



# wwPDB EM Validation Summary Report ⓘ

Nov 23, 2022 – 02:50 AM JST

PDB ID : 7F9O  
EMDB ID : EMD-31498  
Title : PSI-NDH supercomplex of Barley  
Authors : Wang, W.D.; Shen, L.; Tang, K.; Han, G.Y.; Shen, J.R.; Zhang, X.  
Deposited on : 2021-07-04  
Resolution : 4.50 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

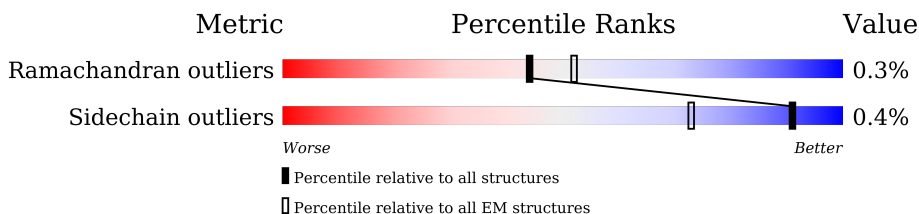
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.50 Å.

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




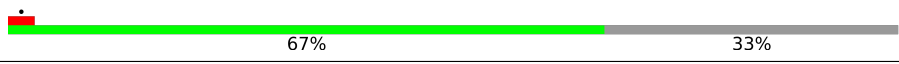
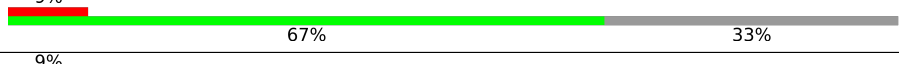


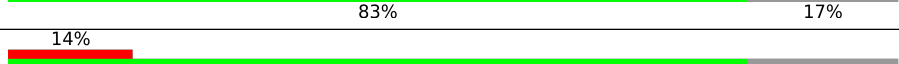
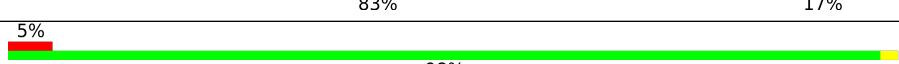
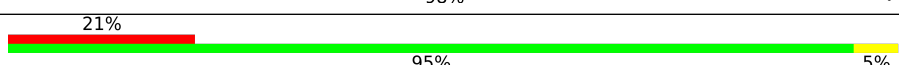
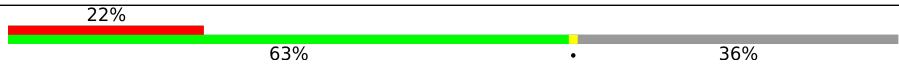


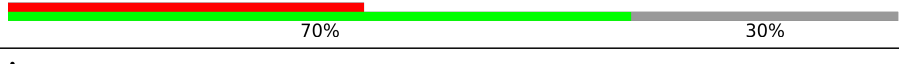
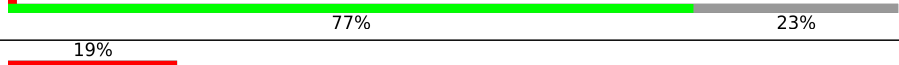

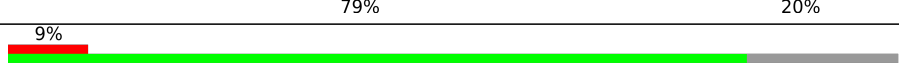


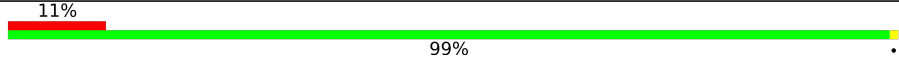
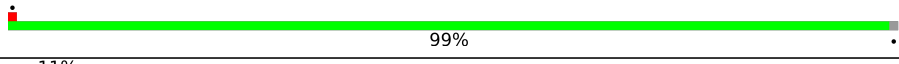
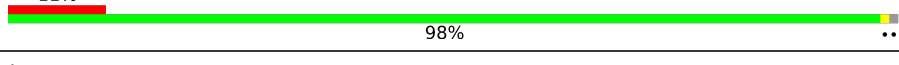
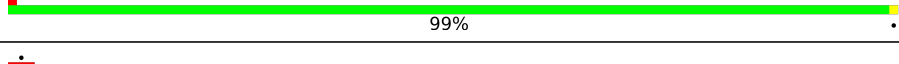
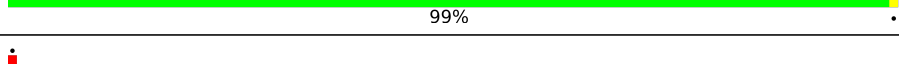



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	750	99%
1	e	750	19% 99%
2	B	734	99%
2	f	734	12% 99%
3	C	81	99%
3	g	81	12% 100%
4	D	205	69% 31%
4	h	205	44% 69% 31%
5	E	147	46% 54%

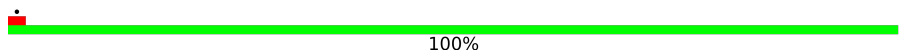

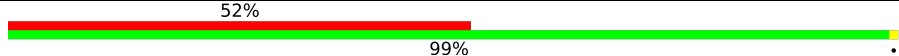

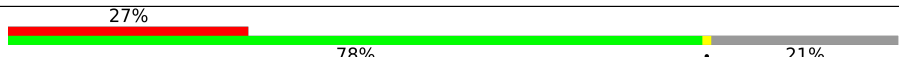
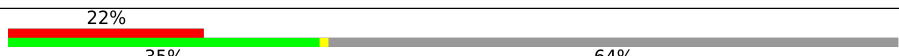
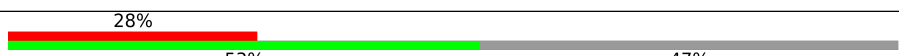
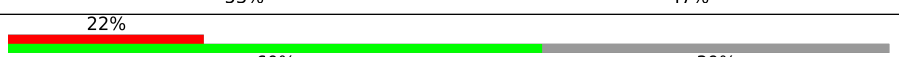

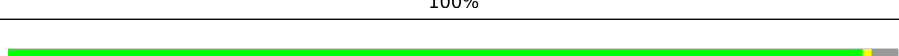
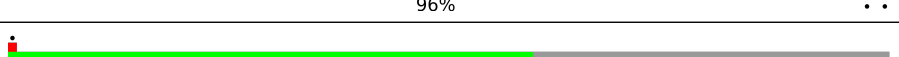

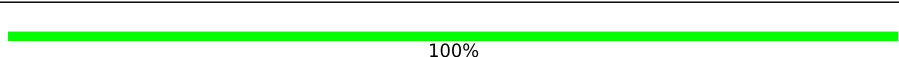
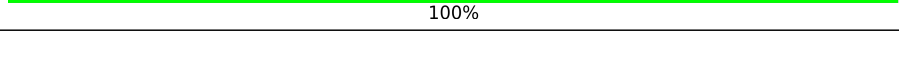
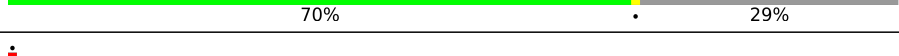


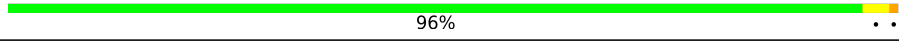
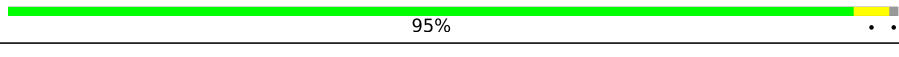
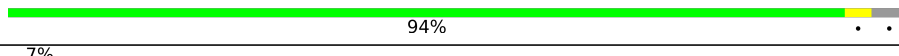
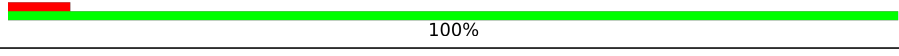
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Mol	Chain	Length	Quality of chain
5	i	147	
6	F	235	
6	j	235	
7	H	143	
7	k	143	
8	I	36	
8	l	36	
9	J	42	
9	m	42	
10	K	131	
10	n	131	
11	L	209	
11	o	209	
12	1	247	
12	p	247	
13	2	255	
14	3	269	
14	q	269	
15	5	257	
16	G	346	
17	M	483	
18	N	117	
19	O	499	
20	P	100	
21	Q	777	

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Mol	Chain	Length	Quality of chain
22	R	176	
23	S	383	
24	T	165	
25	U	159	
26	V	245	
27	W	192	
28	X	213	
29	Y	233	
30	Z	61	
31	a	154	
32	b	216	
33	c	227	
34	4	130	
35	d	243	
36	6	469	
37	7	361	
38	8	119	
39	9	83	
40	0	155	
41	r	197	
42	s	211	

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
43	CL0	A	801	X	-	-	-
43	CL0	e	801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	1	504	X	-	-	-
44	CLA	1	505	X	-	-	-
44	CLA	1	506	X	-	-	-
44	CLA	1	507	X	-	-	-
44	CLA	1	508	X	-	-	-
44	CLA	1	510	X	-	-	-
44	CLA	1	511	X	-	-	-
44	CLA	1	515	X	-	-	-
44	CLA	2	504	X	-	-	-
44	CLA	2	506	X	-	-	-
44	CLA	2	507	X	-	-	-
44	CLA	2	508	X	-	-	-
44	CLA	2	509	X	-	-	-
44	CLA	2	510	X	-	-	-
44	CLA	2	511	X	-	-	-
44	CLA	2	514	X	-	-	-
44	CLA	3	301	X	-	-	-
44	CLA	3	306	X	-	-	-
44	CLA	3	307	X	-	-	-
44	CLA	3	308	X	-	-	-
44	CLA	3	310	X	-	-	-
44	CLA	3	311	X	-	-	-
44	CLA	3	312	X	-	-	-
44	CLA	3	313	X	-	-	-
44	CLA	3	314	X	-	-	-
44	CLA	3	316	X	-	-	-
44	CLA	3	317	X	-	-	-
44	CLA	3	318	X	-	-	-
44	CLA	5	305	X	-	-	-
44	CLA	5	306	X	-	-	-
44	CLA	5	307	X	-	-	-
44	CLA	5	308	X	-	-	-
44	CLA	5	309	X	-	-	-
44	CLA	5	310	X	-	-	-
44	CLA	5	311	X	-	-	-
44	CLA	5	312	X	-	-	-
44	CLA	5	313	X	-	-	-
44	CLA	5	316	X	-	-	-
44	CLA	A	802	X	-	-	-
44	CLA	A	803	X	-	-	-
44	CLA	A	804	X	-	-	-
44	CLA	A	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	A	806	X	-	-	-
44	CLA	A	807	X	-	-	-
44	CLA	A	808	X	-	-	-
44	CLA	A	809	X	-	-	-
44	CLA	A	810	X	-	-	-
44	CLA	A	811	X	-	-	-
44	CLA	A	812	X	-	-	-
44	CLA	A	813	X	-	-	-
44	CLA	A	814	X	-	-	-
44	CLA	A	815	X	-	-	-
44	CLA	A	816	X	-	-	-
44	CLA	A	817	X	-	-	-
44	CLA	A	818	X	-	-	-
44	CLA	A	819	X	-	-	-
44	CLA	A	820	X	-	-	-
44	CLA	A	821	X	-	-	-
44	CLA	A	822	X	-	-	-
44	CLA	A	823	X	-	-	-
44	CLA	A	824	X	-	-	-
44	CLA	A	825	X	-	-	-
44	CLA	A	826	X	-	-	-
44	CLA	A	827	X	-	-	-
44	CLA	A	828	X	-	-	-
44	CLA	A	829	X	-	-	-
44	CLA	A	830	X	-	-	-
44	CLA	A	831	X	-	-	-
44	CLA	A	832	X	-	-	-
44	CLA	A	833	X	-	-	-
44	CLA	A	834	X	-	-	-
44	CLA	A	835	X	-	-	-
44	CLA	A	836	X	-	-	-
44	CLA	A	837	X	-	-	-
44	CLA	A	838	X	-	-	-
44	CLA	A	839	X	-	-	-
44	CLA	A	840	X	-	-	-
44	CLA	A	842	X	-	-	-
44	CLA	A	852	X	-	-	-
44	CLA	B	801	X	-	-	-
44	CLA	B	802	X	-	-	-
44	CLA	B	803	X	-	-	-
44	CLA	B	804	X	-	-	-
44	CLA	B	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	B	806	X	-	-	-
44	CLA	B	807	X	-	-	-
44	CLA	B	808	X	-	-	-
44	CLA	B	809	X	-	-	-
44	CLA	B	810	X	-	-	-
44	CLA	B	811	X	-	-	-
44	CLA	B	812	X	-	-	-
44	CLA	B	813	X	-	-	-
44	CLA	B	814	X	-	-	-
44	CLA	B	815	X	-	-	-
44	CLA	B	816	X	-	-	-
44	CLA	B	817	X	-	-	-
44	CLA	B	818	X	-	-	-
44	CLA	B	819	X	-	-	-
44	CLA	B	820	X	-	-	-
44	CLA	B	821	X	-	-	-
44	CLA	B	822	X	-	-	-
44	CLA	B	823	X	-	-	-
44	CLA	B	824	X	-	-	-
44	CLA	B	825	X	-	-	-
44	CLA	B	826	X	-	-	-
44	CLA	B	827	X	-	-	-
44	CLA	B	828	X	-	-	-
44	CLA	B	829	X	-	-	-
44	CLA	B	830	X	-	-	-
44	CLA	B	831	X	-	-	-
44	CLA	B	832	X	-	-	-
44	CLA	B	833	X	-	-	-
44	CLA	B	834	X	-	-	-
44	CLA	B	835	X	-	-	-
44	CLA	B	837	X	-	-	-
44	CLA	B	838	X	-	-	-
44	CLA	B	839	X	-	-	-
44	CLA	B	840	X	-	-	-
44	CLA	B	841	X	-	-	-
44	CLA	B	842	X	-	-	-
44	CLA	F	802	X	-	-	-
44	CLA	F	803	X	-	-	-
44	CLA	J	101	X	-	-	-
44	CLA	K	201	X	-	-	-
44	CLA	K	202	X	-	-	-
44	CLA	K	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	K	205	X	-	-	-
44	CLA	L	301	X	-	-	-
44	CLA	L	302	X	-	-	-
44	CLA	L	303	X	-	-	-
44	CLA	L	304	X	-	-	-
44	CLA	e	802	X	-	-	-
44	CLA	e	803	X	-	-	-
44	CLA	e	804	X	-	-	-
44	CLA	e	805	X	-	-	-
44	CLA	e	806	X	-	-	-
44	CLA	e	807	X	-	-	-
44	CLA	e	808	X	-	-	-
44	CLA	e	809	X	-	-	-
44	CLA	e	810	X	-	-	-
44	CLA	e	811	X	-	-	-
44	CLA	e	812	X	-	-	-
44	CLA	e	813	X	-	-	-
44	CLA	e	814	X	-	-	-
44	CLA	e	815	X	-	-	-
44	CLA	e	816	X	-	-	-
44	CLA	e	817	X	-	-	-
44	CLA	e	818	X	-	-	-
44	CLA	e	819	X	-	-	-
44	CLA	e	820	X	-	-	-
44	CLA	e	821	X	-	-	-
44	CLA	e	822	X	-	-	-
44	CLA	e	823	X	-	-	-
44	CLA	e	824	X	-	-	-
44	CLA	e	825	X	-	-	-
44	CLA	e	826	X	-	-	-
44	CLA	e	827	X	-	-	-
44	CLA	e	828	X	-	-	-
44	CLA	e	829	X	-	-	-
44	CLA	e	830	X	-	-	-
44	CLA	e	831	X	-	-	-
44	CLA	e	832	X	-	-	-
44	CLA	e	833	X	-	-	-
44	CLA	e	834	X	-	-	-
44	CLA	e	835	X	-	-	-
44	CLA	e	836	X	-	-	-
44	CLA	e	837	X	-	-	-
44	CLA	e	838	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	e	839	X	-	-	-
44	CLA	e	840	X	-	-	-
44	CLA	e	841	X	-	-	-
44	CLA	e	843	X	-	-	-
44	CLA	e	852	X	-	-	-
44	CLA	e	853	X	-	-	-
44	CLA	f	801	X	-	-	-
44	CLA	f	803	X	-	-	-
44	CLA	f	804	X	-	-	-
44	CLA	f	805	X	-	-	-
44	CLA	f	806	X	-	-	-
44	CLA	f	807	X	-	-	-
44	CLA	f	808	X	-	-	-
44	CLA	f	809	X	-	-	-
44	CLA	f	810	X	-	-	-
44	CLA	f	811	X	-	-	-
44	CLA	f	812	X	-	-	-
44	CLA	f	813	X	-	-	-
44	CLA	f	814	X	-	-	-
44	CLA	f	815	X	-	-	-
44	CLA	f	816	X	-	-	-
44	CLA	f	817	X	-	-	-
44	CLA	f	818	X	-	-	-
44	CLA	f	819	X	-	-	-
44	CLA	f	820	X	-	-	-
44	CLA	f	821	X	-	-	-
44	CLA	f	822	X	-	-	-
44	CLA	f	823	X	-	-	-
44	CLA	f	824	X	-	-	-
44	CLA	f	825	X	-	-	-
44	CLA	f	826	X	-	-	-
44	CLA	f	827	X	-	-	-
44	CLA	f	828	X	-	-	-
44	CLA	f	829	X	-	-	-
44	CLA	f	830	X	-	-	-
44	CLA	f	831	X	-	-	-
44	CLA	f	832	X	-	-	-
44	CLA	f	833	X	-	-	-
44	CLA	f	834	X	-	-	-
44	CLA	f	835	X	-	-	-
44	CLA	f	836	X	-	-	-
44	CLA	f	837	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	f	838	X	-	-	-
44	CLA	f	839	X	-	-	-
44	CLA	f	840	X	-	-	-
44	CLA	f	841	X	-	-	-
44	CLA	f	842	X	-	-	-
44	CLA	f	843	X	-	-	-
44	CLA	j	802	X	-	-	-
44	CLA	m	101	X	-	-	-
44	CLA	m	102	X	-	-	-
44	CLA	n	201	X	-	-	-
44	CLA	n	202	X	-	-	-
44	CLA	n	203	X	-	-	-
44	CLA	n	205	X	-	-	-
44	CLA	o	302	X	-	-	-
44	CLA	o	303	X	-	-	-
44	CLA	o	304	X	-	-	-
44	CLA	p	504	X	-	-	-
44	CLA	p	506	X	-	-	-
44	CLA	p	507	X	-	-	-
44	CLA	p	508	X	-	-	-
44	CLA	p	509	X	-	-	-
44	CLA	p	510	X	-	-	-
44	CLA	p	511	X	-	-	-
44	CLA	p	513	X	-	-	-
44	CLA	p	515	X	-	-	-
44	CLA	q	304	X	-	-	-
44	CLA	q	305	X	-	-	-
44	CLA	q	306	X	-	-	-
44	CLA	q	308	X	-	-	-
44	CLA	q	309	X	-	-	-
44	CLA	q	310	X	-	-	-
44	CLA	q	311	X	-	-	-
44	CLA	q	312	X	-	-	-
44	CLA	q	314	X	-	-	-
44	CLA	q	316	X	-	-	-
44	CLA	r	304	X	-	-	-
44	CLA	r	305	X	-	-	-
44	CLA	r	306	X	-	-	-
44	CLA	r	307	X	-	-	-
44	CLA	r	308	X	-	-	-
44	CLA	r	309	X	-	-	-
44	CLA	r	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	r	311	X	-	-	-
44	CLA	r	312	X	-	-	-
44	CLA	r	315	X	-	-	-
44	CLA	r	317	X	-	-	-
44	CLA	s	504	X	-	-	-
44	CLA	s	506	X	-	-	-
44	CLA	s	507	X	-	-	-
44	CLA	s	508	X	-	-	-
44	CLA	s	509	X	-	-	-
44	CLA	s	510	X	-	-	-
44	CLA	s	511	X	-	-	-
44	CLA	s	514	X	-	-	-
51	LUT	p	502	X	-	-	-
52	CHL	1	512	X	-	-	-
52	CHL	1	514	X	-	-	-
52	CHL	1	517	X	-	-	-
52	CHL	2	512	X	-	-	-
52	CHL	2	513	X	-	-	-
52	CHL	2	515	X	-	-	-
52	CHL	2	516	X	-	-	-
52	CHL	3	302	X	-	-	-
52	CHL	3	315	X	-	-	-
52	CHL	5	314	X	-	-	-
52	CHL	5	315	X	-	-	-
52	CHL	5	317	X	-	-	-
52	CHL	p	512	X	-	-	-
52	CHL	p	514	X	-	-	-
52	CHL	p	517	X	-	-	-
52	CHL	q	313	X	-	-	-
52	CHL	r	313	X	-	-	-
52	CHL	r	314	X	-	-	-
52	CHL	r	316	X	-	-	-
52	CHL	s	512	X	-	-	-
52	CHL	s	513	X	-	-	-
52	CHL	s	515	X	-	-	-
52	CHL	s	517	X	-	-	-

## 2 Entry composition [i](#)

There are 54 unique types of molecules in this entry. The entry contains 106329 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	742	Total	C	N	O	S	0	0
			5813	3812	983	1000	18		
1	e	742	Total	C	N	O	S	0	0
			5798	3797	987	996	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	Total	C	N	O	S	0	0
			5851	3835	995	1007	14		
2	f	733	Total	C	N	O	S	0	0
			5840	3832	991	1003	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	81	Total	C	N	O	S	0	0
			610	376	105	117	12		
3	g	81	Total	C	N	O	S	0	0
			613	377	105	119	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	142	Total	C	N	O	S	0	0
			1113	716	193	201	3		
4	h	142	Total	C	N	O	S	0	0
			1111	714	195	199	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			538	341	98	99		
5	i	68	Total	C	N	O	0	0
			539	341	99	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	158	Total	C	N	O	S	0	0
			1204	774	208	219	3		
6	j	158	Total	C	N	O	S	0	0
			1188	768	203	216	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	61	Total	C	N	O	0	0
			454	303	76	75		
7	k	61	Total	C	N	O	0	0
			447	298	73	76		

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	30	Total	C	N	O	0	0	
			232	161	35	36			
8	l	30	Total	C	N	O	S	0	0
			235	163	35	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	42	Total	C	N	O	S	0	0
			333	228	51	53	1		
9	m	42	Total	C	N	O	S	0	0
			332	225	51	55	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			565	359	94	108	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	n	84	576	361	101	110	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	146	1088	716	174	197	1	0	0
11	o	146	1089	720	174	195		0	0

- Molecule 12 is a protein called Chlorophyll a-b binding protein Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	1	191	1422	921	239	258	4	0	0
12	p	193	1484	965	248	269	2	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	73	PHE	UNK	conflict	UNP A0A287WC32
1	74	GLU	UNK	conflict	UNP A0A287WC32
1	75	ARG	UNK	conflict	UNP A0A287WC32
p	73	PHE	UNK	conflict	UNP A0A287WC32
p	74	GLU	UNK	conflict	UNP A0A287WC32
p	75	ARG	UNK	conflict	UNP A0A287WC32

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	2	203	1554	1012	257	282	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	3	222	1631	1064	271	293	3	0	0
14	q	222	1672	1097	272	298	5	0	0

- Molecule 15 is a protein called Chlorophyll a-b binding protein Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	5	205	1486	962	247	270	7	0	0

- Molecule 16 is a protein called NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	G	346	2602	1741	390	463	8	0	0

- Molecule 17 is a protein called NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	M	478	3646	2400	557	665	24	0	0

- Molecule 18 is a protein called NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	N	116	841	575	124	140	2	0	0

- Molecule 19 is a protein called NAD(P)H-quinone oxidoreductase chain 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	O	499	3874	2614	598	639	23	0	0

- Molecule 20 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	P	100	750	486	127	135	2	0	0

- Molecule 21 is a protein called NADH-plastoquinone oxidoreductase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q	671	5041	3367	784	870	20	0	0

- Molecule 22 is a protein called NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	176	Total	C	N	O	S	0	0
			1260	841	194	220	5		

- Molecule 23 is a protein called NAD(P)H-quinone oxidoreductase subunit H, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	383	Total	C	N	O	S	0	0
			2991	1944	493	543	11		

- Molecule 24 is a protein called NAD(P)H-quinone oxidoreductase subunit I, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	165	Total	C	N	O	S	0	0
			1229	772	214	231	12		

- Molecule 25 is a protein called NAD(P)H-quinone oxidoreductase subunit J, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	159	Total	C	N	O	S	0	0
			1258	808	213	233	4		

- Molecule 26 is a protein called NAD(P)H-quinone oxidoreductase subunit K, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	194	Total	C	N	O	S	0	0
			1473	931	250	282	10		

- Molecule 27 is a protein called NAD(P)H-quinone oxidoreductase subunit L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	69	Total	C	N	O	S	0	0
			572	399	89	81	3		

- Molecule 28 is a protein called NAD(P)H-quinone oxidoreductase subunit M, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	112	Total	C	N	O	S	0	0
			876	558	150	162	6		

- Molecule 29 is a protein called NAD(P)H-quinone oxidoreductase subunit N, chloroplastic.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Y	142	1135	741	197	195	2	0	0

- Molecule 30 is a protein called Unidentified stromal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	Z	61	305	183	61	61	0	0

- Molecule 31 is a protein called Photosynthetic NDH subunit of subcomplex L1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	a	150	1185	752	206	227	0	0

- Molecule 32 is a protein called Photosynthetic NDH subunit of subcomplex L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	b	129	915	580	156	175	4	0	0

- Molecule 33 is a protein called Photosynthetic NDH subunit of subcomplex L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	134	989	634	164	187	4	0	0

- Molecule 34 is a protein called Photosynthetic NDH subunit of subcomplex L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	4	130	878	553	153	163	9	0	0

- Molecule 35 is a protein called Photosynthetic NDH subunit of subcomplex L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	d	172	1289	812	229	241	7	0	0

- Molecule 36 is a protein called Photosynthetic NDH subunit of subcomplex B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	6	343	2541	1617	435	474	15	0	0

- Molecule 37 is a protein called Photosynthetic NDH subunit of subcomplex B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	7	317	2302	1436	408	448	10	0	0

- Molecule 38 is a protein called Photosynthetic NDH subunit of subcomplex B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	8	119	828	523	151	147	7	0	0

- Molecule 39 is a protein called Photosynthetic NDH subunit of subcomplex B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	9	82	617	395	101	118	3	0	0

- Molecule 40 is a protein called Photosynthetic NDH subunit of subcomplex B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	0	149	1089	704	175	204	6	0	0

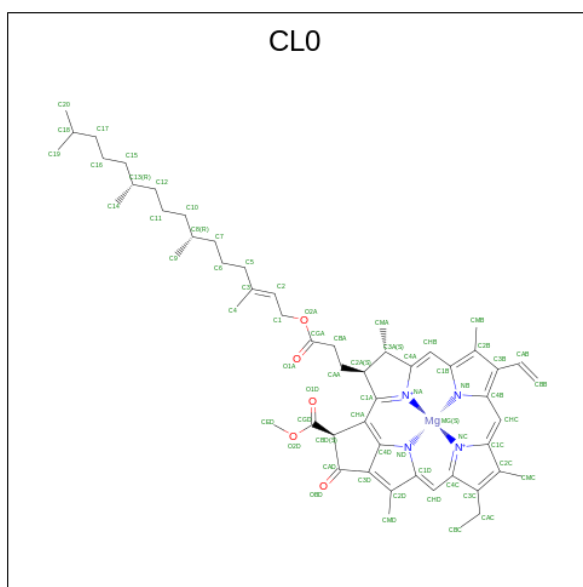
- Molecule 41 is a protein called Chlorophyll a-b binding protein Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	r	197	1529	991	253	282	3	0	0

- Molecule 42 is a protein called Chlorophyll a-b binding protein, chloroplastic.

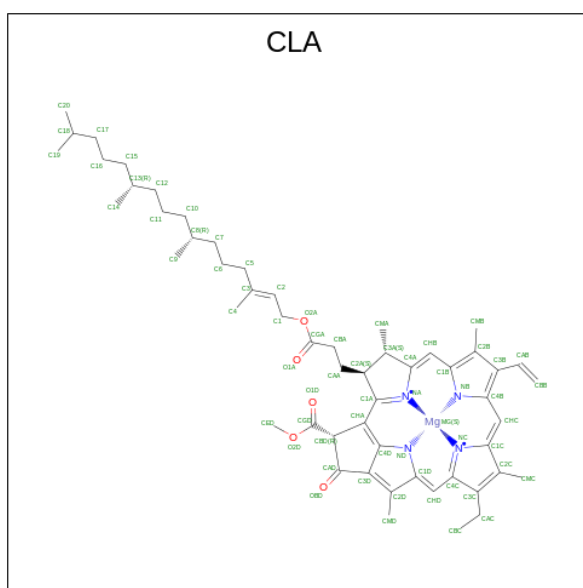
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	s	211	1591	1035	266	283	7	0	0

- Molecule 43 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
43	A	1	61	52	1	4	4	0
43	e	1	61	52	1	4	4	0

- Molecule 44 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0
44	A	1	Total 2024	C 1655	Mg 41	N 164	O 164	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	A	1	2024	1655	41	164	164	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0
44	B	1	2118	1731	42	168	177	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	B	1	Total 2118	C 1731	Mg 42	N 168	O 177	0
44	F	1	Total 83	C 67	Mg 2	N 8	O 6	0
44	F	1	Total 83	C 67	Mg 2	N 8	O 6	0
44	J	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
44	K	1	157	127	4	16	10	0
44	K	1	157	127	4	16	10	0
44	K	1	157	127	4	16	10	0
44	K	1	157	127	4	16	10	0
44	L	1	193	155	4	16	18	0
44	L	1	193	155	4	16	18	0
44	L	1	193	155	4	16	18	0
44	L	1	193	155	4	16	18	0
44	1	1	485	392	10	40	43	0
44	1	1	485	392	10	40	43	0
44	1	1	485	392	10	40	43	0
44	1	1	485	392	10	40	43	0
44	1	1	485	392	10	40	43	0
44	1	1	485	392	10	40	43	0
44	1	1	485	392	10	40	43	0
44	1	1	485	392	10	40	43	0
44	1	1	485	392	10	40	43	0
44	1	1	485	392	10	40	43	0
44	2	1	454	372	9	36	37	0
44	2	1	454	372	9	36	37	0
44	2	1	454	372	9	36	37	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
44	2	1	454	372	9	36	37	0
44	2	1	454	372	9	36	37	0
44	2	1	454	372	9	36	37	0
44	2	1	454	372	9	36	37	0
44	2	1	454	372	9	36	37	0
44	2	1	454	372	9	36	37	0
44	2	1	454	372	9	36	37	0
44	3	1	595	479	13	52	51	0
44	3	1	595	479	13	52	51	0
44	3	1	595	479	13	52	51	0
44	3	1	595	479	13	52	51	0
44	3	1	595	479	13	52	51	0
44	3	1	595	479	13	52	51	0
44	3	1	595	479	13	52	51	0
44	3	1	595	479	13	52	51	0
44	3	1	595	479	13	52	51	0
44	3	1	595	479	13	52	51	0
44	3	1	595	479	13	52	51	0
44	3	1	595	479	13	52	51	0
44	3	1	595	479	13	52	51	0
44	5	1	468	378	10	40	40	0
44	5	1	468	378	10	40	40	0

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Mol	Chain	Residues	Atoms					AltConf
44	5	1	Total 468	C 378	Mg 10	N 40	O 40	0
44	5	1	Total 468	C 378	Mg 10	N 40	O 40	0
44	5	1	Total 468	C 378	Mg 10	N 40	O 40	0
44	5	1	Total 468	C 378	Mg 10	N 40	O 40	0
44	5	1	Total 468	C 378	Mg 10	N 40	O 40	0
44	5	1	Total 468	C 378	Mg 10	N 40	O 40	0
44	5	1	Total 468	C 378	Mg 10	N 40	O 40	0
44	5	1	Total 468	C 378	Mg 10	N 40	O 40	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0
44	e	1	2028	1643	43	172	170	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	e	1	Total 2028	C 1643	Mg 43	N 172	O 170	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	f	1	Total 1921	C 1563	Mg 42	N 168	O 148	0
44	j	1	Total 41	C 33	Mg 1	N 4	O 3	0
44	m	1	Total 83	C 67	Mg 2	N 8	O 6	0
44	m	1	Total 83	C 67	Mg 2	N 8	O 6	0
44	n	1	Total 162	C 130	Mg 4	N 16	O 12	0
44	n	1	Total 162	C 130	Mg 4	N 16	O 12	0
44	n	1	Total 162	C 130	Mg 4	N 16	O 12	0
44	n	1	Total 162	C 130	Mg 4	N 16	O 12	0
44	o	1	Total 145	C 117	Mg 3	N 12	O 13	0
44	o	1	Total 145	C 117	Mg 3	N 12	O 13	0
44	o	1	Total 145	C 117	Mg 3	N 12	O 13	0
44	p	1	Total 474	C 382	Mg 10	N 40	O 42	0
44	p	1	Total 474	C 382	Mg 10	N 40	O 42	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
44	p	1	Total 474	C 382	Mg 10	N 40	O 42	0
44	p	1	Total 474	C 382	Mg 10	N 40	O 42	0
44	p	1	Total 474	C 382	Mg 10	N 40	O 42	0
44	p	1	Total 474	C 382	Mg 10	N 40	O 42	0
44	p	1	Total 474	C 382	Mg 10	N 40	O 42	0
44	p	1	Total 474	C 382	Mg 10	N 40	O 42	0
44	p	1	Total 474	C 382	Mg 10	N 40	O 42	0
44	p	1	Total 474	C 382	Mg 10	N 40	O 42	0
44	q	1	Total 543	C 435	Mg 12	N 48	O 48	0
44	q	1	Total 543	C 435	Mg 12	N 48	O 48	0
44	q	1	Total 543	C 435	Mg 12	N 48	O 48	0
44	q	1	Total 543	C 435	Mg 12	N 48	O 48	0
44	q	1	Total 543	C 435	Mg 12	N 48	O 48	0
44	q	1	Total 543	C 435	Mg 12	N 48	O 48	0
44	q	1	Total 543	C 435	Mg 12	N 48	O 48	0
44	q	1	Total 543	C 435	Mg 12	N 48	O 48	0
44	q	1	Total 543	C 435	Mg 12	N 48	O 48	0
44	q	1	Total 543	C 435	Mg 12	N 48	O 48	0
44	q	1	Total 543	C 435	Mg 12	N 48	O 48	0
44	r	1	Total 525	C 425	Mg 11	N 44	O 45	0

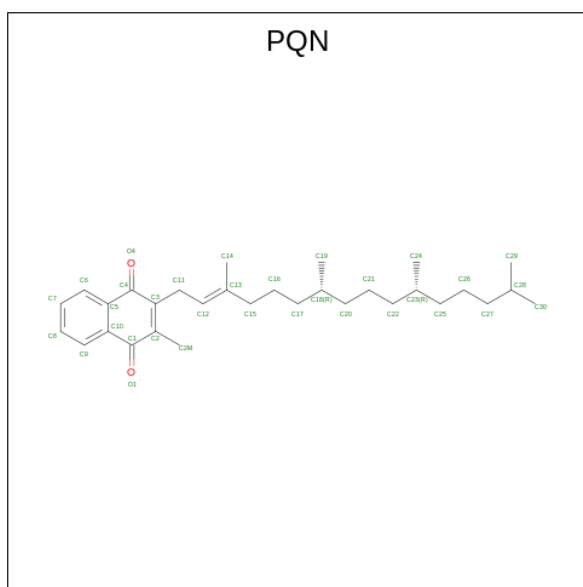
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Mol	Chain	Residues	Atoms					AltConf
44	r	1	Total	C	Mg	N	O	0
			525	425	11	44	45	
44	r	1	Total	C	Mg	N	O	0
			525	425	11	44	45	
44	r	1	Total	C	Mg	N	O	0
			525	425	11	44	45	
44	r	1	Total	C	Mg	N	O	0
			525	425	11	44	45	
44	r	1	Total	C	Mg	N	O	0
			525	425	11	44	45	
44	r	1	Total	C	Mg	N	O	0
			525	425	11	44	45	
44	r	1	Total	C	Mg	N	O	0
			525	425	11	44	45	
44	r	1	Total	C	Mg	N	O	0
			525	425	11	44	45	
44	r	1	Total	C	Mg	N	O	0
			525	425	11	44	45	
44	s	1	Total	C	Mg	N	O	0
			431	349	9	36	37	
44	s	1	Total	C	Mg	N	O	0
			431	349	9	36	37	
44	s	1	Total	C	Mg	N	O	0
			431	349	9	36	37	
44	s	1	Total	C	Mg	N	O	0
			431	349	9	36	37	
44	s	1	Total	C	Mg	N	O	0
			431	349	9	36	37	
44	s	1	Total	C	Mg	N	O	0
			431	349	9	36	37	
44	s	1	Total	C	Mg	N	O	0
			431	349	9	36	37	
44	s	1	Total	C	Mg	N	O	0
			431	349	9	36	37	

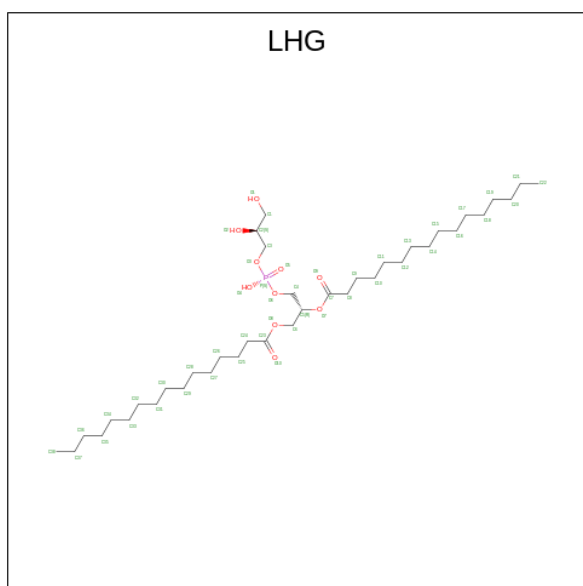
- Molecule 45 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).





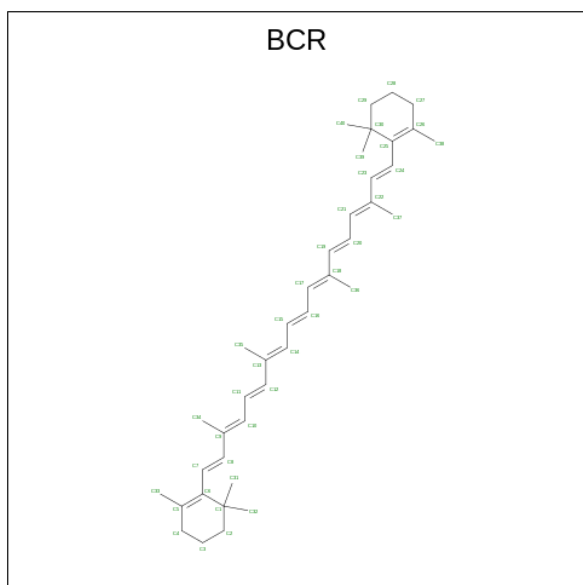
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
45	A	1	33	31	2	0
45	B	1	30	28	2	0
45	e	1	14	12	2	0
45	f	1	16	14	2	0

- Molecule 46 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				AltConf
46	A	1	Total	C	O	P	0
			79	57	20	2	
46	A	1	Total	C	O	P	0
			79	57	20	2	
46	B	1	Total	C	O	P	0
			38	27	10	1	
46	1	1	Total	C	O	P	0
			49	38	10	1	
46	2	1	Total	C	O	P	0
			35	24	10	1	
46	O	1	Total	C	O	P	0
			24	15	8	1	
46	e	1	Total	C	O	P	0
			65	44	19	2	
46	e	1	Total	C	O	P	0
			65	44	19	2	
46	f	1	Total	C	O	P	0
			38	27	10	1	
46	p	1	Total	C	O	P	0
			49	38	10	1	
46	s	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 47 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		AltConf
47	A	1	Total	C	0
			279	279	

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Mol	Chain	Residues	Atoms		AltConf
47	A	1	Total 279	C 279	0
47	A	1	Total 279	C 279	0
47	A	1	Total 279	C 279	0
47	A	1	Total 279	C 279	0
47	A	1	Total 279	C 279	0
47	A	1	Total 279	C 279	0
47	B	1	Total 280	C 280	0
47	B	1	Total 280	C 280	0
47	B	1	Total 280	C 280	0
47	B	1	Total 280	C 280	0
47	B	1	Total 280	C 280	0
47	B	1	Total 280	C 280	0
47	B	1	Total 280	C 280	0
47	B	1	Total 280	C 280	0
47	F	1	Total 80	C 80	0
47	F	1	Total 80	C 80	0
47	I	1	Total 40	C 40	0
47	J	1	Total 40	C 40	0
47	K	1	Total 40	C 40	0
47	L	1	Total 80	C 80	0
47	L	1	Total 80	C 80	0
47	1	1	Total 19	C 19	0

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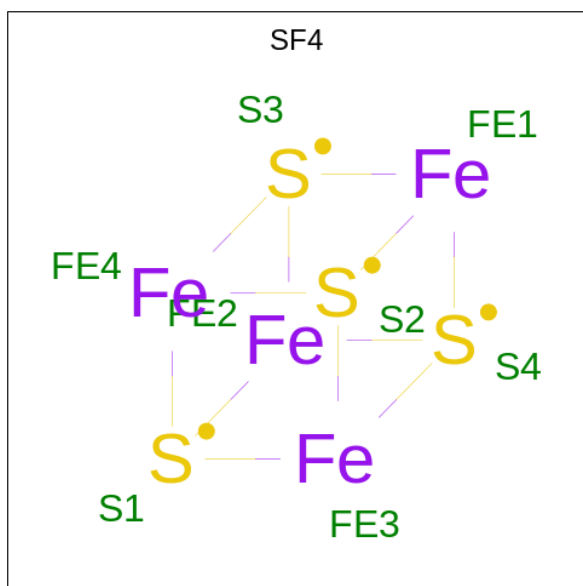
Mol	Chain	Residues	Atoms		AltConf
47	2	1	Total 40	C 40	0
47	3	1	Total 40	C 40	0
47	5	1	Total 40	C 40	0
47	Q	1	Total 39	C 39	0
47	e	1	Total 280	C 280	0
47	e	1	Total 280	C 280	0
47	e	1	Total 280	C 280	0
47	e	1	Total 280	C 280	0
47	e	1	Total 280	C 280	0
47	e	1	Total 280	C 280	0
47	e	1	Total 280	C 280	0
47	e	1	Total 280	C 280	0
47	f	1	Total 239	C 239	0
47	f	1	Total 239	C 239	0
47	f	1	Total 239	C 239	0
47	f	1	Total 239	C 239	0
47	f	1	Total 239	C 239	0
47	f	1	Total 239	C 239	0
47	j	1	Total 80	C 80	0
47	j	1	Total 80	C 80	0
47	l	1	Total 80	C 80	0
47	l	1	Total 80	C 80	0

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Mol	Chain	Residues	Atoms	AltConf
47	m	1	Total C 40 40	0
47	n	1	Total C 40 40	0
47	o	1	Total C 80 80	0
47	o	1	Total C 80 80	0
47	p	1	Total C 11 11	0
47	q	1	Total C 40 40	0
47	r	1	Total C 40 40	0
47	s	1	Total C 40 40	0

- Molecule 48 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



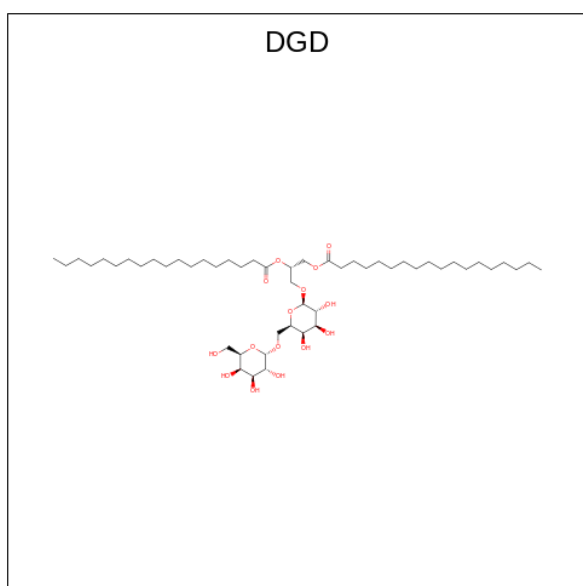
Mol	Chain	Residues	Atoms	AltConf
48	A	1	Total Fe S 8 4 4	0
48	C	1	Total Fe S 16 8 8	0
48	C	1	Total Fe S 16 8 8	0

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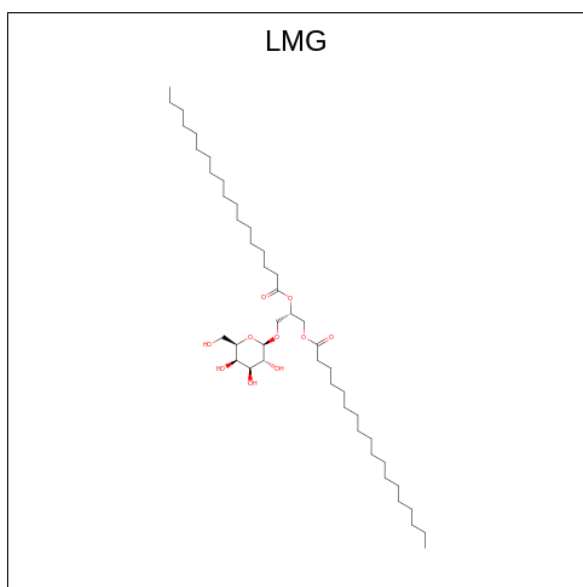
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
48	8	1	8	4	4	0
48	f	1	8	4	4	0
48	g	1	16	8	8	0
48	g	1	16	8	8	0

- Molecule 49 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



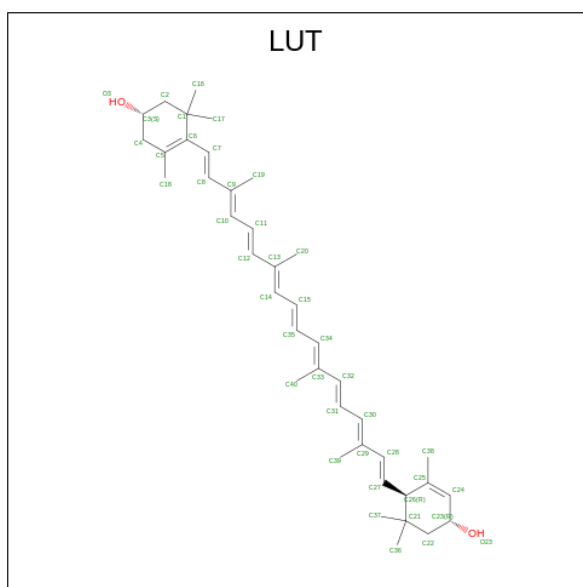
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
49	B	1	59	44	15	0
49	J	1	66	51	15	0
49	f	1	52	37	15	0
49	m	1	66	51	15	0

- Molecule 50 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
50	F	1	75	55	20	0
50	F	1	75	55	20	0
50	2	1	52	35	17	0
50	2	1	52	35	17	0
50	5	1	32	22	10	0
50	m	1	30	20	10	0
50	r	1	18	10	8	0

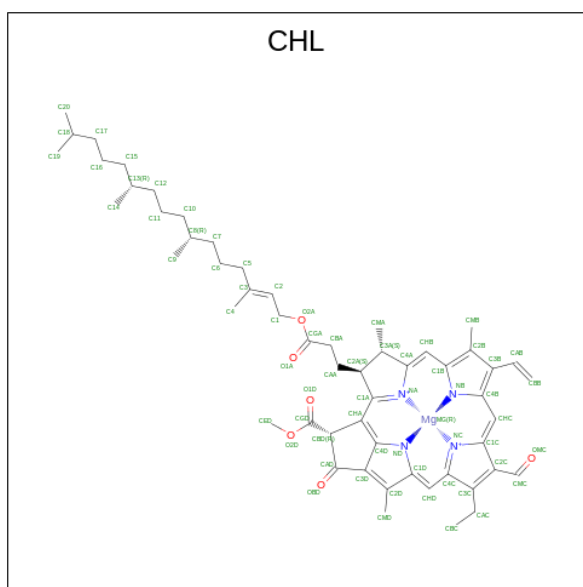
- Molecule 51 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
51	1	1	Total	C	O	0
			84	80	4	
51	1	1	Total	C	O	0
			84	80	4	
51	2	1	Total	C	O	0
			42	40	2	
51	3	1	Total	C	O	0
			84	80	4	
51	3	1	Total	C	O	0
			84	80	4	
51	5	1	Total	C	O	0
			42	40	2	
51	p	1	Total	C	O	0
			84	80	4	
51	p	1	Total	C	O	0
			84	80	4	
51	q	1	Total	C	O	0
			84	80	4	
51	q	1	Total	C	O	0
			84	80	4	
51	r	1	Total	C	O	0
			42	40	2	
51	s	1	Total	C	O	0
			42	40	2	

- Molecule 52 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).





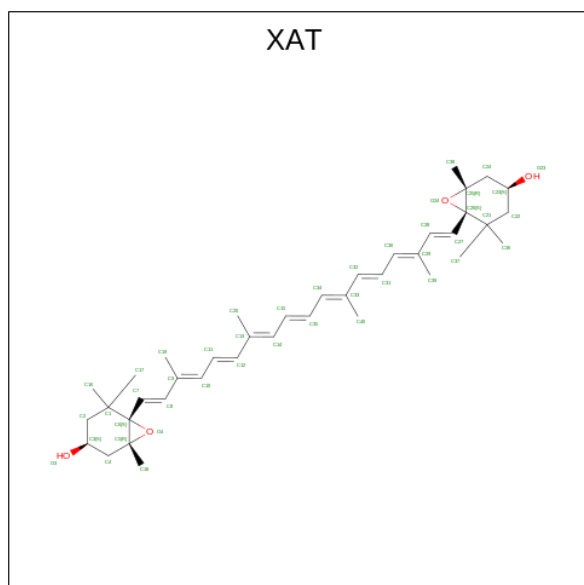
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
52	1	1	Total	C	Mg	N	O	0
			129	100	3	12	14	
52	1	1	Total	C	Mg	N	O	0
			129	100	3	12	14	
52	1	1	Total	C	Mg	N	O	0
			129	100	3	12	14	
52	2	1	Total	C	Mg	N	O	0
			174	135	4	16	19	
52	2	1	Total	C	Mg	N	O	0
			174	135	4	16	19	
52	2	1	Total	C	Mg	N	O	0
			174	135	4	16	19	
52	2	1	Total	C	Mg	N	O	0
			174	135	4	16	19	
52	3	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
52	3	1	Total	C	Mg	N	O	0
			90	70	2	8	10	
52	5	1	Total	C	Mg	N	O	0
			133	102	3	12	16	
52	5	1	Total	C	Mg	N	O	0
			133	102	3	12	16	
52	5	1	Total	C	Mg	N	O	0
			133	102	3	12	16	
52	p	1	Total	C	Mg	N	O	0
			137	106	3	12	16	
52	p	1	Total	C	Mg	N	O	0
			137	106	3	12	16	

*Continued on next page...*

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
52	p	1	Total 137	C 106	Mg 3	N 12	O 16	0
52	q	1	Total 46	C 36	Mg 1	N 4	O 5	0
52	r	1	Total 141	C 110	Mg 3	N 12	O 16	0
52	r	1	Total 141	C 110	Mg 3	N 12	O 16	0
52	r	1	Total 141	C 110	Mg 3	N 12	O 16	0
52	s	1	Total 183	C 141	Mg 4	N 16	O 22	0
52	s	1	Total 183	C 141	Mg 4	N 16	O 22	0
52	s	1	Total 183	C 141	Mg 4	N 16	O 22	0
52	s	1	Total 183	C 141	Mg 4	N 16	O 22	0

- Molecule 53 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



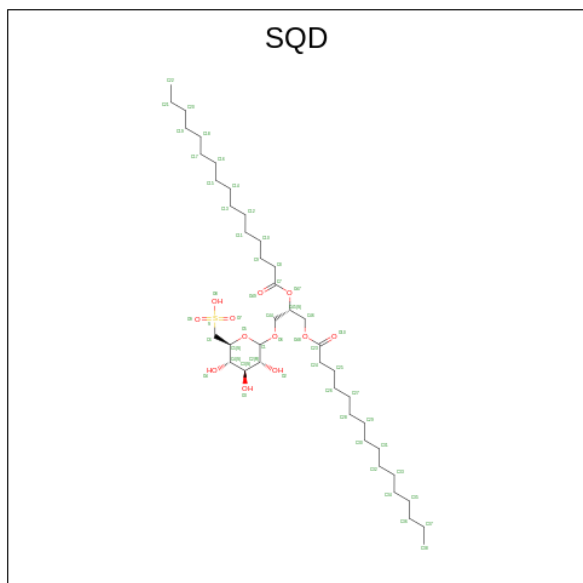
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
53	2	1	Total 44	C 40	O 4	0
53	5	1	Total 44	C 40	O 4	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
53	r	1	44	40	4	0
53	s	1	44	40	4	0

- Molecule 54 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).

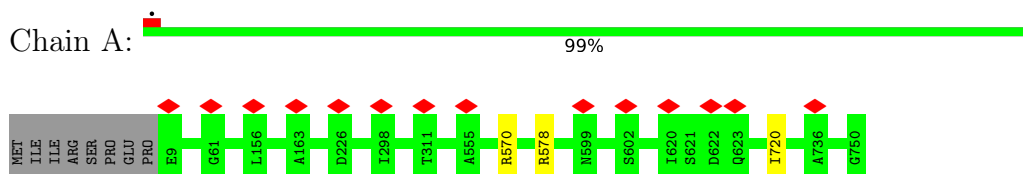


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
54	Q	1	100	74	24	2	0
54	Q	1	100	74	24	2	0

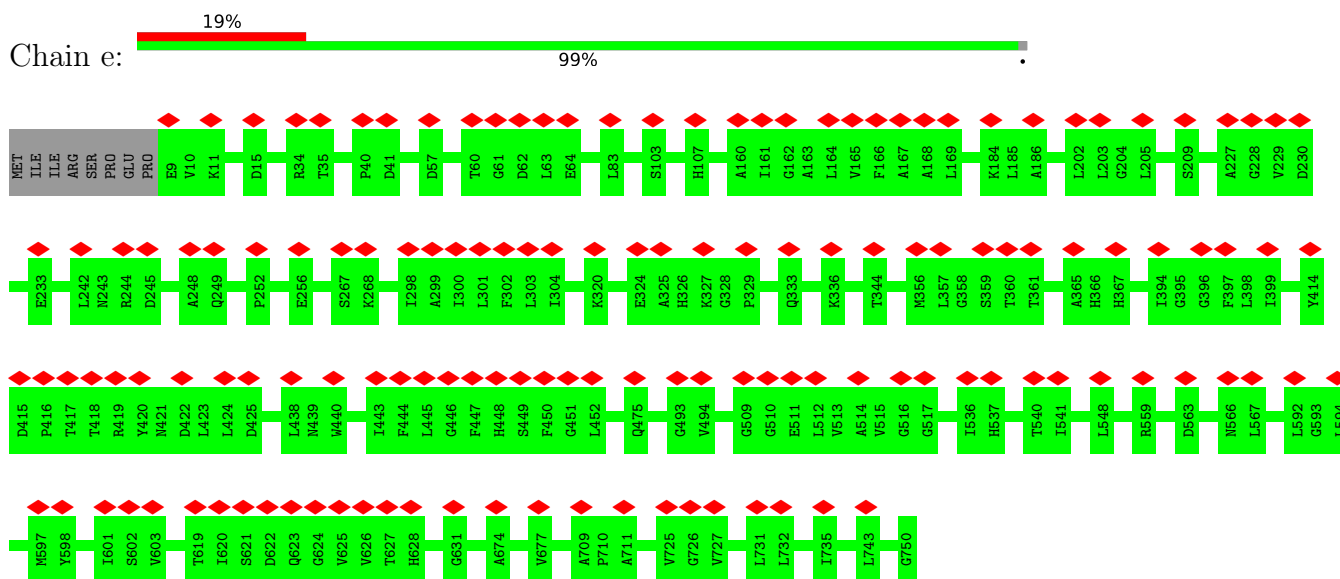
### 3 Residue-property plots [i](#)

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

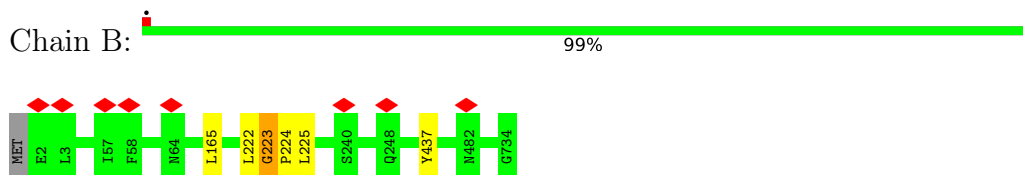
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

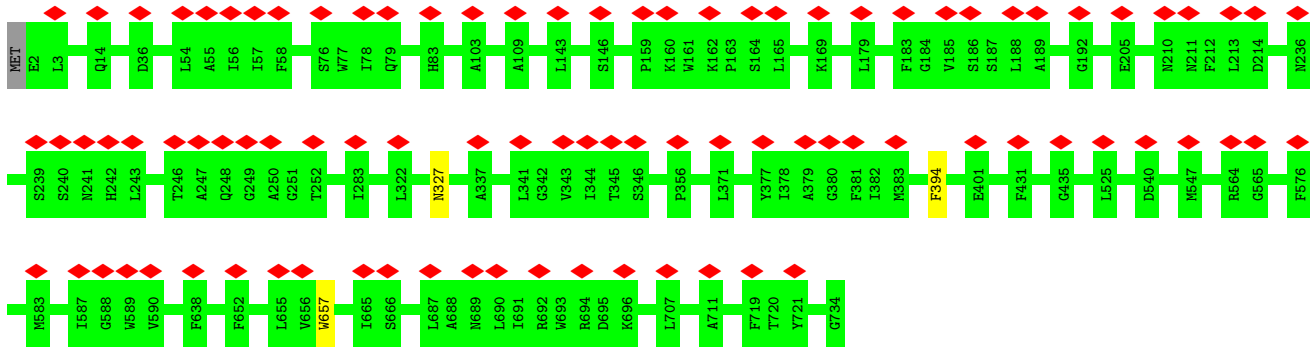


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

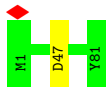


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

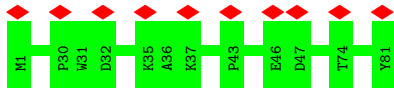




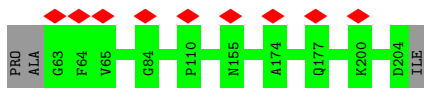
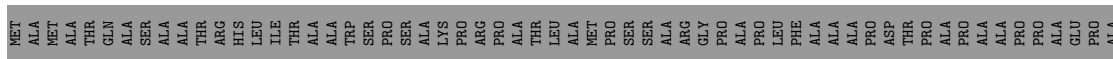
- Molecule 3: Photosystem I iron-sulfur center



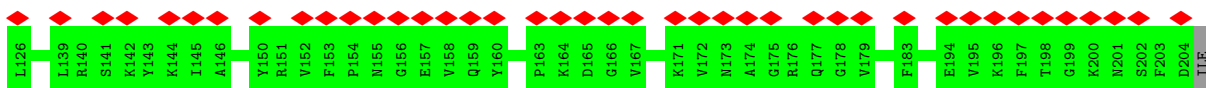
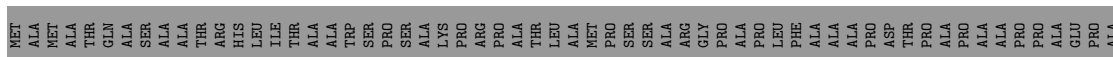
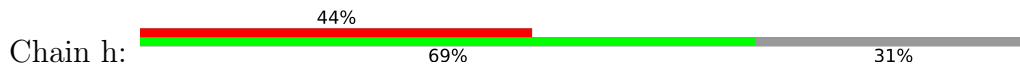
- Molecule 3: Photosystem I iron-sulfur center



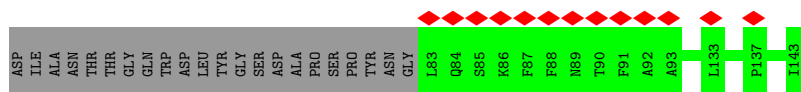
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



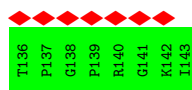
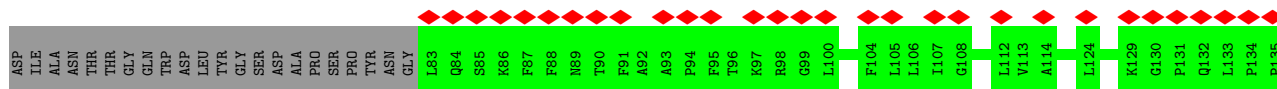
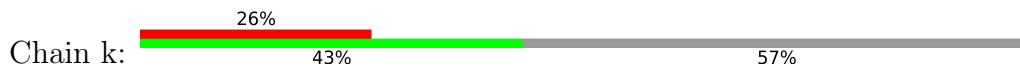
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



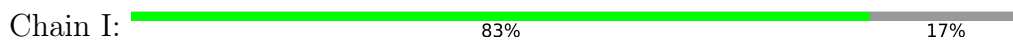




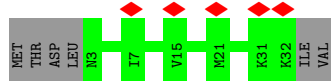
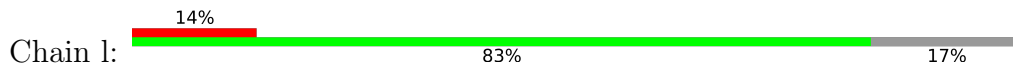
• Molecule 7: Photosystem I reaction center subunit VI, chloroplastic



• Molecule 8: Photosystem I reaction center subunit VIII



• Molecule 8: Photosystem I reaction center subunit VIII



• Molecule 9: Photosystem I reaction center subunit IX

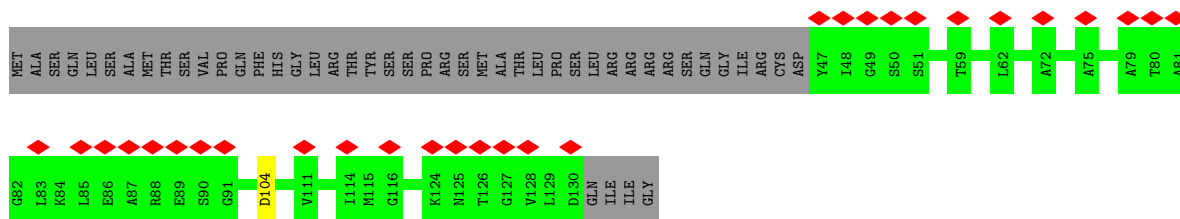


• Molecule 9: Photosystem I reaction center subunit IX

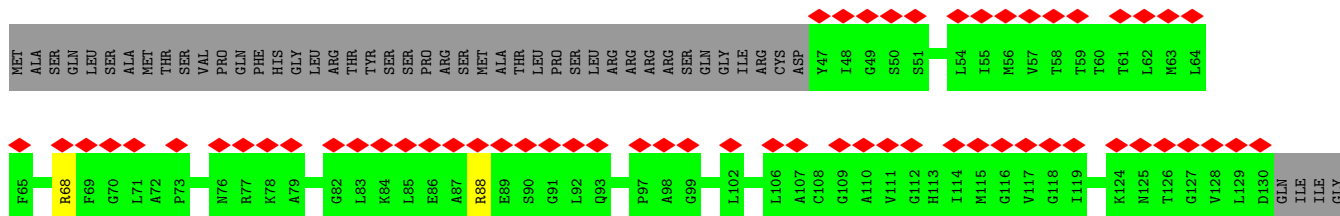


• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

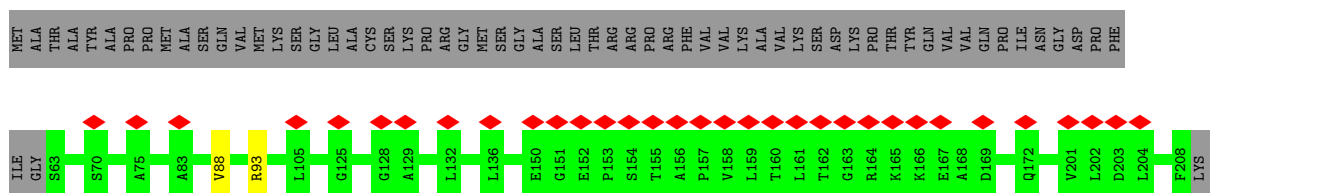




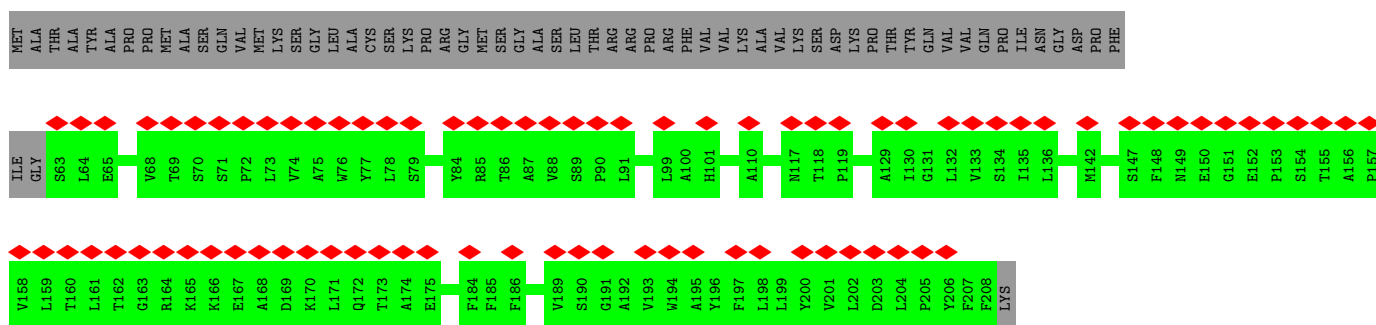
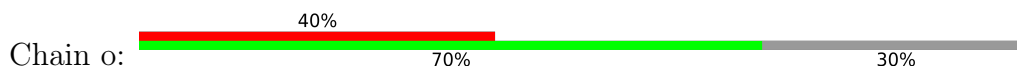
• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic



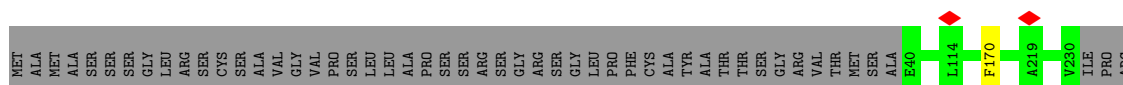
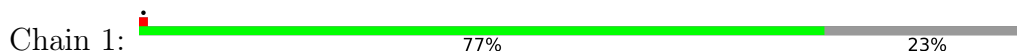
• Molecule 11: Photosystem I reaction center subunit XI, chloroplastic



• Molecule 11: Photosystem I reaction center subunit XI, chloroplastic



• Molecule 12: Chlorophyll a-b binding protein Lhca1

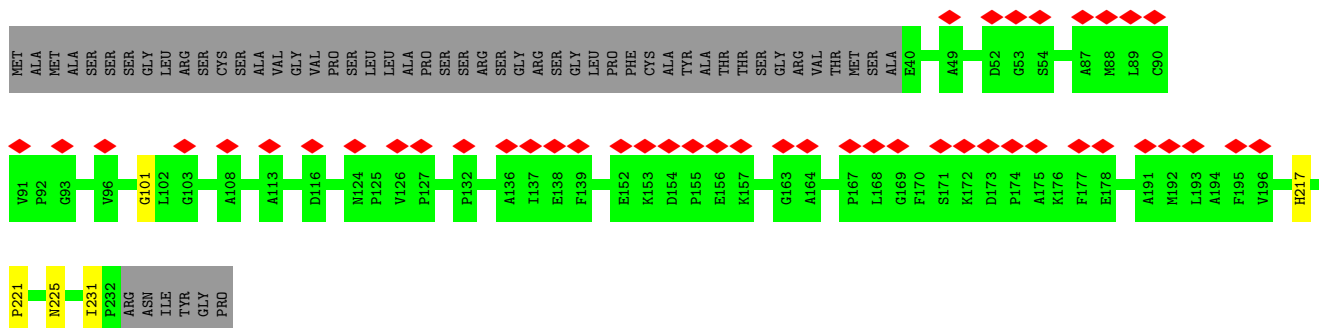




ASN  
ILE  
TYR  
GLY  
PRO

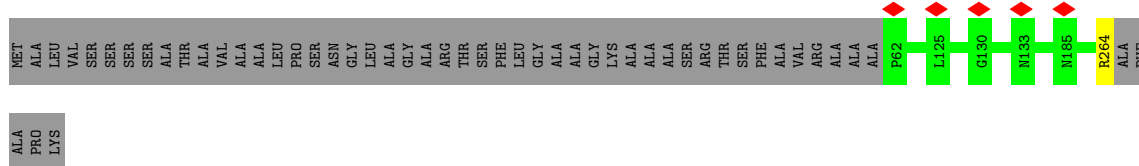
- Molecule 12: Chlorophyll a-b binding protein Lhca1

Chain p: 19% 76% 22%



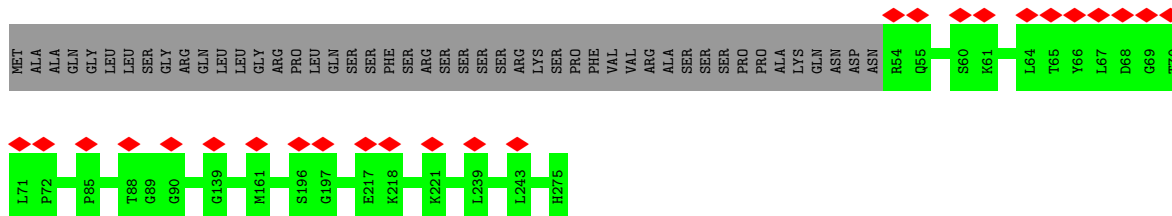
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 2: 79% 20%



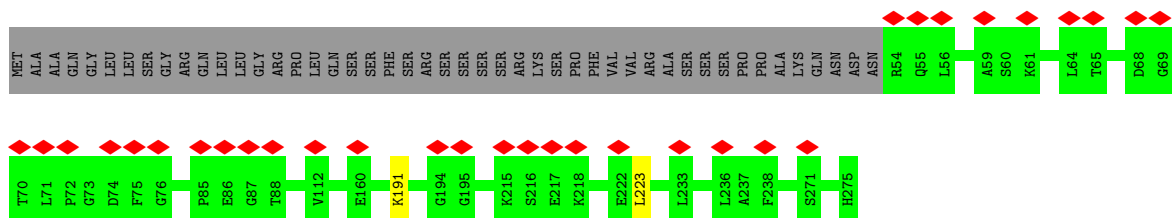
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 9% 83% 17%




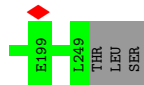
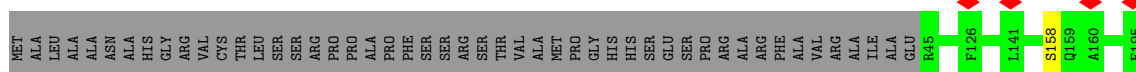
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain q: 12% 82% 17%



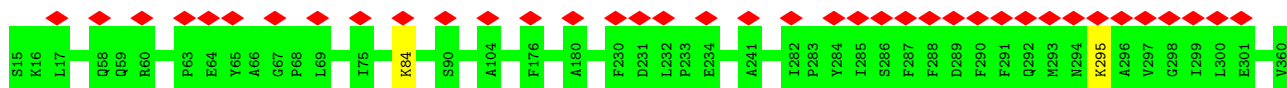
- Molecule 15: Chlorophyll a-b binding protein Lhca5

Chain 5:  79% 20%



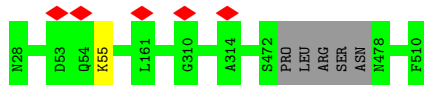
- Molecule 16: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic

Chain G:  11% 99%



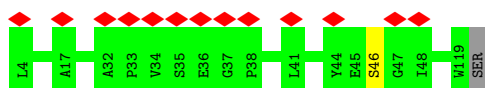
- Molecule 17: NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic

Chain M:  99%



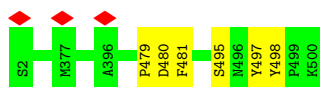
- Molecule 18: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic

Chain N:  11% 98%



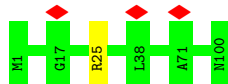
- Molecule 19: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic

Chain O:  99%

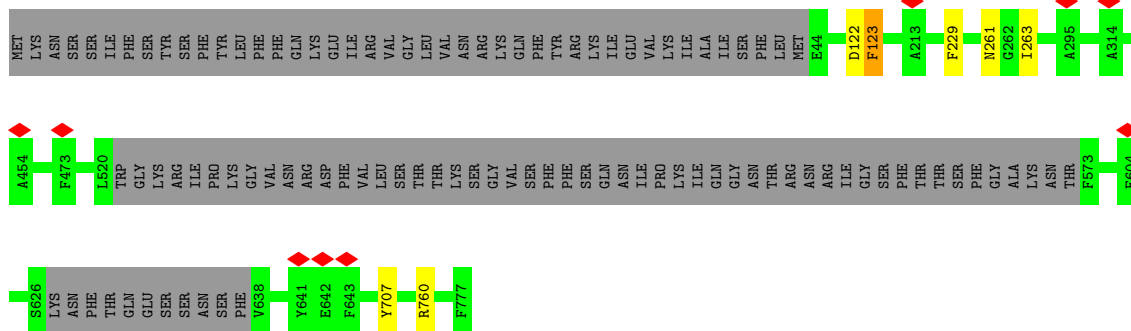
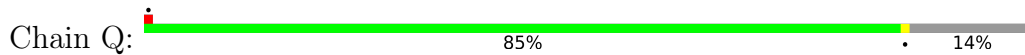


- Molecule 20: NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic

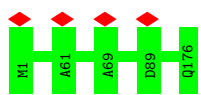
Chain P:  99%



- Molecule 21: NADH-plastoquinone oxidoreductase subunit 5



- Molecule 22: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic

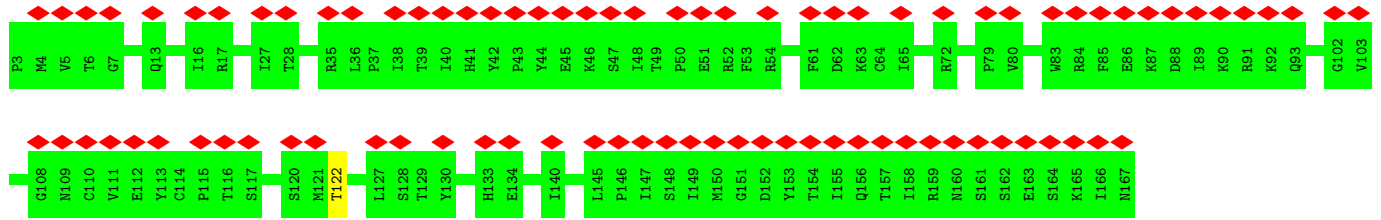


- Molecule 23: NAD(P)H-quinone oxidoreductase subunit H, chloroplastic

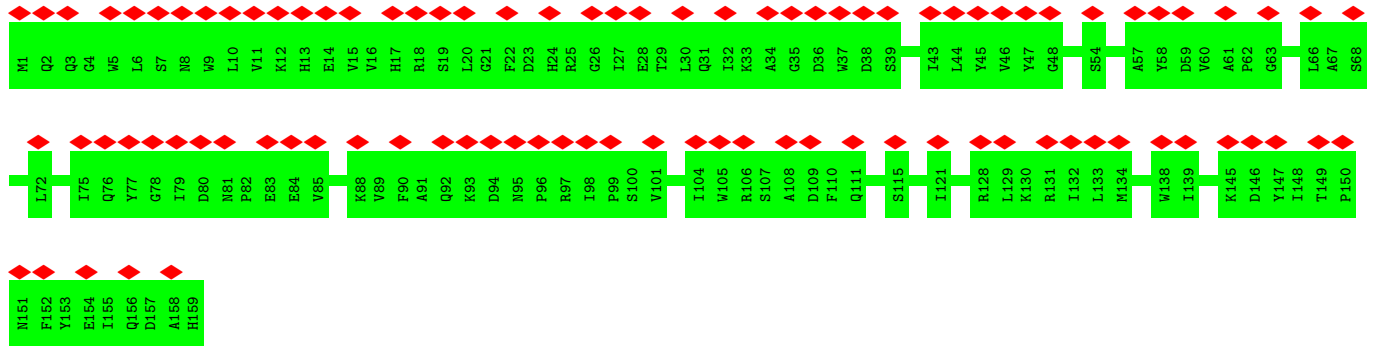


- Molecule 24: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic

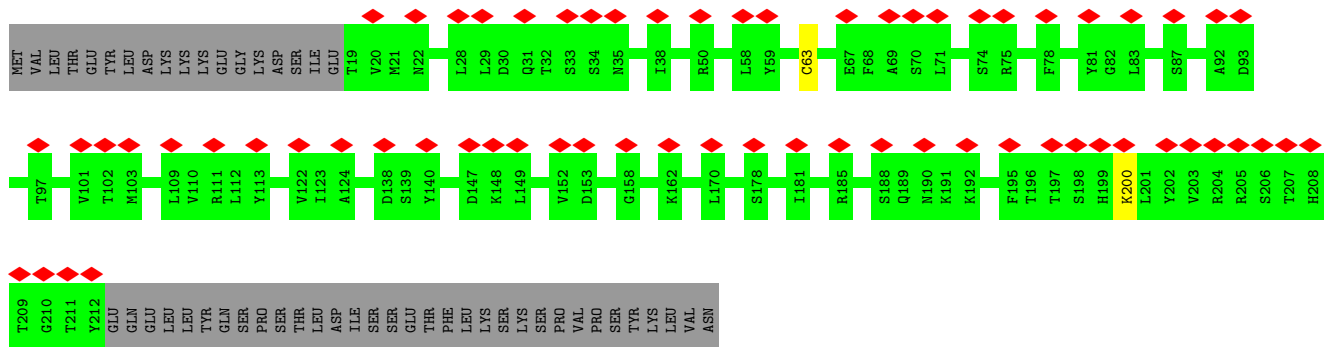
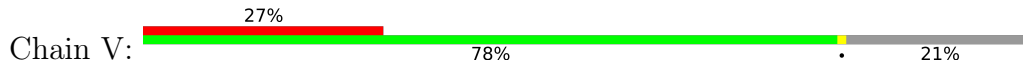




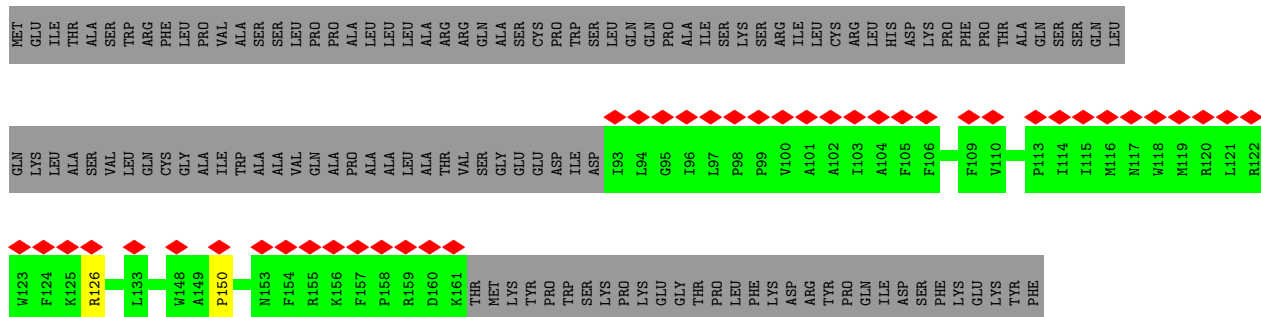
• Molecule 25: NAD(P)H-quinone oxidoreductase subunit J, chloroplastic



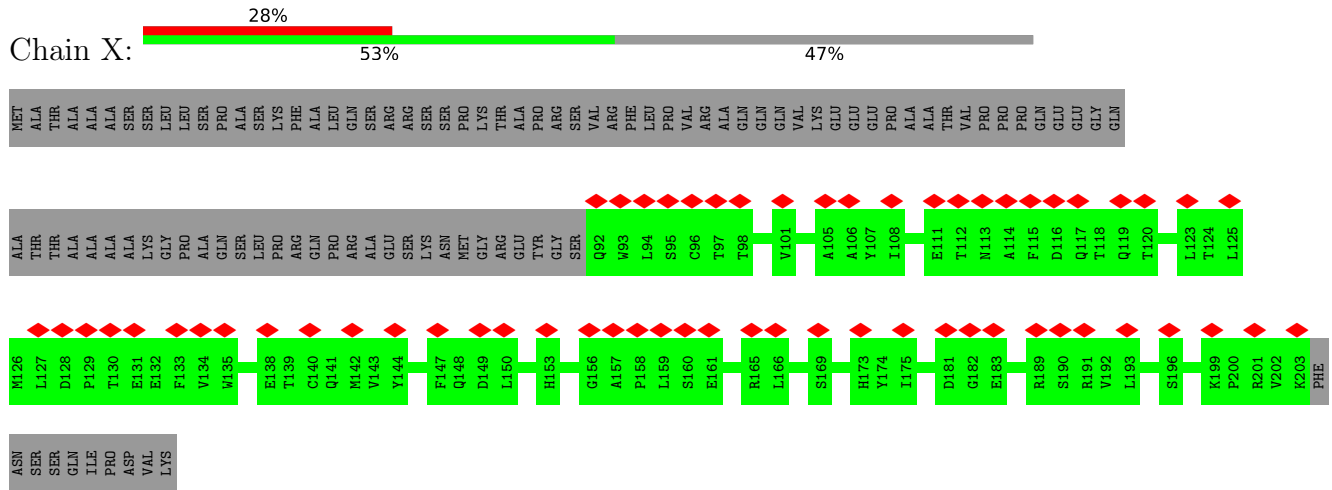
• Molecule 26: NAD(P)H-quinone oxidoreductase subunit K, chloroplastic



• Molecule 27: NAD(P)H-quinone oxidoreductase subunit L, chloroplastic



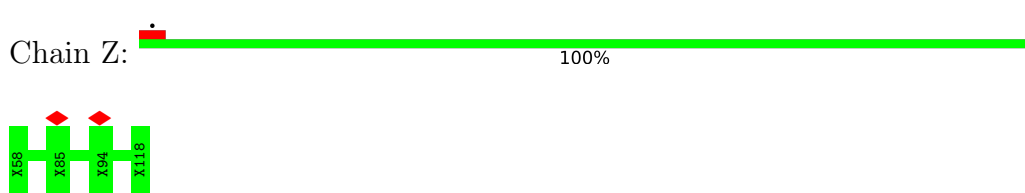
• Molecule 28: NAD(P)H-quinone oxidoreductase subunit M, chloroplastic



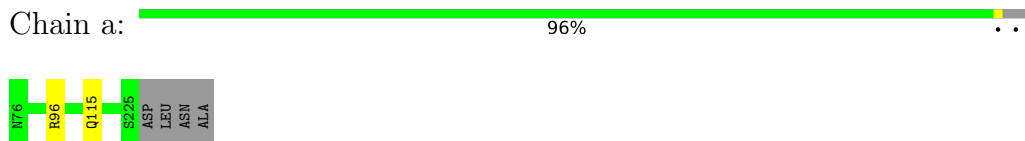
• Molecule 29: NAD(P)H-quinone oxidoreductase subunit N, chloroplastic



• Molecule 30: Unidentified stromal protein

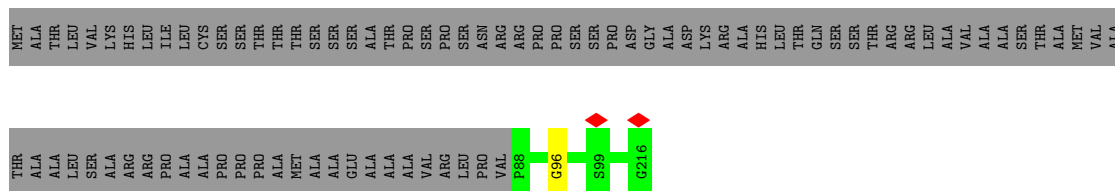


• Molecule 31: Photosynthetic NDH subunit of subcomplex L1

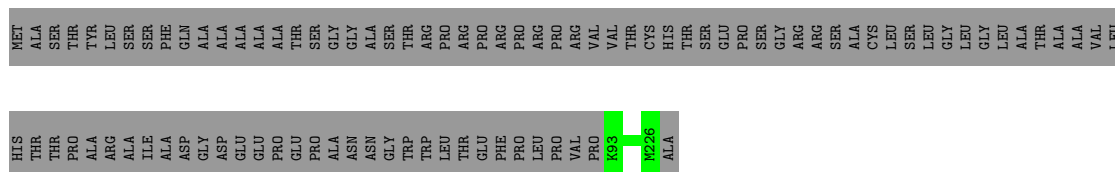


• Molecule 32: Photosynthetic NDH subunit of subcomplex L2





- Molecule 33: Photosynthetic NDH subunit of subcomplex L2

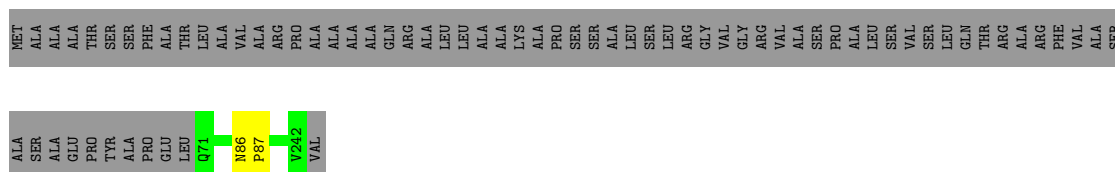


- Molecule 34: Photosynthetic NDH subunit of subcomplex L4

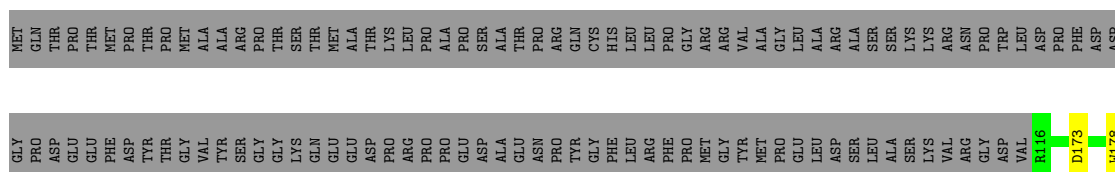


There are no outlier residues recorded for this chain.

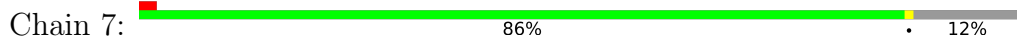
- Molecule 35: Photosynthetic NDH subunit of subcomplex L5

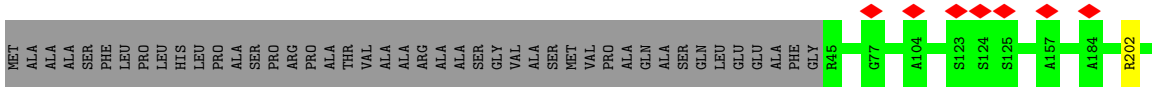


- Molecule 36: Photosynthetic NDH subunit of subcomplex B1

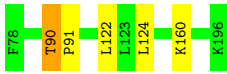


- Molecule 37: Photosynthetic NDH subunit of subcomplex B2





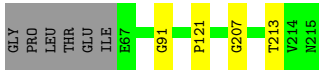
- Molecule 38: Photosynthetic NDH subunit of subcomplex B3



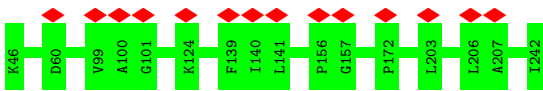
- Molecule 39: Photosynthetic NDH subunit of subcomplex B4



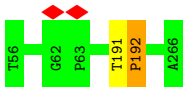
- Molecule 40: Photosynthetic NDH subunit of subcomplex B5



- Molecule 41: Chlorophyll a-b binding protein Lhca4



- Molecule 42: Chlorophyll a-b binding protein, chloroplastic



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103844	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	32.847	Depositor
Minimum map value	-13.195	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.3	Depositor
Map size ( $\text{\AA}$ )	575.08, 575.08, 575.08	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.307, 1.307, 1.307	Depositor



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, CHL, LMG, BCR, SF4, DGD, CLA, PQN, XAT, LUT, LHG, CL0

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	0.66	0/6010	0.49	0/8202
1	e	0.31	0/5993	0.43	0/8178
2	B	0.69	0/6060	0.51	1/8276 (0.0%)
2	f	0.36	3/6052 (0.0%)	0.43	1/8267 (0.0%)
3	C	0.73	0/621	0.53	0/840
3	g	0.30	0/624	0.46	0/844
4	D	0.61	0/1142	0.53	0/1542
4	h	0.27	0/1140	0.47	0/1540
5	E	0.65	0/551	0.49	0/751
5	i	0.30	0/552	0.47	0/751
6	F	0.50	0/1230	0.48	0/1665
6	j	0.26	0/1214	0.45	0/1643
7	H	0.37	0/467	0.46	0/631
7	k	0.26	0/460	0.45	0/623
8	I	0.55	0/238	0.48	0/324
8	l	0.27	0/241	0.41	0/327
9	J	0.54	0/343	0.58	0/467
9	m	0.26	0/342	0.45	0/465
10	K	0.38	0/571	0.55	0/775
10	n	0.26	0/581	0.51	0/786
11	L	0.57	0/1120	0.52	0/1534
11	o	0.27	0/1121	0.46	0/1537
12	1	0.36	0/1467	0.43	0/2008
12	p	0.28	0/1535	0.45	0/2097
13	2	0.42	0/1608	0.46	0/2204
14	3	0.41	0/1684	0.50	0/2298
14	q	0.30	0/1727	0.48	0/2353
15	5	0.45	0/1527	0.50	0/2085
16	G	0.25	0/2664	0.45	0/3637
17	M	0.27	0/3730	0.44	0/5082
18	N	0.30	0/865	0.48	0/1188
19	O	0.37	2/3987 (0.1%)	0.49	2/5427 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	P	0.26	0/759	0.41	0/1028
21	Q	0.29	0/5180	0.46	1/7068 (0.0%)
22	R	0.27	0/1288	0.45	0/1765
23	S	0.25	0/3070	0.46	0/4173
24	T	0.26	0/1254	0.52	0/1702
25	U	0.23	0/1297	0.45	0/1771
26	V	0.25	0/1504	0.47	0/2046
27	W	0.27	0/597	0.46	0/816
28	X	0.23	0/896	0.47	0/1218
29	Y	0.24	0/1170	0.43	0/1592
31	a	0.28	0/1213	0.55	0/1651
32	b	0.25	0/935	0.43	0/1276
33	c	0.26	0/1006	0.43	0/1365
34	4	0.26	0/894	0.54	0/1216
35	d	0.26	0/1314	0.47	0/1771
36	6	0.28	0/2589	0.50	0/3513
37	7	0.28	0/2347	0.57	0/3184
38	8	0.27	0/844	0.54	0/1145
39	9	0.27	0/636	0.48	0/868
40	0	0.27	0/1122	0.54	0/1536
41	r	0.27	0/1577	0.44	0/2153
42	s	0.27	0/1650	0.49	2/2255 (0.1%)
All	All	0.39	5/90609 (0.0%)	0.48	7/123459 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
9	m	0	1
12	p	0	1
19	O	0	1
21	Q	0	1
24	T	0	1
29	Y	0	1
31	a	0	1
32	b	0	1
35	d	0	1
36	6	0	4
37	7	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	8	0	2
40	0	0	3
All	All	0	20

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	657	TRP	CB-CG	-10.12	1.32	1.50
19	O	479	PRO	CA-C	-6.97	1.39	1.52
2	f	657	TRP	C-O	-6.31	1.11	1.23
2	f	657	TRP	CG-CD1	-6.28	1.27	1.36
19	O	481	PHE	N-CA	-5.04	1.36	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	f	657	TRP	CB-CA-C	-5.93	98.55	110.40
42	s	192	PRO	N-CA-C	5.69	126.89	112.10
19	O	481	PHE	N-CA-C	-5.53	96.08	111.00
42	s	192	PRO	C-N-CA	-5.19	108.73	121.70
2	B	223	GLY	N-CA-C	-5.13	100.26	113.10

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	222	LEU	Mainchain
19	O	495	SER	Peptide
21	Q	261	ASN	Peptide
24	T	122	THR	Mainchain
29	Y	125	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	740/750 (99%)	690 (93%)	50 (7%)	0	100	100
1	e	740/750 (99%)	684 (92%)	56 (8%)	0	100	100
2	B	731/734 (100%)	688 (94%)	42 (6%)	1 (0%)	51	85
2	f	731/734 (100%)	680 (93%)	51 (7%)	0	100	100
3	C	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
3	g	79/81 (98%)	68 (86%)	11 (14%)	0	100	100
4	D	140/205 (68%)	118 (84%)	22 (16%)	0	100	100
4	h	140/205 (68%)	125 (89%)	15 (11%)	0	100	100
5	E	66/147 (45%)	61 (92%)	5 (8%)	0	100	100
5	i	66/147 (45%)	61 (92%)	5 (8%)	0	100	100
6	F	156/235 (66%)	150 (96%)	6 (4%)	0	100	100
6	j	156/235 (66%)	148 (95%)	8 (5%)	0	100	100
7	H	59/143 (41%)	58 (98%)	1 (2%)	0	100	100
7	k	59/143 (41%)	56 (95%)	3 (5%)	0	100	100
8	I	28/36 (78%)	28 (100%)	0	0	100	100
8	l	28/36 (78%)	28 (100%)	0	0	100	100
9	J	40/42 (95%)	37 (92%)	2 (5%)	1 (2%)	5	35
9	m	40/42 (95%)	38 (95%)	1 (2%)	1 (2%)	5	35
10	K	82/131 (63%)	73 (89%)	9 (11%)	0	100	100
10	n	82/131 (63%)	75 (92%)	7 (8%)	0	100	100
11	L	144/209 (69%)	135 (94%)	9 (6%)	0	100	100
11	o	144/209 (69%)	134 (93%)	10 (7%)	0	100	100
12	1	189/247 (76%)	179 (95%)	10 (5%)	0	100	100
12	p	191/247 (77%)	171 (90%)	18 (9%)	2 (1%)	15	54
13	2	201/255 (79%)	185 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	3	220/269 (82%)	195 (89%)	25 (11%)	0	100	100
14	q	220/269 (82%)	193 (88%)	27 (12%)	0	100	100
15	5	203/257 (79%)	173 (85%)	30 (15%)	0	100	100
16	G	344/346 (99%)	303 (88%)	40 (12%)	1 (0%)	41	76
17	M	474/483 (98%)	424 (90%)	50 (10%)	0	100	100
18	N	114/117 (97%)	96 (84%)	17 (15%)	1 (1%)	17	56
19	O	497/499 (100%)	447 (90%)	48 (10%)	2 (0%)	34	72
20	P	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
21	Q	665/777 (86%)	598 (90%)	64 (10%)	3 (0%)	29	68
22	R	174/176 (99%)	148 (85%)	26 (15%)	0	100	100
23	S	381/383 (100%)	339 (89%)	42 (11%)	0	100	100
24	T	163/165 (99%)	123 (76%)	40 (24%)	0	100	100
25	U	157/159 (99%)	141 (90%)	16 (10%)	0	100	100
26	V	192/245 (78%)	174 (91%)	17 (9%)	1 (0%)	29	68
27	W	67/192 (35%)	59 (88%)	7 (10%)	1 (2%)	10	46
28	X	110/213 (52%)	92 (84%)	18 (16%)	0	100	100
29	Y	136/233 (58%)	114 (84%)	20 (15%)	2 (2%)	10	46
31	a	148/154 (96%)	112 (76%)	35 (24%)	1 (1%)	22	62
32	b	127/216 (59%)	106 (84%)	21 (16%)	0	100	100
33	c	132/227 (58%)	116 (88%)	16 (12%)	0	100	100
34	4	128/130 (98%)	102 (80%)	26 (20%)	0	100	100
35	d	170/243 (70%)	156 (92%)	13 (8%)	1 (1%)	25	65
36	6	341/469 (73%)	249 (73%)	90 (26%)	2 (1%)	25	65
37	7	315/361 (87%)	226 (72%)	88 (28%)	1 (0%)	41	76
38	8	117/119 (98%)	79 (68%)	34 (29%)	4 (3%)	3	29
39	9	80/83 (96%)	65 (81%)	14 (18%)	1 (1%)	12	48
40	0	147/155 (95%)	98 (67%)	48 (33%)	1 (1%)	22	62
41	r	195/197 (99%)	183 (94%)	12 (6%)	0	100	100
42	s	209/211 (99%)	190 (91%)	17 (8%)	2 (1%)	15	54
All	All	11435/13623 (84%)	10134 (89%)	1272 (11%)	29 (0%)	44	76

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	G	84	LYS
19	O	480	ASP
36	6	275	PRO
42	s	191	THR
42	s	192	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	592/608 (97%)	589 (100%)	3 (0%)	88	93
1	e	588/608 (97%)	588 (100%)	0	100	100
2	B	595/601 (99%)	591 (99%)	4 (1%)	84	90
2	f	589/601 (98%)	587 (100%)	2 (0%)	92	95
3	C	70/71 (99%)	69 (99%)	1 (1%)	67	81
3	g	71/71 (100%)	71 (100%)	0	100	100
4	D	119/160 (74%)	119 (100%)	0	100	100
4	h	118/160 (74%)	118 (100%)	0	100	100
5	E	58/112 (52%)	58 (100%)	0	100	100
5	i	58/112 (52%)	58 (100%)	0	100	100
6	F	121/183 (66%)	121 (100%)	0	100	100
6	j	115/183 (63%)	114 (99%)	1 (1%)	78	87
7	H	48/110 (44%)	48 (100%)	0	100	100
7	k	47/110 (43%)	47 (100%)	0	100	100
8	I	26/33 (79%)	26 (100%)	0	100	100
8	l	27/33 (82%)	27 (100%)	0	100	100
9	J	35/36 (97%)	35 (100%)	0	100	100
9	m	34/36 (94%)	34 (100%)	0	100	100
10	K	52/102 (51%)	51 (98%)	1 (2%)	57	75
10	n	56/102 (55%)	54 (96%)	2 (4%)	35	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	112/166 (68%)	110 (98%)	2 (2%)	59	77
11	o	110/166 (66%)	110 (100%)	0	100	100
12	1	134/196 (68%)	133 (99%)	1 (1%)	84	90
12	p	147/196 (75%)	145 (99%)	2 (1%)	67	81
13	2	155/194 (80%)	154 (99%)	1 (1%)	86	92
14	3	148/216 (68%)	148 (100%)	0	100	100
14	q	159/216 (74%)	157 (99%)	2 (1%)	69	82
15	5	139/202 (69%)	138 (99%)	1 (1%)	84	90
16	G	270/301 (90%)	269 (100%)	1 (0%)	91	94
17	M	397/419 (95%)	396 (100%)	1 (0%)	92	95
18	N	71/100 (71%)	71 (100%)	0	100	100
19	O	399/427 (93%)	399 (100%)	0	100	100
20	P	78/88 (89%)	77 (99%)	1 (1%)	69	82
21	Q	495/674 (73%)	492 (99%)	3 (1%)	86	92
22	R	119/154 (77%)	119 (100%)	0	100	100
23	S	298/336 (89%)	298 (100%)	0	100	100
24	T	123/155 (79%)	123 (100%)	0	100	100
25	U	126/141 (89%)	126 (100%)	0	100	100
26	V	162/226 (72%)	161 (99%)	1 (1%)	86	92
27	W	55/167 (33%)	54 (98%)	1 (2%)	59	77
28	X	86/184 (47%)	86 (100%)	0	100	100
29	Y	115/192 (60%)	115 (100%)	0	100	100
31	a	116/132 (88%)	116 (100%)	0	100	100
32	b	74/181 (41%)	74 (100%)	0	100	100
33	c	92/183 (50%)	92 (100%)	0	100	100
34	4	80/102 (78%)	80 (100%)	0	100	100
35	d	135/191 (71%)	135 (100%)	0	100	100
36	6	250/389 (64%)	250 (100%)	0	100	100
37	7	232/279 (83%)	229 (99%)	3 (1%)	69	82
38	8	69/102 (68%)	69 (100%)	0	100	100
39	9	55/70 (79%)	53 (96%)	2 (4%)	35	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	0	93/137 (68%)	93 (100%)	0	100	100
41	r	156/164 (95%)	156 (100%)	0	100	100
42	s	151/172 (88%)	151 (100%)	0	100	100
All	All	8820/11250 (78%)	8784 (100%)	36 (0%)	91	94

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	f	394	PHE
14	q	223	LEU
6	j	101	LYS
12	p	217	HIS
13	2	264	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
38	8	184	GLN
4	h	148	GLN
40	0	97	HIS
2	f	432	HIS
5	i	135	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

400 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
44	CLA	e	835	1	41,50,73	1.88	7 (17%)	49,85,113	1.54	7 (14%)
47	BCR	e	848	-	41,41,41	0.80	1 (2%)	56,56,56	2.15	20 (35%)
44	CLA	q	312	14	60,68,73	1.54	6 (10%)	70,107,113	1.43	7 (10%)
44	CLA	r	312	-	41,49,73	1.82	6 (14%)	47,84,113	1.65	7 (14%)
44	CLA	B	835	-	60,68,73	1.49	9 (15%)	70,107,113	1.50	11 (15%)
44	CLA	2	509	-	50,58,73	1.60	7 (14%)	58,95,113	1.63	8 (13%)
44	CLA	f	843	46	37,46,73	1.89	5 (13%)	44,80,113	1.67	7 (15%)
52	CHL	2	512	-	46,54,74	2.17	14 (30%)	53,90,114	2.91	20 (37%)
44	CLA	e	828	-	43,51,73	1.78	7 (16%)	48,85,113	1.61	6 (12%)
52	CHL	q	313	-	47,54,74	2.40	15 (31%)	45,89,114	2.89	19 (42%)
44	CLA	A	831	-	63,71,73	1.50	10 (15%)	77,110,113	1.53	12 (15%)
44	CLA	B	834	-	45,53,73	1.73	9 (20%)	52,89,113	1.66	10 (19%)
44	CLA	e	812	-	37,47,73	1.85	7 (18%)	41,80,113	1.75	8 (19%)
44	CLA	e	809	-	50,58,73	1.66	6 (12%)	58,95,113	1.66	9 (15%)
46	LHG	e	844	-	39,39,48	1.00	2 (5%)	42,45,54	1.23	4 (9%)
44	CLA	p	508	-	65,73,73	1.47	6 (9%)	76,113,113	1.33	6 (7%)
52	CHL	s	512	-	47,55,74	2.43	16 (34%)	50,91,114	2.76	19 (38%)
51	LUT	5	303	-	42,43,43	0.95	2 (4%)	51,60,60	1.83	13 (25%)
48	SF4	g	102	-	0,12,12	-	-	-	-	-
44	CLA	F	803	-	41,49,73	1.77	9 (21%)	47,84,113	1.65	8 (17%)
44	CLA	f	818	-	55,63,73	1.58	6 (10%)	64,101,113	1.46	7 (10%)
44	CLA	e	822	-	41,49,73	1.82	7 (17%)	47,84,113	1.70	7 (14%)
44	CLA	f	804	-	43,50,73	2.36	9 (20%)	46,83,113	2.07	9 (19%)
47	BCR	A	851	-	41,41,41	0.91	1 (2%)	56,56,56	2.17	20 (35%)
47	BCR	e	847	-	41,41,41	0.76	0	56,56,56	1.90	17 (30%)
47	BCR	B	849	-	41,41,41	1.07	2 (4%)	56,56,56	2.01	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	CLA	p	509	-	50,58,73	1.50	6 (12%)	58,95,113	2.06	16 (27%)
47	BCR	f	850	-	40,40,41	0.76	0	54,54,56	2.08	15 (27%)
45	PQN	f	844	-	17,17,34	2.13	2 (11%)	21,24,45	1.20	3 (14%)
44	CLA	e	819	-	45,53,73	1.76	6 (13%)	52,89,113	1.61	7 (13%)
44	CLA	f	812	-	39,48,73	1.86	7 (17%)	45,82,113	1.77	8 (17%)
46	LHG	e	845	-	24,24,48	0.96	1 (4%)	26,29,54	1.26	3 (11%)
44	CLA	f	811	2	51,59,73	1.69	7 (13%)	59,96,113	1.52	10 (16%)
47	BCR	e	849	-	41,41,41	0.74	0	56,56,56	2.06	16 (28%)
48	SF4	A	850	1,2	0,12,12	-	-	-	-	-
52	CHL	5	315	-	46,54,74	2.23	15 (32%)	49,90,114	2.89	21 (42%)
44	CLA	B	833	-	65,73,73	1.39	8 (12%)	76,113,113	1.57	10 (13%)
52	CHL	1	512	-	47,55,74	2.31	16 (34%)	50,91,114	2.77	20 (40%)
47	BCR	I	101	-	41,41,41	1.22	3 (7%)	56,56,56	2.08	19 (33%)
48	SF4	g	101	-	0,12,12	-	-	-	-	-
44	CLA	1	515	-	45,52,73	1.81	9 (20%)	47,87,113	1.61	6 (12%)
44	CLA	A	842	46	50,58,73	1.66	10 (20%)	58,95,113	1.52	8 (13%)
44	CLA	B	810	2	39,48,73	1.75	10 (25%)	45,82,113	1.81	9 (20%)
53	XAT	5	304	-	39,47,47	1.24	5 (12%)	54,74,74	2.53	18 (33%)
44	CLA	K	201	-	38,45,73	1.92	9 (23%)	43,78,113	1.66	6 (13%)
44	CLA	A	810	44	54,62,73	1.59	10 (18%)	62,99,113	1.66	7 (11%)
44	CLA	B	806	-	38,47,73	1.98	12 (31%)	46,80,113	1.77	10 (21%)
47	BCR	L	306	-	41,41,41	0.85	1 (2%)	56,56,56	1.96	19 (33%)
44	CLA	q	304	-	40,46,73	2.85	9 (22%)	47,79,113	1.57	8 (17%)
44	CLA	3	301	-	41,49,73	1.80	9 (21%)	47,84,113	1.74	10 (21%)
44	CLA	f	808	-	54,62,73	1.58	6 (11%)	62,99,113	1.51	8 (12%)
44	CLA	s	508	-	40,48,73	1.84	6 (15%)	46,83,113	1.73	8 (17%)
44	CLA	A	818	-	39,48,73	1.75	10 (25%)	45,82,113	1.74	9 (20%)
46	LHG	B	851	-	37,37,48	1.08	2 (5%)	40,43,54	1.17	4 (10%)
44	CLA	A	833	-	39,48,73	1.74	10 (25%)	45,82,113	1.77	9 (20%)
44	CLA	p	511	-	38,47,73	2.06	8 (21%)	46,80,113	1.72	10 (21%)
44	CLA	e	827	-	41,49,73	1.80	8 (19%)	47,84,113	1.64	10 (21%)
44	CLA	f	821	-	55,63,73	1.60	7 (12%)	64,101,113	1.47	7 (10%)
44	CLA	f	816	-	39,46,73	1.83	7 (17%)	44,79,113	1.62	5 (11%)
44	CLA	r	309	-	50,58,73	1.66	6 (12%)	58,95,113	1.54	7 (12%)
44	CLA	A	806	1	65,73,73	1.44	9 (13%)	76,113,113	1.41	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	CLA	s	511	-	50,58,73	1.70	6 (12%)	58,95,113	1.53	8 (13%)
47	BCR	F	801	-	41,41,41	0.99	2 (4%)	56,56,56	2.09	17 (30%)
44	CLA	5	308	-	60,68,73	1.52	9 (15%)	70,107,113	1.57	8 (11%)
52	CHL	s	515	-	40,49,74	2.39	14 (35%)	42,83,114	2.99	19 (45%)
46	LHG	O	601	-	23,23,48	1.32	2 (8%)	26,28,54	1.32	3 (11%)
44	CLA	q	306	-	41,49,73	1.86	6 (14%)	47,84,113	1.69	8 (17%)
47	BCR	J	102	-	41,41,41	1.01	2 (4%)	56,56,56	2.18	24 (42%)
44	CLA	F	802	-	42,50,73	1.78	9 (21%)	48,85,113	1.68	7 (14%)
44	CLA	f	809	-	52,60,73	1.66	8 (15%)	60,97,113	1.47	8 (13%)
44	CLA	e	833	-	41,49,73	1.82	8 (19%)	47,84,113	1.62	9 (19%)
44	CLA	q	309	-	50,58,73	1.67	5 (10%)	58,95,113	1.60	7 (12%)
44	CLA	A	829	-	55,63,73	1.60	10 (18%)	64,101,113	1.59	9 (14%)
52	CHL	3	302	13	47,55,74	2.24	15 (31%)	50,91,114	2.81	18 (36%)
44	CLA	A	817	-	39,47,73	2.03	13 (33%)	42,81,113	1.80	7 (16%)
44	CLA	A	837	-	41,49,73	1.84	11 (26%)	47,84,113	1.87	10 (21%)
44	CLA	f	813	-	54,62,73	1.68	6 (11%)	67,100,113	1.51	10 (14%)
51	LUT	2	501	-	42,43,43	0.94	1 (2%)	51,60,60	1.94	15 (29%)
44	CLA	1	504	-	41,49,73	1.78	7 (17%)	47,84,113	1.60	6 (12%)
44	CLA	f	810	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
44	CLA	B	828	-	41,49,73	1.74	10 (24%)	47,84,113	1.81	12 (25%)
50	LMG	2	519	-	36,36,55	1.09	2 (5%)	44,44,63	1.37	8 (18%)
44	CLA	B	817	-	49,57,73	1.68	11 (22%)	55,93,113	1.59	7 (12%)
44	CLA	3	312	-	41,49,73	1.84	7 (17%)	47,84,113	1.63	8 (17%)
44	CLA	e	806	-	41,49,73	1.81	7 (17%)	47,84,113	1.70	9 (19%)
44	CLA	2	505	-	52,60,73	1.58	7 (13%)	60,97,113	1.53	6 (10%)
44	CLA	A	826	-	60,68,73	1.48	8 (13%)	70,107,113	1.54	9 (12%)
44	CLA	B	819	-	41,49,73	1.77	10 (24%)	47,84,113	1.83	12 (25%)
44	CLA	L	303	-	52,60,73	1.62	9 (17%)	60,97,113	1.73	10 (16%)
51	LUT	p	501	-	42,43,43	0.80	0	51,60,60	1.97	13 (25%)
44	CLA	1	507	12	56,64,73	1.51	9 (16%)	65,102,113	1.52	10 (15%)
44	CLA	B	814	-	41,49,73	1.78	11 (26%)	47,84,113	1.77	12 (25%)
44	CLA	B	807	2	65,73,73	1.46	11 (16%)	76,113,113	1.42	6 (7%)
44	CLA	A	822	-	41,49,73	1.80	9 (21%)	47,84,113	1.79	9 (19%)
44	CLA	L	302	-	41,48,73	1.92	9 (21%)	45,82,113	1.80	8 (17%)
44	CLA	f	827	-	41,48,73	1.96	8 (19%)	45,82,113	1.70	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	BCR	3	305	-	41,41,41	0.90	2 (4%)	56,56,56	1.98	13 (23%)
44	CLA	f	841	-	41,49,73	1.80	7 (17%)	47,84,113	1.69	7 (14%)
44	CLA	e	826	-	64,72,73	1.52	8 (12%)	79,112,113	1.50	9 (11%)
44	CLA	f	834	-	43,51,73	1.77	6 (13%)	49,86,113	1.65	7 (14%)
50	LMG	5	301	-	32,32,55	1.18	2 (6%)	40,40,63	1.15	3 (7%)
44	CLA	r	317	-	50,58,73	1.68	6 (12%)	58,95,113	1.51	9 (15%)
51	LUT	r	302	-	42,43,43	0.76	0	51,60,60	1.90	13 (25%)
50	LMG	r	318	-	18,18,55	1.60	2 (11%)	22,23,63	1.61	2 (9%)
47	BCR	A	846	-	41,41,41	1.05	2 (4%)	56,56,56	2.07	17 (30%)
44	CLA	f	839	-	41,49,73	1.81	5 (12%)	47,84,113	1.72	8 (17%)
47	BCR	F	804	-	41,41,41	1.03	1 (2%)	56,56,56	1.97	18 (32%)
52	CHL	p	514	-	47,55,74	2.42	16 (34%)	50,91,114	2.77	20 (40%)
47	BCR	f	845	-	41,41,41	0.75	0	56,56,56	2.15	19 (33%)
44	CLA	B	827	-	41,49,73	1.78	10 (24%)	47,84,113	1.86	10 (21%)
46	LHG	A	844	44	29,29,48	1.20	3 (10%)	32,35,54	1.19	3 (9%)
44	CLA	3	309	-	41,48,73	2.19	11 (26%)	50,82,113	1.57	6 (12%)
44	CLA	B	803	-	65,73,73	1.45	9 (13%)	76,113,113	1.40	10 (13%)
50	LMG	2	518	-	16,16,55	0.47	0	22,22,63	0.99	2 (9%)
44	CLA	f	840	-	41,49,73	1.81	7 (17%)	47,84,113	1.72	9 (19%)
44	CLA	A	819	-	39,48,73	1.82	9 (23%)	45,82,113	1.67	7 (15%)
44	CLA	f	826	-	65,73,73	1.45	6 (9%)	76,113,113	1.46	8 (10%)
44	CLA	p	507	12	40,48,73	1.88	7 (17%)	50,83,113	1.74	10 (20%)
44	CLA	e	837	-	55,63,73	1.57	6 (10%)	64,101,113	1.54	10 (15%)
44	CLA	s	505	-	46,54,73	1.75	7 (15%)	53,90,113	1.57	6 (11%)
44	CLA	r	310	-	42,50,73	1.84	6 (14%)	48,85,113	1.61	7 (14%)
52	CHL	2	515	-	45,53,74	2.23	14 (31%)	52,89,114	2.82	21 (40%)
44	CLA	A	835	-	51,59,73	1.62	10 (19%)	59,96,113	1.75	9 (15%)
46	LHG	f	852	44	37,37,48	1.05	2 (5%)	40,43,54	1.16	3 (7%)
44	CLA	3	311	-	50,58,73	1.51	7 (14%)	58,95,113	1.74	11 (18%)
47	BCR	5	302	-	41,41,41	0.83	0	56,56,56	1.97	13 (23%)
44	CLA	j	802	-	41,49,73	1.86	6 (14%)	47,84,113	1.63	7 (14%)
44	CLA	f	801	-	64,72,73	1.50	8 (12%)	79,112,113	1.48	8 (10%)
44	CLA	3	313	-	48,56,73	1.71	6 (12%)	55,92,113	1.66	9 (16%)
44	CLA	e	814	-	42,50,73	1.81	7 (16%)	48,85,113	1.59	6 (12%)
47	BCR	f	847	-	41,41,41	0.74	0	56,56,56	2.24	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	CLA	3	317	-	41,49,73	1.79	8 (19%)	47,84,113	1.74	10 (21%)
44	CLA	q	310	-	41,49,73	1.89	6 (14%)	47,84,113	1.65	7 (14%)
44	CLA	A	811	-	39,48,73	1.73	9 (23%)	45,82,113	1.74	10 (22%)
44	CLA	A	813	-	45,53,73	1.69	9 (20%)	52,89,113	1.63	7 (13%)
44	CLA	B	832	-	43,51,73	1.67	9 (20%)	49,86,113	1.62	5 (10%)
44	CLA	L	304	-	45,53,73	1.65	10 (22%)	52,89,113	1.88	11 (21%)
44	CLA	5	312	-	46,54,73	1.73	8 (17%)	53,90,113	1.50	7 (13%)
47	BCR	e	846	-	41,41,41	0.81	1 (2%)	56,56,56	2.19	18 (32%)
44	CLA	B	804	-	65,73,73	1.42	11 (16%)	76,113,113	1.42	6 (7%)
44	CLA	e	815	-	45,53,73	1.81	6 (13%)	52,89,113	1.56	6 (11%)
53	XAT	2	502	-	39,47,47	1.13	4 (10%)	54,74,74	2.84	20 (37%)
44	CLA	m	101	-	41,49,73	1.93	7 (17%)	51,84,113	1.55	6 (11%)
47	BCR	j	801	-	41,41,41	0.74	0	56,56,56	2.22	21 (37%)
44	CLA	A	804	44	52,60,73	1.56	9 (17%)	60,97,113	1.60	7 (11%)
44	CLA	5	305	-	38,46,73	2.22	10 (26%)	47,79,113	1.71	10 (21%)
44	CLA	3	316	-	38,45,73	1.80	5 (13%)	43,78,113	1.82	8 (18%)
44	CLA	B	830	-	56,64,73	1.72	11 (19%)	65,102,113	1.45	7 (10%)
46	LHG	p	516	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	4 (7%)
47	BCR	B	845	-	41,41,41	1.04	1 (2%)	56,56,56	2.07	17 (30%)
44	CLA	m	102	-	42,50,73	1.84	5 (11%)	48,85,113	1.60	6 (12%)
44	CLA	A	830	-	50,58,73	1.59	9 (18%)	58,95,113	1.64	6 (10%)
44	CLA	B	802	-	64,72,73	1.46	10 (15%)	74,111,113	1.49	10 (13%)
44	CLA	s	506	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	6 (7%)
50	LMG	m	105	-	30,30,55	1.20	2 (6%)	38,38,63	1.22	3 (7%)
47	BCR	A	848	-	41,41,41	1.06	2 (4%)	56,56,56	2.00	12 (21%)
44	CLA	3	306	-	52,60,73	1.60	7 (13%)	65,97,113	1.75	11 (16%)
52	CHL	5	314	-	47,55,74	2.22	15 (31%)	50,91,114	2.82	21 (42%)
47	BCR	1	503	-	19,19,41	0.67	0	26,26,56	2.04	7 (26%)
44	CLA	5	306	-	39,48,73	1.78	6 (15%)	44,83,113	1.70	7 (15%)
44	CLA	n	201	-	38,45,73	1.91	7 (18%)	43,78,113	1.64	7 (16%)
47	BCR	A	845	-	41,41,41	1.17	4 (9%)	56,56,56	2.29	20 (35%)
44	CLA	r	308	-	41,49,73	1.83	6 (14%)	47,84,113	1.67	7 (14%)
44	CLA	r	311	-	46,54,73	1.78	7 (15%)	53,90,113	1.54	8 (15%)
52	CHL	1	514	-	40,49,74	2.55	15 (37%)	42,83,114	3.00	19 (45%)
47	BCR	j	803	-	41,41,41	0.76	0	56,56,56	2.16	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	CLA	B	841	-	54,62,73	1.56	10 (18%)	62,99,113	1.53	9 (14%)
44	CLA	2	511	-	39,48,73	1.82	10 (25%)	45,82,113	1.93	11 (24%)
44	CLA	f	831	-	56,64,73	1.59	7 (12%)	65,102,113	1.49	7 (10%)
44	CLA	A	834	1	41,49,73	1.82	9 (21%)	47,84,113	1.62	7 (14%)
44	CLA	s	504	-	40,47,73	2.26	8 (20%)	49,81,113	1.74	9 (18%)
44	CLA	n	203	-	41,49,73	1.80	6 (14%)	47,84,113	1.71	8 (17%)
44	CLA	B	815	-	65,73,73	1.50	11 (16%)	76,113,113	1.44	10 (13%)
44	CLA	o	304	-	45,53,73	1.76	6 (13%)	52,89,113	1.60	6 (11%)
44	CLA	l	506	-	55,63,73	1.62	8 (14%)	64,101,113	1.50	8 (12%)
44	CLA	l	513	-	65,73,73	1.53	7 (10%)	76,113,113	1.36	7 (9%)
44	CLA	q	315	-	45,53,73	1.76	7 (15%)	52,89,113	1.61	7 (13%)
47	BCR	A	847	-	41,41,41	0.97	2 (4%)	56,56,56	2.00	20 (35%)
44	CLA	B	808	-	52,60,73	1.68	9 (17%)	60,97,113	1.57	9 (15%)
44	CLA	l	510	46	46,54,73	1.73	8 (17%)	53,90,113	1.56	7 (13%)
44	CLA	e	836	-	51,59,73	1.65	6 (11%)	59,96,113	1.52	6 (10%)
51	LUT	l	502	-	42,43,43	0.90	2 (4%)	51,60,60	1.68	11 (21%)
52	CHL	5	317	-	41,48,74	2.34	15 (36%)	42,82,114	3.07	22 (52%)
44	CLA	e	834	-	45,53,73	1.74	7 (15%)	52,89,113	1.59	7 (13%)
44	CLA	e	803	44	52,60,73	1.65	6 (11%)	60,97,113	1.55	9 (15%)
44	CLA	e	824	-	56,64,73	1.55	7 (12%)	65,102,113	1.45	9 (13%)
47	BCR	m	103	-	41,41,41	0.77	1 (2%)	56,56,56	2.11	17 (30%)
51	LUT	q	301	-	42,43,43	0.79	0	51,60,60	2.00	11 (21%)
44	CLA	B	818	-	59,67,73	1.50	10 (16%)	68,105,113	1.59	9 (13%)
47	BCR	f	848	-	41,41,41	0.78	1 (2%)	56,56,56	2.04	16 (28%)
44	CLA	r	305	-	50,58,73	1.71	6 (12%)	58,95,113	1.50	8 (13%)
52	CHL	3	315	-	43,51,74	2.17	14 (32%)	45,86,114	3.02	19 (42%)
44	CLA	5	307	15	65,73,73	1.47	8 (12%)	76,113,113	1.35	8 (10%)
48	SF4	C	102	3	0,12,12	-	-	-	-	-
46	LHG	A	843	-	48,48,48	0.90	3 (6%)	51,54,54	1.29	5 (9%)
44	CLA	s	510	-	60,68,73	1.54	6 (10%)	70,107,113	1.38	6 (8%)
44	CLA	A	808	1	65,73,73	1.42	10 (15%)	76,113,113	1.44	7 (9%)
44	CLA	5	316	-	41,49,73	1.73	9 (21%)	47,84,113	1.80	9 (19%)
44	CLA	e	840	-	41,49,73	1.80	6 (14%)	47,84,113	1.70	7 (14%)
44	CLA	B	839	-	47,55,73	1.66	9 (19%)	54,91,113	1.73	9 (16%)
44	CLA	B	812	-	54,62,73	1.59	8 (14%)	67,100,113	1.57	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	CLA	f	829	-	50,58,73	1.64	6 (12%)	58,95,113	1.60	10 (17%)
44	CLA	e	811	-	41,49,73	1.83	8 (19%)	47,84,113	1.64	8 (17%)
47	BCR	B	847	-	41,41,41	1.03	2 (4%)	56,56,56	2.35	19 (33%)
44	CLA	A	814	-	42,50,73	1.82	10 (23%)	48,85,113	1.73	9 (18%)
44	CLA	q	305	-	52,60,73	1.70	6 (11%)	60,97,113	1.52	10 (16%)
44	CLA	2	506	-	65,73,73	1.44	9 (13%)	76,113,113	1.51	7 (9%)
45	PQN	B	843	-	31,31,34	1.36	2 (6%)	38,41,45	1.49	5 (13%)
48	SF4	f	802	-	0,12,12	-	-	-	-	-
44	CLA	f	803	-	40,49,73	1.73	6 (15%)	44,83,113	1.64	6 (13%)
44	CLA	f	814	-	43,51,73	1.77	7 (16%)	49,86,113	1.61	6 (12%)
44	CLA	B	840	-	41,49,73	1.75	9 (21%)	47,84,113	1.80	8 (17%)
47	BCR	e	854	-	41,41,41	0.70	0	56,56,56	2.26	19 (33%)
44	CLA	B	811	-	55,63,73	1.58	11 (20%)	64,101,113	1.53	7 (10%)
44	CLA	3	310	-	45,53,73	1.77	7 (15%)	52,89,113	1.63	9 (17%)
44	CLA	A	815	-	45,53,73	1.71	9 (20%)	52,89,113	1.61	8 (15%)
44	CLA	q	314	-	39,48,73	1.84	6 (15%)	45,82,113	1.84	8 (17%)
44	CLA	e	807	-	42,50,73	1.81	6 (14%)	48,85,113	1.66	7 (14%)
44	CLA	B	820	-	53,61,73	1.68	10 (18%)	61,98,113	1.48	8 (13%)
44	CLA	A	840	-	41,49,73	1.82	9 (21%)	47,84,113	1.64	8 (17%)
44	CLA	e	816	-	60,68,73	1.55	6 (10%)	70,107,113	1.41	6 (8%)
44	CLA	B	831	-	43,51,73	1.80	9 (20%)	49,86,113	1.62	7 (14%)
44	CLA	2	510	46	60,68,73	1.50	7 (11%)	70,107,113	1.51	9 (12%)
44	CLA	f	823	-	41,49,73	1.84	8 (19%)	47,84,113	1.66	7 (14%)
44	CLA	r	306	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	8 (10%)
43	CL0	A	801	-	61,69,73	1.64	10 (16%)	70,107,113	2.21	16 (22%)
44	CLA	B	821	-	50,58,73	1.71	9 (18%)	58,95,113	1.62	8 (13%)
52	CHL	s	517	42	47,55,74	2.27	15 (31%)	50,91,114	2.81	19 (38%)
44	CLA	5	313	15	39,48,73	1.80	9 (23%)	45,82,113	1.64	8 (17%)
54	SQD	Q	802	-	53,54,54	1.18	4 (7%)	62,65,65	1.04	4 (6%)
44	CLA	A	807	-	37,47,73	1.78	10 (27%)	41,80,113	1.76	8 (19%)
44	CLA	A	821	-	42,50,73	1.78	9 (21%)	48,85,113	1.79	8 (16%)
44	CLA	f	822	-	41,49,73	1.85	6 (14%)	47,84,113	1.62	8 (17%)
47	BCR	B	846	-	41,41,41	1.05	3 (7%)	56,56,56	2.31	18 (32%)
44	CLA	1	511	-	46,54,73	1.71	9 (19%)	53,90,113	1.61	7 (13%)
44	CLA	f	817	-	43,51,73	1.77	7 (16%)	49,86,113	1.57	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	CLA	f	842	-	41,49,73	1.83	8 (19%)	47,84,113	1.69	8 (17%)
44	CLA	s	507	-	41,49,73	1.82	7 (17%)	47,84,113	1.66	8 (17%)
44	CLA	p	506	-	55,63,73	1.61	6 (10%)	64,101,113	1.42	9 (14%)
44	CLA	p	513	-	52,60,73	1.68	6 (11%)	60,97,113	1.51	8 (13%)
44	CLA	B	813	-	43,51,73	1.72	9 (20%)	49,86,113	1.69	9 (18%)
47	BCR	o	301	-	41,41,41	0.75	1 (2%)	56,56,56	2.04	17 (30%)
44	CLA	f	835	-	45,53,73	1.74	7 (15%)	52,89,113	1.63	9 (17%)
47	BCR	o	305	-	41,41,41	0.71	0	56,56,56	2.18	18 (32%)
44	CLA	5	309	-	45,53,73	1.72	8 (17%)	52,89,113	1.65	7 (13%)
44	CLA	p	515	-	39,48,73	1.93	7 (17%)	45,82,113	1.74	8 (17%)
44	CLA	B	805	-	41,49,73	1.79	9 (21%)	47,84,113	1.75	10 (21%)
44	CLA	p	510	-	46,54,73	1.76	7 (15%)	53,90,113	1.49	6 (11%)
44	CLA	f	815	-	43,51,73	1.78	6 (13%)	49,86,113	1.51	6 (12%)
44	CLA	B	842	-	57,65,73	1.55	8 (14%)	66,103,113	1.46	7 (10%)
44	CLA	e	839	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	9 (11%)
44	CLA	r	304	-	38,47,73	1.90	7 (18%)	48,81,113	1.93	10 (20%)
46	LHG	2	517	44	34,34,48	1.07	2 (5%)	37,40,54	1.21	4 (10%)
44	CLA	3	308	-	55,63,73	1.49	9 (16%)	64,101,113	1.54	9 (14%)
44	CLA	3	318	-	45,53,73	1.67	7 (15%)	56,89,113	1.59	8 (14%)
52	CHL	p	512	-	47,55,74	2.44	16 (34%)	50,91,114	2.79	22 (44%)
44	CLA	A	827	-	65,73,73	1.42	12 (18%)	76,113,113	1.51	9 (11%)
44	CLA	A	839	-	42,50,73	1.81	10 (23%)	48,85,113	1.73	7 (14%)
44	CLA	o	303	-	60,68,73	1.51	6 (10%)	70,107,113	1.43	7 (10%)
51	LUT	p	502	-	42,43,43	2.39	1 (2%)	51,60,60	1.81	9 (17%)
44	CLA	A	836	-	55,63,73	1.65	10 (18%)	64,101,113	1.60	10 (15%)
44	CLA	B	823	-	42,50,73	1.76	9 (21%)	48,85,113	1.68	7 (14%)
44	CLA	e	820	-	41,49,73	1.78	6 (14%)	47,84,113	1.71	7 (14%)
44	CLA	e	838	-	52,60,73	1.60	7 (13%)	60,97,113	1.57	8 (13%)
53	XAT	s	502	-	39,47,47	0.91	0	54,74,74	2.89	22 (40%)
44	CLA	r	307	-	60,68,73	1.52	6 (10%)	70,107,113	1.47	8 (11%)
44	CLA	3	314	14	60,68,73	1.51	6 (10%)	70,107,113	1.49	10 (14%)
49	DGD	f	851	-	53,53,67	0.93	2 (3%)	67,67,81	1.06	3 (4%)
44	CLA	3	307	-	39,48,73	2.01	9 (23%)	45,82,113	1.58	7 (15%)
47	BCR	B	852	-	41,41,41	1.22	3 (7%)	56,56,56	2.06	18 (32%)
44	CLA	f	824	-	42,50,73	1.81	7 (16%)	48,85,113	1.62	6 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	SF4	C	101	3	0,12,12	-	-	-		
47	BCR	f	849	-	41,41,41	0.79	1 (2%)	56,56,56	2.02	16 (28%)
44	CLA	s	514	-	39,48,73	1.83	6 (15%)	45,82,113	1.74	8 (17%)
44	CLA	e	830	-	50,58,73	1.69	8 (16%)	58,95,113	1.51	8 (13%)
44	CLA	f	806	-	41,49,73	1.81	6 (14%)	47,84,113	1.62	7 (14%)
44	CLA	q	307	14	39,48,73	1.90	5 (12%)	45,82,113	1.71	8 (17%)
44	CLA	B	801	-	65,73,73	1.47	11 (16%)	76,113,113	1.47	10 (13%)
44	CLA	e	802	-	39,48,73	1.87	7 (17%)	45,82,113	1.76	8 (17%)
44	CLA	e	852	-	57,65,73	1.57	7 (12%)	66,103,113	1.43	7 (10%)
50	LMG	F	806	-	45,45,55	0.95	2 (4%)	53,53,63	1.07	4 (7%)
51	LUT	q	302	-	42,43,43	0.77	0	51,60,60	1.85	16 (31%)
44	CLA	e	821	-	42,50,73	1.76	7 (16%)	48,85,113	1.64	6 (12%)
43	CL0	e	801	-	61,69,73	1.64	10 (16%)	70,107,113	2.21	16 (22%)
48	SF4	8	201	38	0,12,12	-	-	-		
47	BCR	r	301	-	41,41,41	0.72	0	56,56,56	1.85	14 (25%)
44	CLA	5	310	-	50,58,73	1.65	8 (16%)	58,95,113	1.59	8 (13%)
44	CLA	f	837	-	42,50,73	1.84	6 (14%)	48,85,113	1.58	6 (12%)
44	CLA	B	825	-	42,50,73	1.70	10 (23%)	48,85,113	1.69	7 (14%)
44	CLA	B	826	-	62,70,73	1.40	10 (16%)	72,109,113	1.52	10 (13%)
44	CLA	e	805	-	46,54,73	1.73	6 (13%)	53,90,113	1.57	6 (11%)
44	CLA	A	802	-	58,66,73	1.54	9 (15%)	67,104,113	1.51	7 (10%)
49	DGD	m	104	-	67,67,67	0.84	2 (2%)	81,81,81	0.88	3 (3%)
47	BCR	Q	801	-	40,40,41	0.77	0	54,54,56	2.99	21 (38%)
44	CLA	A	825	-	59,67,73	1.55	10 (16%)	68,105,113	1.47	8 (11%)
44	CLA	f	833	-	43,51,73	1.77	6 (13%)	49,86,113	1.55	6 (12%)
47	BCR	e	851	-	41,41,41	0.71	0	56,56,56	2.16	19 (33%)
44	CLA	e	843	-	49,57,73	1.75	6 (12%)	61,94,113	1.67	8 (13%)
44	CLA	5	311	-	42,50,73	1.72	7 (16%)	48,85,113	1.74	8 (16%)
44	CLA	e	813	-	42,50,73	1.83	7 (16%)	48,85,113	1.57	7 (14%)
44	CLA	f	828	-	41,49,73	1.81	8 (19%)	47,84,113	1.74	7 (14%)
44	CLA	s	509	-	50,58,73	1.71	5 (10%)	58,95,113	1.54	9 (15%)
54	SQD	Q	803	-	45,46,54	1.28	4 (8%)	54,57,65	1.15	7 (12%)
49	DGD	B	850	-	60,60,67	0.88	2 (3%)	74,74,81	1.39	11 (14%)
44	CLA	f	838	-	39,48,73	1.83	7 (17%)	45,82,113	1.71	8 (17%)
44	CLA	A	816	-	59,67,73	1.47	8 (13%)	68,105,113	1.56	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	CLA	1	505	-	42,50,73	1.86	7 (16%)	48,85,113	1.58	8 (16%)
47	BCR	l	102	-	41,41,41	0.70	0	56,56,56	2.15	16 (28%)
44	CLA	A	832	-	44,53,73	1.68	10 (22%)	52,88,113	1.78	8 (15%)
49	DGD	J	103	-	67,67,67	0.83	2 (2%)	81,81,81	1.11	4 (4%)
50	LMG	F	805	-	30,30,55	1.22	2 (6%)	38,38,63	1.21	3 (7%)
47	BCR	A	853	-	41,41,41	0.97	2 (4%)	56,56,56	2.24	18 (32%)
44	CLA	B	836	-	42,50,73	1.84	9 (21%)	48,85,113	1.56	7 (14%)
45	PQN	e	842	-	15,15,34	1.44	2 (13%)	22,22,45	0.87	2 (9%)
44	CLA	K	205	10	37,47,73	1.93	7 (18%)	42,81,113	1.73	8 (19%)
44	CLA	B	829	-	39,48,73	1.77	11 (28%)	45,82,113	1.73	9 (20%)
52	CHL	1	517	12	40,49,74	2.29	14 (35%)	42,83,114	3.16	20 (47%)
44	CLA	K	202	-	41,49,73	1.75	8 (19%)	47,84,113	1.70	8 (17%)
44	CLA	e	853	-	45,53,73	1.74	7 (15%)	52,89,113	1.66	8 (15%)
44	CLA	q	311	-	48,56,73	1.72	6 (12%)	55,92,113	1.54	7 (12%)
44	CLA	B	837	-	50,58,73	1.62	10 (20%)	58,95,113	1.62	10 (17%)
44	CLA	r	315	41	41,49,73	1.85	6 (14%)	47,84,113	1.70	10 (21%)
44	CLA	A	824	-	39,48,73	1.77	8 (20%)	45,82,113	1.68	8 (17%)
46	LHG	s	516	-	34,34,48	1.08	2 (5%)	37,40,54	1.14	3 (8%)
44	CLA	f	807	-	41,49,73	1.80	6 (14%)	47,84,113	1.69	9 (19%)
44	CLA	1	509	-	50,58,73	1.63	7 (14%)	58,95,113	1.60	7 (12%)
44	CLA	e	825	-	41,49,73	1.78	6 (14%)	47,84,113	1.71	8 (17%)
47	BCR	f	846	-	41,41,41	0.73	0	56,56,56	1.96	14 (25%)
52	CHL	2	513	-	40,48,74	2.49	16 (40%)	37,81,114	3.16	19 (51%)
44	CLA	2	507	13	47,56,73	1.97	9 (19%)	54,91,113	1.81	10 (18%)
44	CLA	A	820	-	57,65,73	1.53	8 (14%)	66,103,113	1.69	9 (13%)
51	LUT	1	501	-	42,43,43	0.89	1 (2%)	51,60,60	1.65	11 (21%)
44	CLA	A	838	-	65,73,73	1.46	10 (15%)	76,113,113	1.45	10 (13%)
47	BCR	L	305	-	41,41,41	1.00	1 (2%)	56,56,56	2.16	18 (32%)
44	CLA	q	308	-	42,50,73	1.81	5 (11%)	48,85,113	1.69	6 (12%)
47	BCR	B	844	-	41,41,41	0.85	1 (2%)	56,56,56	2.59	19 (33%)
44	CLA	f	805	-	37,46,73	1.83	7 (18%)	40,79,113	1.88	7 (17%)
44	CLA	e	831	-	56,64,73	1.56	6 (10%)	65,102,113	1.46	7 (10%)
52	CHL	s	513	-	48,56,74	2.31	16 (33%)	51,92,114	2.77	22 (43%)
44	CLA	B	824	-	45,53,73	1.74	9 (20%)	52,89,113	1.54	6 (11%)
44	CLA	B	809	-	39,48,73	1.81	10 (25%)	45,82,113	1.69	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	CLA	n	202	-	45,53,73	1.78	5 (11%)	52,89,113	1.57	9 (17%)
51	LUT	s	501	-	42,43,43	0.78	0	51,60,60	1.89	13 (25%)
44	CLA	A	828	-	41,49,73	1.76	10 (24%)	47,84,113	1.68	7 (14%)
52	CHL	p	517	-	43,51,74	2.37	15 (34%)	45,86,114	2.90	19 (42%)
46	LHG	1	516	44	48,48,48	0.91	2 (4%)	51,54,54	1.16	4 (7%)
44	CLA	A	812	-	42,50,73	1.75	10 (23%)	48,85,113	1.76	10 (20%)
44	CLA	A	809	1	38,47,73	1.83	9 (23%)	39,80,113	1.63	5 (12%)
44	CLA	e	832	-	43,51,73	1.80	6 (13%)	49,86,113	1.56	8 (16%)
44	CLA	J	101	9	42,50,73	1.79	6 (14%)	48,85,113	1.68	7 (14%)
51	LUT	3	304	-	42,43,43	0.91	2 (4%)	51,60,60	1.56	10 (19%)
47	BCR	K	204	-	41,41,41	0.99	2 (4%)	56,56,56	2.02	16 (28%)
44	CLA	A	852	-	57,65,73	1.61	9 (15%)	66,103,113	1.43	9 (13%)
52	CHL	r	316	-	43,51,74	2.30	14 (32%)	45,86,114	2.85	19 (42%)
44	CLA	B	838	-	65,73,73	1.47	10 (15%)	76,113,113	1.49	8 (10%)
44	CLA	e	804	-	65,73,73	1.44	7 (10%)	76,113,113	1.42	6 (7%)
44	CLA	f	836	-	59,66,73	1.68	7 (11%)	64,103,113	1.42	8 (12%)
44	CLA	B	816	-	43,51,73	1.67	9 (20%)	49,86,113	1.66	6 (12%)
45	PQN	A	841	-	34,34,34	1.38	2 (5%)	42,45,45	1.24	4 (9%)
44	CLA	1	508	-	39,48,73	1.83	6 (15%)	45,82,113	1.71	7 (15%)
44	CLA	2	514	-	55,63,73	1.55	10 (18%)	64,101,113	1.47	8 (12%)
47	BCR	l	101	-	41,41,41	0.80	1 (2%)	56,56,56	2.29	21 (37%)
44	CLA	A	805	-	64,72,73	1.50	12 (18%)	74,111,113	1.57	10 (13%)
47	BCR	B	848	-	41,41,41	1.05	2 (4%)	56,56,56	1.98	18 (32%)
44	CLA	p	505	-	46,54,73	1.65	6 (13%)	53,90,113	1.54	8 (15%)
44	CLA	e	808	1	41,49,73	1.85	7 (17%)	47,84,113	1.67	8 (17%)
47	BCR	2	503	-	41,41,41	0.89	1 (2%)	56,56,56	3.62	27 (48%)
44	CLA	f	820	-	50,58,73	1.65	7 (14%)	58,95,113	1.57	8 (13%)
47	BCR	A	849	-	40,40,41	1.04	2 (5%)	54,54,56	1.90	15 (27%)
51	LUT	3	303	-	42,43,43	0.89	2 (4%)	51,60,60	1.51	10 (19%)
44	CLA	n	205	-	37,47,73	1.97	6 (16%)	42,81,113	1.63	7 (16%)
44	CLA	f	819	-	41,49,73	1.83	6 (14%)	47,84,113	1.63	8 (17%)
47	BCR	p	503	-	10,11,41	0.69	0	15,16,56	1.94	4 (26%)
44	CLA	2	504	13	34,44,73	2.06	10 (29%)	42,76,113	1.87	10 (23%)
44	CLA	e	810	44	55,63,73	1.61	8 (14%)	64,101,113	1.45	8 (12%)
52	CHL	2	516	13	43,51,74	2.19	13 (30%)	49,86,114	3.04	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
44	CLA	K	203	-	39,48,73	1.71	10 (25%)	45,82,113	1.68	8 (17%)
47	BCR	s	503	-	41,41,41	0.71	0	56,56,56	3.61	30 (53%)
44	CLA	e	818	-	40,47,73	2.03	7 (17%)	44,81,113	2.14	12 (27%)
44	CLA	f	825	-	42,50,73	1.79	7 (16%)	48,85,113	1.59	6 (12%)
44	CLA	o	302	-	40,48,73	1.93	6 (15%)	50,83,113	1.88	9 (18%)
44	CLA	B	822	-	47,55,73	1.72	10 (21%)	54,91,113	1.75	7 (12%)
47	BCR	e	850	-	41,41,41	0.81	2 (4%)	56,56,56	2.33	20 (35%)
53	XAT	r	303	-	39,47,47	0.88	0	54,74,74	2.72	20 (37%)
44	CLA	e	823	-	42,50,73	1.83	7 (16%)	52,85,113	1.74	9 (17%)
44	CLA	f	832	-	39,48,73	1.86	7 (17%)	45,82,113	1.76	8 (17%)
44	CLA	L	301	-	56,64,73	1.59	11 (19%)	65,102,113	1.50	8 (12%)
44	CLA	e	841	-	41,49,73	1.83	8 (19%)	47,84,113	1.66	8 (17%)
44	CLA	e	829	-	58,66,73	1.60	8 (13%)	67,104,113	1.46	7 (10%)
44	CLA	p	504	-	41,49,73	1.84	7 (17%)	47,84,113	1.73	9 (19%)
44	CLA	A	803	-	41,49,73	1.80	10 (24%)	47,84,113	1.79	10 (21%)
47	BCR	q	303	-	41,41,41	0.79	1 (2%)	56,56,56	2.00	18 (32%)
52	CHL	r	314	-	51,59,74	2.14	15 (29%)	55,96,114	2.75	20 (36%)
44	CLA	A	823	-	55,62,73	1.74	11 (20%)	60,99,113	1.54	10 (16%)
44	CLA	e	817	-	39,47,73	1.86	7 (17%)	42,81,113	1.73	8 (19%)
44	CLA	2	508	-	47,55,73	1.72	7 (14%)	54,91,113	1.49	6 (11%)
47	BCR	n	204	-	41,41,41	0.70	0	56,56,56	2.09	18 (32%)
52	CHL	r	313	-	47,55,74	2.39	16 (34%)	50,91,114	2.74	20 (40%)
44	CLA	q	316	-	46,54,73	1.77	6 (13%)	53,90,113	1.49	7 (13%)
44	CLA	f	830	-	38,47,73	1.93	8 (21%)	48,81,113	1.81	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	e	835	1	1/1/10/20	2/7/85/115	-
47	BCR	e	848	-	-	6/29/63/63	0/2/2/2
44	CLA	q	312	14	1/1/14/20	12/31/109/115	-
44	CLA	r	312	-	1/1/10/20	3/8/86/115	-
44	CLA	B	835	-	1/1/14/20	6/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	2	509	-	1/1/12/20	10/19/97/115	-
44	CLA	f	843	46	1/1/9/20	0/2/80/115	-
52	CHL	2	512	-	3/3/16/26	3/17/113/137	-
44	CLA	e	828	-	1/1/10/20	5/10/88/115	-
52	CHL	q	313	-	3/3/15/26	11/17/111/137	-
44	CLA	A	831	-	1/1/14/20	17/35/111/115	-
44	CLA	B	834	-	1/1/11/20	6/13/91/115	-
44	CLA	e	812	-	1/1/8/20	3/5/79/115	-
44	CLA	e	809	-	1/1/12/20	4/19/97/115	-
46	LHG	e	844	-	-	8/44/44/53	-
44	CLA	p	508	-	1/1/15/20	17/37/115/115	-
52	CHL	s	512	-	3/3/16/26	5/17/115/137	-
51	LUT	5	303	-	-	2/29/67/67	0/2/2/2
48	SF4	g	102	-	-	-	0/6/5/5
44	CLA	F	803	-	1/1/10/20	3/8/86/115	-
44	CLA	f	818	-	1/1/13/20	9/25/103/115	-
44	CLA	e	822	-	1/1/10/20	1/8/86/115	-
44	CLA	f	804	-	1/1/9/20	4/10/84/115	-
47	BCR	A	851	-	-	6/29/63/63	0/2/2/2
47	BCR	e	847	-	-	0/29/63/63	0/2/2/2
47	BCR	B	849	-	-	3/29/63/63	0/2/2/2
44	CLA	p	509	-	1/1/12/20	8/19/97/115	-
47	BCR	f	850	-	-	2/27/61/63	0/2/2/2
45	PQN	f	844	-	-	0/3/23/43	0/2/2/2
44	CLA	e	819	-	1/1/11/20	5/13/91/115	-
44	CLA	f	812	-	1/1/9/20	4/8/82/115	-
46	LHG	e	845	-	-	10/28/28/53	-
44	CLA	f	811	2	1/1/12/20	6/21/99/115	-
47	BCR	e	849	-	-	7/29/63/63	0/2/2/2
48	SF4	A	850	1,2	-	-	0/6/5/5
52	CHL	5	315	-	3/3/16/26	4/15/113/137	-
44	CLA	B	833	-	1/1/15/20	4/37/115/115	-
52	CHL	1	512	-	3/3/16/26	8/17/115/137	-
47	BCR	I	101	-	-	4/29/63/63	0/2/2/2
48	SF4	g	101	-	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	1	515	-	1/1/10/20	6/13/87/115	-
44	CLA	A	842	46	1/1/12/20	9/19/97/115	-
44	CLA	B	810	2	1/1/9/20	2/8/82/115	-
53	XAT	5	304	-	-	2/31/93/93	0/4/4/4
44	CLA	K	201	-	1/1/8/20	0/2/76/115	-
44	CLA	A	810	44	1/1/12/20	5/24/102/115	-
44	CLA	B	806	-	1/1/8/20	4/8/79/115	-
47	BCR	L	306	-	-	6/29/63/63	0/2/2/2
44	CLA	q	304	-	1/1/10/20	0/6/84/115	-
44	CLA	3	301	-	1/1/10/20	2/8/86/115	-
44	CLA	f	808	-	1/1/12/20	6/23/101/115	-
44	CLA	s	508	-	1/1/10/20	2/6/84/115	-
44	CLA	A	818	-	1/1/9/20	4/8/82/115	-
46	LHG	B	851	-	-	18/42/42/53	-
44	CLA	A	833	-	1/1/9/20	1/8/82/115	-
44	CLA	p	511	-	1/1/8/20	2/8/79/115	-
44	CLA	e	827	-	1/1/10/20	1/8/86/115	-
44	CLA	f	821	-	1/1/13/20	8/25/103/115	-
44	CLA	f	816	-	1/1/8/20	1/4/78/115	-
44	CLA	r	309	-	1/1/12/20	7/19/97/115	-
44	CLA	A	806	1	1/1/15/20	20/37/115/115	-
44	CLA	s	511	-	1/1/12/20	7/19/97/115	-
47	BCR	F	801	-	-	6/29/63/63	0/2/2/2
44	CLA	5	308	-	1/1/14/20	14/31/109/115	-
52	CHL	s	515	-	3/3/14/26	4/10/104/137	-
46	LHG	O	601	-	-	3/27/27/53	-
44	CLA	q	306	-	1/1/10/20	3/8/86/115	-
47	BCR	J	102	-	-	3/29/63/63	0/2/2/2
44	CLA	F	802	-	1/1/10/20	2/10/88/115	-
44	CLA	f	809	-	1/1/12/20	3/22/100/115	-
44	CLA	e	833	-	1/1/10/20	4/8/86/115	-
44	CLA	q	309	-	1/1/12/20	5/19/97/115	-
44	CLA	A	829	-	1/1/13/20	6/25/103/115	-
52	CHL	3	302	13	3/3/16/26	3/17/115/137	-
44	CLA	A	817	-	1/1/9/20	0/2/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	A	837	-	1/1/10/20	4/8/86/115	-
44	CLA	f	813	-	1/1/13/20	10/25/101/115	-
51	LUT	2	501	-	-	0/29/67/67	0/2/2/2
44	CLA	1	504	-	1/1/10/20	5/8/86/115	-
44	CLA	f	810	-	1/1/15/20	10/37/115/115	-
44	CLA	B	828	-	1/1/10/20	3/8/86/115	-
50	LMG	2	519	-	-	14/31/51/70	0/1/1/1
44	CLA	B	817	-	1/1/11/20	7/18/96/115	-
44	CLA	3	312	-	1/1/10/20	5/8/86/115	-
44	CLA	e	806	-	1/1/10/20	1/8/86/115	-
44	CLA	2	505	-	-	11/22/100/115	-
44	CLA	A	826	-	1/1/14/20	13/31/109/115	-
44	CLA	B	819	-	1/1/10/20	0/8/86/115	-
44	CLA	L	303	-	1/1/12/20	12/22/100/115	-
51	LUT	p	501	-	-	2/29/67/67	0/2/2/2
44	CLA	1	507	12	1/1/13/20	6/27/105/115	-
44	CLA	B	814	-	1/1/10/20	5/8/86/115	-
44	CLA	B	807	2	1/1/15/20	11/37/115/115	-
44	CLA	A	822	-	1/1/10/20	2/8/86/115	-
44	CLA	L	302	-	1/1/9/20	1/8/82/115	-
44	CLA	f	827	-	1/1/9/20	1/8/82/115	-
47	BCR	3	305	-	-	8/29/63/63	0/2/2/2
44	CLA	f	841	-	1/1/10/20	3/8/86/115	-
44	CLA	e	826	-	1/1/15/20	18/37/113/115	-
44	CLA	f	834	-	1/1/10/20	3/11/89/115	-
50	LMG	5	301	-	-	8/27/47/70	0/1/1/1
44	CLA	r	317	-	1/1/12/20	7/19/97/115	-
51	LUT	r	302	-	-	2/29/67/67	0/2/2/2
50	LMG	r	318	-	-	11/11/28/70	0/1/1/1
47	BCR	A	846	-	-	7/29/63/63	0/2/2/2
44	CLA	f	839	-	1/1/10/20	4/8/86/115	-
47	BCR	F	804	-	-	2/29/63/63	0/2/2/2
52	CHL	p	514	-	3/3/16/26	7/17/115/137	-
47	BCR	f	845	-	-	7/29/63/63	0/2/2/2
44	CLA	B	827	-	1/1/10/20	3/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	LHG	A	844	44	-	11/34/34/53	-
44	CLA	3	309	-	-	4/10/86/115	-
44	CLA	B	803	-	1/1/15/20	16/37/115/115	-
50	LMG	2	518	-	-	3/7/27/70	0/1/1/1
44	CLA	f	840	-	1/1/10/20	4/8/86/115	-
44	CLA	A	819	-	1/1/9/20	3/8/82/115	-
44	CLA	f	826	-	1/1/15/20	11/37/115/115	-
44	CLA	p	507	12	1/1/10/20	4/8/84/115	-
44	CLA	e	837	-	1/1/13/20	11/25/103/115	-
44	CLA	s	505	-	-	9/15/93/115	-
44	CLA	r	310	-	1/1/10/20	3/10/88/115	-
52	CHL	2	515	-	3/3/16/26	6/15/111/137	-
44	CLA	A	835	-	1/1/12/20	12/21/99/115	-
46	LHG	f	852	44	-	13/42/42/53	-
44	CLA	3	311	-	1/1/12/20	8/19/97/115	-
47	BCR	5	302	-	-	9/29/63/63	0/2/2/2
44	CLA	j	802	-	1/1/10/20	2/8/86/115	-
44	CLA	f	801	-	1/1/15/20	13/37/113/115	-
44	CLA	3	313	-	1/1/11/20	10/17/95/115	-
44	CLA	e	814	-	1/1/10/20	5/10/88/115	-
47	BCR	f	847	-	-	6/29/63/63	0/2/2/2
44	CLA	3	317	-	1/1/10/20	4/8/86/115	-
44	CLA	q	310	-	1/1/10/20	3/8/86/115	-
44	CLA	A	811	-	1/1/9/20	2/8/82/115	-
44	CLA	A	813	-	1/1/11/20	9/13/91/115	-
44	CLA	B	832	-	1/1/10/20	3/11/89/115	-
44	CLA	L	304	-	1/1/11/20	6/13/91/115	-
44	CLA	5	312	-	1/1/11/20	7/15/93/115	-
47	BCR	e	846	-	-	4/29/63/63	0/2/2/2
44	CLA	B	804	-	1/1/15/20	14/37/115/115	-
44	CLA	e	815	-	1/1/11/20	7/13/91/115	-
53	XAT	2	502	-	-	6/31/93/93	0/4/4/4
44	CLA	m	101	-	1/1/10/20	6/10/86/115	-
47	BCR	j	801	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	A	804	44	1/1/12/20	5/22/100/115	-
44	CLA	5	305	-	1/1/9/20	1/8/80/115	-
44	CLA	3	316	-	1/1/8/20	0/2/76/115	-
44	CLA	B	830	-	1/1/13/20	11/27/105/115	-
46	LHG	p	516	-	-	12/53/53/53	-
47	BCR	B	845	-	-	6/29/63/63	0/2/2/2
44	CLA	m	102	-	1/1/10/20	4/10/88/115	-
44	CLA	A	830	-	1/1/12/20	3/19/97/115	-
44	CLA	B	802	-	1/1/14/20	6/35/113/115	-
44	CLA	s	506	-	1/1/15/20	19/37/115/115	-
50	LMG	m	105	-	-	5/25/45/70	0/1/1/1
47	BCR	A	848	-	-	6/29/63/63	0/2/2/2
44	CLA	3	306	-	1/1/13/20	14/23/99/115	-
52	CHL	5	314	-	3/3/16/26	7/17/115/137	-
47	BCR	1	503	-	-	4/11/28/63	0/1/1/2
44	CLA	5	306	-	1/1/10/20	2/6/84/115	-
44	CLA	n	201	-	1/1/8/20	0/2/76/115	-
47	BCR	A	845	-	-	6/29/63/63	0/2/2/2
44	CLA	r	308	-	1/1/10/20	4/8/86/115	-
44	CLA	r	311	-	1/1/11/20	4/15/93/115	-
52	CHL	1	514	-	3/3/14/26	4/10/104/137	-
47	BCR	j	803	-	-	2/29/63/63	0/2/2/2
44	CLA	B	841	-	1/1/12/20	8/24/102/115	-
44	CLA	2	511	-	1/1/9/20	1/8/82/115	-
44	CLA	f	831	-	1/1/13/20	5/27/105/115	-
44	CLA	A	834	1	1/1/10/20	4/8/86/115	-
44	CLA	s	504	-	1/1/10/20	3/8/84/115	-
44	CLA	n	203	-	1/1/10/20	4/8/86/115	-
44	CLA	B	815	-	1/1/15/20	7/37/115/115	-
44	CLA	o	304	-	1/1/11/20	6/13/91/115	-
44	CLA	1	506	-	1/1/13/20	9/25/103/115	-
44	CLA	1	513	-	-	19/37/115/115	-
44	CLA	q	315	-	-	8/13/91/115	-
47	BCR	A	847	-	-	2/29/63/63	0/2/2/2
44	CLA	B	808	-	1/1/12/20	7/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	1	510	46	1/1/11/20	7/15/93/115	-
44	CLA	e	836	-	1/1/12/20	6/21/99/115	-
52	CHL	5	317	-	3/3/14/26	4/8/102/137	-
51	LUT	1	502	-	-	4/29/67/67	0/2/2/2
44	CLA	e	834	-	1/1/11/20	5/13/91/115	-
44	CLA	e	803	44	1/1/12/20	5/22/100/115	-
44	CLA	e	824	-	1/1/13/20	9/27/105/115	-
47	BCR	m	103	-	-	2/29/63/63	0/2/2/2
51	LUT	q	301	-	-	6/29/67/67	0/2/2/2
44	CLA	B	818	-	1/1/13/20	16/30/108/115	-
47	BCR	f	848	-	-	0/29/63/63	0/2/2/2
44	CLA	r	305	-	1/1/12/20	6/19/97/115	-
52	CHL	3	315	-	3/3/15/26	3/12/110/137	-
44	CLA	5	307	15	1/1/15/20	17/37/115/115	-
48	SF4	C	102	3	-	-	0/6/5/5
46	LHG	A	843	-	-	13/53/53/53	-
44	CLA	s	510	-	1/1/14/20	11/31/109/115	-
44	CLA	A	808	1	1/1/15/20	8/37/115/115	-
44	CLA	5	316	-	1/1/10/20	2/8/86/115	-
44	CLA	e	840	-	1/1/10/20	1/8/86/115	-
44	CLA	B	839	-	1/1/11/20	5/16/94/115	-
44	CLA	B	812	-	1/1/13/20	6/25/101/115	-
44	CLA	f	829	-	1/1/12/20	9/19/97/115	-
44	CLA	e	811	-	1/1/10/20	4/8/86/115	-
47	BCR	B	847	-	-	5/29/63/63	0/2/2/2
44	CLA	A	814	-	1/1/10/20	1/10/88/115	-
44	CLA	q	305	-	1/1/12/20	7/22/100/115	-
44	CLA	2	506	-	1/1/15/20	16/37/115/115	-
45	PQN	B	843	-	-	7/20/40/43	0/2/2/2
48	SF4	f	802	-	-	-	0/6/5/5
44	CLA	f	803	-	1/1/10/20	3/10/88/115	-
44	CLA	f	814	-	1/1/10/20	4/11/89/115	-
44	CLA	B	840	-	1/1/10/20	1/8/86/115	-
47	BCR	e	854	-	-	4/29/63/63	0/2/2/2
44	CLA	B	811	-	1/1/13/20	12/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	3	310	-	1/1/11/20	4/13/91/115	-
44	CLA	A	815	-	1/1/11/20	4/13/91/115	-
44	CLA	q	314	-	1/1/9/20	2/8/82/115	-
44	CLA	e	807	-	1/1/10/20	2/10/88/115	-
44	CLA	B	820	-	1/1/12/20	5/23/101/115	-
44	CLA	A	840	-	1/1/10/20	2/8/86/115	-
44	CLA	e	816	-	1/1/14/20	11/31/109/115	-
44	CLA	B	831	-	1/1/10/20	1/11/89/115	-
44	CLA	2	510	46	1/1/14/20	16/31/109/115	-
44	CLA	f	823	-	1/1/10/20	2/8/86/115	-
44	CLA	r	306	-	1/1/15/20	16/37/115/115	-
43	CLO	A	801	-	3/3/18/25	5/33/125/135	-
44	CLA	B	821	-	1/1/12/20	5/19/97/115	-
52	CHL	s	517	42	3/3/16/26	3/17/115/137	-
44	CLA	5	313	15	1/1/9/20	2/8/82/115	-
54	SQD	Q	802	-	-	9/49/69/69	0/1/1/1
44	CLA	A	807	-	1/1/8/20	1/5/79/115	-
44	CLA	A	821	-	1/1/10/20	2/10/88/115	-
44	CLA	f	822	-	1/1/10/20	0/8/86/115	-
47	BCR	B	846	-	-	6/29/63/63	0/2/2/2
44	CLA	l	511	-	1/1/11/20	5/15/93/115	-
44	CLA	f	817	-	1/1/10/20	5/11/89/115	-
44	CLA	f	842	-	1/1/10/20	0/8/86/115	-
44	CLA	s	507	-	1/1/10/20	2/8/86/115	-
44	CLA	p	506	-	1/1/13/20	10/25/103/115	-
44	CLA	p	513	-	1/1/12/20	5/22/100/115	-
44	CLA	B	813	-	1/1/10/20	3/11/89/115	-
47	BCR	o	301	-	-	2/29/63/63	0/2/2/2
44	CLA	f	835	-	1/1/11/20	8/13/91/115	-
47	BCR	o	305	-	-	2/29/63/63	0/2/2/2
44	CLA	5	309	-	1/1/11/20	5/13/91/115	-
44	CLA	p	515	-	1/1/9/20	3/8/82/115	-
44	CLA	B	805	-	1/1/10/20	2/8/86/115	-
44	CLA	p	510	-	1/1/11/20	7/15/93/115	-
44	CLA	f	815	-	1/1/10/20	4/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	B	842	-	1/1/13/20	15/28/106/115	-
44	CLA	e	839	-	1/1/15/20	16/37/115/115	-
44	CLA	r	304	-	1/1/9/20	3/8/80/115	-
46	LHG	2	517	44	-	5/39/39/53	-
44	CLA	3	308	-	1/1/13/20	14/25/103/115	-
44	CLA	3	318	-	1/1/11/20	6/15/91/115	-
52	CHL	p	512	-	3/3/16/26	3/17/115/137	-
44	CLA	A	827	-	1/1/15/20	17/37/115/115	-
44	CLA	A	839	-	1/1/10/20	3/10/88/115	-
44	CLA	o	303	-	1/1/14/20	12/31/109/115	-
51	LUT	p	502	-	1/1/12/27	9/29/67/67	0/2/2/2
44	CLA	A	836	-	1/1/13/20	11/25/103/115	-
44	CLA	B	823	-	1/1/10/20	4/10/88/115	-
44	CLA	e	820	-	1/1/10/20	3/8/86/115	-
44	CLA	e	838	-	1/1/12/20	4/22/100/115	-
53	XAT	s	502	-	-	6/31/93/93	0/4/4/4
44	CLA	r	307	-	1/1/14/20	12/31/109/115	-
44	CLA	3	314	14	1/1/14/20	15/31/109/115	-
49	DGD	f	851	-	-	9/41/81/95	0/2/2/2
44	CLA	3	307	-	1/1/9/20	3/8/82/115	-
47	BCR	B	852	-	-	6/29/63/63	0/2/2/2
44	CLA	f	824	-	1/1/10/20	4/10/88/115	-
48	SF4	C	101	3	-	-	0/6/5/5
47	BCR	f	849	-	-	0/29/63/63	0/2/2/2
44	CLA	s	514	-	1/1/9/20	2/8/82/115	-
44	CLA	e	830	-	1/1/12/20	6/19/97/115	-
44	CLA	f	806	-	1/1/10/20	2/8/86/115	-
44	CLA	q	307	14	-	3/8/82/115	-
44	CLA	B	801	-	1/1/15/20	9/37/115/115	-
44	CLA	e	802	-	1/1/9/20	4/8/82/115	-
44	CLA	e	852	-	1/1/13/20	9/28/106/115	-
50	LMG	F	806	-	-	18/40/60/70	0/1/1/1
51	LUT	q	302	-	-	6/29/67/67	0/2/2/2
44	CLA	e	821	-	1/1/10/20	5/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	CL0	e	801	-	3/3/18/25	5/33/125/135	-
48	SF4	8	201	38	-	-	0/6/5/5
47	BCR	r	301	-	-	6/29/63/63	0/2/2/2
44	CLA	5	310	-	1/1/12/20	10/19/97/115	-
44	CLA	f	837	-	1/1/10/20	3/10/88/115	-
44	CLA	B	825	-	1/1/10/20	3/10/88/115	-
44	CLA	B	826	-	1/1/14/20	8/34/112/115	-
44	CLA	e	805	-	1/1/11/20	4/15/93/115	-
44	CLA	A	802	-	1/1/13/20	12/29/107/115	-
49	DGD	m	104	-	-	14/55/95/95	0/2/2/2
47	BCR	Q	801	-	-	10/27/61/63	0/2/2/2
44	CLA	A	825	-	1/1/13/20	8/30/108/115	-
44	CLA	f	833	-	1/1/10/20	3/11/89/115	-
47	BCR	e	851	-	-	4/29/63/63	0/2/2/2
44	CLA	e	843	-	1/1/12/20	9/19/95/115	-
44	CLA	5	311	-	1/1/10/20	4/10/88/115	-
44	CLA	e	813	-	1/1/10/20	4/10/88/115	-
44	CLA	f	828	-	1/1/10/20	4/8/86/115	-
44	CLA	s	509	-	1/1/12/20	6/19/97/115	-
54	SQD	Q	803	-	-	9/41/61/69	0/1/1/1
49	DGD	B	850	-	-	19/48/88/95	0/2/2/2
44	CLA	f	838	-	1/1/9/20	5/8/82/115	-
44	CLA	A	816	-	1/1/13/20	12/29/107/115	-
44	CLA	l	505	-	1/1/10/20	3/10/88/115	-
47	BCR	l	102	-	-	8/29/63/63	0/2/2/2
44	CLA	A	832	-	1/1/10/20	5/11/89/115	-
49	DGD	J	103	-	-	26/55/95/95	0/2/2/2
50	LMG	F	805	-	-	4/25/45/70	0/1/1/1
47	BCR	A	853	-	-	2/29/63/63	0/2/2/2
44	CLA	B	836	-	-	4/10/88/115	-
45	PQN	e	842	-	-	-	0/2/2/2
44	CLA	K	205	10	1/1/9/20	0/6/80/115	-
44	CLA	B	829	-	1/1/9/20	2/8/82/115	-
52	CHL	l	517	12	3/3/14/26	5/10/104/137	-
44	CLA	K	202	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	e	853	-	1/1/11/20	8/13/91/115	-
44	CLA	q	311	-	1/1/11/20	8/17/95/115	-
44	CLA	B	837	-	1/1/12/20	5/19/97/115	-
44	CLA	r	315	41	1/1/10/20	2/8/86/115	-
44	CLA	A	824	-	1/1/9/20	5/8/82/115	-
46	LHG	s	516	-	-	6/39/39/53	-
44	CLA	f	807	-	1/1/10/20	2/8/86/115	-
44	CLA	l	509	-	-	6/19/97/115	-
44	CLA	e	825	-	1/1/10/20	0/8/86/115	-
52	CHL	2	513	-	3/3/13/26	5/10/100/137	-
47	BCR	f	846	-	-	7/29/63/63	0/2/2/2
44	CLA	2	507	13	2/2/11/20	5/14/88/115	-
44	CLA	A	820	-	1/1/13/20	10/28/106/115	-
51	LUT	l	501	-	-	2/29/67/67	0/2/2/2
44	CLA	A	838	-	1/1/15/20	15/37/115/115	-
47	BCR	L	305	-	-	9/29/63/63	0/2/2/2
44	CLA	q	308	-	1/1/10/20	5/10/88/115	-
47	BCR	B	844	-	-	4/29/63/63	0/2/2/2
44	CLA	f	805	-	1/1/8/20	0/2/78/115	-
44	CLA	e	831	-	1/1/13/20	7/27/105/115	-
52	CHL	s	513	-	3/3/16/26	5/18/116/137	-
44	CLA	B	824	-	1/1/11/20	6/13/91/115	-
44	CLA	B	809	-	1/1/9/20	2/8/82/115	-
44	CLA	n	202	-	1/1/11/20	8/13/91/115	-
51	LUT	s	501	-	-	4/29/67/67	0/2/2/2
44	CLA	A	828	-	1/1/10/20	2/8/86/115	-
52	CHL	p	517	-	3/3/15/26	5/12/110/137	-
46	LHG	l	516	44	-	23/53/53/53	-
44	CLA	A	812	-	1/1/10/20	3/10/88/115	-
44	CLA	A	809	1	1/1/9/20	1/4/84/115	-
44	CLA	e	832	-	1/1/10/20	6/11/89/115	-
44	CLA	J	101	9	1/1/10/20	7/10/88/115	-
51	LUT	3	304	-	-	2/29/67/67	0/2/2/2
47	BCR	K	204	-	-	8/29/63/63	0/2/2/2
44	CLA	A	852	-	1/1/13/20	9/28/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	CHL	r	316	-	3/3/15/26	3/12/110/137	-
44	CLA	B	838	-	1/1/15/20	4/37/115/115	-
44	CLA	e	804	-	1/1/15/20	16/37/115/115	-
44	CLA	f	836	-	1/1/12/20	11/29/103/115	-
44	CLA	B	816	-	1/1/10/20	4/11/89/115	-
45	PQN	A	841	-	-	13/23/43/43	0/2/2/2
44	CLA	1	508	-	1/1/9/20	3/8/82/115	-
44	CLA	2	514	-	1/1/13/20	8/25/103/115	-
47	BCR	l	101	-	-	6/29/63/63	0/2/2/2
44	CLA	A	805	-	1/1/14/20	18/36/114/115	-
47	BCR	B	848	-	-	2/29/63/63	0/2/2/2
44	CLA	p	505	-	-	5/15/93/115	-
44	CLA	e	808	1	1/1/10/20	4/8/86/115	-
47	BCR	2	503	-	-	8/29/63/63	0/2/2/2
44	CLA	f	820	-	1/1/12/20	11/19/97/115	-
47	BCR	A	849	-	-	2/27/61/63	0/2/2/2
51	LUT	3	303	-	-	2/29/67/67	0/2/2/2
44	CLA	n	205	-	1/1/9/20	0/6/80/115	-
44	CLA	f	819	-	1/1/10/20	2/8/86/115	-
47	BCR	p	503	-	-	1/1/19/63	0/1/1/2
44	CLA	2	504	13	1/1/7/20	0/2/73/115	-
44	CLA	e	810	44	1/1/13/20	10/25/103/115	-
52	CHL	2	516	13	3/3/15/26	8/13/109/137	-
44	CLA	K	203	-	1/1/9/20	5/8/82/115	-
47	BCR	s	503	-	-	7/29/63/63	0/2/2/2
44	CLA	e	818	-	1/1/9/20	4/6/80/115	-
44	CLA	f	825	-	1/1/10/20	3/10/88/115	-
44	CLA	o	302	-	1/1/10/20	2/8/84/115	-
44	CLA	B	822	-	1/1/11/20	4/16/94/115	-
47	BCR	e	850	-	-	6/29/63/63	0/2/2/2
53	XAT	r	303	-	-	2/31/93/93	0/4/4/4
44	CLA	e	823	-	1/1/10/20	3/11/87/115	-
44	CLA	f	832	-	1/1/9/20	2/8/82/115	-
44	CLA	L	301	-	1/1/13/20	5/27/105/115	-
44	CLA	e	841	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	e	829	-	1/1/13/20	13/29/107/115	-
44	CLA	p	504	-	1/1/10/20	5/8/86/115	-
44	CLA	A	803	-	1/1/10/20	0/8/86/115	-
47	BCR	q	303	-	-	7/29/63/63	0/2/2/2
52	CHL	r	314	-	3/3/17/26	4/21/119/137	-
44	CLA	A	823	-	1/1/12/20	13/25/99/115	-
44	CLA	e	817	-	1/1/9/20	0/2/82/115	-
44	CLA	2	508	-	1/1/11/20	2/15/93/115	-
47	BCR	n	204	-	-	9/29/63/63	0/2/2/2
52	CHL	r	313	-	3/3/16/26	5/17/115/137	-
44	CLA	q	316	-	1/1/11/20	7/15/93/115	-
44	CLA	f	830	-	1/1/9/20	3/8/80/115	-

