



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 05:30 PM JST

PDB ID : 8WMJ
EMDB ID : EMD-37654
Title : structure of PSI-11CAC complex at Logrithmic growth phase
Authors : Zhang, S.M.; Si, L.; Li, M.
Deposited on : 2023-10-03
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

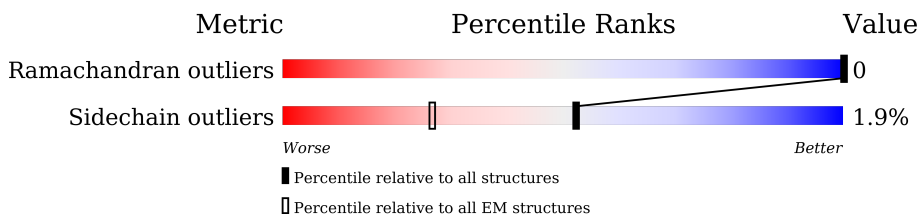
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	752	
2	B	734	
3	C	81	
4	D	141	
5	E	64	
6	F	188	
7	I	36	
8	J	42	
9	L	153	

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Mol	Chain	Length	Quality of chain
10	M	30	 100%
11	K	87	 79% 21%
12	s	269	 57% 43%
13	c	216	 79% 21%
14	a	216	 77% 19%
15	b	223	 86% 13%
16	h	225	 70% 28%
17	j	212	 80% 19%
17	m	212	 81% 18%
18	l	238	 72% 26%
19	k	241	 73% 25%
20	i	218	 79% 20%
21	d	213	 59% 39%
22	R	129	 70% 30%
23	n	219	 82% 17%
24	Q	234	 9% 70% 28%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	801	X	-	-	-
25	CLA	A	802	X	-	-	-
25	CLA	A	804	X	-	-	-
25	CLA	A	805	X	-	-	-
25	CLA	A	807	X	-	-	-
25	CLA	A	808	X	-	-	-
25	CLA	A	810	X	-	-	-
25	CLA	A	812	X	-	-	-
25	CLA	A	817	X	-	-	-
25	CLA	A	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	820	X	-	-	-
25	CLA	A	824	X	-	-	-
25	CLA	A	826	X	-	-	-
25	CLA	A	829	X	-	-	-
25	CLA	A	833	X	-	-	-
25	CLA	A	834	X	-	-	-
25	CLA	A	835	X	-	-	-
25	CLA	A	837	X	-	-	-
25	CLA	A	838	X	-	-	-
25	CLA	A	839	X	-	-	-
25	CLA	A	841	X	-	-	-
25	CLA	A	842	X	-	-	-
25	CLA	A	843	X	-	-	-
25	CLA	A	853	X	-	-	-
25	CLA	A	854	X	-	-	-
25	CLA	A	855	X	-	-	-
25	CLA	A	856	X	-	-	-
25	CLA	B	803	X	-	-	-
25	CLA	B	804	X	-	-	-
25	CLA	B	805	X	-	-	-
25	CLA	B	806	X	-	-	-
25	CLA	B	807	X	-	-	-
25	CLA	B	808	X	-	-	-
25	CLA	B	809	X	-	-	-
25	CLA	B	810	X	-	-	-
25	CLA	B	811	X	-	-	-
25	CLA	B	812	X	-	-	-
25	CLA	B	813	X	-	-	-
25	CLA	B	814	X	-	-	-
25	CLA	B	816	X	-	-	-
25	CLA	B	817	X	-	-	-
25	CLA	B	818	X	-	-	-
25	CLA	B	822	X	-	-	-
25	CLA	B	824	X	-	-	-
25	CLA	B	825	X	-	-	-
25	CLA	B	826	X	-	-	-
25	CLA	B	832	X	-	-	-
25	CLA	B	833	X	-	-	-
25	CLA	B	834	X	-	-	-
25	CLA	B	835	X	-	-	-
25	CLA	B	837	X	-	-	-
25	CLA	B	839	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	840	X	-	-	-
25	CLA	B	841	X	-	-	-
25	CLA	B	850	X	-	-	-
25	CLA	F	201	X	-	-	-
25	CLA	J	103	X	-	-	-
25	CLA	K	101	X	-	-	-
25	CLA	K	102	X	-	-	-
25	CLA	L	202	X	-	-	-
25	CLA	Q	302	X	-	-	-
25	CLA	Q	303	X	-	-	-
25	CLA	R	202	X	-	-	-
25	CLA	a	303	X	-	-	-
25	CLA	a	304	X	-	-	-
25	CLA	a	305	X	-	-	-
25	CLA	a	306	X	-	-	-
25	CLA	a	308	X	-	-	-
25	CLA	a	309	X	-	-	-
25	CLA	a	310	X	-	-	-
25	CLA	a	311	X	-	-	-
25	CLA	a	313	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	c	601	X	-	-	-
25	CLA	c	602	X	-	-	-
25	CLA	c	603	X	-	-	-
25	CLA	c	604	X	-	-	-
25	CLA	c	605	X	-	-	-
25	CLA	c	607	X	-	-	-
25	CLA	c	608	X	-	-	-
25	CLA	c	609	X	-	-	-
25	CLA	c	612	X	-	-	-
25	CLA	d	301	X	-	-	-
25	CLA	d	302	X	-	-	-
25	CLA	d	303	X	-	-	-
25	CLA	d	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	d	305	X	-	-	-
25	CLA	d	306	X	-	-	-
25	CLA	d	307	X	-	-	-
25	CLA	d	308	X	-	-	-
25	CLA	d	309	X	-	-	-
25	CLA	d	312	X	-	-	-
25	CLA	h	302	X	-	-	-
25	CLA	h	303	X	-	-	-
25	CLA	h	304	X	-	-	-
25	CLA	h	305	X	-	-	-
25	CLA	h	306	X	-	-	-
25	CLA	h	307	X	-	-	-
25	CLA	h	308	X	-	-	-
25	CLA	h	313	X	-	-	-
25	CLA	i	302	X	-	-	-
25	CLA	i	303	X	-	-	-
25	CLA	i	304	X	-	-	-
25	CLA	i	306	X	-	-	-
25	CLA	i	307	X	-	-	-
25	CLA	i	308	X	-	-	-
25	CLA	i	309	X	-	-	-
25	CLA	i	311	X	-	-	-
25	CLA	i	312	X	-	-	-
25	CLA	j	601	X	-	-	-
25	CLA	j	603	X	-	-	-
25	CLA	j	605	X	-	-	-
25	CLA	j	606	X	-	-	-
25	CLA	j	607	X	-	-	-
25	CLA	j	608	X	-	-	-
25	CLA	j	609	X	-	-	-
25	CLA	j	611	X	-	-	-
25	CLA	j	612	X	-	-	-
25	CLA	k	601	X	-	-	-
25	CLA	k	602	X	-	-	-
25	CLA	k	603	X	-	-	-
25	CLA	k	605	X	-	-	-
25	CLA	k	607	X	-	-	-
25	CLA	k	608	X	-	-	-
25	CLA	k	609	X	-	-	-
25	CLA	k	610	X	-	-	-
25	CLA	l	303	X	-	-	-
25	CLA	l	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	l	305	X	-	-	-
25	CLA	l	307	X	-	-	-
25	CLA	l	308	X	-	-	-
25	CLA	l	309	X	-	-	-
25	CLA	l	310	X	-	-	-
25	CLA	l	312	X	-	-	-
25	CLA	m	601	X	-	-	-
25	CLA	m	602	X	-	-	-
25	CLA	m	603	X	-	-	-
25	CLA	m	606	X	-	-	-
25	CLA	m	608	X	-	-	-
25	CLA	m	609	X	-	-	-
25	CLA	m	610	X	-	-	-
25	CLA	m	613	X	-	-	-
25	CLA	n	302	X	-	-	-
25	CLA	n	303	X	-	-	-
25	CLA	n	304	X	-	-	-
25	CLA	n	305	X	-	-	-
25	CLA	n	306	X	-	-	-
25	CLA	n	307	X	-	-	-
25	CLA	n	308	X	-	-	-
25	CLA	n	309	X	-	-	-
25	CLA	n	310	X	-	-	-
25	CLA	s	202	X	-	-	-
25	CLA	s	209	X	-	-	-

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 52744 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	5825	3802	994	1001	28	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	732	5820	3840	981	984	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	592	361	103	116	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	139	1084	692	186	203	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	60	485	309	84	92	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	161	1254	814	212	226	2	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	34	264	182	35	45	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	42	351	240	49	59	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	151	1146	753	182	208	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	30	232	155	38	38	1	0	0

- Molecule 11 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	69	488	319	80	87	2	0	0

- Molecule 12 is a protein called chain s.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	s	154	1140	719	195	217	9	0	0

- Molecule 13 is a protein called CAC-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	c	170	1357	897	221	236	3	0	0

- Molecule 14 is a protein called CAC-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	a	175	1361	889	217	245	10	0	0

- Molecule 15 is a protein called CAC-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	b	194	1439	916	251	258	14	0	0

- Molecule 16 is a protein called CAC-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	h	162	1200	778	202	214	6	0	0

- Molecule 17 is a protein called CAC-j.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	m	174	1309	846	214	241	8	0	0
17	j	172	1293	834	212	239	8	0	0

- Molecule 18 is a protein called CAC-l.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	l	175	1344	869	230	238	7	0	0

- Molecule 19 is a protein called CAC-k.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	k	180	1346	872	223	239	12	0	0

- Molecule 20 is a protein called CAC-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	i	175	1324	849	227	237	11	0	0

- Molecule 21 is a protein called CAC-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	d	129	974	624	169	171	10	0	0

- Molecule 22 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	90	664	434	105	124	1	0	0

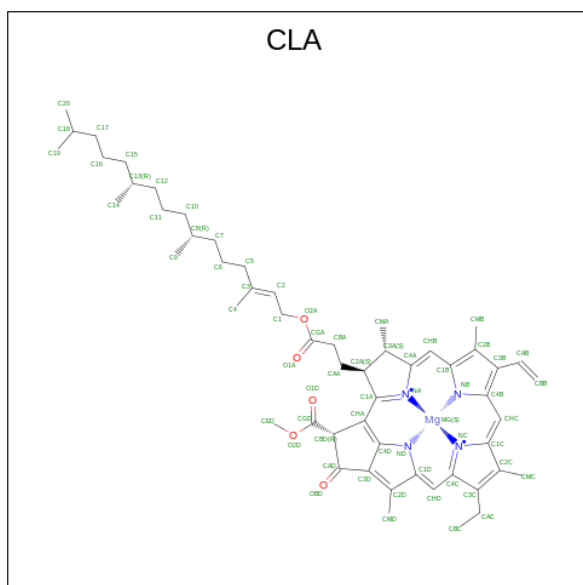
- Molecule 23 is a protein called CAC-n.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	n	181	1350	870	228	242	10	0	0

- Molecule 24 is a protein called PsaQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	169	1226	775	208	238	5	0	0

- Molecule 25 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	
25	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	A	1	65	55	1	4	5	0
25	A	1	55	45	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	56	46	1	4	5	0
25	A	1	62	52	1	4	5	0
25	A	1	54	44	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	45	35	1	4	5	0
25	A	1	50	40	1	4	5	0
25	A	1	45	35	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	45	35	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	49	39	1	4	5	0
25	A	1	51	41	1	4	5	0

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	65	55	1	4	5	0
25	A	1	41	33	1	4	3	0
25	B	1	65	55	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	54	44	1	4	5	0
25	B	1	55	45	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	60	50	1	4	5	0
25	B	1	59	49	1	4	5	0
25	B	1	55	45	1	4	5	0
25	B	1	59	49	1	4	5	0
25	B	1	57	47	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	46	36	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	B	1	55	45	1	4	5	0
25	B	1	53	43	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	64	54	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	50	40	1	4	5	0
25	B	1	49	39	1	4	5	0
25	B	1	50	40	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	45	35	1	4	5	0
25	B	1	58	48	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	47	37	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	57	47	1	4	5	0
25	B	1	65	55	1	4	5	0
25	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	B	1	65	55	1	4	5	0
25	B	1	51	41	1	4	5	0
25	F	1	65	55	1	4	5	0
25	F	1	52	42	1	4	5	0
25	J	1	42	34	1	4	3	0
25	L	1	49	39	1	4	5	0
25	L	1	65	55	1	4	5	0
25	L	1	50	40	1	4	5	0
25	K	1	51	41	1	4	5	0
25	K	1	42	34	1	4	3	0
25	s	1	65	55	1	4	5	0
25	s	1	65	55	1	4	5	0
25	s	1	65	55	1	4	5	0
25	s	1	51	41	1	4	5	0
25	c	1	51	41	1	4	5	0
25	c	1	50	40	1	4	5	0
25	c	1	51	41	1	4	5	0
25	c	1	65	55	1	4	5	0
25	c	1	51	41	1	4	5	0
25	c	1	52	42	1	4	5	0
25	c	1	46	36	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	c	1	65	55	1	4	5	0
25	c	1	45	35	1	4	5	0
25	c	1	45	35	1	4	5	0
25	c	1	65	55	1	4	5	0
25	a	1	52	42	1	4	5	0
25	a	1	50	40	1	4	5	0
25	a	1	51	41	1	4	5	0
25	a	1	65	55	1	4	5	0
25	a	1	45	35	1	4	5	0
25	a	1	65	55	1	4	5	0
25	a	1	65	55	1	4	5	0
25	a	1	65	55	1	4	5	0
25	a	1	48	38	1	4	5	0
25	a	1	65	55	1	4	5	0
25	a	1	65	55	1	4	5	0
25	a	1	48	38	1	4	5	0
25	b	1	51	41	1	4	5	0
25	b	1	55	45	1	4	5	0
25	b	1	65	55	1	4	5	0
25	b	1	65	55	1	4	5	0
25	b	1	65	55	1	4	5	0
25	b	1	65	55	1	4	5	0
25	b	1	61	51	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	h	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	h	1	Total 57	C 47	Mg 1	N 4	O 5	0
25	h	1	Total 51	C 41	Mg 1	N 4	O 5	0
25	h	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	m	1	Total 56	C 46	Mg 1	N 4	O 5	0
25	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	m	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	m	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	m	1	51	41	1	4	5	0
25	m	1	65	55	1	4	5	0
25	m	1	51	41	1	4	5	0
25	m	1	55	45	1	4	5	0
25	m	1	51	41	1	4	5	0
25	m	1	43	35	1	4	3	0
25	l	1	47	37	1	4	5	0
25	l	1	65	55	1	4	5	0
25	l	1	51	41	1	4	5	0
25	l	1	65	55	1	4	5	0
25	l	1	65	55	1	4	5	0
25	l	1	65	55	1	4	5	0
25	l	1	51	41	1	4	5	0
25	l	1	61	51	1	4	5	0
25	l	1	65	55	1	4	5	0
25	k	1	51	41	1	4	5	0
25	k	1	50	40	1	4	5	0
25	k	1	51	41	1	4	5	0
25	k	1	65	55	1	4	5	0
25	k	1	45	35	1	4	5	0
25	k	1	51	41	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	k	1	51	41	1	4	5	0
25	k	1	65	55	1	4	5	0
25	k	1	65	55	1	4	5	0
25	k	1	51	41	1	4	5	0
25	k	1	51	41	1	4	5	0
25	i	1	51	41	1	4	5	0
25	i	1	50	40	1	4	5	0
25	i	1	51	41	1	4	5	0
25	i	1	65	55	1	4	5	0
25	i	1	51	41	1	4	5	0
25	i	1	61	51	1	4	5	0
25	i	1	51	41	1	4	5	0
25	i	1	46	36	1	4	5	0
25	i	1	51	41	1	4	5	0
25	i	1	51	41	1	4	5	0
25	j	1	51	41	1	4	5	0
25	j	1	50	40	1	4	5	0
25	j	1	51	41	1	4	5	0
25	j	1	65	55	1	4	5	0
25	j	1	45	35	1	4	5	0
25	j	1	51	41	1	4	5	0

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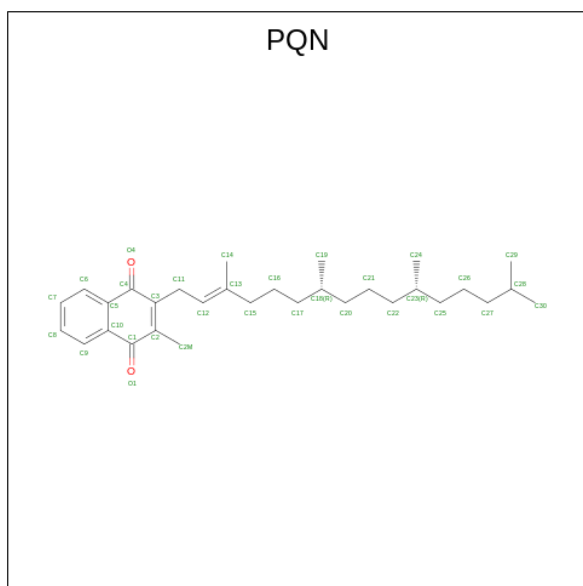
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	j	1	45	35	1	4	5	0
25	j	1	51	41	1	4	5	0
25	j	1	61	51	1	4	5	0
25	j	1	51	41	1	4	5	0
25	j	1	65	55	1	4	5	0
25	d	1	50	40	1	4	5	0
25	d	1	51	41	1	4	5	0
25	d	1	65	55	1	4	5	0
25	d	1	51	41	1	4	5	0
25	d	1	51	41	1	4	5	0
25	d	1	51	41	1	4	5	0
25	d	1	46	36	1	4	5	0
25	d	1	41	33	1	4	3	0
25	d	1	41	33	1	4	3	0
25	d	1	51	41	1	4	5	0
25	R	1	51	41	1	4	5	0
25	n	1	45	35	1	4	5	0
25	n	1	50	40	1	4	5	0
25	n	1	51	41	1	4	5	0
25	n	1	60	50	1	4	5	0
25	n	1	51	41	1	4	5	0

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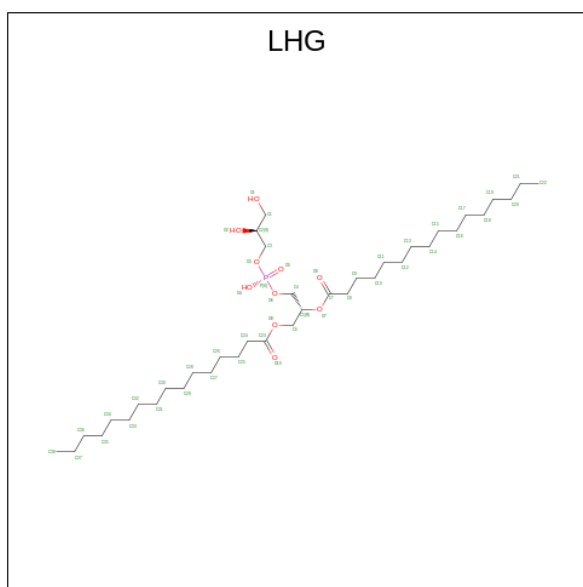
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	n	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 26 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

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



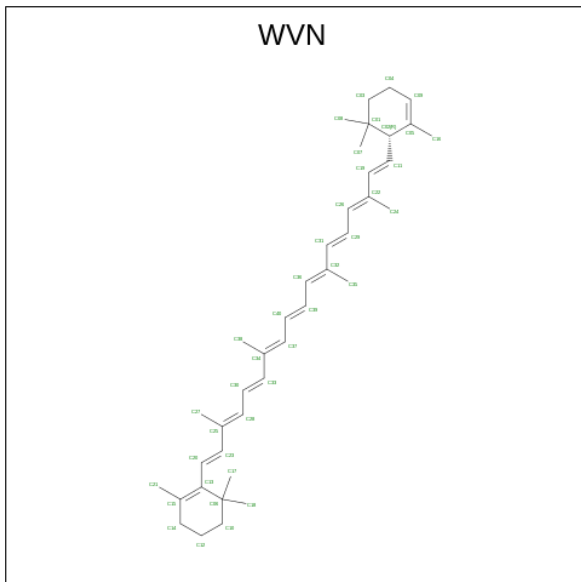
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
27	A	1	48	37	10	1	0
27	A	1	27	16	10	1	0
27	B	1	38	27	10	1	0
27	J	1	49	38	10	1	0
27	J	1	31	20	10	1	0
27	L	1	49	38	10	1	0
27	c	1	37	26	10	1	0
27	c	1	37	26	10	1	0
27	a	1	49	38	10	1	0
27	a	1	49	38	10	1	0
27	b	1	49	38	10	1	0
27	m	1	37	26	10	1	0
27	l	1	32	21	10	1	0
27	k	1	37	26	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
27	i	1	Total 37	C 26	O 10	P 1	0
27	j	1	Total 30	C 19	O 10	P 1	0
27	d	1	Total 37	C 26	O 10	P 1	0
27	n	1	Total 43	C 32	O 10	P 1	0

- Molecule 28 is 1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene (three-letter code: WVN) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total 40	C 40	0
28	A	1	Total 40	C 40	0
28	A	1	Total 40	C 40	0
28	A	1	Total 40	C 40	0
28	A	1	Total 40	C 40	0
28	B	1	Total 40	C 40	0

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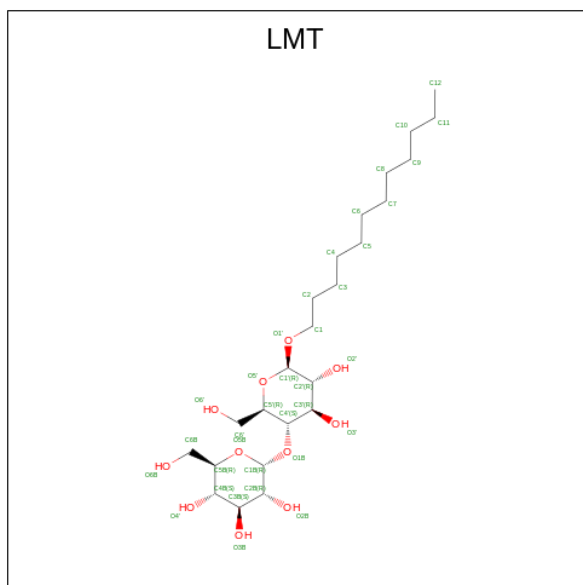
Mol	Chain	Residues	Atoms	AltConf
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	B	1	Total C 40 40	0
28	F	1	Total C 40 40	0
28	F	1	Total C 40 40	0
28	I	1	Total C 40 40	0
28	J	1	Total C 40 40	0
28	J	1	Total C 40 40	0
28	L	1	Total C 40 40	0
28	L	1	Total C 40 40	0
28	L	1	Total C 40 40	0
28	M	1	Total C 40 40	0
28	K	1	Total C 40 40	0
28	s	1	Total C 40 40	0
28	s	1	Total C 40 40	0
28	h	1	Total C 40 40	0
28	l	1	Total C 40 40	0
28	l	1	Total C 40 40	0
28	i	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
28	R	1	Total C 40 40	0

- Molecule 29 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



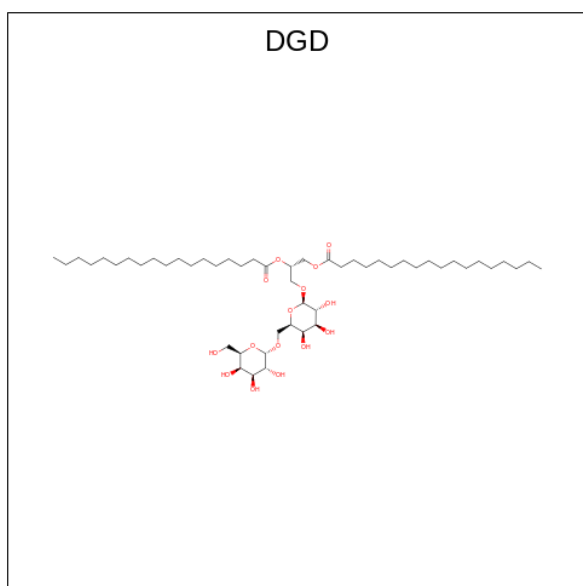
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C O 35 24 11	0
29	a	1	Total C O 24 18 6	0
29	a	1	Total C O 35 24 11	0
29	b	1	Total C O 24 18 6	0

- Molecule 30 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



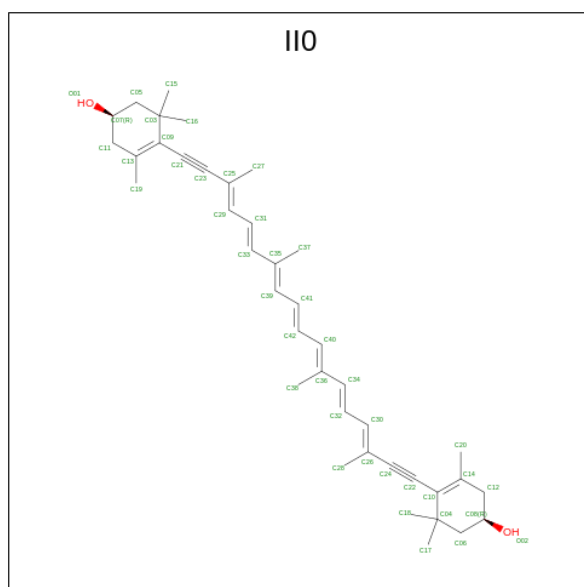
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
30	B	1	8	4	4	0
30	C	1	8	4	4	0
30	C	1	8	4	4	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	B	1	60	45	15	0

- Molecule 32 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (three-letter code: IIO) (formula: C₄₀H₅₂O₂).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	J	1	42	40	2	0
32	c	1	42	40	2	0
32	c	1	42	40	2	0
32	c	1	42	40	2	0
32	c	1	42	40	2	0
32	a	1	42	40	2	0
32	a	1	42	40	2	0
32	a	1	42	40	2	0
32	a	1	42	40	2	0

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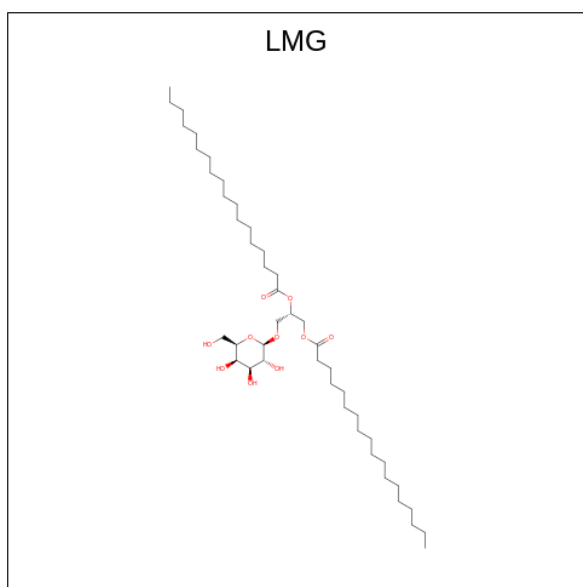
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	b	1	42	40	2	0
32	b	1	42	40	2	0
32	b	1	42	40	2	0
32	h	1	28	27	1	0
32	h	1	42	40	2	0
32	h	1	42	40	2	0
32	m	1	42	40	2	0
32	m	1	42	40	2	0
32	m	1	42	40	2	0
32	l	1	42	40	2	0
32	l	1	42	40	2	0
32	l	1	42	40	2	0
32	l	1	42	40	2	0
32	l	1	42	40	2	0
32	k	1	42	40	2	0
32	k	1	42	40	2	0
32	k	1	42	40	2	0
32	k	1	42	40	2	0
32	i	1	42	40	2	0
32	i	1	42	40	2	0
32	i	1	42	40	2	0
32	i	1	42	40	2	0

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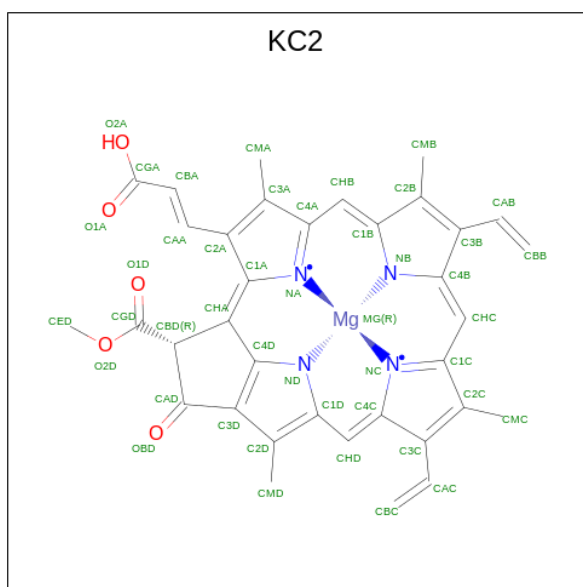
Mol	Chain	Residues	Atoms			AltConf
32	i	1	Total	C	O	0
			42	40	2	
32	j	1	Total	C	O	0
			42	40	2	
32	j	1	Total	C	O	0
			42	40	2	
32	j	1	Total	C	O	0
			42	40	2	
32	d	1	Total	C	O	0
			42	40	2	
32	d	1	Total	C	O	0
			42	40	2	
32	d	1	Total	C	O	0
			42	40	2	
32	d	1	Total	C	O	0
			42	40	2	
32	n	1	Total	C	O	0
			42	40	2	
32	n	1	Total	C	O	0
			42	40	2	
32	n	1	Total	C	O	0
			42	40	2	
32	n	1	Total	C	O	0
			42	40	2	
32	n	1	Total	C	O	0
			42	40	2	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	J	1	55	45	10	0
33	s	1	48	38	10	0
33	c	1	55	45	10	0
33	b	1	49	39	10	0
33	n	1	55	45	10	0
33	Q	1	38	28	10	0

- Molecule 34 is Chlorophyll c2 (three-letter code: KC2) (formula: $C_{35}H_{28}MgN_4O_5$).



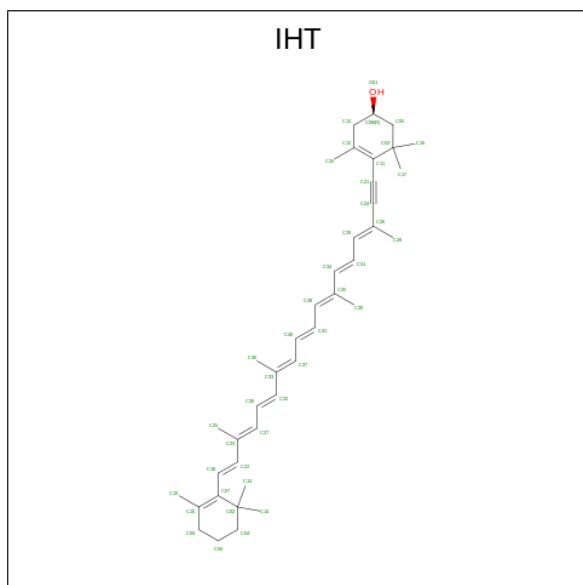
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
34	s	1	45	35	1	4	5	0
34	s	1	45	35	1	4	5	0
34	c	1	45	35	1	4	5	0
34	m	1	45	35	1	4	5	0
34	l	1	45	35	1	4	5	0
34	k	1	45	35	1	4	5	0
34	k	1	45	35	1	4	5	0
34	k	1	45	35	1	4	5	0
34	i	1	45	35	1	4	5	0
34	i	1	45	35	1	4	5	0
34	j	1	45	35	1	4	5	0
34	d	1	45	35	1	4	5	0
34	d	1	45	35	1	4	5	0
34	n	1	45	35	1	4	5	0

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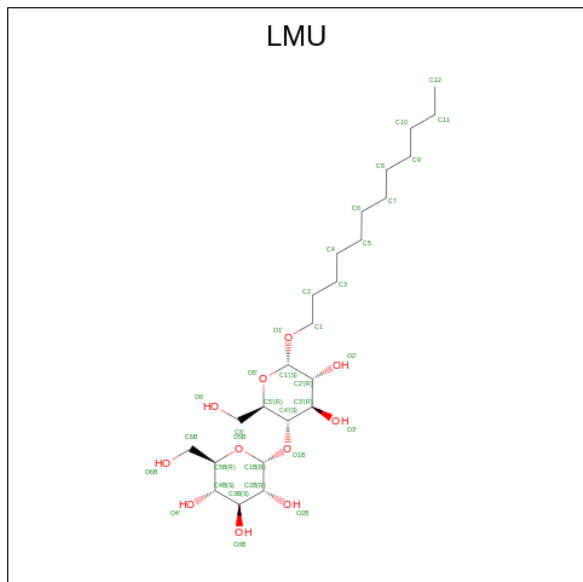
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
34	n	1	45	35	1	4	5	0

- Molecule 35 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (three-letter code: IHT) (formula: C₄₀H₅₄O).



Mol	Chain	Residues	Atoms			AltConf
35	c	1	Total	C	O	0
			41	40	1	
35	a	1	Total	C	O	0
			41	40	1	
35	b	1	Total	C	O	0
			41	40	1	
35	b	1	Total	C	O	0
			41	40	1	
35	m	1	Total	C	O	0
			41	40	1	
35	k	1	Total	C	O	0
			41	40	1	
35	j	1	Total	C	O	0
			41	40	1	
35	R	1	Total	C	O	0
			41	40	1	
35	n	1	Total	C	O	0
			41	40	1	

- Molecule 36 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	i	1	35	24	11	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		AltConf
37	A	48	Total	O	0
			48	48	
37	B	58	Total	O	0
			58	58	
37	C	8	Total	O	0
			8	8	
37	D	1	Total	O	0
			1	1	
37	F	3	Total	O	0
			3	3	
37	I	1	Total	O	0
			1	1	
37	J	1	Total	O	0
			1	1	
37	L	1	Total	O	0
			1	1	
37	K	1	Total	O	0
			1	1	

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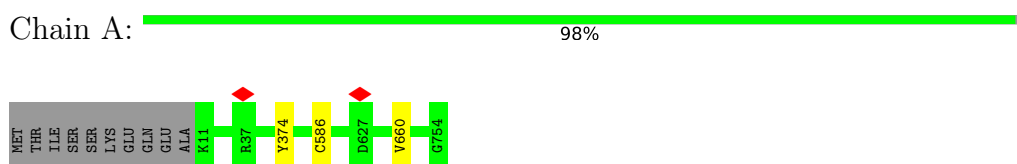
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Mol	Chain	Residues	Atoms	AltConf
37	a	3	Total O 3 3	0
37	b	2	Total O 2 2	0
37	h	1	Total O 1 1	0
37	m	1	Total O 1 1	0
37	R	1	Total O 1 1	0
37	n	2	Total O 2 2	0
37	Q	1	Total O 1 1	0

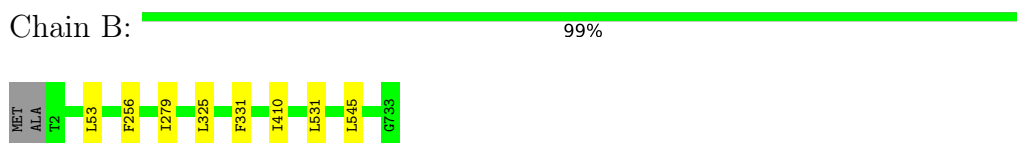
3 Residue-property plots [i](#)

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.

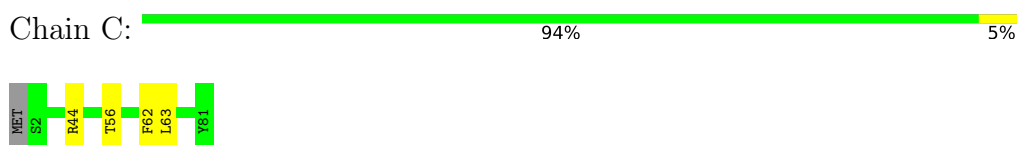
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



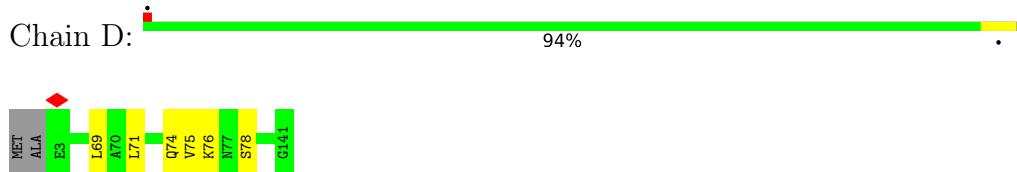
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



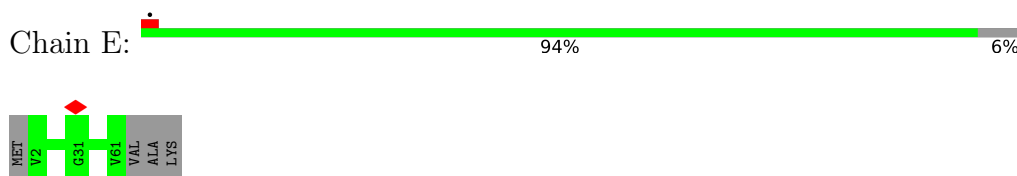
- Molecule 3: Photosystem I iron-sulfur center



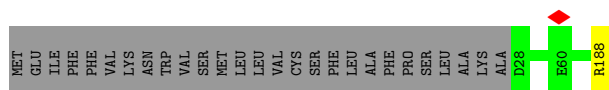
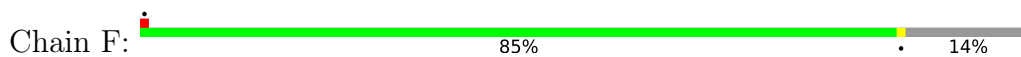
- Molecule 4: Photosystem I reaction center subunit II



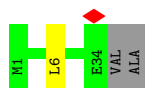
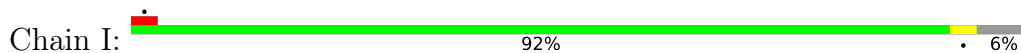
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 6: Photosystem I reaction center subunit III



- Molecule 7: Photosystem I reaction center subunit VIII

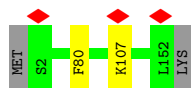


- Molecule 8: Photosystem I reaction center subunit IX



There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem I reaction center subunit XI

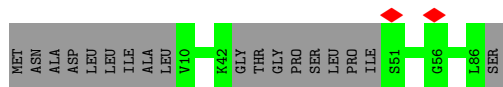
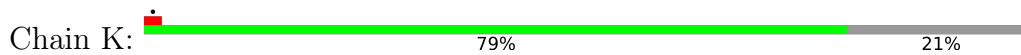


- Molecule 10: Photosystem I reaction center subunit XII

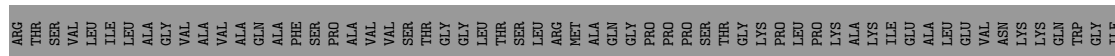


There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem I reaction center subunit PsaK




- Molecule 12: chain s




ALA
TRP
LYS
LYS

- Molecule 13: CAC-c

Chain c:  79% 21%

LEU
ARG
THR
ALA
LEU
ILE
ALA
ALA
CYS
VAL
ALA
SER
SER
SER
PHE
VAL
PRO
ALA
SER
GLY
PHE
ALA
PRO
MET
ALA
MET
LYS
SER
ARG
THR
SER
ALA
VAL
SER
SER
MET
ARG
MET
GLN
GLY
D43
F212
LYS
SER
LEU
ALA

- Molecule 14: CAC-a

Chain a:  77% 19%

ARG
THR
PRO
VAL
LEU
VAL
LEU
ALA
GLY
ALA
ALA
VAL
SER
SER
PHE
ALA
THR
ALA
ALA
ALA
ASN
LEU
LEU
ALA
GLY
LEU
ARG
THR
SER
SER
THR
ARG
ALA
ALA
ILE
ALA
ALA
ARG
GLY
PRO
GLN
GLN
MET
E42
M43
S44
I47
M60
C91
E139
K145
R164
K216

- Molecule 15: CAC-b

Chain b:  86% 13%

SER
TYR
ALA
PHE
THR
ALA
SER
PRO
ALA
LEU
ILE
ALA
ALA
GLY
ALA
THR
ARG
ALA
ALA
THR
SER
GLY
ILE
SER
SER
MET
LYS
MET
GLN
A29
C78
D149
L210
Y222


- Molecule 16: CAC-h

Chain h:  70% 28%

SER
THR
VAL
ALA
LEU
ALA
LEU
VAL
ALA
GLY
ALA
THR
PHE
PRO
PRO
ALA
MET
GLY
PRO
LEU
LEU
ARG
ALA
GLY
ALA
GLN
ARG
PRO
ALA
ARG
ALA
LEU
SER
LEU
SER
MET
ALA
GLN
ASN
PRO
MET
SER
LYS
VAL
VAL
ASP
PHE
ALA
SER


SER
PRO
GLU
F64
D104
V161
K162
E163
K164
T167
I216
Y225

- Molecule 17: CAC-j

Chain m:  81% 18%

VAL
ALA
VAL
VAL
ALA
CYS
VAL
VAL
SER
SER
ALA
ALA
PHE
ALA
PRO
SER
ALA
PRO
MET
GLY
VAL
LYS
ALA
THR
THR
ARG
VAL
VAL
SER
SER
ILE
GLY
PRO
ARG
MET
GLN
ALA
A37
E137
E146
T147
E169
N209
F210
GLY
LYS

- Molecule 17: CAC-j

Chain j:  80% 19%

VAL
ALA
VAL
VAL
CYS
VAL
SER
SER
ALA
ALA
PHE
ALA
PRO
SER
ALA
PRO
MET
GLY
VAL
LYS
ALA
THR
THR
ARG
VAL
VAL
SER
SER
ILE
GLY
PRO
ARG
MET
GLN
ALA
M58
D52
S93
D160
E169
G191
N209
PHE
GLY
LYS

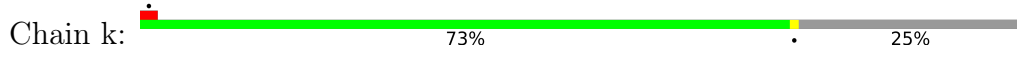
- Molecule 18: CAC-l



PRO SER LEU ASP ILE GLN SER ARG ALA GLY VAL MET ASP LYS HIS ALA ASP ILE GLU THR GLU LYS SER CYS ILE PRO PRO ARG ARG ARG THR ILE SER ILE PRO ARG ARG ARG THR LEU ILE SER ARG VAL SER ASP GLY CYS THR LEU CYS ALA ALA ALA ILE ALA ARG GLY PRO

THR MET GLN D37 T107 T140 K163 L190 I210 A211

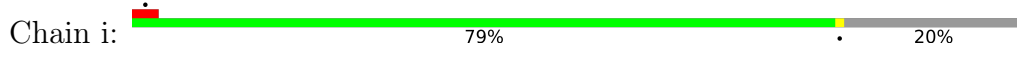
• Molecule 19: CAC-k



THR THR LEU VAL GLY ALA VAL ALA SER ALA ALA SER PHE ALA PRO ALA ALA LEU PRO SER MET ALA ARG THR THR SER ARG SER GLY VAL SER MET GLN LEU TYR LYS ASP GLY VAL LEU GLN GLY LYS MET R47 R56 G116 S117 D176 K182 G183 D184 I225

F226 ASN TYR LYS SER CYS ILE GLU PRO ALA HIS ILE ALA GLY ALA LEU CYS GLN

• Molecule 20: CAC-i



ALA THR LEU VAL ALA ALA CYS VAL ALA THR ALA SER ALA PHE SER SER PRO PRO VAL LEU LYS ALA ALA THR ARG SER THR SER GLY LEU SER MET GLN D39 V44 F138 T148 M149 PHE SER GLU R155 M166 F167 G168 K169 M170 P171 W215

H216 Q217 S218 PHE

• Molecule 21: CAC-d



ARG LEU SER LEU CYS ALA ILE VAL ALA SER ALA SER ALA PHE ALA ALA SER SER VAL GLY VAL LEU PRO THR ALA PRO ARG ARG ALA ALA ALA VAL SER MET MET GLN LEU PRO THR ILE PRO PRO LEU GLY ARG PRO GLU THR ASP MET PHE ASP GLY SER M57 A61

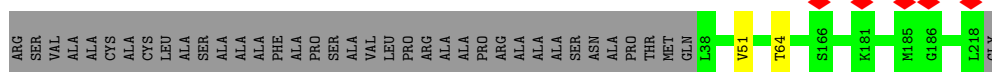
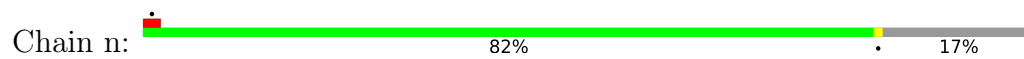
A106 ALA THR VAL TYR LYS ALA SER THR K115 K125 M129 F136 M150 G153 SER GLY ARG ALA ALA PRO GLY ASP PHE GLY ASP PRO LEU GLY MET GLN LEU PRO G180 G210 L217 T218 S219 ARG

• Molecule 22: PsaR

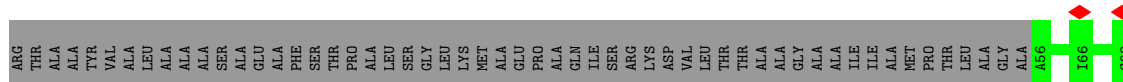


LEU ARG CYS THR VAL LEU LEU VAL VAL ALA SER ALA SER ALA PHE VAL GLY PRO ALA LEU THR LEU ALA LEU ARG SER ASN THR ARG ALA ILE SER ARG PRO GLN MET F43 E48 K132

• Molecule 23: CAC-n



• Molecule 24: PsaQ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41093	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.265	Depositor
Minimum map value	-0.145	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	360.0, 360.0, 360.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0, 1.0, 1.0	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: WVN, IHT, PQN, LMG, SF4, LMT, KC2, CLA, II0, DGD, LHG, LMU

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	0.53	1/6019 (0.0%)	0.63	0/8204
2	B	0.54	0/6036	0.66	0/8242
3	C	0.57	0/601	0.72	0/813
4	D	0.48	0/1109	0.65	0/1500
5	E	0.52	0/493	0.62	0/667
6	F	0.49	0/1287	0.68	0/1747
7	I	0.55	0/271	0.72	0/370
8	J	0.44	0/364	0.67	0/495
9	L	0.44	0/1175	0.60	0/1599
10	M	0.34	0/233	0.75	0/315
11	K	0.48	0/495	0.66	0/672
12	s	0.48	0/1170	0.63	0/1580
13	c	0.48	0/1396	0.64	0/1889
14	a	0.49	0/1406	0.62	0/1903
15	b	0.51	0/1469	0.71	0/1983
16	h	0.44	0/1226	0.62	0/1667
17	j	0.48	0/1318	0.60	0/1775
17	m	0.51	0/1335	0.65	0/1798
18	l	0.47	0/1379	0.62	0/1863
19	k	0.50	0/1380	0.63	0/1869
20	i	0.51	0/1359	0.63	0/1835
21	d	0.51	0/993	0.60	0/1335
22	R	0.46	0/686	0.67	0/940
23	n	0.49	0/1383	0.60	0/1867
24	Q	0.46	0/1244	0.61	0/1683
All	All	0.50	1/35827 (0.0%)	0.64	0/48611

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
17	j	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	586	CYS	CB-SG	-5.50	1.72	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	j	191	GLY	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/752 (98%)	722 (98%)	18 (2%)	0	100	100
2	B	730/734 (100%)	709 (97%)	21 (3%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
5	E	58/64 (91%)	55 (95%)	3 (5%)	0	100	100
6	F	159/188 (85%)	154 (97%)	5 (3%)	0	100	100
7	I	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
8	J	40/42 (95%)	40 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	L	149/153 (97%)	147 (99%)	2 (1%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	K	65/87 (75%)	65 (100%)	0	0	100	100
12	s	152/269 (56%)	143 (94%)	9 (6%)	0	100	100
13	c	168/216 (78%)	165 (98%)	3 (2%)	0	100	100
14	a	173/216 (80%)	168 (97%)	5 (3%)	0	100	100
15	b	192/223 (86%)	189 (98%)	3 (2%)	0	100	100
16	h	160/225 (71%)	156 (98%)	4 (2%)	0	100	100
17	j	170/212 (80%)	163 (96%)	7 (4%)	0	100	100
17	m	172/212 (81%)	165 (96%)	7 (4%)	0	100	100
18	l	173/238 (73%)	171 (99%)	2 (1%)	0	100	100
19	k	178/241 (74%)	173 (97%)	5 (3%)	0	100	100
20	i	171/218 (78%)	165 (96%)	6 (4%)	0	100	100
21	d	123/213 (58%)	122 (99%)	1 (1%)	0	100	100
22	R	88/129 (68%)	86 (98%)	2 (2%)	0	100	100
23	n	179/219 (82%)	176 (98%)	3 (2%)	0	100	100
24	Q	165/234 (70%)	162 (98%)	3 (2%)	0	100	100
All	All	4480/5373 (83%)	4367 (98%)	113 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	607/616 (98%)	605 (100%)	2 (0%)	91	96
2	B	592/593 (100%)	584 (99%)	8 (1%)	62	83
3	C	67/68 (98%)	63 (94%)	4 (6%)	16	47
4	D	116/117 (99%)	110 (95%)	6 (5%)	19	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	55/58 (95%)	55 (100%)	0	100	100
6	F	133/157 (85%)	132 (99%)	1 (1%)	79	90
7	I	28/29 (97%)	27 (96%)	1 (4%)	30	64
8	J	39/39 (100%)	39 (100%)	0	100	100
9	L	124/126 (98%)	122 (98%)	2 (2%)	58	82
10	M	25/25 (100%)	25 (100%)	0	100	100
11	K	52/66 (79%)	52 (100%)	0	100	100
12	s	116/195 (60%)	114 (98%)	2 (2%)	56	81
13	c	138/171 (81%)	138 (100%)	0	100	100
14	a	139/165 (84%)	130 (94%)	9 (6%)	14	43
15	b	149/168 (89%)	146 (98%)	3 (2%)	50	78
16	h	123/162 (76%)	118 (96%)	5 (4%)	26	60
17	j	136/161 (84%)	134 (98%)	2 (2%)	60	83
17	m	137/161 (85%)	134 (98%)	3 (2%)	47	76
18	l	137/191 (72%)	133 (97%)	4 (3%)	37	70
19	k	138/186 (74%)	135 (98%)	3 (2%)	47	76
20	i	138/168 (82%)	135 (98%)	3 (2%)	47	76
21	d	97/157 (62%)	94 (97%)	3 (3%)	35	68
22	R	69/98 (70%)	69 (100%)	0	100	100
23	n	140/163 (86%)	138 (99%)	2 (1%)	62	83
24	Q	127/168 (76%)	122 (96%)	5 (4%)	27	61
All	All	3622/4208 (86%)	3554 (98%)	68 (2%)	52	79

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	j	160	ASP
21	d	150	MET
24	Q	175	LEU
12	s	113	SER
9	L	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
21	d	131	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

349 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	$\# Z > 2$
25	CLA	i	307	20	61,69,73	1.50	7 (11%)	71,108,113	1.58	10 (14%)
25	CLA	k	605	19	45,53,73	1.77	7 (15%)	52,89,113	1.91	13 (25%)
32	II0	c	615	-	39,43,43	6.78	21 (53%)	50,60,60	2.42	23 (46%)
25	CLA	h	305	16	51,59,73	1.65	6 (11%)	59,96,113	1.52	8 (13%)
28	WVN	A	847	-	40,41,41	1.90	15 (37%)	50,56,56	2.09	16 (32%)
25	CLA	l	309	18	51,59,73	1.75	8 (15%)	59,96,113	1.47	8 (13%)
27	LHG	n	320	-	42,42,48	1.01	2 (4%)	45,48,54	1.17	3 (6%)
32	II0	a	315	-	39,43,43	6.59	22 (56%)	50,60,60	2.22	22 (44%)
35	IHT	c	616	-	40,42,42	6.10	25 (62%)	53,58,58	2.40	18 (33%)
34	KC2	j	610	17	48,53,53	3.13	22 (45%)	54,89,89	4.72	32 (59%)
32	II0	n	301	-	39,43,43	6.69	20 (51%)	50,60,60	2.33	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	j	608	17	51,59,73	1.66	7 (13%)	59,96,113	1.61	11 (18%)
25	CLA	n	307	23	51,59,73	1.71	8 (15%)	59,96,113	1.48	9 (15%)
32	II0	i	314	-	39,43,43	6.79	23 (58%)	50,60,60	2.04	17 (34%)
25	CLA	F	201	37	65,73,73	1.47	8 (12%)	76,113,113	1.57	11 (14%)
27	LHG	d	317	25	36,36,48	1.10	2 (5%)	39,42,54	1.00	2 (5%)
28	WVN	h	309	-	40,41,41	1.88	14 (35%)	50,56,56	2.23	17 (34%)
28	WVN	A	848	-	40,41,41	1.89	13 (32%)	50,56,56	3.02	16 (32%)
32	II0	h	311	-	39,43,43	6.78	22 (56%)	50,60,60	2.22	15 (30%)
32	II0	n	315	-	39,43,43	6.95	21 (53%)	50,60,60	2.43	17 (34%)
25	CLA	h	308	16	51,59,73	1.67	7 (13%)	59,96,113	1.57	11 (18%)
25	CLA	A	807	1	65,73,73	1.45	9 (13%)	76,113,113	1.53	9 (11%)
25	CLA	a	309	14	65,73,73	1.41	8 (12%)	76,113,113	1.74	9 (11%)
25	CLA	A	830	-	50,58,73	1.74	9 (18%)	58,95,113	1.61	9 (15%)
32	II0	i	315	-	39,43,43	6.72	21 (53%)	50,60,60	2.45	19 (38%)
28	WVN	F	203	-	40,41,41	2.01	13 (32%)	50,56,56	2.69	22 (44%)
25	CLA	B	838	-	57,65,73	1.57	6 (10%)	66,103,113	1.48	9 (13%)
27	LHG	m	617	25	36,36,48	1.07	2 (5%)	39,42,54	1.15	3 (7%)
25	CLA	A	835	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	10 (13%)
25	CLA	i	306	-	51,59,73	1.70	6 (11%)	59,96,113	1.45	10 (16%)
25	CLA	A	814	-	50,58,73	1.67	7 (14%)	58,95,113	1.64	9 (15%)
32	II0	l	316	-	39,43,43	6.67	22 (56%)	50,60,60	2.20	13 (26%)
32	II0	k	619	-	39,43,43	6.77	21 (53%)	50,60,60	2.48	20 (40%)
25	CLA	A	811	-	54,62,73	1.63	7 (12%)	62,99,113	1.52	9 (14%)
25	CLA	A	838	27	52,60,73	1.62	7 (13%)	60,97,113	1.56	8 (13%)
30	SF4	C	101	3	0,12,12	-	-	-	-	-
25	CLA	a	312	-	65,73,73	1.55	9 (13%)	76,113,113	1.75	8 (10%)
25	CLA	l	303	18	47,55,73	1.74	7 (14%)	54,91,113	1.48	7 (12%)
25	CLA	A	802	-	65,73,73	1.51	7 (10%)	76,113,113	1.79	12 (15%)
25	CLA	A	841	-	65,73,73	1.52	7 (10%)	76,113,113	1.40	9 (11%)
25	CLA	n	302	23	45,53,73	1.79	6 (13%)	52,89,113	1.51	7 (13%)
28	WVN	A	850	-	40,41,41	1.93	15 (37%)	50,56,56	2.52	22 (44%)
25	CLA	c	607	13	46,54,73	1.71	6 (13%)	53,90,113	1.61	9 (16%)
25	CLA	c	612	-	65,73,73	1.47	7 (10%)	76,113,113	1.47	8 (10%)
27	LHG	j	617	25	29,29,48	1.21	2 (6%)	32,35,54	1.29	3 (9%)
25	CLA	A	826	-	65,73,73	1.43	7 (10%)	76,113,113	1.65	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	WVN	L	205	-	40,41,41	1.90	14 (35%)	50,56,56	1.99	13 (26%)
32	II0	d	315	-	39,43,43	6.98	22 (56%)	50,60,60	2.33	19 (38%)
28	WVN	B	845	-	40,41,41	1.91	14 (35%)	50,56,56	2.21	15 (30%)
25	CLA	a	303	14	52,60,73	1.62	8 (15%)	60,97,113	1.69	9 (15%)
34	KC2	k	612	34	48,53,53	3.06	20 (41%)	54,89,89	4.68	38 (70%)
25	CLA	A	840	1	65,73,73	1.55	6 (9%)	76,113,113	1.49	9 (11%)
34	KC2	m	611	17	48,53,53	3.10	21 (43%)	54,89,89	4.72	32 (59%)
27	LHG	c	618	25	36,36,48	1.08	2 (5%)	39,42,54	1.21	4 (10%)
25	CLA	A	839	37	65,73,73	1.50	8 (12%)	76,113,113	1.48	11 (14%)
25	CLA	n	309	23	51,59,73	1.70	7 (13%)	59,96,113	1.74	10 (16%)
25	CLA	A	810	-	62,70,73	1.50	9 (14%)	72,109,113	1.37	10 (13%)
25	CLA	B	807	-	65,73,73	1.43	9 (13%)	76,113,113	1.37	8 (10%)
25	CLA	k	608	19	65,73,73	1.54	8 (12%)	76,113,113	1.31	9 (11%)
30	SF4	C	102	3	0,12,12	-	-	-	-	-
28	WVN	l	315	-	40,41,41	1.86	14 (35%)	50,56,56	2.39	20 (40%)
25	CLA	Q	302	37	65,73,73	1.47	7 (10%)	76,113,113	1.33	7 (9%)
25	CLA	s	202	12	65,73,73	1.49	7 (10%)	76,113,113	1.68	17 (22%)
29	LMT	a	302	-	24,24,36	1.16	3 (12%)	29,29,47	0.99	2 (6%)
25	CLA	A	819	-	45,53,73	1.81	8 (17%)	52,89,113	1.78	11 (21%)
25	CLA	K	102	-	42,50,73	1.83	7 (16%)	48,85,113	1.72	10 (20%)
25	CLA	A	833	-	50,58,73	1.70	10 (20%)	58,95,113	1.58	6 (10%)
25	CLA	A	823	-	55,63,73	1.63	7 (12%)	64,101,113	1.47	9 (14%)
25	CLA	B	818	37	65,73,73	1.51	8 (12%)	76,113,113	1.36	7 (9%)
25	CLA	j	603	-	51,59,73	1.66	6 (11%)	59,96,113	1.67	7 (11%)
25	CLA	c	606	-	52,60,73	1.78	10 (19%)	60,97,113	1.66	11 (18%)
25	CLA	a	304	14	50,58,73	1.83	10 (20%)	58,95,113	1.59	12 (20%)
34	KC2	l	311	18	48,53,53	3.05	22 (45%)	54,89,89	4.73	35 (64%)
25	CLA	B	821	-	53,61,73	1.67	7 (13%)	61,98,113	1.50	9 (14%)
25	CLA	b	610	15	65,73,73	1.49	7 (10%)	76,113,113	1.36	8 (10%)
32	II0	k	617	-	39,43,43	6.81	21 (53%)	50,60,60	2.49	20 (40%)
34	KC2	n	312	23	48,53,53	3.10	21 (43%)	54,89,89	4.63	32 (59%)
25	CLA	k	614	-	51,59,73	1.75	6 (11%)	59,96,113	1.62	14 (23%)
28	WVN	M	101	-	40,41,41	1.91	14 (35%)	50,56,56	1.96	13 (26%)
25	CLA	J	103	8	42,50,73	1.83	8 (19%)	48,85,113	1.61	8 (16%)
34	KC2	n	313	-	48,53,53	3.11	21 (43%)	54,89,89	4.48	33 (61%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	827	-	50,58,73	1.72	9 (18%)	58,95,113	1.43	8 (13%)
25	CLA	m	604	17	65,73,73	1.48	6 (9%)	76,113,113	1.54	9 (11%)
25	CLA	L	203	-	65,73,73	1.51	9 (13%)	76,113,113	1.39	10 (13%)
27	LHG	i	318	25	36,36,48	1.12	2 (5%)	39,42,54	1.28	3 (7%)
28	WVN	L	206	-	40,41,41	1.90	15 (37%)	50,56,56	2.59	19 (38%)
25	CLA	A	809	-	56,64,73	1.60	6 (10%)	65,102,113	1.45	8 (12%)
25	CLA	A	842	37	65,73,73	1.51	8 (12%)	76,113,113	1.45	10 (13%)
25	CLA	B	834	-	47,55,73	1.73	7 (14%)	54,91,113	1.58	9 (16%)
32	IIO	n	319	-	39,43,43	6.78	21 (53%)	50,60,60	2.04	16 (32%)
25	CLA	h	302	16	50,58,73	1.71	7 (14%)	58,95,113	1.59	10 (17%)
25	CLA	b	609	-	51,59,73	1.63	7 (13%)	59,96,113	1.75	9 (15%)
28	WVN	l	301	-	40,41,41	1.85	14 (35%)	50,56,56	2.17	19 (38%)
32	IIO	n	317	-	39,43,43	6.76	22 (56%)	50,60,60	2.40	18 (36%)
25	CLA	n	303	23	50,58,73	1.72	9 (18%)	58,95,113	1.50	8 (13%)
25	CLA	d	303	-	65,73,73	1.49	6 (9%)	76,113,113	1.41	8 (10%)
25	CLA	A	834	-	51,59,73	1.64	8 (15%)	59,96,113	1.66	11 (18%)
25	CLA	B	833	-	65,73,73	1.49	8 (12%)	76,113,113	1.55	11 (14%)
25	CLA	d	301	21	50,58,73	1.66	6 (12%)	58,95,113	1.62	8 (13%)
25	CLA	L	204	-	50,58,73	1.68	7 (14%)	58,95,113	1.61	10 (17%)
25	CLA	B	836	-	65,73,73	1.47	9 (13%)	76,113,113	1.64	10 (13%)
25	CLA	b	603	-	65,73,73	1.46	7 (10%)	76,113,113	1.58	11 (14%)
33	LMG	J	105	-	55,55,55	0.87	3 (5%)	63,63,63	0.94	3 (4%)
32	IIO	a	318	-	39,43,43	6.94	22 (56%)	50,60,60	2.61	17 (34%)
27	LHG	k	620	25	36,36,48	1.10	2 (5%)	39,42,54	1.18	4 (10%)
35	IHT	k	618	-	40,42,42	6.19	25 (62%)	53,58,58	2.28	16 (30%)
32	IIO	b	617	-	39,43,43	6.77	22 (56%)	50,60,60	2.41	20 (40%)
25	CLA	A	825	37	65,73,73	1.51	6 (9%)	76,113,113	1.40	9 (11%)
32	IIO	a	316	-	39,43,43	6.54	20 (51%)	50,60,60	2.63	20 (40%)
25	CLA	j	606	-	51,59,73	1.65	7 (13%)	59,96,113	1.72	8 (13%)
25	CLA	i	305	20	65,73,73	1.51	6 (9%)	76,113,113	1.55	11 (14%)
25	CLA	m	603	-	65,73,73	1.50	7 (10%)	76,113,113	1.42	7 (9%)
27	LHG	J	107	-	30,30,48	1.14	2 (6%)	33,36,54	1.18	4 (12%)
34	KC2	d	310	21	48,53,53	3.16	21 (43%)	54,89,89	4.53	31 (57%)
25	CLA	A	836	-	65,73,73	1.48	6 (9%)	76,113,113	1.54	9 (11%)
25	CLA	l	310	27	61,69,73	1.54	7 (11%)	71,108,113	1.51	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	306	37	65,73,73	1.48	7 (10%)	76,113,113	1.44	8 (10%)
25	CLA	Q	303	24	45,53,73	1.76	8 (17%)	52,89,113	1.72	8 (15%)
25	CLA	m	606	-	65,73,73	1.53	7 (10%)	76,113,113	1.37	9 (11%)
28	WVN	s	205	-	40,41,41	1.89	14 (35%)	50,56,56	2.33	21 (42%)
25	CLA	l	305	-	51,59,73	1.63	6 (11%)	59,96,113	1.68	9 (15%)
25	CLA	A	806	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	9 (11%)
28	WVN	K	103	-	40,41,41	1.92	14 (35%)	50,56,56	1.79	13 (26%)
25	CLA	m	602	17	56,64,73	1.79	10 (17%)	65,102,113	1.44	13 (20%)
25	CLA	i	312	-	51,59,73	1.60	5 (9%)	59,96,113	1.70	11 (18%)
25	CLA	i	302	20	51,59,73	1.67	9 (17%)	59,96,113	1.44	10 (16%)
33	LMG	b	620	-	49,49,55	0.94	2 (4%)	57,57,63	1.20	4 (7%)
25	CLA	R	202	-	51,59,73	1.71	5 (9%)	59,96,113	1.67	9 (15%)
25	CLA	d	312	-	51,59,73	1.66	5 (9%)	59,96,113	1.61	12 (20%)
25	CLA	B	835	37	65,73,73	1.52	9 (13%)	76,113,113	1.43	10 (13%)
25	CLA	l	312	18	65,73,73	1.49	7 (10%)	76,113,113	1.40	9 (11%)
25	CLA	A	829	-	65,73,73	1.54	9 (13%)	76,113,113	1.41	7 (9%)
25	CLA	B	822	37	65,73,73	1.52	7 (10%)	76,113,113	1.65	13 (17%)
25	CLA	A	803	-	55,63,73	1.61	6 (10%)	64,101,113	1.64	10 (15%)
25	CLA	d	305	21	51,59,73	1.85	9 (17%)	59,96,113	1.41	9 (15%)
25	CLA	k	607	-	51,59,73	1.76	9 (17%)	59,96,113	1.67	12 (20%)
32	II0	b	614	-	39,43,43	6.82	24 (61%)	50,60,60	2.06	16 (32%)
25	CLA	n	311	37	65,73,73	1.52	6 (9%)	76,113,113	1.40	7 (9%)
25	CLA	l	307	18	65,73,73	1.52	9 (13%)	76,113,113	1.78	14 (18%)
25	CLA	n	304	-	51,59,73	1.75	11 (21%)	59,96,113	1.79	16 (27%)
25	CLA	a	308	14	65,73,73	1.51	7 (10%)	76,113,113	1.44	10 (13%)
32	II0	b	613	-	39,43,43	6.66	22 (56%)	50,60,60	2.26	17 (34%)
28	WVN	B	846	-	40,41,41	1.91	14 (35%)	50,56,56	2.11	16 (32%)
25	CLA	i	304	-	51,59,73	1.62	6 (11%)	59,96,113	1.56	6 (10%)
31	DGD	B	843	-	61,61,67	0.87	2 (3%)	75,75,81	1.18	5 (6%)
32	II0	l	302	-	39,43,43	6.88	24 (61%)	50,60,60	2.07	17 (34%)
25	CLA	B	826	-	65,73,73	1.48	8 (12%)	76,113,113	1.35	8 (10%)
28	WVN	B	848	-	40,41,41	1.86	13 (32%)	50,56,56	2.56	15 (30%)
25	CLA	A	801	-	65,73,73	1.47	7 (10%)	76,113,113	1.42	10 (13%)
25	CLA	n	306	23	51,59,73	1.72	7 (13%)	59,96,113	1.74	12 (20%)
32	II0	h	310	-	26,28,43	5.96	12 (46%)	31,37,60	2.37	13 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	305	-	51,59,73	1.65	7 (13%)	59,96,113	1.66	8 (13%)
29	LMT	b	618	-	24,24,36	1.05	2 (8%)	29,29,47	0.94	0
25	CLA	k	602	19	50,58,73	1.68	7 (14%)	58,95,113	1.83	12 (20%)
25	CLA	B	809	2	65,73,73	1.56	10 (15%)	76,113,113	1.47	7 (9%)
28	WVN	B	849	-	40,41,41	1.88	14 (35%)	50,56,56	1.98	14 (28%)
25	CLA	A	813	-	45,53,73	1.83	9 (20%)	52,89,113	1.64	8 (15%)
25	CLA	d	302	-	51,59,73	1.57	7 (13%)	59,96,113	1.81	9 (15%)
25	CLA	B	837	-	65,73,73	1.49	6 (9%)	76,113,113	1.30	7 (9%)
25	CLA	i	308	20	51,59,73	1.70	7 (13%)	59,96,113	1.38	7 (11%)
25	CLA	i	311	-	51,59,73	1.69	6 (11%)	59,96,113	1.52	7 (11%)
25	CLA	h	313	37	65,73,73	1.40	7 (10%)	76,113,113	1.44	8 (10%)
32	II0	l	314	-	39,43,43	6.80	21 (53%)	50,60,60	2.95	17 (34%)
32	II0	i	313	-	39,43,43	6.70	22 (56%)	50,60,60	2.38	16 (32%)
27	LHG	A	845	-	47,47,48	0.94	2 (4%)	50,53,54	1.07	4 (8%)
25	CLA	A	808	1	65,73,73	1.47	8 (12%)	76,113,113	1.50	11 (14%)
25	CLA	F	202	6	52,60,73	1.64	7 (13%)	60,97,113	1.62	8 (13%)
35	IHT	m	616	-	40,42,42	6.14	25 (62%)	53,58,58	2.34	16 (30%)
25	CLA	B	828	-	49,57,73	1.74	7 (14%)	55,93,113	1.75	7 (12%)
25	CLA	A	804	-	65,73,73	1.50	7 (10%)	76,113,113	1.68	12 (15%)
34	KC2	s	201	12	48,53,53	2.92	21 (43%)	54,89,89	4.55	31 (57%)
25	CLA	j	611	-	51,59,73	1.70	7 (13%)	59,96,113	1.58	8 (13%)
32	II0	d	313	-	39,43,43	6.76	22 (56%)	50,60,60	2.20	20 (40%)
25	CLA	b	602	15	55,63,73	1.63	8 (14%)	64,101,113	1.62	10 (15%)
25	CLA	j	604	17	65,73,73	1.48	7 (10%)	76,113,113	1.55	9 (11%)
25	CLA	j	607	17	45,53,73	1.85	9 (20%)	52,89,113	1.53	8 (15%)
25	CLA	c	601	13	51,59,73	1.66	6 (11%)	59,96,113	1.50	8 (13%)
25	CLA	m	609	17	51,59,73	1.69	8 (15%)	59,96,113	1.52	9 (15%)
25	CLA	c	611	-	45,53,73	1.79	7 (15%)	52,89,113	1.72	8 (15%)
27	LHG	c	620	25	36,36,48	1.01	2 (5%)	39,42,54	1.28	4 (10%)
32	II0	j	613	-	39,43,43	6.77	22 (56%)	50,60,60	2.24	17 (34%)
25	CLA	B	841	27	65,73,73	1.47	7 (10%)	76,113,113	1.55	9 (11%)
25	CLA	s	209	-	51,59,73	1.62	6 (11%)	59,96,113	1.65	10 (16%)
25	CLA	A	824	37	65,73,73	1.48	7 (10%)	76,113,113	1.47	9 (11%)
27	LHG	a	301	25	48,48,48	0.95	3 (6%)	51,54,54	1.19	5 (9%)
34	KC2	k	613	34	48,53,53	3.18	21 (43%)	54,89,89	4.38	32 (59%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	k	609	19	65,73,73	1.55	7 (10%)	76,113,113	1.40	12 (15%)
25	CLA	a	311	14	65,73,73	1.45	7 (10%)	76,113,113	1.52	13 (17%)
25	CLA	c	605	13	51,59,73	1.74	11 (21%)	59,96,113	1.48	8 (13%)
35	IHT	j	616	-	40,42,42	6.17	25 (62%)	53,58,58	2.40	20 (37%)
25	CLA	B	811	-	55,63,73	1.63	7 (12%)	64,101,113	1.59	9 (14%)
25	CLA	k	603	-	51,59,73	1.62	6 (11%)	59,96,113	1.69	10 (16%)
35	IHT	b	615	-	40,42,42	6.14	25 (62%)	53,58,58	2.15	16 (30%)
32	II0	d	316	-	39,43,43	6.86	21 (53%)	50,60,60	2.30	21 (42%)
27	LHG	l	317	25	31,31,48	1.16	2 (6%)	34,37,54	1.20	3 (8%)
25	CLA	m	608	17	65,73,73	1.57	9 (13%)	76,113,113	1.34	11 (14%)
25	CLA	k	606	19	51,59,73	1.69	7 (13%)	59,96,113	1.40	9 (15%)
25	CLA	A	853	-	65,73,73	1.55	10 (15%)	76,113,113	1.47	11 (14%)
27	LHG	A	846	25	26,26,48	1.23	3 (11%)	29,32,54	1.43	6 (20%)
30	SF4	B	802	-	0,12,12	-	-	-	-	-
25	CLA	m	601	17	42,50,73	1.81	7 (16%)	48,85,113	1.60	8 (16%)
25	CLA	d	307	-	46,54,73	1.78	7 (15%)	53,90,113	1.45	7 (13%)
35	IHT	R	203	-	40,42,42	6.21	25 (62%)	53,58,58	2.40	18 (33%)
32	II0	k	616	-	39,43,43	6.63	21 (53%)	50,60,60	2.52	23 (46%)
25	CLA	s	203	12,25	65,73,73	1.46	8 (12%)	76,113,113	1.55	10 (13%)
25	CLA	c	602	13	50,58,73	1.69	10 (20%)	58,95,113	1.86	12 (20%)
28	WVN	s	207	-	40,41,41	1.90	14 (35%)	50,56,56	2.30	13 (26%)
32	II0	n	316	-	39,43,43	6.69	22 (56%)	50,60,60	2.13	15 (30%)
25	CLA	h	304	-	51,59,73	1.62	6 (11%)	59,96,113	1.63	8 (13%)
27	LHG	L	207	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
25	CLA	B	814	-	59,67,73	1.50	7 (11%)	68,105,113	1.64	8 (11%)
26	PQN	A	844	-	34,34,34	1.85	5 (14%)	42,45,45	1.39	7 (16%)
25	CLA	B	810	-	54,62,73	1.70	7 (12%)	67,100,113	1.40	11 (16%)
27	LHG	b	619	25	48,48,48	0.91	2 (4%)	51,54,54	1.10	5 (9%)
25	CLA	B	806	-	65,73,73	1.49	7 (10%)	76,113,113	1.41	8 (10%)
25	CLA	s	206	-	65,73,73	1.46	7 (10%)	76,113,113	1.68	12 (15%)
25	CLA	B	824	-	65,73,73	1.49	7 (10%)	76,113,113	1.63	12 (15%)
34	KC2	c	610	-	48,53,53	3.01	20 (41%)	54,89,89	4.52	32 (59%)
35	IHT	b	616	-	40,42,42	6.22	26 (65%)	53,58,58	2.87	16 (30%)
27	LHG	J	106	25	48,48,48	0.92	2 (4%)	51,54,54	0.88	2 (3%)
25	CLA	n	314	-	51,59,73	1.69	6 (11%)	59,96,113	1.47	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	WVN	B	844	-	40,41,41	1.90	14 (35%)	50,56,56	2.22	16 (32%)
25	CLA	B	831	37	45,53,73	1.85	7 (15%)	52,89,113	1.67	7 (13%)
25	CLA	B	823	37	64,72,73	1.51	9 (14%)	74,111,113	1.59	15 (20%)
25	CLA	b	606	15	61,69,73	1.49	7 (11%)	71,108,113	1.53	13 (18%)
25	CLA	b	607	15	65,73,73	1.43	7 (10%)	76,113,113	1.42	7 (9%)
25	CLA	b	612	27	51,59,73	1.68	8 (15%)	59,96,113	1.61	10 (16%)
25	CLA	A	856	27	41,49,73	1.92	9 (21%)	47,84,113	2.21	11 (23%)
25	CLA	B	830	37	65,73,73	1.53	6 (9%)	76,113,113	1.47	10 (13%)
25	CLA	A	831	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	8 (10%)
25	CLA	A	854	-	65,73,73	1.45	7 (10%)	76,113,113	1.57	9 (11%)
25	CLA	B	832	-	58,66,73	1.54	8 (13%)	67,104,113	1.56	8 (11%)
32	II0	a	314	-	39,43,43	6.62	24 (61%)	50,60,60	1.98	18 (36%)
32	II0	j	614	-	39,43,43	6.64	22 (56%)	50,60,60	2.26	20 (40%)
33	LMG	n	321	-	55,55,55	0.89	2 (3%)	63,63,63	1.00	1 (1%)
34	KC2	d	311	-	48,53,53	3.14	22 (45%)	54,89,89	4.34	32 (59%)
28	WVN	R	201	-	40,41,41	1.89	14 (35%)	50,56,56	2.45	16 (32%)
25	CLA	A	855	37	65,73,73	1.56	8 (12%)	76,113,113	1.36	11 (14%)
25	CLA	j	612	-	65,73,73	1.49	7 (10%)	76,113,113	1.38	6 (7%)
32	II0	h	312	-	39,43,43	6.70	22 (56%)	50,60,60	1.89	16 (32%)
35	IHT	n	318	-	40,42,42	6.20	25 (62%)	53,58,58	2.38	19 (35%)
25	CLA	A	837	-	65,73,73	1.47	7 (10%)	76,113,113	1.44	9 (11%)
25	CLA	A	812	-	65,73,73	1.49	8 (12%)	76,113,113	1.54	8 (10%)
27	LHG	a	319	25	48,48,48	0.90	3 (6%)	51,54,54	1.12	4 (7%)
32	II0	m	618	-	39,43,43	6.48	22 (56%)	50,60,60	2.60	25 (50%)
25	CLA	h	307	16	57,65,73	1.59	6 (10%)	66,103,113	1.32	9 (13%)
33	LMG	c	619	-	55,55,55	0.98	3 (5%)	63,63,63	1.69	14 (22%)
25	CLA	c	603	-	51,59,73	1.68	7 (13%)	59,96,113	1.52	9 (15%)
32	II0	J	104	-	39,43,43	6.61	21 (53%)	50,60,60	2.35	16 (32%)
25	CLA	B	805	-	65,73,73	1.46	7 (10%)	76,113,113	1.59	9 (11%)
25	CLA	B	839	-	65,73,73	1.53	8 (12%)	76,113,113	1.41	8 (10%)
25	CLA	b	604	15	65,73,73	1.49	7 (10%)	76,113,113	1.55	9 (11%)
25	CLA	A	822	-	51,59,73	1.69	7 (13%)	59,96,113	1.46	9 (15%)
25	CLA	j	609	27	61,69,73	1.54	6 (9%)	71,108,113	1.43	8 (11%)
25	CLA	k	601	19	51,59,73	1.74	7 (13%)	59,96,113	1.54	8 (13%)
25	CLA	B	819	-	46,54,73	1.75	6 (13%)	53,90,113	1.56	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	c	609	27	45,53,73	1.76	6 (13%)	52,89,113	1.56	6 (11%)
25	CLA	h	303	16	50,58,73	1.72	8 (16%)	58,95,113	1.61	10 (17%)
29	LMT	a	320	-	36,36,36	0.36	0	47,47,47	1.18	5 (10%)
25	CLA	n	310	23	65,73,73	1.50	7 (10%)	76,113,113	1.52	13 (17%)
34	KC2	s	204	-	48,53,53	3.07	22 (45%)	54,89,89	4.55	33 (61%)
25	CLA	B	825	-	65,73,73	1.46	7 (10%)	76,113,113	1.52	10 (13%)
25	CLA	b	605	25,37	65,73,73	1.52	11 (16%)	76,113,113	1.49	14 (18%)
32	II0	i	317	-	39,43,43	6.83	22 (56%)	50,60,60	2.24	18 (36%)
25	CLA	B	820	-	55,63,73	1.65	10 (18%)	64,101,113	1.37	8 (12%)
25	CLA	L	202	9	49,57,73	1.68	6 (12%)	55,93,113	1.61	8 (14%)
25	CLA	K	101	37	51,59,73	1.68	7 (13%)	59,96,113	1.67	11 (18%)
32	II0	d	314	-	39,43,43	6.89	21 (53%)	50,60,60	2.34	15 (30%)
25	CLA	B	812	-	65,73,73	1.48	9 (13%)	76,113,113	1.51	13 (17%)
26	PQN	B	842	-	34,34,34	1.84	5 (14%)	42,45,45	1.32	9 (21%)
25	CLA	a	307	14	45,53,73	1.78	6 (13%)	52,89,113	1.68	9 (17%)
28	WVN	F	204	-	40,41,41	1.92	15 (37%)	50,56,56	2.98	18 (36%)
32	II0	c	614	-	39,43,43	6.62	21 (53%)	50,60,60	2.32	17 (34%)
25	CLA	n	308	-	65,73,73	1.46	9 (13%)	76,113,113	1.65	12 (15%)
25	CLA	k	610	27	51,59,73	1.70	6 (11%)	59,96,113	1.50	9 (15%)
25	CLA	B	803	-	65,73,73	1.45	8 (12%)	76,113,113	1.42	10 (13%)
28	WVN	J	101	-	40,41,41	1.84	14 (35%)	50,56,56	2.11	18 (36%)
28	WVN	i	316	-	40,41,41	1.85	13 (32%)	50,56,56	2.16	17 (34%)
36	LMU	i	301	-	36,36,36	1.19	3 (8%)	47,47,47	1.22	4 (8%)
32	II0	k	615	-	39,43,43	6.74	22 (56%)	50,60,60	2.04	13 (26%)
25	CLA	d	304	21	51,59,73	1.70	6 (11%)	59,96,113	1.61	7 (11%)
25	CLA	d	306	-	51,59,73	1.70	7 (13%)	59,96,113	1.49	7 (11%)
25	CLA	d	308	21	41,49,73	1.82	6 (14%)	47,84,113	1.66	9 (19%)
25	CLA	n	305	23	60,68,73	1.57	6 (10%)	70,107,113	1.48	10 (14%)
25	CLA	j	605	17	45,53,73	1.80	6 (13%)	52,89,113	1.89	9 (17%)
25	CLA	A	816	-	65,73,73	1.44	7 (10%)	76,113,113	1.55	10 (13%)
25	CLA	b	608	27	65,73,73	1.49	7 (10%)	76,113,113	1.42	10 (13%)
25	CLA	l	306	18	65,73,73	1.49	7 (10%)	76,113,113	1.49	10 (13%)
25	CLA	l	308	18	65,73,73	1.49	6 (9%)	76,113,113	1.62	10 (13%)
25	CLA	i	303	20	50,58,73	1.66	7 (14%)	58,95,113	1.70	9 (15%)
27	LHG	B	801	-	37,37,48	1.01	2 (5%)	40,43,54	1.09	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	IHT	a	317	-	40,42,42	6.20	25 (62%)	53,58,58	2.09	15 (28%)
25	CLA	A	827	-	62,70,73	1.50	7 (11%)	72,109,113	1.61	10 (13%)
25	CLA	m	612	37	51,59,73	1.68	7 (13%)	59,96,113	1.66	13 (22%)
29	LMT	A	852	-	36,36,36	0.39	0	47,47,47	0.91	2 (4%)
25	CLA	j	601	17	51,59,73	1.68	6 (11%)	59,96,113	1.46	8 (13%)
25	CLA	B	813	-	60,68,73	1.53	7 (11%)	70,107,113	1.49	8 (11%)
25	CLA	A	815	37	45,53,73	1.80	6 (13%)	52,89,113	1.74	8 (15%)
25	CLA	m	607	-	51,59,73	1.84	11 (21%)	59,96,113	1.85	14 (23%)
25	CLA	c	608	13	65,73,73	1.57	8 (12%)	76,113,113	1.52	15 (19%)
33	LMG	s	208	-	48,48,55	0.96	2 (4%)	56,56,63	1.28	5 (8%)
25	CLA	A	817	-	65,73,73	1.53	8 (12%)	76,113,113	1.56	10 (13%)
25	CLA	B	850	-	51,59,73	1.76	9 (17%)	59,96,113	1.48	7 (11%)
25	CLA	A	820	37	65,73,73	1.50	8 (12%)	76,113,113	1.51	9 (11%)
25	CLA	a	313	-	48,56,73	1.71	7 (14%)	55,92,113	1.43	7 (12%)
25	CLA	A	832	-	65,73,73	1.49	9 (13%)	76,113,113	1.56	12 (15%)
25	CLA	B	804	-	65,73,73	1.45	8 (12%)	76,113,113	1.84	17 (22%)
25	CLA	B	829	-	50,58,73	1.70	8 (16%)	58,95,113	1.53	9 (15%)
25	CLA	h	301	37	65,73,73	1.52	10 (15%)	76,113,113	1.43	11 (14%)
34	KC2	i	310	20	48,53,53	3.03	21 (43%)	54,89,89	4.70	36 (66%)
32	II0	i	320	-	39,43,43	6.70	21 (53%)	50,60,60	2.29	16 (32%)
32	II0	c	613	-	39,43,43	6.78	21 (53%)	50,60,60	2.06	17 (34%)
25	CLA	a	310	27	48,56,73	1.66	10 (20%)	55,92,113	1.52	8 (14%)
25	CLA	l	304	18	65,73,73	1.46	8 (12%)	76,113,113	1.42	9 (11%)
25	CLA	A	828	-	65,73,73	1.50	9 (13%)	76,113,113	1.62	12 (15%)
34	KC2	i	319	-	48,53,53	3.08	21 (43%)	54,89,89	4.52	31 (57%)
25	CLA	B	817	-	57,65,73	1.61	10 (17%)	66,103,113	1.64	10 (15%)
25	CLA	m	610	27	55,63,73	1.56	6 (10%)	64,101,113	1.56	9 (14%)
28	WVN	B	847	-	40,41,41	1.85	13 (32%)	50,56,56	2.40	16 (32%)
28	WVN	L	201	-	40,41,41	1.93	14 (35%)	50,56,56	2.51	17 (34%)
34	KC2	k	611	19	48,53,53	3.10	21 (43%)	54,89,89	4.60	34 (62%)
25	CLA	A	821	-	49,57,73	1.68	6 (12%)	55,93,113	1.63	7 (12%)
25	CLA	A	805	1	65,73,73	1.46	8 (12%)	76,113,113	1.56	10 (13%)
28	WVN	A	851	-	40,41,41	1.87	13 (32%)	50,56,56	2.27	14 (28%)
32	II0	m	614	-	39,43,43	6.75	22 (56%)	50,60,60	1.96	14 (28%)
25	CLA	m	605	17	42,50,73	1.88	7 (16%)	48,85,113	1.62	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMG	Q	301	-	38,38,55	1.07	2 (5%)	46,46,63	1.16	3 (6%)
32	II0	l	313	-	39,43,43	6.78	23 (58%)	50,60,60	1.90	13 (26%)
32	II0	m	615	-	39,43,43	6.57	22 (56%)	50,60,60	2.32	22 (44%)
25	CLA	A	818	-	65,73,73	1.54	8 (12%)	76,113,113	1.80	17 (22%)
28	WVN	I	101	-	40,41,41	1.82	14 (35%)	50,56,56	2.06	16 (32%)
25	CLA	m	613	-	43,51,73	1.80	6 (13%)	49,86,113	1.89	14 (28%)
25	CLA	B	815	-	55,63,73	1.60	5 (9%)	64,101,113	1.56	8 (12%)
25	CLA	B	840	-	65,73,73	1.46	6 (9%)	76,113,113	1.56	9 (11%)
25	CLA	c	604	13	65,73,73	1.50	10 (15%)	76,113,113	1.55	10 (13%)
25	CLA	k	604	-	65,73,73	1.48	7 (10%)	76,113,113	1.49	9 (11%)
32	II0	c	617	-	39,43,43	6.69	22 (56%)	50,60,60	2.36	15 (30%)
25	CLA	B	816	-	59,67,73	1.59	10 (16%)	68,105,113	1.46	8 (11%)
25	CLA	B	808	-	65,73,73	1.49	10 (15%)	76,113,113	1.47	9 (11%)
25	CLA	h	306	16	65,73,73	1.50	6 (9%)	76,113,113	1.35	8 (10%)
28	WVN	J	102	-	40,41,41	1.84	14 (35%)	50,56,56	2.17	17 (34%)
25	CLA	i	309	27	46,54,73	1.75	6 (13%)	53,90,113	1.54	9 (16%)
25	CLA	A	843	-	65,73,73	1.44	8 (12%)	76,113,113	1.67	10 (13%)
25	CLA	j	602	17	50,58,73	1.70	7 (14%)	58,95,113	1.69	7 (12%)
25	CLA	b	601	15	51,59,73	1.62	7 (13%)	59,96,113	1.61	8 (13%)
25	CLA	b	611	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	9 (11%)
28	WVN	A	849	-	40,41,41	1.89	14 (35%)	50,56,56	2.10	20 (40%)
32	II0	j	615	-	39,43,43	6.77	20 (51%)	50,60,60	2.19	16 (32%)
25	CLA	d	309	27	41,49,73	1.85	6 (14%)	47,84,113	1.71	7 (14%)

