



## wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 08:25 PM UTC

PDB ID : 6LY5 / pdb\_00006ly5  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

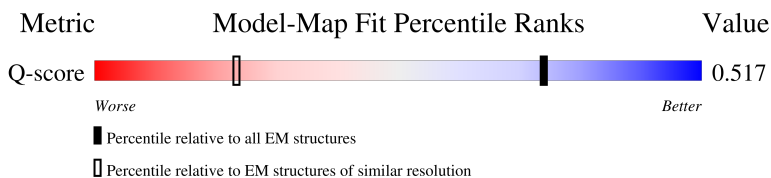
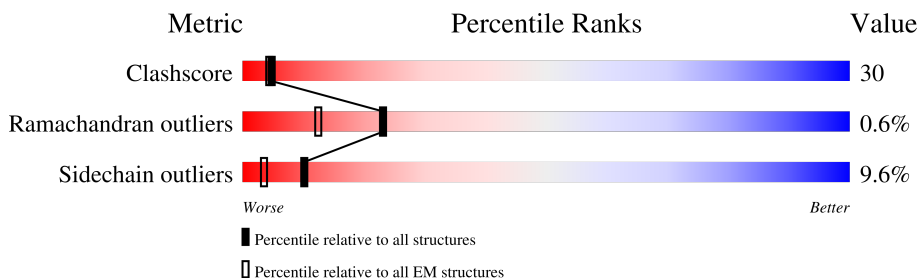
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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.





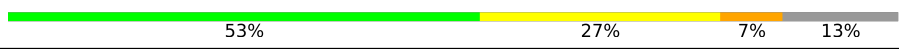


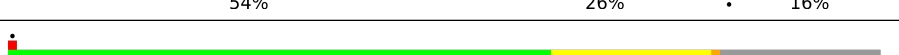
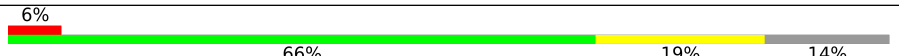
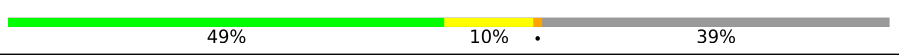


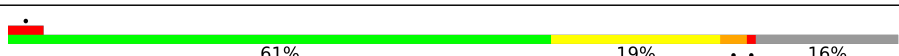









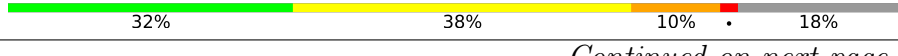



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4811 ( 1.88 - 2.88 )

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

Mol	Chain	Length	Quality of chain
1	A	168	
2	B	223	
3	C	198	
4	D	207	






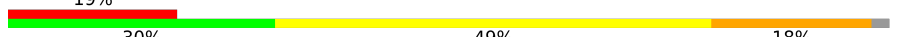
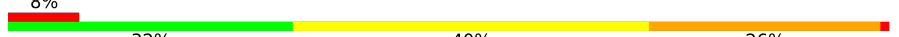
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Mol	Chain	Length	Quality of chain
5	E	222	
6	F	215	
7	G	245	
8	H	203	
9	I	195	
10	J	200	
11	K	207	
12	L	229	
13	M	306	
14	N	219	
15	O	205	
15	P	205	
15	Q	205	
16	R	246	
17	S	254	
18	T	207	
19	W	198	
19	X	198	
20	a	743	
21	b	733	
22	c	80	
23	d	132	
24	e	63	
25	f	162	
26	i	40	

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Mol	Chain	Length	Quality of chain
27	j	42	
28	l	172	
29	m	29	
30	g	134	
31	h	139	
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
34	DD6	L	305	-	-	X	-
34	DD6	W	204	-	-	X	-
34	DD6	W	205	-	-	X	-
35	A86	Q	316	-	-	X	-
35	A86	S	304	-	-	X	-
35	A86	V	301	-	-	X	-
35	A86	X	314	-	-	X	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	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	-	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	-	X	-
36	CLA	G	316	X	-	-	-
36	CLA	G	319	X	-	-	-
36	CLA	H	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
36	CLA	I	308	X	-	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	-	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	-	X	-
36	CLA	L	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	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	-	-	-
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	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	V	305	X	-	X	-
36	CLA	V	306	X	-	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	-	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	-	-	-
36	CLA	W	211	X	-	-	-
36	CLA	W	212	-	-	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	X	315	-	-	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	-	X	-
36	CLA	a	817	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-
39	LMT	F	321	-	-	X	-
39	LMT	h	205	-	-	X	-
41	LHG	E	322	-	-	X	-
41	LHG	f	808	-	-	X	-
41	LHG	i	104	-	-	X	-
42	LMG	J	318	-	-	X	-
42	LMG	V	316	-	-	X	-
42	LMG	j	105	-	-	X	-
45	SF4	b	803	-	-	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		

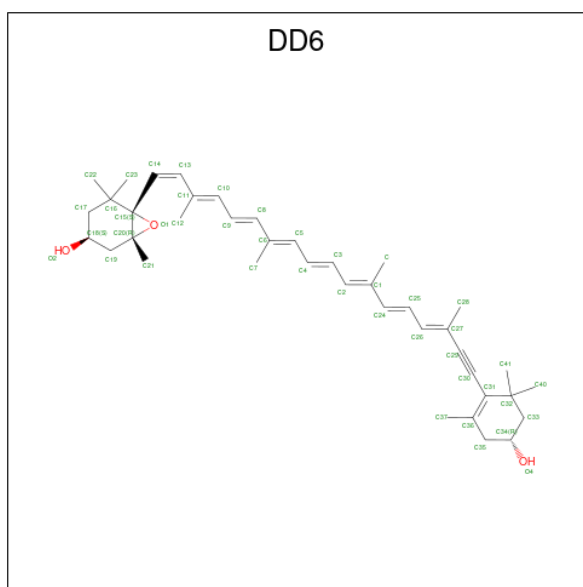
- Molecule 32 is a protein called FCPI-2.

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 (CCD ID: DD6) (formula: C<sub>40</sub>H<sub>54</sub>O<sub>3</sub>).



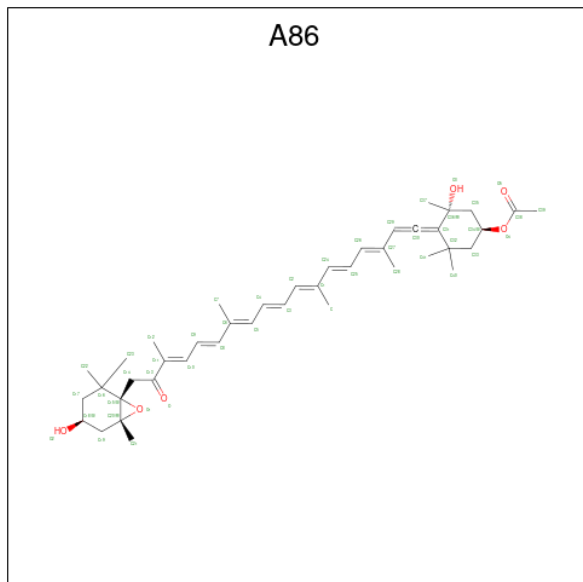
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			43	40	3	
34	A	1	Total	C	O	0
			43	40	3	
34	A	1	Total	C	O	0
			43	40	3	
34	B	1	Total	C	O	0
			43	40	3	
34	B	1	Total	C	O	0
			43	40	3	
34	C	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	D	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	
34	E	1	Total	C	O	0
			43	40	3	

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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	43	40	3	0
34	H	1	43	40	3	0
34	I	1	43	40	3	0
34	J	1	43	40	3	0
34	K	1	43	40	3	0
34	K	1	43	40	3	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	43	40	3	0
34	R	1	43	40	3	0
34	S	1	43	40	3	0
34	S	1	43	40	3	0
34	W	1	43	40	3	0
34	W	1	43	40	3	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 (CCD ID: A86) (formula: C<sub>42</sub>H<sub>58</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			48	42	6	
35	A	1	Total	C	O	0
			48	42	6	
35	B	1	Total	C	O	0
			48	42	6	
35	B	1	Total	C	O	0
			48	42	6	
35	C	1	Total	C	O	0
			48	42	6	
35	C	1	Total	C	O	0
			48	42	6	
35	C	1	Total	C	O	0
			48	42	6	
35	D	1	Total	C	O	0
			48	42	6	
35	E	1	Total	C	O	0
			48	42	6	
35	E	1	Total	C	O	0
			48	42	6	
35	E	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
35	F	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	
35	F	1	Total	C	O	0
			48	42	6	
35	G	1	Total	C	O	0
			48	42	6	
35	G	1	Total	C	O	0
			48	42	6	
35	G	1	Total	C	O	0
			48	42	6	
35	G	1	Total	C	O	0
			48	42	6	
35	H	1	Total	C	O	0
			48	42	6	
35	H	1	Total	C	O	0
			48	42	6	
35	I	1	Total	C	O	0
			48	42	6	
35	I	1	Total	C	O	0
			48	42	6	
35	I	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	J	1	Total	C	O	0
			48	42	6	
35	K	1	Total	C	O	0
			48	42	6	
35	K	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	K	1	48	42	6	0
35	K	1	48	42	6	0
35	L	1	48	42	6	0
35	L	1	48	42	6	0
35	L	1	48	42	6	0
35	L	1	48	42	6	0
35	L	1	48	42	6	0
35	L	1	48	42	6	0
35	M	1	48	42	6	0
35	M	1	48	42	6	0
35	M	1	48	42	6	0
35	M	1	48	42	6	0
35	M	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	O	1	48	42	6	0
35	O	1	48	42	6	0
35	O	1	48	42	6	0

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Mol	Chain	Residues	Atoms			AltConf
35	O	1	Total	C	O	0
			48	42	6	
35	O	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	P	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	Q	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	R	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	
35	S	1	Total	C	O	0
			48	42	6	

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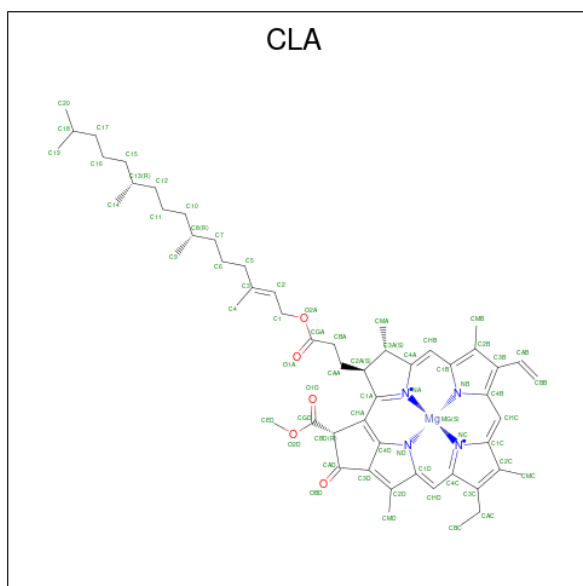
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	S	1	48	42	6	0
35	S	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	W	1	48	42	6	0
35	W	1	48	42	6	0
35	X	1	48	42	6	0
35	X	1	48	42	6	0
35	X	1	48	42	6	0
35	X	1	48	42	6	0
35	X	1	48	42	6	0
35	X	1	48	42	6	0
35	X	1	48	42	6	0
35	h	1	48	42	6	0
35	h	1	48	42	6	0
35	U	1	48	42	6	0
35	U	1	48	42	6	0

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Mol	Chain	Residues	Atoms			AltConf
35	U	1	Total	C	O	0
			48	42	6	
35	U	1	Total	C	O	0
			48	42	6	
35	V	1	Total	C	O	0
			48	42	6	
35	V	1	Total	C	O	0
			48	42	6	
35	V	1	Total	C	O	0
			48	42	6	
35	V	1	Total	C	O	0
			48	42	6	

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



Mol	Chain	Residues	Atoms				AltConf	
36	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	C	1	Total 43	C 35	Mg 1	N 4	O 3	0
36	C	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	C	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
36	D	1	Total 61	C 51	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	D	1	65	55	1	4	5	0
36	D	1	55	45	1	4	5	0
36	D	1	65	55	1	4	5	0
36	D	1	46	36	1	4	5	0
36	D	1	65	55	1	4	5	0
36	D	1	65	55	1	4	5	0
36	D	1	41	33	1	4	3	0
36	D	1	52	42	1	4	5	0
36	D	1	58	48	1	4	5	0
36	E	1	49	39	1	4	5	0
36	E	1	65	55	1	4	5	0
36	E	1	65	55	1	4	5	0
36	E	1	65	55	1	4	5	0
36	E	1	65	55	1	4	5	0
36	E	1	65	55	1	4	5	0
36	E	1	65	55	1	4	5	0
36	E	1	65	55	1	4	5	0
36	E	1	46	36	1	4	5	0
36	F	1	65	55	1	4	5	0
36	F	1	56	46	1	4	5	0
36	F	1	52	42	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	F	1	65	55	1	4	5	0
36	F	1	52	42	1	4	5	0
36	F	1	65	55	1	4	5	0
36	F	1	41	33	1	4	3	0
36	F	1	56	46	1	4	5	0
36	G	1	42	34	1	4	3	0
36	G	1	65	55	1	4	5	0
36	G	1	65	55	1	4	5	0
36	G	1	65	55	1	4	5	0
36	G	1	58	48	1	4	5	0
36	G	1	65	55	1	4	5	0
36	G	1	41	33	1	4	3	0
36	G	1	56	46	1	4	5	0
36	G	1	49	39	1	4	5	0
36	G	1	50	40	1	4	5	0
36	H	1	48	38	1	4	5	0
36	H	1	61	51	1	4	5	0
36	H	1	60	50	1	4	5	0
36	H	1	64	54	1	4	5	0
36	H	1	65	55	1	4	5	0
36	H	1	46	36	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	H	1	65	55	1	4	5	0
36	H	1	65	55	1	4	5	0
36	H	1	41	33	1	4	3	0
36	H	1	65	55	1	4	5	0
36	H	1	65	55	1	4	5	0
36	H	1	65	55	1	4	5	0
36	H	1	50	40	1	4	5	0
36	I	1	61	51	1	4	5	0
36	I	1	65	55	1	4	5	0
36	I	1	54	44	1	4	5	0
36	I	1	65	55	1	4	5	0
36	I	1	46	36	1	4	5	0
36	I	1	65	55	1	4	5	0
36	I	1	65	55	1	4	5	0
36	I	1	52	42	1	4	5	0
36	I	1	41	33	1	4	3	0
36	I	1	41	33	1	4	3	0
36	J	1	61	51	1	4	5	0
36	J	1	61	51	1	4	5	0
36	J	1	65	55	1	4	5	0
36	J	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	J	1	46	36	1	4	5	0
36	J	1	65	55	1	4	5	0
36	J	1	65	55	1	4	5	0
36	J	1	41	33	1	4	3	0
36	J	1	46	36	1	4	5	0
36	J	1	47	37	1	4	5	0
36	K	1	61	51	1	4	5	0
36	K	1	65	55	1	4	5	0
36	K	1	59	49	1	4	5	0
36	K	1	62	52	1	4	5	0
36	K	1	46	36	1	4	5	0
36	K	1	65	55	1	4	5	0
36	K	1	65	55	1	4	5	0
36	K	1	41	33	1	4	3	0
36	K	1	65	55	1	4	5	0
36	L	1	61	51	1	4	5	0
36	L	1	65	55	1	4	5	0
36	L	1	54	44	1	4	5	0
36	L	1	65	55	1	4	5	0
36	L	1	46	36	1	4	5	0
36	L	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	L	1	65	55	1	4	5	0
36	L	1	41	33	1	4	3	0
36	L	1	65	55	1	4	5	0
36	M	1	55	45	1	4	5	0
36	M	1	65	55	1	4	5	0
36	M	1	52	42	1	4	5	0
36	M	1	65	55	1	4	5	0
36	M	1	46	36	1	4	5	0
36	M	1	65	55	1	4	5	0
36	M	1	47	37	1	4	5	0
36	M	1	41	33	1	4	3	0
36	M	1	47	37	1	4	5	0
36	M	1	42	34	1	4	3	0
36	N	1	61	51	1	4	5	0
36	N	1	65	55	1	4	5	0
36	N	1	51	41	1	4	5	0
36	N	1	41	33	1	4	3	0
36	N	1	46	36	1	4	5	0
36	N	1	47	37	1	4	5	0
36	N	1	41	33	1	4	3	0
36	N	1	41	33	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	N	1	65	55	1	4	5	0
36	N	1	54	44	1	4	5	0
36	N	1	47	37	1	4	5	0
36	N	1	42	34	1	4	3	0
36	O	1	61	51	1	4	5	0
36	O	1	65	55	1	4	5	0
36	O	1	65	55	1	4	5	0
36	O	1	65	55	1	4	5	0
36	O	1	46	36	1	4	5	0
36	O	1	58	48	1	4	5	0
36	O	1	40	32	1	4	3	0
36	O	1	41	33	1	4	3	0
36	O	1	65	55	1	4	5	0
36	P	1	65	55	1	4	5	0
36	P	1	42	34	1	4	3	0
36	P	1	61	51	1	4	5	0
36	P	1	65	55	1	4	5	0
36	P	1	65	55	1	4	5	0
36	P	1	65	55	1	4	5	0
36	P	1	46	36	1	4	5	0
36	P	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
36	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	P	1	Total 51	C 41	Mg 1	N 4	O 5	0
36	P	1	Total 60	C 50	Mg 1	N 4	O 5	0
36	Q	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	Q	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	R	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	R	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	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	
36	R	1	45	35	1	4	5	0
36	R	1	65	55	1	4	5	0
36	R	1	52	42	1	4	5	0
36	S	1	61	51	1	4	5	0
36	S	1	65	55	1	4	5	0
36	S	1	46	36	1	4	5	0
36	S	1	65	55	1	4	5	0
36	S	1	46	36	1	4	5	0
36	S	1	65	55	1	4	5	0
36	S	1	45	37	1	4	3	0
36	S	1	41	33	1	4	3	0
36	S	1	42	34	1	4	3	0
36	S	1	65	55	1	4	5	0
36	S	1	65	55	1	4	5	0
36	S	1	52	42	1	4	5	0
36	T	1	61	51	1	4	5	0
36	T	1	65	55	1	4	5	0
36	T	1	65	55	1	4	5	0
36	T	1	46	36	1	4	5	0
36	T	1	65	55	1	4	5	0
36	T	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	T	1	41	33	1	4	3	0
36	W	1	48	38	1	4	5	0
36	W	1	61	51	1	4	5	0
36	W	1	65	55	1	4	5	0
36	W	1	45	35	1	4	5	0
36	W	1	57	47	1	4	5	0
36	W	1	46	36	1	4	5	0
36	W	1	65	55	1	4	5	0
36	W	1	65	55	1	4	5	0
36	W	1	41	33	1	4	3	0
36	W	1	48	38	1	4	5	0
36	W	1	45	35	1	4	5	0
36	W	1	43	35	1	4	3	0
36	X	1	61	51	1	4	5	0
36	X	1	50	40	1	4	5	0
36	X	1	47	37	1	4	5	0
36	X	1	45	35	1	4	5	0
36	X	1	41	33	1	4	3	0
36	X	1	41	33	1	4	3	0
36	X	1	42	34	1	4	3	0
36	X	1	41	33	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	55	45	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	56	46	1	4	5	0
36	a	1	62	52	1	4	5	0
36	a	1	54	44	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	45	35	1	4	5	0
36	a	1	50	40	1	4	5	0
36	a	1	45	35	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	45	35	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	49	39	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	a	1	51	41	1	4	5	0
36	a	1	55	45	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	62	52	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	50	40	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	50	40	1	4	5	0
36	a	1	45	35	1	4	5	0
36	a	1	51	41	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	65	55	1	4	5	0
36	a	1	52	42	1	4	5	0
36	a	1	65	55	1	4	5	0
36	b	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	b	1	65	55	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	45	35	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	54	44	1	4	5	0
36	b	1	55	45	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	60	50	1	4	5	0
36	b	1	59	49	1	4	5	0
36	b	1	55	45	1	4	5	0
36	b	1	59	49	1	4	5	0
36	b	1	60	50	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	46	36	1	4	5	0
36	b	1	55	45	1	4	5	0
36	b	1	53	43	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	b	1	65	55	1	4	5	0
36	b	1	64	54	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	50	40	1	4	5	0
36	b	1	49	39	1	4	5	0
36	b	1	58	48	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	45	35	1	4	5	0
36	b	1	58	48	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	47	37	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	65	55	1	4	5	0
36	b	1	65	55	1	4	5	0
36	f	1	65	55	1	4	5	0
36	f	1	65	55	1	4	5	0
36	f	1	65	55	1	4	5	0
36	f	1	52	42	1	4	5	0

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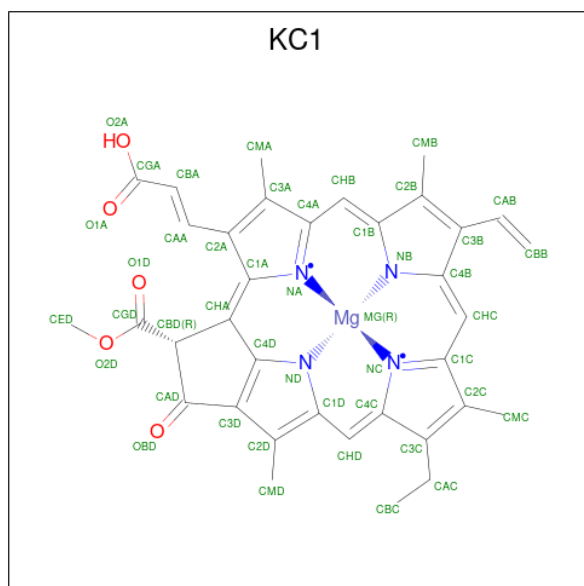
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	j	1	Total 42	C 34	Mg 1	N 4	O 3	0
36	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	l	1	Total 49	C 39	Mg 1	N 4	O 5	0
36	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	l	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	U	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	U	1	Total 50	C 40	Mg 1	N 4	O 5	0
36	U	1	Total 56	C 46	Mg 1	N 4	O 5	0
36	U	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	U	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	V	1	Total 61	C 51	Mg 1	N 4	O 5	0
36	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	V	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
36	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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



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

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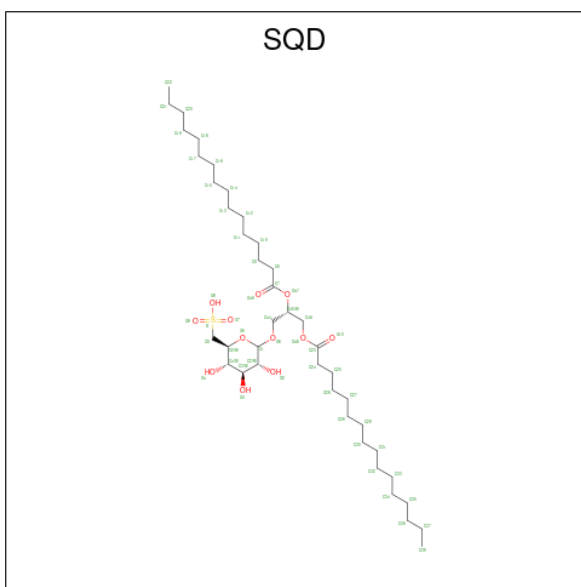
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	F	1	45	35	1	4	5	0
37	F	1	45	35	1	4	5	0
37	G	1	45	35	1	4	5	0
37	G	1	45	35	1	4	5	0
37	G	1	45	35	1	4	5	0
37	H	1	45	35	1	4	5	0
37	J	1	45	35	1	4	5	0
37	K	1	45	35	1	4	5	0
37	L	1	45	35	1	4	5	0
37	L	1	45	35	1	4	5	0
37	M	1	45	35	1	4	5	0
37	M	1	45	35	1	4	5	0
37	M	1	45	35	1	4	5	0
37	N	1	45	35	1	4	5	0
37	O	1	45	35	1	4	5	0
37	O	1	45	35	1	4	5	0
37	P	1	45	35	1	4	5	0
37	P	1	45	35	1	4	5	0
37	Q	1	45	35	1	4	5	0
37	Q	1	45	35	1	4	5	0
37	R	1	45	35	1	4	5	0

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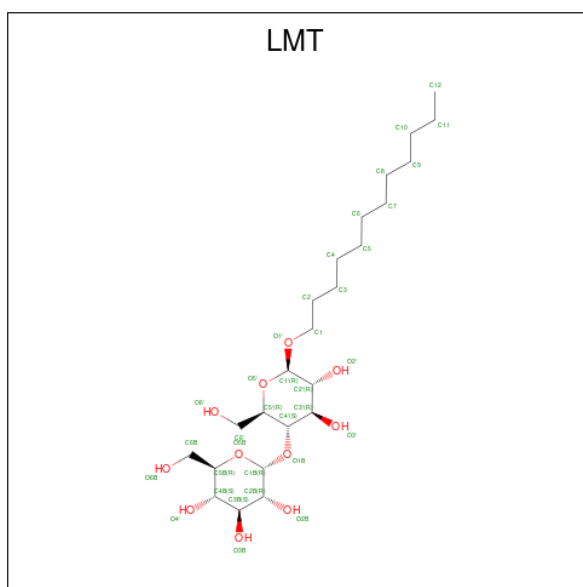
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	U	1	Total 45	C 35	Mg 1	N 4	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 (CCD ID: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>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 (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



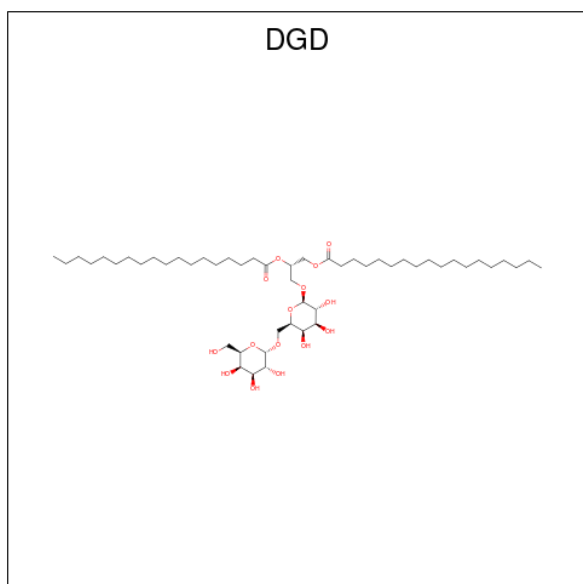
Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			35	24	11	
39	B	1	Total	C	O	0
			35	24	11	
39	E	1	Total	C	O	0
			35	24	11	
39	E	1	Total	C	O	0
			23	17	6	
39	E	1	Total	C	O	0
			35	24	11	
39	F	1	Total	C	O	0
			35	24	11	
39	F	1	Total	C	O	0
			33	22	11	
39	G	1	Total	C	O	0
			35	24	11	
39	G	1	Total	C	O	0
			35	24	11	
39	I	1	Total	C	O	0
			35	24	11	
39	I	1	Total	C	O	0
			35	24	11	
39	K	1	Total	C	O	0
			31	20	11	
39	K	1	Total	C	O	0
			35	24	11	
39	L	1	Total	C	O	0
			35	24	11	

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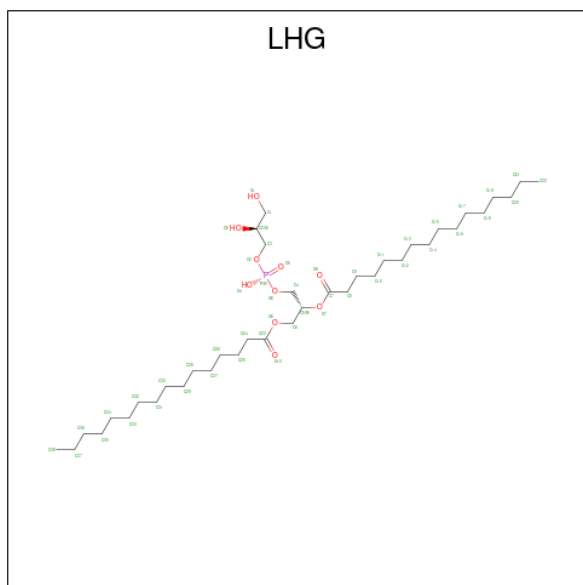
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	L	1	Total 31	C 20	O 11	0
39	P	1	Total 23	C 17	O 6	0
39	P	1	Total 23	C 17	O 6	0
39	a	1	Total 35	C 24	O 11	0
39	a	1	Total 32	C 21	O 11	0
39	a	1	Total 35	C 24	O 11	0
39	b	1	Total 35	C 24	O 11	0
39	b	1	Total 24	C 19	O 5	0
39	f	1	Total 24	C 18	O 6	0
39	h	1	Total 35	C 24	O 11	0
39	U	1	Total 35	C 24	O 11	0
39	U	1	Total 35	C 24	O 11	0

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



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

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



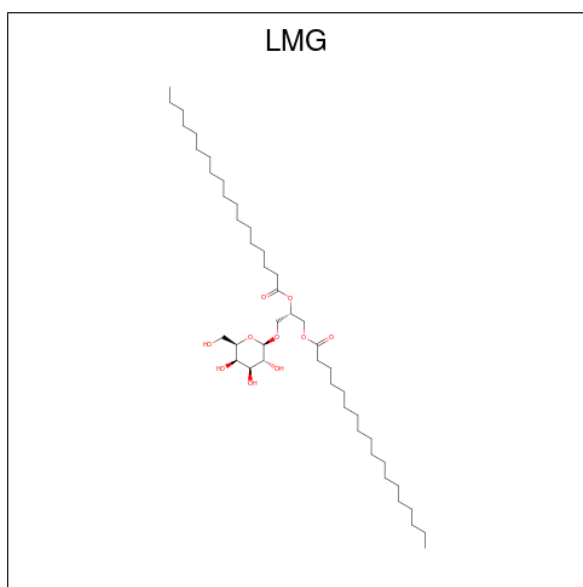
Mol	Chain	Residues	Atoms				AltConf
41	D	1	Total	C	O	P	0
			46	35	10	1	
41	D	1	Total	C	O	P	0
			49	38	10	1	
41	E	1	Total	C	O	P	0
			49	38	10	1	
41	F	1	Total	C	O	P	0
			33	24	8	1	
41	F	1	Total	C	O	P	0
			41	30	10	1	
41	G	1	Total	C	O	P	0
			49	38	10	1	
41	G	1	Total	C	O	P	0
			40	29	10	1	
41	G	1	Total	C	O	P	0
			47	36	10	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
41	I	1	49	38	10	1	0
41	O	1	42	31	10	1	0
41	O	1	49	38	10	1	0
41	Q	1	49	38	10	1	0
41	R	1	49	38	10	1	0
41	a	1	48	37	10	1	0
41	a	1	27	16	10	1	0
41	a	1	47	36	10	1	0
41	b	1	49	38	10	1	0
41	f	1	49	38	10	1	0
41	f	1	42	31	10	1	0
41	i	1	46	35	10	1	0
41	j	1	49	38	10	1	0
41	l	1	48	37	10	1	0

- Molecule 42 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



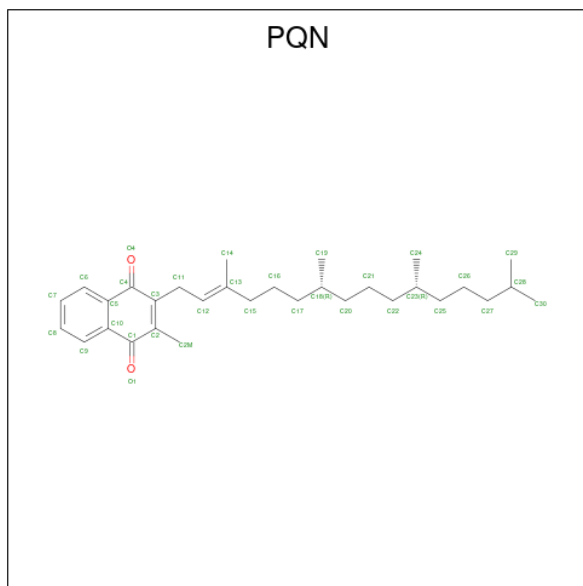
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
42	D	1	46	36	10	0
42	D	1	37	27	10	0
42	E	1	46	36	10	0
42	E	1	40	30	10	0
42	G	1	55	45	10	0
42	G	1	55	45	10	0
42	I	1	55	45	10	0
42	J	1	55	45	10	0
42	J	1	44	34	10	0
42	L	1	33	23	10	0
42	a	1	54	44	10	0
42	j	1	52	42	10	0
42	m	1	37	27	10	0
42	h	1	45	35	10	0

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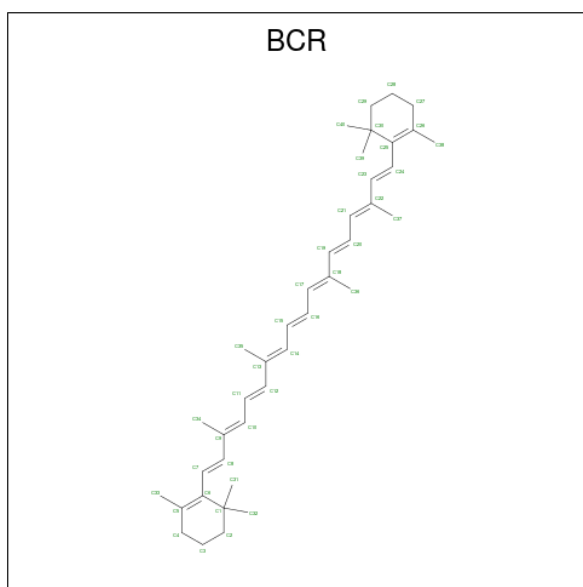
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
42	V	1	46	36	10	0
42	V	1	46	36	10	0

- Molecule 43 is PHYLLOQUINONE (CCD ID: 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 (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



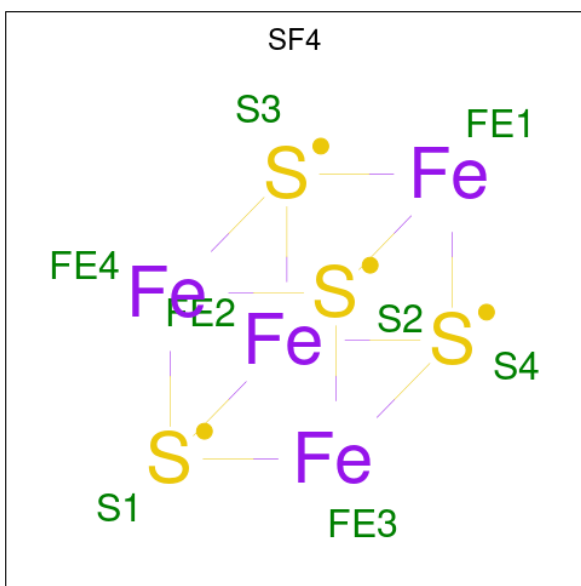
Mol	Chain	Residues	Atoms	AltConf
44	a	1	Total C 40 40	0
44	a	1	Total C 40 40	0
44	a	1	Total C 40 40	0
44	a	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	b	1	Total C 40 40	0
44	f	1	Total C 40 40	0
44	f	1	Total C 40 40	0
44	i	1	Total C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

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

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (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 8 4 4	0
45	c	1	Total Fe S 8 4 4	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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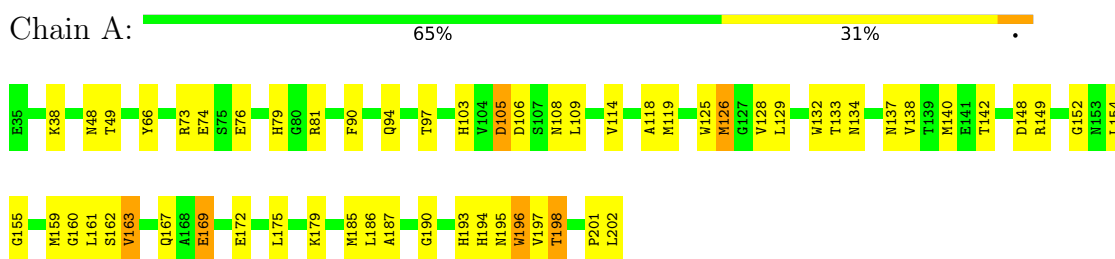
*Continued from previous page...*

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

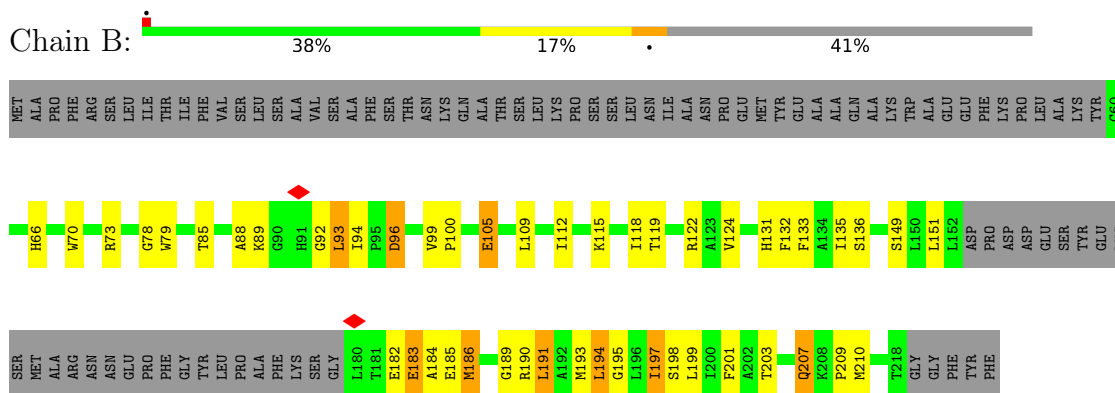
### 3 Residue-property plots [i](#)

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.

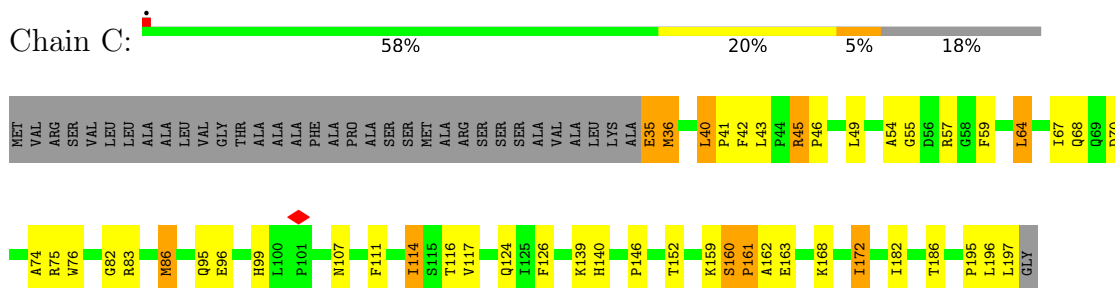
- Molecule 1: FCPI-7



- Molecule 2: FCPI-1

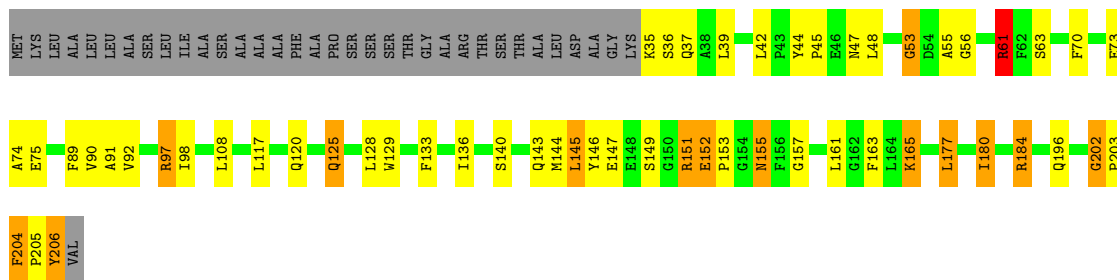


- Molecule 3: FCPI-11

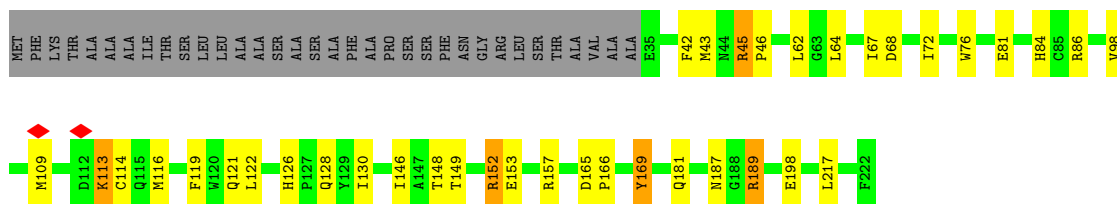


- Molecule 4: FCPI-6

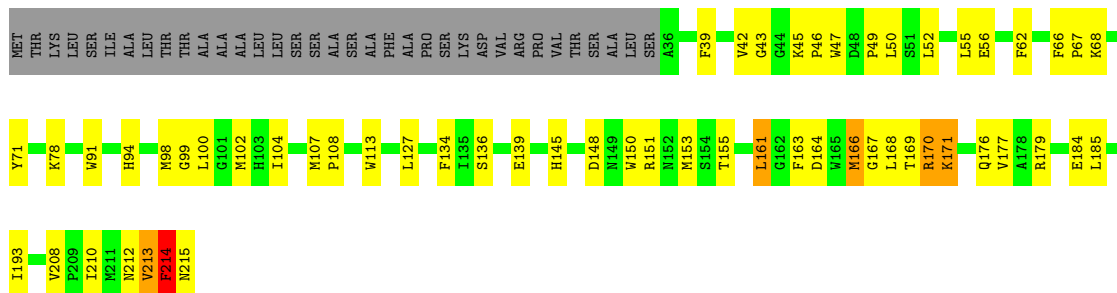




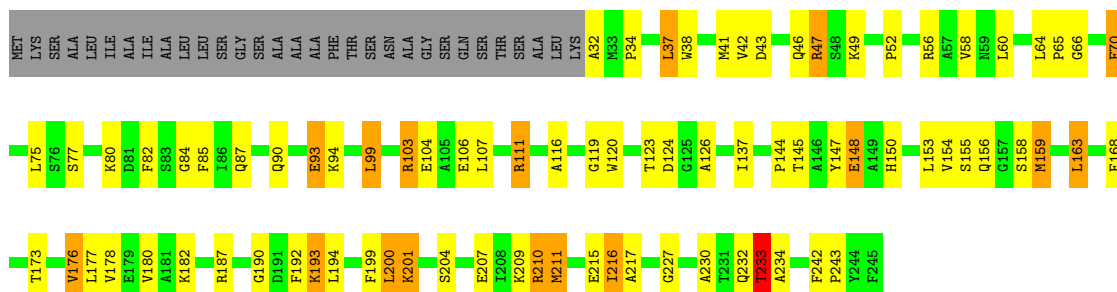
• Molecule 5: FCPI-5



• Molecule 6: FCPI-8

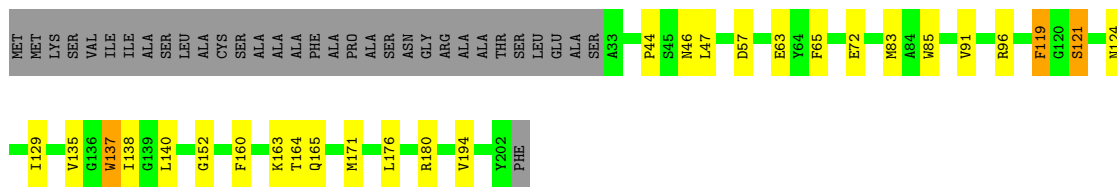


• Molecule 7: FCPI-4

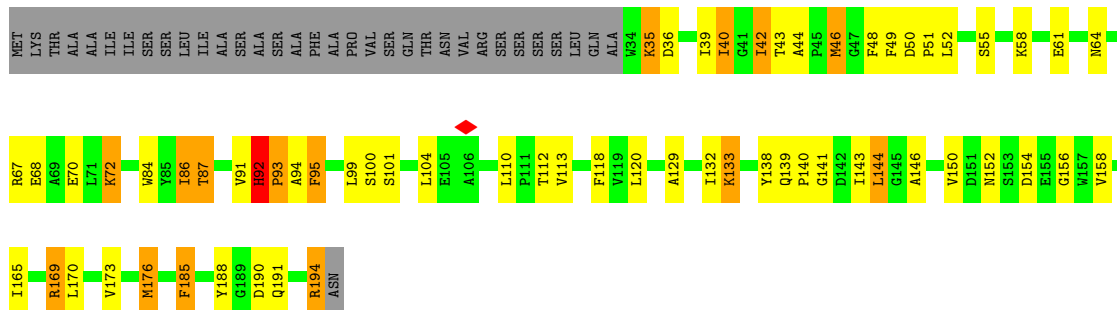


• Molecule 8: FCPI-10

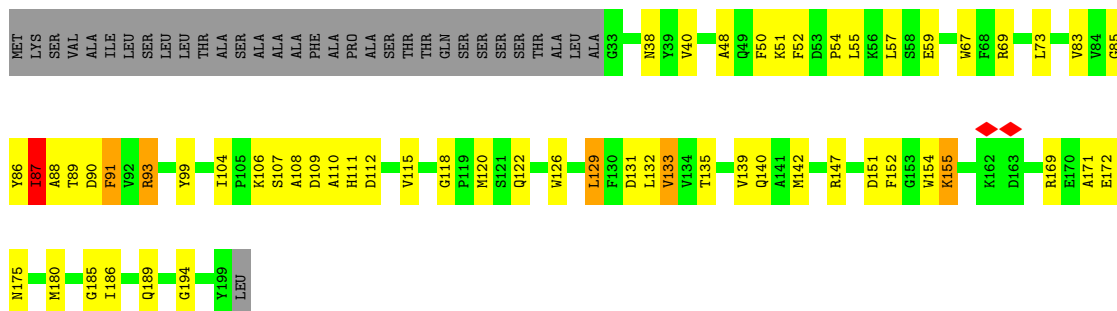




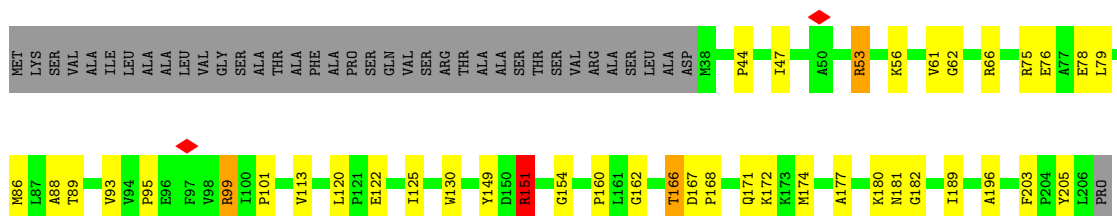
• Molecule 9: FCPI-3



• Molecule 10: FCPI-9

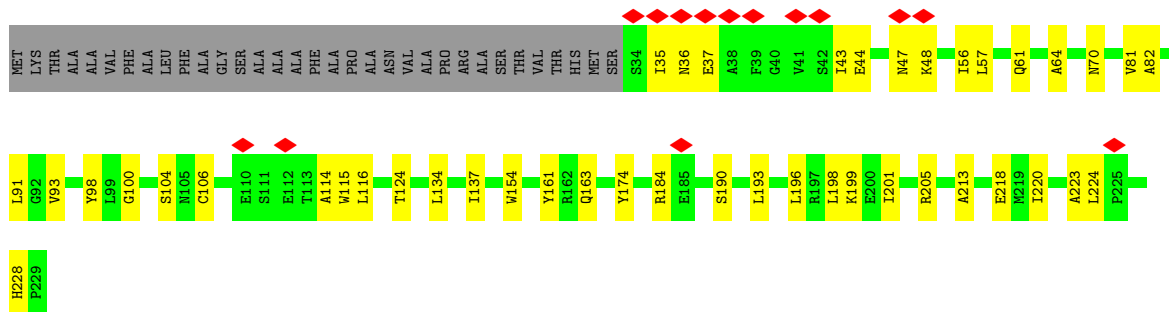


• Molecule 11: FCPI-13

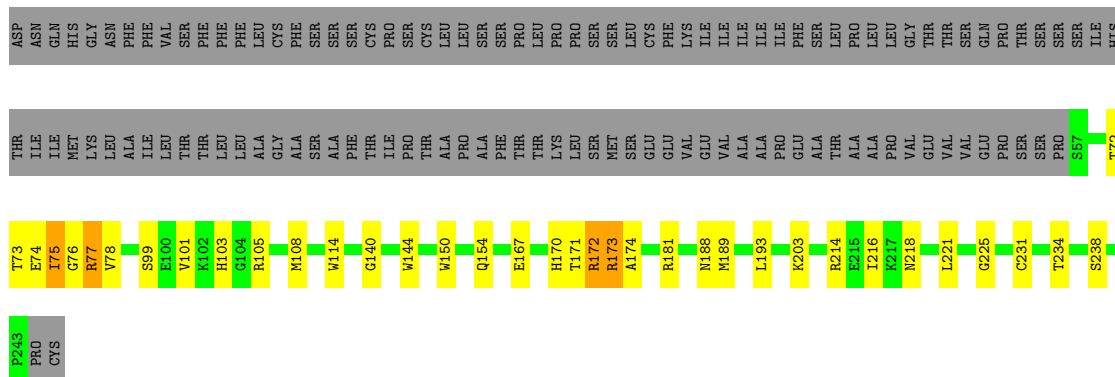


• Molecule 12: FCPI-14

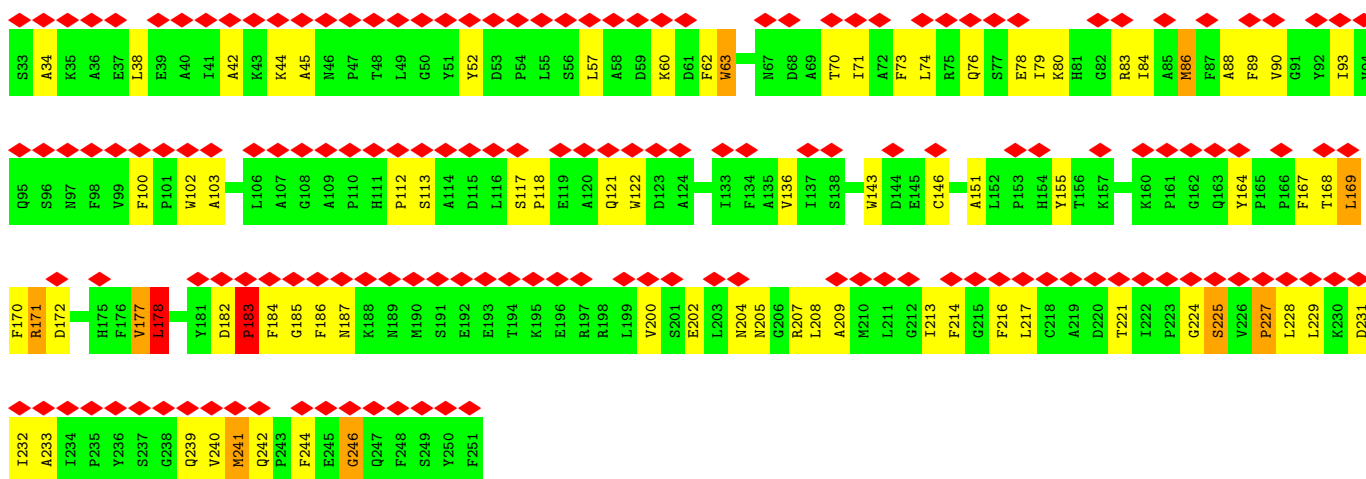




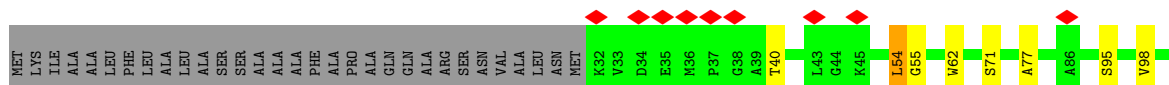
• Molecule 13: FCPI-16

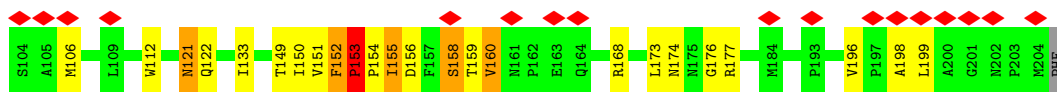


• Molecule 14: FCPI-21

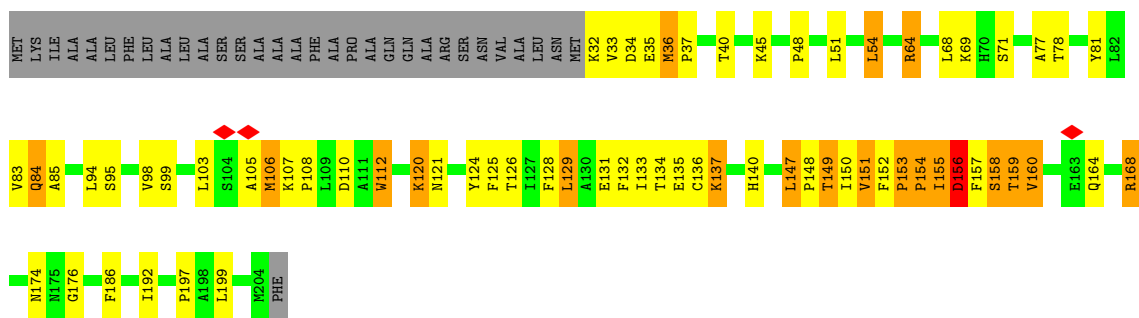


• Molecule 15: FCPI

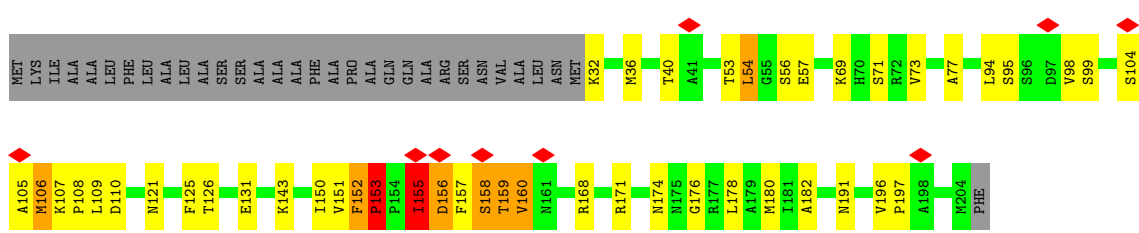




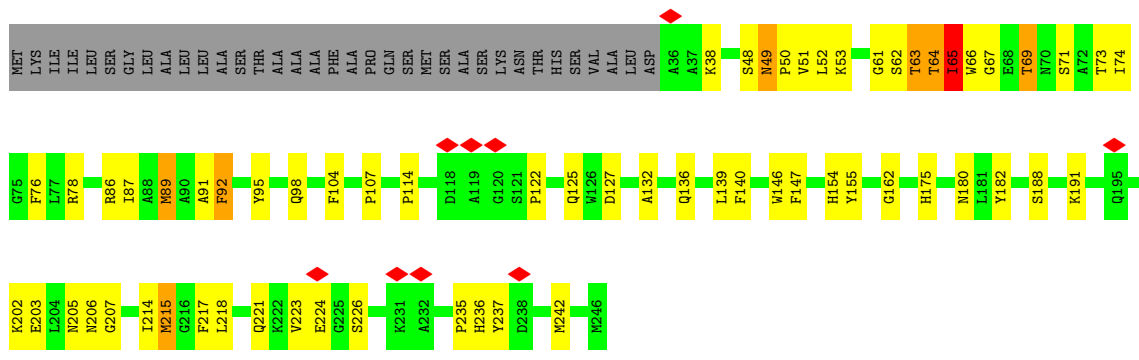
• Molecule 15: FCPI



• Molecule 15: FCPI

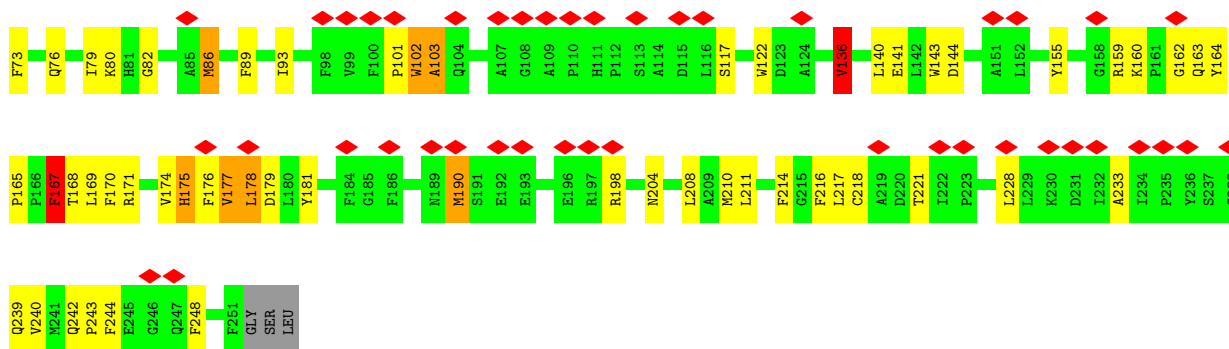


• Molecule 16: FCPI-24

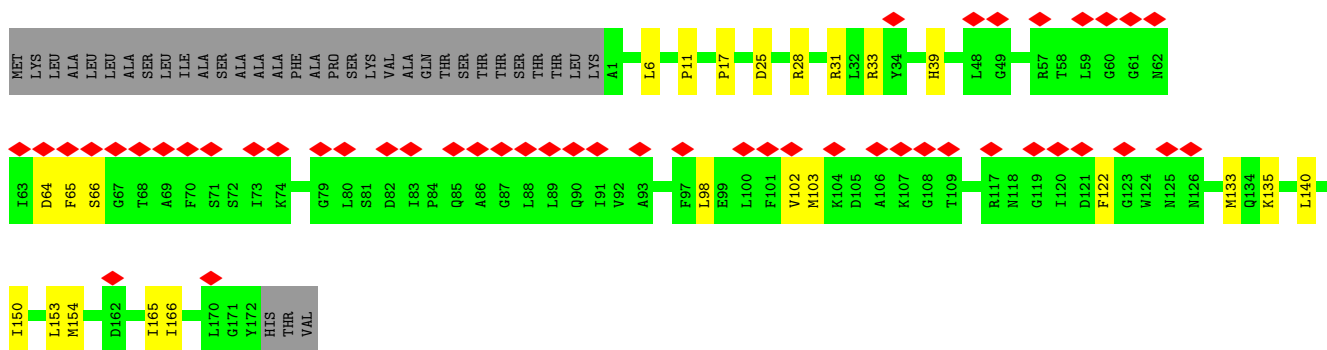


• Molecule 17: FCPI-23

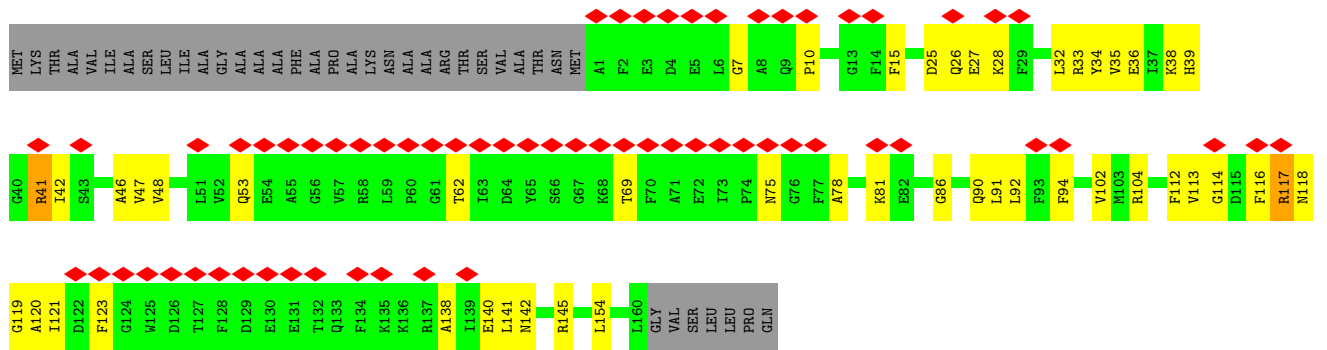




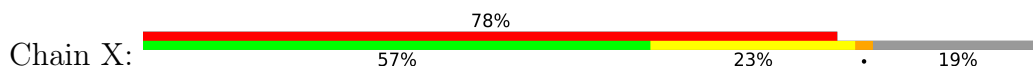
• Molecule 18: FCPI-12

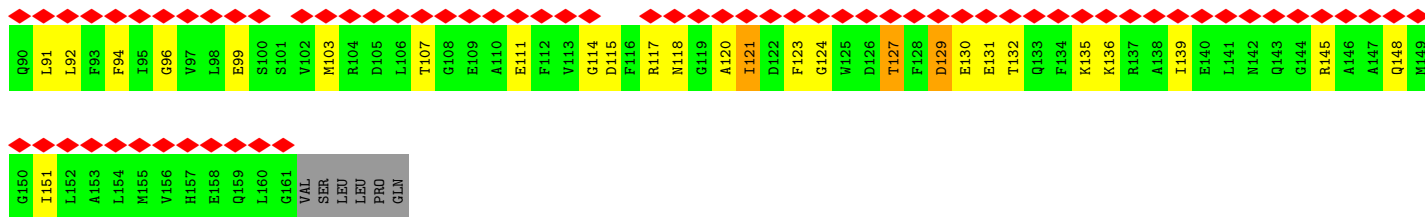


• Molecule 19: FCPI-17

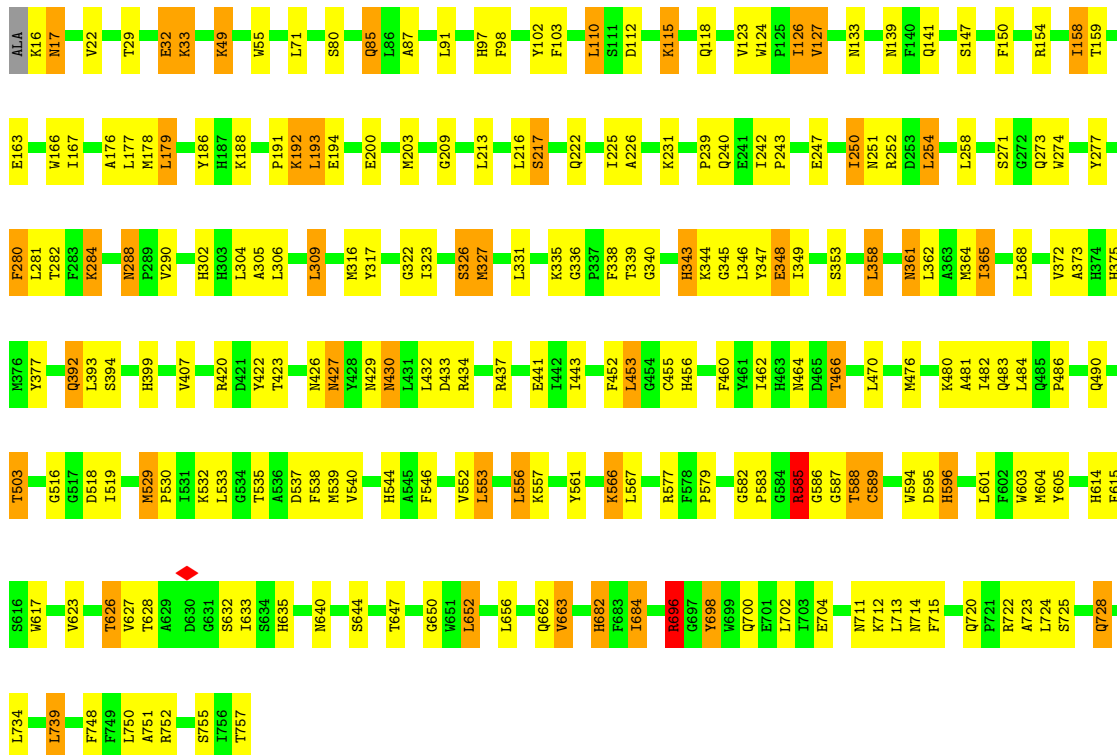


• Molecule 19: FCPI-17

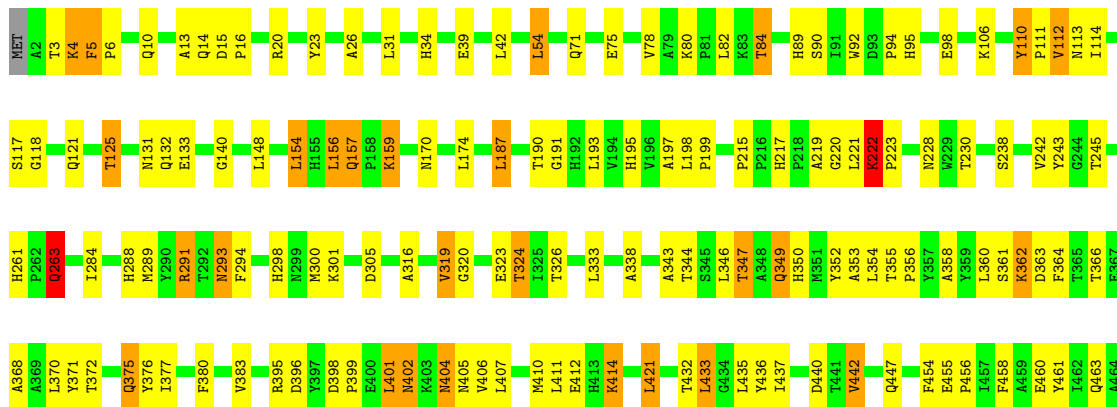


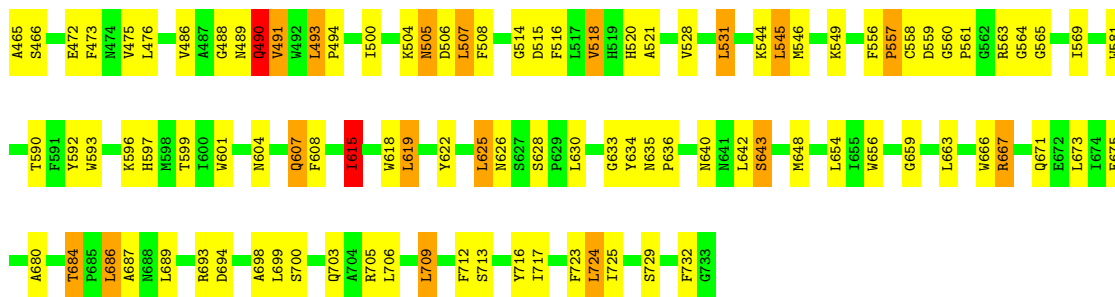


• Molecule 20: PsaA

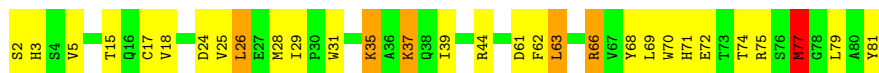


• Molecule 21: PsaB





• Molecule 22: PsaC



• Molecule 23: PsaD



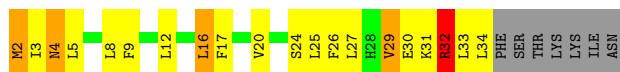
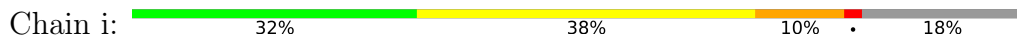
• Molecule 24: PsaE



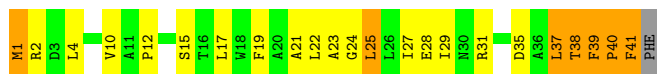
• Molecule 25: PsaF



• Molecule 26: PsaI



• Molecule 27: PsaJ



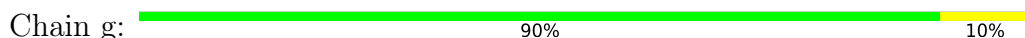
• Molecule 28: PsaL



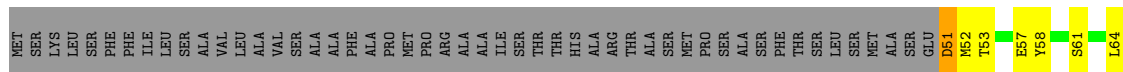
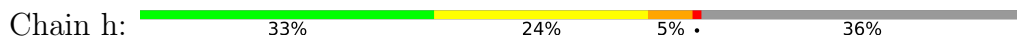
• Molecule 29: PsaM



• Molecule 30: PsaS

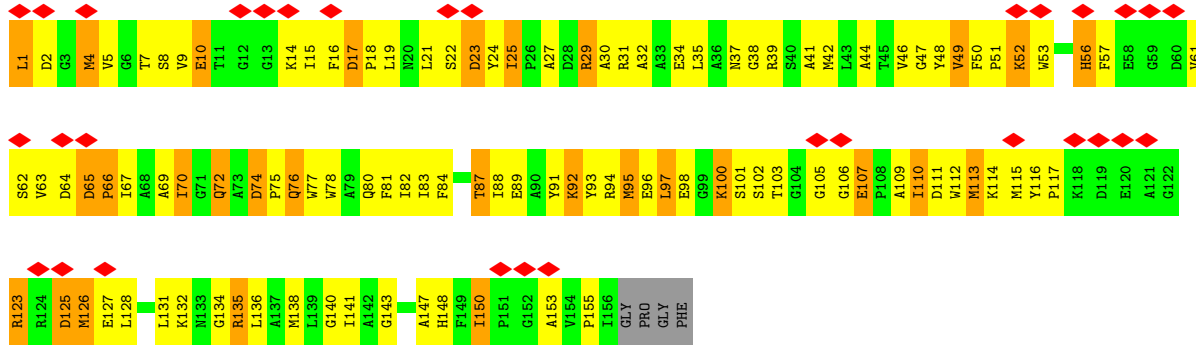


• Molecule 31: PsaR

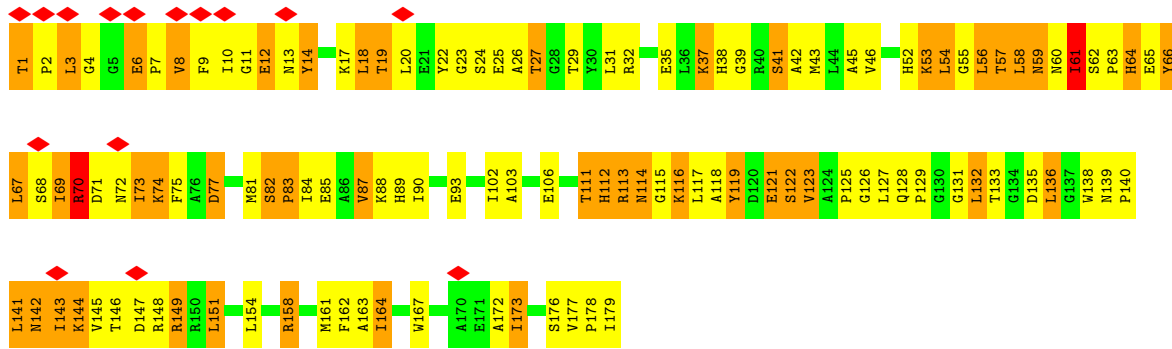


• Molecule 32: FCPI-2





• 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

### 5.1 Standard geometry

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

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	0.50	0/1319	0.80	0/1786
2	B	0.87	2/1039 (0.2%)	1.16	11/1412 (0.8%)
3	C	0.41	0/1275	0.77	3/1726 (0.2%)
4	D	0.49	0/1373	0.84	5/1860 (0.3%)
5	E	0.48	0/1439	0.70	1/1944 (0.1%)
6	F	0.43	0/1411	0.84	5/1908 (0.3%)
7	G	0.45	0/1714	0.79	2/2321 (0.1%)
8	H	0.48	0/1326	0.80	1/1798 (0.1%)
9	I	0.44	0/1285	1.00	6/1746 (0.3%)
10	J	0.50	1/1339 (0.1%)	0.94	4/1811 (0.2%)
11	K	0.49	0/1346	0.84	4/1826 (0.2%)
12	L	0.45	0/1571	0.71	0/2141
13	M	0.40	0/1464	0.74	3/1982 (0.2%)
14	N	0.48	0/1770	1.01	7/2405 (0.3%)
15	O	0.47	0/1335	0.92	7/1817 (0.4%)
15	P	0.47	1/1329 (0.1%)	1.31	11/1810 (0.6%)
15	Q	0.48	0/1335	0.92	8/1817 (0.4%)
16	R	0.35	0/1680	0.72	1/2282 (0.0%)
17	S	0.40	0/1776	0.89	3/2413 (0.1%)
18	T	0.34	0/1353	0.62	0/1823
19	W	0.48	1/1265 (0.1%)	0.85	3/1707 (0.2%)
19	X	0.50	2/1282 (0.2%)	0.93	7/1729 (0.4%)
20	a	0.47	0/6053	0.80	19/8238 (0.2%)
21	b	0.48	2/6031 (0.0%)	0.85	20/8231 (0.2%)
22	c	0.45	0/607	0.82	2/822 (0.2%)
23	d	4.08	2/1086 (0.2%)	1.45	9/1461 (0.6%)
24	e	0.40	0/517	0.58	0/701
25	f	0.47	0/1248	0.75	2/1687 (0.1%)
26	i	0.60	0/262	1.24	2/356 (0.6%)
27	j	0.57	0/333	0.82	1/455 (0.2%)
28	l	0.48	0/1121	0.83	2/1520 (0.1%)
29	m	0.57	0/198	0.82	0/269

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	h	0.49	0/698	1.08	10/951 (1.1%)
32	U	0.59	0/1225	2.00	10/1657 (0.6%)
33	V	0.38	0/1393	0.88	5/1894 (0.3%)
All	All	0.76	11/51798 (0.0%)	0.92	174/70306 (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 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	151[A]	LYS	CA-C	94.74	2.66	1.52
23	d	151[B]	LYS	CA-C	94.74	2.66	1.52
2	B	186	MET	C-N	22.66	1.54	1.33
15	P	156	ASP	C-N	9.60	1.48	1.33
2	B	183	GLU	C-N	-8.62	1.21	1.33

The worst 5 of 174 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	U	65	ASP	CA-C-N	48.07	179.93	119.84
32	U	65	ASP	C-N-CA	48.07	179.93	119.84
23	d	151[A]	LYS	CB-CA-C	-26.47	64.81	109.80
23	d	151[B]	LYS	CB-CA-C	-26.47	64.81	109.80
15	P	156	ASP	O-C-N	-23.88	90.36	123.07

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](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1287	0	1265	83	0
2	B	1013	0	1016	100	0
3	C	1247	0	1240	72	0
4	D	1337	0	1310	69	0
5	E	1411	0	1376	46	0
6	F	1375	0	1345	82	0
7	G	1668	0	1631	110	0
8	H	1291	0	1258	47	0
9	I	1250	0	1196	79	0
10	J	1301	0	1256	66	0
11	K	1304	0	1281	48	0
12	L	1523	0	1488	71	0
13	M	1423	0	1397	37	0
14	N	1716	0	1658	139	0
15	O	1302	0	1296	64	0
15	P	1296	0	1291	125	0
15	Q	1302	0	1300	115	0
16	R	1628	0	1588	115	0
17	S	1722	0	1670	149	0
18	T	1326	0	1304	18	0
19	W	1239	0	1208	55	0
19	X	1253	0	1232	91	0
20	a	5858	0	5689	242	0
21	b	5820	0	5647	270	0
22	c	597	0	583	29	0
23	d	1056	0	1074	108	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	e	507	0	504	23	0
25	f	1223	0	1238	79	0
26	i	256	0	284	29	0
27	j	324	0	338	48	0
28	l	1094	0	1129	55	0
29	m	198	0	213	27	0
30	g	670	0	143	23	0
31	h	676	0	662	75	0
32	U	1194	0	1160	221	0
33	V	1361	0	1354	361	0
34	A	129	0	0	14	0
34	B	86	0	0	15	0
34	C	43	0	0	4	0
34	D	172	0	0	19	0
34	E	172	0	0	12	0
34	F	43	0	0	3	0
34	G	43	0	0	2	0
34	H	86	0	0	6	0
34	I	43	0	0	6	0
34	J	43	0	0	4	0
34	K	86	0	0	8	0
34	L	43	0	0	25	0
34	M	43	0	0	18	0
34	O	43	0	0	6	0
34	P	43	0	0	6	0
34	Q	43	0	0	19	0
34	R	86	0	0	16	0
34	S	86	0	0	3	0
34	W	86	0	0	45	0
34	a	43	0	0	1	0
34	j	43	0	0	4	0
35	A	96	0	0	3	0
35	B	96	0	0	19	0
35	C	144	0	0	16	0
35	D	48	0	0	6	0
35	E	144	0	0	18	0
35	F	288	0	0	12	0
35	G	192	0	0	9	0
35	H	96	0	0	7	0
35	I	144	0	0	21	0
35	J	240	0	0	29	0
35	K	192	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	L	240	0	0	14	0
35	M	192	0	0	12	0
35	N	336	0	0	55	0
35	O	240	0	0	27	0
35	P	192	0	0	6	0
35	Q	192	0	0	42	0
35	R	336	0	0	10	0
35	S	288	0	0	27	0
35	T	336	0	0	9	0
35	U	192	0	0	35	0
35	V	192	0	0	46	0
35	W	96	0	0	1	0
35	X	288	0	0	27	0
35	h	96	0	0	9	0
36	A	517	0	509	59	0
36	B	329	0	299	34	0
36	C	516	0	513	41	0
36	D	618	0	591	45	0
36	E	550	0	576	54	0
36	F	452	0	431	57	0
36	G	556	0	526	75	0
36	H	760	0	747	60	0
36	I	555	0	520	91	0
36	J	562	0	540	30	0
36	K	529	0	532	61	0
36	L	527	0	523	54	0
36	M	525	0	462	38	0
36	N	601	0	503	65	0
36	O	506	0	492	34	0
36	P	686	0	666	50	0
36	Q	458	0	441	78	0
36	R	661	0	616	25	0
36	S	658	0	611	46	0
36	T	408	0	409	27	0
36	U	449	0	427	96	0
36	V	545	0	565	145	0
36	W	629	0	552	49	0
36	X	368	0	273	36	0
36	a	2437	0	2463	146	0
36	b	2337	0	2371	117	0
36	f	247	0	259	39	0
36	h	65	0	72	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	i	65	0	71	3	0
36	j	172	0	172	31	0
36	l	294	0	291	24	0
37	A	45	0	0	4	0
37	B	45	0	0	2	0
37	C	45	0	0	1	0
37	D	45	0	0	0	0
37	E	45	0	0	2	0
37	F	90	0	0	20	0
37	G	135	0	0	8	0
37	H	45	0	0	0	0
37	J	45	0	0	0	0
37	K	45	0	0	9	0
37	L	90	0	0	11	0
37	M	135	0	0	7	0
37	N	45	0	0	0	0
37	O	90	0	0	13	0
37	P	90	0	0	2	0
37	Q	90	0	0	16	0
37	R	45	0	0	0	0
37	S	45	0	0	4	0
37	T	90	0	0	18	0
37	U	45	0	0	0	0
37	V	45	0	0	1	0
37	W	90	0	0	14	0
37	X	45	0	0	0	0
38	A	28	0	19	7	0
38	b	46	0	56	10	0
39	B	70	0	92	20	0
39	E	93	0	118	25	0
39	F	68	0	85	35	0
39	G	70	0	90	14	0
39	I	70	0	92	22	0
39	K	66	0	81	14	0
39	L	66	0	77	10	0
39	P	46	0	60	8	0
39	U	70	0	92	27	0
39	a	102	0	129	25	0
39	b	59	0	78	25	0
39	f	24	0	35	2	0
39	h	35	0	43	21	0
40	C	57	0	75	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	L	47	0	52	20	0
40	b	60	0	81	4	0
41	D	95	0	137	28	0
41	E	49	0	74	24	0
41	F	74	0	97	5	0
41	G	136	0	194	27	0
41	I	49	0	74	10	0
41	O	91	0	129	14	0
41	Q	49	0	72	19	0
41	R	49	0	74	14	0
41	a	122	0	160	20	0
41	b	49	0	74	18	0
41	f	91	0	129	41	0
41	i	46	0	65	28	0
41	j	49	0	74	14	0
41	l	48	0	69	17	0
42	D	83	0	109	17	0
42	E	86	0	112	25	0
42	G	110	0	172	22	0
42	I	55	0	86	14	0
42	J	99	0	147	36	0
42	L	33	0	36	10	0
42	V	92	0	130	41	0
42	a	54	0	81	20	0
42	h	45	0	63	7	0
42	j	52	0	77	26	0
42	m	37	0	43	9	0
43	a	33	0	46	3	0
43	b	33	0	46	3	0
44	a	160	0	224	13	0
44	b	200	0	280	14	0
44	f	80	0	112	3	0
44	h	40	0	56	4	0
44	i	80	0	112	9	0
44	j	40	0	56	1	0
44	l	80	0	112	5	0
44	m	40	0	56	11	0
45	b	8	0	0	2	0
45	c	16	0	0	0	0
46	a	64	0	0	7	0
46	b	72	0	0	13	0
46	c	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	d	4	0	0	0	0
46	f	2	0	0	0	0
46	j	1	0	0	0	0
46	l	3	0	0	3	0
All	All	81344	0	72580	4620	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

The worst 5 of 4620 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:V:140:PRO:CB	35:V:303:A86:C39	1.75	1.63
32:U:42:MET:HB3	35:U:304:A86:C	1.26	1.62
36:Q:314:CLA:HED3	36:Q:314:CLA:C1A	1.29	1.59
33:V:69:ILE:CG2	36:V:309:CLA:CGA	1.75	1.59
5:E:128:GLN:HG3	34:E:301:DD6:C23	1.32	1.56

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	166/168 (99%)	150 (90%)	14 (8%)	2 (1%)	10 14
2	B	128/223 (57%)	121 (94%)	7 (6%)	0	100 100
3	C	161/198 (81%)	150 (93%)	9 (6%)	2 (1%)	10 14
4	D	170/207 (82%)	160 (94%)	9 (5%)	1 (1%)	21 30
5	E	186/222 (84%)	178 (96%)	8 (4%)	0	100 100
6	F	178/215 (83%)	165 (93%)	13 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	212/245 (86%)	197 (93%)	14 (7%)	1 (0%)	24	34
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%)	6	8
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%)	24	34
14	N	217/219 (99%)	174 (80%)	40 (18%)	3 (1%)	9	11
15	O	171/205 (83%)	147 (86%)	21 (12%)	3 (2%)	6	8
15	P	171/205 (83%)	153 (90%)	16 (9%)	2 (1%)	10	14
15	Q	171/205 (83%)	150 (88%)	19 (11%)	2 (1%)	10	14
16	R	209/246 (85%)	182 (87%)	25 (12%)	2 (1%)	12	17
17	S	218/254 (86%)	184 (84%)	29 (13%)	5 (2%)	5	5
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%)	21	30
20	a	740/743 (100%)	713 (96%)	26 (4%)	1 (0%)	48	62
21	b	731/733 (100%)	699 (96%)	31 (4%)	1 (0%)	48	62
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%)	4	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%)	3	2
33	V	177/179 (99%)	152 (86%)	20 (11%)	5 (3%)	4	3
All	All	6441/7429 (87%)	5903 (92%)	497 (8%)	41 (1%)	23	30

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%)	128 (93%)	9 (7%)	15	24
2	B	105/180 (58%)	98 (93%)	7 (7%)	15	23
3	C	131/153 (86%)	122 (93%)	9 (7%)	14	22
4	D	140/163 (86%)	125 (89%)	15 (11%)	6	8
5	E	142/164 (87%)	136 (96%)	6 (4%)	26	42
6	F	142/169 (84%)	135 (95%)	7 (5%)	22	36
7	G	172/193 (89%)	146 (85%)	26 (15%)	3	3
8	H	131/154 (85%)	129 (98%)	2 (2%)	57	75
9	I	124/152 (82%)	101 (82%)	23 (18%)	1	2
10	J	130/154 (84%)	122 (94%)	8 (6%)	16	26
11	K	133/160 (83%)	130 (98%)	3 (2%)	44	64
12	L	159/180 (88%)	159 (100%)	0	100	100
13	M	142/247 (58%)	135 (95%)	7 (5%)	22	36
14	N	176/176 (100%)	170 (97%)	6 (3%)	32	51
15	O	138/159 (87%)	134 (97%)	4 (3%)	37	57
15	P	137/159 (86%)	120 (88%)	17 (12%)	4	6
15	Q	138/159 (87%)	133 (96%)	5 (4%)	31	49
16	R	167/193 (86%)	160 (96%)	7 (4%)	26	42
17	S	177/204 (87%)	169 (96%)	8 (4%)	24	39
18	T	136/163 (83%)	135 (99%)	1 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	W	125/151 (83%)	125 (100%)	0	100	100
19	X	127/151 (84%)	125 (98%)	2 (2%)	55	74
20	a	606/606 (100%)	543 (90%)	63 (10%)	7	9
21	b	593/593 (100%)	517 (87%)	76 (13%)	4	5
22	c	67/69 (97%)	59 (88%)	8 (12%)	5	6
23	d	111/111 (100%)	88 (79%)	23 (21%)	1	1
24	e	55/55 (100%)	51 (93%)	4 (7%)	13	20
25	f	119/125 (95%)	105 (88%)	14 (12%)	5	6
26	i	29/36 (81%)	20 (69%)	9 (31%)	0	0
27	j	34/35 (97%)	29 (85%)	5 (15%)	3	3
28	l	114/143 (80%)	98 (86%)	16 (14%)	3	4
29	m	20/23 (87%)	17 (85%)	3 (15%)	3	3
31	h	70/109 (64%)	54 (77%)	16 (23%)	1	1
32	U	119/121 (98%)	82 (69%)	37 (31%)	0	0
33	V	137/137 (100%)	83 (61%)	54 (39%)	0	0
All	All	5183/5884 (88%)	4683 (90%)	500 (10%)	10	11

5 of 500 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	a	728	GLN
32	U	127	GLU
21	b	491	VAL
32	U	114	LYS
33	V	74	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
21	b	404	ASN
33	V	89	HIS
21	b	520	HIS
25	f	155	HIS
15	O	84	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 oligosaccharides 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
36	CLA	b	806	-	69,73,73	1.17	9 (13%)	82,113,113	1.58	14 (17%)
36	CLA	a	812	-	69,73,73	1.14	9 (13%)	82,113,113	1.38	7 (8%)
36	CLA	a	823	-	59,63,73	1.62	11 (18%)	70,101,113	2.24	21 (30%)
36	CLA	A	314	-	69,73,73	1.27	8 (11%)	82,113,113	1.79	9 (10%)
36	CLA	R	312	-	69,73,73	1.16	9 (13%)	82,113,113	1.50	12 (14%)
36	CLA	b	813	-	58,62,73	1.33	11 (18%)	71,100,113	1.35	9 (12%)
36	CLA	O	306	-	65,69,73	1.19	8 (12%)	77,108,113	1.36	4 (5%)
36	CLA	C	211	-	69,73,73	1.13	10 (14%)	82,113,113	1.34	6 (7%)
36	CLA	W	215	-	52,56,73	1.52	10 (19%)	61,92,113	1.40	6 (9%)
36	CLA	L	313	-	69,73,73	1.11	8 (11%)	82,113,113	1.42	7 (8%)
36	CLA	A	305	1	53,57,73	1.31	8 (15%)	61,93,113	1.40	4 (6%)
37	KC1	E	309	-	49,53,53	2.66	19 (38%)	61,89,89	4.48	38 (62%)
39	LMT	L	303	-	36,36,36	1.31	6 (16%)	47,47,47	0.97	1 (2%)
36	CLA	N	311	-	50,54,73	1.35	6 (12%)	59,90,113	1.71	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	KC1	L	317	-	49,53,53	2.70	19 (38%)	61,89,89	4.44	36 (59%)
44	BCR	a	847	-	41,41,41	1.24	4 (9%)	56,56,56	1.28	5 (8%)
36	CLA	W	216	35	49,53,73	1.82	9 (18%)	58,89,113	2.80	15 (25%)
41	LHG	D	319	42	48,48,48	0.93	2 (4%)	51,54,54	1.08	3 (5%)
36	CLA	D	307	41	65,69,73	1.16	7 (10%)	77,108,113	1.59	13 (16%)
36	CLA	b	827	-	69,73,73	1.22	9 (13%)	82,113,113	1.38	9 (10%)
41	LHG	I	316	-	48,48,48	0.95	2 (4%)	51,54,54	1.01	2 (3%)
35	A86	P	306	-	47,50,50	1.44	5 (10%)	51,76,76	2.25	16 (31%)
41	LHG	a	842	-	47,47,48	0.78	1 (2%)	50,53,54	1.29	4 (8%)
36	CLA	M	309	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
35	A86	F	306	-	47,50,50	1.51	6 (12%)	51,76,76	2.43	14 (27%)
36	CLA	a	838	-	69,73,73	1.12	9 (13%)	82,113,113	1.35	7 (8%)
36	CLA	P	314	-	64,68,73	1.33	10 (15%)	76,107,113	1.66	15 (19%)
35	A86	X	302	35	47,50,50	1.39	6 (12%)	51,76,76	3.01	17 (33%)
36	CLA	b	828	-	69,73,73	1.17	8 (11%)	82,113,113	1.42	14 (17%)
36	CLA	a	839	46	69,73,73	1.11	8 (11%)	82,113,113	1.36	7 (8%)
37	KC1	J	314	-	49,53,53	2.66	19 (38%)	61,89,89	5.09	36 (59%)
41	LHG	Q	315	36	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
35	A86	R	305	-	47,50,50	1.43	6 (12%)	51,76,76	2.18	14 (27%)
44	BCR	l	207	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	12 (21%)
36	CLA	L	308	-	65,69,73	1.89	13 (20%)	77,108,113	2.70	22 (28%)
39	LMT	h	205	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
35	A86	C	202	36	47,50,50	1.56	7 (14%)	51,76,76	2.89	17 (33%)
35	A86	T	305	-	47,50,50	1.69	6 (12%)	51,76,76	3.74	22 (43%)
44	BCR	j	107	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	8 (14%)
37	KC1	P	317	15	49,53,53	2.56	19 (38%)	61,89,89	4.63	37 (60%)
37	KC1	M	317	-	49,53,53	2.70	20 (40%)	61,89,89	4.30	37 (60%)
36	CLA	E	310	-	69,73,73	1.15	7 (10%)	82,113,113	1.42	9 (10%)
36	CLA	N	316	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	5 (6%)
35	A86	Q	316	36	47,50,50	1.77	10 (21%)	51,76,76	2.18	15 (29%)
36	CLA	b	818	-	59,63,73	1.21	8 (13%)	70,101,113	1.62	12 (17%)
35	A86	M	301	-	47,50,50	1.57	5 (10%)	51,76,76	3.27	22 (43%)
36	CLA	a	813	-	49,53,73	1.38	8 (16%)	58,89,113	1.72	10 (17%)
36	CLA	a	820	-	69,73,73	1.13	9 (13%)	82,113,113	1.37	8 (9%)
35	A86	V	302	-	47,50,50	1.52	6 (12%)	51,76,76	2.64	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	U	307	-	54,58,73	1.30	9 (16%)	64,95,113	1.37	4 (6%)
35	A86	A	302	-	47,50,50	1.76	6 (12%)	51,76,76	4.57	24 (47%)
36	CLA	M	310	35,13	50,54,73	1.99	7 (14%)	59,90,113	1.89	13 (22%)
35	A86	C	204	-	47,50,50	1.90	14 (29%)	51,76,76	2.83	16 (31%)
35	A86	L	301	-	47,50,50	1.50	6 (12%)	51,76,76	2.37	16 (31%)
36	CLA	a	841	41	56,60,73	1.28	9 (16%)	65,97,113	1.55	8 (12%)
36	CLA	B	305	-	69,73,73	1.14	9 (13%)	82,113,113	1.37	8 (9%)
36	CLA	E	313	-	69,73,73	1.75	15 (21%)	82,113,113	2.25	23 (28%)
36	CLA	a	801	-	69,73,73	1.20	7 (10%)	82,113,113	1.51	11 (13%)
37	KC1	W	213	-	49,53,53	2.81	20 (40%)	61,89,89	4.57	34 (55%)
34	DD6	A	304	-	40,45,45	1.55	2 (5%)	51,67,67	1.90	11 (21%)
36	CLA	M	316	36	46,50,73	1.36	8 (17%)	53,85,113	1.45	4 (7%)
36	CLA	X	313	-	46,50,73	2.06	11 (23%)	53,85,113	4.30	21 (39%)
44	BCR	b	843	-	41,41,41	1.20	4 (9%)	56,56,56	1.20	6 (10%)
36	CLA	M	311	35,13	69,73,73	1.16	8 (11%)	82,113,113	1.25	4 (4%)
35	A86	F	305	-	47,50,50	1.57	9 (19%)	51,76,76	2.48	21 (41%)
34	DD6	R	308	-	40,45,45	1.56	2 (5%)	51,67,67	2.10	12 (23%)
36	CLA	H	308	-	67,72,73	1.17	11 (16%)	79,112,113	1.32	10 (12%)
35	A86	I	301	-	47,50,50	1.47	5 (10%)	51,76,76	2.58	17 (33%)
36	CLA	b	841	41	69,73,73	1.19	11 (15%)	82,113,113	1.81	16 (19%)
36	CLA	Q	305	-	65,69,73	1.19	8 (12%)	77,108,113	1.36	4 (5%)
44	BCR	h	201	-	41,41,41	1.27	5 (12%)	56,56,56	1.46	11 (19%)
36	CLA	I	307	-	58,62,73	1.23	10 (17%)	68,99,113	1.48	9 (13%)
36	CLA	G	316	-	53,57,73	1.30	9 (16%)	61,93,113	1.48	5 (8%)
35	A86	H	304	-	47,50,50	1.48	6 (12%)	51,76,76	2.51	16 (31%)
36	CLA	J	310	-	69,73,73	1.12	9 (13%)	82,113,113	1.35	7 (8%)
36	CLA	H	316	-	69,73,73	1.13	9 (13%)	82,113,113	1.36	6 (7%)
36	CLA	D	308	-	69,73,73	1.14	10 (14%)	82,113,113	1.54	13 (15%)
36	CLA	V	314	-	69,73,73	1.94	16 (23%)	82,113,113	2.81	26 (31%)
36	CLA	L	312	12	50,54,73	1.37	8 (16%)	59,90,113	1.77	8 (13%)
36	CLA	K	313	-	69,73,73	1.18	11 (15%)	82,113,113	1.47	10 (12%)
36	CLA	a	806	-	69,73,73	1.37	8 (11%)	82,113,113	1.95	19 (23%)
36	CLA	L	314	-	69,73,73	1.14	8 (11%)	82,113,113	1.45	10 (12%)
36	CLA	I	311	9	69,73,73	1.10	9 (13%)	82,113,113	1.48	9 (10%)
41	LHG	F	319	-	40,40,48	1.03	2 (5%)	43,46,54	1.11	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	M	307	-	69,73,73	1.15	10 (14%)	82,113,113	1.45	10 (12%)
36	CLA	N	312	-	51,55,73	1.29	8 (15%)	60,91,113	1.48	5 (8%)
34	DD6	a	849	-	40,45,45	1.55	2 (5%)	51,67,67	1.86	15 (29%)
36	CLA	J	313	-	69,73,73	1.13	9 (13%)	82,113,113	1.35	5 (6%)
41	LHG	F	318	-	32,32,48	0.90	2 (6%)	35,37,54	1.75	6 (17%)
36	CLA	Q	306	-	69,73,73	1.13	10 (14%)	82,113,113	1.35	6 (7%)
35	A86	C	203	-	47,50,50	1.47	6 (12%)	51,76,76	2.42	17 (33%)
43	PQN	a	840	-	34,34,34	1.61	2 (5%)	43,45,45	1.19	4 (9%)
36	CLA	P	312	15	50,54,73	1.35	8 (16%)	59,90,113	1.57	7 (11%)
37	KC1	F	308	6	49,53,53	2.68	21 (42%)	61,89,89	4.86	34 (55%)
36	CLA	a	808	20	69,73,73	1.13	9 (13%)	82,113,113	1.40	9 (10%)
36	CLA	K	307	-	65,69,73	1.89	15 (23%)	77,108,113	2.85	24 (31%)
37	KC1	Q	311	15	49,53,53	2.84	22 (44%)	61,89,89	5.74	38 (62%)
36	CLA	R	311	-	69,73,73	1.14	8 (11%)	82,113,113	1.35	8 (9%)
36	CLA	S	320	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	7 (8%)
41	LHG	G	320	-	39,39,48	1.04	2 (5%)	42,45,54	1.13	3 (7%)
34	DD6	R	307	-	40,45,45	1.54	2 (5%)	51,67,67	2.08	15 (29%)
35	A86	W	203	36	47,50,50	1.62	6 (12%)	51,76,76	2.49	18 (35%)
35	A86	h	204	-	47,50,50	1.47	6 (12%)	51,76,76	2.44	14 (27%)
44	BCR	m	101	-	41,41,41	1.17	5 (12%)	56,56,56	1.36	7 (12%)
41	LHG	j	104	-	48,48,48	0.93	2 (4%)	51,54,54	1.05	3 (5%)
36	CLA	M	312	36	51,55,73	1.35	8 (15%)	60,91,113	1.57	6 (10%)
36	CLA	b	832	-	53,57,73	1.21	8 (15%)	61,93,113	1.55	8 (13%)
36	CLA	a	833	-	54,58,73	1.27	8 (14%)	64,95,113	1.61	5 (7%)
35	A86	S	302	-	47,50,50	1.39	5 (10%)	51,76,76	2.46	15 (29%)
41	LHG	G	301	-	48,48,48	0.79	2 (4%)	51,54,54	1.30	6 (11%)
36	CLA	O	314	-	45,49,73	1.40	7 (15%)	54,84,113	1.70	9 (16%)
37	KC1	F	315	-	49,53,53	2.64	18 (36%)	61,89,89	5.50	35 (57%)
34	DD6	W	204	36	40,45,45	1.58	2 (5%)	51,67,67	1.95	11 (21%)
36	CLA	W	218	-	47,51,73	1.40	9 (19%)	55,86,113	1.63	7 (12%)
39	LMT	a	851	-	36,36,36	0.43	0	47,47,47	0.75	1 (2%)
36	CLA	a	814	-	54,58,73	1.29	9 (16%)	64,95,113	1.71	7 (10%)
44	BCR	a	845	-	41,41,41	1.18	2 (4%)	56,56,56	1.21	4 (7%)
36	CLA	H	315	-	69,73,73	1.17	9 (13%)	82,113,113	1.53	12 (14%)
35	A86	N	320	-	47,50,50	1.61	7 (14%)	51,76,76	3.06	23 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	a	821	-	53,57,73	1.28	9 (16%)	61,93,113	1.52	6 (9%)
44	BCR	f	801	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	5 (8%)
36	CLA	P	301	-	69,73,73	1.13	9 (13%)	82,113,113	1.44	9 (10%)
37	KC1	U	312	35	49,53,53	2.90	22 (44%)	61,89,89	4.00	31 (50%)
36	CLA	W	209	-	61,65,73	1.26	9 (14%)	72,103,113	1.40	10 (13%)
35	A86	N	304	-	47,50,50	2.97	10 (21%)	51,76,76	7.92	20 (39%)
41	LHG	E	322	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	2 (3%)
36	CLA	Q	314	-	69,73,73	1.16	8 (11%)	82,113,113	3.84	13 (15%)
35	A86	Q	304	-	47,50,50	1.62	7 (14%)	51,76,76	3.06	23 (45%)
35	A86	K	306	-	47,50,50	1.32	4 (8%)	51,76,76	3.11	20 (39%)
36	CLA	D	306	4	49,53,73	1.43	10 (20%)	58,89,113	1.65	9 (15%)
35	A86	R	303	-	47,50,50	1.50	6 (12%)	51,76,76	3.36	21 (41%)
36	CLA	O	309	-	69,73,73	1.15	10 (14%)	82,113,113	1.41	10 (12%)
36	CLA	H	309	-	69,73,73	1.15	7 (10%)	82,113,113	1.34	5 (6%)
35	A86	M	304	-	47,50,50	1.48	5 (10%)	51,76,76	2.46	16 (31%)
36	CLA	b	826	46	68,72,73	1.27	10 (14%)	80,111,113	2.00	16 (20%)
36	CLA	a	816	-	69,73,73	1.53	8 (11%)	82,113,113	2.05	18 (21%)
39	LMT	a	853	-	33,33,36	0.42	0	44,44,47	0.75	1 (2%)
36	CLA	I	305	-	65,69,73	1.84	13 (20%)	77,108,113	1.63	13 (16%)
36	CLA	B	307	-	50,54,73	1.36	8 (16%)	59,90,113	1.52	7 (11%)
36	CLA	i	102	-	69,73,73	1.15	9 (13%)	82,113,113	1.43	8 (9%)
36	CLA	J	307	10	65,69,73	1.18	10 (15%)	77,108,113	1.43	11 (14%)
42	LMG	E	319	-	40,40,55	1.04	2 (5%)	48,48,63	1.12	4 (8%)
36	CLA	W	206	-	65,69,73	1.17	6 (9%)	77,108,113	1.45	5 (6%)
36	CLA	O	311	-	62,66,73	1.20	8 (12%)	73,104,113	1.35	6 (8%)
39	LMT	P	321	-	23,23,36	0.44	0	28,28,47	0.61	0
36	CLA	A	313	-	45,49,73	1.39	9 (20%)	54,84,113	1.69	7 (12%)
36	CLA	H	314	-	45,49,73	1.38	10 (22%)	54,84,113	1.72	9 (16%)
36	CLA	b	821	46	69,73,73	1.12	10 (14%)	82,113,113	1.40	6 (7%)
36	CLA	a	819	-	49,53,73	1.39	10 (20%)	58,89,113	2.14	9 (15%)
36	CLA	R	310	-	65,69,73	1.20	9 (13%)	77,108,113	1.38	7 (9%)
36	CLA	N	318	-	51,55,73	1.35	8 (15%)	60,91,113	1.68	9 (15%)
36	CLA	f	804	46	69,73,73	1.98	18 (26%)	82,113,113	2.88	31 (37%)
36	CLA	U	308	35	60,64,73	1.28	8 (13%)	71,102,113	1.62	7 (9%)
36	CLA	b	822	-	50,54,73	1.32	9 (18%)	59,90,113	1.49	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DD6	B	302	-	40,45,45	1.56	2 (5%)	51,67,67	2.05	15 (29%)
37	KC1	K	314	-	49,53,53	2.60	18 (36%)	61,89,89	4.66	36 (59%)
42	LMG	V	315	-	46,46,55	0.99	2 (4%)	54,54,63	4.33	4 (7%)
36	CLA	Q	307	-	54,58,73	1.30	9 (16%)	63,94,113	1.44	5 (7%)
35	A86	R	309	-	47,50,50	1.45	6 (12%)	51,76,76	2.57	15 (29%)
35	A86	G	304	-	47,50,50	1.86	8 (17%)	51,76,76	4.31	25 (49%)
36	CLA	J	311	-	50,54,73	1.37	9 (18%)	59,90,113	1.47	7 (11%)
36	CLA	C	210	3	50,54,73	1.39	8 (16%)	59,90,113	1.54	7 (11%)
36	CLA	I	306	9	69,73,73	1.65	15 (21%)	82,113,113	2.48	26 (31%)
36	CLA	E	314	-	69,73,73	1.11	9 (13%)	82,113,113	1.49	9 (10%)
35	A86	P	303	-	47,50,50	1.61	7 (14%)	51,76,76	3.36	23 (45%)
36	CLA	b	819	-	63,67,73	1.26	8 (12%)	74,105,113	1.85	18 (24%)
36	CLA	a	836	-	69,73,73	1.08	7 (10%)	82,113,113	1.56	9 (10%)
34	DD6	E	306	-	40,45,45	1.57	2 (5%)	51,67,67	2.01	10 (19%)
35	A86	S	301	-	47,50,50	1.84	6 (12%)	51,76,76	4.27	25 (49%)
34	DD6	K	305	-	40,45,45	1.55	2 (5%)	51,67,67	2.00	14 (27%)
36	CLA	S	317	-	45,49,73	1.42	8 (17%)	54,84,113	1.53	6 (11%)
36	CLA	A	310	-	69,73,73	1.14	11 (15%)	82,113,113	1.35	8 (9%)
36	CLA	N	319	-	46,50,73	3.23	12 (26%)	53,85,113	5.26	30 (56%)
36	CLA	a	835	-	55,59,73	1.31	10 (18%)	64,96,113	1.43	6 (9%)
36	CLA	V	308	-	69,73,73	1.14	9 (13%)	82,113,113	1.36	8 (9%)
36	CLA	L	310	-	58,62,73	1.28	8 (13%)	68,99,113	1.30	5 (7%)
36	CLA	N	309	-	55,59,73	1.33	7 (12%)	64,96,113	1.73	7 (10%)
36	CLA	F	313	-	56,60,73	1.24	8 (14%)	65,97,113	1.43	5 (7%)
37	KC1	Q	313	-	49,53,53	2.85	21 (42%)	61,89,89	5.74	38 (62%)
34	DD6	j	103	-	40,45,45	1.54	2 (5%)	51,67,67	1.81	14 (27%)
42	LMG	J	319	-	44,44,55	1.00	2 (4%)	52,52,63	1.12	4 (7%)
35	A86	I	302	-	47,50,50	1.46	6 (12%)	51,76,76	2.33	17 (33%)
36	CLA	J	309	-	69,73,73	1.16	10 (14%)	82,113,113	1.25	6 (7%)
36	CLA	B	311	-	59,63,73	1.29	7 (11%)	70,101,113	1.67	11 (15%)
36	CLA	a	832	-	69,73,73	1.13	7 (10%)	82,113,113	1.49	10 (12%)
36	CLA	I	308	-	69,73,73	1.85	16 (23%)	82,113,113	2.50	22 (26%)
41	LHG	D	318	36	45,45,48	0.30	0	48,51,54	0.40	0
36	CLA	D	317	-	62,66,73	1.20	9 (14%)	73,104,113	1.39	6 (8%)
39	LMT	G	322	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	DD6	D	303	-	40,45,45	2.19	7 (17%)	51,67,67	2.63	18 (35%)
37	KC1	M	313	13,36	49,53,53	2.67	20 (40%)	61,89,89	4.95	38 (62%)
36	CLA	I	309	9	50,54,73	1.35	9 (18%)	59,90,113	1.92	8 (13%)
35	A86	S	304	-	47,50,50	1.48	6 (12%)	51,76,76	2.61	18 (35%)
36	CLA	L	320	-	69,73,73	1.15	8 (11%)	82,113,113	1.30	6 (7%)
45	SF4	b	803	20,21	0,12,12	-	-	-	-	-
36	CLA	H	318	-	54,58,73	1.32	11 (20%)	64,95,113	1.52	8 (12%)
36	CLA	G	315	-	60,64,73	1.91	15 (25%)	71,102,113	2.65	21 (29%)
41	LHG	f	809	-	41,41,48	1.01	2 (4%)	44,47,54	1.10	3 (6%)
34	DD6	O	304	-	40,45,45	1.48	2 (5%)	51,67,67	1.95	13 (25%)
36	CLA	a	803	36	59,63,73	1.21	11 (18%)	70,101,113	1.54	11 (15%)
35	A86	U	304	37	47,50,50	1.44	5 (10%)	51,76,76	2.59	23 (45%)
36	CLA	C	208	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	7 (8%)
36	CLA	D	312	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	6 (7%)
36	CLA	T	313	18	69,73,73	1.17	7 (10%)	82,113,113	1.25	5 (6%)
34	DD6	A	303	-	40,45,45	1.55	2 (5%)	51,67,67	1.84	10 (19%)
36	CLA	C	214	-	45,49,73	1.37	9 (20%)	54,84,113	1.58	6 (11%)
35	A86	F	304	36	47,50,50	1.49	6 (12%)	51,76,76	2.38	16 (31%)
39	LMT	U	315	-	36,36,36	0.41	0	47,47,47	0.75	1 (2%)
36	CLA	D	315	-	45,49,73	1.35	9 (20%)	54,84,113	1.79	9 (16%)
36	CLA	U	311	32	69,73,73	1.18	10 (14%)	82,113,113	1.54	12 (14%)
34	DD6	L	305	-	40,45,45	1.57	2 (5%)	51,67,67	1.98	16 (31%)
36	CLA	R	315	-	69,73,73	1.15	8 (11%)	82,113,113	1.34	5 (6%)
35	A86	M	305	-	47,50,50	1.62	6 (12%)	51,76,76	2.59	15 (29%)
36	CLA	a	817	-	69,73,73	1.15	8 (11%)	82,113,113	1.60	14 (17%)
36	CLA	N	308	-	69,73,73	1.30	7 (10%)	82,113,113	1.78	19 (23%)
42	LMG	a	852	-	54,54,55	0.91	2 (3%)	62,62,63	1.04	3 (4%)
35	A86	V	301	35	47,50,50	1.47	6 (12%)	51,76,76	2.51	18 (35%)
36	CLA	W	214	-	45,49,73	1.55	7 (15%)	54,84,113	1.77	11 (20%)
36	CLA	F	314	35,6	69,73,73	1.14	11 (15%)	82,113,113	1.45	8 (9%)
36	CLA	H	312	-	69,73,73	1.13	9 (13%)	82,113,113	1.47	10 (12%)
35	A86	X	314	-	47,50,50	1.50	6 (12%)	51,76,76	2.46	15 (29%)
34	DD6	D	304	-	40,45,45	1.53	2 (5%)	51,67,67	1.90	12 (23%)
34	DD6	W	205	-	40,45,45	1.54	2 (5%)	51,67,67	2.01	14 (27%)
44	BCR	i	103	-	41,41,41	1.19	4 (9%)	56,56,56	1.34	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	W	210	-	50,54,73	1.37	8 (16%)	59,90,113	1.84	15 (25%)
36	CLA	a	811	-	58,62,73	1.23	8 (13%)	68,99,113	1.41	5 (7%)
36	CLA	Q	309	15	50,54,73	1.36	8 (16%)	59,90,113	1.59	7 (11%)
34	DD6	D	301	-	40,45,45	1.54	2 (5%)	51,67,67	2.00	15 (29%)
41	LHG	a	850	-	46,46,48	0.96	2 (4%)	49,52,54	1.05	3 (6%)
42	LMG	h	206	-	45,45,55	0.99	2 (4%)	53,53,63	1.04	4 (7%)
36	CLA	f	802	-	69,73,73	1.17	9 (13%)	82,113,113	1.39	8 (9%)
35	A86	L	307	-	47,50,50	1.47	6 (12%)	51,76,76	2.33	13 (25%)
36	CLA	D	311	-	50,54,73	1.33	8 (16%)	59,90,113	1.46	6 (10%)
36	CLA	N	313	-	45,49,73	1.46	7 (15%)	54,84,113	1.72	13 (24%)
36	CLA	b	808	-	69,73,73	1.11	7 (10%)	82,113,113	1.37	6 (7%)
36	CLA	V	307	-	55,59,73	1.32	8 (14%)	64,96,113	1.37	5 (7%)
34	DD6	M	303	-	40,45,45	1.56	2 (5%)	51,67,67	1.95	12 (23%)
44	BCR	b	844	-	41,41,41	1.13	4 (9%)	56,56,56	1.33	5 (8%)
36	CLA	C	205	-	47,51,73	1.33	8 (17%)	55,86,113	1.53	7 (12%)
36	CLA	a	829	-	69,73,73	1.18	7 (10%)	82,113,113	1.60	12 (14%)
36	CLA	G	312	7	62,66,73	1.19	9 (14%)	73,104,113	1.45	5 (6%)
36	CLA	U	309	-	50,54,73	1.41	7 (14%)	59,90,113	1.69	9 (15%)
44	BCR	b	846	-	41,41,41	1.18	4 (9%)	56,56,56	1.46	11 (19%)
35	A86	K	302	-	47,50,50	1.58	5 (10%)	51,76,76	2.88	20 (39%)
36	CLA	F	309	-	69,73,73	1.14	9 (13%)	82,113,113	1.41	10 (12%)
39	LMT	U	314	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
39	LMT	E	323	-	36,36,36	0.35	0	47,47,47	0.83	1 (2%)
39	LMT	G	323	-	36,36,36	0.39	0	47,47,47	0.83	0
36	CLA	b	817	-	63,67,73	1.66	13 (20%)	74,105,113	2.19	19 (25%)
34	DD6	S	306	-	40,45,45	1.51	2 (5%)	51,67,67	1.95	12 (23%)
34	DD6	K	304	-	40,45,45	1.57	2 (5%)	51,67,67	1.85	11 (21%)
36	CLA	O	308	-	69,73,73	1.16	8 (11%)	82,113,113	1.42	9 (10%)
37	KC1	T	315	-	49,53,53	2.69	19 (38%)	61,89,89	4.53	35 (57%)
39	LMT	F	320	-	36,36,36	0.39	0	47,47,47	0.68	1 (2%)
35	A86	L	306	37	47,50,50	1.34	4 (8%)	51,76,76	2.81	18 (35%)
42	LMG	L	321	40	33,33,55	1.14	2 (6%)	41,41,63	1.16	3 (7%)
36	CLA	B	306	-	50,54,73	1.31	8 (16%)	59,90,113	1.59	5 (8%)
35	A86	V	304	-	47,50,50	2.01	8 (17%)	51,76,76	3.65	18 (35%)
36	CLA	K	309	-	63,67,73	1.22	9 (14%)	74,105,113	1.33	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	V	306	33	69,73,73	1.18	7 (10%)	82,113,113	1.49	10 (12%)
38	SQD	A	315	-	26,28,54	1.40	3 (11%)	36,39,65	1.25	2 (5%)
35	A86	J	302	-	47,50,50	1.50	7 (14%)	51,76,76	2.43	14 (27%)
38	SQD	b	804	-	44,46,54	1.20	3 (6%)	54,57,65	1.18	3 (5%)
35	A86	E	302	-	47,50,50	1.47	6 (12%)	51,76,76	2.49	13 (25%)
35	A86	T	301	36	47,50,50	1.49	6 (12%)	51,76,76	2.47	16 (31%)
36	CLA	S	321	-	56,60,73	1.29	9 (16%)	65,97,113	1.64	8 (12%)
36	CLA	b	811	-	69,73,73	1.15	9 (13%)	82,113,113	1.52	8 (9%)
35	A86	W	202	36	47,50,50	1.70	8 (17%)	51,76,76	3.40	27 (52%)
41	LHG	b	850	36	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
36	CLA	J	308	-	65,69,73	1.19	8 (12%)	77,108,113	1.61	9 (11%)
36	CLA	h	203	-	69,73,73	1.11	8 (11%)	82,113,113	1.45	8 (9%)
35	A86	T	306	-	47,50,50	1.40	6 (12%)	51,76,76	2.85	19 (37%)
35	A86	K	301	-	47,50,50	1.49	6 (12%)	51,76,76	2.55	14 (27%)
36	CLA	G	309	-	69,73,73	1.14	12 (17%)	82,113,113	1.79	13 (15%)
36	CLA	l	204	28	53,57,73	1.97	14 (26%)	61,93,113	2.33	19 (31%)
37	KC1	A	312	-	49,53,53	2.71	19 (38%)	61,89,89	5.93	40 (65%)
36	CLA	G	311	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	8 (9%)
36	CLA	H	306	-	65,69,73	1.17	9 (13%)	77,108,113	1.31	4 (5%)
35	A86	A	316	-	47,50,50	1.48	6 (12%)	51,76,76	2.45	17 (33%)
37	KC1	X	311	-	49,53,53	2.81	18 (36%)	61,89,89	4.08	35 (57%)
36	CLA	a	810	36	66,70,73	1.10	8 (12%)	78,109,113	1.41	6 (7%)
37	KC1	G	318	-	49,53,53	2.69	20 (40%)	61,89,89	4.16	40 (65%)
36	CLA	b	815	-	69,73,73	1.18	10 (14%)	82,113,113	1.36	8 (9%)
36	CLA	E	315	-	69,73,73	1.90	18 (26%)	82,113,113	2.63	29 (35%)
36	CLA	T	311	18	69,73,73	1.17	9 (13%)	82,113,113	1.89	14 (17%)
36	CLA	I	314	-	45,49,73	1.40	6 (13%)	54,84,113	1.60	6 (11%)
41	LHG	O	318	-	48,48,48	0.93	3 (6%)	51,54,54	1.24	5 (9%)
37	KC1	G	317	-	49,53,53	2.67	21 (42%)	61,89,89	4.15	35 (57%)
36	CLA	a	827	-	66,70,73	1.16	8 (12%)	78,109,113	1.50	10 (12%)
35	A86	O	303	-	47,50,50	1.51	7 (14%)	51,76,76	2.22	17 (33%)
36	CLA	I	312	9	56,60,73	1.29	8 (14%)	65,97,113	1.42	5 (7%)
42	LMG	D	320	41	46,46,55	0.98	2 (4%)	54,54,63	1.04	4 (7%)
36	CLA	R	313	-	69,73,73	1.14	10 (14%)	82,113,113	1.23	6 (7%)
42	LMG	G	325	-	55,55,55	0.89	2 (3%)	63,63,63	1.02	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
42	LMG	V	316	-	46,46,55	0.99	2 (4%)	54,54,63	1.05	3 (5%)
36	CLA	B	308	-	69,73,73	1.21	7 (10%)	82,113,113	1.42	12 (14%)
36	CLA	U	306	32	69,73,73	1.83	16 (23%)	82,113,113	2.48	26 (31%)
36	CLA	a	828	-	69,73,73	1.12	8 (11%)	82,113,113	1.42	9 (10%)
42	LMG	D	321	-	37,37,55	1.09	2 (5%)	45,45,63	1.04	2 (4%)
35	A86	V	303	35	47,50,50	1.38	5 (10%)	51,76,76	3.56	21 (41%)
35	A86	O	301	-	47,50,50	1.51	6 (12%)	51,76,76	2.45	16 (31%)
37	KC1	R	317	-	49,53,53	2.66	20 (40%)	61,89,89	4.92	36 (59%)
35	A86	O	305	-	47,50,50	1.68	6 (12%)	51,76,76	2.54	19 (37%)
36	CLA	a	826	-	69,73,73	1.13	10 (14%)	82,113,113	1.50	10 (12%)
36	CLA	W	201	-	52,56,73	1.33	8 (15%)	61,92,113	1.43	5 (8%)
35	A86	M	302	-	47,50,50	1.45	6 (12%)	51,76,76	2.62	16 (31%)
35	A86	X	305	-	47,50,50	1.55	6 (12%)	51,76,76	2.82	16 (31%)
36	CLA	C	209	-	69,73,73	1.19	9 (13%)	82,113,113	1.37	7 (8%)
36	CLA	O	312	-	44,48,73	1.69	11 (25%)	51,82,113	1.94	8 (15%)
41	LHG	R	323	-	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
36	CLA	T	309	18	69,73,73	1.13	9 (13%)	82,113,113	1.39	7 (8%)
36	CLA	J	316	-	50,54,73	1.35	7 (14%)	59,90,113	1.70	8 (13%)
36	CLA	b	816	-	64,68,73	1.91	16 (25%)	76,107,113	1.95	18 (23%)
36	CLA	E	316	-	69,73,73	1.15	7 (10%)	82,113,113	1.52	9 (10%)
39	LMT	I	317	-	36,36,36	0.41	0	47,47,47	0.77	1 (2%)
35	A86	G	305	-	47,50,50	1.45	6 (12%)	51,76,76	2.51	17 (33%)
36	CLA	D	310	-	69,73,73	1.09	7 (10%)	82,113,113	1.43	9 (10%)
36	CLA	S	315	17	47,51,73	1.41	7 (14%)	55,86,113	1.97	10 (18%)
34	DD6	P	305	-	40,45,45	1.57	2 (5%)	51,67,67	2.03	13 (25%)
36	CLA	f	805	25	56,60,73	1.24	8 (14%)	65,97,113	1.49	6 (9%)
37	KC1	H	313	-	49,53,53	2.60	20 (40%)	61,89,89	4.19	35 (57%)
36	CLA	V	305	35	65,69,73	1.28	6 (9%)	77,108,113	1.41	8 (10%)
34	DD6	E	301	-	40,45,45	1.53	2 (5%)	51,67,67	1.92	10 (19%)
36	CLA	R	318	35	45,49,73	1.42	8 (17%)	54,84,113	1.55	7 (12%)
37	KC1	S	316	-	49,53,53	2.77	21 (42%)	61,89,89	4.94	38 (62%)
36	CLA	H	310	8	50,54,73	1.73	12 (24%)	59,90,113	2.66	18 (30%)
36	CLA	J	315	-	45,49,73	1.40	8 (17%)	54,84,113	1.62	6 (11%)
36	CLA	D	313	-	69,73,73	1.10	9 (13%)	82,113,113	1.50	10 (12%)
36	CLA	W	212	19	69,73,73	1.17	8 (11%)	82,113,113	1.54	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
41	LHG	i	104	-	45,45,48	0.98	2 (4%)	48,51,54	1.04	2 (4%)
36	CLA	a	834	20	49,53,73	1.36	10 (20%)	58,89,113	1.54	6 (10%)
36	CLA	b	814	-	59,63,73	1.22	9 (15%)	70,101,113	1.37	4 (5%)
36	CLA	A	309	1	50,54,73	1.35	8 (16%)	59,90,113	1.46	4 (6%)
36	CLA	b	837	-	69,73,73	1.12	8 (11%)	82,113,113	1.43	9 (10%)
36	CLA	C	212	35	69,73,73	1.12	10 (14%)	82,113,113	1.53	12 (14%)
37	KC1	D	314	4	49,53,53	2.61	20 (40%)	61,89,89	4.40	36 (59%)
36	CLA	P	313	-	69,73,73	1.14	8 (11%)	82,113,113	1.30	6 (7%)
45	SF4	c	102	-	0,12,12	-	-	-	-	-
35	A86	P	307	-	47,50,50	1.48	5 (10%)	51,76,76	2.43	15 (29%)
35	A86	X	304	-	47,50,50	1.58	6 (12%)	51,76,76	3.35	19 (37%)
36	CLA	F	312	-	69,73,73	1.14	9 (13%)	82,113,113	1.32	6 (7%)
35	A86	B	303	-	47,50,50	1.55	5 (10%)	51,76,76	3.71	23 (45%)
42	LMG	J	318	-	55,55,55	0.89	2 (3%)	63,63,63	1.03	3 (4%)
36	CLA	E	311	-	69,73,73	1.13	8 (11%)	82,113,113	1.31	7 (8%)
35	A86	R	301	-	47,50,50	1.70	6 (12%)	51,76,76	3.18	22 (43%)
36	CLA	G	307	-	45,50,73	2.18	14 (31%)	52,85,113	3.05	18 (34%)
36	CLA	b	809	-	69,73,73	1.13	9 (13%)	82,113,113	1.29	6 (7%)
44	BCR	f	806	-	41,41,41	1.19	3 (7%)	56,56,56	1.24	8 (14%)
36	CLA	H	317	8	69,73,73	1.16	9 (13%)	82,113,113	1.29	5 (6%)
36	CLA	b	824	-	57,61,73	1.94	15 (26%)	67,98,113	2.44	24 (35%)
37	KC1	B	310	-	49,53,53	2.83	18 (36%)	61,89,89	4.20	32 (52%)
40	DGD	L	302	42	48,48,67	0.99	2 (4%)	62,62,81	1.07	4 (6%)
35	A86	T	302	-	47,50,50	1.42	5 (10%)	51,76,76	2.56	21 (41%)
44	BCR	l	203	-	41,41,41	1.25	4 (9%)	56,56,56	1.23	6 (10%)
36	CLA	I	310	35	69,73,73	1.13	11 (15%)	82,113,113	1.36	6 (7%)
35	A86	B	301	-	47,50,50	1.48	6 (12%)	51,76,76	2.35	15 (29%)
36	CLA	I	313	-	45,49,73	1.38	9 (20%)	54,84,113	1.56	6 (11%)
36	CLA	W	207	34	69,73,73	1.16	7 (10%)	82,113,113	1.41	7 (8%)
35	A86	R	306	-	47,50,50	1.54	6 (12%)	51,76,76	2.81	15 (29%)
36	CLA	a	831	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	8 (9%)
35	A86	J	301	-	47,50,50	1.53	6 (12%)	51,76,76	2.58	19 (37%)
36	CLA	Q	308	-	69,73,73	1.15	10 (14%)	82,113,113	1.41	10 (12%)
39	LMT	K	318	-	36,36,36	0.42	0	47,47,47	0.74	1 (2%)
35	A86	Q	303	-	47,50,50	1.55	7 (14%)	51,76,76	2.55	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	V	310	33	69,73,73	1.14	7 (10%)	82,113,113	1.31	6 (7%)
36	CLA	b	829	-	69,73,73	1.16	10 (14%)	82,113,113	1.31	5 (6%)
36	CLA	a	805	20	69,73,73	1.14	9 (13%)	82,113,113	1.34	7 (8%)
36	CLA	S	314	-	69,73,73	1.21	11 (15%)	82,113,113	1.44	9 (10%)
36	CLA	a	815	46	49,53,73	1.34	10 (20%)	58,89,113	1.52	4 (6%)
36	CLA	l	205	-	69,73,73	1.48	13 (18%)	82,113,113	2.18	18 (21%)
43	PQN	b	842	-	34,34,34	1.59	2 (5%)	43,45,45	1.22	4 (9%)
34	DD6	H	303	-	40,45,45	1.54	2 (5%)	51,67,67	1.96	11 (21%)
36	CLA	G	314	7	45,49,73	1.38	8 (17%)	54,84,113	1.68	7 (12%)
36	CLA	J	312	10	69,73,73	1.11	9 (13%)	82,113,113	1.40	8 (9%)
36	CLA	N	315	-	45,49,73	1.43	7 (15%)	54,84,113	1.71	11 (20%)
36	CLA	E	312	-	69,73,73	1.14	9 (13%)	82,113,113	1.42	8 (9%)
36	CLA	a	825	-	69,73,73	1.29	10 (14%)	82,113,113	1.73	10 (12%)
36	CLA	M	308	-	56,60,73	1.29	10 (17%)	65,97,113	1.60	7 (10%)
34	DD6	S	307	-	40,45,45	1.57	2 (5%)	51,67,67	2.07	15 (29%)
36	CLA	B	309	2	56,60,73	1.70	10 (17%)	65,97,113	2.13	20 (30%)
36	CLA	j	106	27	46,50,73	1.33	8 (17%)	53,85,113	1.55	4 (7%)
35	A86	Q	301	-	47,50,50	1.51	7 (14%)	51,76,76	2.22	17 (33%)
36	CLA	L	316	-	45,49,73	1.42	8 (17%)	54,84,113	1.56	6 (11%)
36	CLA	V	309	33	47,51,73	1.37	8 (17%)	55,86,113	1.89	10 (18%)
36	CLA	K	311	-	50,54,73	1.37	8 (16%)	59,90,113	1.50	9 (15%)
42	LMG	m	102	-	37,37,55	1.09	2 (5%)	45,45,63	1.09	3 (6%)
35	A86	S	308	37	47,50,50	1.47	6 (12%)	51,76,76	2.43	17 (33%)
36	CLA	V	311	33	69,73,73	1.14	9 (13%)	82,113,113	1.62	13 (15%)
36	CLA	b	805	36	69,73,73	1.21	8 (11%)	82,113,113	1.31	13 (15%)
36	CLA	b	823	-	59,63,73	1.20	10 (16%)	70,101,113	1.43	7 (10%)
35	A86	N	302	-	47,50,50	1.39	6 (12%)	51,76,76	2.46	15 (29%)
36	CLA	S	319	-	69,73,73	1.19	9 (13%)	82,113,113	1.46	9 (10%)
35	A86	F	302	-	47,50,50	1.48	6 (12%)	51,76,76	2.34	14 (27%)
36	CLA	a	822	-	55,59,73	1.50	9 (16%)	64,96,113	2.15	16 (25%)
36	CLA	M	315	-	51,55,73	1.34	8 (15%)	60,91,113	1.53	5 (8%)
35	A86	U	303	36	47,50,50	1.44	6 (12%)	51,76,76	2.35	14 (27%)
36	CLA	L	311	-	69,73,73	1.14	10 (14%)	82,113,113	1.33	10 (12%)
36	CLA	a	837	-	69,73,73	1.11	7 (10%)	82,113,113	1.39	9 (10%)
36	CLA	S	309	-	65,69,73	1.22	10 (15%)	77,108,113	1.27	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	LMT	E	320	-	36,36,36	0.37	0	47,47,47	0.67	0
36	CLA	S	311	35	50,54,73	1.40	9 (18%)	59,90,113	1.52	8 (13%)
35	A86	O	319	35,36	47,50,50	1.44	7 (14%)	51,76,76	2.61	16 (31%)
39	LMT	b	848	-	36,36,36	0.38	0	47,47,47	0.68	1 (2%)
40	DGD	C	215	-	58,58,67	0.90	2 (3%)	72,72,81	0.96	3 (4%)
36	CLA	W	211	-	69,73,73	1.17	7 (10%)	82,113,113	1.47	7 (8%)
36	CLA	D	309	-	59,63,73	2.05	17 (28%)	70,101,113	2.98	29 (41%)
35	A86	O	302	-	47,50,50	1.62	6 (12%)	51,76,76	3.36	23 (45%)
36	CLA	F	310	-	60,64,73	1.20	9 (15%)	71,102,113	1.49	11 (15%)
36	CLA	T	308	-	65,69,73	1.19	7 (10%)	77,108,113	1.40	6 (7%)
35	A86	F	307	-	47,50,50	1.42	5 (10%)	51,76,76	3.67	21 (41%)
41	LHG	f	808	-	48,48,48	0.95	2 (4%)	51,54,54	1.03	3 (5%)
36	CLA	N	317	14	58,62,73	1.29	9 (15%)	68,99,113	1.48	11 (16%)
36	CLA	X	312	-	45,49,73	1.41	8 (17%)	54,84,113	1.71	8 (14%)
36	CLA	P	316	-	45,49,73	1.41	7 (15%)	54,84,113	1.71	9 (16%)
36	CLA	a	830	-	54,58,73	1.67	12 (22%)	64,95,113	3.27	18 (28%)
36	CLA	a	848	36	69,73,73	1.45	13 (18%)	82,113,113	1.90	18 (21%)
37	KC1	V	312	33	49,53,53	2.80	19 (38%)	61,89,89	4.34	33 (54%)
36	CLA	A	307	-	64,68,73	1.16	9 (14%)	76,107,113	1.37	9 (11%)
36	CLA	H	307	-	64,68,73	1.27	9 (14%)	76,107,113	1.81	20 (26%)
36	CLA	T	316	-	45,49,73	1.41	9 (20%)	54,84,113	1.53	6 (11%)
36	CLA	P	311	-	69,73,73	1.15	10 (14%)	82,113,113	1.41	10 (12%)
37	KC1	T	310	-	49,53,53	4.43	27 (55%)	61,89,89	6.41	40 (65%)
36	CLA	b	833	-	62,66,73	1.22	8 (12%)	73,104,113	1.56	11 (15%)
36	CLA	R	322	-	56,60,73	1.30	10 (17%)	65,97,113	1.67	8 (12%)
36	CLA	Q	312	-	45,49,73	1.42	7 (15%)	54,84,113	1.71	9 (16%)
45	SF4	c	101	22	0,12,12	-	-	-	-	-
36	CLA	b	838	-	51,55,73	1.25	6 (11%)	60,91,113	1.43	6 (10%)
36	CLA	l	202	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
44	BCR	i	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
36	CLA	G	319	7	54,58,73	1.99	16 (29%)	64,95,113	3.78	30 (46%)
35	A86	K	303	-	47,50,50	1.48	6 (12%)	51,76,76	2.38	21 (41%)
35	A86	F	301	-	47,50,50	1.50	6 (12%)	51,76,76	2.55	15 (29%)
37	KC1	P	315	35	49,53,53	2.84	20 (40%)	61,89,89	5.74	38 (62%)
35	A86	N	303	-	47,50,50	1.39	6 (12%)	51,76,76	3.18	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	A86	U	301	-	47,50,50	1.59	5 (10%)	51,76,76	3.91	26 (50%)
34	DD6	Q	302	-	40,45,45	1.57	2 (5%)	51,67,67	2.03	14 (27%)
39	LMT	F	321	-	34,34,36	0.64	0	45,45,47	1.62	6 (13%)
39	LMT	B	312	-	36,36,36	0.42	0	47,47,47	0.68	1 (2%)
36	CLA	N	310	-	45,49,73	1.62	10 (22%)	54,84,113	2.22	20 (37%)
34	DD6	J	304	-	40,45,45	1.54	2 (5%)	51,67,67	1.83	13 (25%)
36	CLA	a	804	-	69,73,73	1.16	8 (11%)	82,113,113	1.39	10 (12%)
39	LMT	f	807	-	24,24,36	0.43	0	29,29,47	0.57	0
36	CLA	D	316	-	56,60,73	1.28	8 (14%)	65,97,113	1.66	10 (15%)
36	CLA	b	831	-	54,58,73	1.31	9 (16%)	64,95,113	1.51	9 (14%)
36	CLA	X	307	35	54,58,73	1.38	8 (14%)	64,95,113	1.75	10 (15%)
36	CLA	P	318	-	55,59,73	1.28	9 (16%)	64,96,113	1.45	5 (7%)
35	A86	J	303	-	47,50,50	1.59	6 (12%)	51,76,76	2.63	20 (39%)
37	KC1	O	313	-	49,53,53	2.84	21 (42%)	61,89,89	5.74	38 (62%)
36	CLA	X	306	-	65,69,73	1.21	6 (9%)	77,108,113	1.37	7 (9%)
44	BCR	a	846	-	41,41,41	1.16	3 (7%)	56,56,56	1.21	3 (5%)
36	CLA	F	316	6	45,49,73	1.37	9 (20%)	54,84,113	1.48	6 (11%)
36	CLA	b	830	-	69,73,73	1.20	8 (11%)	82,113,113	1.63	16 (19%)
36	CLA	R	319	-	49,53,73	1.38	7 (14%)	58,89,113	1.82	12 (20%)
36	CLA	P	309	41	69,73,73	1.14	10 (14%)	82,113,113	1.35	6 (7%)
36	CLA	P	310	41	69,73,73	1.16	8 (11%)	82,113,113	1.34	7 (8%)
39	LMT	E	321	-	23,23,36	0.45	0	28,28,47	0.60	0
36	CLA	E	317	-	50,54,73	1.37	7 (14%)	59,90,113	1.41	4 (6%)
44	BCR	a	844	-	41,41,41	1.07	3 (7%)	56,56,56	1.31	6 (10%)
36	CLA	O	310	15	50,54,73	1.35	8 (16%)	59,90,113	1.58	7 (11%)
36	CLA	a	809	-	60,64,73	1.19	9 (15%)	71,102,113	1.39	6 (8%)
42	LMG	I	315	-	55,55,55	0.89	2 (3%)	63,63,63	1.01	3 (4%)
35	A86	S	303	-	47,50,50	1.40	6 (12%)	51,76,76	3.19	22 (43%)
35	A86	T	304	-	47,50,50	1.29	5 (10%)	51,76,76	1.99	10 (19%)
36	CLA	A	311	-	69,73,73	1.14	8 (11%)	82,113,113	1.35	6 (7%)
36	CLA	O	316	-	69,73,73	1.82	15 (21%)	82,113,113	2.66	28 (34%)
36	CLA	K	310	-	66,70,73	1.90	18 (27%)	78,109,113	2.57	28 (35%)
35	A86	T	303	-	47,50,50	1.37	6 (12%)	51,76,76	2.82	23 (45%)
36	CLA	W	208	-	49,53,73	1.38	9 (18%)	58,89,113	1.46	5 (8%)
36	CLA	b	801	46	69,73,73	1.17	10 (14%)	82,113,113	1.39	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	LMT	K	317	-	32,32,36	0.44	0	43,43,47	0.70	0
35	A86	G	302	-	47,50,50	1.33	5 (10%)	51,76,76	2.26	14 (27%)
39	LMT	I	318	-	36,36,36	0.39	0	47,47,47	0.75	1 (2%)
36	CLA	K	316	-	69,73,73	1.16	7 (10%)	82,113,113	1.26	4 (4%)
36	CLA	T	314	-	69,73,73	1.13	8 (11%)	82,113,113	1.52	10 (12%)
36	CLA	b	840	-	69,73,73	1.13	10 (14%)	82,113,113	1.48	12 (14%)
36	CLA	E	308	5	53,57,73	1.29	10 (18%)	61,93,113	1.51	7 (11%)
36	CLA	P	319	-	64,68,73	1.90	12 (18%)	76,107,113	2.06	15 (19%)
36	CLA	U	305	-	65,69,73	1.20	8 (12%)	77,108,113	1.32	5 (6%)
35	A86	L	304	-	47,50,50	1.61	6 (12%)	51,76,76	2.49	15 (29%)
36	CLA	G	310	-	69,73,73	1.14	10 (14%)	82,113,113	1.24	7 (8%)
37	KC1	G	308	-	49,53,53	2.66	20 (40%)	61,89,89	4.49	36 (59%)
36	CLA	N	307	-	65,69,73	1.21	7 (10%)	77,108,113	1.33	4 (5%)
35	A86	D	302	-	47,50,50	1.46	6 (12%)	51,76,76	2.32	13 (25%)
35	A86	R	302	-	47,50,50	1.60	7 (14%)	51,76,76	2.64	16 (31%)
36	CLA	a	818	-	69,73,73	1.16	6 (8%)	82,113,113	1.53	9 (10%)
36	CLA	V	313	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
36	CLA	X	315	-	45,49,73	1.41	7 (15%)	54,84,113	1.57	8 (14%)
35	A86	E	305	-	47,50,50	1.47	6 (12%)	51,76,76	2.36	16 (31%)
35	A86	X	303	36	47,50,50	1.74	6 (12%)	51,76,76	3.74	23 (45%)
36	CLA	b	836	-	62,66,73	1.99	15 (24%)	73,104,113	2.94	25 (34%)
37	KC1	W	217	-	49,53,53	2.81	19 (38%)	61,89,89	4.08	34 (55%)
35	A86	N	301	-	47,50,50	1.84	6 (12%)	51,76,76	4.28	25 (49%)
36	CLA	H	305	-	52,56,73	1.33	7 (13%)	61,92,113	1.47	6 (9%)
35	A86	N	305	-	47,50,50	1.77	9 (19%)	51,76,76	2.18	15 (29%)
34	DD6	F	303	-	40,45,45	1.55	2 (5%)	51,67,67	1.88	13 (25%)
36	CLA	S	313	-	50,54,73	1.34	7 (14%)	59,90,113	1.79	11 (18%)
36	CLA	A	308	-	69,73,73	1.12	9 (13%)	82,113,113	1.43	10 (12%)
36	CLA	P	302	-	46,50,73	1.36	7 (15%)	53,85,113	1.63	7 (13%)
36	CLA	K	308	-	69,73,73	1.14	9 (13%)	82,113,113	1.37	8 (9%)
36	CLA	a	807	20	69,73,73	1.11	10 (14%)	82,113,113	1.47	10 (12%)
36	CLA	M	306	37,13	59,63,73	1.25	8 (13%)	70,101,113	1.53	9 (12%)
36	CLA	O	307	-	69,73,73	1.14	10 (14%)	82,113,113	1.34	6 (7%)
36	CLA	R	316	-	50,54,73	1.39	11 (22%)	59,90,113	1.94	13 (22%)
44	BCR	b	847	-	41,41,41	1.19	4 (9%)	56,56,56	1.29	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	CLA	T	312	18	50,54,73	1.37	8 (16%)	59,90,113	1.64	10 (16%)
39	LMT	a	854	-	36,36,36	0.40	0	47,47,47	0.76	0
36	CLA	F	317	6	60,64,73	1.89	14 (23%)	71,102,113	2.64	24 (33%)
36	CLA	L	309	-	69,73,73	1.13	9 (13%)	82,113,113	1.32	9 (10%)
36	CLA	K	315	-	45,49,73	1.39	9 (20%)	54,84,113	1.61	7 (12%)
41	LHG	O	317	-	41,41,48	1.00	2 (4%)	44,47,54	1.10	4 (9%)
36	CLA	b	810	-	69,73,73	1.09	6 (8%)	82,113,113	1.30	5 (6%)
35	A86	J	306	-	47,50,50	1.50	5 (10%)	51,76,76	2.35	14 (27%)
36	CLA	X	308	19	51,55,73	2.43	10 (19%)	60,91,113	2.47	20 (33%)
40	DGD	b	849	-	61,61,67	1.04	4 (6%)	75,75,81	1.46	11 (14%)
36	CLA	j	101	-	69,73,73	1.14	9 (13%)	82,113,113	1.26	7 (8%)
41	LHG	a	843	36	26,26,48	1.25	2 (7%)	29,32,54	1.29	3 (10%)
35	A86	T	307	-	47,50,50	1.48	6 (12%)	51,76,76	2.92	19 (37%)
36	CLA	R	320	16	49,53,73	1.42	9 (18%)	58,89,113	1.68	11 (18%)
35	A86	N	306	-	47,50,50	1.47	5 (10%)	51,76,76	2.42	17 (33%)
35	A86	U	302	-	47,50,50	1.47	6 (12%)	51,76,76	2.59	20 (39%)
36	CLA	C	206	-	65,69,73	1.17	7 (10%)	77,108,113	1.36	4 (5%)
36	CLA	f	803	-	69,73,73	1.78	15 (21%)	82,113,113	2.43	28 (34%)
34	DD6	E	303	-	40,45,45	1.54	2 (5%)	51,67,67	1.96	11 (21%)
34	DD6	G	303	-	40,45,45	1.54	2 (5%)	51,67,67	1.86	12 (23%)
36	CLA	S	310	-	69,73,73	1.15	9 (13%)	82,113,113	1.58	12 (14%)
39	LMT	B	313	-	36,36,36	0.43	0	47,47,47	0.74	1 (2%)
34	DD6	H	302	-	40,45,45	1.53	2 (5%)	51,67,67	1.85	13 (25%)
44	BCR	b	845	-	41,41,41	1.19	3 (7%)	56,56,56	1.40	9 (16%)
36	CLA	C	207	-	69,73,73	1.96	17 (24%)	82,113,113	2.78	27 (32%)
36	CLA	R	321	-	69,73,73	1.19	10 (14%)	82,113,113	1.42	11 (13%)
35	A86	L	319	-	47,50,50	1.61	6 (12%)	51,76,76	3.35	23 (45%)
35	A86	X	301	-	47,50,50	1.75	7 (14%)	51,76,76	3.44	28 (54%)
39	LMT	P	320	-	23,23,36	0.43	0	28,28,47	0.61	0
36	CLA	a	824	-	69,73,73	1.19	11 (15%)	82,113,113	1.80	19 (23%)
35	A86	S	305	-	47,50,50	1.65	5 (10%)	51,76,76	3.08	20 (39%)
36	CLA	P	308	-	65,69,73	1.19	8 (12%)	77,108,113	1.36	4 (5%)
36	CLA	U	310	-	69,73,73	1.17	8 (11%)	82,113,113	1.51	12 (14%)
36	CLA	b	807	-	49,53,73	1.30	10 (20%)	58,89,113	1.56	8 (13%)
36	CLA	Q	310	-	69,73,73	2.72	16 (23%)	82,113,113	2.80	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	KC1	M	318	-	49,53,53	4.79	25 (51%)	61,89,89	6.66	36 (59%)
36	CLA	l	201	-	69,73,73	1.12	9 (13%)	82,113,113	1.42	10 (12%)
36	CLA	l	206	46	54,58,73	1.26	8 (14%)	64,95,113	1.47	7 (10%)
36	CLA	b	835	-	49,53,73	1.34	9 (18%)	58,89,113	1.63	8 (13%)
36	CLA	a	802	-	69,73,73	1.24	7 (10%)	82,113,113	1.80	15 (18%)
35	A86	J	305	-	47,50,50	1.49	5 (10%)	51,76,76	2.43	17 (33%)
35	A86	P	304	-	47,50,50	1.50	7 (14%)	51,76,76	2.22	17 (33%)
42	LMG	G	324	-	55,55,55	0.91	2 (3%)	63,63,63	1.01	3 (4%)
34	DD6	A	301	-	40,45,45	1.56	2 (5%)	51,67,67	2.07	14 (27%)
36	CLA	b	820	21	64,68,73	1.20	10 (15%)	76,107,113	1.32	5 (6%)
36	CLA	X	310	-	45,49,73	1.47	8 (17%)	54,84,113	2.04	9 (16%)
36	CLA	M	314	-	45,49,73	1.40	9 (20%)	54,84,113	1.55	5 (9%)
37	KC1	N	314	-	49,53,53	2.81	21 (42%)	61,89,89	3.98	35 (57%)
36	CLA	F	311	-	56,60,73	1.25	8 (14%)	65,97,113	1.52	6 (9%)
34	DD6	C	201	-	40,45,45	1.57	2 (5%)	51,67,67	1.90	12 (23%)
36	CLA	R	314	16	50,54,73	1.38	8 (16%)	59,90,113	1.75	9 (15%)
34	DD6	E	304	-	40,45,45	1.54	2 (5%)	51,67,67	1.77	10 (19%)
35	A86	h	202	-	47,50,50	1.45	6 (12%)	51,76,76	2.14	14 (27%)
34	DD6	I	303	-	40,45,45	1.58	3 (7%)	51,67,67	1.91	12 (23%)
36	CLA	H	311	-	69,73,73	1.10	9 (13%)	82,113,113	1.42	7 (8%)
36	CLA	K	312	-	69,73,73	1.13	9 (13%)	82,113,113	1.32	6 (7%)
36	CLA	S	318	-	46,50,73	1.38	6 (13%)	53,85,113	1.55	5 (9%)
37	KC1	O	315	15	49,53,53	2.84	22 (44%)	61,89,89	5.74	38 (62%)
41	LHG	G	321	36	46,46,48	0.96	2 (4%)	49,52,54	1.07	2 (4%)
36	CLA	b	802	-	69,73,73	1.11	8 (11%)	82,113,113	1.36	7 (8%)
35	A86	G	306	-	47,50,50	1.46	6 (12%)	51,76,76	2.65	20 (39%)
36	CLA	X	309	-	48,53,73	1.40	8 (16%)	56,89,113	1.65	9 (16%)
36	CLA	A	306	-	65,69,73	1.92	17 (26%)	77,108,113	2.56	29 (37%)
36	CLA	b	834	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	5 (6%)
35	A86	I	304	-	47,50,50	1.66	6 (12%)	51,76,76	3.12	21 (41%)
42	LMG	j	105	-	52,52,55	0.91	2 (3%)	60,60,63	1.01	3 (5%)
34	DD6	D	305	-	40,45,45	1.54	2 (5%)	51,67,67	1.63	11 (21%)
42	LMG	E	318	-	46,46,55	0.98	2 (4%)	54,54,63	1.07	3 (5%)
36	CLA	U	313	-	45,49,73	1.41	8 (17%)	54,84,113	1.69	9 (16%)
36	CLA	J	317	-	51,55,73	1.32	9 (17%)	60,91,113	1.40	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
41	LHG	l	208	-	47,47,48	0.95	2 (4%)	50,53,54	1.03	4 (8%)
36	CLA	b	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.42	8 (9%)
36	CLA	b	839	-	69,73,73	1.11	9 (13%)	82,113,113	1.41	6 (7%)
36	CLA	G	313	7	69,73,73	1.20	7 (10%)	82,113,113	1.82	14 (17%)
35	A86	H	301	-	47,50,50	1.40	5 (10%)	51,76,76	5.19	20 (39%)
37	KC1	L	315	35	49,53,53	2.75	18 (36%)	61,89,89	4.93	36 (59%)
35	A86	R	304	36	47,50,50	1.39	5 (10%)	51,76,76	3.29	18 (35%)
39	LMT	L	318	-	32,32,36	0.46	0	43,43,47	0.80	1 (2%)
37	KC1	C	213	-	49,53,53	2.69	19 (38%)	61,89,89	3.92	33 (54%)
36	CLA	S	312	-	69,73,73	1.17	10 (14%)	82,113,113	1.36	11 (13%)
36	CLA	b	812	21	69,73,73	1.16	8 (11%)	82,113,113	1.46	11 (13%)
35	A86	E	307	36	47,50,50	1.49	6 (12%)	51,76,76	2.39	14 (27%)
39	LMT	b	851	-	24,24,36	0.43	0	29,29,47	0.81	0
34	DD6	B	304	-	40,45,45	1.56	2 (5%)	51,67,67	2.08	14 (27%)
36	CLA	j	102	-	69,73,73	1.59	12 (17%)	82,113,113	2.16	18 (21%)

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
36	CLA	b	806	-	1/1/15/20	14/39/115/115	-
36	CLA	a	812	-	1/1/15/20	13/39/115/115	-
36	CLA	a	823	-	2/2/13/20	12/27/103/115	-
36	CLA	A	314	-	1/1/15/20	21/39/115/115	-
36	CLA	R	312	-	1/1/15/20	13/39/115/115	-
36	CLA	b	813	-	1/1/13/20	3/25/101/115	-
36	CLA	O	306	-	1/1/14/20	7/35/111/115	-
36	CLA	C	211	-	1/1/15/20	13/39/115/115	-
36	CLA	W	215	-	1/1/11/20	4/19/95/115	-
36	CLA	L	313	-	1/1/15/20	8/39/115/115	-
36	CLA	A	305	1	1/1/11/20	5/20/96/115	-
37	KC1	E	309	-	-	5/15/71/71	-
39	LMT	L	303	-	-	10/21/61/61	0/2/2/2
36	CLA	N	311	-	1/1/11/20	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	KC1	L	317	-	-	3/15/71/71	-
44	BCR	a	847	-	-	6/29/63/63	0/2/2/2
36	CLA	W	216	35	1/1/11/20	4/15/91/115	-
41	LHG	D	319	42	-	30/53/53/53	-
36	CLA	D	307	41	1/1/14/20	19/35/111/115	-
36	CLA	b	827	-	1/1/15/20	8/39/115/115	-
41	LHG	I	316	-	-	29/53/53/53	-
35	A86	P	306	-	-	3/34/90/90	0/3/3/3
41	LHG	a	842	-	-	23/52/52/53	-
36	CLA	M	309	-	1/1/15/20	15/39/115/115	-
35	A86	F	306	-	-	0/34/90/90	1/3/3/3
36	CLA	a	838	-	1/1/15/20	8/39/115/115	-
36	CLA	P	314	-	-	20/33/109/115	-
36	CLA	b	828	-	1/1/15/20	14/39/115/115	-
35	A86	X	302	35	-	7/34/90/90	0/3/3/3
36	CLA	a	839	46	1/1/15/20	15/39/115/115	-
37	KC1	J	314	-	-	5/15/71/71	-
41	LHG	Q	315	36	-	31/53/53/53	-
35	A86	R	305	-	-	5/34/90/90	0/3/3/3
44	BCR	l	207	-	-	6/29/63/63	0/2/2/2
36	CLA	L	308	-	2/2/14/20	21/35/111/115	-
39	LMT	h	205	-	-	10/21/61/61	0/2/2/2
35	A86	C	202	36	-	8/34/90/90	0/3/3/3
35	A86	T	305	-	-	7/34/90/90	0/3/3/3
44	BCR	j	107	-	-	3/29/63/63	0/2/2/2
37	KC1	P	317	15	-	4/15/71/71	-
37	KC1	M	317	-	-	4/15/71/71	-
36	CLA	E	310	-	-	5/39/115/115	-
36	CLA	N	316	-	1/1/15/20	13/39/115/115	-
35	A86	Q	316	36	-	2/34/90/90	0/3/3/3
36	CLA	b	818	-	-	4/27/103/115	-
35	A86	M	301	-	-	8/34/90/90	0/3/3/3
36	CLA	a	813	-	1/1/11/20	0/15/91/115	-
36	CLA	a	820	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	U	307	-	1/1/12/20	2/21/97/115	-
35	A86	V	302	-	-	5/34/90/90	0/3/3/3
35	A86	A	302	-	-	9/34/90/90	0/3/3/3
36	CLA	M	310	35,13	1/1/11/20	6/17/93/115	-
35	A86	C	204	-	-	11/34/90/90	0/3/3/3
35	A86	L	301	-	-	5/34/90/90	1/3/3/3
36	CLA	a	841	41	1/1/12/20	6/24/100/115	-
36	CLA	B	305	-	1/1/15/20	21/39/115/115	-
36	CLA	E	313	-	2/2/15/20	10/39/115/115	-
36	CLA	a	801	-	1/1/15/20	10/39/115/115	-
37	KC1	W	213	-	-	5/15/71/71	-
34	DD6	A	304	-	-	4/26/80/80	0/3/3/3
36	CLA	M	316	36	1/1/10/20	6/12/88/115	-
36	CLA	X	313	-	-	6/12/88/115	-
44	BCR	b	843	-	-	9/29/63/63	0/2/2/2
36	CLA	M	311	35,13	1/1/15/20	9/39/115/115	-
35	A86	F	305	-	-	8/34/90/90	0/3/3/3
34	DD6	R	308	-	-	11/26/80/80	0/3/3/3
36	CLA	H	308	-	1/1/15/20	14/37/113/115	-
35	A86	I	301	-	-	11/34/90/90	0/3/3/3
36	CLA	b	841	41	1/1/15/20	7/39/115/115	-
36	CLA	Q	305	-	1/1/14/20	7/35/111/115	-
44	BCR	h	201	-	-	9/29/63/63	0/2/2/2
36	CLA	I	307	-	1/1/12/20	4/26/102/115	-
36	CLA	G	316	-	1/1/11/20	10/20/96/115	-
35	A86	H	304	-	-	8/34/90/90	0/3/3/3
36	CLA	J	310	-	1/1/15/20	10/39/115/115	-
36	CLA	H	316	-	1/1/15/20	18/39/115/115	-
36	CLA	V	314	-	1/1/15/20	18/39/115/115	-
36	CLA	D	308	-	1/1/15/20	14/39/115/115	-
36	CLA	L	312	12	-	7/17/93/115	-
36	CLA	K	313	-	1/1/15/20	11/39/115/115	-
36	CLA	a	806	-	2/2/15/20	11/39/115/115	-
36	CLA	L	314	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	I	311	9	1/1/15/20	14/39/115/115	-
41	LHG	F	319	-	-	32/45/45/53	-
36	CLA	M	307	-	1/1/15/20	12/39/115/115	-
36	CLA	N	312	-	1/1/11/20	9/18/94/115	-
34	DD6	a	849	-	-	6/26/80/80	0/3/3/3
36	CLA	J	313	-	1/1/15/20	14/39/115/115	-
41	LHG	F	318	-	-	15/34/34/53	-
36	CLA	Q	306	-	1/1/15/20	14/39/115/115	-
35	A86	C	203	-	-	7/34/90/90	1/3/3/3
43	PQN	a	840	-	-	7/23/43/43	0/2/2/2
36	CLA	P	312	15	1/1/11/20	9/17/93/115	-
37	KC1	F	308	6	-	7/15/71/71	-
36	CLA	a	808	20	1/1/15/20	11/39/115/115	-
36	CLA	K	307	-	2/2/14/20	21/35/111/115	-
37	KC1	Q	311	15	-	1/15/71/71	-
36	CLA	R	311	-	1/1/15/20	12/39/115/115	-
36	CLA	S	320	-	-	12/39/115/115	-
41	LHG	G	320	-	-	16/44/44/53	-
34	DD6	R	307	-	-	11/26/80/80	0/3/3/3
35	A86	W	203	36	-	6/34/90/90	0/3/3/3
35	A86	h	204	-	-	1/34/90/90	0/3/3/3
44	BCR	m	101	-	-	9/29/63/63	0/2/2/2
41	LHG	j	104	-	-	31/53/53/53	-
36	CLA	M	312	36	1/1/11/20	12/18/94/115	-
36	CLA	b	832	-	1/1/11/20	4/20/96/115	-
36	CLA	a	833	-	1/1/12/20	3/21/97/115	-
35	A86	S	302	-	-	6/34/90/90	0/3/3/3
41	LHG	G	301	-	-	24/53/53/53	-
36	CLA	O	314	-	1/1/10/20	4/10/86/115	-
37	KC1	F	315	-	-	3/15/71/71	-
34	DD6	W	204	36	-	7/26/80/80	0/3/3/3
36	CLA	W	218	-	1/1/10/20	6/13/89/115	-
39	LMT	a	851	-	-	15/21/61/61	0/2/2/2
36	CLA	a	814	-	1/1/12/20	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	BCR	a	845	-	-	7/29/63/63	0/2/2/2
36	CLA	H	315	-	1/1/15/20	15/39/115/115	-
36	CLA	a	821	-	1/1/11/20	4/20/96/115	-
35	A86	N	320	-	-	10/34/90/90	0/3/3/3
44	BCR	f	801	-	-	5/29/63/63	0/2/2/2
36	CLA	P	301	-	1/1/15/20	18/39/115/115	-
37	KC1	U	312	35	-	4/15/71/71	-
36	CLA	W	209	-	1/1/13/20	15/30/106/115	-
35	A86	N	304	-	-	8/34/90/90	0/3/3/3
41	LHG	E	322	-	-	28/53/53/53	-
36	CLA	Q	314	-	1/1/15/20	22/39/115/115	-
35	A86	Q	304	-	-	10/34/90/90	0/3/3/3
36	CLA	D	306	4	1/1/11/20	5/15/91/115	-
35	A86	K	306	-	-	9/34/90/90	0/3/3/3
35	A86	R	303	-	-	7/34/90/90	0/3/3/3
36	CLA	O	309	-	1/1/15/20	17/39/115/115	-
36	CLA	H	309	-	1/1/15/20	17/39/115/115	-
35	A86	M	304	-	-	14/34/90/90	0/3/3/3
36	CLA	b	826	46	1/1/14/20	11/38/114/115	-
36	CLA	a	816	-	1/1/15/20	20/39/115/115	-
39	LMT	a	853	-	-	10/18/58/61	0/2/2/2
36	CLA	I	305	-	2/2/14/20	11/35/111/115	-
36	CLA	B	307	-	1/1/11/20	7/17/93/115	-
36	CLA	i	102	-	1/1/15/20	17/39/115/115	-
36	CLA	J	307	10	1/1/14/20	11/35/111/115	-
42	LMG	E	319	-	-	22/35/55/70	0/1/1/1
36	CLA	W	206	-	1/1/14/20	8/35/111/115	-
36	CLA	O	311	-	1/1/13/20	9/31/107/115	-
39	LMT	P	321	-	-	10/14/34/61	0/1/1/2
36	CLA	A	313	-	1/1/10/20	4/10/86/115	-
36	CLA	H	314	-	1/1/10/20	2/10/86/115	-
36	CLA	b	821	46	1/1/15/20	11/39/115/115	-
36	CLA	a	819	-	1/1/11/20	5/15/91/115	-
36	CLA	R	310	-	1/1/14/20	15/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	N	318	-	1/1/11/20	7/18/94/115	-
36	CLA	f	804	46	2/2/15/20	10/39/115/115	-
36	CLA	U	308	35	1/1/13/20	11/29/105/115	-
36	CLA	b	822	-	1/1/11/20	4/17/93/115	-
34	DD6	B	302	-	-	4/26/80/80	0/3/3/3
37	KC1	K	314	-	-	5/15/71/71	-
42	LMG	V	315	-	-	24/41/61/70	0/1/1/1
36	CLA	Q	307	-	1/1/11/20	5/21/97/115	-
35	A86	R	309	-	-	8/34/90/90	0/3/3/3
35	A86	G	304	-	-	8/34/90/90	0/3/3/3
36	CLA	J	311	-	1/1/11/20	5/17/93/115	-
36	CLA	C	210	3	1/1/11/20	6/17/93/115	-
36	CLA	I	306	9	2/2/15/20	15/39/115/115	-
36	CLA	E	314	-	1/1/15/20	8/39/115/115	-
35	A86	P	303	-	-	9/34/90/90	0/3/3/3
36	CLA	b	819	-	1/1/13/20	7/32/108/115	-
36	CLA	a	836	-	1/1/15/20	11/39/115/115	-
34	DD6	E	306	-	-	4/26/80/80	0/3/3/3
35	A86	S	301	-	-	9/34/90/90	0/3/3/3
34	DD6	K	305	-	-	0/26/80/80	0/3/3/3
36	CLA	S	317	-	1/1/10/20	4/10/86/115	-
36	CLA	A	310	-	1/1/15/20	11/39/115/115	-
36	CLA	N	319	-	1/1/10/20	6/12/88/115	-
36	CLA	a	835	-	1/1/12/20	3/23/99/115	-
36	CLA	V	308	-	1/1/15/20	16/39/115/115	-
36	CLA	L	310	-	1/1/12/20	4/26/102/115	-
36	CLA	N	309	-	1/1/12/20	8/23/99/115	-
36	CLA	F	313	-	1/1/12/20	8/24/100/115	-
37	KC1	Q	313	-	-	1/15/71/71	-
34	DD6	j	103	-	-	8/26/80/80	0/3/3/3
42	LMG	J	319	-	-	22/39/59/70	0/1/1/1
35	A86	I	302	-	-	7/34/90/90	0/3/3/3
36	CLA	J	309	-	1/1/15/20	8/39/115/115	-
36	CLA	B	311	-	1/1/13/20	12/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	a	832	-	1/1/15/20	15/39/115/115	-
36	CLA	I	308	-	1/1/15/20	17/39/115/115	-
41	LHG	D	318	36	-	29/50/50/53	-
36	CLA	D	317	-	1/1/13/20	11/31/107/115	-
39	LMT	G	322	-	-	17/21/61/61	0/2/2/2
34	DD6	D	303	-	-	9/26/80/80	0/3/3/3
37	KC1	M	313	13,36	-	5/15/71/71	-
36	CLA	I	309	9	1/1/11/20	8/17/93/115	-
35	A86	S	304	-	-	8/34/90/90	0/3/3/3
36	CLA	L	320	-	1/1/15/20	10/39/115/115	-
45	SF4	b	803	20,21	-	-	0/6/5/5
36	CLA	H	318	-	1/1/12/20	7/21/97/115	-
36	CLA	G	315	-	2/2/13/20	12/29/105/115	-
41	LHG	f	809	-	-	28/46/46/53	-
34	DD6	O	304	-	-	5/26/80/80	0/3/3/3
36	CLA	a	803	36	1/1/13/20	5/27/103/115	-
35	A86	U	304	37	-	10/34/90/90	0/3/3/3
36	CLA	C	208	-	1/1/15/20	19/39/115/115	-
36	CLA	D	312	-	1/1/15/20	13/39/115/115	-
36	CLA	T	313	18	1/1/15/20	8/39/115/115	-
34	DD6	A	303	-	-	5/26/80/80	0/3/3/3
36	CLA	C	214	-	1/1/10/20	4/10/86/115	-
35	A86	F	304	36	-	4/34/90/90	0/3/3/3
39	LMT	U	315	-	-	17/21/61/61	0/2/2/2
36	CLA	D	315	-	1/1/10/20	2/10/86/115	-
36	CLA	U	311	32	1/1/15/20	20/39/115/115	-
34	DD6	L	305	-	-	6/26/80/80	0/3/3/3
36	CLA	R	315	-	1/1/15/20	14/39/115/115	-
36	CLA	a	817	-	1/1/15/20	16/39/115/115	-
35	A86	M	305	-	-	8/34/90/90	0/3/3/3
36	CLA	N	308	-	1/1/15/20	15/39/115/115	-
42	LMG	a	852	-	-	26/49/69/70	0/1/1/1
35	A86	V	301	35	-	10/34/90/90	1/3/3/3
36	CLA	W	214	-	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	F	314	35,6	1/1/15/20	16/39/115/115	-
36	CLA	H	312	-	1/1/15/20	17/39/115/115	-
35	A86	X	314	-	-	3/34/90/90	1/3/3/3
34	DD6	D	304	-	-	8/26/80/80	0/3/3/3
34	DD6	W	205	-	-	8/26/80/80	0/3/3/3
44	BCR	i	103	-	-	11/29/63/63	0/2/2/2
36	CLA	W	210	-	1/1/11/20	8/17/93/115	-
36	CLA	a	811	-	1/1/12/20	5/26/102/115	-
36	CLA	Q	309	15	1/1/11/20	9/17/93/115	-
34	DD6	D	301	-	-	11/26/80/80	0/3/3/3
41	LHG	a	850	-	-	36/51/51/53	-
42	LMG	h	206	-	-	24/40/60/70	0/1/1/1
36	CLA	f	802	-	1/1/15/20	12/39/115/115	-
35	A86	L	307	-	-	8/34/90/90	1/3/3/3
36	CLA	D	311	-	-	7/17/93/115	-
36	CLA	N	313	-	1/1/10/20	0/10/86/115	-
36	CLA	b	808	-	1/1/15/20	13/39/115/115	-
36	CLA	V	307	-	1/1/12/20	6/23/99/115	-
34	DD6	M	303	-	-	3/26/80/80	0/3/3/3
44	BCR	b	844	-	-	6/29/63/63	0/2/2/2
36	CLA	C	205	-	1/1/10/20	4/13/89/115	-
36	CLA	a	829	-	1/1/15/20	12/39/115/115	-
36	CLA	G	312	7	1/1/13/20	6/31/107/115	-
36	CLA	U	309	-	-	6/17/93/115	-
44	BCR	b	846	-	-	8/29/63/63	0/2/2/2
35	A86	K	302	-	-	8/34/90/90	0/3/3/3
36	CLA	F	309	-	1/1/15/20	13/39/115/115	-
39	LMT	U	314	-	-	14/21/61/61	0/2/2/2
39	LMT	E	323	-	-	11/21/61/61	0/2/2/2
39	LMT	G	323	-	-	17/21/61/61	0/2/2/2
36	CLA	b	817	-	2/2/13/20	9/32/108/115	-
34	DD6	S	306	-	-	5/26/80/80	0/3/3/3
34	DD6	K	304	-	-	2/26/80/80	0/3/3/3
36	CLA	O	308	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	KC1	T	315	-	-	7/15/71/71	-
39	LMT	F	320	-	-	12/21/61/61	0/2/2/2
35	A86	L	306	37	-	10/34/90/90	0/3/3/3
42	LMG	L	321	40	-	15/28/48/70	0/1/1/1
36	CLA	B	306	-	1/1/11/20	6/17/93/115	-
35	A86	V	304	-	-	8/34/90/90	0/3/3/3
36	CLA	K	309	-	1/1/13/20	13/32/108/115	-
36	CLA	V	306	33	1/1/15/20	17/39/115/115	-
38	SQD	A	315	-	-	13/22/42/69	0/1/1/1
35	A86	J	302	-	-	5/34/90/90	1/3/3/3
38	SQD	b	804	-	-	23/41/61/69	0/1/1/1
35	A86	E	302	-	-	4/34/90/90	0/3/3/3
35	A86	T	301	36	-	4/34/90/90	1/3/3/3
36	CLA	S	321	-	-	10/24/100/115	-
36	CLA	b	811	-	1/1/15/20	12/39/115/115	-
35	A86	W	202	36	-	9/34/90/90	0/3/3/3
41	LHG	b	850	36	-	26/53/53/53	-
36	CLA	h	203	-	1/1/15/20	17/39/115/115	-
36	CLA	J	308	-	-	12/35/111/115	-
35	A86	K	301	-	-	6/34/90/90	1/3/3/3
35	A86	T	306	-	-	7/34/90/90	0/3/3/3
36	CLA	G	309	-	1/1/15/20	13/39/115/115	-
36	CLA	l	204	28	-	10/20/96/115	-
37	KC1	A	312	-	-	2/15/71/71	-
36	CLA	G	311	-	1/1/15/20	16/39/115/115	-
36	CLA	H	306	-	1/1/14/20	6/35/111/115	-
35	A86	A	316	-	-	9/34/90/90	0/3/3/3
37	KC1	X	311	-	-	2/15/71/71	-
36	CLA	a	810	36	1/1/14/20	16/36/112/115	-
37	KC1	G	318	-	-	7/15/71/71	-
36	CLA	b	815	-	1/1/15/20	15/39/115/115	-
36	CLA	E	315	-	2/2/15/20	16/39/115/115	-
36	CLA	T	311	18	1/1/15/20	13/39/115/115	-
36	CLA	I	314	-	1/1/10/20	2/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LHG	O	318	-	-	30/53/53/53	-
37	KC1	G	317	-	-	6/15/71/71	-
36	CLA	a	827	-	1/1/14/20	13/36/112/115	-
35	A86	O	303	-	-	6/34/90/90	0/3/3/3
36	CLA	I	312	9	1/1/12/20	4/24/100/115	-
42	LMG	D	320	41	-	24/41/61/70	0/1/1/1
36	CLA	R	313	-	1/1/15/20	14/39/115/115	-
42	LMG	G	325	-	-	27/50/70/70	0/1/1/1
42	LMG	V	316	-	-	25/41/61/70	0/1/1/1
36	CLA	B	308	-	1/1/15/20	14/39/115/115	-
36	CLA	U	306	32	1/1/15/20	19/39/115/115	-
36	CLA	a	828	-	1/1/15/20	14/39/115/115	-
42	LMG	D	321	-	-	21/32/52/70	0/1/1/1
35	A86	V	303	35	-	8/34/90/90	0/3/3/3
35	A86	O	301	-	-	4/34/90/90	0/3/3/3
37	KC1	R	317	-	-	3/15/71/71	-
35	A86	O	305	-	-	13/34/90/90	0/3/3/3
36	CLA	a	826	-	1/1/15/20	10/39/115/115	-
36	CLA	W	201	-	1/1/11/20	4/19/95/115	-
36	CLA	C	209	-	1/1/15/20	11/39/115/115	-
35	A86	M	302	-	-	7/34/90/90	0/3/3/3
35	A86	X	305	-	-	8/34/90/90	0/3/3/3
36	CLA	O	312	-	-	4/10/82/115	-
41	LHG	R	323	-	-	27/53/53/53	-
36	CLA	T	309	18	1/1/15/20	19/39/115/115	-
36	CLA	J	316	-	1/1/11/20	8/17/93/115	-
36	CLA	b	816	-	2/2/14/20	15/33/109/115	-
36	CLA	E	316	-	1/1/15/20	15/39/115/115	-
39	LMT	I	317	-	-	13/21/61/61	0/2/2/2
36	CLA	D	310	-	1/1/15/20	7/39/115/115	-
36	CLA	S	315	17	1/1/10/20	5/13/89/115	-
35	A86	G	305	-	-	4/34/90/90	0/3/3/3
34	DD6	P	305	-	-	3/26/80/80	0/3/3/3
36	CLA	f	805	25	1/1/12/20	9/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	KC1	H	313	-	-	6/15/71/71	-
36	CLA	V	305	35	1/1/14/20	11/35/111/115	-
34	DD6	E	301	-	-	3/26/80/80	0/3/3/3
36	CLA	R	318	35	1/1/10/20	4/10/86/115	-
37	KC1	S	316	-	-	6/15/71/71	-
36	CLA	H	310	8	1/1/11/20	7/17/93/115	-
36	CLA	J	315	-	1/1/10/20	2/10/86/115	-
36	CLA	D	313	-	1/1/15/20	8/39/115/115	-
36	CLA	W	212	19	-	12/39/115/115	-
41	LHG	i	104	-	-	29/50/50/53	-
36	CLA	a	834	20	1/1/11/20	5/15/91/115	-
36	CLA	b	814	-	1/1/13/20	5/27/103/115	-
36	CLA	A	309	1	1/1/11/20	7/17/93/115	-
36	CLA	b	837	-	1/1/15/20	7/39/115/115	-
36	CLA	C	212	35	1/1/15/20	22/39/115/115	-
37	KC1	D	314	4	-	4/15/71/71	-
36	CLA	P	313	-	1/1/15/20	10/39/115/115	-
45	SF4	c	102	-	-	-	0/6/5/5
35	A86	P	307	-	-	2/34/90/90	0/3/3/3
35	A86	X	304	-	-	7/34/90/90	0/3/3/3
36	CLA	F	312	-	1/1/15/20	21/39/115/115	-
35	A86	B	303	-	-	13/34/90/90	0/3/3/3
42	LMG	J	318	-	-	28/50/70/70	0/1/1/1
36	CLA	E	311	-	1/1/15/20	16/39/115/115	-
36	CLA	b	809	-	1/1/15/20	16/39/115/115	-
35	A86	R	301	-	-	9/34/90/90	0/3/3/3
36	CLA	G	307	-	-	4/11/87/115	-
44	BCR	f	806	-	-	9/29/63/63	0/2/2/2
36	CLA	H	317	8	1/1/15/20	10/39/115/115	-
36	CLA	b	824	-	1/1/12/20	12/25/101/115	-
37	KC1	B	310	-	-	3/15/71/71	-
40	DGD	L	302	42	-	21/36/76/95	0/2/2/2
35	A86	T	302	-	-	7/34/90/90	0/3/3/3
44	BCR	l	203	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	I	310	35	1/1/15/20	11/39/115/115	-
36	CLA	I	313	-	1/1/10/20	4/10/86/115	-
35	A86	B	301	-	-	10/34/90/90	0/3/3/3
36	CLA	W	207	34	1/1/15/20	15/39/115/115	-
36	CLA	a	831	-	1/1/15/20	16/39/115/115	-
35	A86	R	306	-	-	8/34/90/90	0/3/3/3
35	A86	J	301	-	-	10/34/90/90	0/3/3/3
36	CLA	Q	308	-	1/1/15/20	17/39/115/115	-
39	LMT	K	318	-	-	12/21/61/61	0/2/2/2
35	A86	Q	303	-	-	8/34/90/90	0/3/3/3
36	CLA	V	310	33	1/1/15/20	6/39/115/115	-
36	CLA	b	829	-	1/1/15/20	11/39/115/115	-
36	CLA	a	805	20	1/1/15/20	17/39/115/115	-
36	CLA	a	815	46	1/1/11/20	2/15/91/115	-
36	CLA	l	205	-	2/2/15/20	12/39/115/115	-
36	CLA	S	314	-	-	11/39/115/115	-
43	PQN	b	842	-	-	11/23/43/43	0/2/2/2
34	DD6	H	303	-	-	6/26/80/80	0/3/3/3
36	CLA	G	314	7	1/1/10/20	4/10/86/115	-
36	CLA	J	312	10	1/1/15/20	9/39/115/115	-
36	CLA	N	315	-	-	0/10/86/115	-
36	CLA	E	312	-	1/1/15/20	14/39/115/115	-
36	CLA	a	825	-	2/2/15/20	15/39/115/115	-
36	CLA	M	308	-	1/1/12/20	6/24/100/115	-
36	CLA	B	309	2	1/1/12/20	7/24/100/115	-
34	DD6	S	307	-	-	6/26/80/80	0/3/3/3
36	CLA	j	106	27	1/1/10/20	6/12/88/115	-
36	CLA	V	309	33	1/1/10/20	4/13/89/115	-
36	CLA	L	316	-	1/1/10/20	3/10/86/115	-
35	A86	Q	301	-	-	6/34/90/90	0/3/3/3
36	CLA	K	311	-	1/1/11/20	8/17/93/115	-
42	LMG	m	102	-	-	14/32/52/70	0/1/1/1
35	A86	S	308	37	-	12/34/90/90	0/3/3/3
36	CLA	V	311	33	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	b	805	36	1/1/15/20	15/39/115/115	-
36	CLA	b	823	-	1/1/13/20	5/27/103/115	-
36	CLA	a	822	-	1/1/12/20	4/23/99/115	-
36	CLA	S	319	-	1/1/15/20	7/39/115/115	-
35	A86	F	302	-	-	8/34/90/90	0/3/3/3
35	A86	N	302	-	-	6/34/90/90	0/3/3/3
36	CLA	M	315	-	-	6/18/94/115	-
35	A86	U	303	36	-	16/34/90/90	0/3/3/3
36	CLA	L	311	-	1/1/15/20	13/39/115/115	-
36	CLA	a	837	-	1/1/15/20	8/39/115/115	-
36	CLA	S	309	-	1/1/14/20	8/35/111/115	-
39	LMT	E	320	-	-	13/21/61/61	0/2/2/2
36	CLA	S	311	35	1/1/11/20	4/17/93/115	-
35	A86	O	319	35,36	-	8/34/90/90	0/3/3/3
39	LMT	b	848	-	-	12/21/61/61	0/2/2/2
40	DGD	C	215	-	-	31/46/86/95	0/2/2/2
36	CLA	W	211	-	1/1/15/20	10/39/115/115	-
36	CLA	D	309	-	2/2/13/20	7/27/103/115	-
35	A86	O	302	-	-	9/34/90/90	0/3/3/3
36	CLA	F	310	-	1/1/13/20	9/29/105/115	-
36	CLA	T	308	-	1/1/14/20	8/35/111/115	-
35	A86	F	307	-	-	7/34/90/90	0/3/3/3
41	LHG	f	808	-	-	28/53/53/53	-
36	CLA	N	317	14	1/1/12/20	10/26/102/115	-
36	CLA	X	312	-	1/1/10/20	2/10/86/115	-
36	CLA	P	316	-	1/1/10/20	4/10/86/115	-
36	CLA	a	830	-	-	11/21/97/115	-
36	CLA	a	848	36	2/2/15/20	12/39/115/115	-
37	KC1	V	312	33	-	6/15/71/71	-
36	CLA	A	307	-	1/1/14/20	8/33/109/115	-
36	CLA	H	307	-	1/1/14/20	5/33/109/115	-
36	CLA	T	316	-	1/1/10/20	2/10/86/115	-
36	CLA	P	311	-	1/1/15/20	17/39/115/115	-
37	KC1	T	310	-	-	8/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	b	833	-	1/1/13/20	11/31/107/115	-
36	CLA	R	322	-	1/1/12/20	9/24/100/115	-
36	CLA	Q	312	-	1/1/10/20	4/10/86/115	-
45	SF4	c	101	22	-	-	0/6/5/5
36	CLA	b	838	-	1/1/11/20	2/18/94/115	-
36	CLA	l	202	-	1/1/15/20	13/39/115/115	-
44	BCR	i	101	-	-	1/29/63/63	0/2/2/2
36	CLA	G	319	7	1/1/12/20	8/21/97/115	-
35	A86	K	303	-	-	5/34/90/90	0/3/3/3
35	A86	F	301	-	-	5/34/90/90	0/3/3/3
37	KC1	P	315	35	-	1/15/71/71	-
35	A86	N	303	-	-	5/34/90/90	0/3/3/3
35	A86	U	301	-	-	8/34/90/90	0/3/3/3
34	DD6	Q	302	-	-	8/26/80/80	0/3/3/3
39	LMT	F	321	-	-	10/19/59/61	0/2/2/2
39	LMT	B	312	-	-	14/21/61/61	0/2/2/2
36	CLA	N	310	-	1/1/10/20	1/10/86/115	-
34	DD6	J	304	-	-	4/26/80/80	0/3/3/3
36	CLA	a	804	-	1/1/15/20	16/39/115/115	-
39	LMT	f	807	-	-	6/15/35/61	0/1/1/2
36	CLA	D	316	-	1/1/12/20	10/24/100/115	-
36	CLA	b	831	-	1/1/12/20	7/21/97/115	-
36	CLA	X	307	35	-	5/21/97/115	-
36	CLA	P	318	-	1/1/12/20	8/23/99/115	-
35	A86	J	303	-	-	7/34/90/90	0/3/3/3
37	KC1	O	313	-	-	1/15/71/71	-
36	CLA	X	306	-	1/1/14/20	9/35/111/115	-
44	BCR	a	846	-	-	7/29/63/63	0/2/2/2
36	CLA	F	316	6	1/1/10/20	2/10/86/115	-
36	CLA	b	830	-	1/1/15/20	7/39/115/115	-
36	CLA	R	319	-	1/1/11/20	6/15/91/115	-
36	CLA	P	309	41	1/1/15/20	14/39/115/115	-
36	CLA	P	310	41	1/1/15/20	11/39/115/115	-
39	LMT	E	321	-	-	9/15/35/61	0/1/1/2
36	CLA	E	317	-	1/1/11/20	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	BCR	a	844	-	-	6/29/63/63	0/2/2/2
36	CLA	O	310	15	1/1/11/20	9/17/93/115	-
36	CLA	a	809	-	1/1/13/20	8/29/105/115	-
42	LMG	I	315	-	-	32/50/70/70	0/1/1/1
35	A86	S	303	-	-	5/34/90/90	0/3/3/3
35	A86	T	304	-	-	0/34/90/90	0/3/3/3
36	CLA	A	311	-	1/1/15/20	20/39/115/115	-
36	CLA	O	316	-	1/1/15/20	29/39/115/115	-
36	CLA	K	310	-	2/2/14/20	15/36/112/115	-
35	A86	T	303	-	-	6/34/90/90	0/3/3/3
36	CLA	W	208	-	1/1/11/20	6/15/91/115	-
36	CLA	b	801	46	1/1/15/20	8/39/115/115	-
39	LMT	K	317	-	-	14/17/57/61	0/2/2/2
35	A86	G	302	-	-	7/34/90/90	0/3/3/3
39	LMT	I	318	-	-	17/21/61/61	0/2/2/2
36	CLA	K	316	-	1/1/15/20	11/39/115/115	-
36	CLA	T	314	-	1/1/15/20	13/39/115/115	-
36	CLA	b	840	-	1/1/15/20	12/39/115/115	-
36	CLA	E	308	5	1/1/11/20	8/20/96/115	-
36	CLA	P	319	-	1/1/14/20	15/33/109/115	-
36	CLA	U	305	-	1/1/14/20	11/35/111/115	-
35	A86	L	304	-	-	7/34/90/90	0/3/3/3
36	CLA	G	310	-	1/1/15/20	5/39/115/115	-
37	KC1	G	308	-	-	6/15/71/71	-
36	CLA	N	307	-	1/1/14/20	9/35/111/115	-
35	A86	D	302	-	-	7/34/90/90	0/3/3/3
35	A86	R	302	-	-	6/34/90/90	0/3/3/3
36	CLA	a	818	-	1/1/15/20	11/39/115/115	-
36	CLA	V	313	-	1/1/15/20	14/39/115/115	-
36	CLA	b	836	-	1/1/13/20	8/31/107/115	-
35	A86	E	305	-	-	5/34/90/90	0/3/3/3
35	A86	X	303	36	-	9/34/90/90	0/3/3/3
36	CLA	X	315	-	-	2/10/86/115	-
37	KC1	W	217	-	-	4/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	N	301	-	-	9/34/90/90	0/3/3/3
36	CLA	H	305	-	1/1/11/20	5/19/95/115	-
35	A86	N	305	-	-	2/34/90/90	0/3/3/3
34	DD6	F	303	-	-	8/26/80/80	0/3/3/3
36	CLA	S	313	-	1/1/11/20	8/17/93/115	-
36	CLA	A	308	-	1/1/15/20	12/39/115/115	-
36	CLA	P	302	-	-	4/12/88/115	-
36	CLA	K	308	-	1/1/15/20	9/39/115/115	-
36	CLA	a	807	20	1/1/15/20	14/39/115/115	-
36	CLA	M	306	37,13	1/1/13/20	8/27/103/115	-
36	CLA	O	307	-	1/1/15/20	14/39/115/115	-
36	CLA	R	316	-	1/1/11/20	8/17/93/115	-
44	BCR	b	847	-	-	8/29/63/63	0/2/2/2
36	CLA	T	312	18	1/1/11/20	6/17/93/115	-
39	LMT	a	854	-	-	16/21/61/61	0/2/2/2
36	CLA	F	317	6	2/2/13/20	10/29/105/115	-
36	CLA	L	309	-	1/1/15/20	11/39/115/115	-
36	CLA	K	315	-	1/1/10/20	2/10/86/115	-
41	LHG	O	317	-	-	32/46/46/53	-
36	CLA	b	810	-	1/1/15/20	9/39/115/115	-
36	CLA	X	308	19	1/1/11/20	11/18/94/115	-
35	A86	J	306	-	-	7/34/90/90	0/3/3/3
40	DGD	b	849	-	-	21/49/89/95	0/2/2/2
36	CLA	j	101	-	1/1/15/20	17/39/115/115	-
41	LHG	a	843	36	-	9/31/31/53	-
35	A86	T	307	-	-	9/34/90/90	0/3/3/3
36	CLA	R	320	16	1/1/11/20	4/15/91/115	-
36	CLA	C	206	-	1/1/14/20	17/35/111/115	-
36	CLA	f	803	-	2/2/15/20	11/39/115/115	-
35	A86	N	306	-	-	8/34/90/90	0/3/3/3
35	A86	U	302	-	-	9/34/90/90	0/3/3/3
36	CLA	S	310	-	1/1/15/20	17/39/115/115	-
34	DD6	E	303	-	-	7/26/80/80	0/3/3/3
34	DD6	G	303	-	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LMT	B	313	-	-	16/21/61/61	0/2/2/2
34	DD6	H	302	-	-	1/26/80/80	0/3/3/3
44	BCR	b	845	-	-	6/29/63/63	0/2/2/2
36	CLA	C	207	-	1/1/15/20	16/39/115/115	-
36	CLA	R	321	-	-	10/39/115/115	-
35	A86	L	319	-	-	9/34/90/90	0/3/3/3
35	A86	X	301	-	-	9/34/90/90	0/3/3/3
39	LMT	P	320	-	-	8/14/34/61	0/1/1/2
36	CLA	a	824	-	1/1/15/20	11/39/115/115	-
35	A86	S	305	-	-	9/34/90/90	0/3/3/3
36	CLA	P	308	-	1/1/14/20	7/35/111/115	-
36	CLA	U	310	-	1/1/15/20	19/39/115/115	-
36	CLA	b	807	-	1/1/11/20	3/15/91/115	-
36	CLA	Q	310	-	-	20/39/115/115	-
37	KC1	M	318	-	-	9/15/71/71	-
36	CLA	l	201	-	1/1/15/20	14/39/115/115	-
36	CLA	l	206	46	1/1/12/20	6/21/97/115	-
36	CLA	b	835	-	1/1/11/20	5/15/91/115	-
36	CLA	a	802	-	2/2/15/20	11/39/115/115	-
35	A86	J	305	-	-	6/34/90/90	0/3/3/3
35	A86	P	304	-	-	6/34/90/90	0/3/3/3
42	LMG	G	324	-	-	31/50/70/70	0/1/1/1
34	DD6	A	301	-	-	6/26/80/80	0/3/3/3
36	CLA	b	820	21	1/1/14/20	17/33/109/115	-
36	CLA	X	310	-	1/1/10/20	4/10/86/115	-
36	CLA	M	314	-	1/1/10/20	4/10/86/115	-
37	KC1	N	314	-	-	7/15/71/71	-
36	CLA	F	311	-	1/1/12/20	9/24/100/115	-
34	DD6	C	201	-	-	7/26/80/80	0/3/3/3
36	CLA	H	311	-	1/1/15/20	9/39/115/115	-
36	CLA	R	314	16	1/1/11/20	9/17/93/115	-
36	CLA	K	312	-	1/1/15/20	6/39/115/115	-
34	DD6	E	304	-	-	4/26/80/80	0/3/3/3
34	DD6	I	303	-	-	3/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	h	202	-	-	3/34/90/90	1/3/3/3
36	CLA	S	318	-	1/1/10/20	7/12/88/115	-
37	KC1	O	315	15	-	1/15/71/71	-
41	LHG	G	321	36	-	28/51/51/53	-
36	CLA	b	802	-	1/1/15/20	9/39/115/115	-
35	A86	G	306	-	-	6/34/90/90	1/3/3/3
36	CLA	X	309	-	-	7/15/91/115	-
36	CLA	A	306	-	2/2/14/20	17/35/111/115	-
36	CLA	b	834	-	1/1/15/20	8/39/115/115	-
35	A86	I	304	-	-	9/34/90/90	0/3/3/3
42	LMG	j	105	-	-	31/47/67/70	0/1/1/1
34	DD6	D	305	-	-	2/26/80/80	0/3/3/3
42	LMG	E	318	-	-	25/41/61/70	0/1/1/1
36	CLA	U	313	-	1/1/10/20	4/10/86/115	-
36	CLA	J	317	-	1/1/11/20	5/18/94/115	-
41	LHG	l	208	-	-	34/52/52/53	-
36	CLA	b	825	-	1/1/15/20	12/39/115/115	-
36	CLA	b	839	-	1/1/15/20	4/39/115/115	-
36	CLA	G	313	7	1/1/15/20	14/39/115/115	-
35	A86	H	301	-	-	5/34/90/90	0/3/3/3
37	KC1	L	315	35	-	6/15/71/71	-
35	A86	R	304	36	-	8/34/90/90	0/3/3/3
39	LMT	L	318	-	-	12/17/57/61	0/2/2/2
37	KC1	C	213	-	-	5/15/71/71	-
36	CLA	S	312	-	-	15/39/115/115	-
36	CLA	b	812	21	1/1/15/20	6/39/115/115	-
35	A86	E	307	36	-	3/34/90/90	0/3/3/3
39	LMT	b	851	-	-	7/15/35/61	0/1/1/2
34	DD6	B	304	-	-	3/26/80/80	0/3/3/3
36	CLA	j	102	-	1/1/15/20	14/39/115/115	-

The worst 5 of 4548 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Q	310	CLA	CAA-C2A	16.11	1.83	1.54
37	M	318	KC1	C4C-NC	15.94	1.63	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	M	318	KC1	C1A-NA	14.76	1.68	1.38
37	T	310	KC1	C1A-NA	13.47	1.66	1.38
35	N	304	A86	C19-C18	-13.40	1.33	1.52

The worst 5 of 7109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	N	304	A86	O1-C20-C21	-50.47	58.64	115.05
36	Q	314	CLA	C4-C3-C5	-23.62	74.22	115.23
37	M	318	KC1	C1D-ND-C4D	-23.03	90.15	106.31
42	V	315	LMG	O7-C10-C11	22.21	159.53	111.48
35	A	302	A86	C33-C32-C31	-21.39	88.43	109.21

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 5875 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	301	DD6	C10-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
34	A	303	DD6	C12-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