The worst 5 of 2637 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	p	502	LUT	C24-C25	14.61	1.51	1.33
44	q	304	CLA	C3B-C4B	9.98	1.49	1.43
44	s	504	CLA	C3B-C4B	8.58	1.49	1.39
44	q	304	CLA	C2B-C1B	8.49	1.49	1.39
44	f	804	CLA	CHB-C4A	8.43	1.41	1.34

The worst 5 of 3924 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	2	503	BCR	C40-C30-C25	-12.70	89.71	110.30
47	s	503	BCR	C40-C30-C25	-12.39	90.20	110.30
43	A	801	CL0	C4A-NA-C1A	10.86	111.59	106.71
43	e	801	CL0	C4A-NA-C1A	10.83	111.58	106.71
47	Q	801	BCR	C11-C10-C9	-10.58	112.21	127.31

5 of 341 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
43	A	801	CL0	ND
43	A	801	CL0	NA
43	A	801	CL0	NC
43	e	801	CL0	ND
43	e	801	CL0	NA



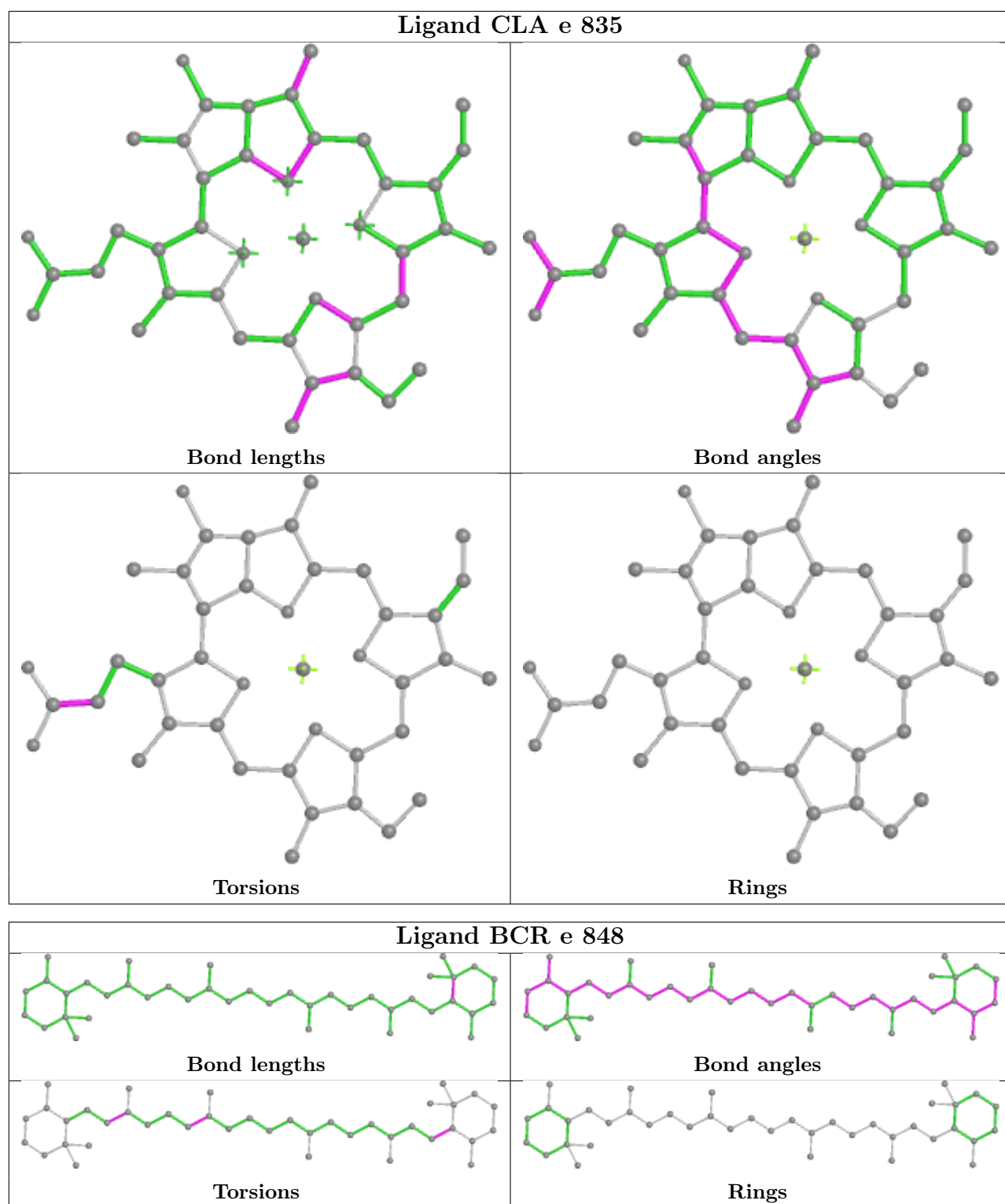
5 of 2327 torsion outliers are listed below:

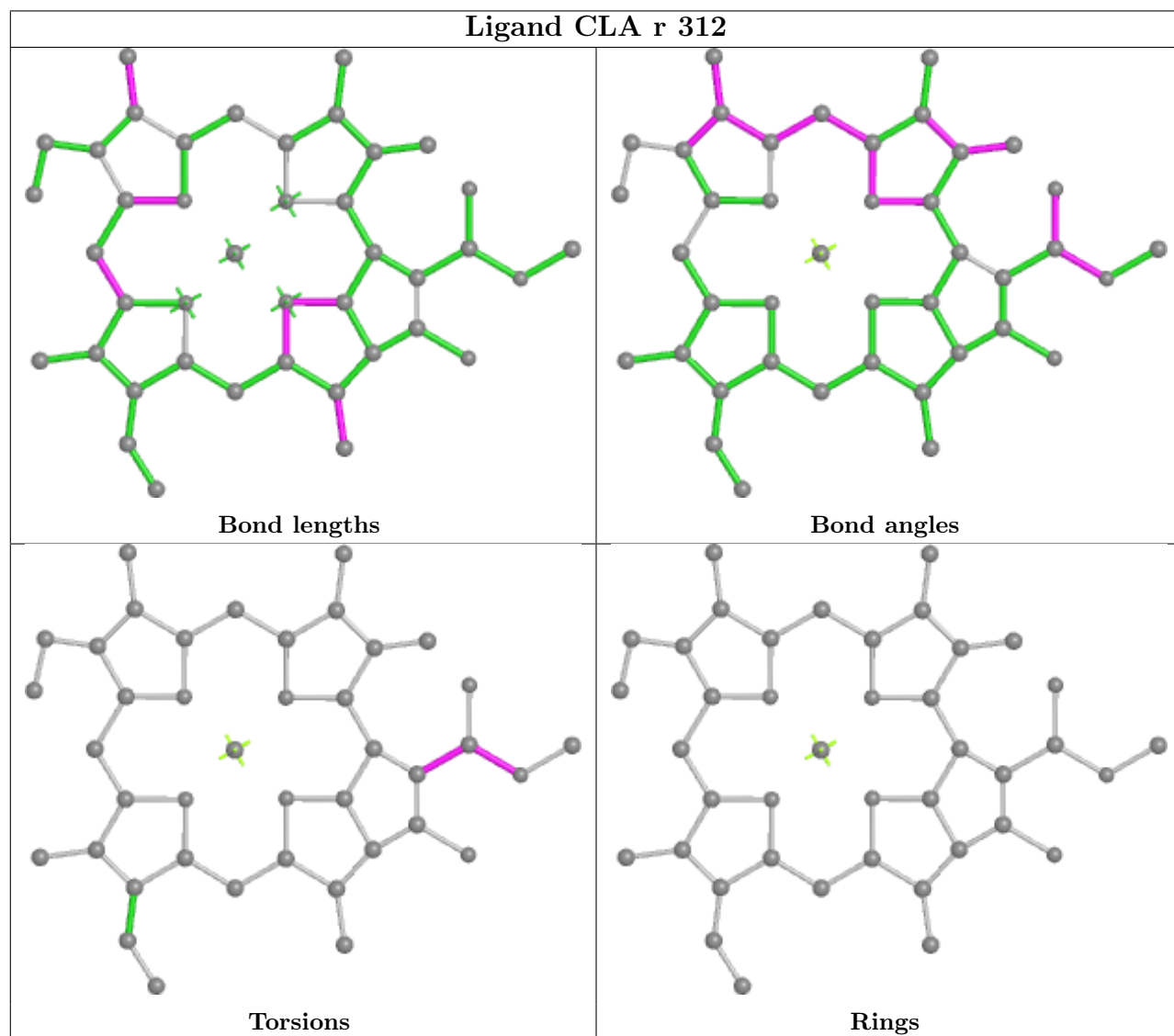
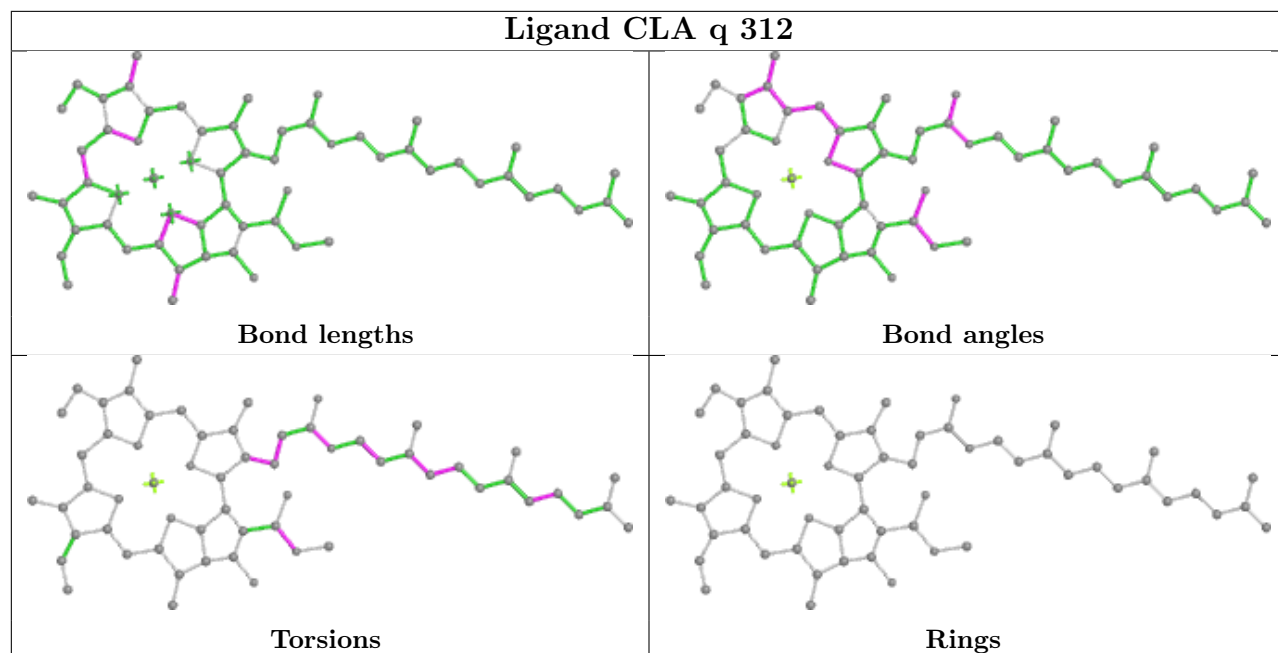
Mol	Chain	Res	Type	Atoms
43	A	801	CL0	C1A-C2A-CAA-CBA
43	A	801	CL0	CHA-CBD-CGD-O2D
43	e	801	CL0	C1A-C2A-CAA-CBA
43	e	801	CL0	CHA-CBD-CGD-O2D
44	A	802	CLA	CHA-CBD-CGD-O1D

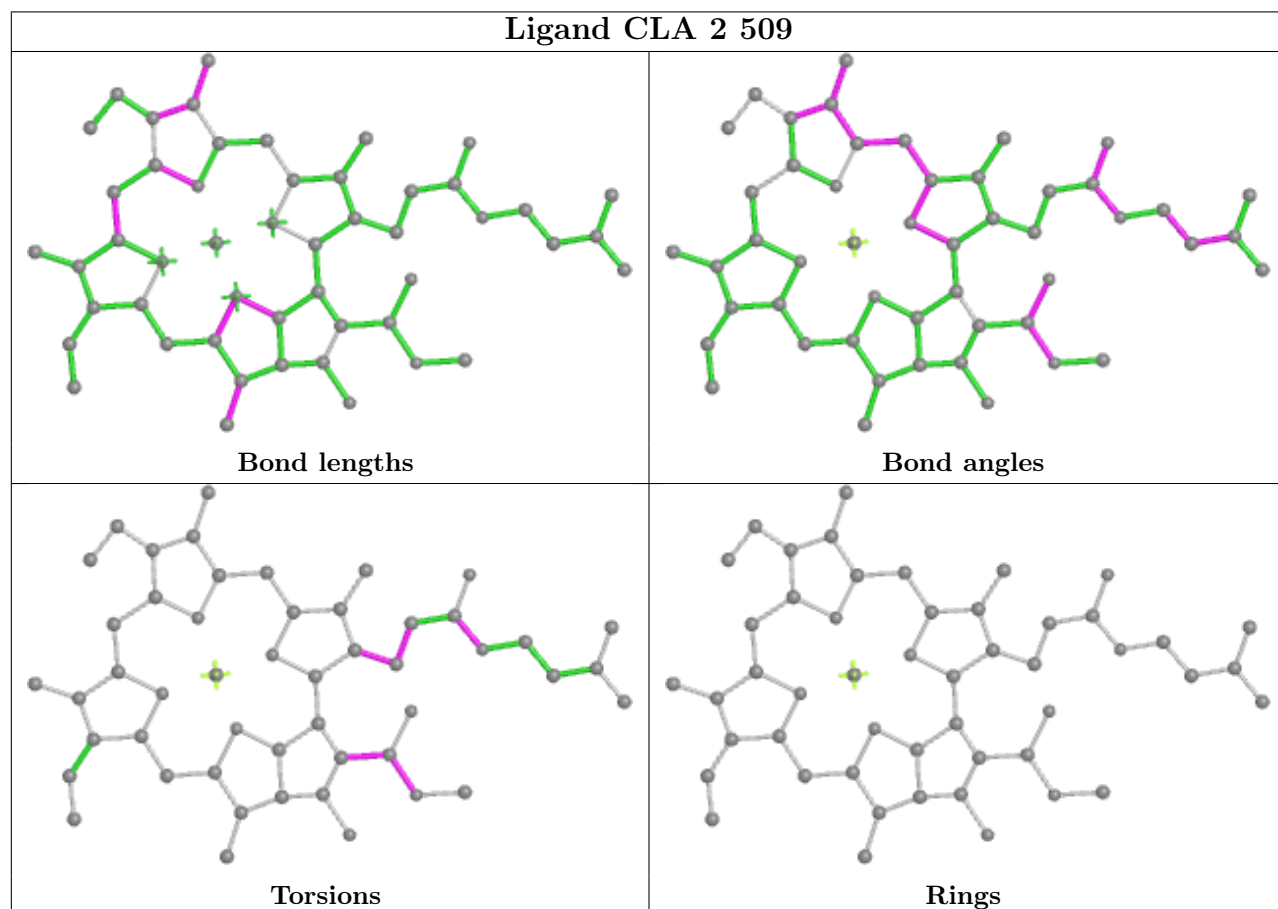
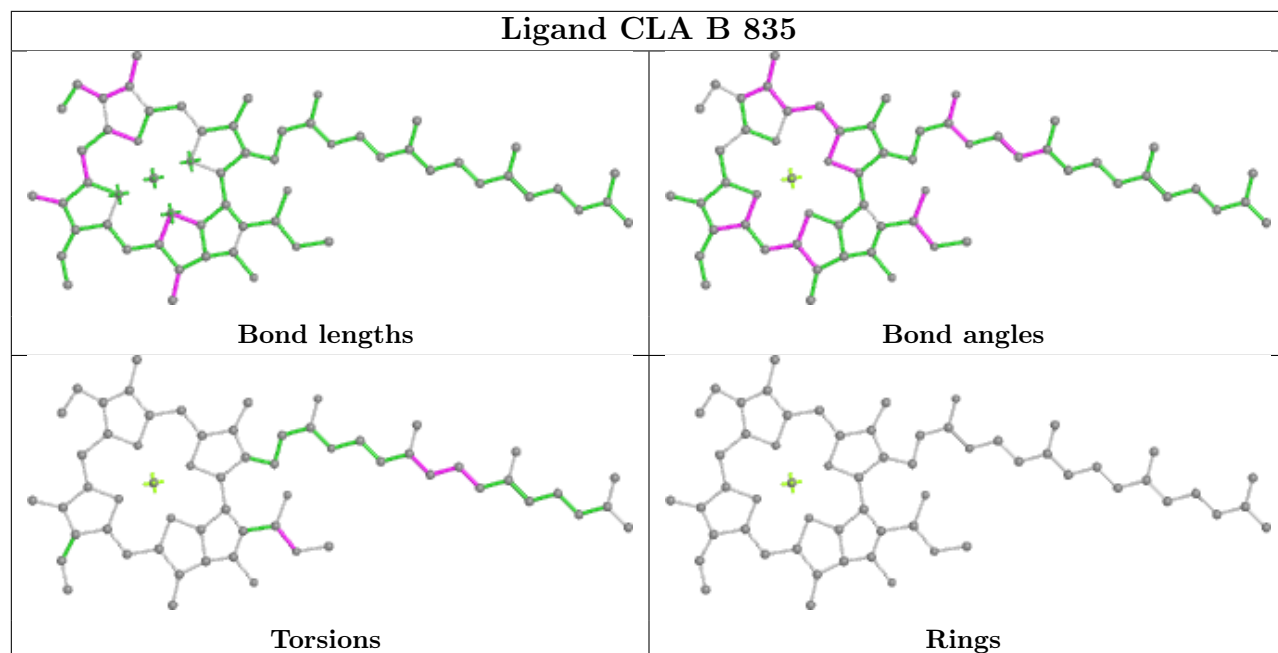
There are no ring outliers.

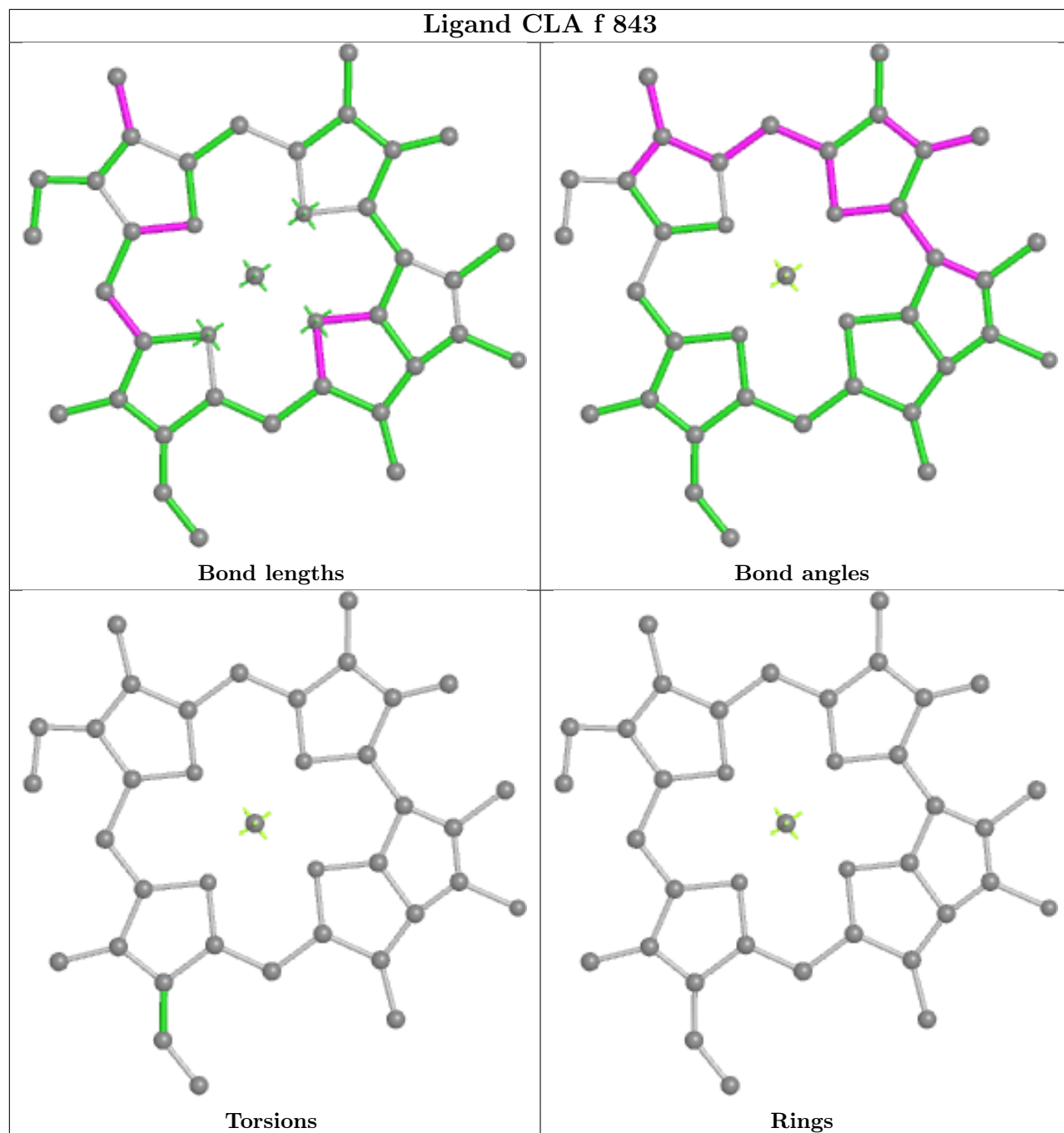
No monomer is involved in short contacts.

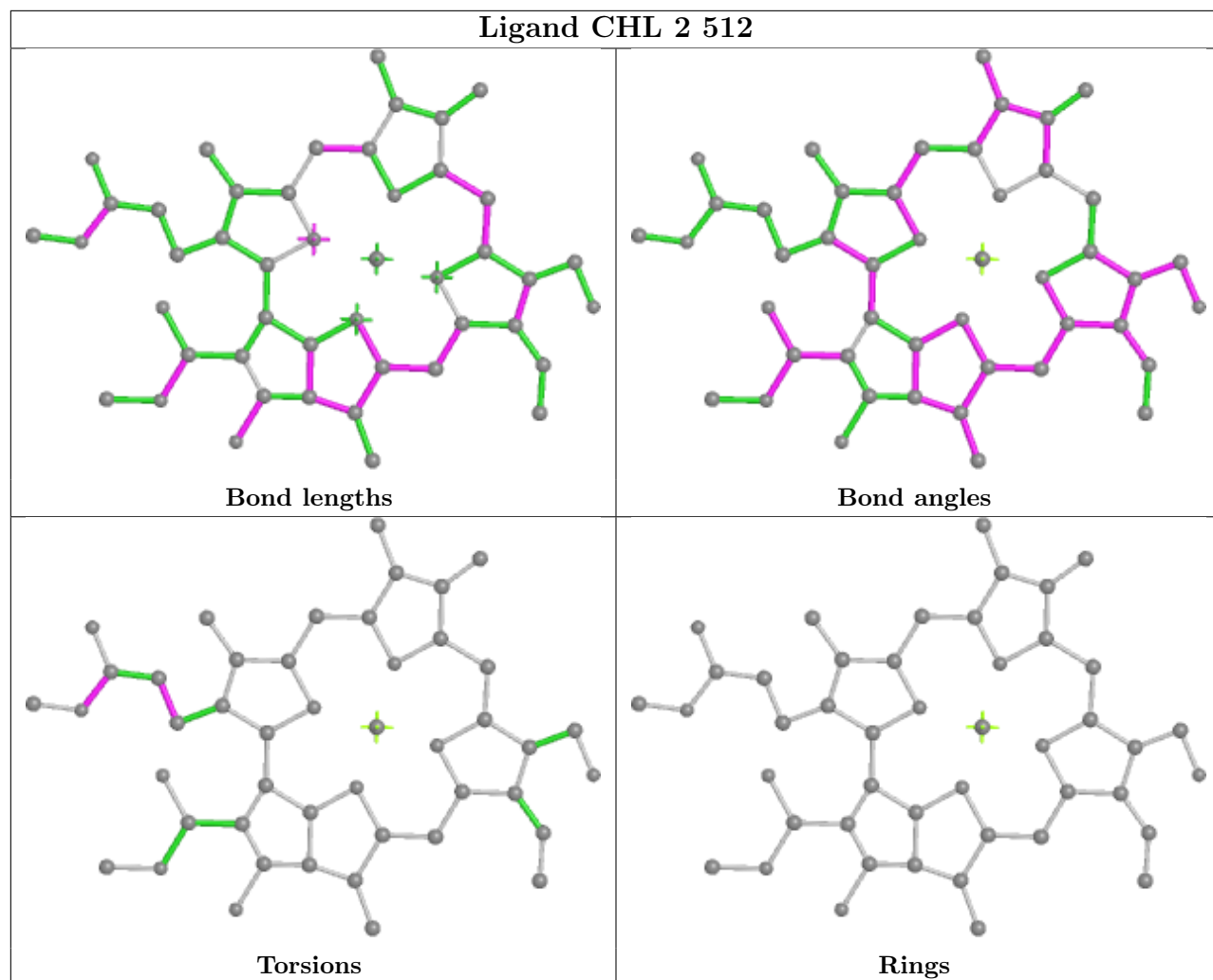
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

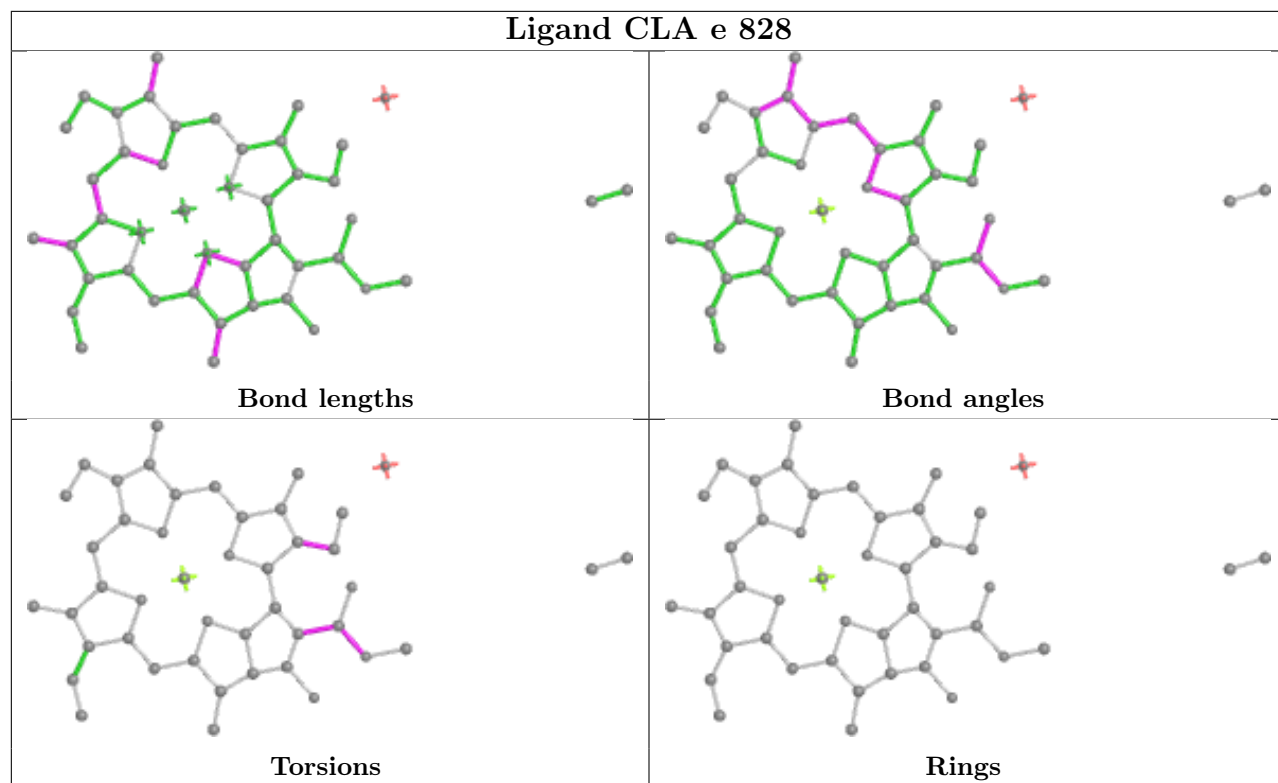


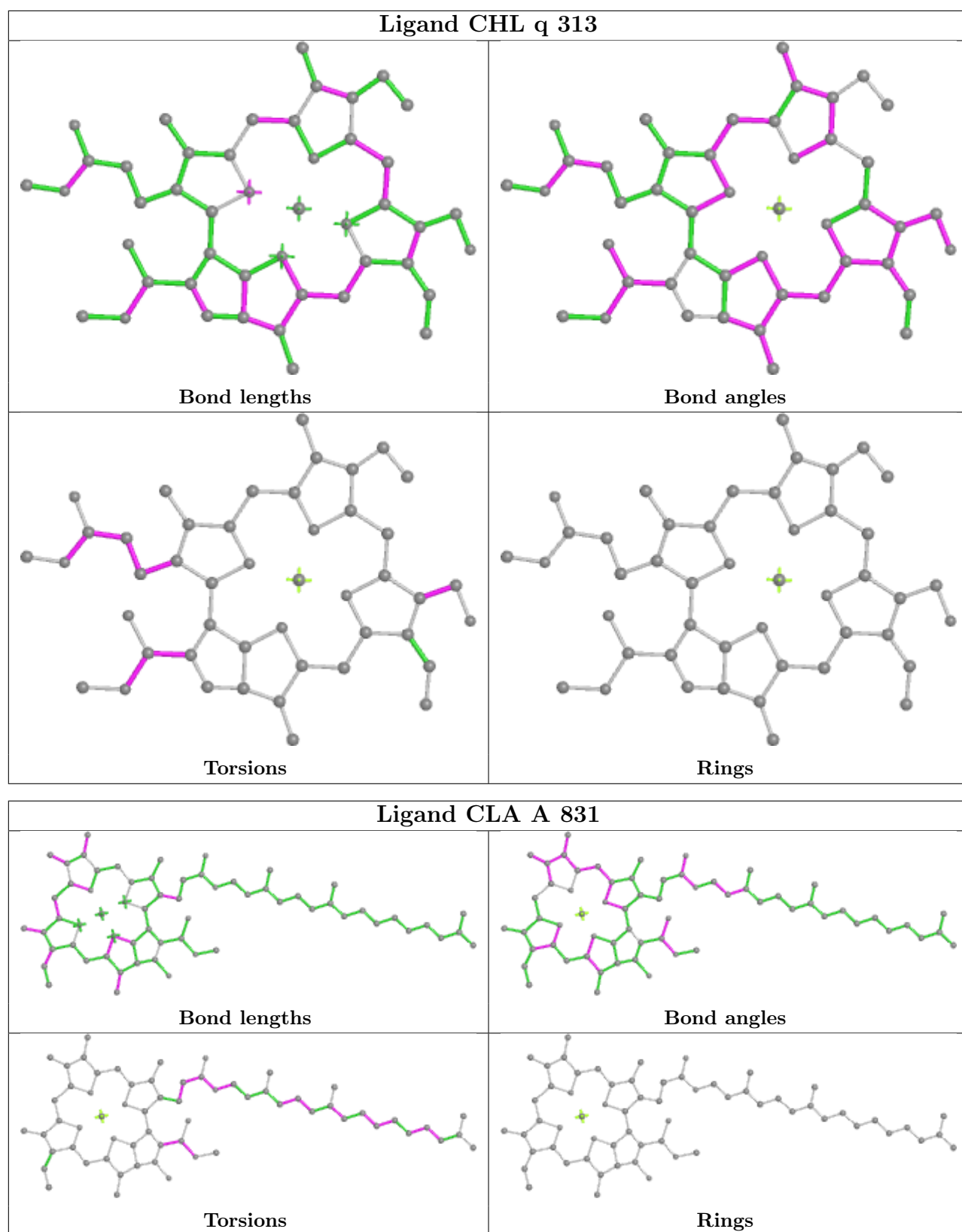




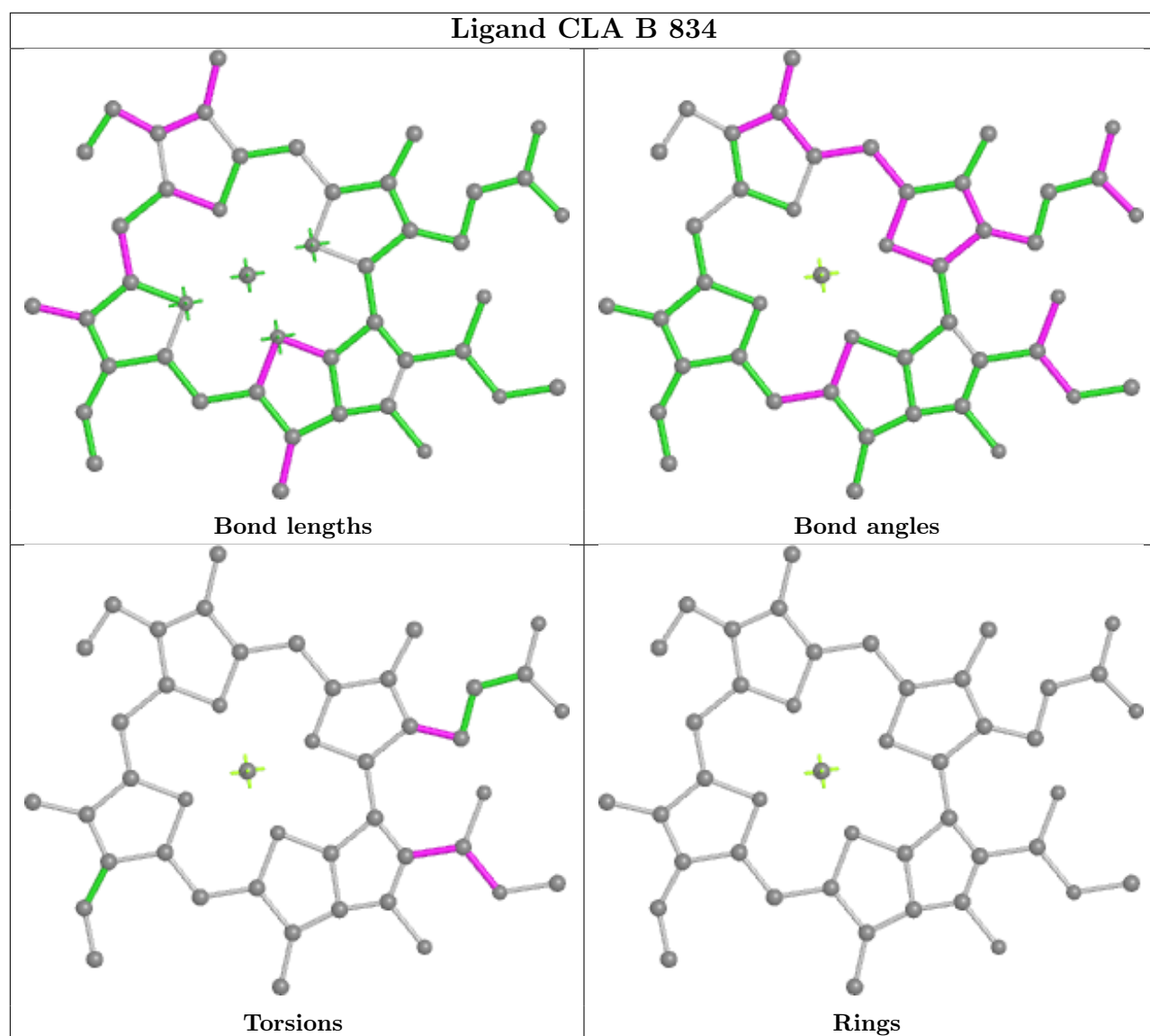


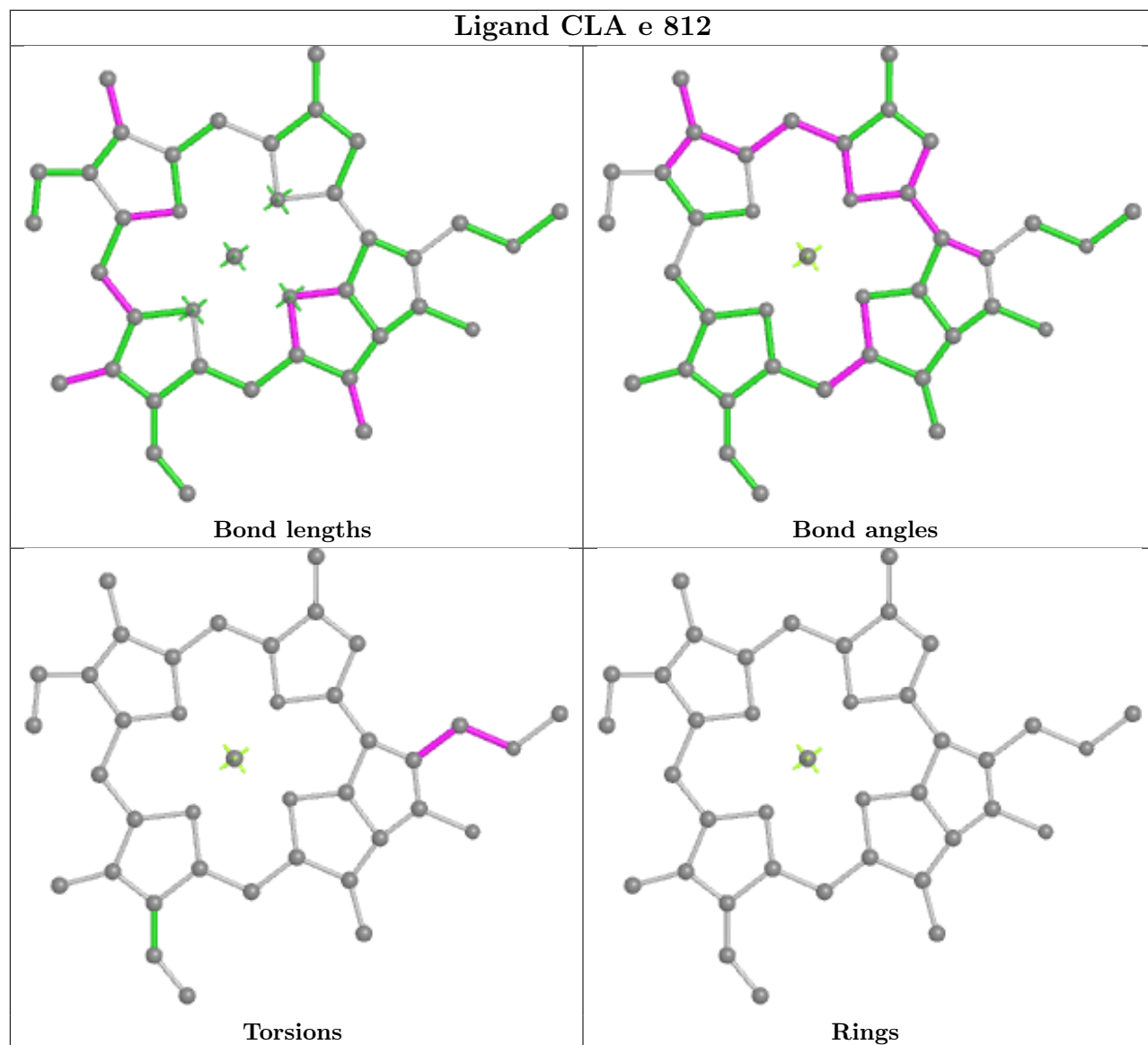


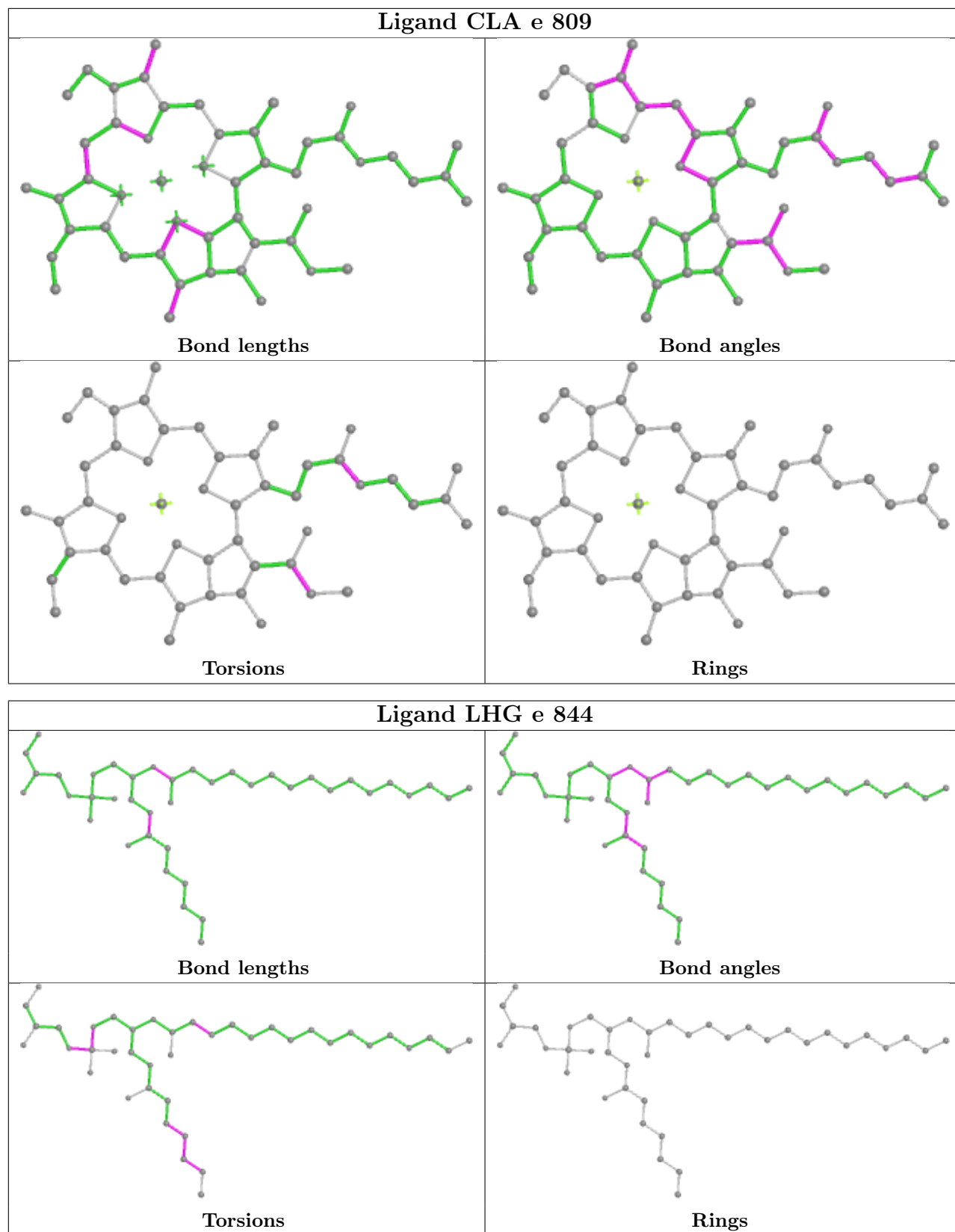


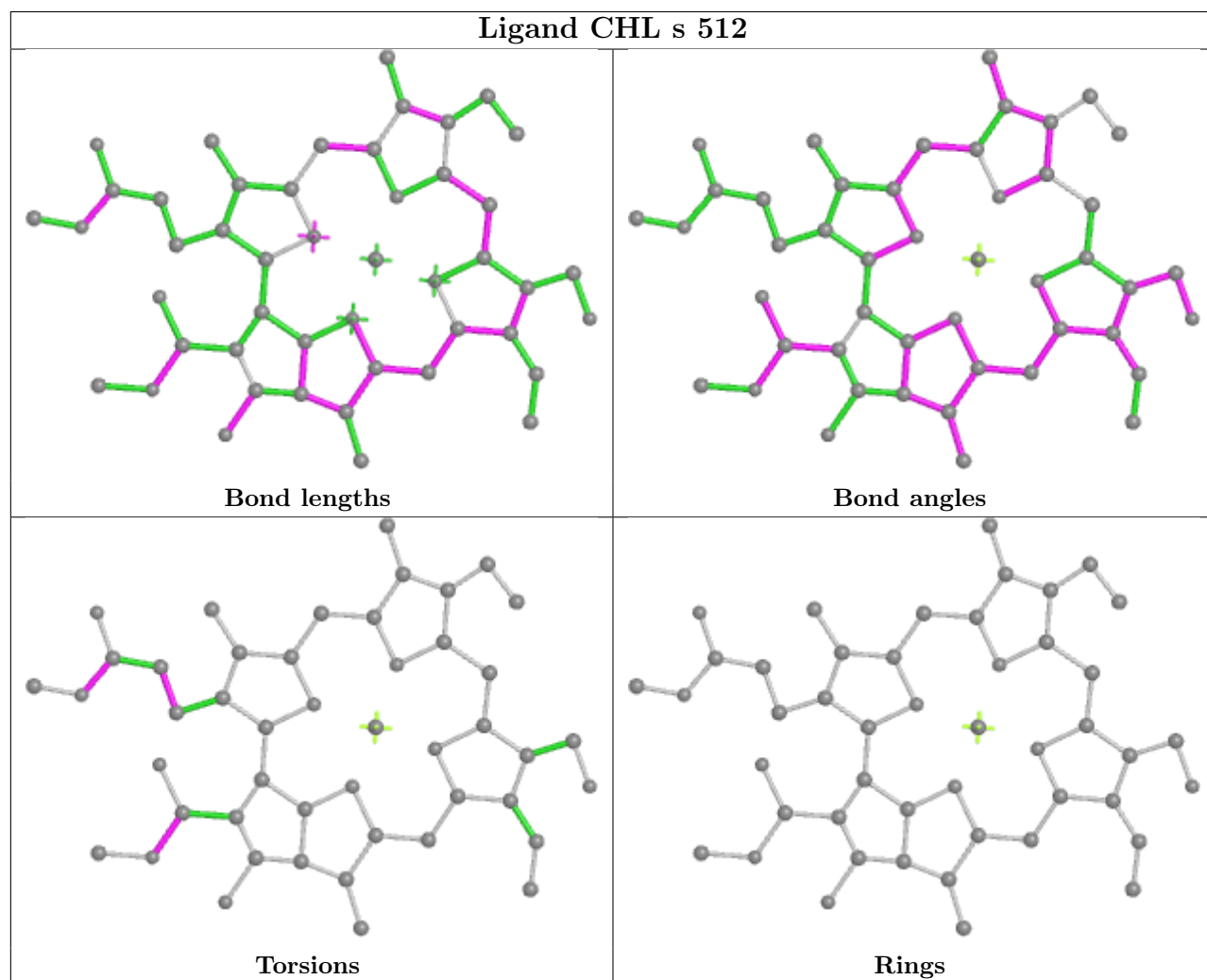
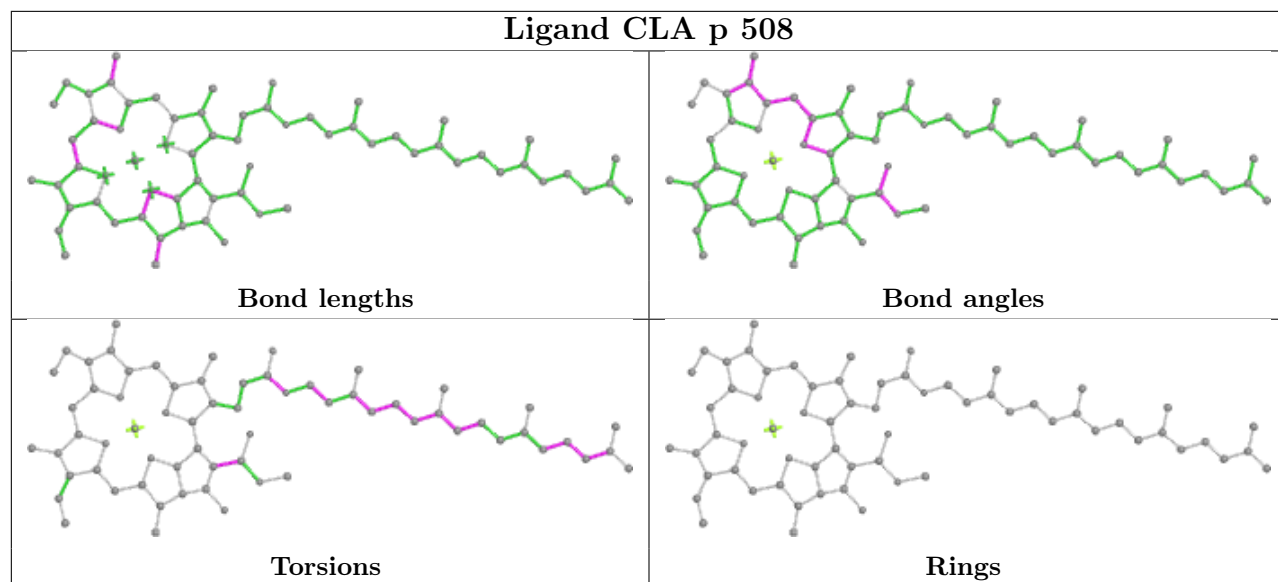


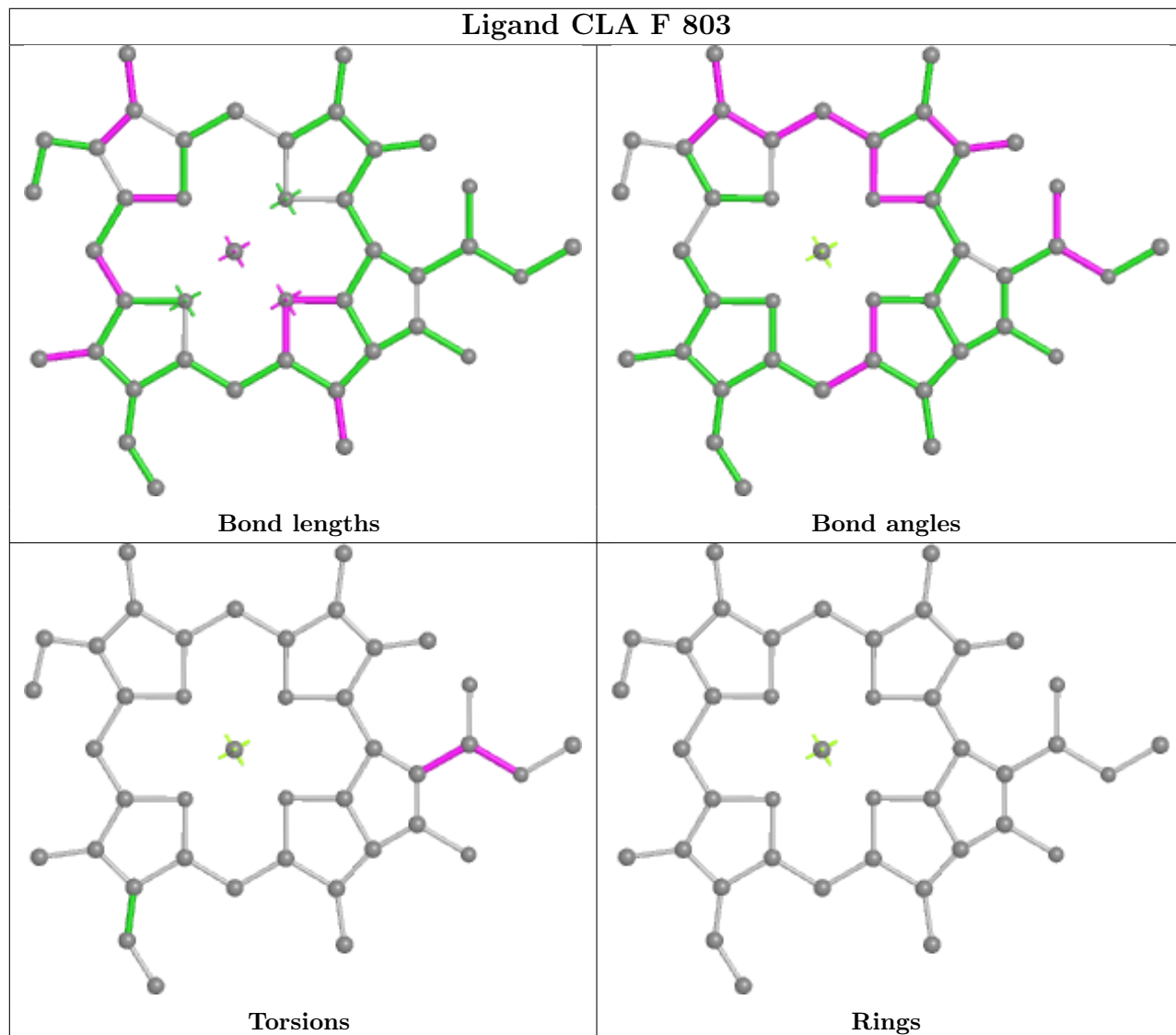
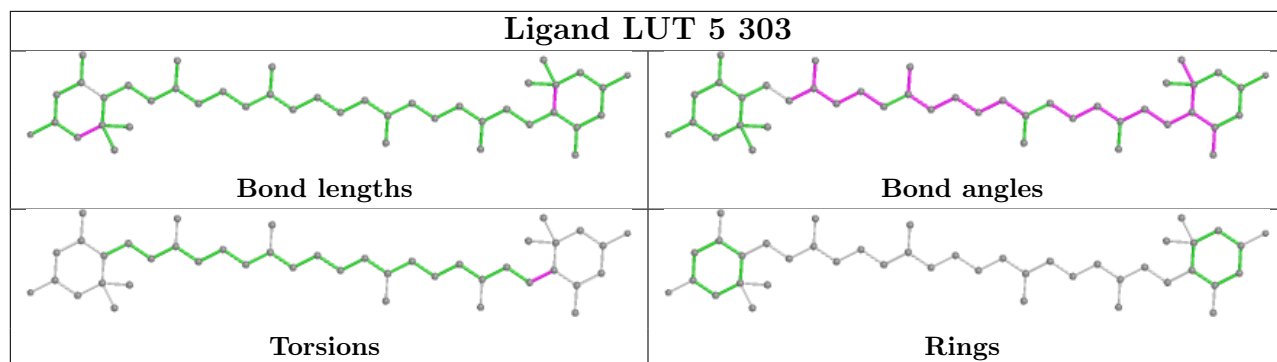


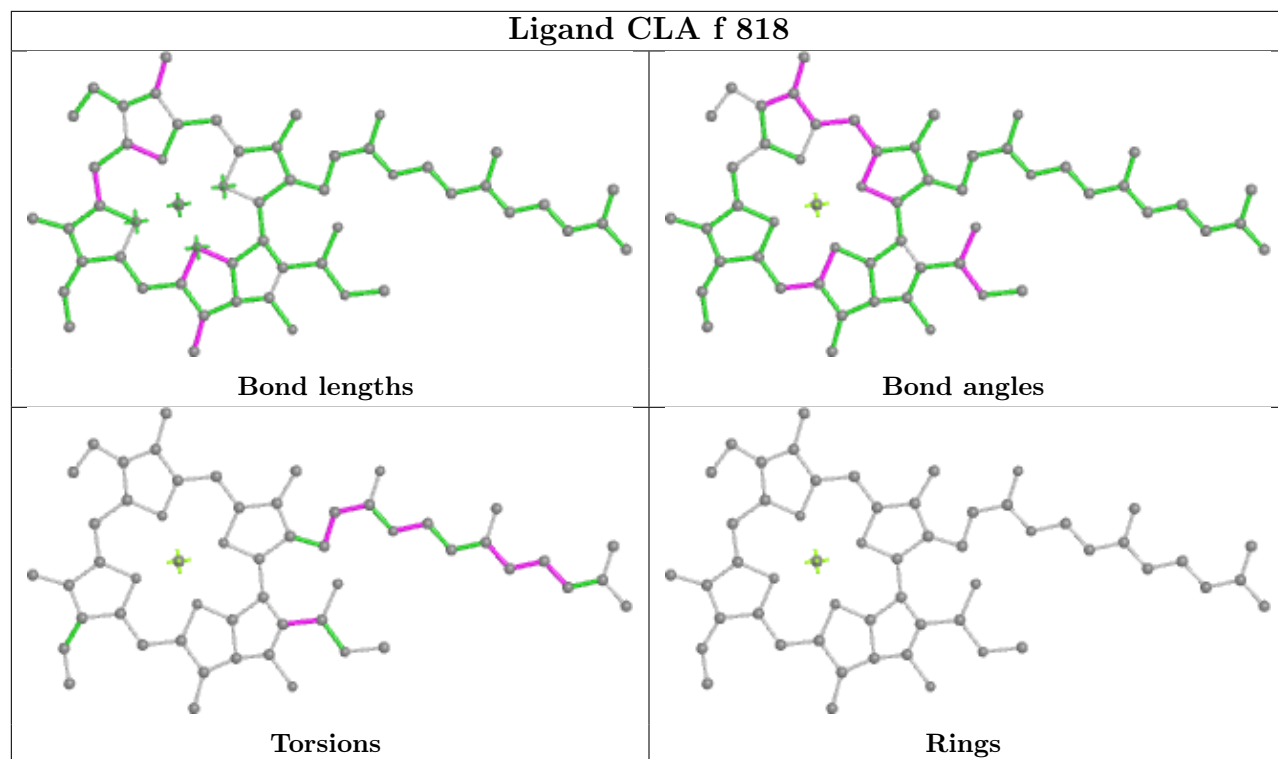


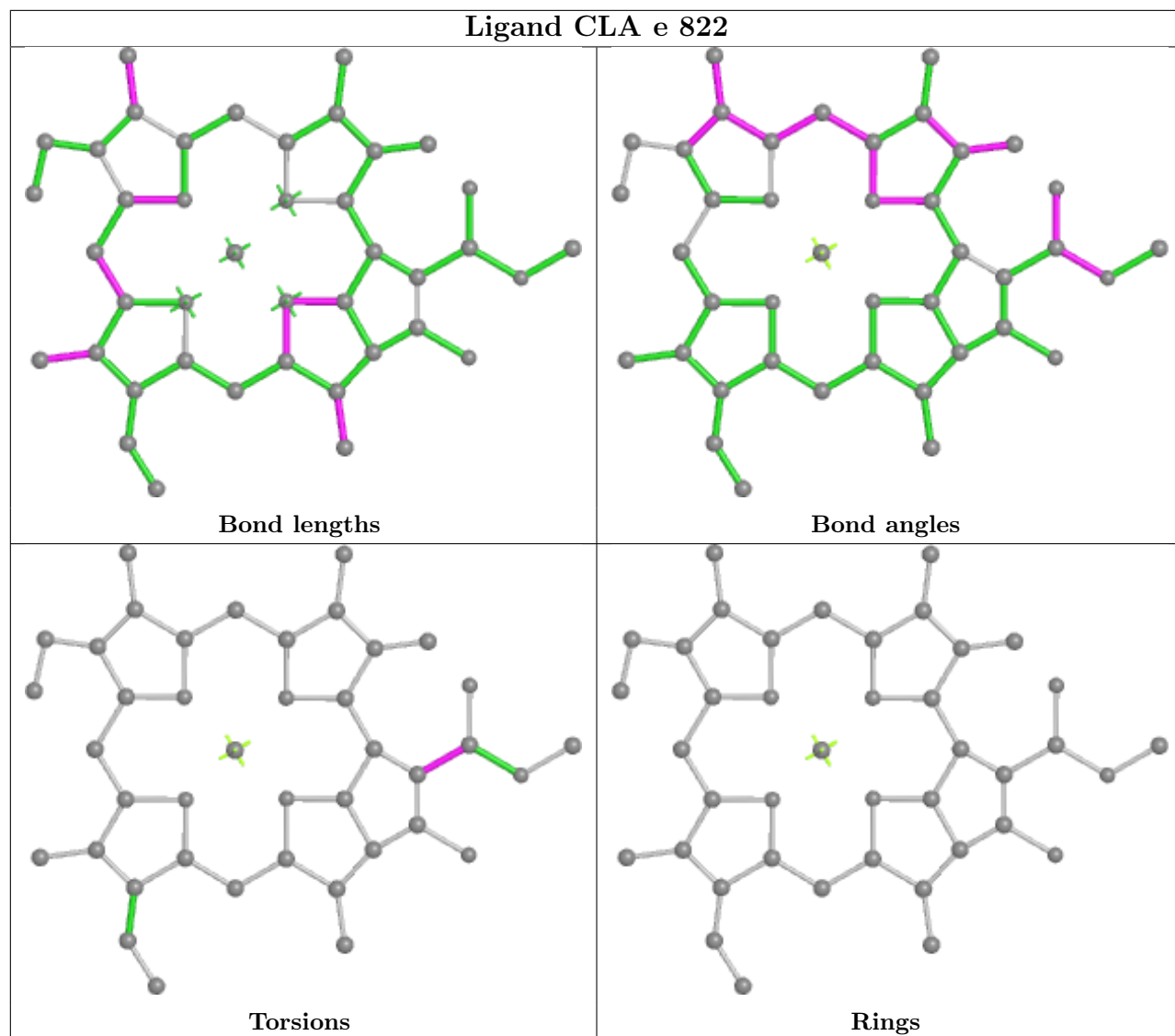


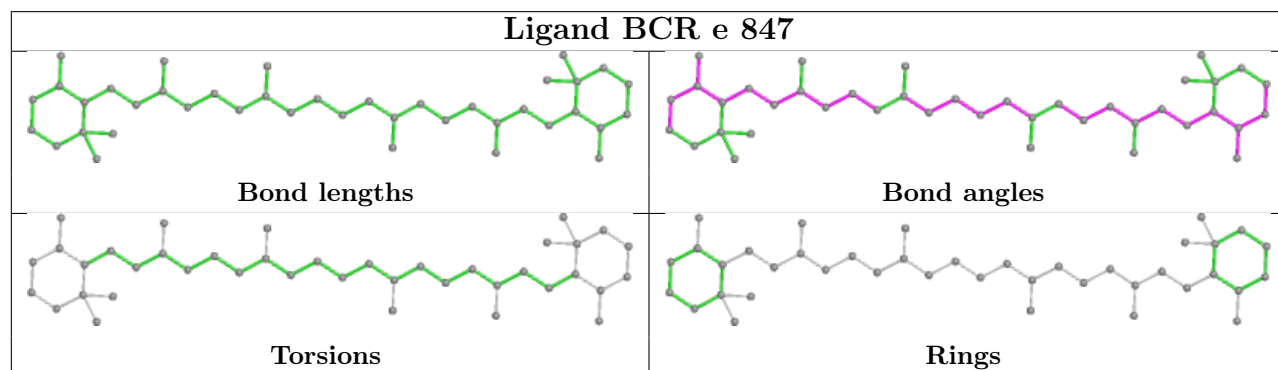
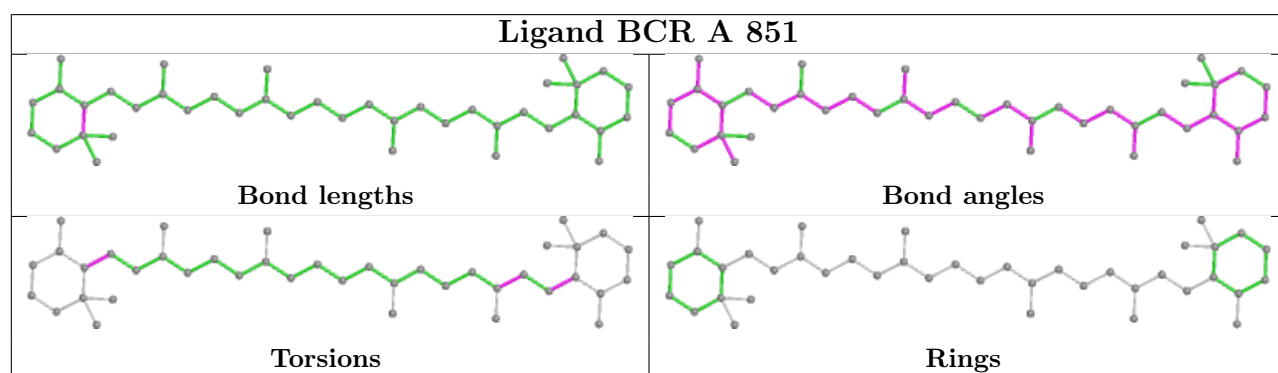
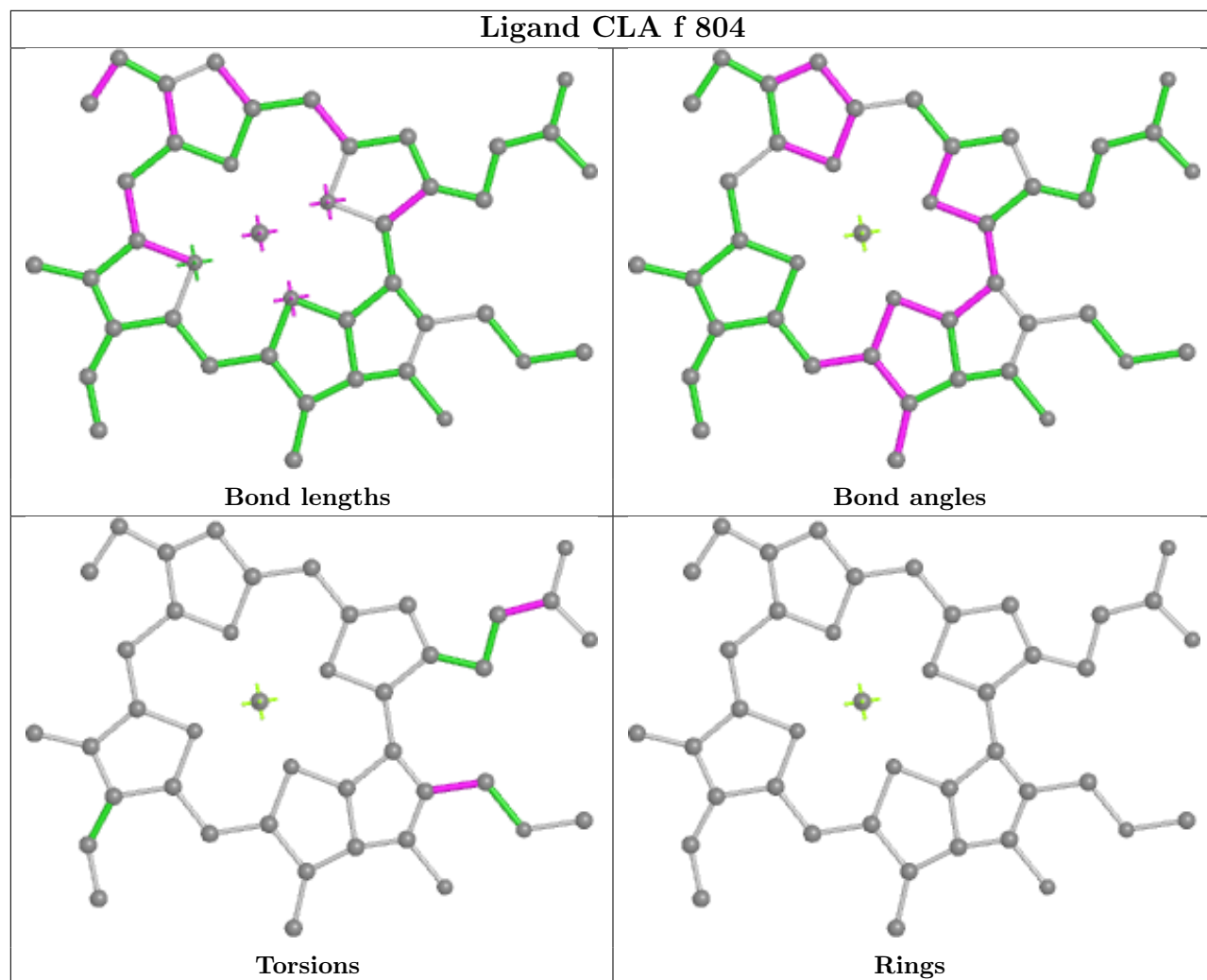




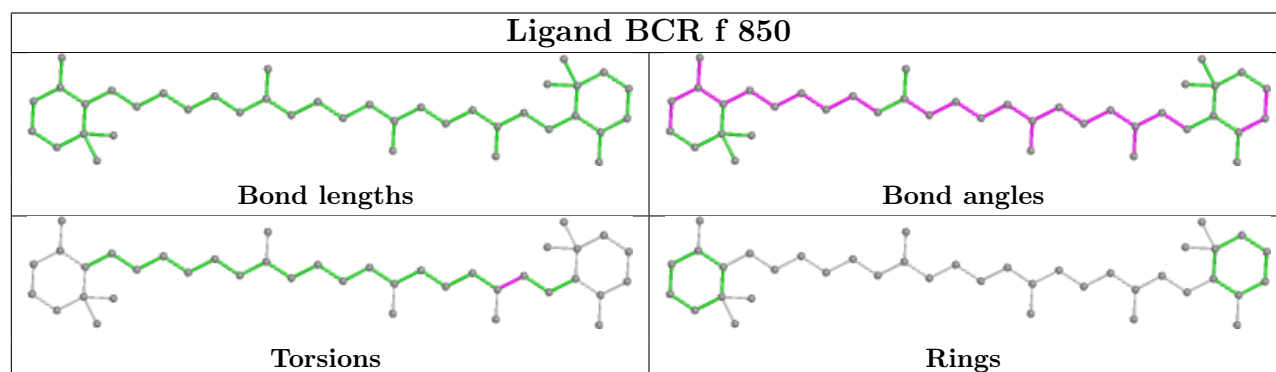
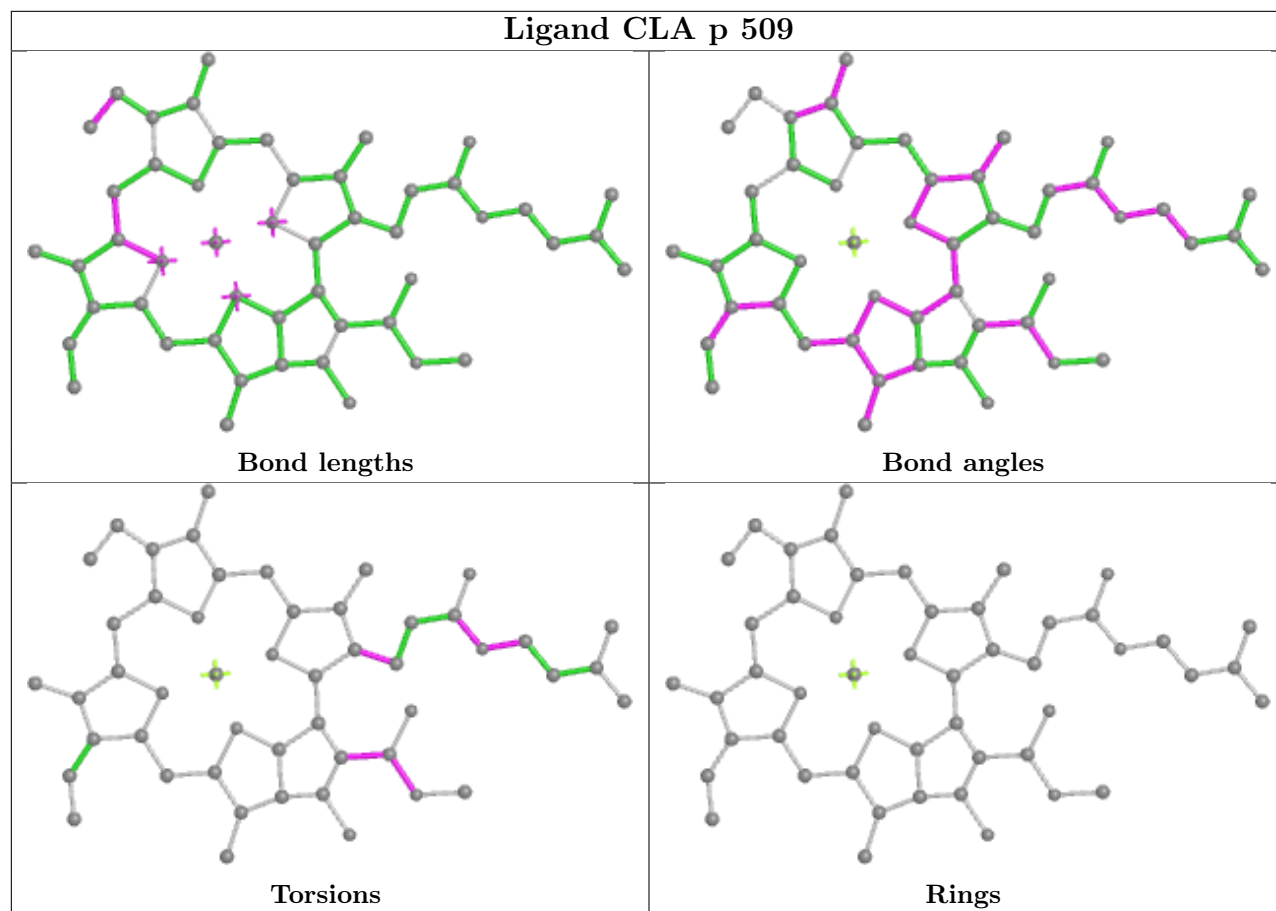
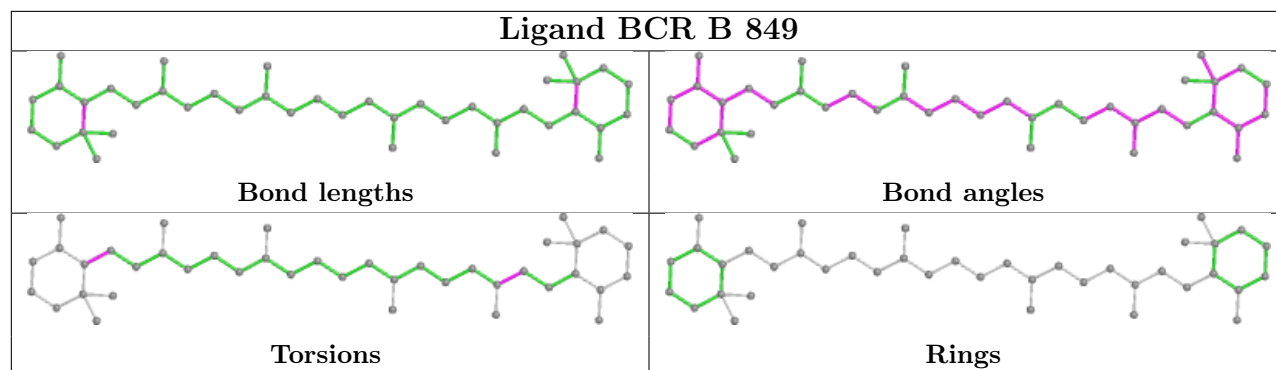