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
25	CLA	i	307	20	1/1/14/20	13/33/111/115	-
25	CLA	k	605	19	1/1/11/20	7/13/91/115	-
32	II0	c	615	-	-	5/21/67/67	0/2/2/2
25	CLA	h	305	16	1/1/12/20	7/21/99/115	-
28	WVN	A	847	-	-	9/29/63/63	0/2/2/2
25	CLA	l	309	18	1/1/12/20	5/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	n	320	-	-	16/47/47/53	-
32	II0	a	315	-	-	3/21/67/67	0/2/2/2
35	IHT	c	616	-	-	9/25/65/65	0/2/2/2
34	KC2	j	610	17	-	7/15/71/71	-
32	II0	n	301	-	-	4/21/67/67	0/2/2/2
25	CLA	j	608	17	1/1/12/20	0/21/99/115	-
25	CLA	n	307	23	1/1/12/20	4/21/99/115	-
32	II0	i	314	-	-	6/21/67/67	0/2/2/2
25	CLA	F	201	37	1/1/15/20	12/37/115/115	-
27	LHG	d	317	25	-	16/41/41/53	-
28	WVN	h	309	-	-	8/29/63/63	0/2/2/2
28	WVN	A	848	-	-	12/29/63/63	0/2/2/2
32	II0	h	311	-	-	8/21/67/67	0/2/2/2
32	II0	n	315	-	-	1/21/67/67	0/2/2/2
25	CLA	h	308	16	1/1/12/20	9/21/99/115	-
25	CLA	A	807	1	1/1/15/20	14/37/115/115	-
25	CLA	a	309	14	1/1/15/20	8/37/115/115	-
25	CLA	A	830	-	-	6/19/97/115	-
32	II0	i	315	-	-	6/21/67/67	0/2/2/2
28	WVN	F	203	-	-	11/29/63/63	0/2/2/2
25	CLA	B	838	-	-	11/28/106/115	-
27	LHG	m	617	25	-	19/41/41/53	-
25	CLA	A	835	-	1/1/15/20	17/37/115/115	-
25	CLA	i	306	-	1/1/12/20	9/21/99/115	-
25	CLA	A	814	-	-	9/19/97/115	-
32	II0	l	316	-	-	5/21/67/67	0/2/2/2
32	II0	k	619	-	-	6/21/67/67	0/2/2/2
25	CLA	A	838	27	1/1/12/20	6/22/100/115	-
25	CLA	A	811	-	-	8/24/102/115	-
30	SF4	C	101	3	-	-	0/6/5/5
25	CLA	a	312	-	-	20/37/115/115	-
25	CLA	l	303	18	1/1/11/20	7/16/94/115	-
25	CLA	A	802	-	1/1/15/20	12/37/115/115	-
25	CLA	A	841	-	1/1/15/20	18/37/115/115	-
25	CLA	n	302	23	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	WVN	A	850	-	-	8/29/63/63	0/2/2/2
25	CLA	c	607	13	1/1/11/20	6/15/93/115	-
25	CLA	c	612	-	1/1/15/20	14/37/115/115	-
27	LHG	j	617	25	-	5/34/34/53	-
25	CLA	A	826	-	1/1/15/20	12/37/115/115	-
28	WVN	L	205	-	-	6/29/63/63	0/2/2/2
32	IIO	d	315	-	-	6/21/67/67	0/2/2/2
28	WVN	B	845	-	-	0/29/63/63	0/2/2/2
25	CLA	a	303	14	1/1/12/20	9/22/100/115	-
34	KC2	k	612	34	-	8/15/71/71	-
25	CLA	A	840	1	-	19/37/115/115	-
34	KC2	m	611	17	-	7/15/71/71	-
27	LHG	c	618	25	-	14/41/41/53	-
25	CLA	A	839	37	1/1/15/20	17/37/115/115	-
25	CLA	n	309	23	1/1/12/20	5/21/99/115	-
25	CLA	A	810	-	1/1/14/20	8/34/112/115	-
25	CLA	B	807	-	1/1/15/20	14/37/115/115	-
25	CLA	k	608	19	1/1/15/20	15/37/115/115	-
30	SF4	C	102	3	-	-	0/6/5/5
28	WVN	l	315	-	-	9/29/63/63	0/2/2/2
25	CLA	Q	302	37	1/1/15/20	13/37/115/115	-
25	CLA	s	202	12	1/1/15/20	18/37/115/115	-
29	LMT	a	302	-	-	4/15/35/61	0/1/1/2
25	CLA	A	819	-	-	6/13/91/115	-
25	CLA	K	102	-	1/1/10/20	5/10/88/115	-
25	CLA	A	833	-	1/1/12/20	5/19/97/115	-
25	CLA	A	823	-	-	14/25/103/115	-
25	CLA	B	818	37	1/1/15/20	19/37/115/115	-
25	CLA	j	603	-	1/1/12/20	8/21/99/115	-
25	CLA	c	606	-	-	11/22/100/115	-
25	CLA	a	304	14	1/1/12/20	3/19/97/115	-
34	KC2	l	311	18	-	10/15/71/71	-
25	CLA	B	821	-	-	9/23/101/115	-
25	CLA	b	610	15	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	II0	k	617	-	-	2/21/67/67	0/2/2/2
34	KC2	n	312	23	-	4/15/71/71	-
25	CLA	k	614	-	-	9/21/99/115	-
28	WVN	M	101	-	-	9/29/63/63	0/2/2/2
25	CLA	J	103	8	1/1/10/20	2/10/88/115	-
34	KC2	n	313	-	-	7/15/71/71	-
25	CLA	B	827	-	-	7/19/97/115	-
25	CLA	m	604	17	-	19/37/115/115	-
25	CLA	L	203	-	-	14/37/115/115	-
27	LHG	i	318	25	-	13/41/41/53	-
28	WVN	L	206	-	-	3/29/63/63	0/2/2/2
25	CLA	A	809	-	-	10/27/105/115	-
25	CLA	A	842	37	1/1/15/20	17/37/115/115	-
25	CLA	B	834	-	1/1/11/20	2/16/94/115	-
32	II0	n	319	-	-	6/21/67/67	0/2/2/2
25	CLA	h	302	16	1/1/12/20	8/19/97/115	-
25	CLA	b	609	-	-	5/21/99/115	-
28	WVN	l	301	-	-	3/29/63/63	0/2/2/2
32	II0	n	317	-	-	3/21/67/67	0/2/2/2
25	CLA	n	303	23	1/1/12/20	7/19/97/115	-
25	CLA	d	303	-	1/1/15/20	18/37/115/115	-
25	CLA	A	834	-	1/1/12/20	7/21/99/115	-
25	CLA	B	833	-	1/1/15/20	16/37/115/115	-
25	CLA	d	301	21	1/1/12/20	2/19/97/115	-
25	CLA	b	603	-	1/1/15/20	8/37/115/115	-
25	CLA	B	836	-	-	23/37/115/115	-
25	CLA	L	204	-	-	8/19/97/115	-
33	LMG	J	105	-	-	13/50/70/70	0/1/1/1
32	II0	a	318	-	-	7/21/67/67	0/2/2/2
27	LHG	k	620	25	-	12/41/41/53	-
35	IHT	k	618	-	-	10/25/65/65	0/2/2/2
32	II0	b	617	-	-	0/21/67/67	0/2/2/2
25	CLA	A	825	37	-	9/37/115/115	-
32	II0	a	316	-	-	2/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	j	606	-	1/1/12/20	9/21/99/115	-
25	CLA	i	305	20	-	13/37/115/115	-
25	CLA	m	603	-	1/1/15/20	21/37/115/115	-
27	LHG	J	107	-	-	9/35/35/53	-
34	KC2	d	310	21	-	8/15/71/71	-
25	CLA	A	836	-	-	16/37/115/115	-
25	CLA	l	310	27	1/1/14/20	15/33/111/115	-
25	CLA	a	306	37	1/1/15/20	15/37/115/115	-
25	CLA	Q	303	24	1/1/11/20	8/13/91/115	-
25	CLA	m	606	-	1/1/15/20	12/37/115/115	-
28	WVN	s	205	-	-	4/29/63/63	0/2/2/2
25	CLA	l	305	-	1/1/12/20	4/21/99/115	-
25	CLA	A	806	-	-	12/37/115/115	-
28	WVN	K	103	-	-	6/29/63/63	0/2/2/2
25	CLA	m	602	17	1/1/13/20	9/27/105/115	-
25	CLA	i	312	-	1/1/12/20	7/21/99/115	-
25	CLA	i	302	20	1/1/12/20	6/21/99/115	-
33	LMG	b	620	-	-	17/44/64/70	0/1/1/1
25	CLA	R	202	-	1/1/12/20	10/21/99/115	-
25	CLA	d	312	-	1/1/12/20	8/21/99/115	-
25	CLA	B	835	37	1/1/15/20	12/37/115/115	-
25	CLA	l	312	18	1/1/15/20	11/37/115/115	-
25	CLA	A	829	-	1/1/15/20	18/37/115/115	-
25	CLA	B	822	37	1/1/15/20	17/37/115/115	-
25	CLA	d	305	21	1/1/12/20	5/21/99/115	-
25	CLA	A	803	-	-	8/25/103/115	-
25	CLA	k	607	-	1/1/12/20	9/21/99/115	-
32	II0	b	614	-	-	9/21/67/67	0/2/2/2
25	CLA	n	311	37	-	16/37/115/115	-
25	CLA	l	307	18	1/1/15/20	17/37/115/115	-
25	CLA	n	304	-	1/1/12/20	8/21/99/115	-
25	CLA	a	308	14	1/1/15/20	16/37/115/115	-
32	II0	b	613	-	-	2/21/67/67	0/2/2/2
28	WVN	B	846	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	i	304	-	1/1/12/20	4/21/99/115	-
31	DGD	B	843	-	-	5/49/89/95	0/2/2/2
32	II0	l	302	-	-	8/21/67/67	0/2/2/2
25	CLA	B	826	-	1/1/15/20	15/37/115/115	-
28	WVN	B	848	-	-	7/29/63/63	0/2/2/2
25	CLA	A	801	-	1/1/15/20	12/37/115/115	-
25	CLA	n	306	23	1/1/12/20	8/21/99/115	-
32	II0	h	310	-	-	2/17/40/67	0/1/1/2
25	CLA	a	305	-	1/1/12/20	7/21/99/115	-
29	LMT	b	618	-	-	9/15/35/61	0/1/1/2
25	CLA	k	602	19	1/1/12/20	8/19/97/115	-
25	CLA	B	809	2	1/1/15/20	15/37/115/115	-
28	WVN	B	849	-	-	12/29/63/63	0/2/2/2
25	CLA	A	813	-	-	7/13/91/115	-
25	CLA	d	302	-	1/1/12/20	6/21/99/115	-
25	CLA	B	837	-	1/1/15/20	16/37/115/115	-
25	CLA	i	308	20	1/1/12/20	9/21/99/115	-
25	CLA	i	311	-	1/1/12/20	11/21/99/115	-
25	CLA	h	313	37	1/1/15/20	9/37/115/115	-
32	II0	l	314	-	-	7/21/67/67	0/2/2/2
32	II0	i	313	-	-	7/21/67/67	0/2/2/2
27	LHG	A	845	-	-	22/52/52/53	-
25	CLA	A	808	1	1/1/15/20	13/37/115/115	-
25	CLA	F	202	6	-	8/22/100/115	-
35	IHT	m	616	-	-	7/25/65/65	0/2/2/2
25	CLA	B	828	-	-	5/18/96/115	-
25	CLA	A	804	-	1/1/15/20	15/37/115/115	-
34	KC2	s	201	12	-	9/15/71/71	-
25	CLA	j	611	-	1/1/12/20	9/21/99/115	-
32	II0	d	313	-	-	7/21/67/67	0/2/2/2
25	CLA	b	602	15	1/1/13/20	11/25/103/115	-
25	CLA	j	604	17	-	16/37/115/115	-
25	CLA	j	607	17	1/1/11/20	5/13/91/115	-
25	CLA	c	601	13	1/1/12/20	10/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	m	609	17	1/1/12/20	9/21/99/115	-
25	CLA	c	611	-	-	10/13/91/115	-
27	LHG	c	620	25	-	25/41/41/53	-
32	II0	j	613	-	-	7/21/67/67	0/2/2/2
25	CLA	B	841	27	1/1/15/20	13/37/115/115	-
25	CLA	s	209	-	1/1/12/20	4/21/99/115	-
25	CLA	A	824	37	1/1/15/20	11/37/115/115	-
27	LHG	a	301	25	-	14/53/53/53	-
34	KC2	k	613	34	-	13/15/71/71	-
25	CLA	k	609	19	1/1/15/20	16/37/115/115	-
25	CLA	a	311	14	1/1/15/20	11/37/115/115	-
25	CLA	c	605	13	1/1/12/20	7/21/99/115	-
35	IHT	j	616	-	-	7/25/65/65	0/2/2/2
25	CLA	B	811	-	1/1/13/20	8/25/103/115	-
25	CLA	k	603	-	1/1/12/20	7/21/99/115	-
35	IHT	b	615	-	-	6/25/65/65	0/2/2/2
32	II0	d	316	-	-	7/21/67/67	0/2/2/2
27	LHG	l	317	25	-	14/36/36/53	-
25	CLA	m	608	17	1/1/15/20	17/37/115/115	-
25	CLA	k	606	19	-	10/21/99/115	-
25	CLA	A	853	-	1/1/15/20	11/37/115/115	-
27	LHG	A	846	25	-	7/31/31/53	-
30	SF4	B	802	-	-	-	0/6/5/5
25	CLA	m	601	17	1/1/10/20	1/10/88/115	-
25	CLA	d	307	-	1/1/11/20	4/15/93/115	-
35	IHT	R	203	-	-	4/25/65/65	0/2/2/2
32	II0	k	616	-	-	9/21/67/67	0/2/2/2
25	CLA	s	203	12,25	-	15/37/115/115	-
25	CLA	c	602	13	1/1/12/20	9/19/97/115	-
28	WVN	s	207	-	-	7/29/63/63	0/2/2/2
32	II0	n	316	-	-	3/21/67/67	0/2/2/2
25	CLA	h	304	-	1/1/12/20	6/21/99/115	-
27	LHG	L	207	-	-	22/53/53/53	-
25	CLA	B	814	-	1/1/13/20	15/30/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PQN	A	844	-	-	9/23/43/43	0/2/2/2
25	CLA	B	810	-	1/1/13/20	4/25/101/115	-
27	LHG	b	619	25	-	22/53/53/53	-
25	CLA	B	806	-	1/1/15/20	20/37/115/115	-
25	CLA	s	206	-	-	15/37/115/115	-
25	CLA	B	824	-	1/1/15/20	13/37/115/115	-
34	KC2	c	610	-	-	7/15/71/71	-
35	IHT	b	616	-	-	6/25/65/65	0/2/2/2
27	LHG	J	106	25	-	21/53/53/53	-
25	CLA	n	314	-	-	9/21/99/115	-
28	WVN	B	844	-	-	6/29/63/63	0/2/2/2
25	CLA	B	831	37	-	2/13/91/115	-
25	CLA	B	823	37	-	15/36/114/115	-
25	CLA	b	606	15	1/1/14/20	11/33/111/115	-
25	CLA	b	607	15	1/1/15/20	15/37/115/115	-
25	CLA	b	612	27	-	5/21/99/115	-
25	CLA	A	856	27	1/1/10/20	4/8/86/115	-
25	CLA	B	830	37	-	18/37/115/115	-
25	CLA	A	831	-	-	12/37/115/115	-
25	CLA	A	854	-	1/1/15/20	21/37/115/115	-
25	CLA	B	832	-	1/1/13/20	10/29/107/115	-
32	II0	a	314	-	-	4/21/67/67	0/2/2/2
32	II0	j	614	-	-	4/21/67/67	0/2/2/2
33	LMG	n	321	-	-	9/50/70/70	0/1/1/1
34	KC2	d	311	-	-	6/15/71/71	-
28	WVN	R	201	-	-	10/29/63/63	0/2/2/2
25	CLA	A	855	37	1/1/15/20	28/37/115/115	-
25	CLA	j	612	-	1/1/15/20	11/37/115/115	-
32	II0	h	312	-	-	7/21/67/67	0/2/2/2
35	IHT	n	318	-	-	9/25/65/65	0/2/2/2
25	CLA	A	837	-	1/1/15/20	18/37/115/115	-
25	CLA	A	812	-	1/1/15/20	24/37/115/115	-
27	LHG	a	319	25	-	15/53/53/53	-
32	II0	m	618	-	-	4/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	h	307	16	1/1/13/20	8/28/106/115	-
33	LMG	c	619	-	-	20/50/70/70	0/1/1/1
25	CLA	c	603	-	1/1/12/20	9/21/99/115	-
32	II0	J	104	-	-	7/21/67/67	0/2/2/2
25	CLA	B	805	-	1/1/15/20	9/37/115/115	-
25	CLA	B	839	-	1/1/15/20	21/37/115/115	-
25	CLA	b	604	15	-	15/37/115/115	-
25	CLA	A	822	-	-	8/21/99/115	-
25	CLA	j	609	27	1/1/14/20	14/33/111/115	-
25	CLA	k	601	19	1/1/12/20	7/21/99/115	-
25	CLA	c	609	27	1/1/11/20	8/13/91/115	-
25	CLA	B	819	-	-	4/15/93/115	-
25	CLA	h	303	16	1/1/12/20	7/19/97/115	-
29	LMT	a	320	-	-	9/21/61/61	0/2/2/2
25	CLA	n	310	23	1/1/15/20	16/37/115/115	-
34	KC2	s	204	-	-	6/15/71/71	-
25	CLA	B	825	-	1/1/15/20	14/37/115/115	-
25	CLA	b	605	25,37	1/1/15/20	10/37/115/115	-
32	II0	i	317	-	-	6/21/67/67	0/2/2/2
25	CLA	B	820	-	-	10/25/103/115	-
25	CLA	L	202	9	1/1/11/20	9/18/96/115	-
25	CLA	K	101	37	1/1/12/20	7/21/99/115	-
32	II0	d	314	-	-	3/21/67/67	0/2/2/2
25	CLA	B	812	-	1/1/15/20	21/37/115/115	-
26	PQN	B	842	-	-	12/23/43/43	0/2/2/2
25	CLA	a	307	14	-	7/13/91/115	-
28	WVN	F	204	-	-	11/29/63/63	0/2/2/2
32	II0	c	614	-	-	1/21/67/67	0/2/2/2
25	CLA	n	308	-	1/1/15/20	15/37/115/115	-
25	CLA	k	610	27	1/1/12/20	8/21/99/115	-
25	CLA	B	803	-	1/1/15/20	20/37/115/115	-
28	WVN	J	101	-	-	8/29/63/63	0/2/2/2
28	WVN	i	316	-	-	9/29/63/63	0/2/2/2
36	LMU	i	301	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	II0	k	615	-	-	6/21/67/67	0/2/2/2
25	CLA	d	304	21	1/1/12/20	9/21/99/115	-
25	CLA	d	306	-	1/1/12/20	10/21/99/115	-
25	CLA	d	308	21	1/1/10/20	3/8/86/115	-
25	CLA	n	305	23	1/1/14/20	10/31/109/115	-
25	CLA	j	605	17	1/1/11/20	9/13/91/115	-
25	CLA	A	816	-	-	18/37/115/115	-
25	CLA	b	608	27	1/1/15/20	11/37/115/115	-
25	CLA	l	306	18	-	20/37/115/115	-
25	CLA	l	308	18	1/1/15/20	9/37/115/115	-
25	CLA	i	303	20	1/1/12/20	10/19/97/115	-
27	LHG	B	801	-	-	27/42/42/53	-
35	IHT	a	317	-	-	10/25/65/65	0/2/2/2
25	CLA	A	827	-	-	17/34/112/115	-
25	CLA	m	612	37	-	8/21/99/115	-
29	LMT	A	852	-	-	13/21/61/61	0/2/2/2
25	CLA	j	601	17	1/1/12/20	5/21/99/115	-
25	CLA	B	813	-	1/1/14/20	16/31/109/115	-
25	CLA	A	815	37	-	7/13/91/115	-
25	CLA	m	607	-	-	5/21/99/115	-
25	CLA	c	608	13	1/1/15/20	14/37/115/115	-
33	LMG	s	208	-	-	11/43/63/70	0/1/1/1
25	CLA	A	817	-	1/1/15/20	18/37/115/115	-
25	CLA	B	850	-	1/1/12/20	5/21/99/115	-
25	CLA	A	820	37	1/1/15/20	15/37/115/115	-
25	CLA	a	313	-	1/1/11/20	8/17/95/115	-
25	CLA	A	832	-	-	11/37/115/115	-
25	CLA	B	804	-	1/1/15/20	14/37/115/115	-
25	CLA	B	829	-	-	5/19/97/115	-
25	CLA	h	301	37	-	12/37/115/115	-
34	KC2	i	310	20	-	9/15/71/71	-
32	II0	i	320	-	-	6/21/67/67	0/2/2/2
32	II0	c	613	-	-	4/21/67/67	0/2/2/2
25	CLA	a	310	27	1/1/11/20	9/17/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	l	304	18	1/1/15/20	16/37/115/115	-
25	CLA	A	828	-	-	6/37/115/115	-
34	KC2	i	319	-	-	6/15/71/71	-
25	CLA	B	817	-	1/1/13/20	10/28/106/115	-
25	CLA	m	610	27	1/1/13/20	13/25/103/115	-
28	WVN	B	847	-	-	10/29/63/63	0/2/2/2
28	WVN	L	201	-	-	9/29/63/63	0/2/2/2
34	KC2	k	611	19	-	9/15/71/71	-
25	CLA	A	821	-	-	9/18/96/115	-
25	CLA	A	805	1	1/1/15/20	11/37/115/115	-
28	WVN	A	851	-	-	14/29/63/63	0/2/2/2
32	II0	m	614	-	-	3/21/67/67	0/2/2/2
25	CLA	m	605	17	-	5/10/88/115	-
33	LMG	Q	301	-	-	10/33/53/70	0/1/1/1
32	II0	l	313	-	-	4/21/67/67	0/2/2/2
32	II0	m	615	-	-	7/21/67/67	0/2/2/2
25	CLA	A	818	-	1/1/15/20	22/37/115/115	-
28	WVN	I	101	-	-	9/29/63/63	0/2/2/2
25	CLA	m	613	-	1/1/10/20	8/11/89/115	-
25	CLA	B	815	-	-	9/25/103/115	-
25	CLA	B	840	-	1/1/15/20	17/37/115/115	-
25	CLA	c	604	13	1/1/15/20	19/37/115/115	-
25	CLA	k	604	-	-	17/37/115/115	-
32	II0	c	617	-	-	4/21/67/67	0/2/2/2
25	CLA	B	816	-	1/1/13/20	10/30/108/115	-
25	CLA	B	808	-	1/1/15/20	14/37/115/115	-
25	CLA	h	306	16	1/1/15/20	17/37/115/115	-
28	WVN	J	102	-	-	8/29/63/63	0/2/2/2
25	CLA	i	309	27	1/1/11/20	4/15/93/115	-
25	CLA	A	843	-	1/1/15/20	22/37/115/115	-
25	CLA	j	602	17	-	4/19/97/115	-
25	CLA	b	601	15	1/1/12/20	7/21/99/115	-
25	CLA	b	611	-	1/1/15/20	17/37/115/115	-
28	WVN	A	849	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	II0	j	615	-	-	9/21/67/67	0/2/2/2
25	CLA	d	309	27	1/1/10/20	4/8/86/115	-

The worst 5 of 3548 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	R	203	IHT	C15-C11	25.22	1.63	1.34
35	b	616	IHT	C15-C11	25.18	1.63	1.34
35	a	317	IHT	C15-C11	25.04	1.62	1.34
35	k	618	IHT	C15-C11	24.88	1.62	1.34
35	n	318	IHT	C15-C11	24.85	1.62	1.34

The worst 5 of 4083 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	m	611	KC2	C1A-NA-C4A	-12.79	100.95	106.71
34	j	610	KC2	C1A-NA-C4A	-12.62	101.03	106.71
34	s	204	KC2	C1A-NA-C4A	-12.36	101.15	106.71
34	l	311	KC2	C1A-NA-C4A	-12.13	101.25	106.71
34	n	312	KC2	C1A-NA-C4A	-12.10	101.27	106.71

5 of 161 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	801	CLA	ND
25	A	802	CLA	ND
25	A	804	CLA	ND
25	A	805	CLA	ND
25	A	807	CLA	ND

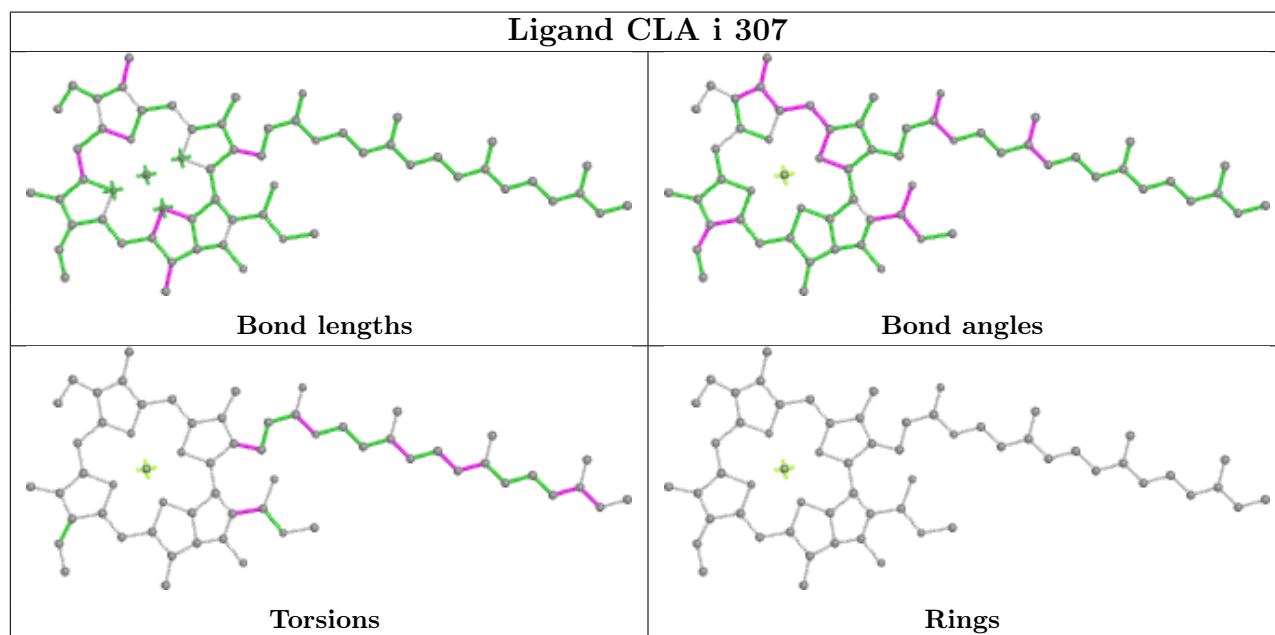
5 of 3458 torsion outliers are listed below:

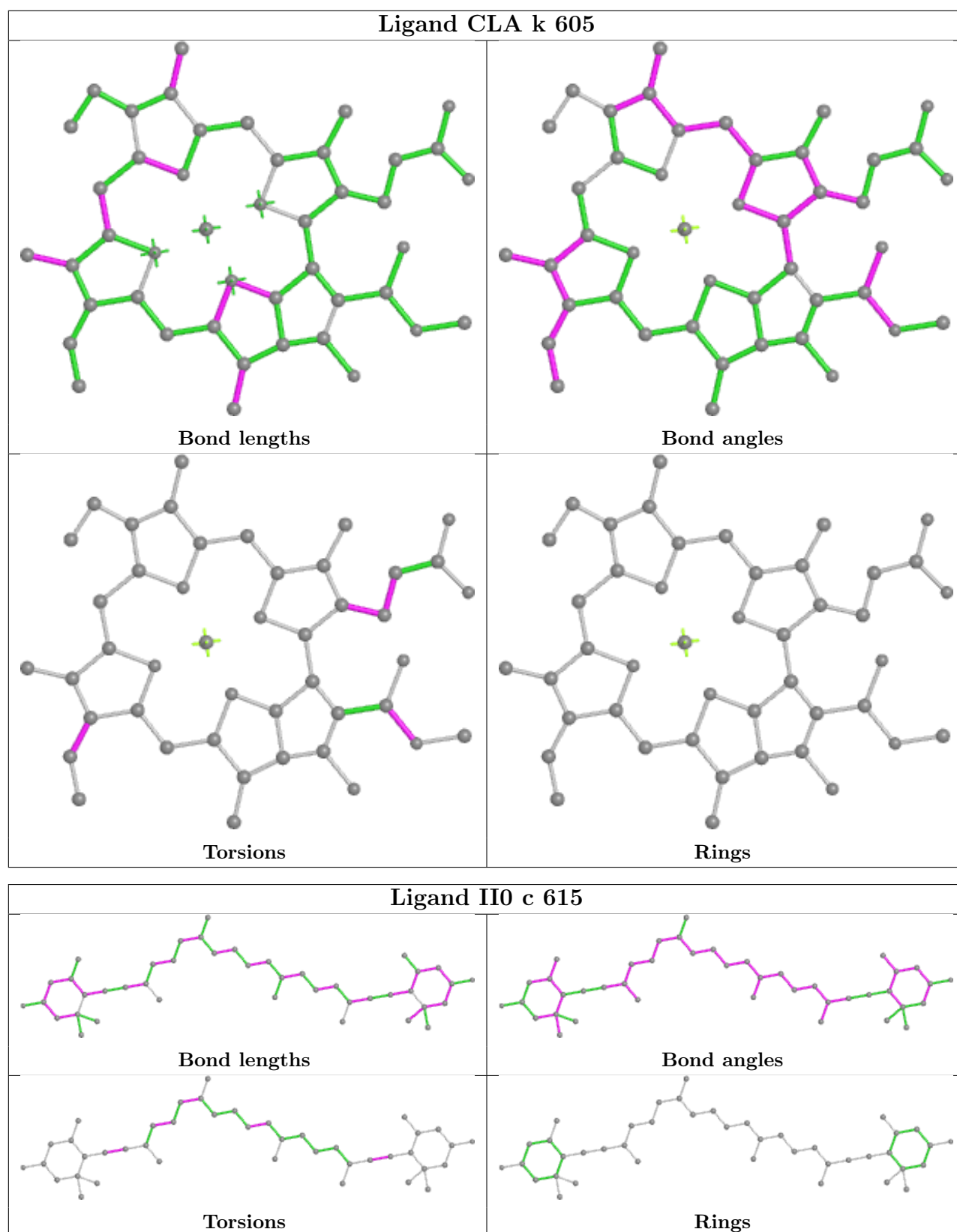
Mol	Chain	Res	Type	Atoms
25	A	801	CLA	CBD-CGD-O2D-CED
25	A	802	CLA	CBA-CGA-O2A-C1
25	A	802	CLA	O1A-CGA-O2A-C1
25	A	803	CLA	C1A-C2A-CAA-CBA
25	A	803	CLA	C3A-C2A-CAA-CBA

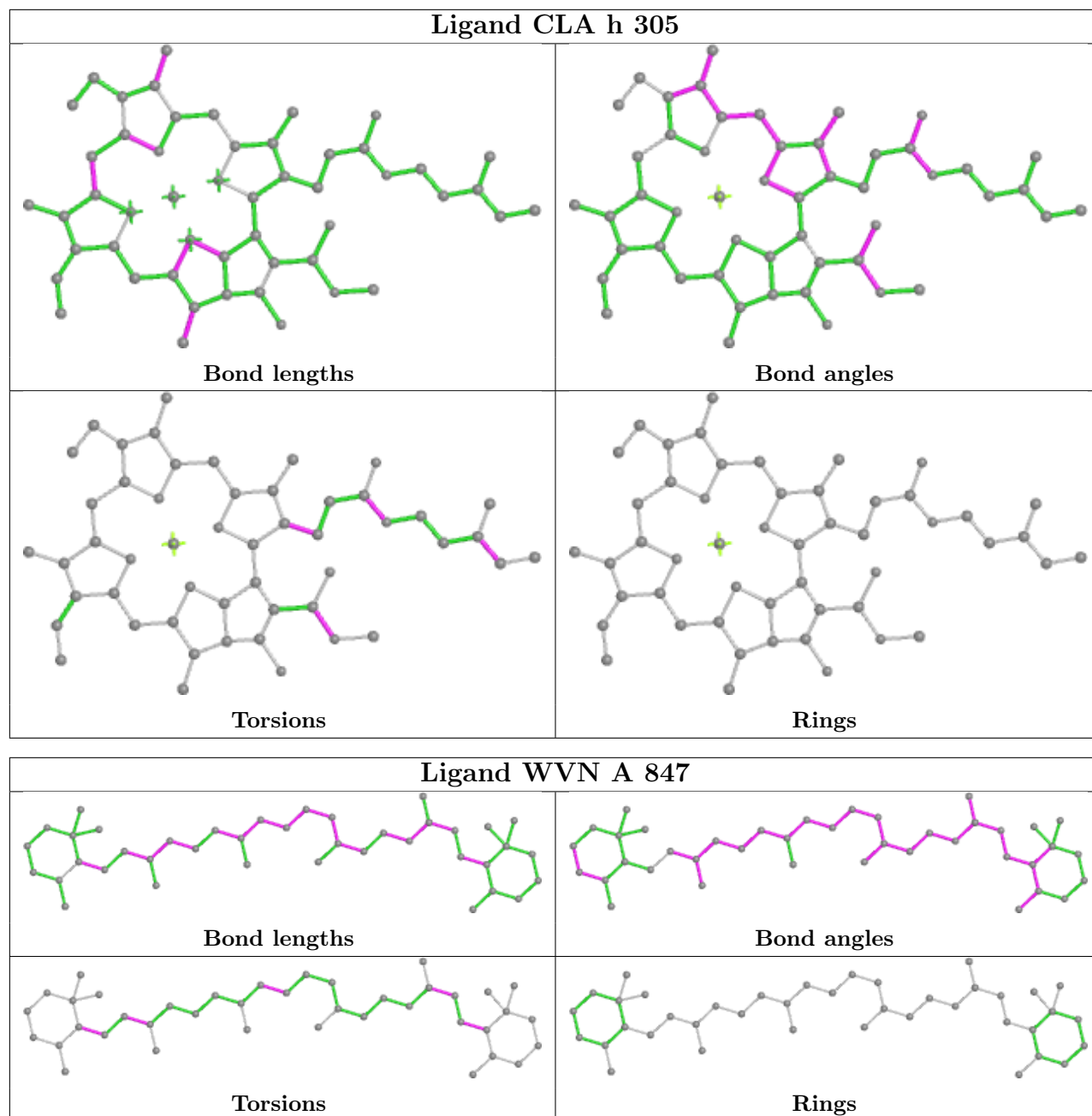
There are no ring outliers.

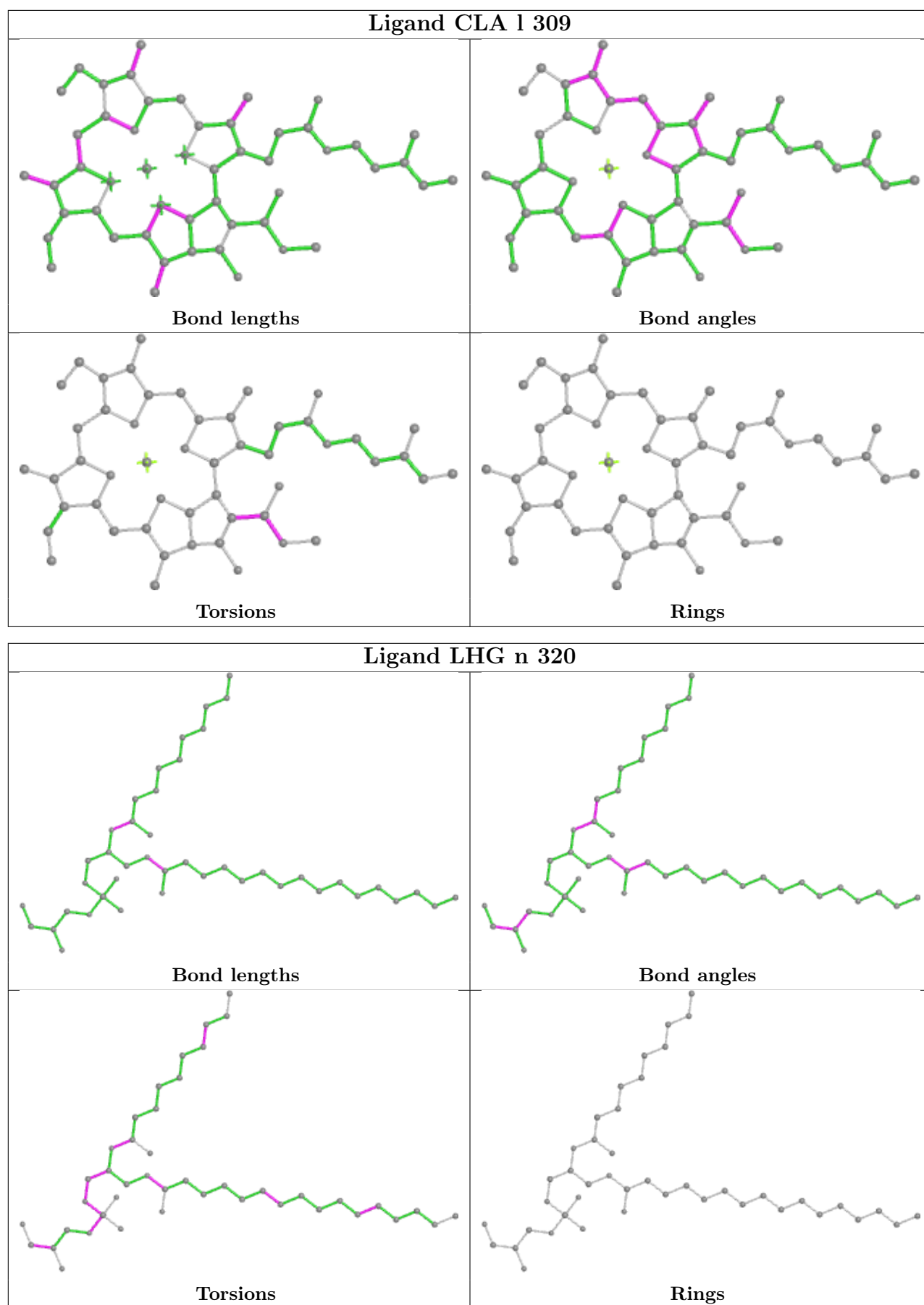
No monomer is involved in short contacts.

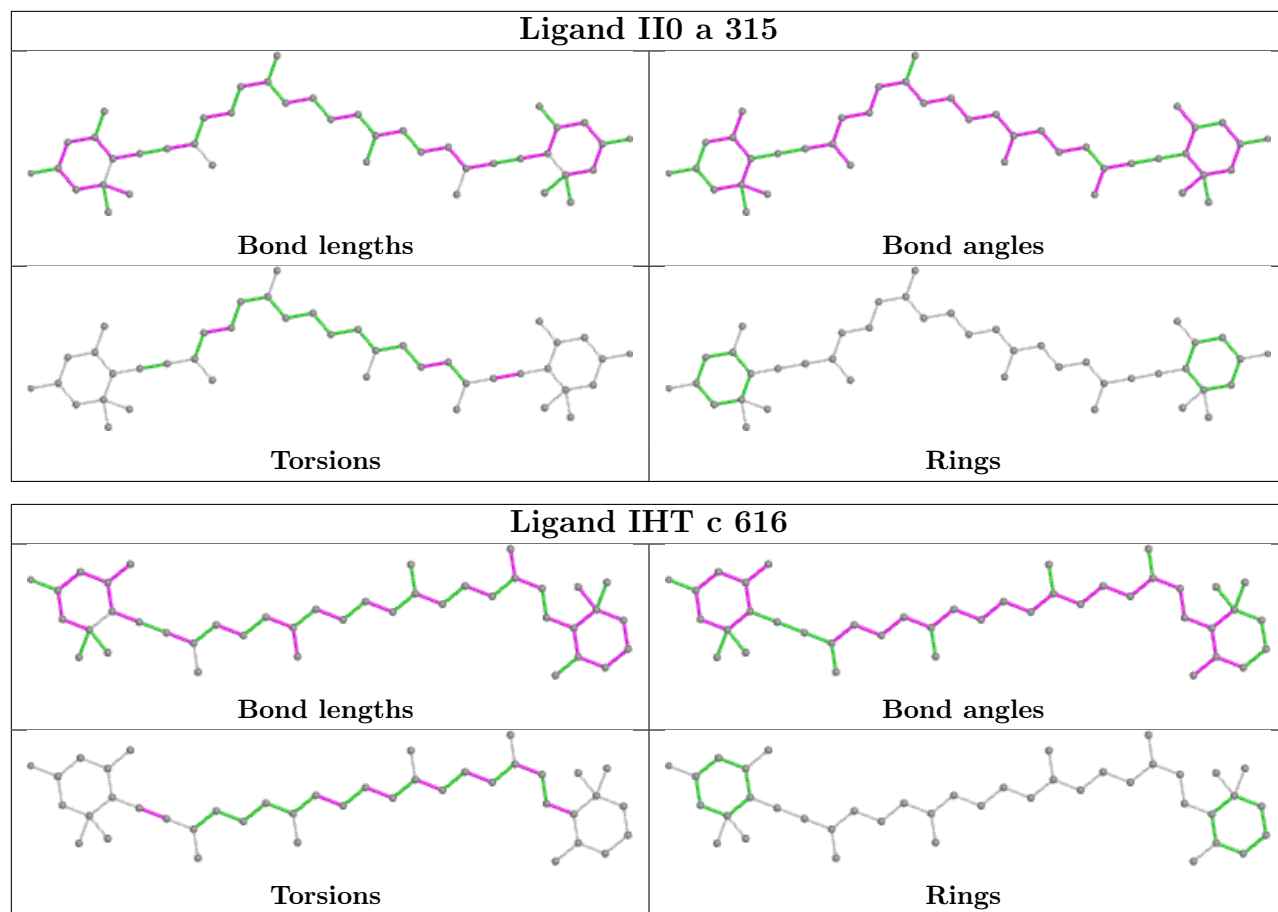
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

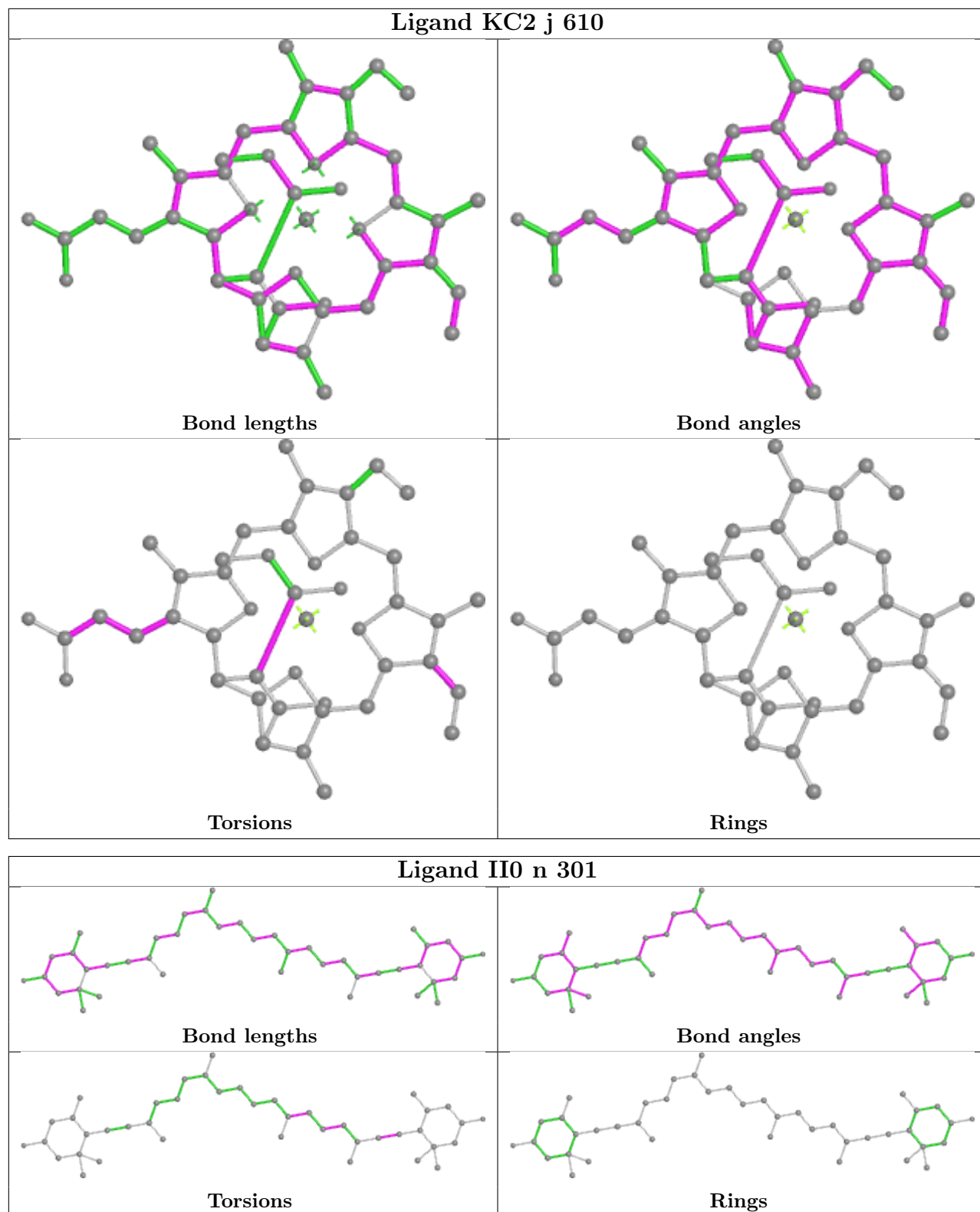


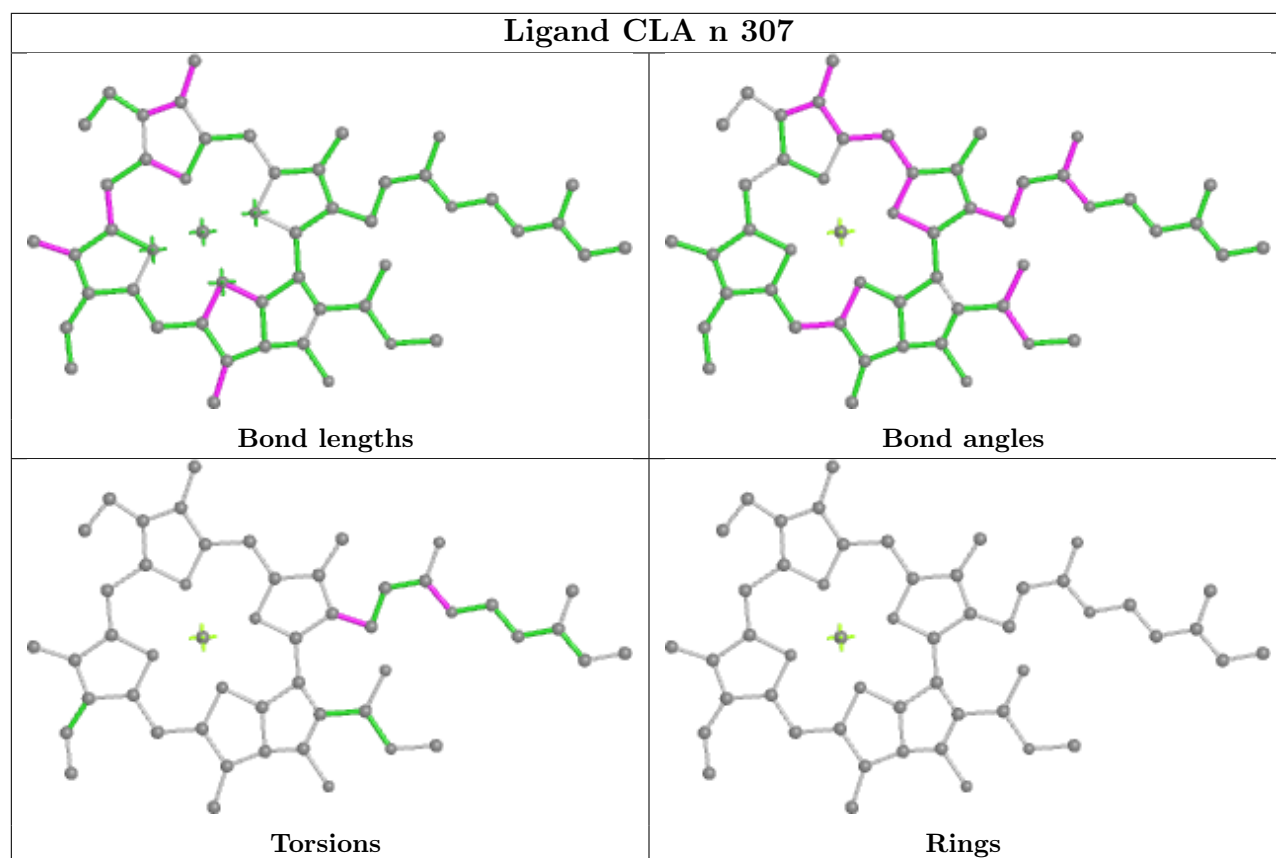
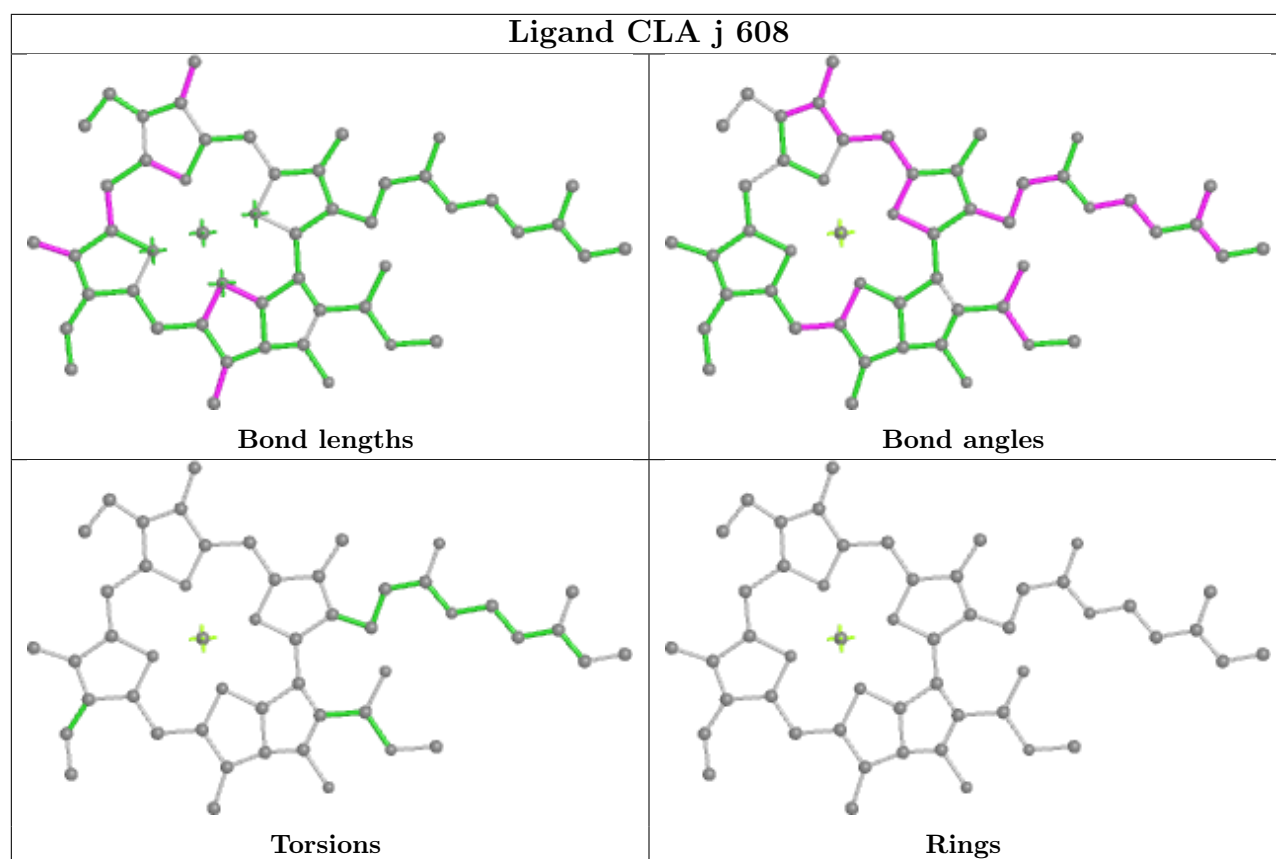


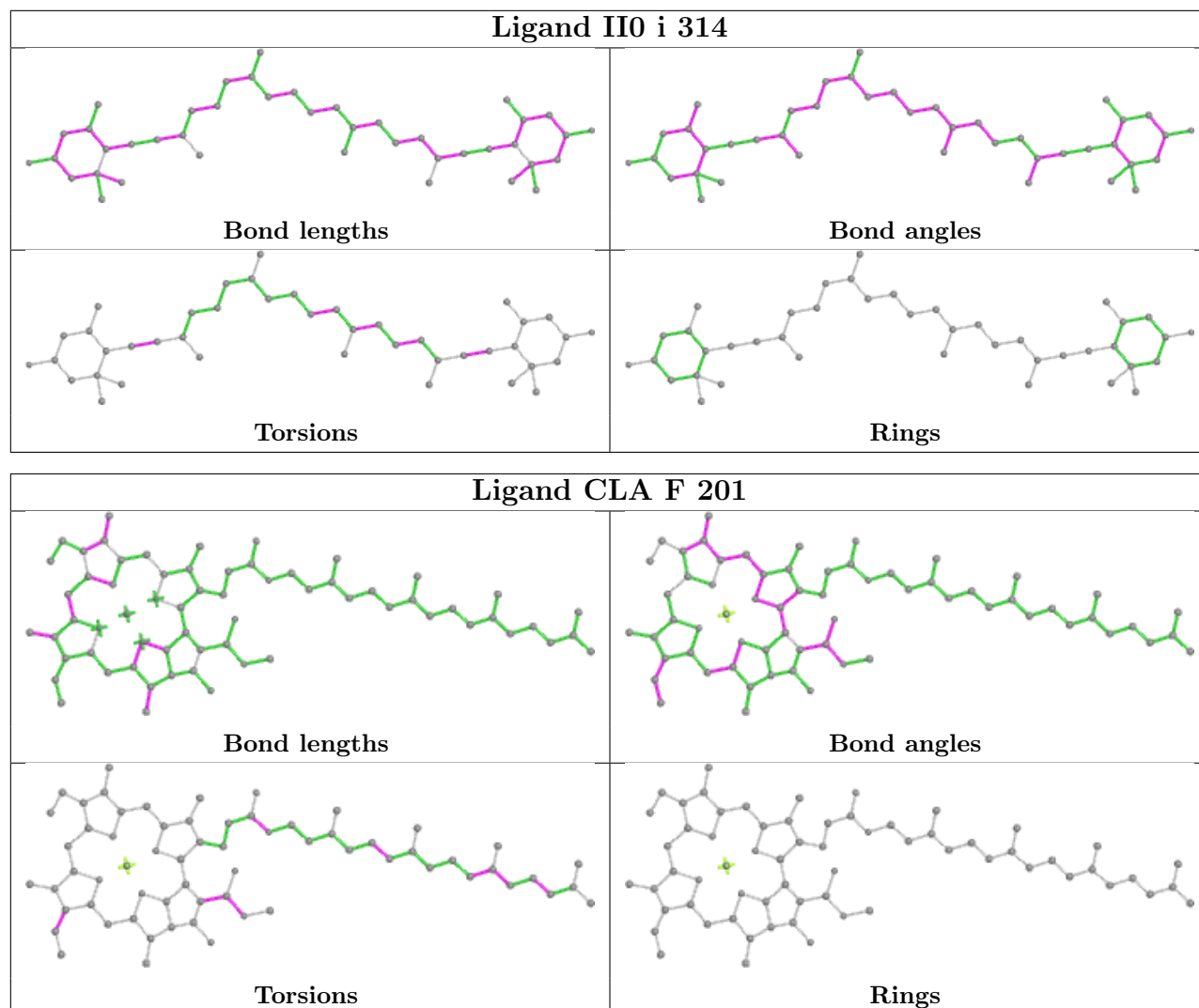


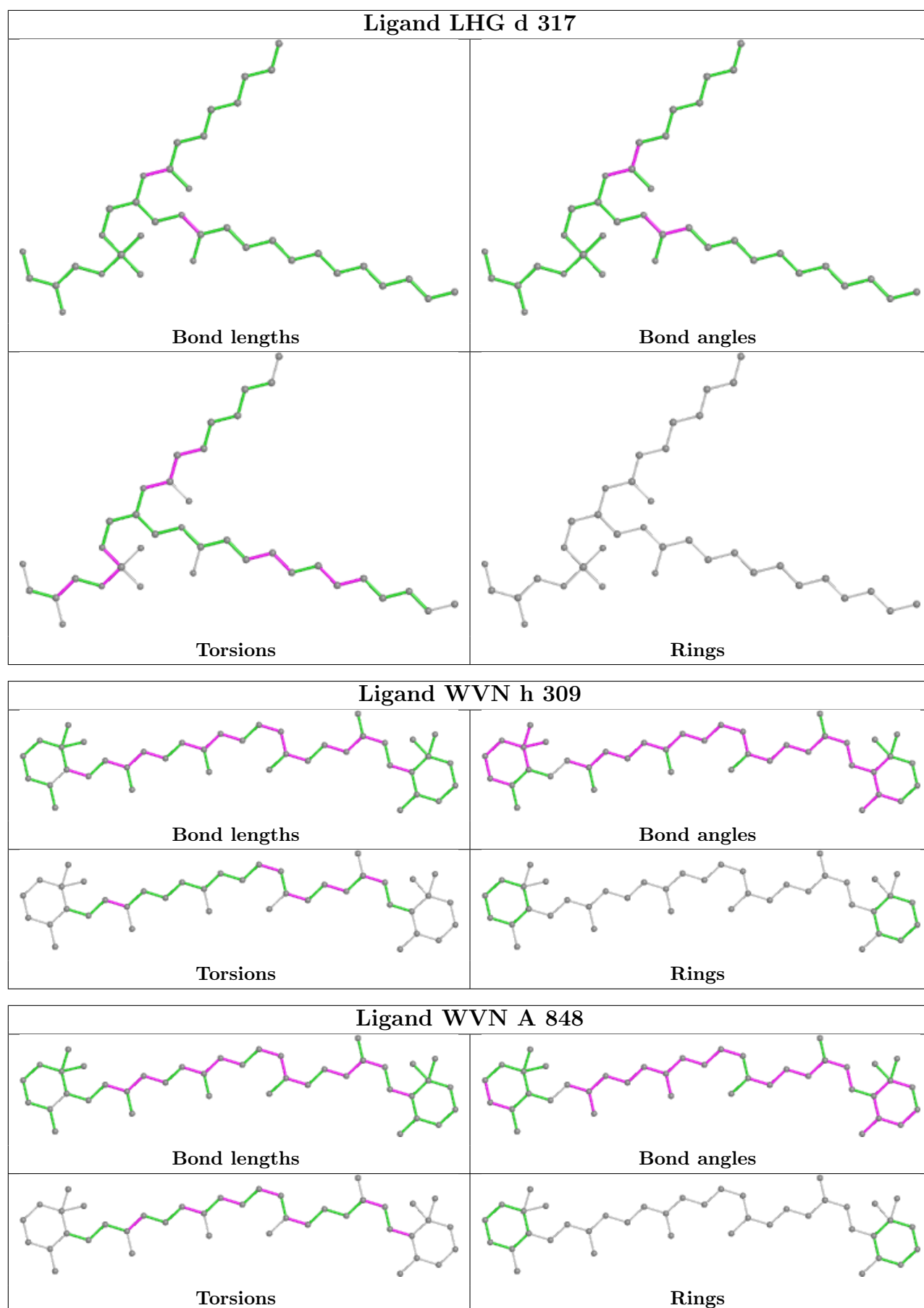


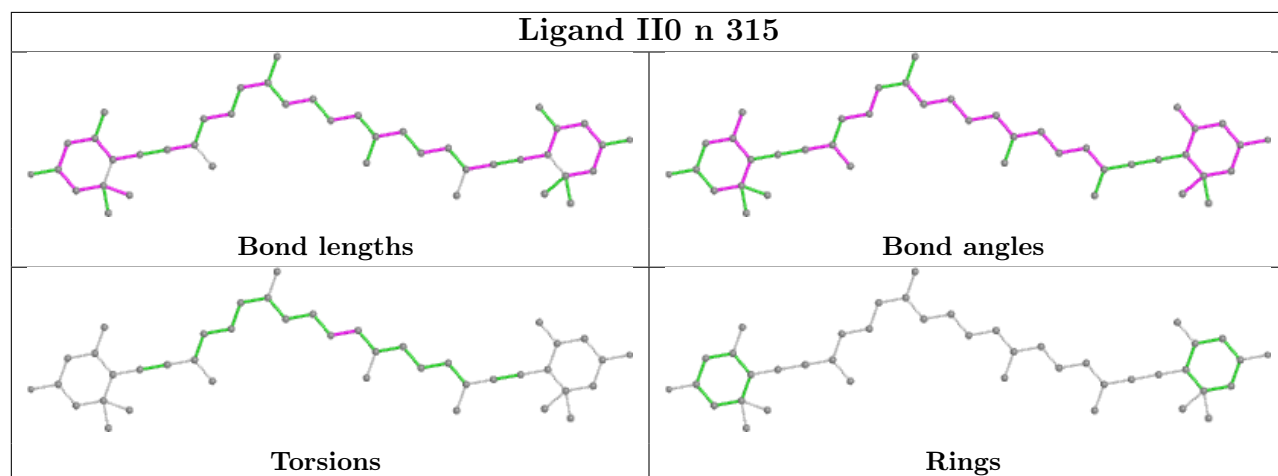
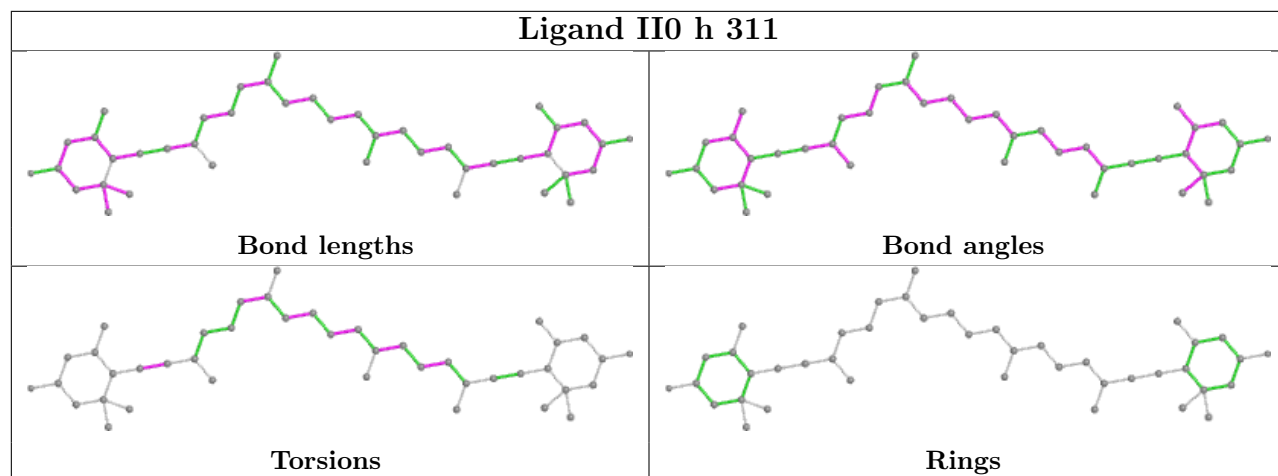