498 monomers are involved in 2733 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	b	806	CLA	2	0
36	a	812	CLA	1	0
36	a	823	CLA	1	0
36	A	314	CLA	20	0
36	b	813	CLA	1	0
36	O	306	CLA	1	0
36	C	211	CLA	1	0
36	W	215	CLA	3	0
36	A	305	CLA	4	0
37	E	309	KC1	2	0
39	L	303	LMT	1	0
37	L	317	KC1	2	0
44	a	847	BCR	1	0
36	W	216	CLA	1	0
41	D	319	LHG	12	0
36	D	307	CLA	12	0
41	I	316	LHG	10	0
35	P	306	A86	4	0
36	M	309	CLA	8	0
36	a	838	CLA	1	0
36	P	314	CLA	5	0
35	X	302	A86	1	0
36	b	828	CLA	4	0
36	a	839	CLA	1	0
41	Q	315	LHG	19	0
35	R	305	A86	7	0
44	l	207	BCR	4	0
36	L	308	CLA	36	0
39	h	205	LMT	21	0
44	j	107	BCR	1	0
36	E	310	CLA	1	0
36	N	316	CLA	6	0
35	Q	316	A86	27	0
36	b	818	CLA	3	0
36	a	813	CLA	12	0
36	U	307	CLA	11	0
35	A	302	A86	1	0
36	M	310	CLA	1	0
35	C	204	A86	4	0
35	L	301	A86	5	0
36	a	841	CLA	3	0
36	B	305	CLA	3	0
36	E	313	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	a	801	CLA	6	0
34	A	304	DD6	2	0
36	M	316	CLA	3	0
44	b	843	BCR	6	0
36	M	311	CLA	3	0
34	R	308	DD6	5	0
36	H	308	CLA	19	0
35	I	301	A86	4	0
36	b	841	CLA	7	0
36	Q	305	CLA	4	0
44	h	201	BCR	4	0
36	I	307	CLA	6	0
36	G	316	CLA	3	0
35	H	304	A86	7	0
36	J	310	CLA	4	0
36	H	316	CLA	2	0
36	D	308	CLA	6	0
36	V	314	CLA	31	0
36	L	312	CLA	1	0
36	K	313	CLA	6	0
36	a	806	CLA	19	0
36	L	314	CLA	2	0
36	I	311	CLA	1	0
41	F	319	LHG	4	0
36	M	307	CLA	18	0
36	N	312	CLA	6	0
34	a	849	DD6	1	0
36	J	313	CLA	5	0
41	F	318	LHG	1	0
36	Q	306	CLA	3	0
35	C	203	A86	12	0
43	a	840	PQN	3	0
37	F	308	KC1	15	0
36	a	808	CLA	7	0
36	K	307	CLA	15	0
37	Q	311	KC1	8	0
36	R	311	CLA	1	0
36	S	320	CLA	2	0
41	G	320	LHG	14	0
34	R	307	DD6	11	0
35	W	203	A86	1	0
35	h	204	A86	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	m	101	BCR	11	0
41	j	104	LHG	14	0
36	M	312	CLA	3	0
36	a	833	CLA	2	0
35	S	302	A86	1	0
41	G	301	LHG	3	0
37	F	315	KC1	5	0
34	W	204	DD6	22	0
36	W	218	CLA	4	0
39	a	851	LMT	8	0
44	a	845	BCR	3	0
36	H	315	CLA	3	0
36	a	821	CLA	2	0
44	f	801	BCR	2	0
36	P	301	CLA	9	0
36	W	209	CLA	7	0
35	N	304	A86	14	0
41	E	322	LHG	24	0
36	Q	314	CLA	50	0
35	Q	304	A86	1	0
36	D	306	CLA	5	0
35	R	303	A86	1	0
36	O	309	CLA	8	0
35	M	304	A86	12	0
36	b	826	CLA	1	0
36	a	816	CLA	30	0
39	a	853	LMT	12	0
36	I	305	CLA	5	0
36	B	307	CLA	1	0
36	i	102	CLA	3	0
36	J	307	CLA	1	0
42	E	319	LMG	6	0
36	W	206	CLA	1	0
36	O	311	CLA	3	0
39	P	321	LMT	2	0
36	A	313	CLA	3	0
36	H	314	CLA	6	0
36	b	821	CLA	1	0
36	a	819	CLA	10	0
36	R	310	CLA	9	0
36	N	318	CLA	15	0
36	f	804	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	U	308	CLA	19	0
36	b	822	CLA	2	0
34	B	302	DD6	5	0
37	K	314	KC1	9	0
42	V	315	LMG	14	0
36	Q	307	CLA	5	0
36	J	311	CLA	3	0
36	C	210	CLA	6	0
36	I	306	CLA	14	0
36	E	314	CLA	4	0
36	b	819	CLA	3	0
36	a	836	CLA	6	0
34	E	306	DD6	4	0
34	K	305	DD6	4	0
36	A	310	CLA	1	0
36	N	319	CLA	14	0
36	a	835	CLA	1	0
36	V	308	CLA	12	0
36	L	310	CLA	1	0
36	N	309	CLA	6	0
36	F	313	CLA	6	0
37	Q	313	KC1	8	0
34	j	103	DD6	4	0
42	J	319	LMG	12	0
35	I	302	A86	17	0
36	J	309	CLA	2	0
36	B	311	CLA	7	0
36	a	832	CLA	3	0
36	I	308	CLA	29	0
41	D	318	LHG	16	0
36	D	317	CLA	1	0
39	G	322	LMT	10	0
34	D	303	DD6	5	0
37	M	313	KC1	1	0
36	I	309	CLA	17	0
35	S	304	A86	21	0
36	L	320	CLA	2	0
45	b	803	SF4	2	0
36	H	318	CLA	4	0
36	G	315	CLA	24	0
41	f	809	LHG	20	0
34	O	304	DD6	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	a	803	CLA	5	0
35	U	304	A86	15	0
36	C	208	CLA	5	0
36	D	312	CLA	2	0
36	T	313	CLA	13	0
34	A	303	DD6	4	0
39	U	315	LMT	17	0
36	D	315	CLA	1	0
36	U	311	CLA	16	0
34	L	305	DD6	25	0
36	a	817	CLA	3	0
36	N	308	CLA	4	0
42	a	852	LMG	20	0
35	V	301	A86	27	0
36	F	314	CLA	6	0
36	H	312	CLA	2	0
35	X	314	A86	24	0
34	D	304	DD6	2	0
34	W	205	DD6	23	0
44	i	103	BCR	5	0
36	a	811	CLA	3	0
34	D	301	DD6	12	0
41	a	850	LHG	15	0
42	h	206	LMG	7	0
36	f	802	CLA	4	0
35	L	307	A86	8	0
36	D	311	CLA	5	0
36	N	313	CLA	5	0
36	b	808	CLA	1	0
36	V	307	CLA	1	0
34	M	303	DD6	18	0
44	b	844	BCR	2	0
36	C	205	CLA	14	0
36	a	829	CLA	1	0
36	U	309	CLA	4	0
44	b	846	BCR	4	0
36	F	309	CLA	5	0
39	U	314	LMT	15	0
39	E	323	LMT	5	0
39	G	323	LMT	4	0
36	b	817	CLA	6	0
34	S	306	DD6	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	K	304	DD6	4	0
36	O	308	CLA	6	0
37	T	315	KC1	1	0
39	F	320	LMT	19	0
42	L	321	LMG	10	0
35	V	304	A86	6	0
36	K	309	CLA	6	0
36	V	306	CLA	22	0
38	A	315	SQD	7	0
35	J	302	A86	3	0
38	b	804	SQD	10	0
35	T	301	A86	2	0
36	S	321	CLA	7	0
36	b	811	CLA	1	0
41	b	850	LHG	18	0
36	J	308	CLA	8	0
36	h	203	CLA	11	0
35	T	306	A86	1	0
35	K	301	A86	4	0
36	G	309	CLA	4	0
36	l	204	CLA	6	0
37	A	312	KC1	4	0
36	G	311	CLA	11	0
35	A	316	A86	2	0
36	a	810	CLA	4	0
36	b	815	CLA	2	0
36	E	315	CLA	29	0
36	T	311	CLA	4	0
36	I	314	CLA	2	0
41	O	318	LHG	6	0
37	G	317	KC1	6	0
36	a	827	CLA	2	0
36	I	312	CLA	16	0
42	D	320	LMG	12	0
36	R	313	CLA	2	0
42	G	325	LMG	14	0
42	V	316	LMG	28	0
36	B	308	CLA	7	0
36	U	306	CLA	31	0
36	a	828	CLA	1	0
42	D	321	LMG	5	0
35	V	303	A86	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	O	301	A86	13	0
35	O	305	A86	13	0
36	a	826	CLA	2	0
36	W	201	CLA	1	0
35	X	305	A86	2	0
36	C	209	CLA	1	0
36	O	312	CLA	2	0
41	R	323	LHG	14	0
36	T	309	CLA	4	0
36	b	816	CLA	9	0
36	E	316	CLA	3	0
39	I	317	LMT	15	0
35	G	305	A86	3	0
36	D	310	CLA	1	0
36	S	315	CLA	15	0
34	P	305	DD6	6	0
36	f	805	CLA	20	0
36	V	305	CLA	32	0
34	E	301	DD6	4	0
37	S	316	KC1	4	0
36	H	310	CLA	9	0
36	J	315	CLA	3	0
36	D	313	CLA	3	0
36	W	212	CLA	23	0
41	i	104	LHG	28	0
36	a	834	CLA	2	0
36	b	814	CLA	2	0
36	A	309	CLA	6	0
36	b	837	CLA	2	0
36	C	212	CLA	6	0
36	P	313	CLA	7	0
35	P	307	A86	2	0
36	F	312	CLA	6	0
35	B	303	A86	8	0
42	J	318	LMG	24	0
36	E	311	CLA	6	0
36	G	307	CLA	12	0
36	b	809	CLA	2	0
44	f	806	BCR	1	0
36	H	317	CLA	1	0
36	b	824	CLA	4	0
37	B	310	KC1	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	L	302	DGD	20	0
44	l	203	BCR	1	0
36	I	310	CLA	4	0
35	B	301	A86	11	0
36	I	313	CLA	2	0
36	W	207	CLA	8	0
36	a	831	CLA	1	0
35	J	301	A86	14	0
36	Q	308	CLA	7	0
39	K	318	LMT	8	0
35	Q	303	A86	14	0
36	V	310	CLA	15	0
36	b	829	CLA	3	0
36	a	805	CLA	1	0
36	S	314	CLA	3	0
36	a	815	CLA	3	0
36	l	205	CLA	3	0
43	b	842	PQN	3	0
34	H	303	DD6	5	0
36	G	314	CLA	1	0
36	J	312	CLA	5	0
36	N	315	CLA	1	0
36	E	312	CLA	1	0
36	a	825	CLA	2	0
34	S	307	DD6	1	0
36	B	309	CLA	16	0
36	j	106	CLA	1	0
36	V	309	CLA	7	0
36	K	311	CLA	5	0
42	m	102	LMG	9	0
35	S	308	A86	5	0
36	V	311	CLA	16	0
36	b	805	CLA	2	0
36	b	823	CLA	11	0
35	N	302	A86	4	0
36	S	319	CLA	2	0
35	F	302	A86	2	0
36	a	822	CLA	3	0
36	M	315	CLA	2	0
35	U	303	A86	15	0
36	L	311	CLA	2	0
36	S	309	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	E	320	LMT	16	0
36	S	311	CLA	8	0
35	O	319	A86	1	0
39	b	848	LMT	5	0
40	C	215	DGD	19	0
36	W	211	CLA	1	0
36	D	309	CLA	10	0
36	T	308	CLA	3	0
41	f	808	LHG	23	0
36	N	317	CLA	3	0
36	P	316	CLA	4	0
36	a	830	CLA	4	0
36	a	848	CLA	10	0
37	V	312	KC1	1	0
36	A	307	CLA	3	0
36	H	307	CLA	10	0
36	T	316	CLA	1	0
37	T	310	KC1	17	0
36	b	833	CLA	8	0
36	R	322	CLA	1	0
36	b	838	CLA	1	0
36	l	202	CLA	8	0
44	i	101	BCR	4	0
36	G	319	CLA	4	0
35	K	303	A86	2	0
35	F	301	A86	10	0
37	P	315	KC1	2	0
35	N	303	A86	15	0
35	U	301	A86	1	0
34	Q	302	DD6	19	0
39	F	321	LMT	25	0
39	B	312	LMT	15	0
36	N	310	CLA	6	0
34	J	304	DD6	4	0
36	a	804	CLA	3	0
39	f	807	LMT	2	0
36	D	316	CLA	1	0
36	b	831	CLA	2	0
36	X	307	CLA	3	0
36	P	318	CLA	1	0
37	O	313	KC1	1	0
44	a	846	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	F	316	CLA	3	0
36	b	830	CLA	1	0
36	P	309	CLA	2	0
36	P	310	CLA	2	0
39	E	321	LMT	8	0
36	E	317	CLA	1	0
44	a	844	BCR	7	0
36	a	809	CLA	5	0
42	I	315	LMG	14	0
35	T	304	A86	5	0
36	A	311	CLA	3	0
36	O	316	CLA	22	0
36	K	310	CLA	21	0
35	T	303	A86	1	0
36	W	208	CLA	1	0
36	b	801	CLA	1	0
39	K	317	LMT	6	0
35	G	302	A86	2	0
39	I	318	LMT	7	0
36	K	316	CLA	3	0
36	T	314	CLA	1	0
36	b	840	CLA	3	0
36	E	308	CLA	3	0
36	P	319	CLA	13	0
36	U	305	CLA	3	0
35	L	304	A86	1	0
36	G	310	CLA	1	0
37	G	308	KC1	2	0
35	D	302	A86	6	0
36	a	818	CLA	3	0
36	V	313	CLA	12	0
36	X	315	CLA	24	0
35	E	305	A86	4	0
36	b	836	CLA	20	0
37	W	217	KC1	14	0
35	N	301	A86	2	0
36	H	305	CLA	2	0
35	N	305	A86	20	0
34	F	303	DD6	3	0
36	S	313	CLA	1	0
36	A	308	CLA	2	0
36	P	302	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	K	308	CLA	2	0
36	a	807	CLA	1	0
36	M	306	CLA	1	0
36	R	316	CLA	1	0
44	b	847	BCR	1	0
36	T	312	CLA	1	0
39	a	854	LMT	5	0
36	F	317	CLA	29	0
36	L	309	CLA	10	0
36	K	315	CLA	2	0
41	O	317	LHG	8	0
36	b	810	CLA	2	0
35	J	306	A86	6	0
36	X	308	CLA	4	0
40	b	849	DGD	4	0
36	j	101	CLA	11	0
41	a	843	LHG	5	0
36	R	320	CLA	7	0
35	N	306	A86	1	0
35	U	302	A86	4	0
36	C	206	CLA	3	0
36	f	803	CLA	3	0
34	E	303	DD6	4	0
34	G	303	DD6	2	0
39	B	313	LMT	5	0
34	H	302	DD6	1	0
44	b	845	BCR	1	0
36	C	207	CLA	7	0
36	R	321	CLA	2	0
39	P	320	LMT	6	0
36	a	824	CLA	2	0
36	P	308	CLA	1	0
36	U	310	CLA	15	0
36	b	807	CLA	4	0
36	Q	310	CLA	9	0
37	M	318	KC1	6	0
36	l	201	CLA	6	0
36	l	206	CLA	1	0
36	a	802	CLA	4	0
35	J	305	A86	6	0
42	G	324	LMG	17	0
34	A	301	DD6	8	0

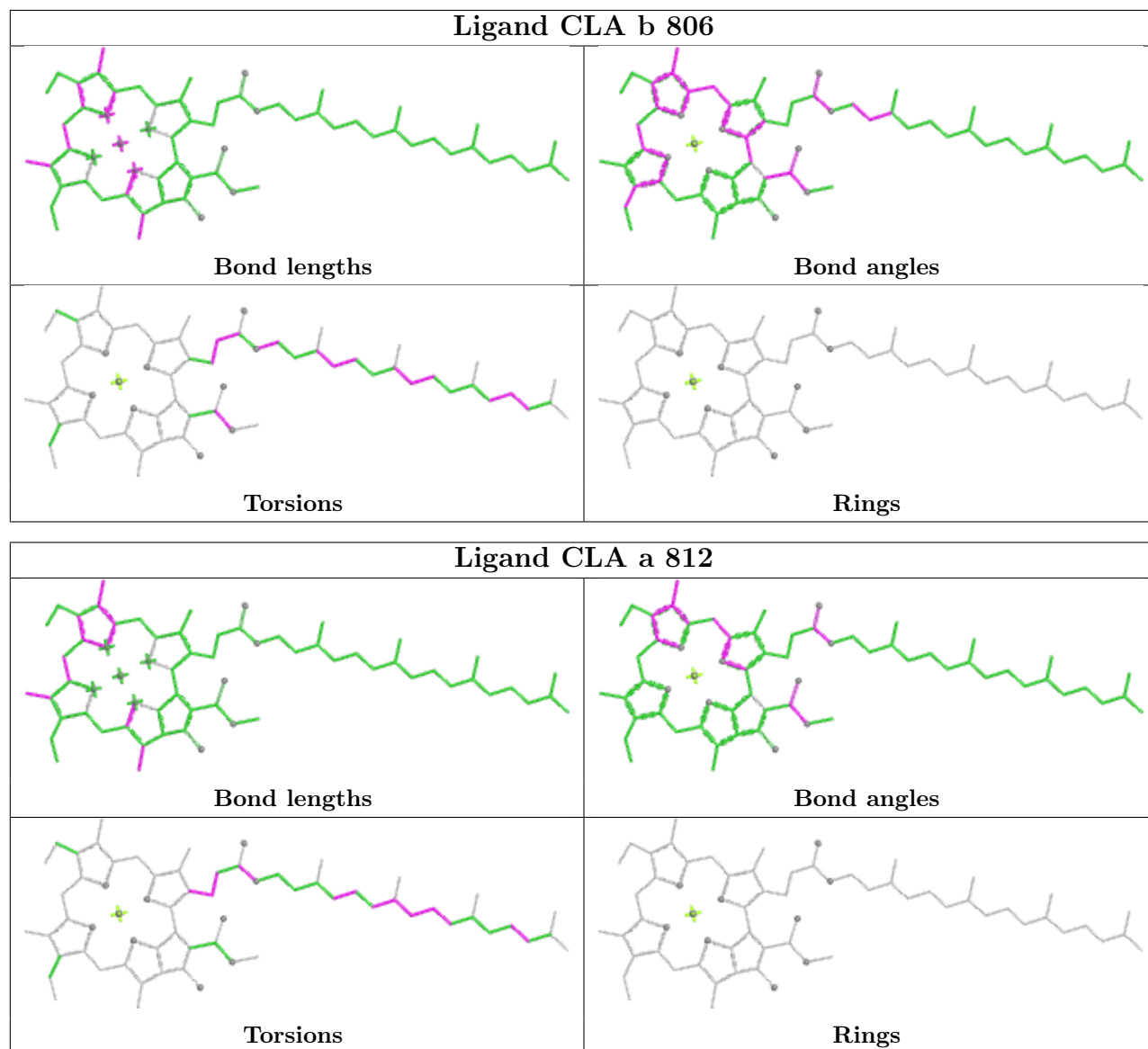
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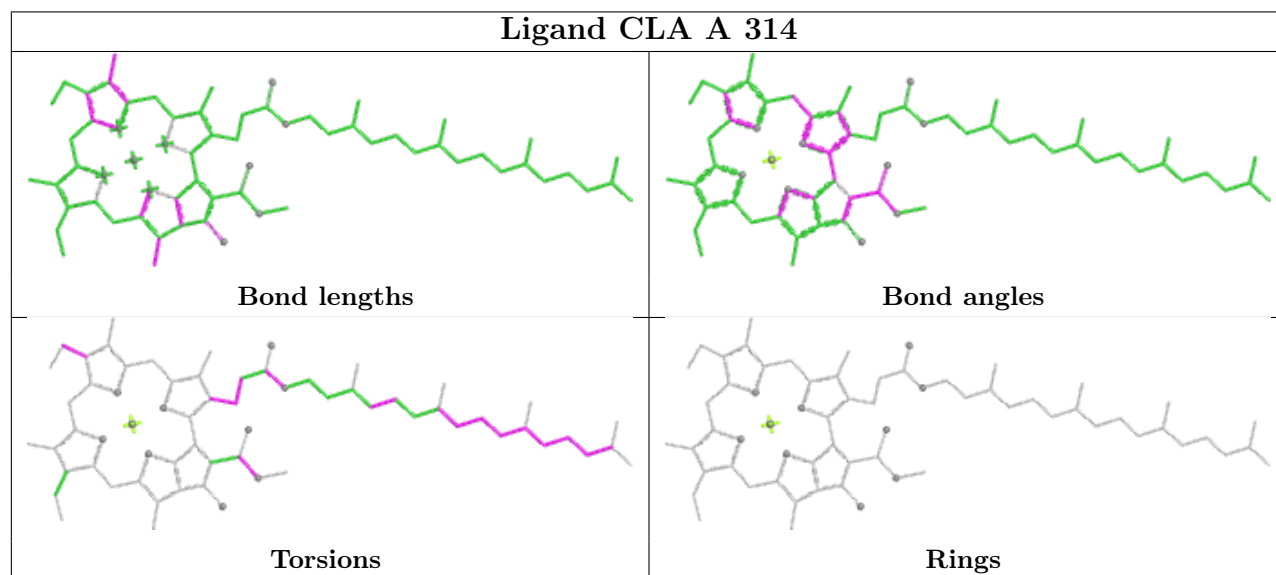
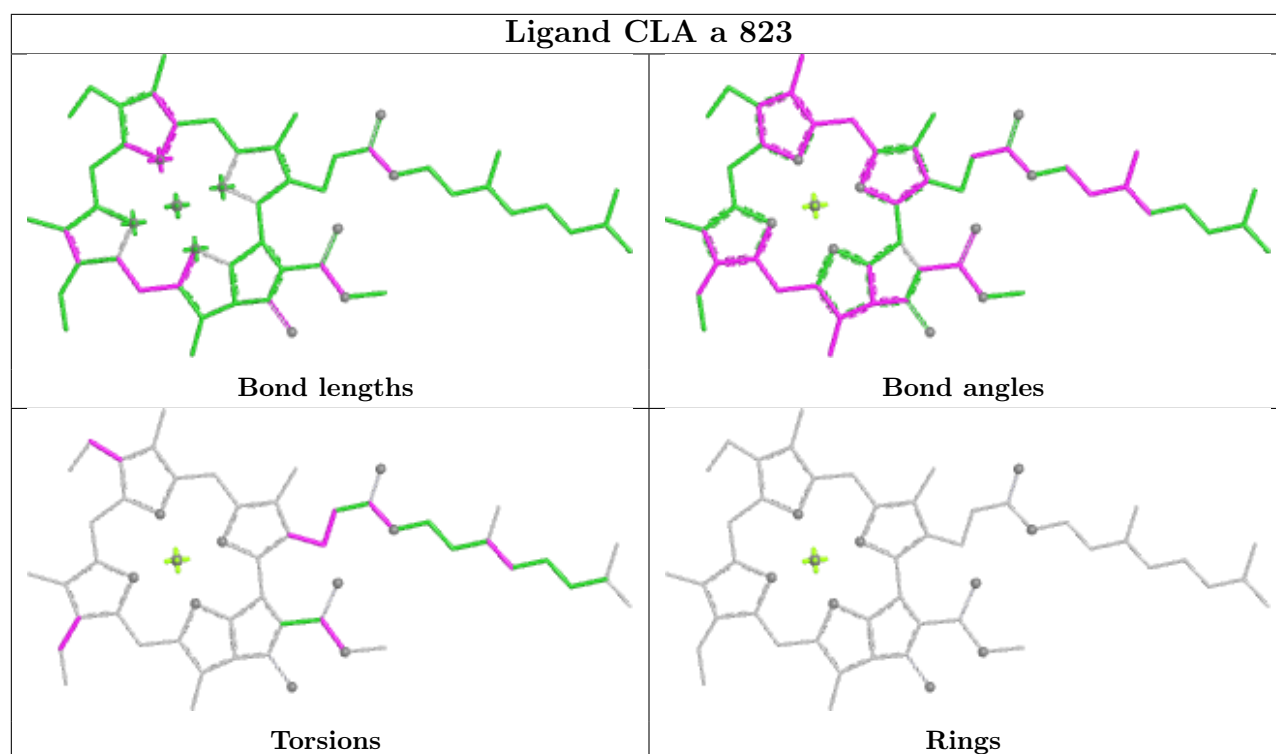
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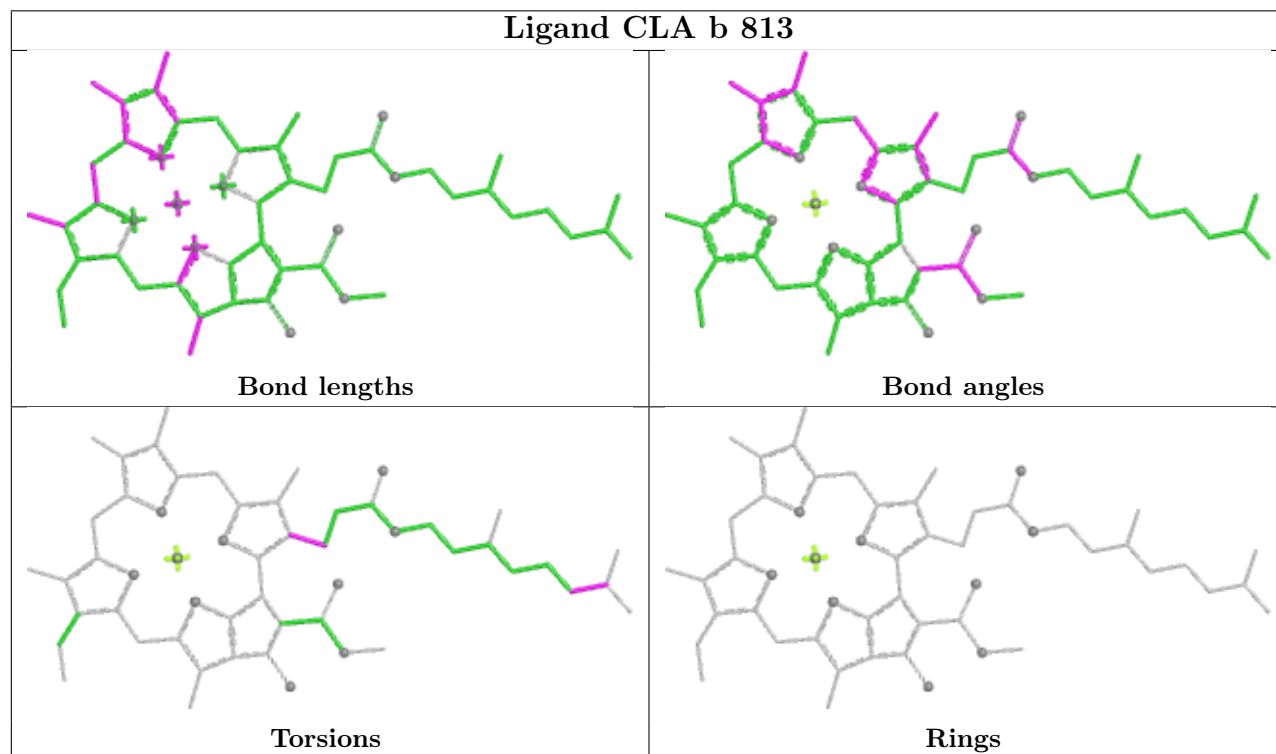
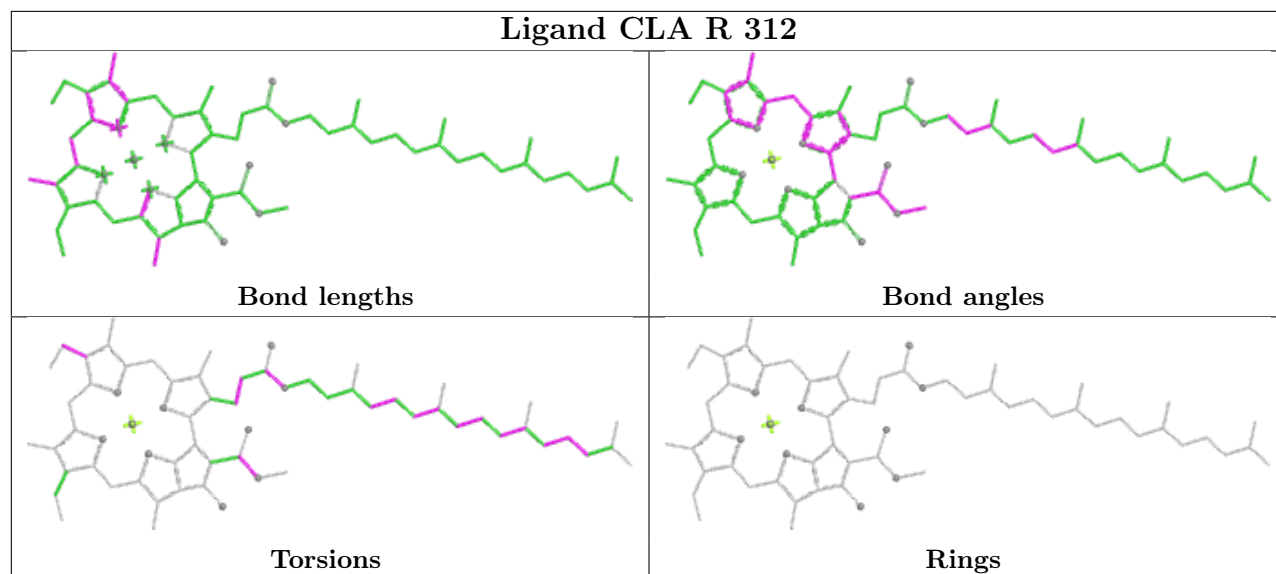
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	b	820	CLA	6	0
36	X	310	CLA	3	0
36	F	311	CLA	2	0
34	C	201	DD6	4	0
36	R	314	CLA	3	0
35	h	202	A86	5	0
34	I	303	DD6	6	0
36	H	311	CLA	3	0
36	K	312	CLA	3	0
36	S	318	CLA	3	0
37	O	315	KC1	12	0
41	G	321	LHG	10	0
36	b	802	CLA	3	0
35	G	306	A86	4	0
36	X	309	CLA	2	0
36	A	306	CLA	17	0
36	b	834	CLA	3	0
42	j	105	LMG	26	0
42	E	318	LMG	19	0
36	U	313	CLA	1	0
36	J	317	CLA	1	0
41	l	208	LHG	17	0
36	b	825	CLA	3	0
36	b	839	CLA	1	0
36	G	313	CLA	18	0
37	L	315	KC1	9	0
35	R	304	A86	2	0
39	L	318	LMT	9	0
37	C	213	KC1	1	0
36	S	312	CLA	3	0
36	b	812	CLA	2	0
35	E	307	A86	14	0
39	b	851	LMT	20	0
34	B	304	DD6	10	0
36	j	102	CLA	19	0

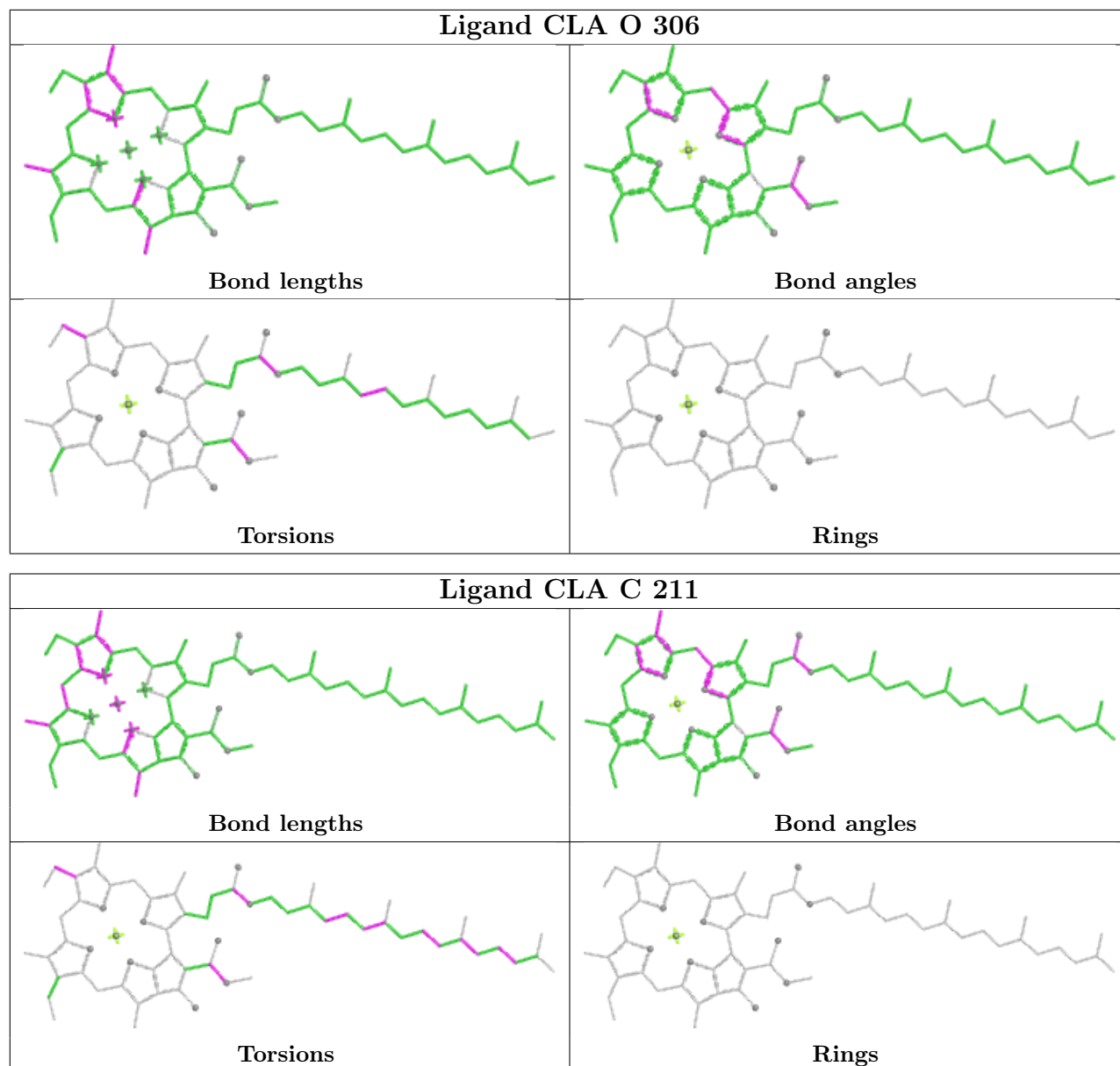
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

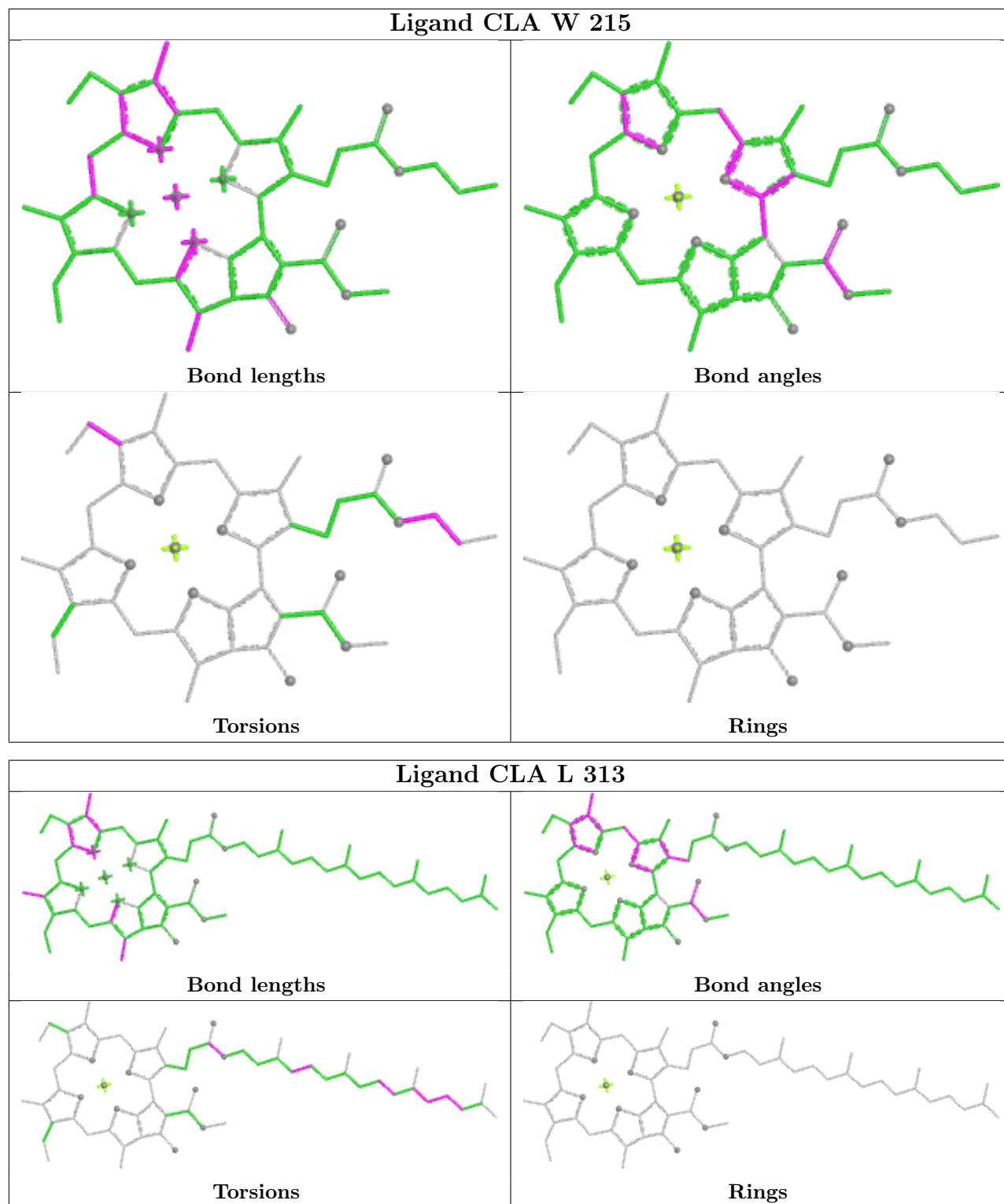
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

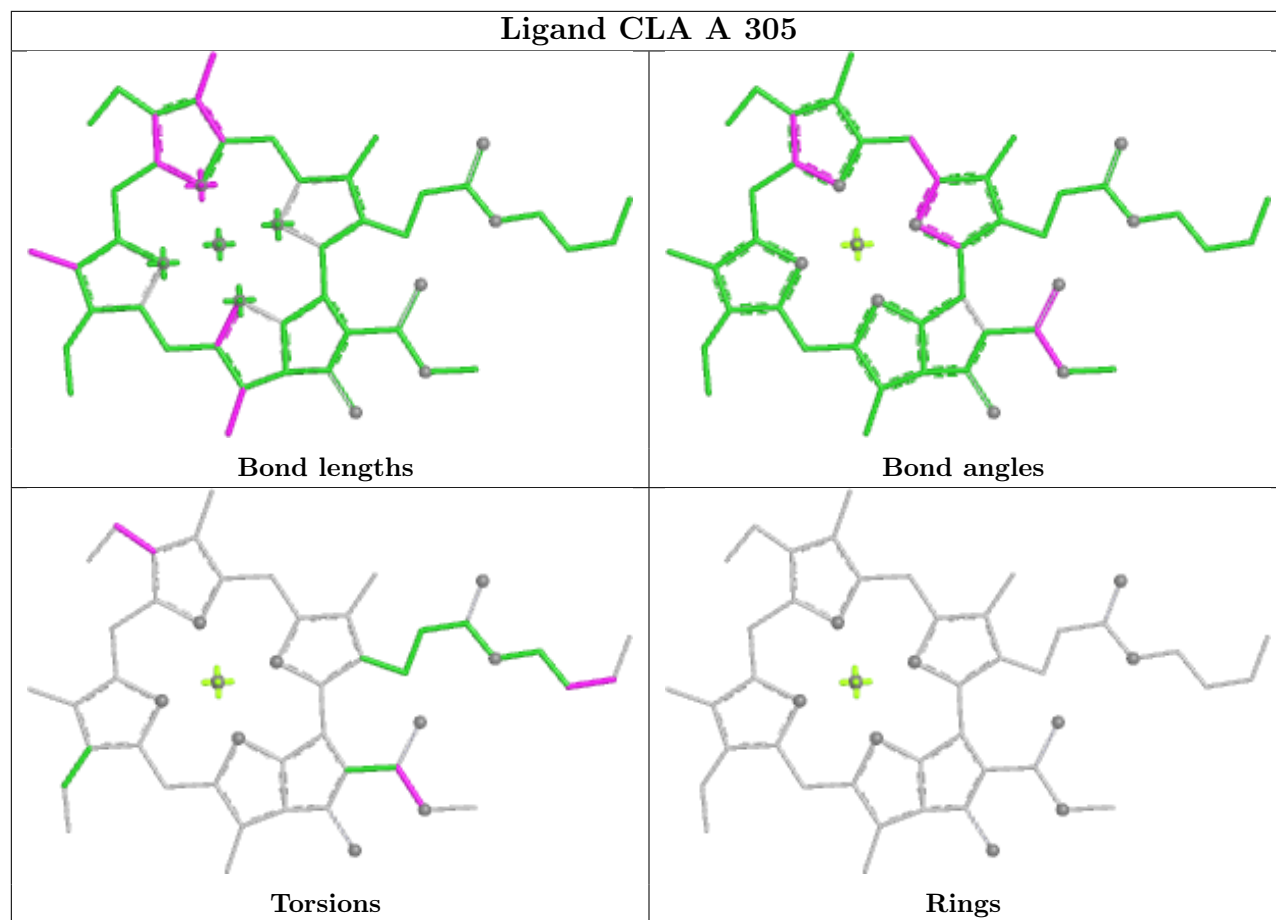


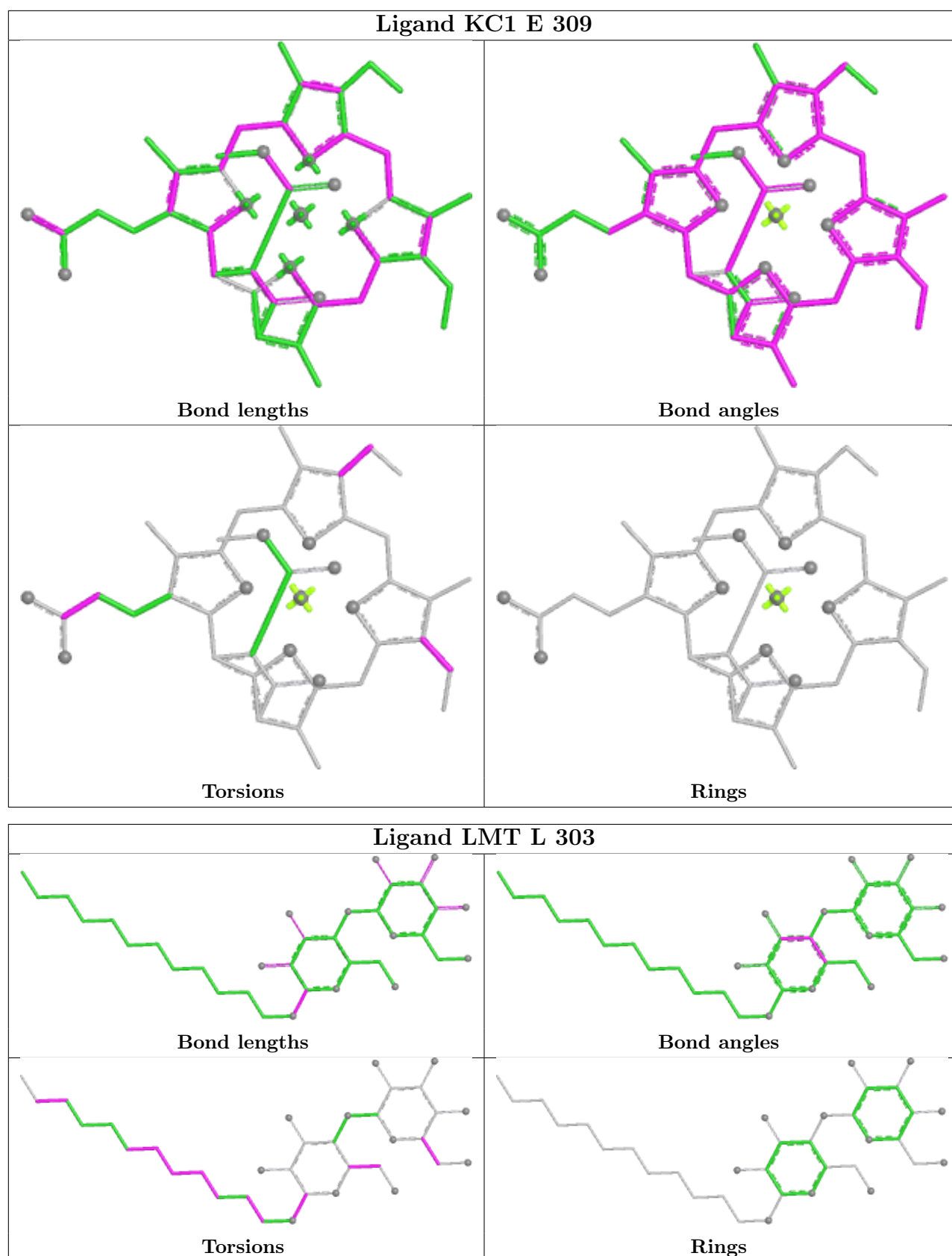


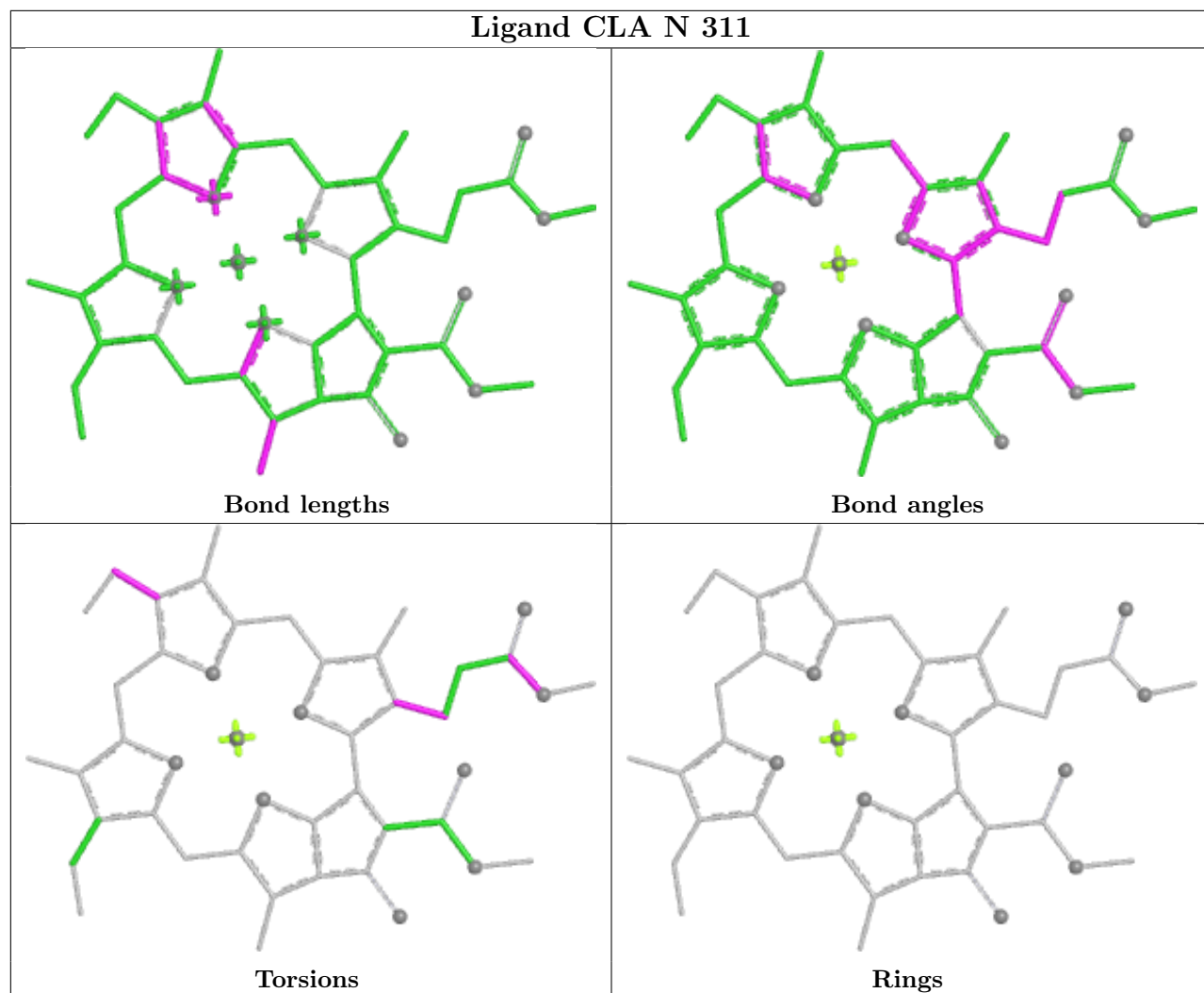


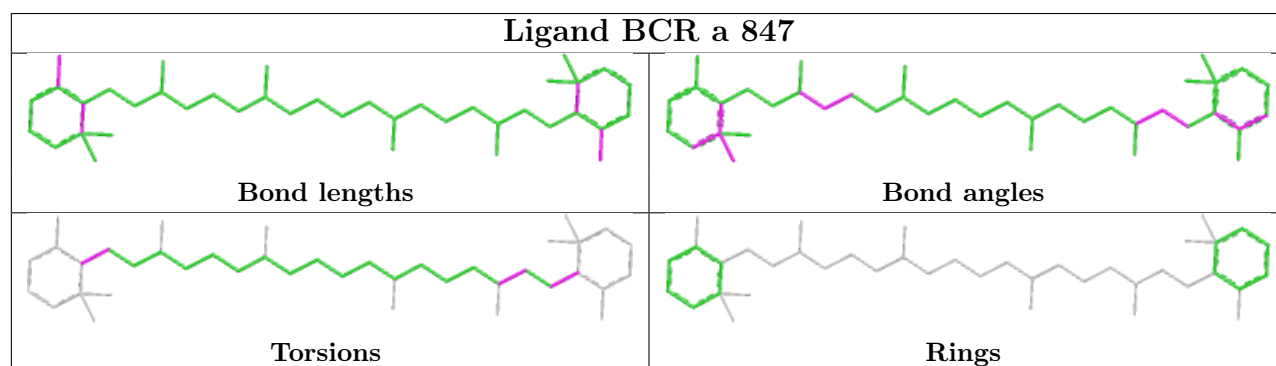
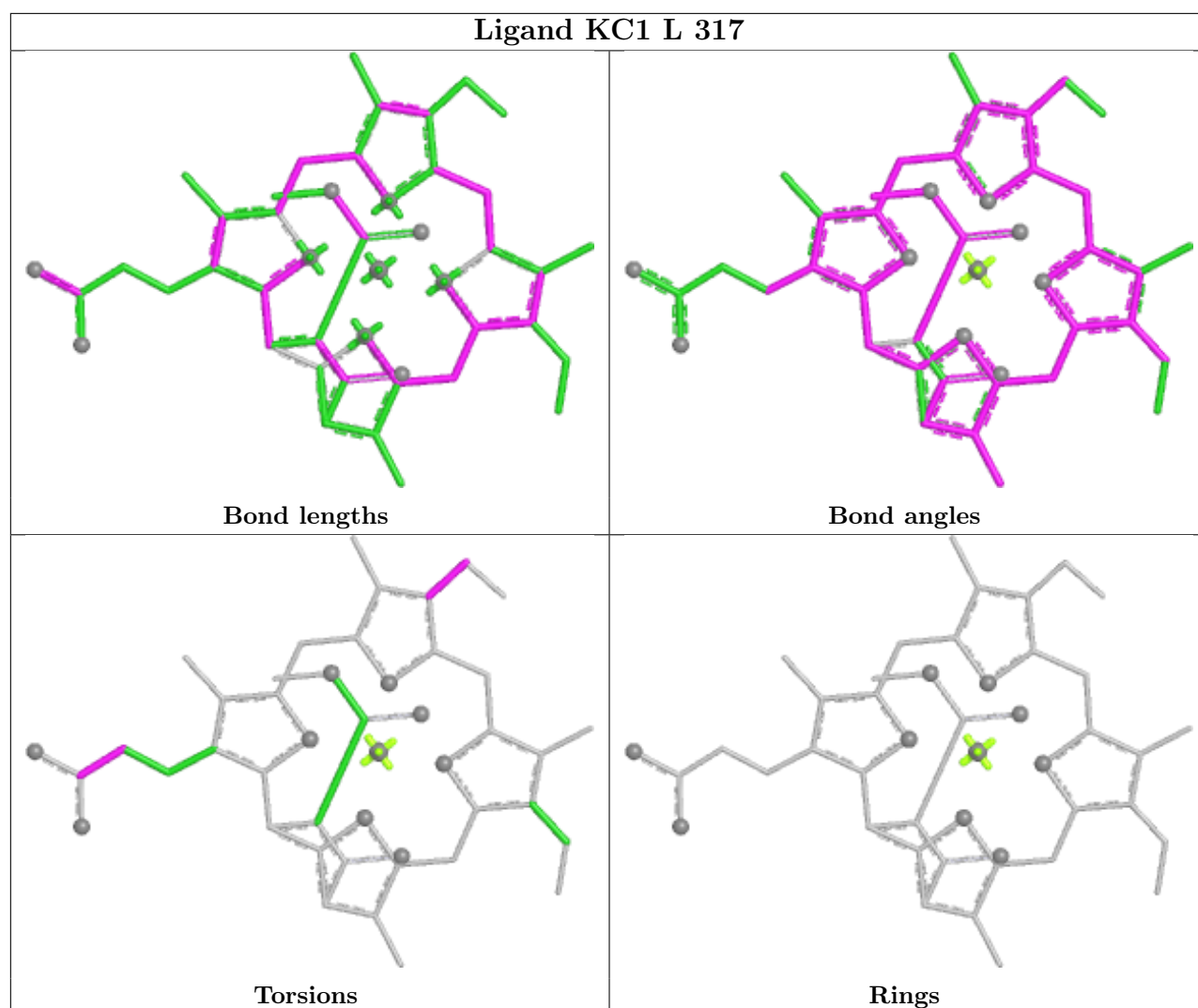


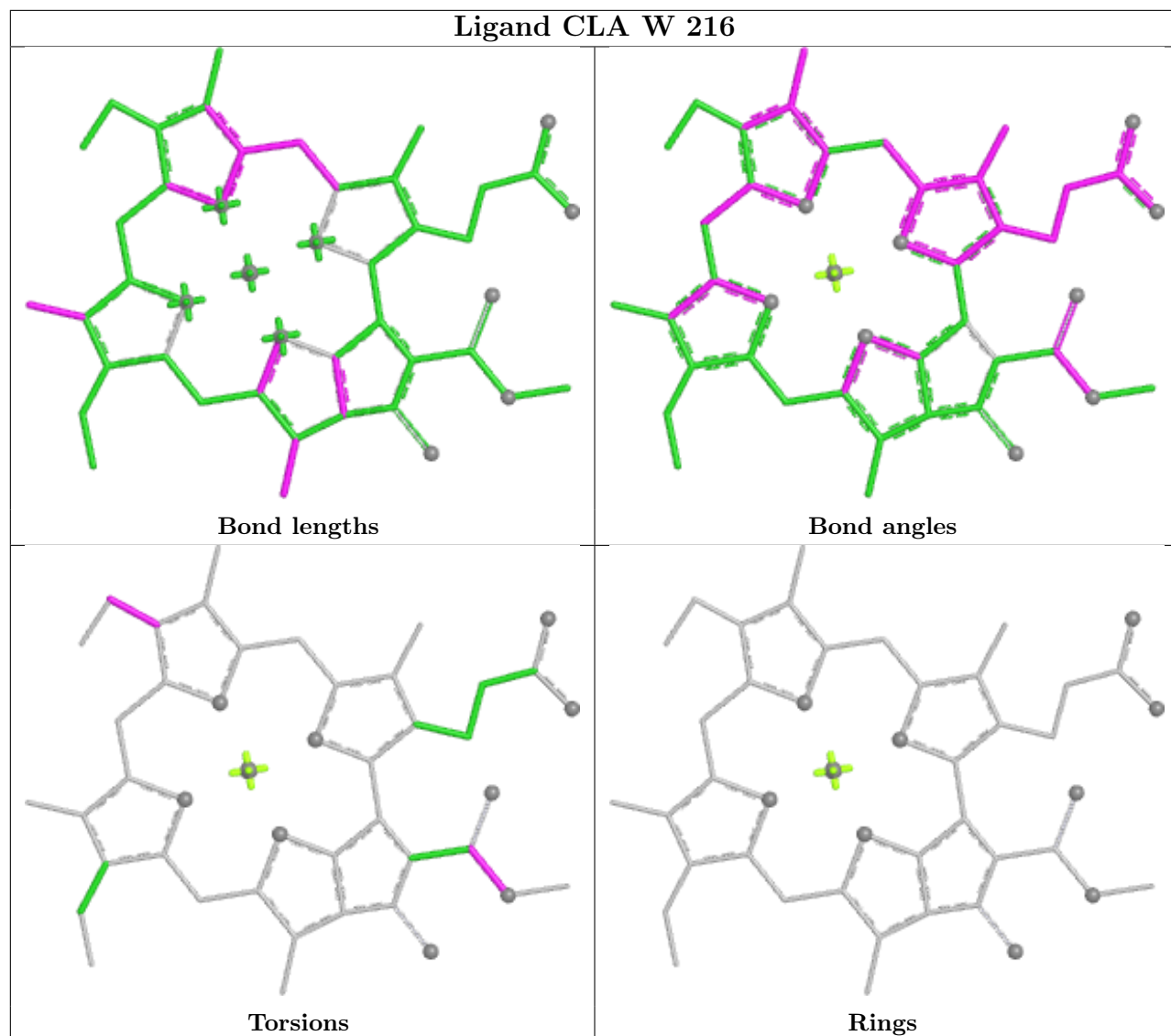


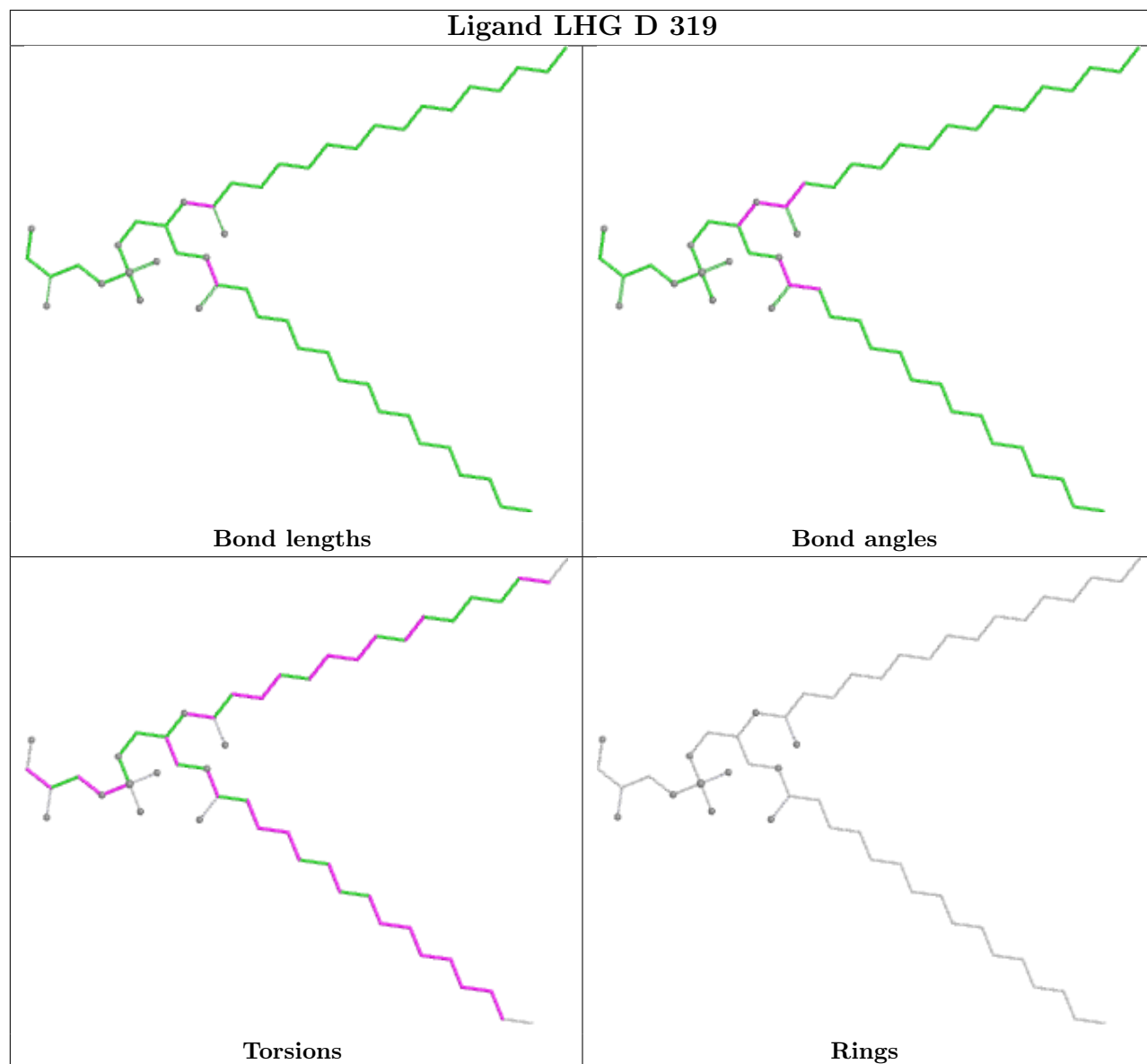


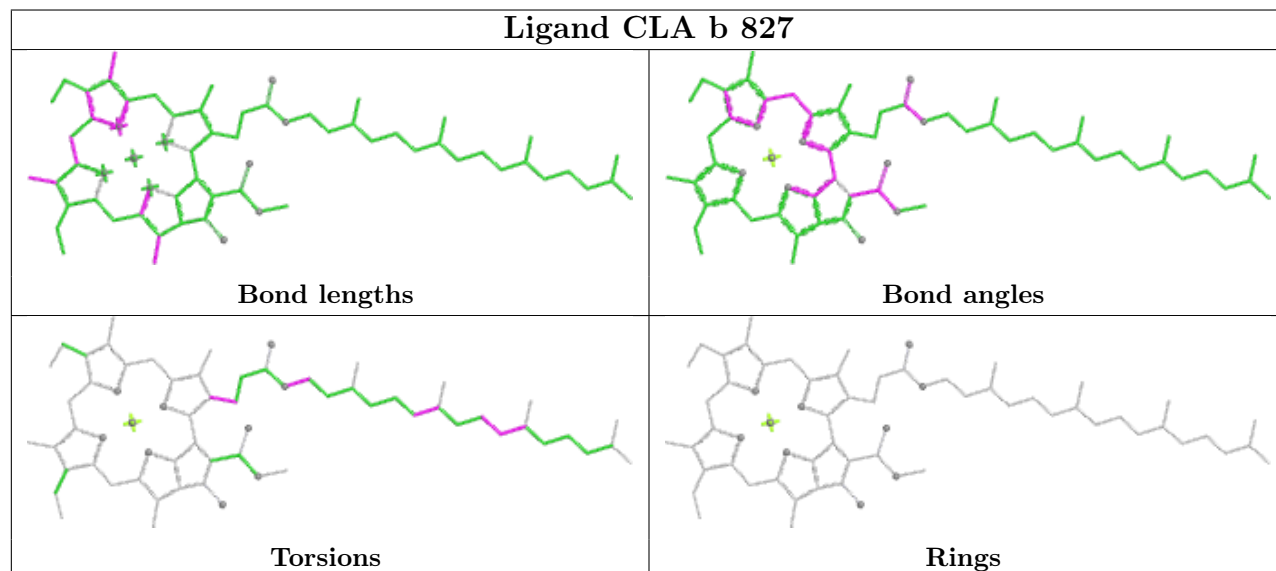
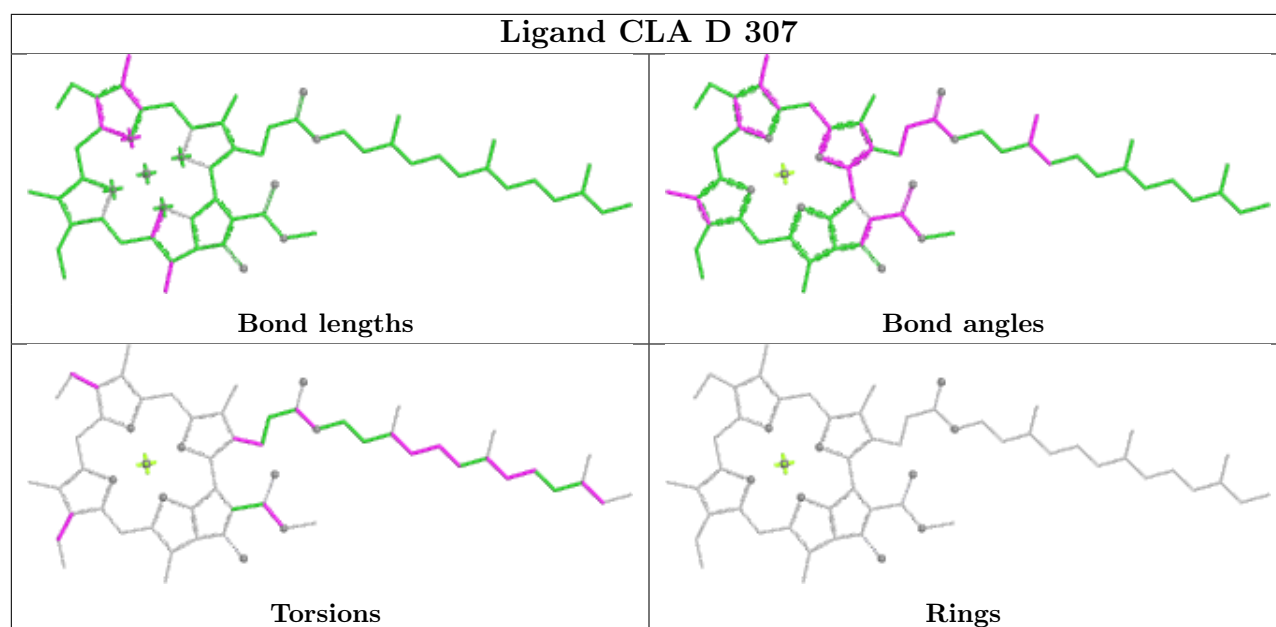


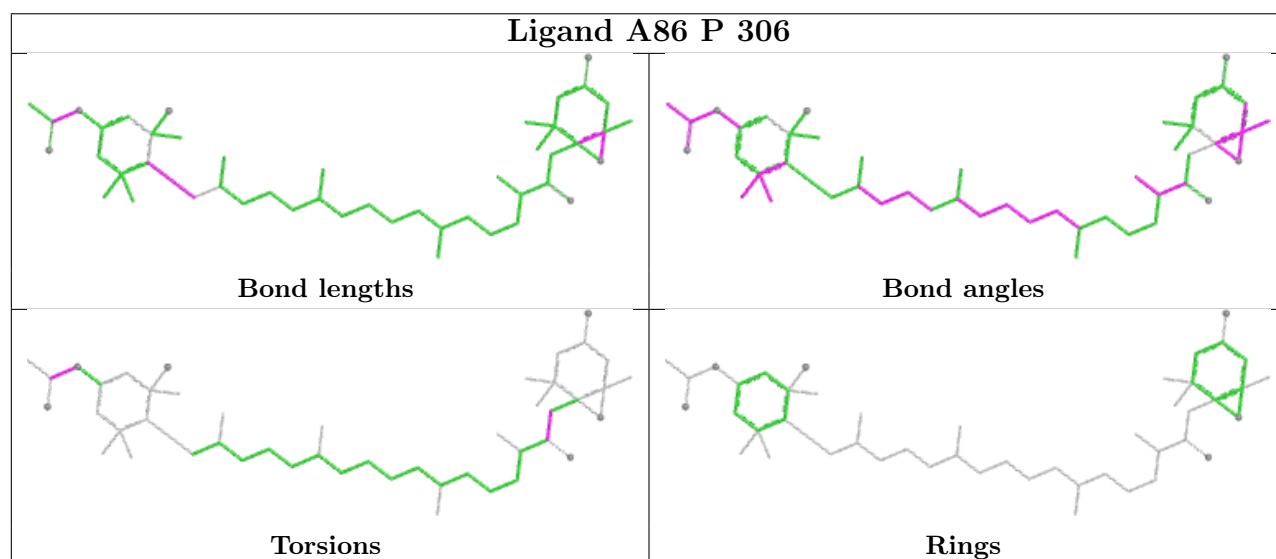
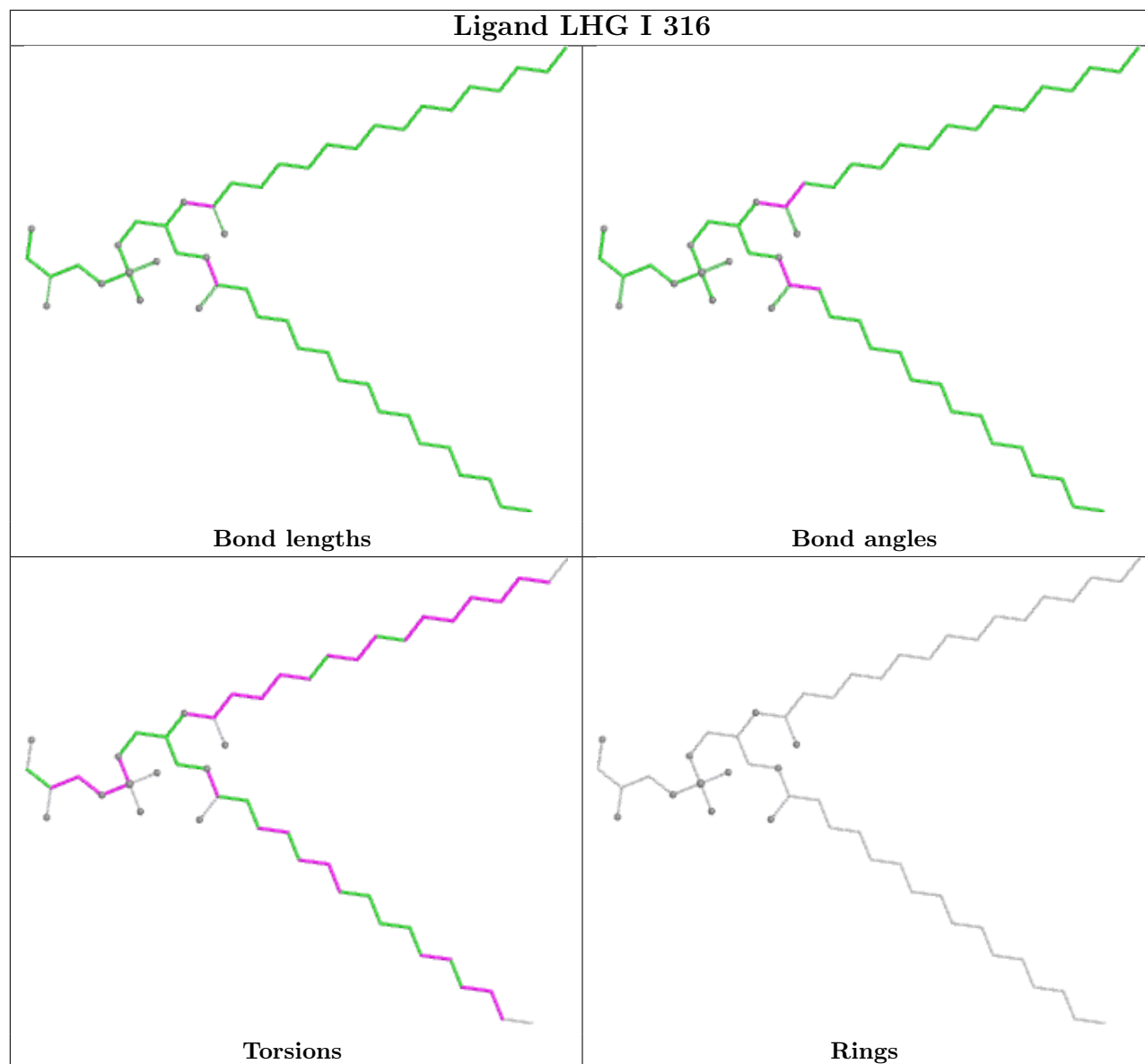


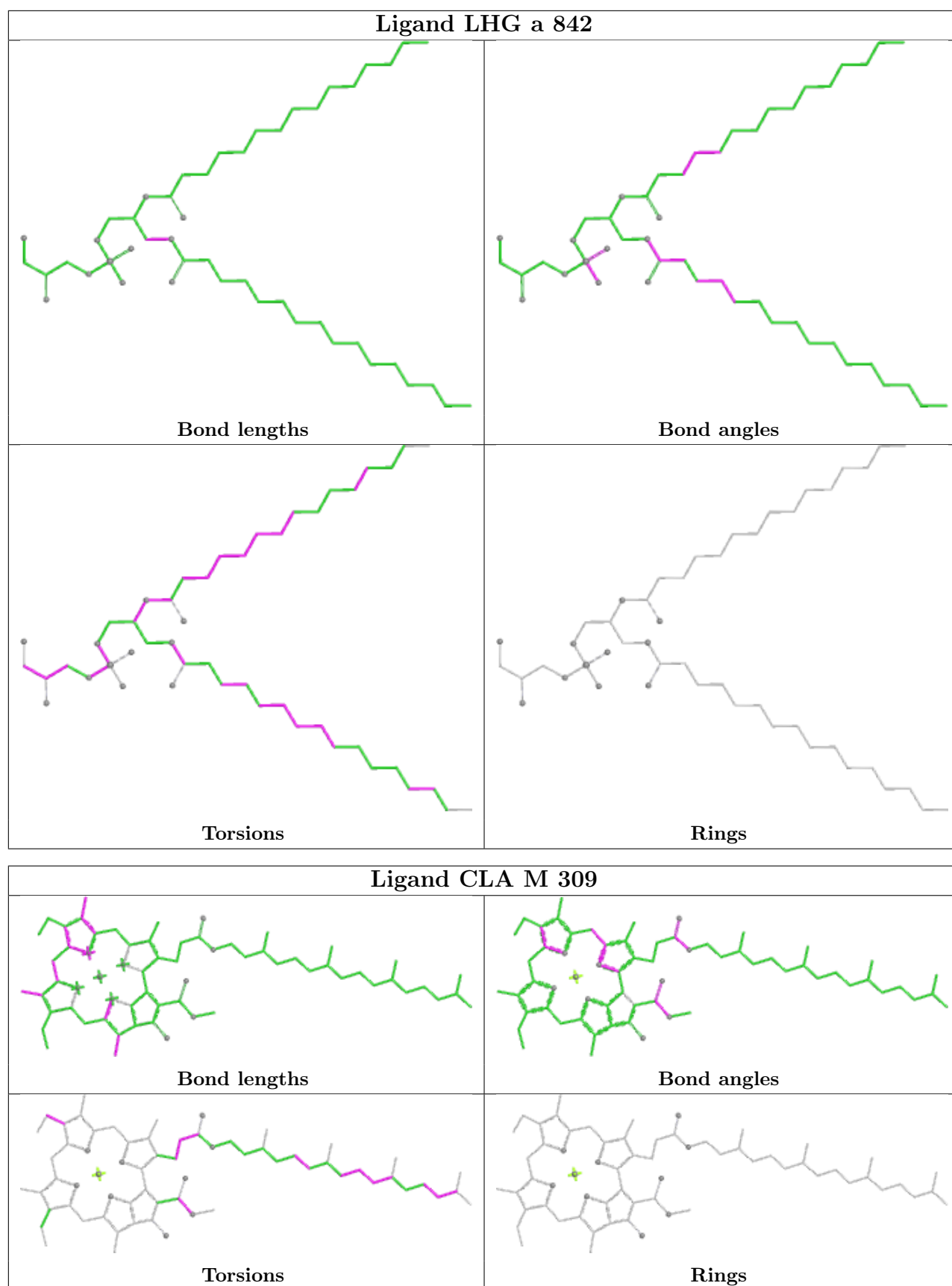


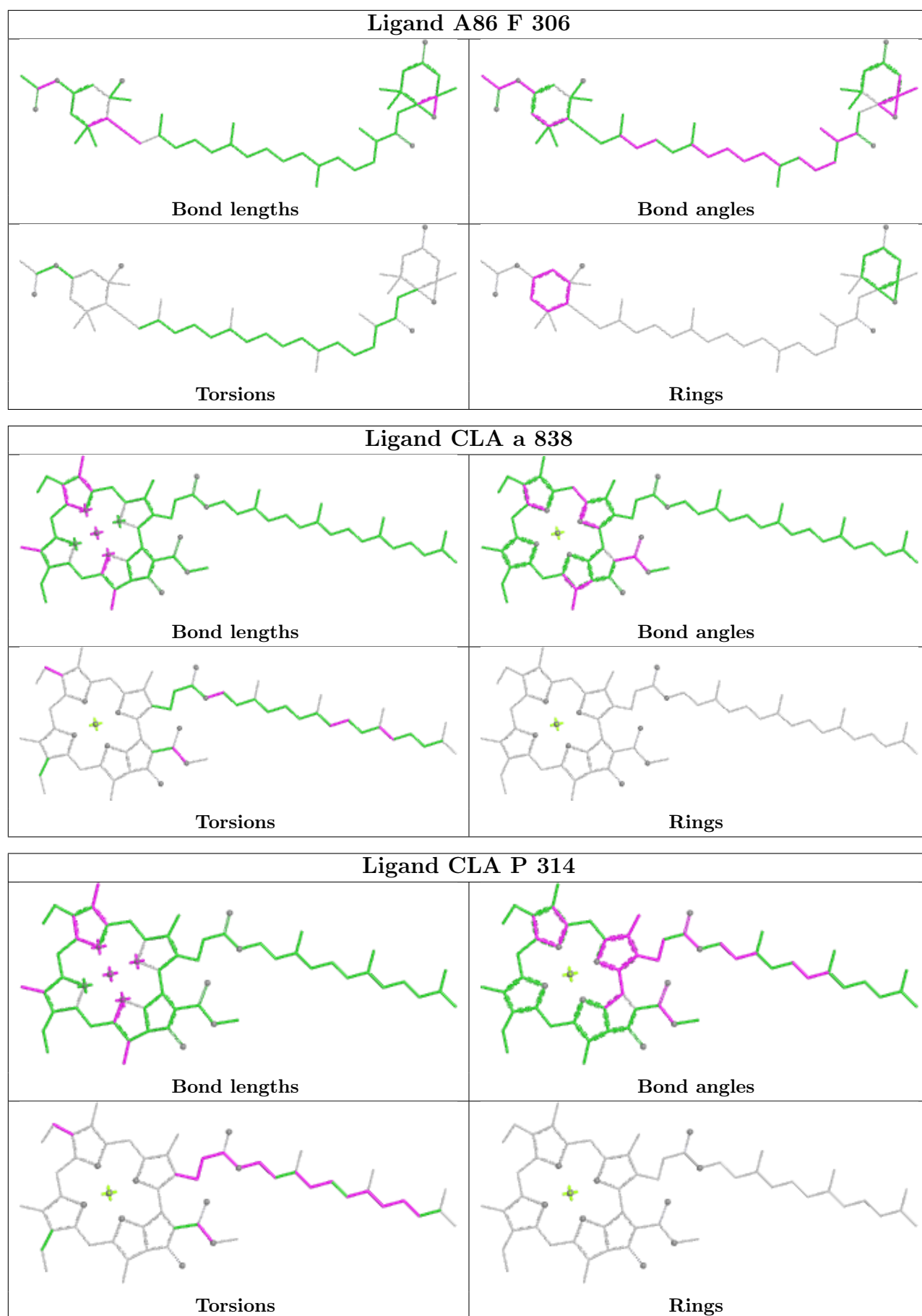


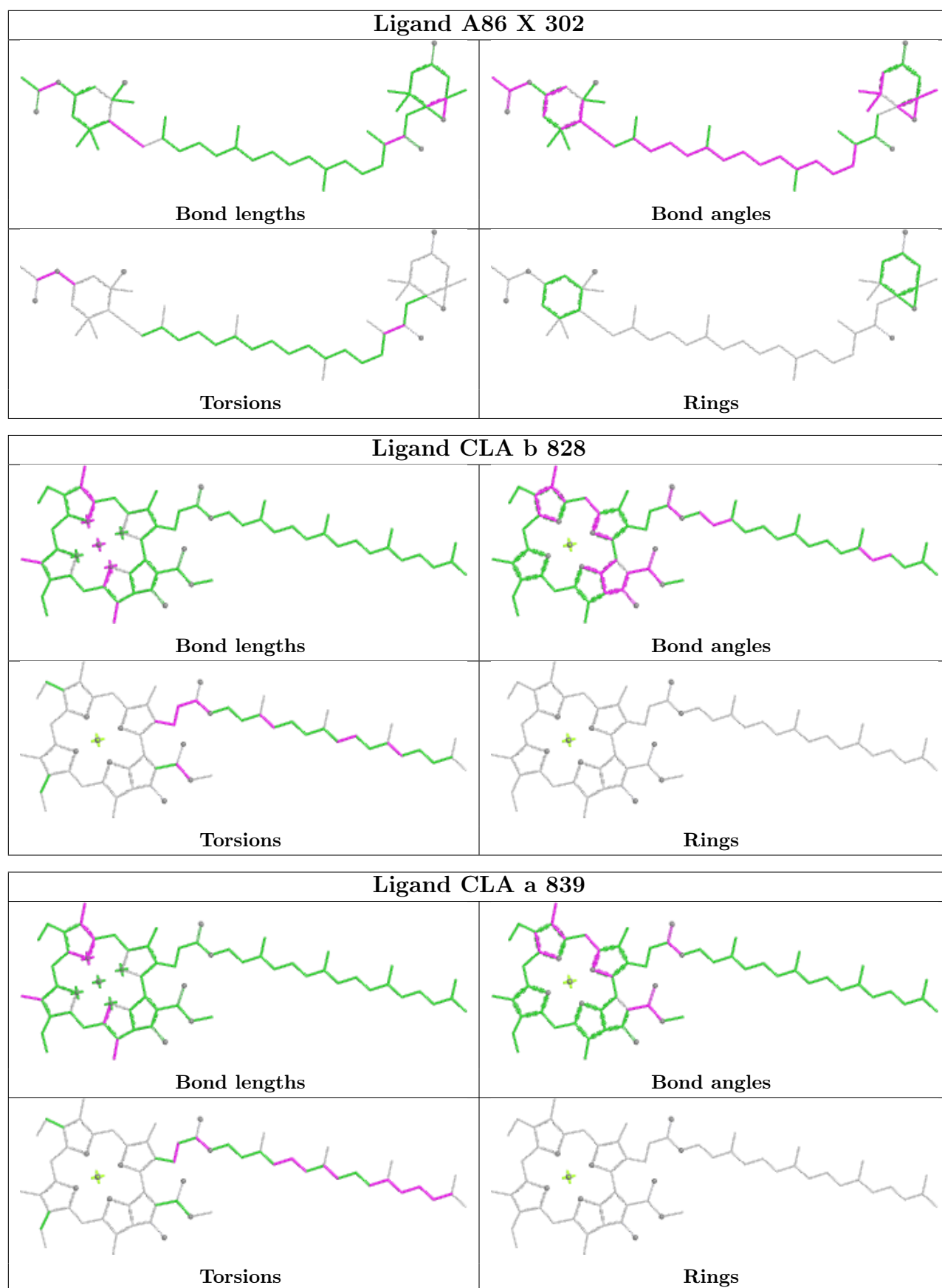


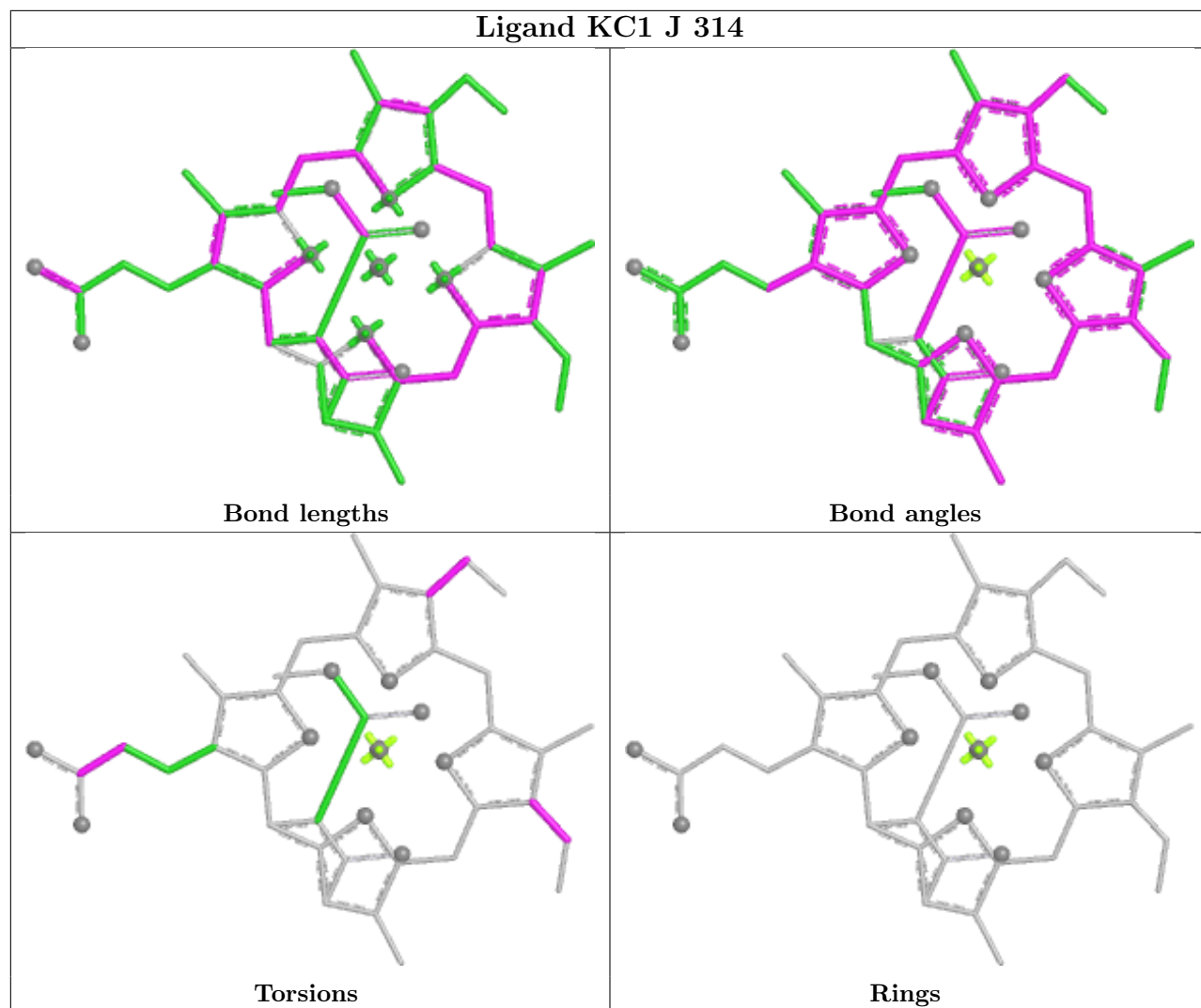


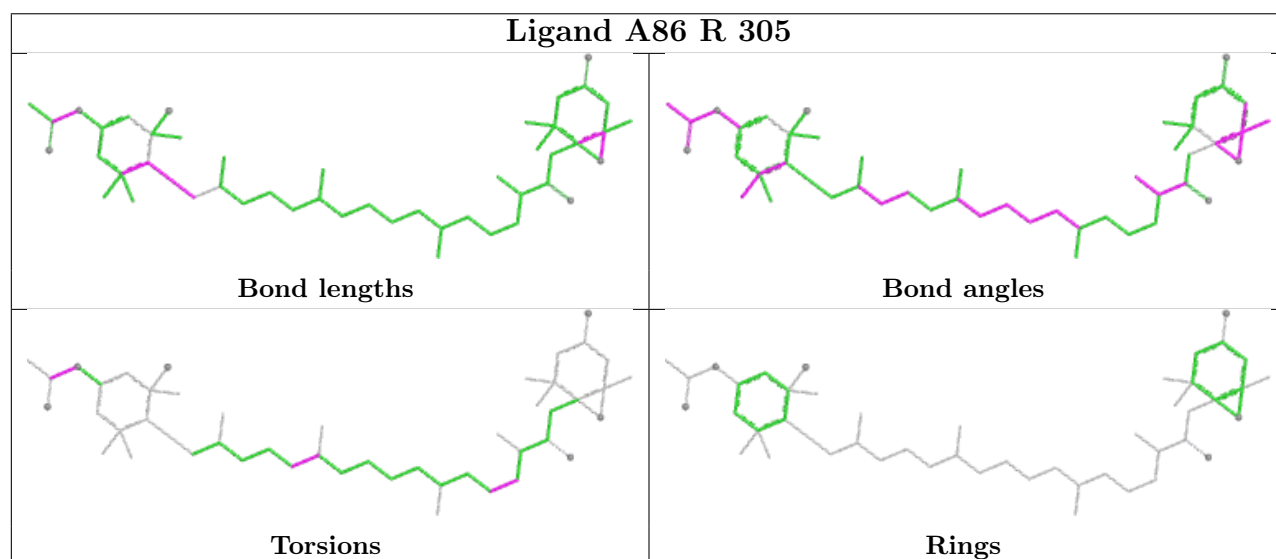
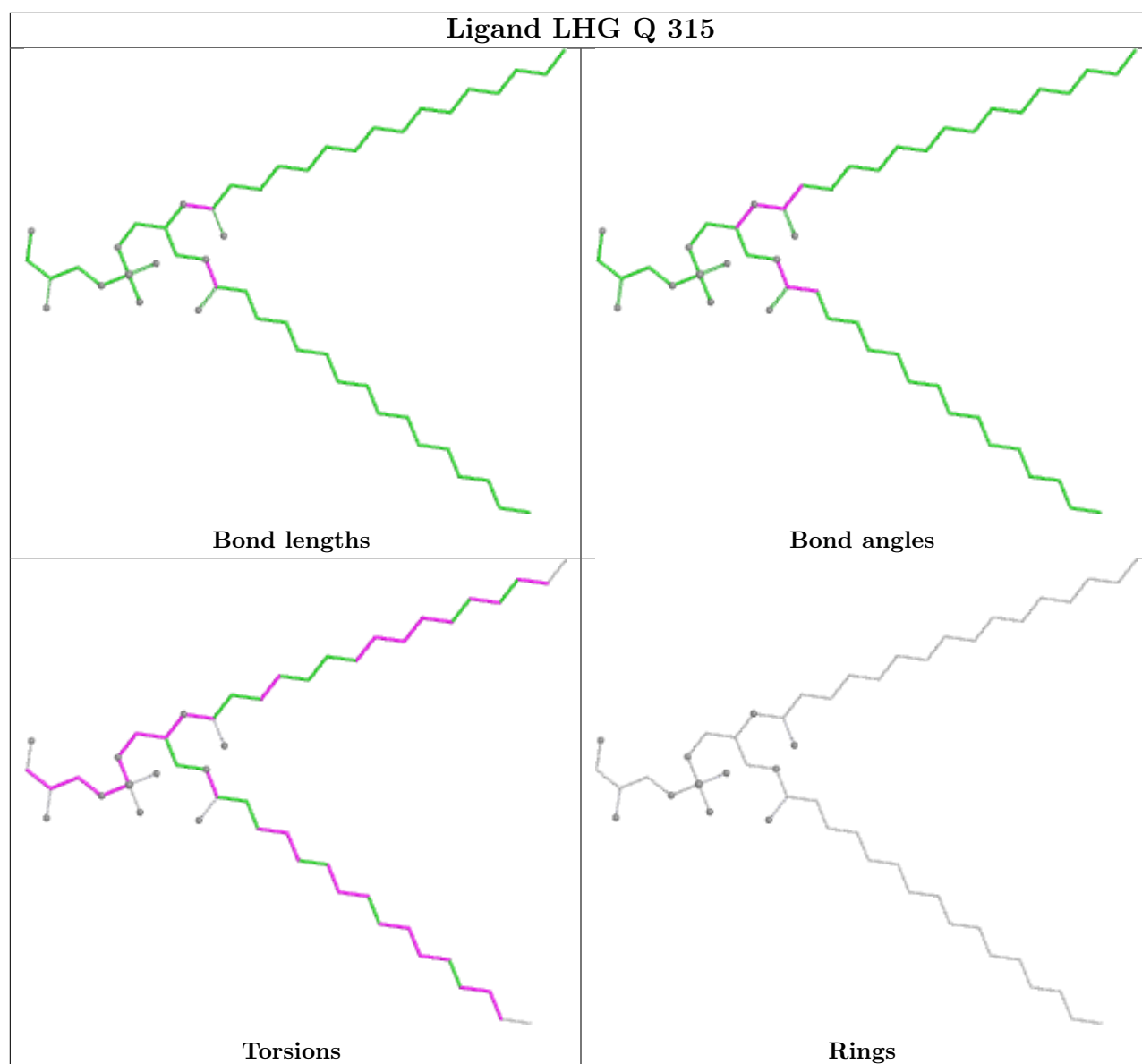


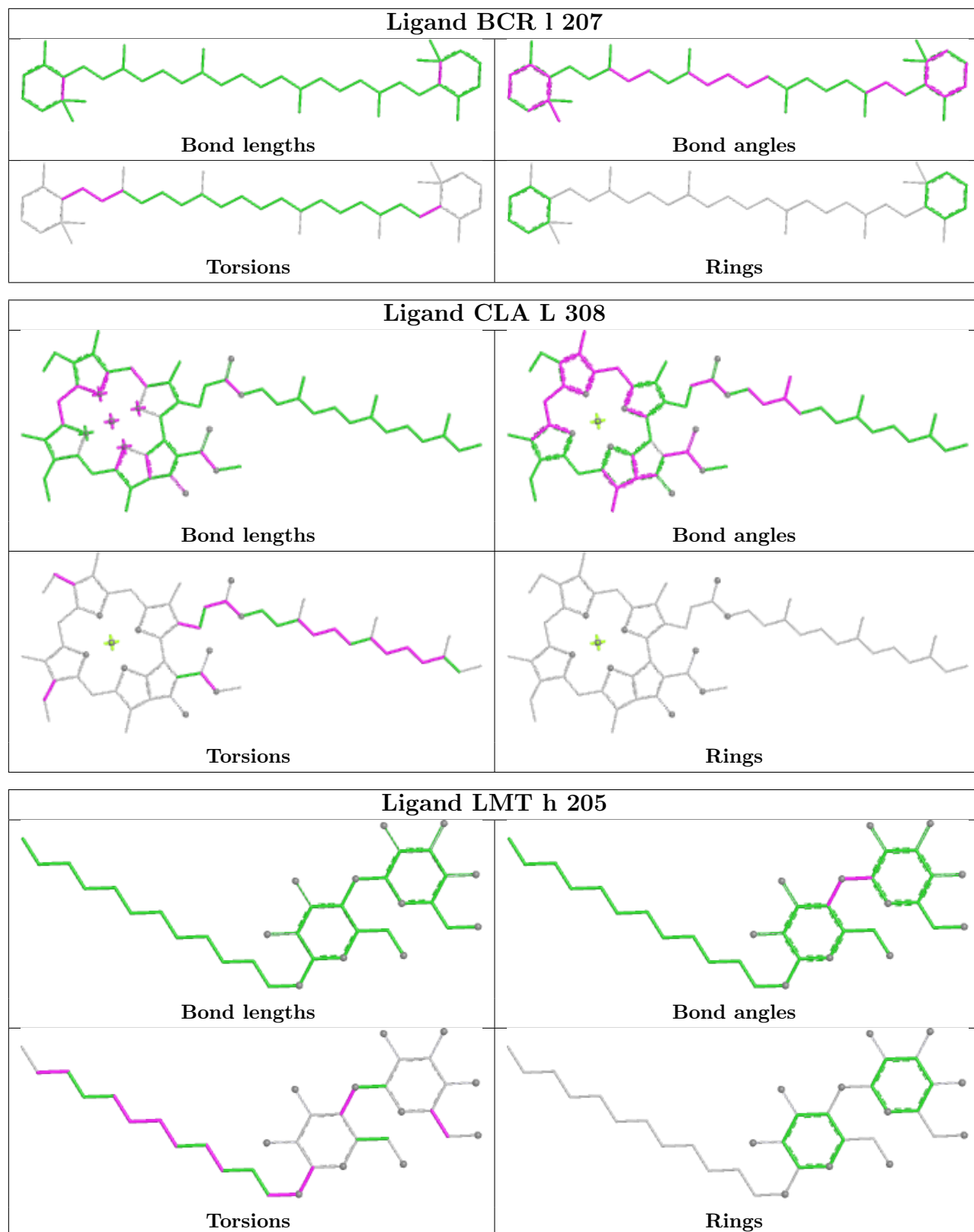


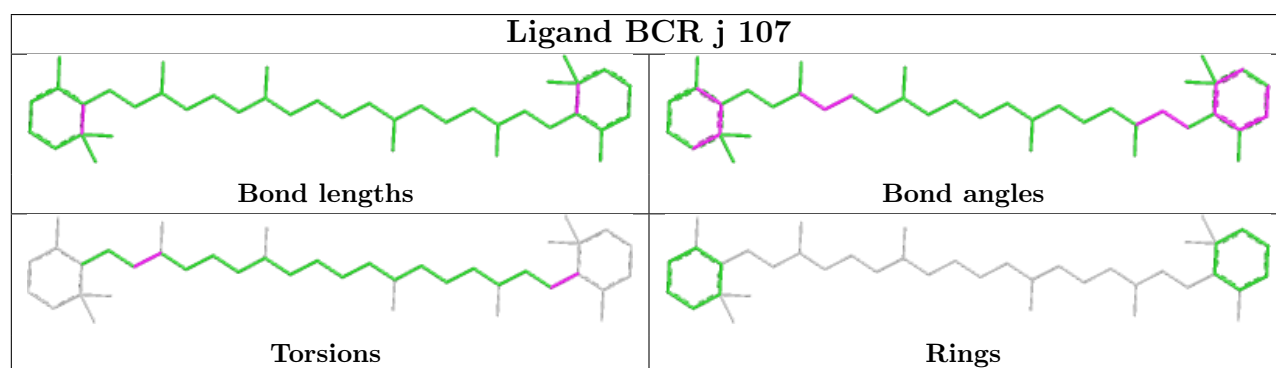
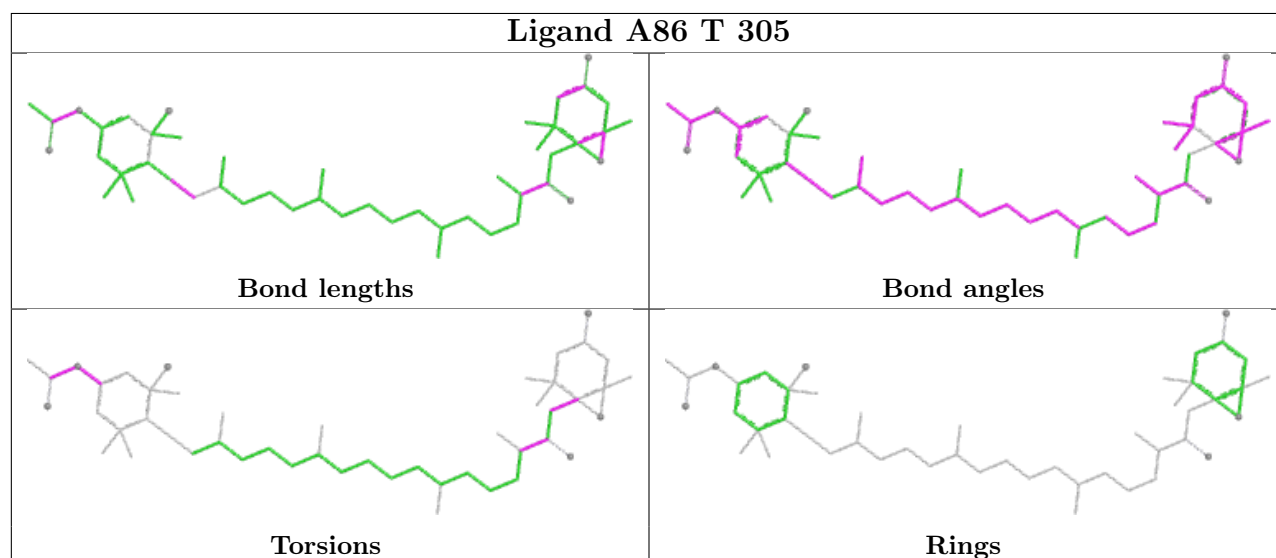
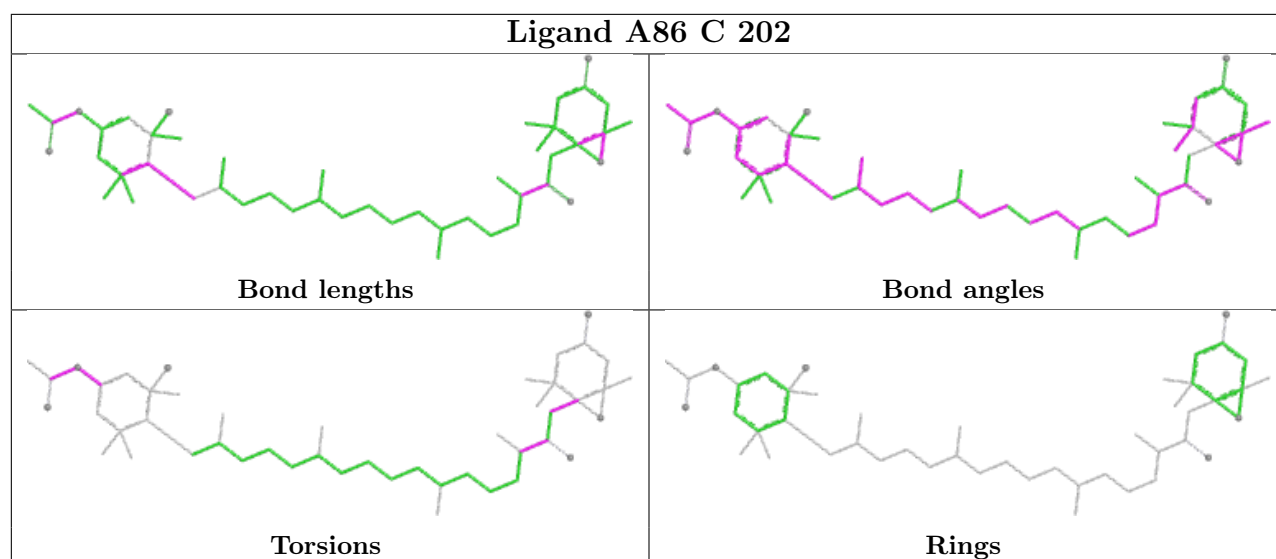


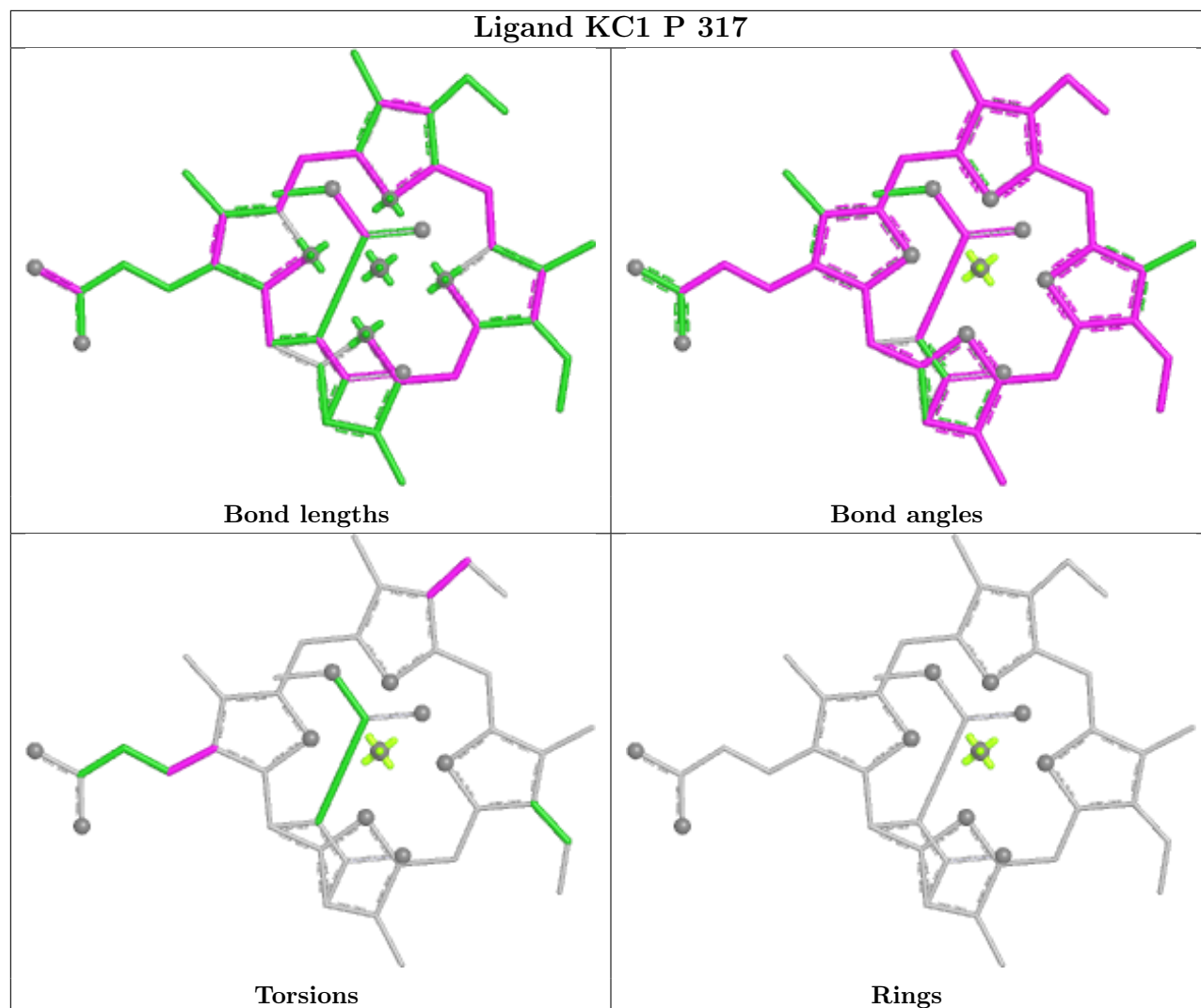


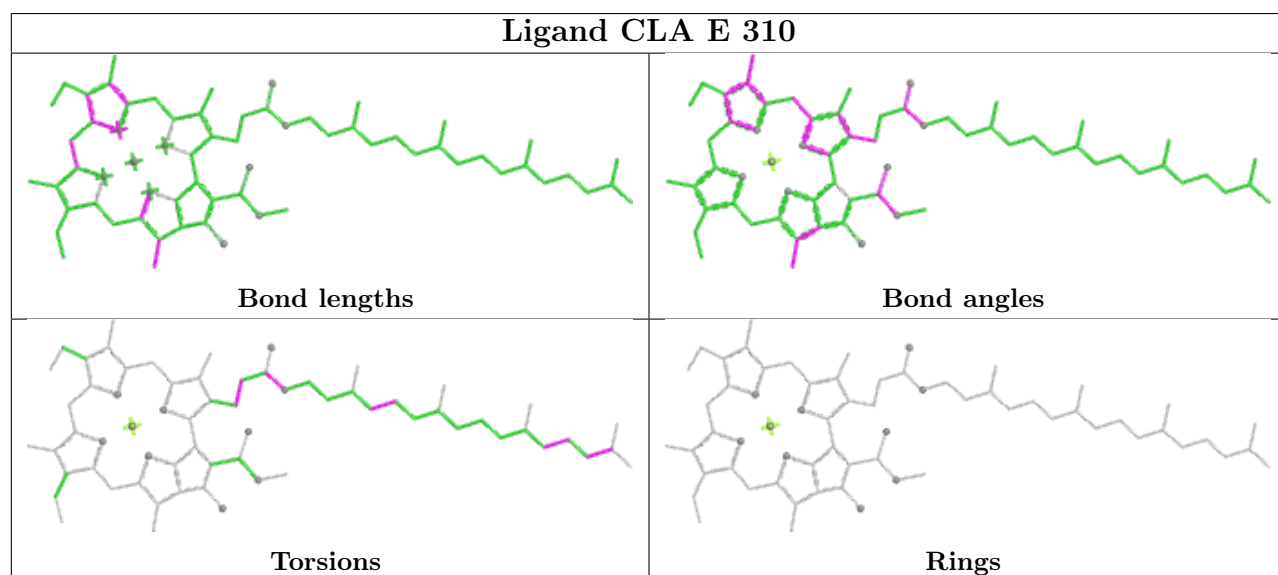
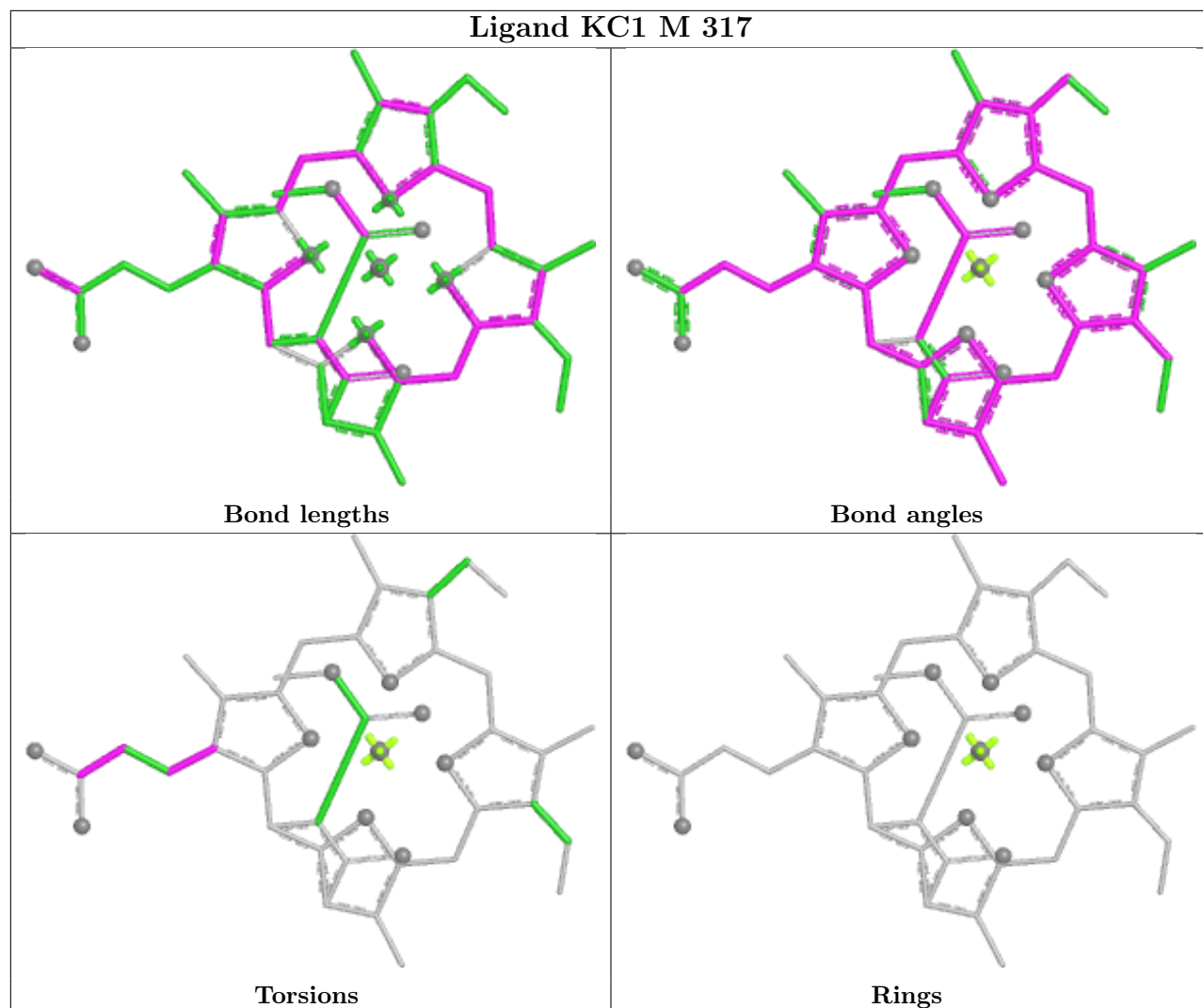


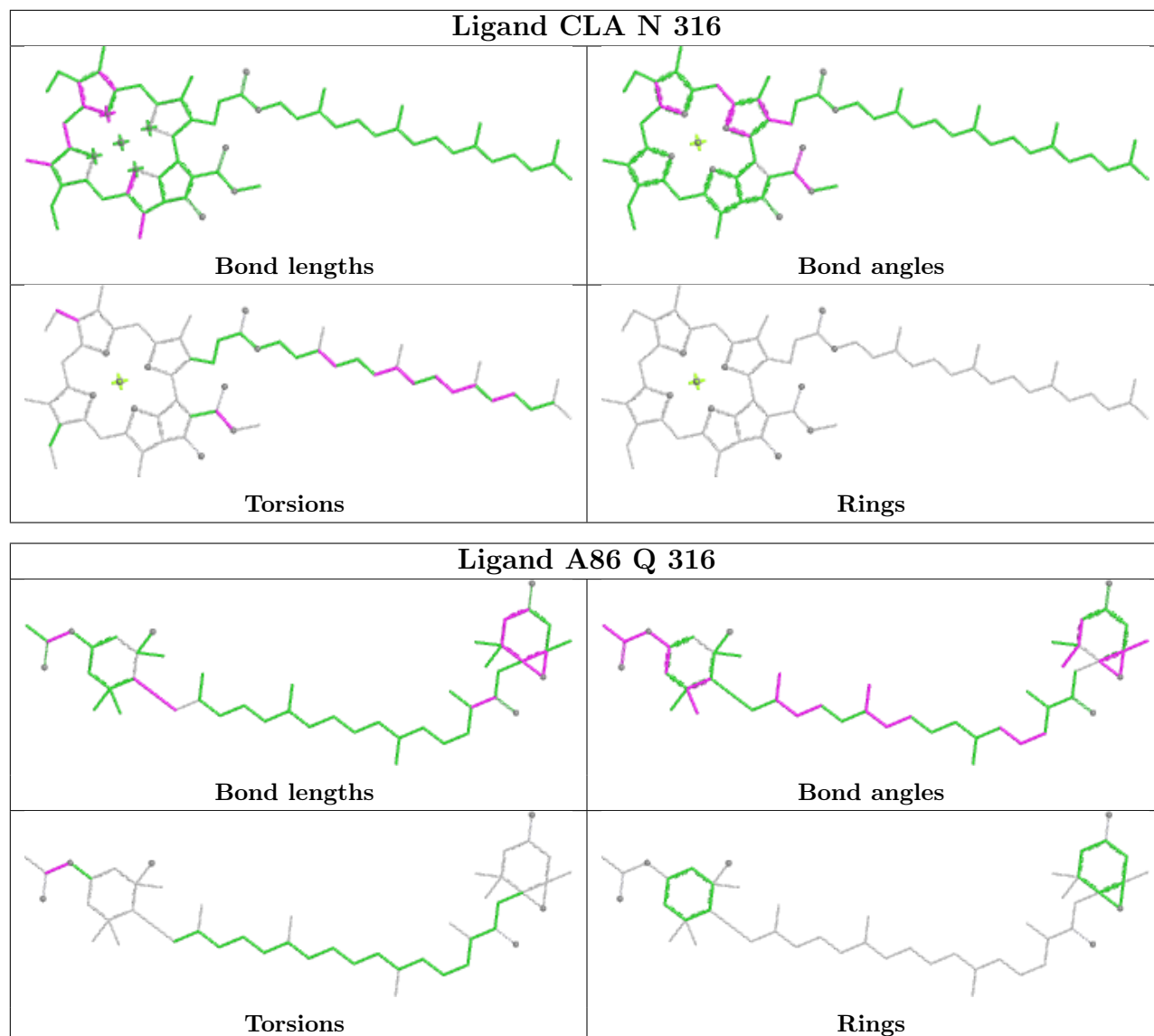


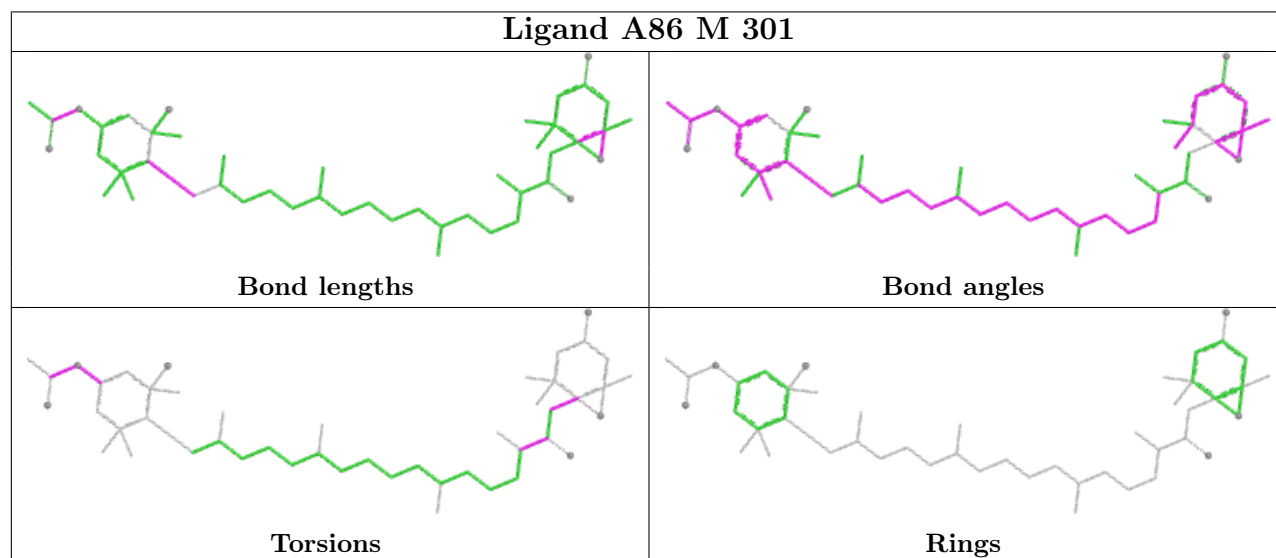
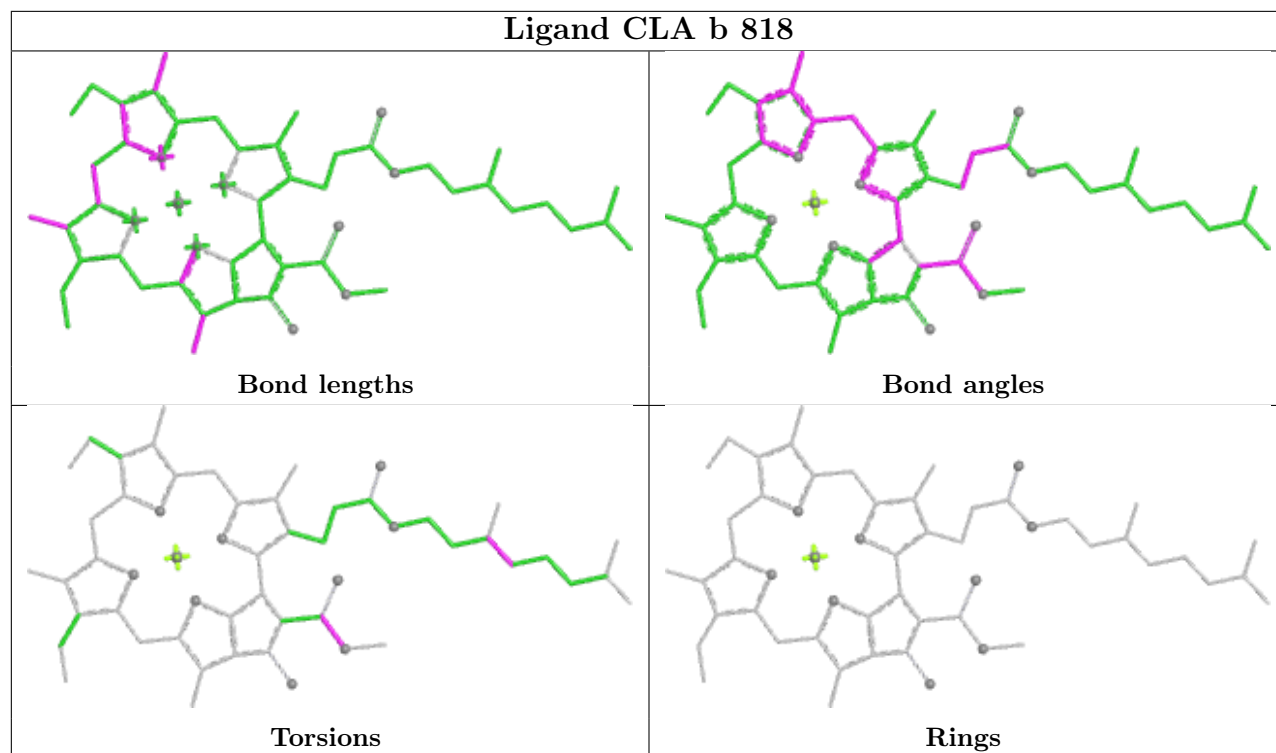


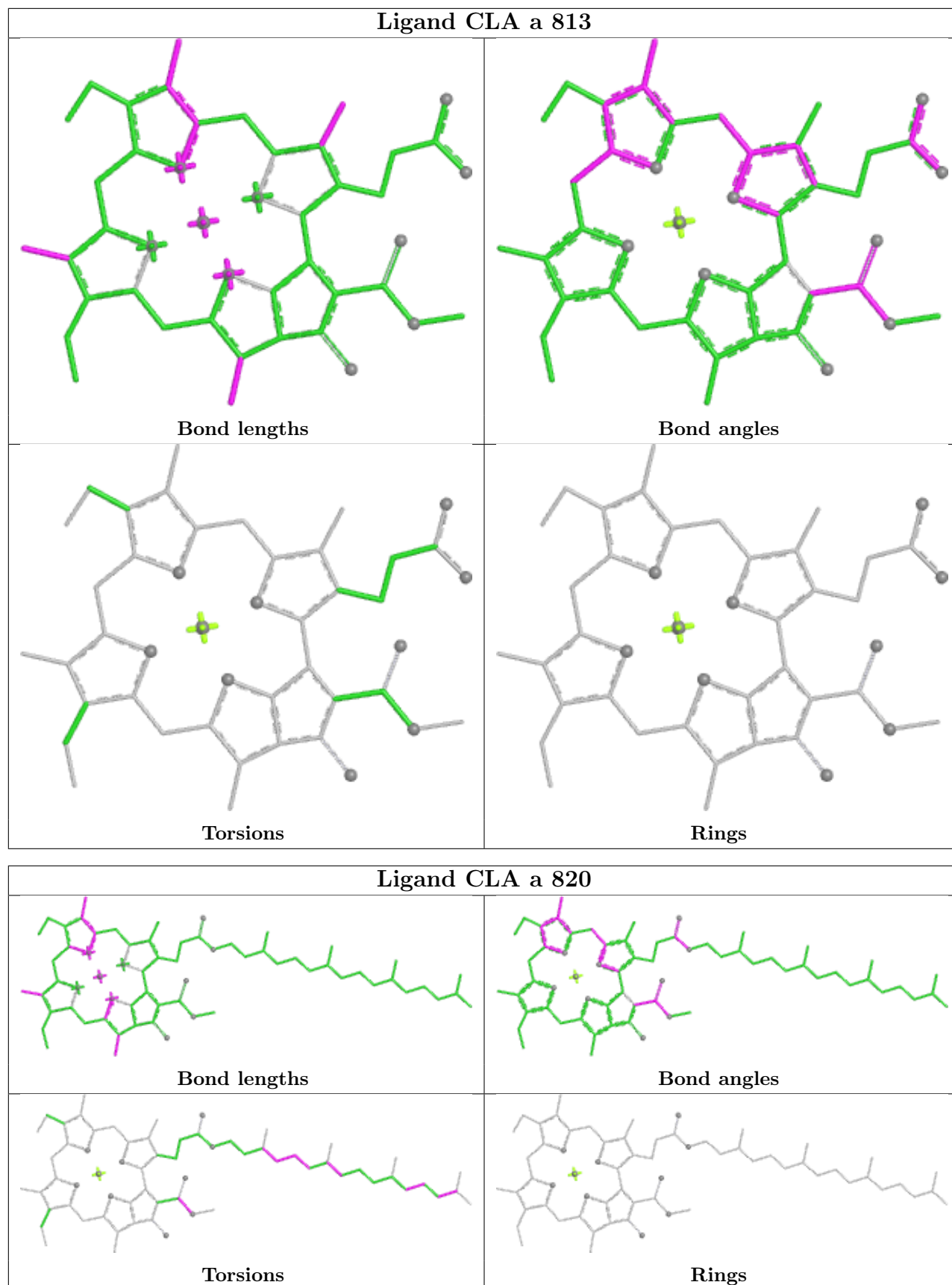


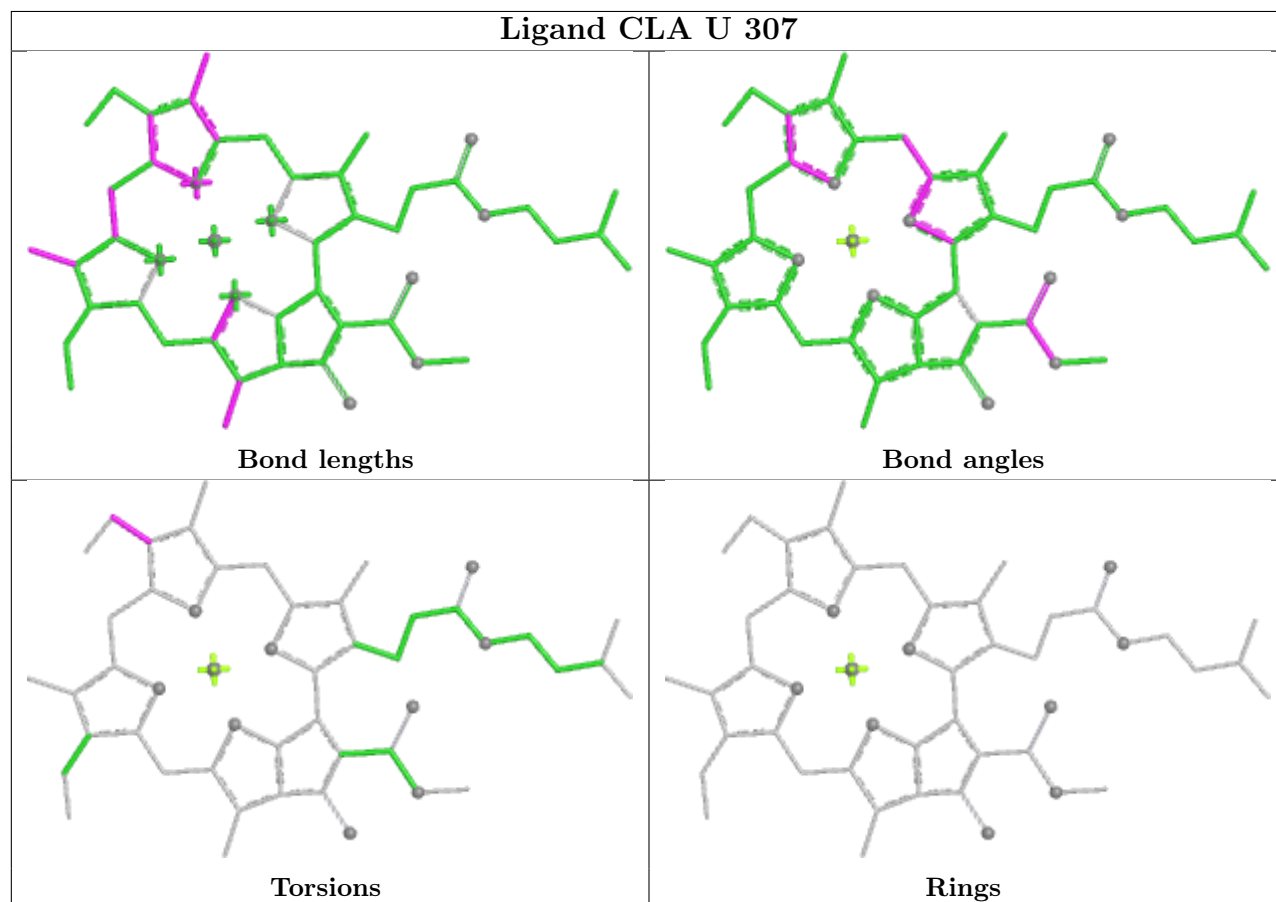
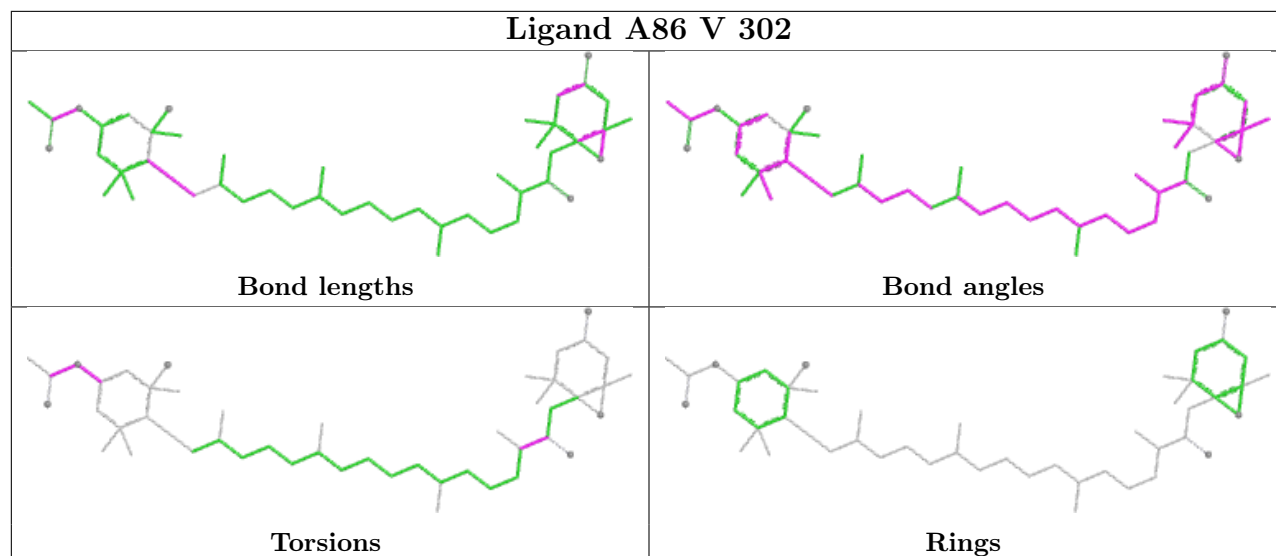


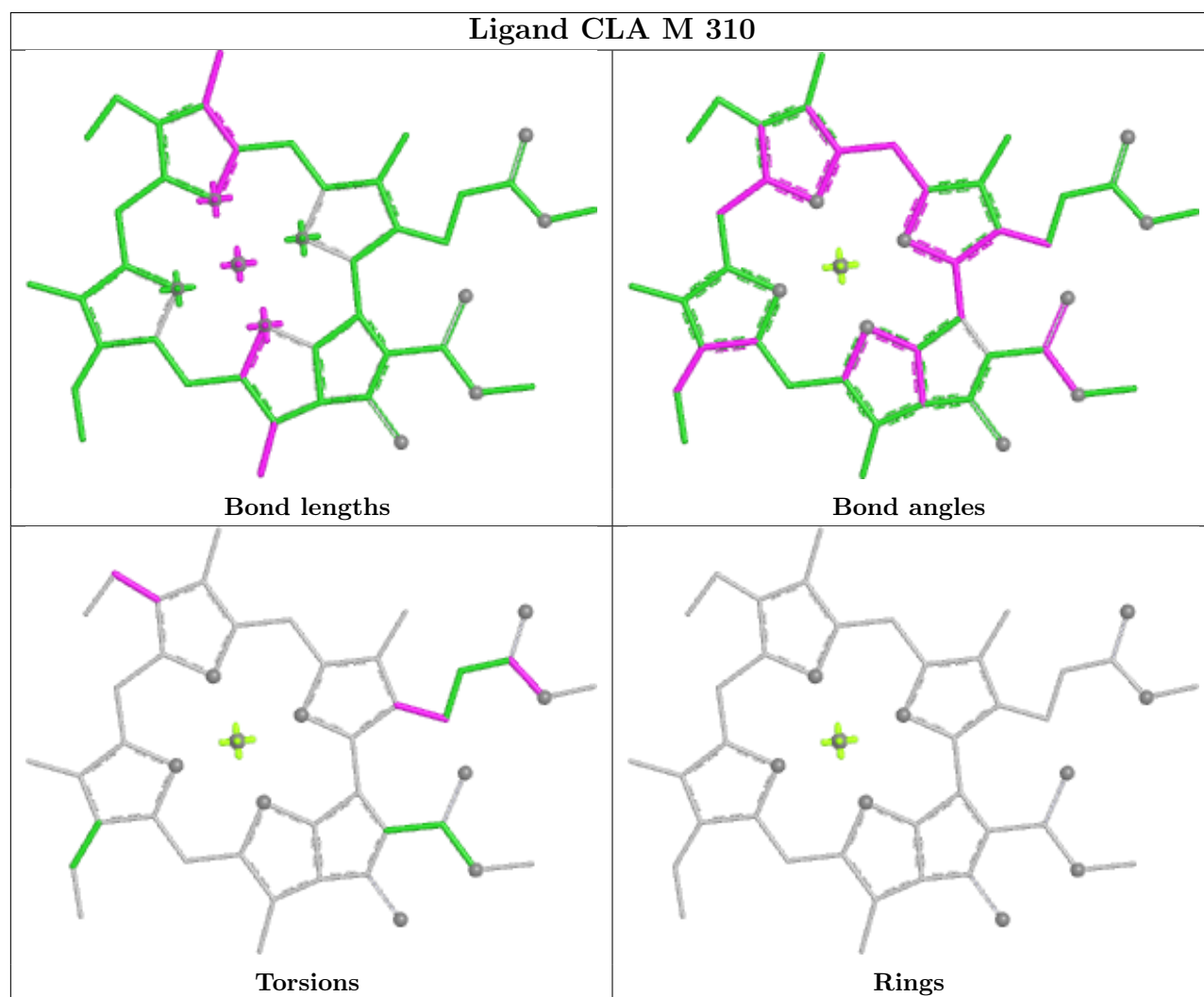
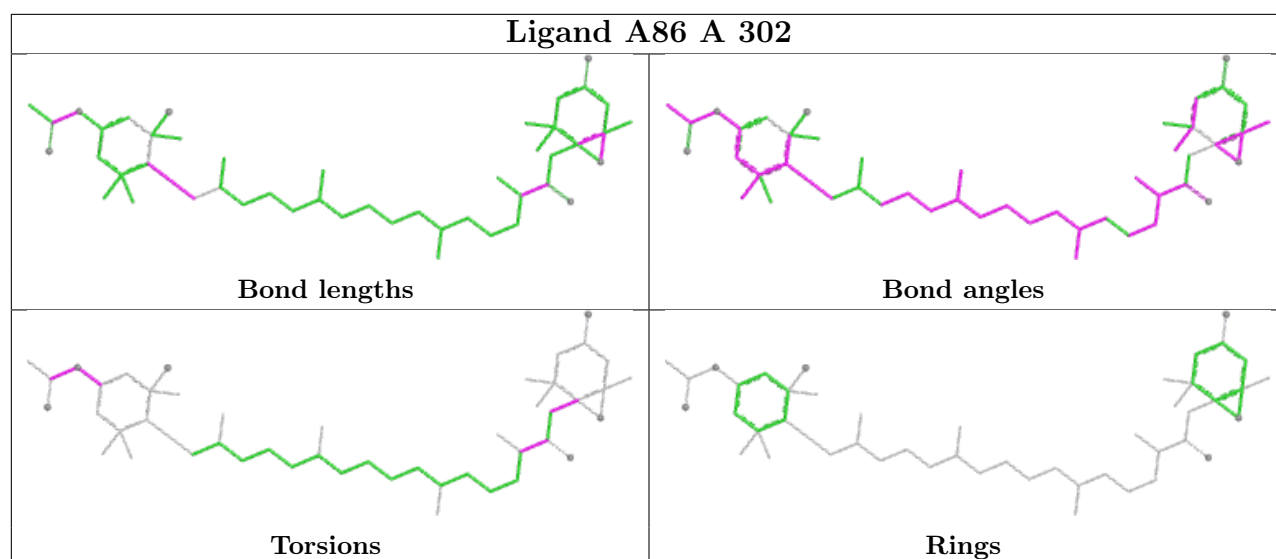


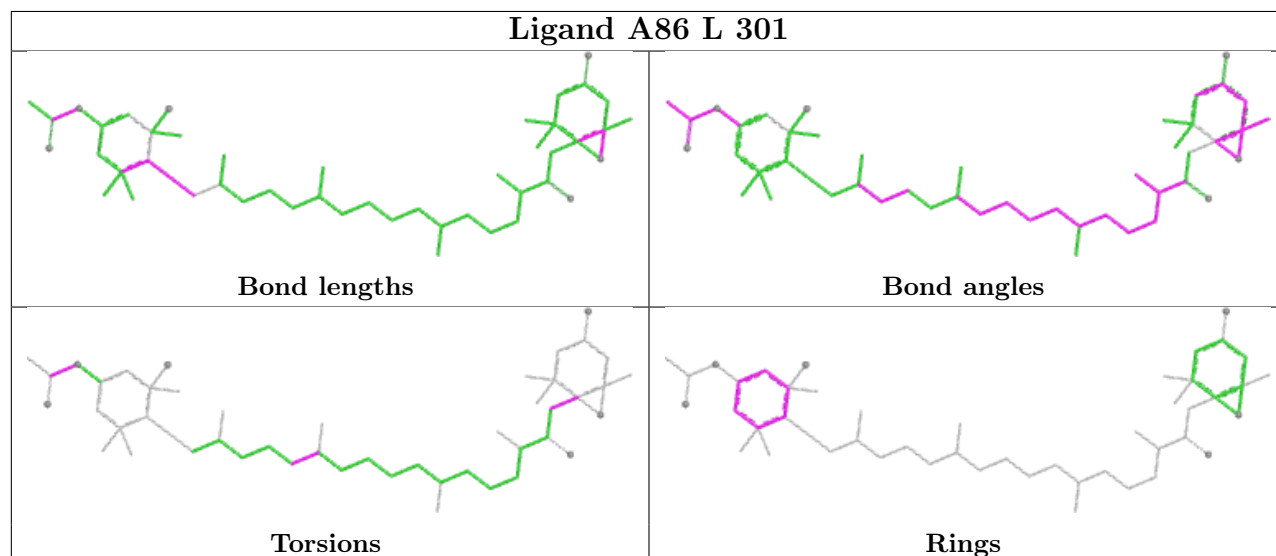
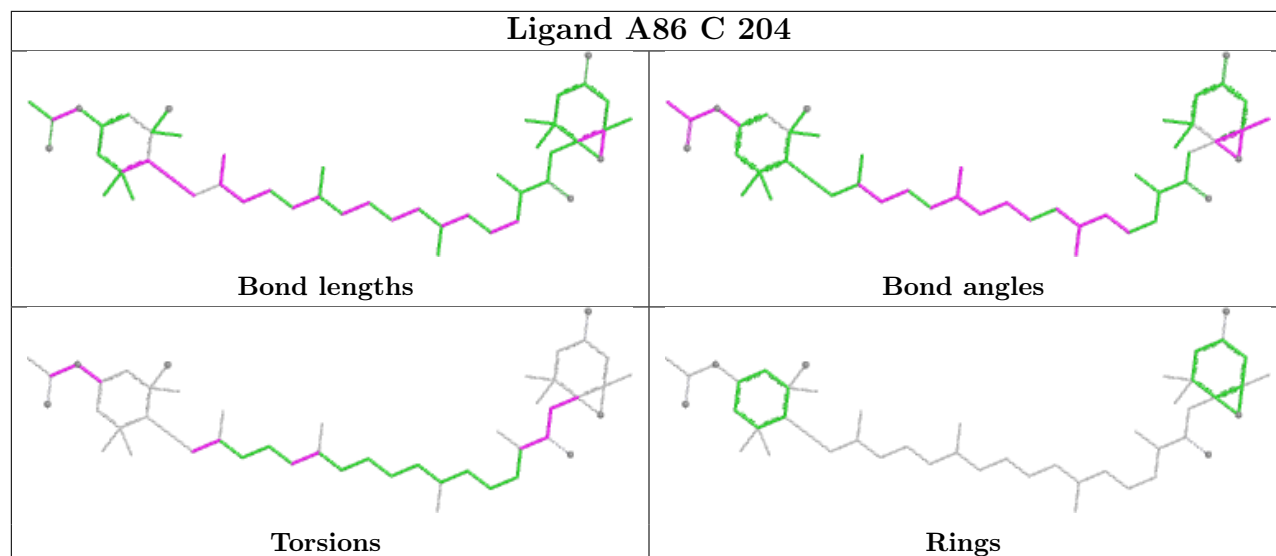


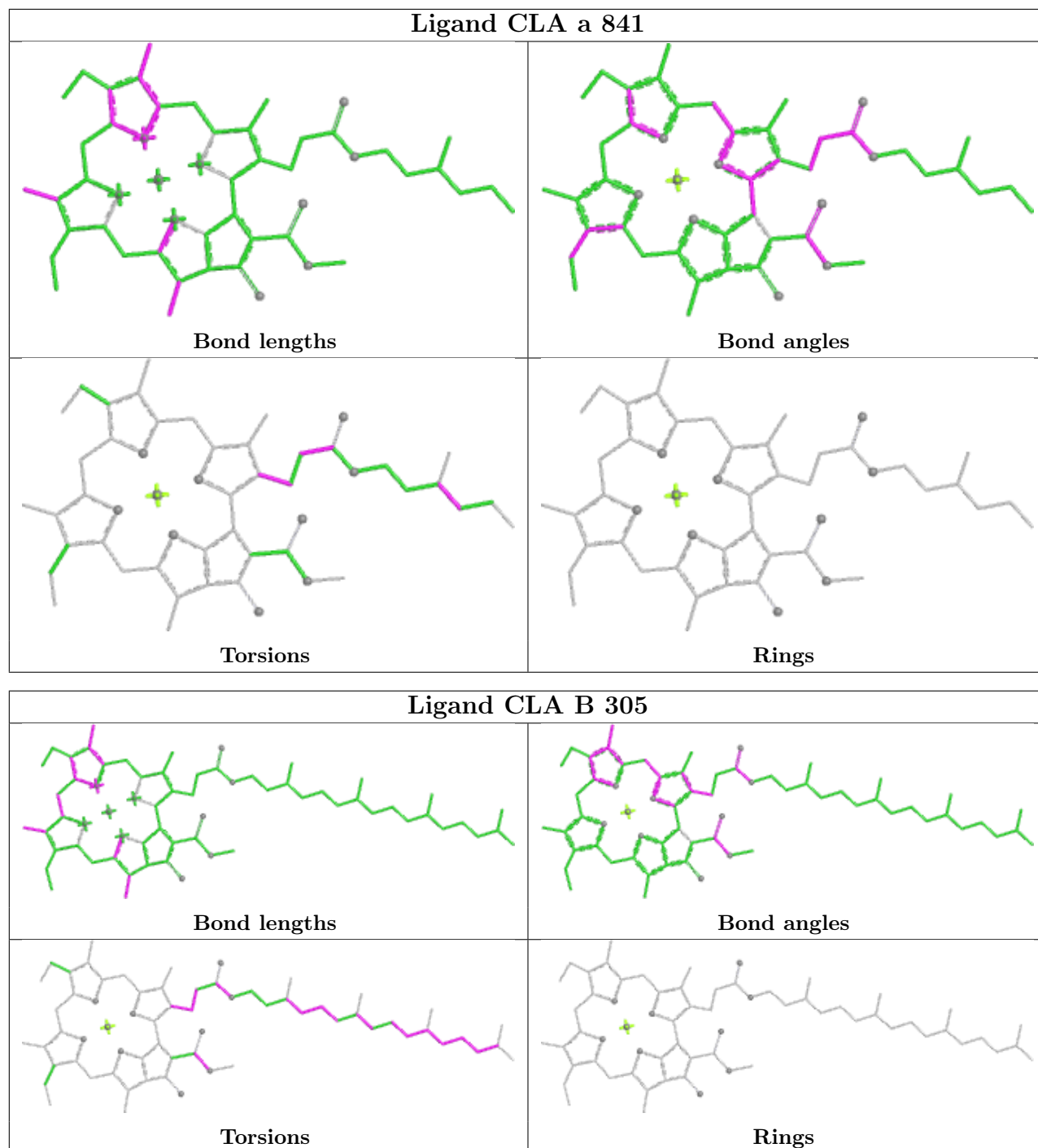


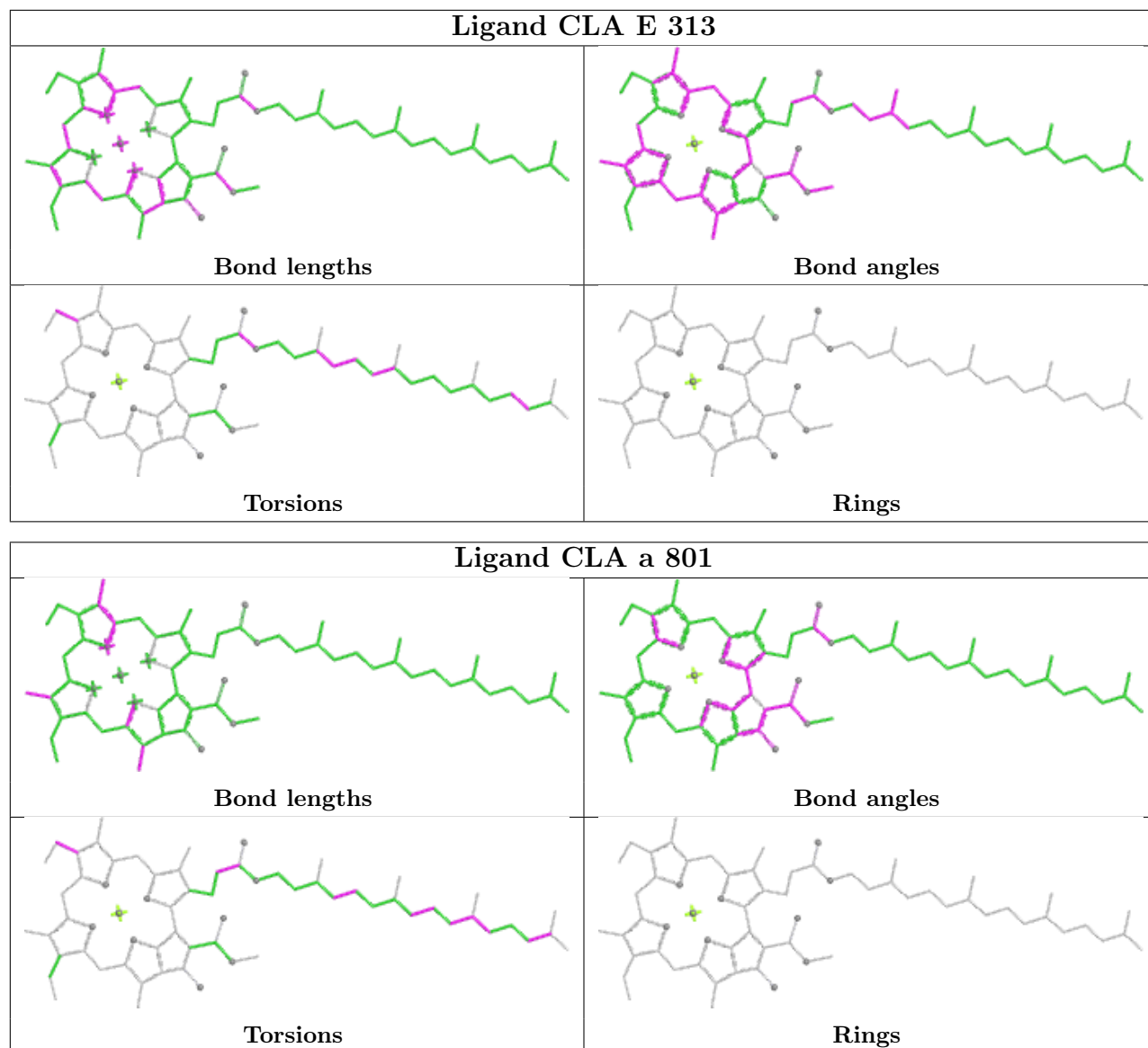


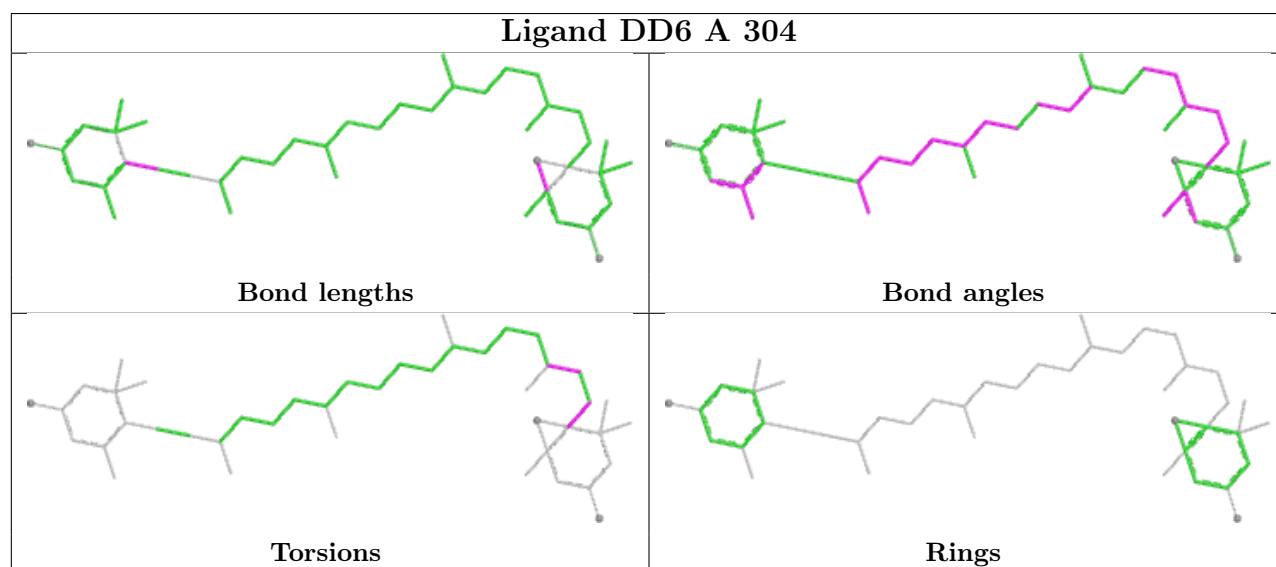
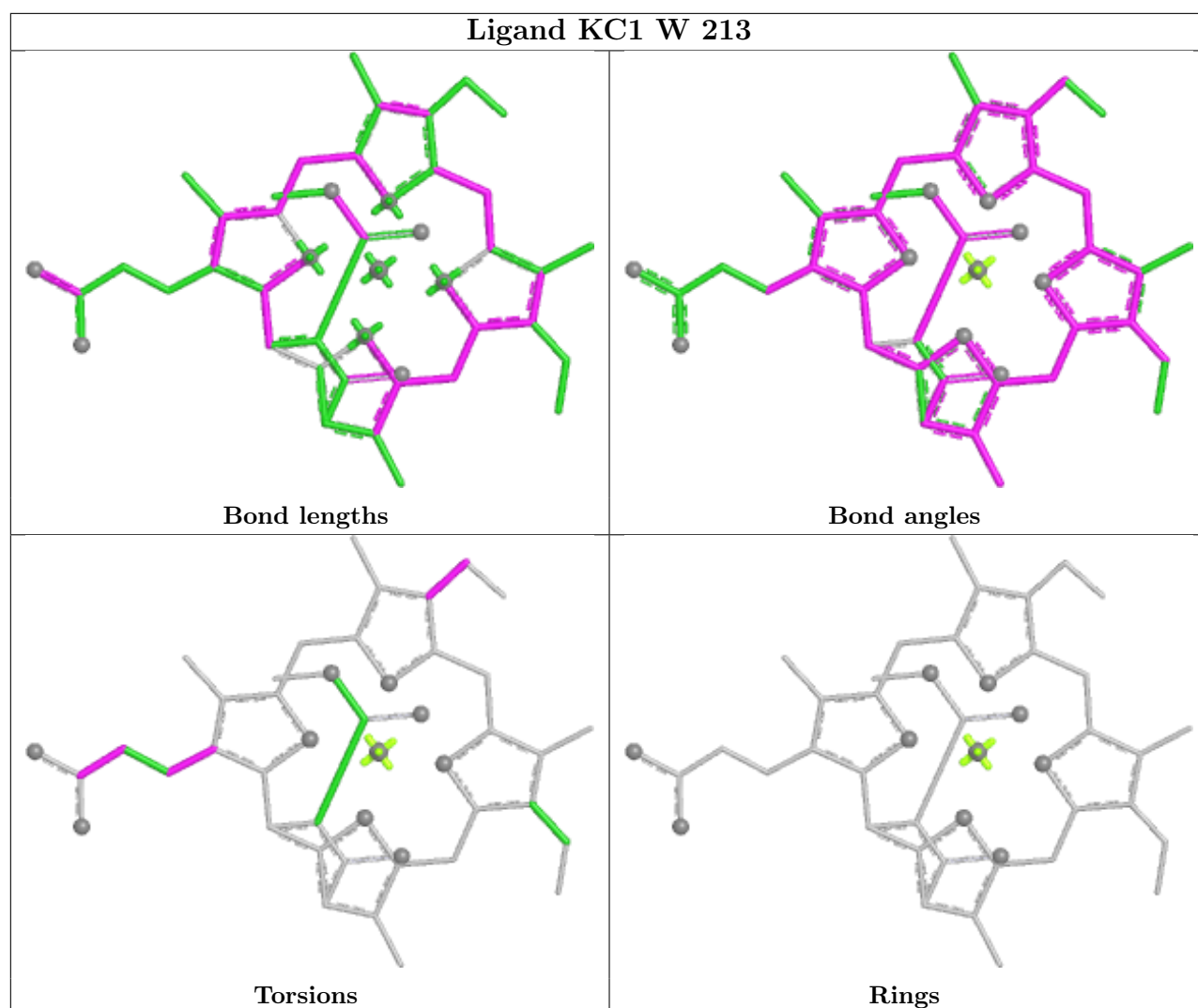


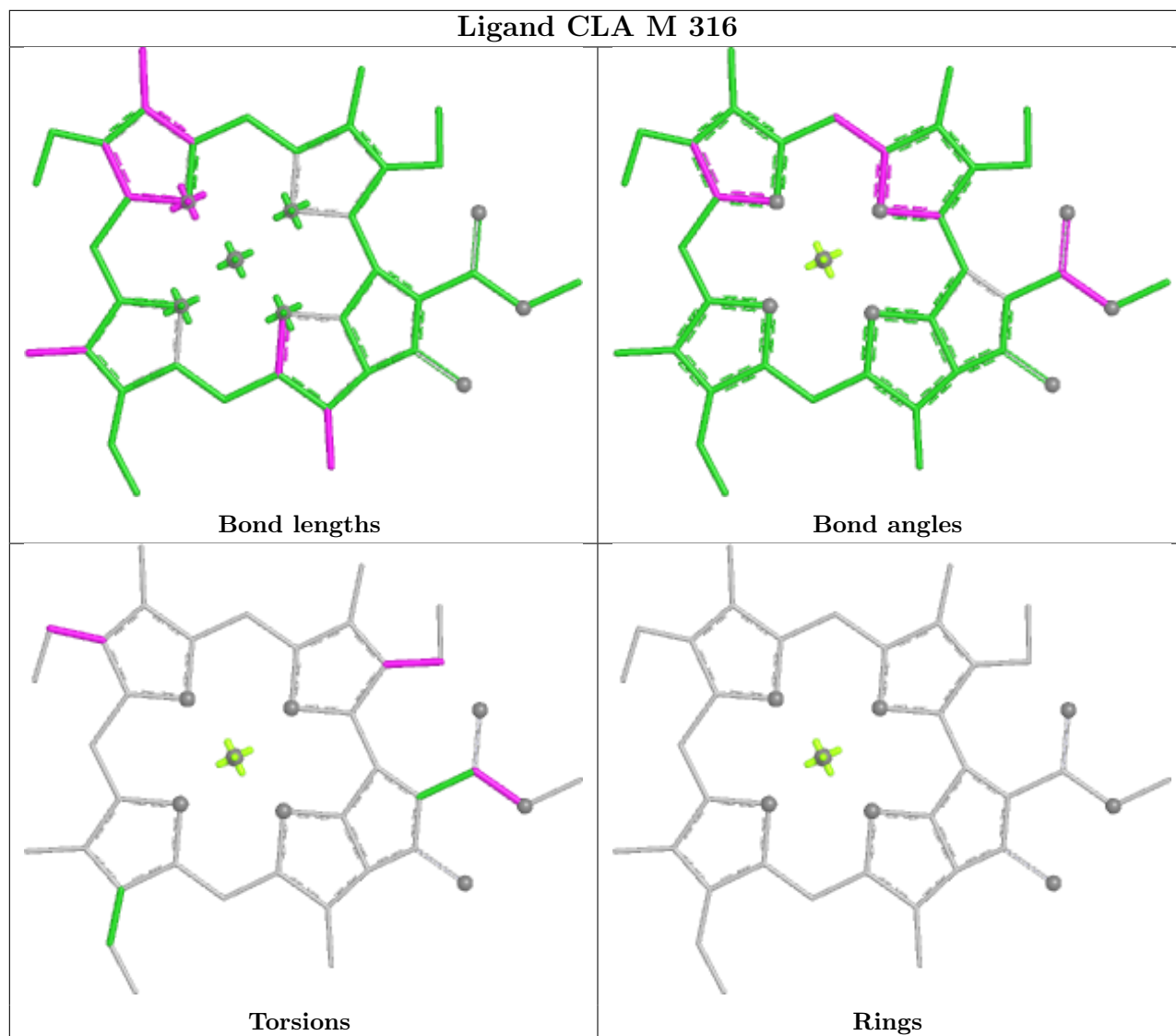


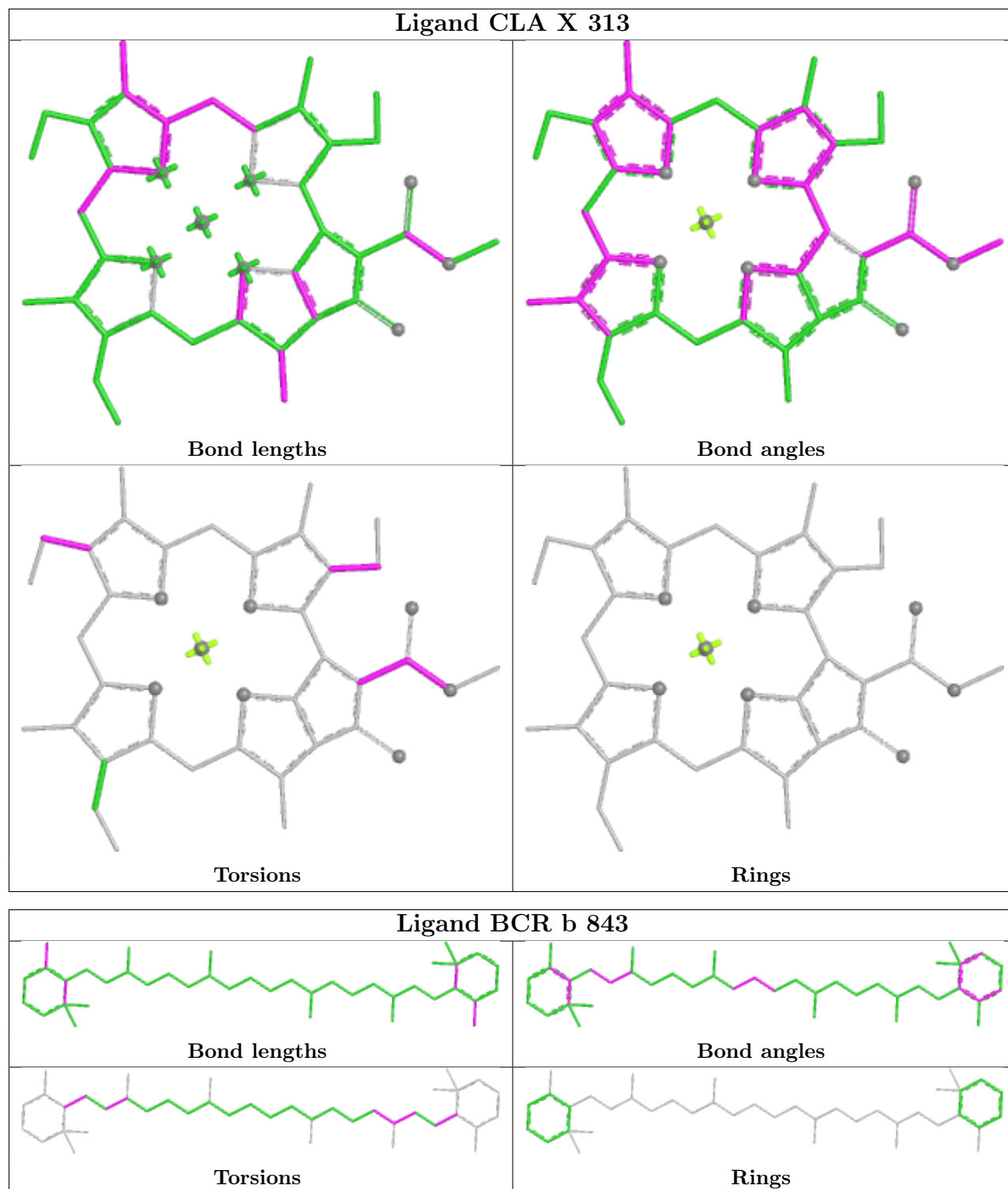


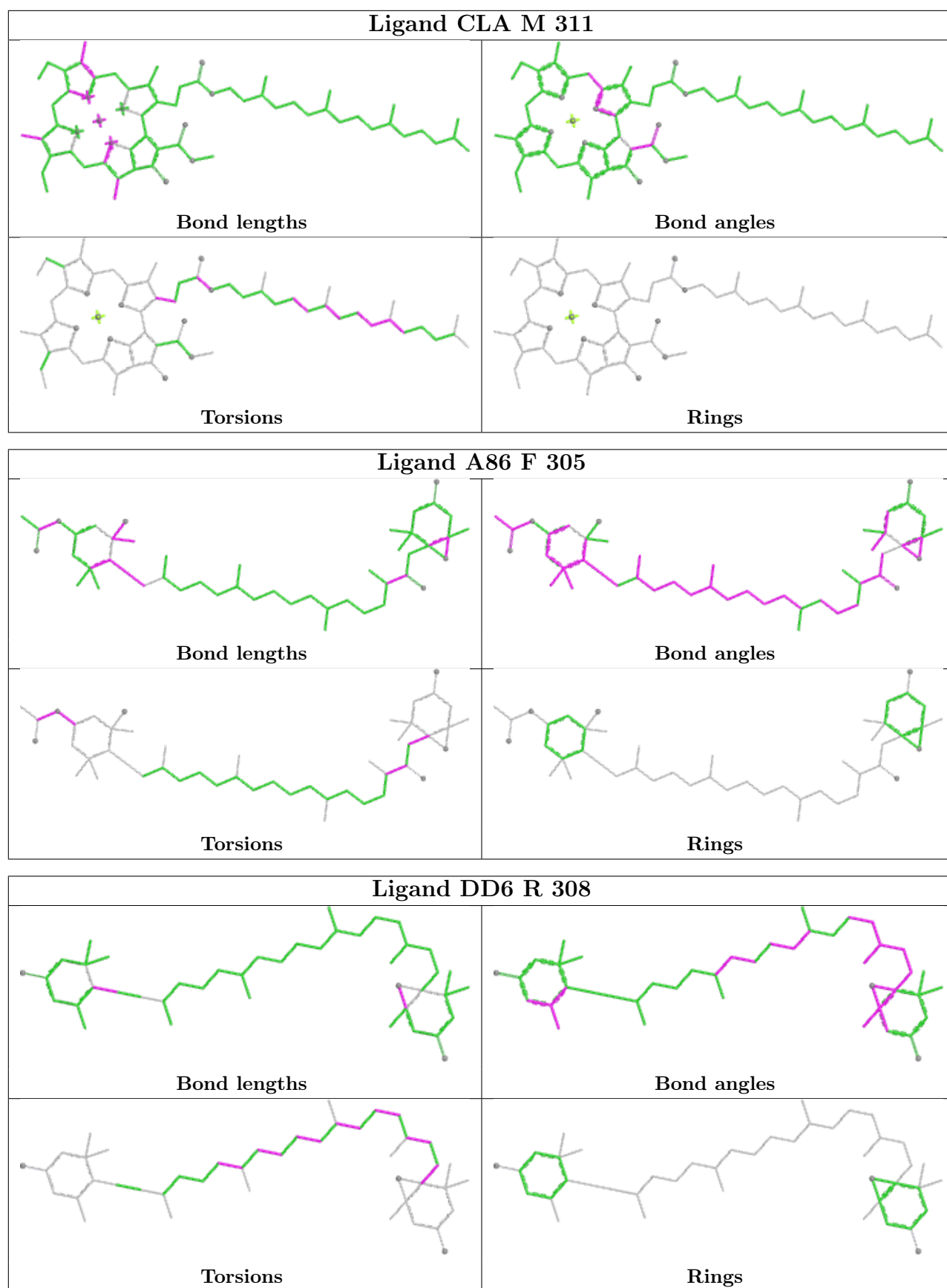


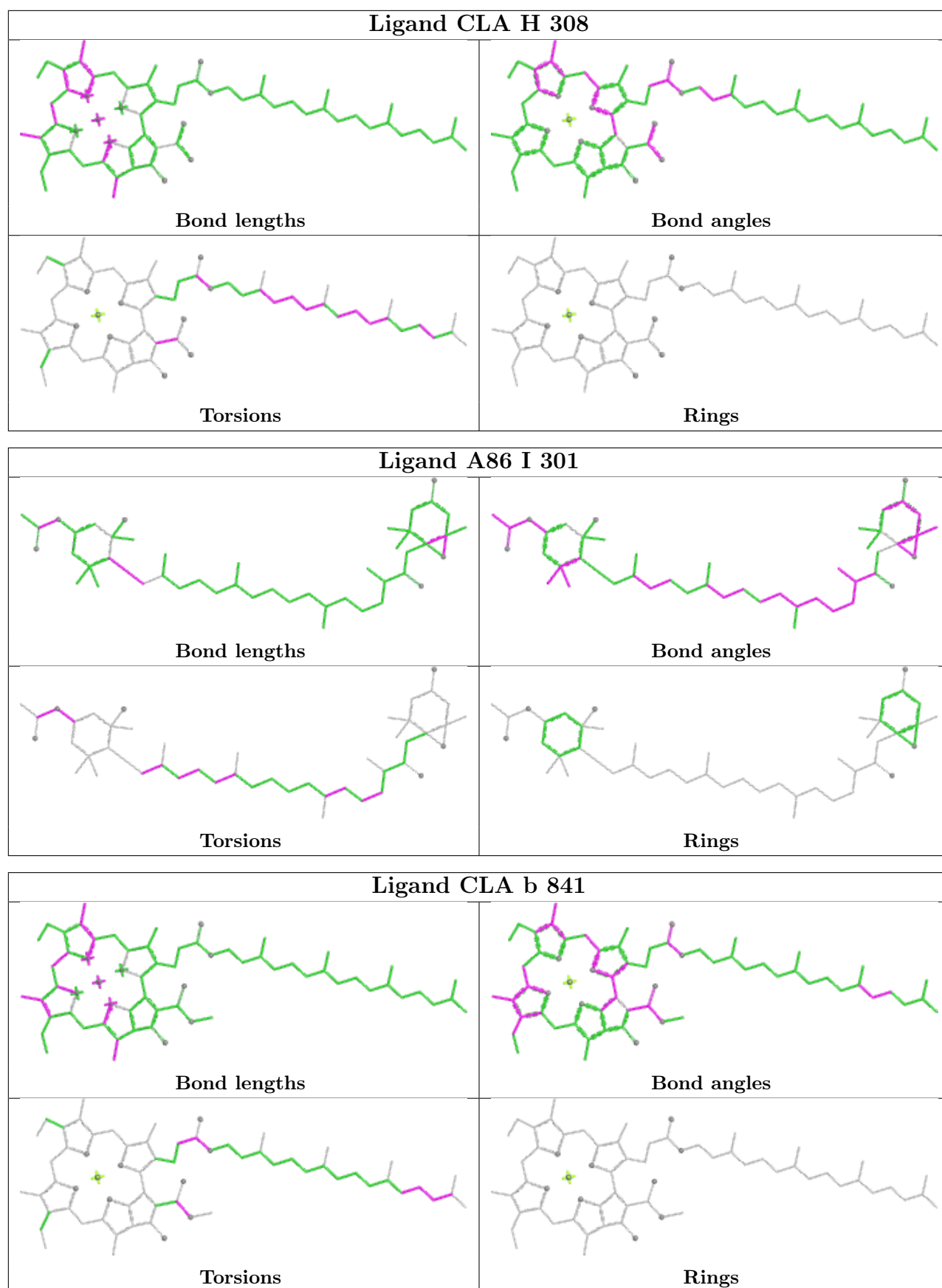


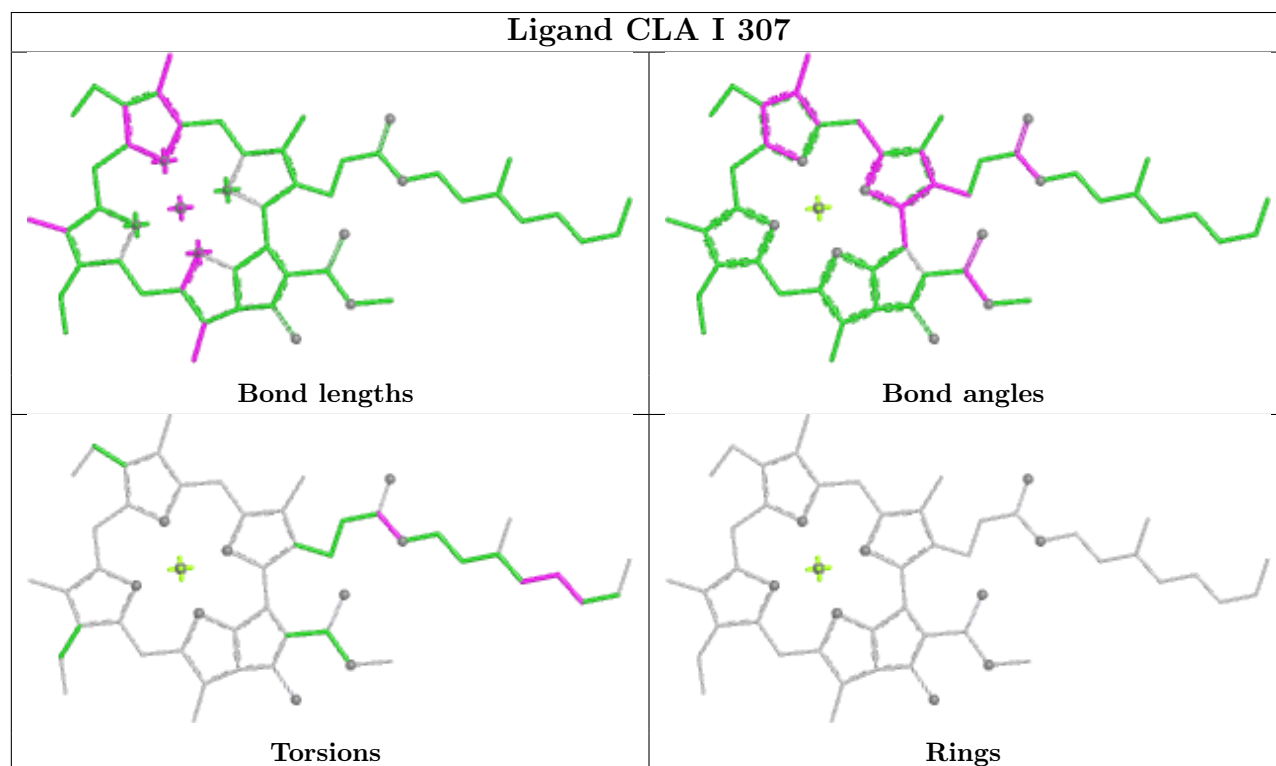
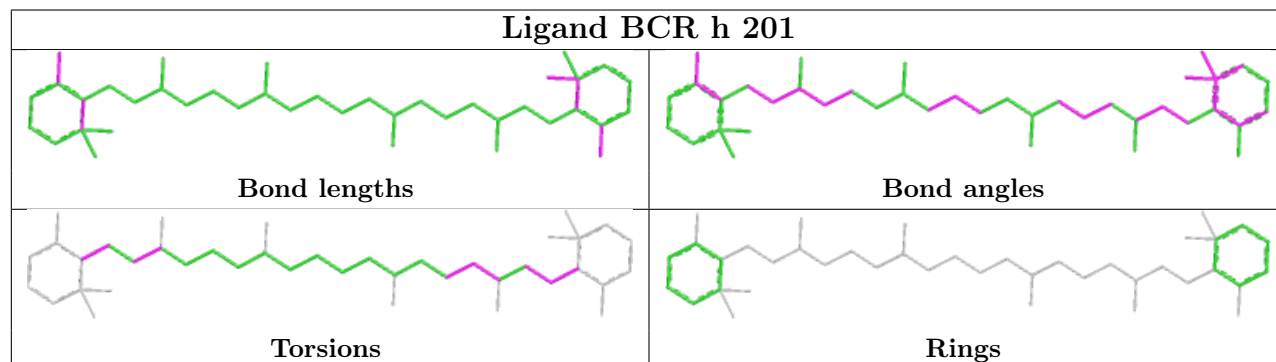
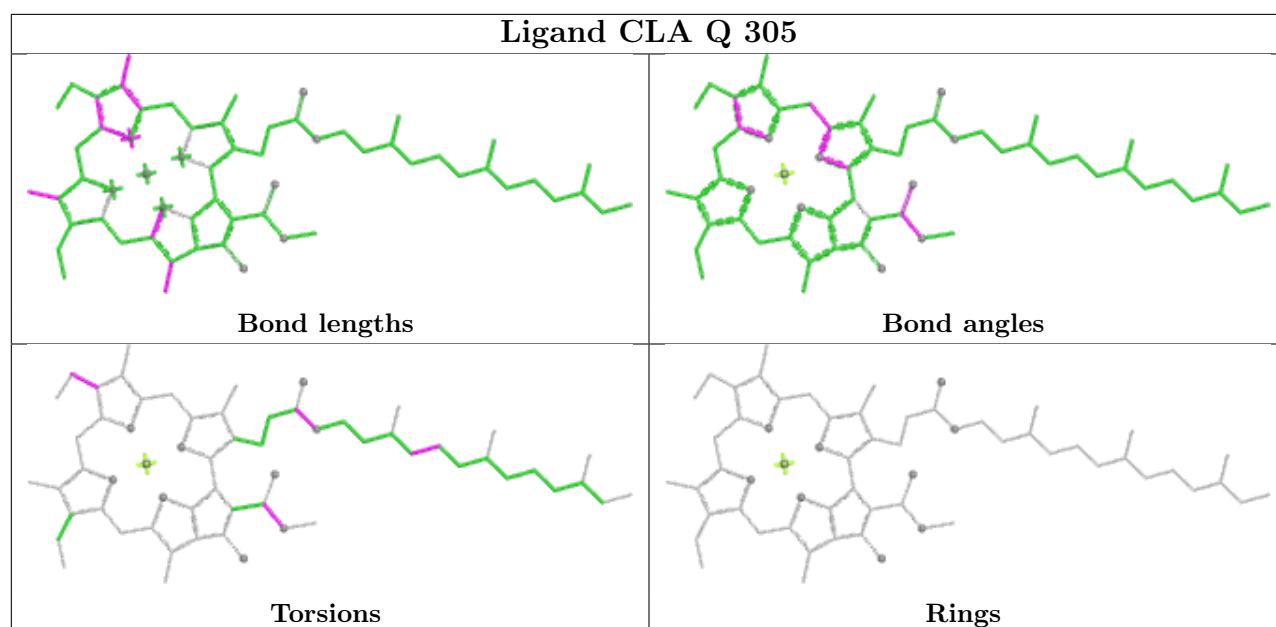


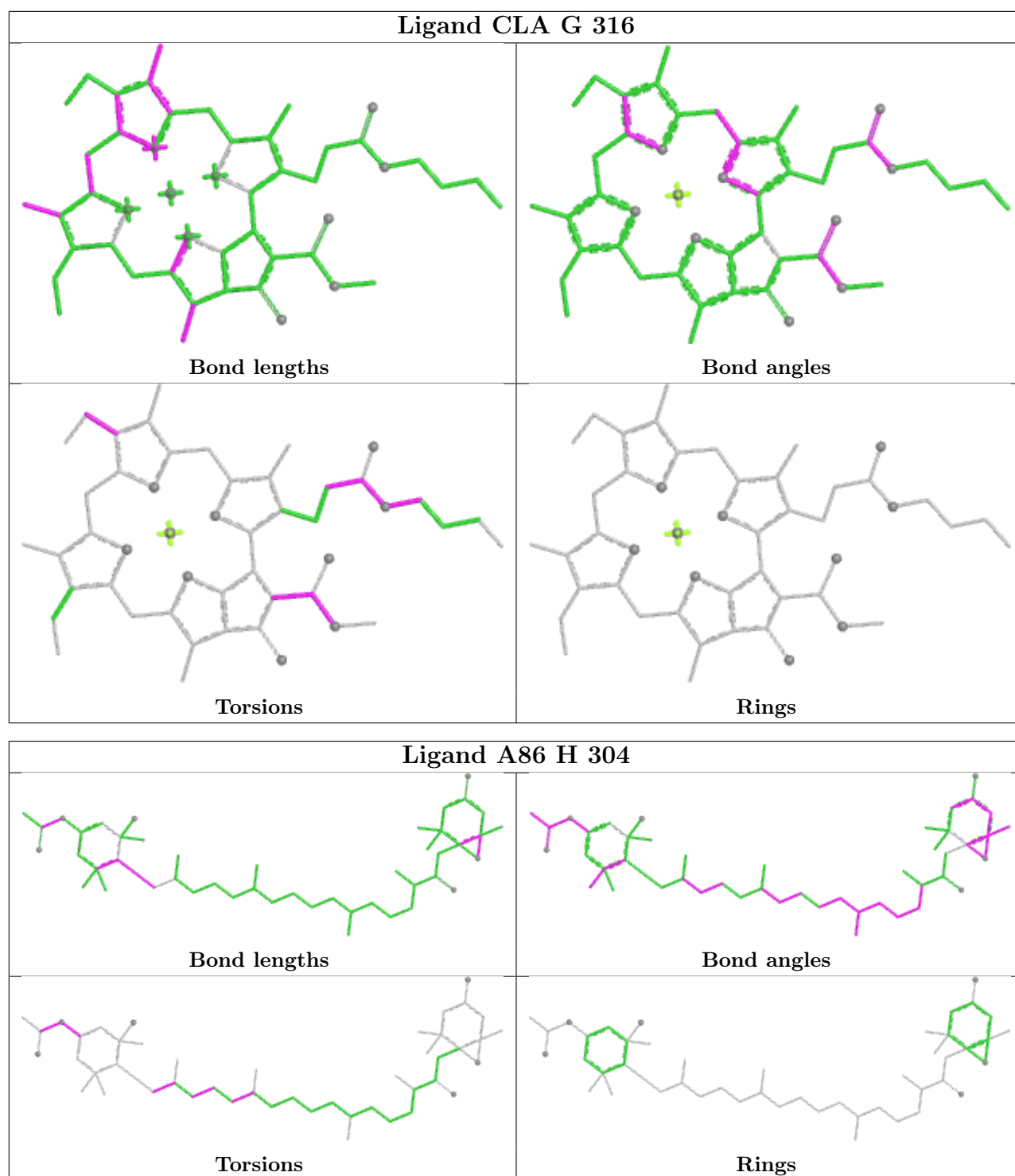


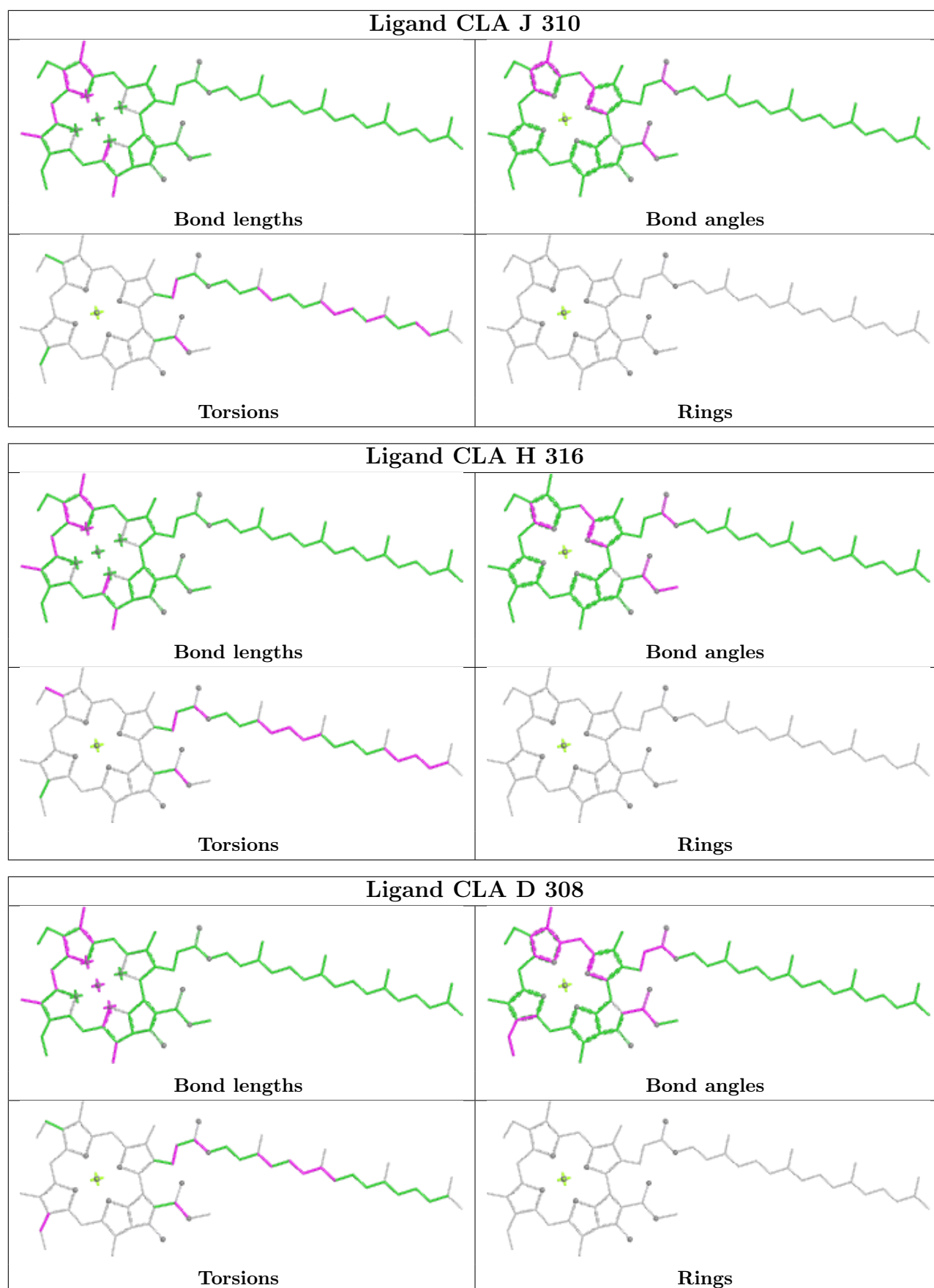


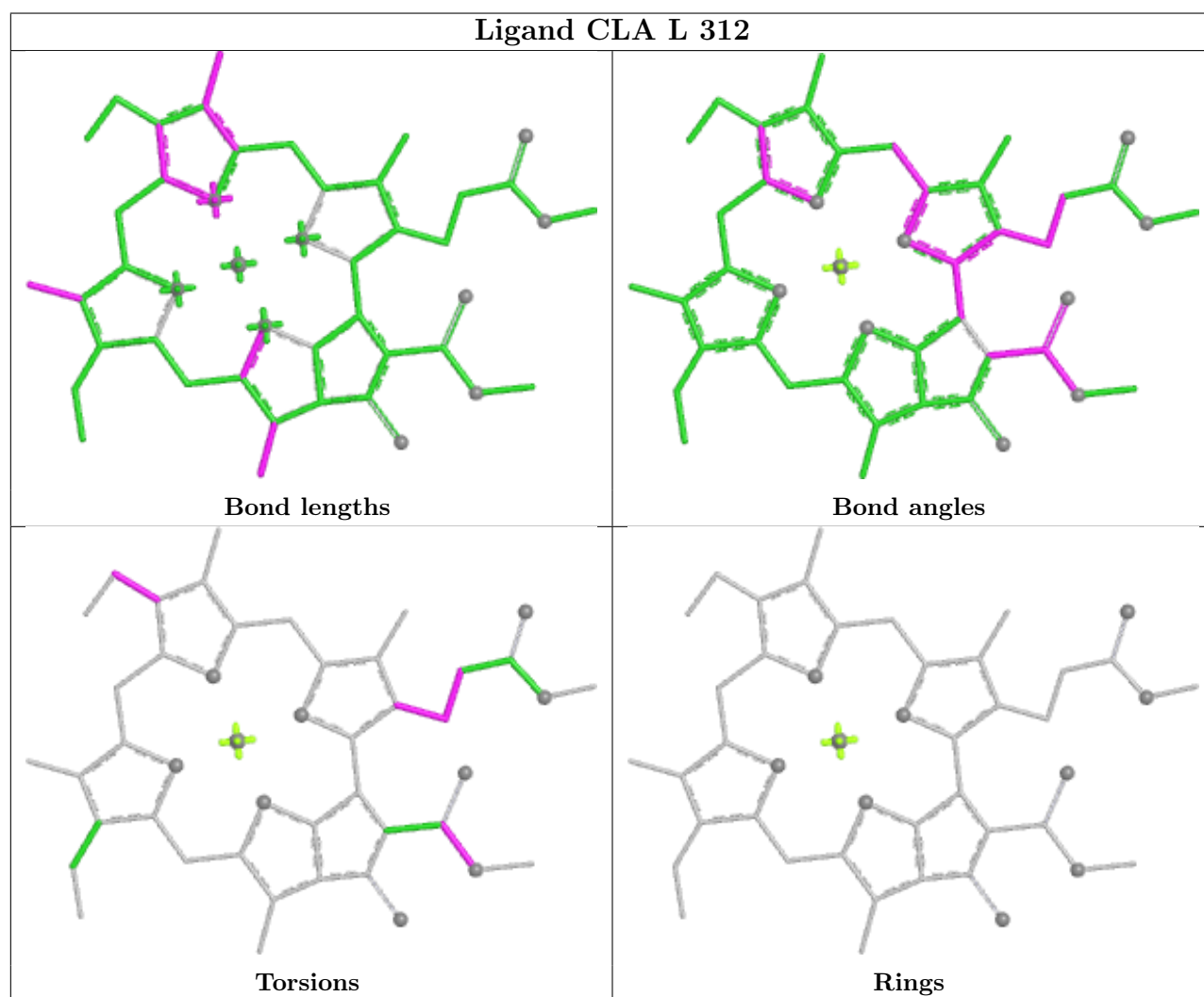
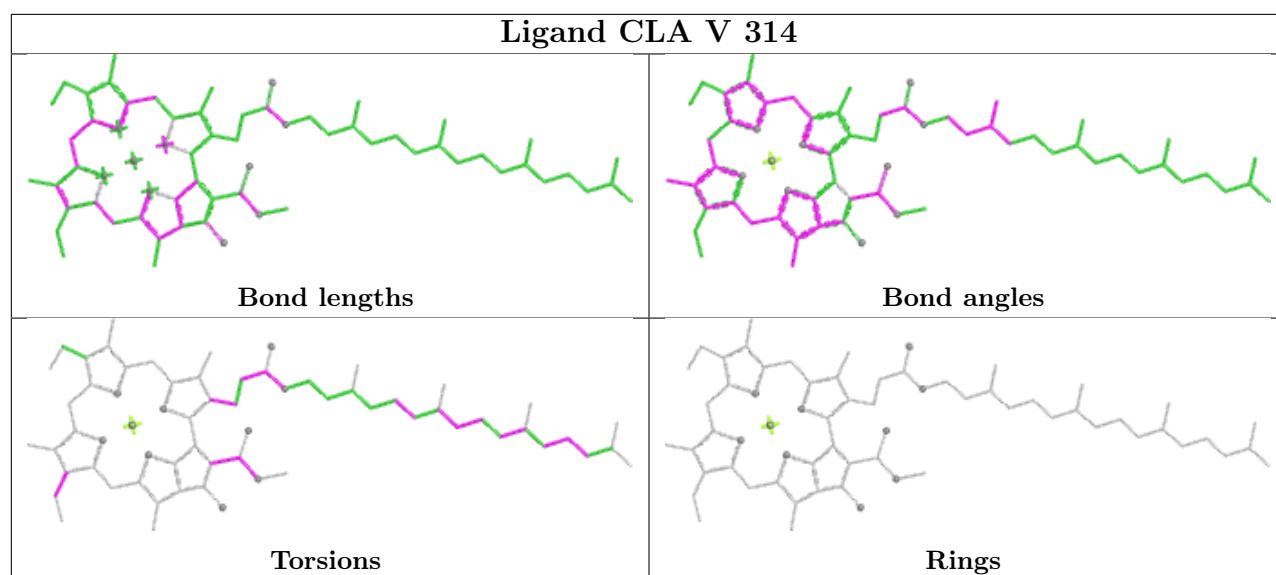


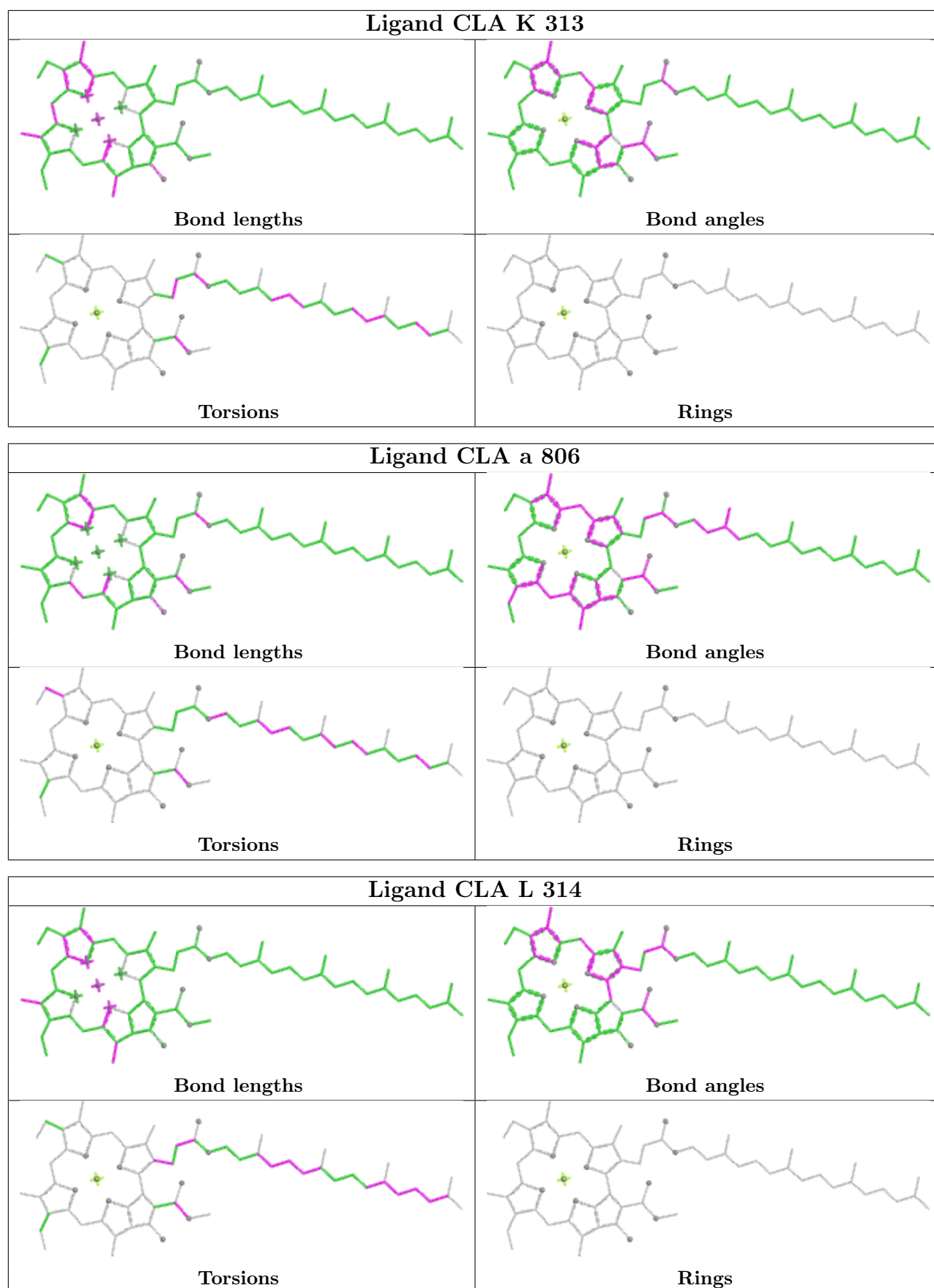


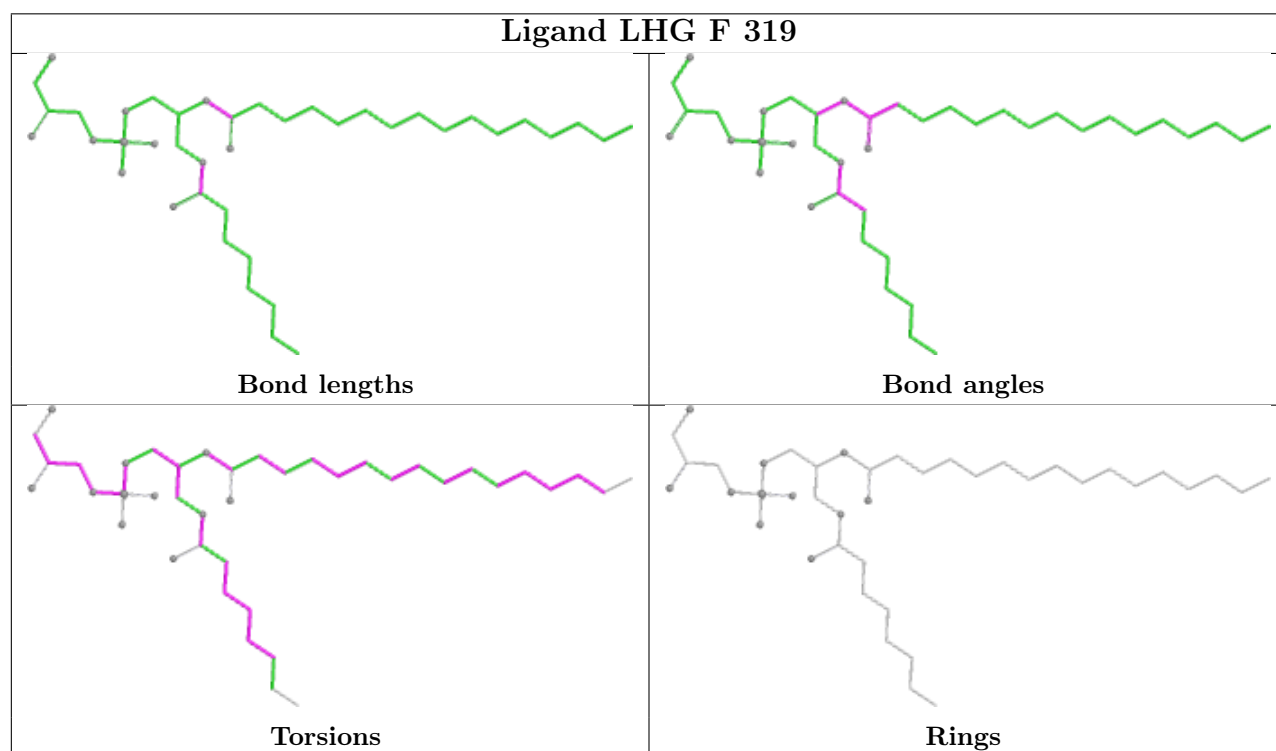
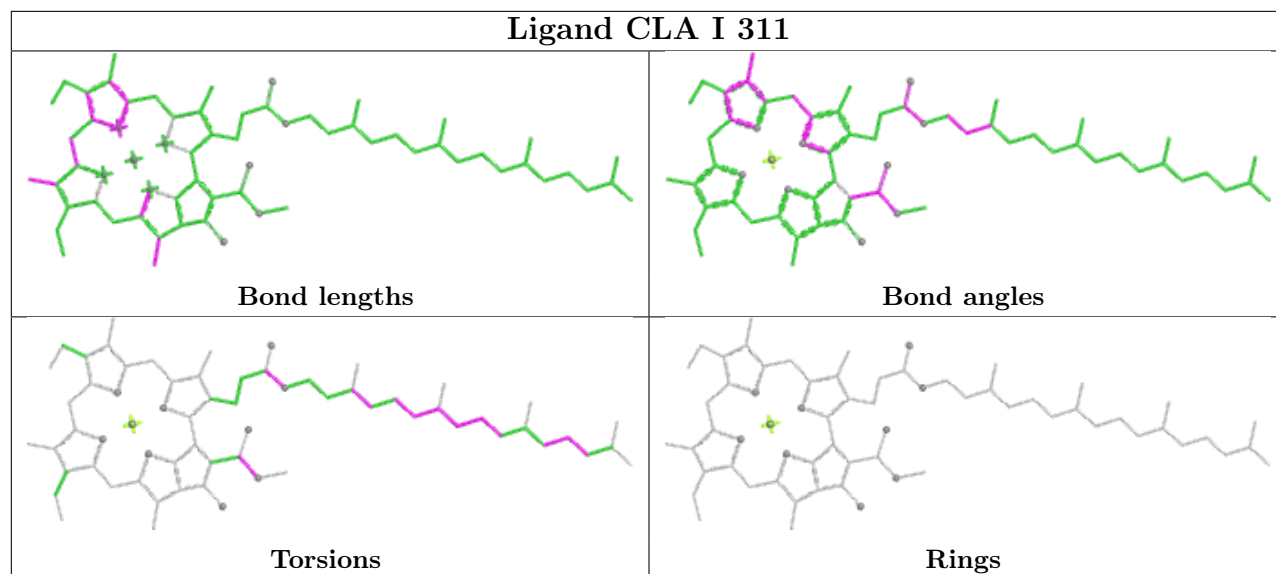