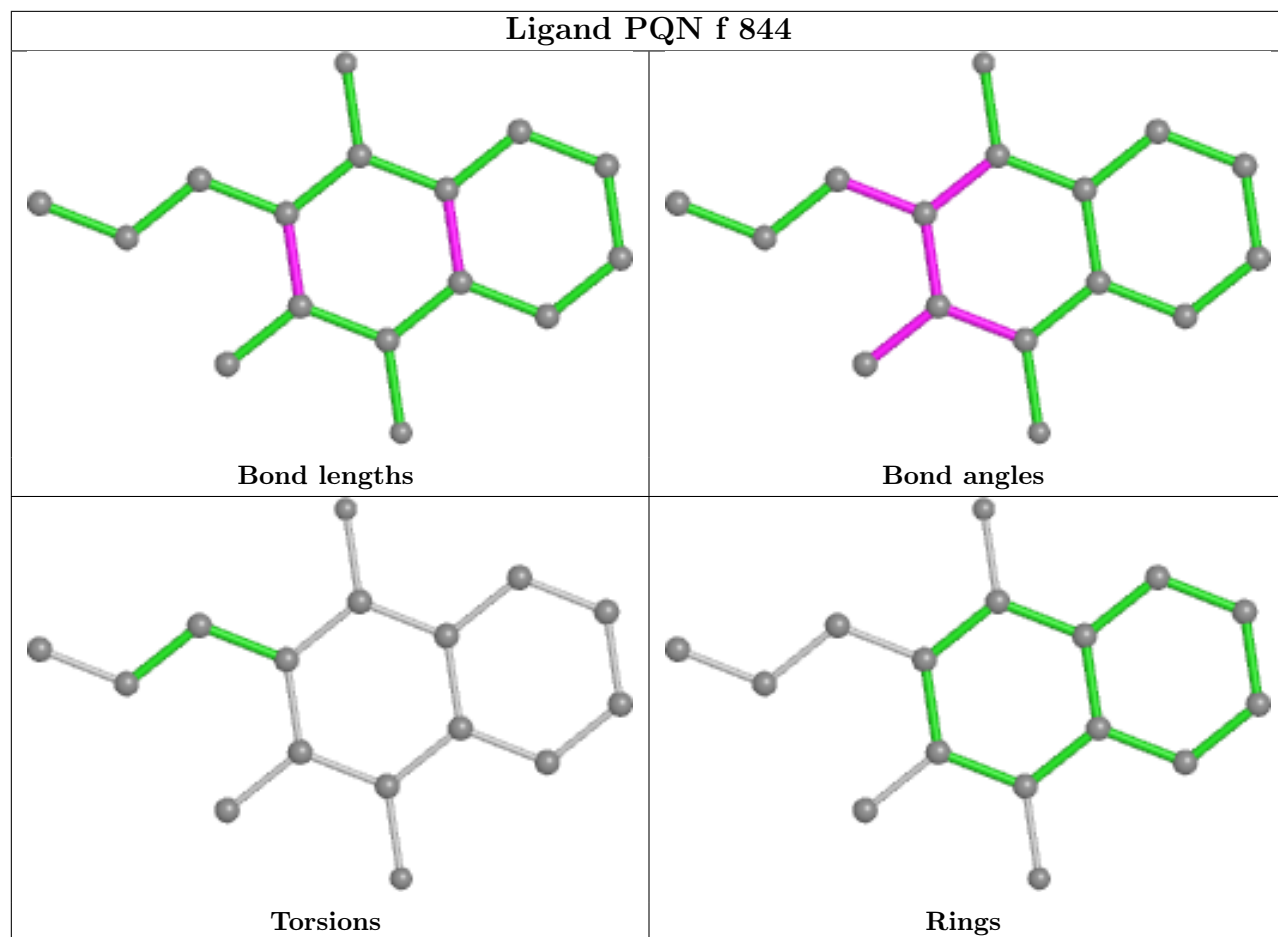


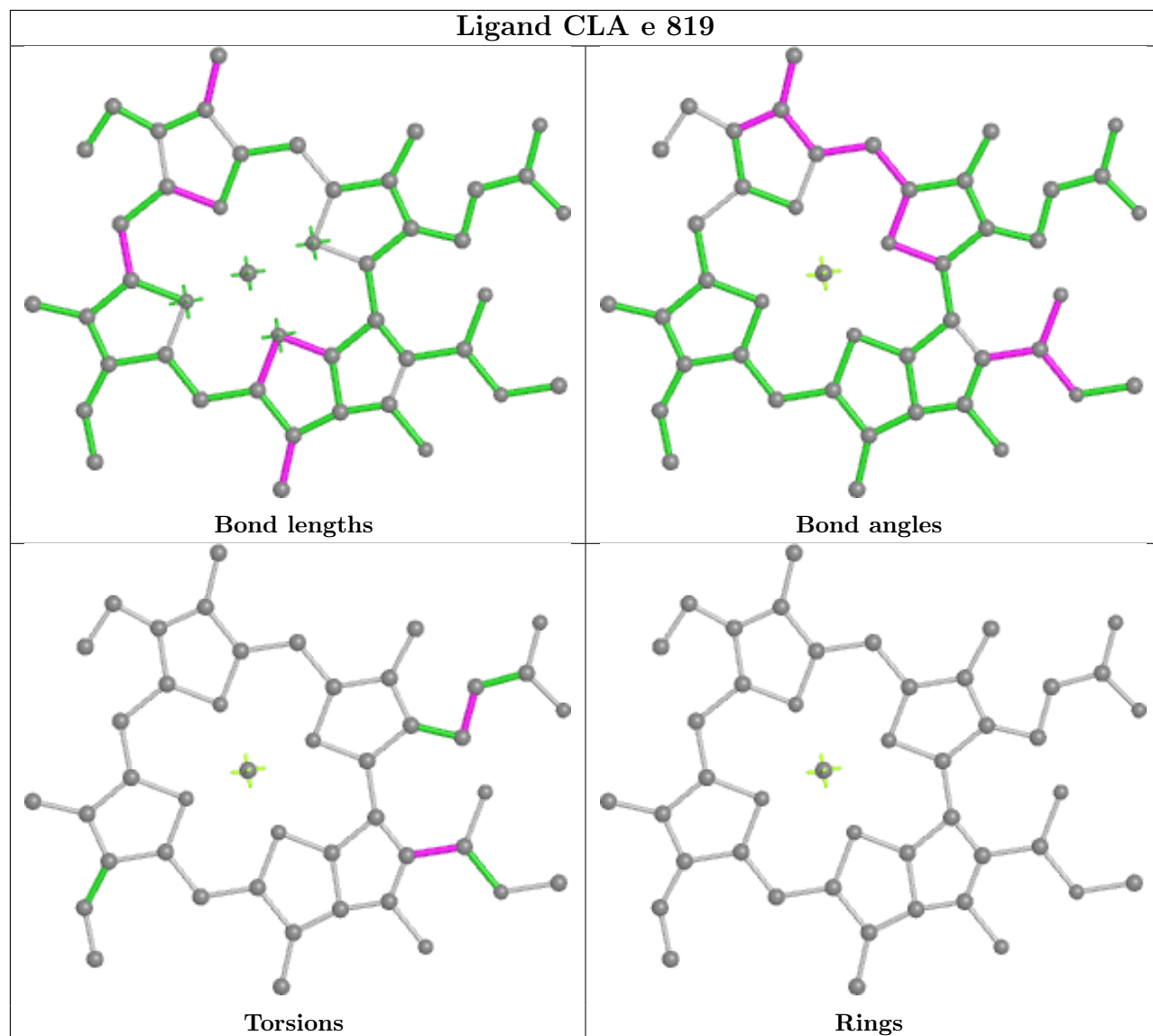


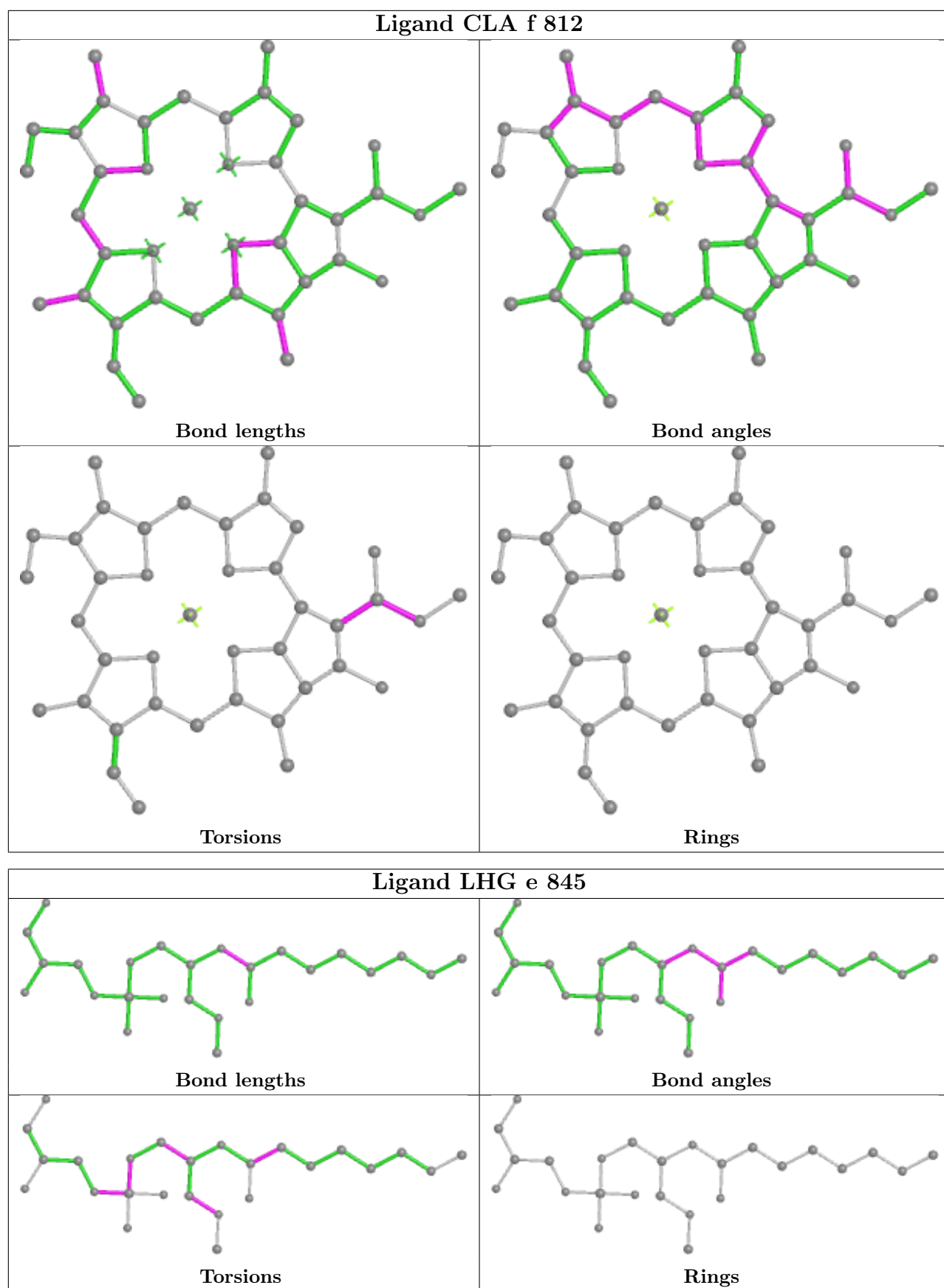


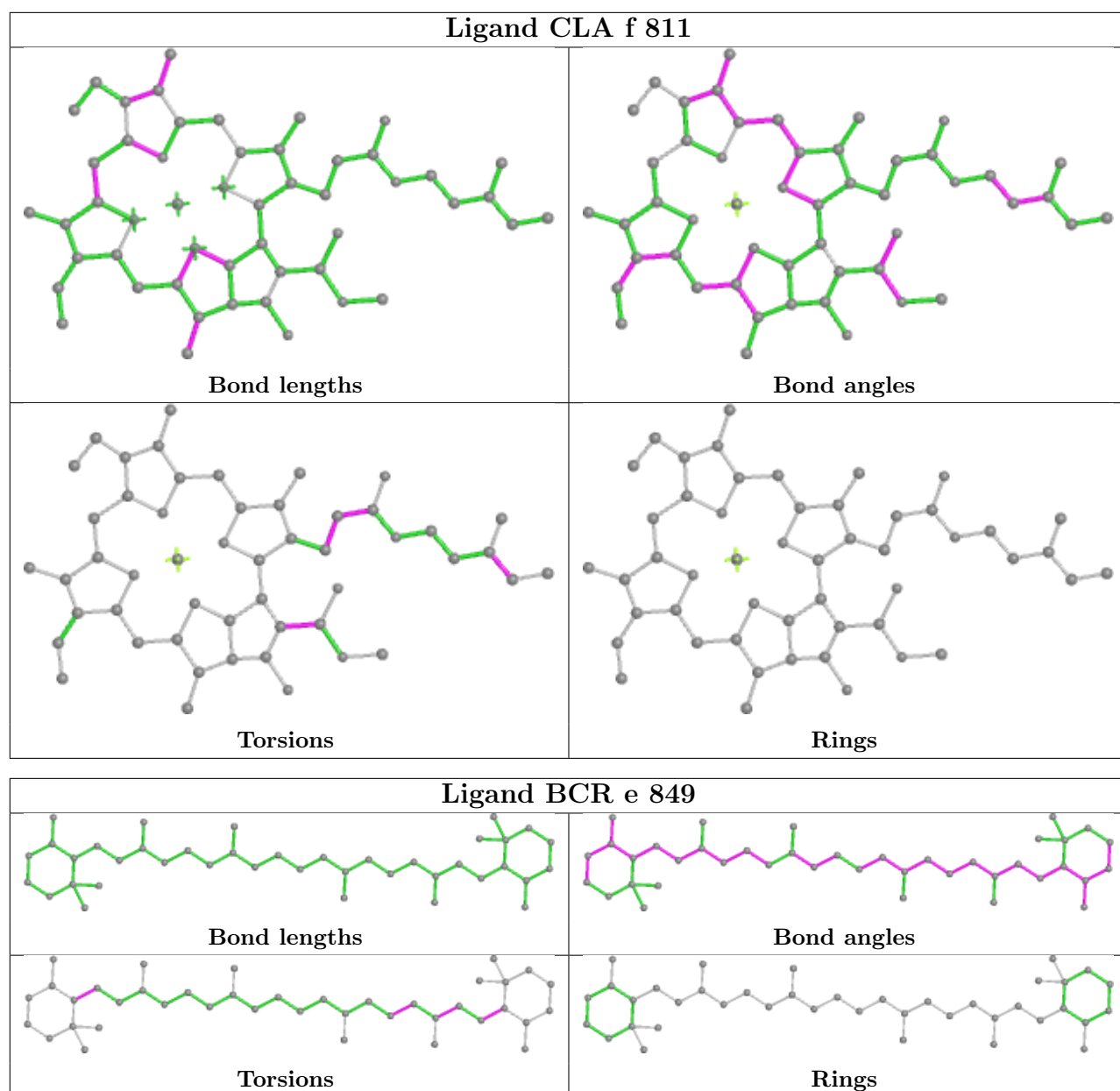


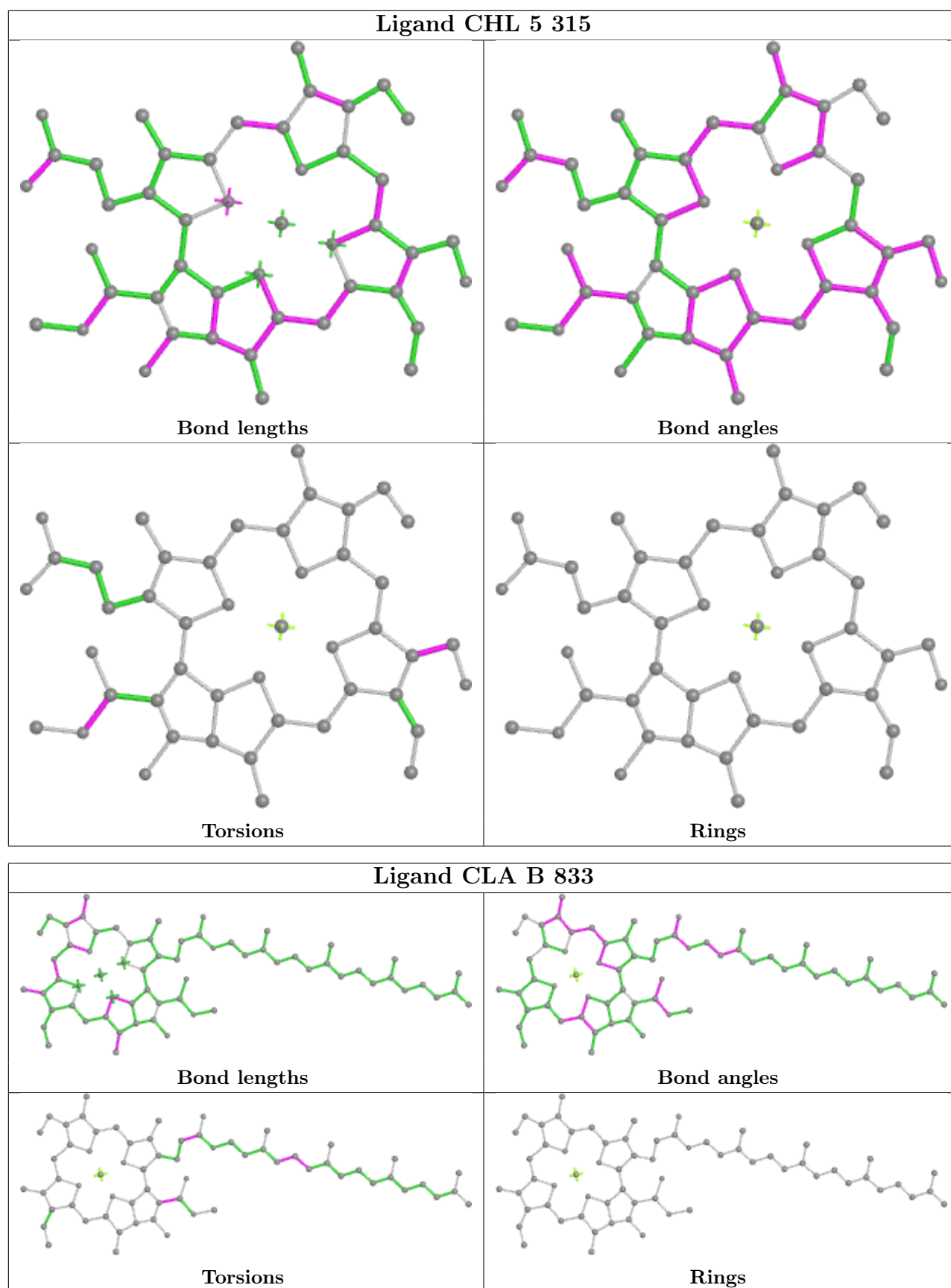


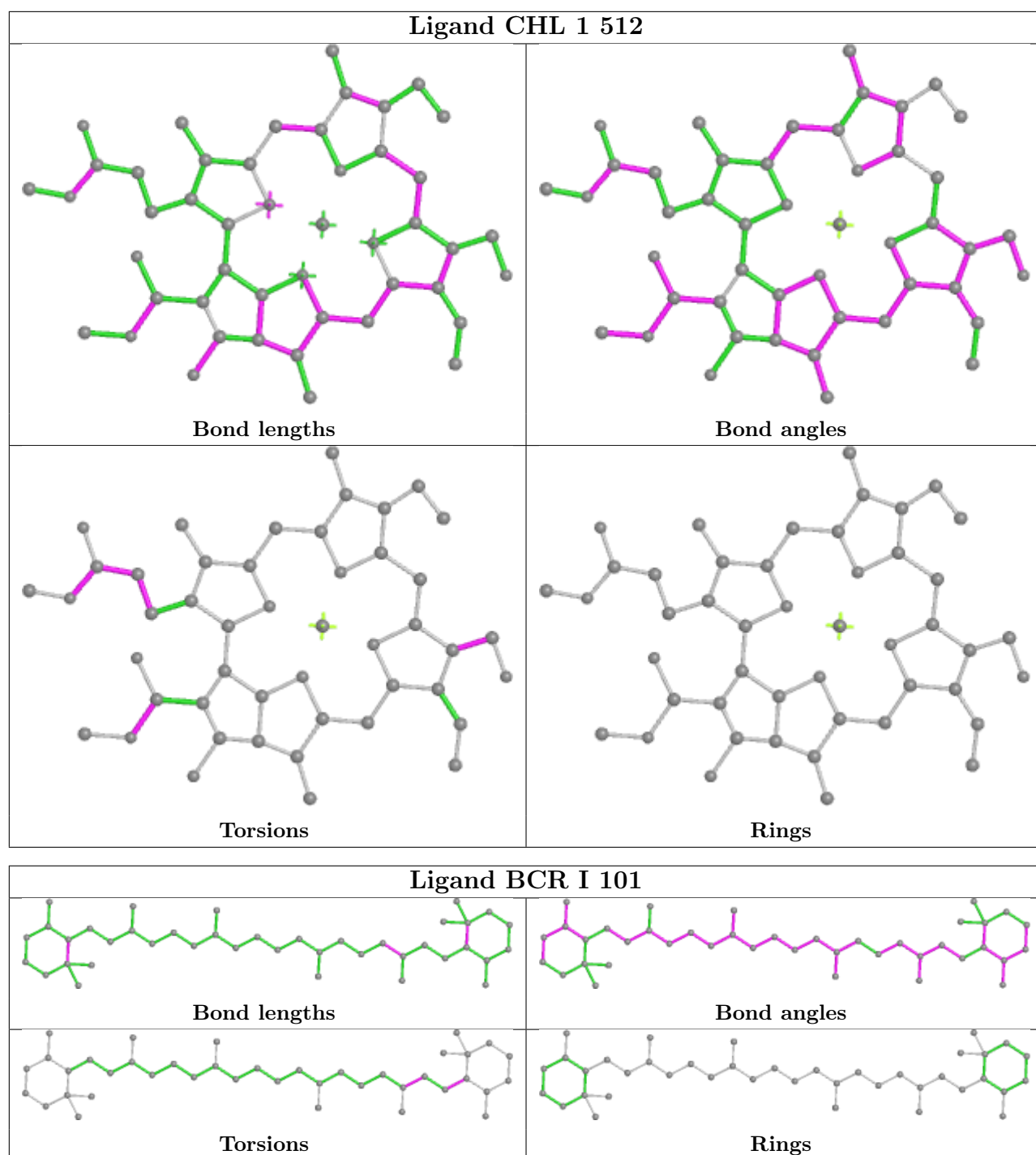


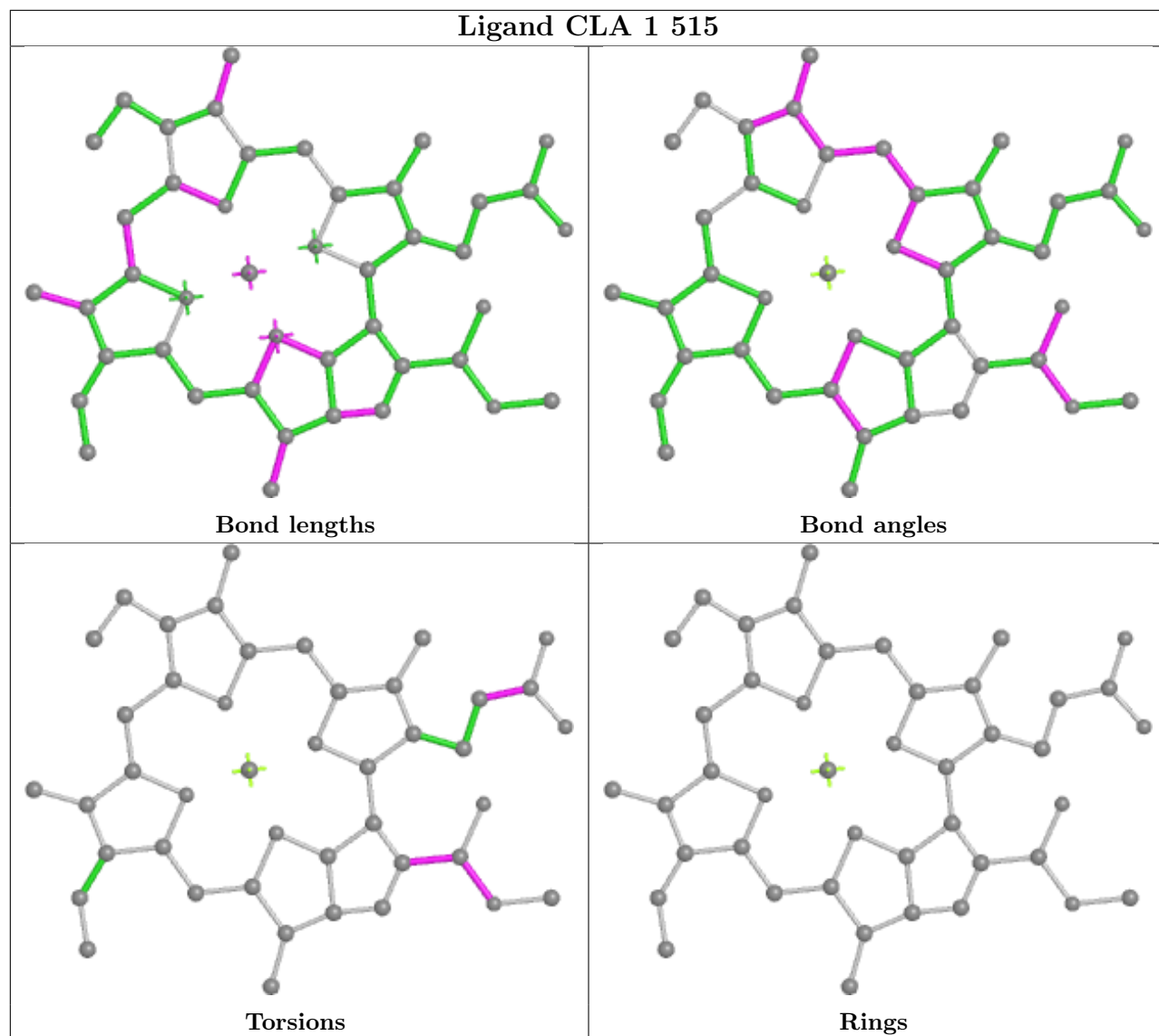




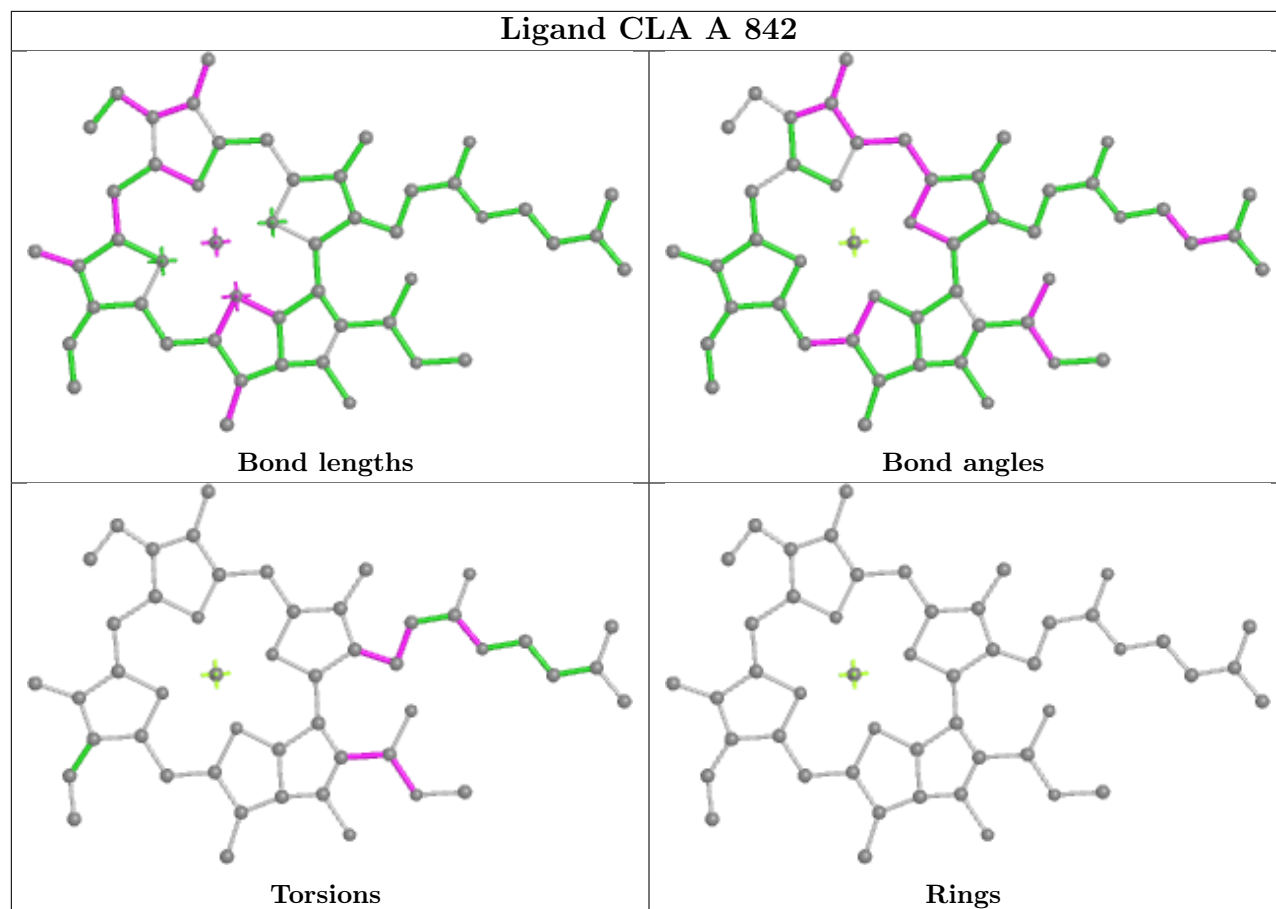


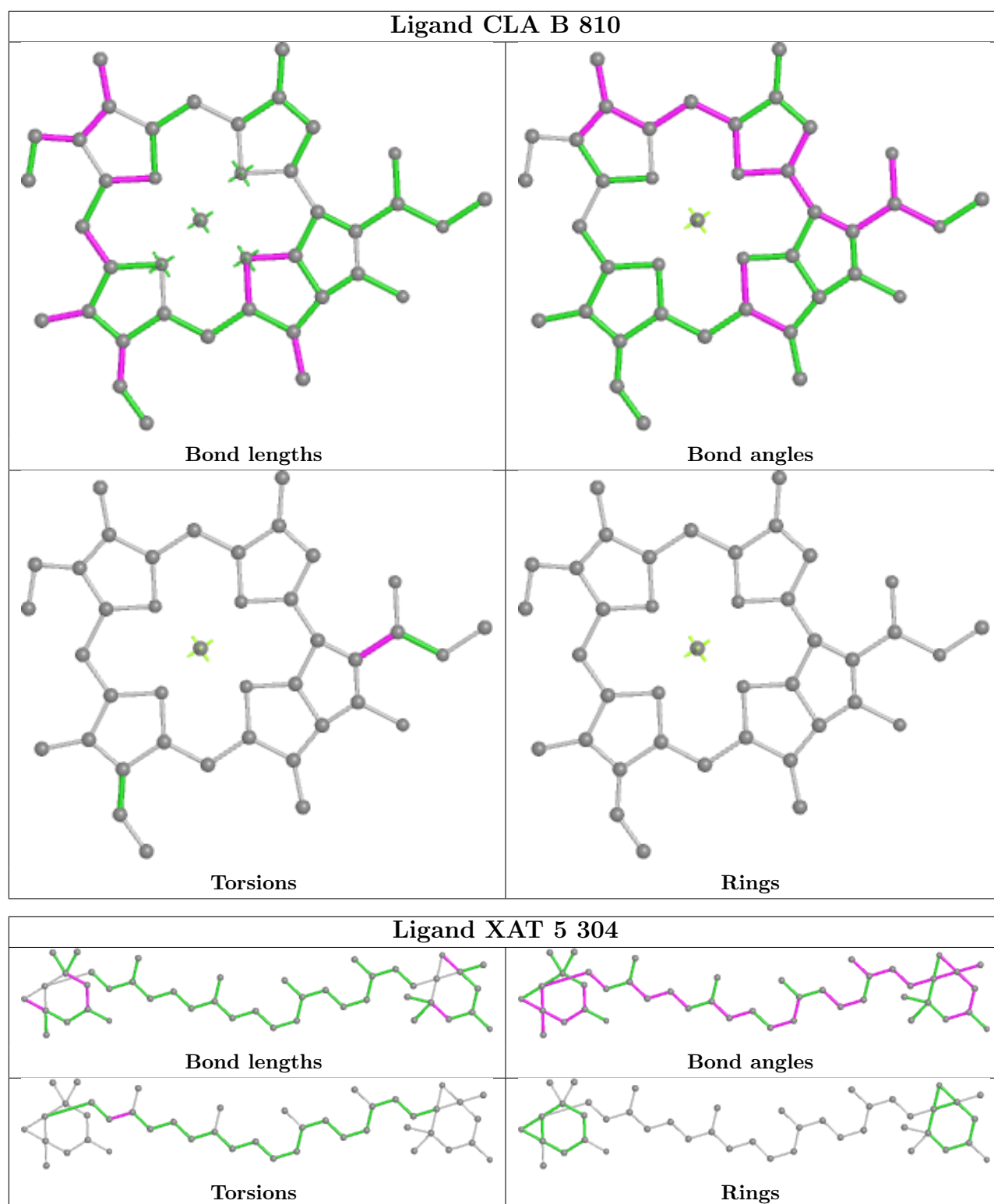


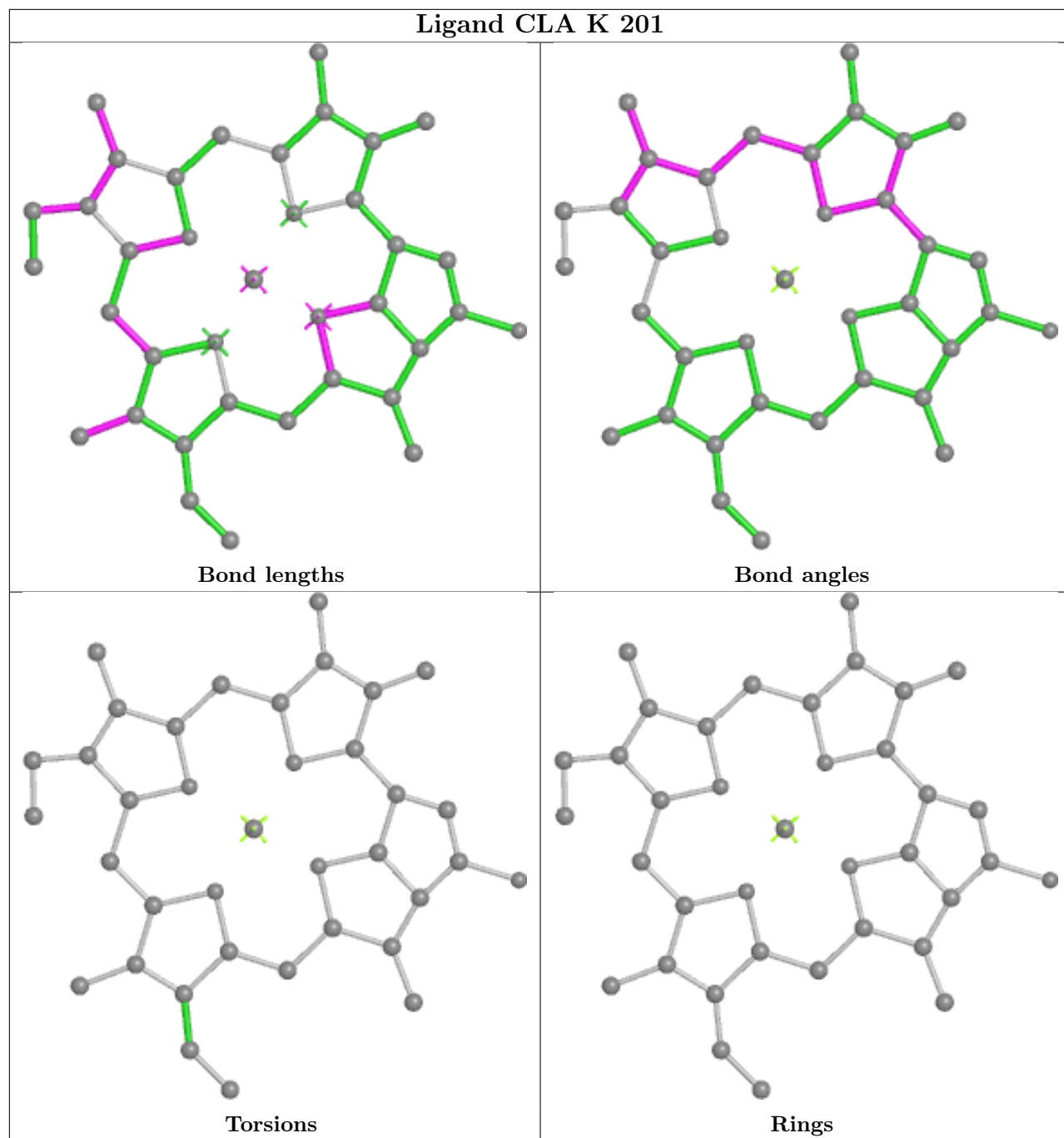


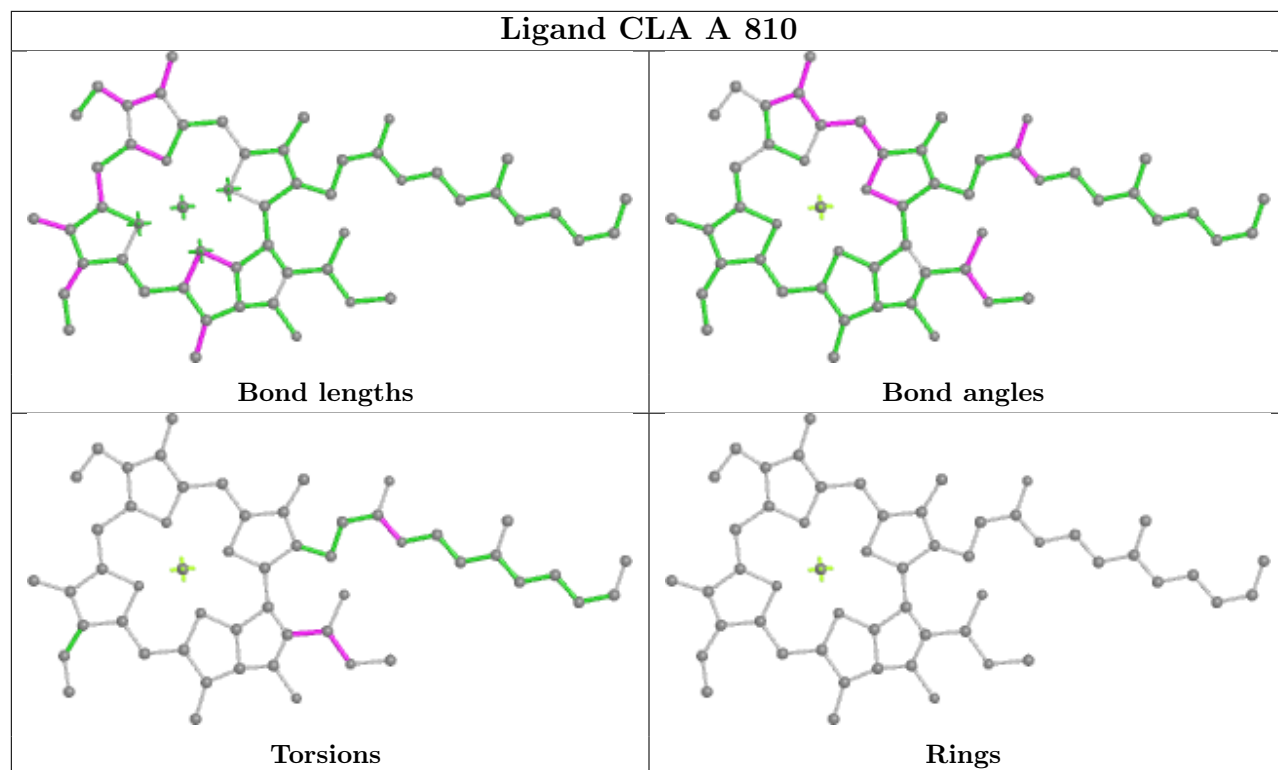


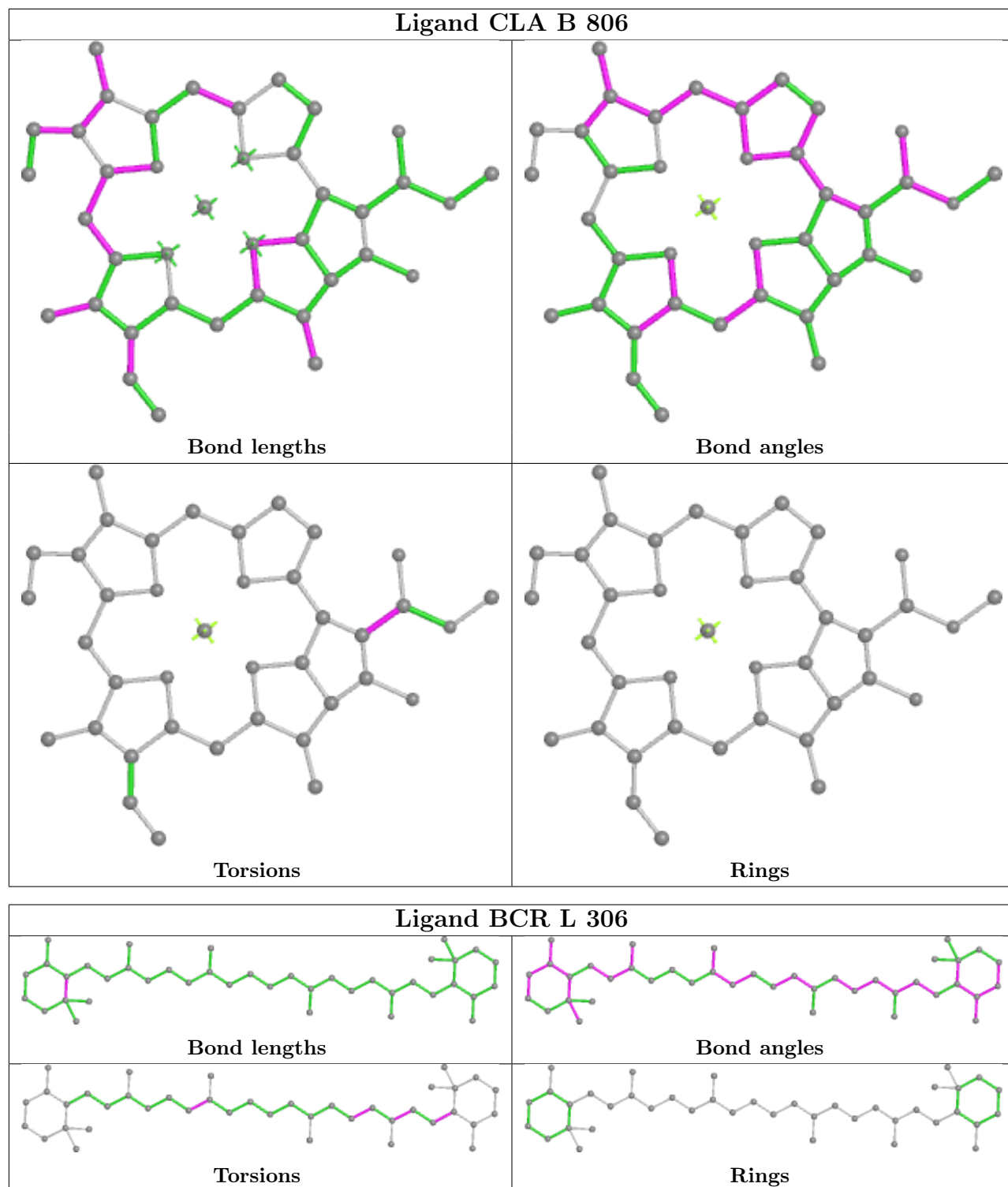


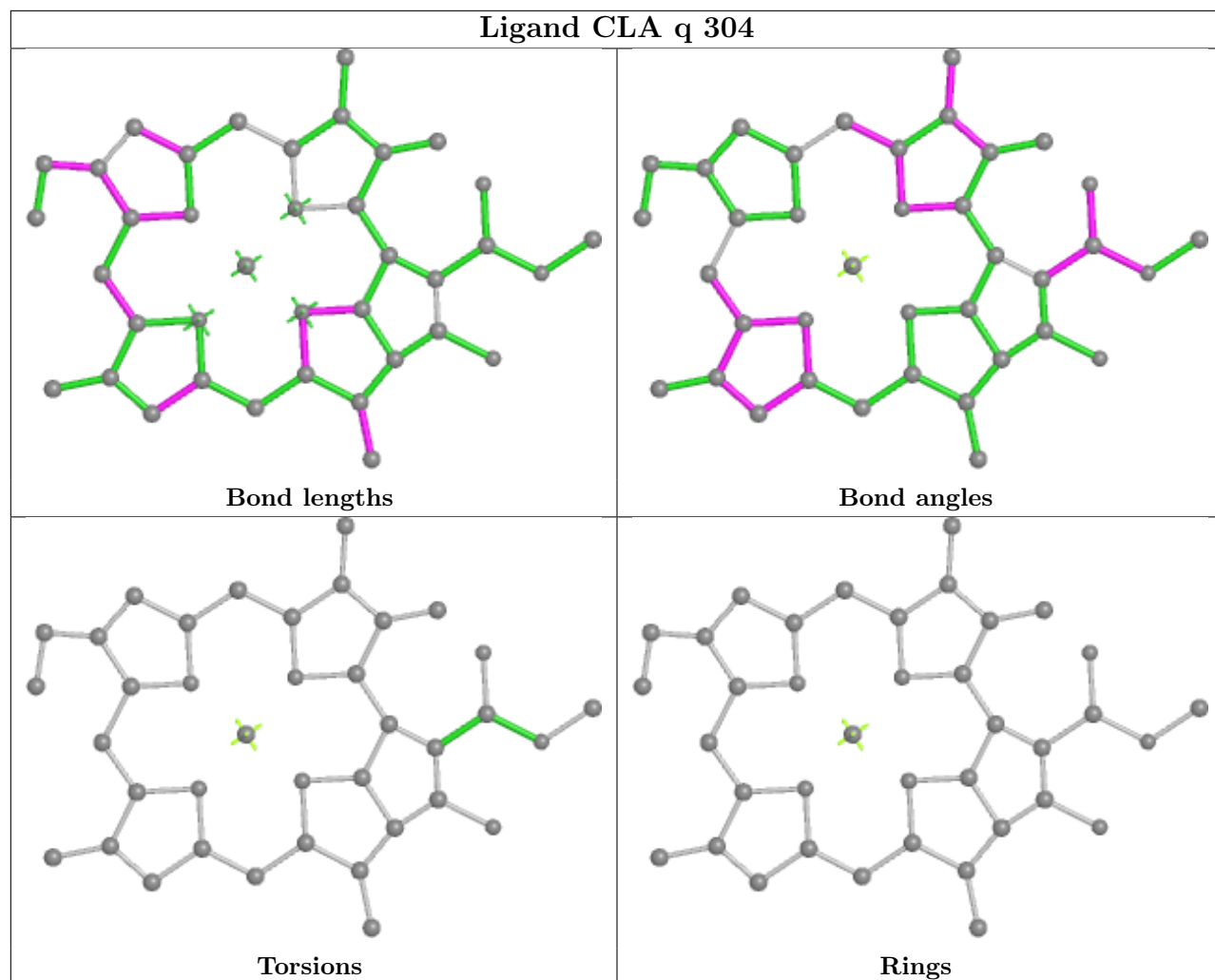


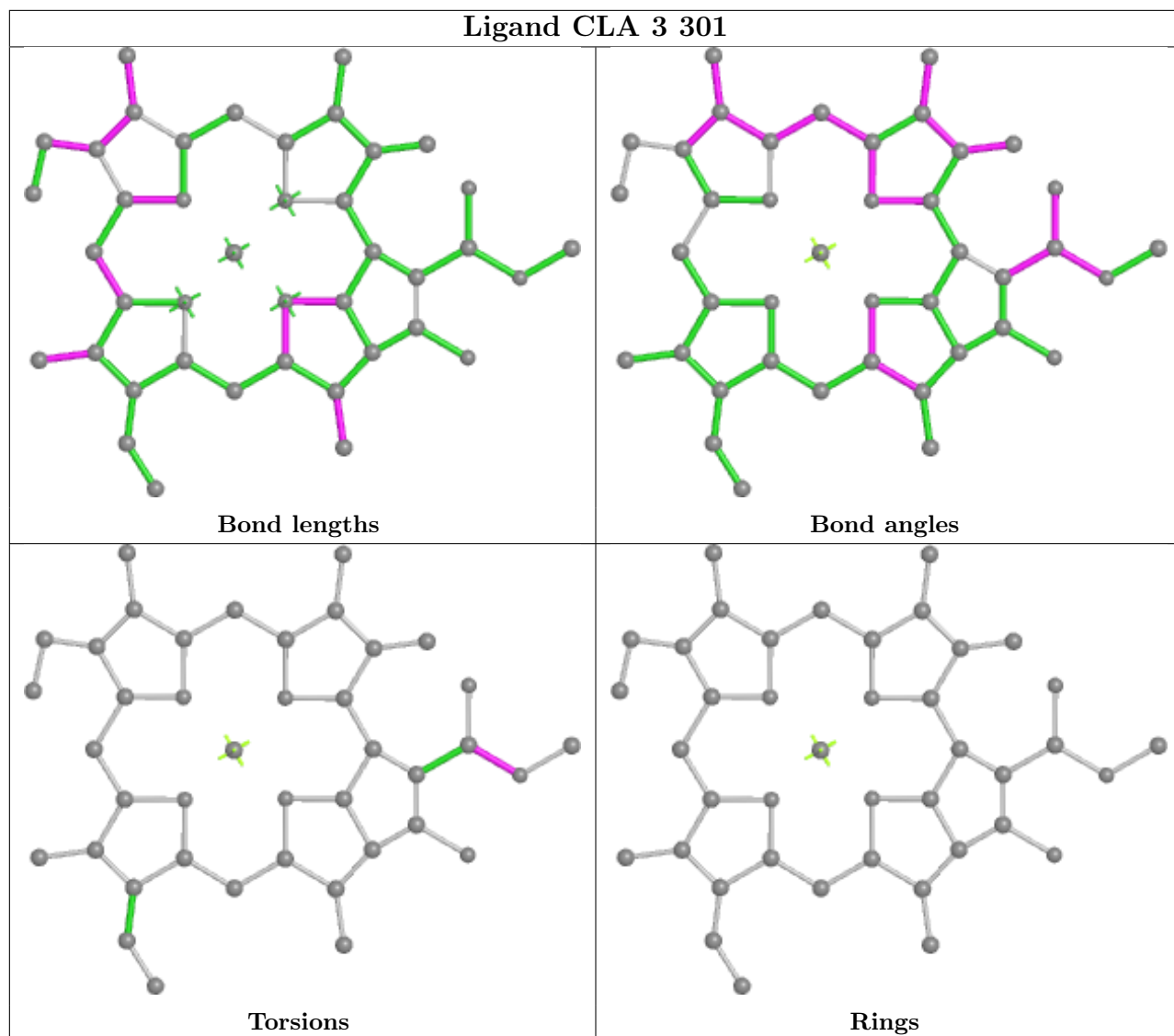


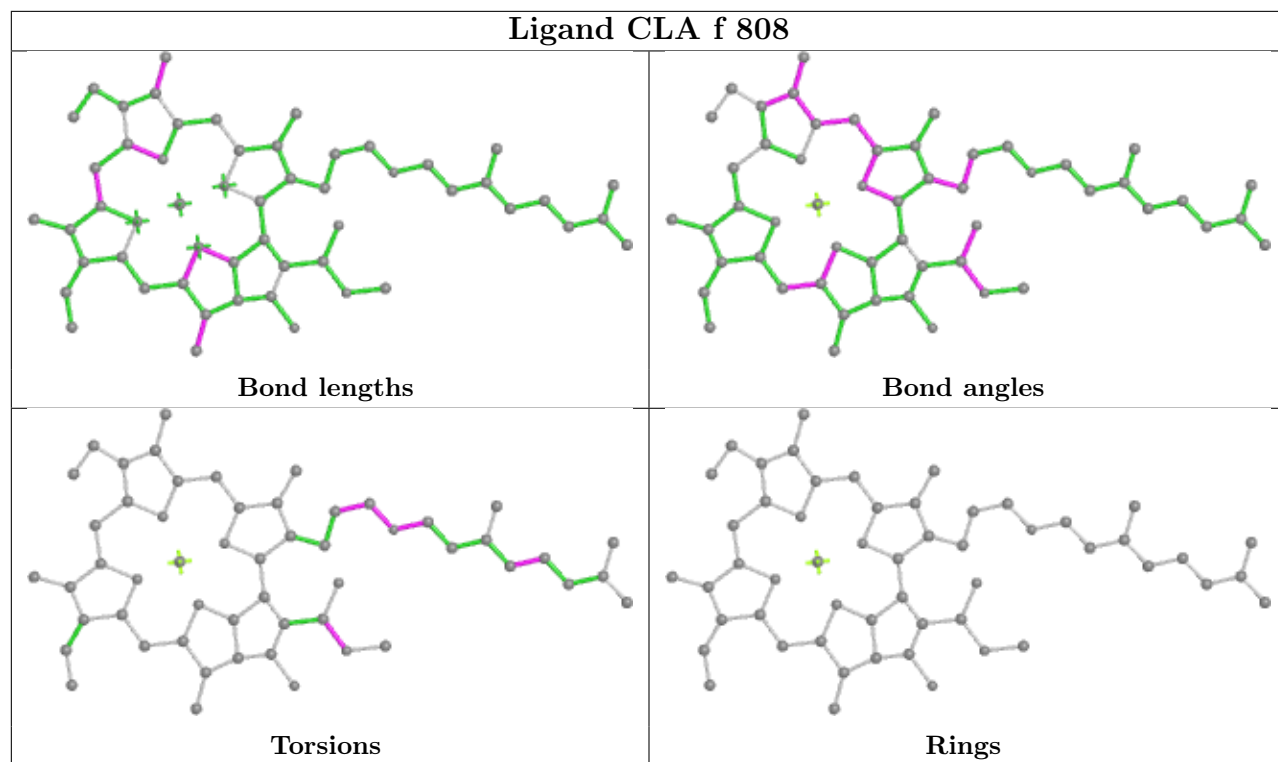




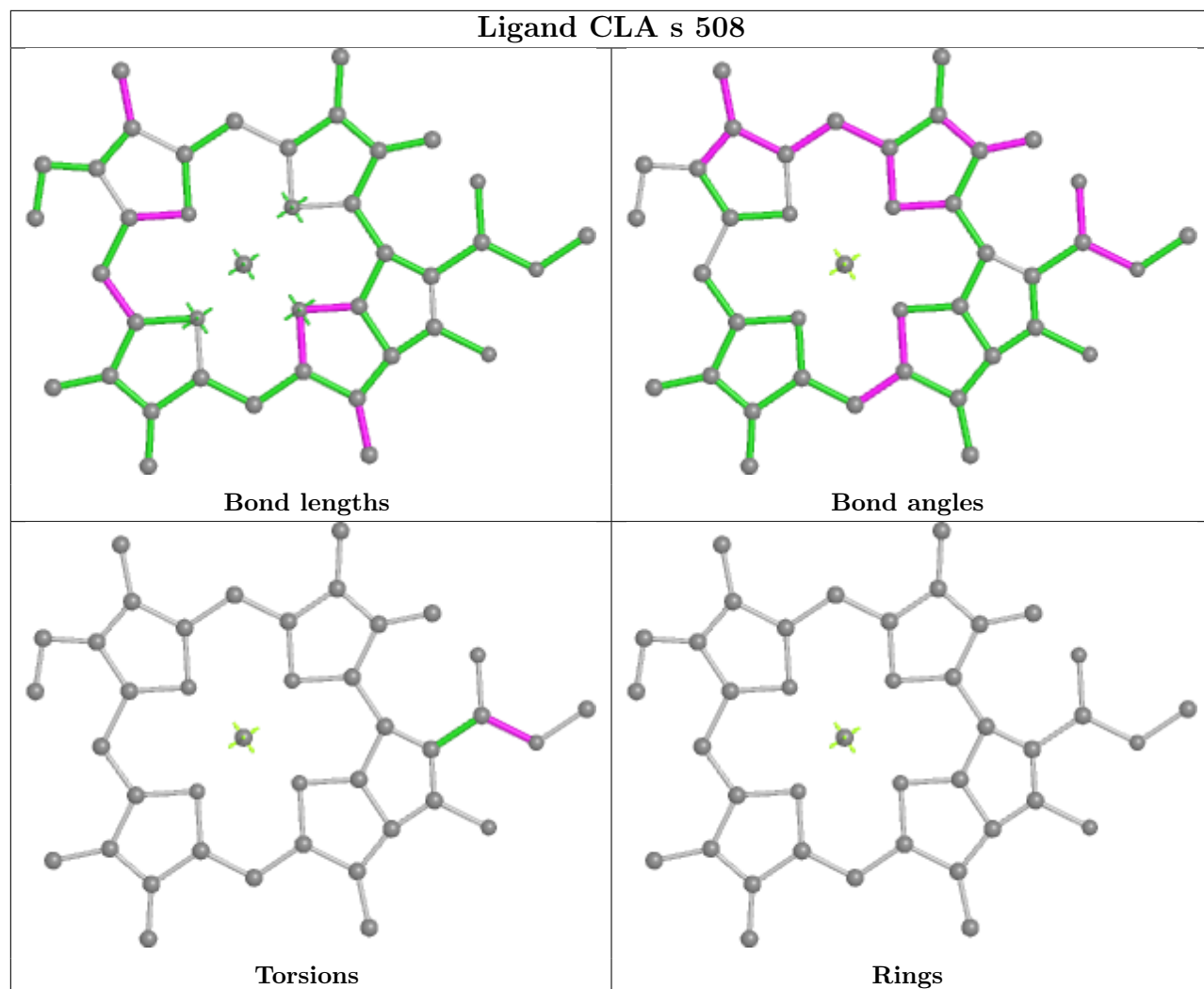


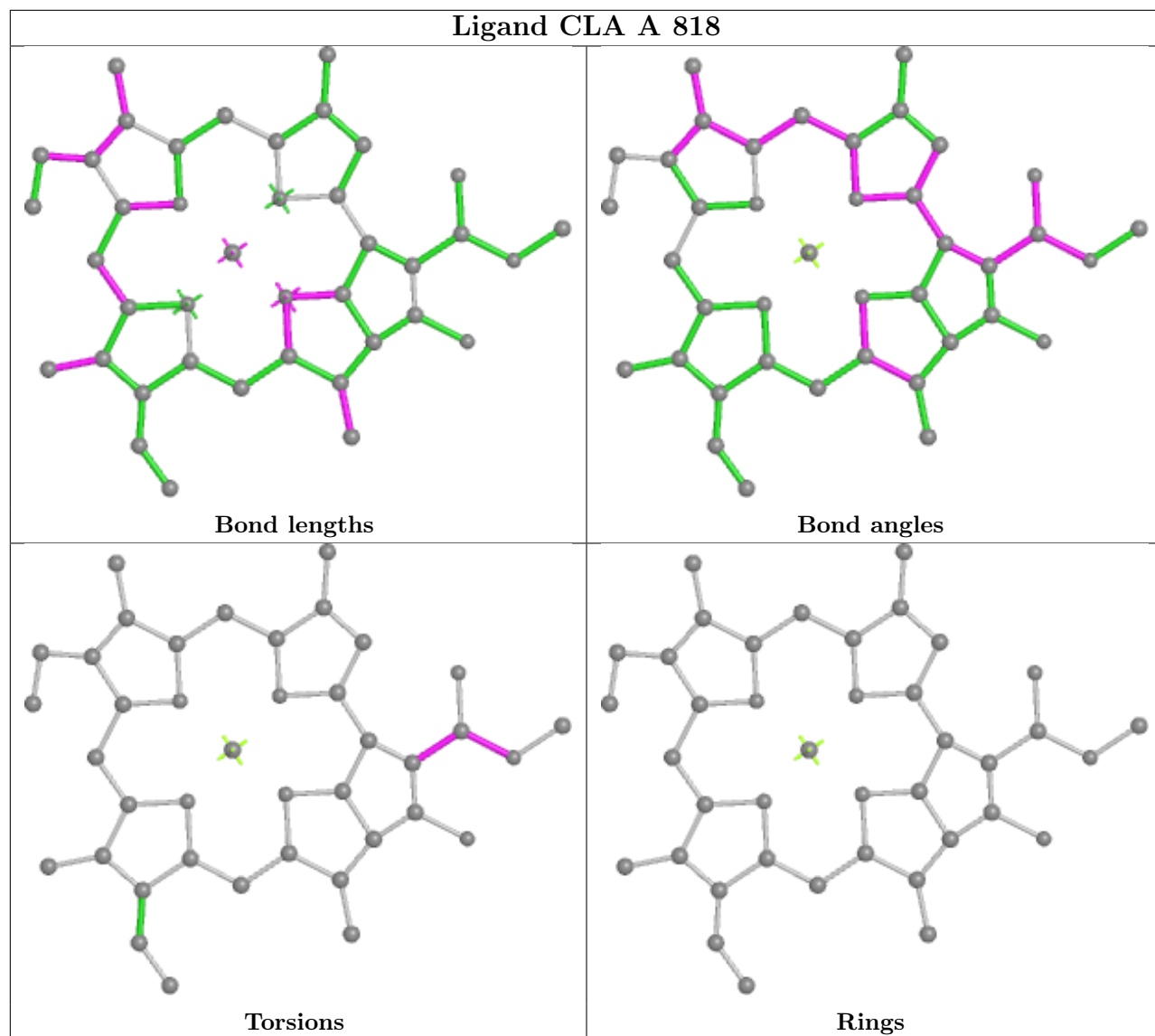


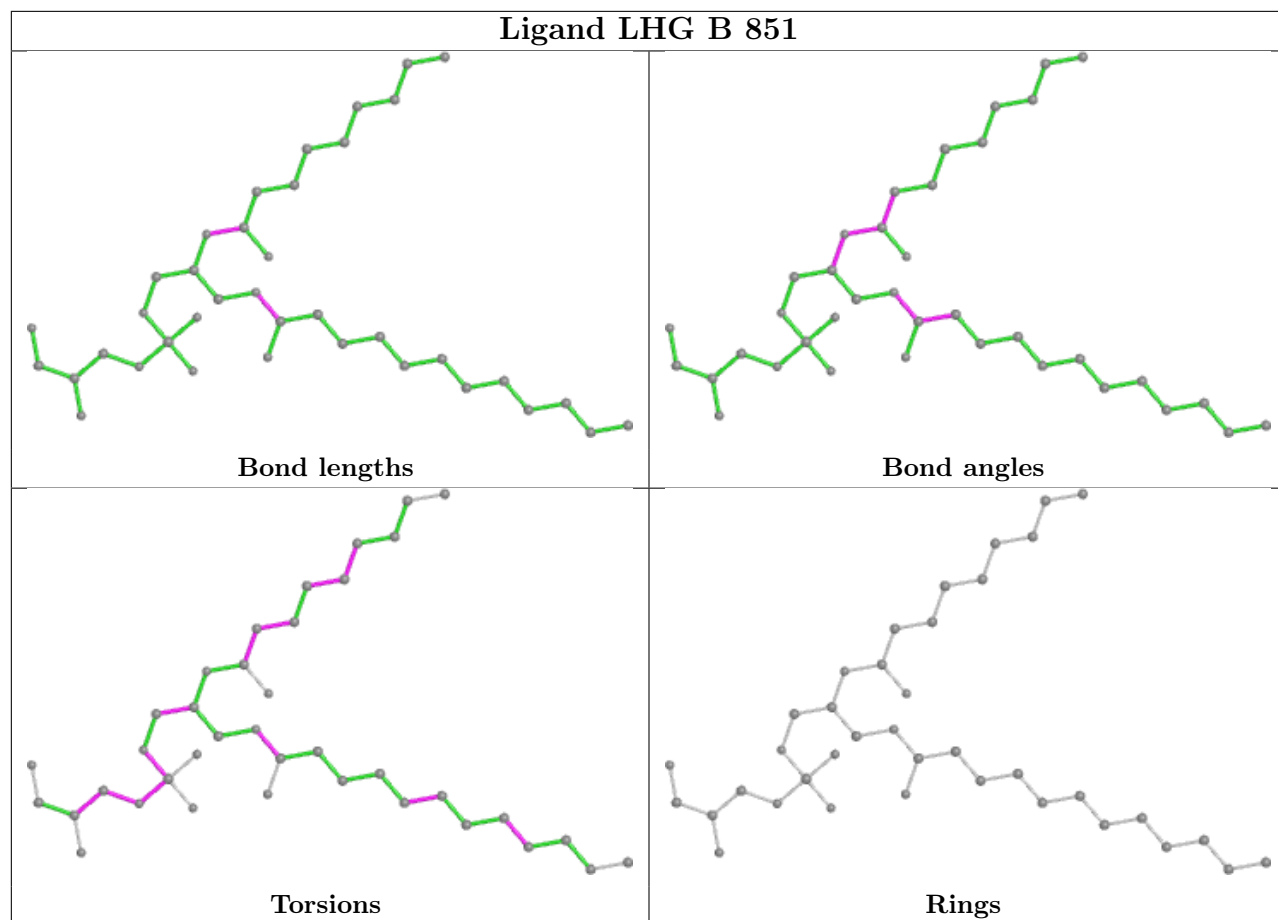


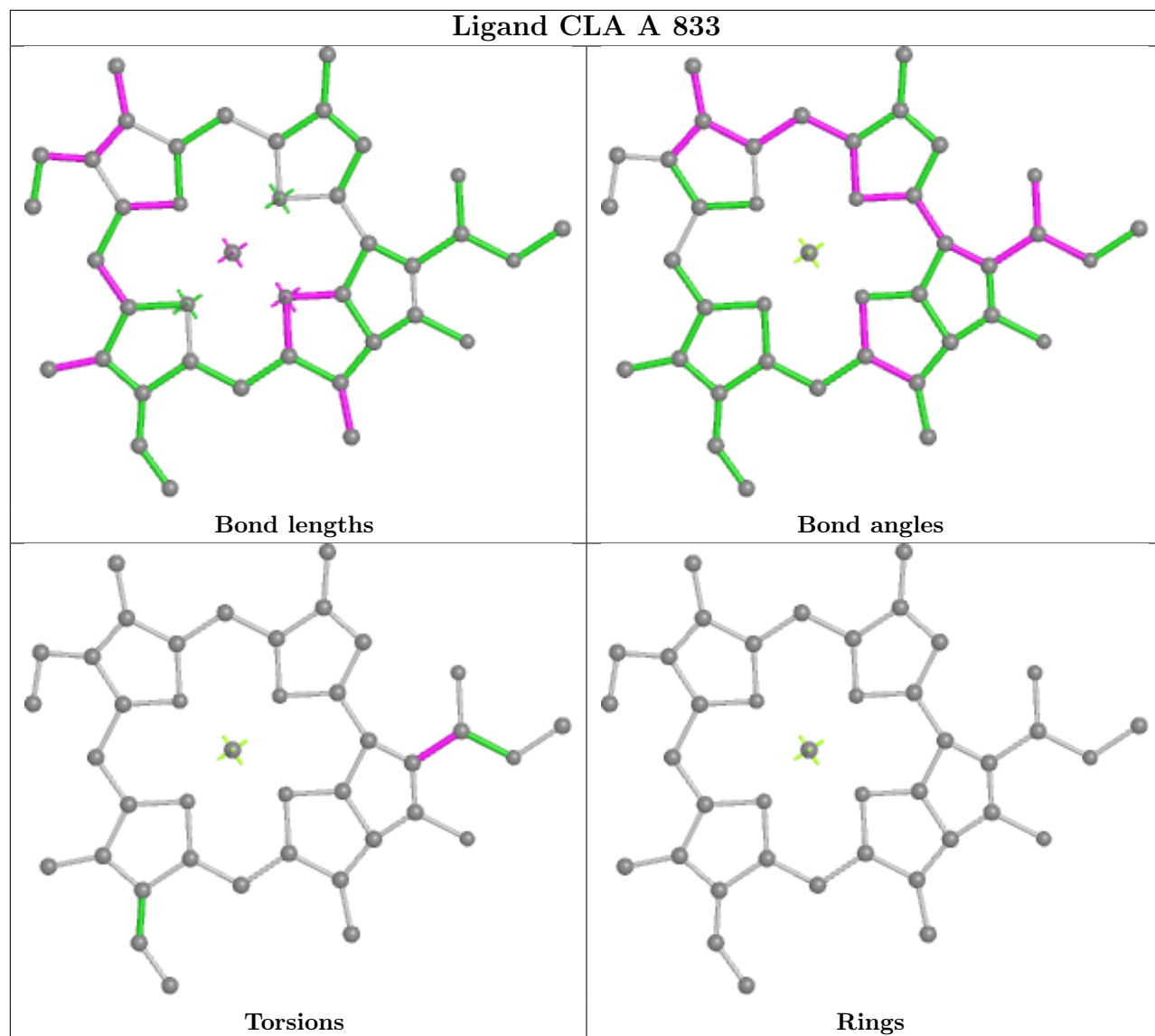


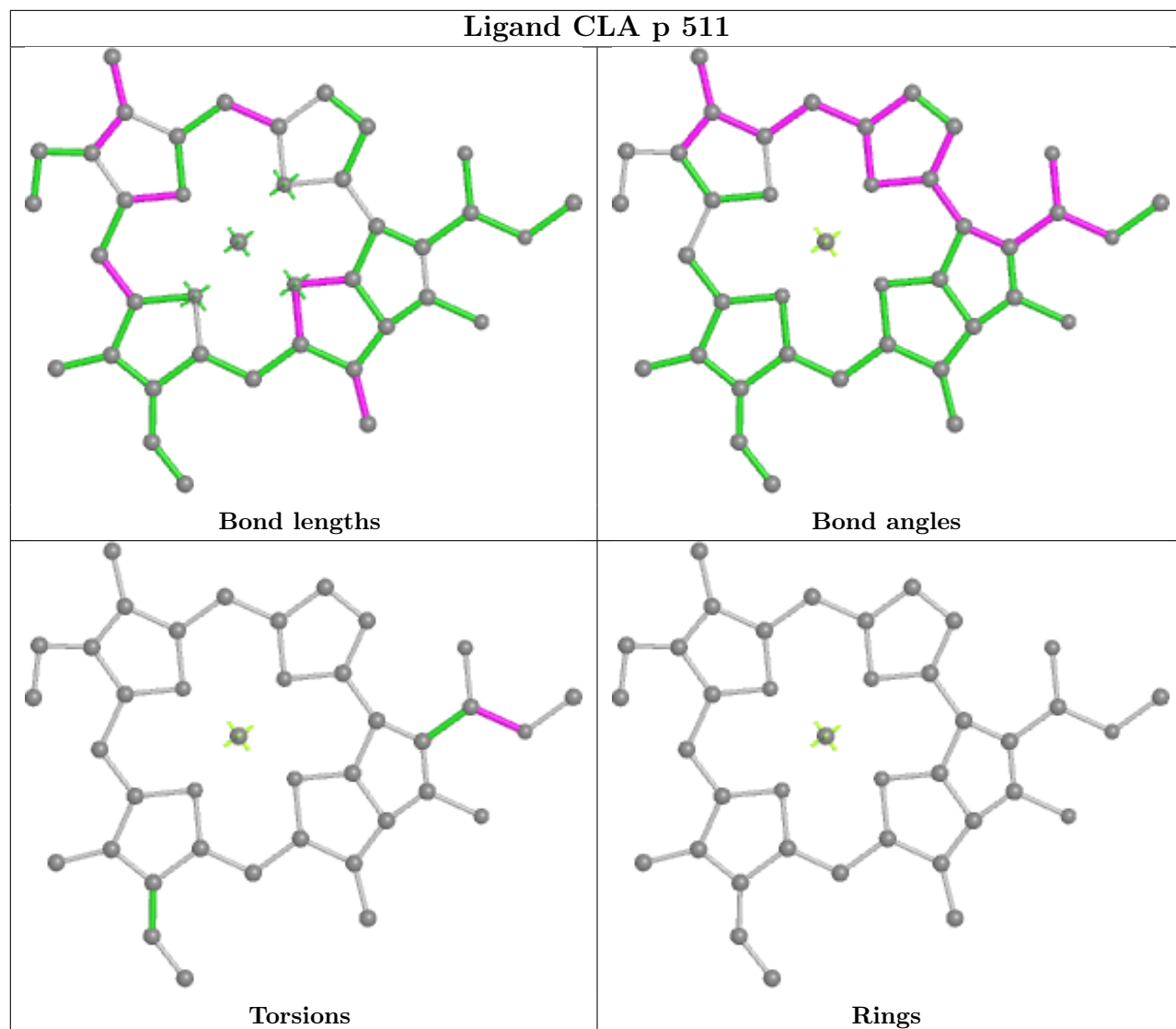


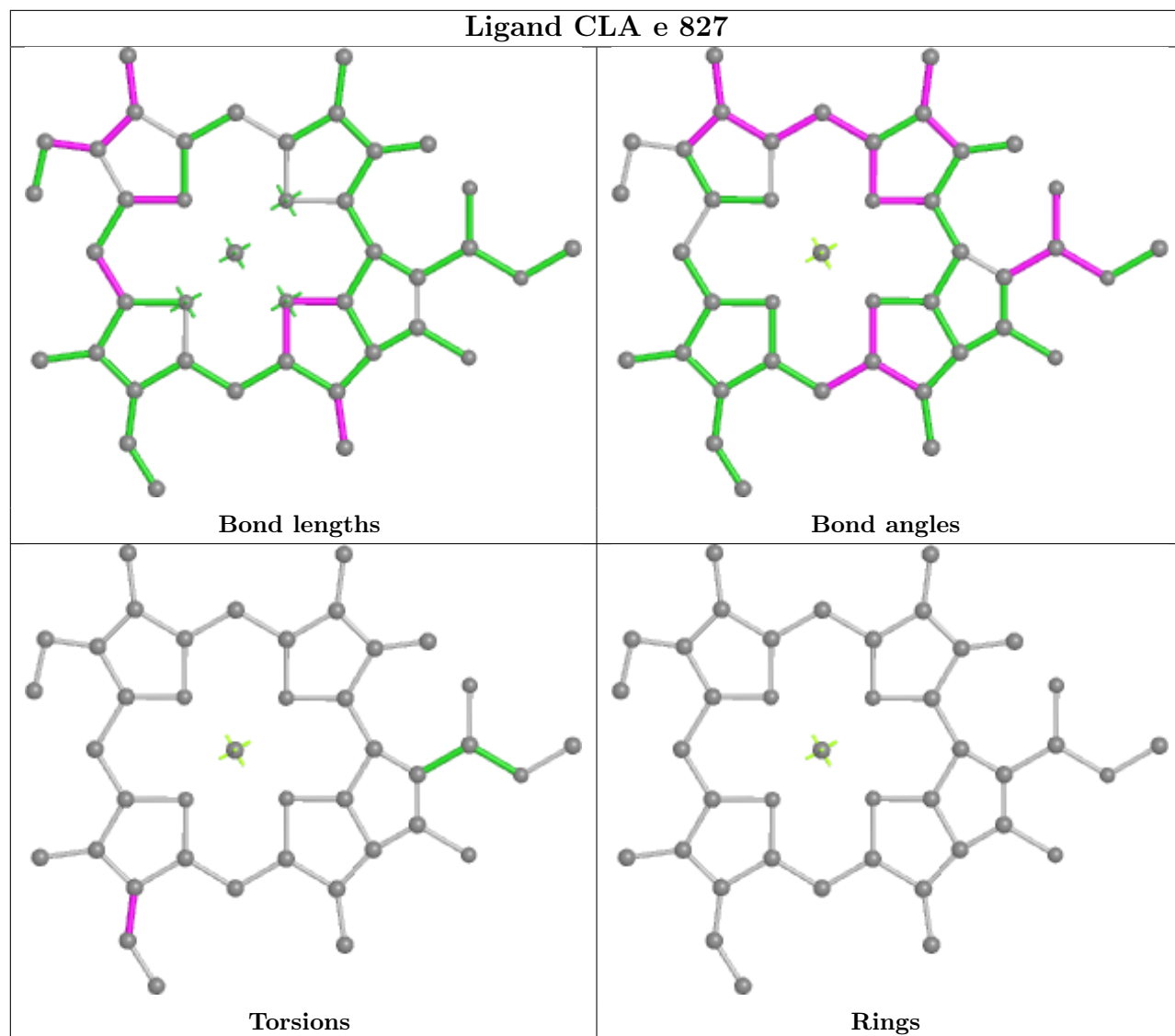


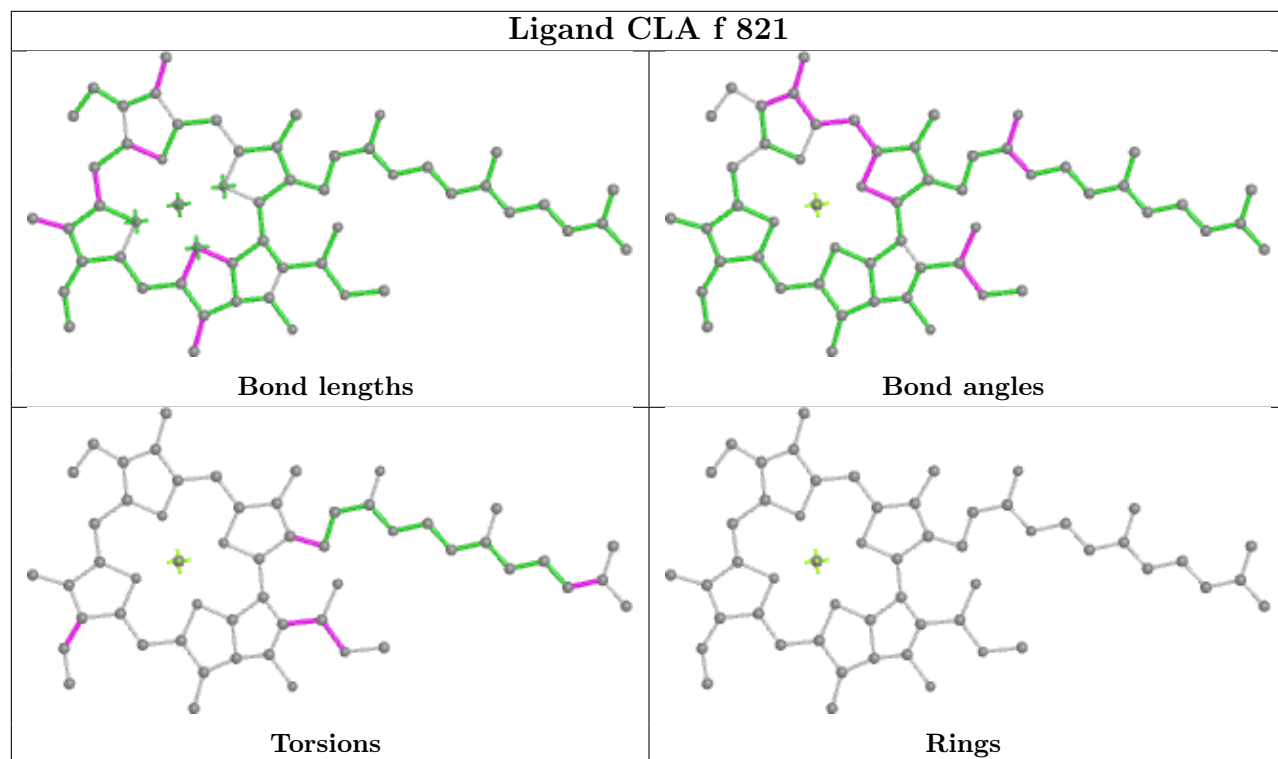


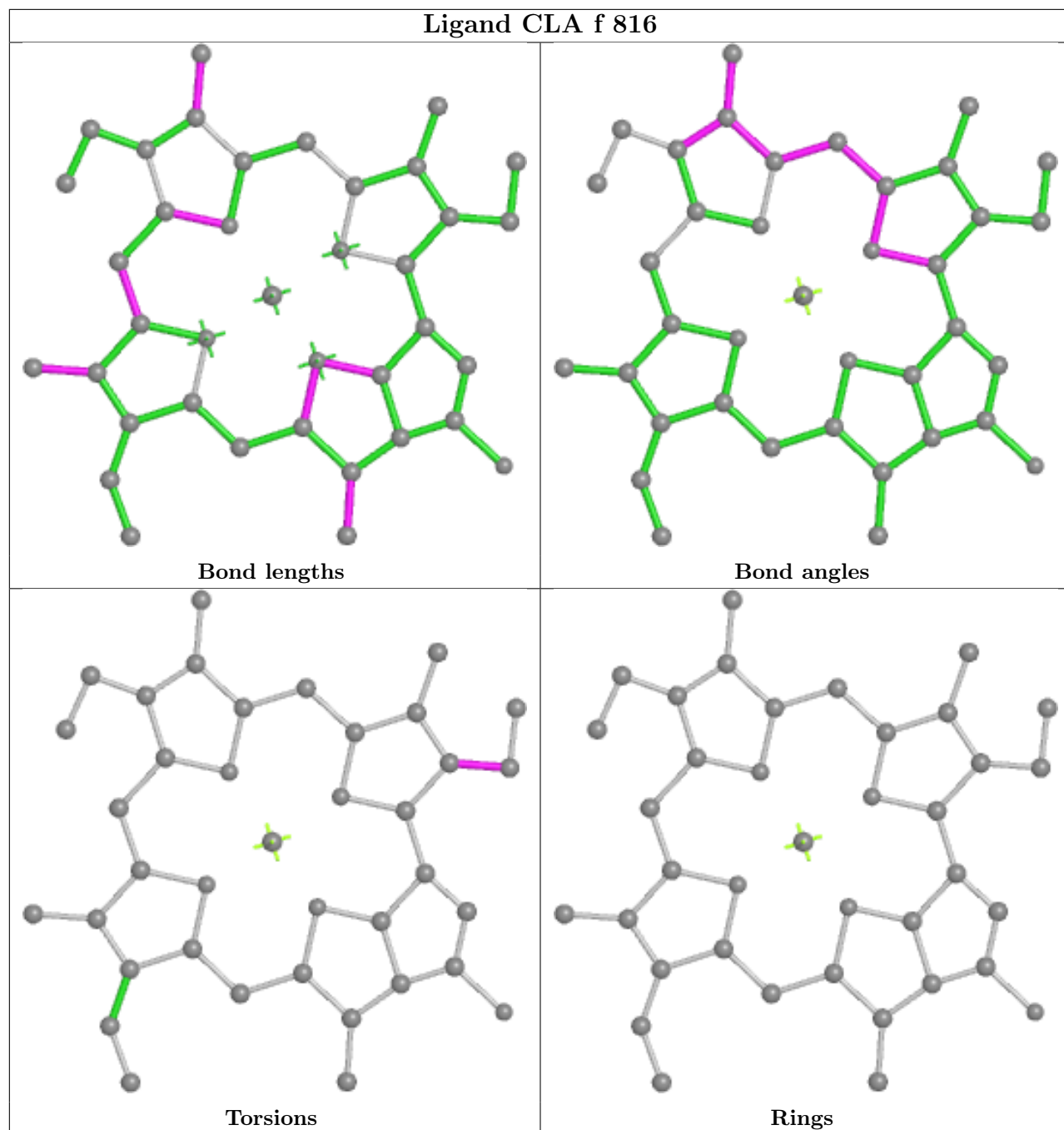




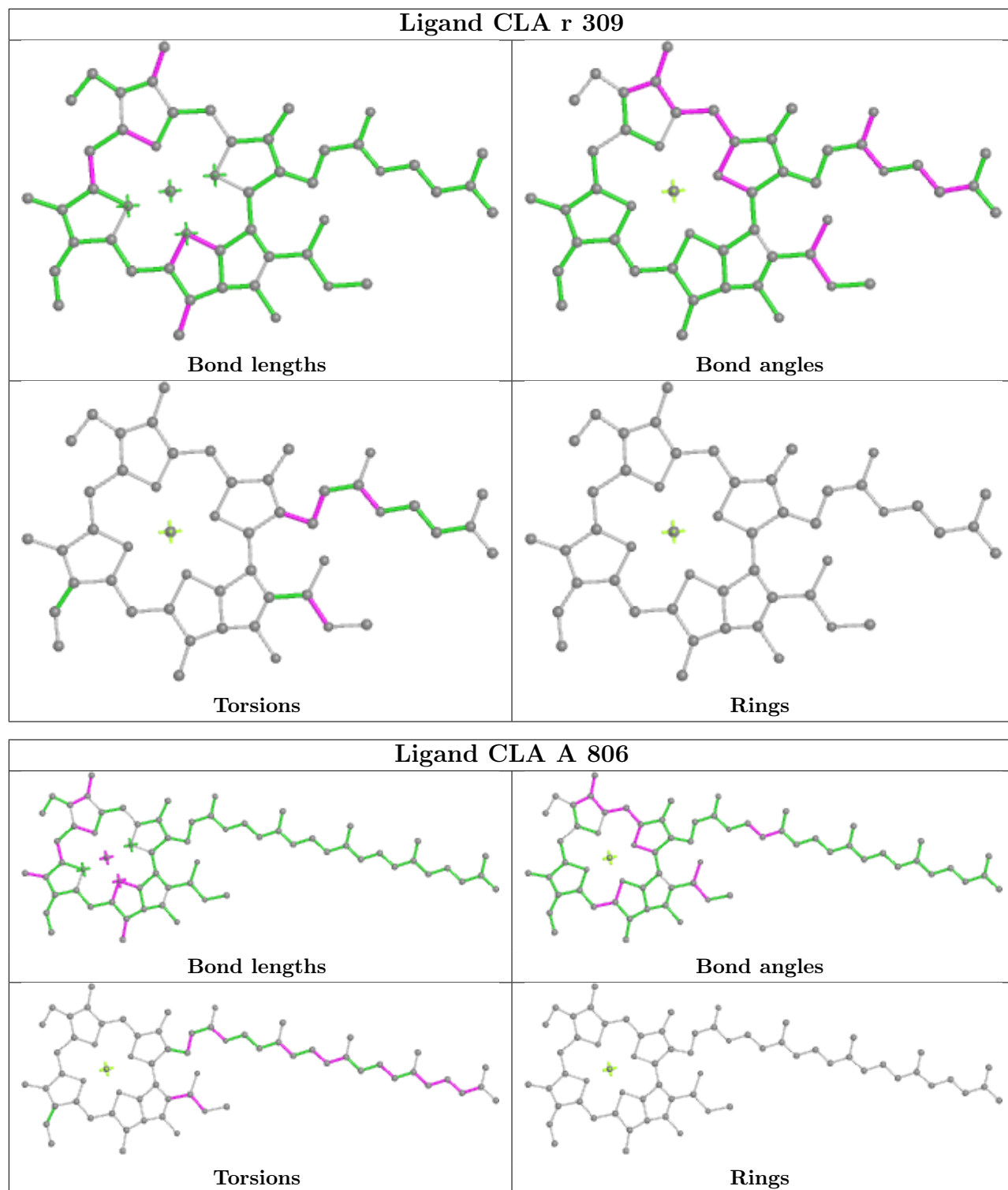


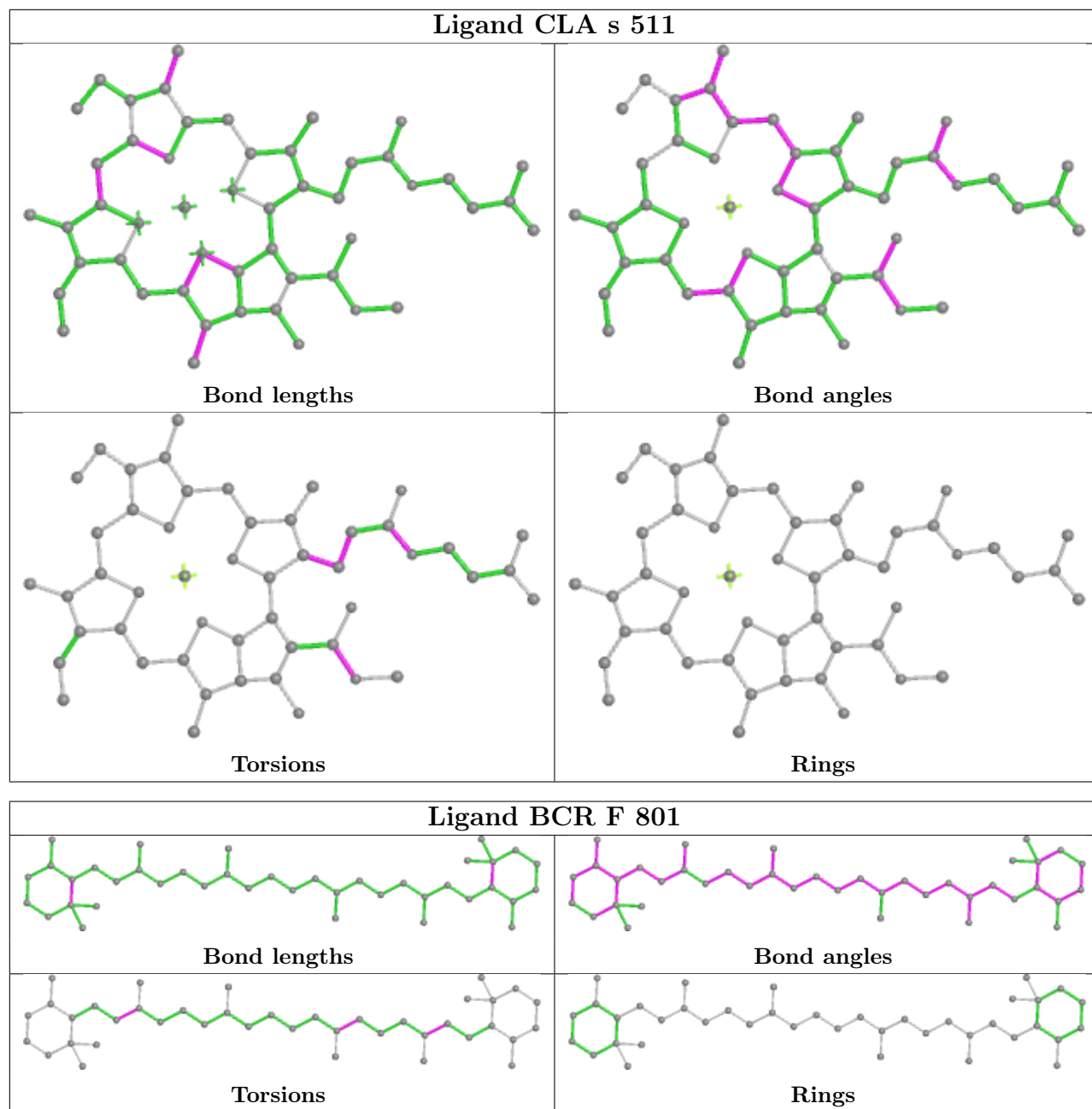


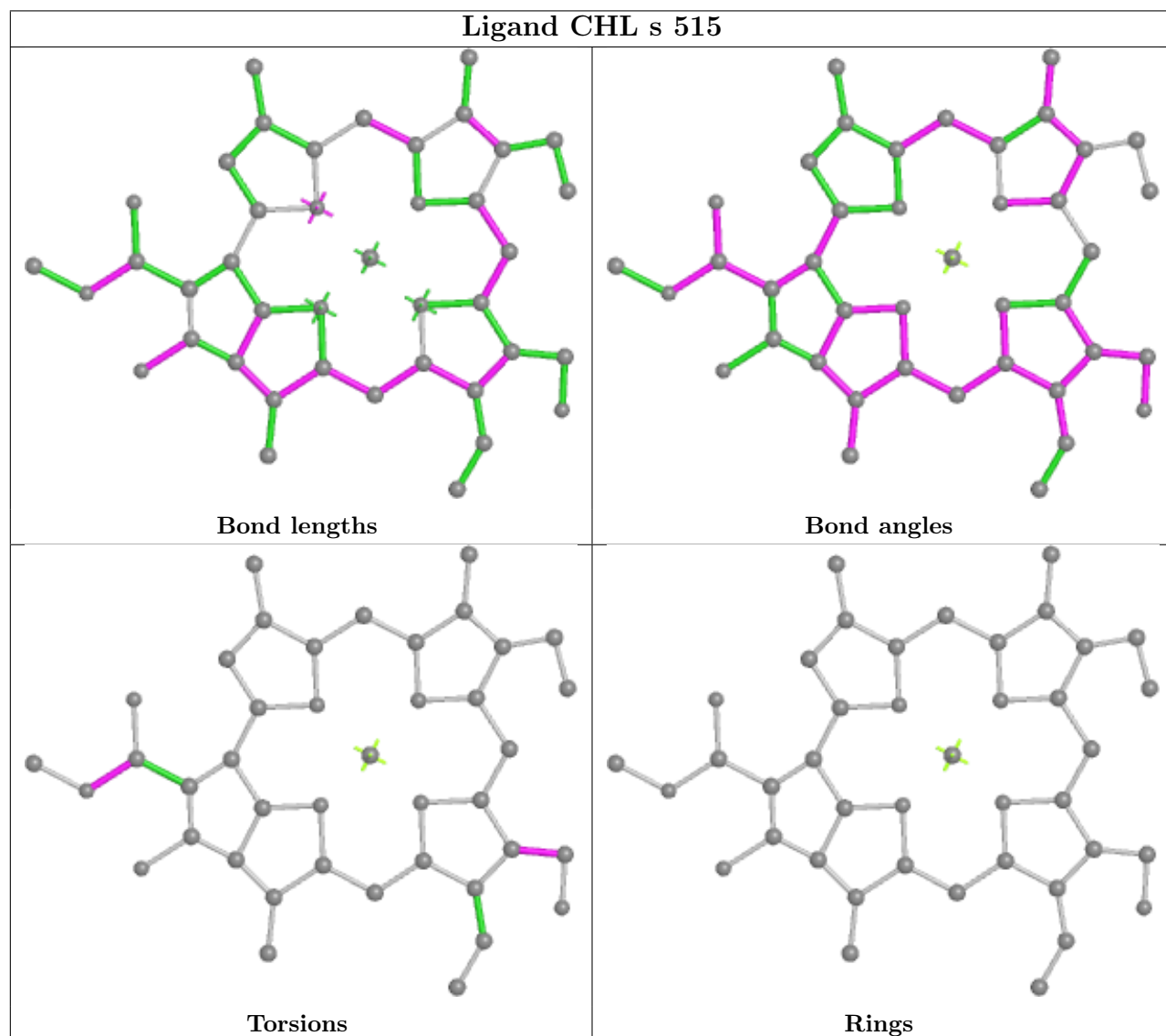
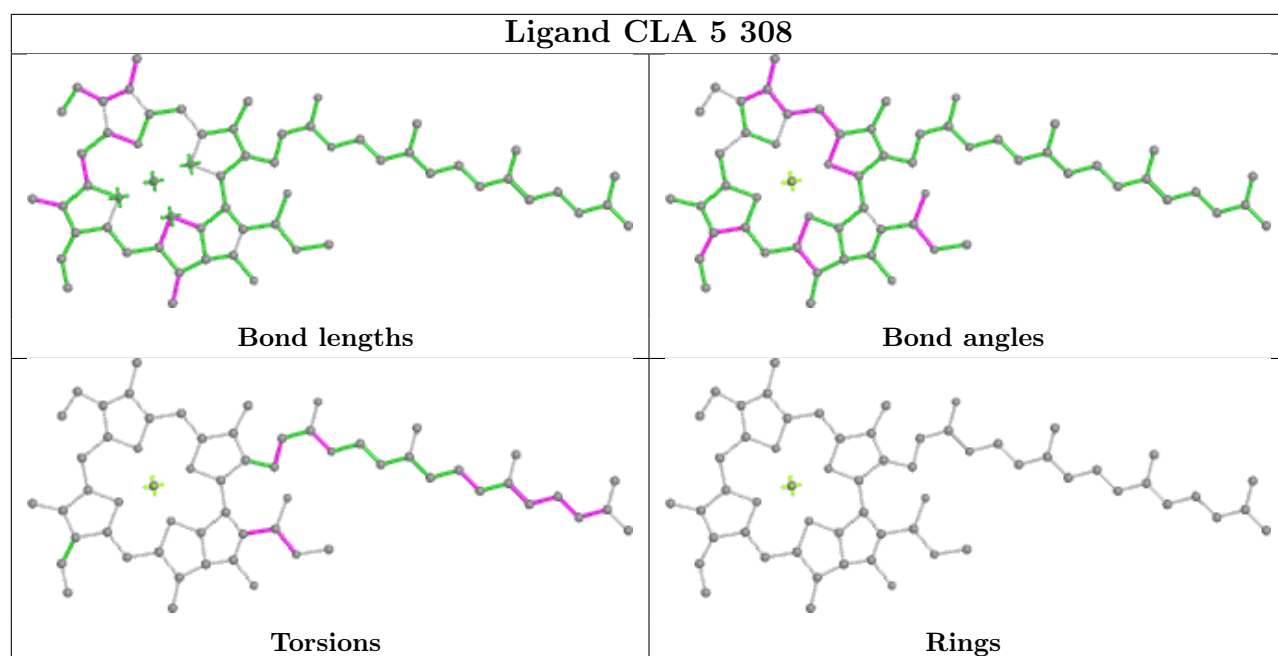


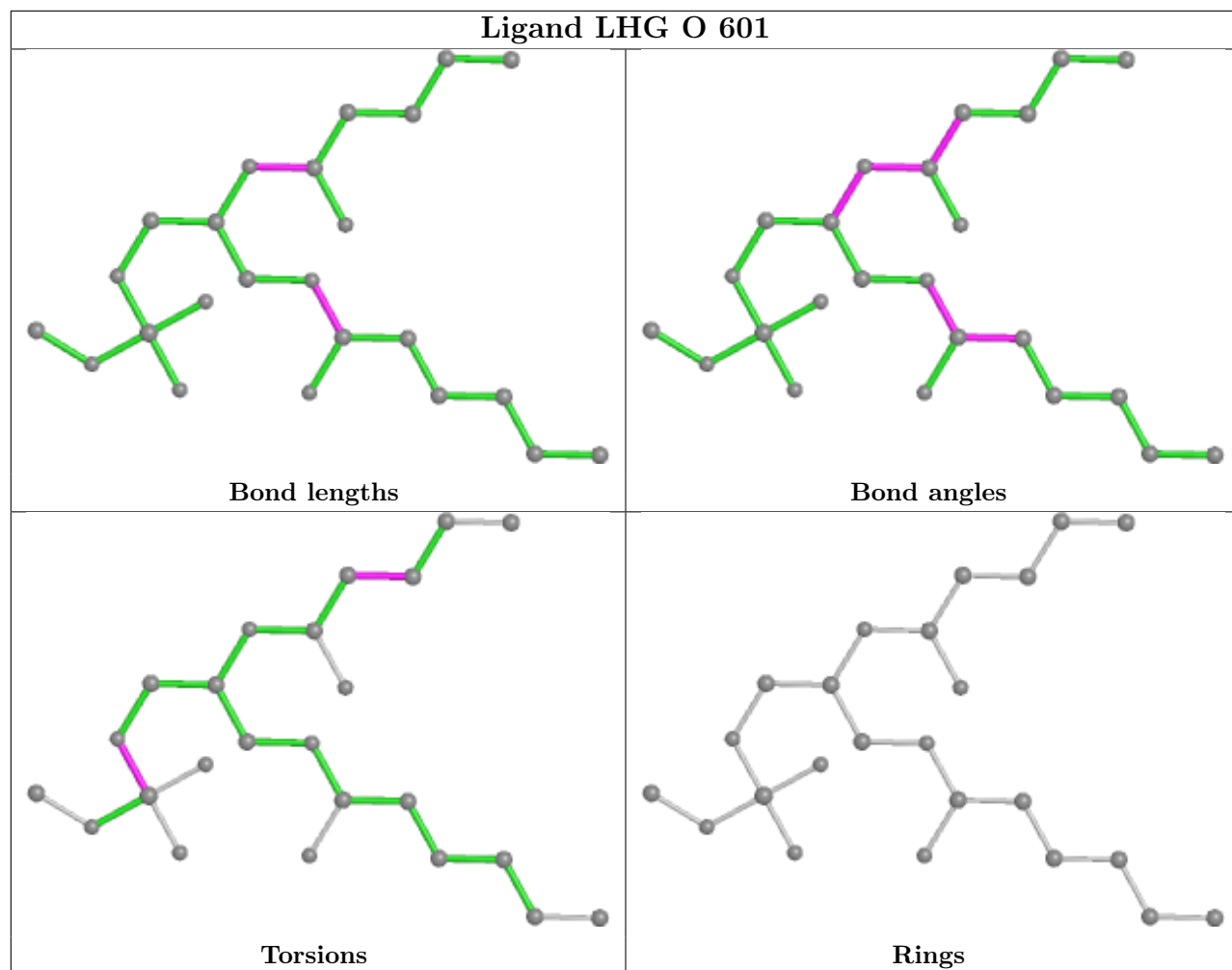


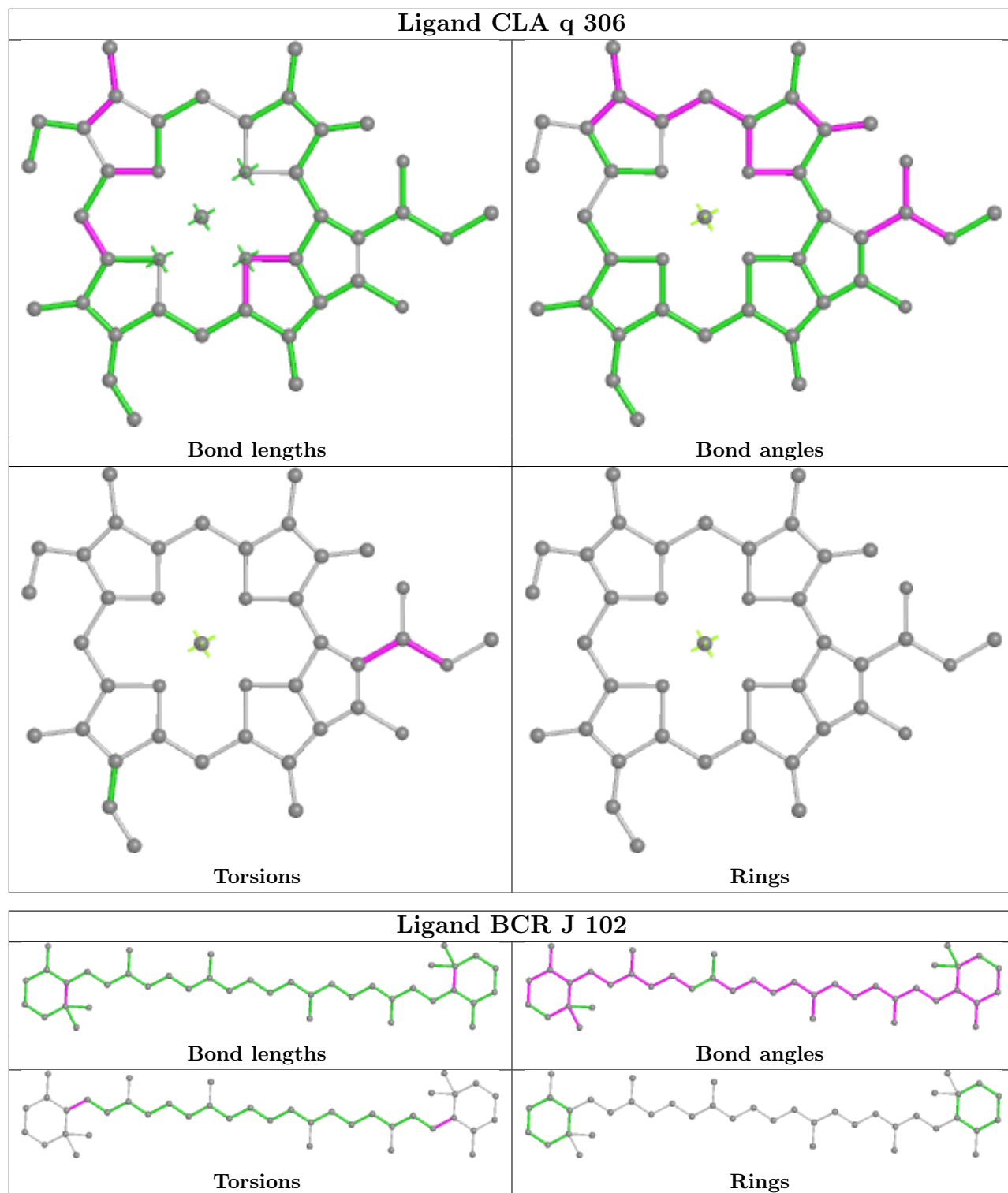


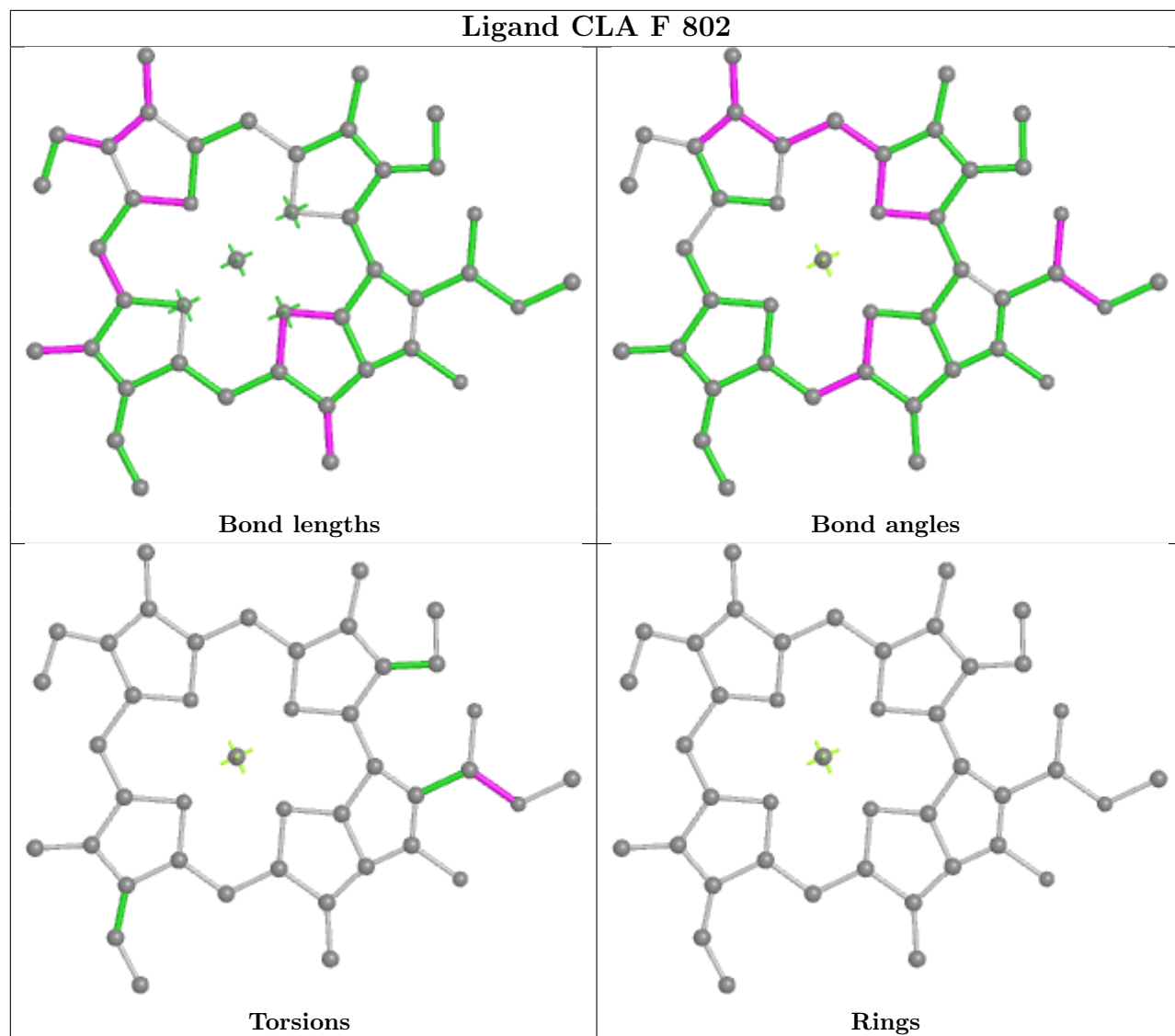


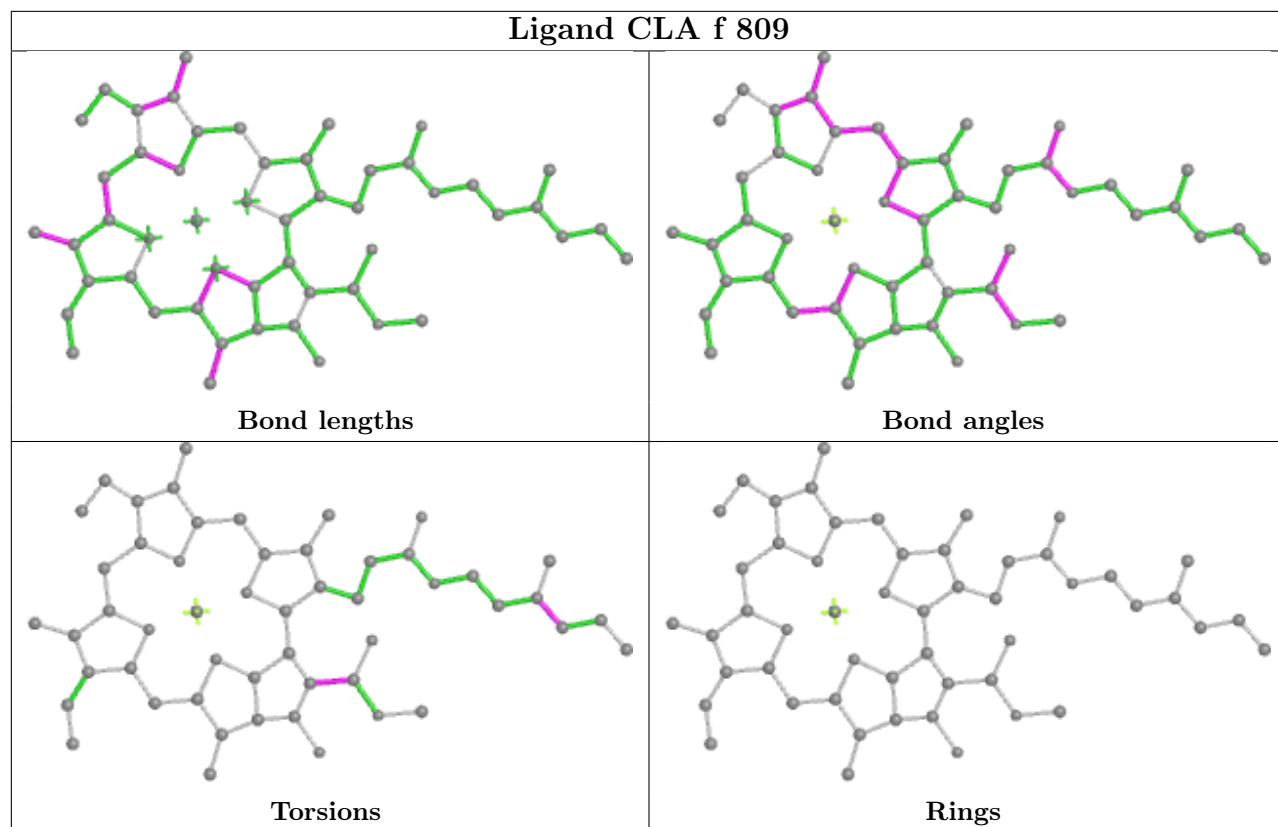


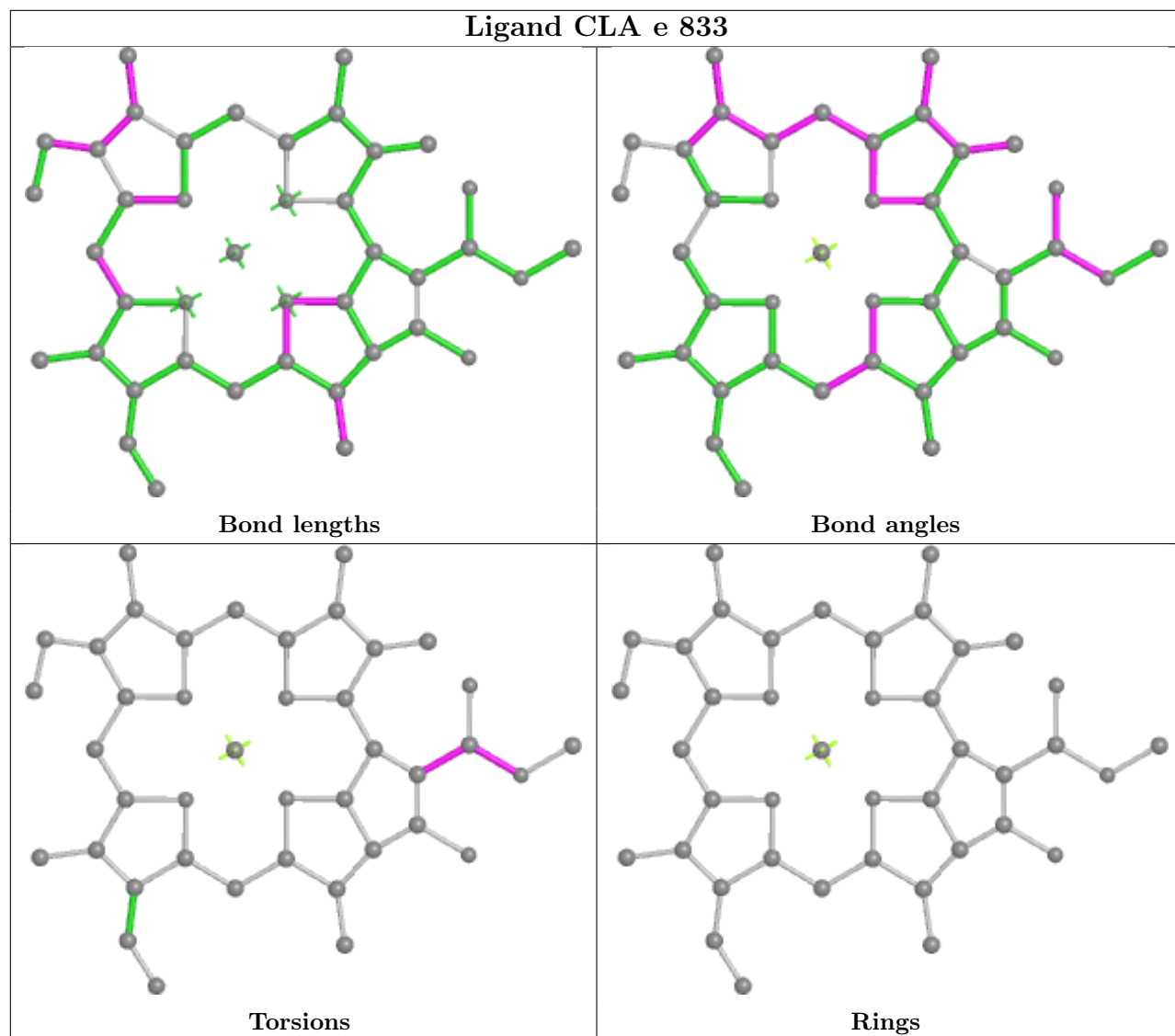




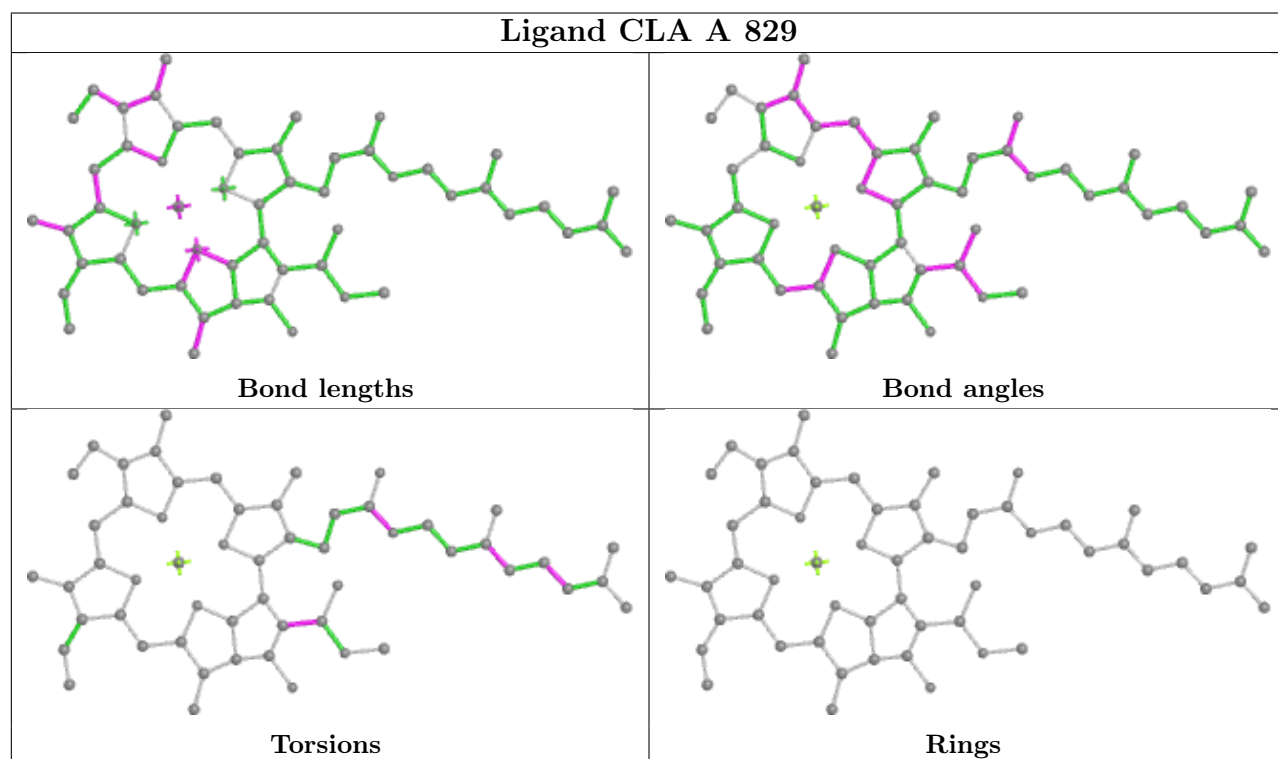
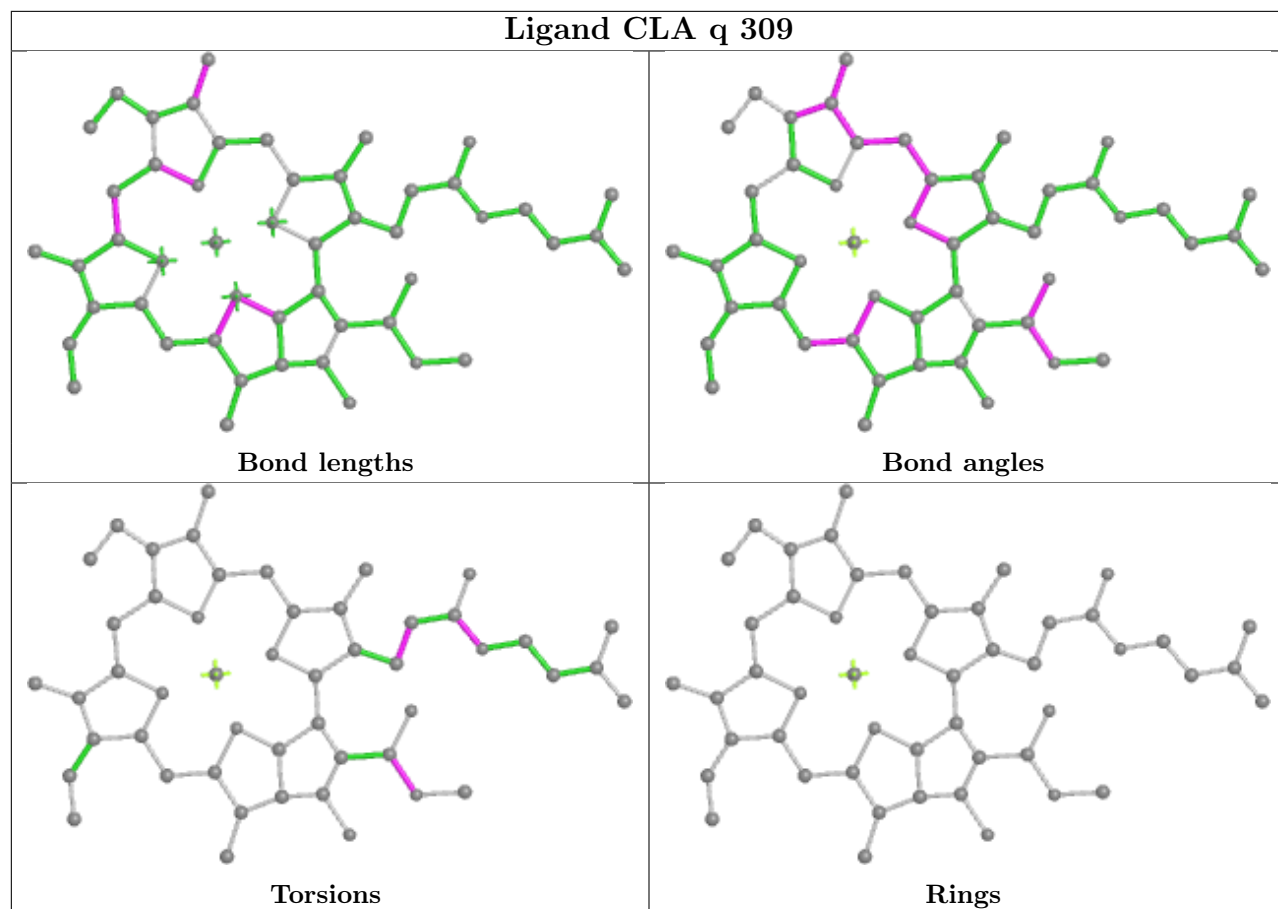


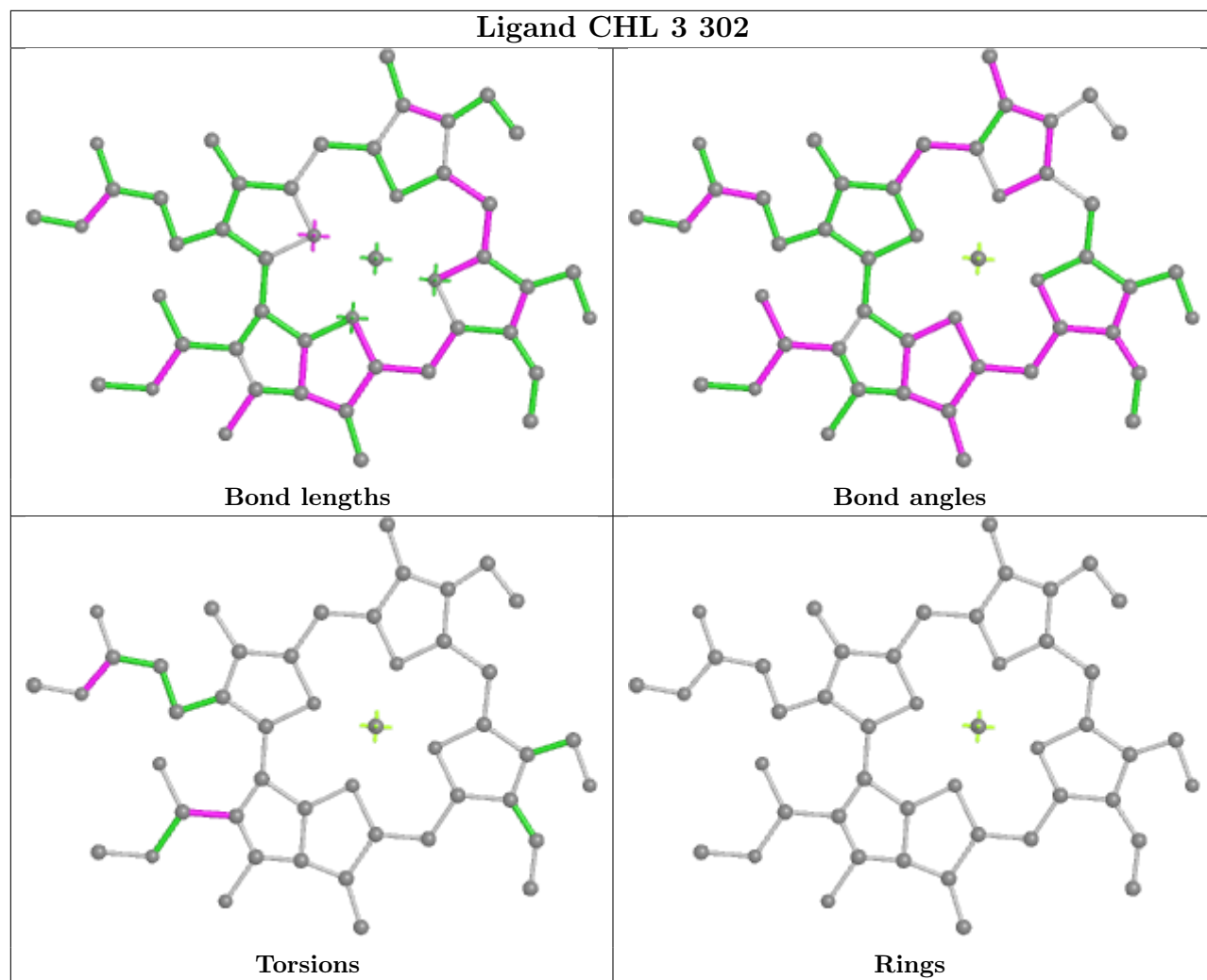


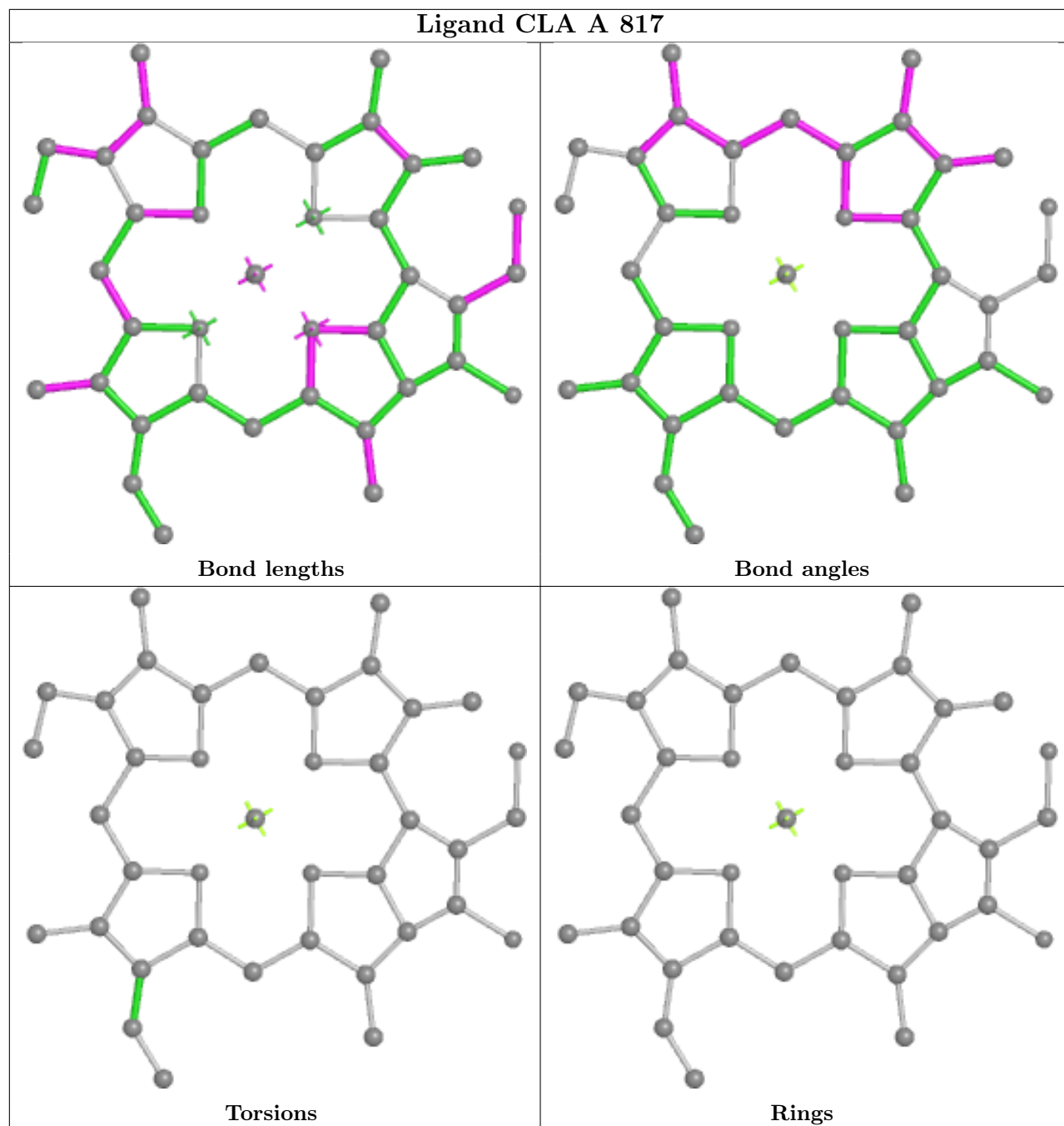


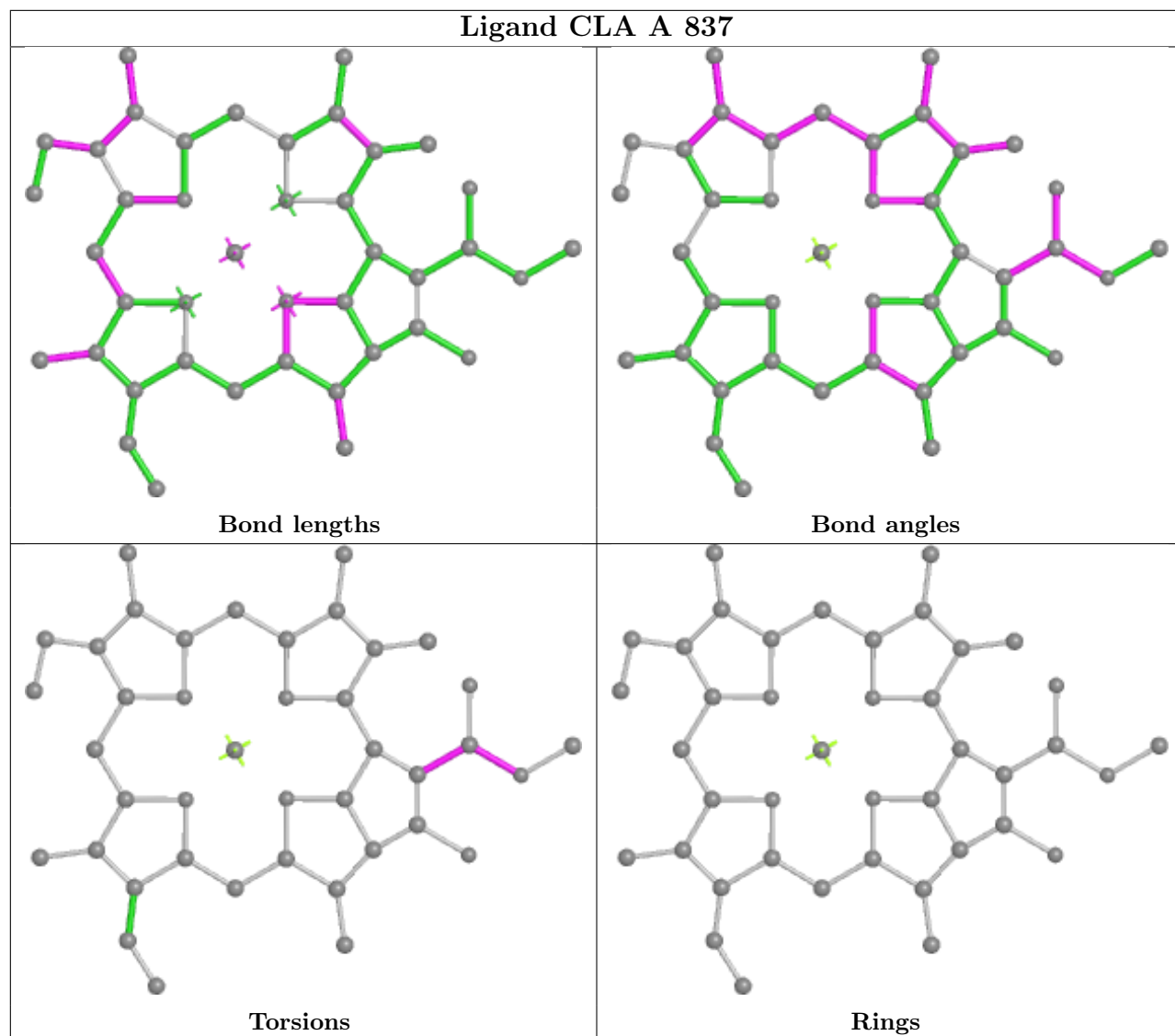


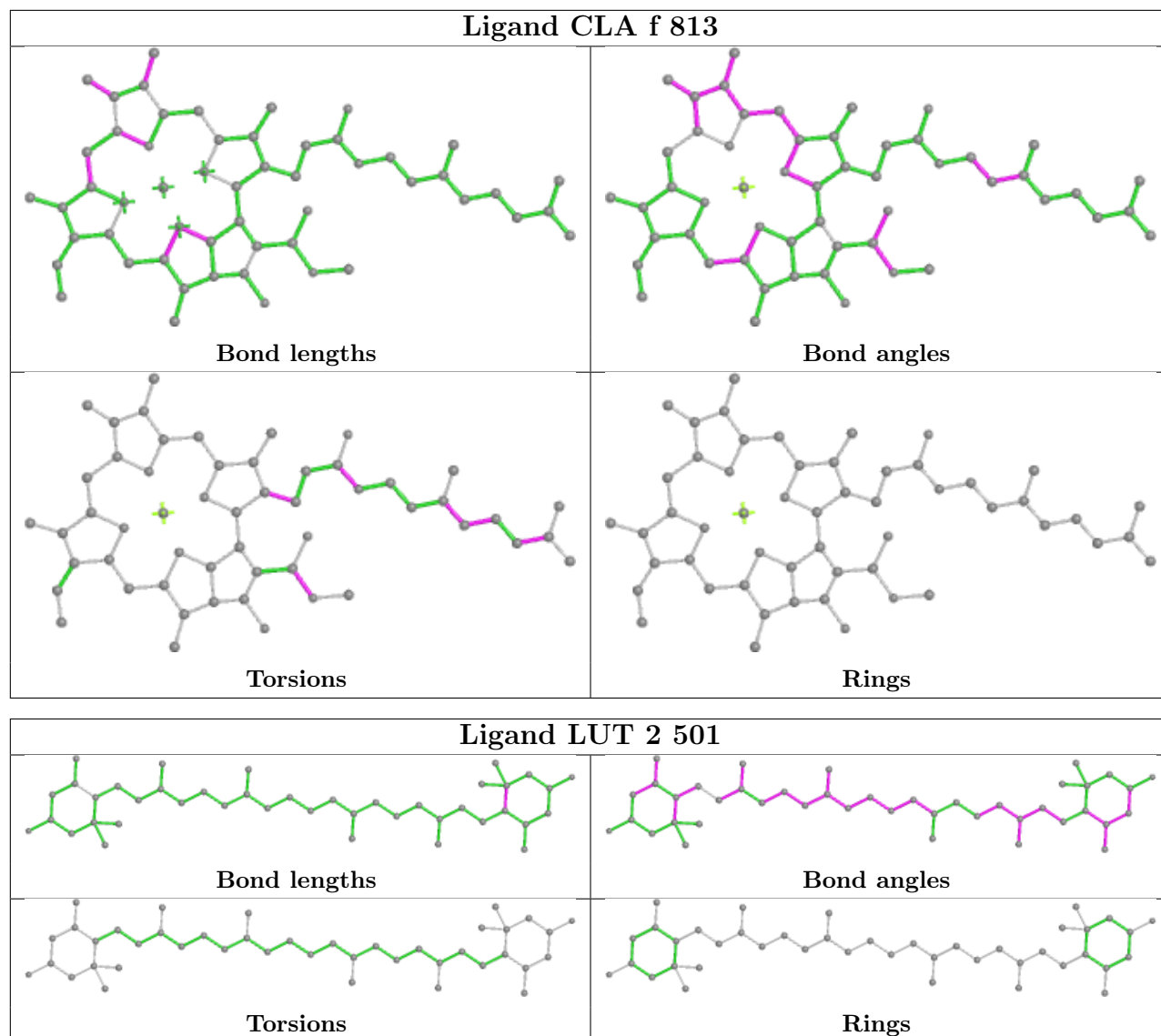


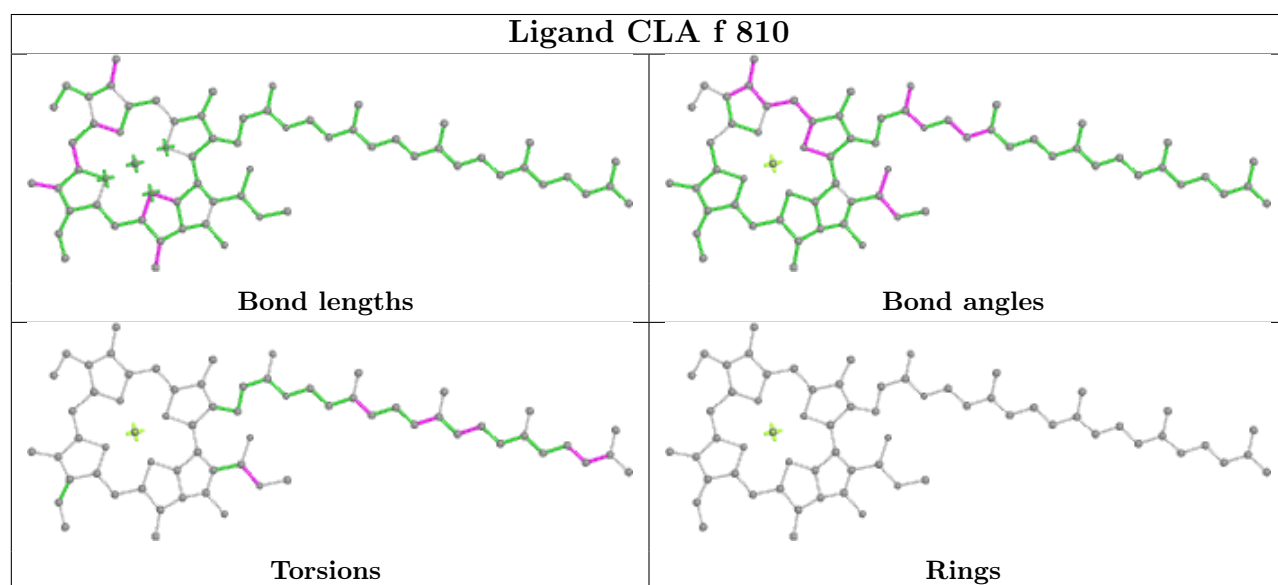
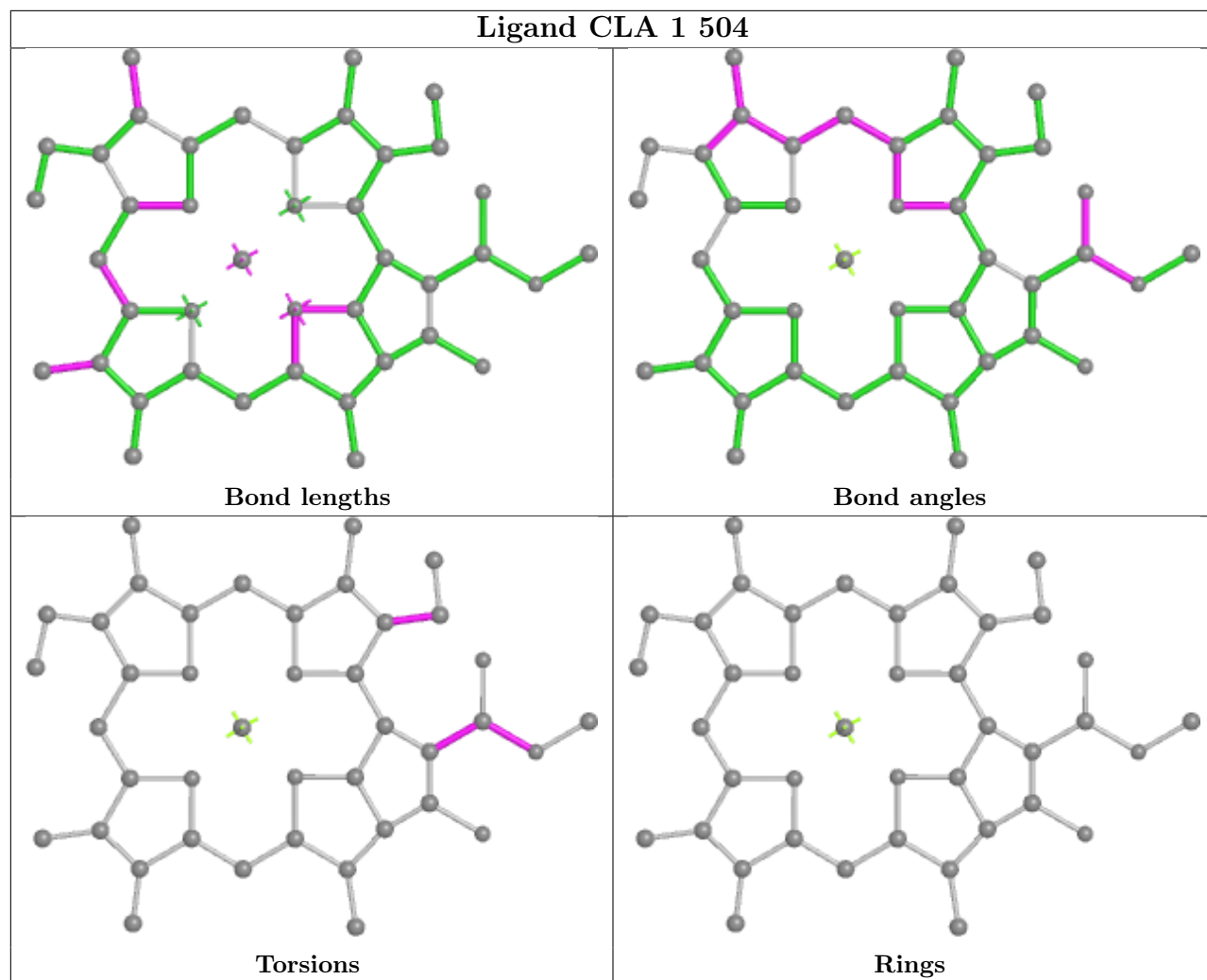


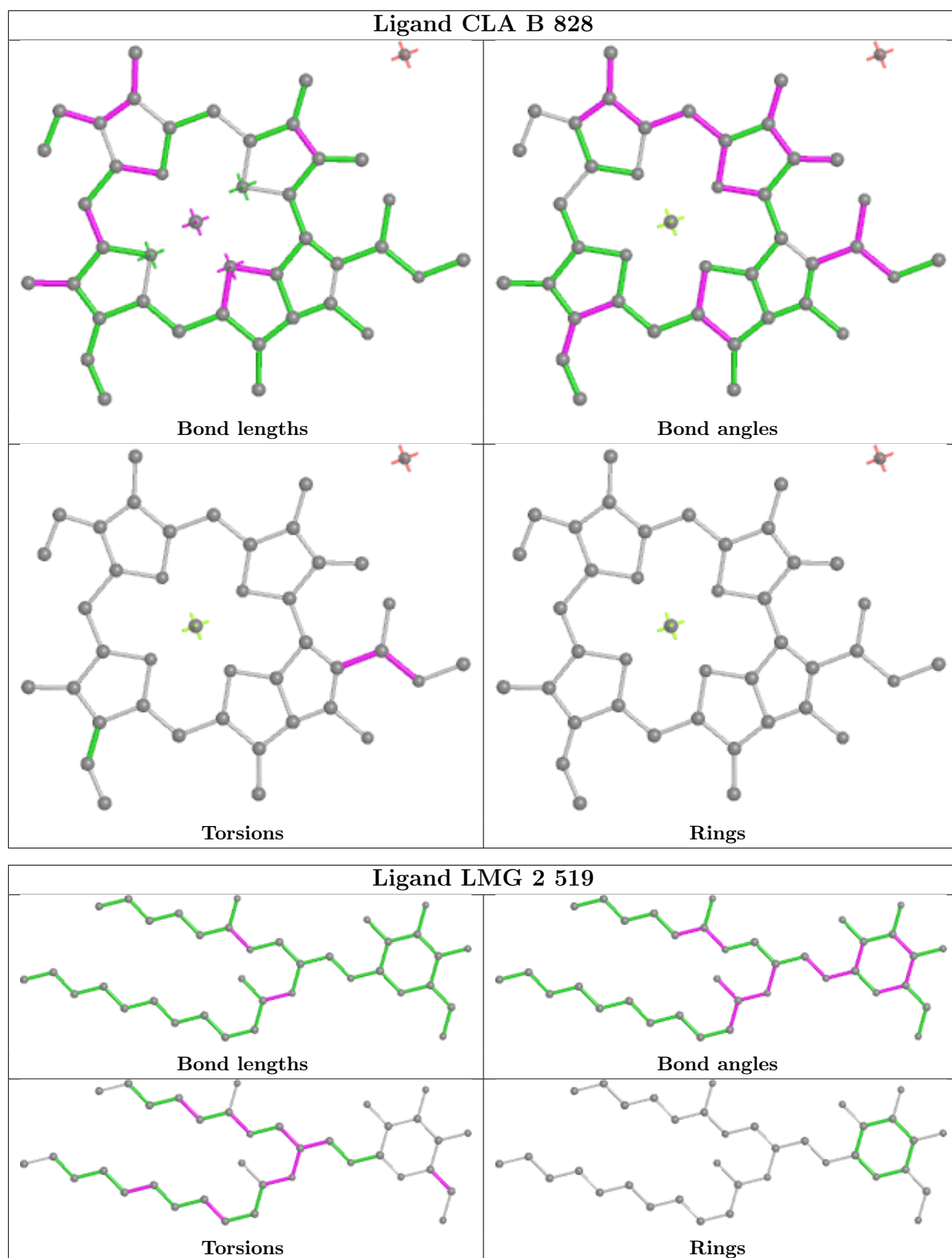


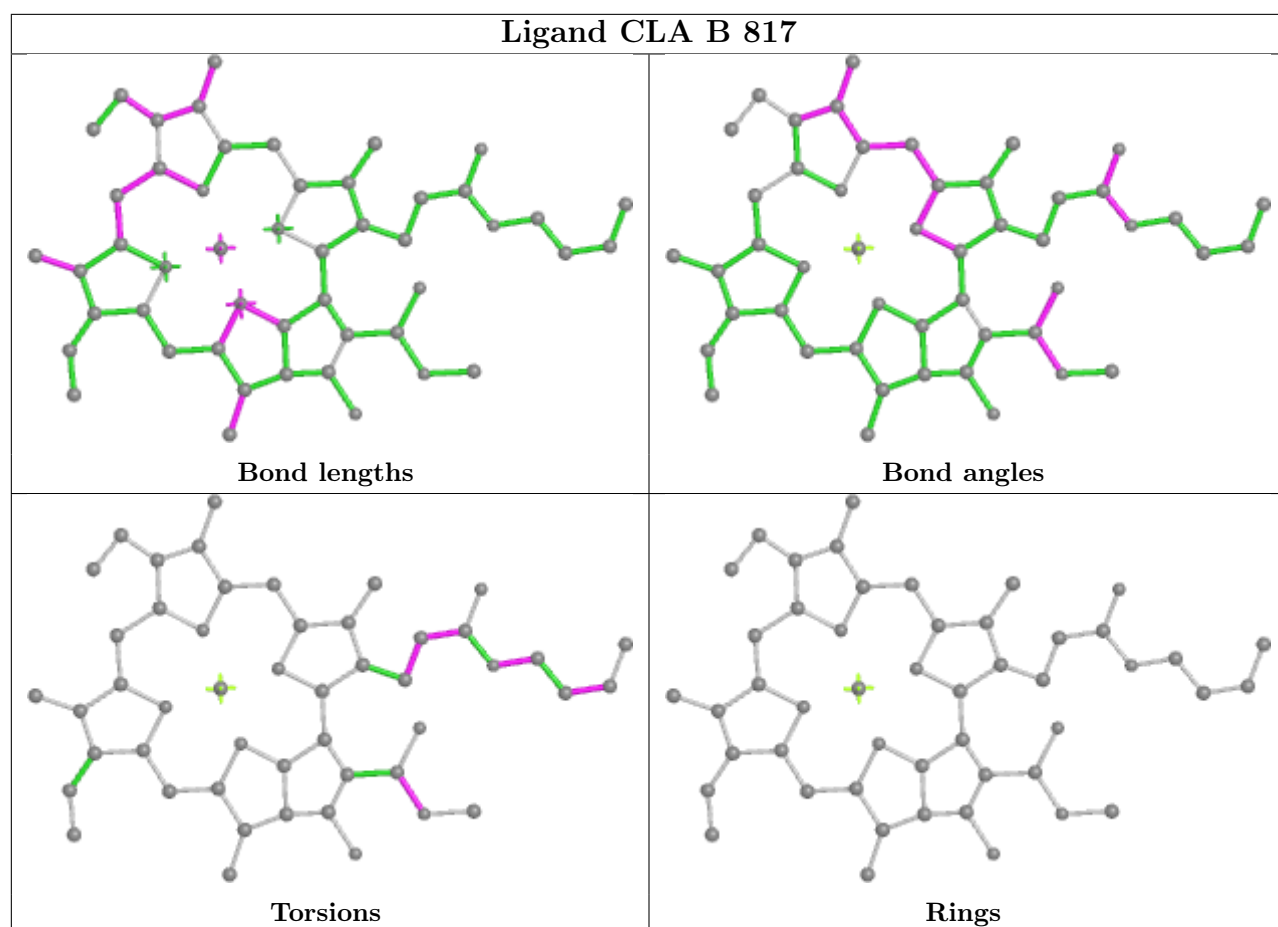




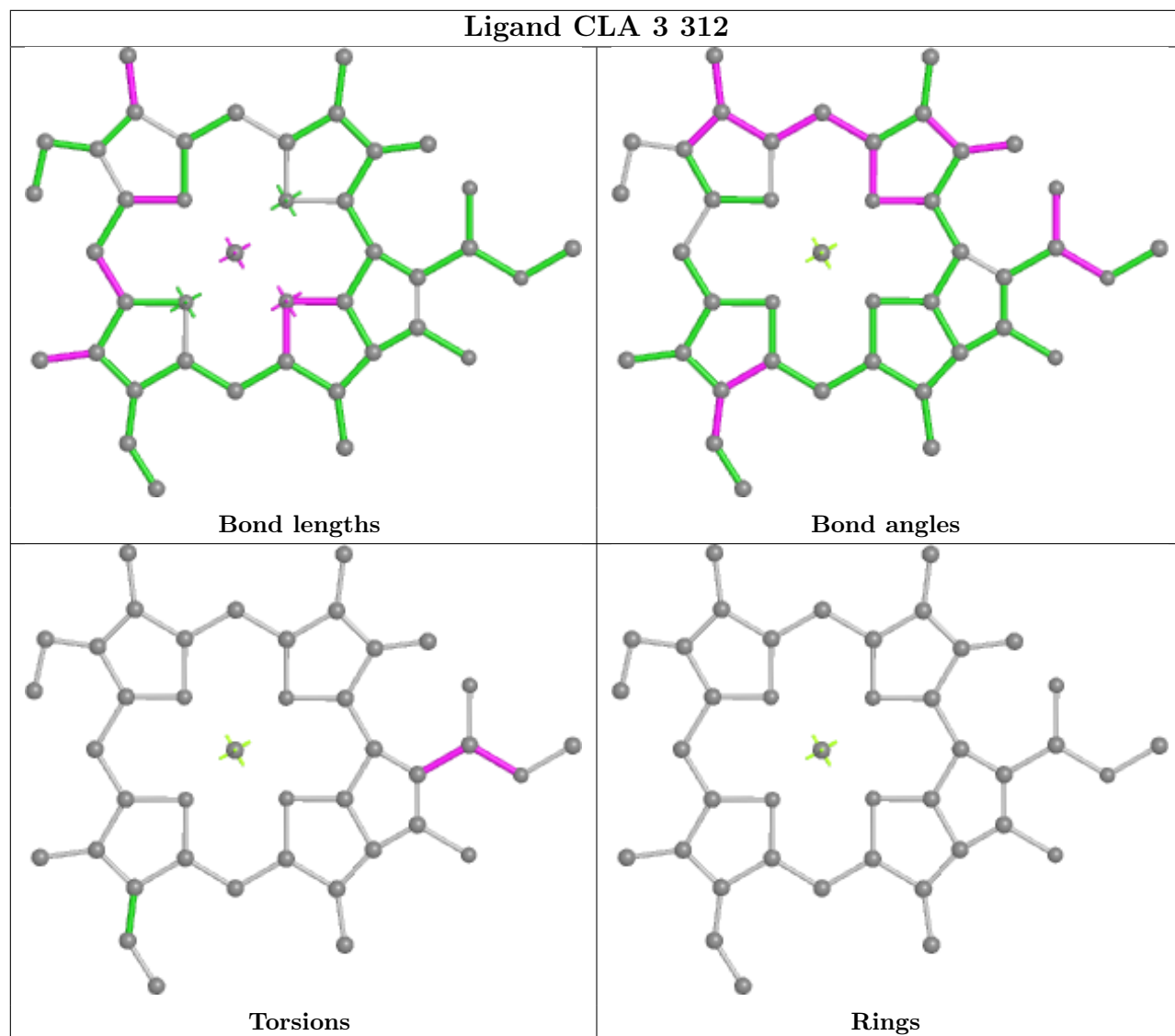


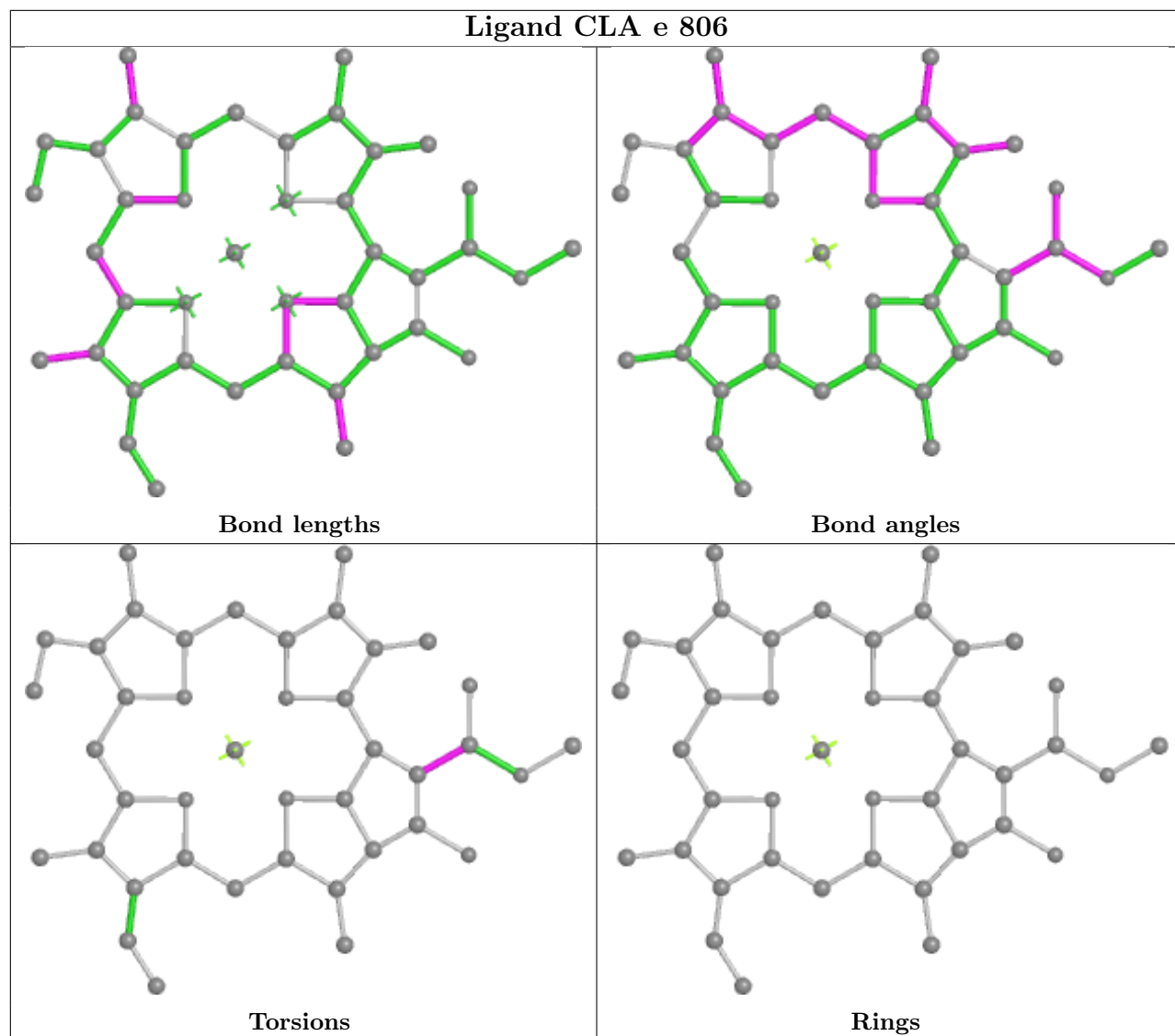


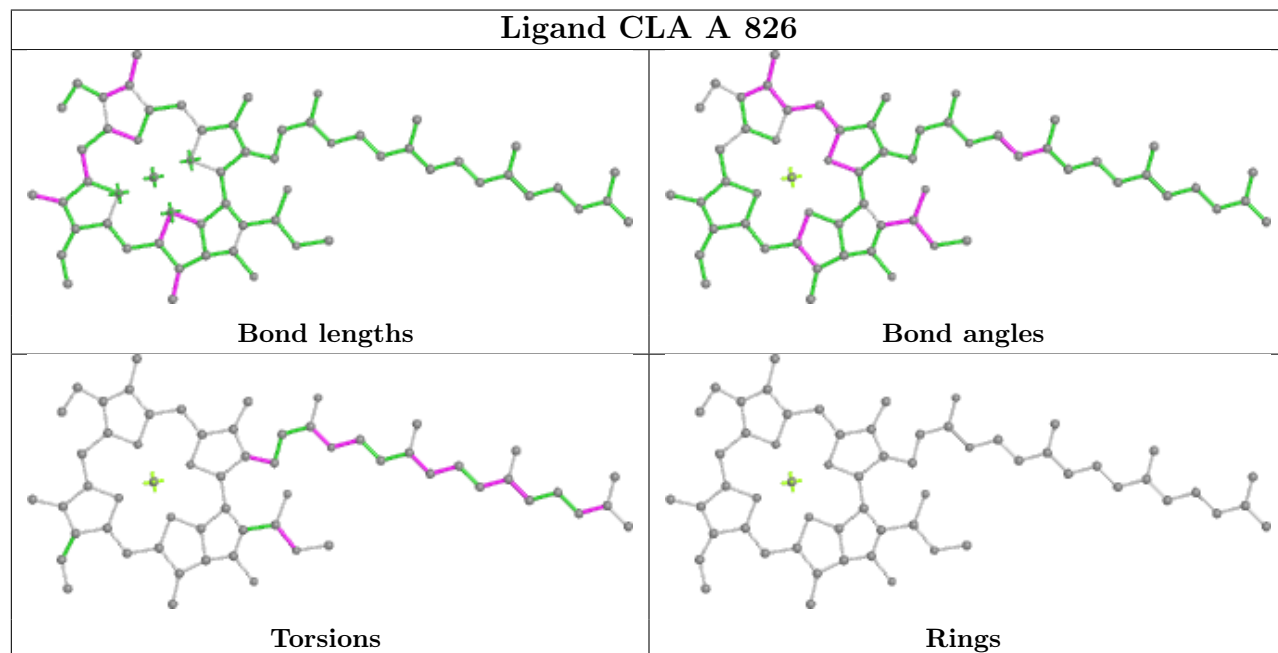
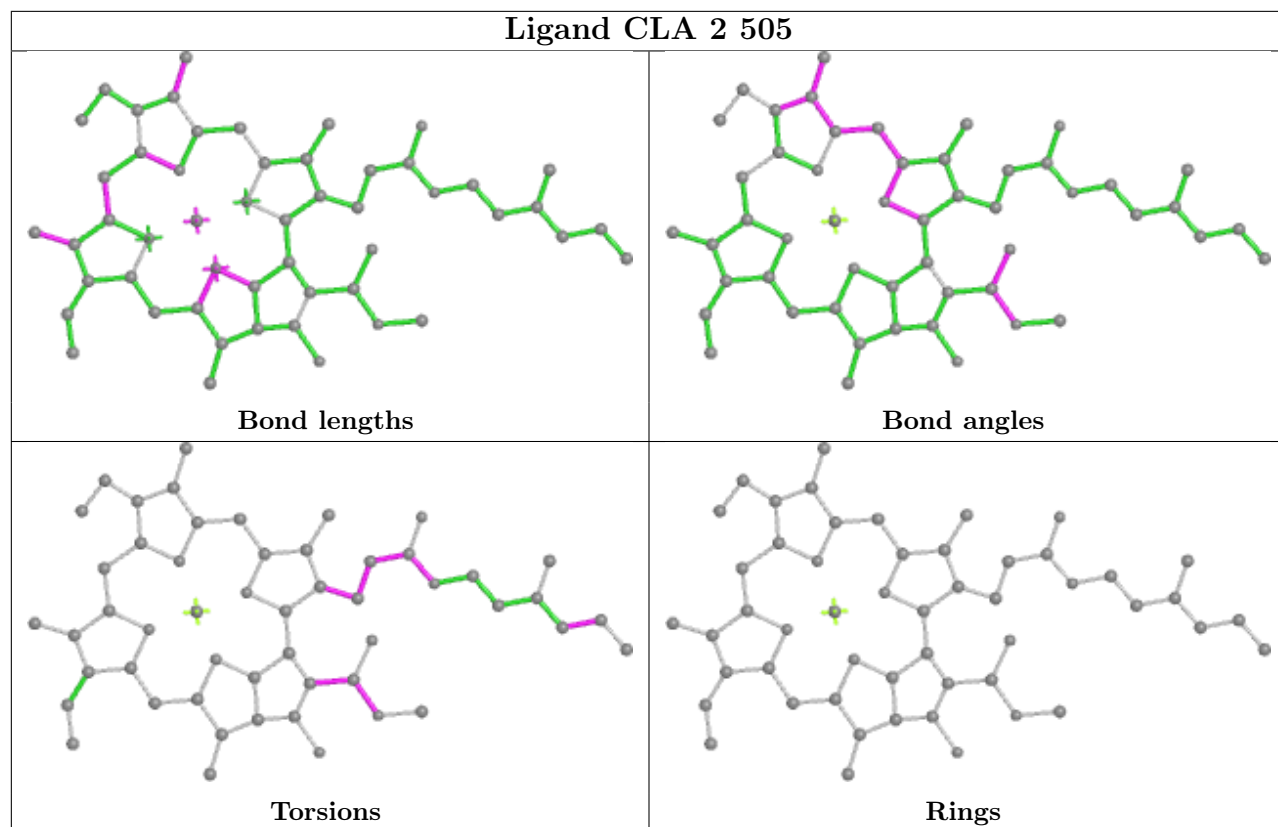