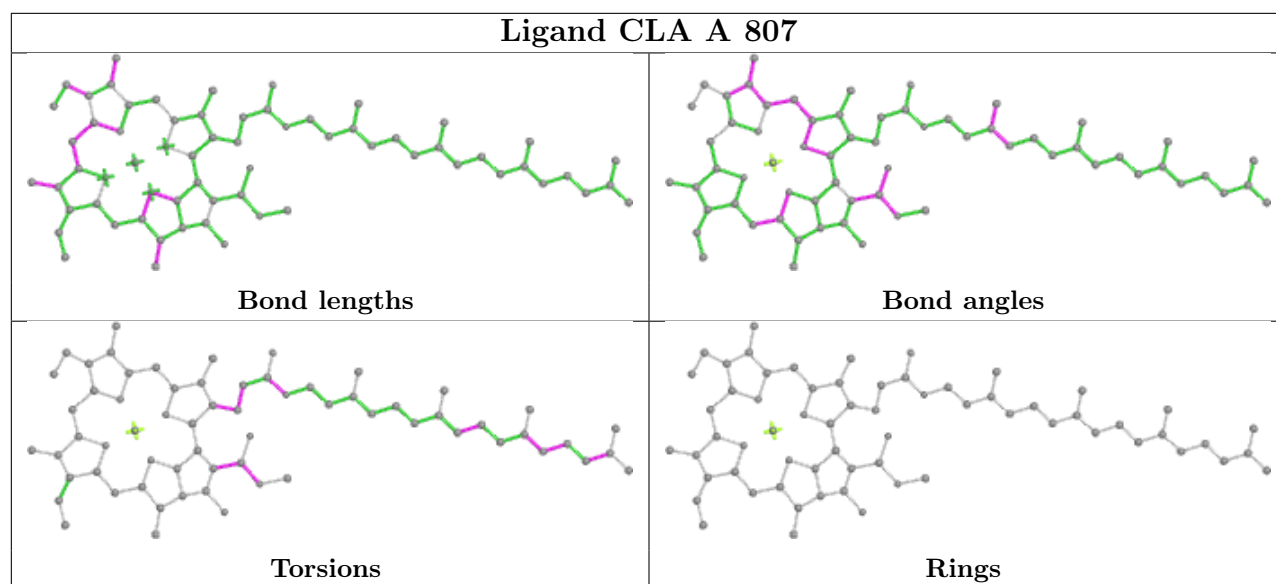
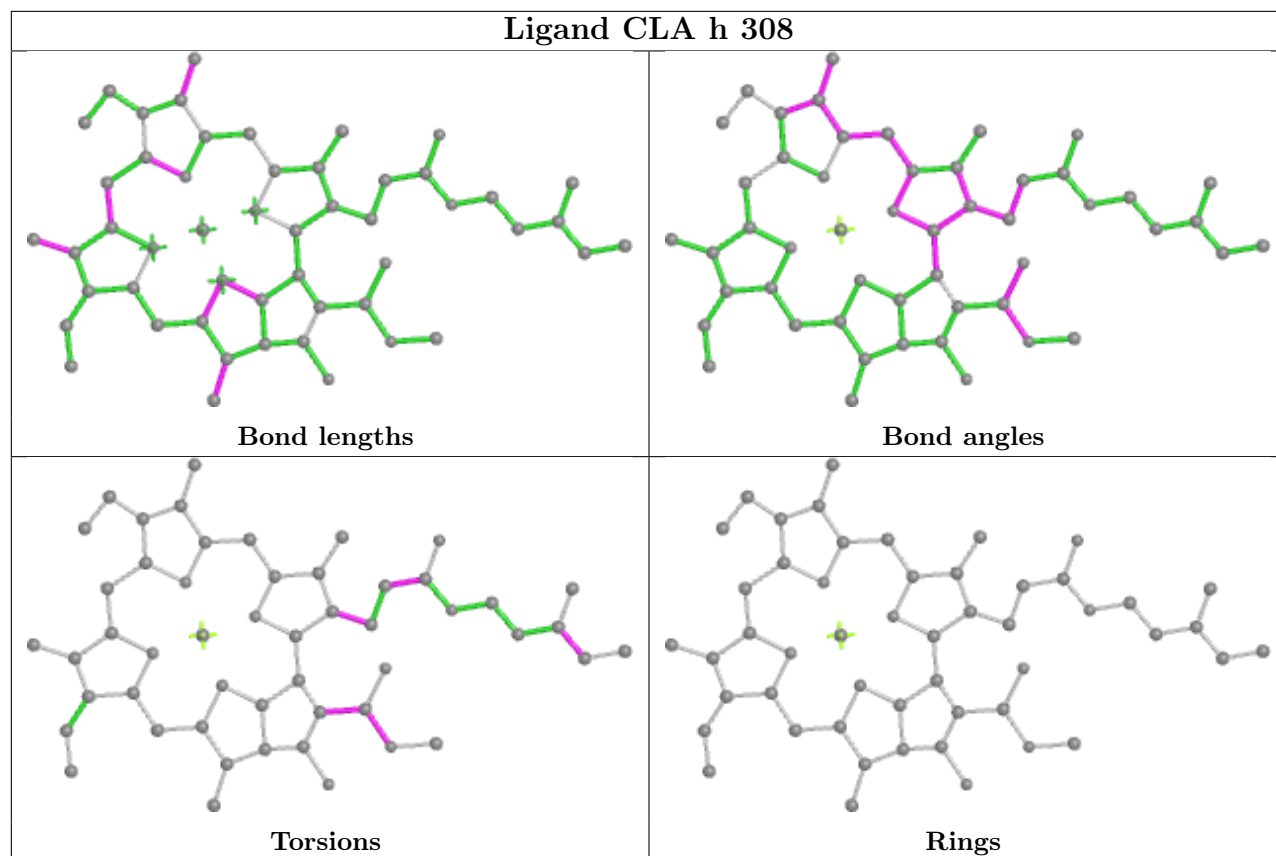


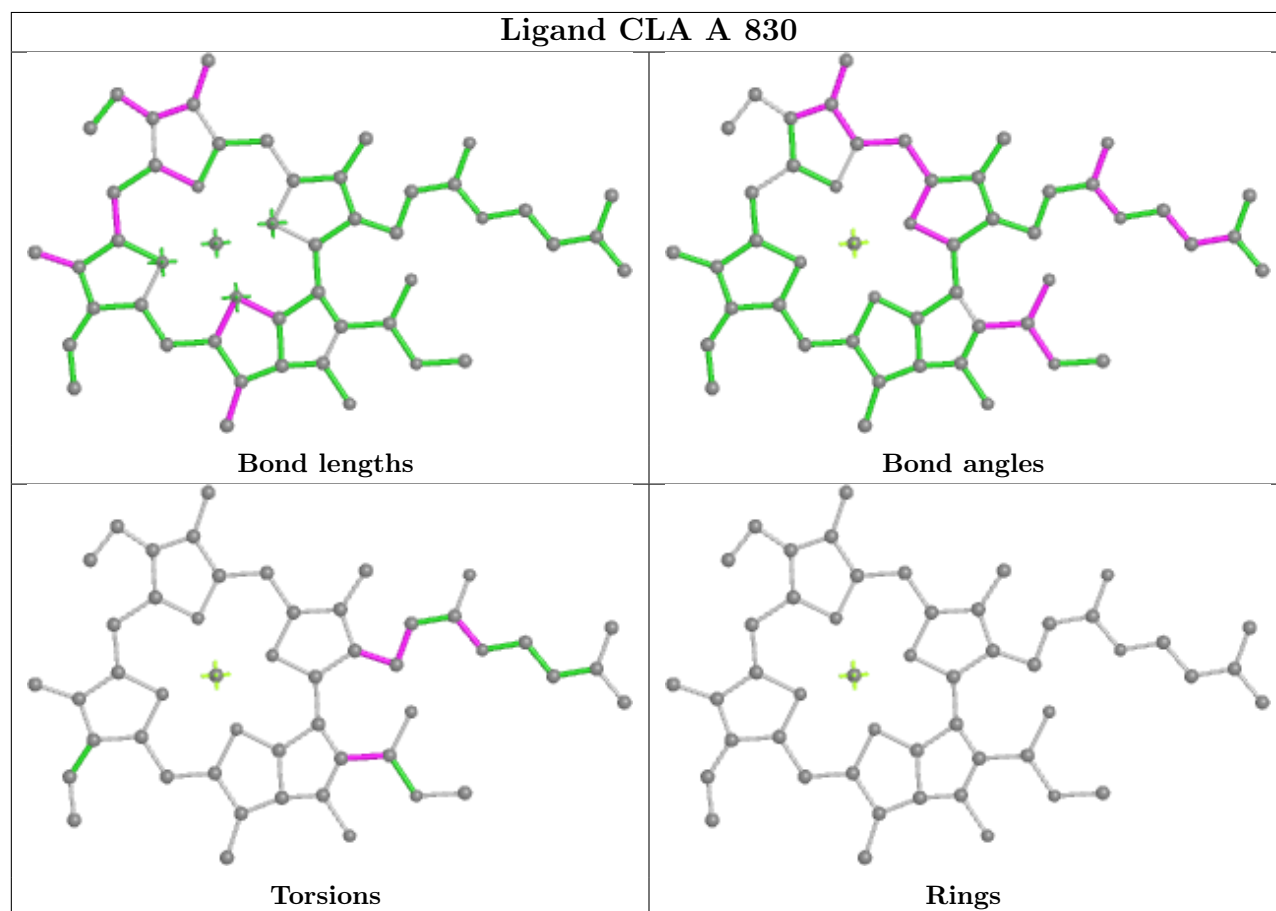
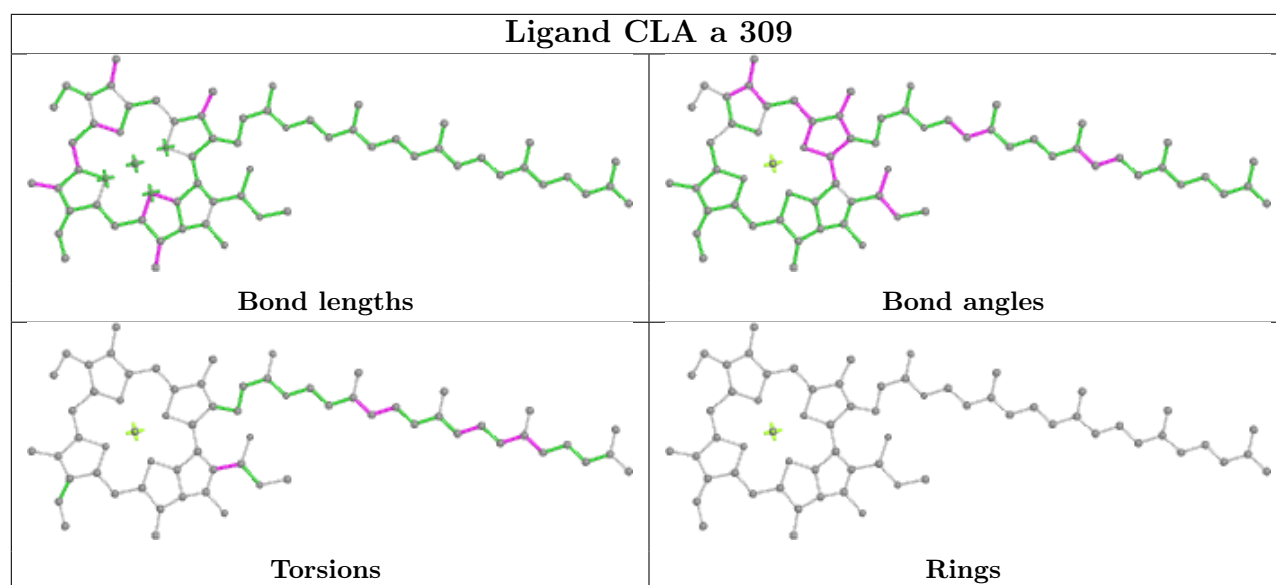


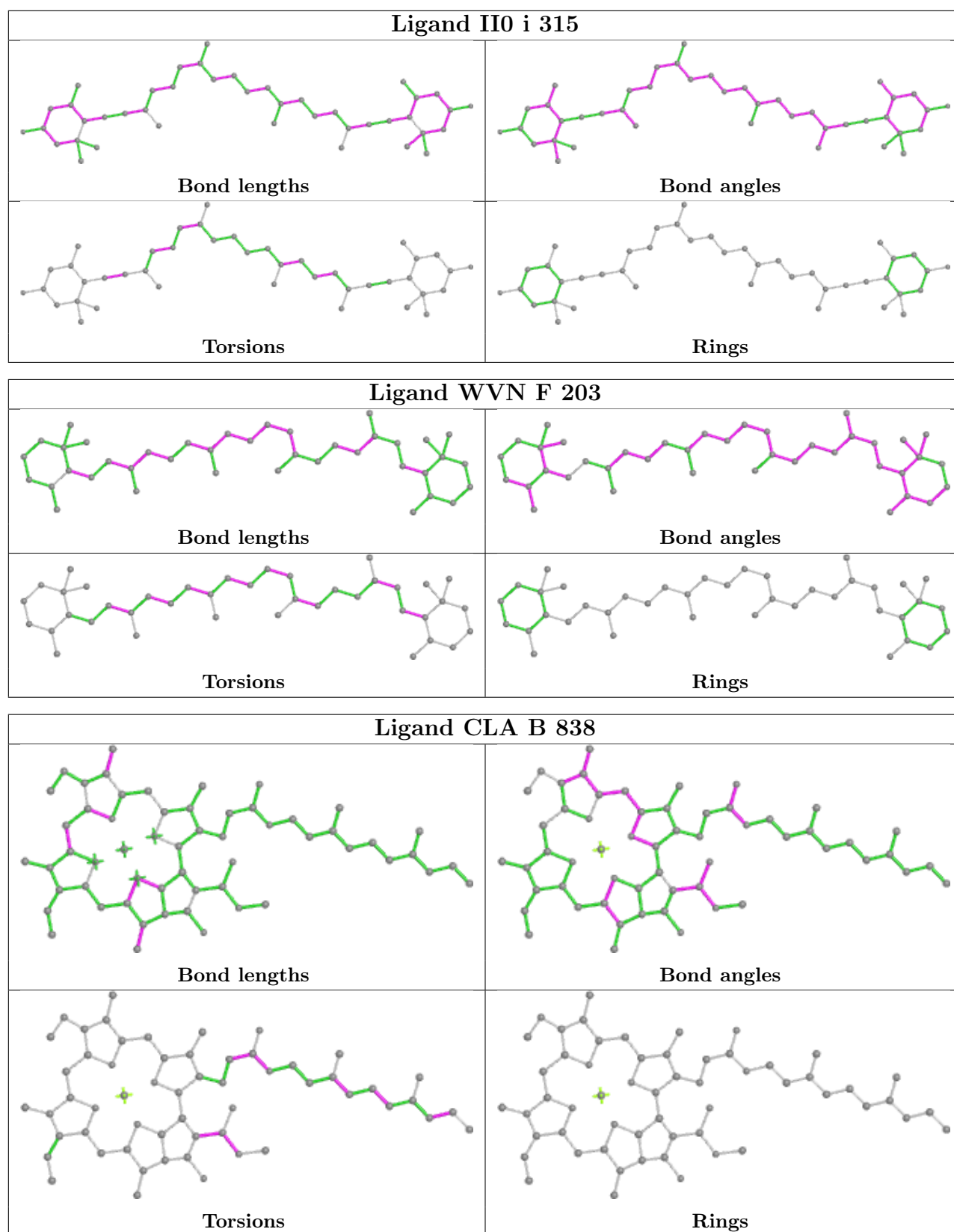


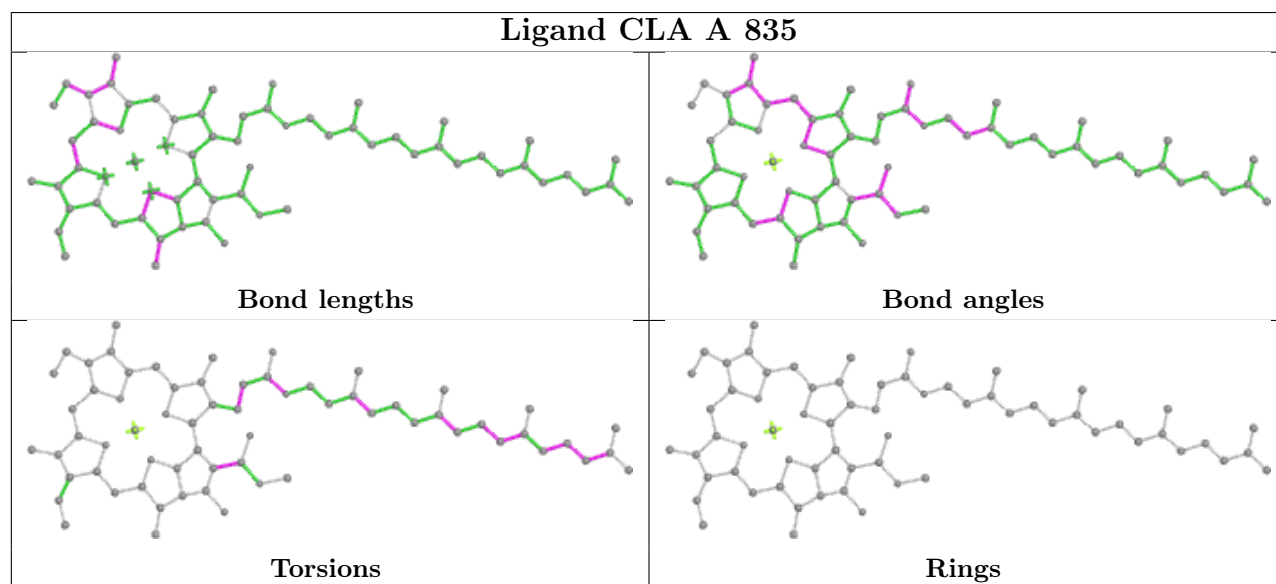
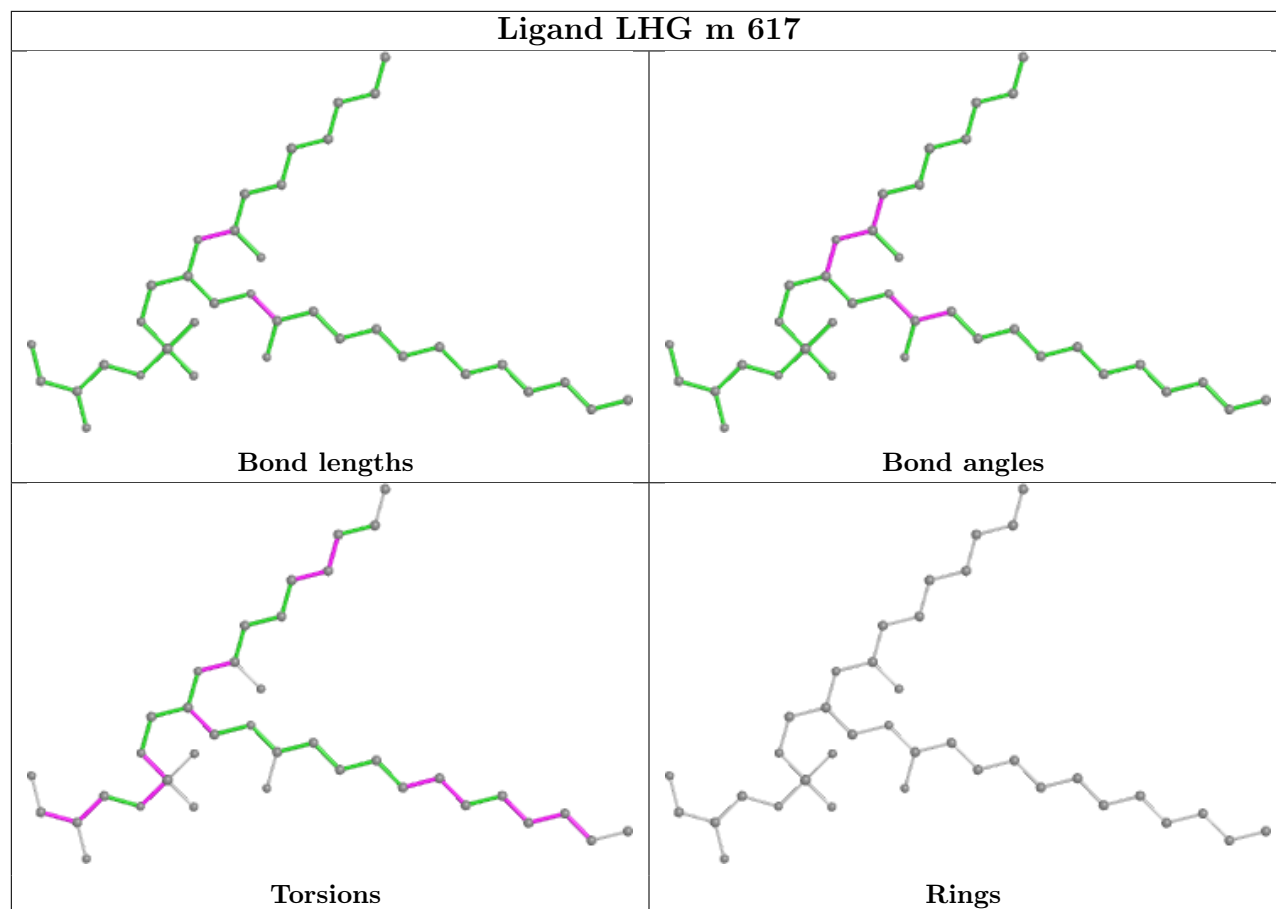


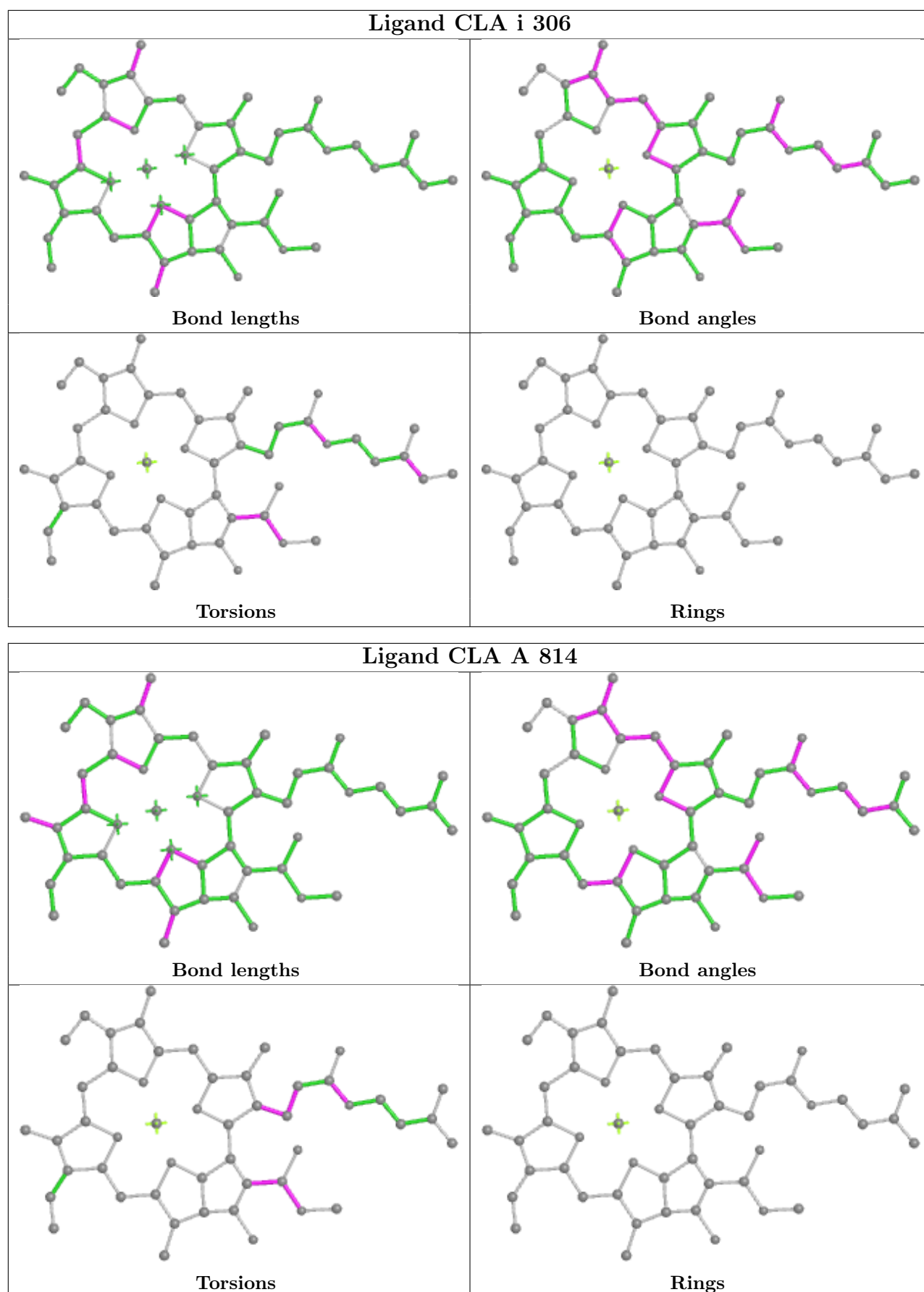


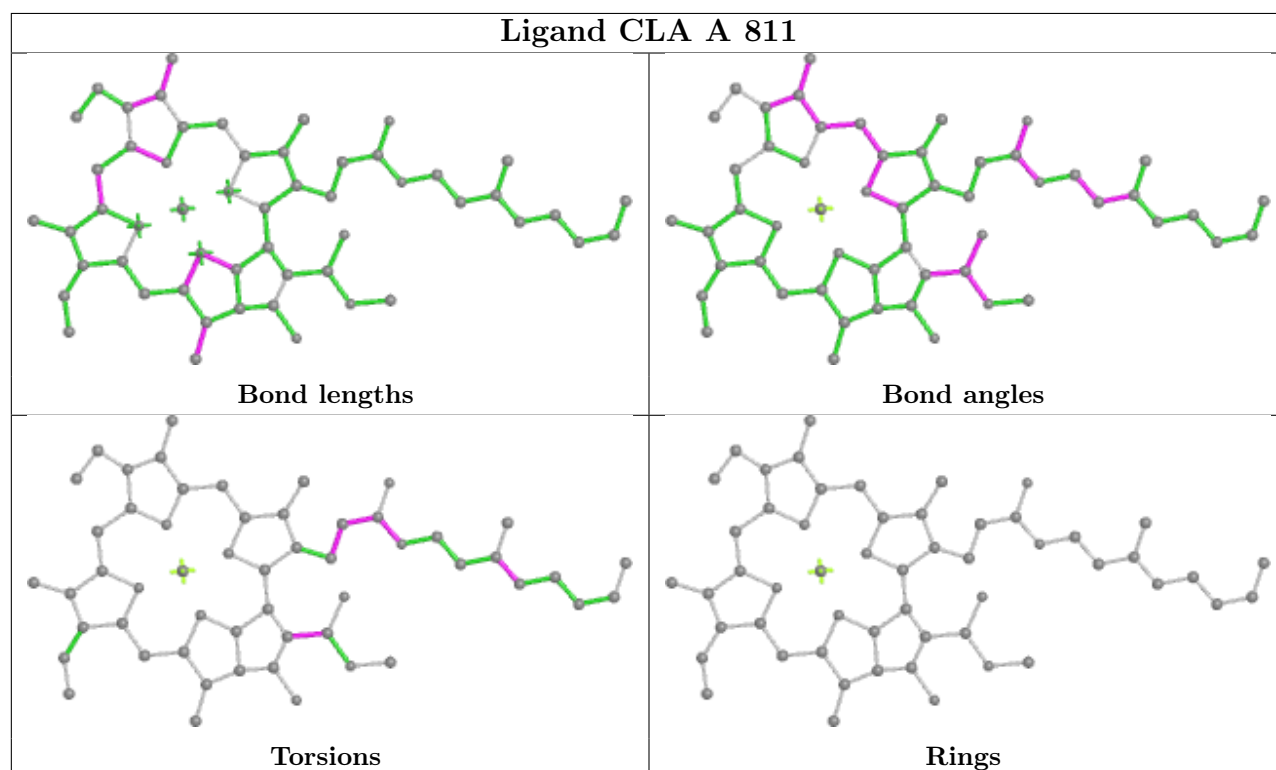
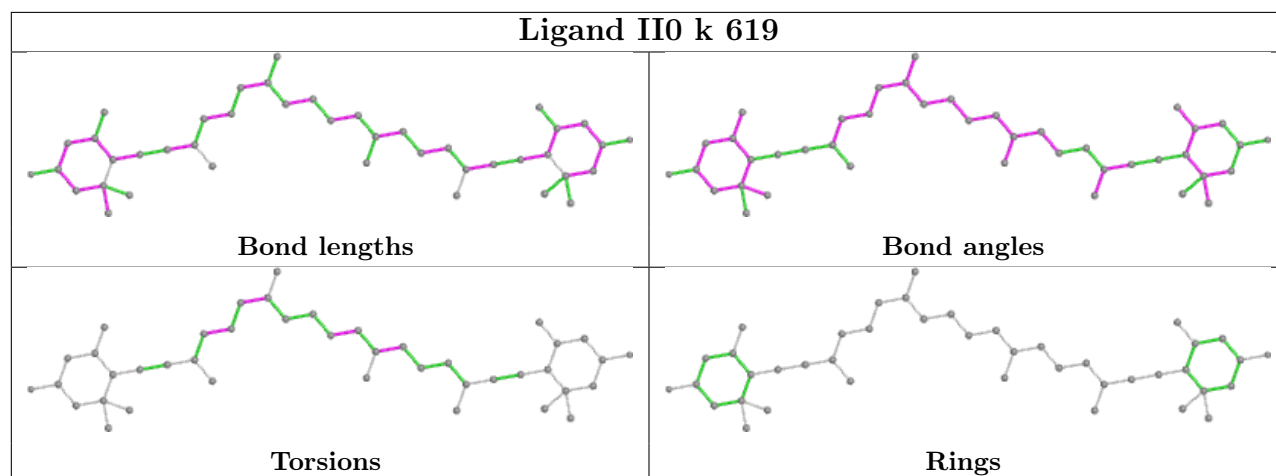
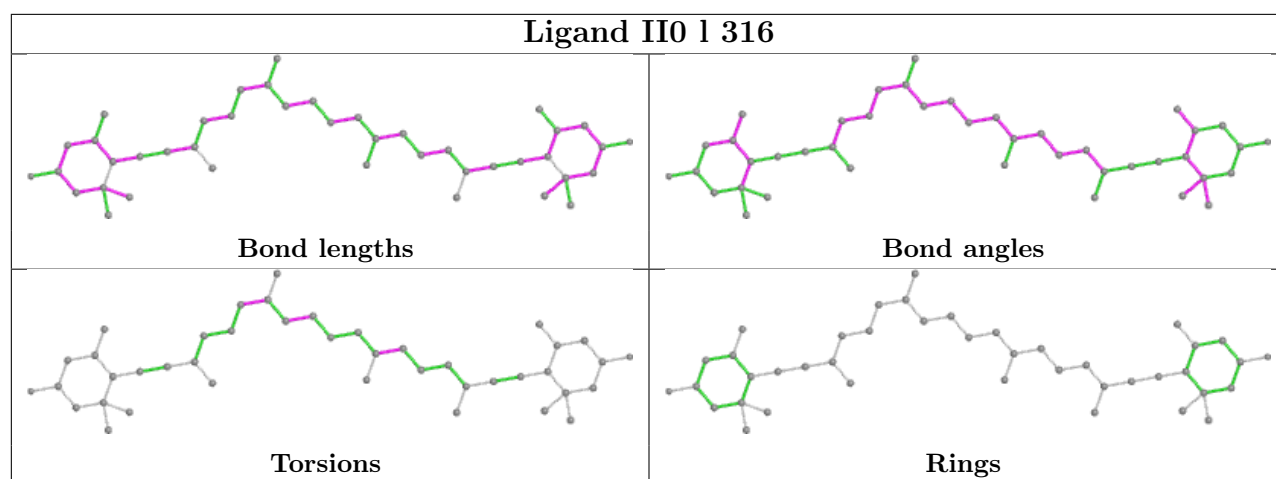


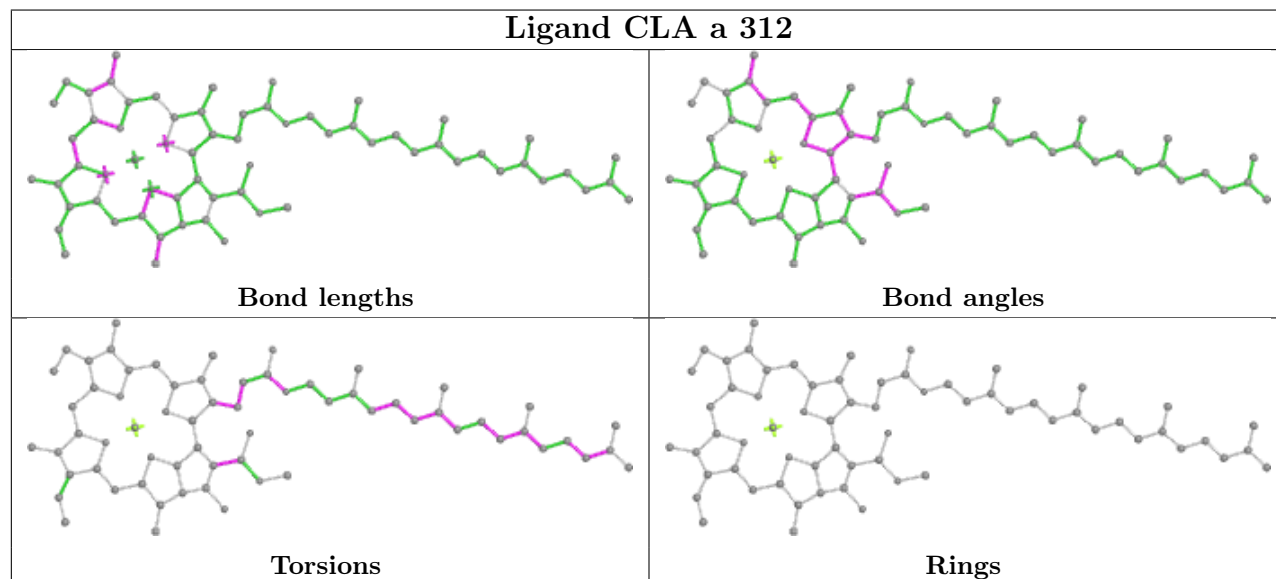
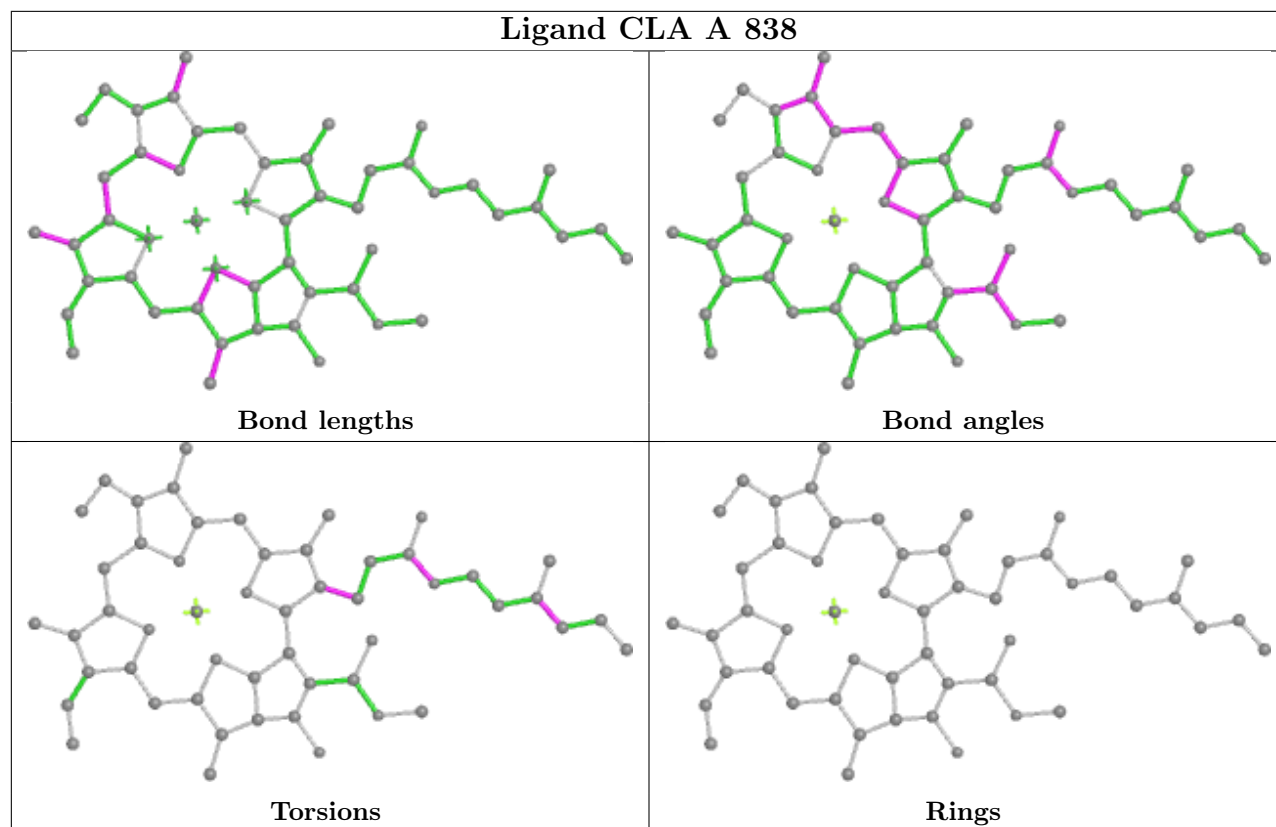


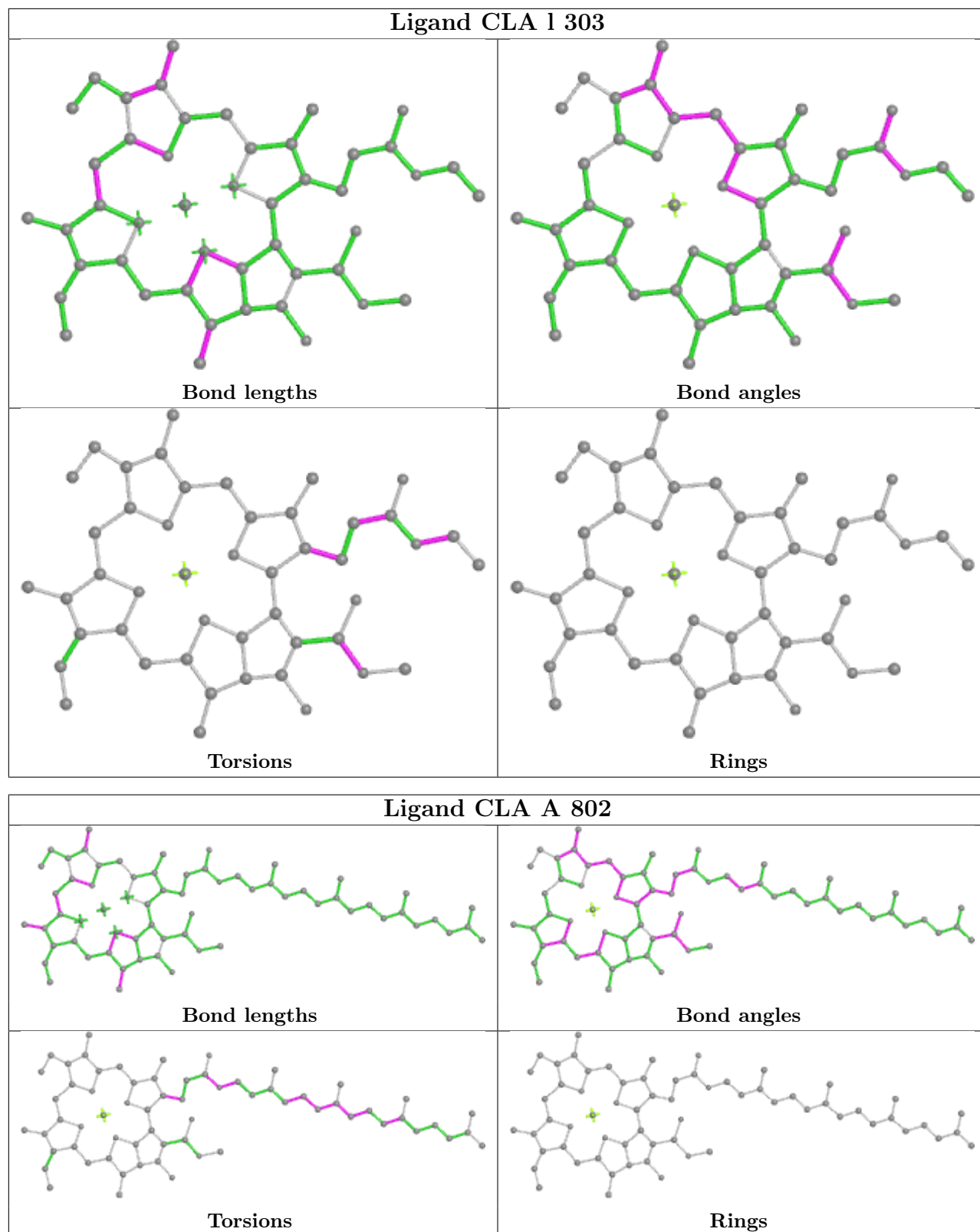


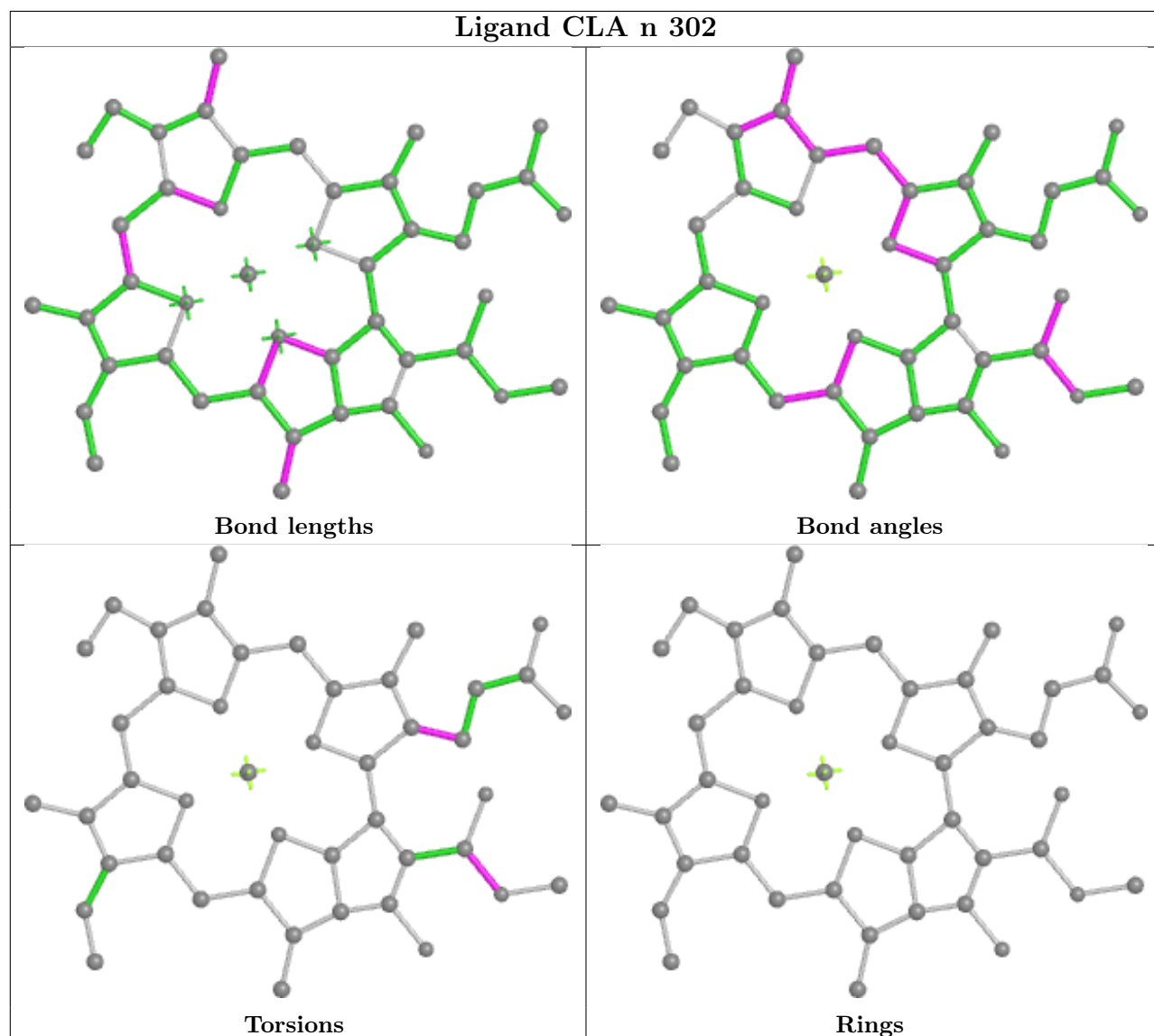
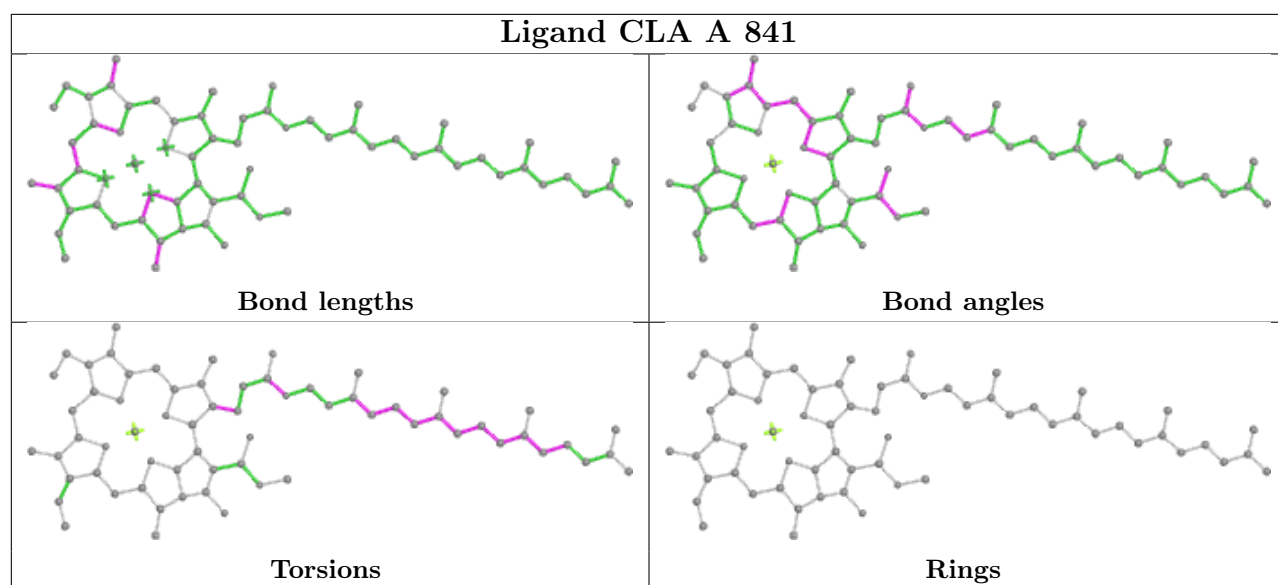


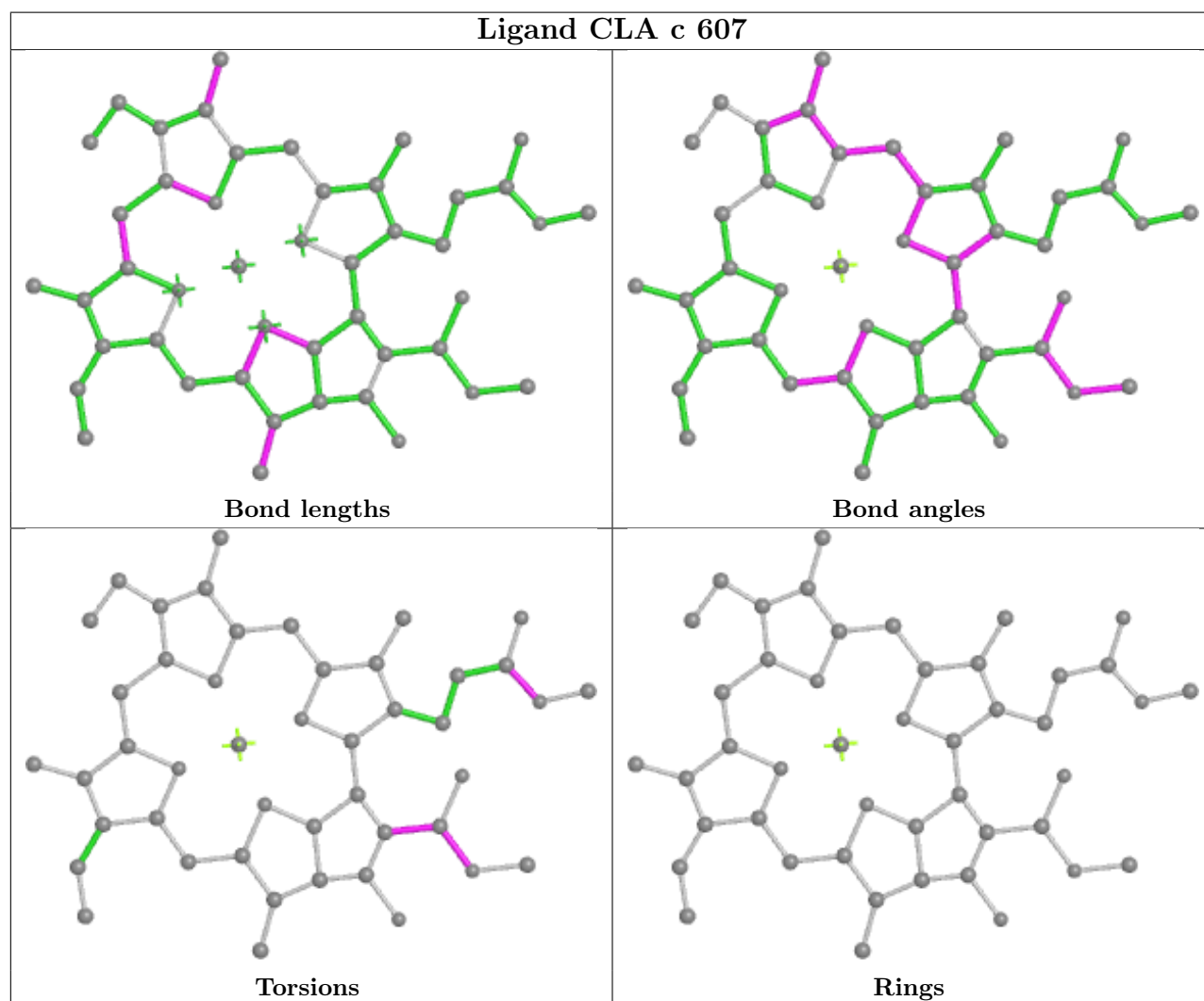
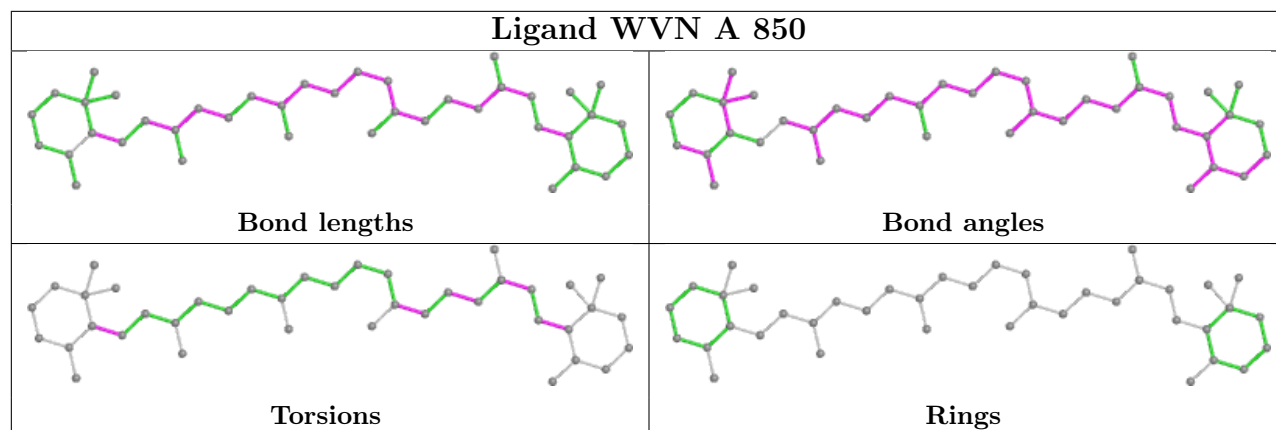


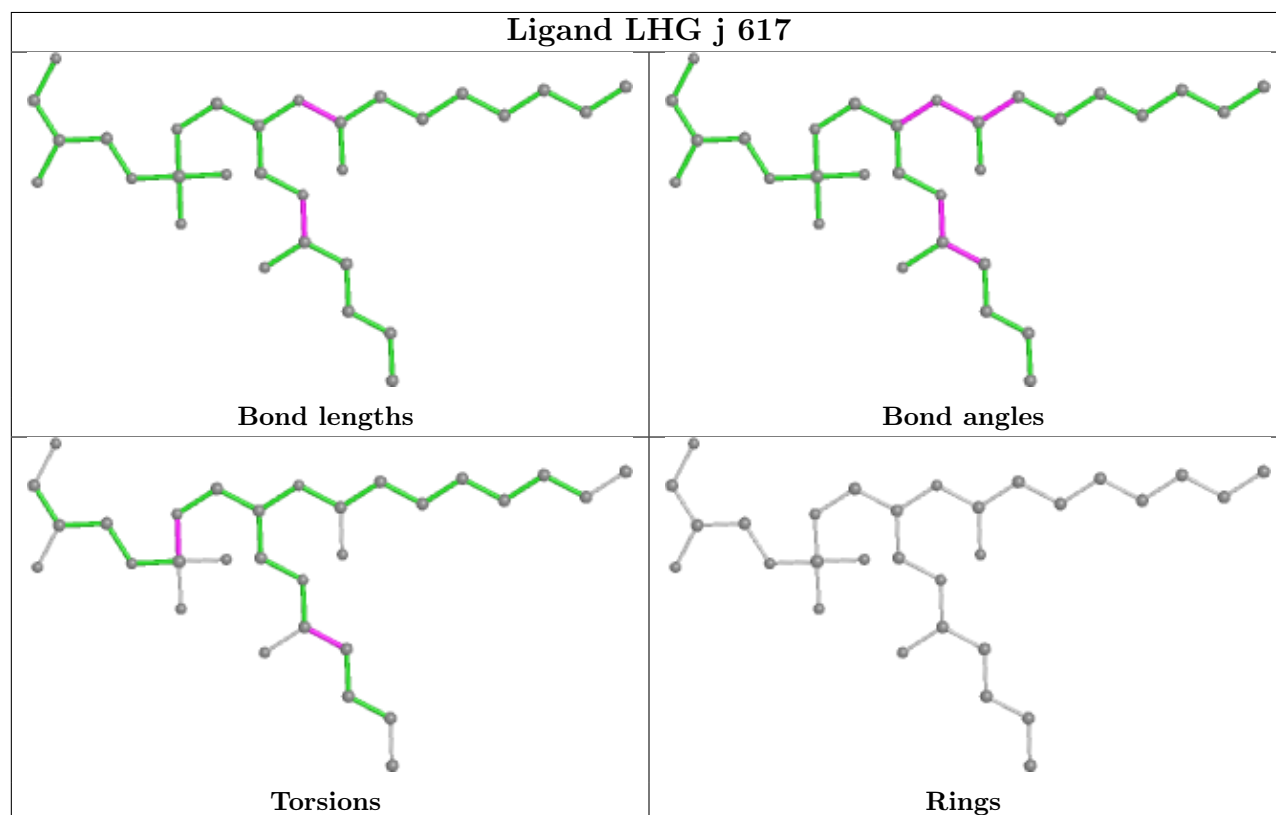
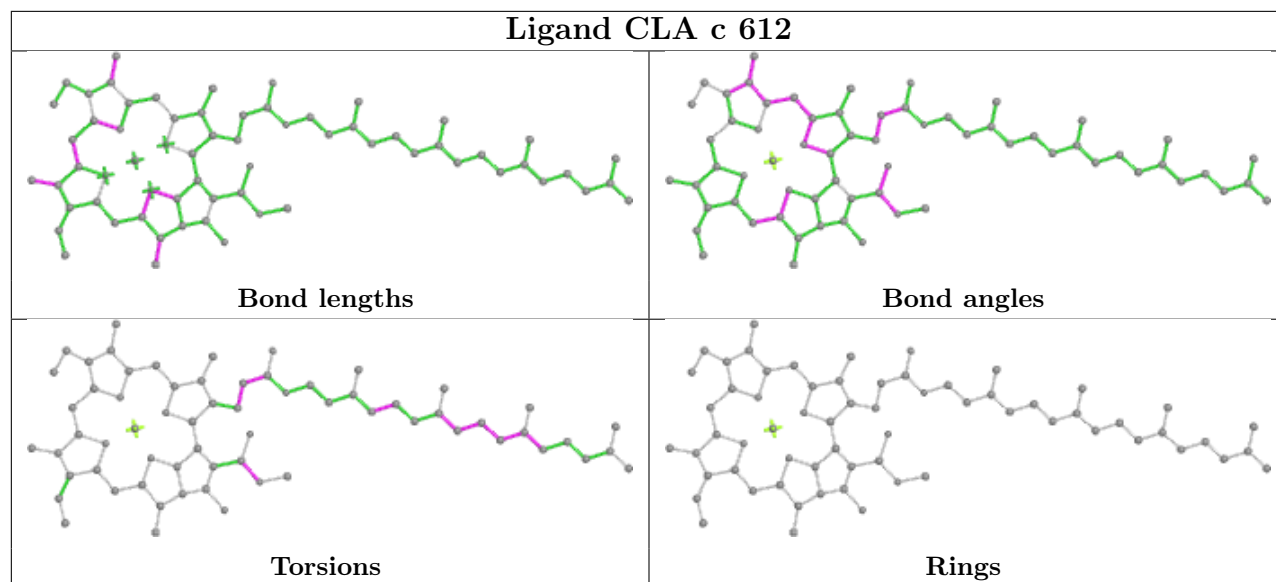


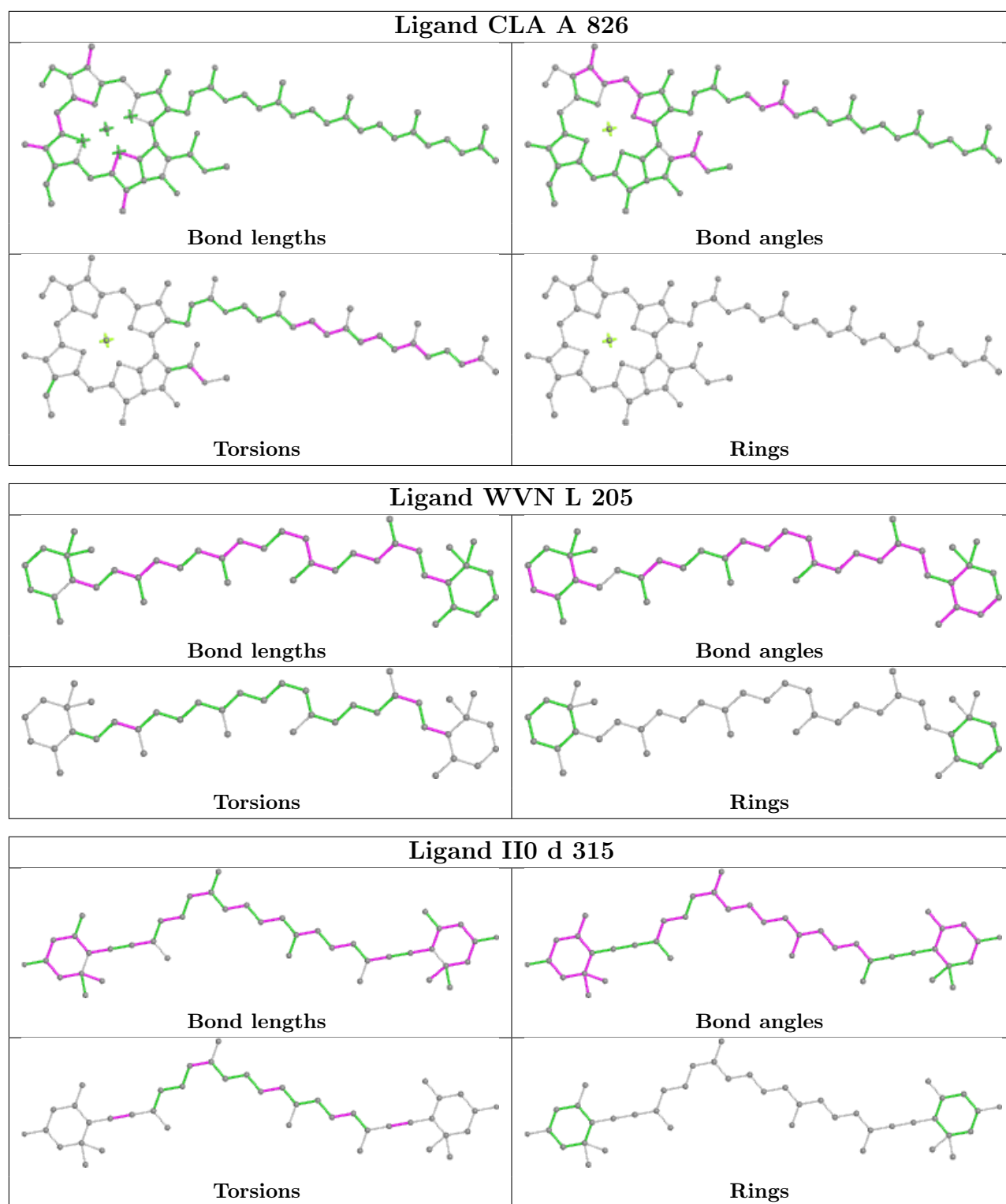


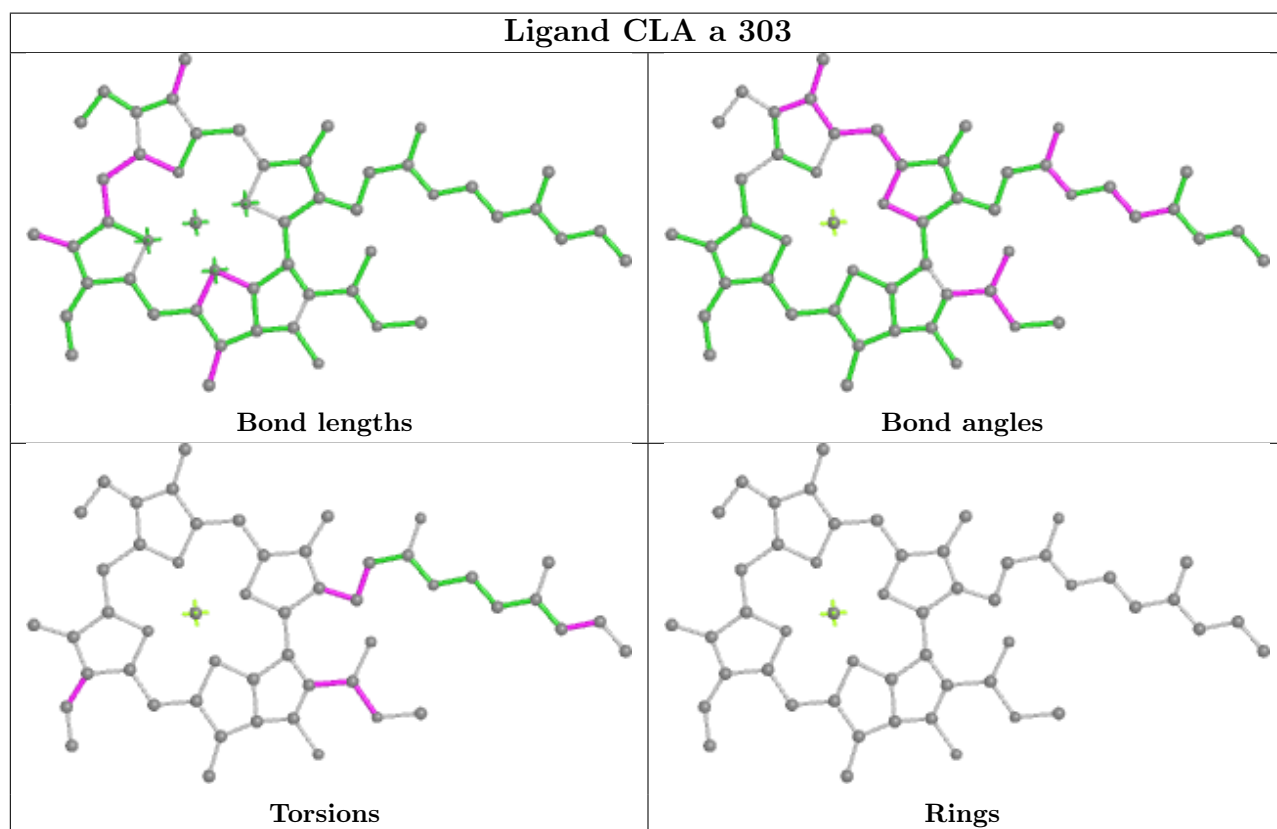
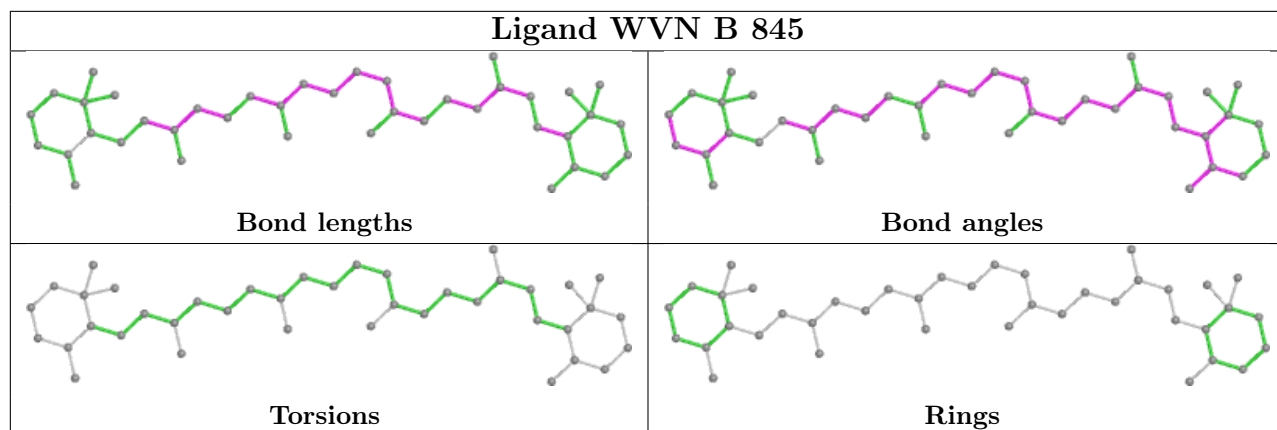