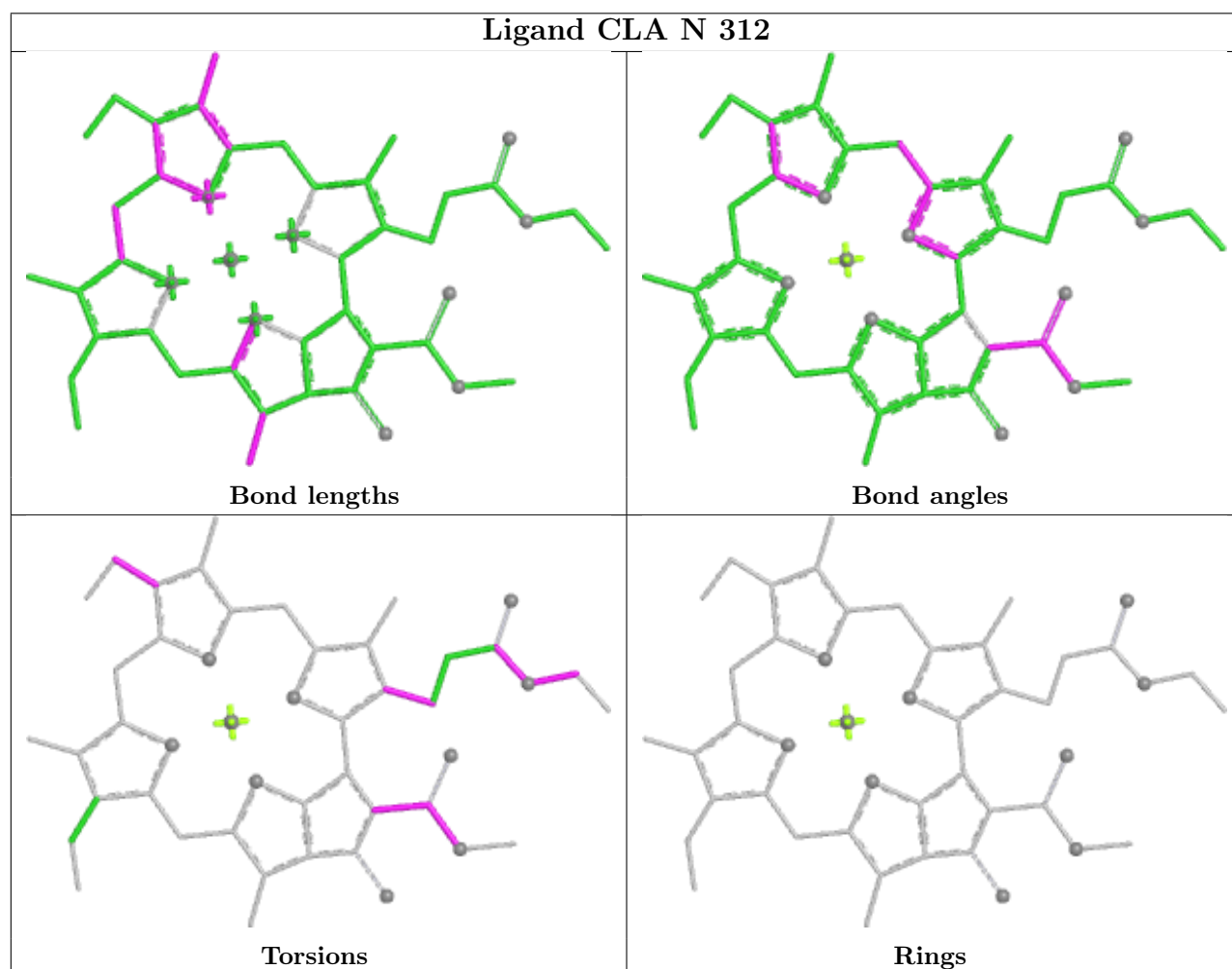
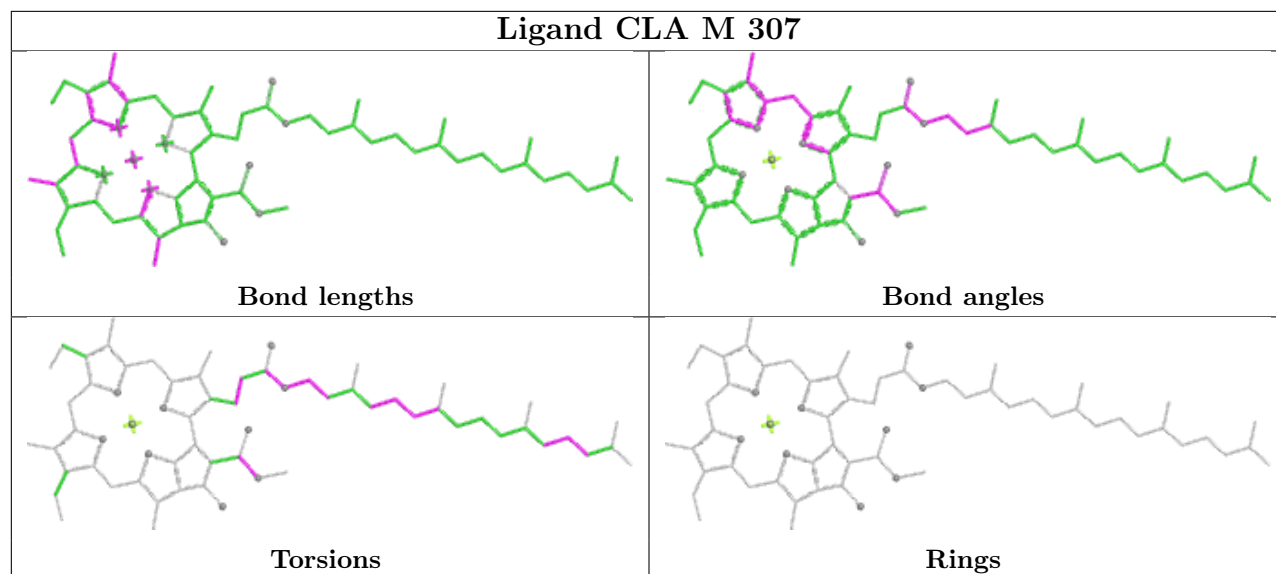


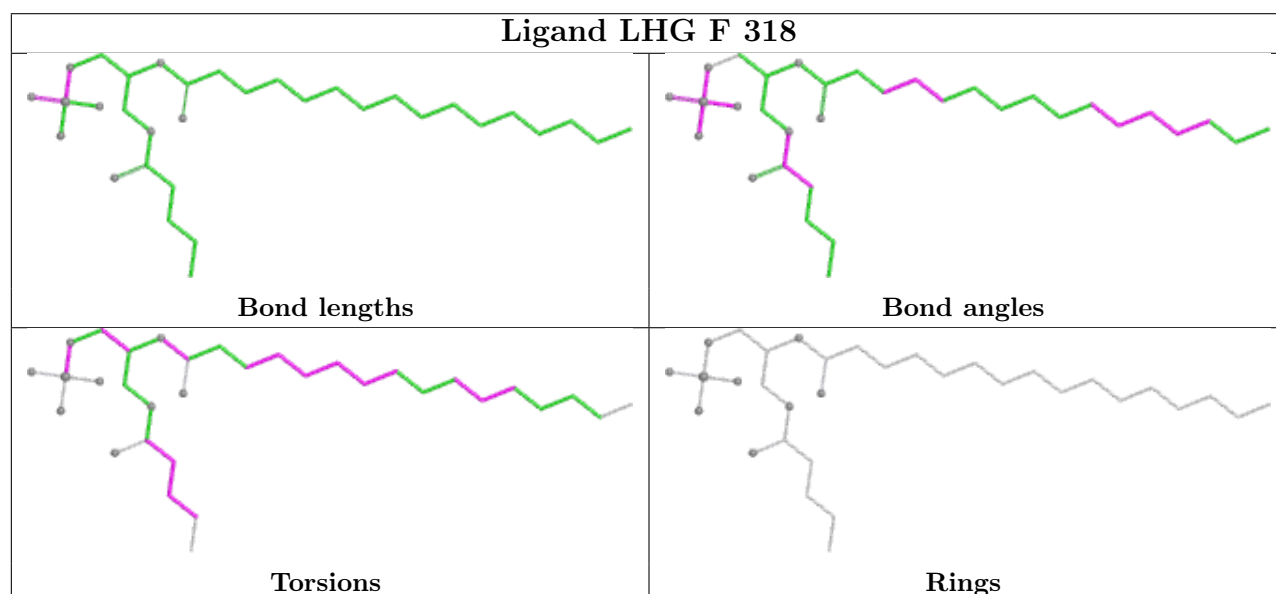
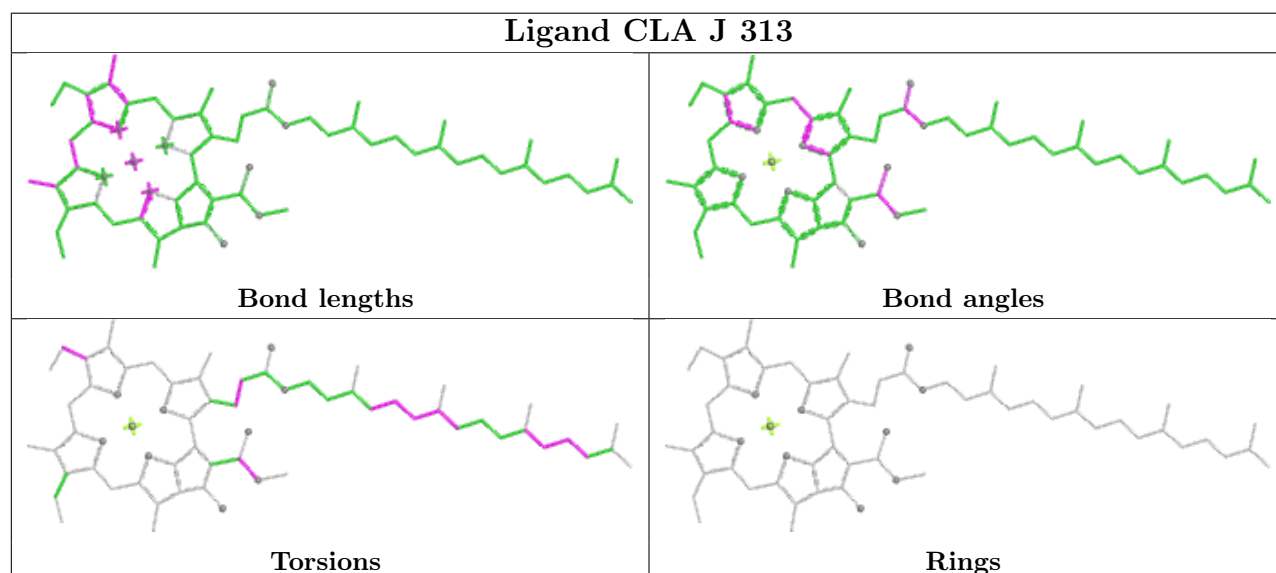
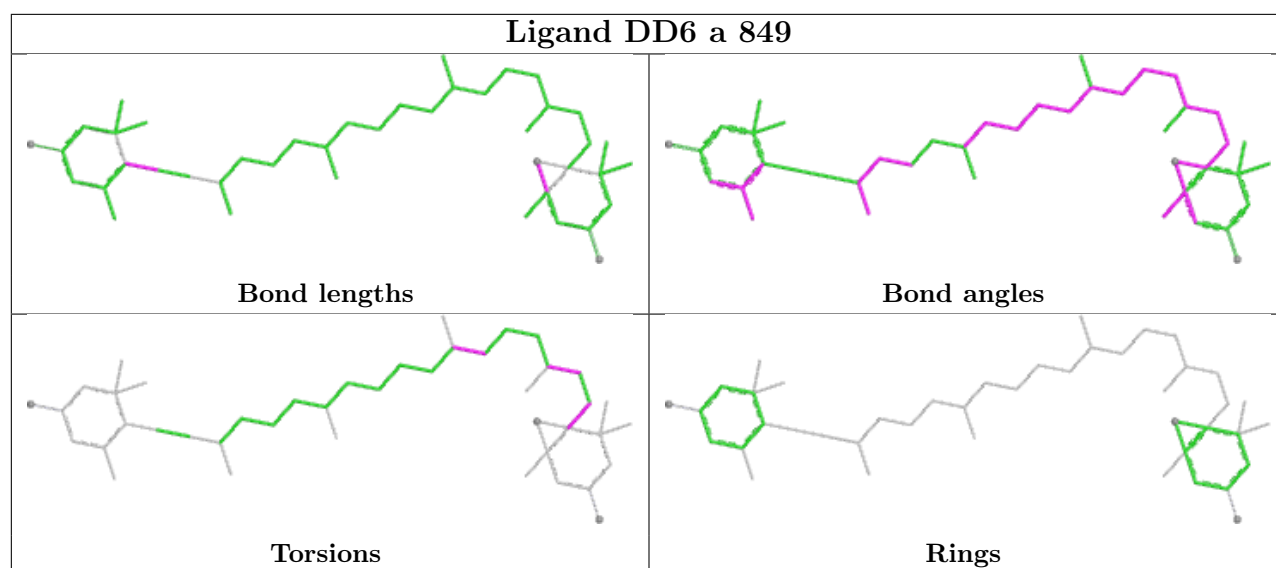


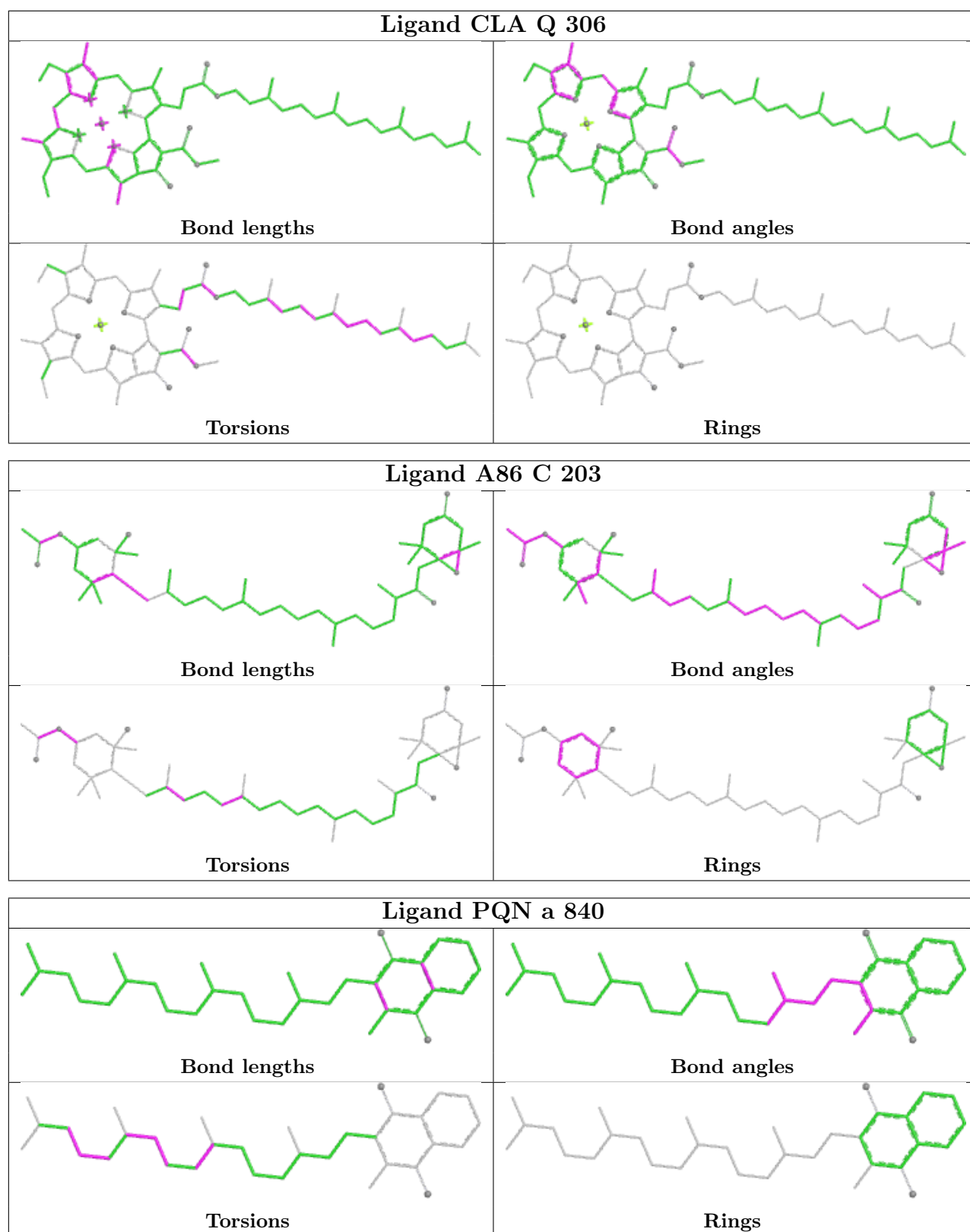


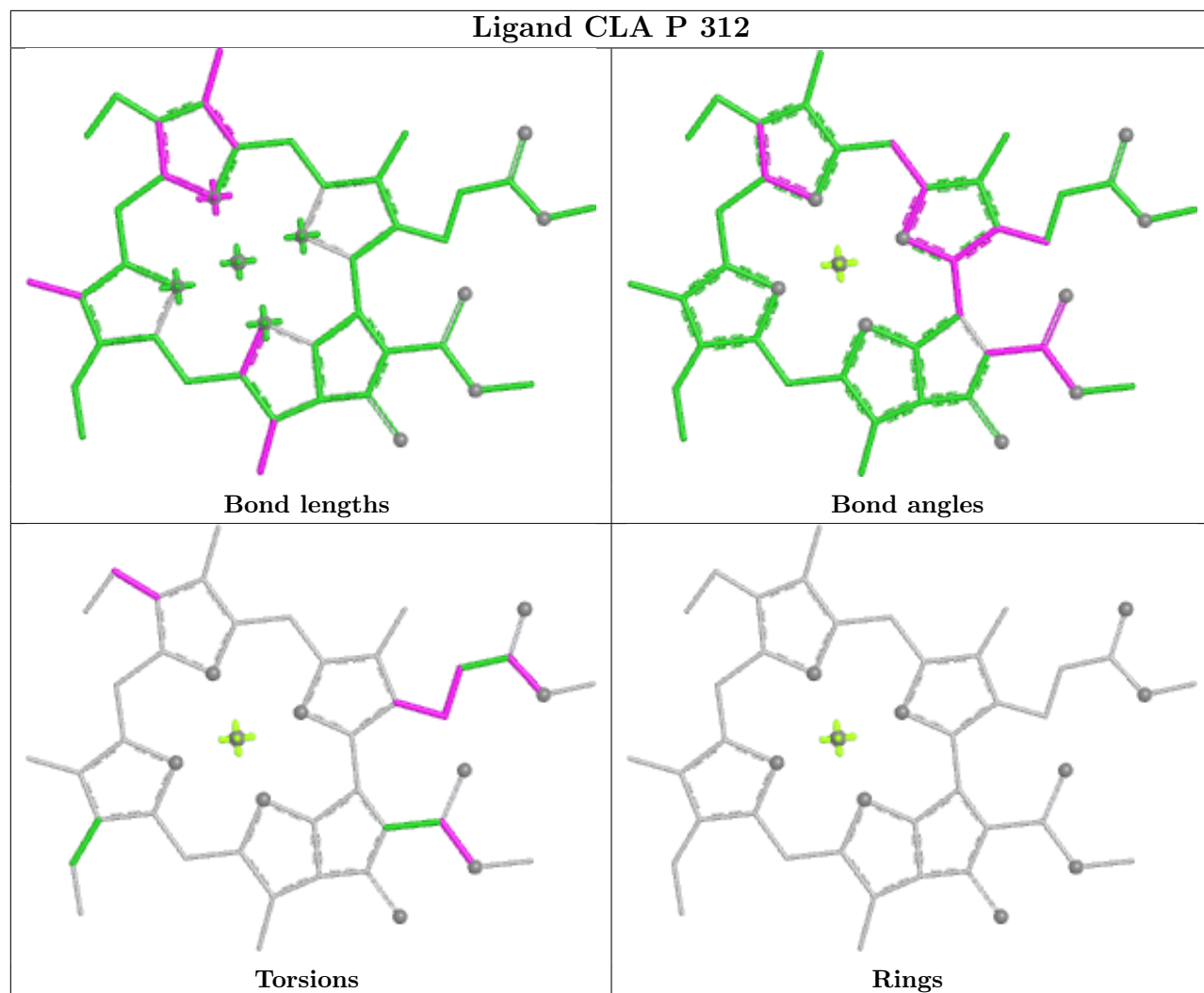


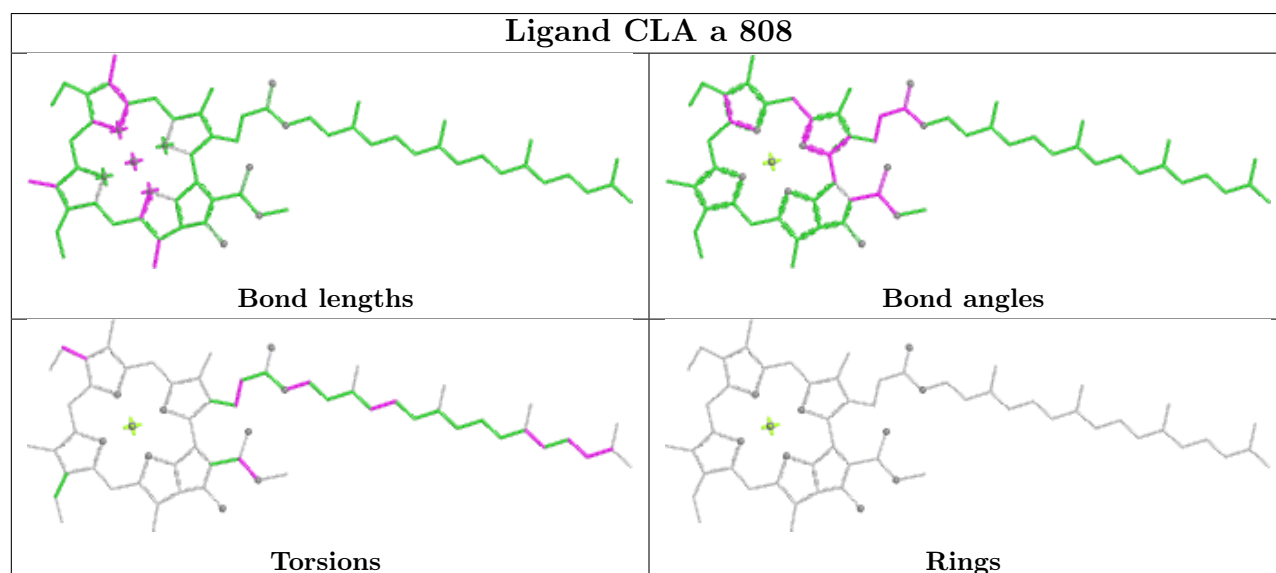
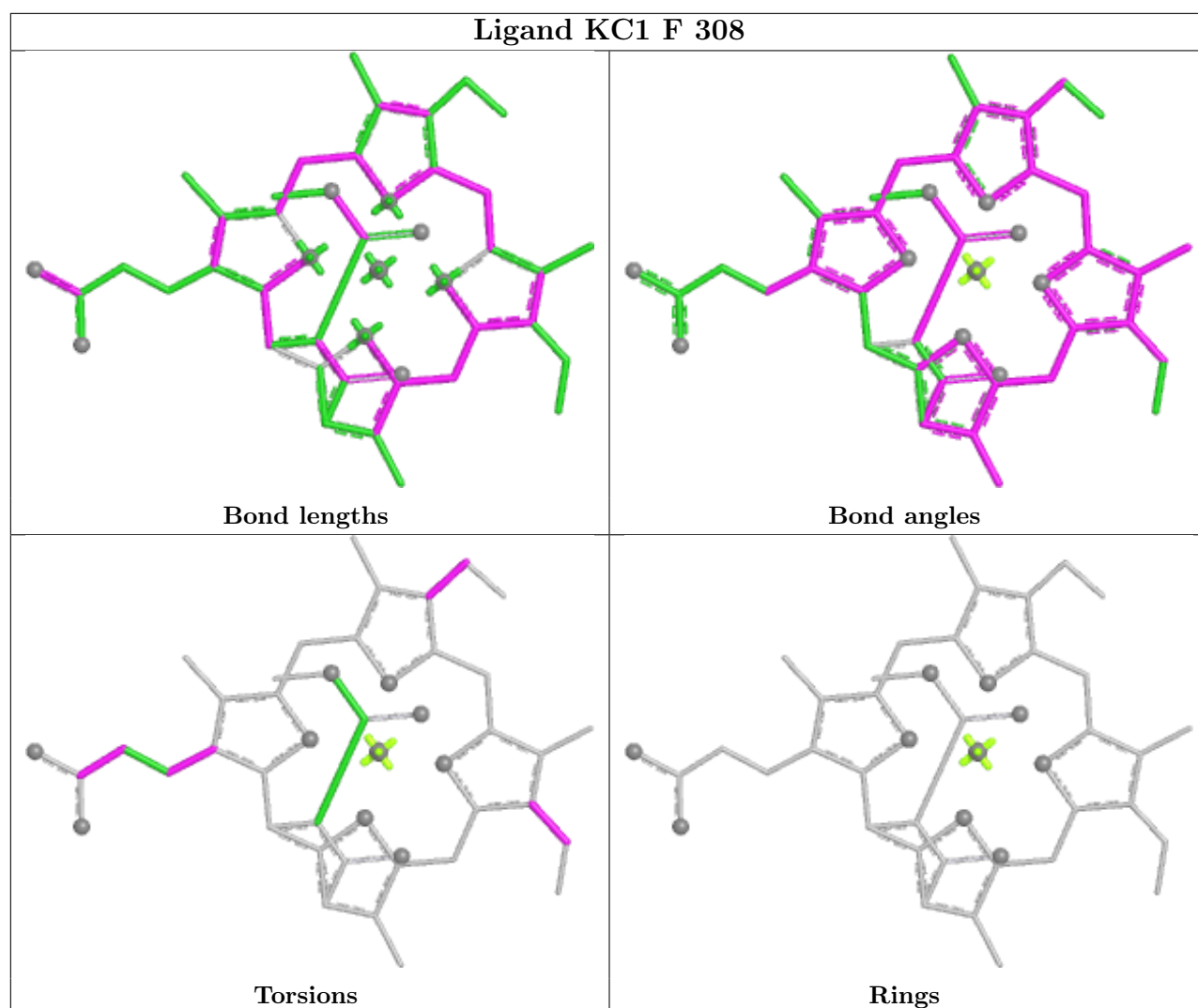


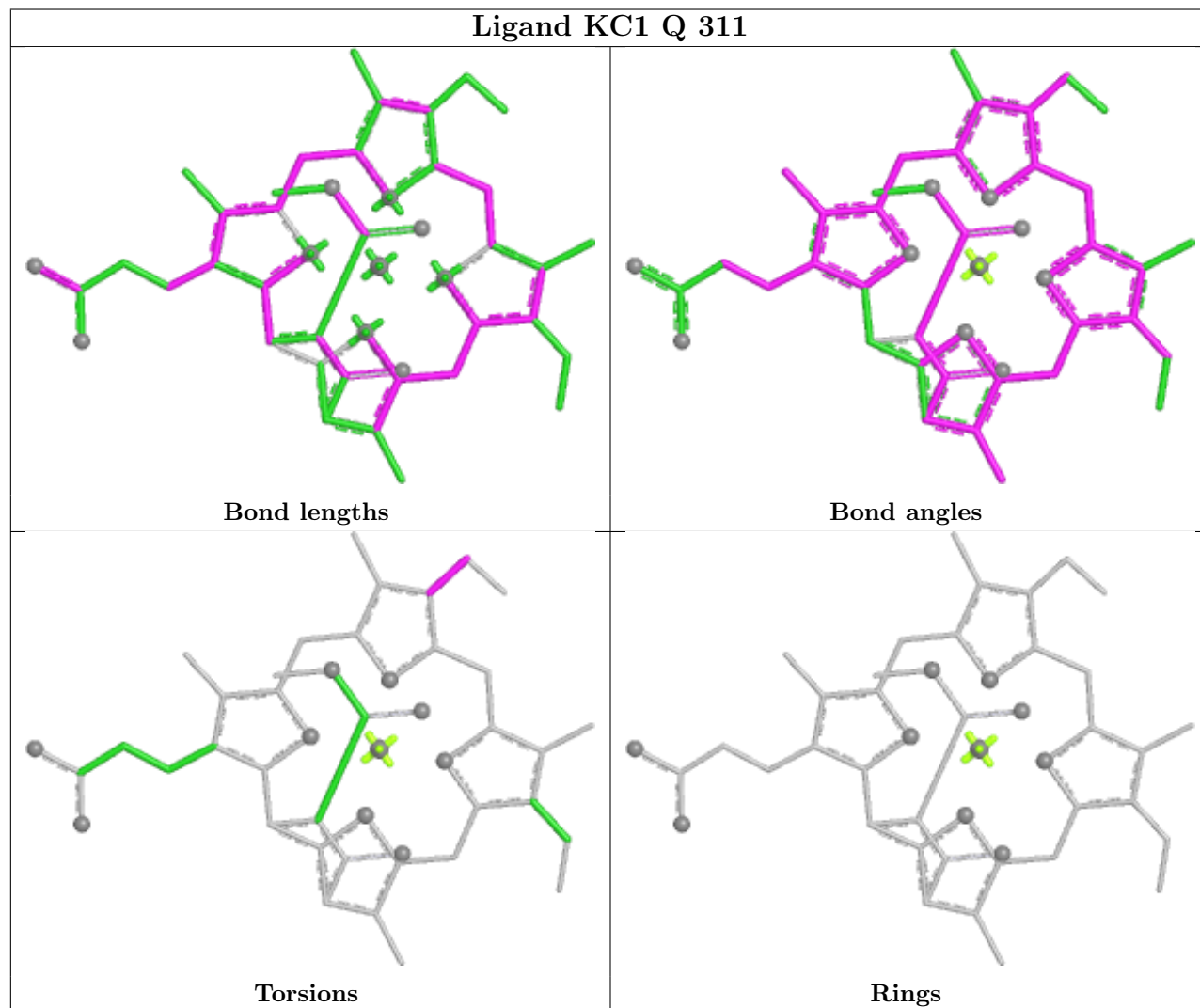
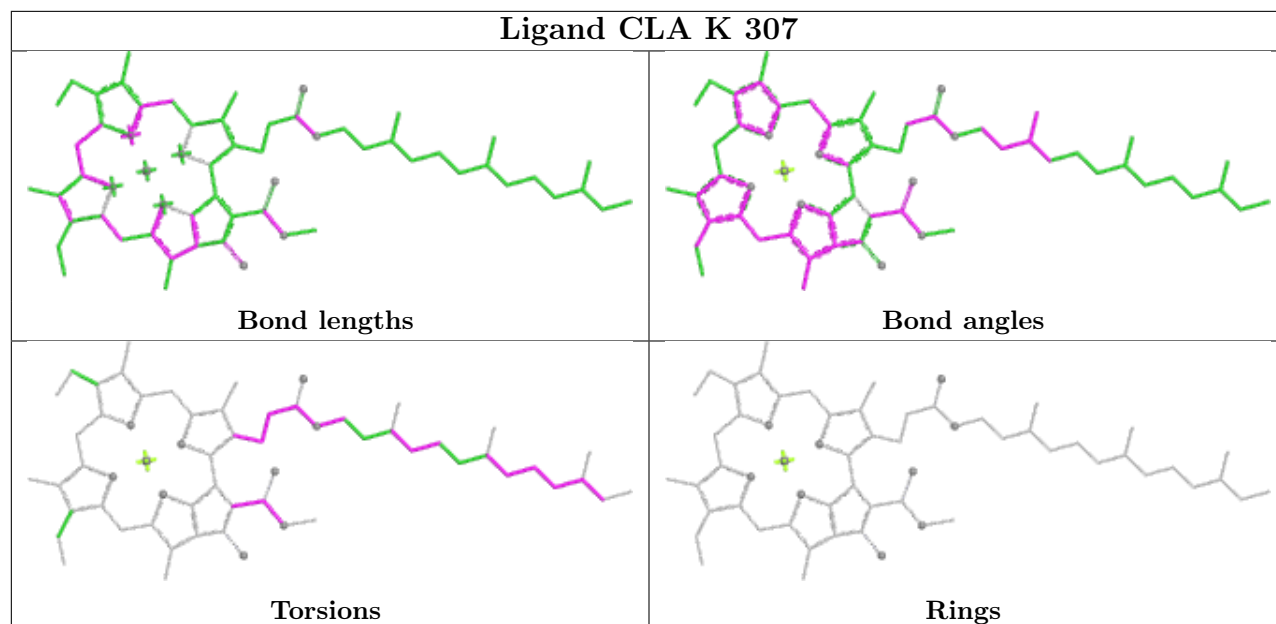


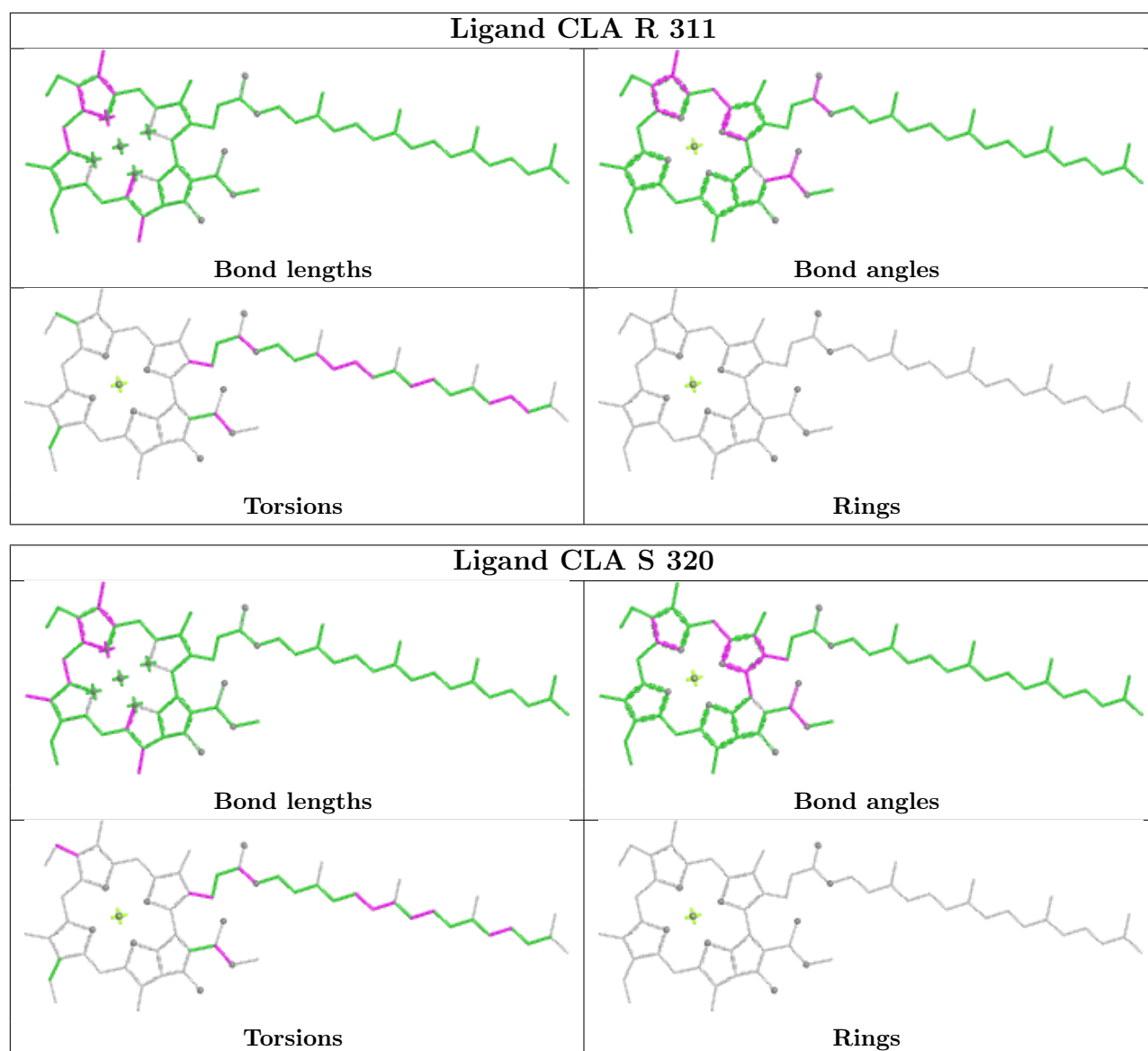


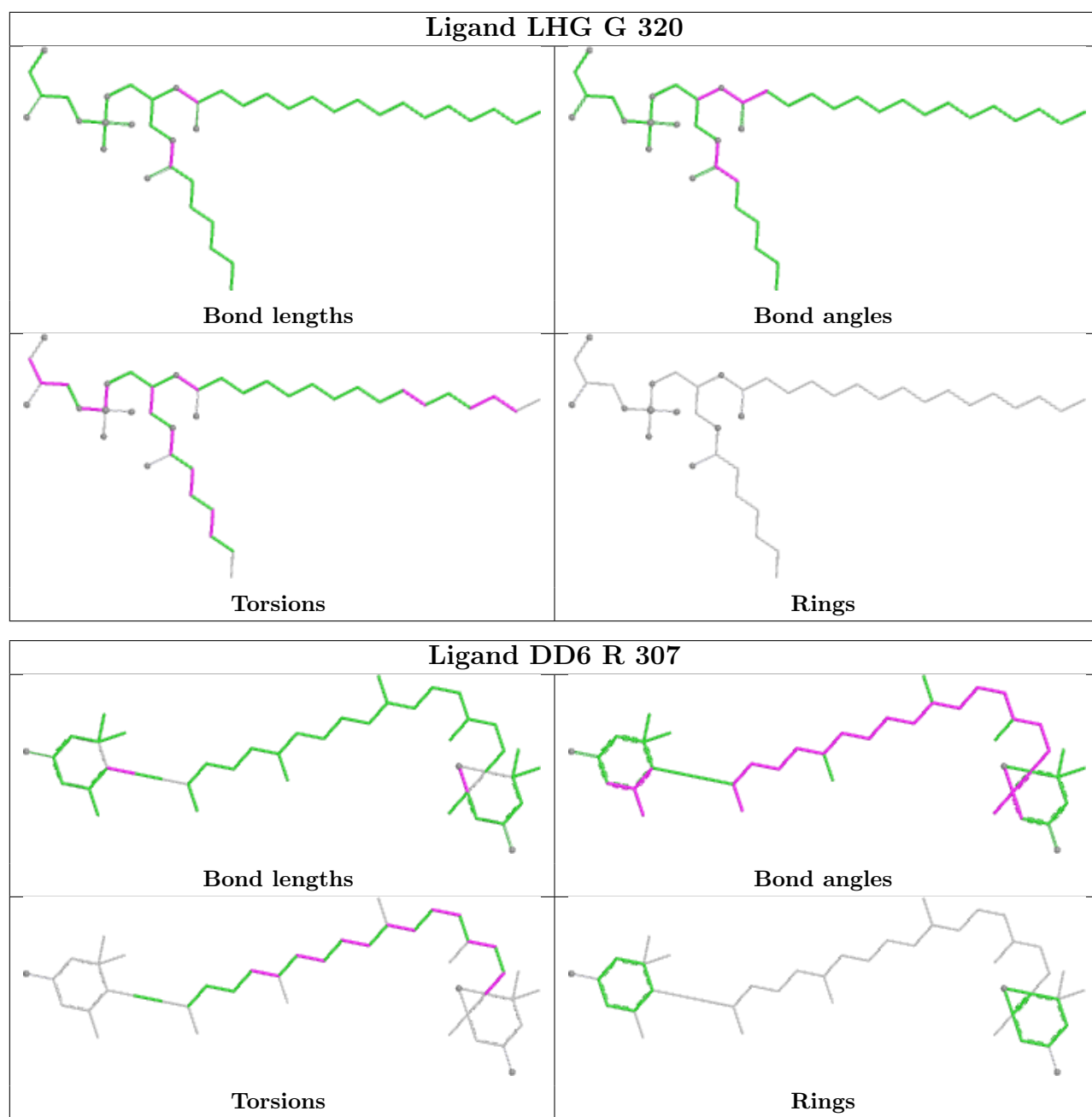


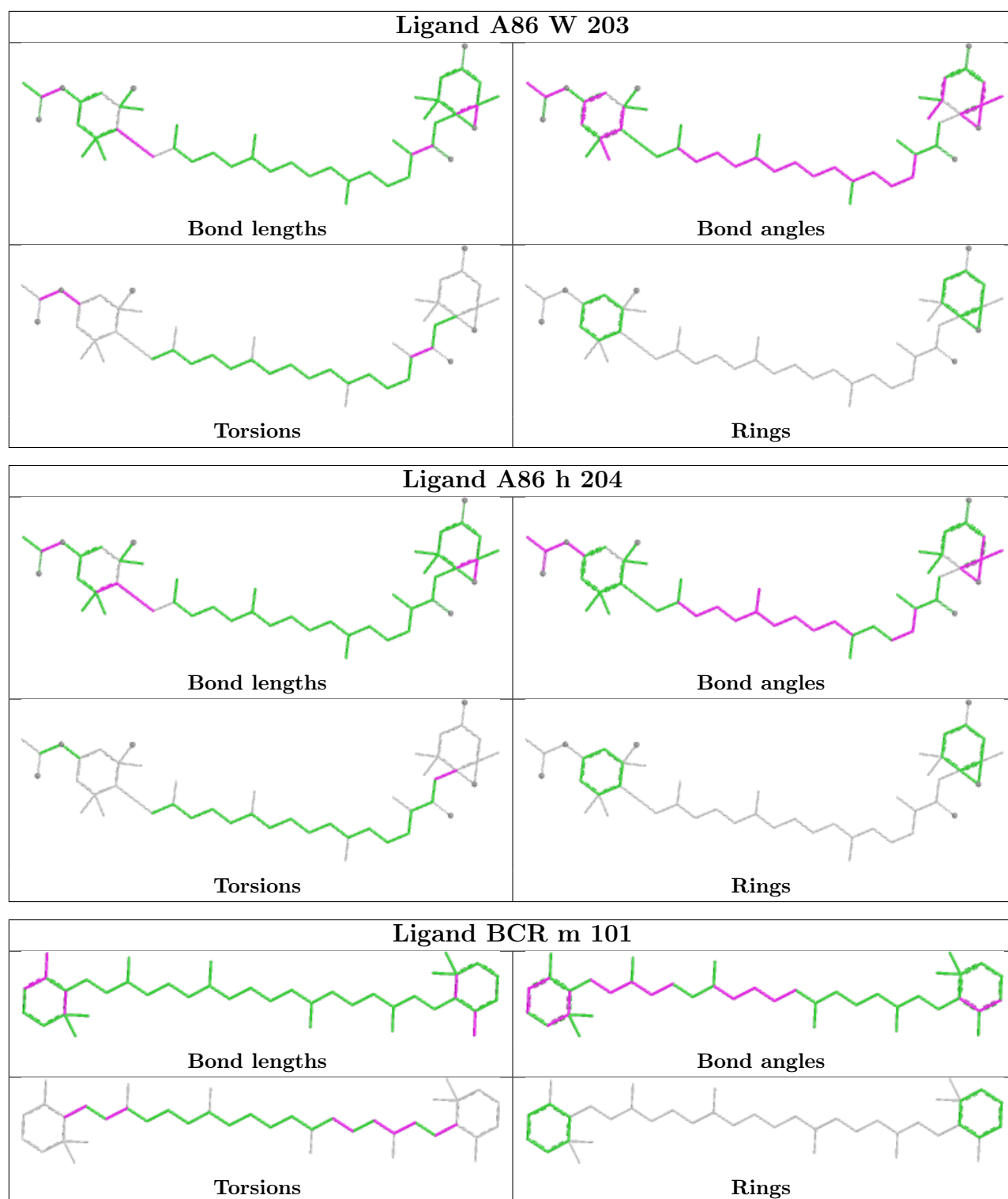


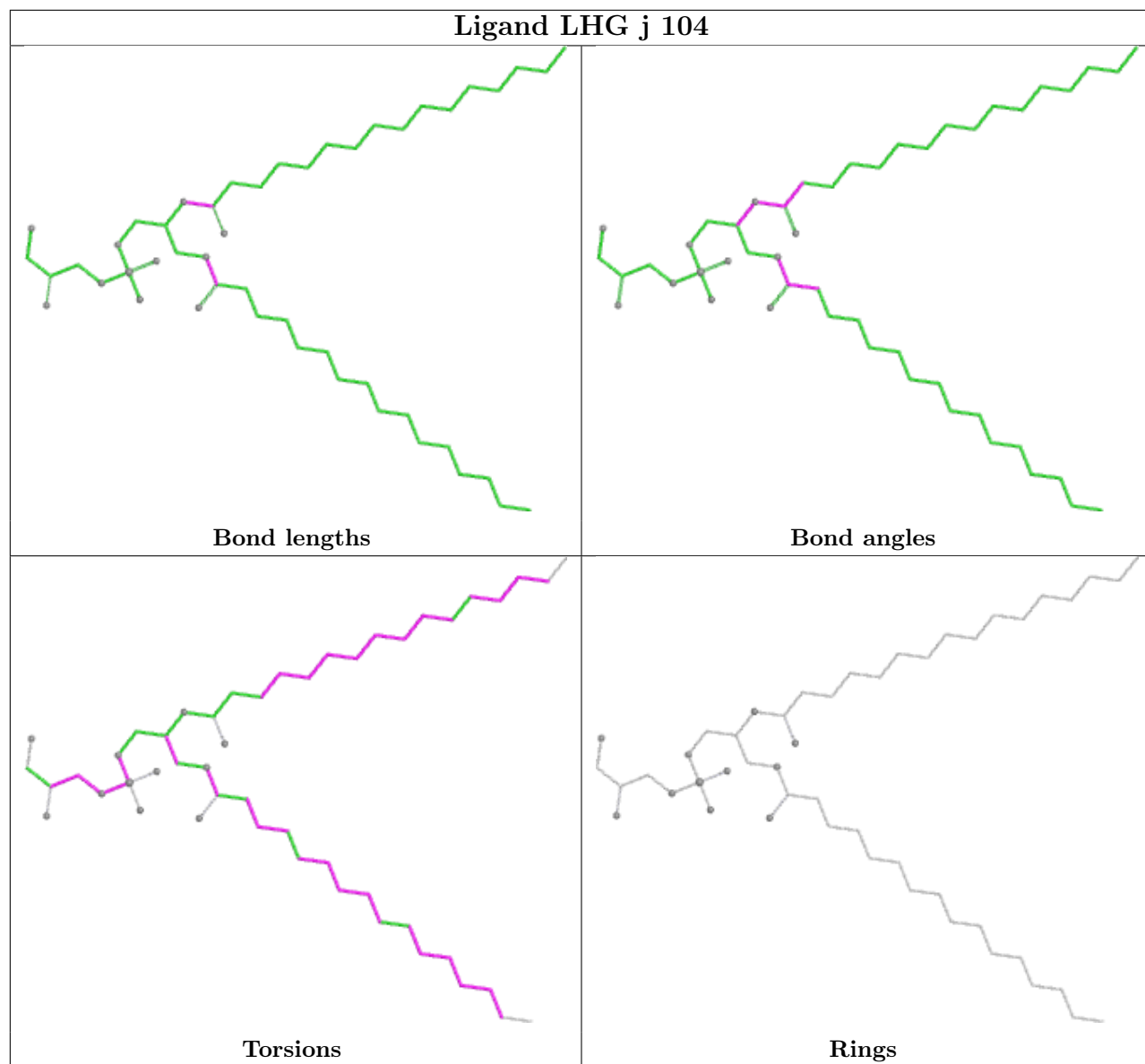


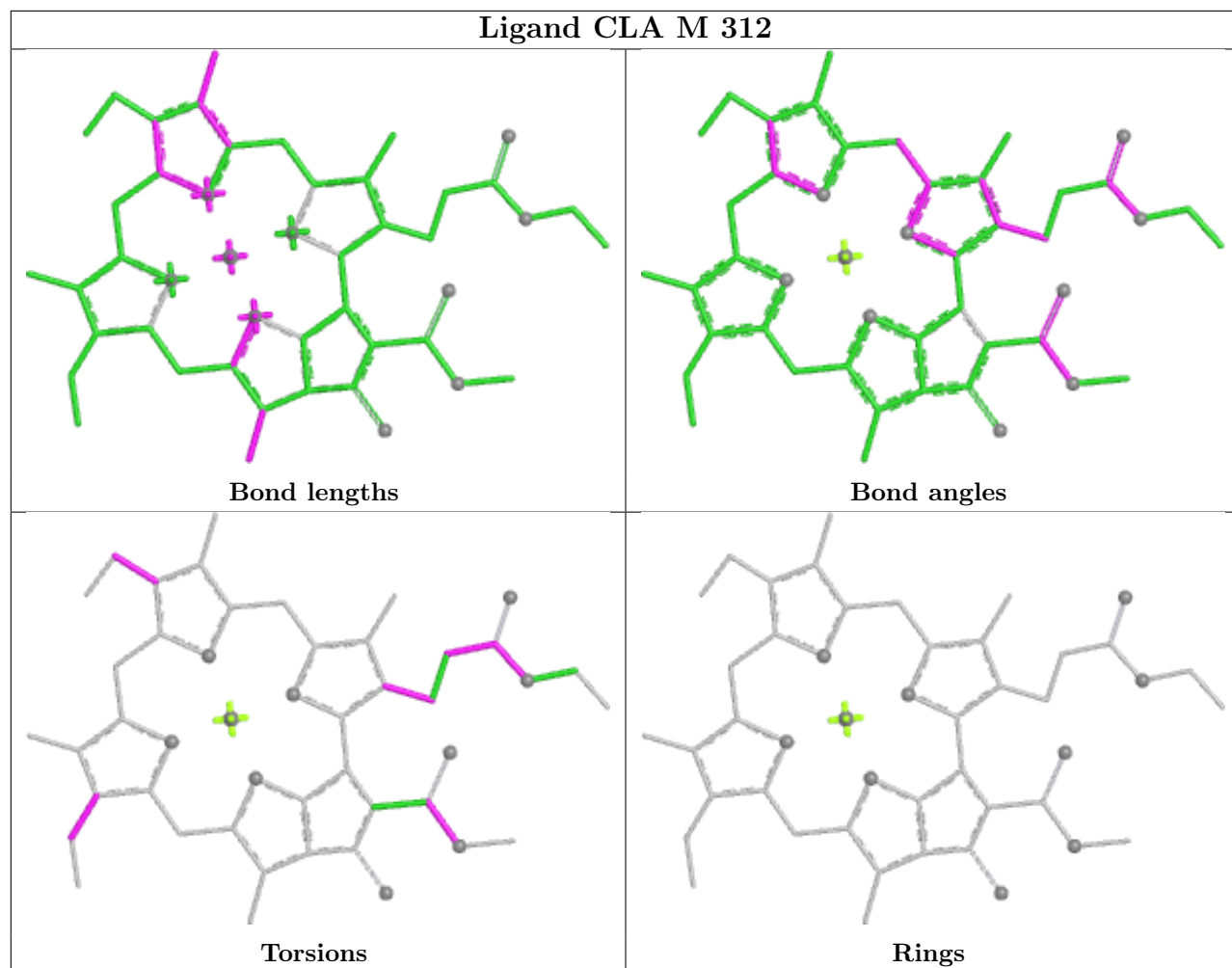


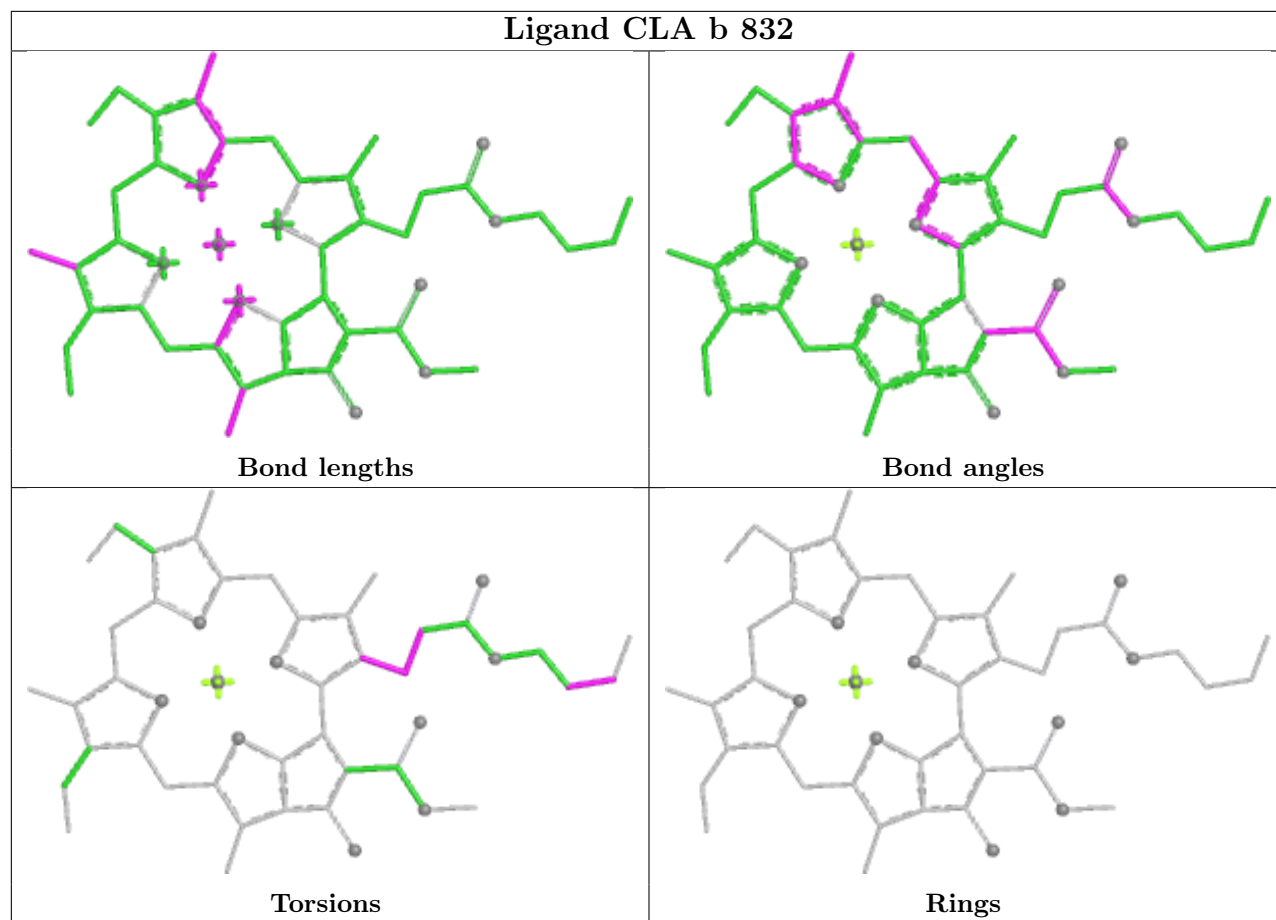


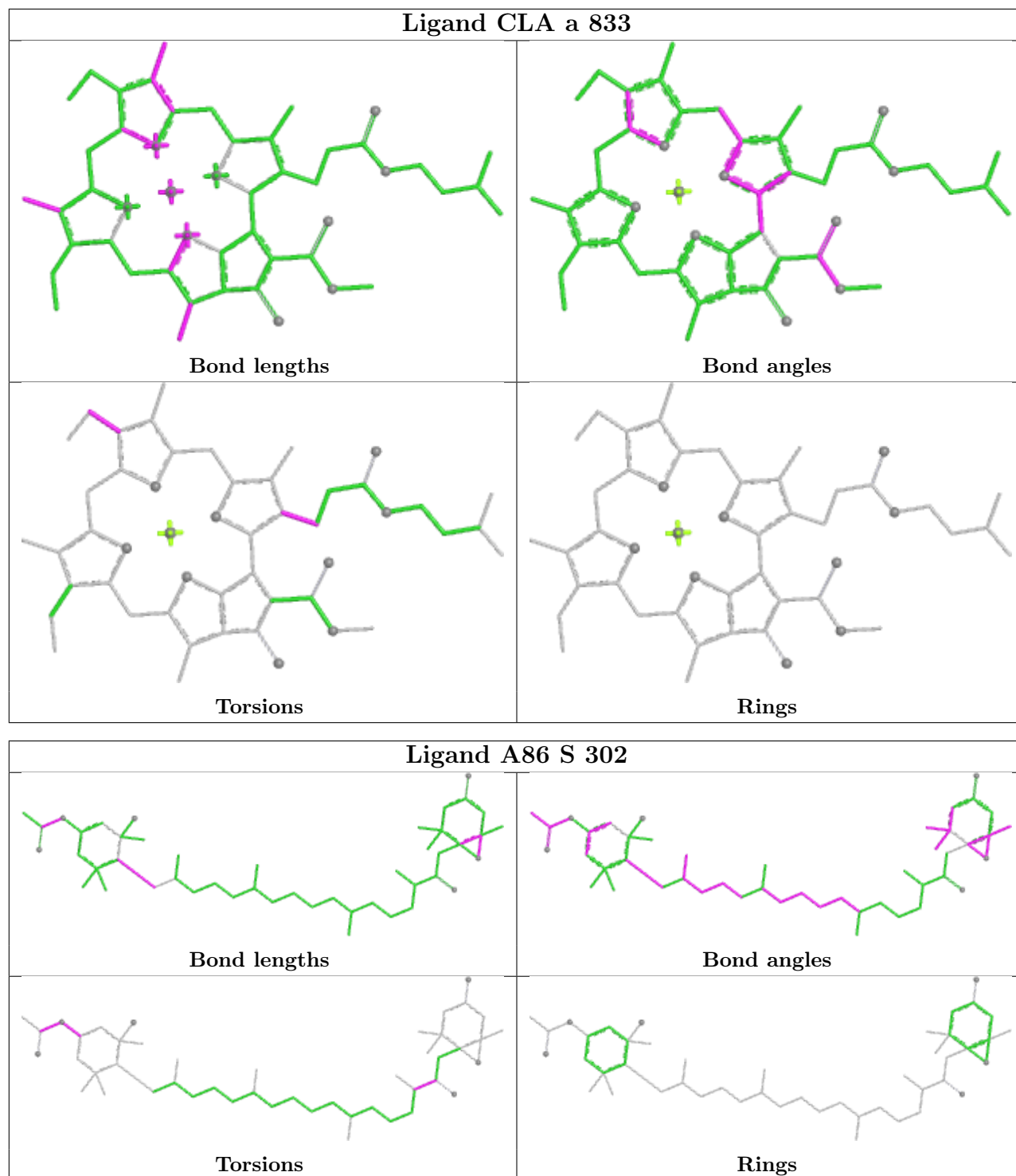


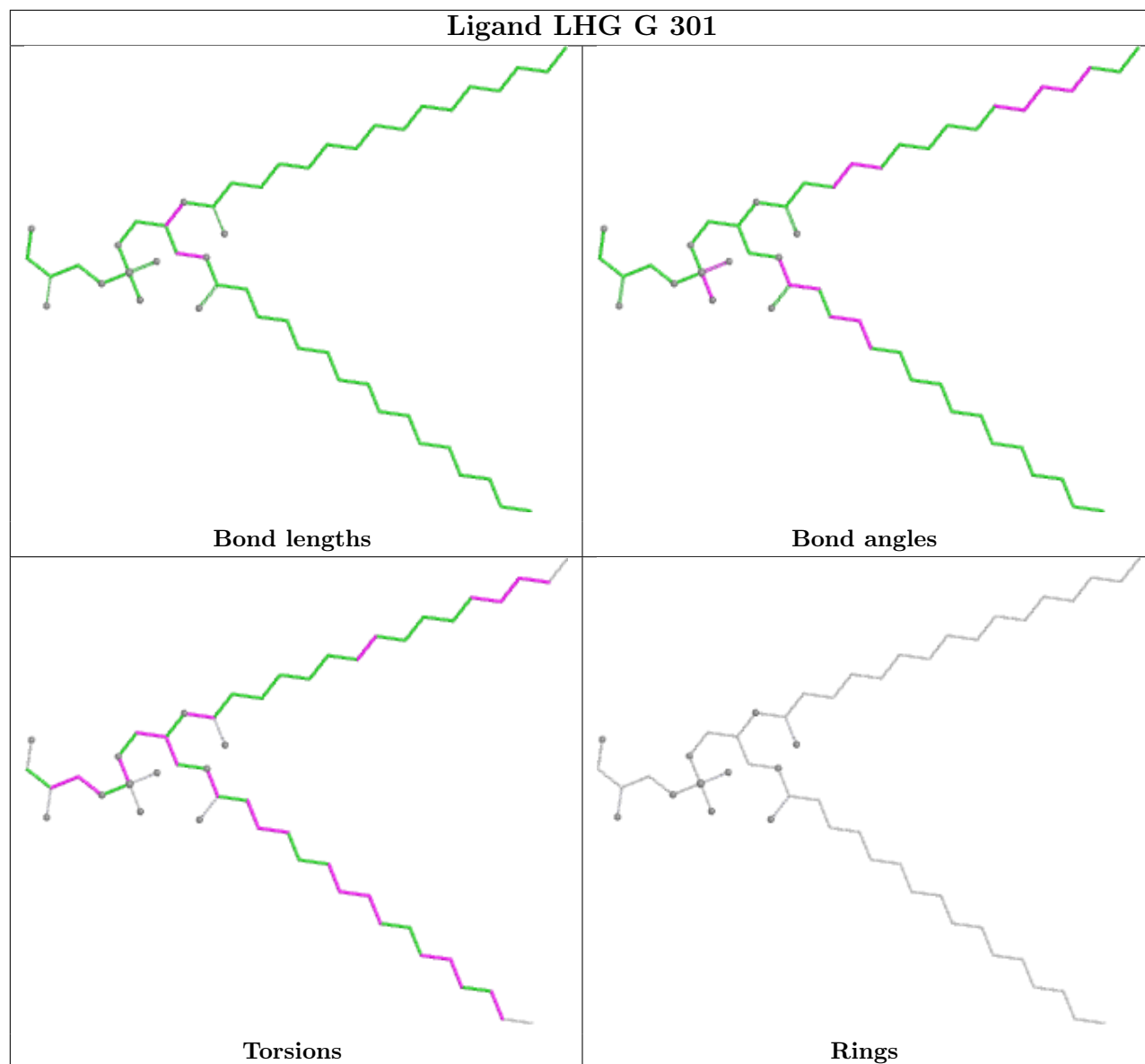


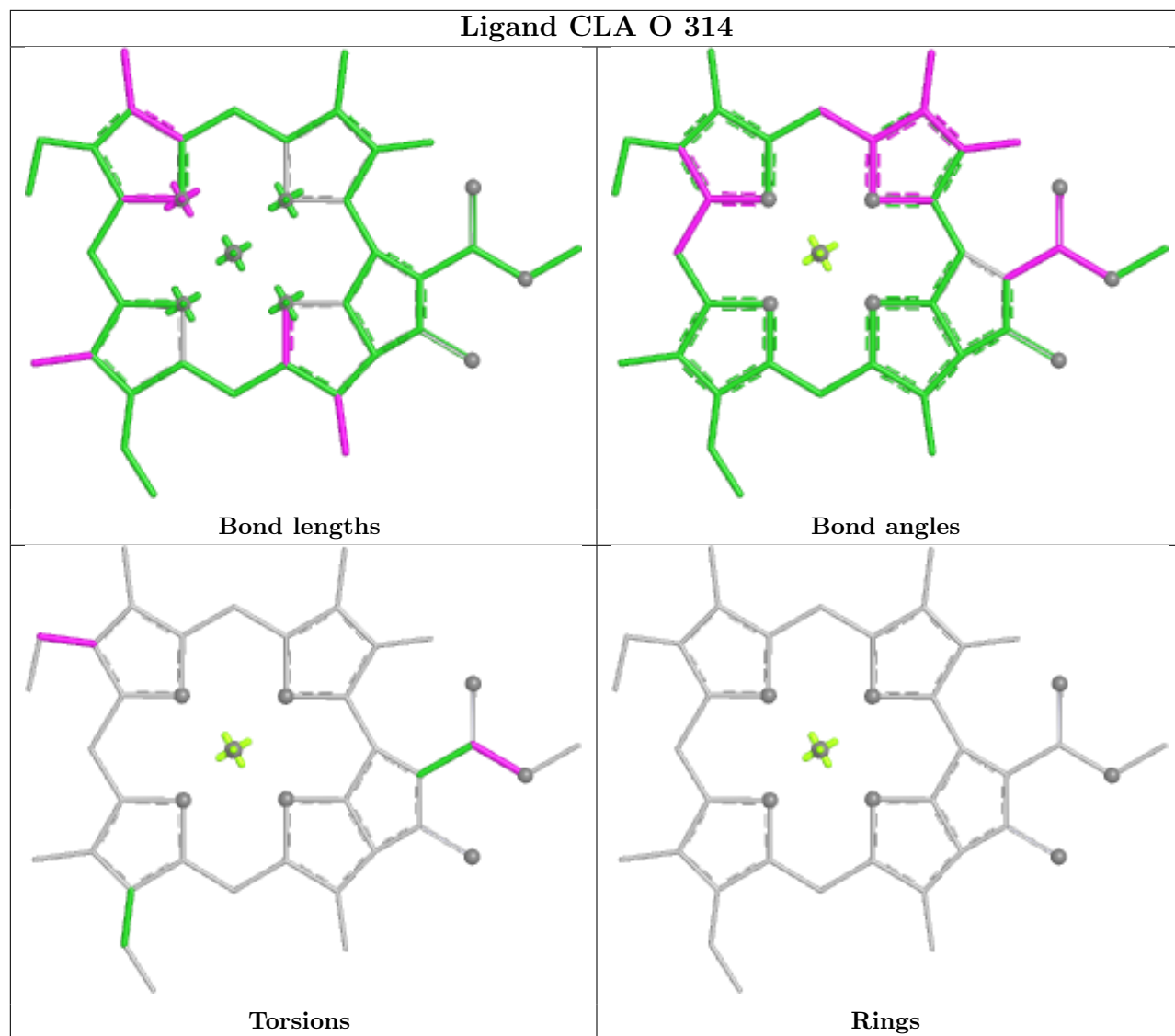


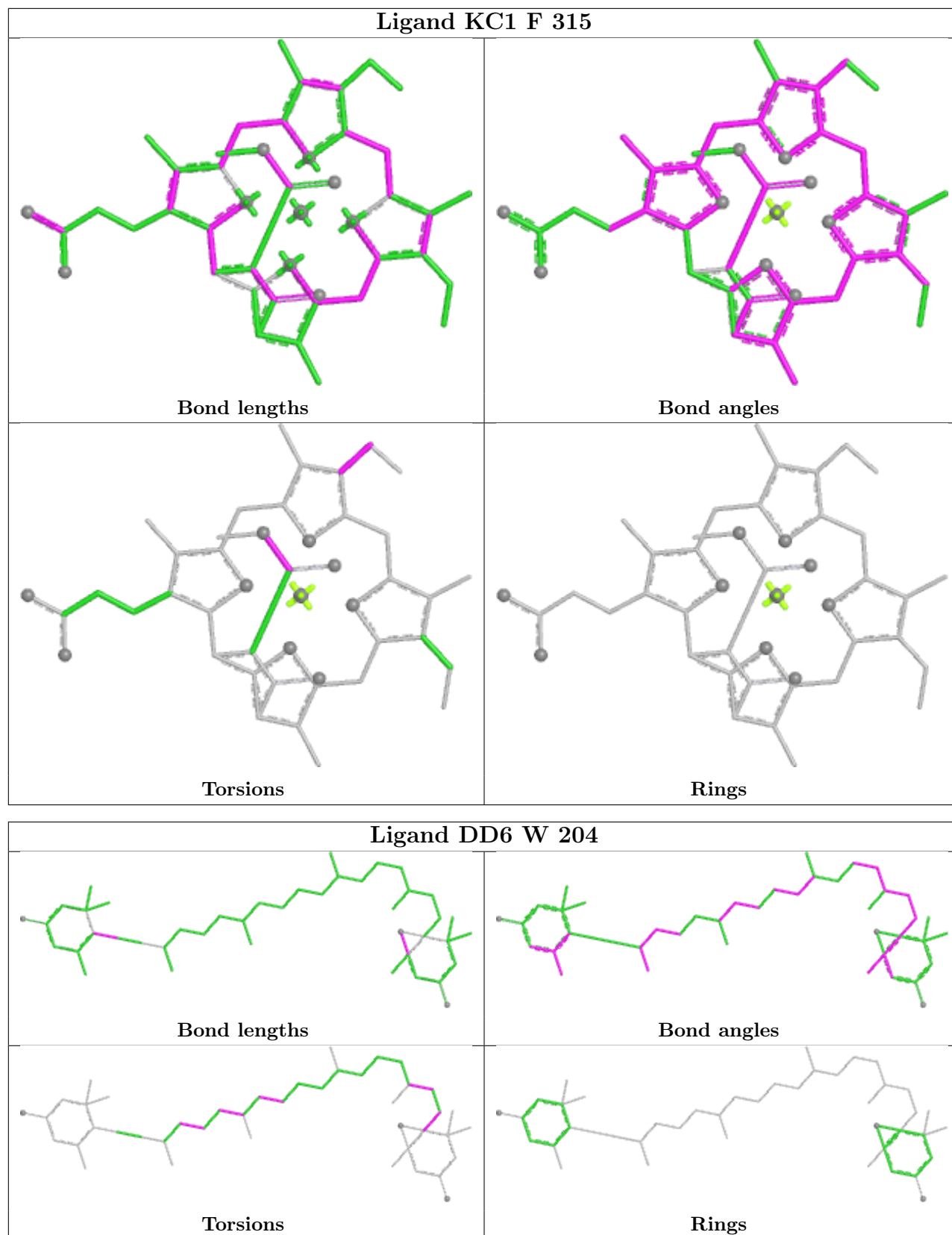


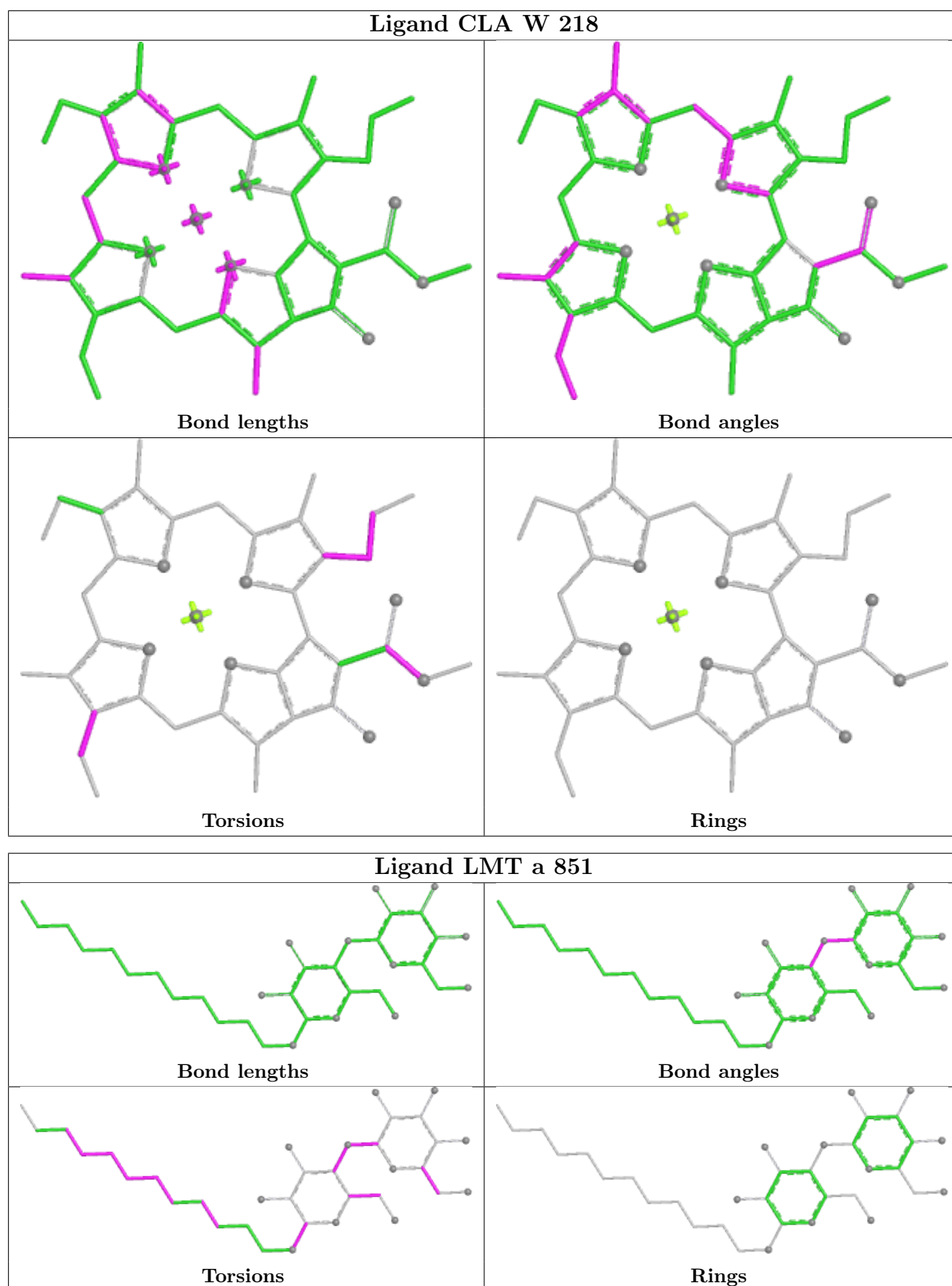


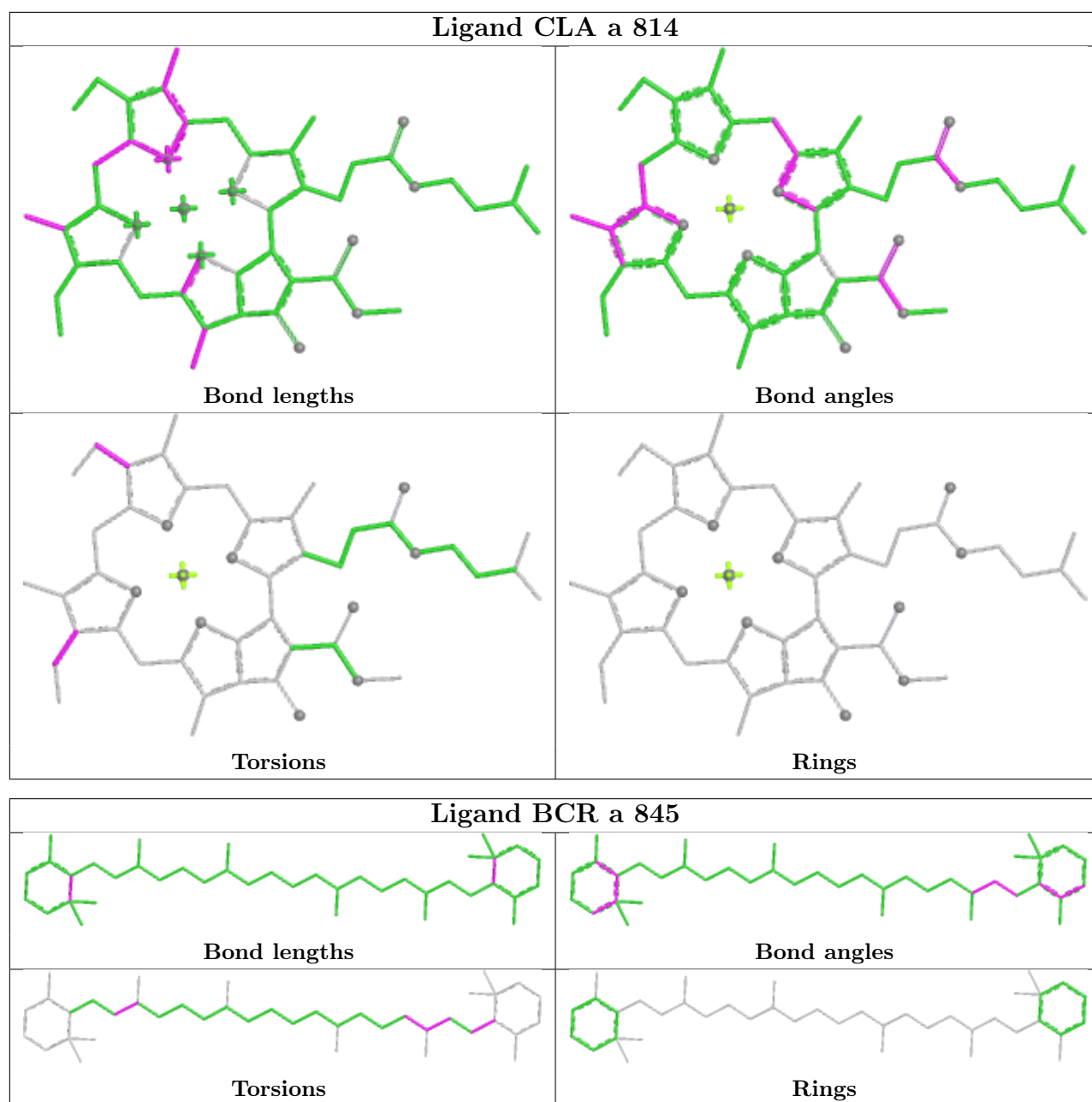


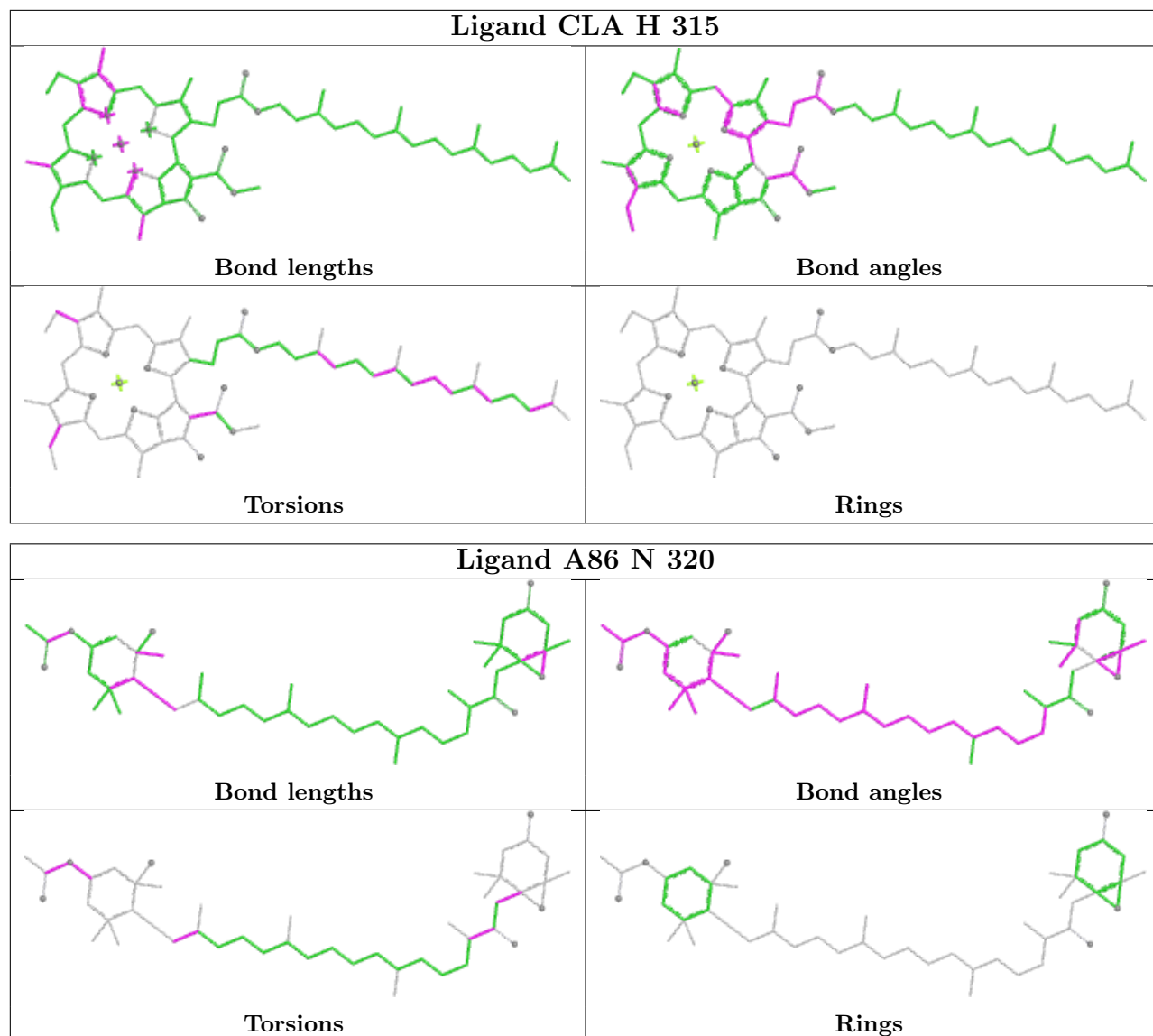


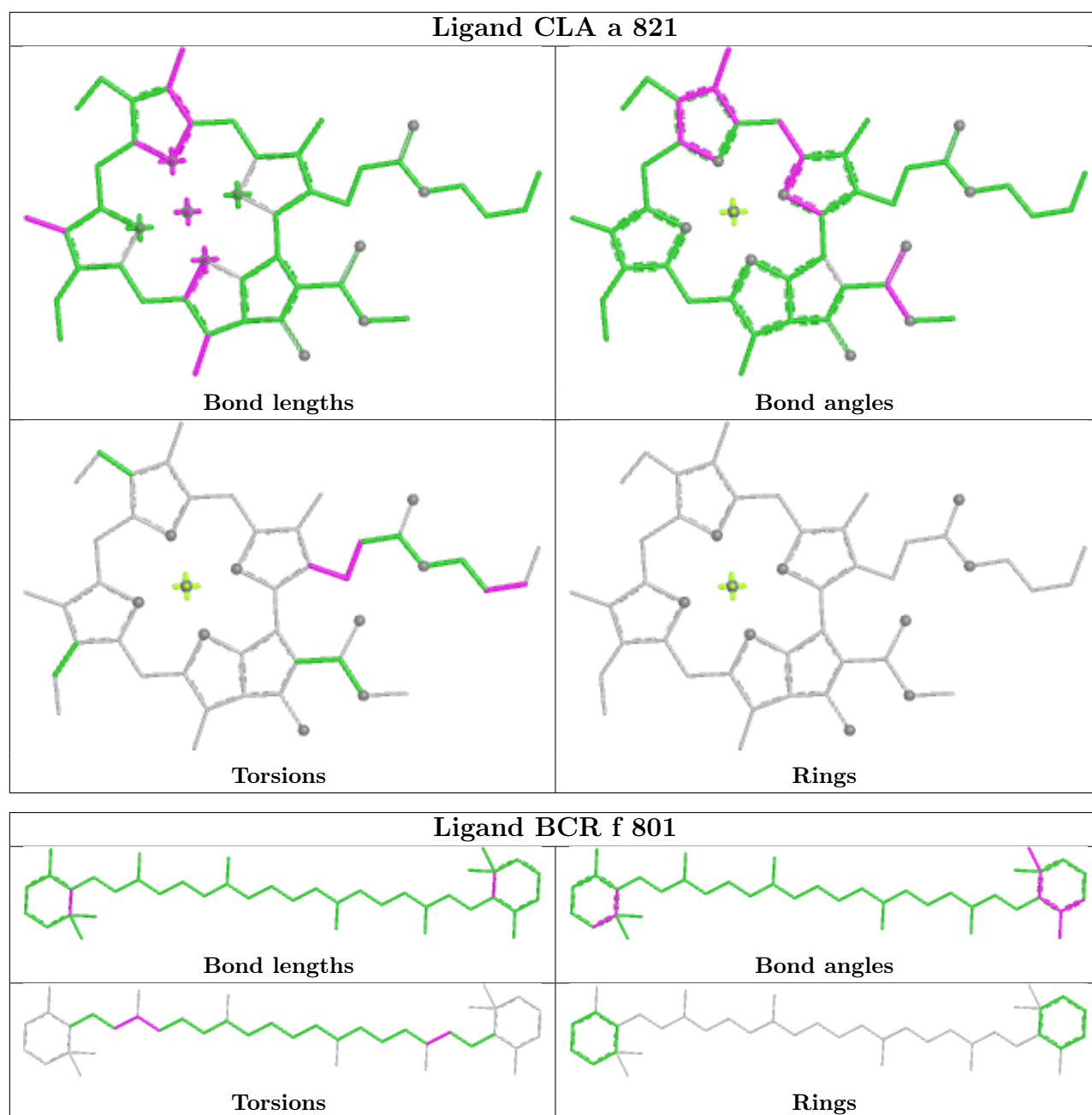


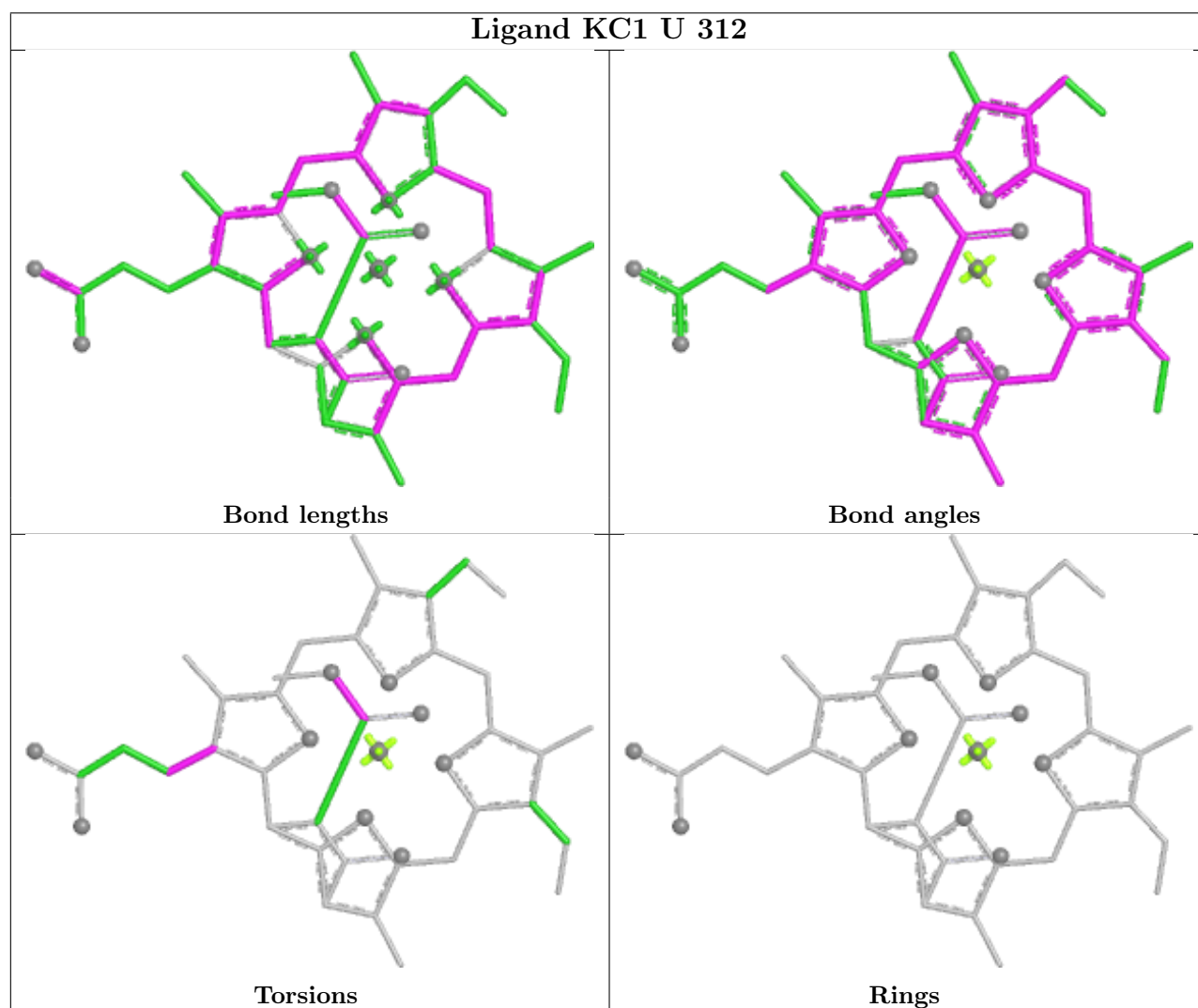
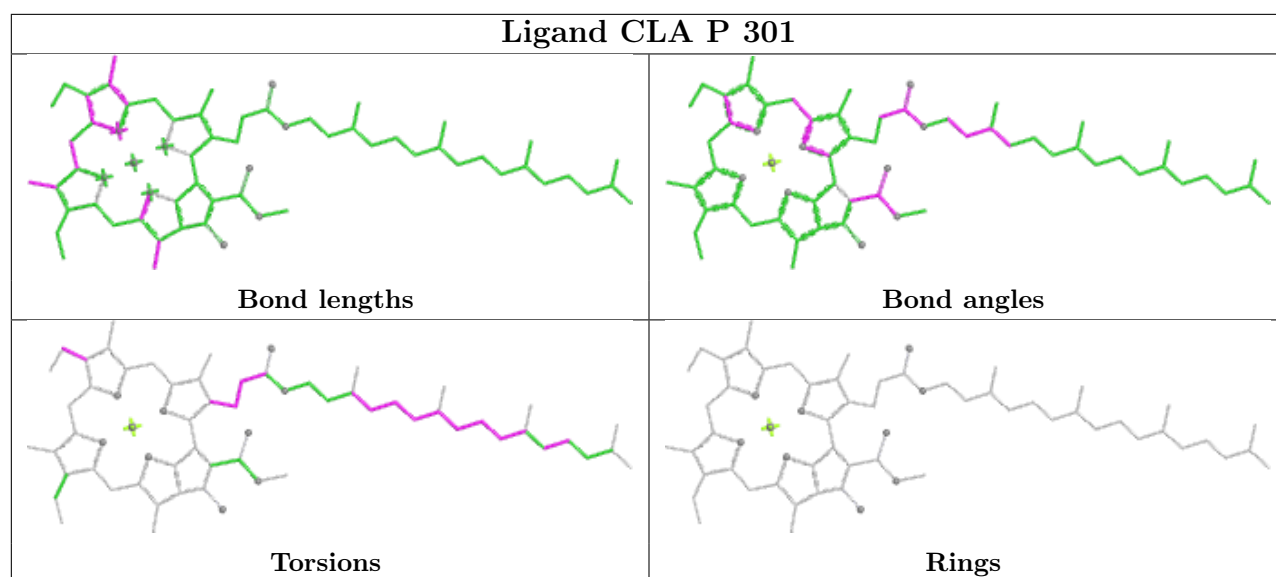


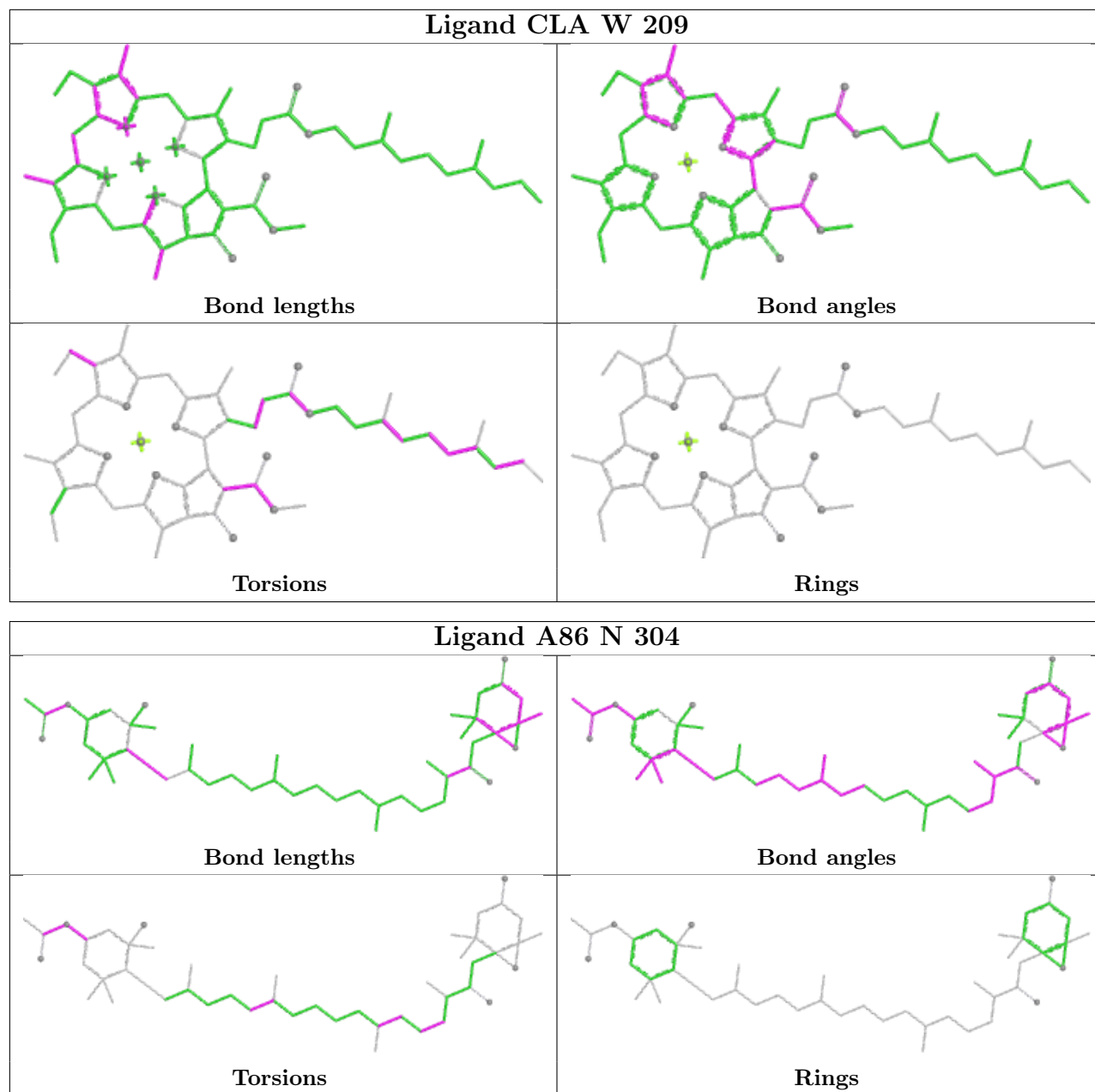


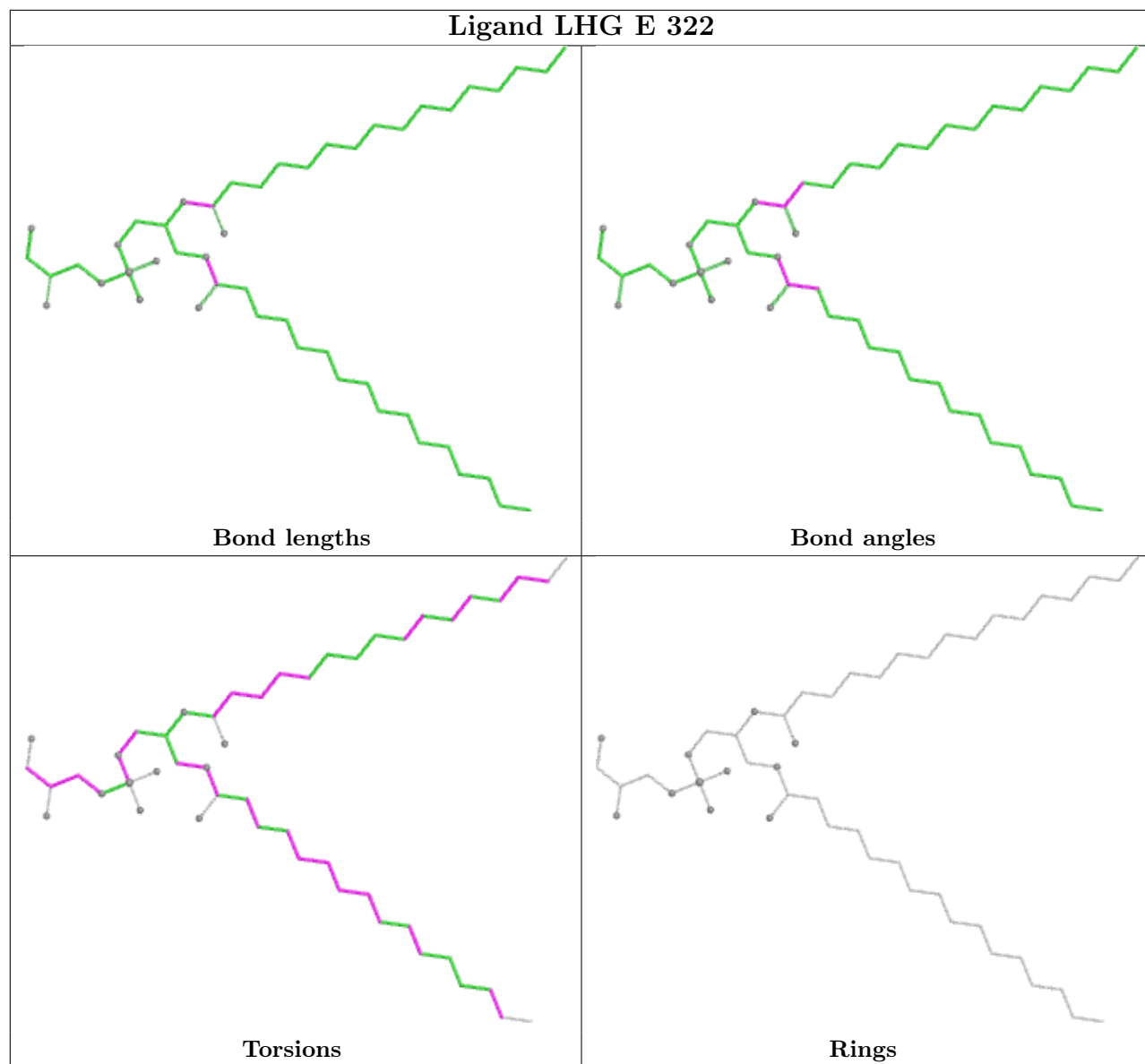


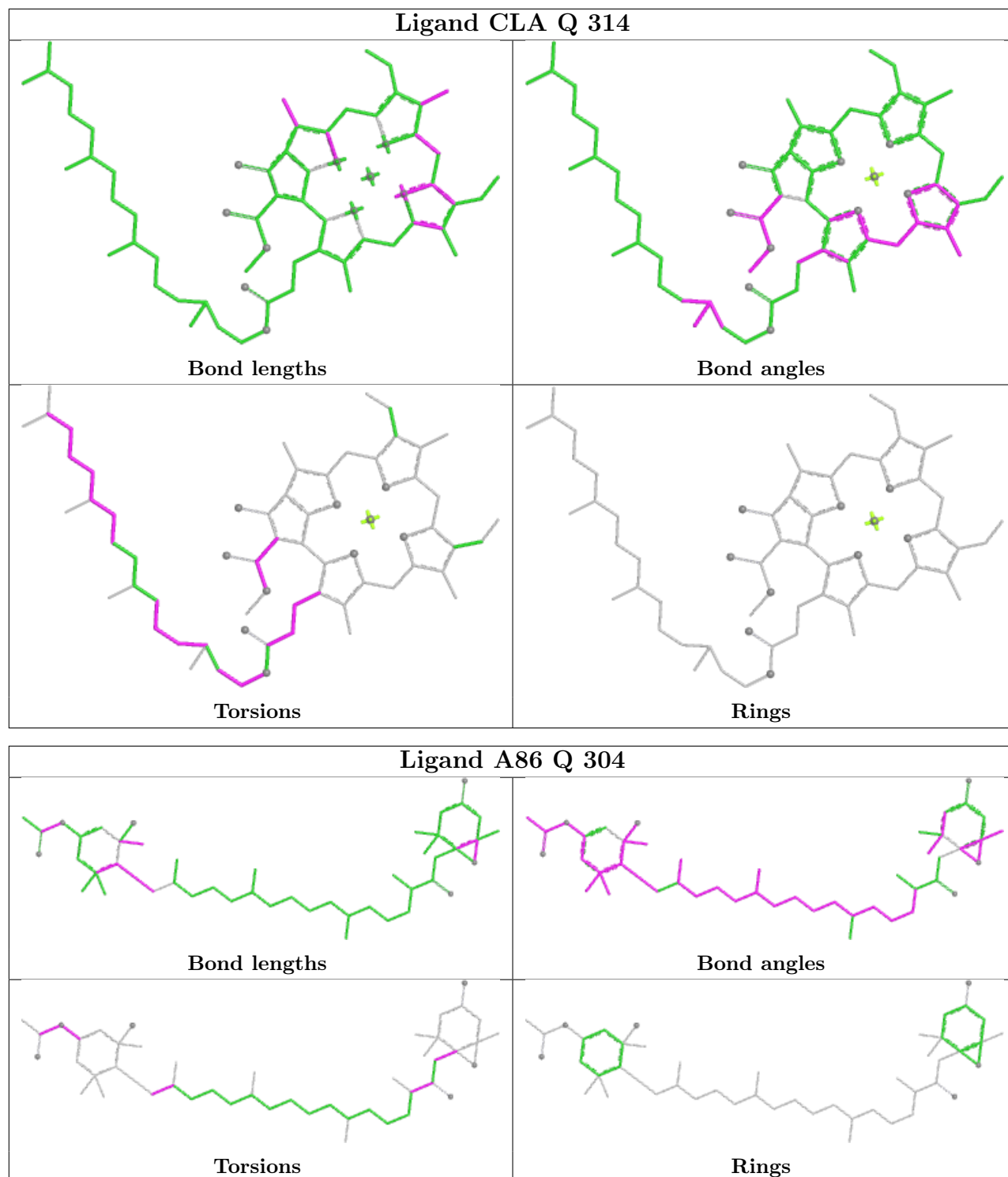


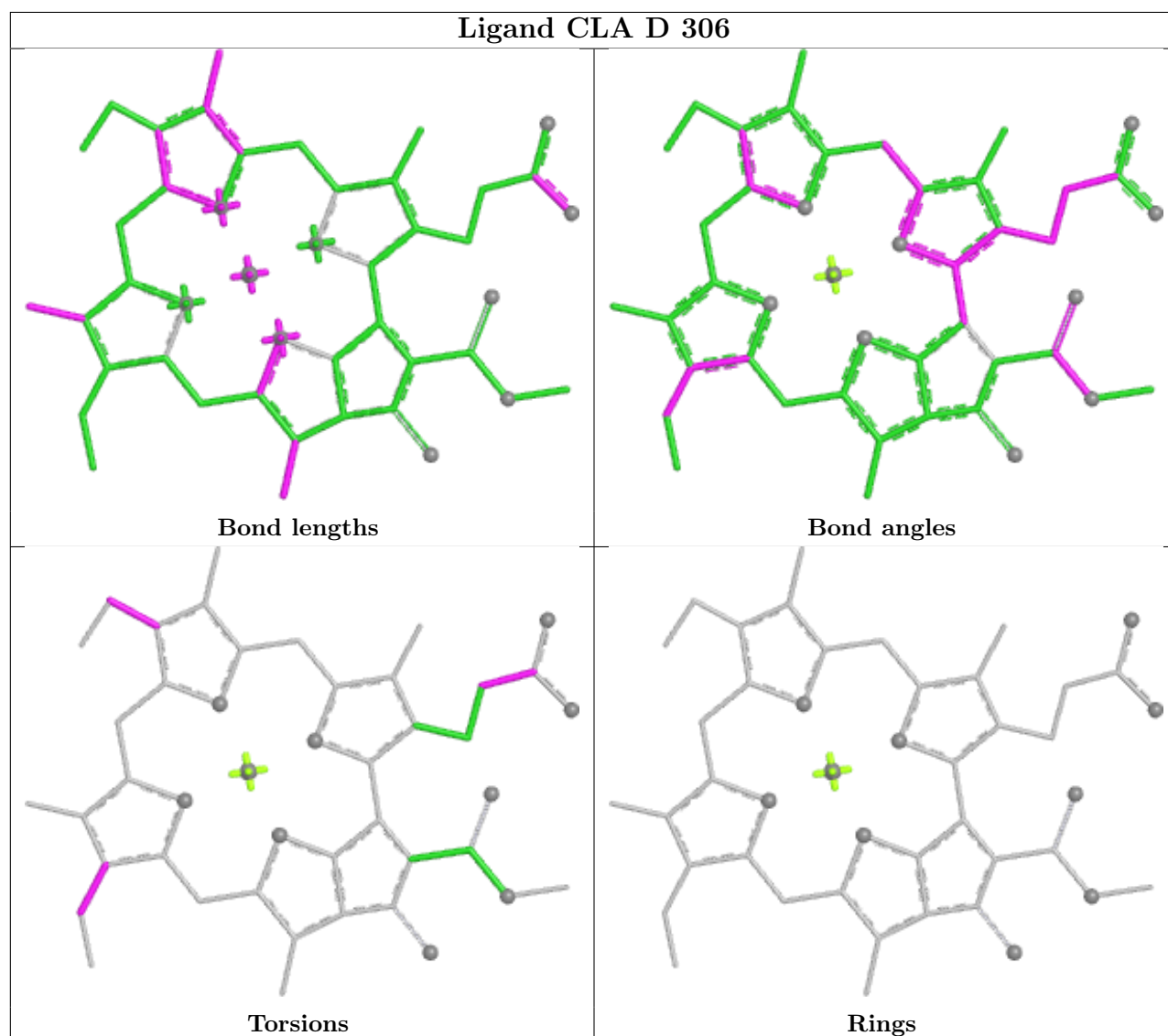
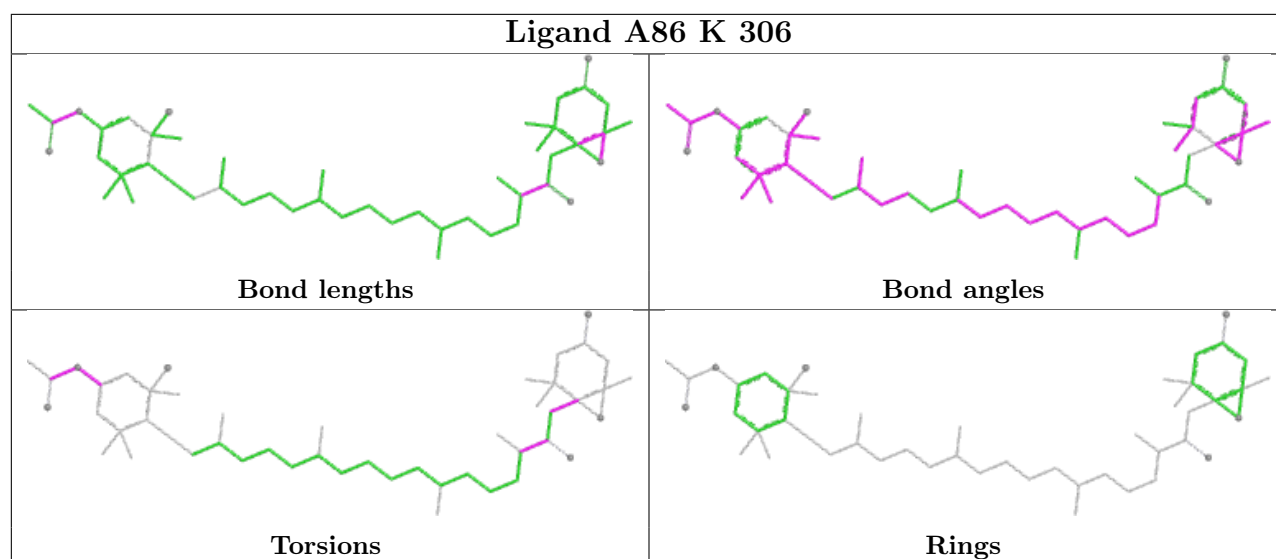


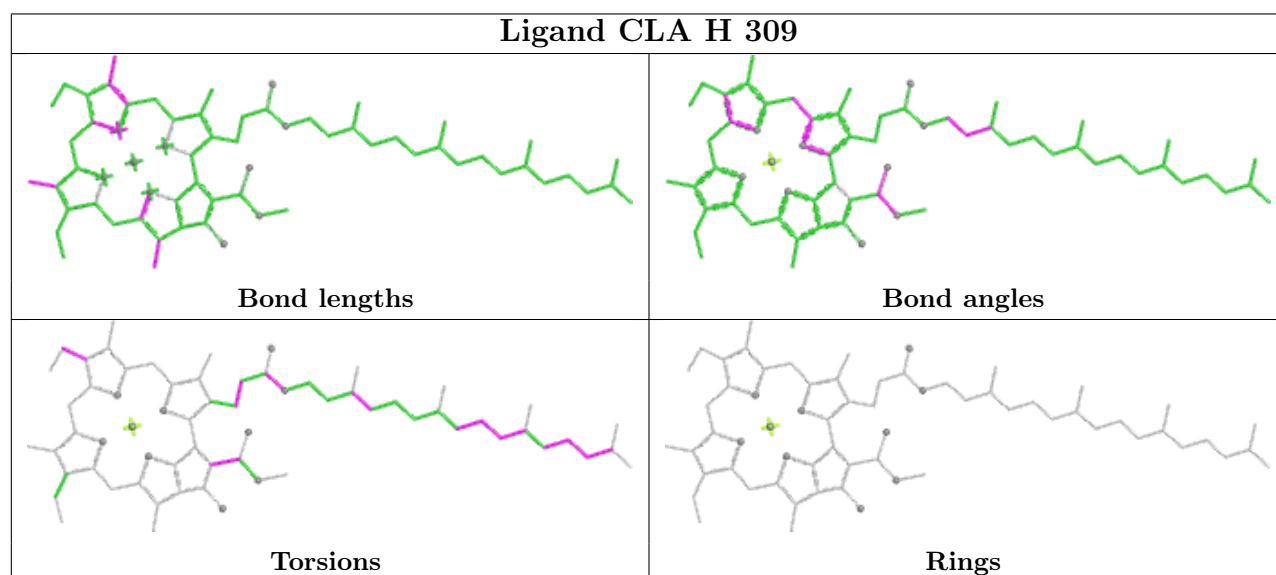
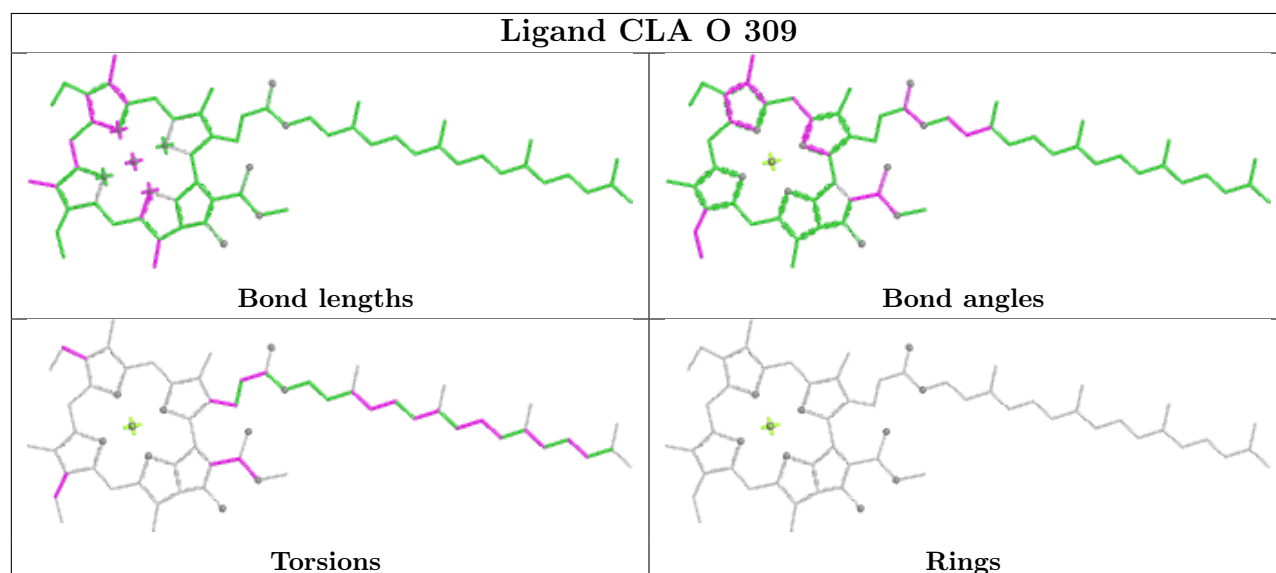
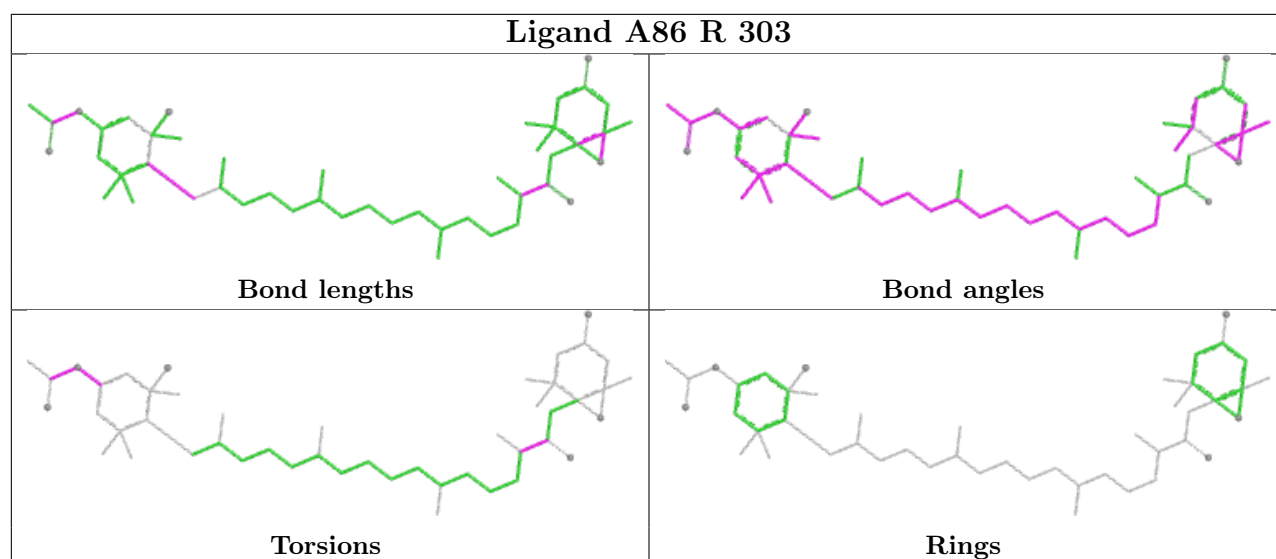


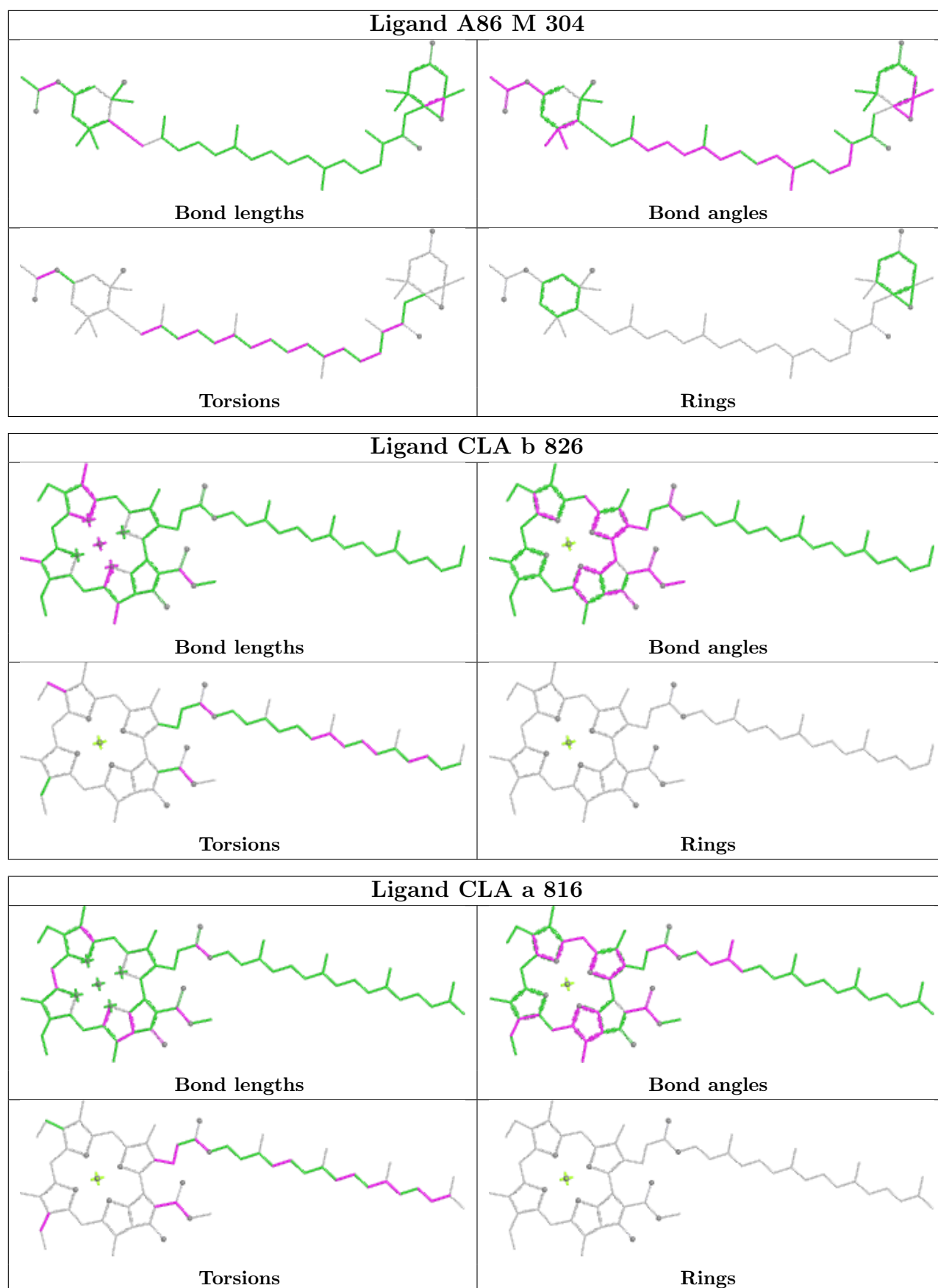


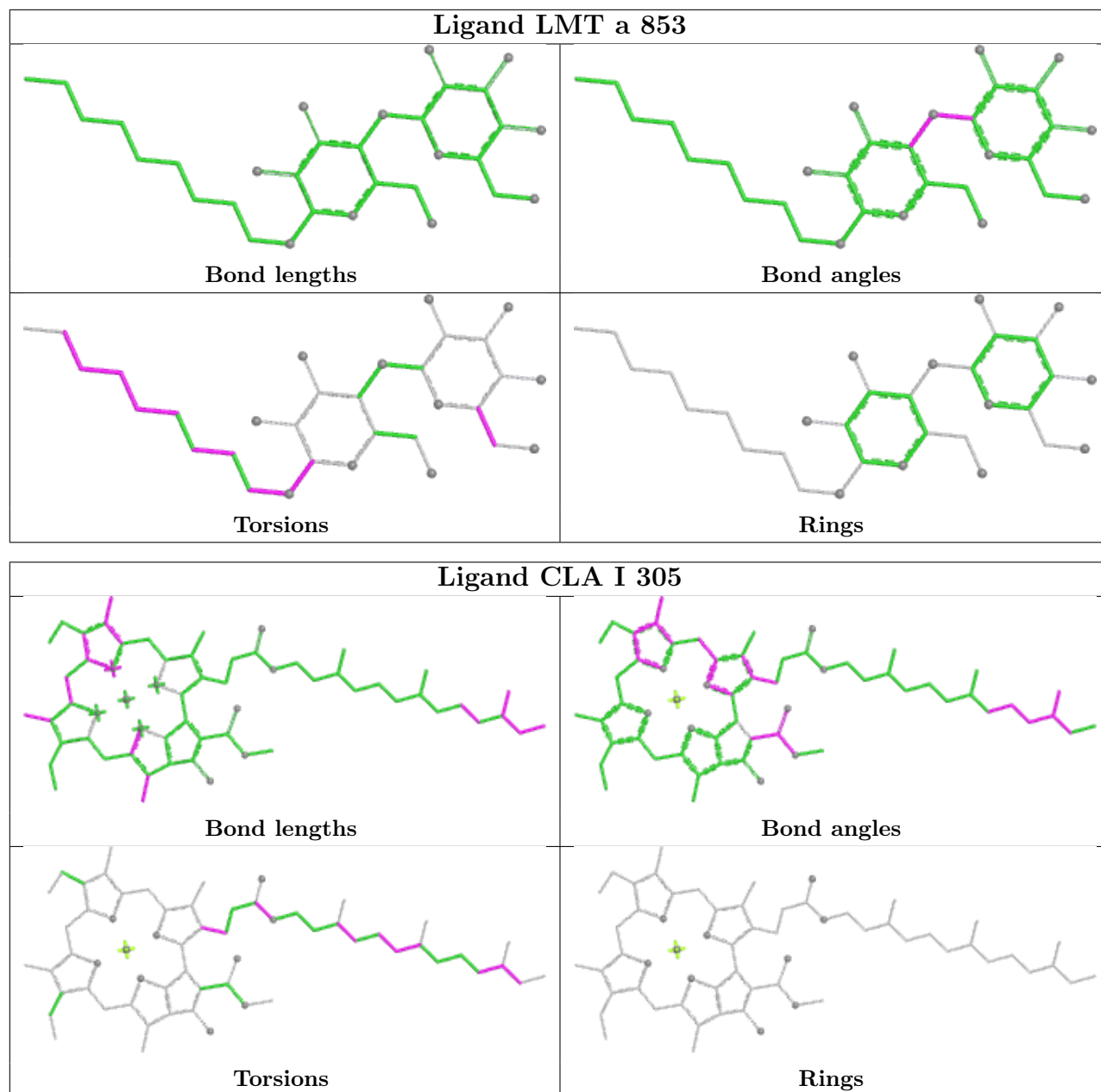


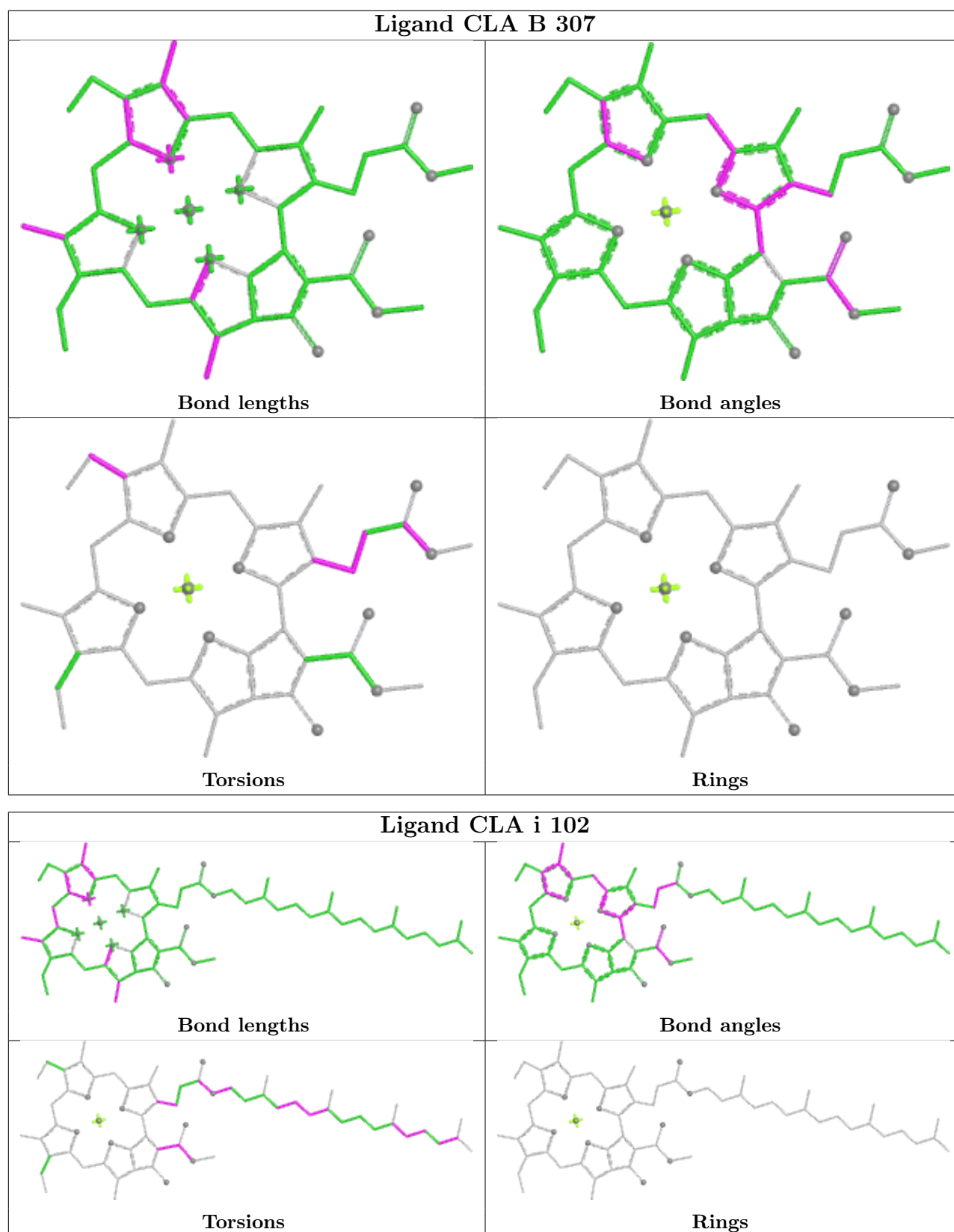


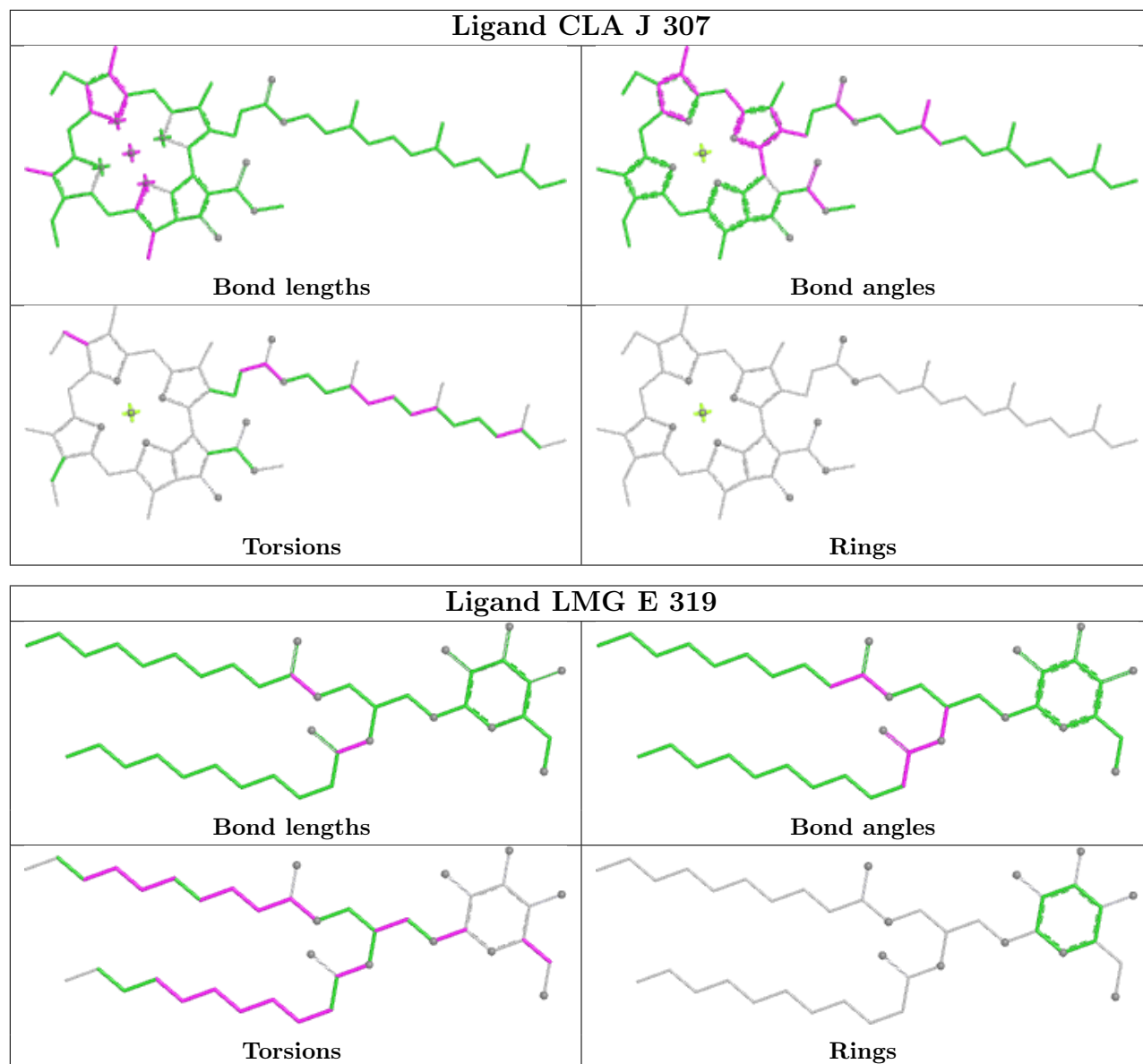


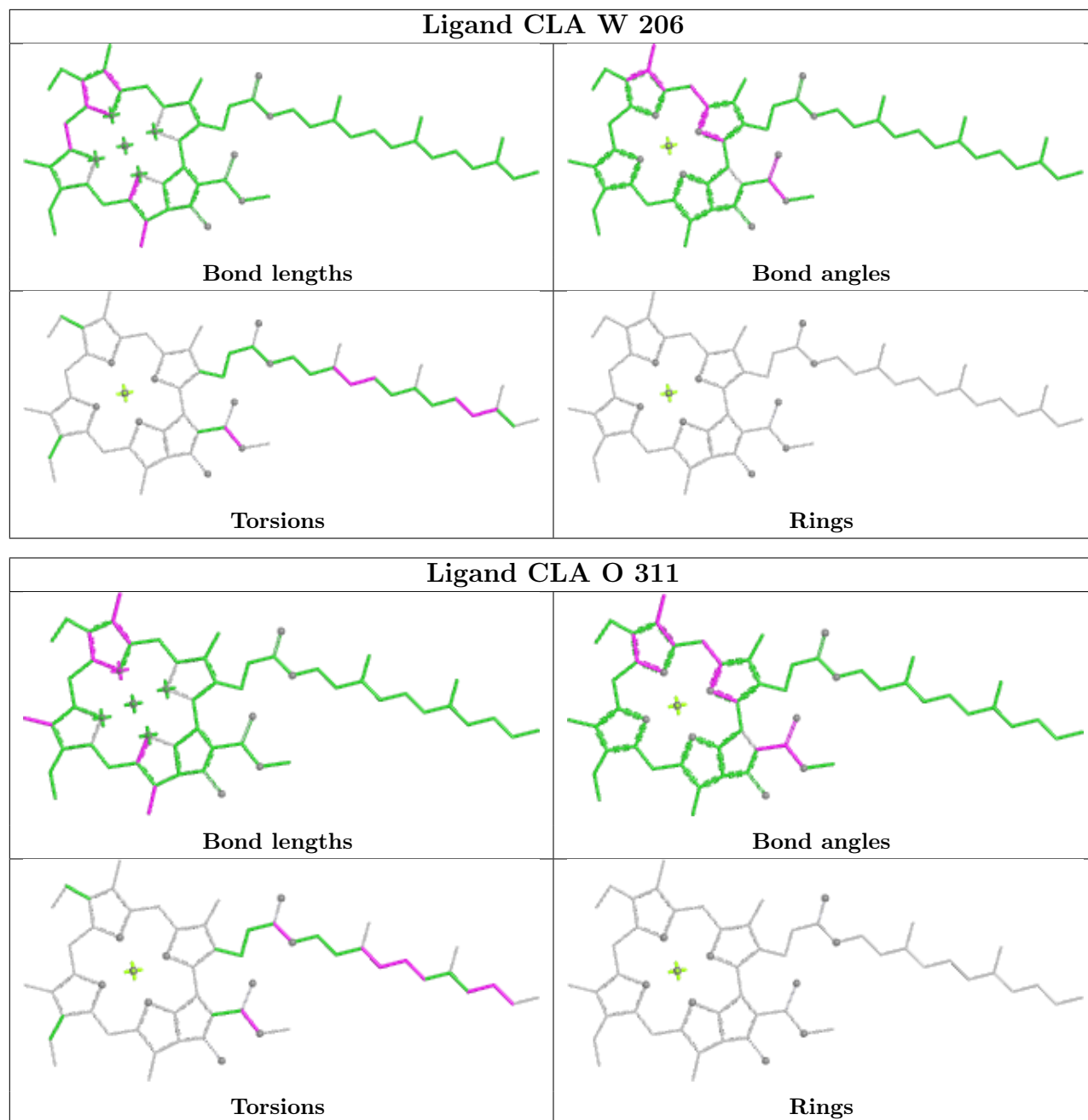


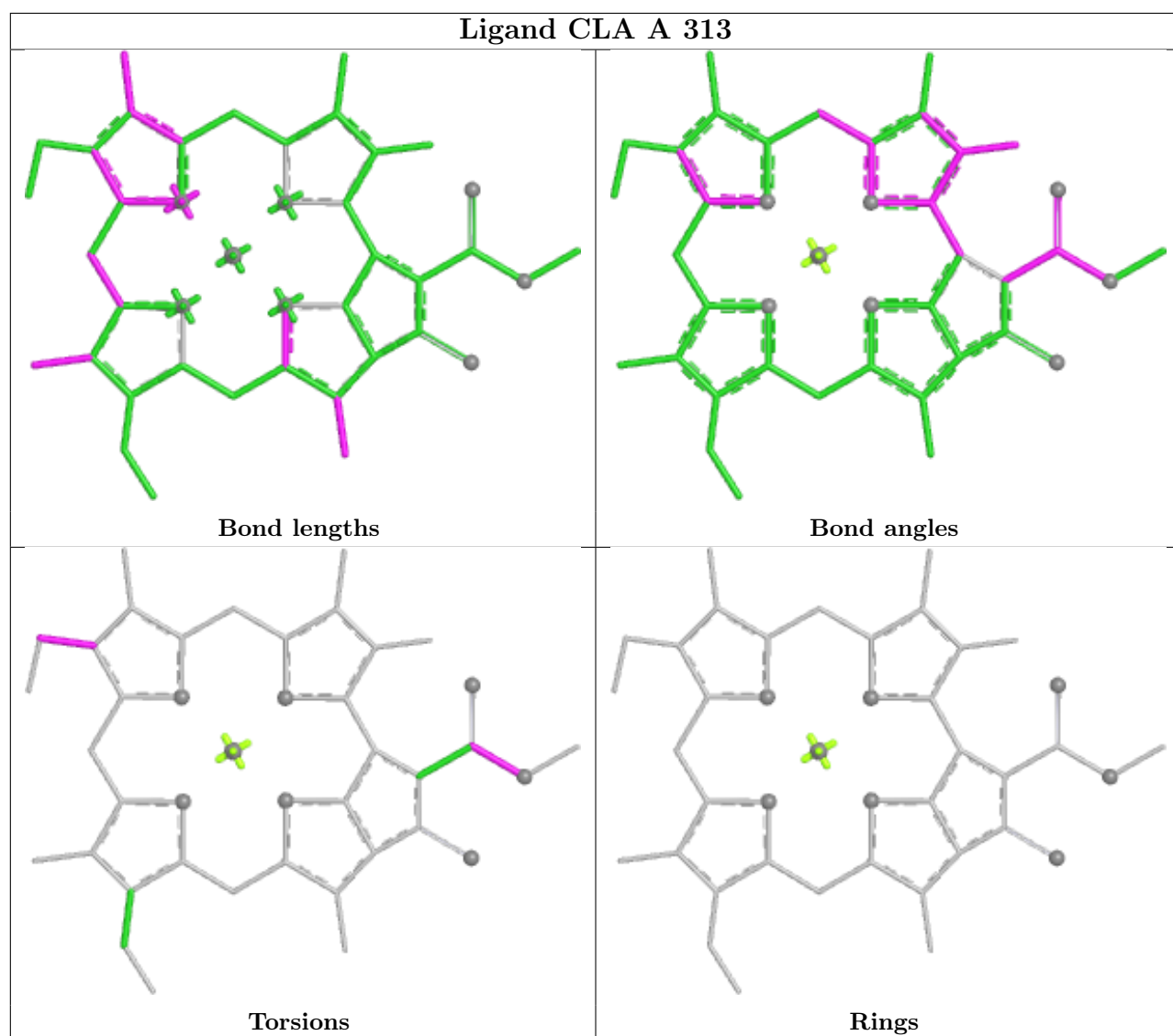
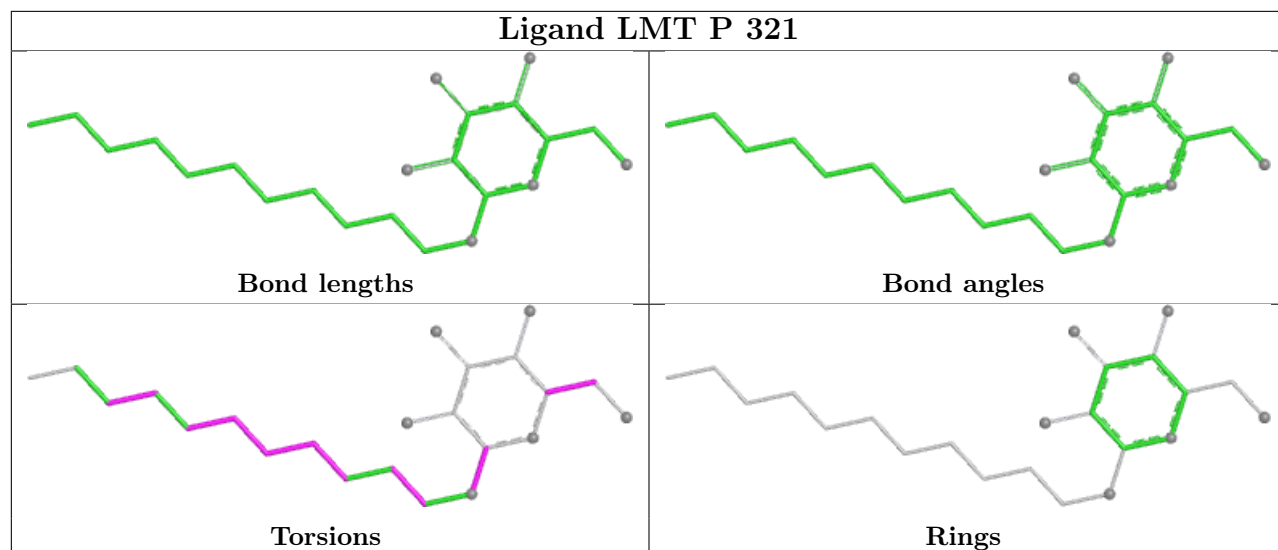


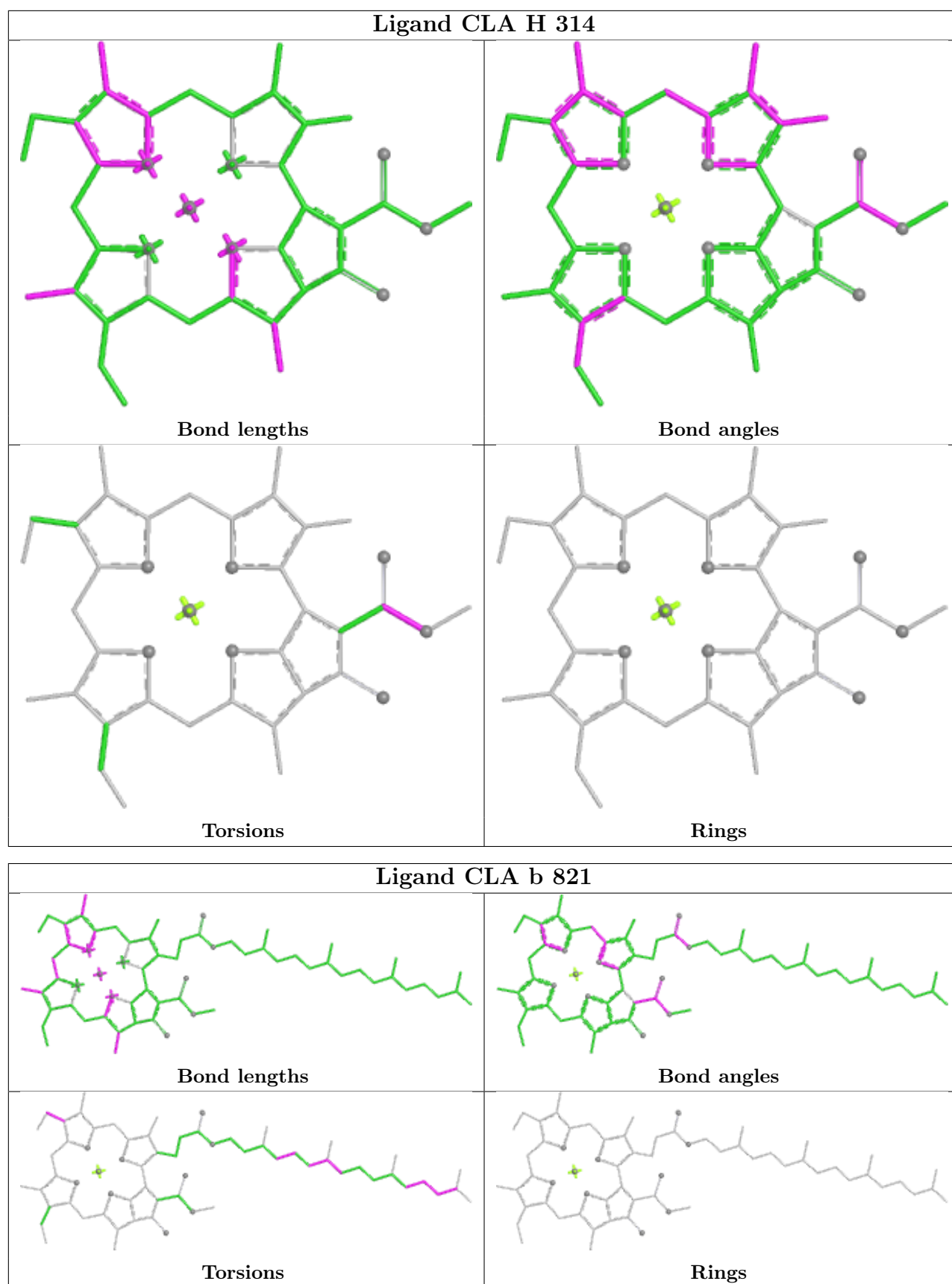


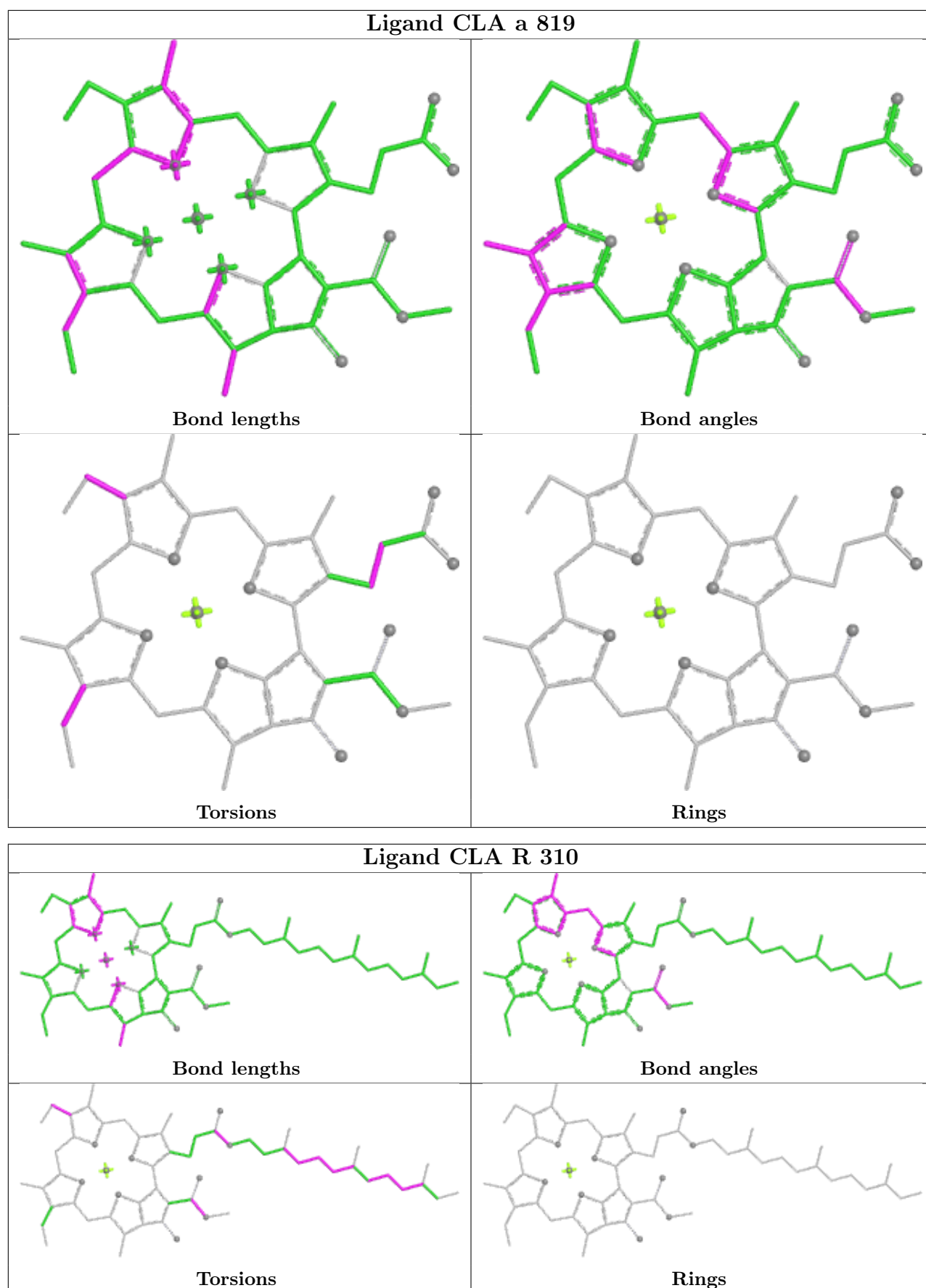


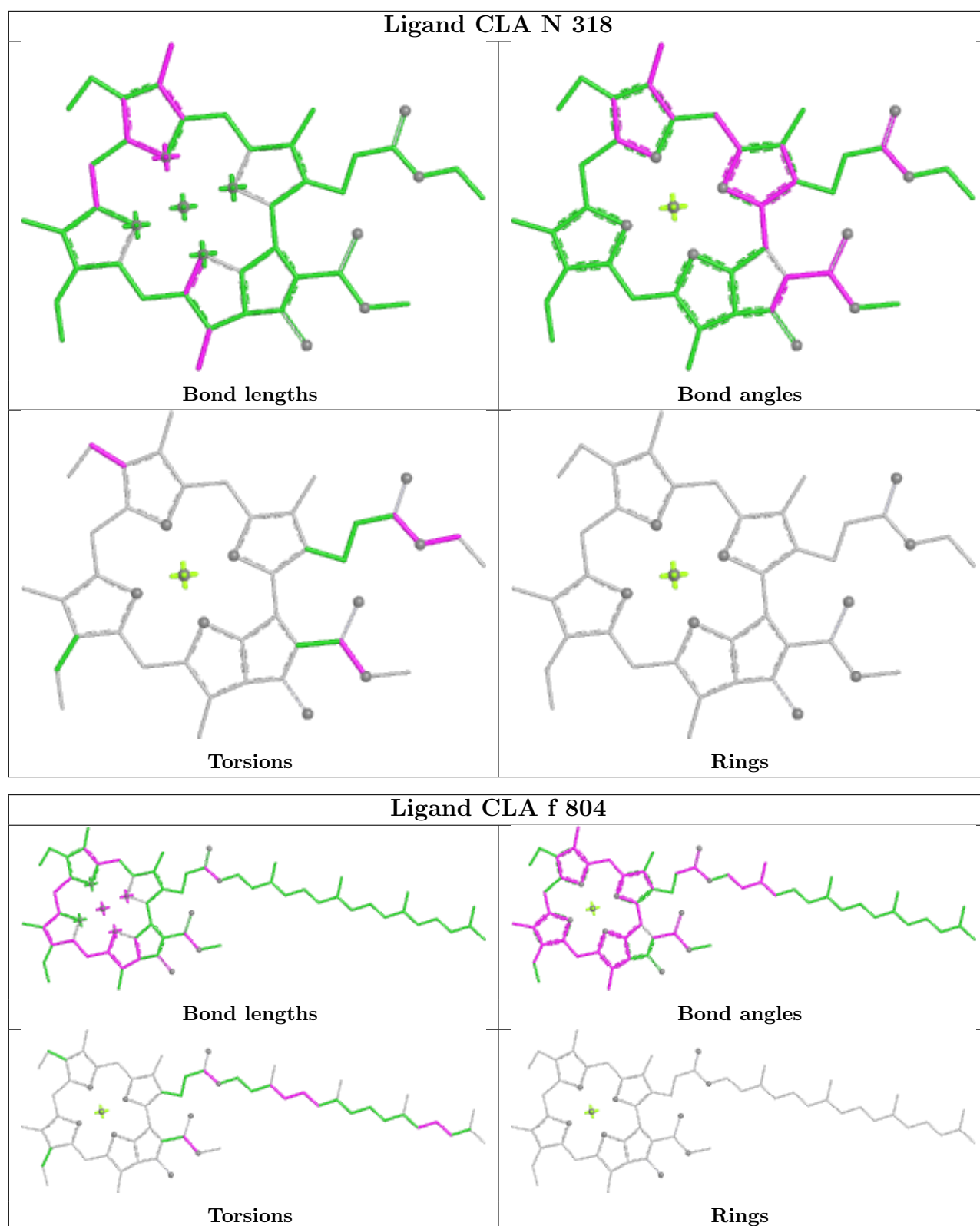


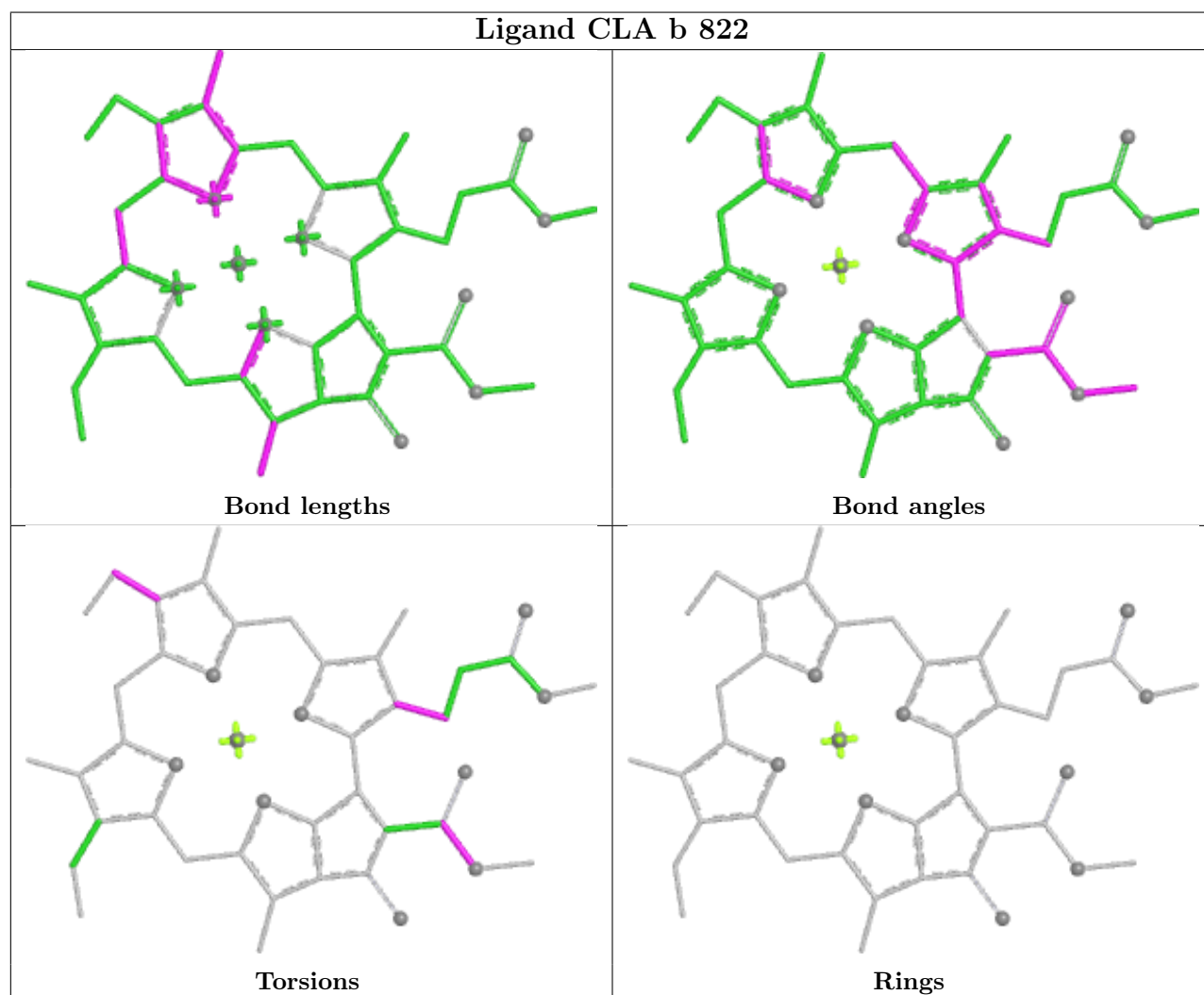
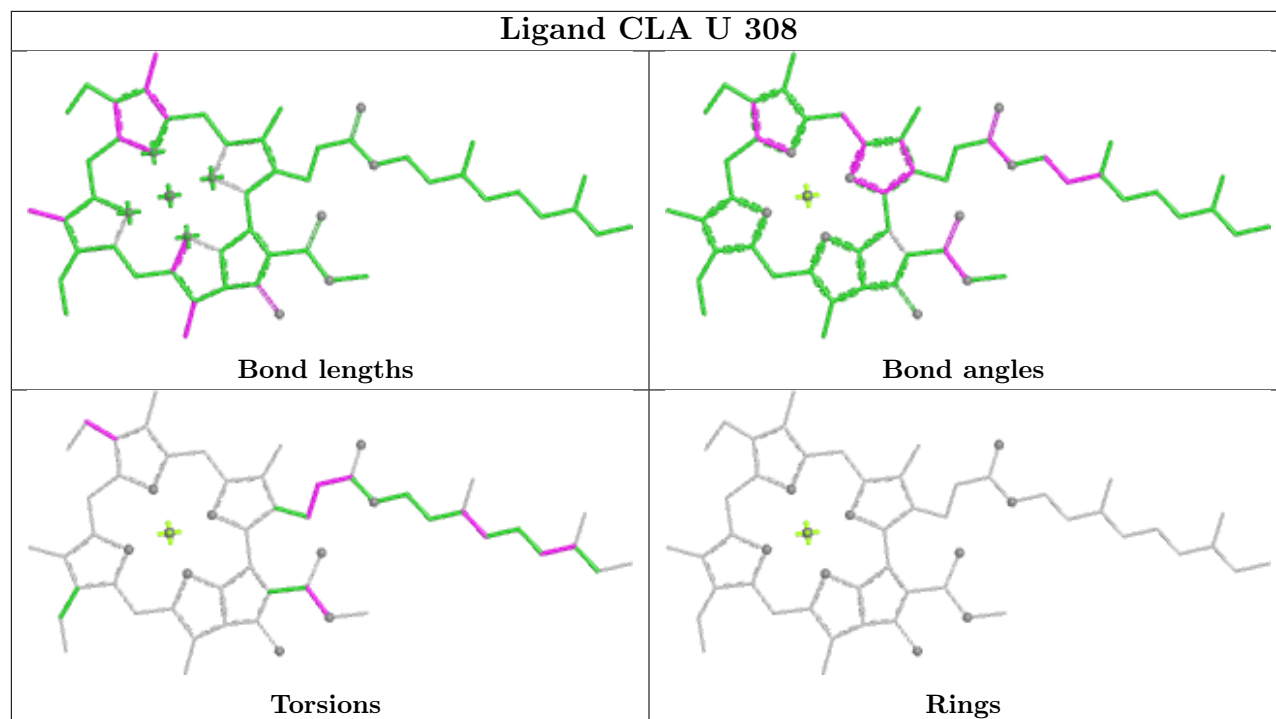


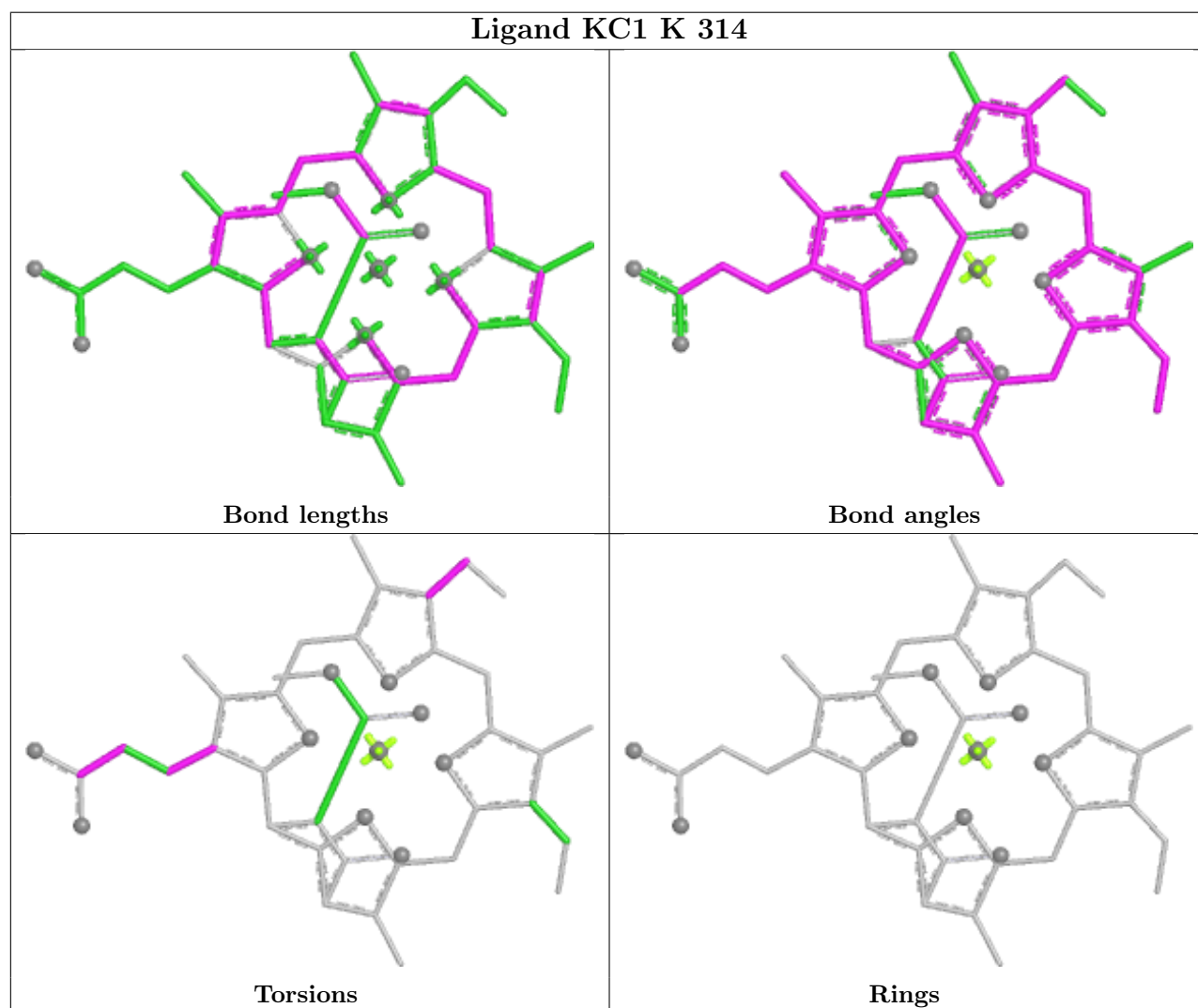
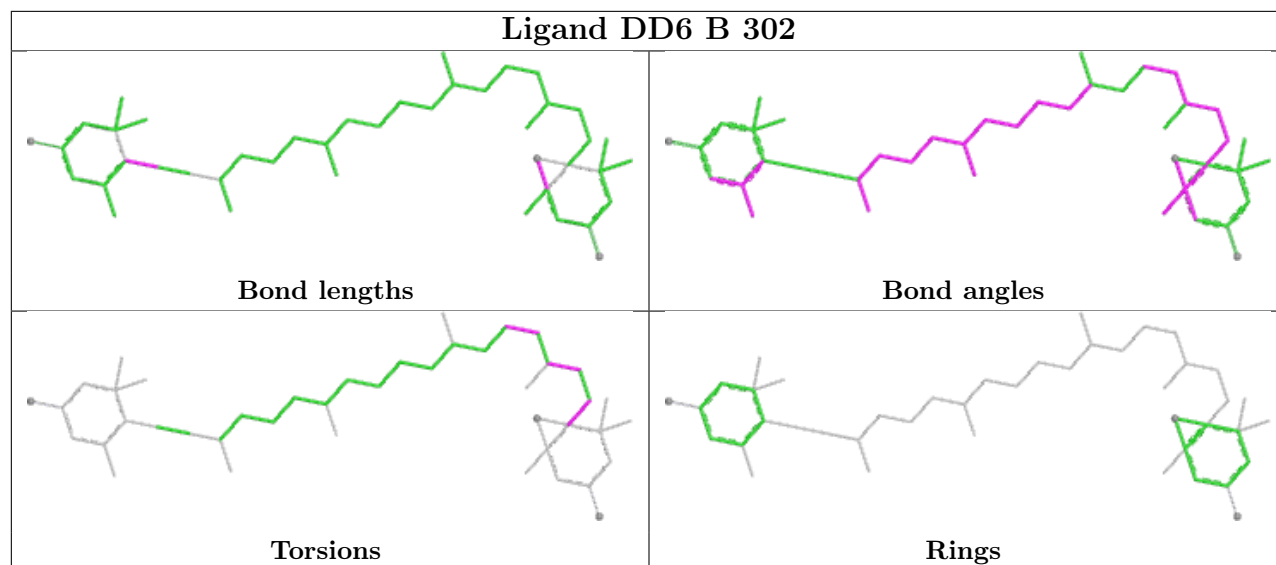


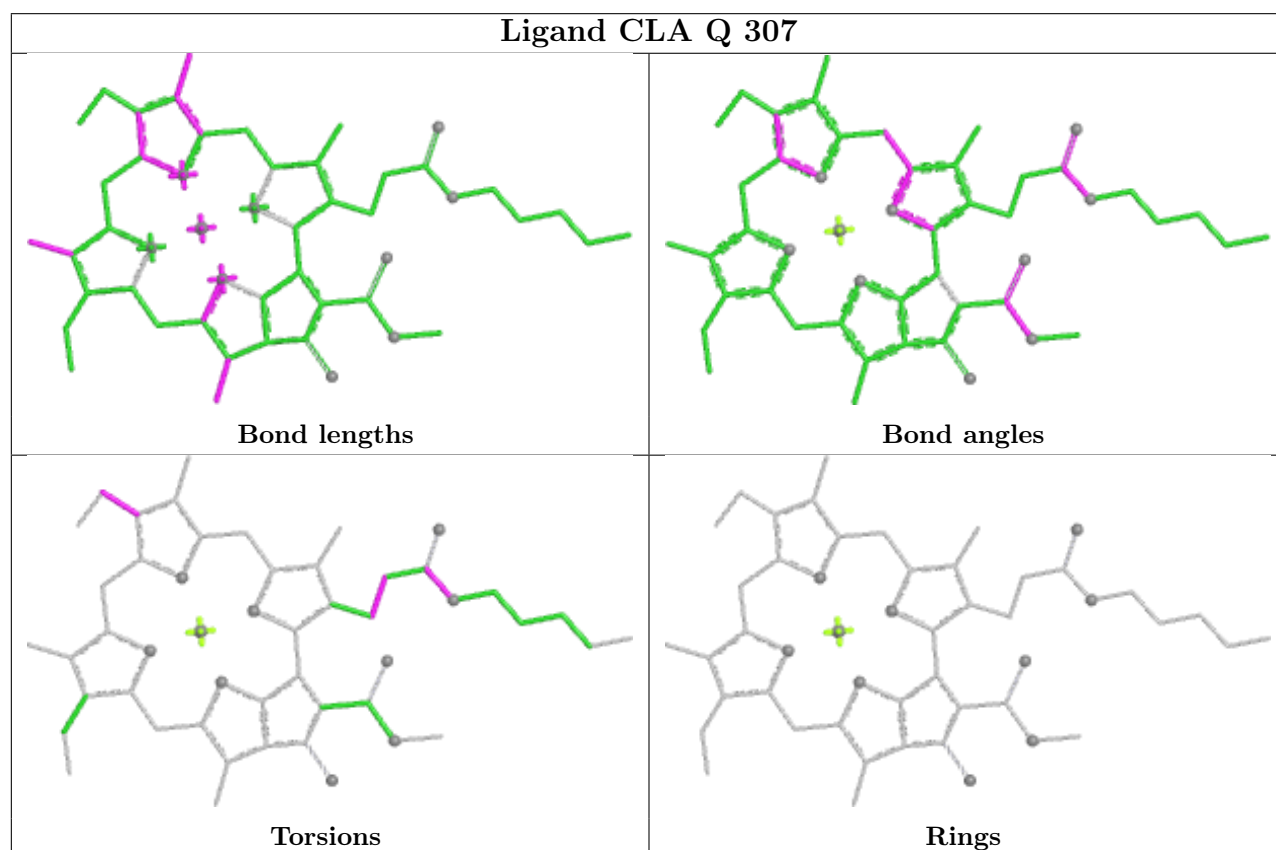
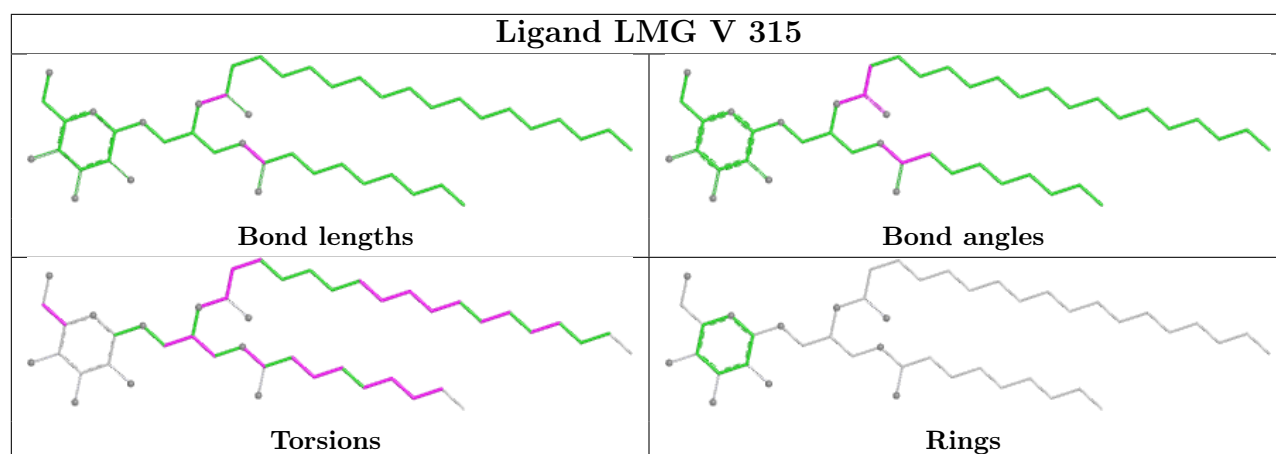


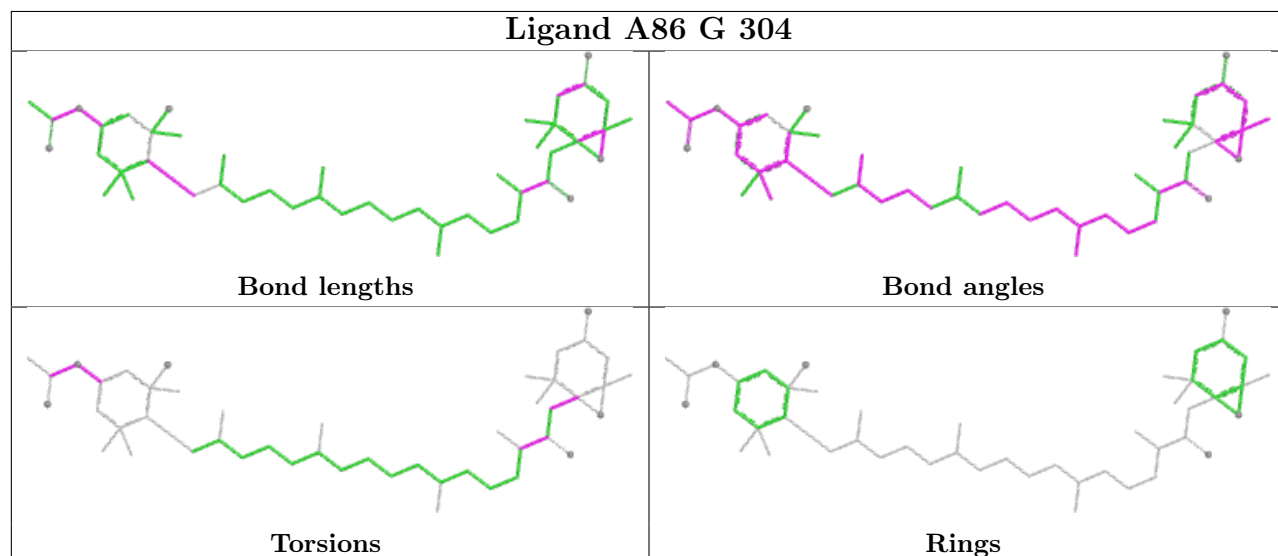
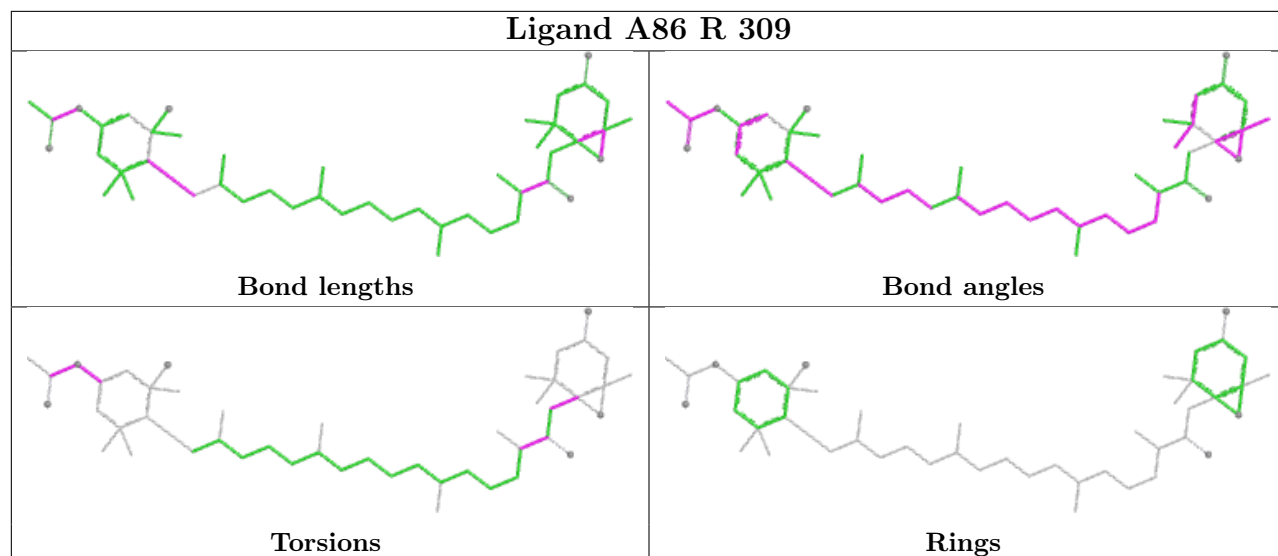


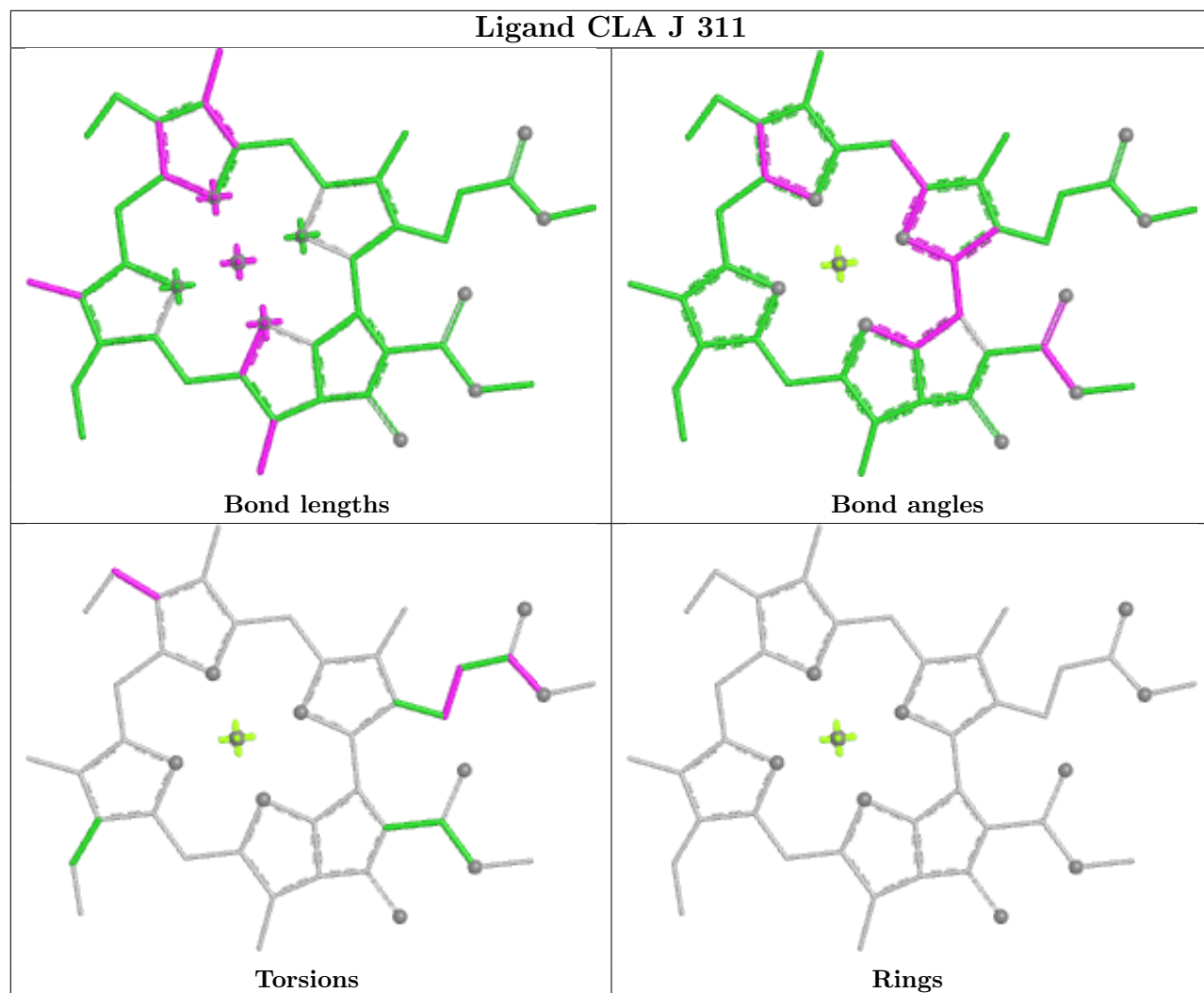


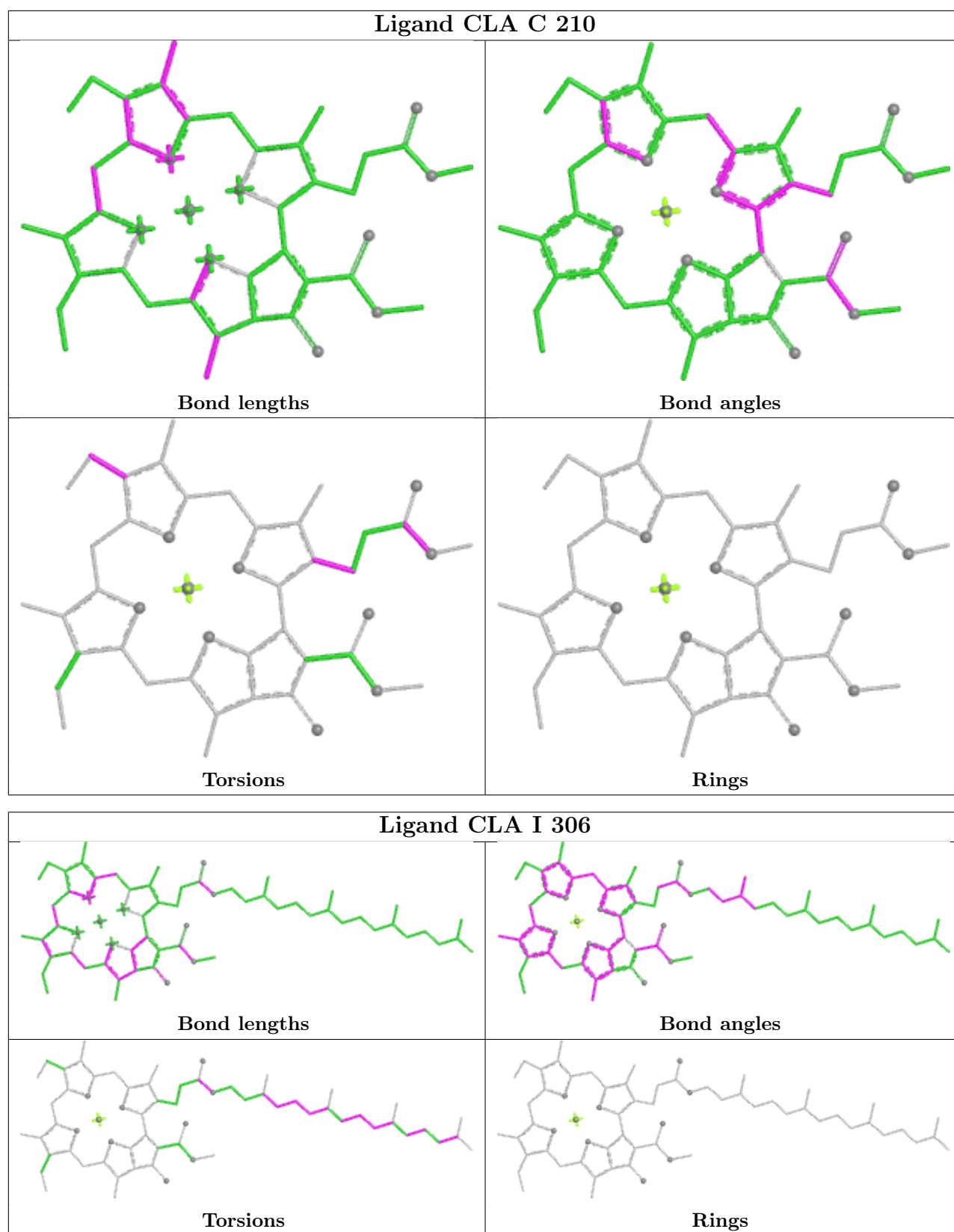


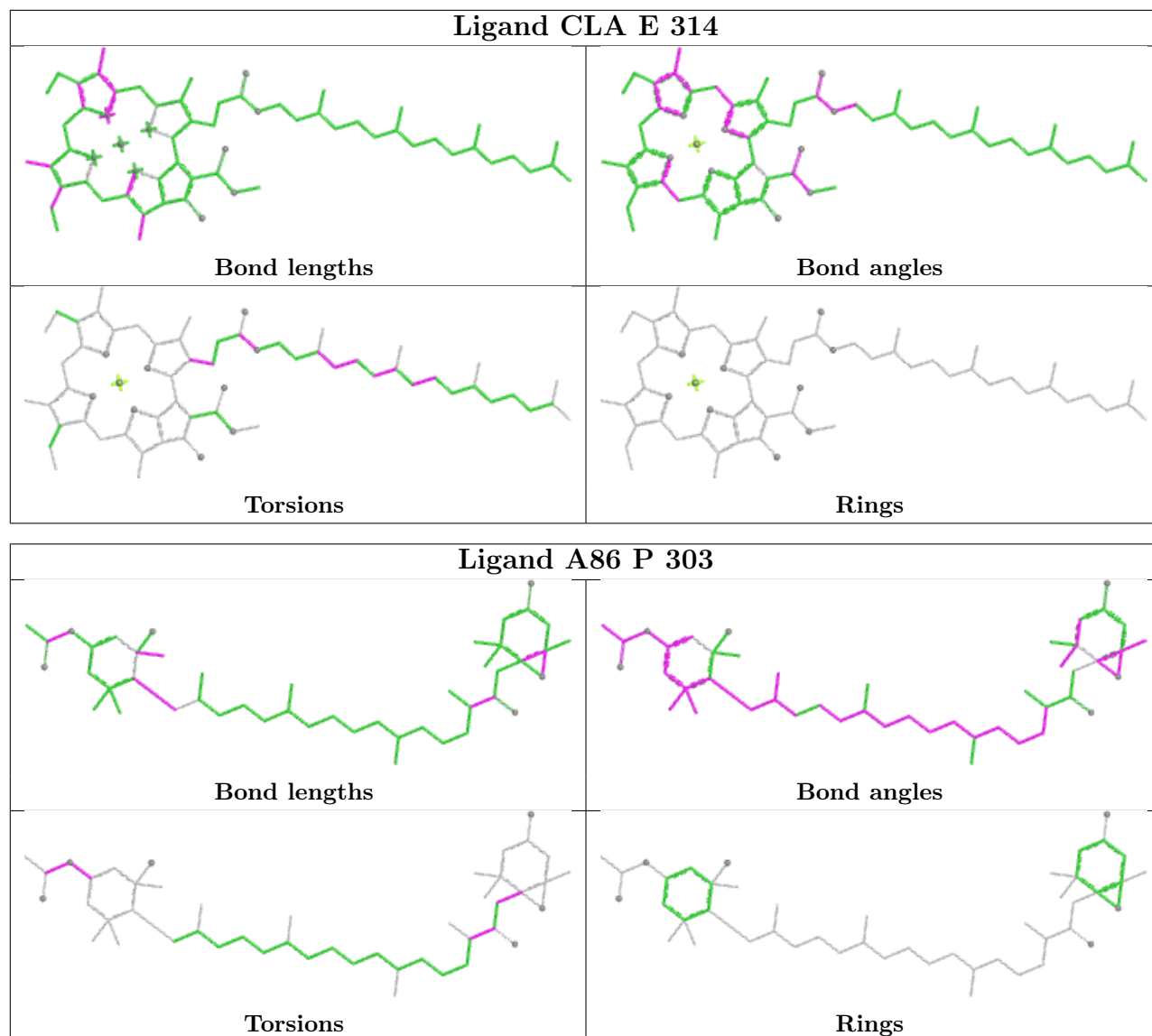


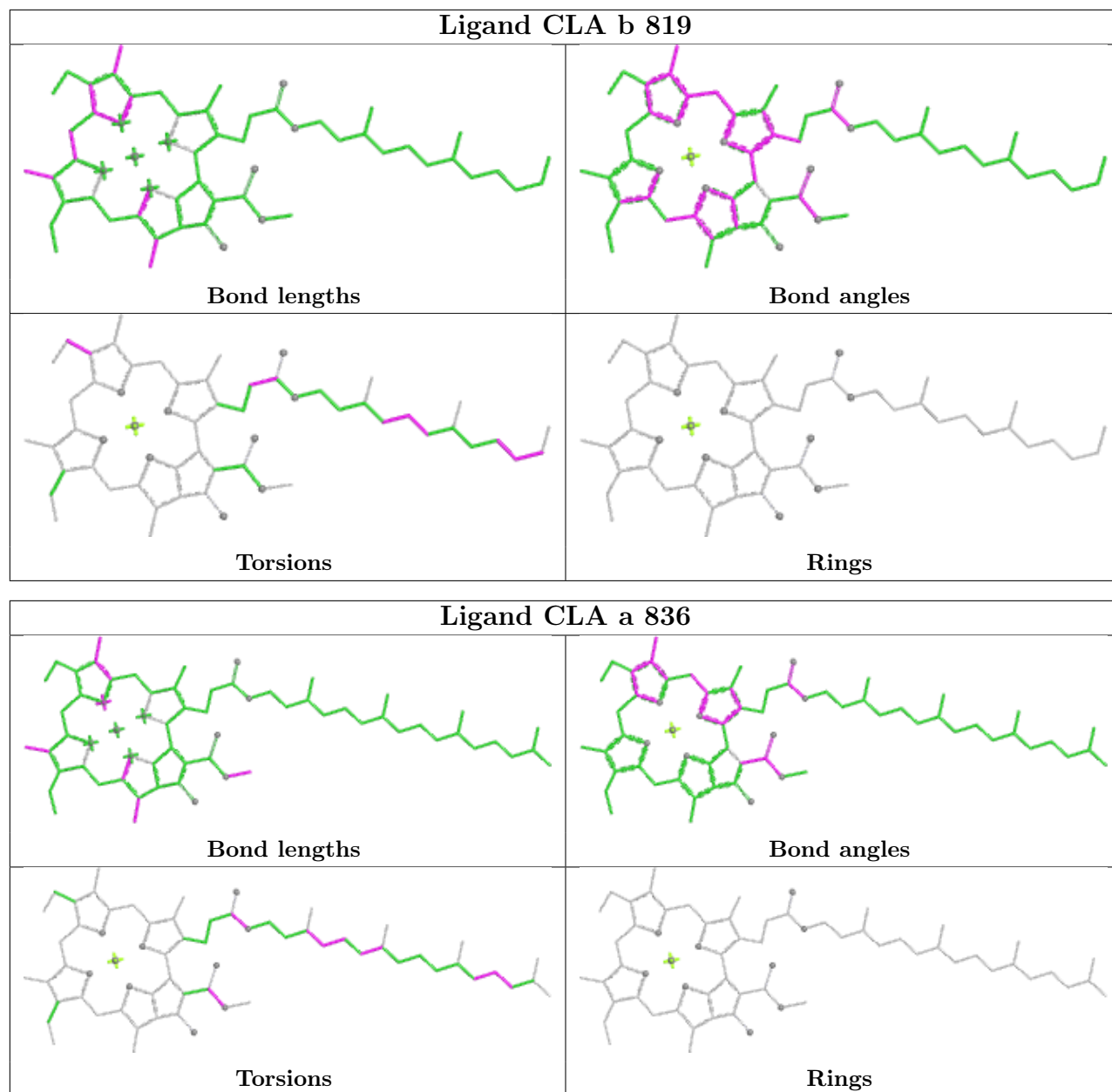


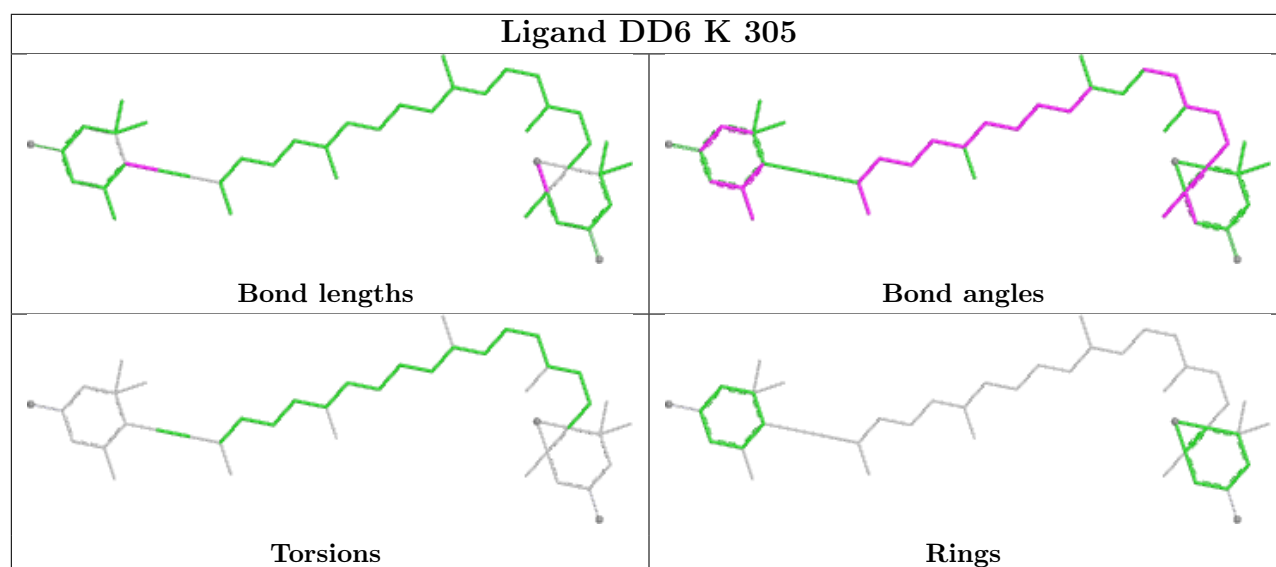
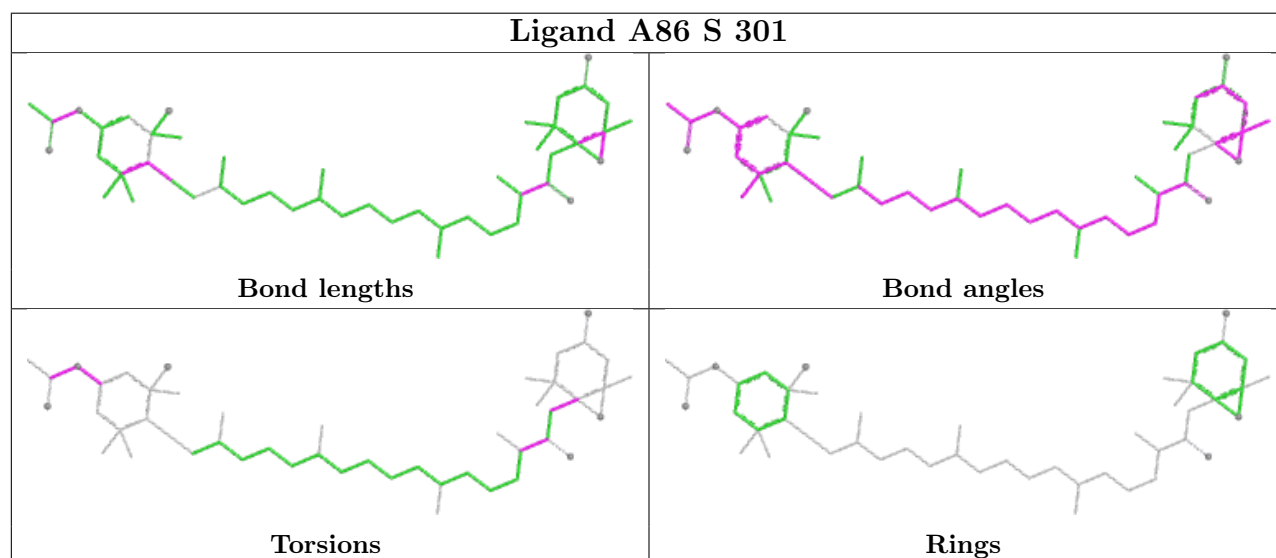
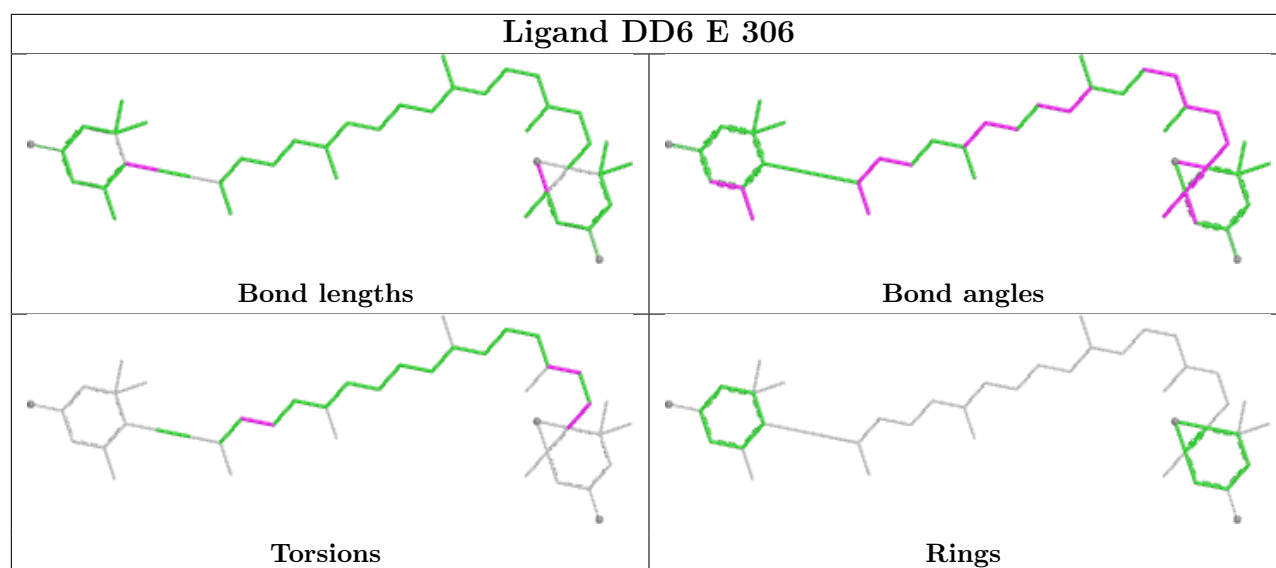