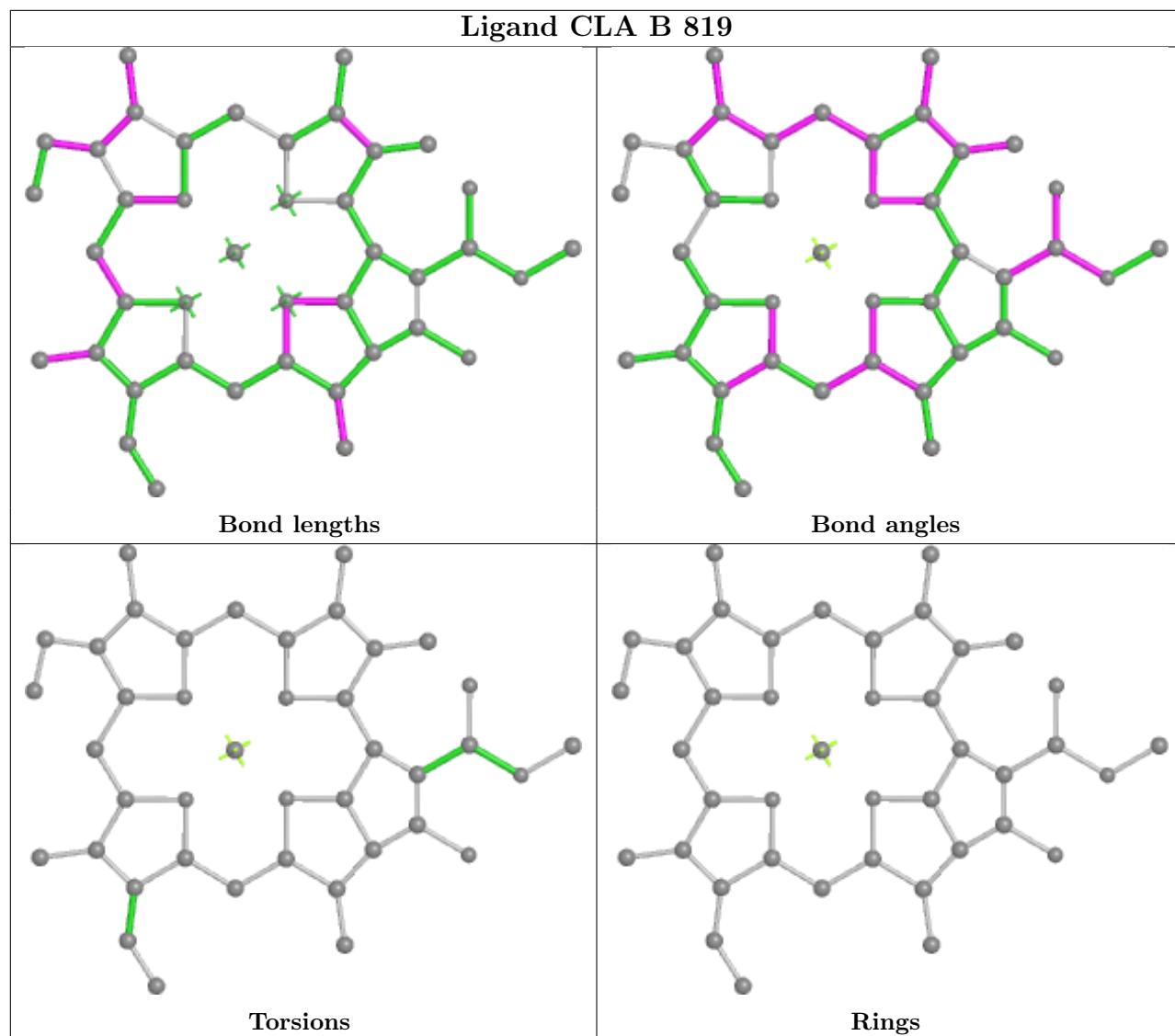


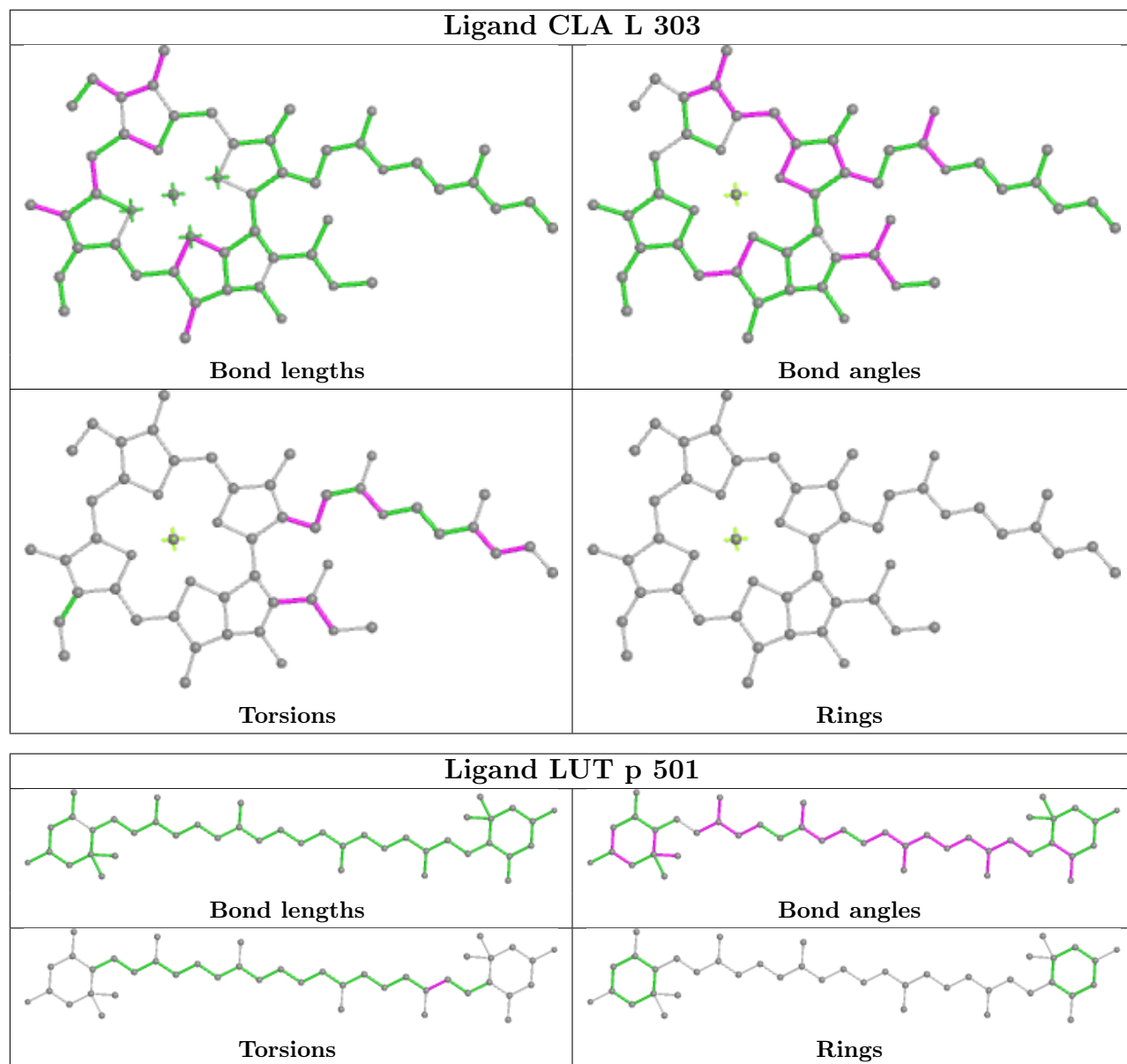


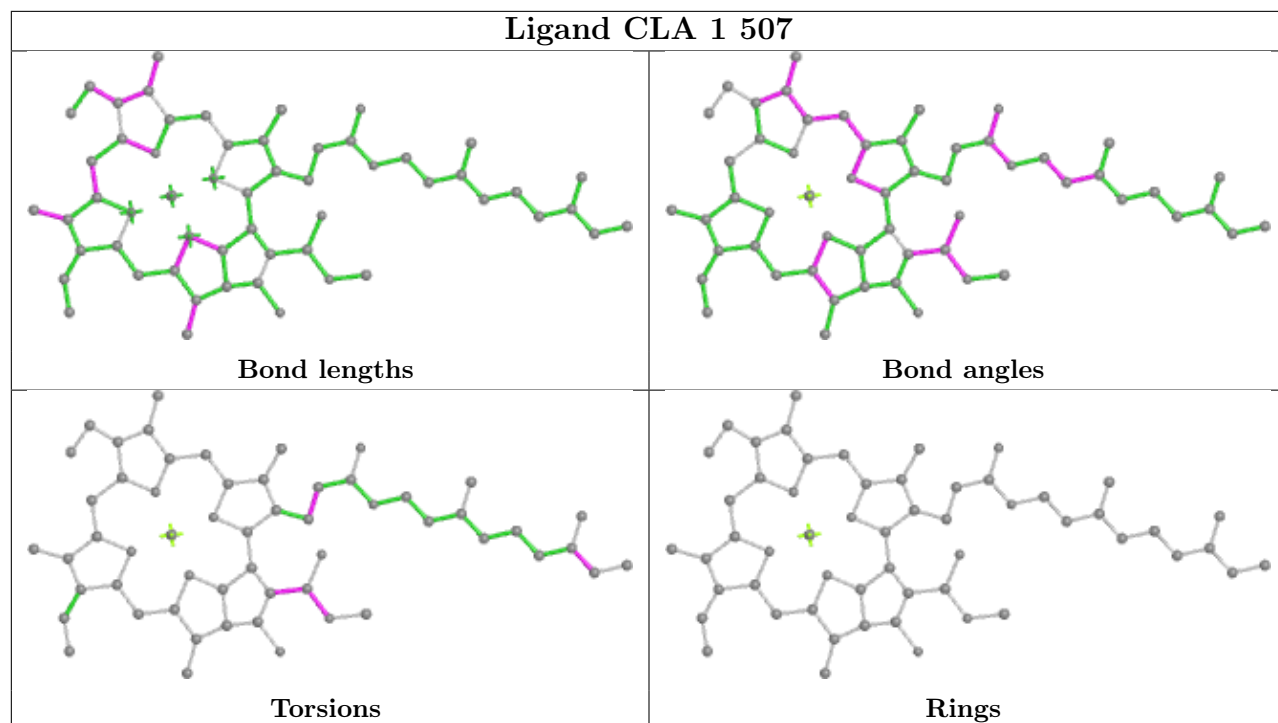


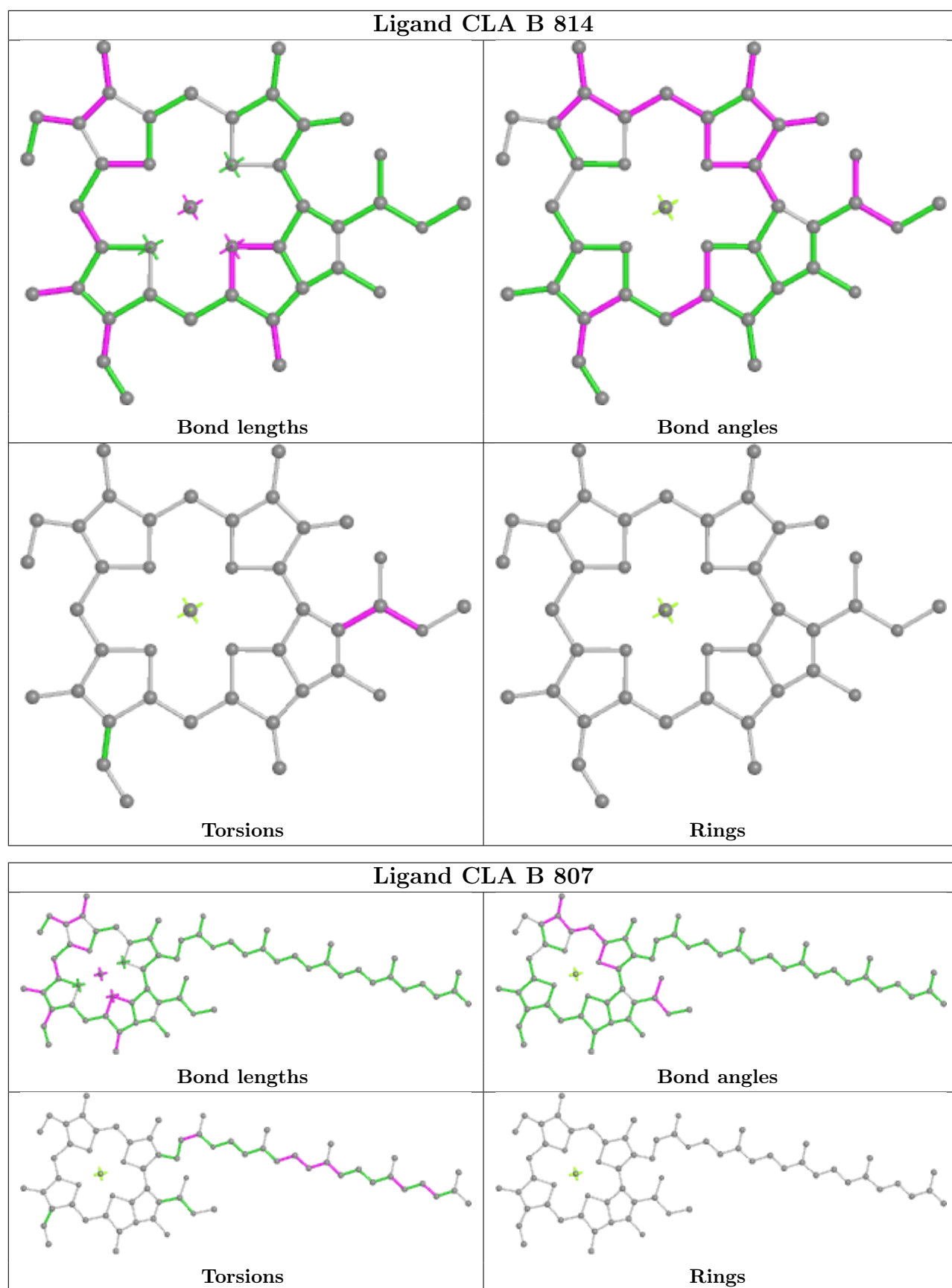


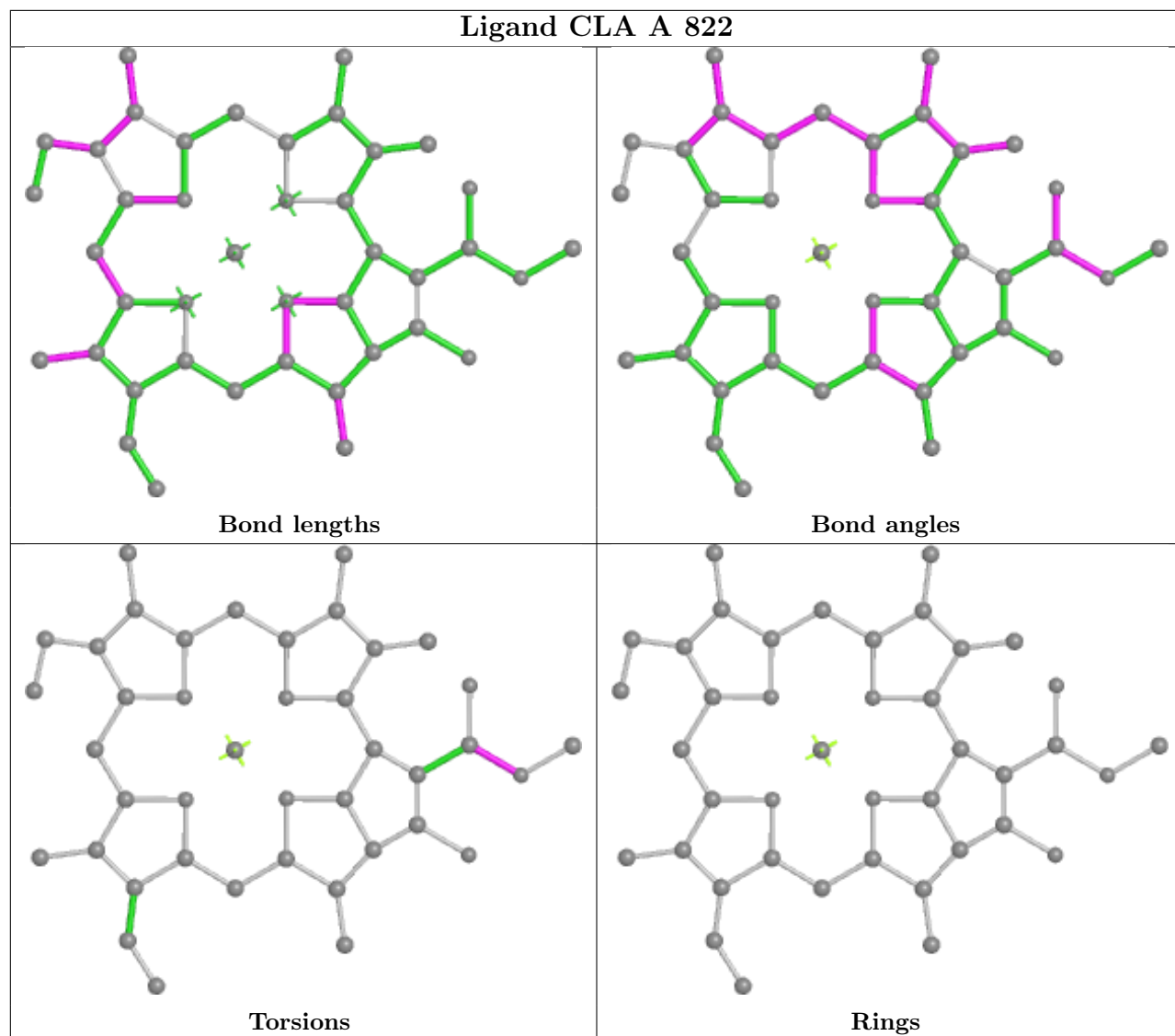




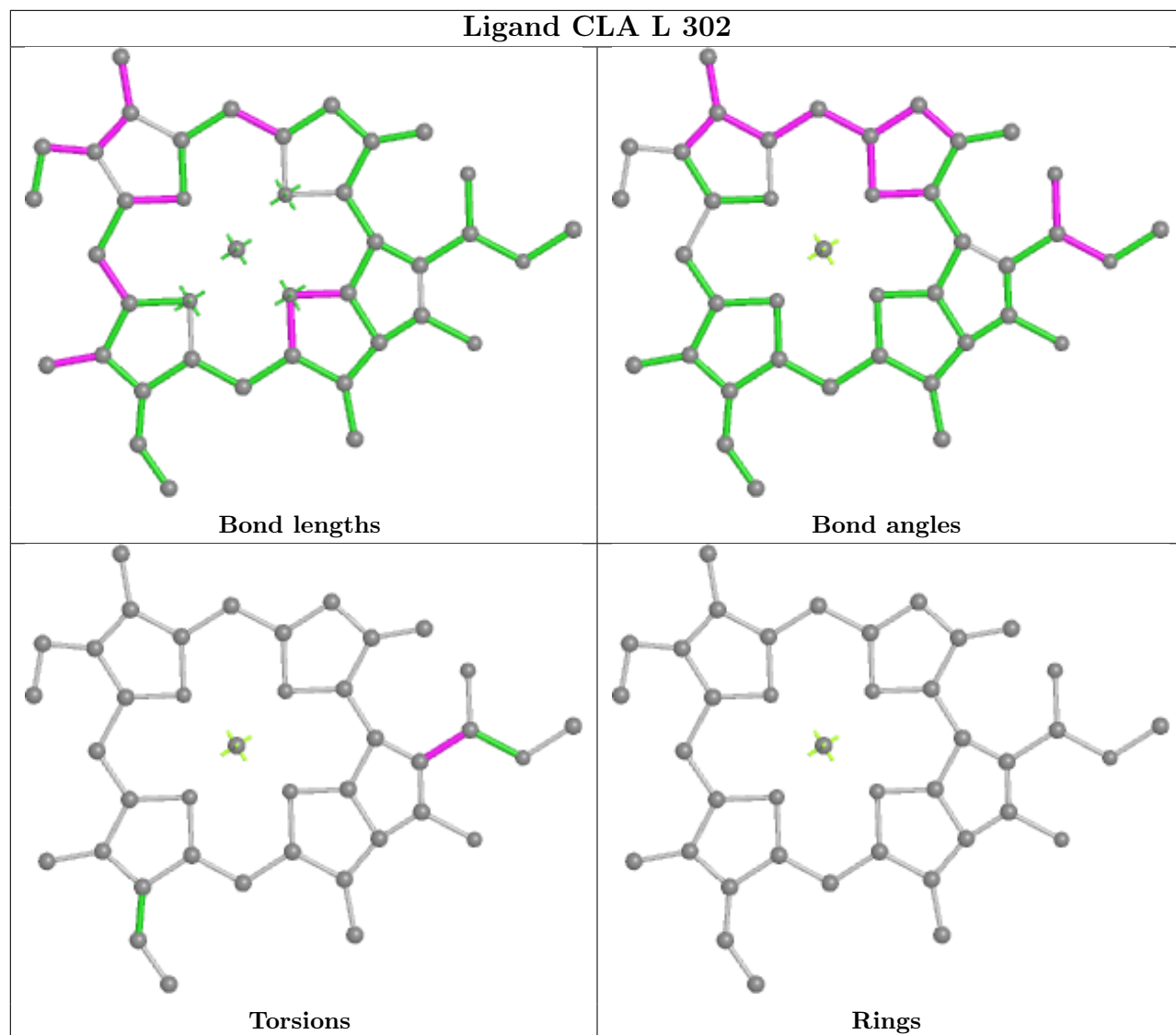


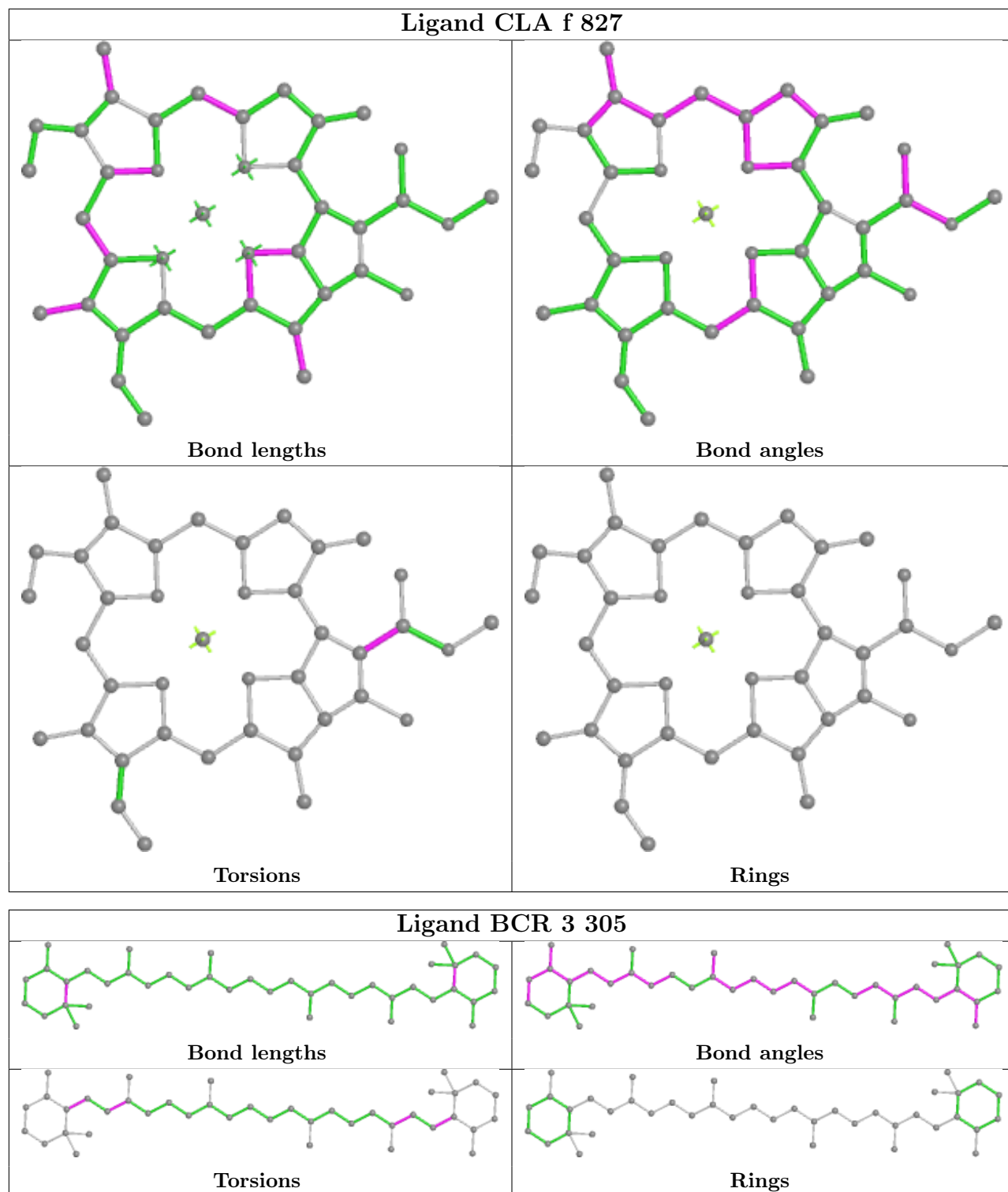


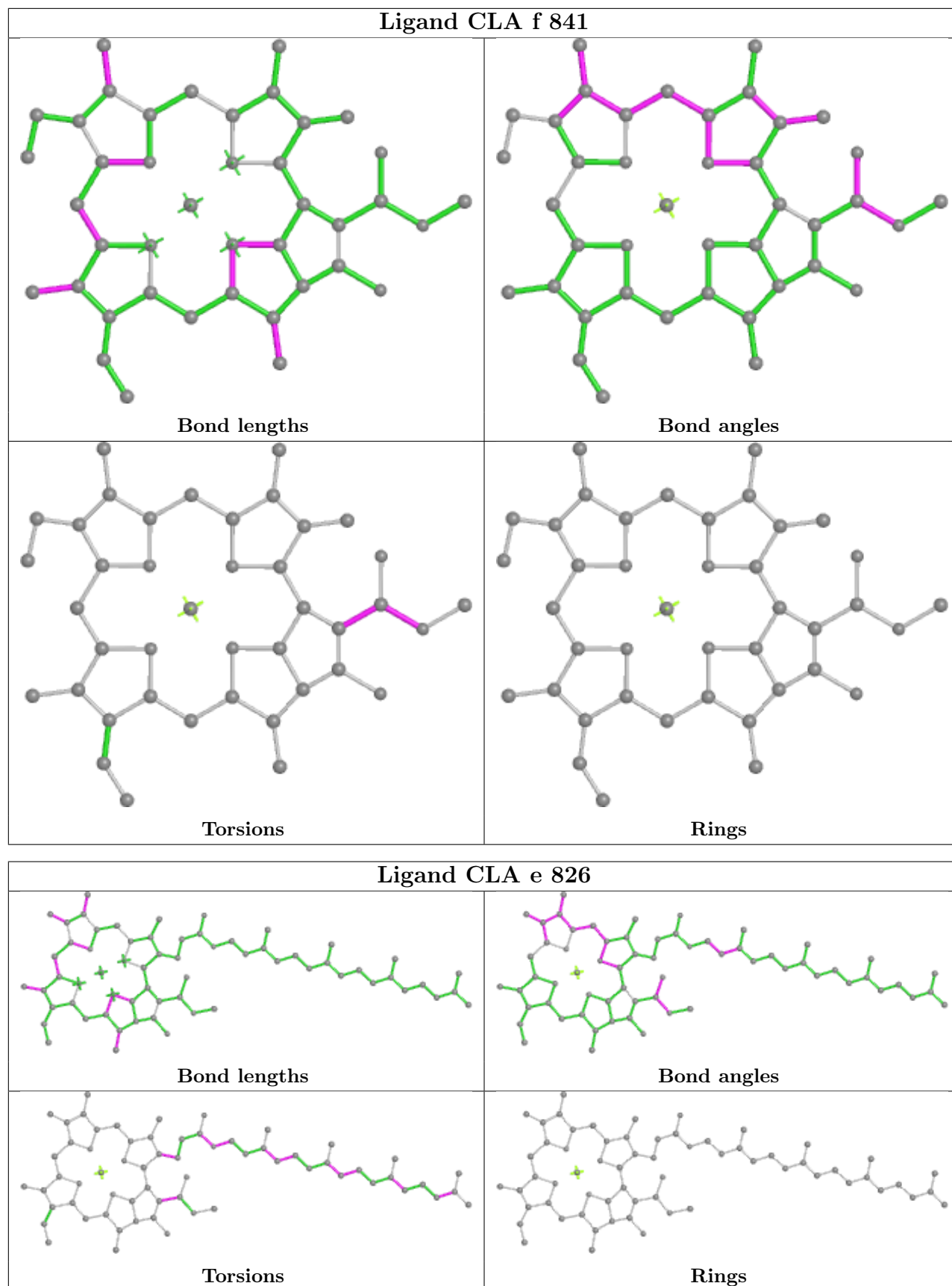


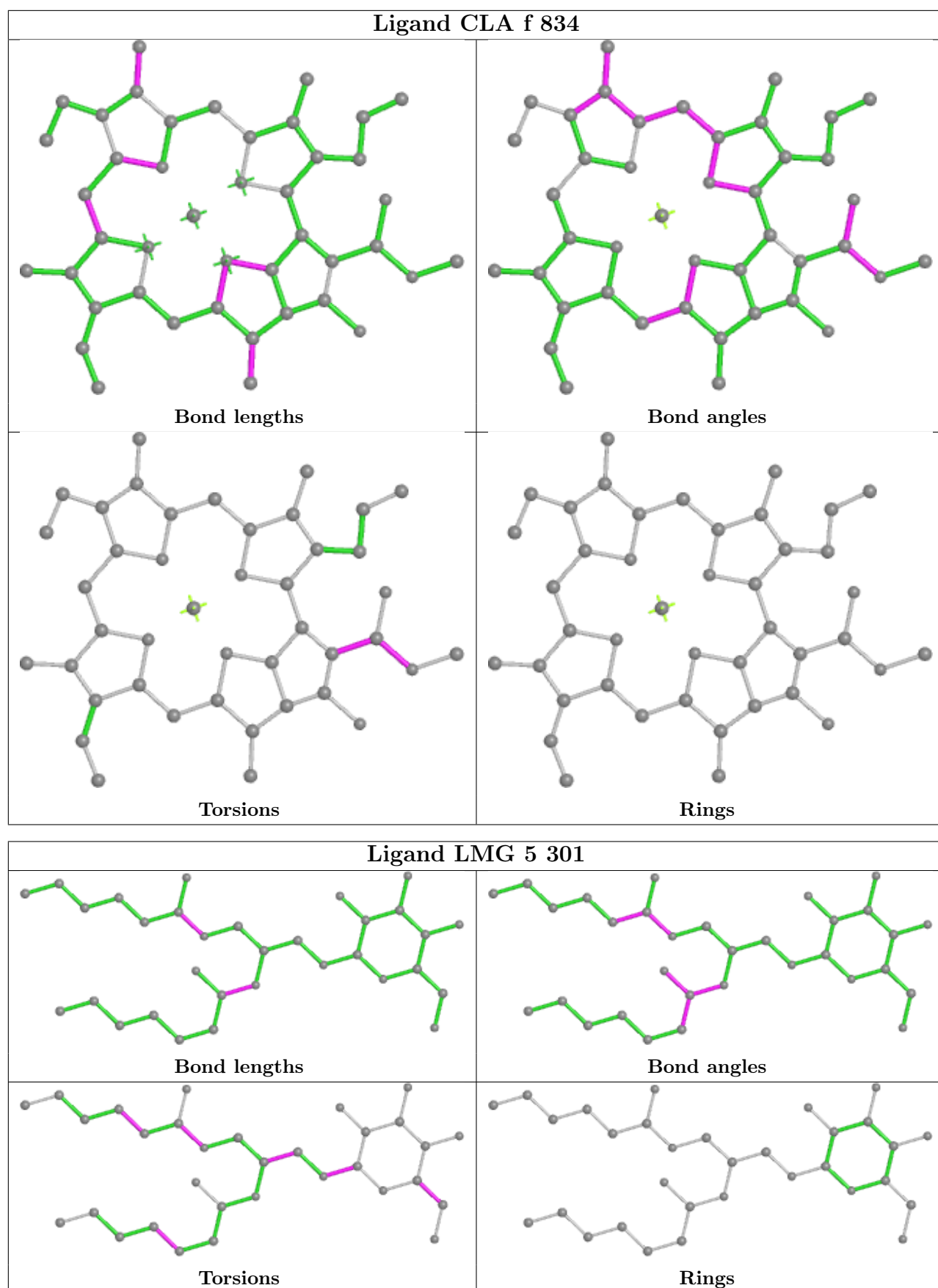


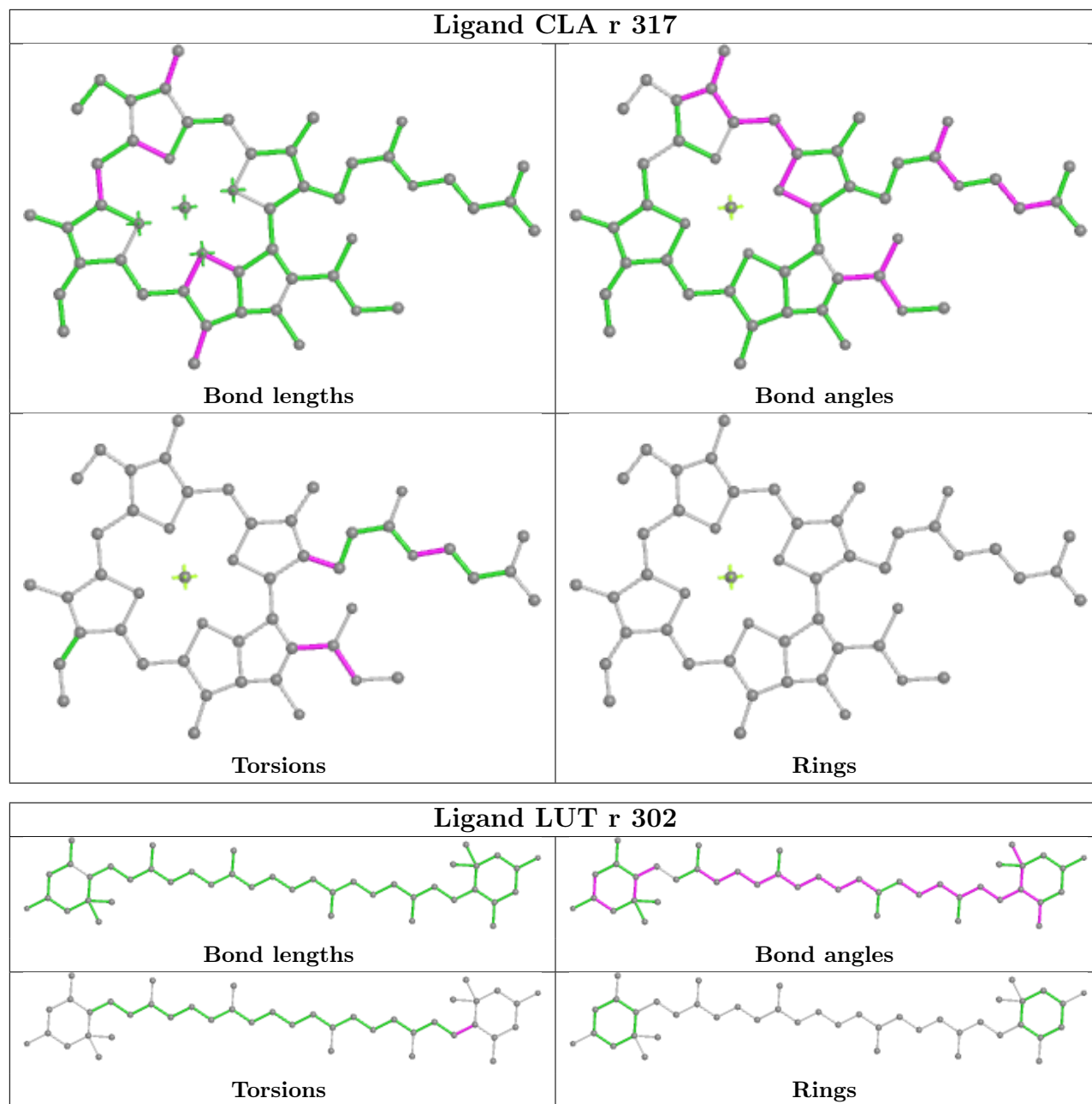


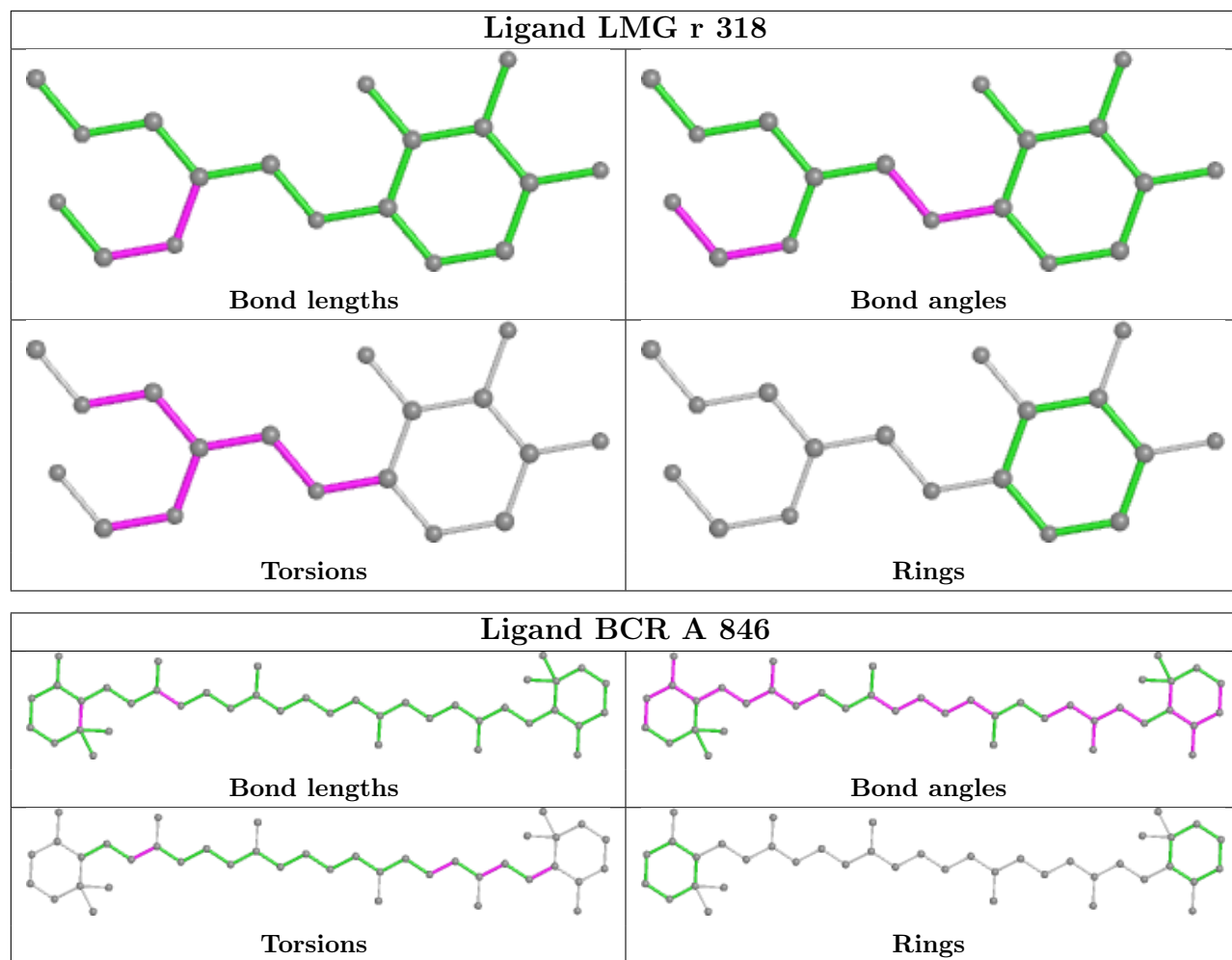


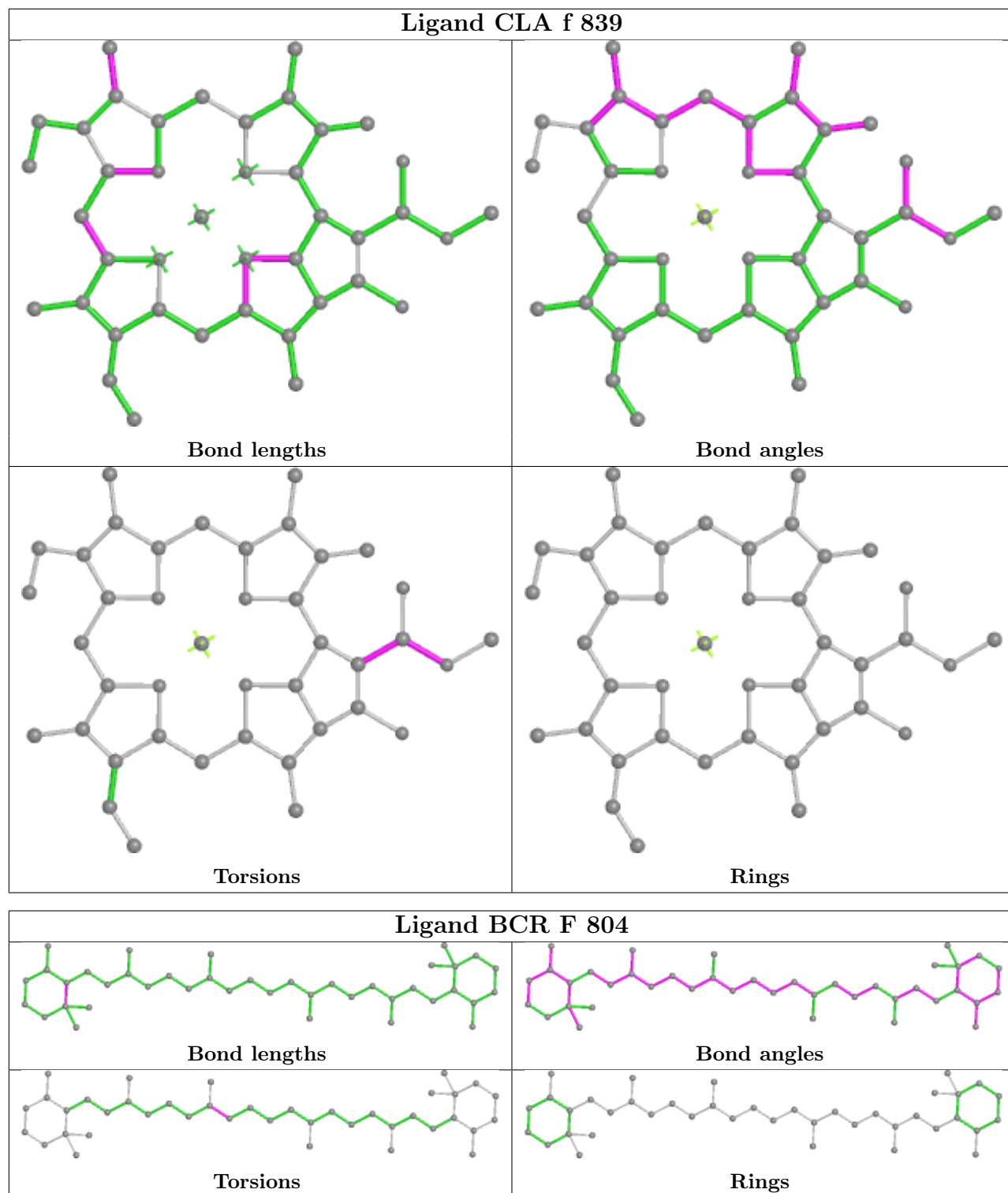


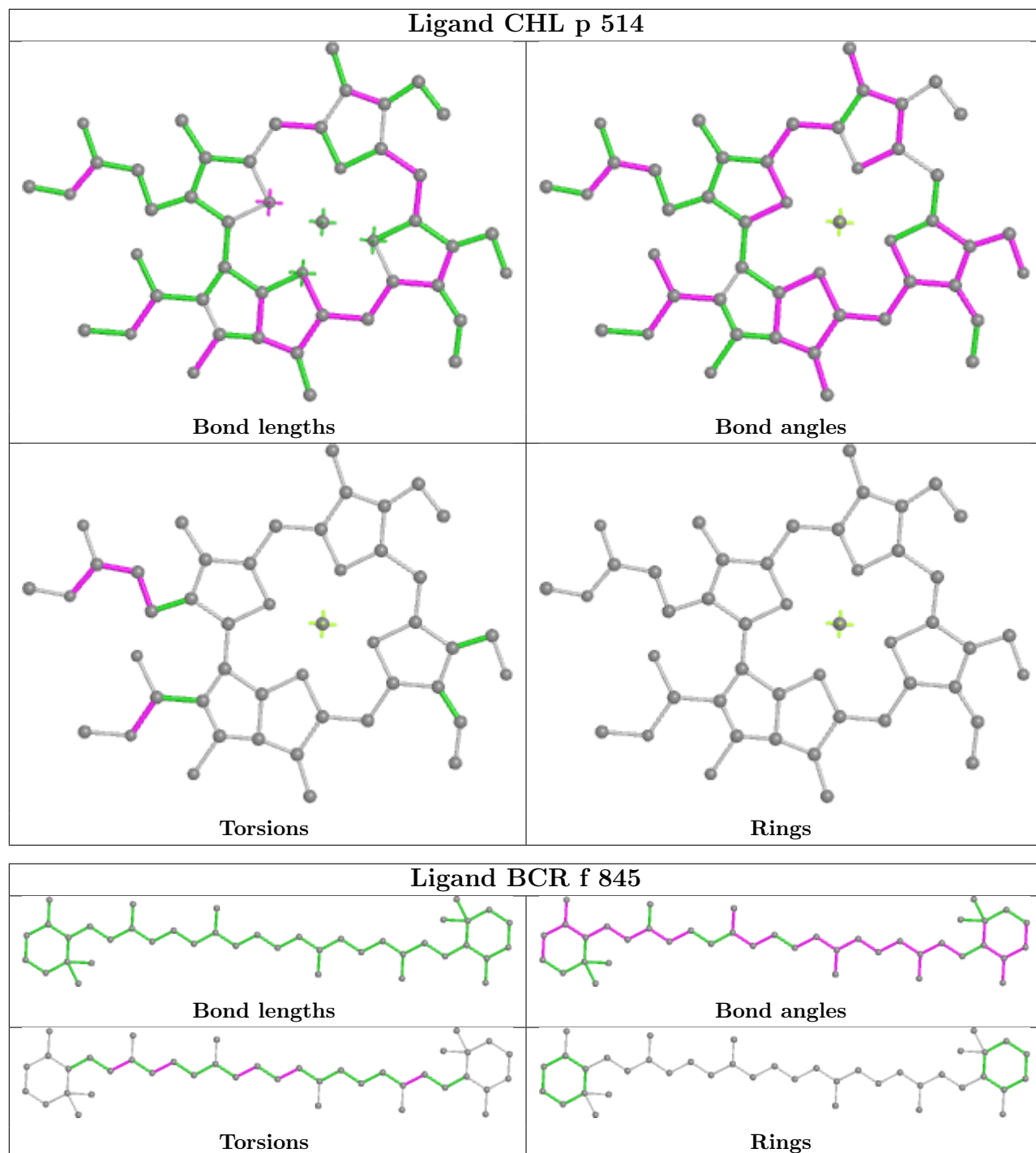




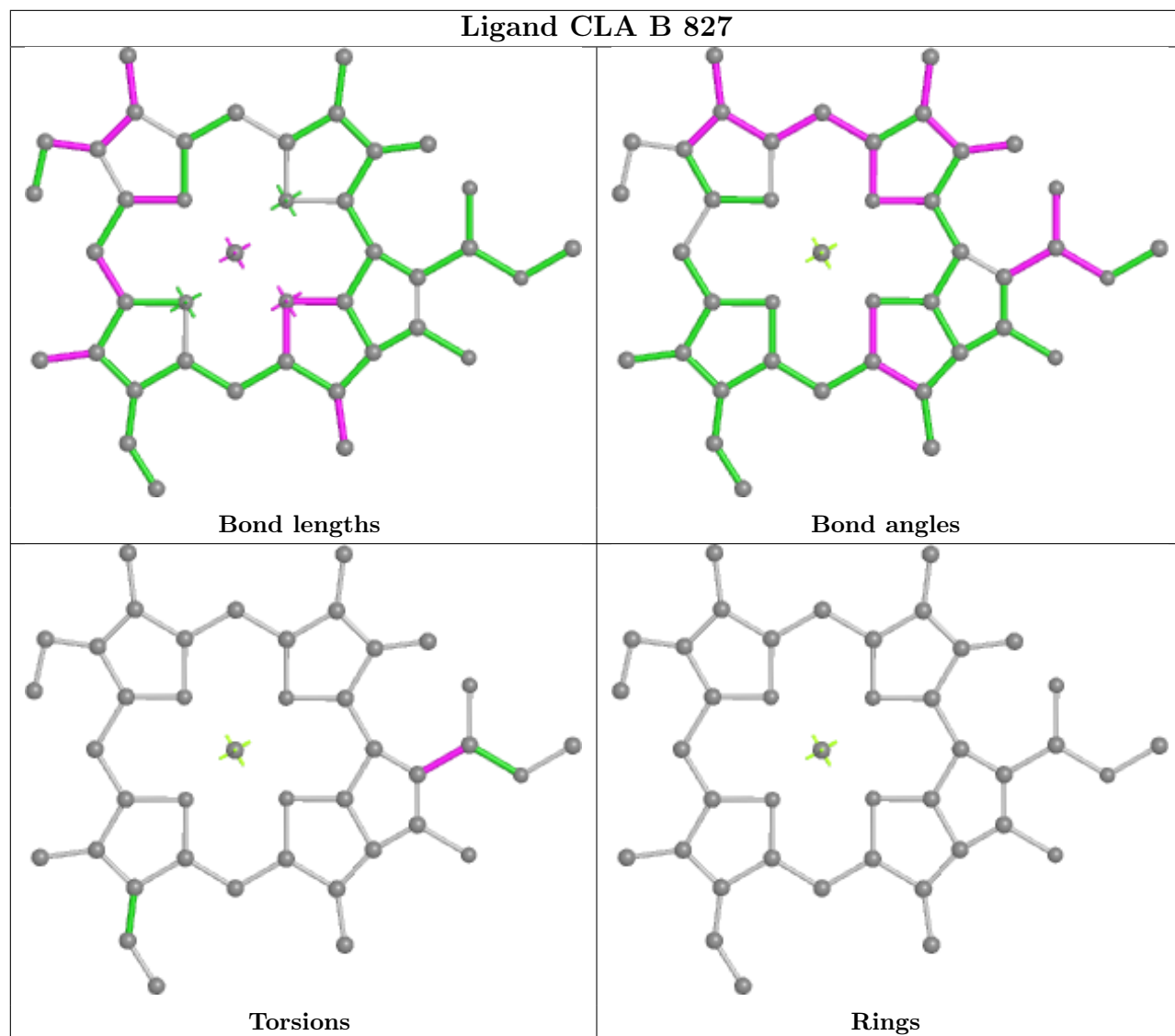


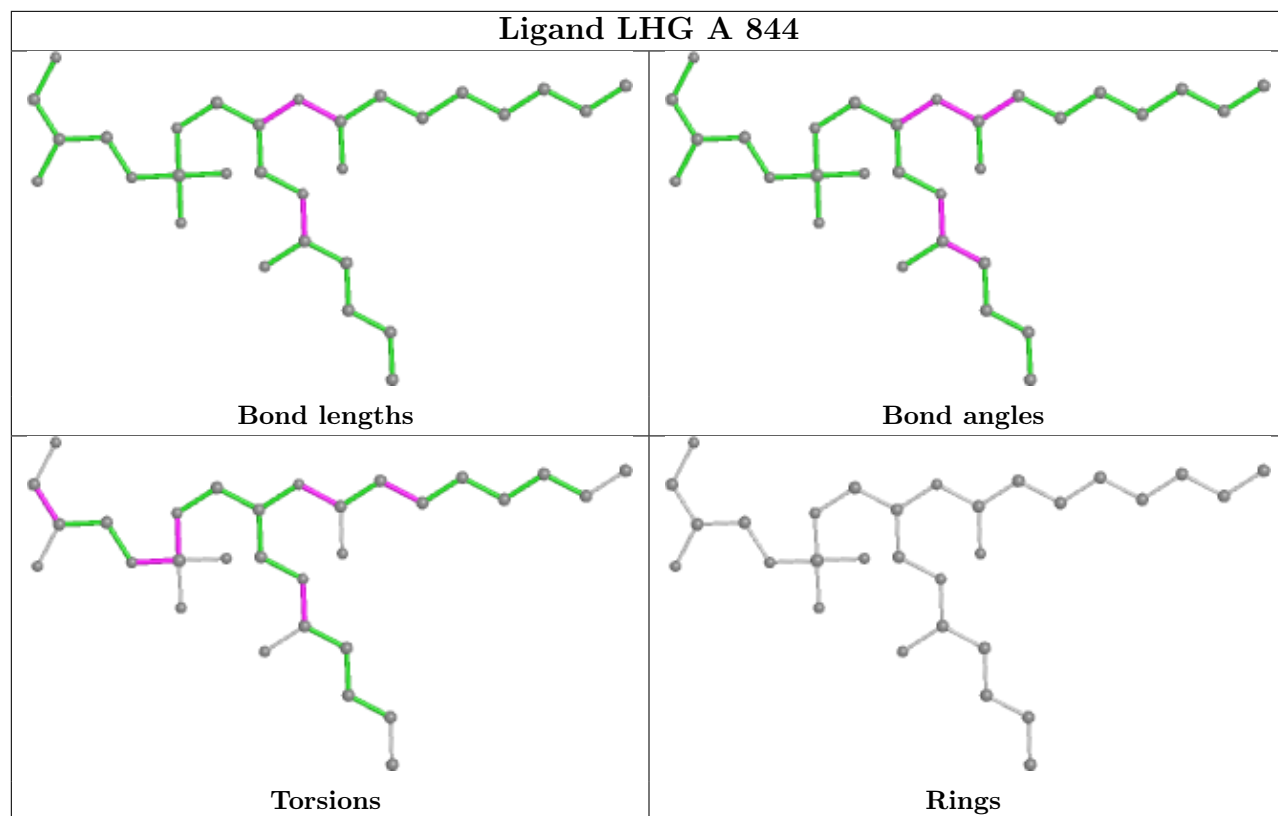


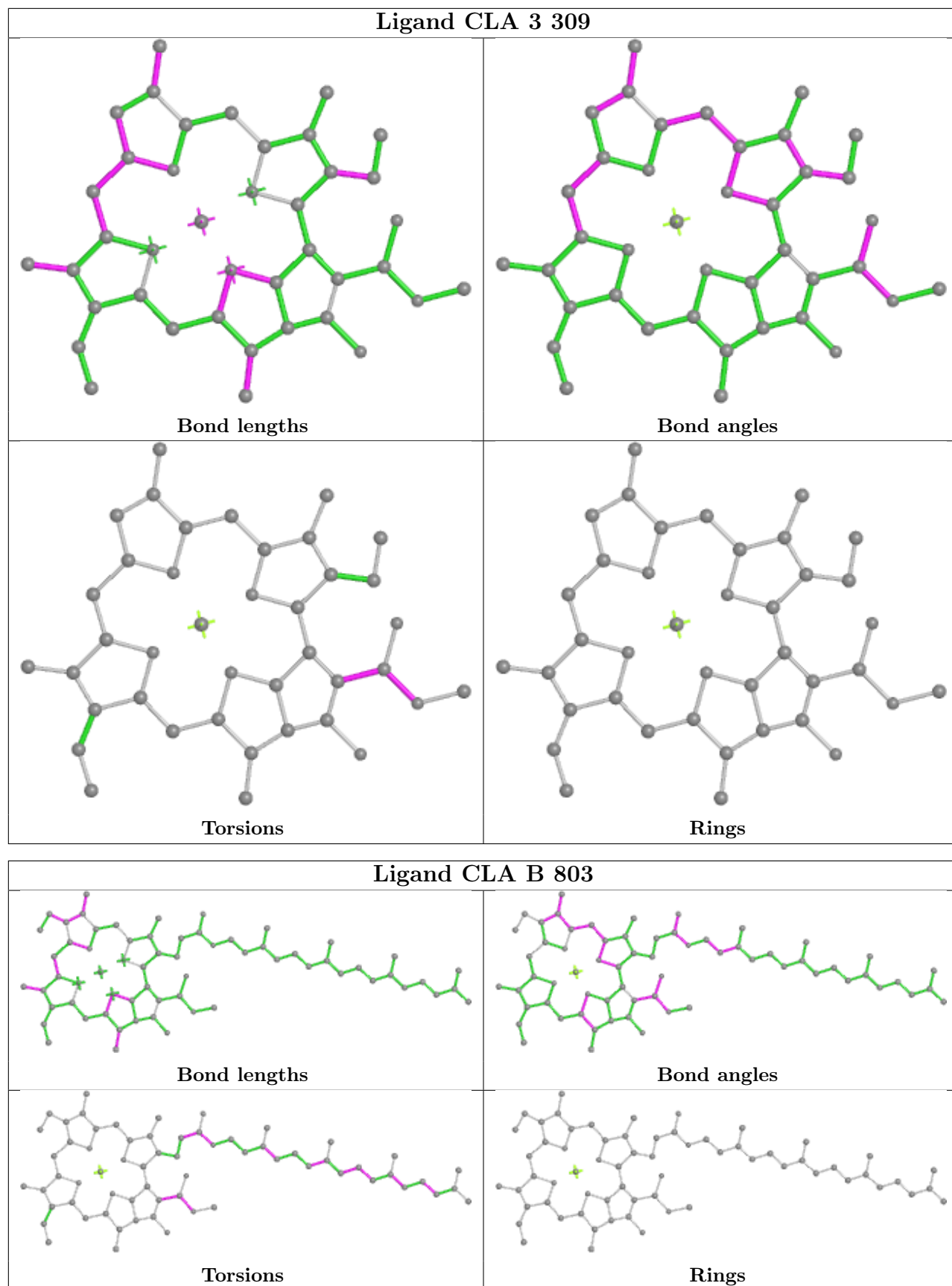


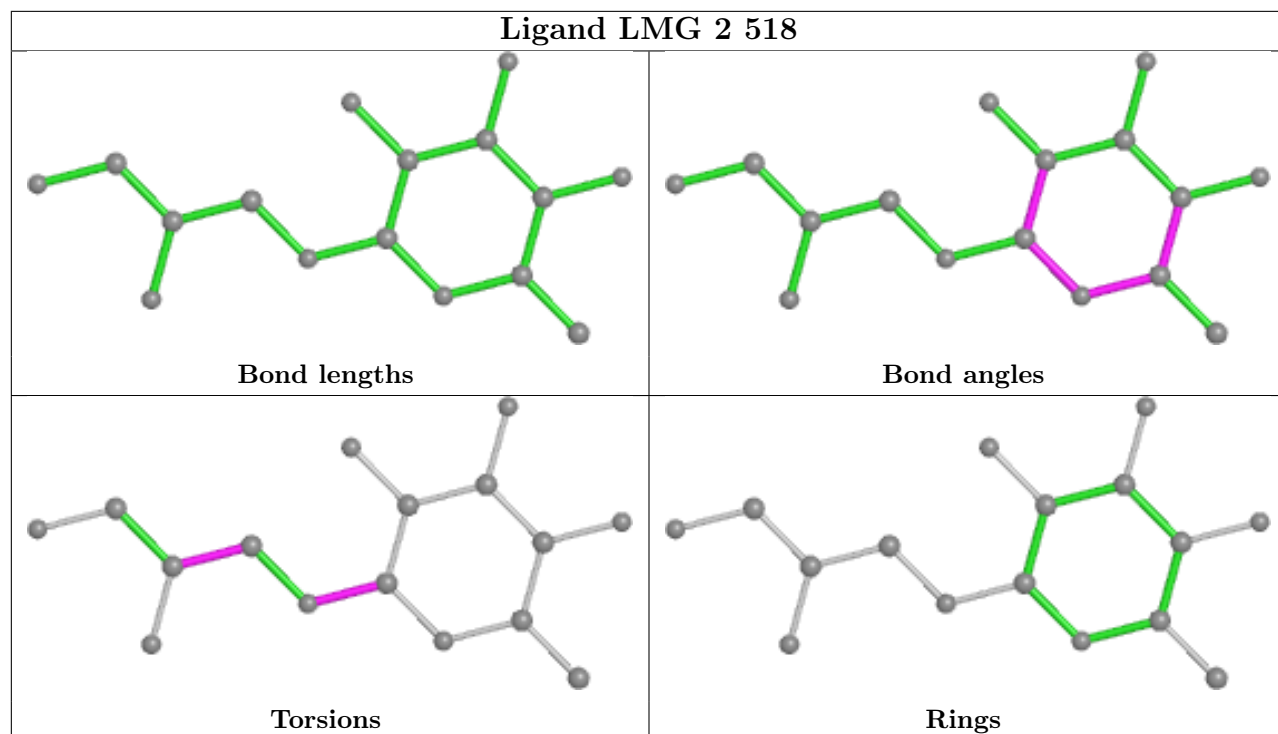


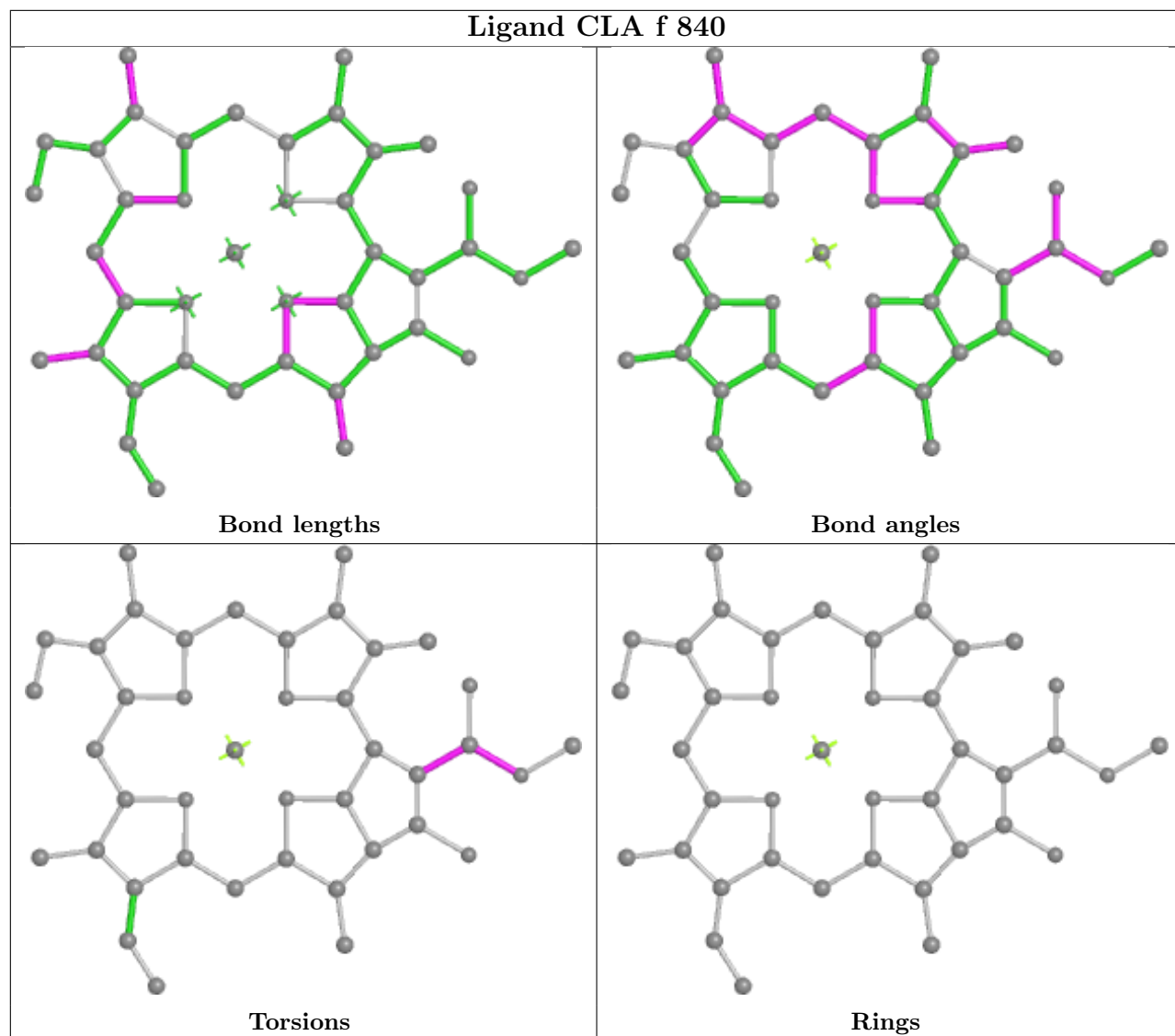


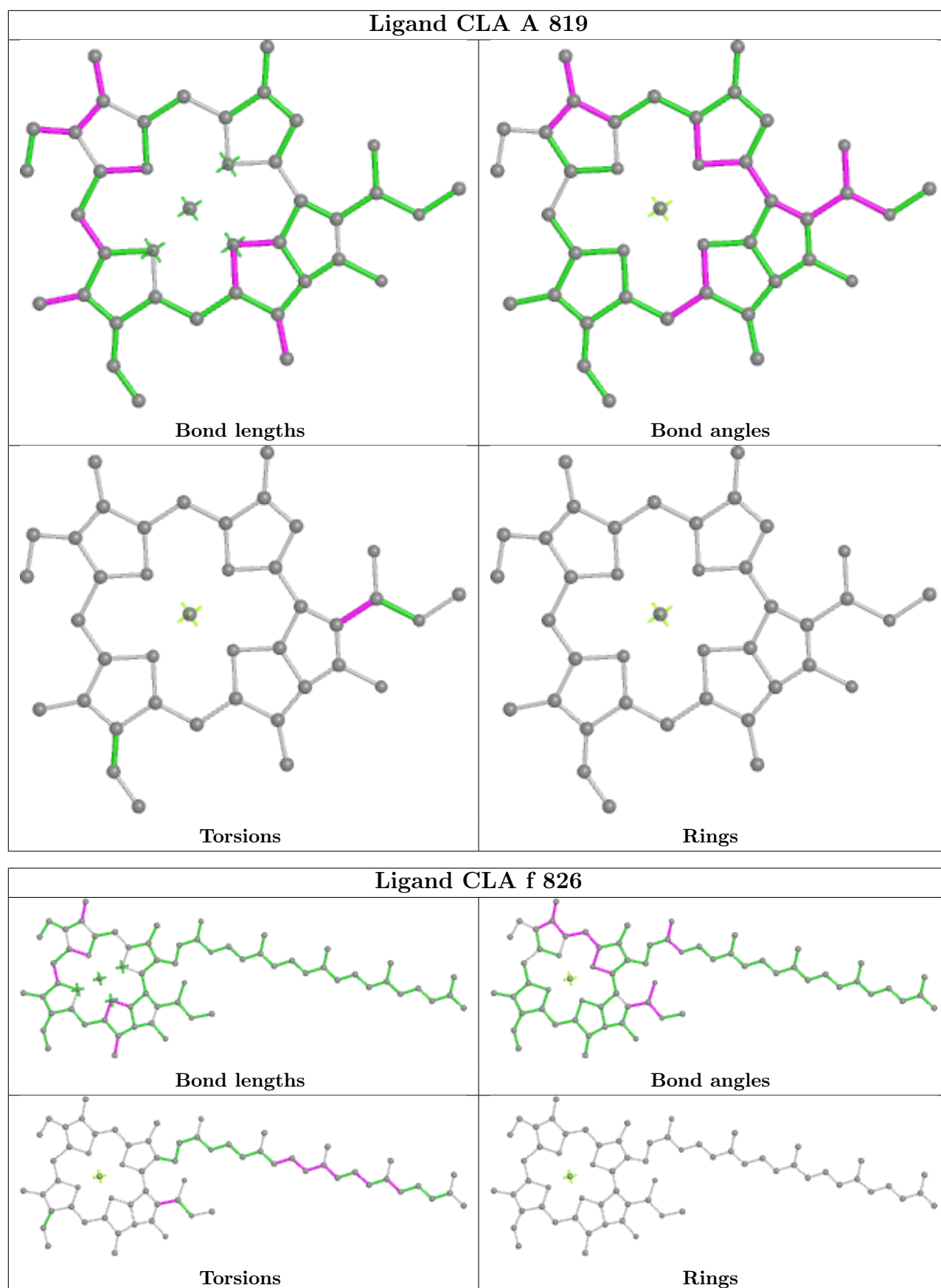


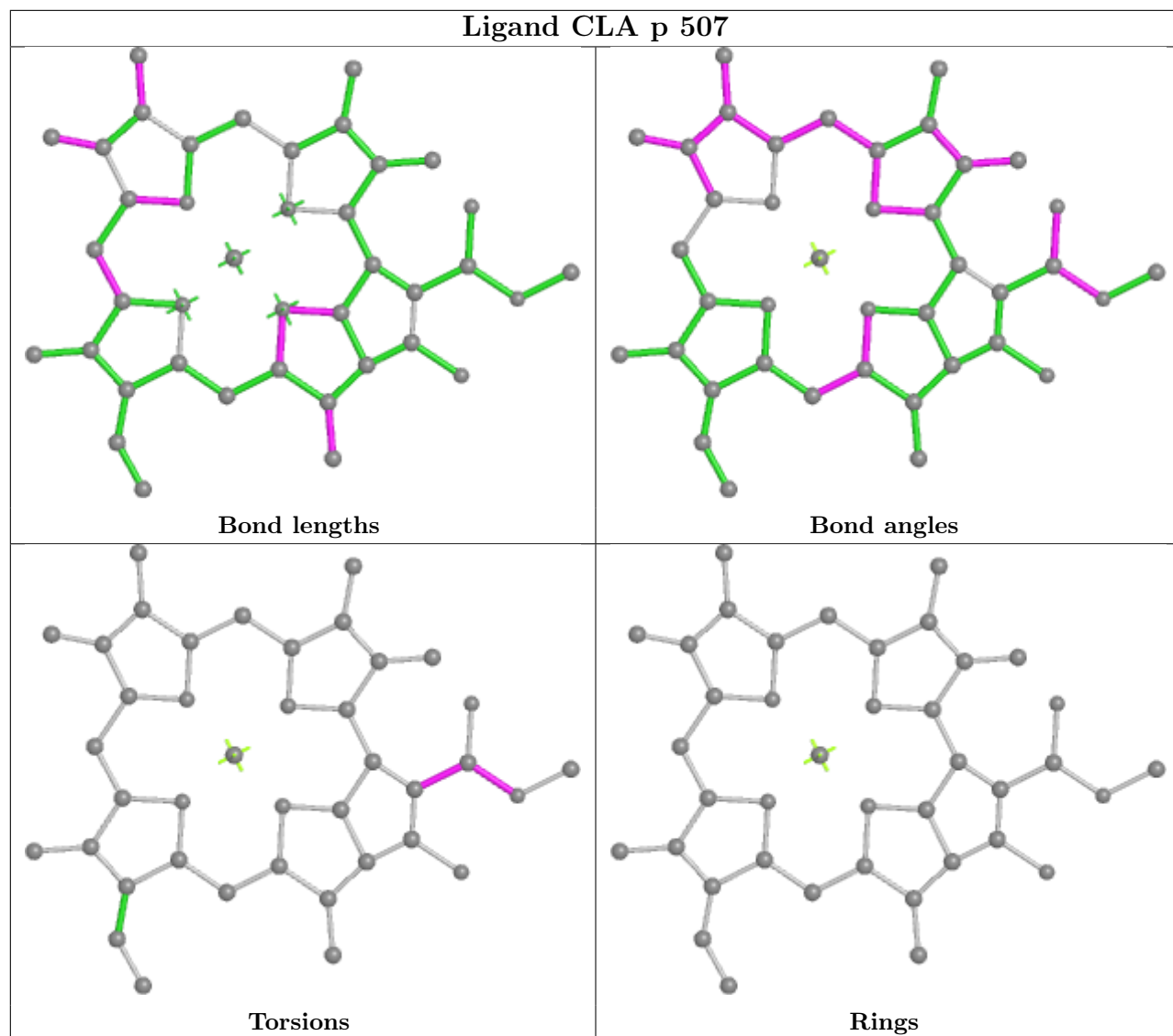


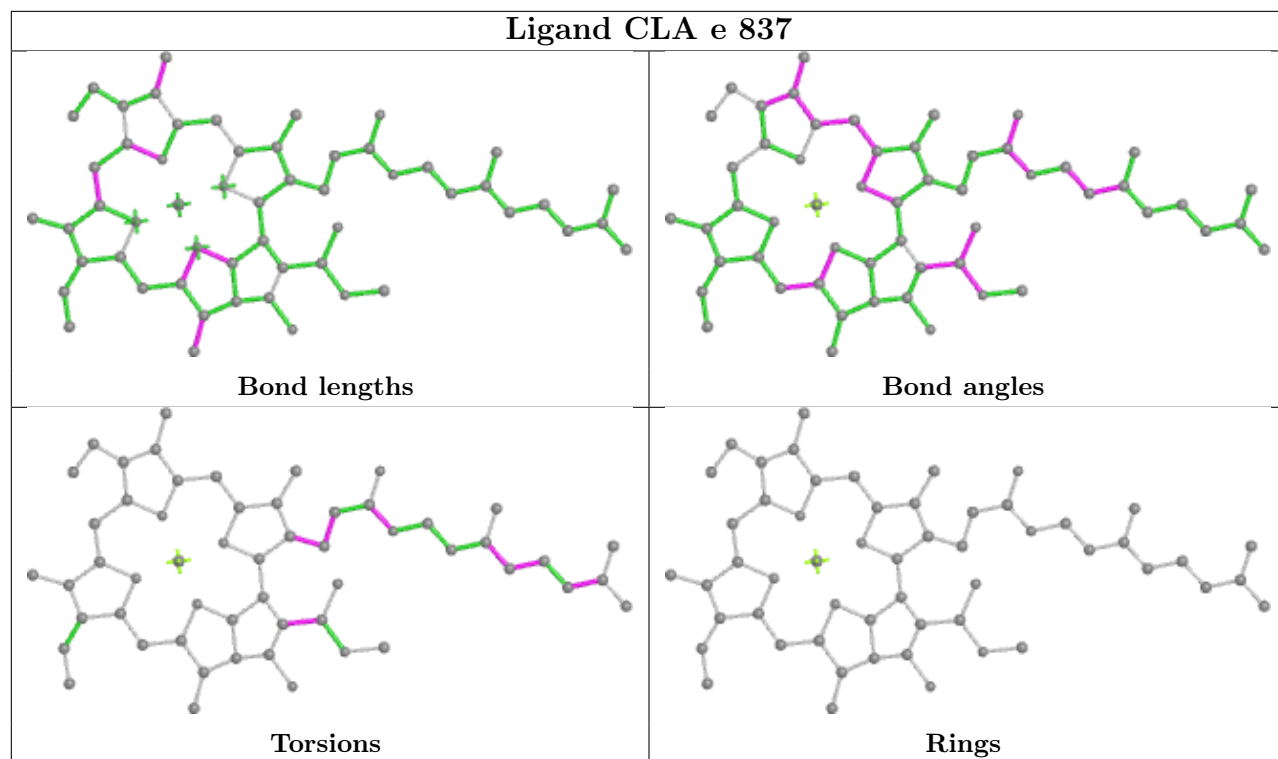




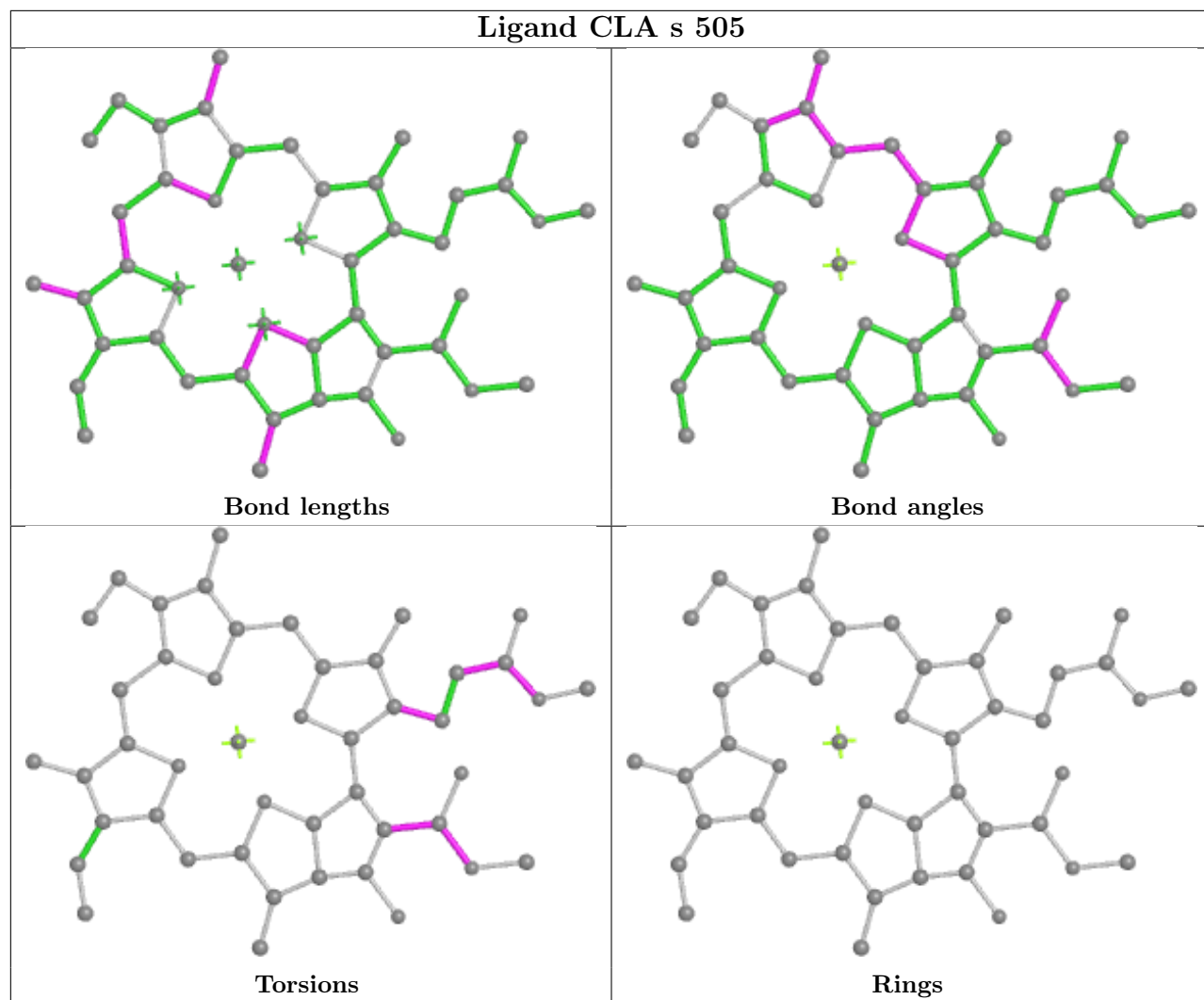


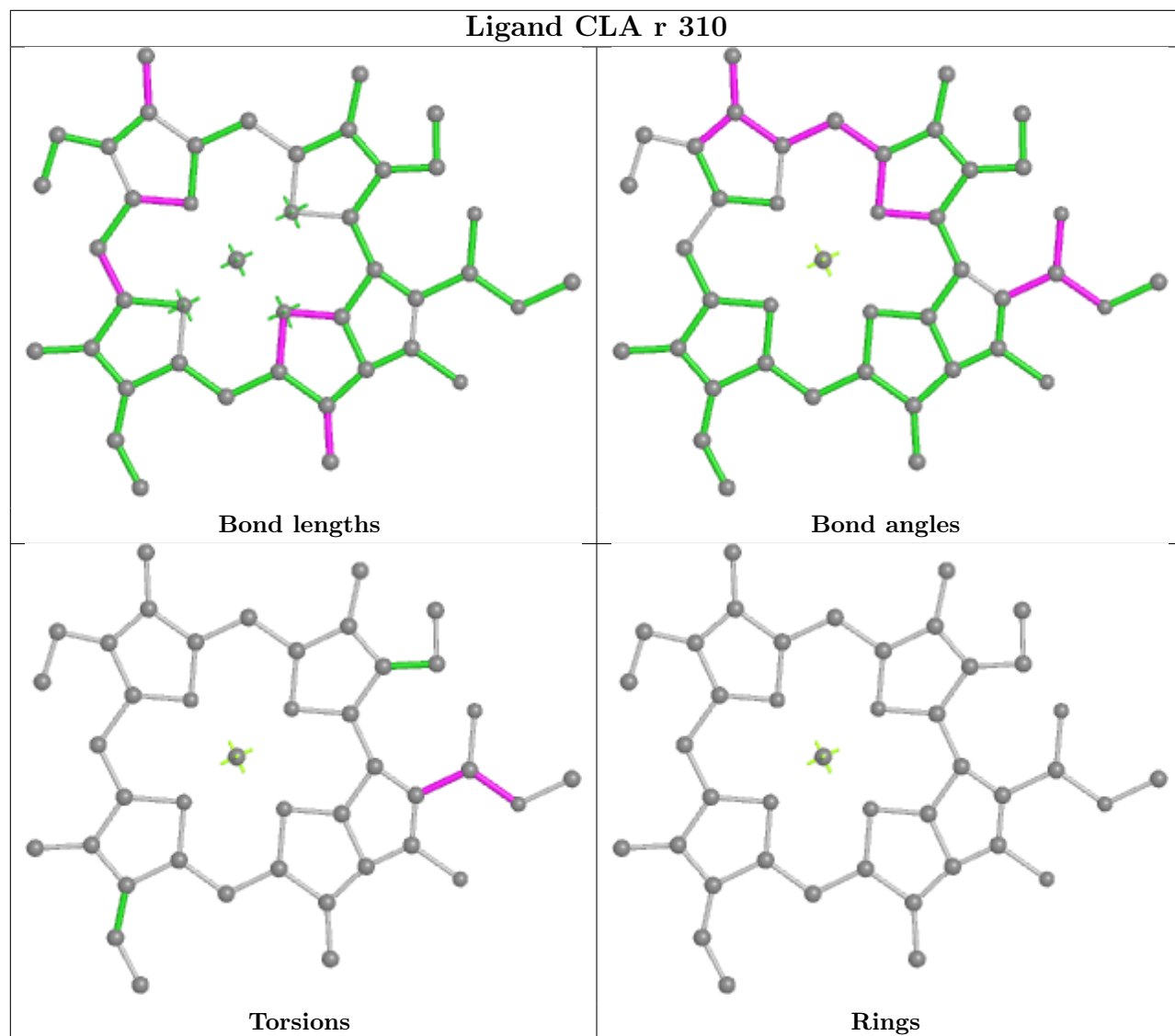


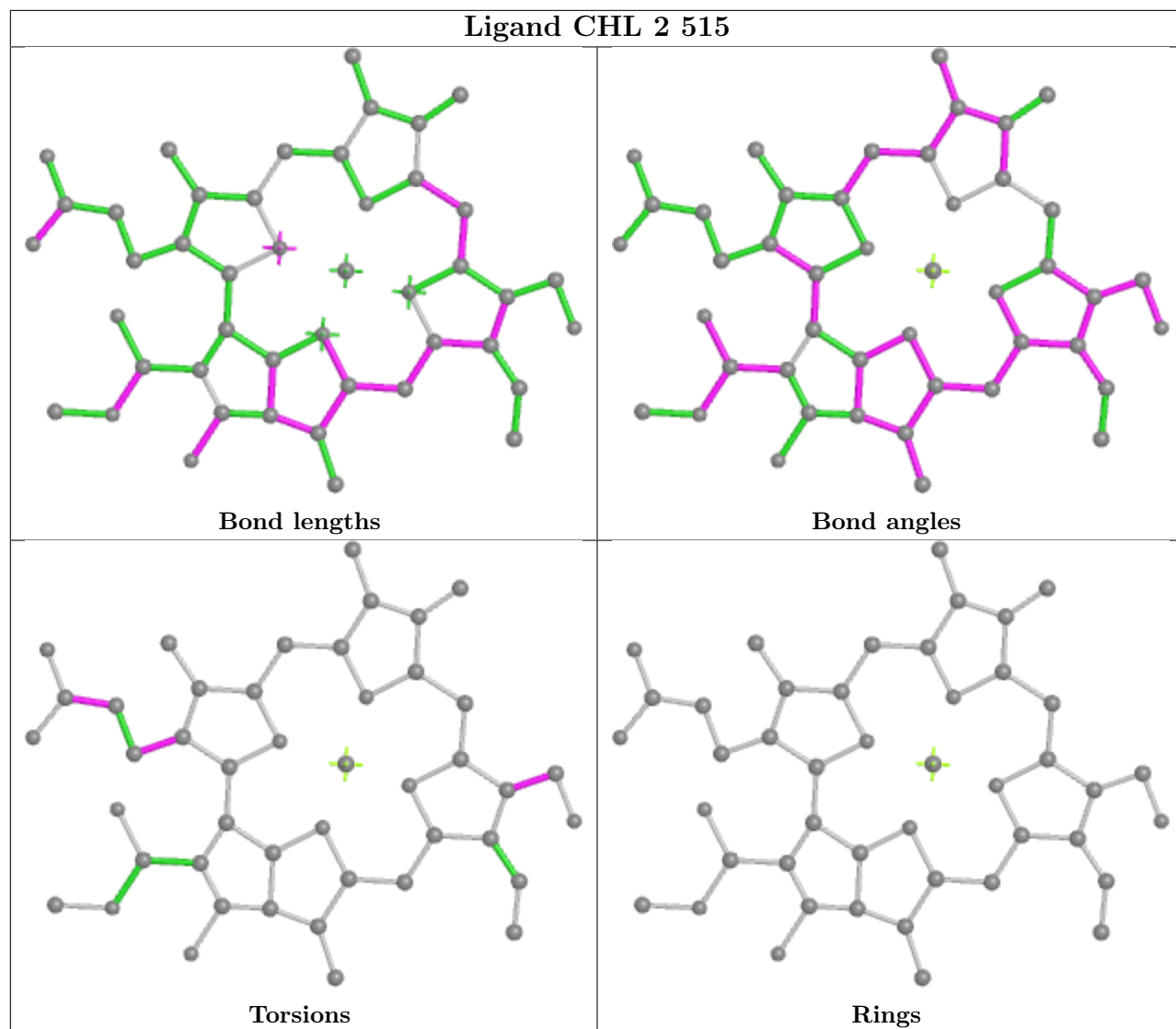


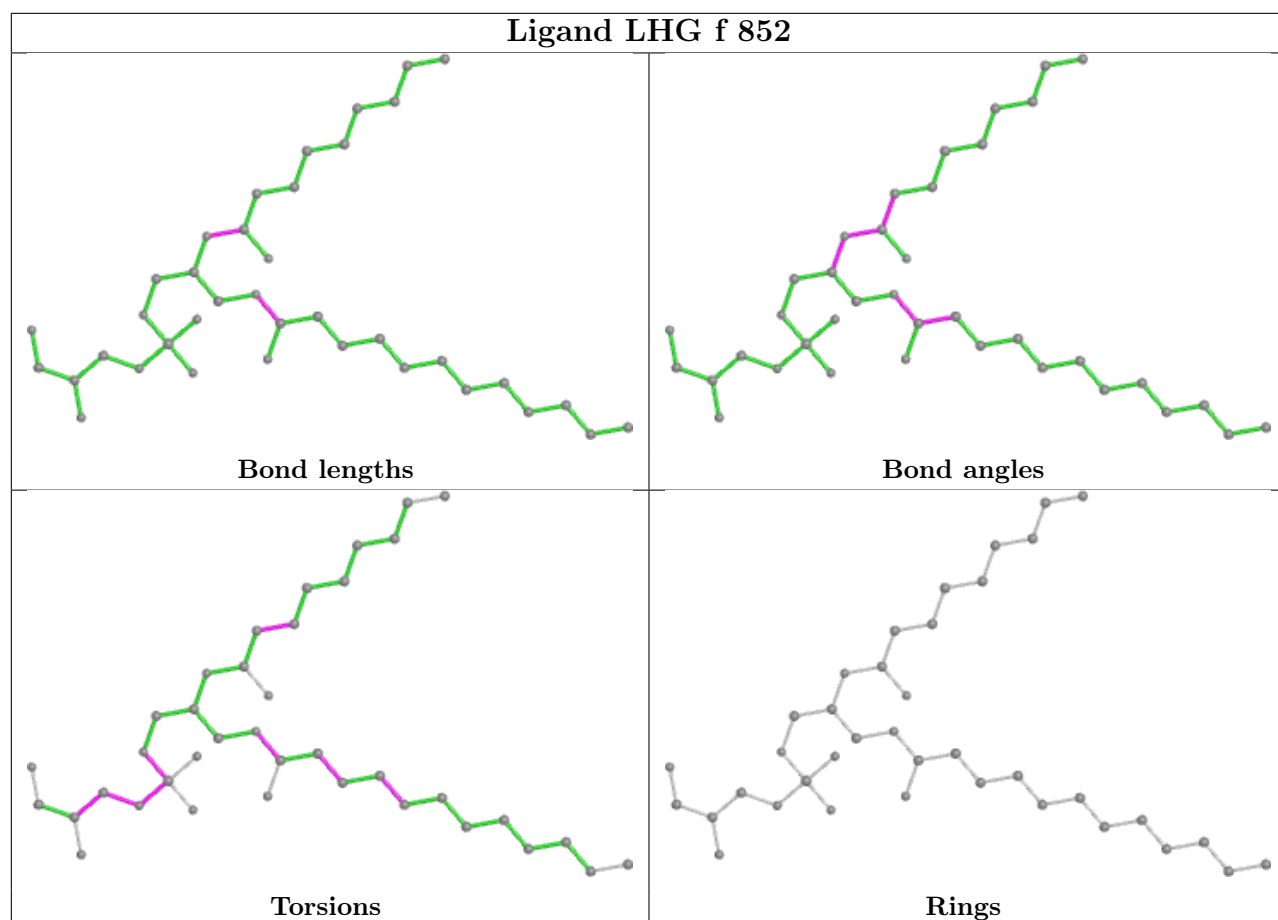
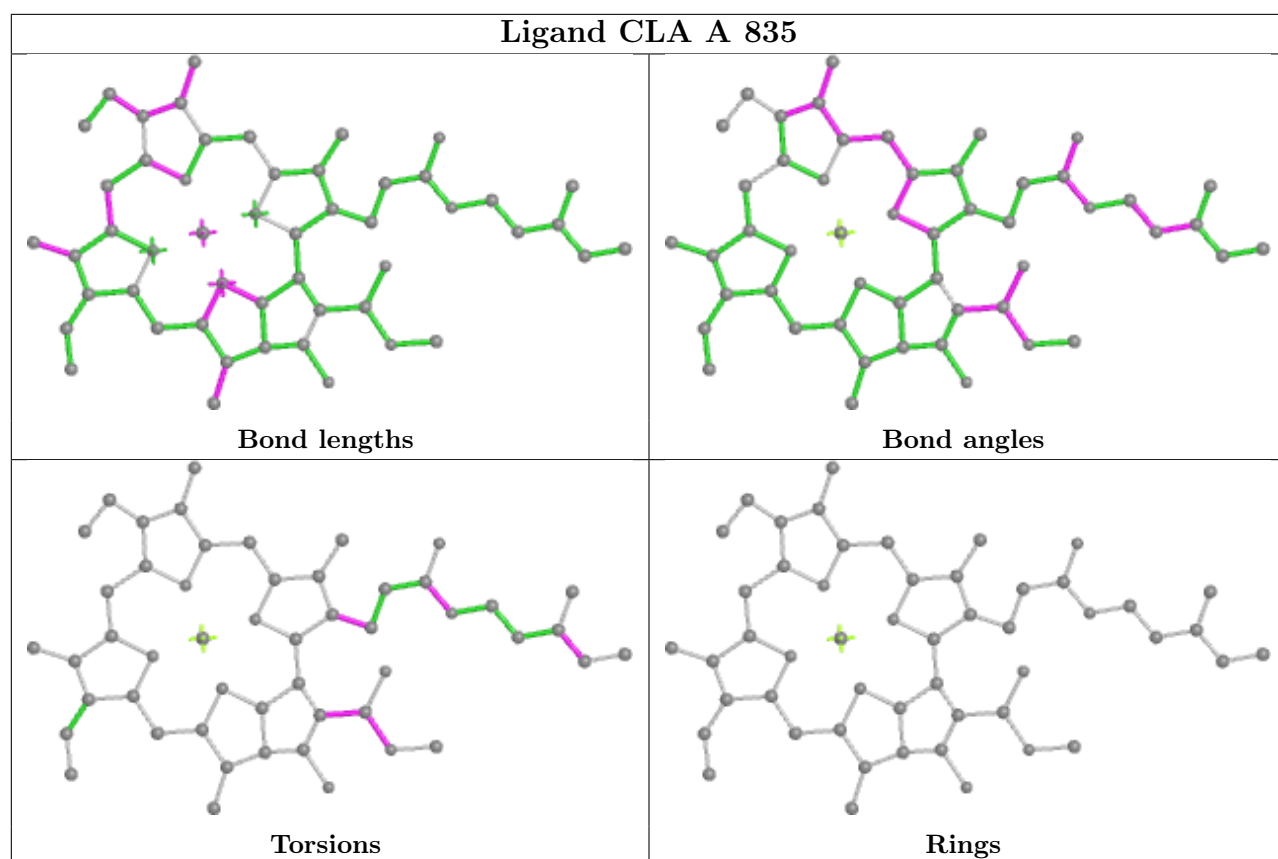


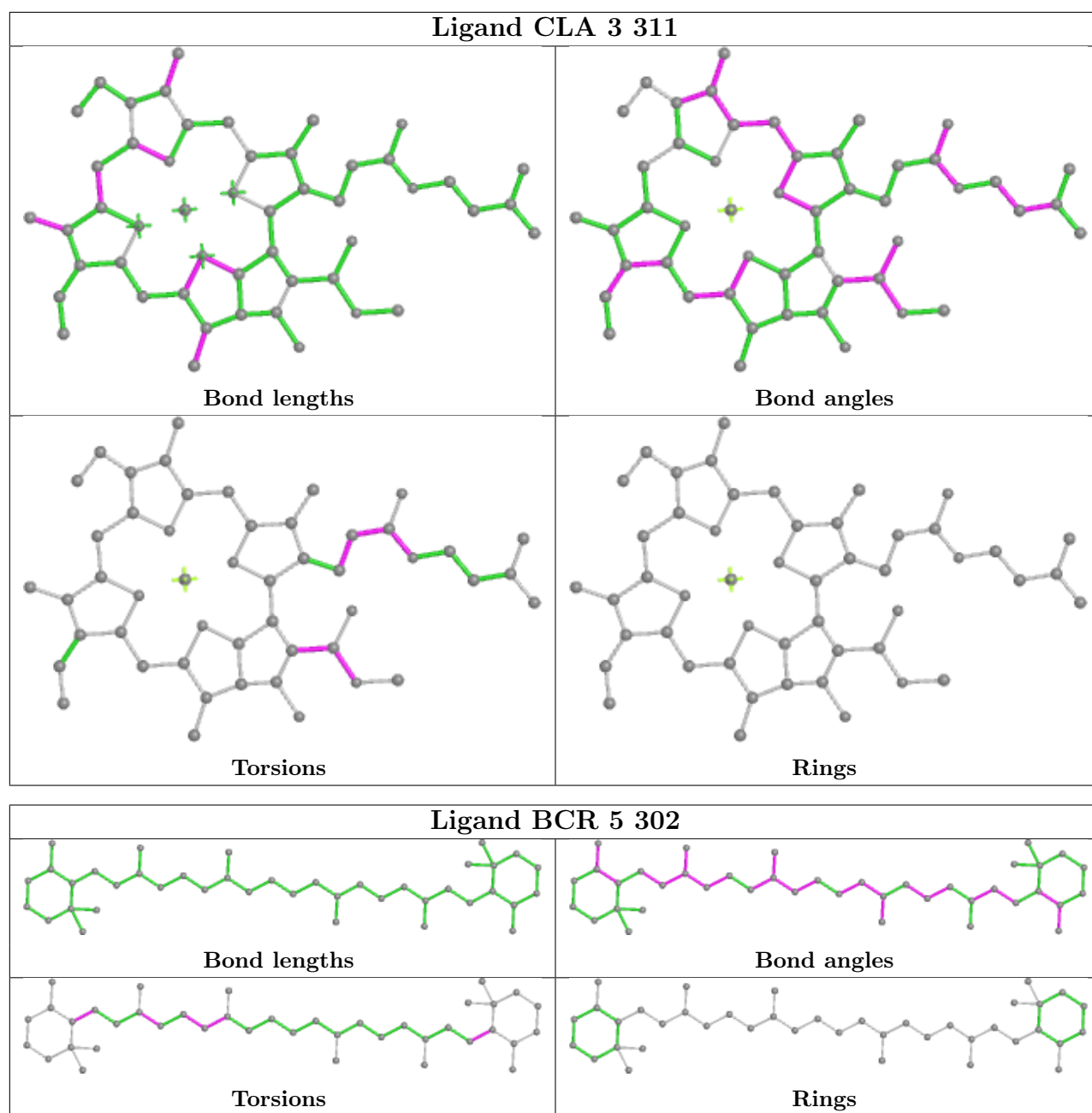


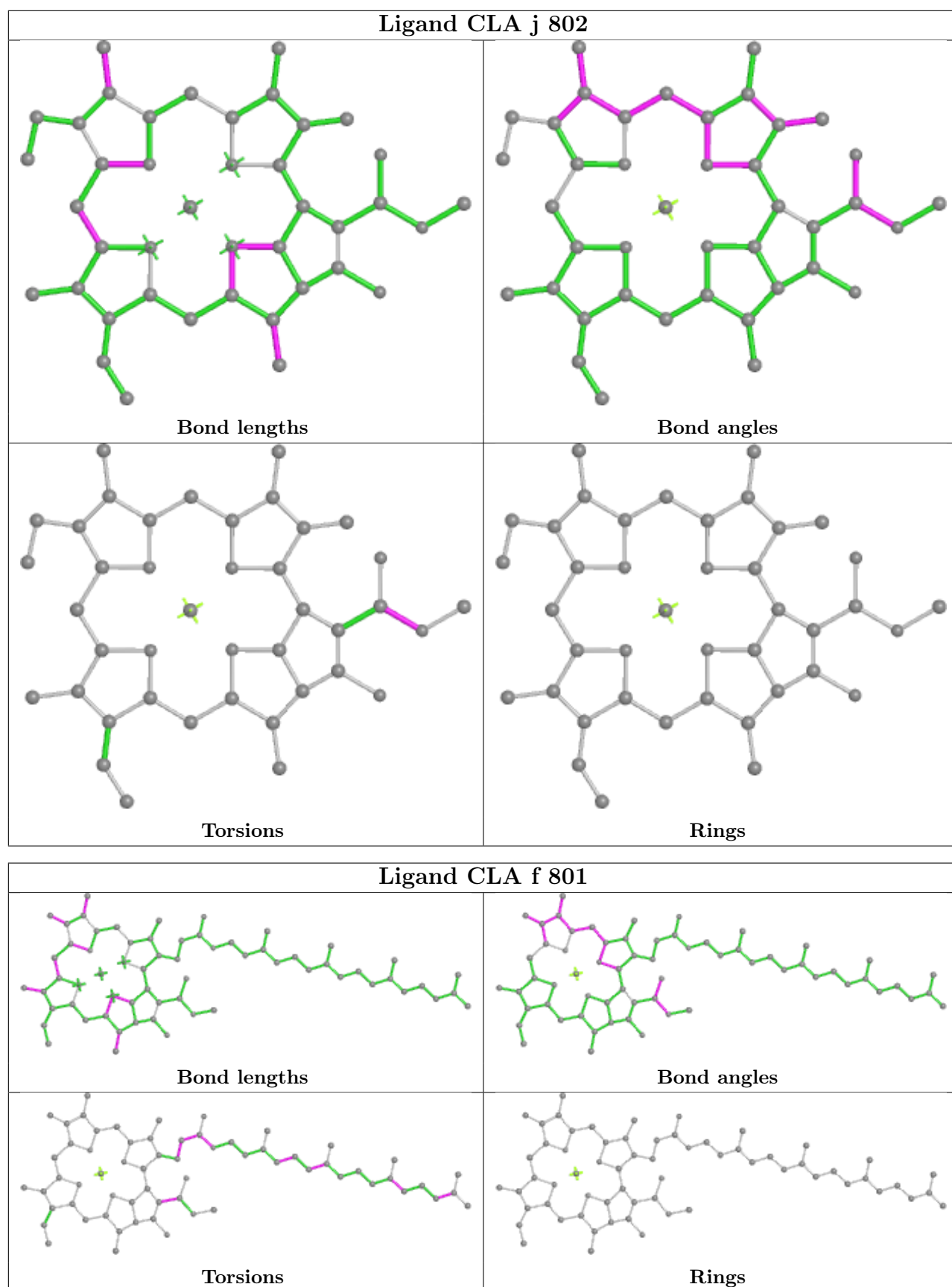


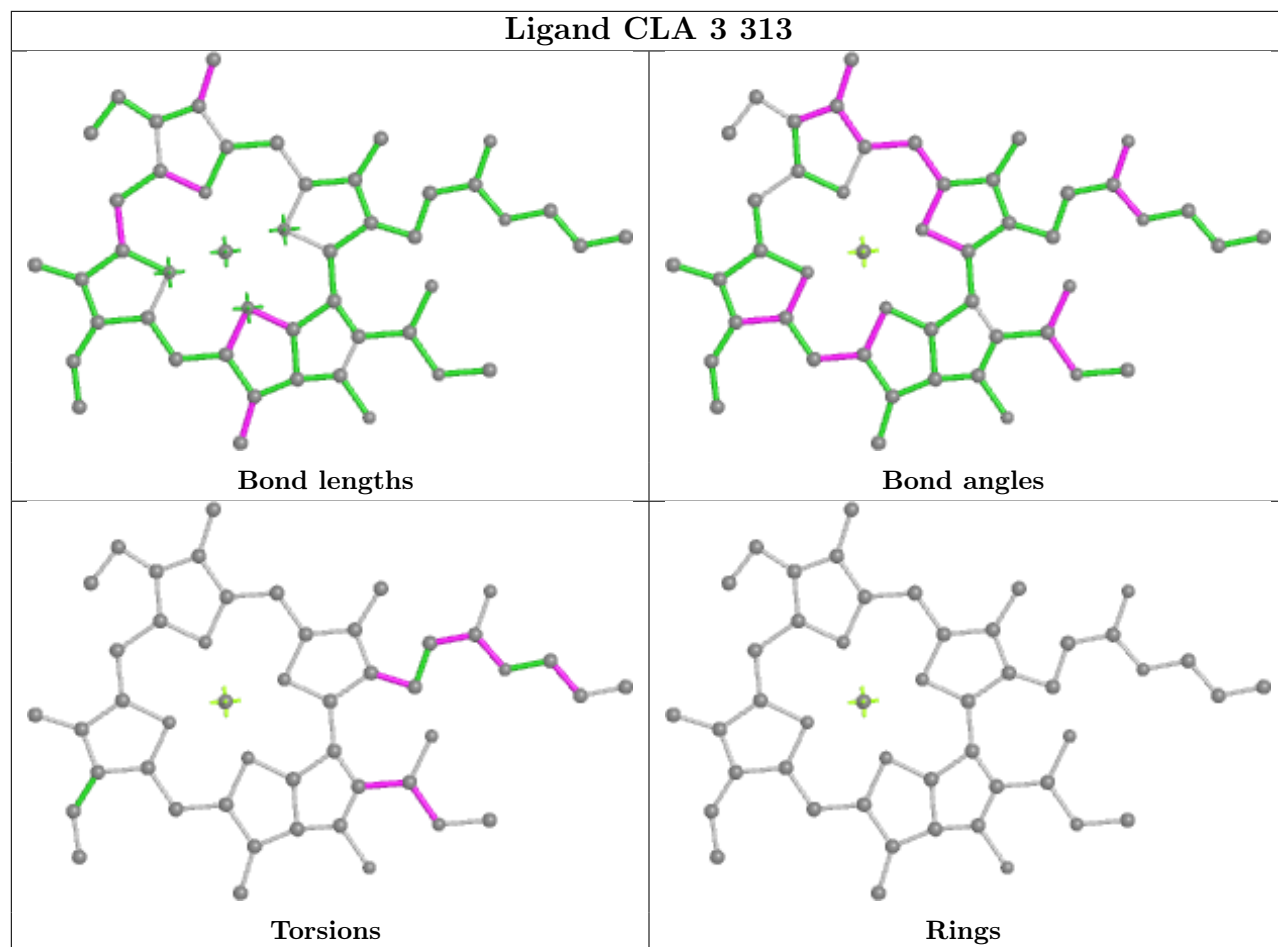


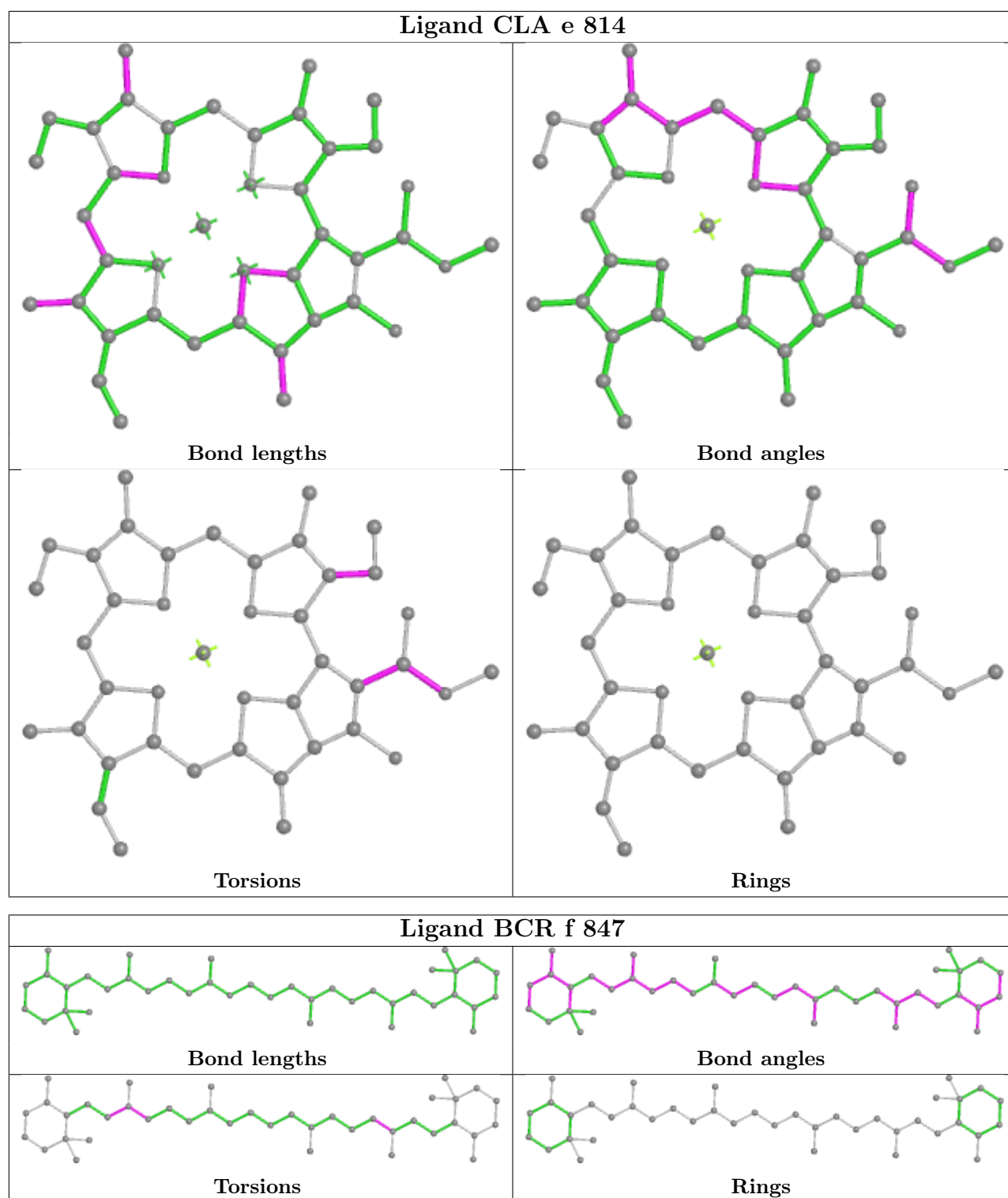




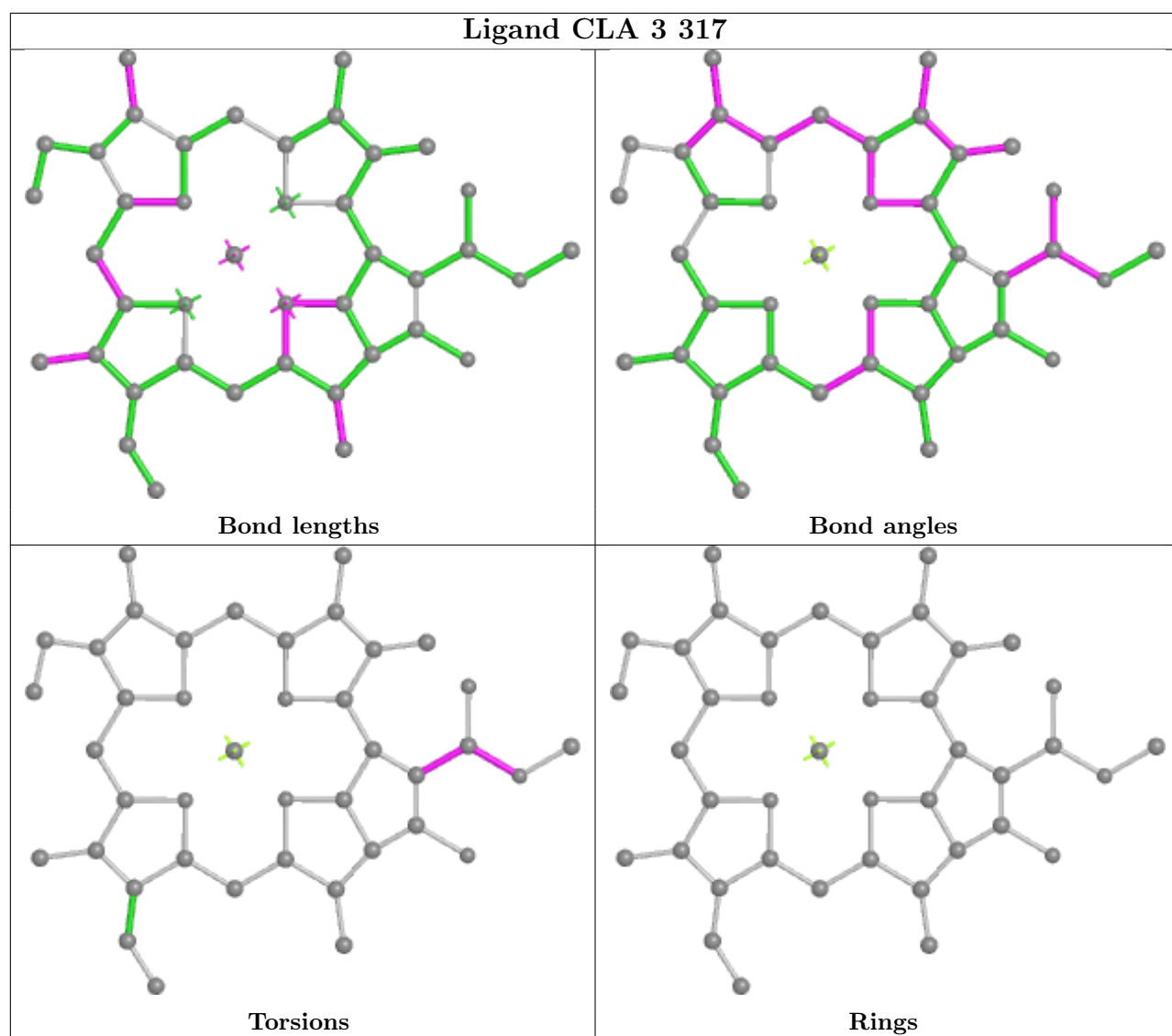


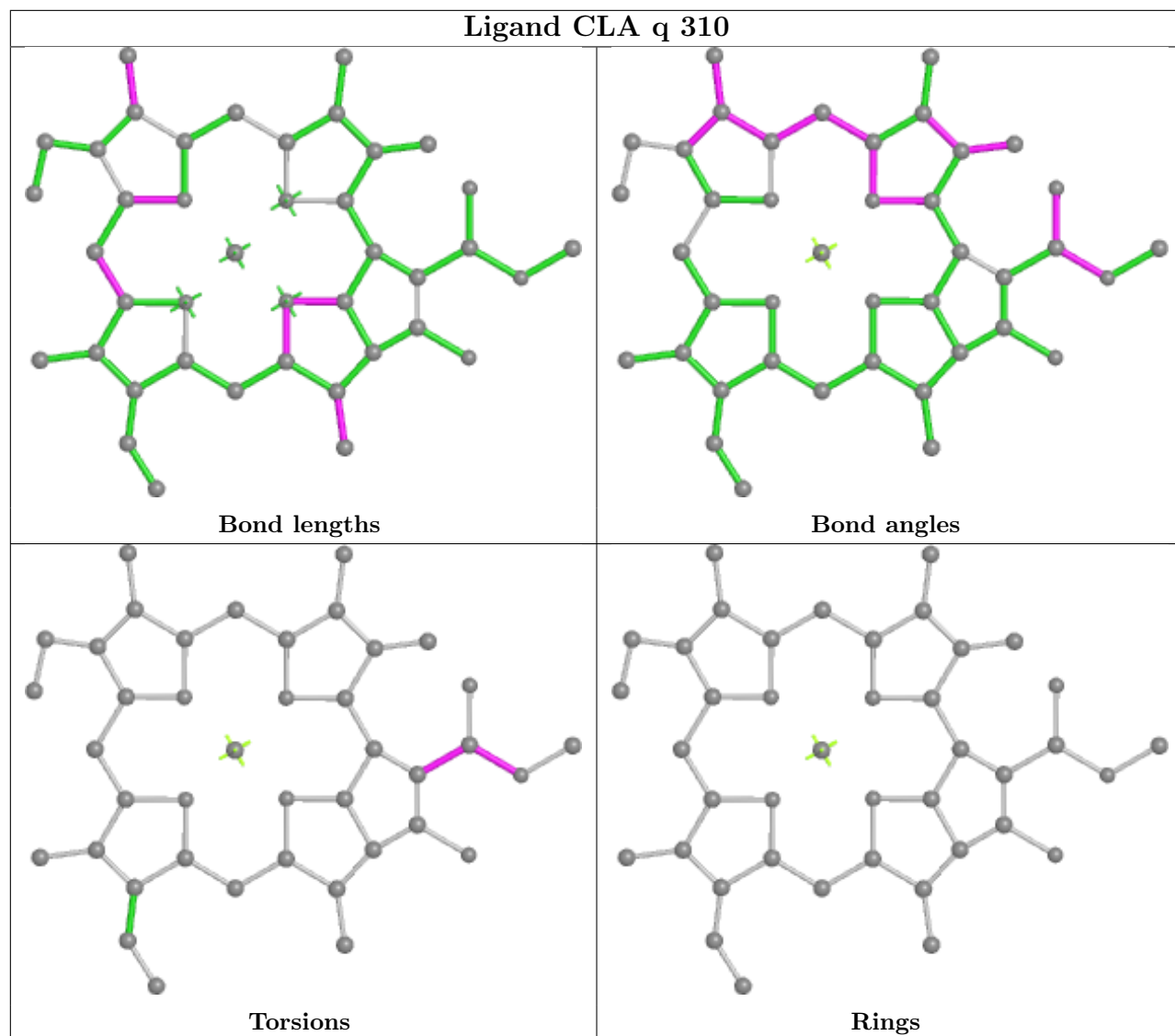


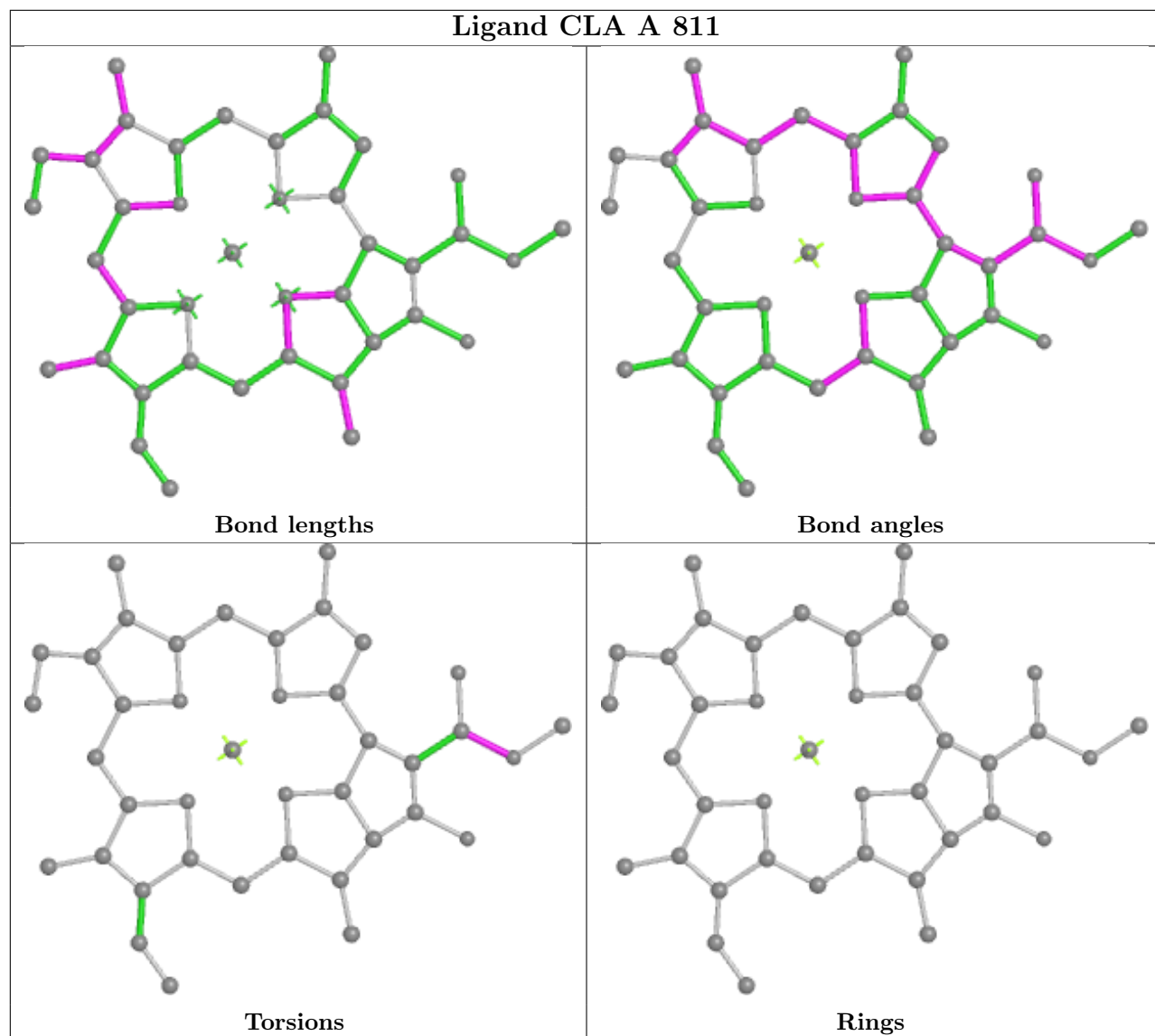


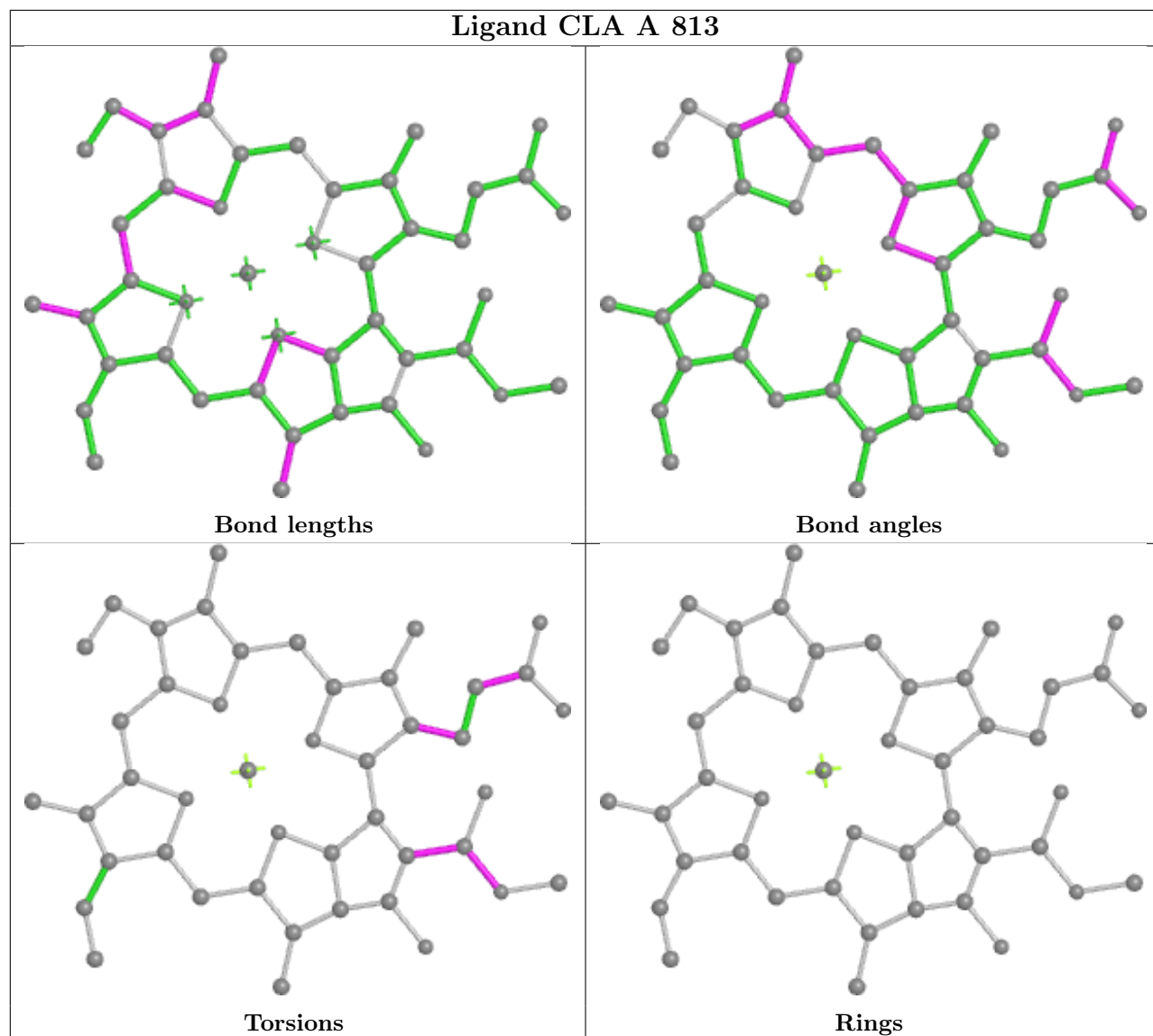


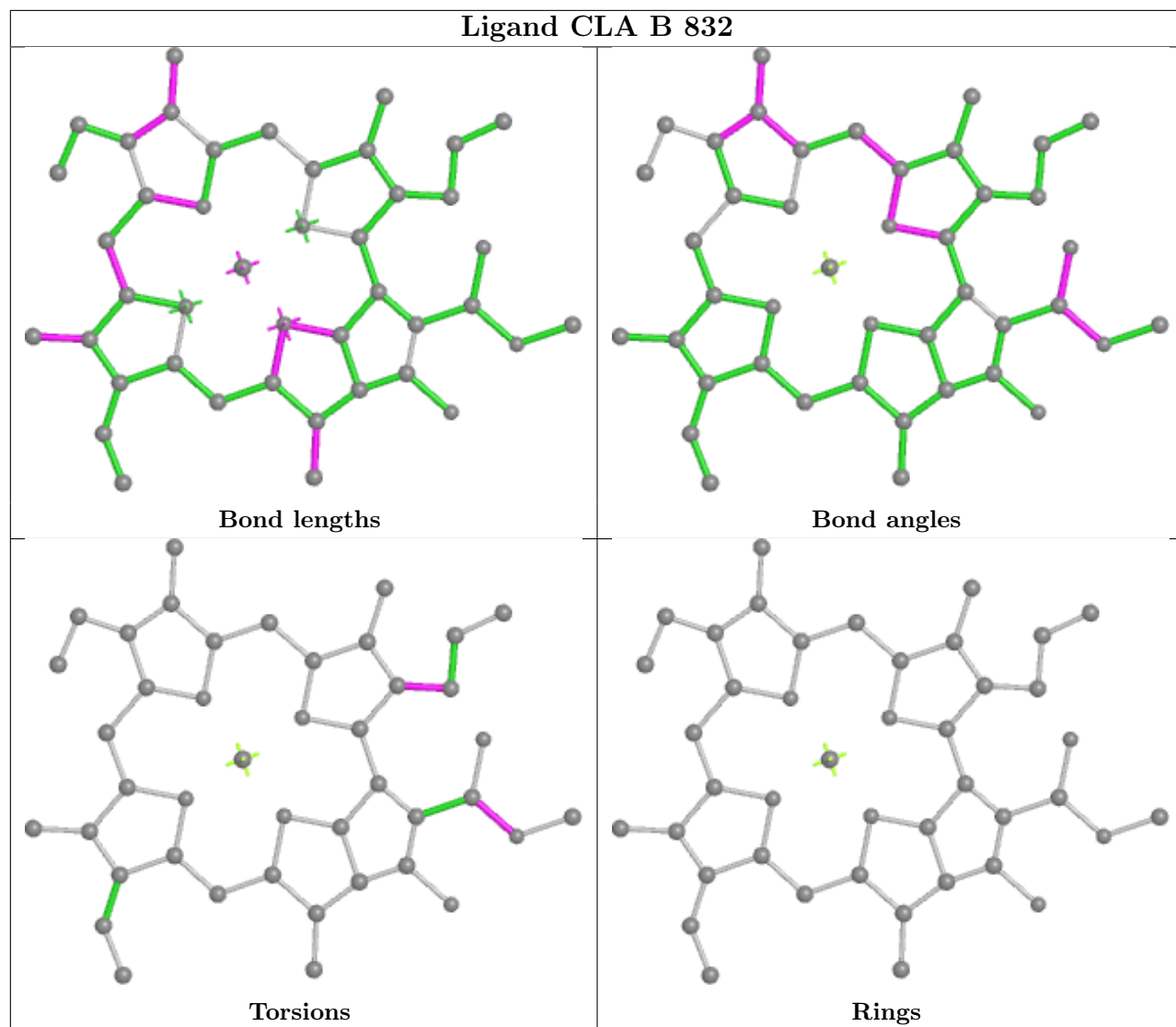


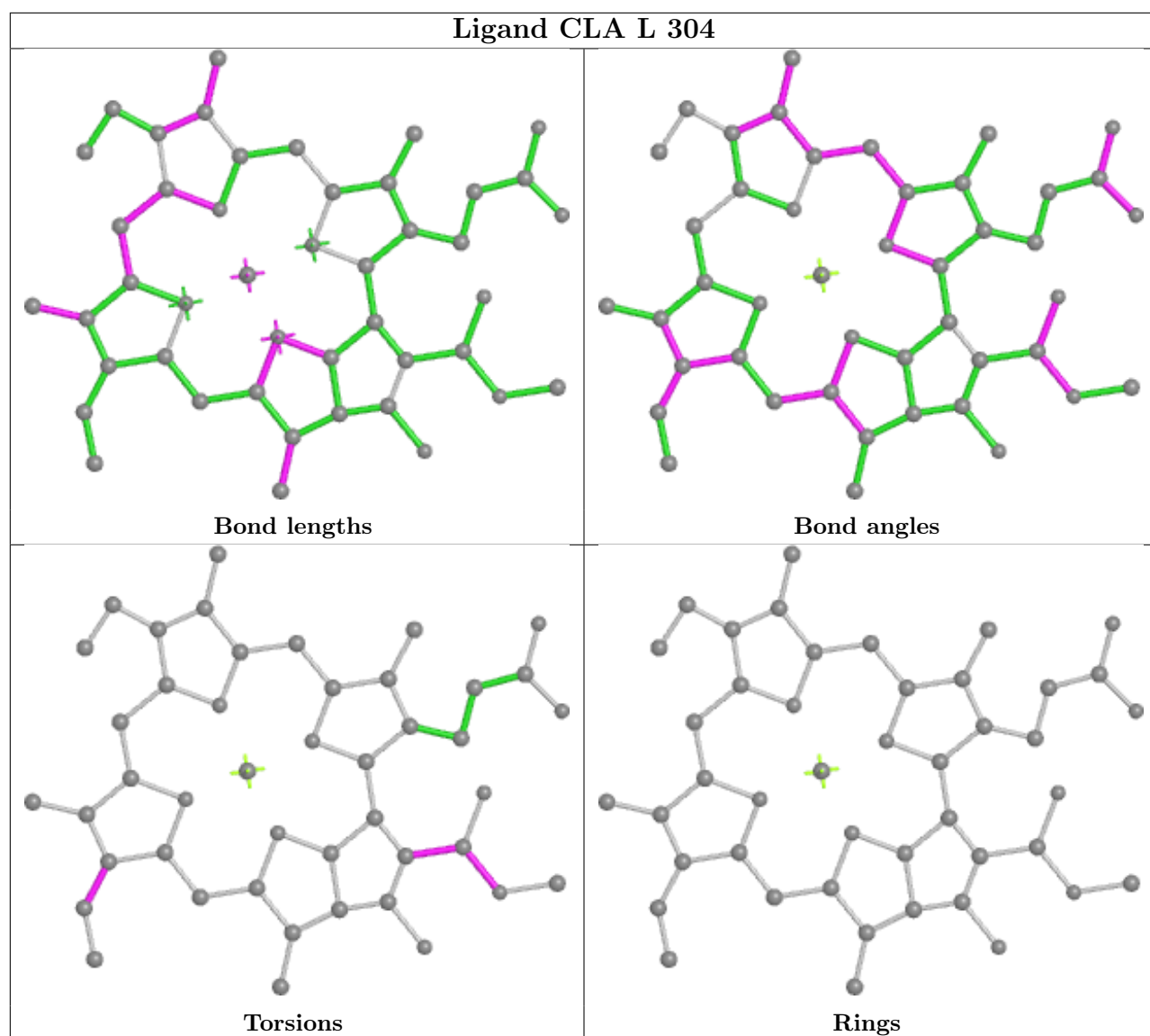


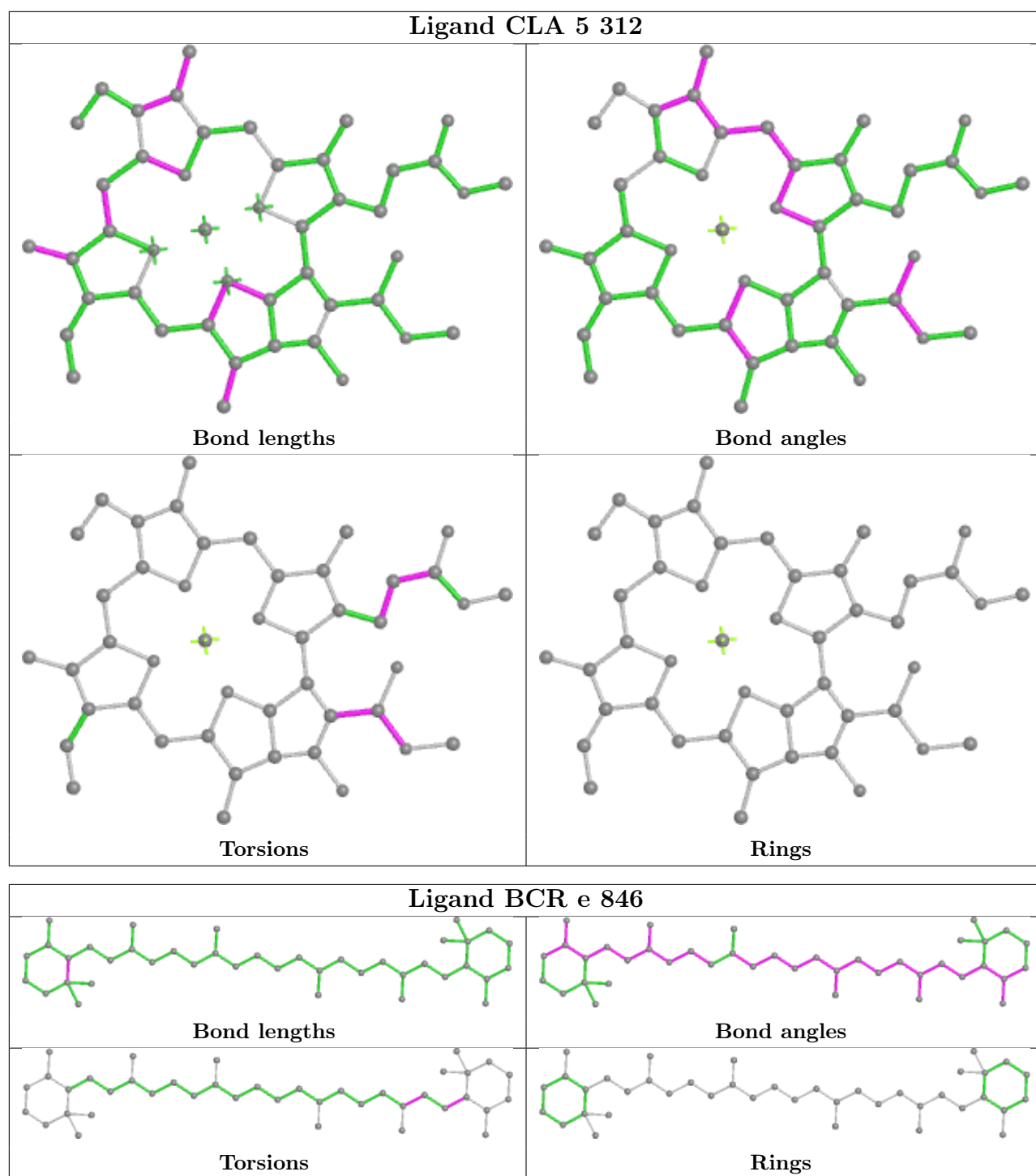


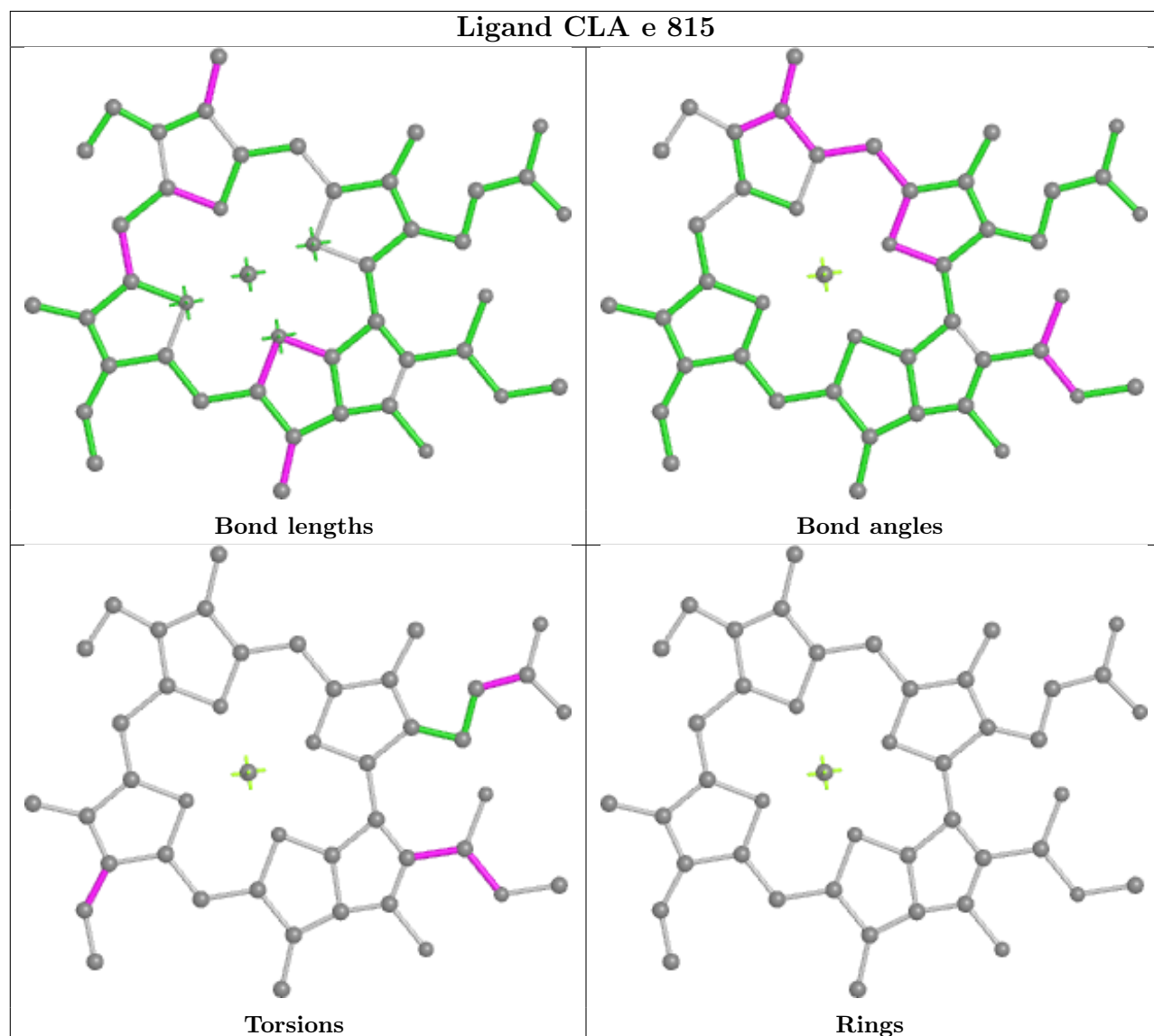
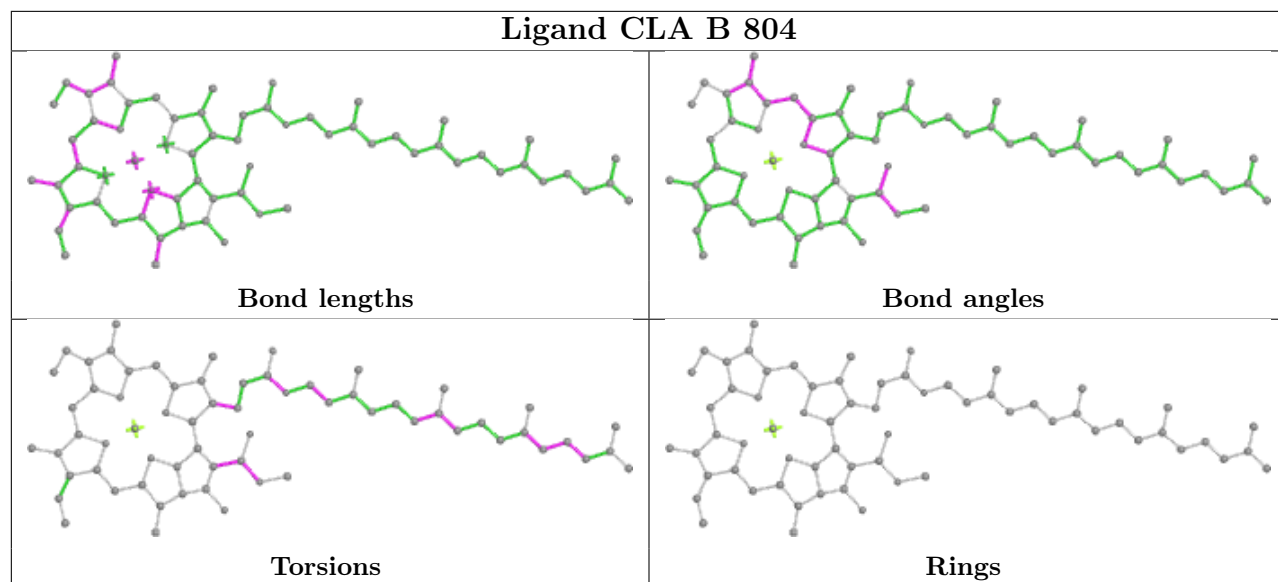




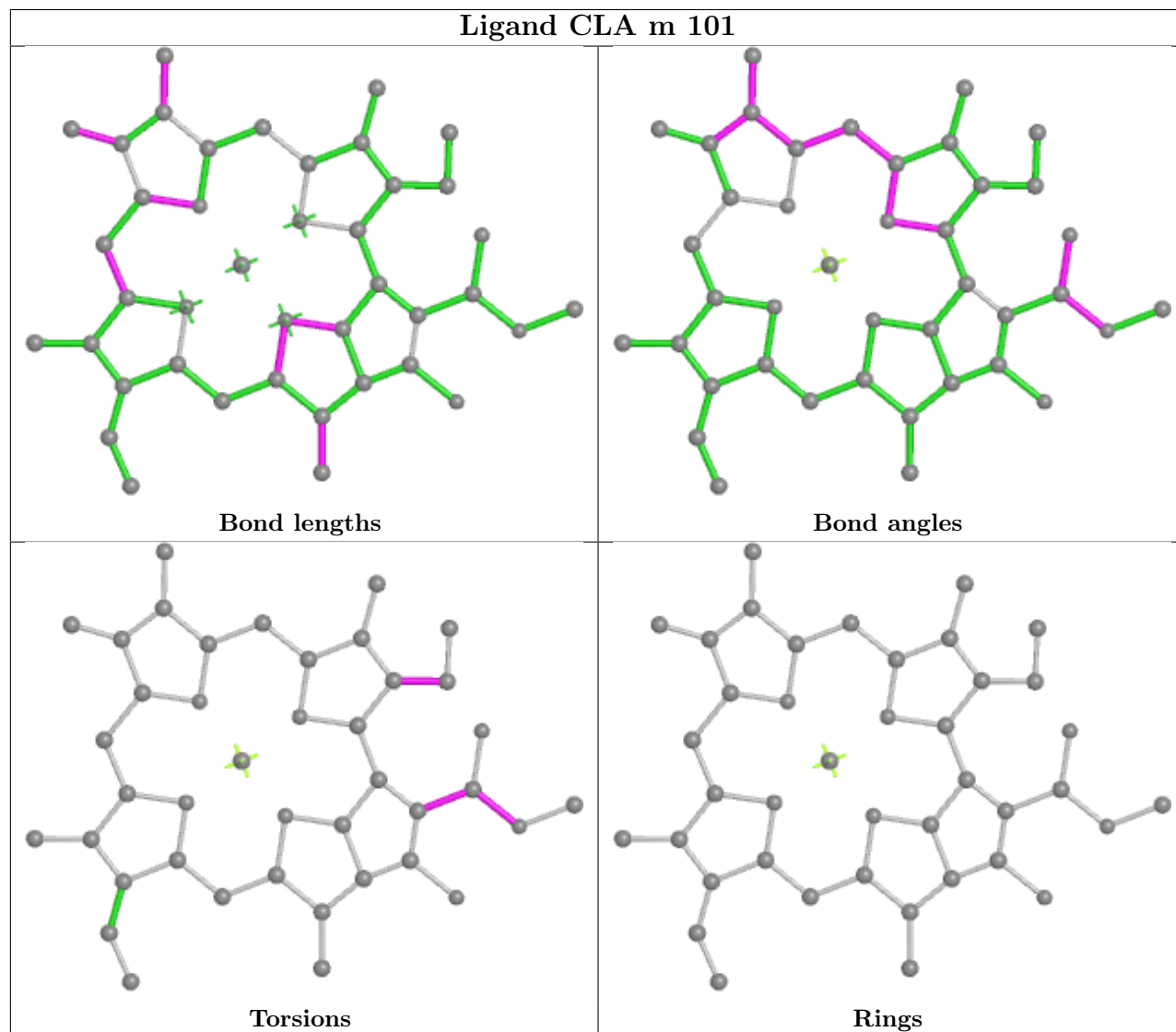
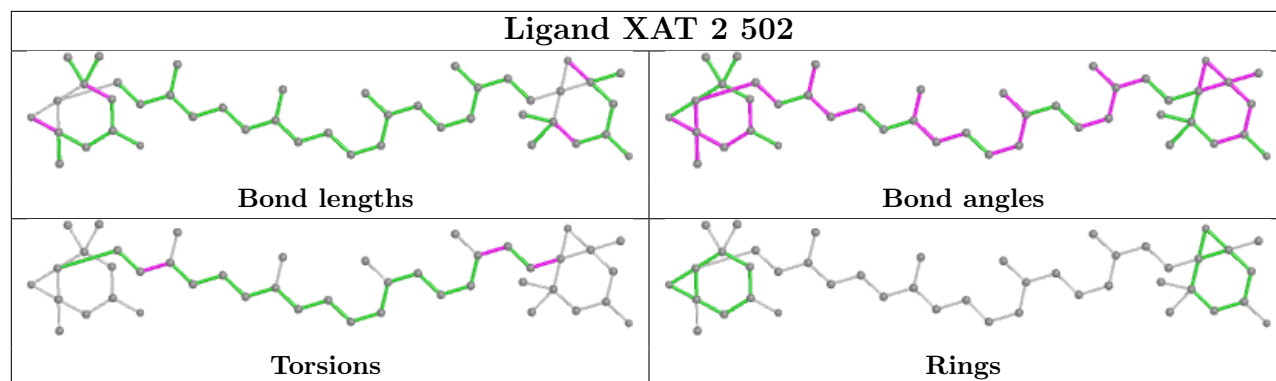


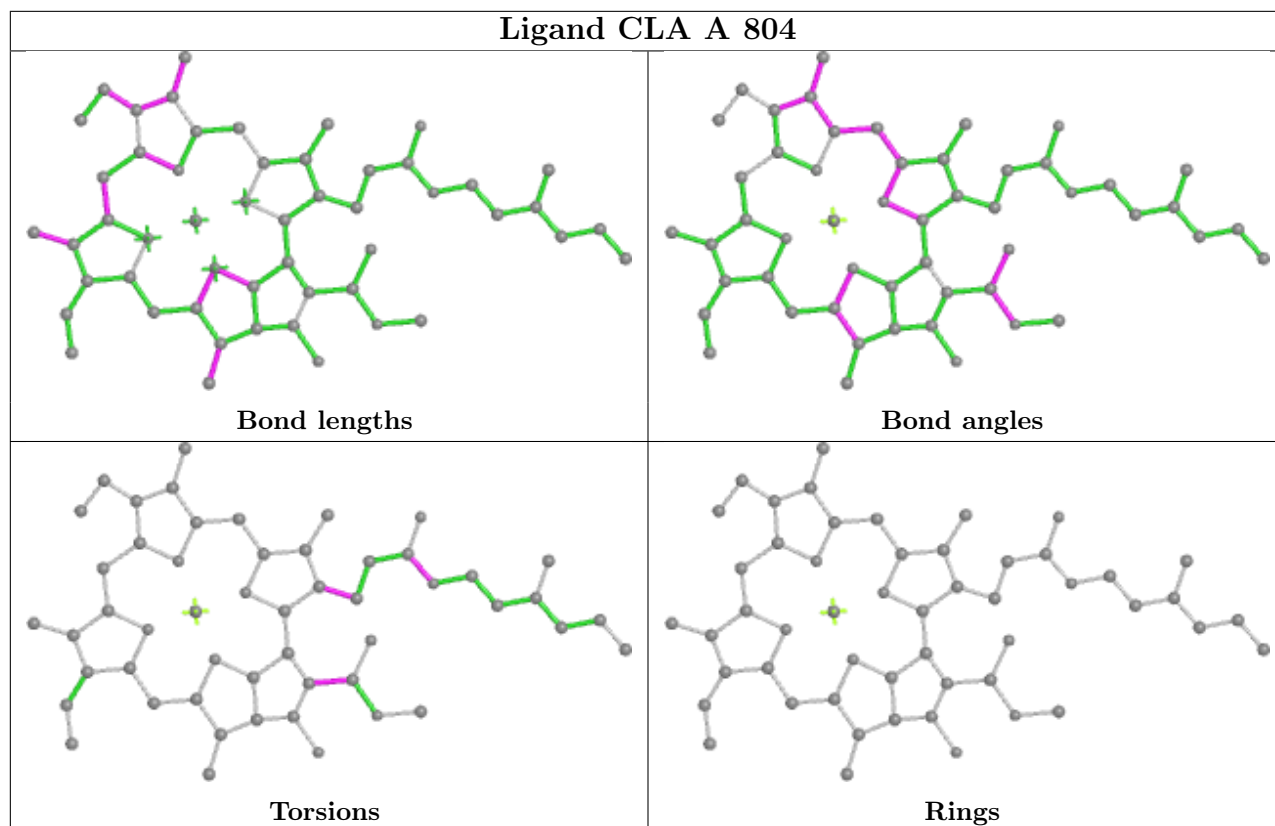
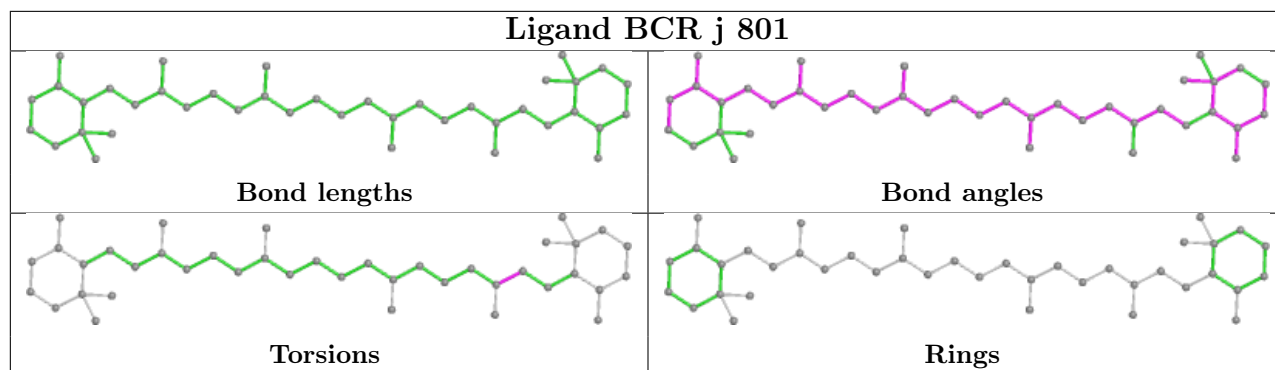


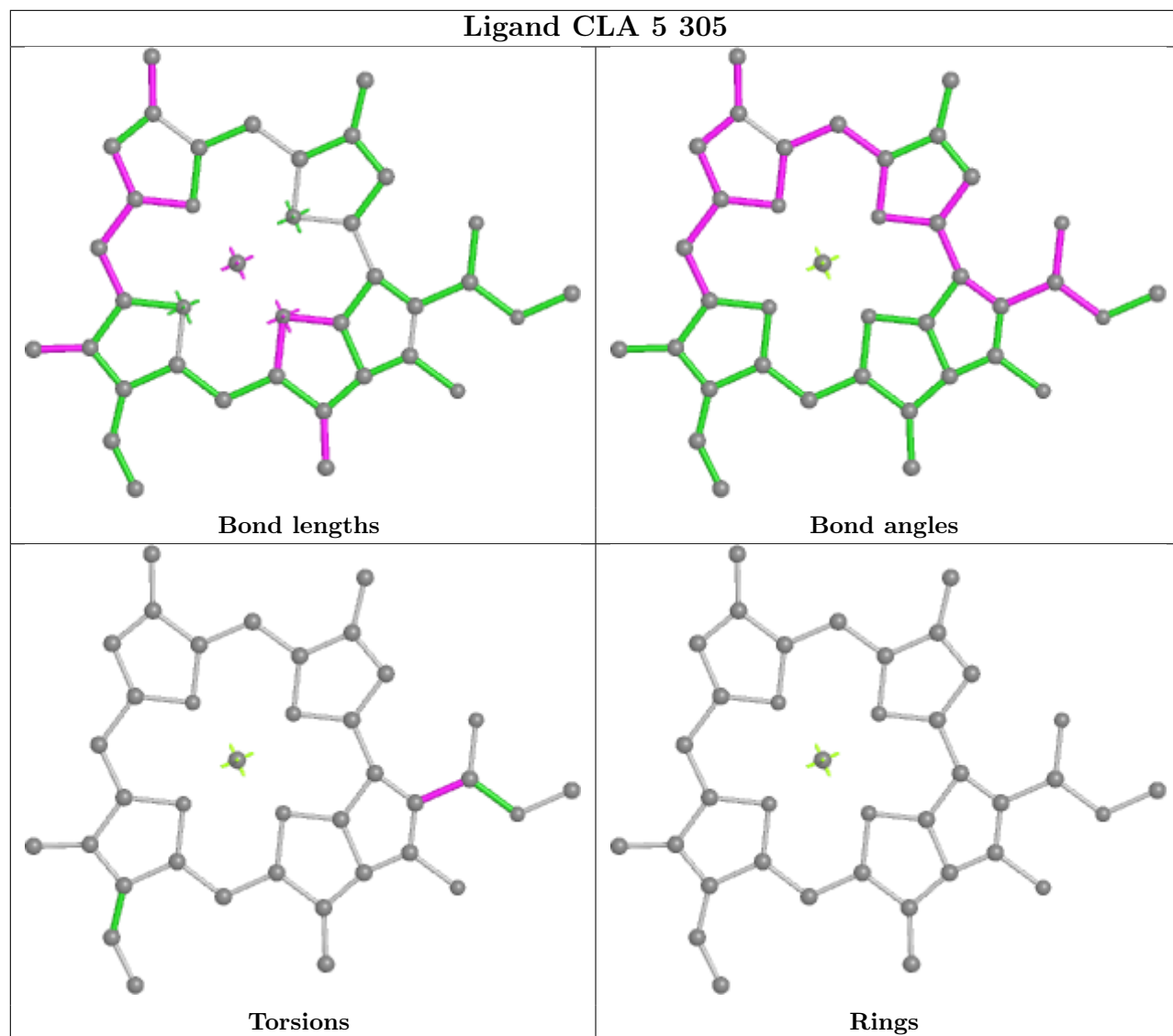


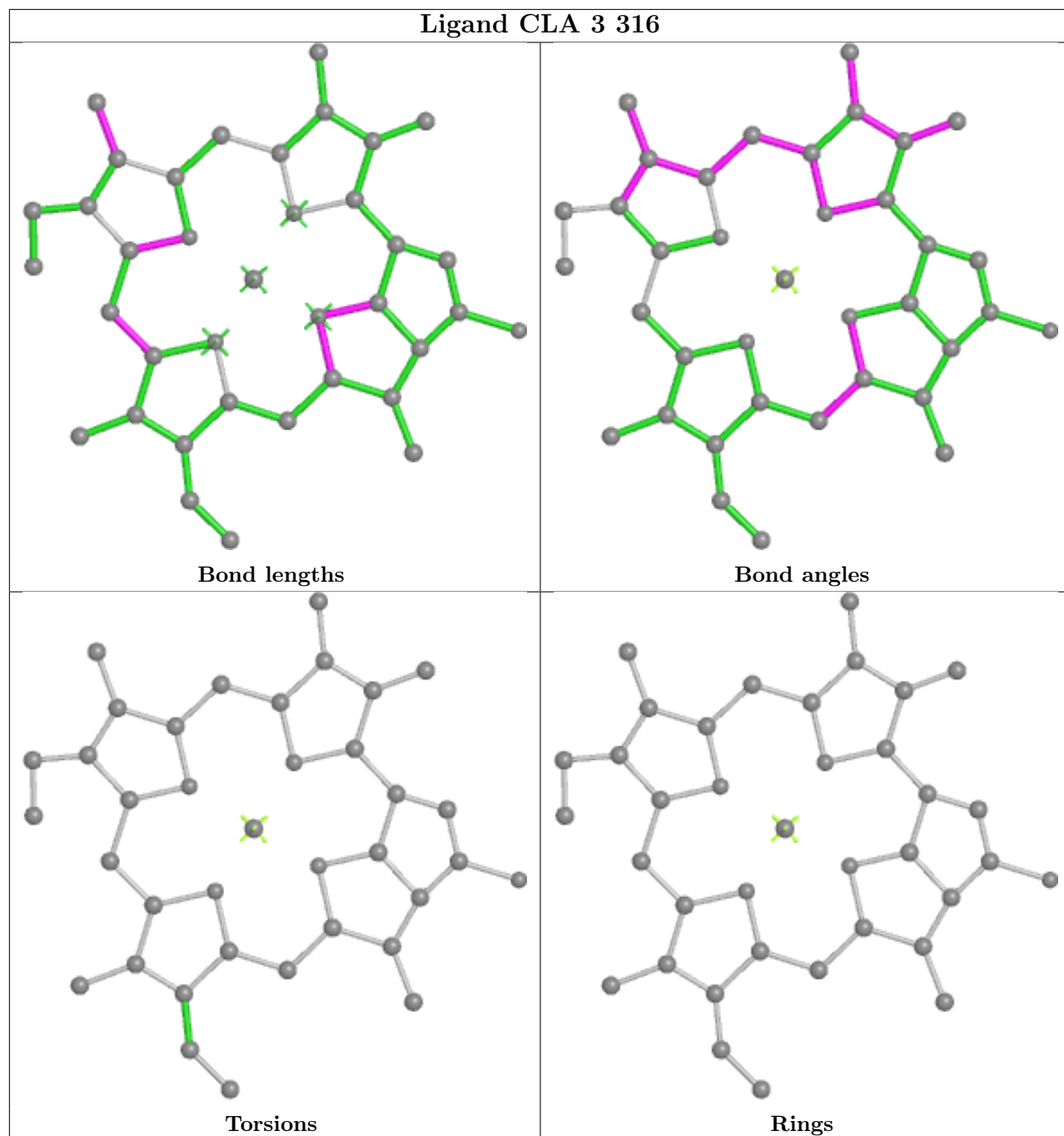


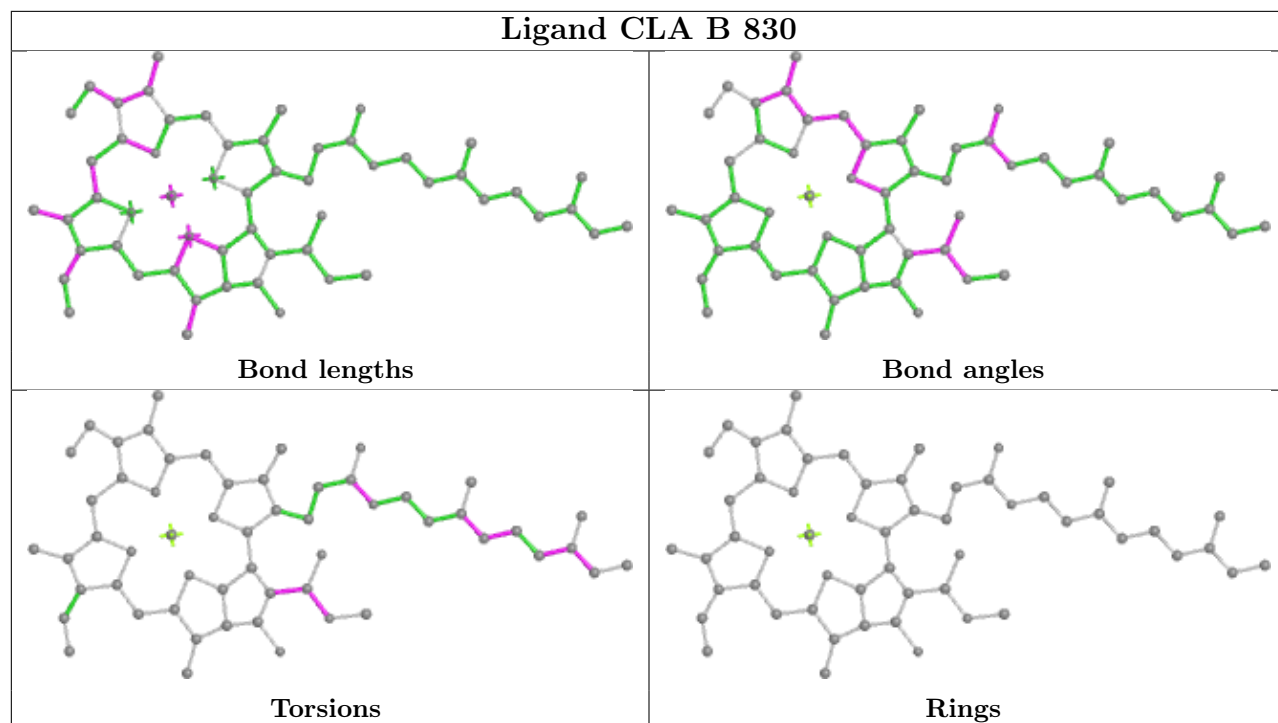


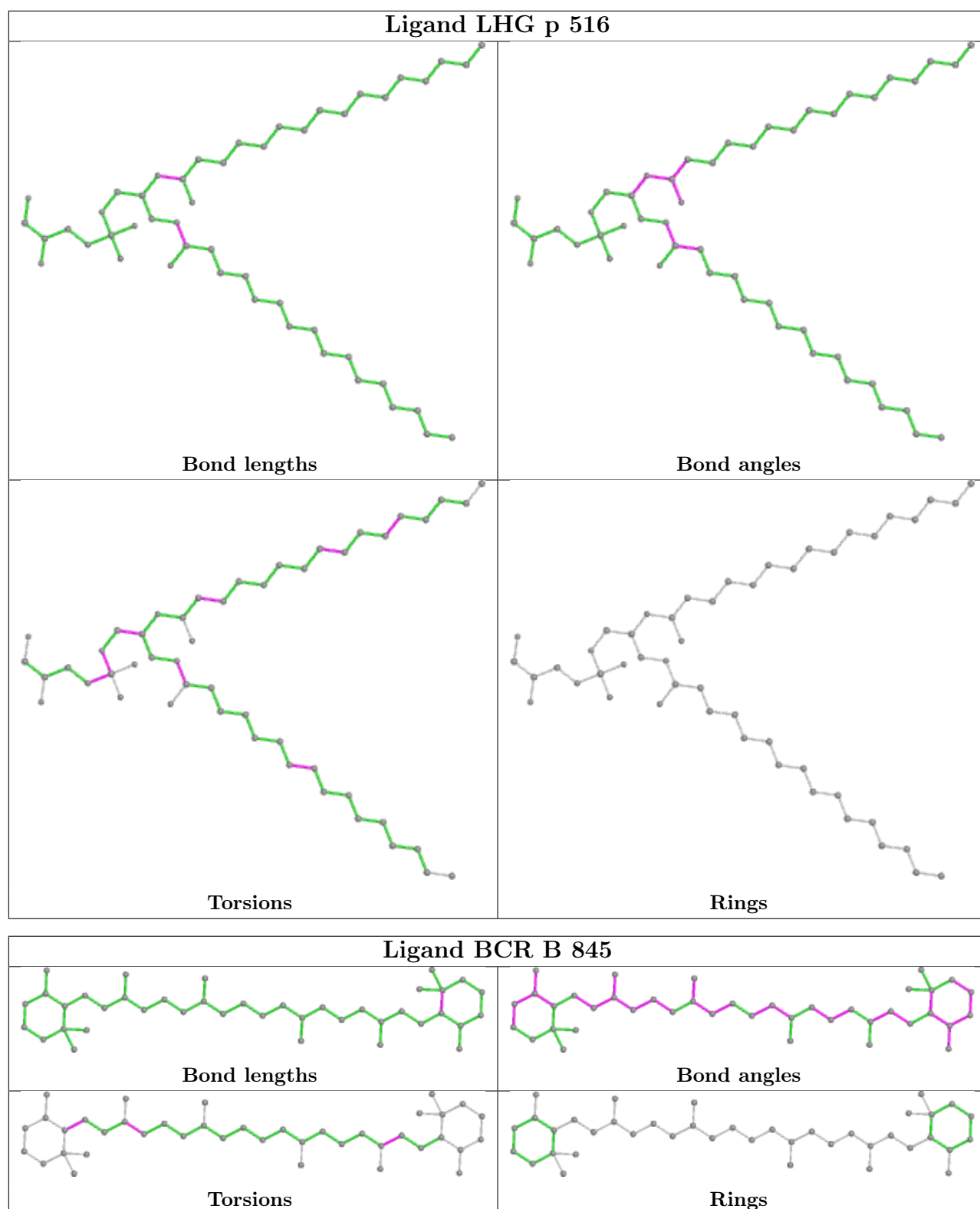


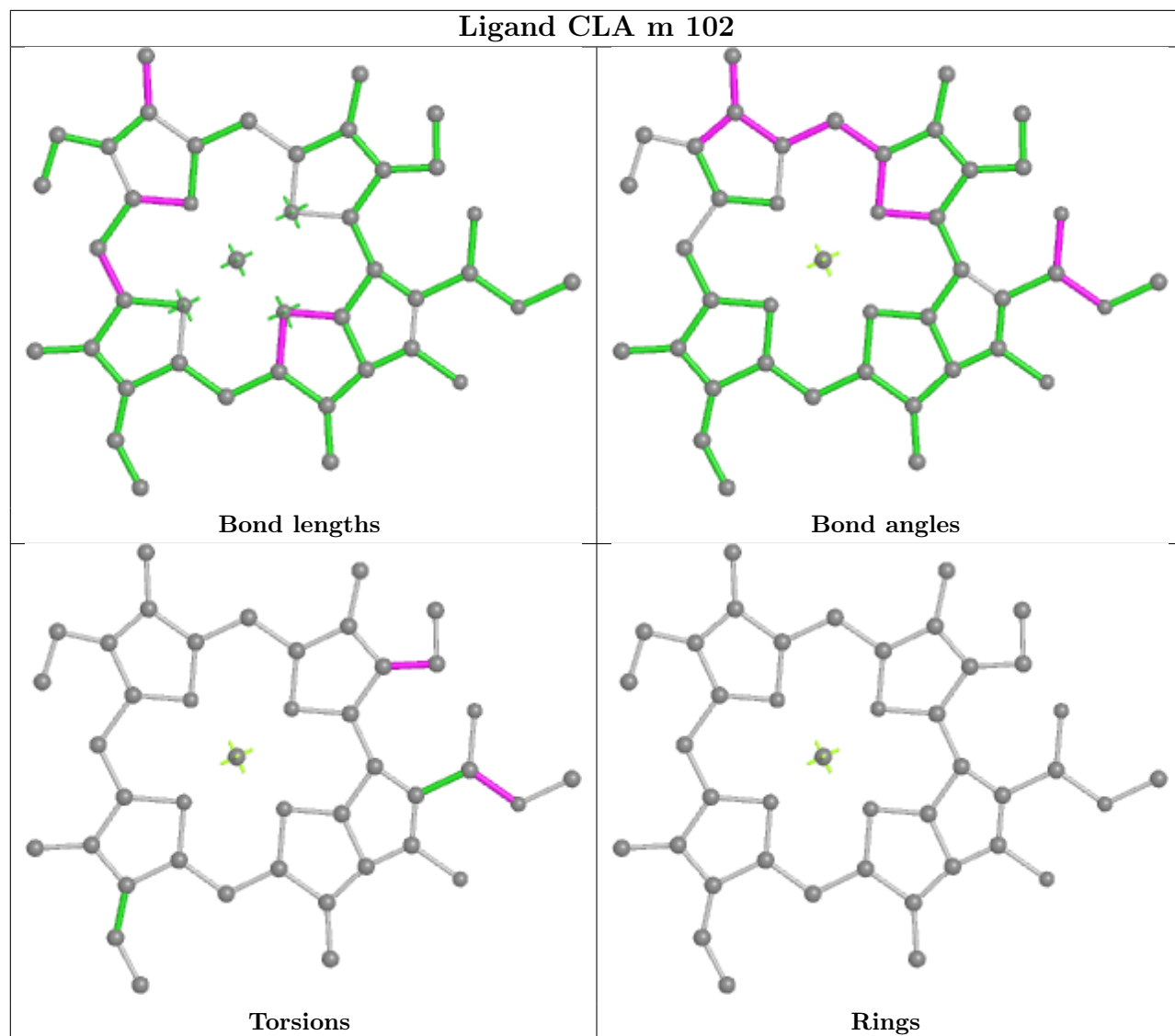


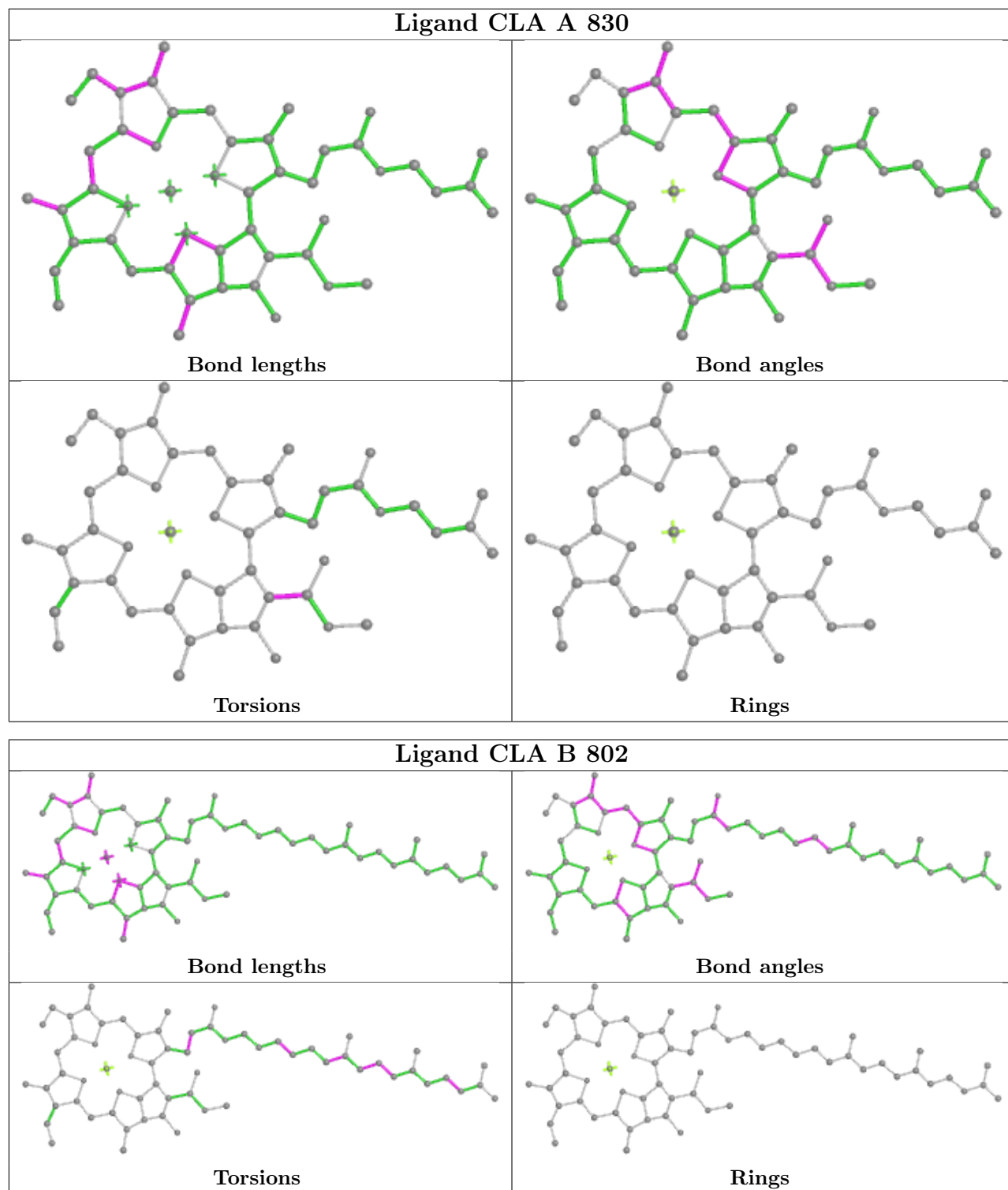




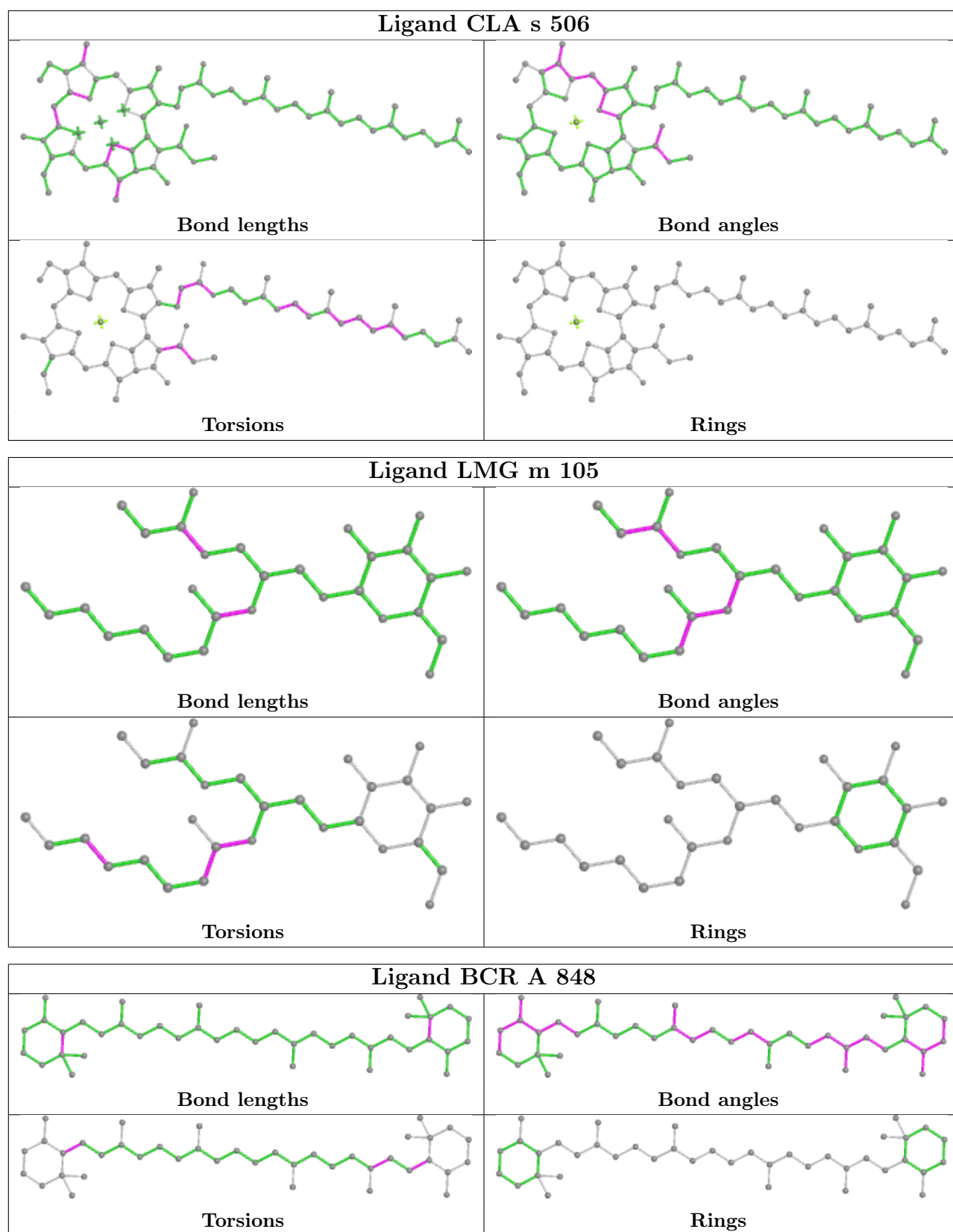


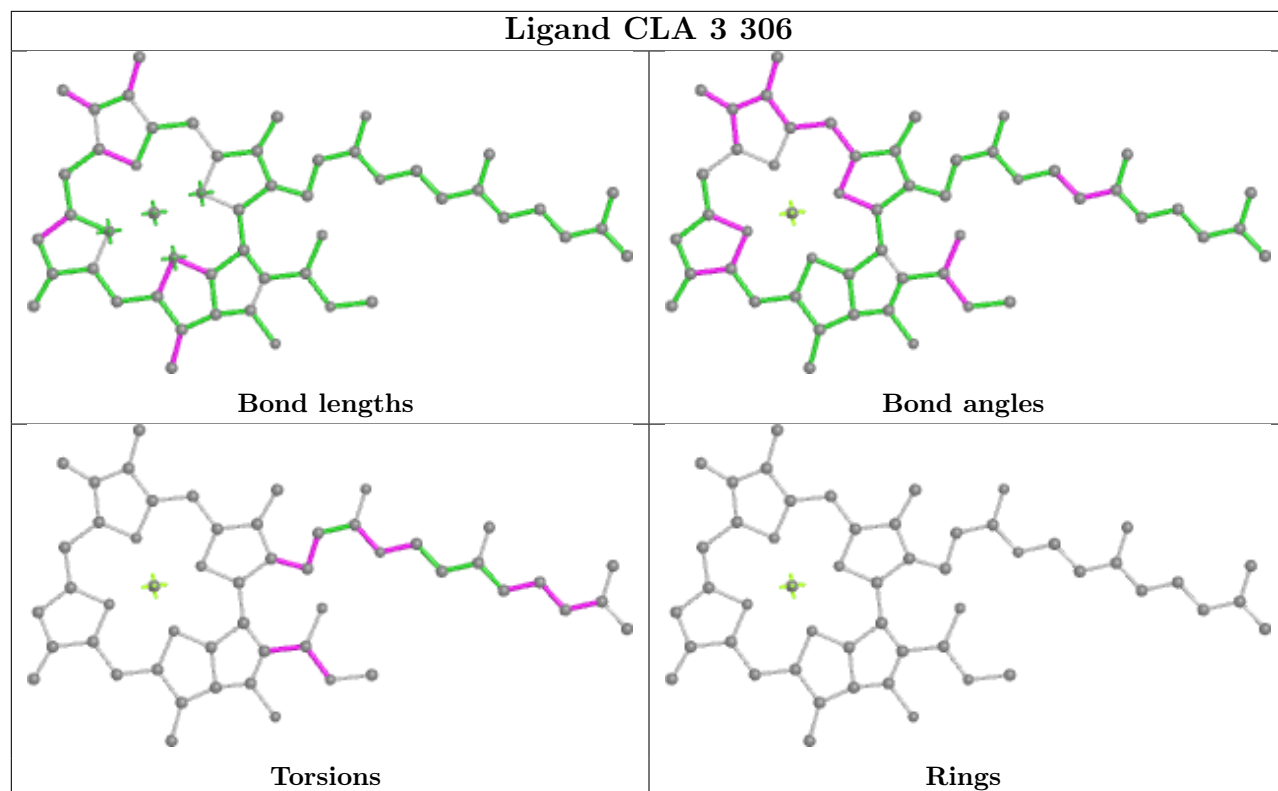


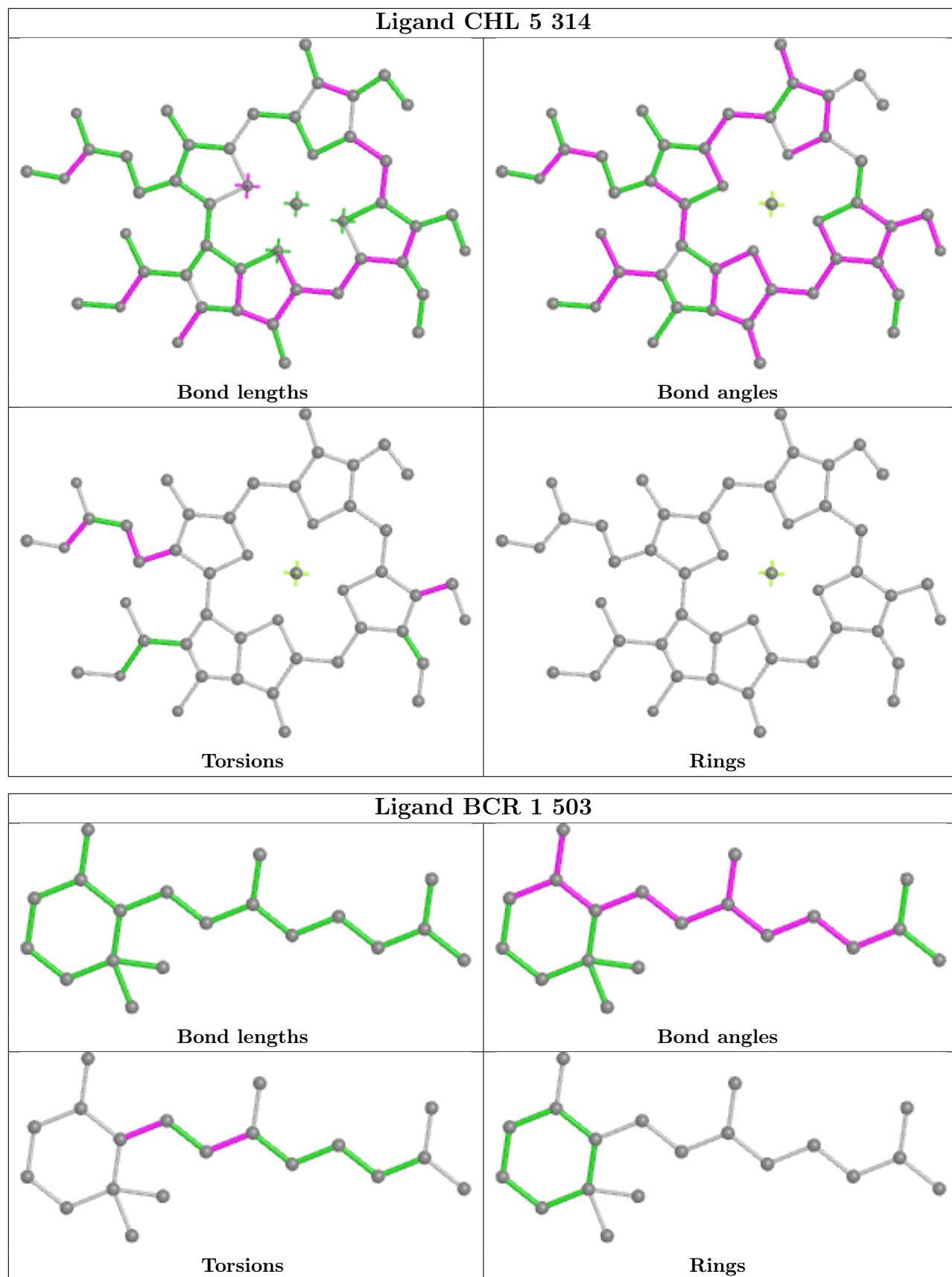


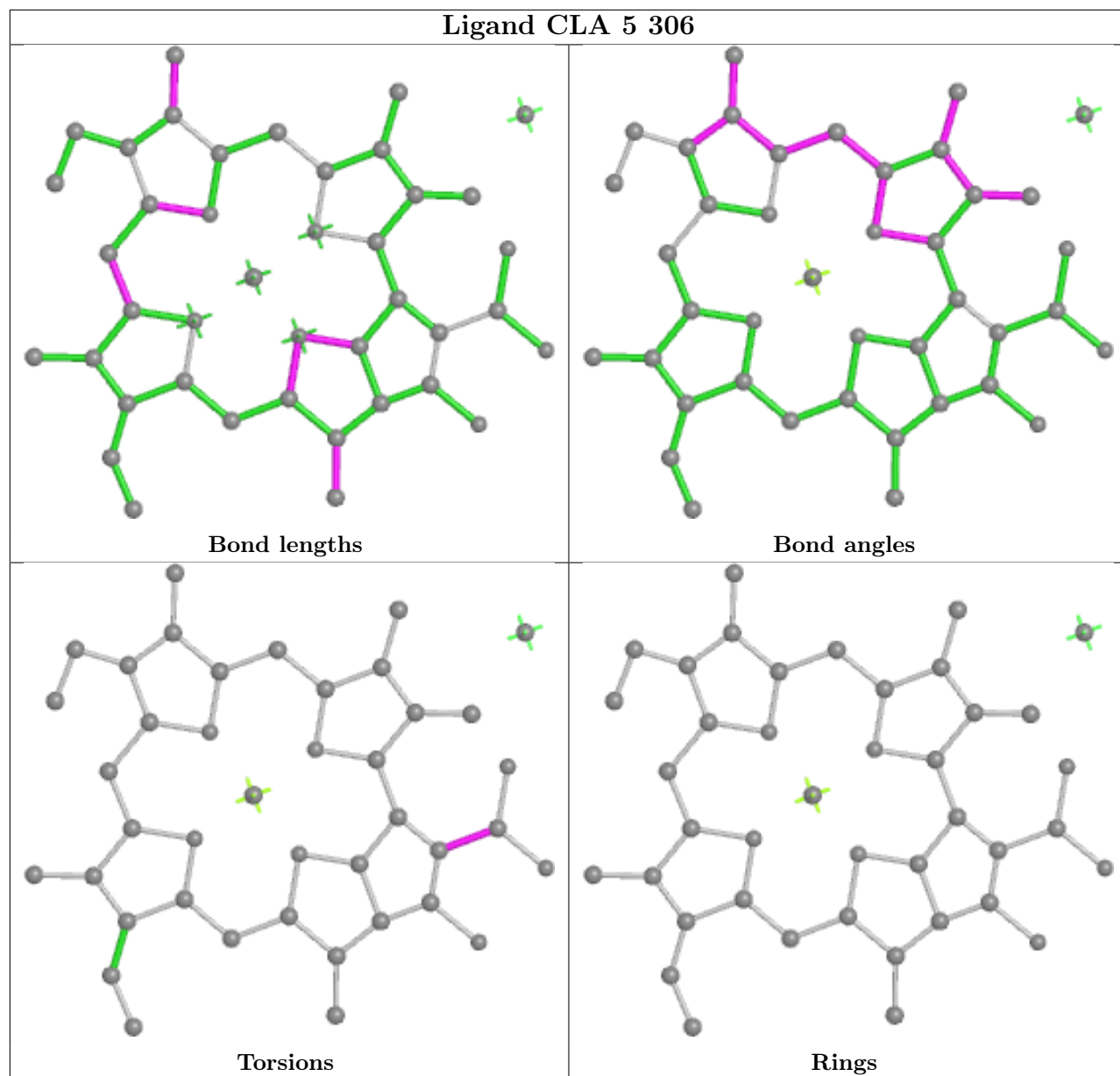


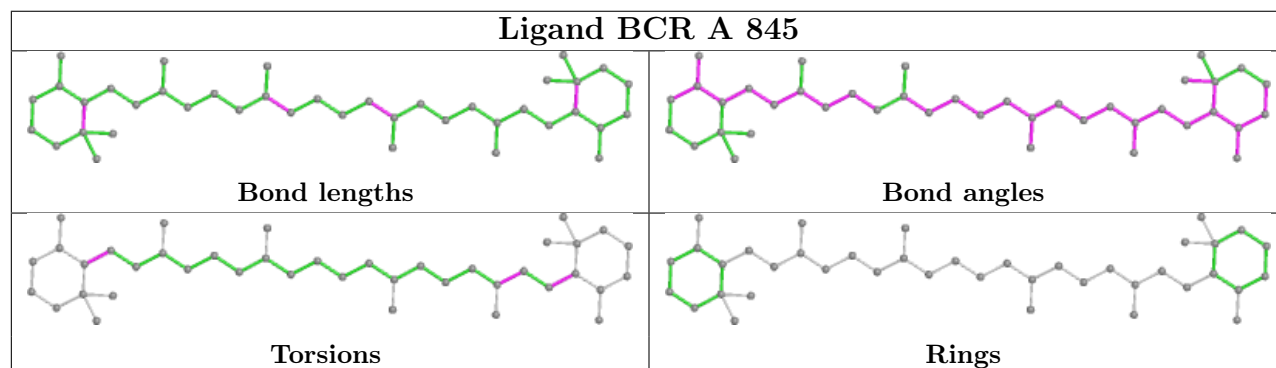
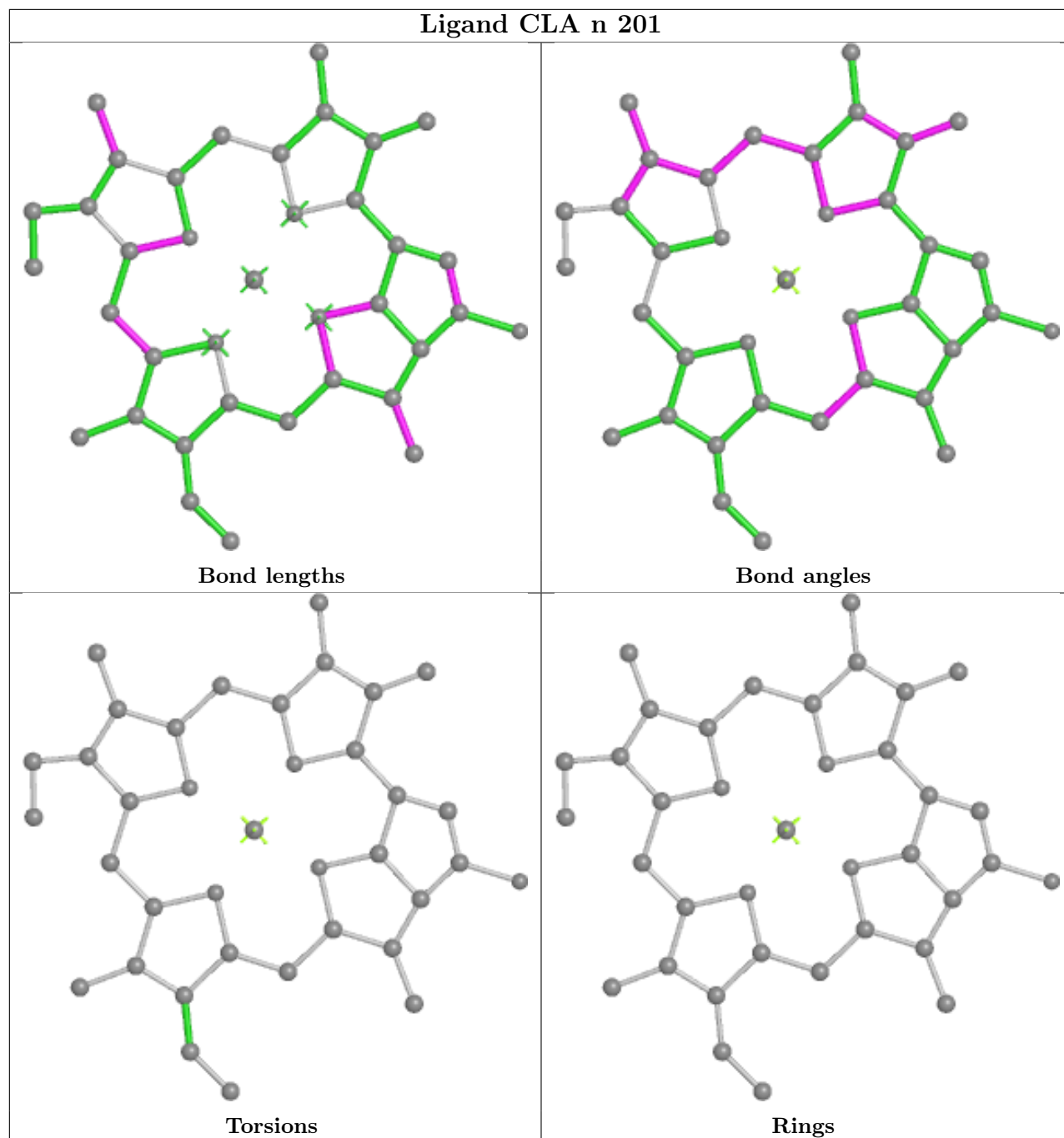


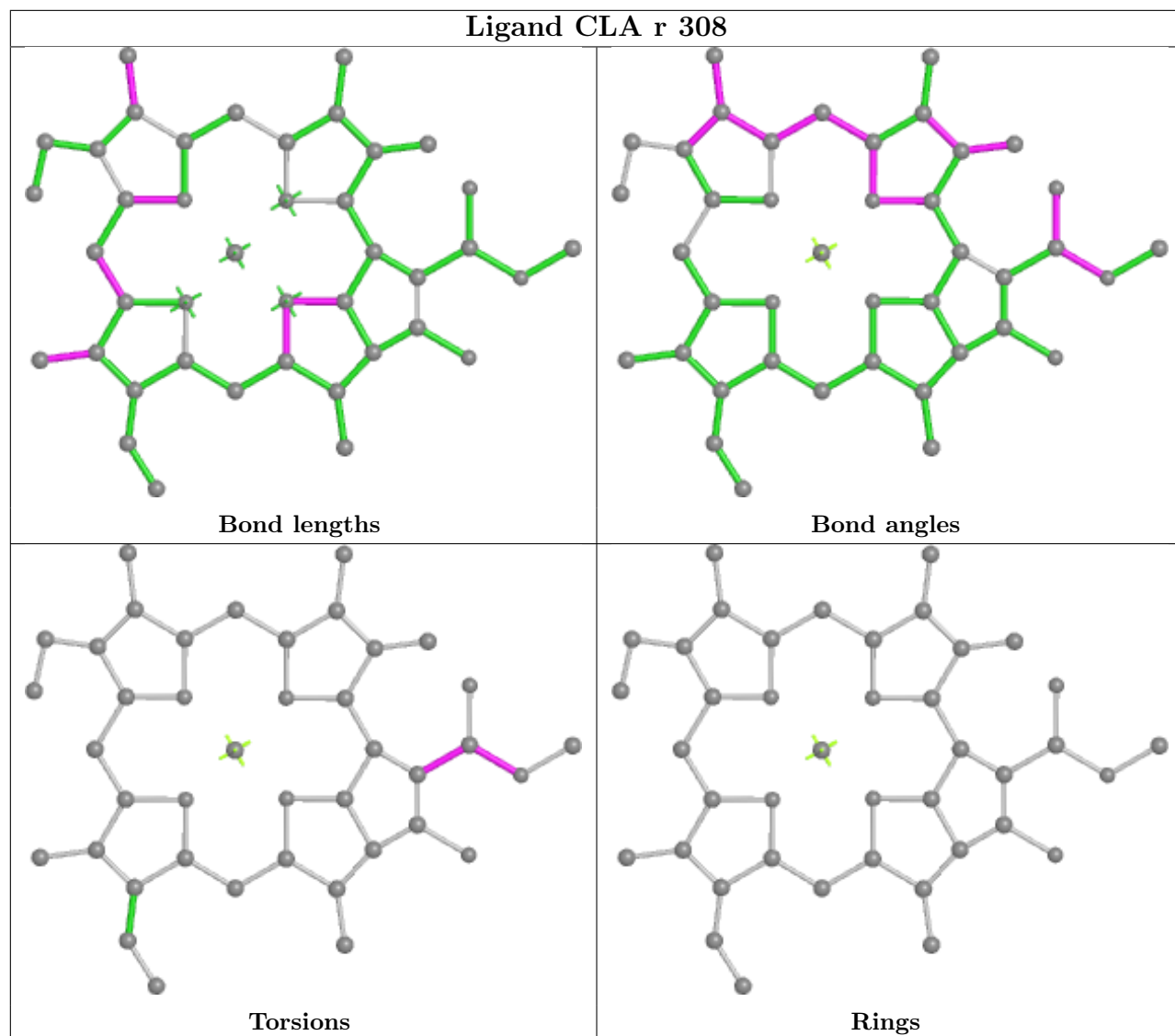


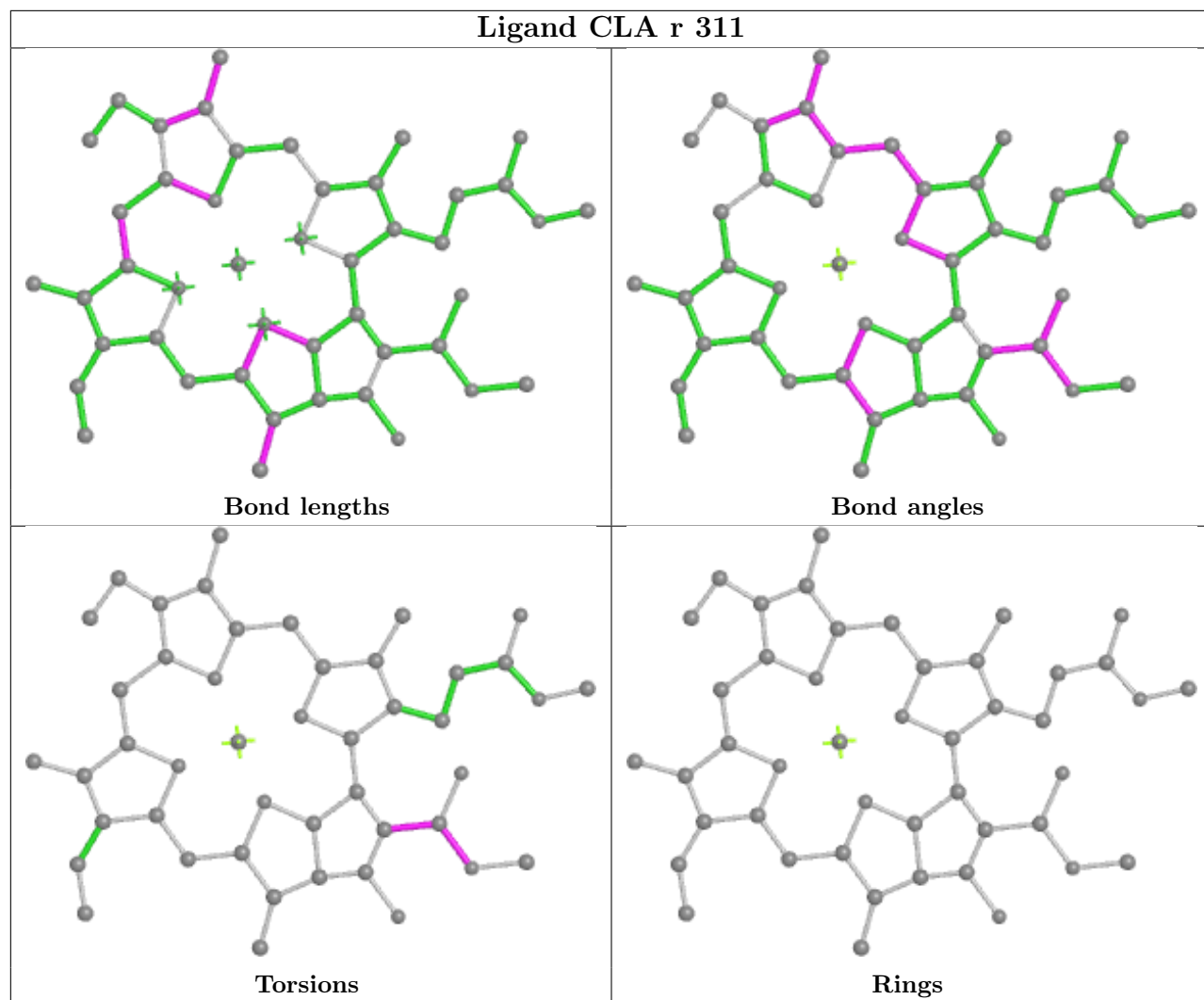


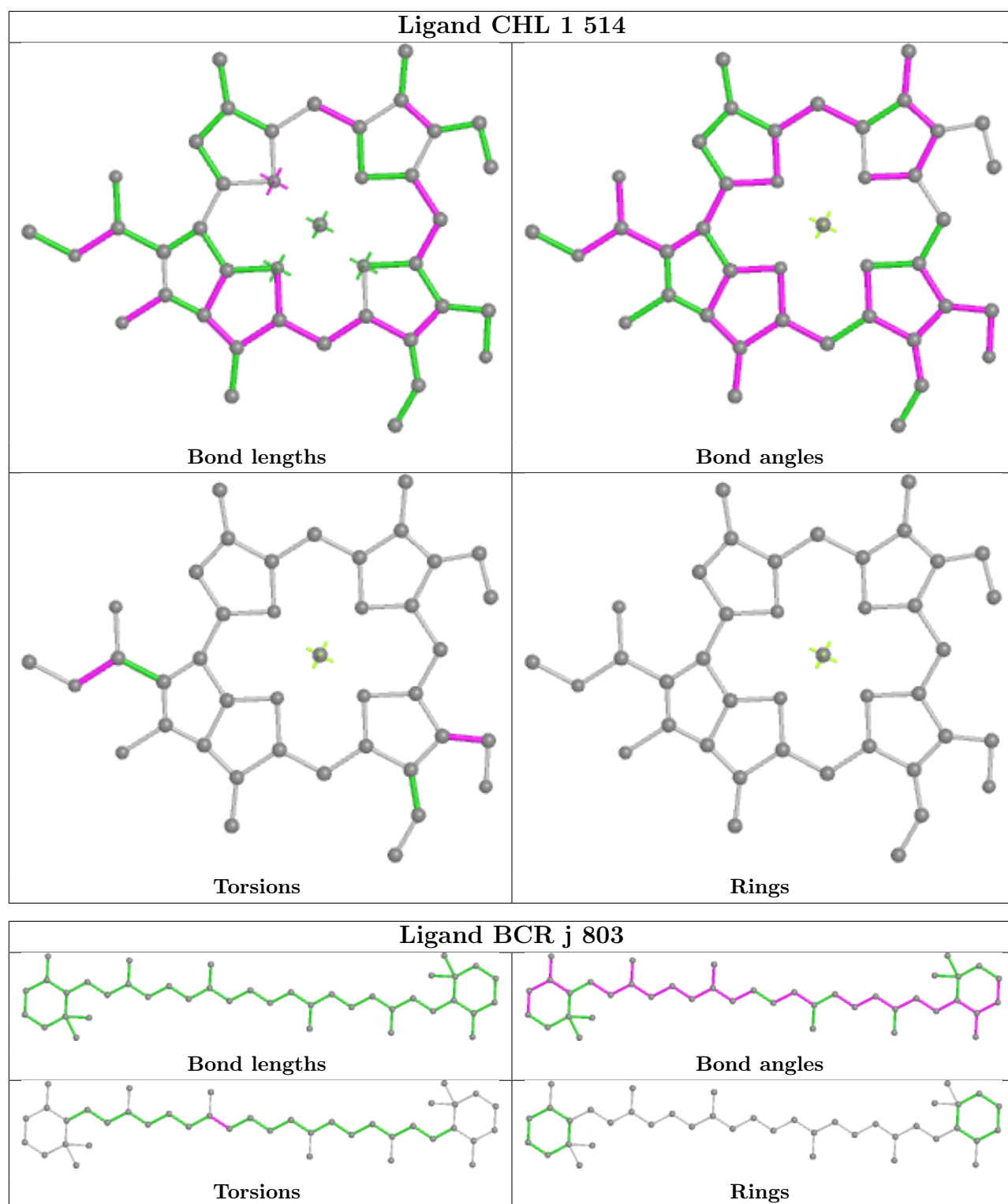




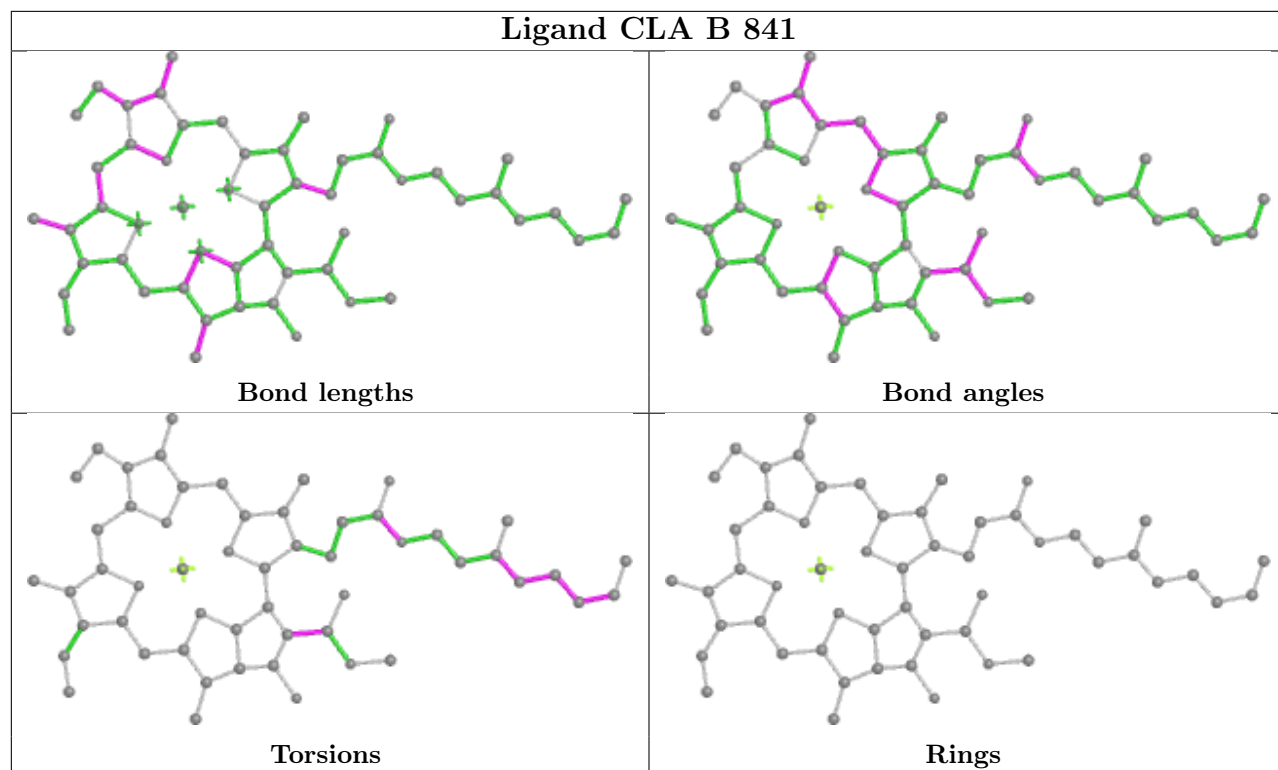


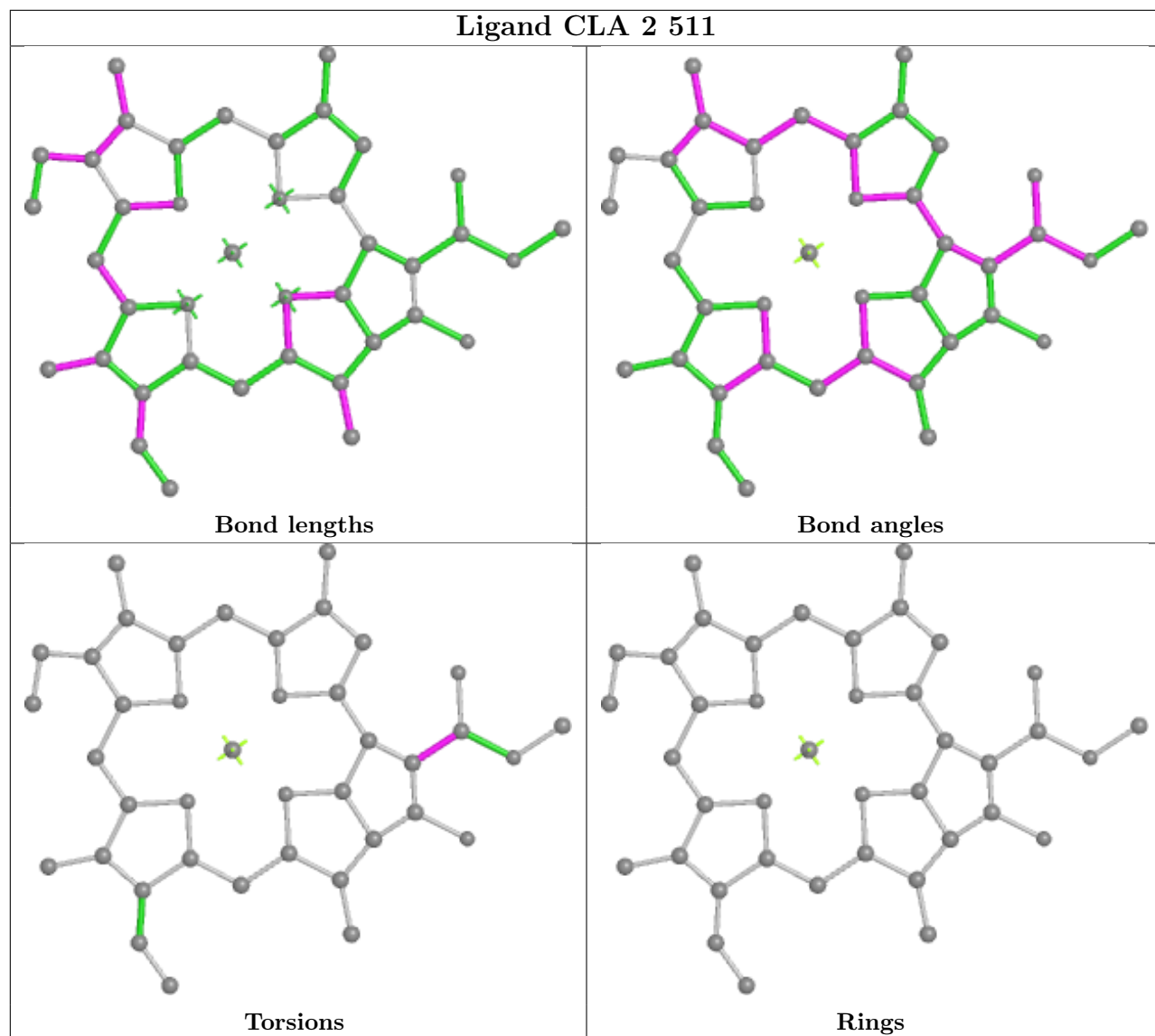


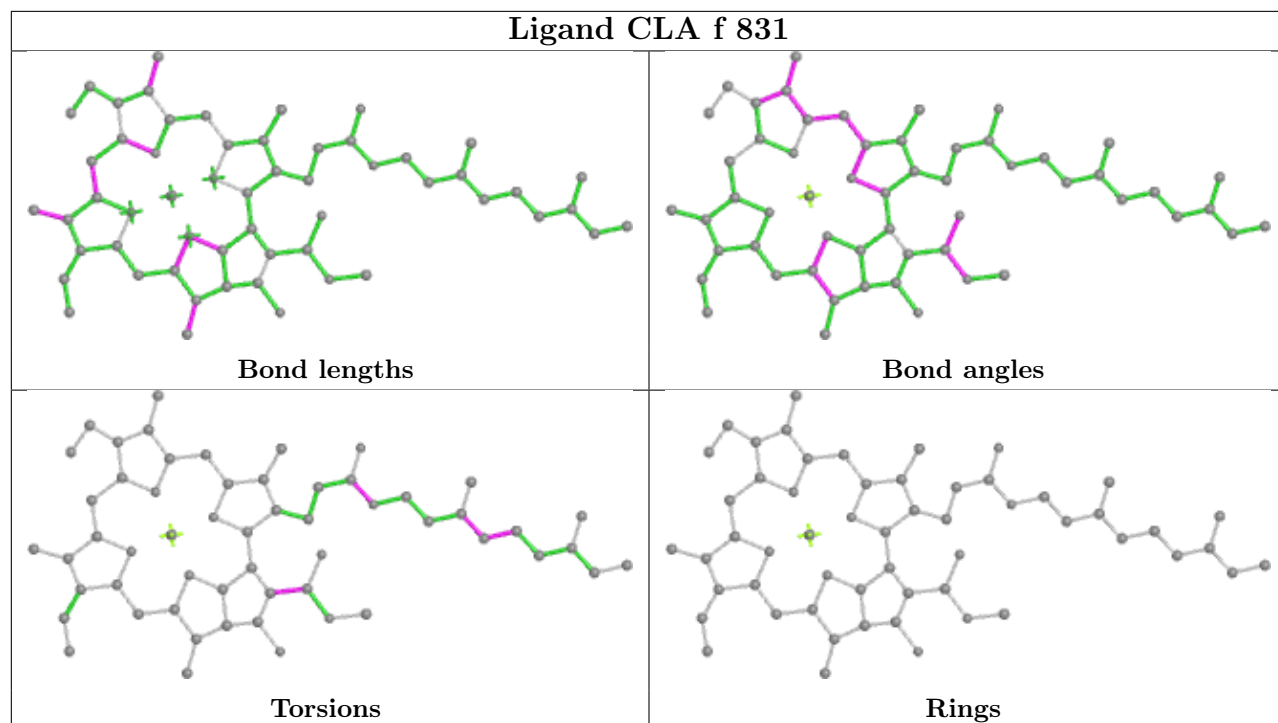


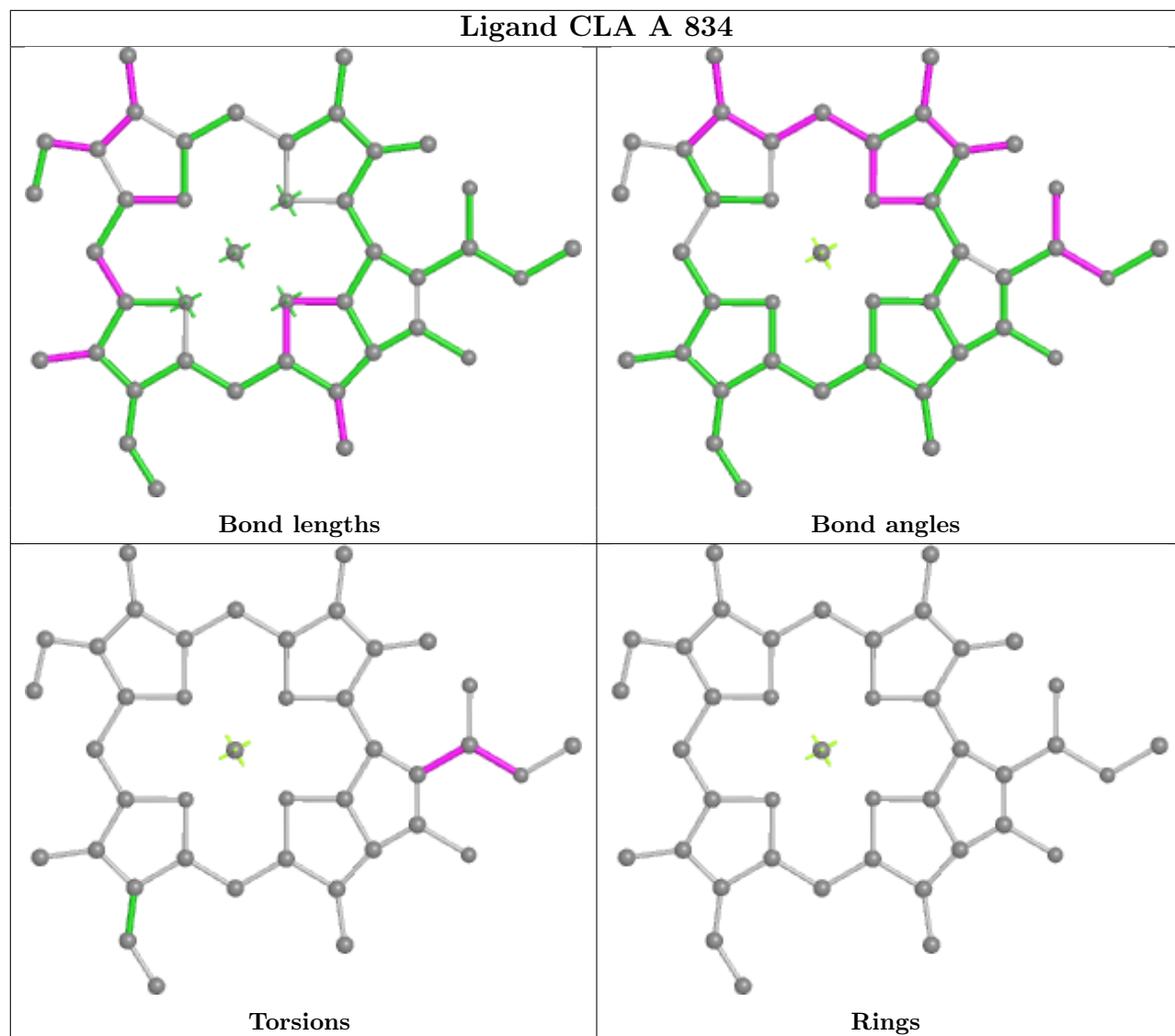


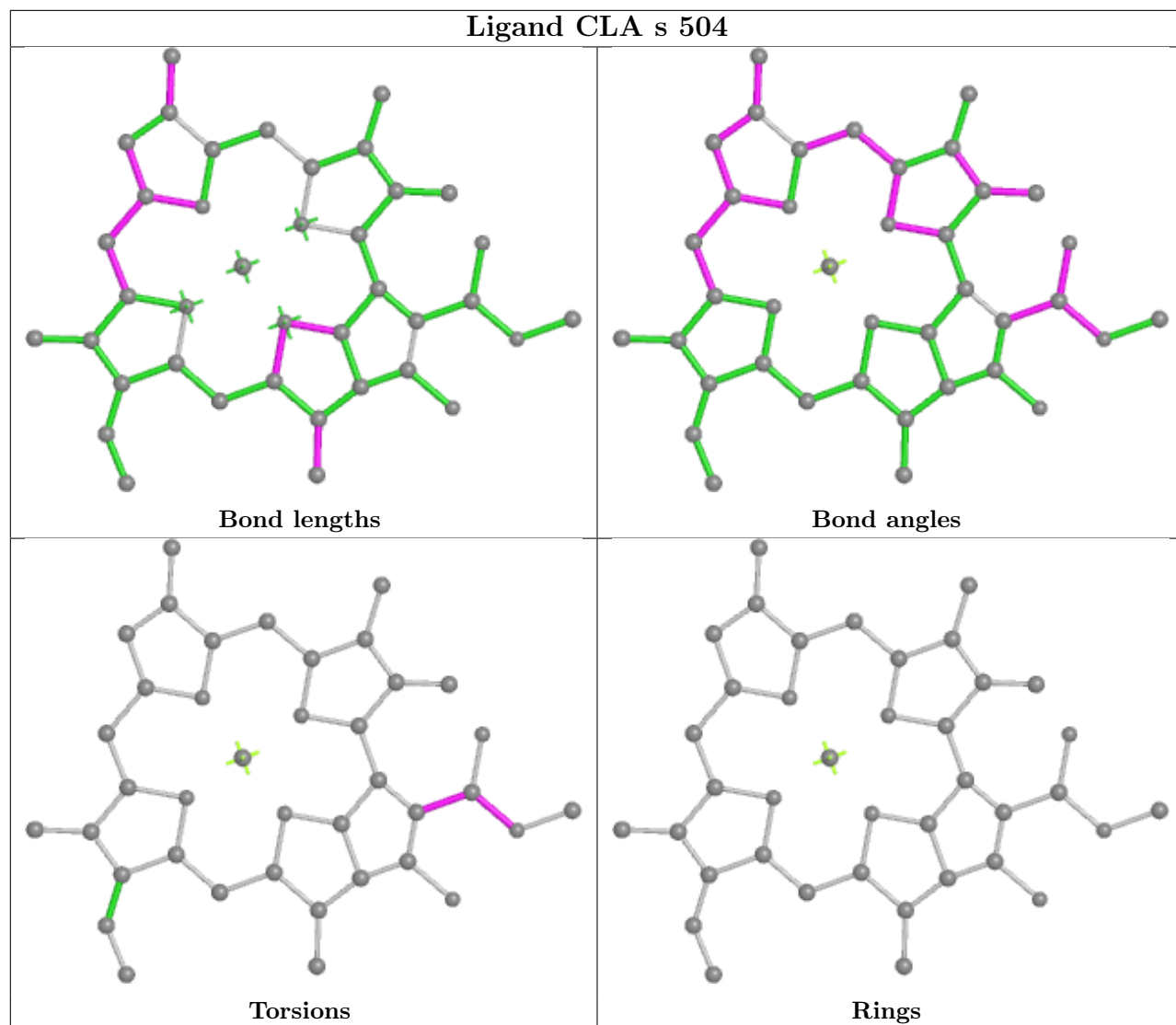


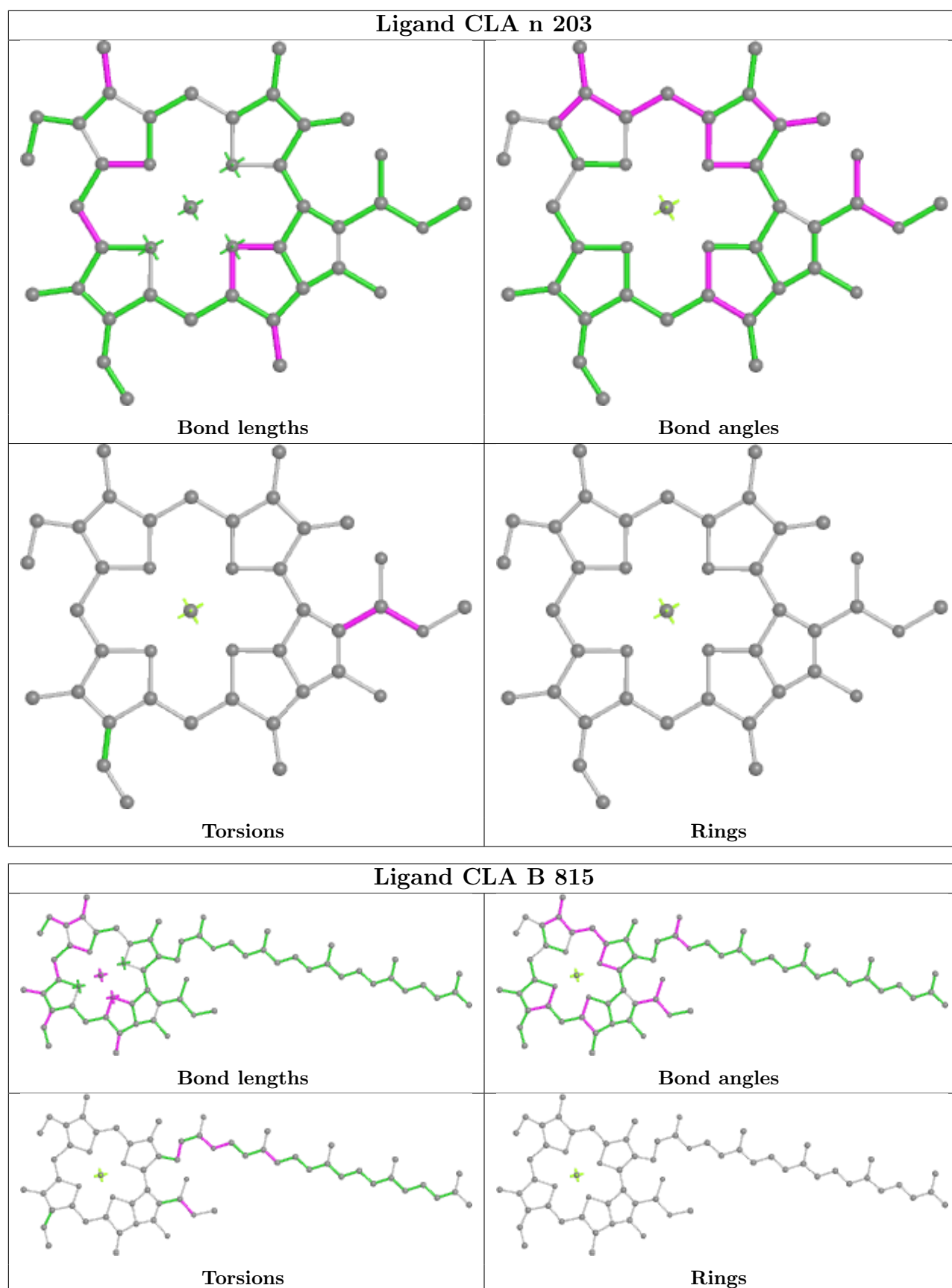


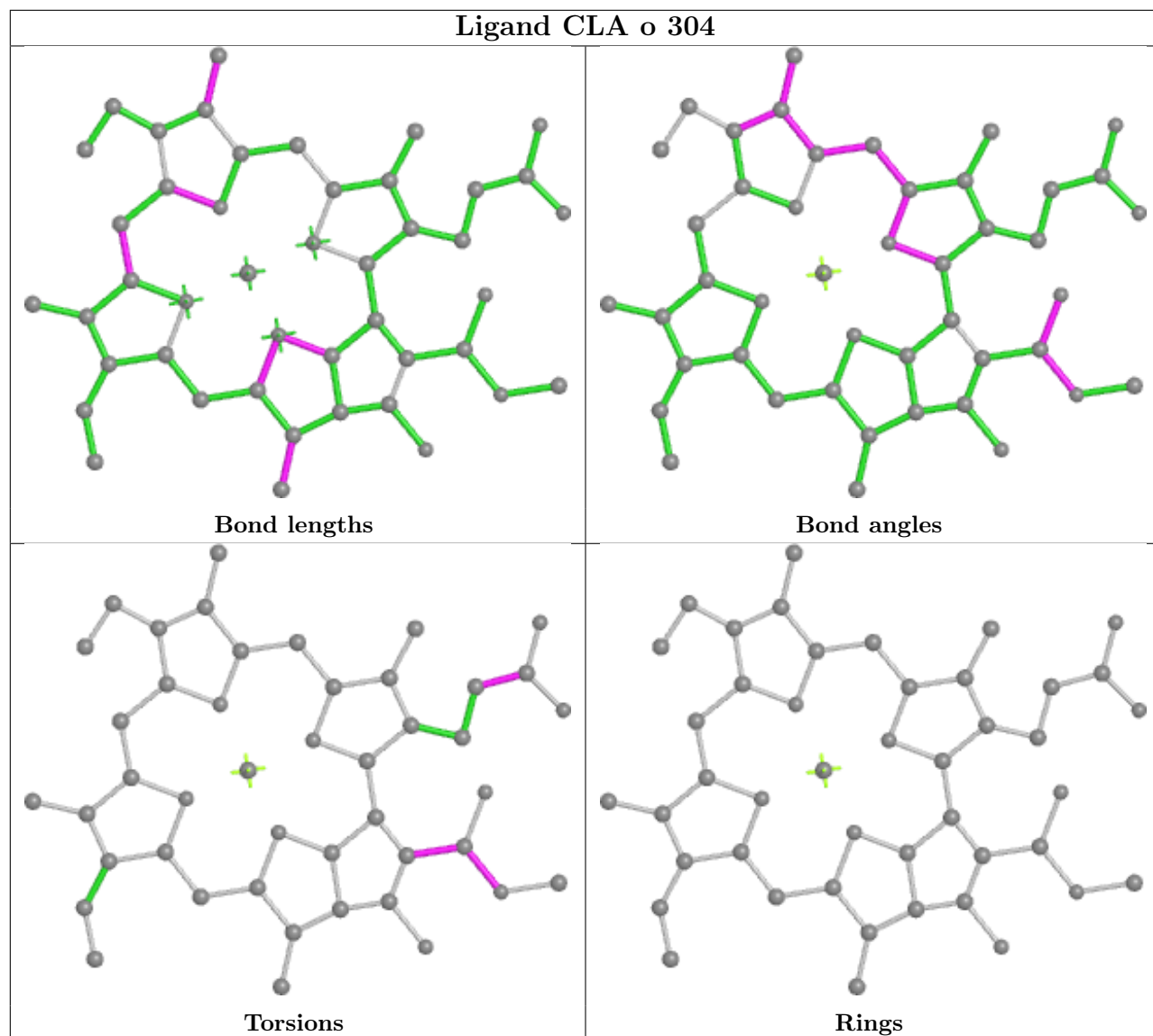


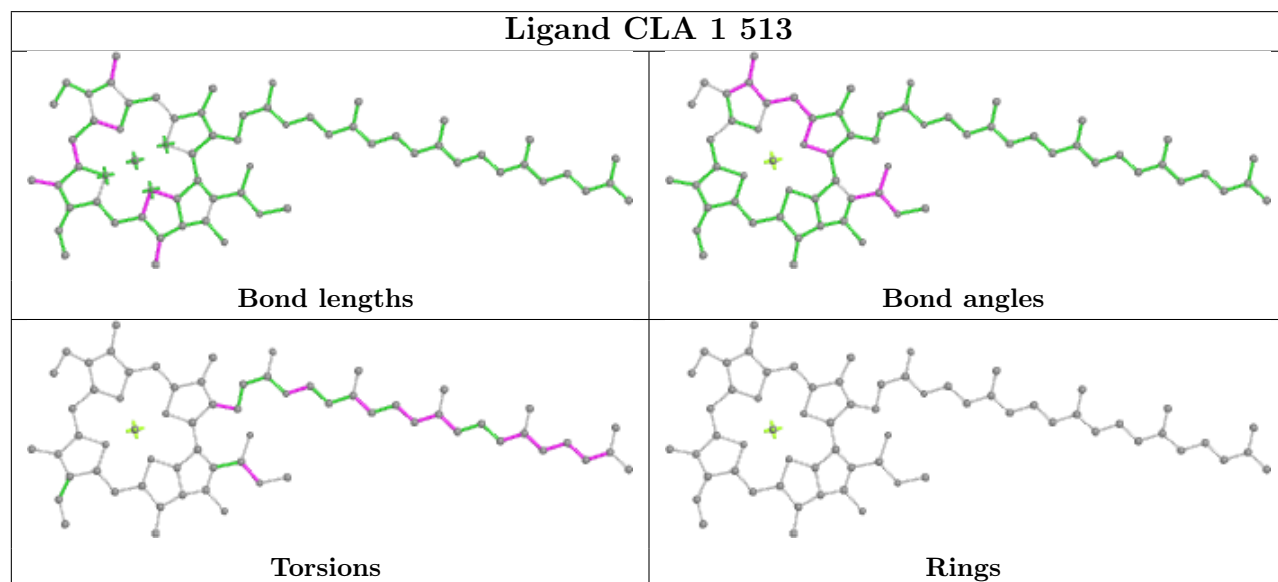
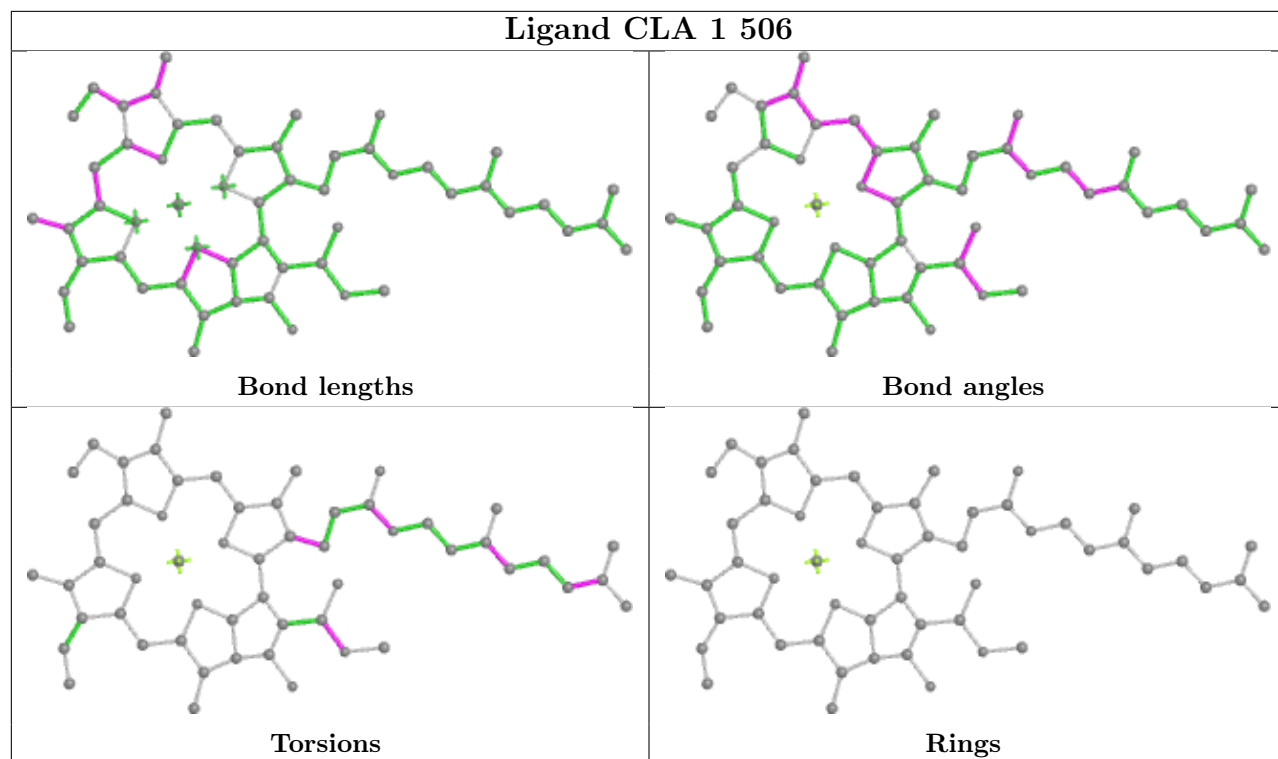