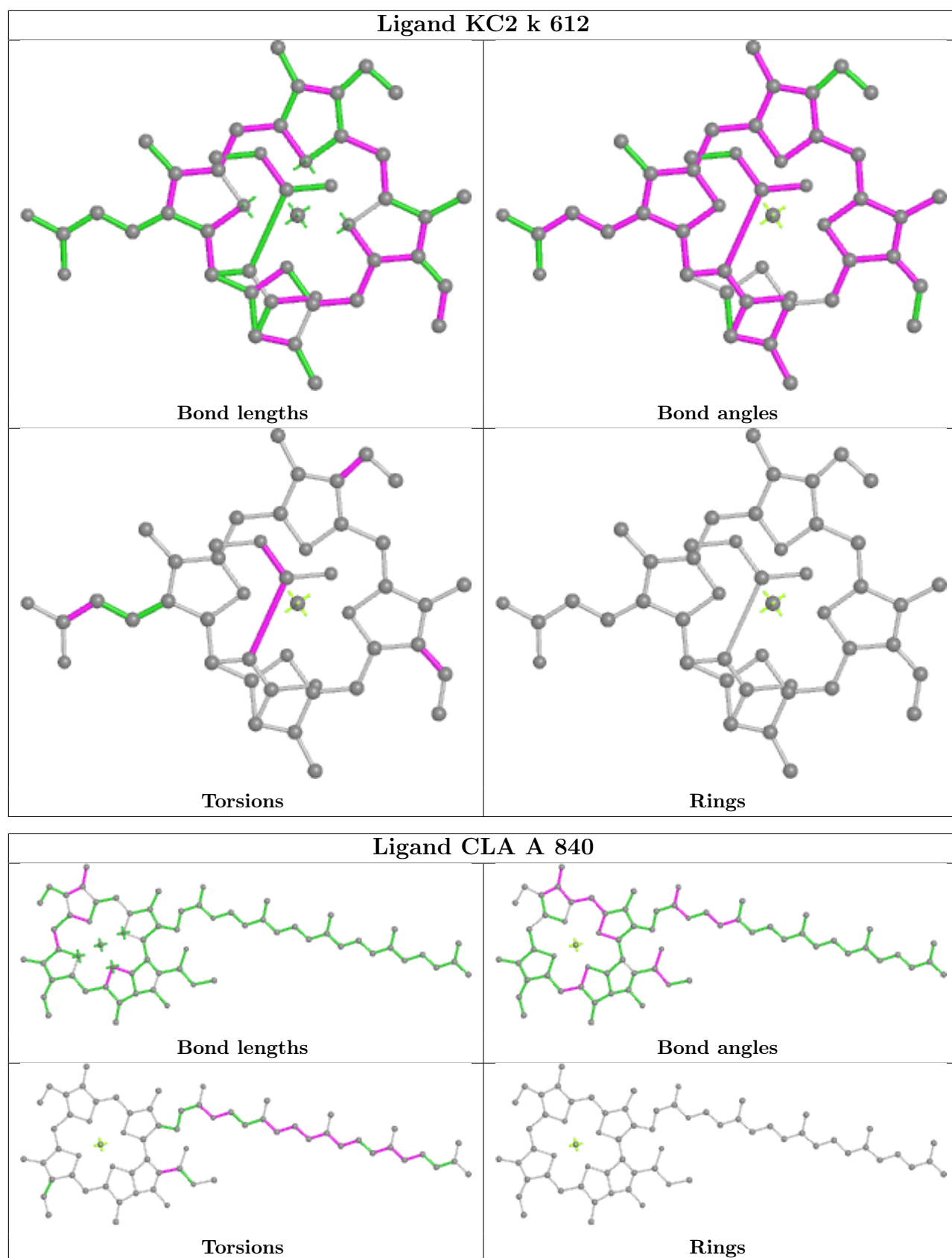


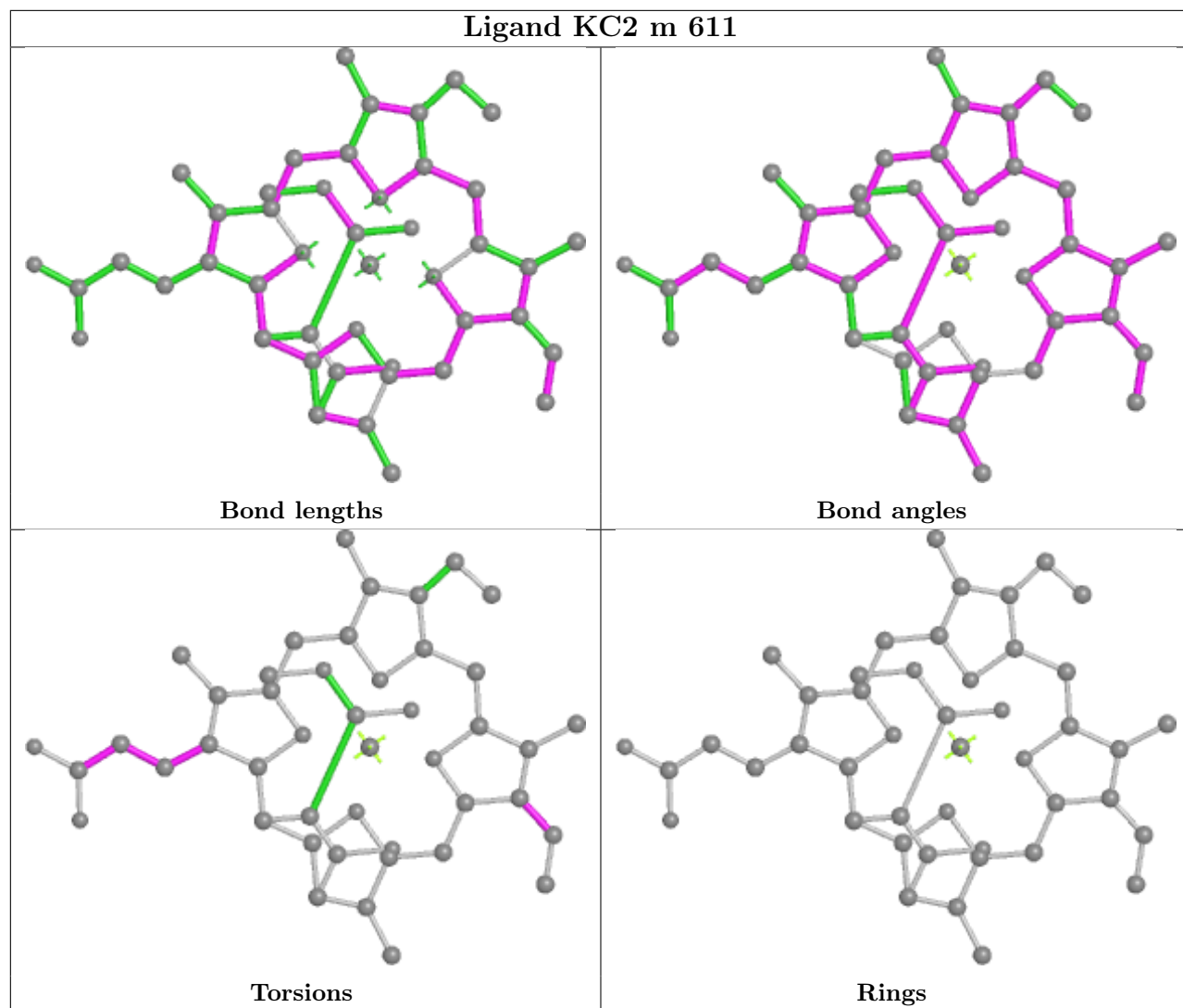


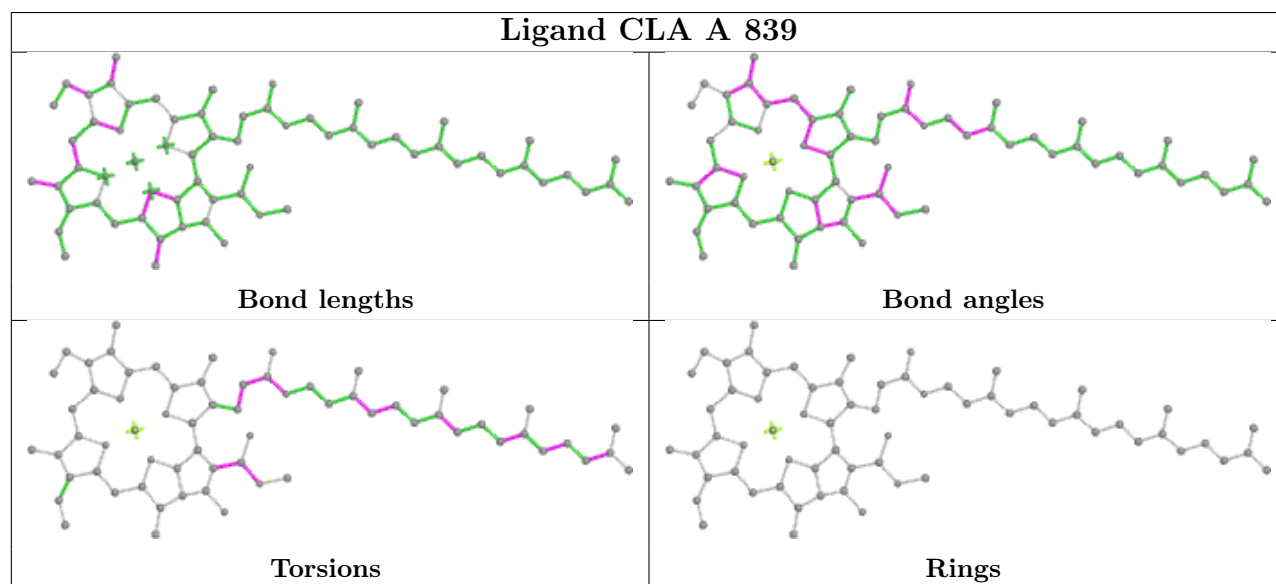
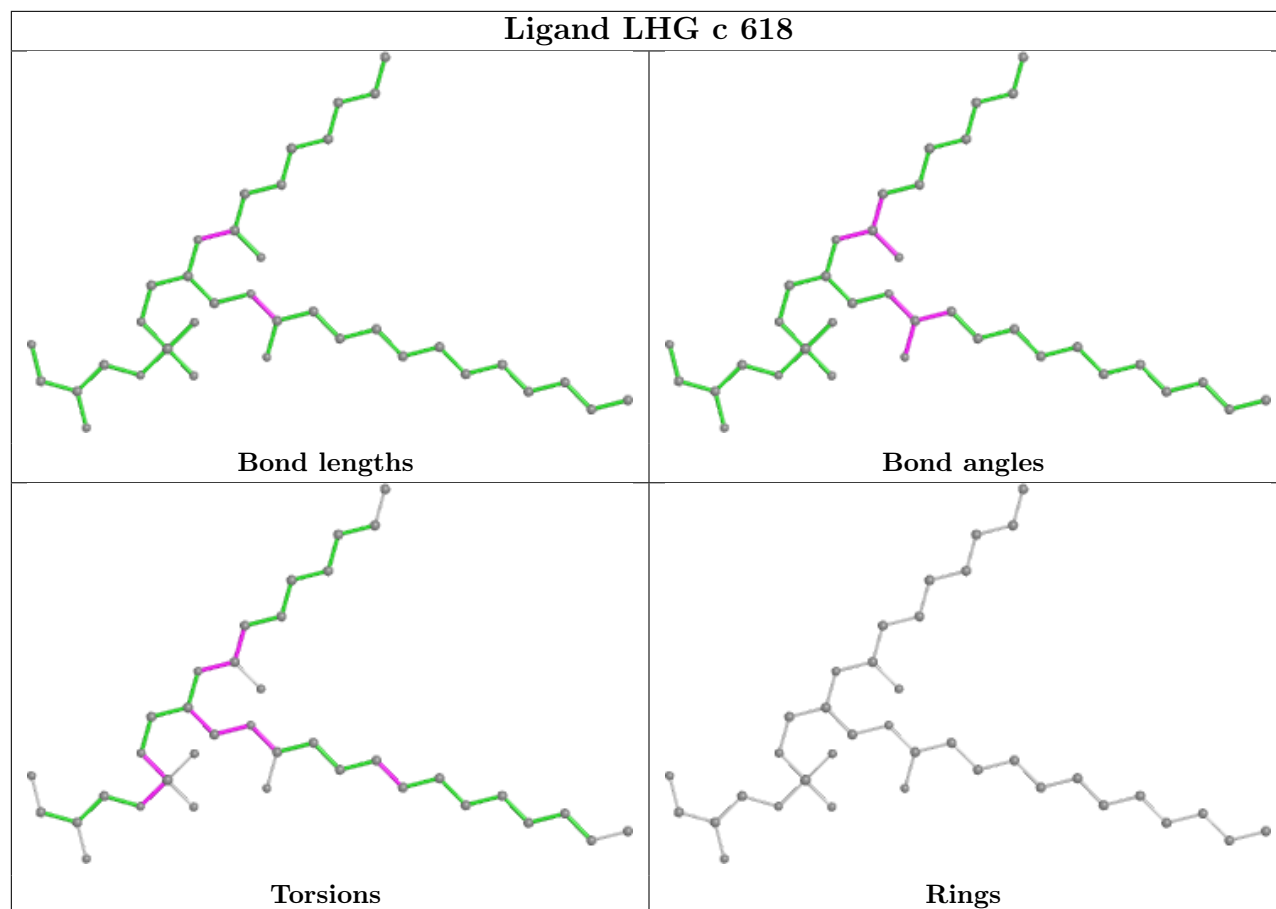


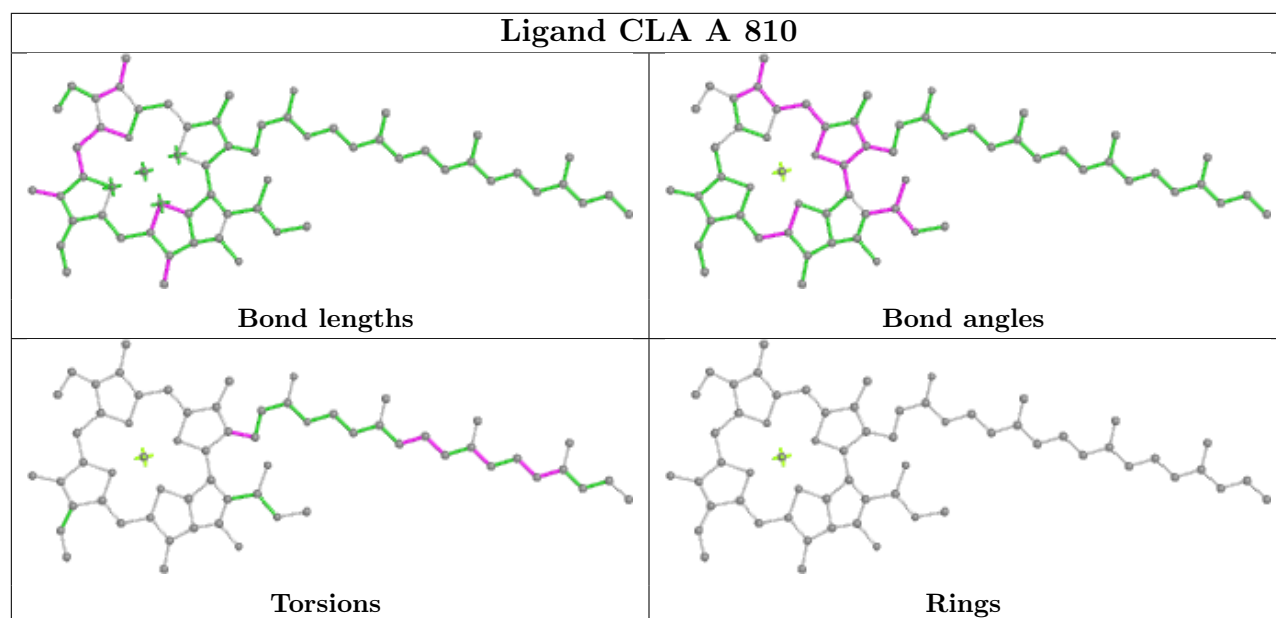
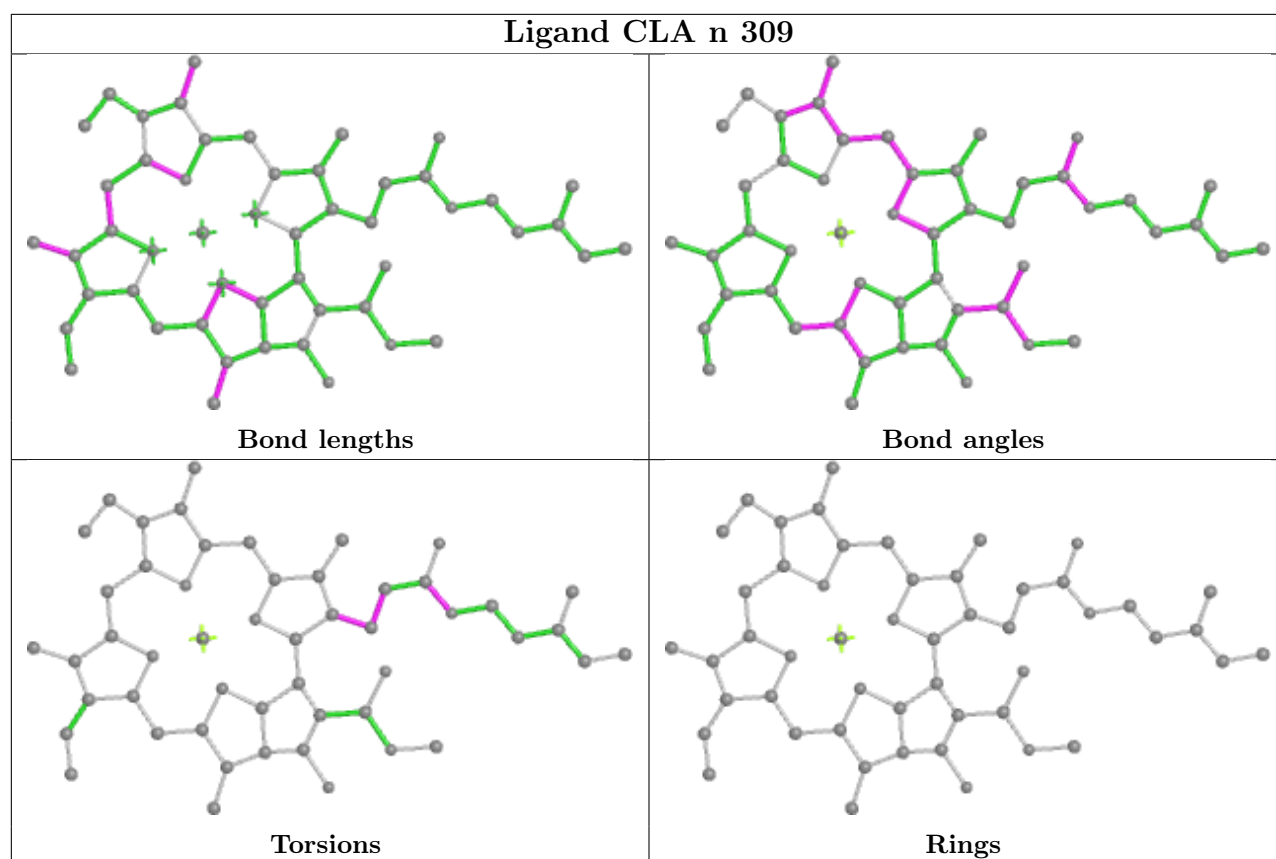


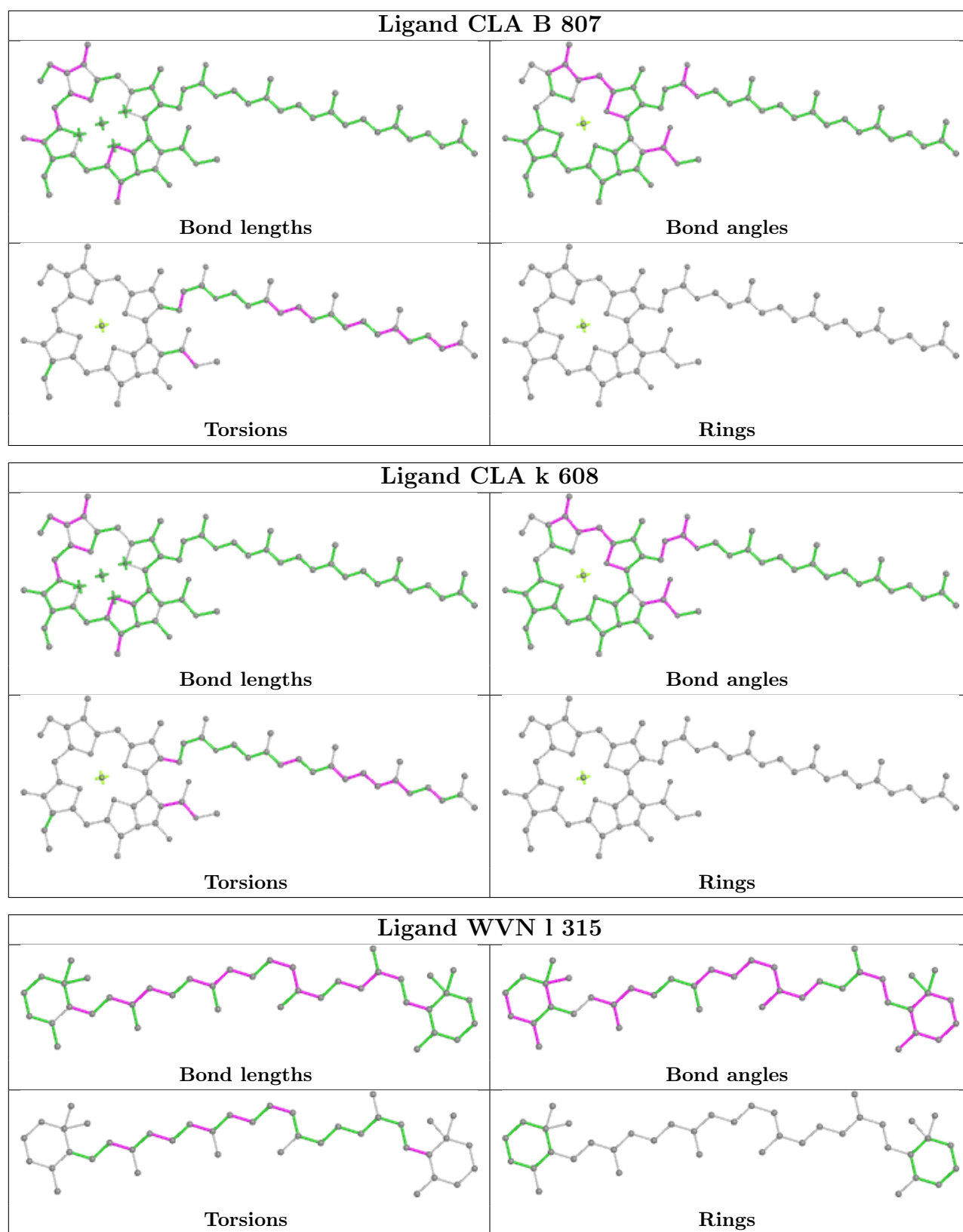


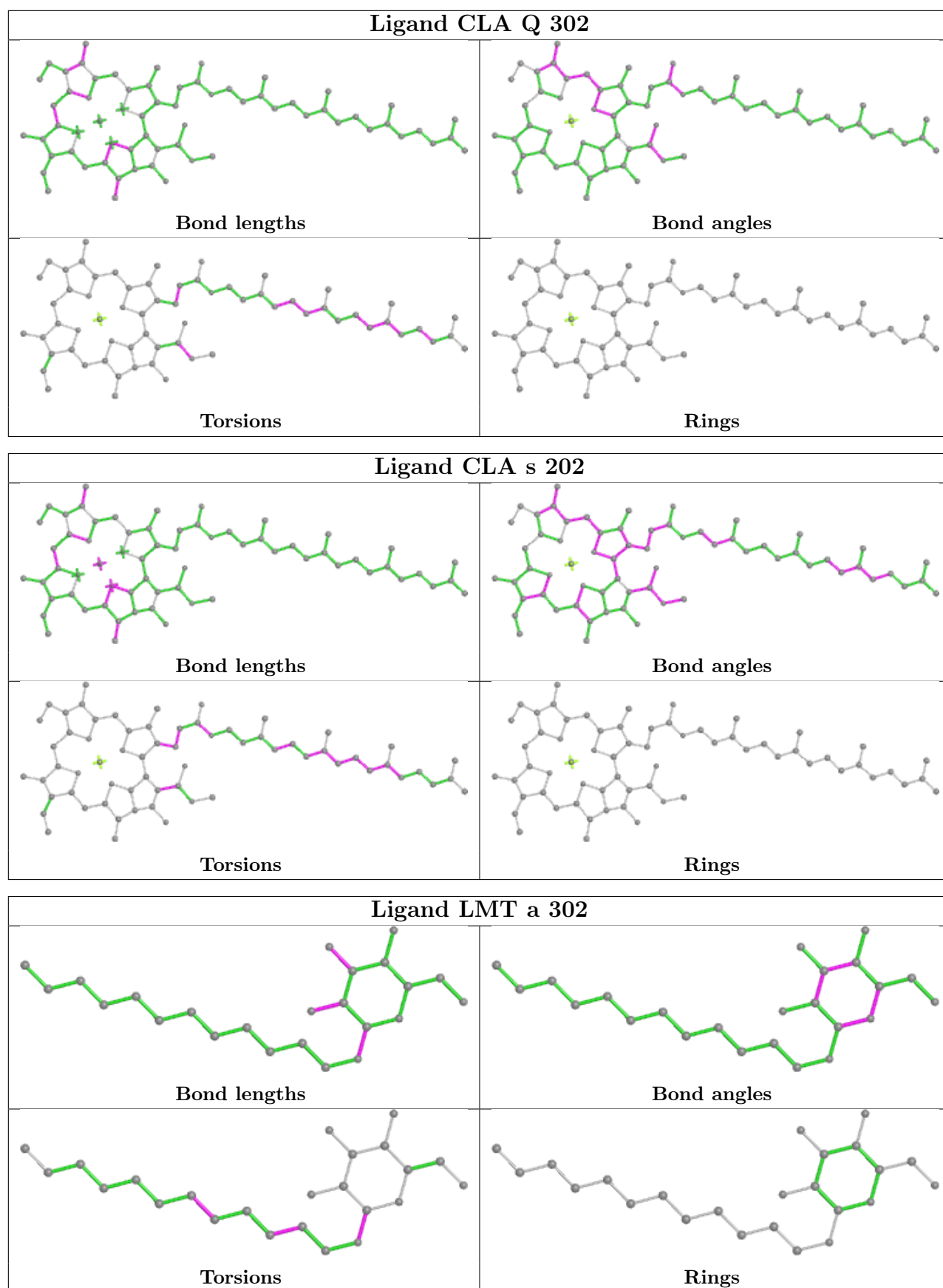


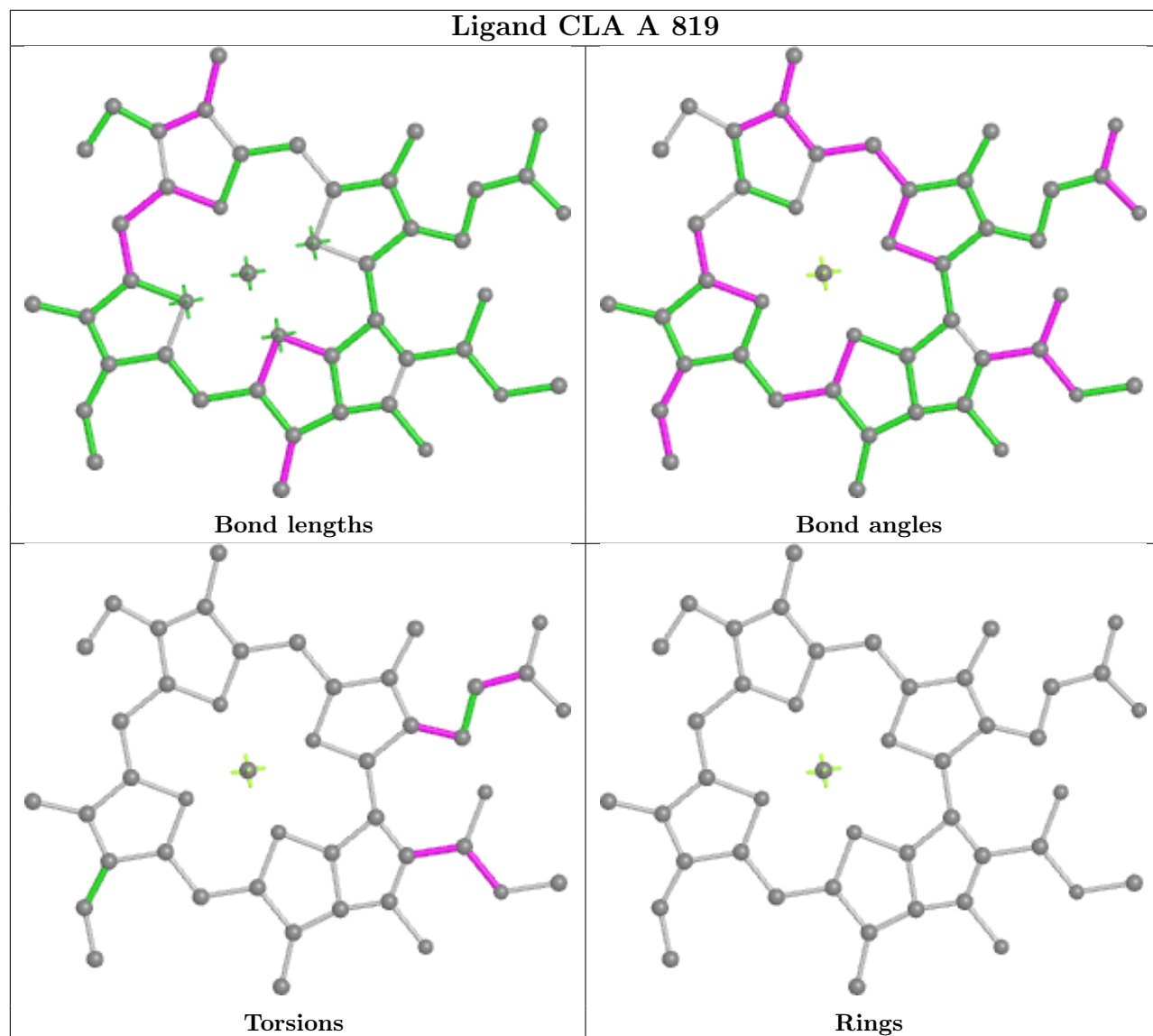


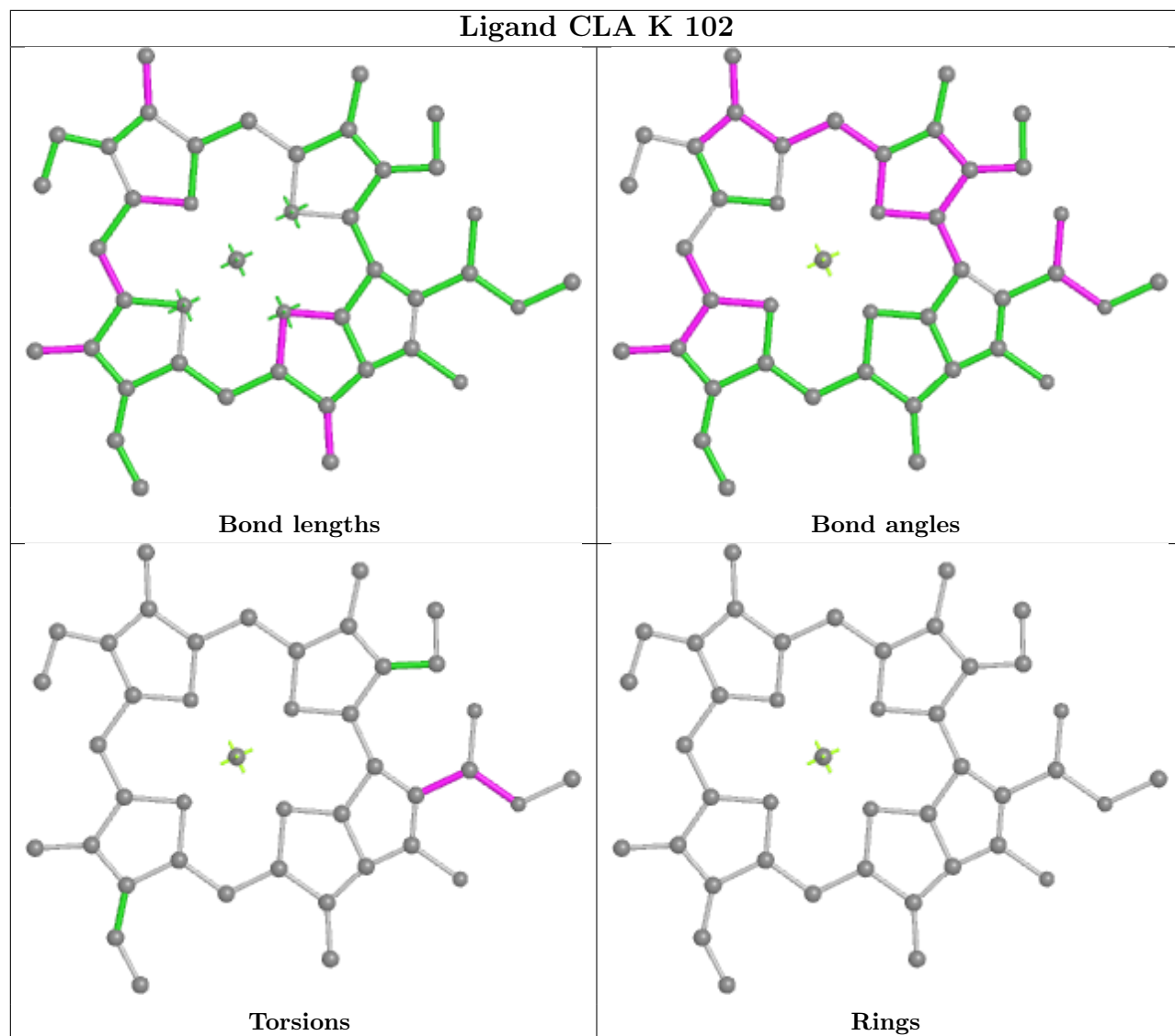


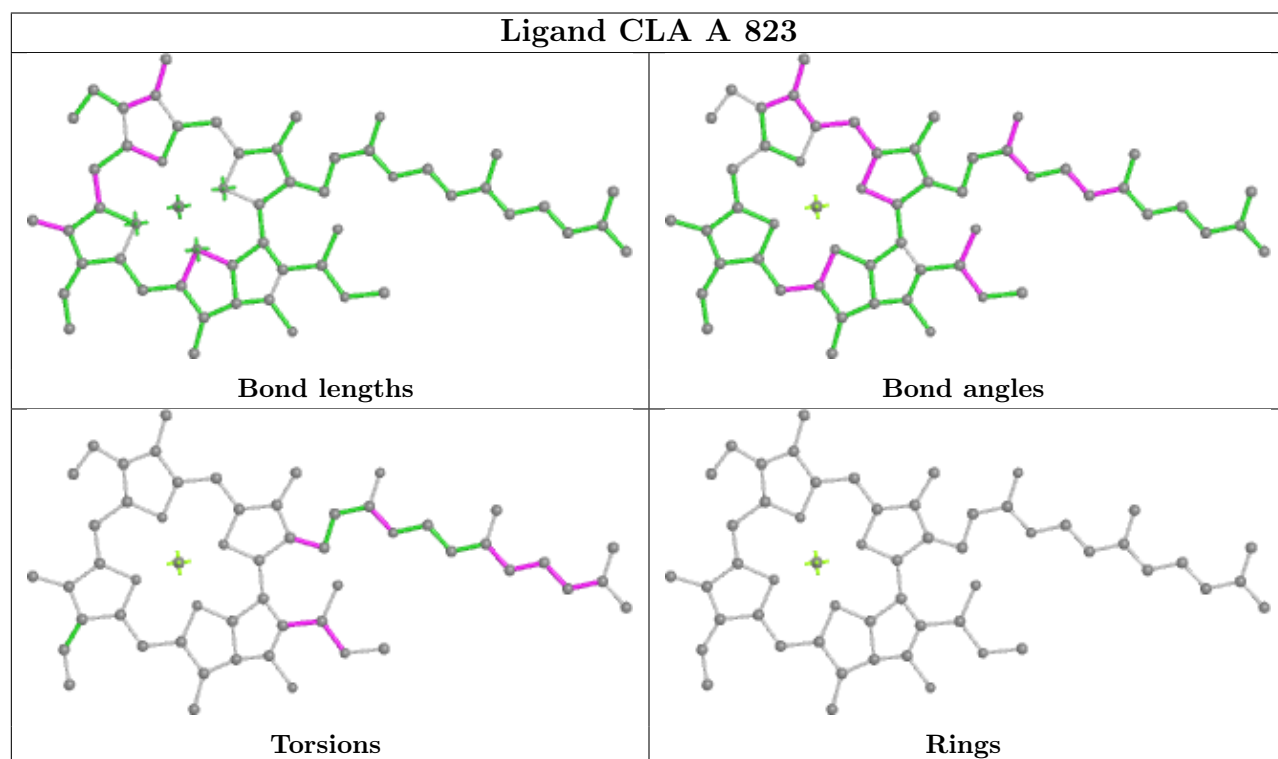
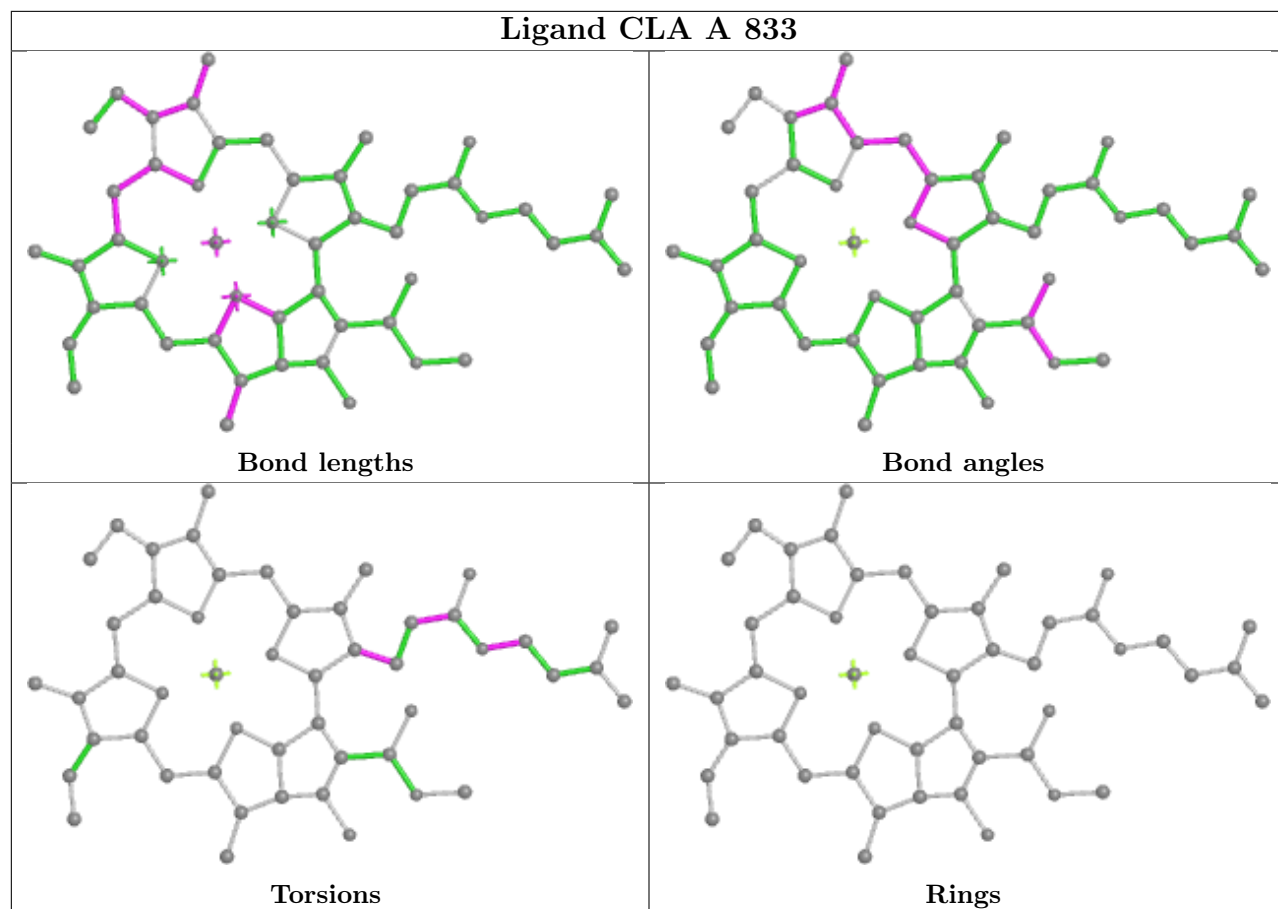


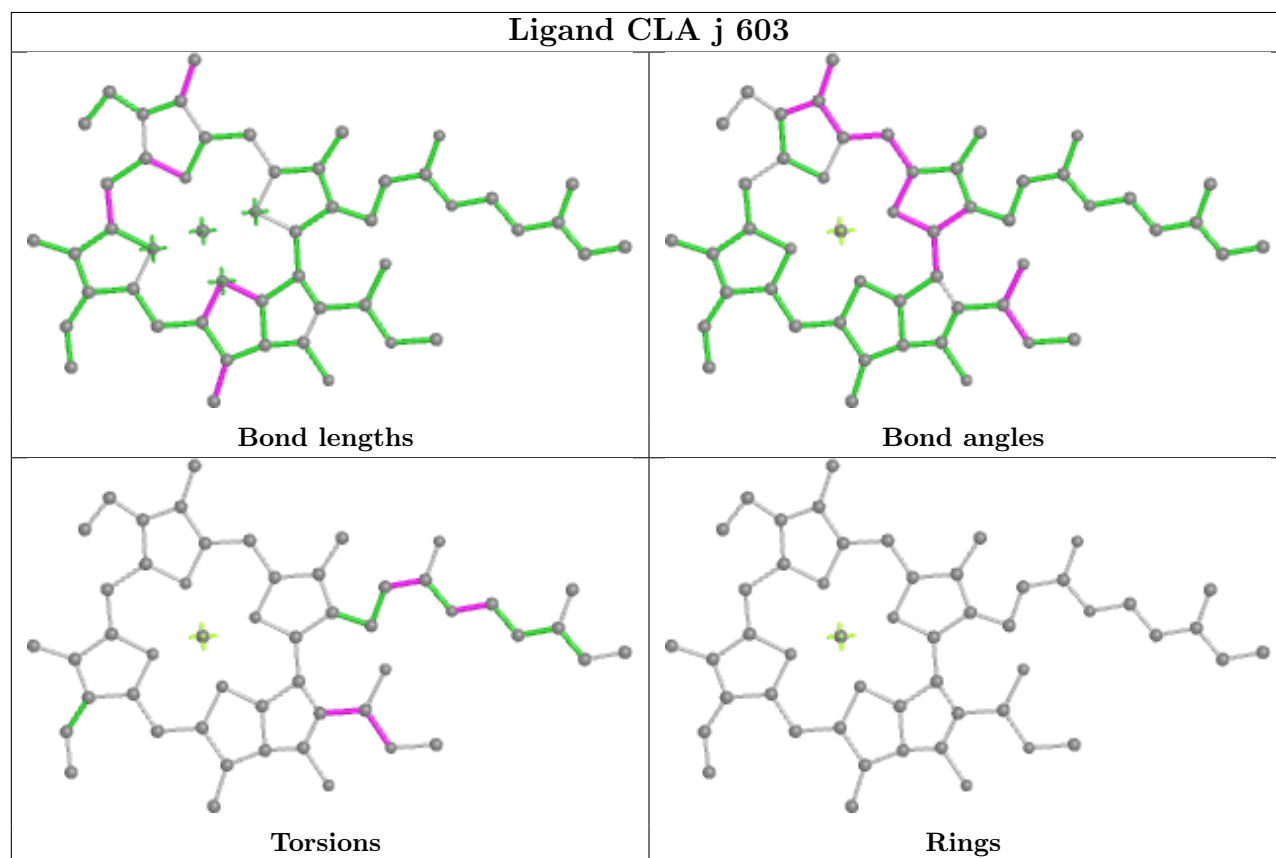
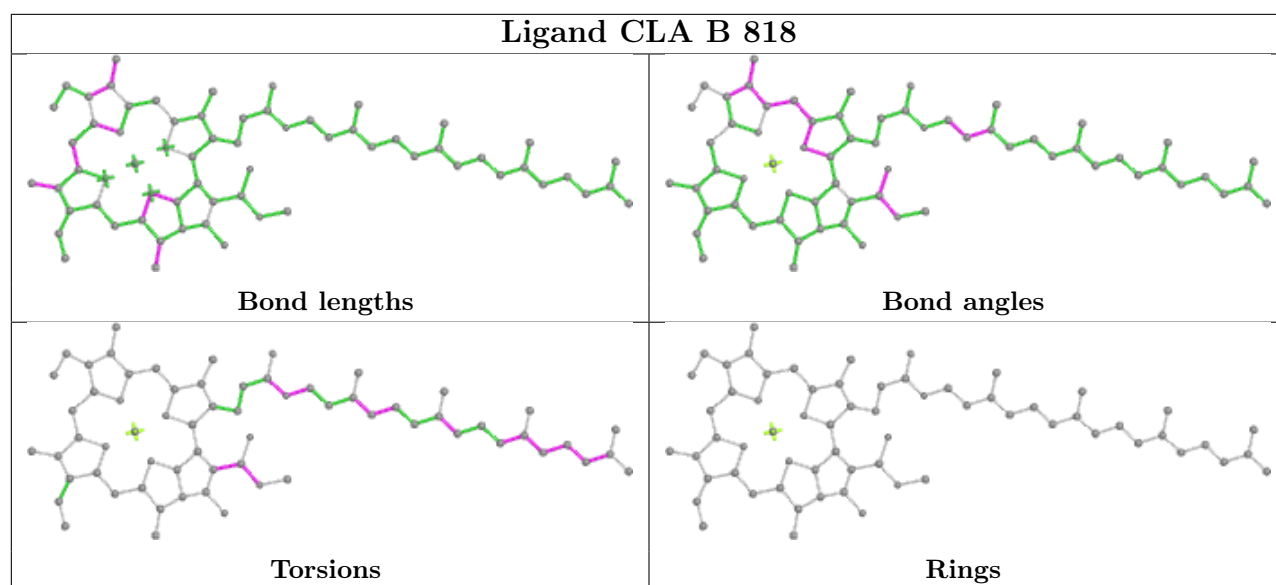


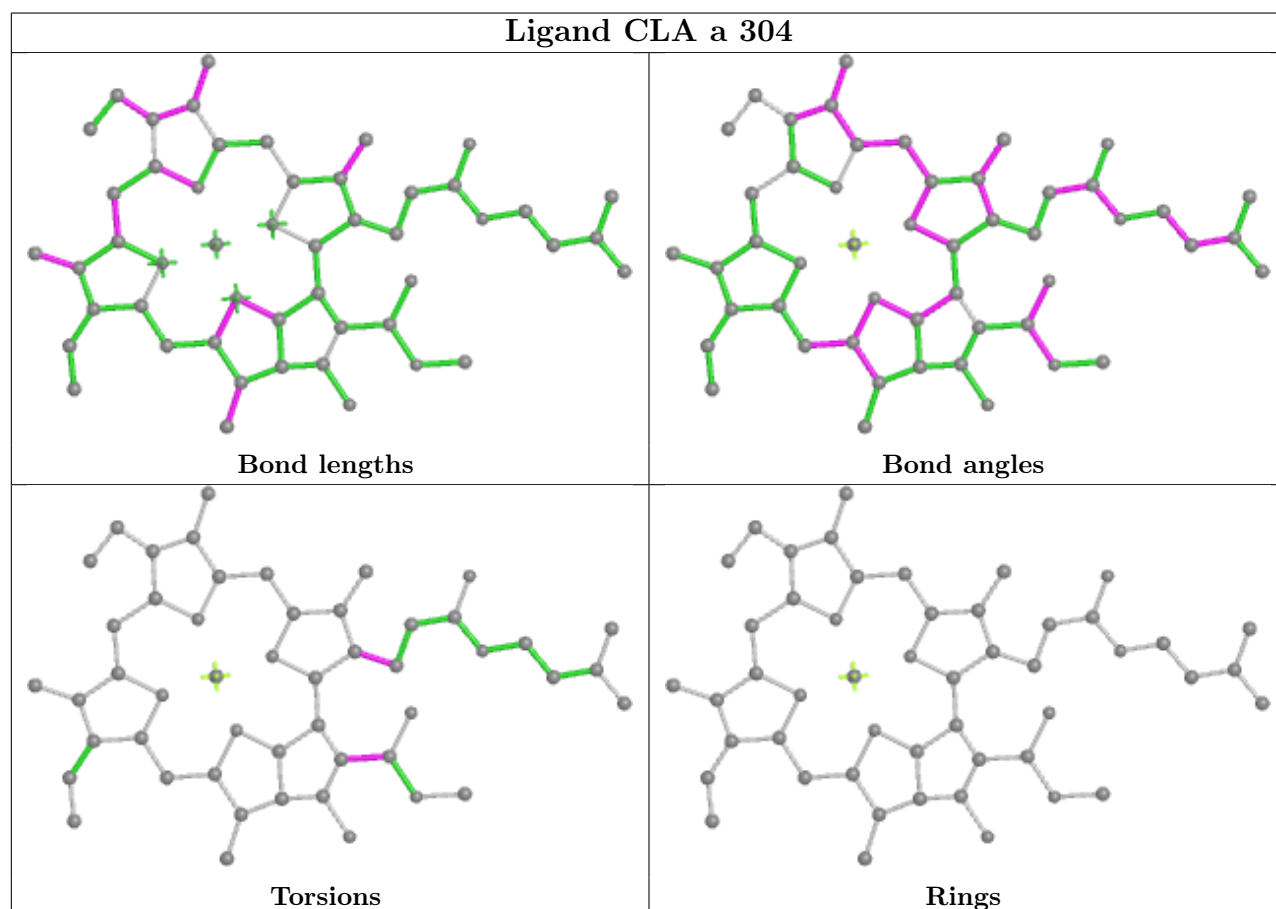
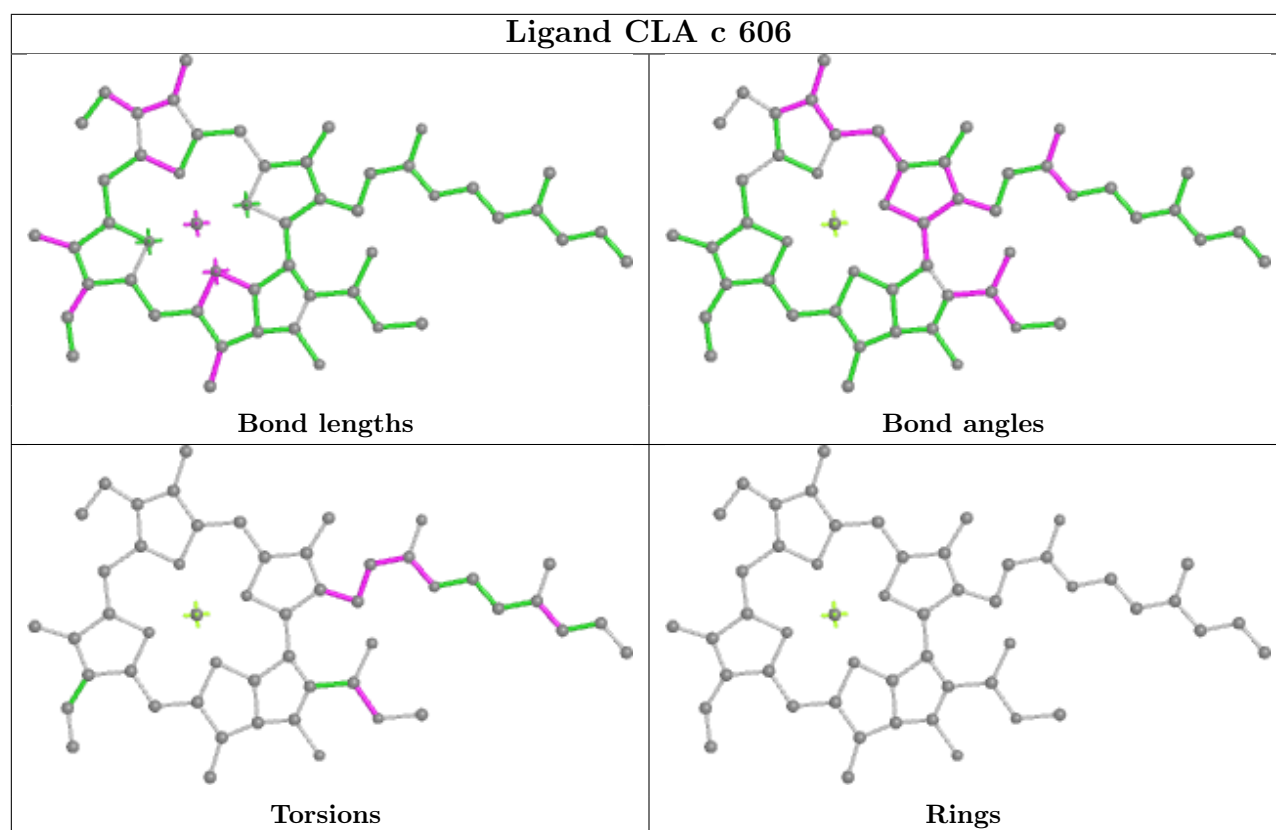


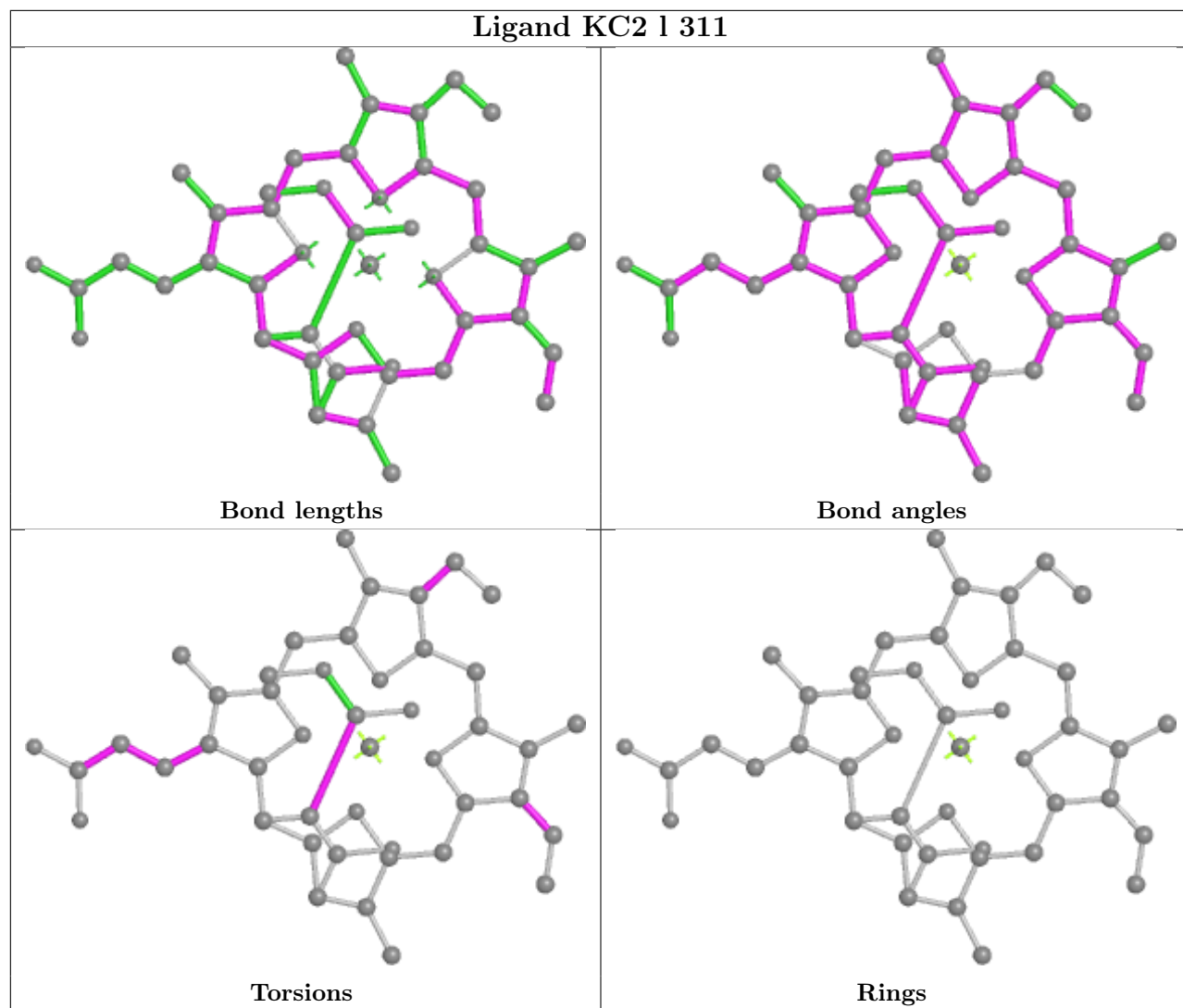


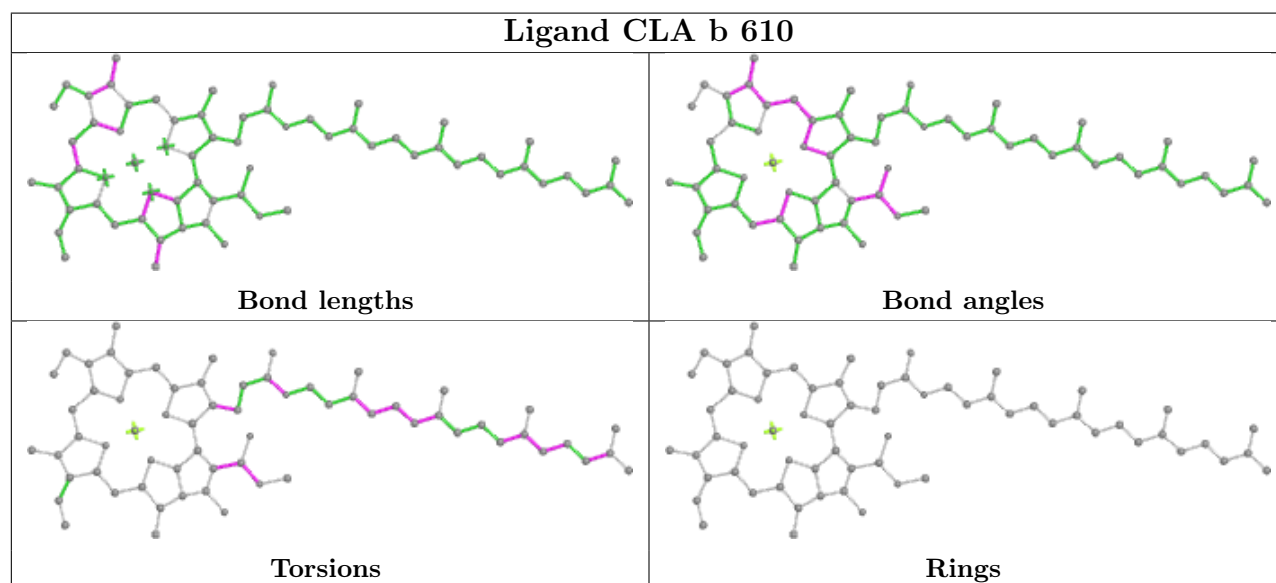
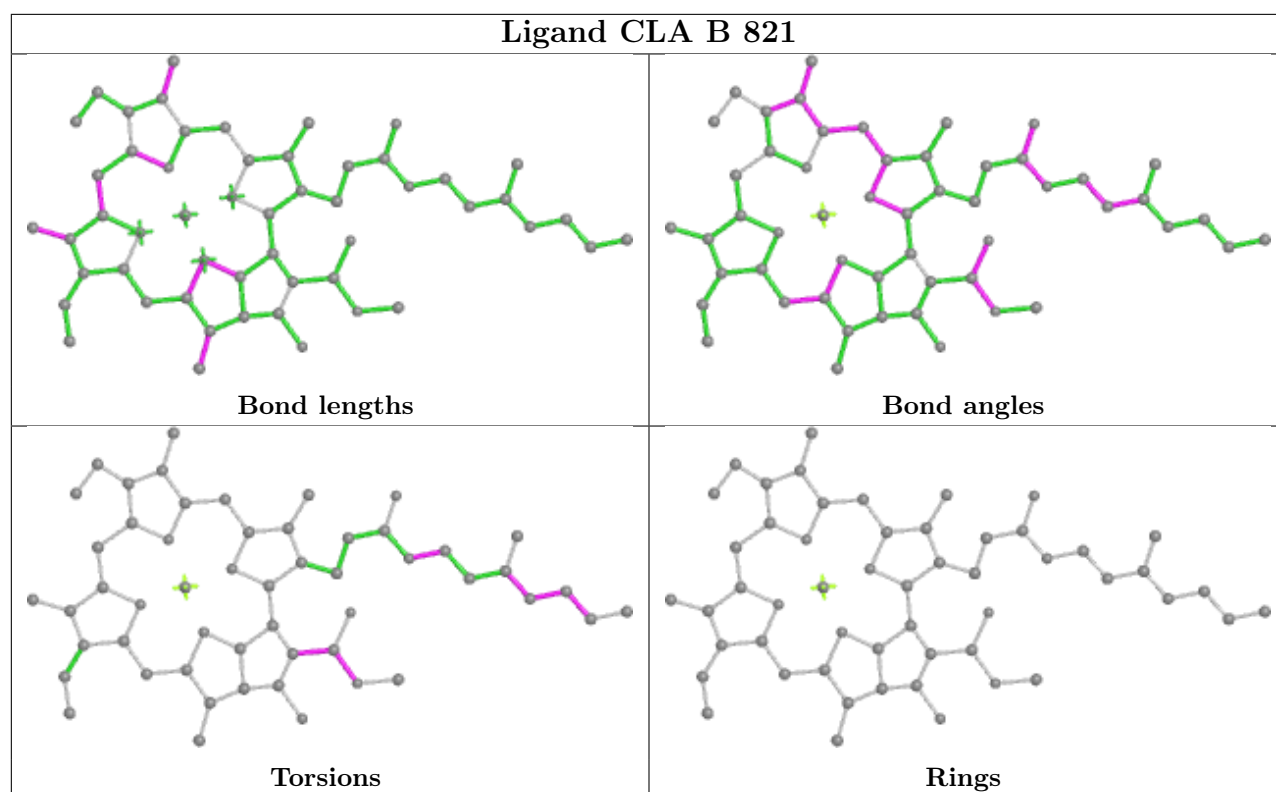


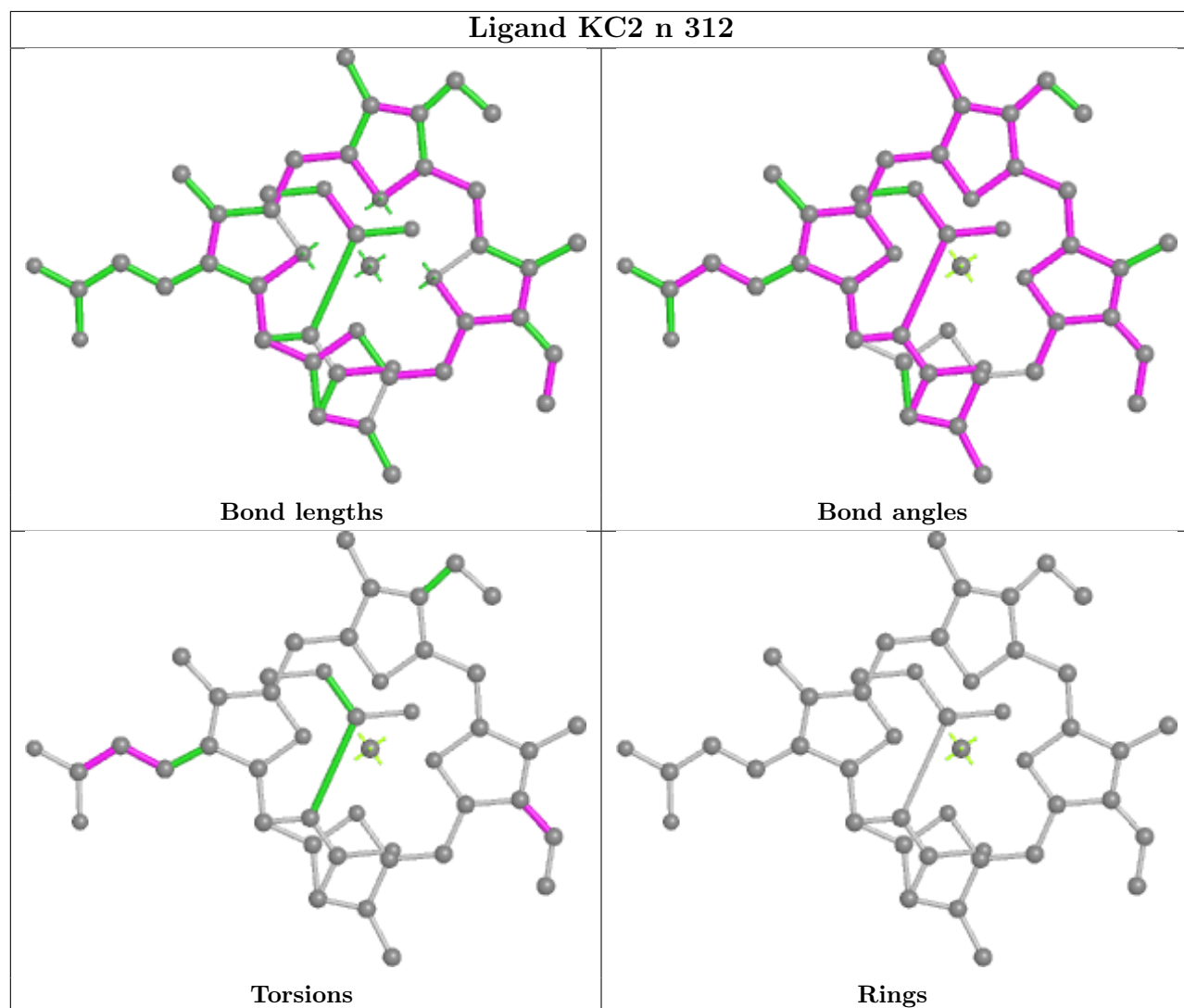
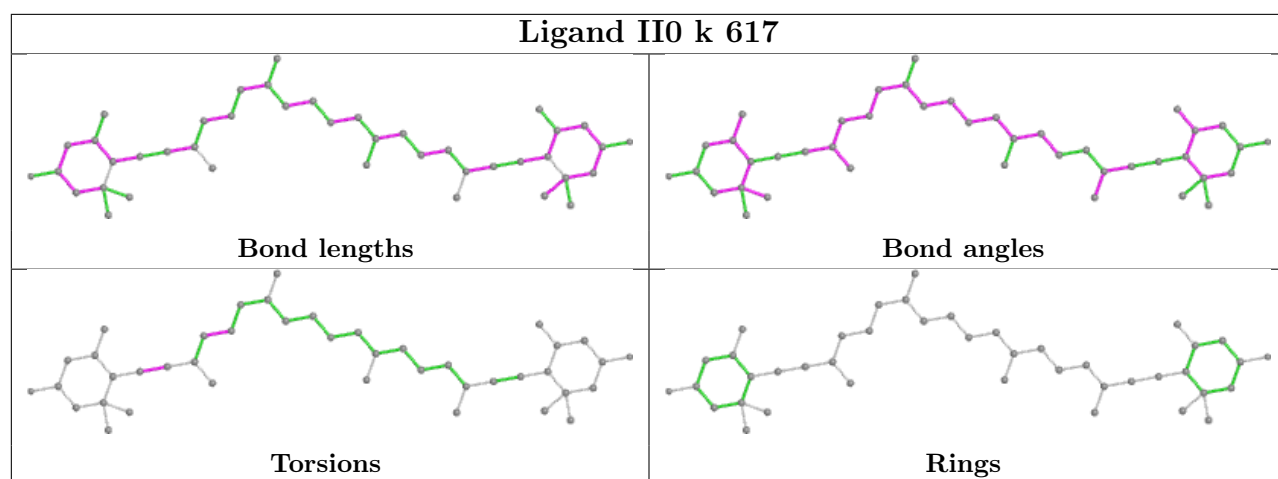