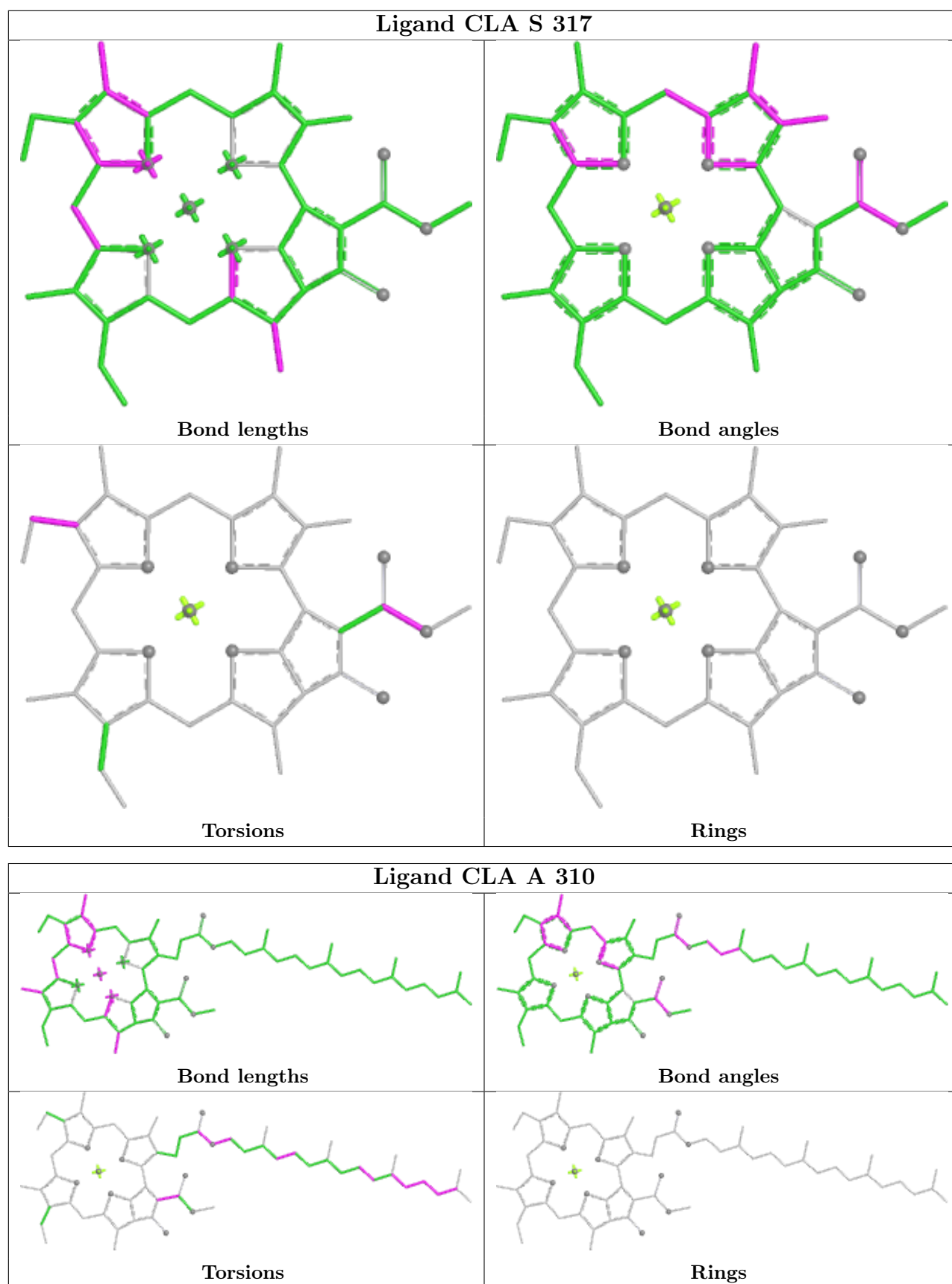


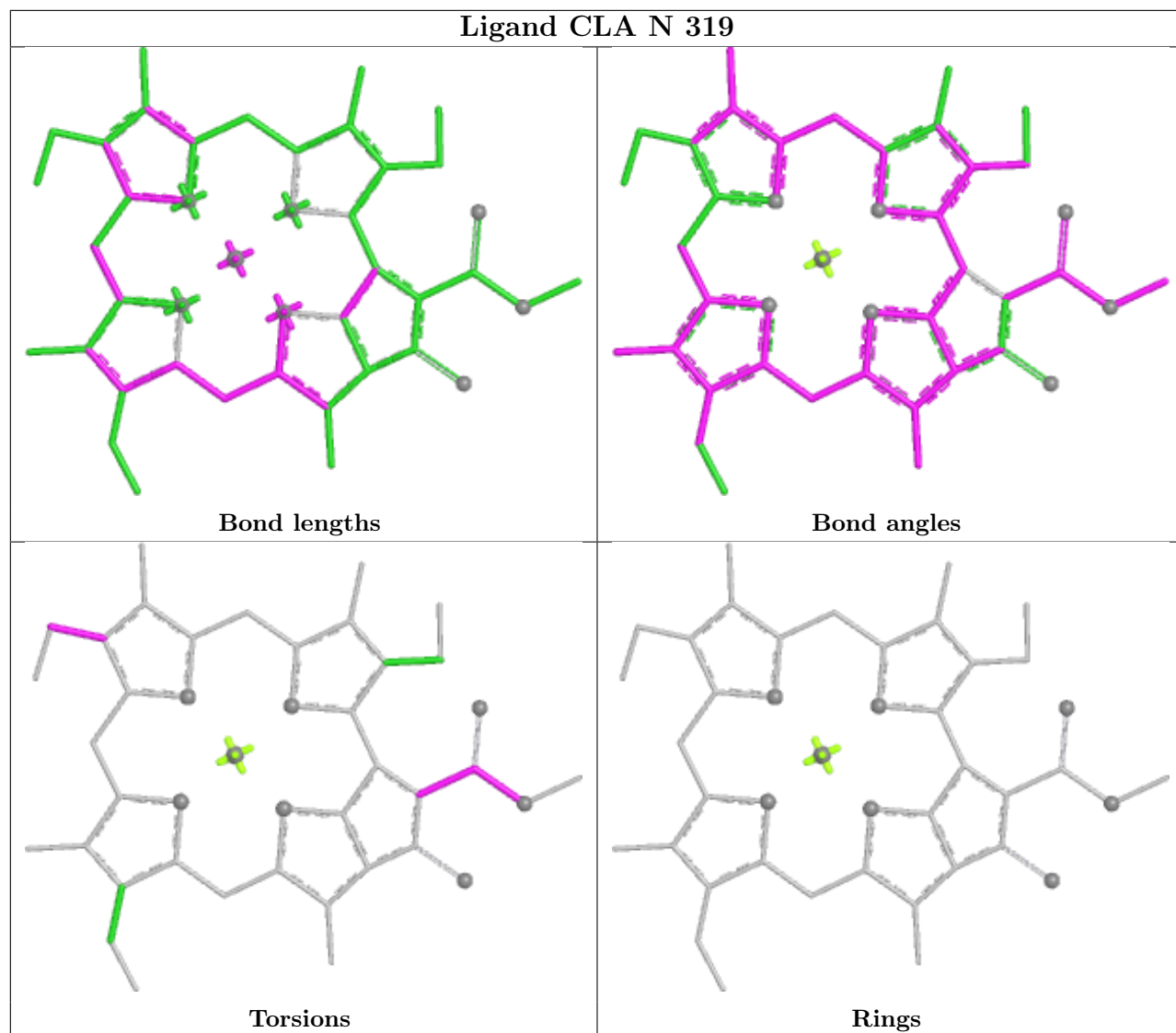


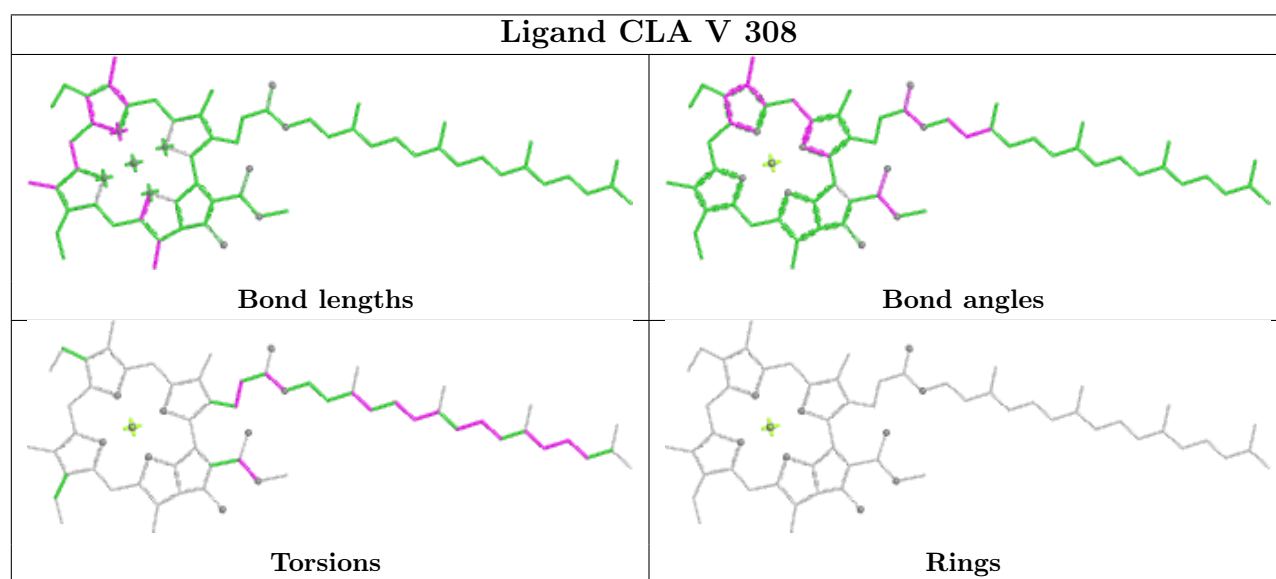
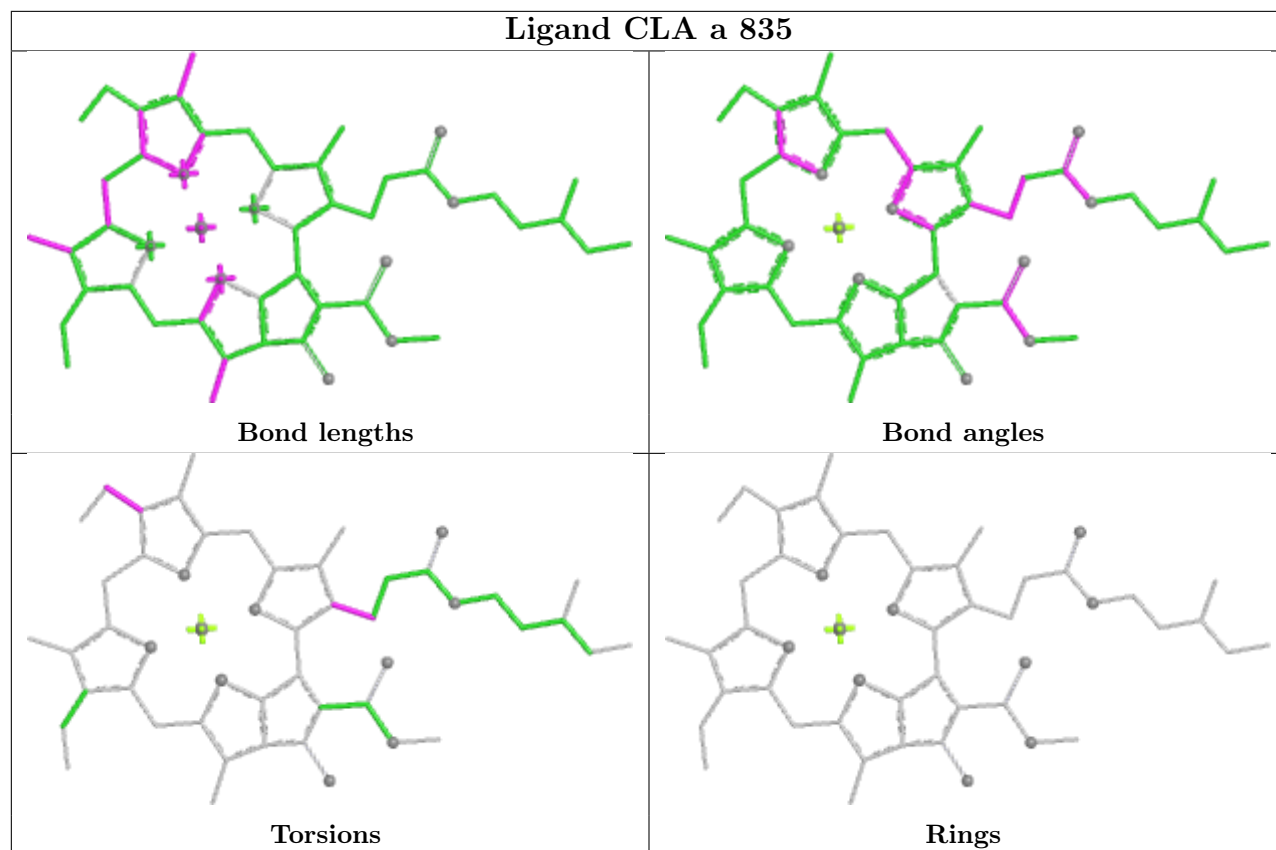


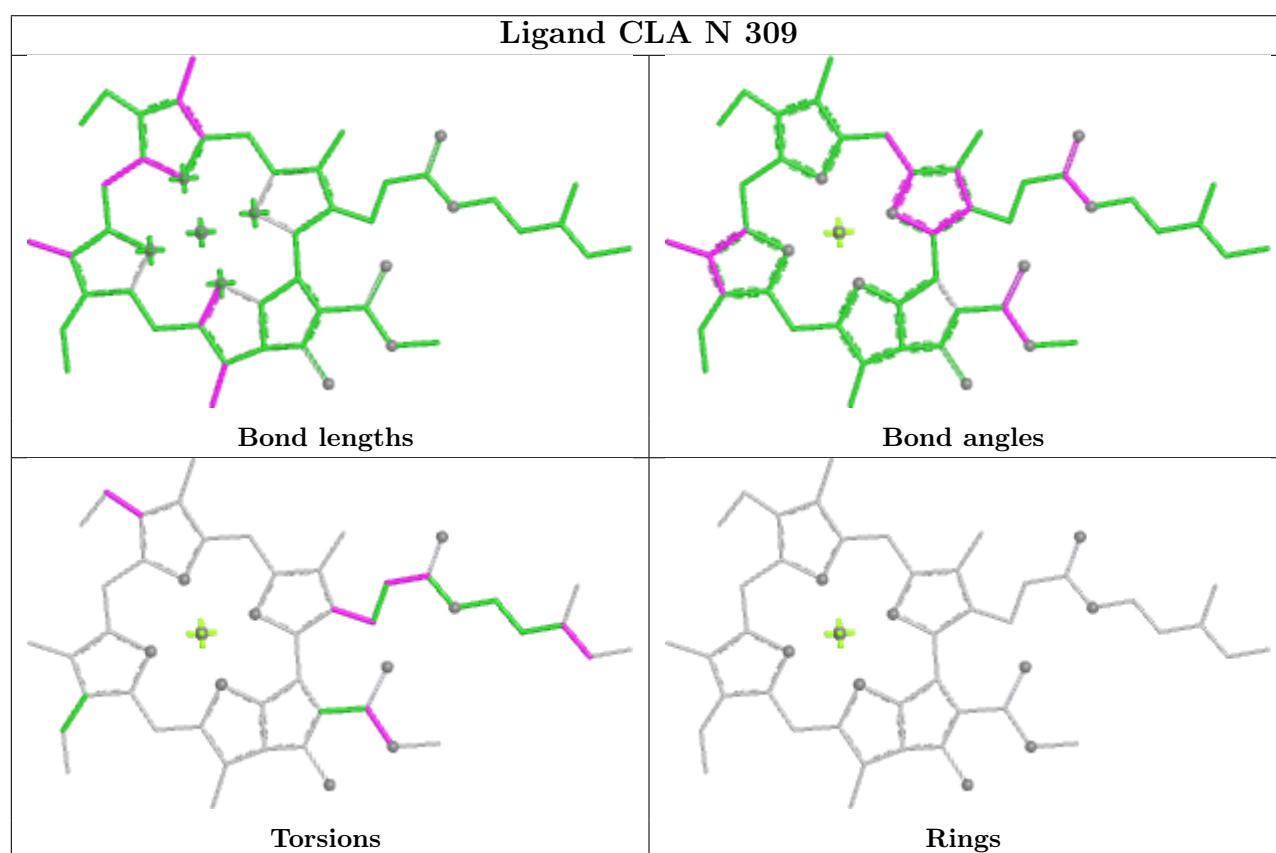
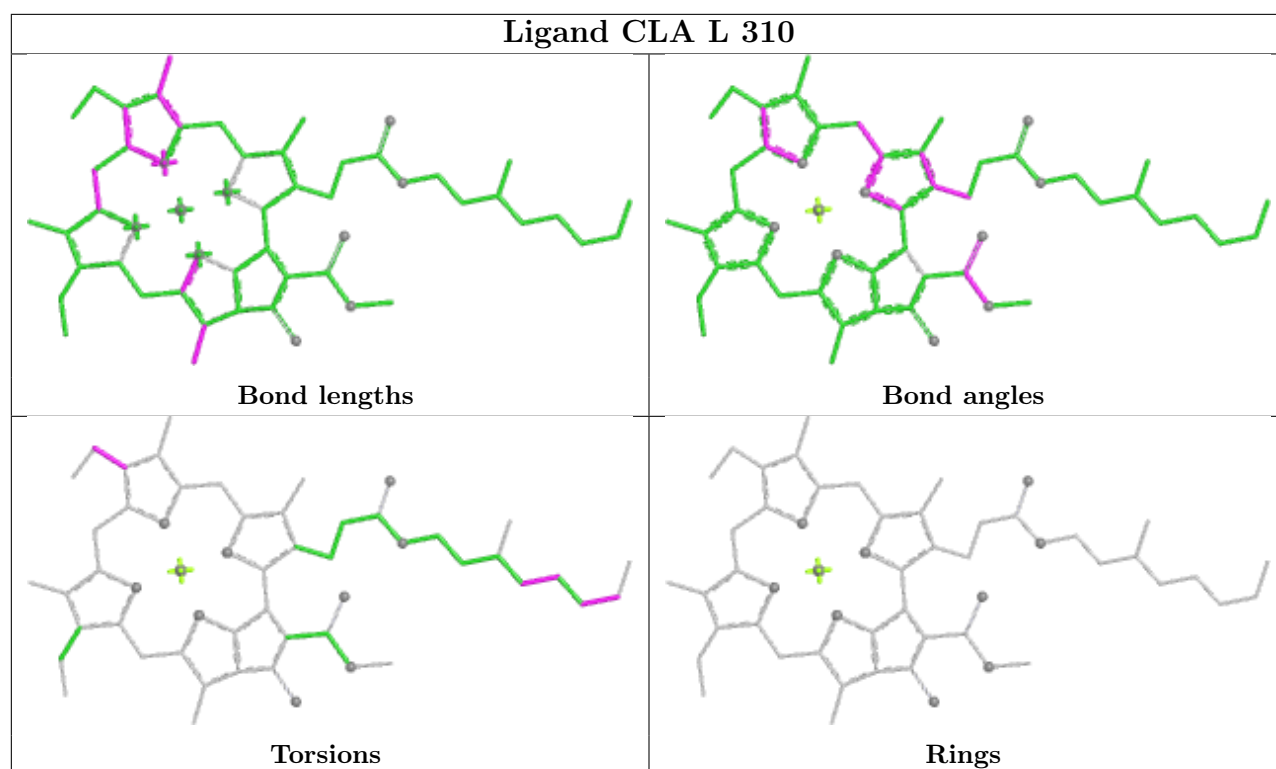


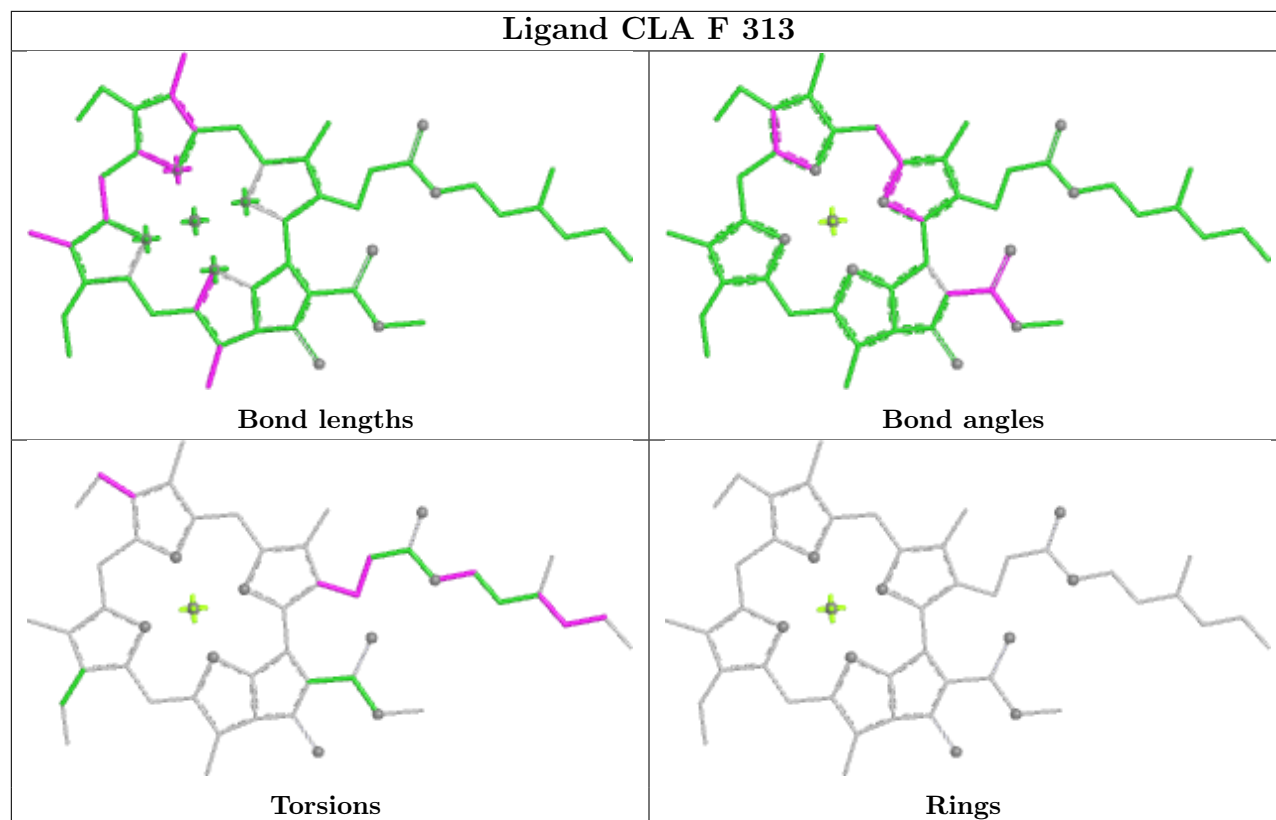


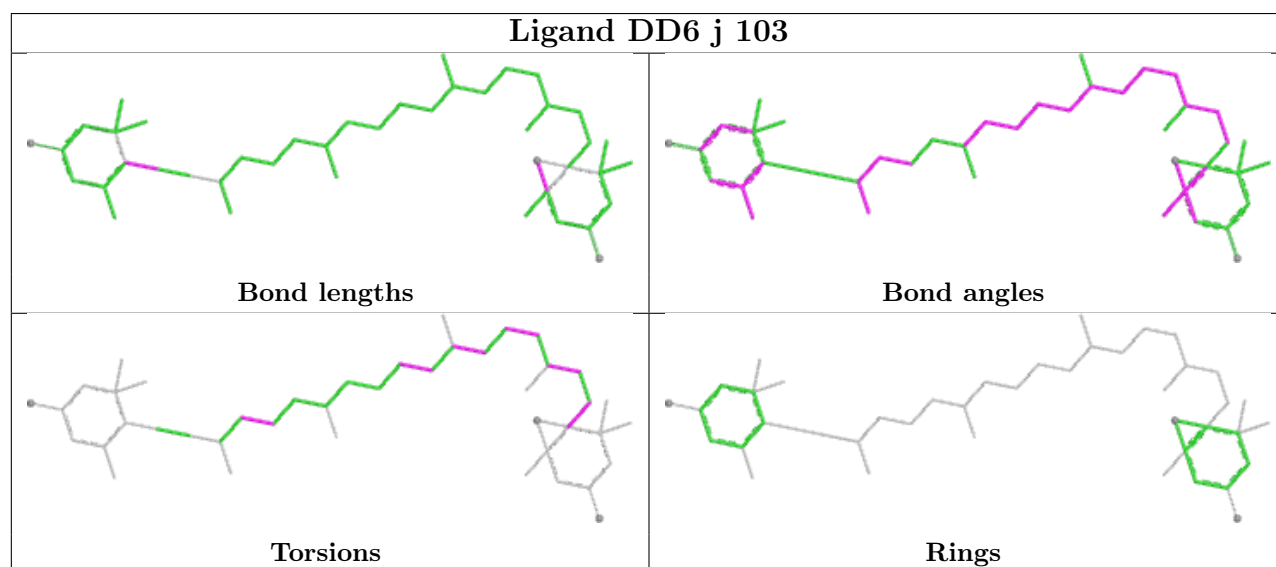
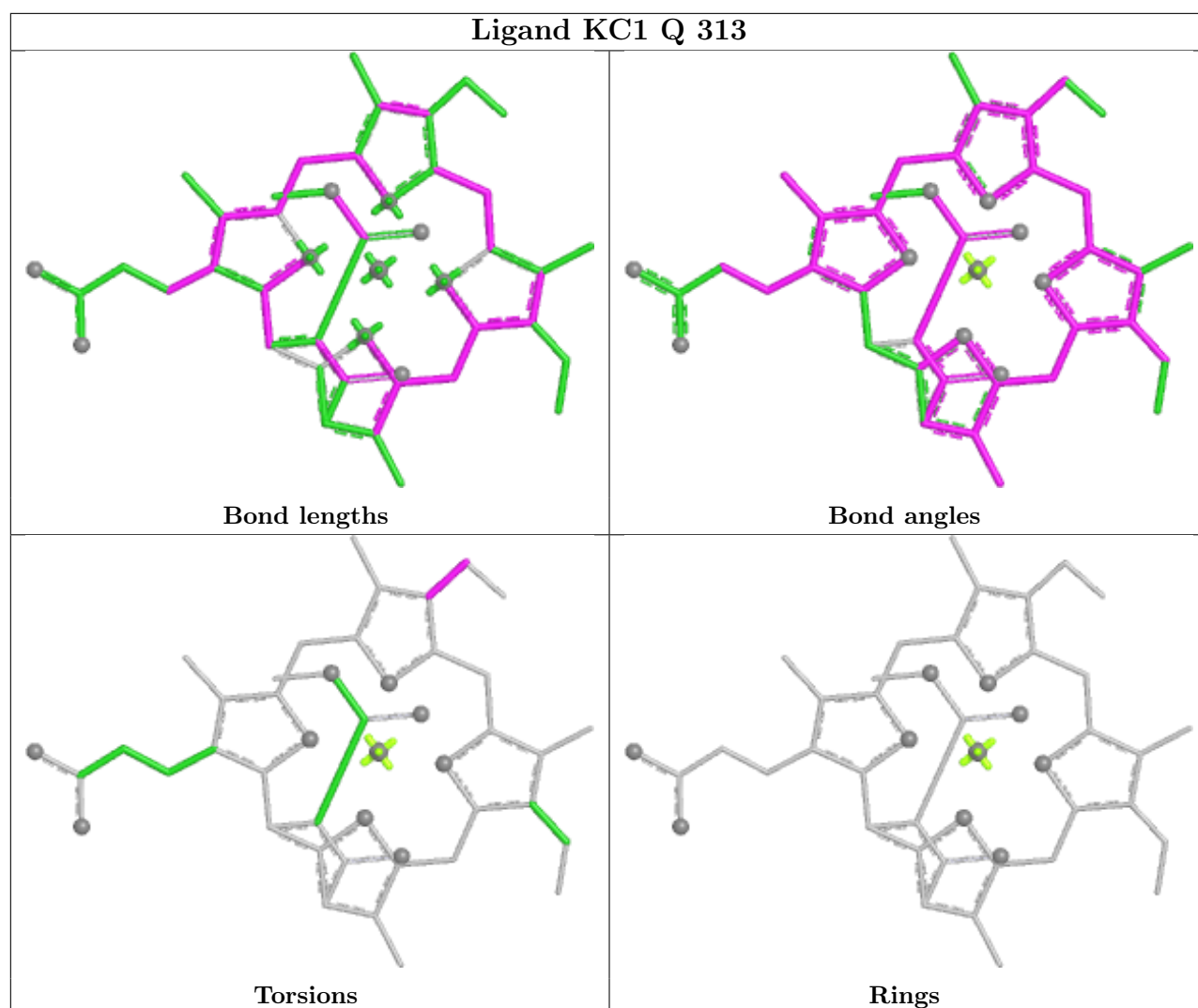


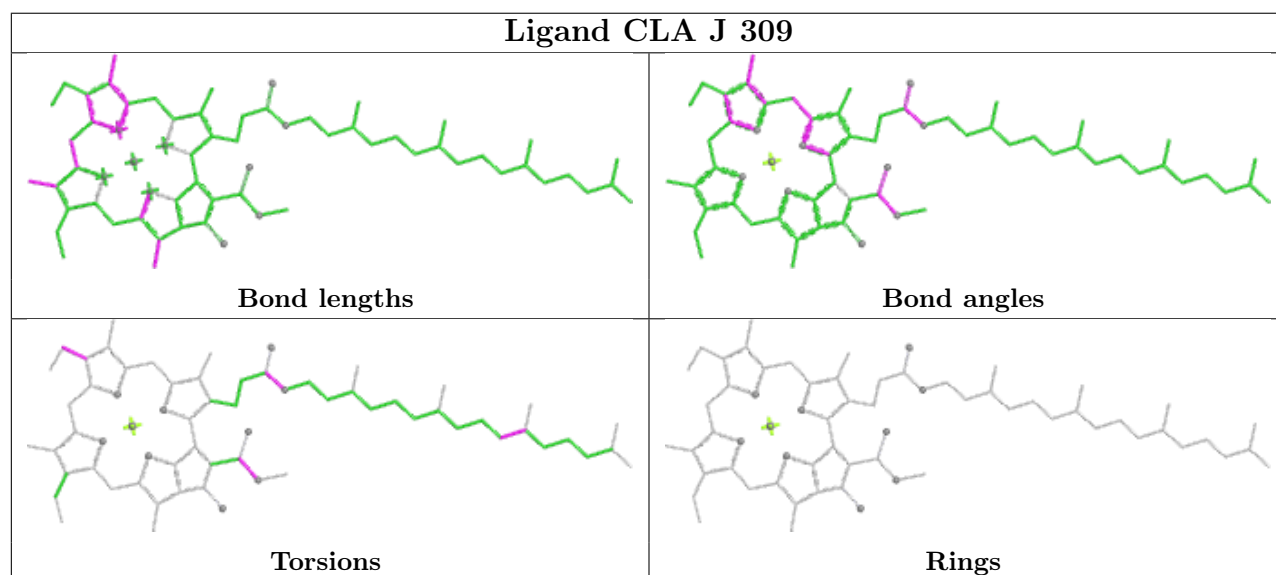
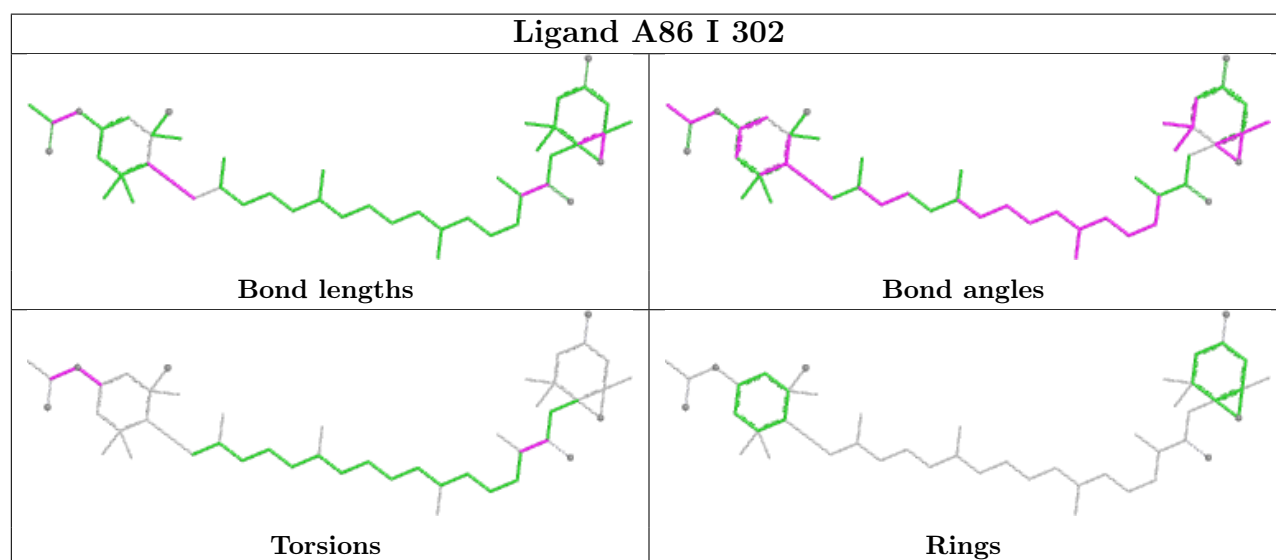
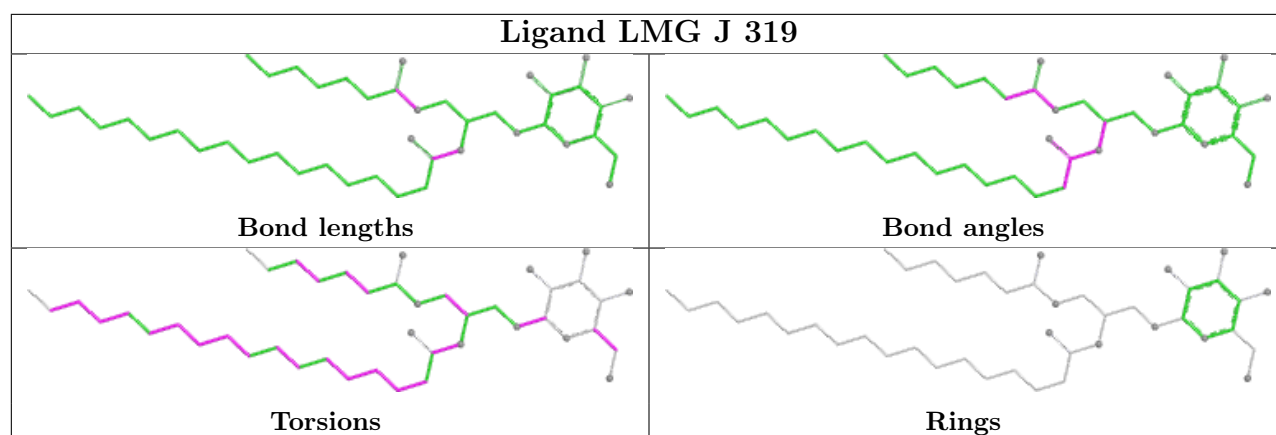


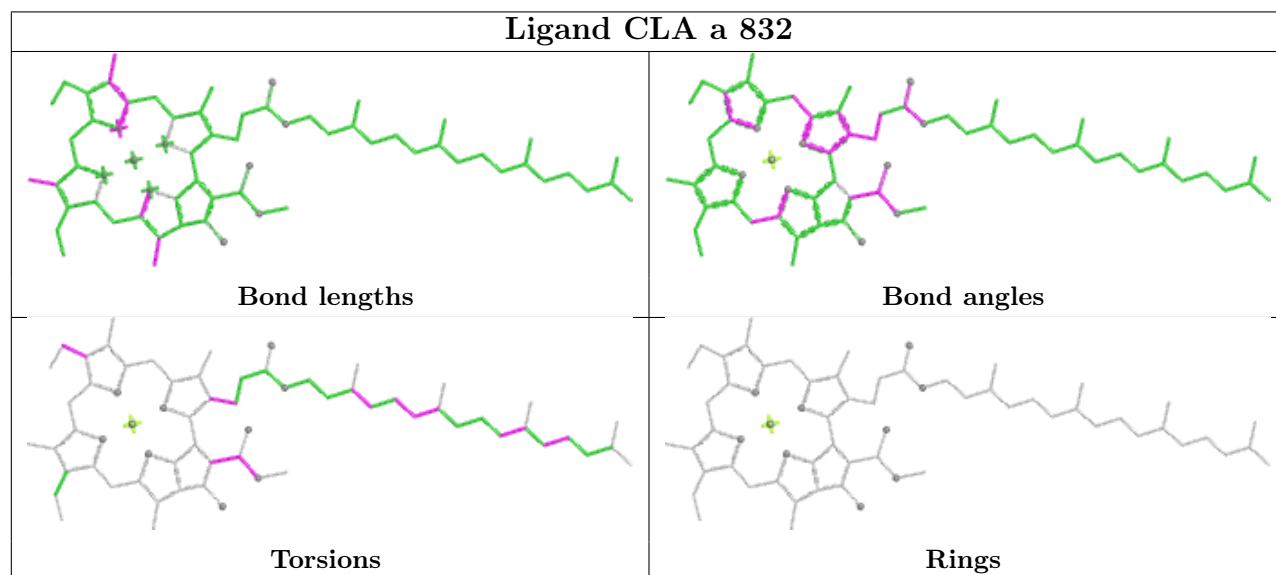
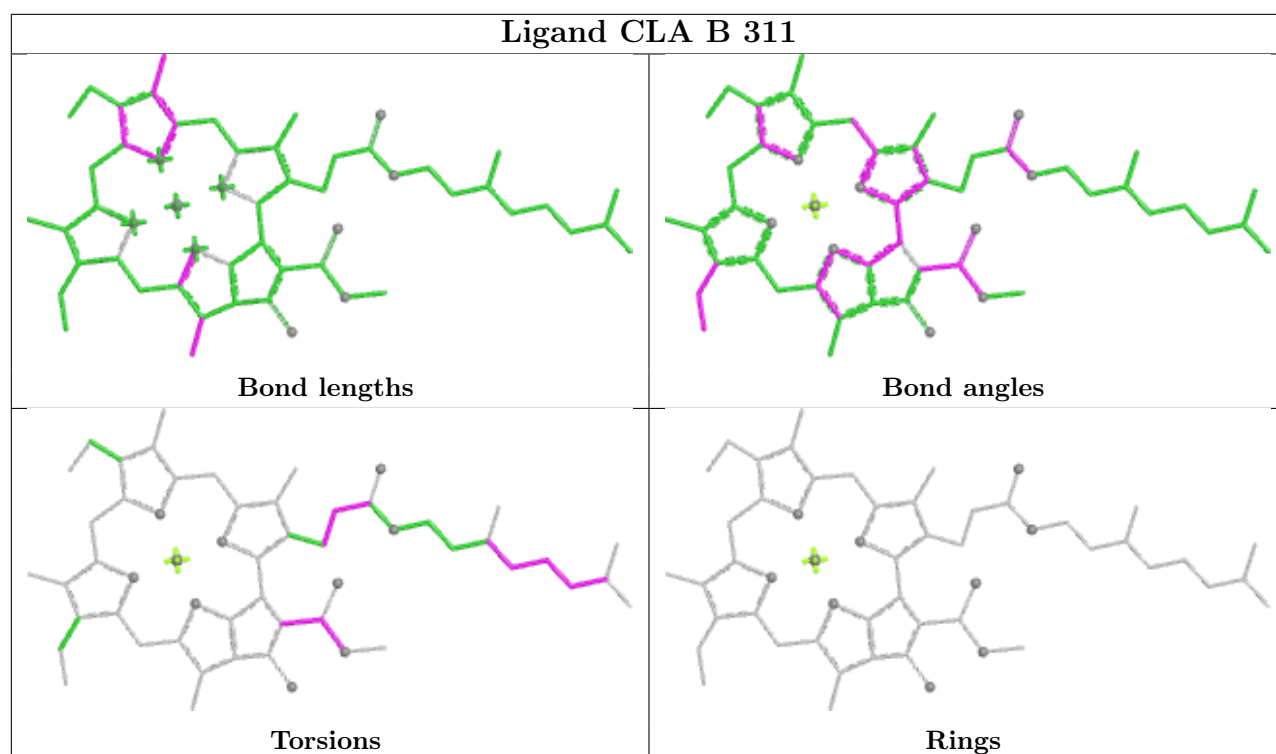


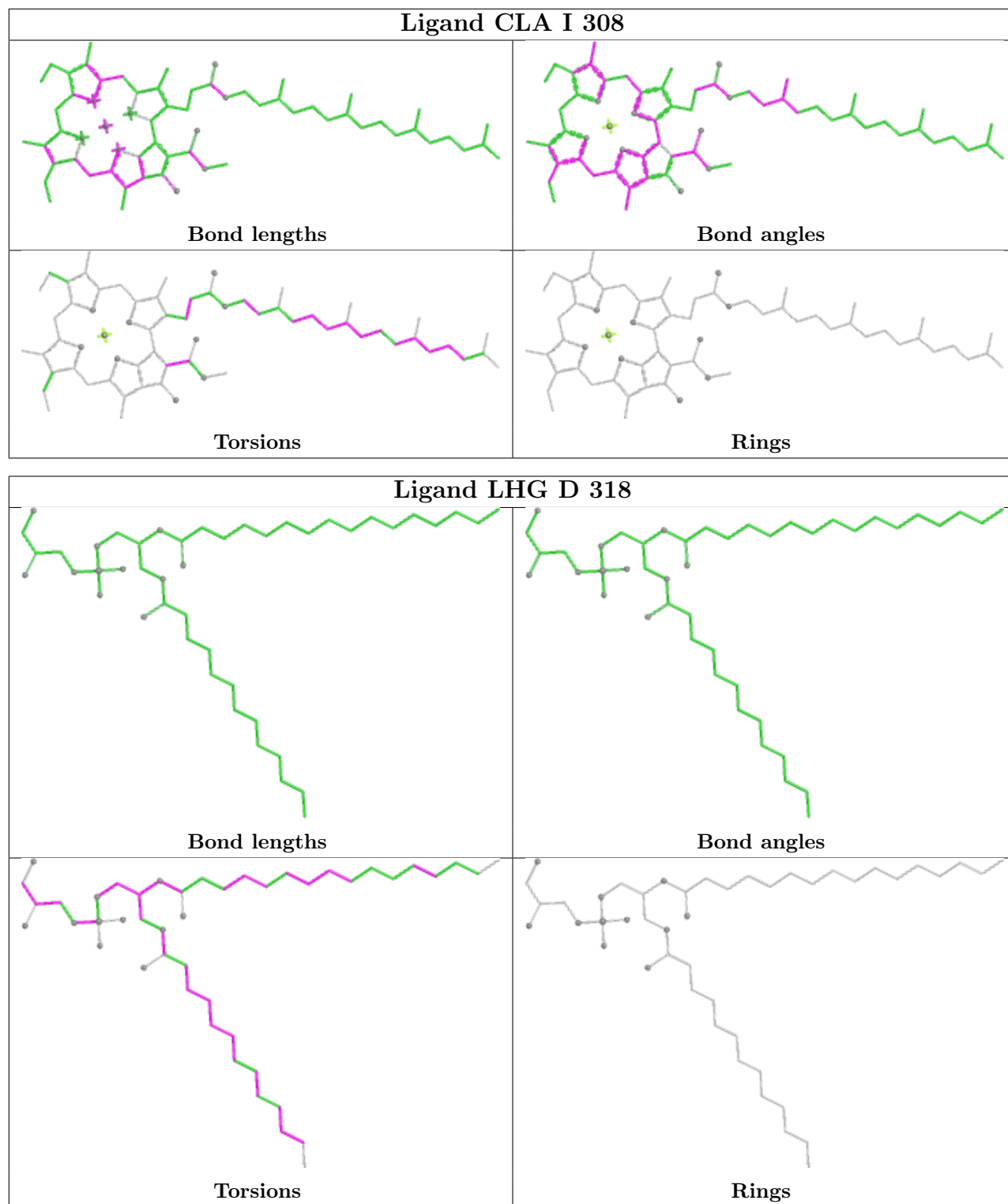


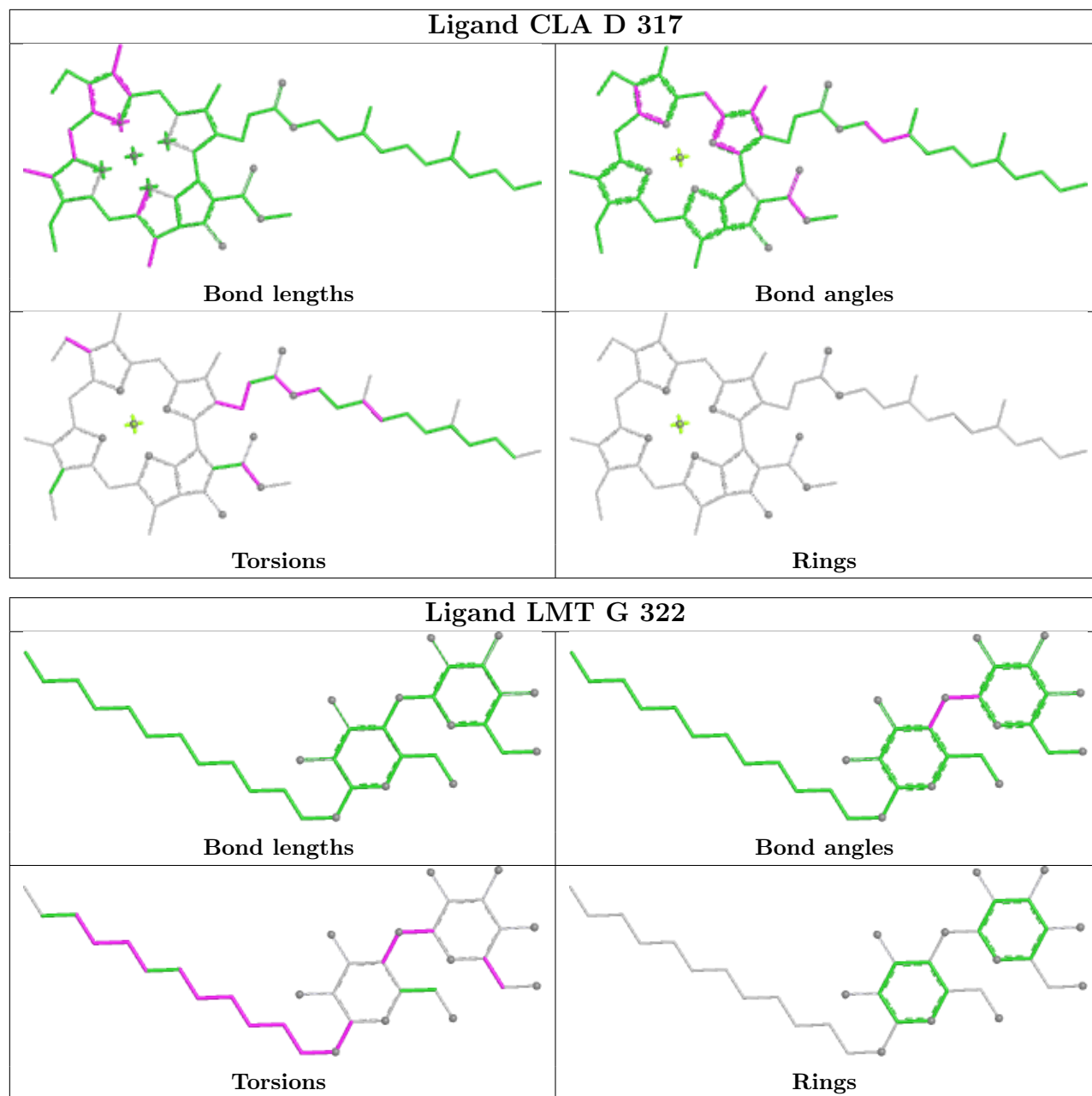


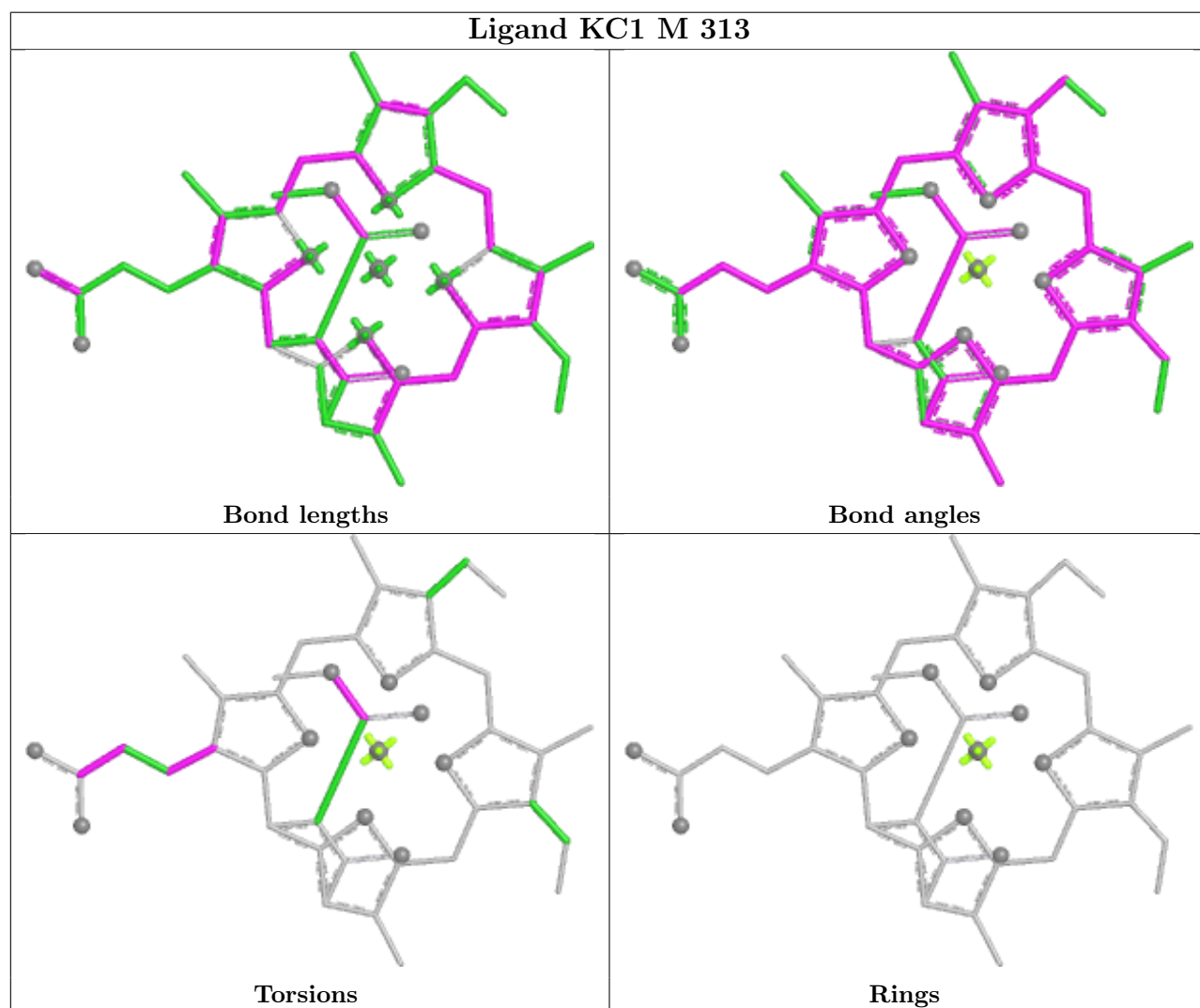
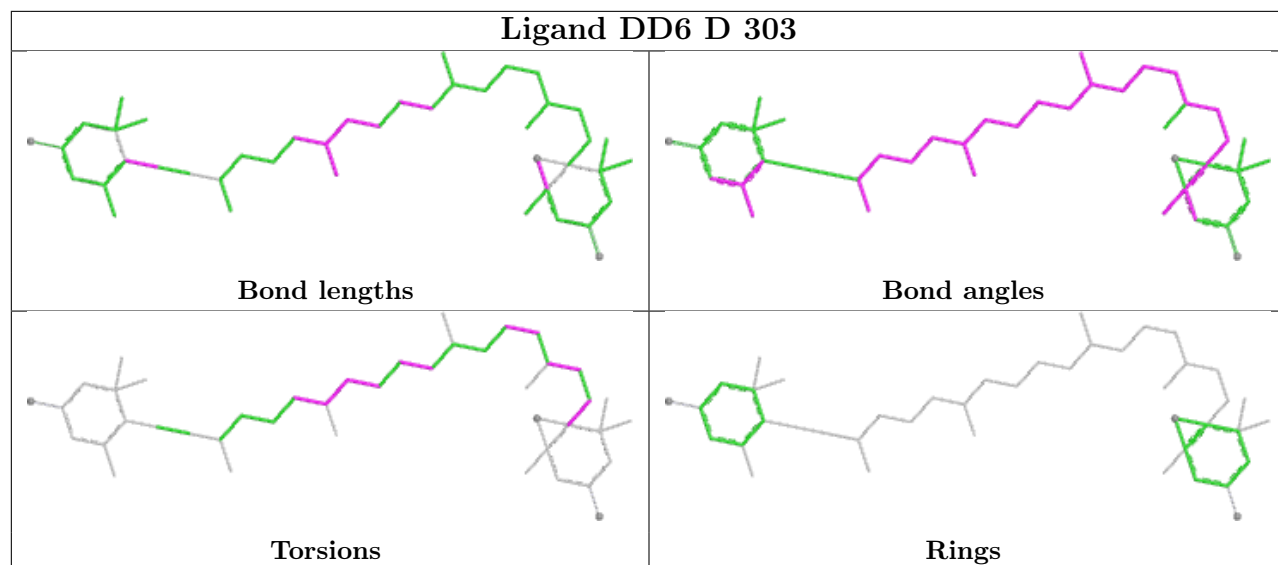


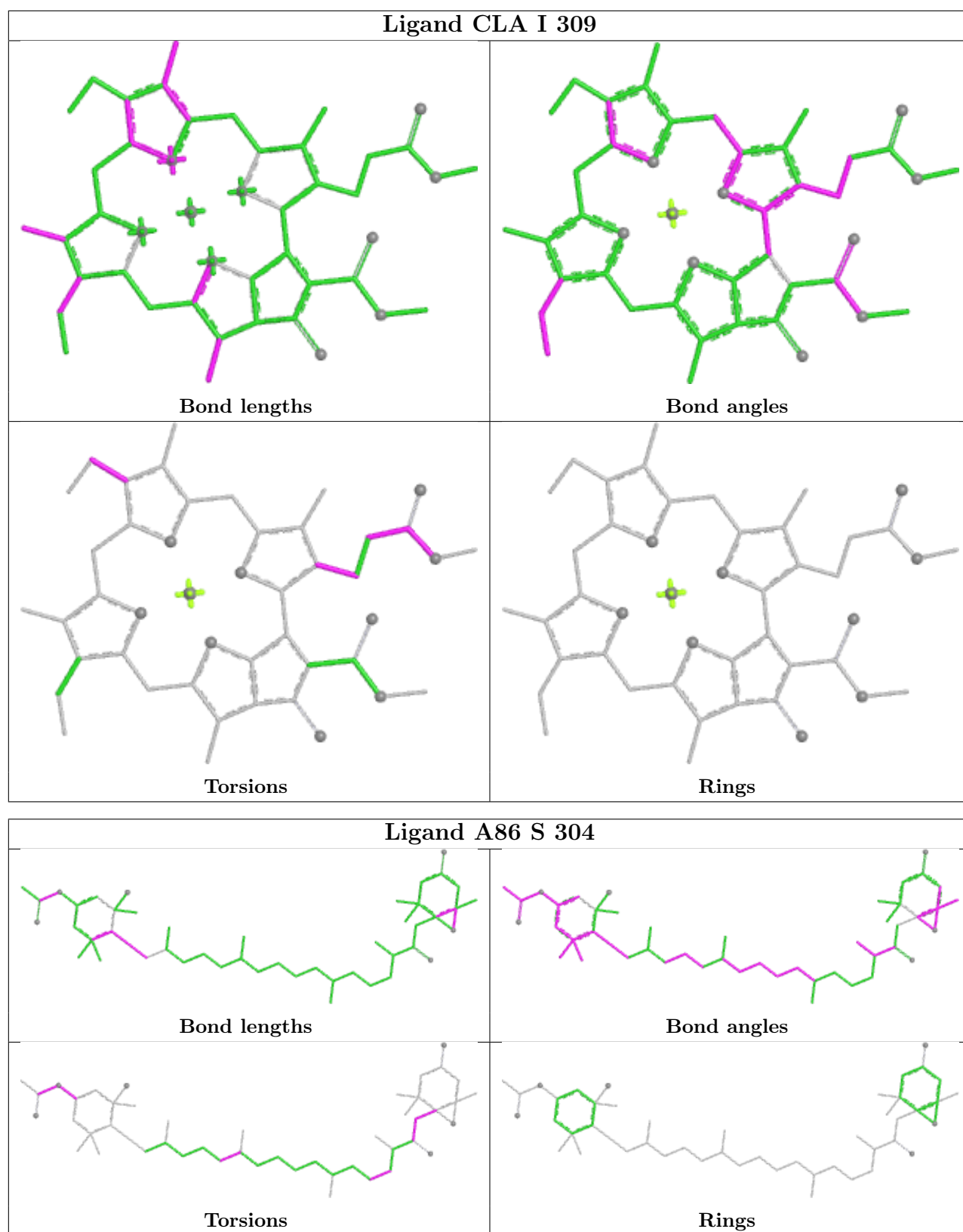


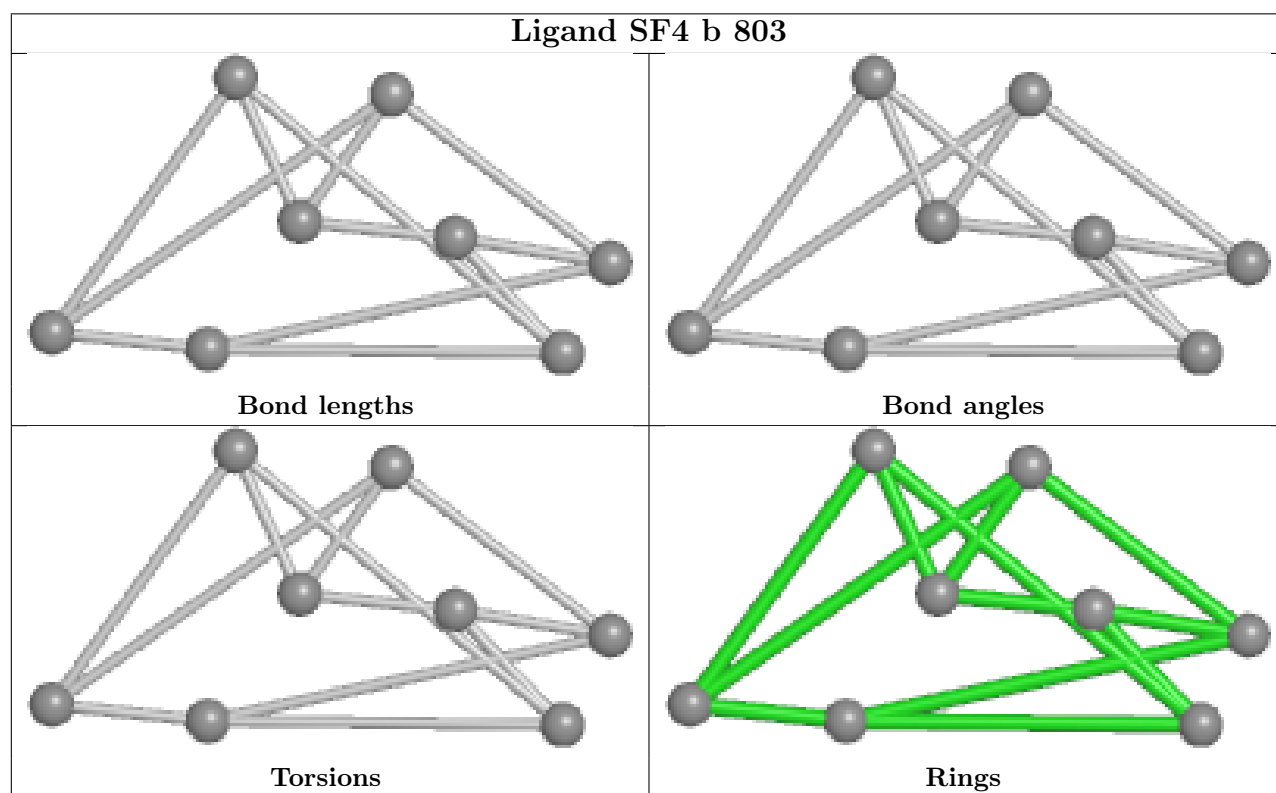
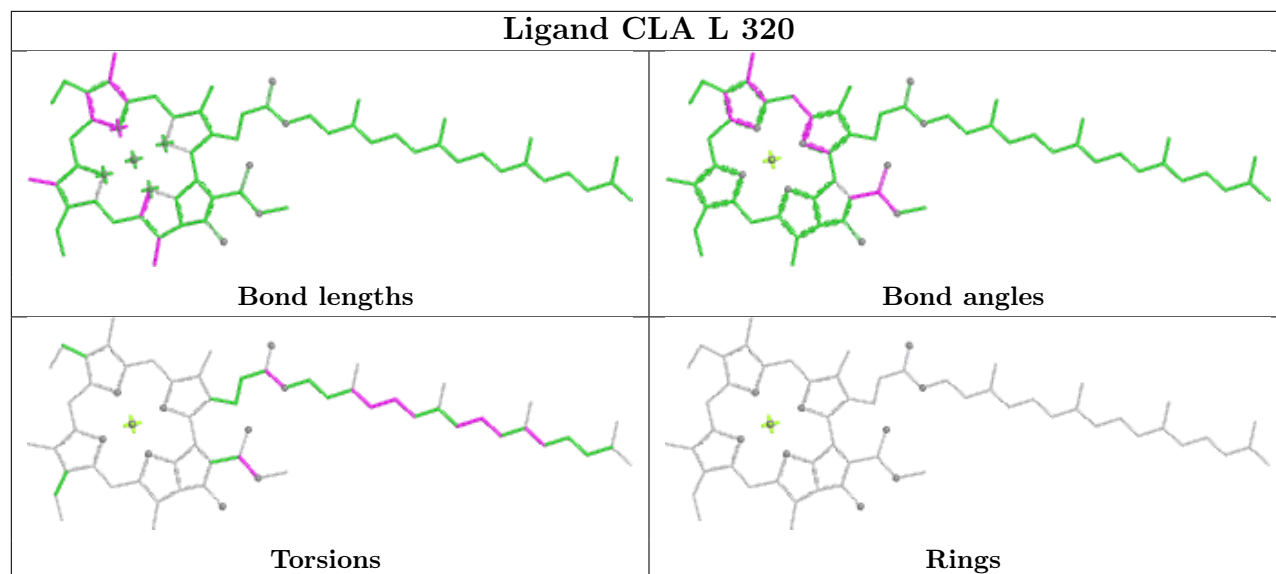


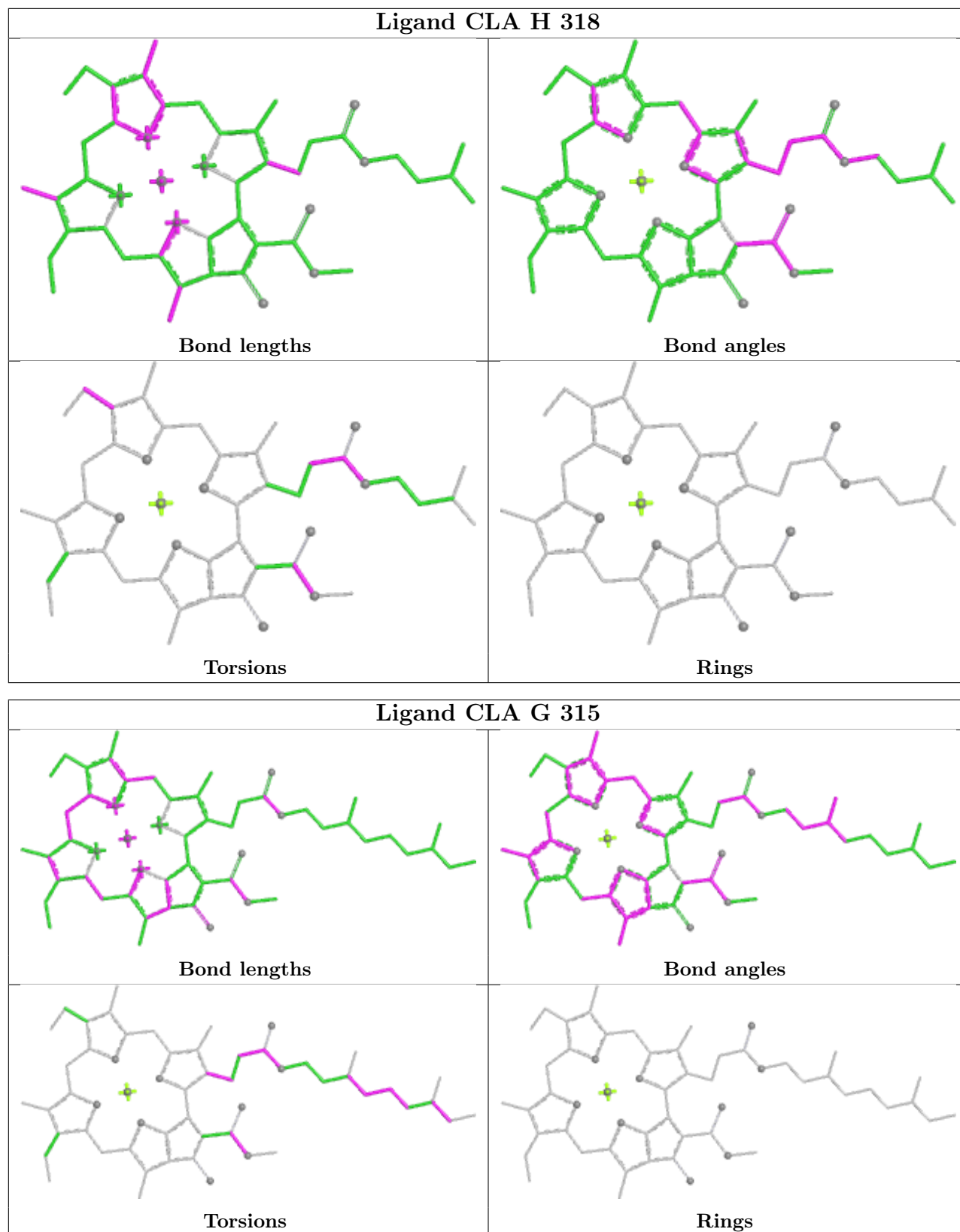


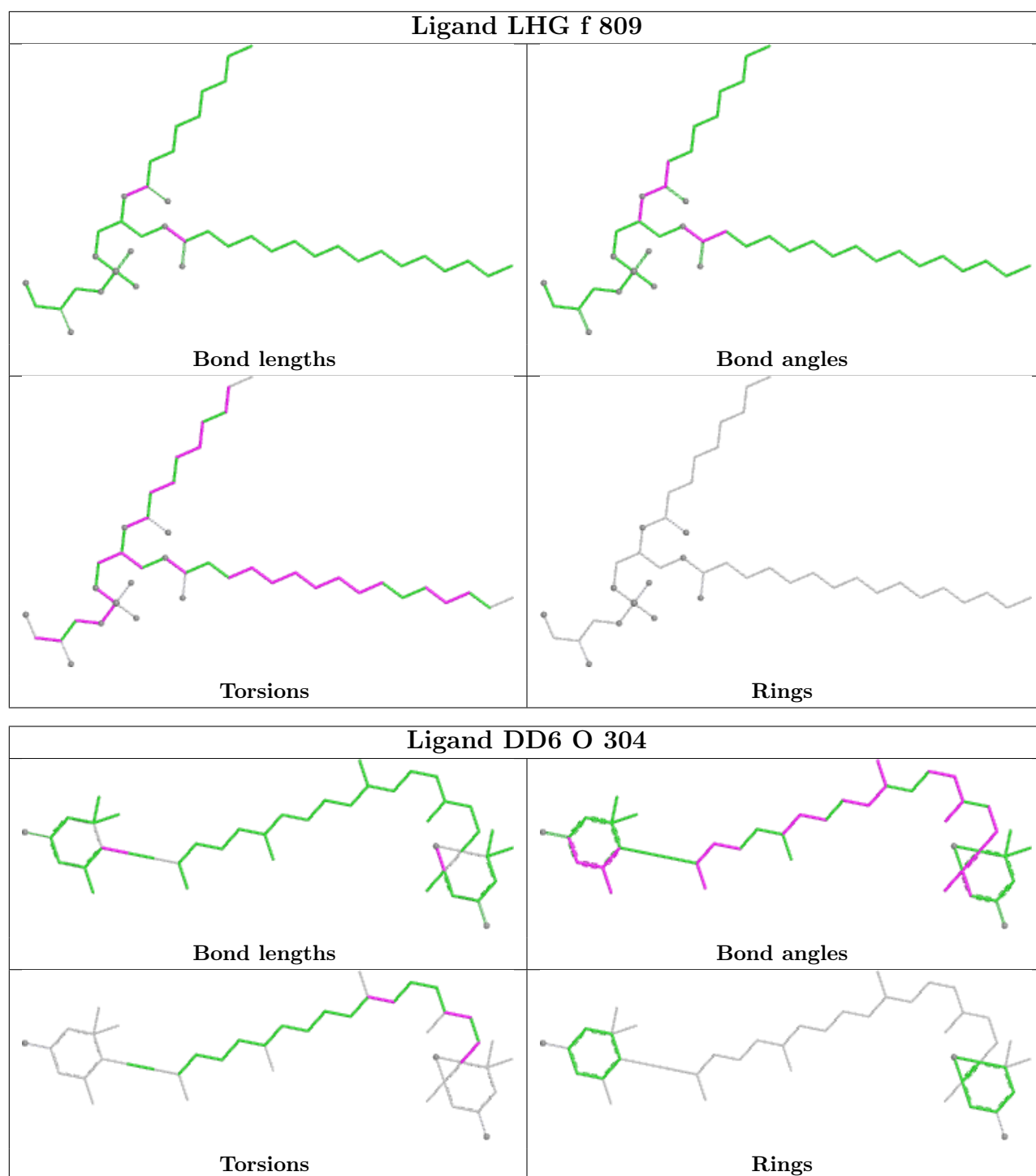


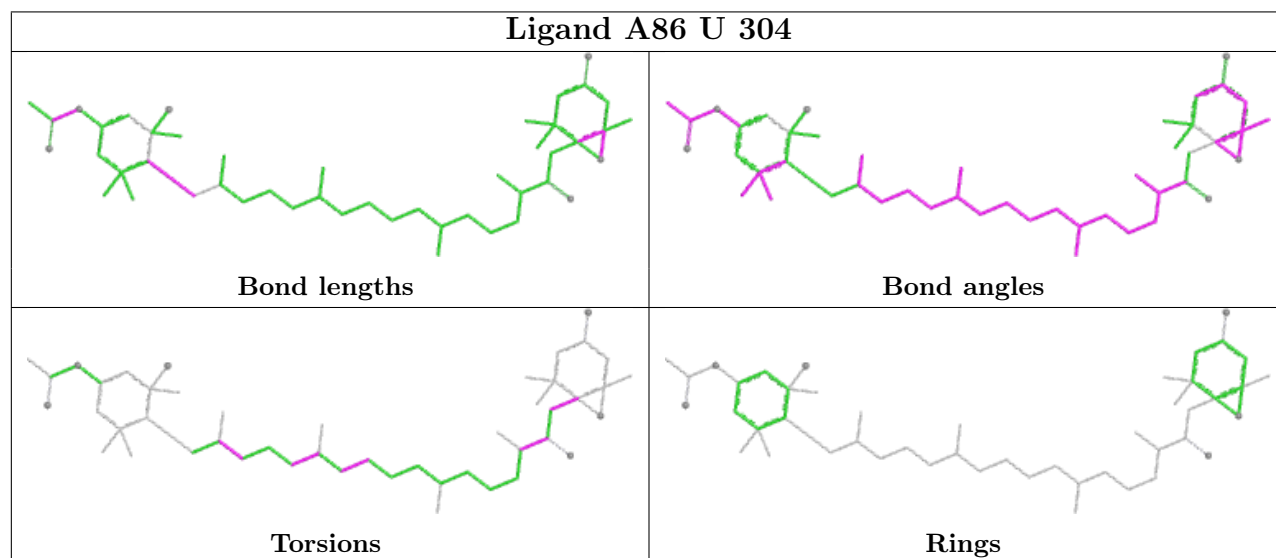
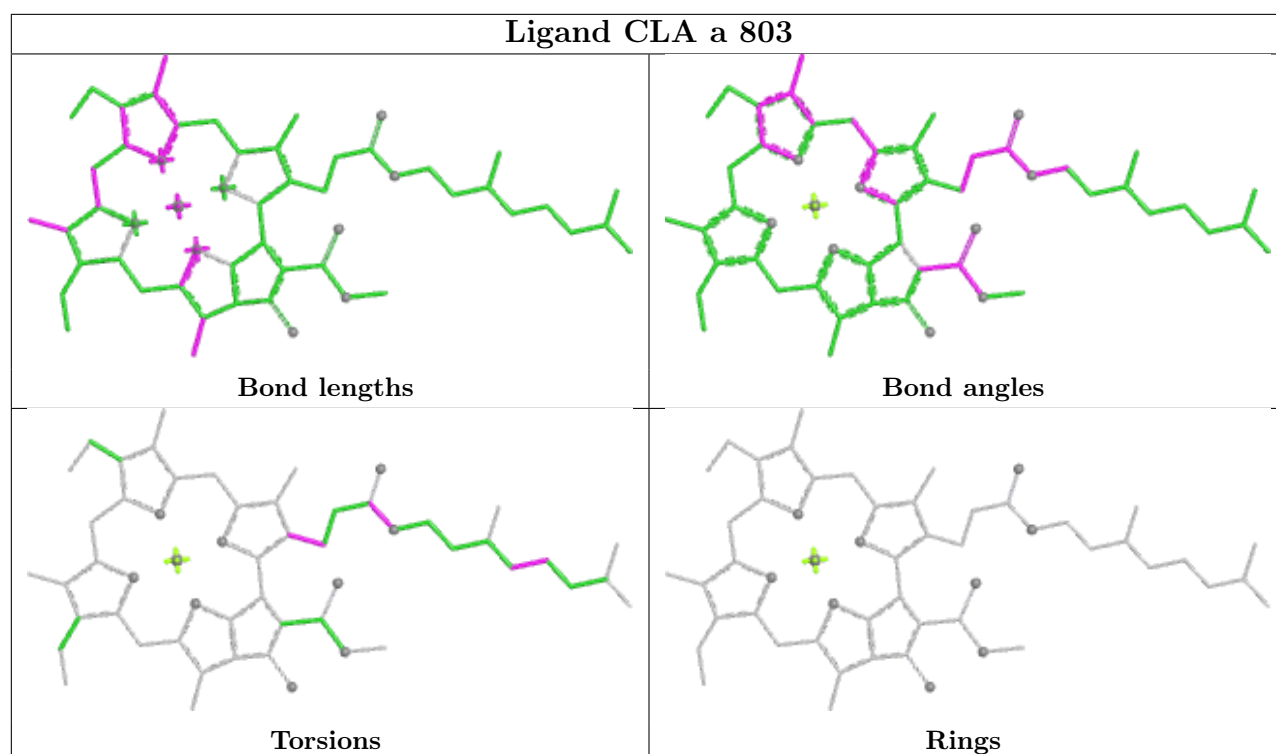


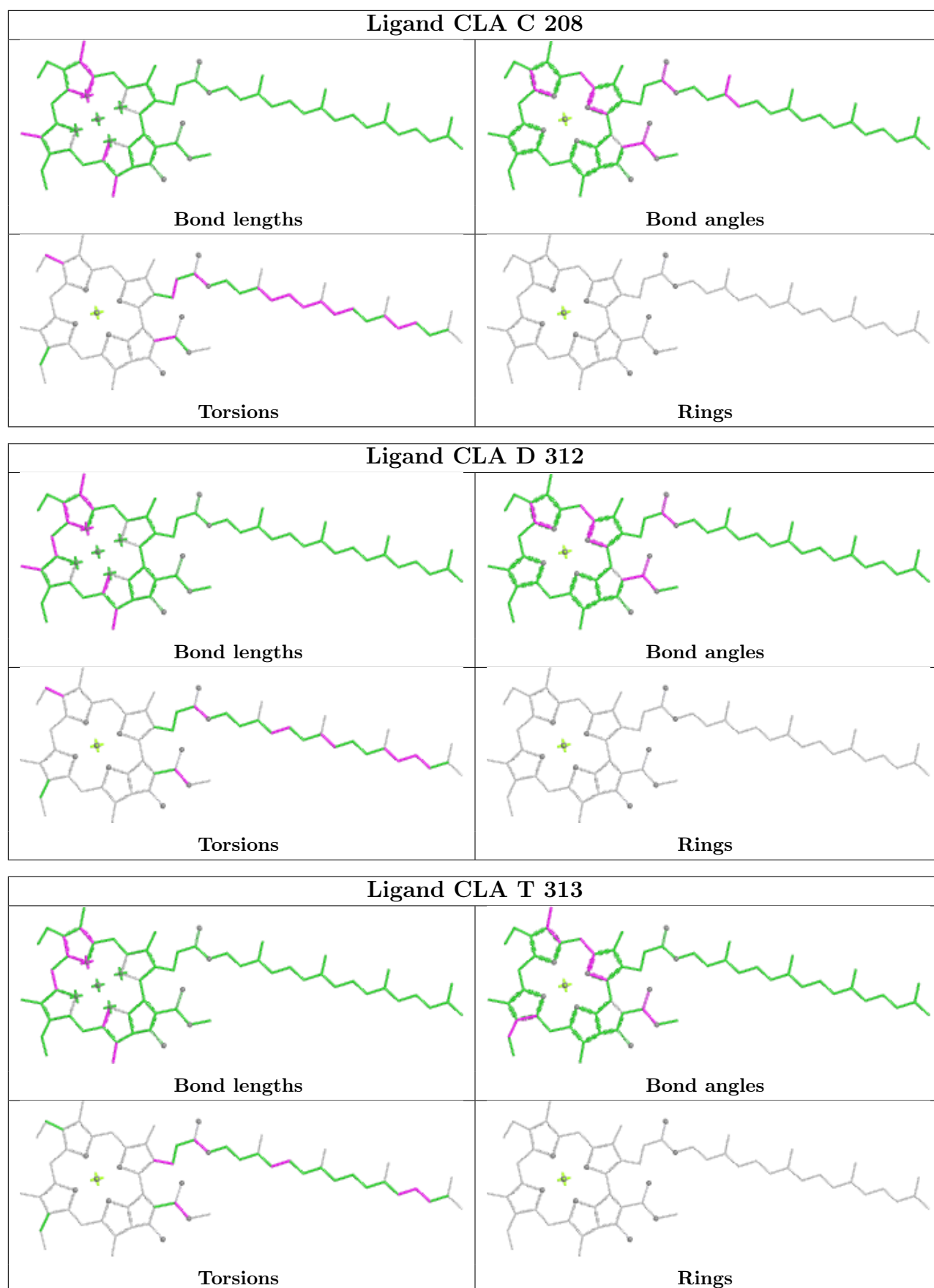


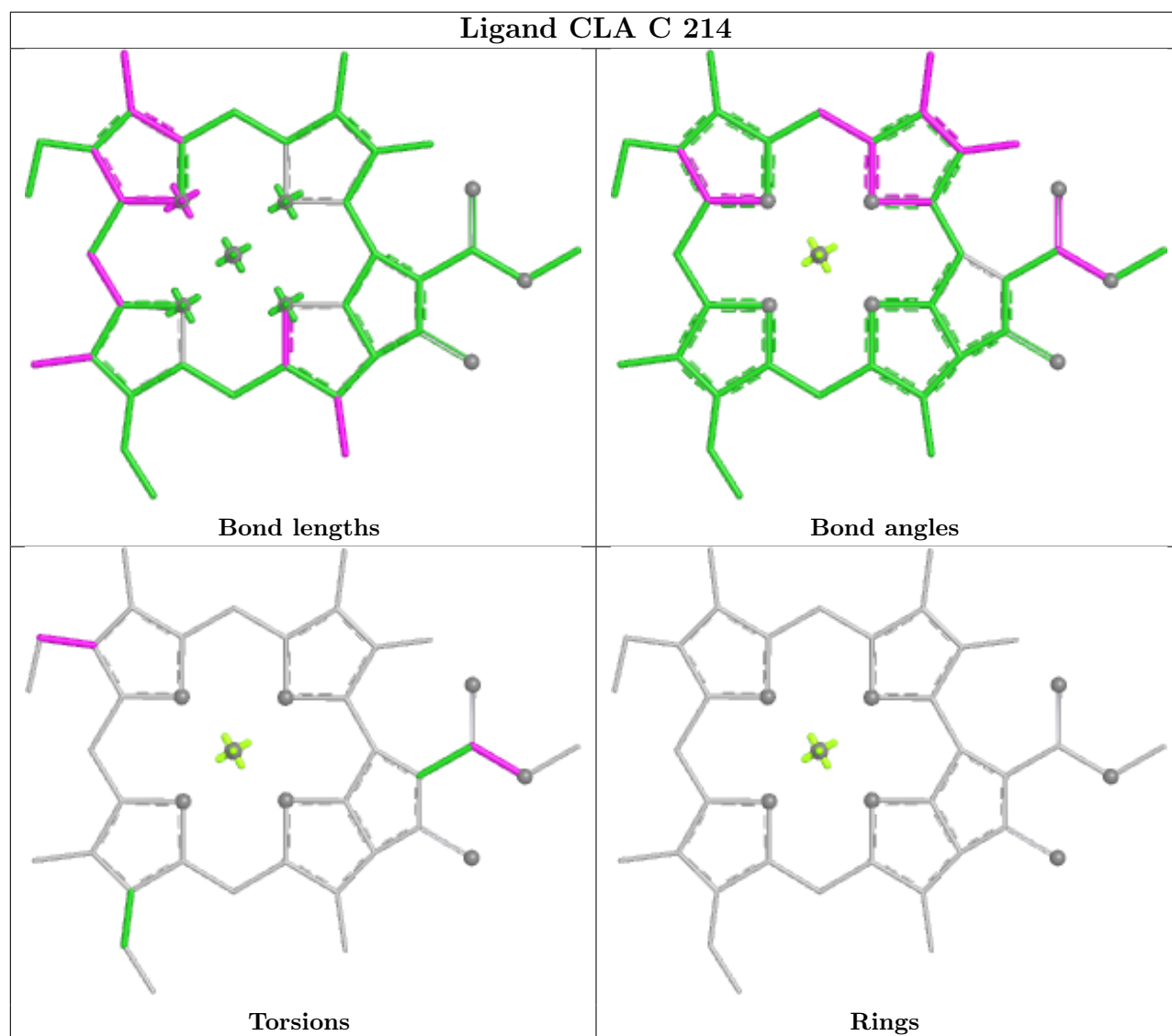
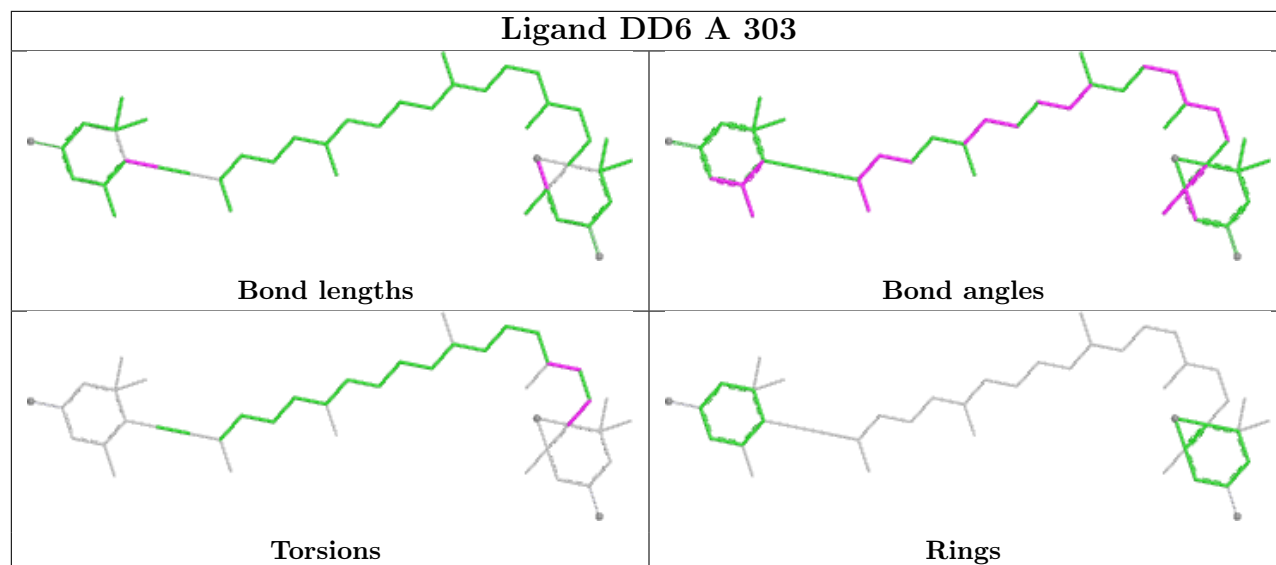


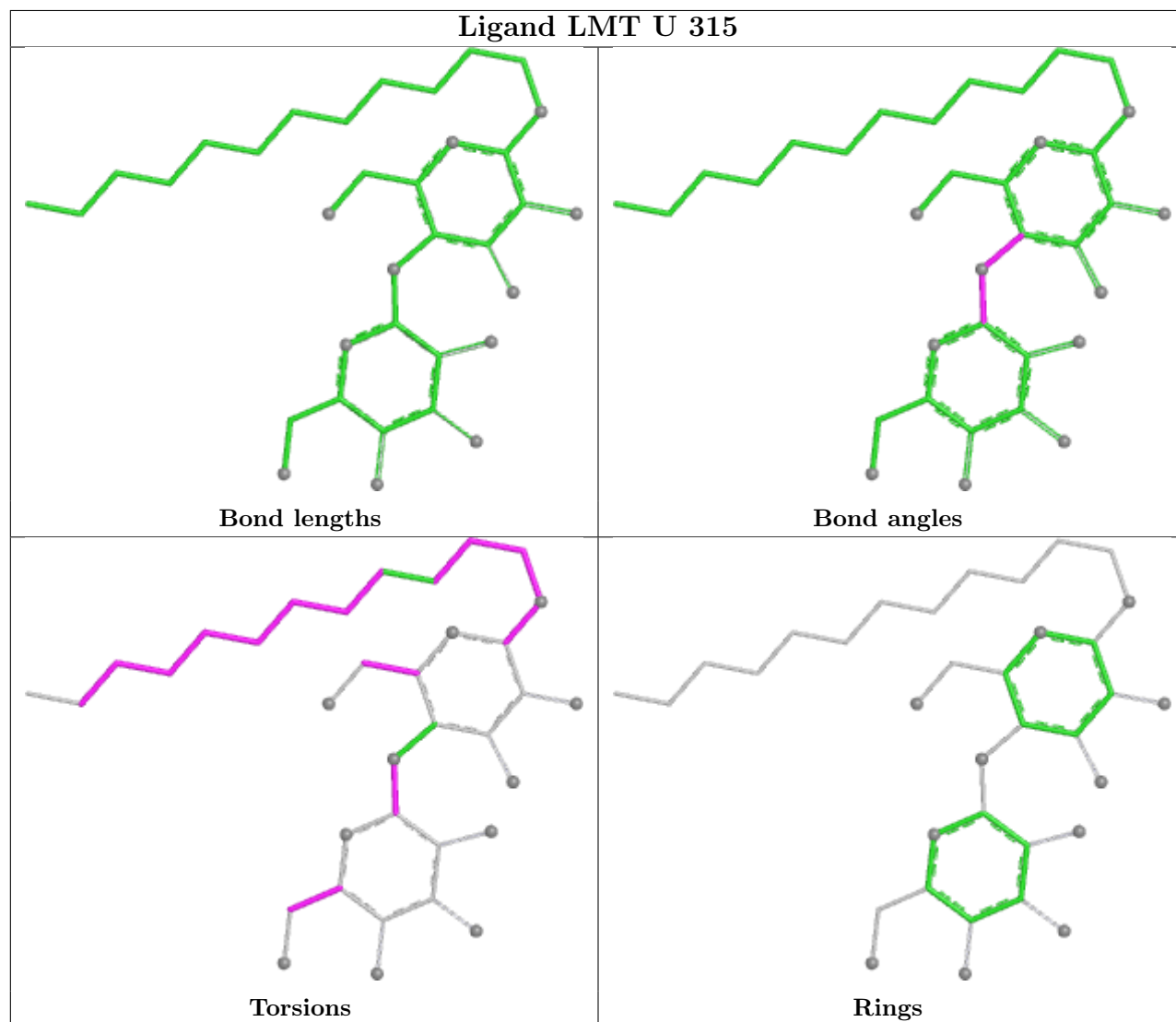
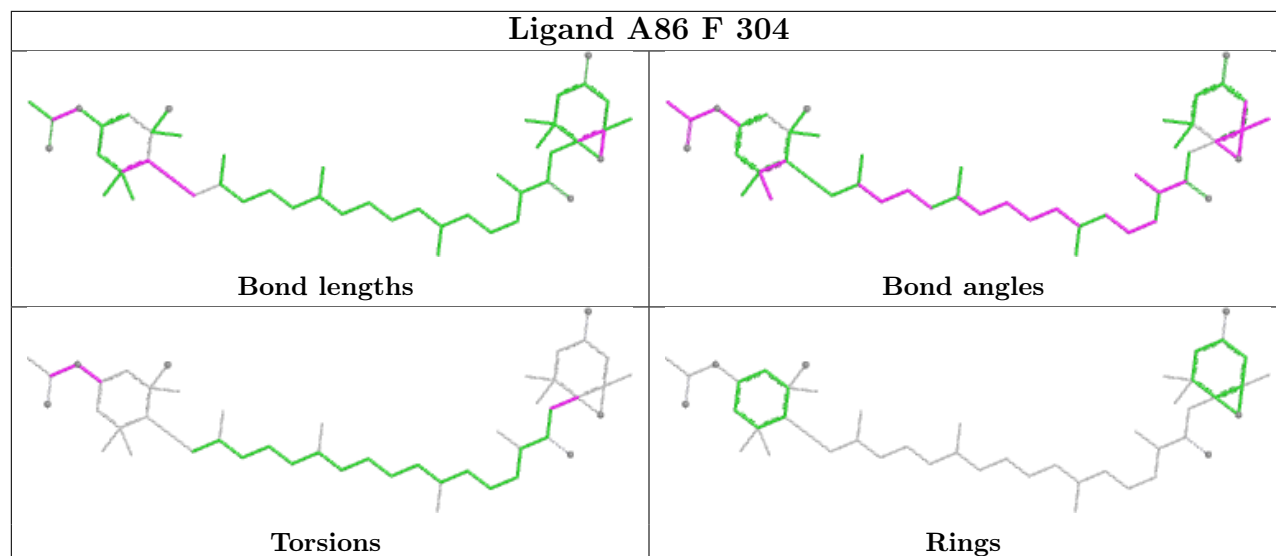


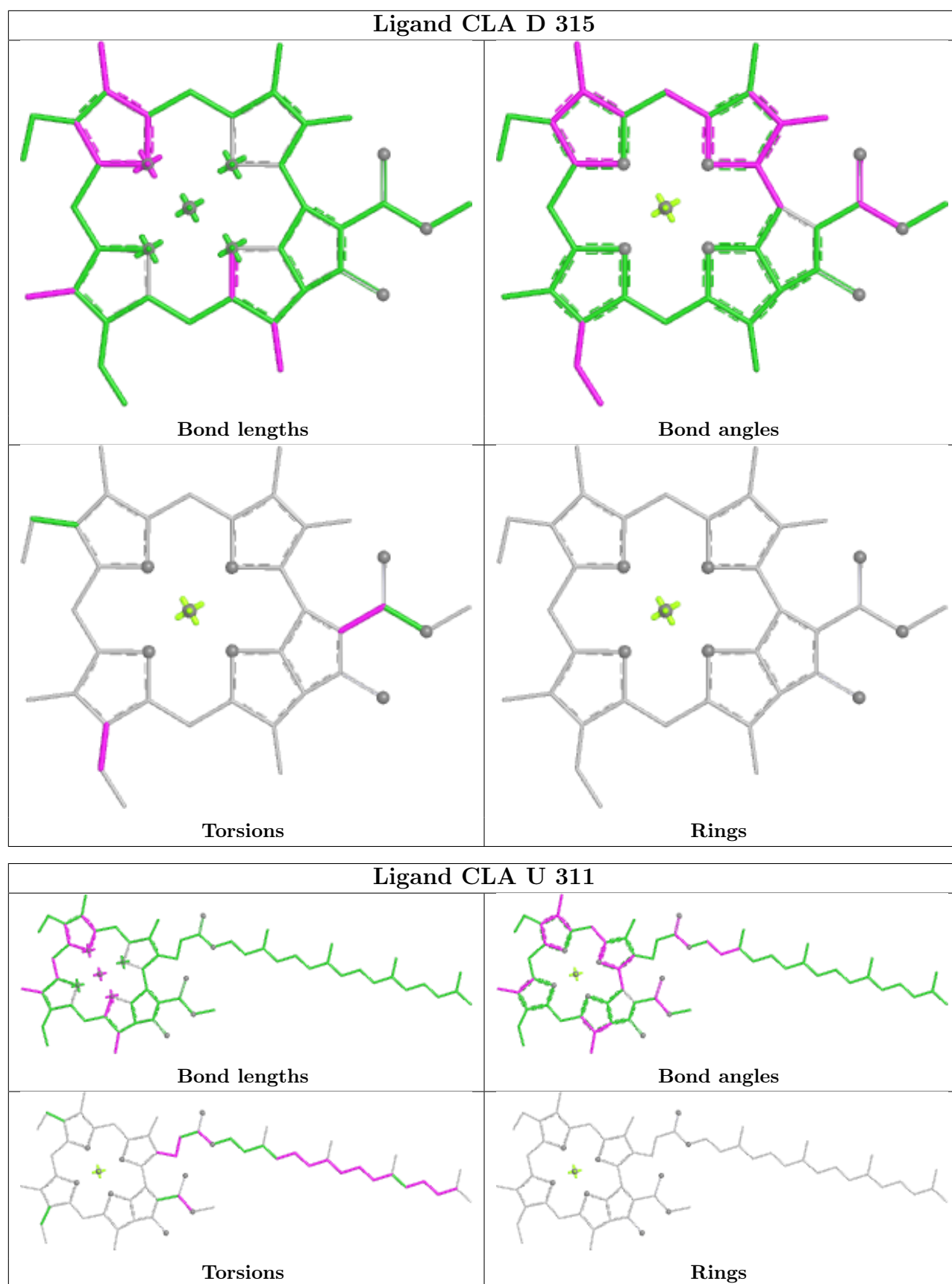


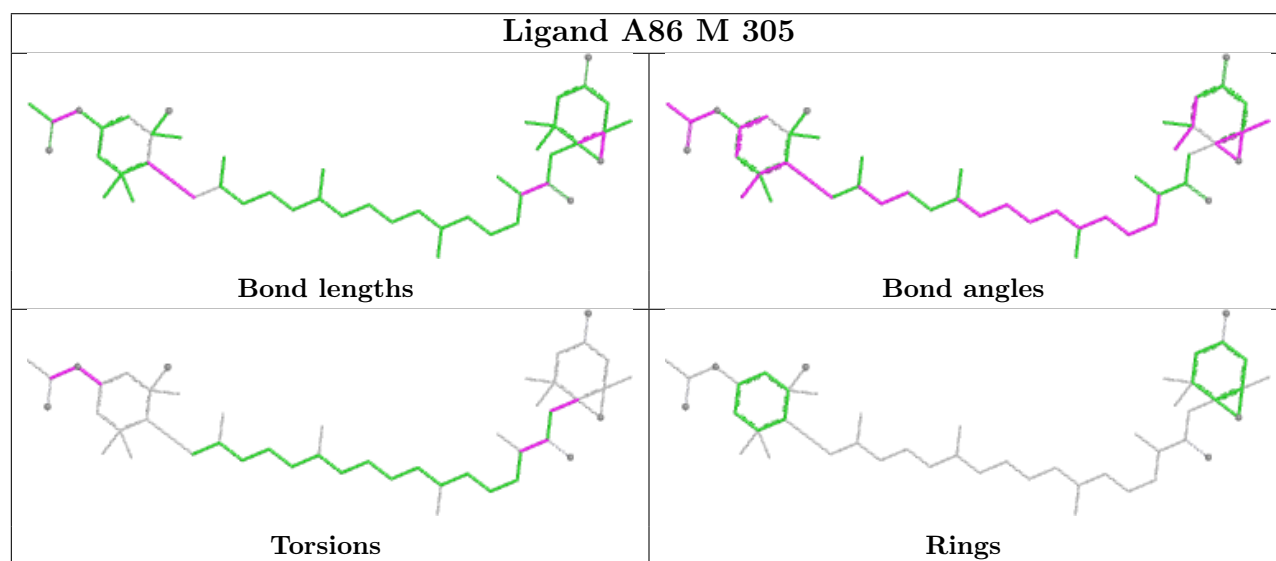
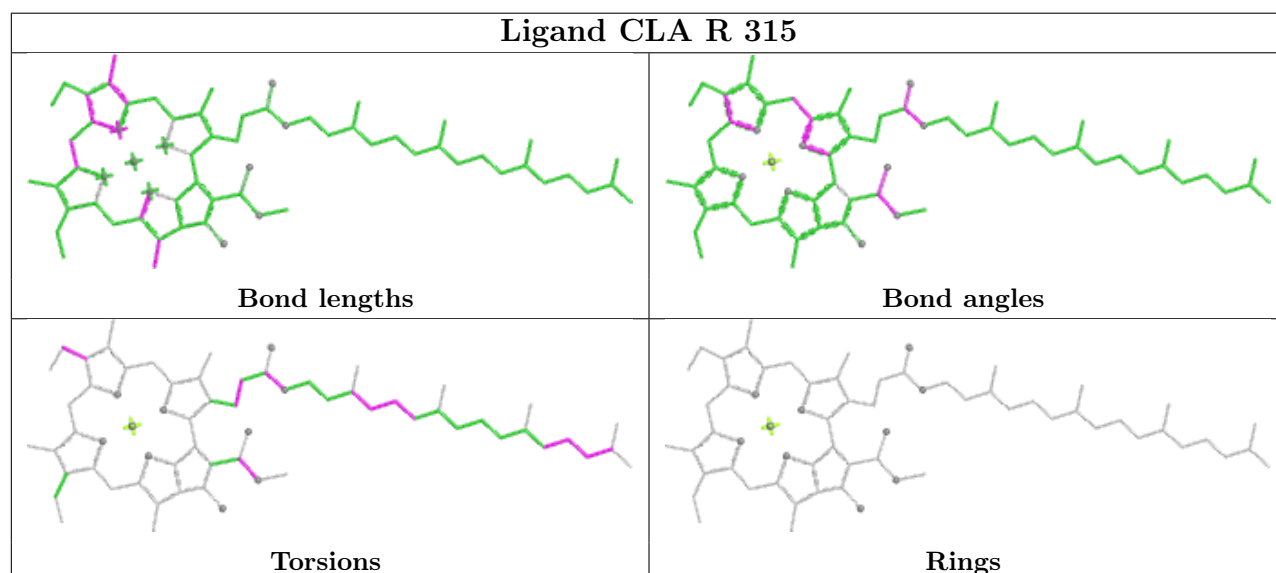
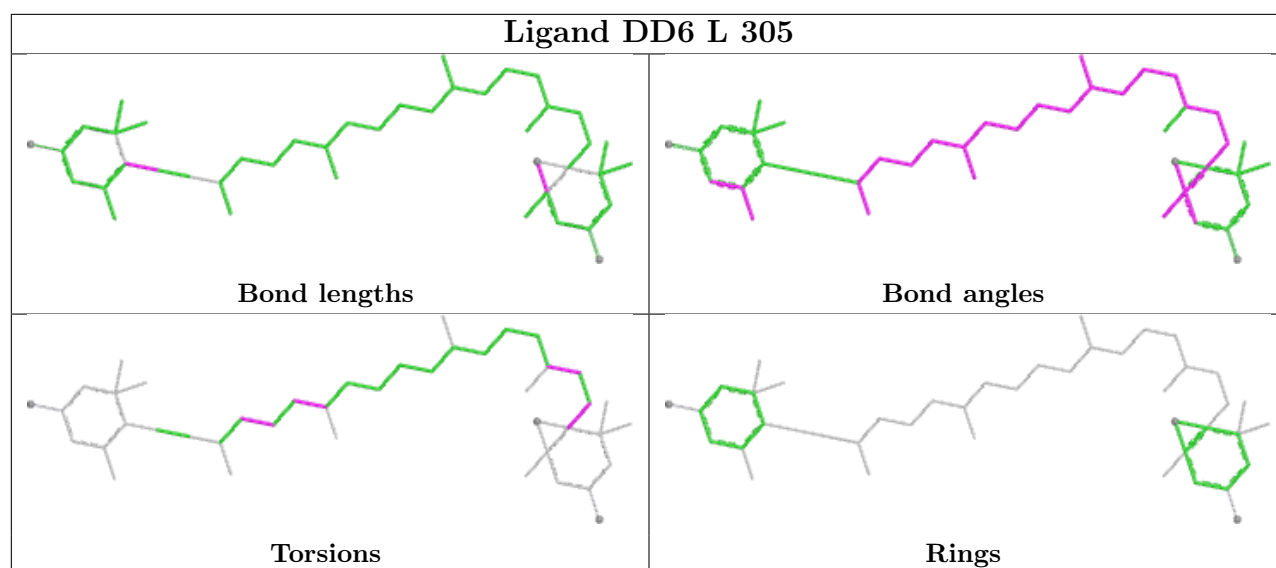


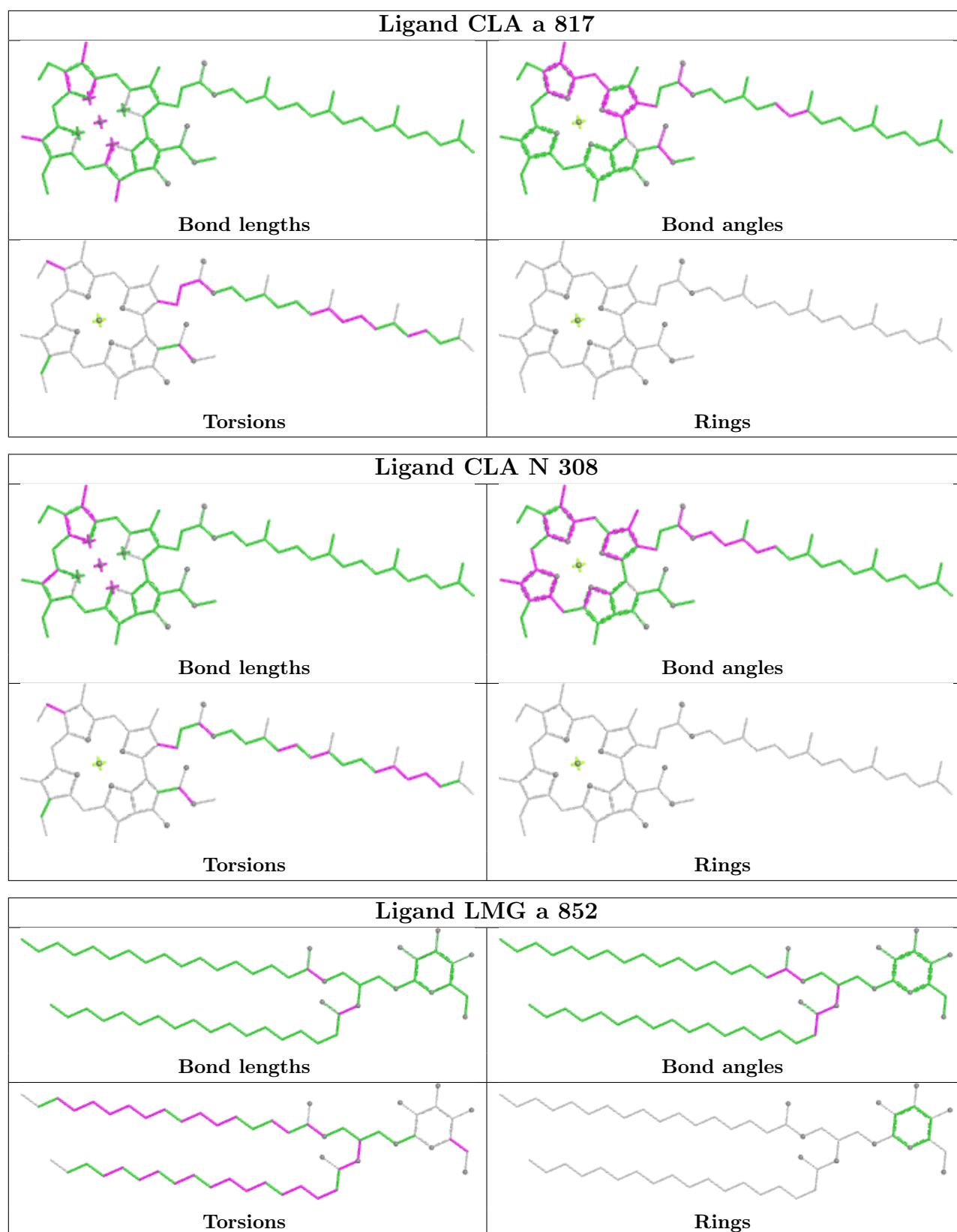


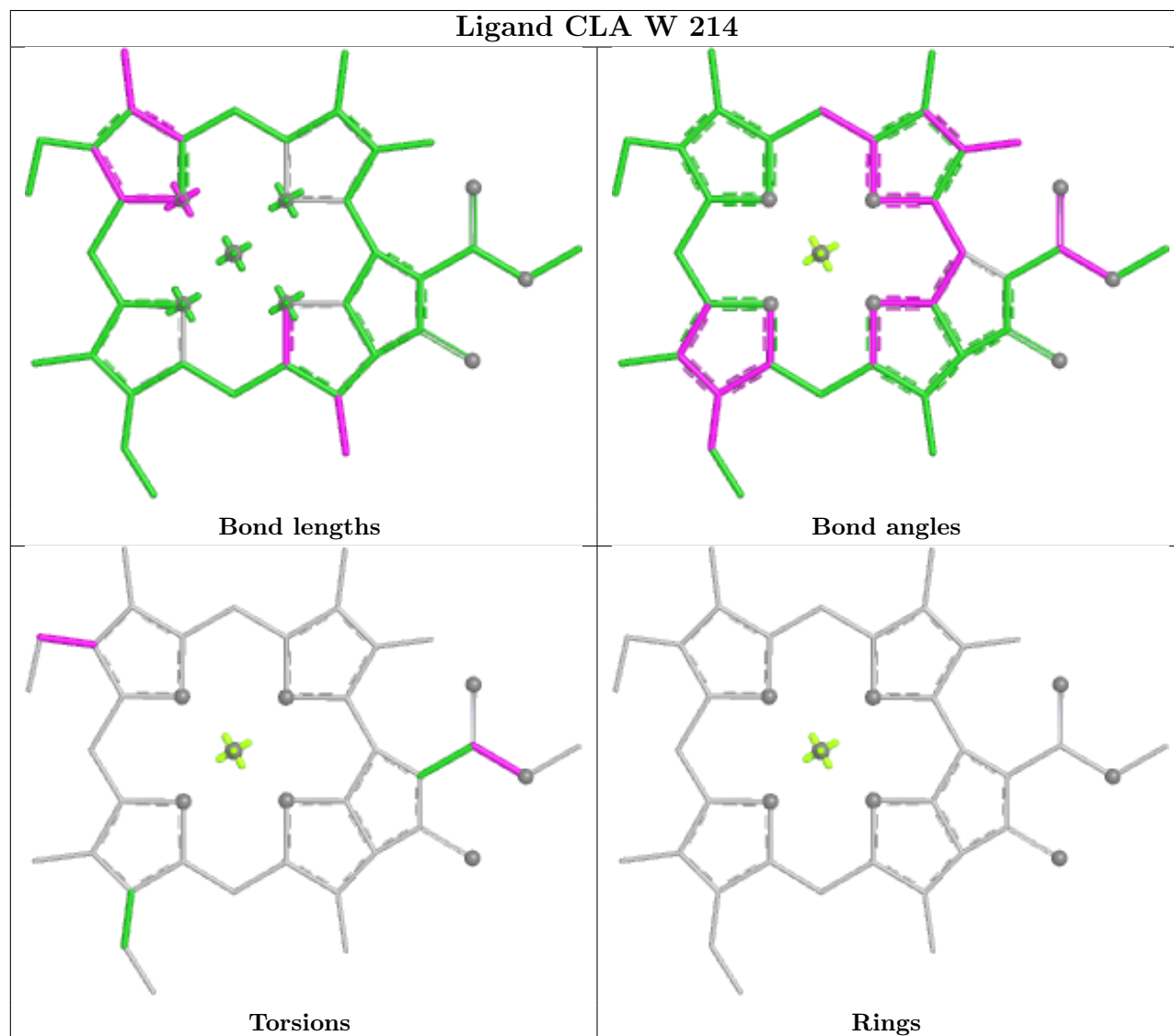
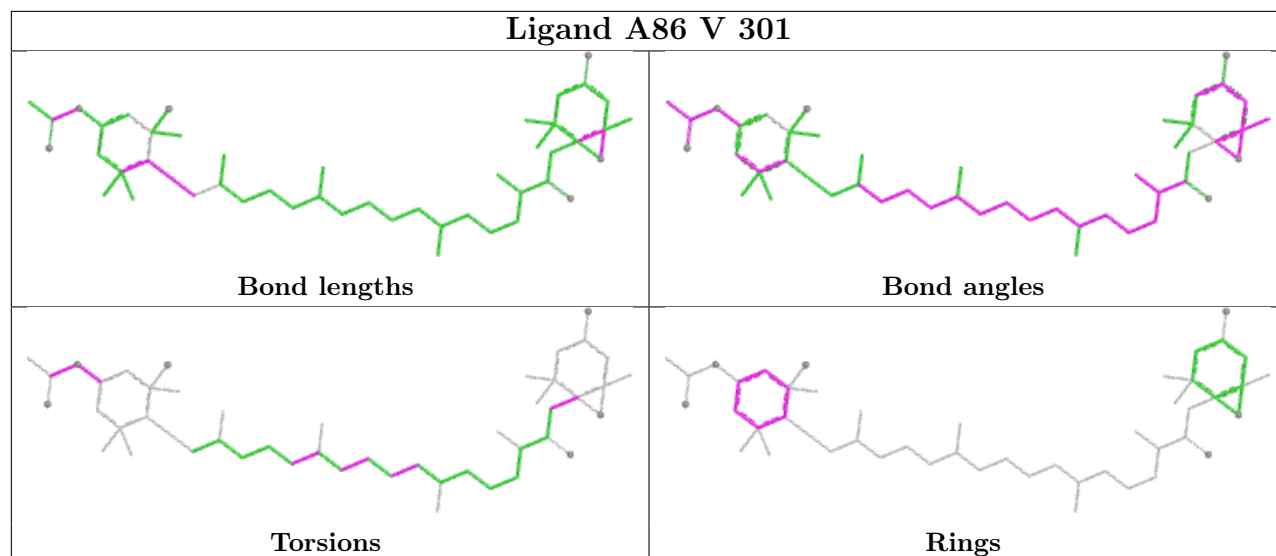


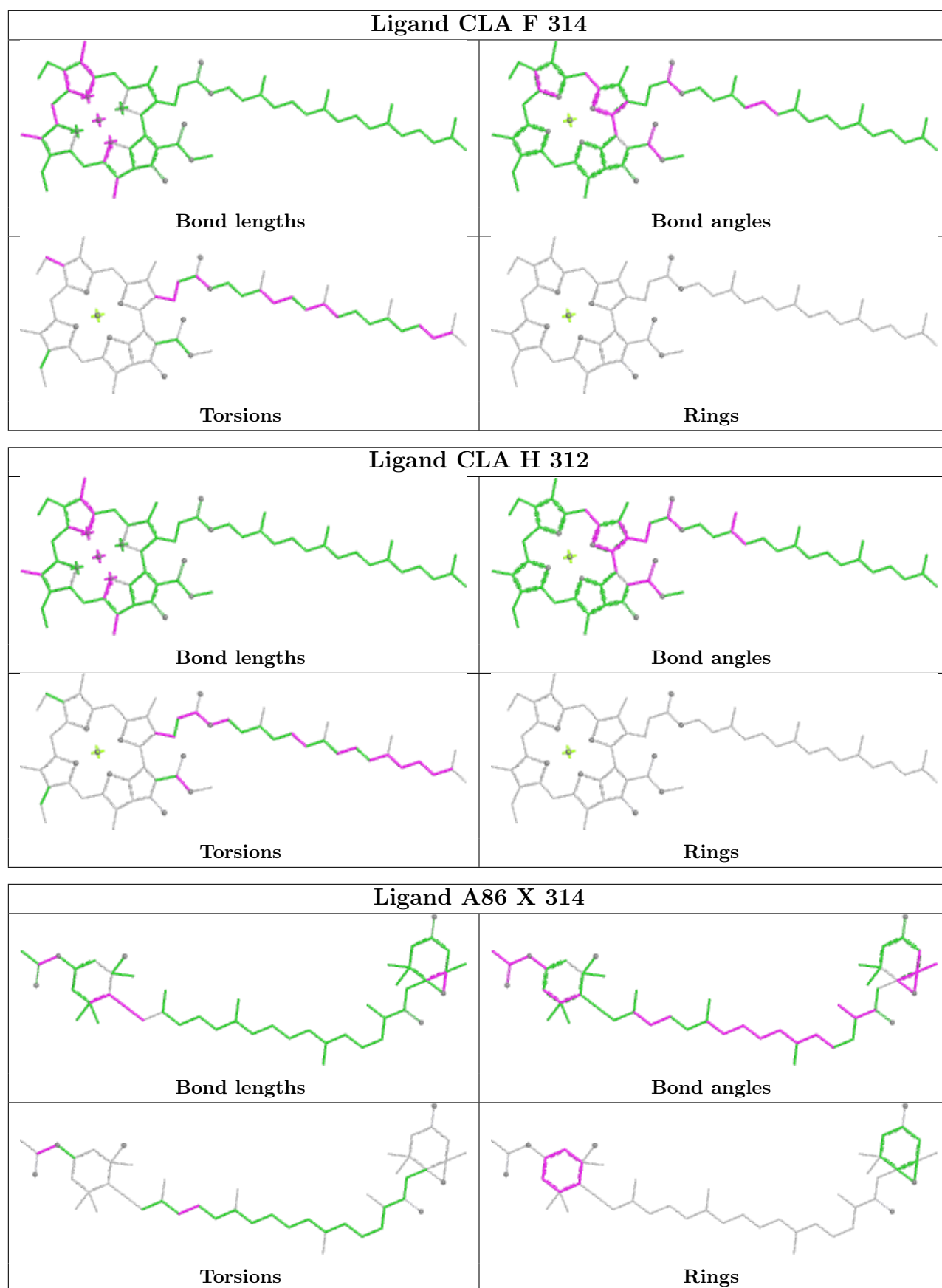


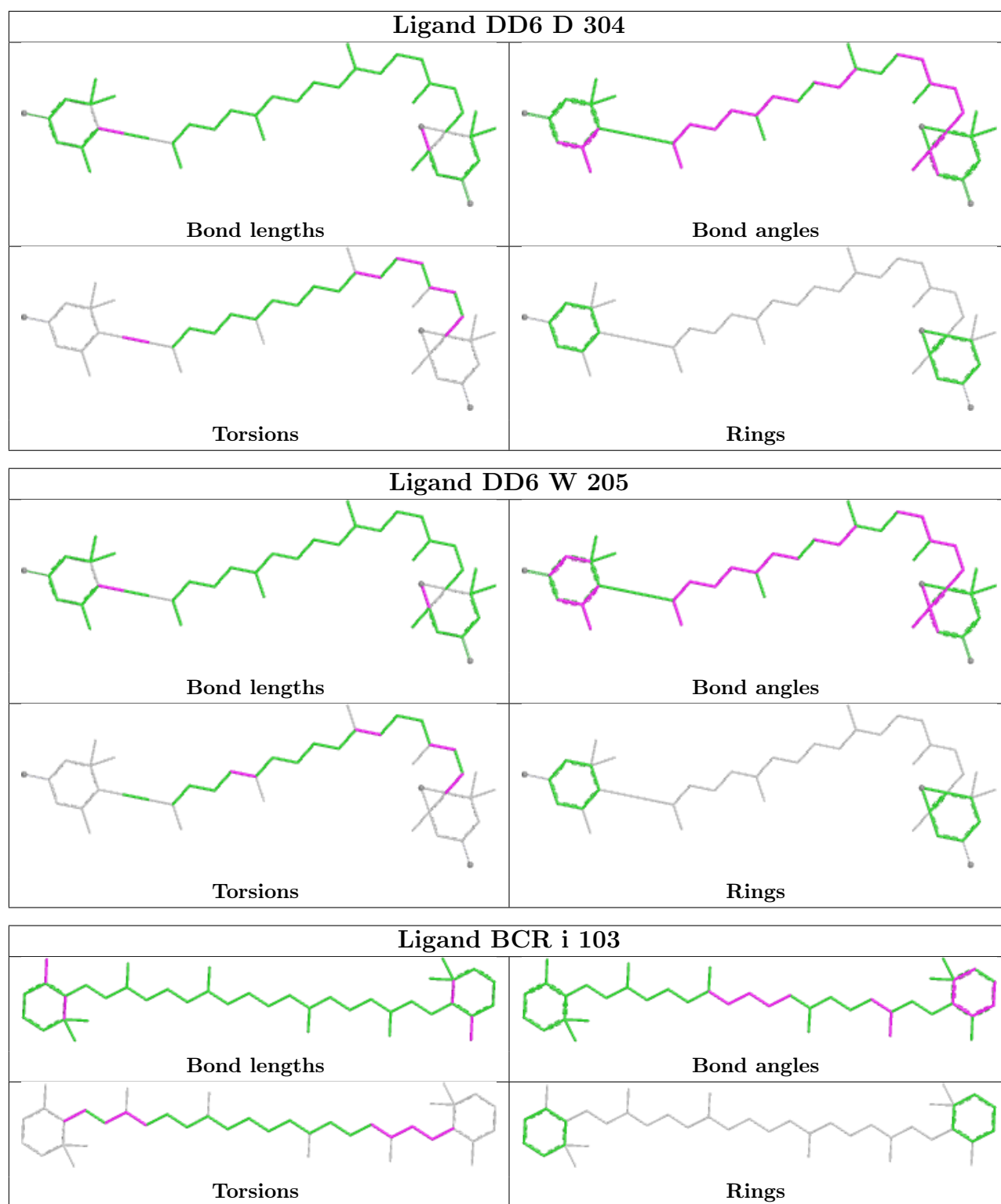


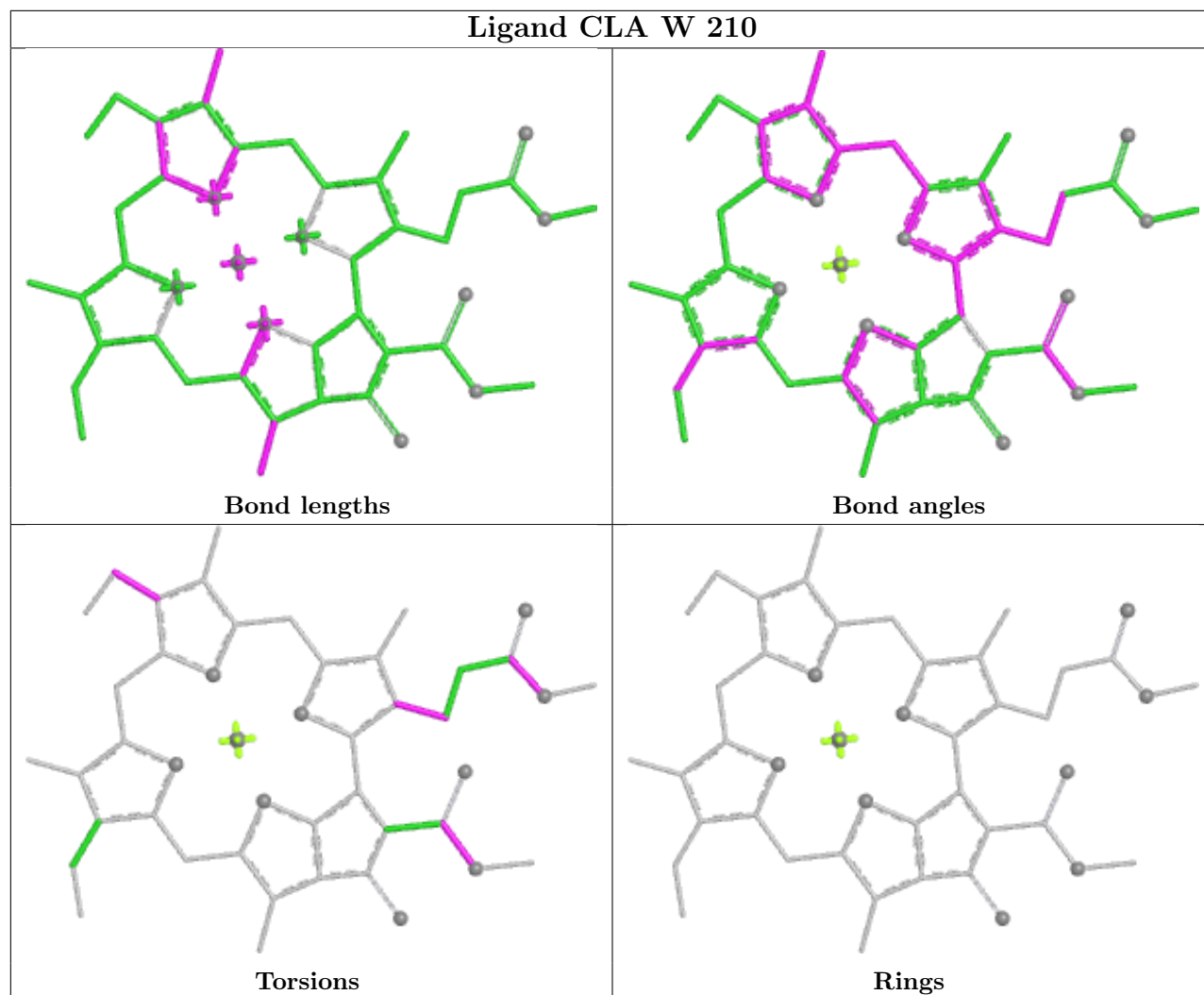


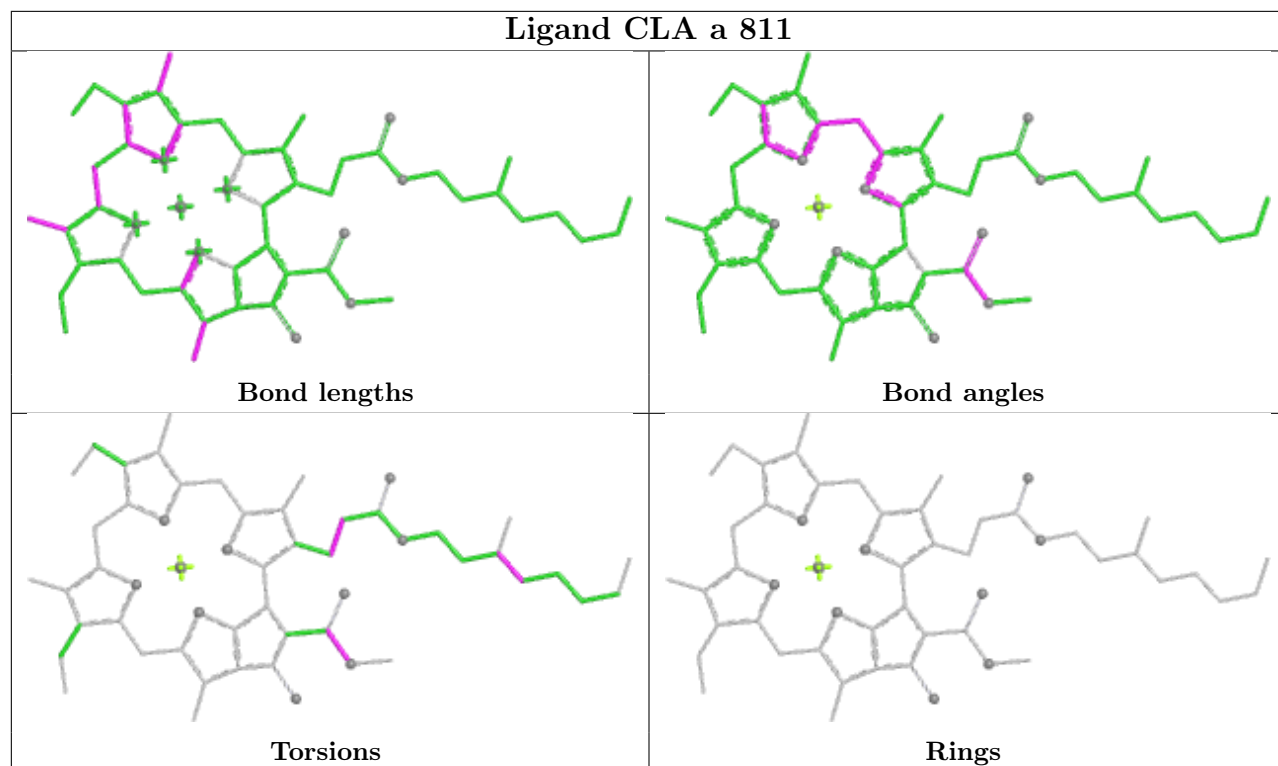


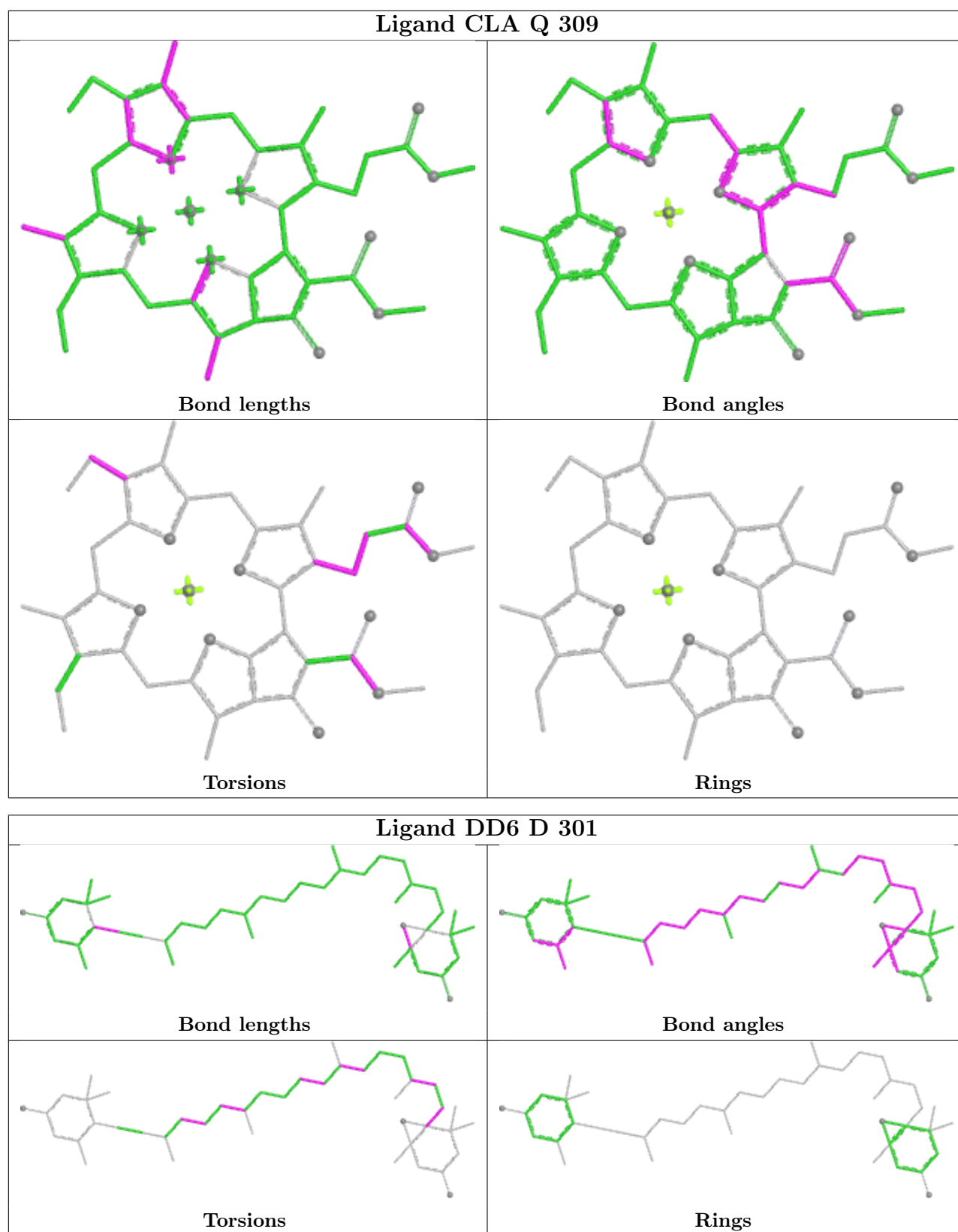


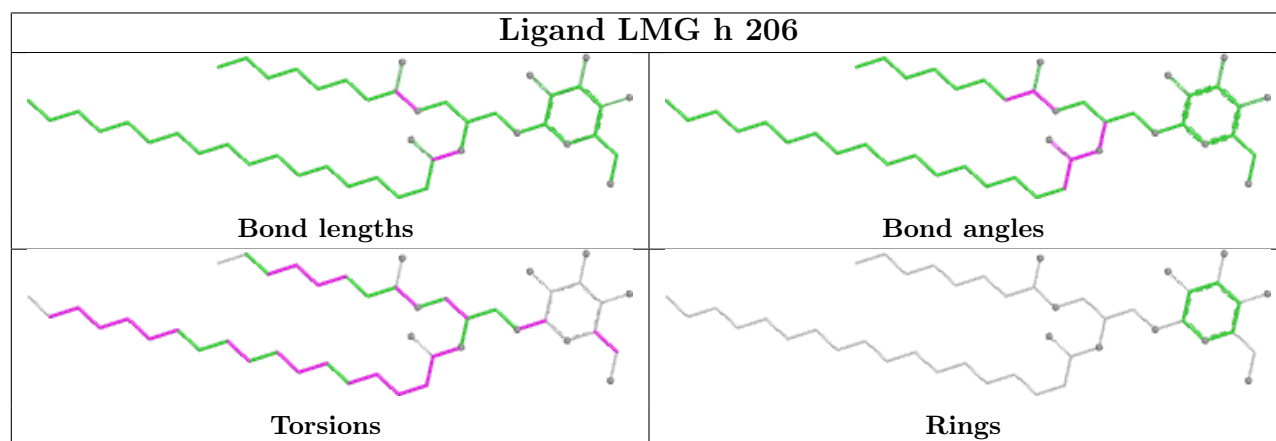
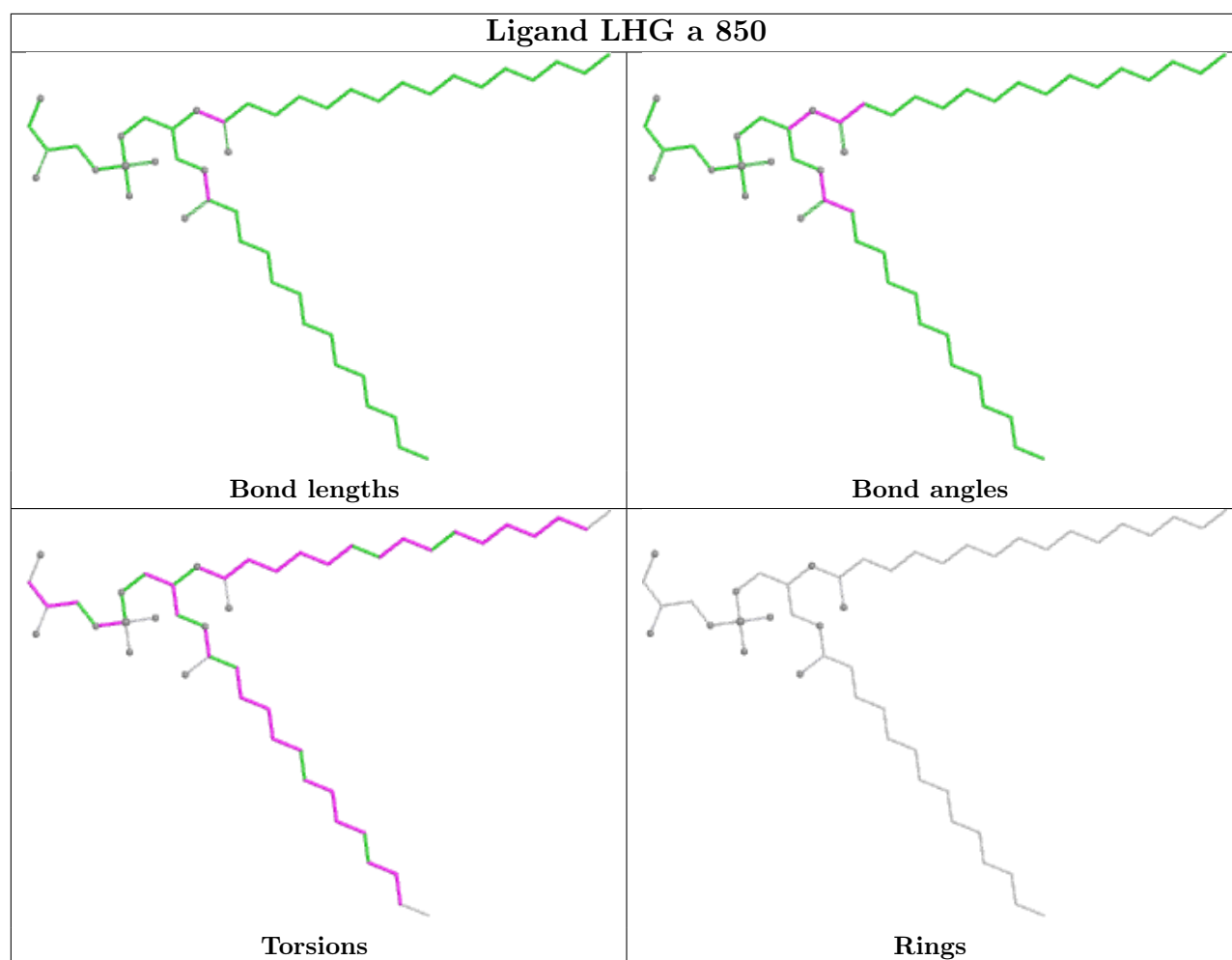


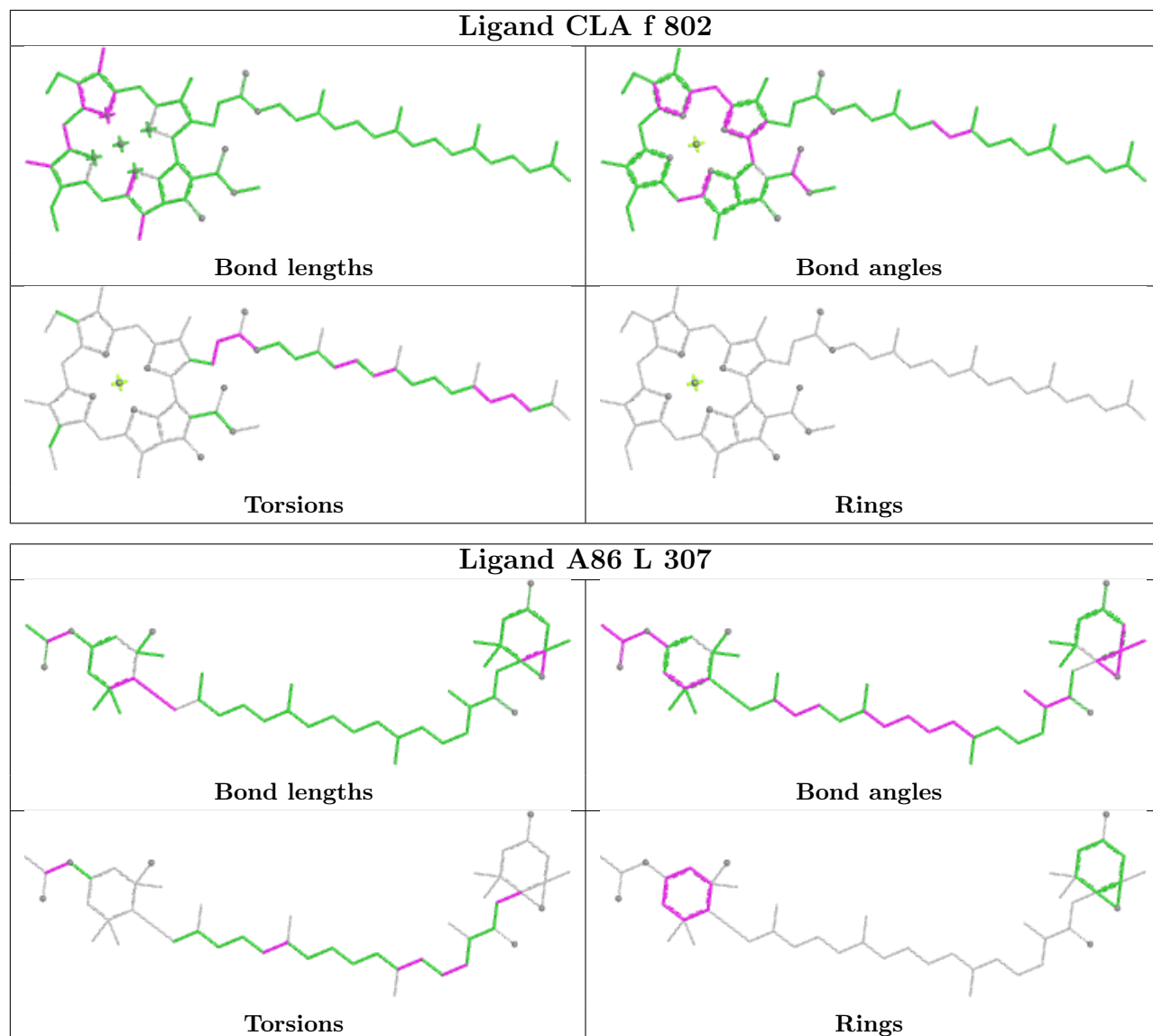


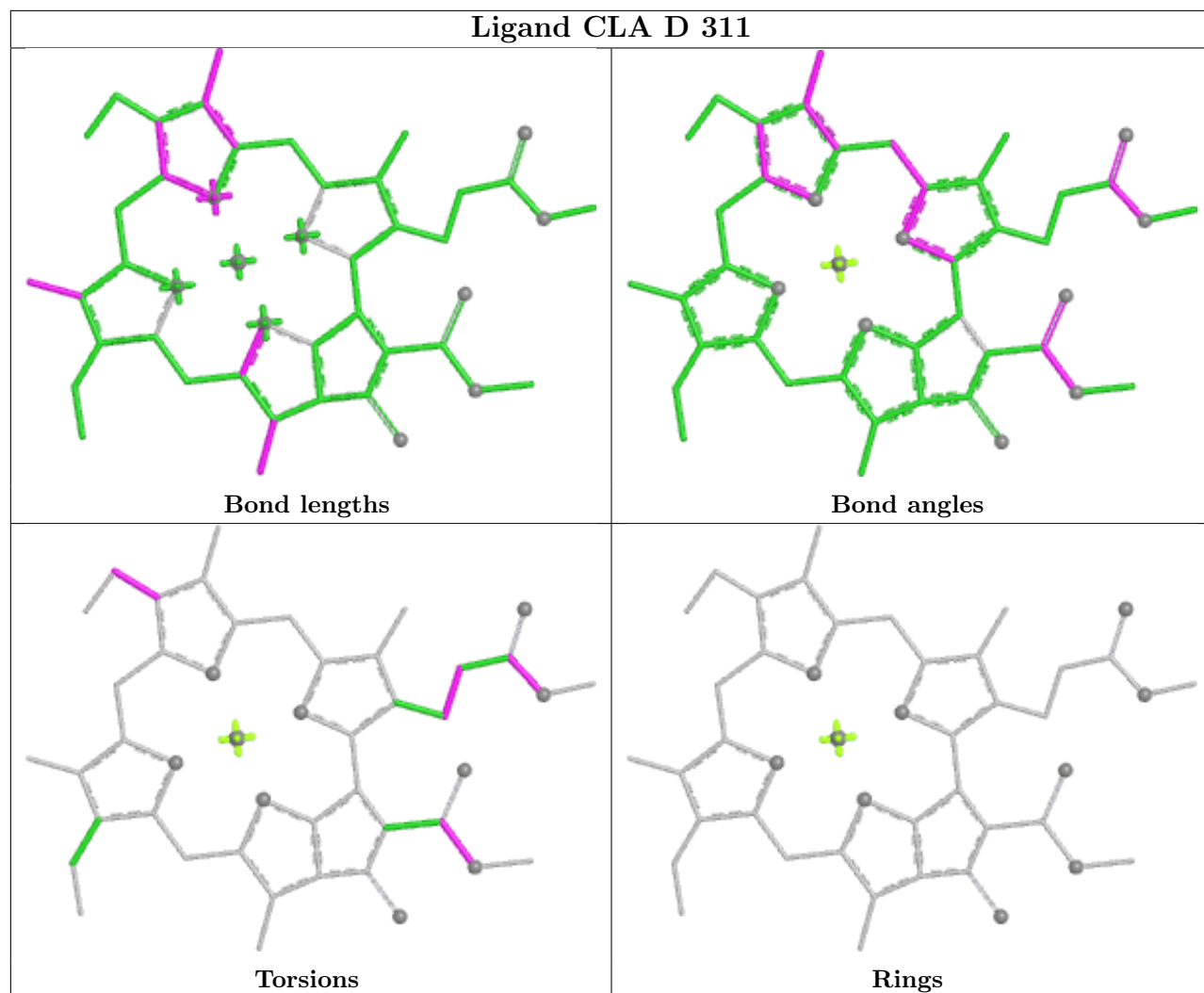


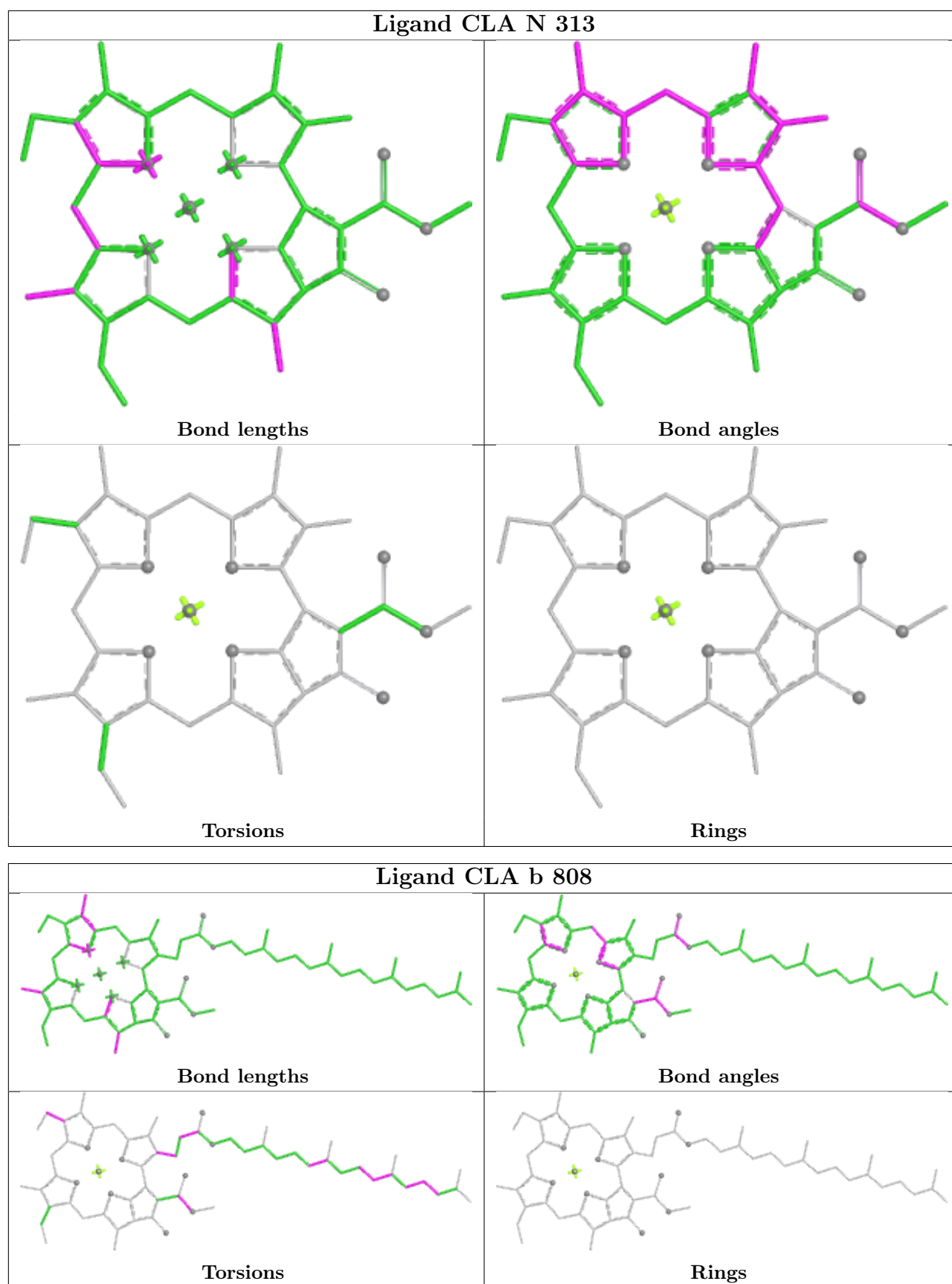


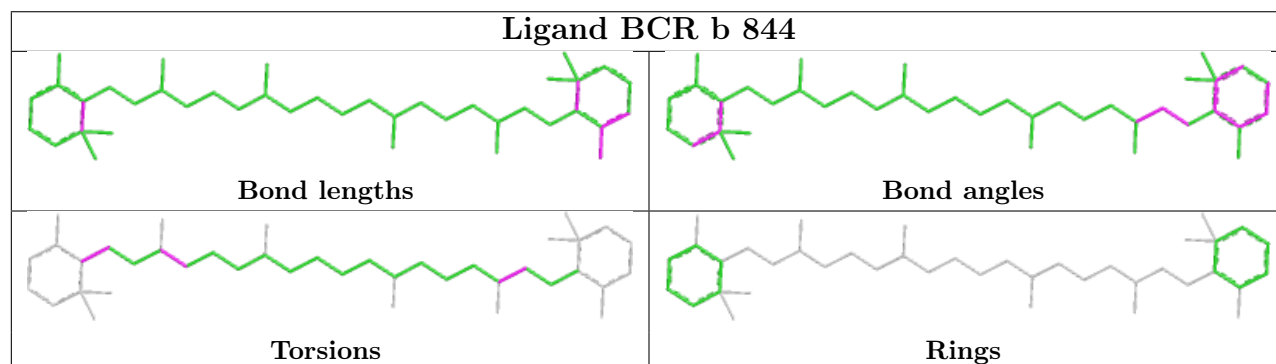
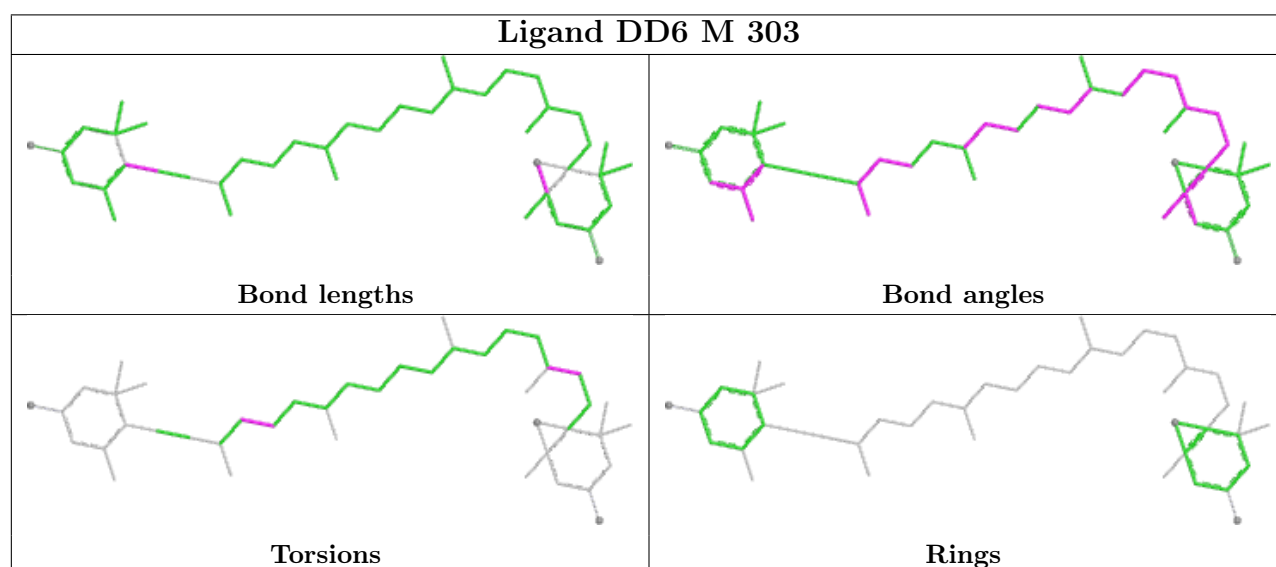
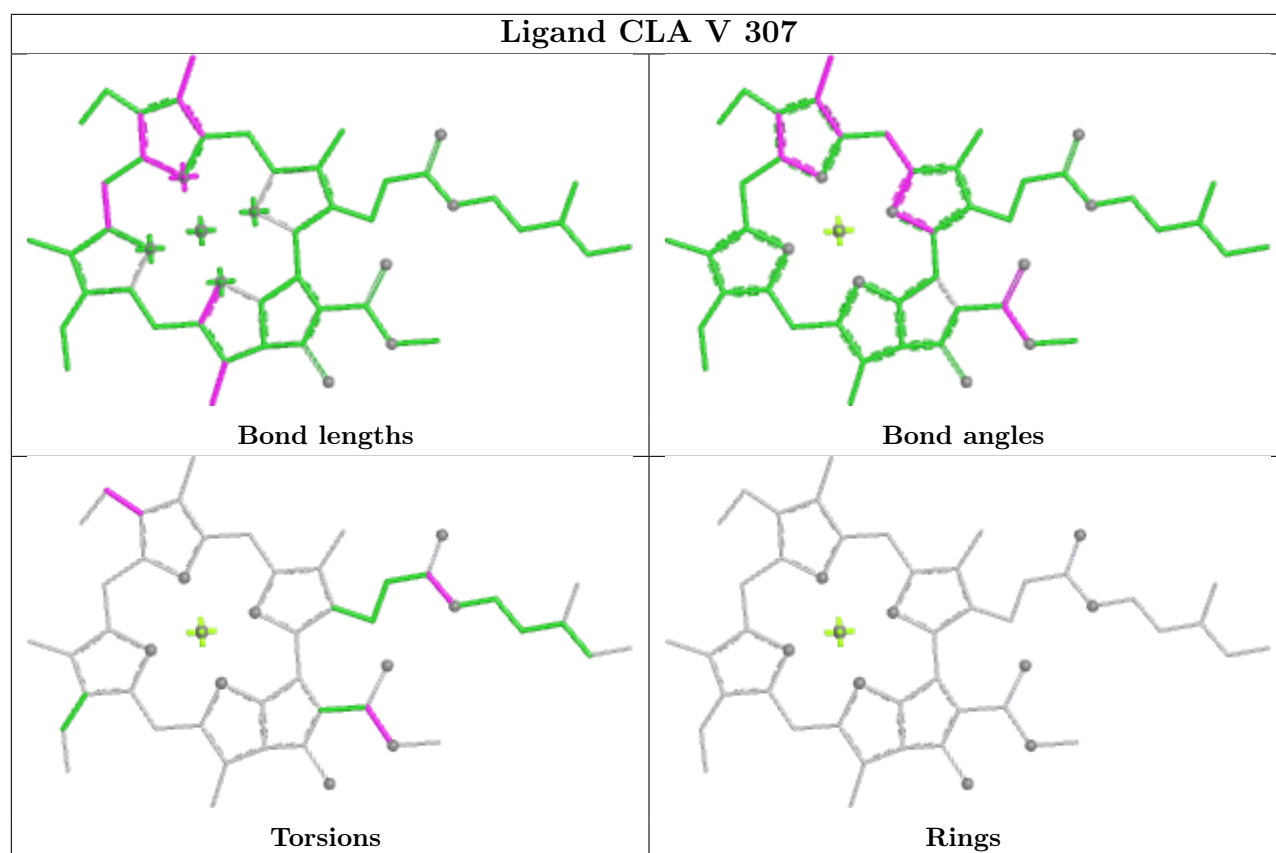


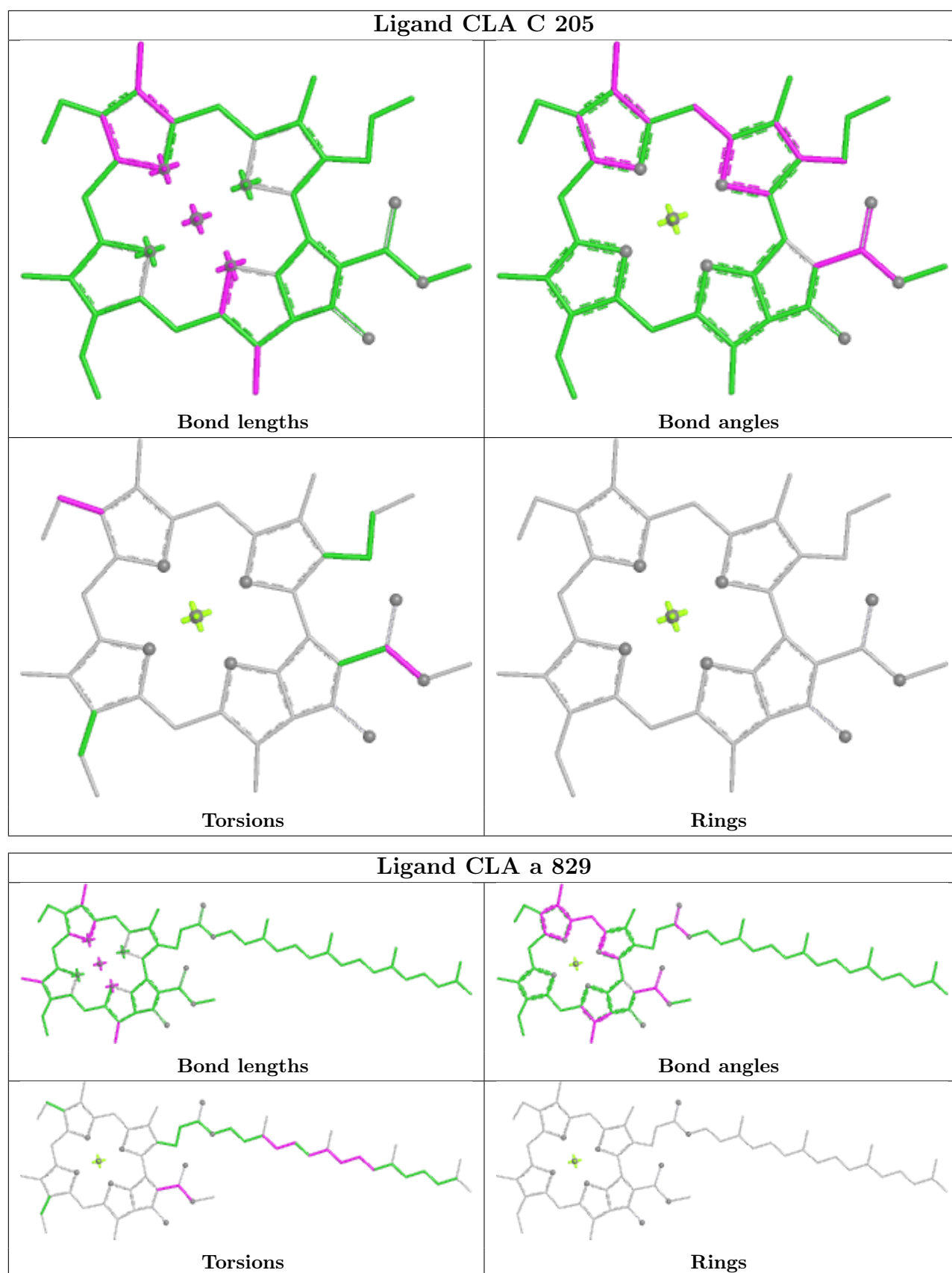


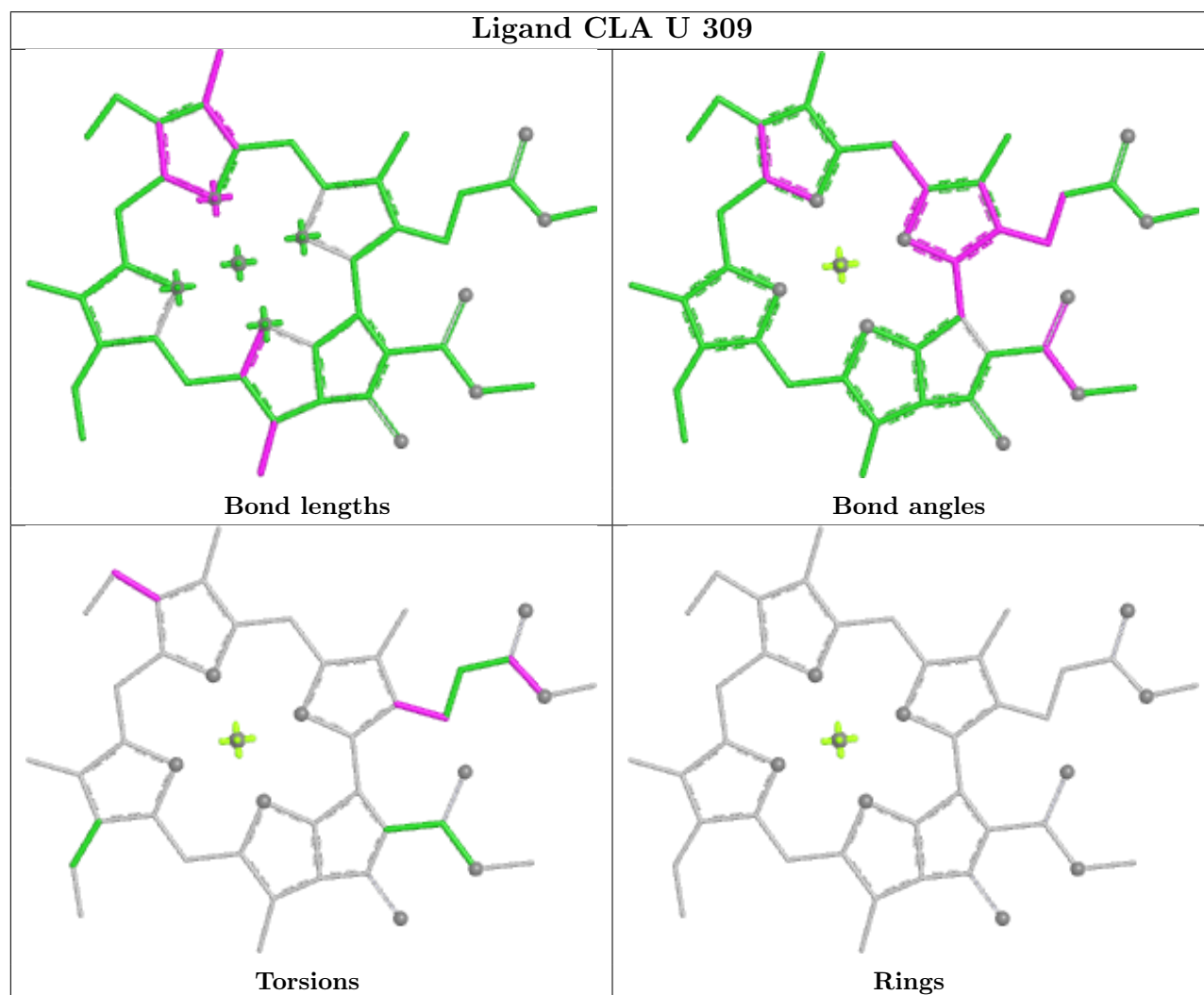
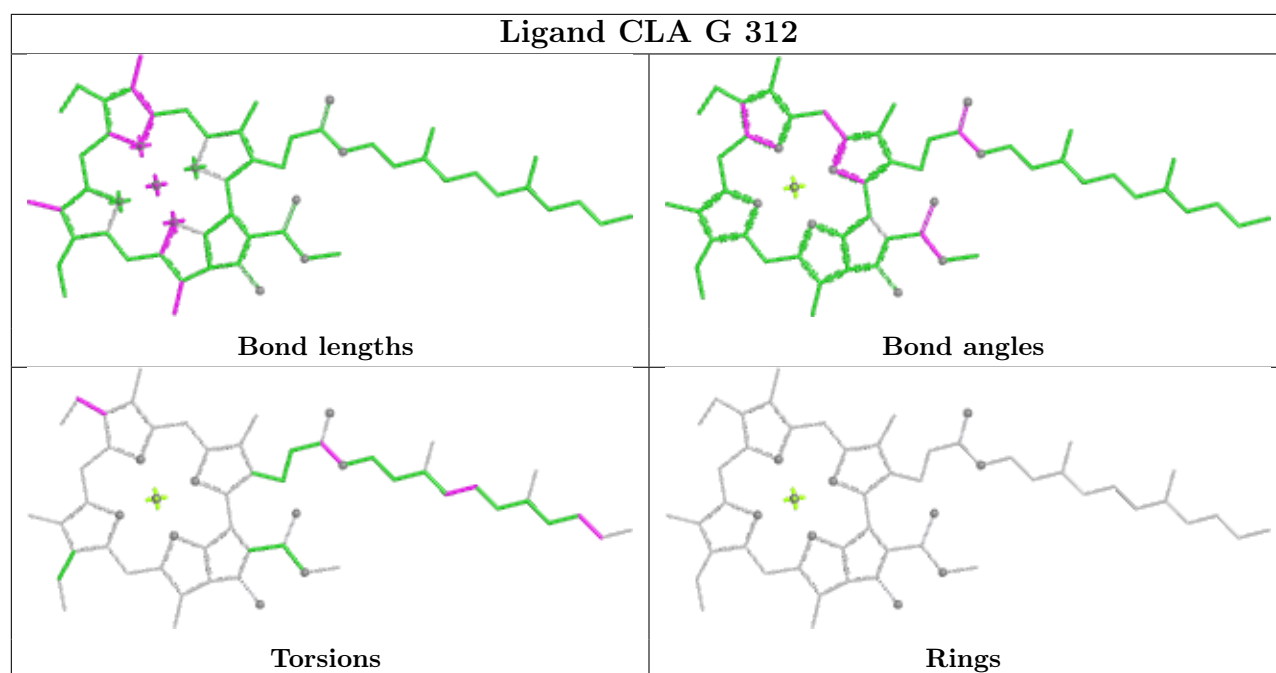


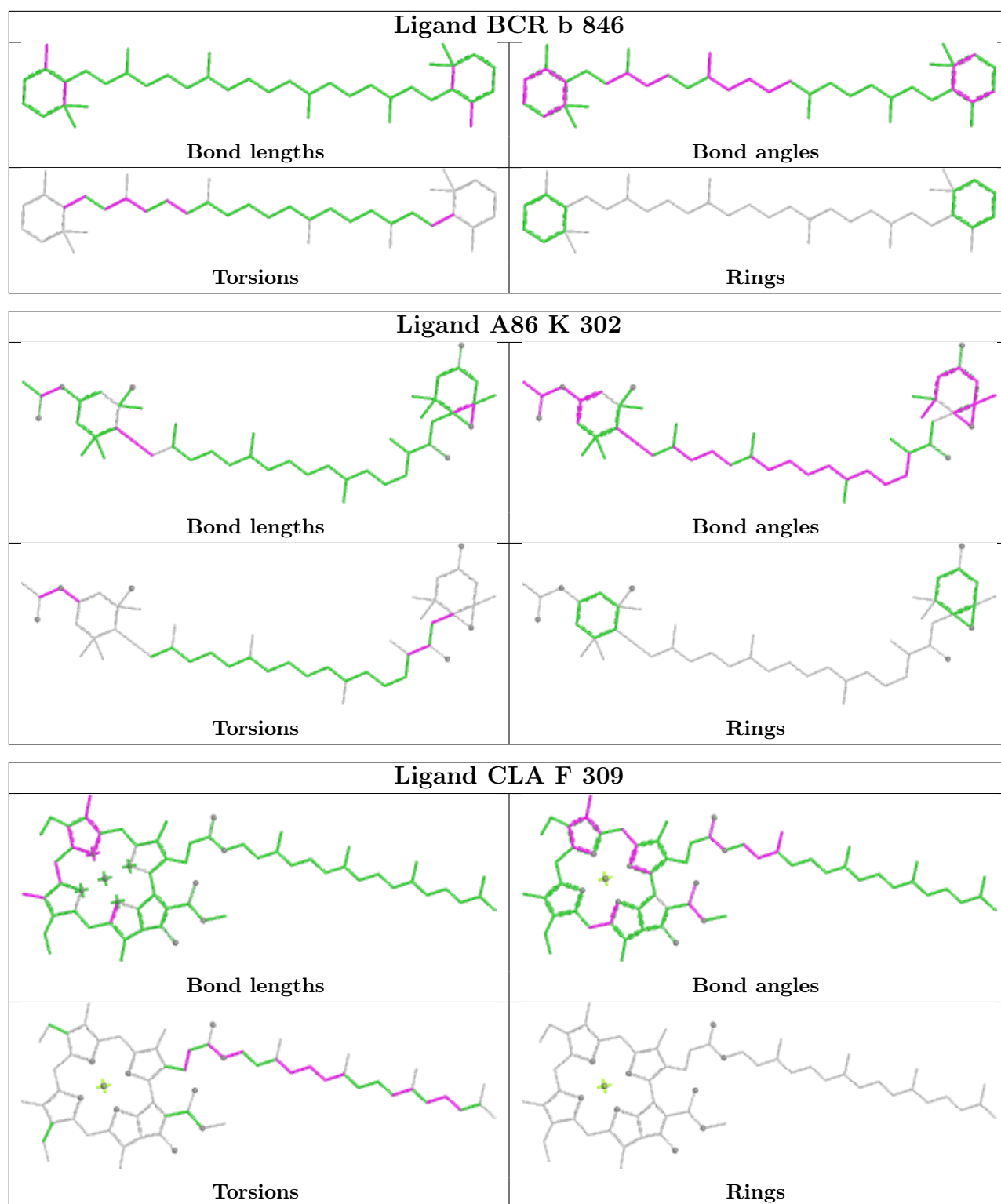


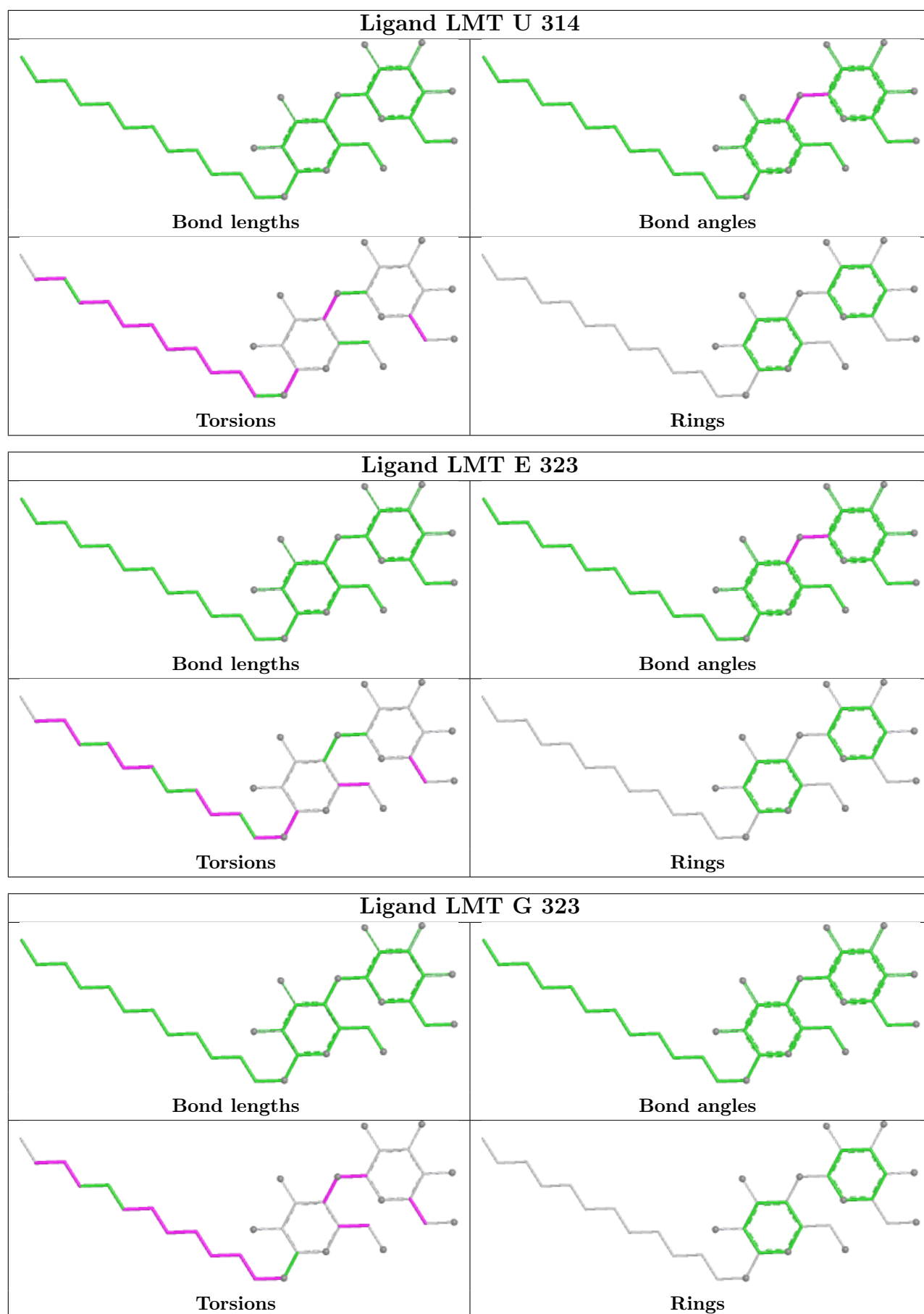


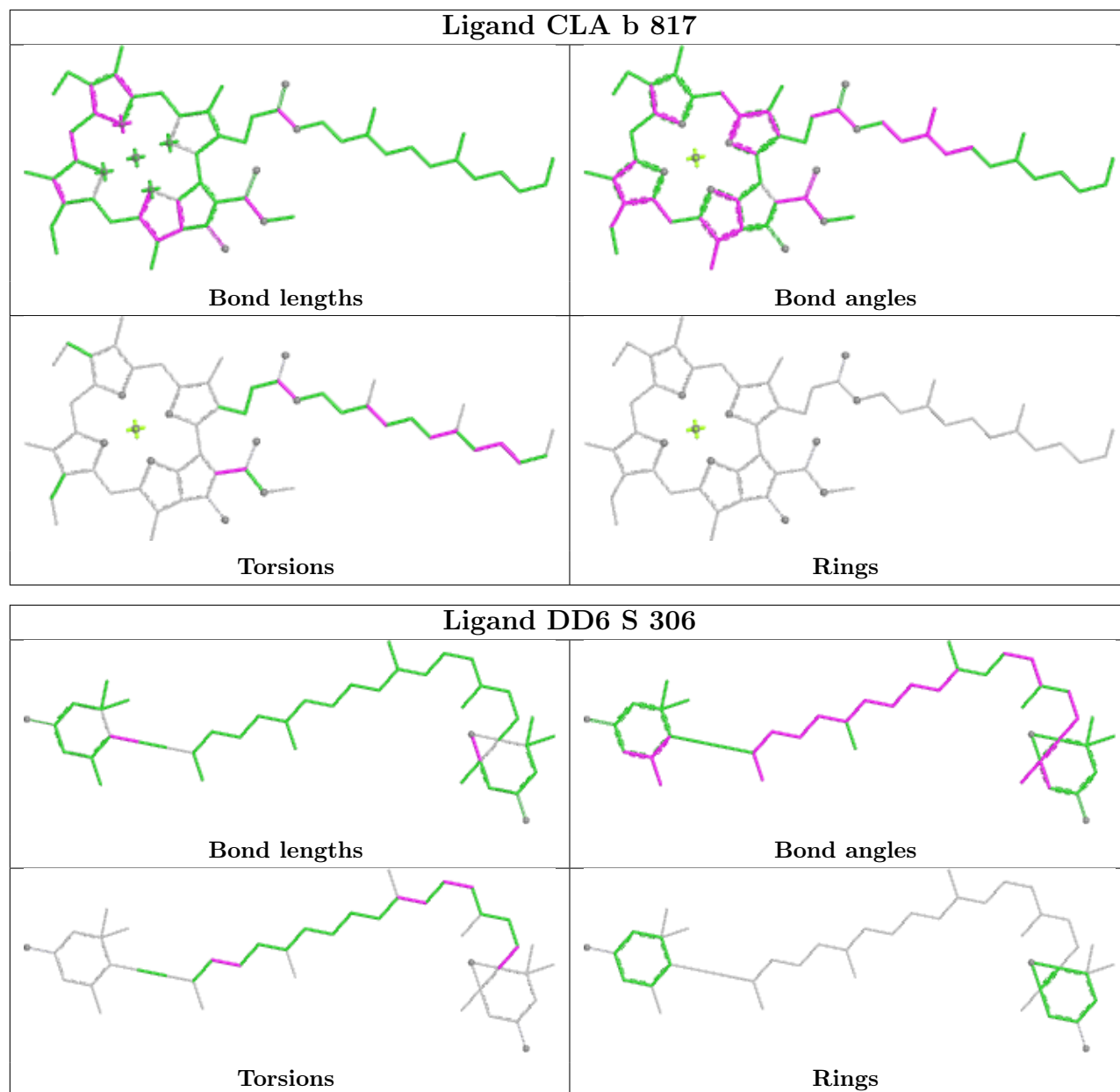


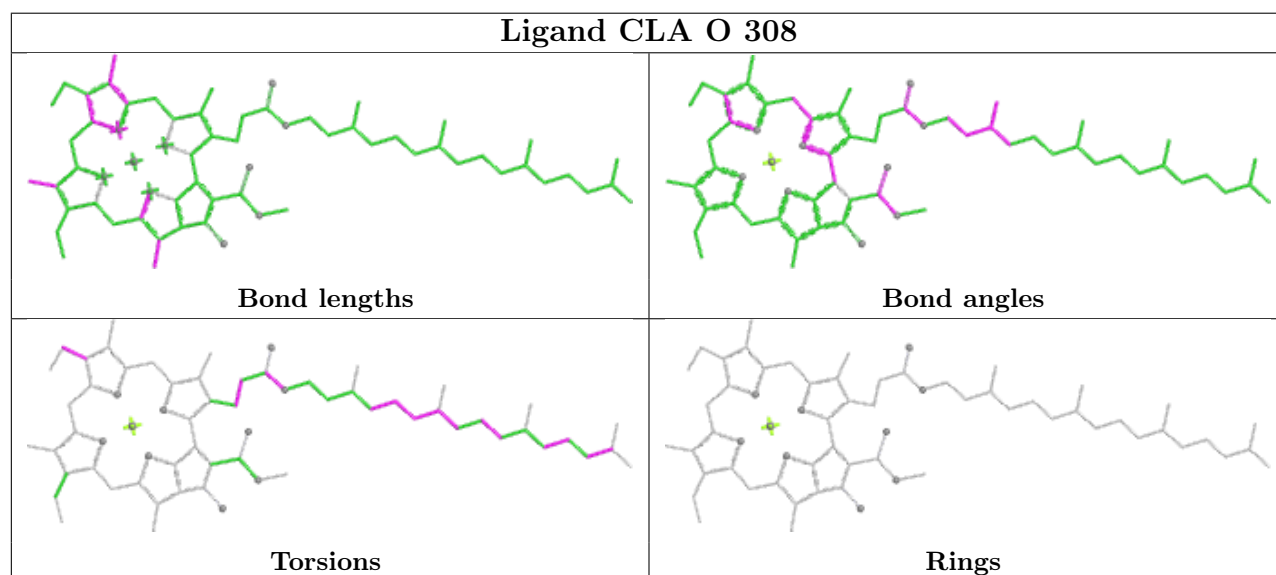
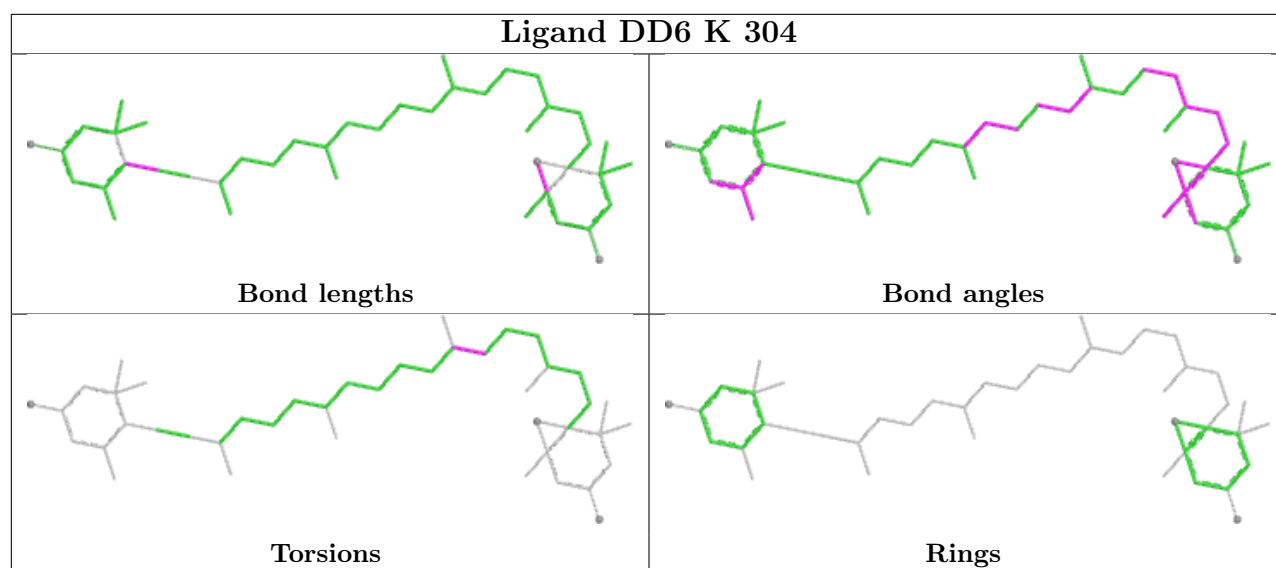


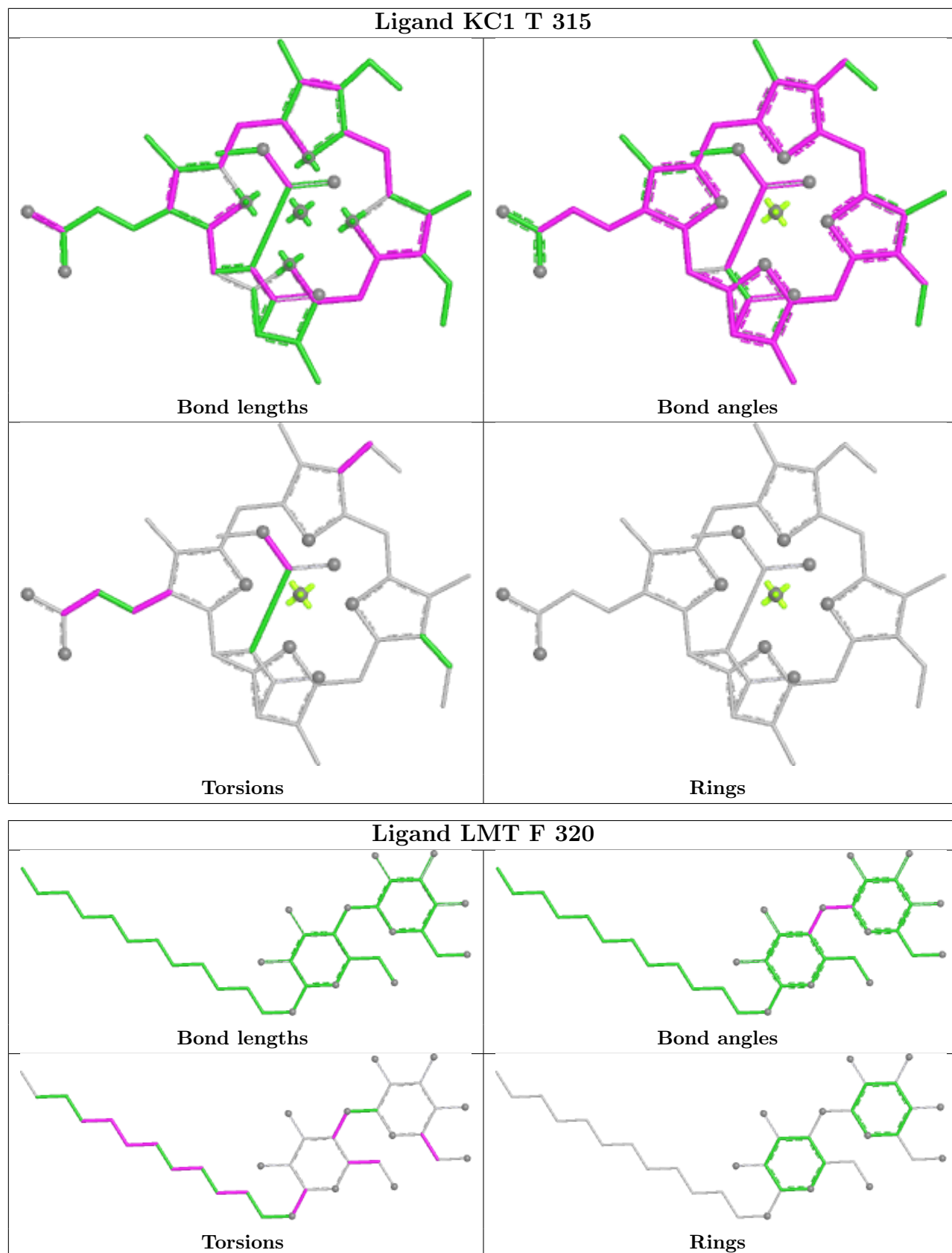


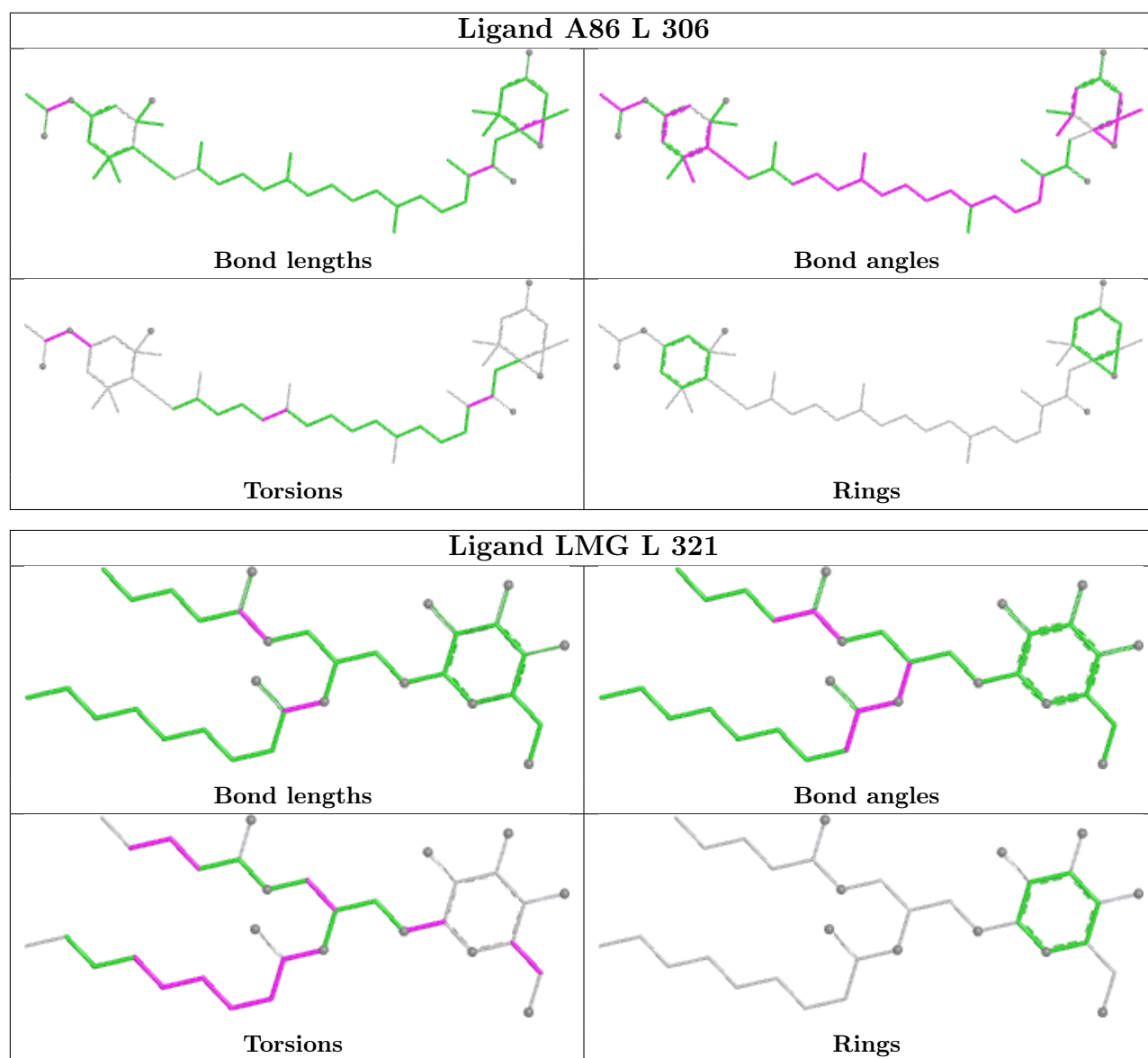


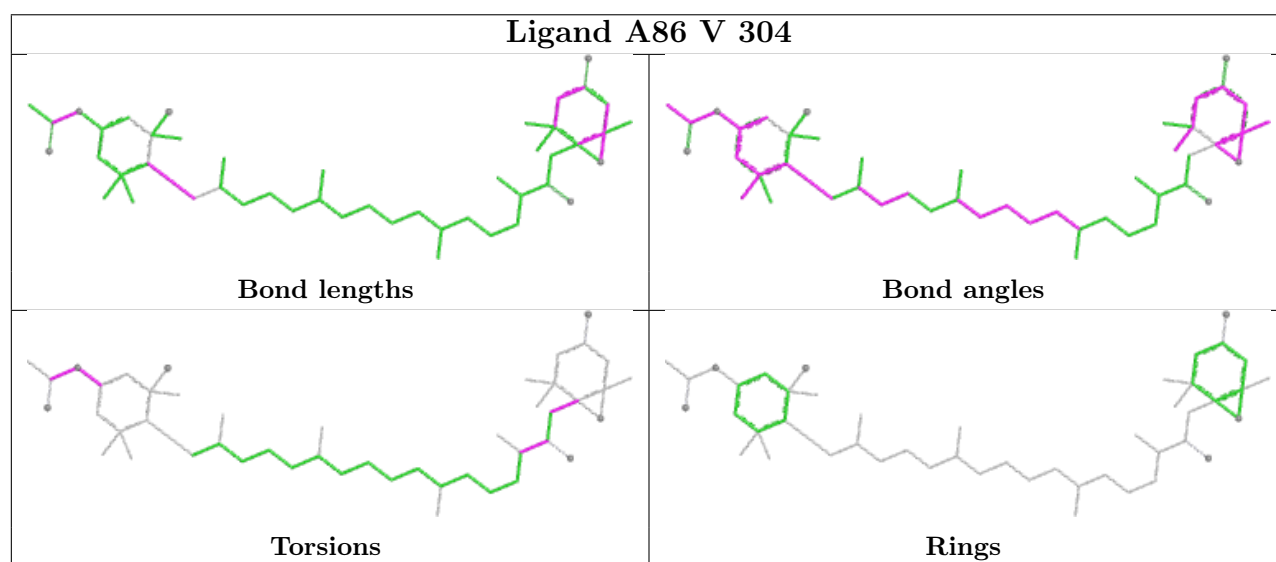
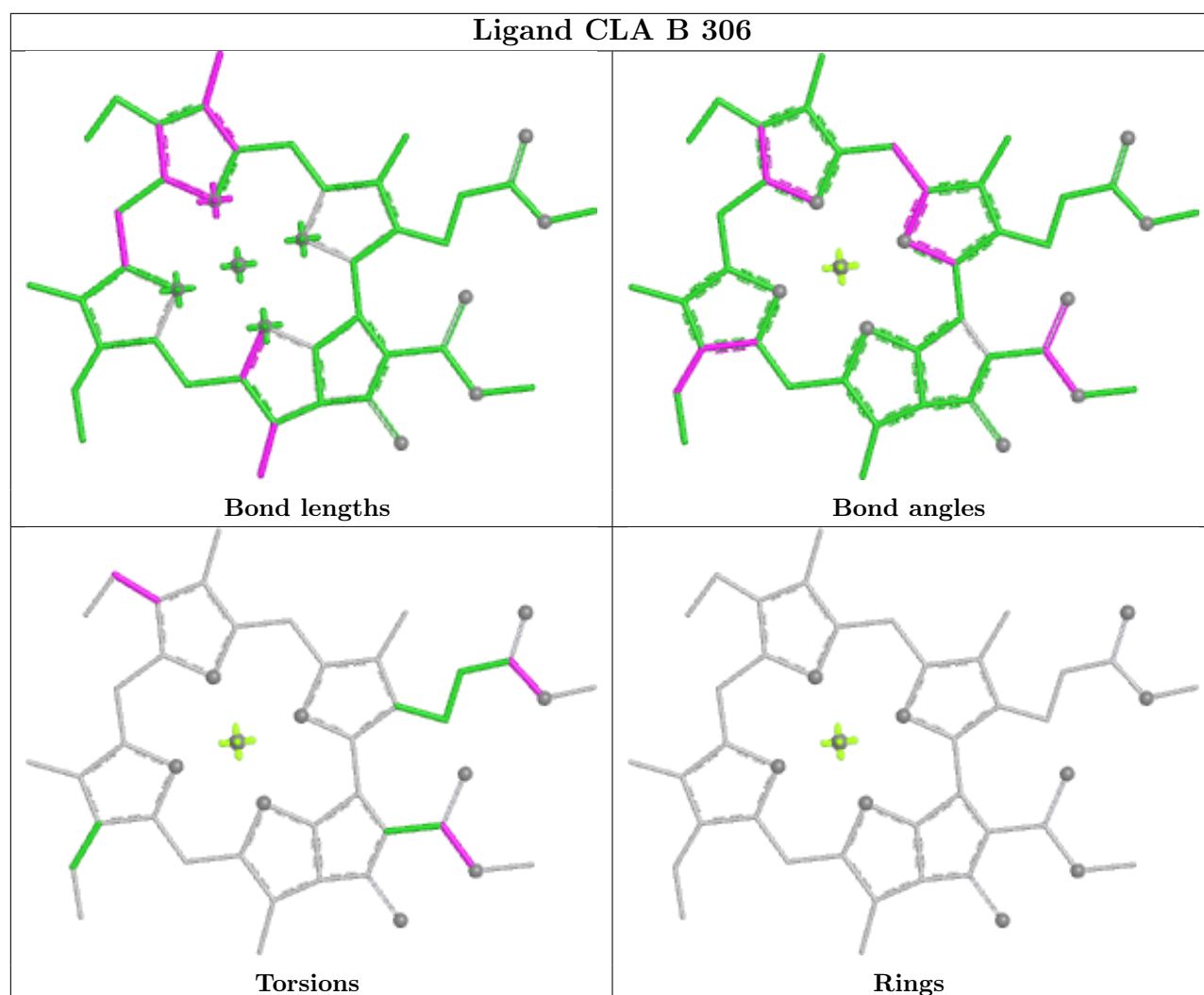