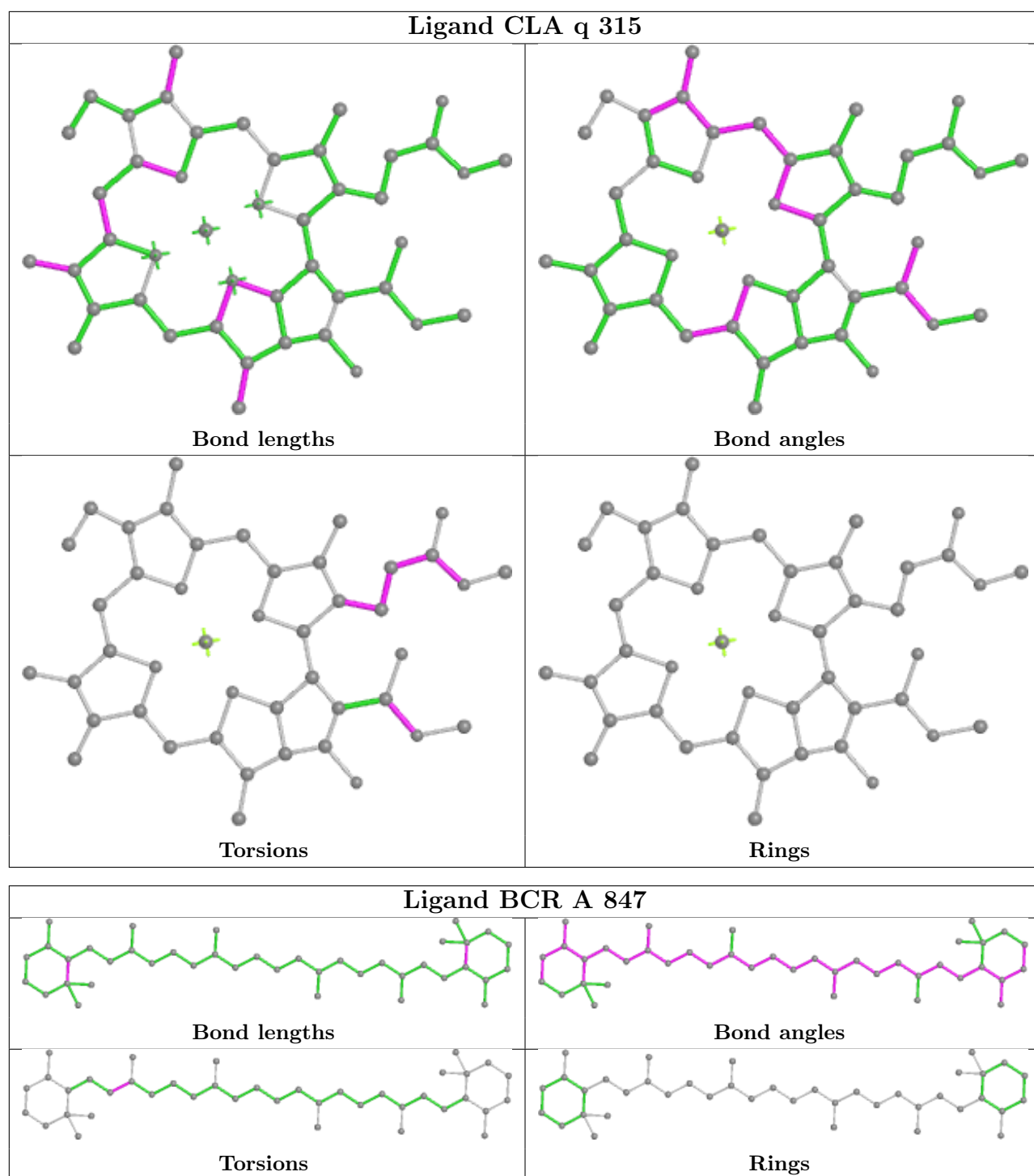


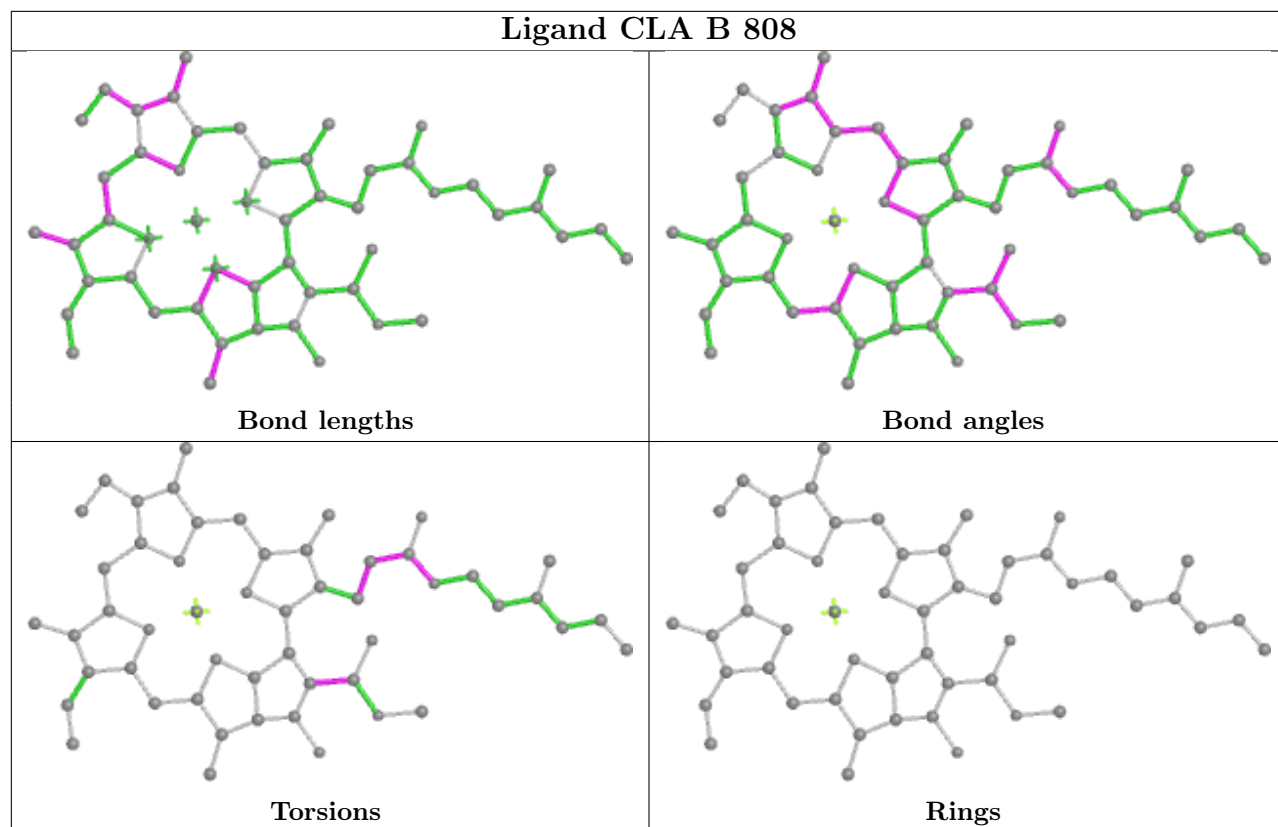


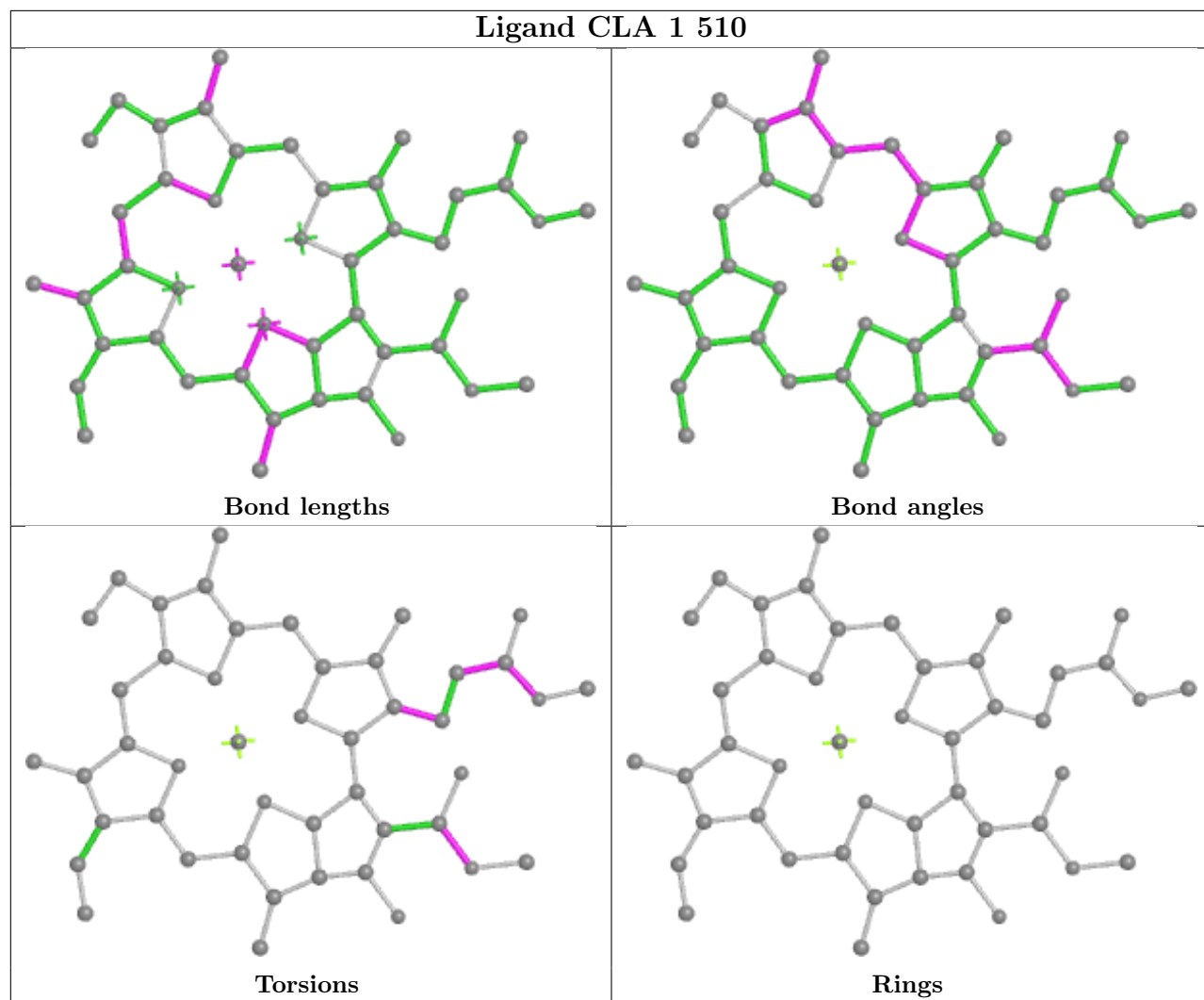


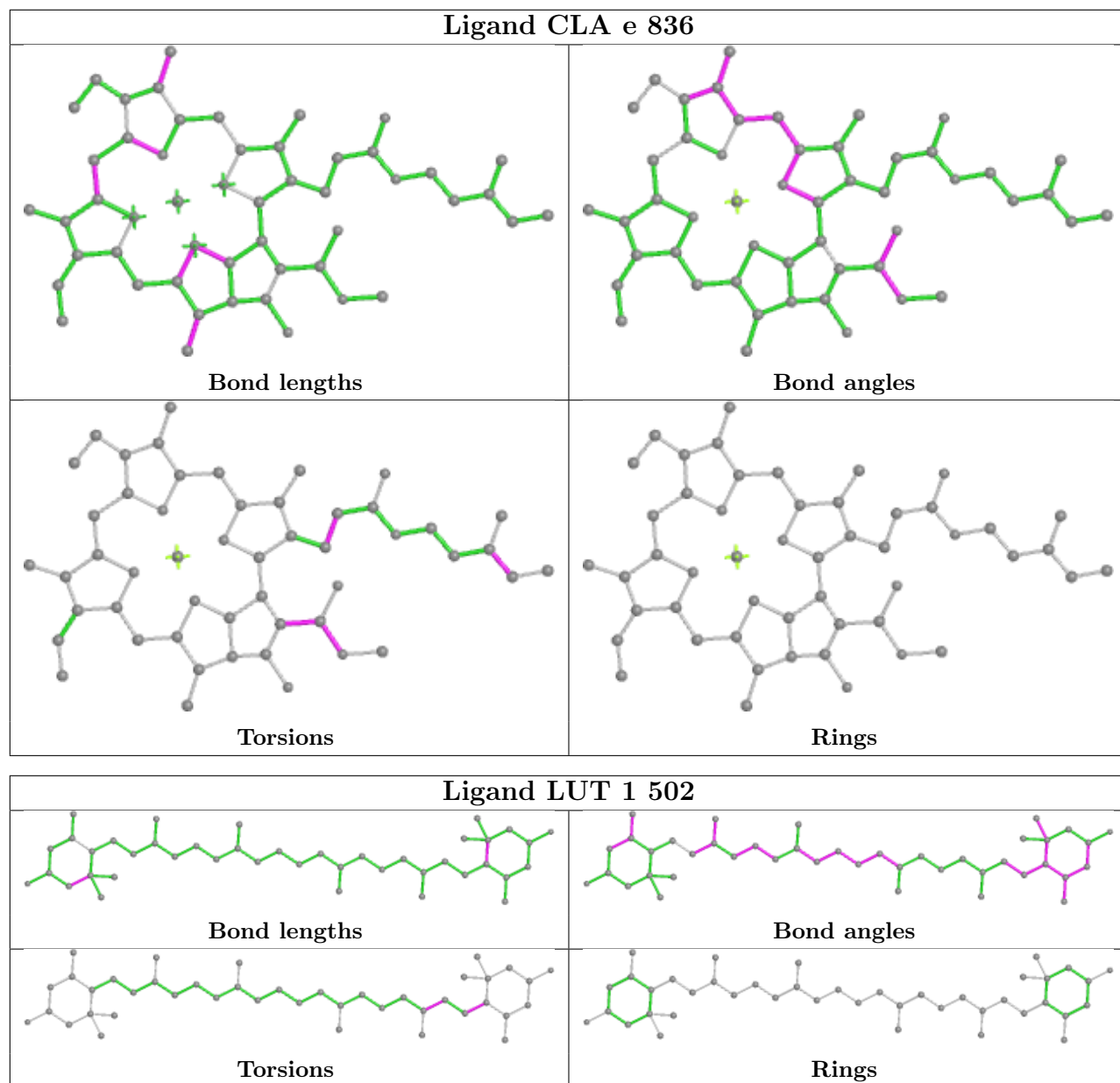


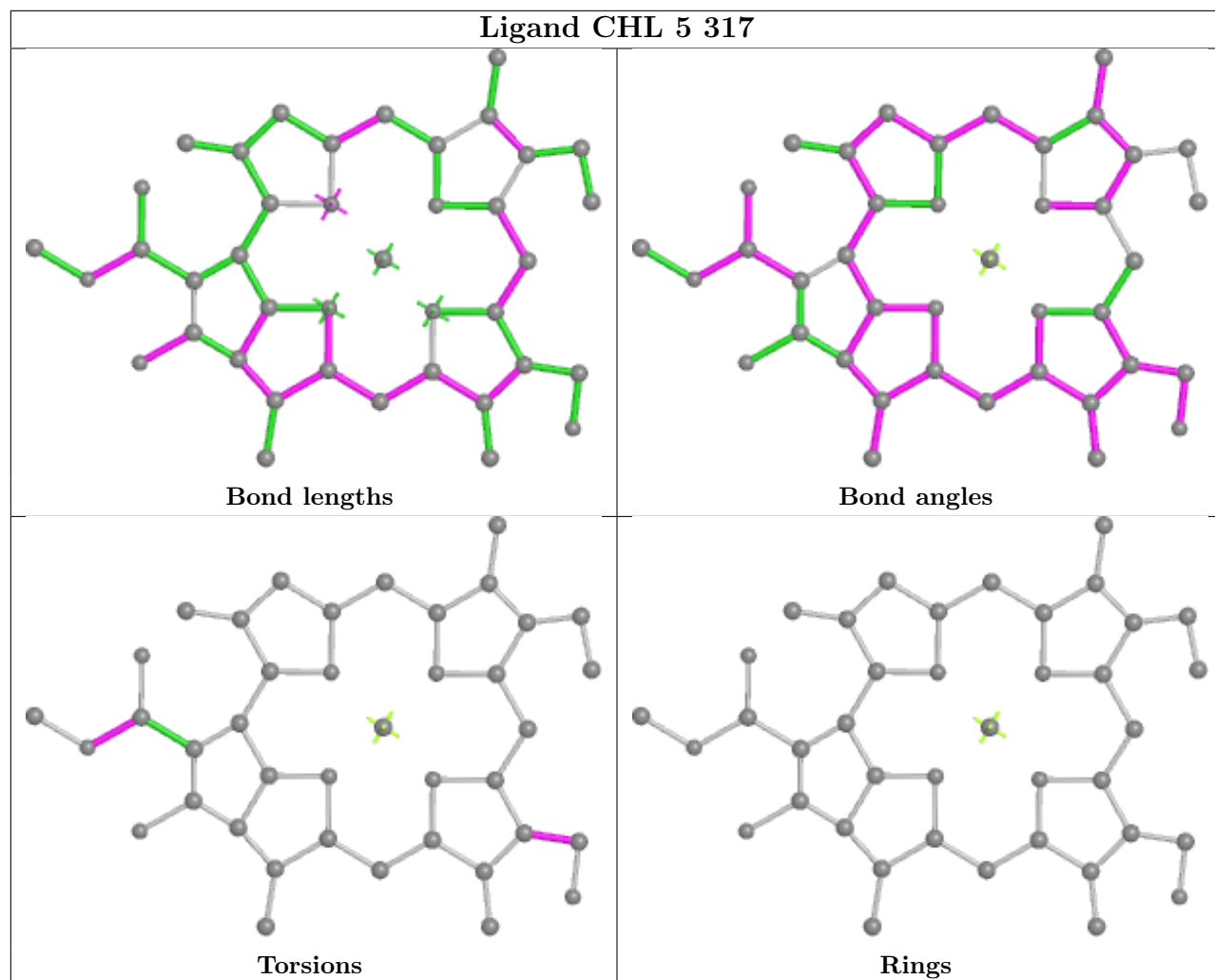


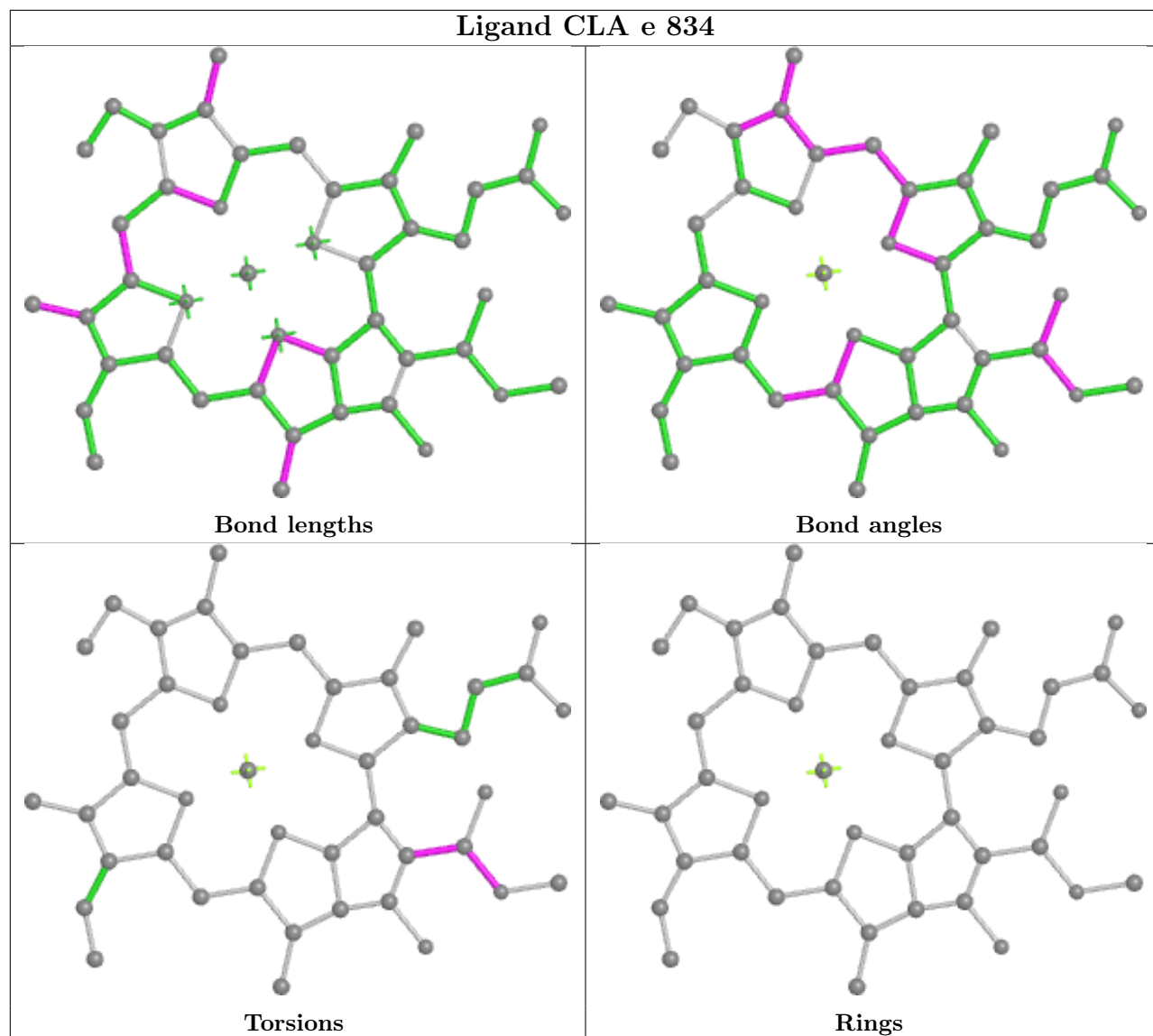


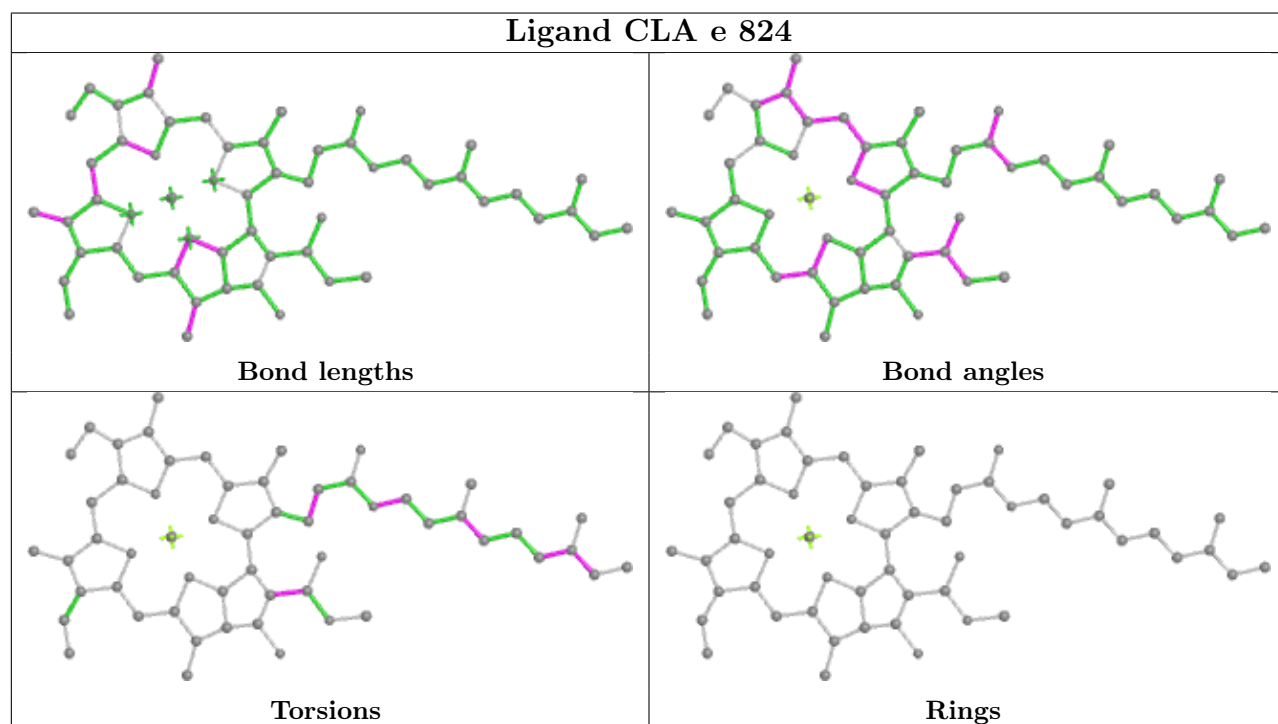
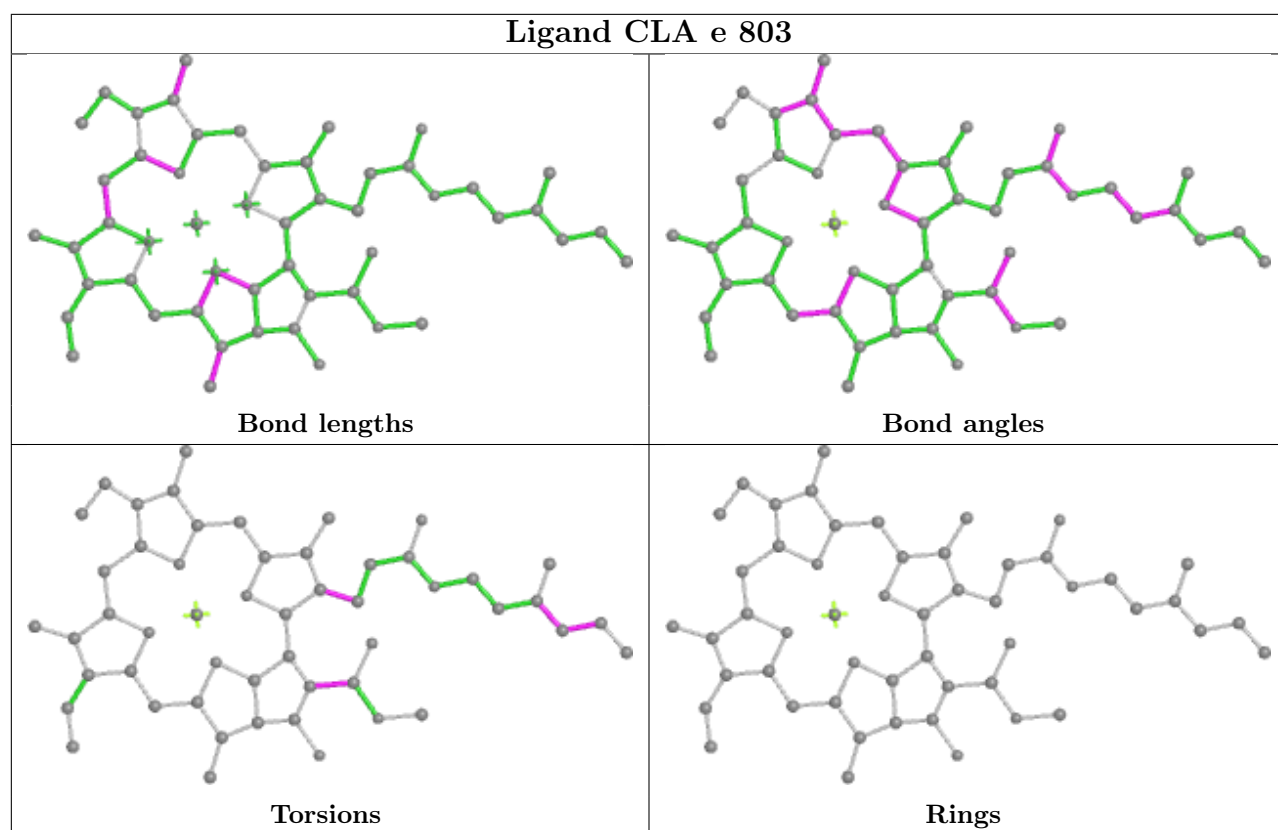


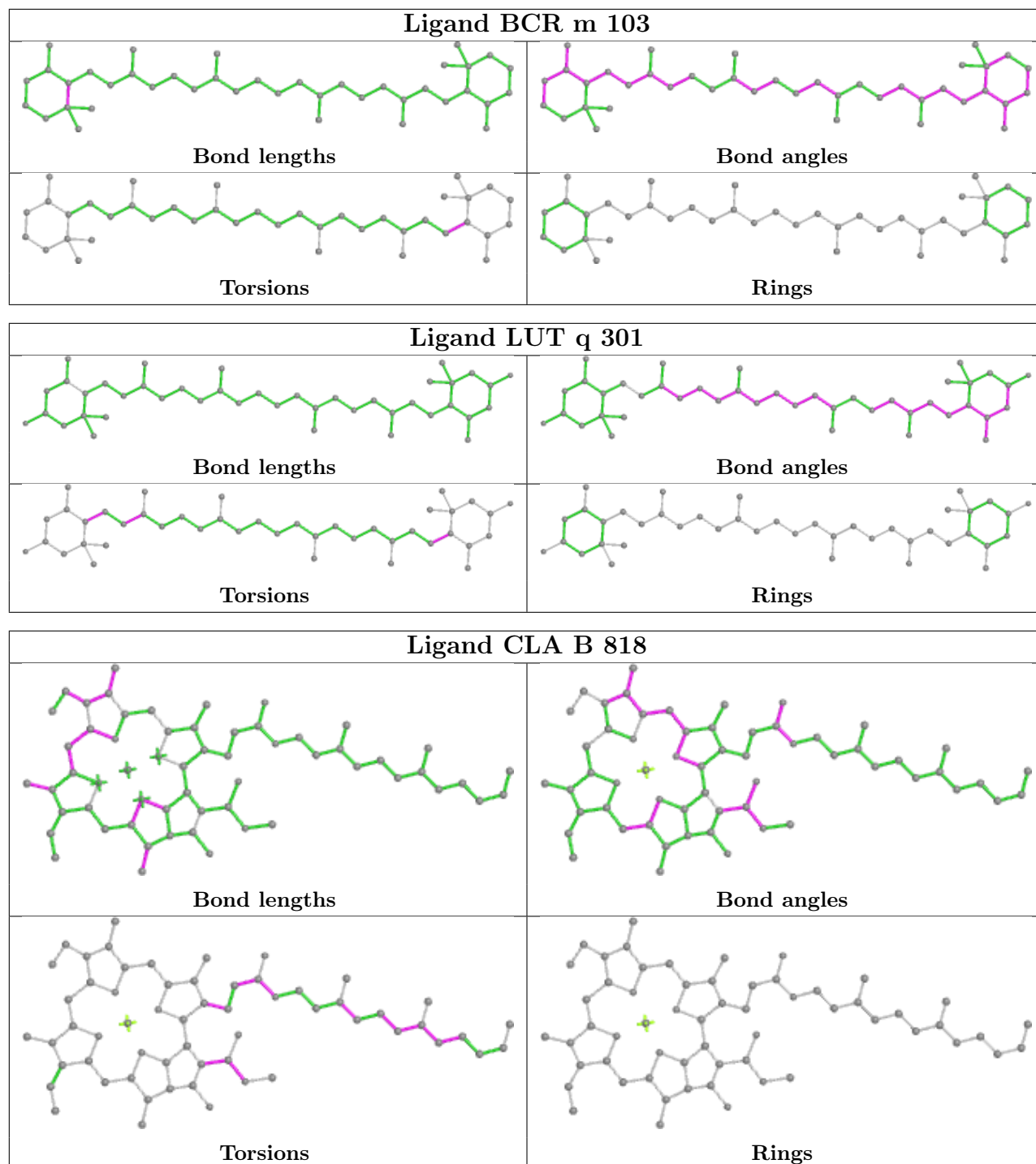




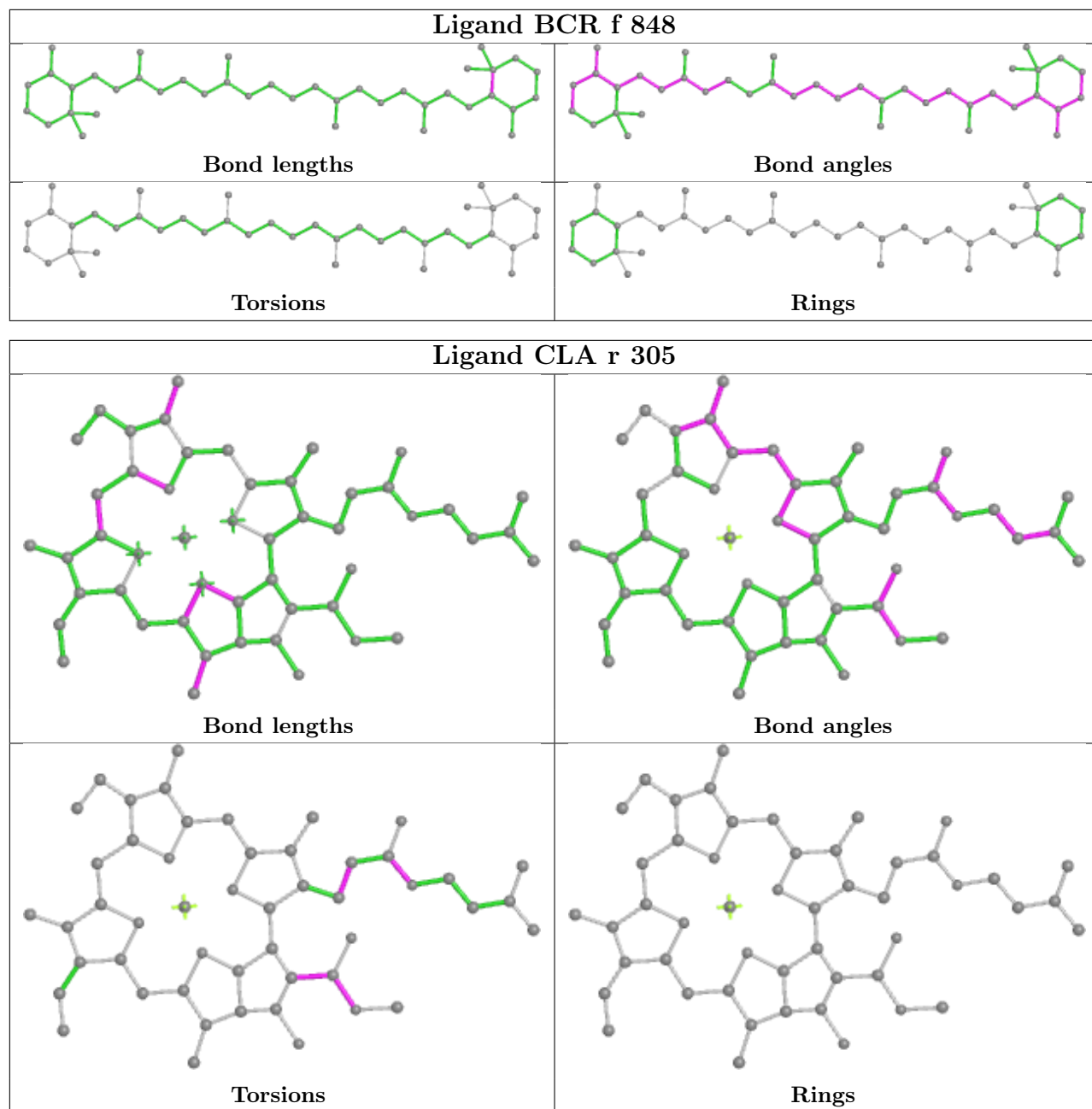


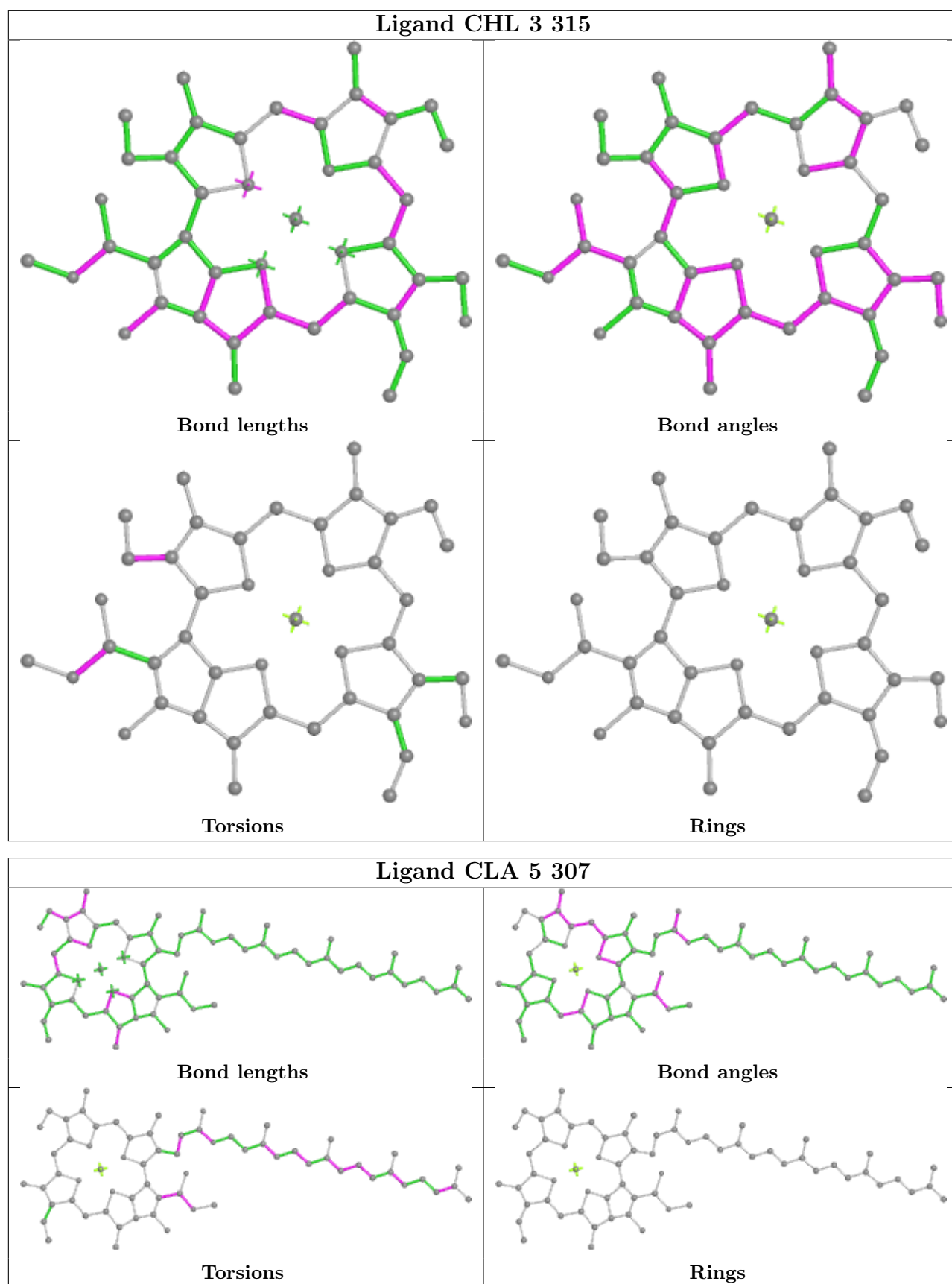


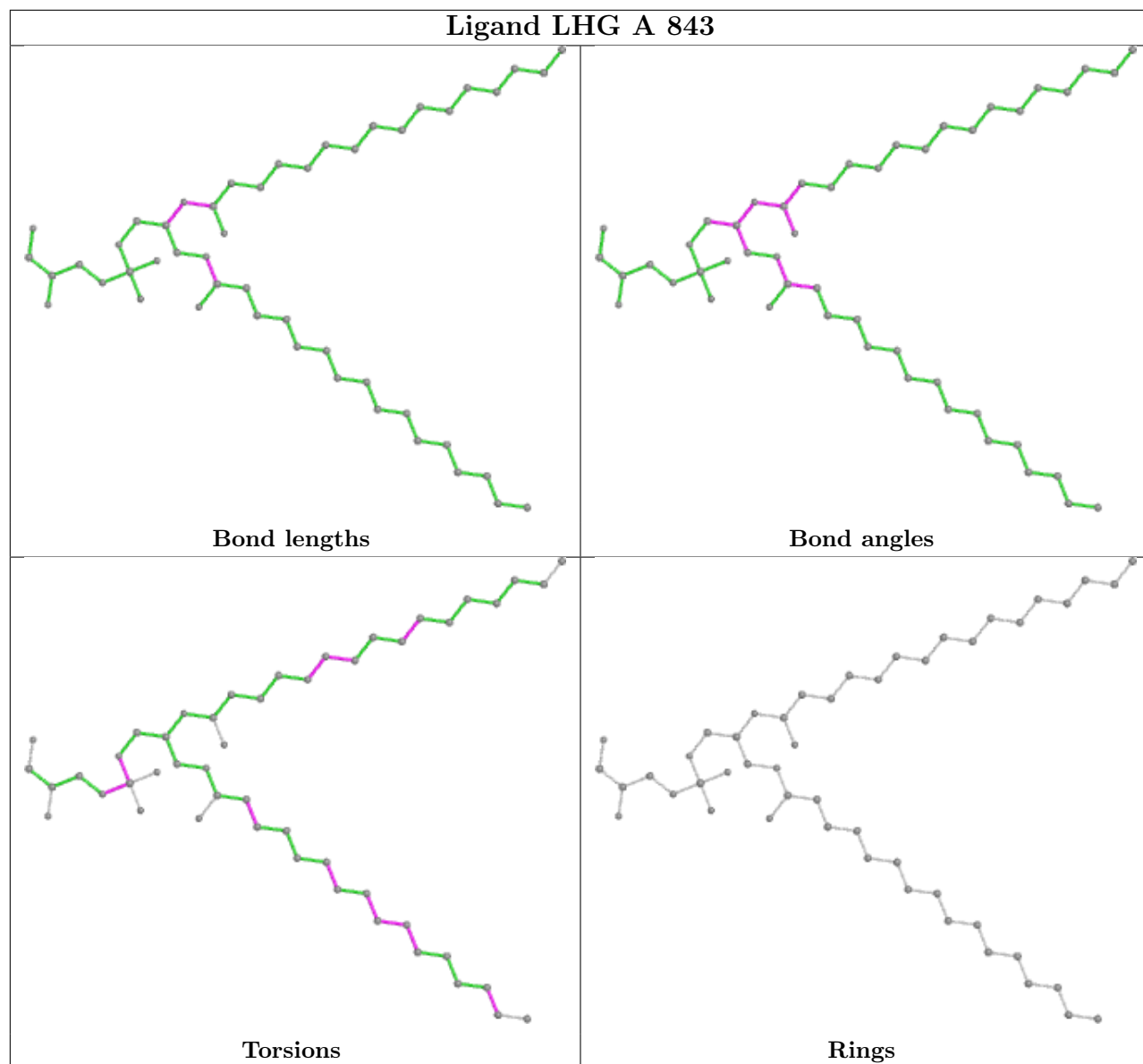


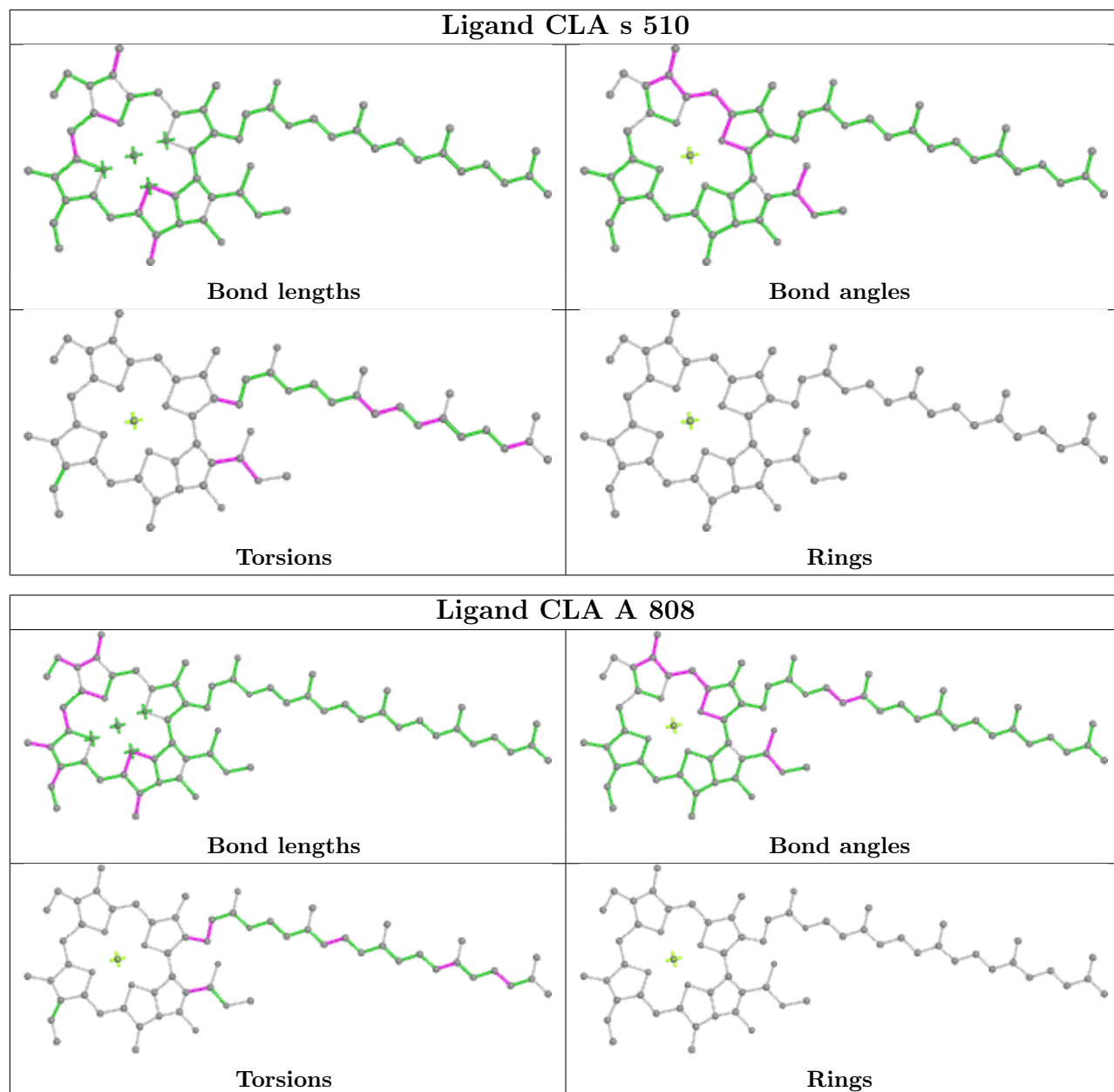


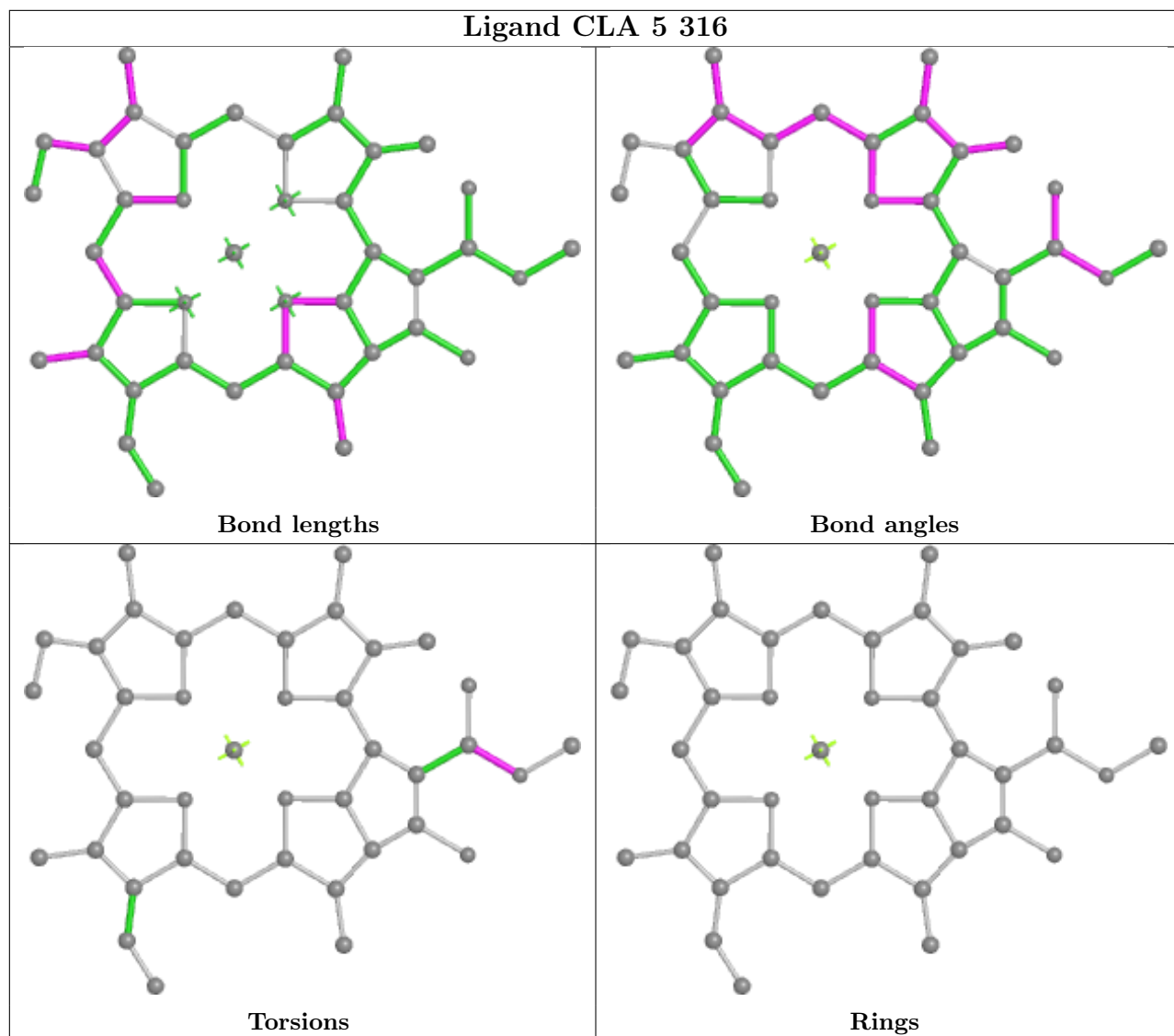


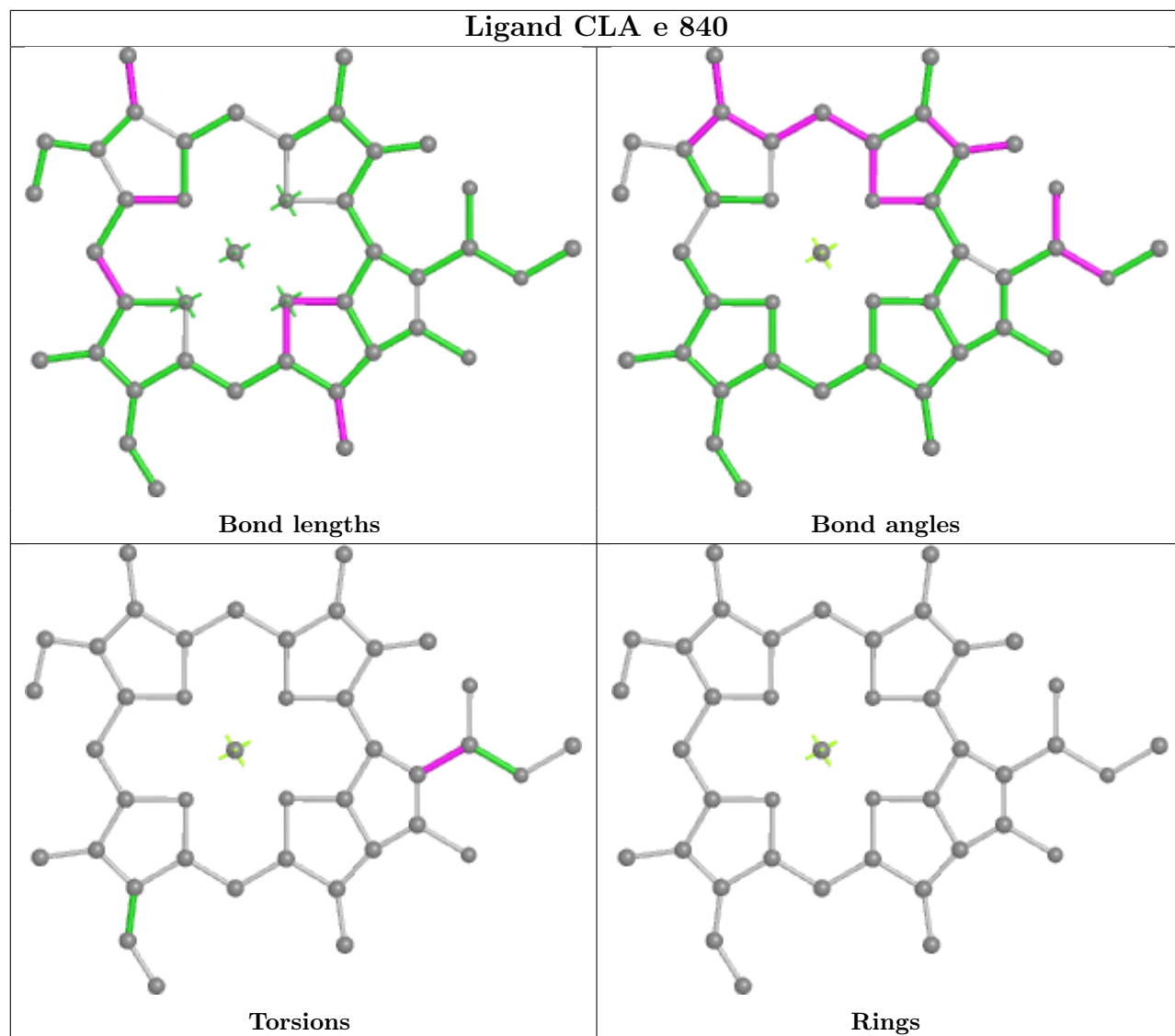


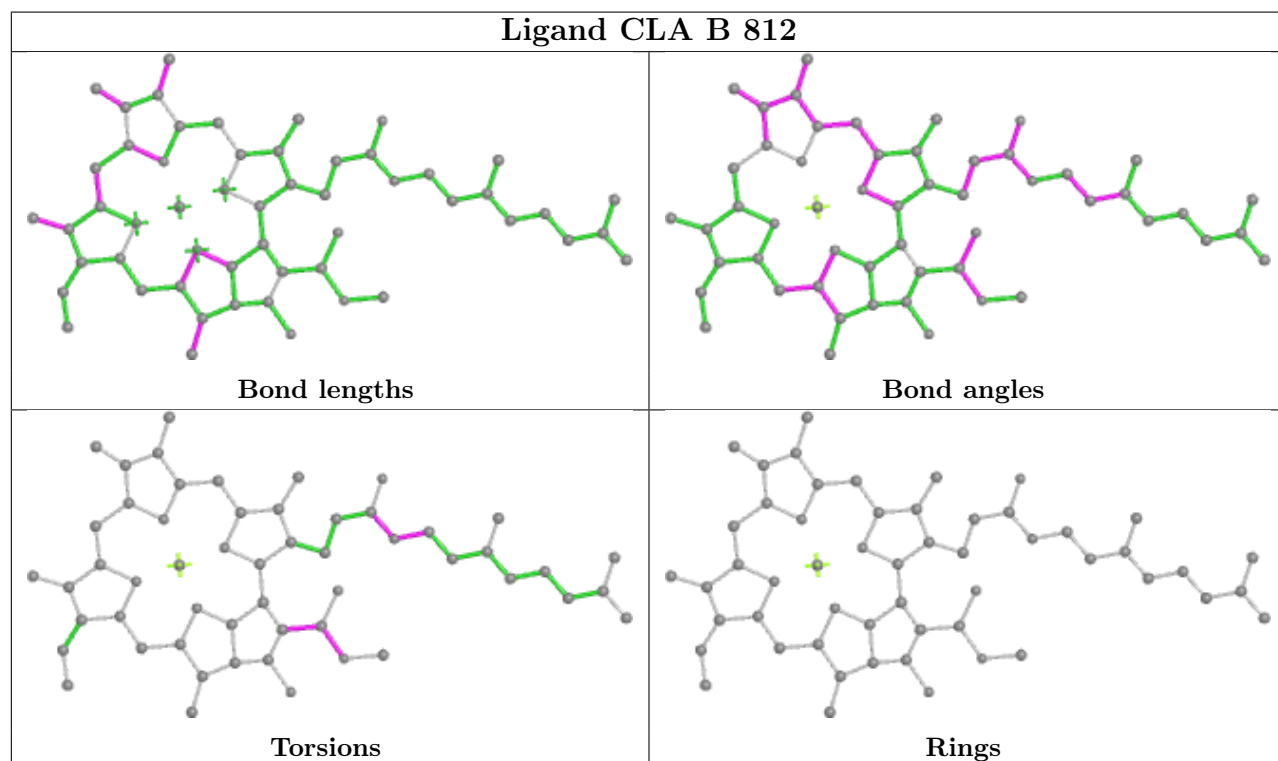
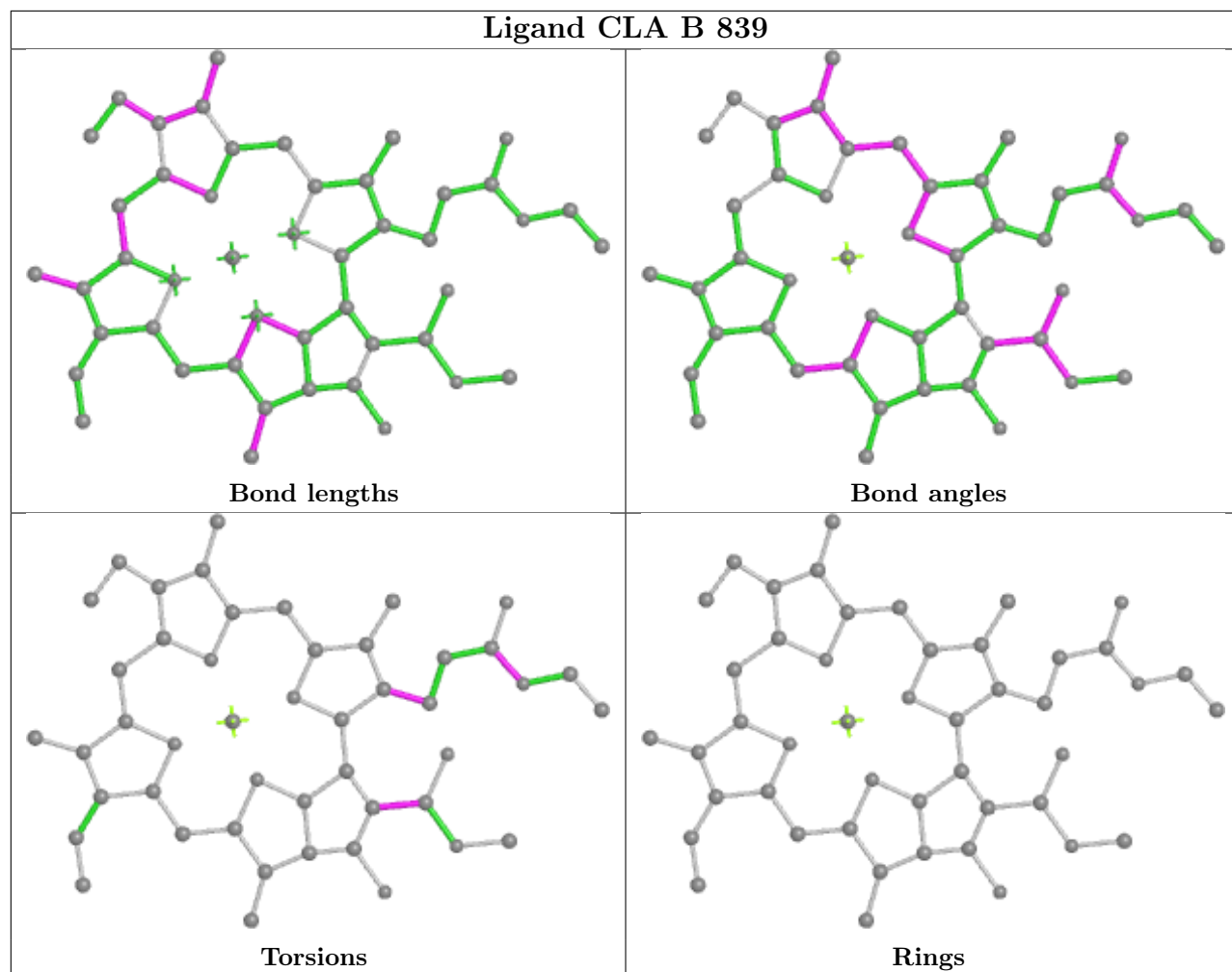


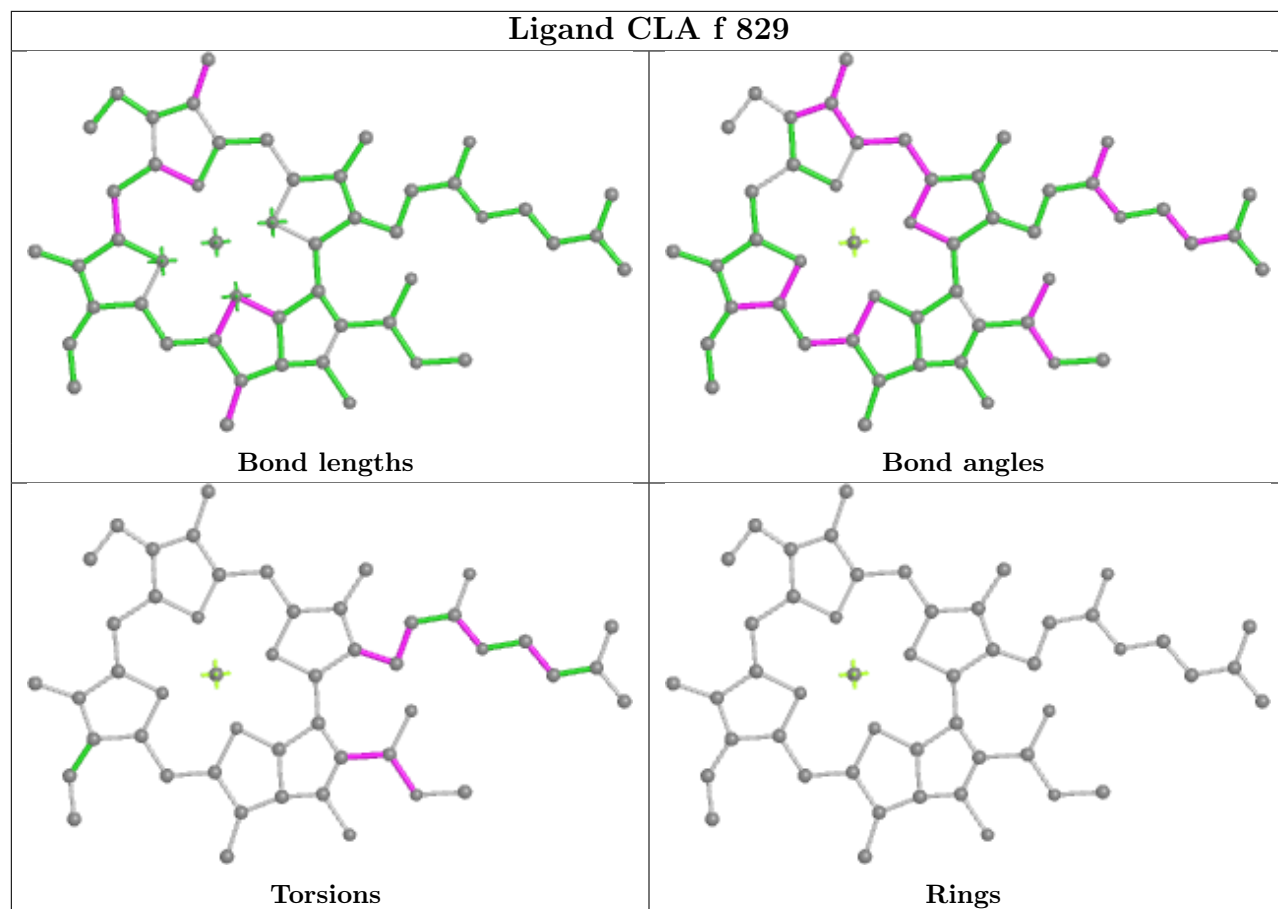




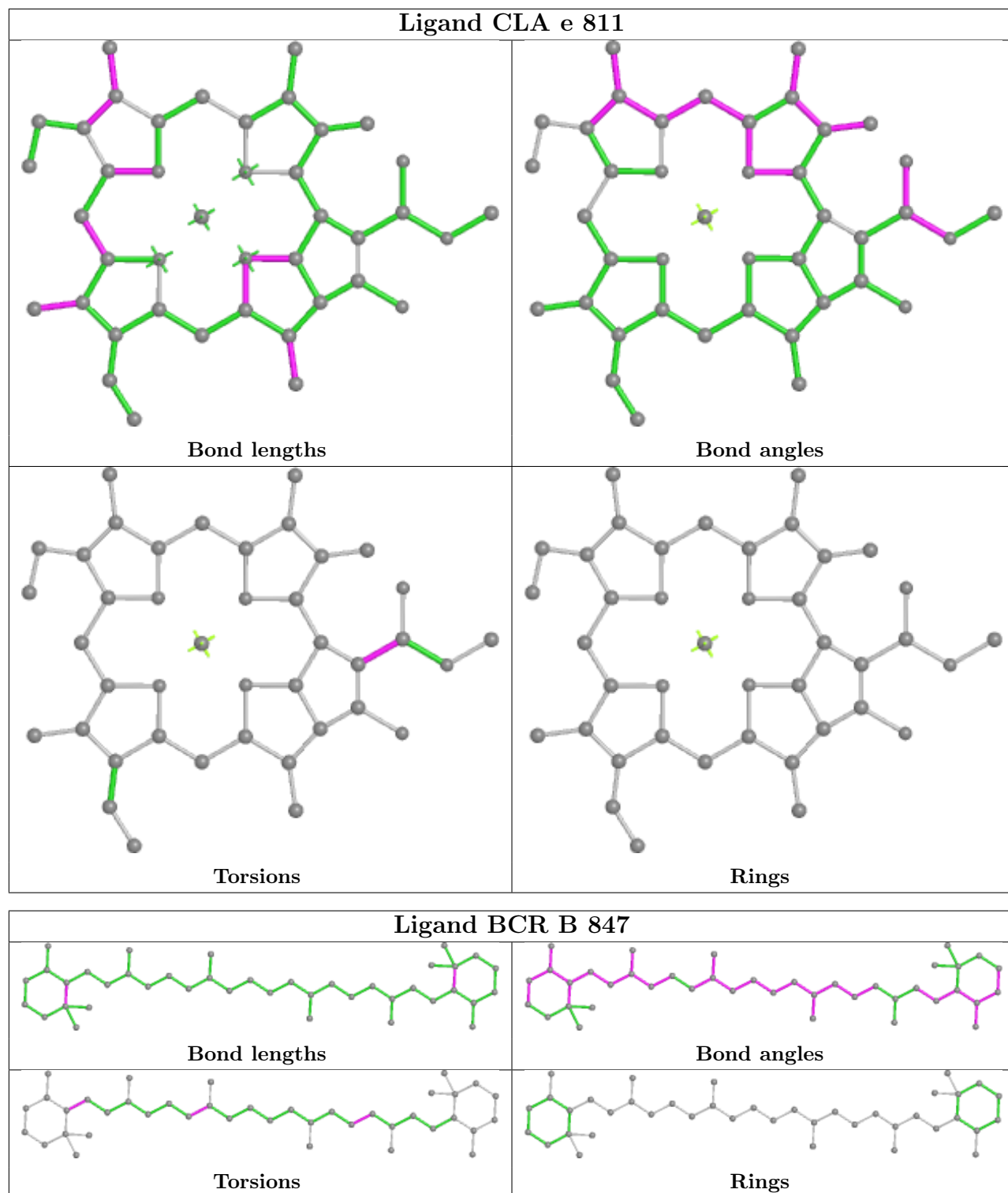


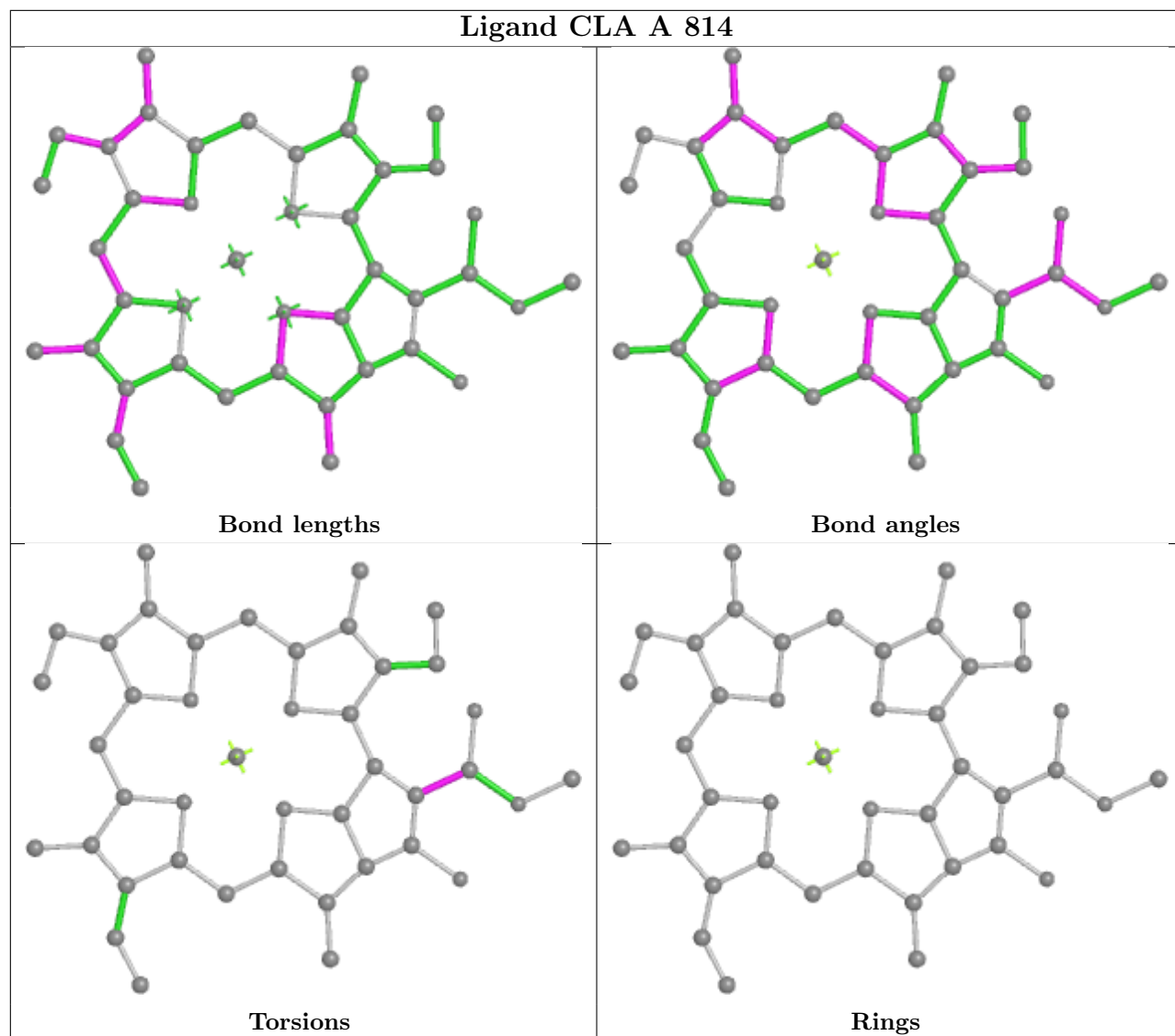


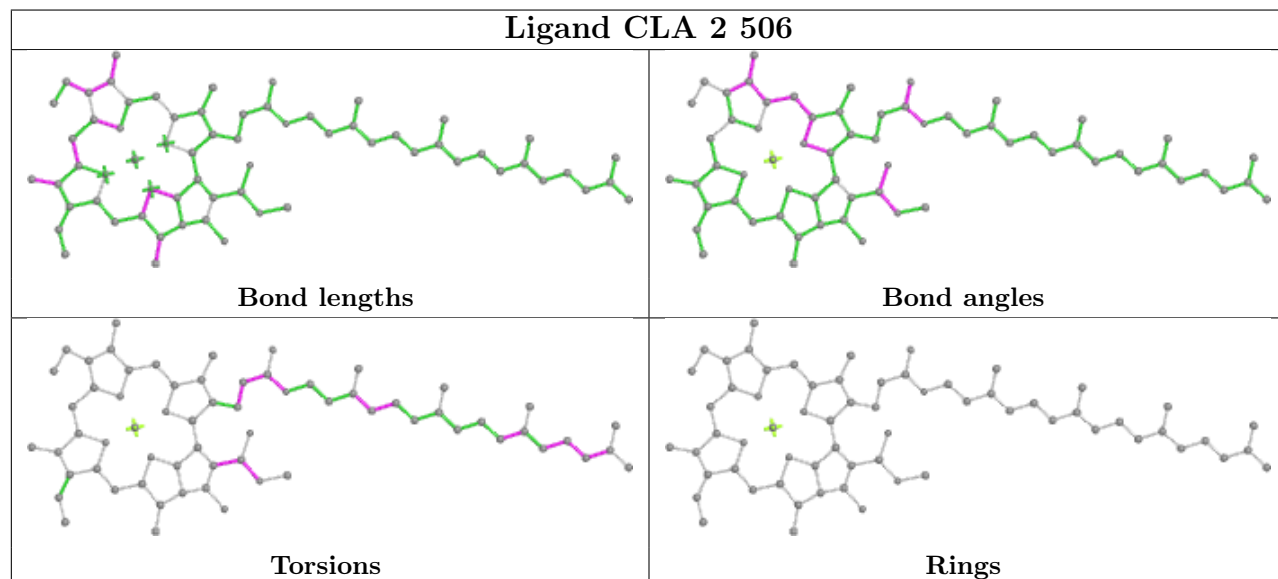
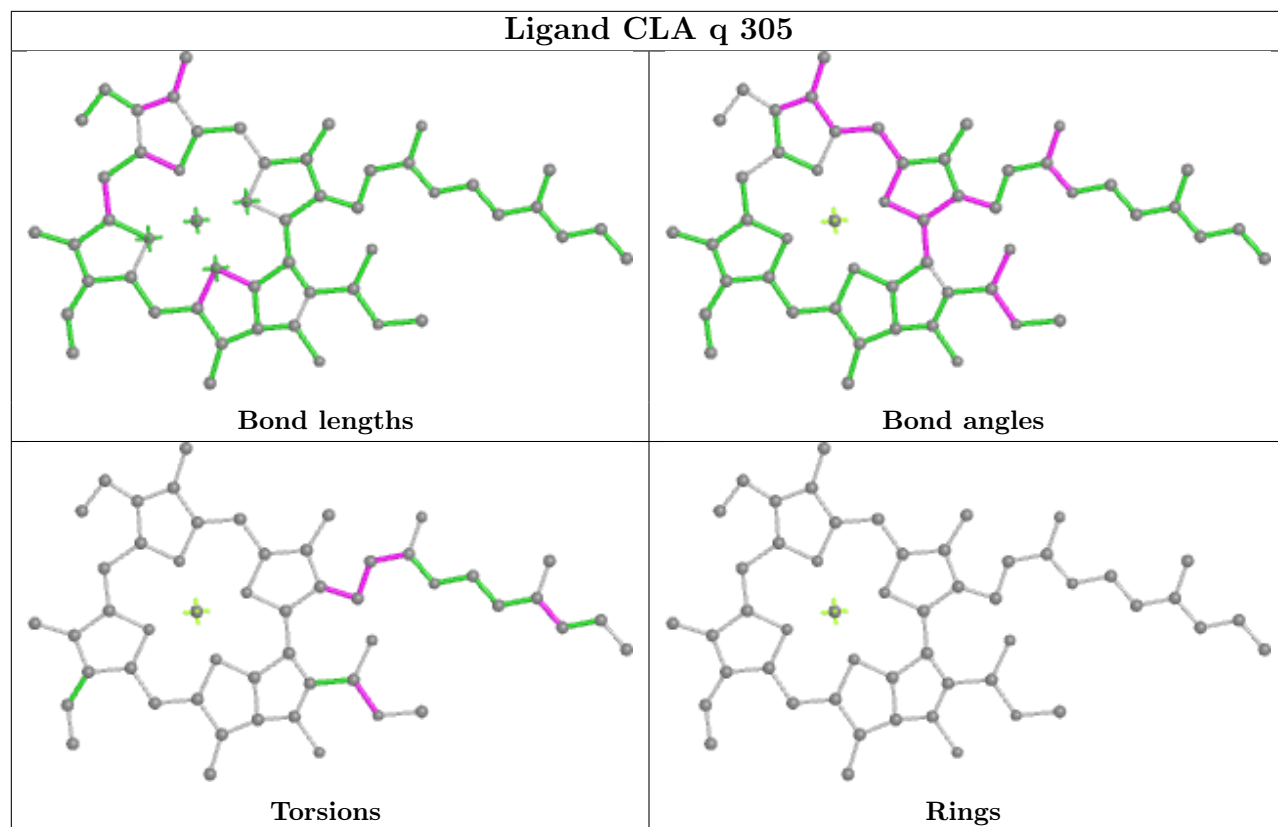


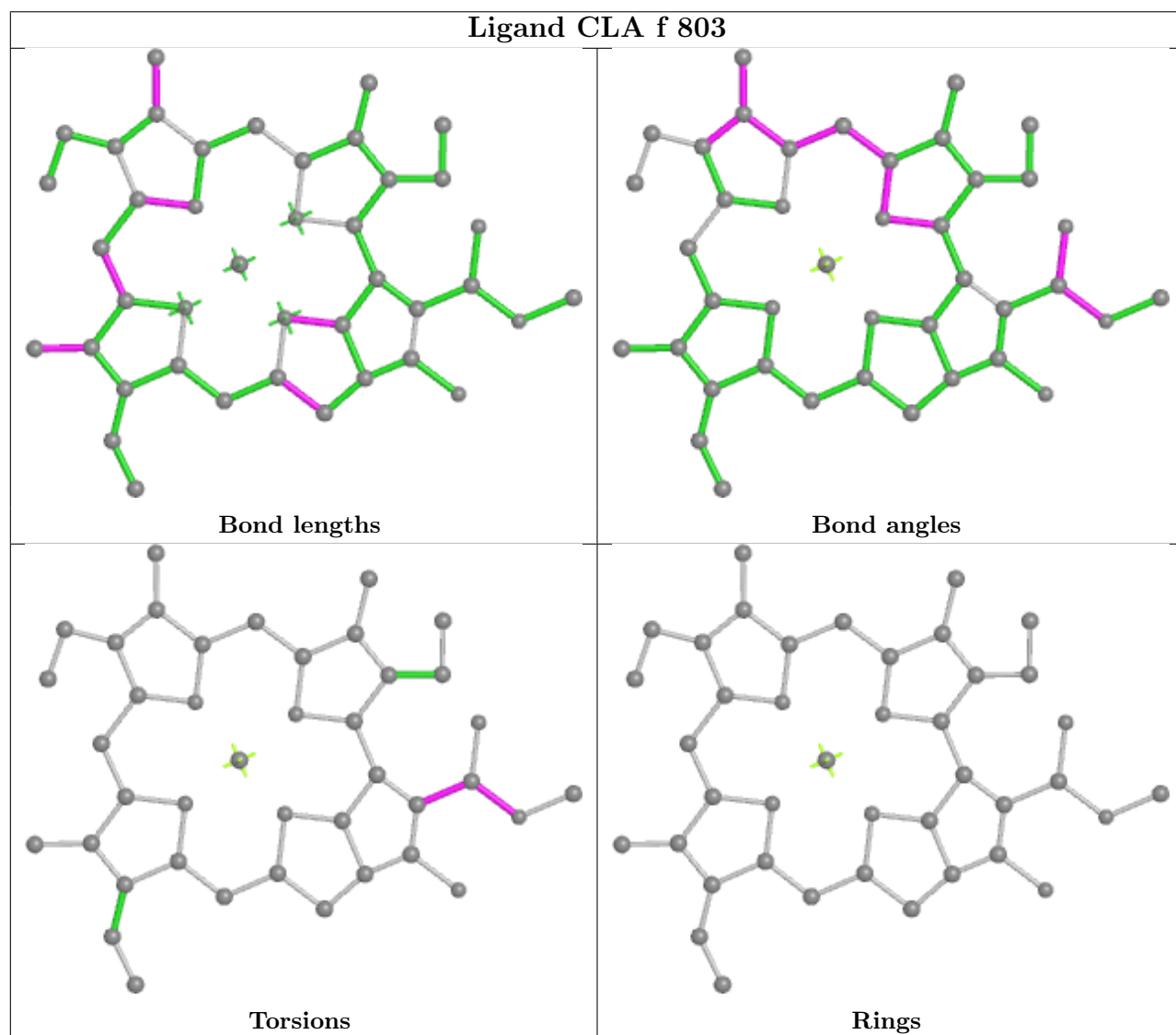
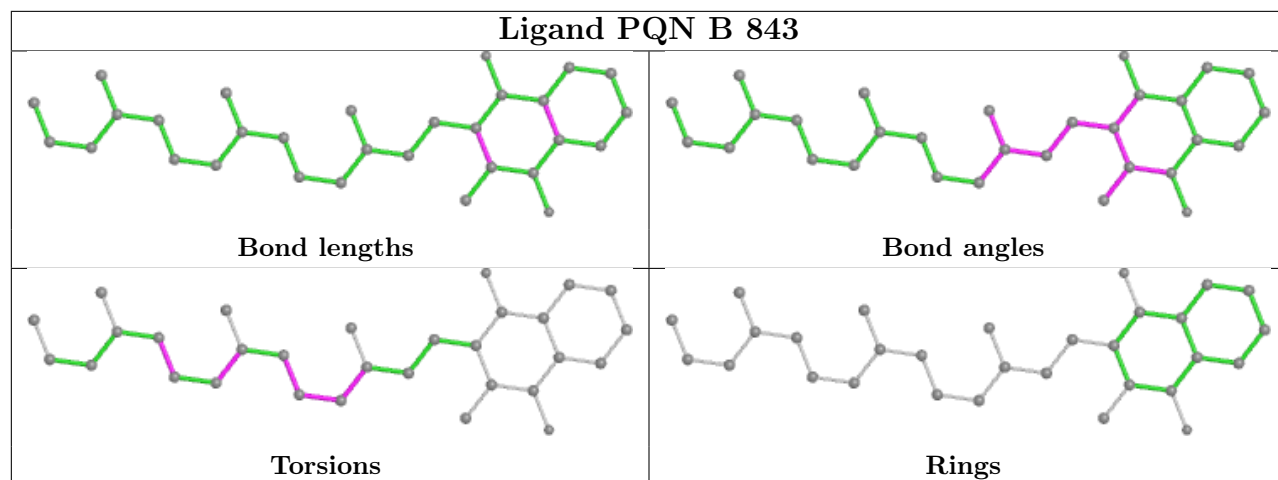


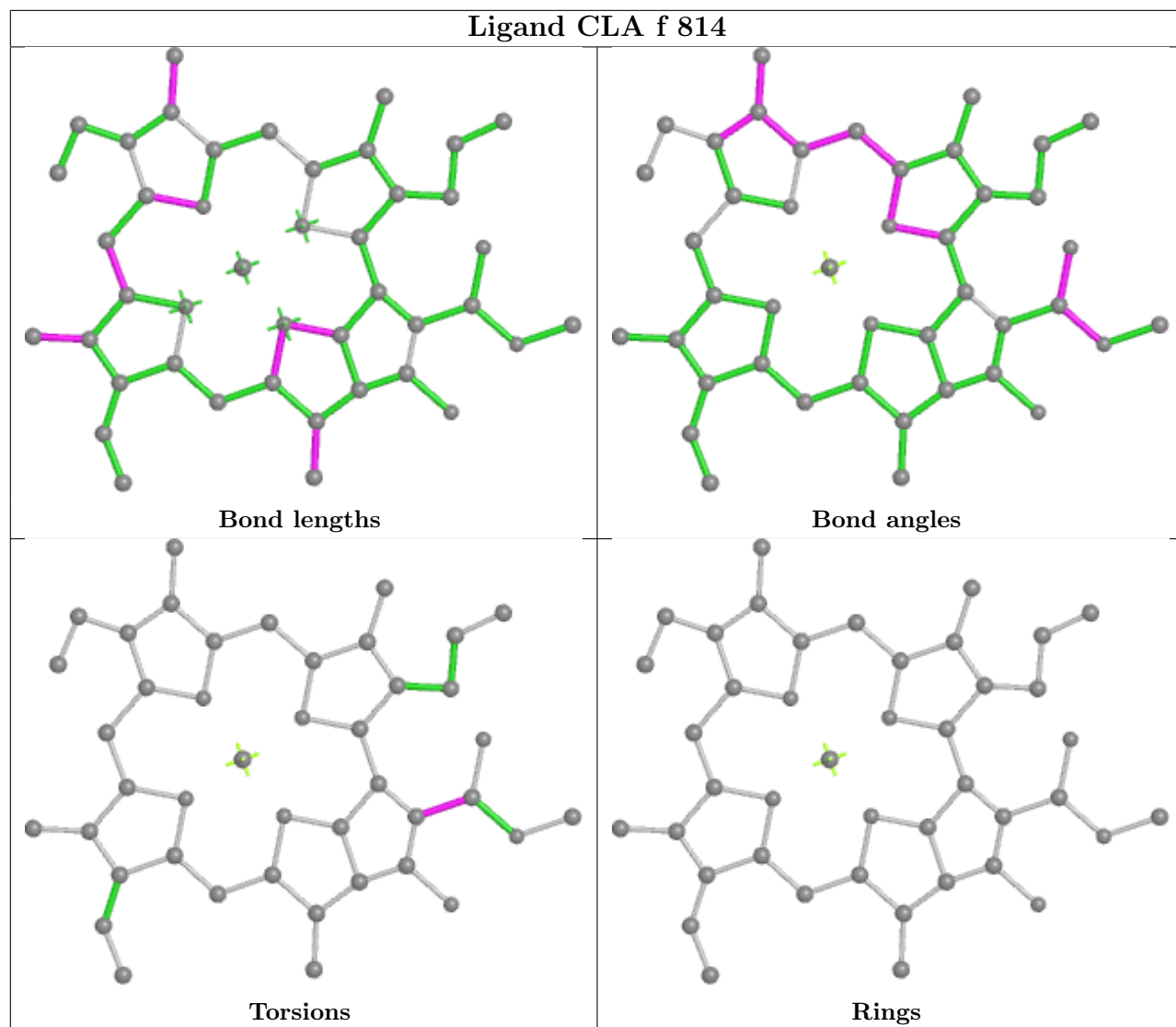


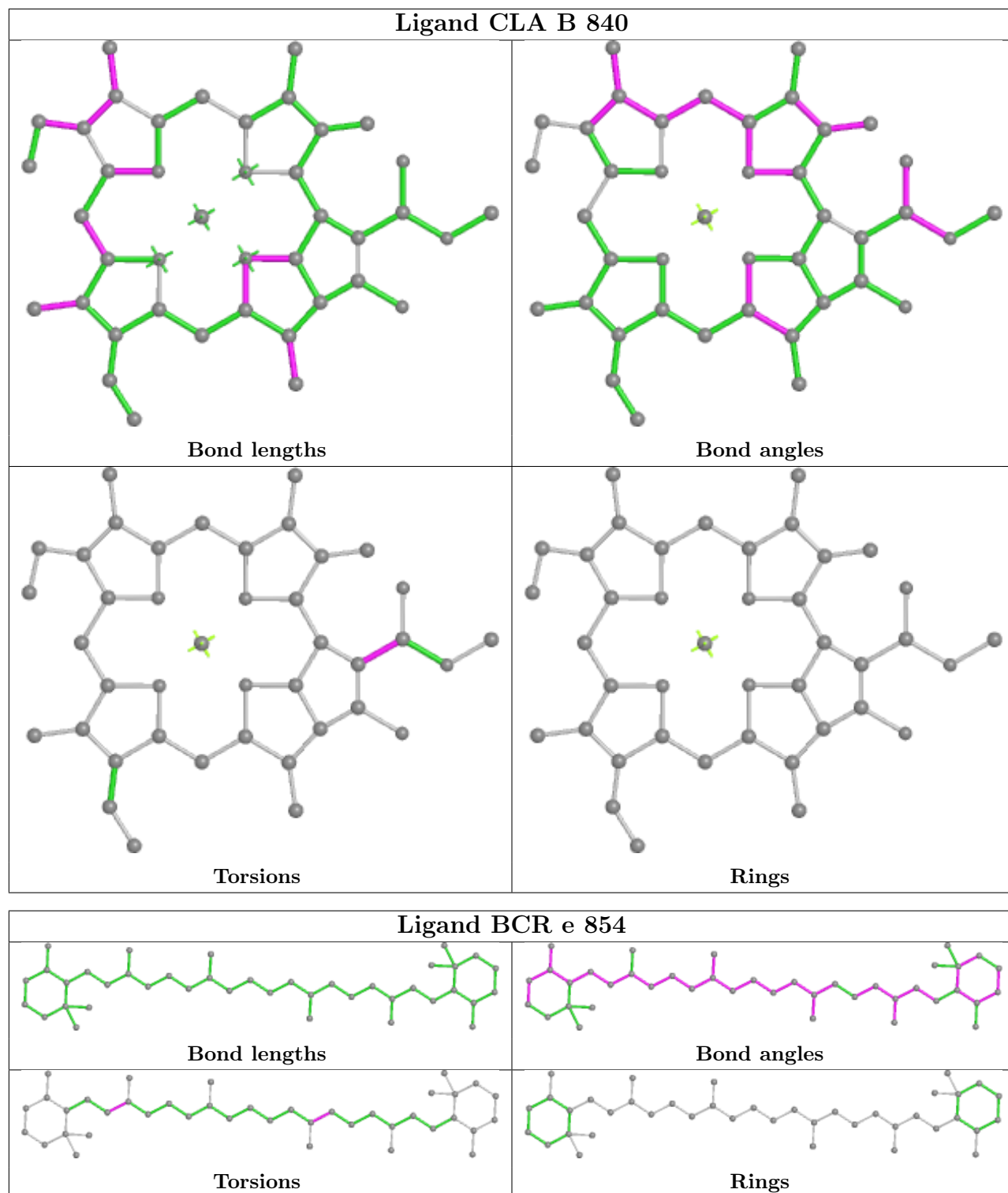


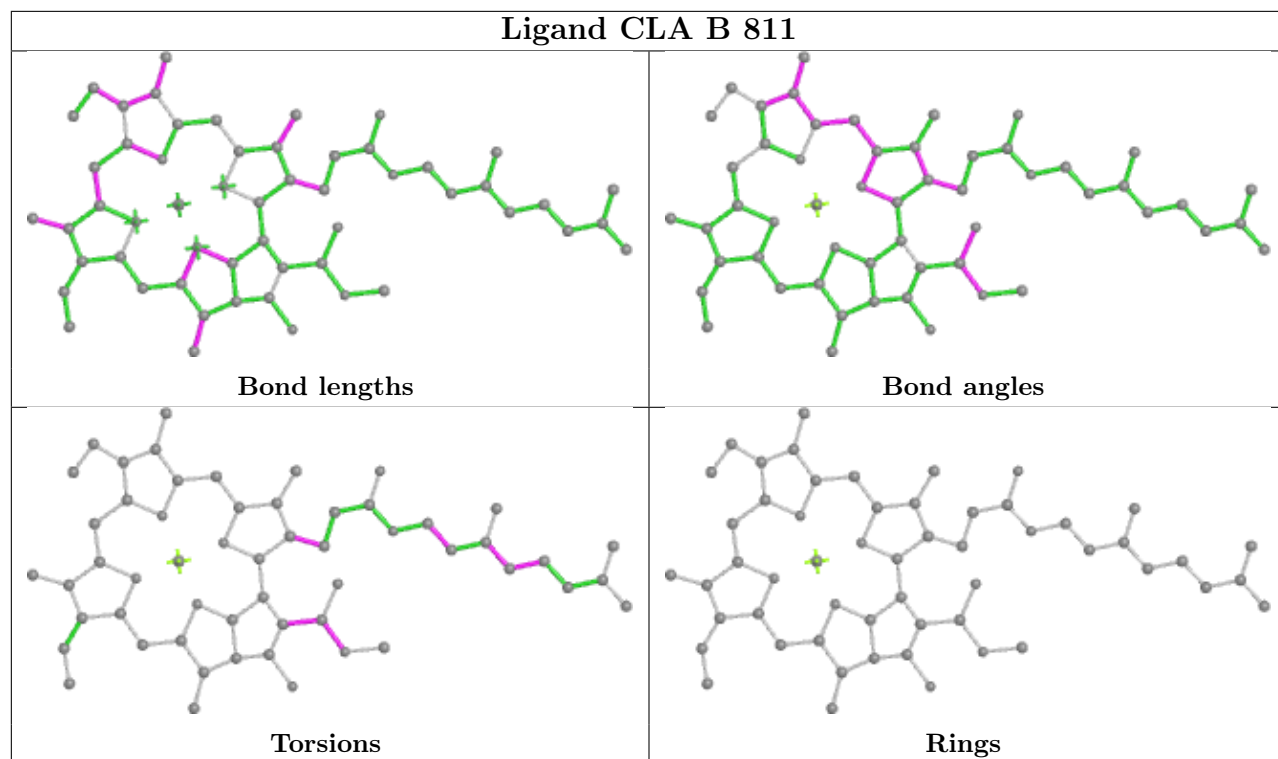


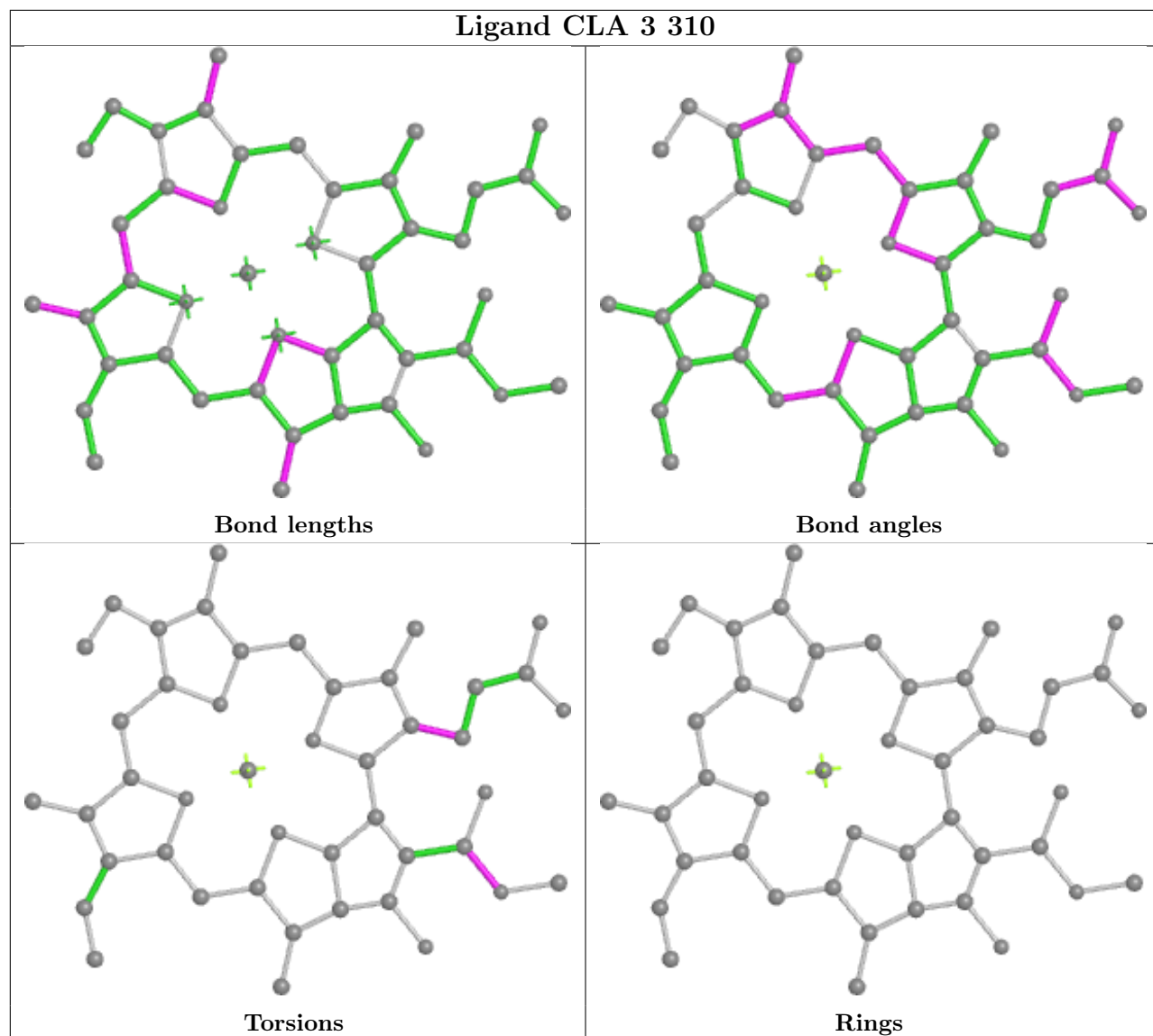




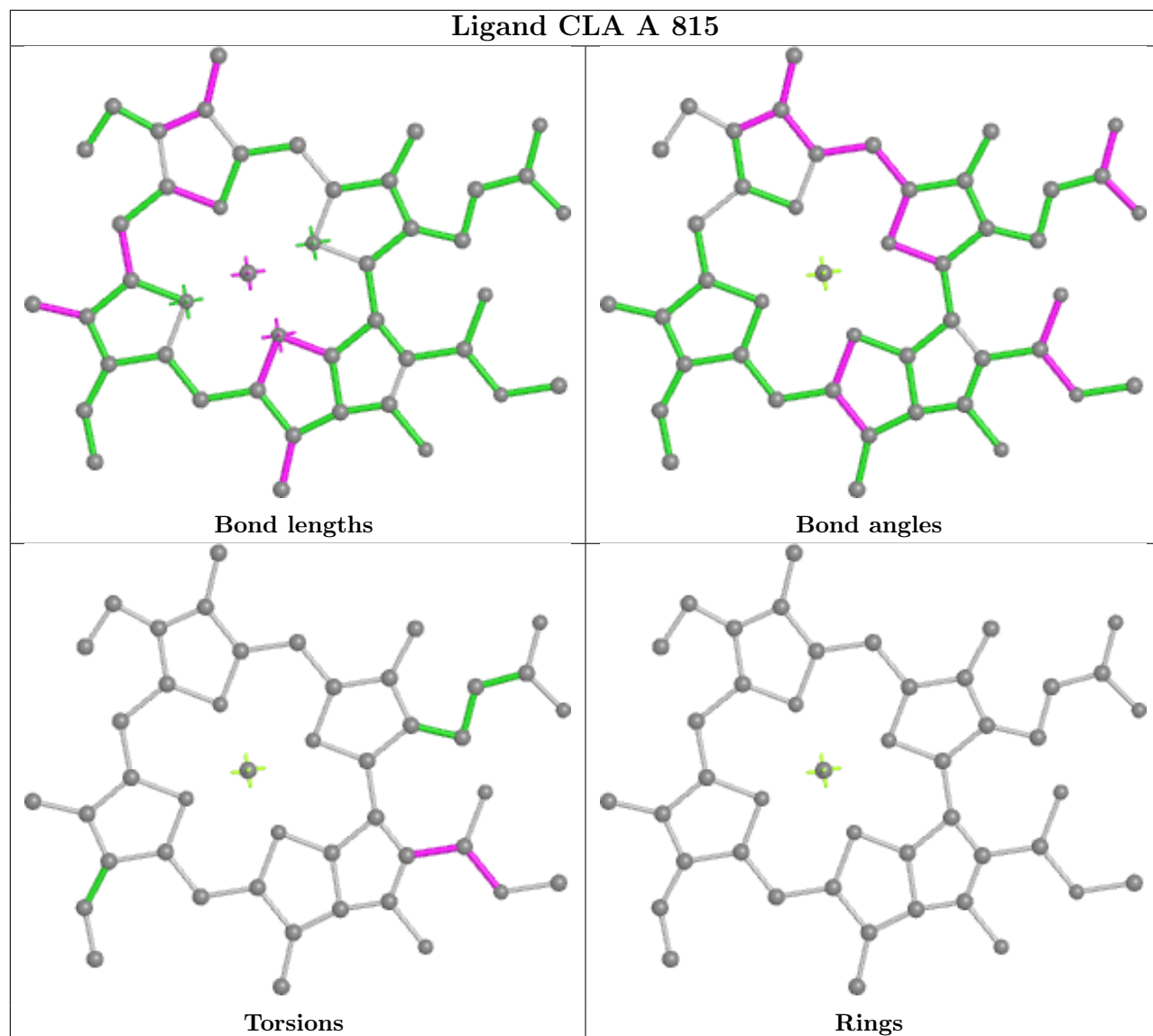


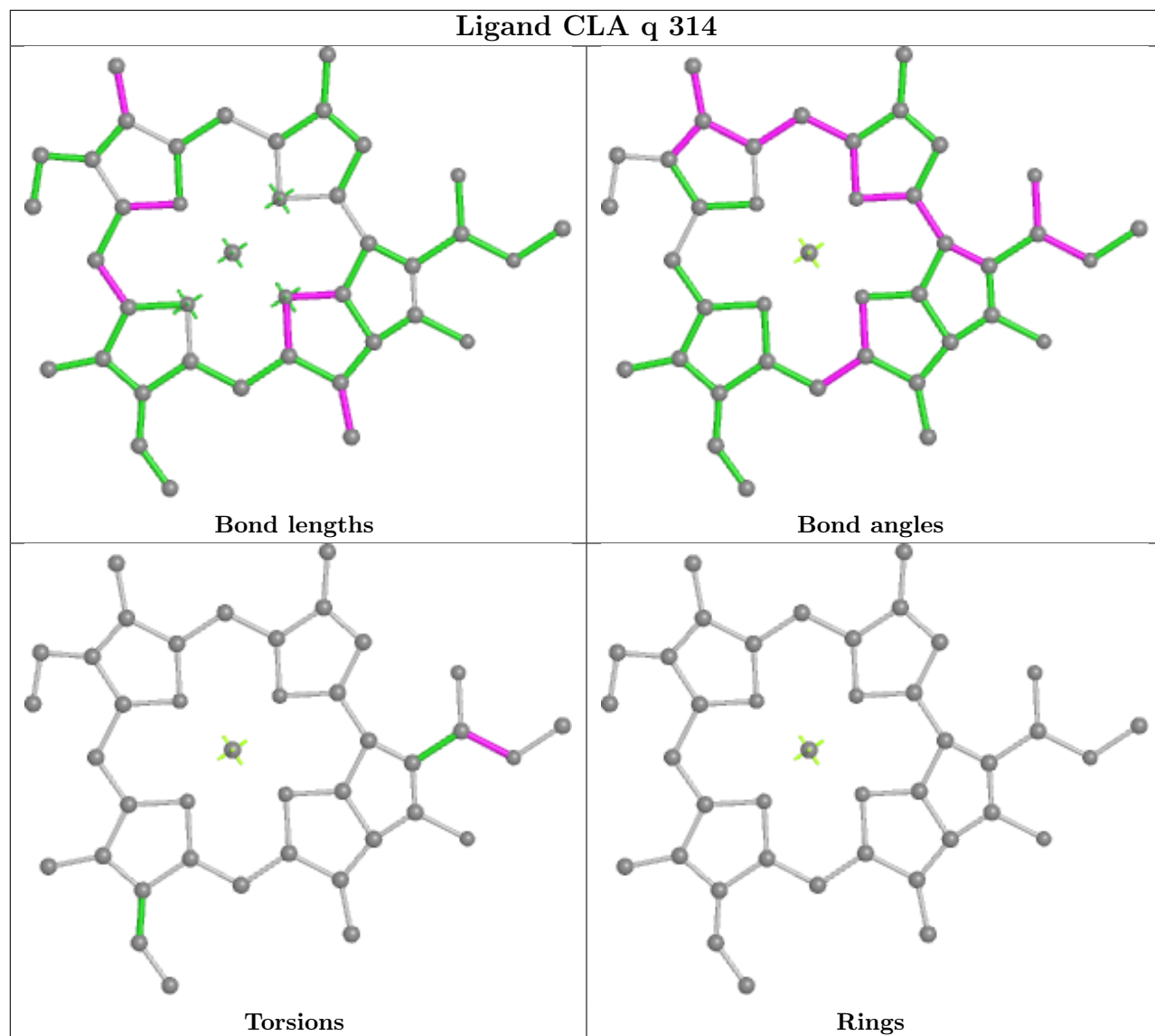


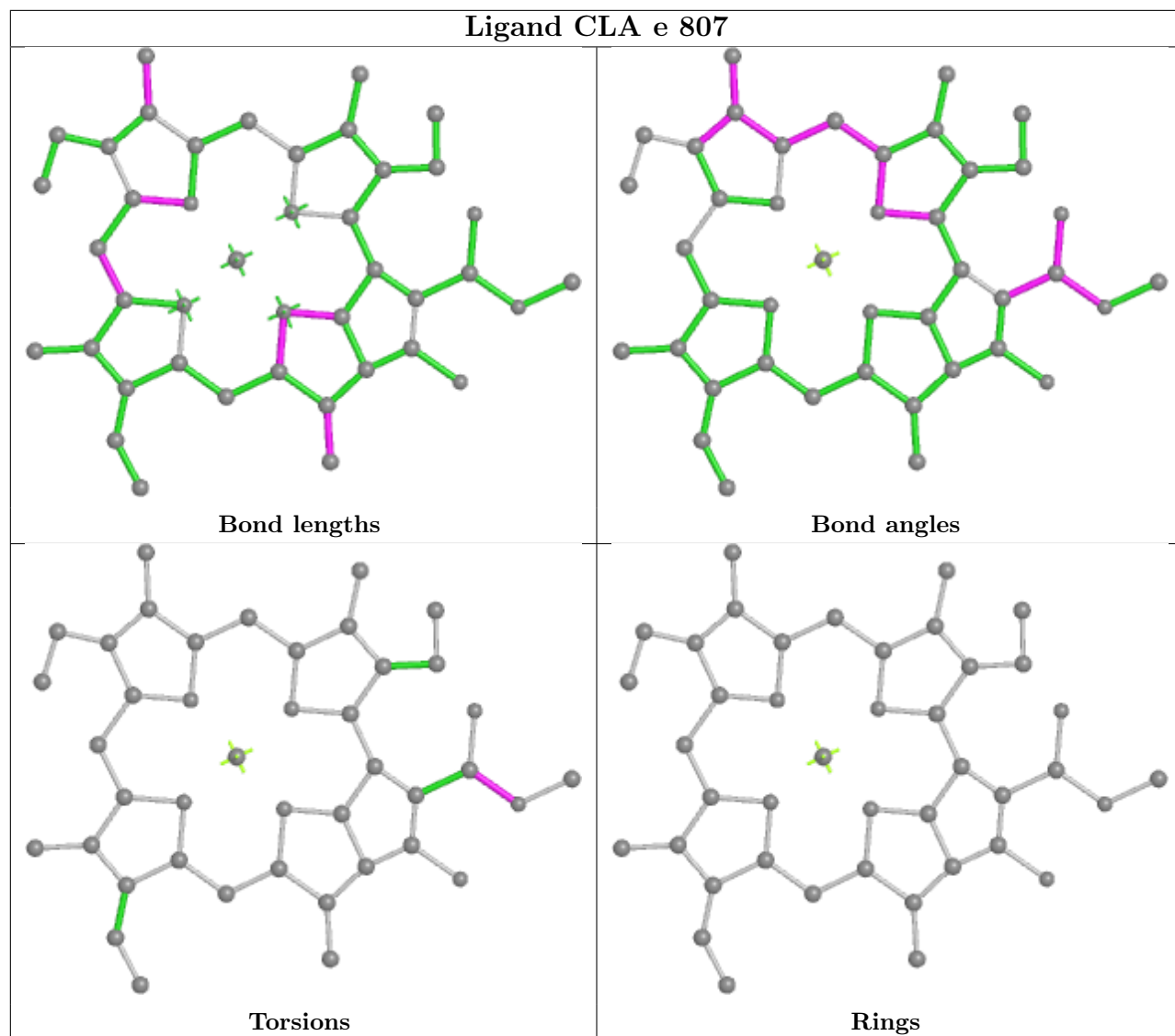


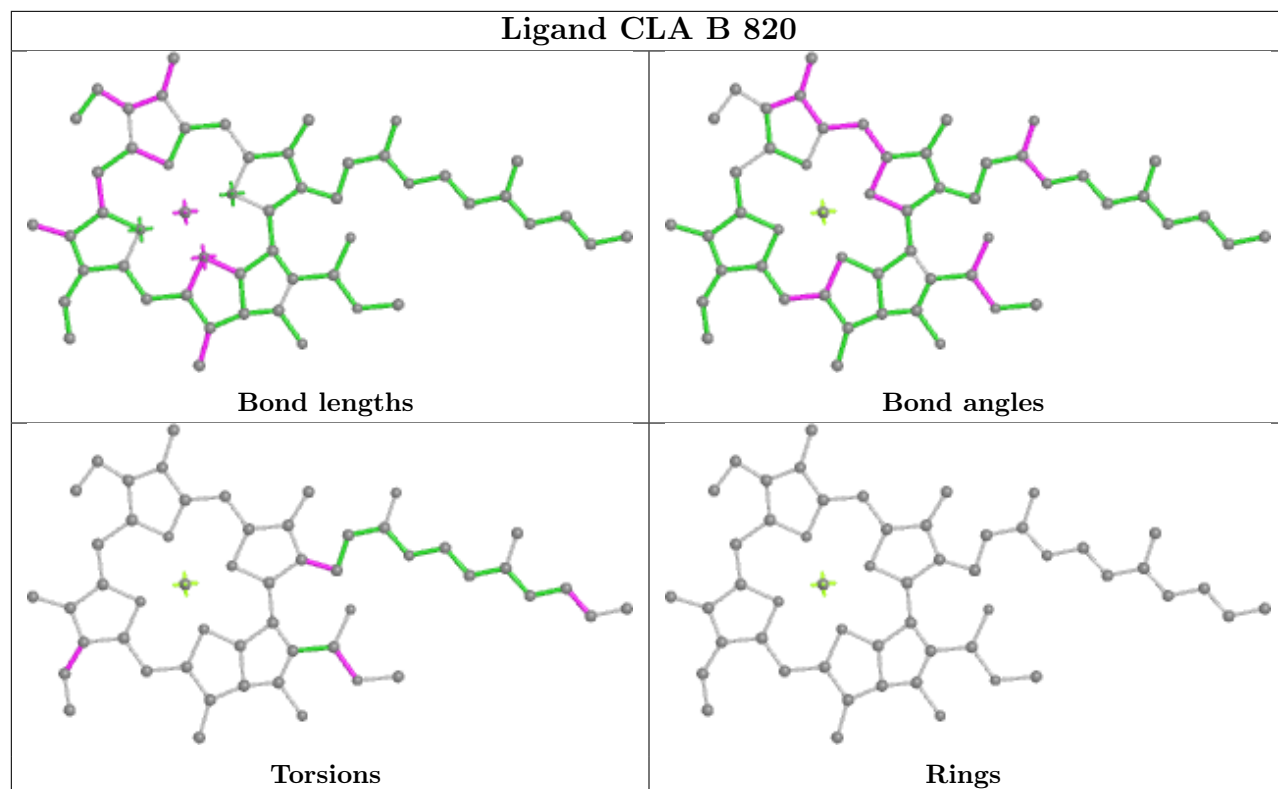


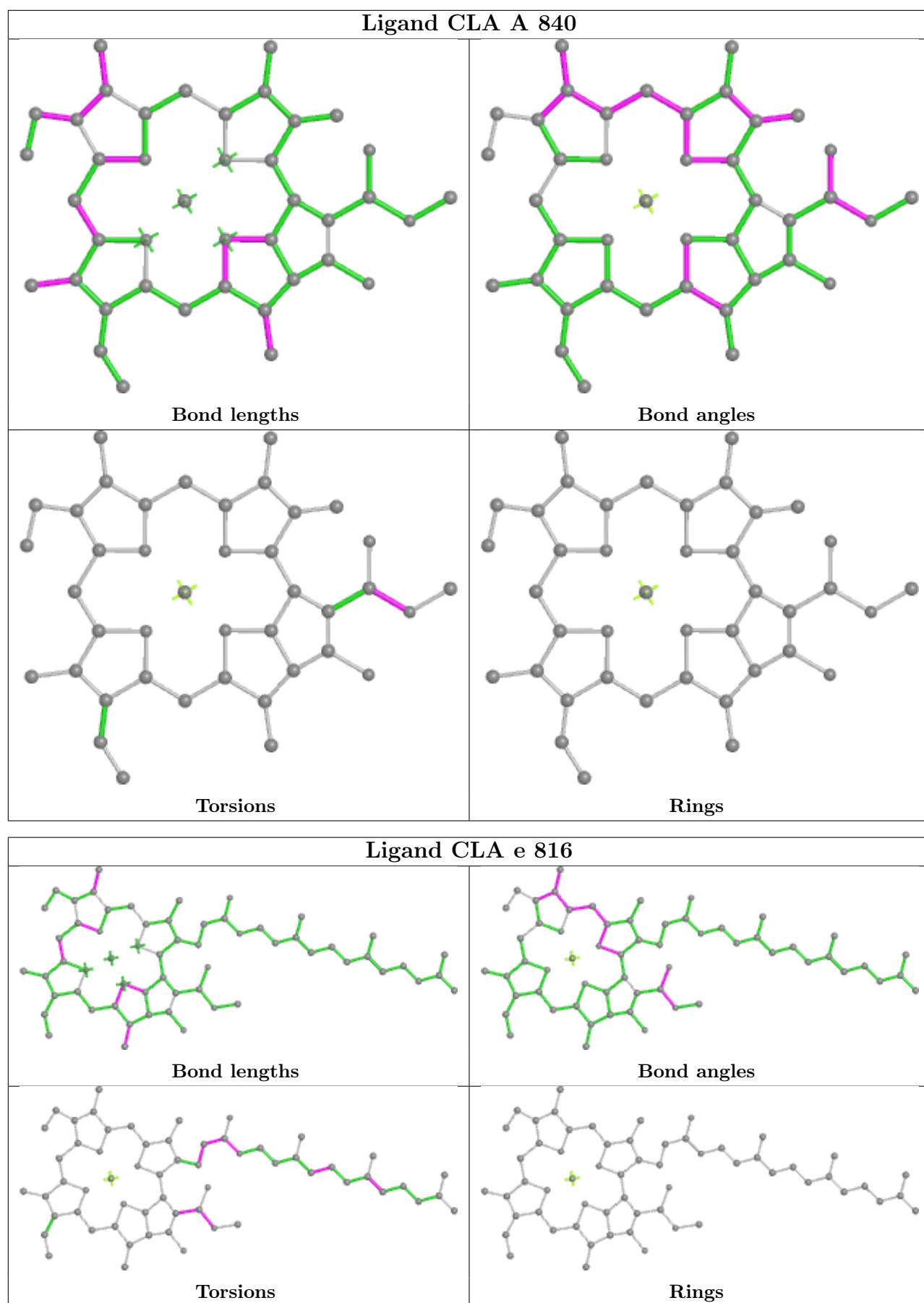


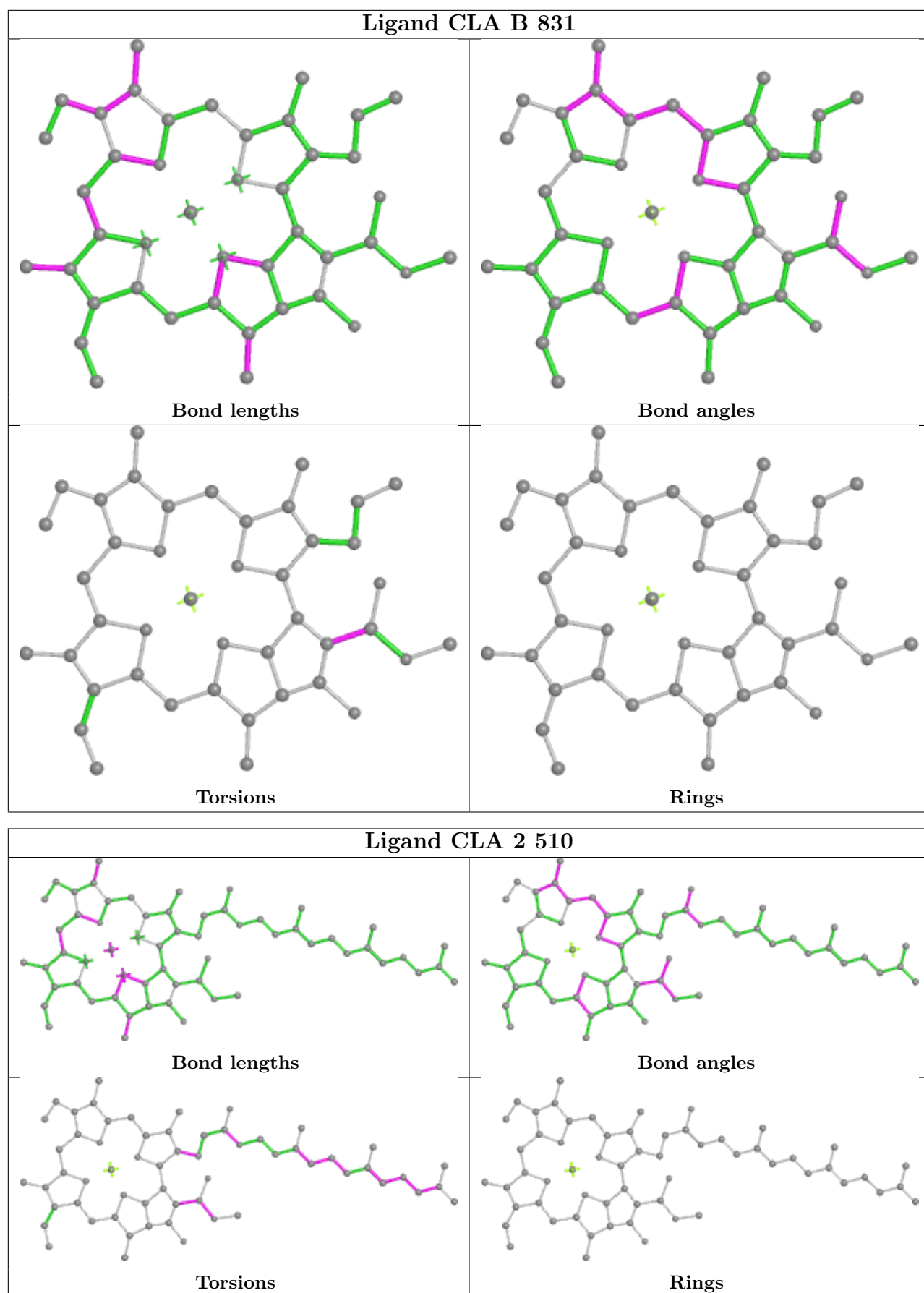


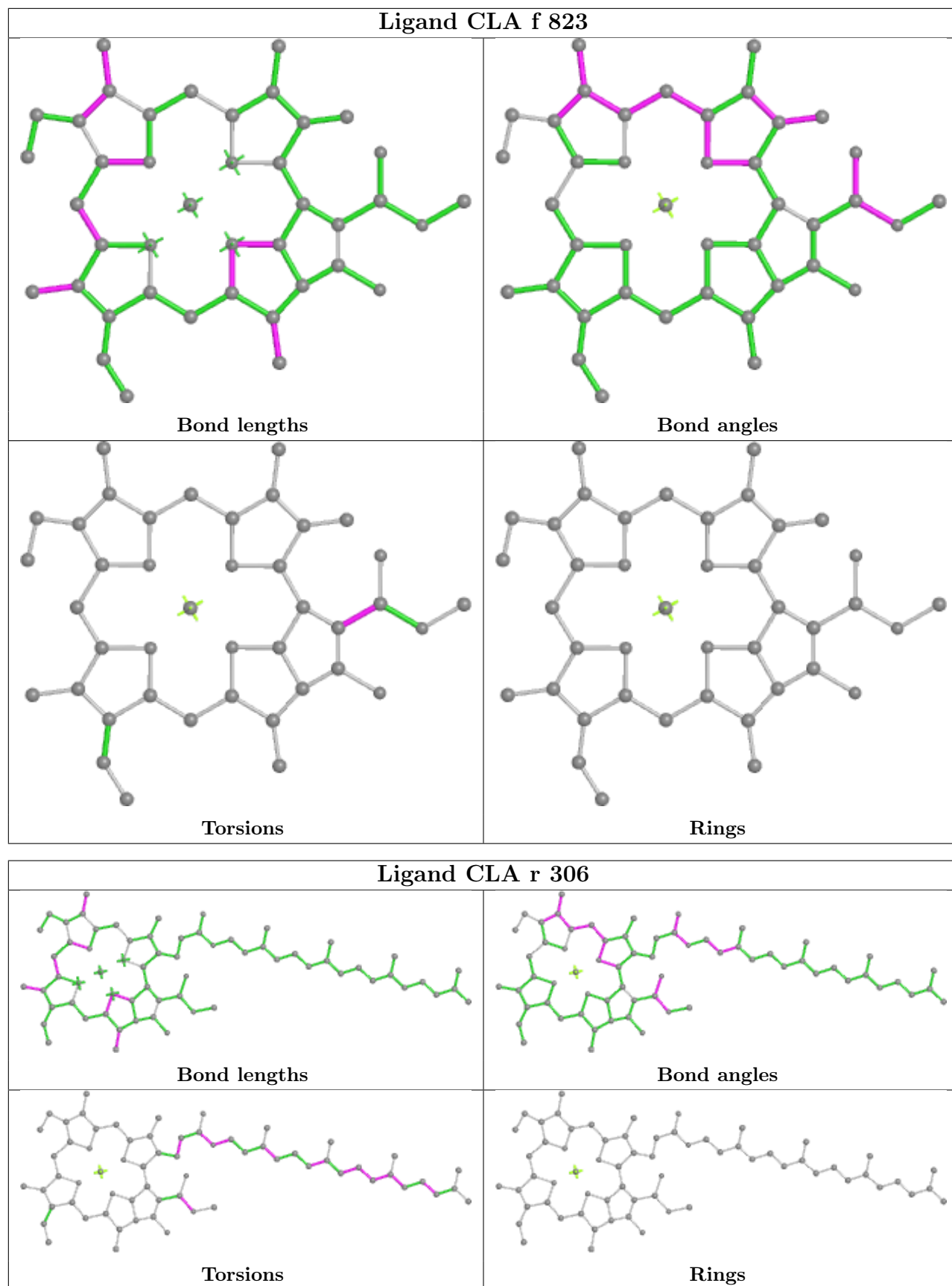


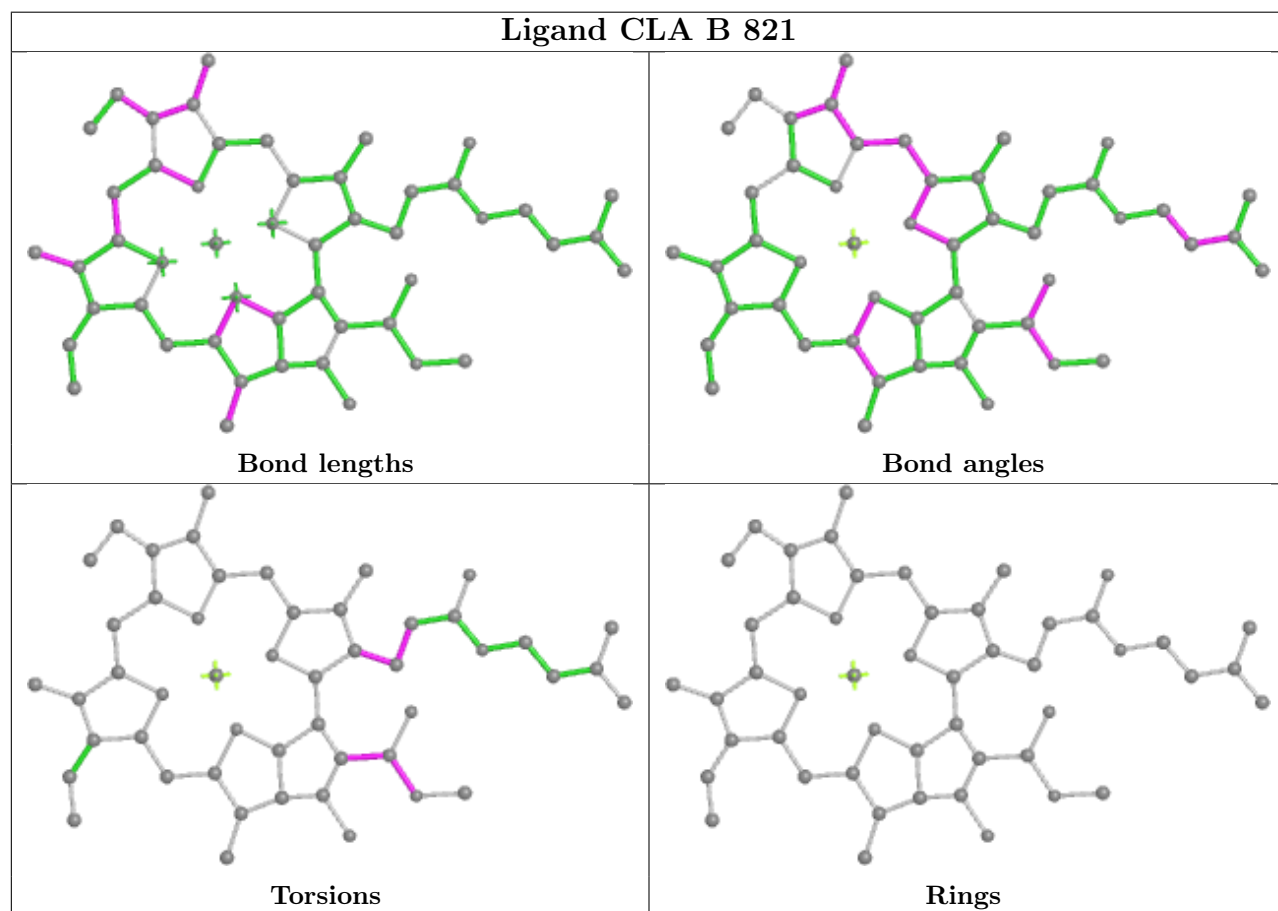
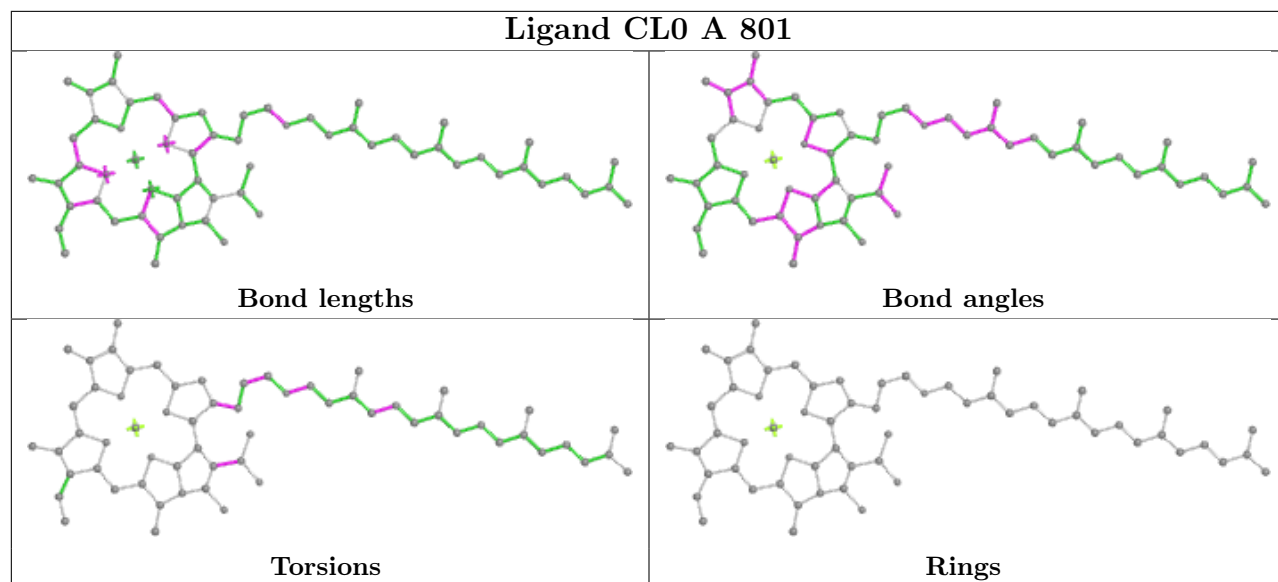