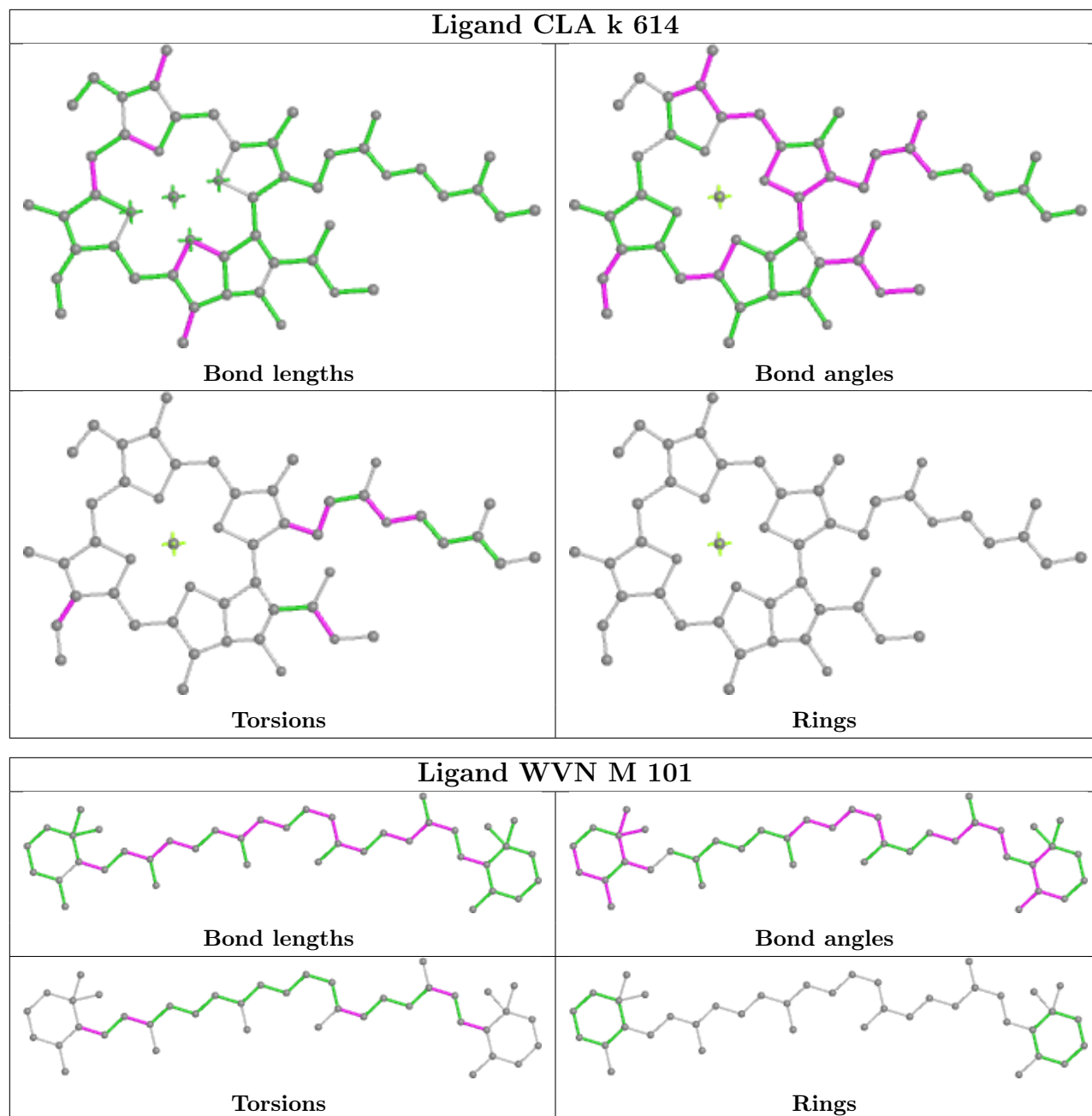


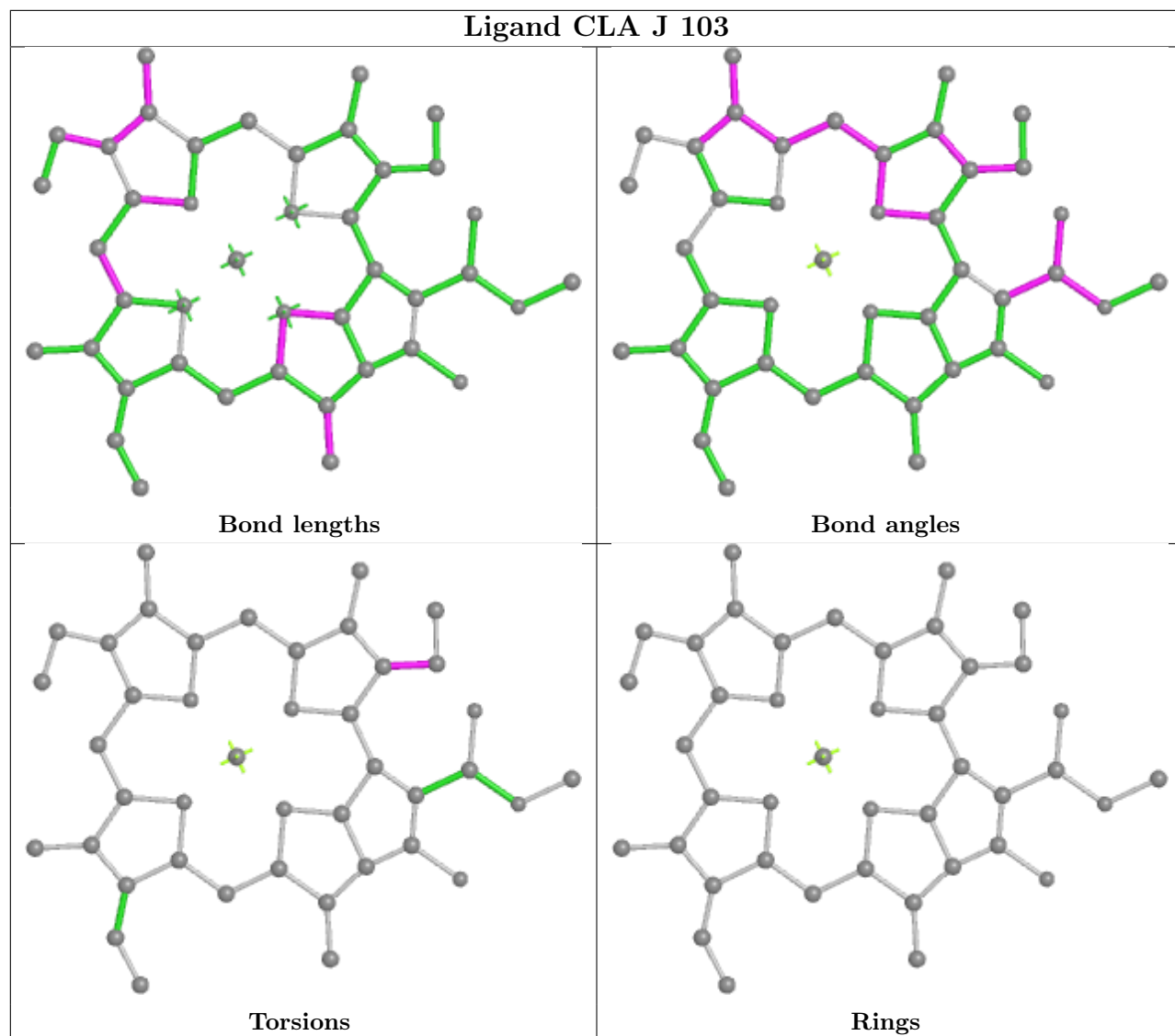


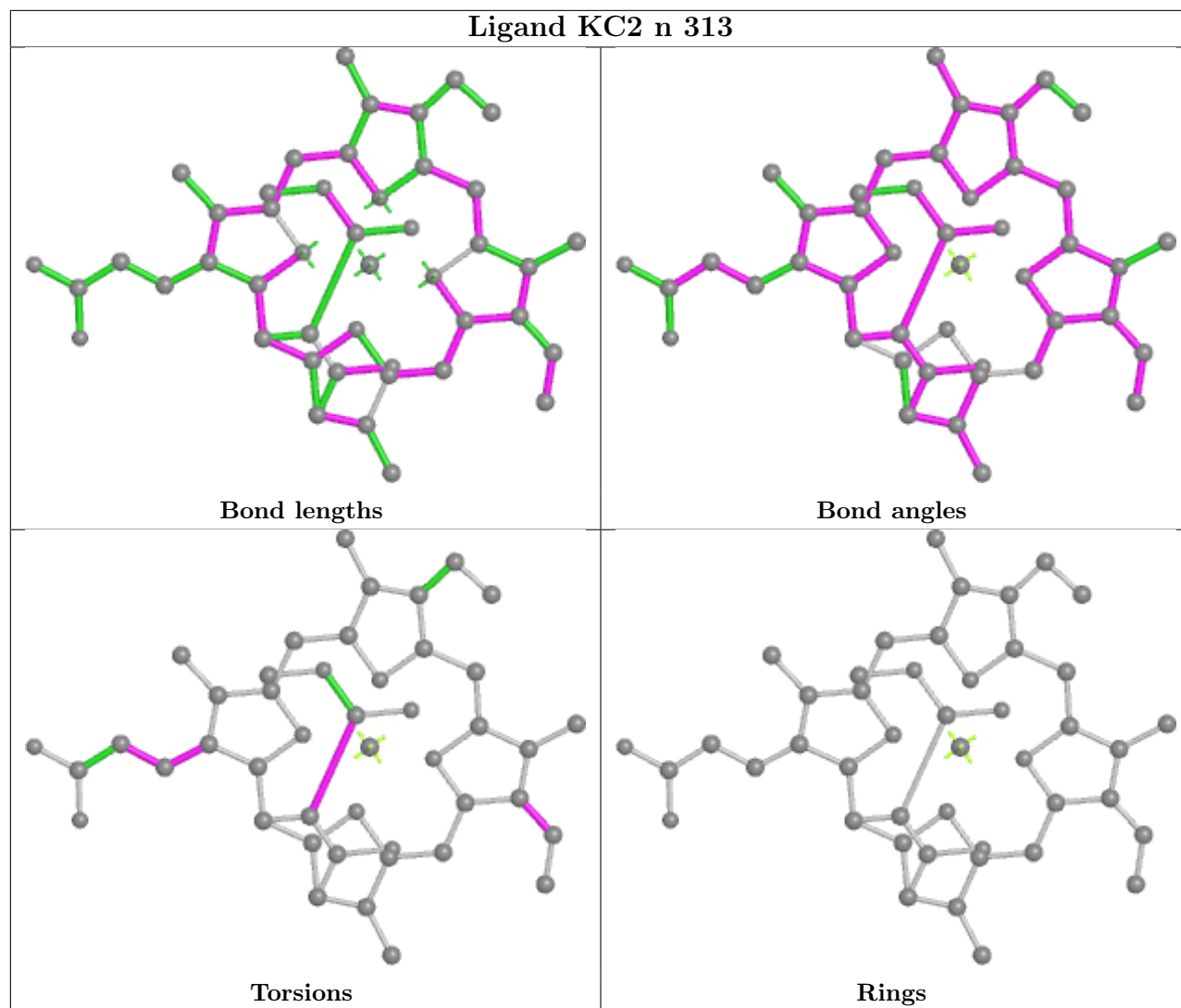


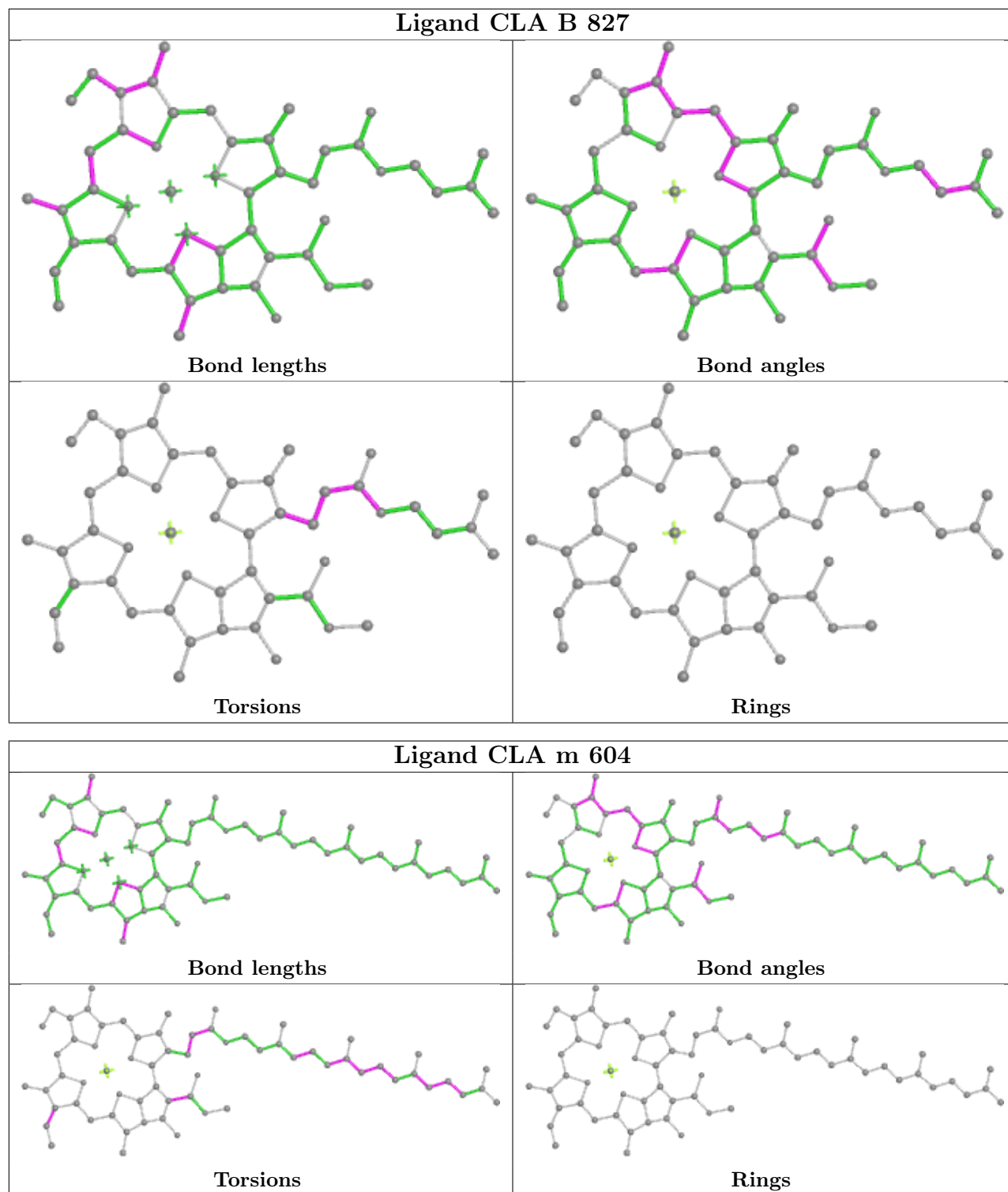


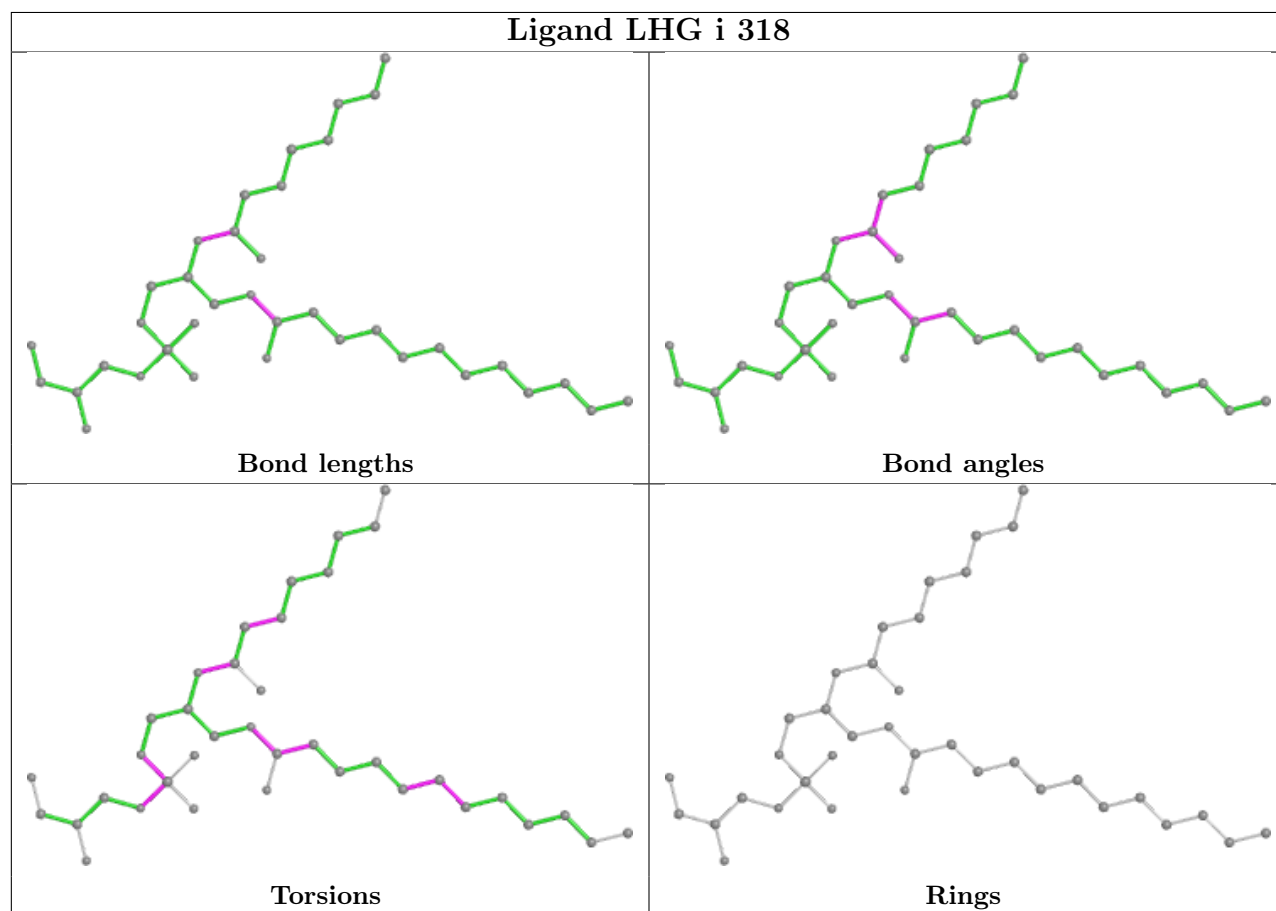
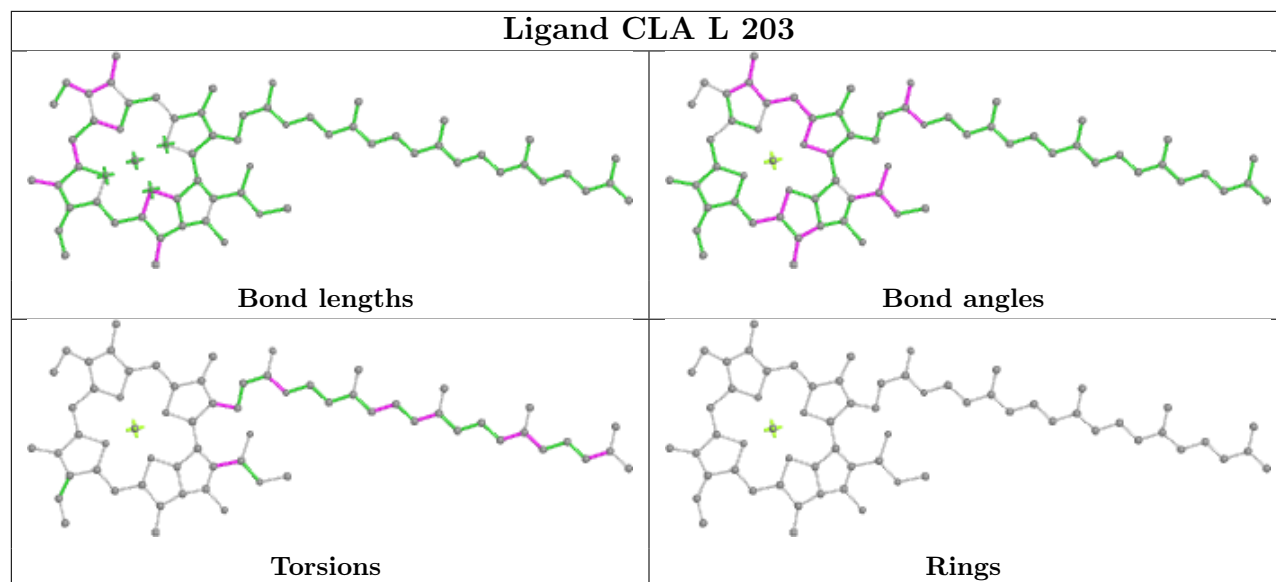


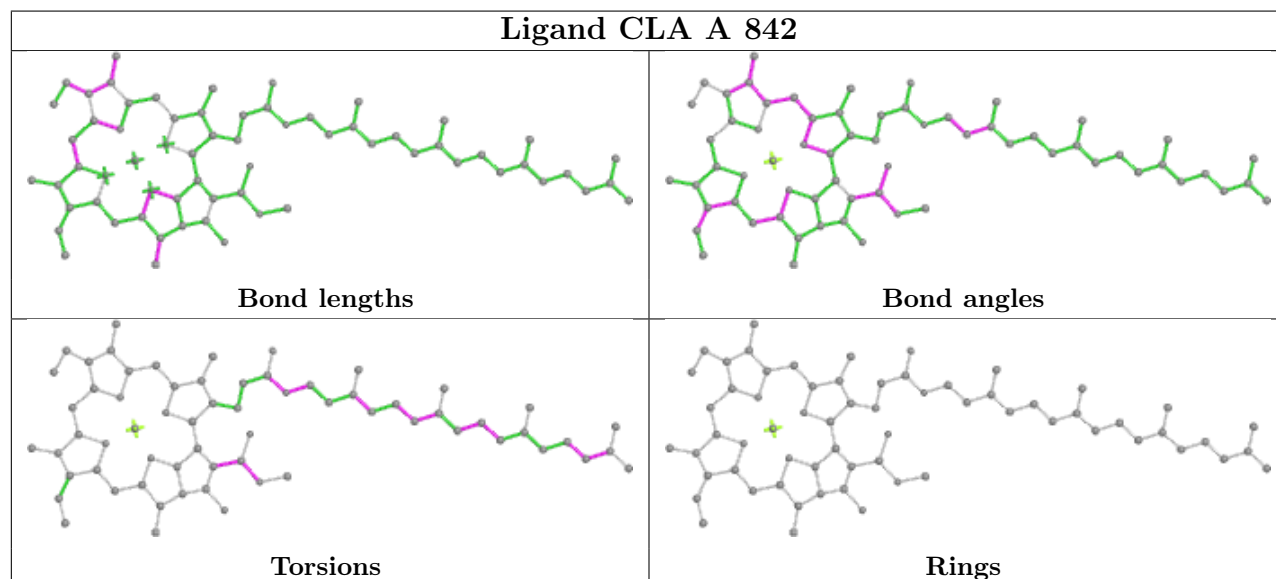
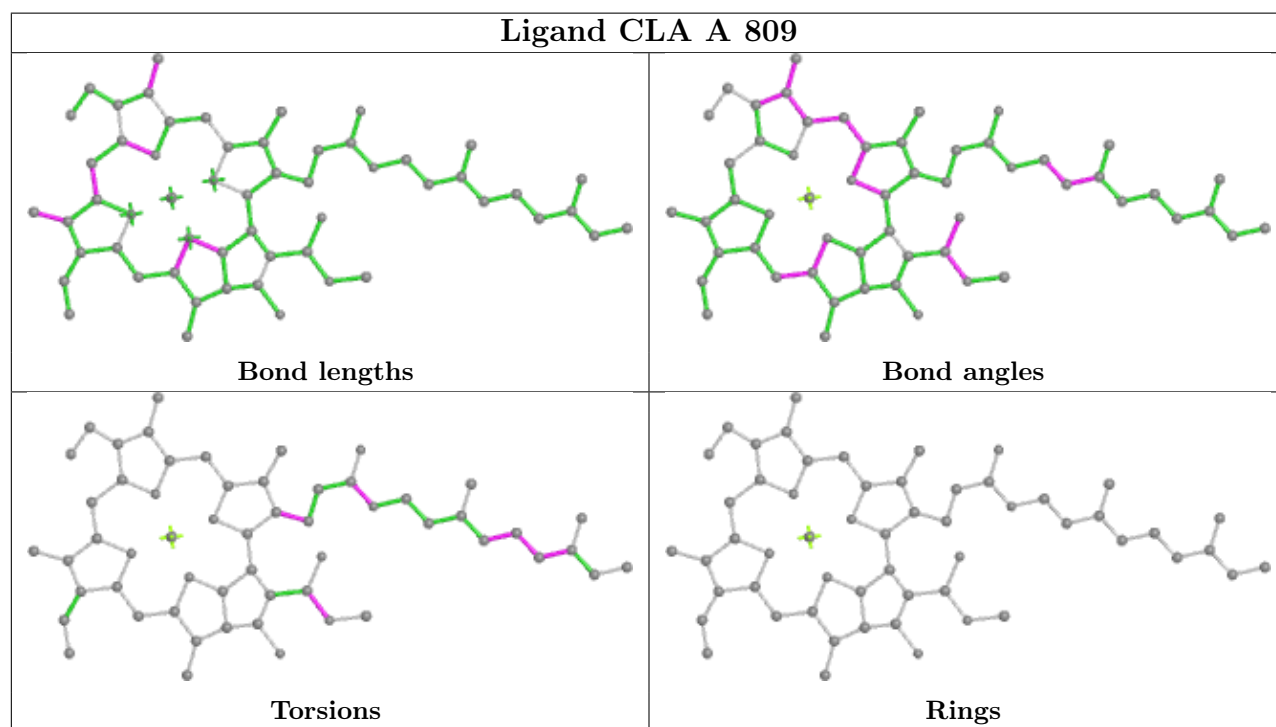
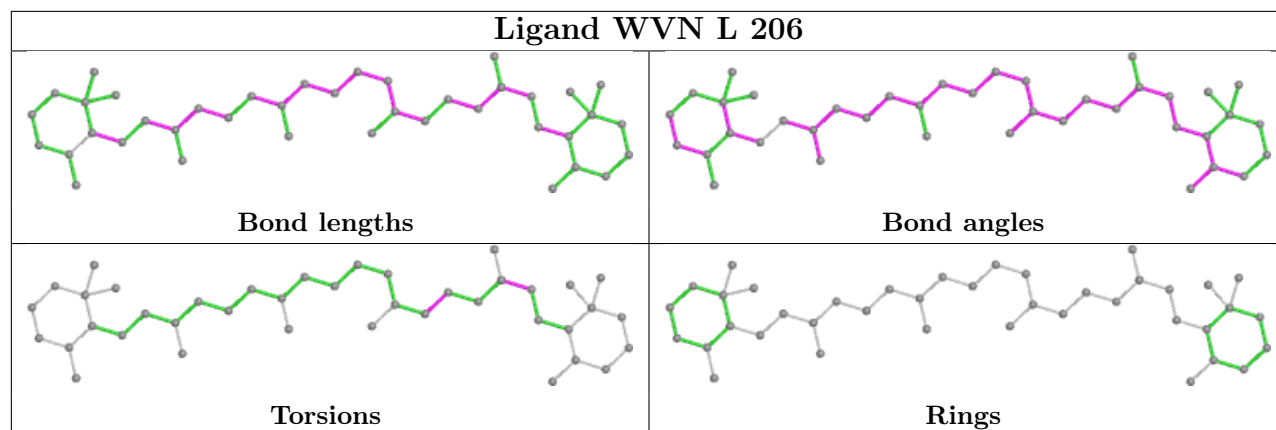


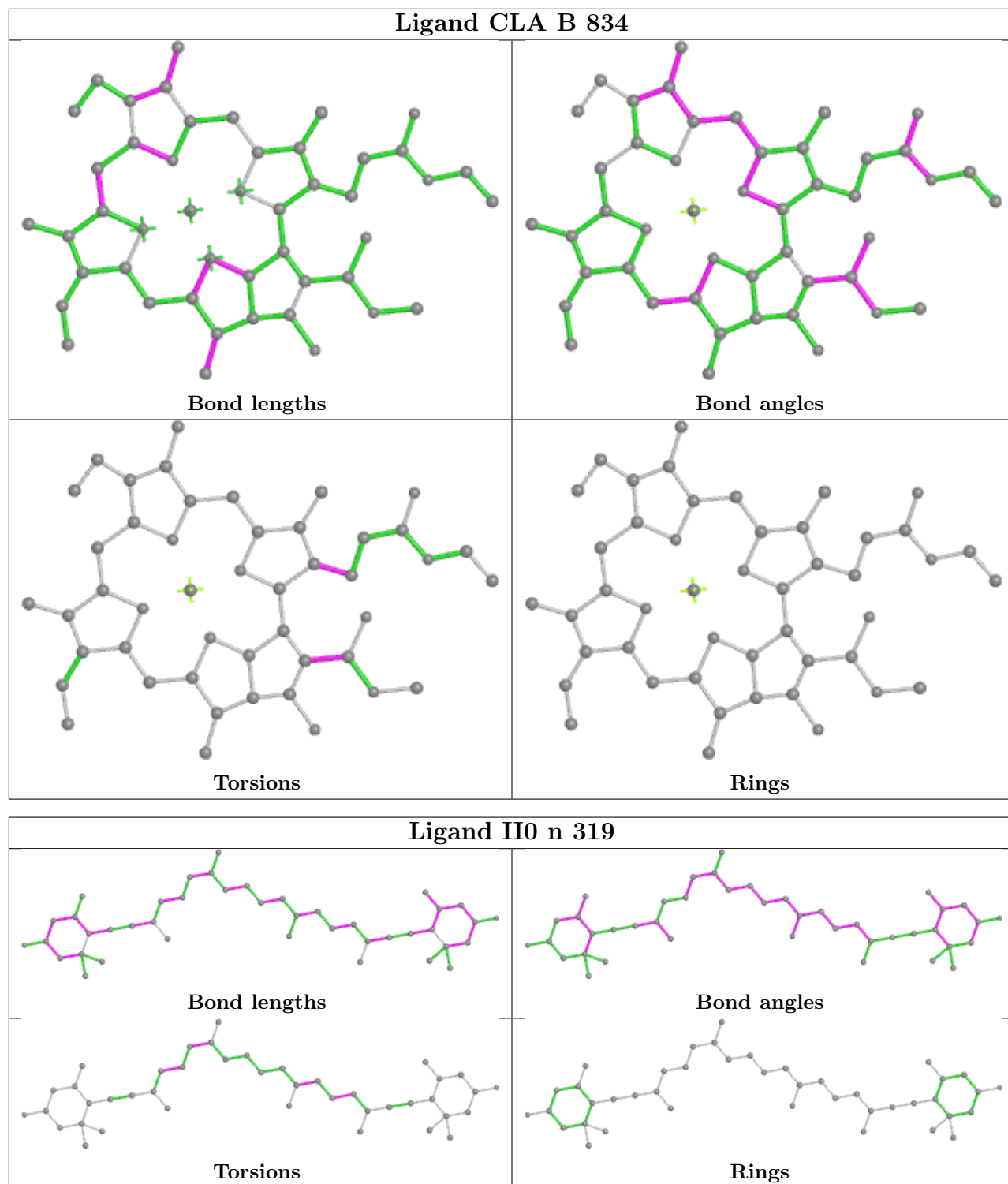


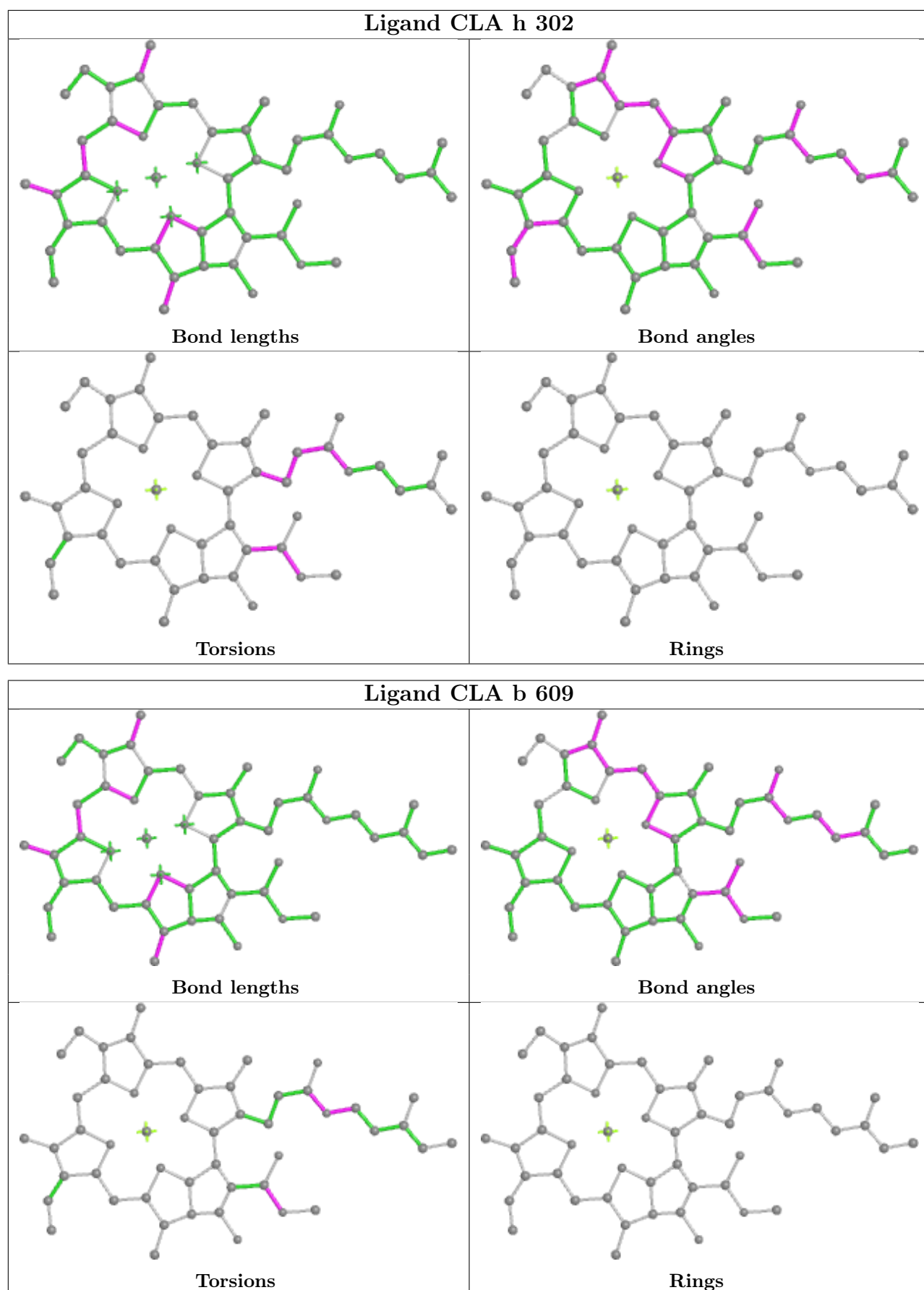


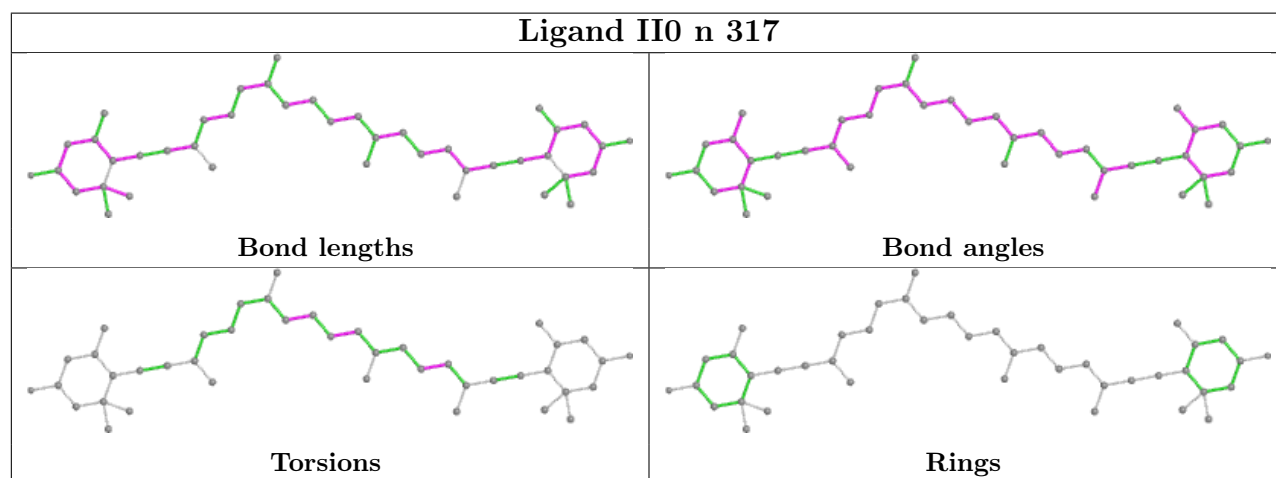
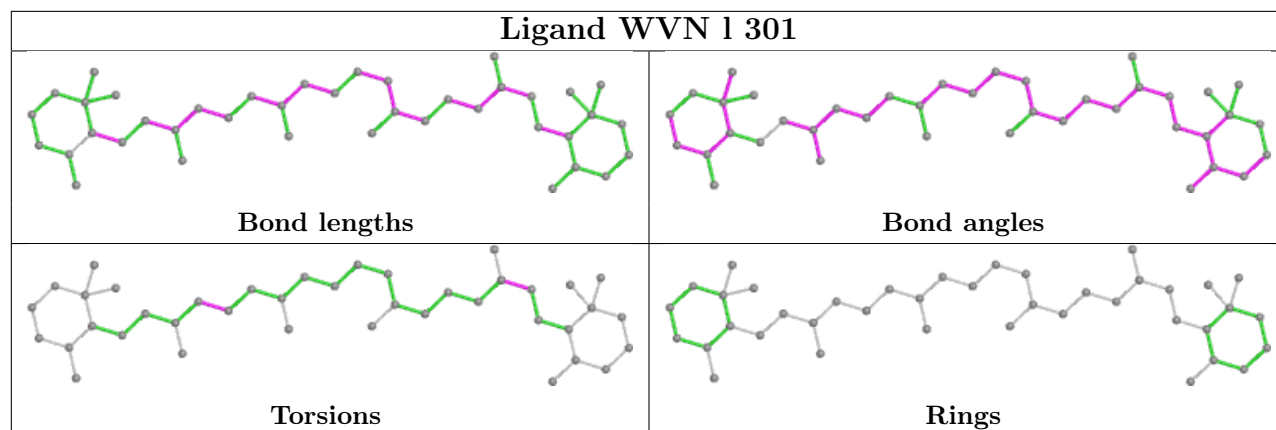


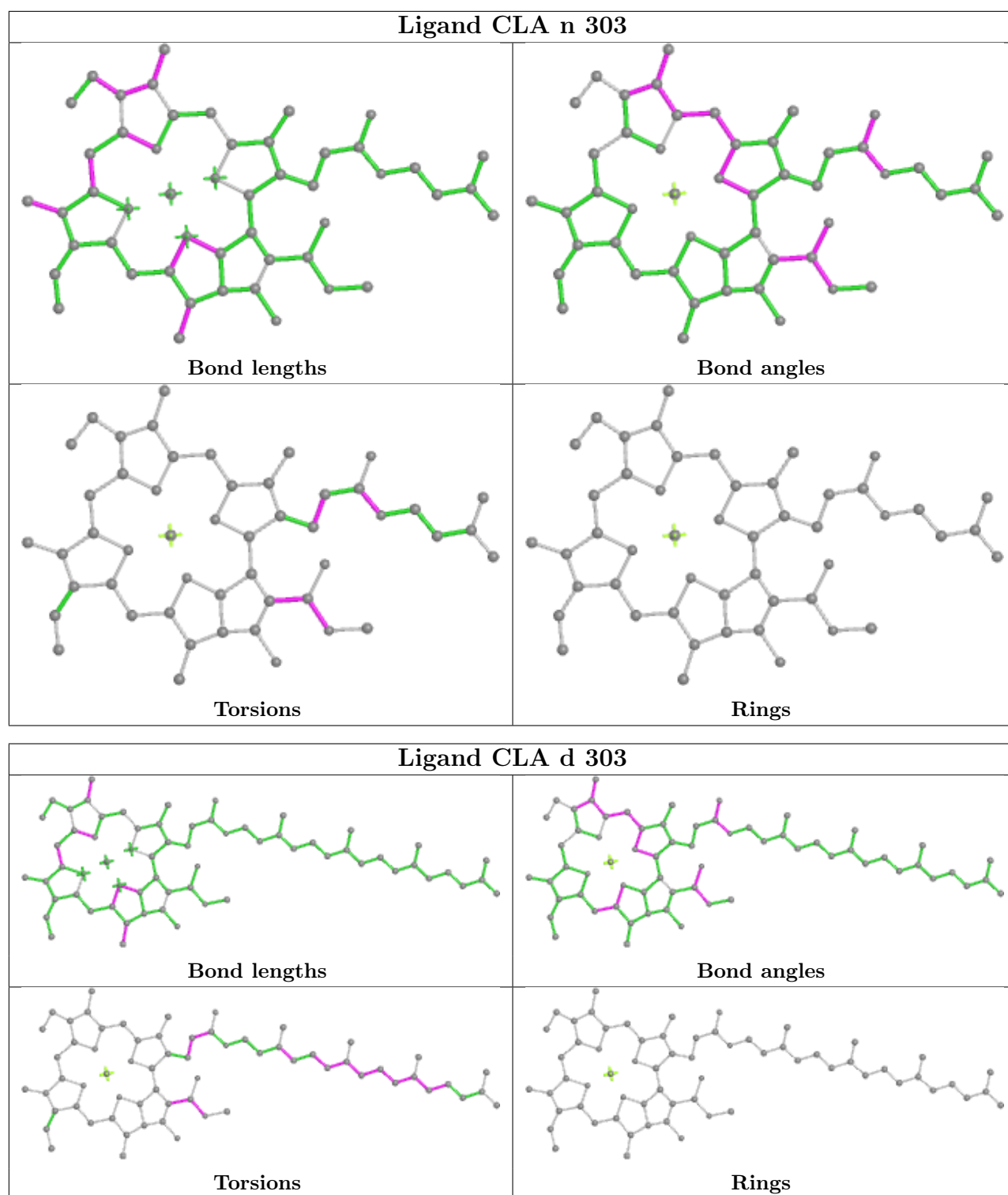


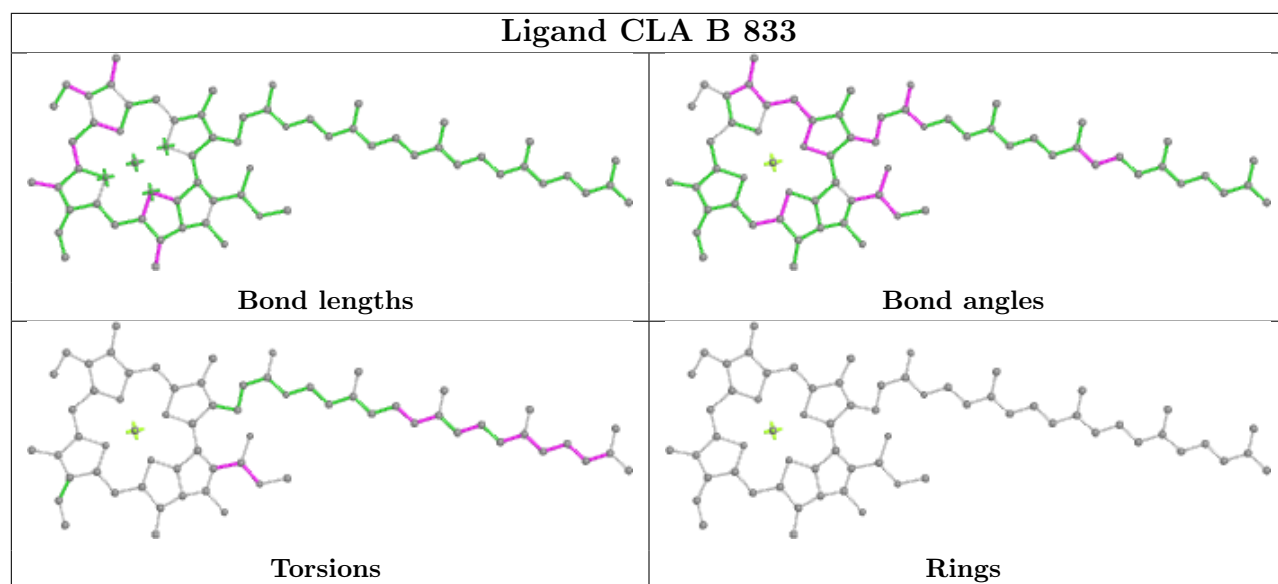
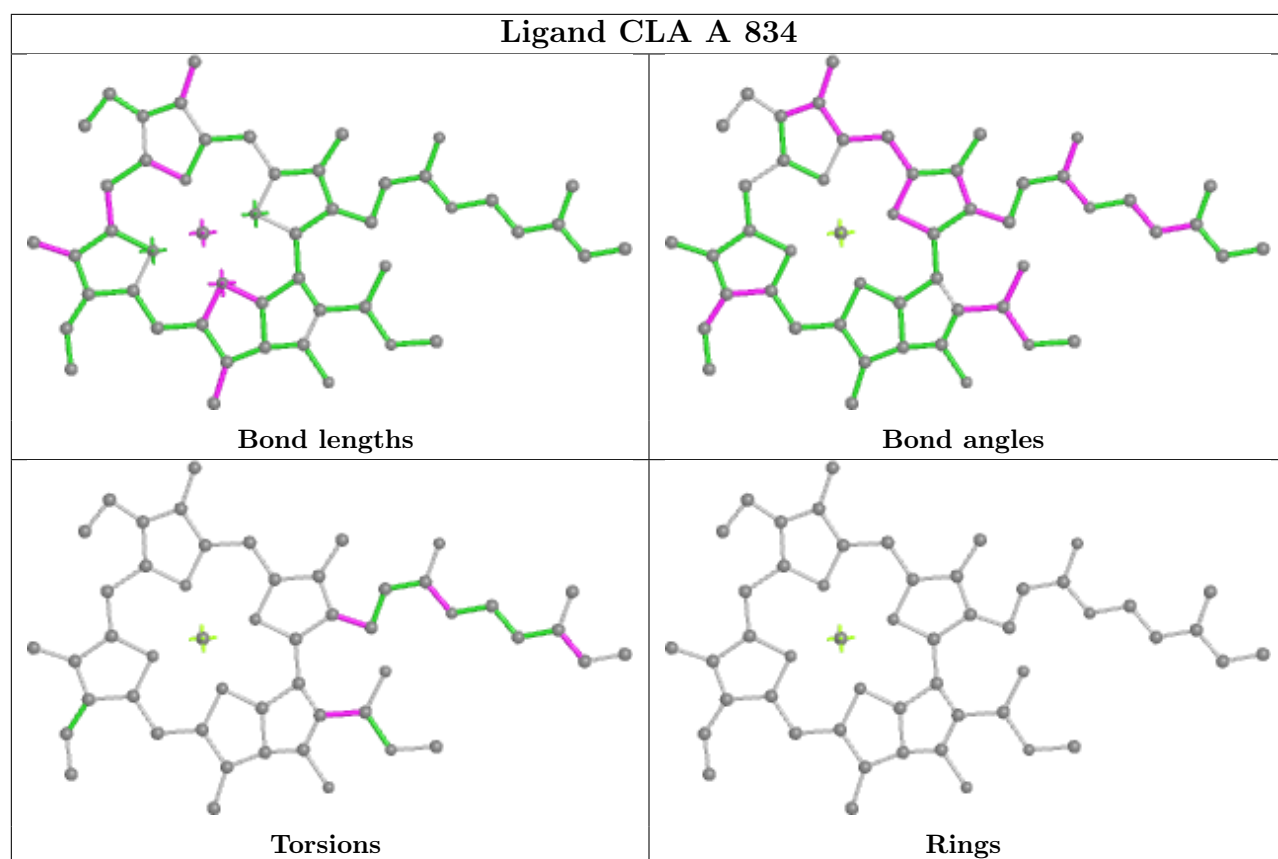


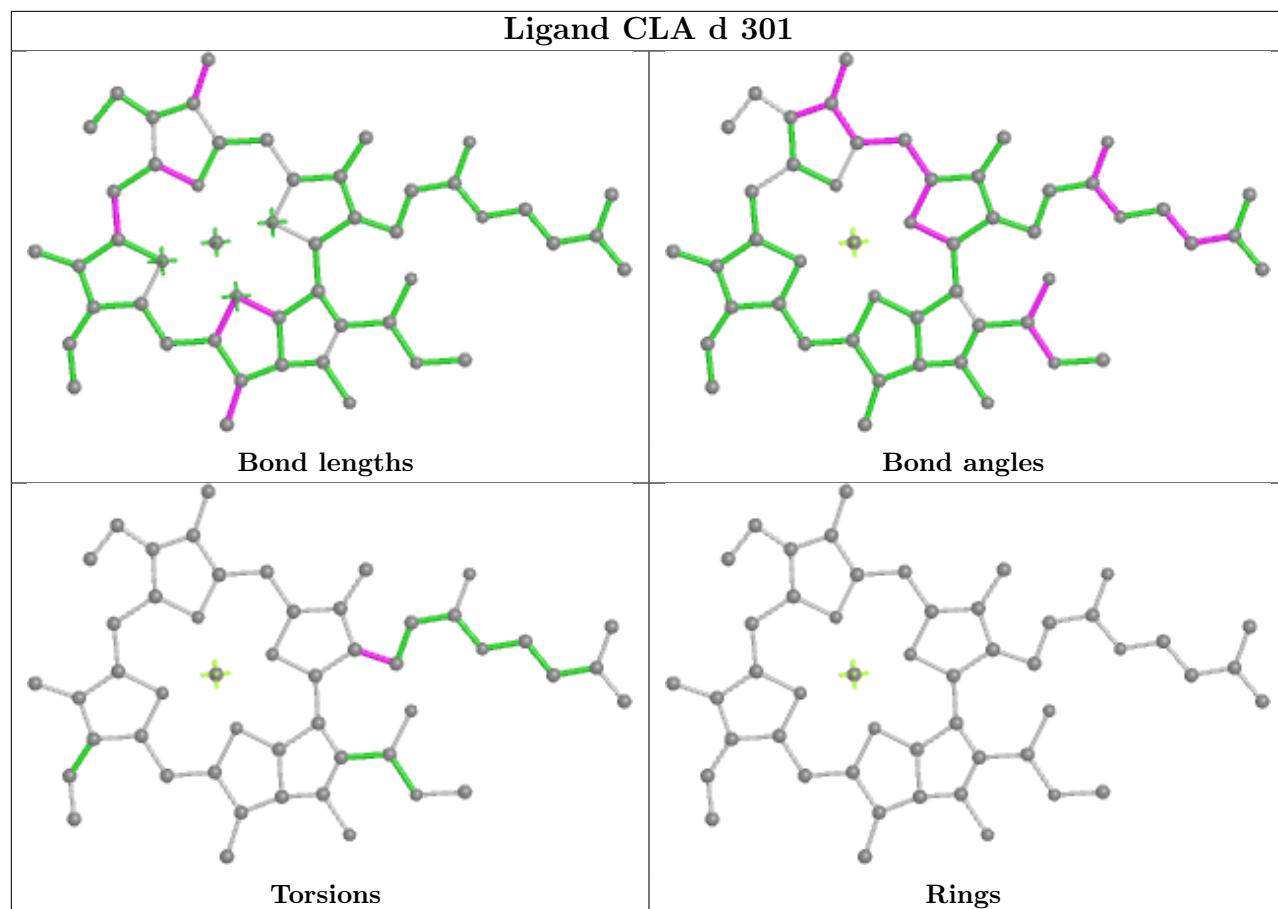


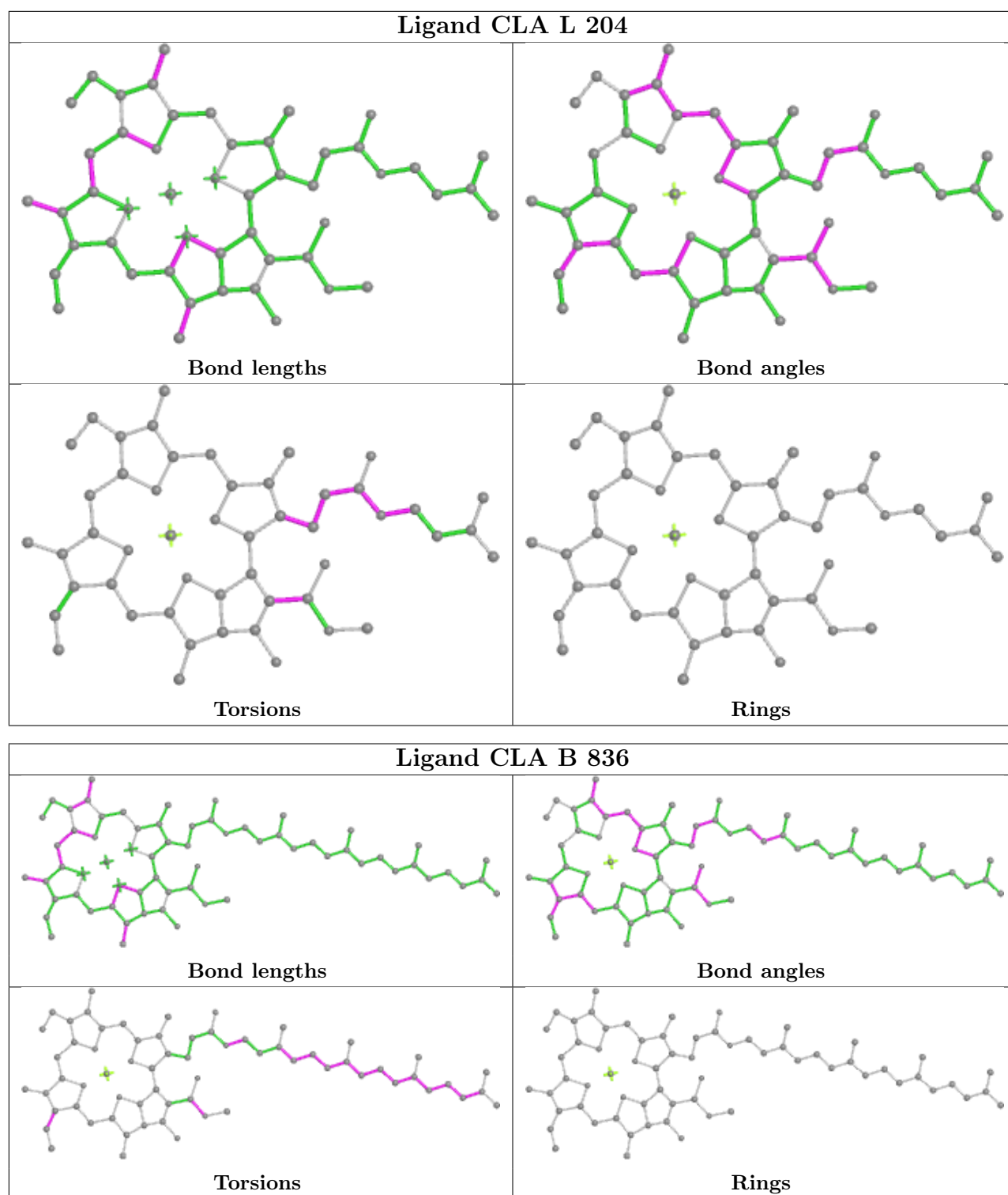


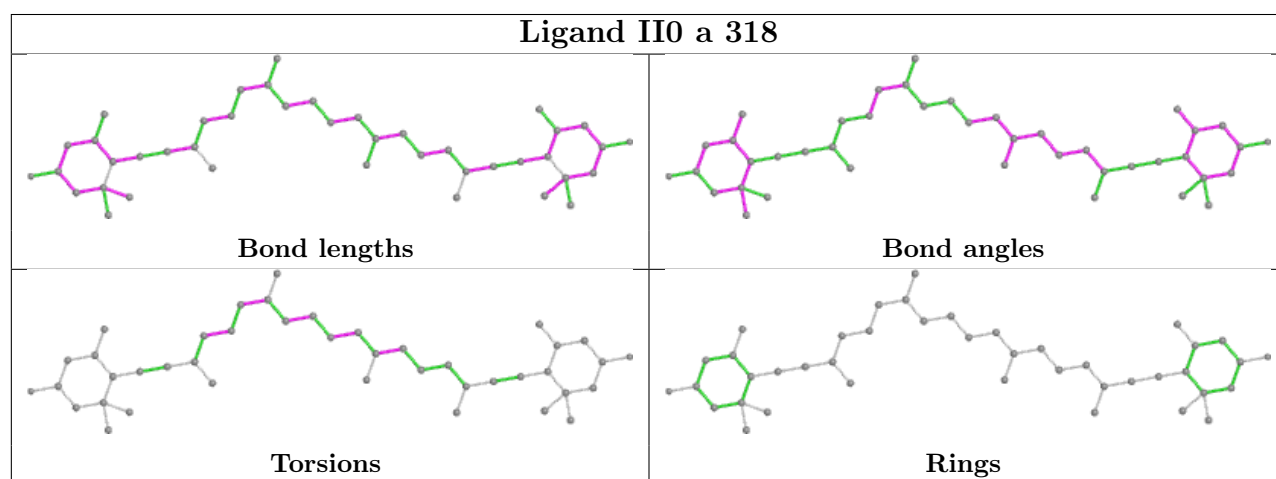
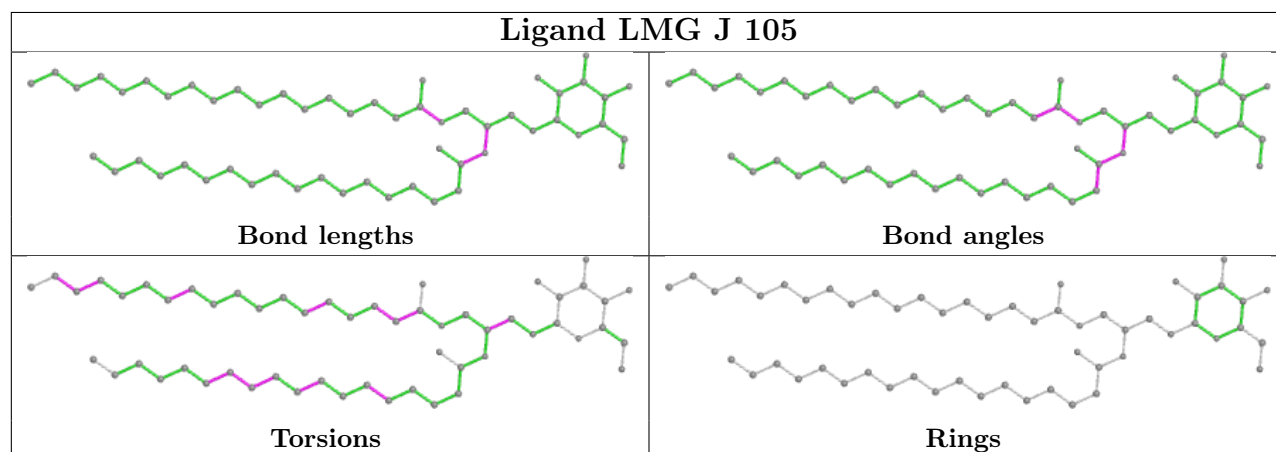
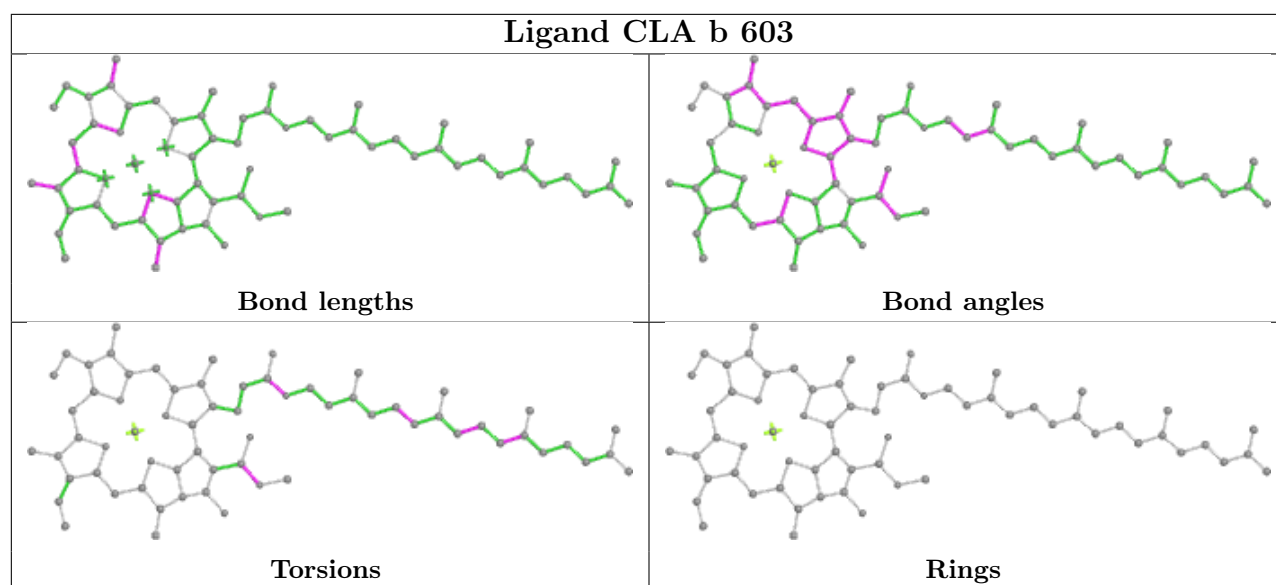


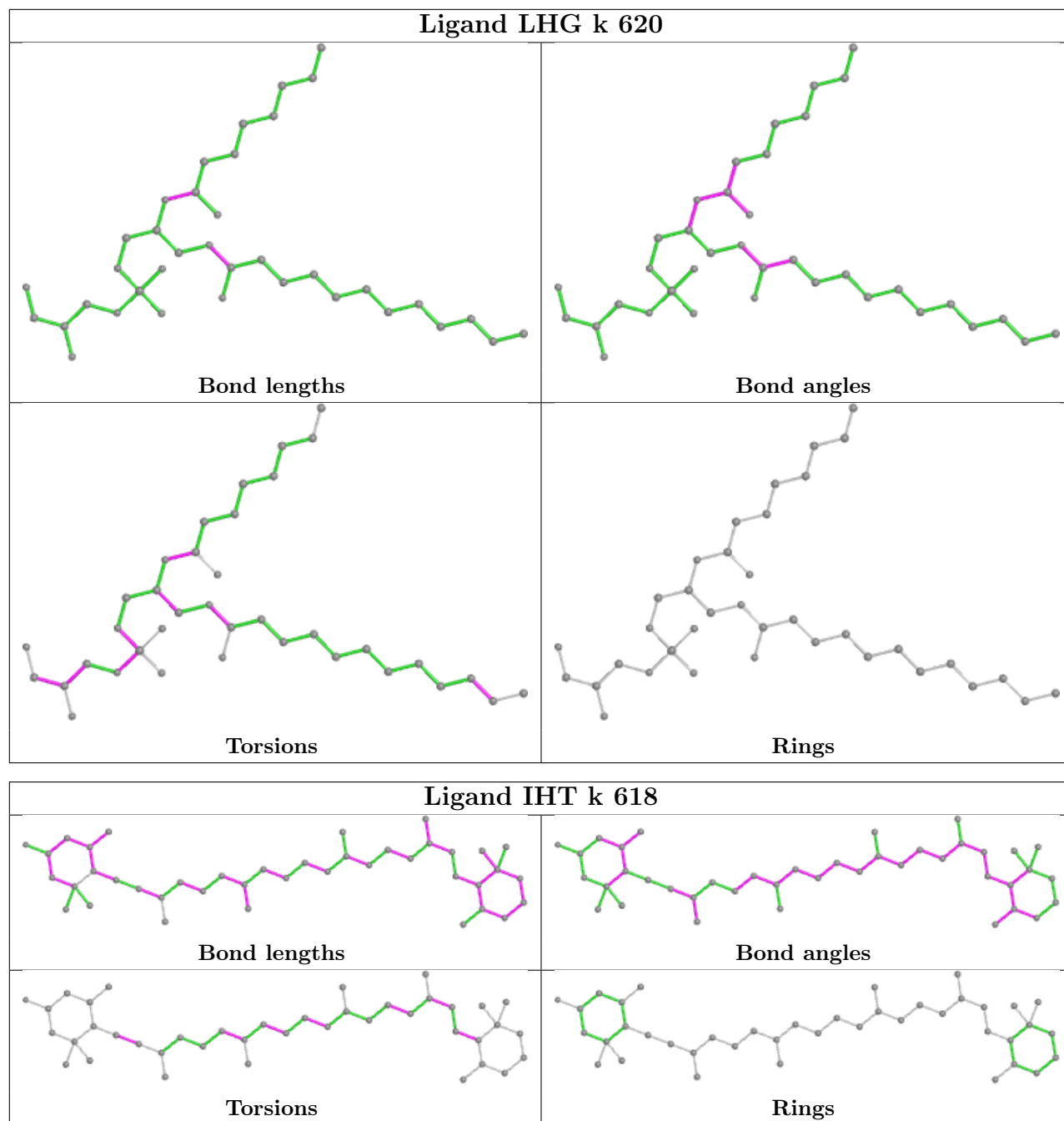


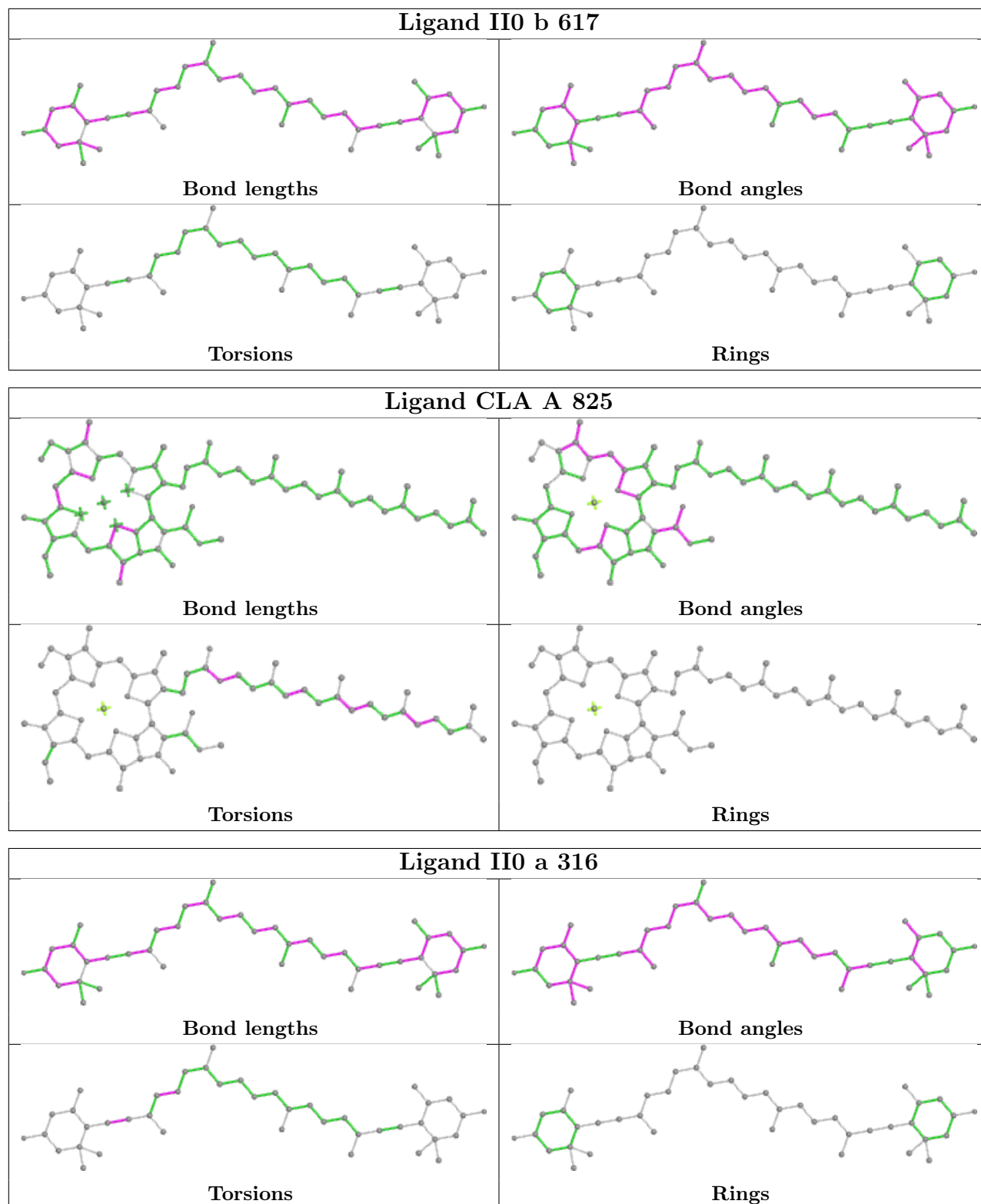


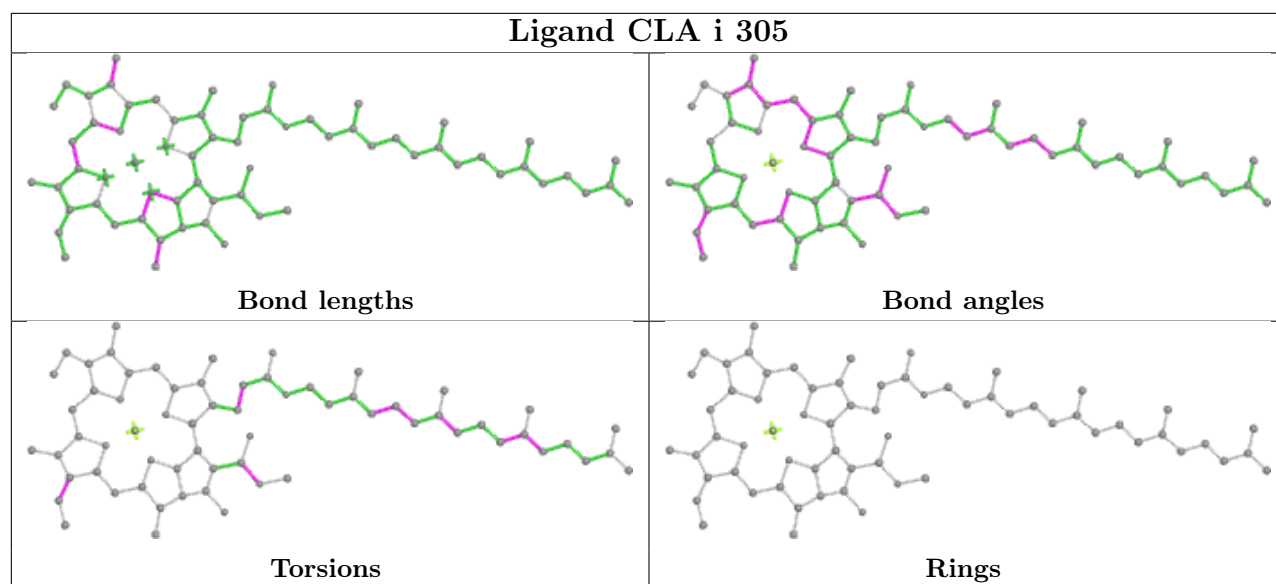
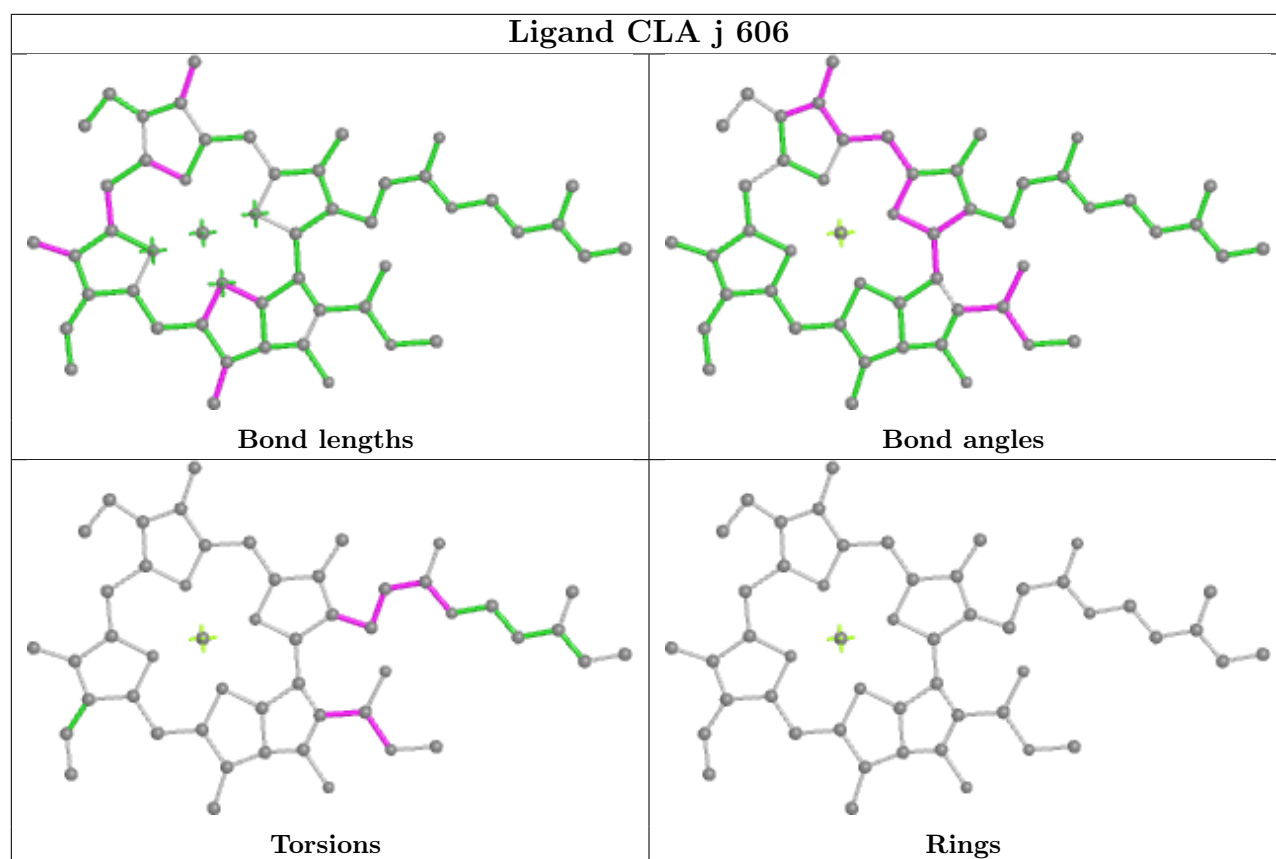


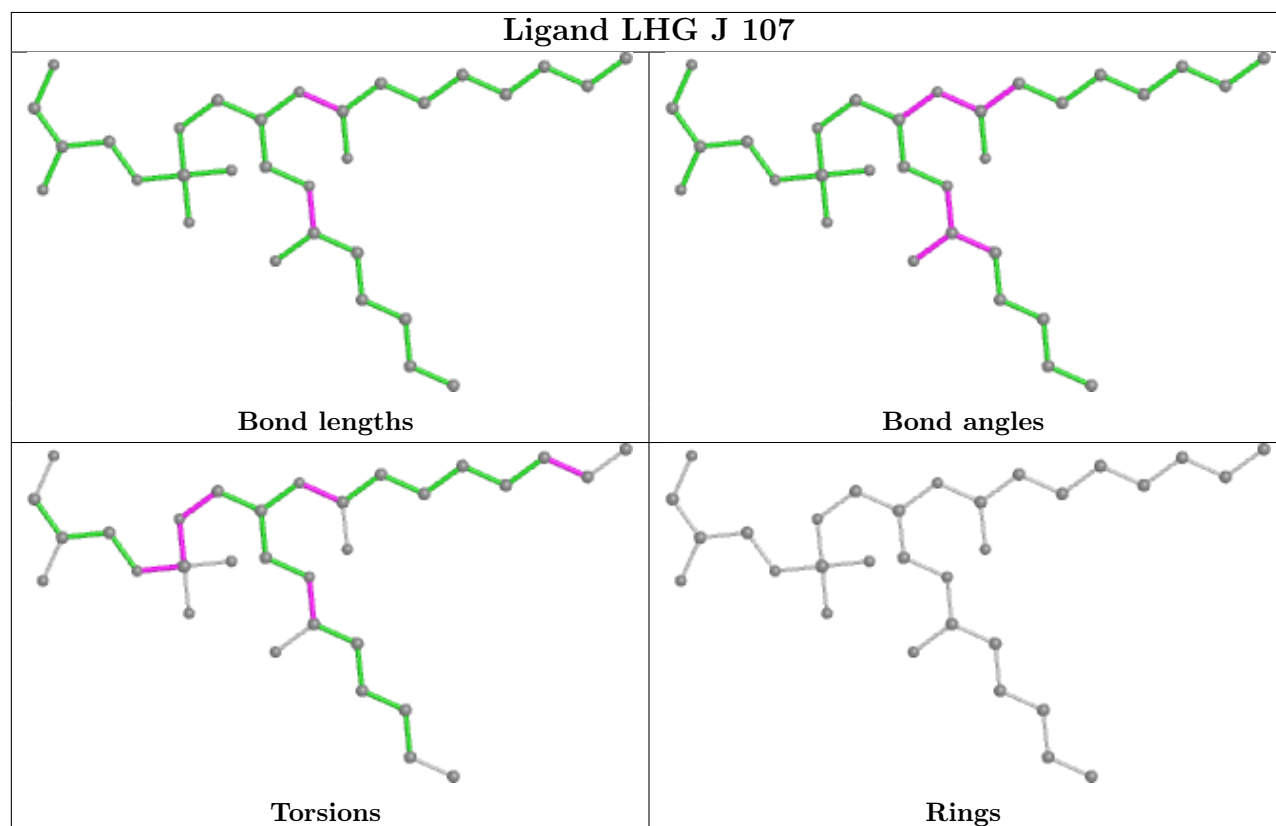
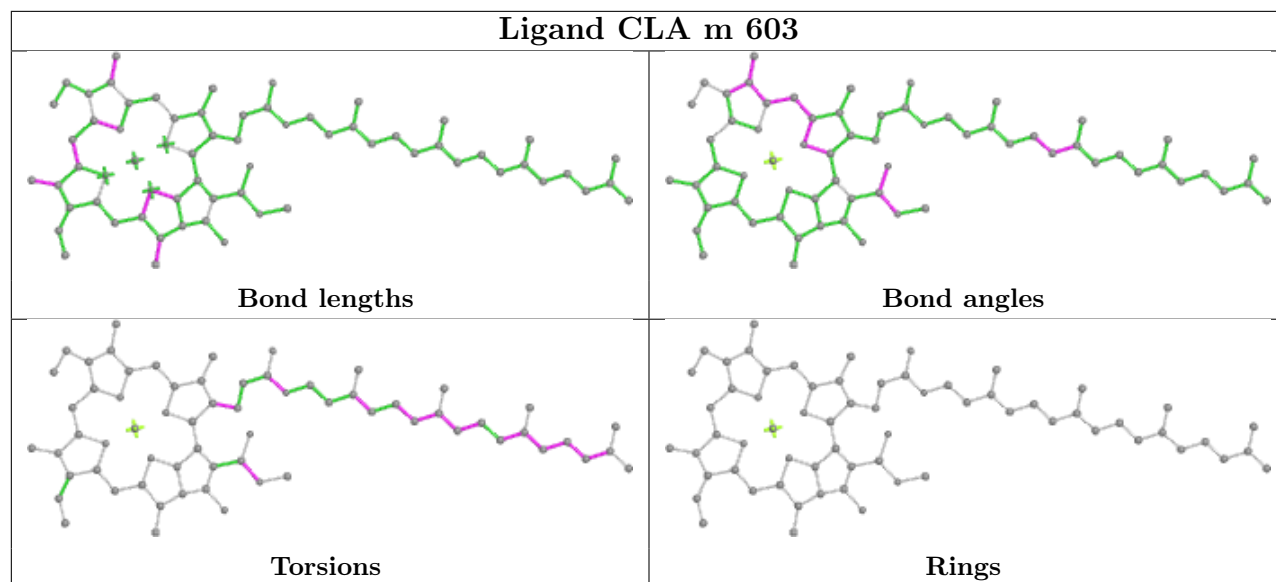