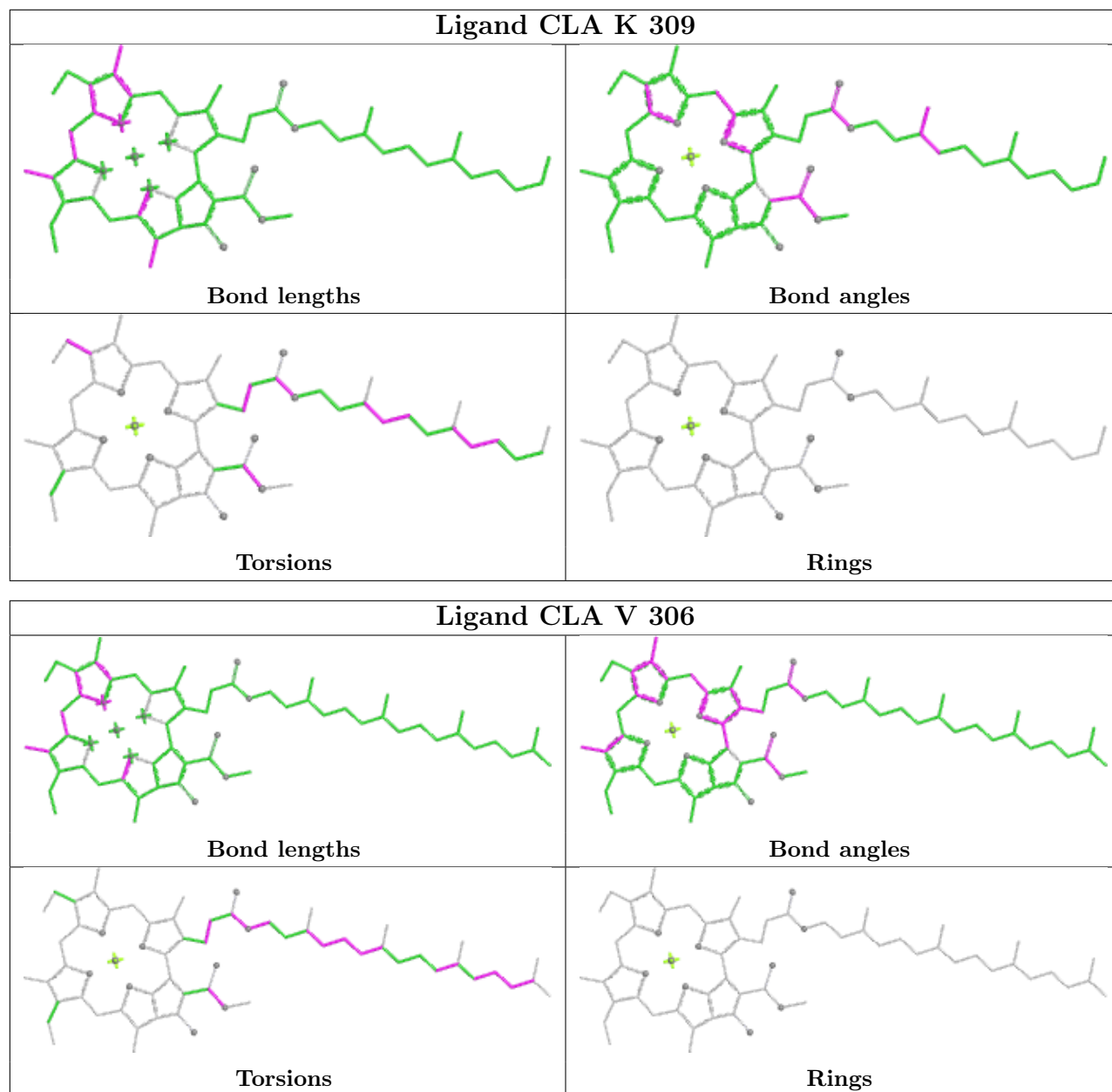


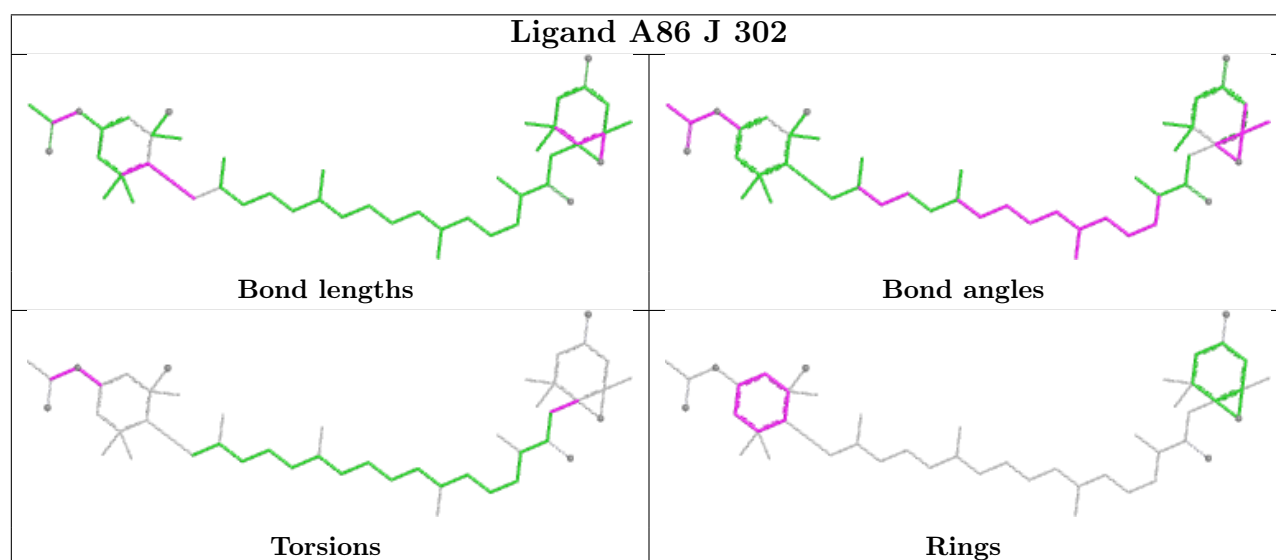
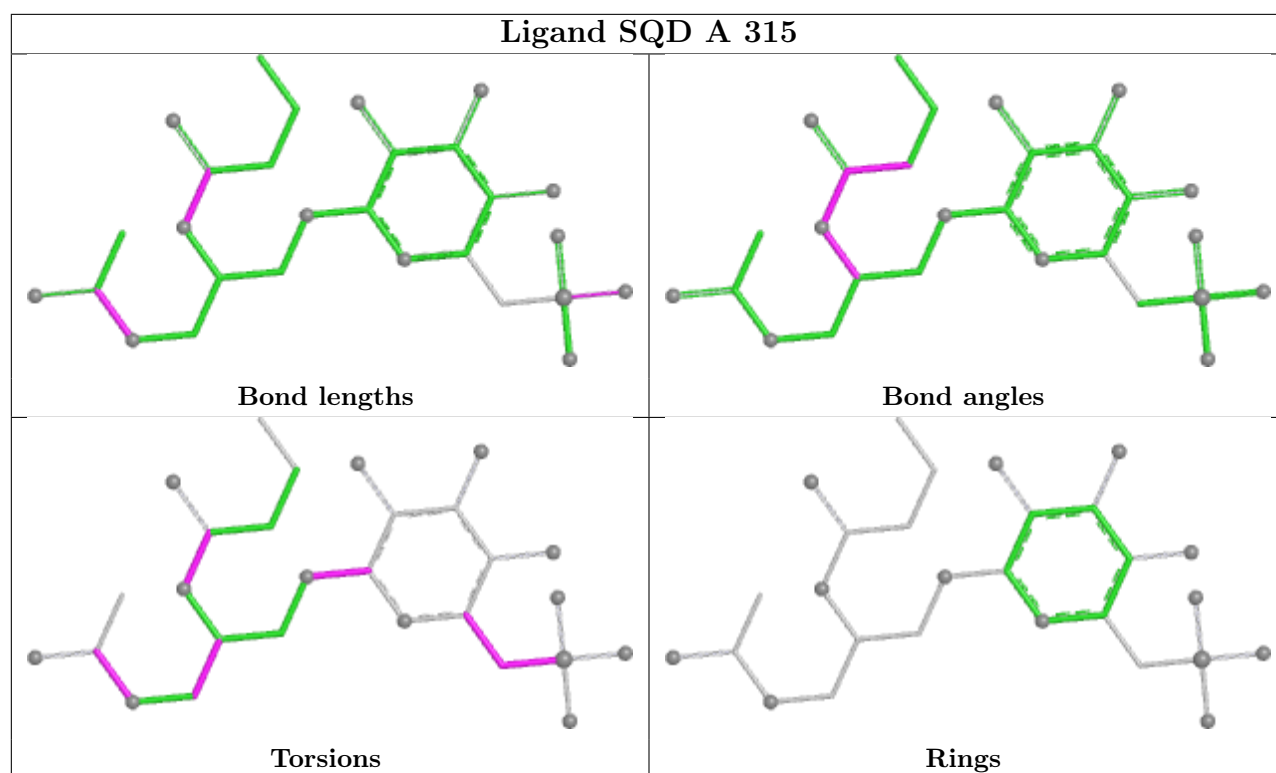


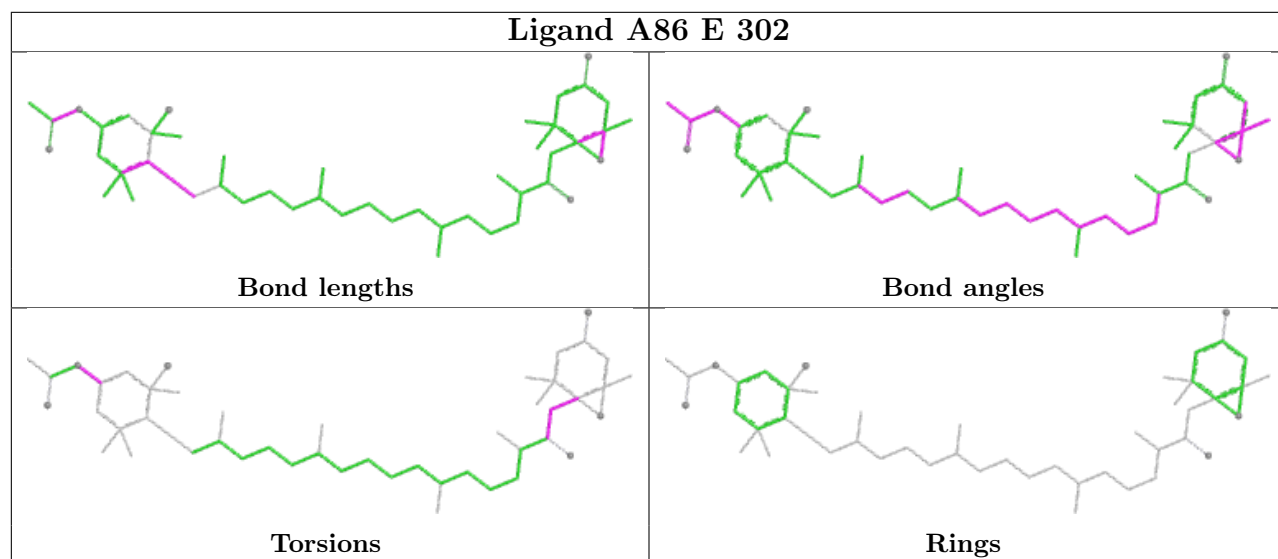
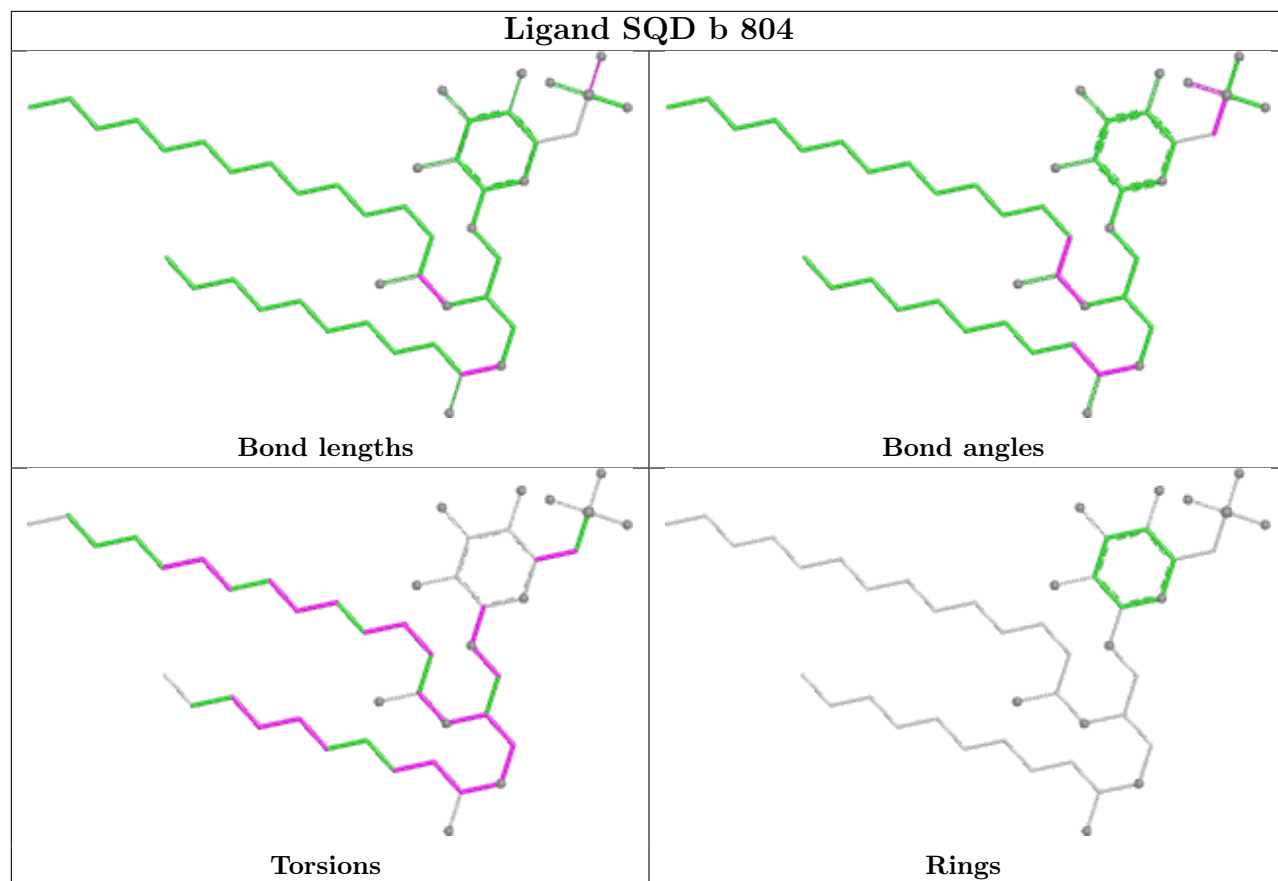


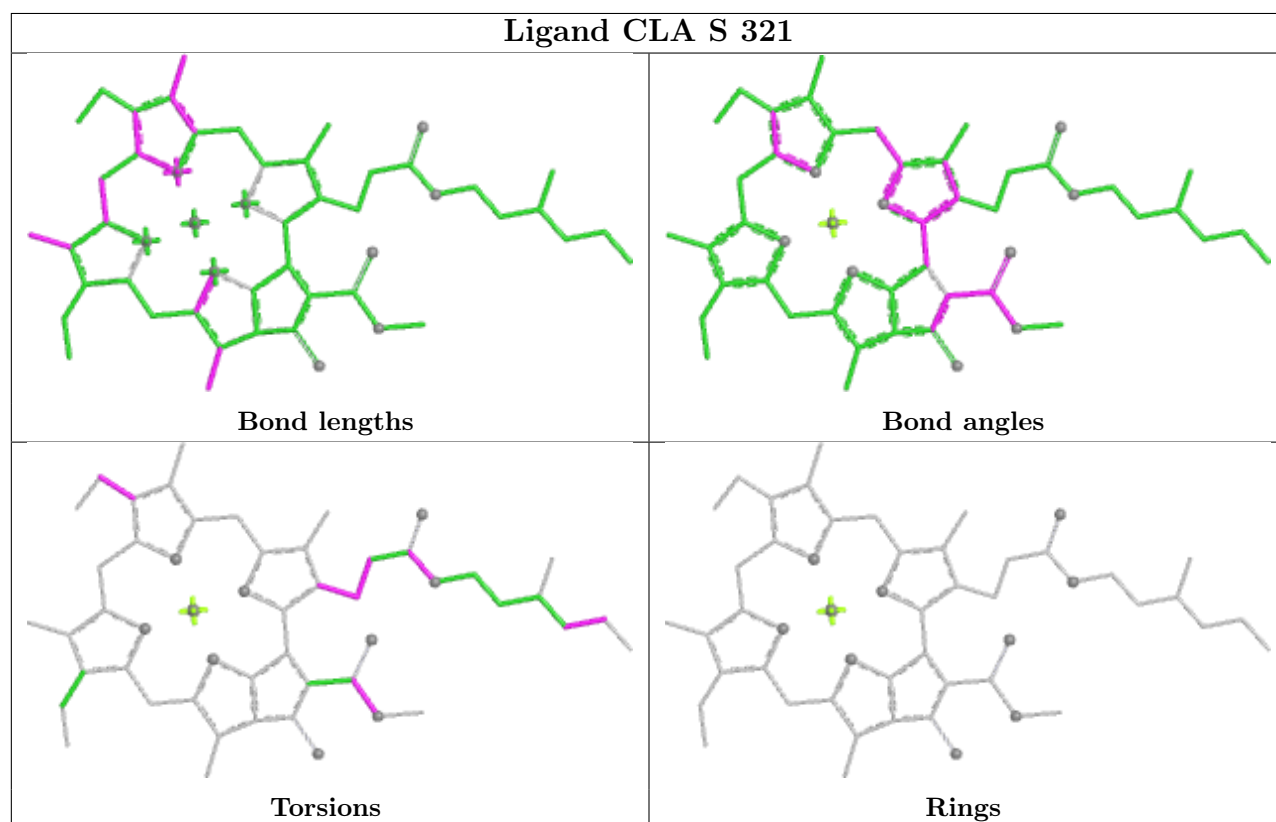
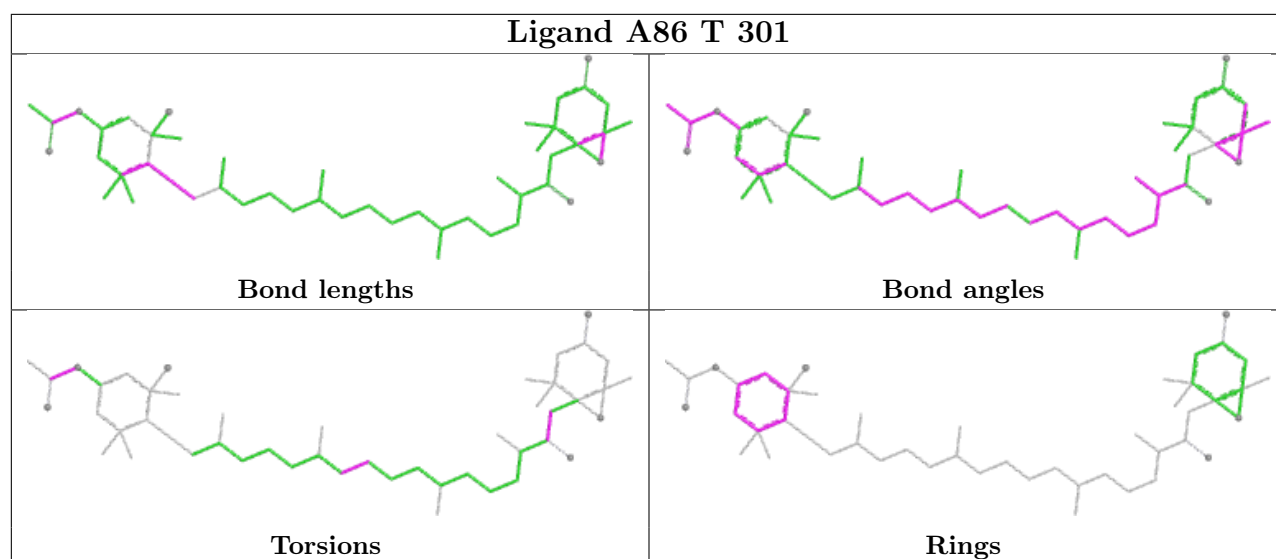


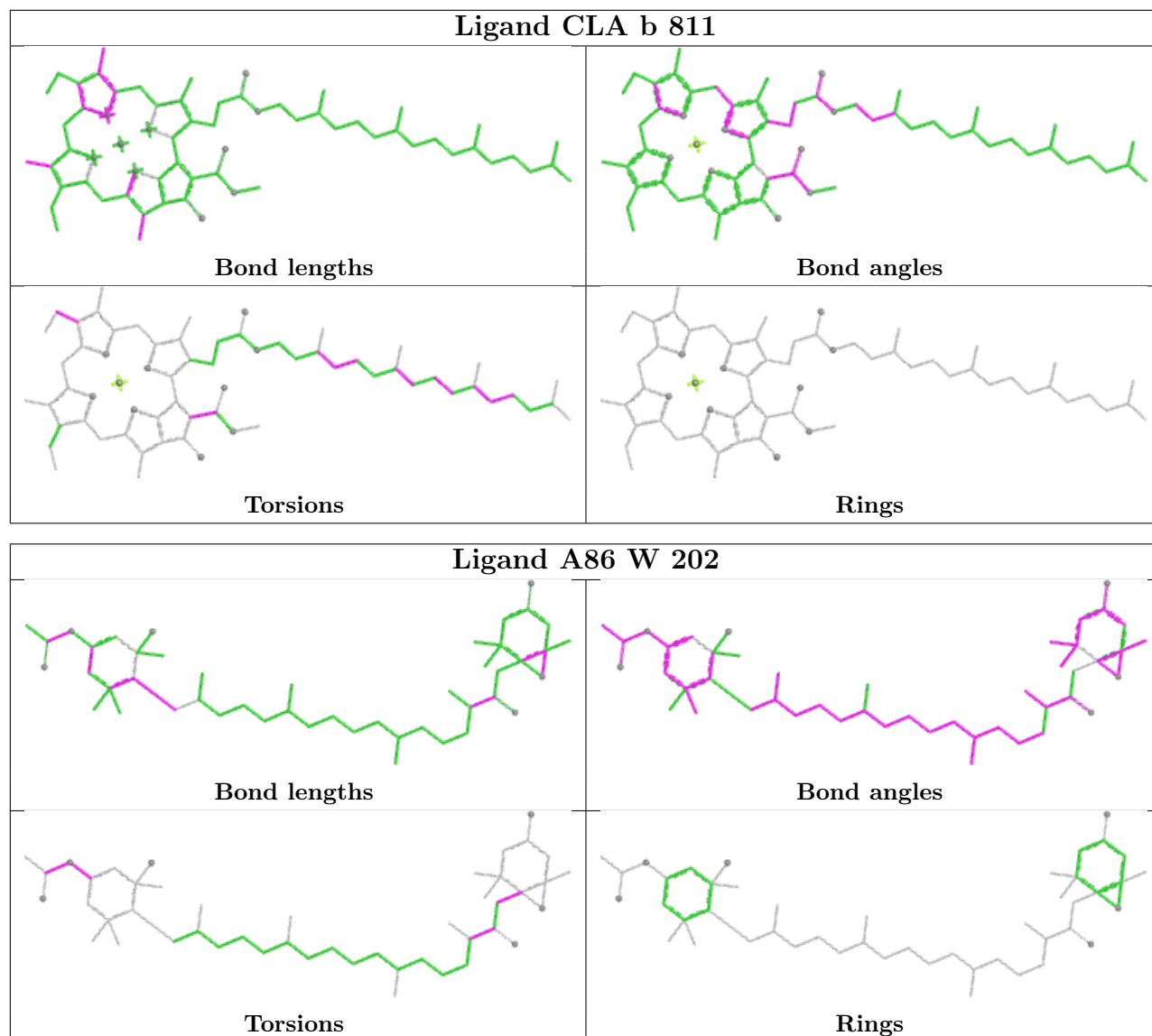


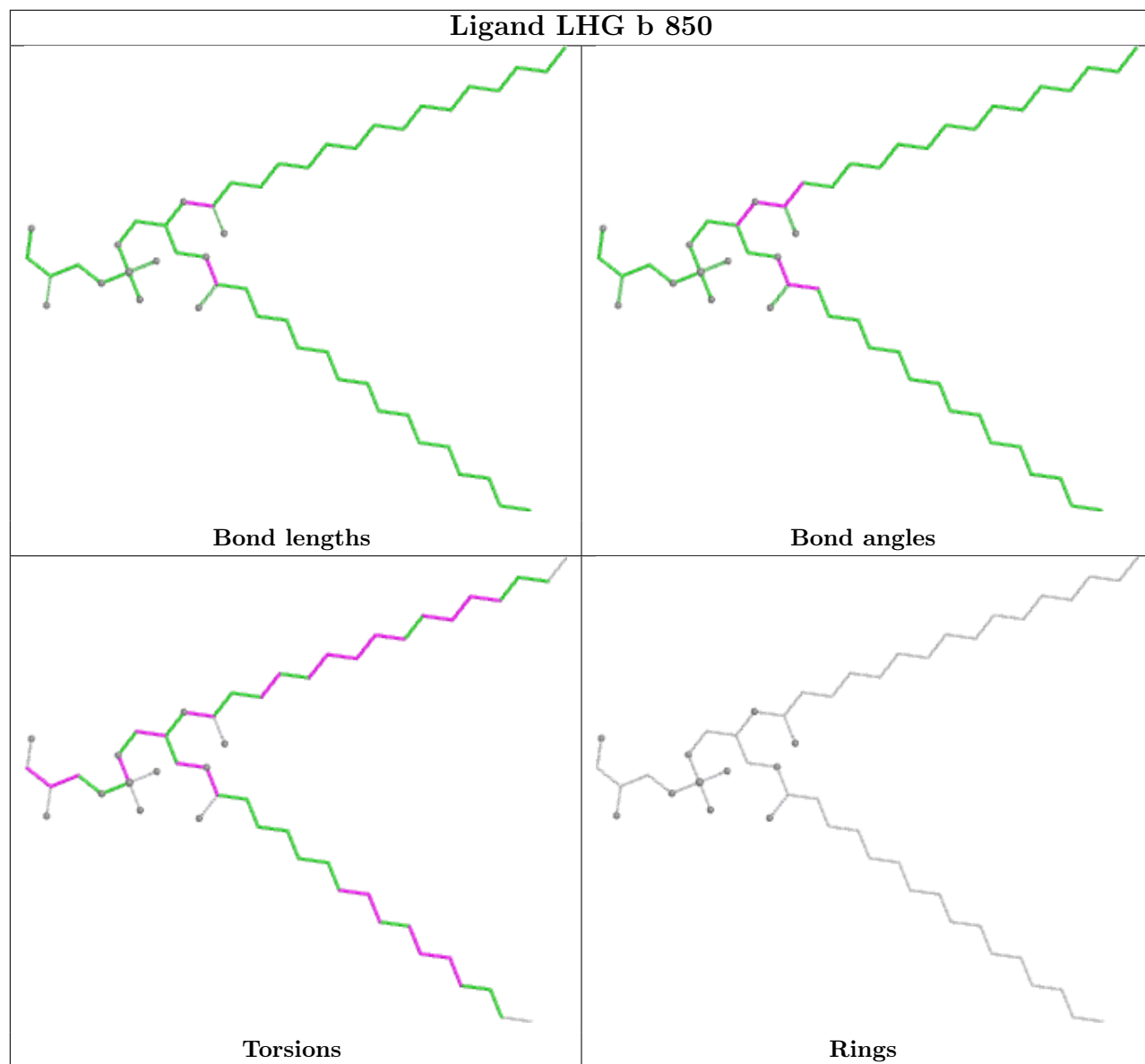


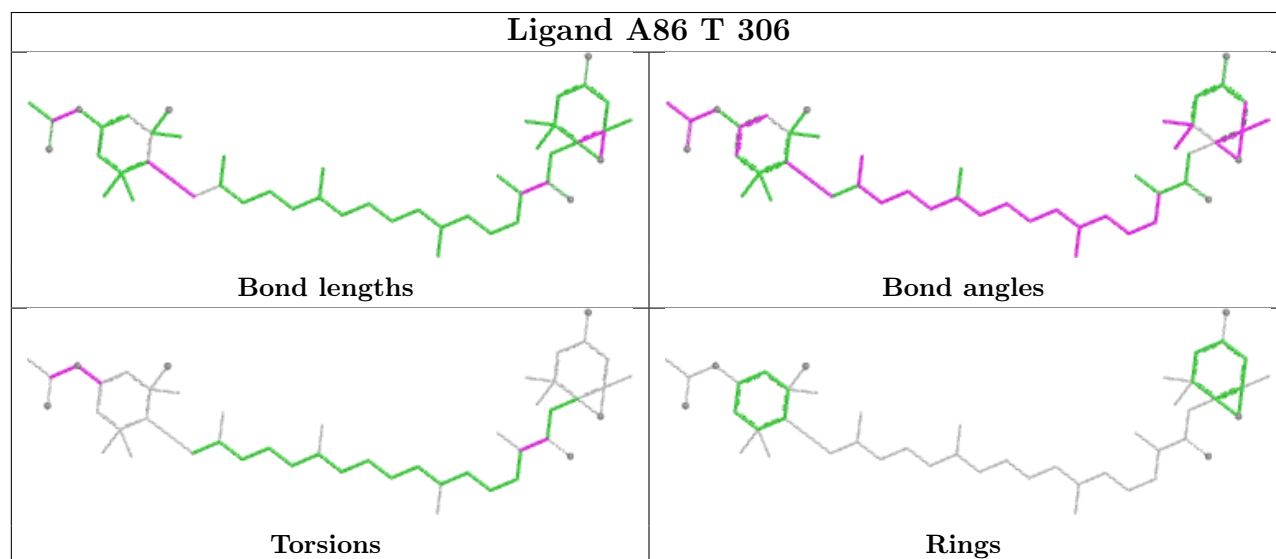
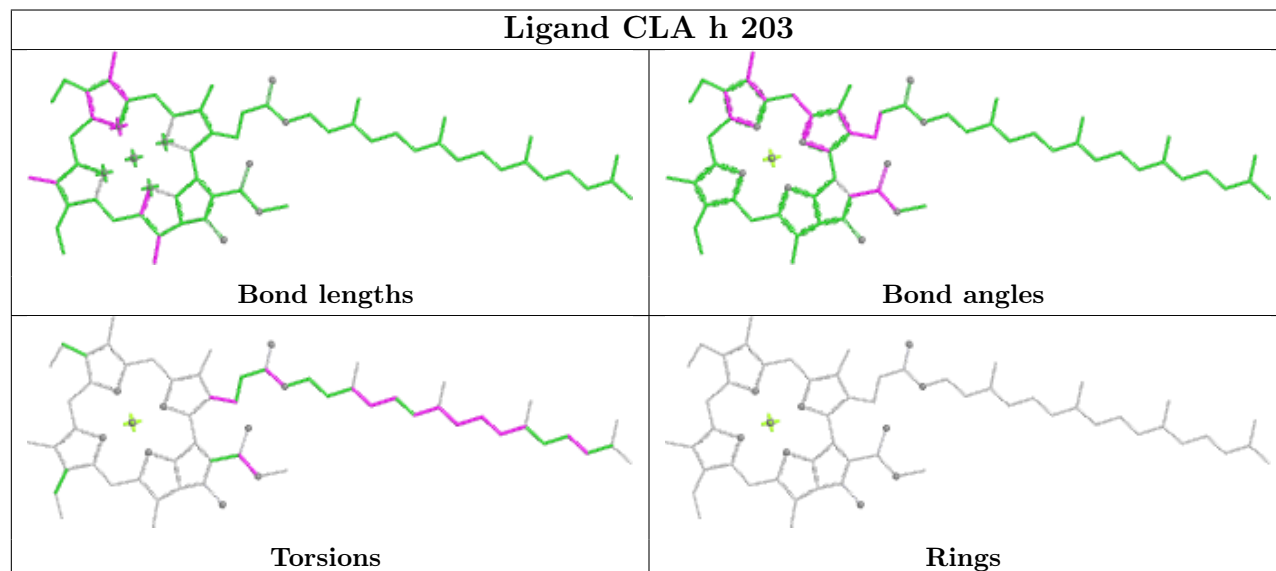
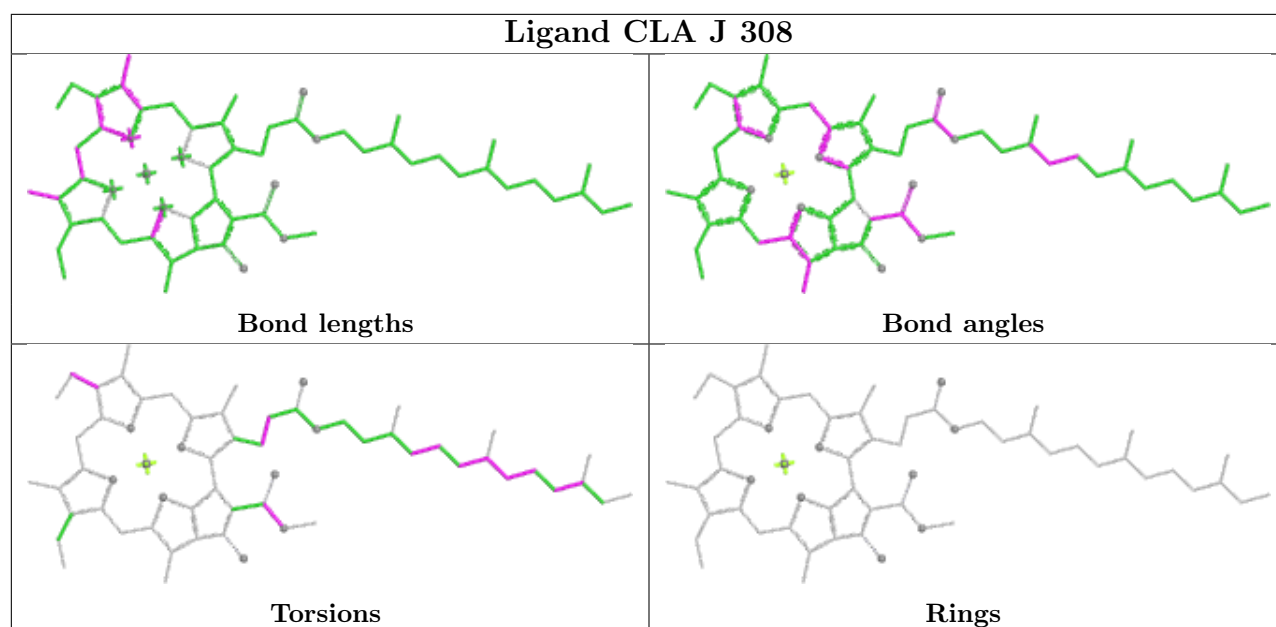


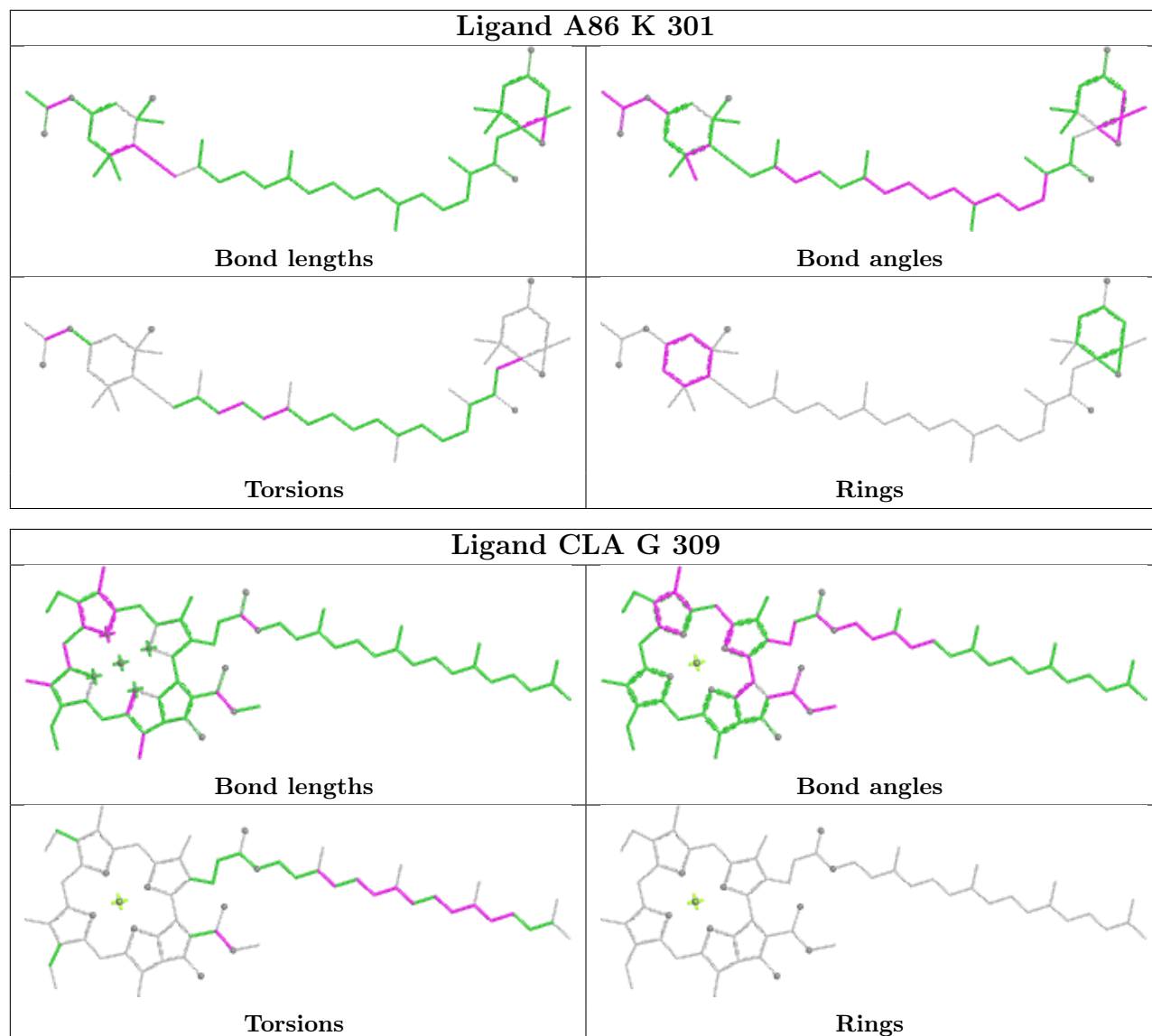


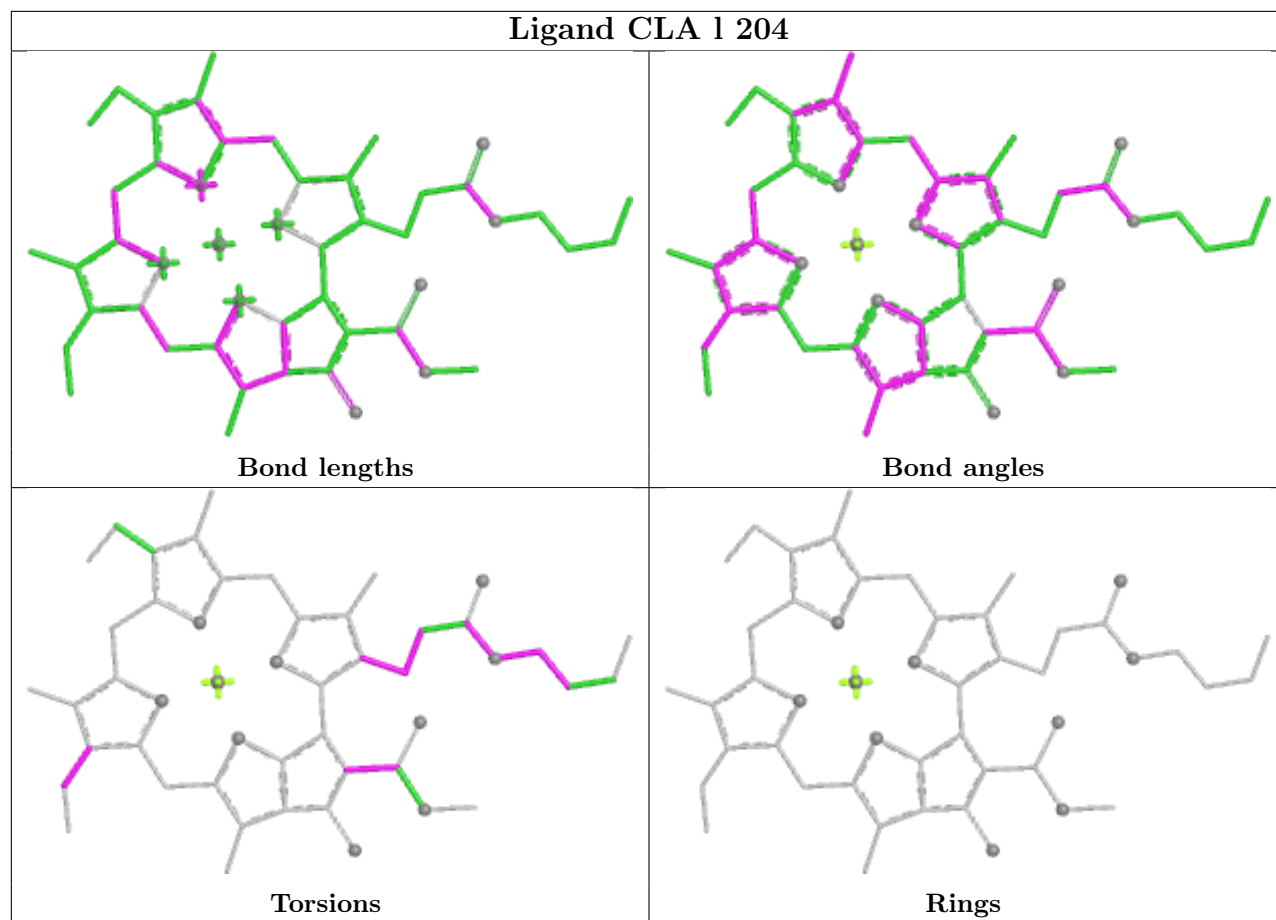


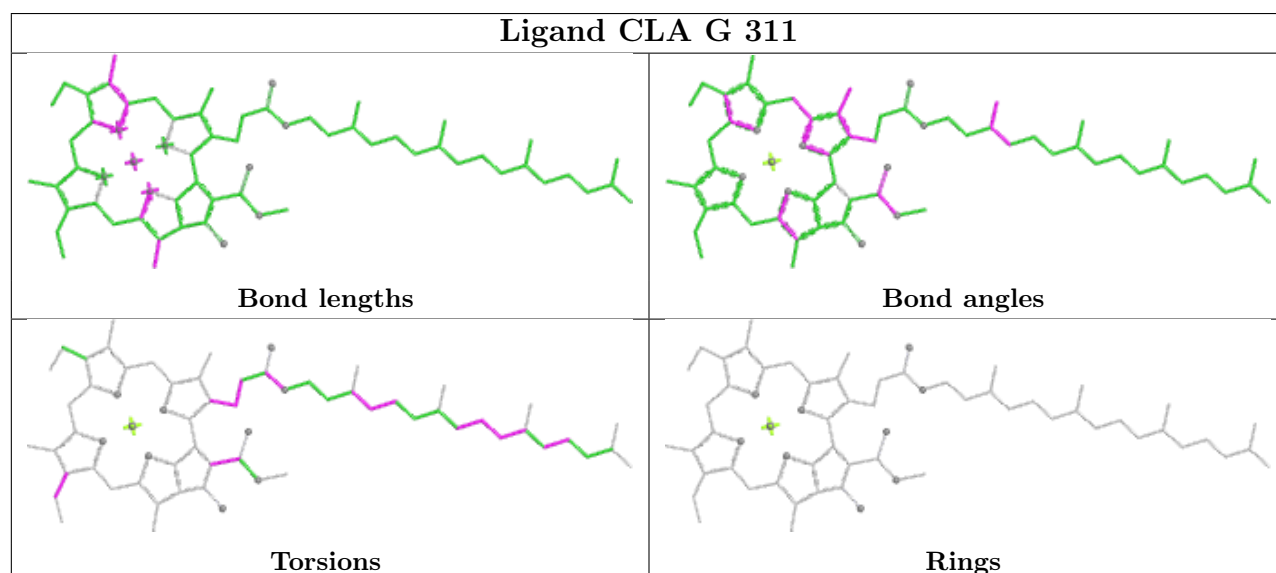
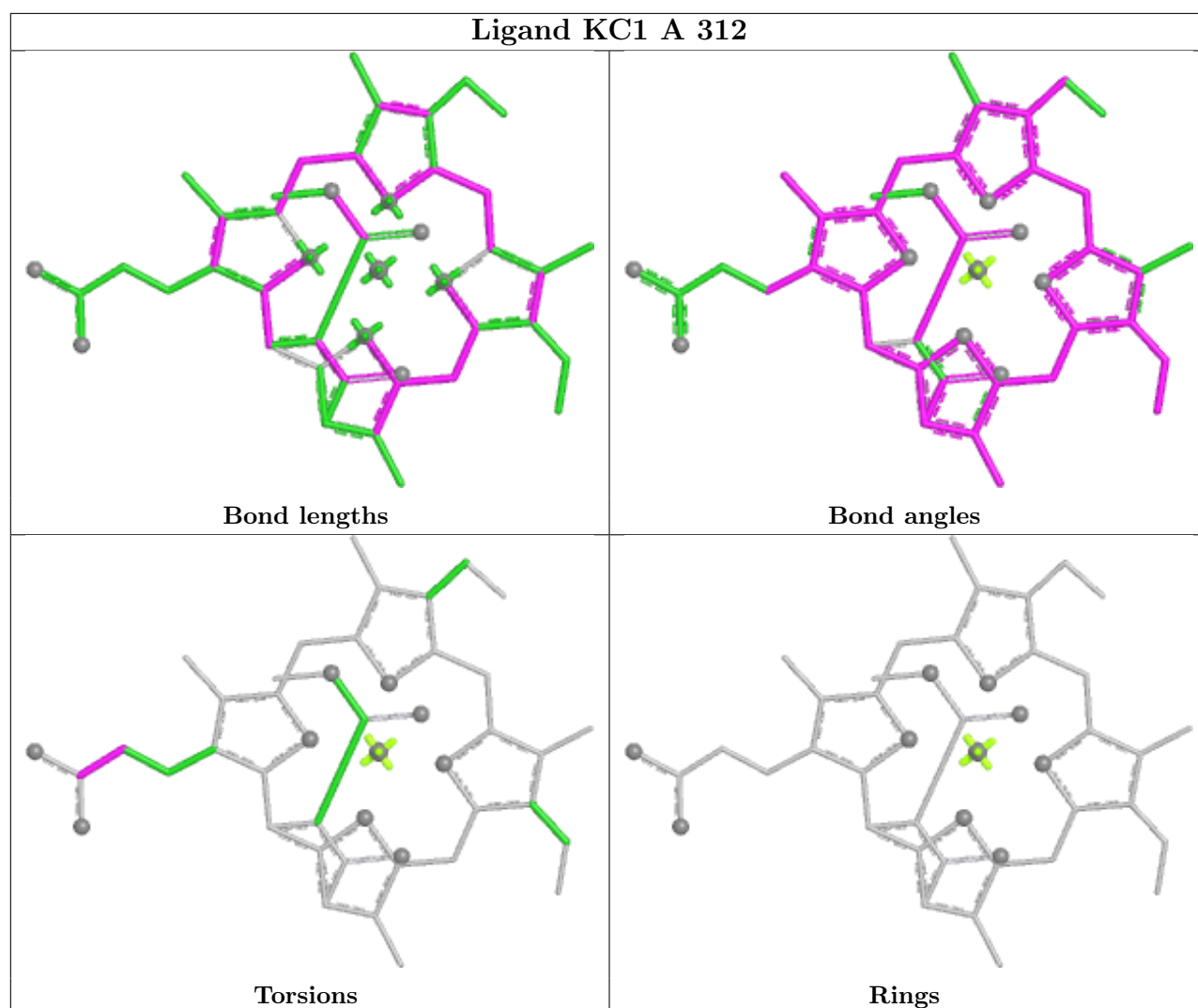


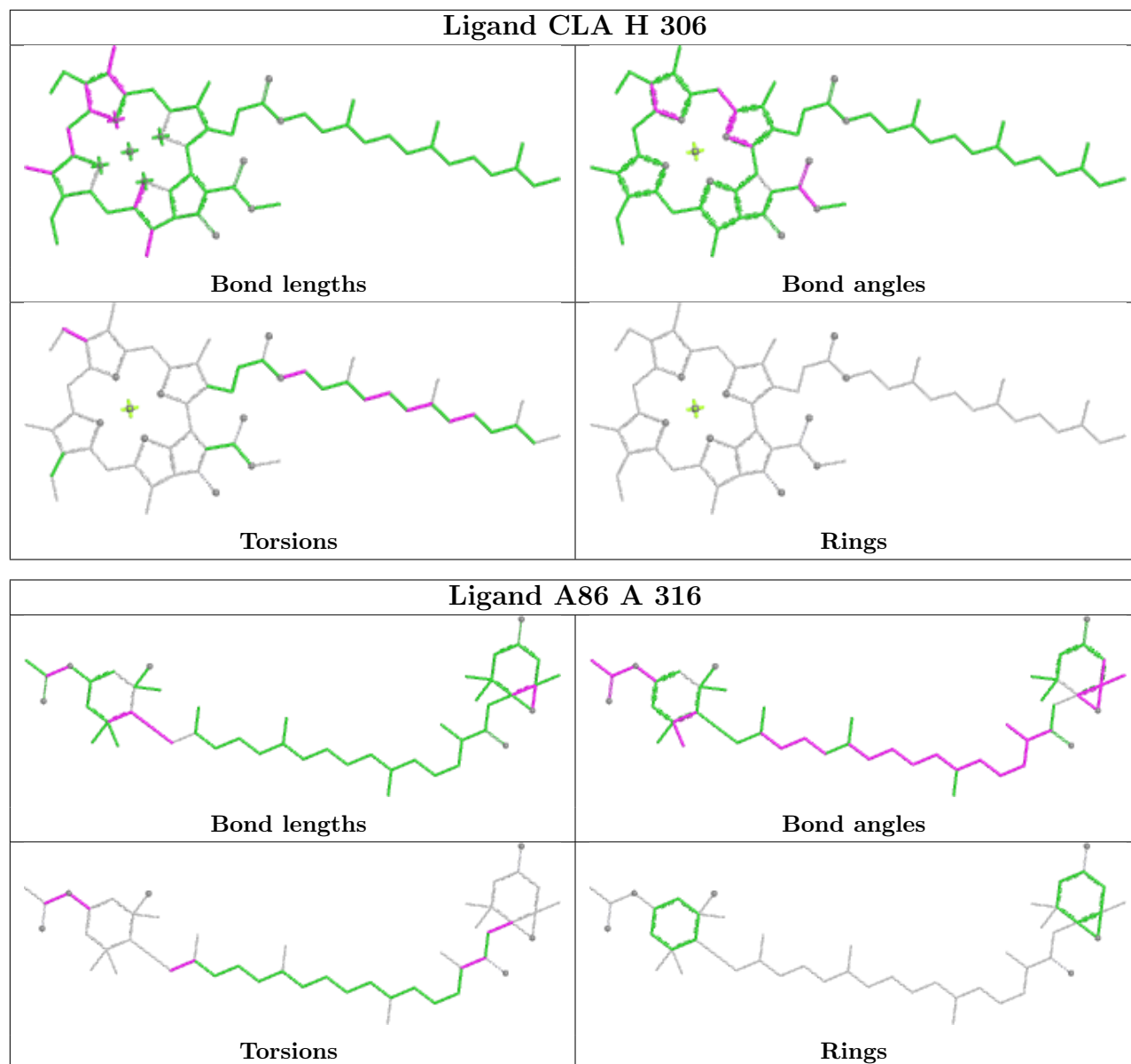


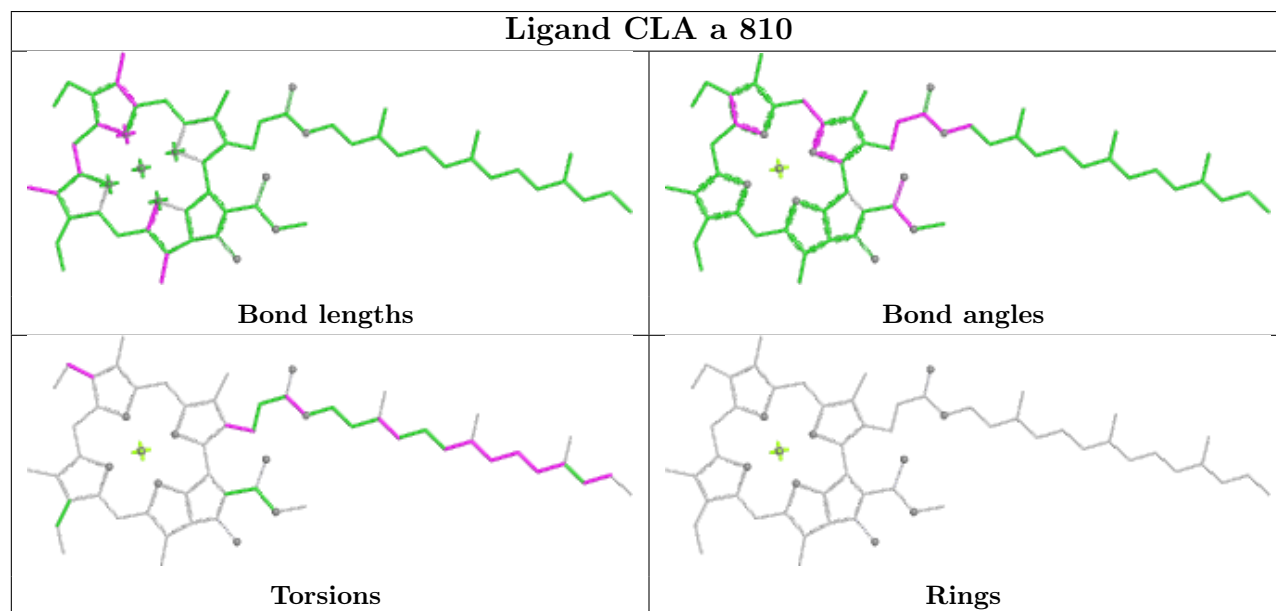
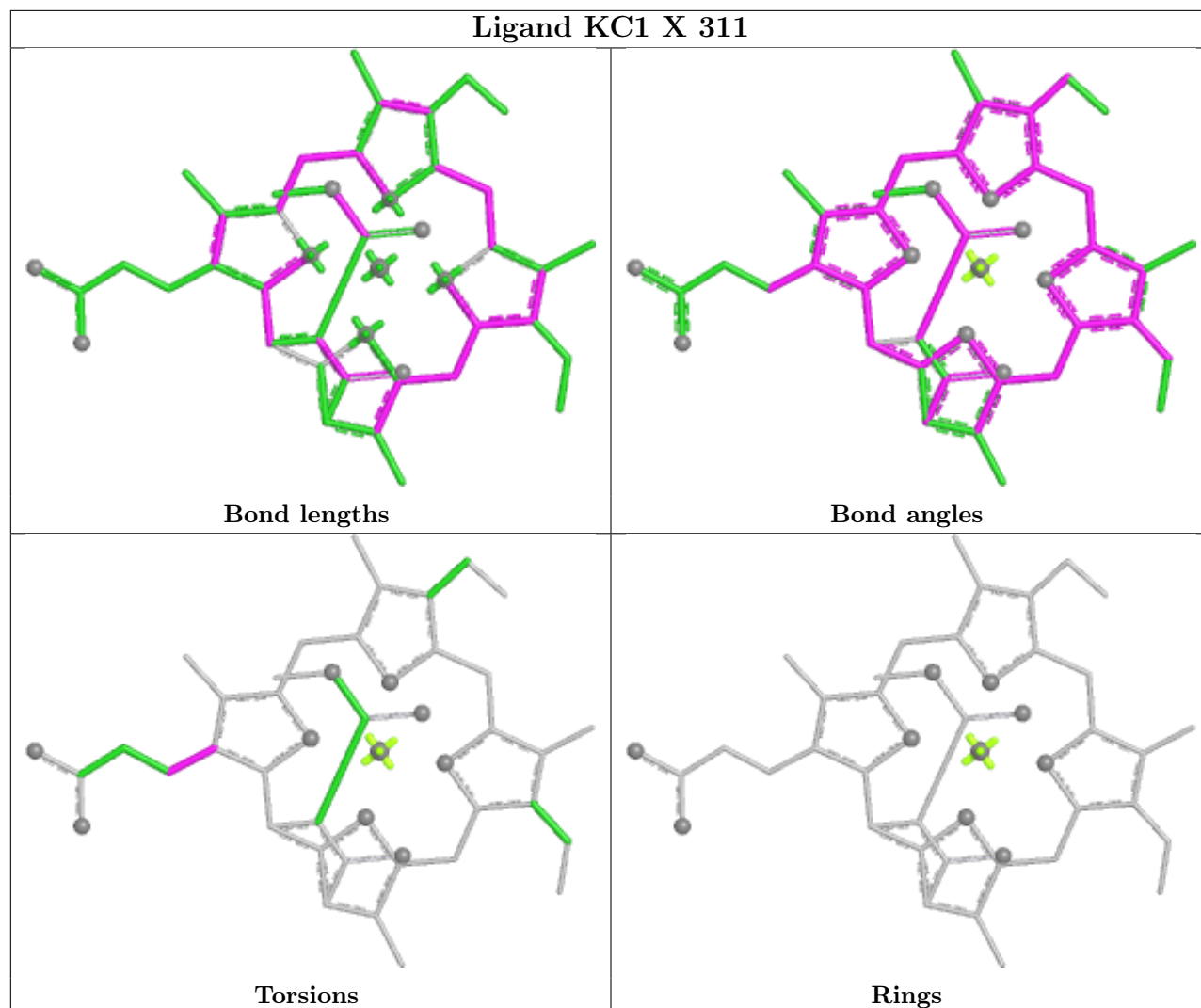


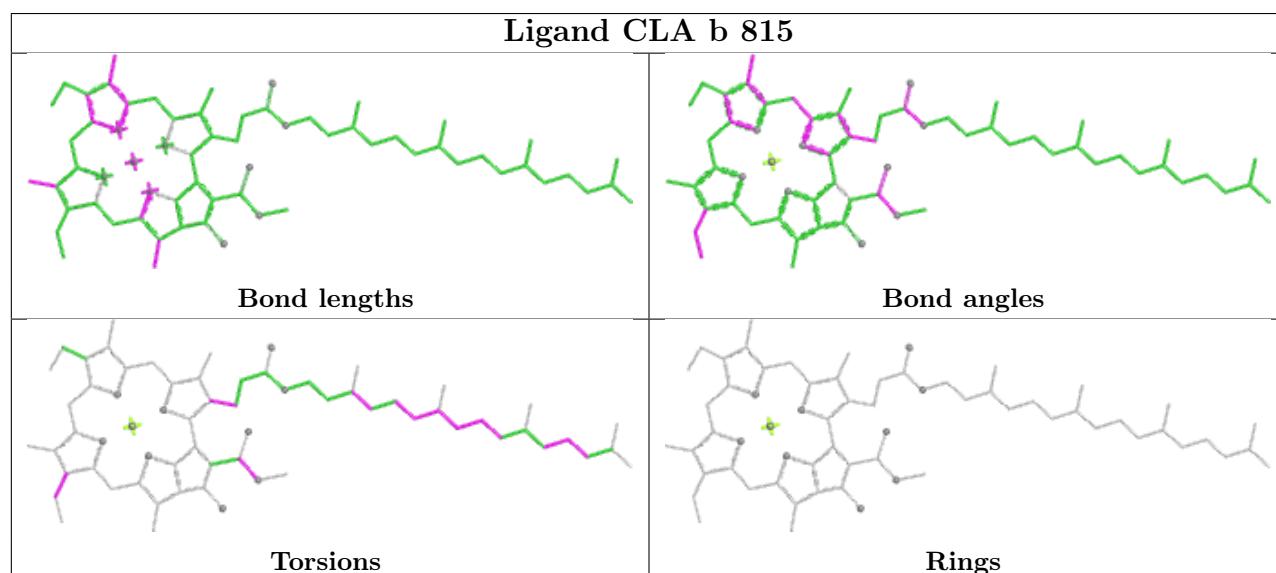
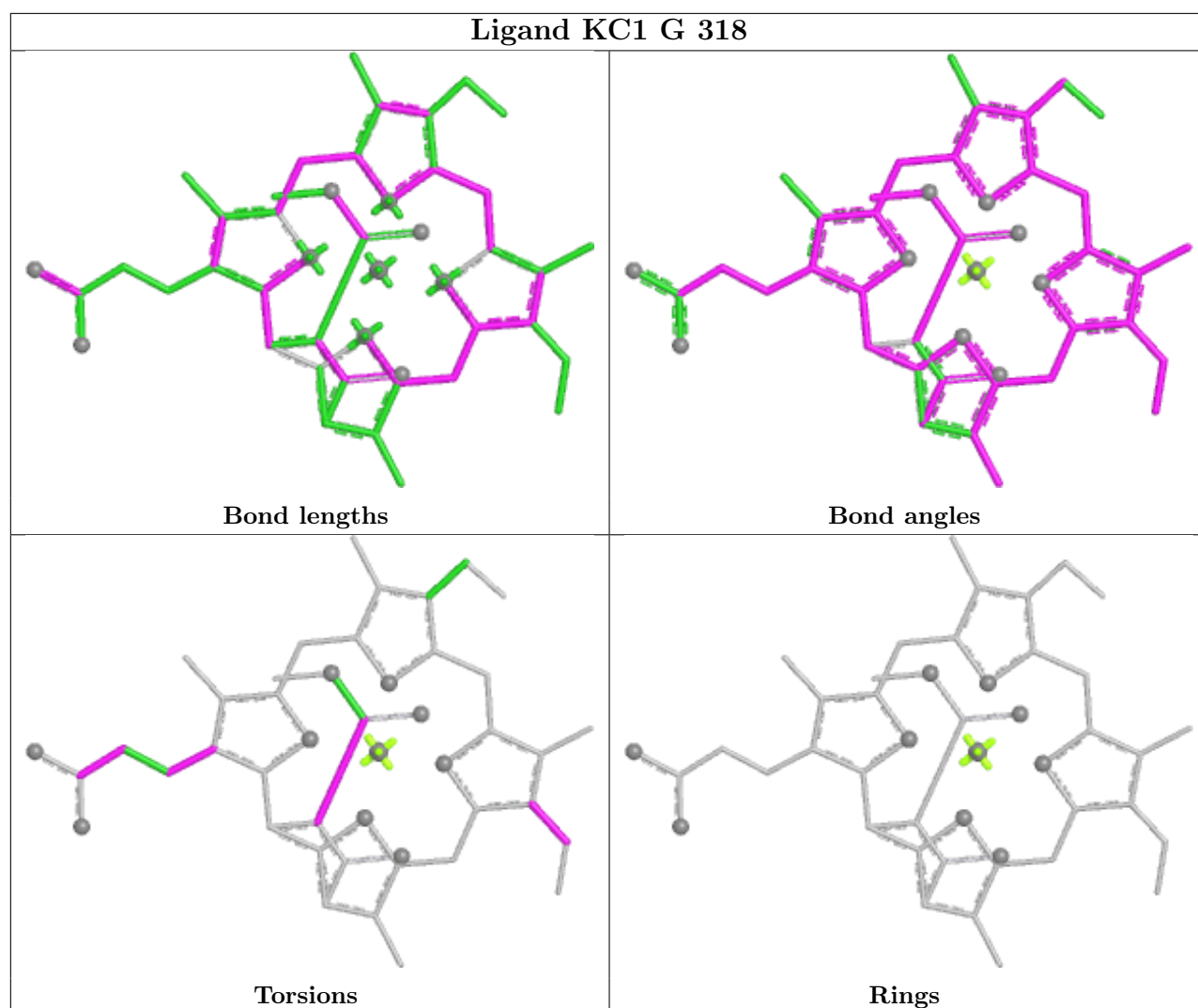


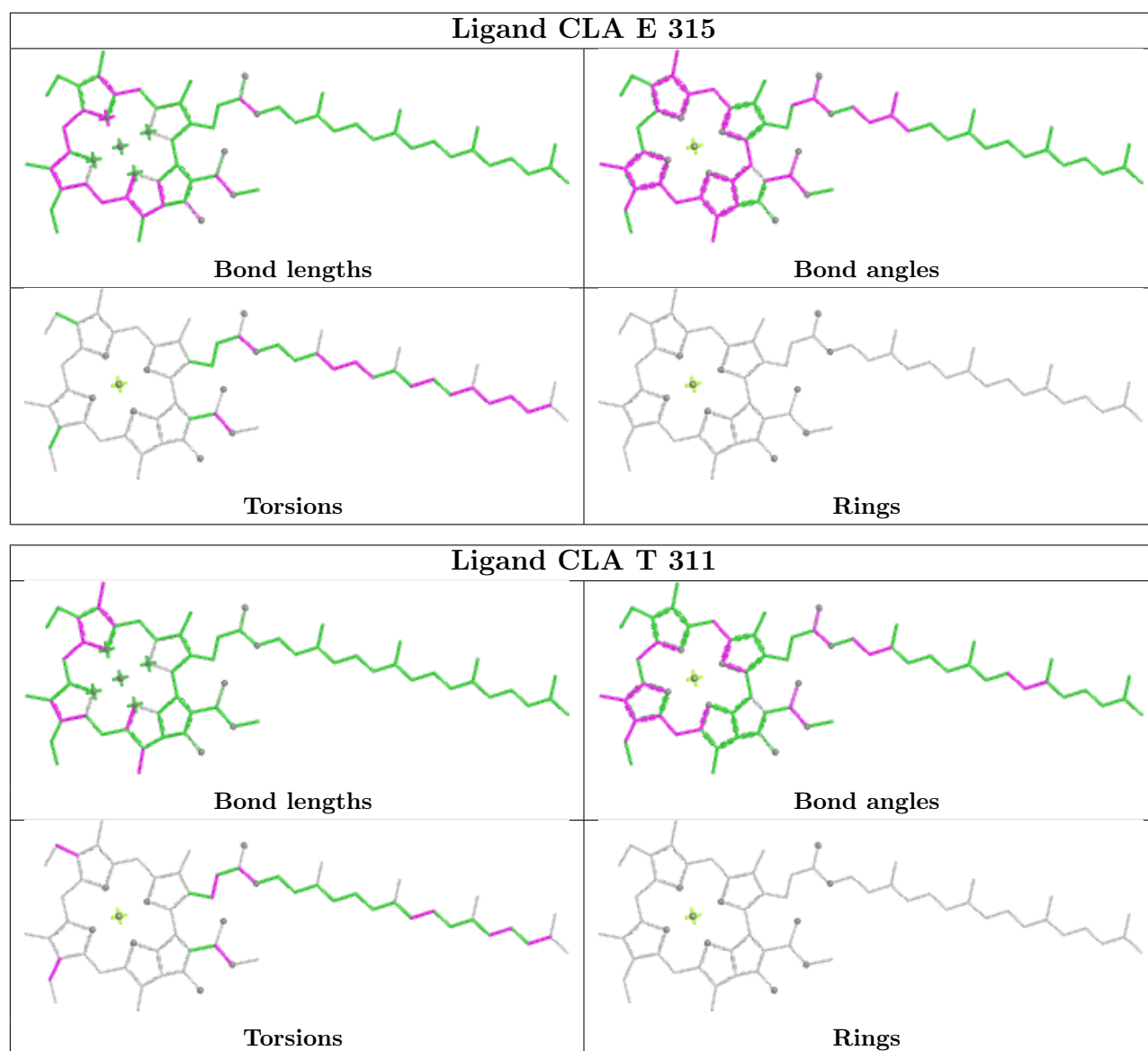


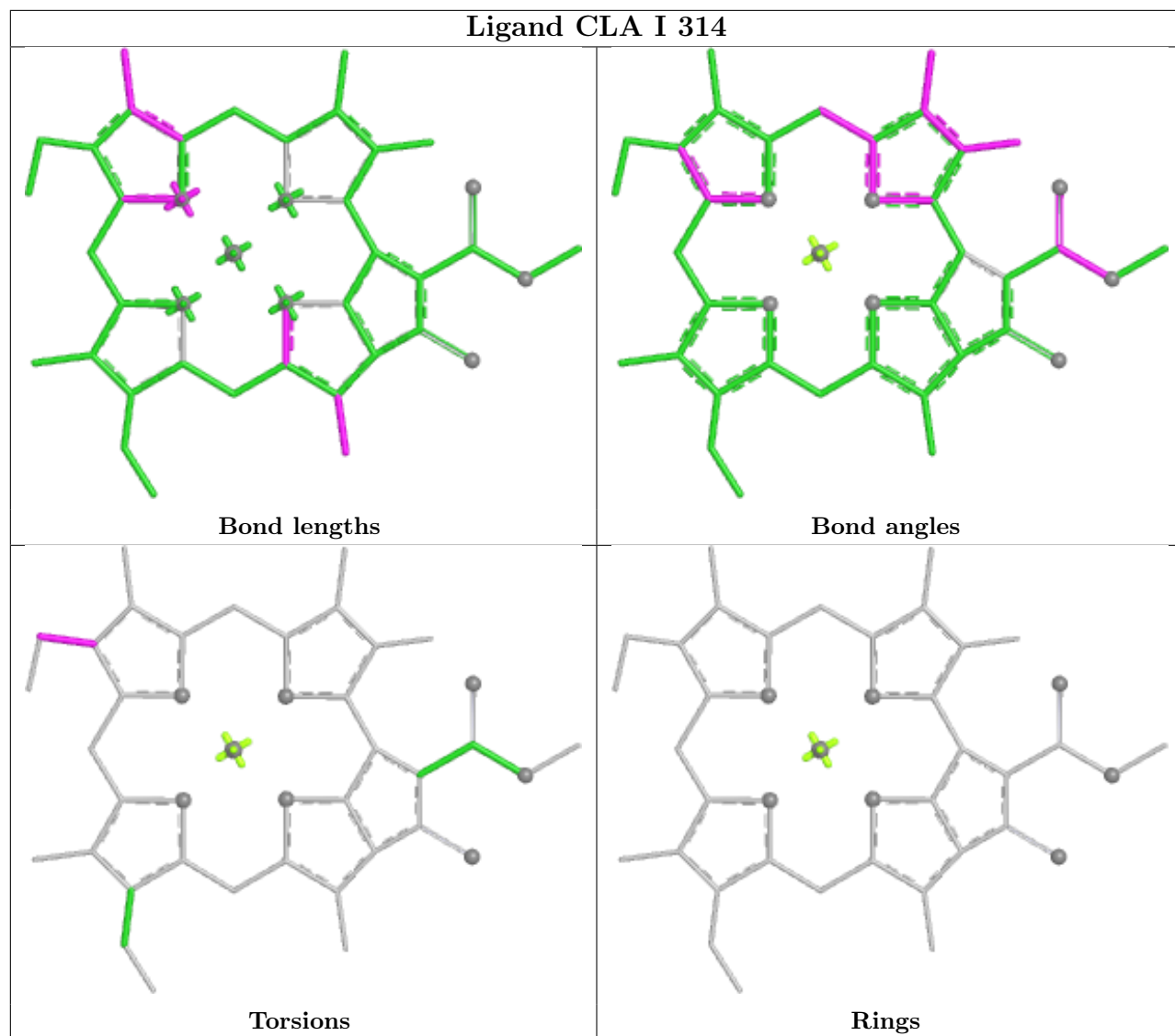


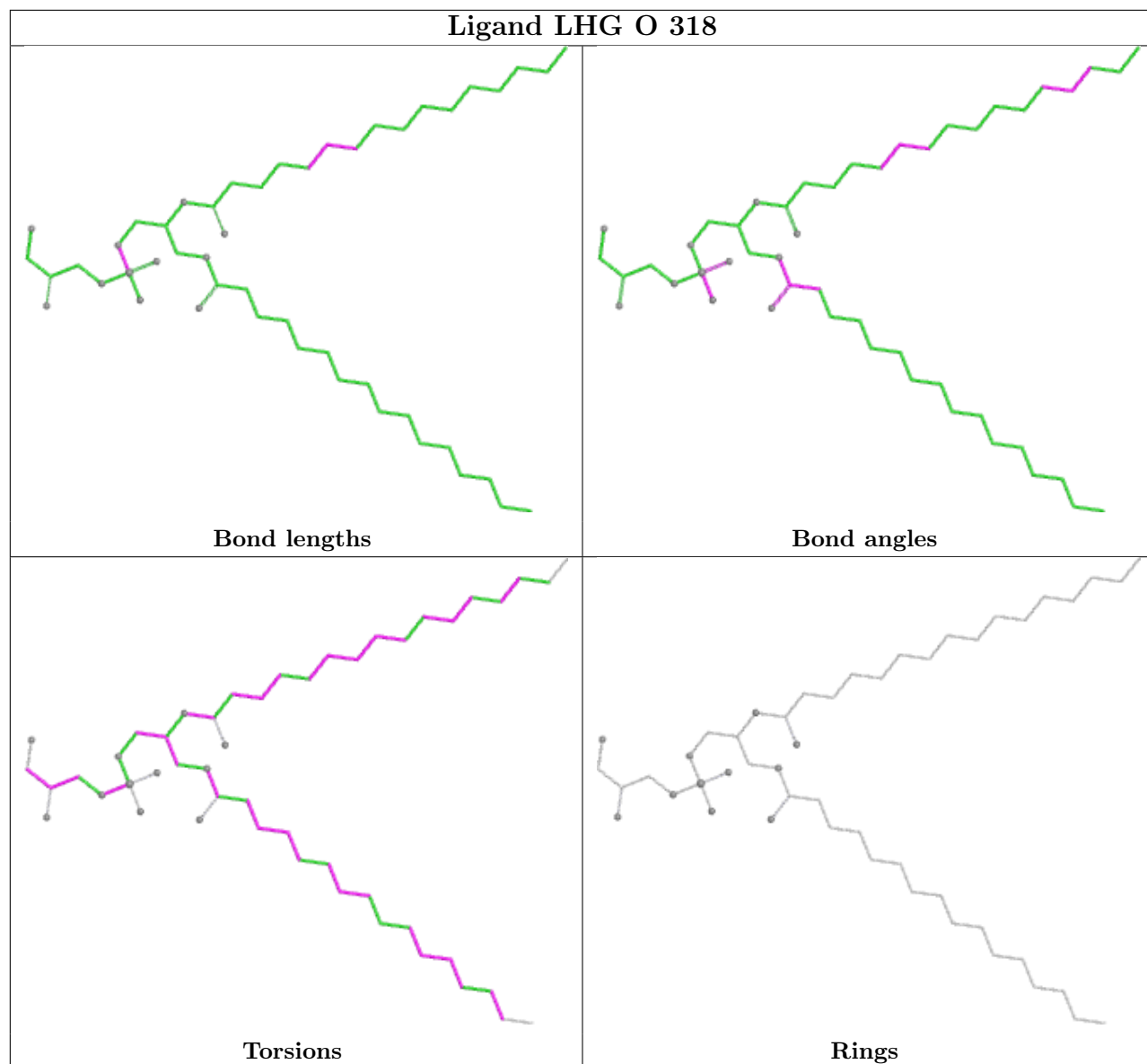


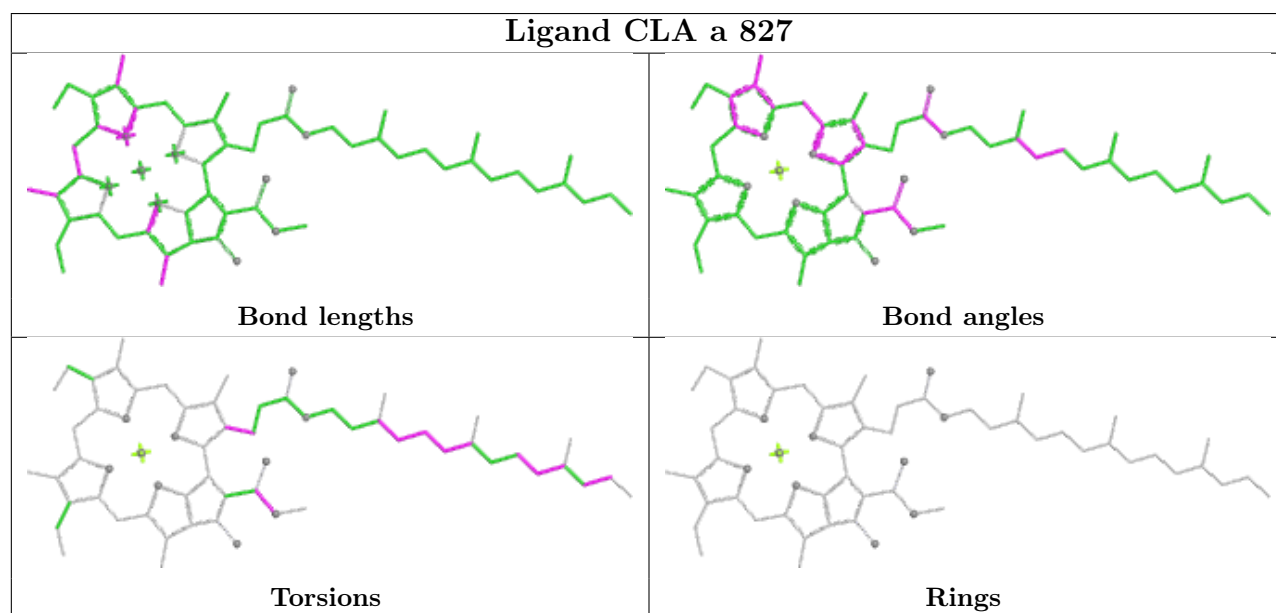
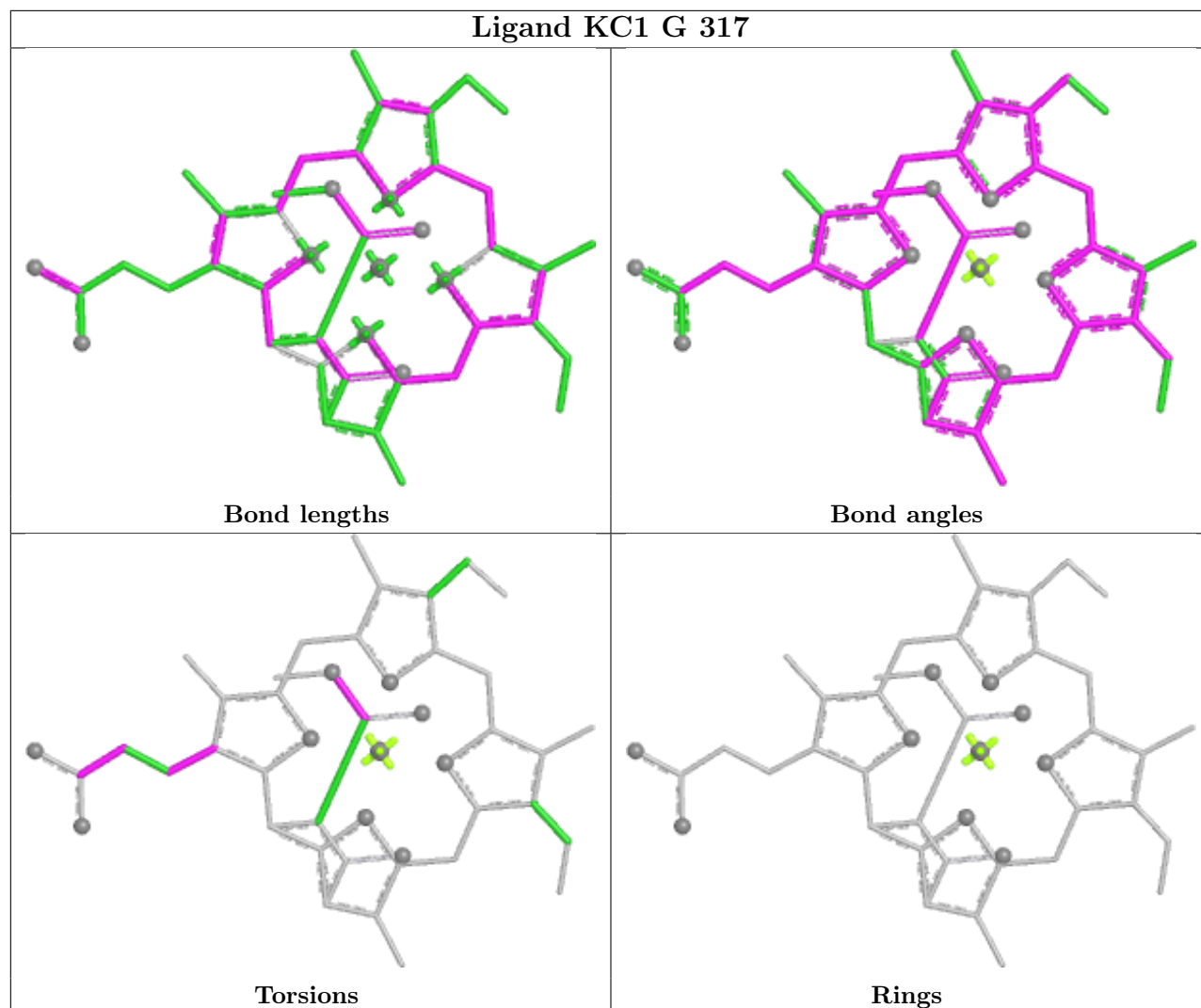


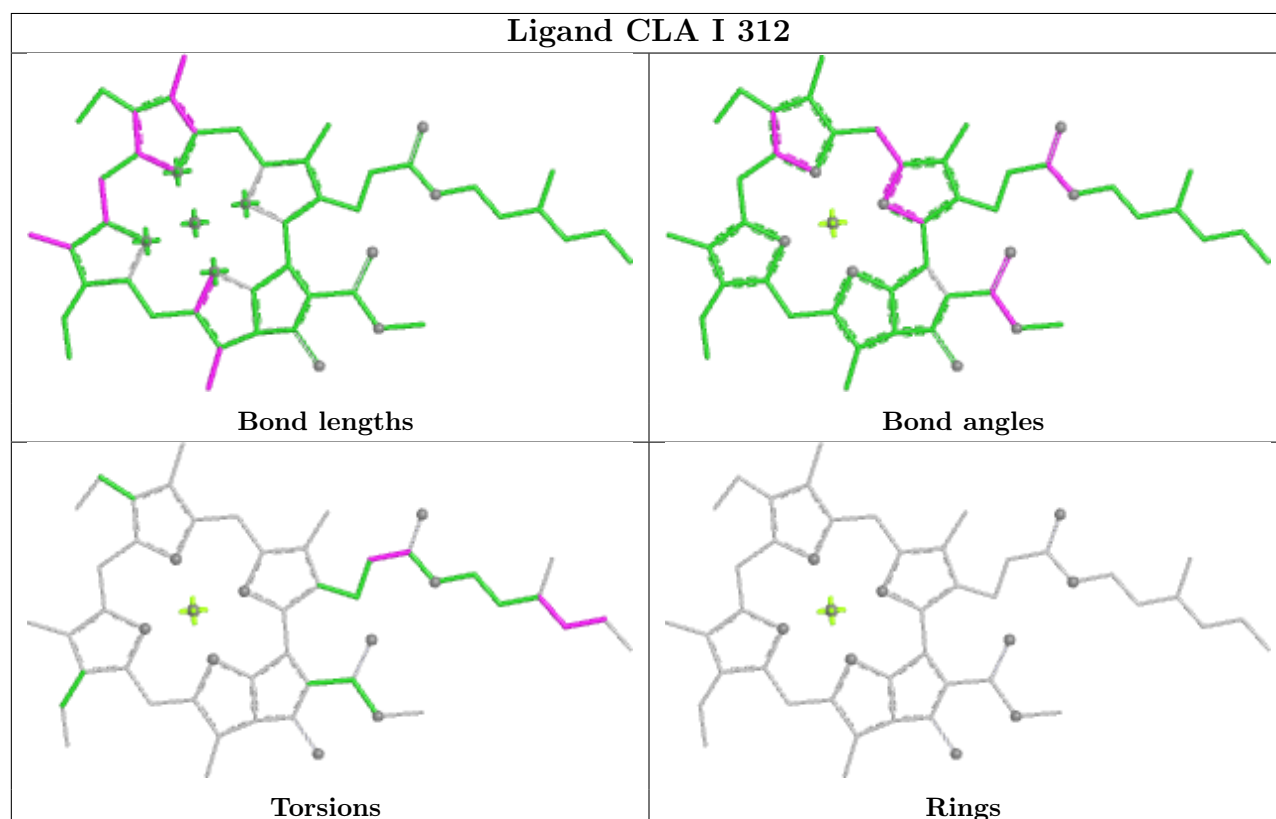
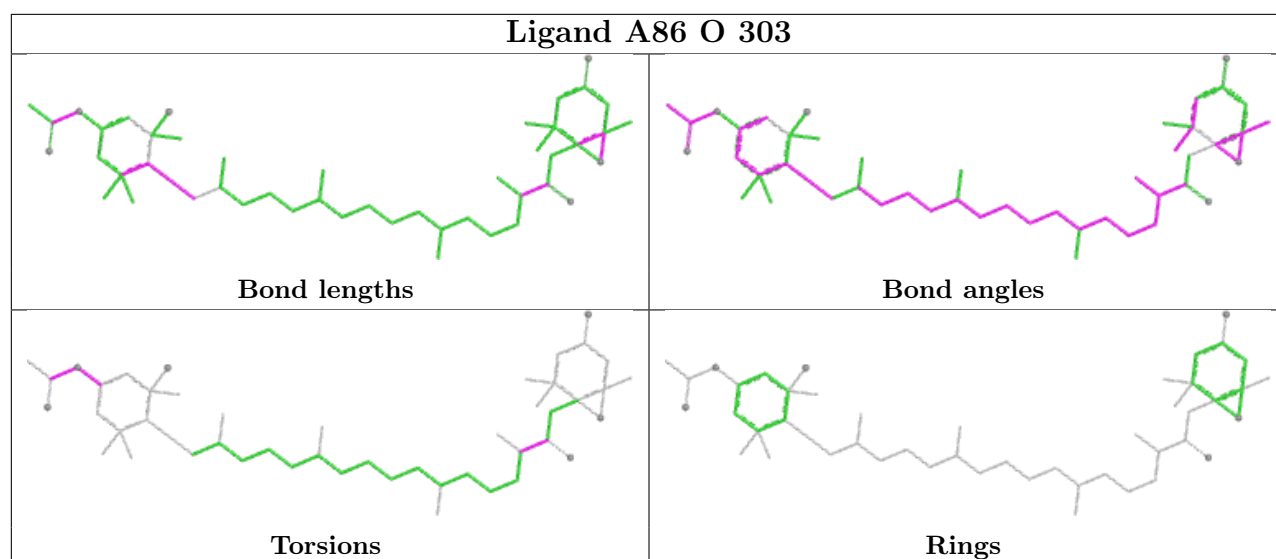


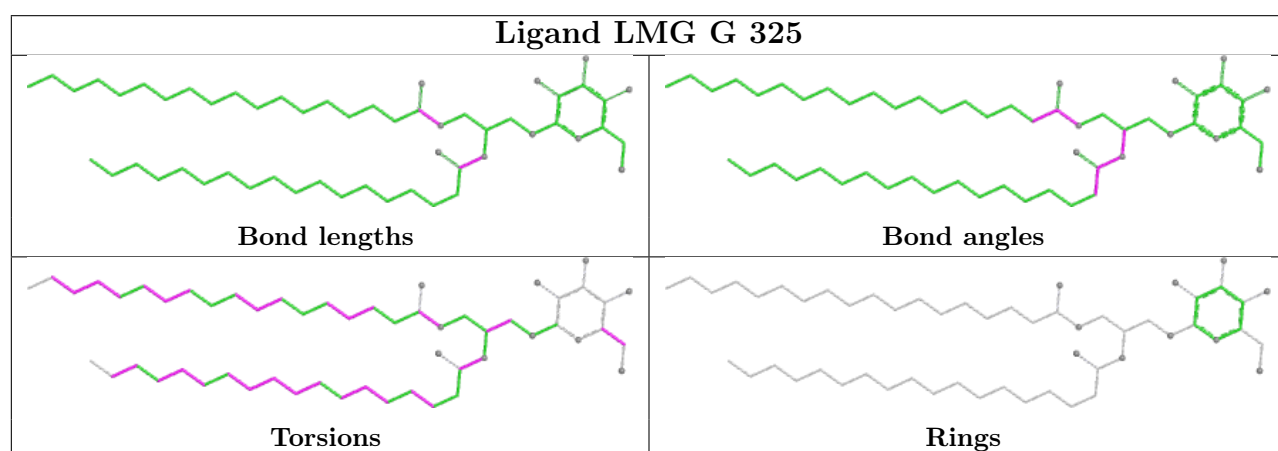
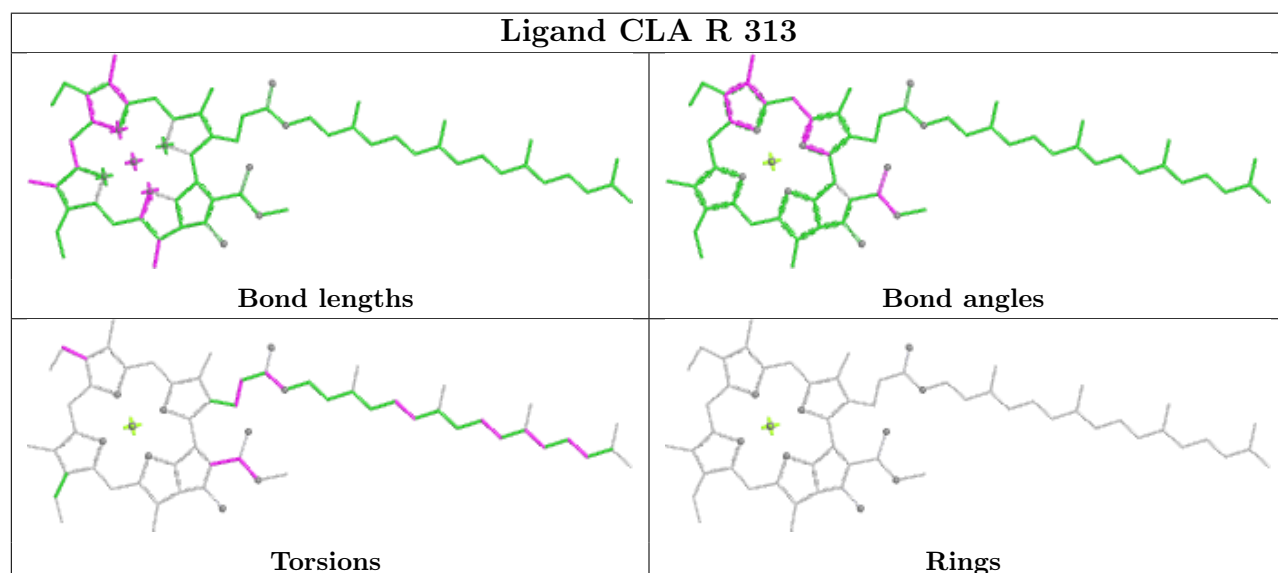
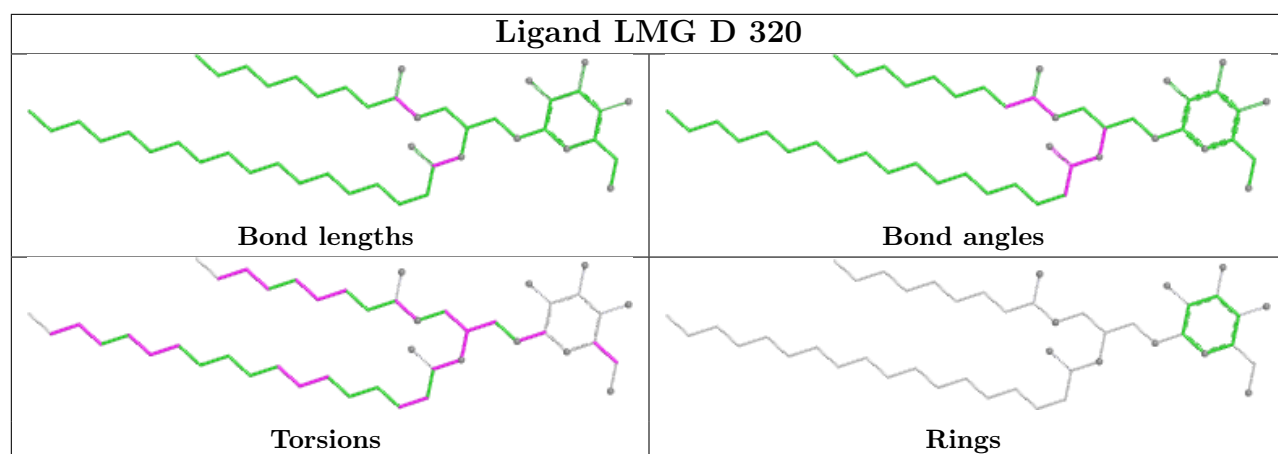


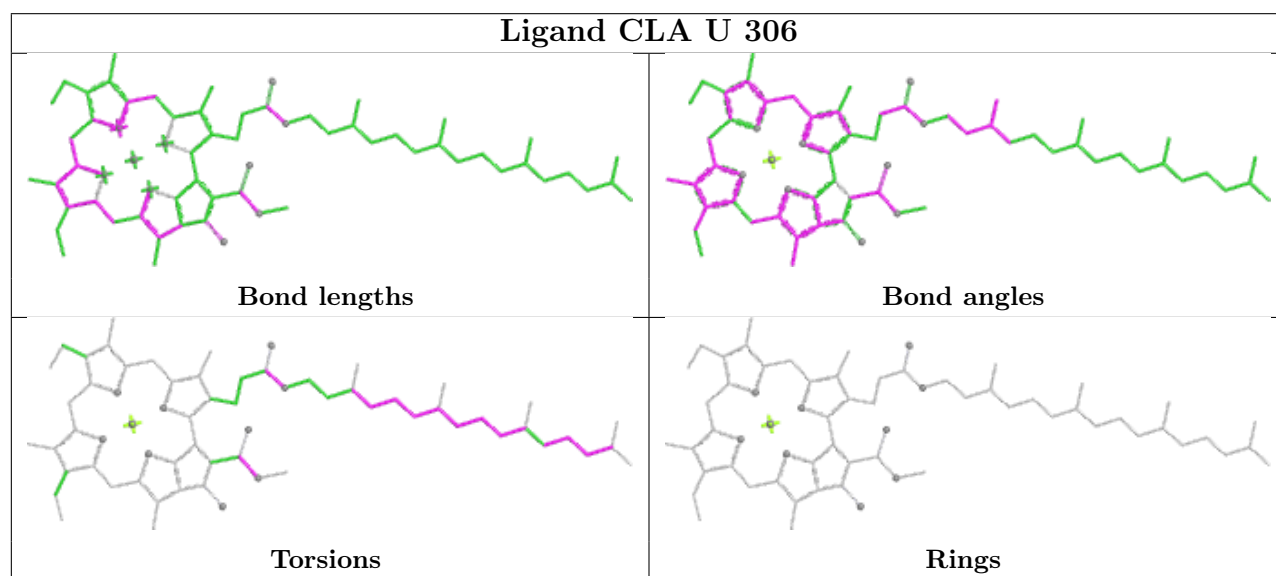
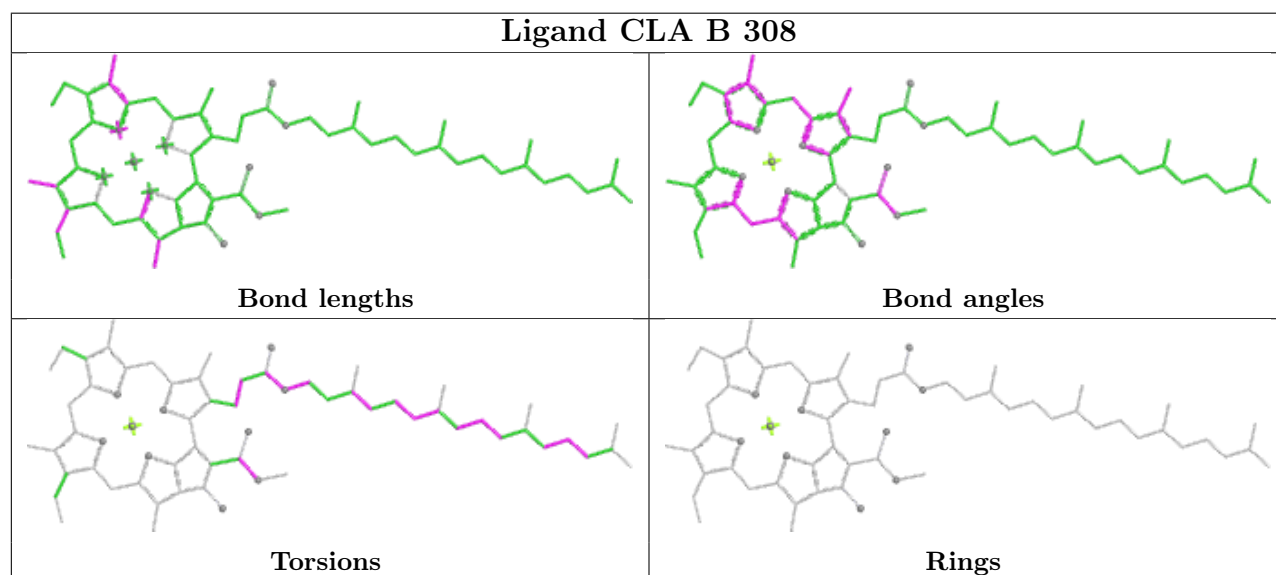
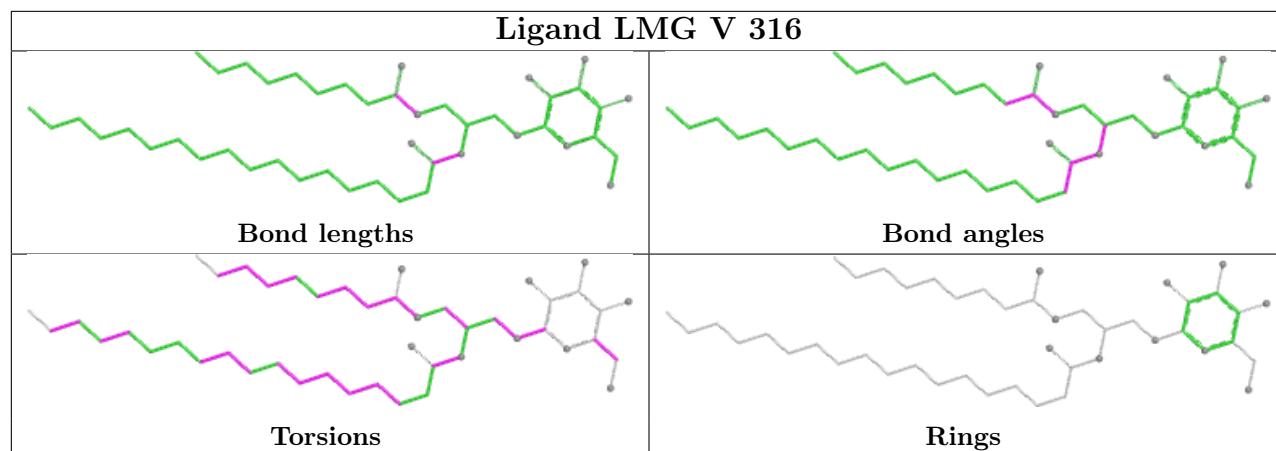


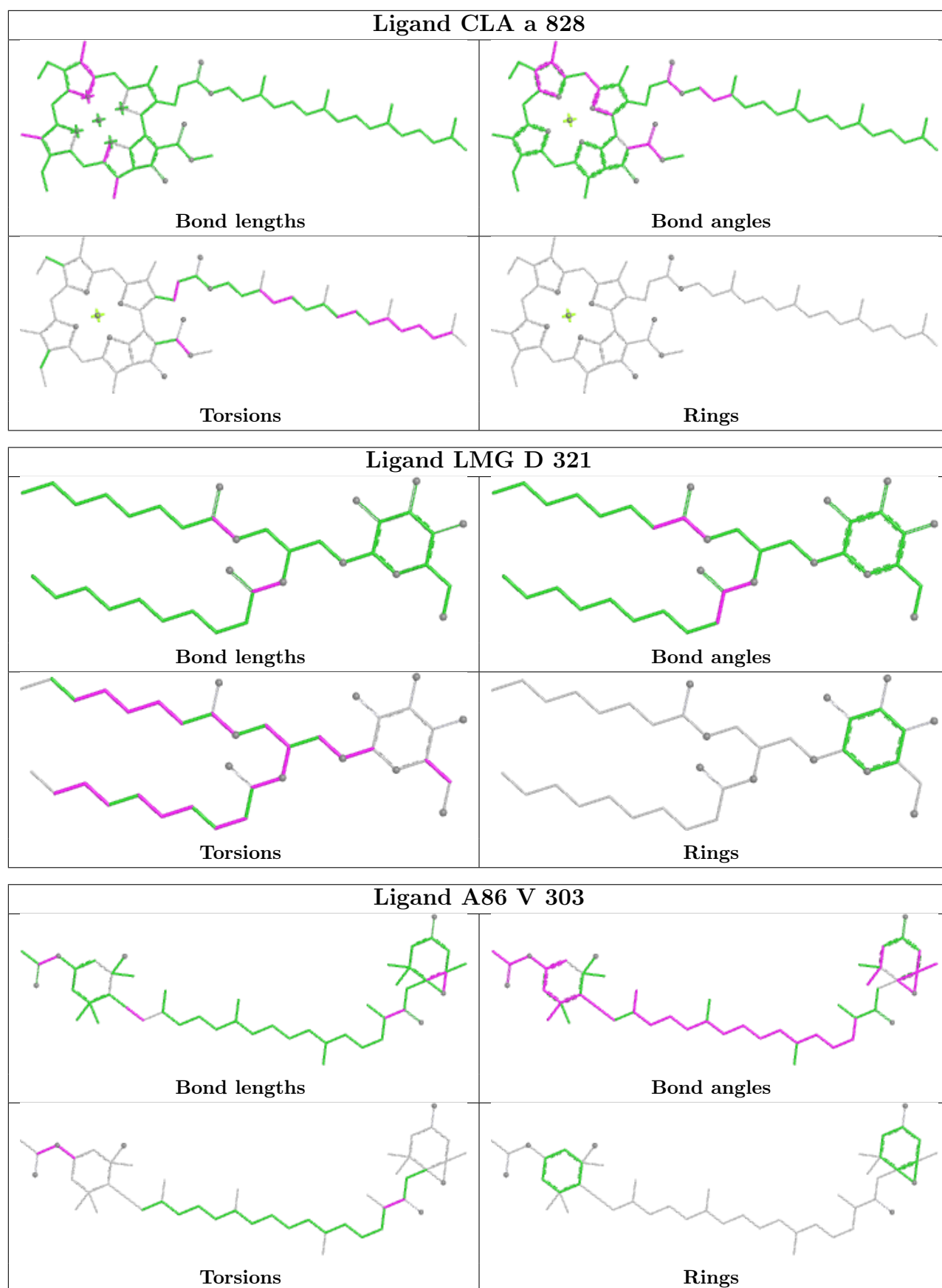


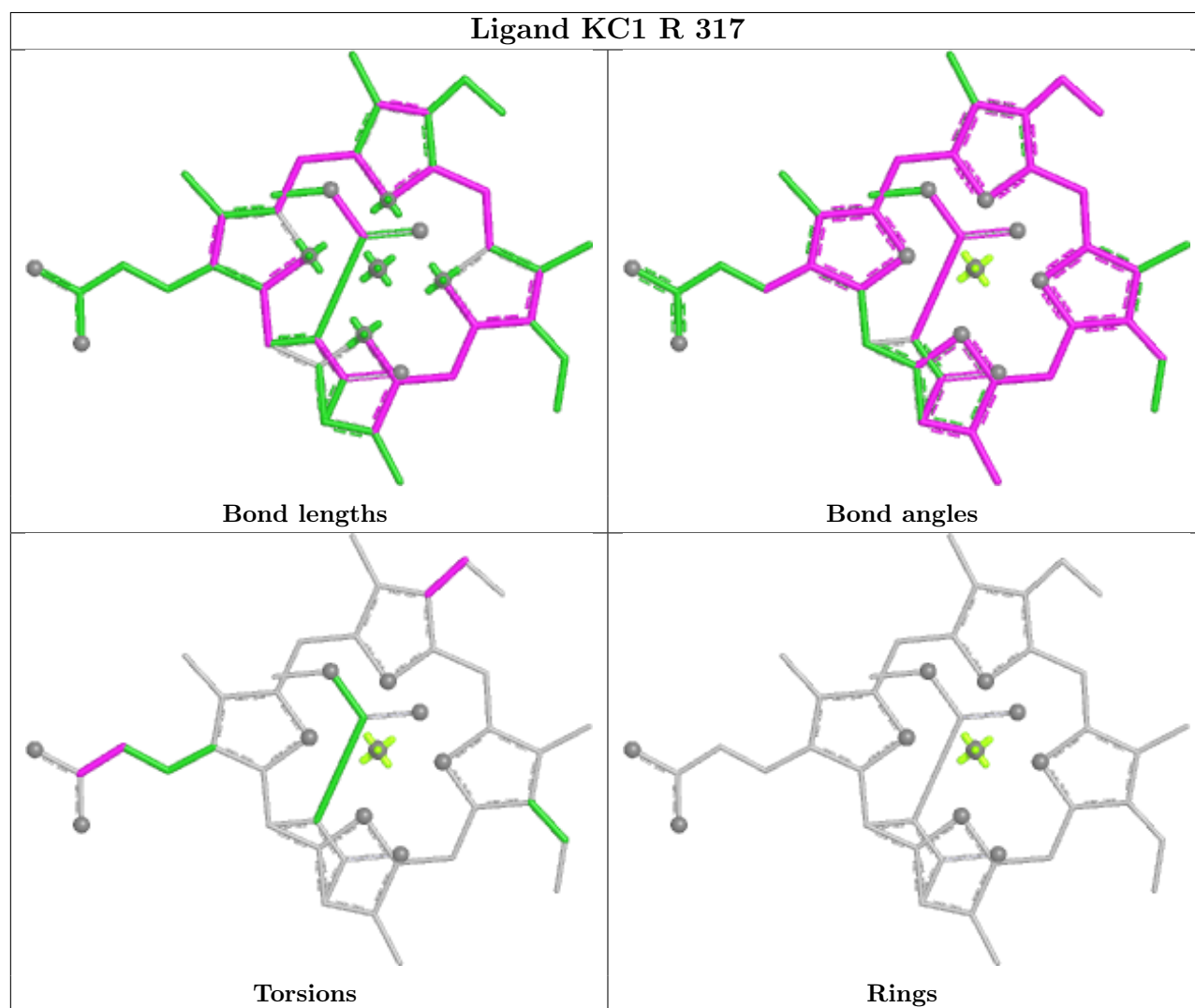
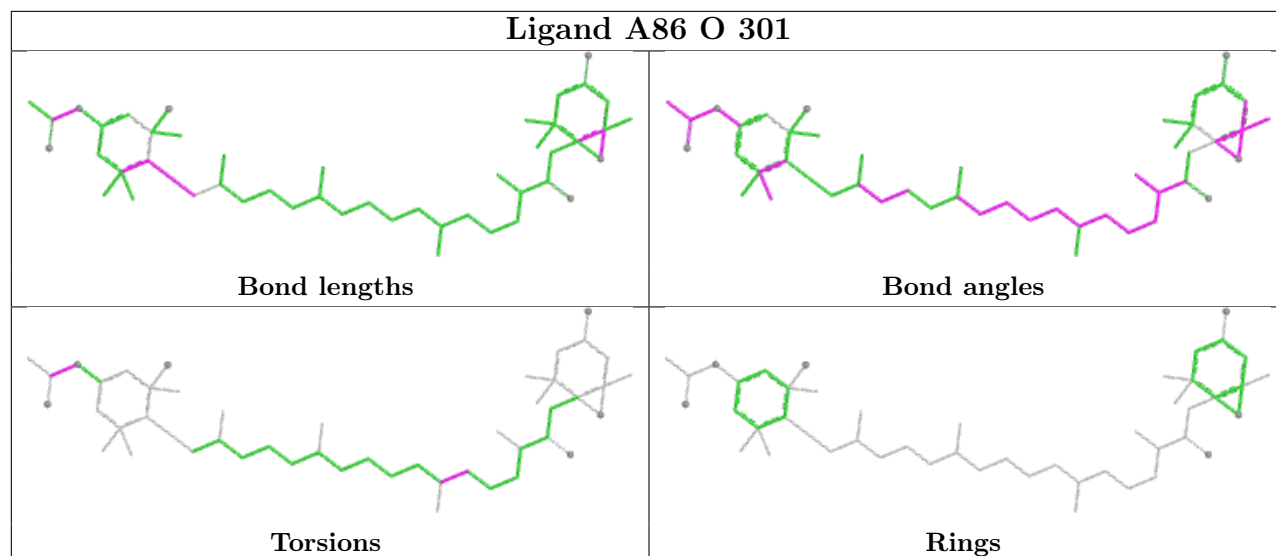


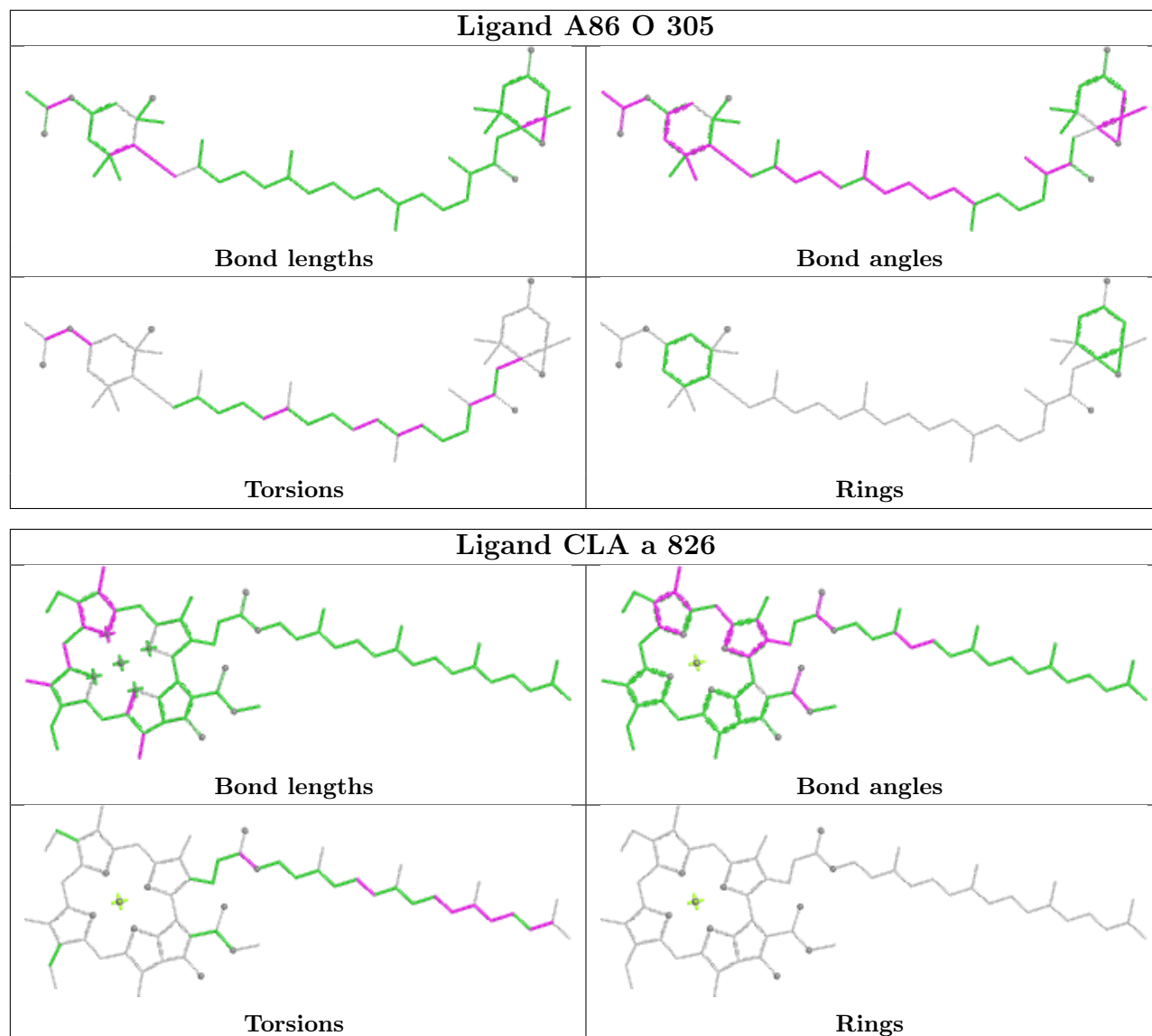


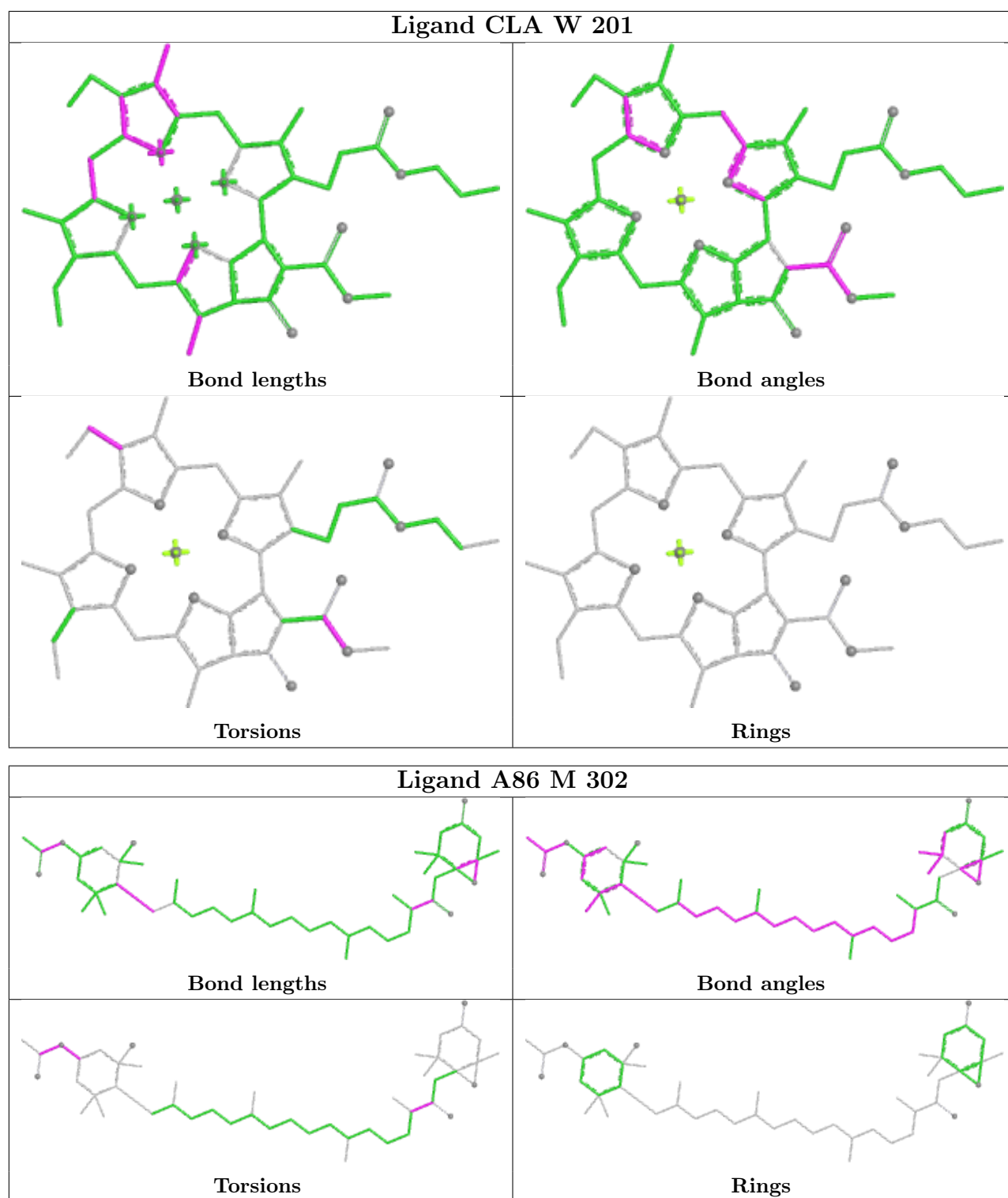


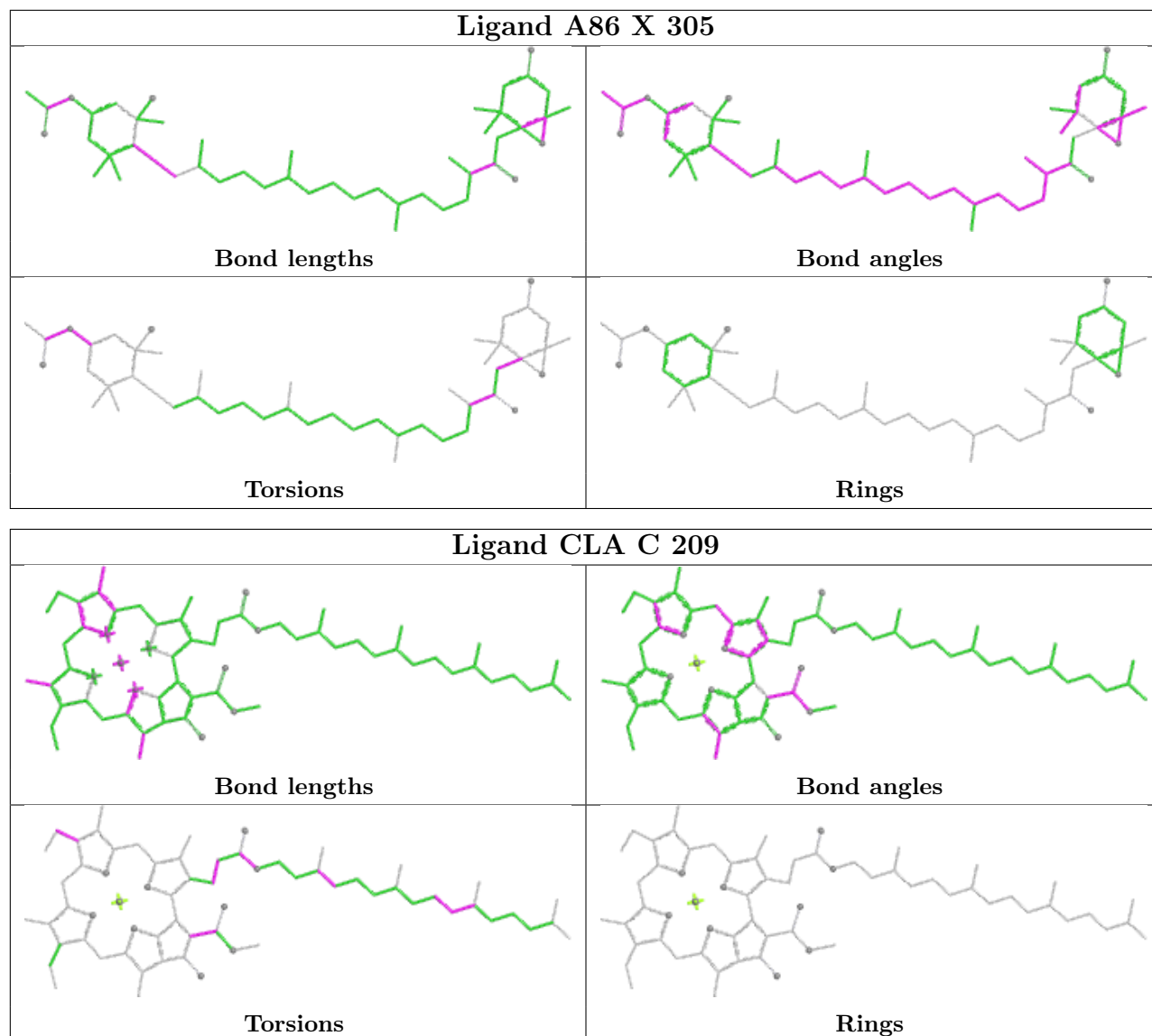


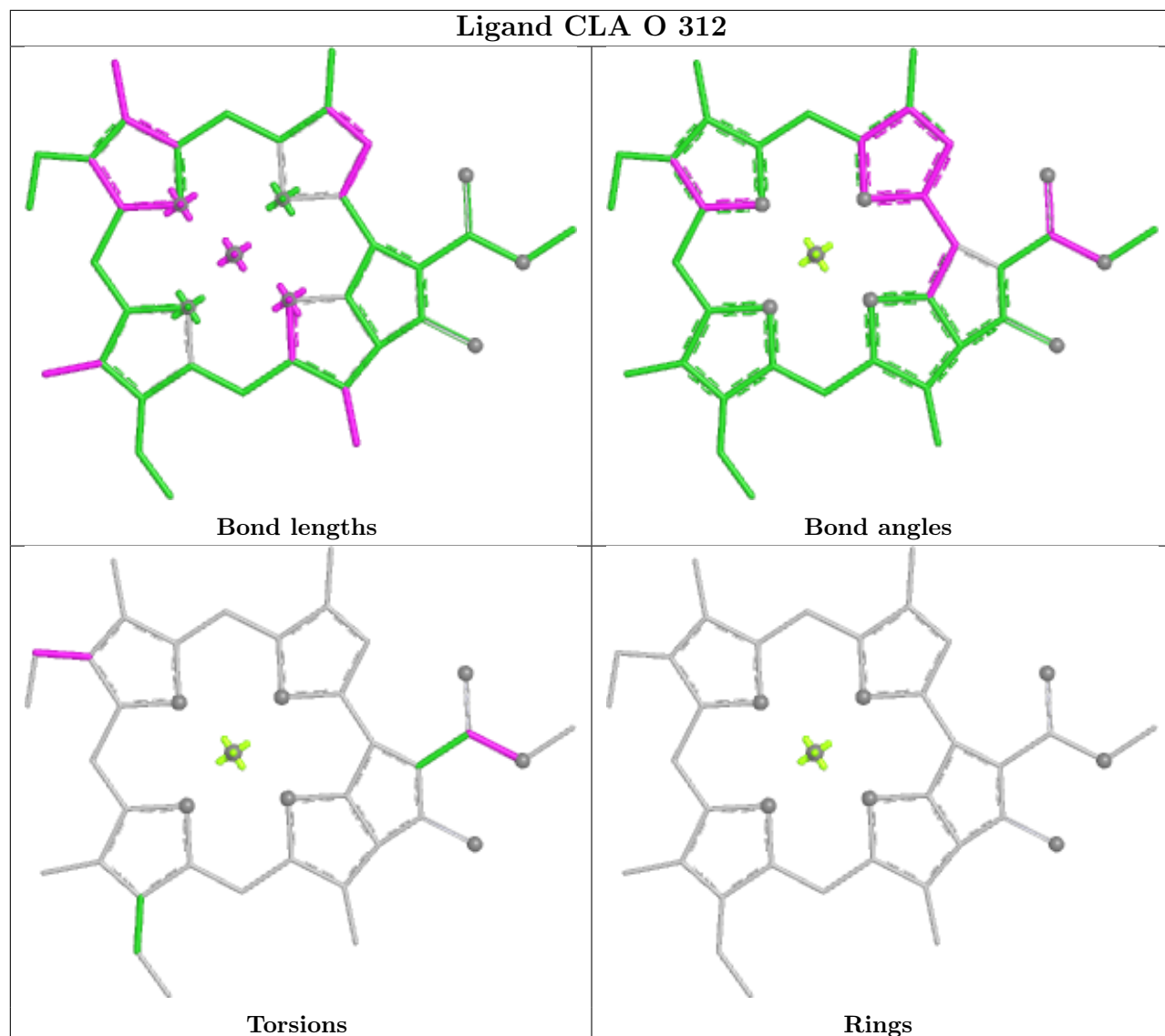


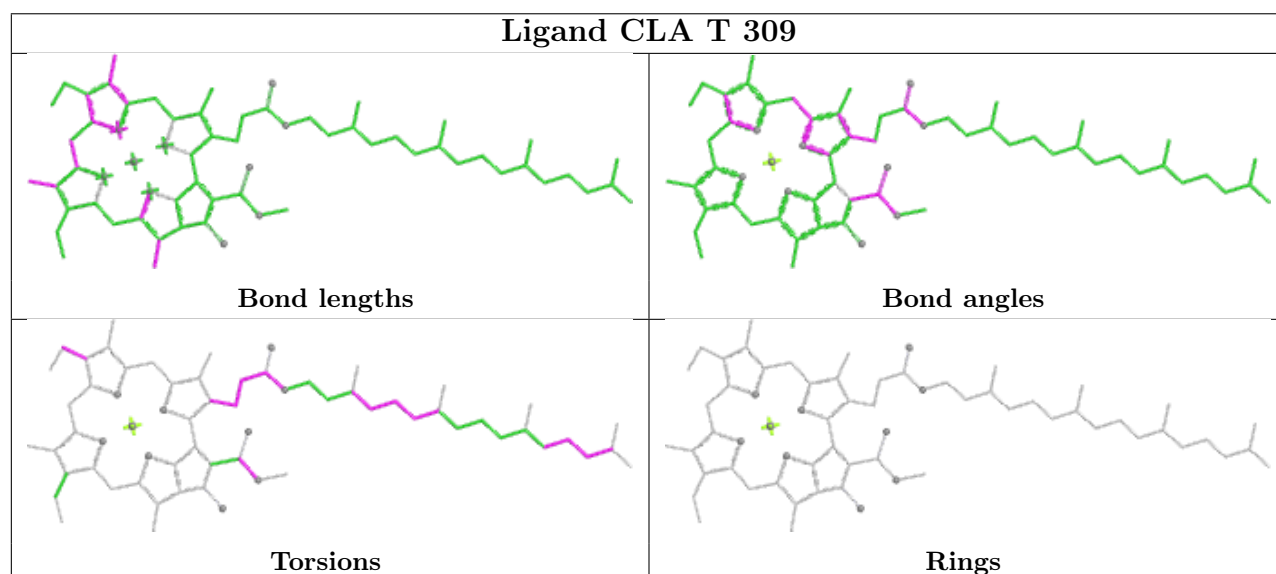
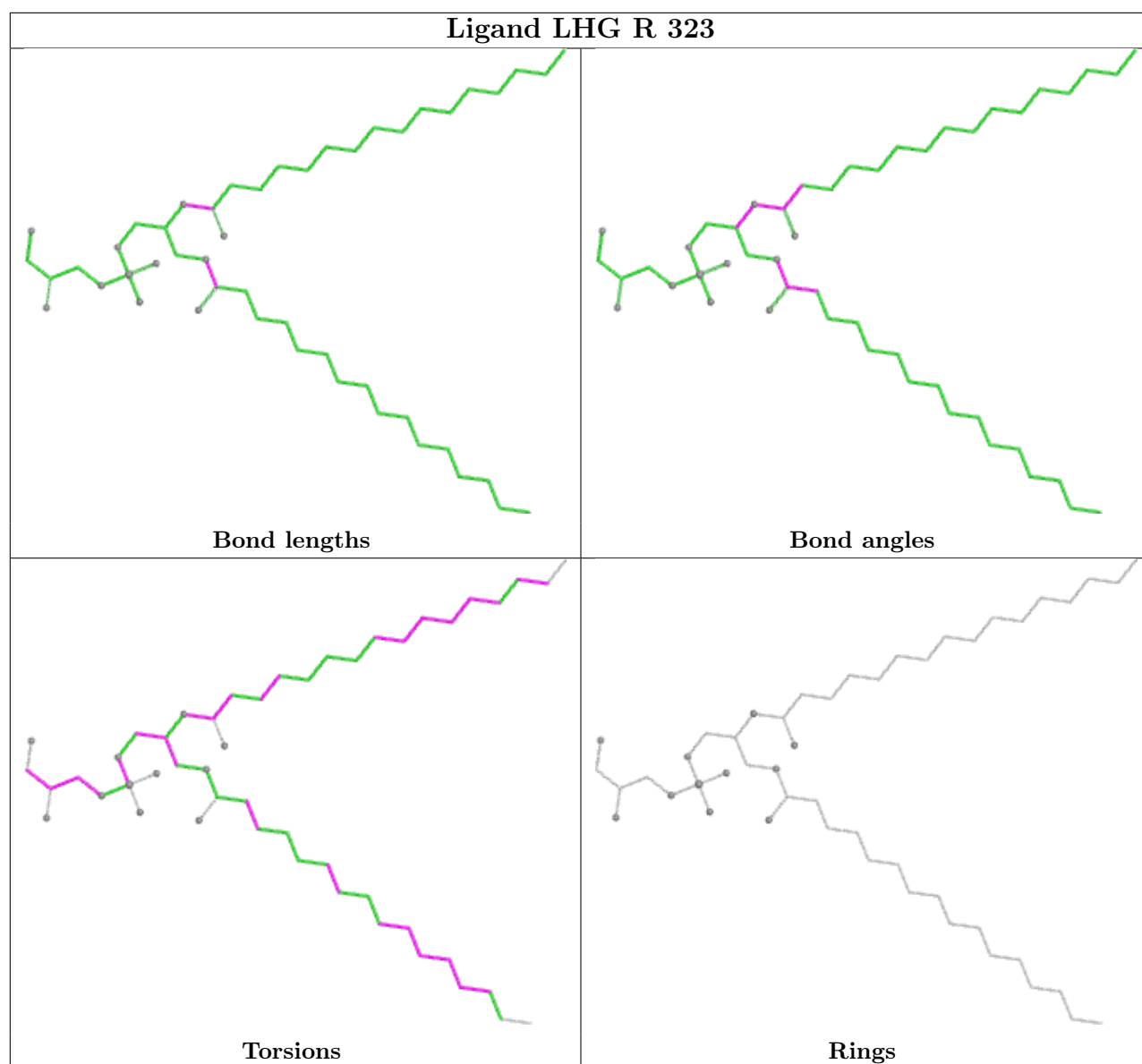


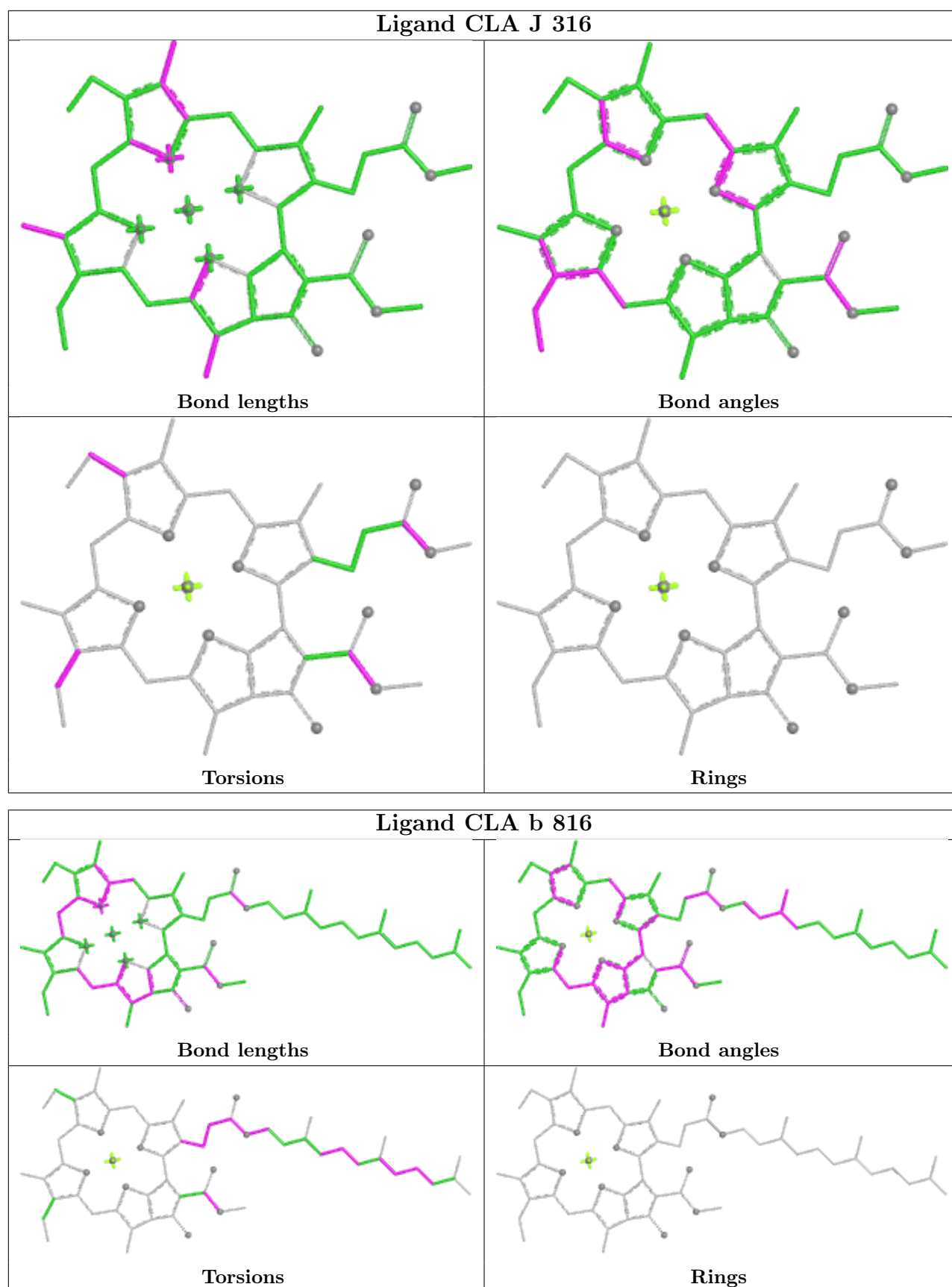


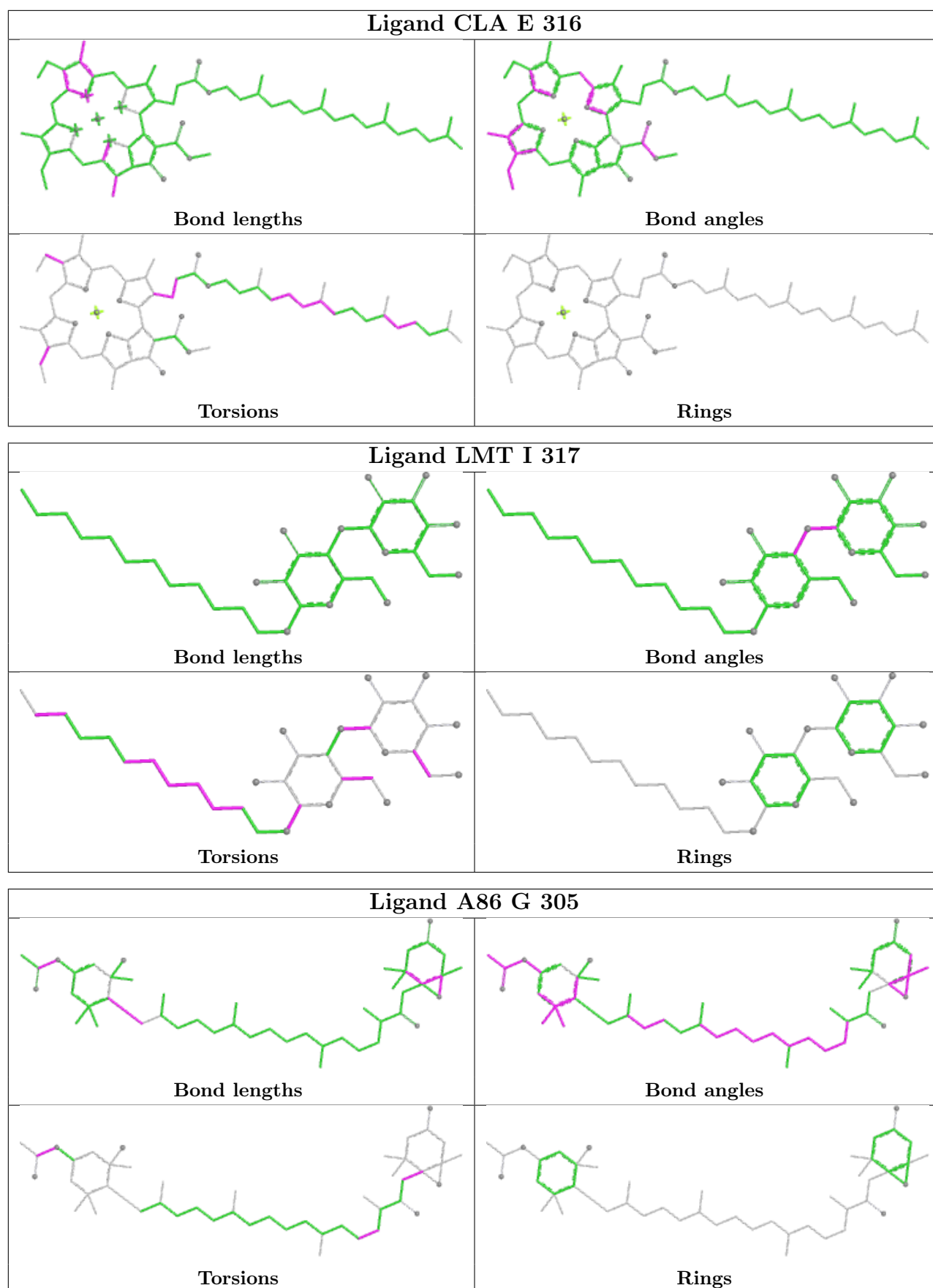


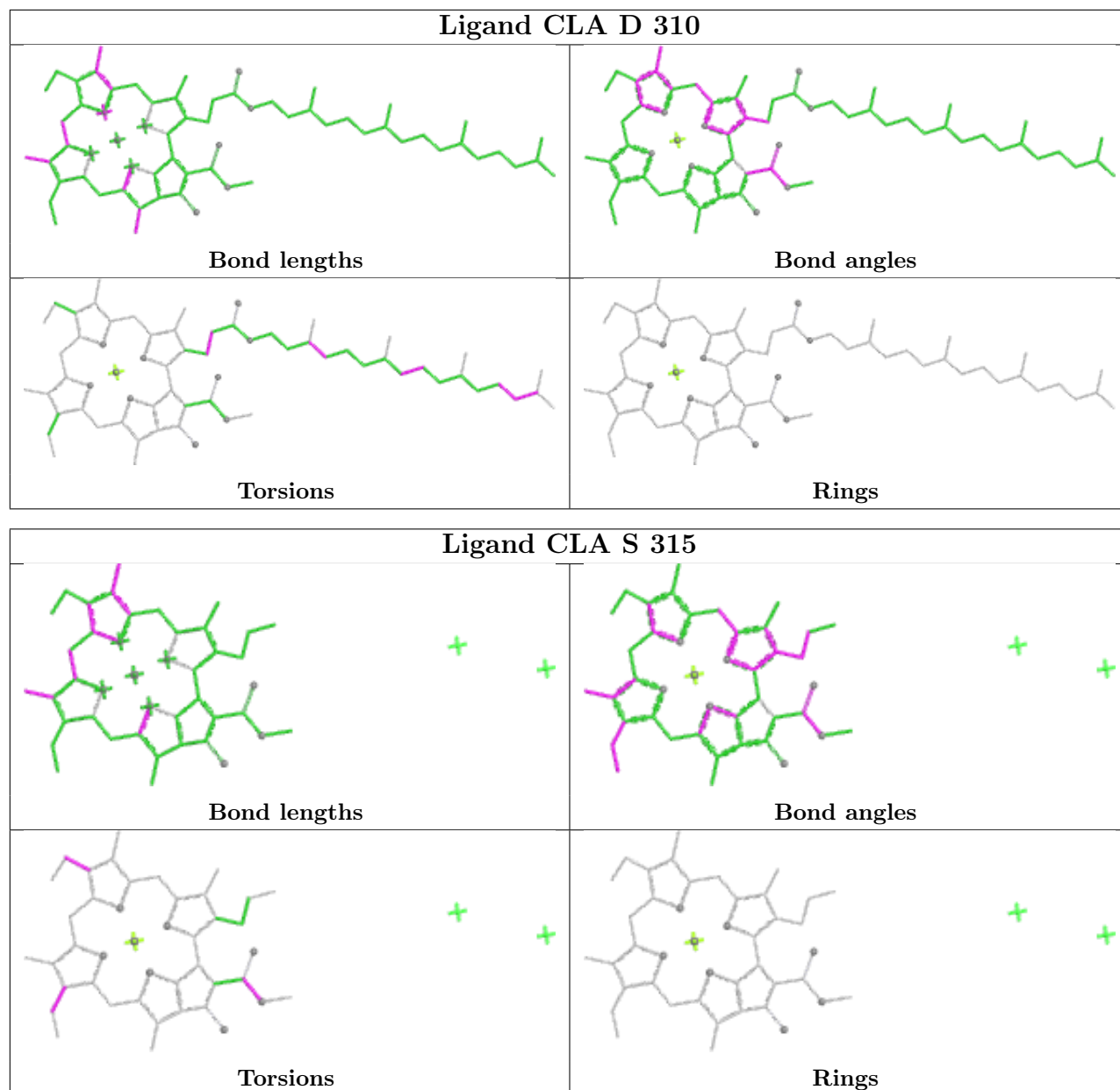


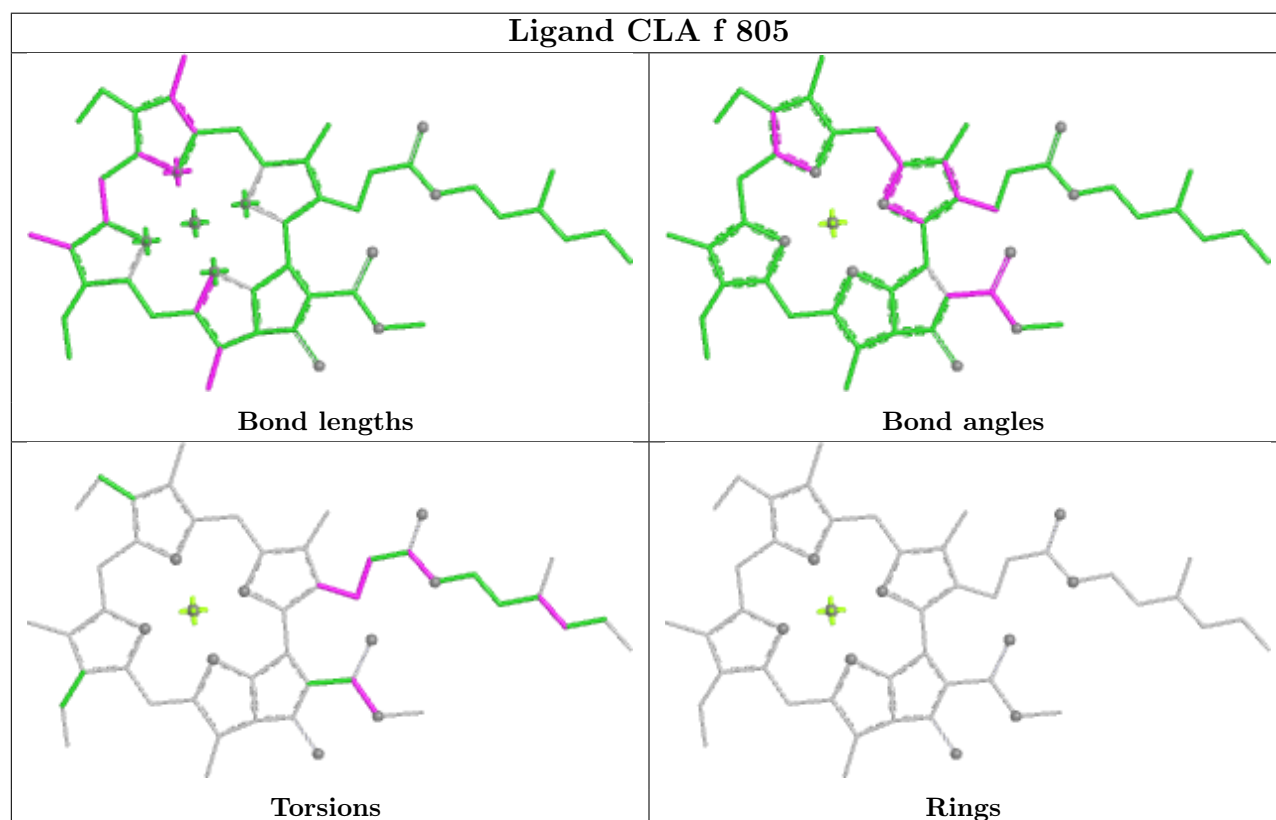
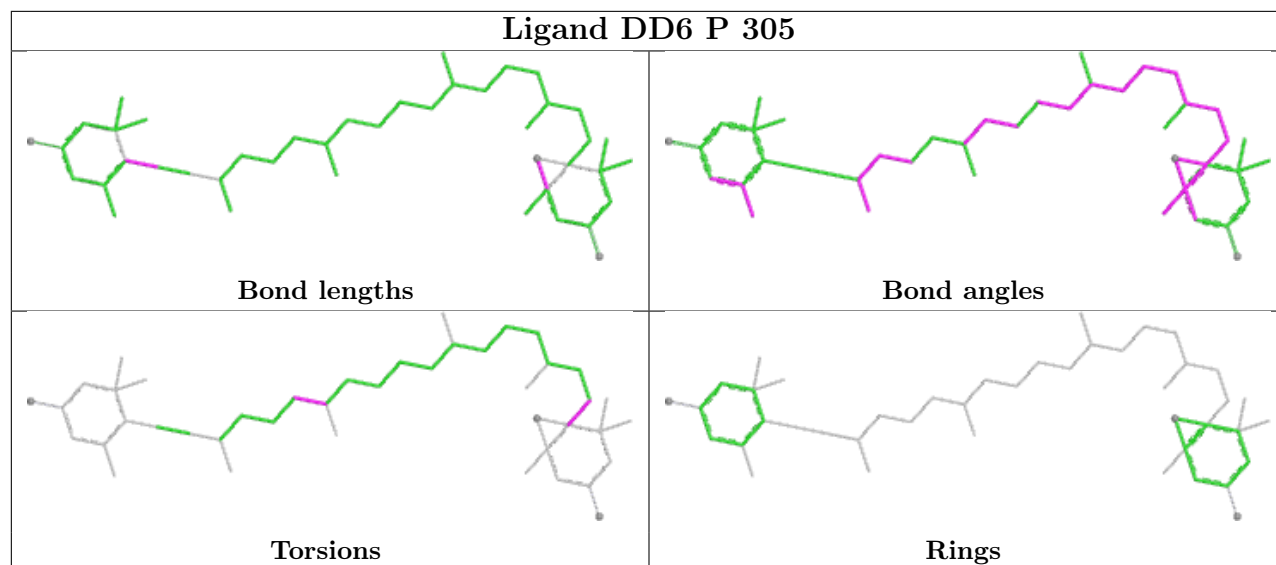


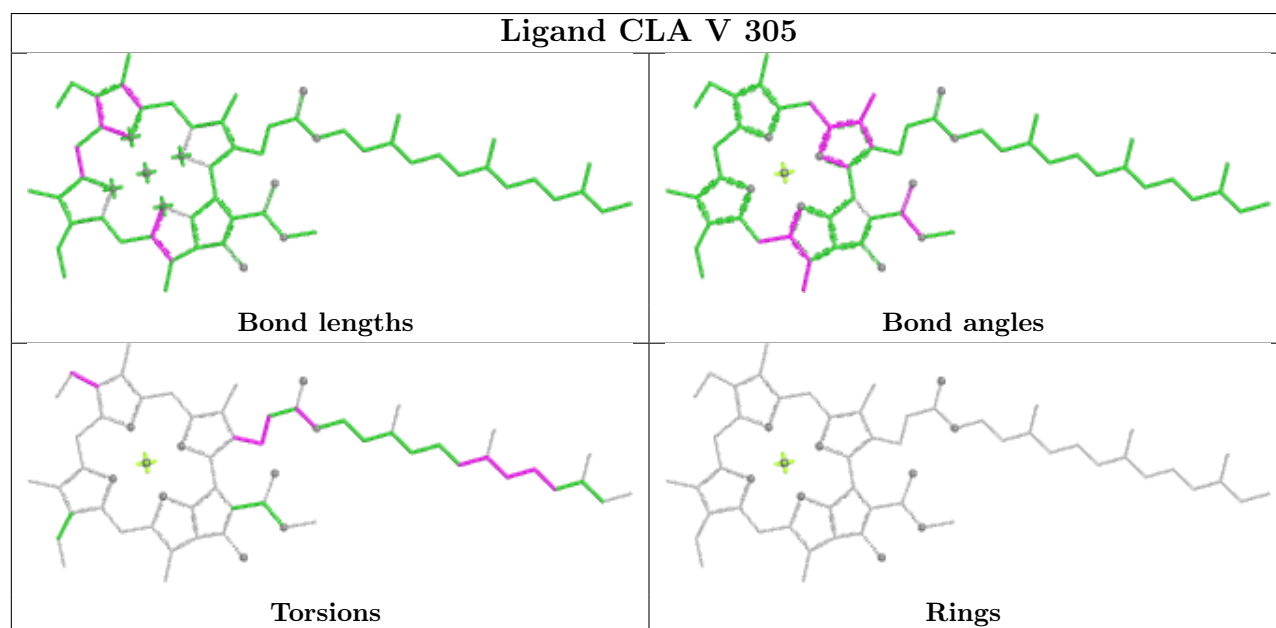
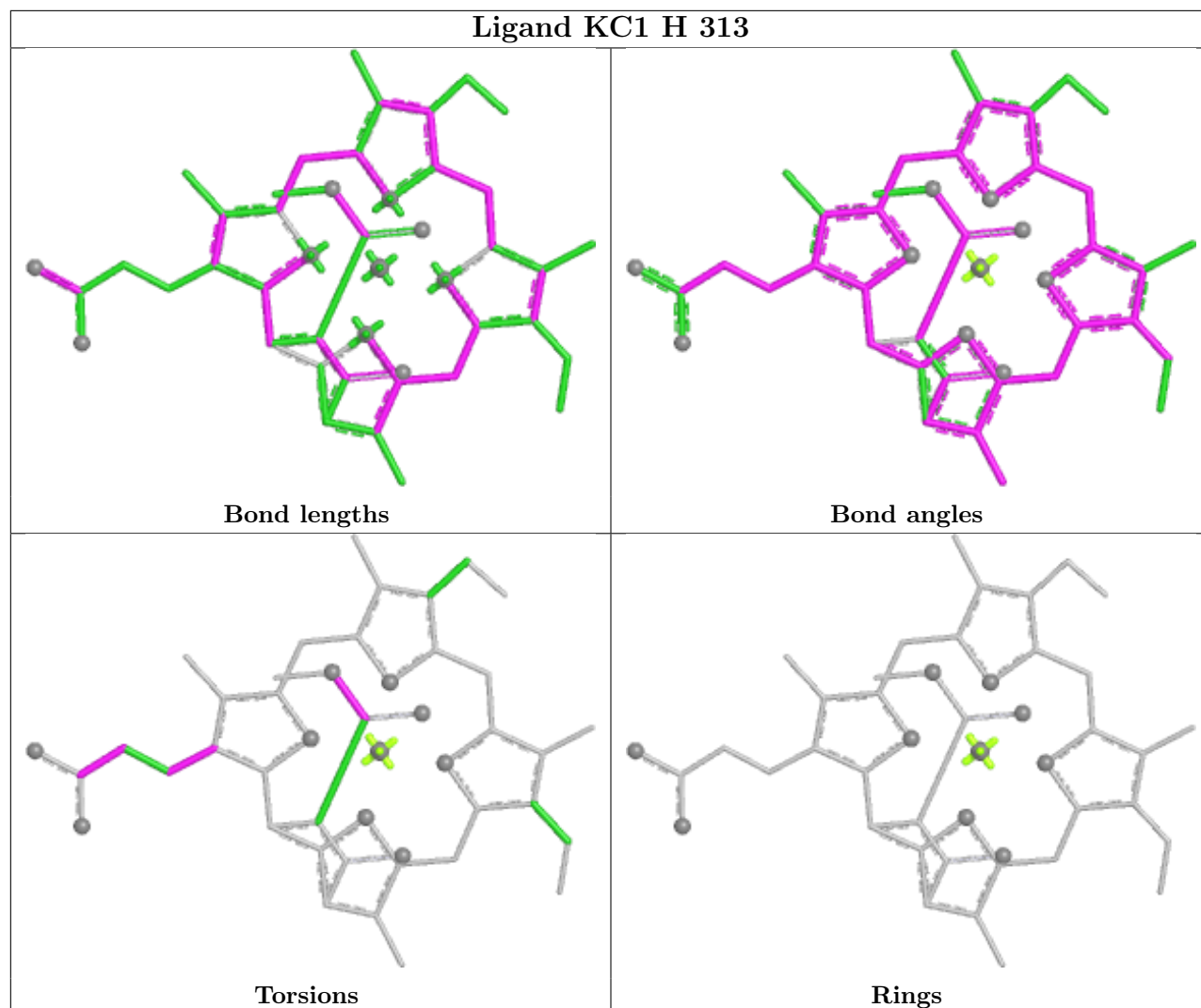


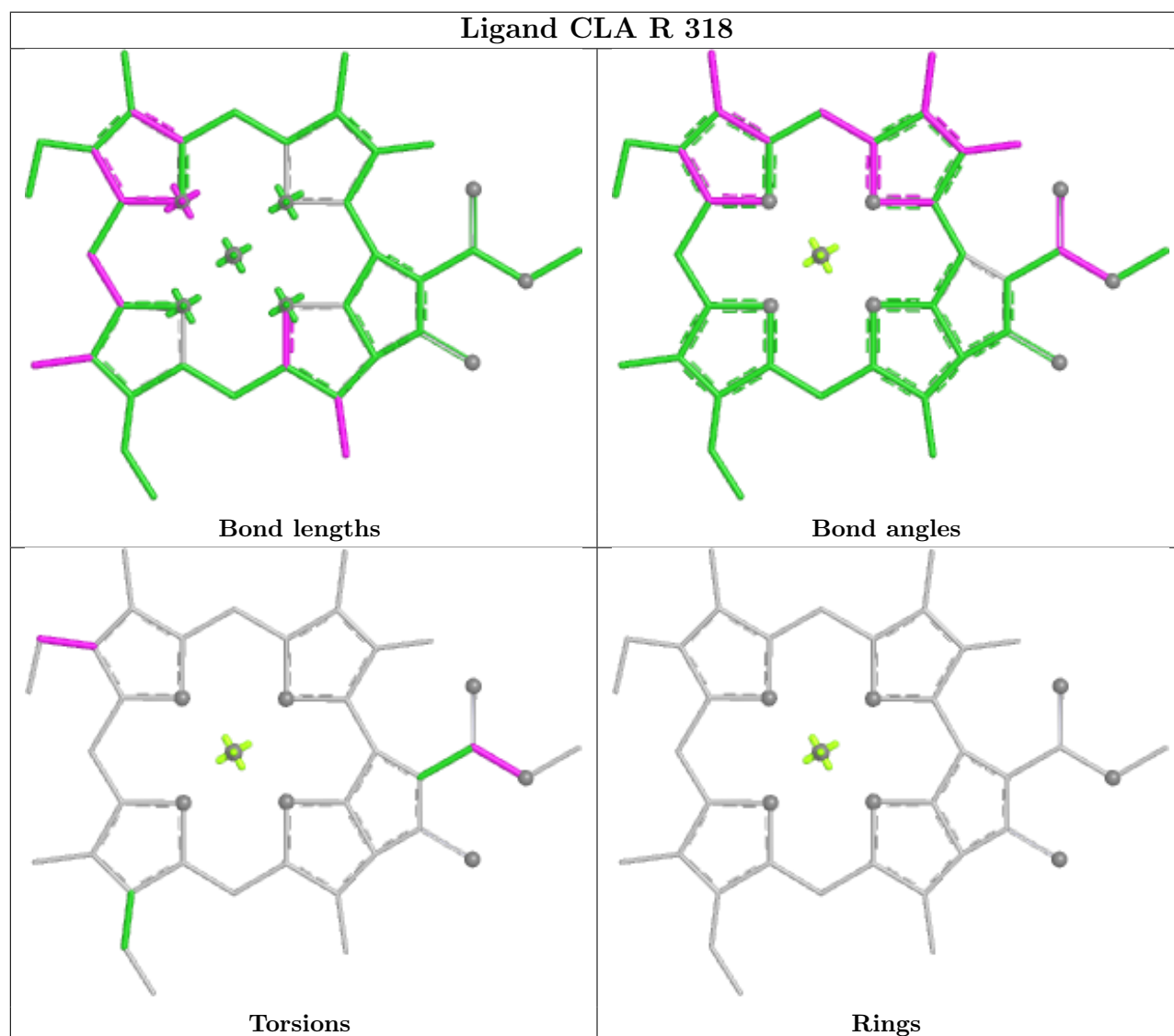
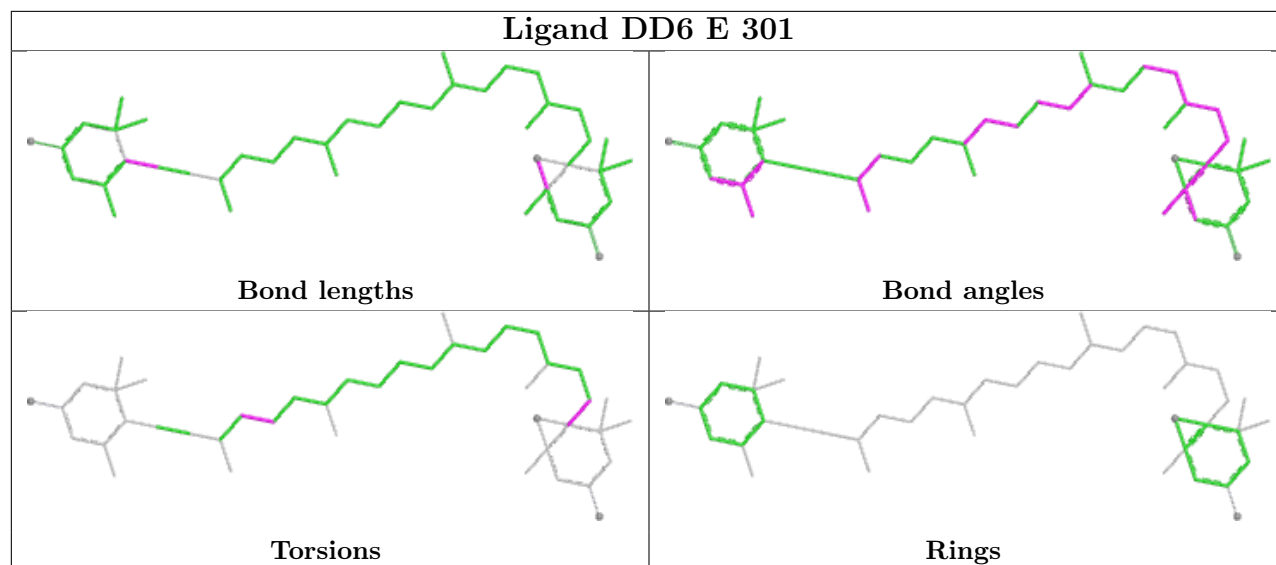


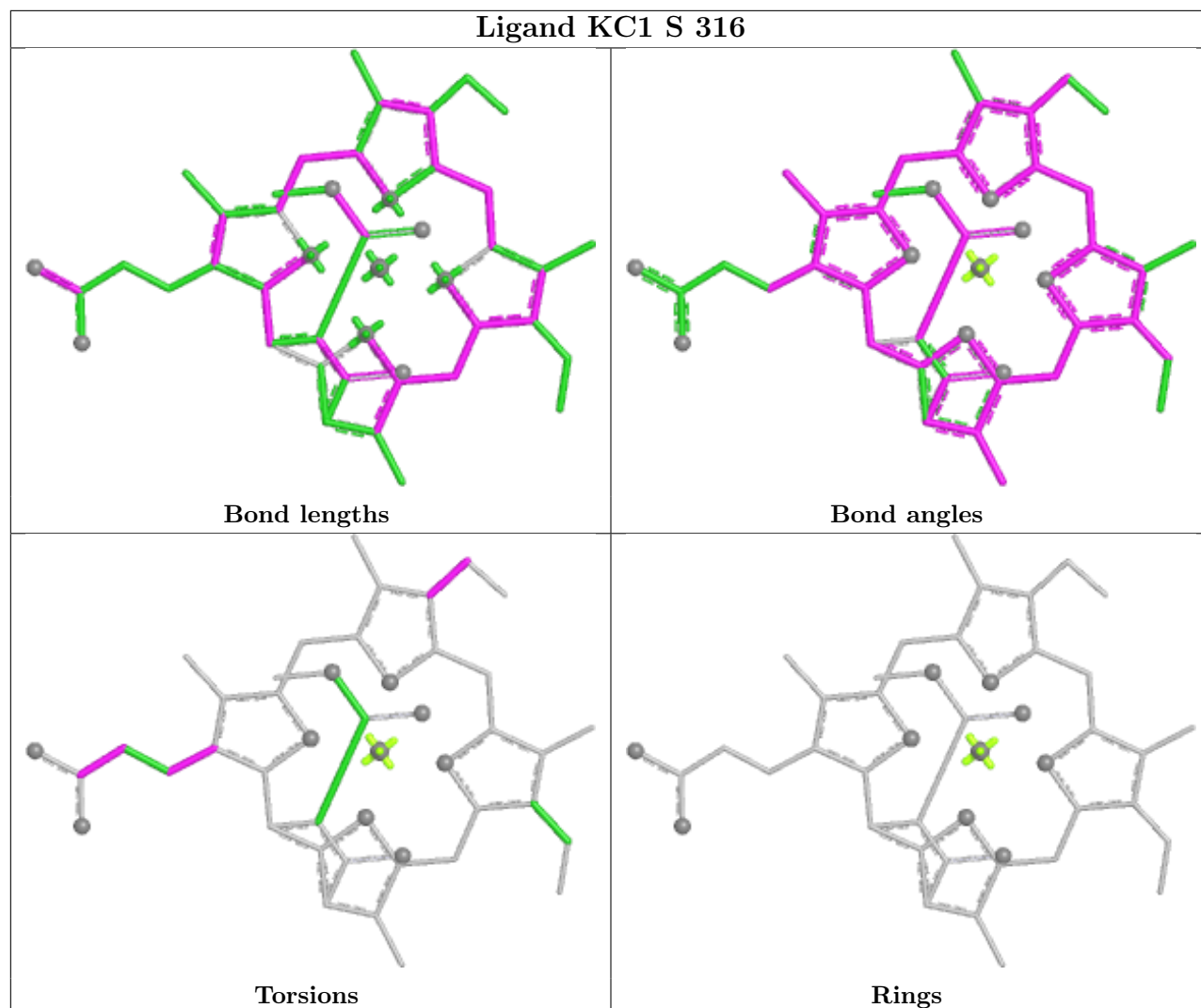


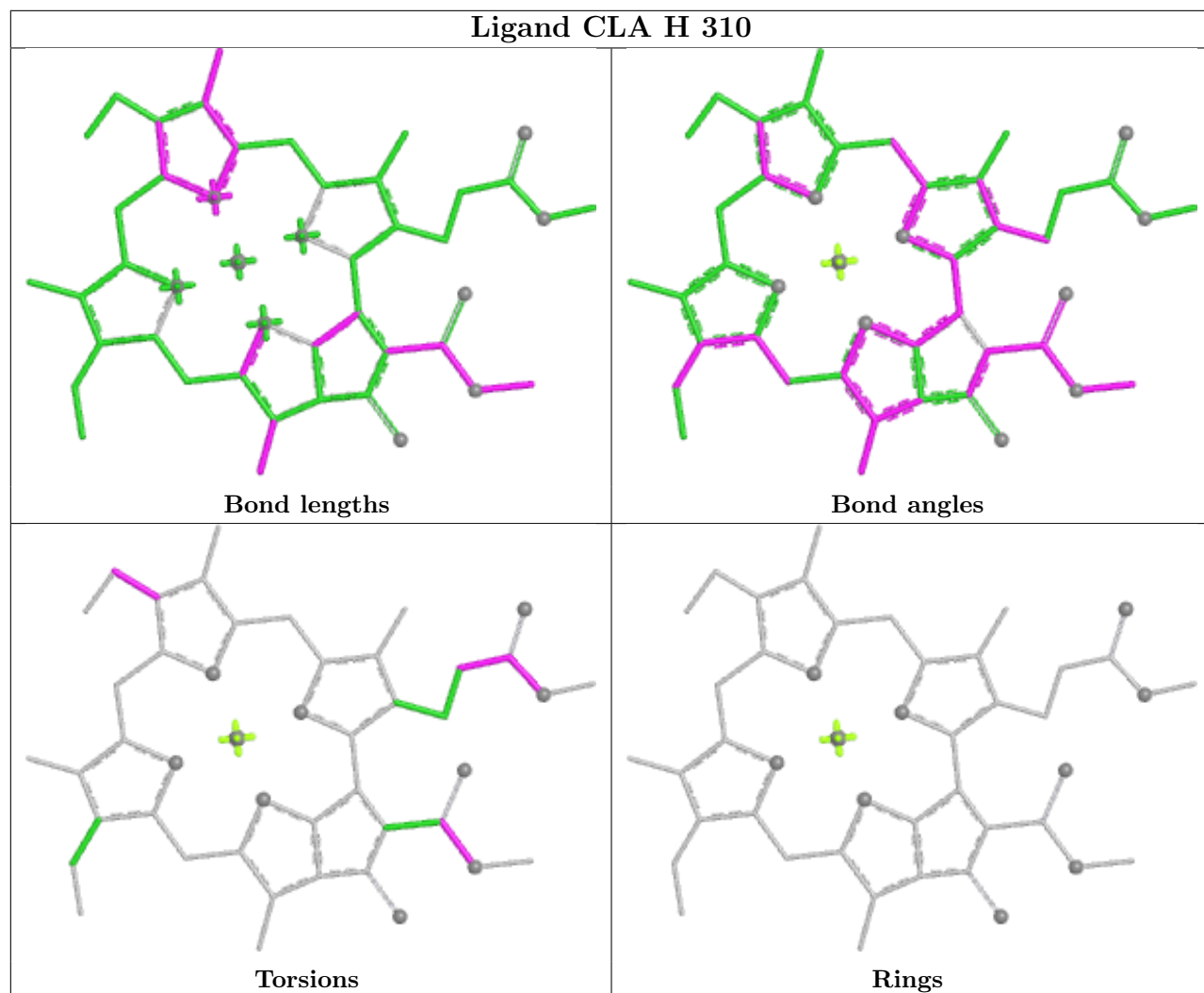


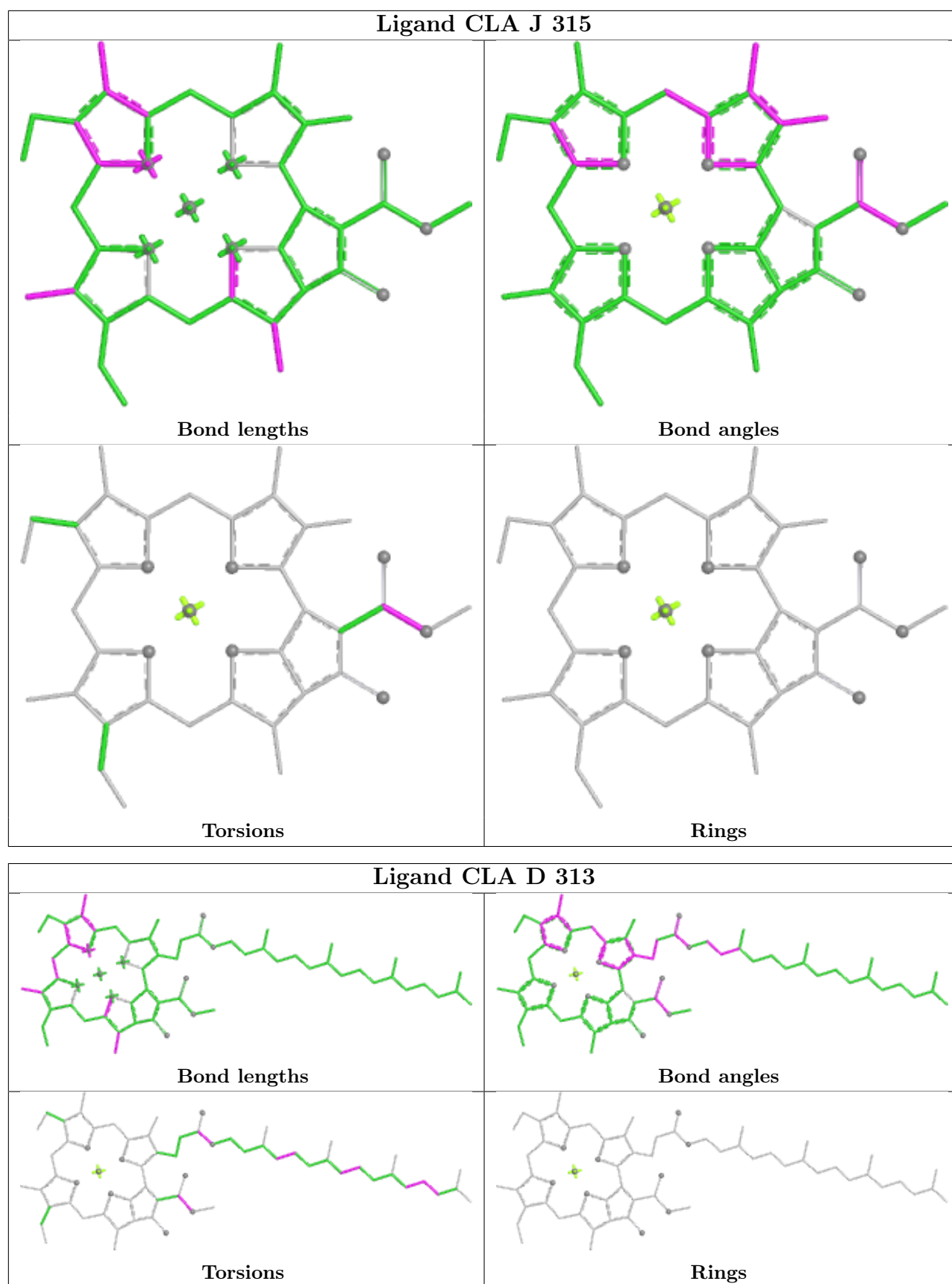


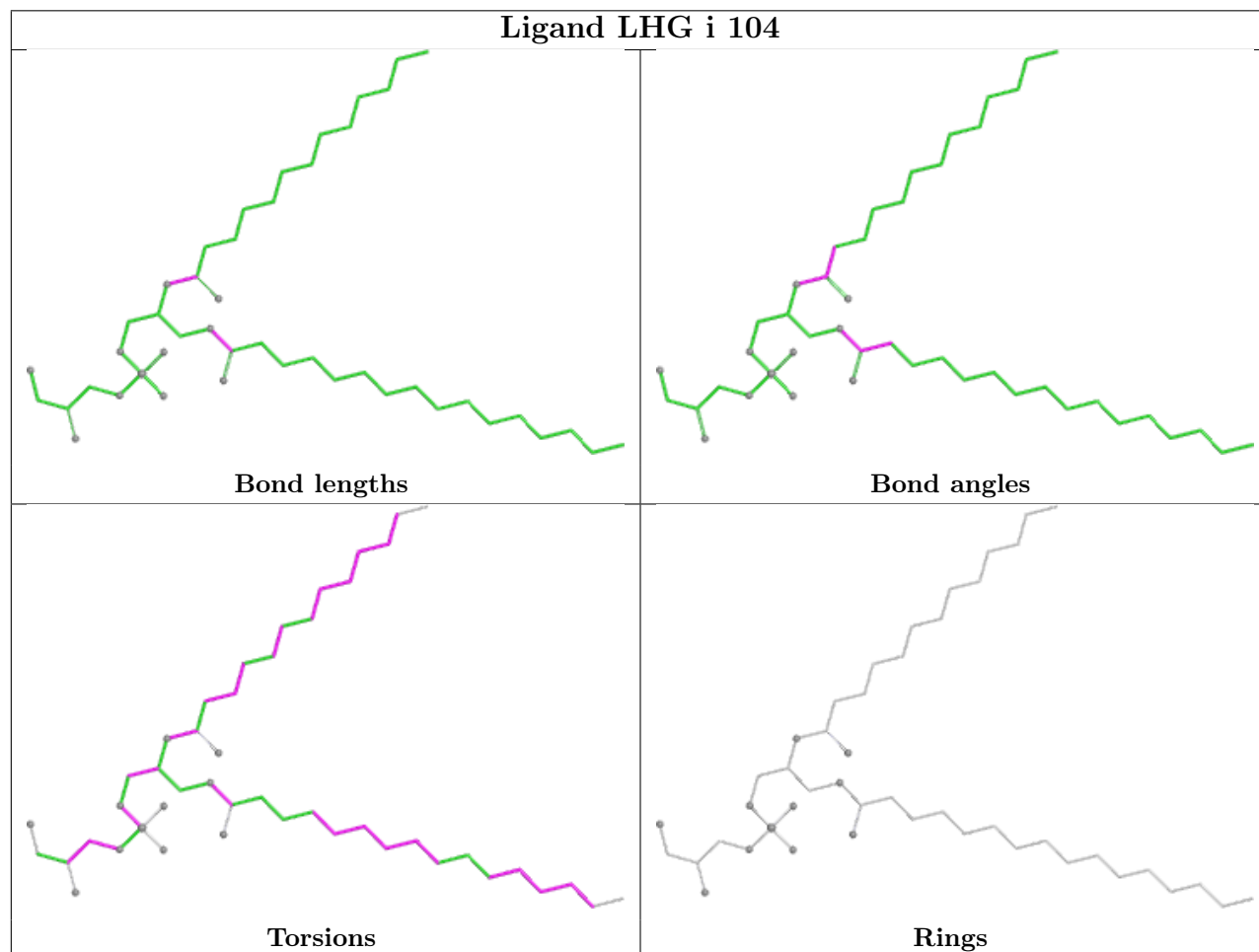
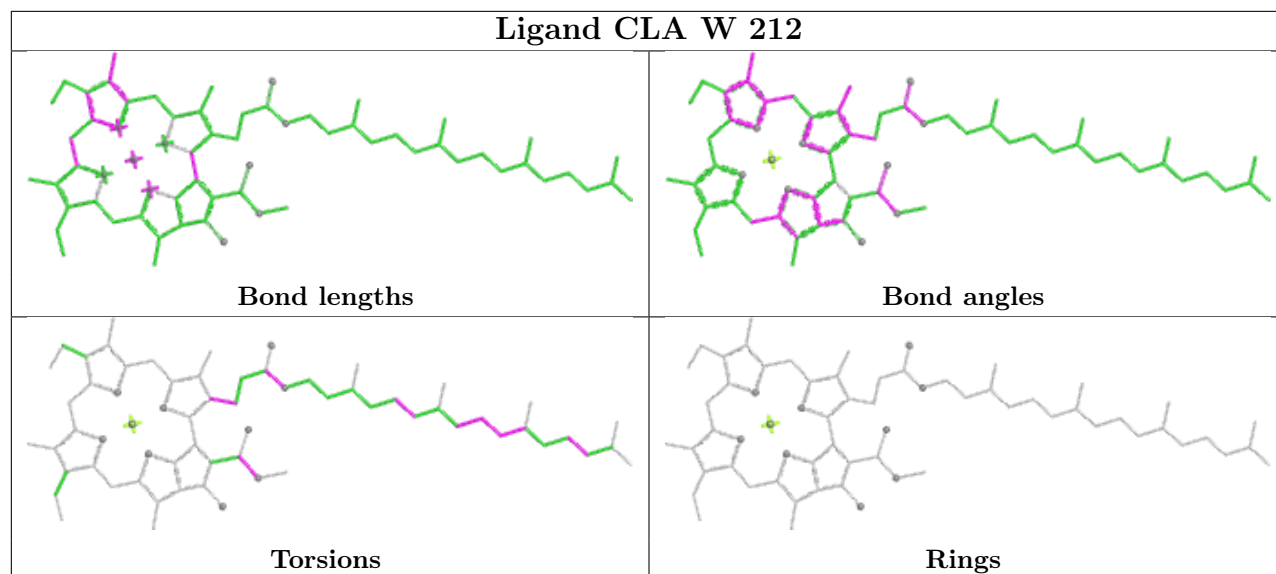


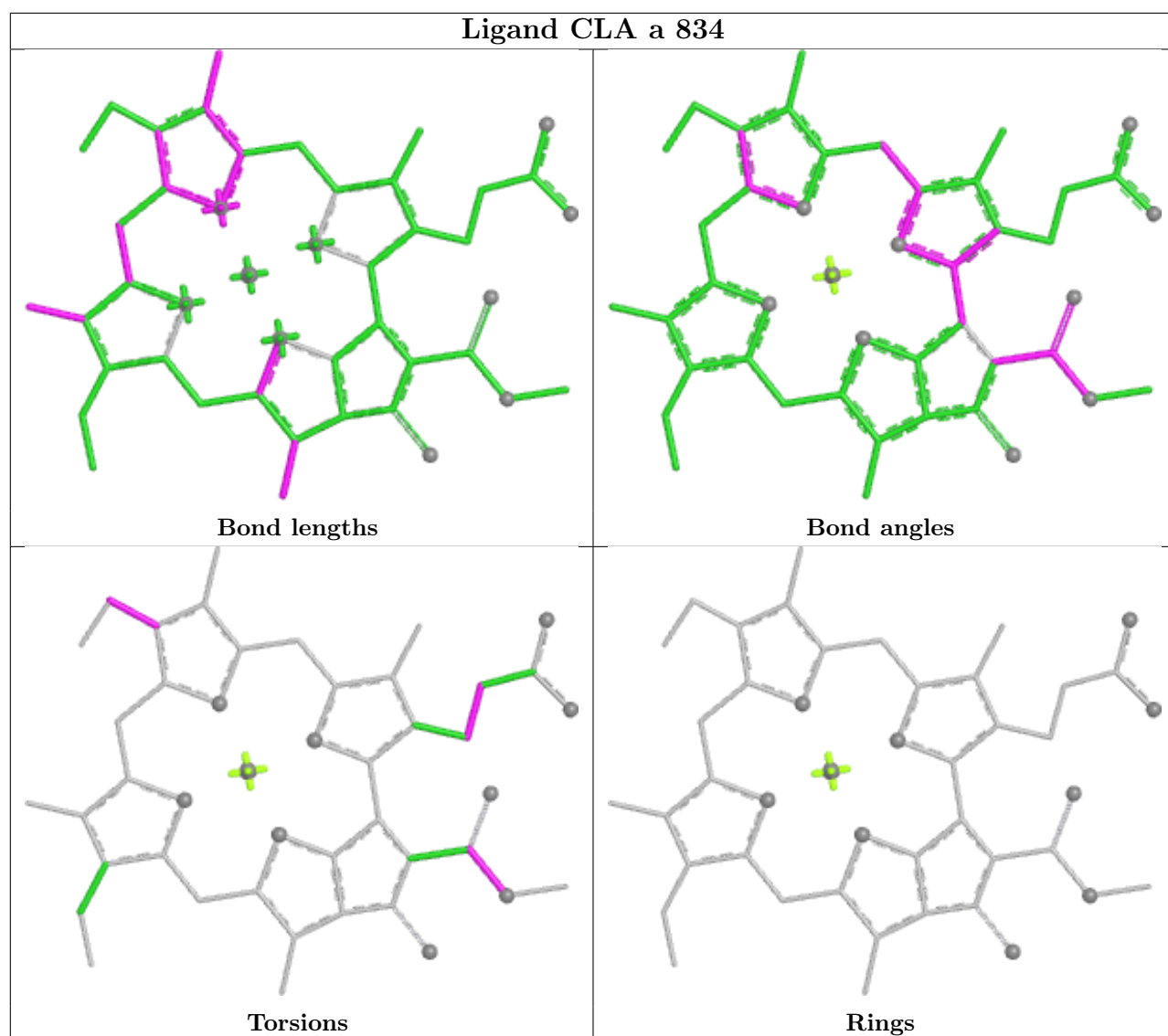


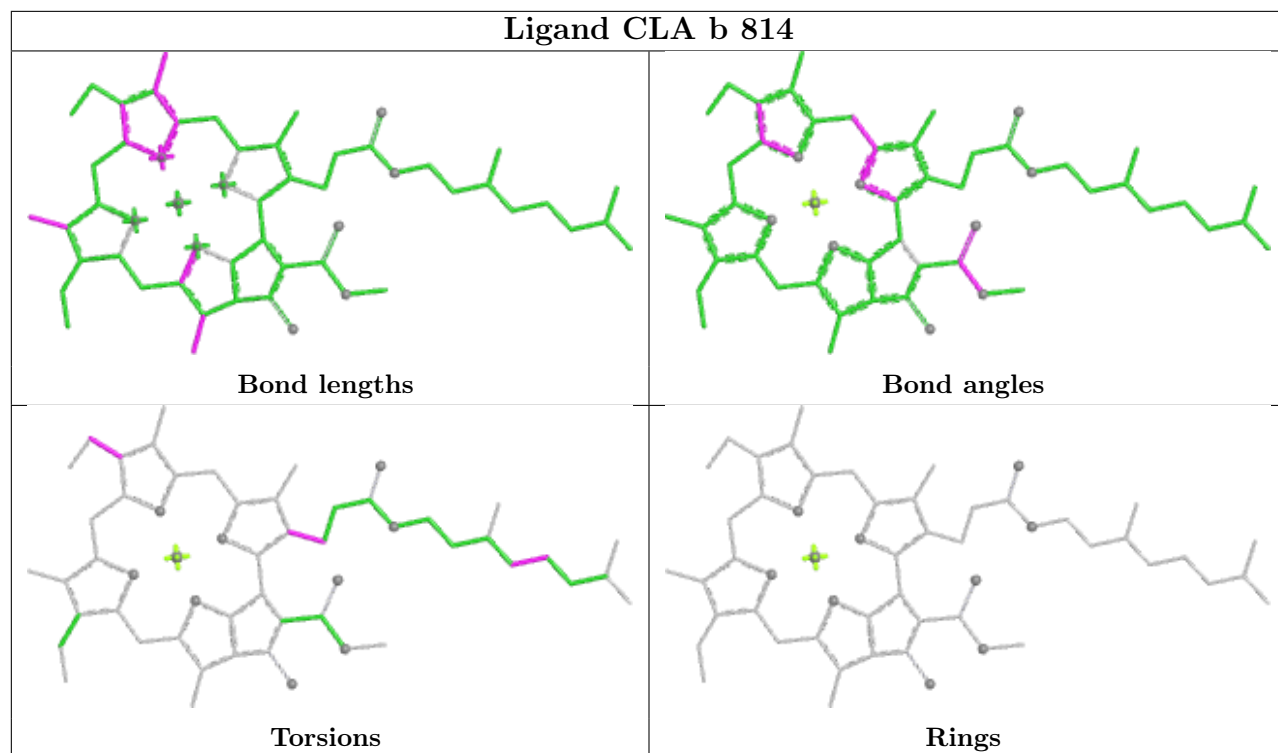


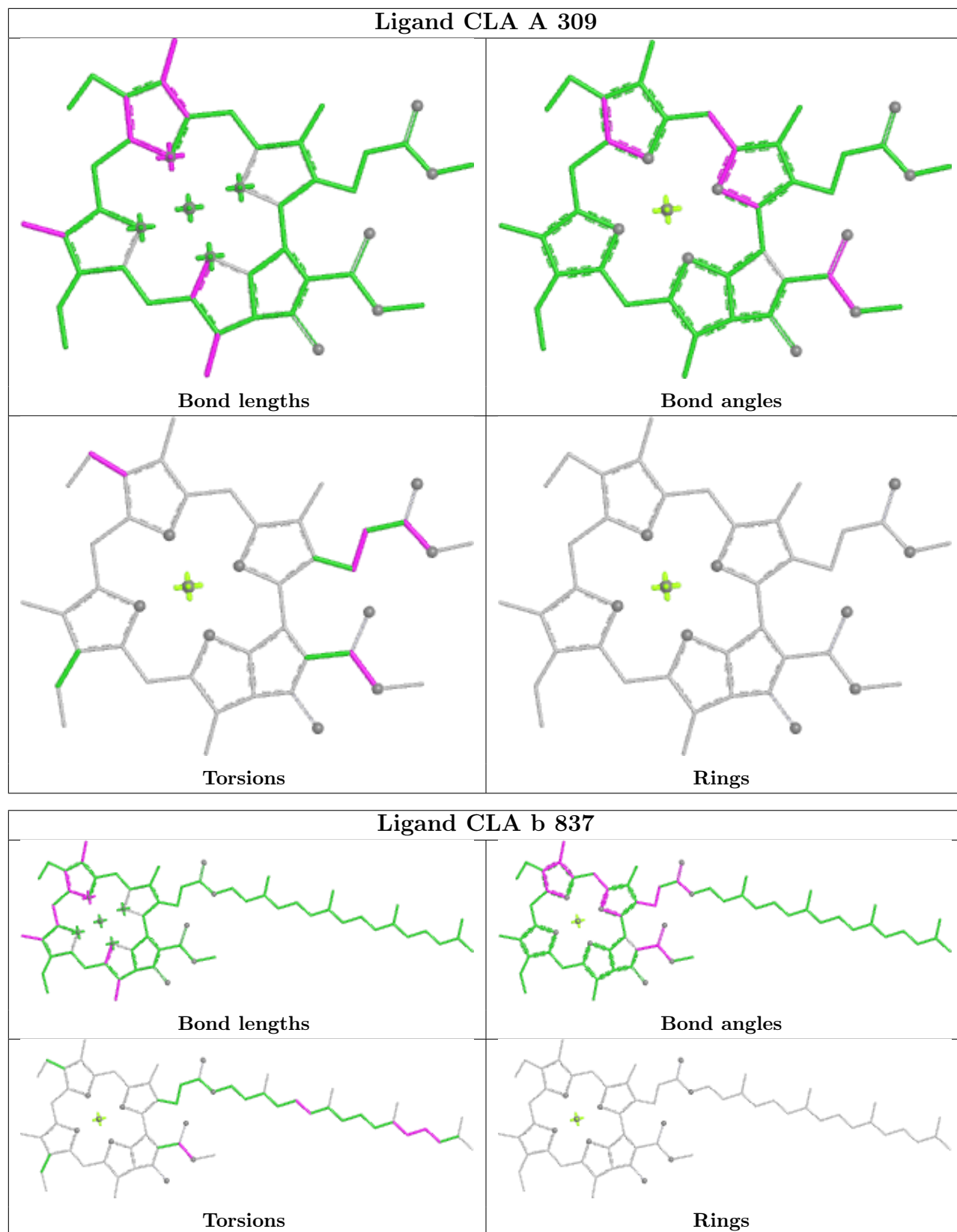


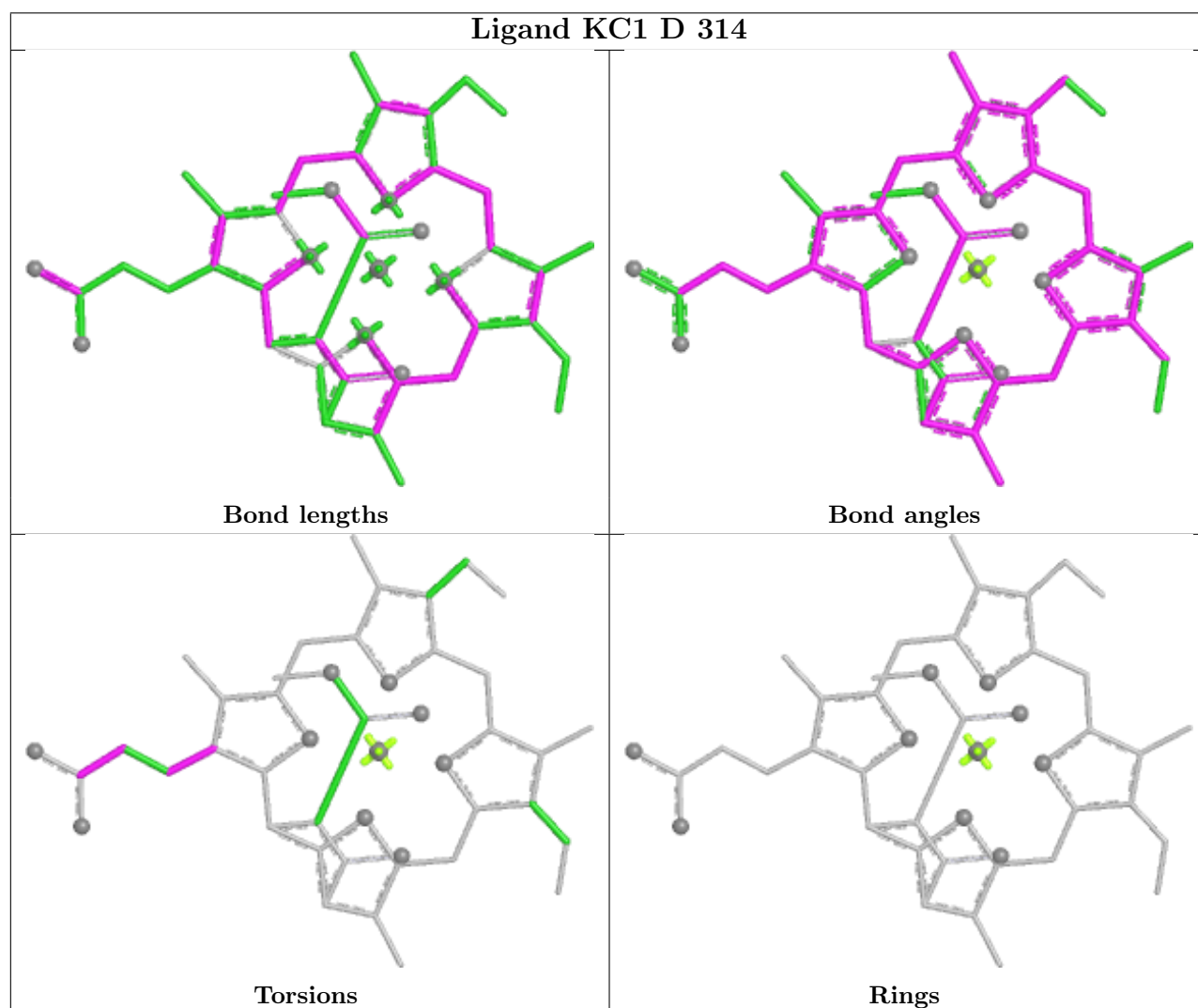
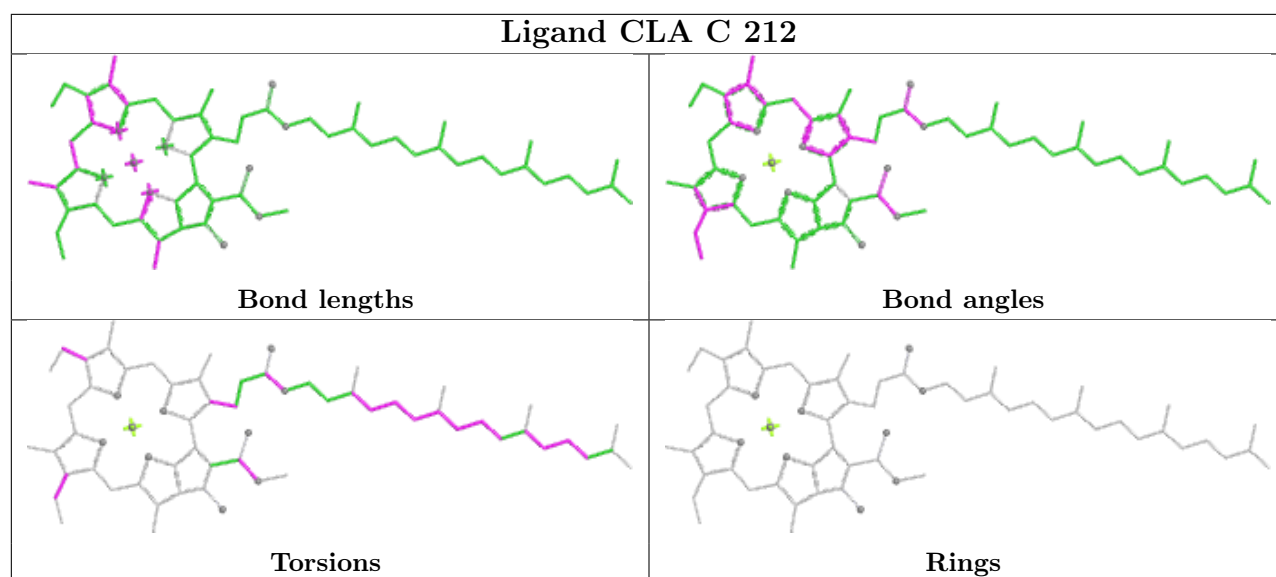


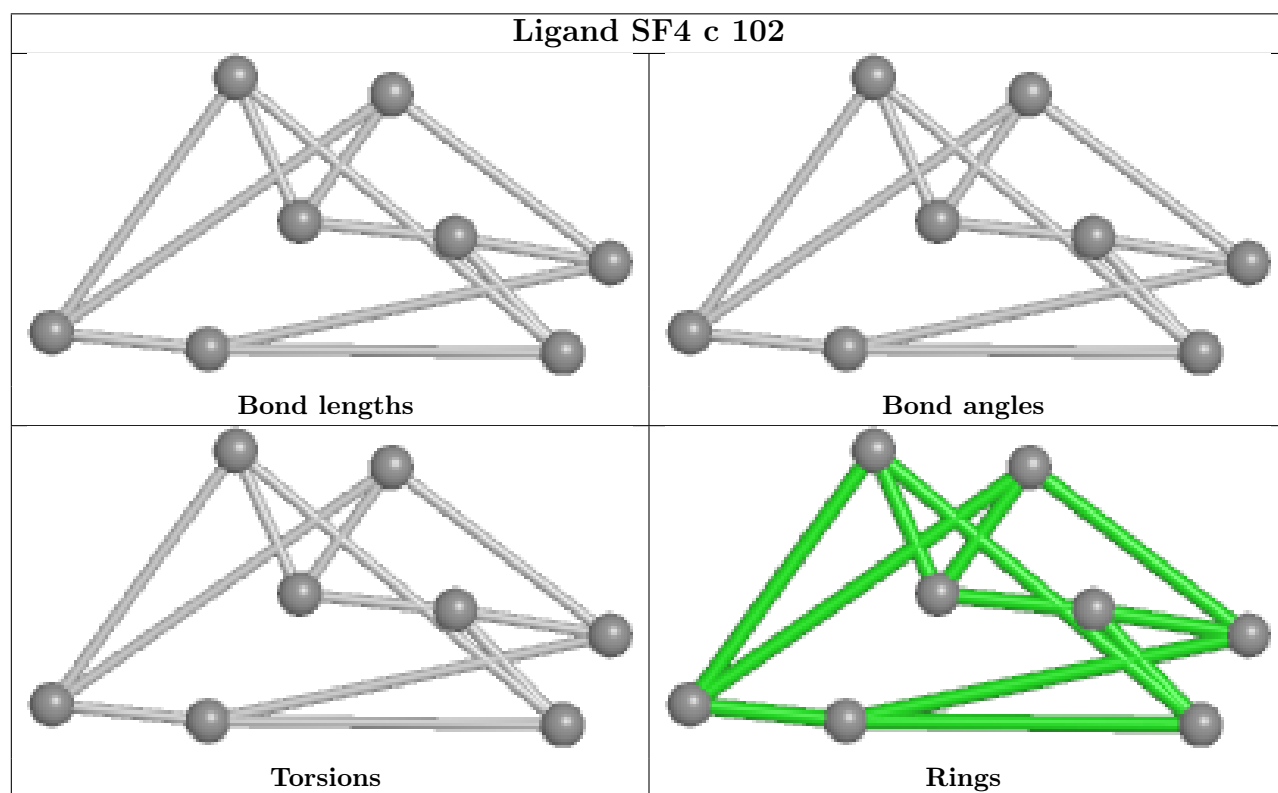
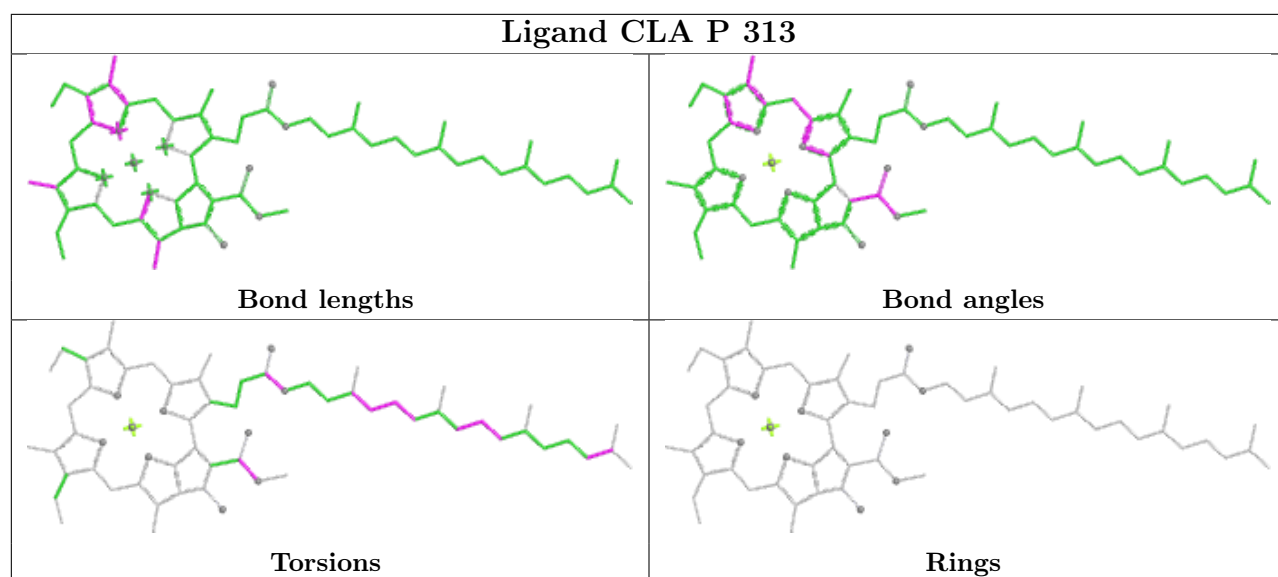