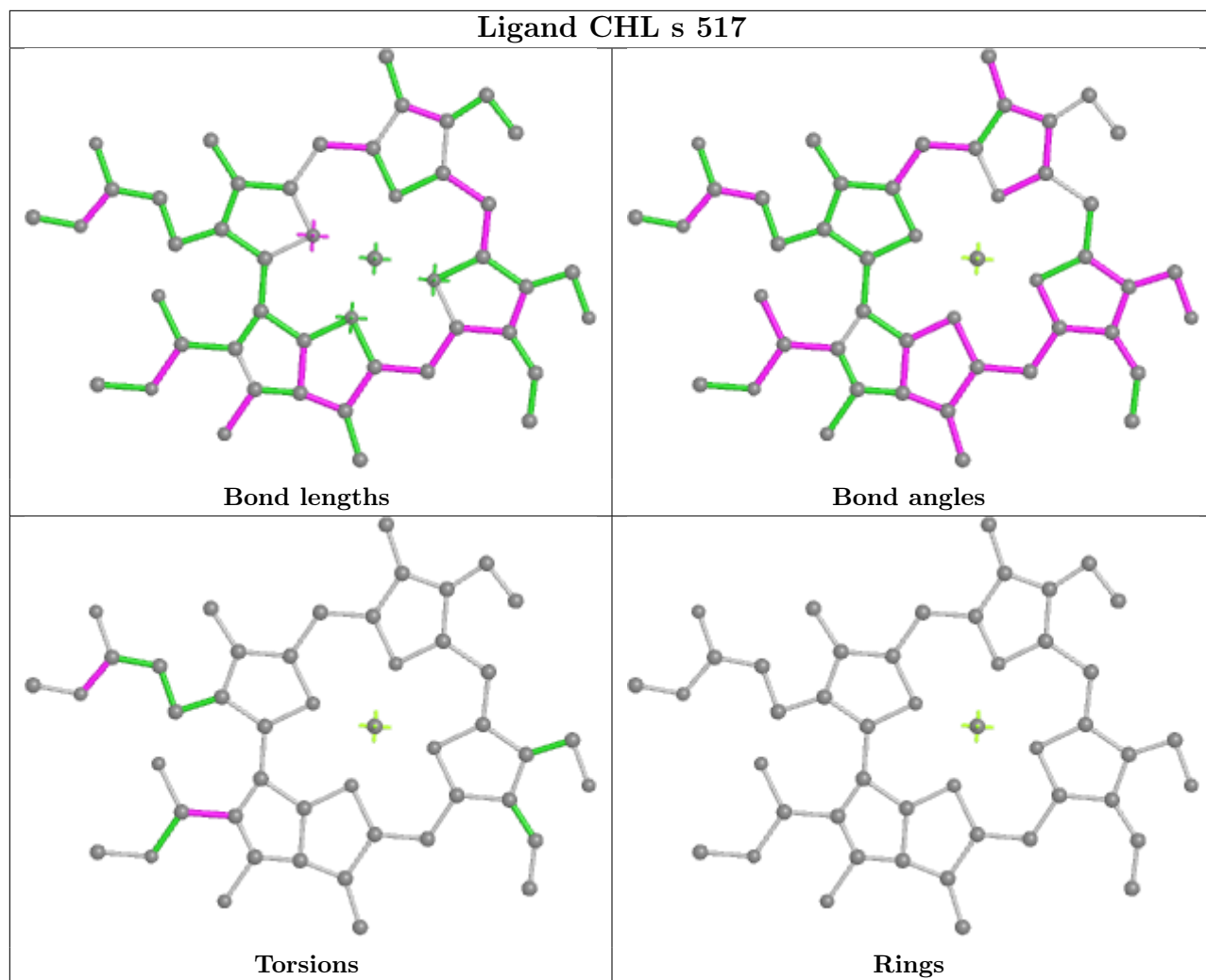


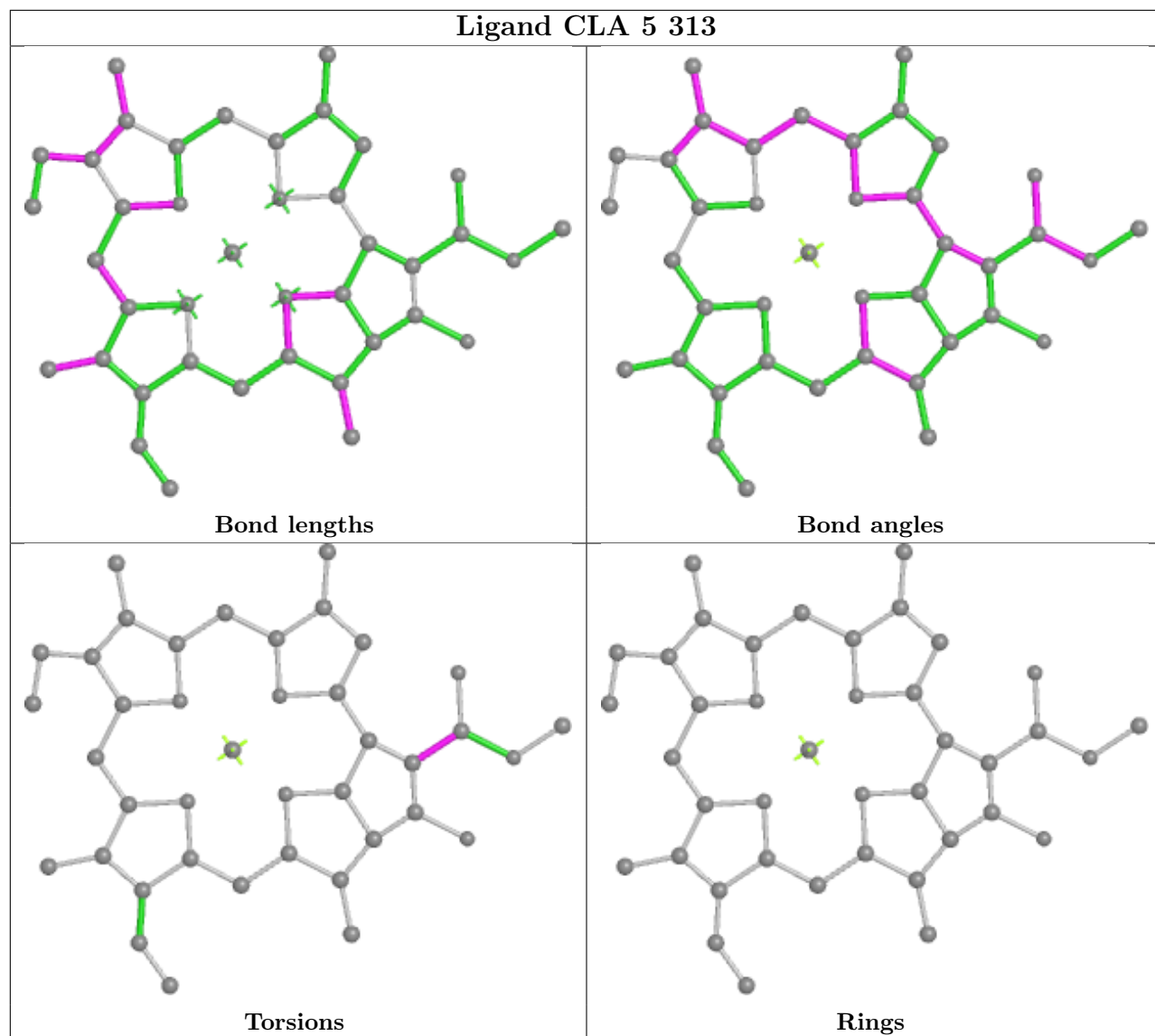


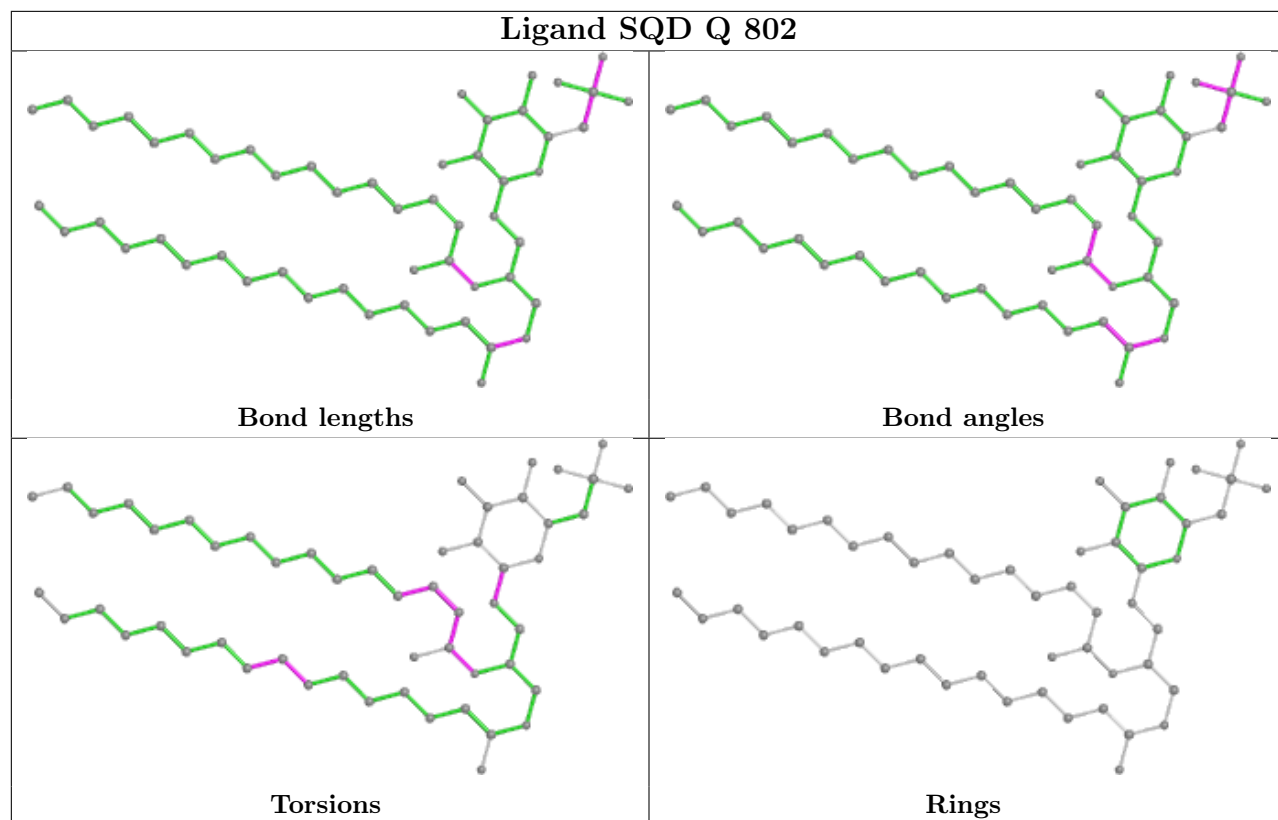


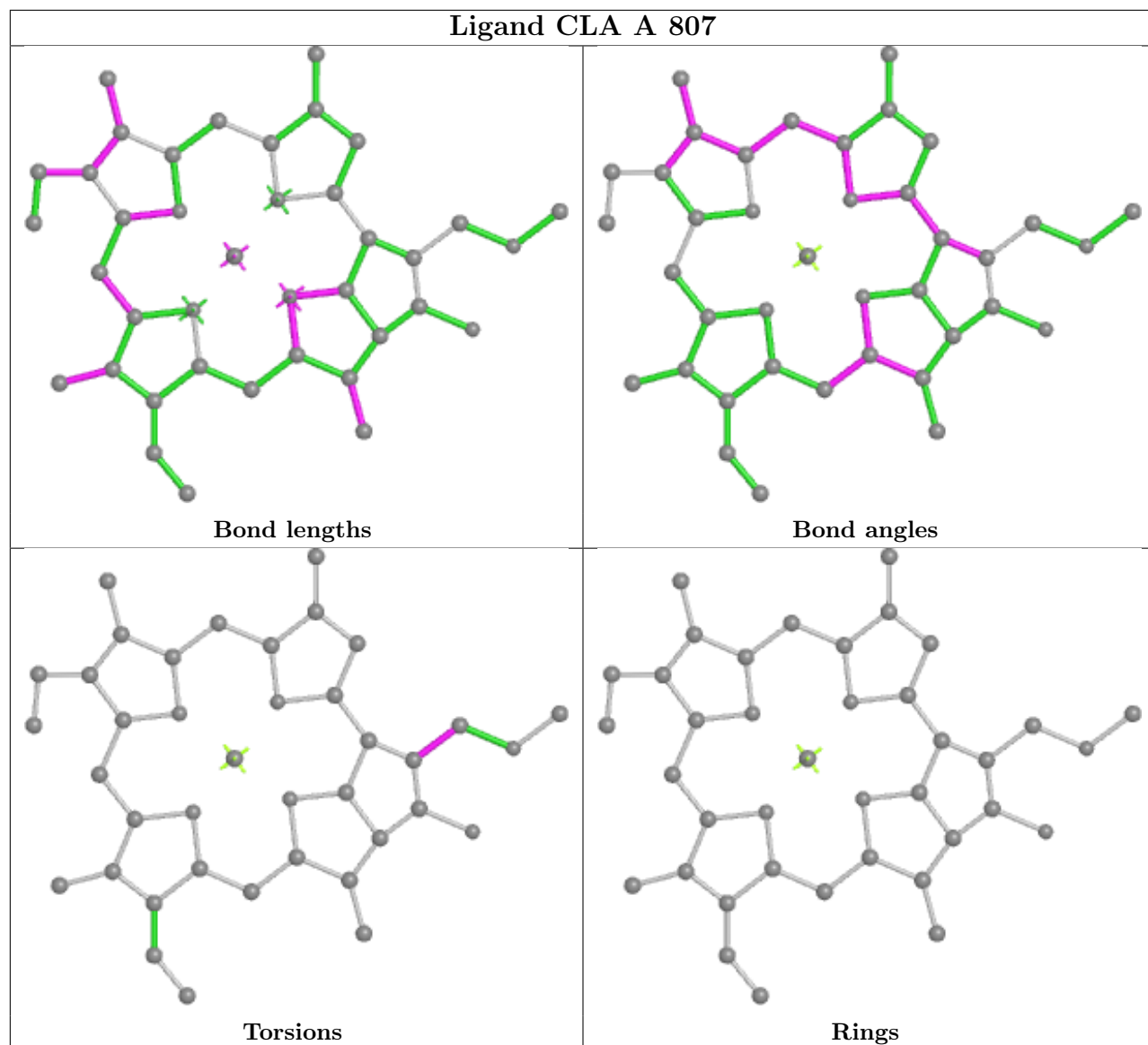


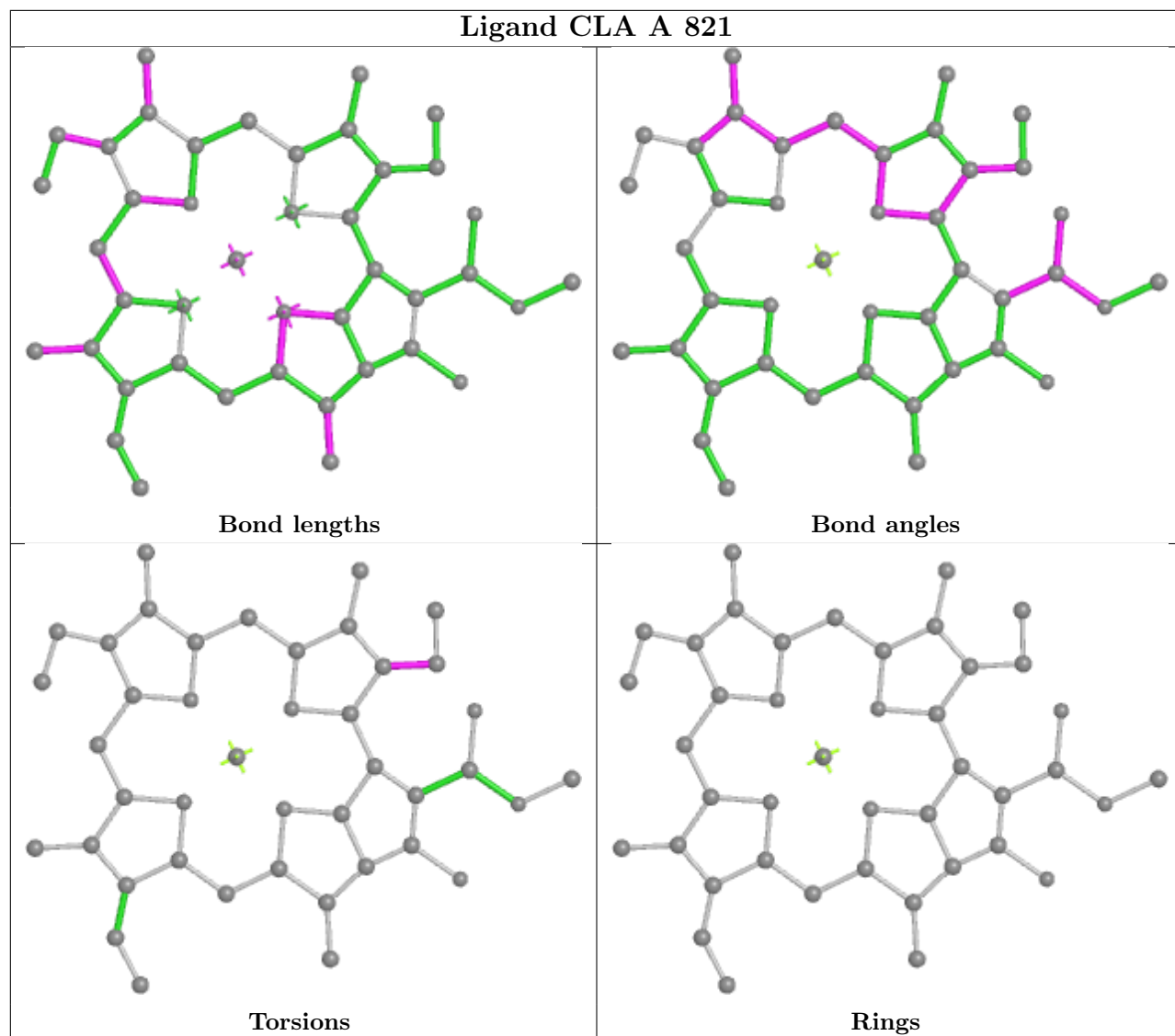


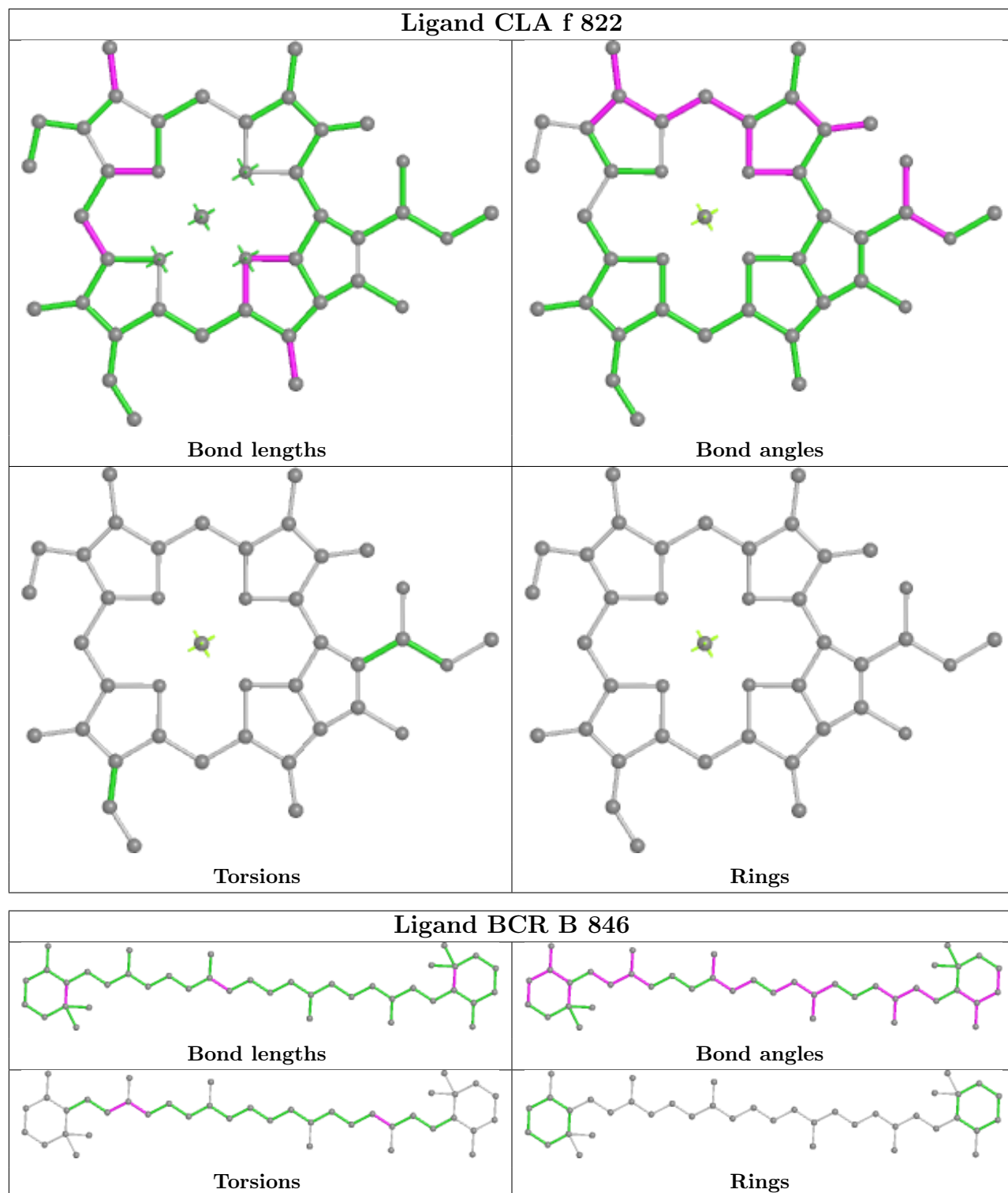


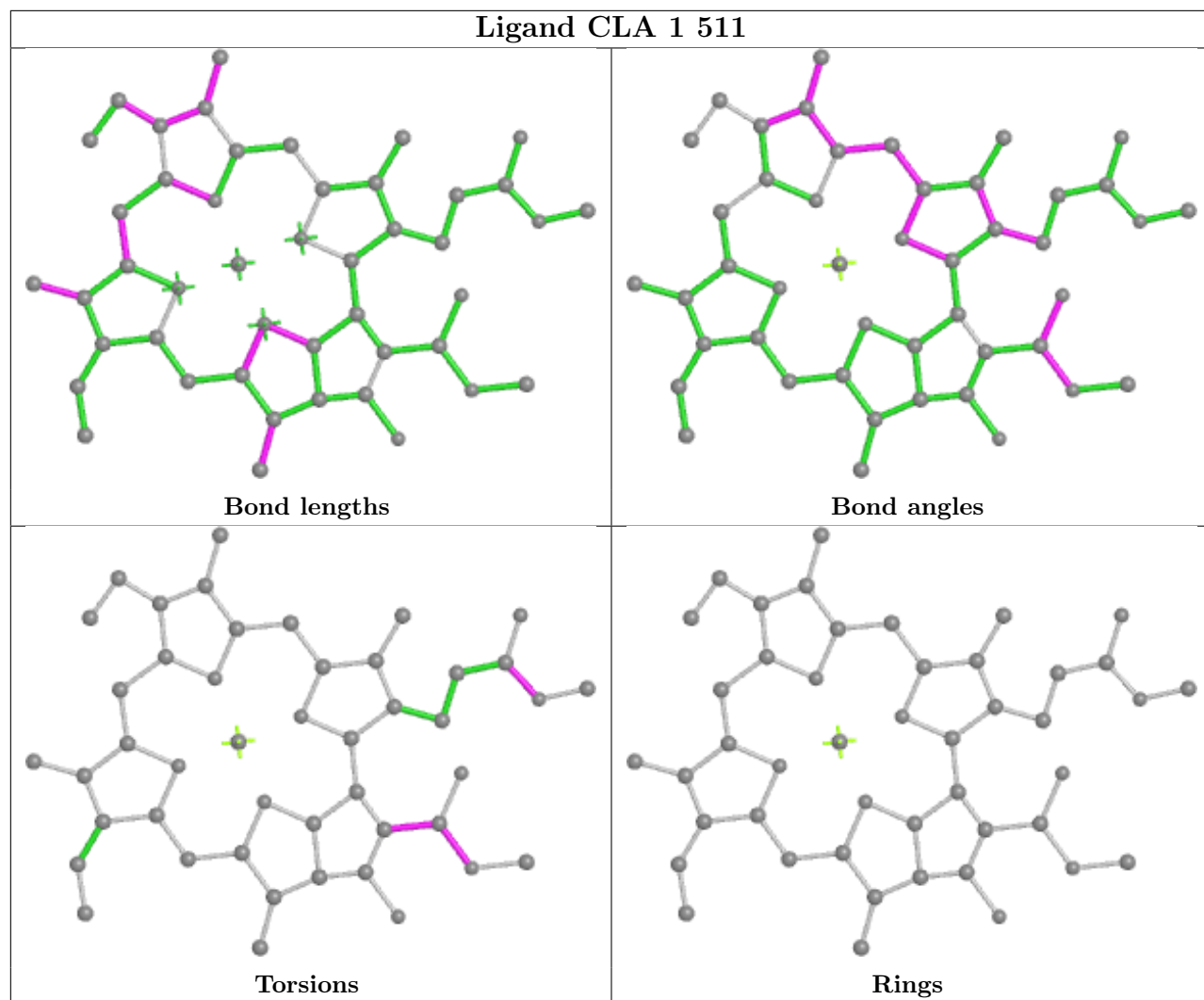


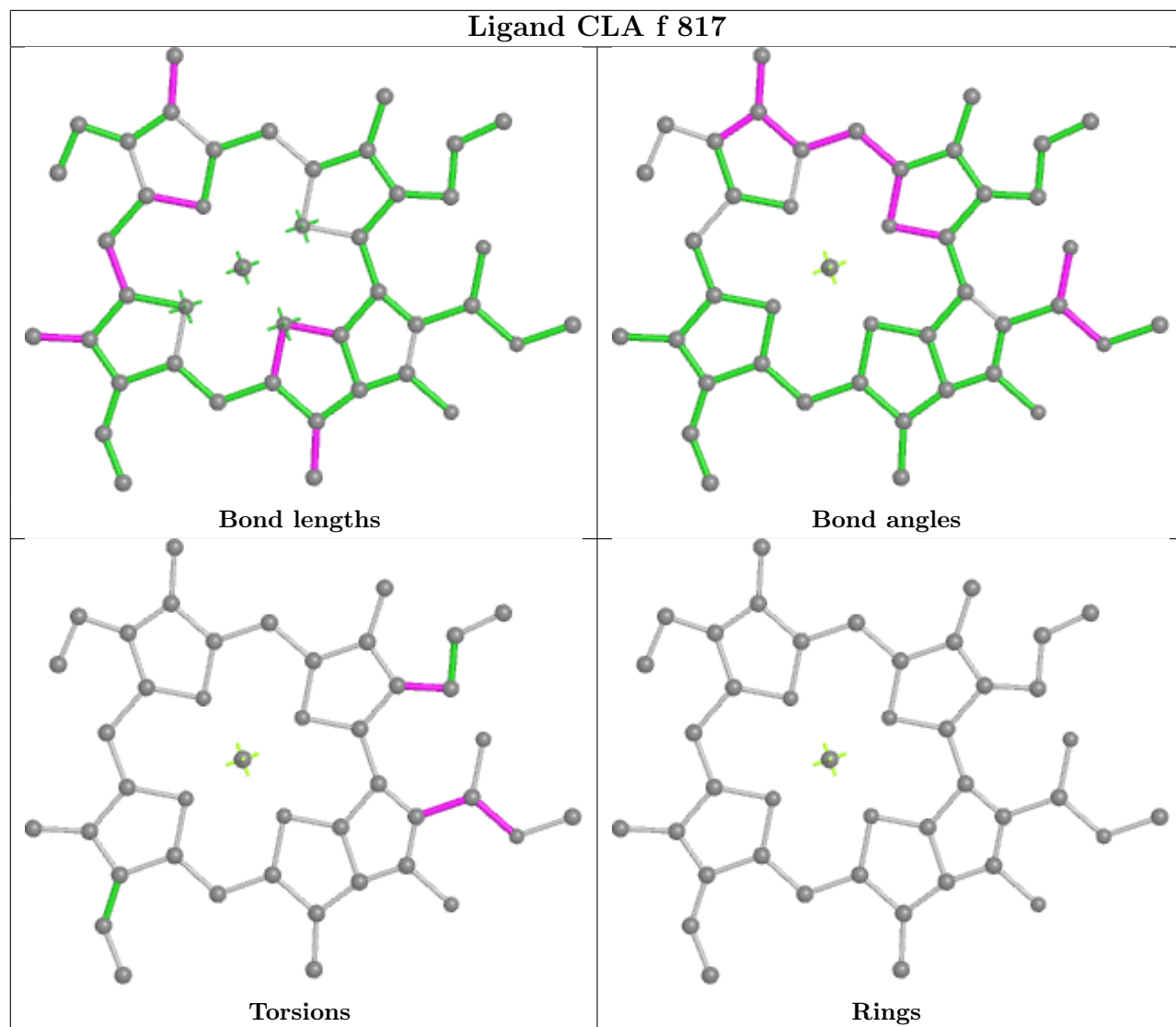




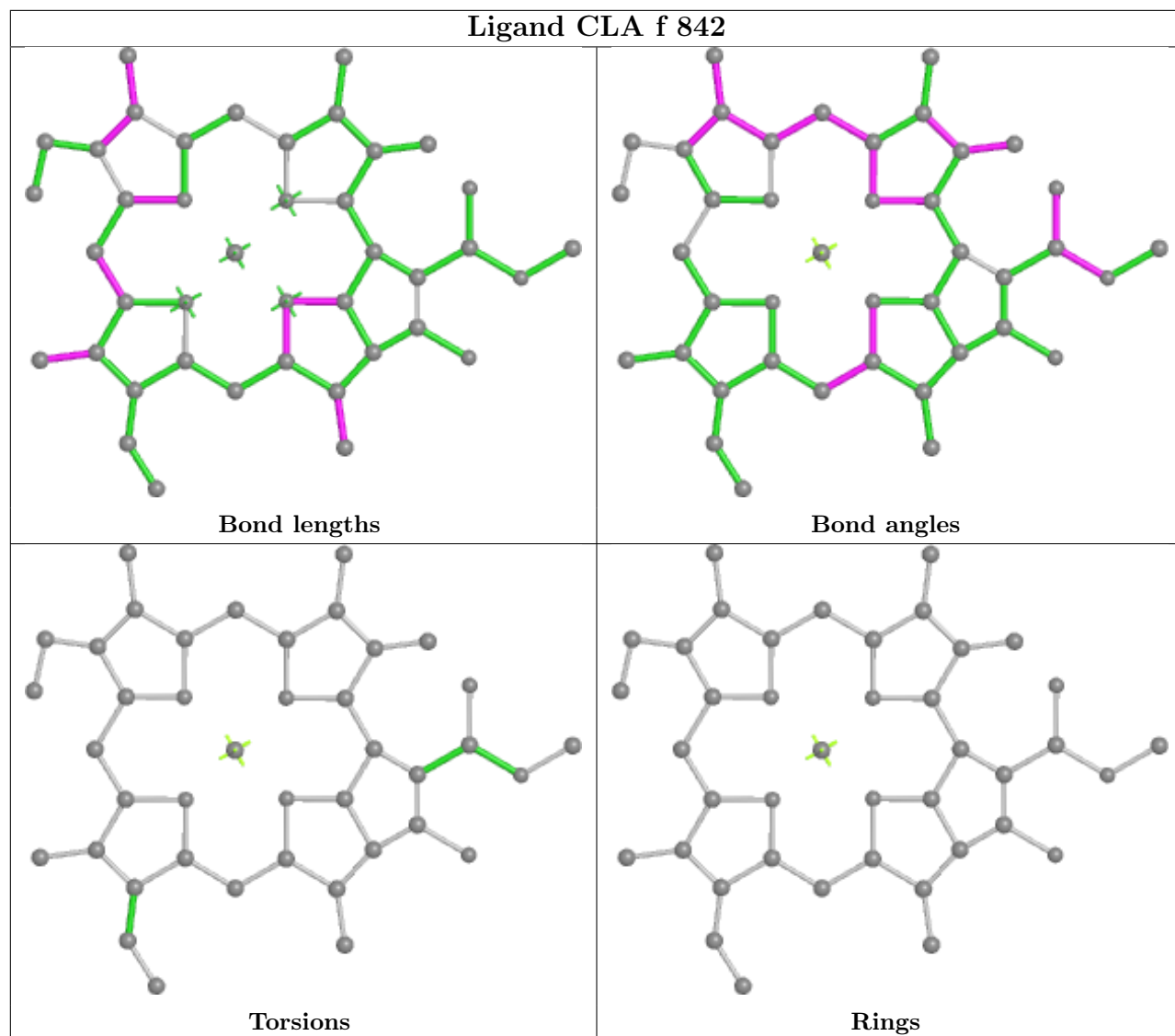


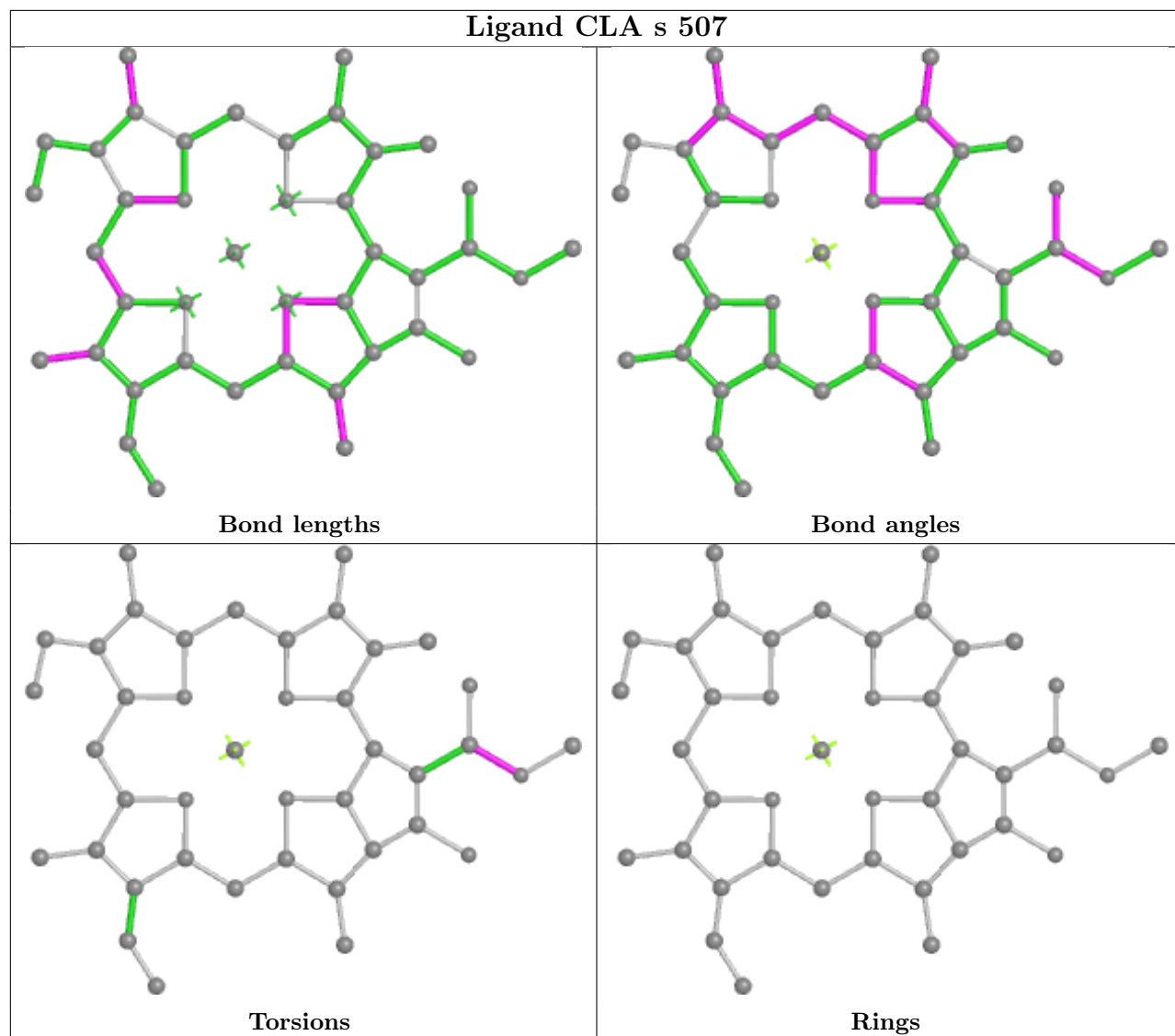


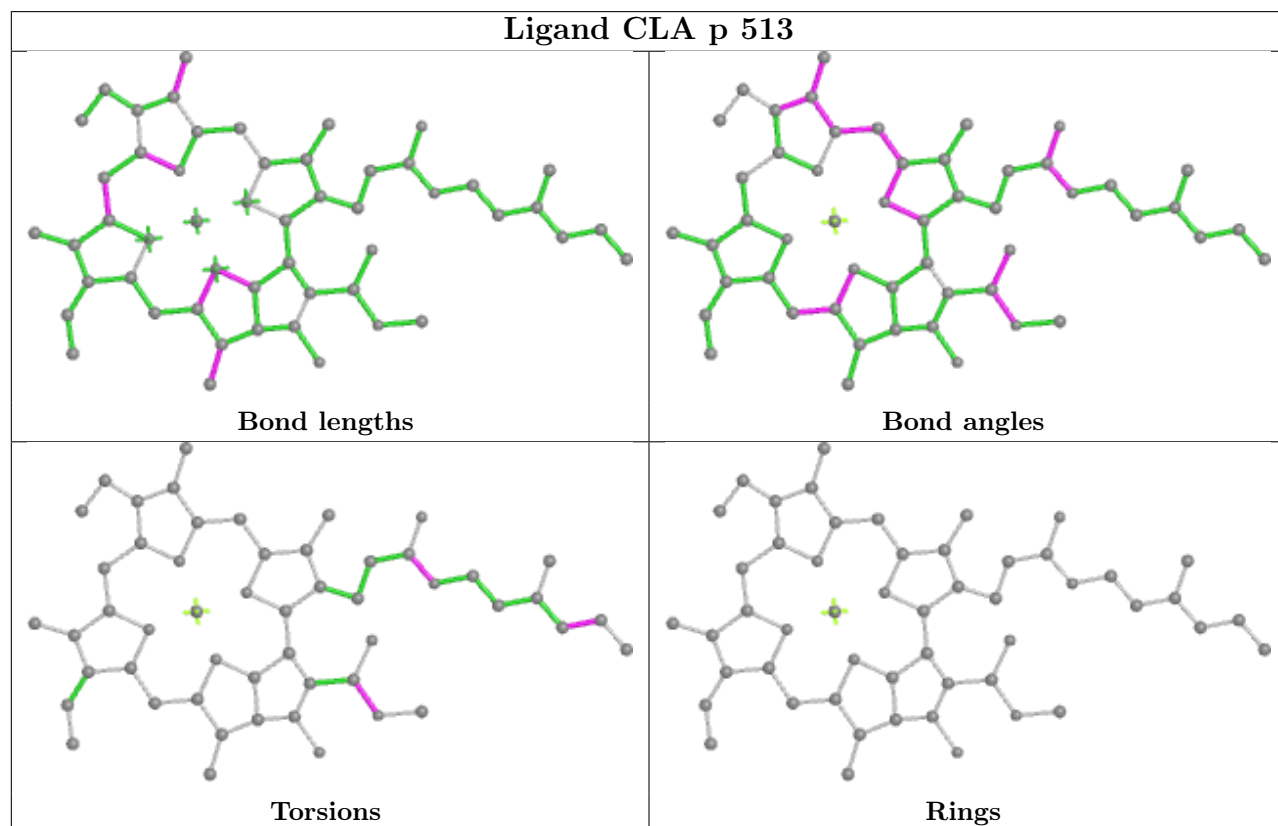
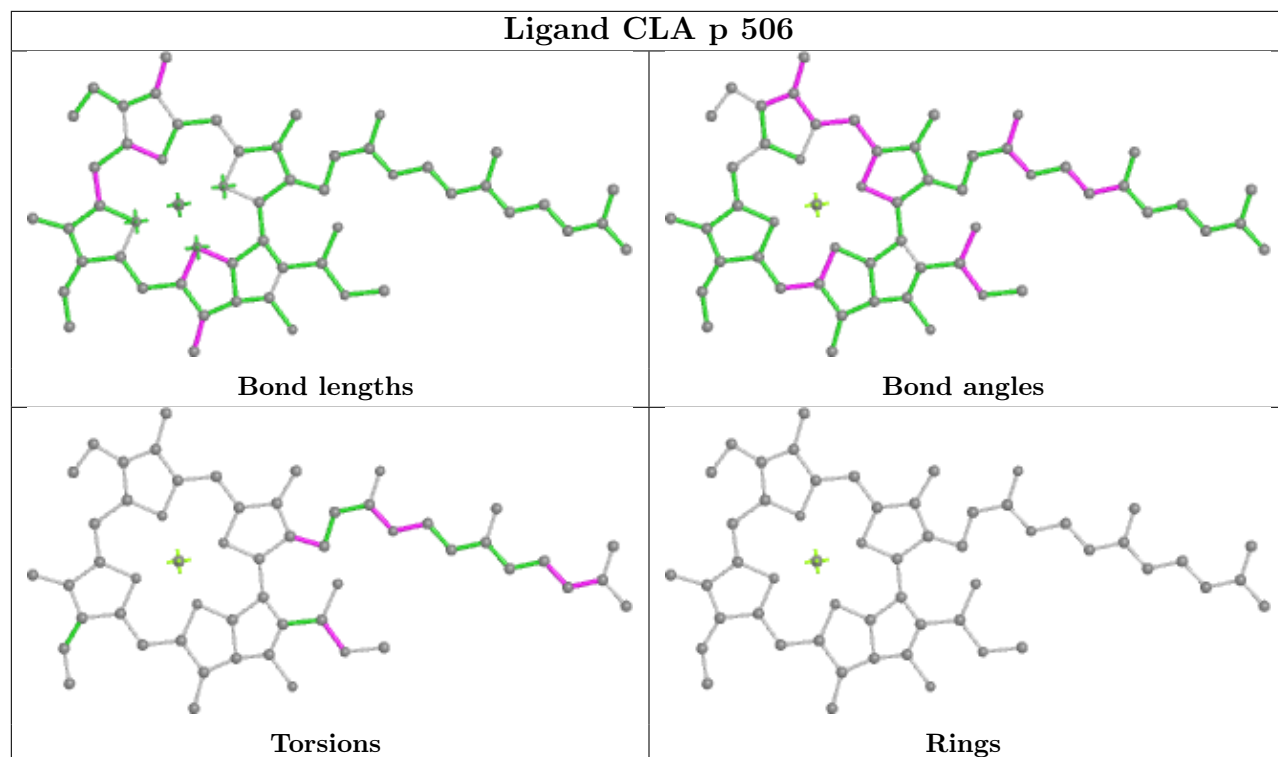


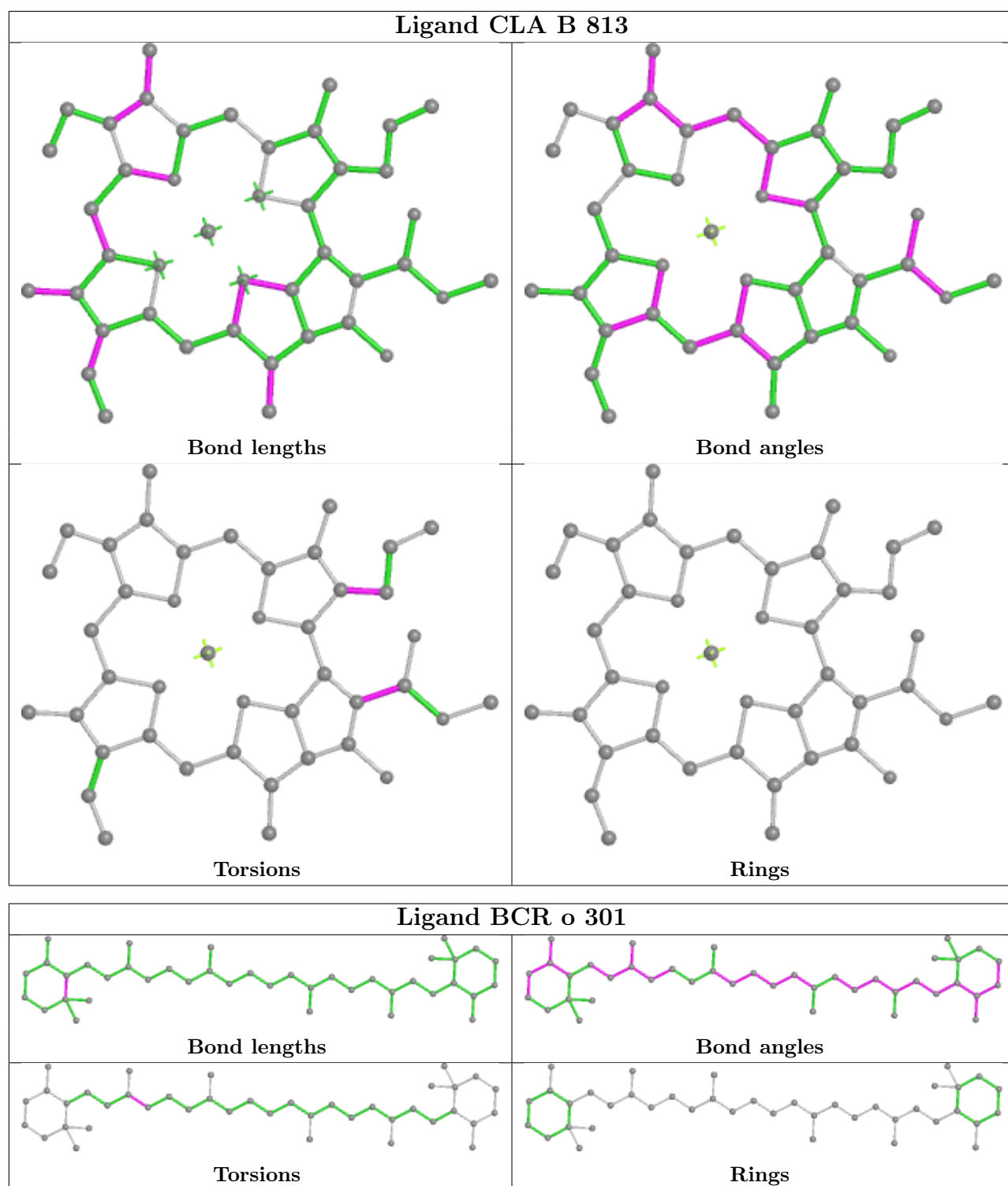


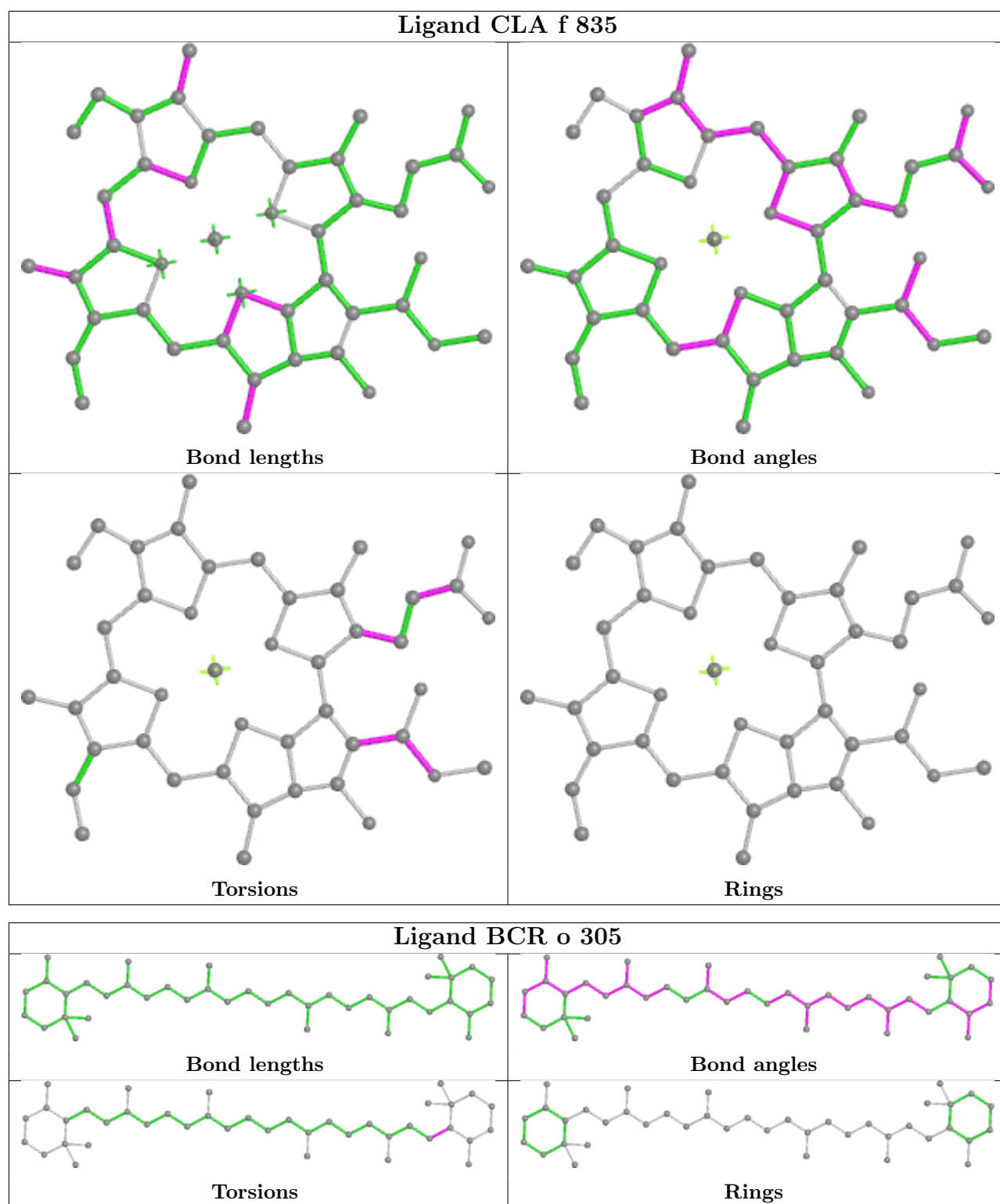


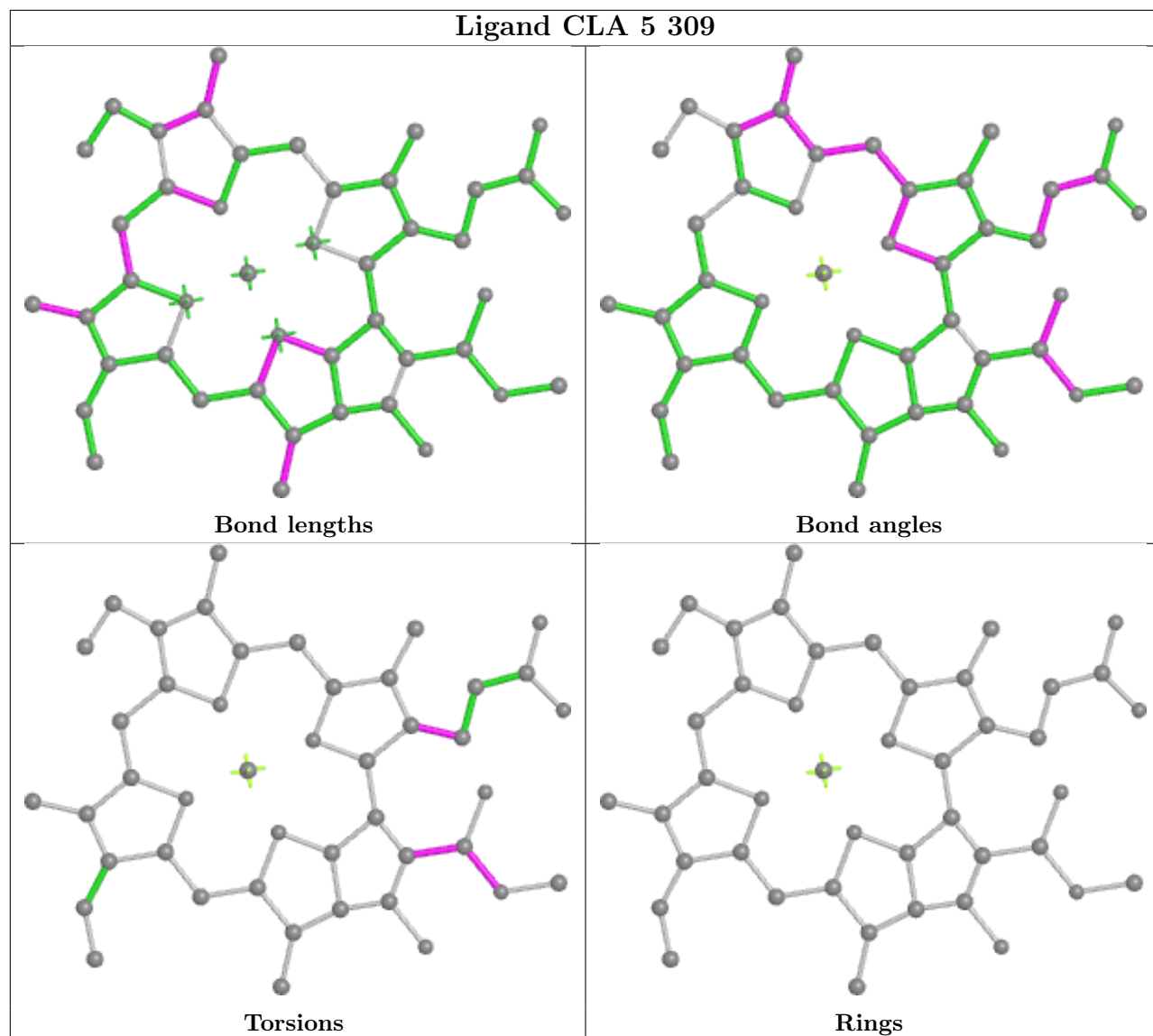


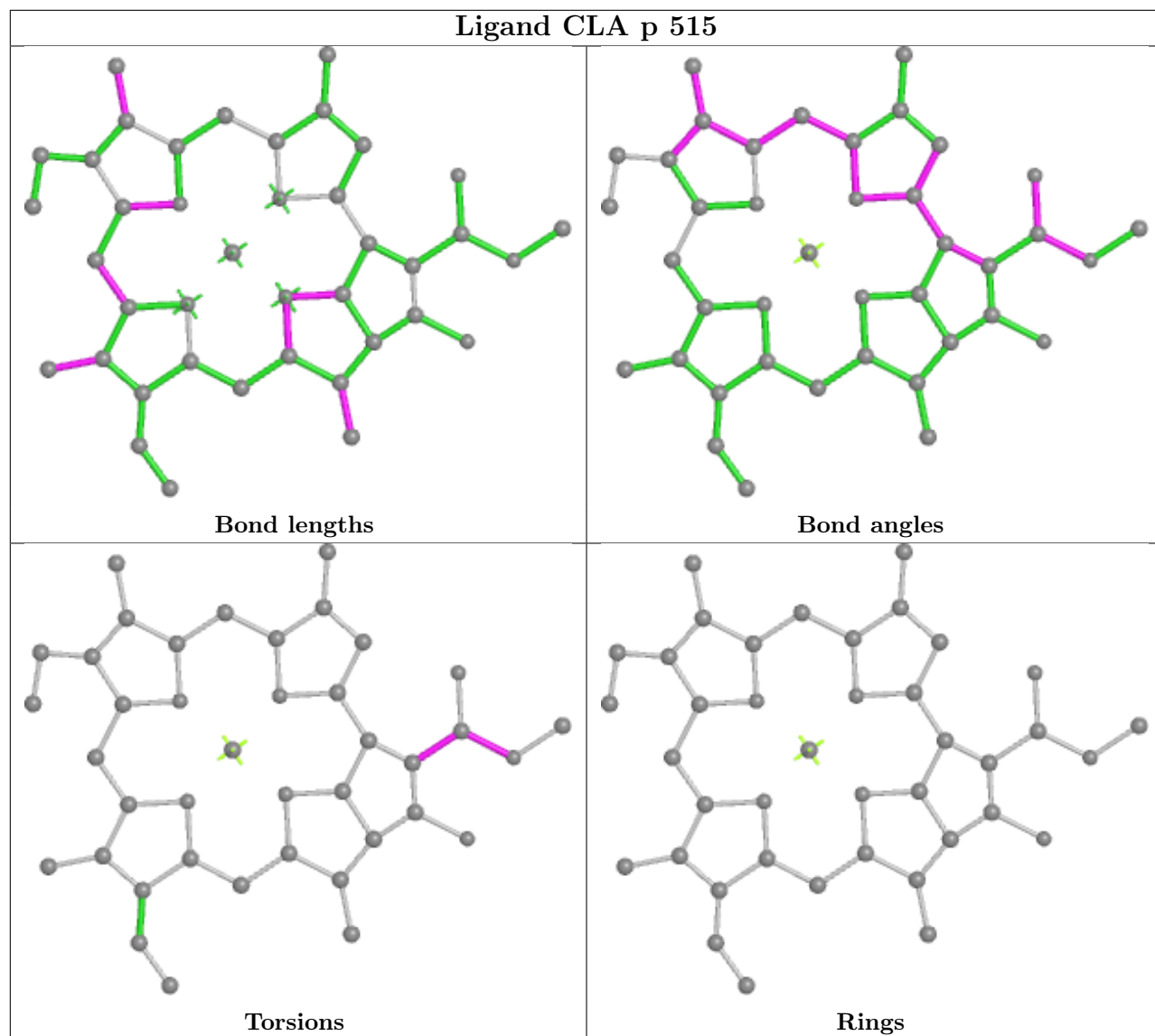


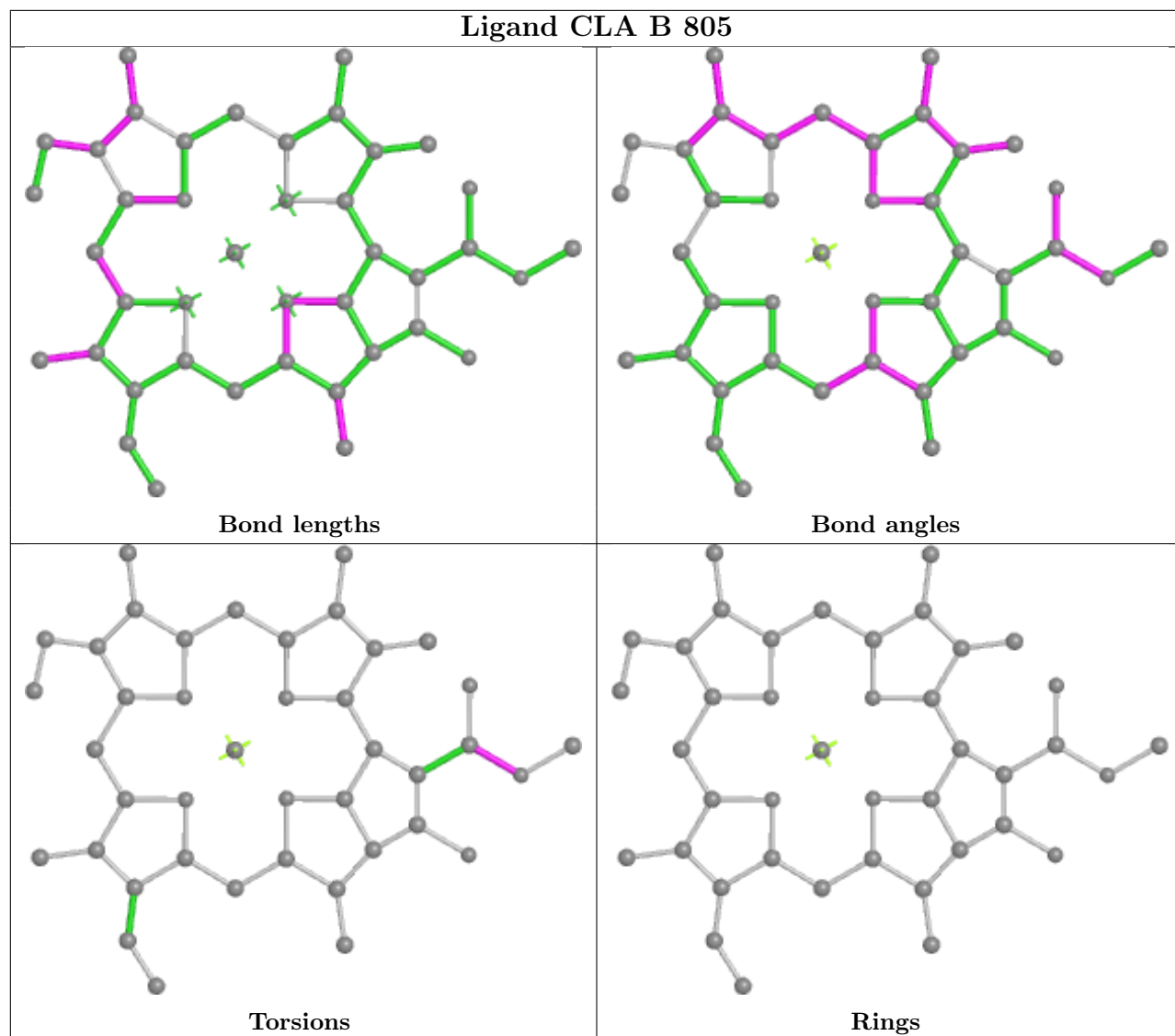




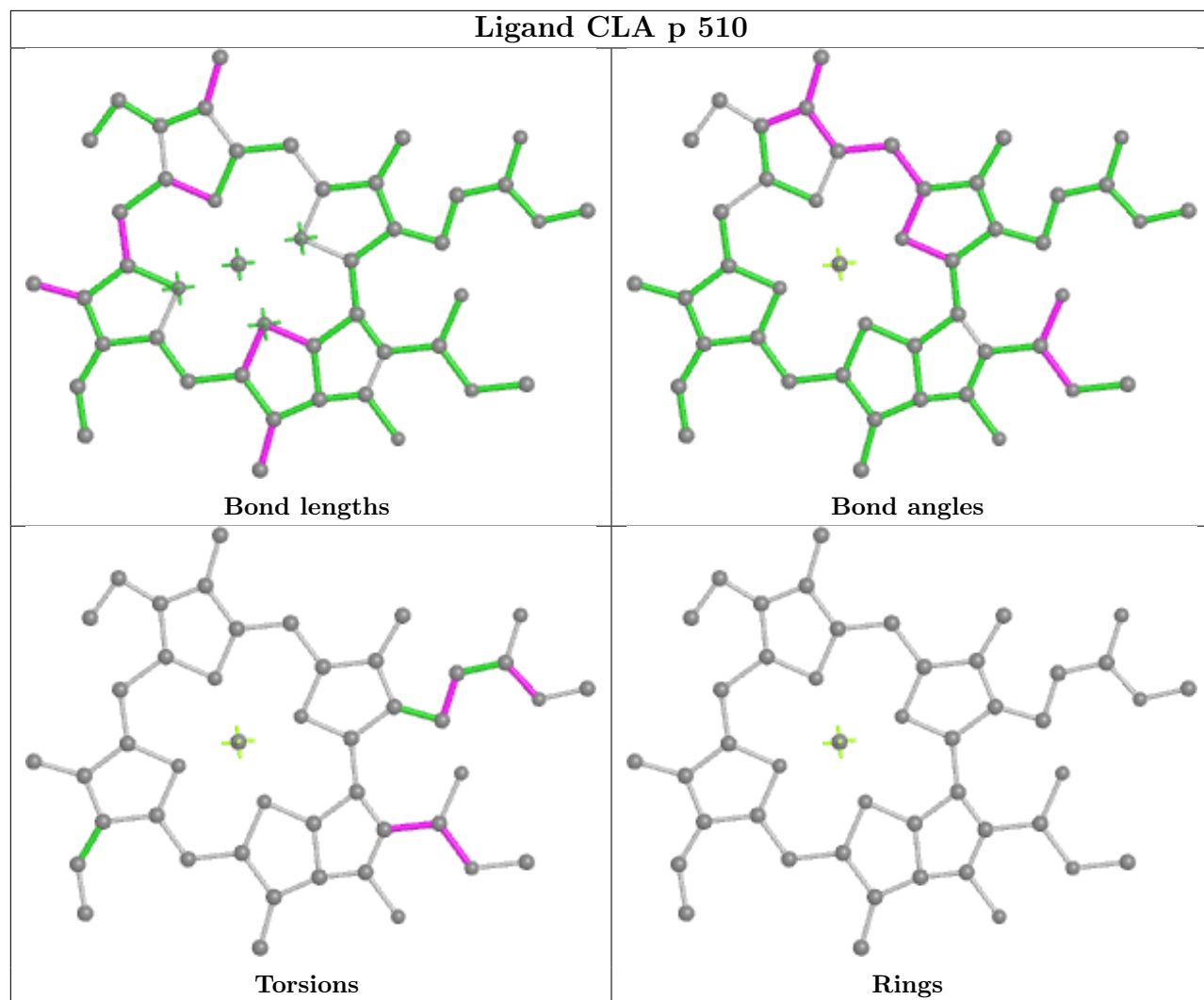


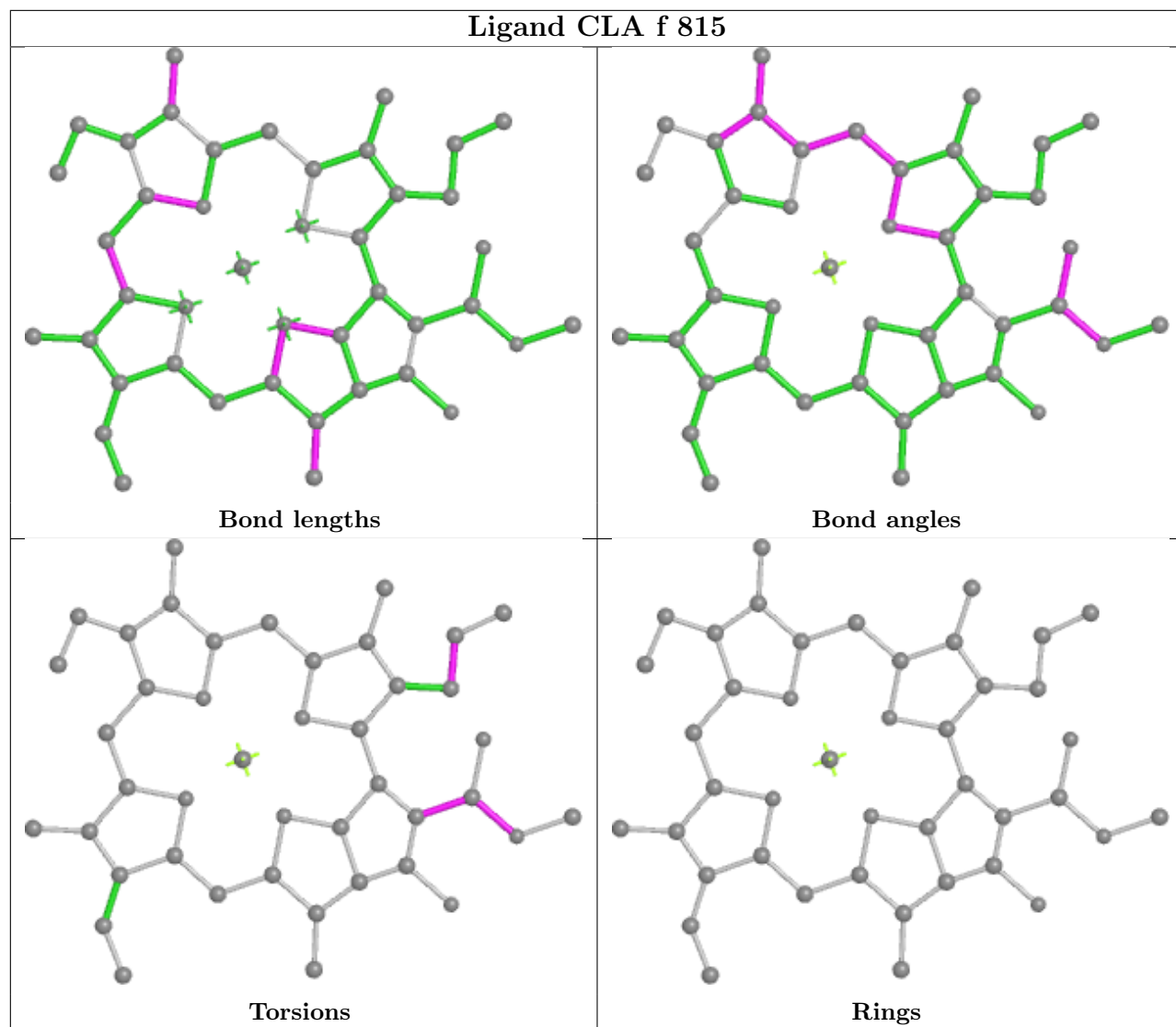


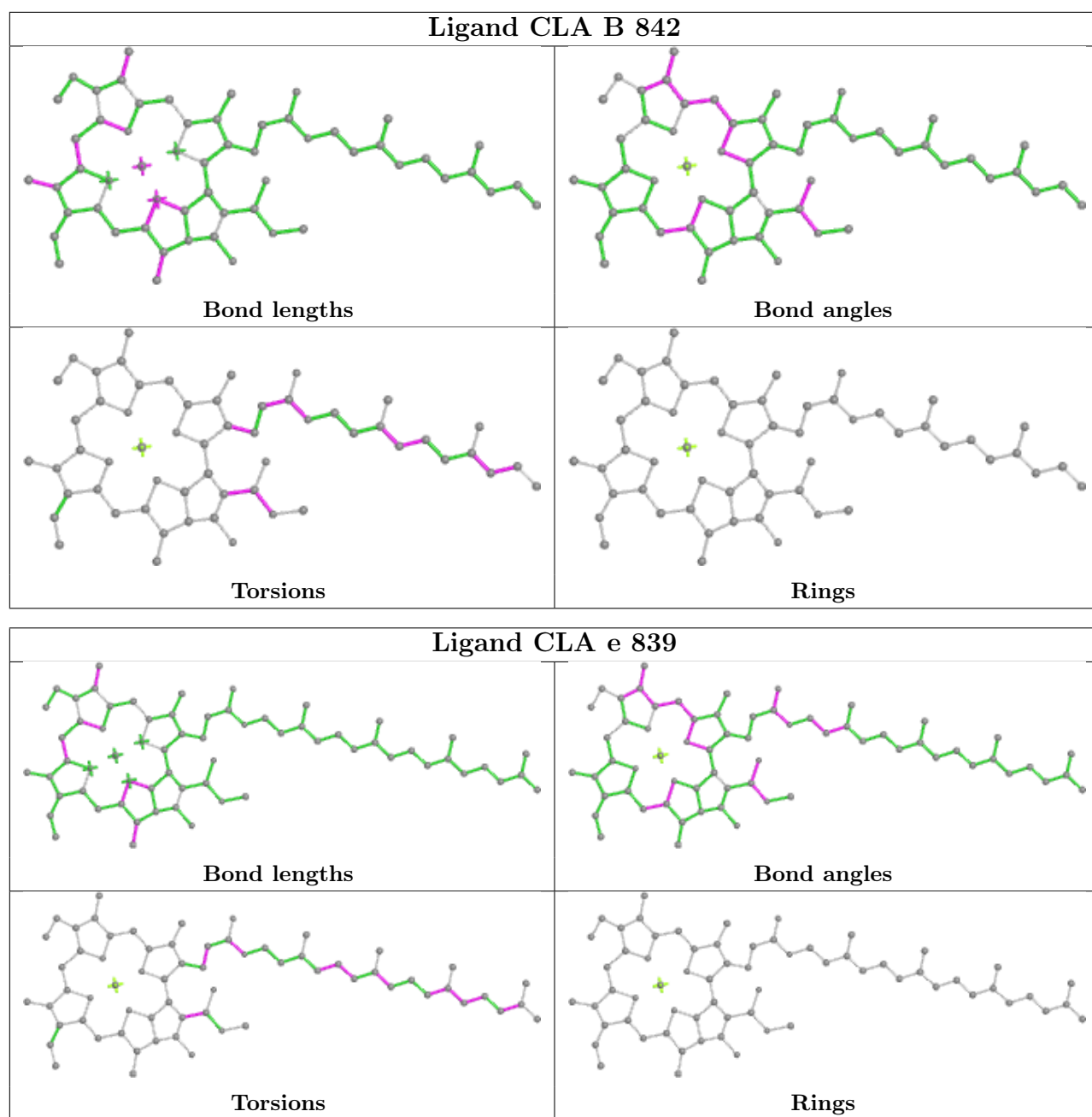


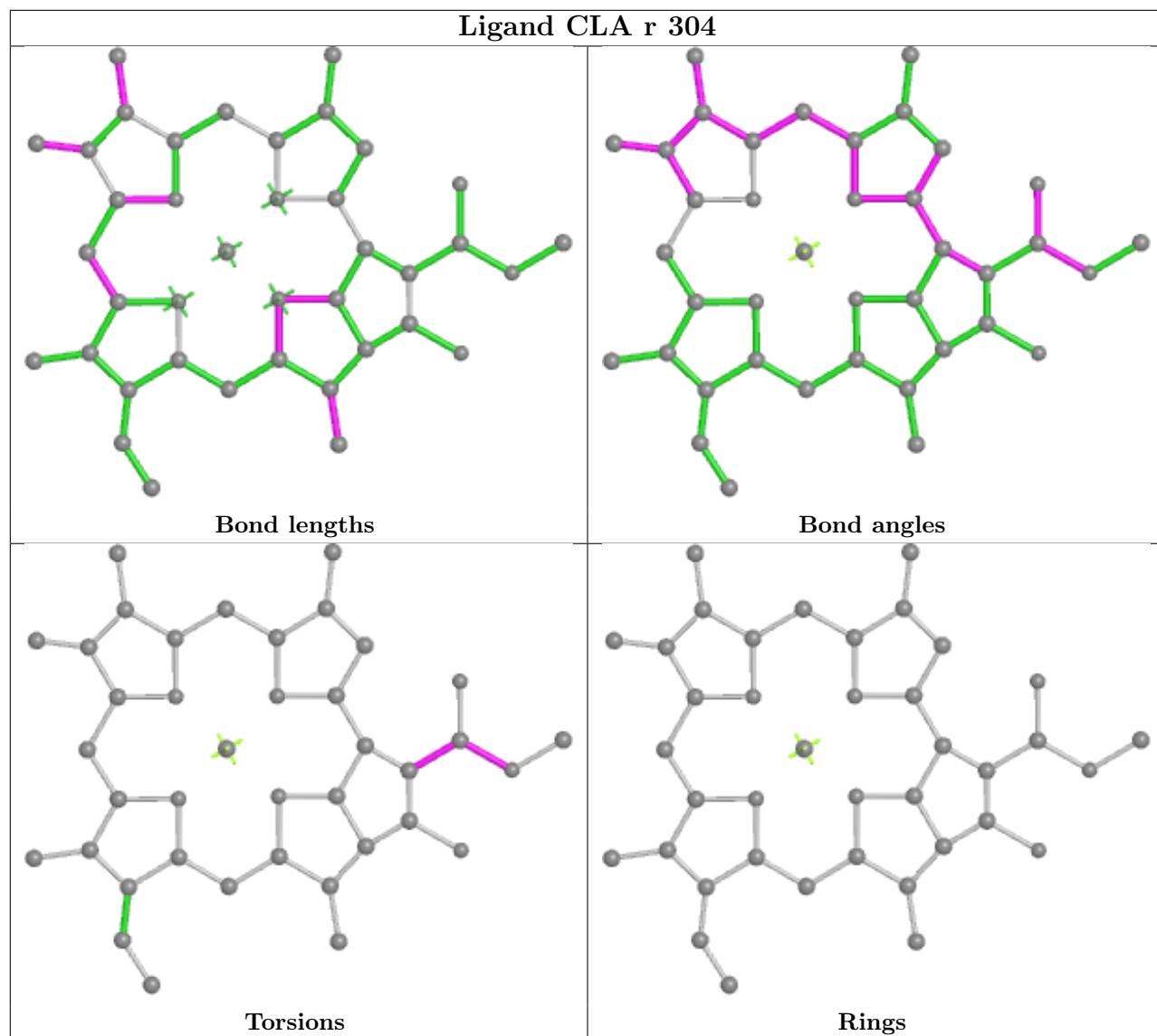


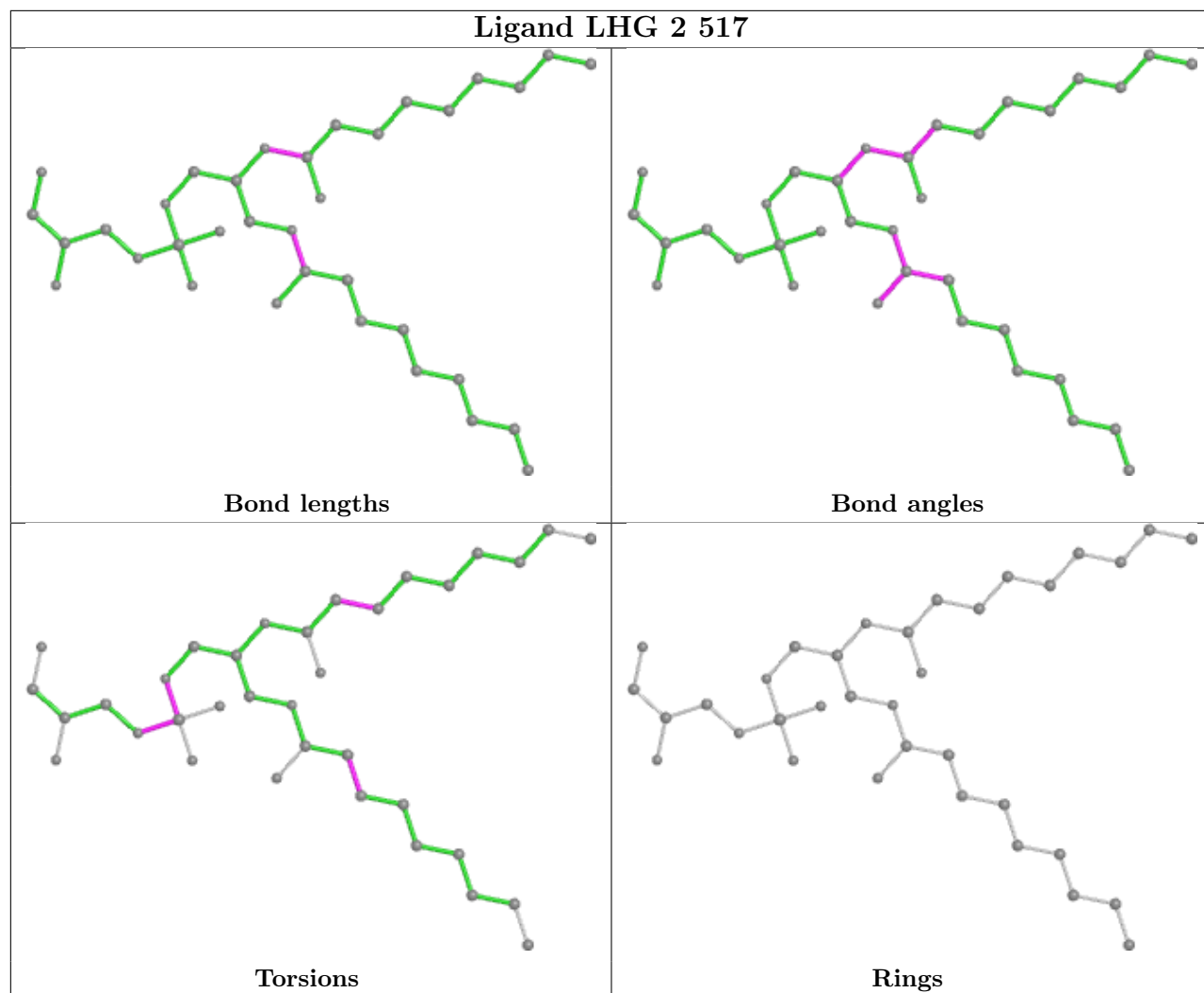


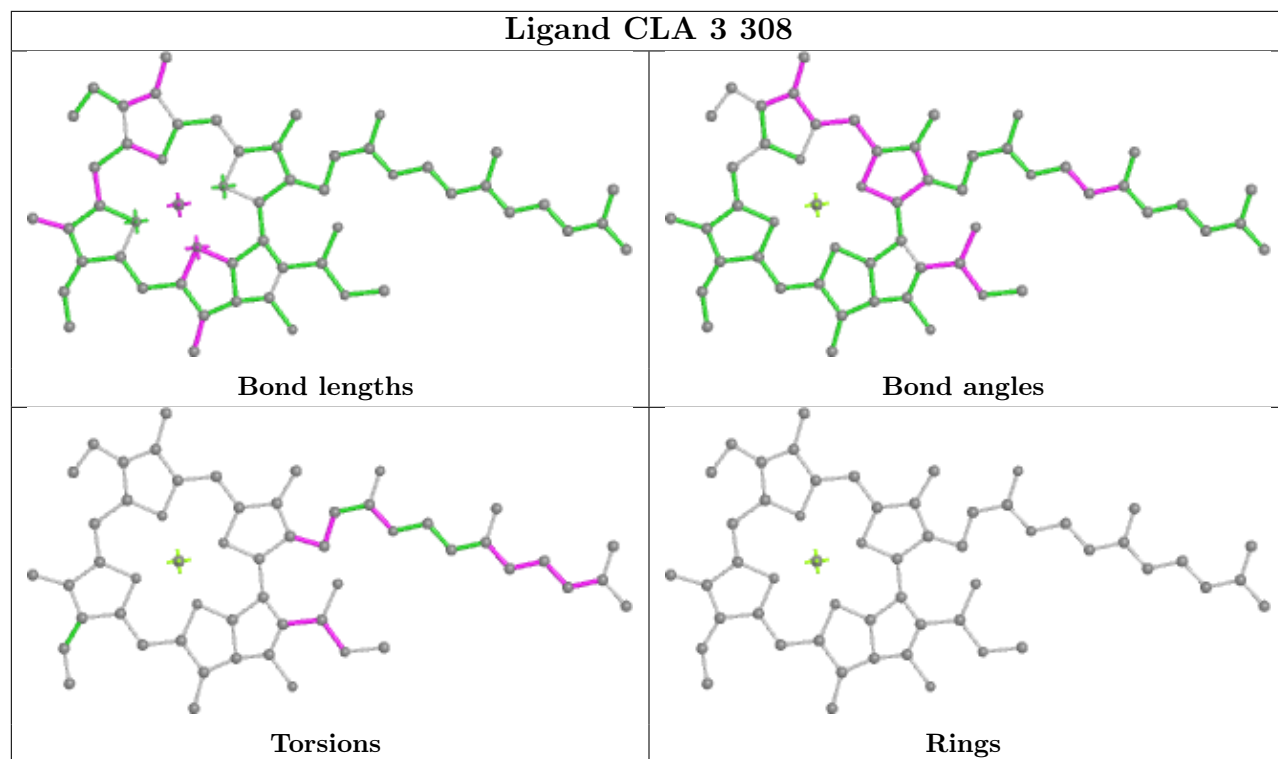


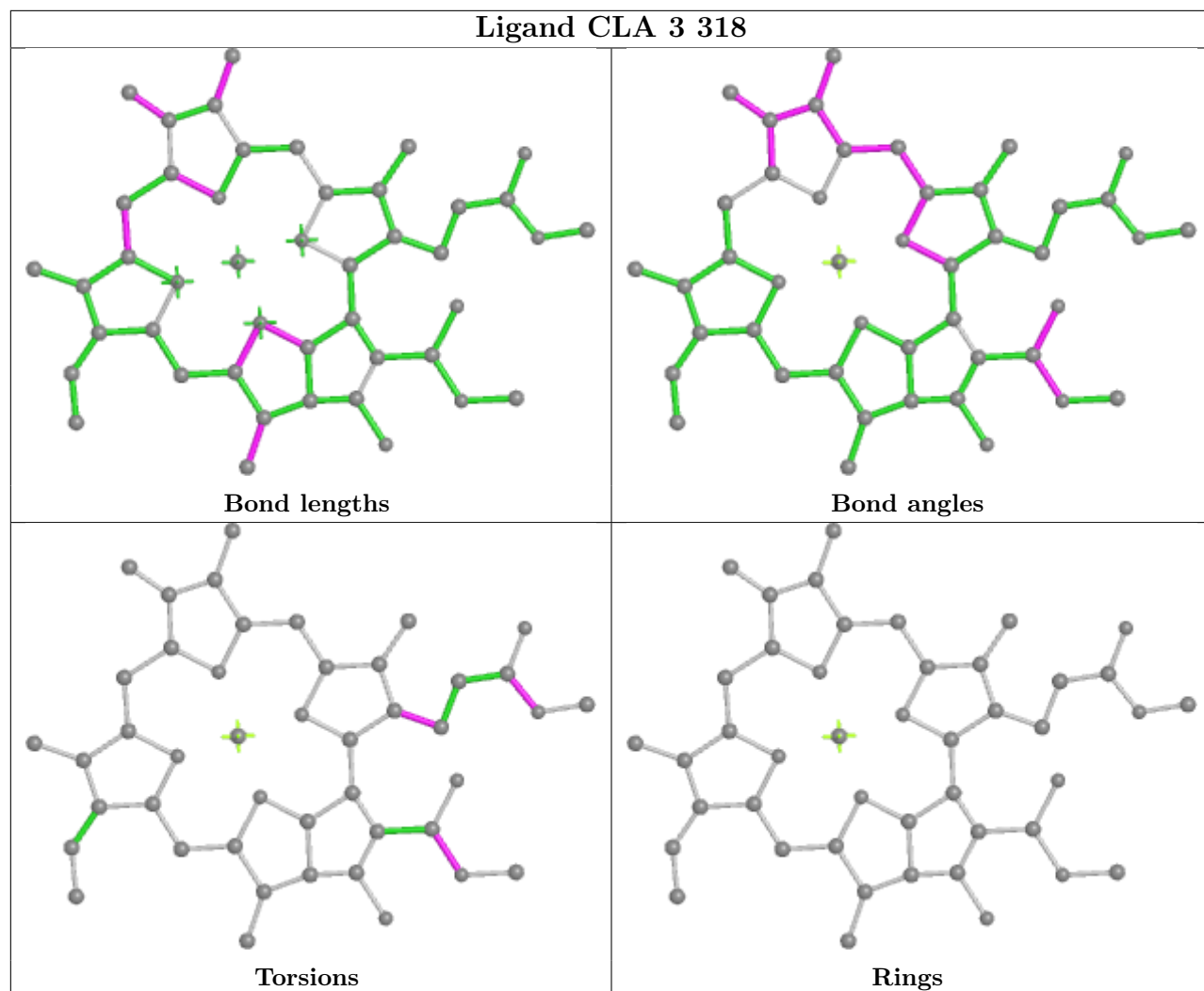


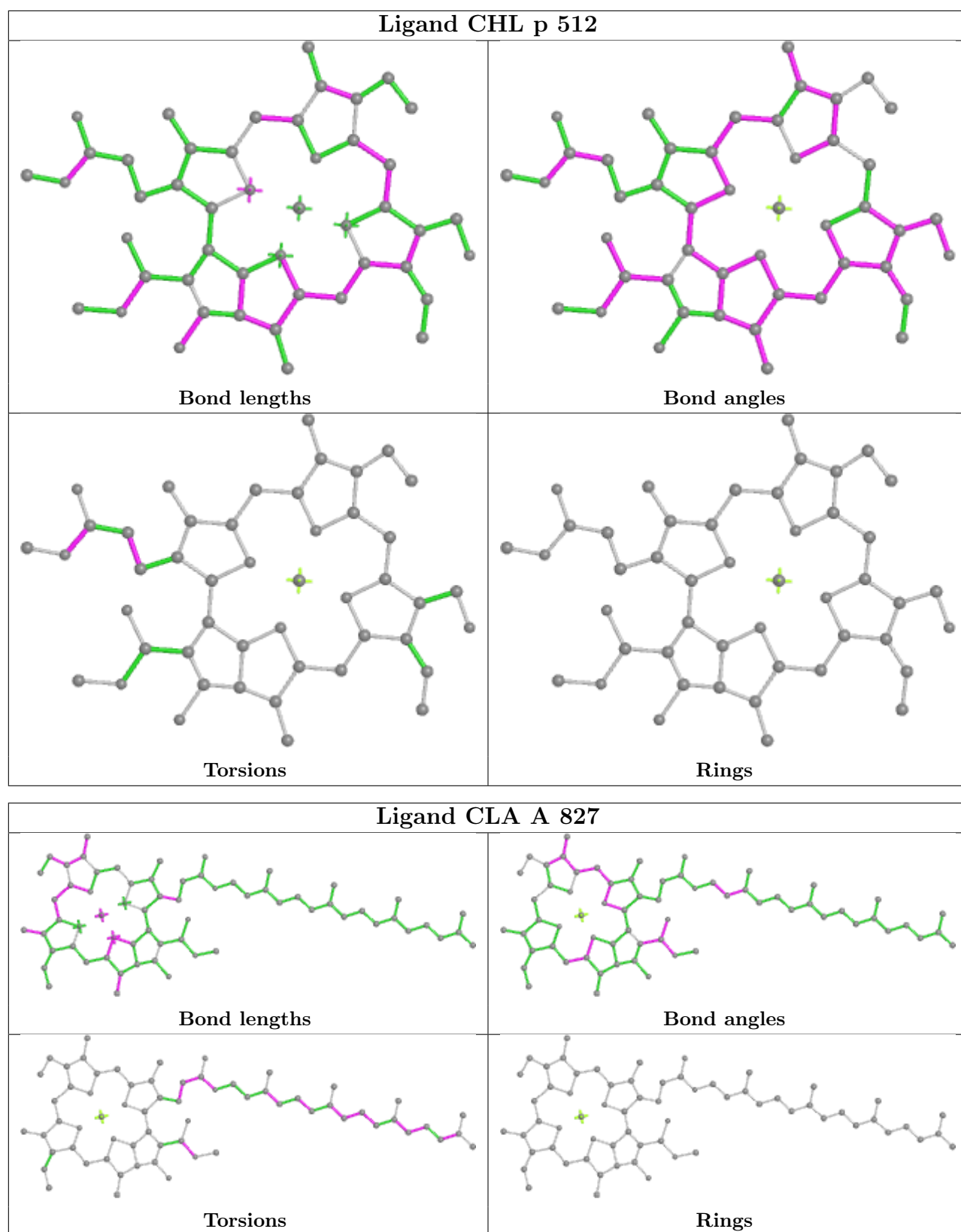




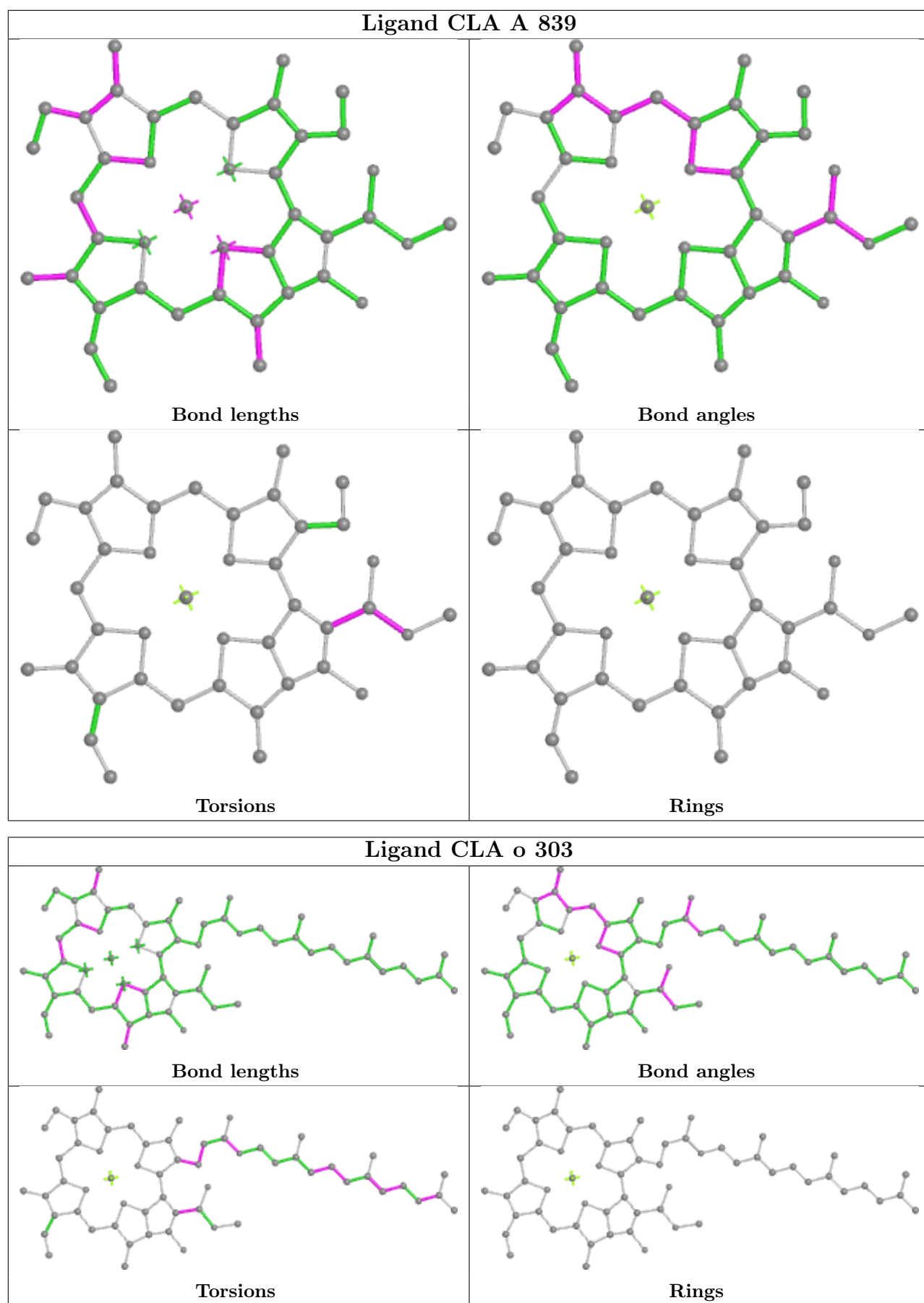


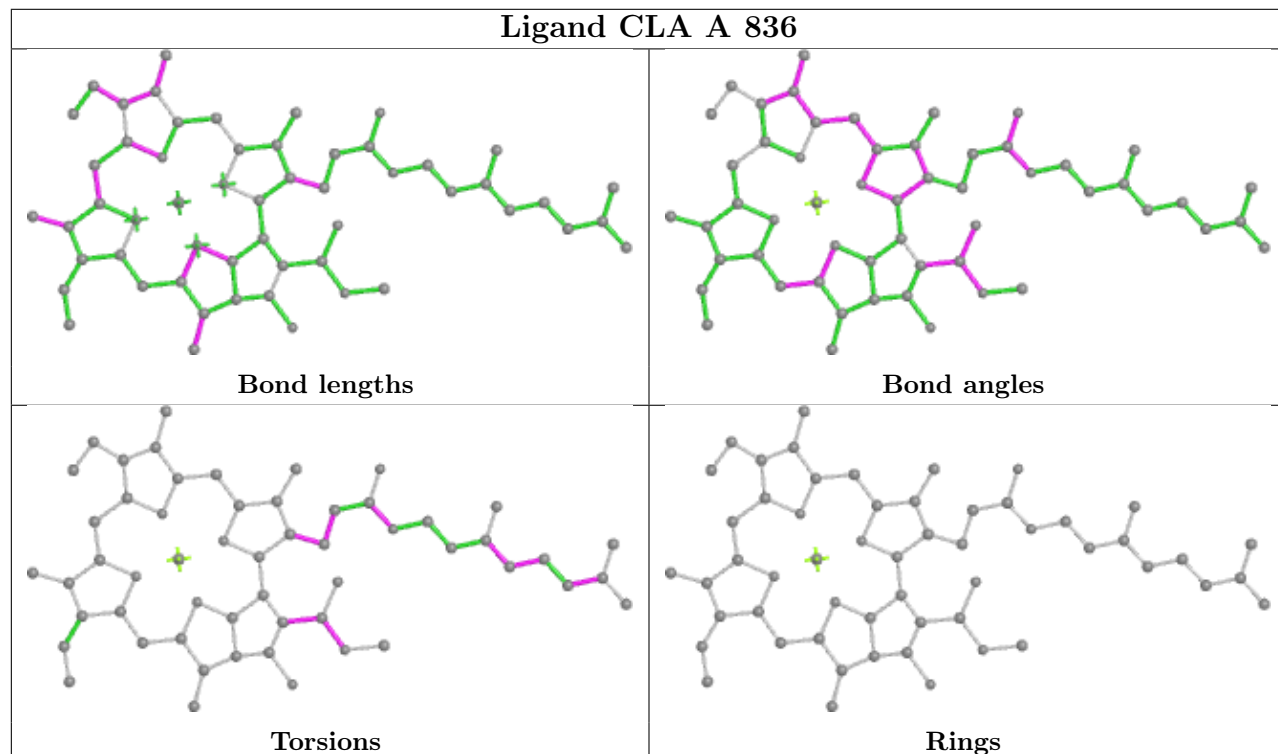
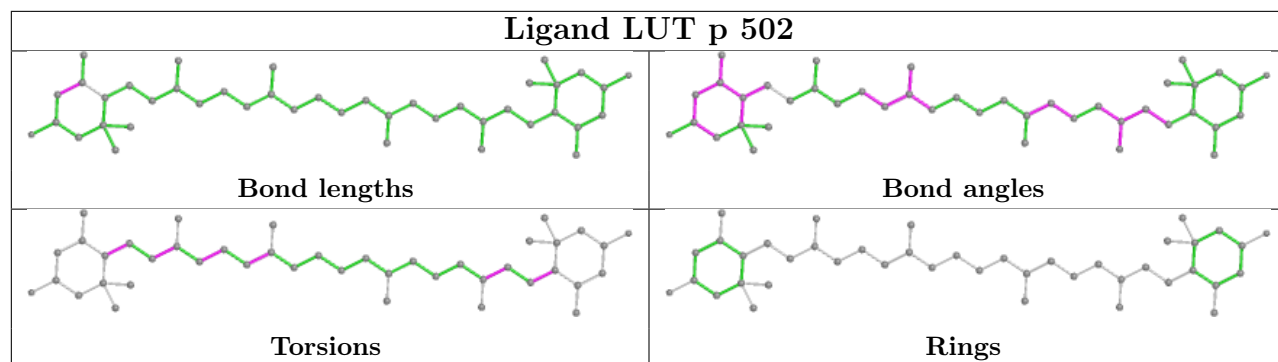


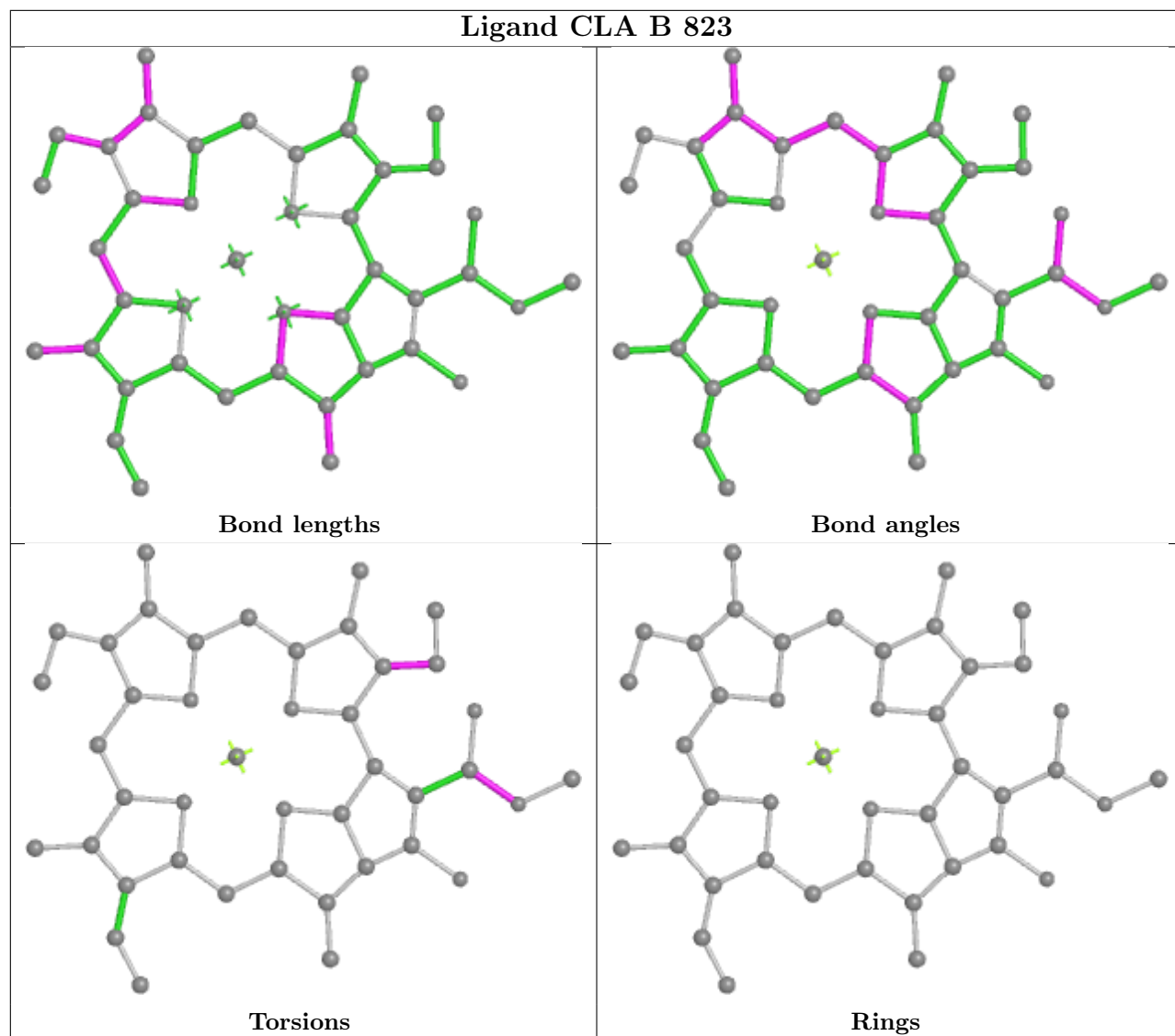


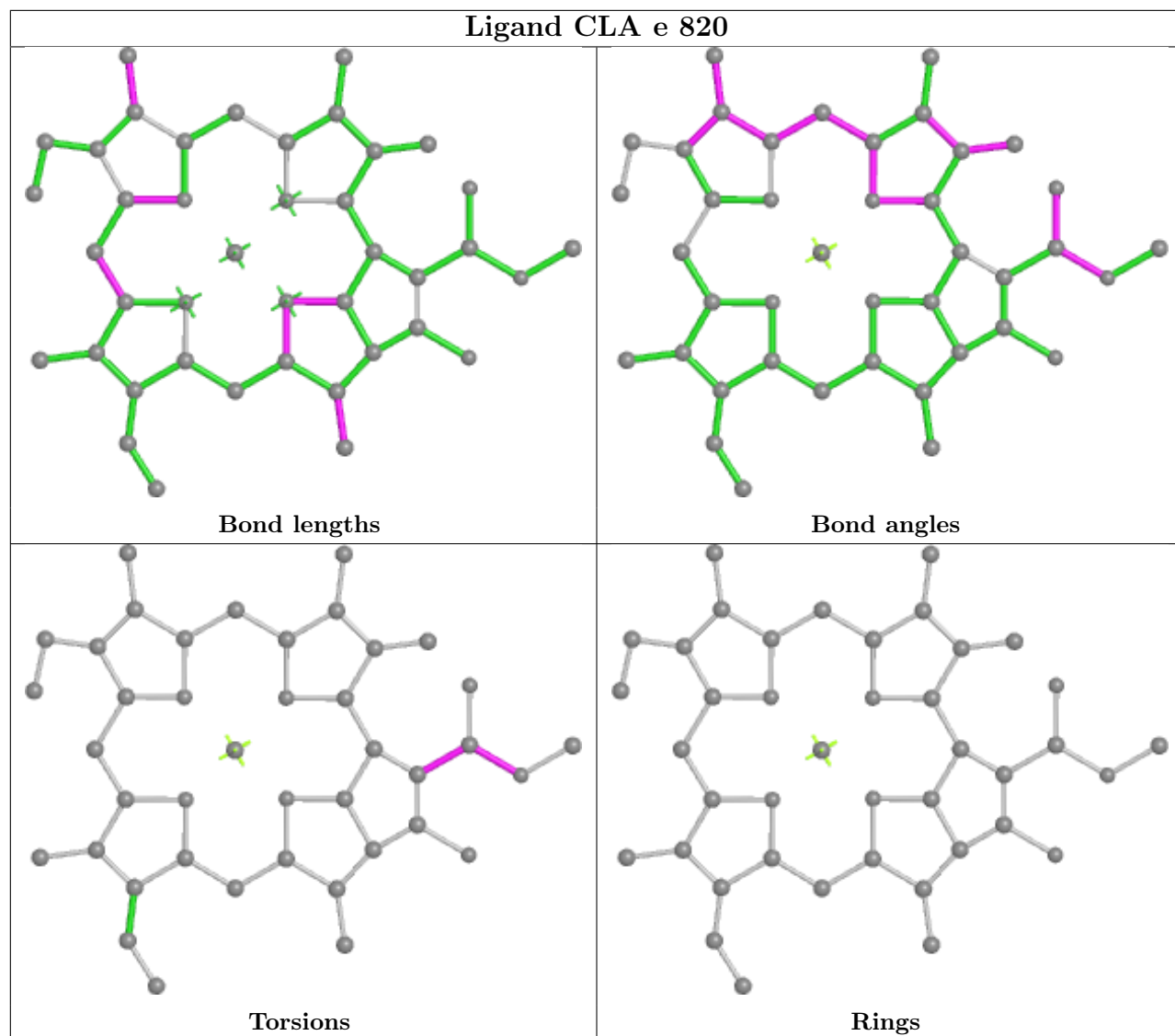


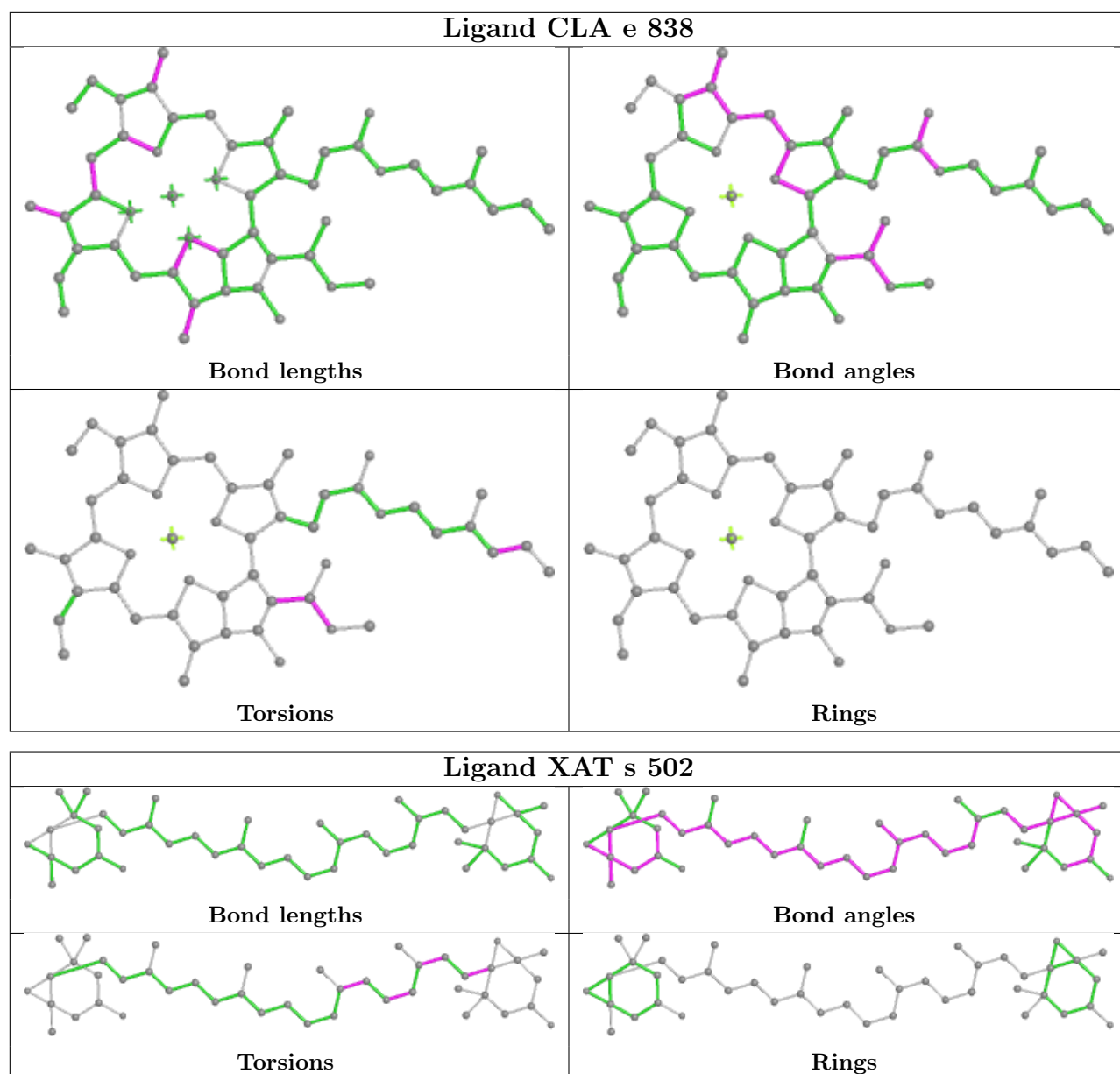


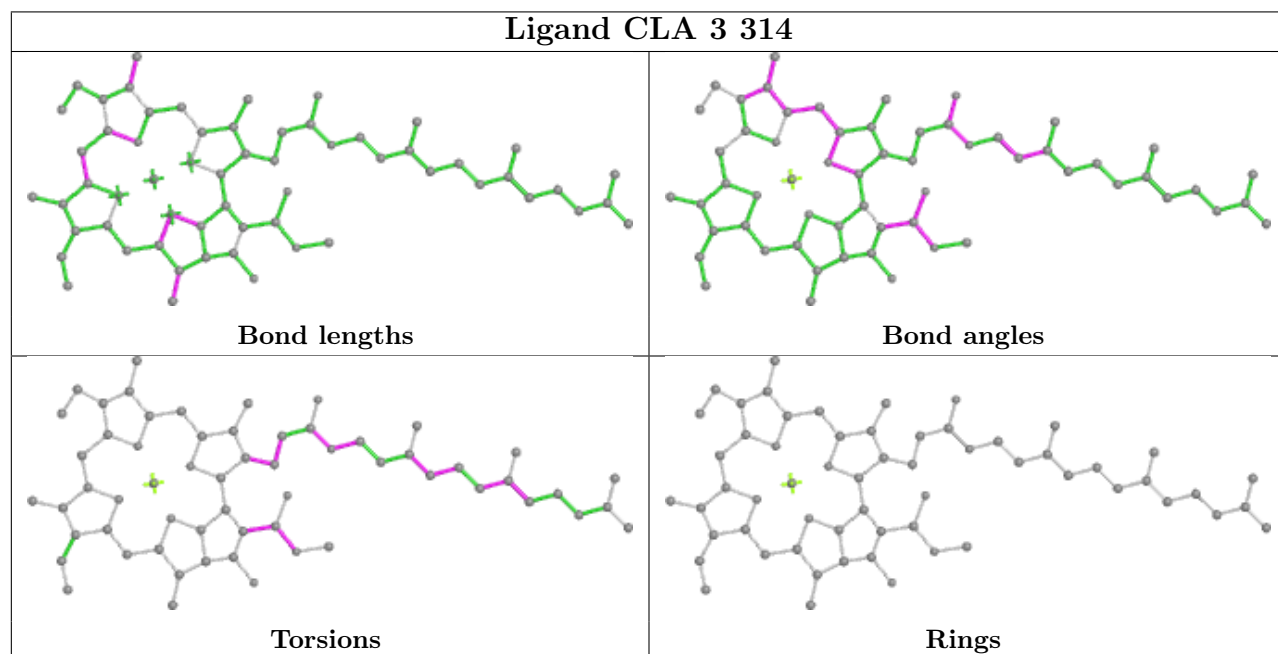
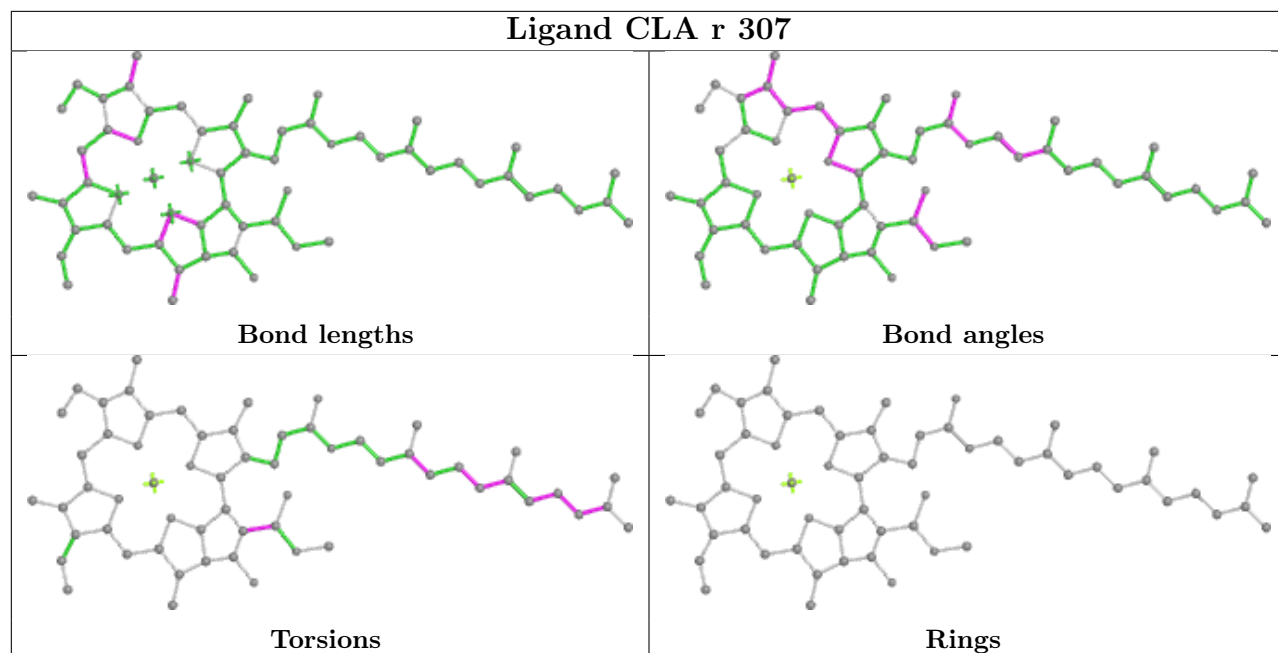


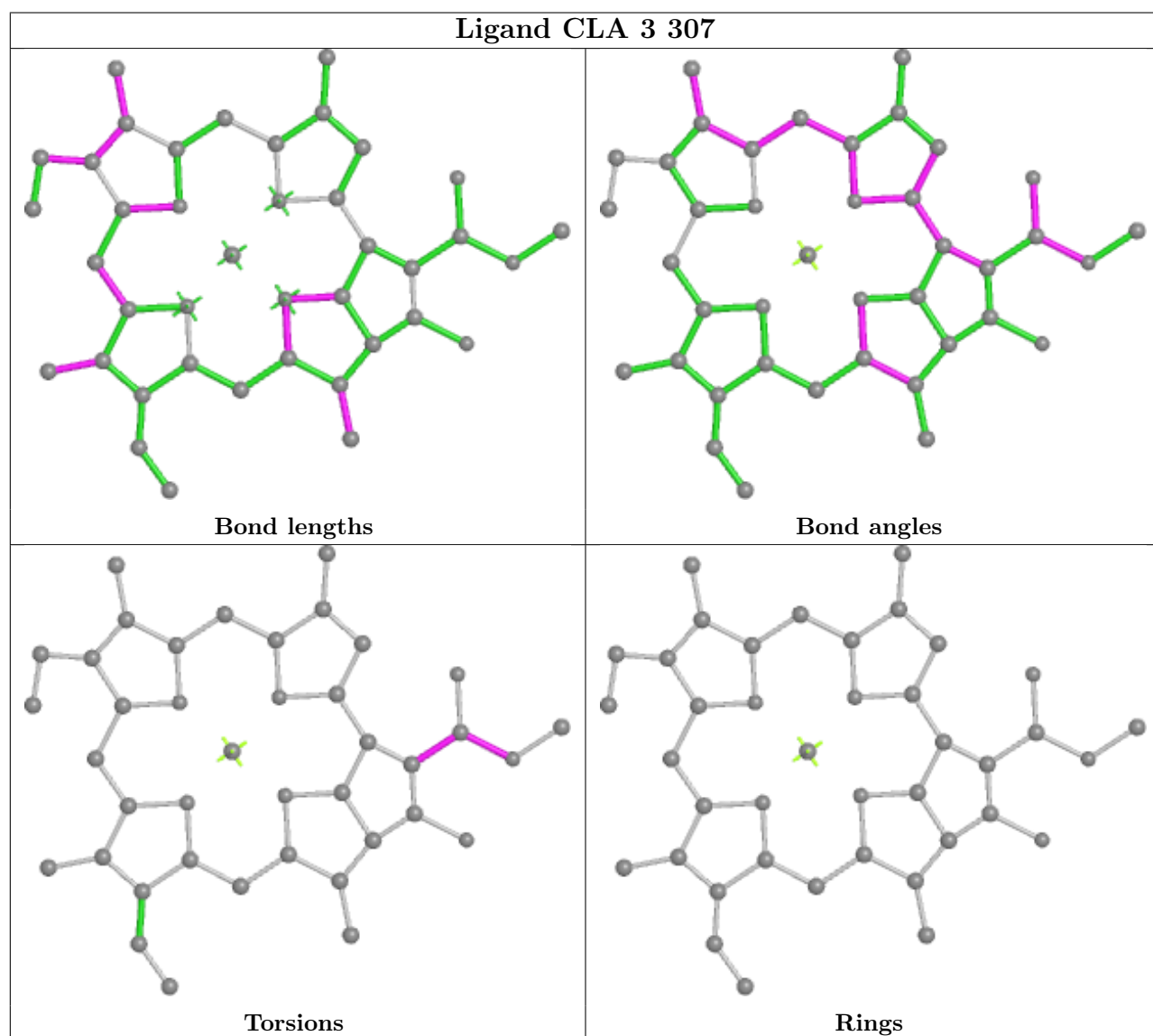
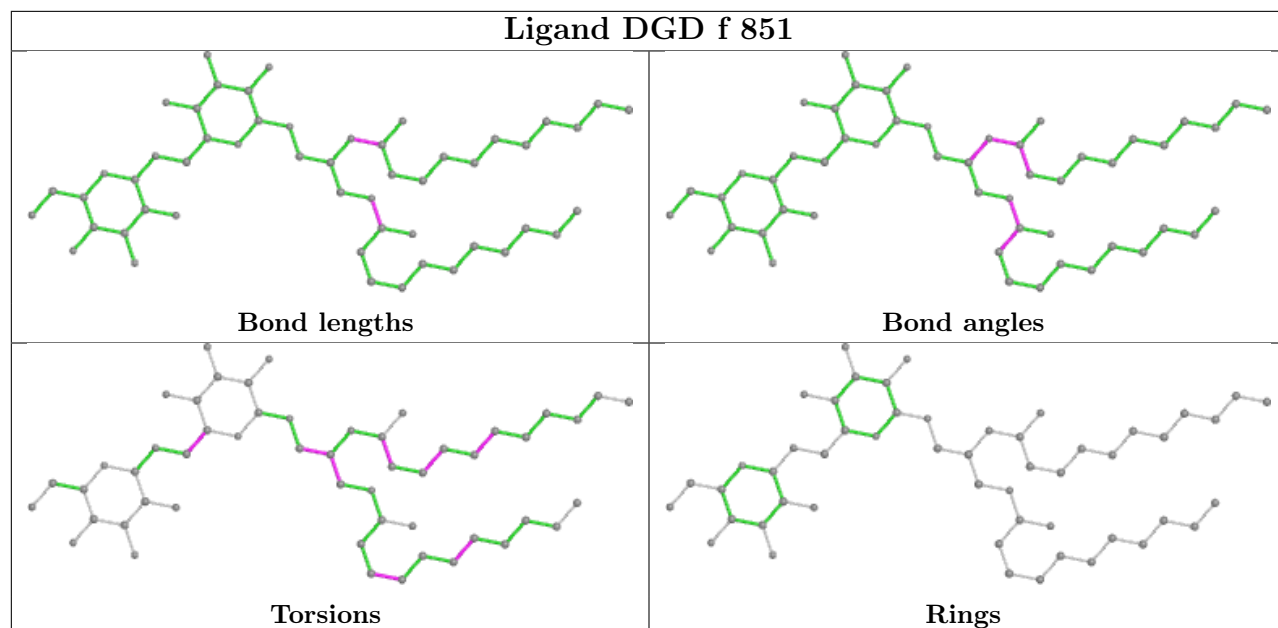


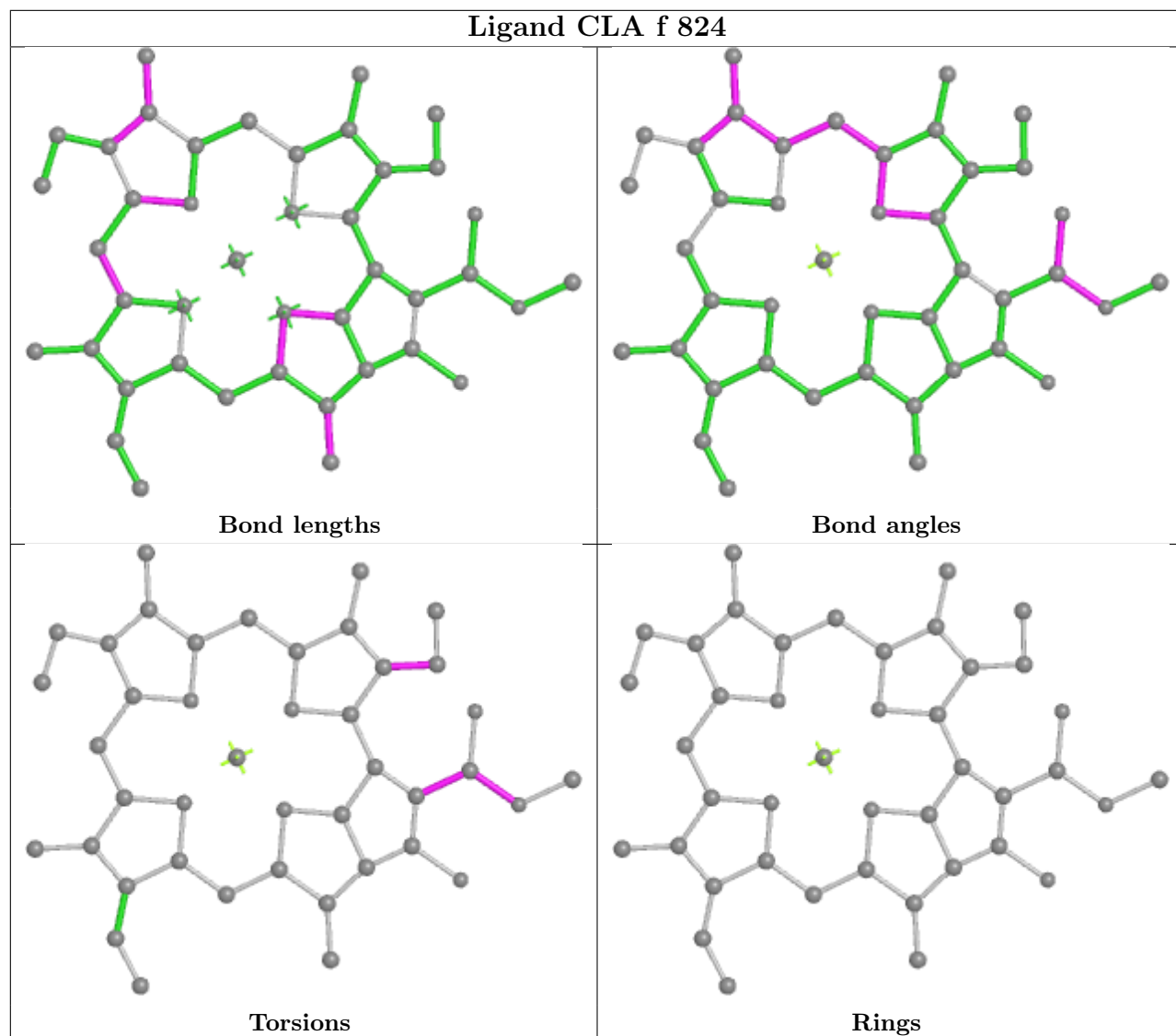
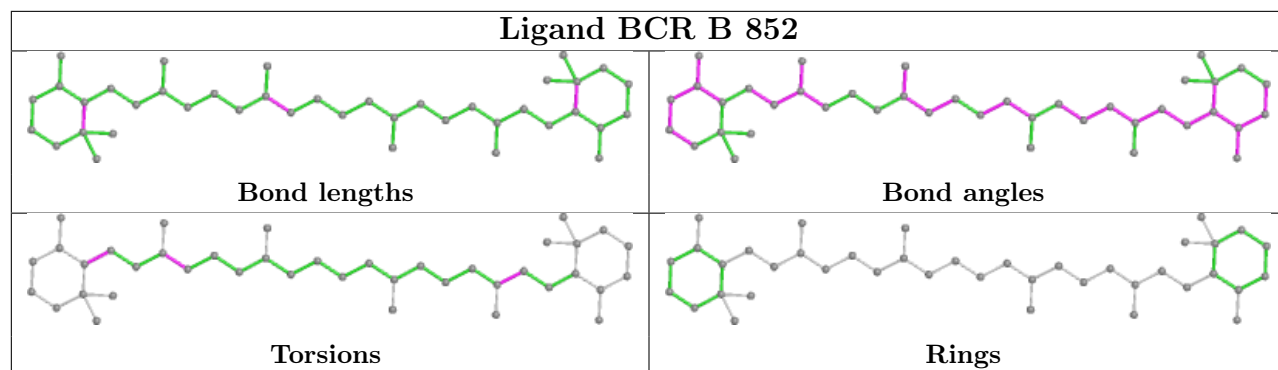




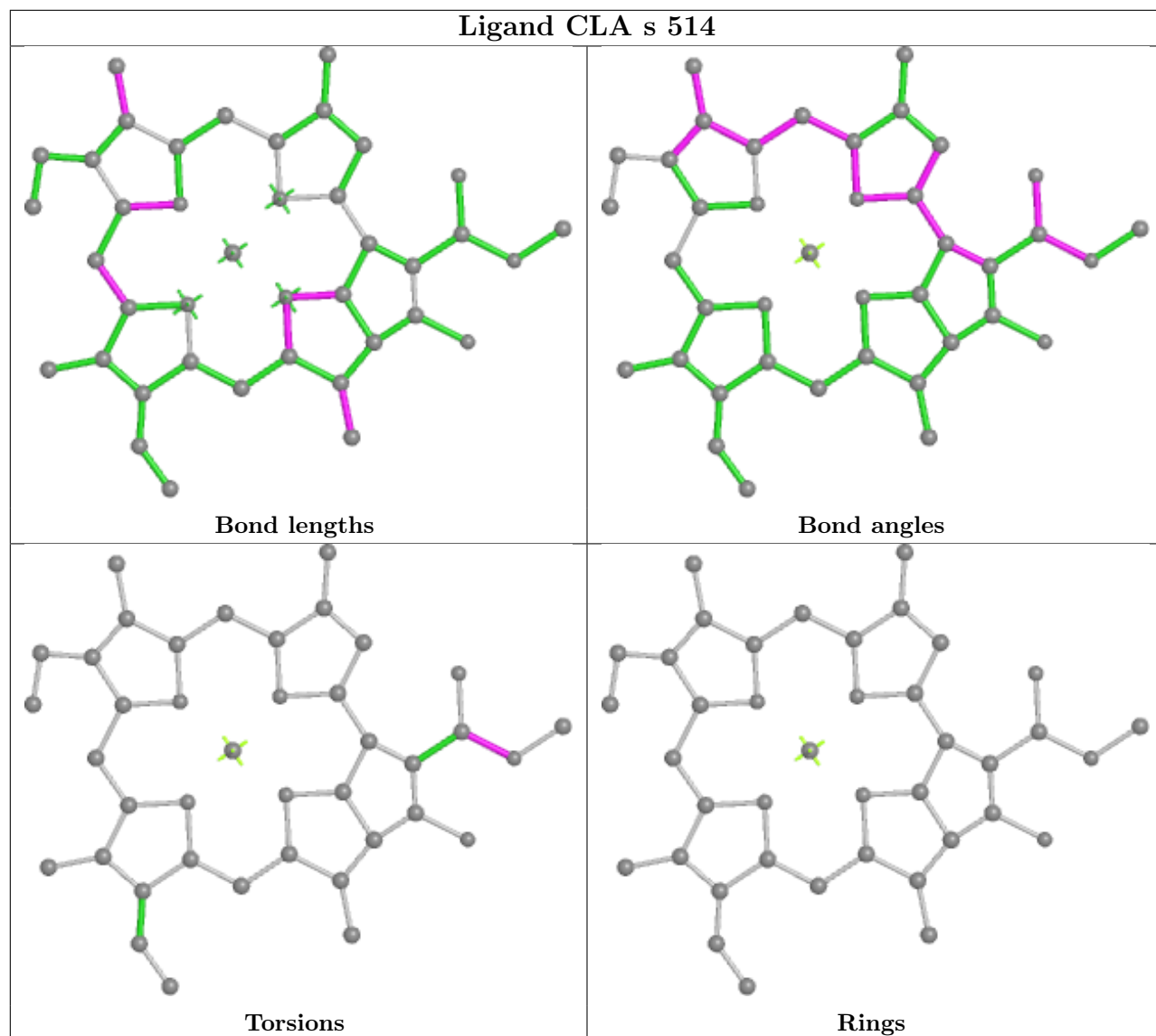
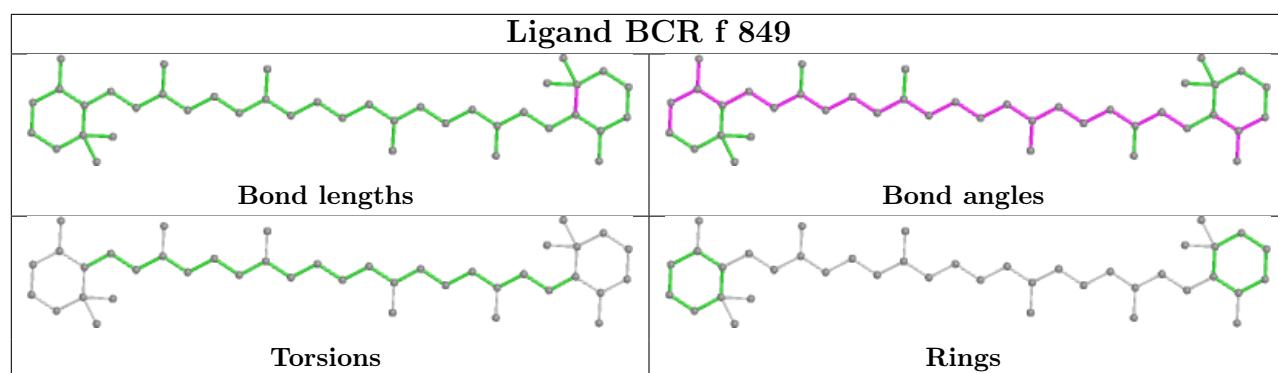


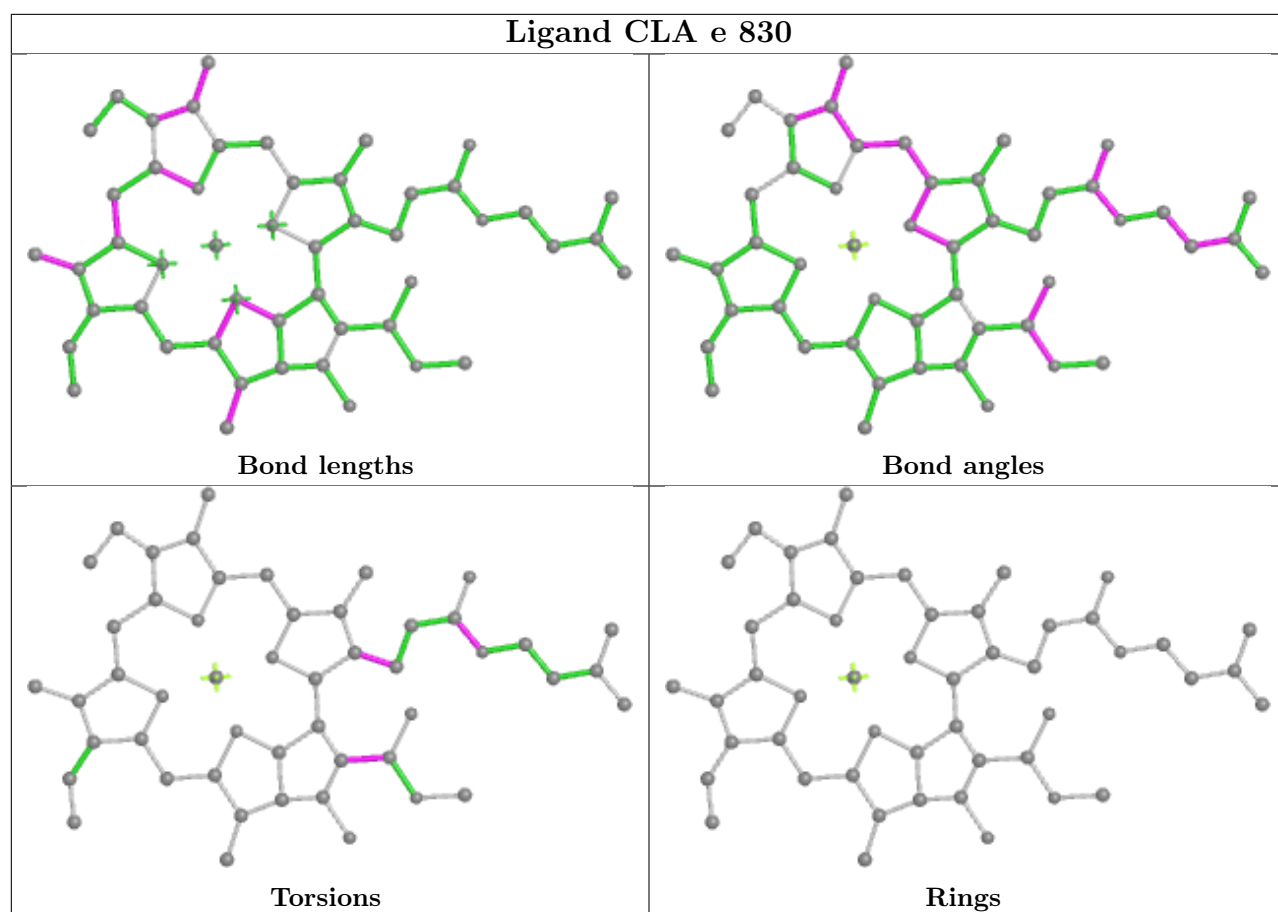


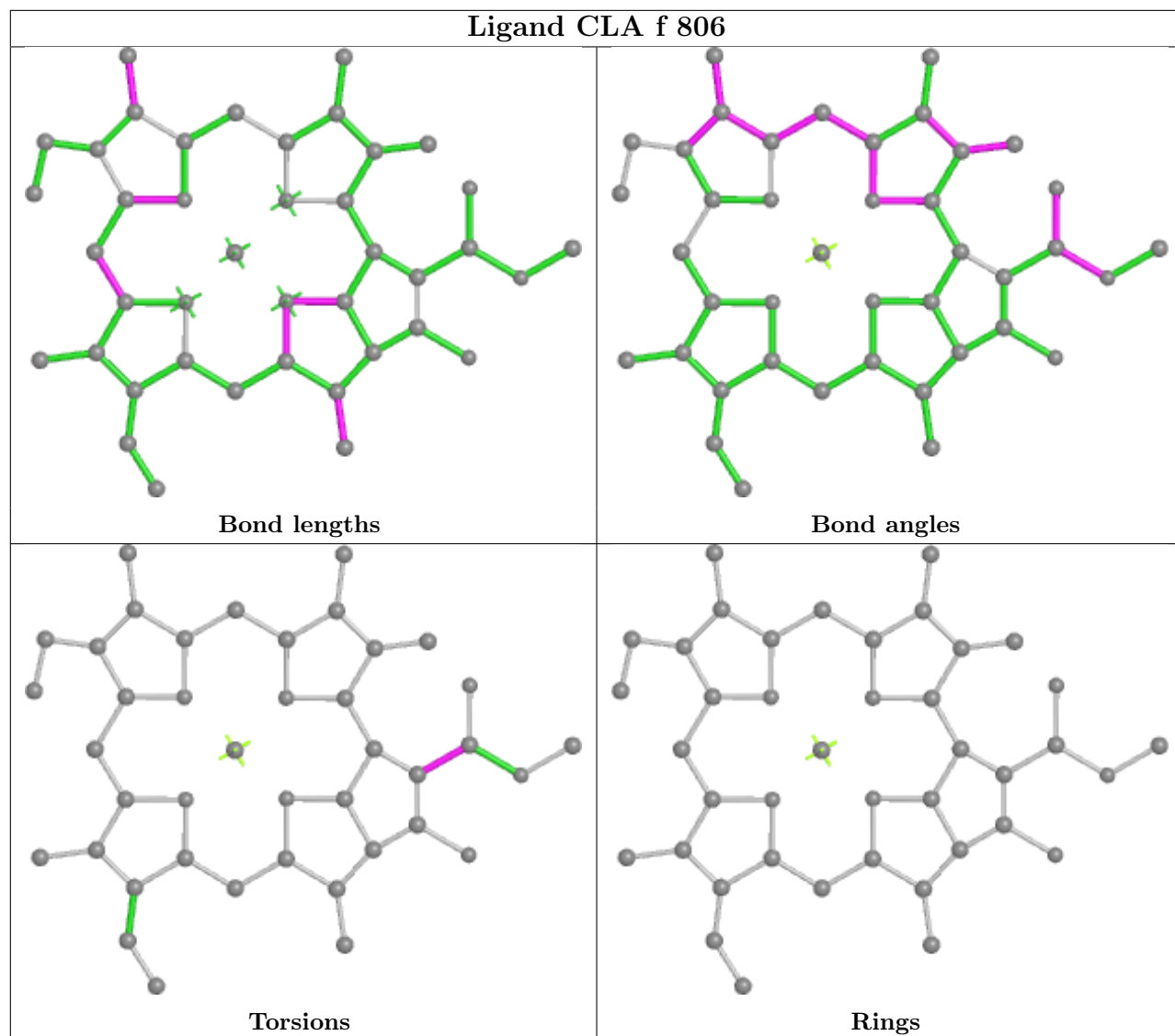


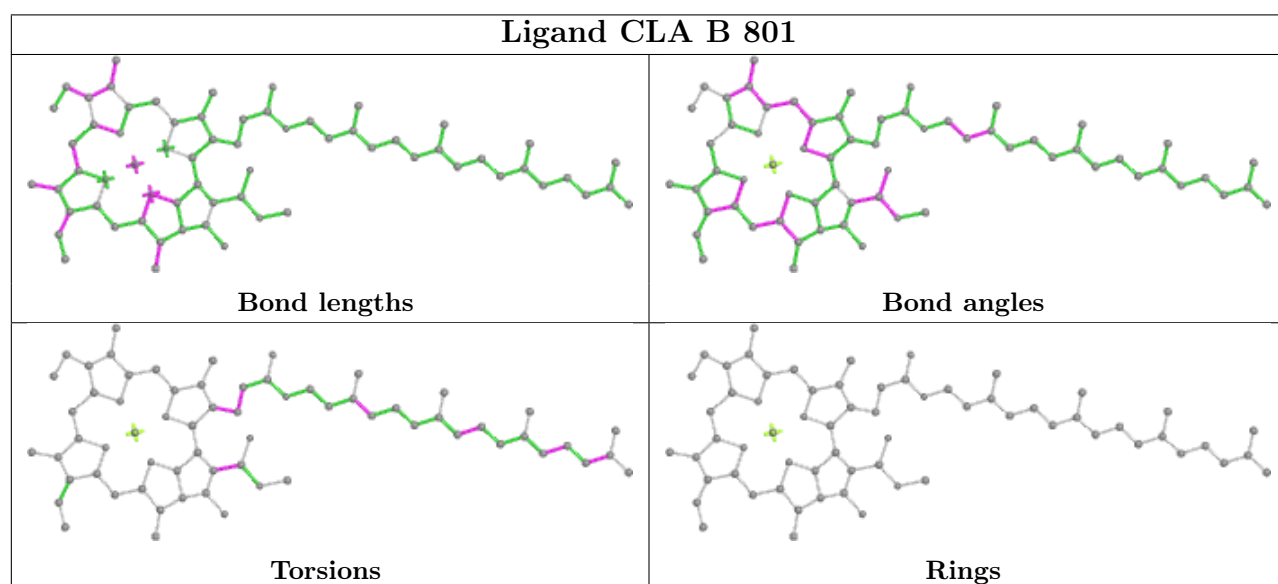
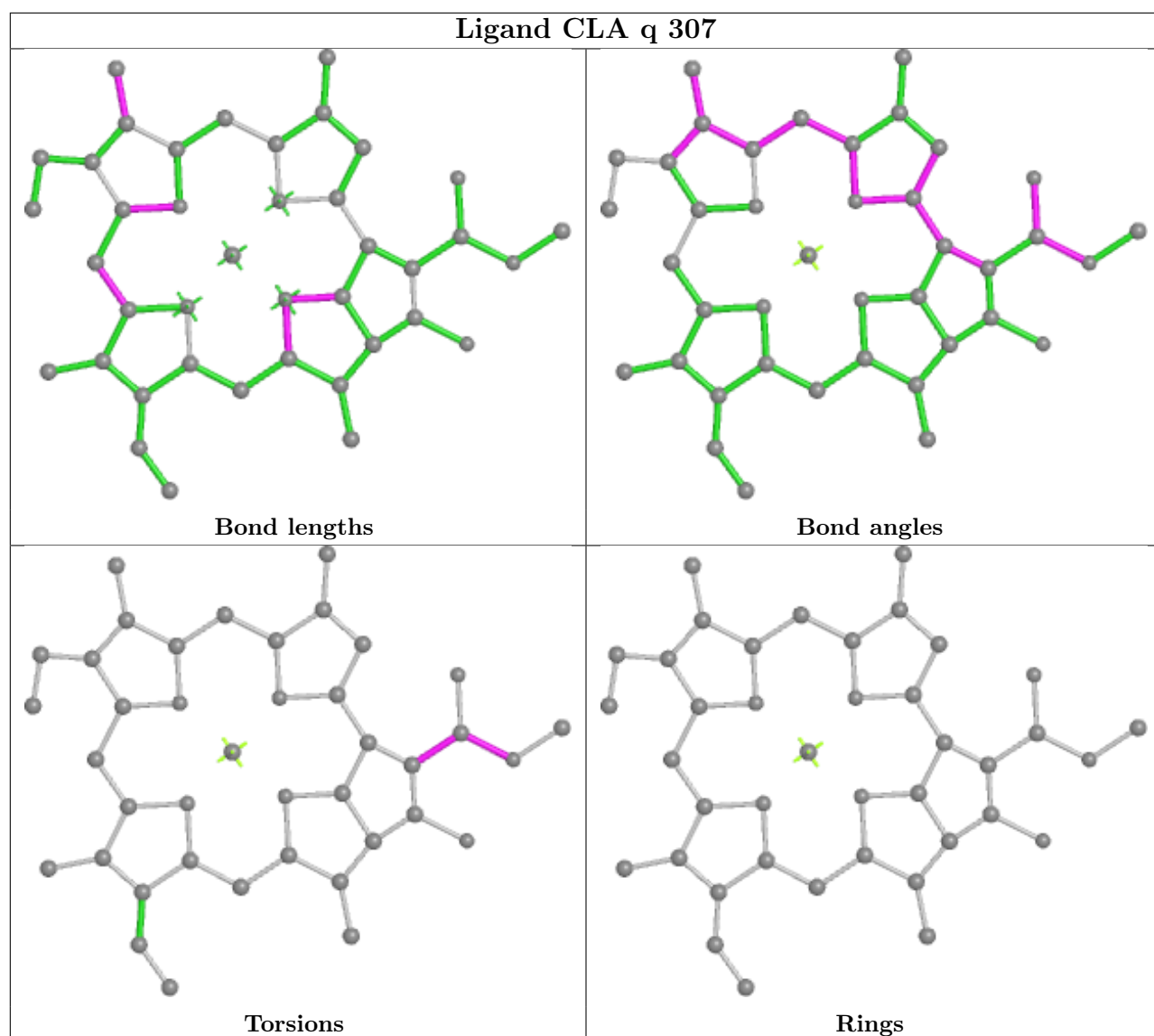


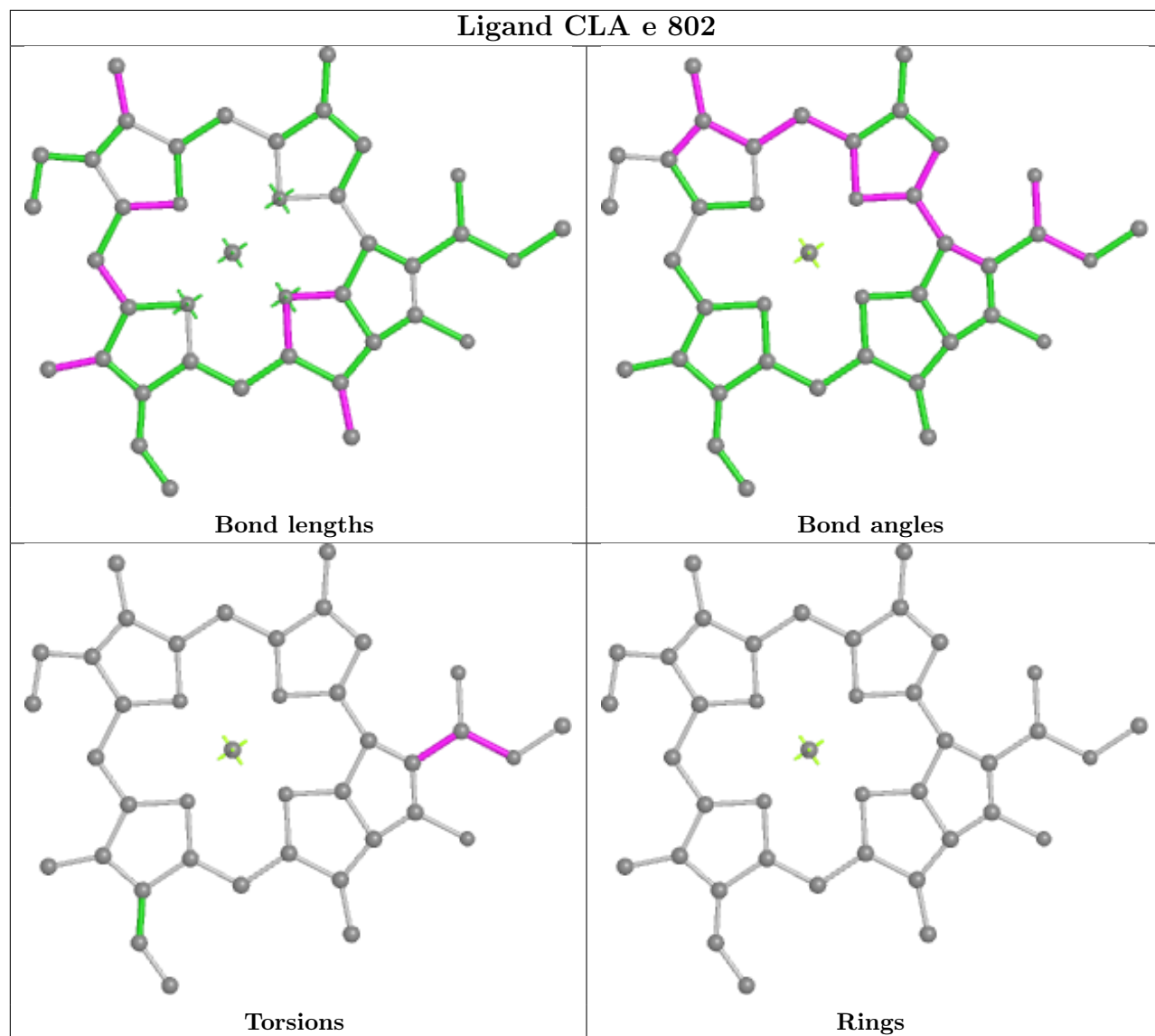


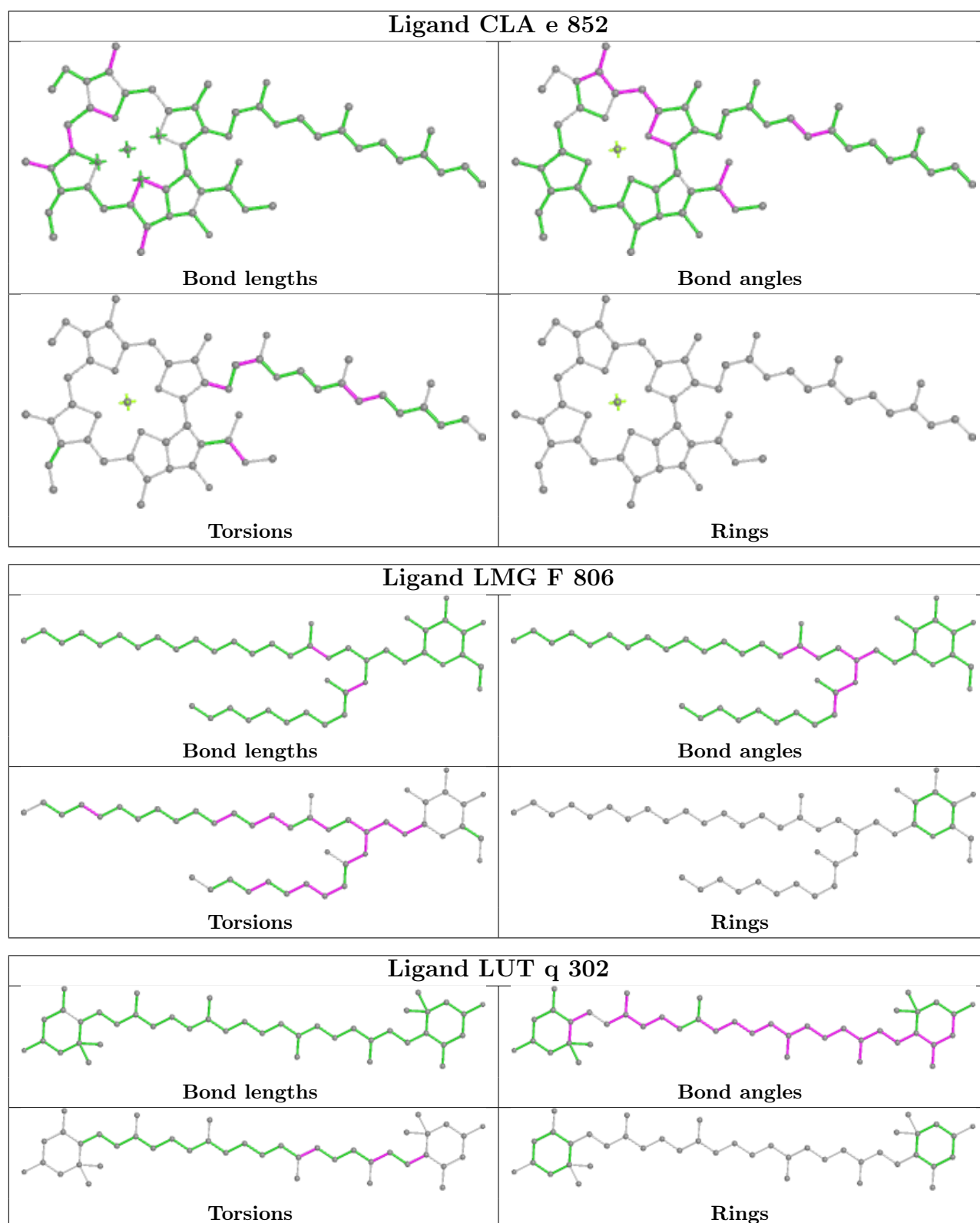


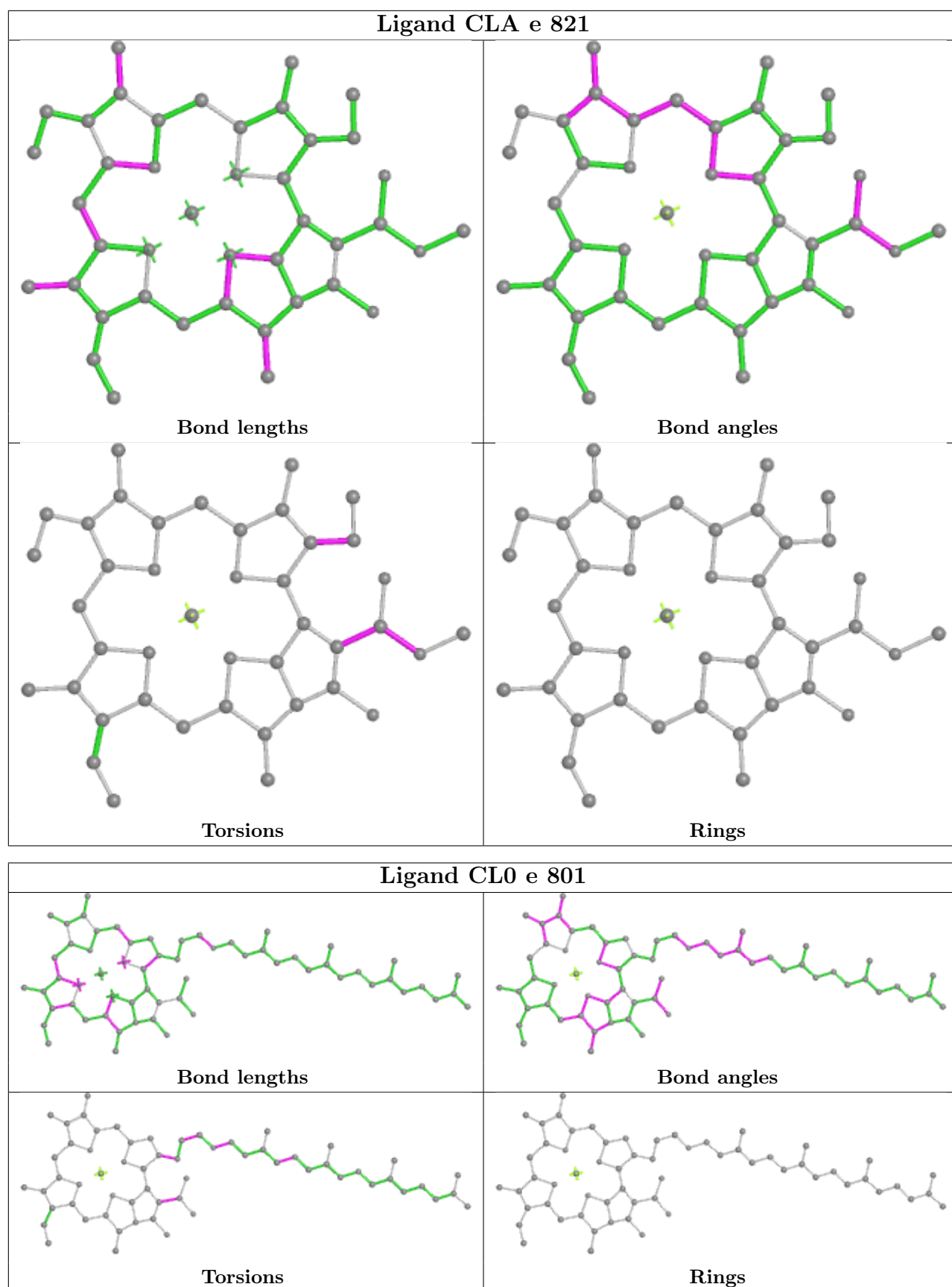


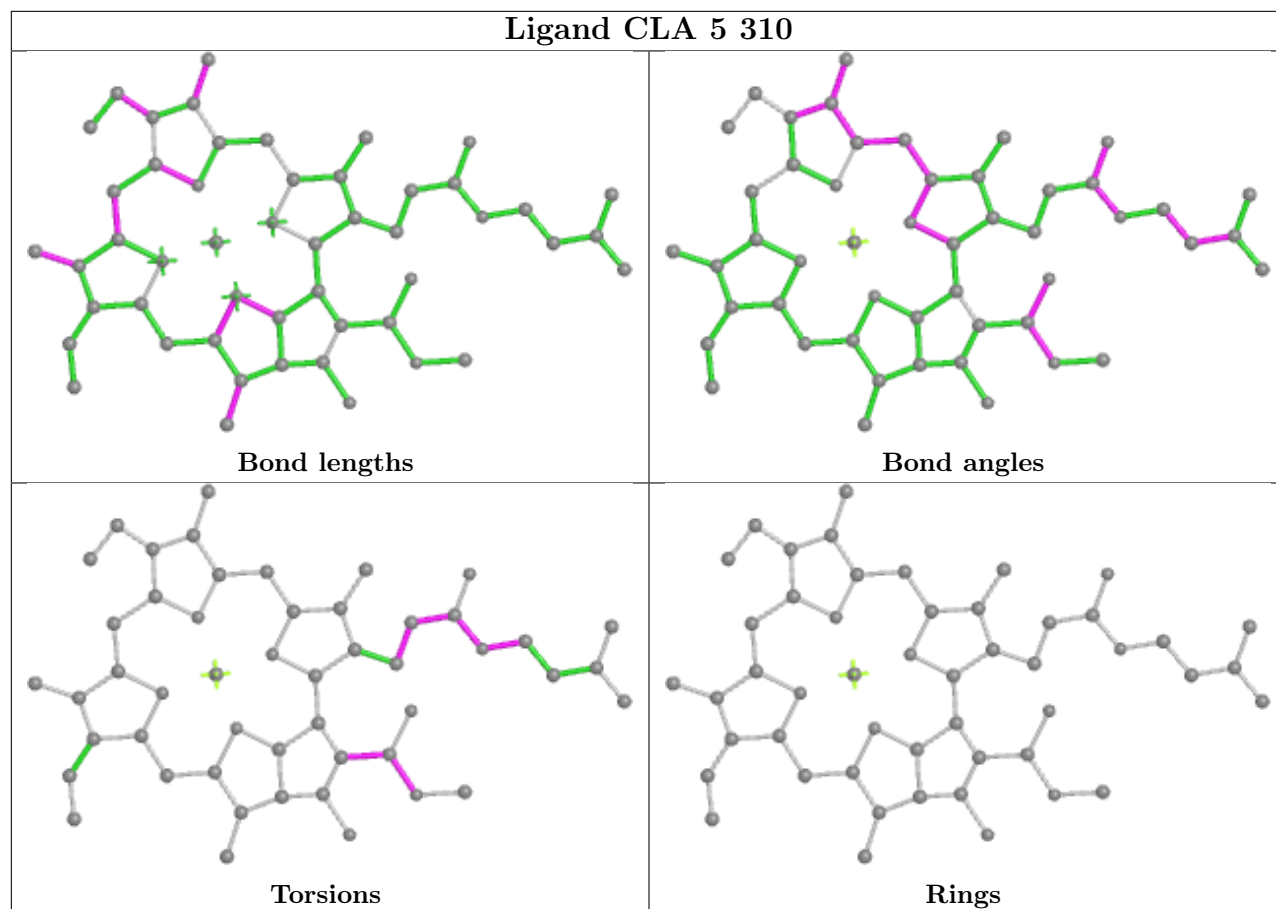
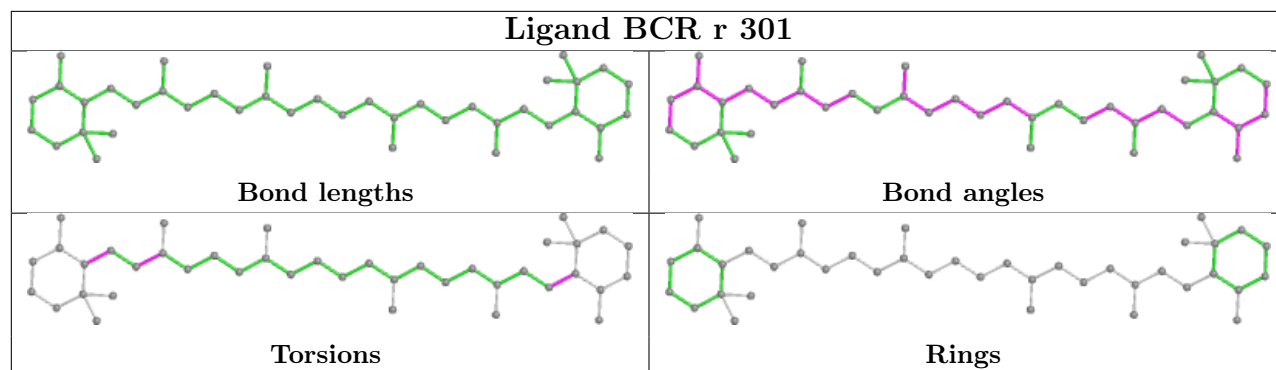




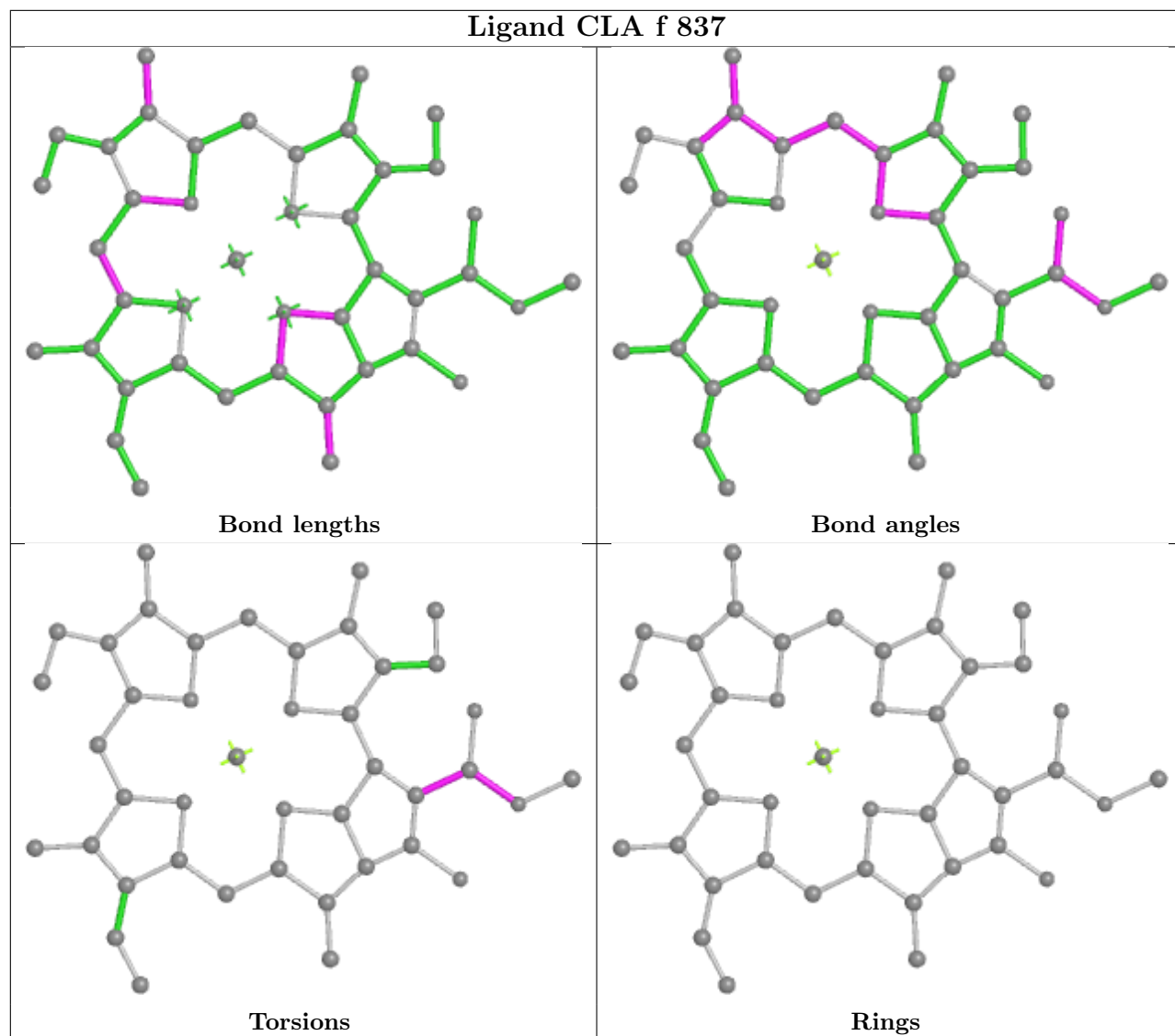


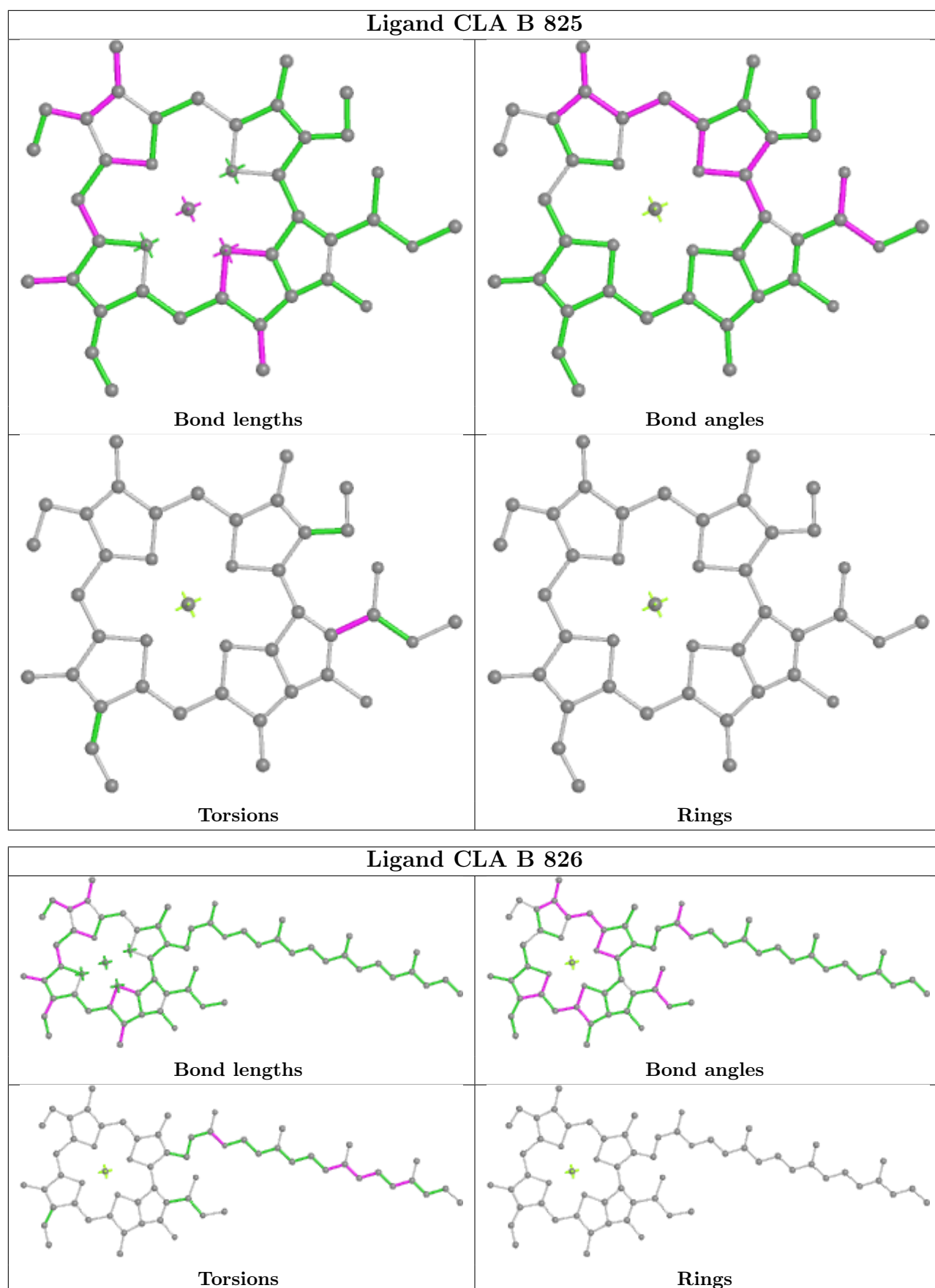


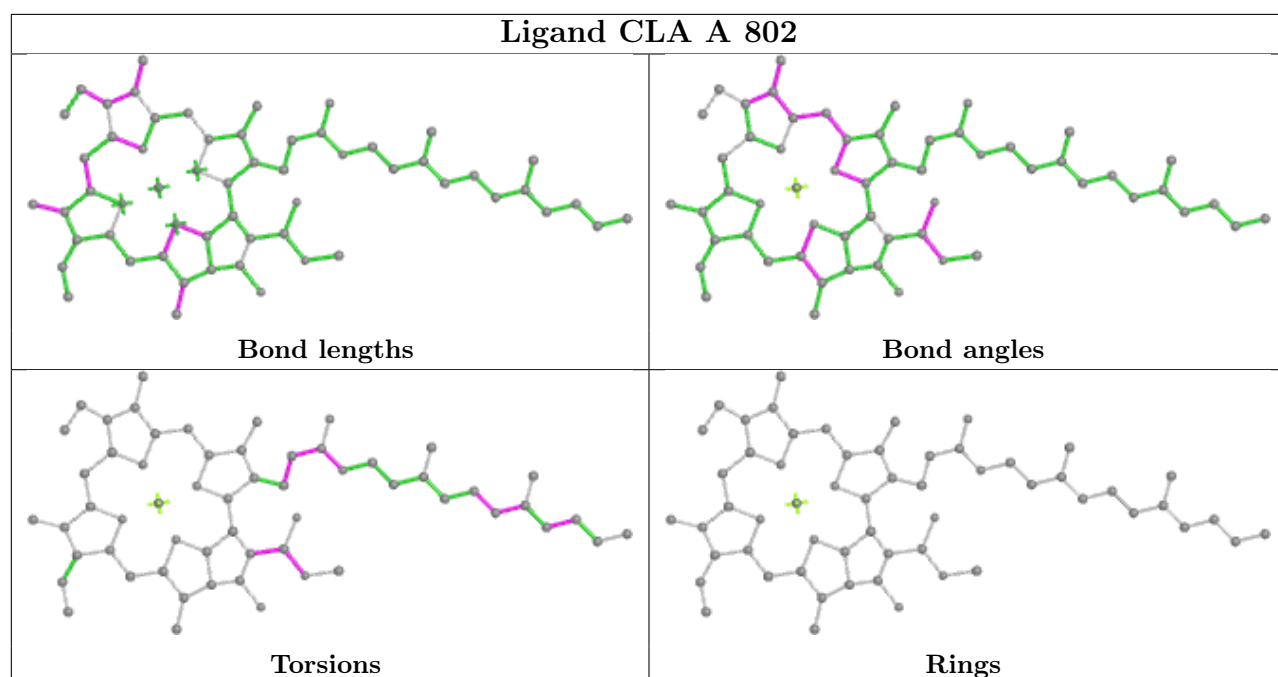
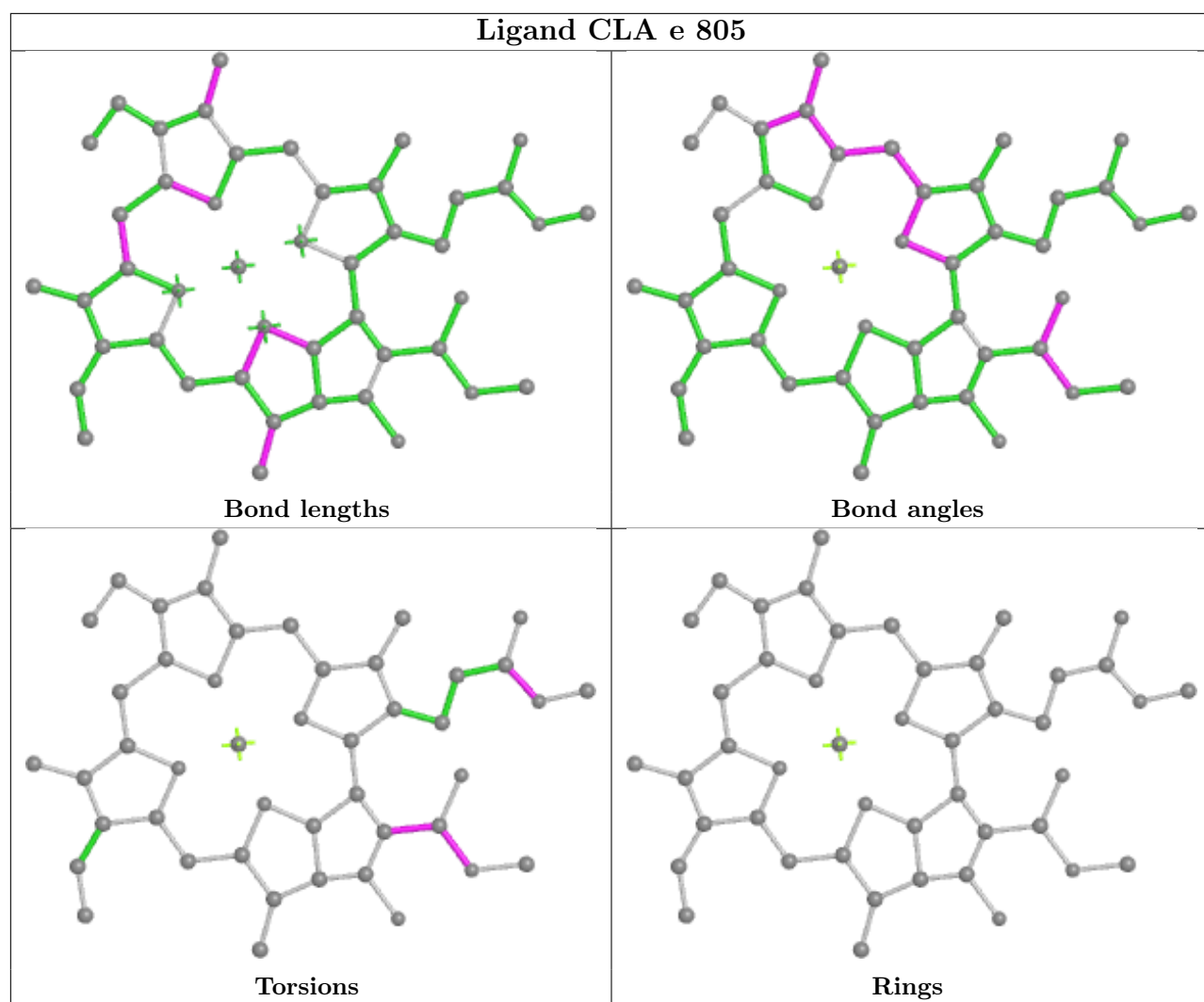