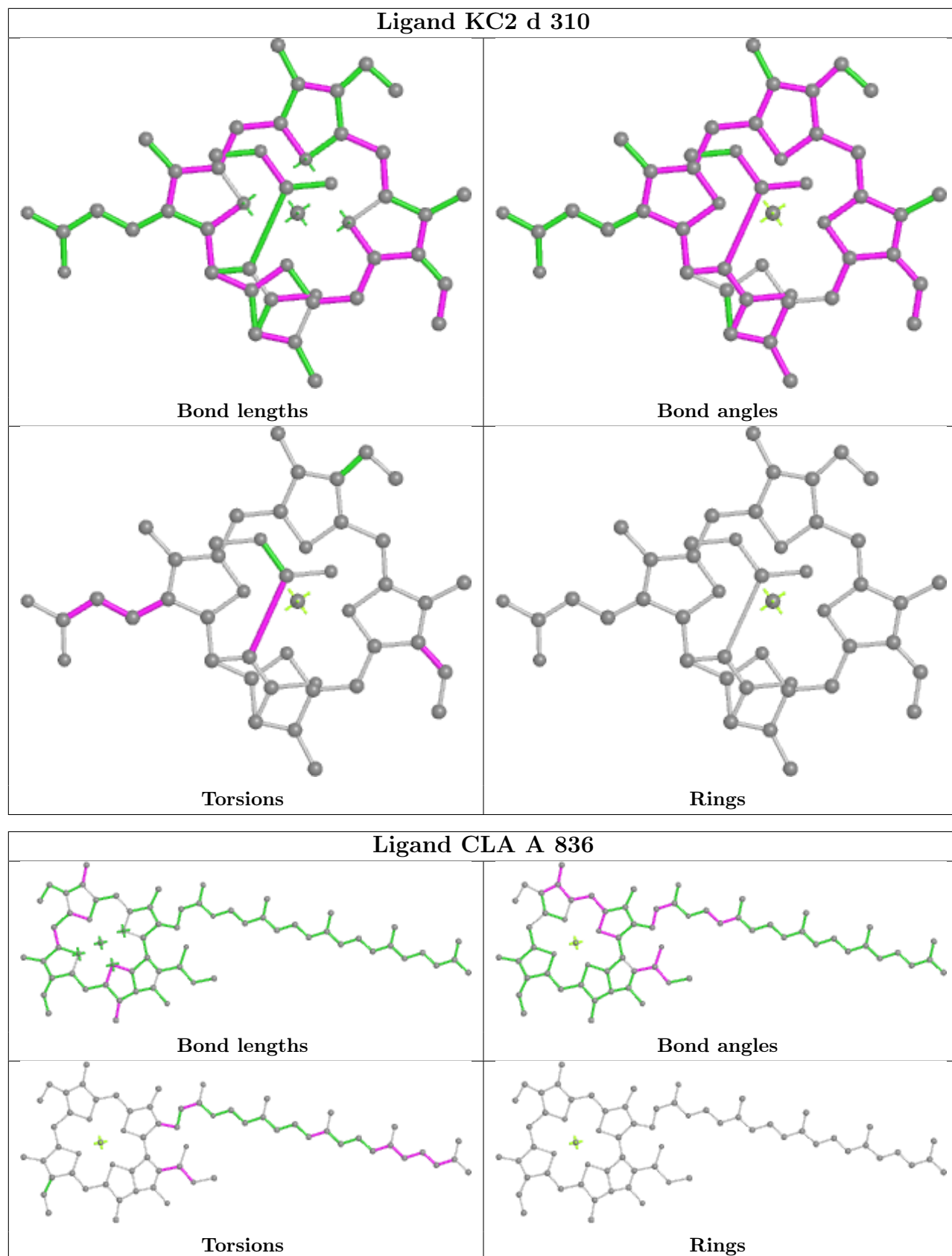


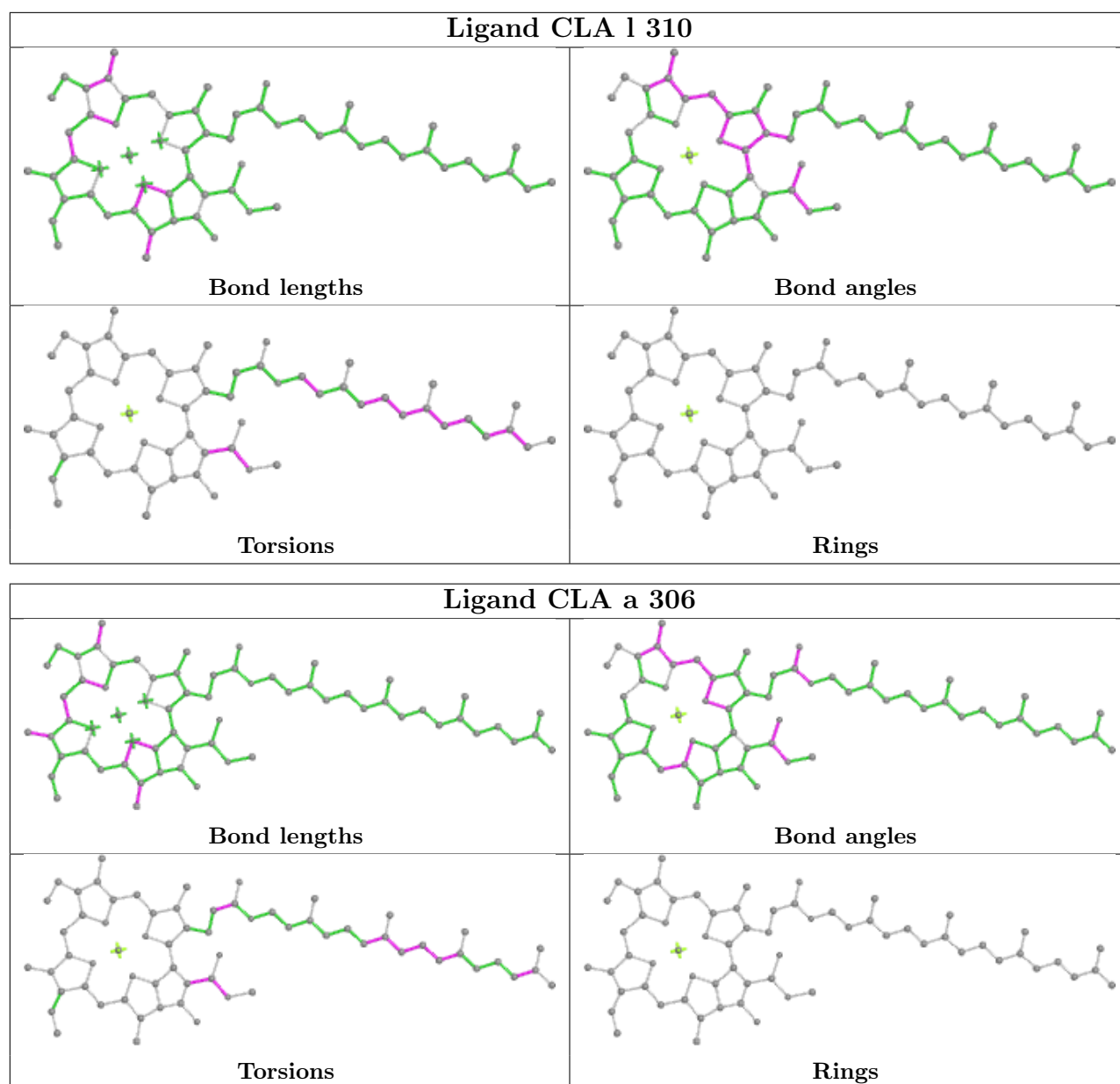


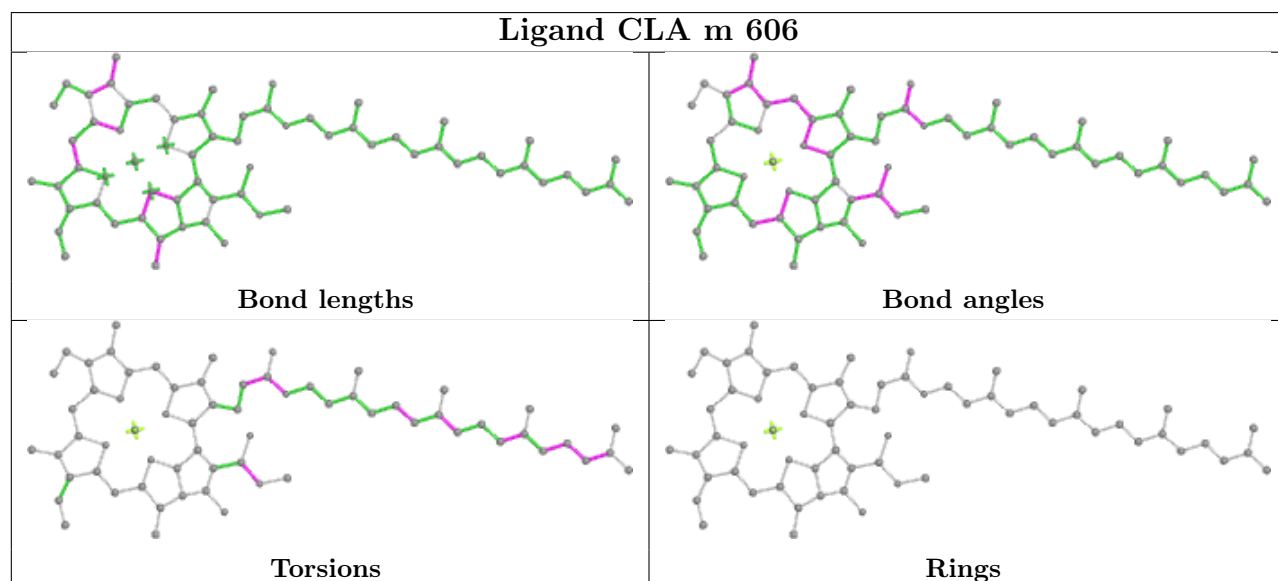
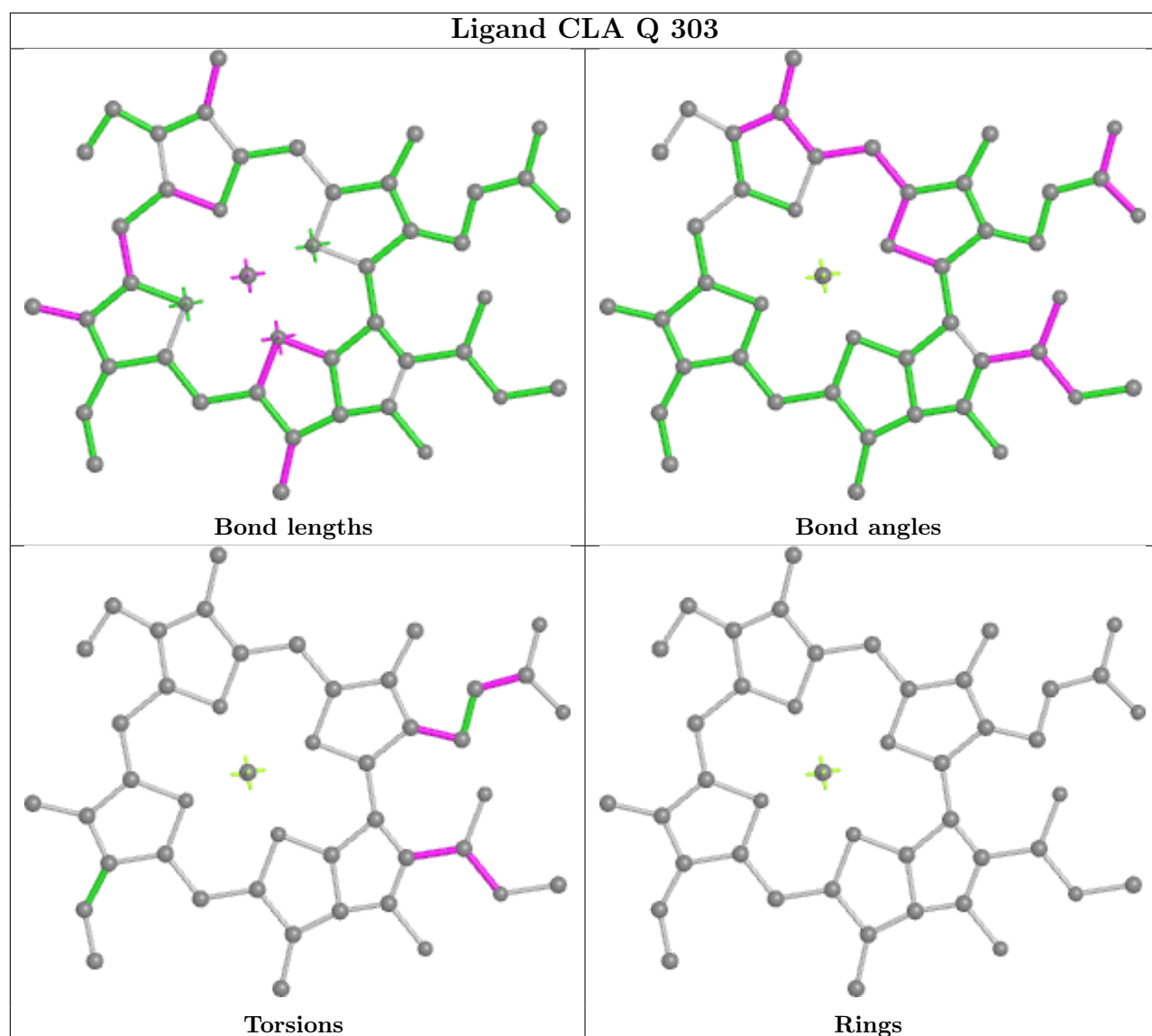


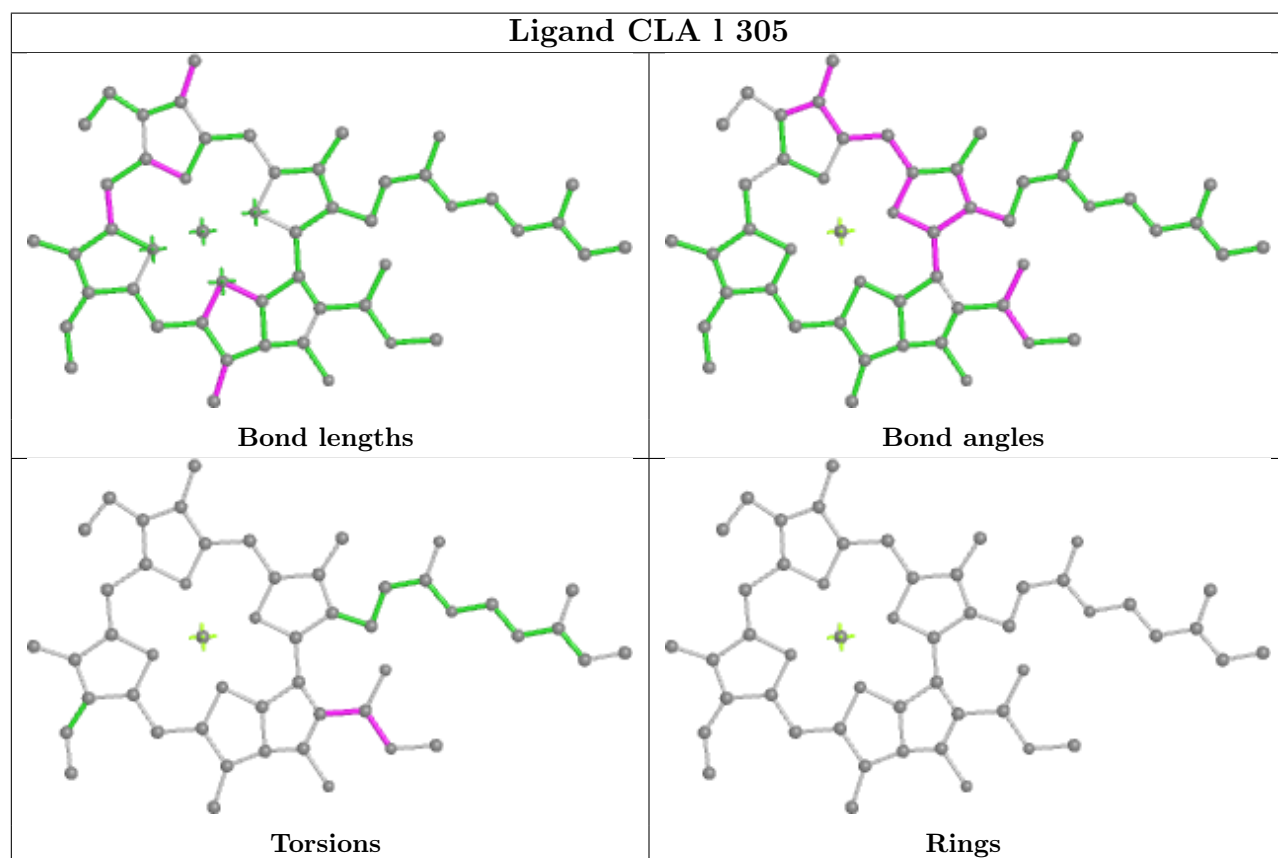
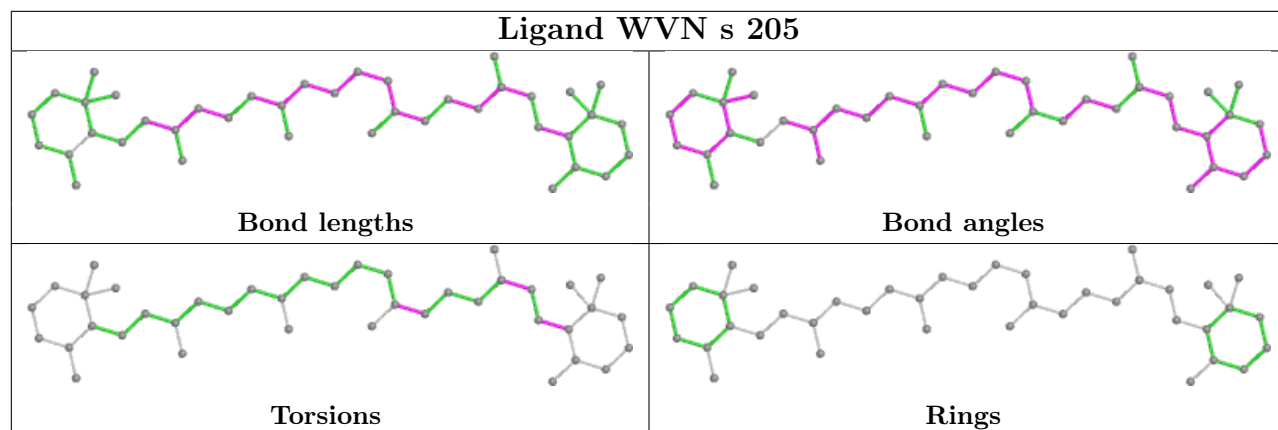


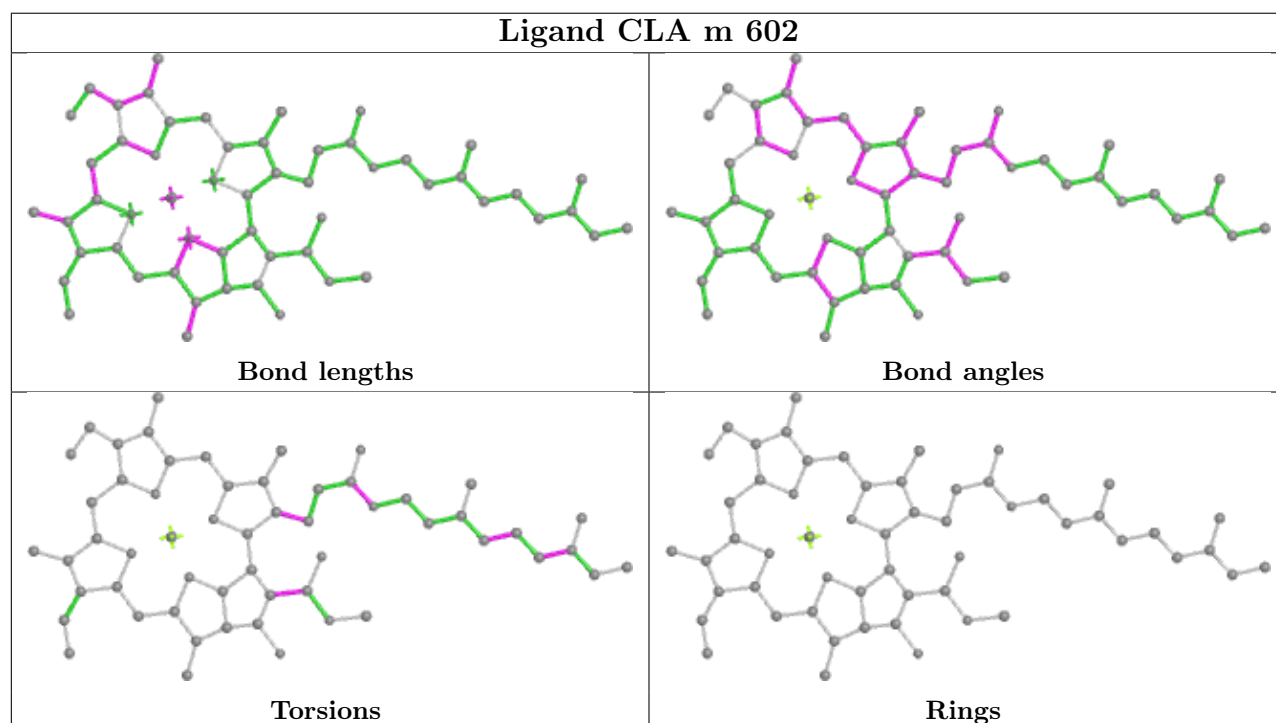
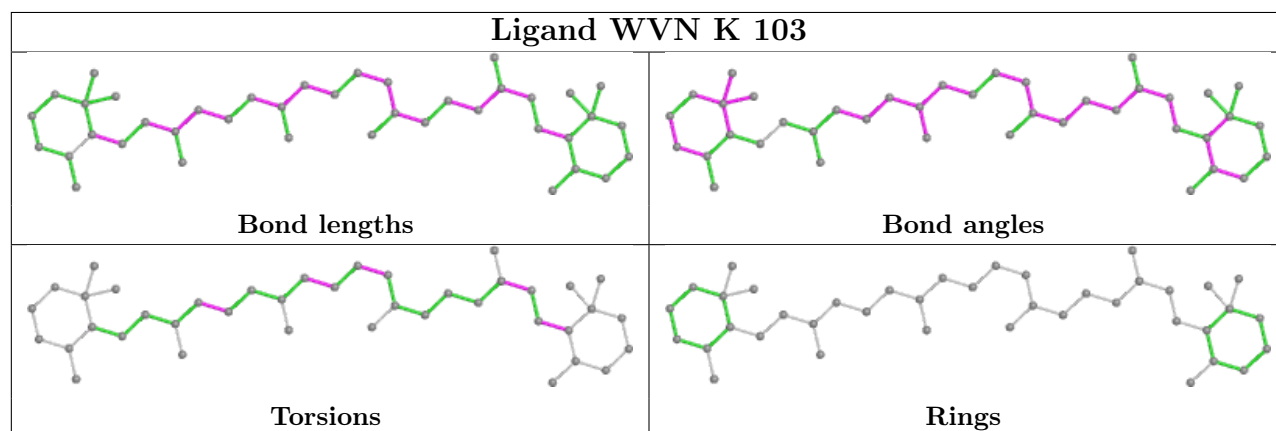
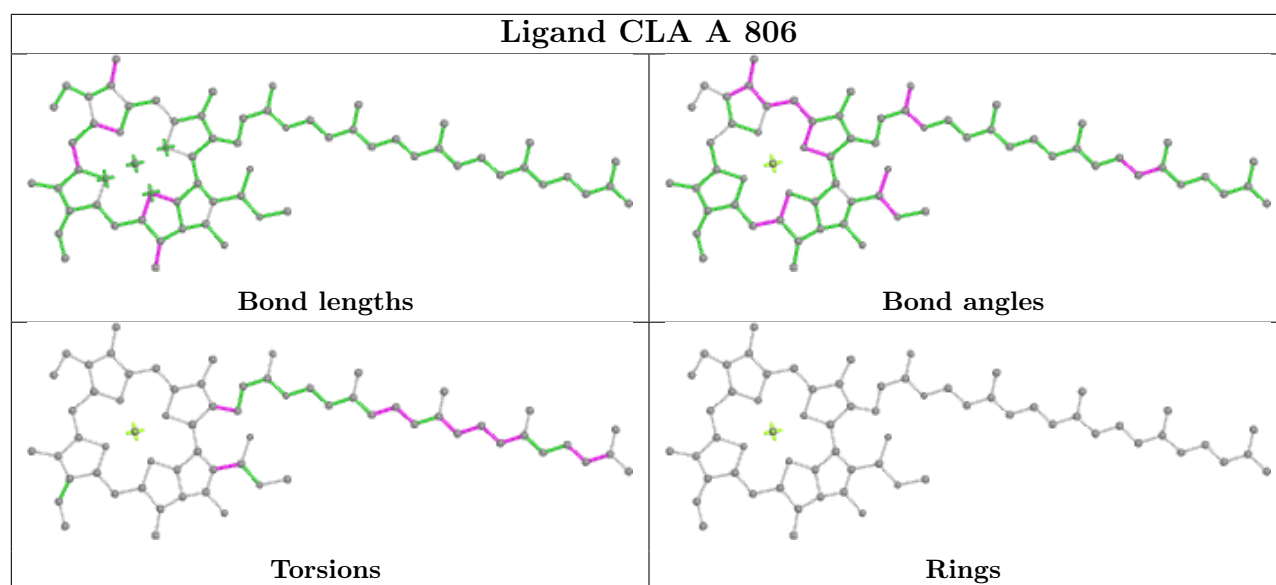


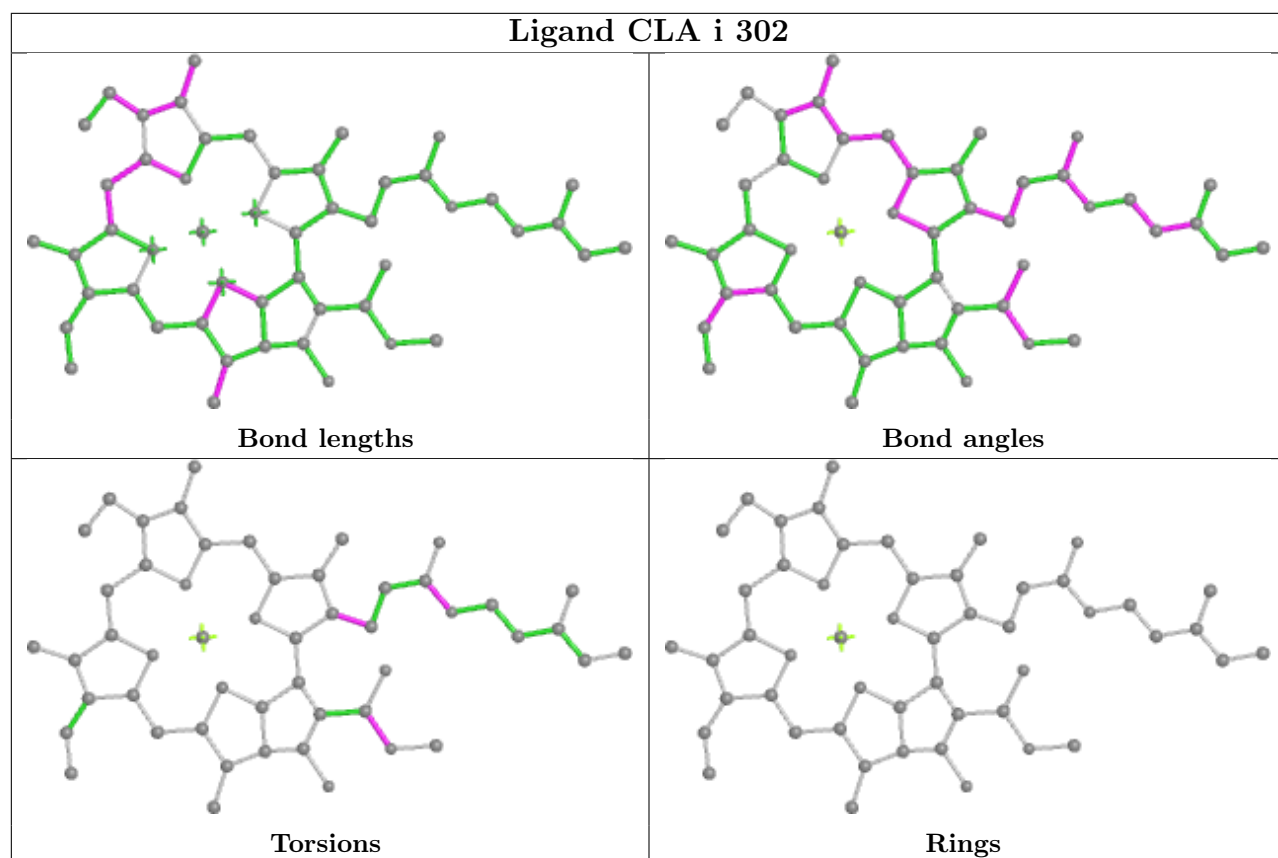
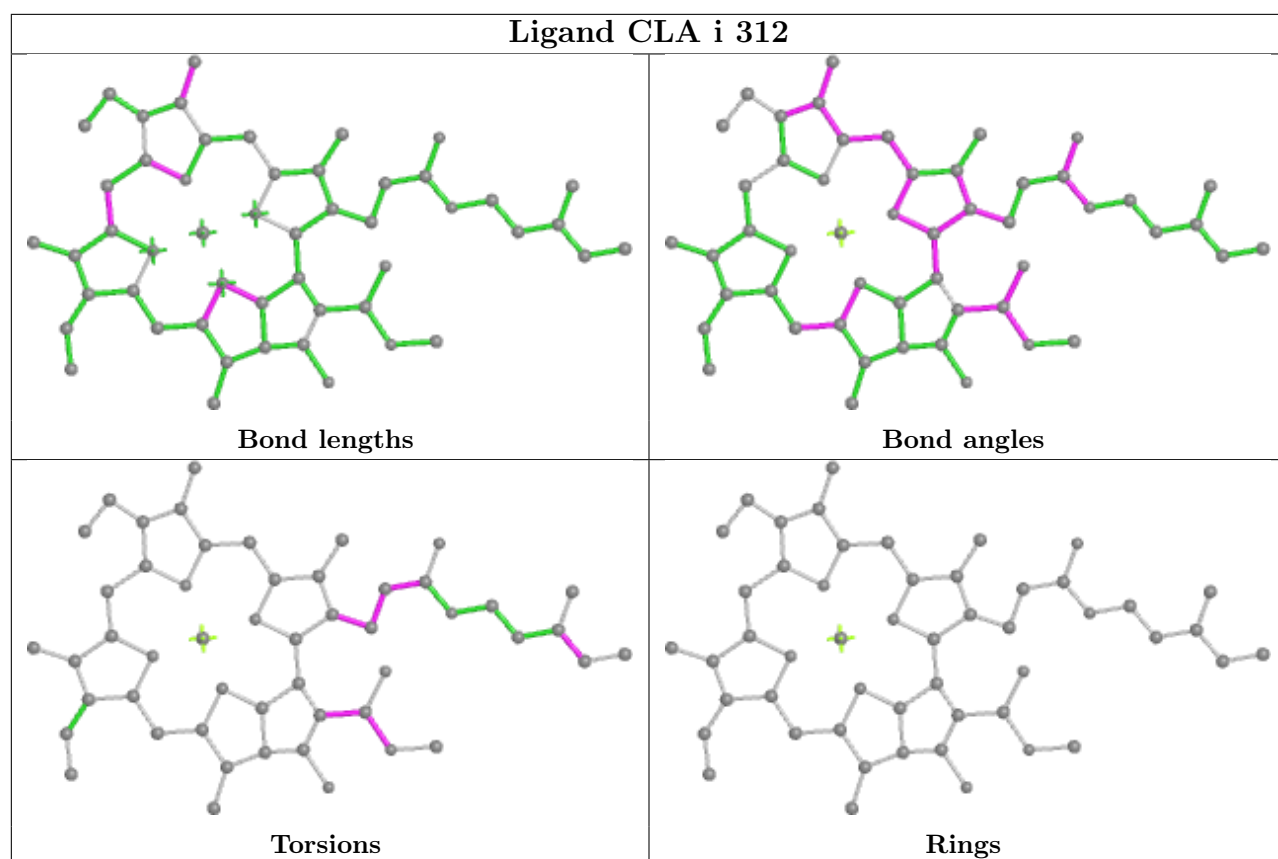


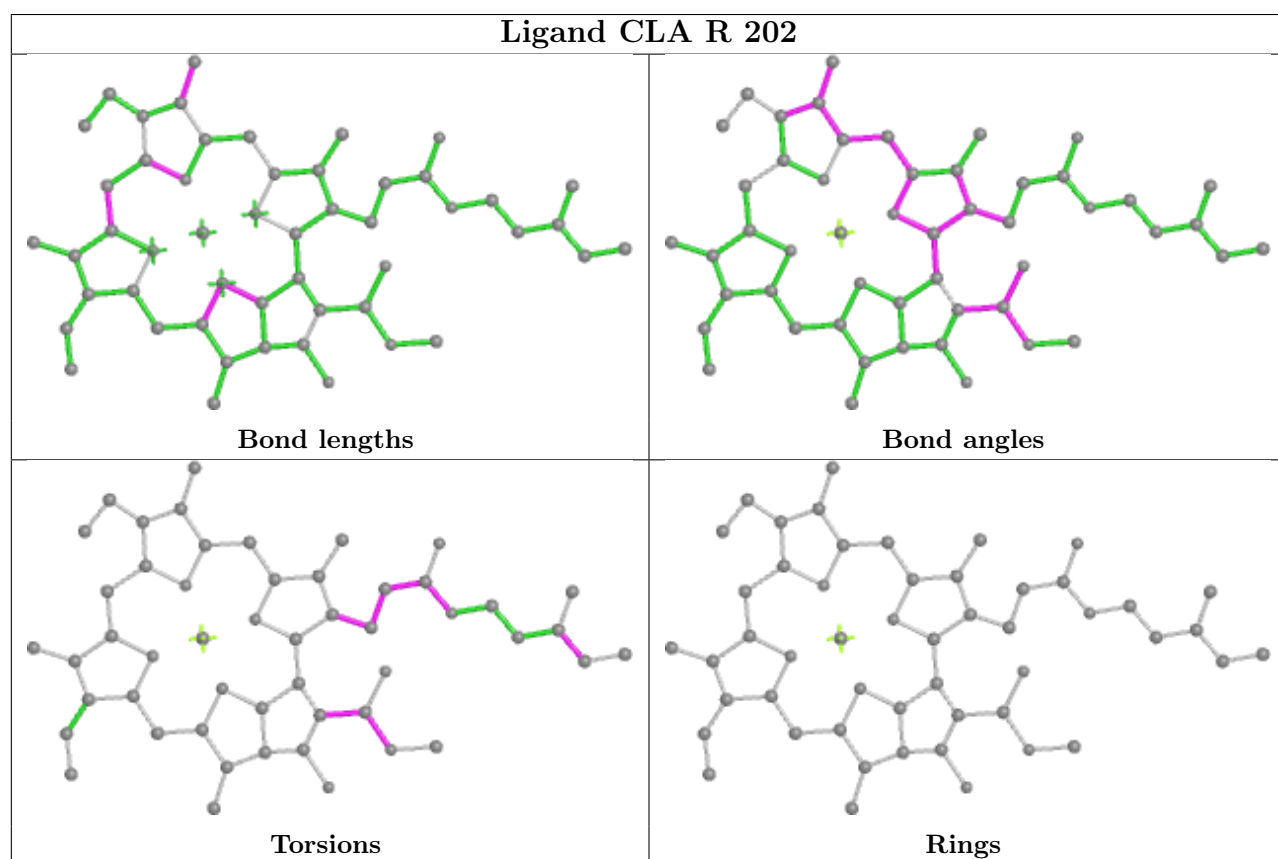
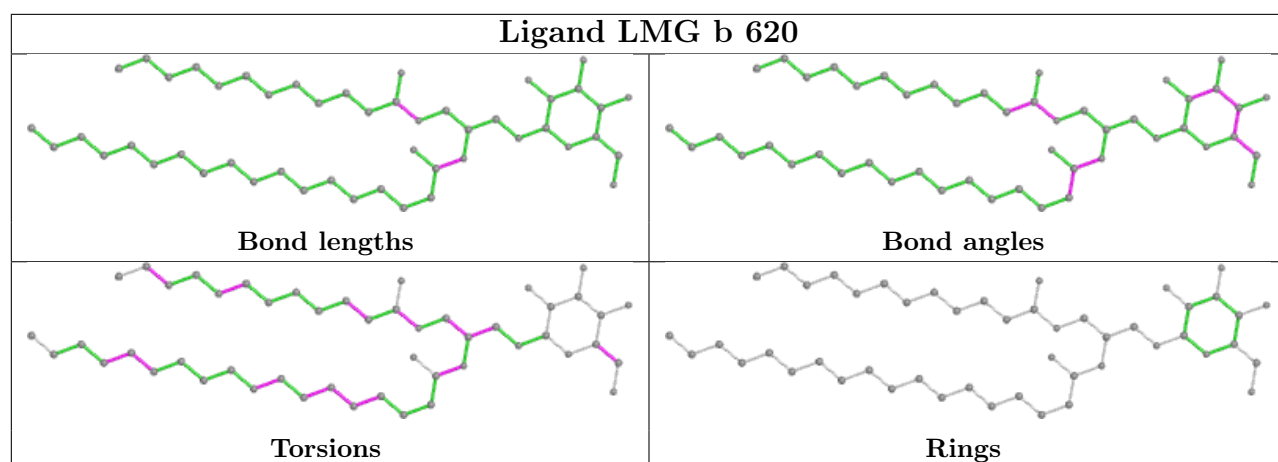


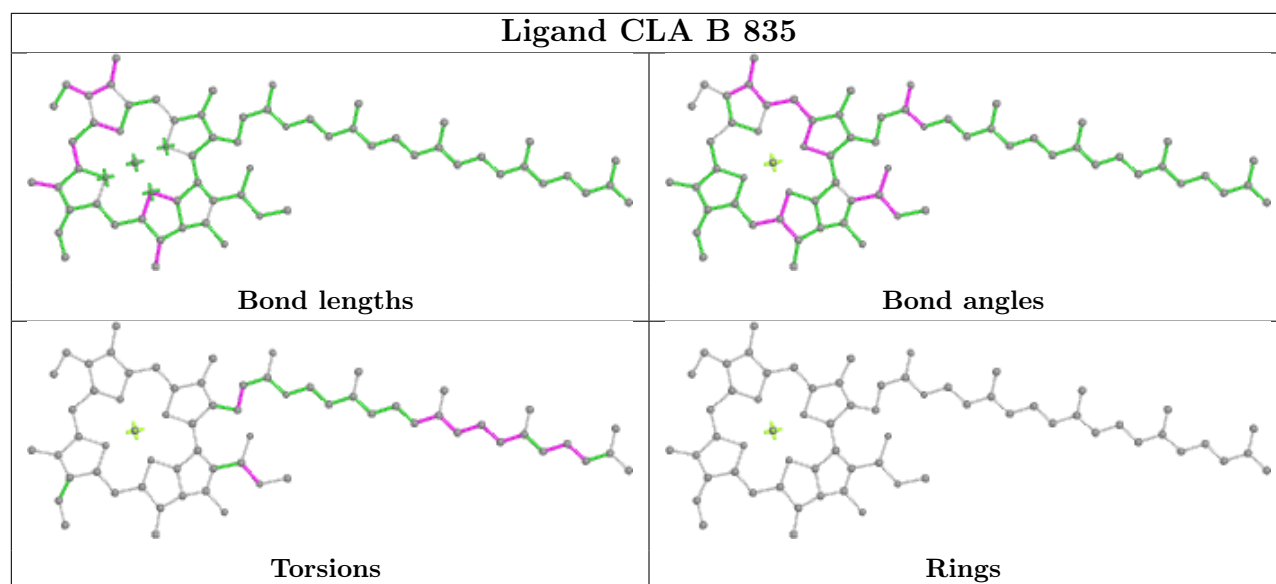
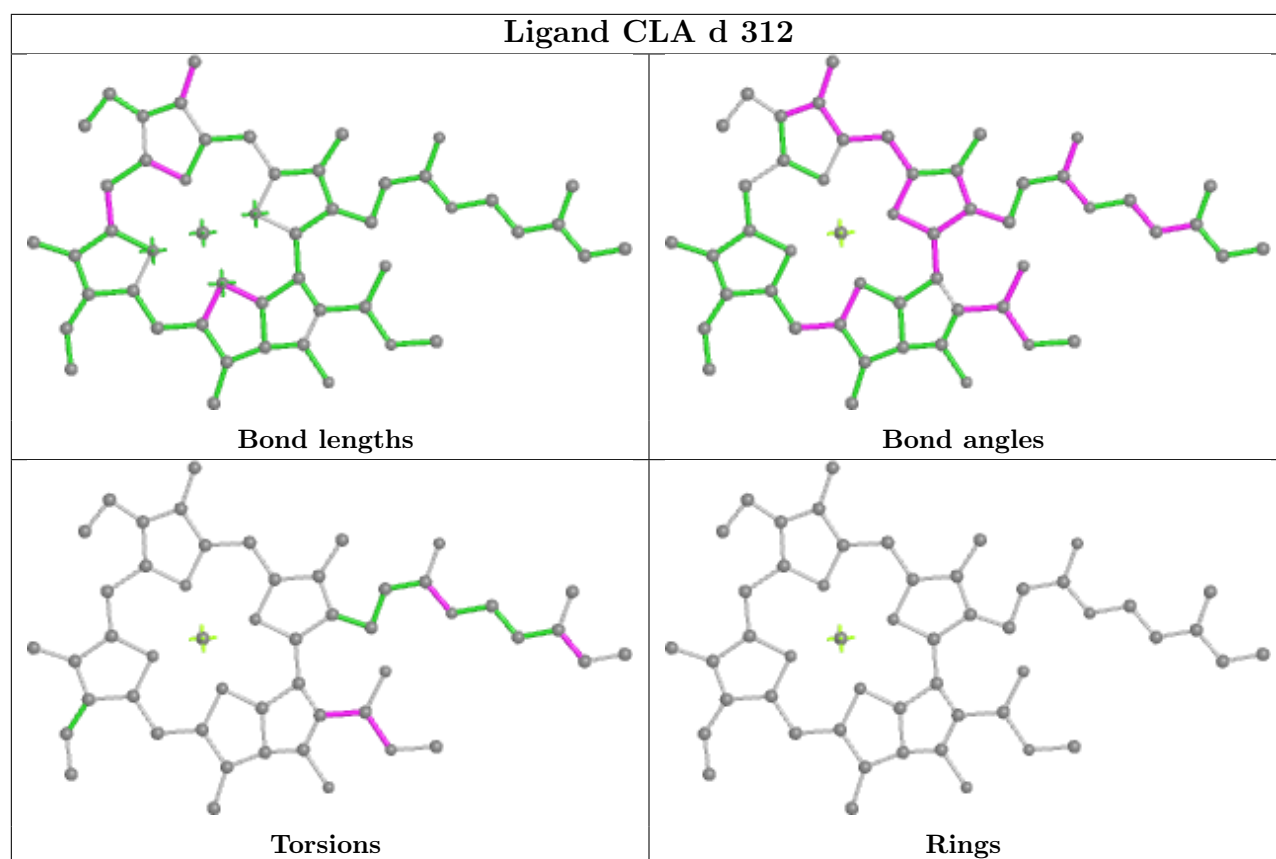


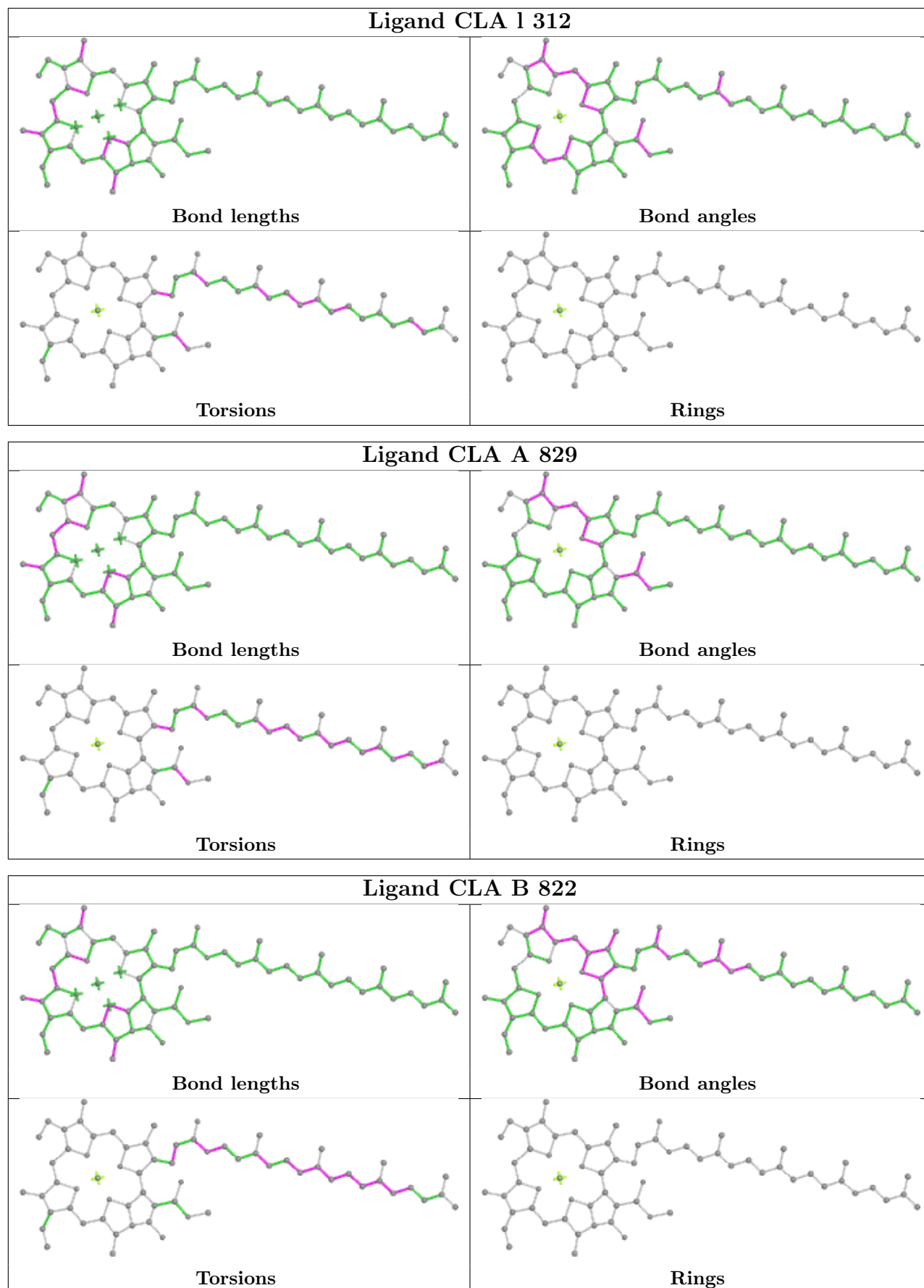


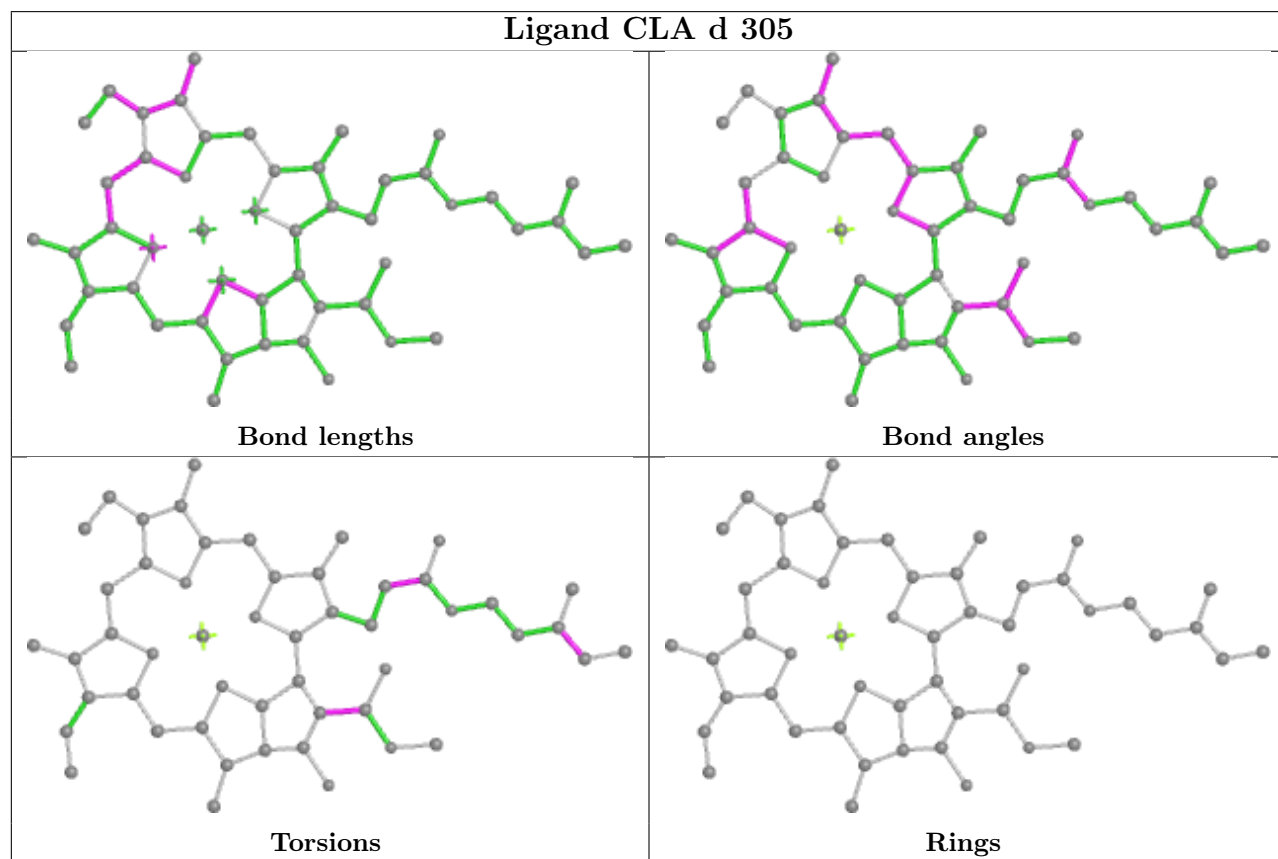
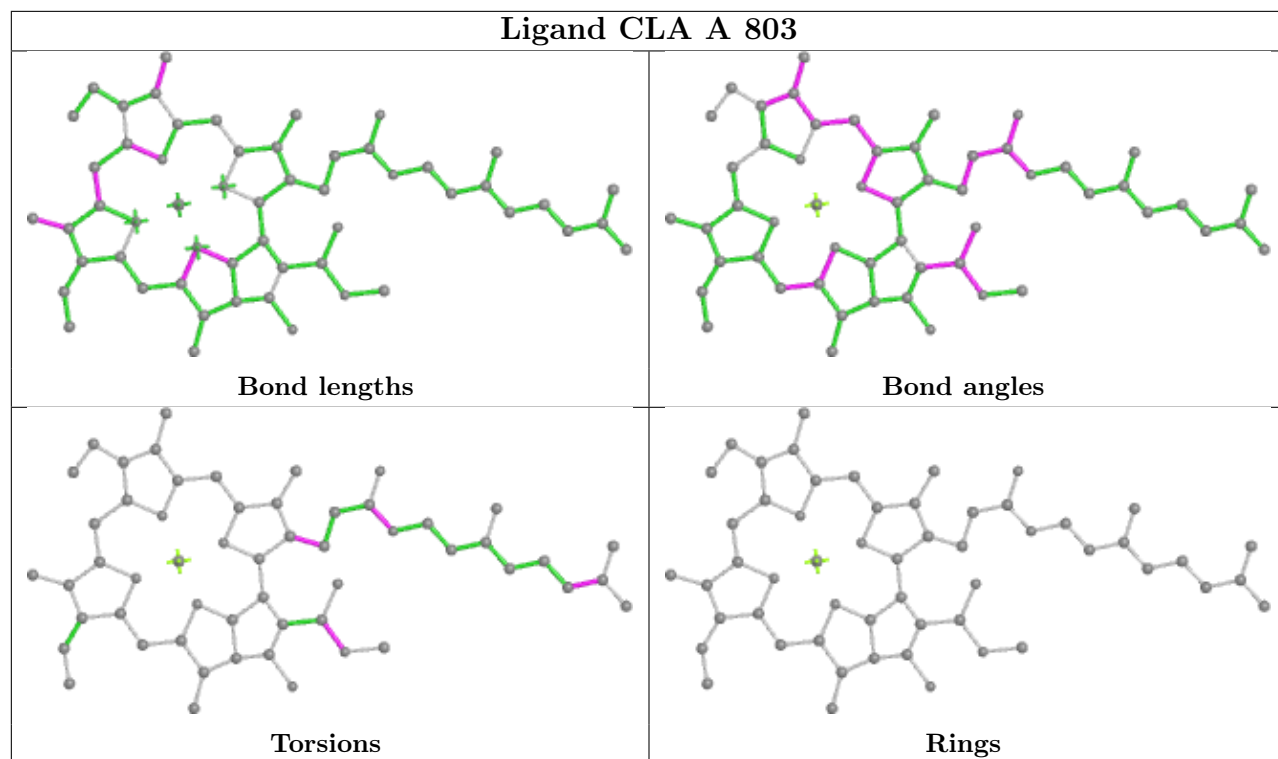


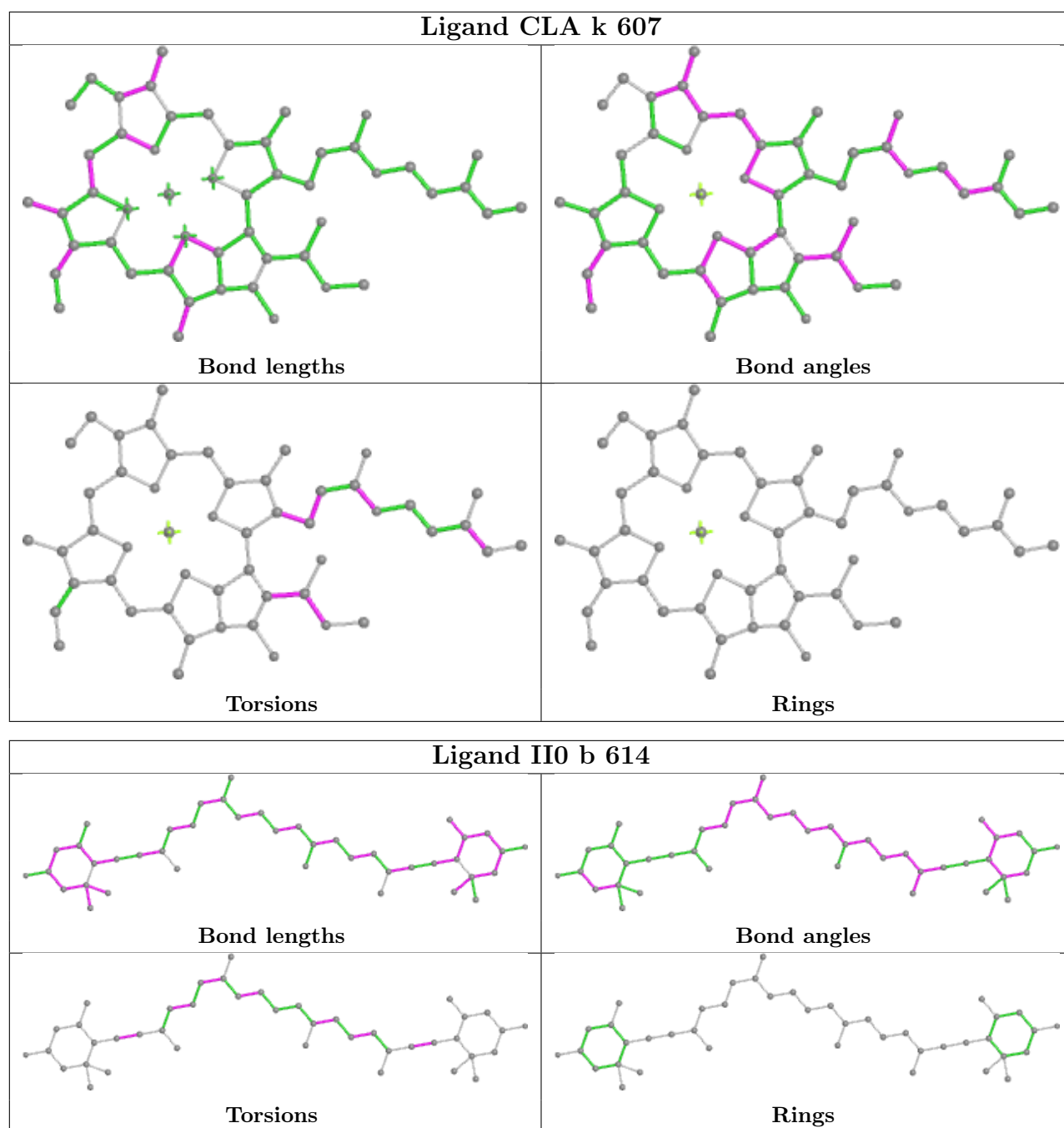


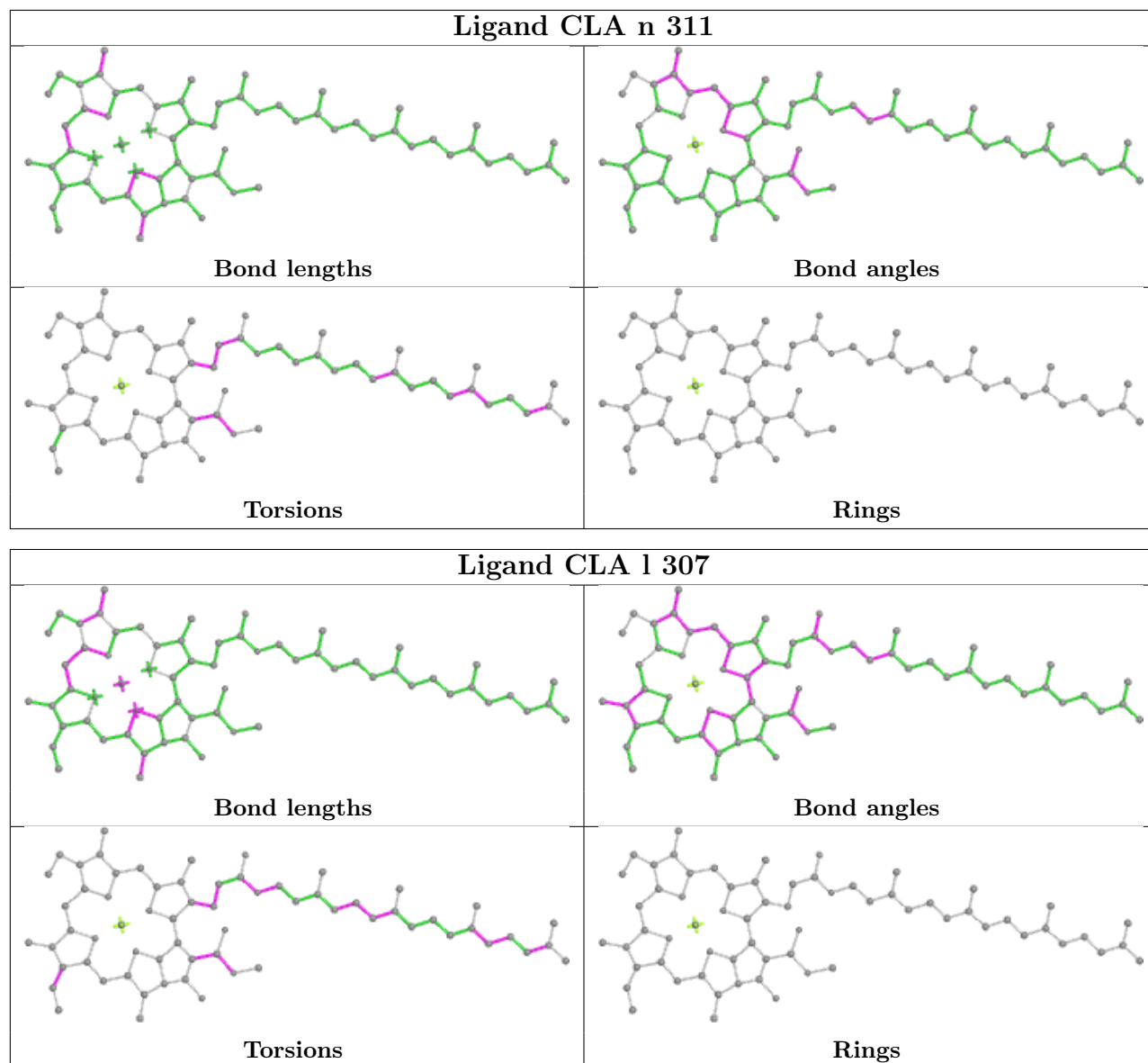


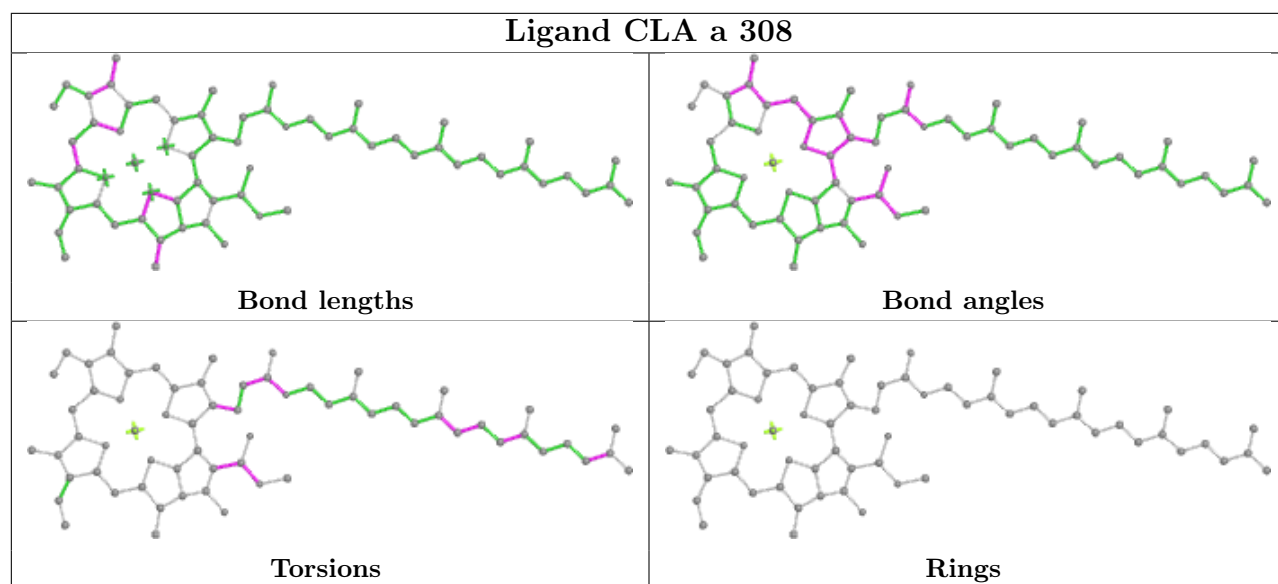
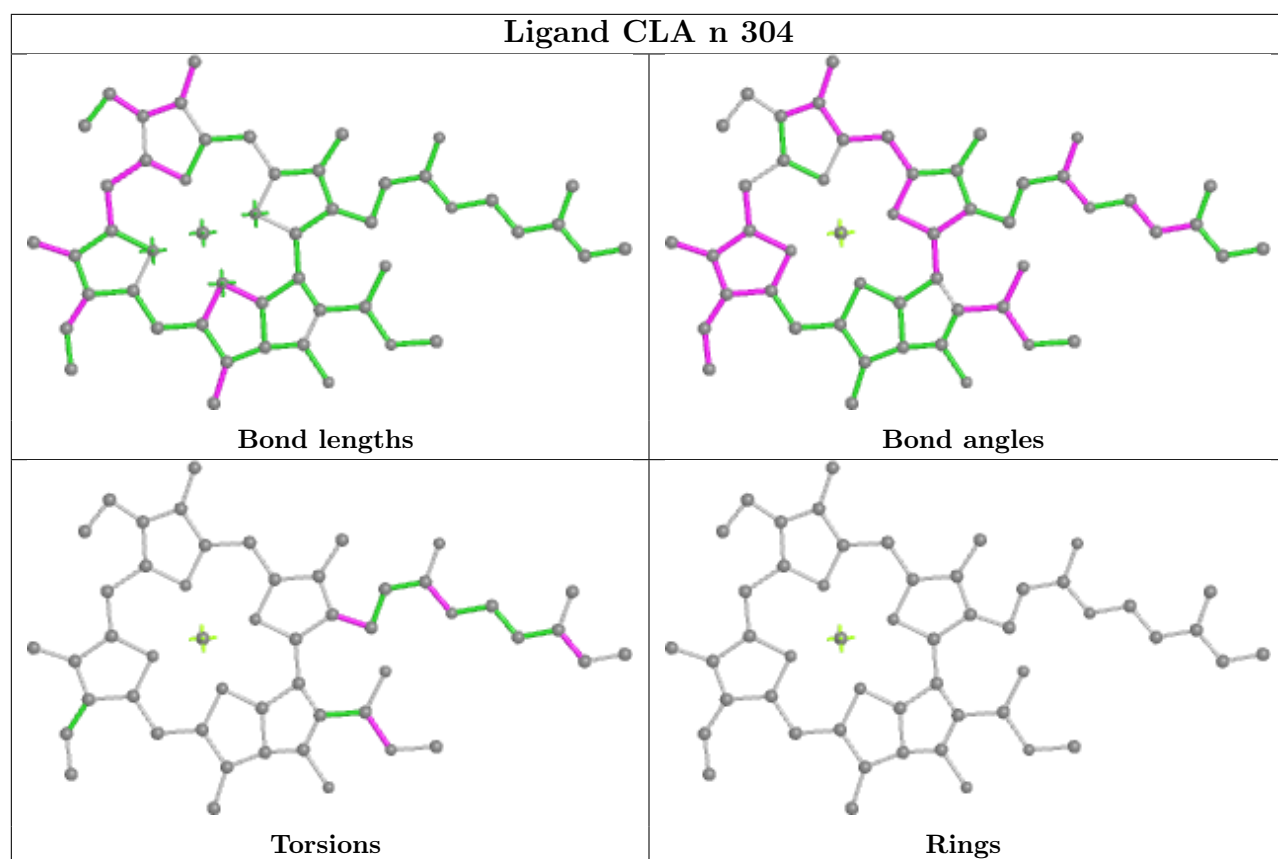