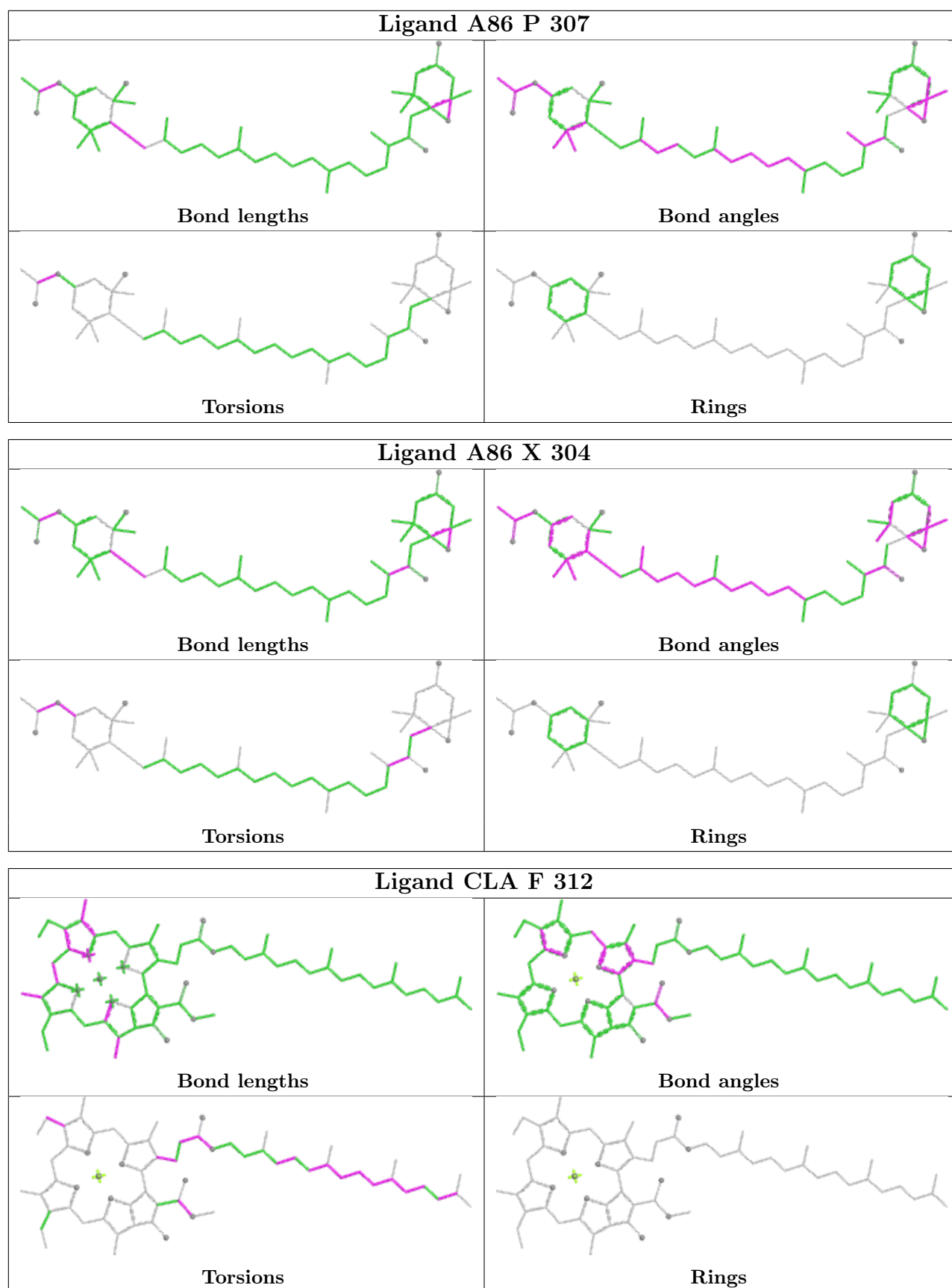


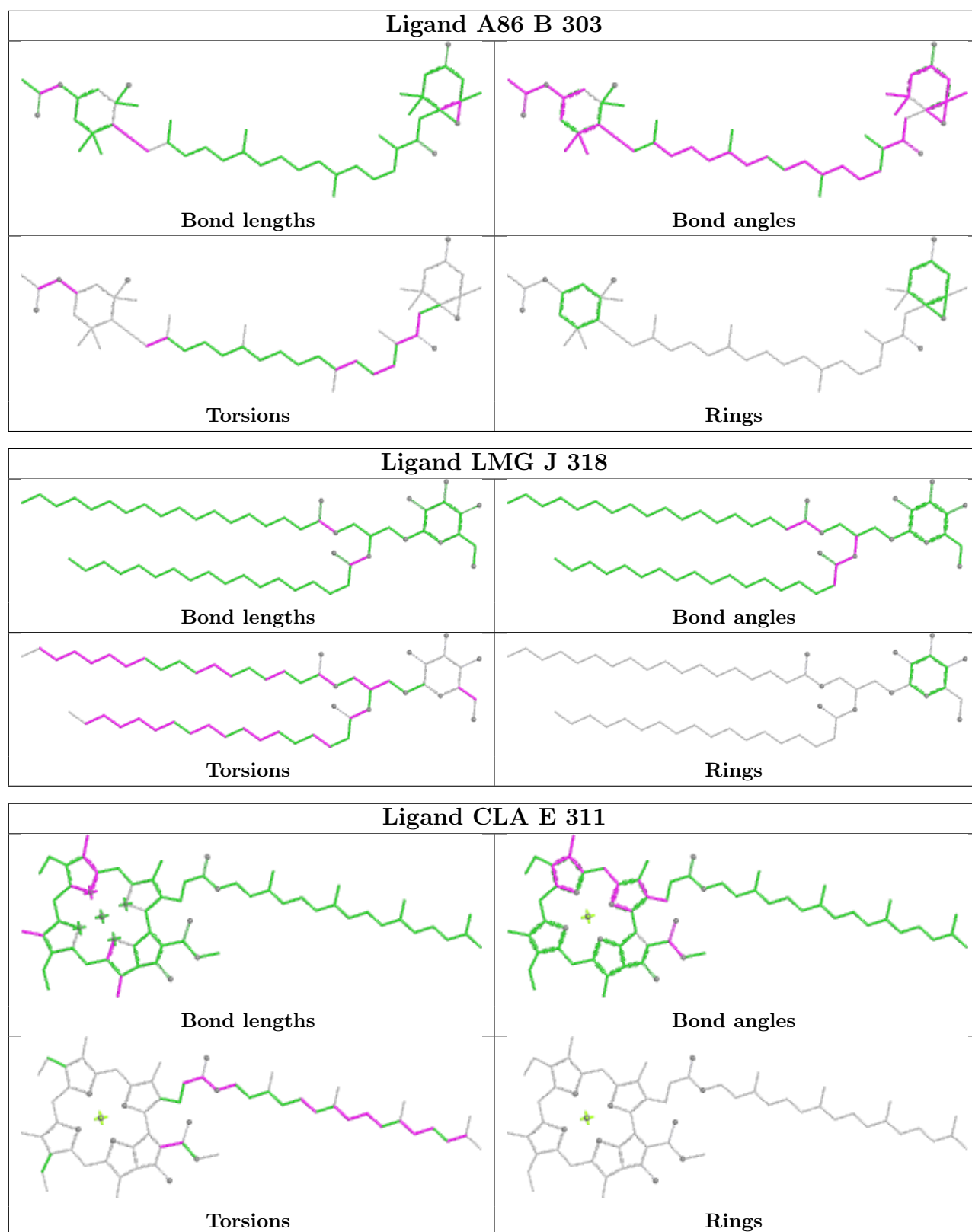


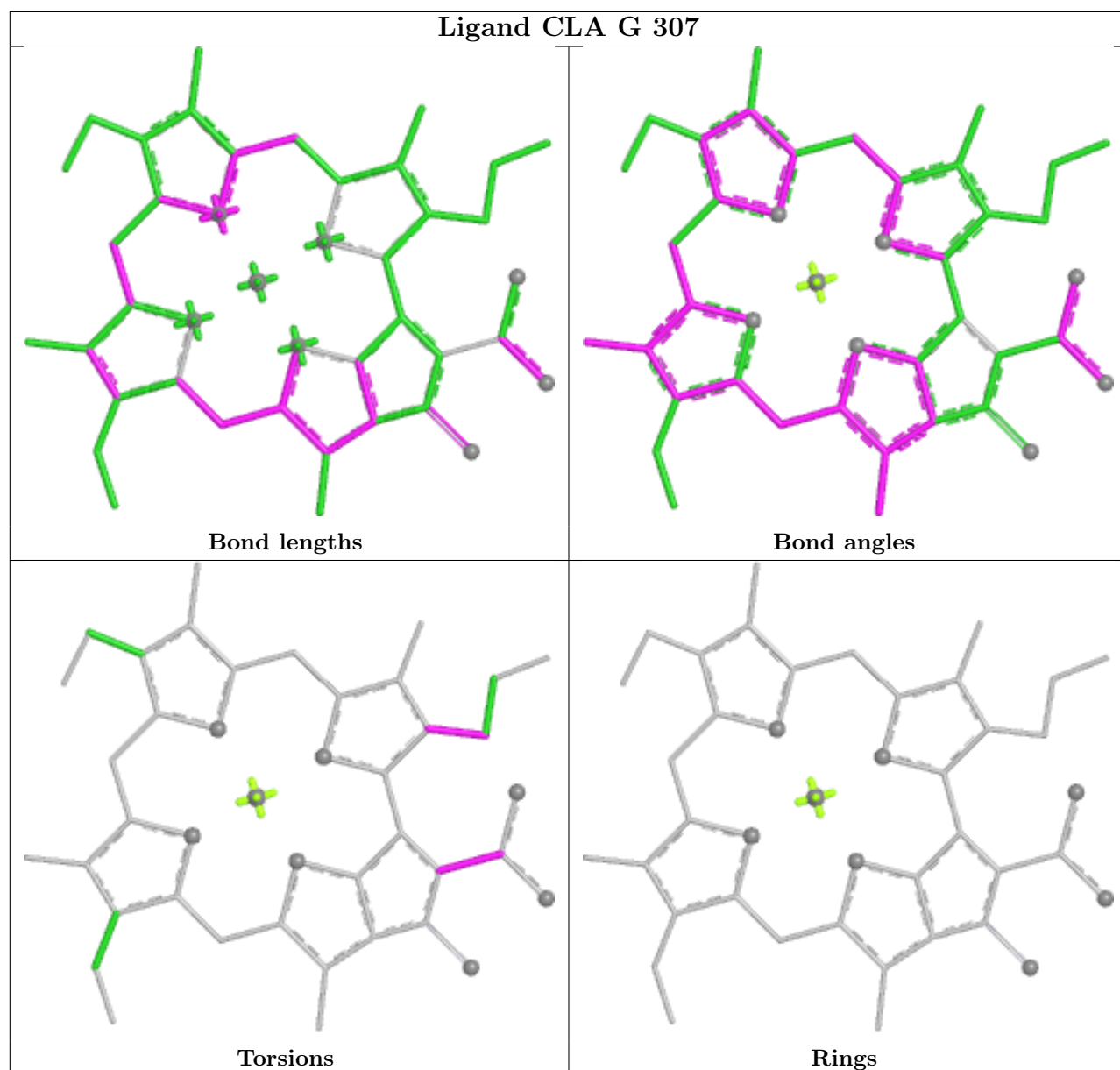
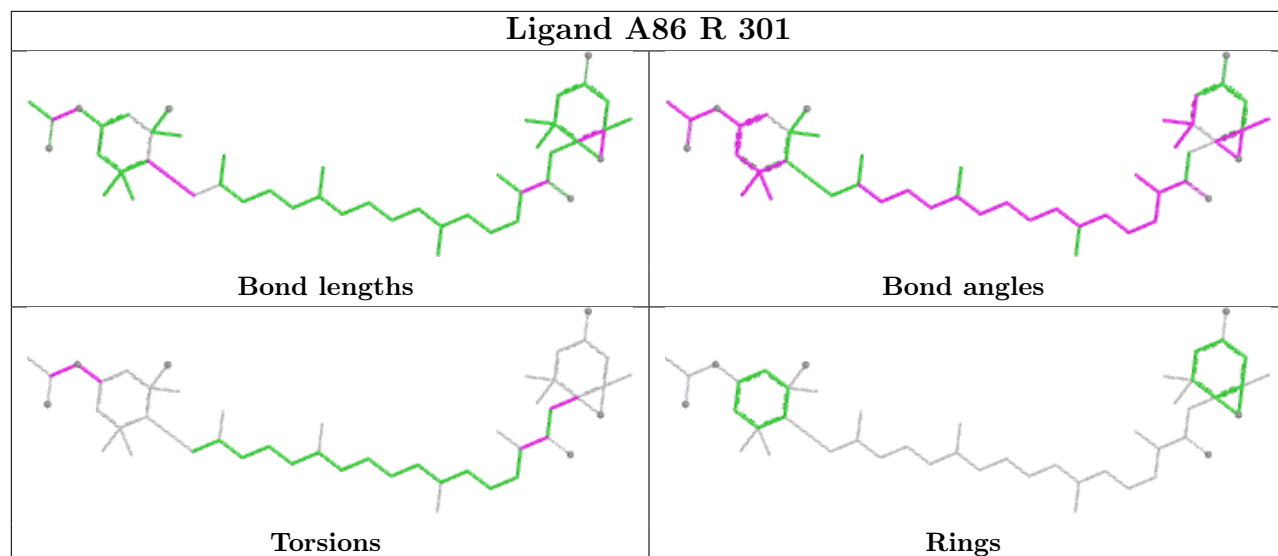


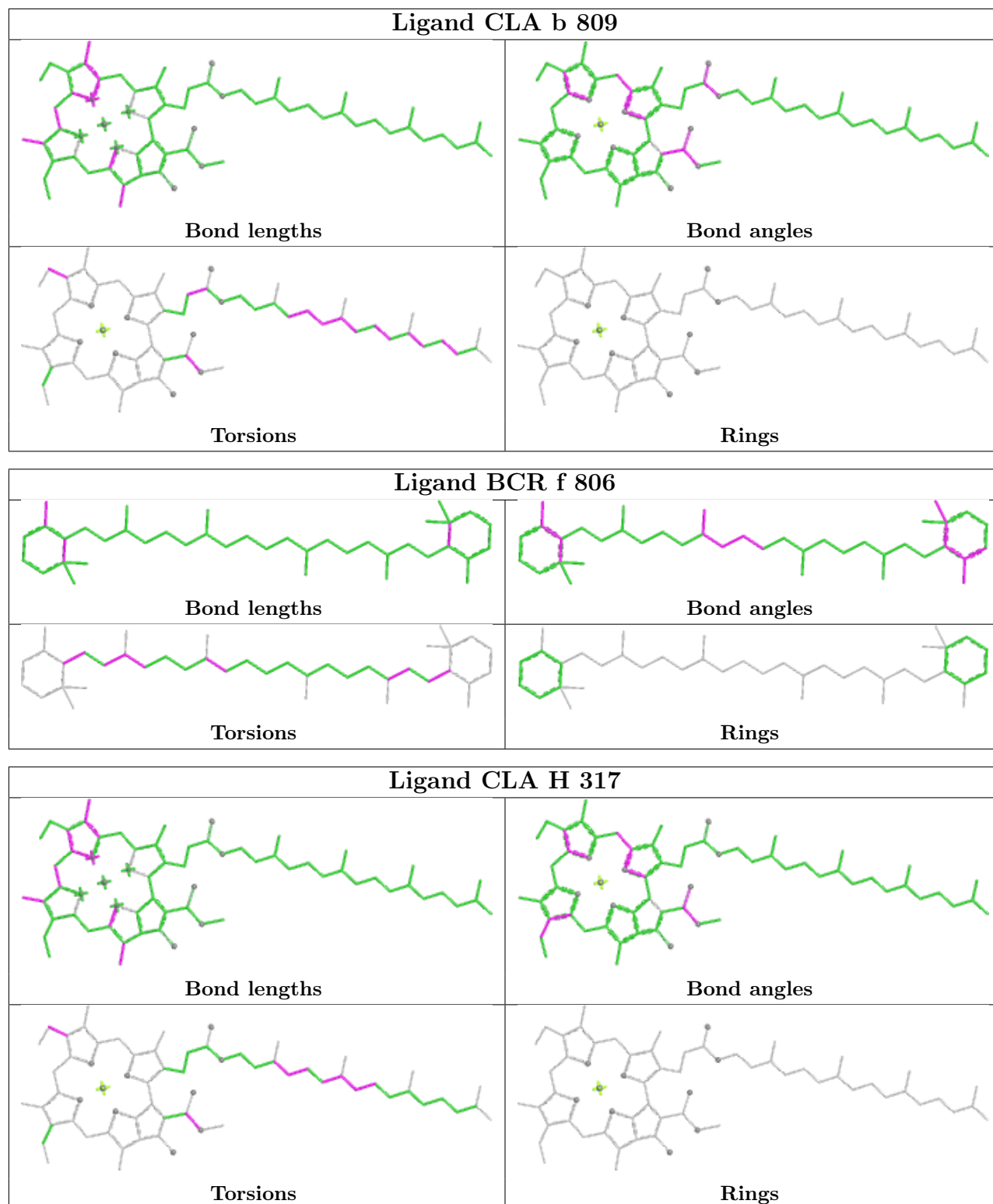


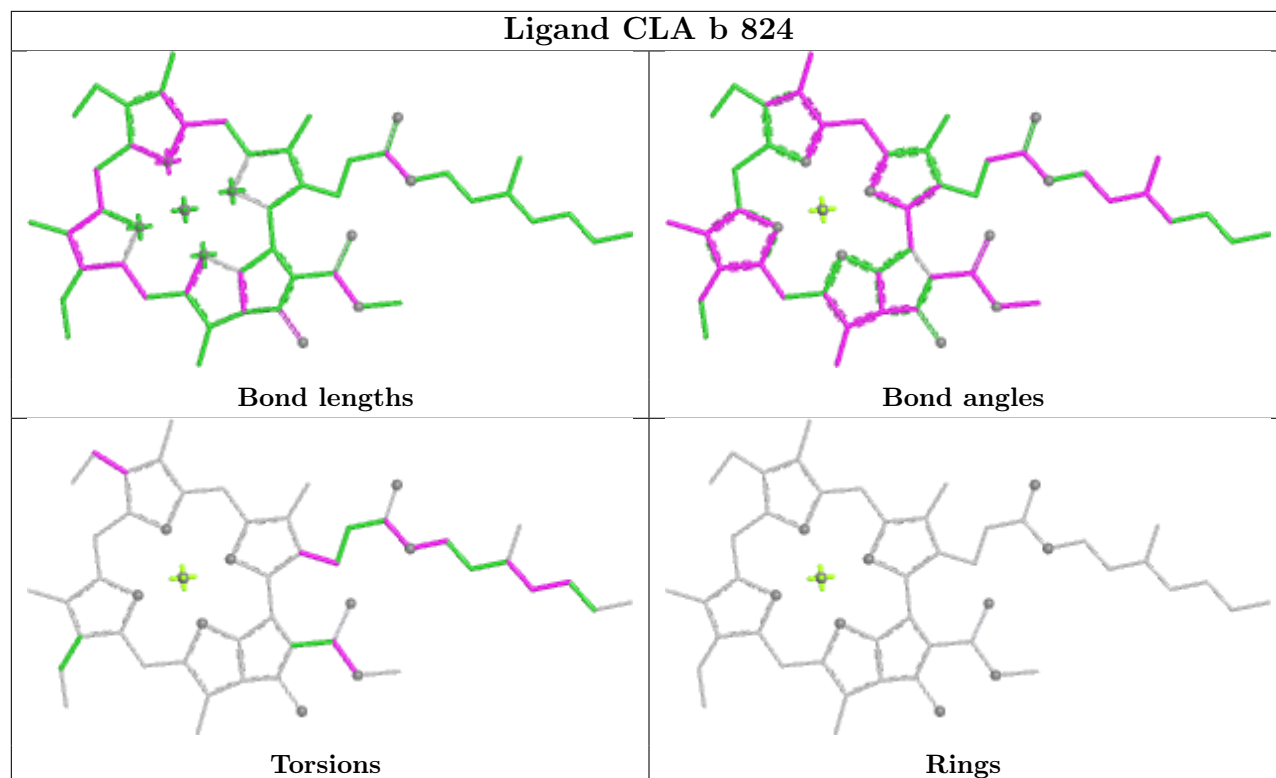


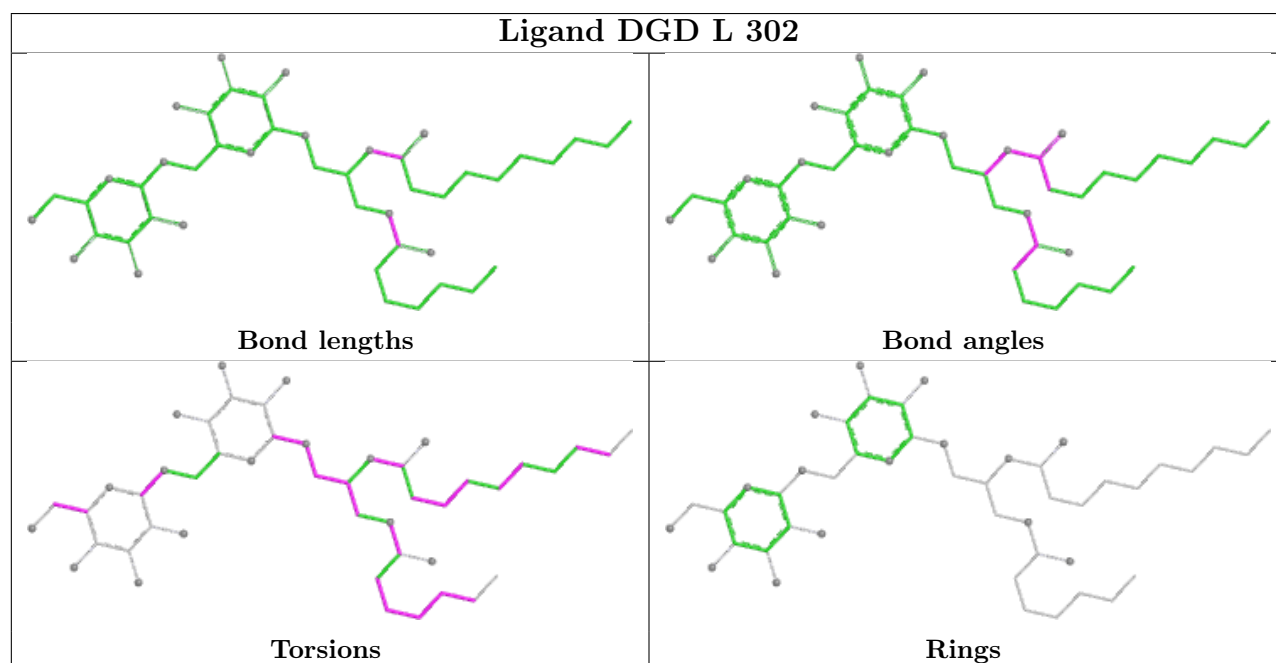
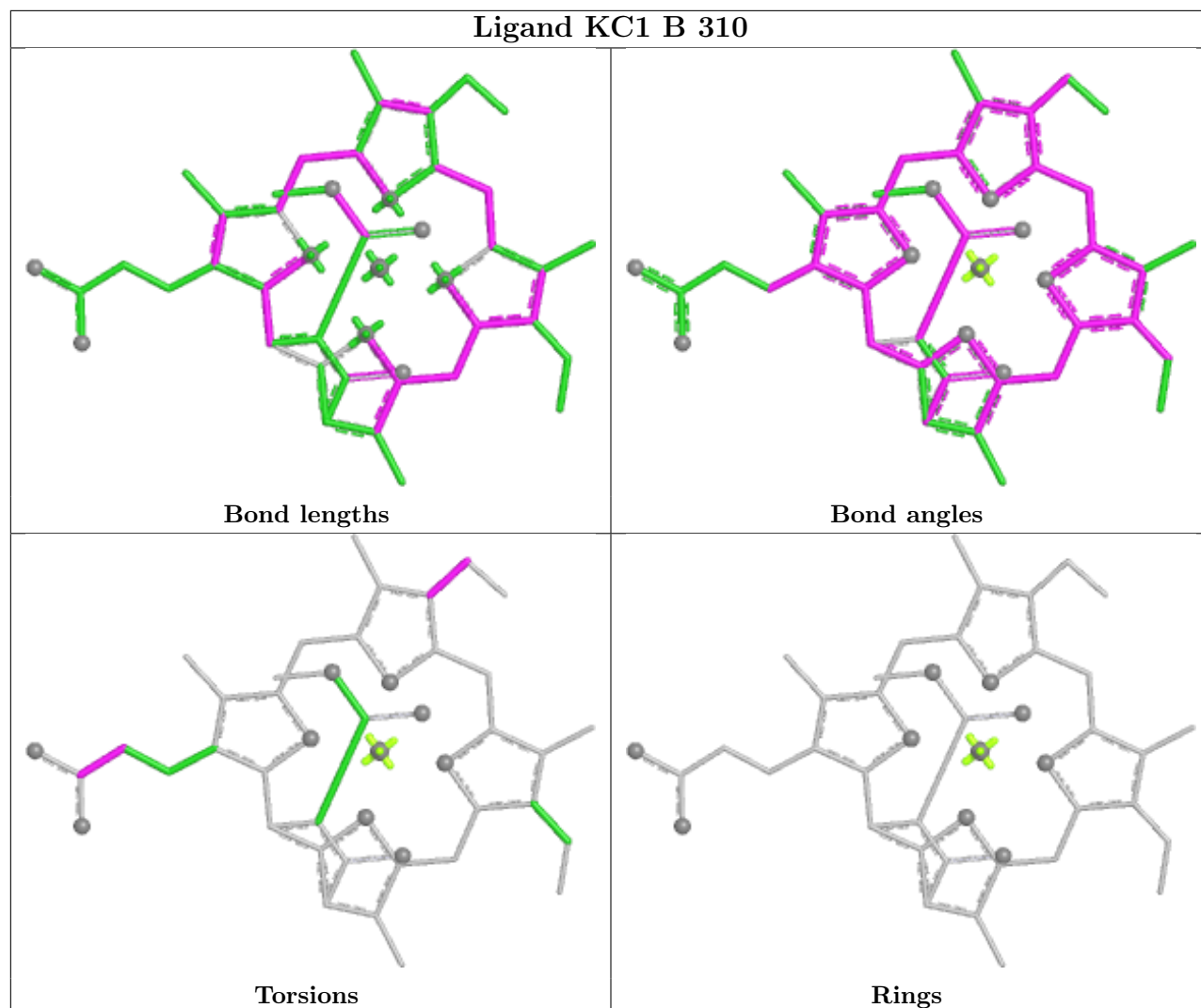


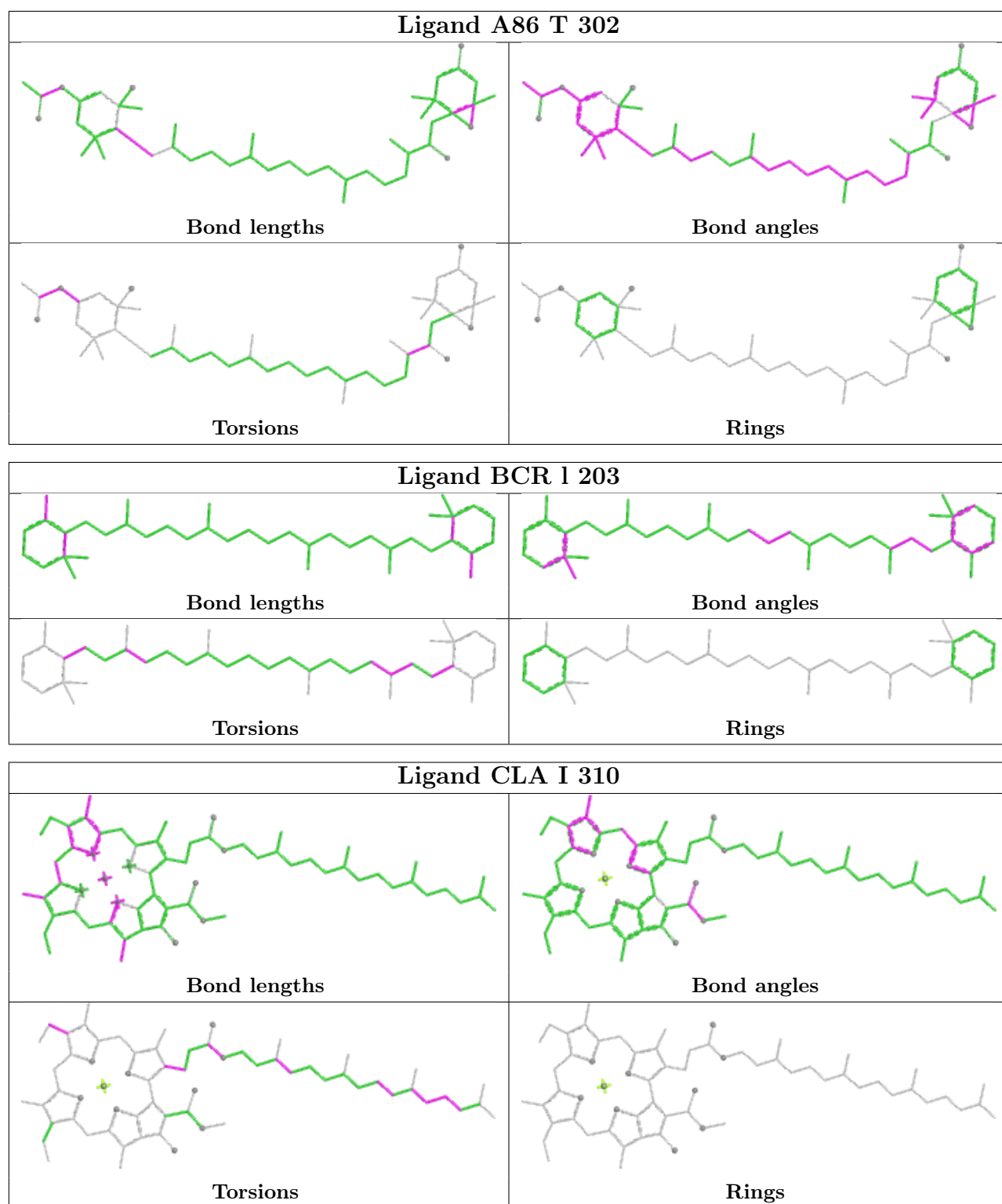


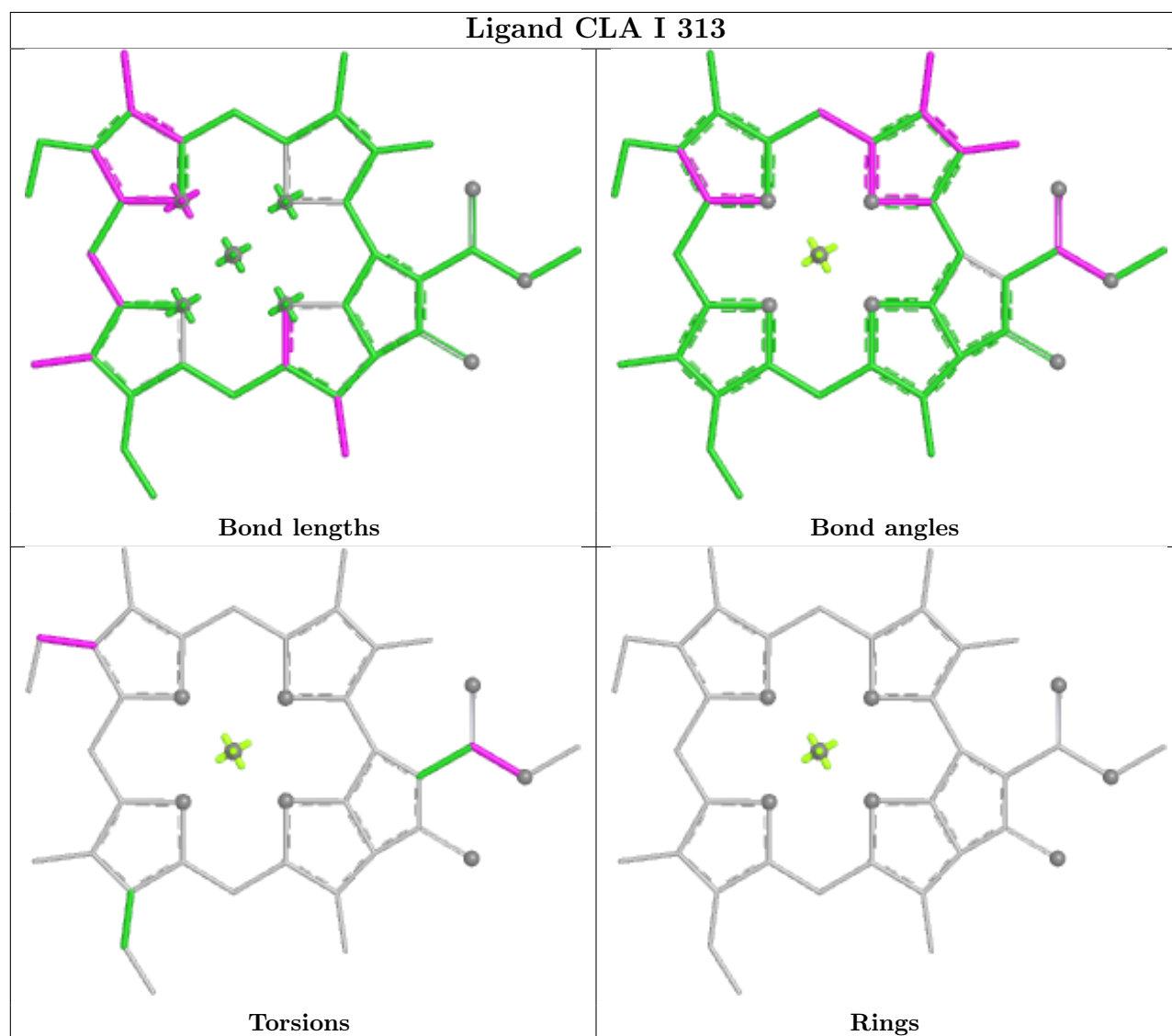
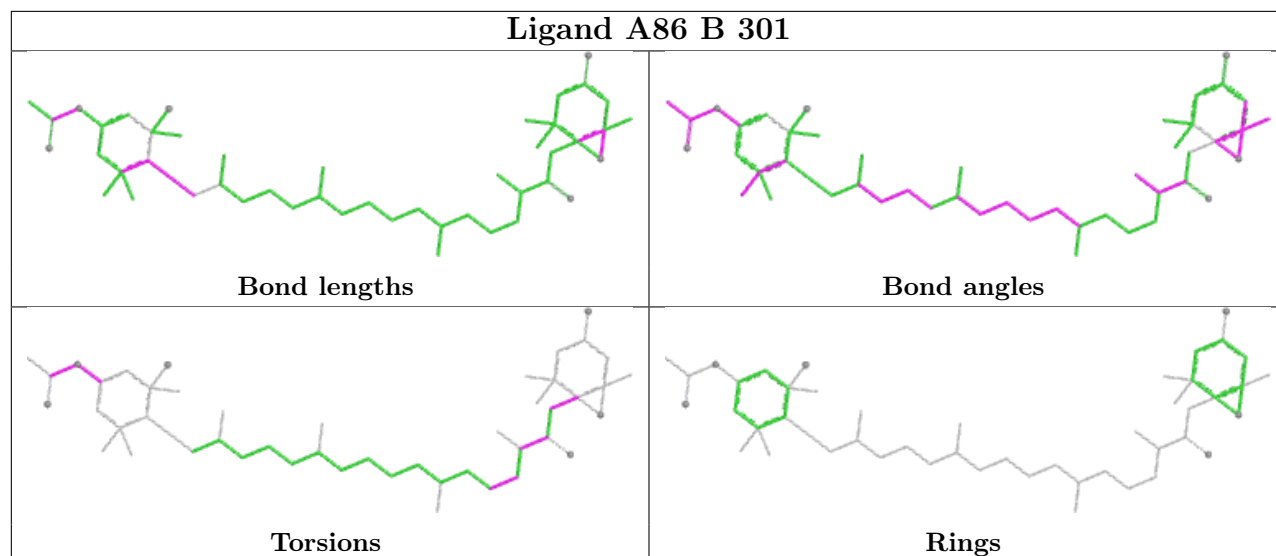


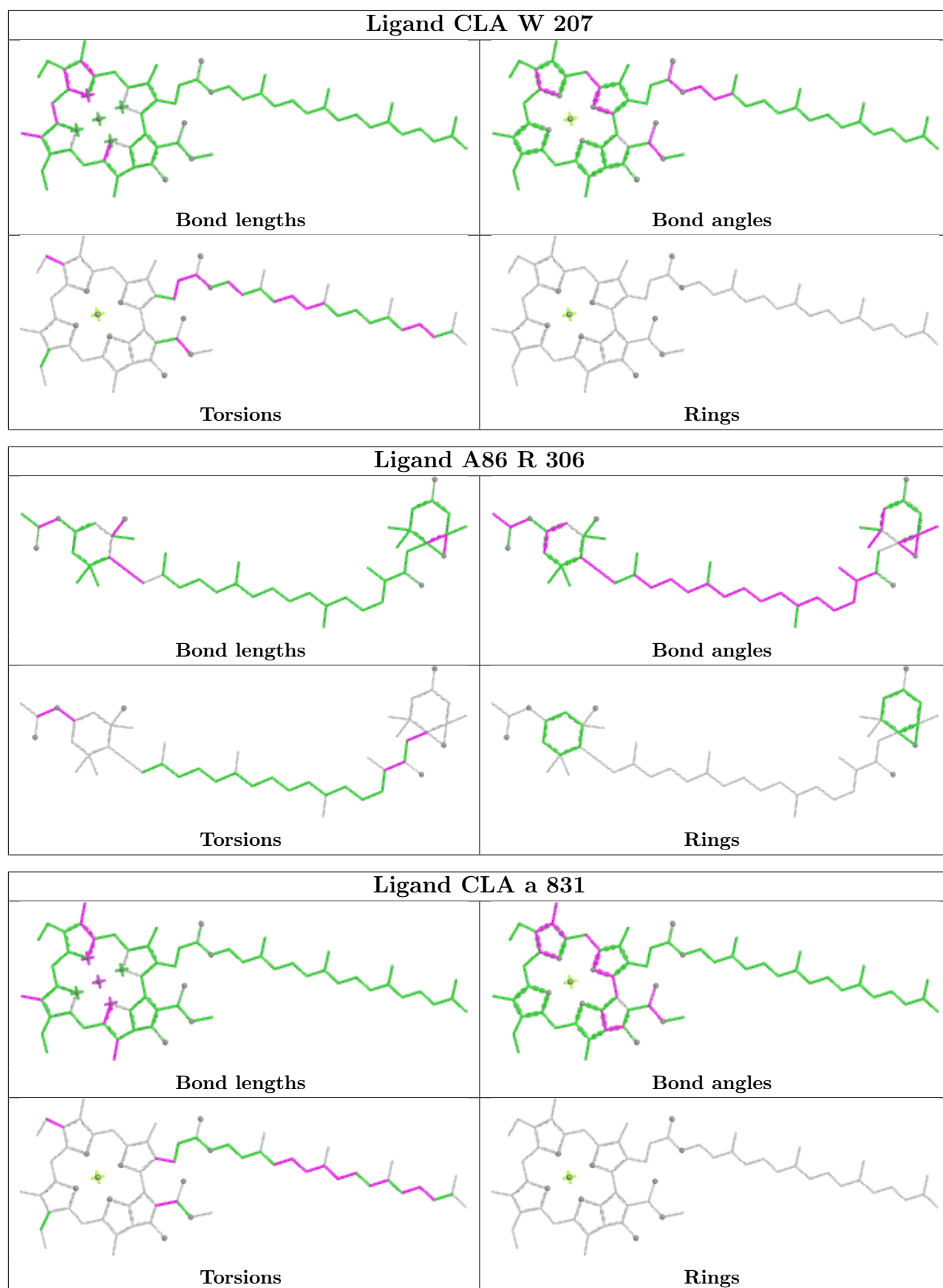


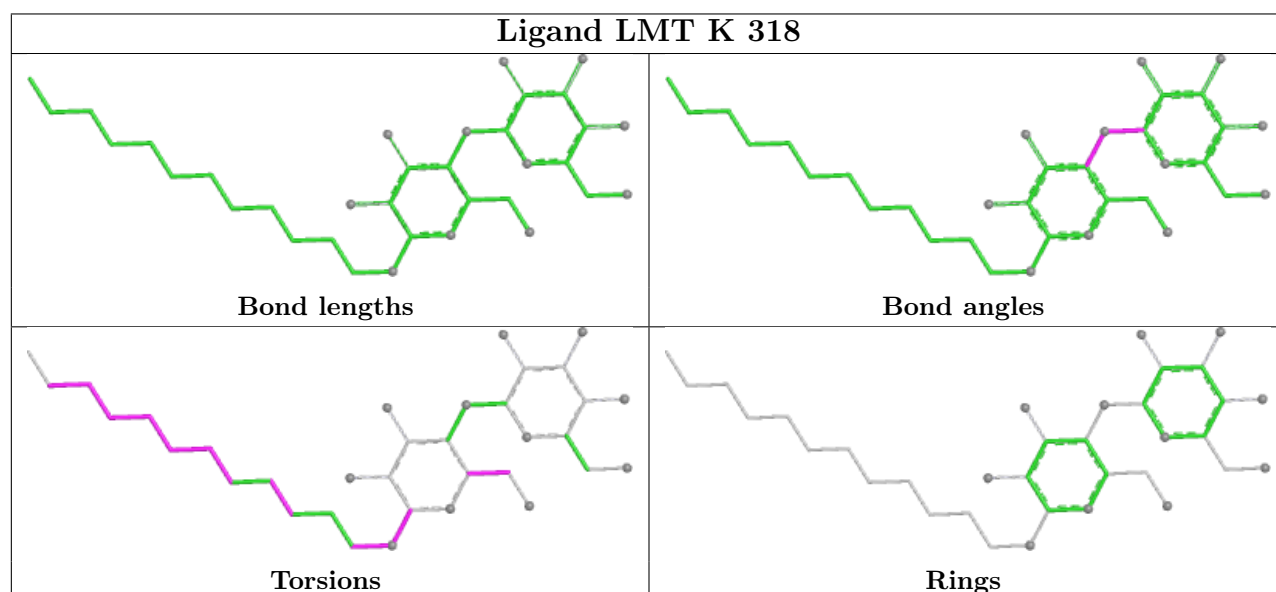
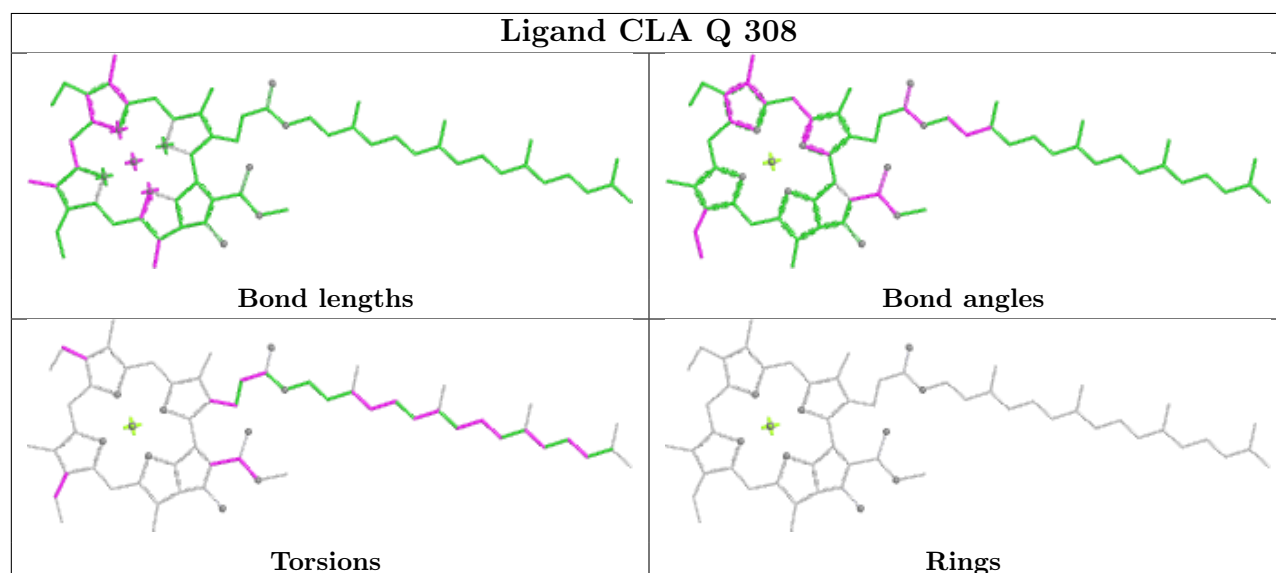


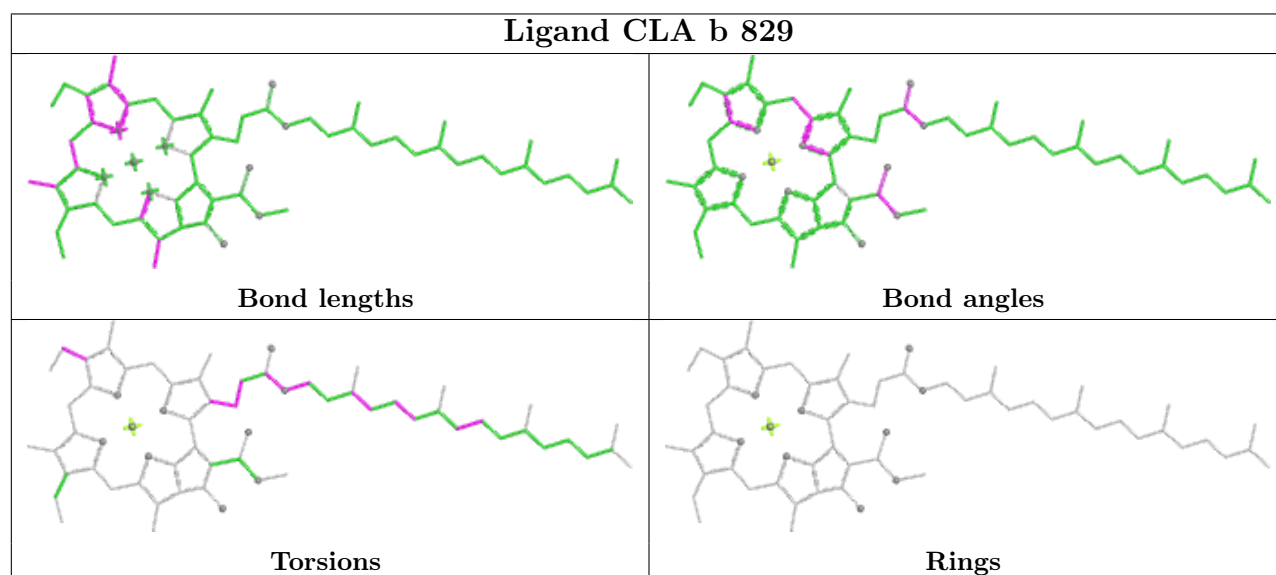
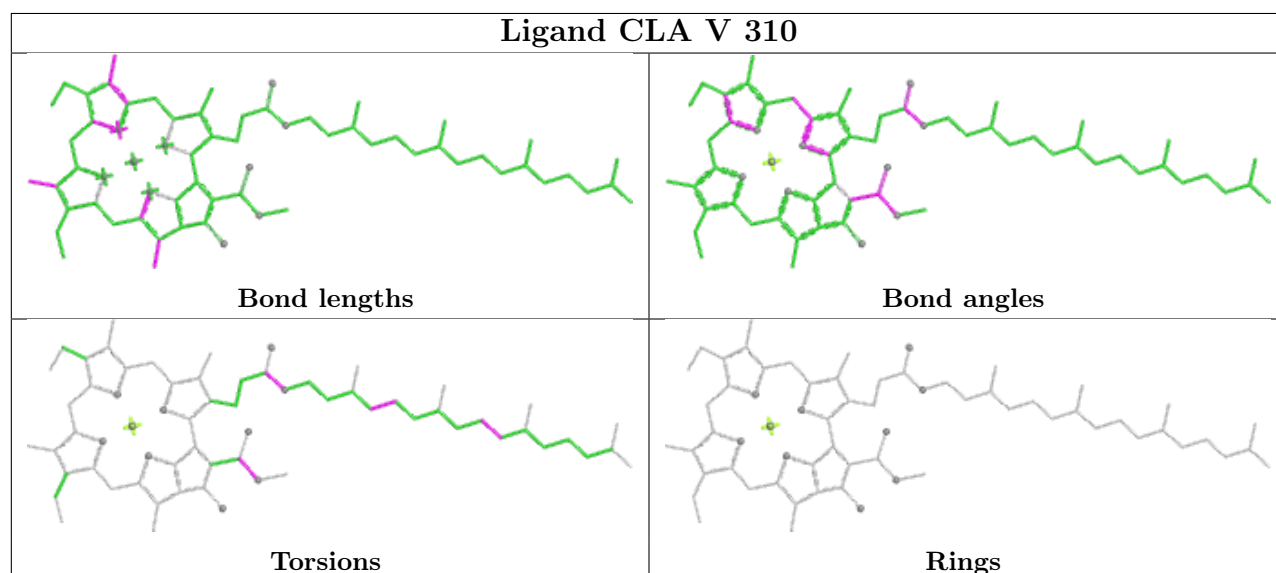
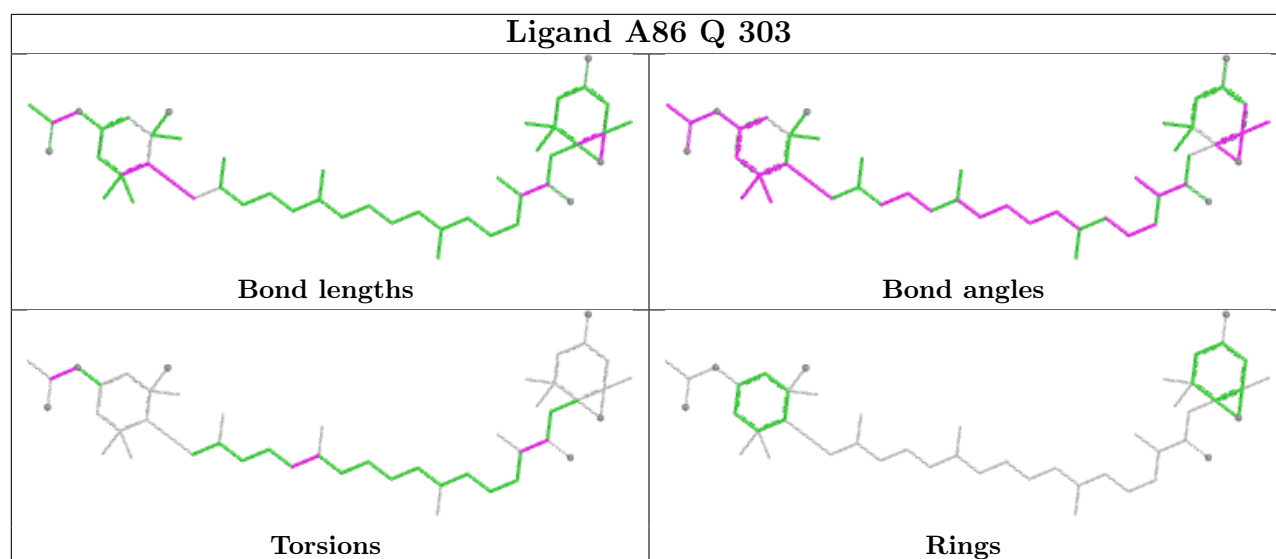


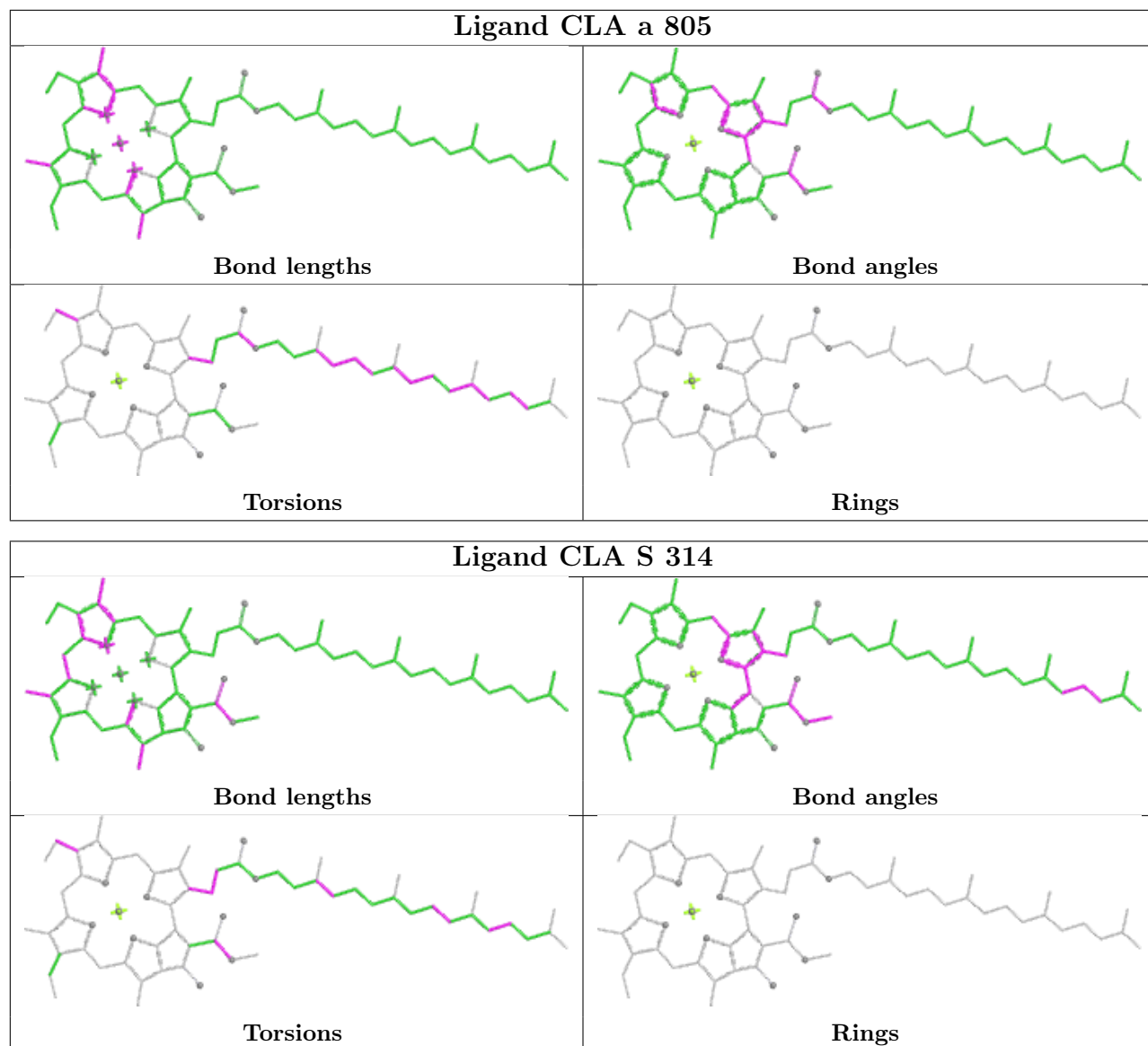


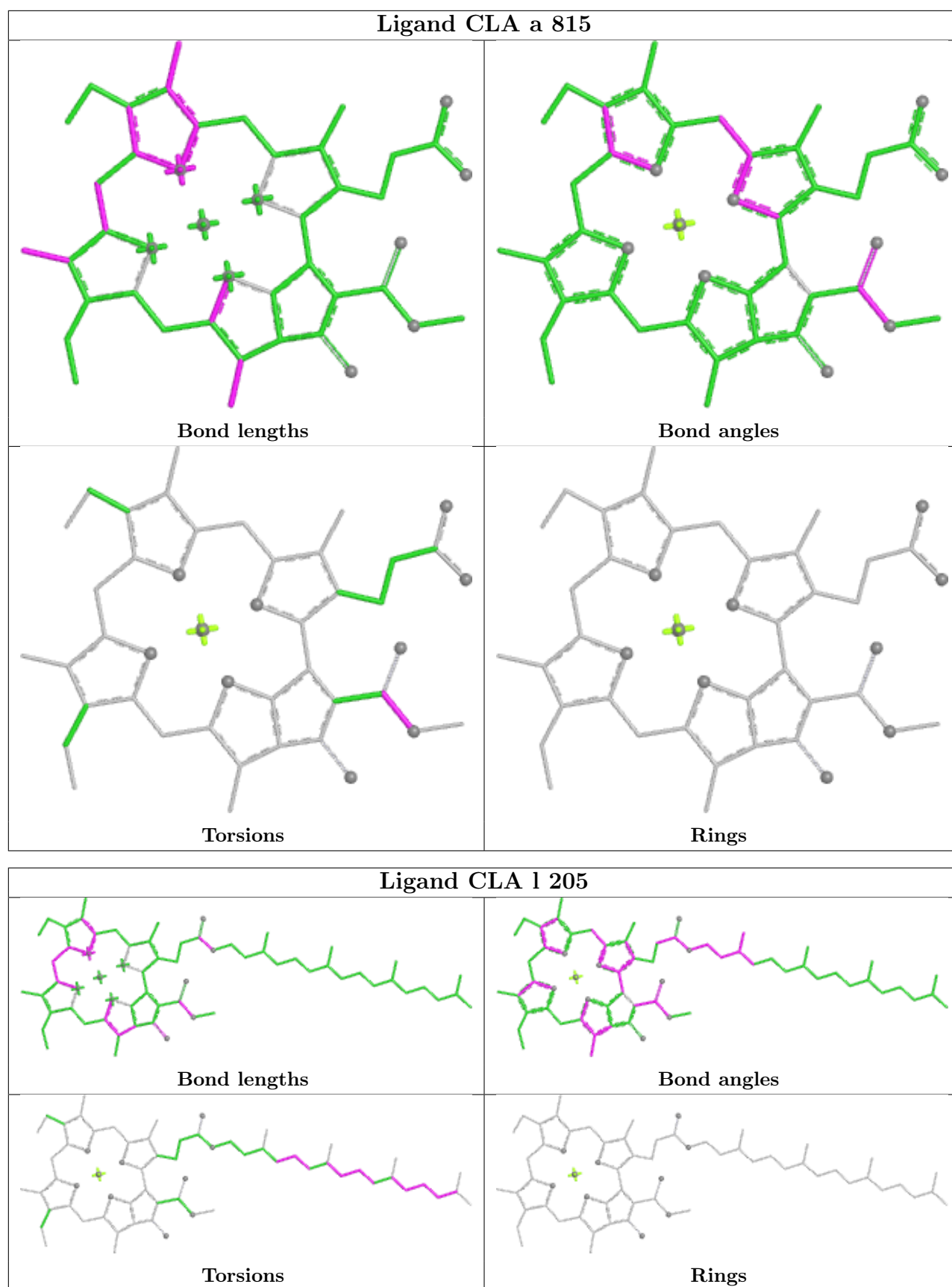


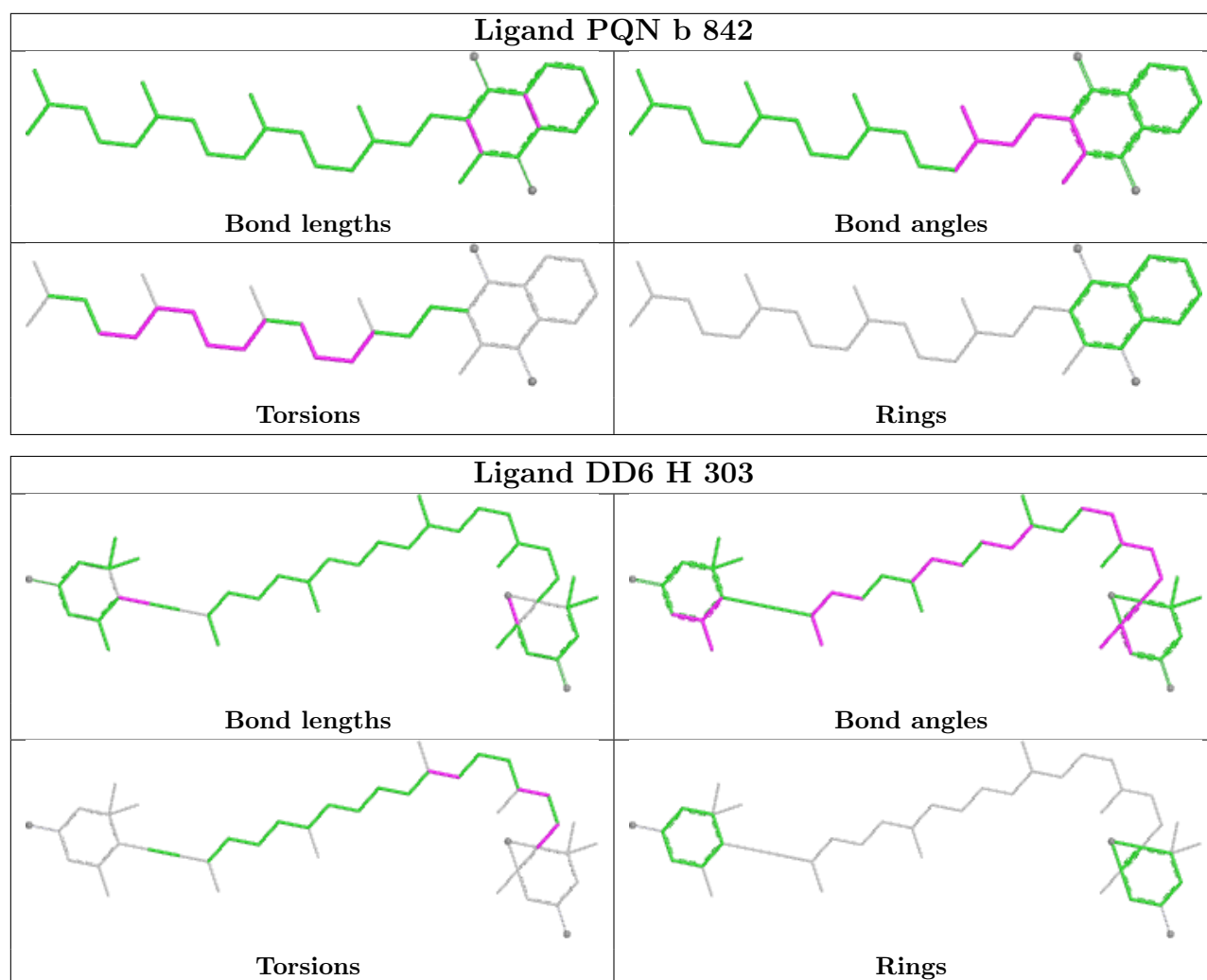


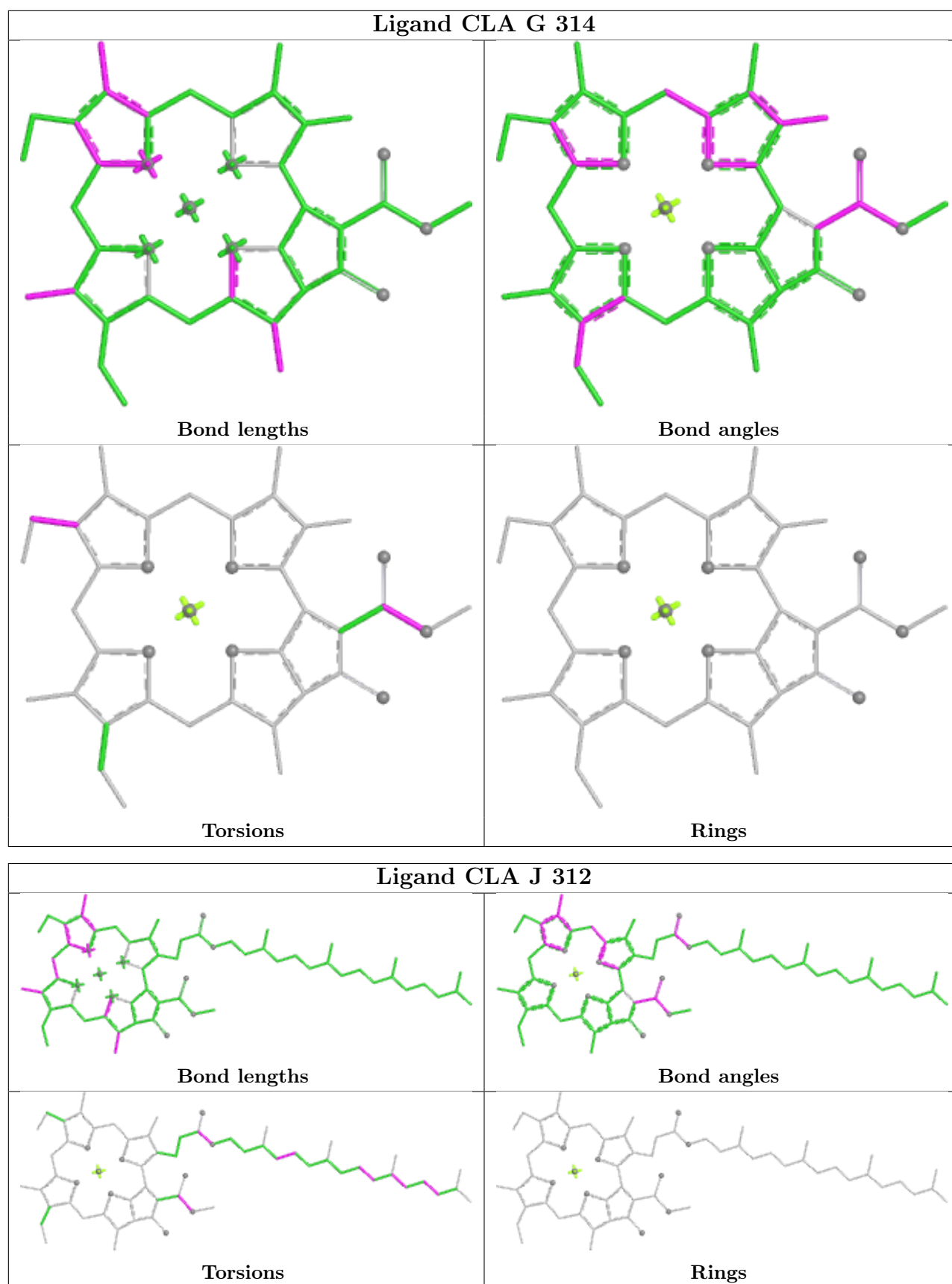


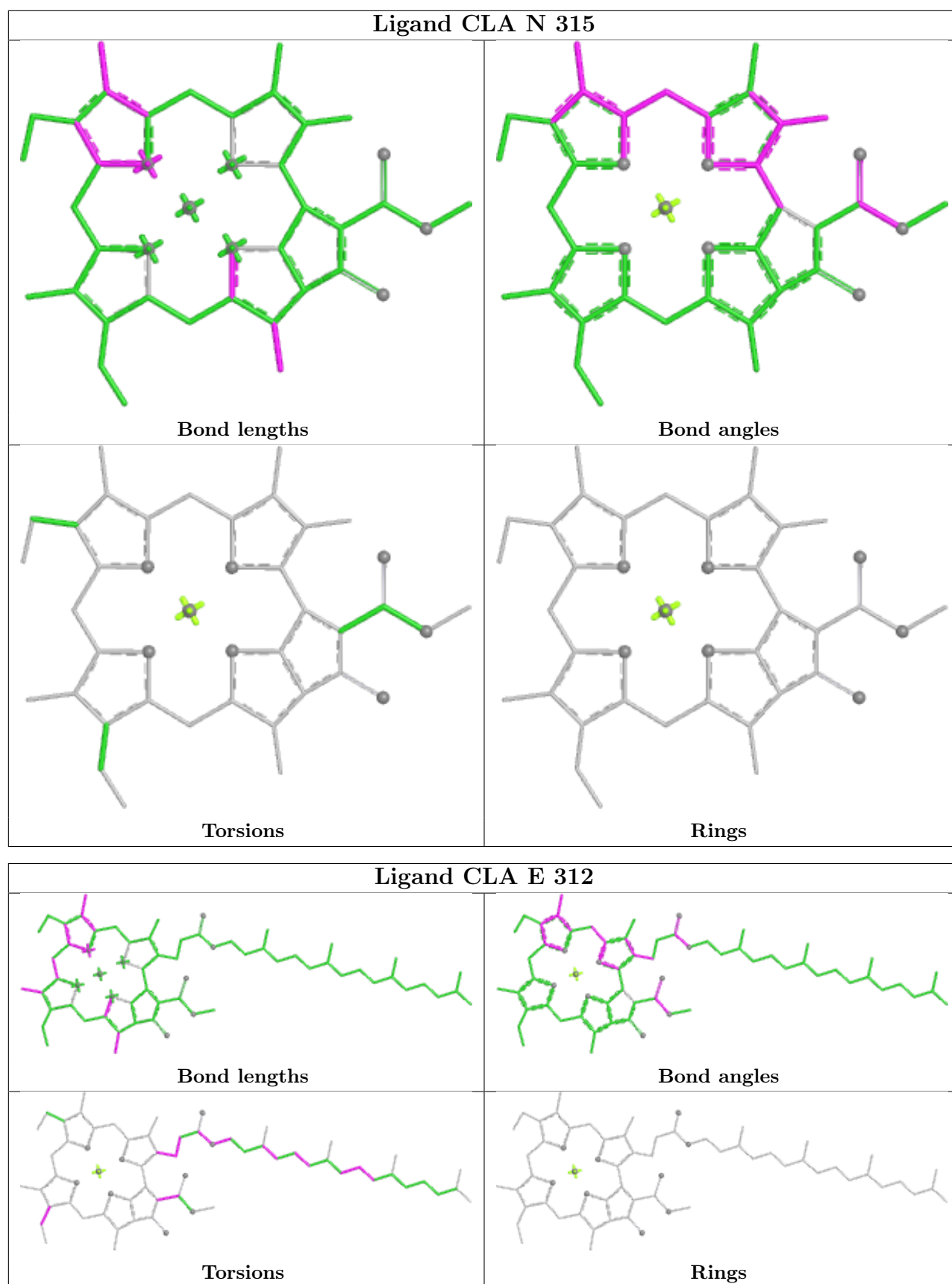


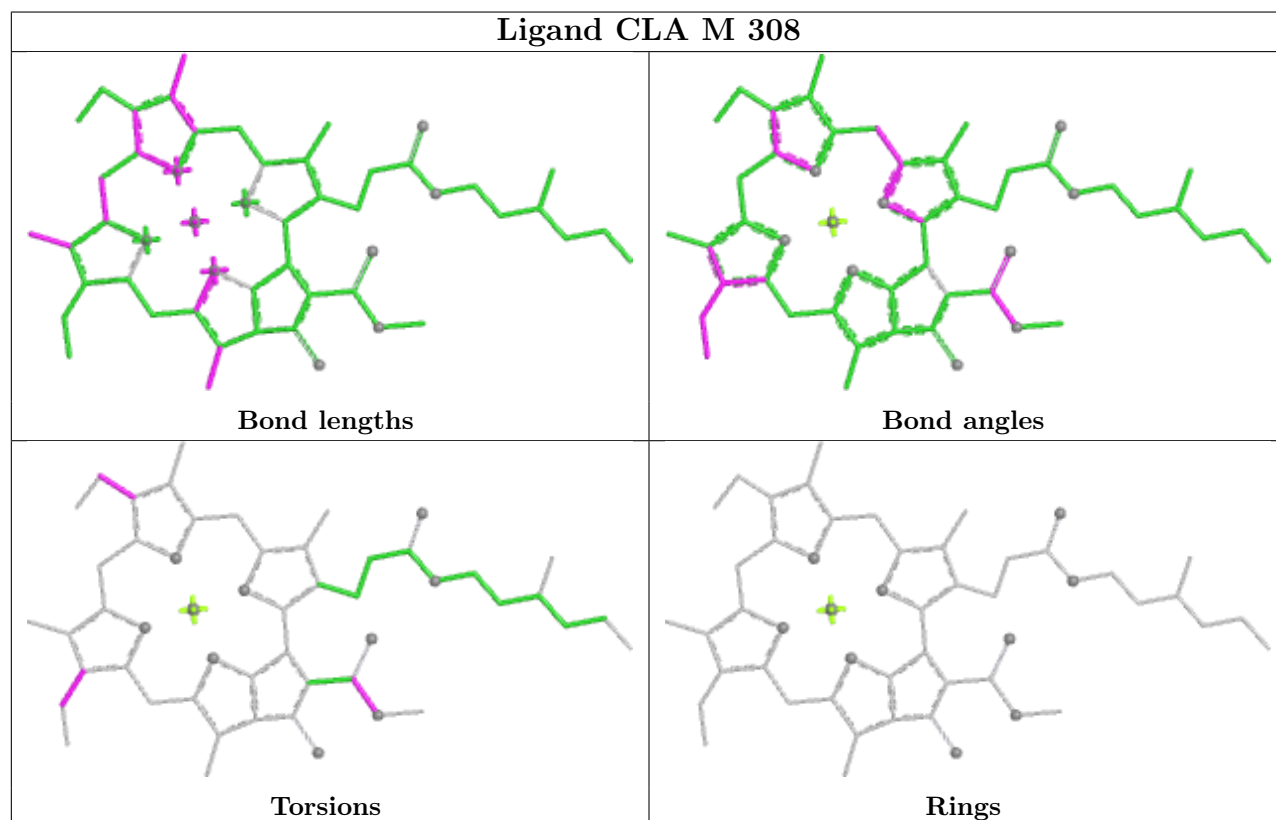
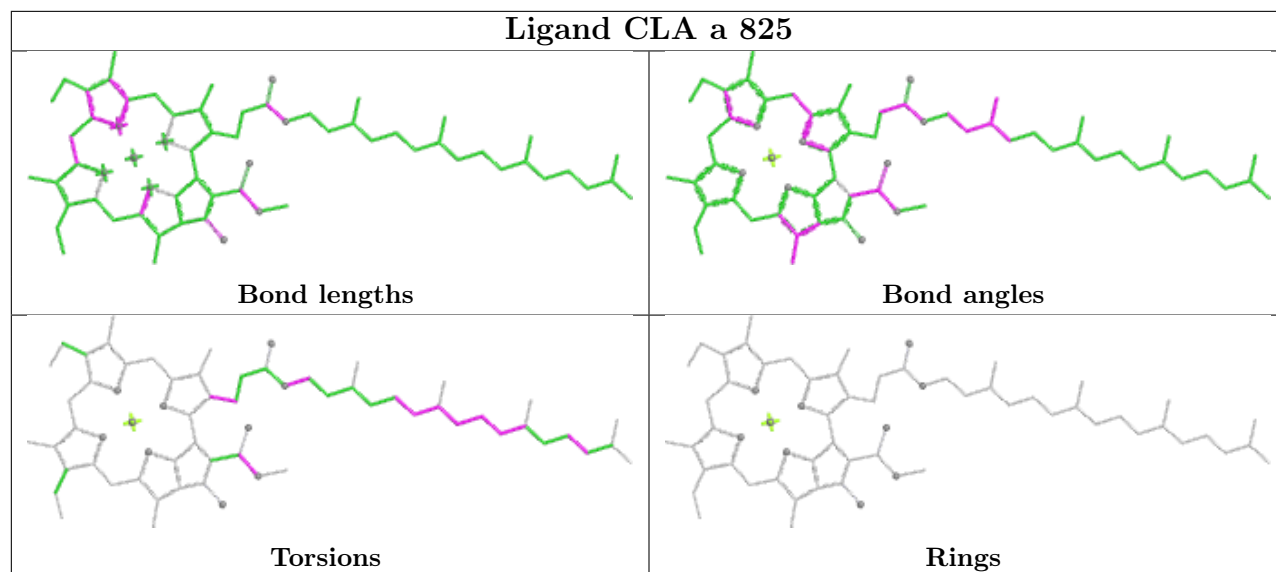


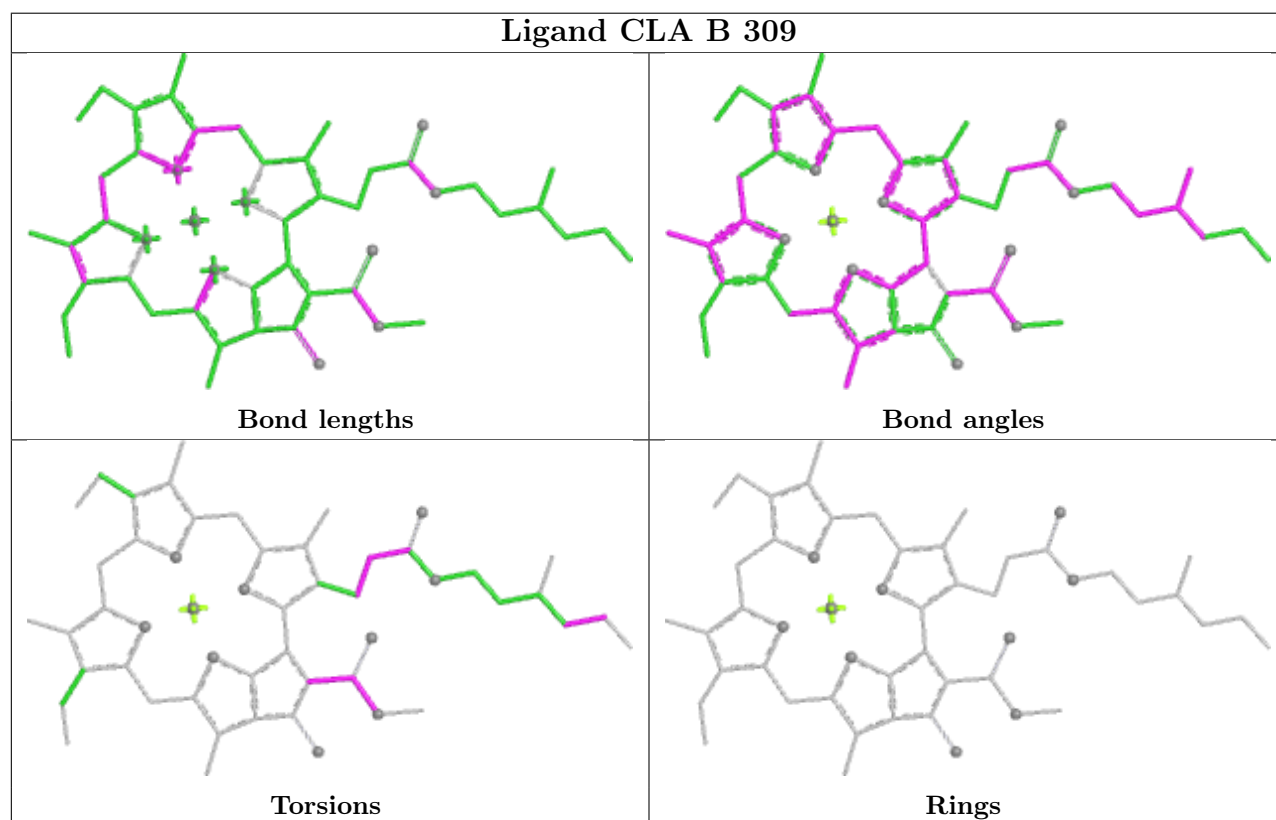
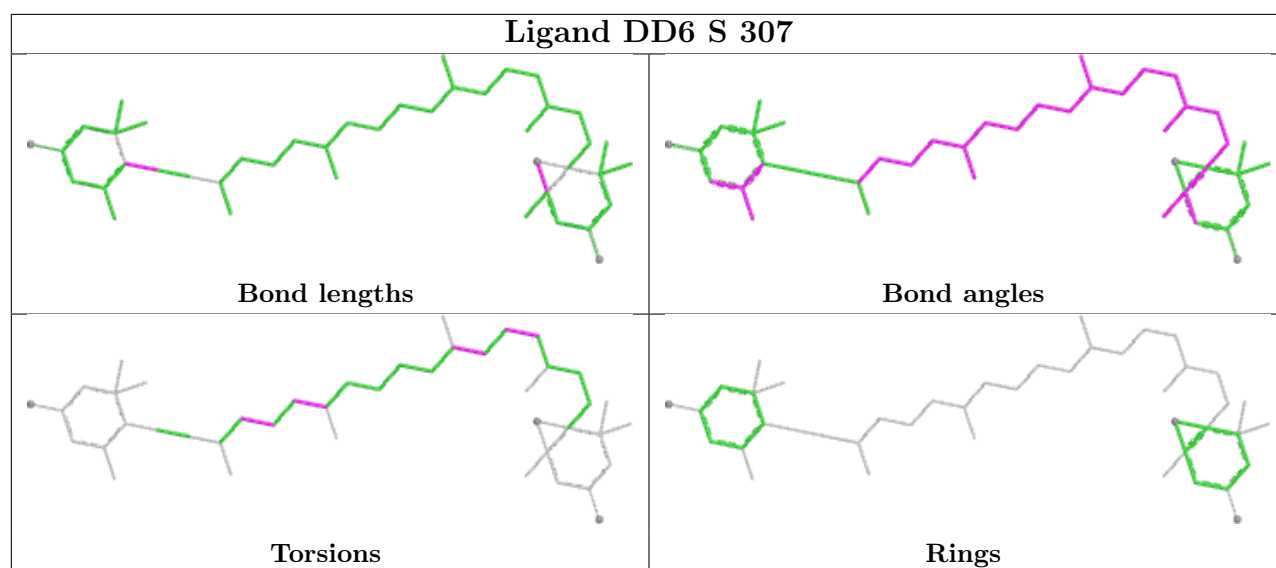


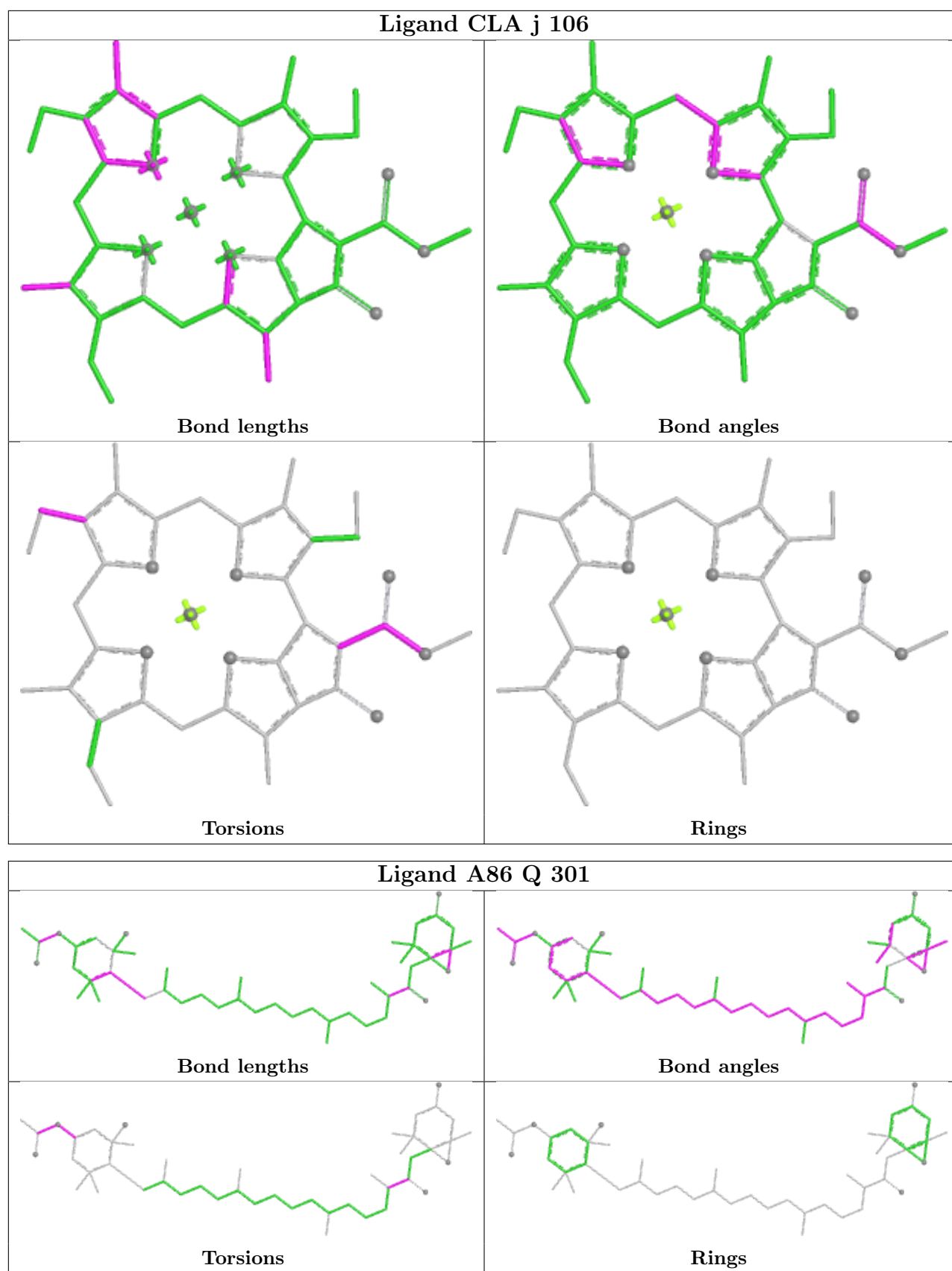


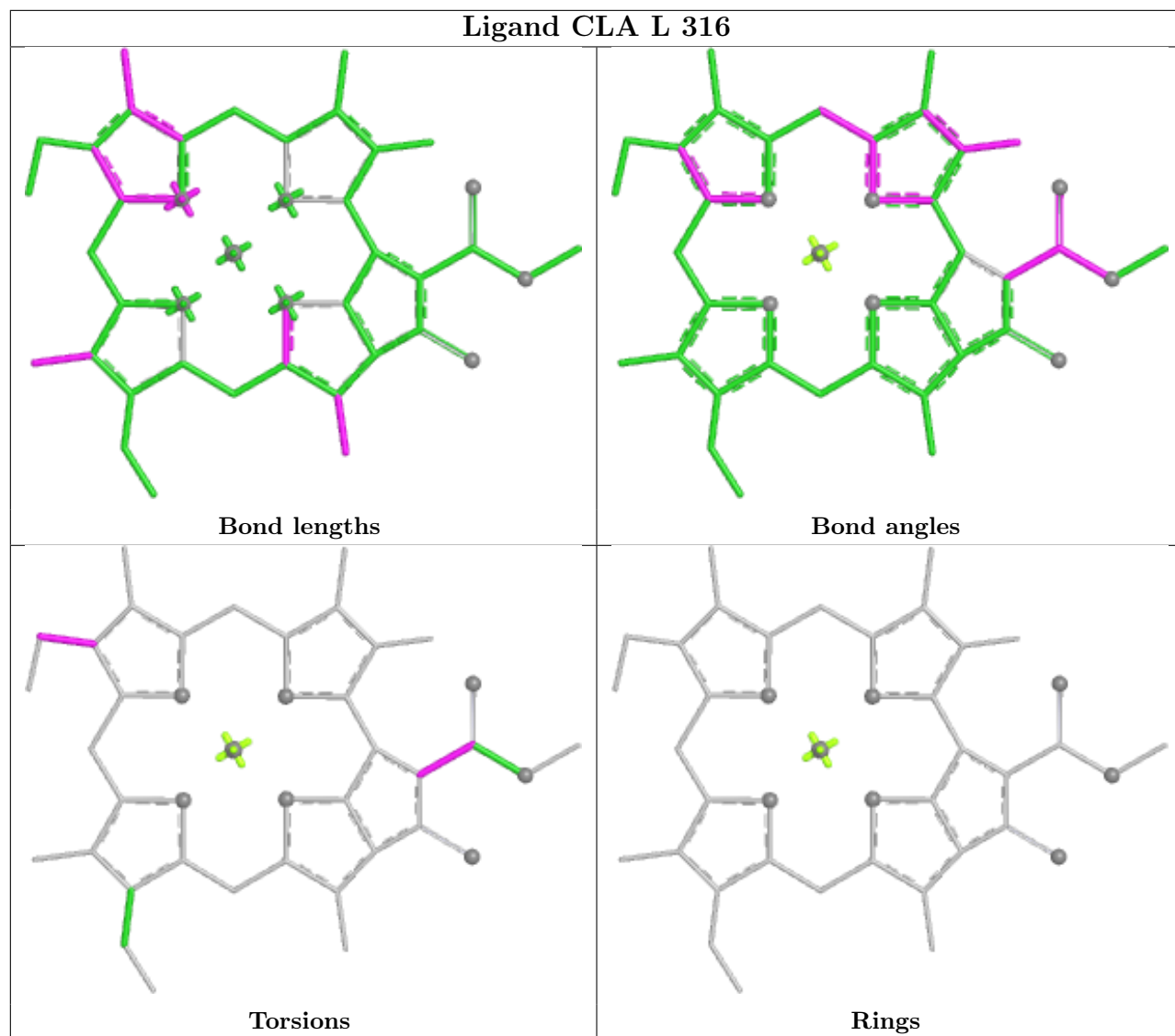


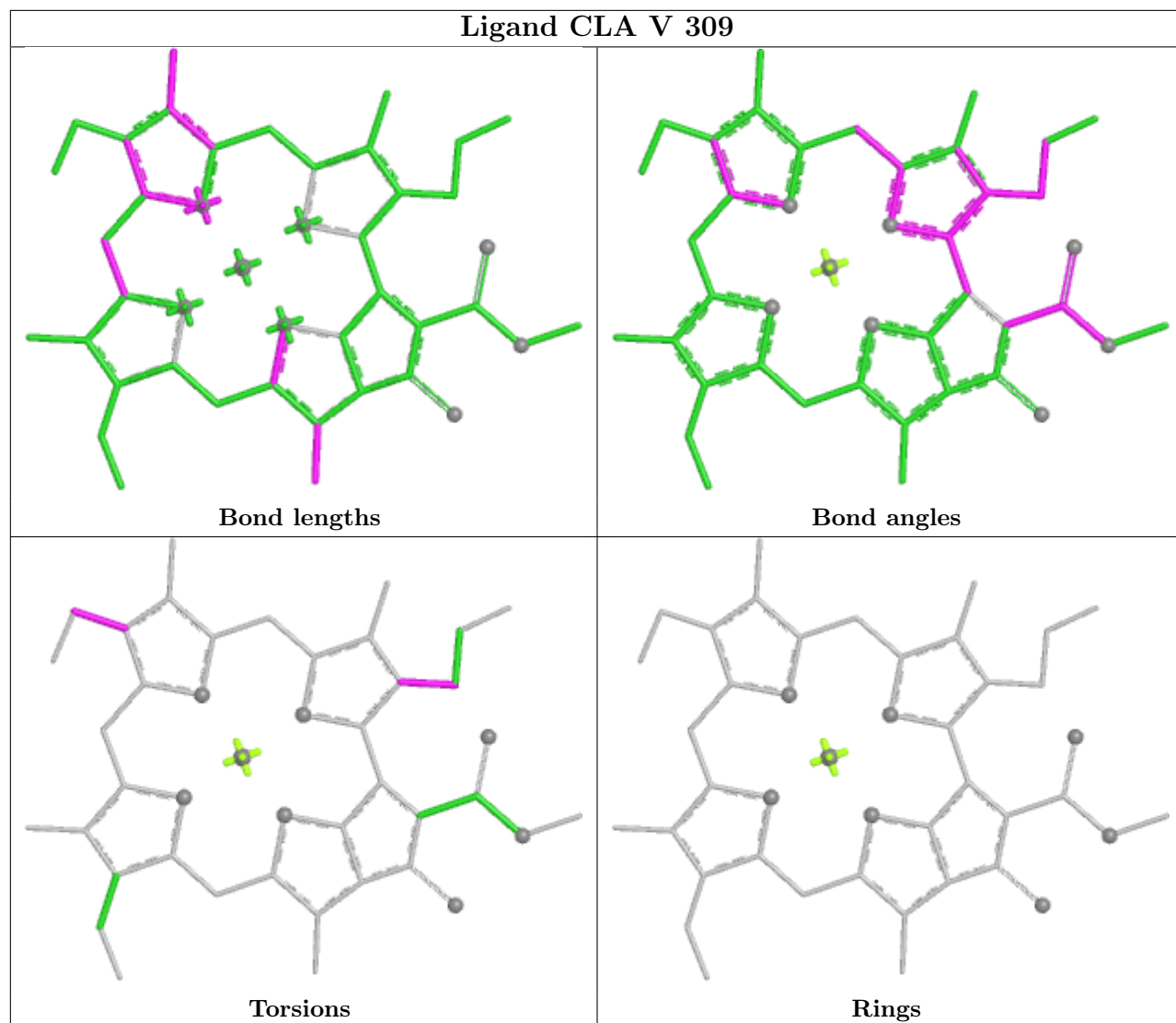


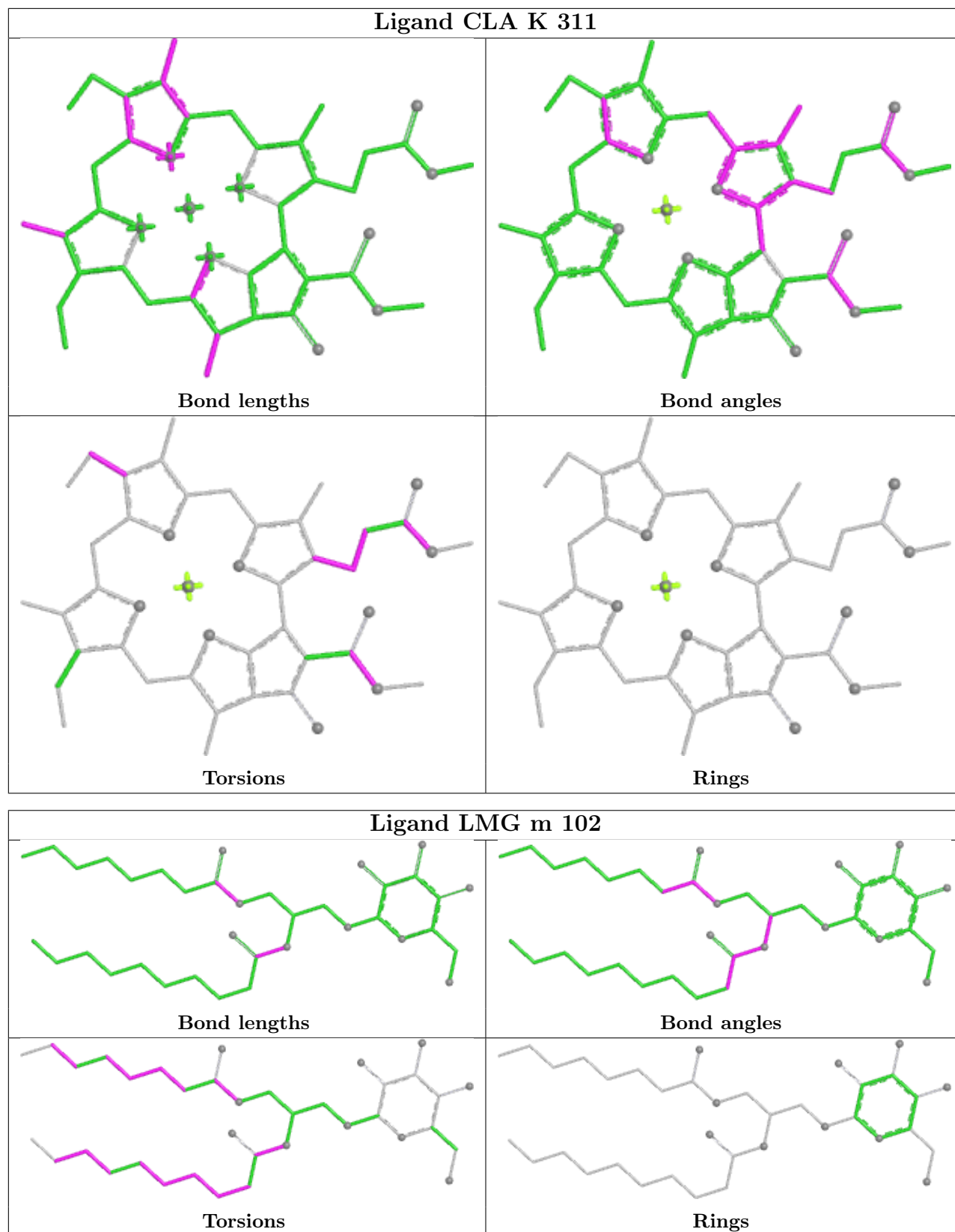


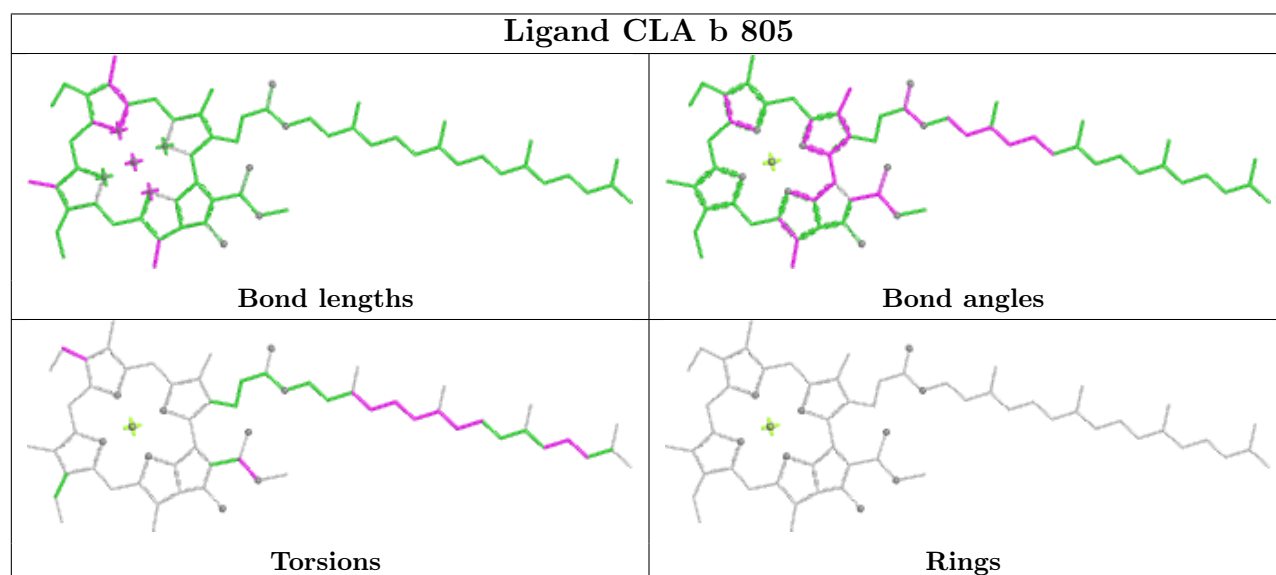
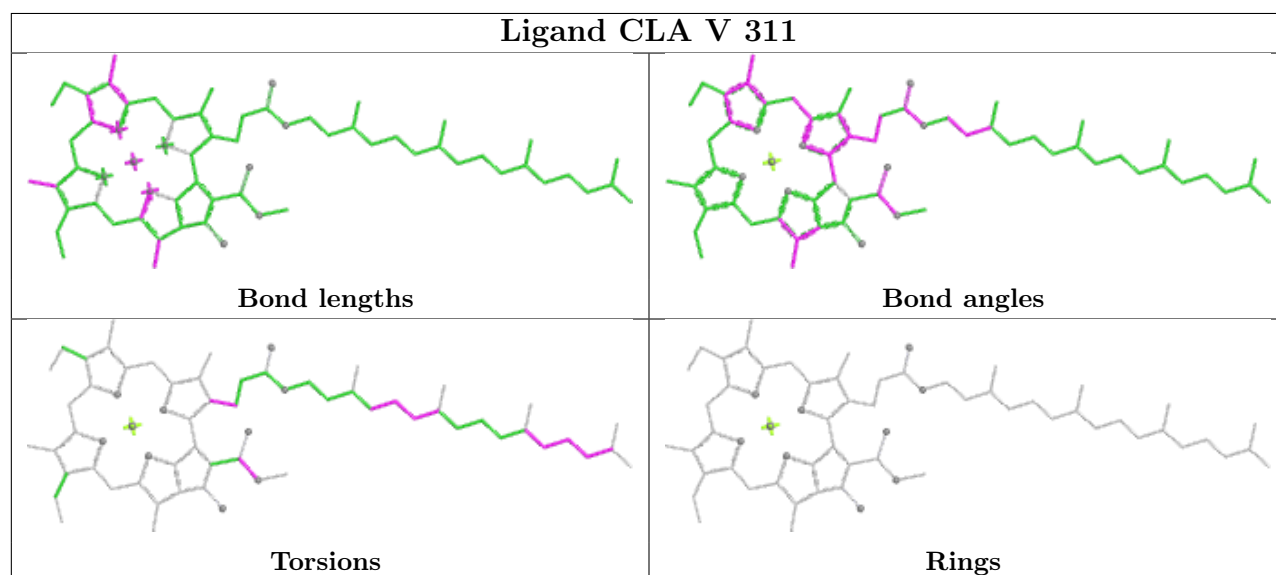
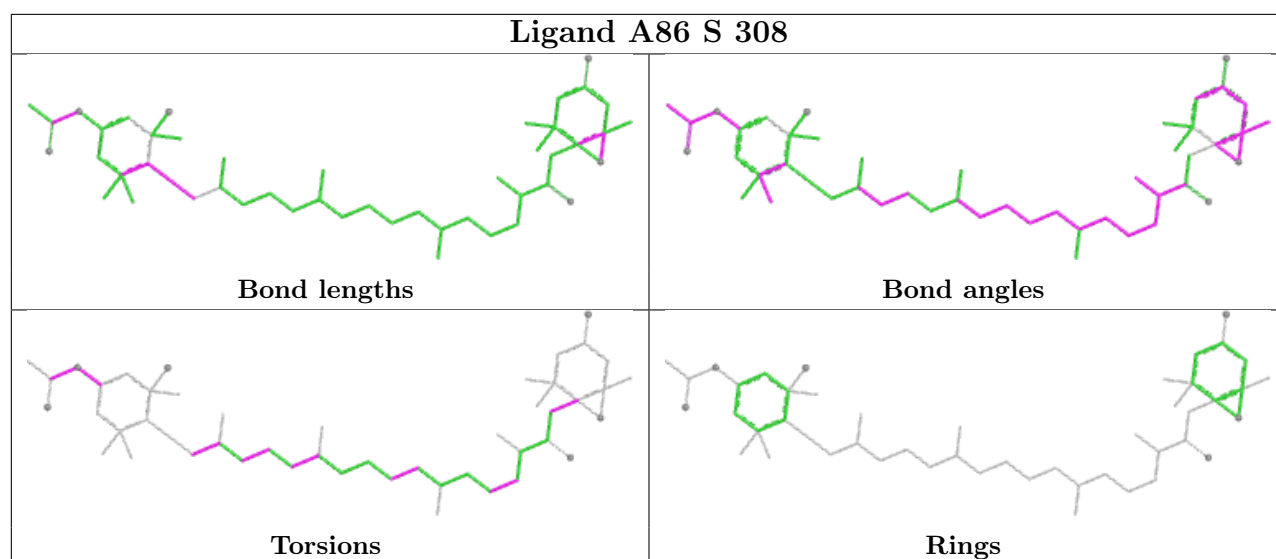


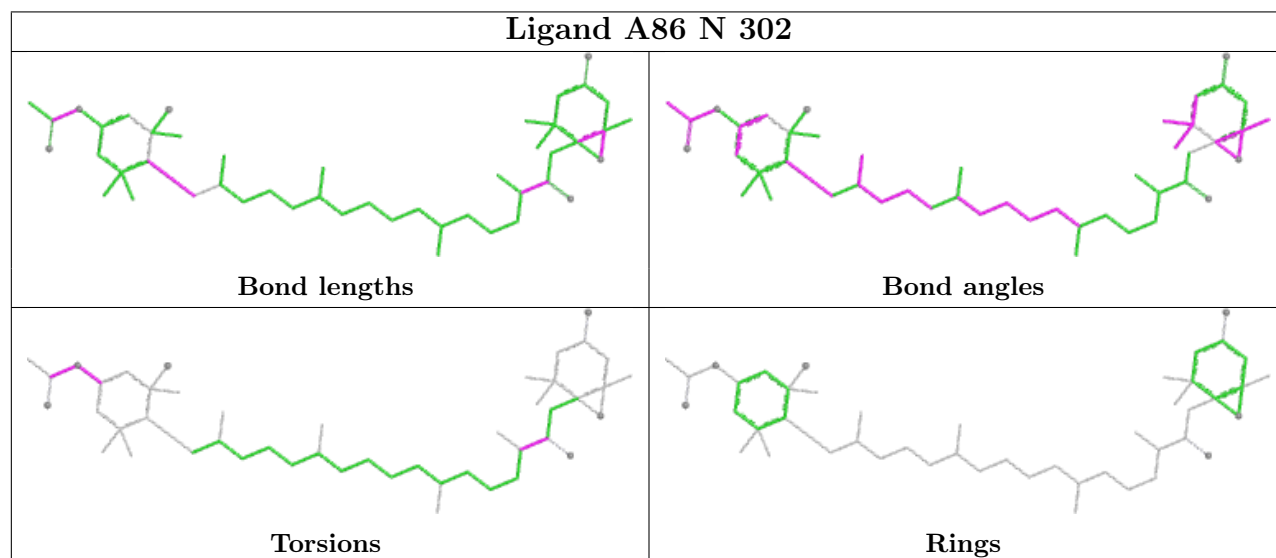
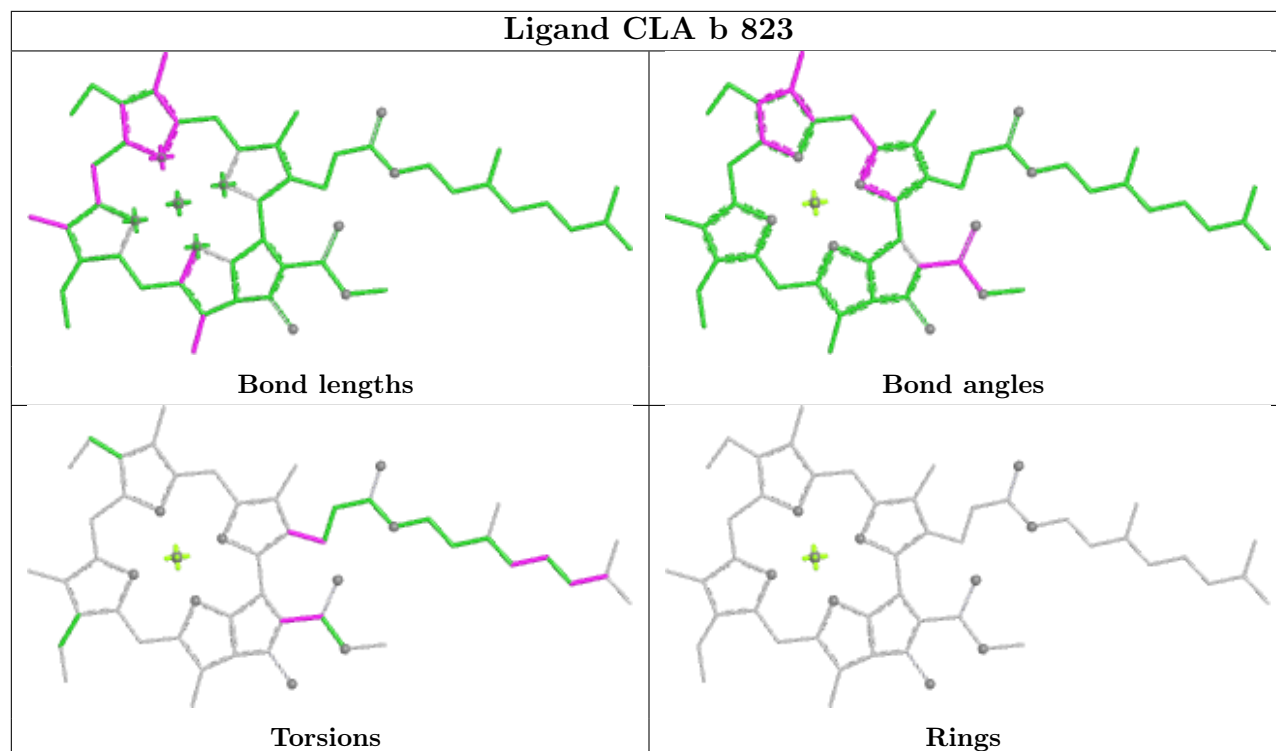


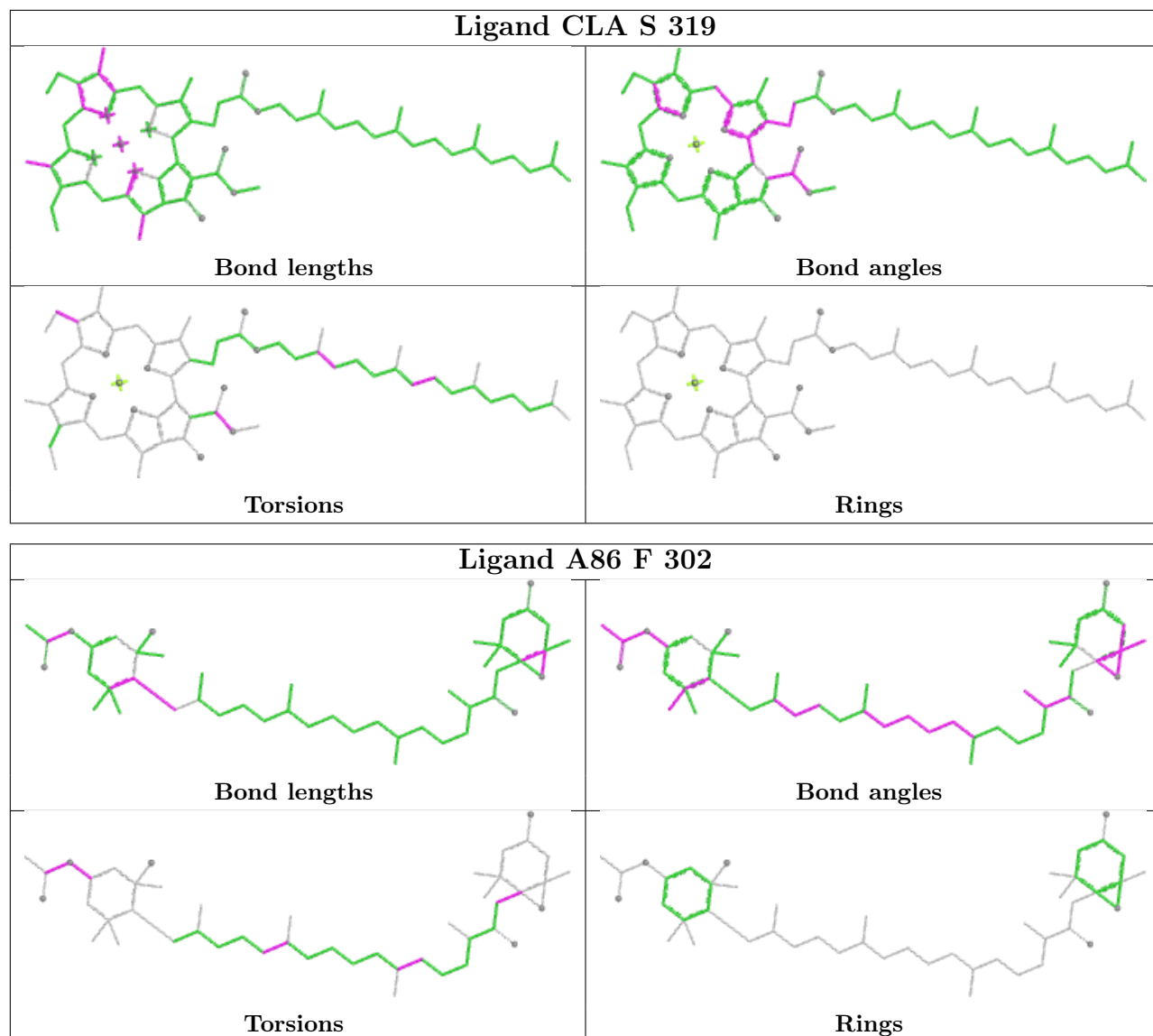


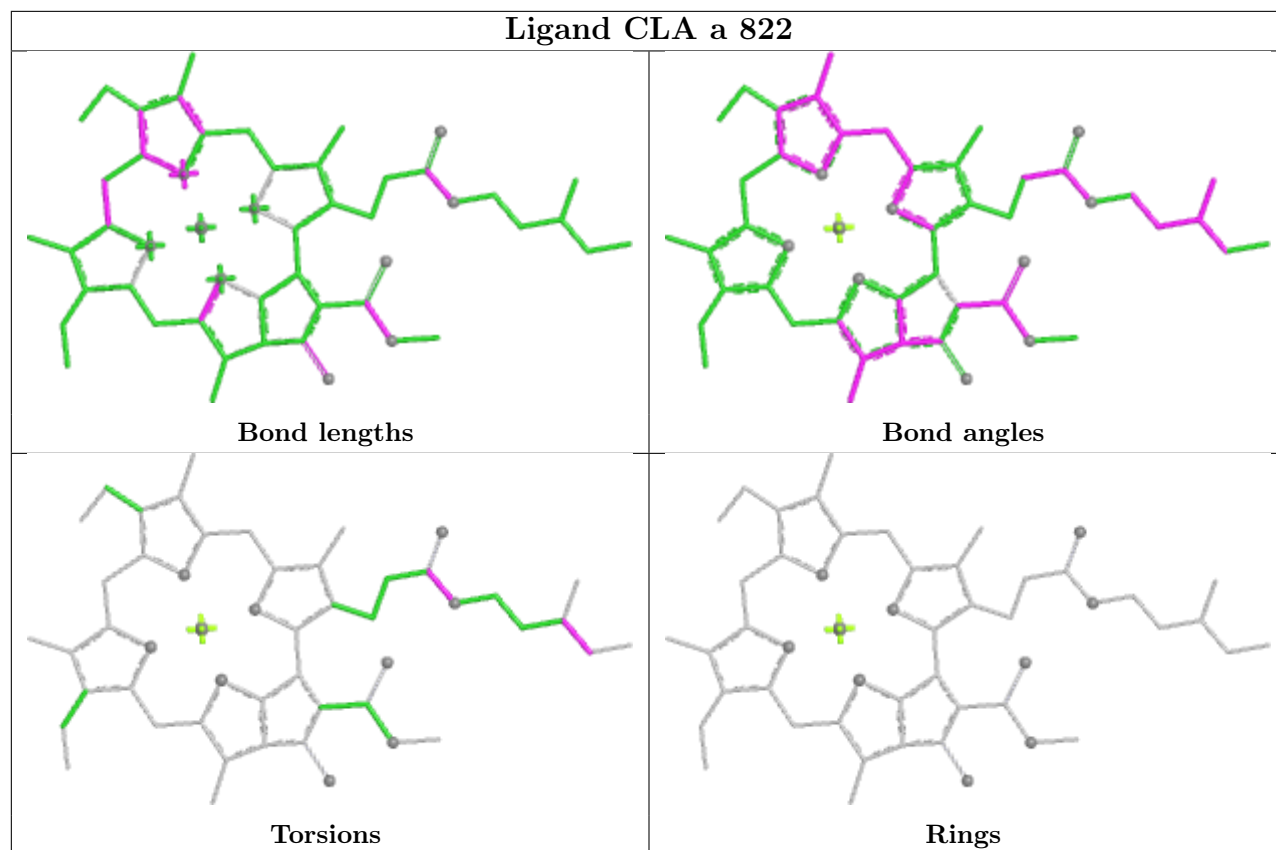


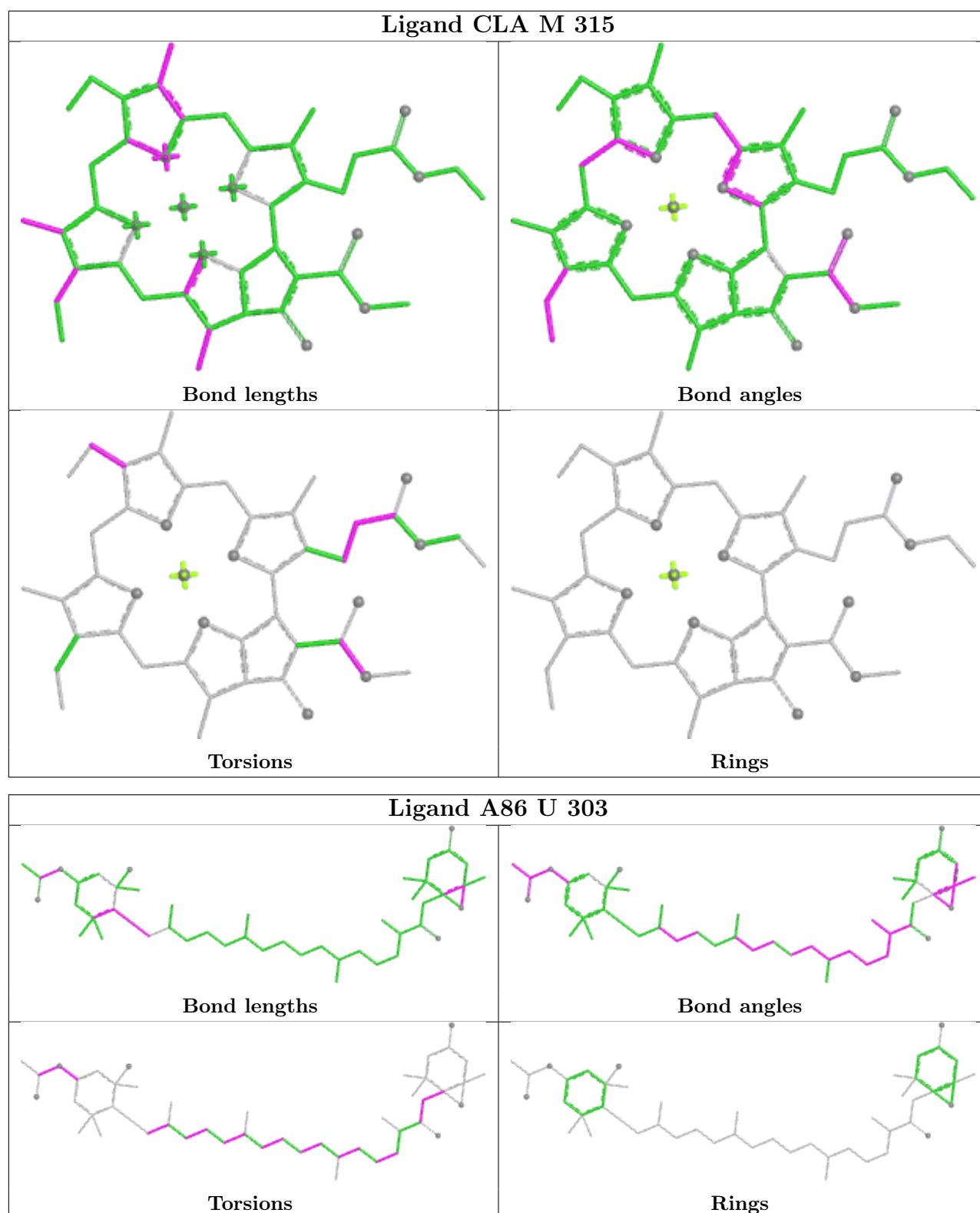


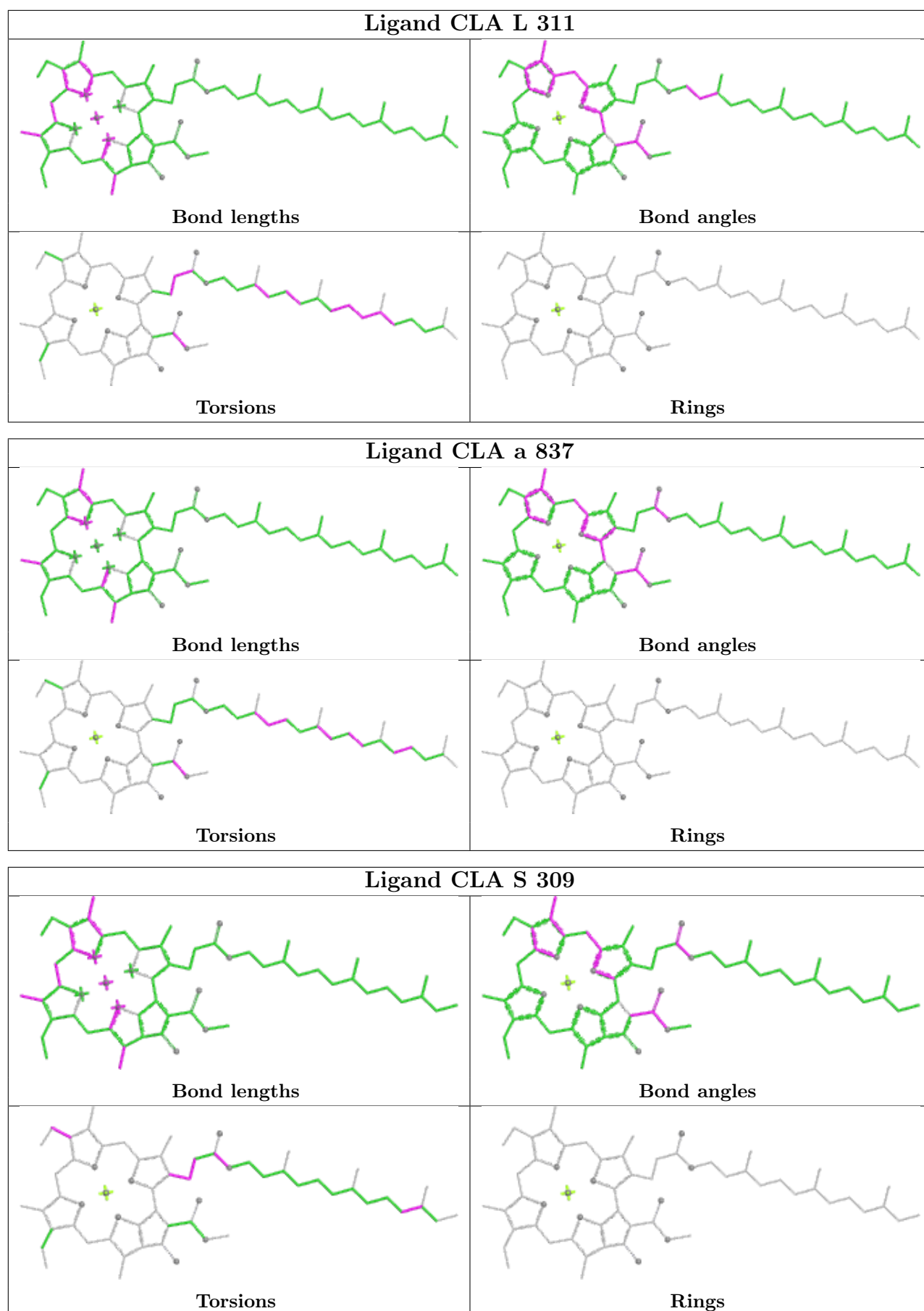


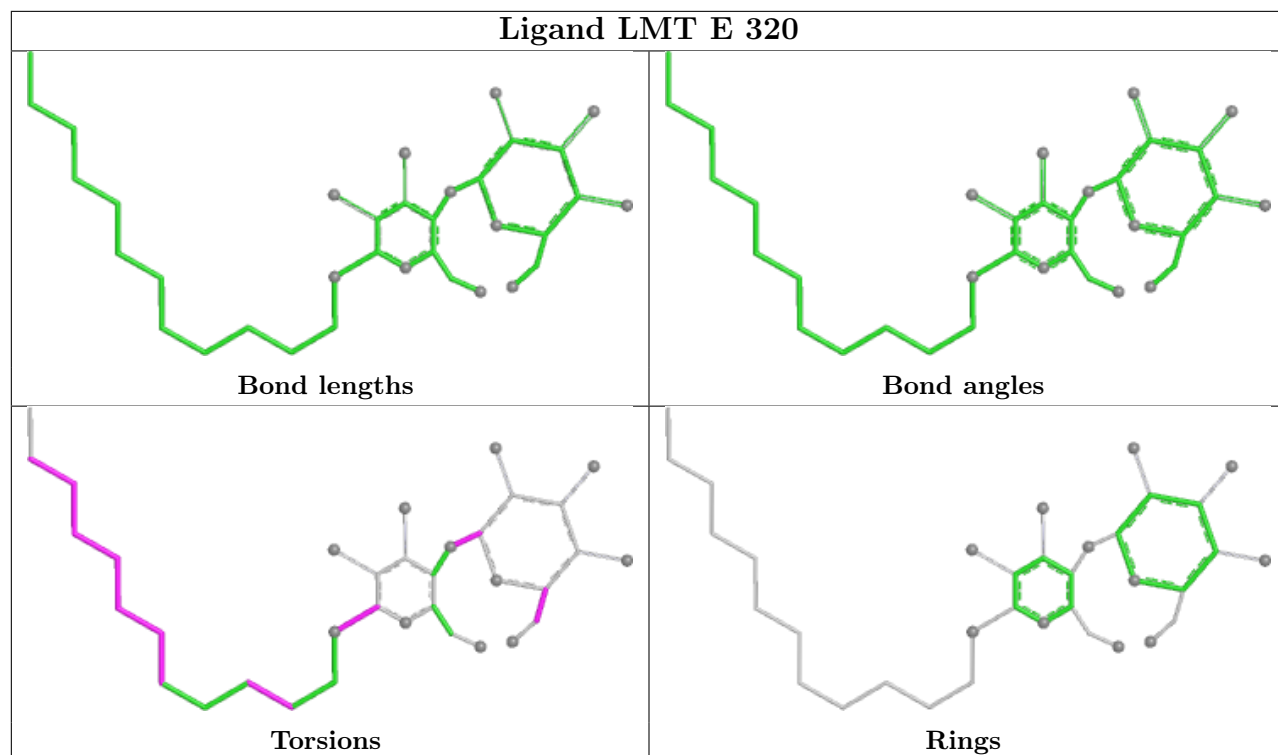


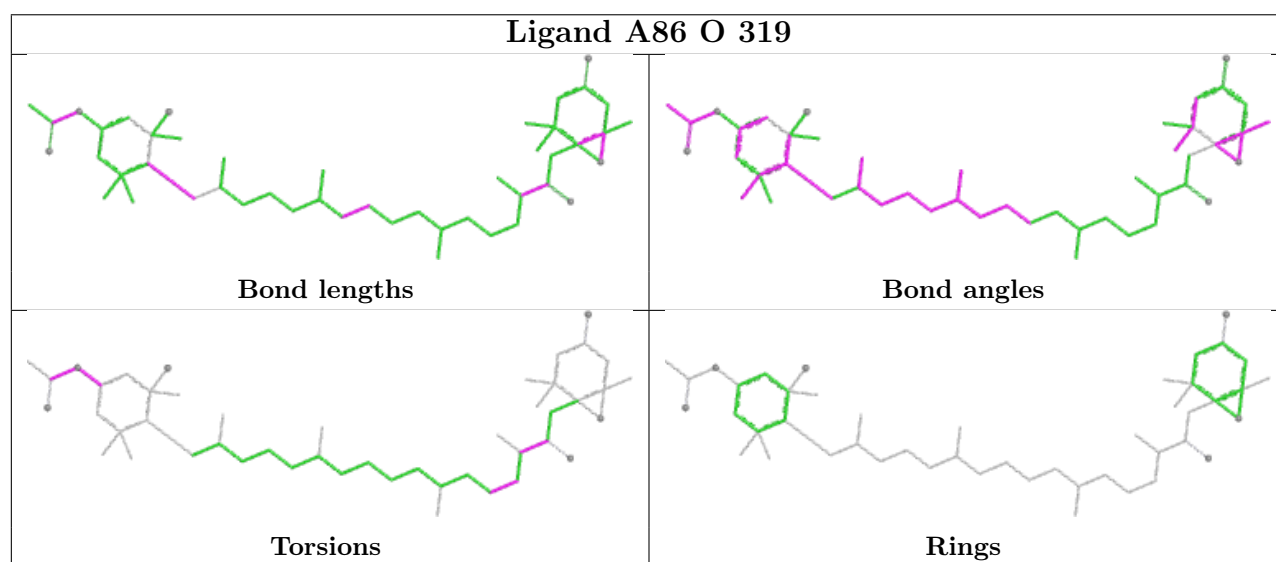
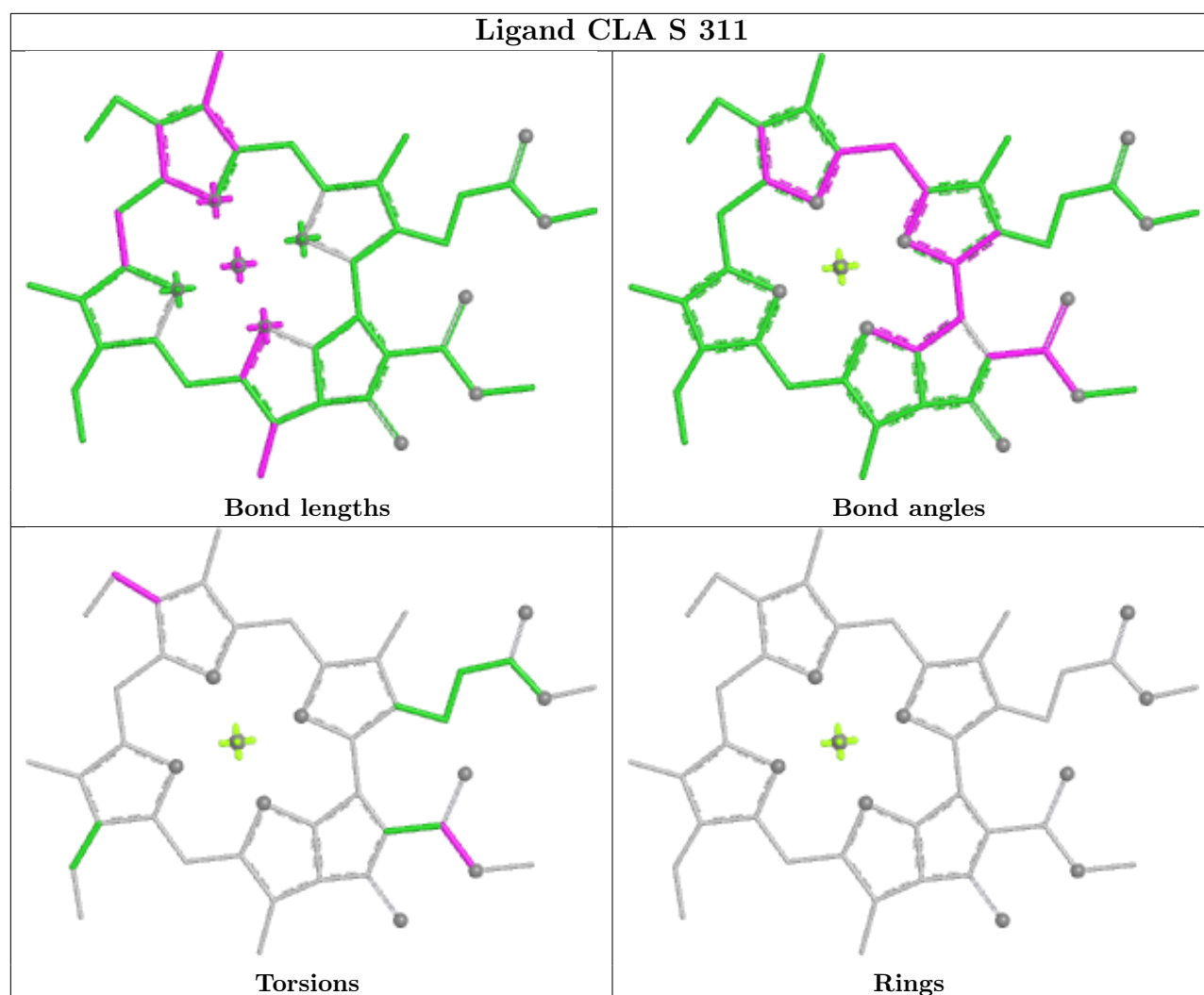


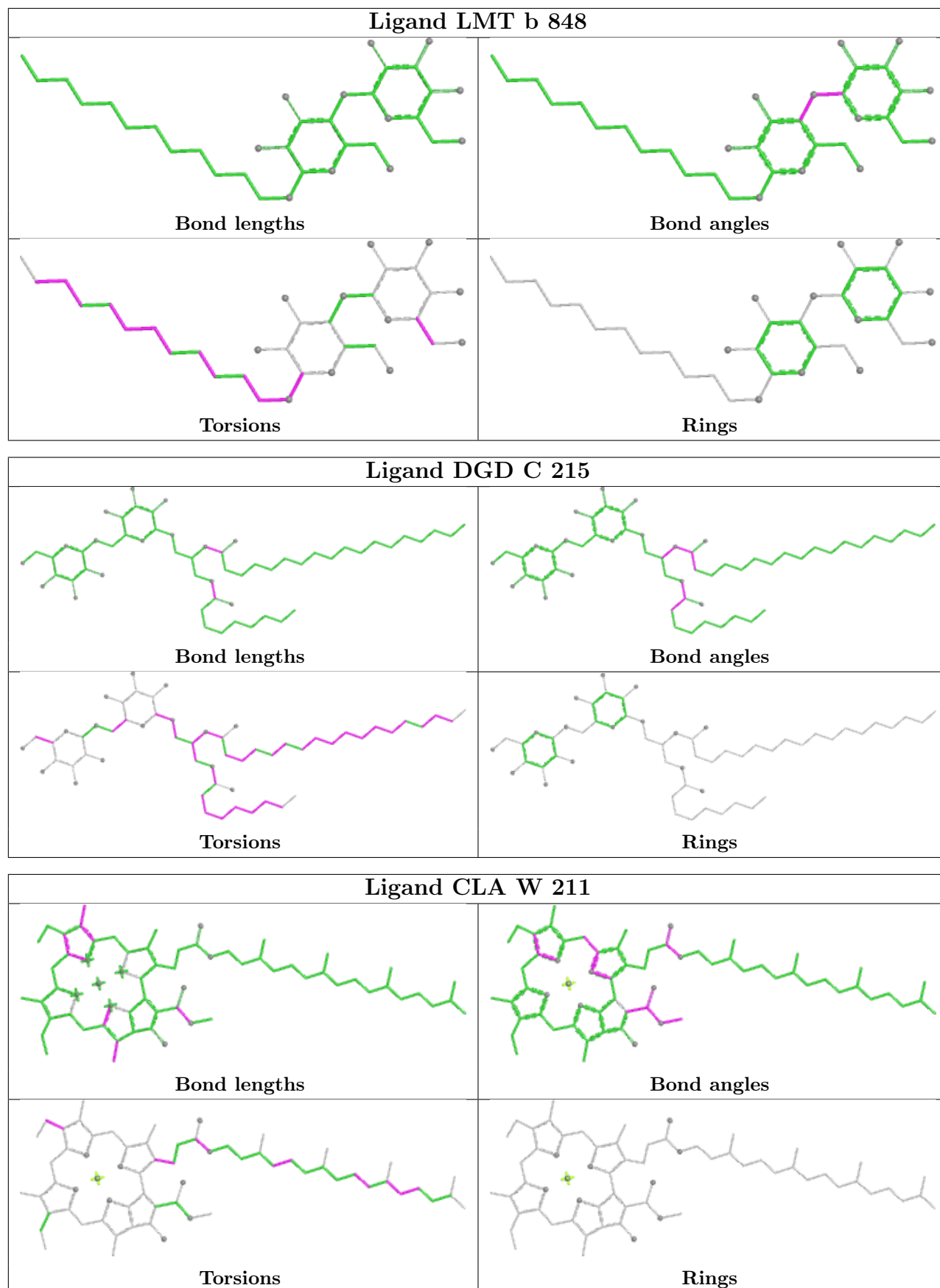


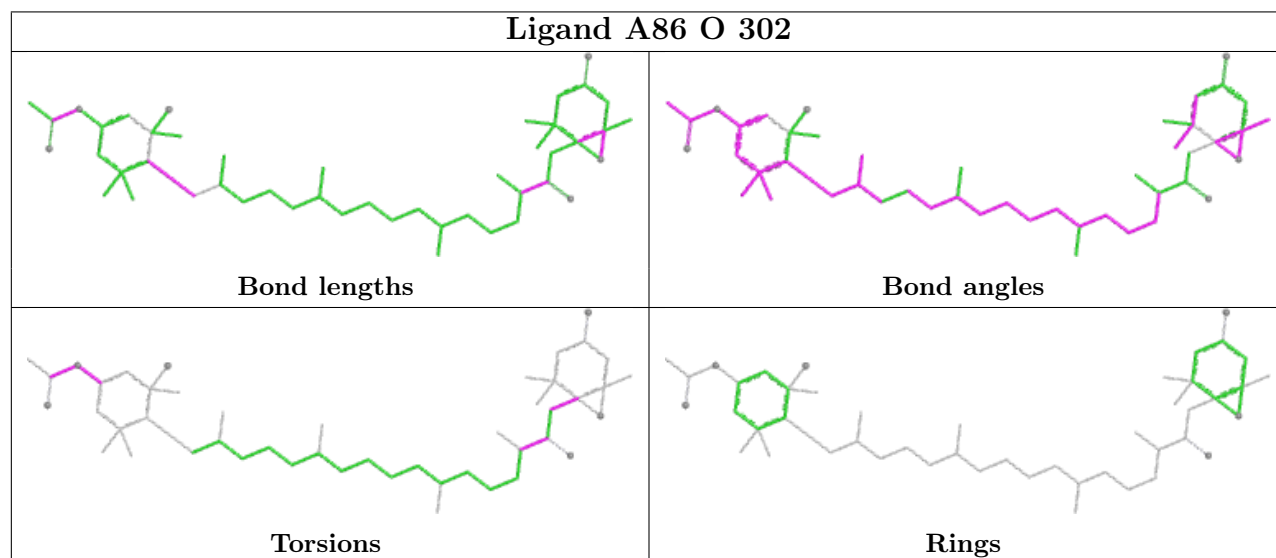
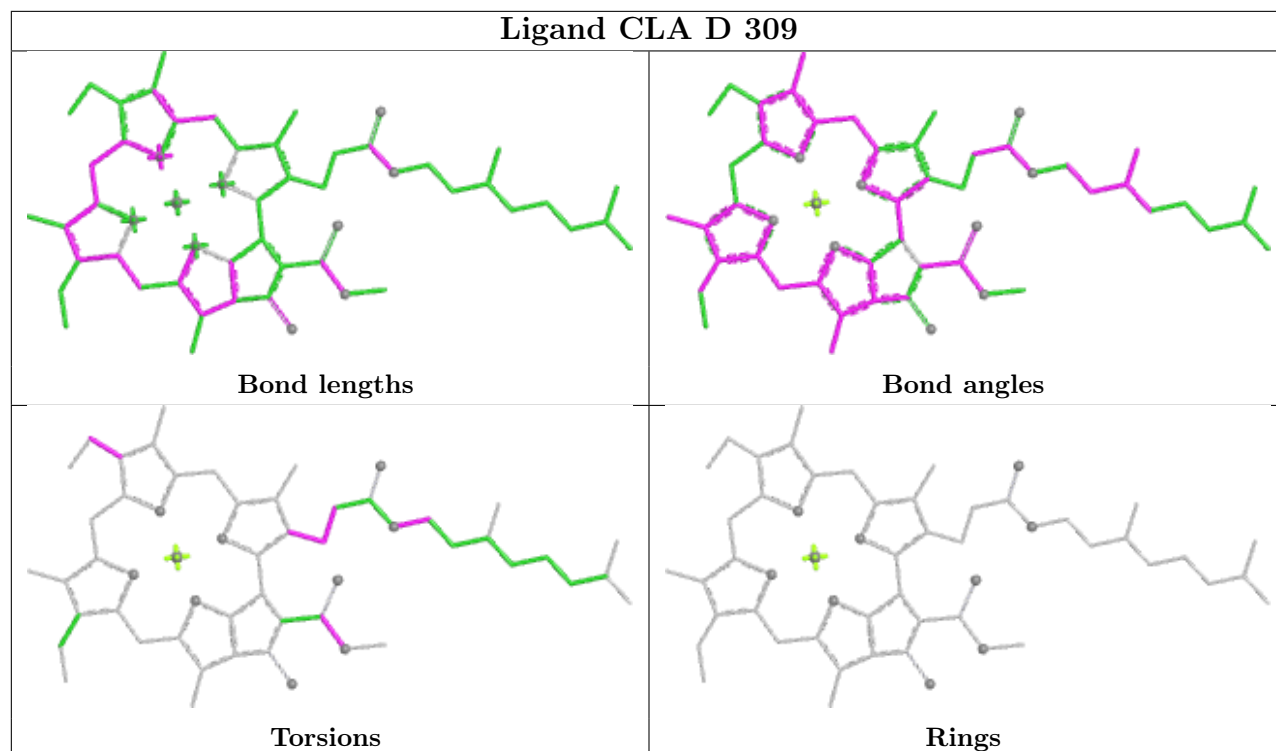


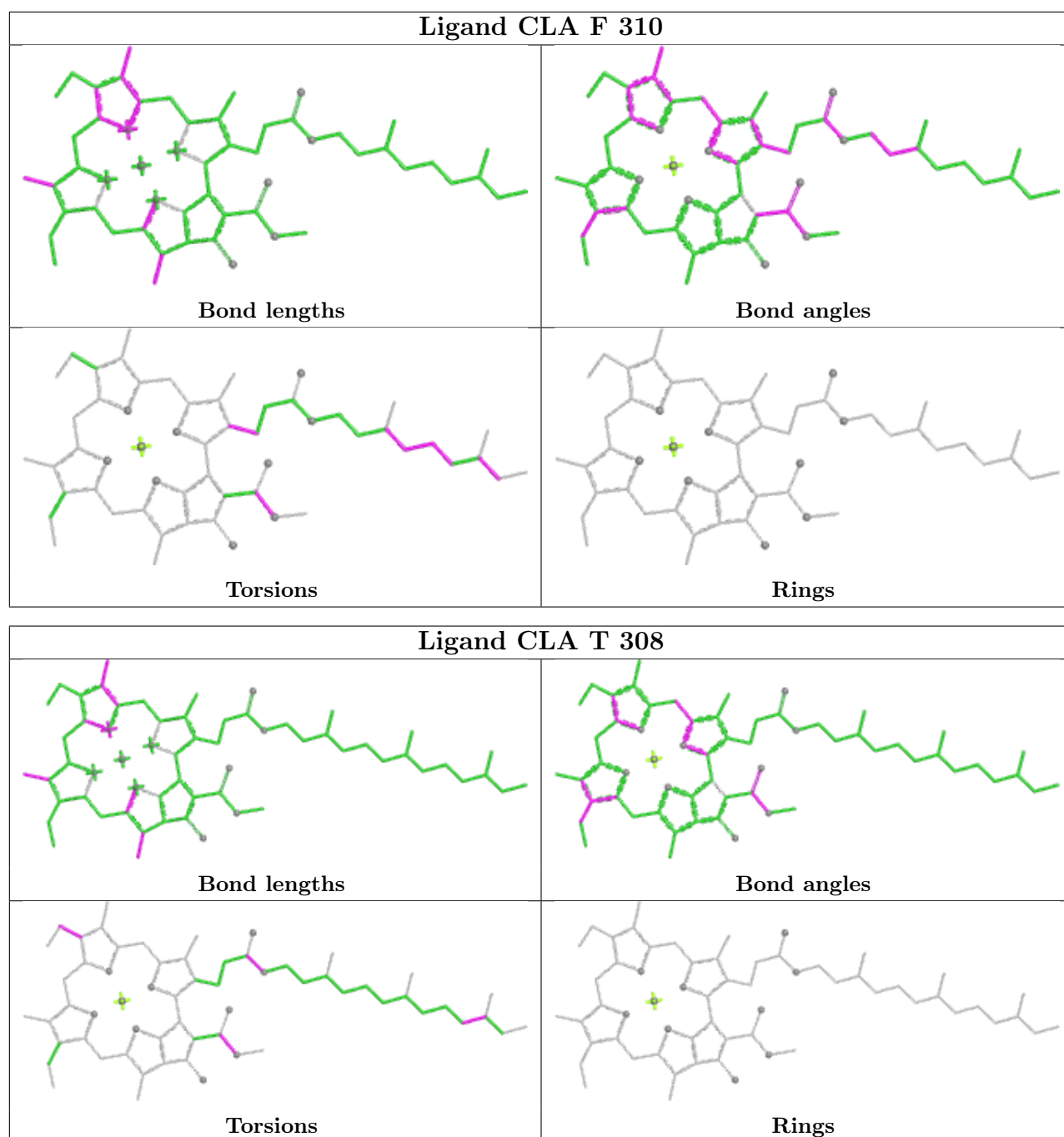


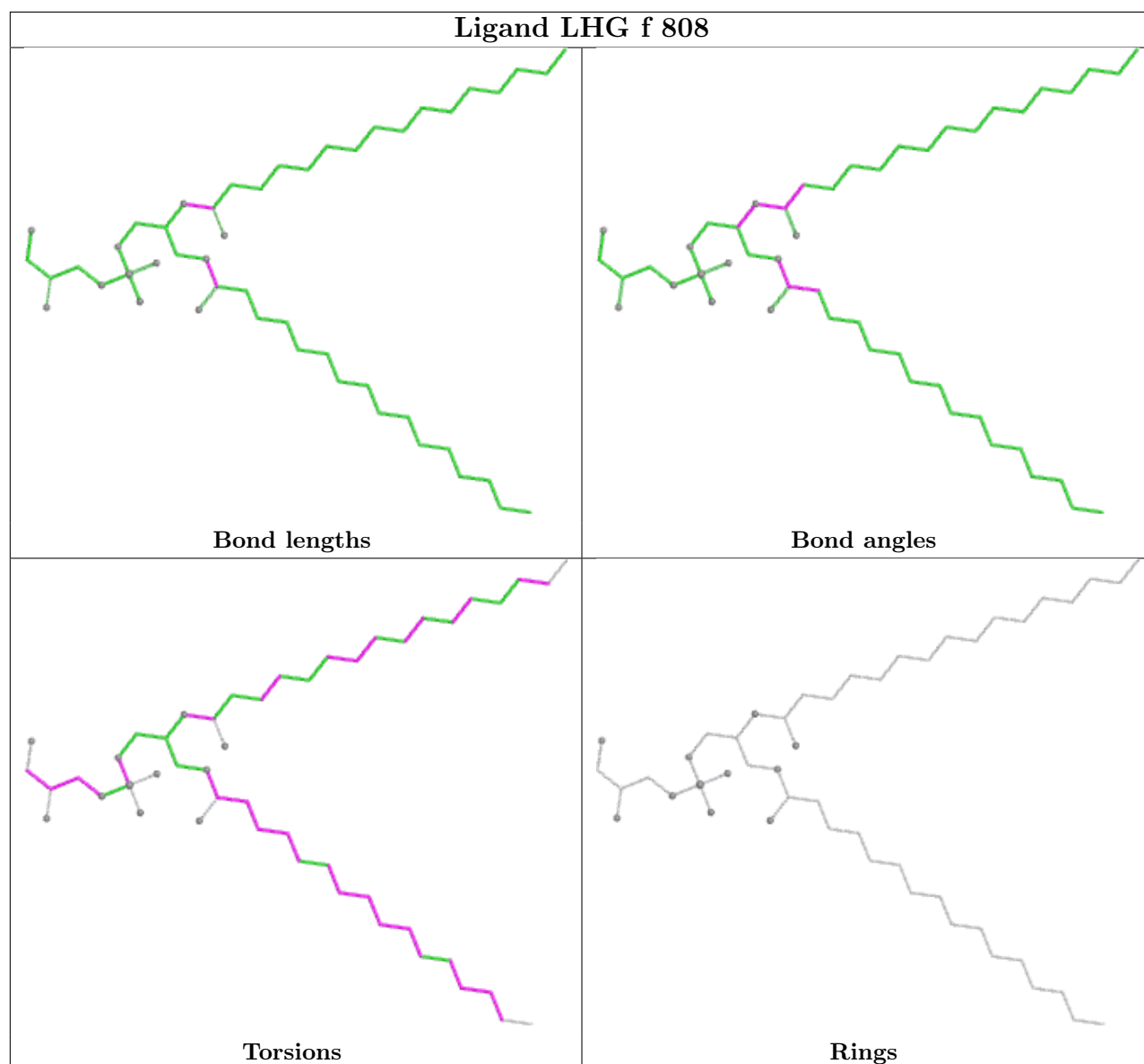
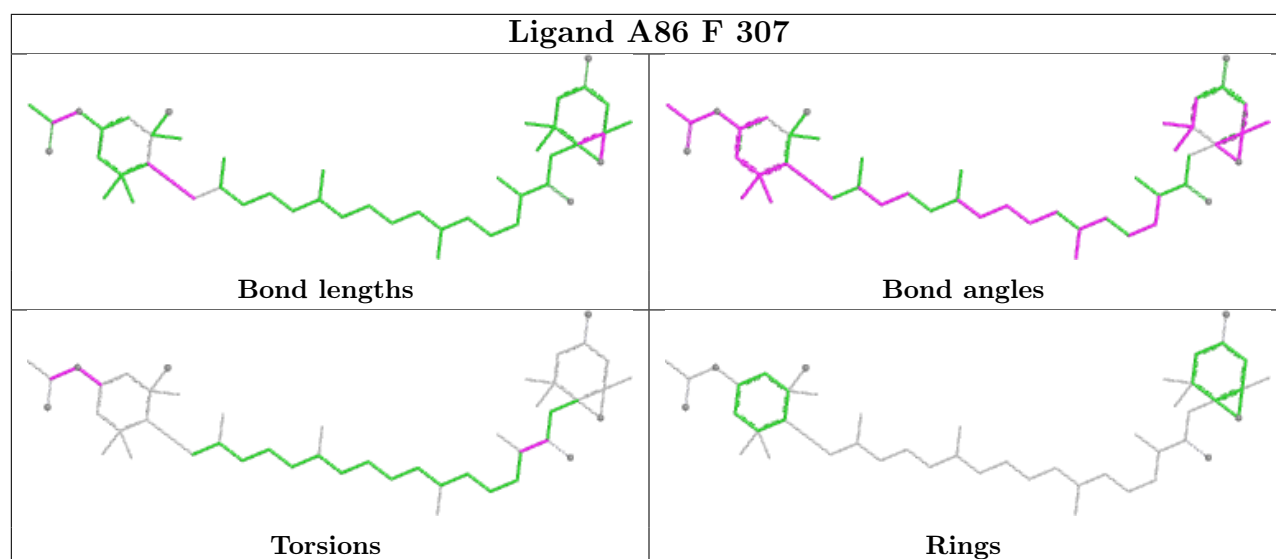


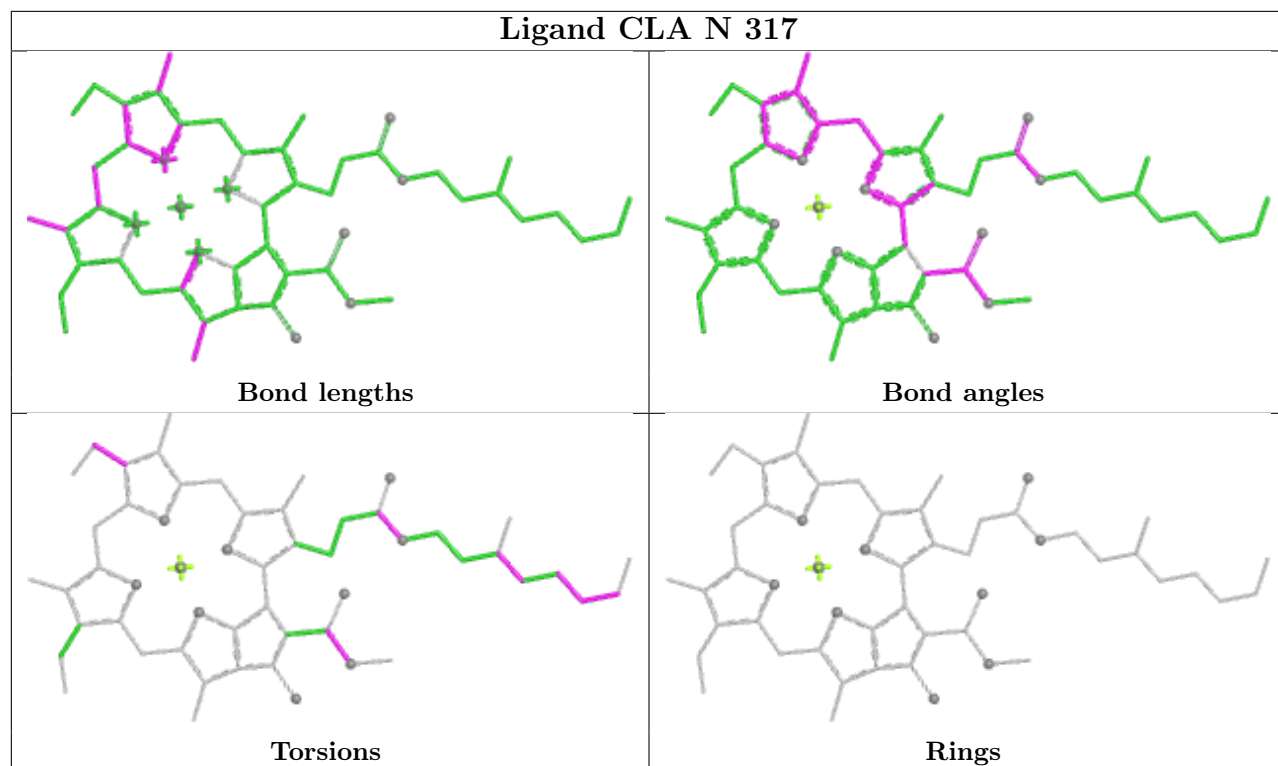


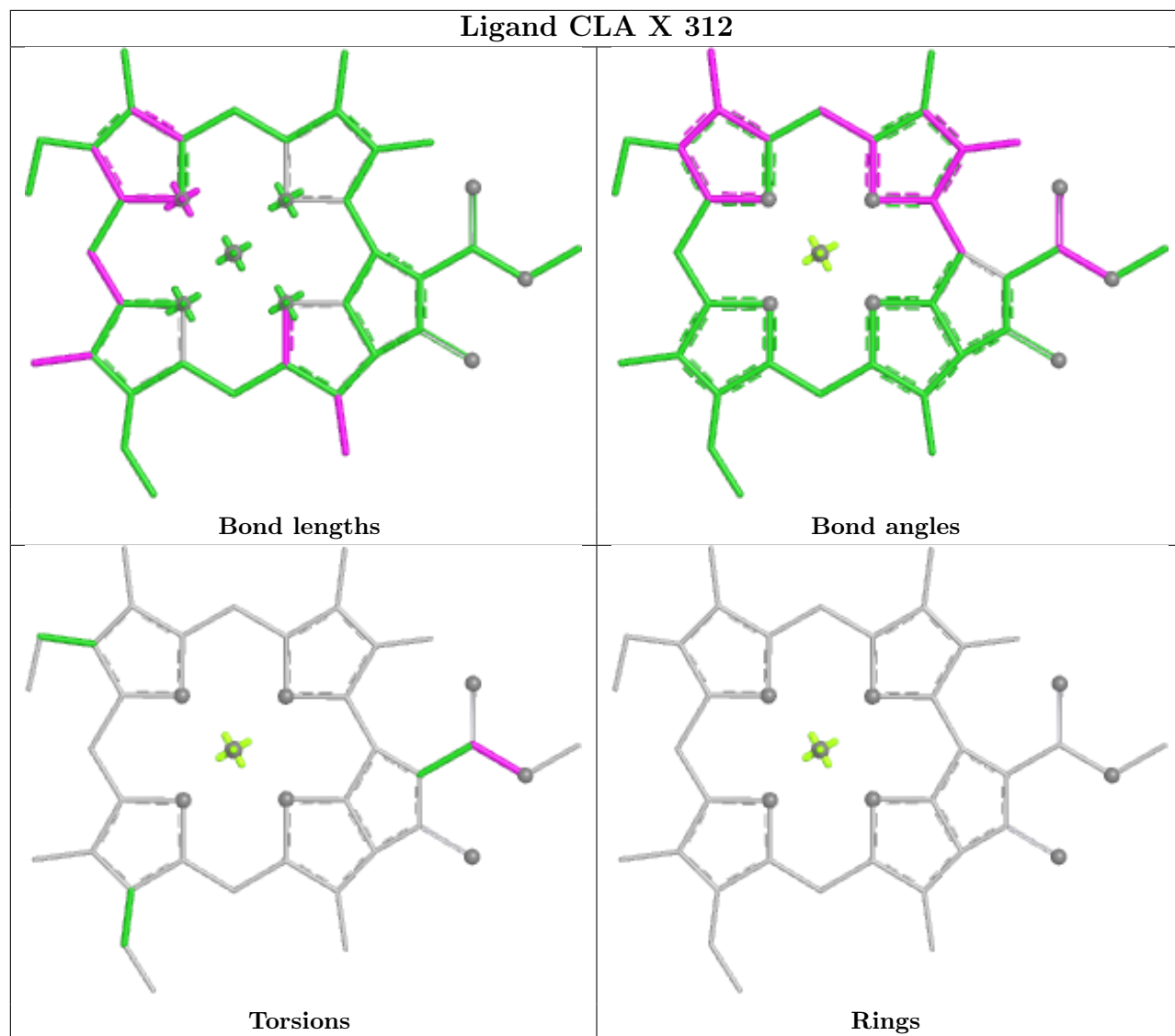


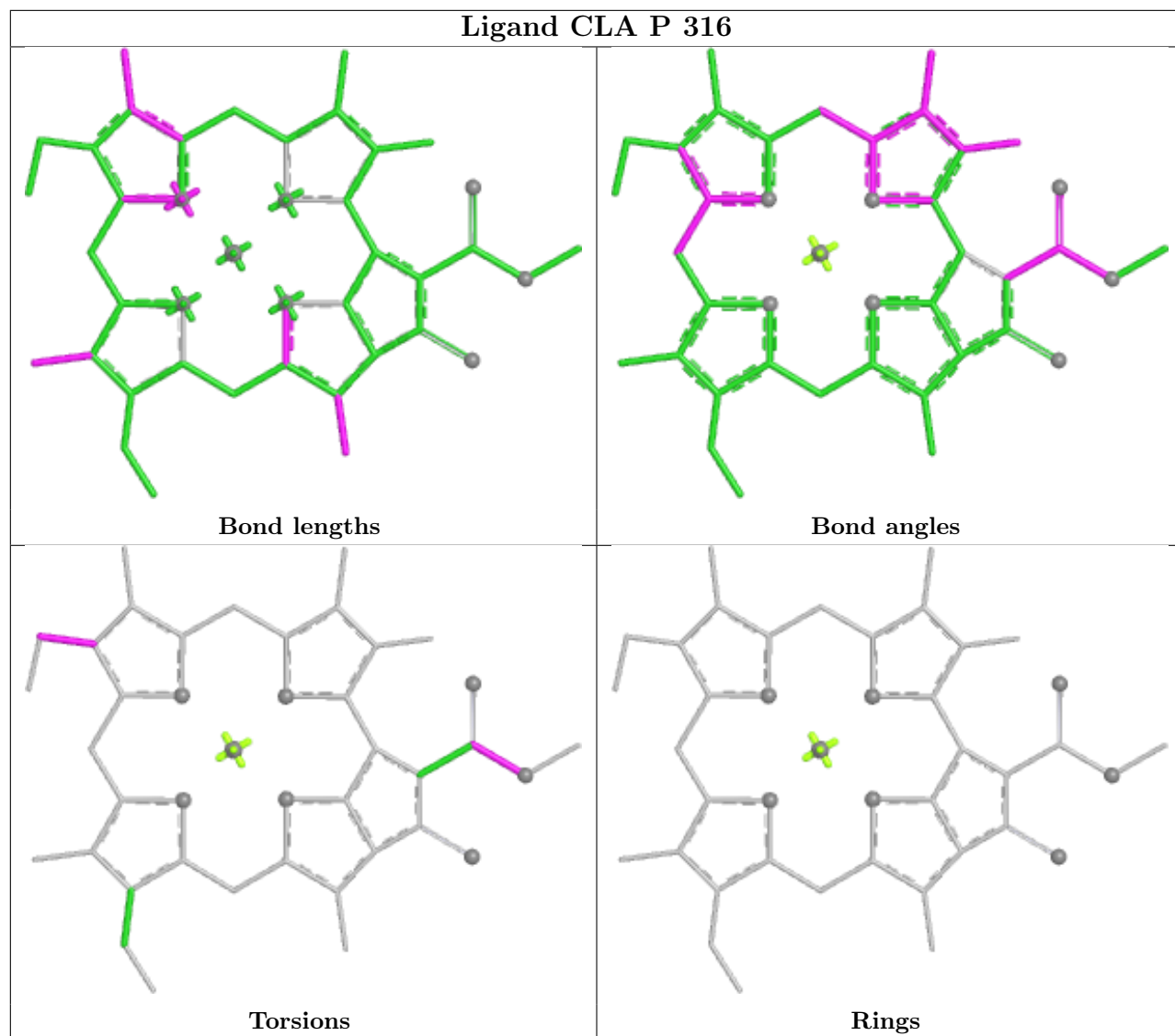


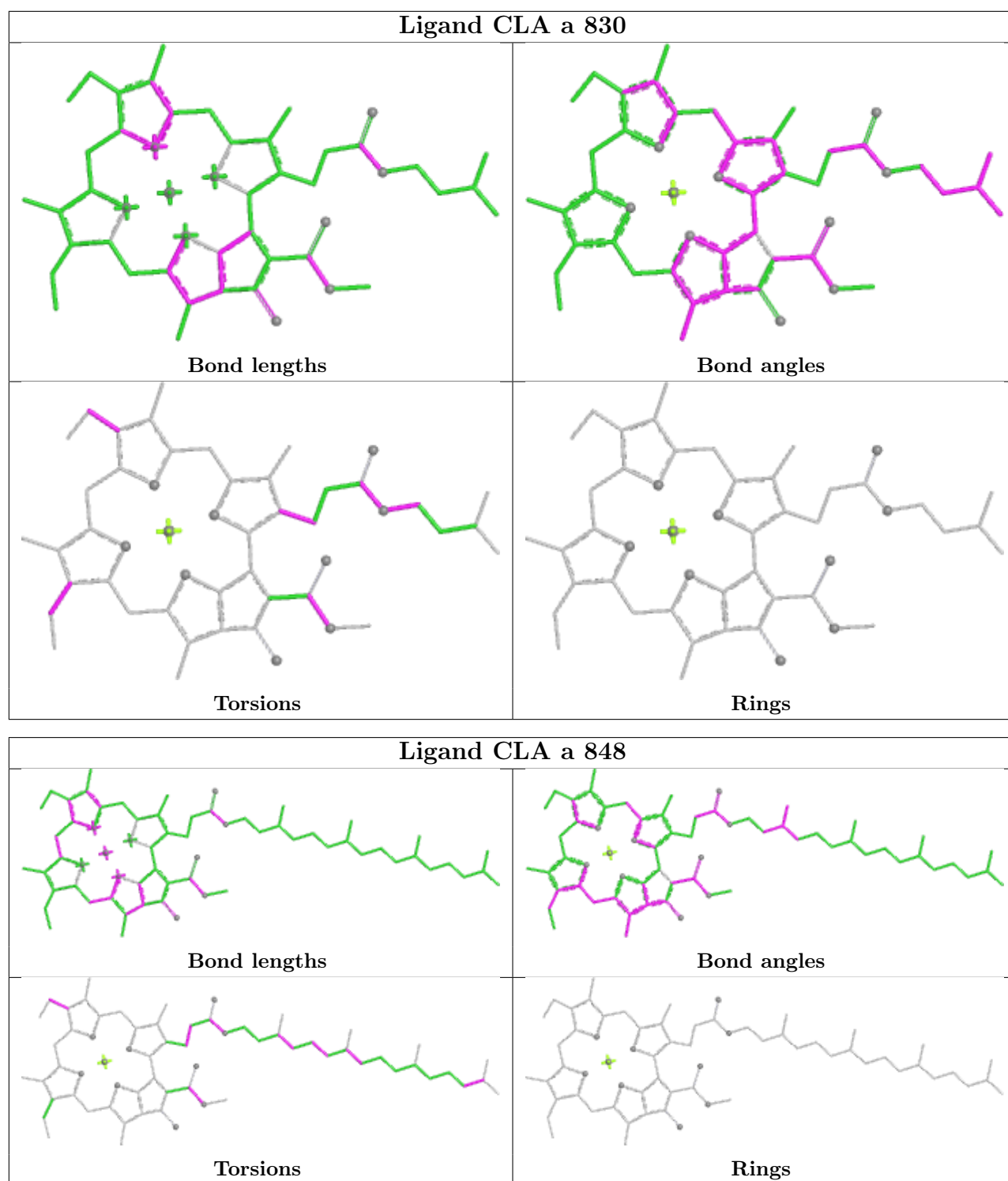


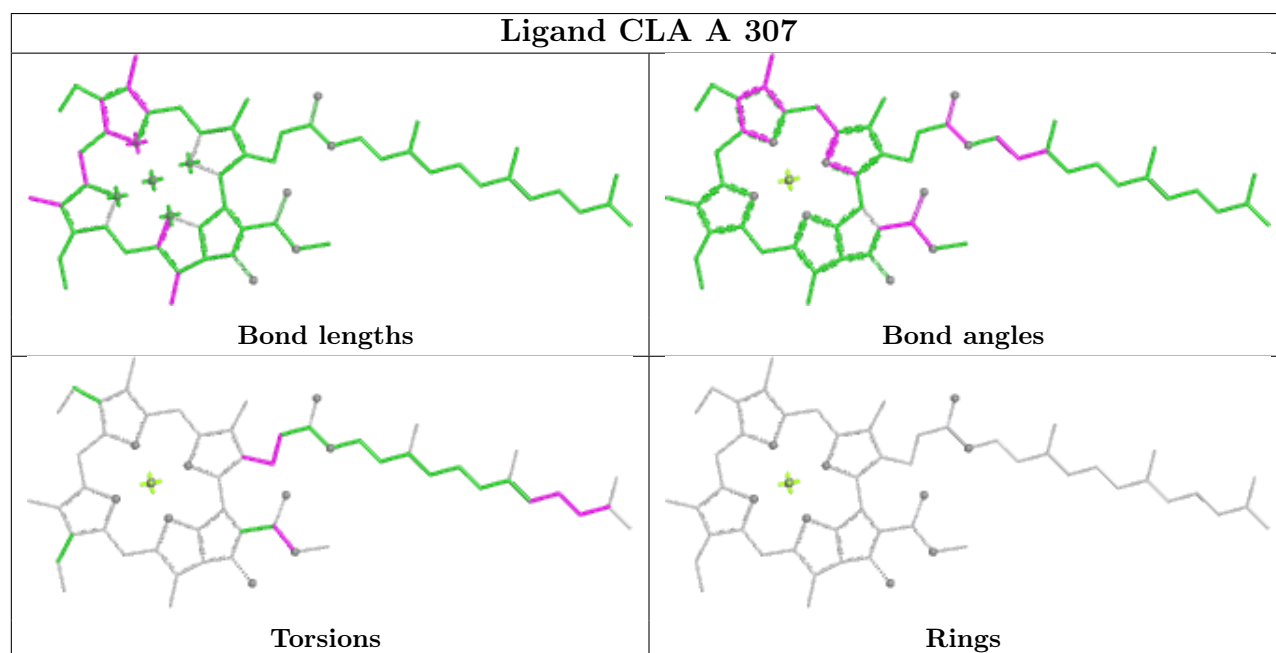
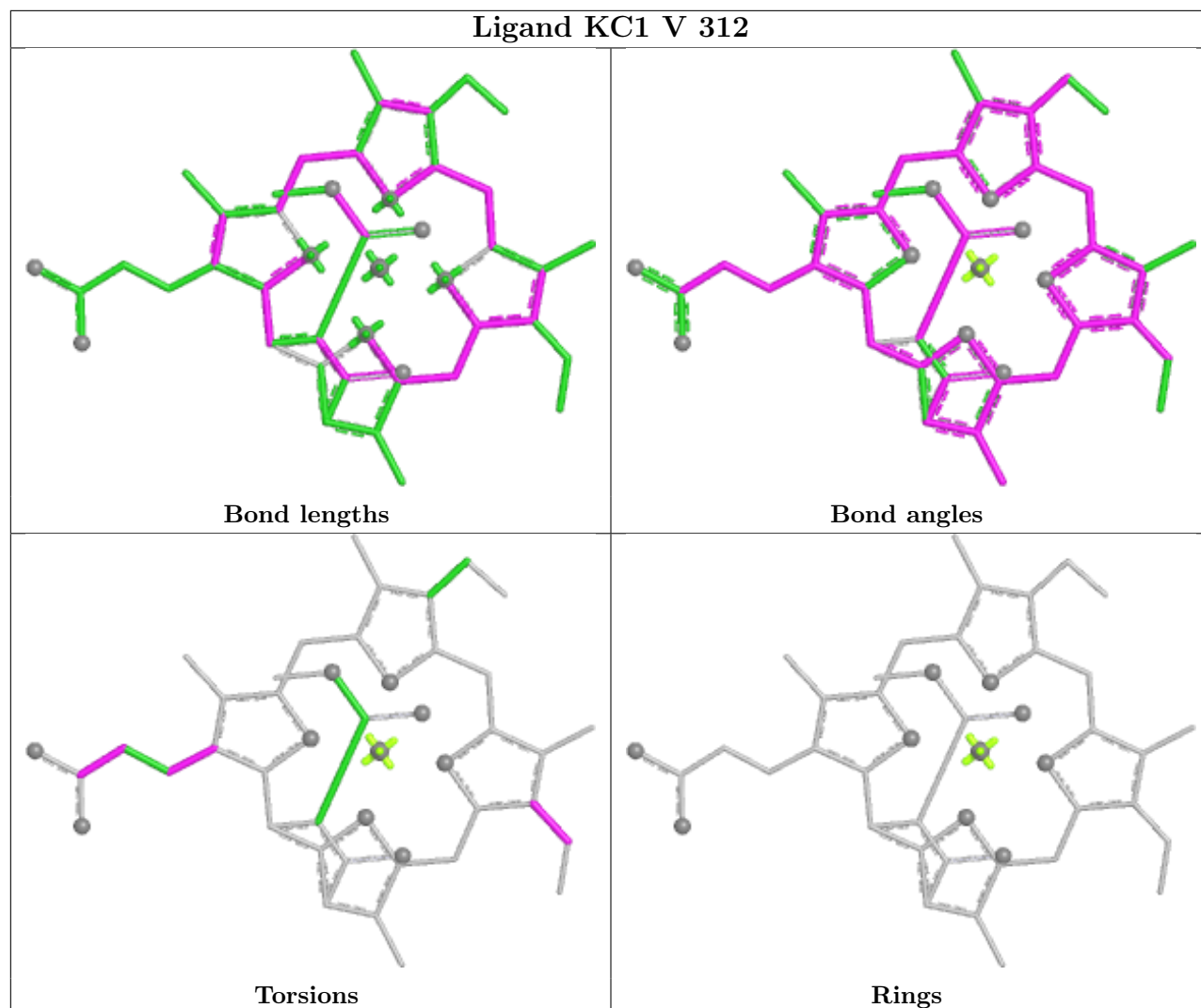


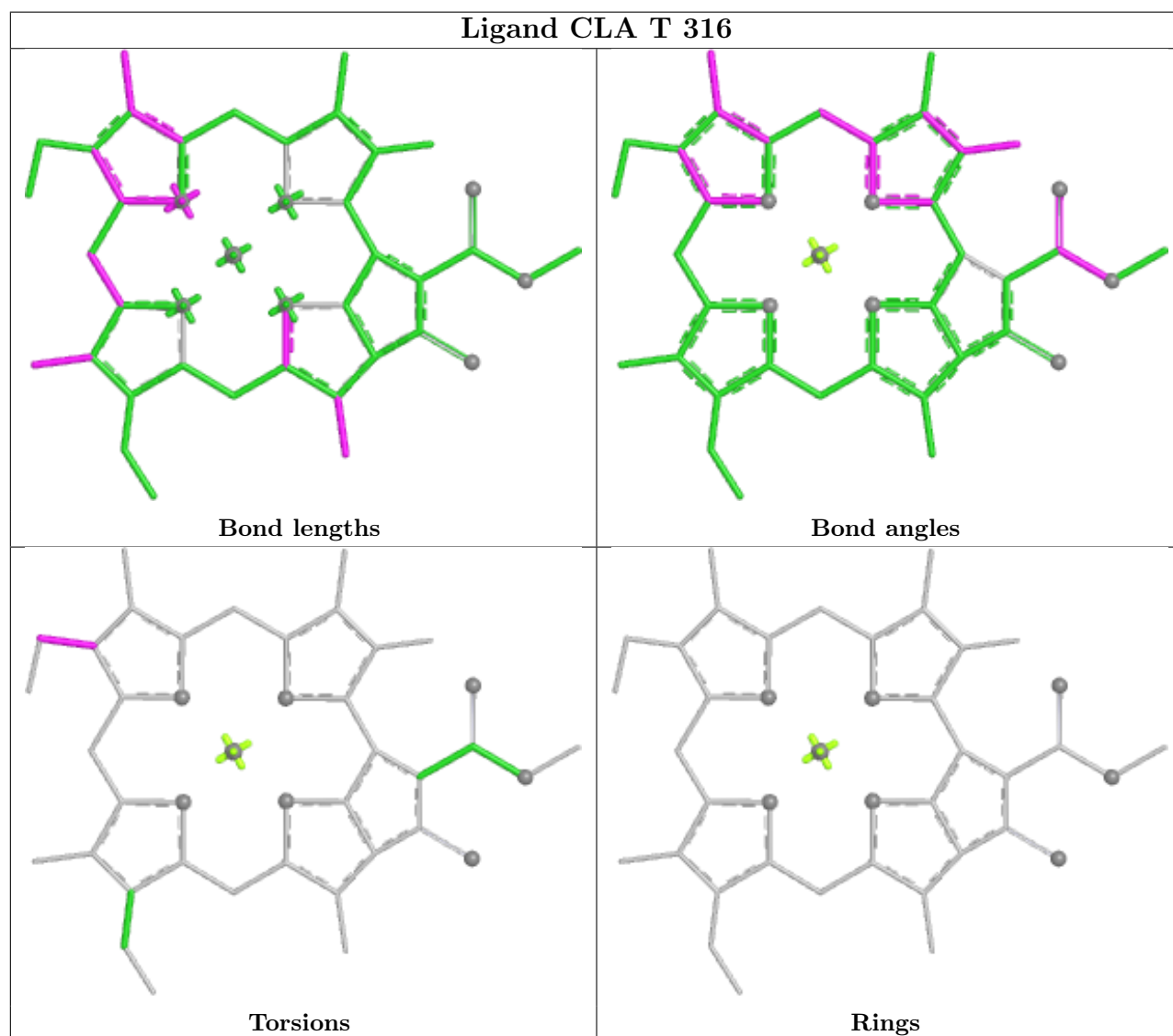
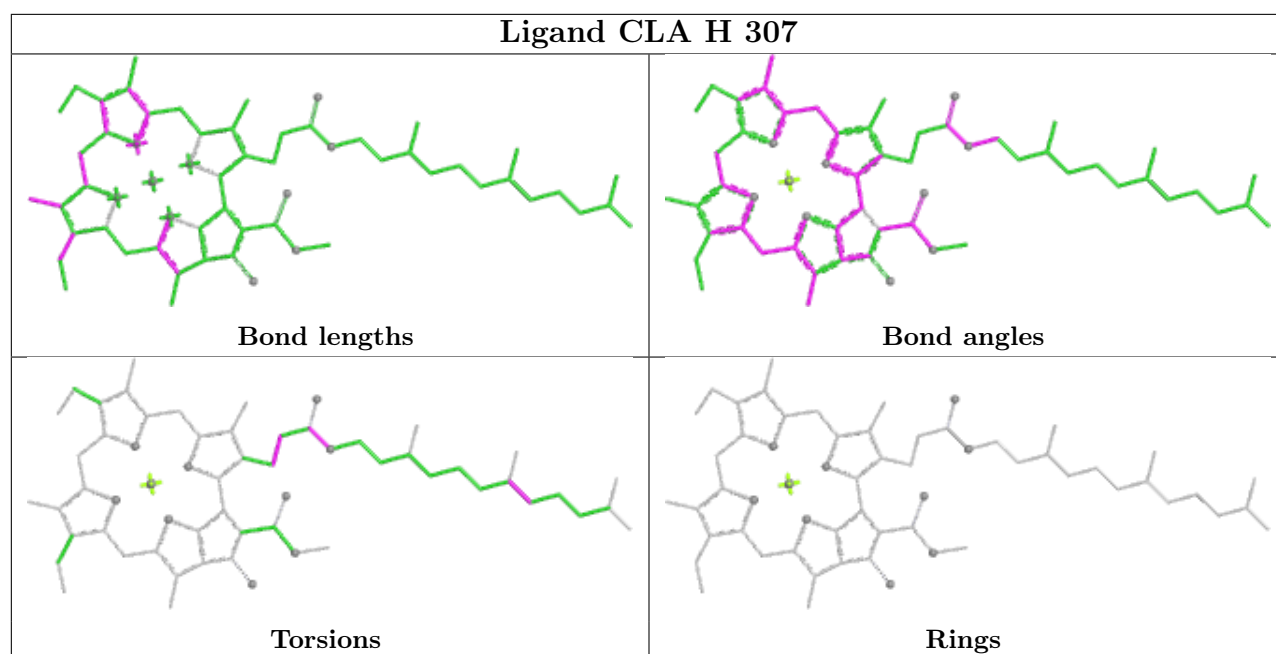


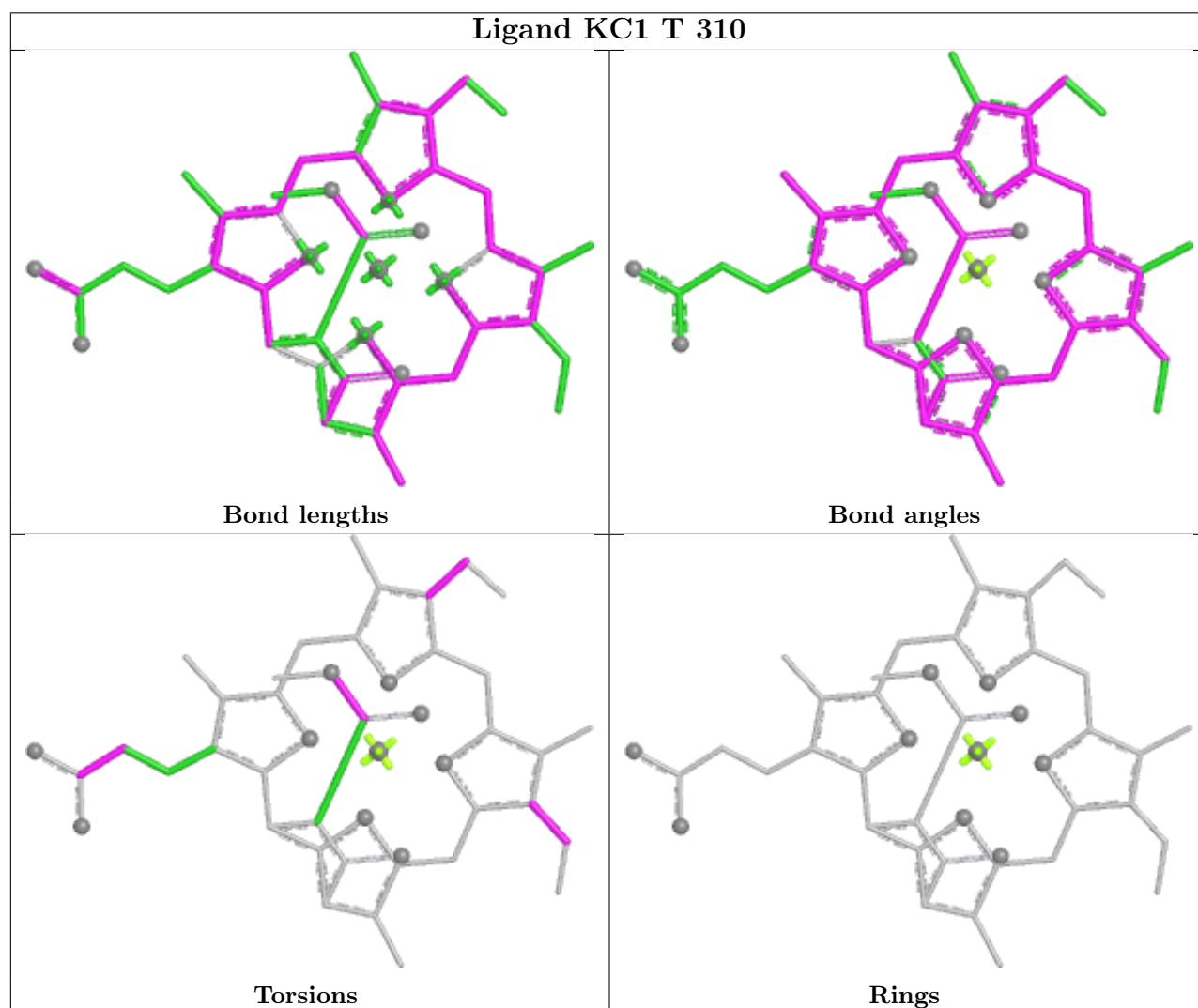
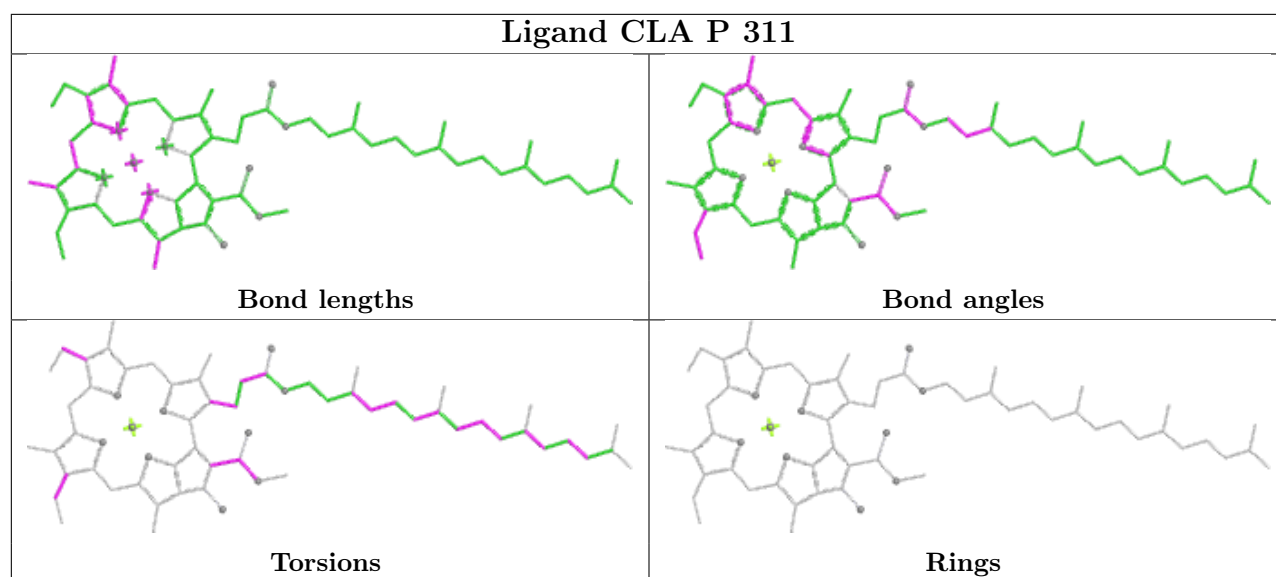


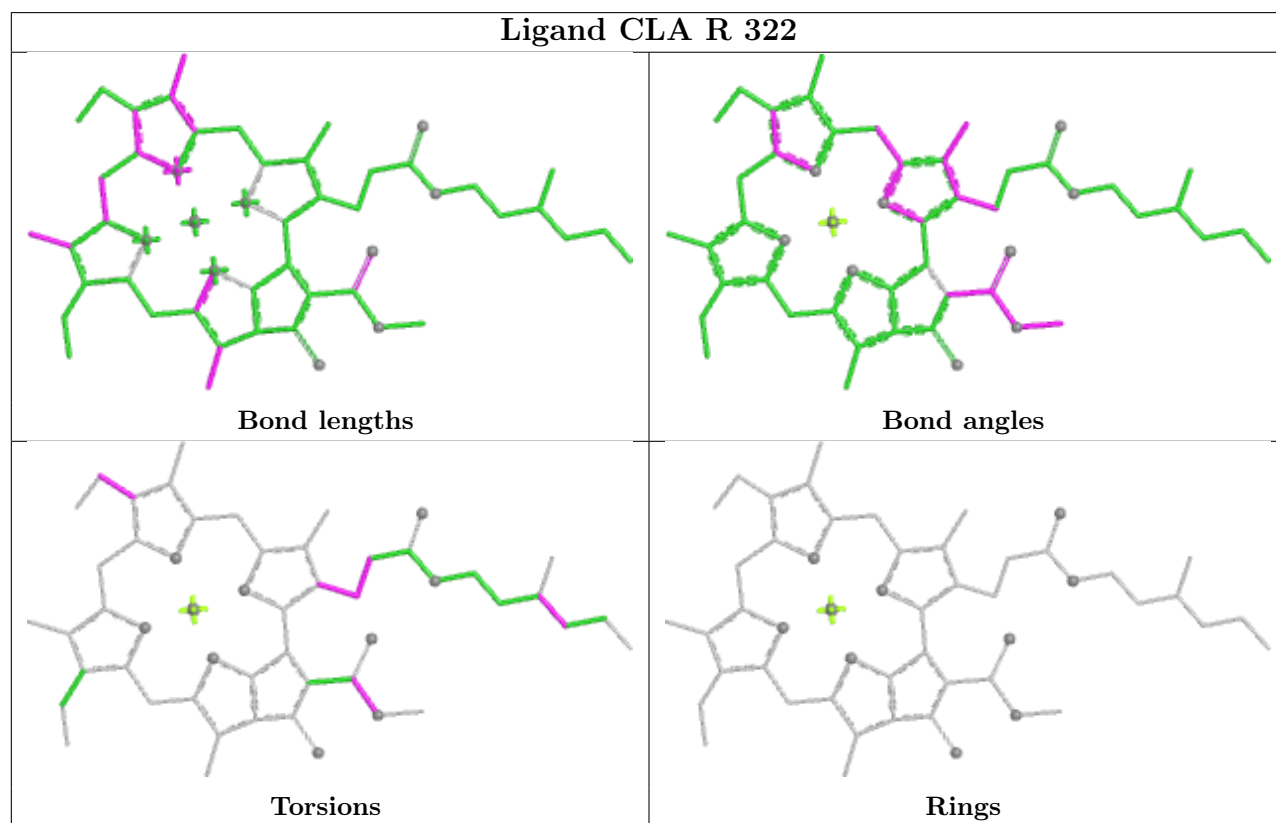
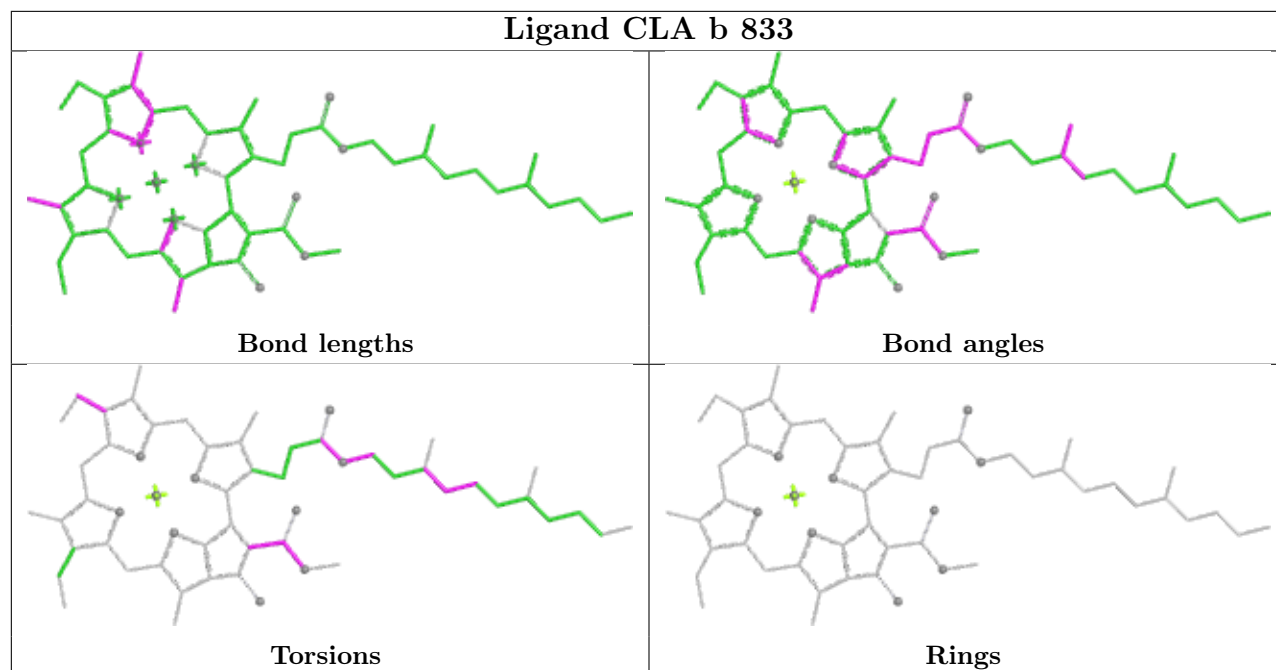