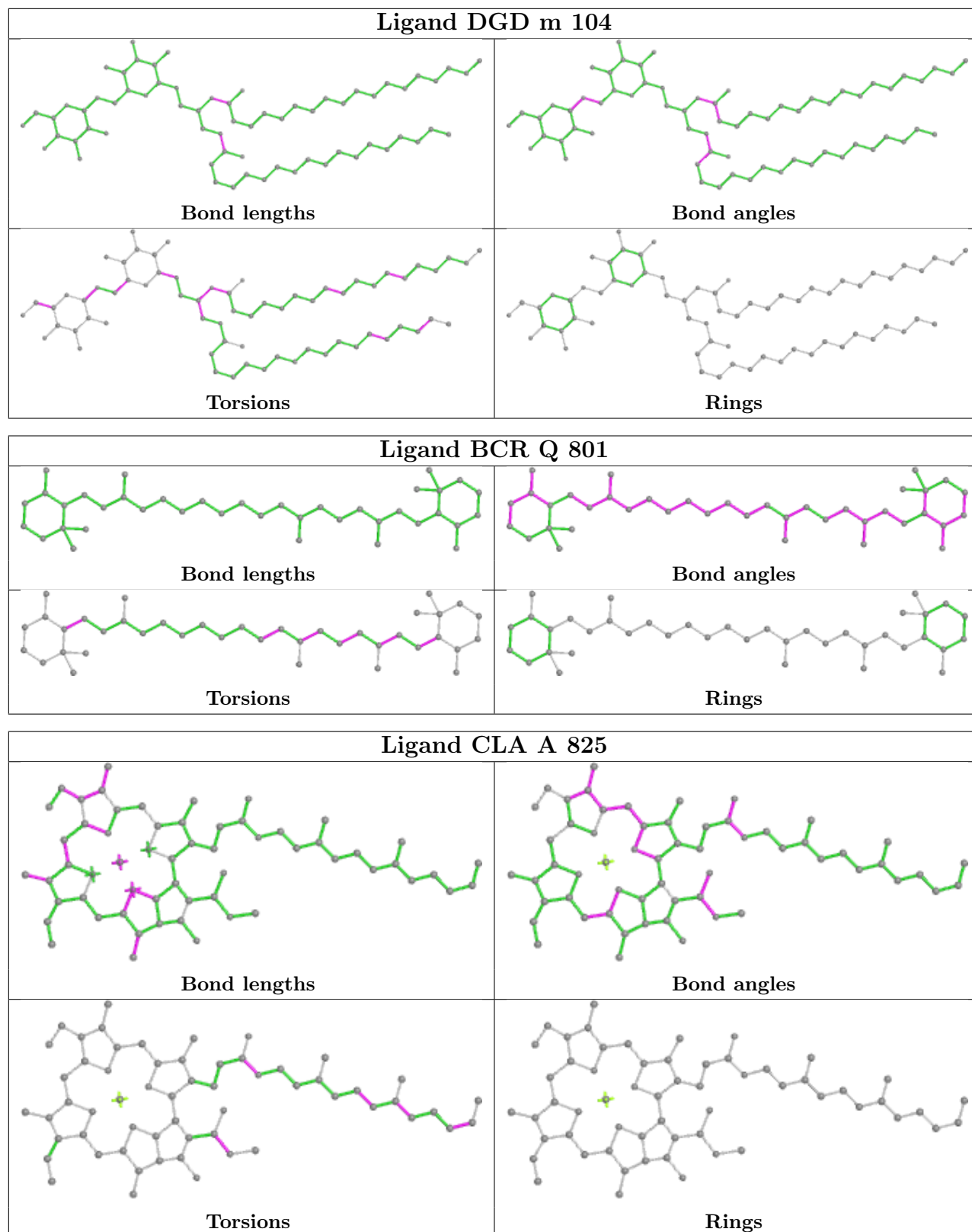


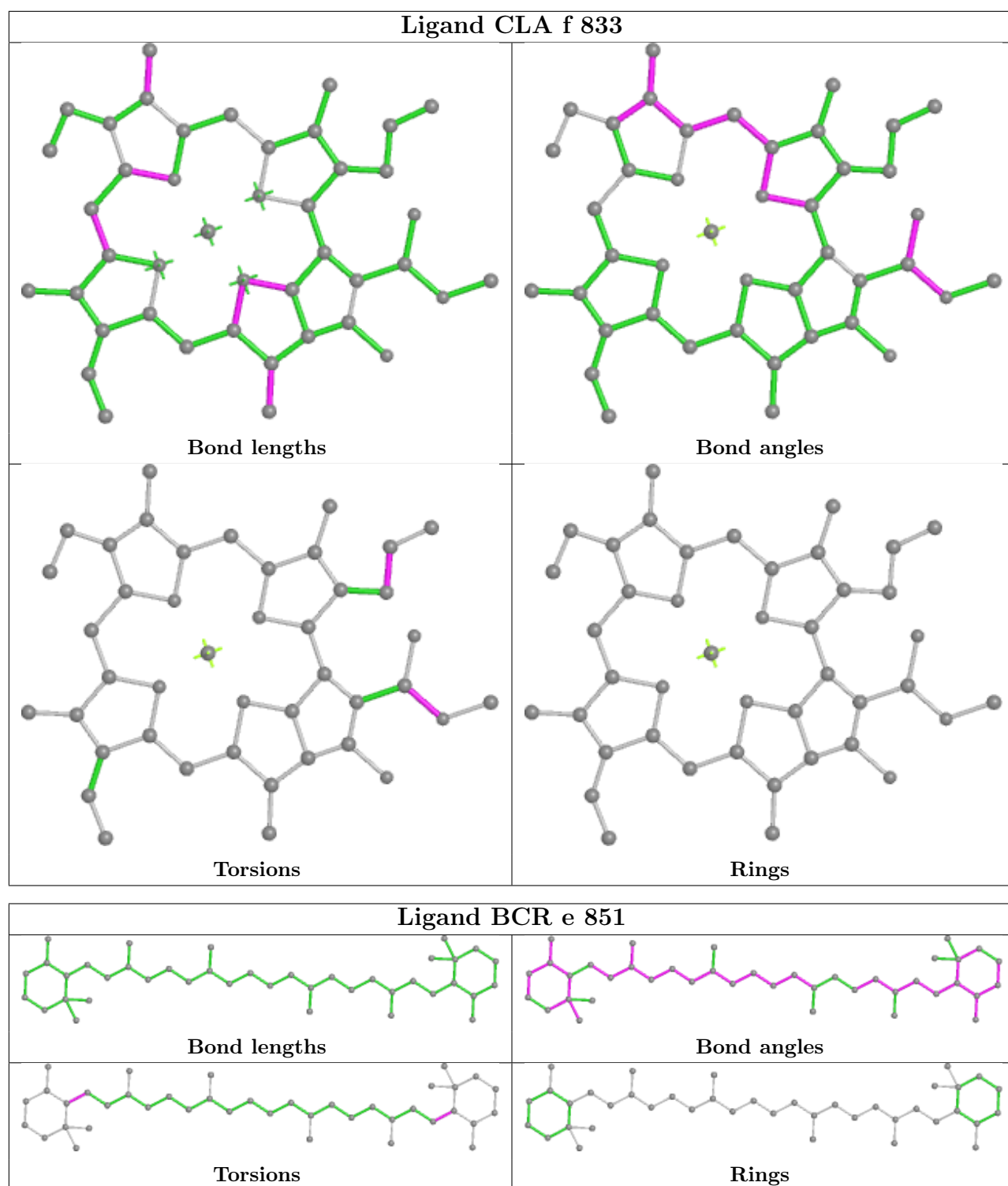


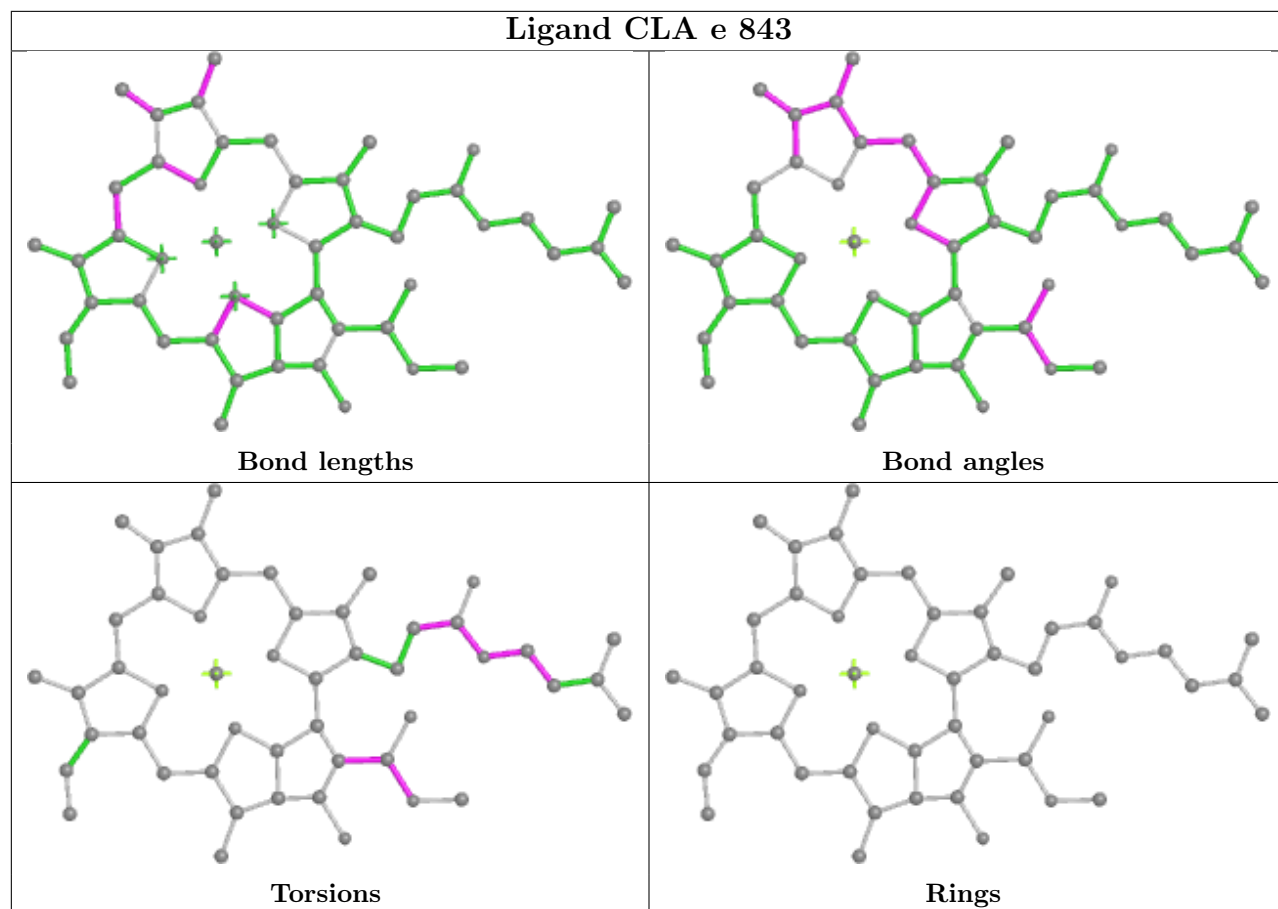




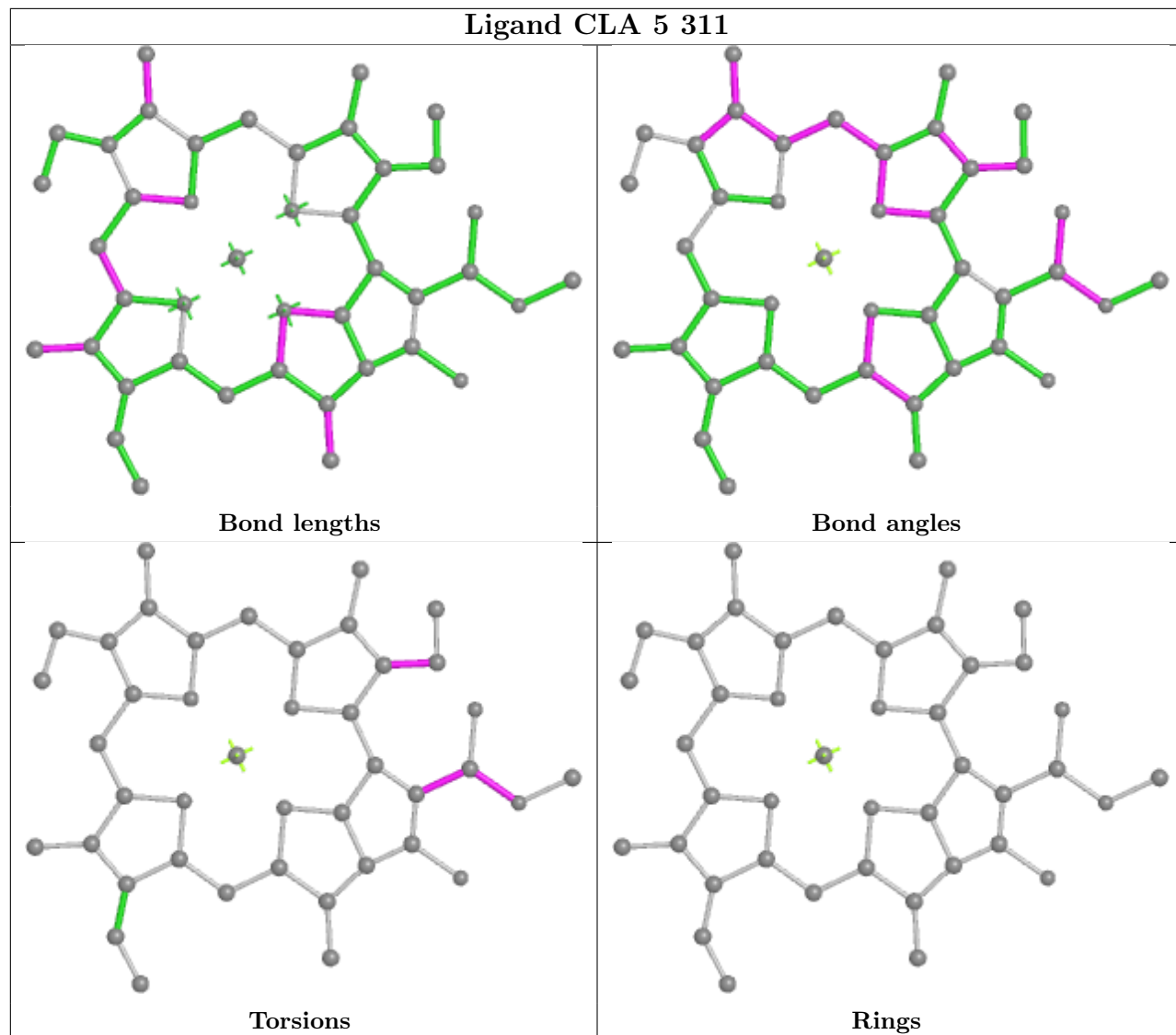


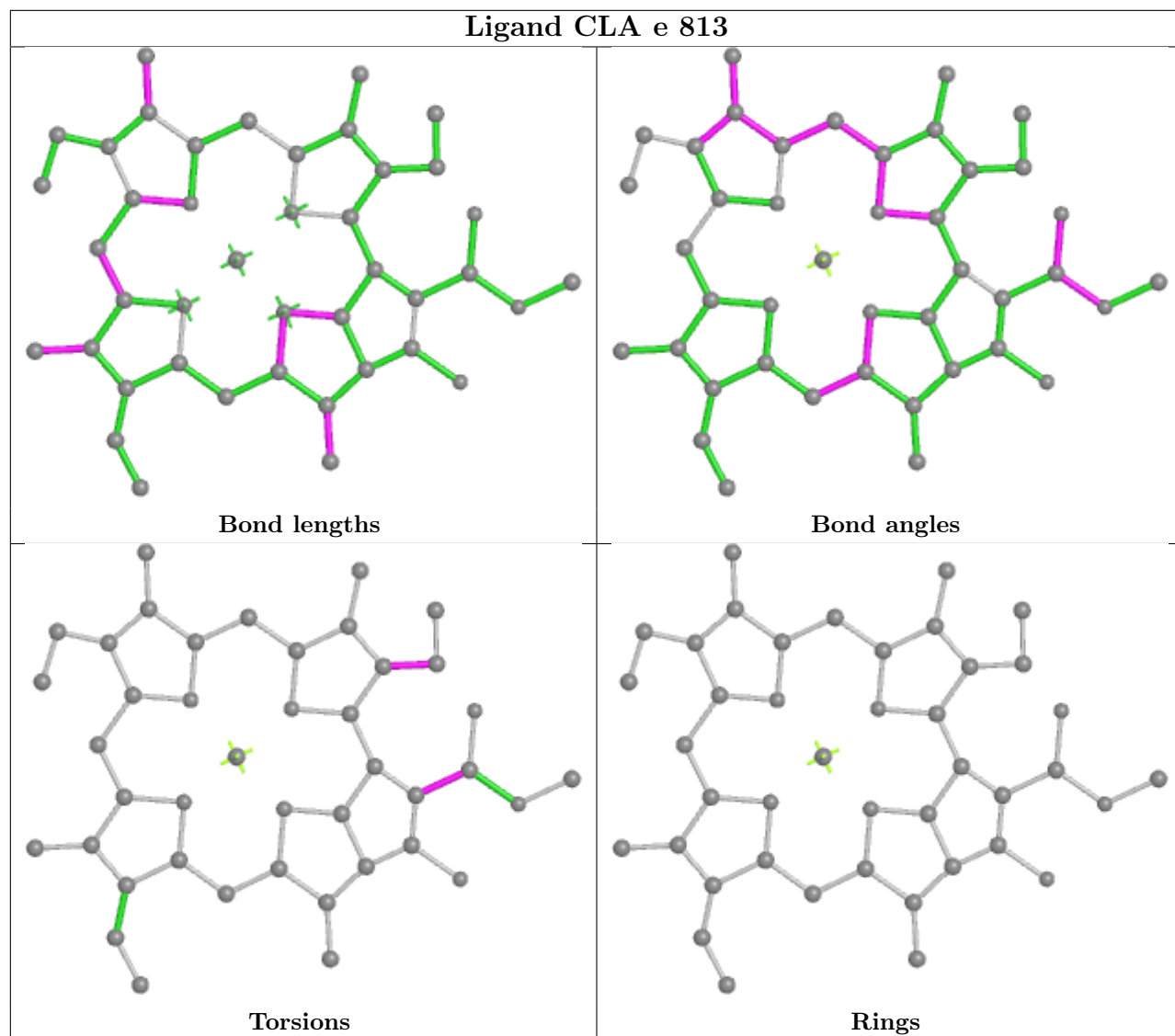




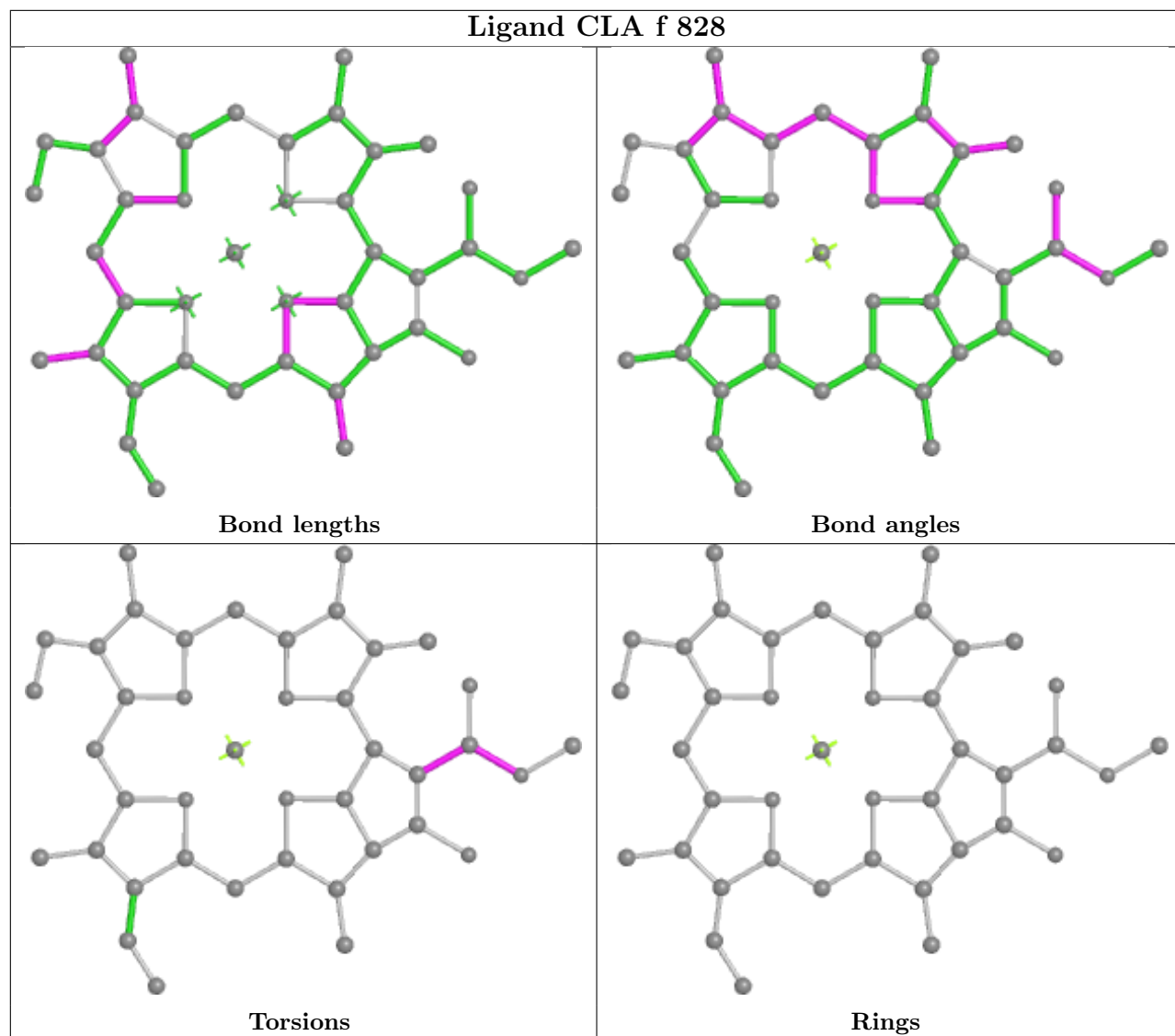


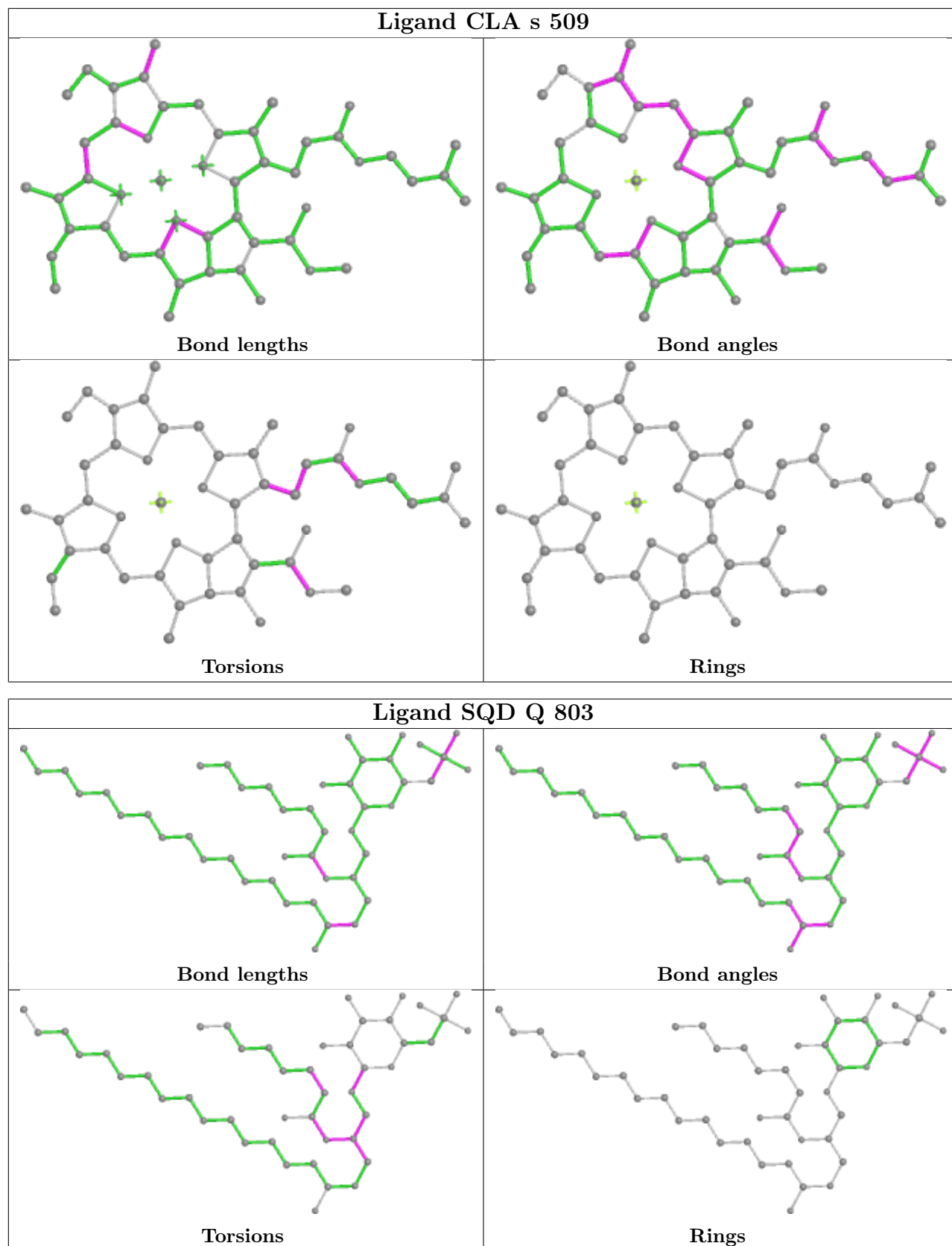
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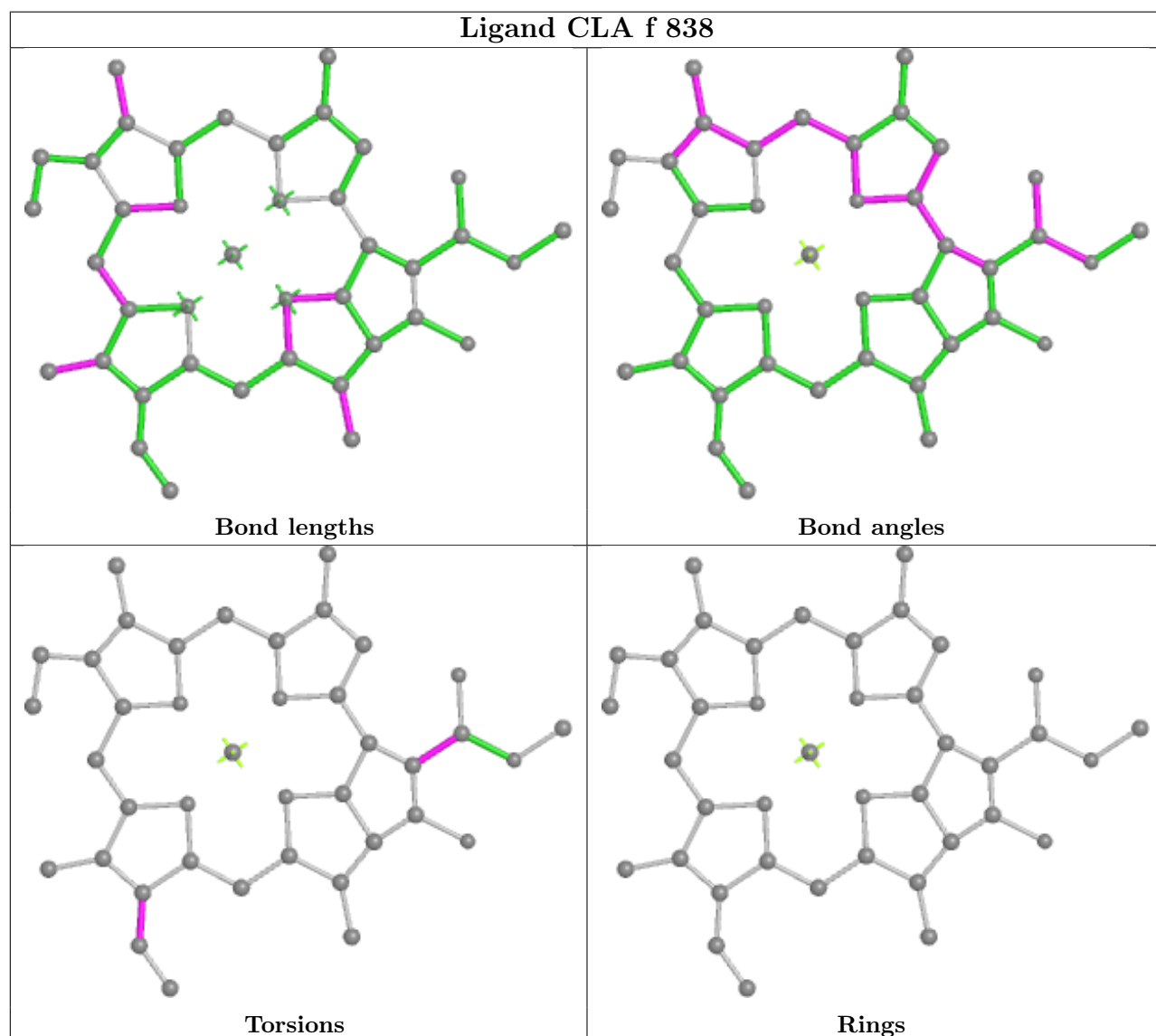
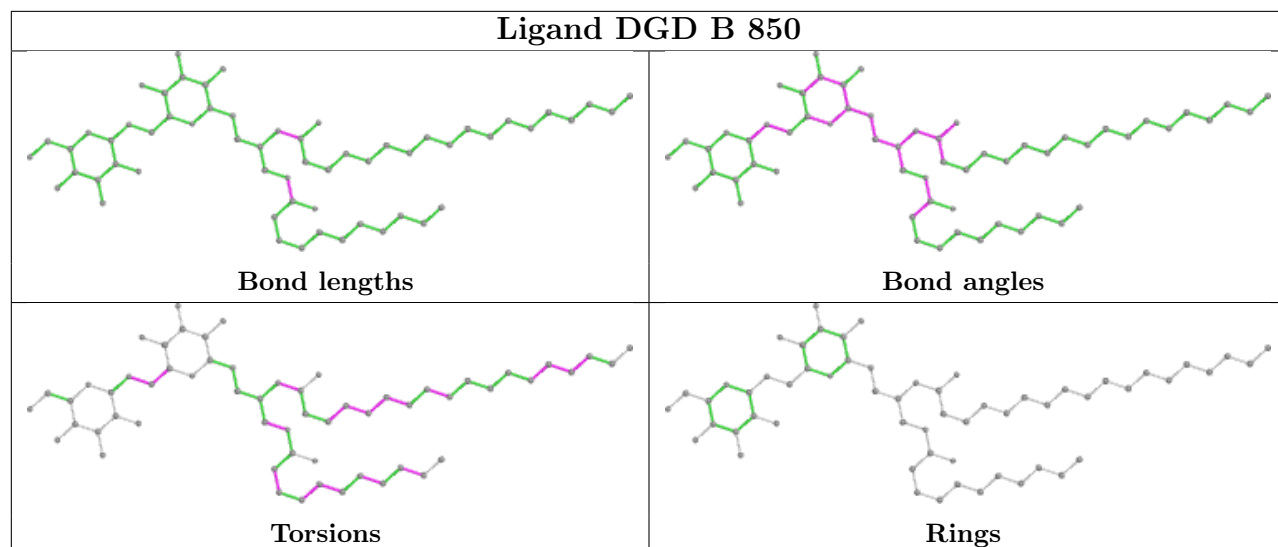


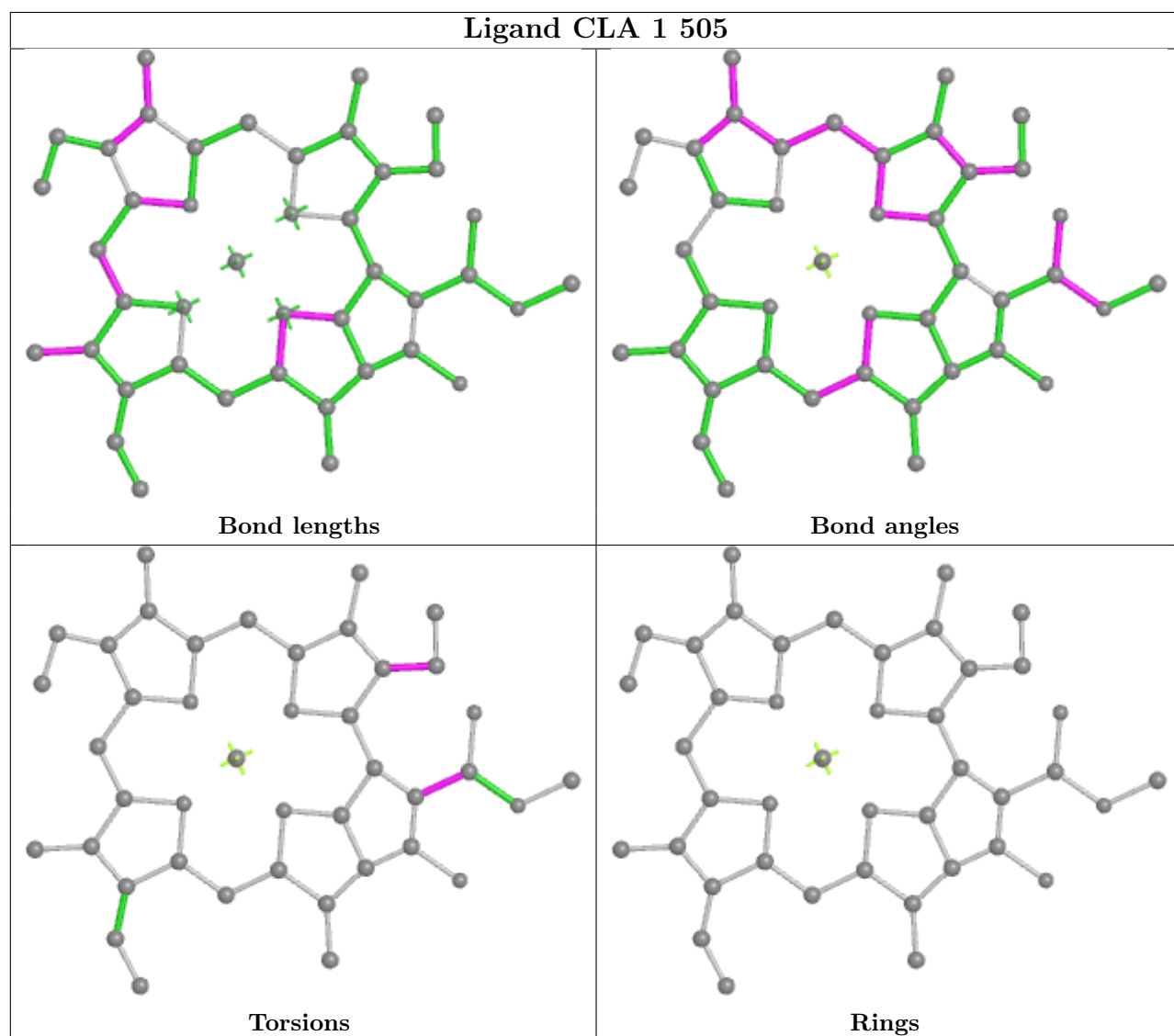
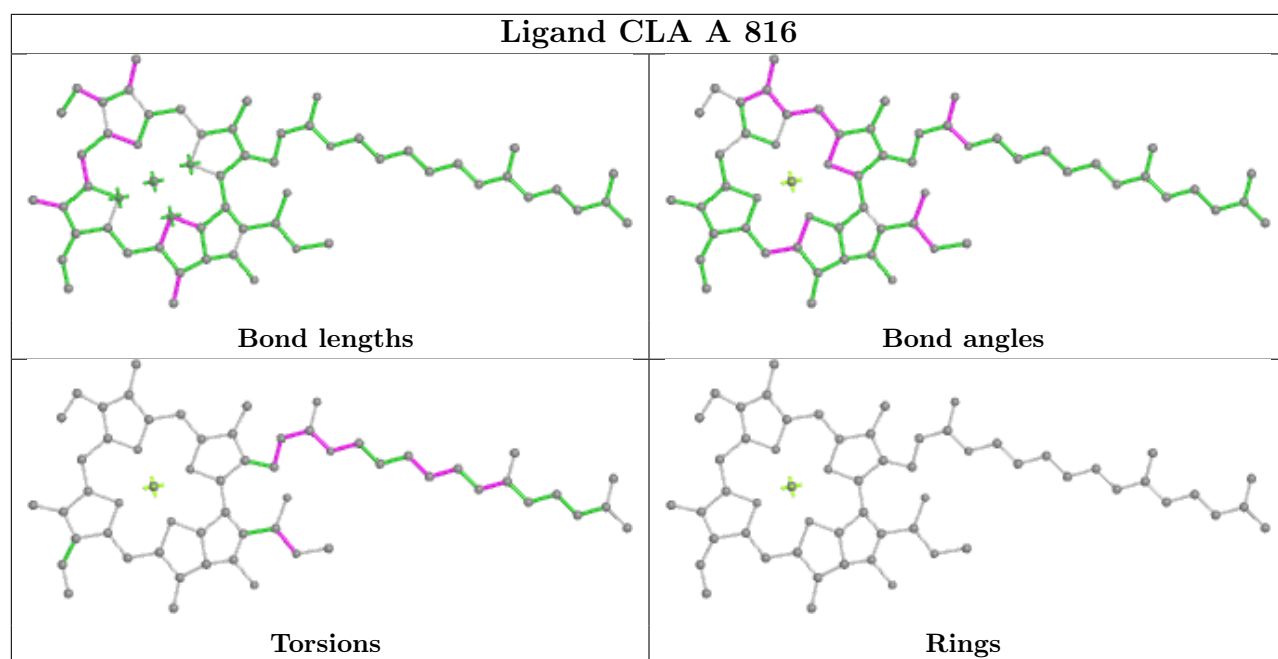


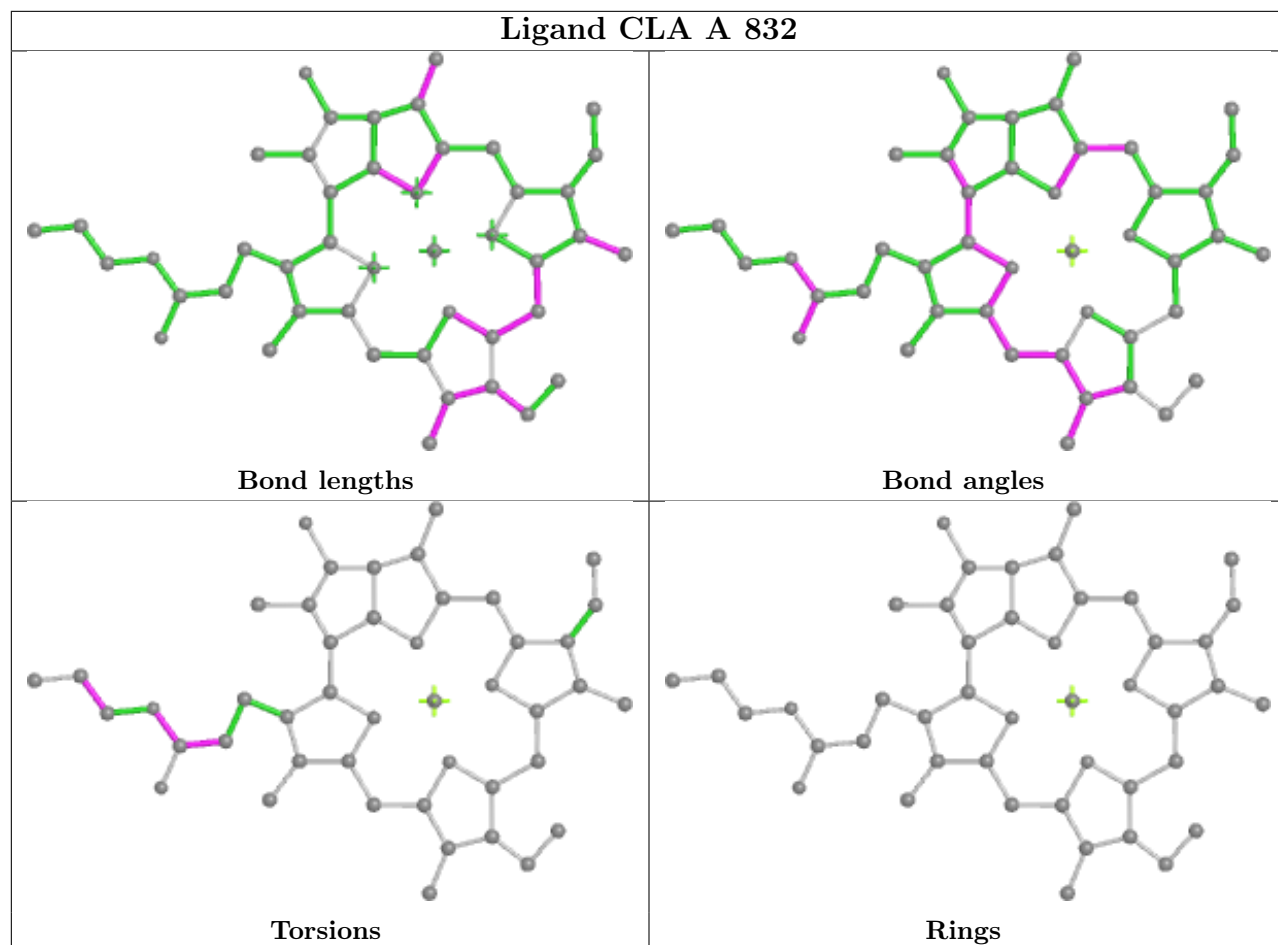
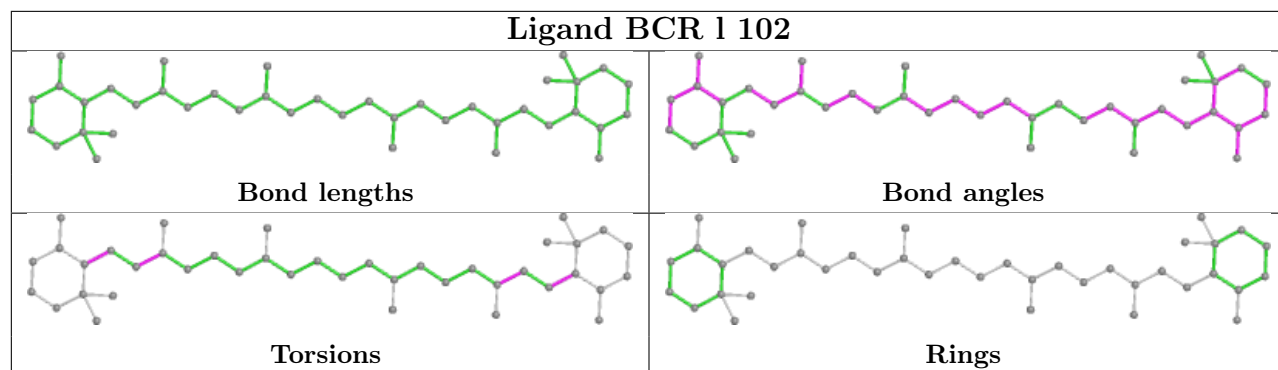


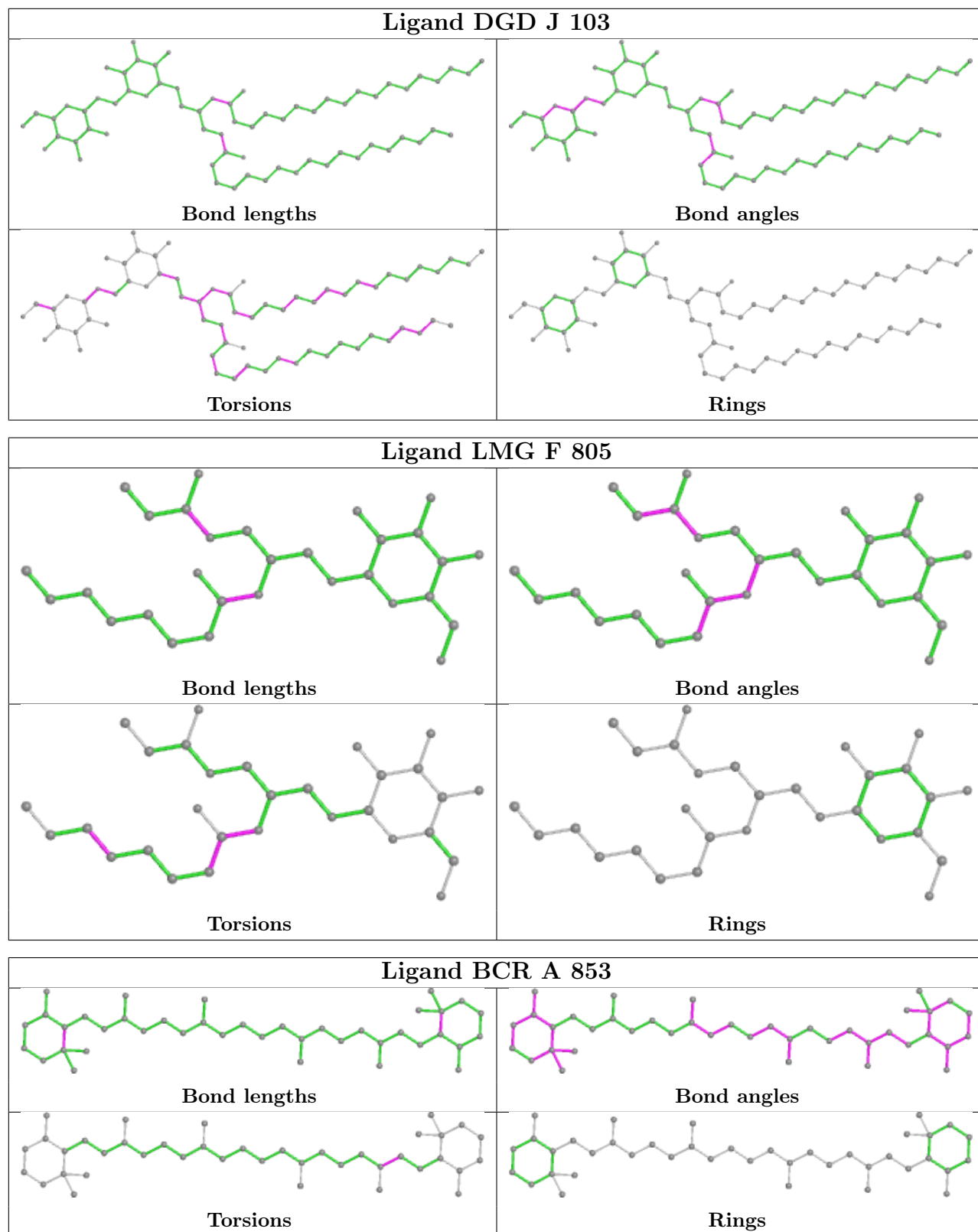


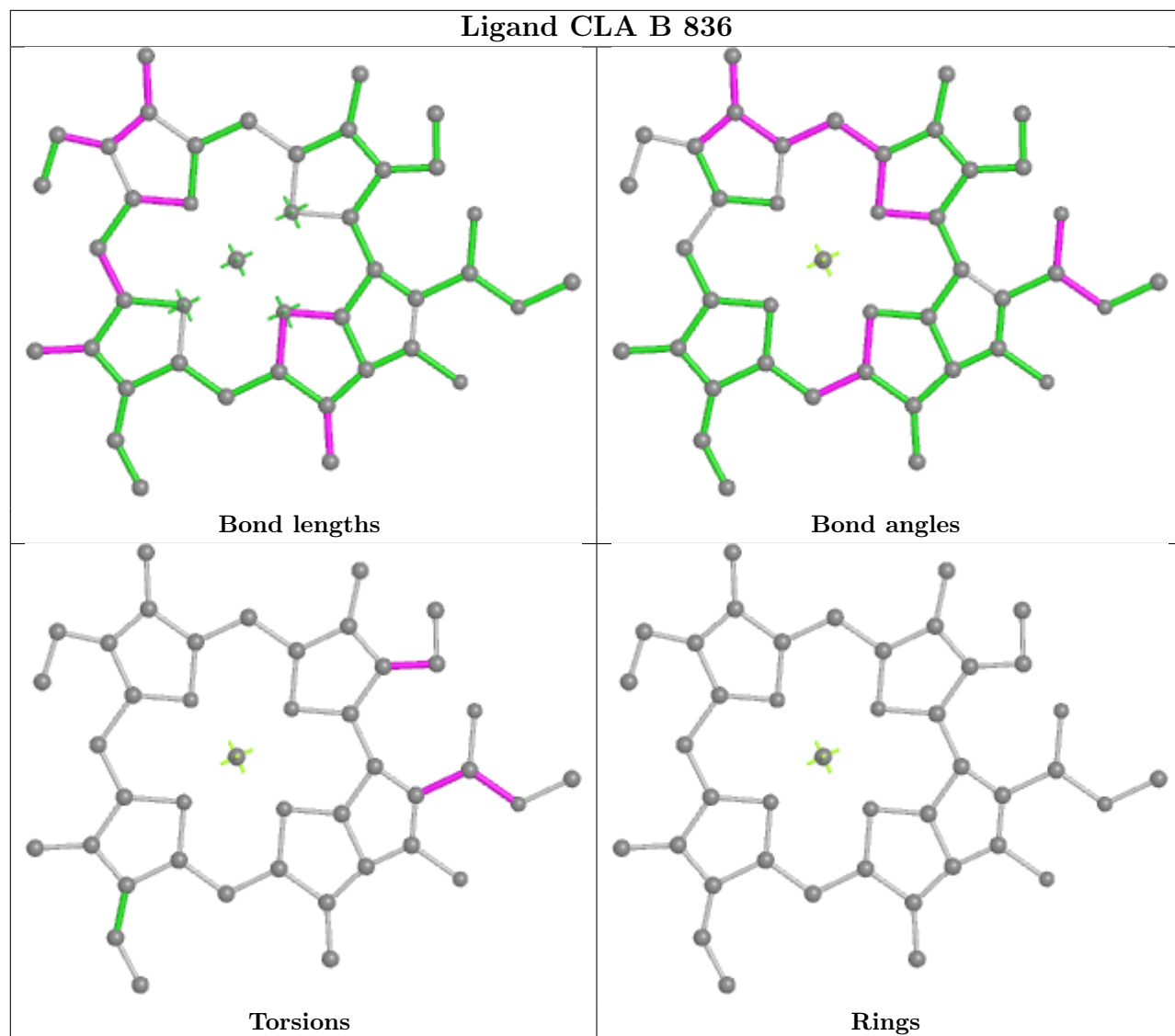


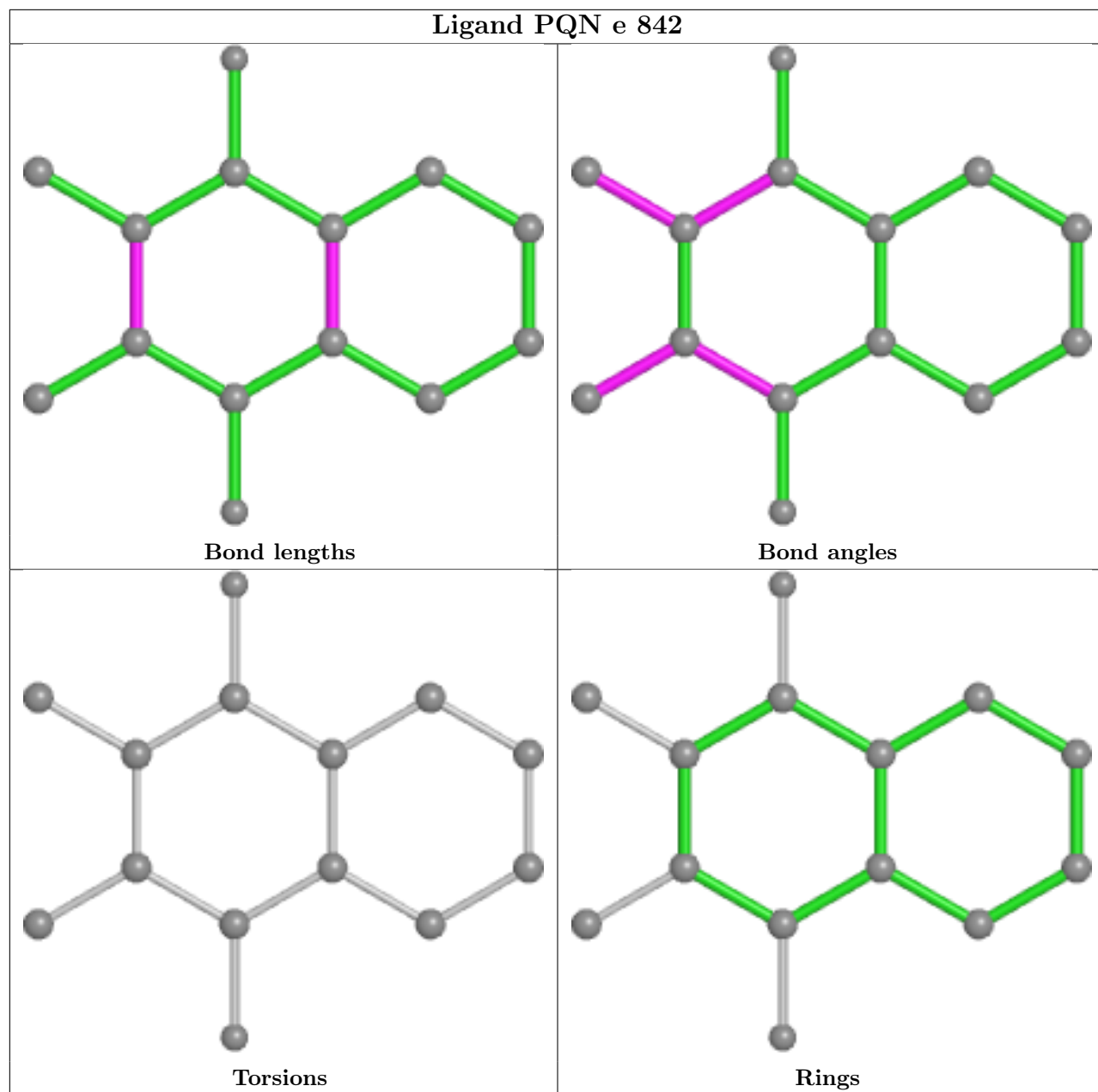




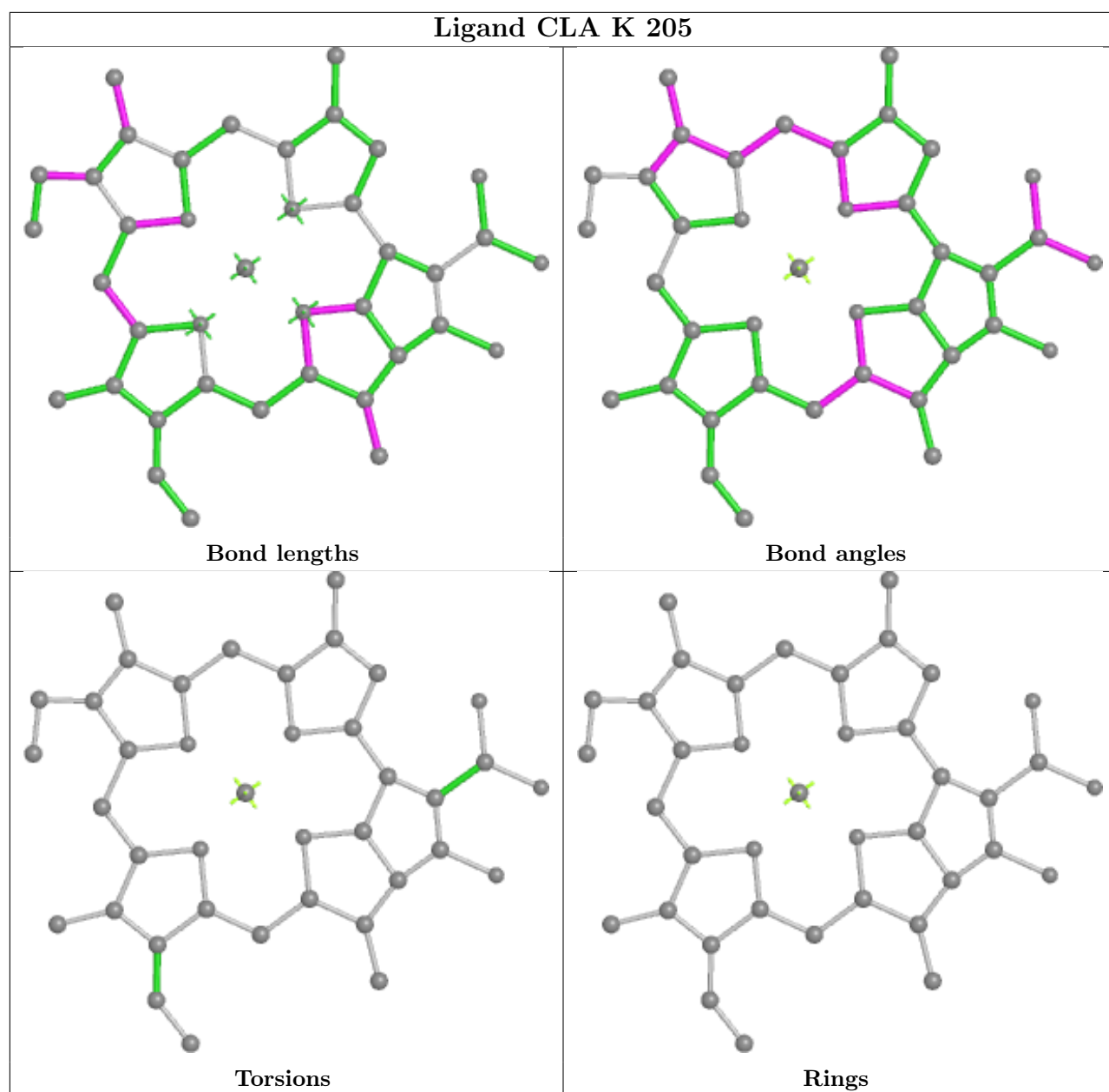


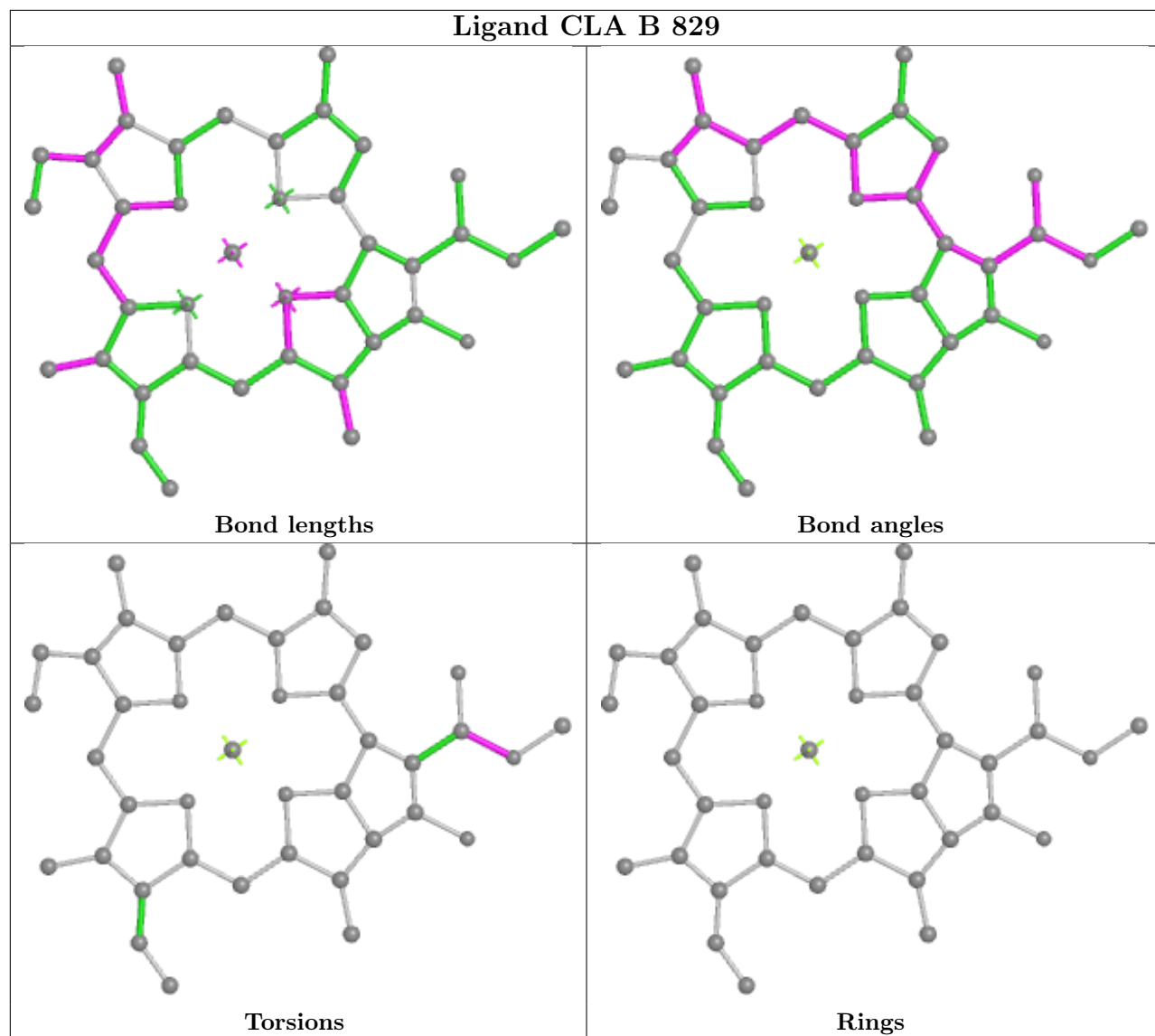


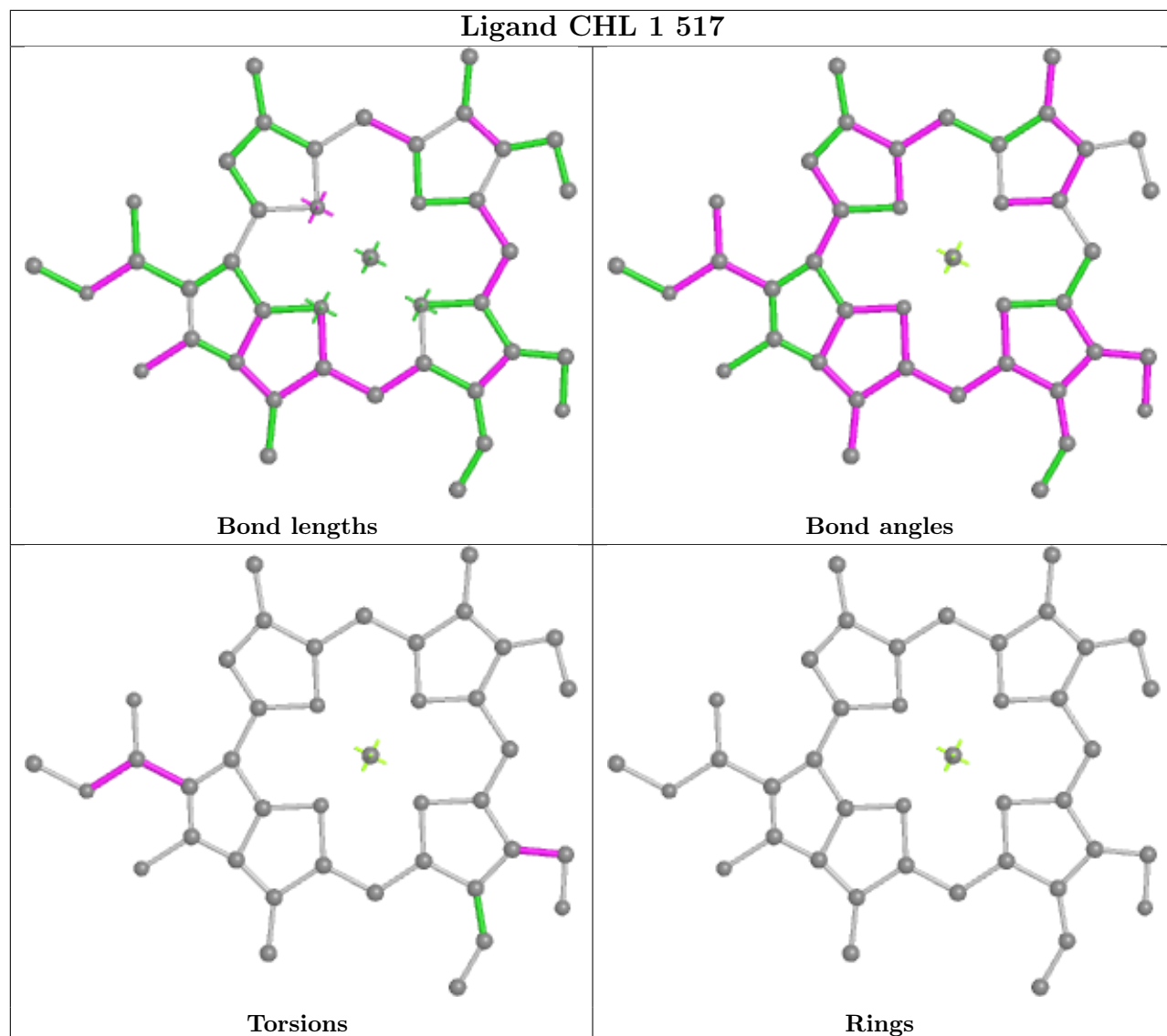


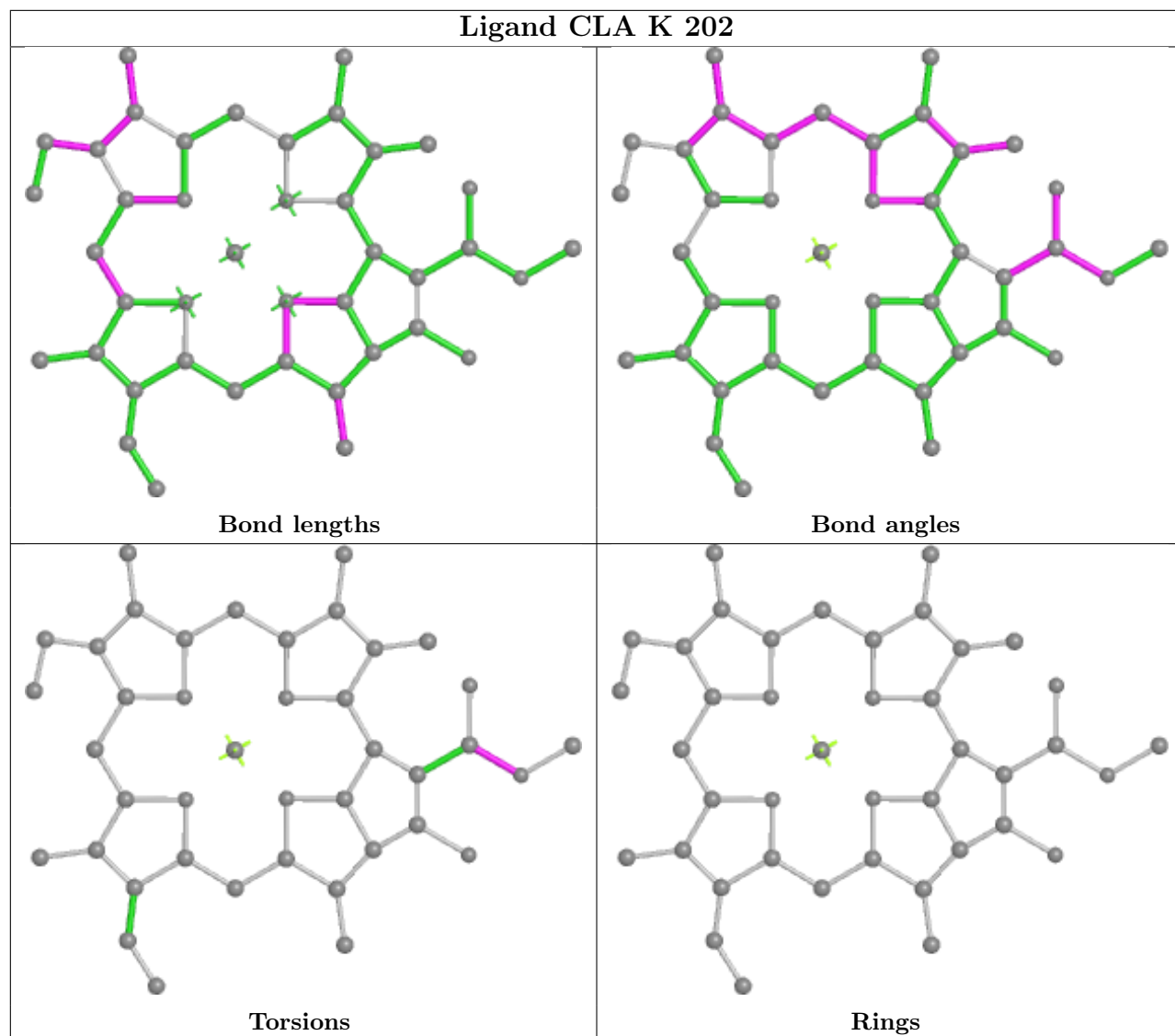


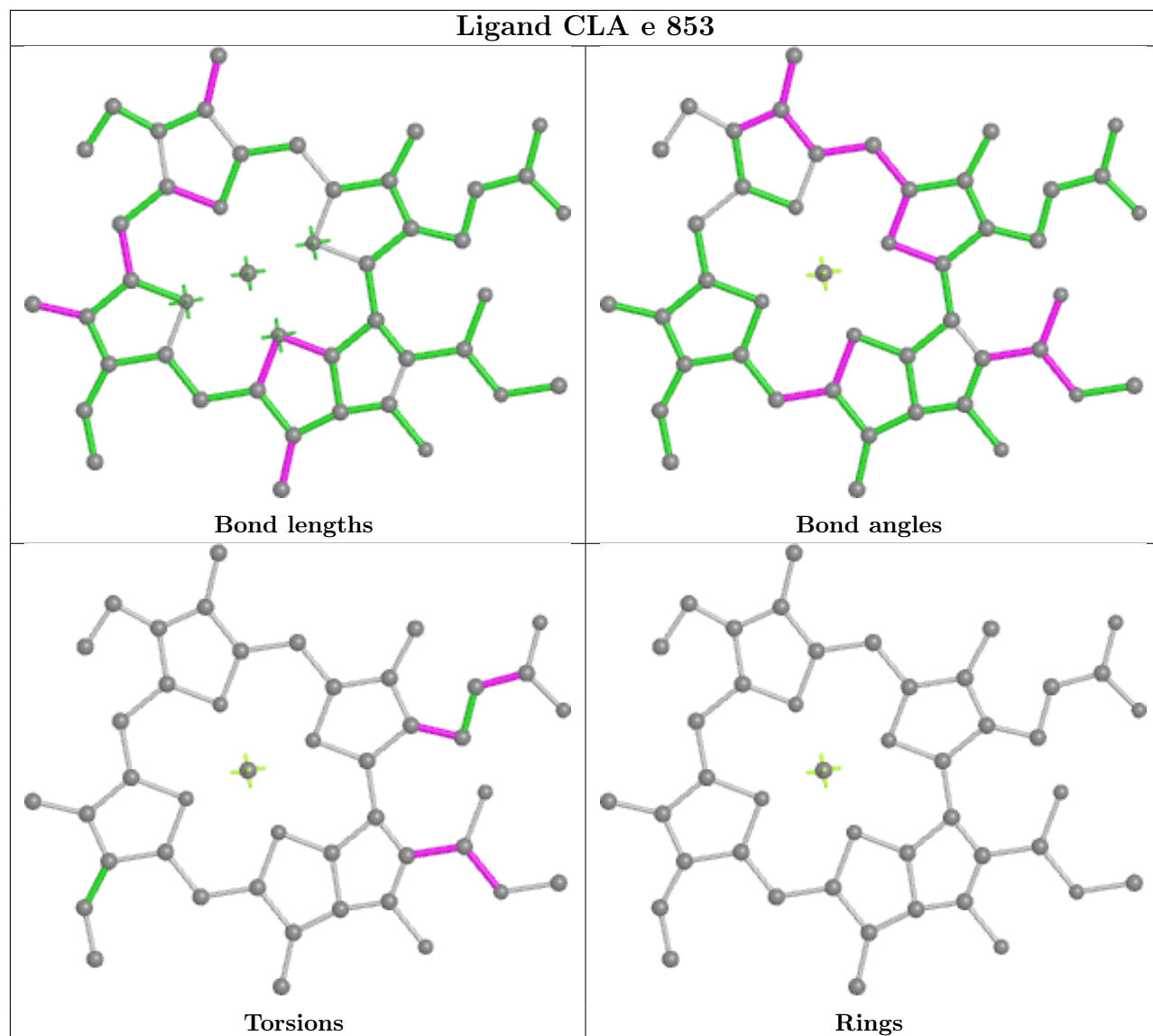


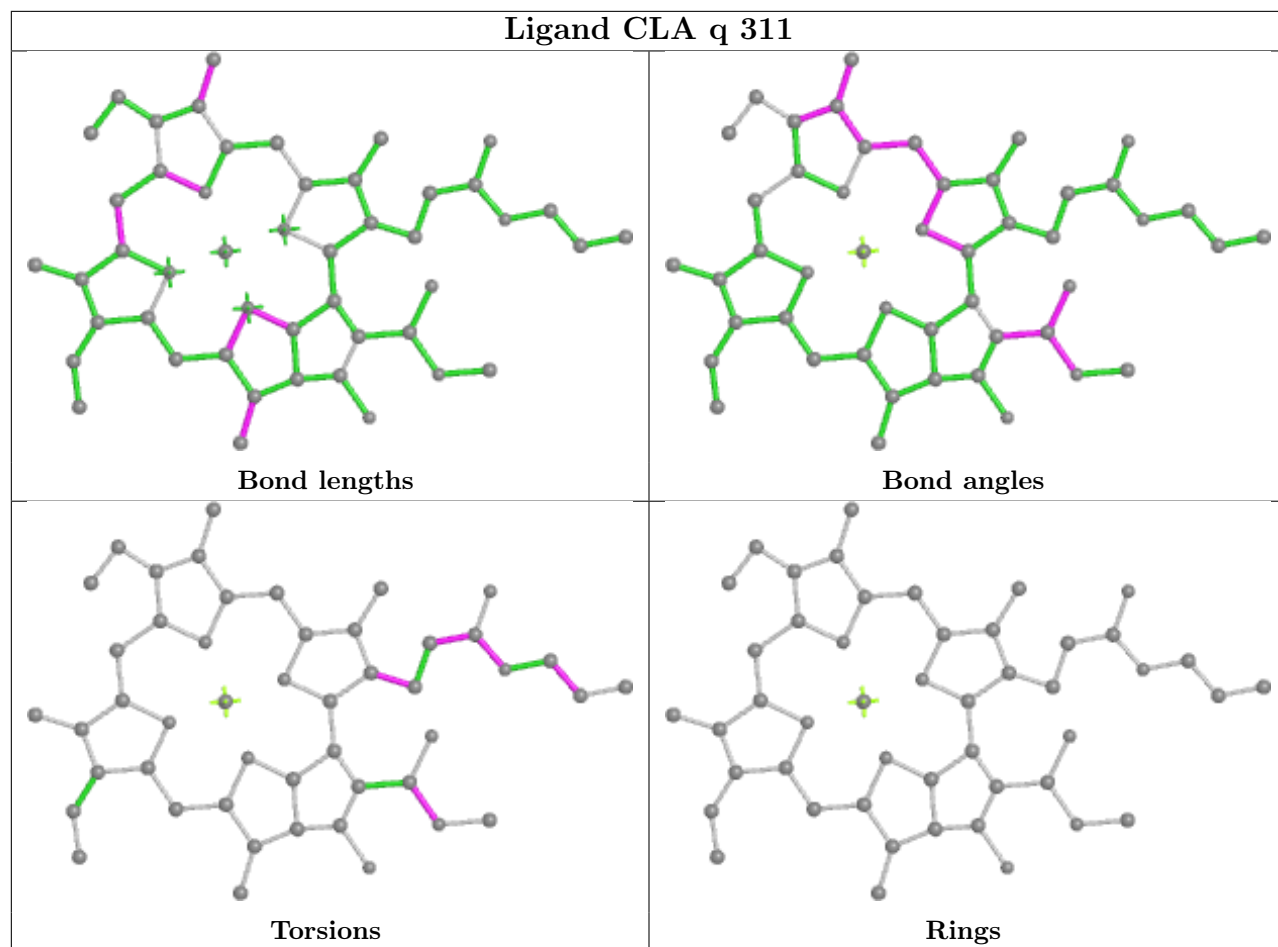


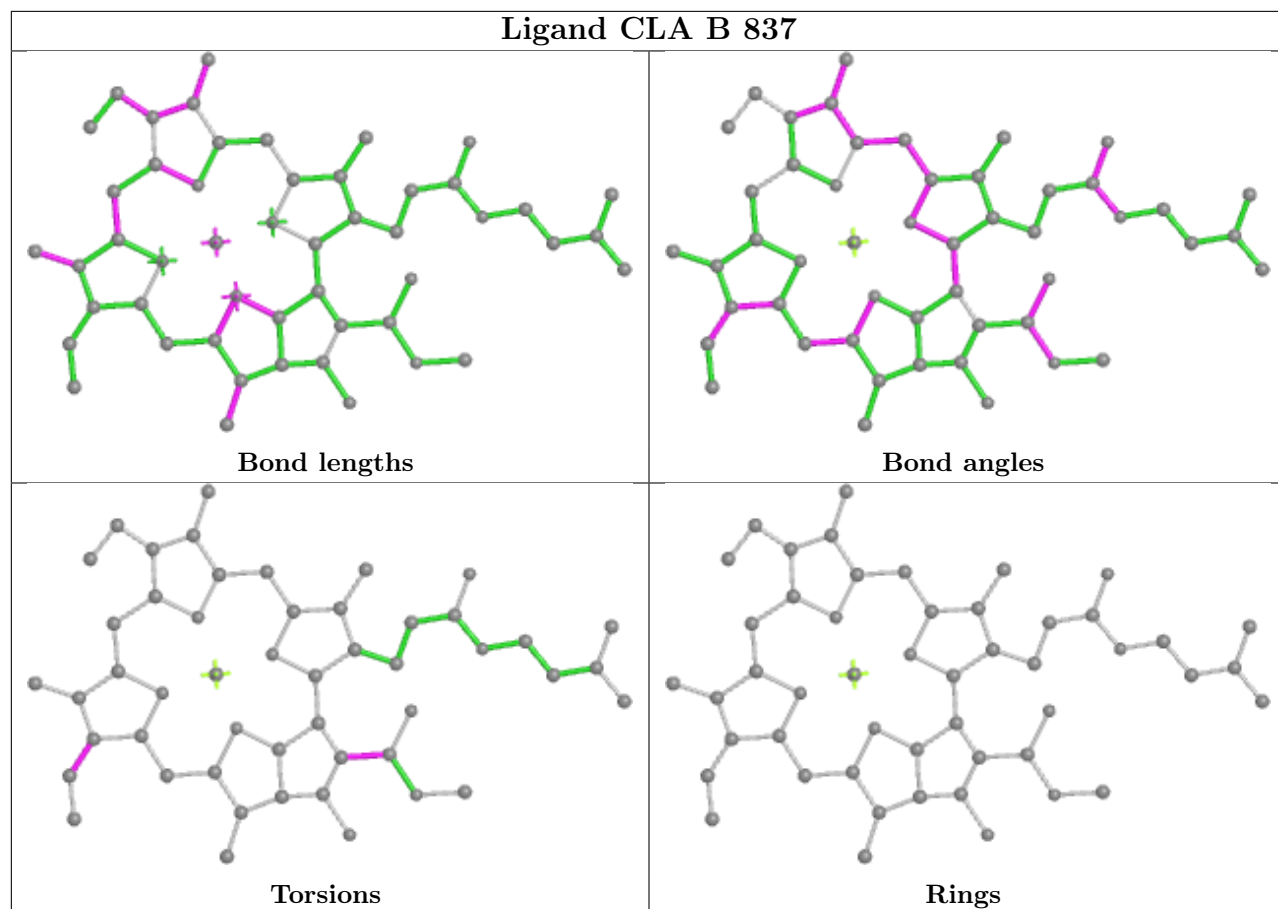


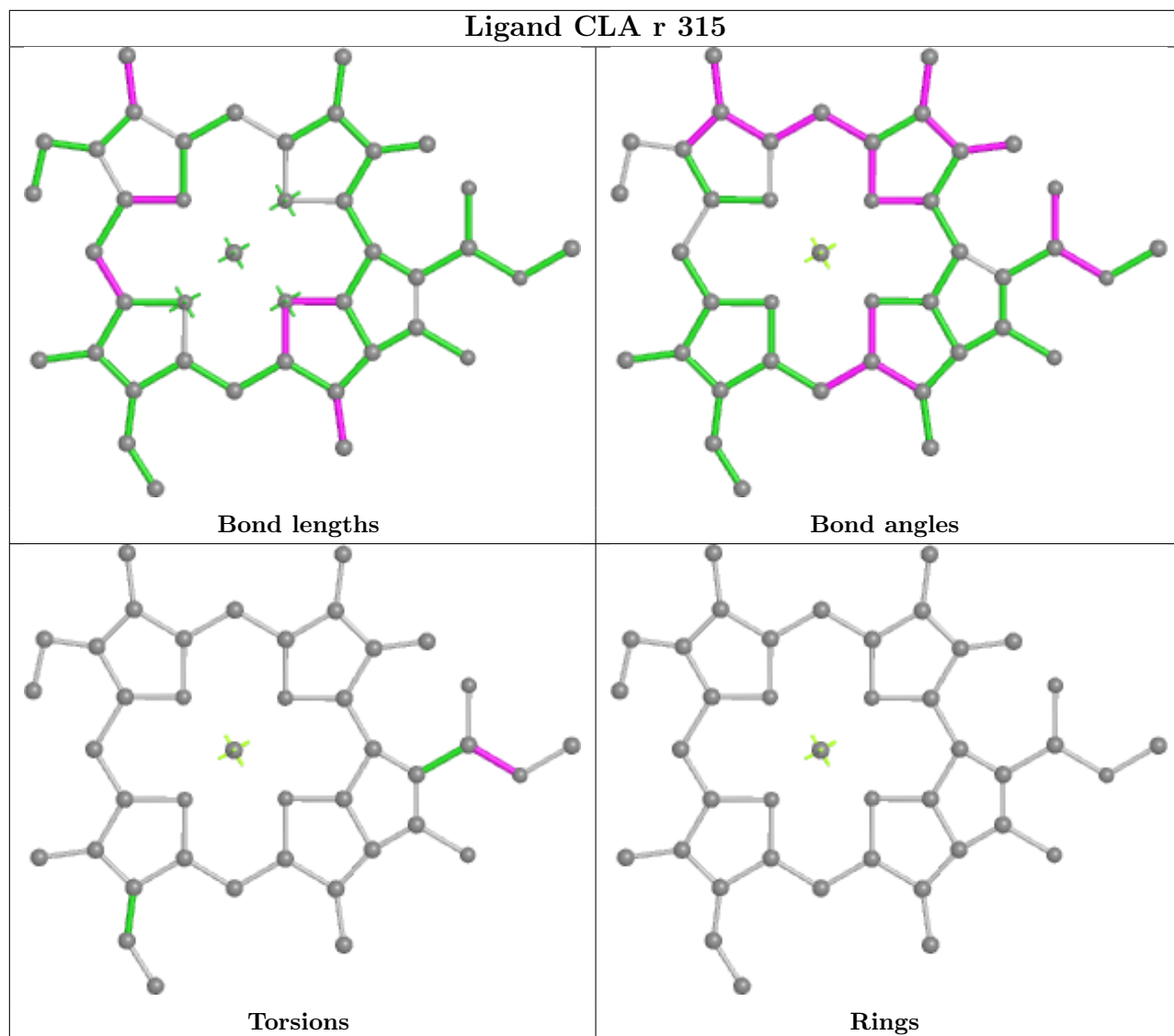




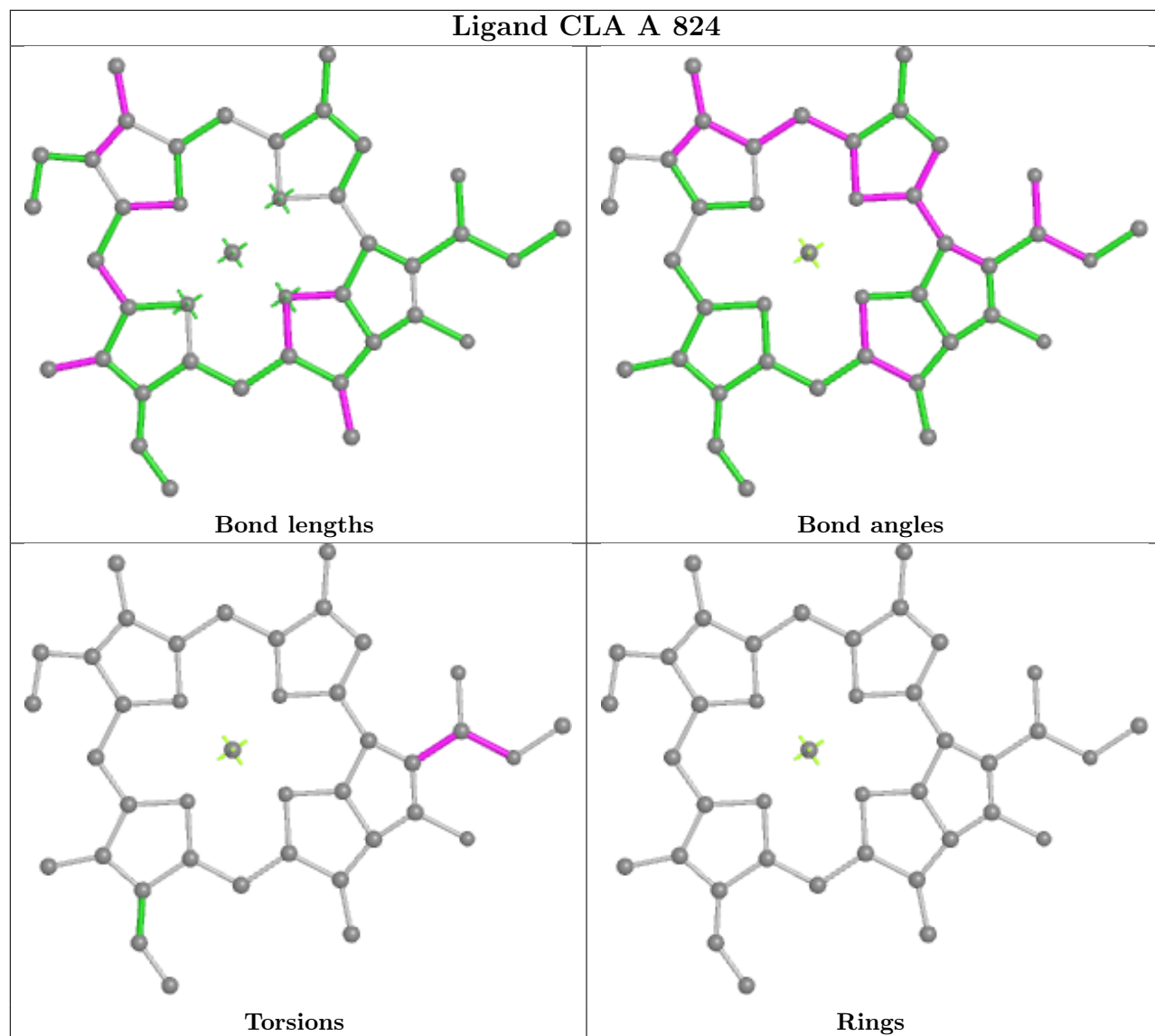


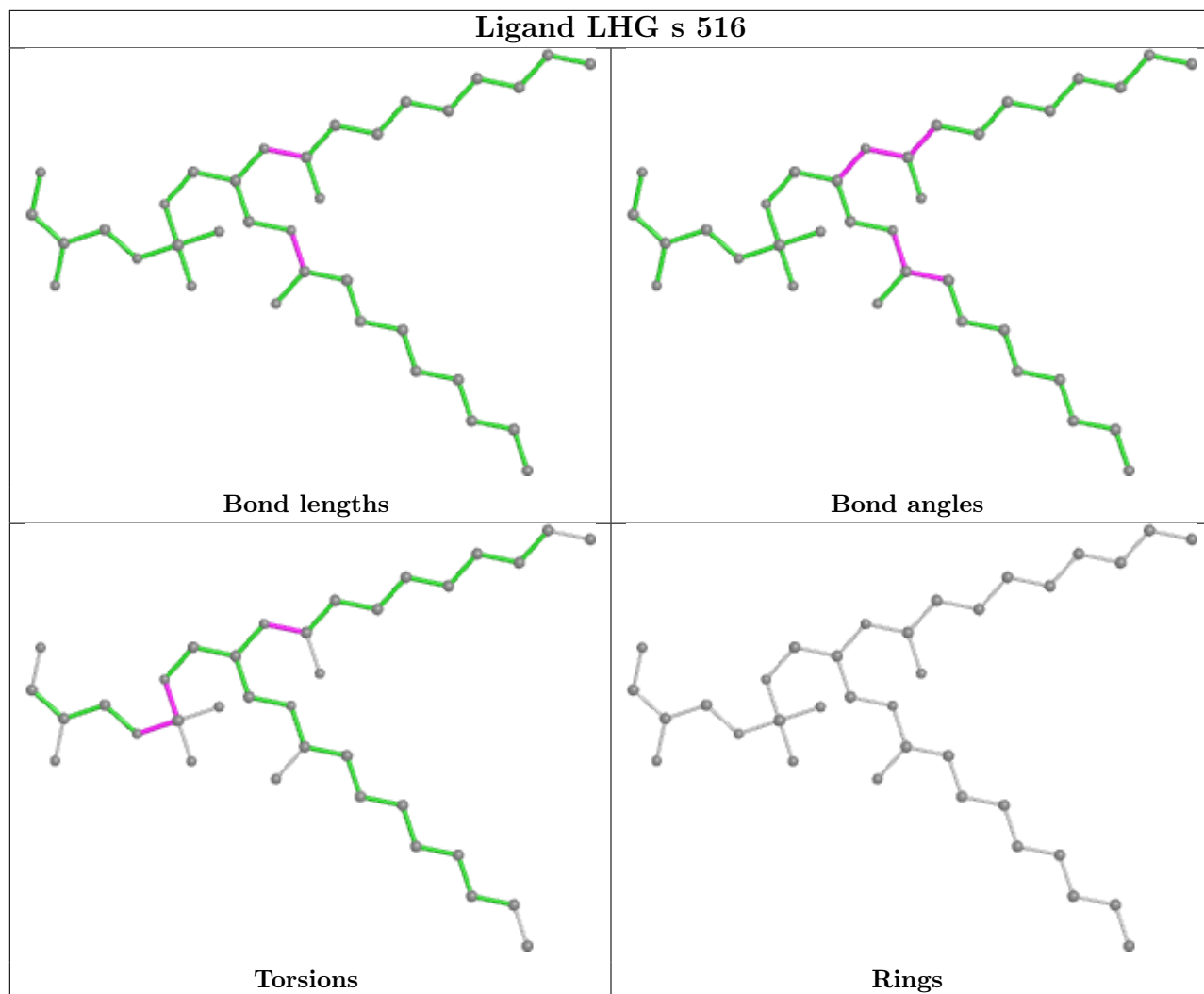


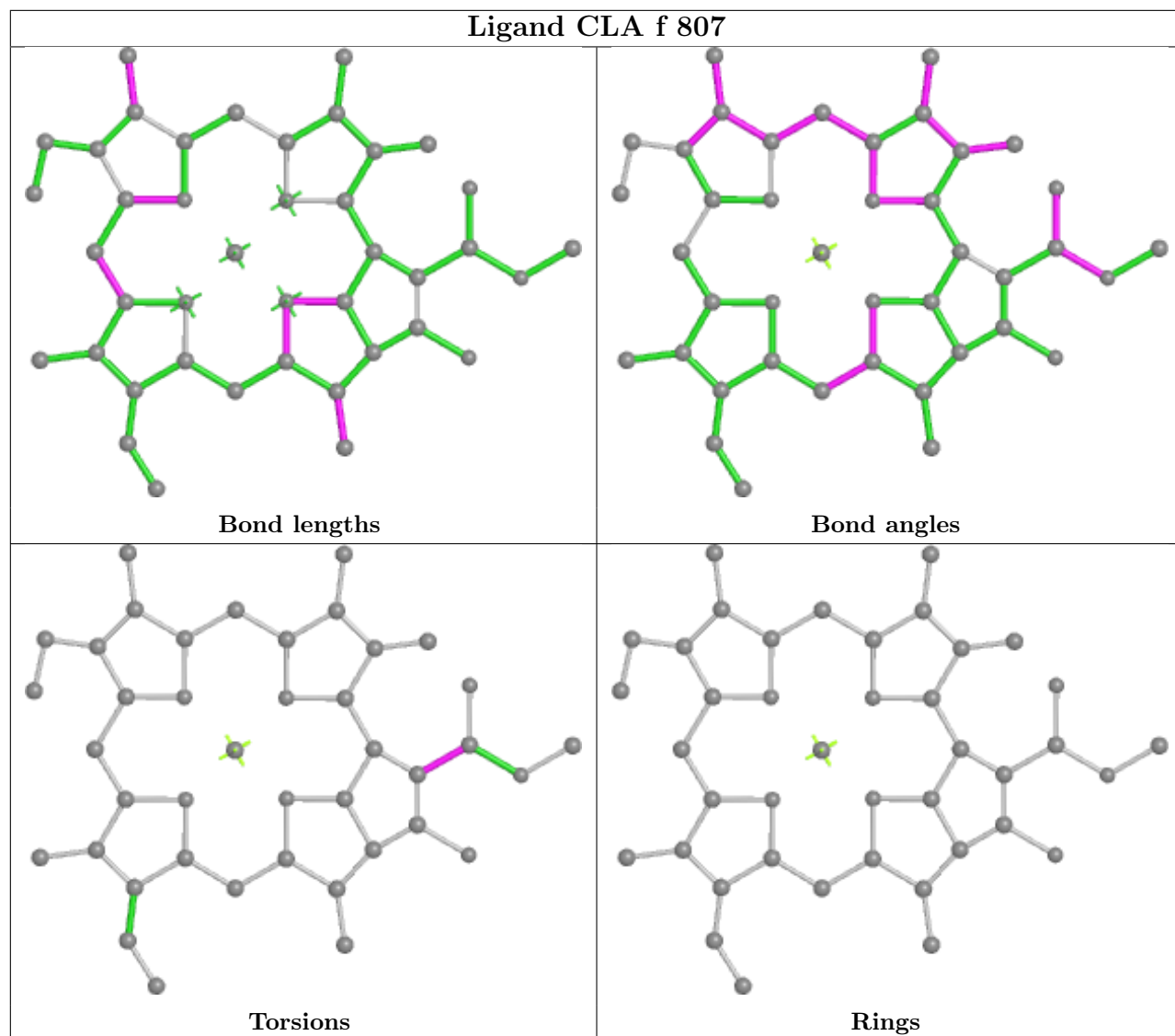


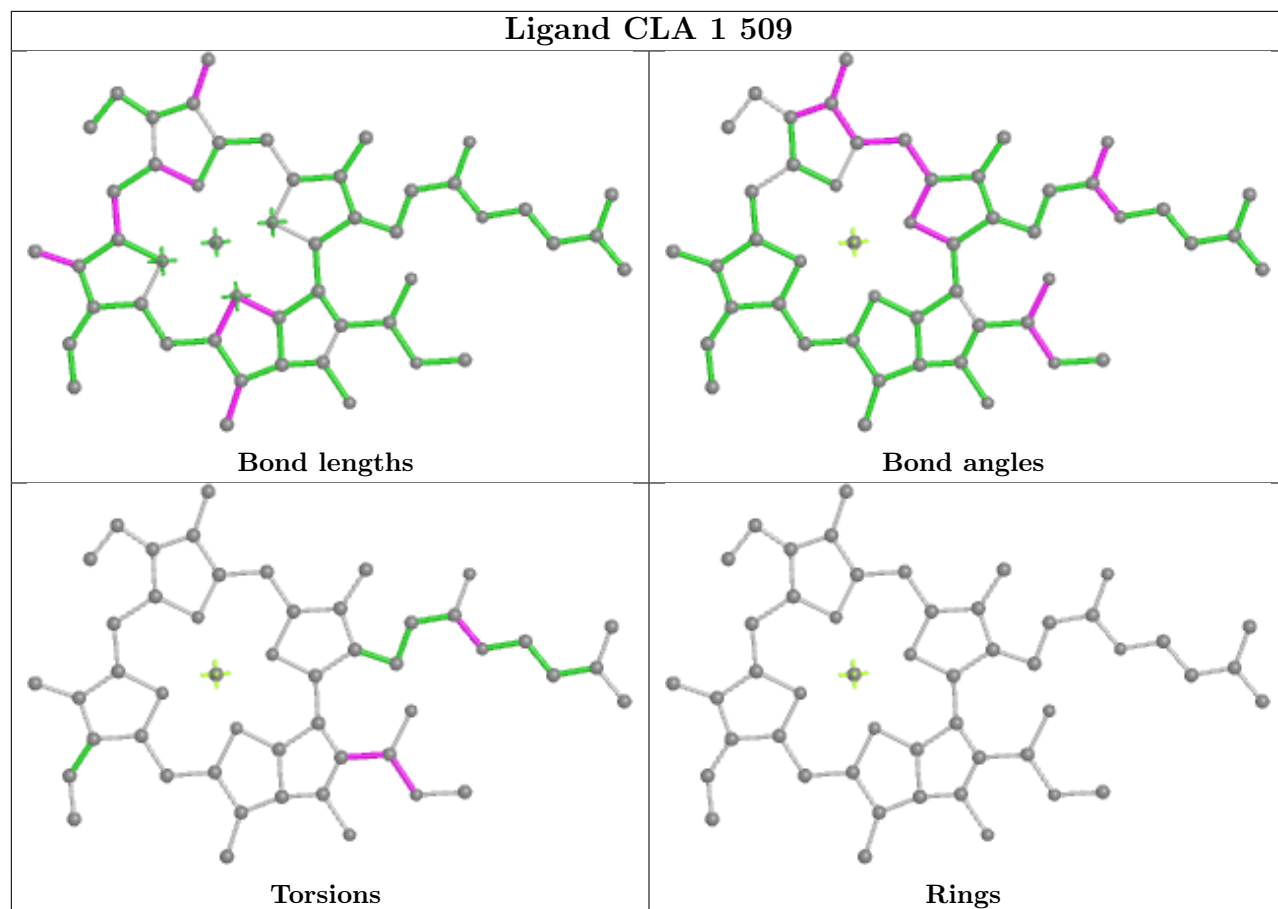


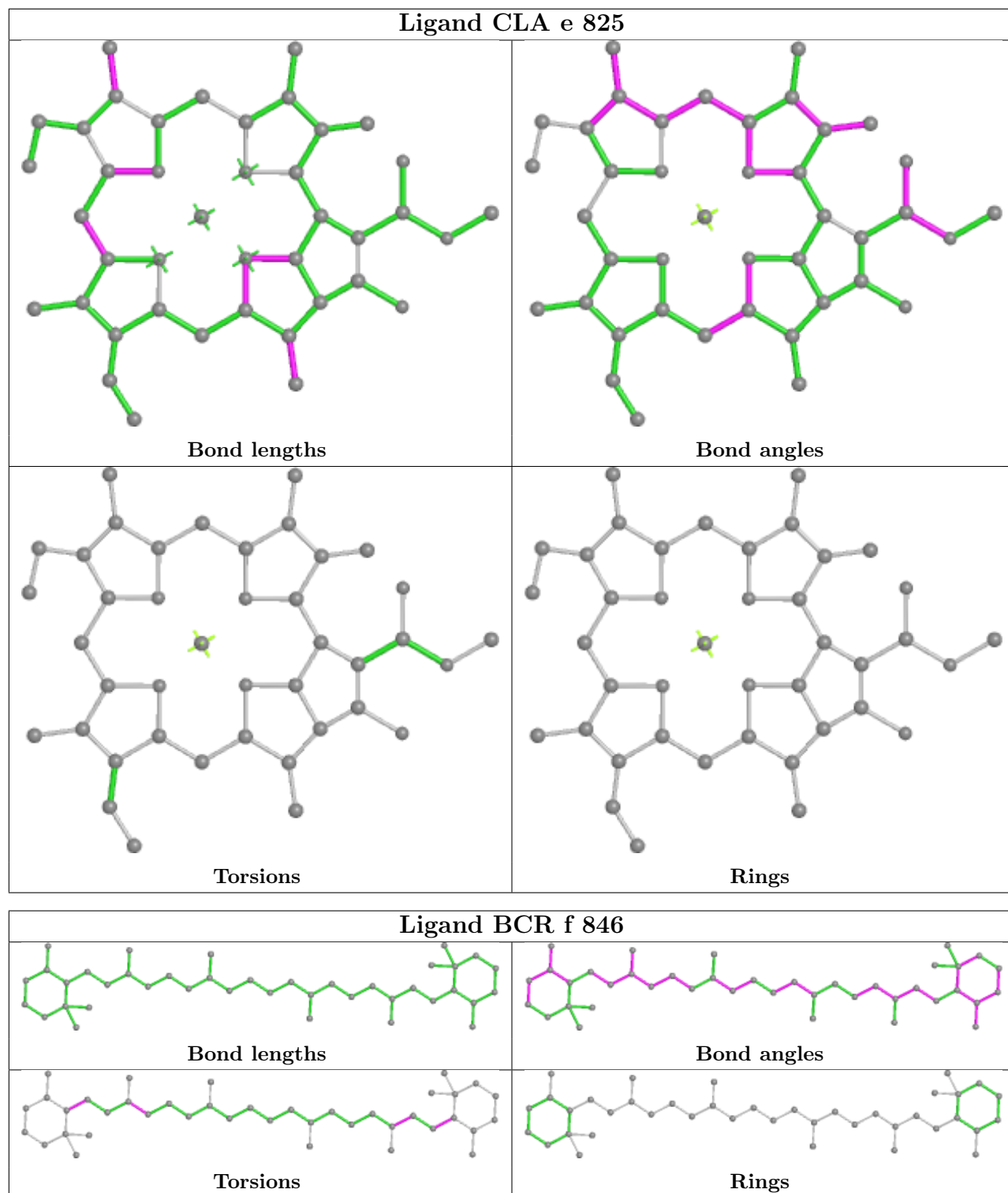


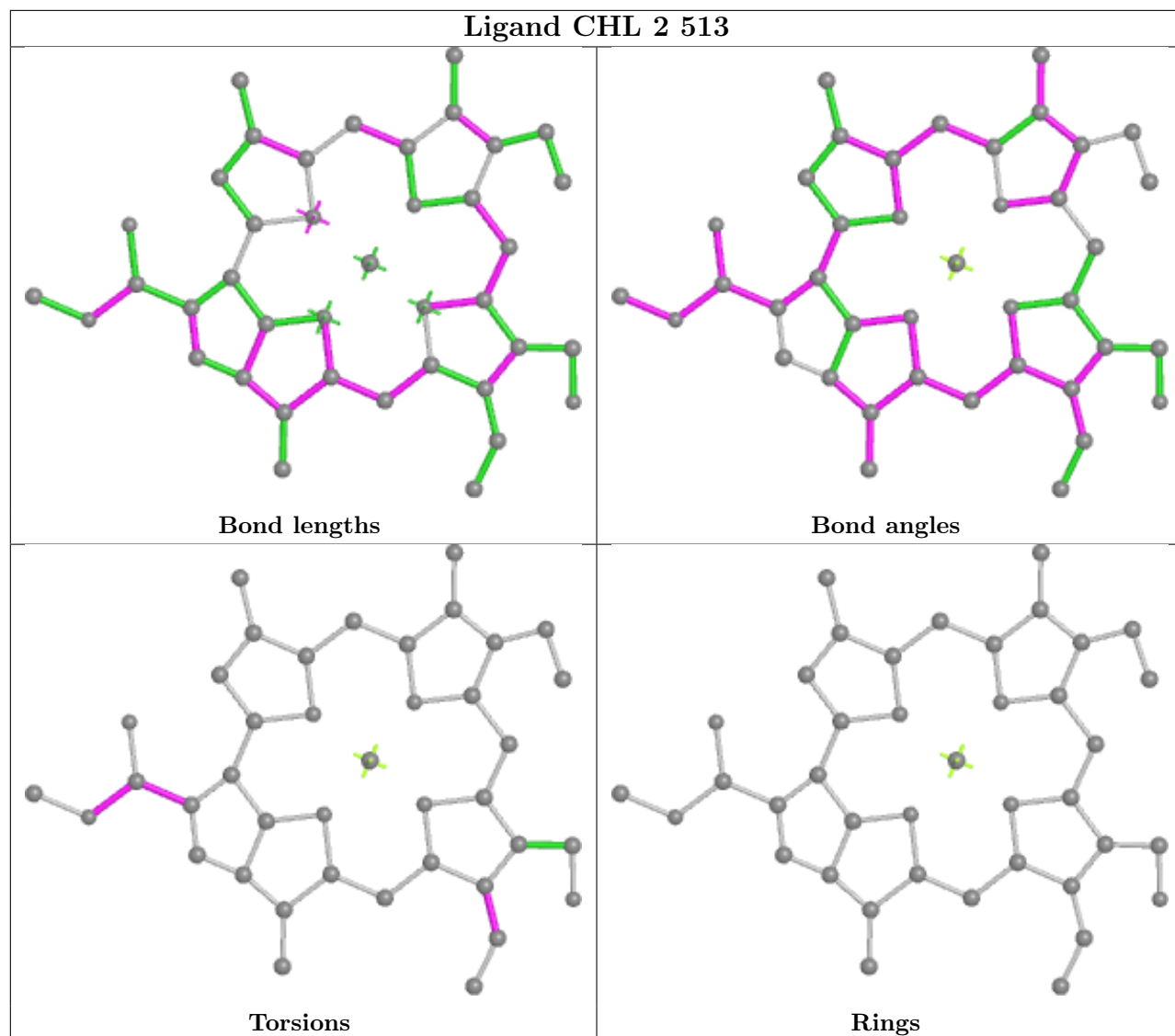


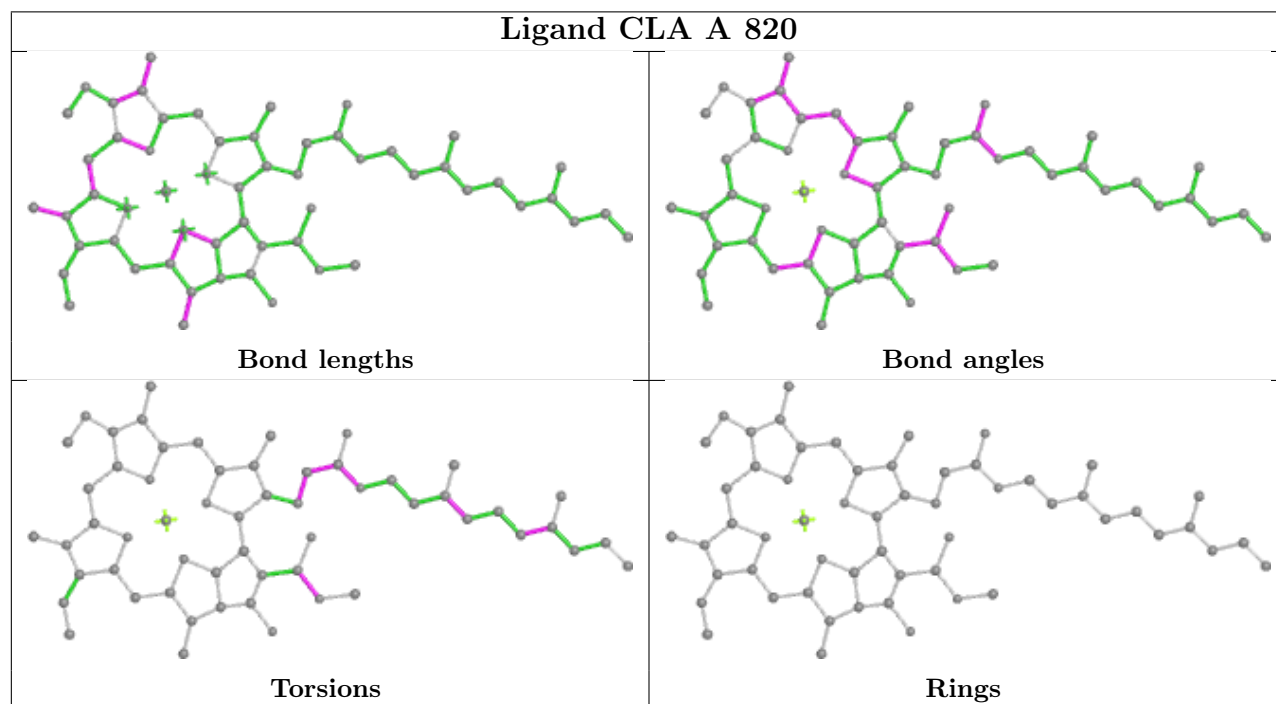
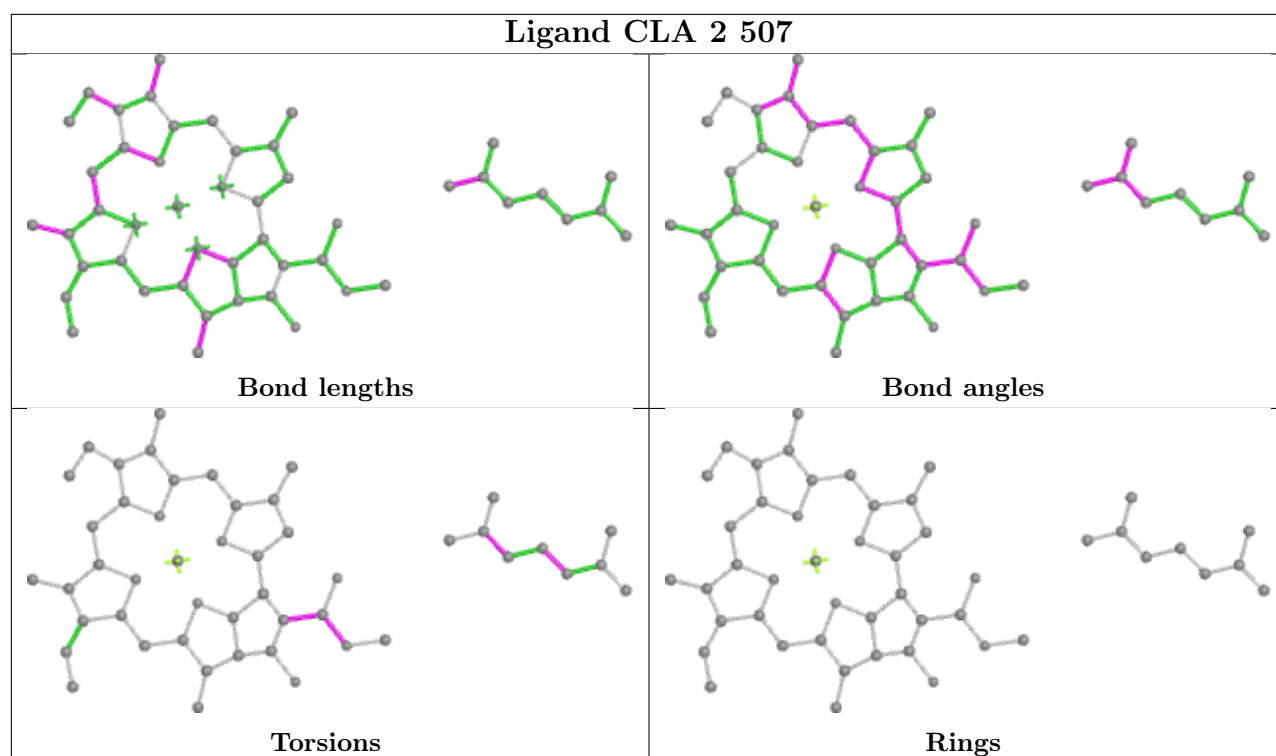


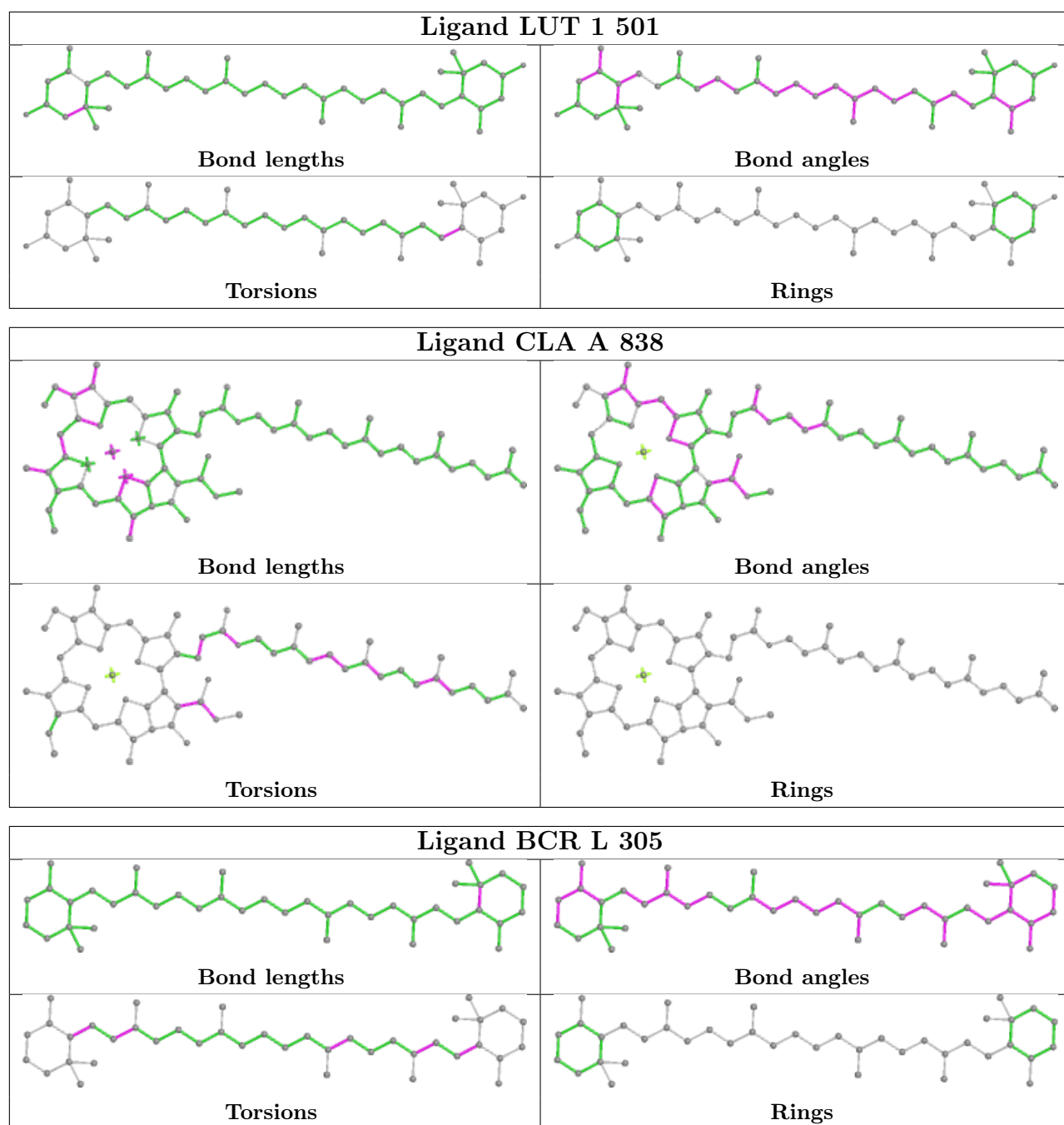




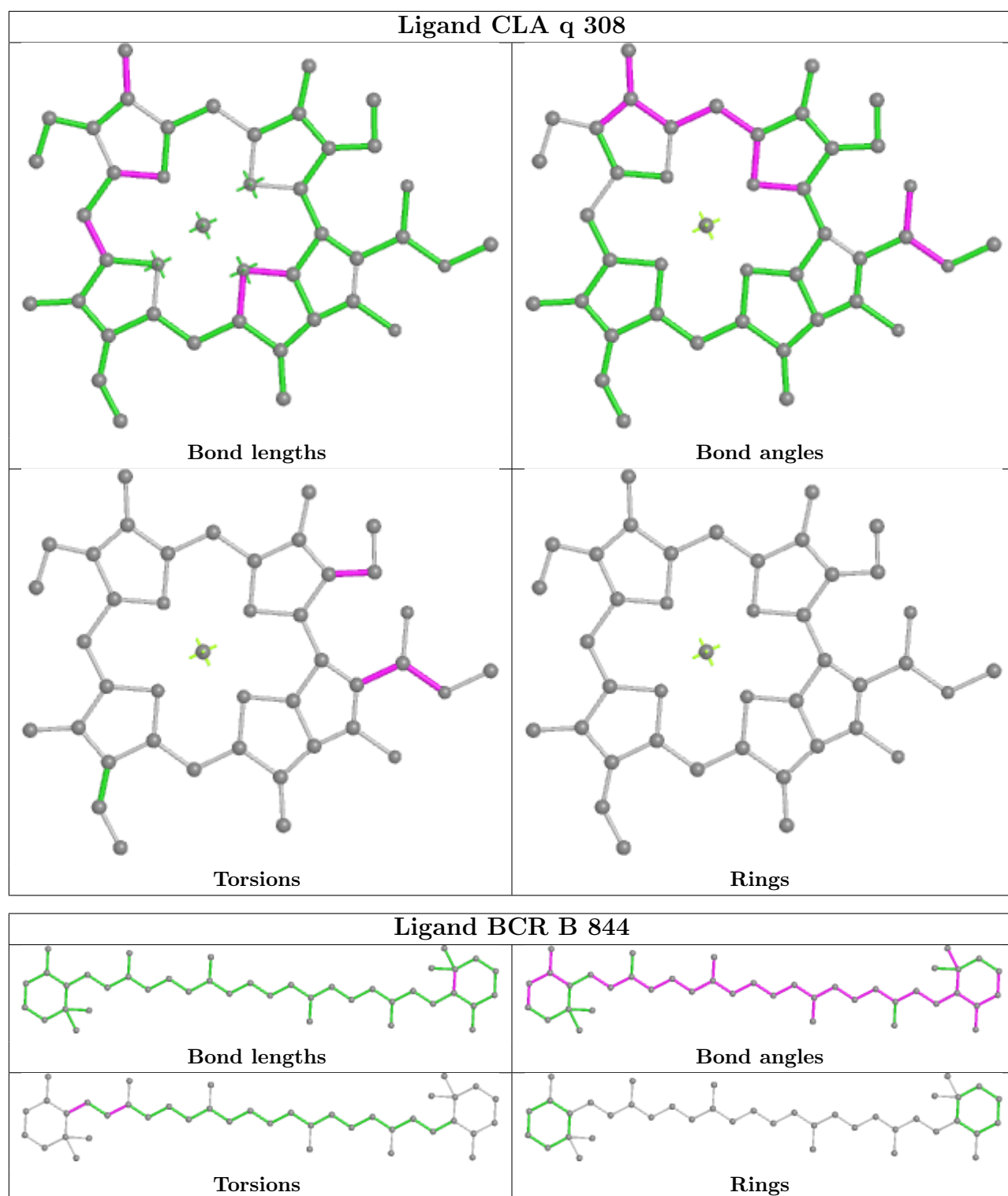


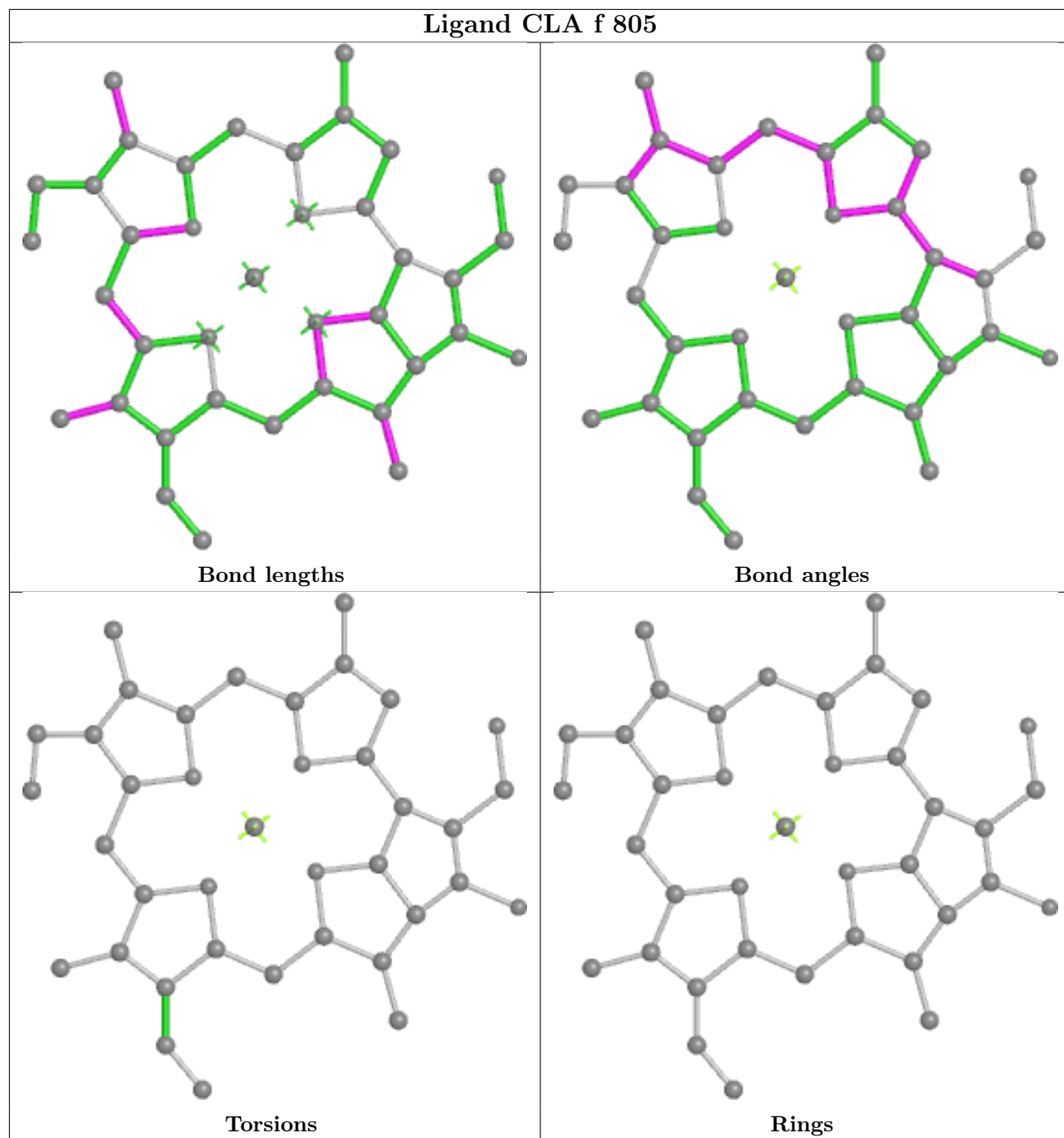


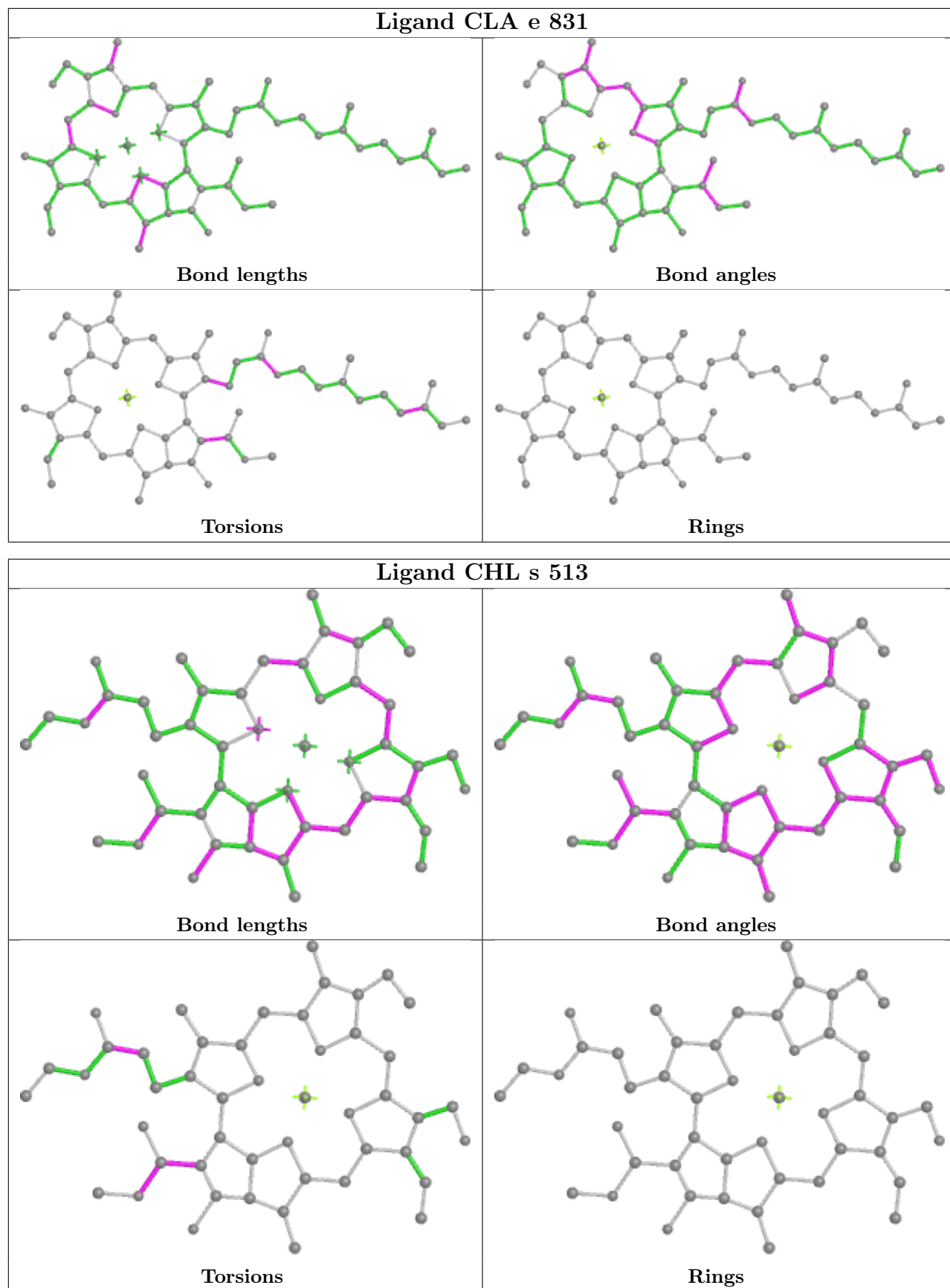


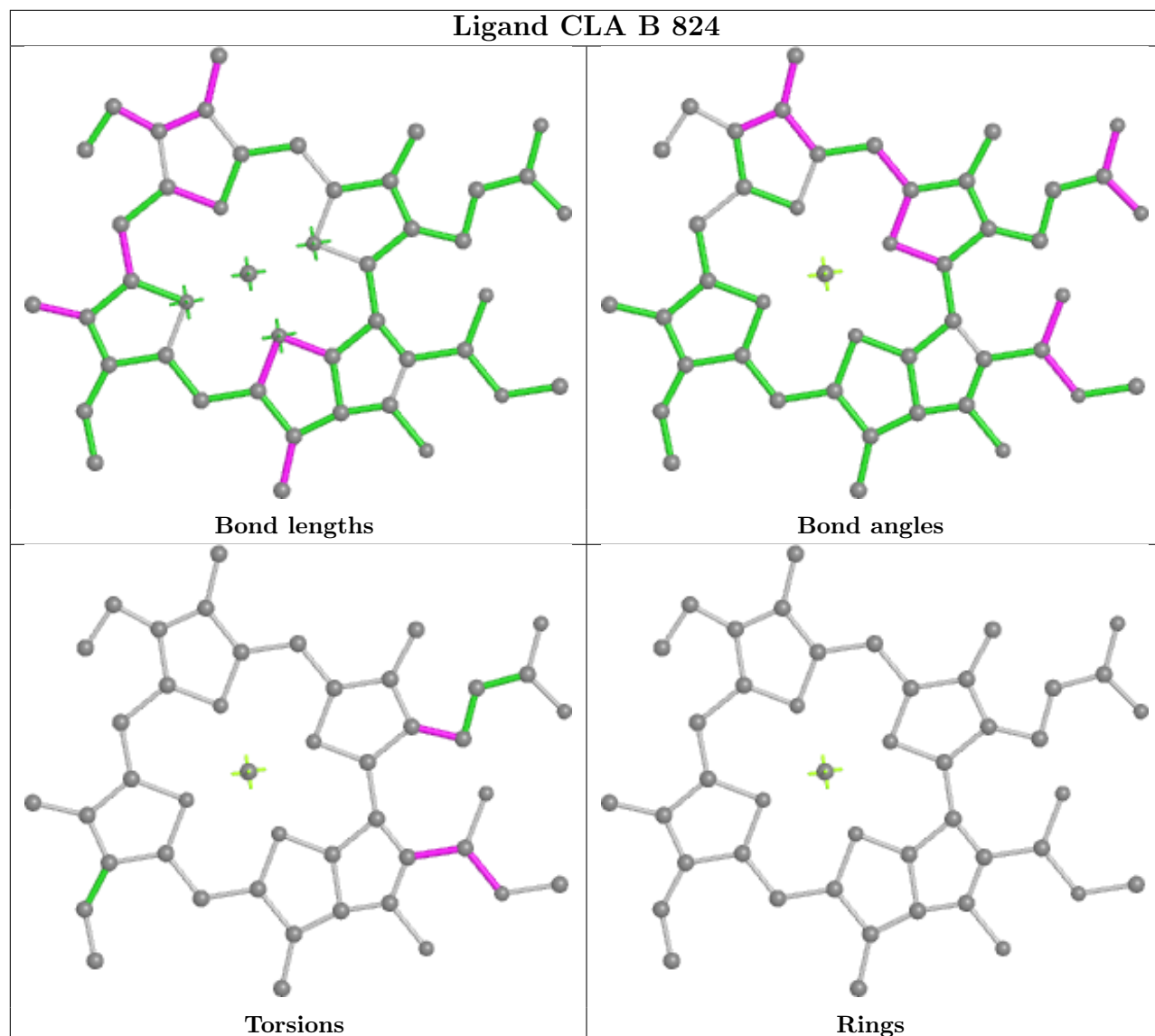


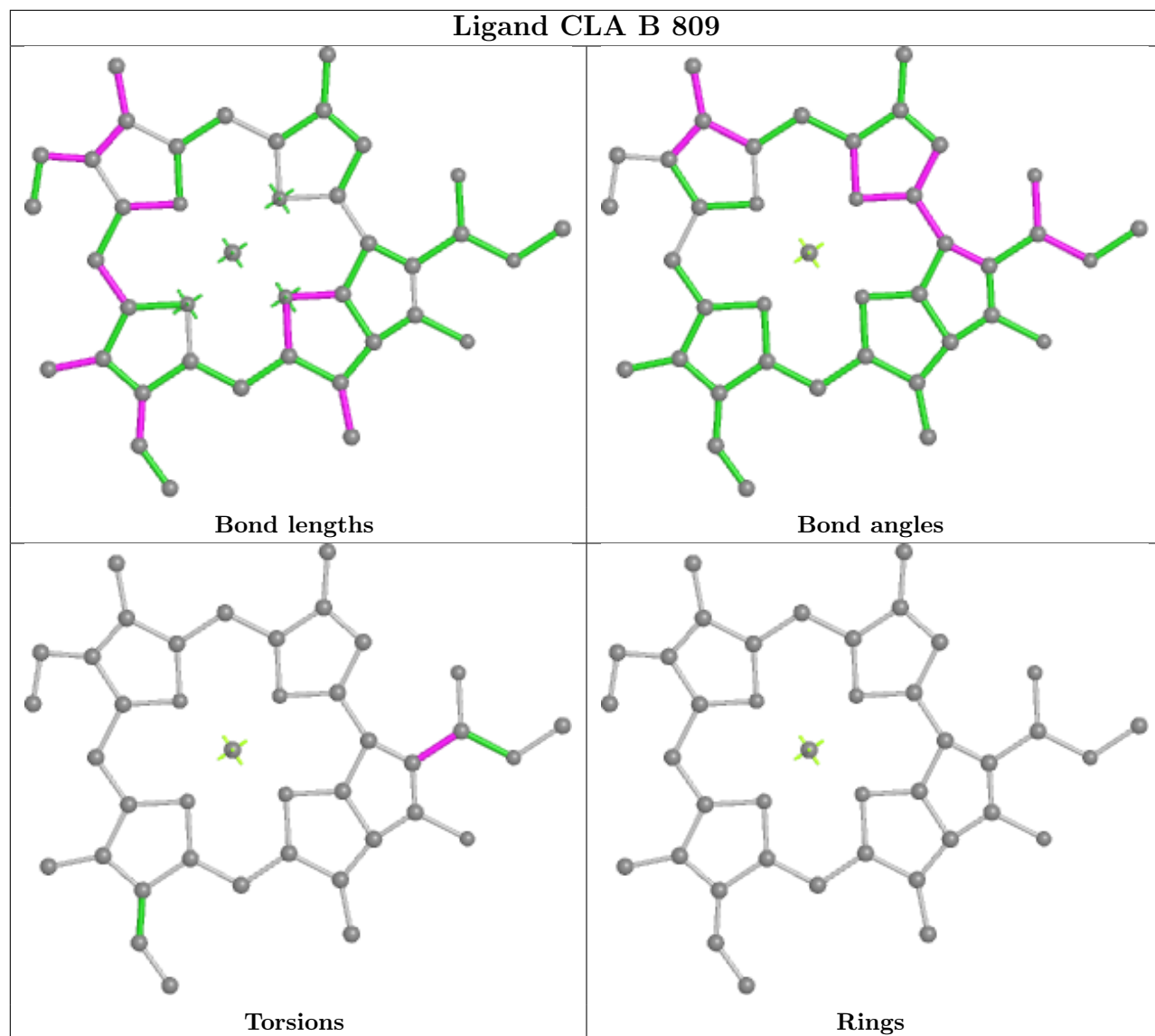


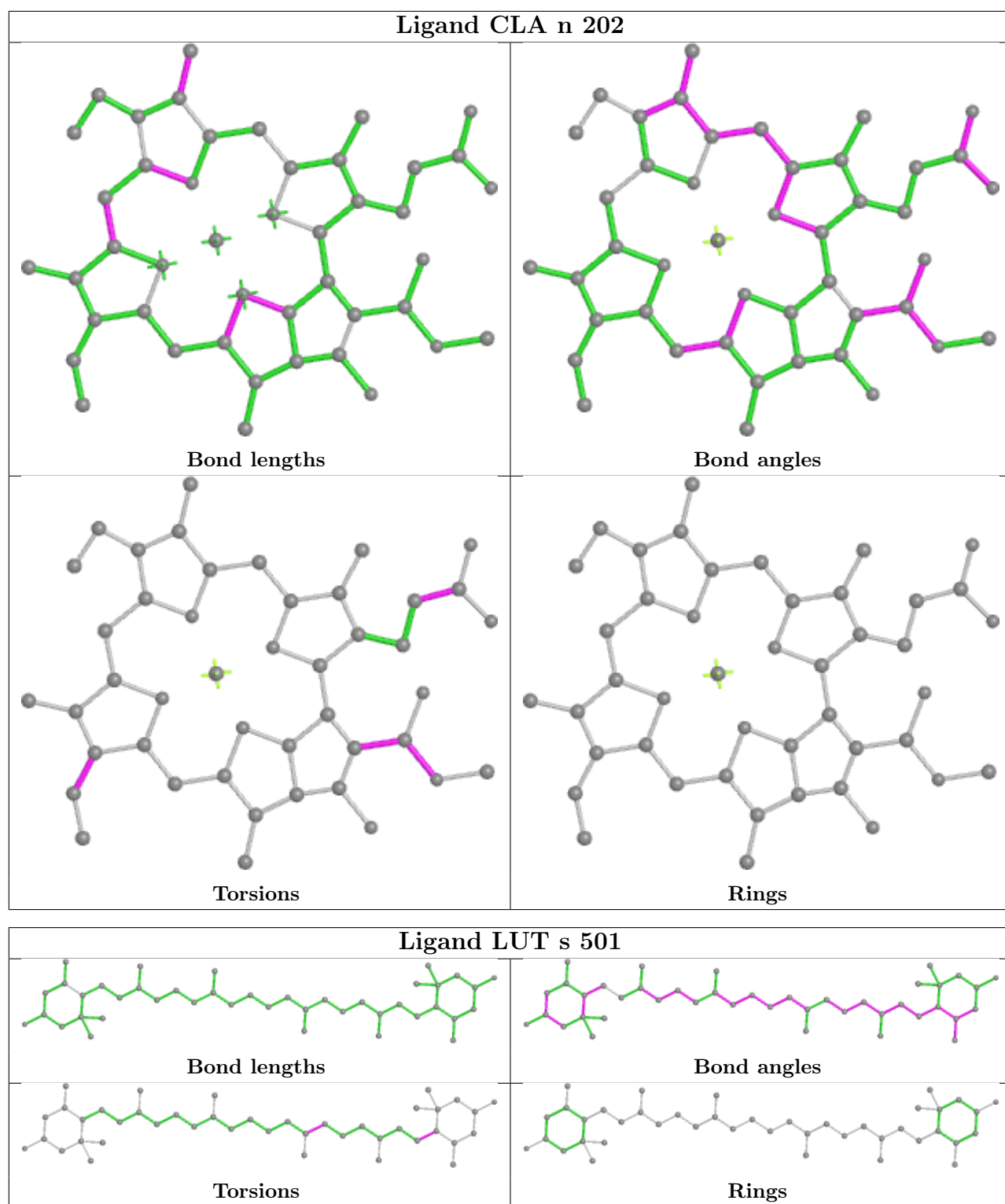


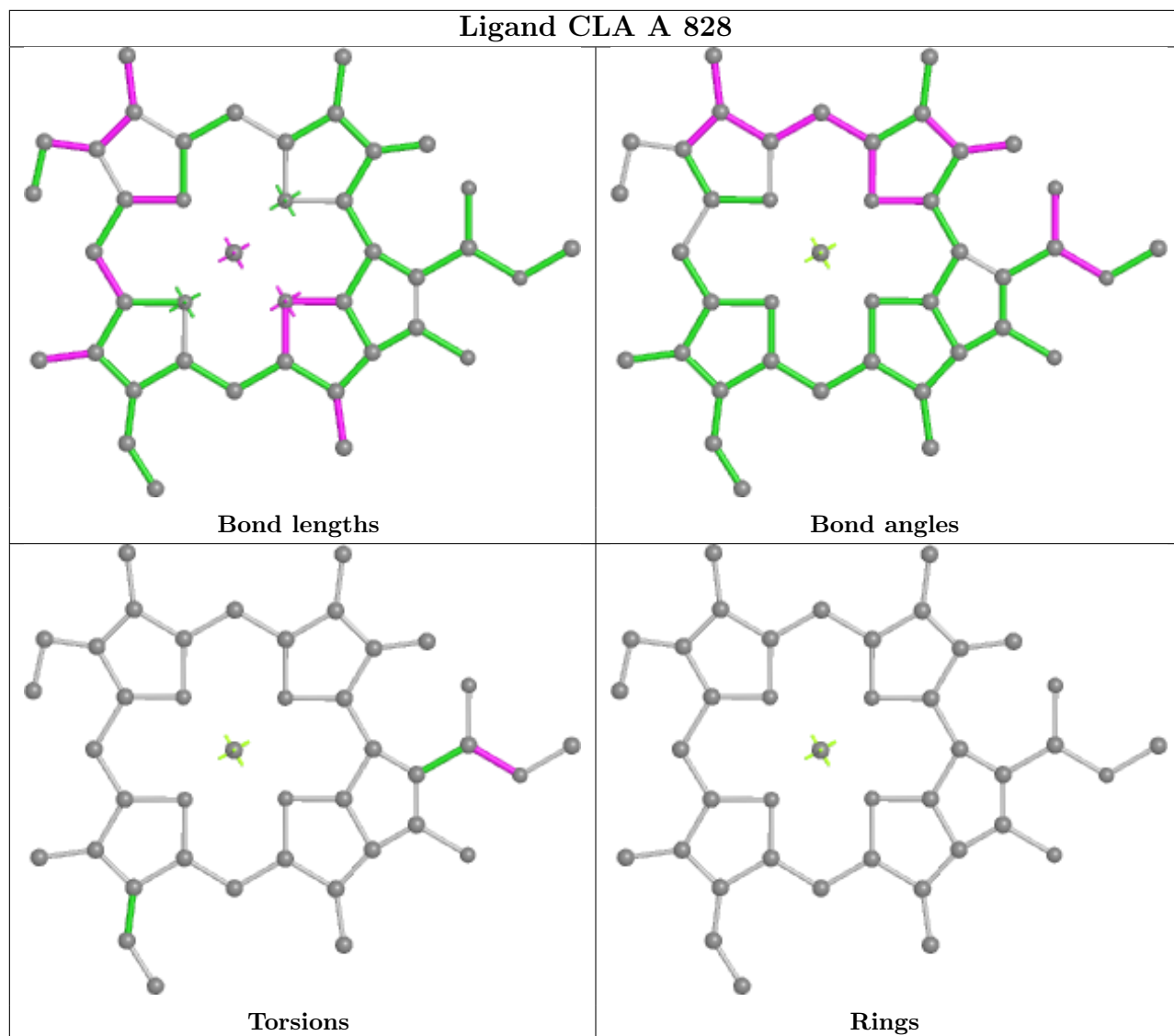


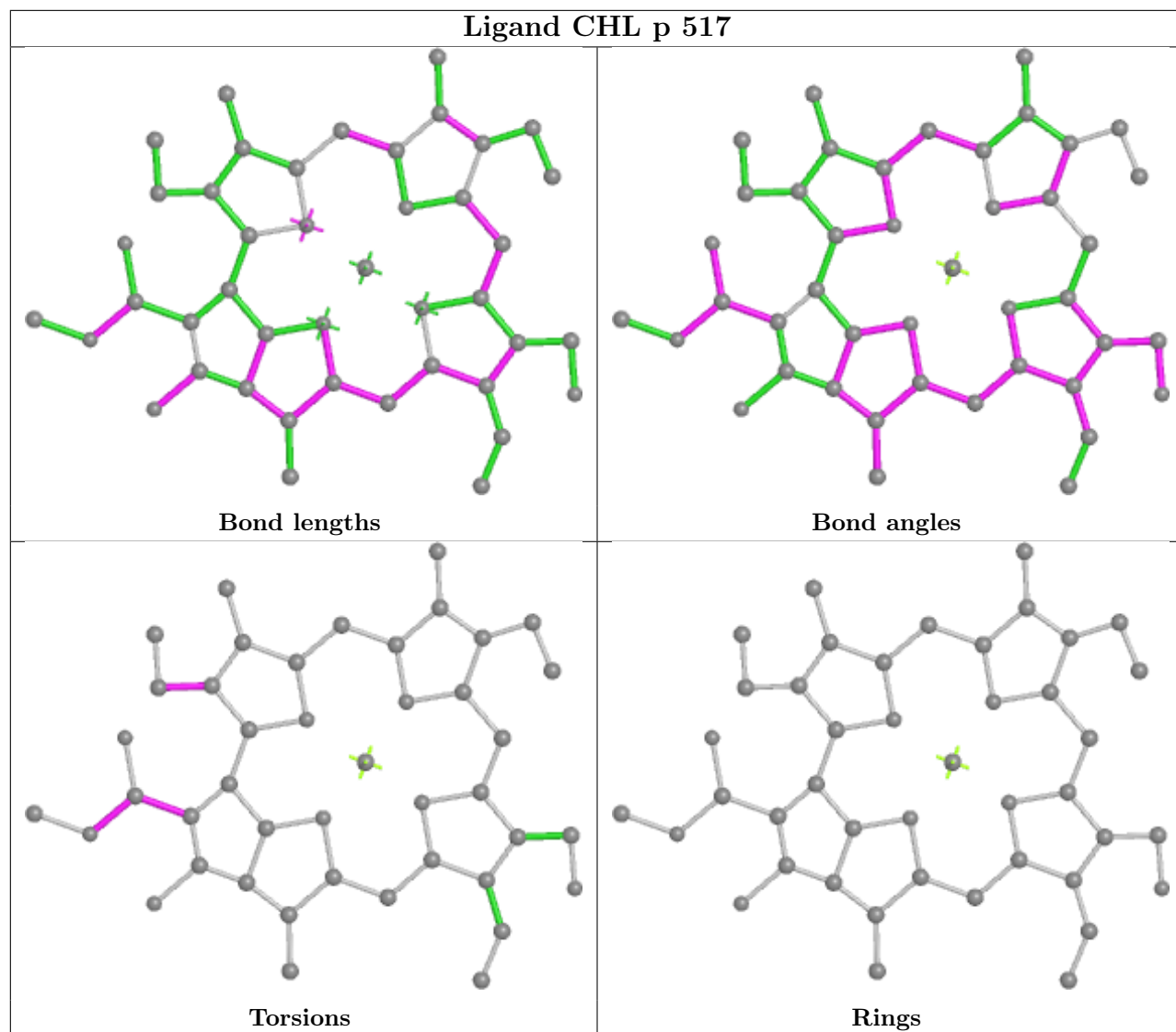




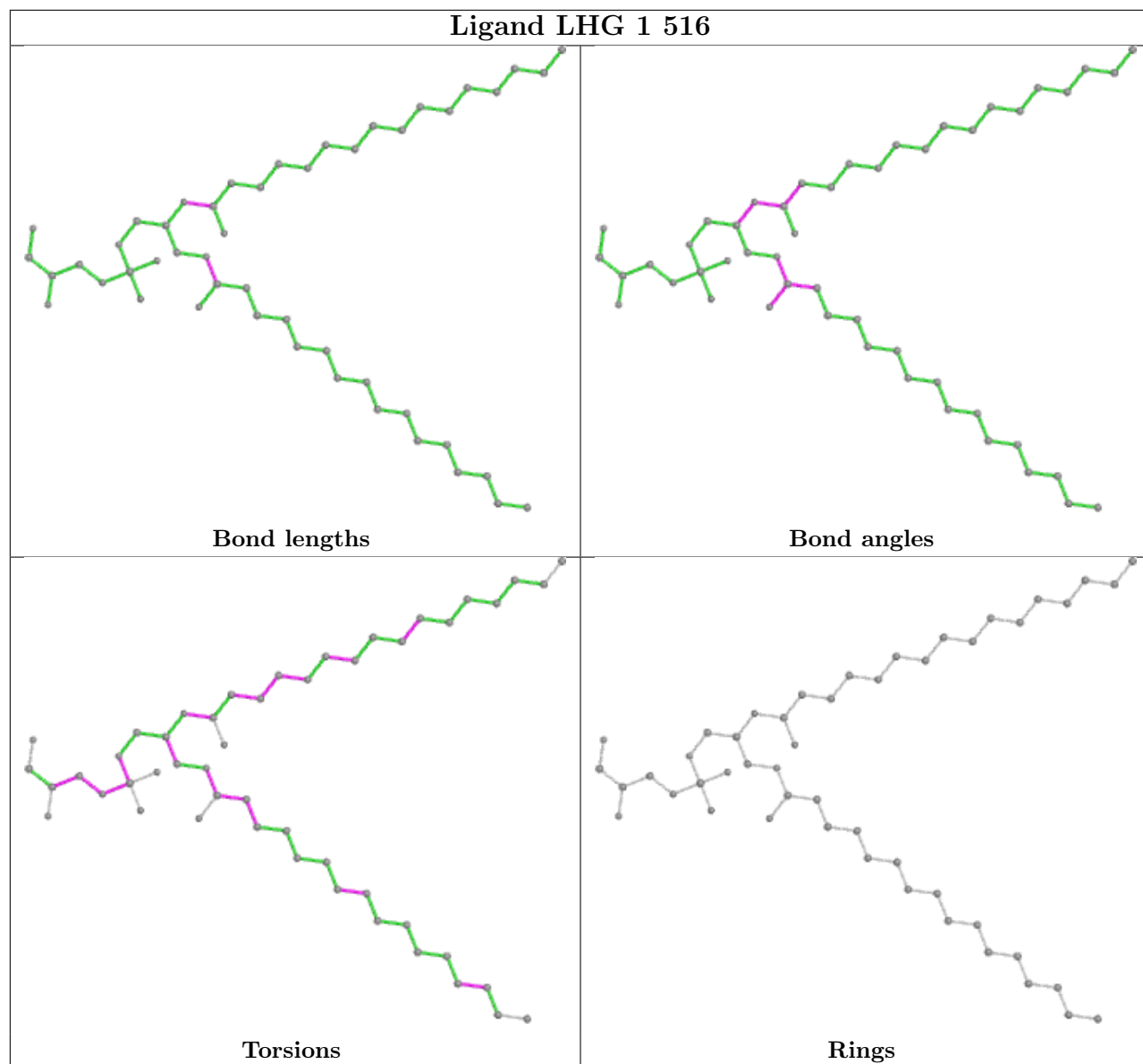


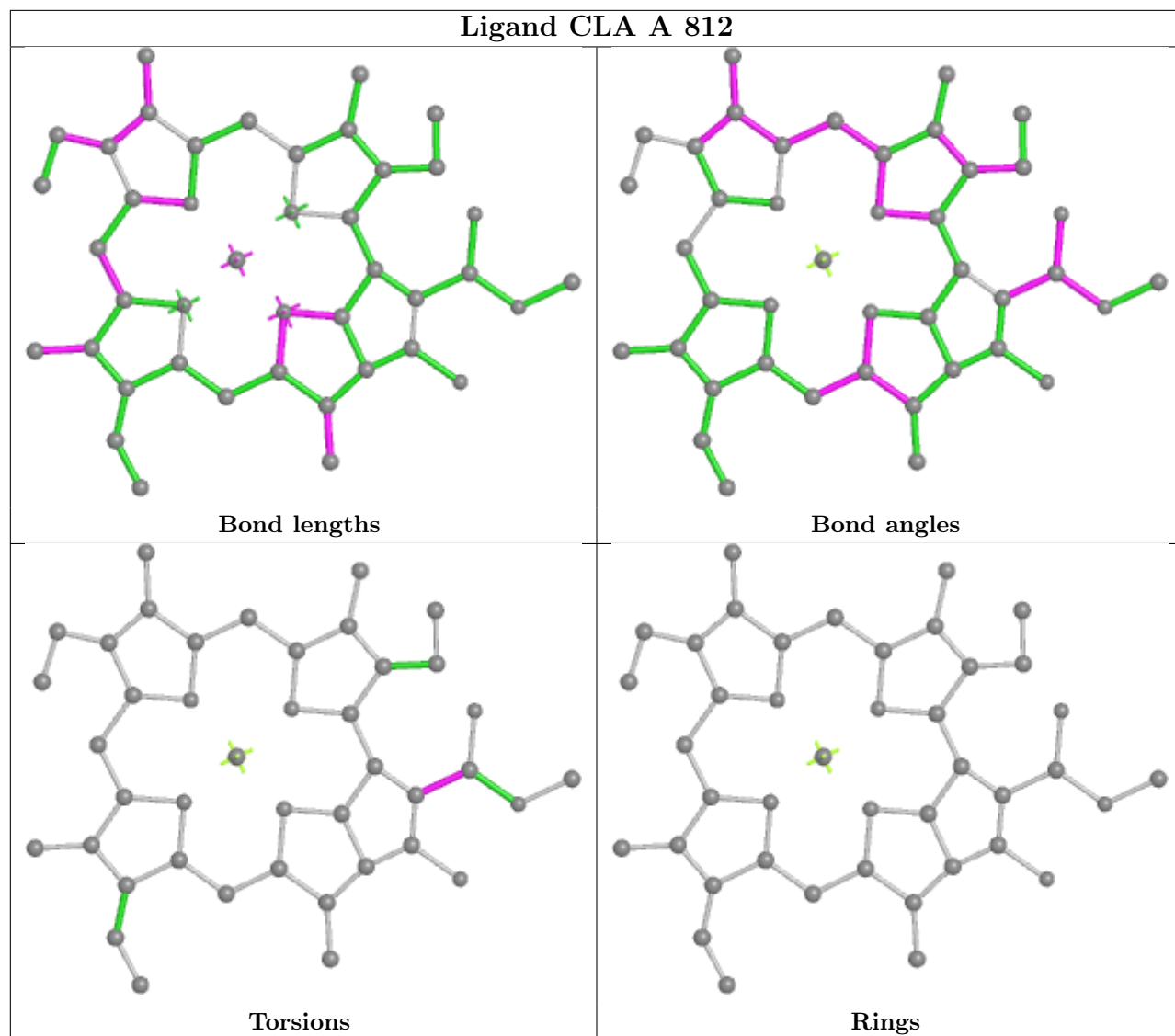


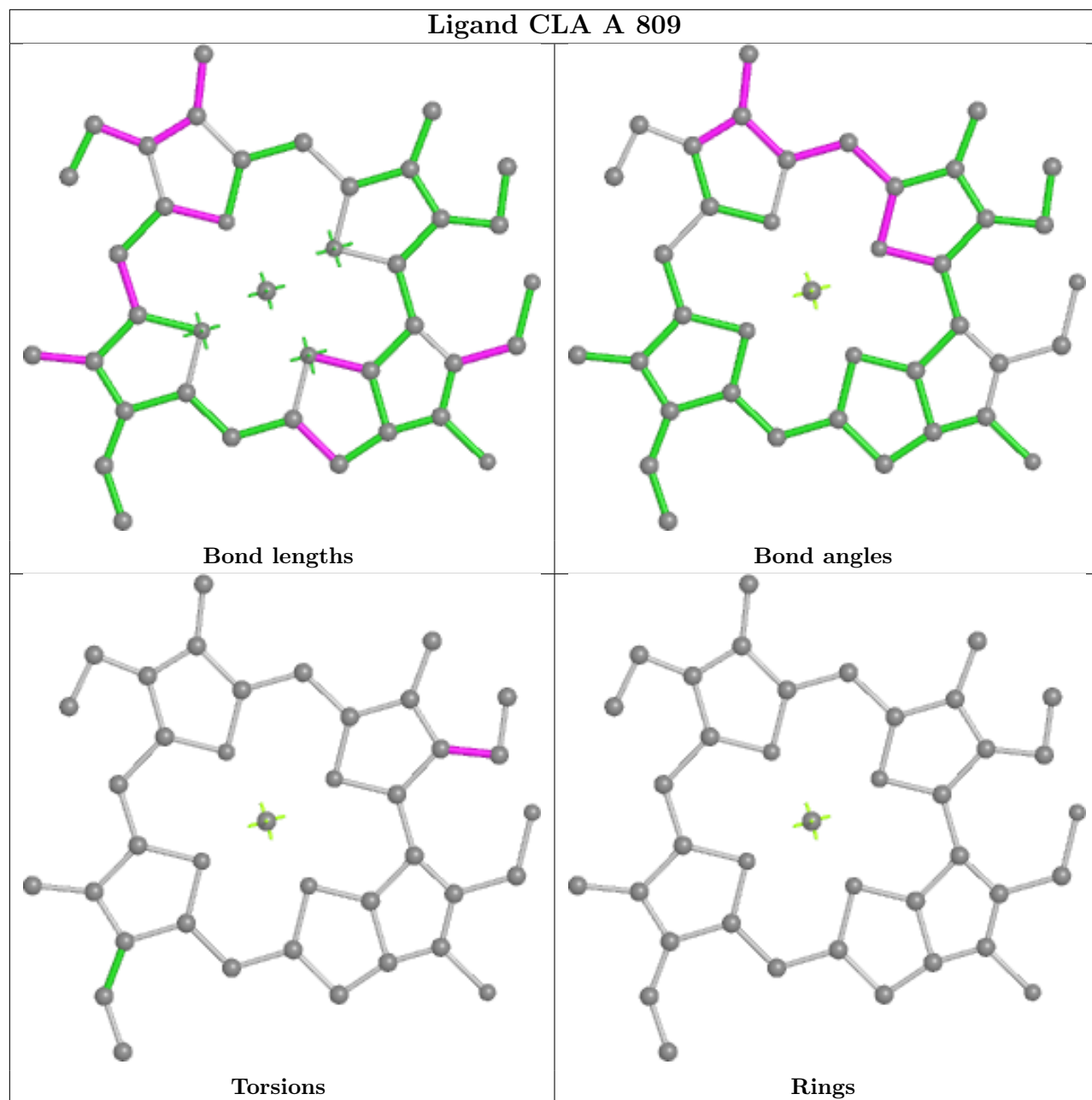


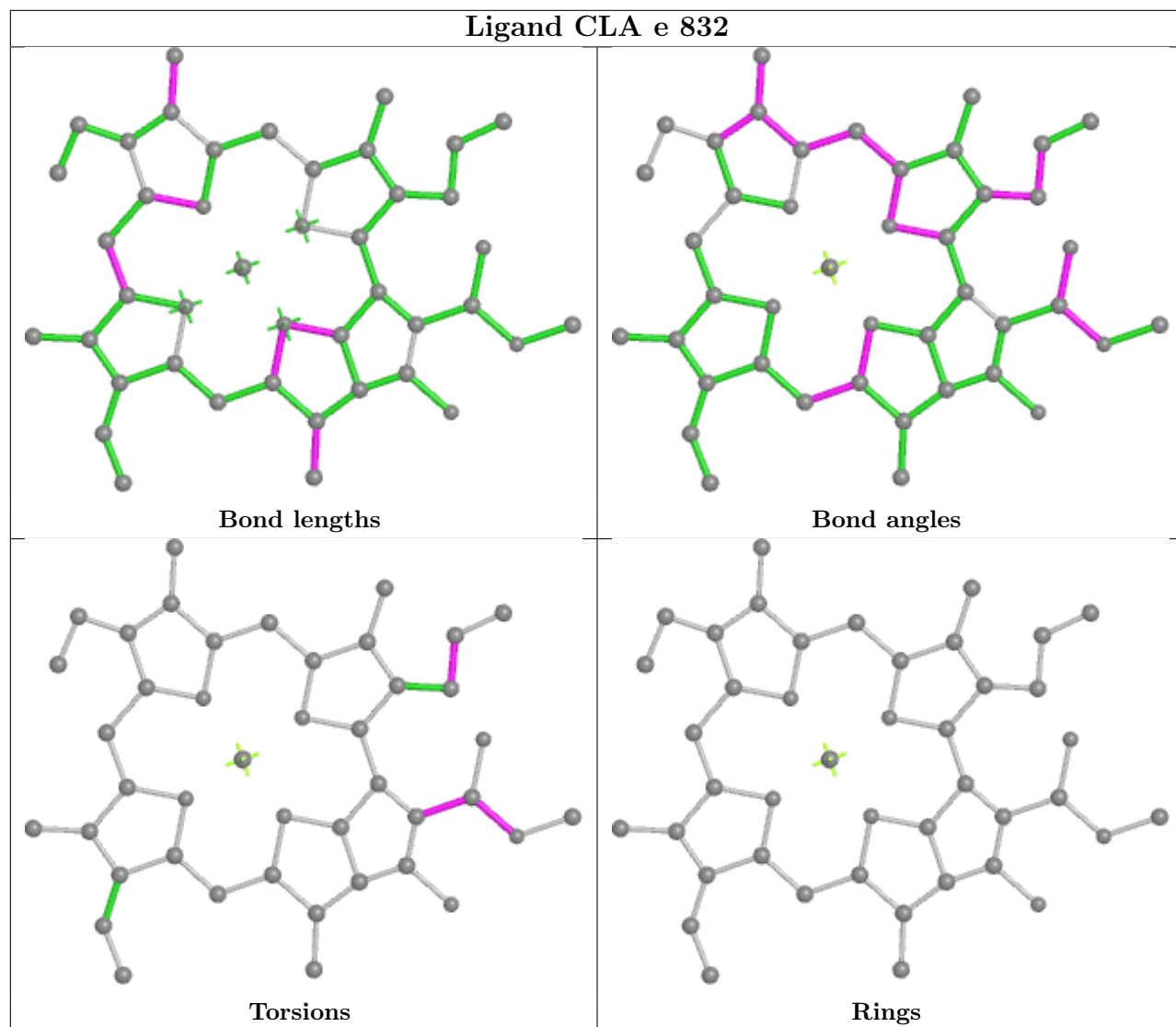


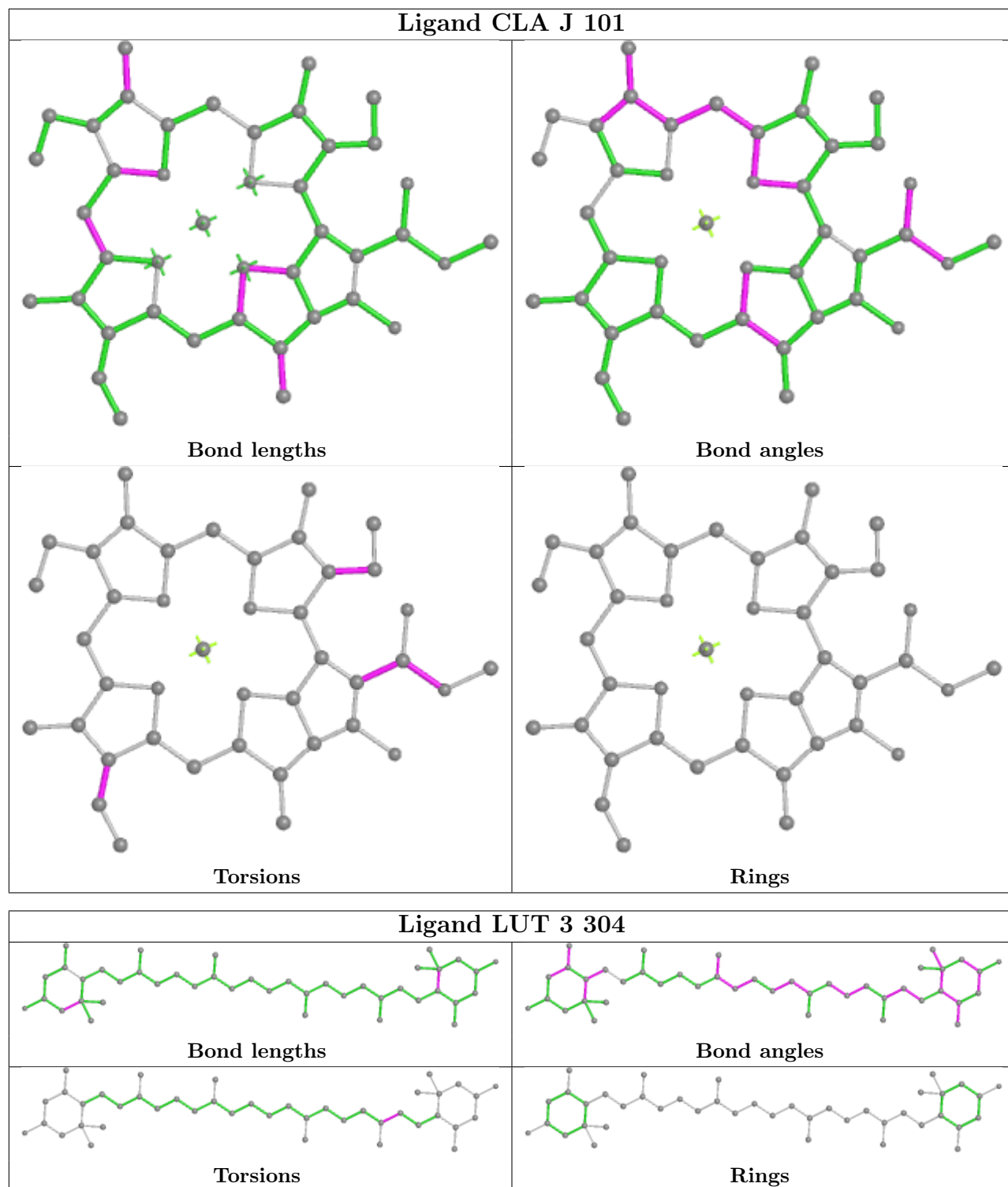


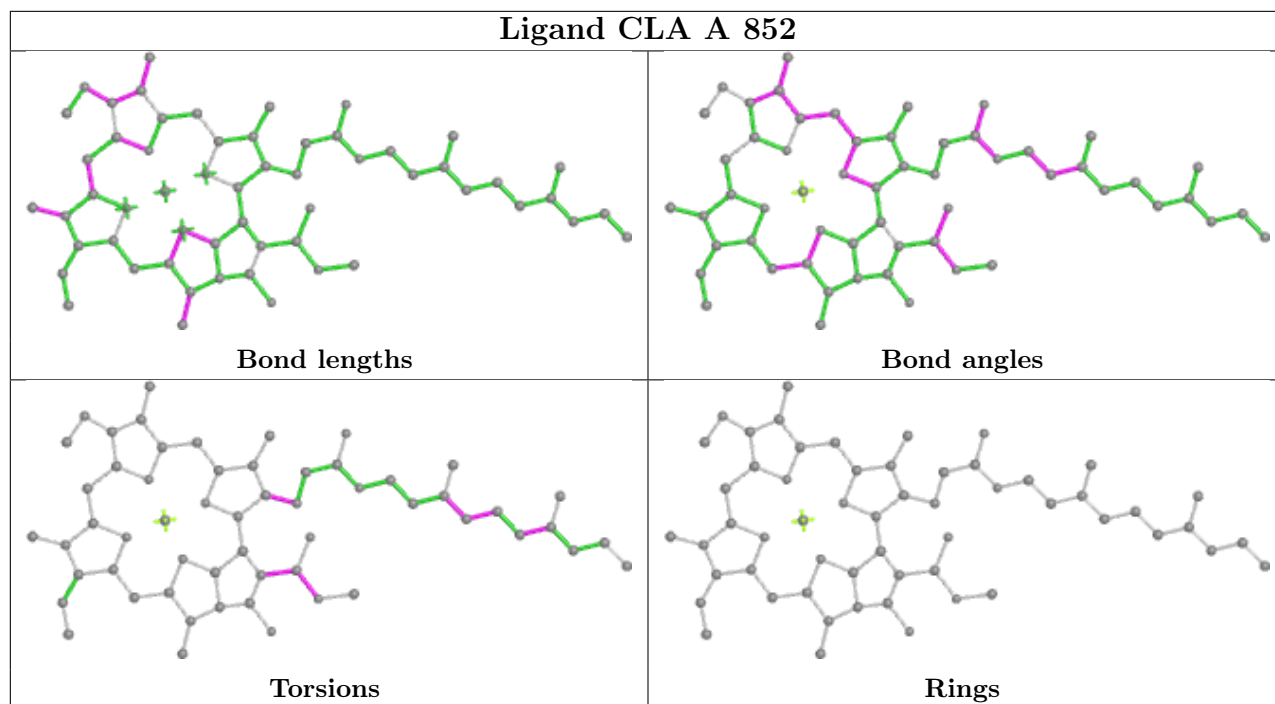
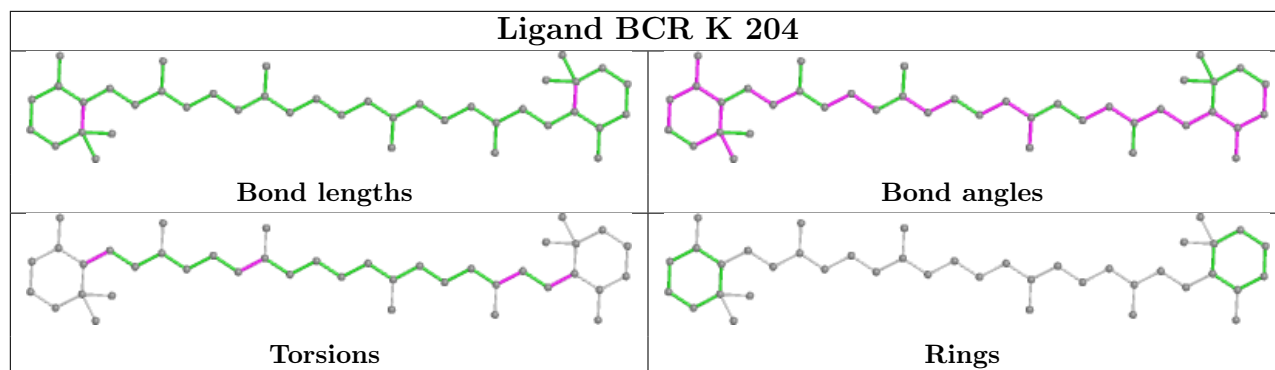