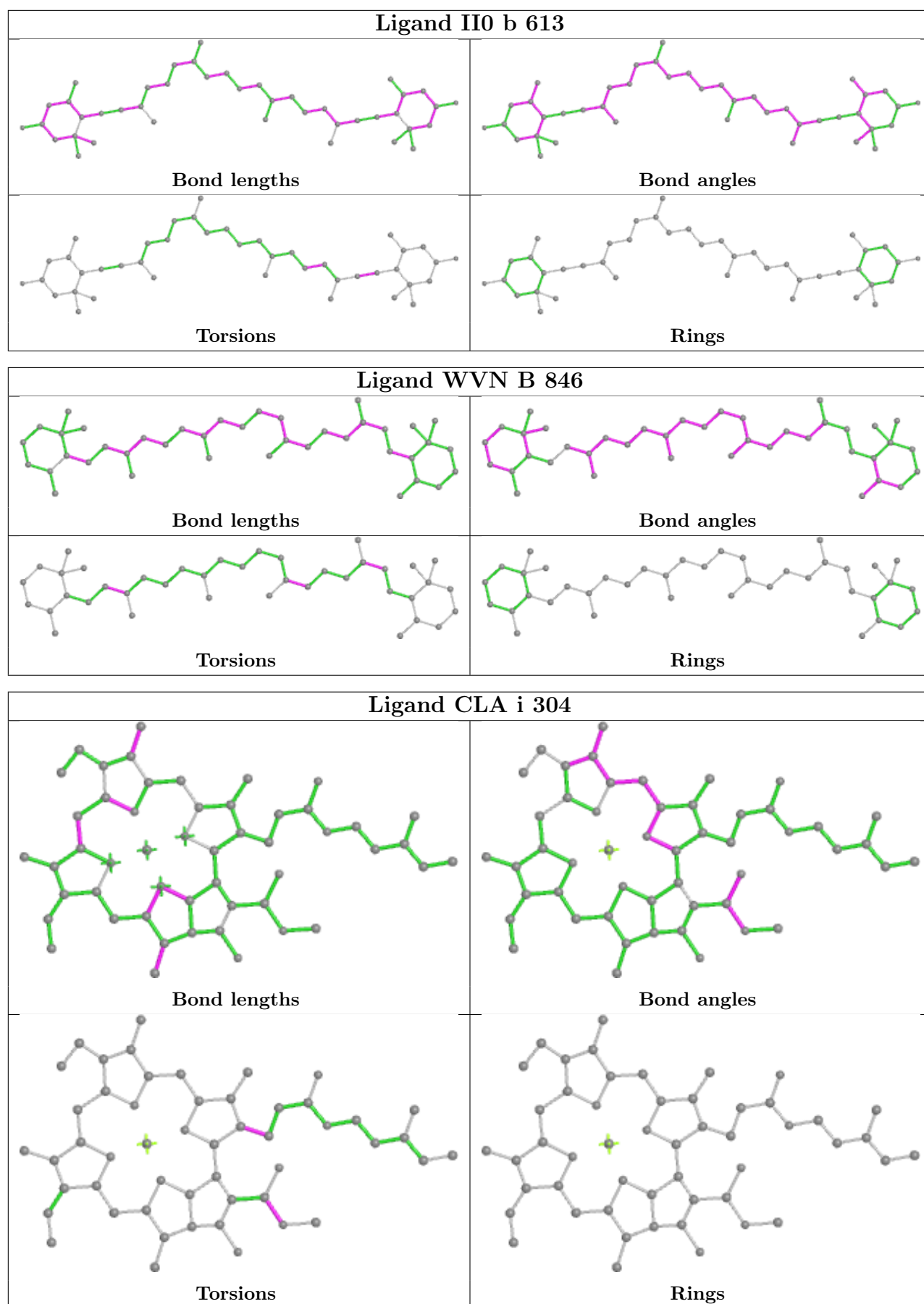


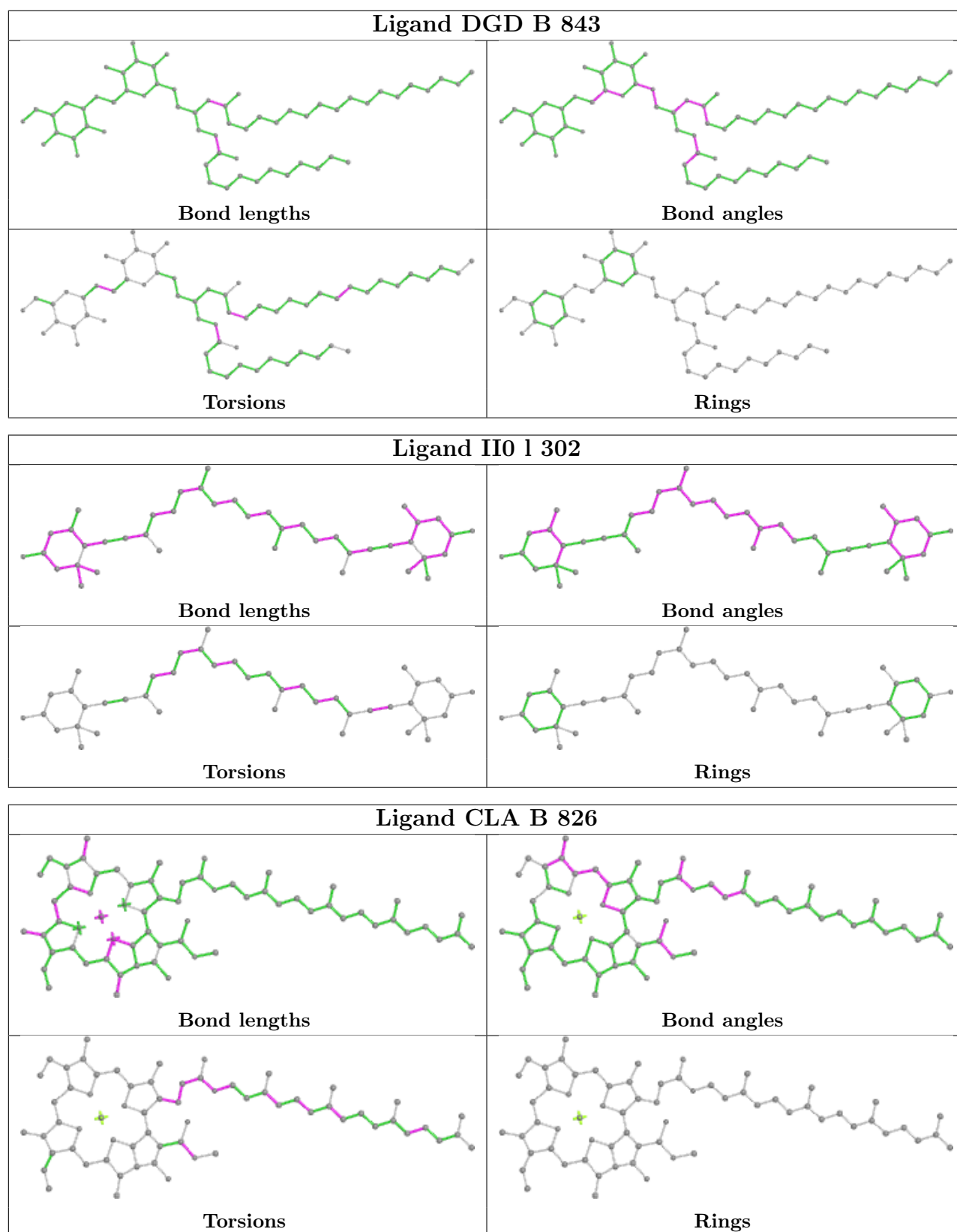


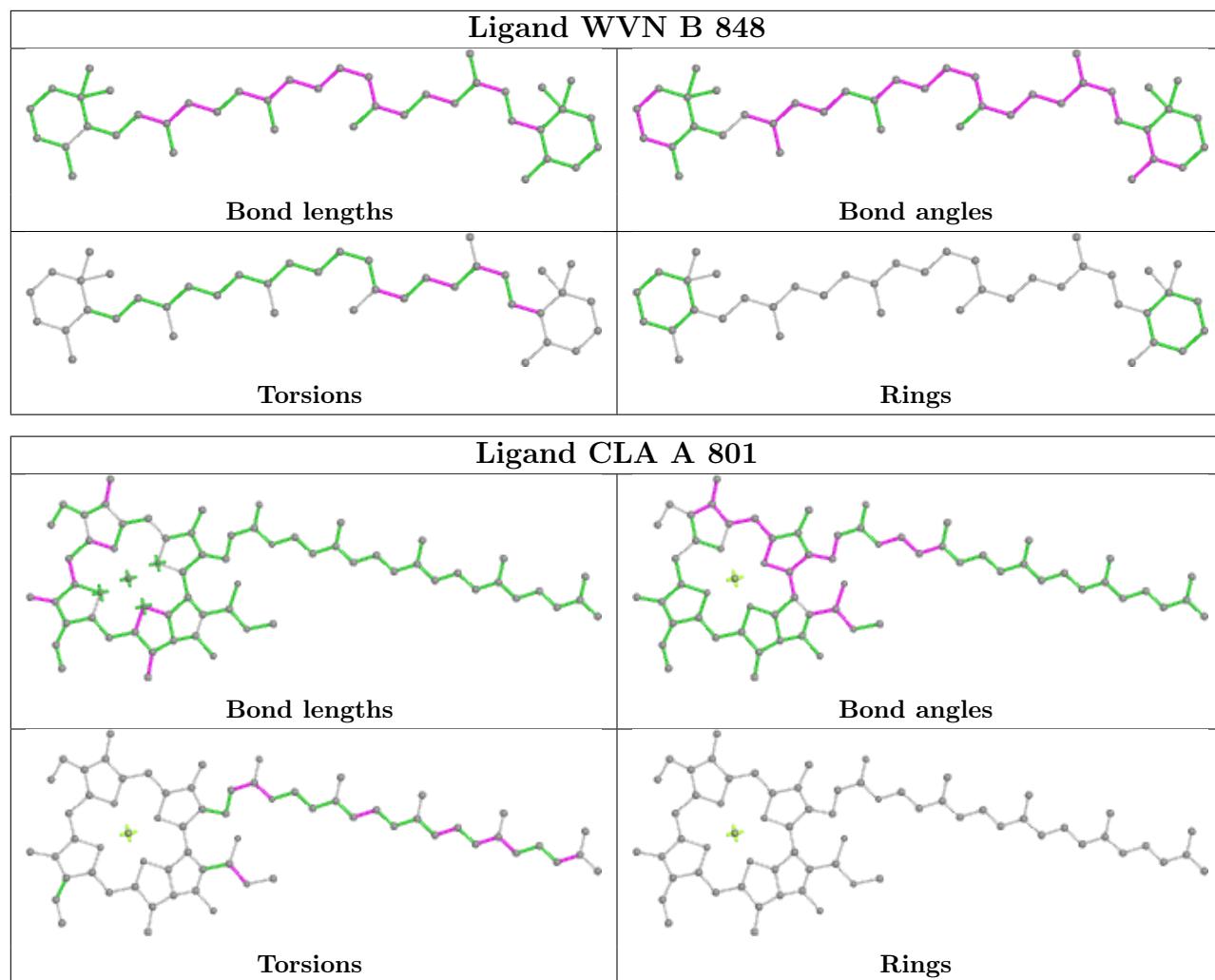


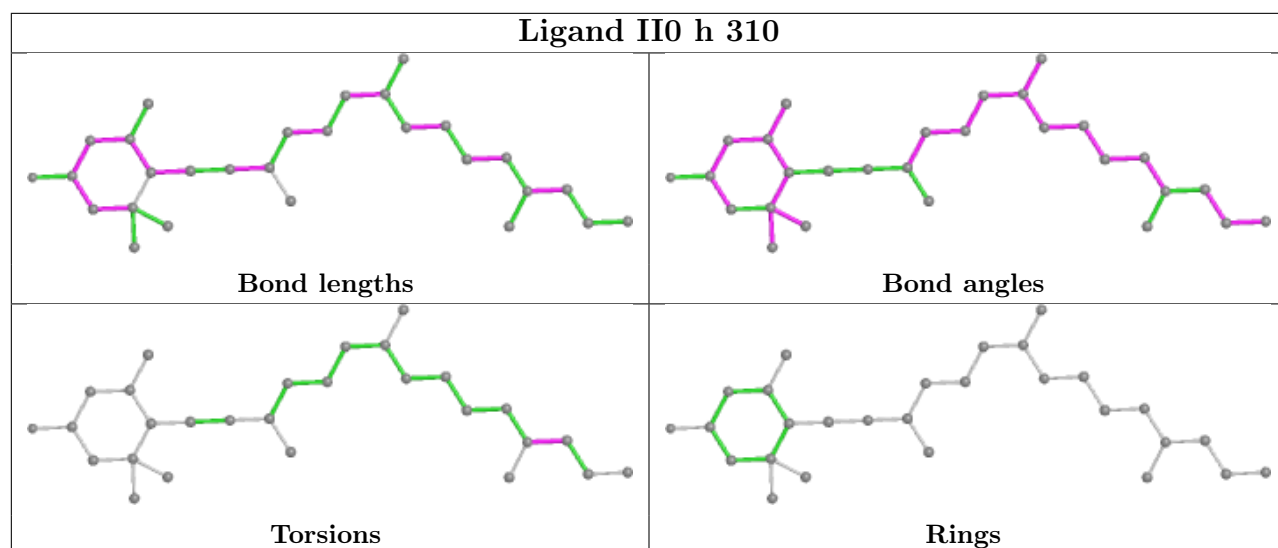
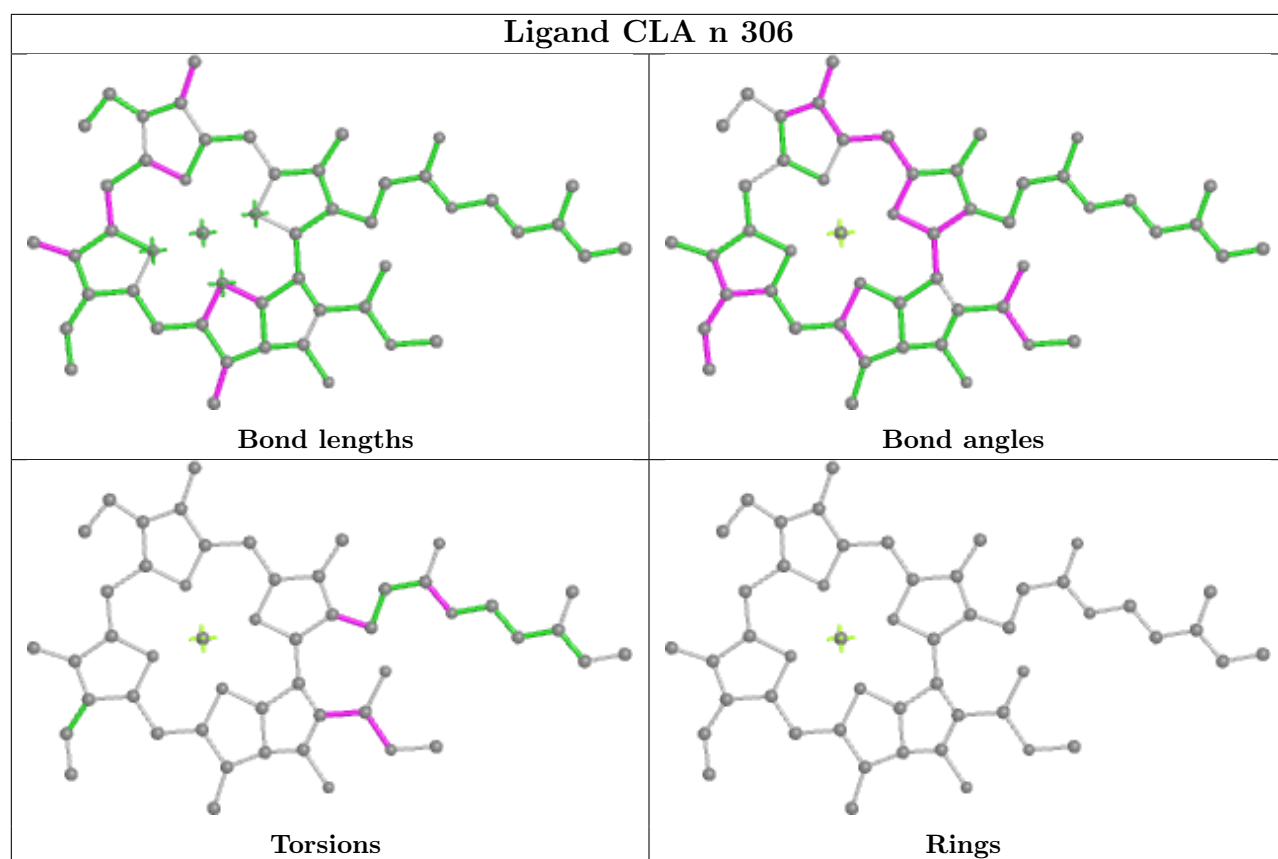


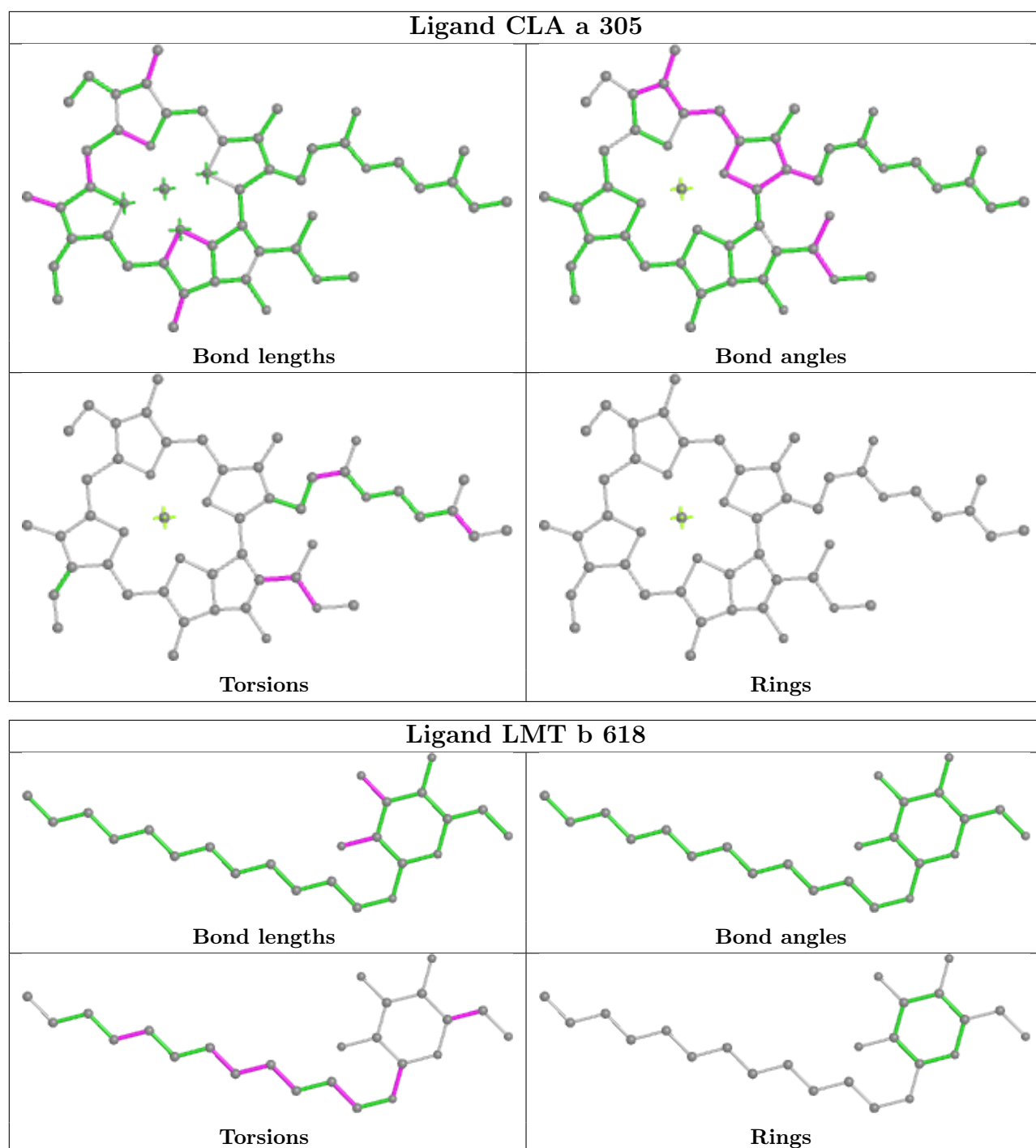


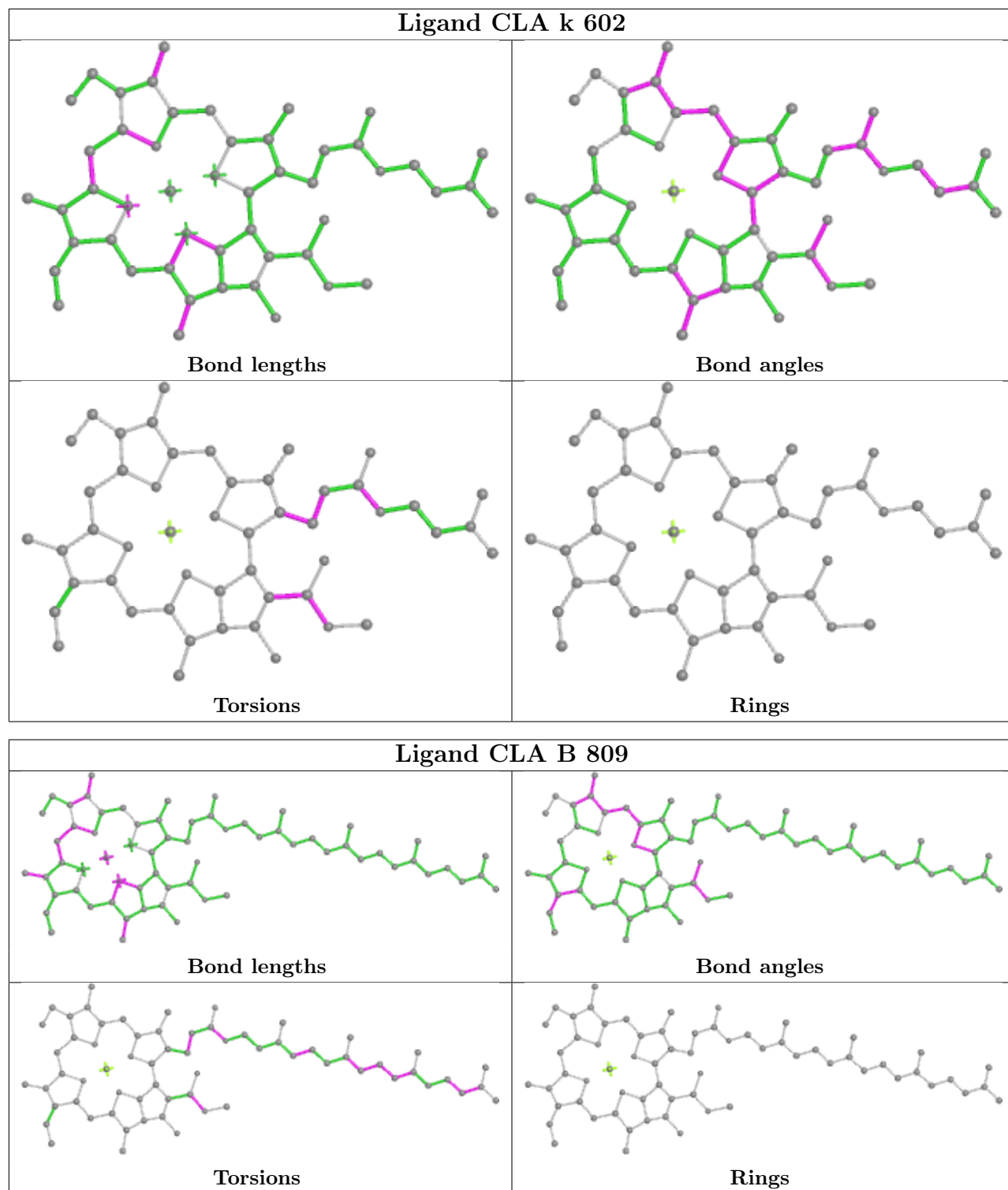


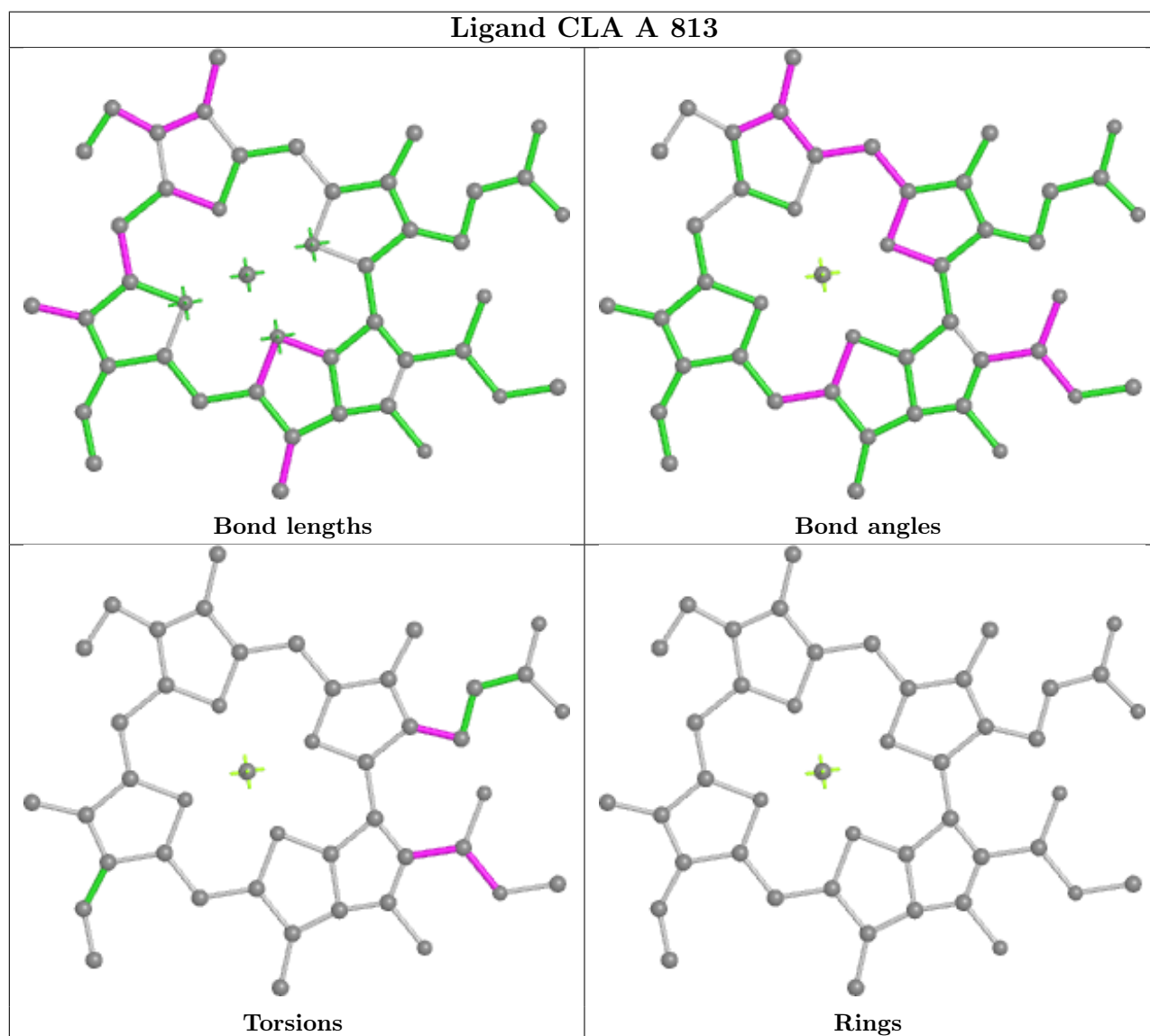
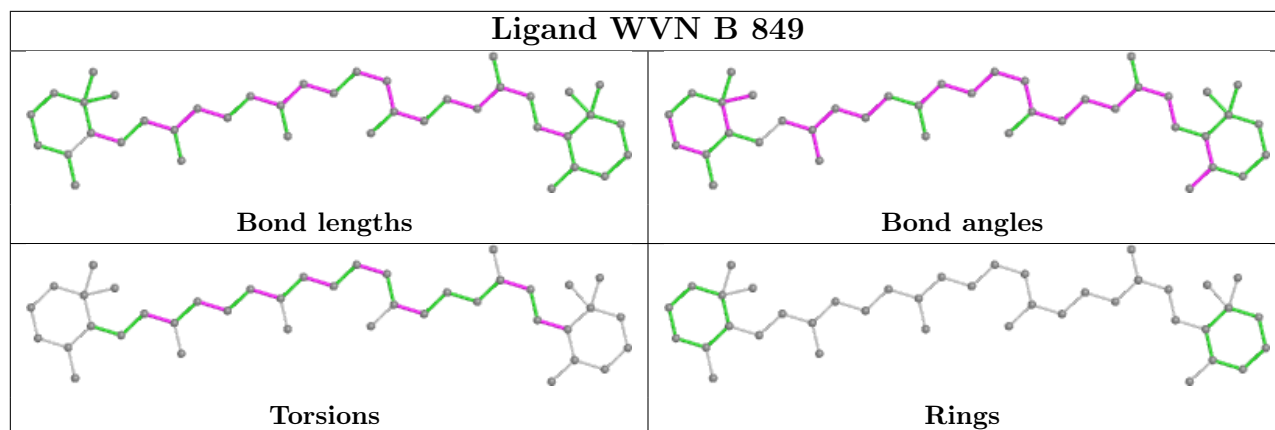


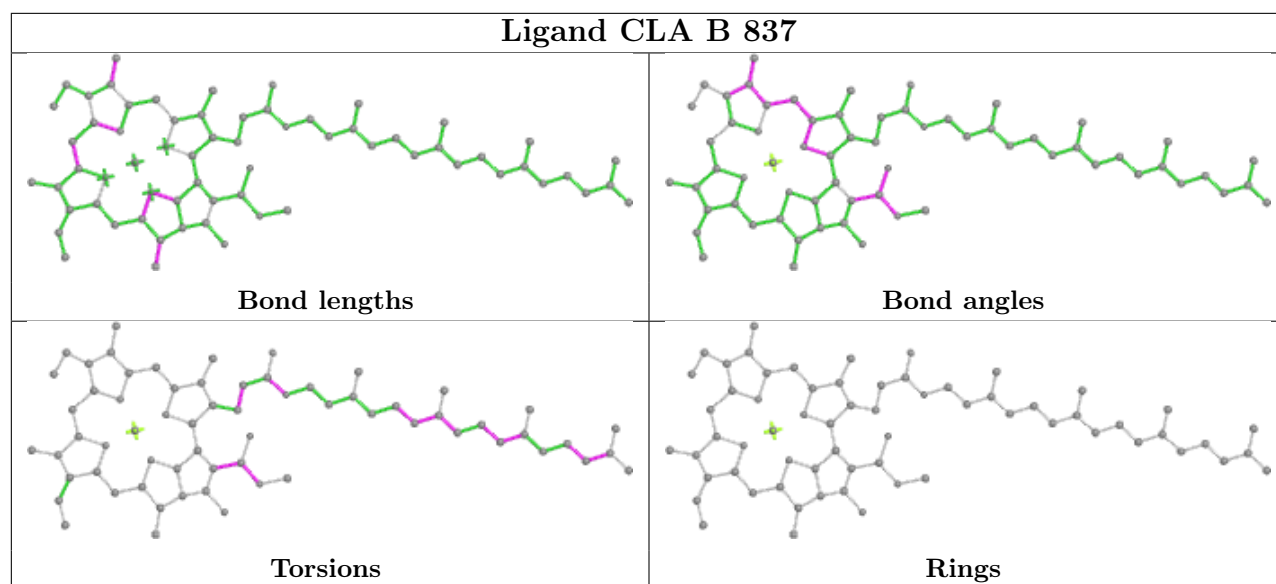
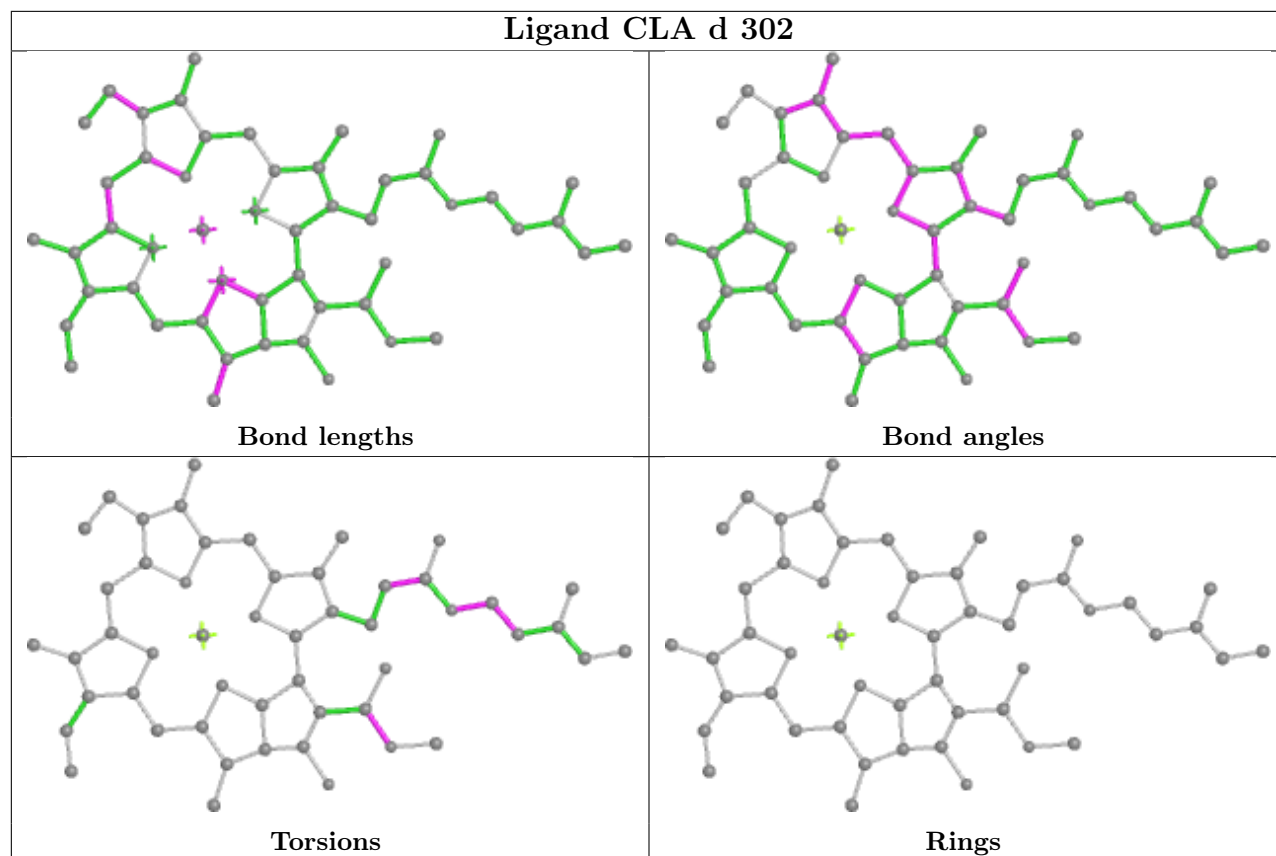


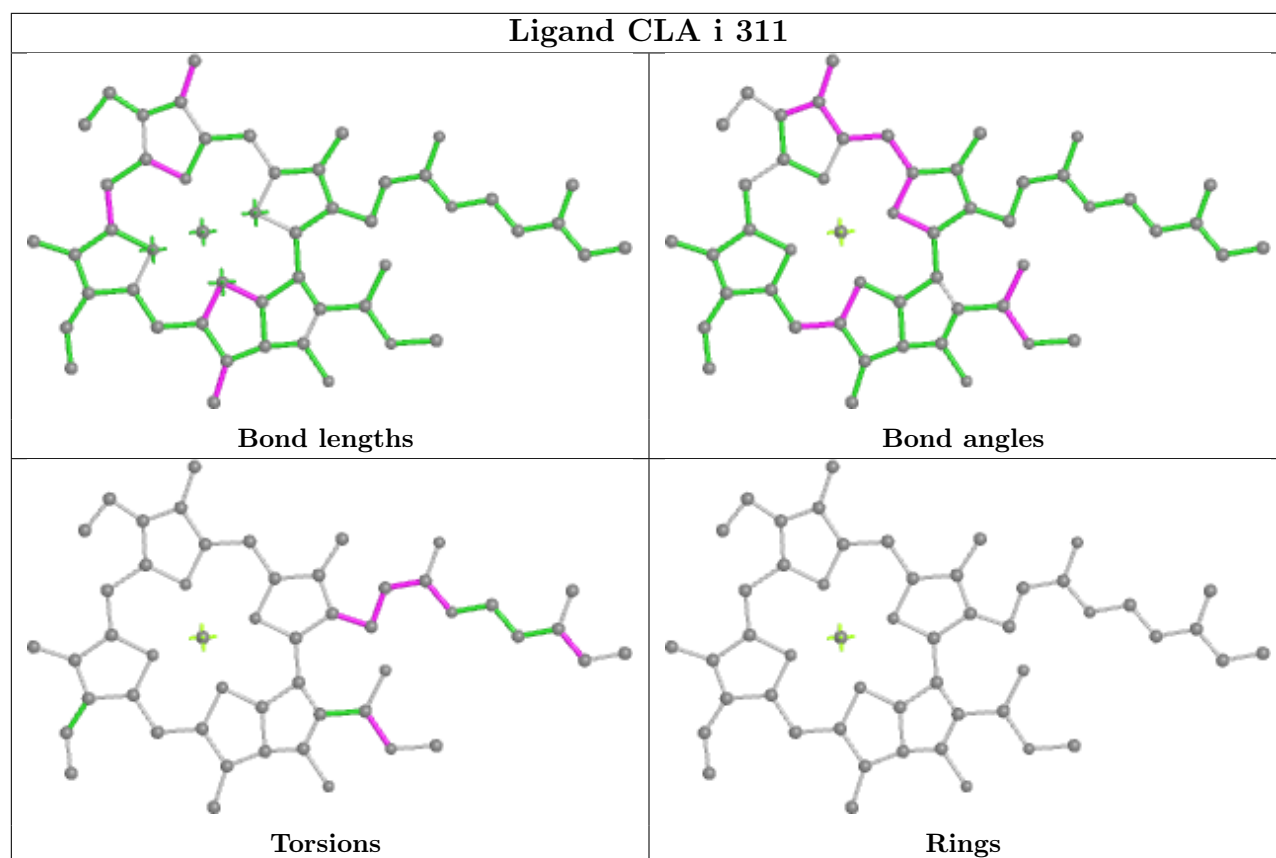
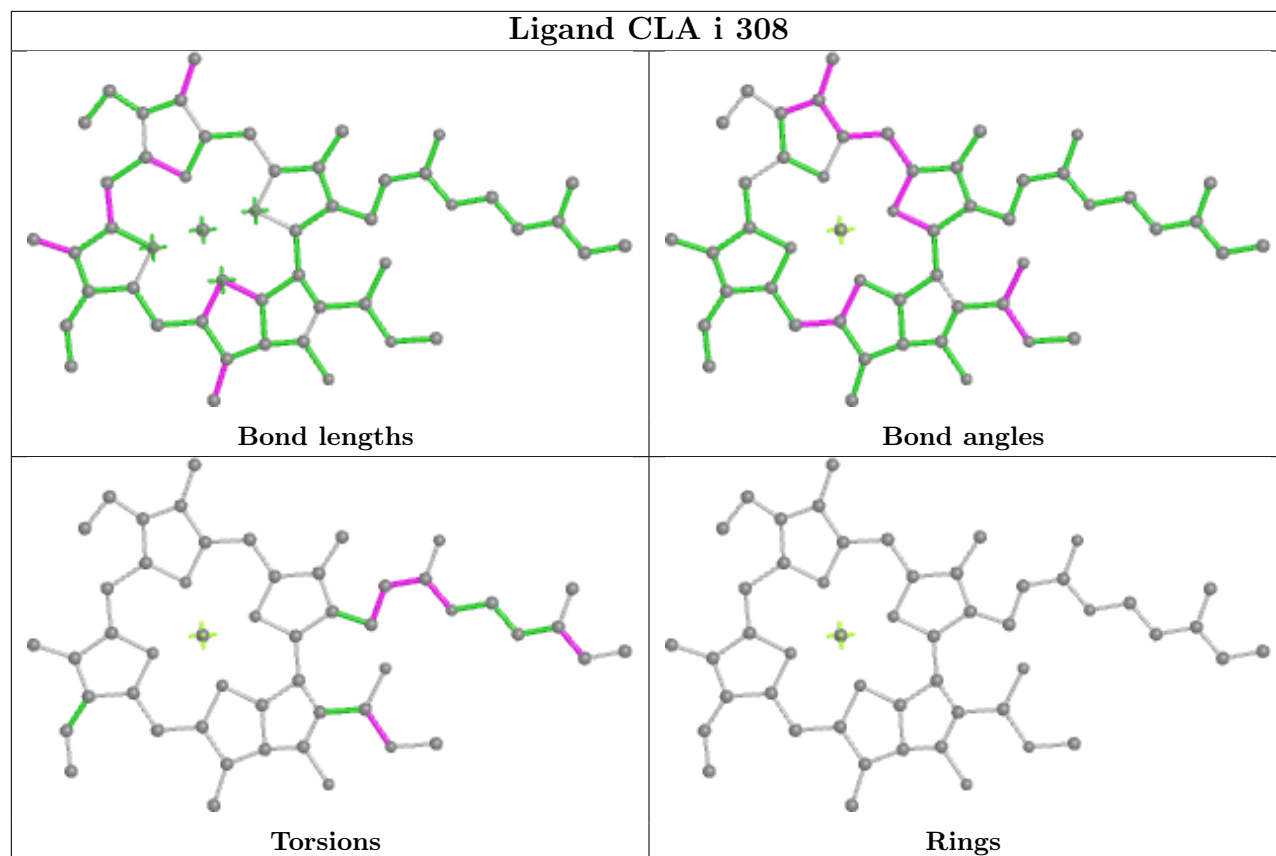


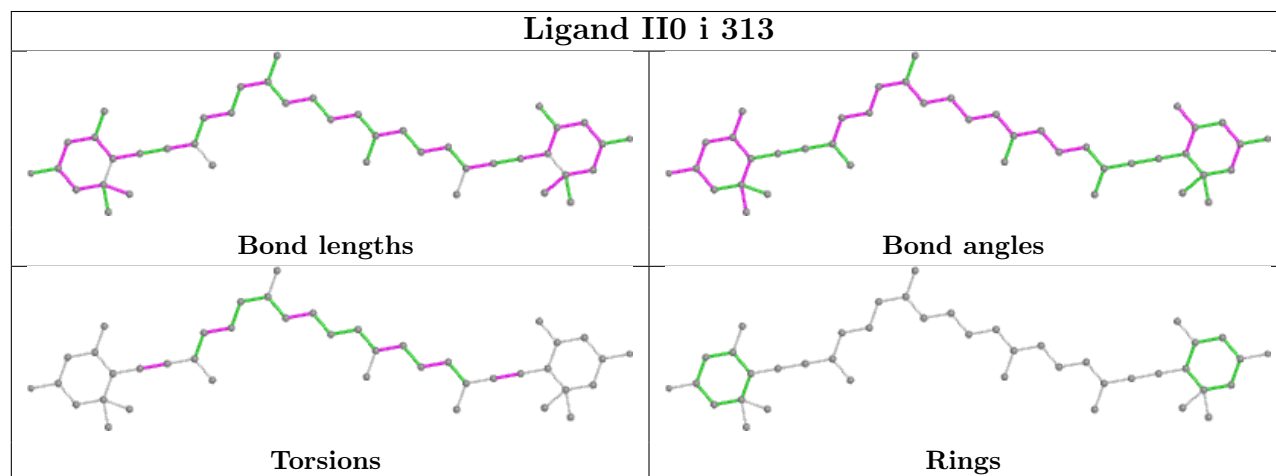
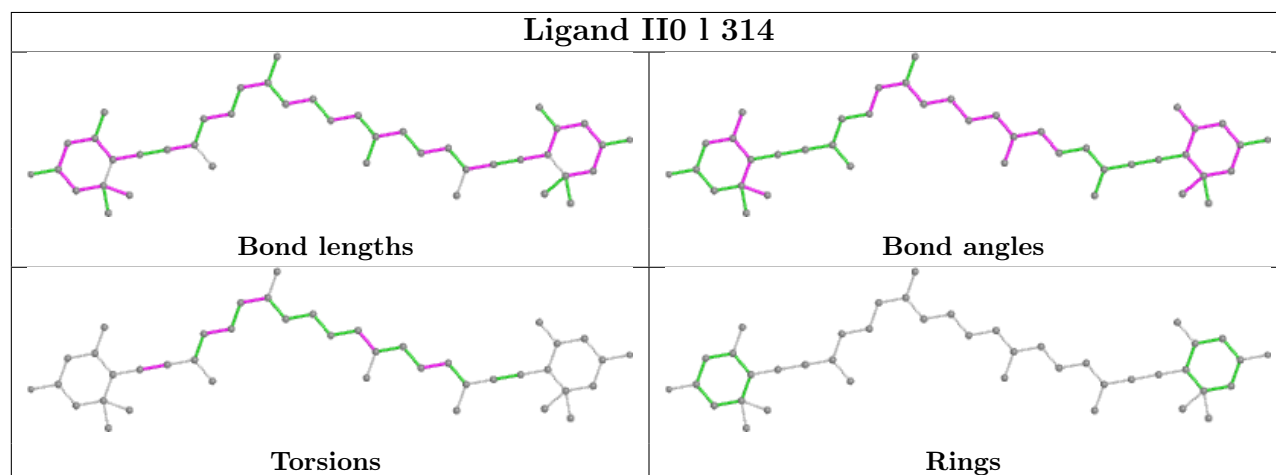
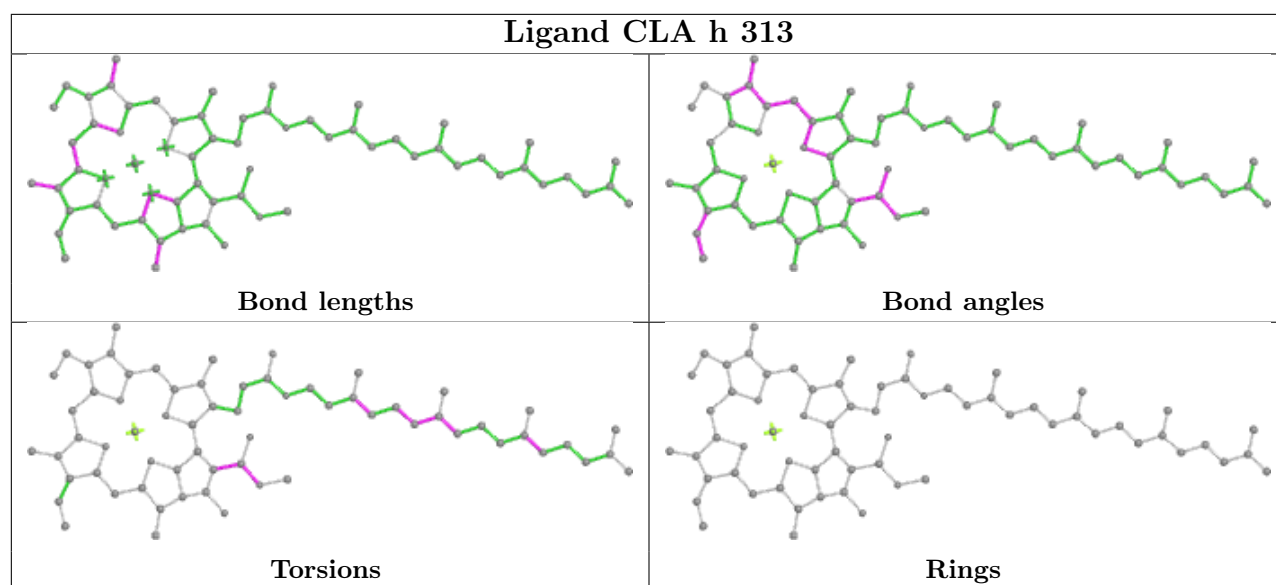


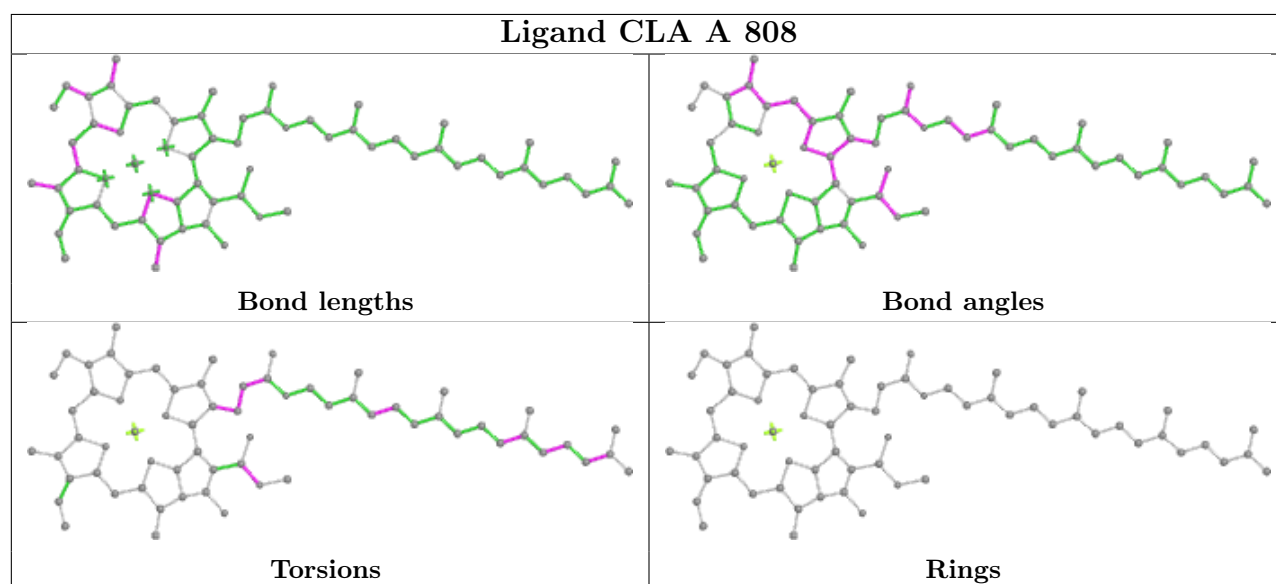
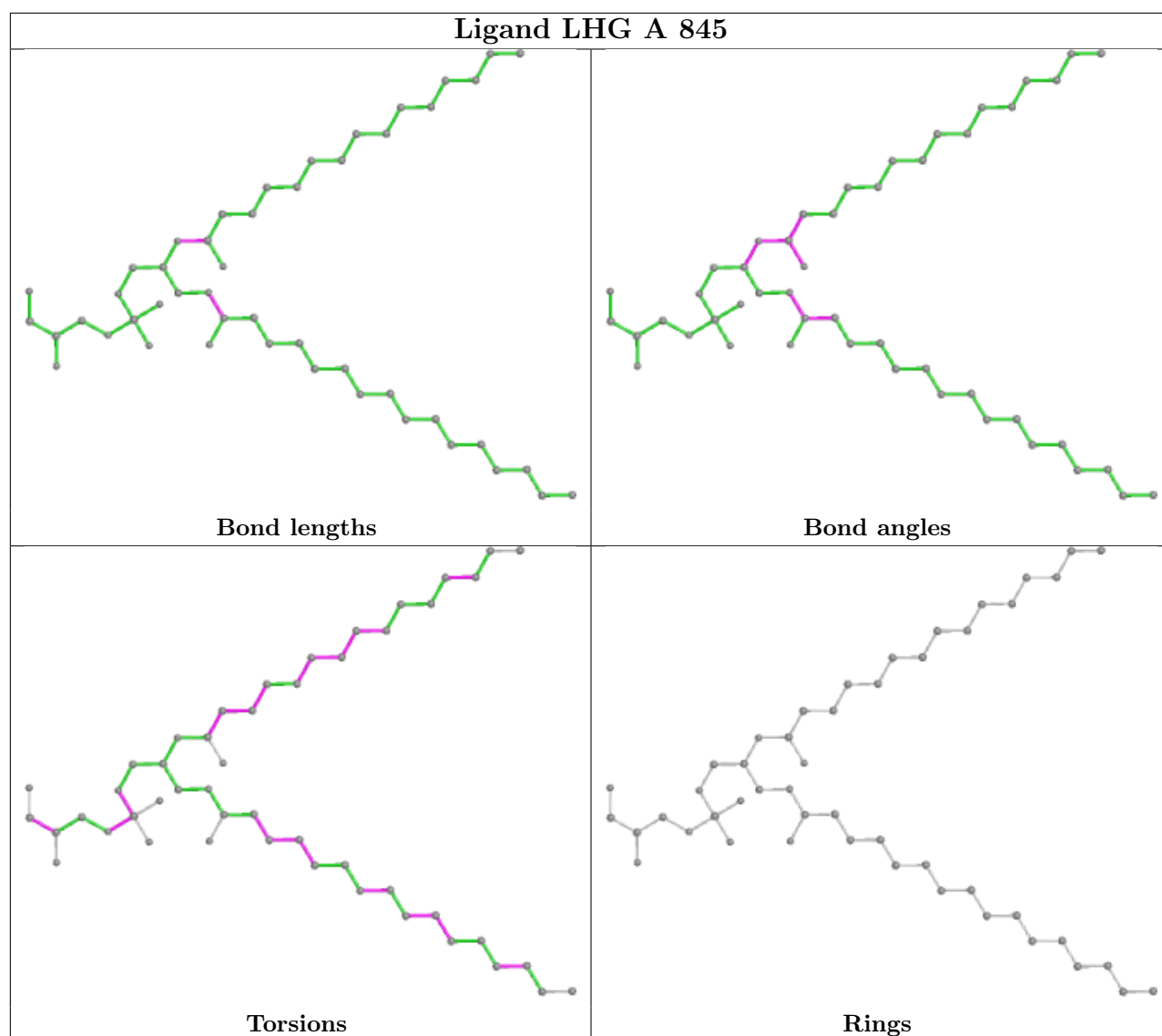


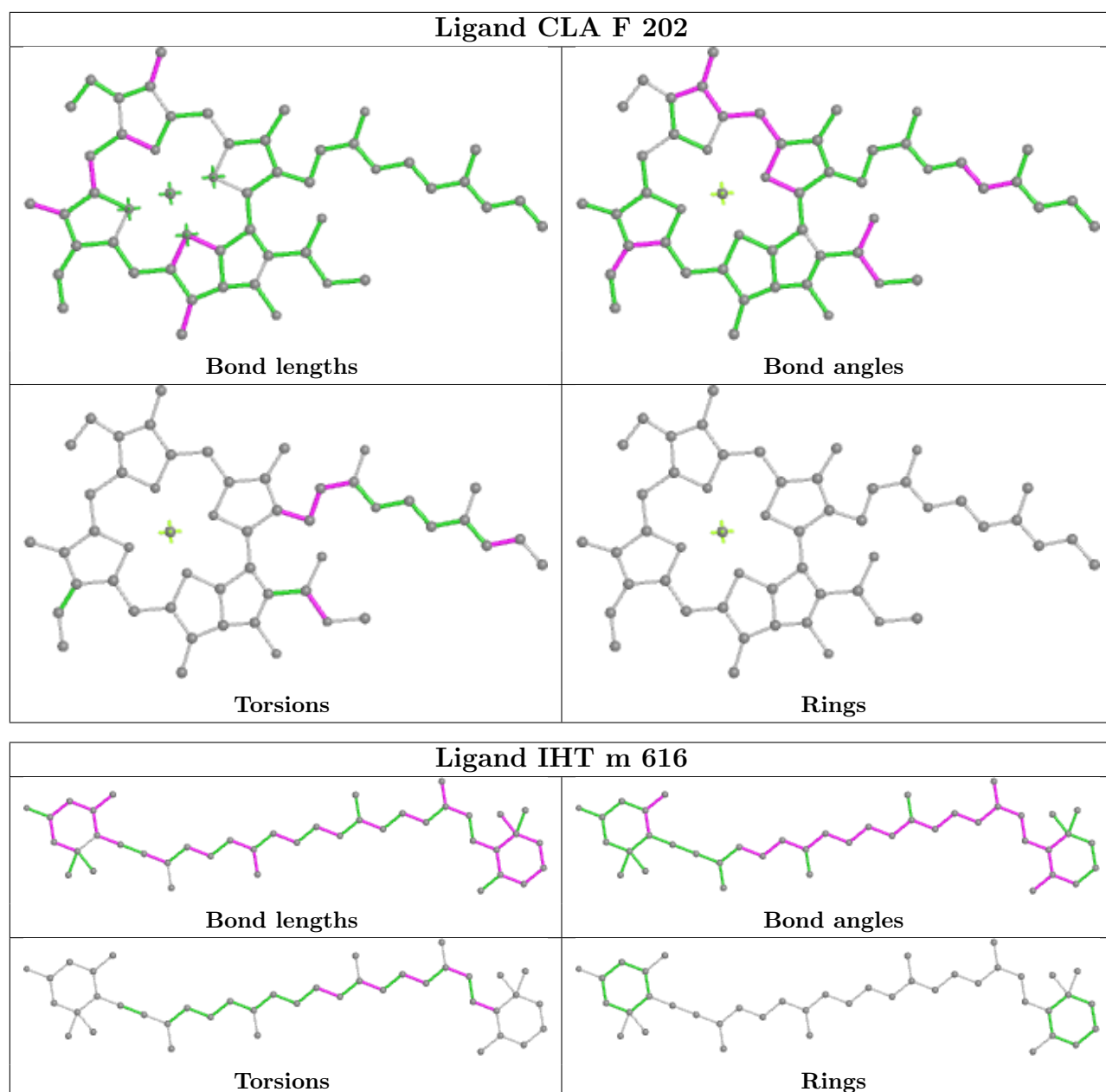


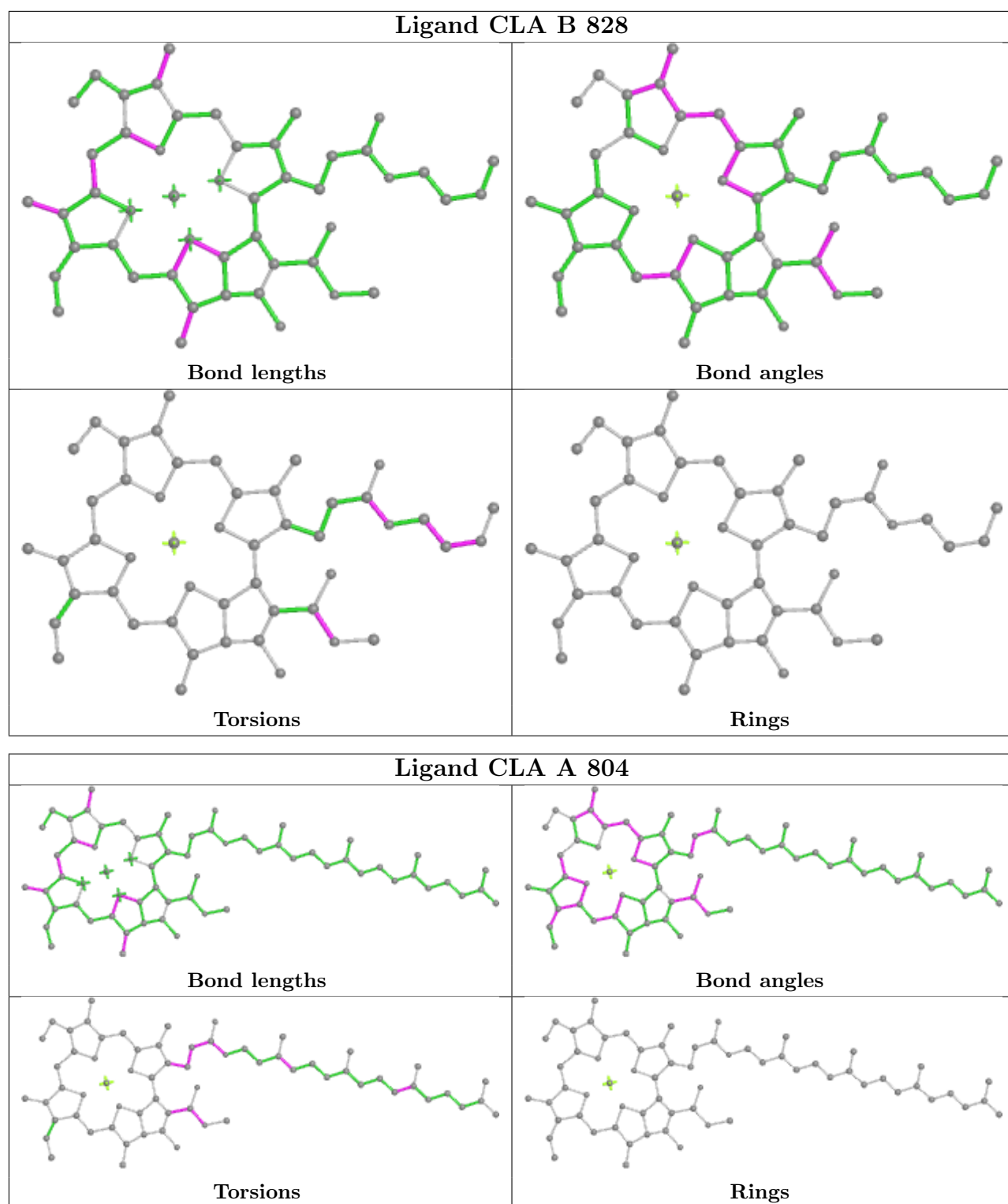


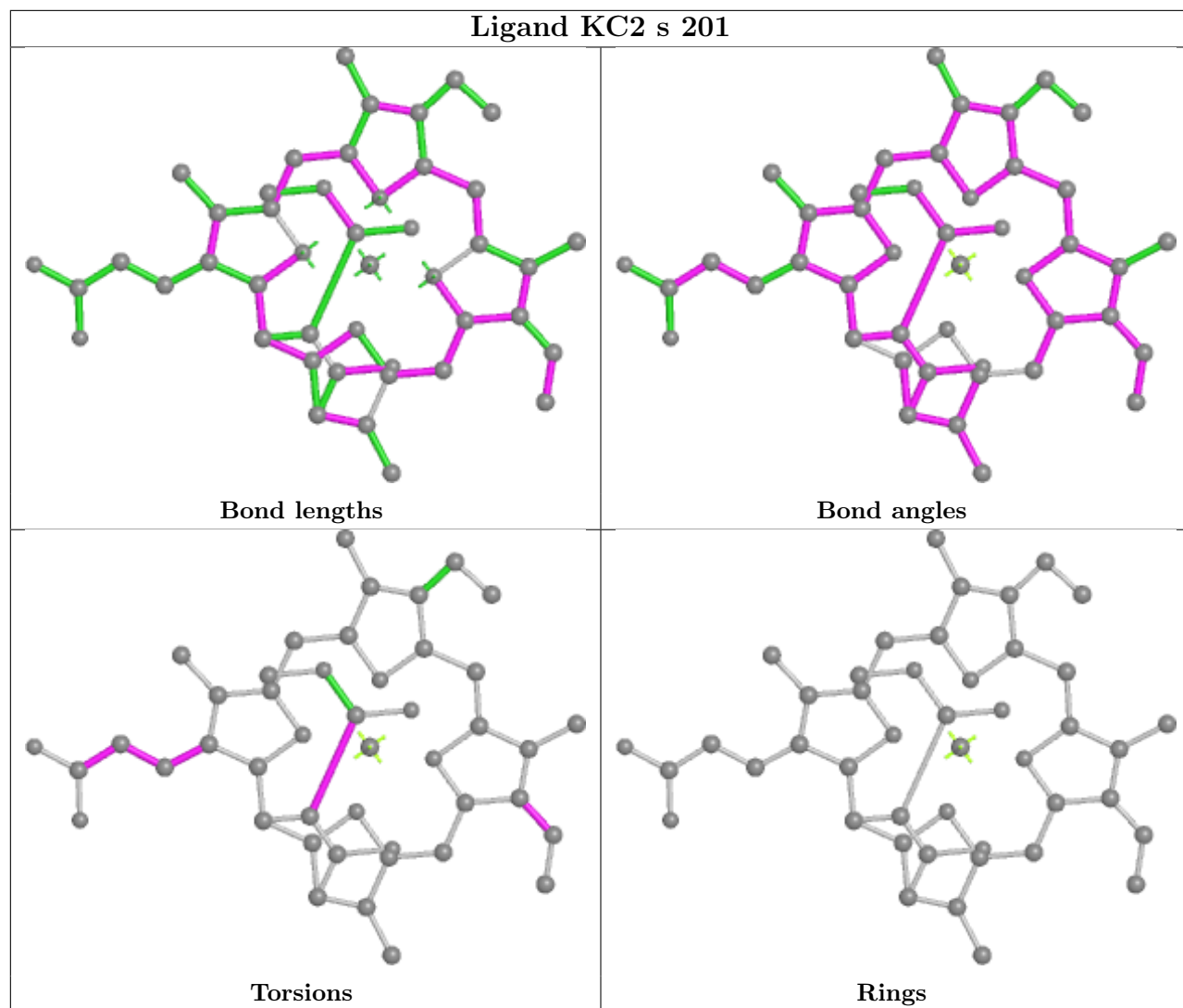


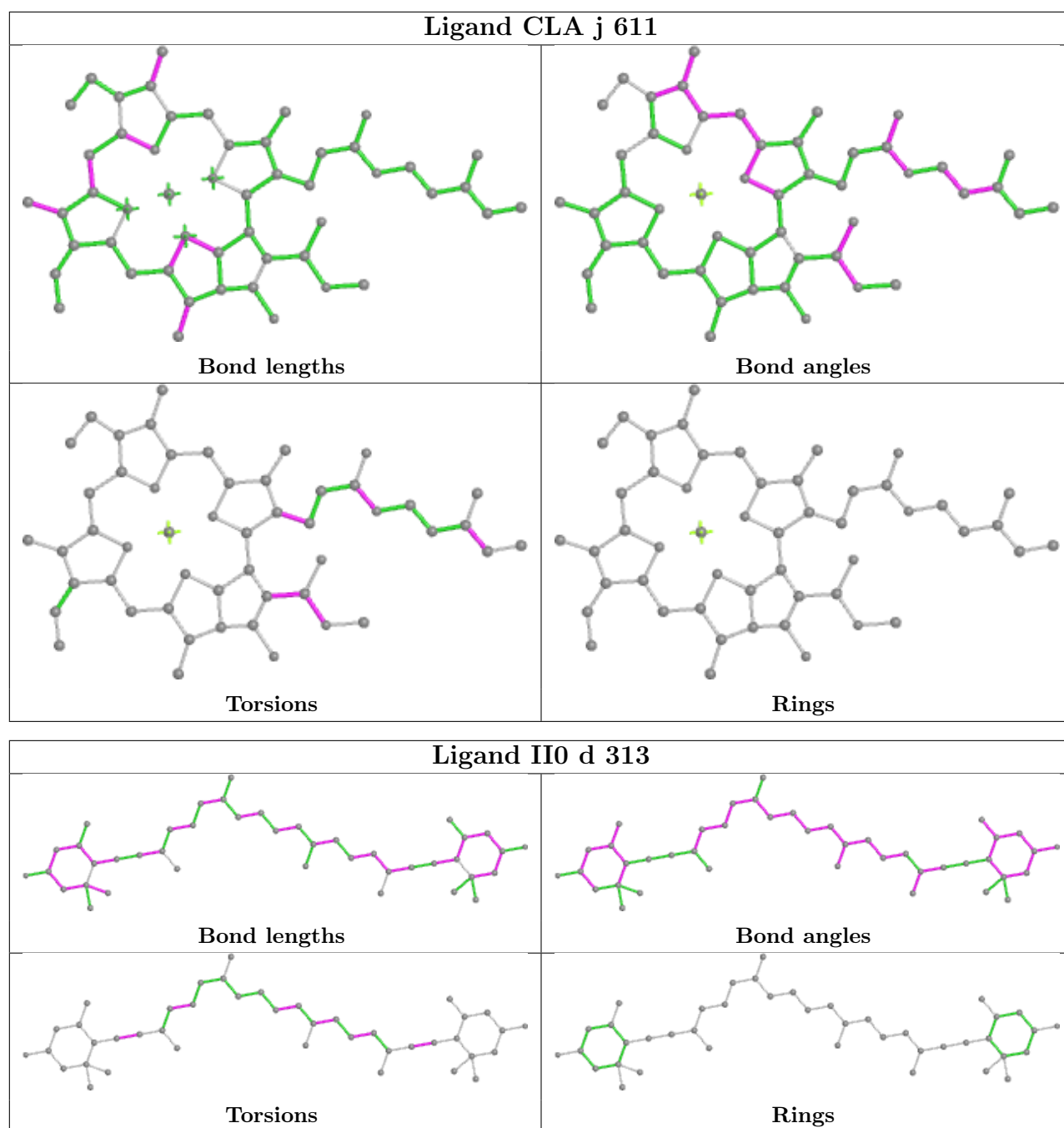


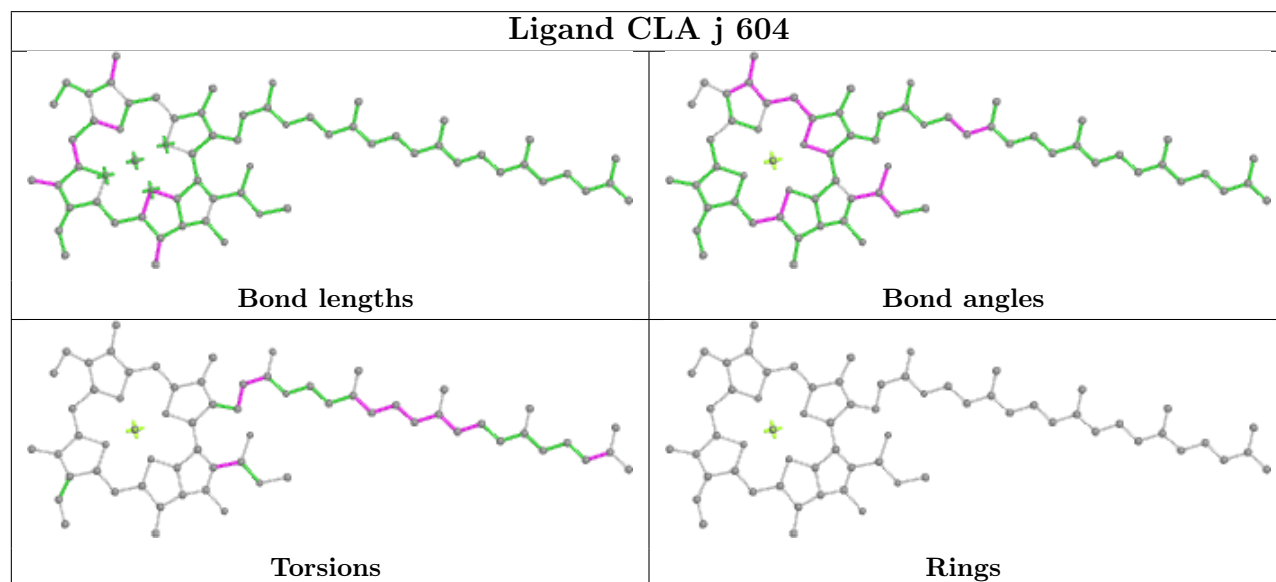
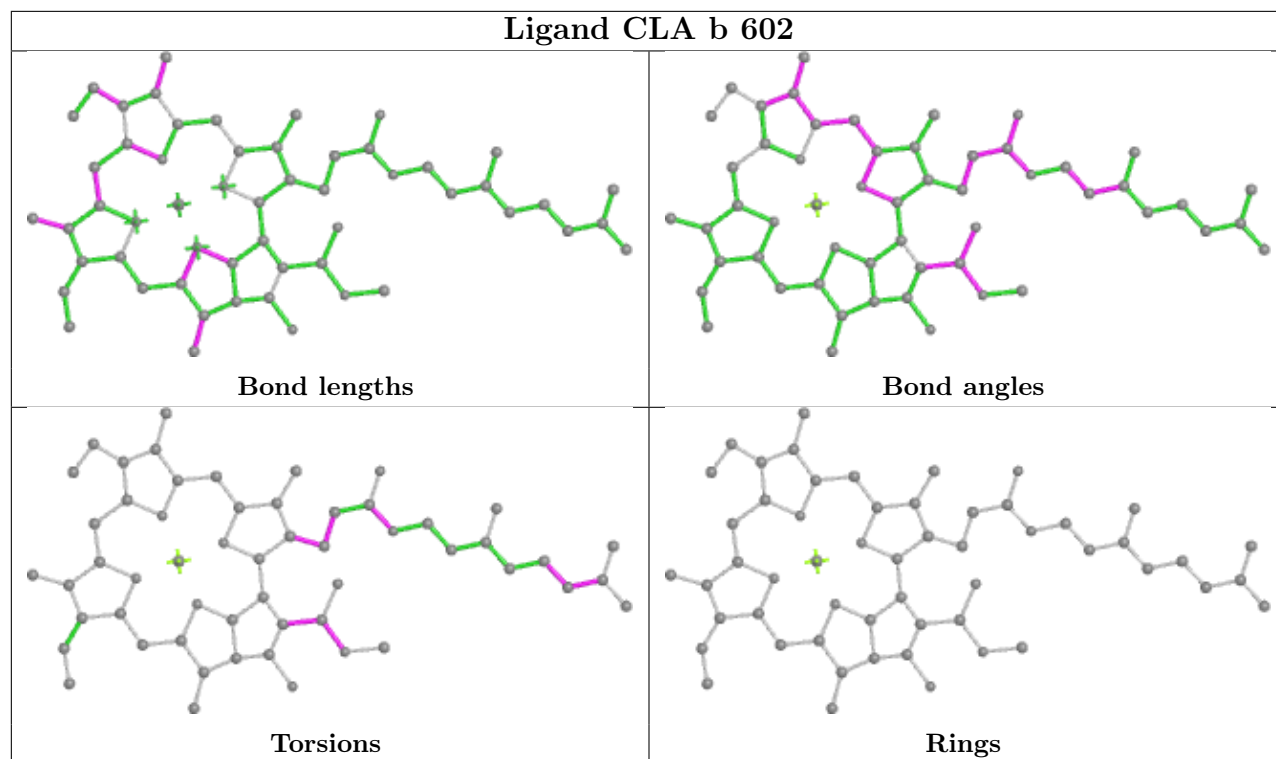


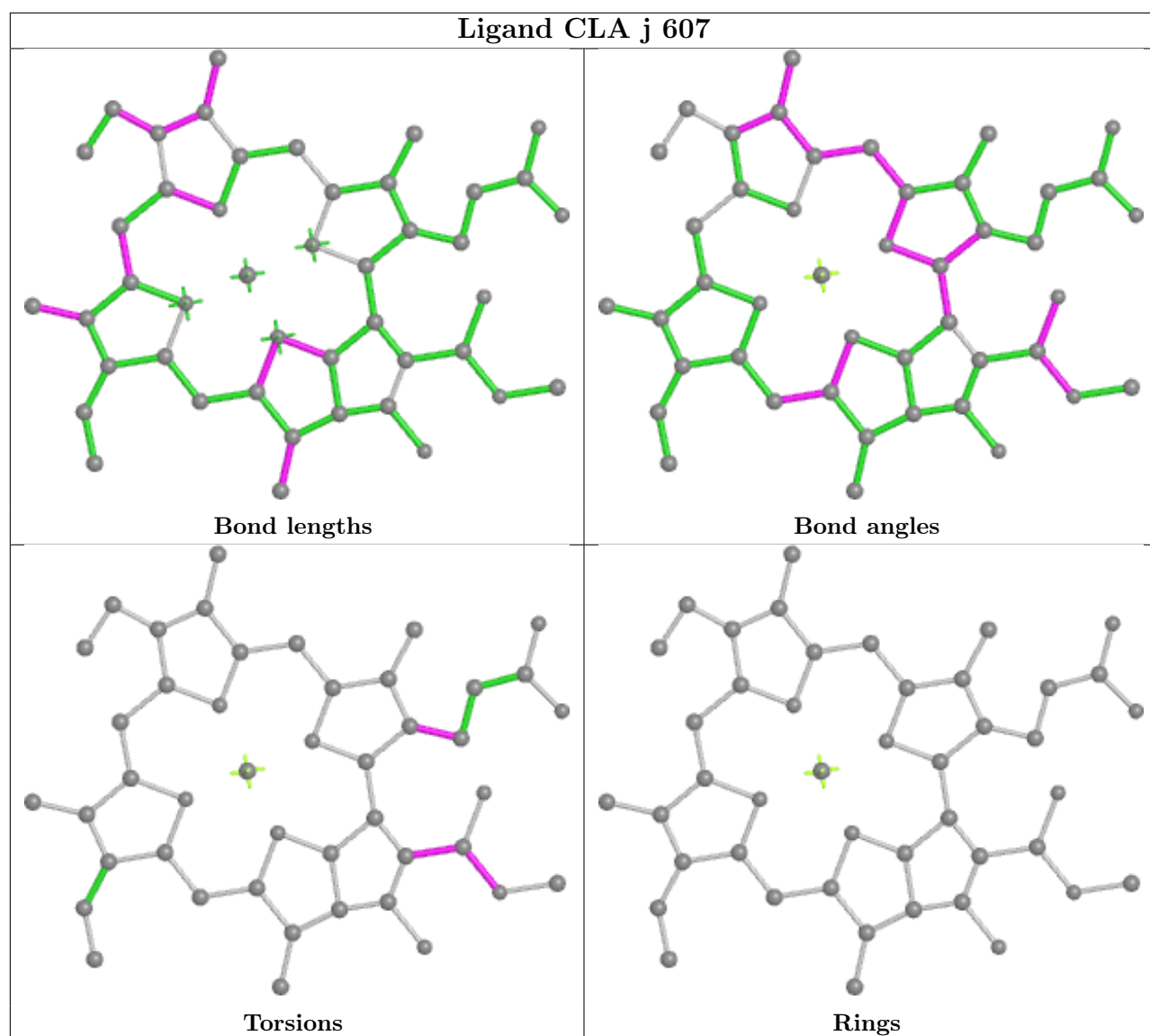


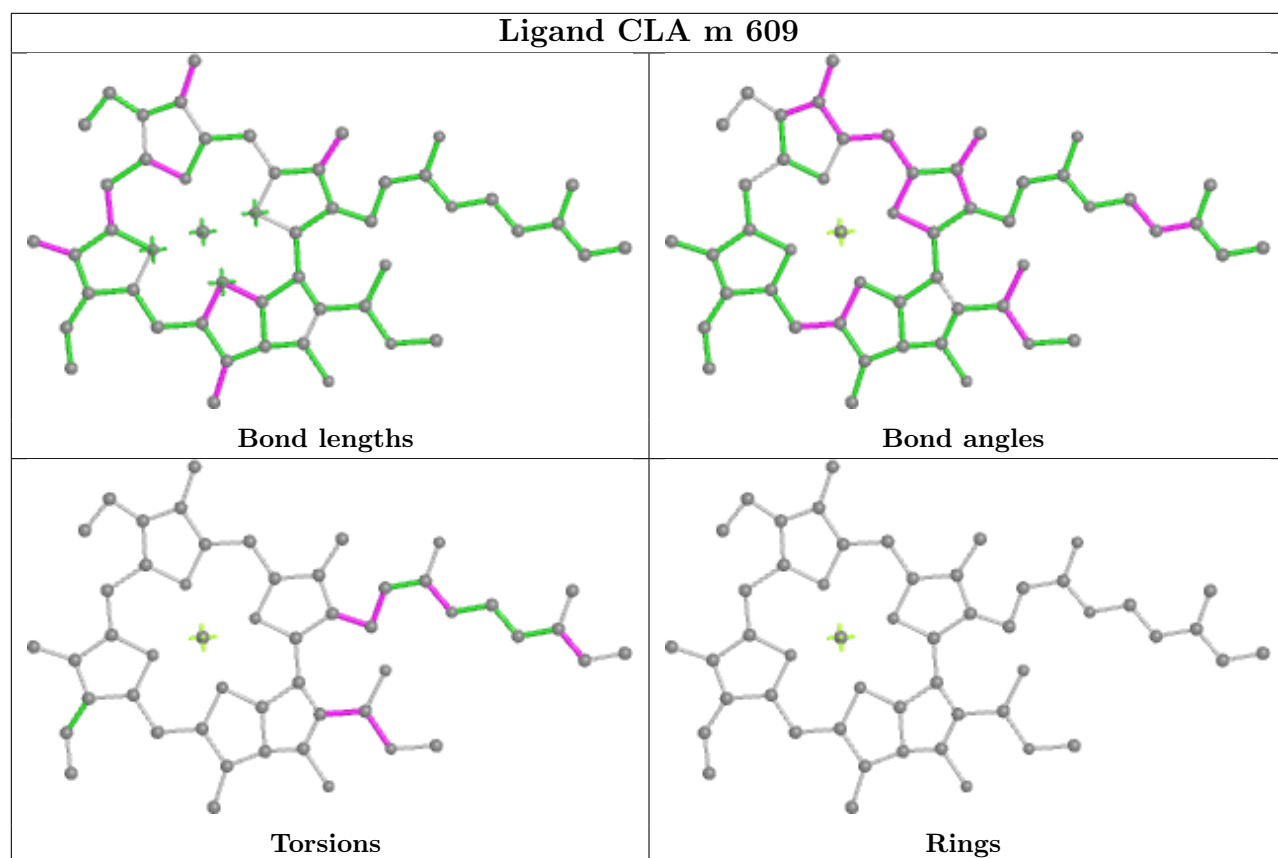
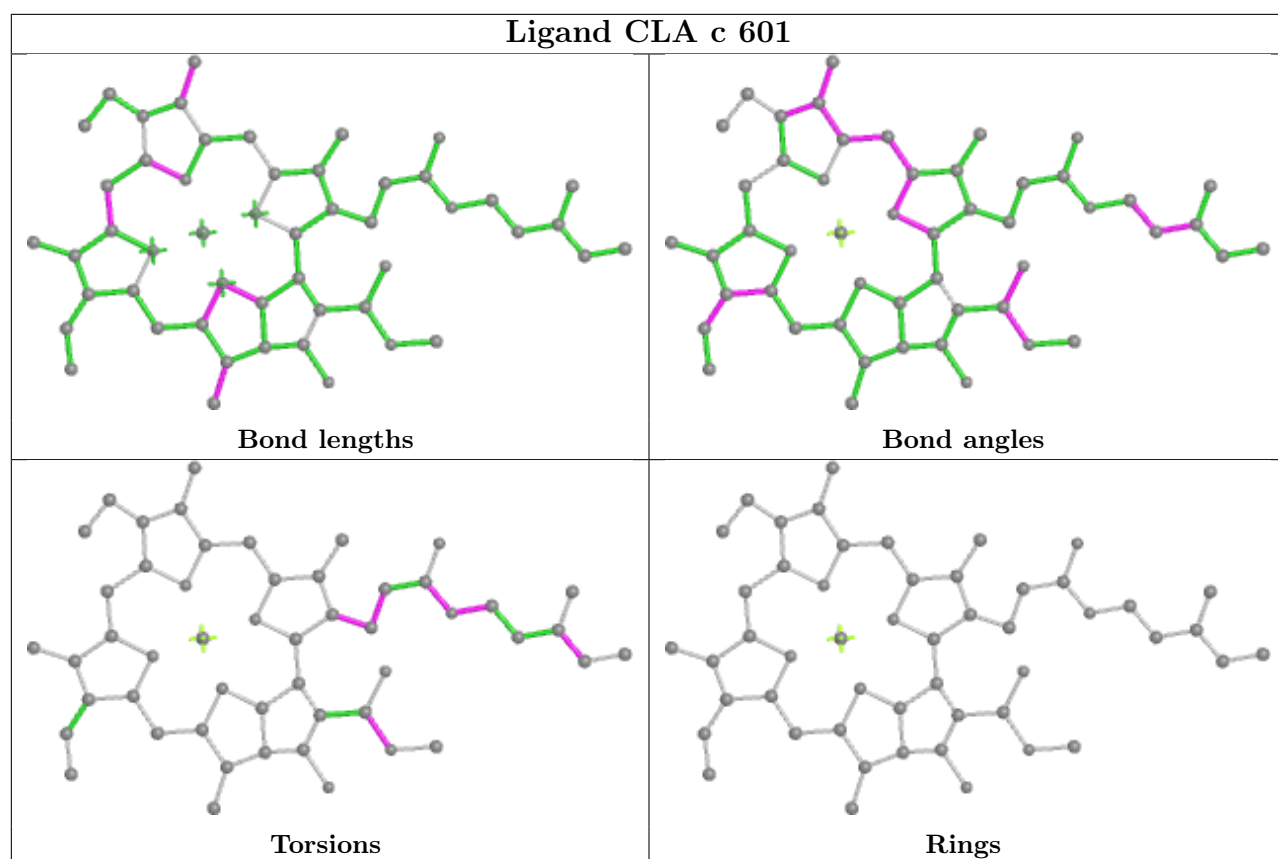