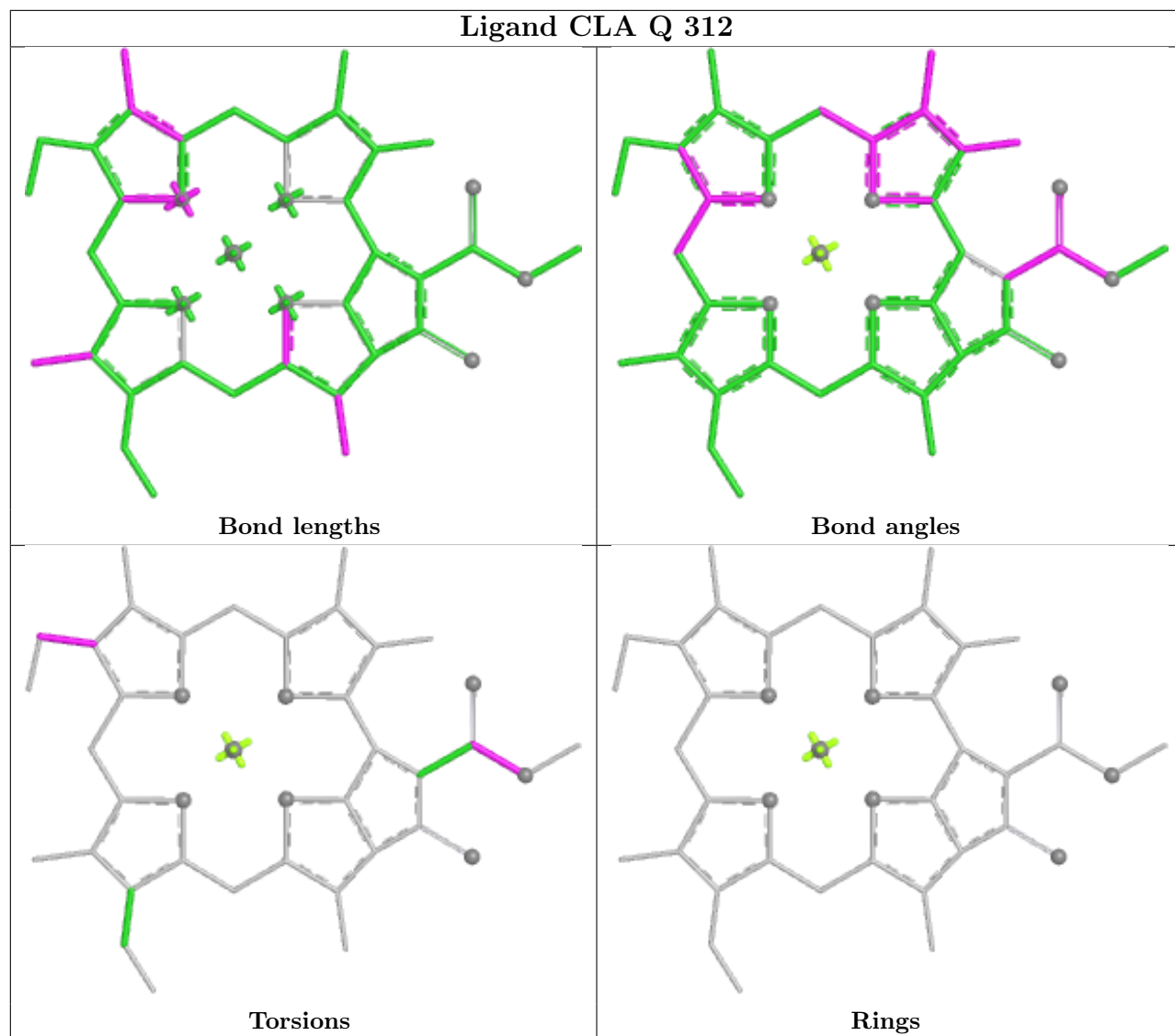


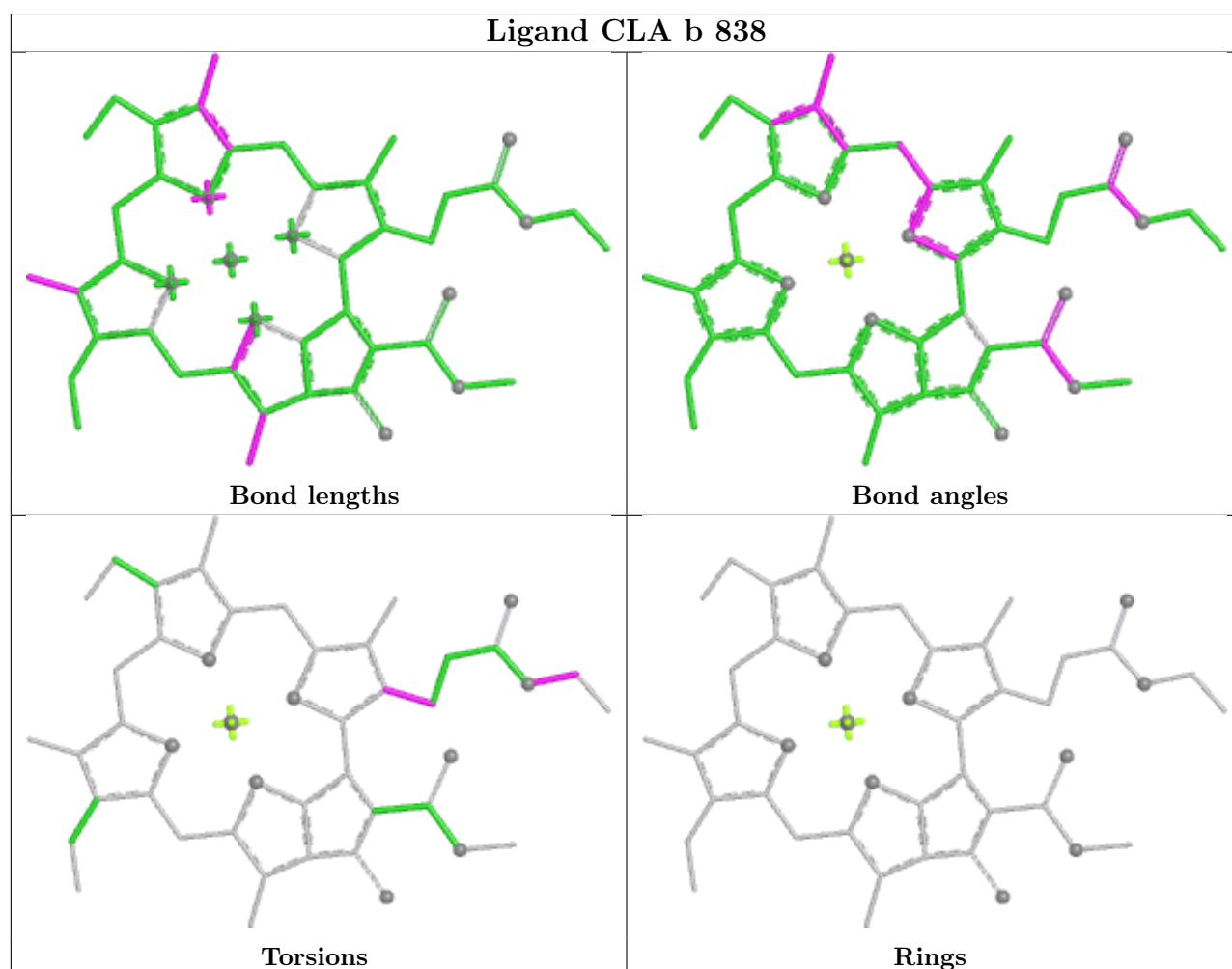
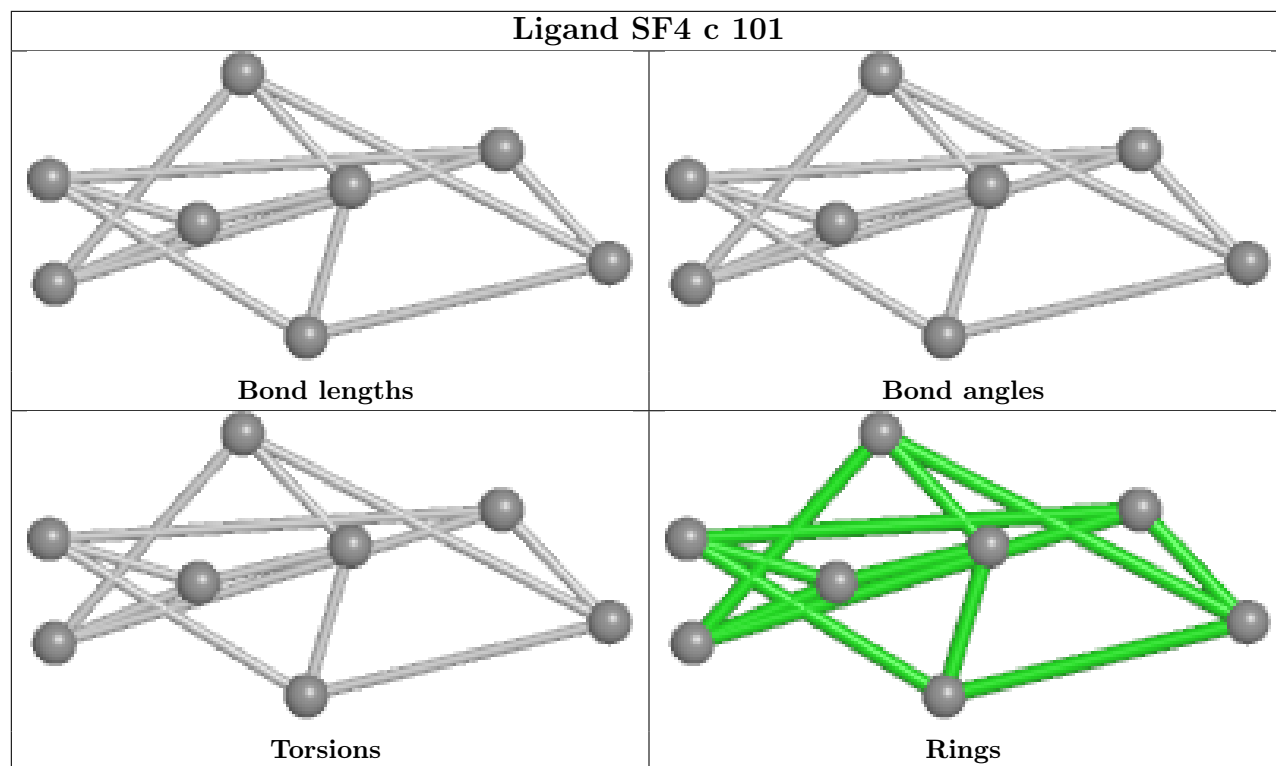


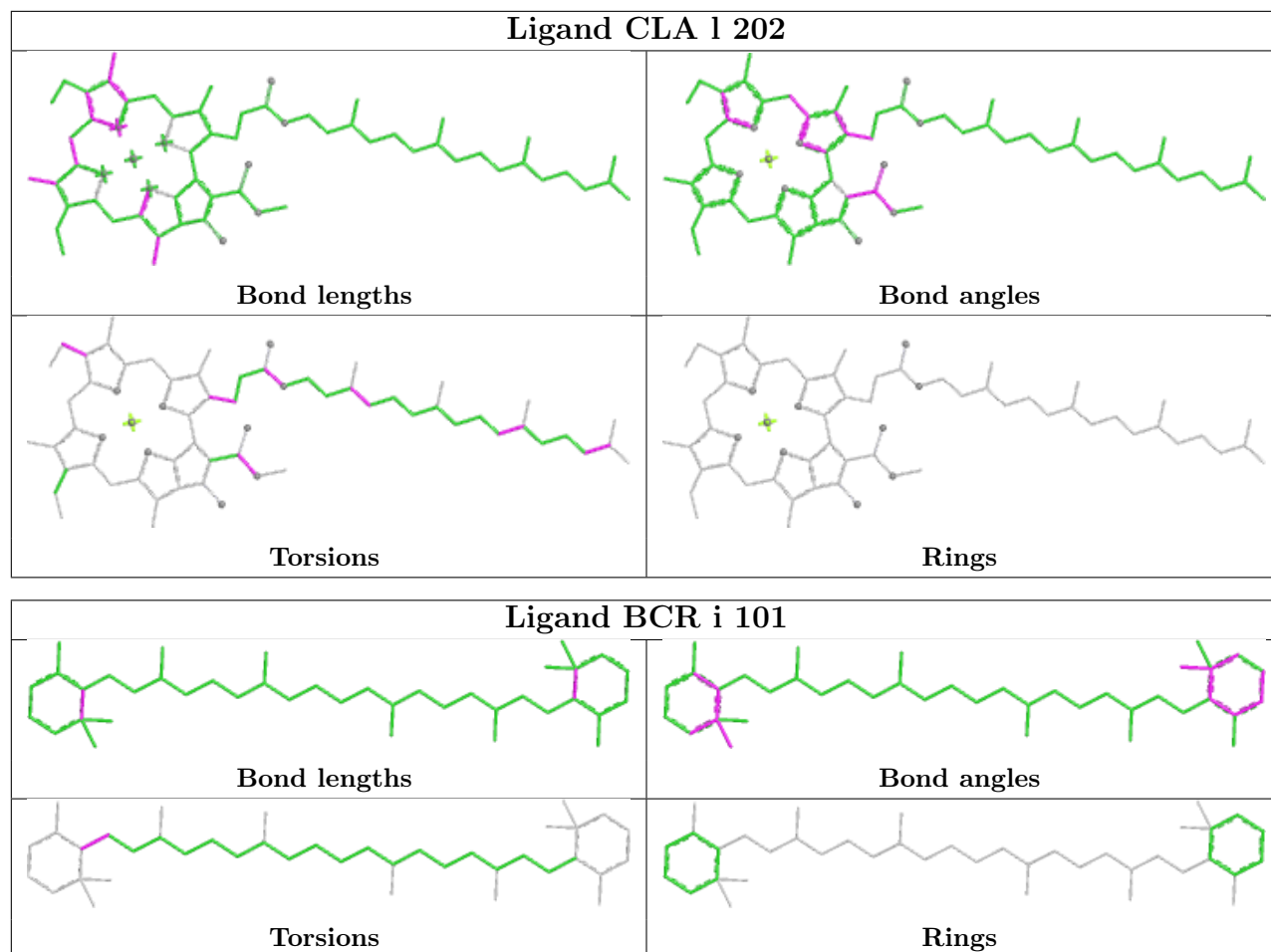


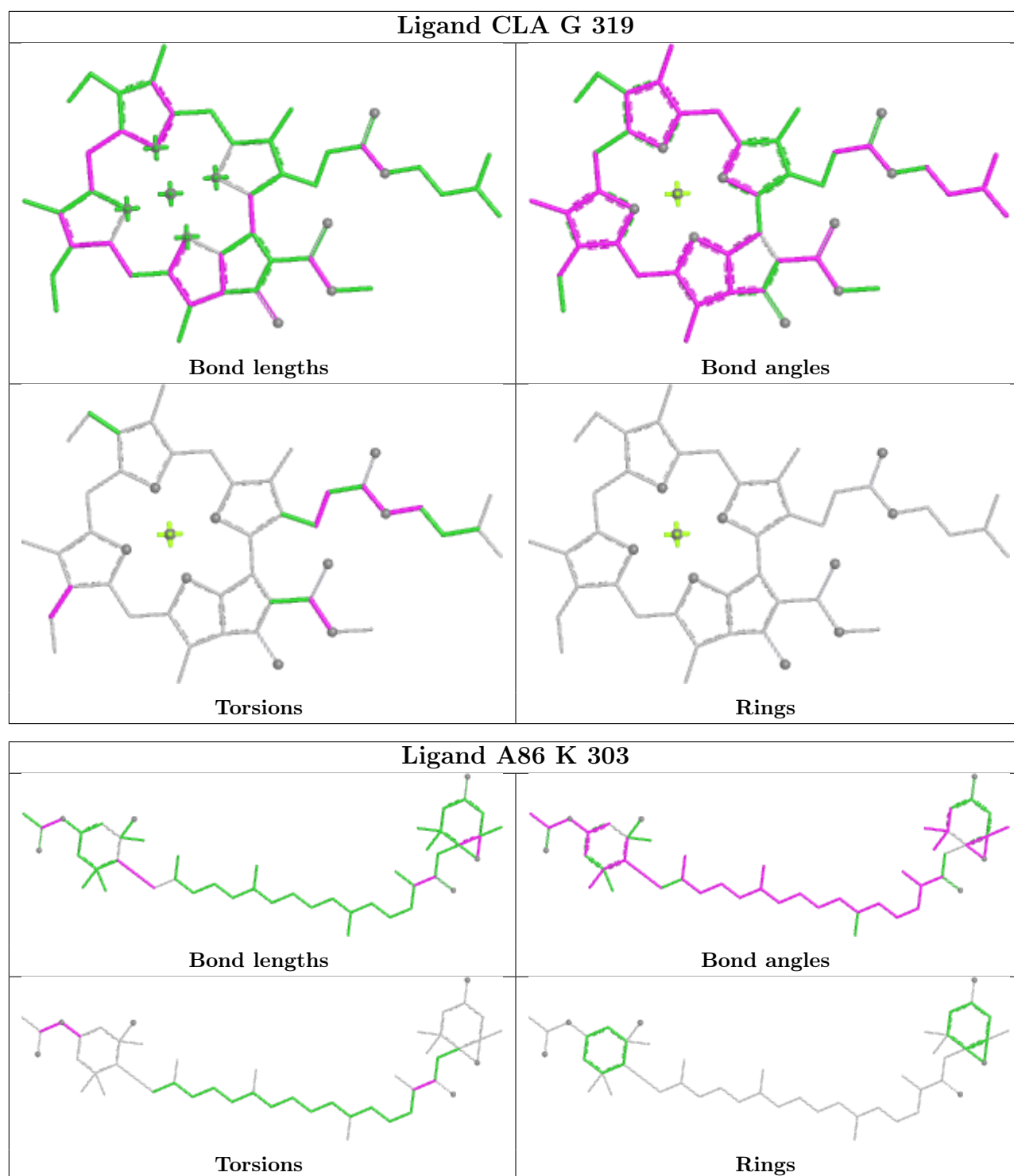


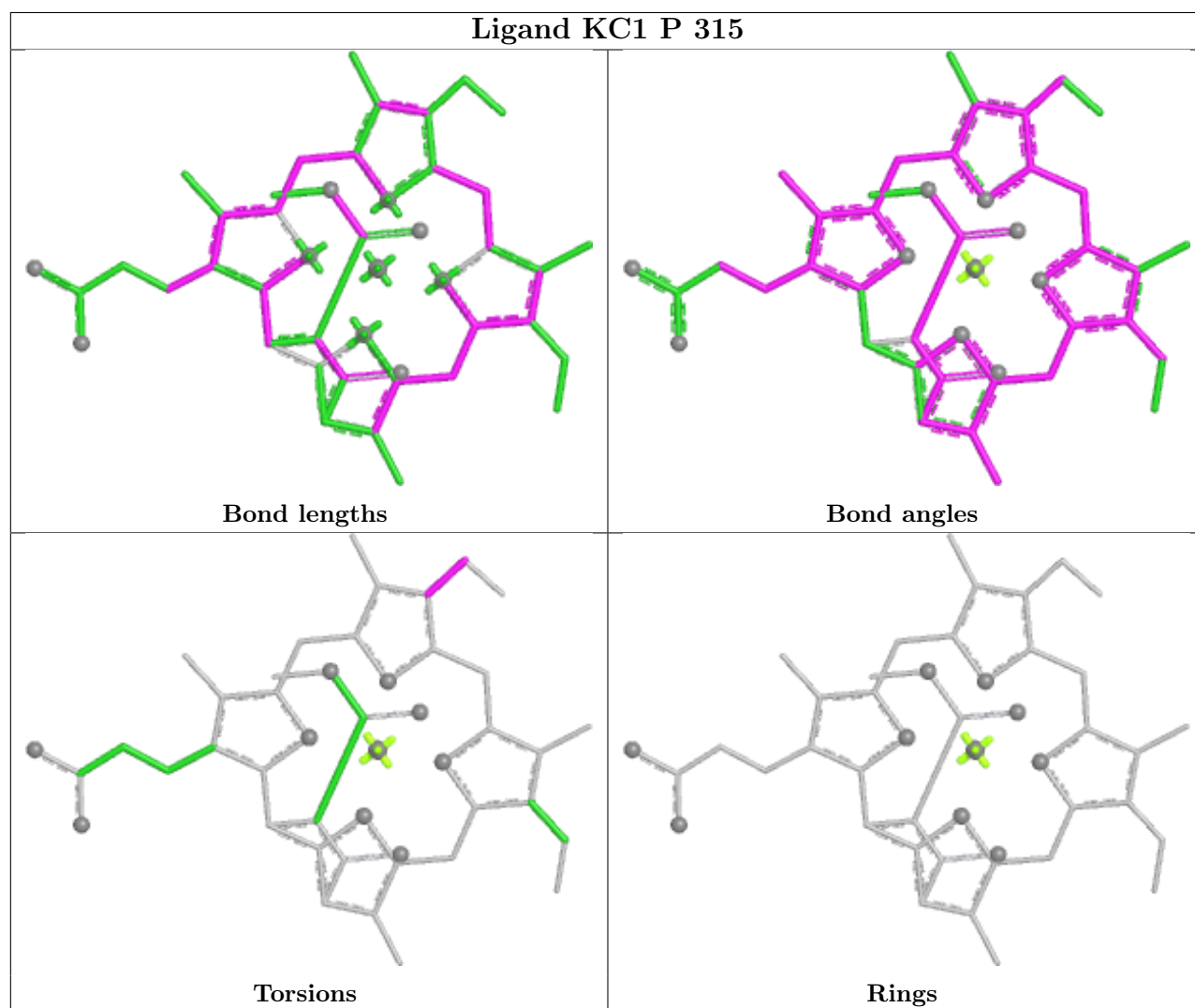
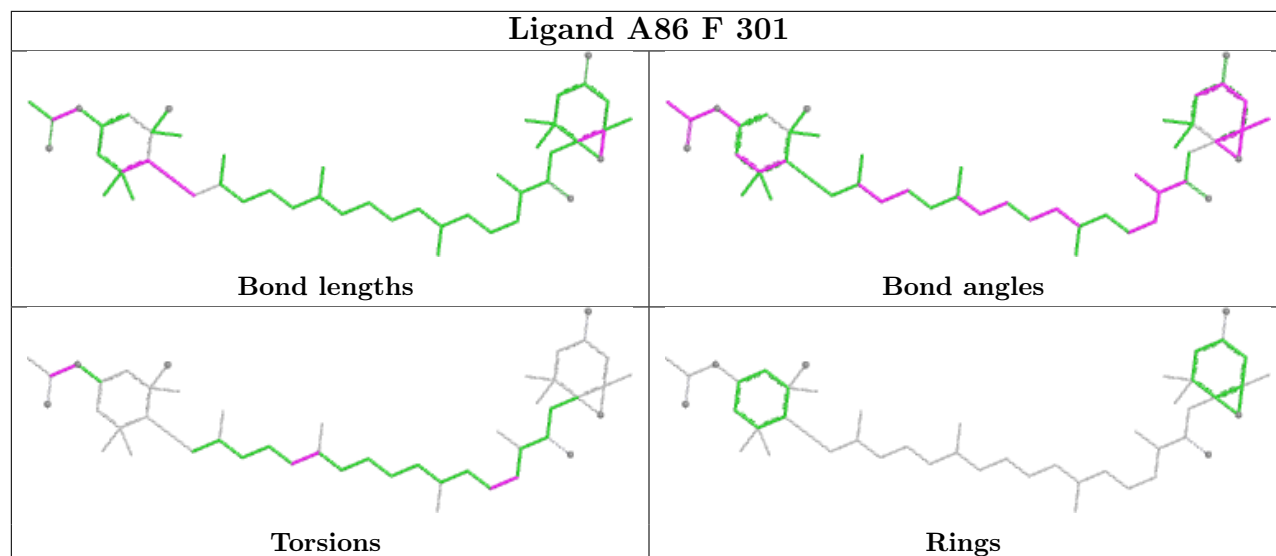


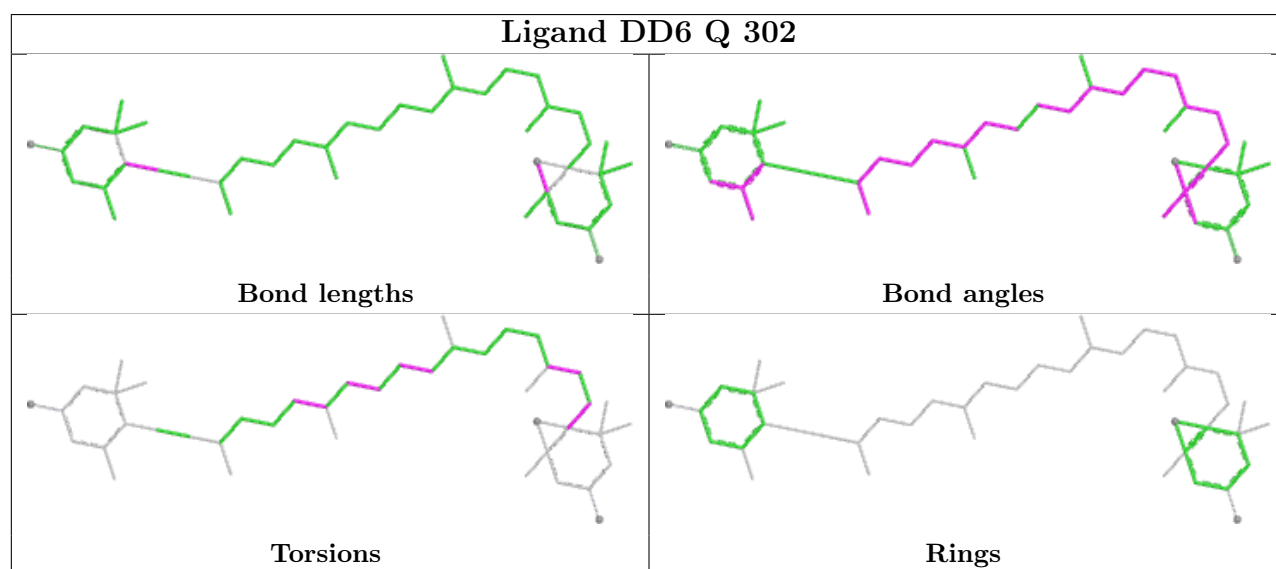
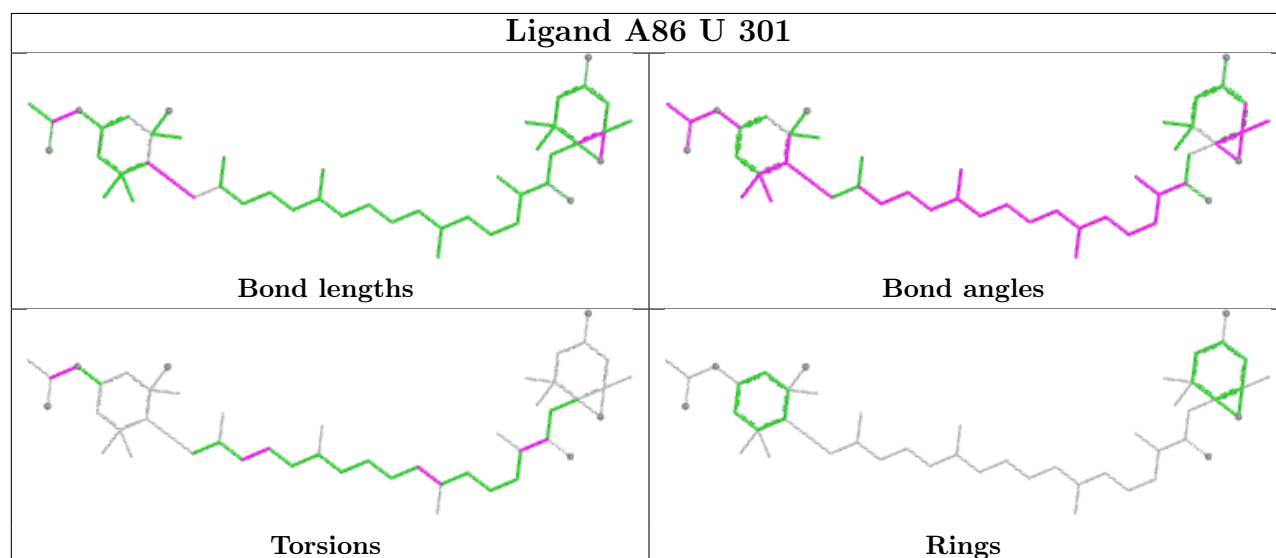
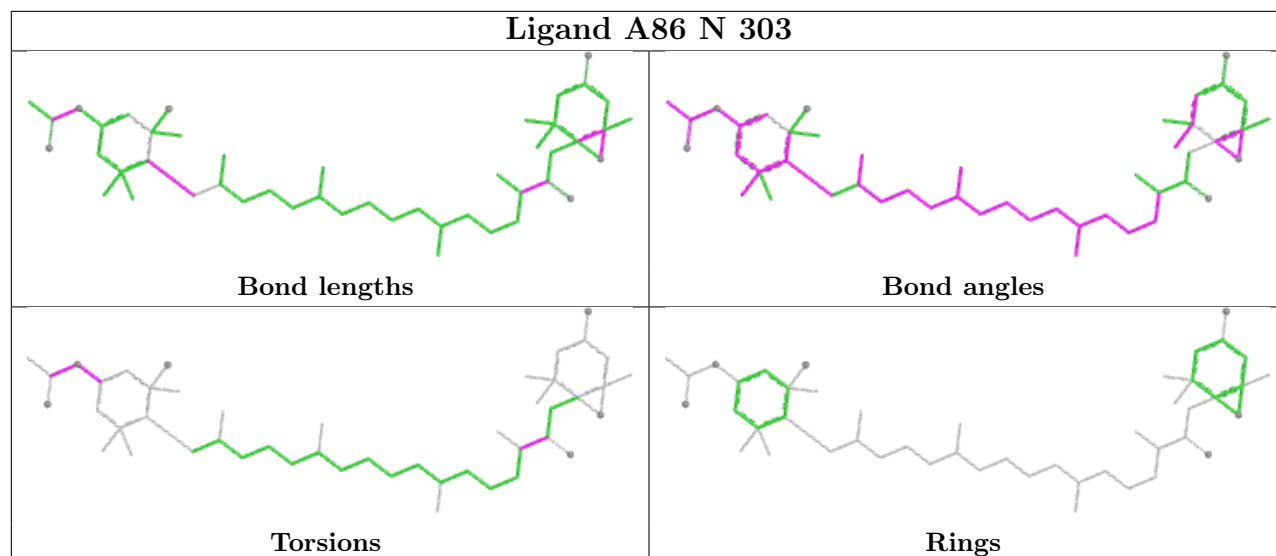


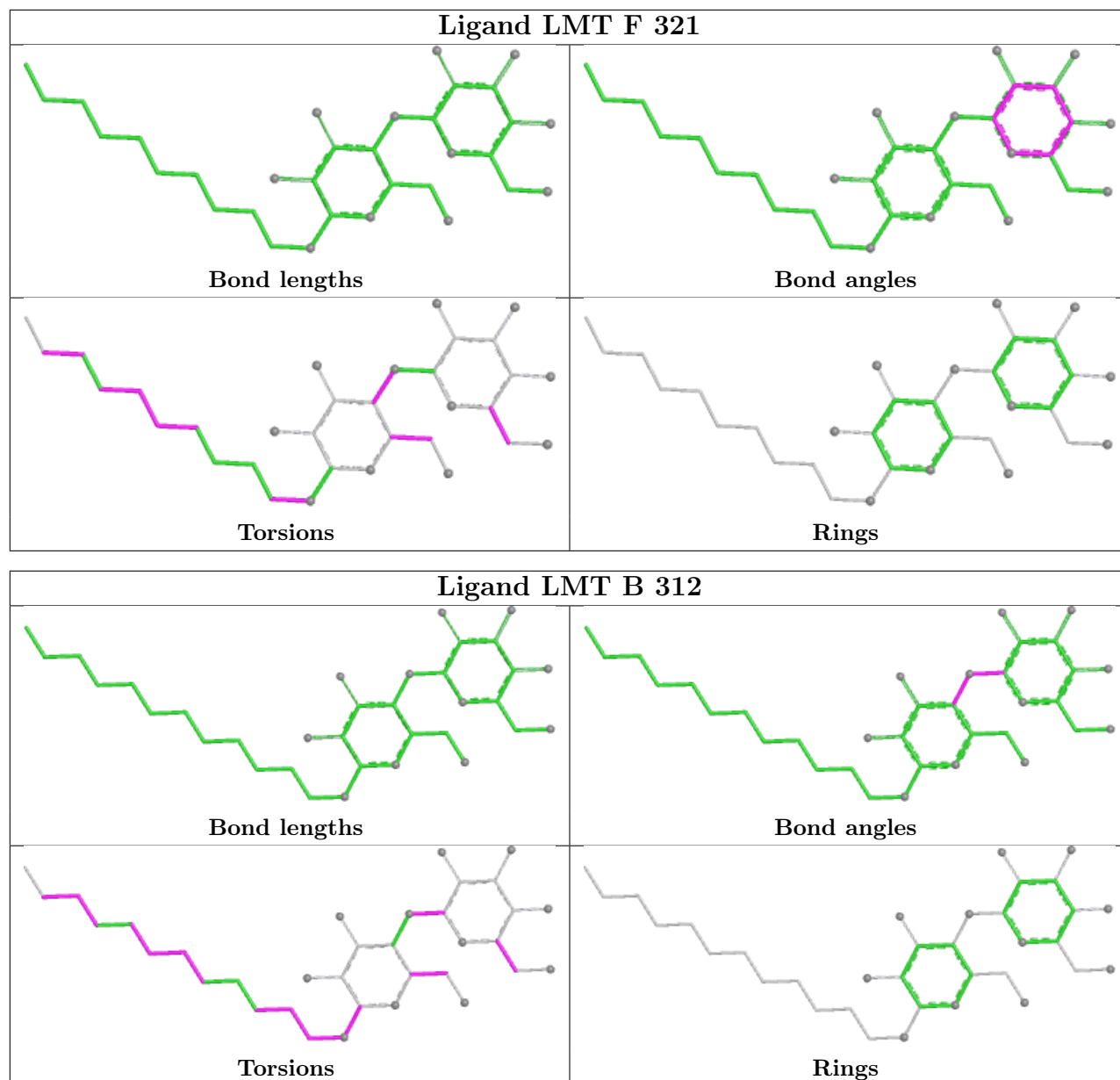


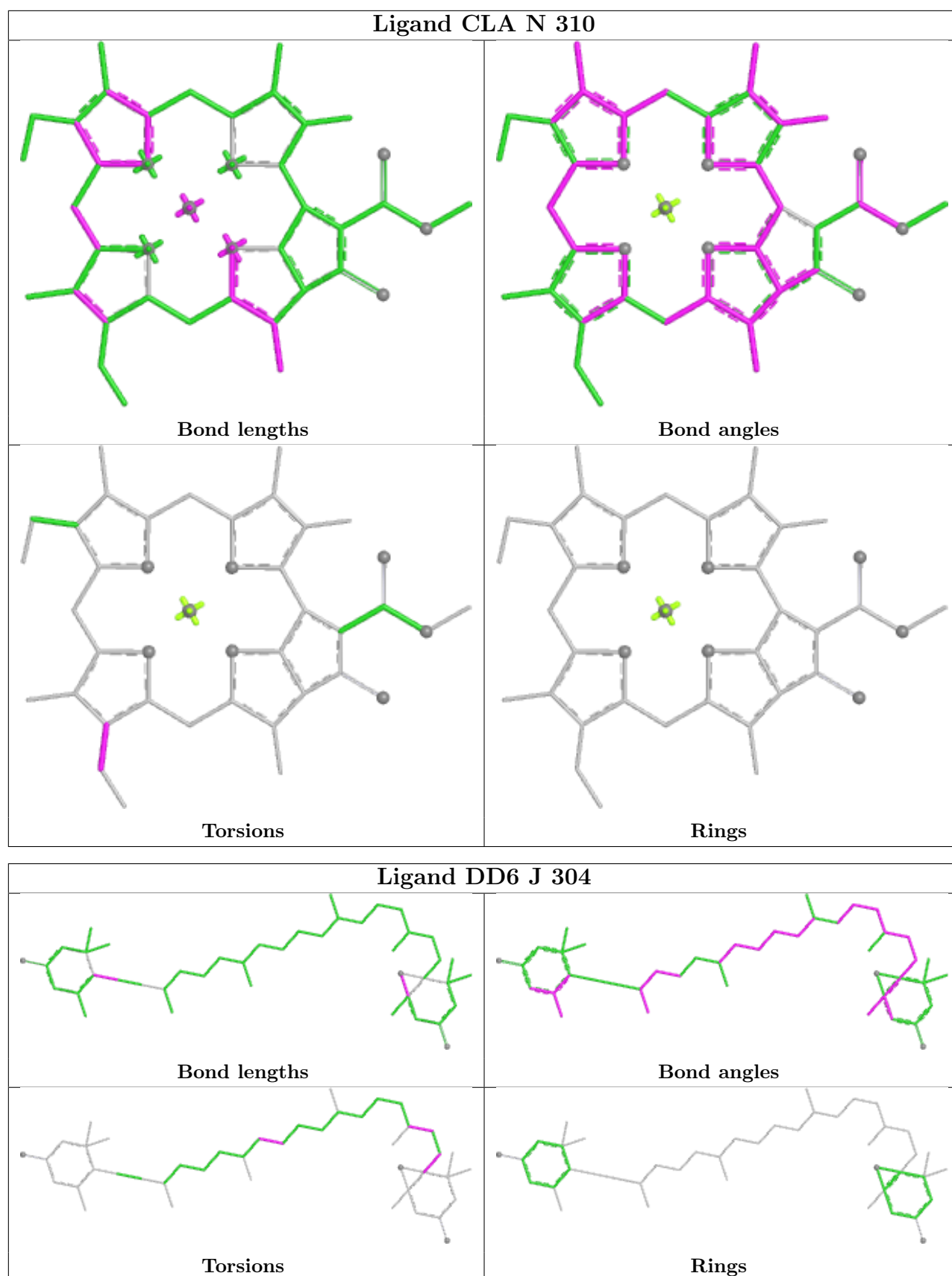


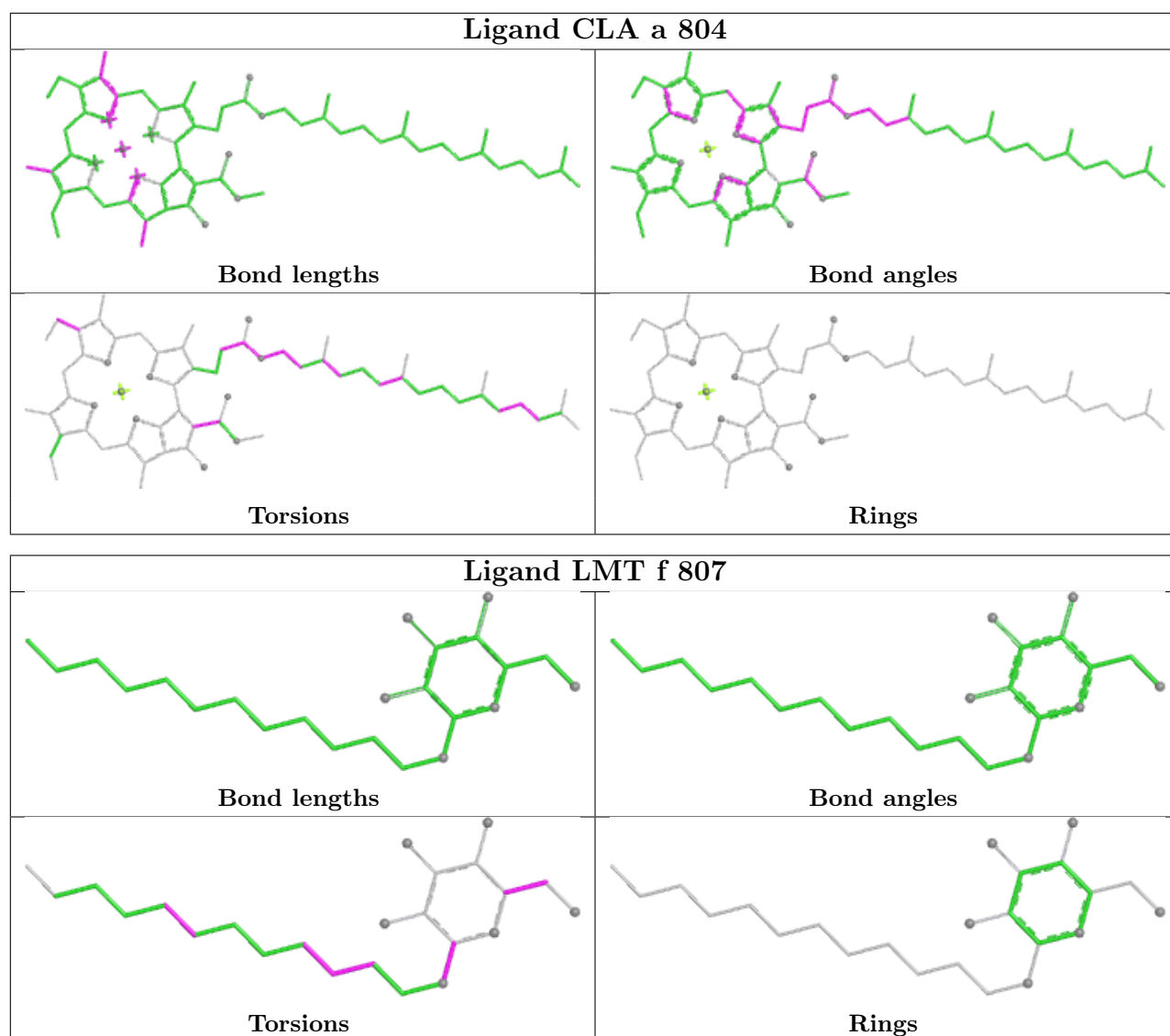


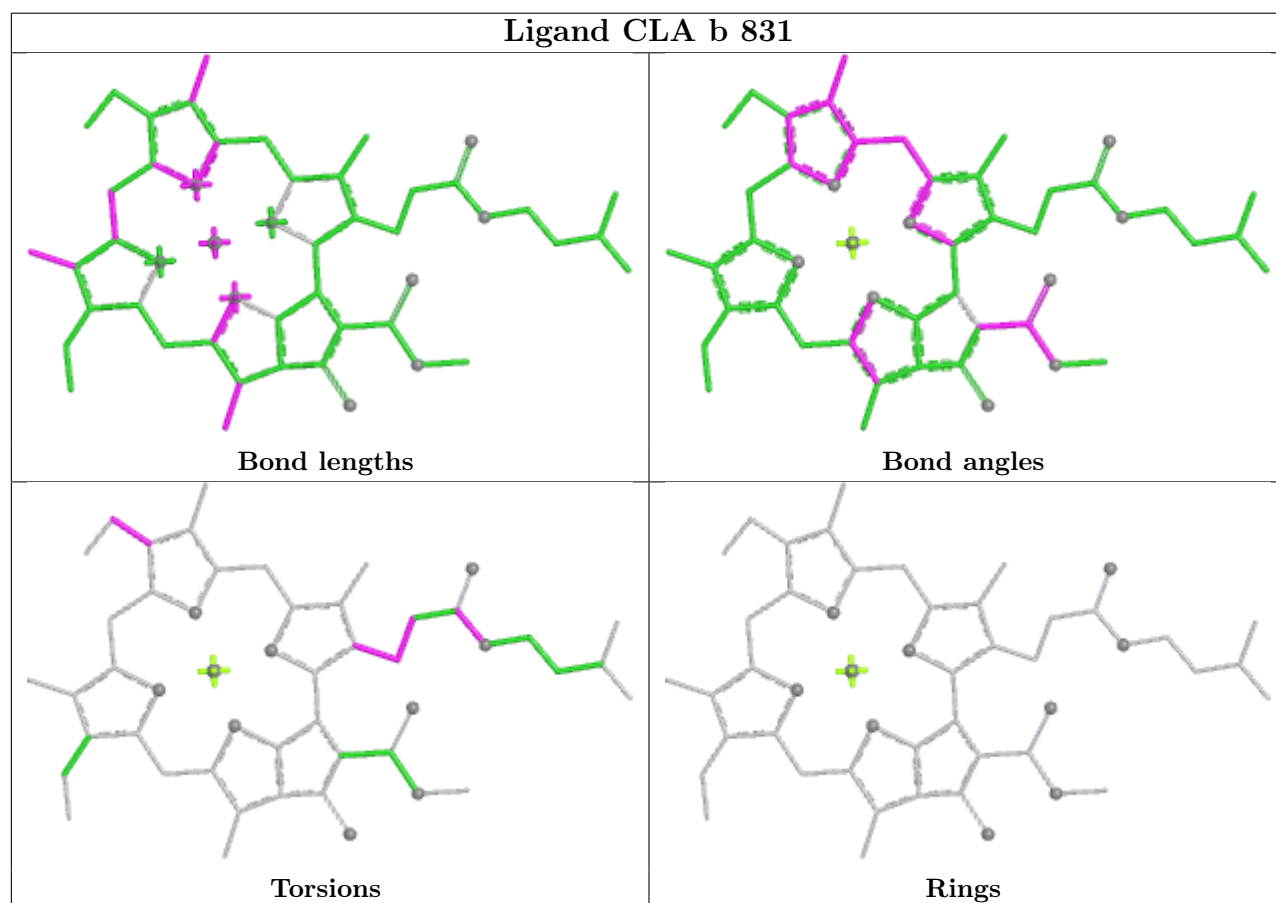
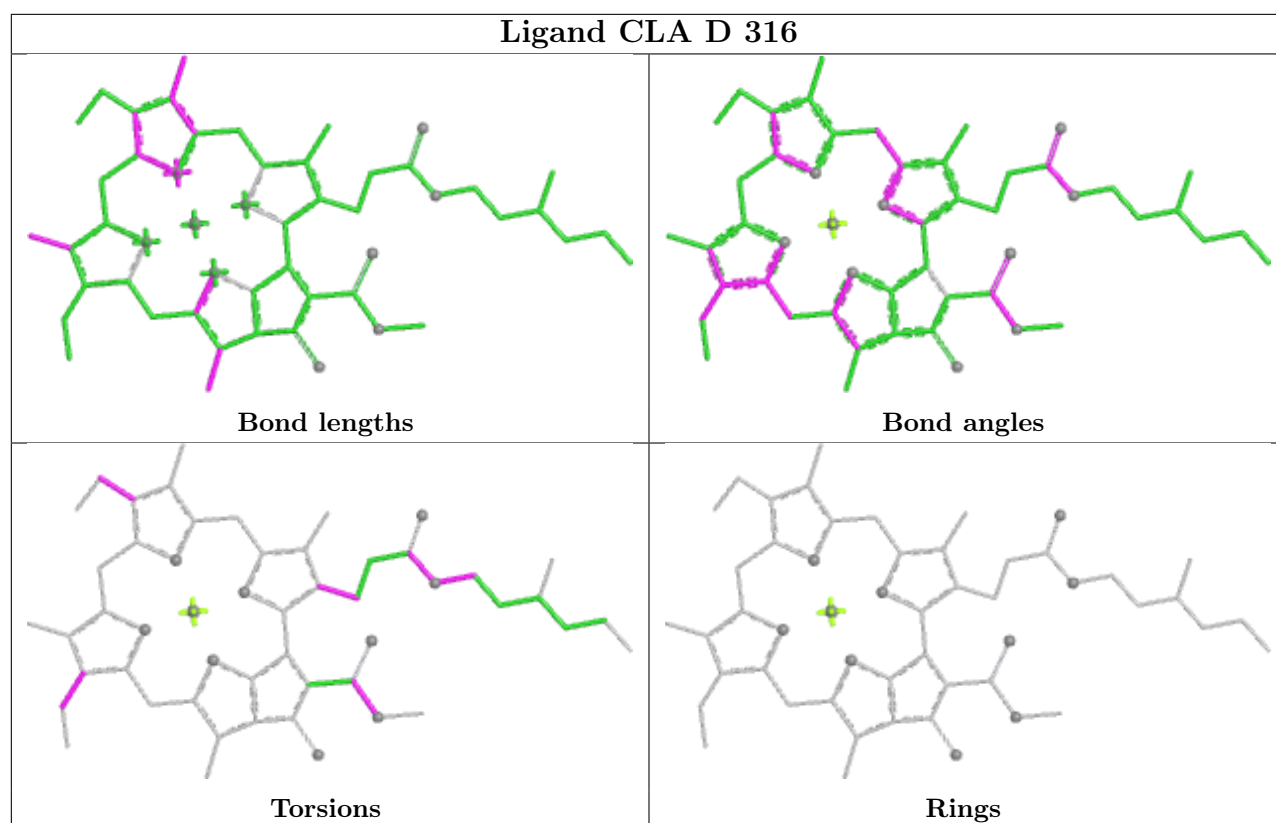


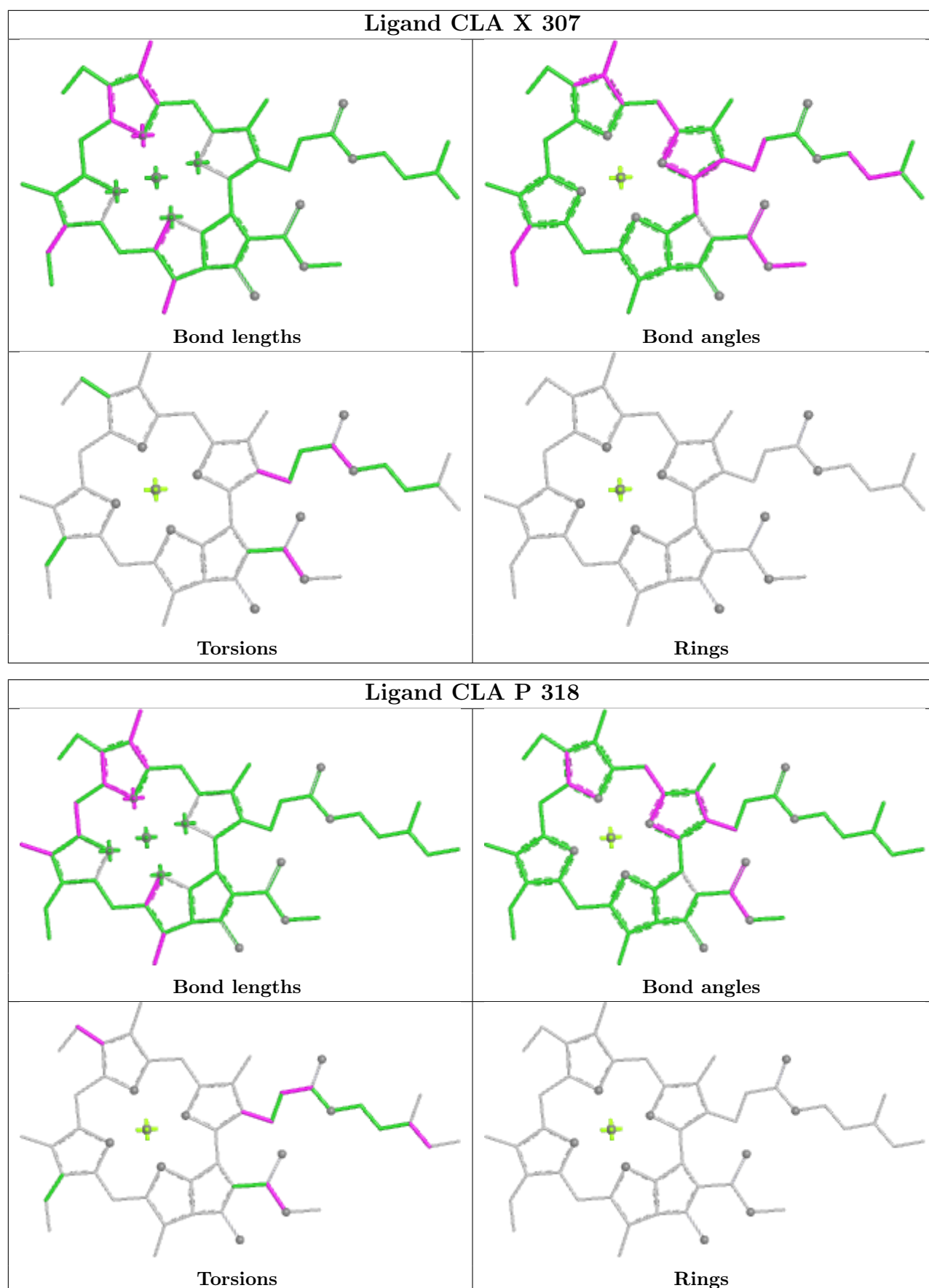


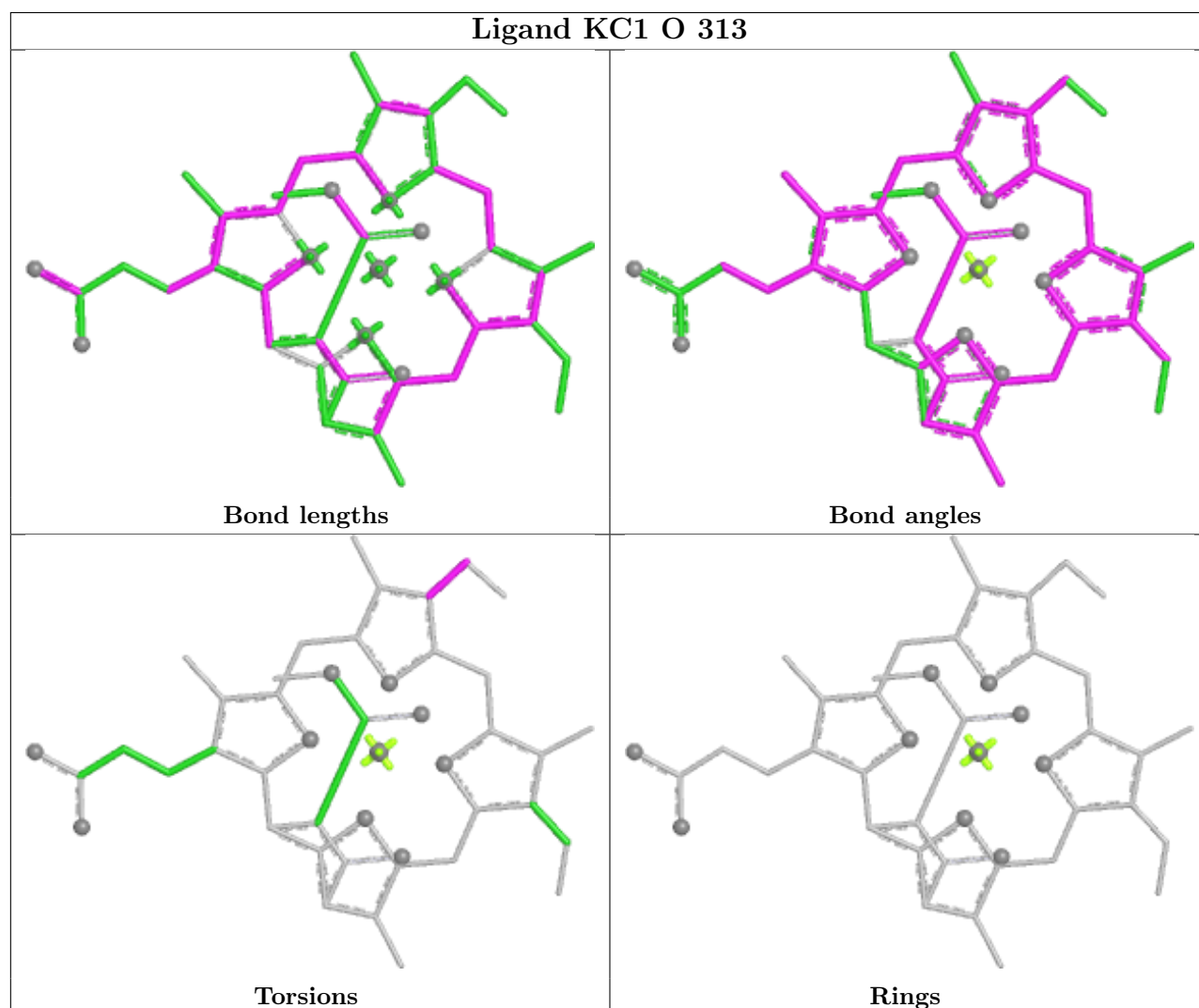
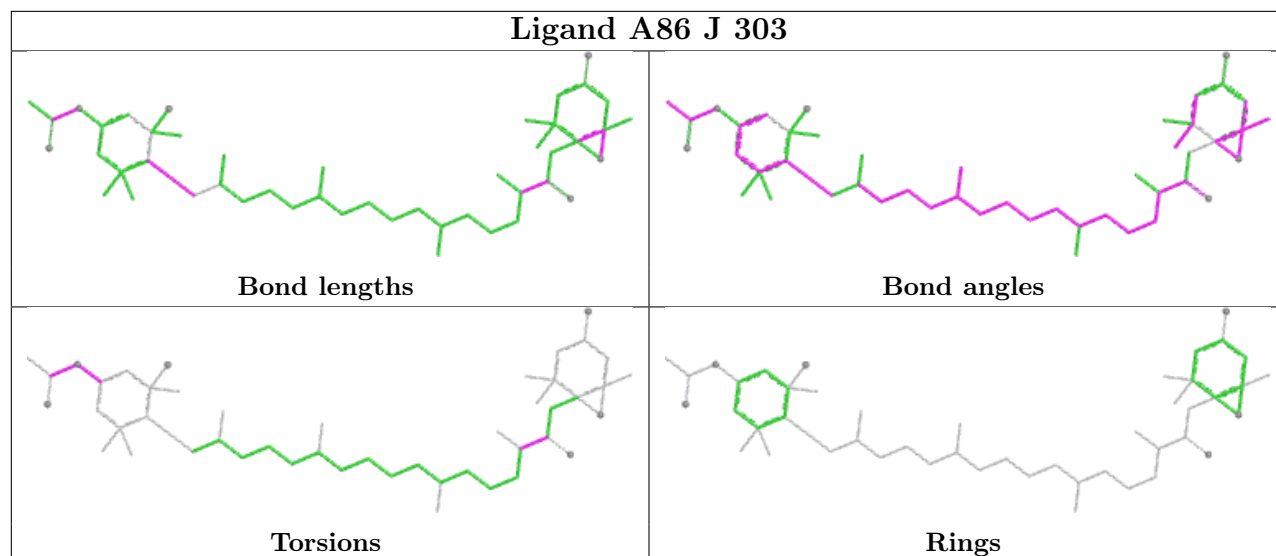


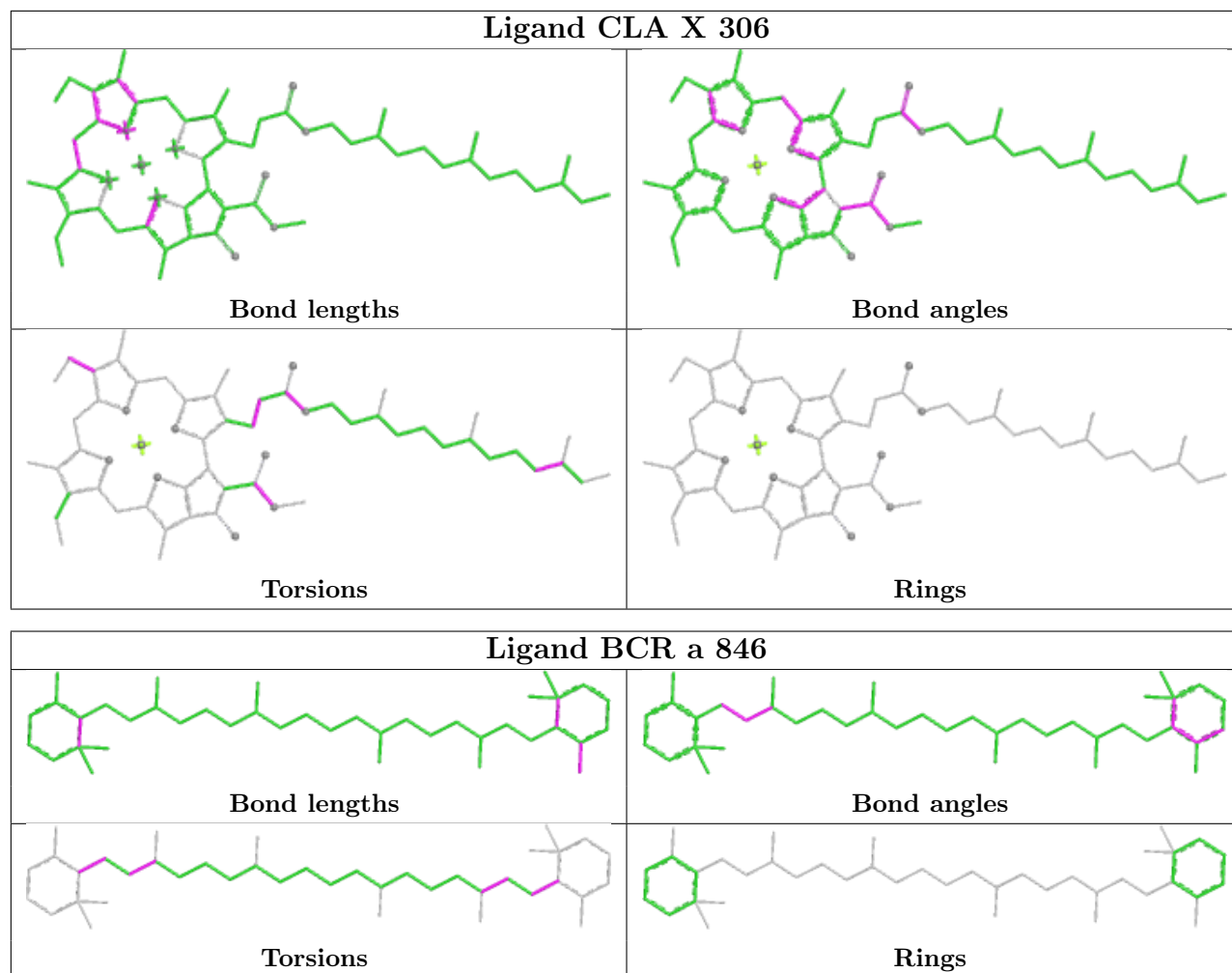


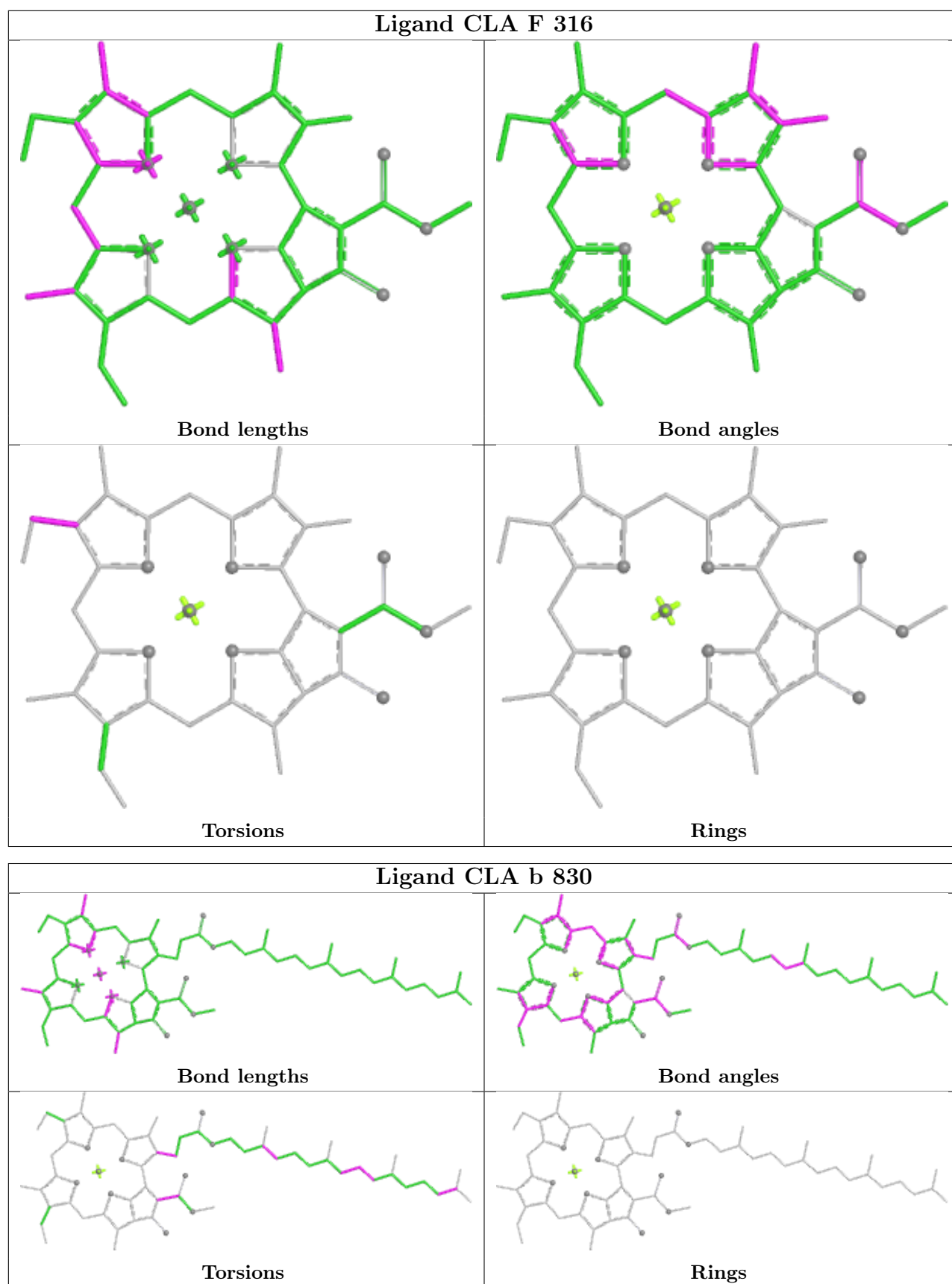


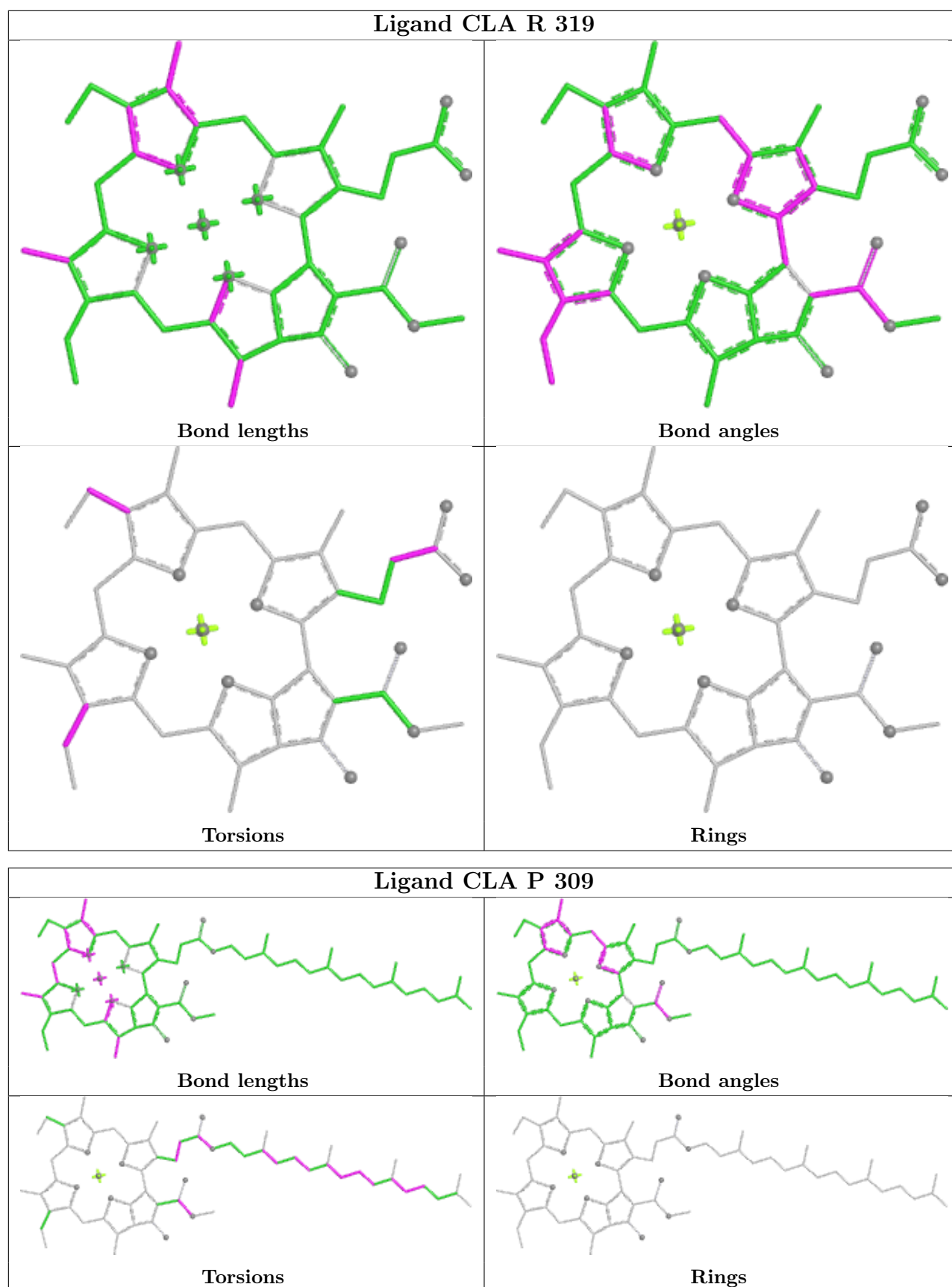


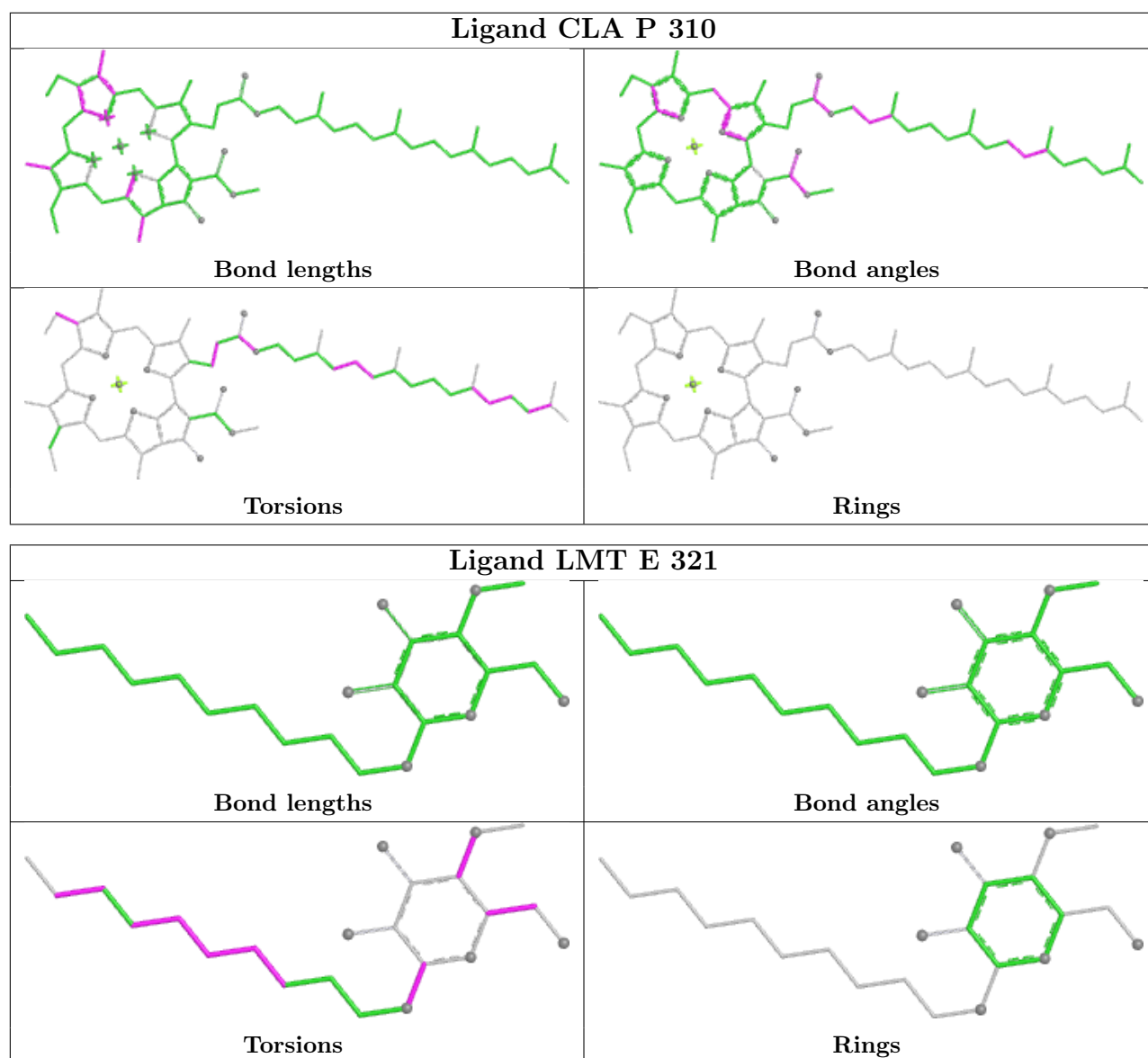


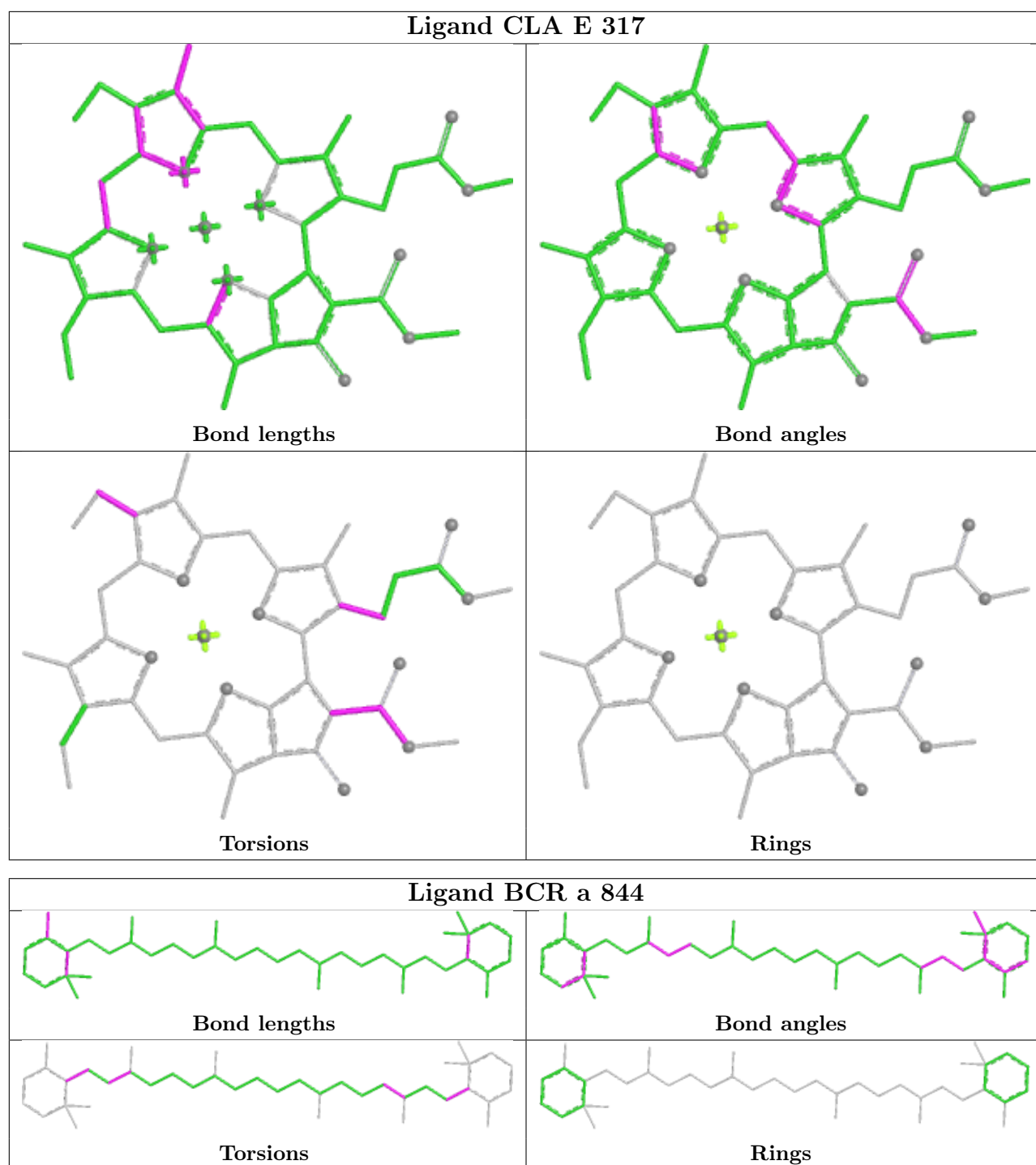


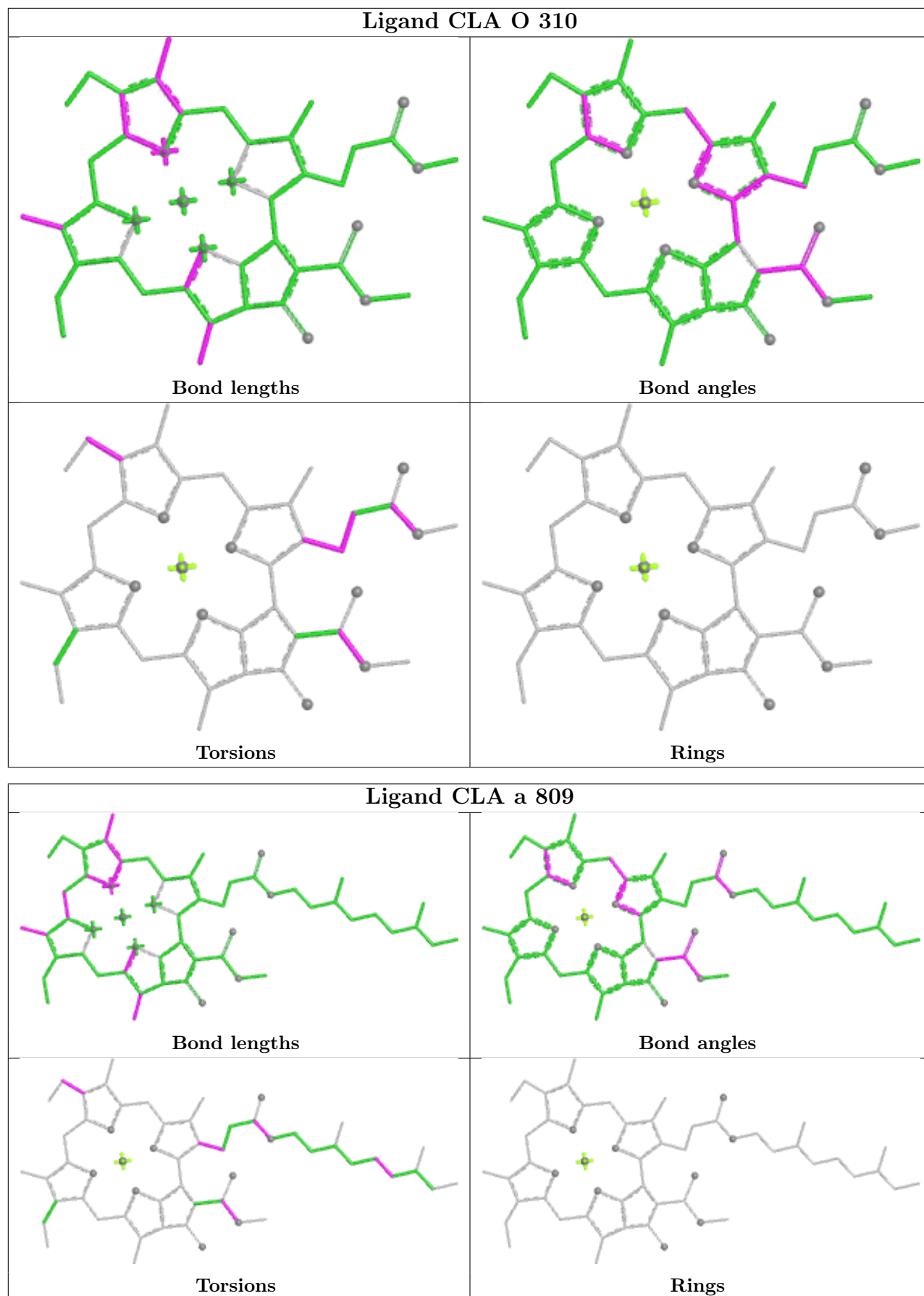


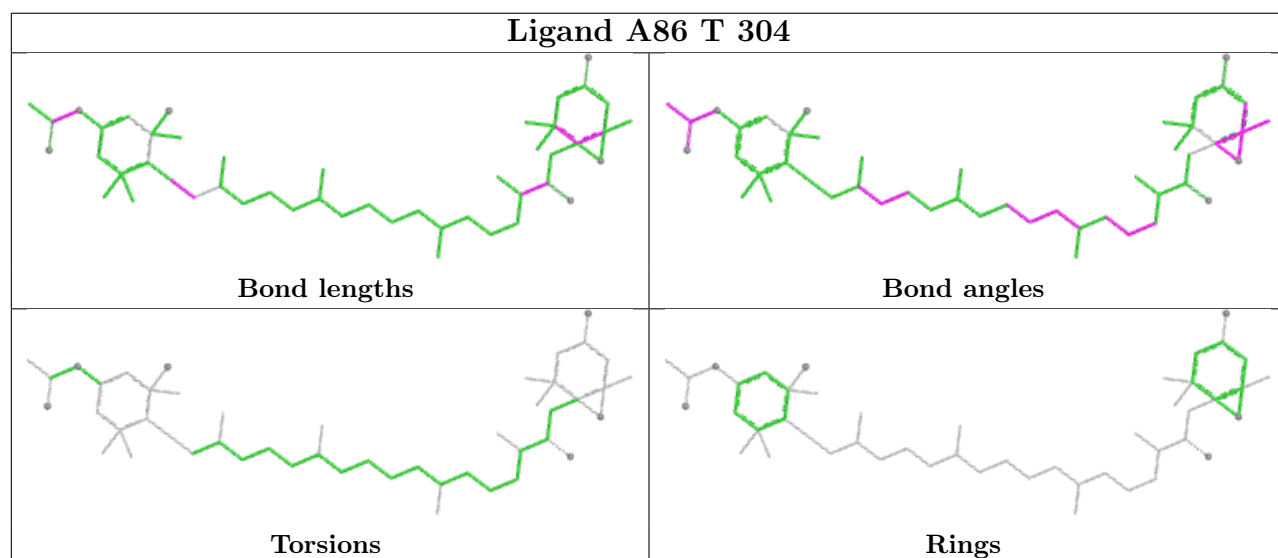
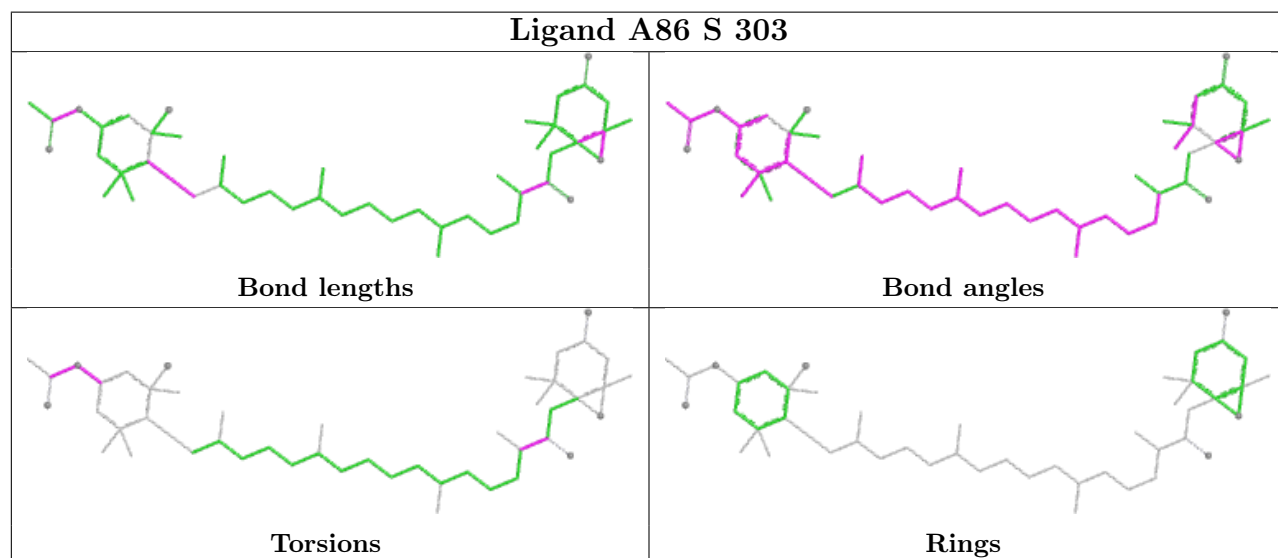
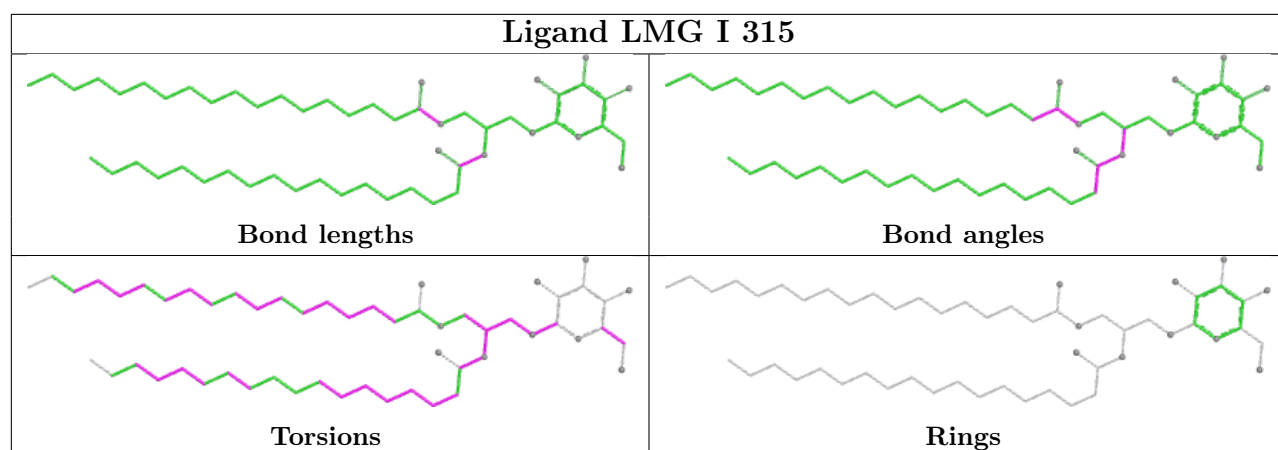


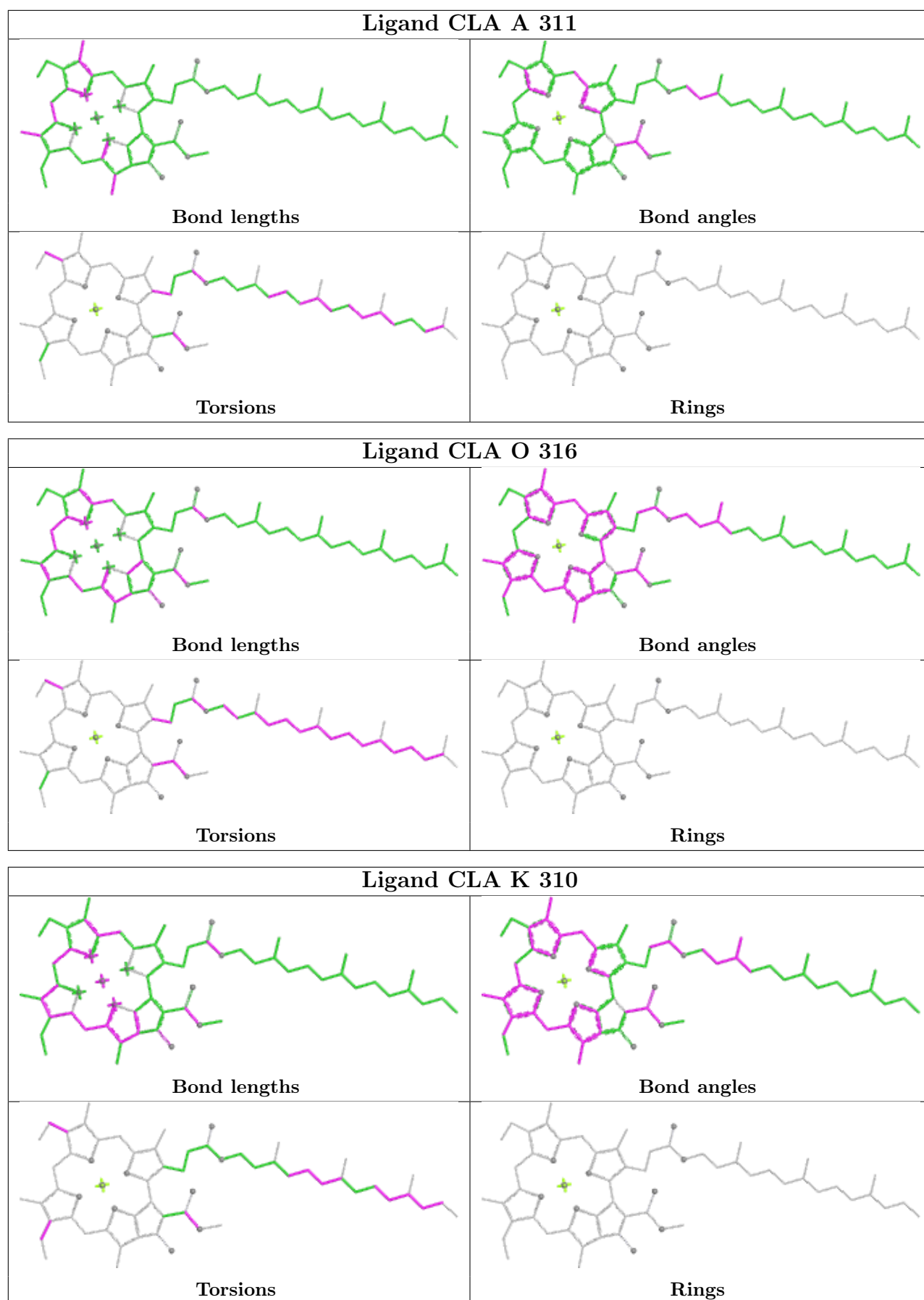


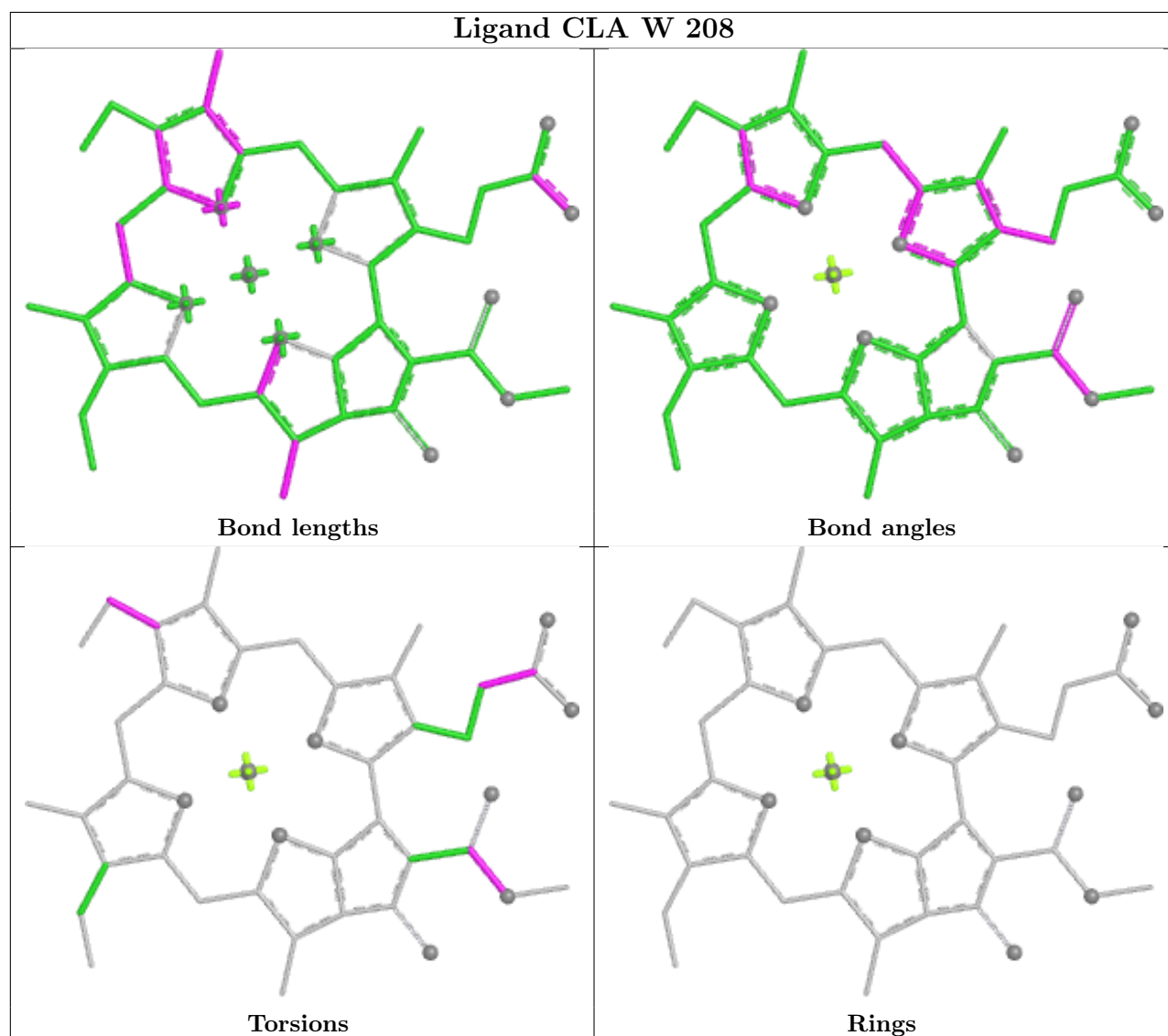
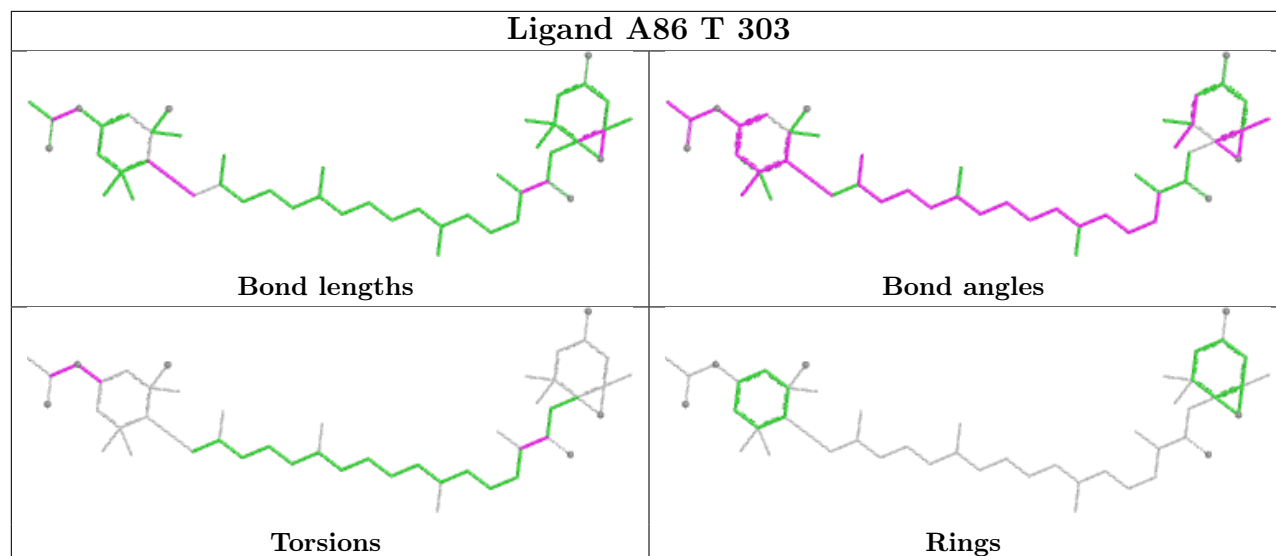


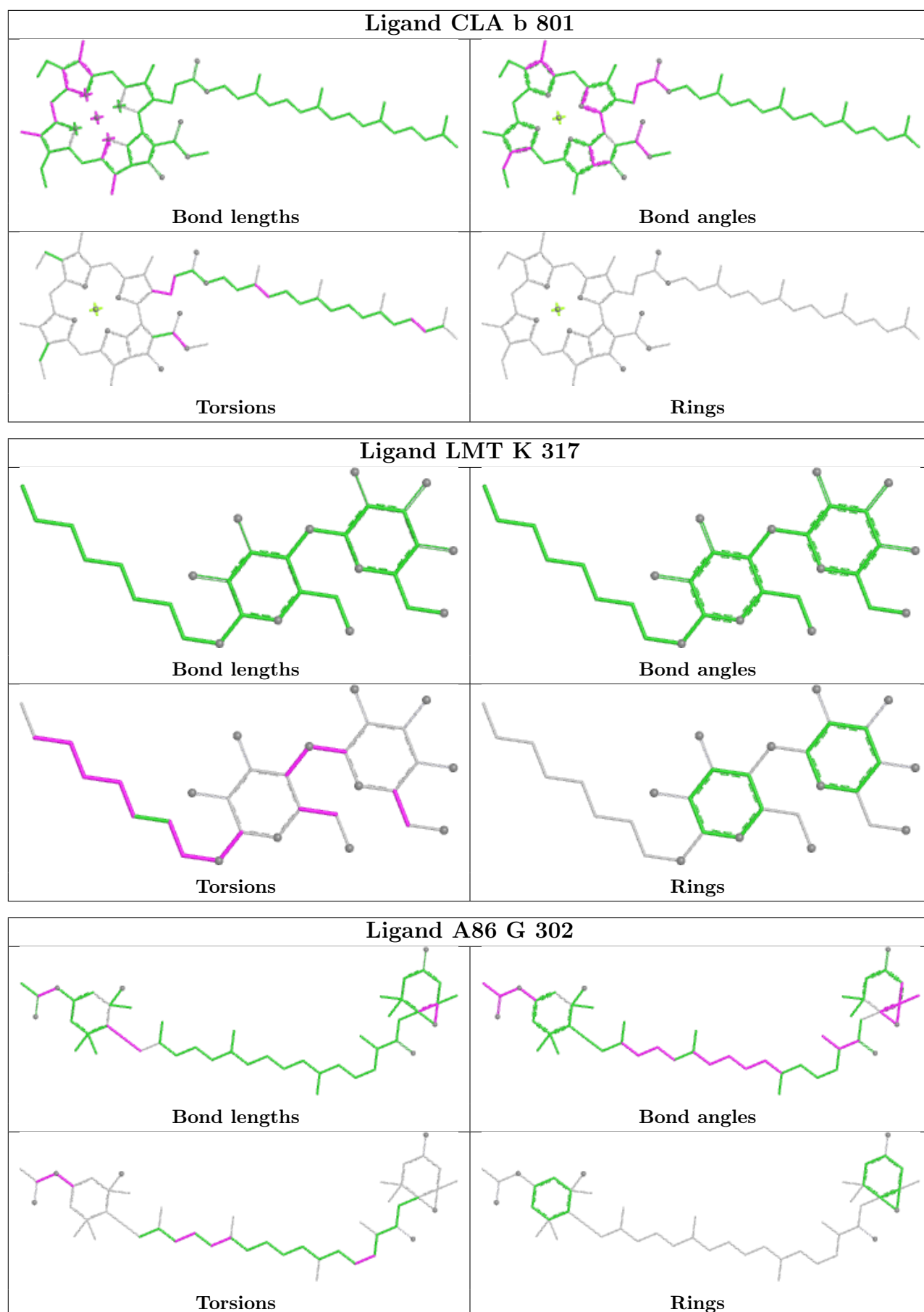


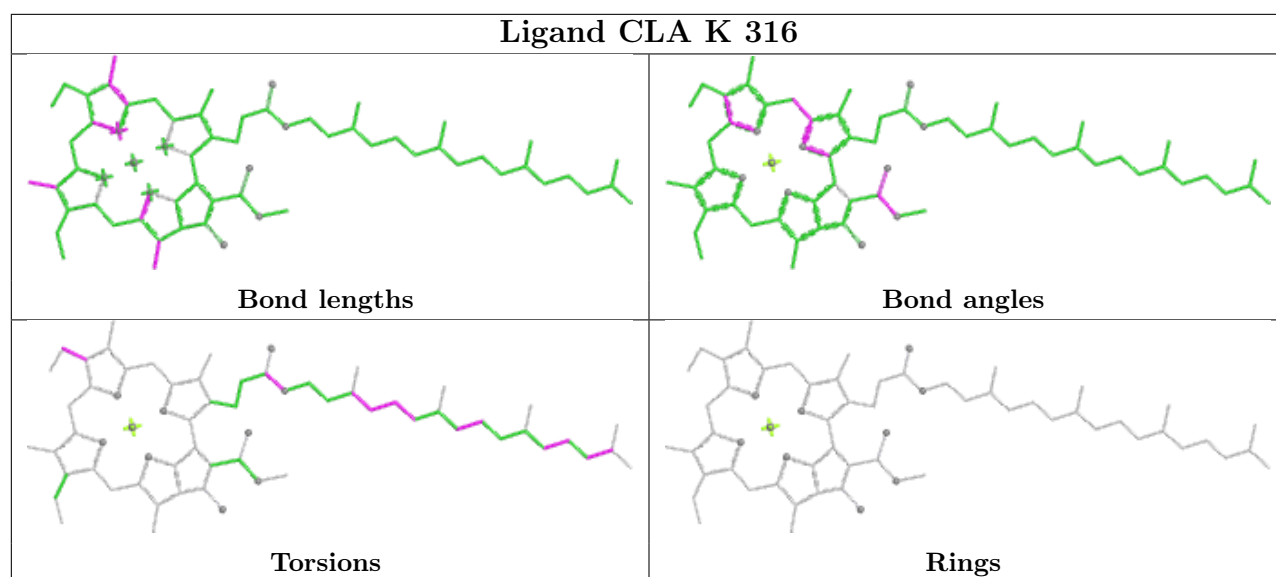
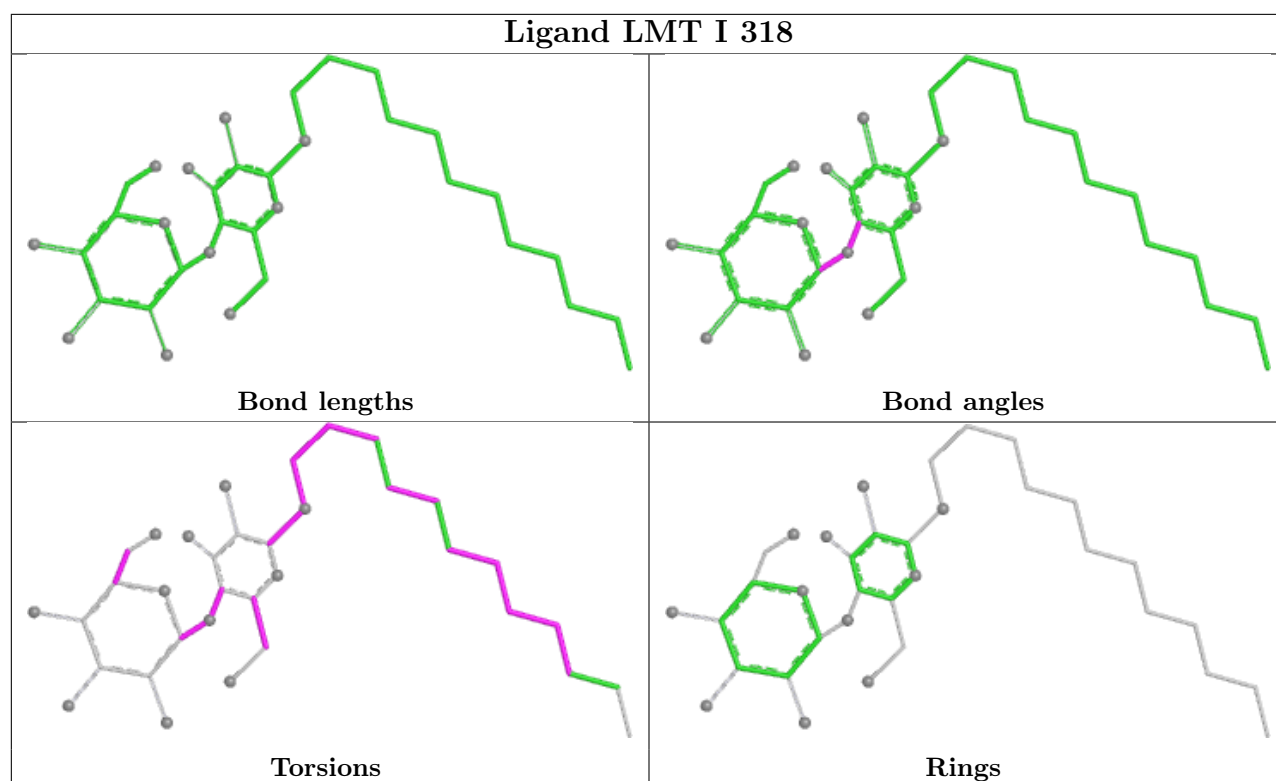


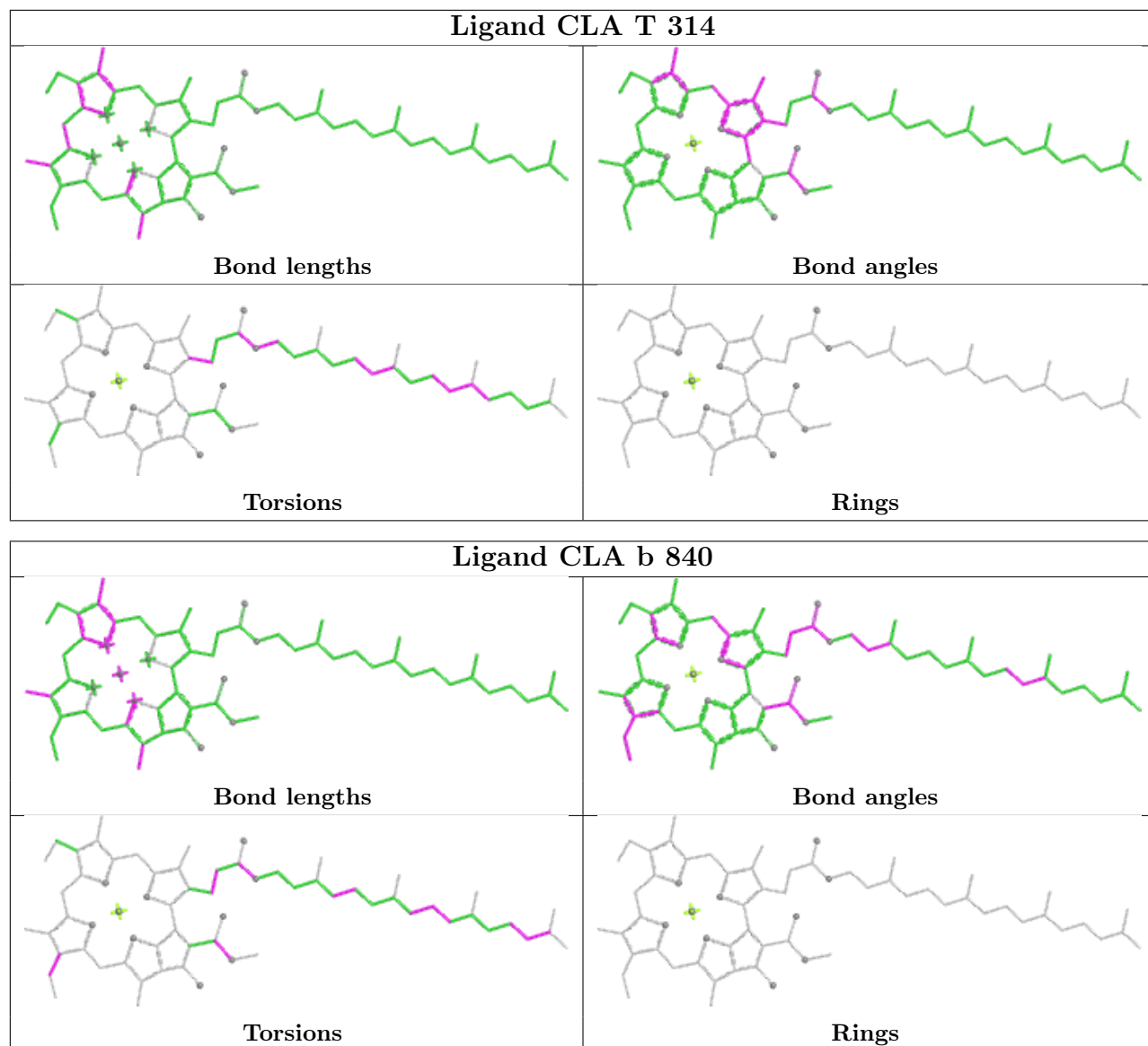


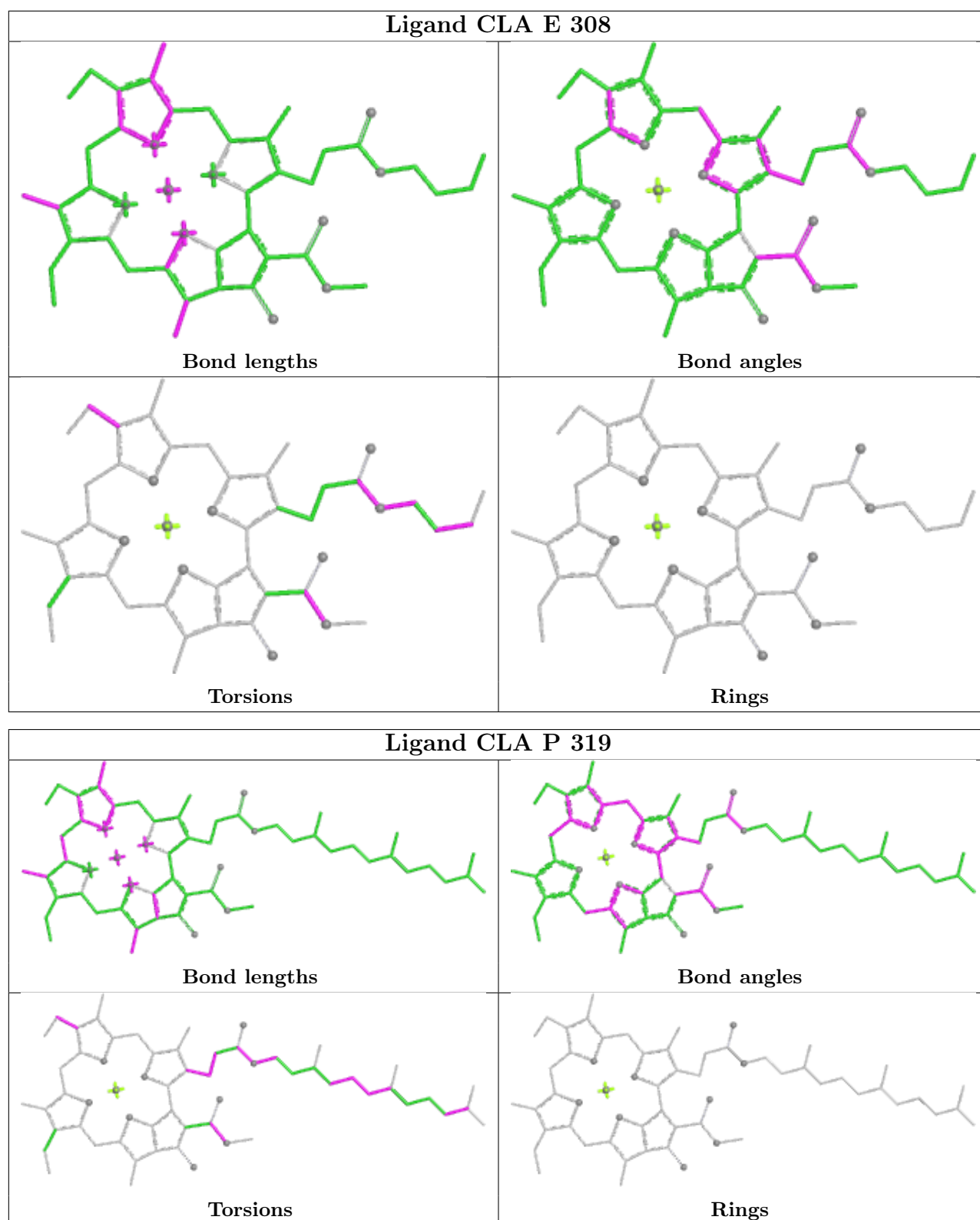


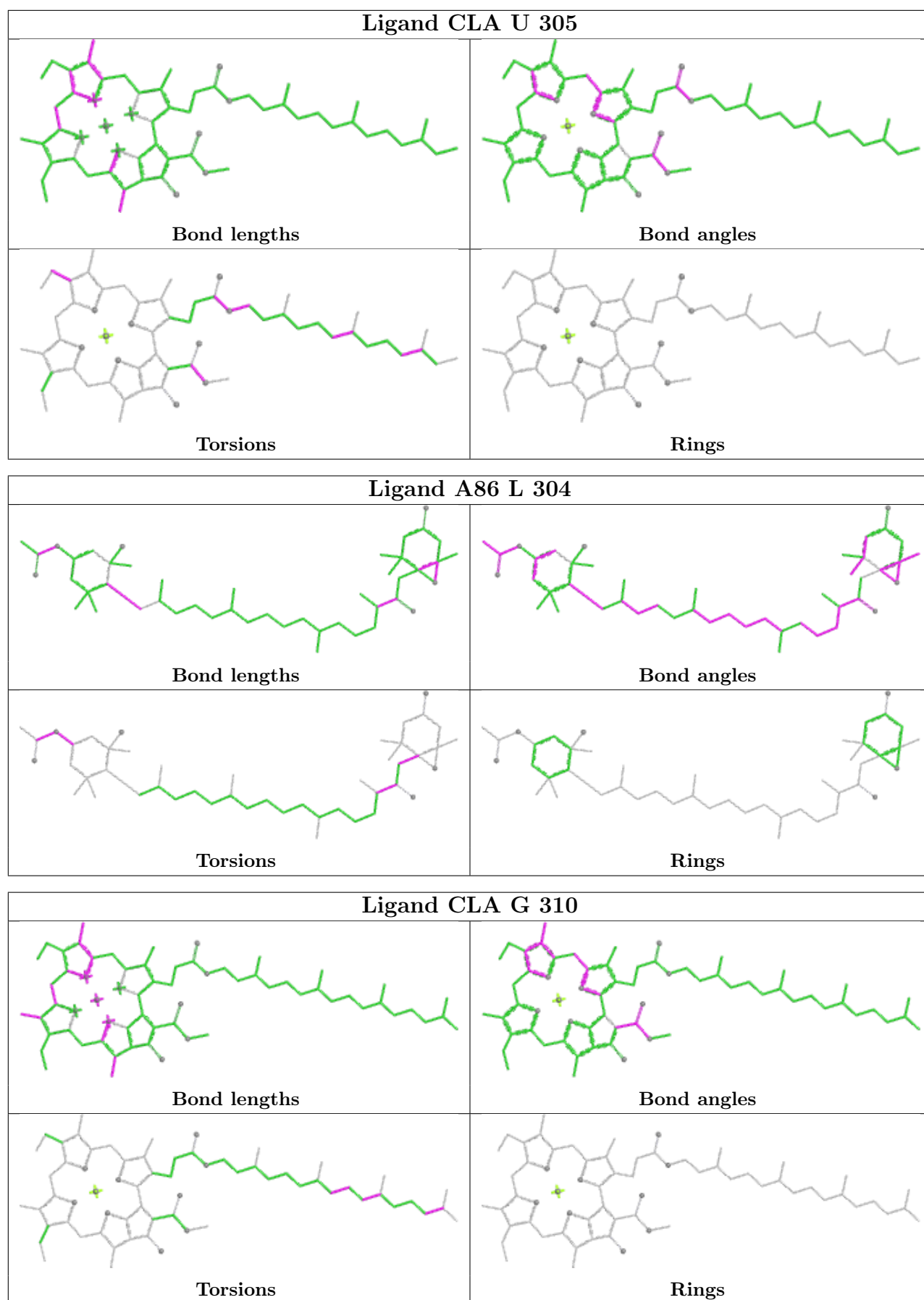


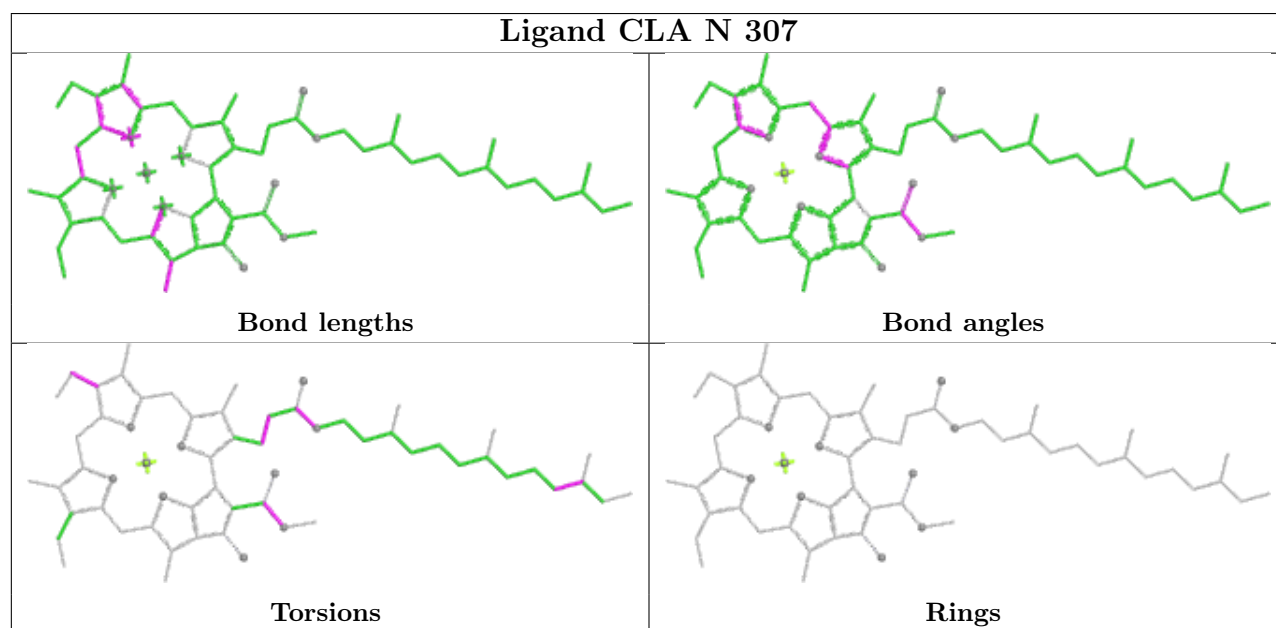
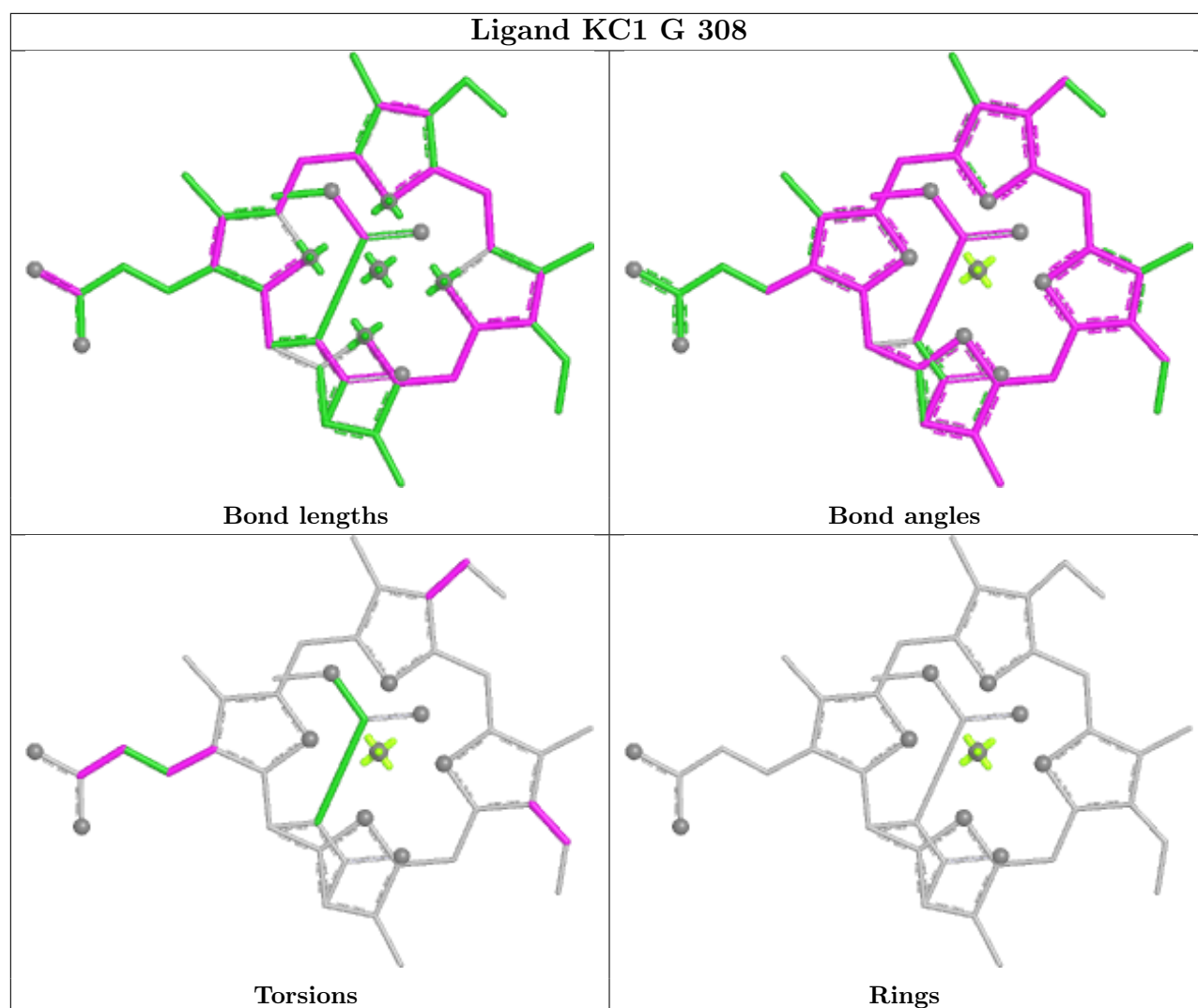


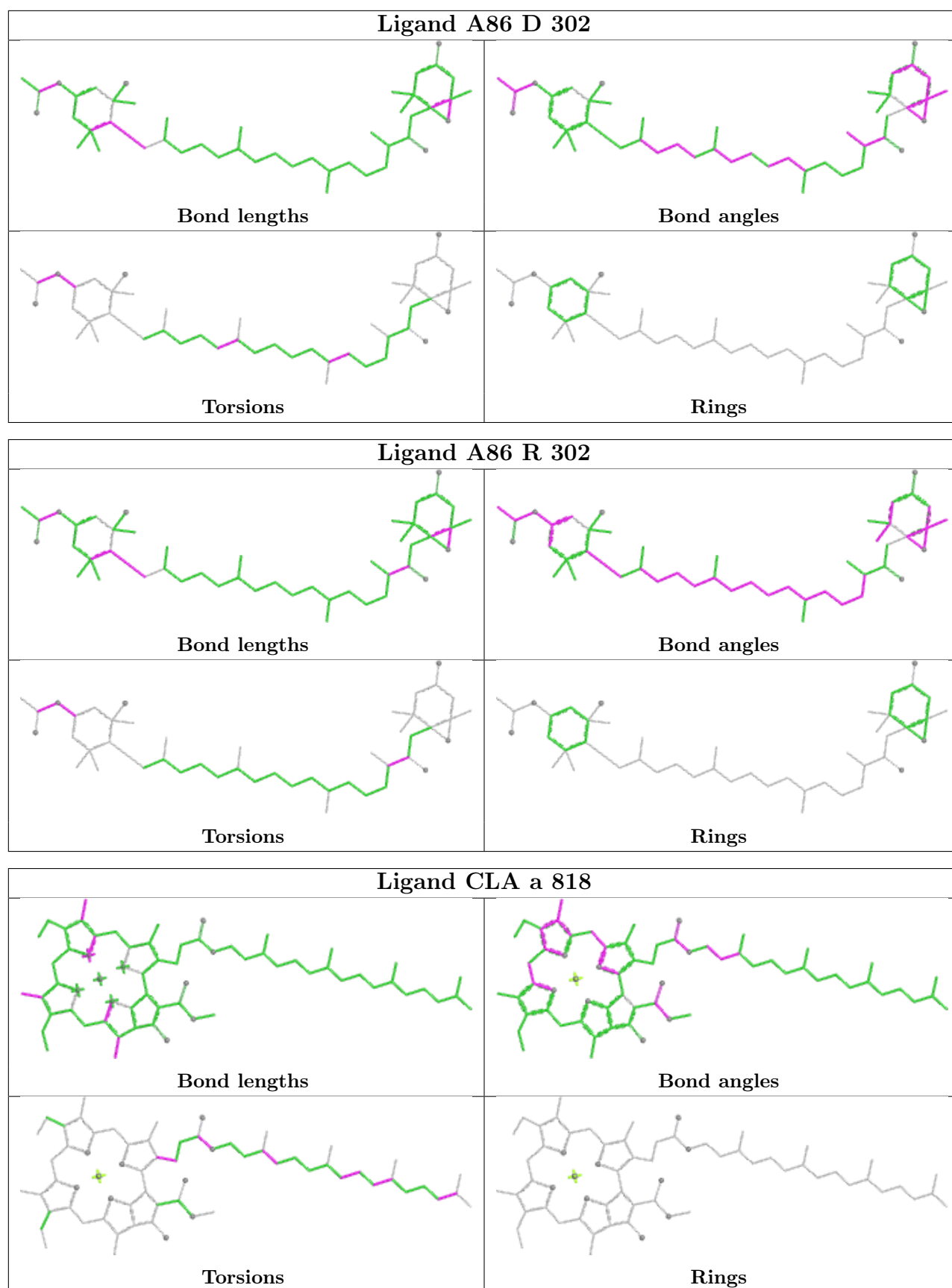


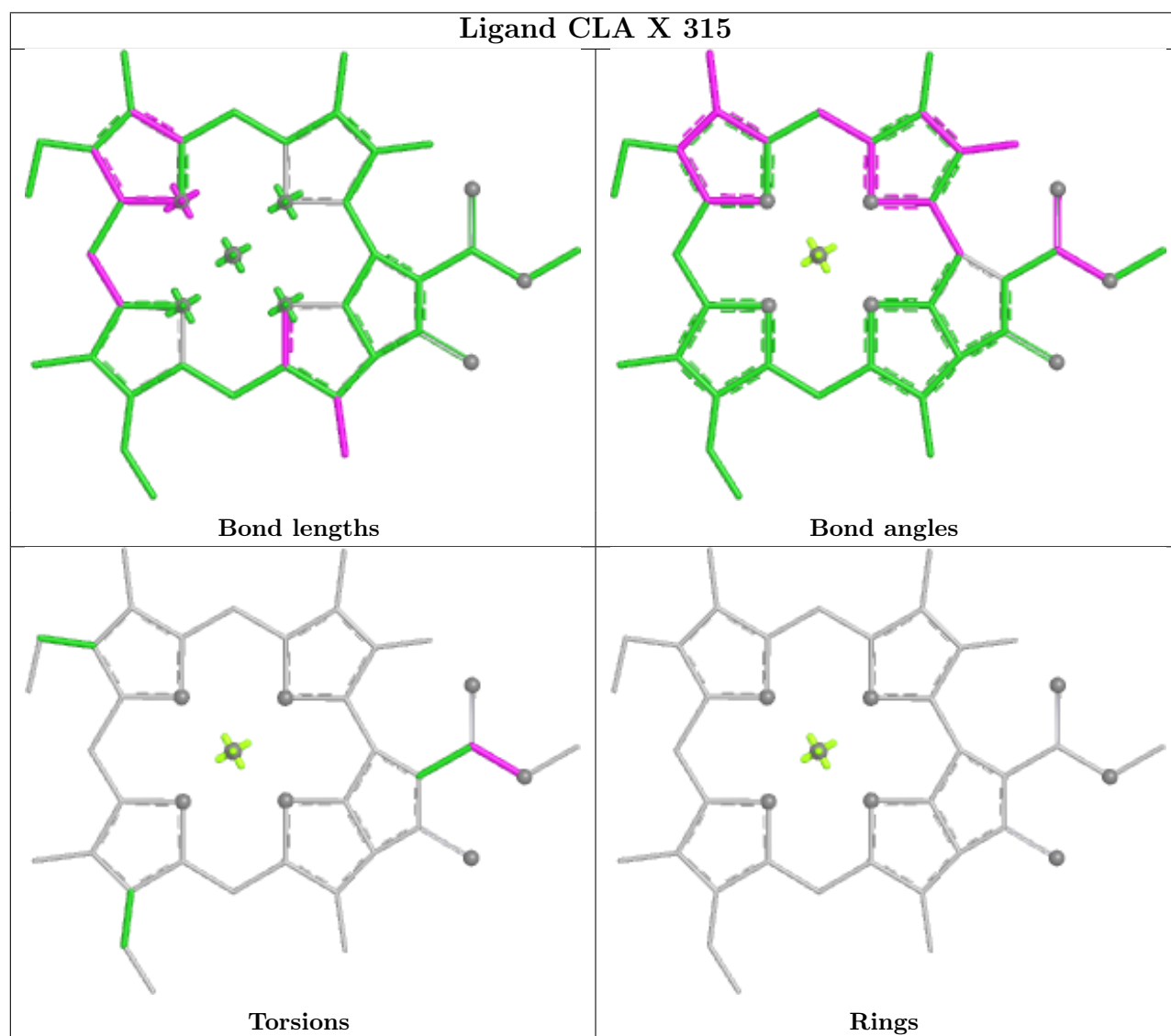
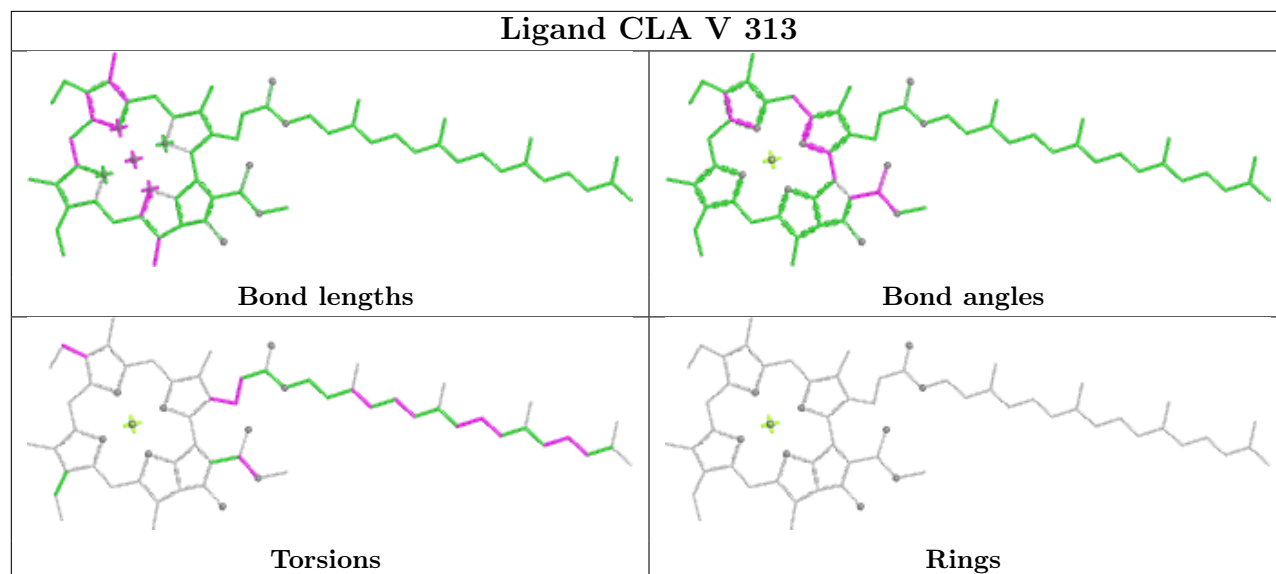


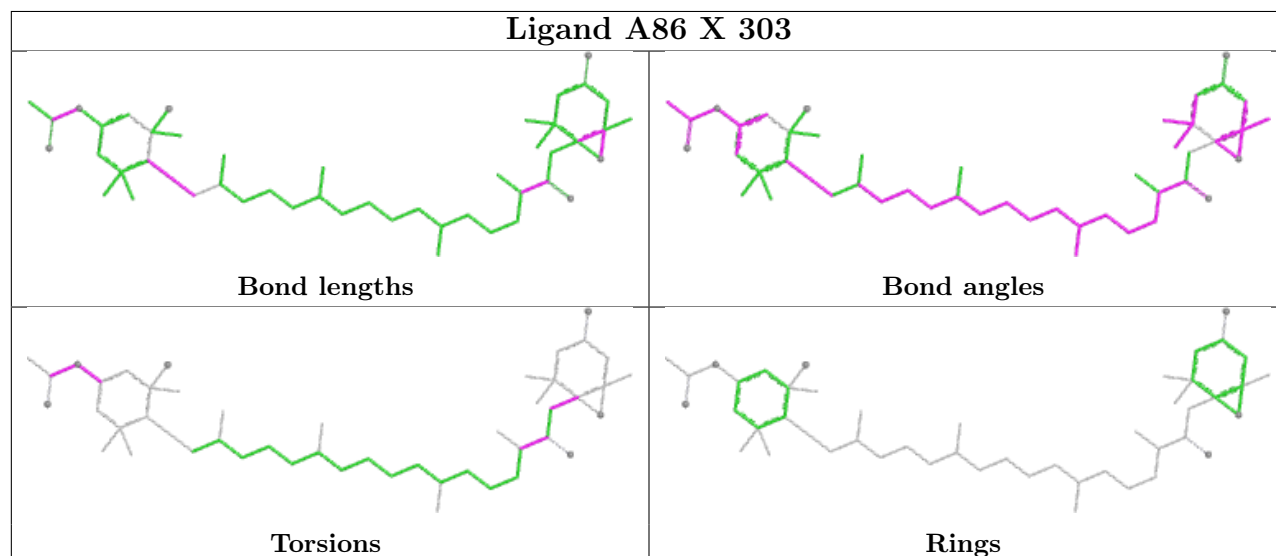
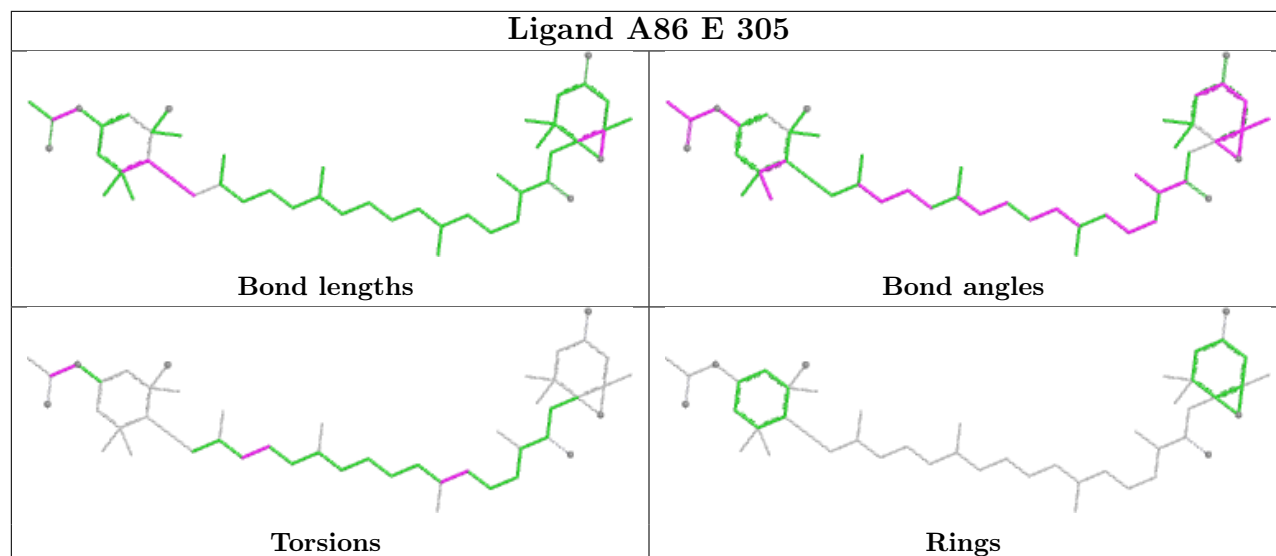


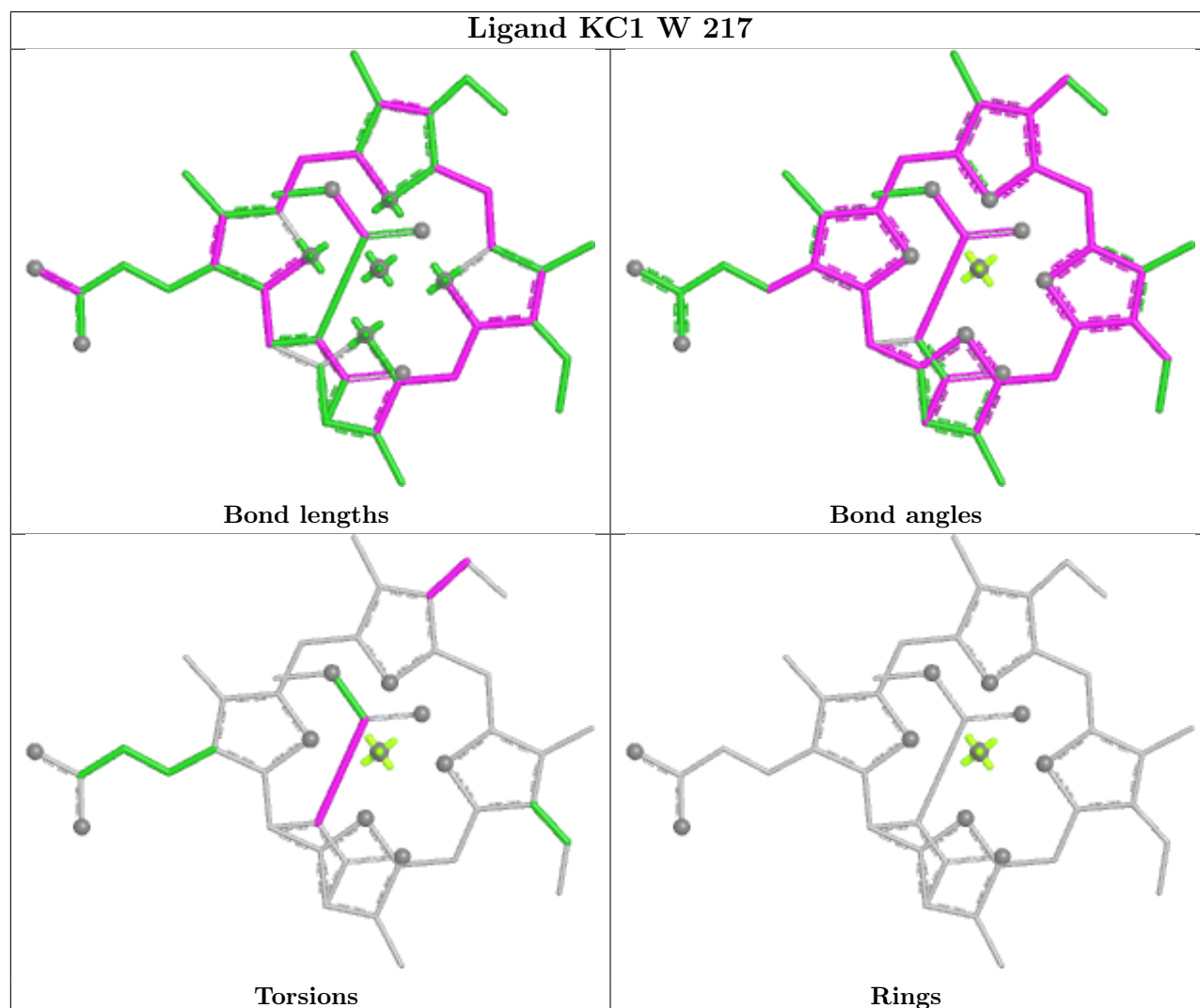
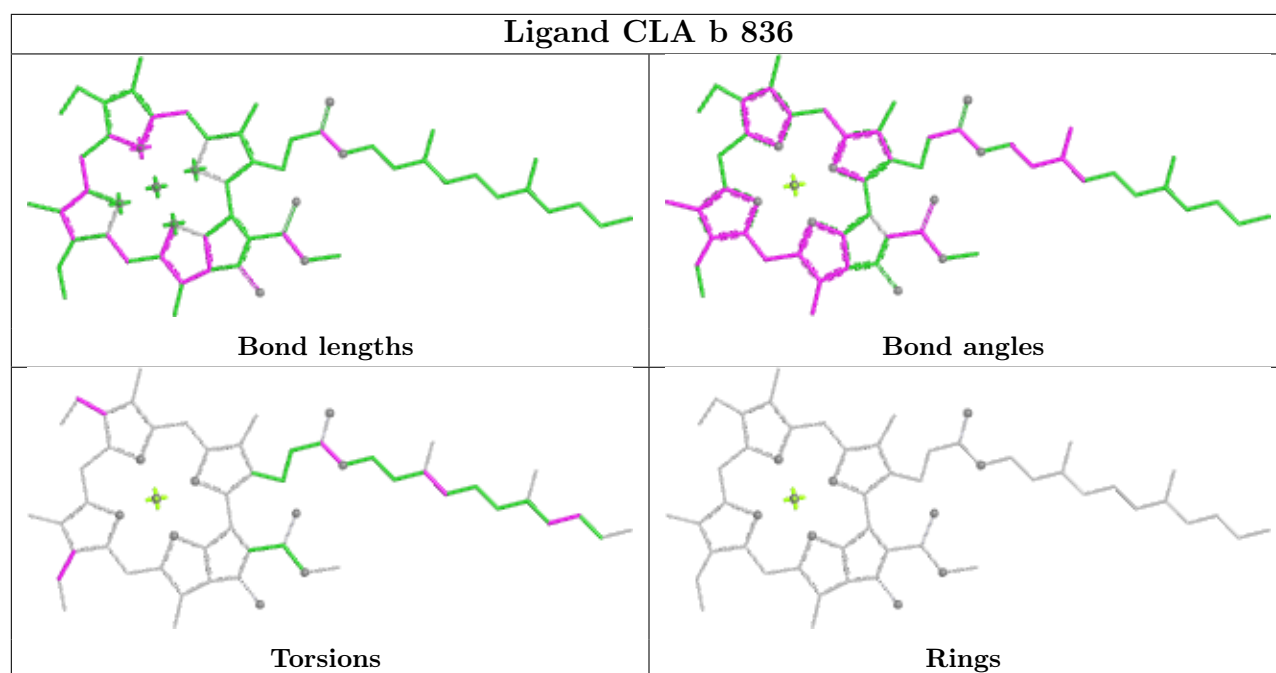


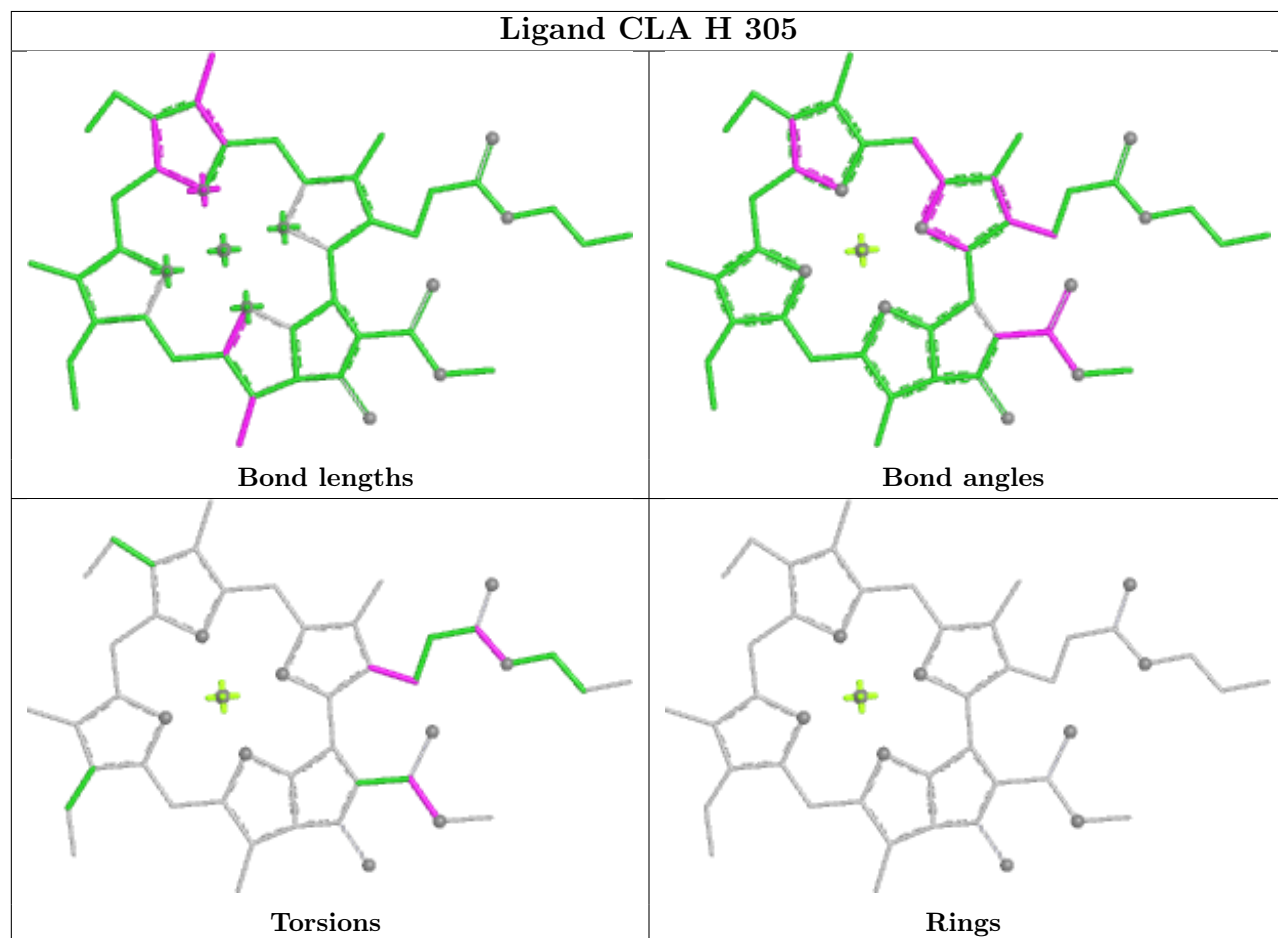
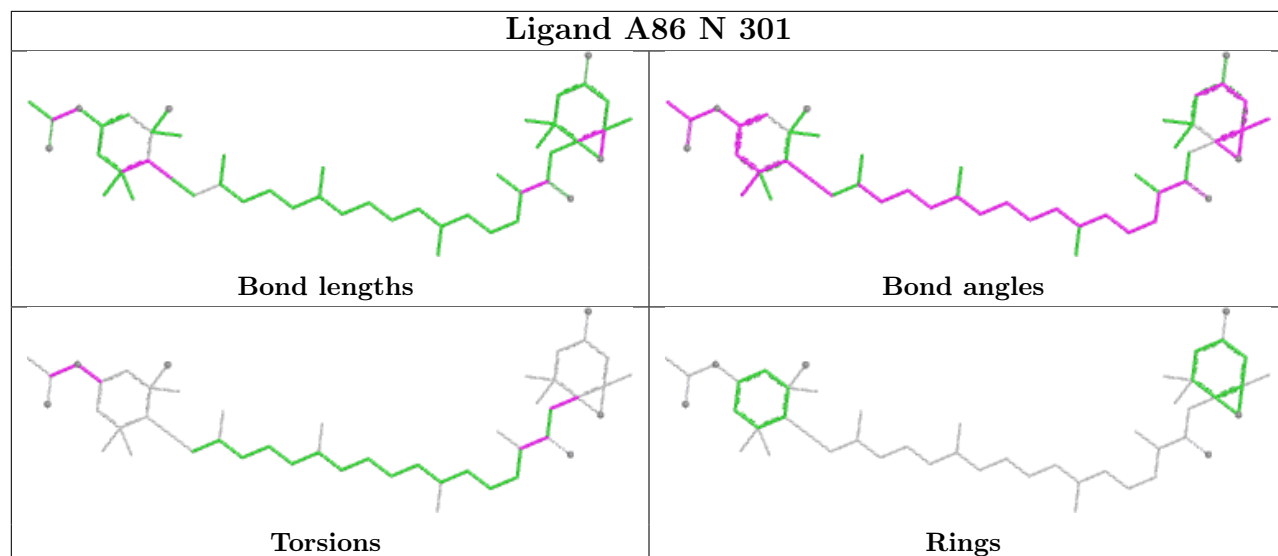


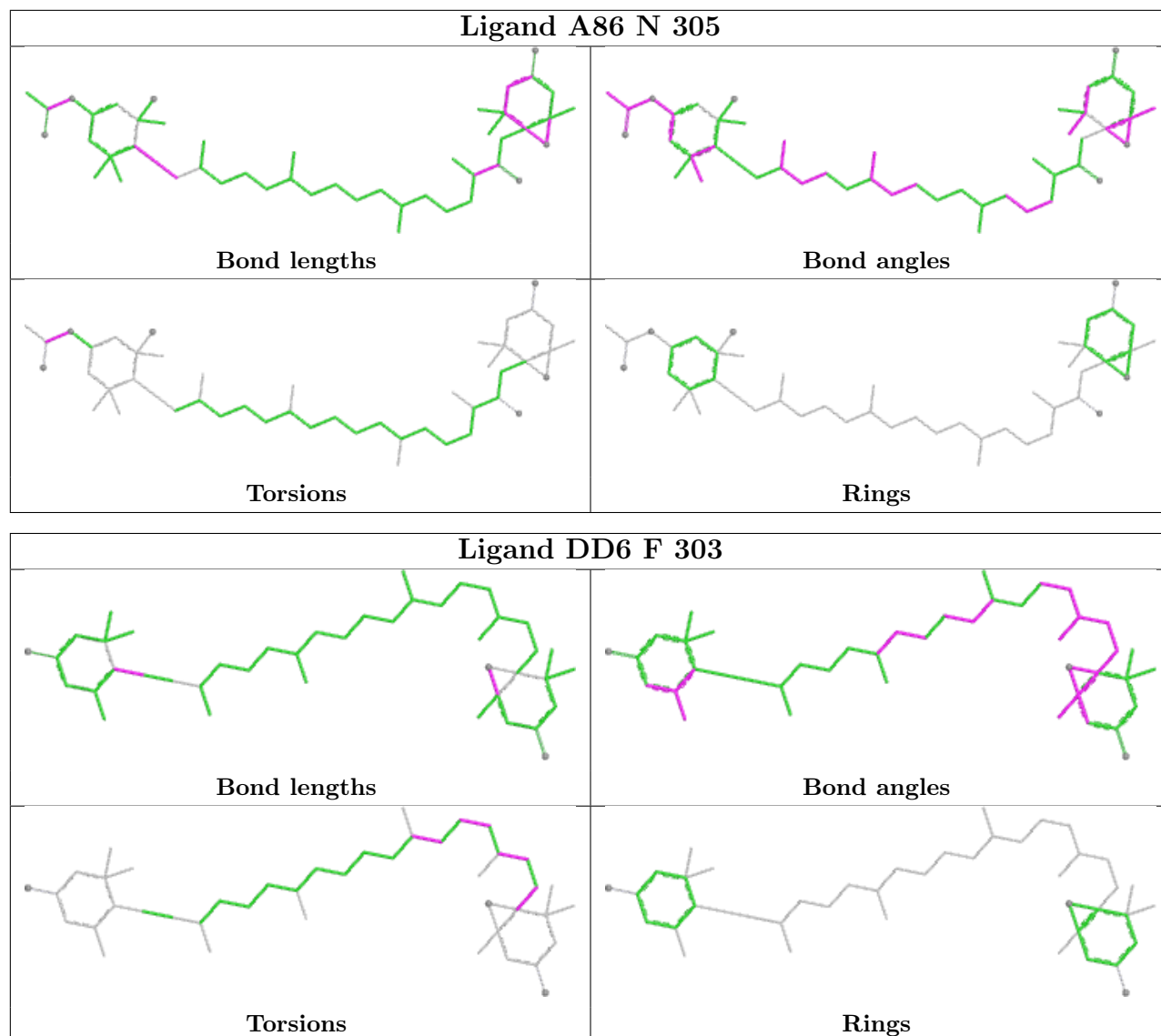


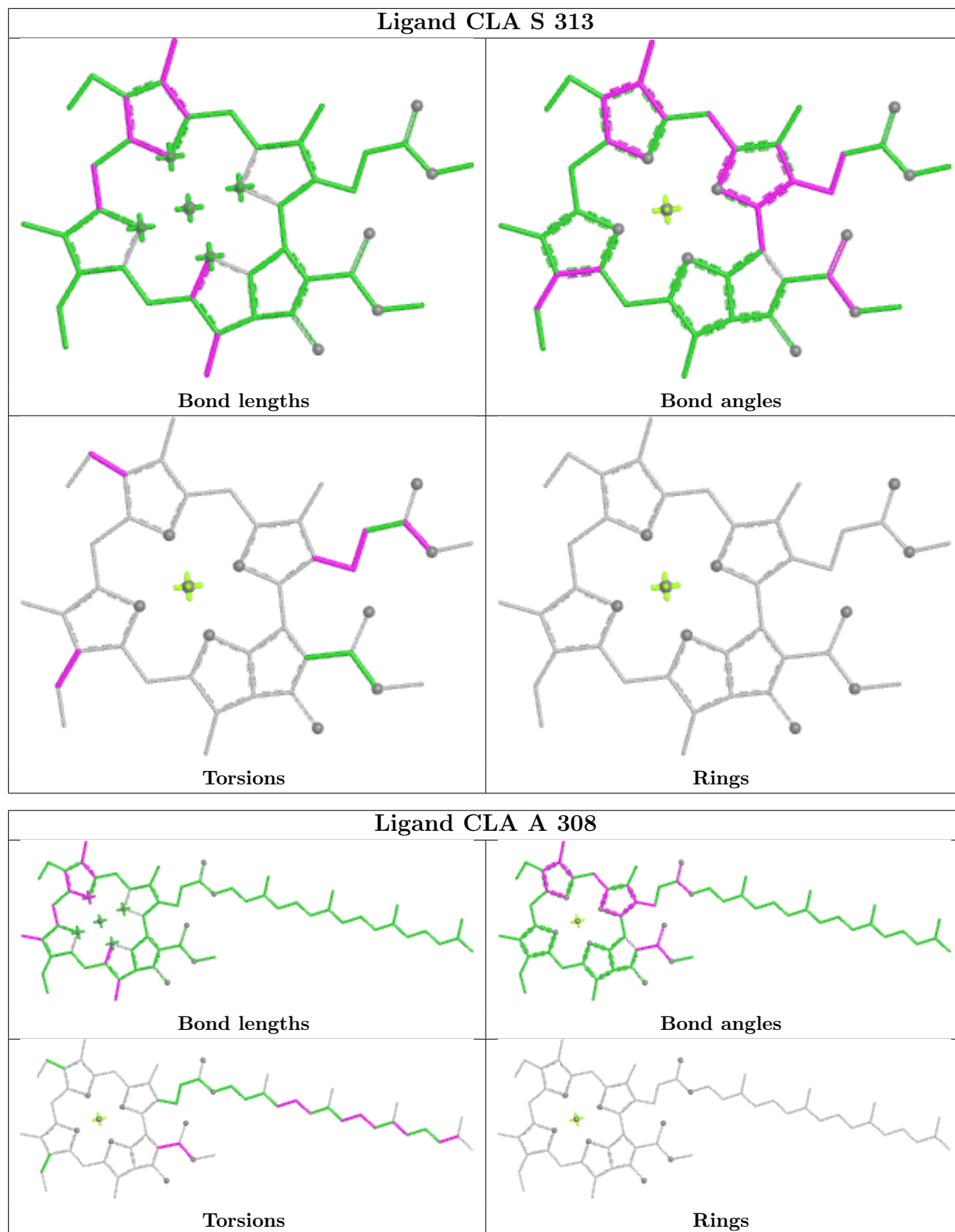


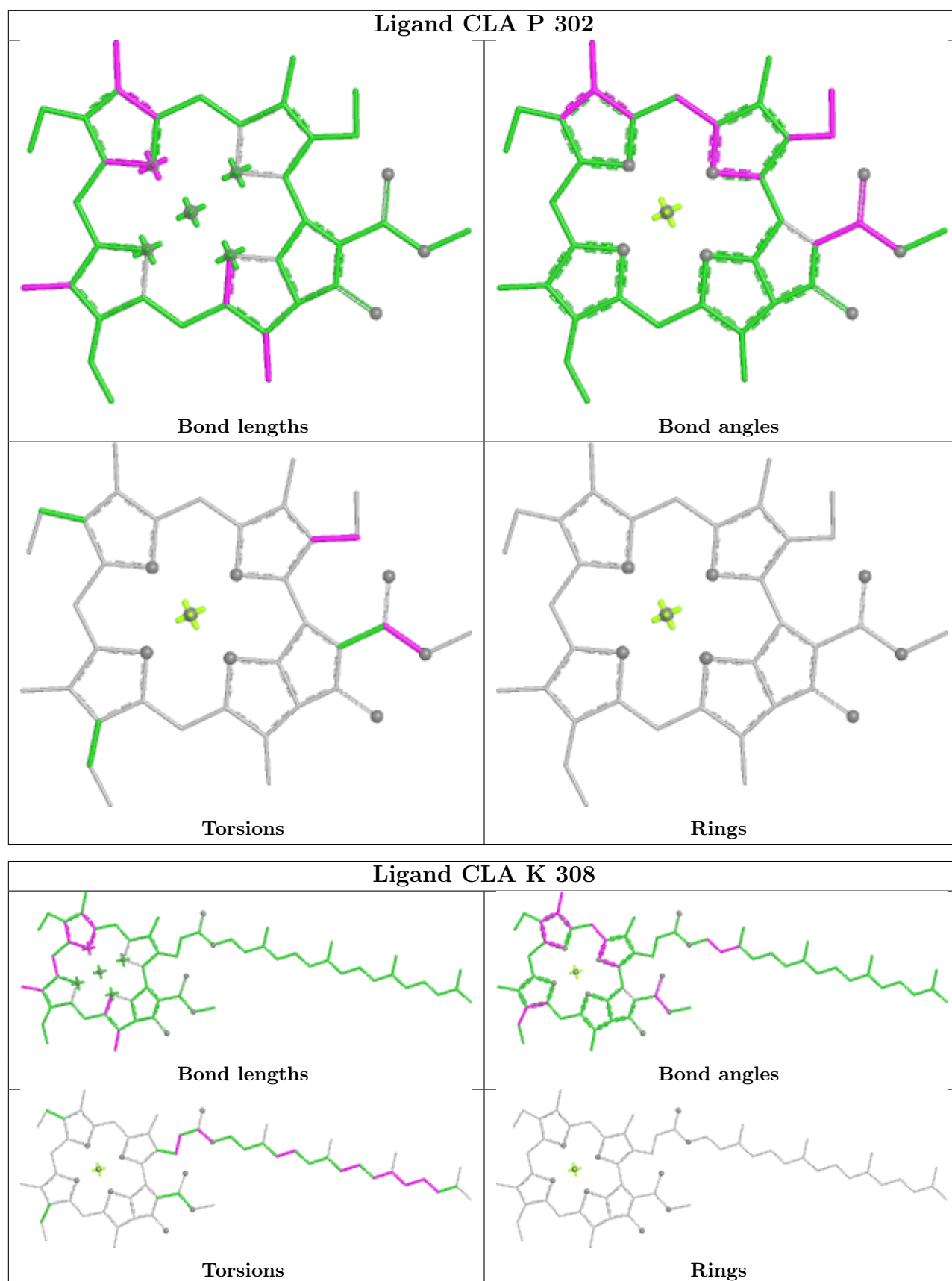


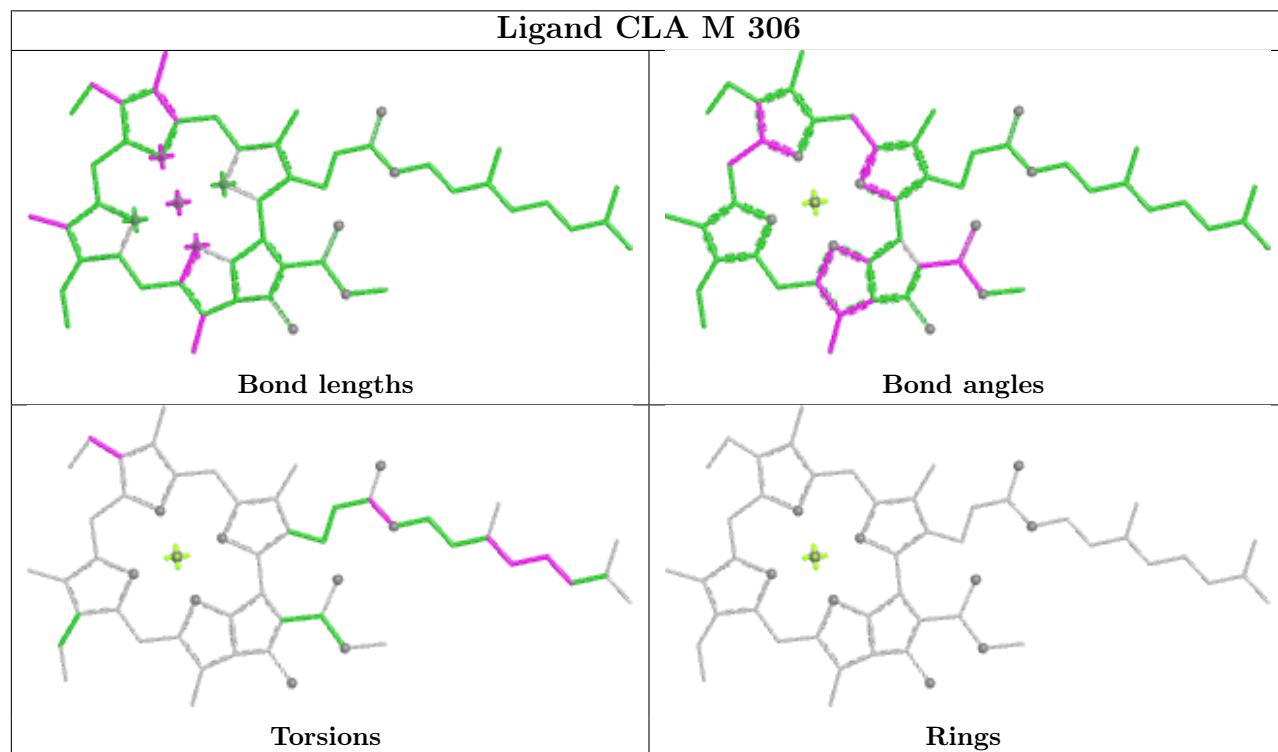
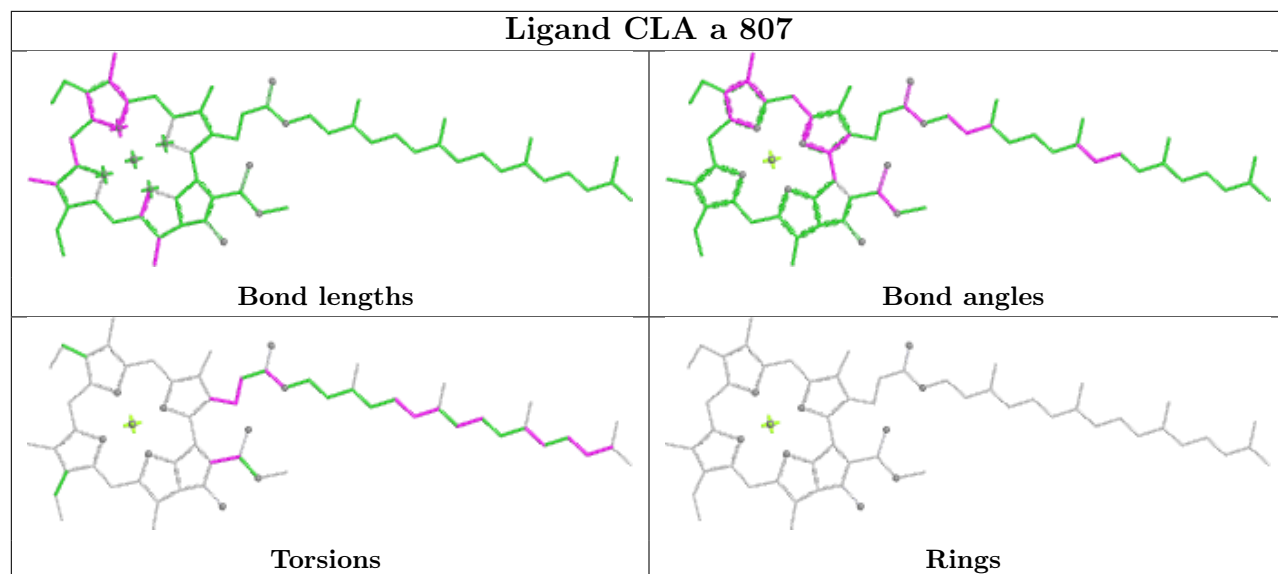


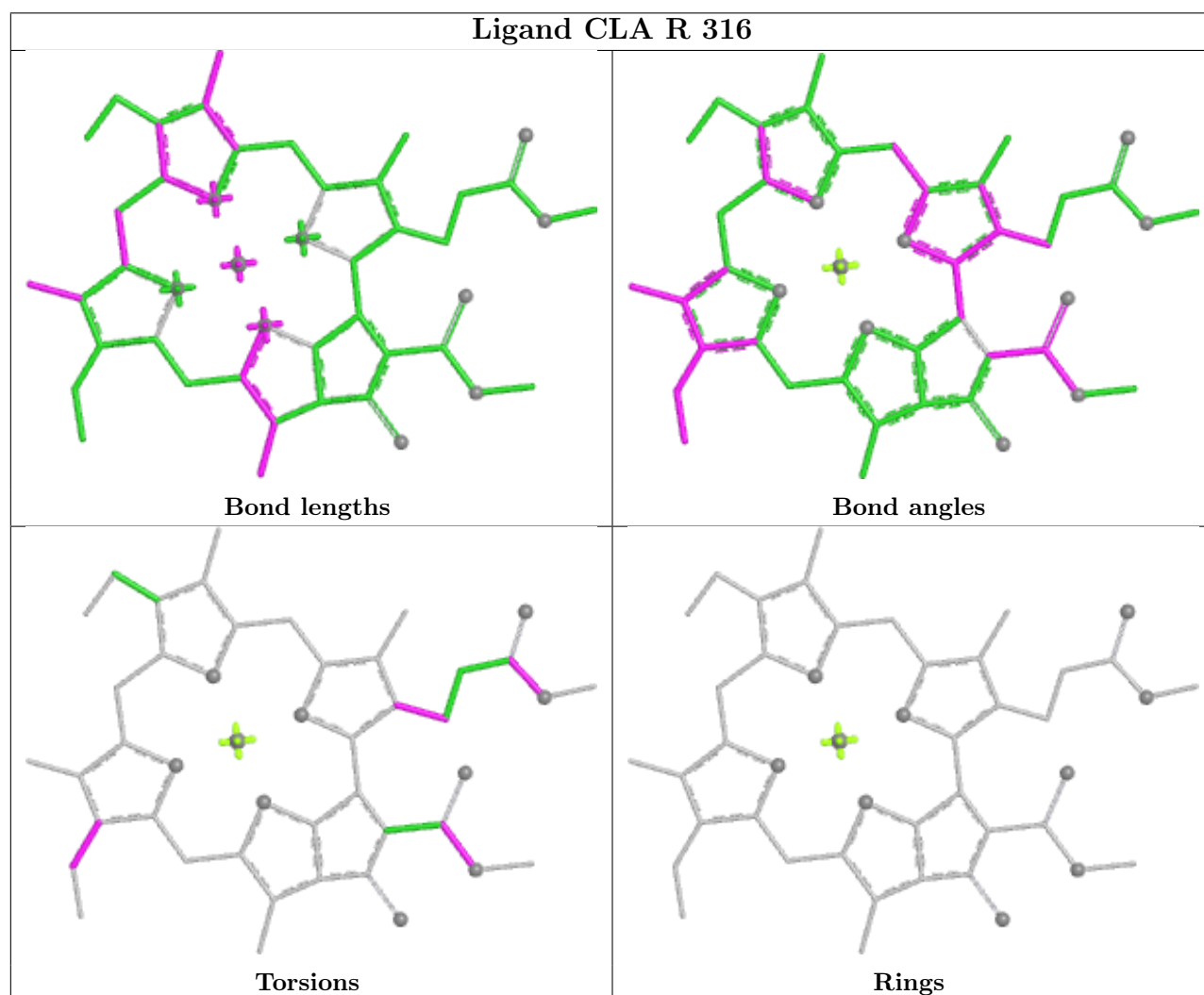
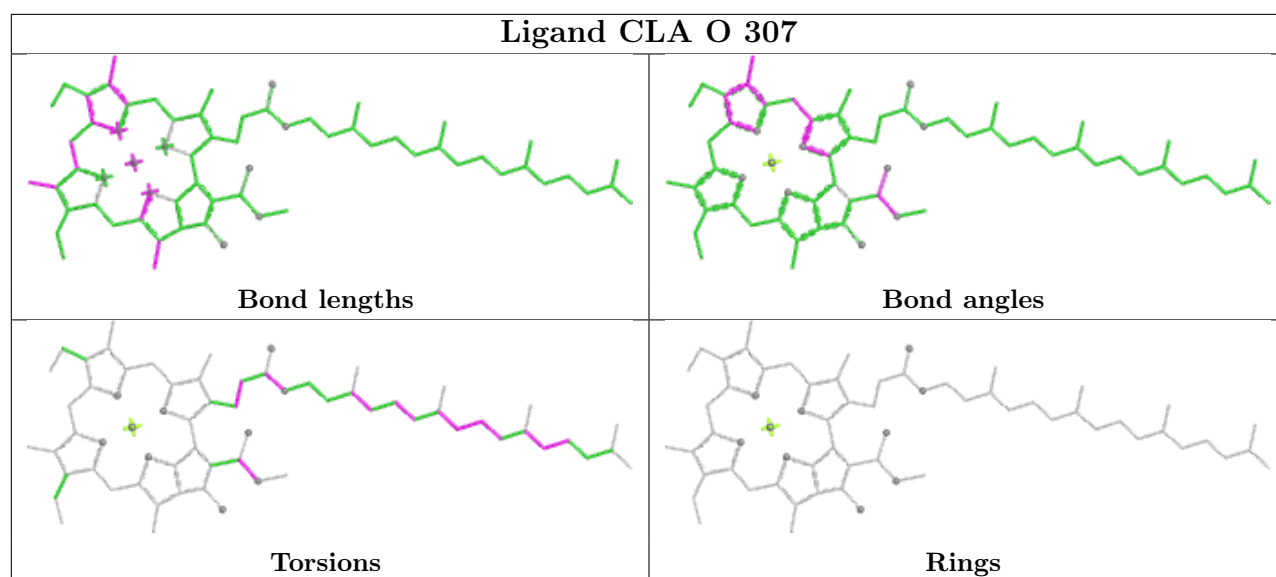


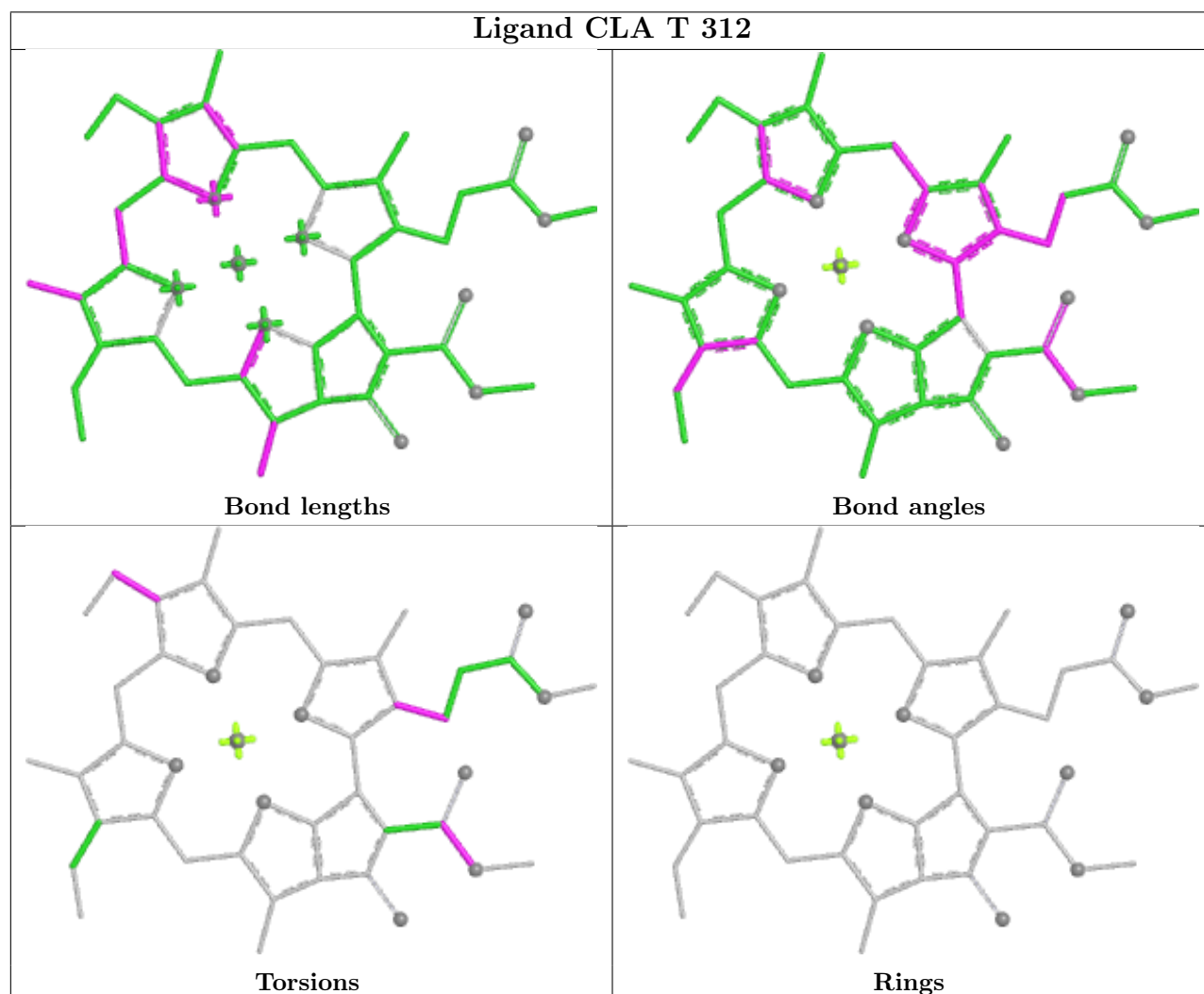
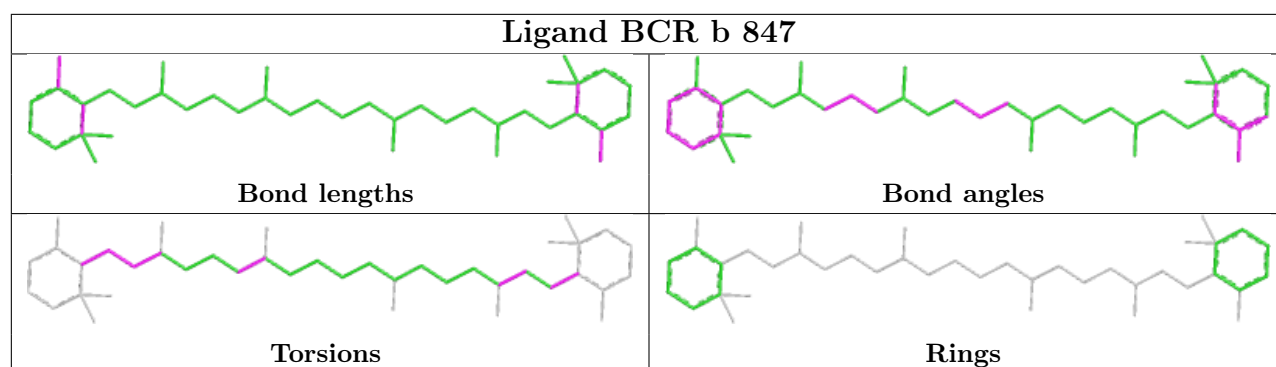


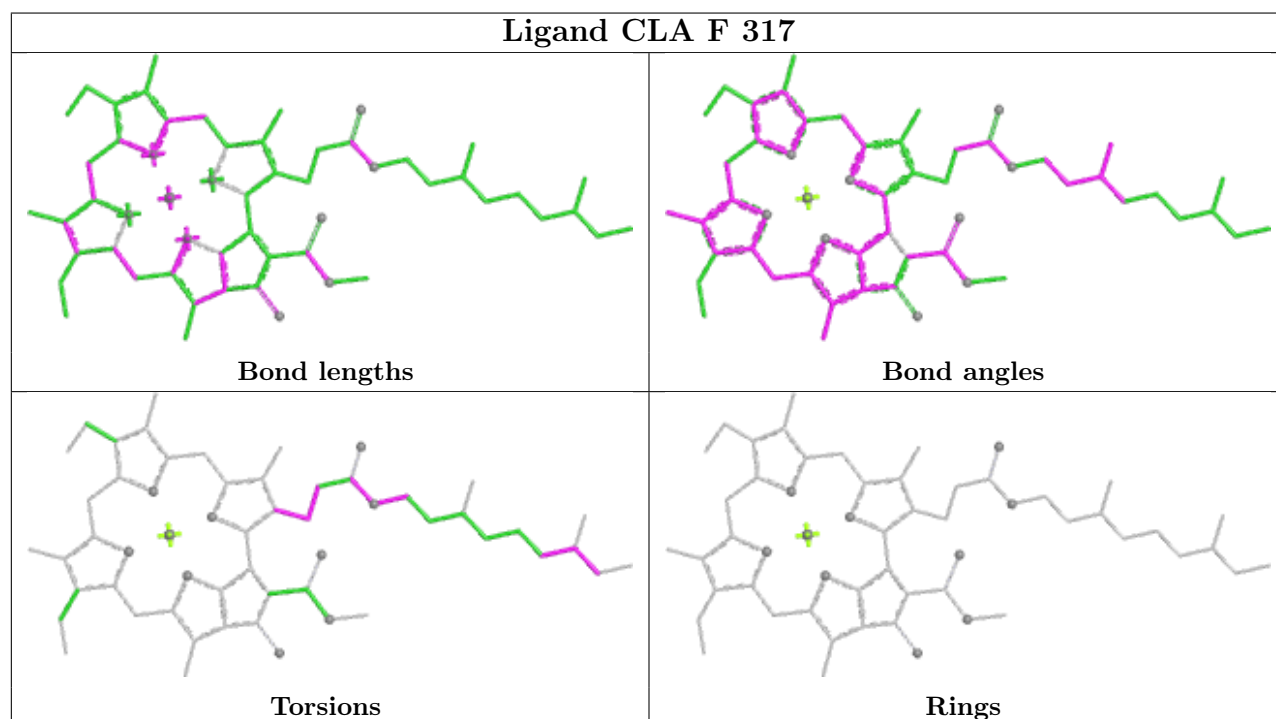
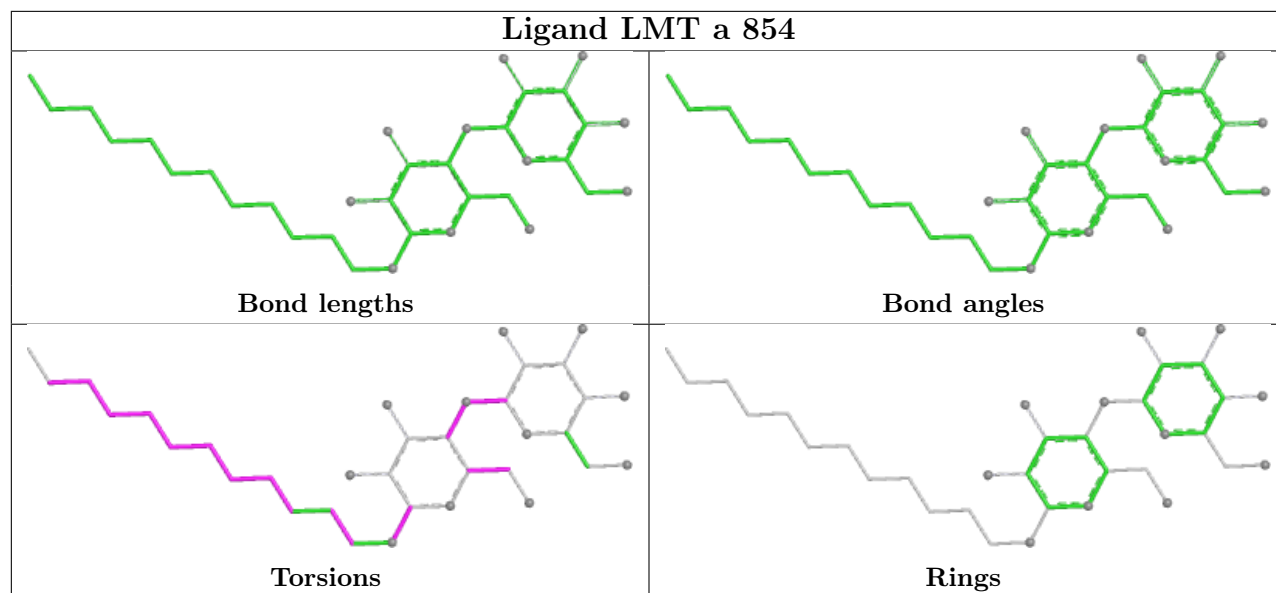


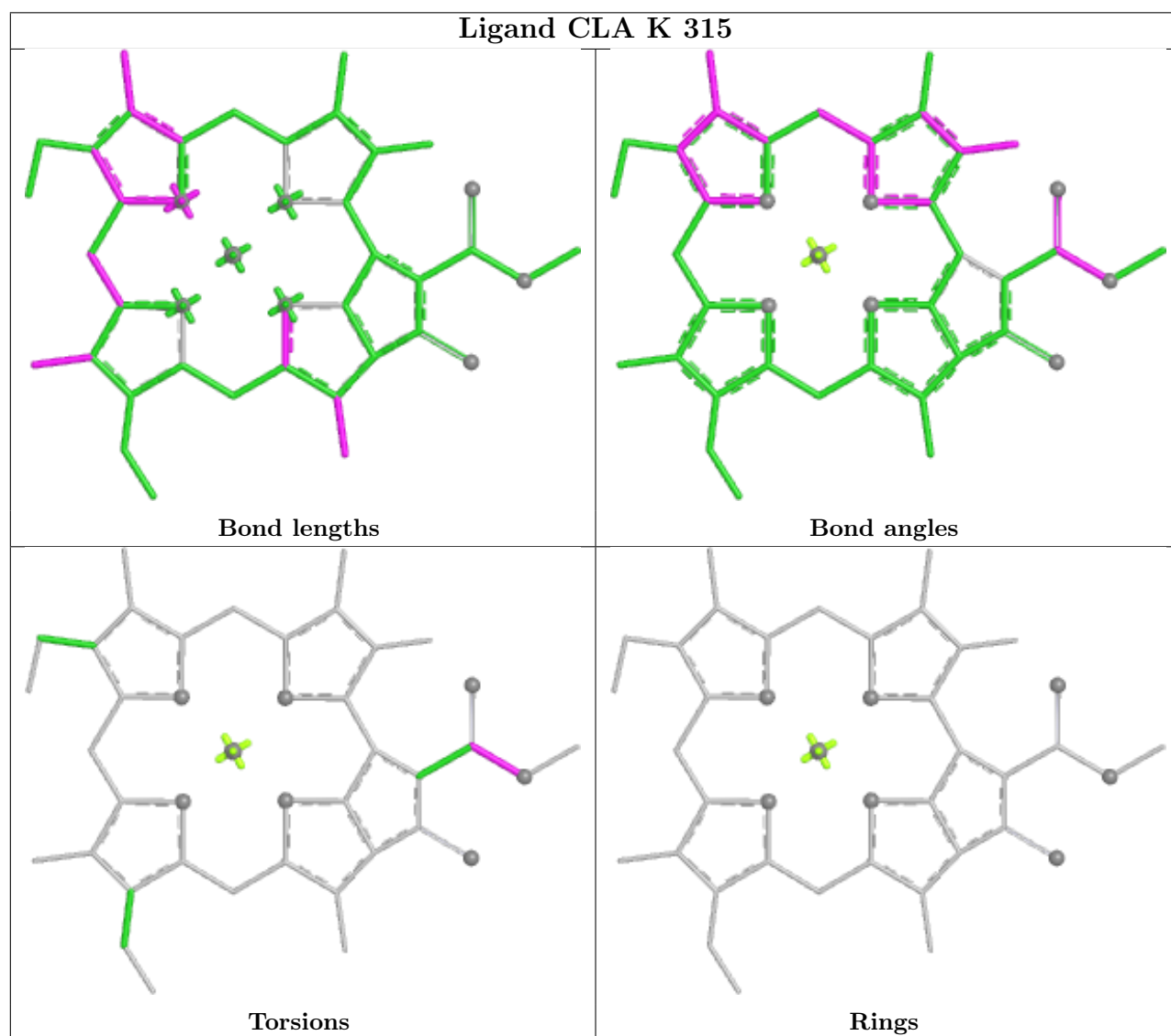
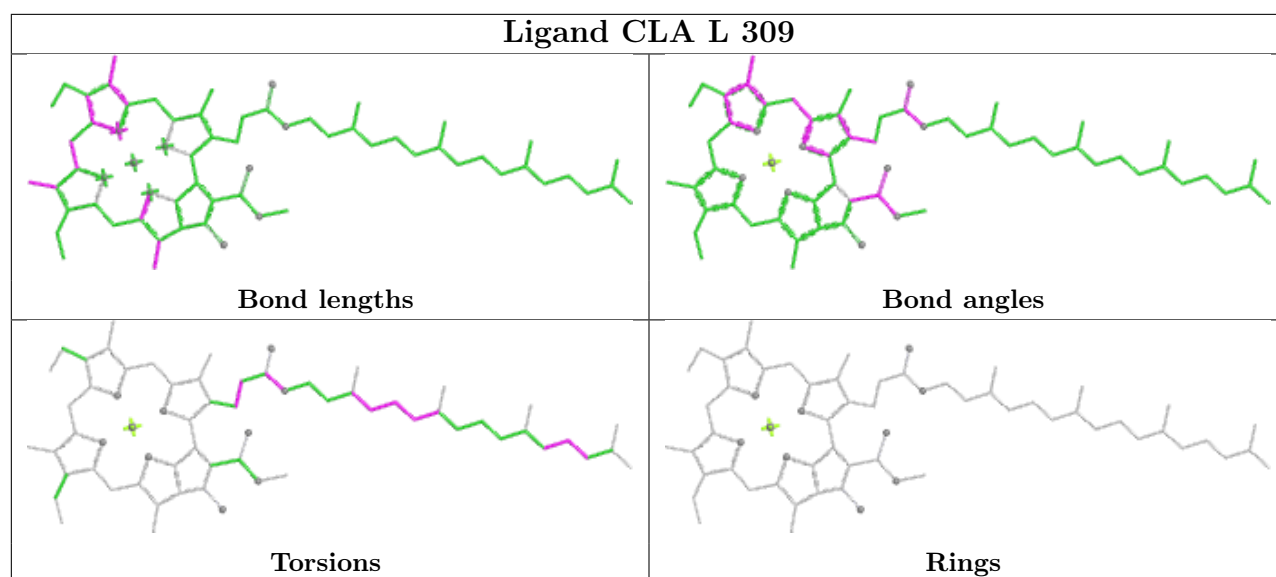


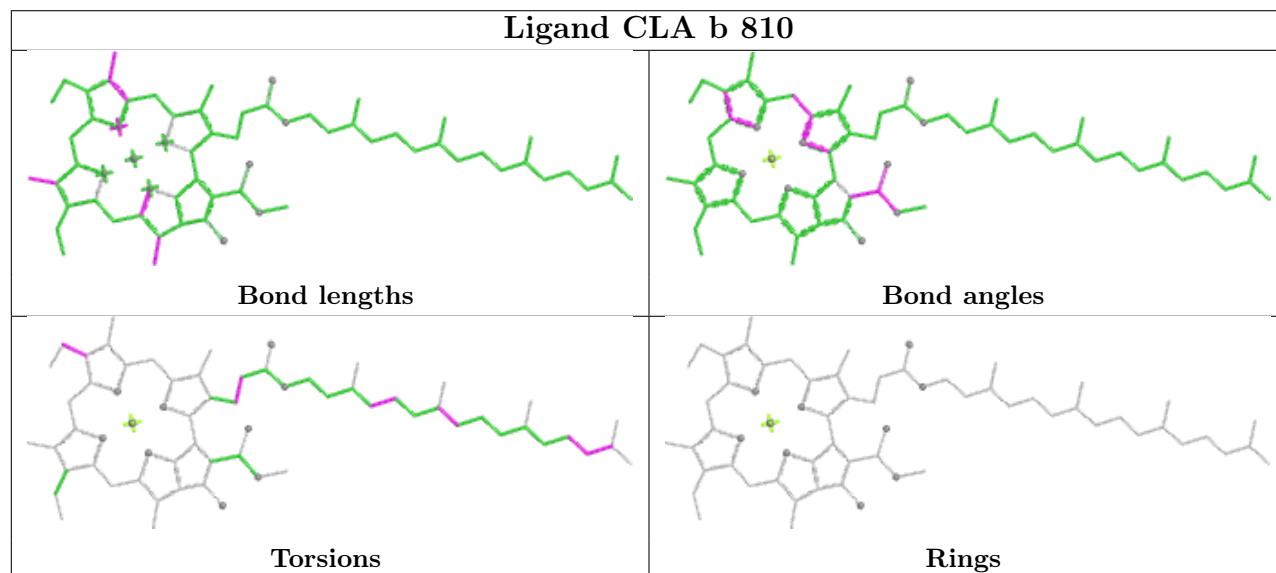
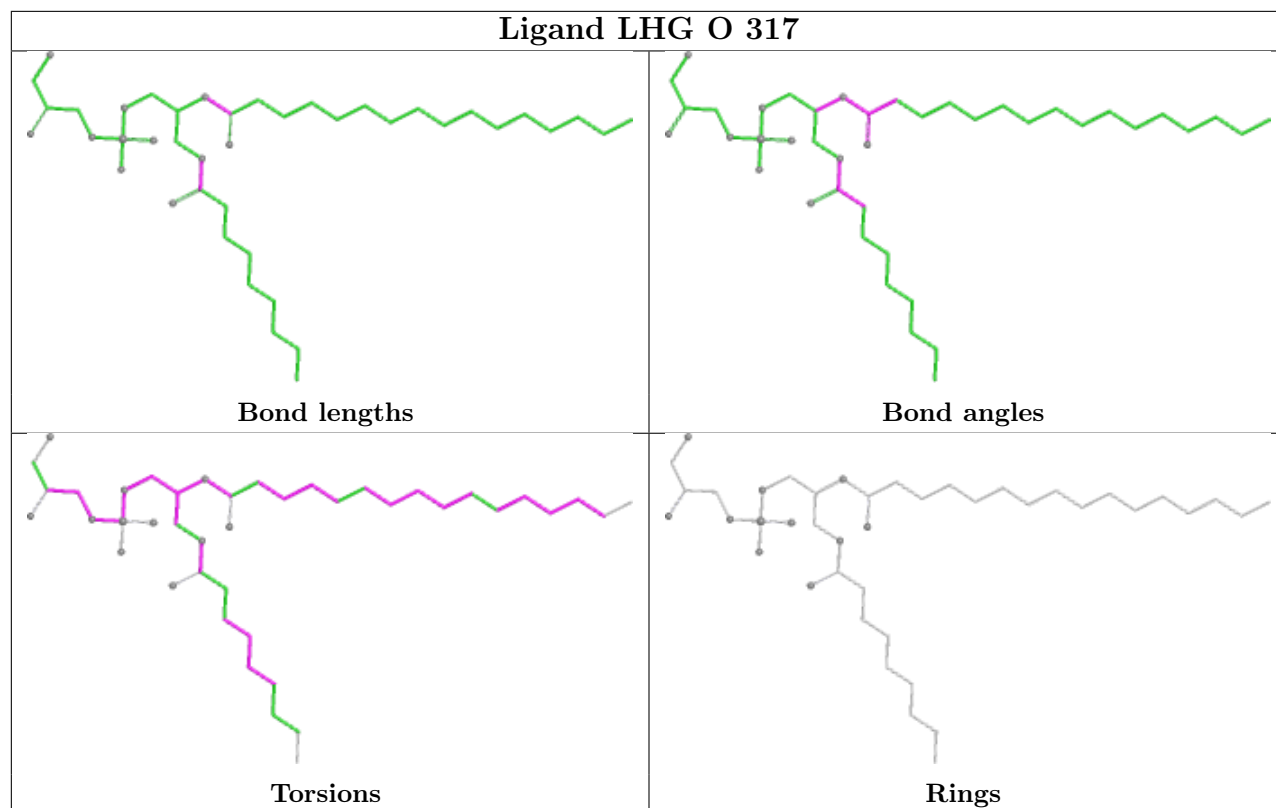


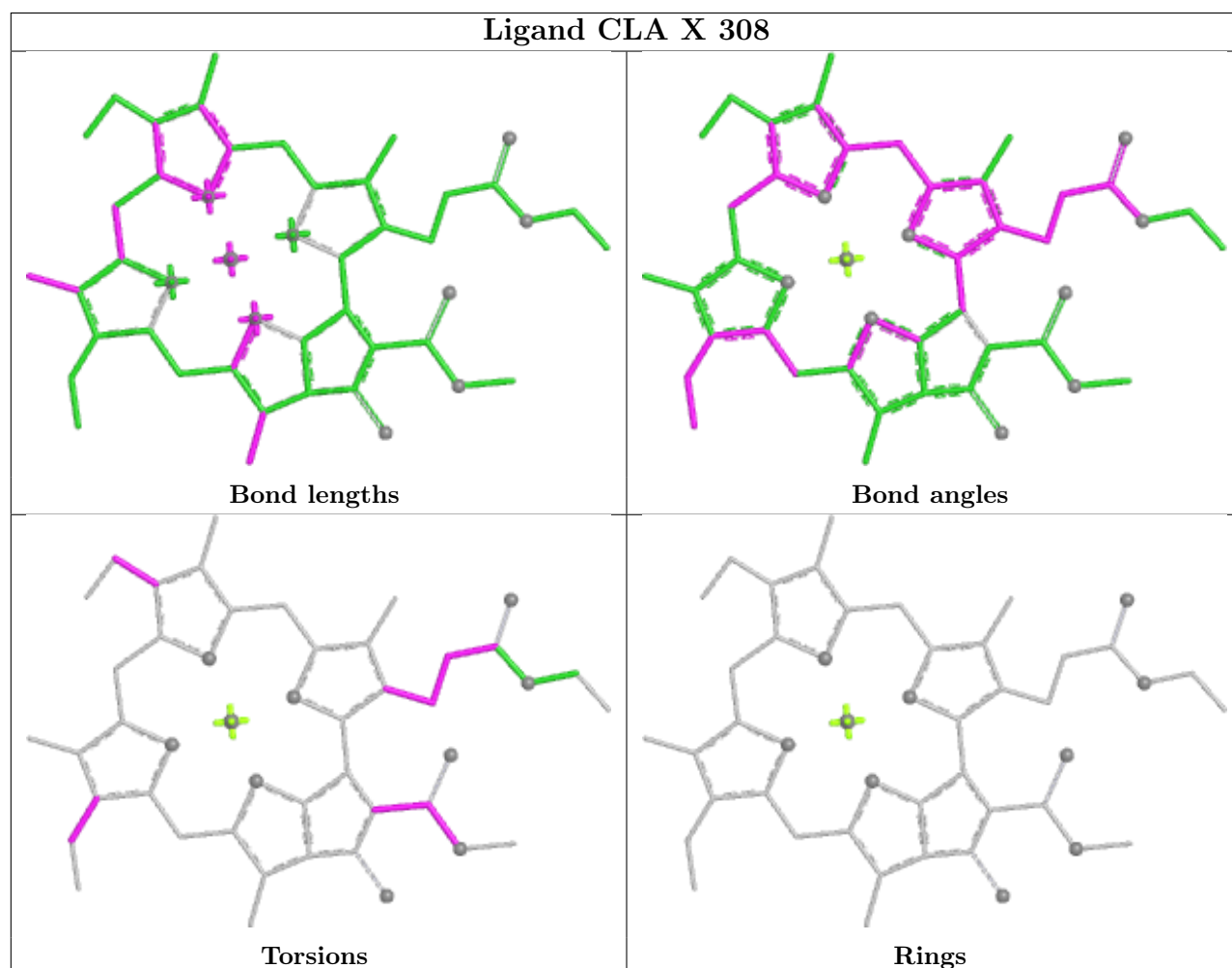
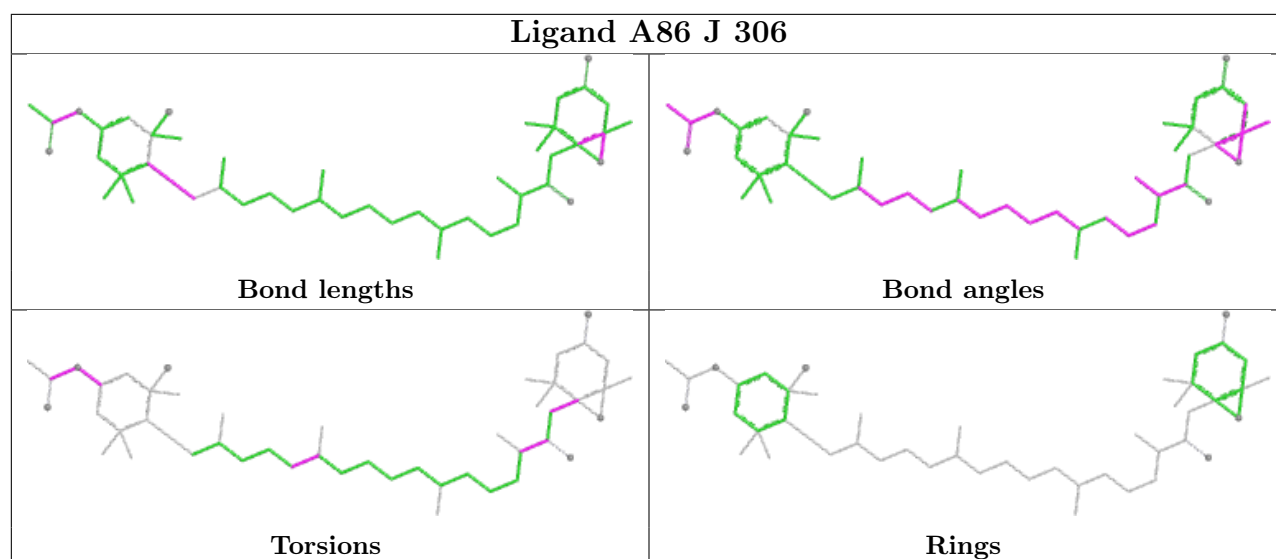