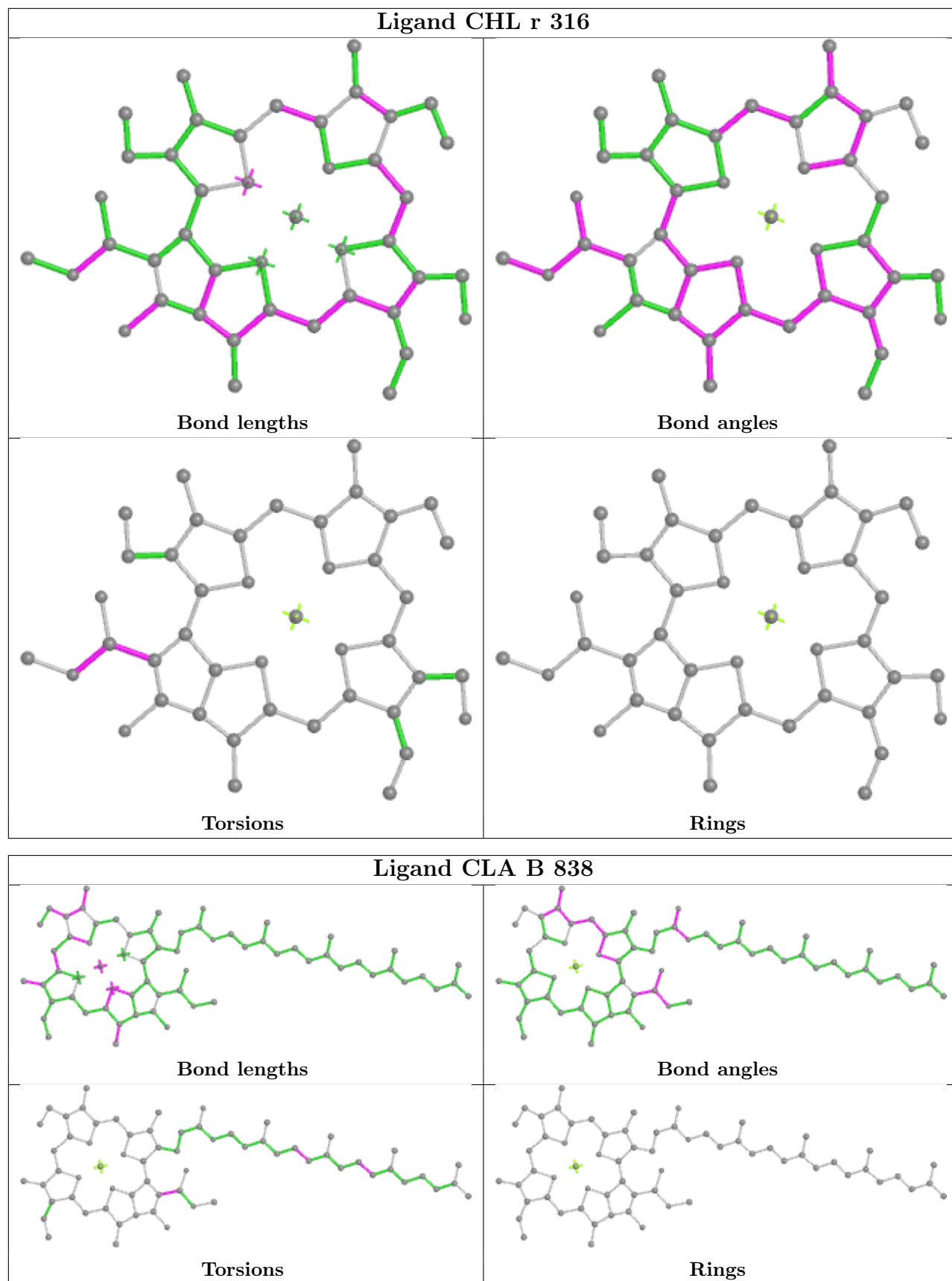


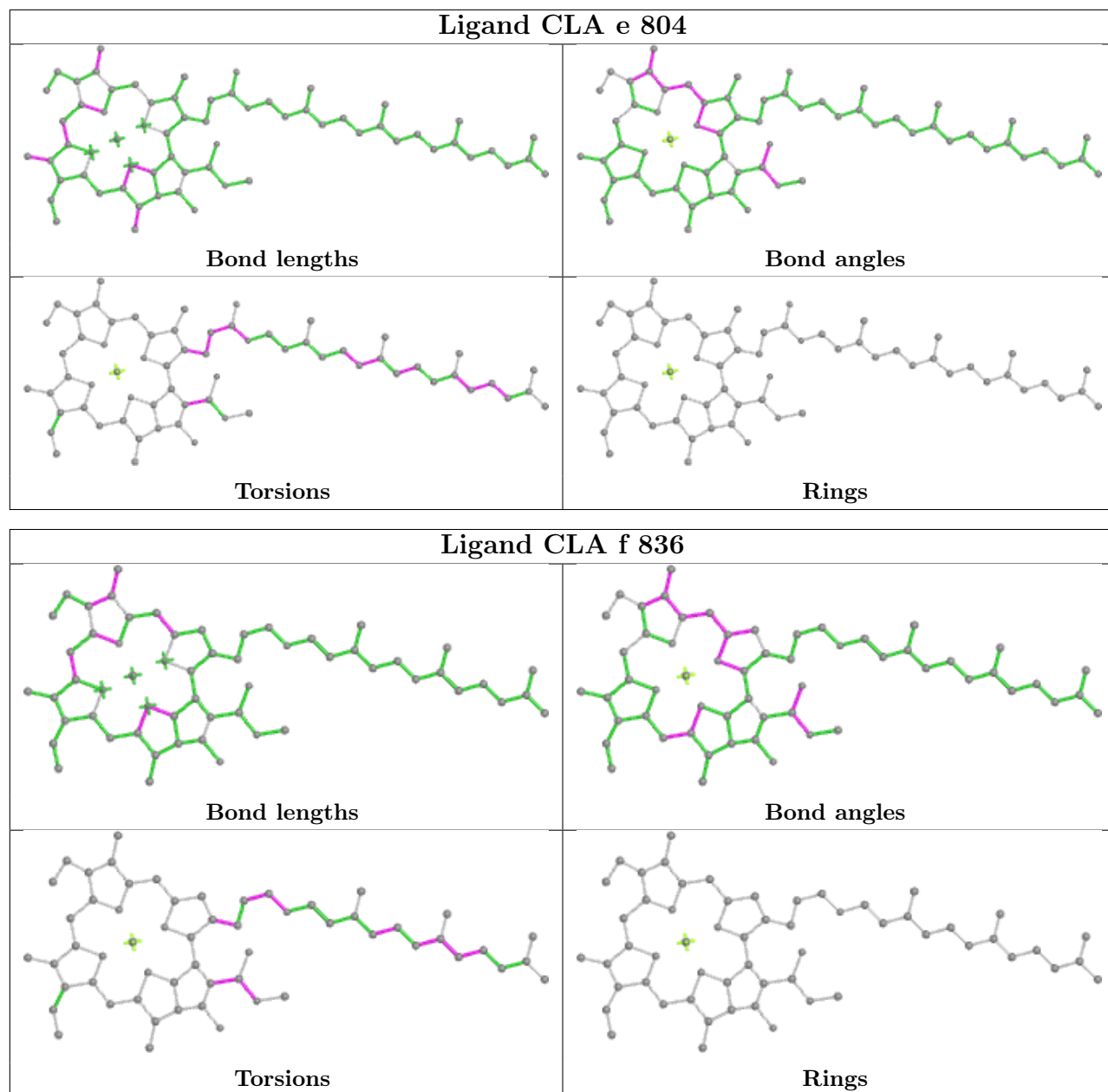




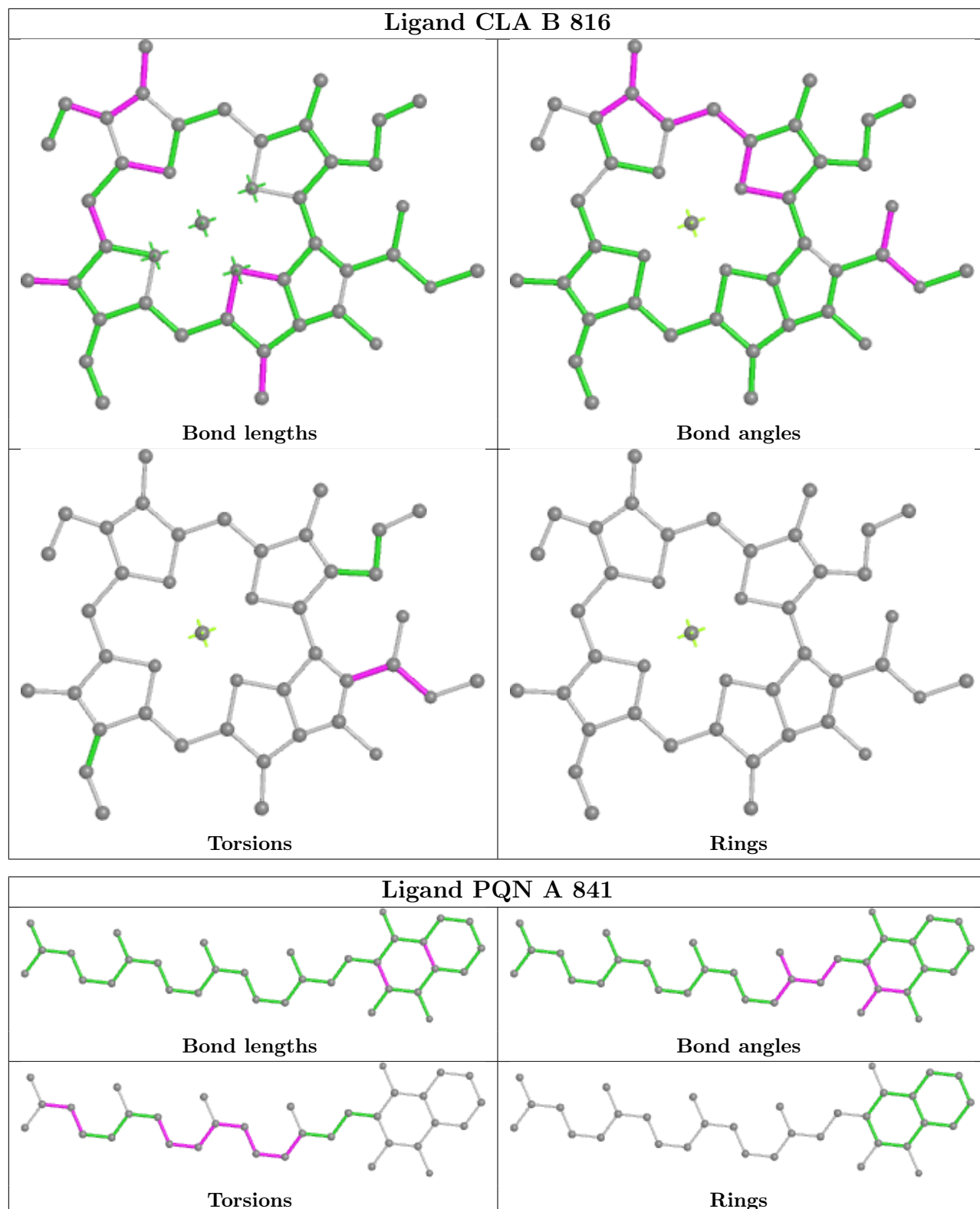


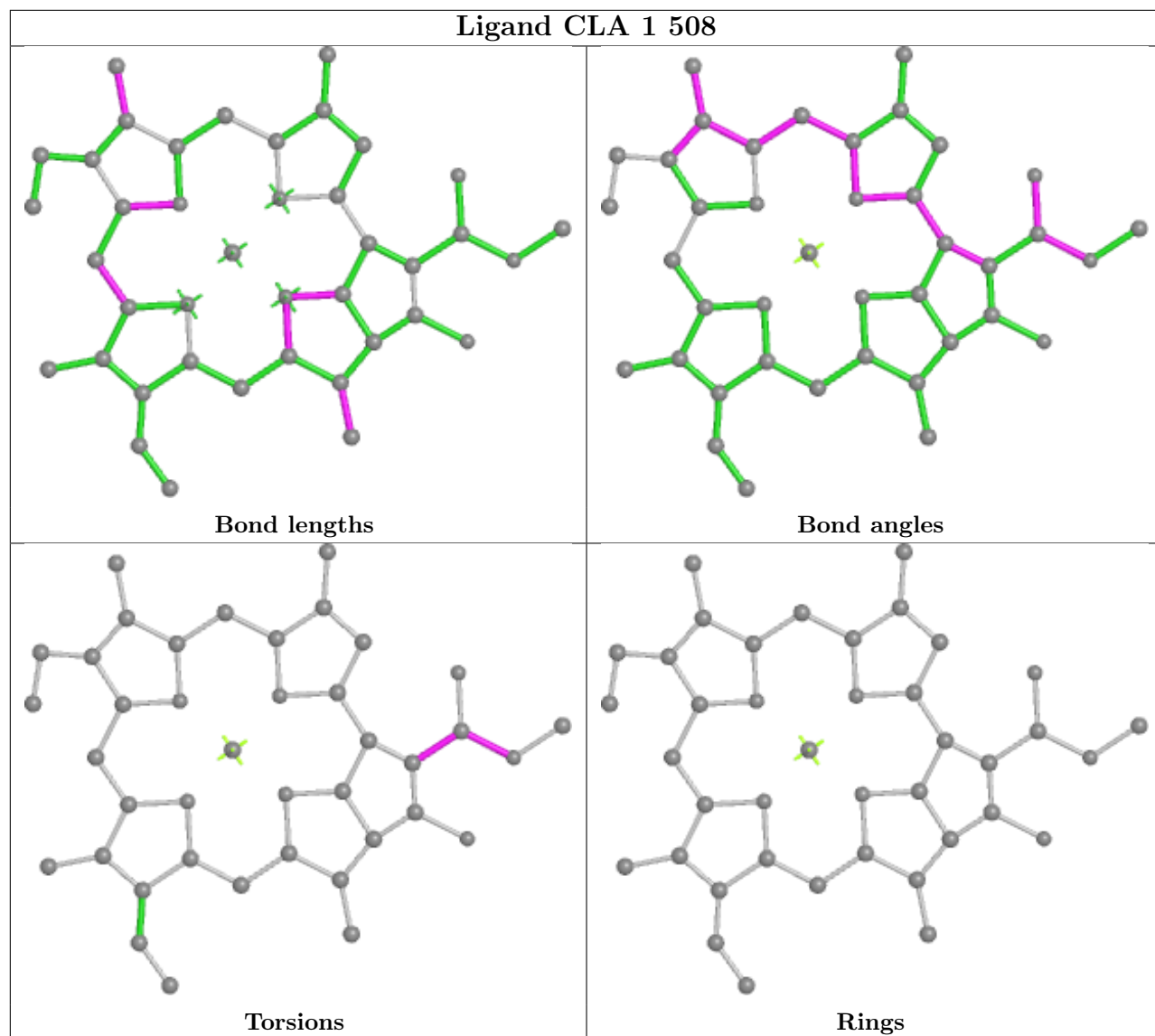


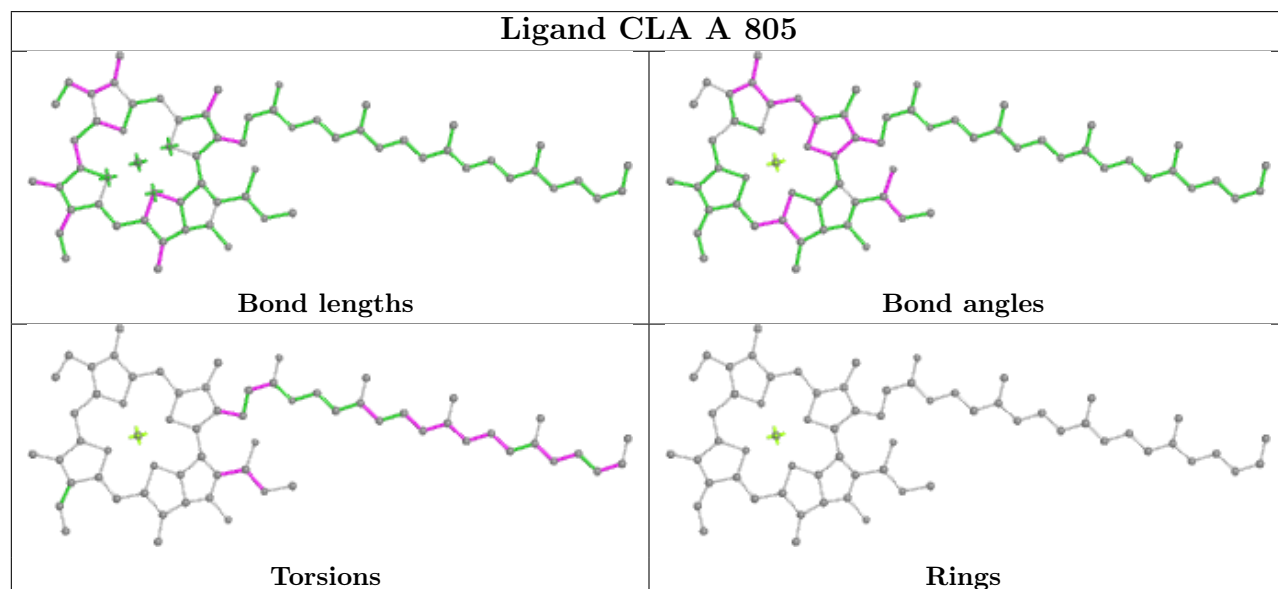
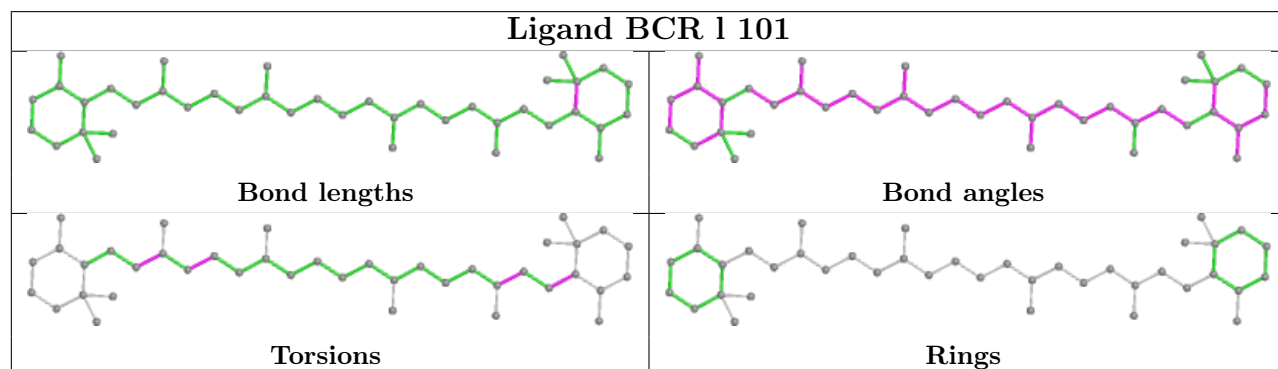
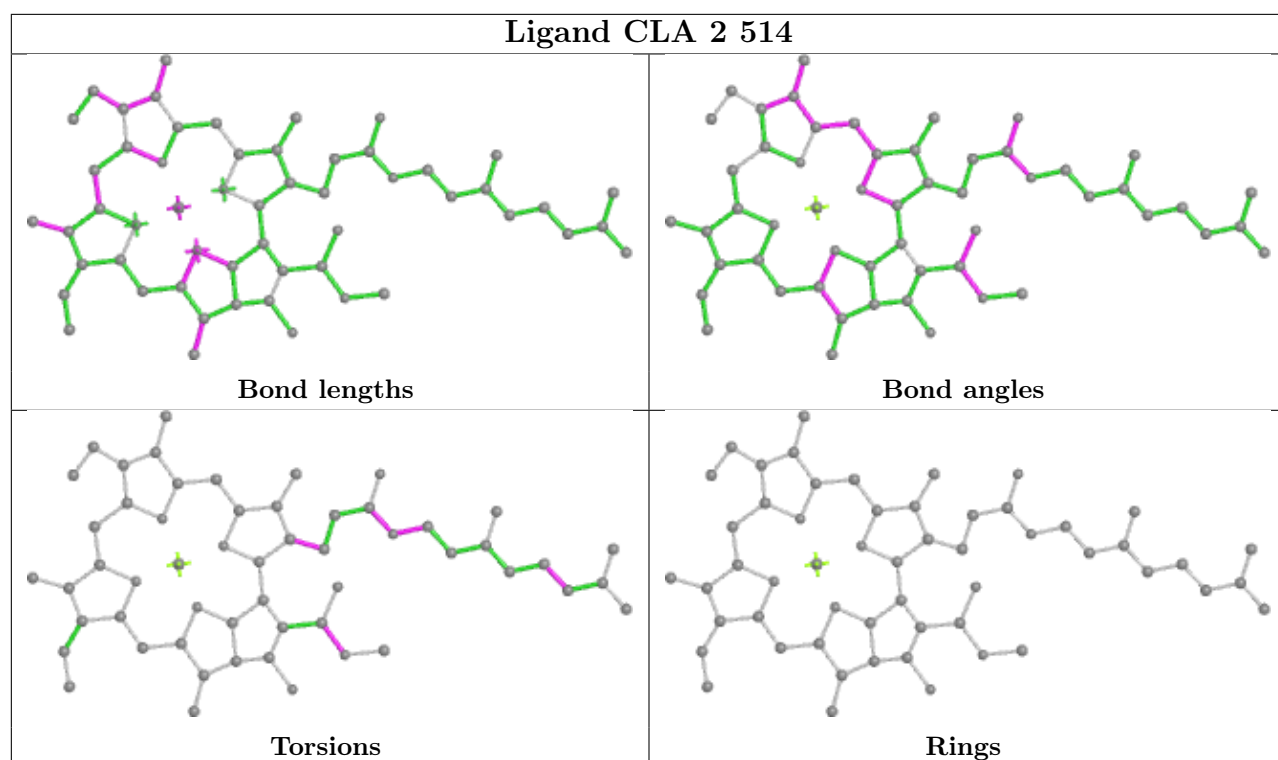


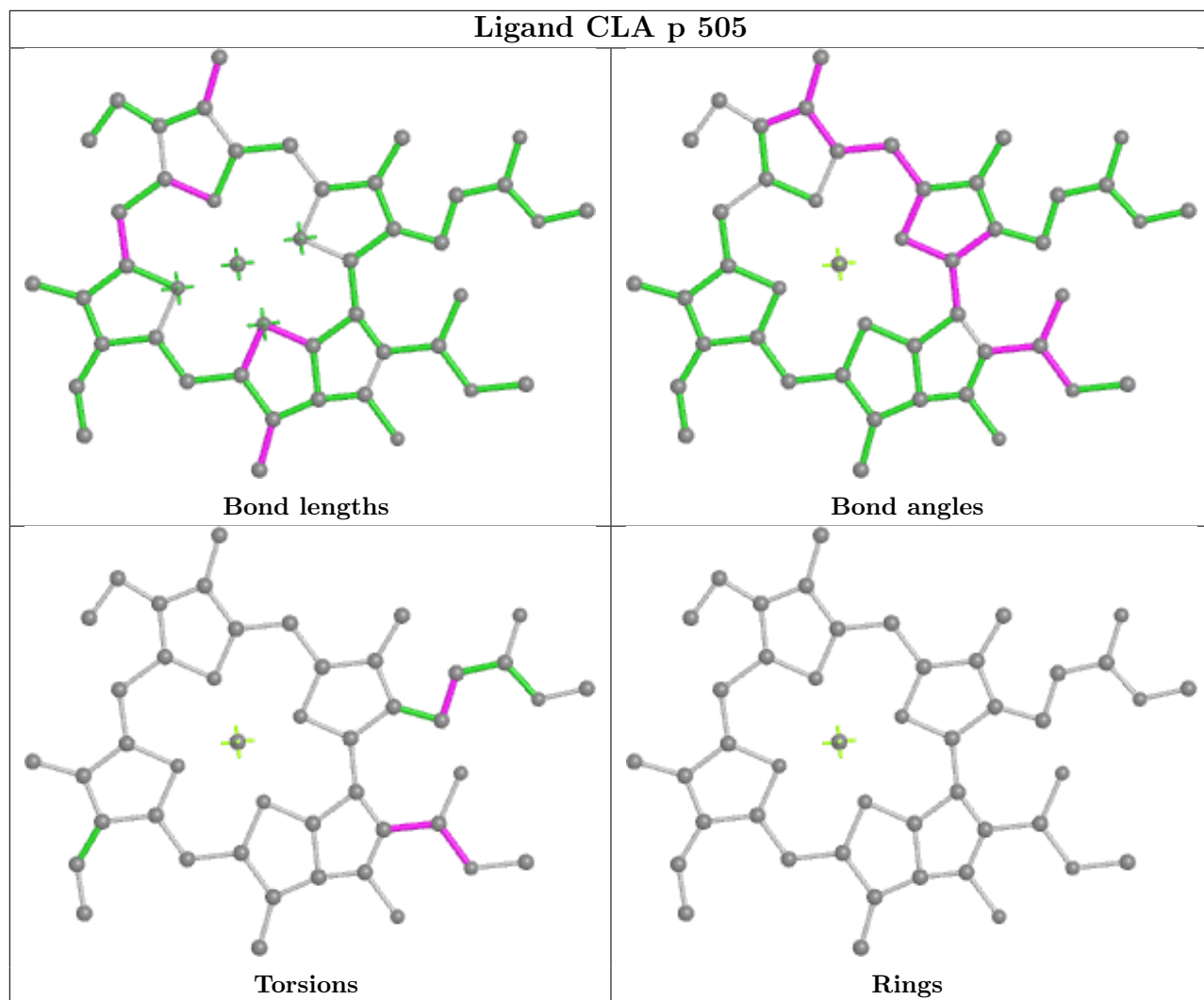
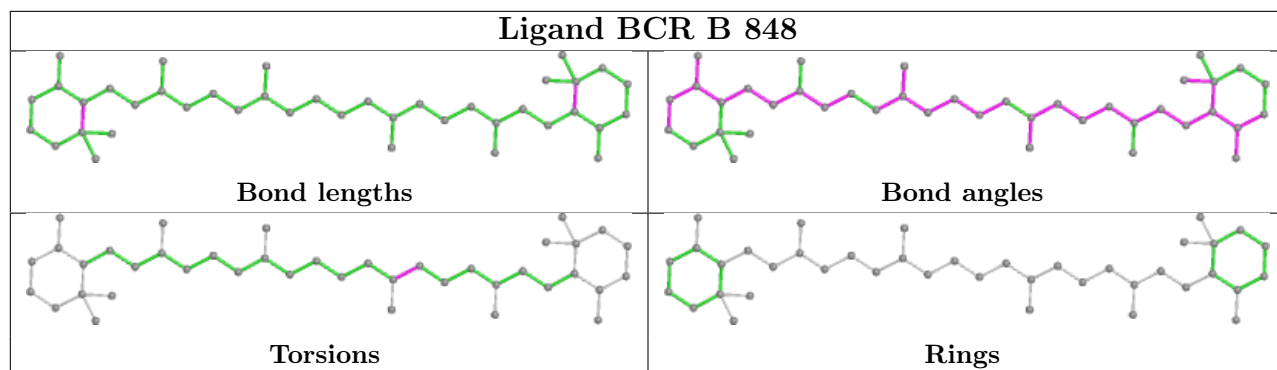


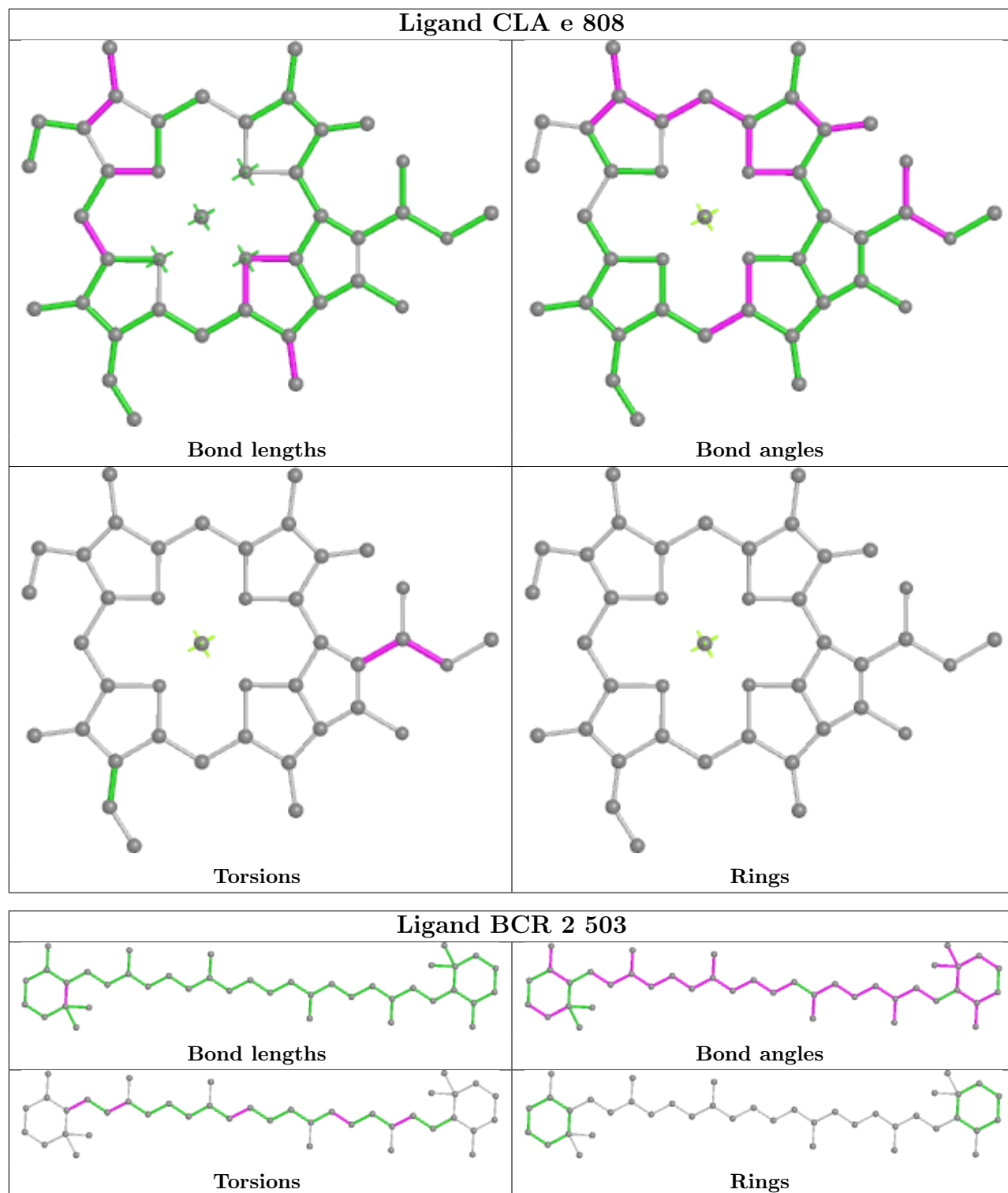


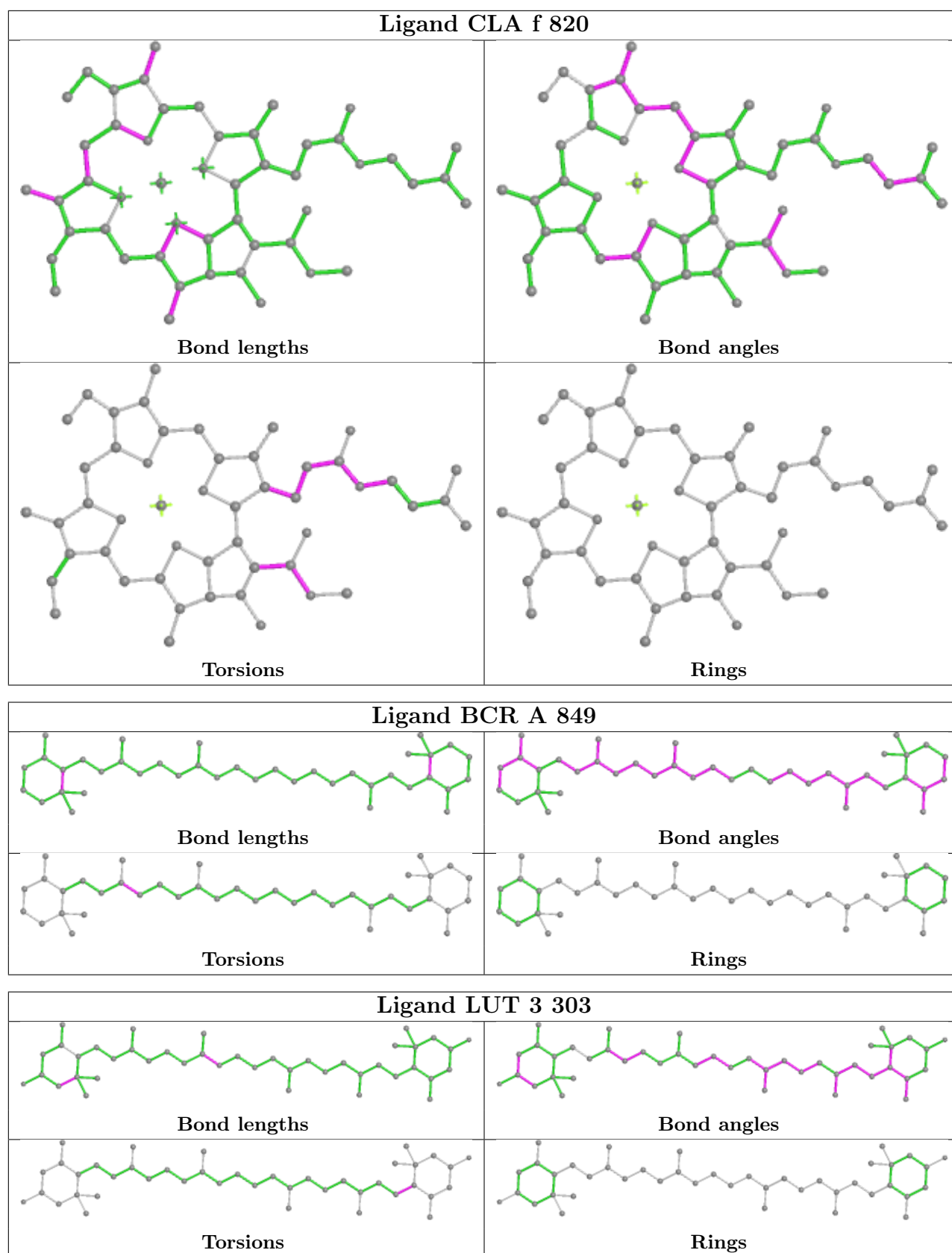


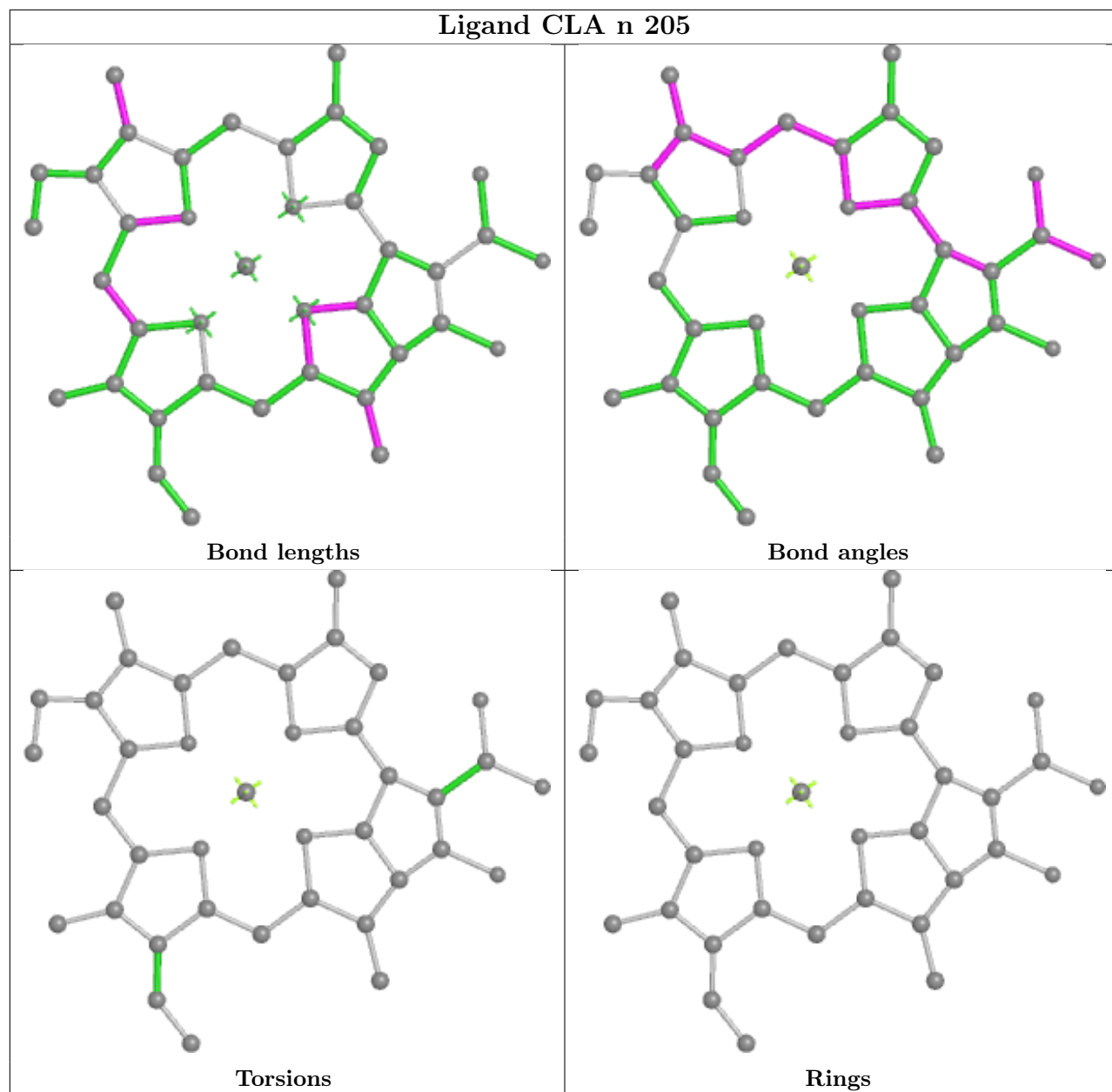


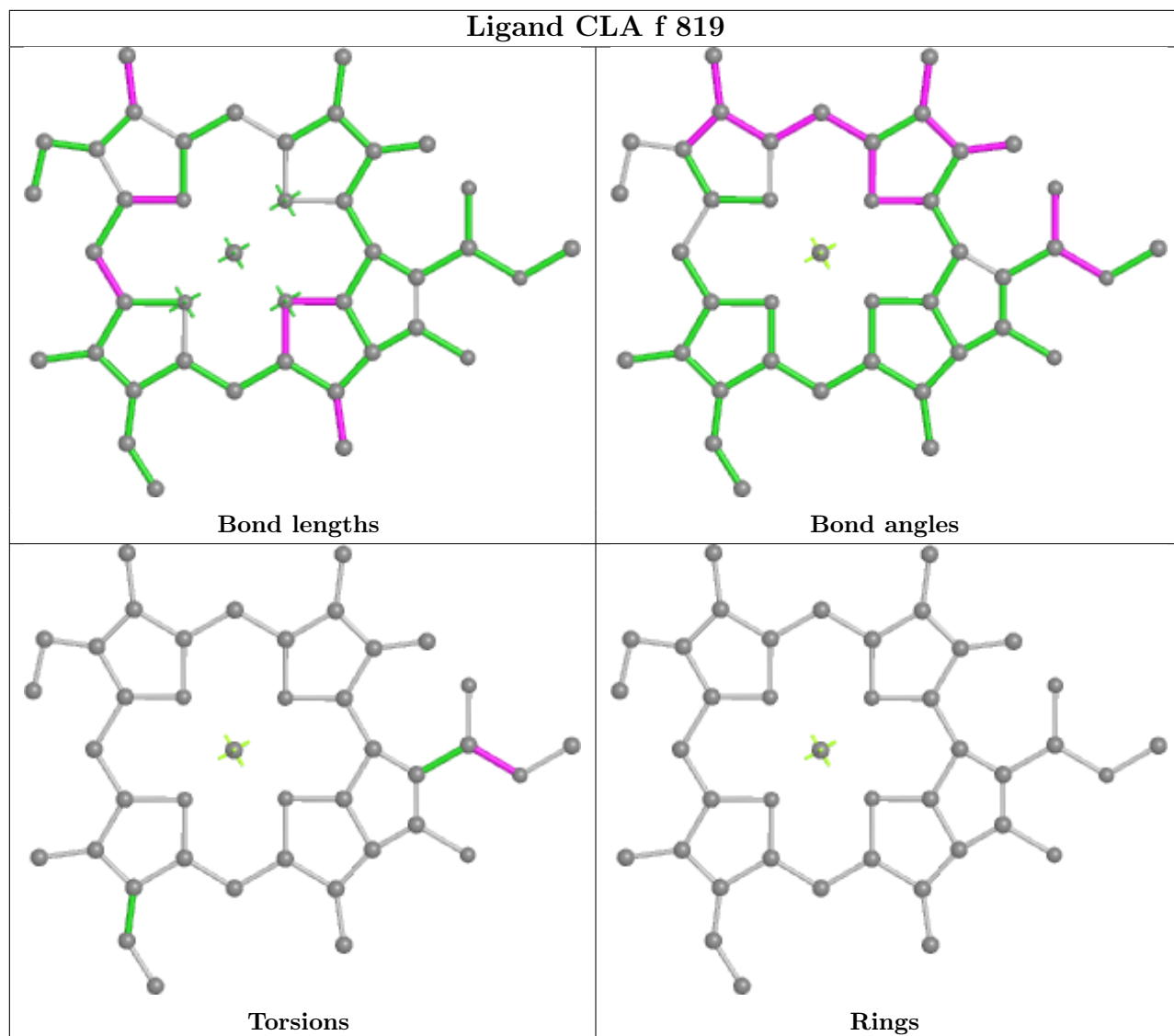




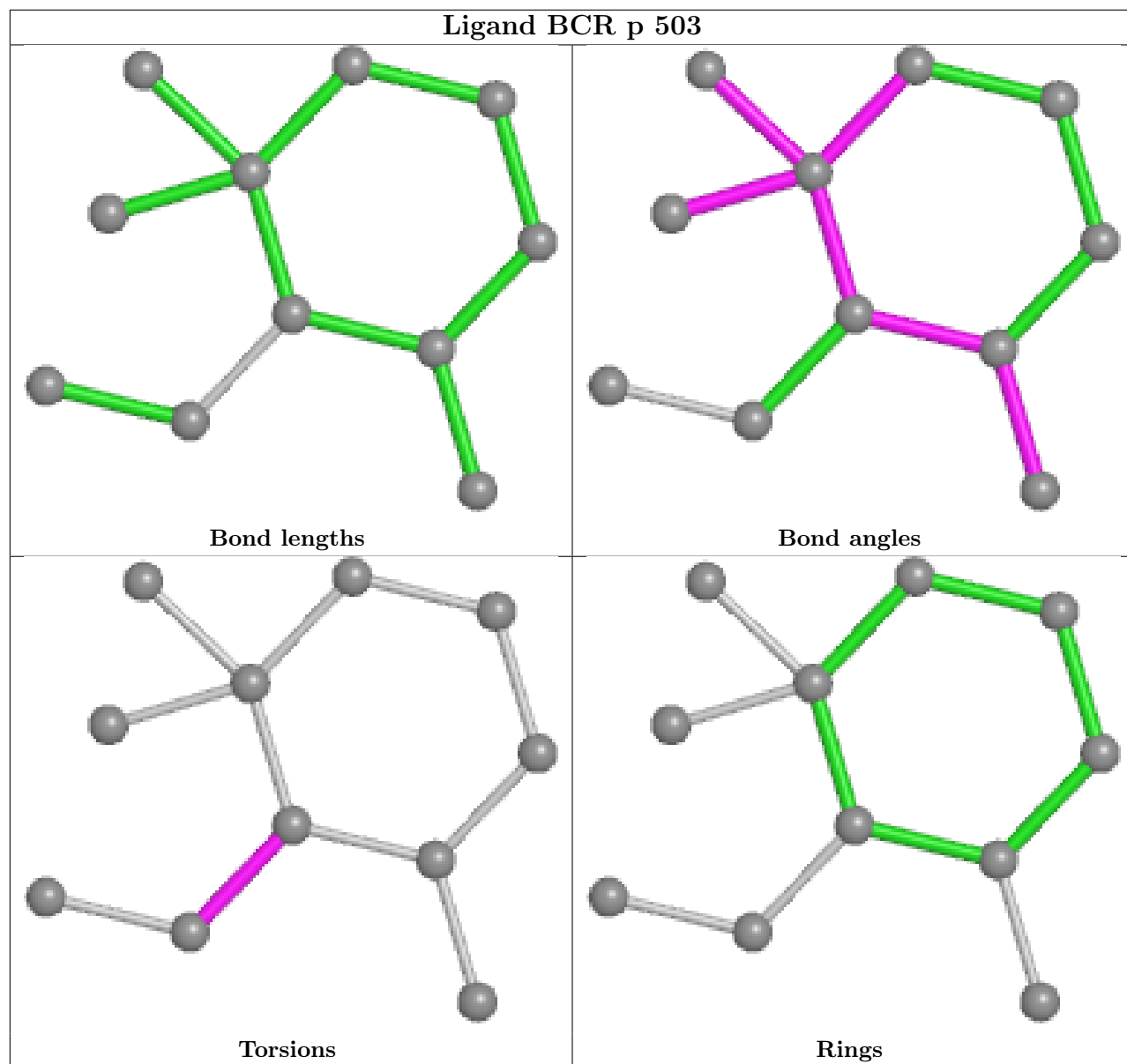


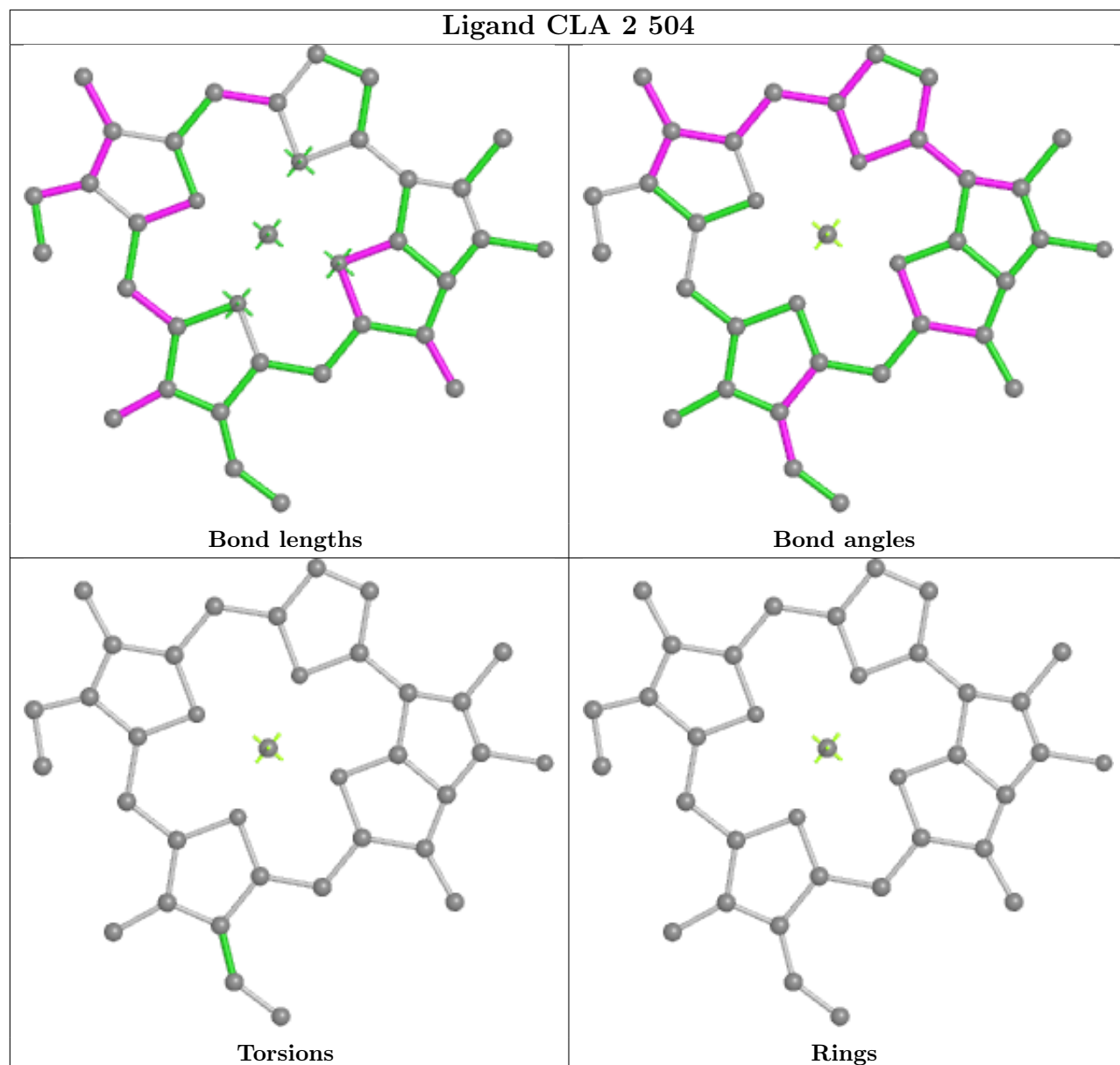


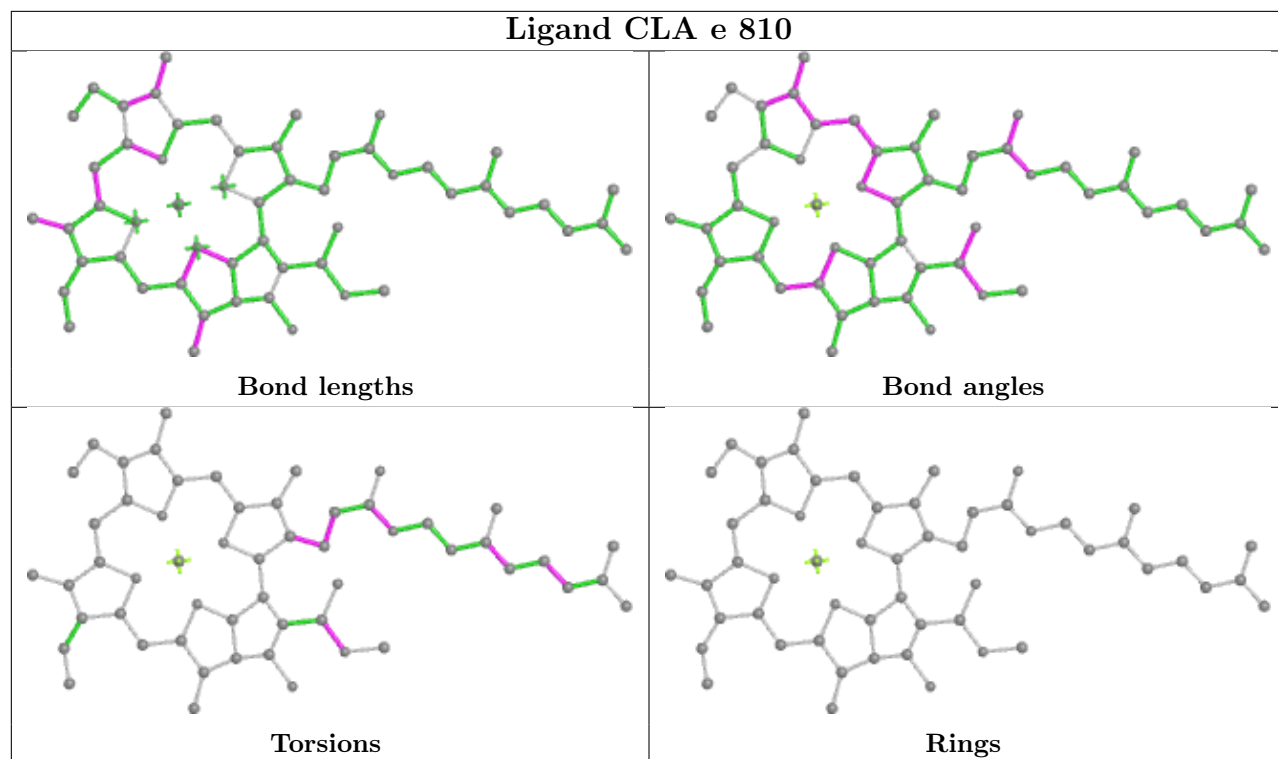


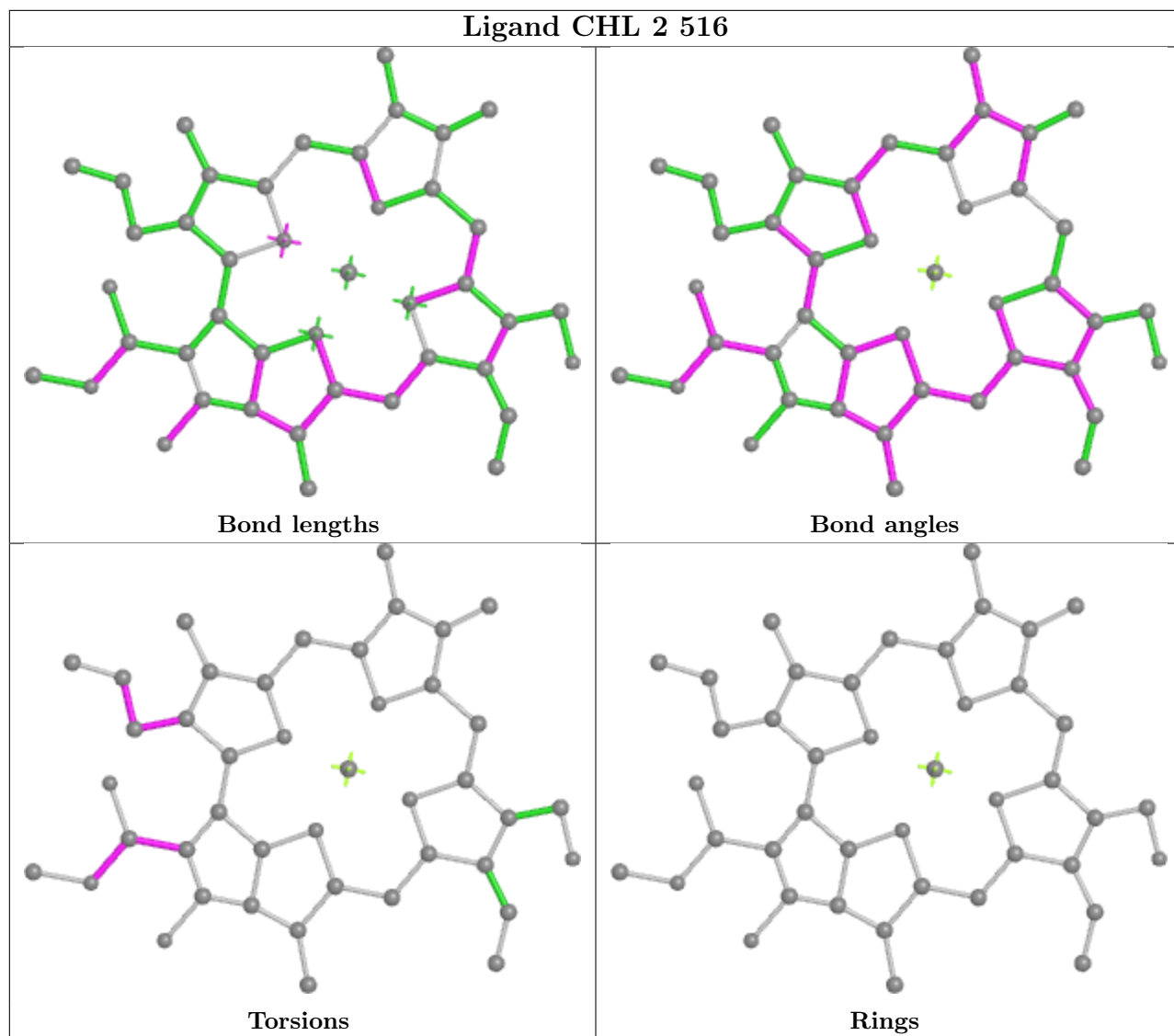


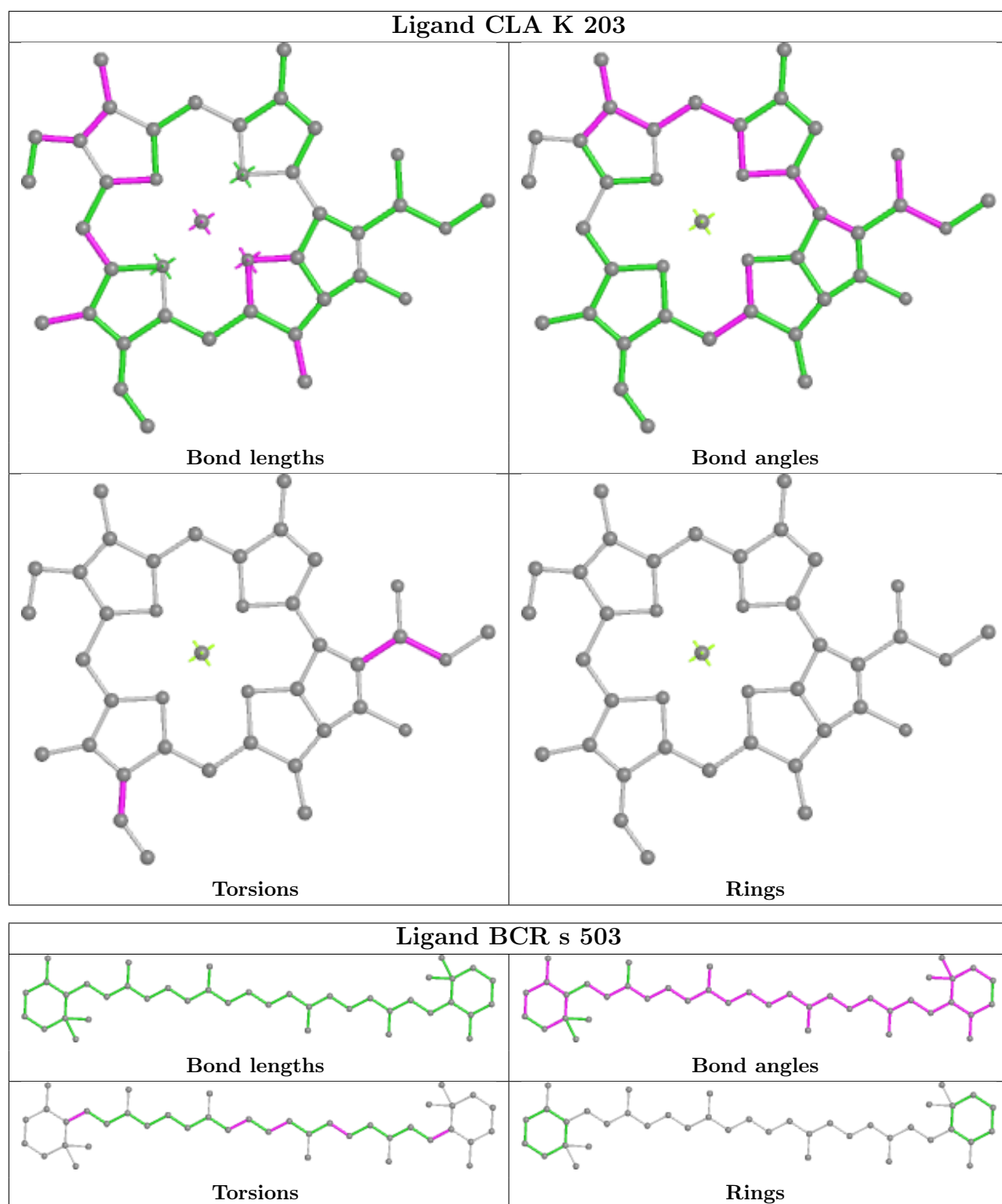


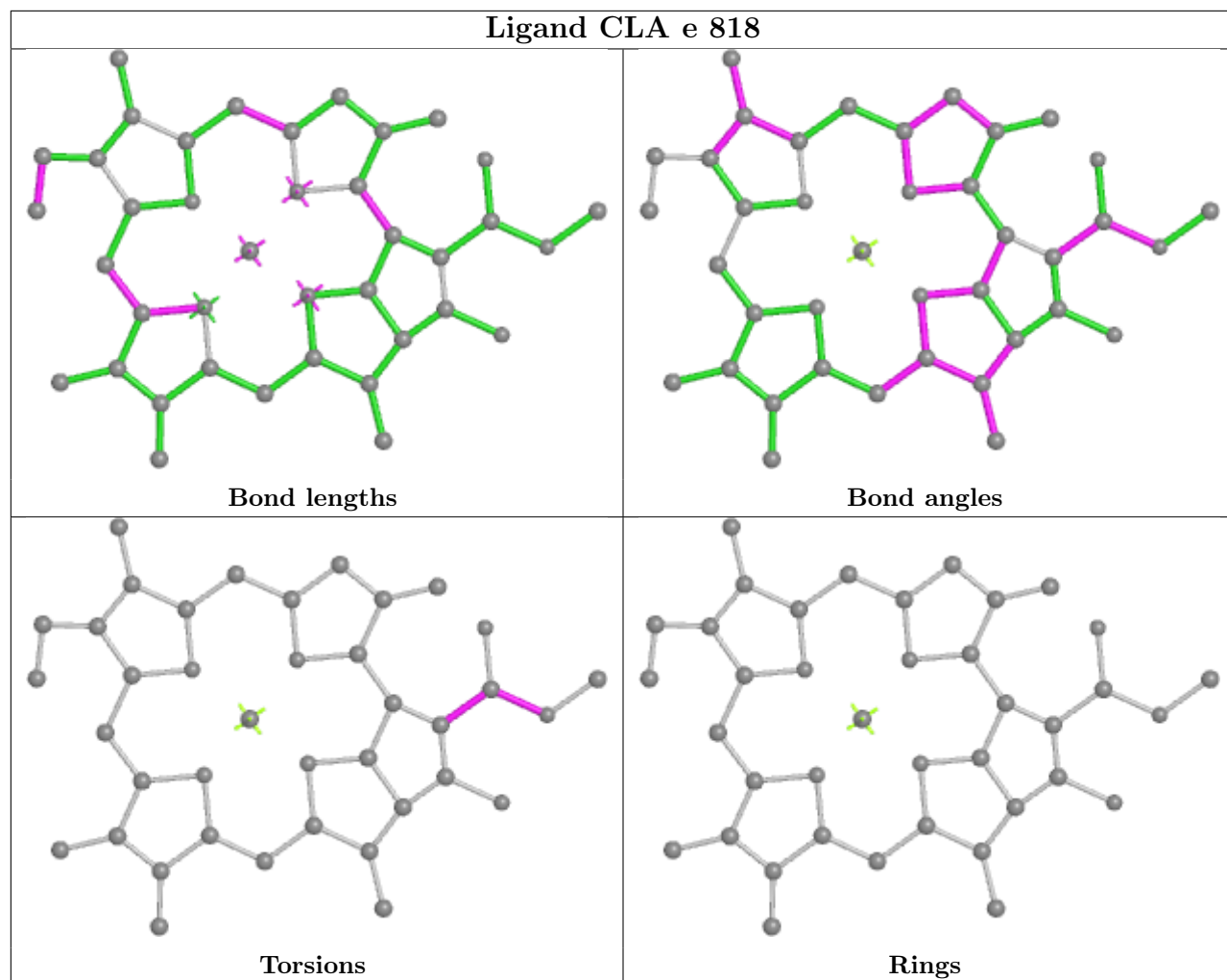


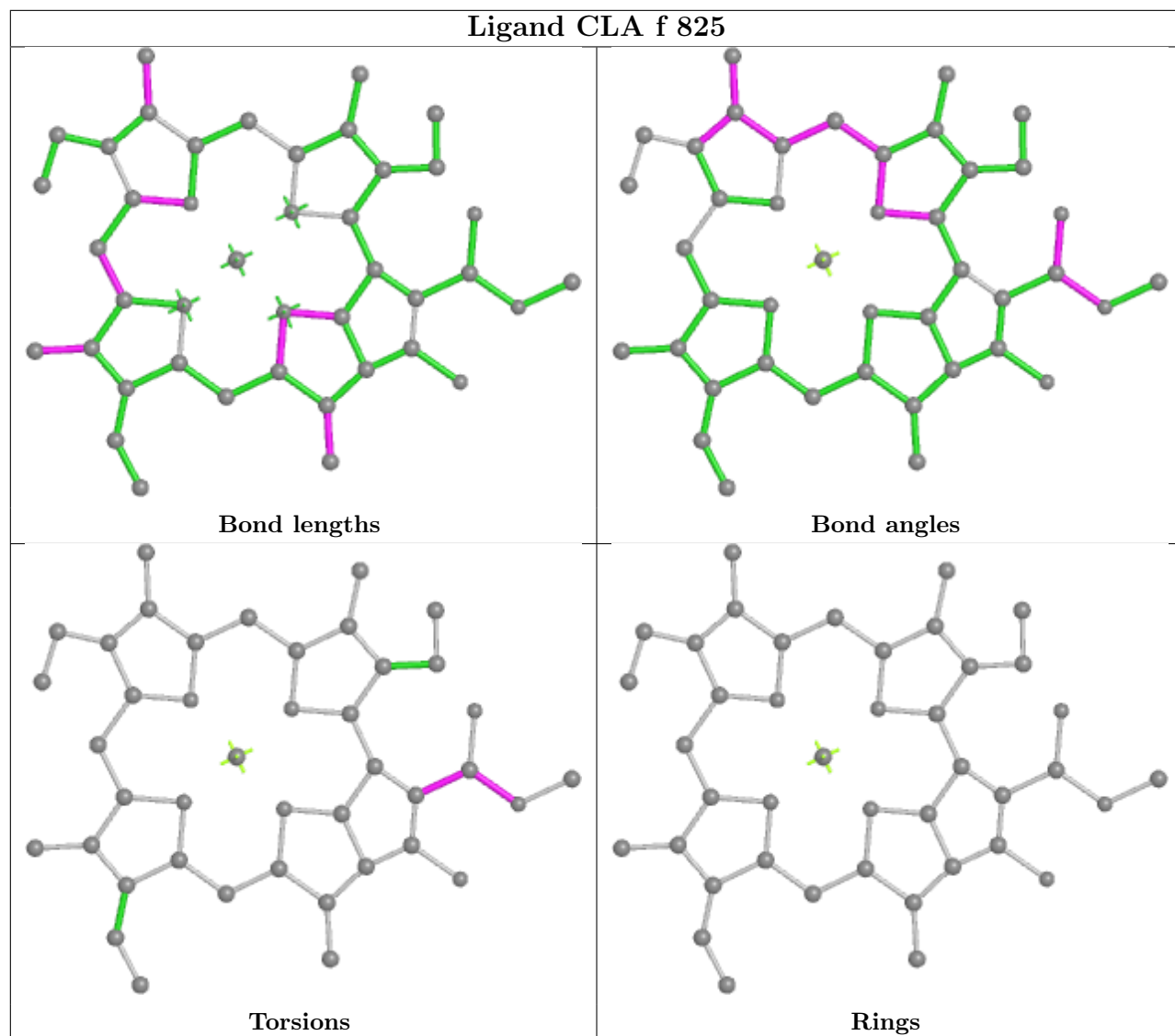


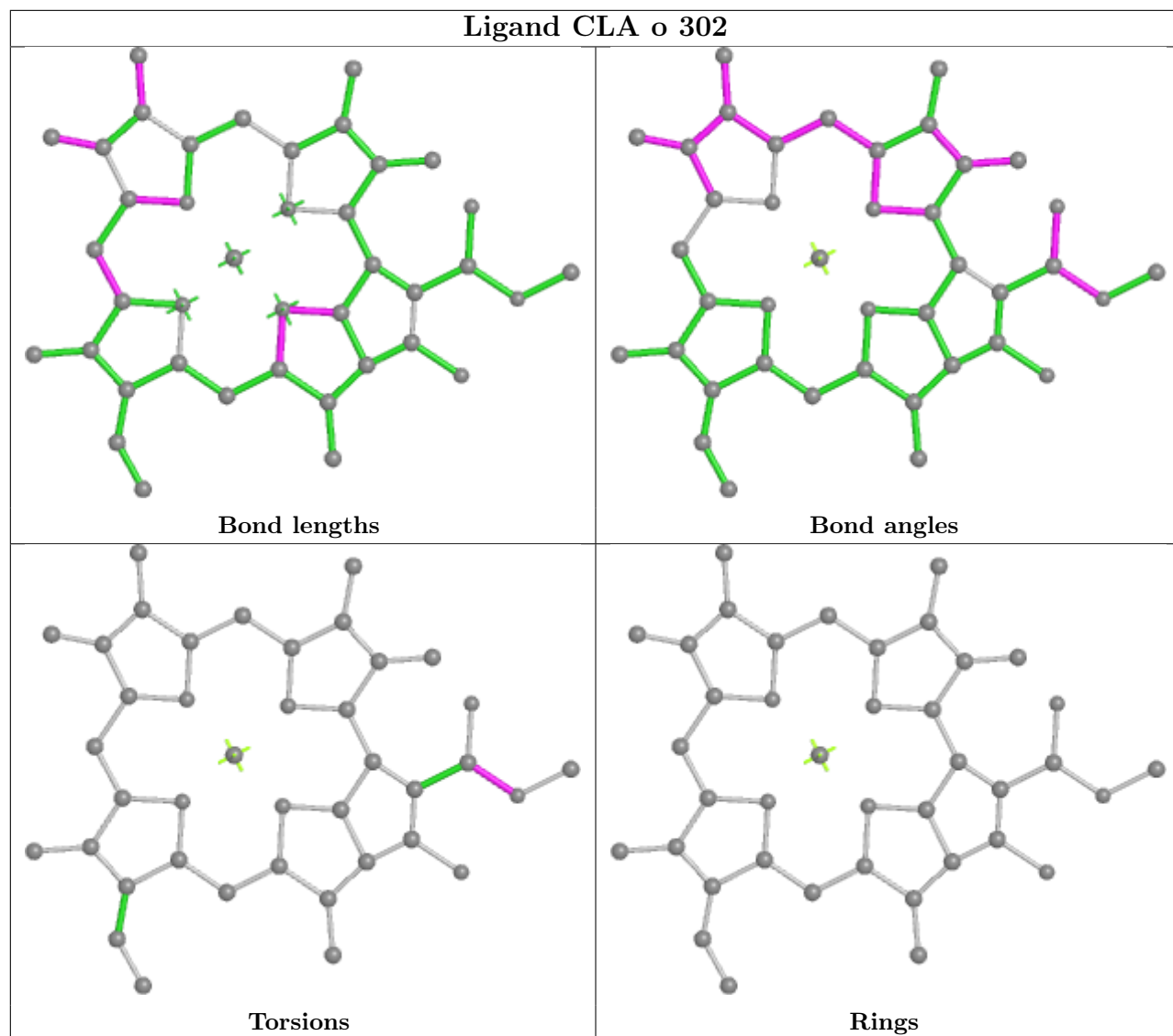




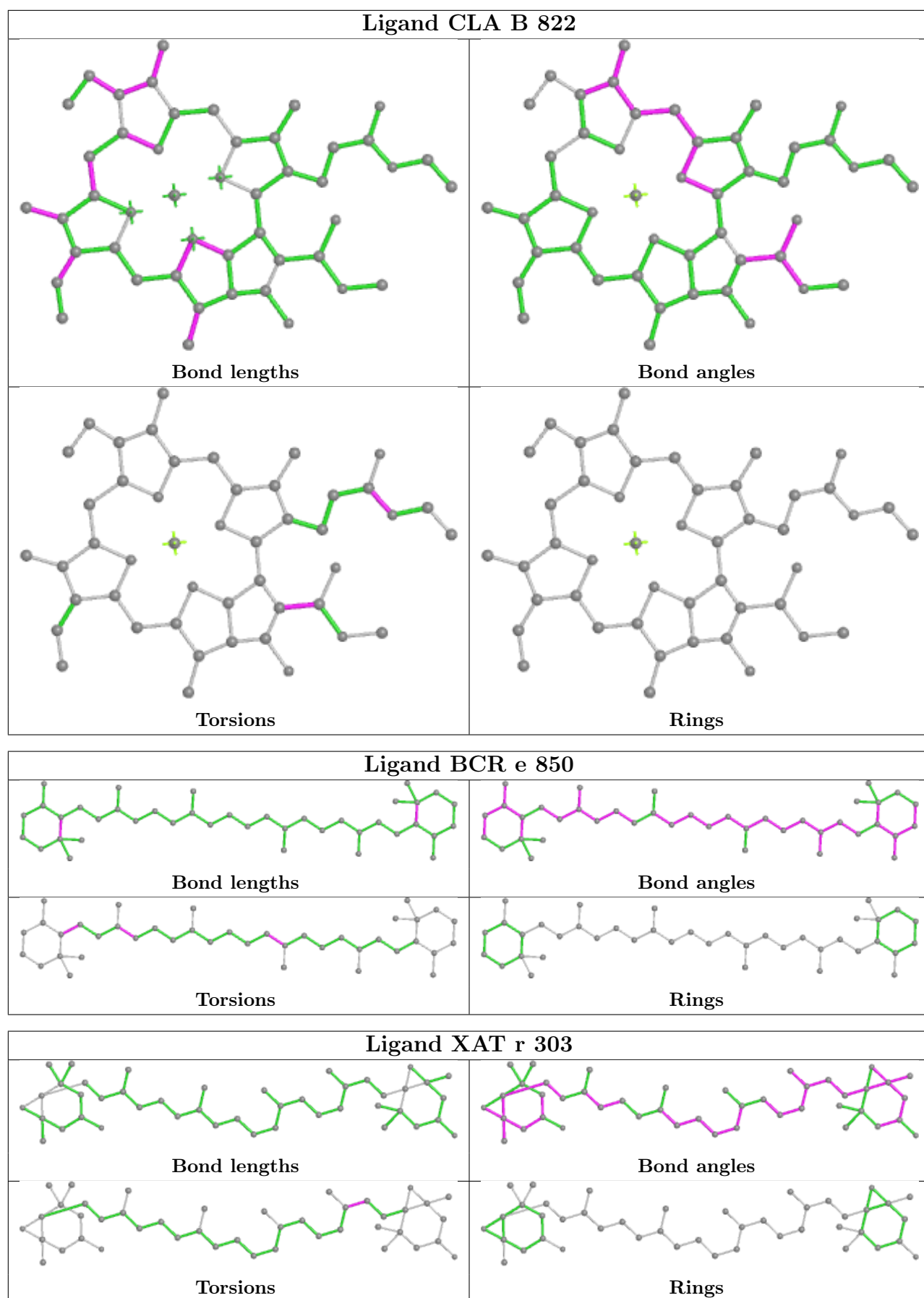


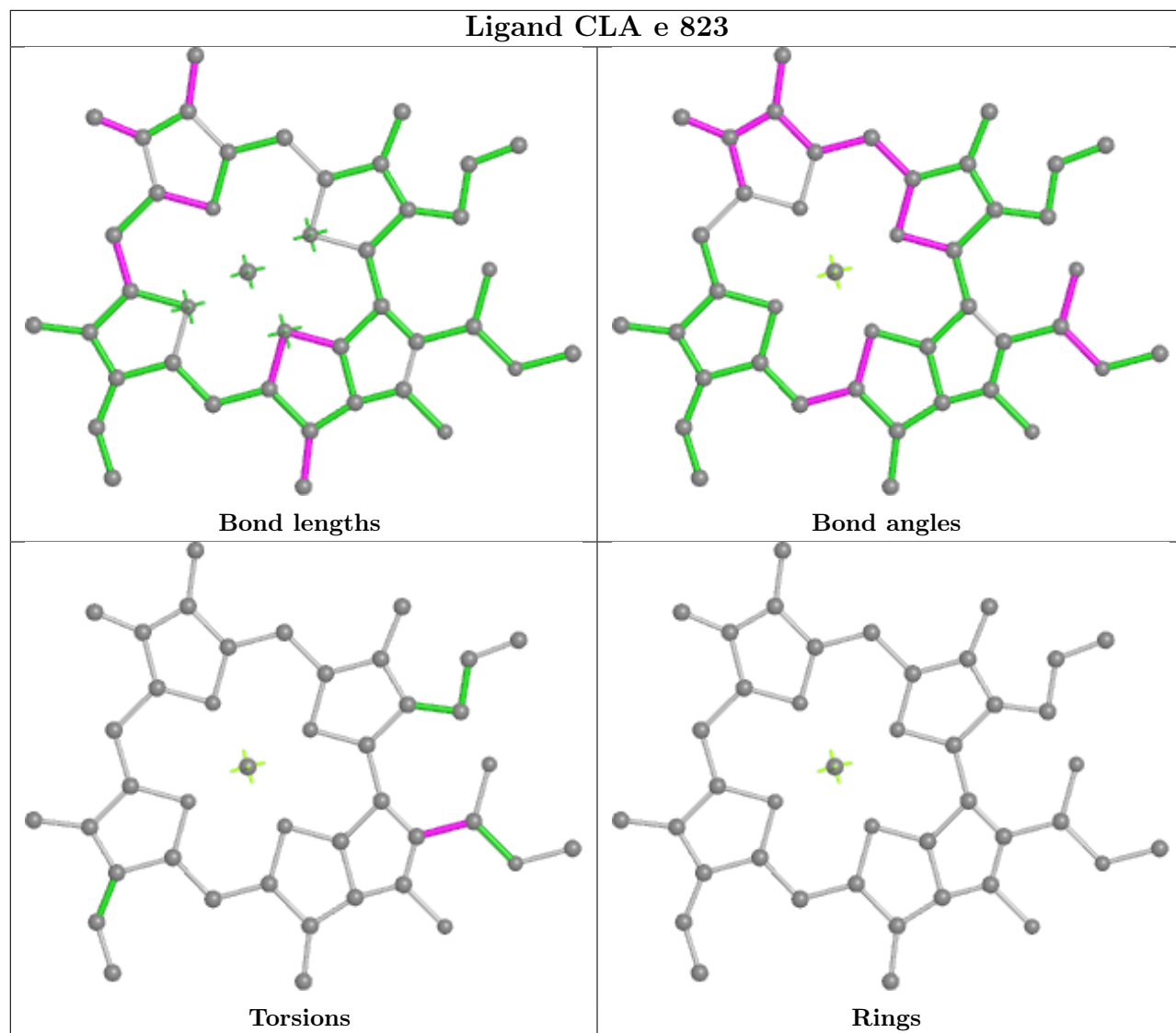


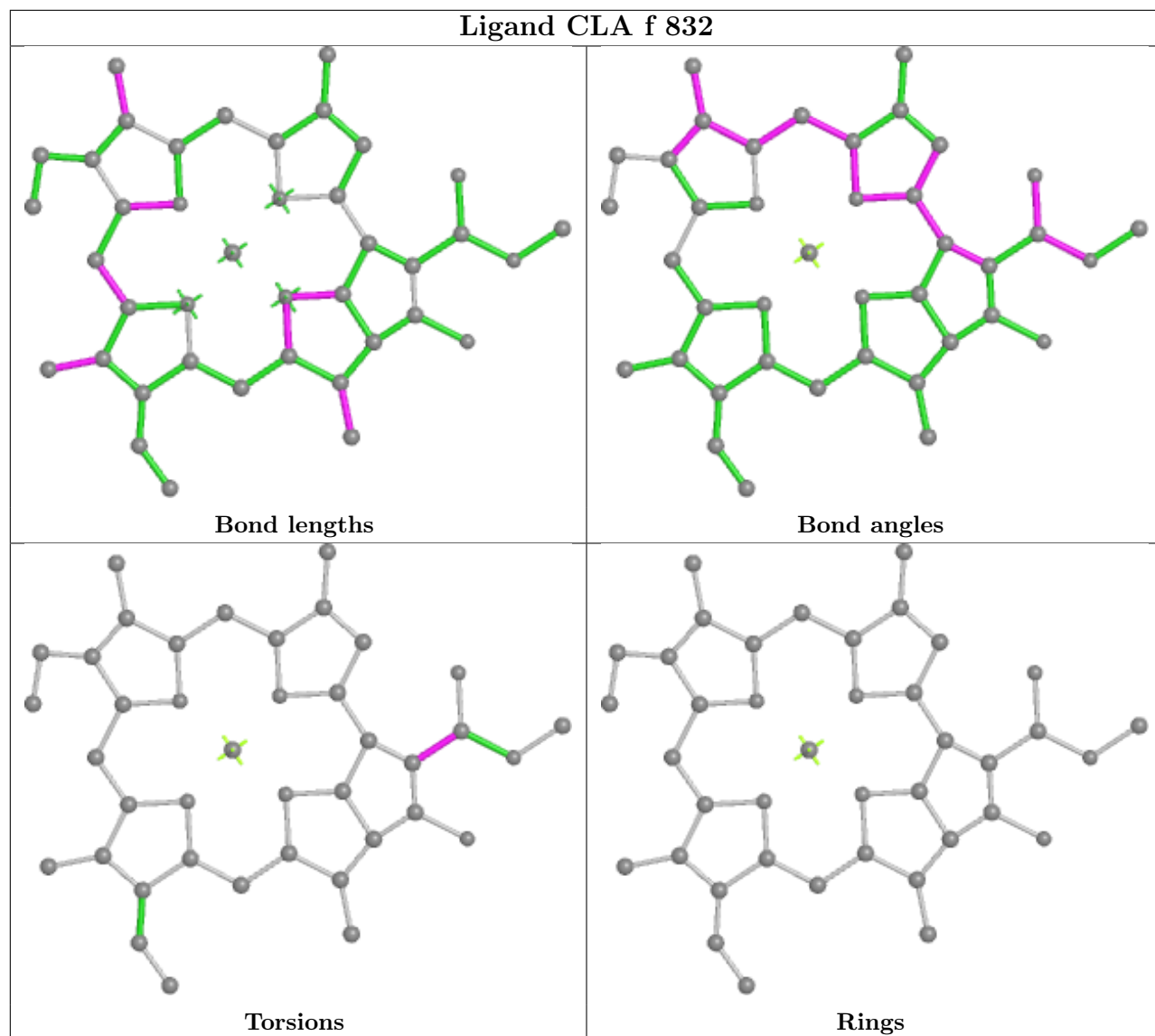


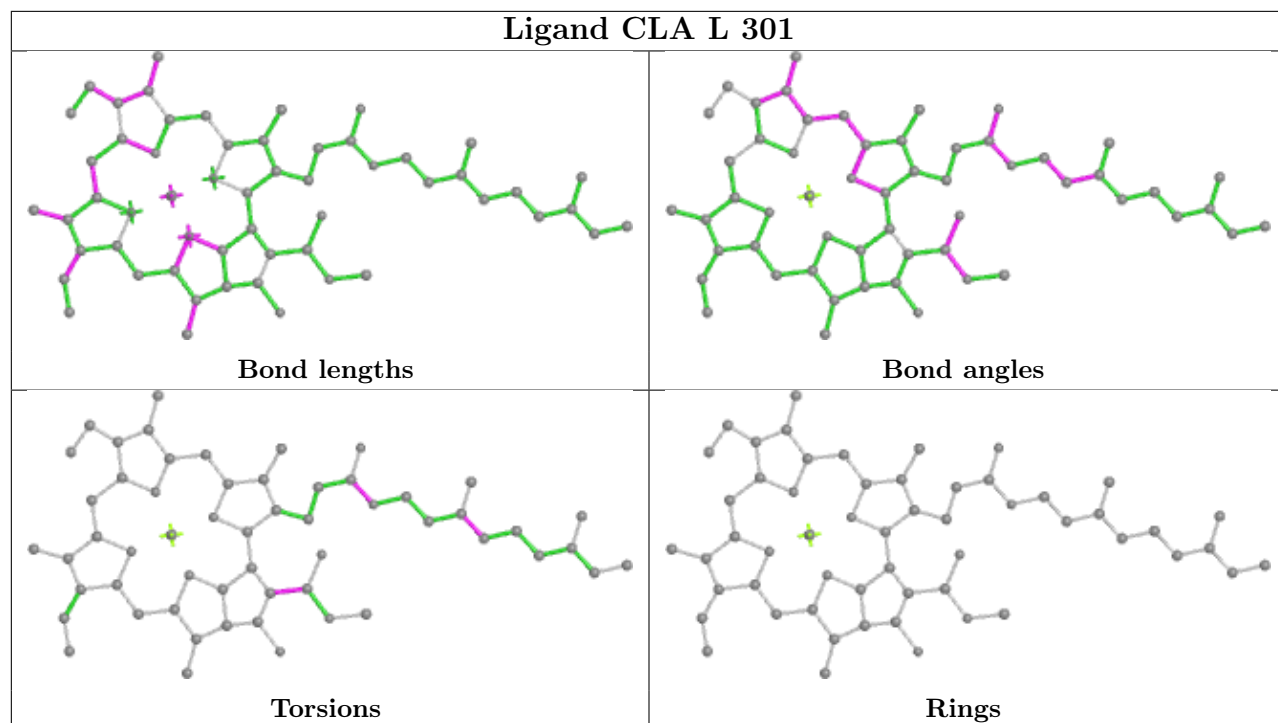


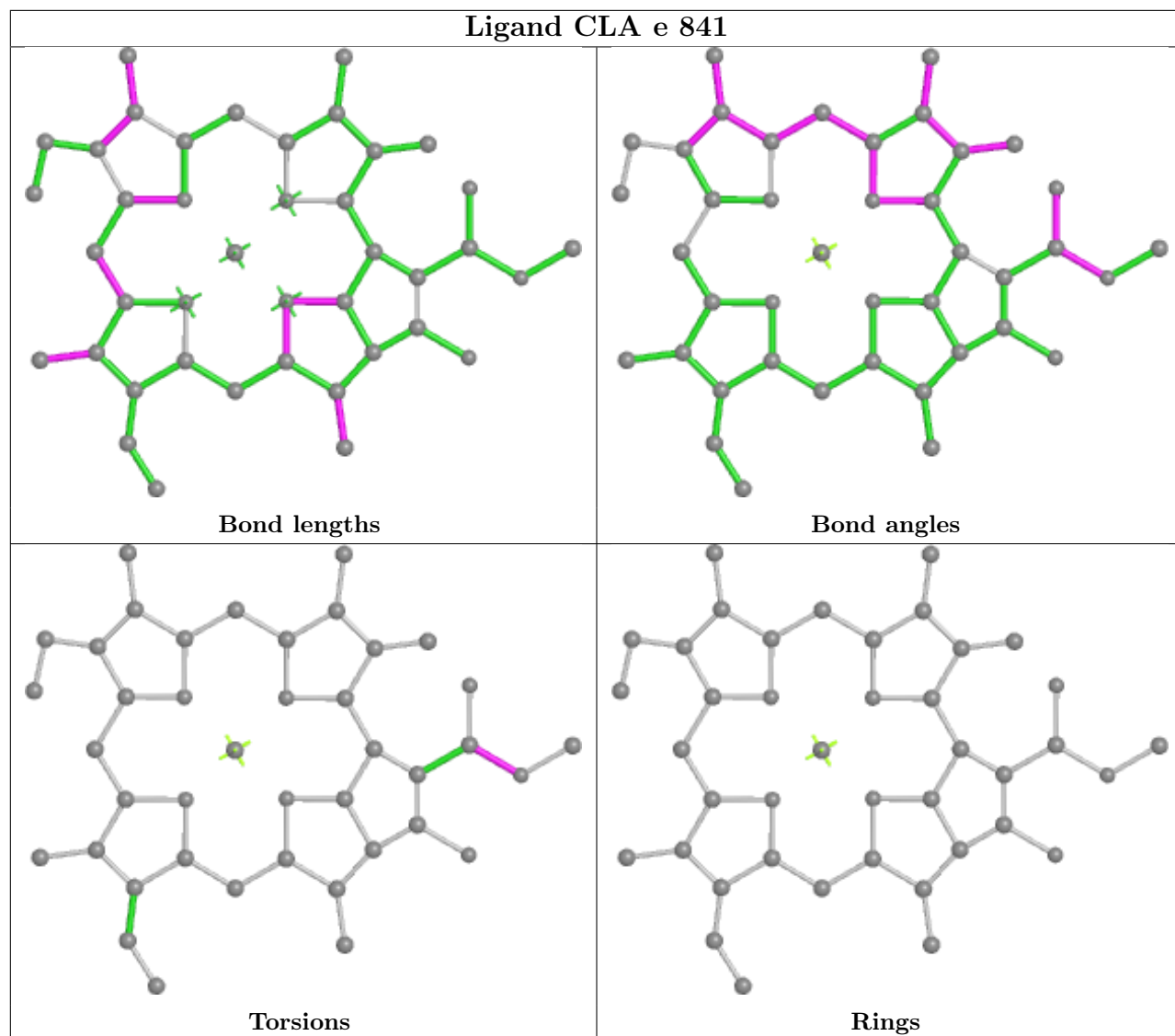


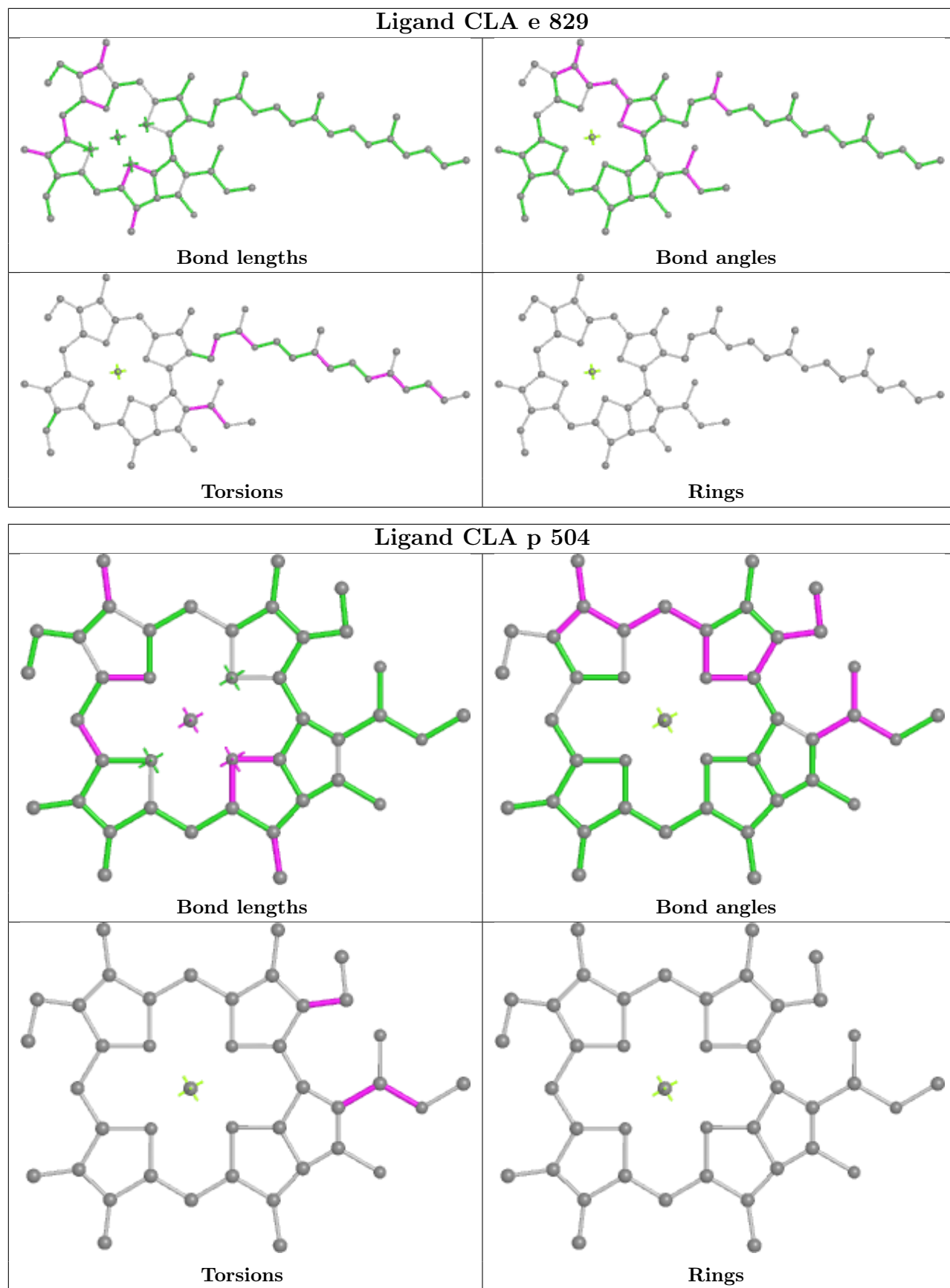


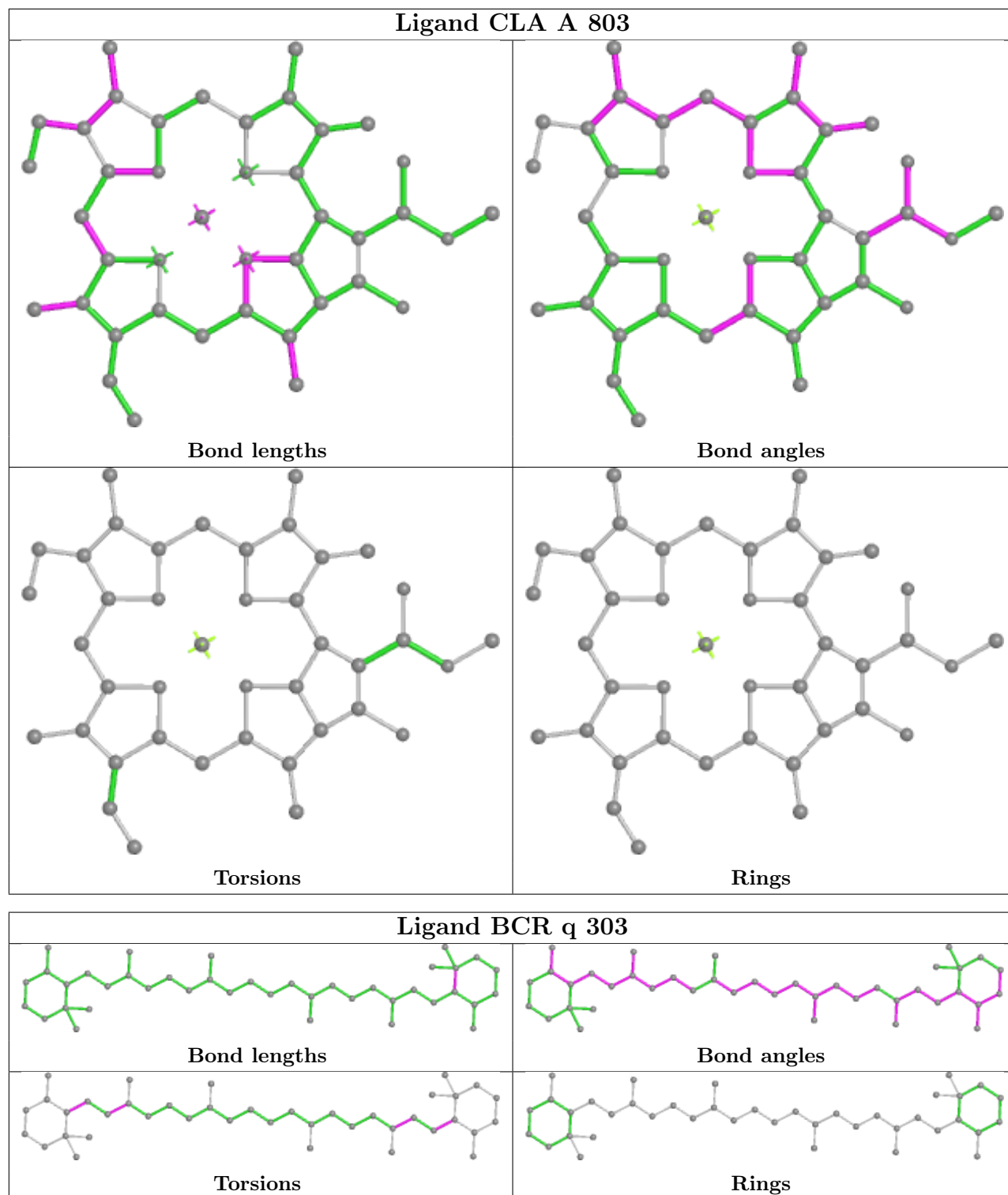


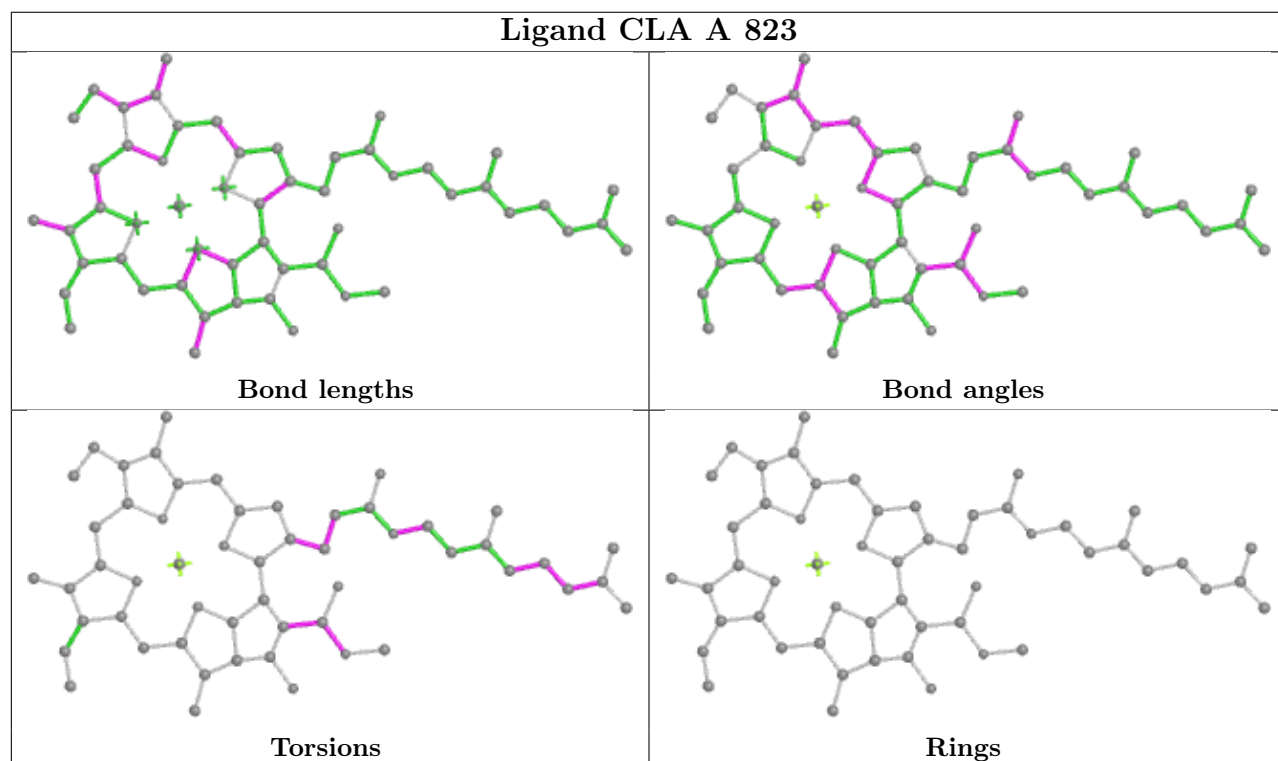
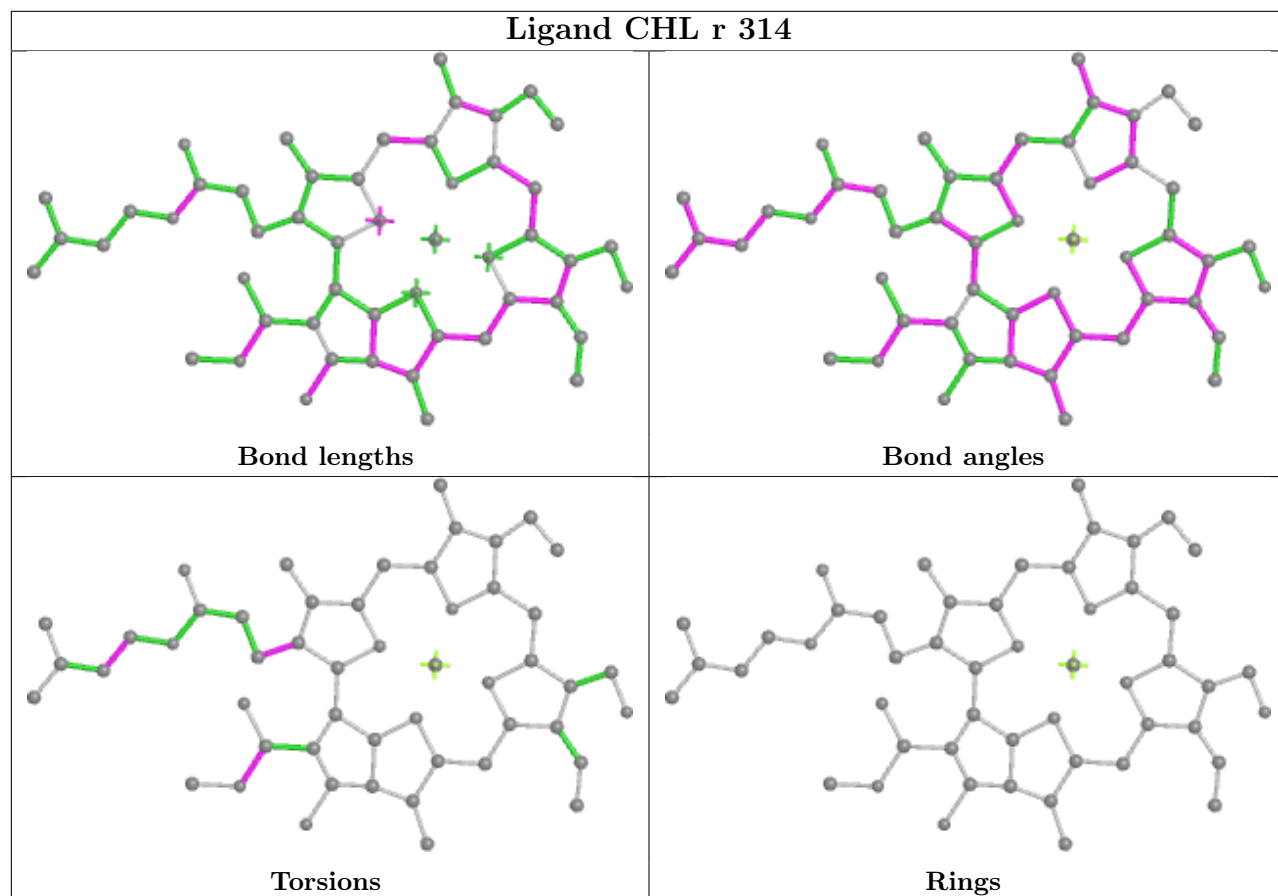




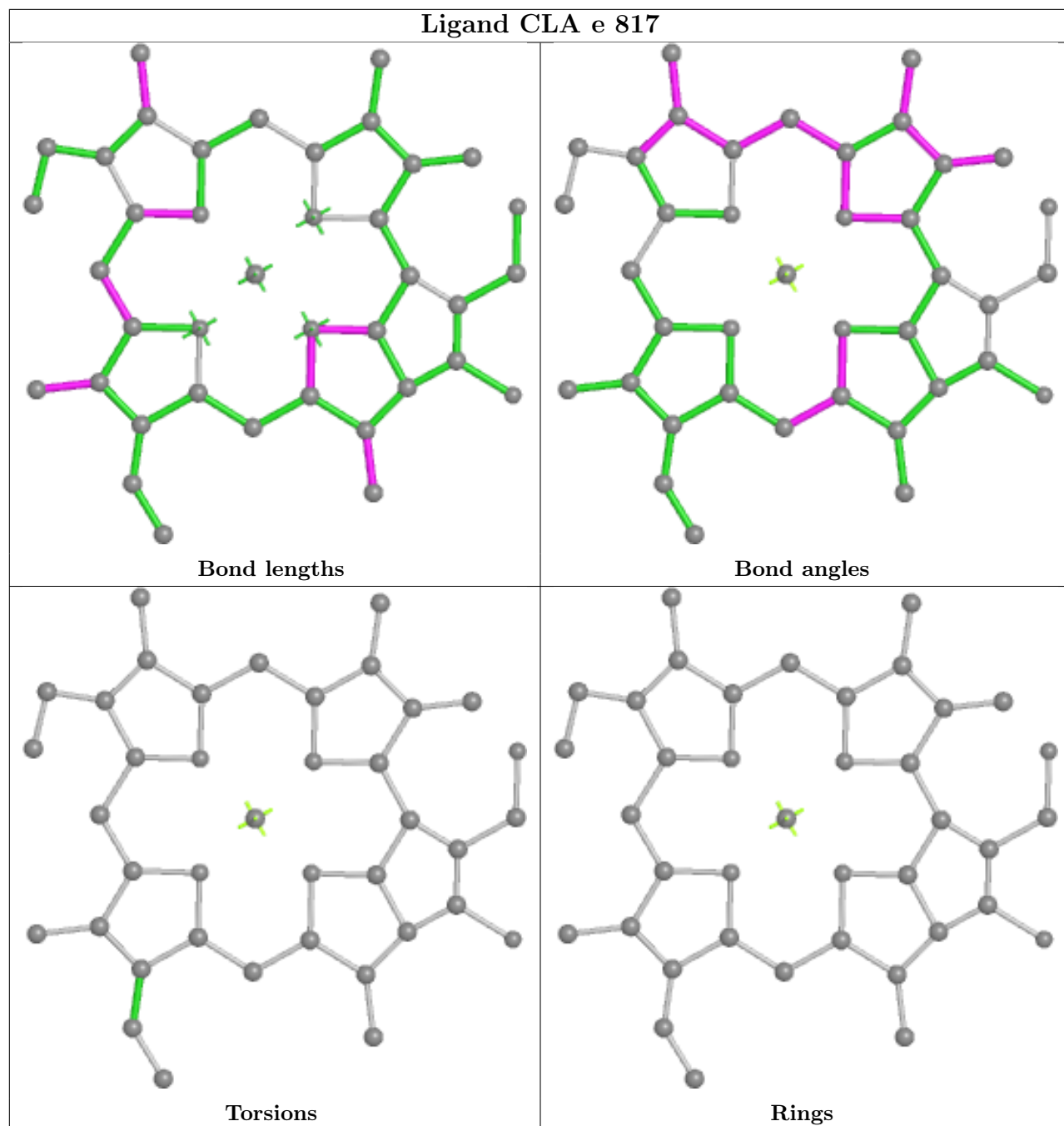


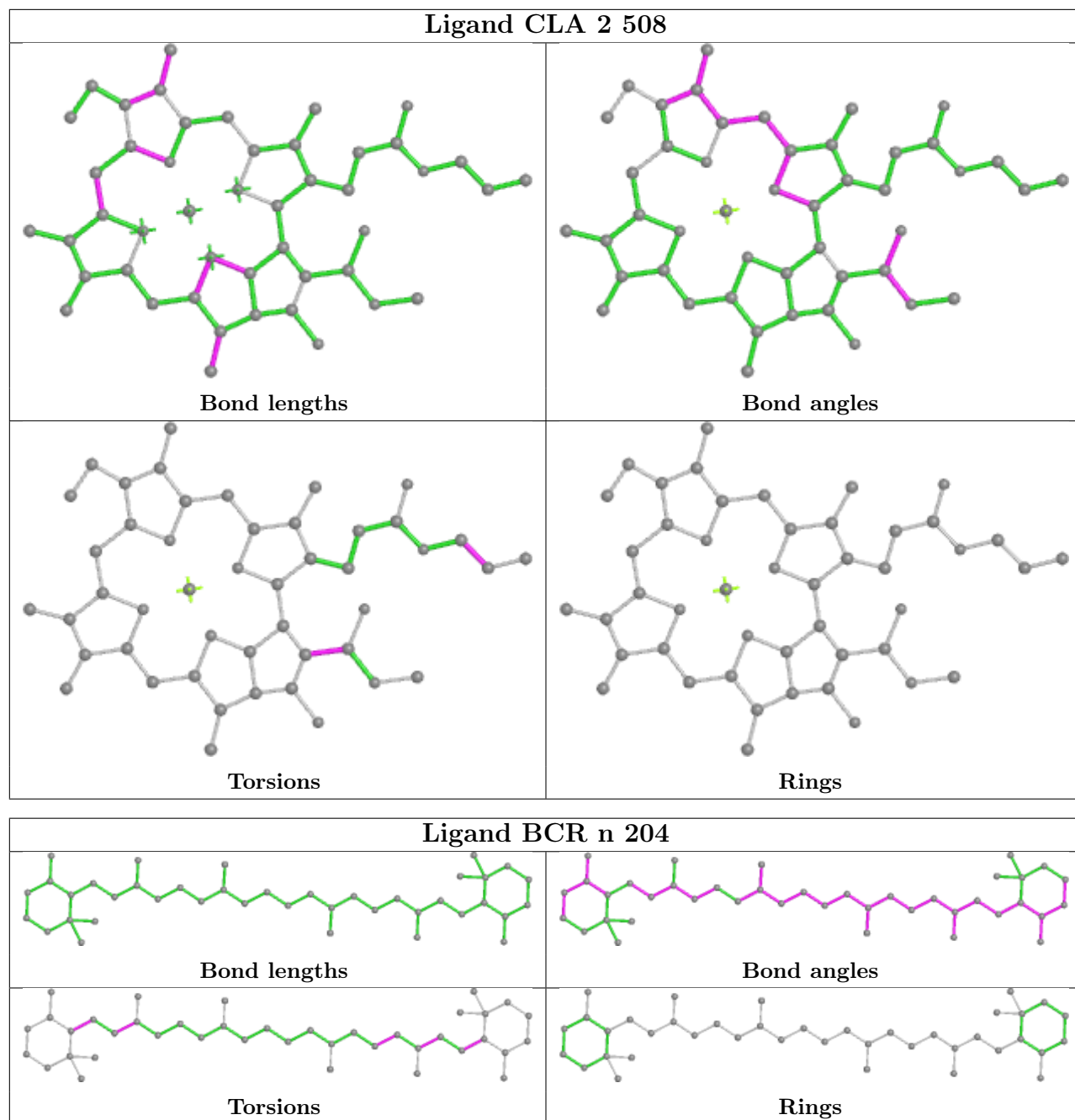


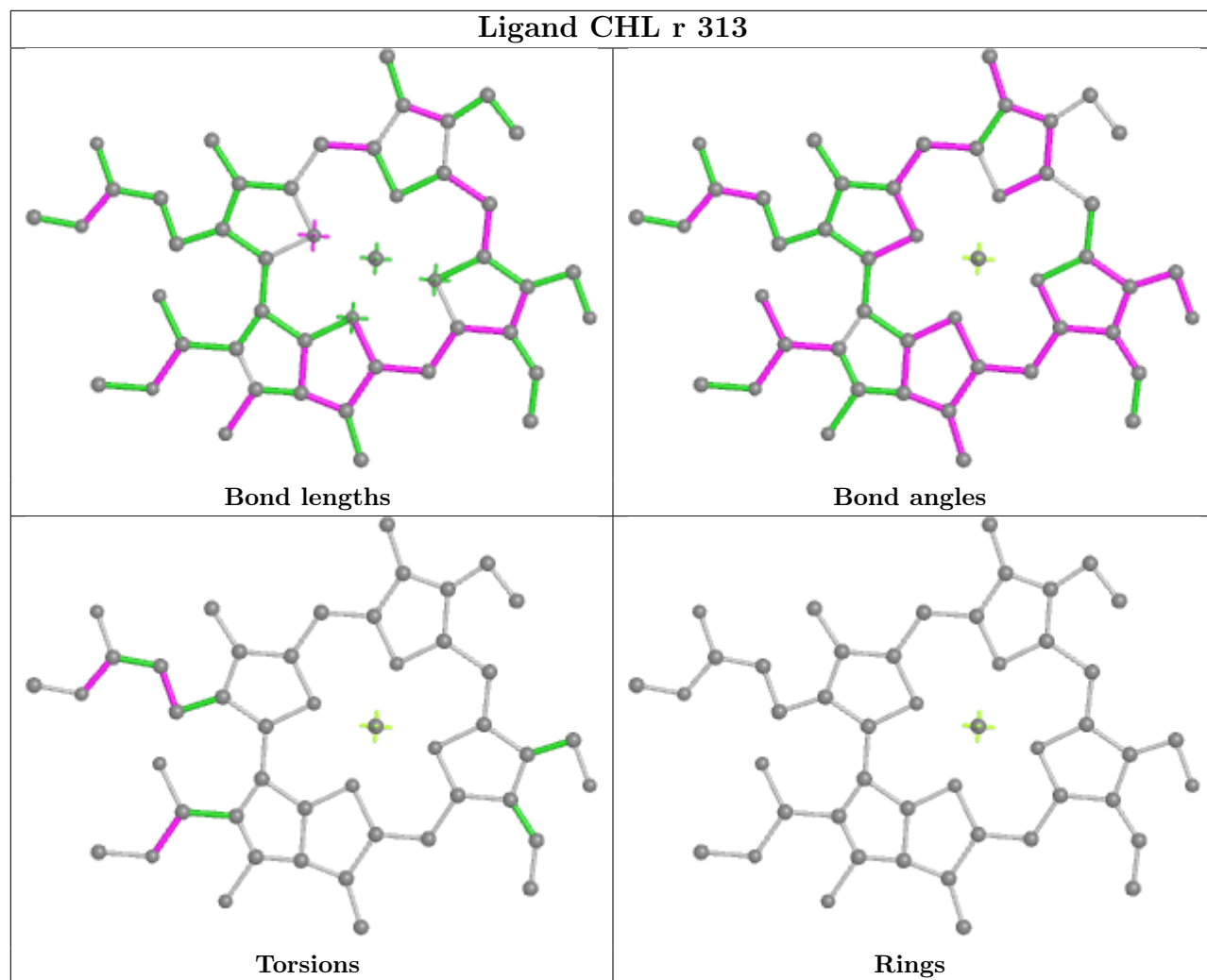


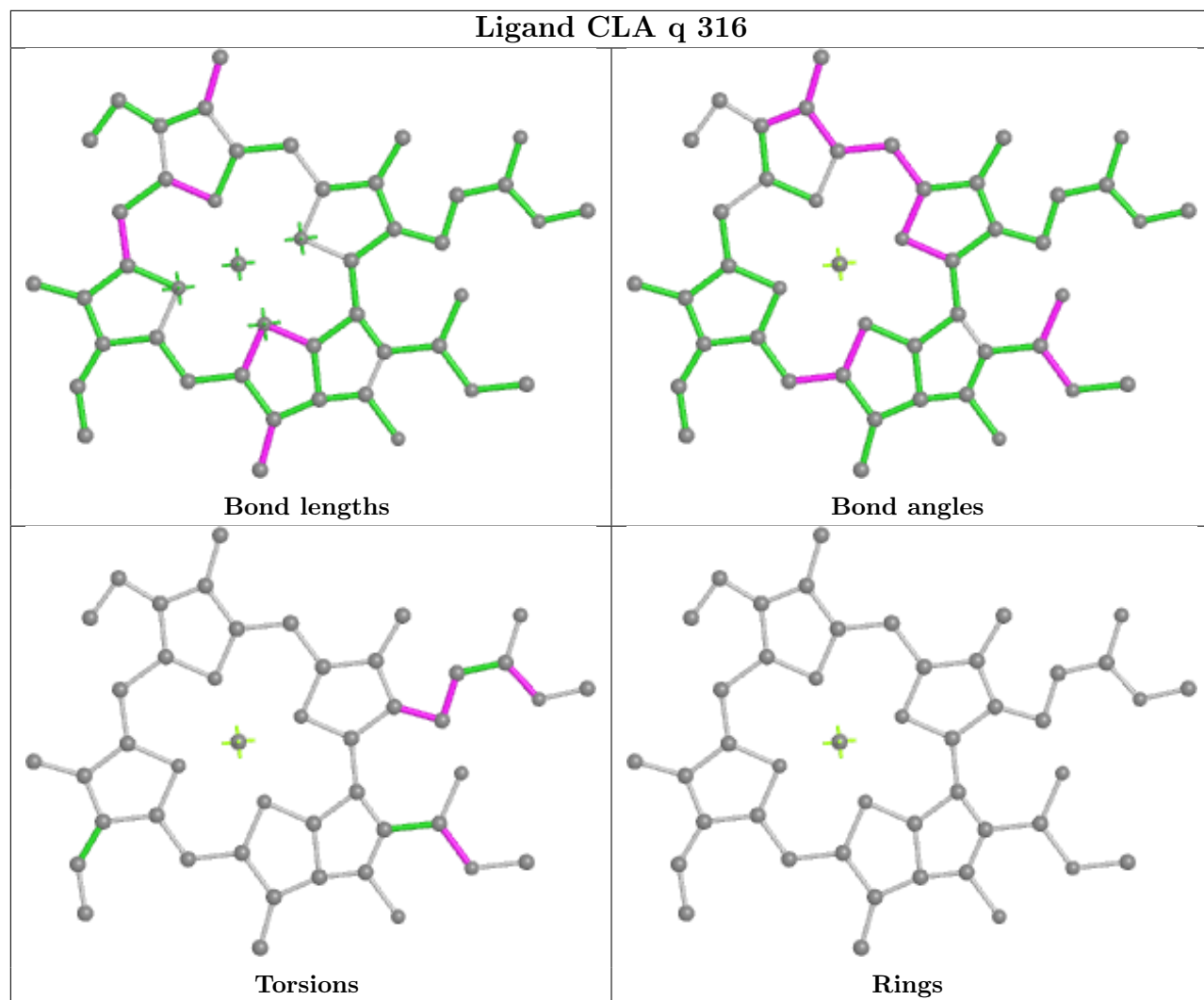


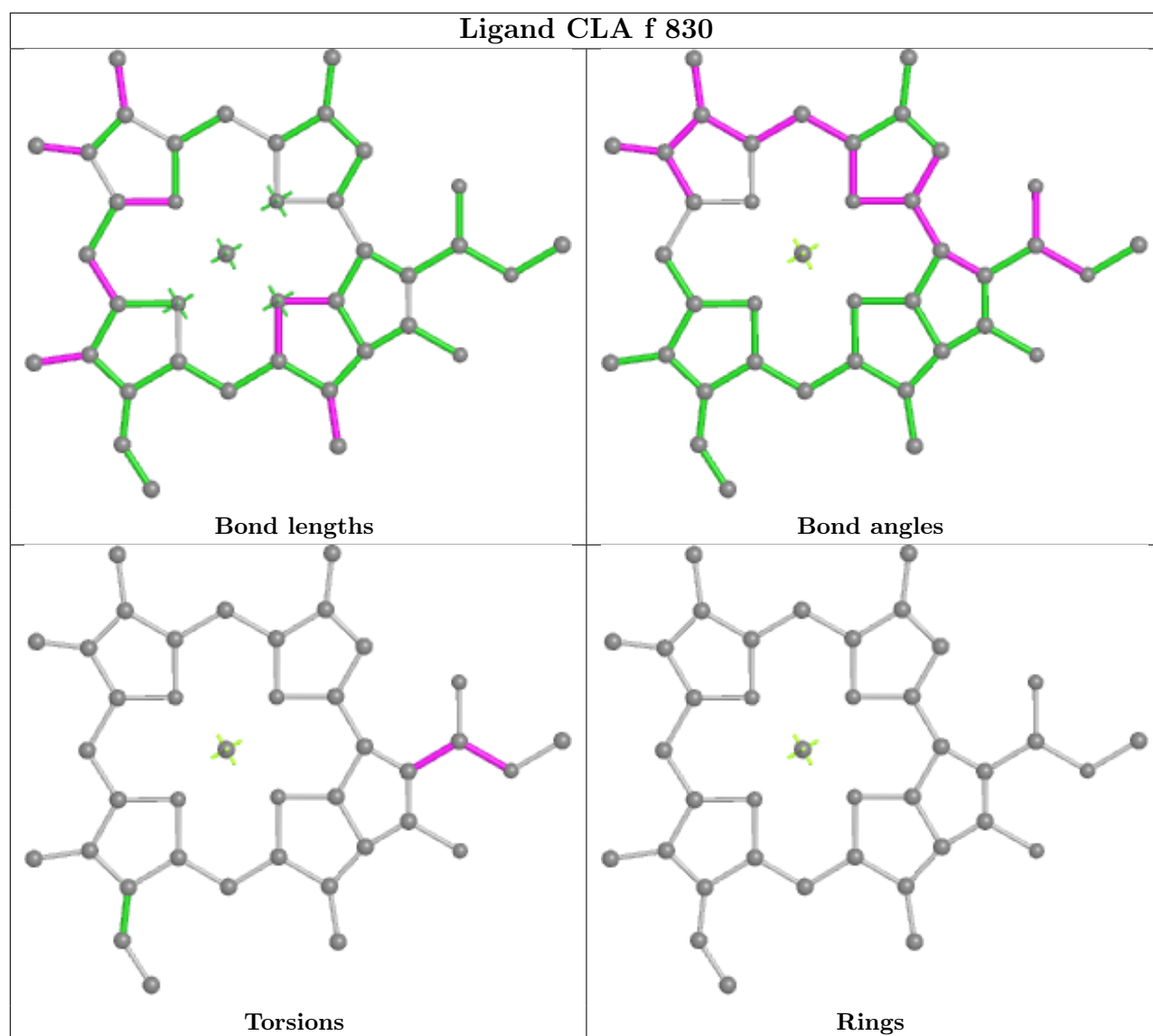












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

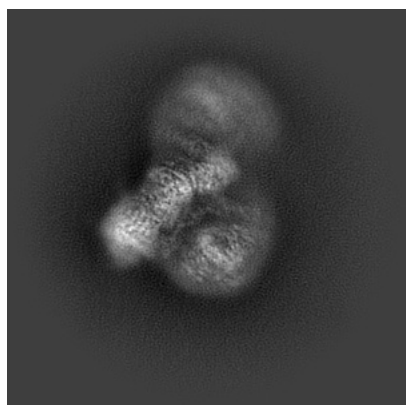
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31498. These allow visual inspection of the internal detail of the map and identification of artifacts.

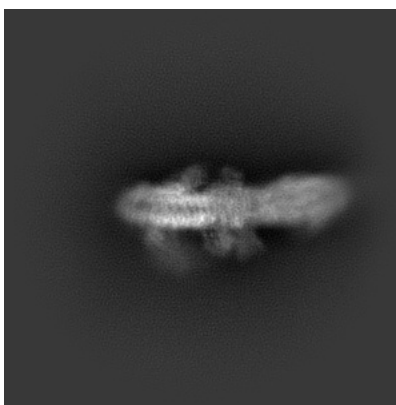
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

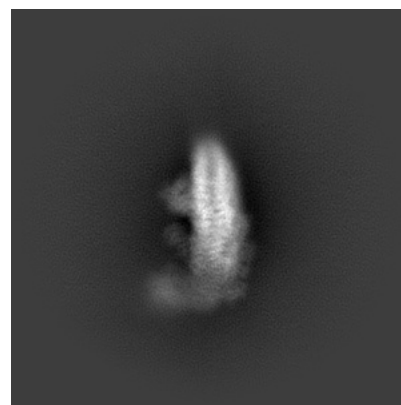
#### 6.1.1 Primary map



X



Y

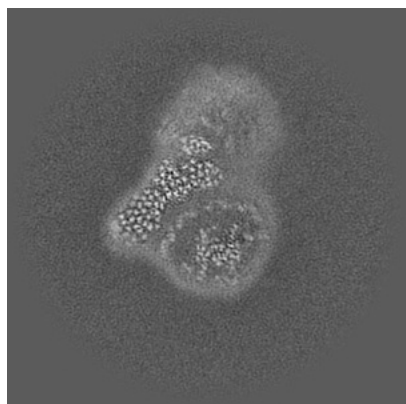


Z

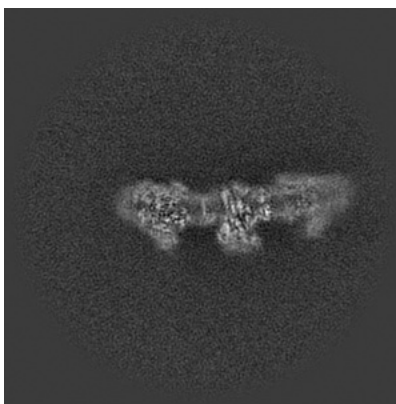
The images above show the map projected in three orthogonal directions.

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

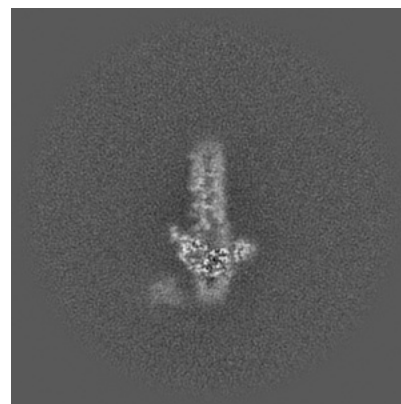
#### 6.2.1 Primary map



X Index: 220



Y Index: 220

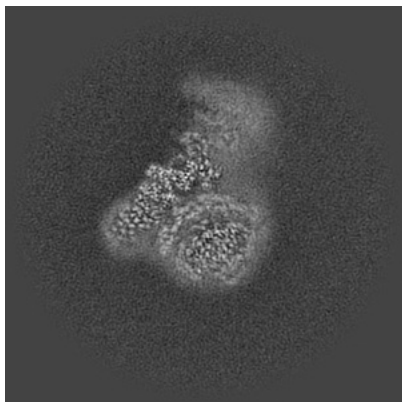


Z Index: 220

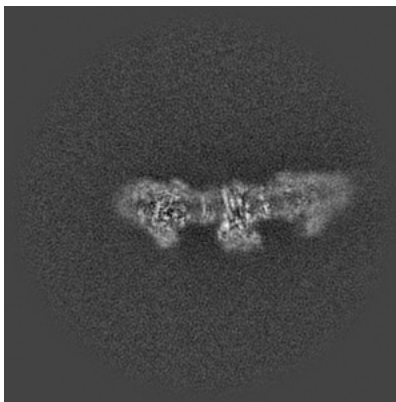
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 209



Y Index: 221



Z Index: 196

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

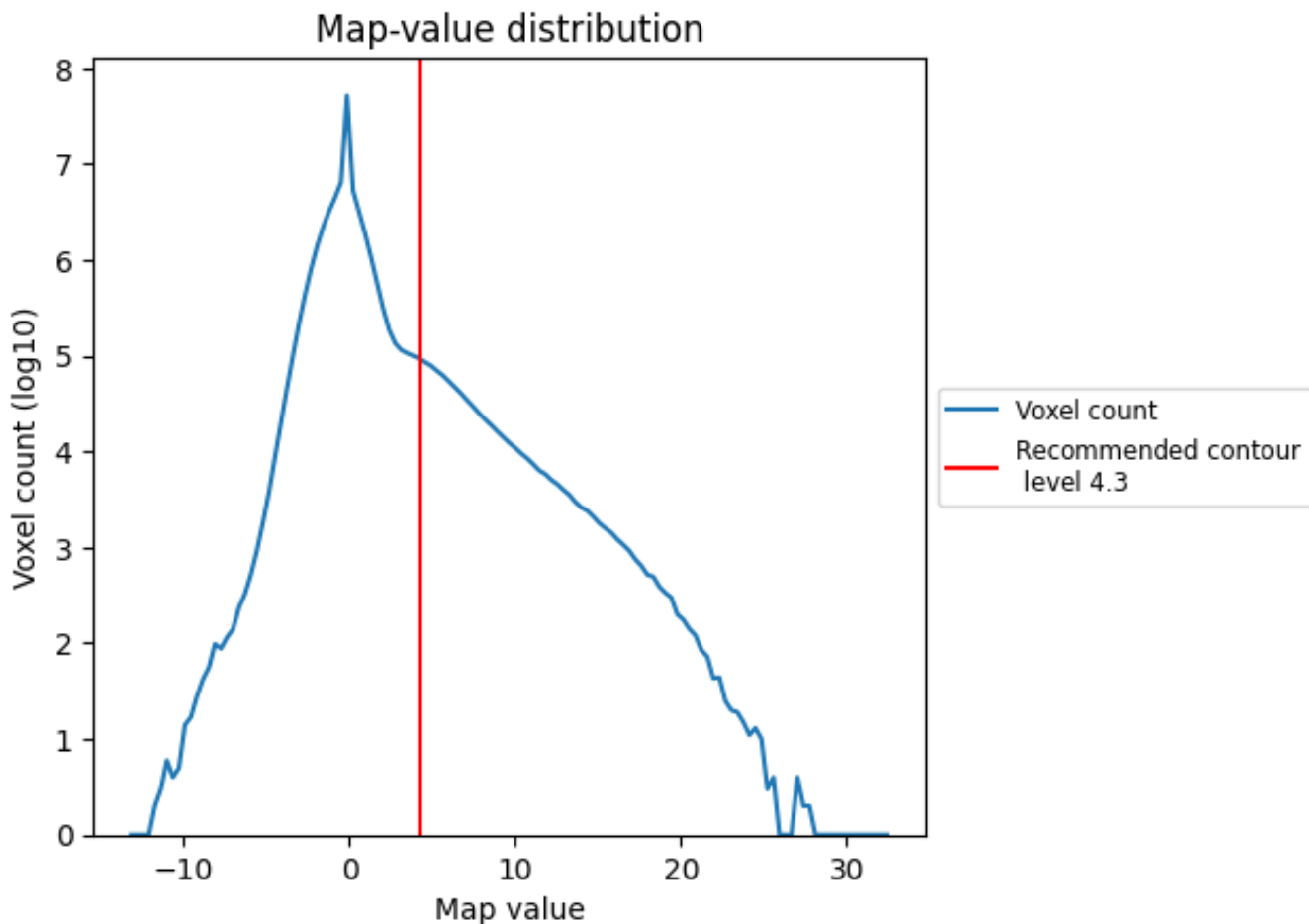
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

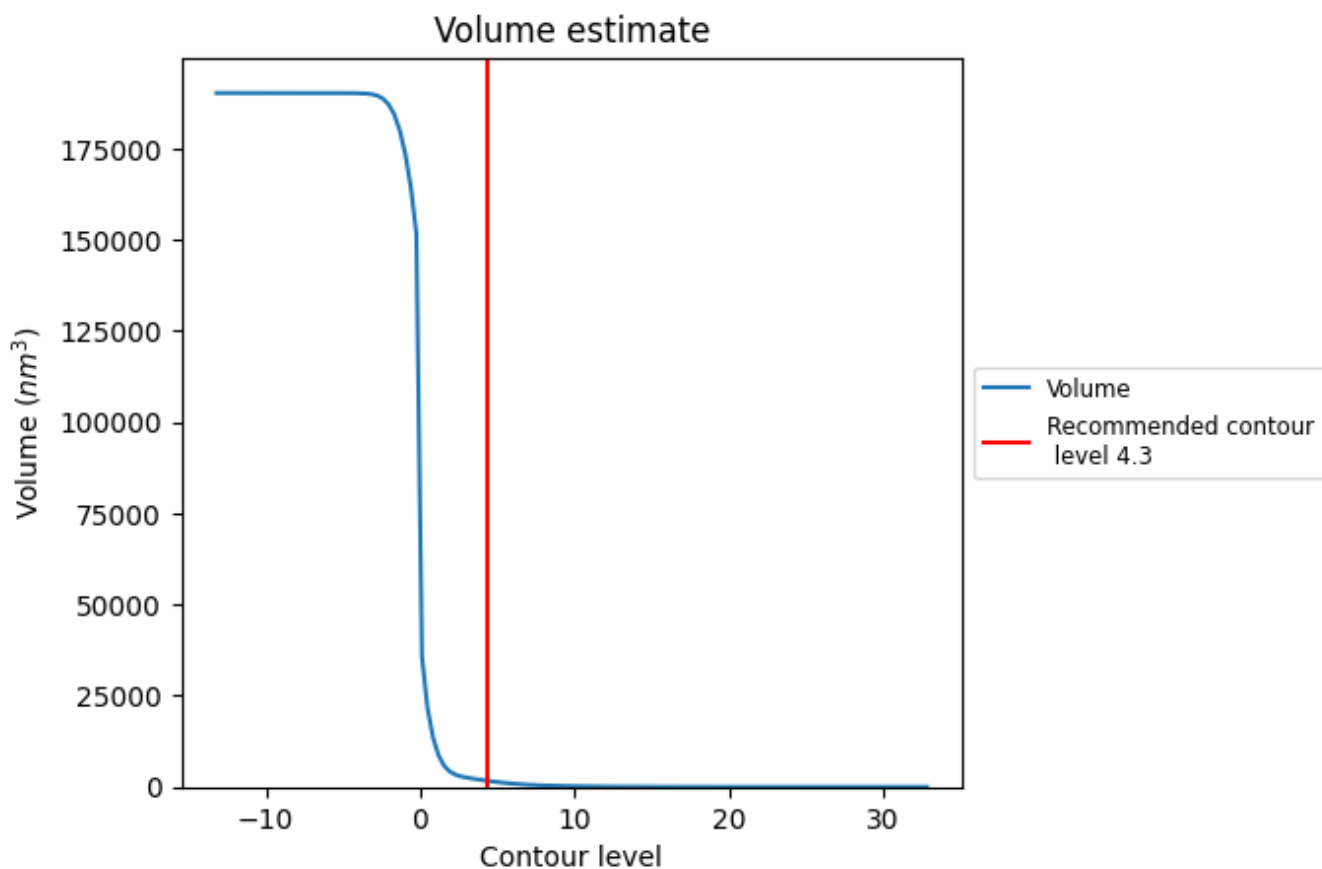
This section contains the results of statistical analysis of the map.

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



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

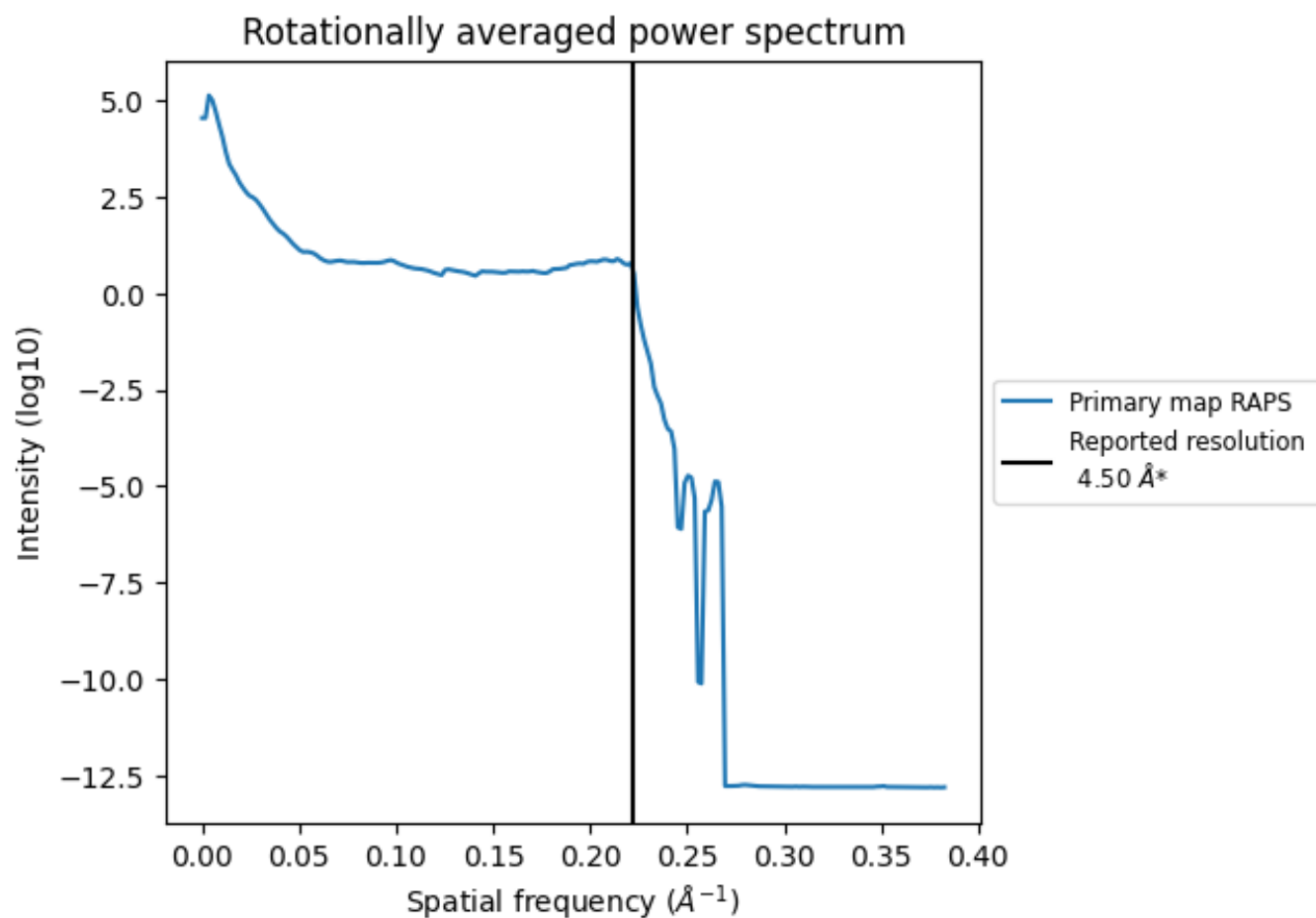
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1712 nm<sup>3</sup>; this corresponds to an approximate mass of 1547 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  $0.222 \text{\AA}^{-1}$

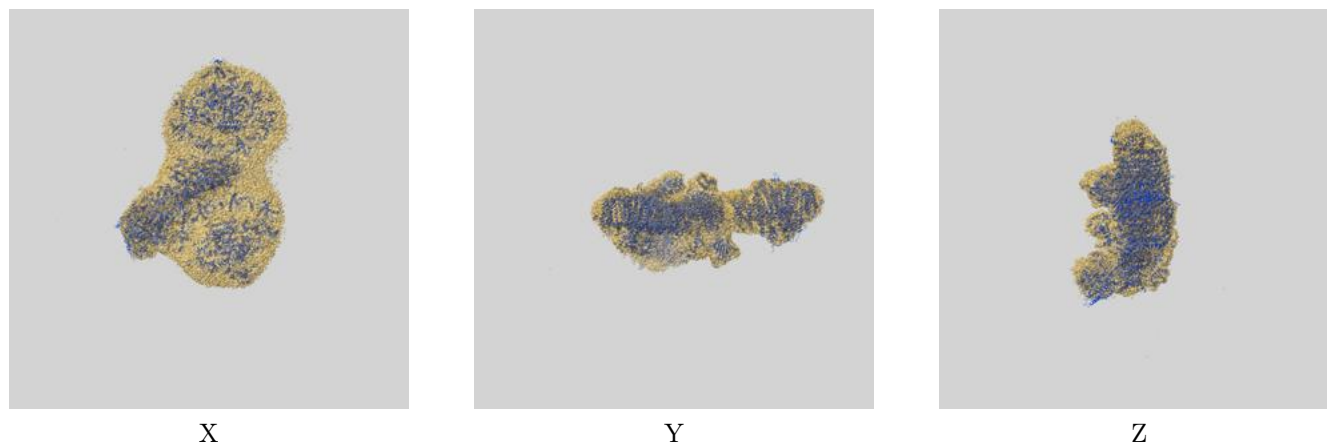
## 8 Fourier-Shell correlation

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

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

This section contains information regarding the fit between EMDB map EMD-31498 and PDB model 7F9O. Per-residue inclusion information can be found in section [3](#) on page [44](#).

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



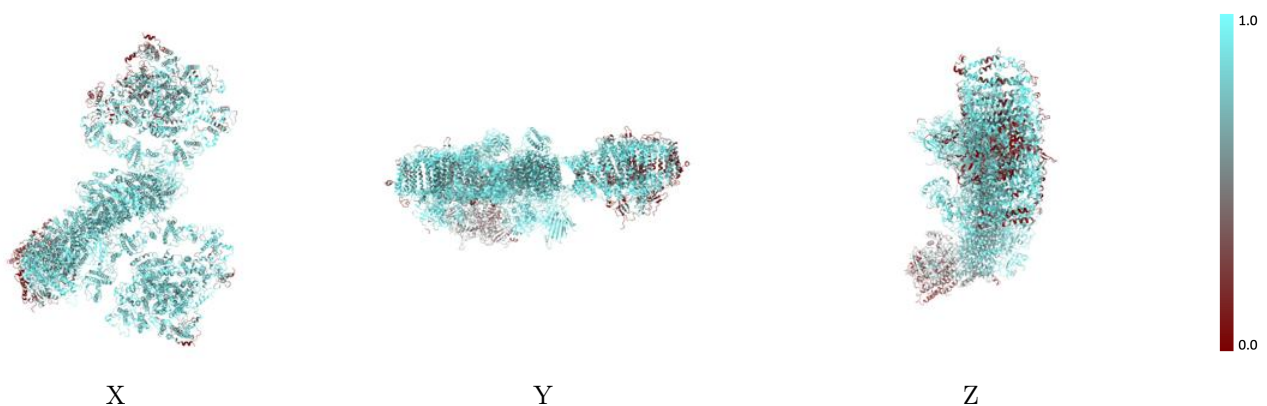
The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



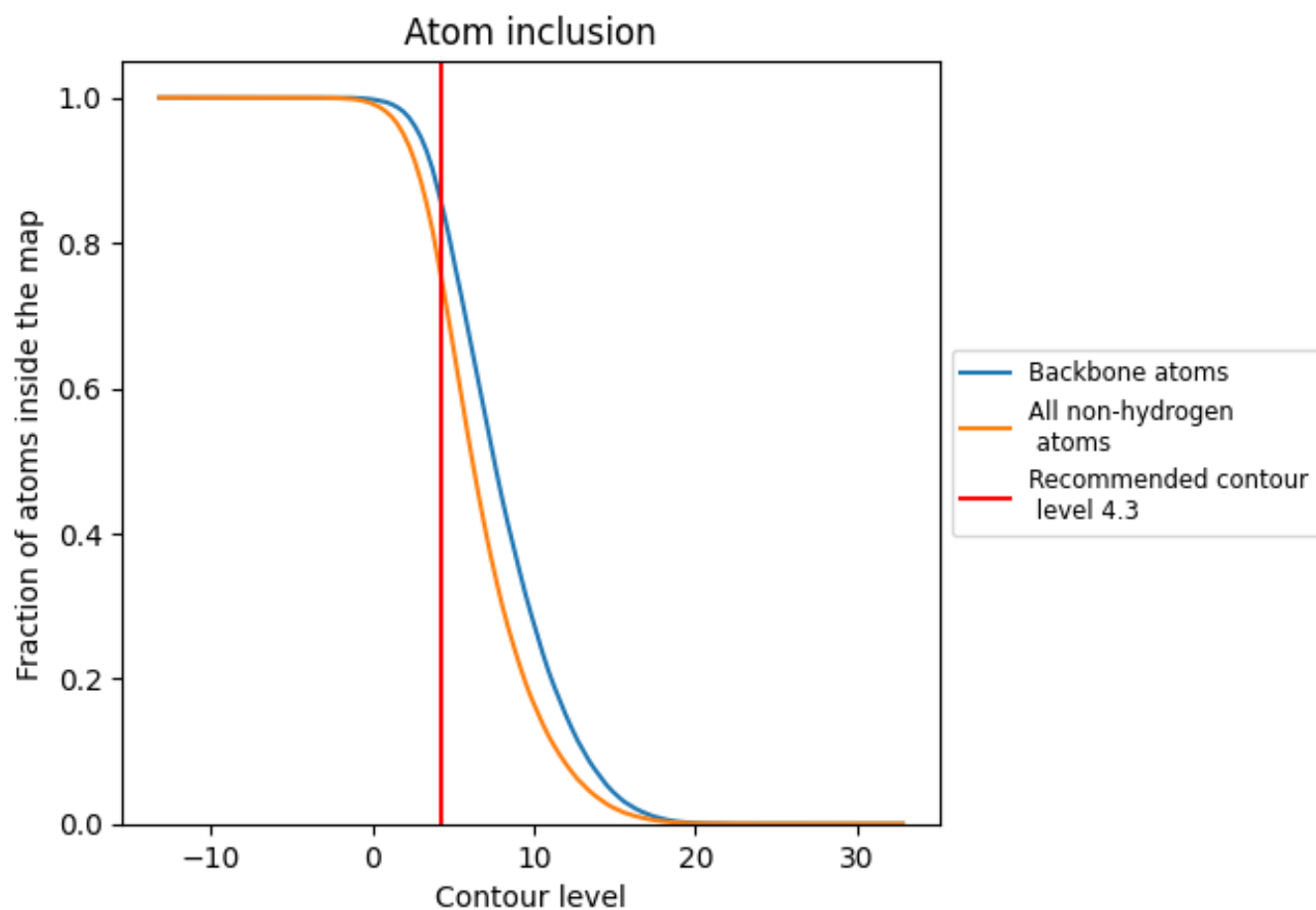
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.3).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 75% 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 (4.3) and Q-score for the entire model and for each chain.











































Chain	Atom inclusion	Q-score
All	 0.7483	 0.1530
0	 0.9115	 0.2790
1	 0.8683	 0.1670
2	 0.8142	 0.1560
3	 0.7631	 0.1310
4	 0.9469	 0.2970
5	 0.8447	 0.2040
6	 0.9222	 0.2590
7	 0.9032	 0.1660
8	 0.9294	 0.2190
9	 0.9387	 0.3030
A	 0.7971	 0.2100
B	 0.8350	 0.1920
C	 0.9297	 0.1900
D	 0.8104	 0.1390
E	 0.8462	 0.2510
F	 0.7912	 0.2080
G	 0.7714	 0.1410
H	 0.6080	 0.0710
I	 0.7269	 0.1620
J	 0.7655	 0.2130
K	 0.5680	 0.0740
L	 0.6438	 0.0840
M	 0.8567	 0.2760
N	 0.8002	 0.1930
O	 0.8712	 0.2910
P	 0.8108	 0.2610
Q	 0.8352	 0.2470
R	 0.8328	 0.2580
S	 0.3304	 0.0480
T	 0.4226	 0.0480
U	 0.3667	 0.0450
V	 0.5323	 0.0910
W	 0.3674	 0.0230
X	 0.4143	 0.0630



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Chain	Atom inclusion	Q-score
Y	 0.5344	 0.0660
Z	 0.9213	 0.2760
a	 0.9322	 0.2200
b	 0.9430	 0.2340
c	 0.9384	 0.2400
d	 0.9196	 0.2580
e	 0.6787	 0.0550
f	 0.7365	 0.0470
g	 0.7545	 0.0570
h	 0.3024	 0.0450
i	 0.3877	 0.1030
j	 0.7207	 0.0960
k	 0.2973	 0.0220
l	 0.5892	 0.0140
m	 0.6505	 0.1240
n	 0.2751	 0.0030
o	 0.3411	 0.0070
p	 0.6931	 0.0230
q	 0.7065	 0.0930
r	 0.7971	 0.0940
s	 0.8690	 0.2290