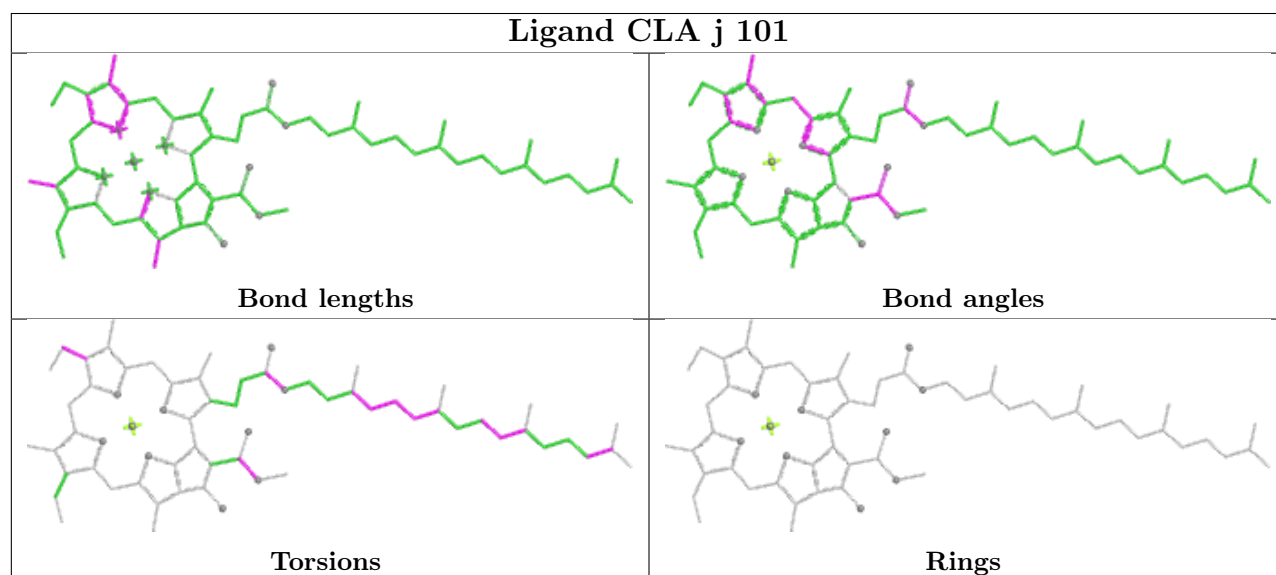
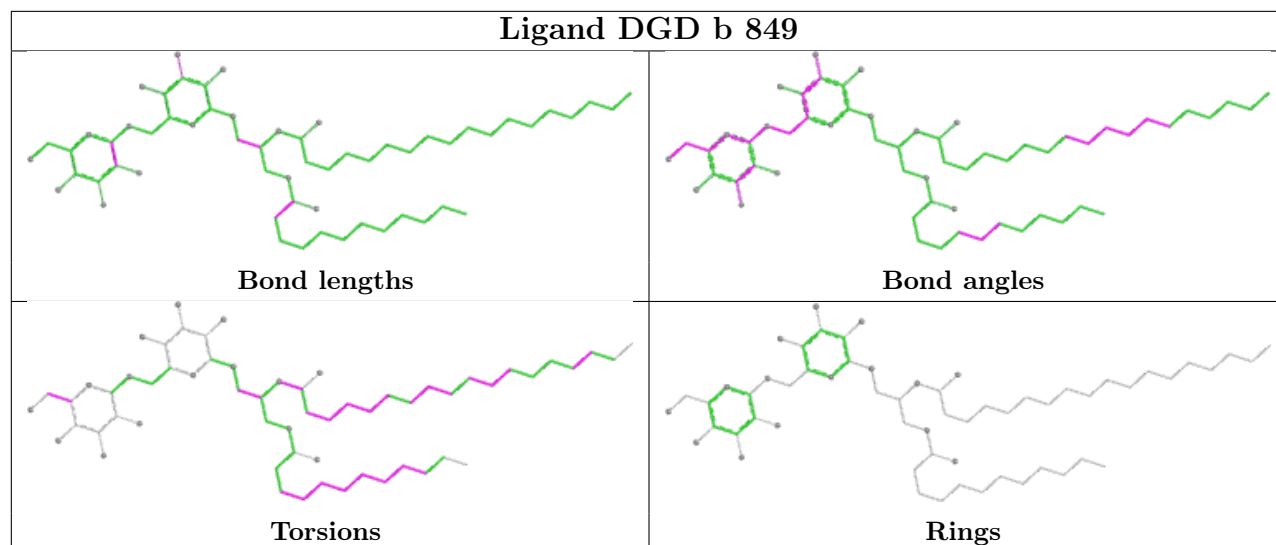


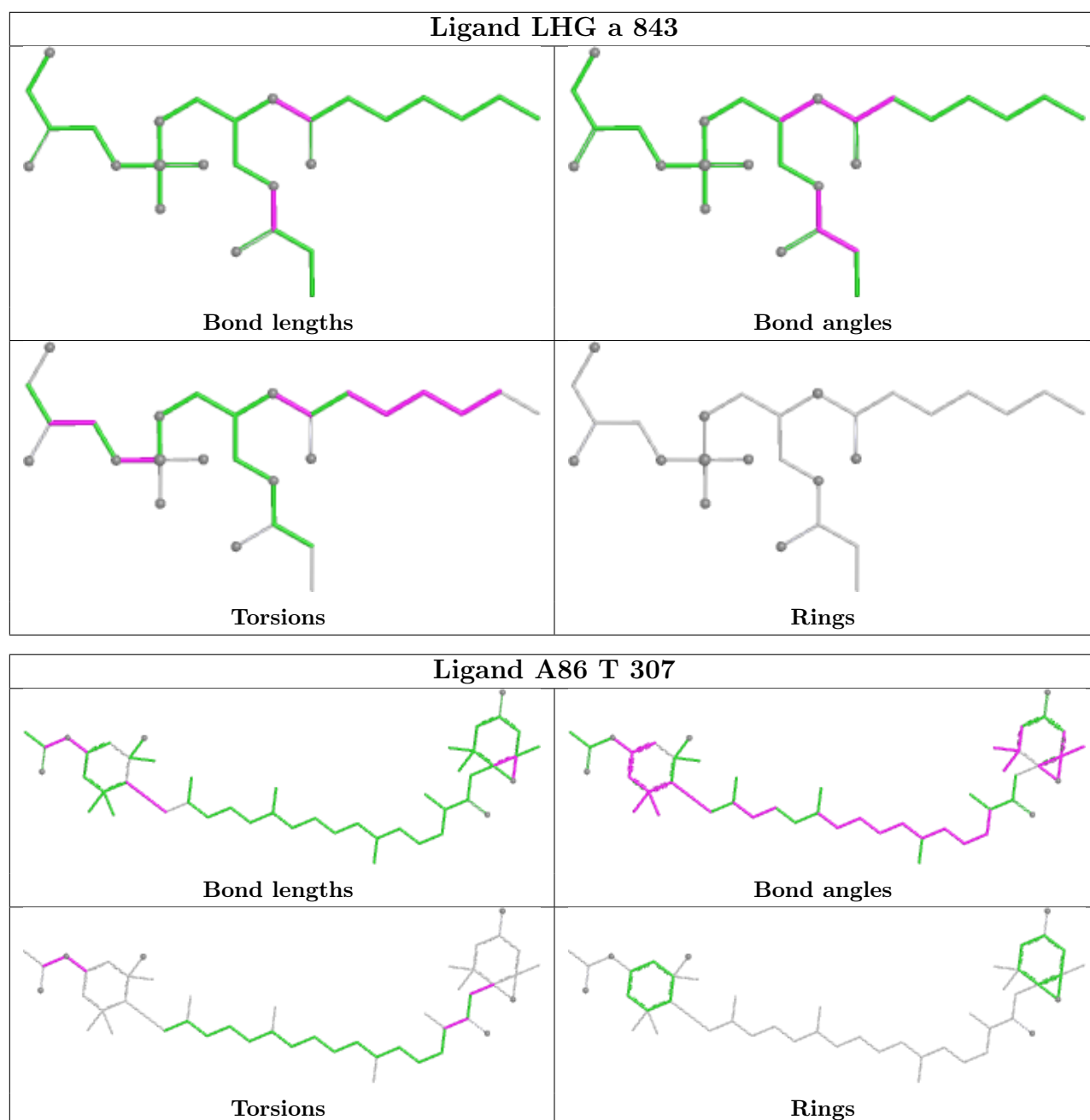


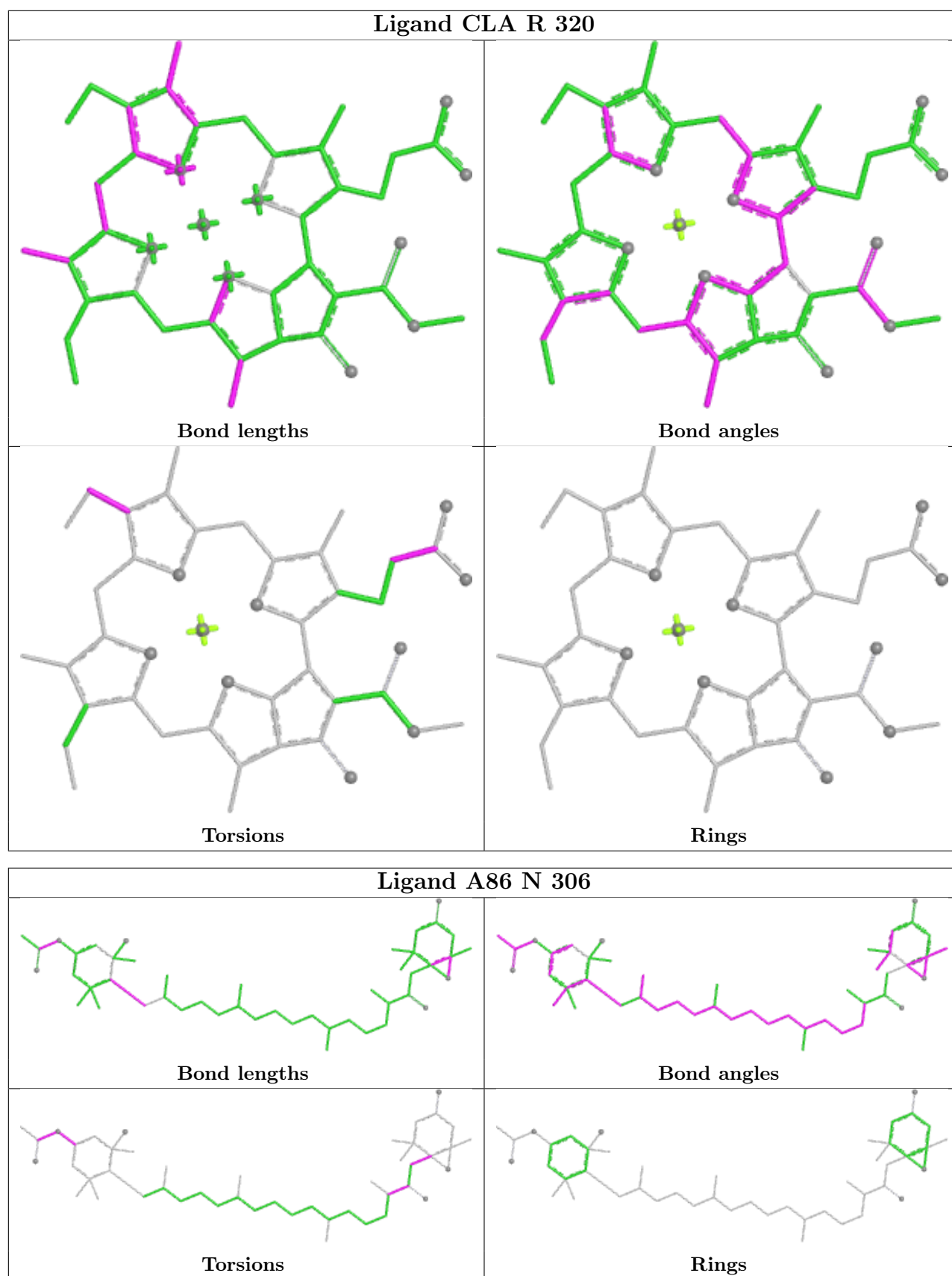


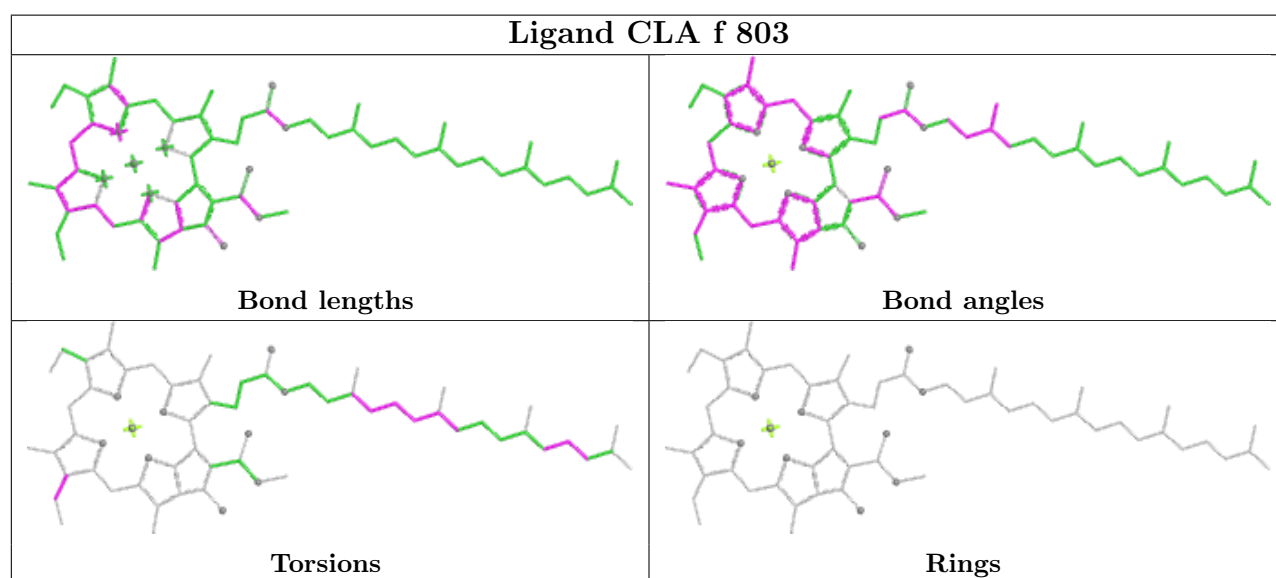
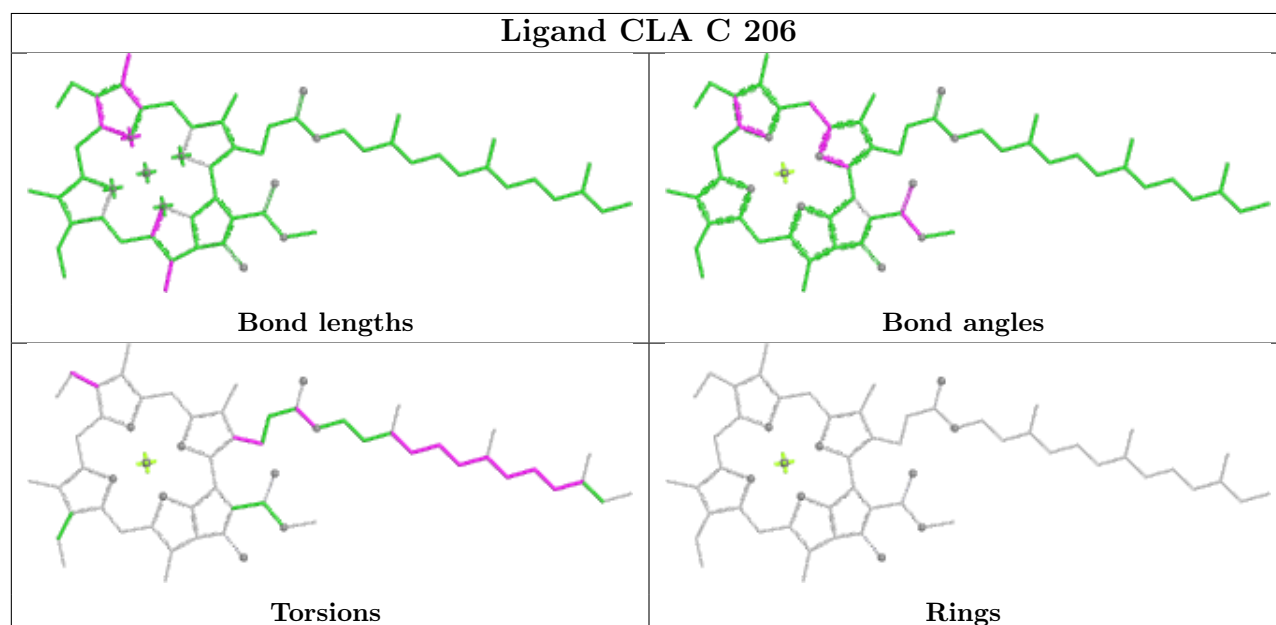
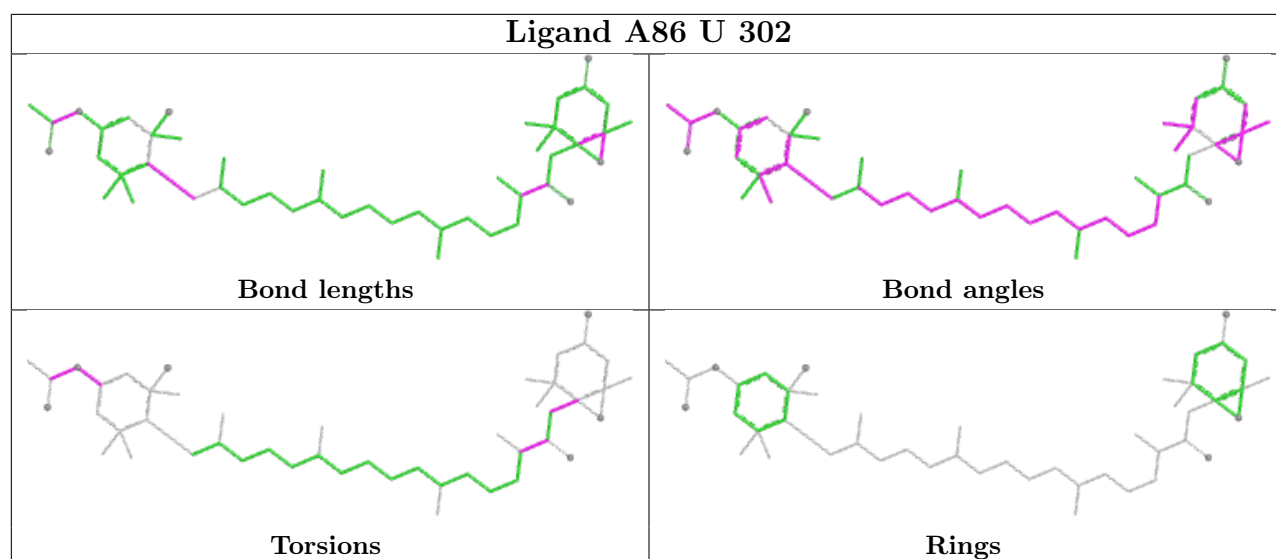


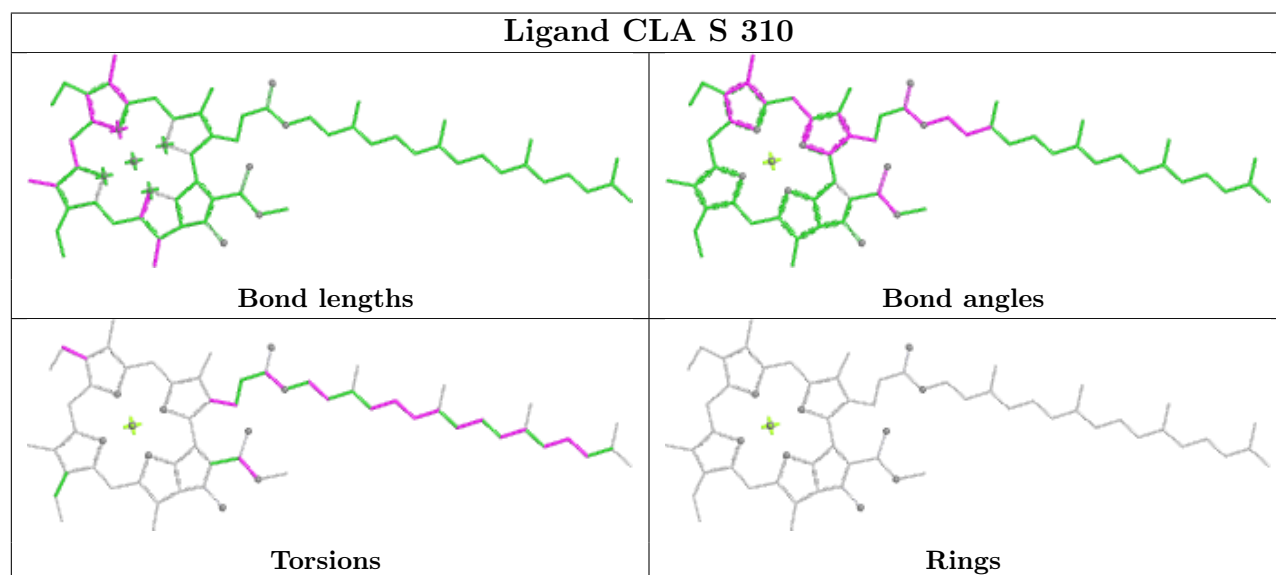
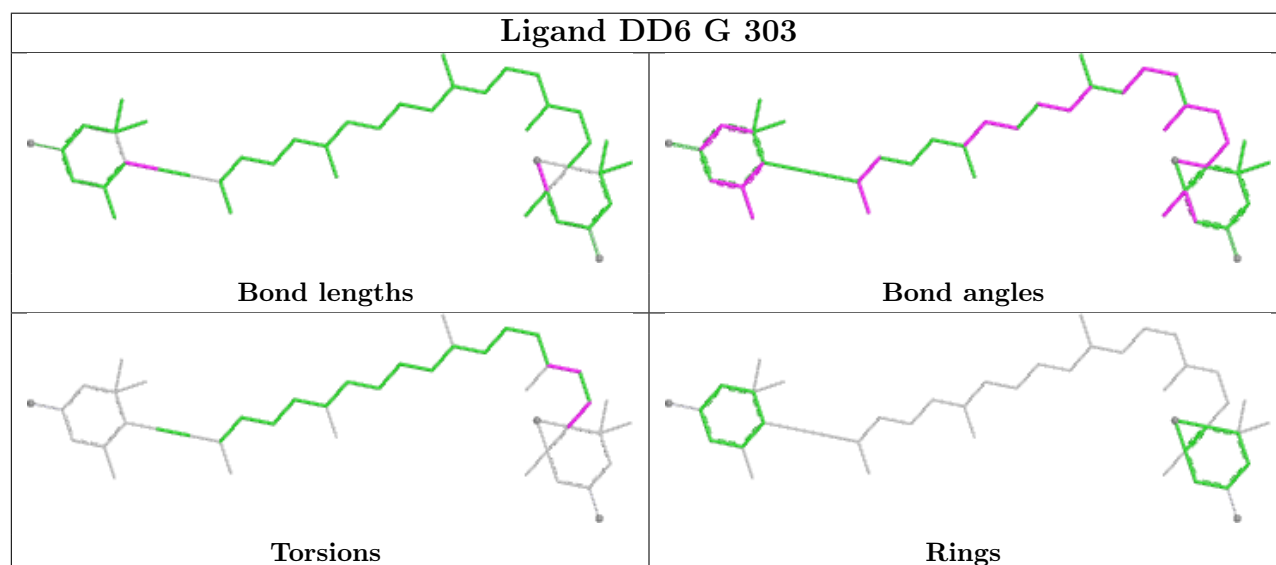
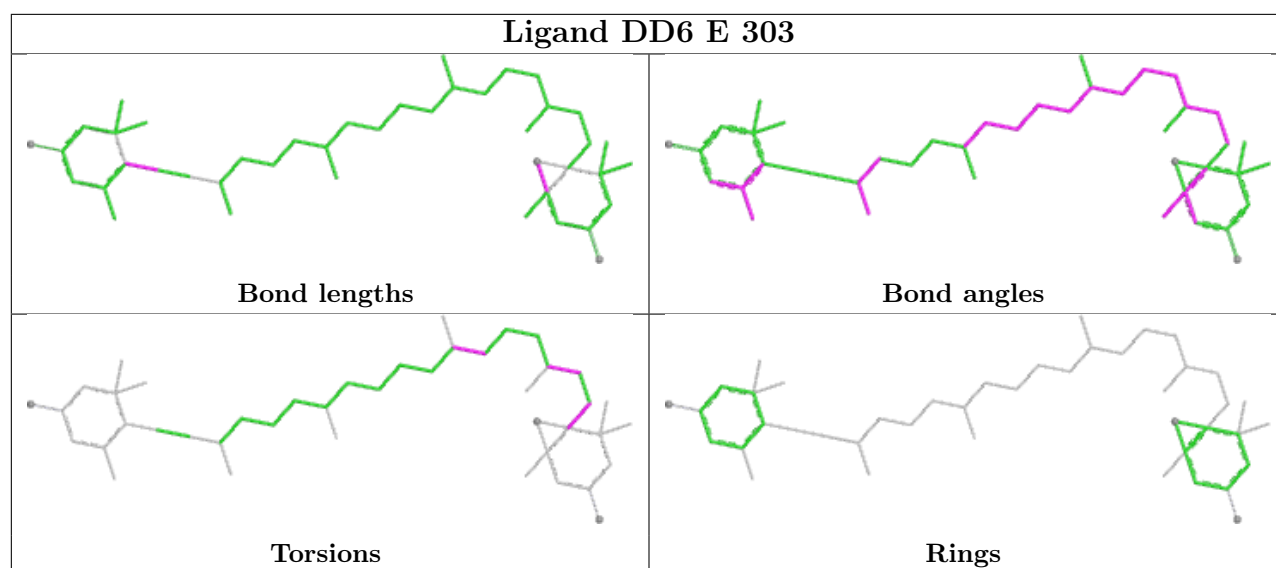


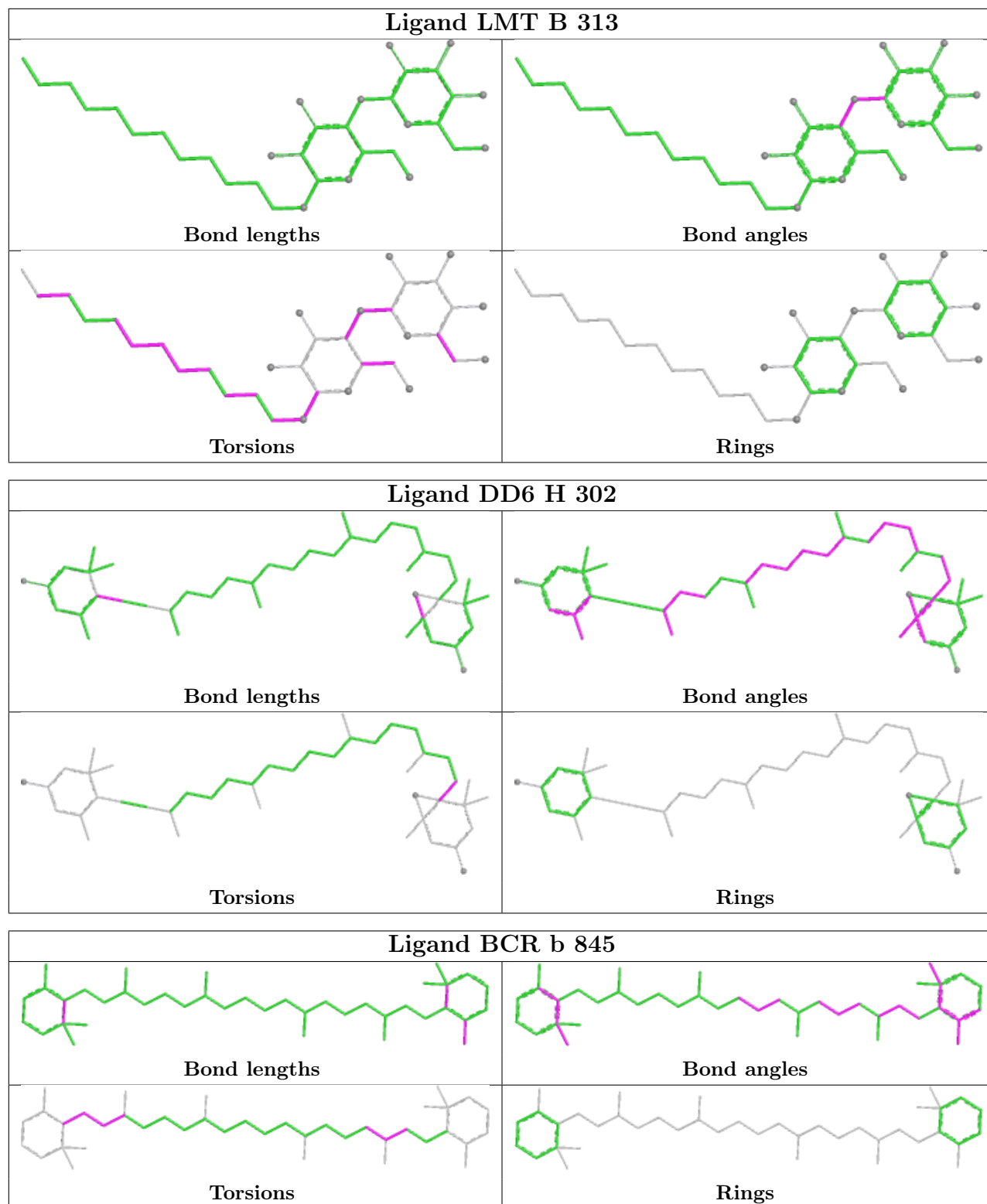


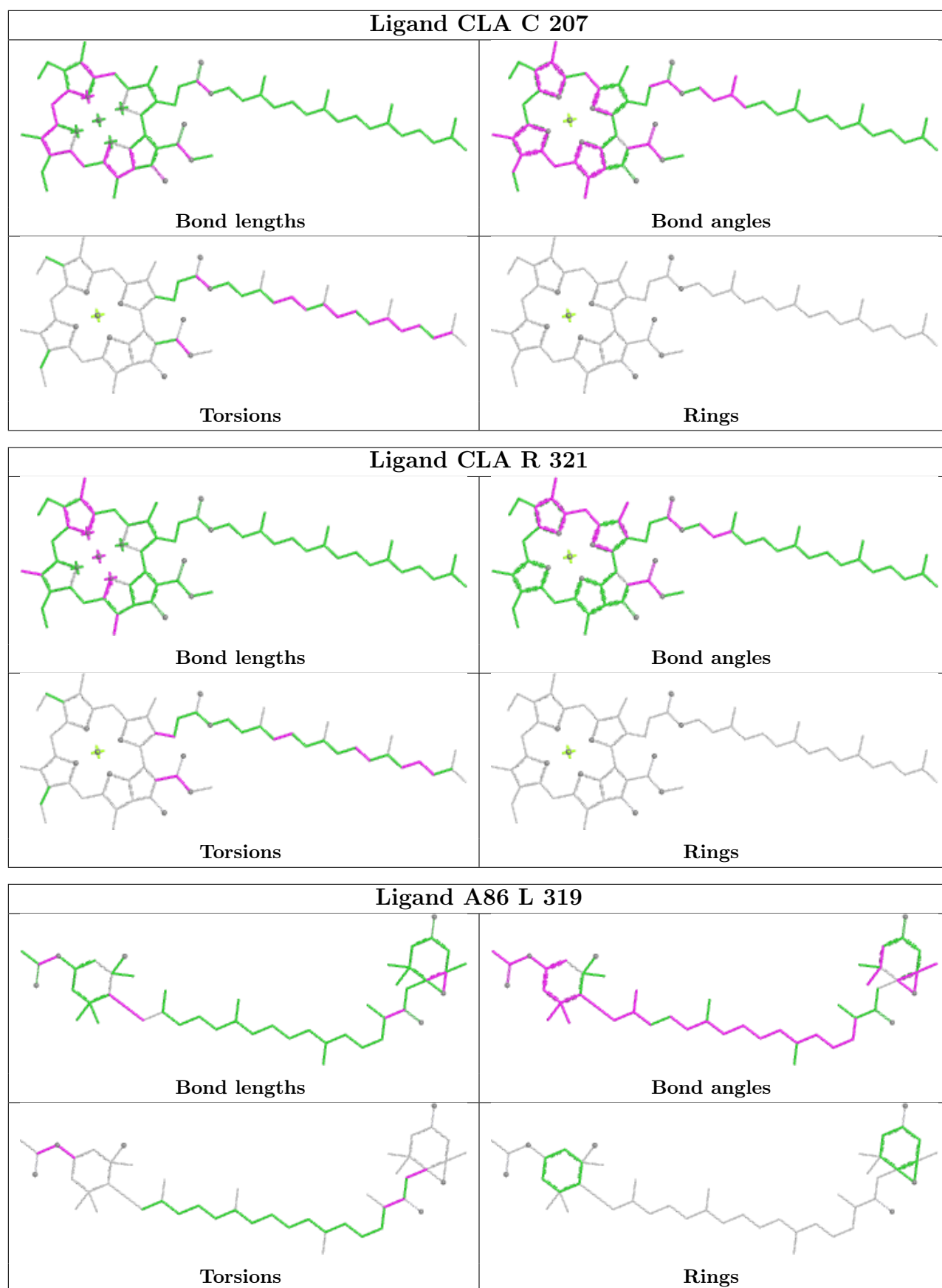


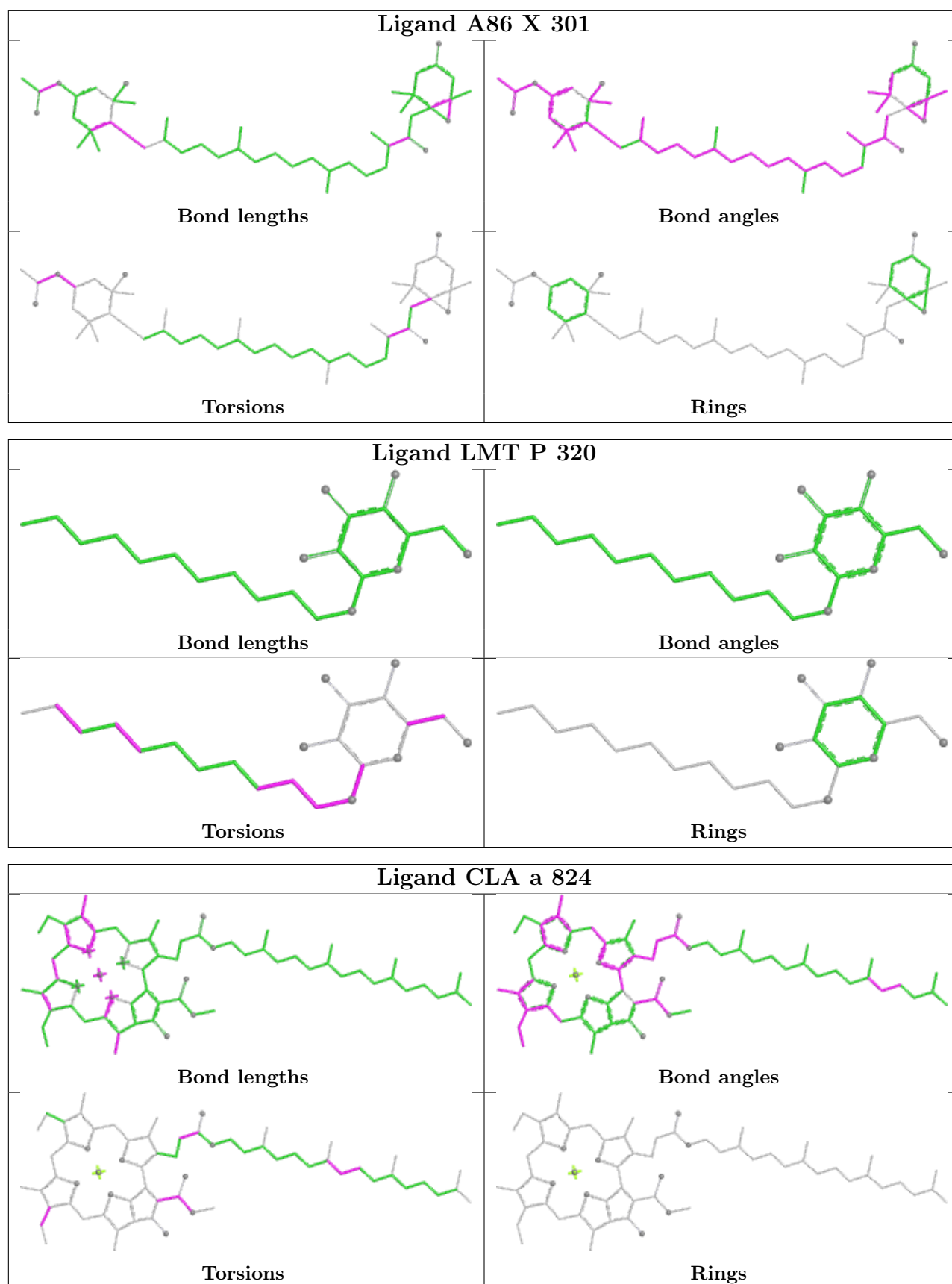


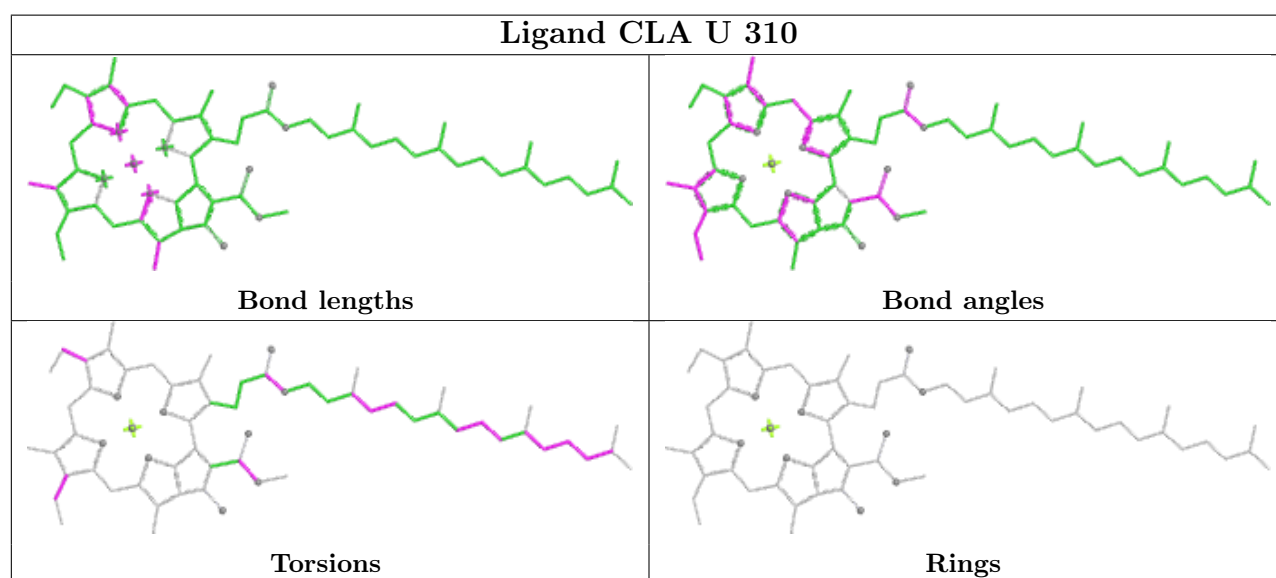
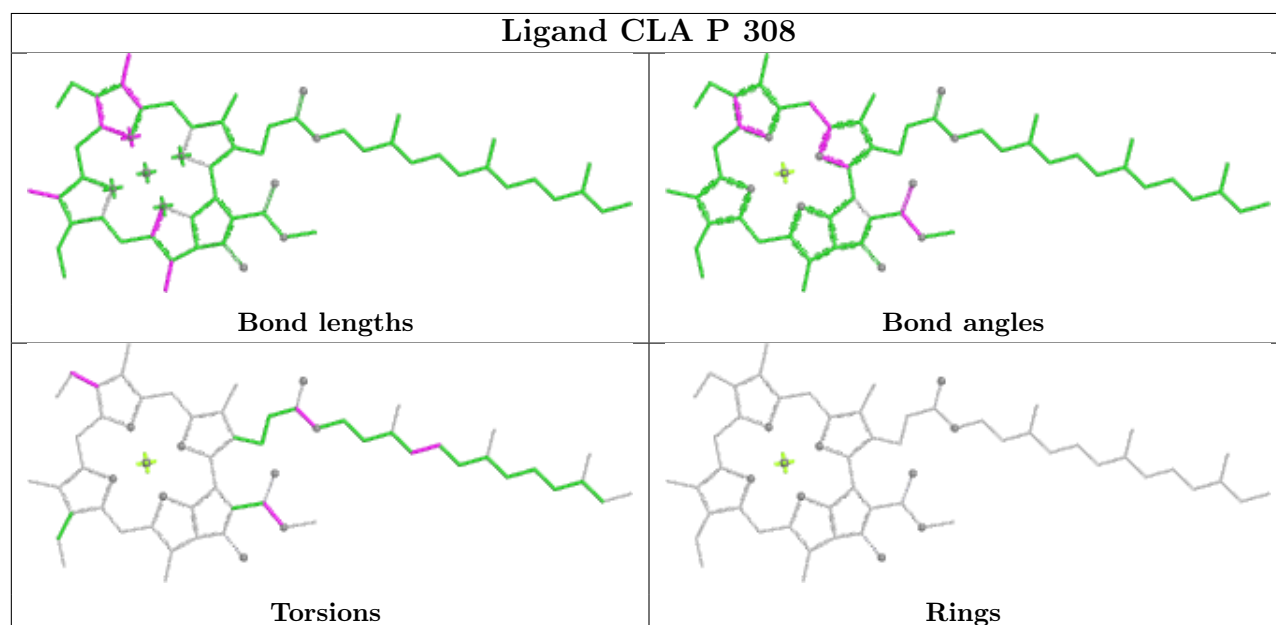
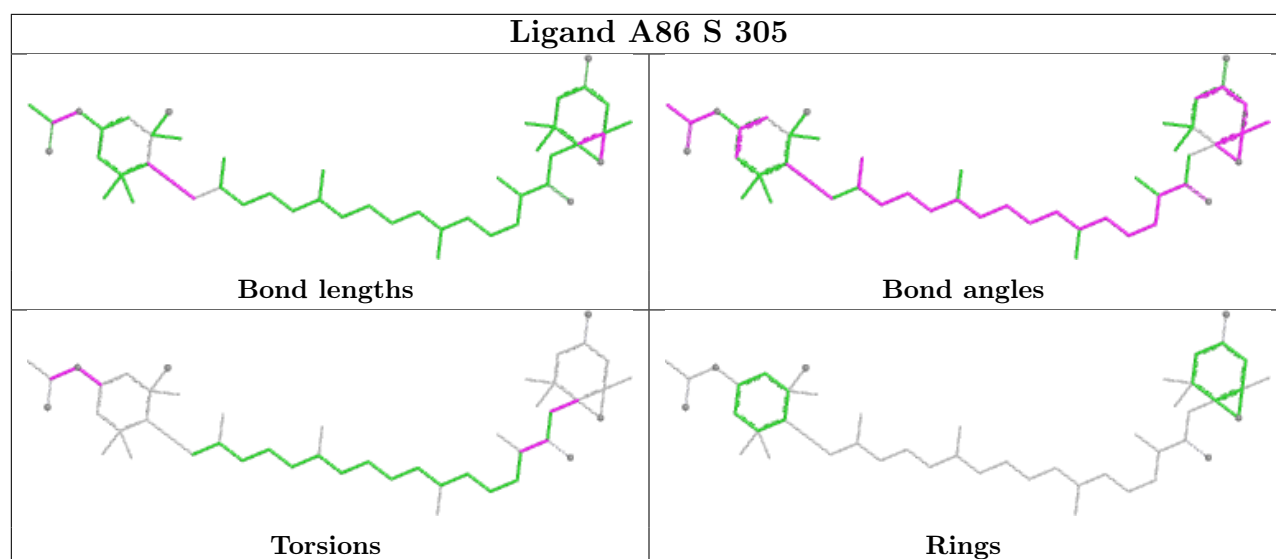


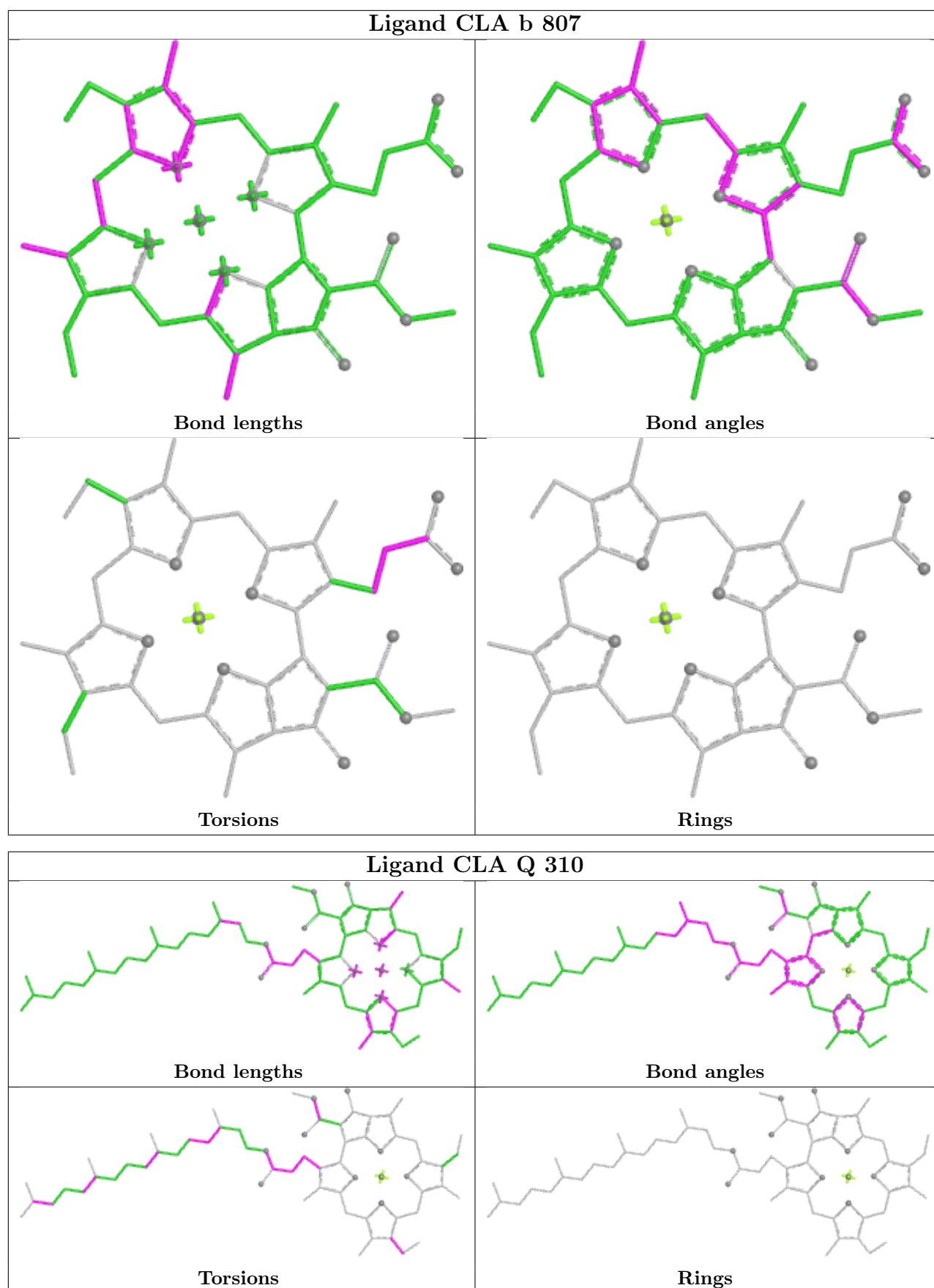


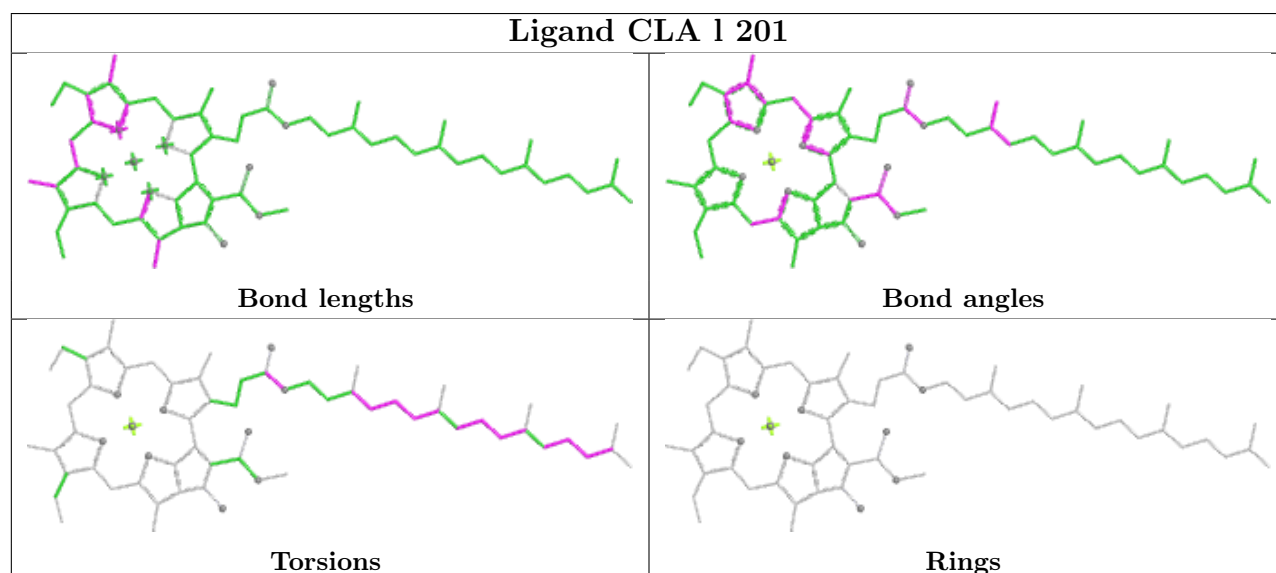
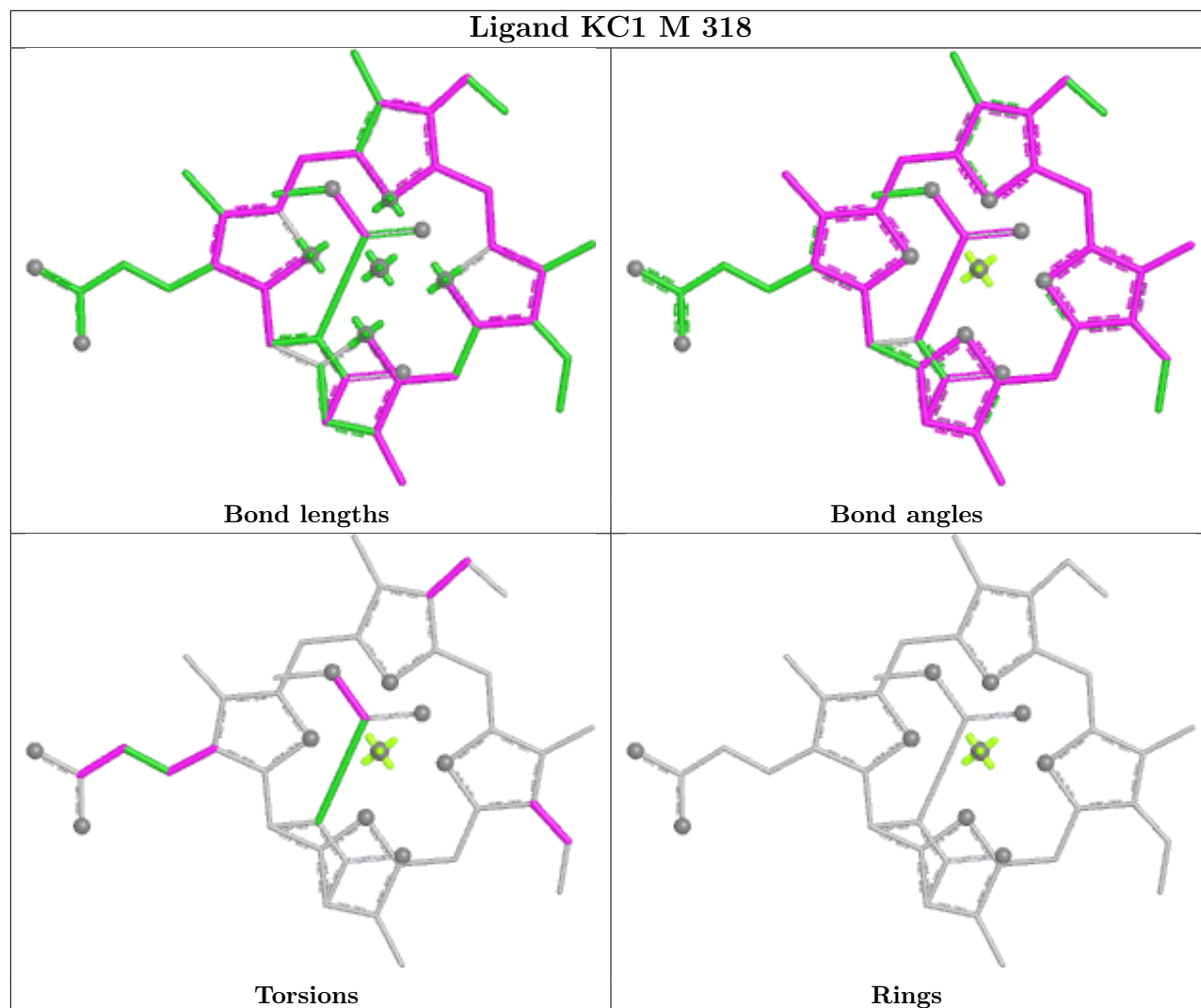


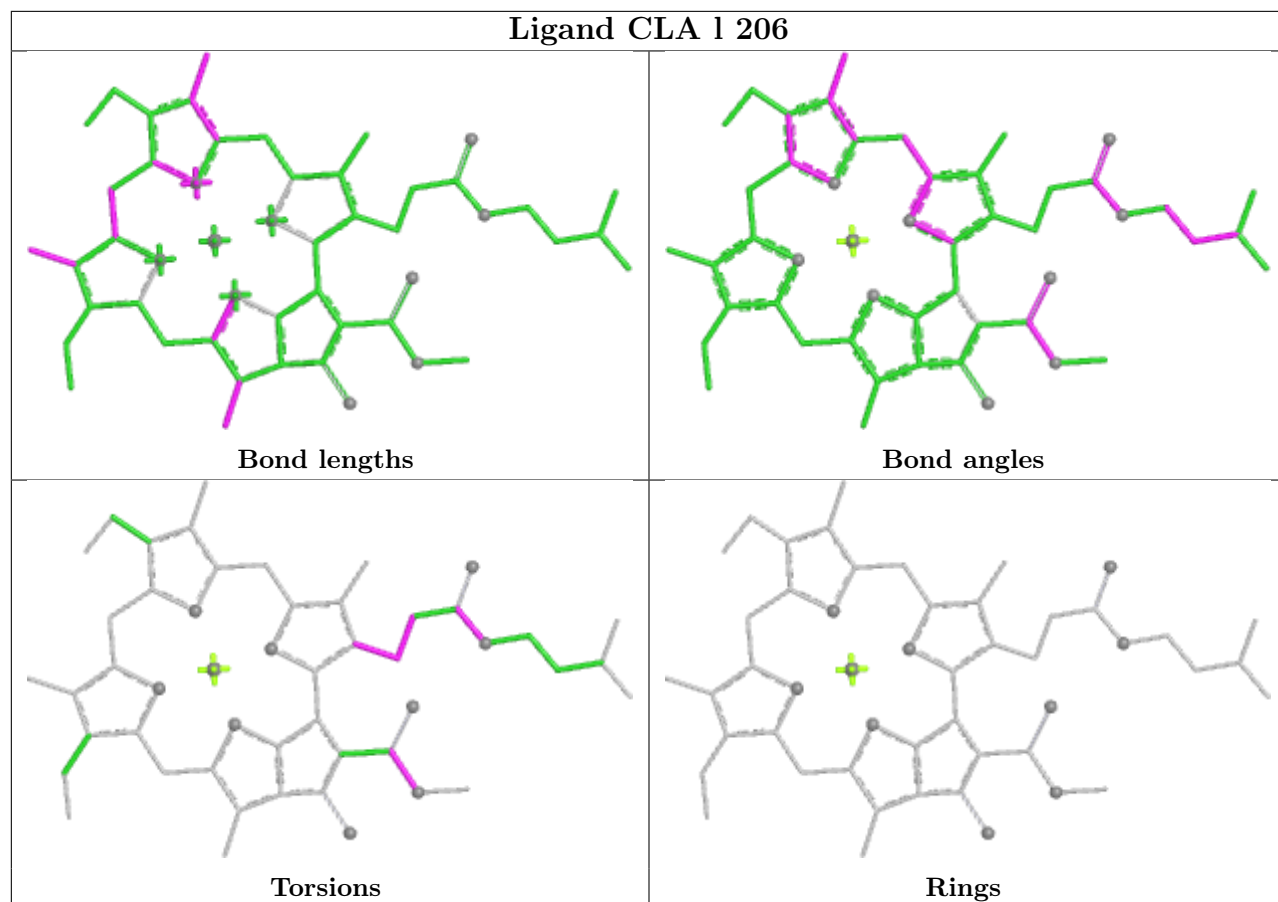


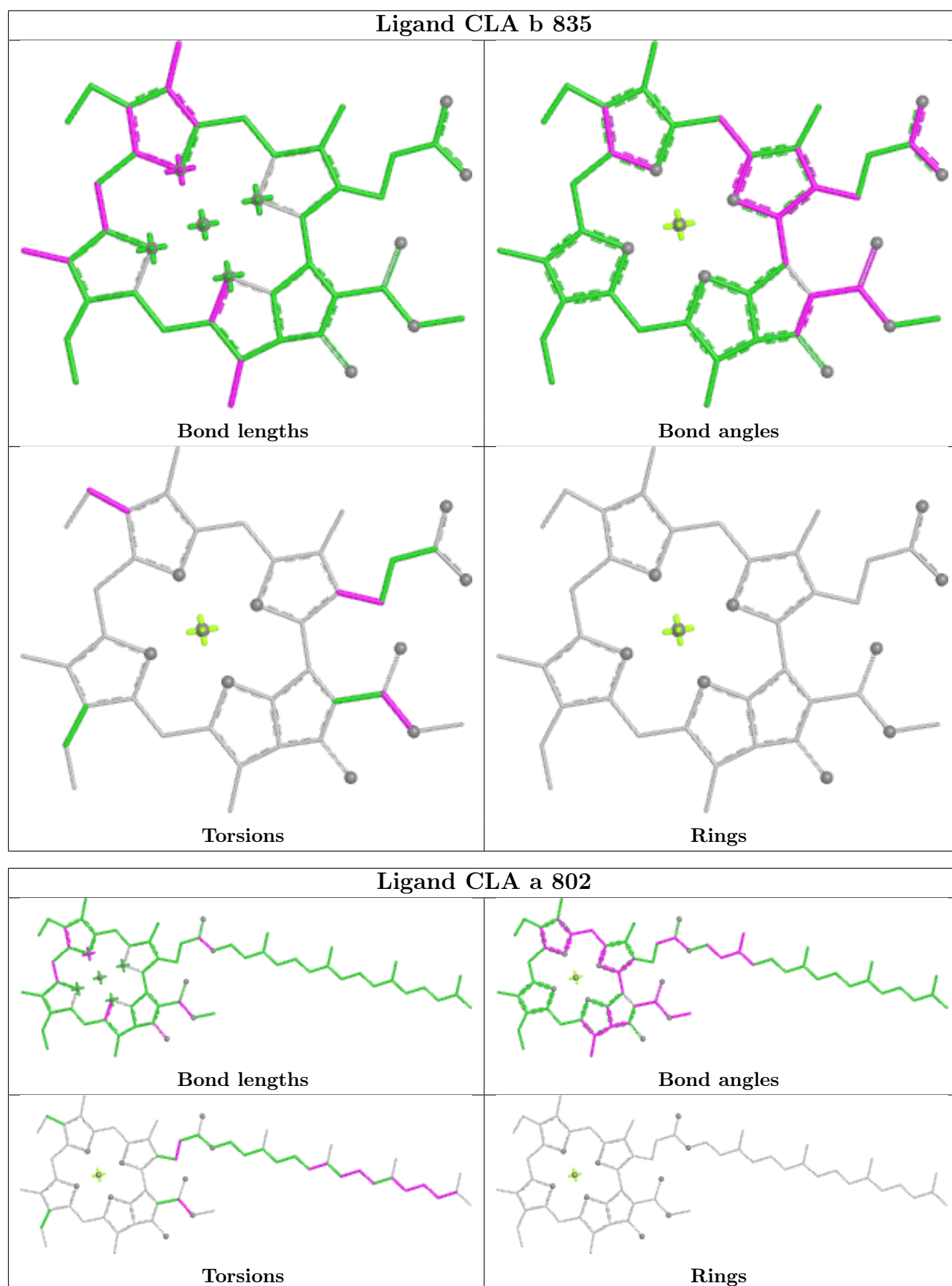


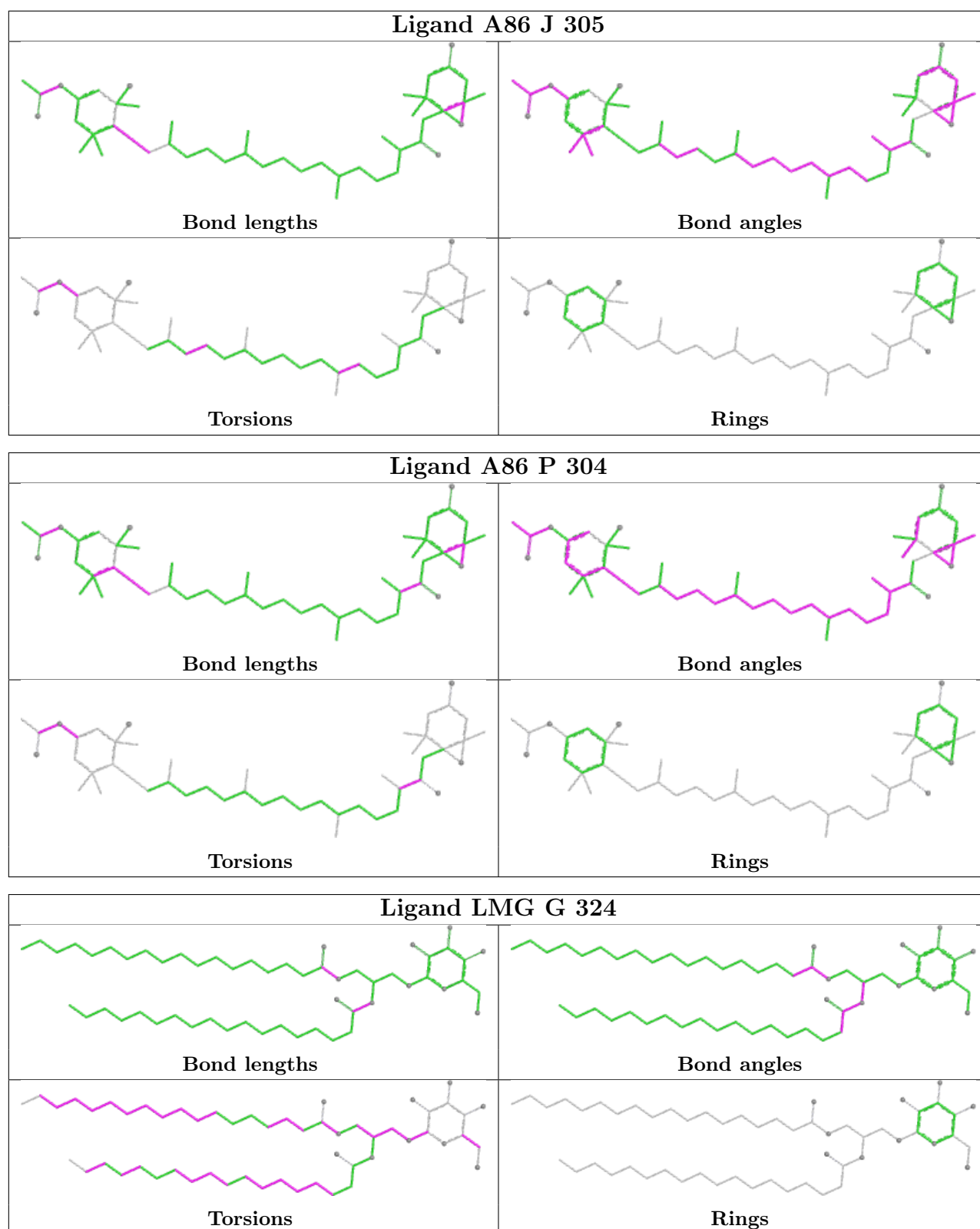


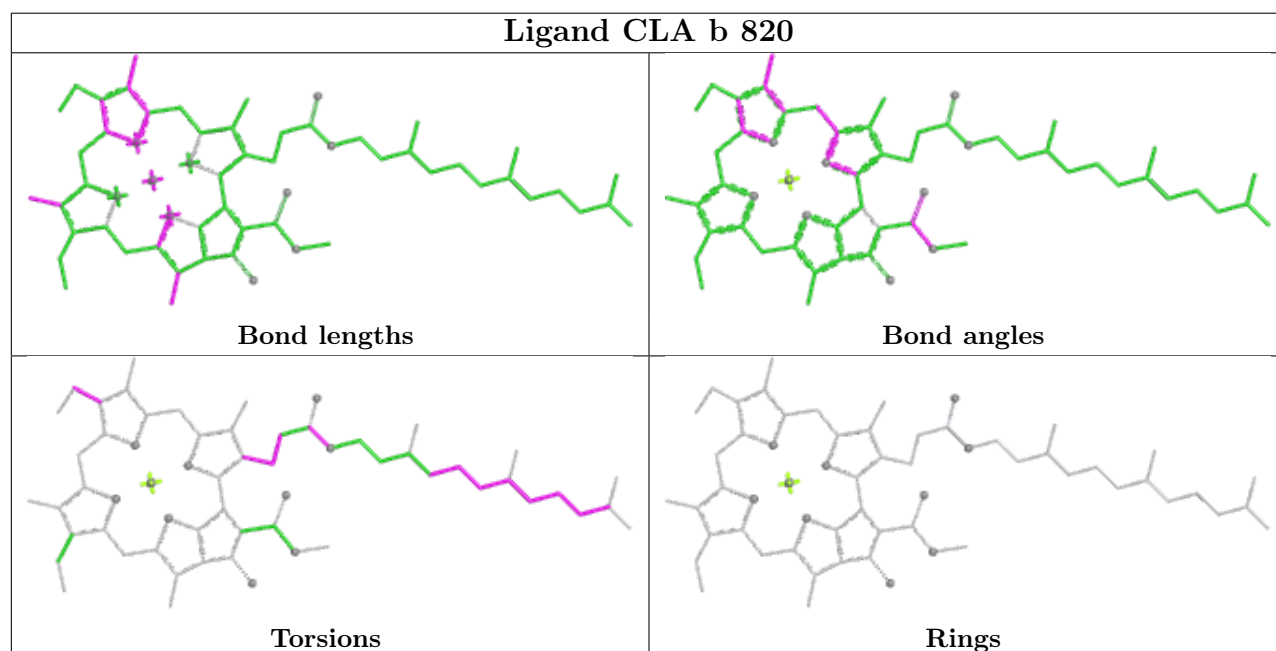
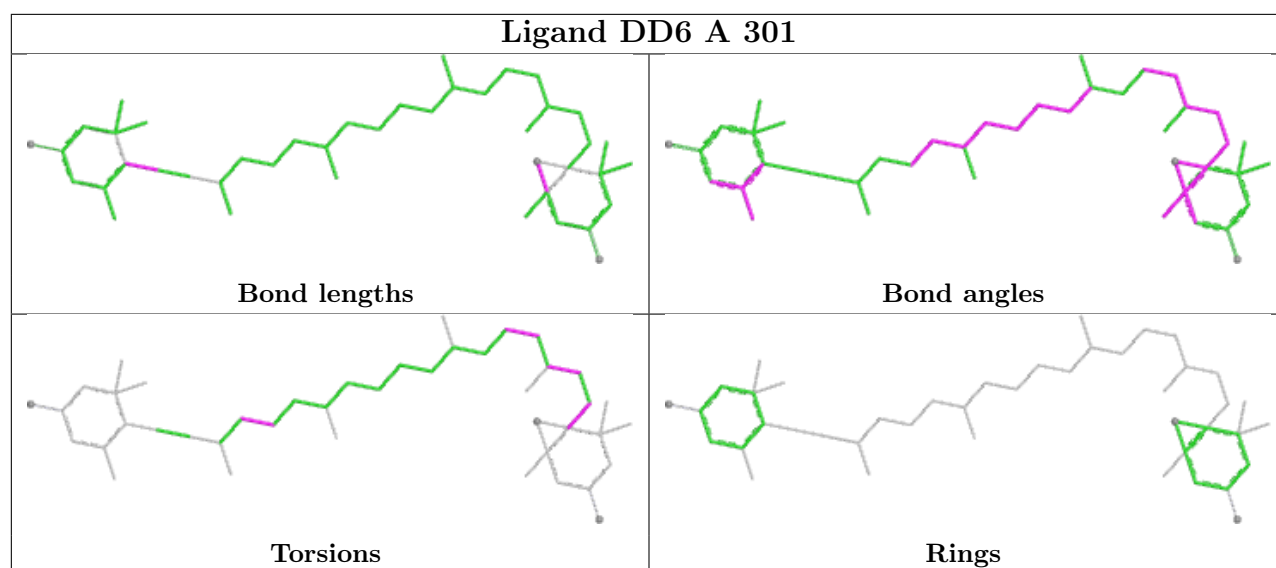


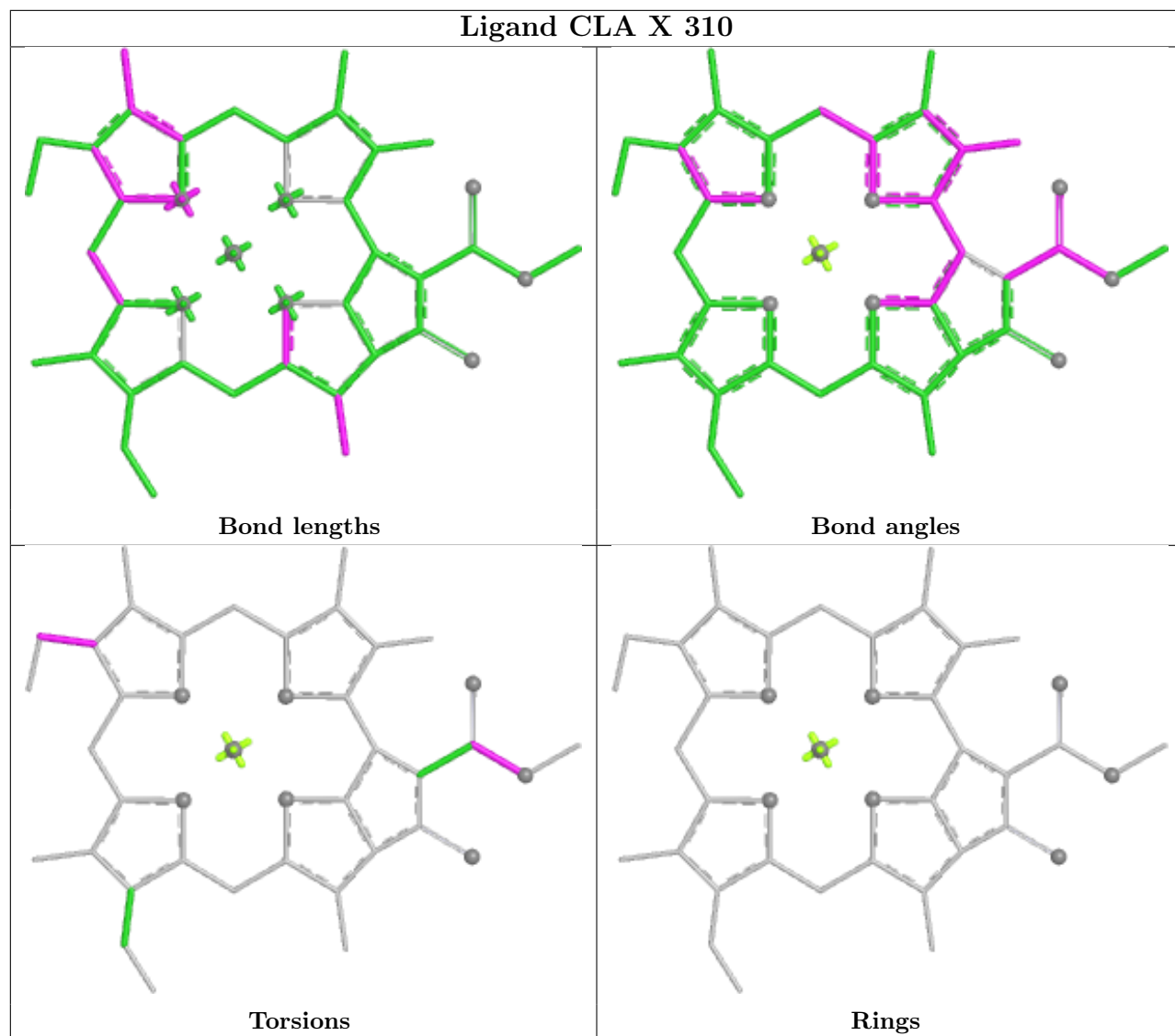


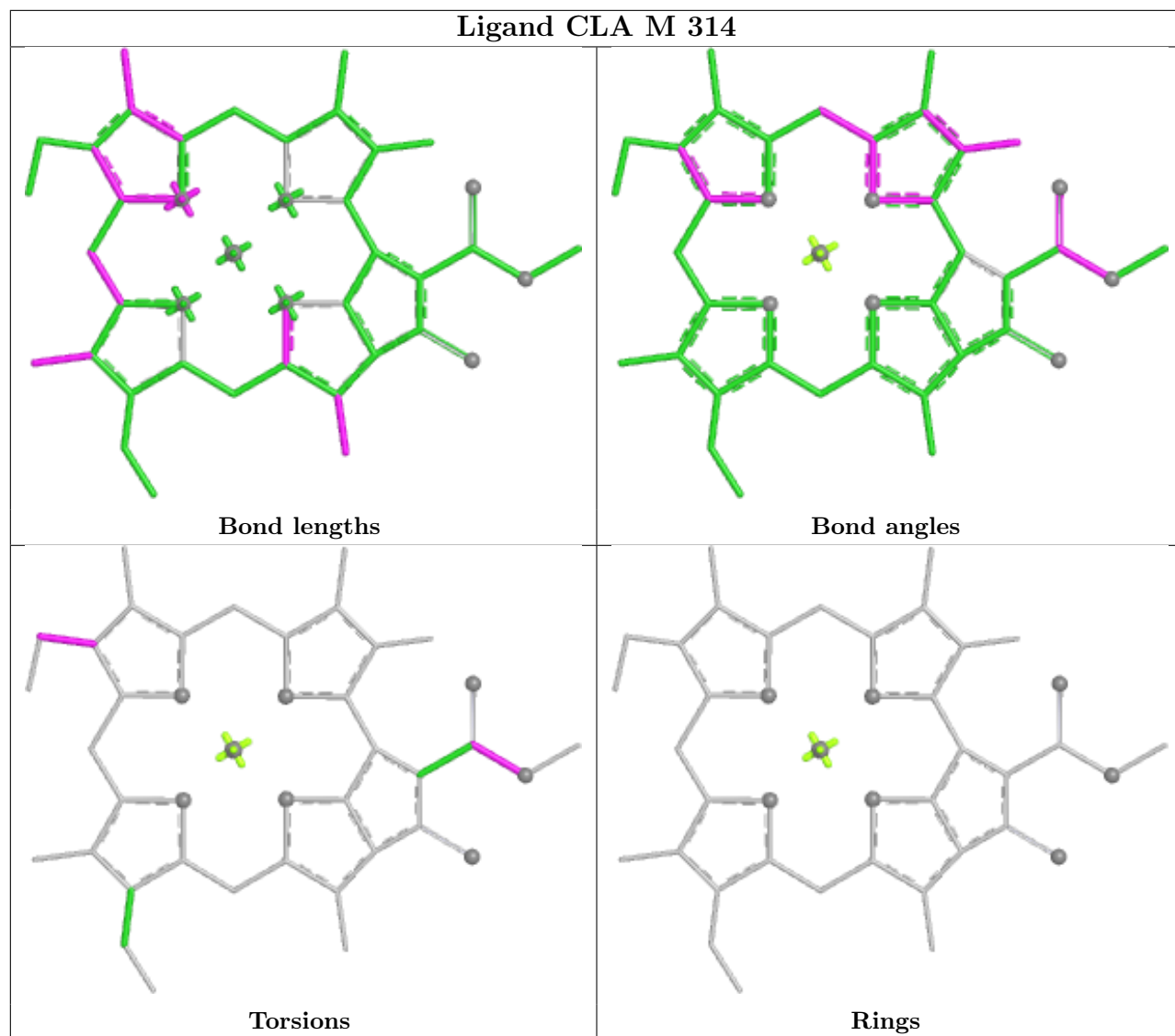


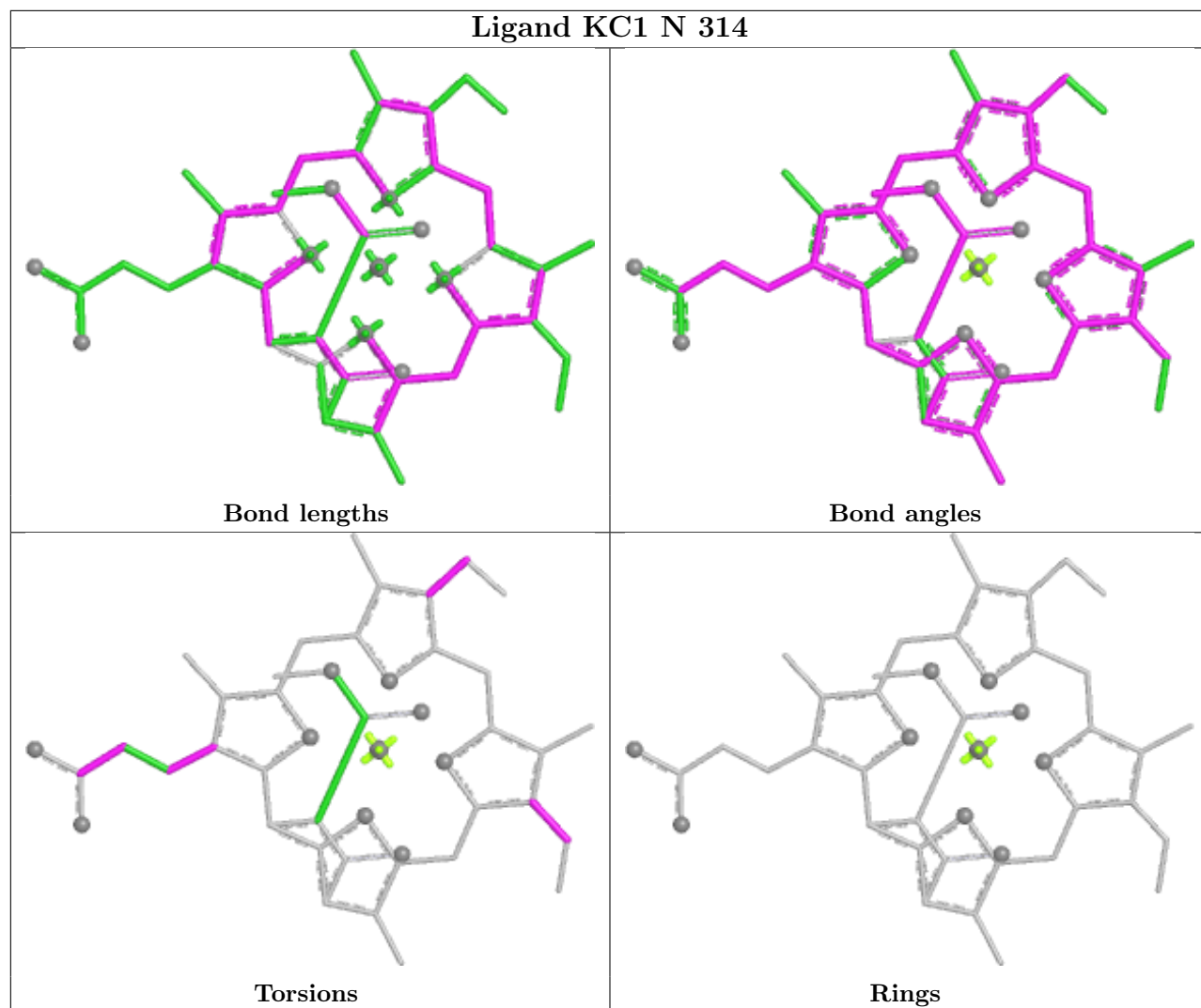


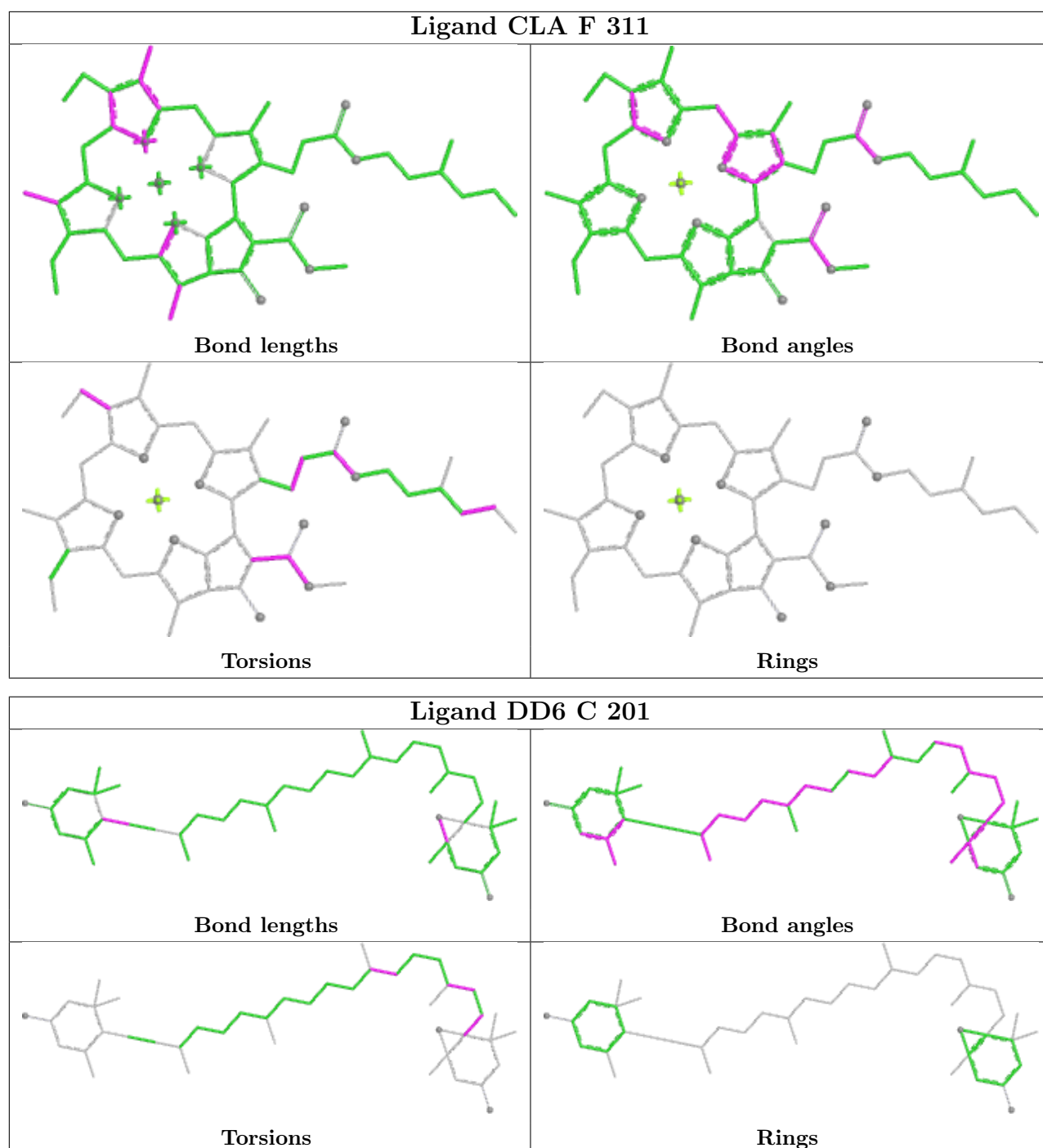


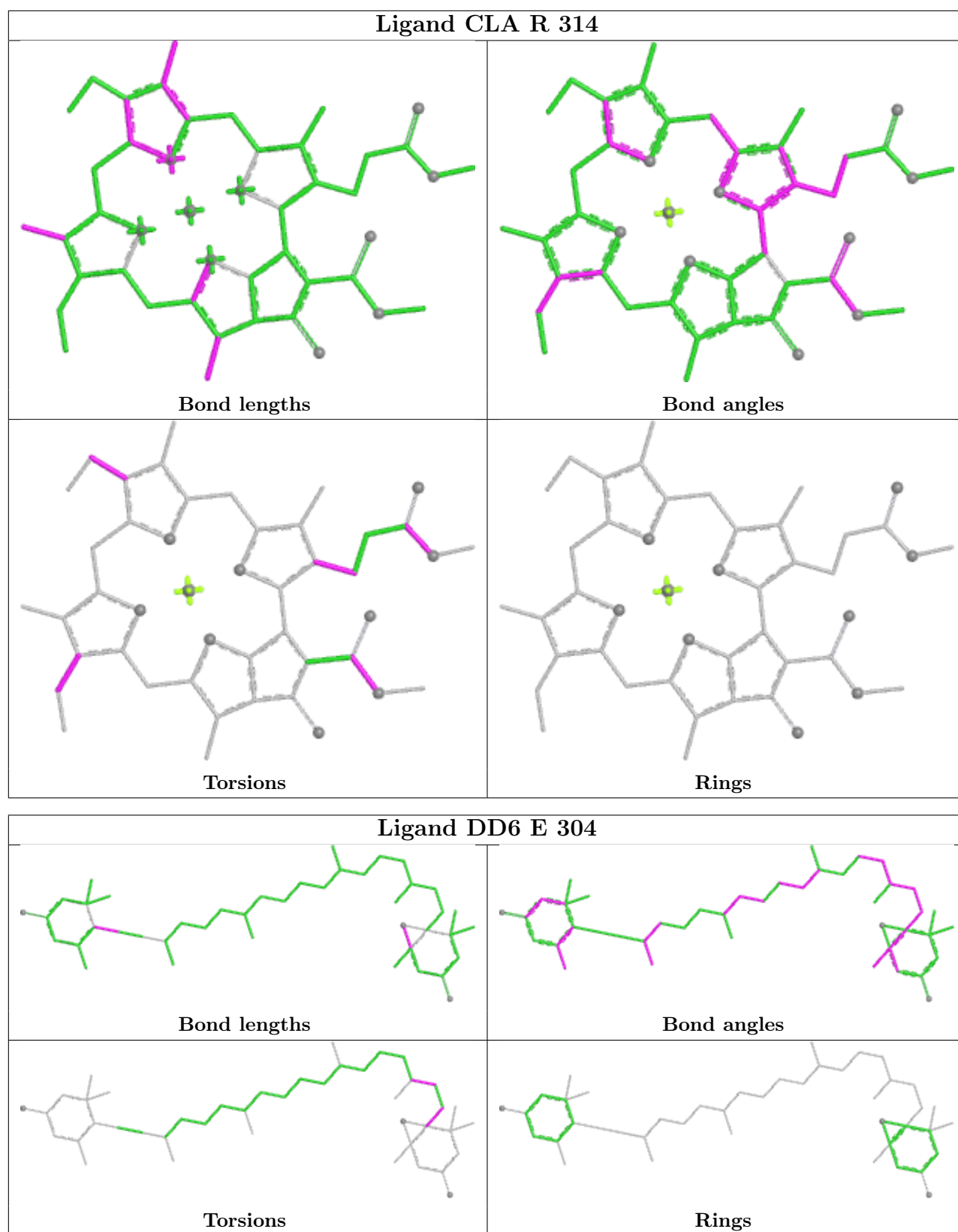


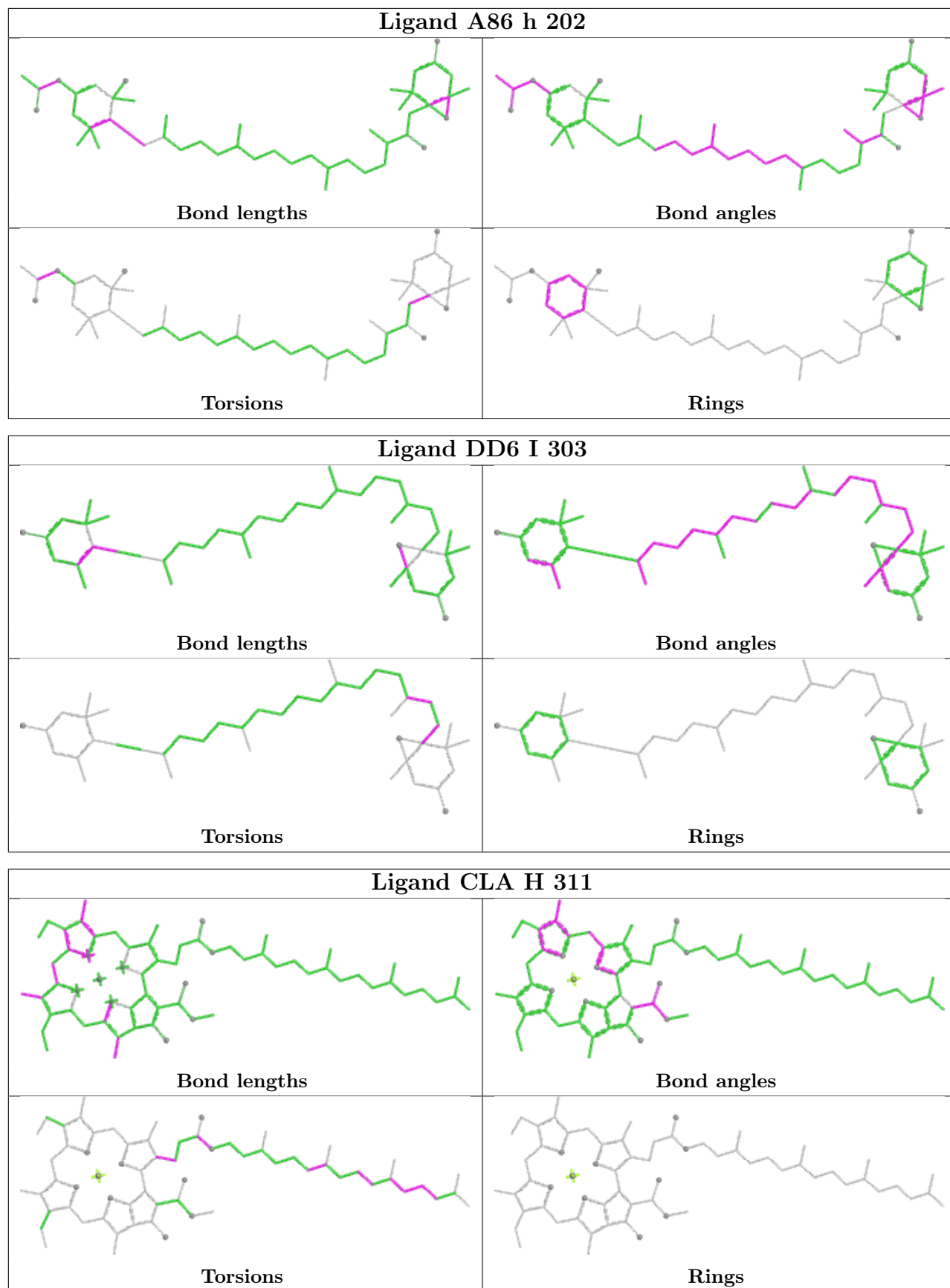


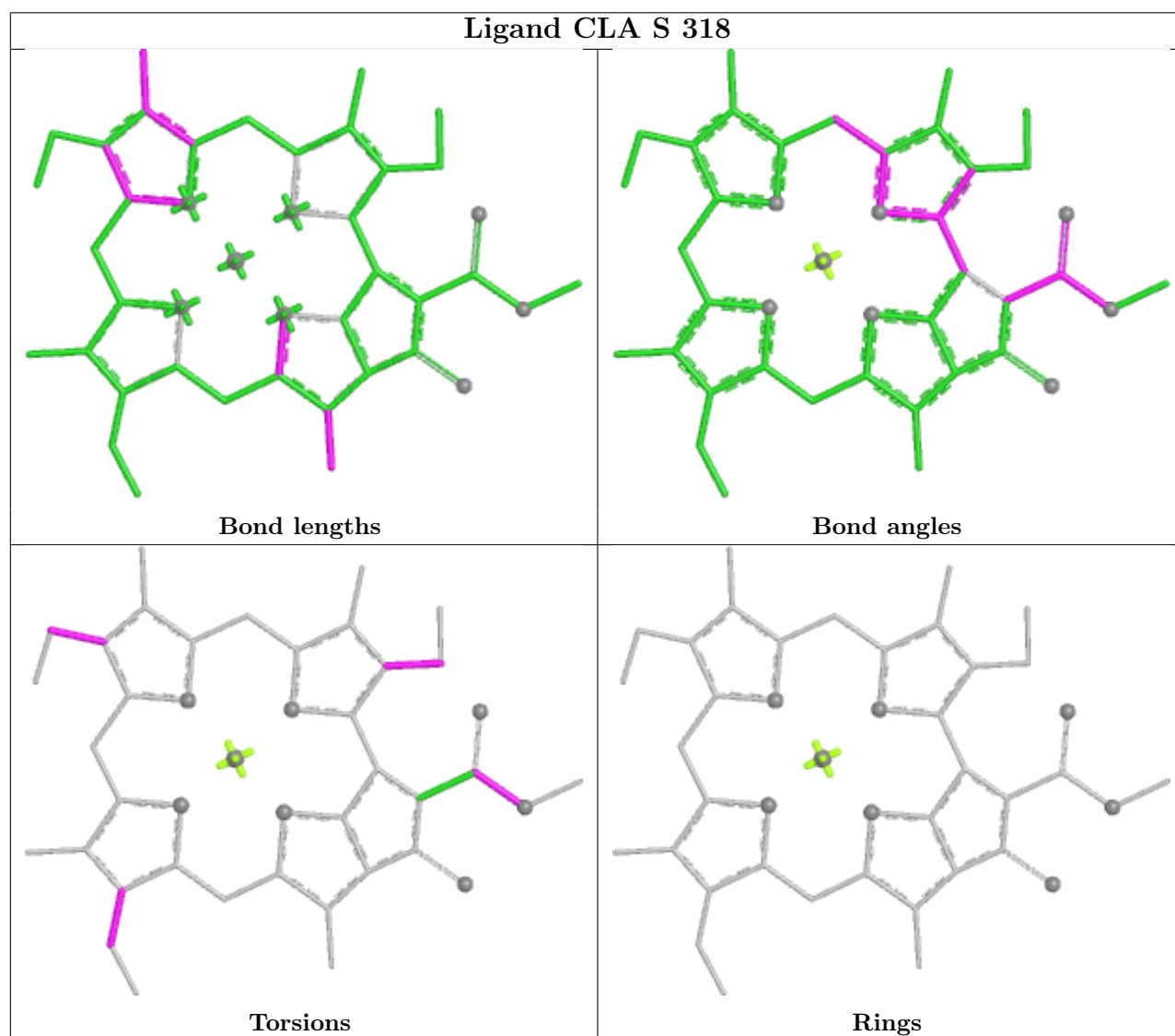
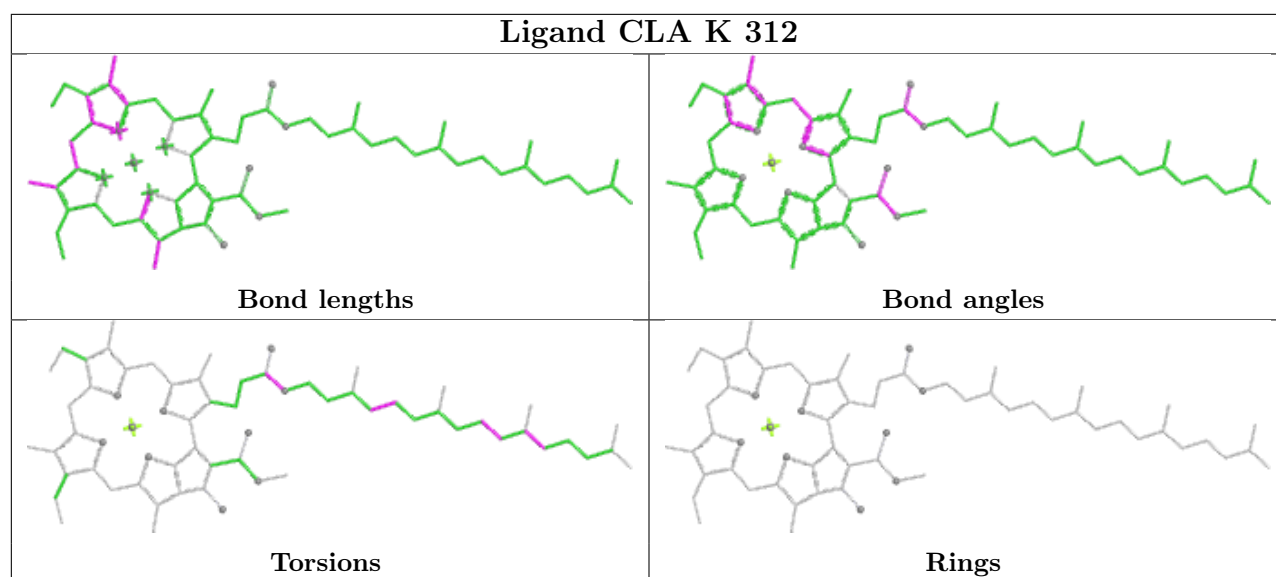


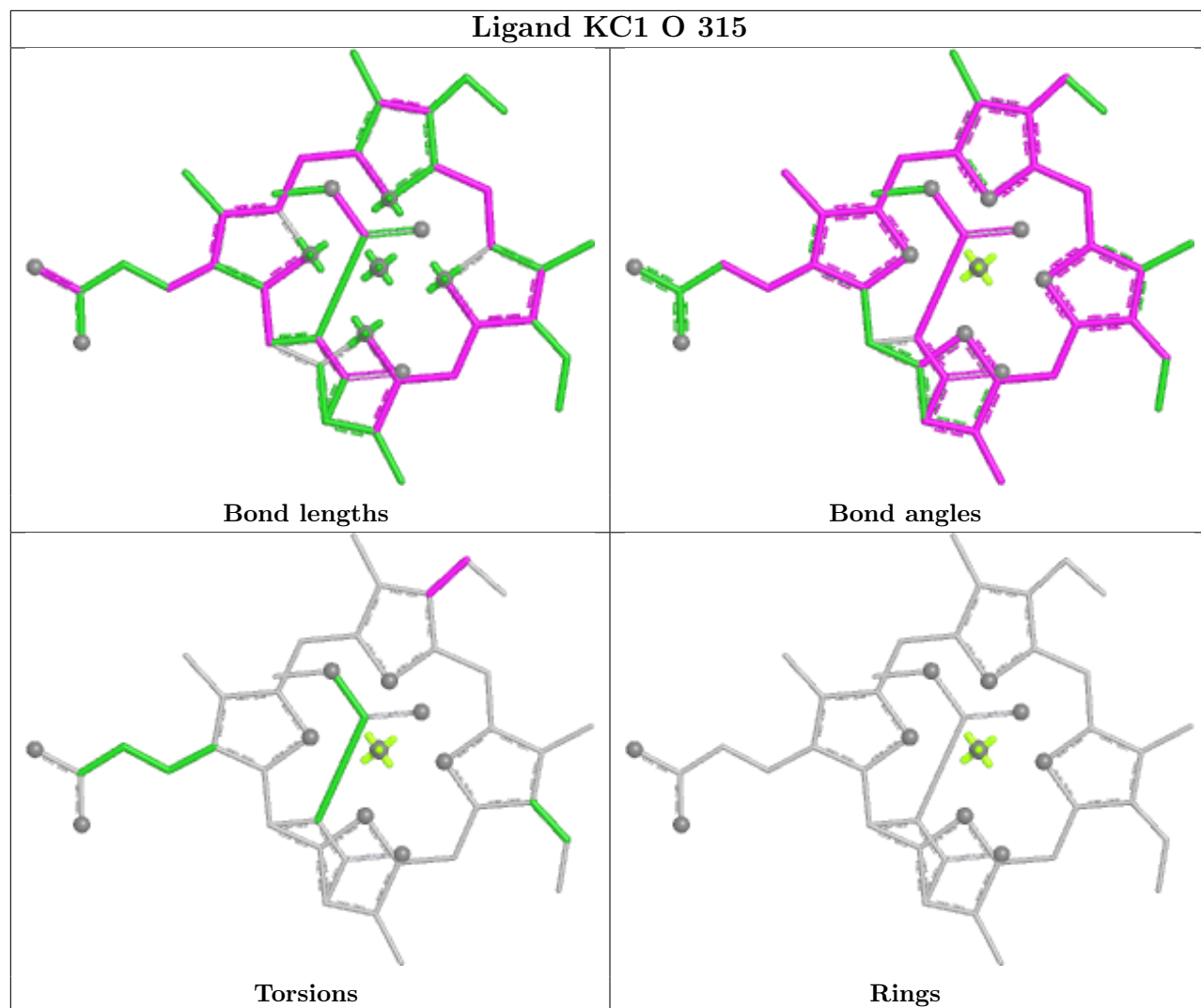


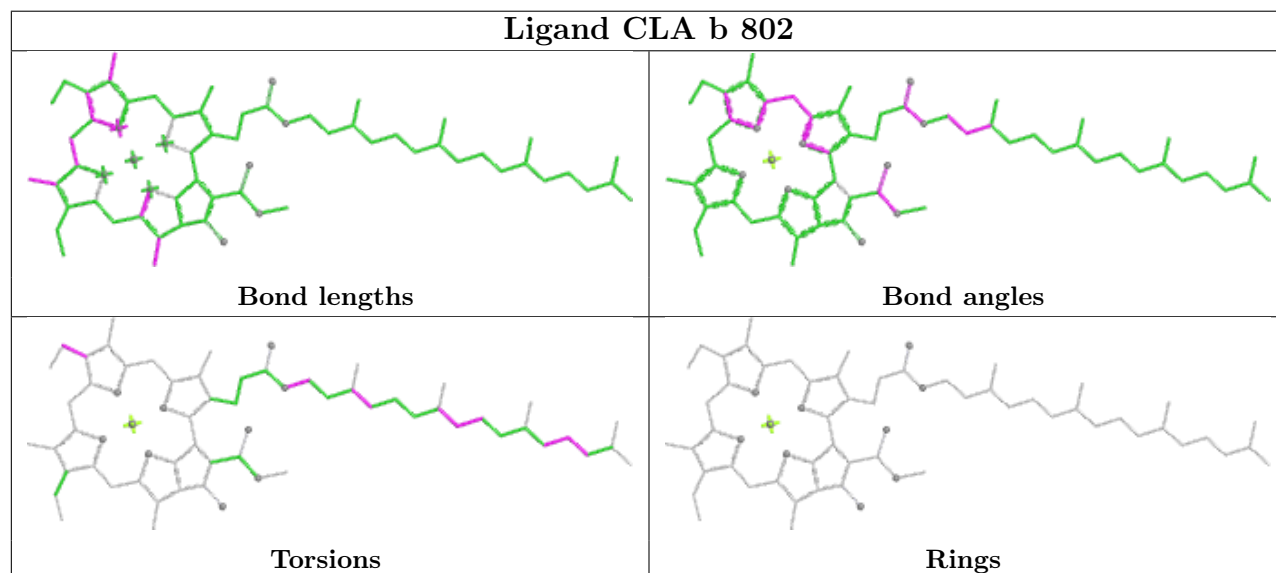
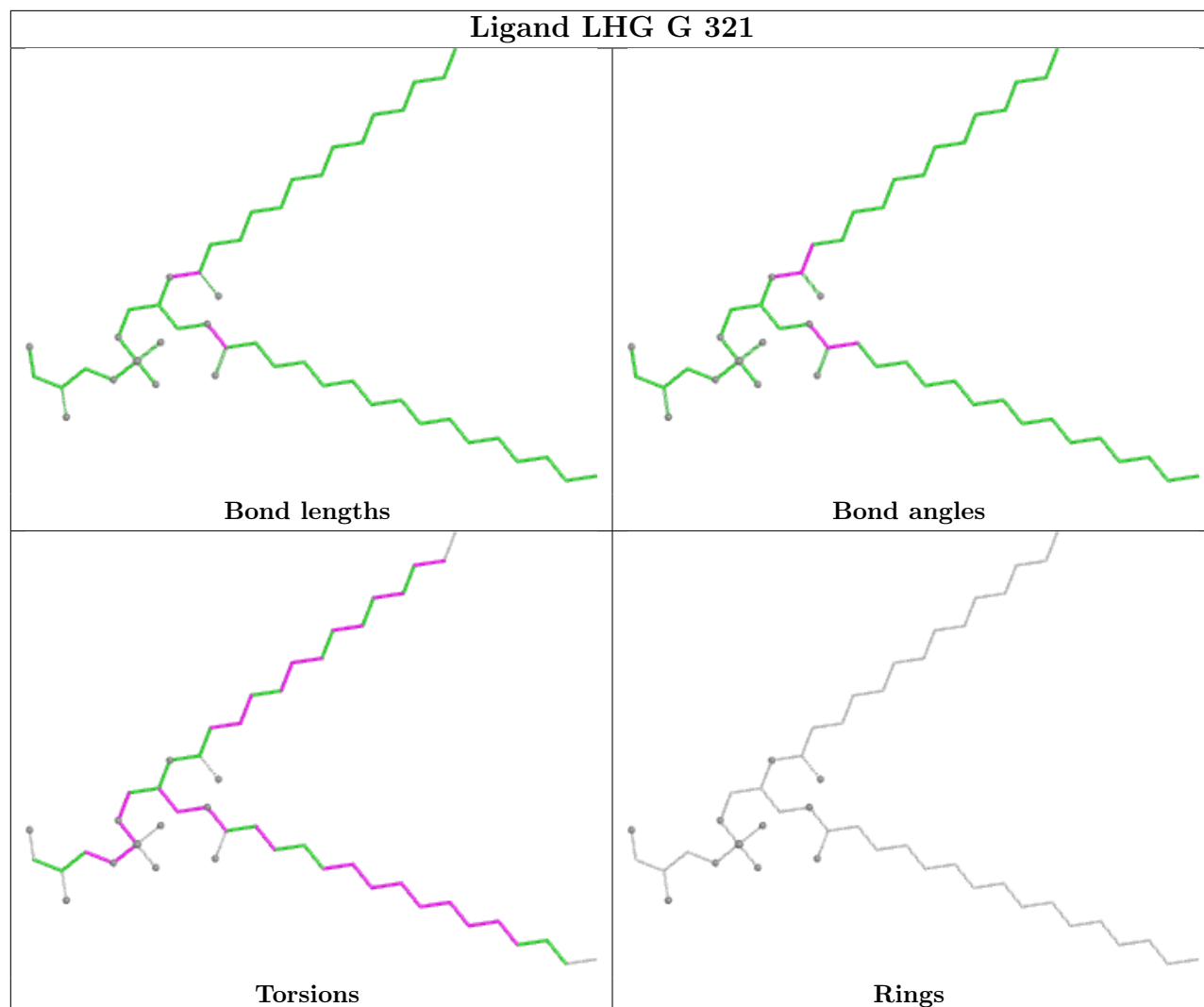


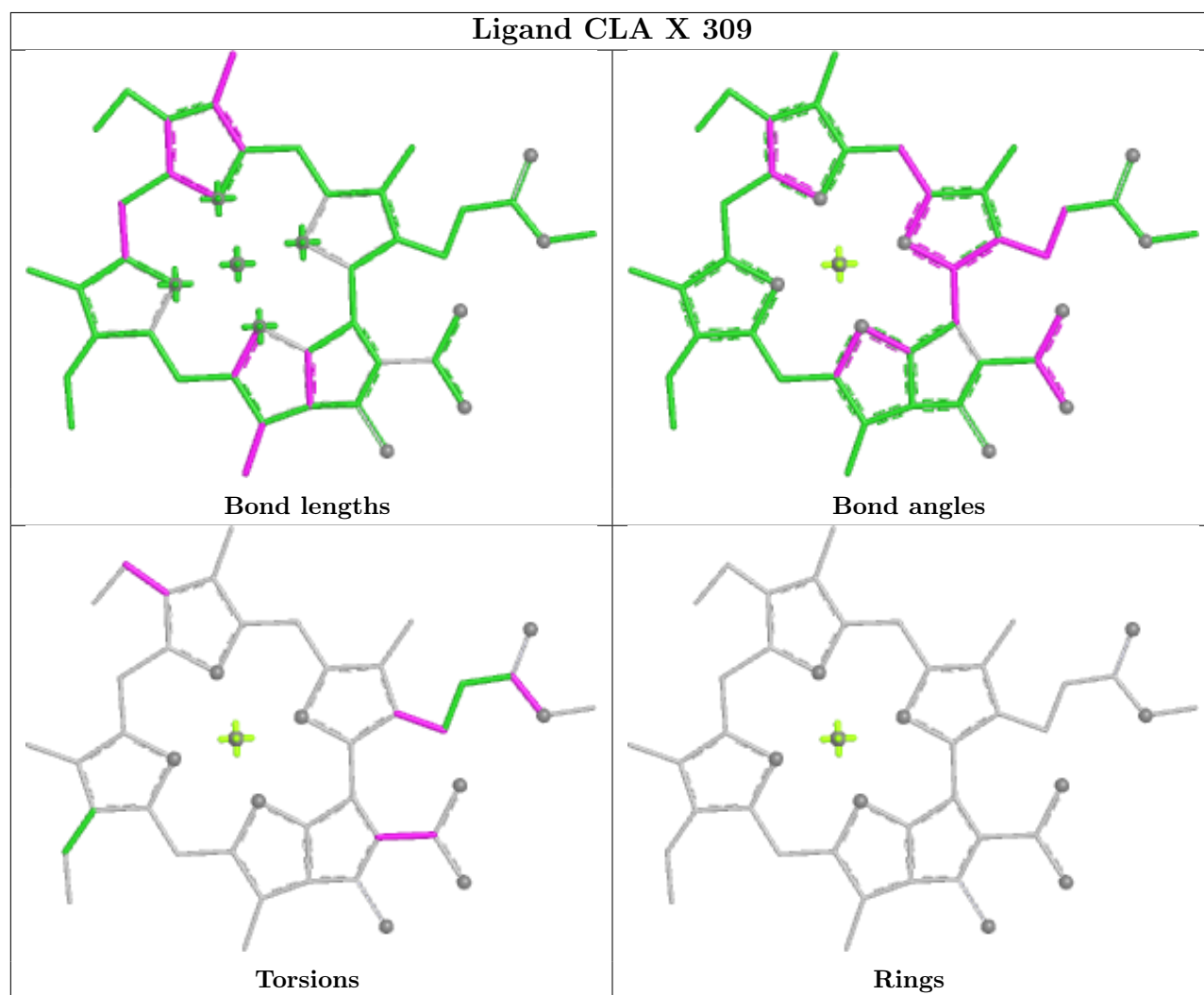
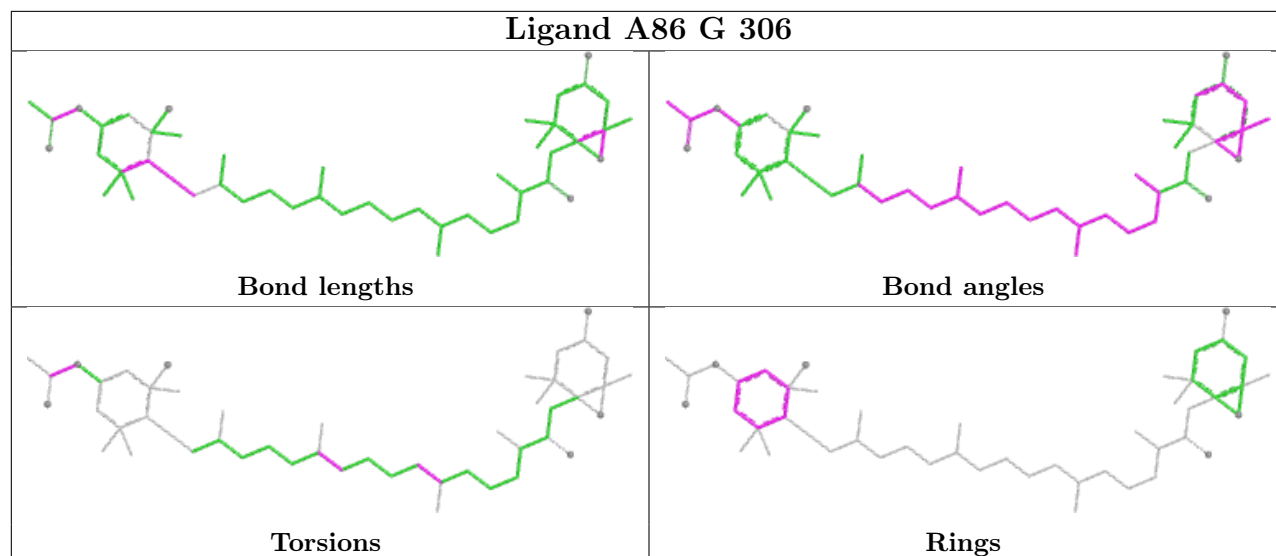


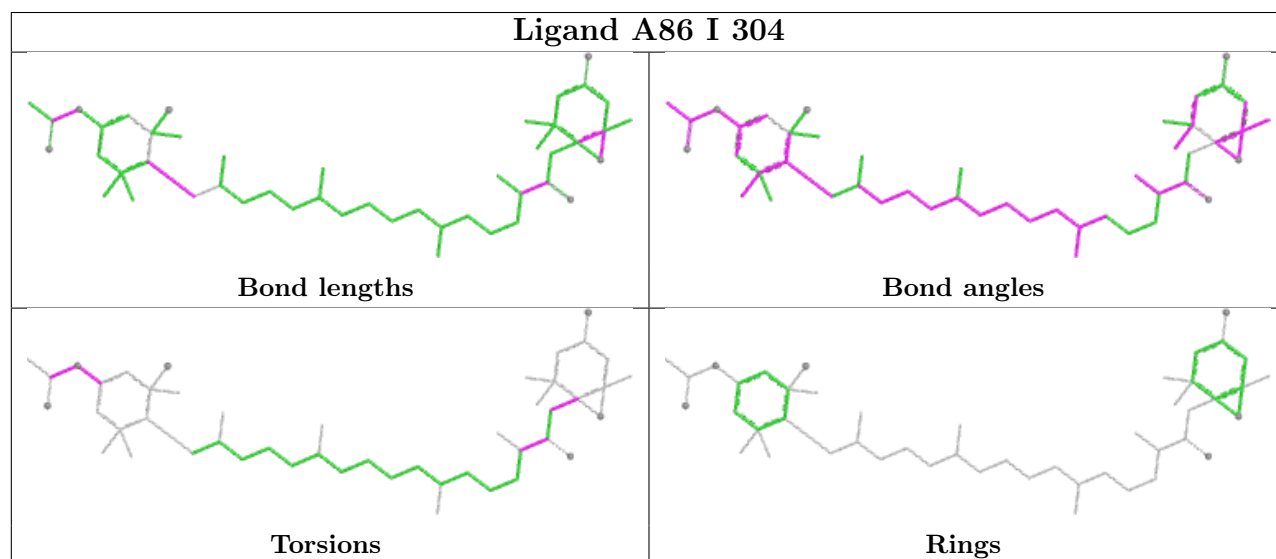
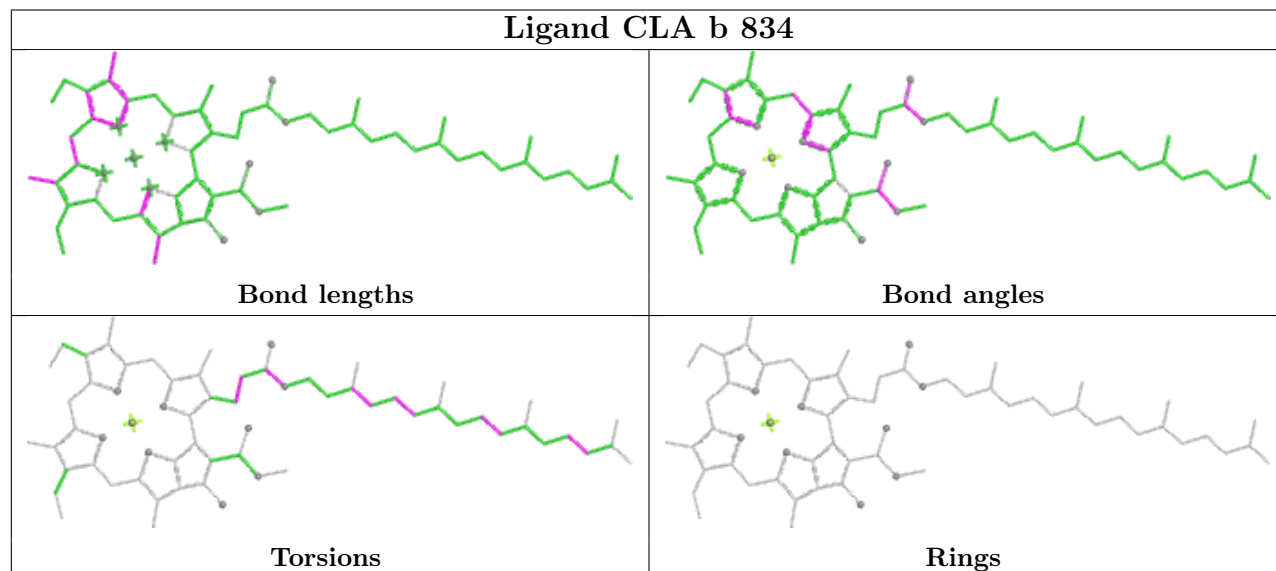
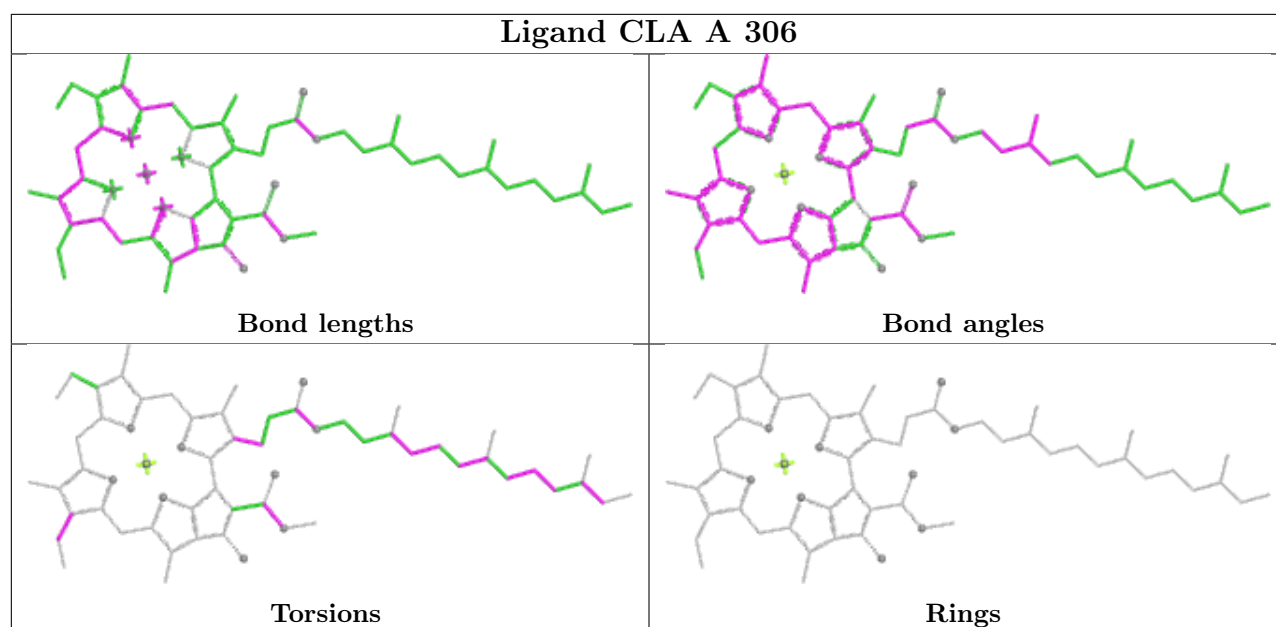


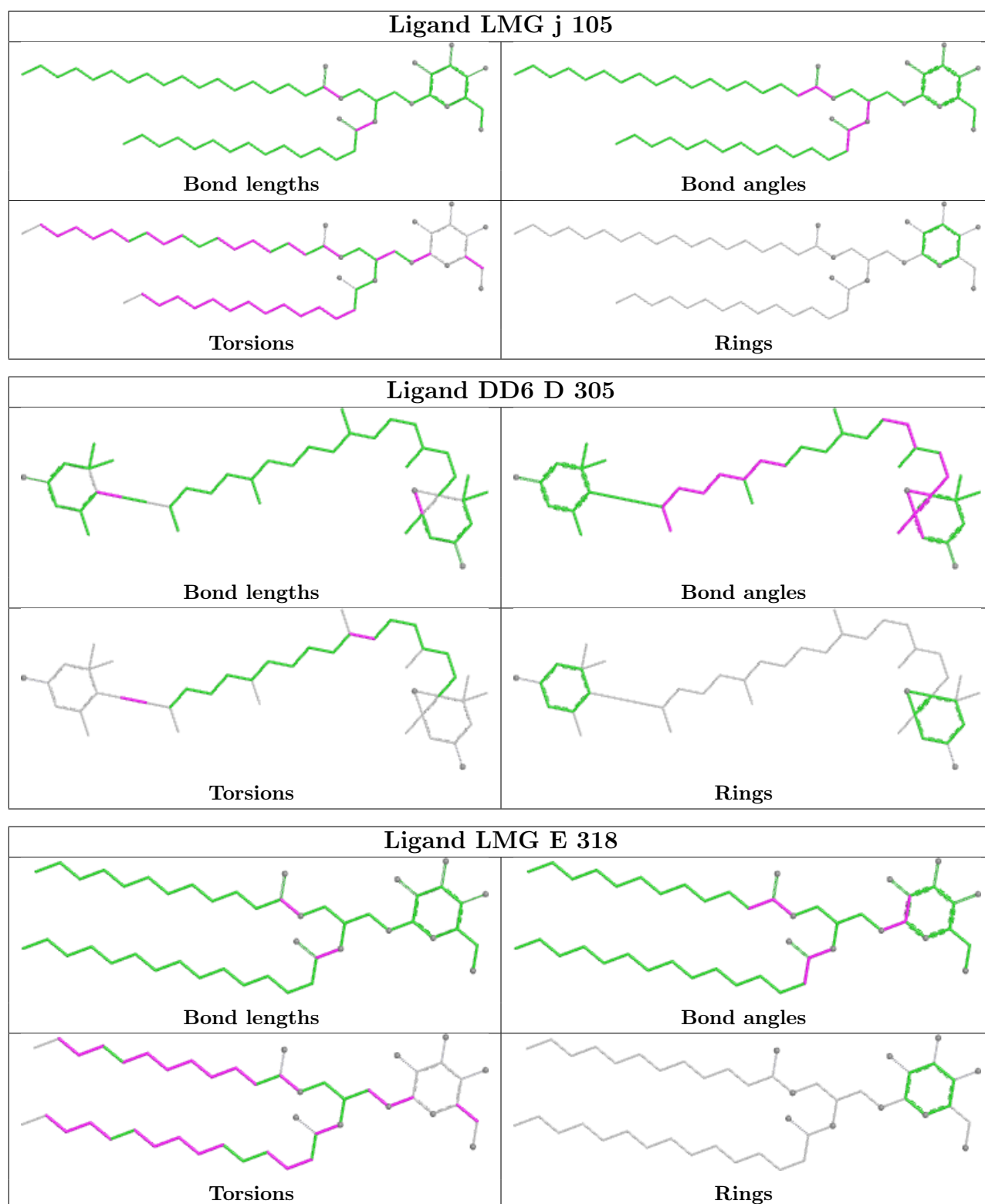


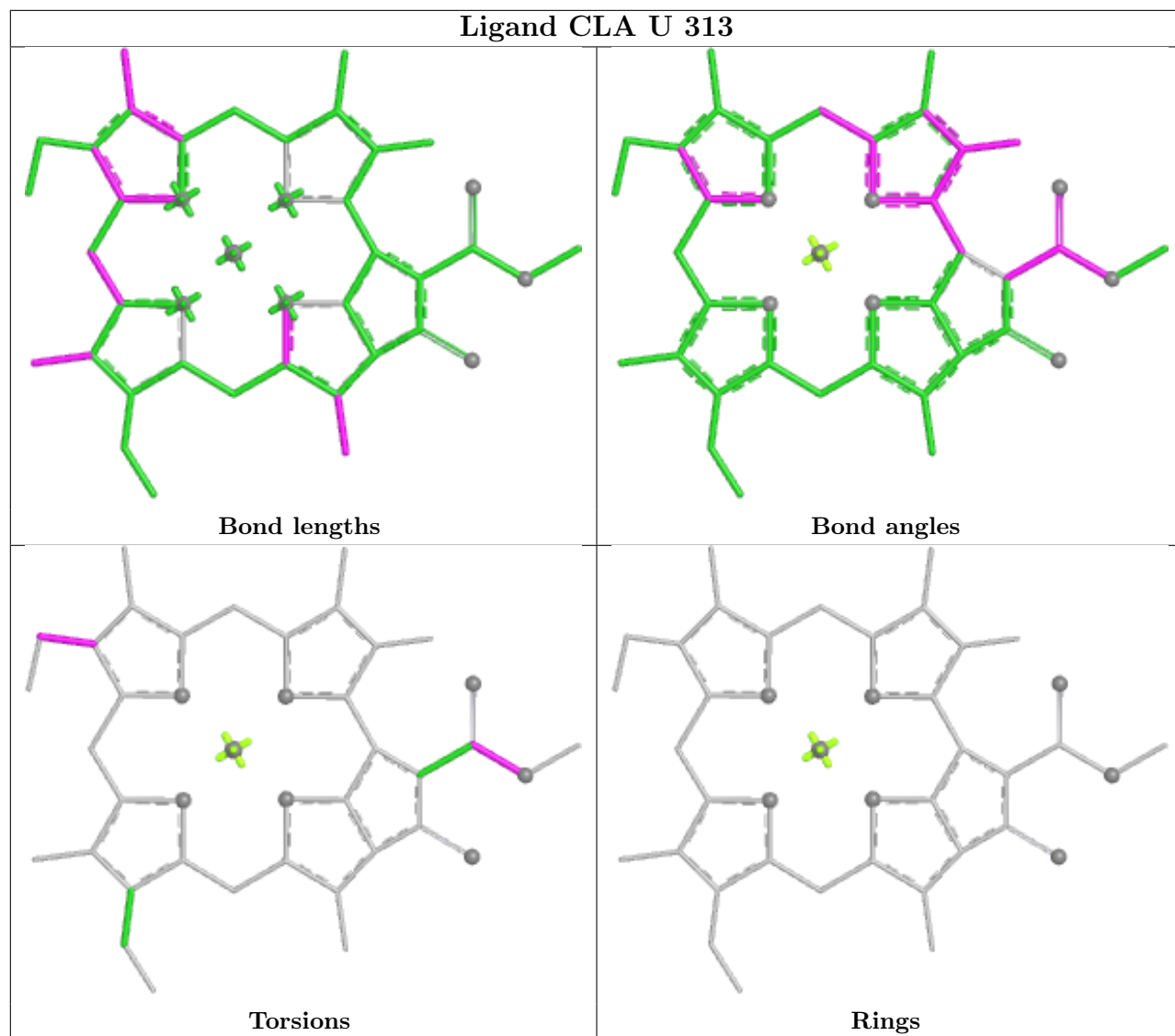


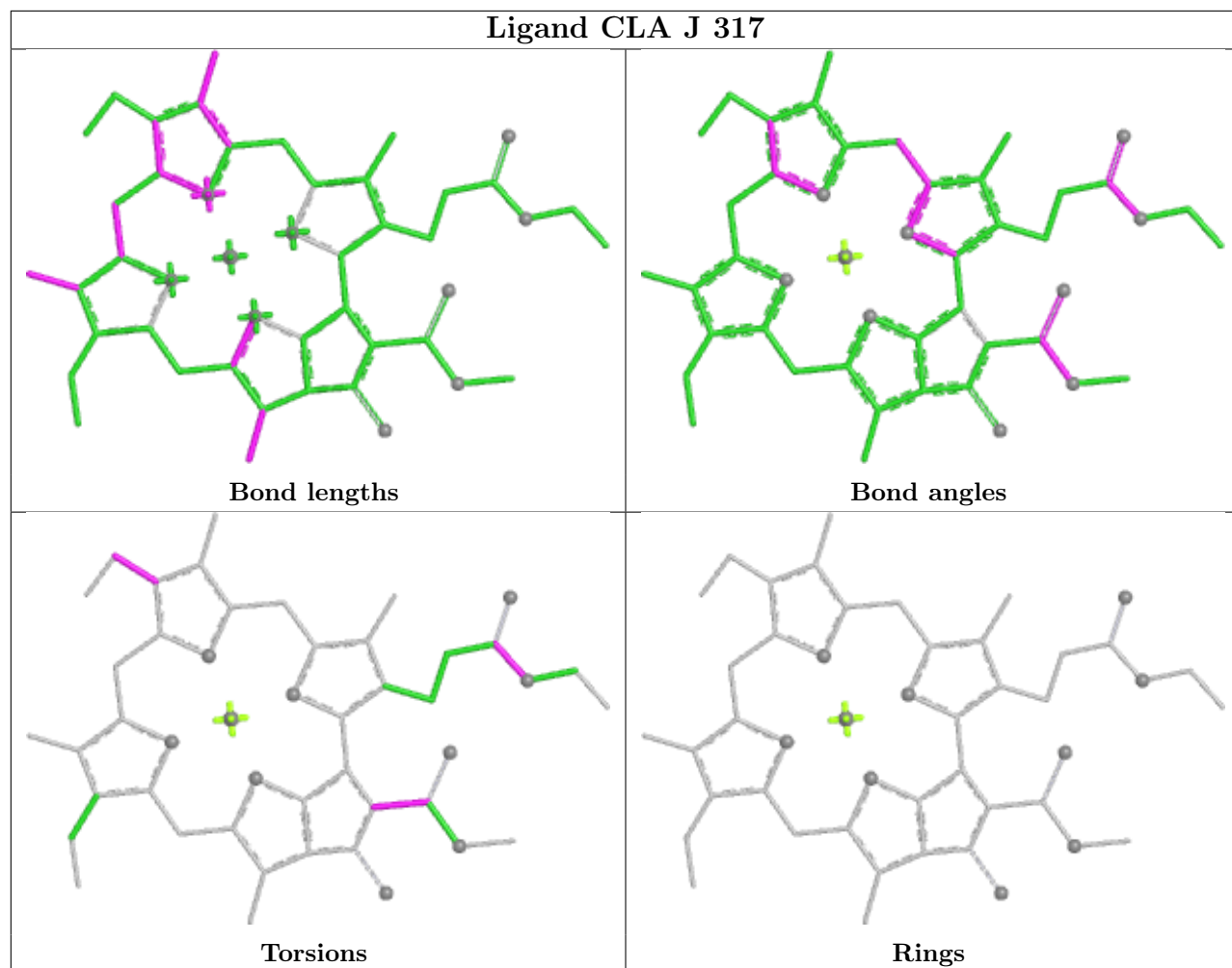


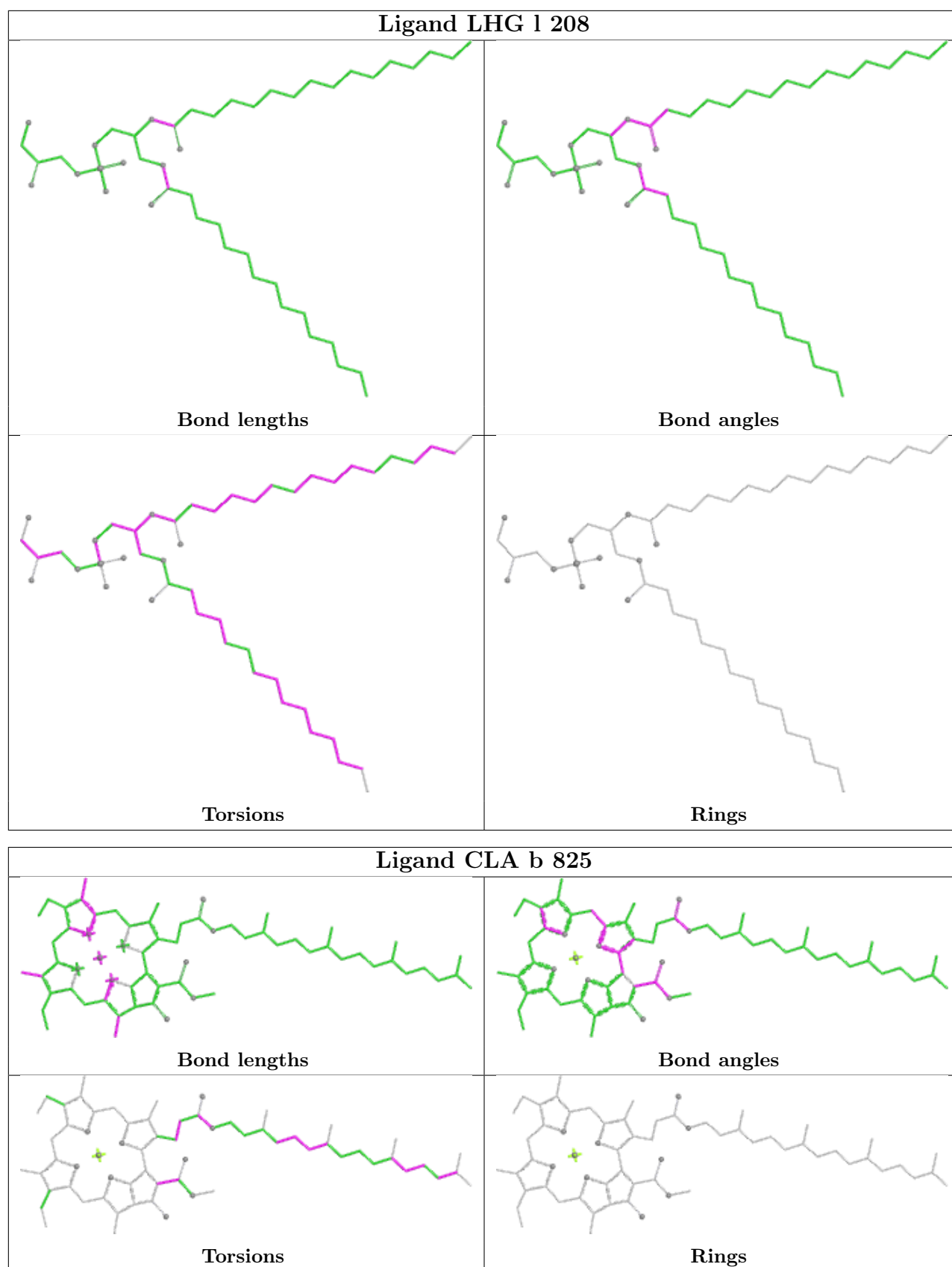


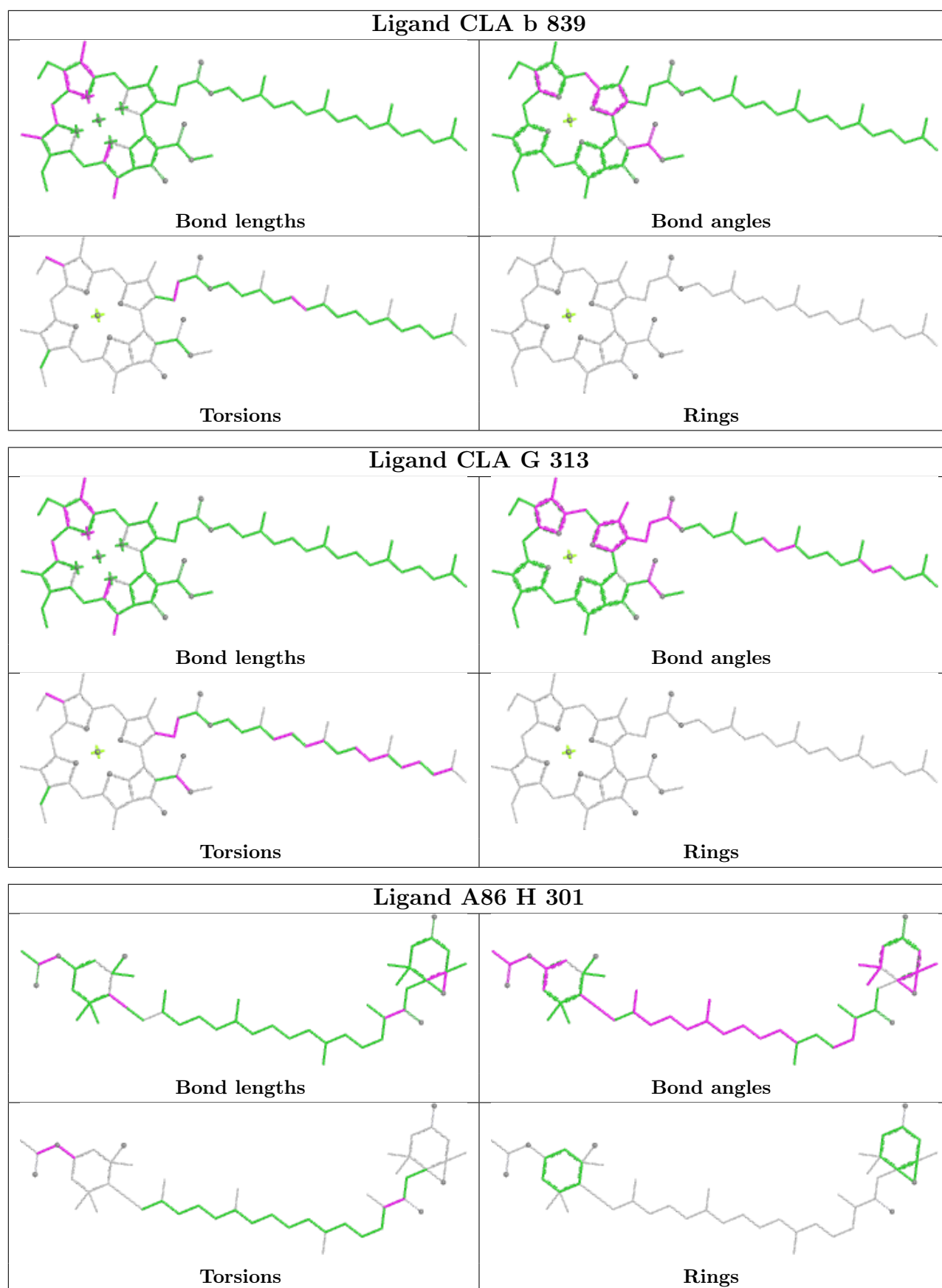


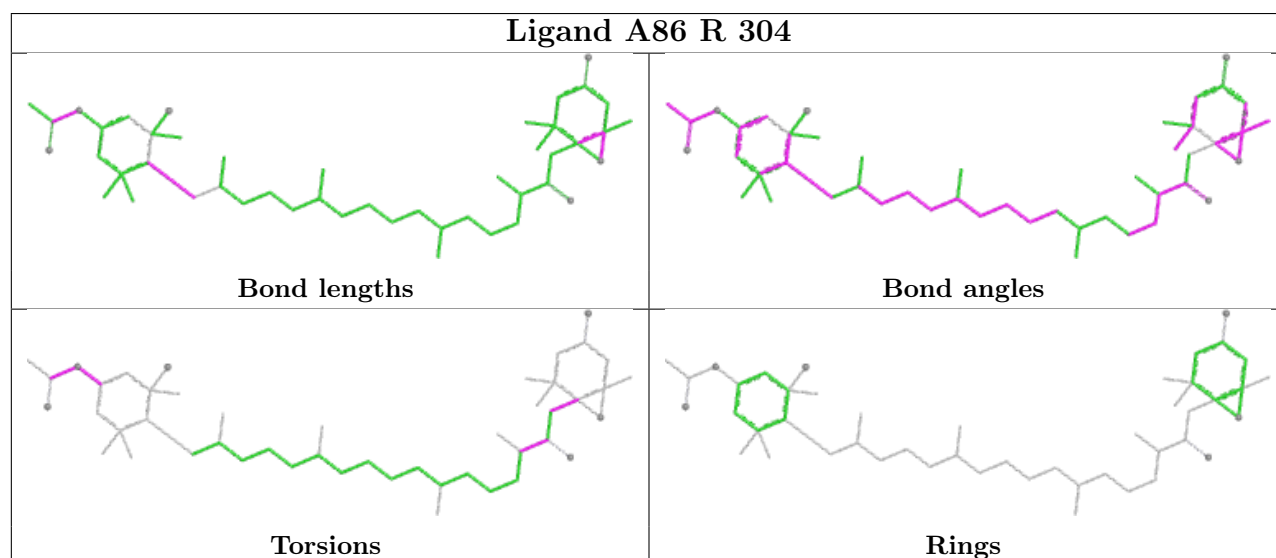
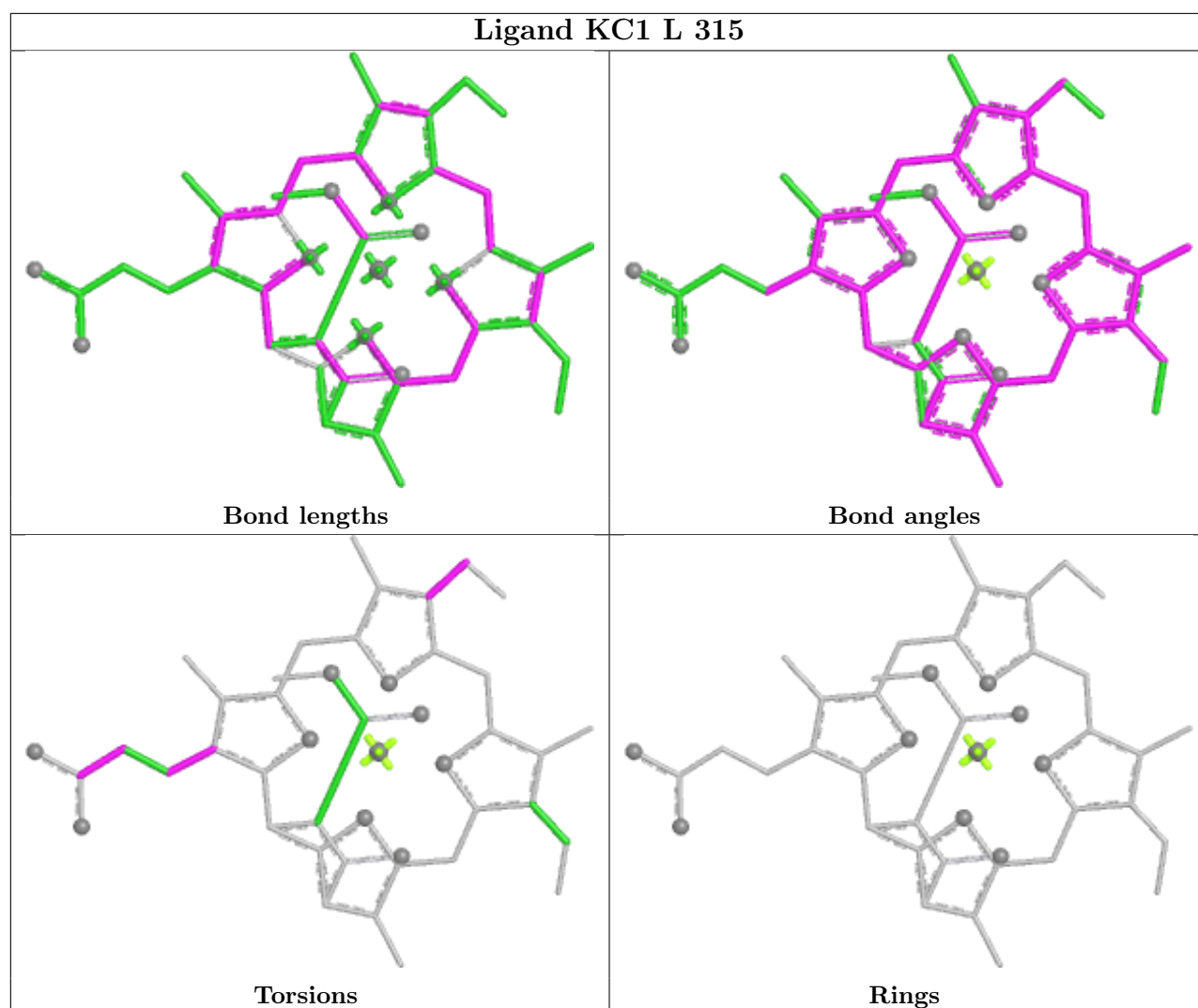


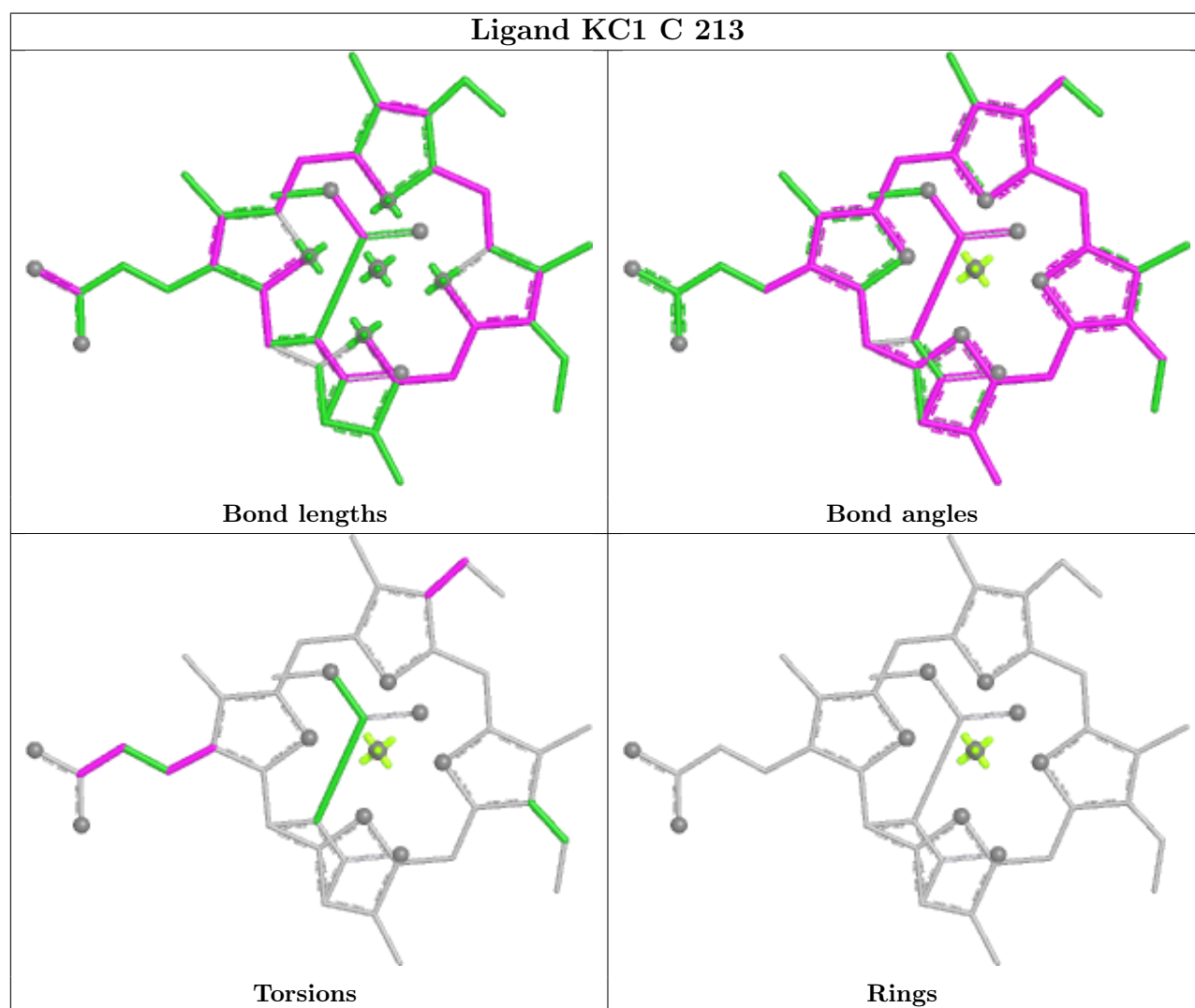
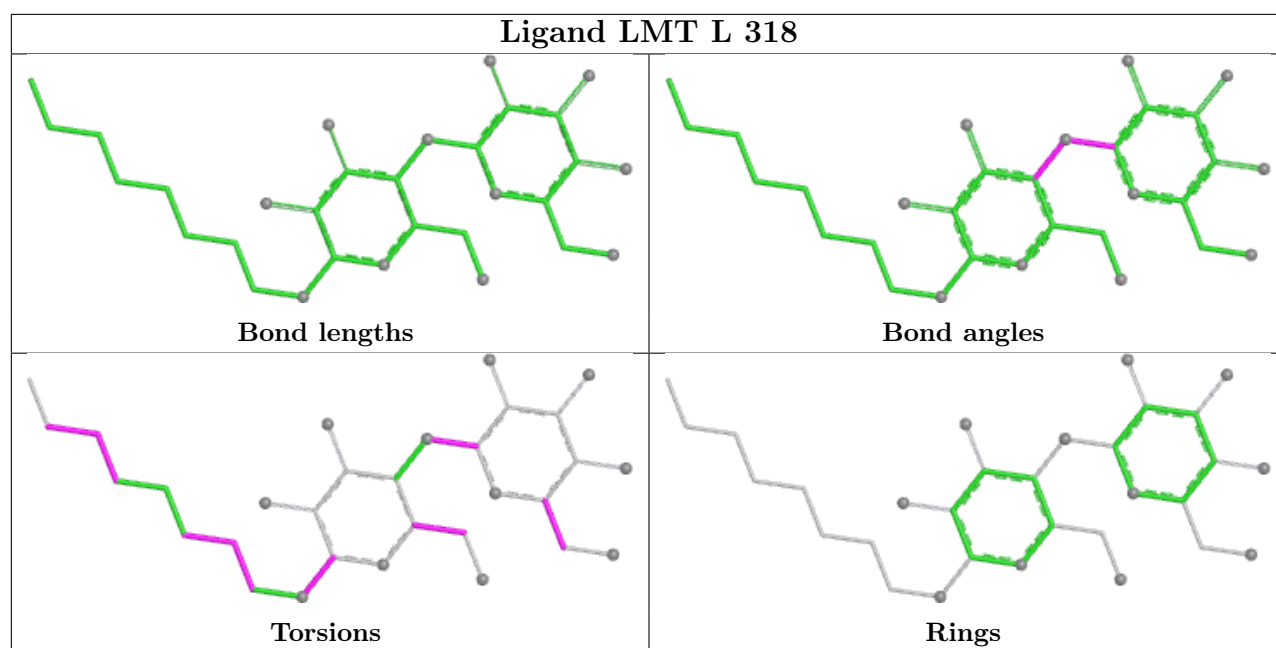


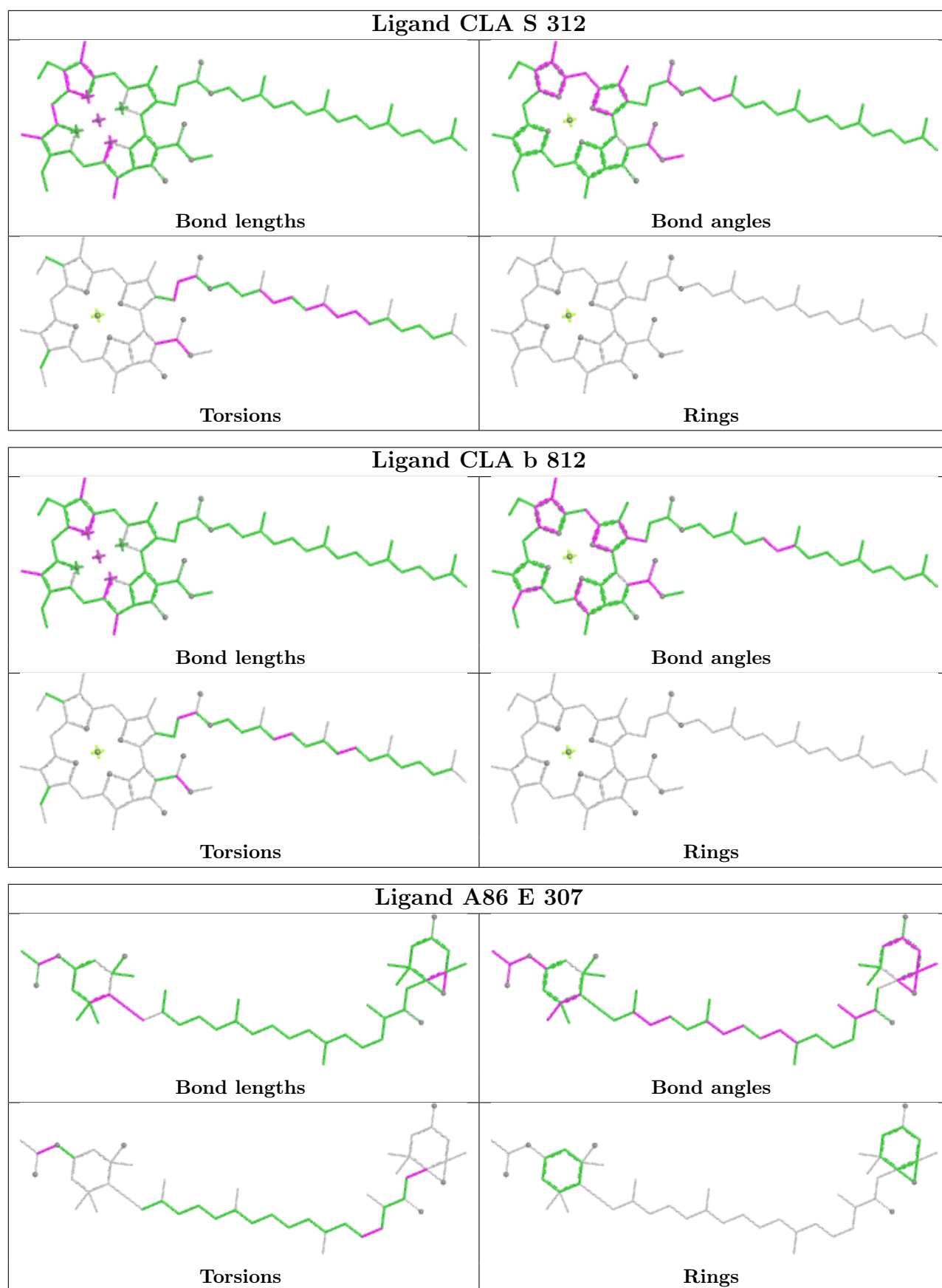


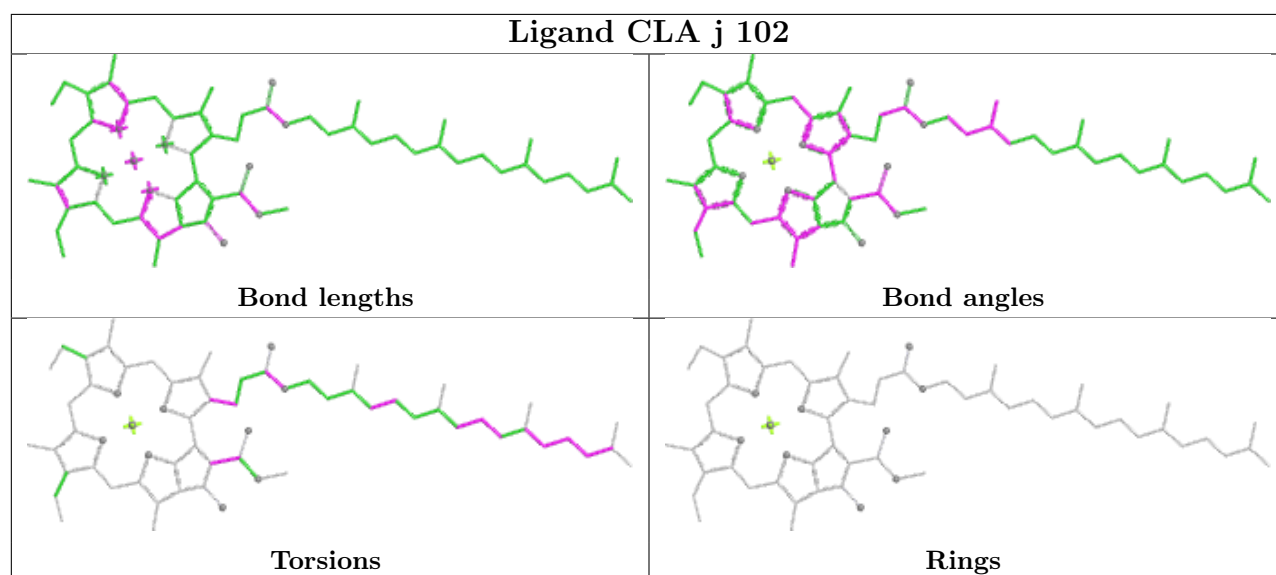
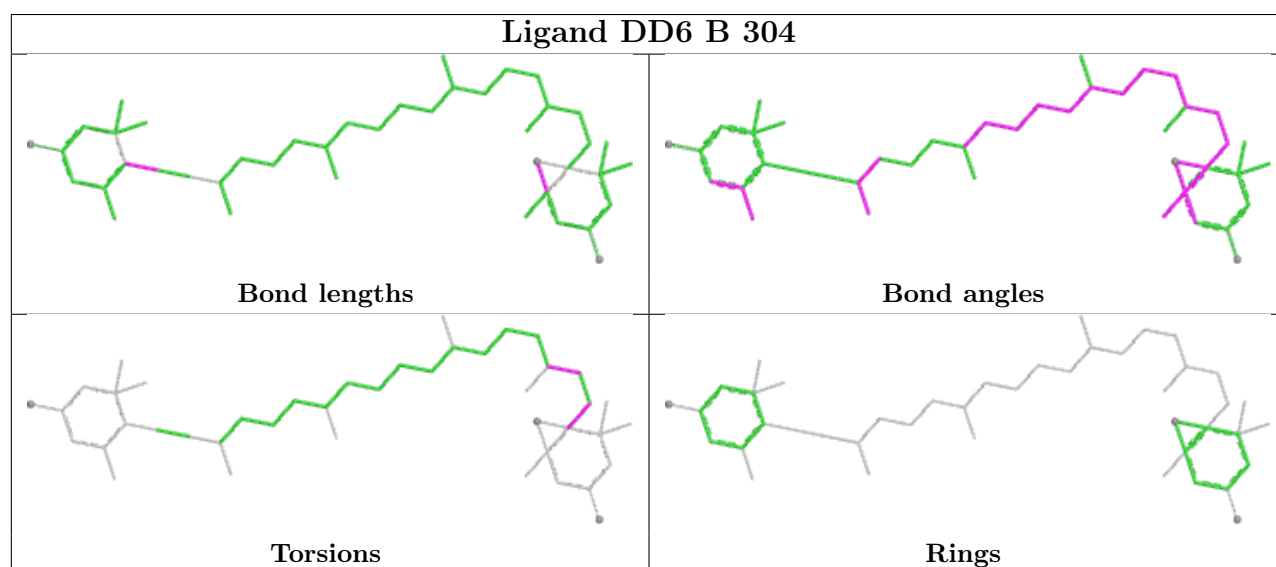
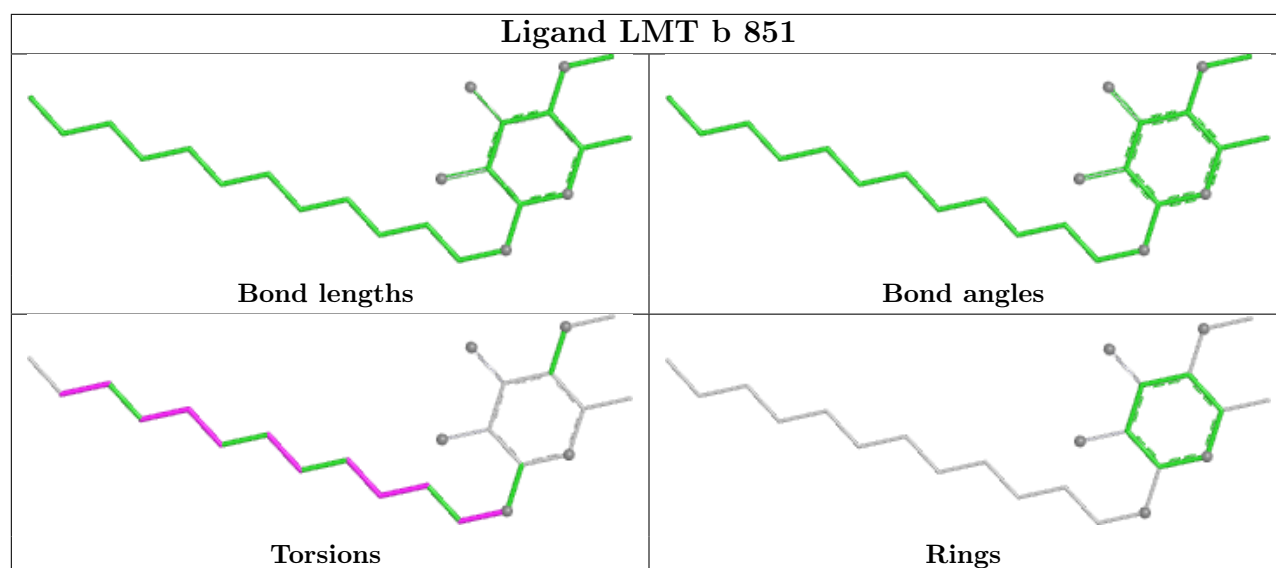












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

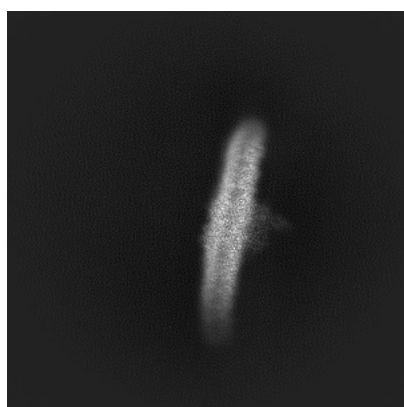
## 6 Map visualisation [i](#)

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.

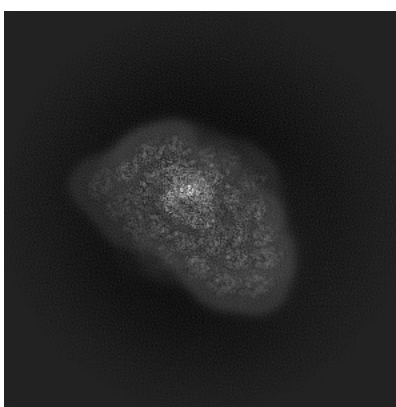
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

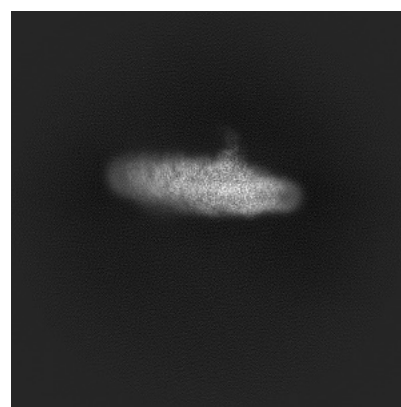
#### 6.1.1 Primary map



X



Y

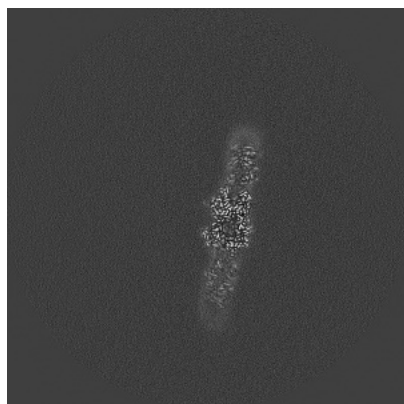


Z

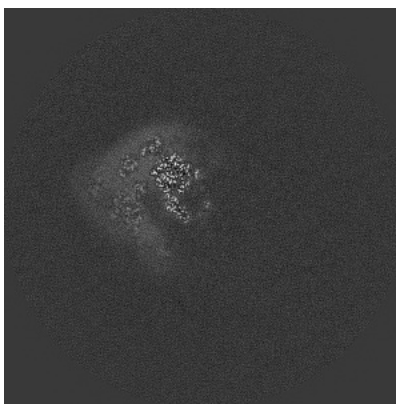
The images above show the map projected in three orthogonal directions.

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

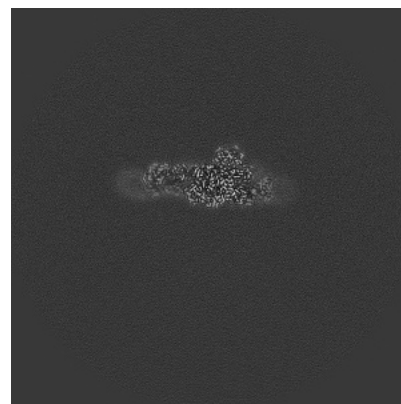
#### 6.2.1 Primary map



X Index: 260



Y Index: 260

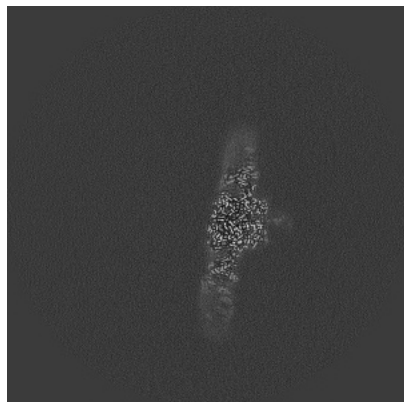


Z Index: 260

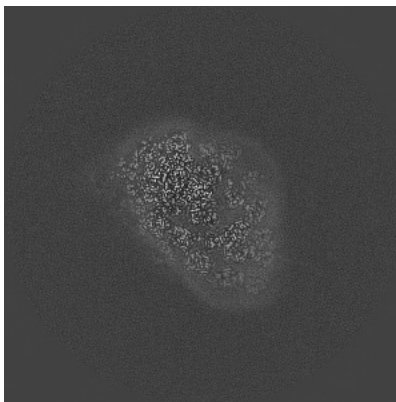
The images above show central slices of the map in three orthogonal directions.

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

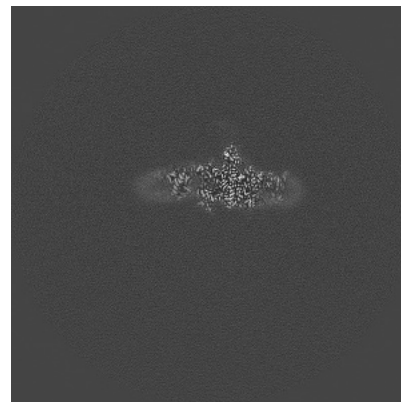
### 6.3.1 Primary map



X Index: 278



Y Index: 294

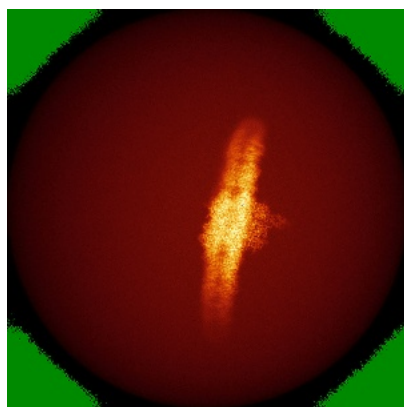


Z Index: 231

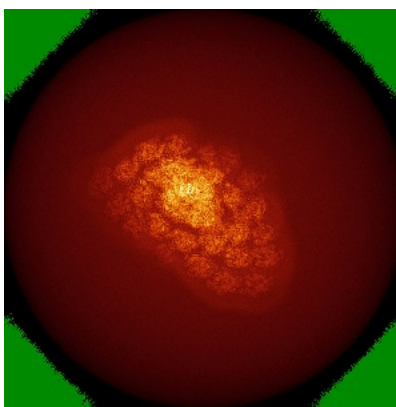
The images above show the largest variance slices of the map in three orthogonal directions.

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

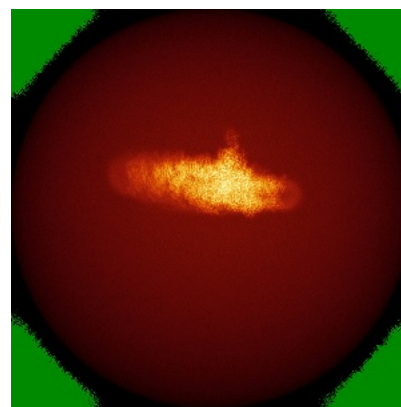
### 6.4.1 Primary map



X



Y

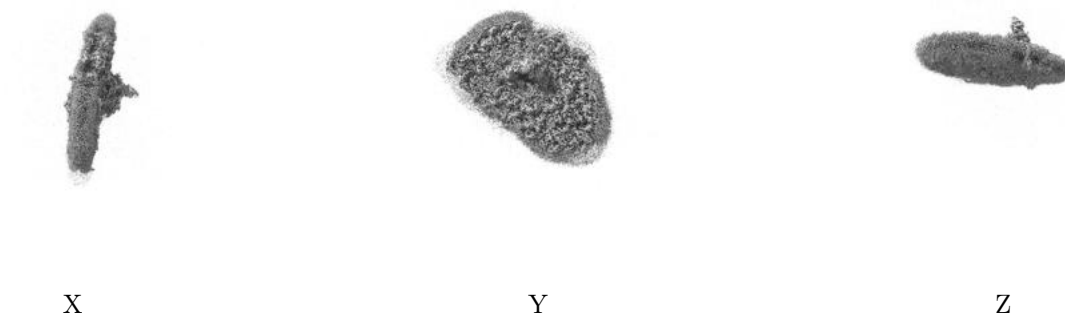


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



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

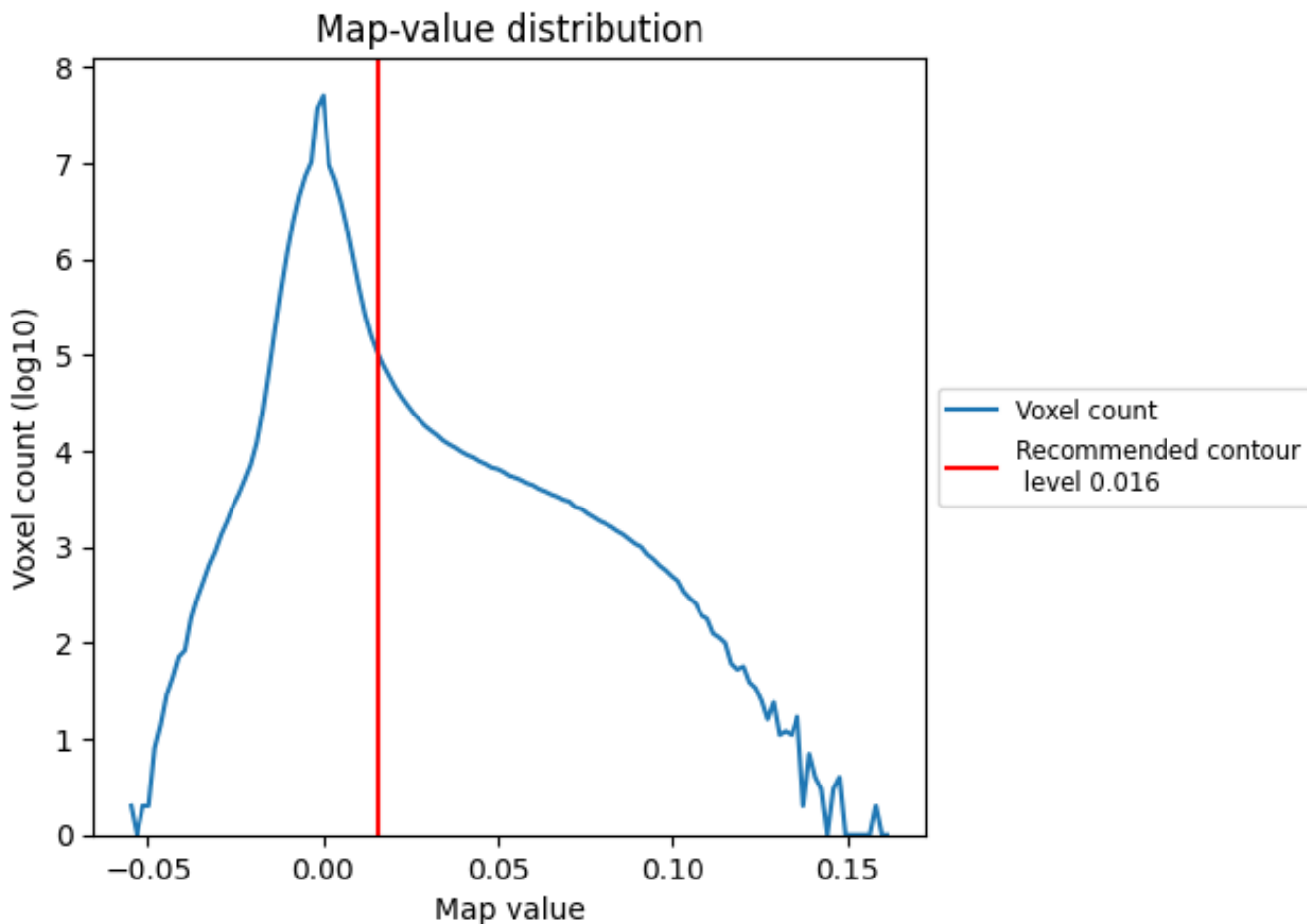
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

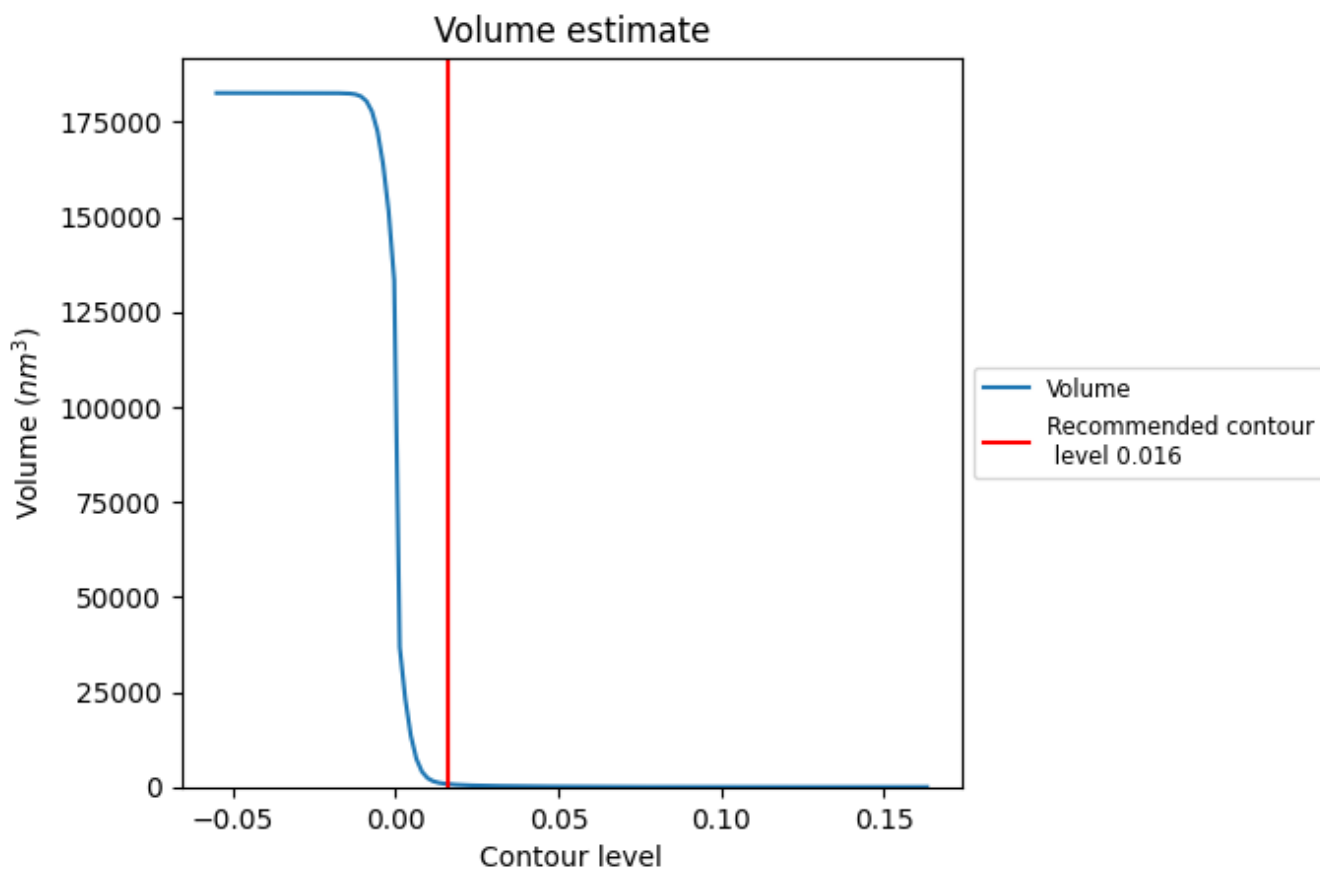
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

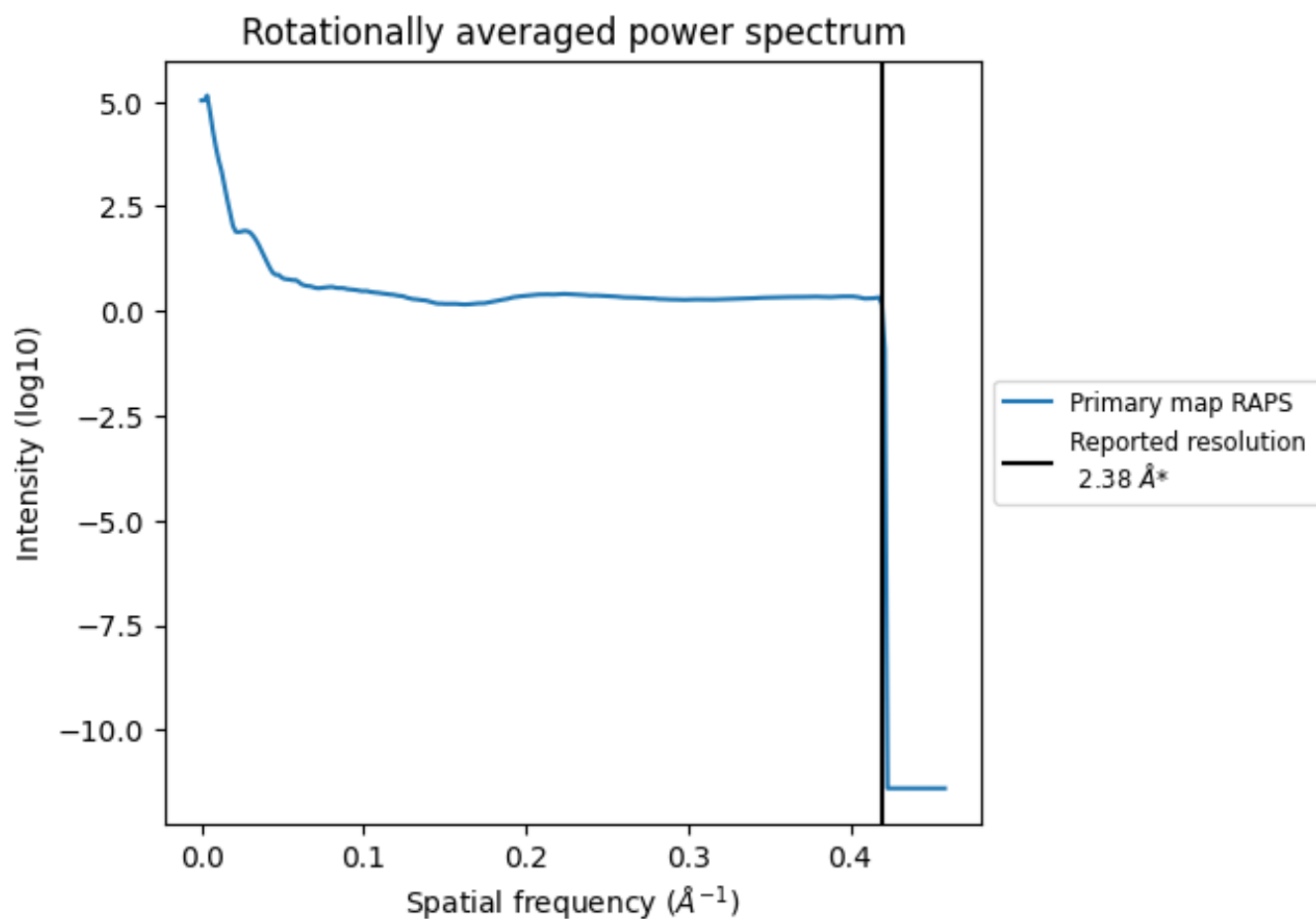
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 778  $\text{nm}^3$ ; 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<sup>-1</sup>

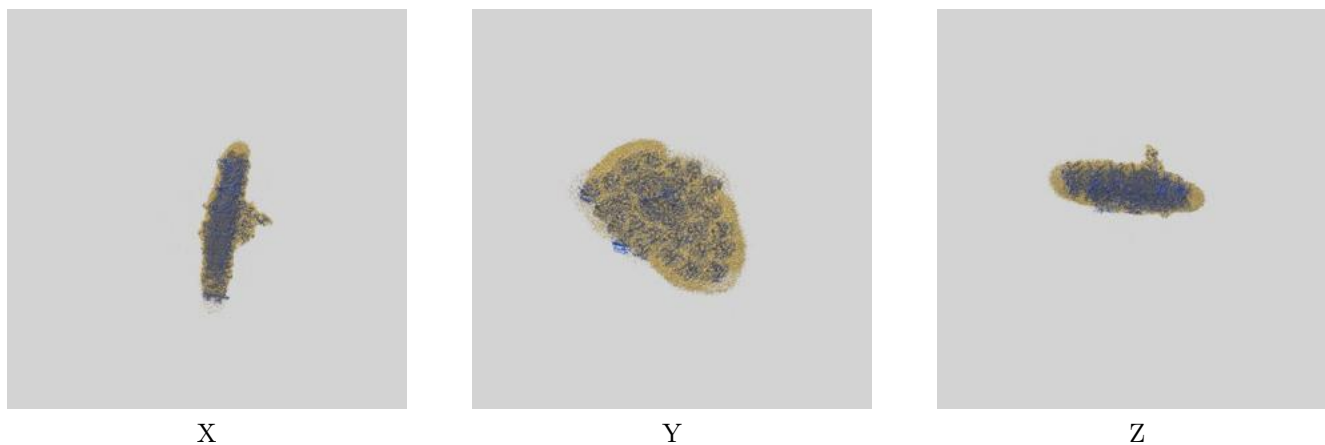
## 8 Fourier-Shell correlation

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

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

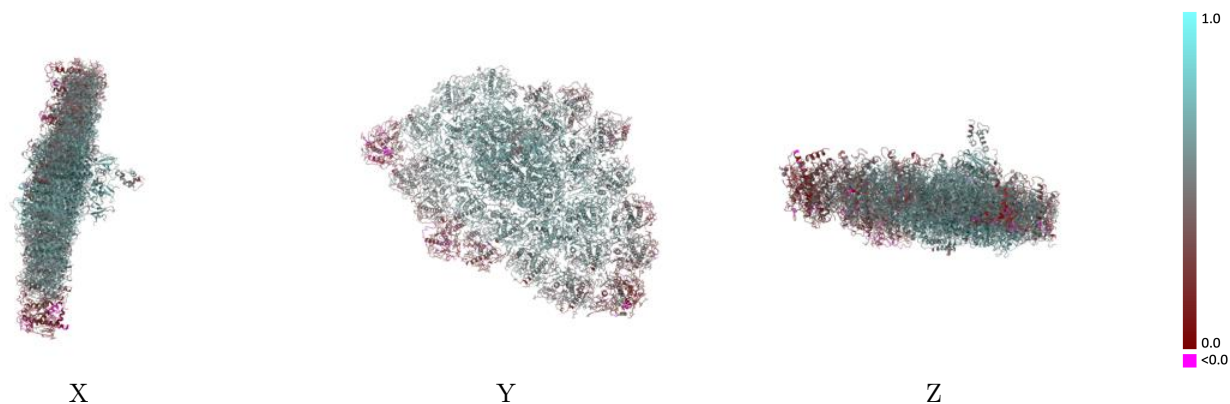
This section contains information regarding the fit between EMDB map EMD-30012 and PDB model 6LY5. Per-residue inclusion information can be found in section [3](#) on page [52](#).

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



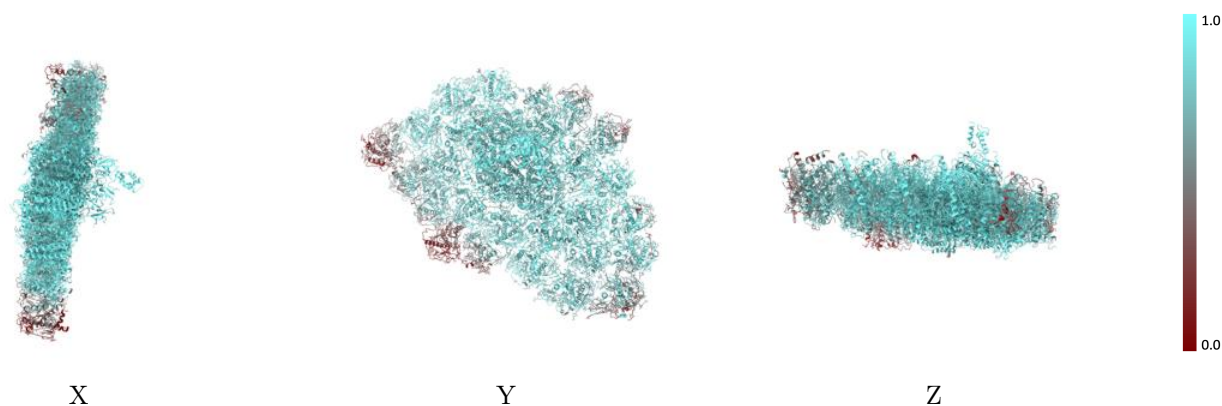
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



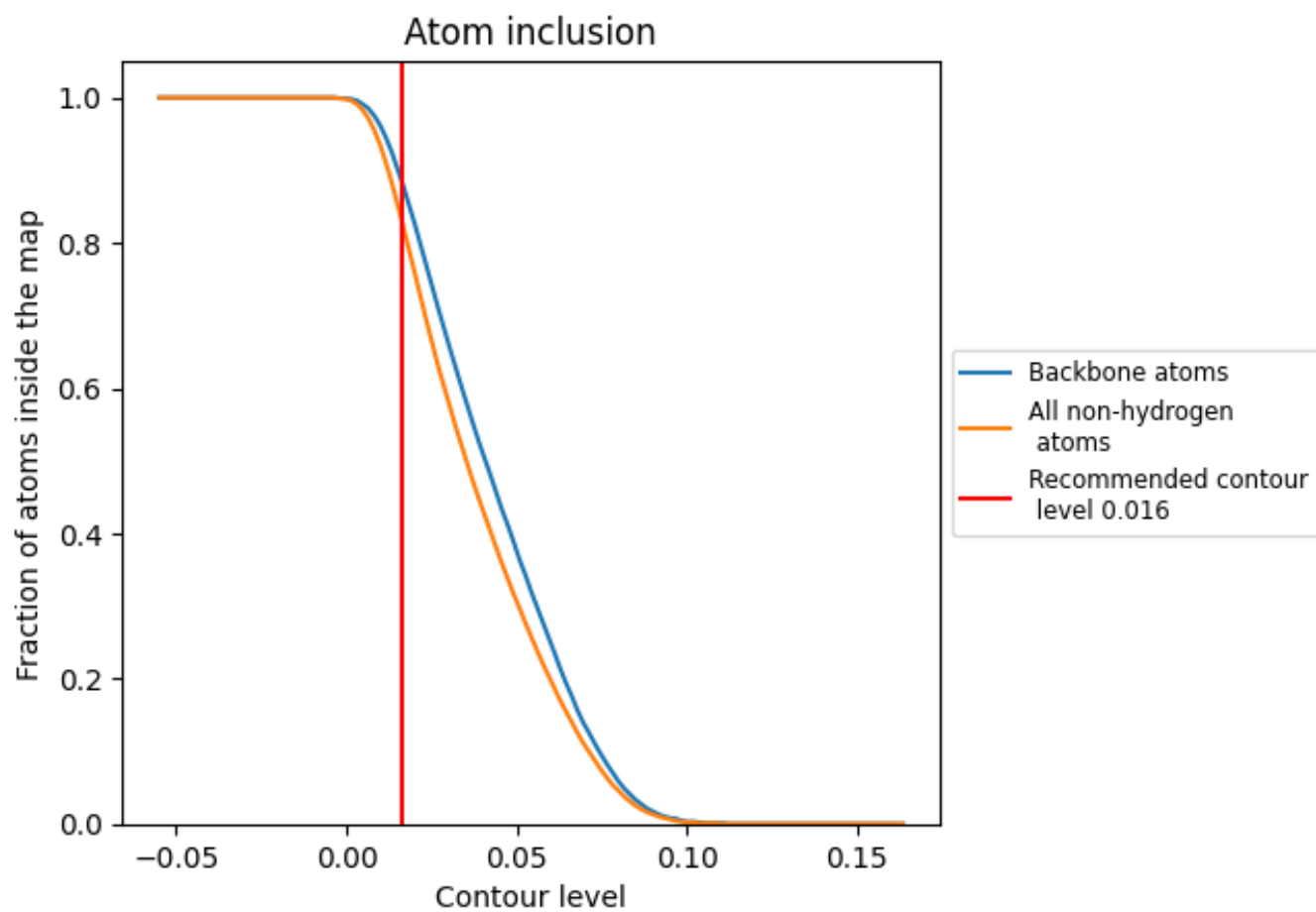
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.9410	 0.5810
B	 0.8370	 0.4930
C	 0.8980	 0.5340
D	 0.9340	 0.5870
E	 0.9530	 0.6050
F	 0.9430	 0.5960
G	 0.9570	 0.6150
H	 0.8900	 0.5450
I	 0.9240	 0.5640
J	 0.9060	 0.5400
K	 0.8890	 0.5170
L	 0.8050	 0.4220
M	 0.8700	 0.4820
N	 0.3040	 0.1740
O	 0.6670	 0.4100
P	 0.8980	 0.5260
Q	 0.7760	 0.3880
R	 0.7930	 0.4220
S	 0.5670	 0.2610
T	 0.6280	 0.3920
U	 0.6600	 0.3880
V	 0.7550	 0.4470
W	 0.4970	 0.2640
X	 0.1530	 0.1400
a	 0.9830	 0.6690
b	 0.9910	 0.6730
c	 0.9770	 0.6620
d	 0.9460	 0.6200
e	 0.9210	 0.5940
f	 0.9320	 0.6150
g	 0.8870	 0.4480
h	 0.9690	 0.6040
i	 0.9430	 0.6250
j	 0.9380	 0.6250



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
l	 0.9580	 0.6310
m	 0.9420	 0.6140