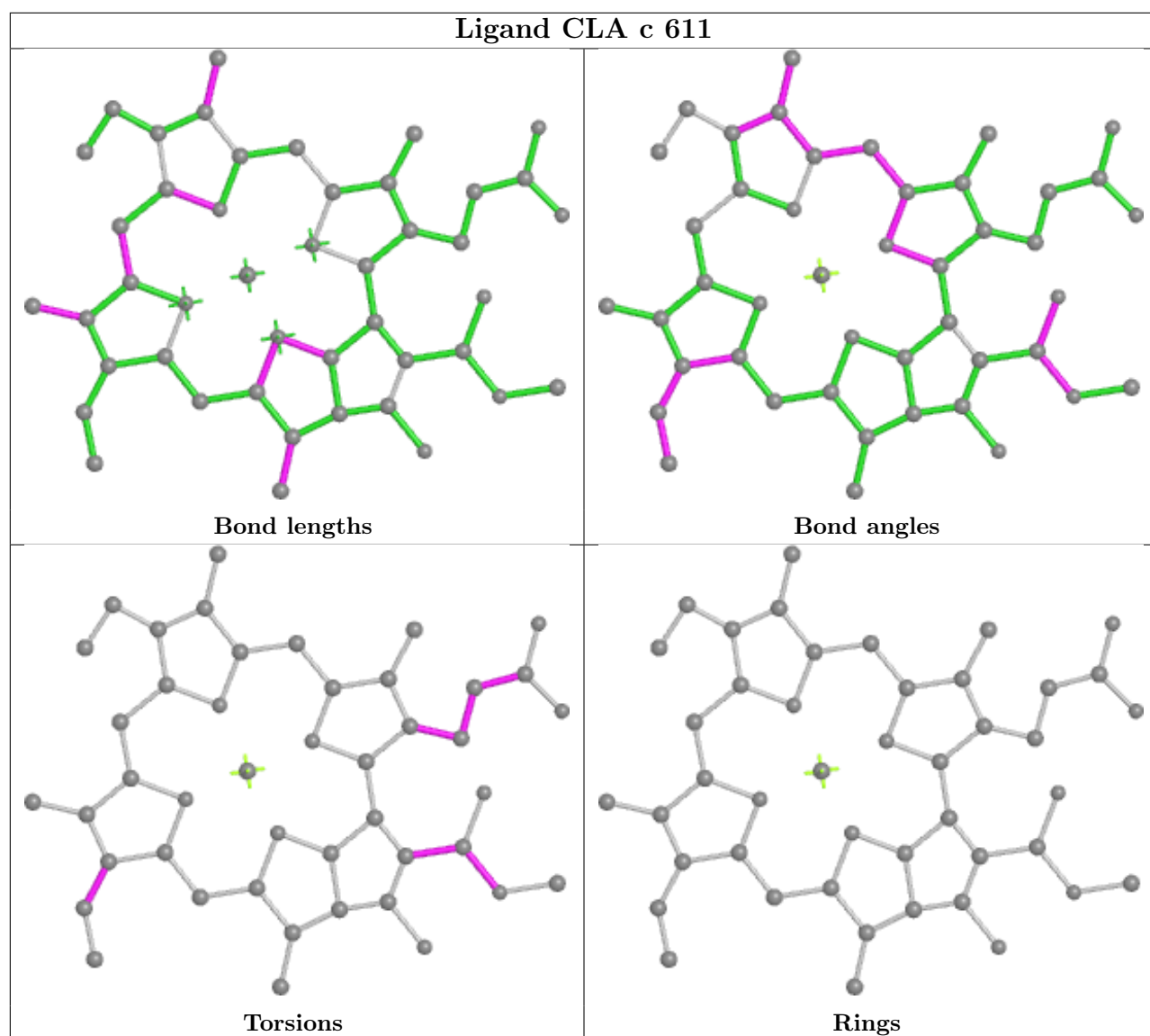


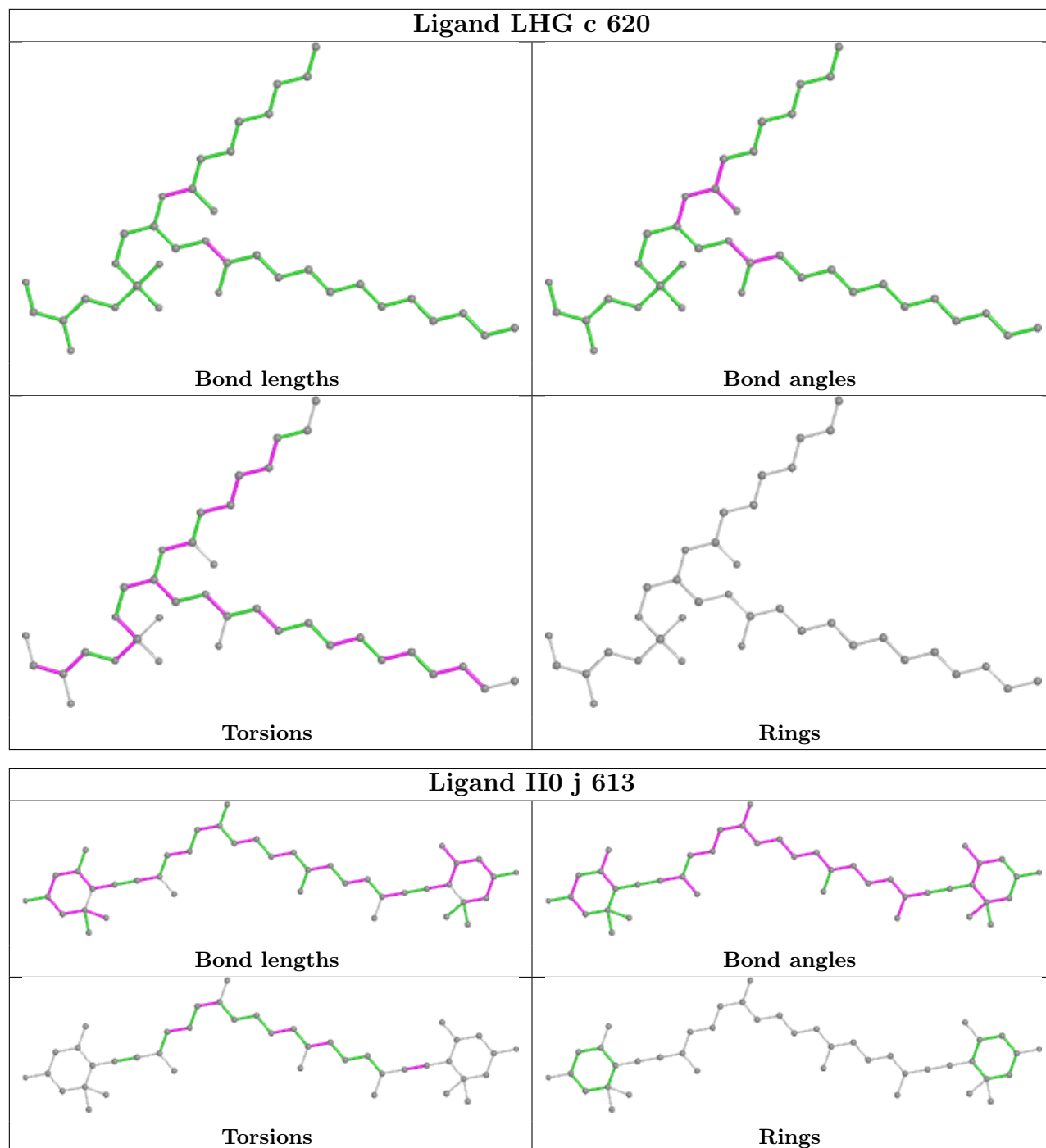


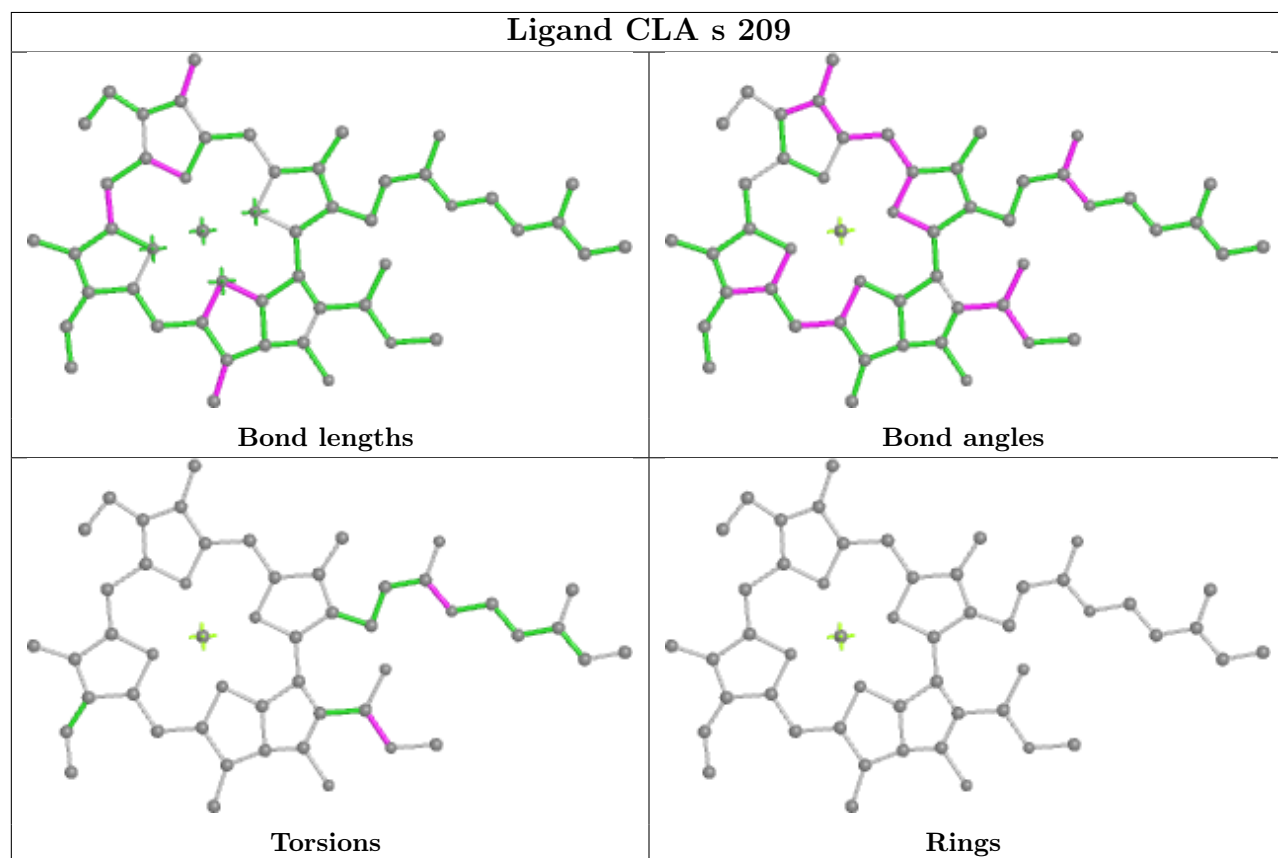
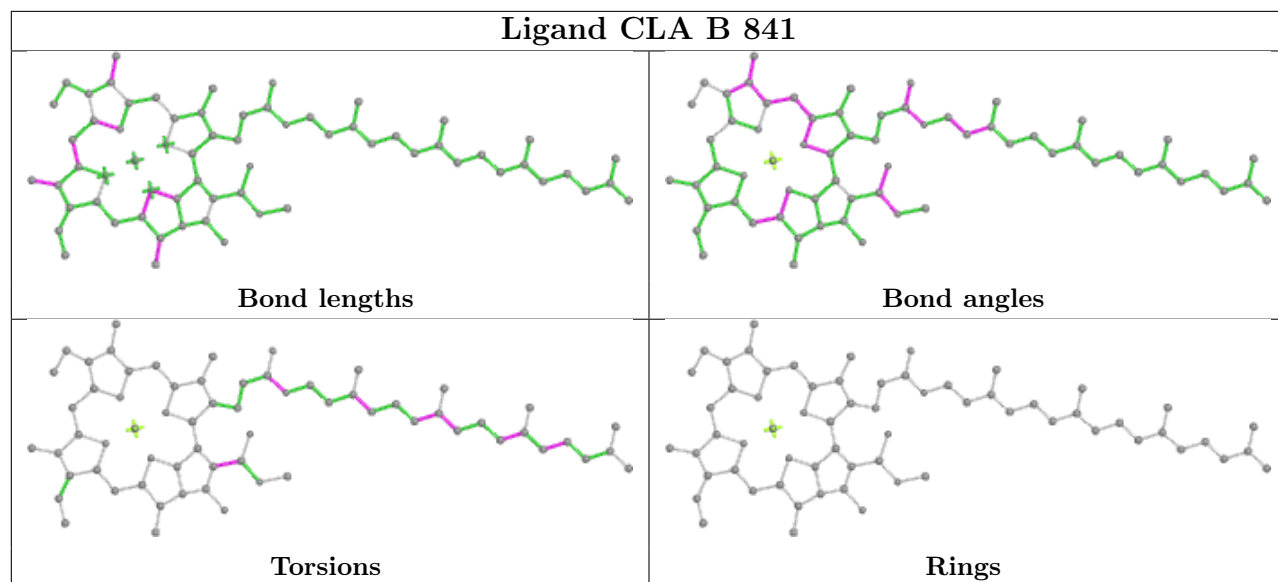


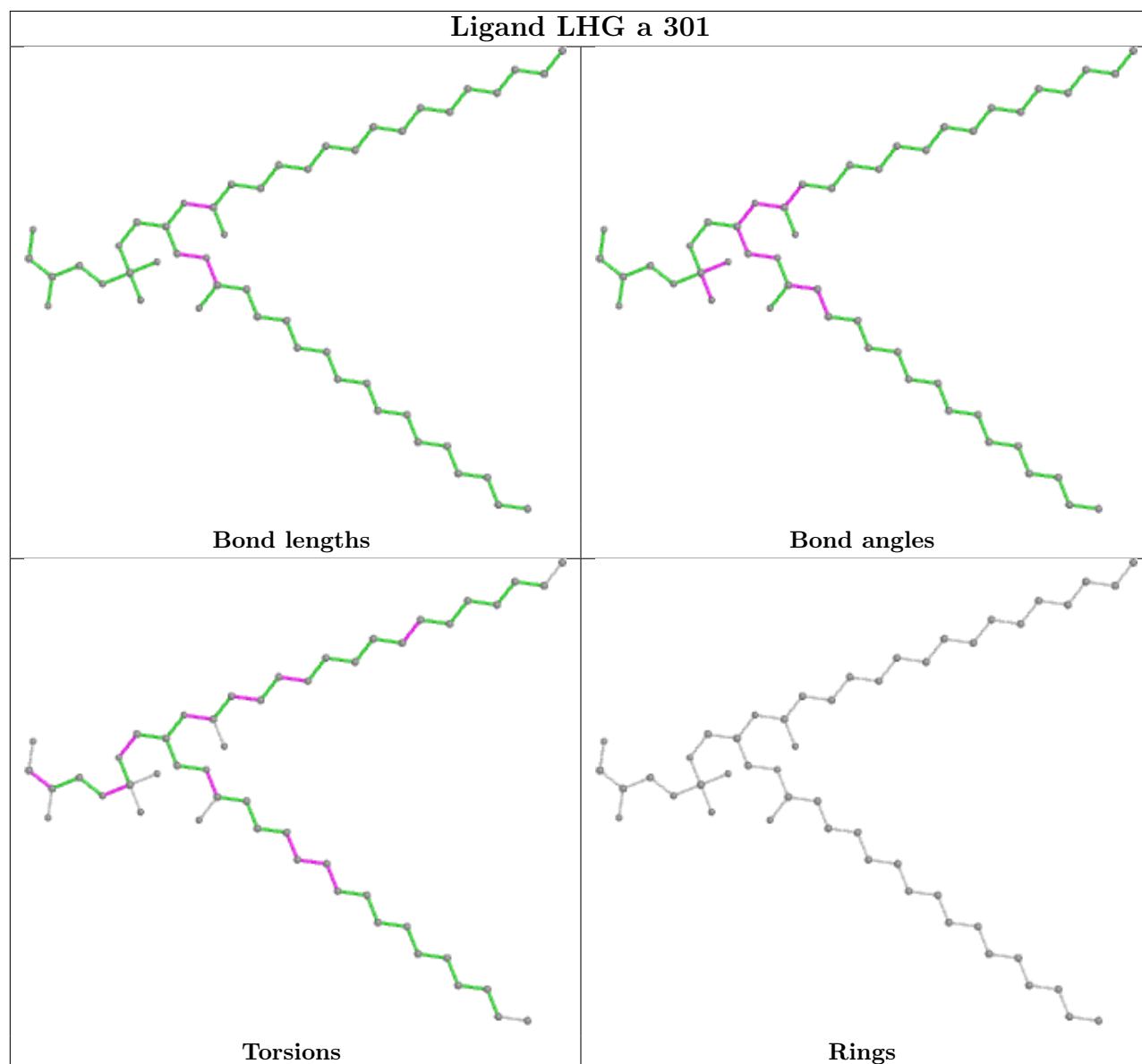
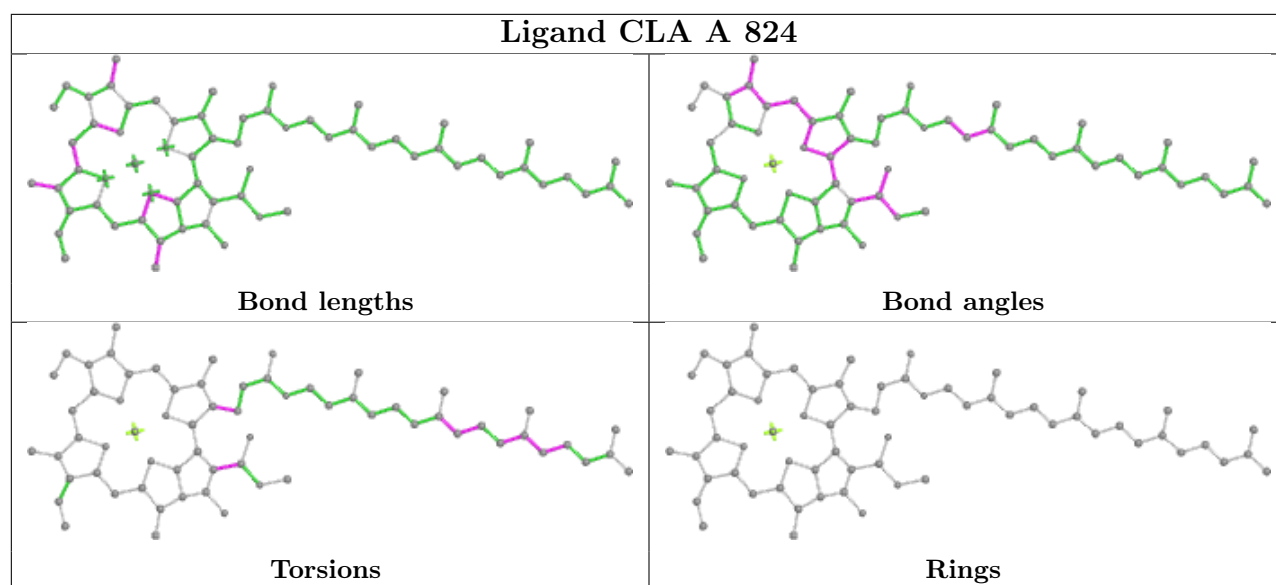


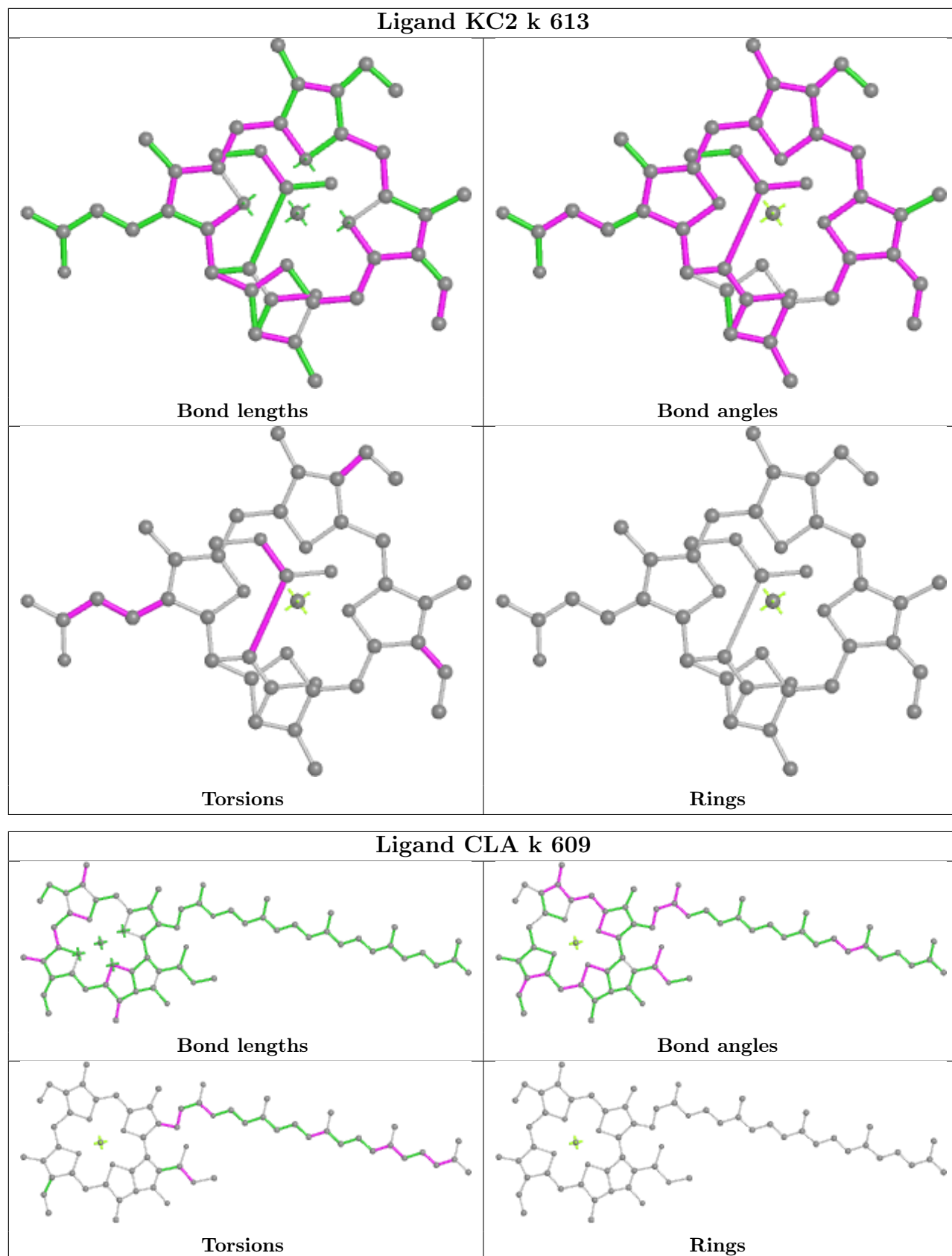


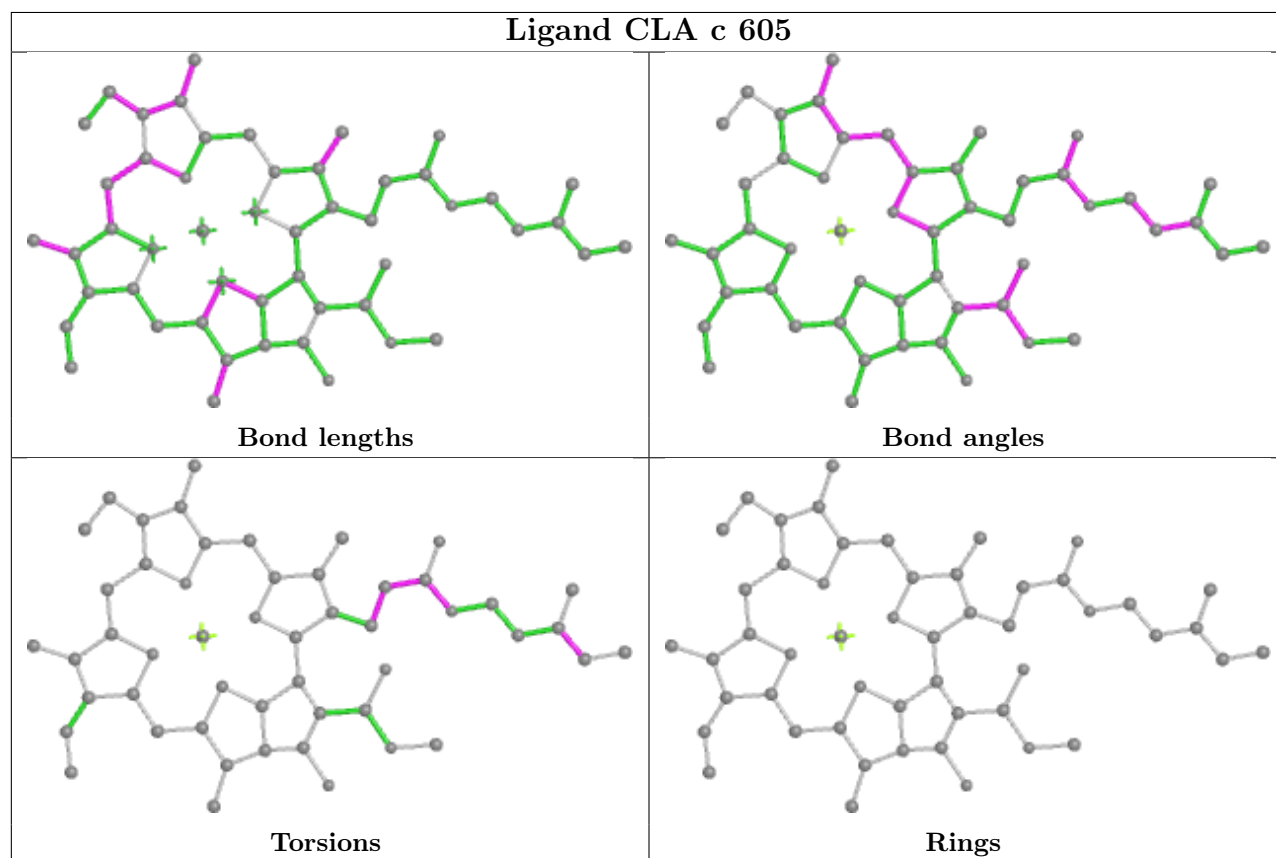
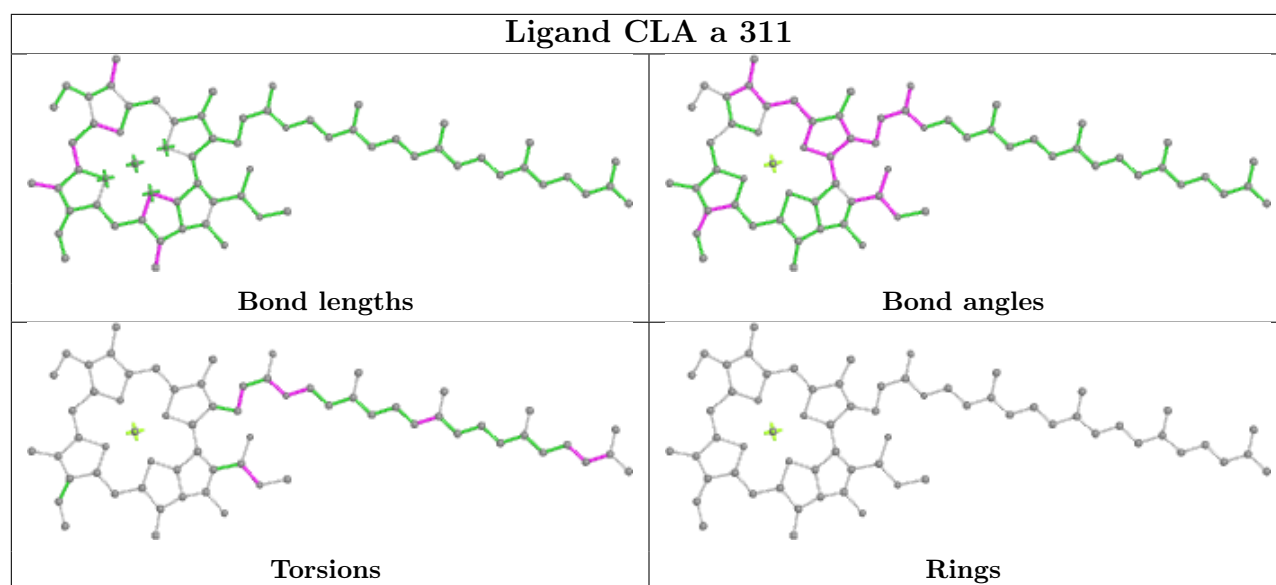


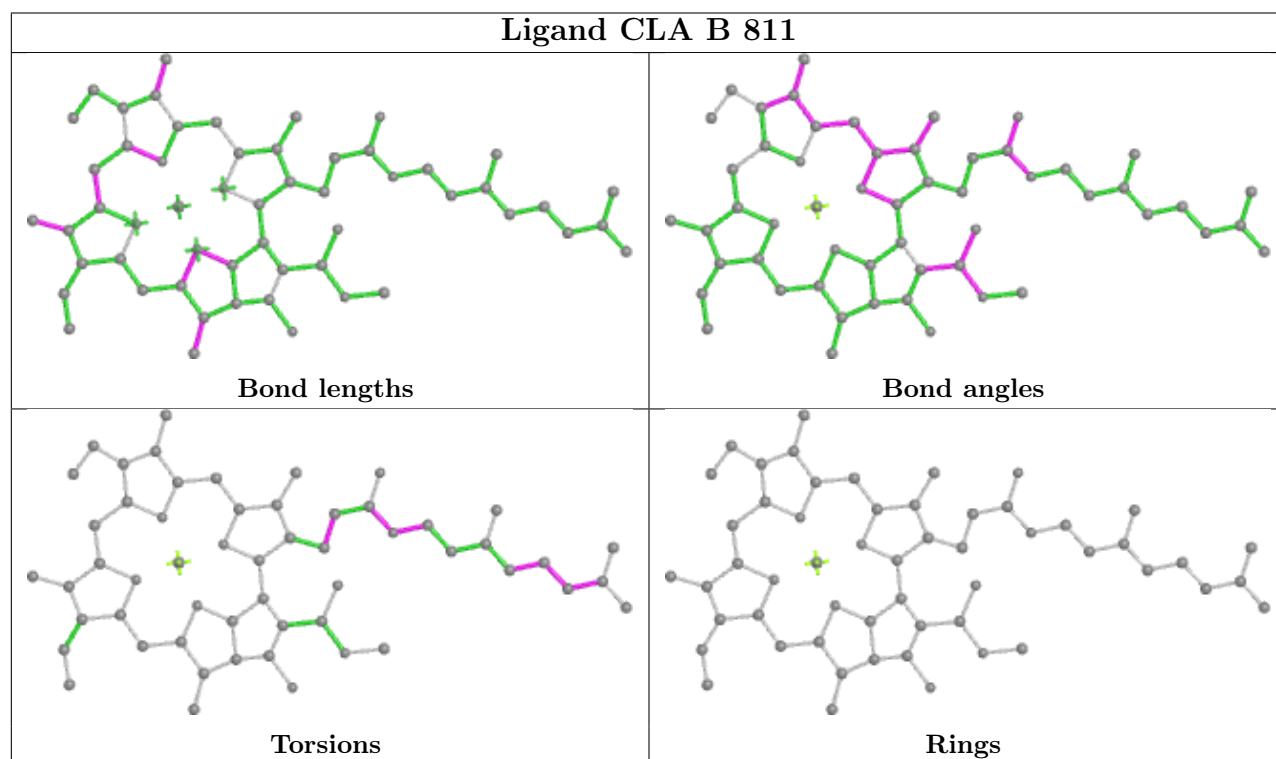
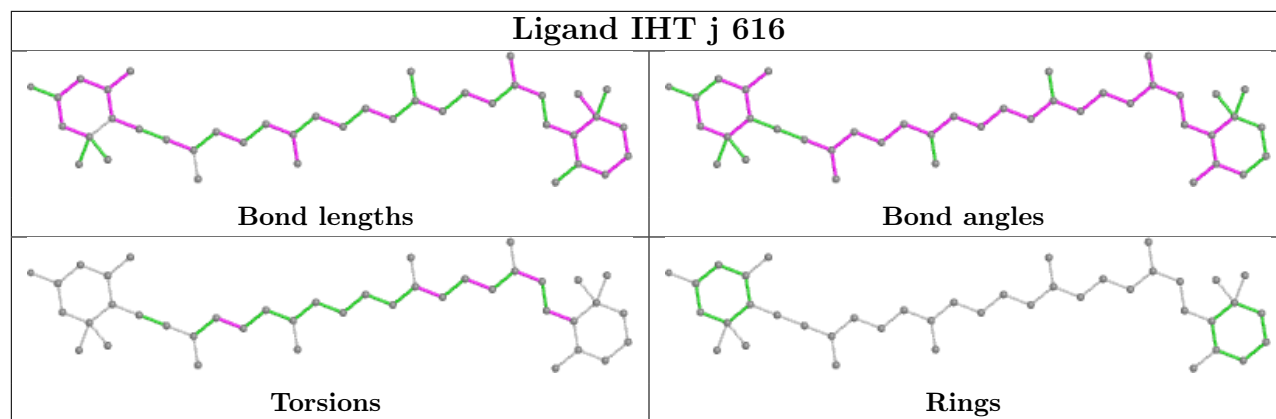


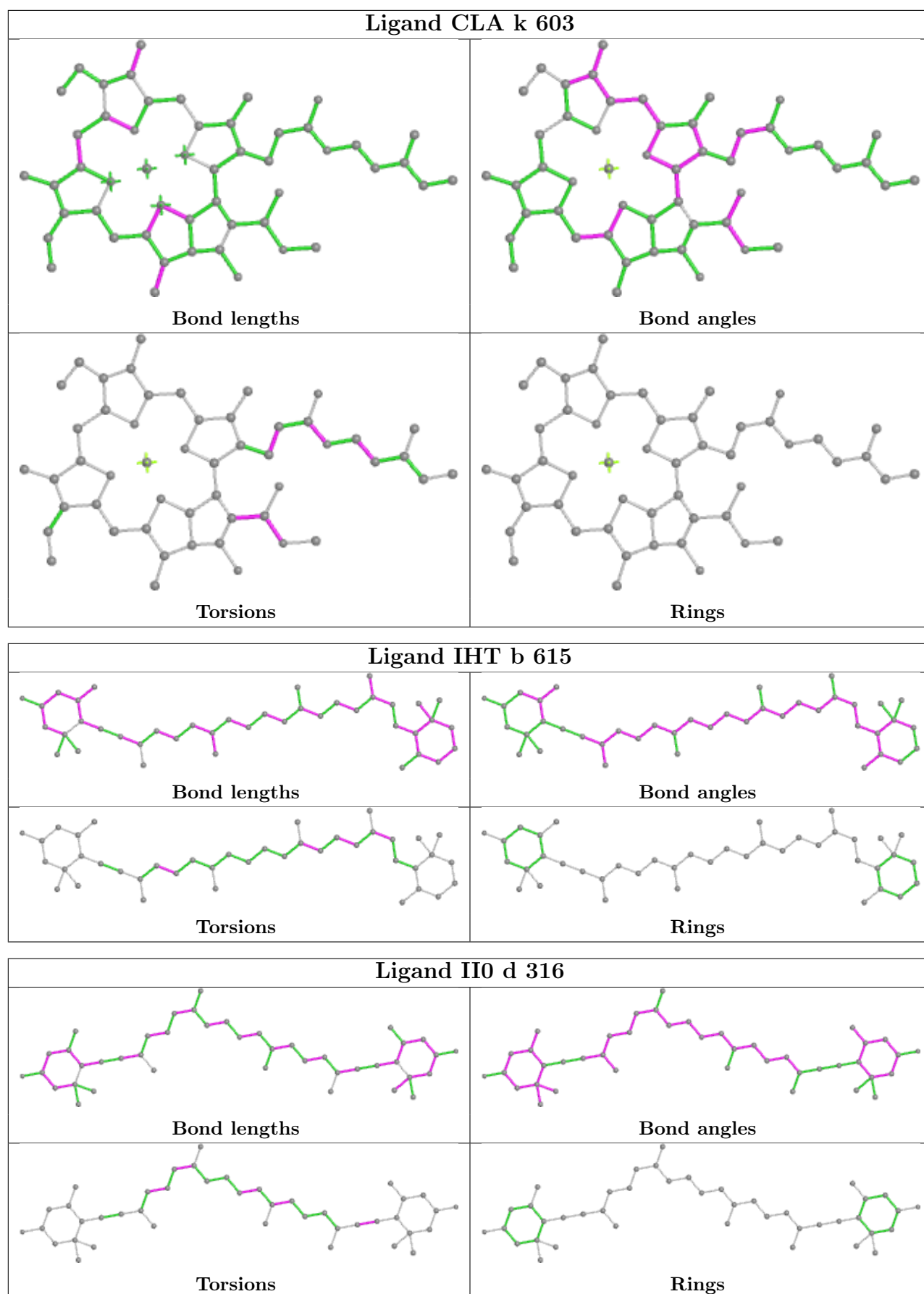


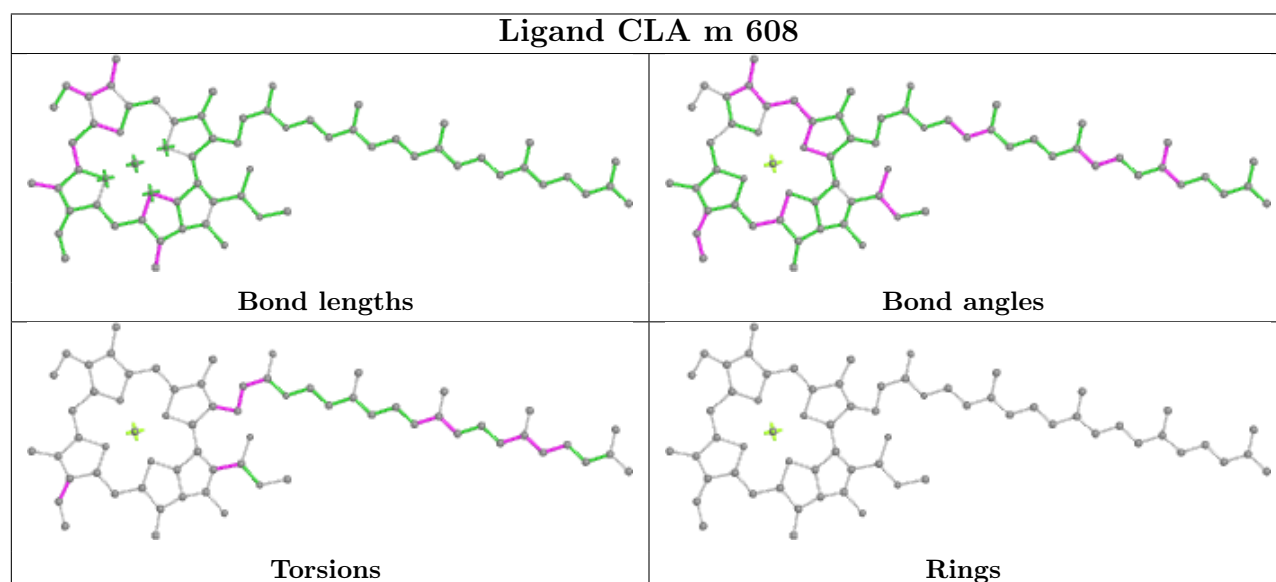
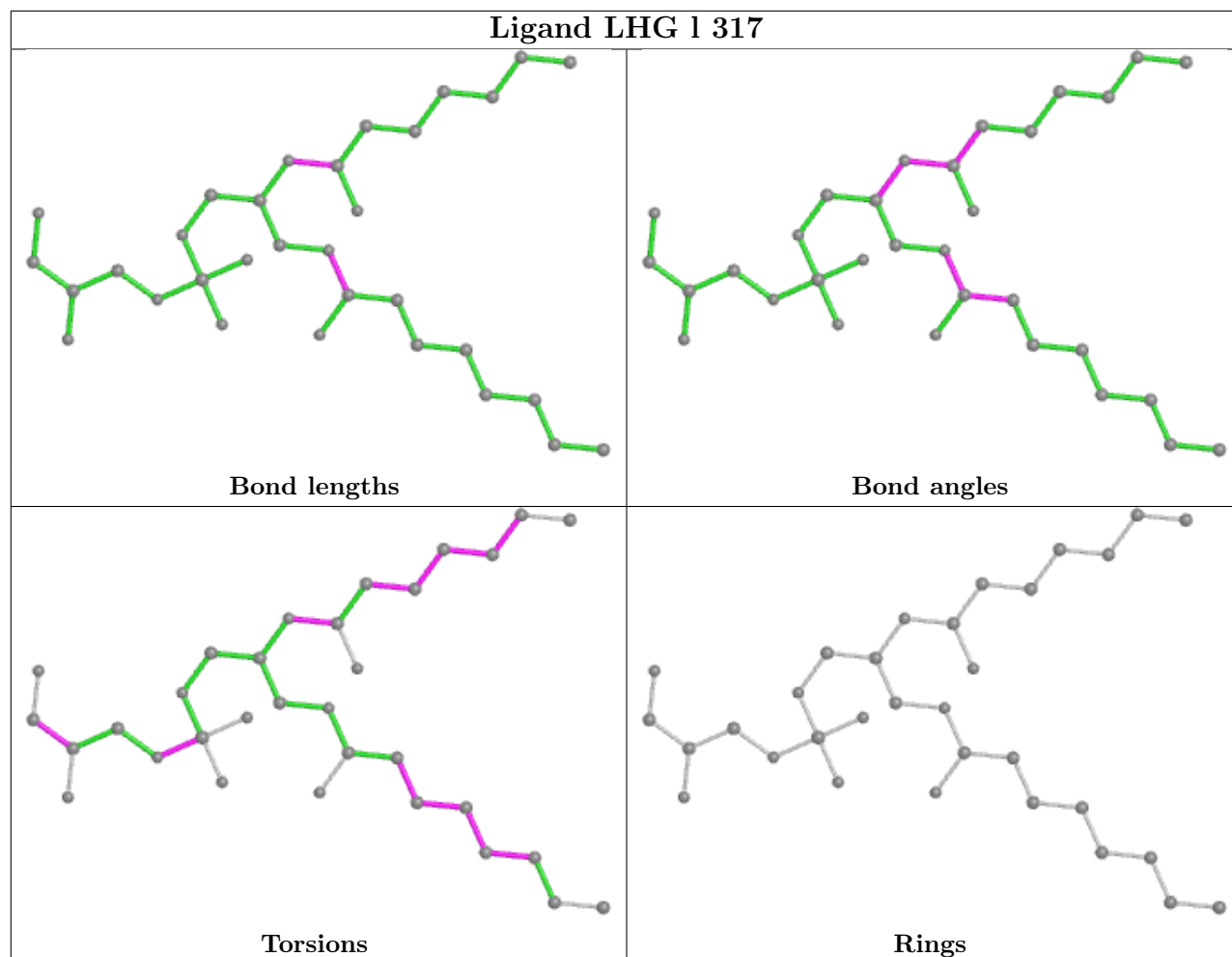


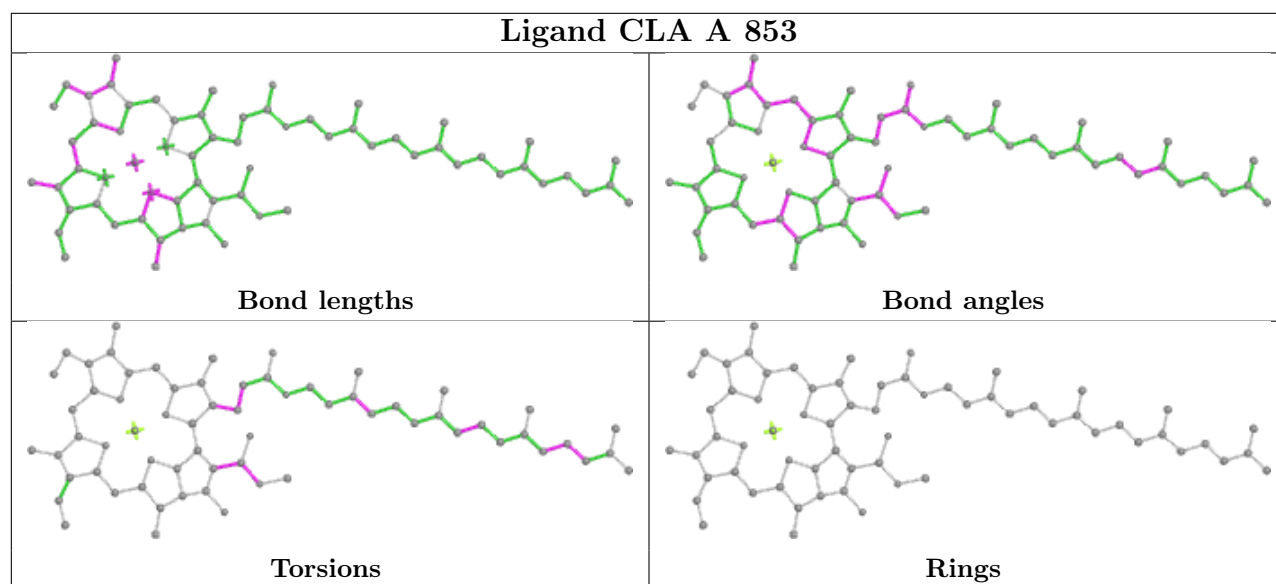
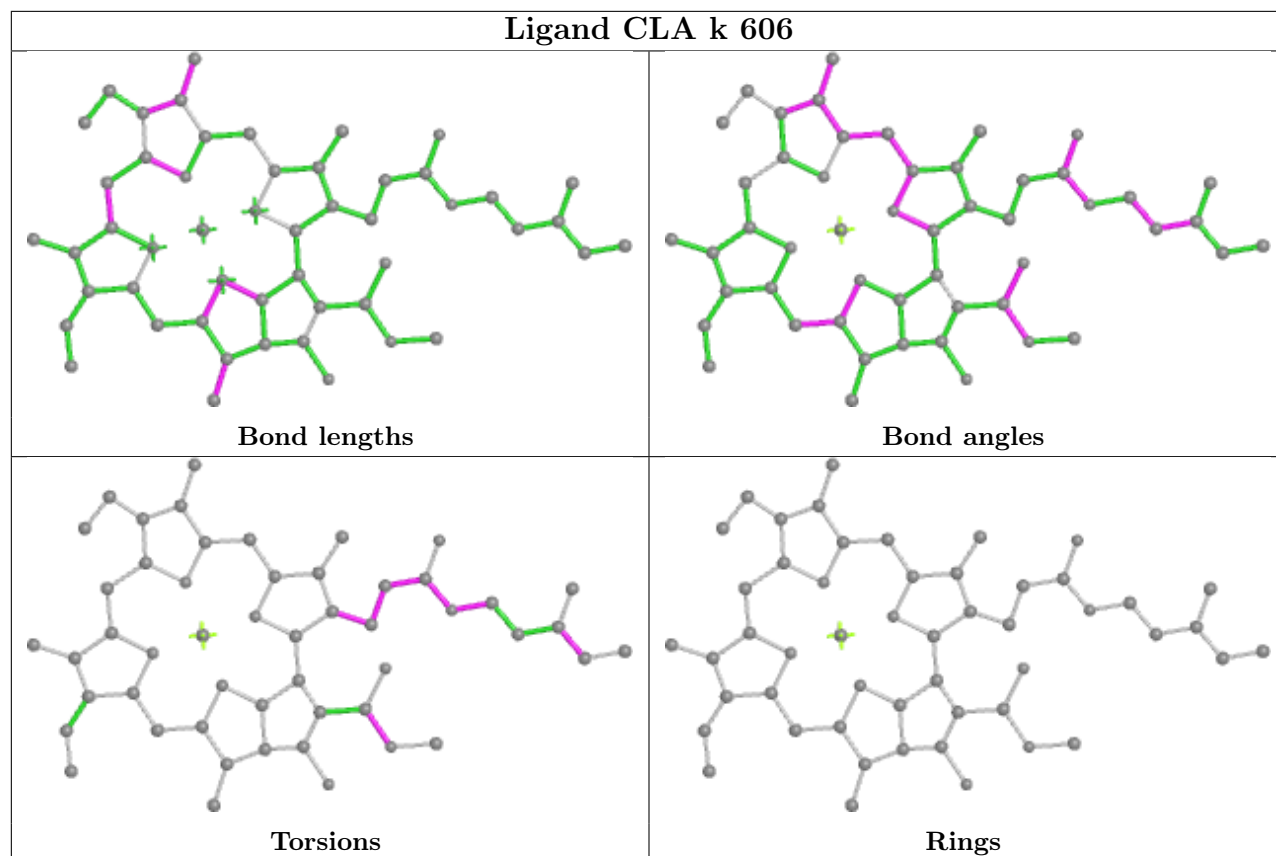


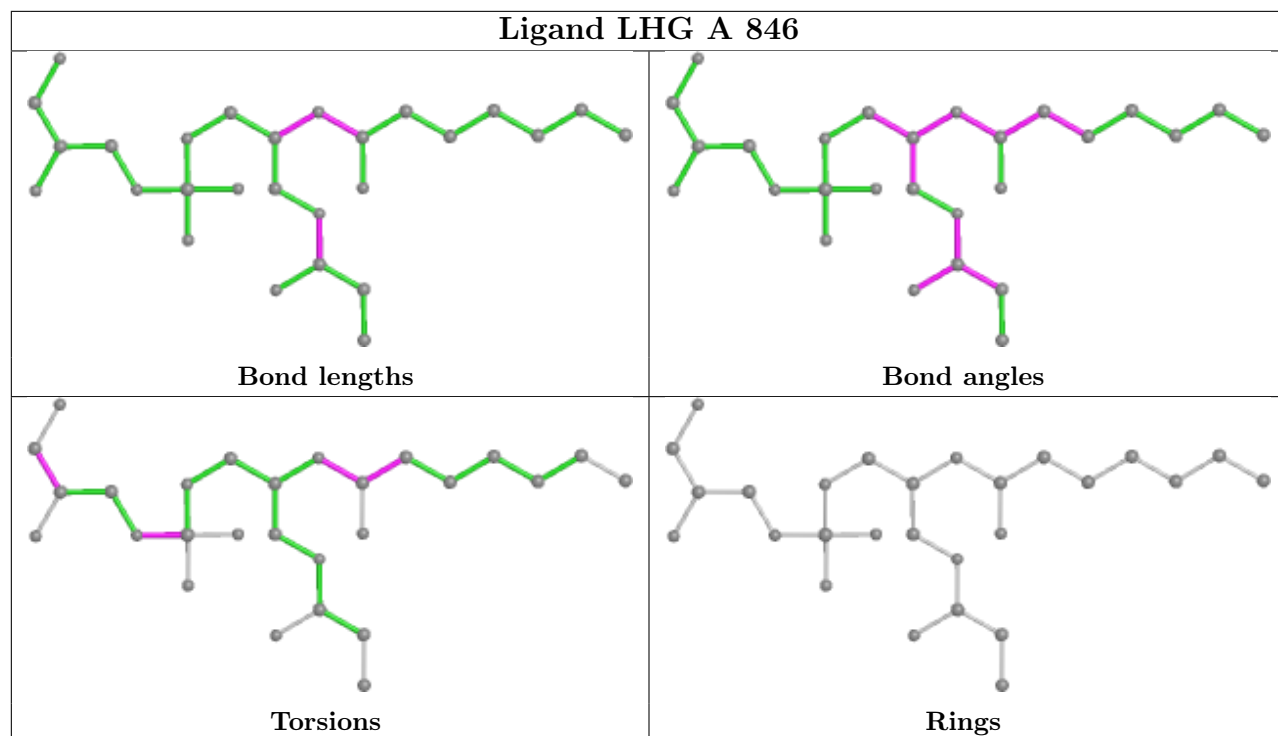


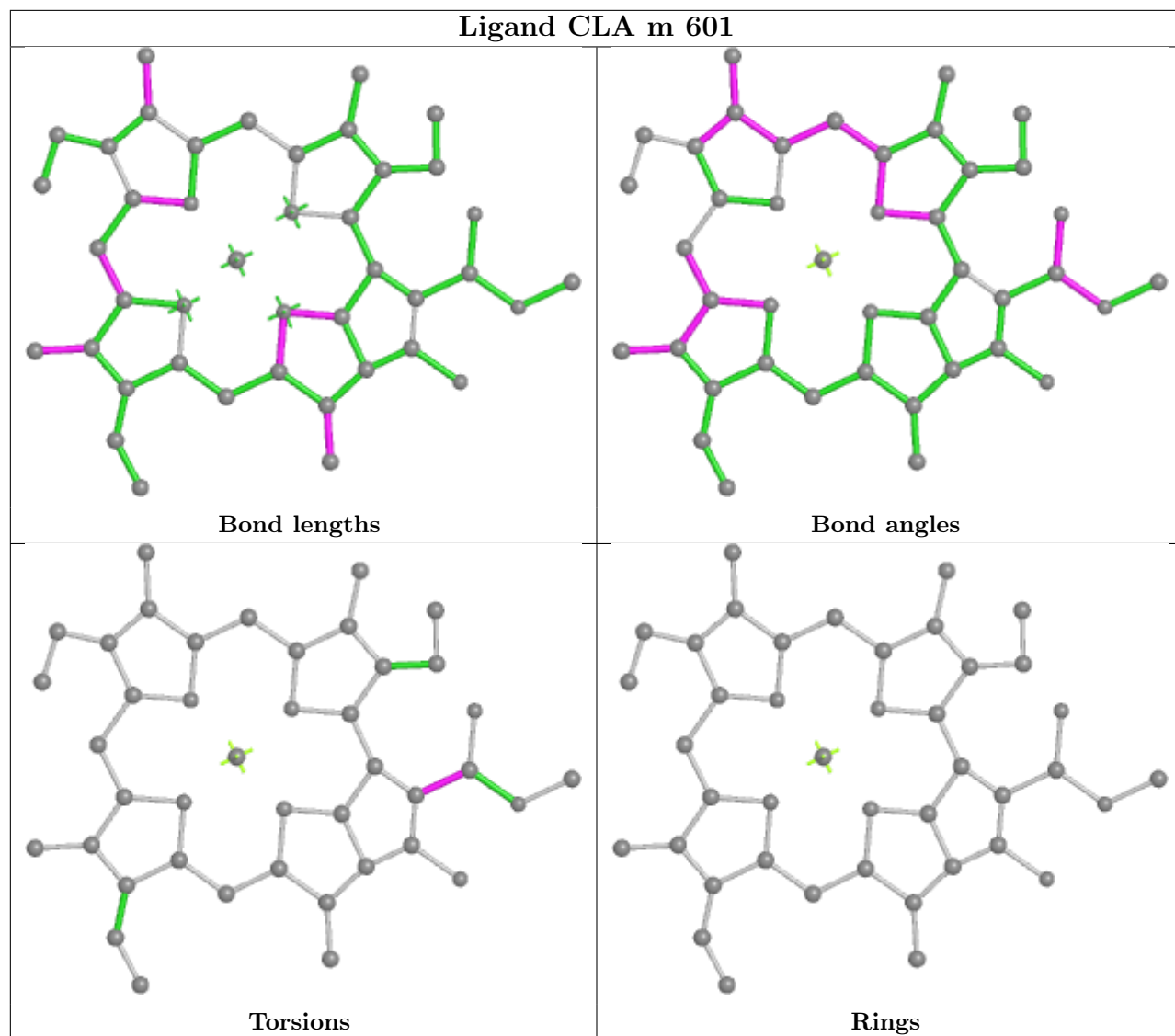


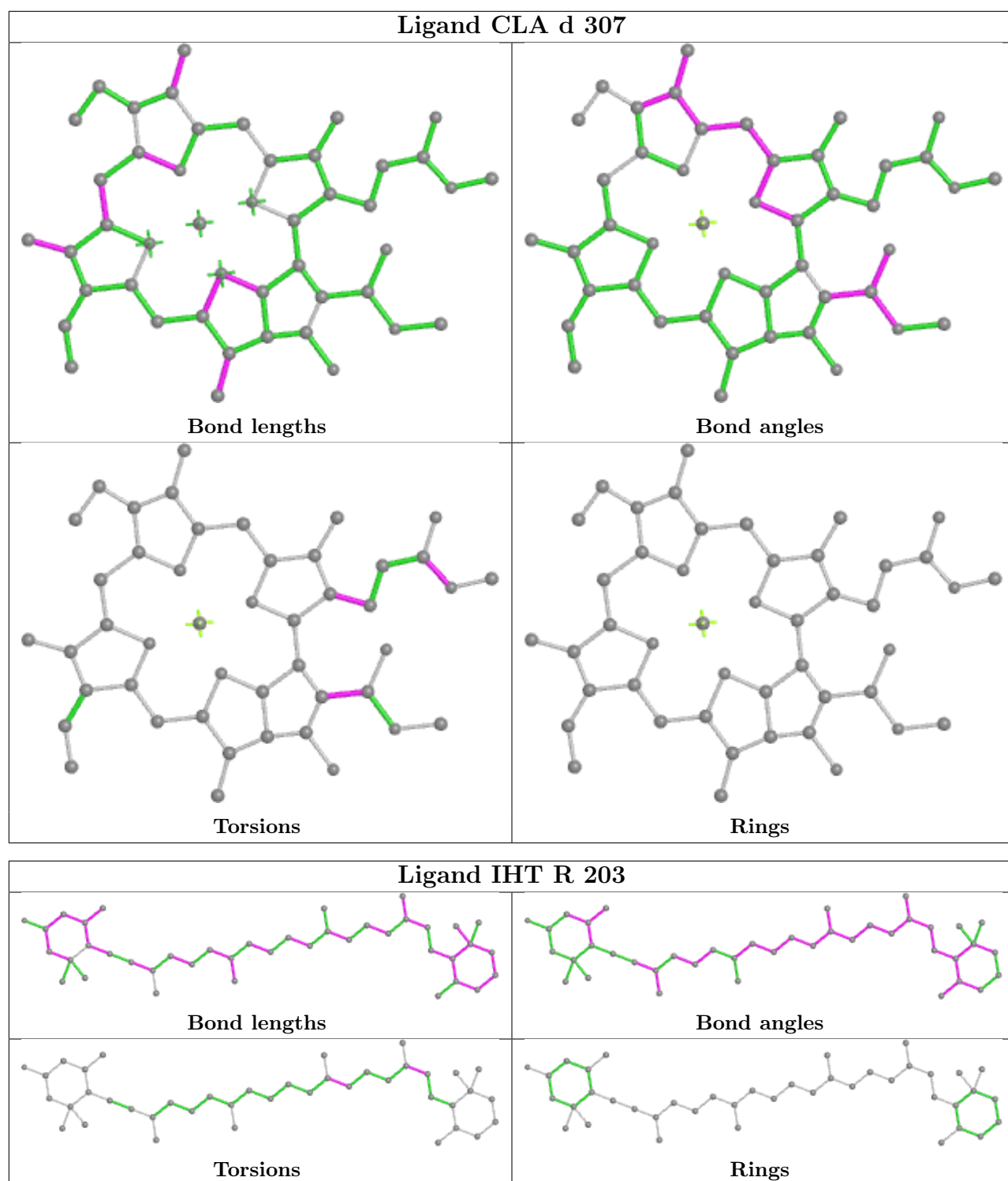


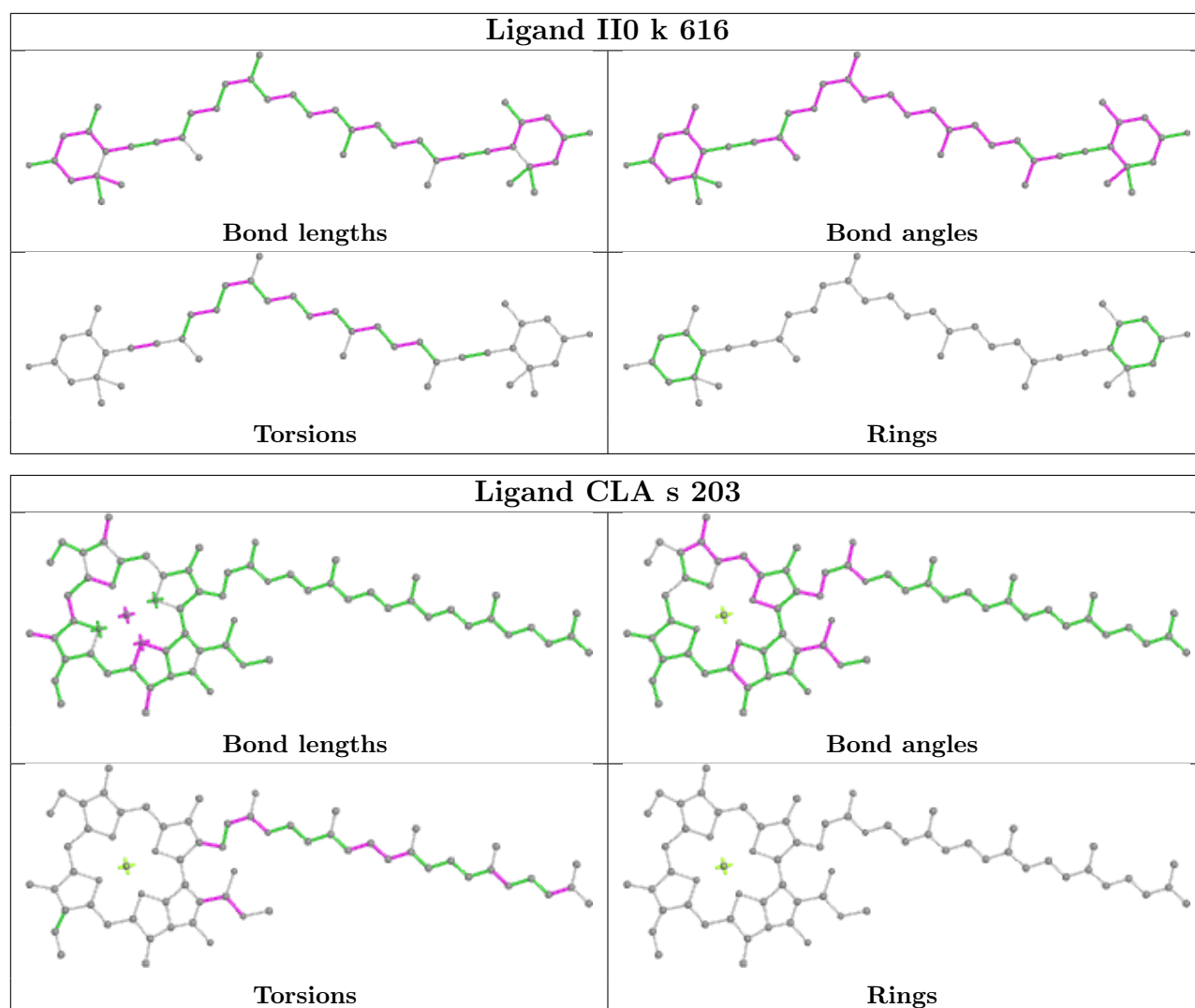


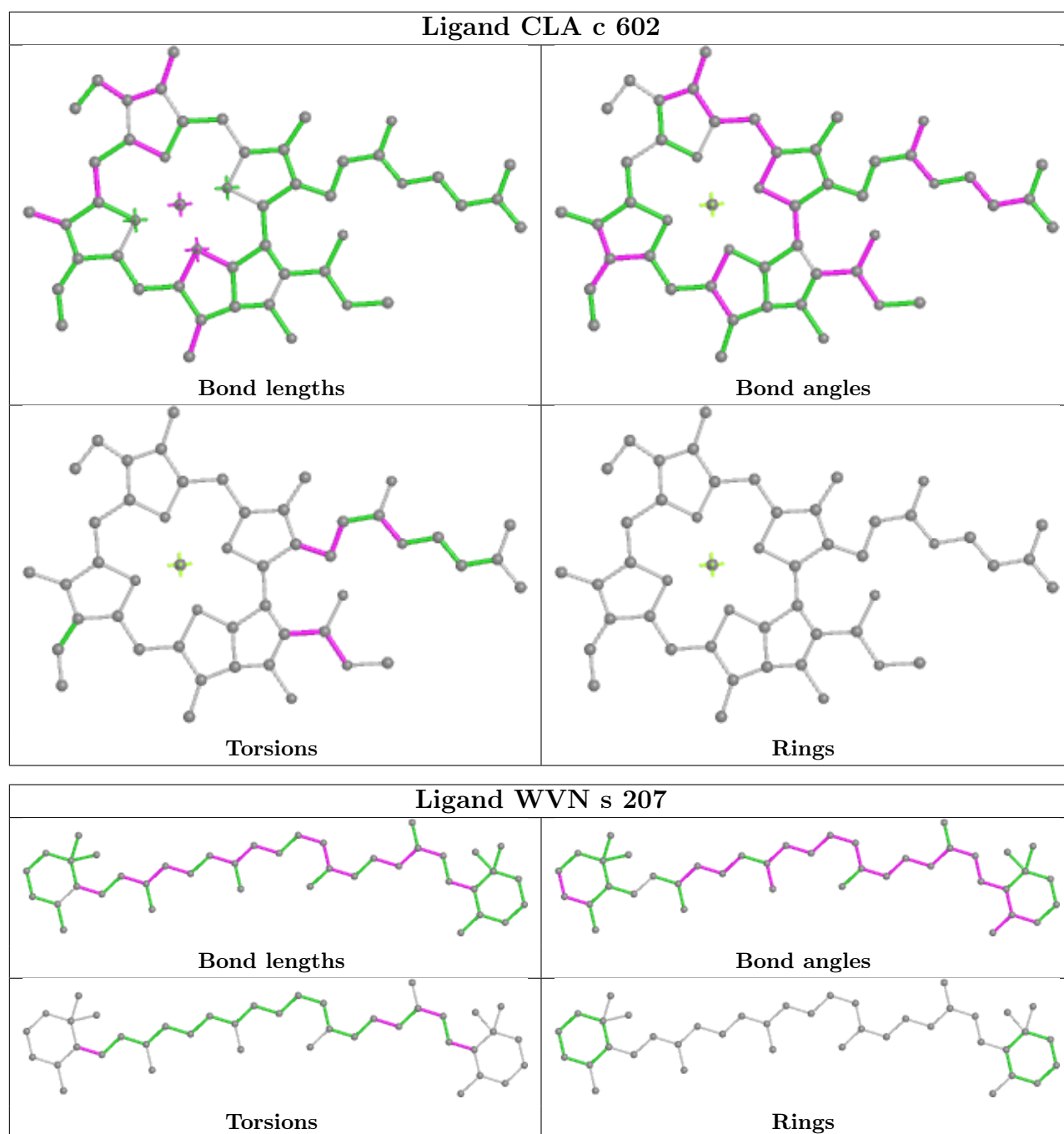


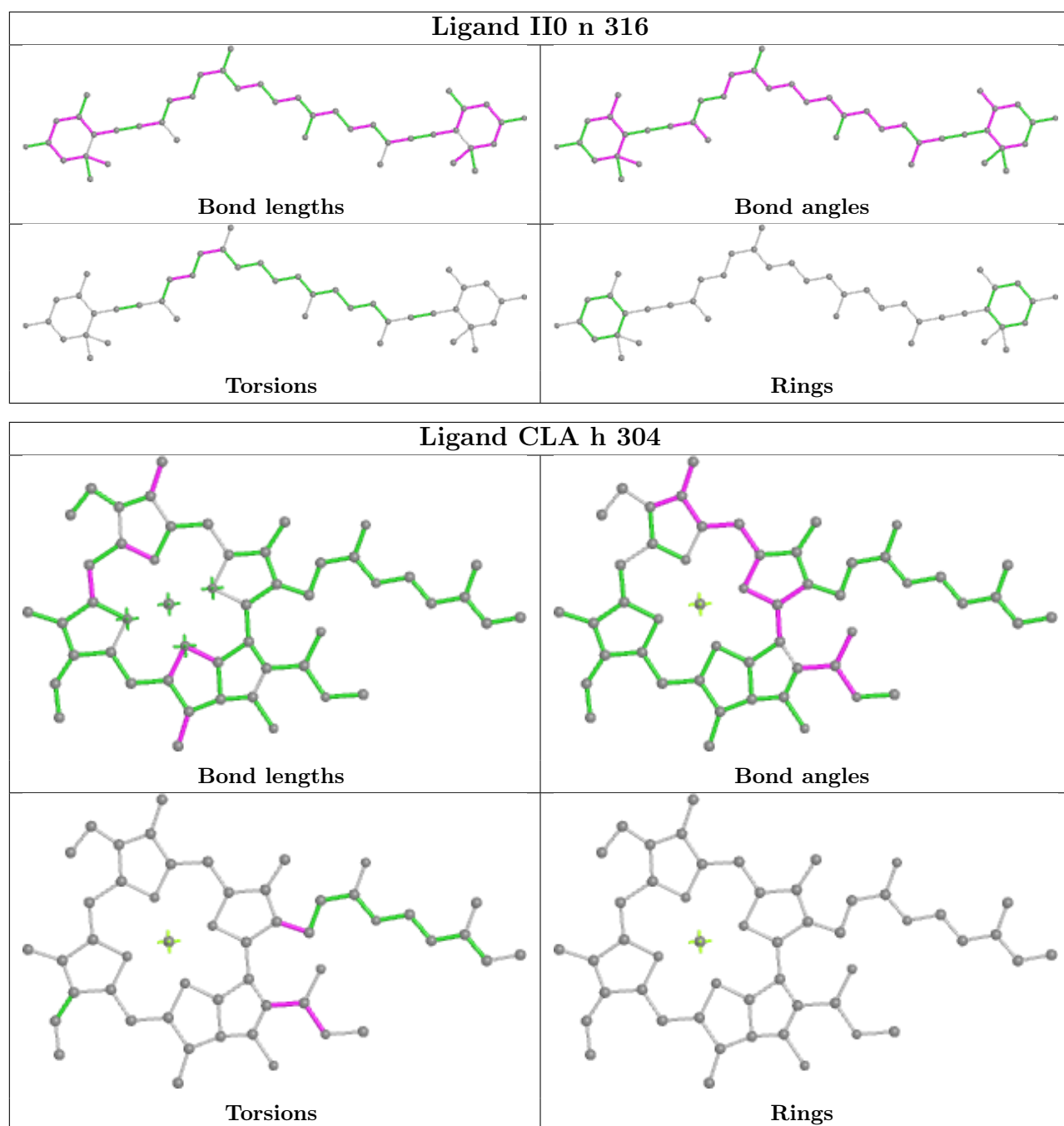


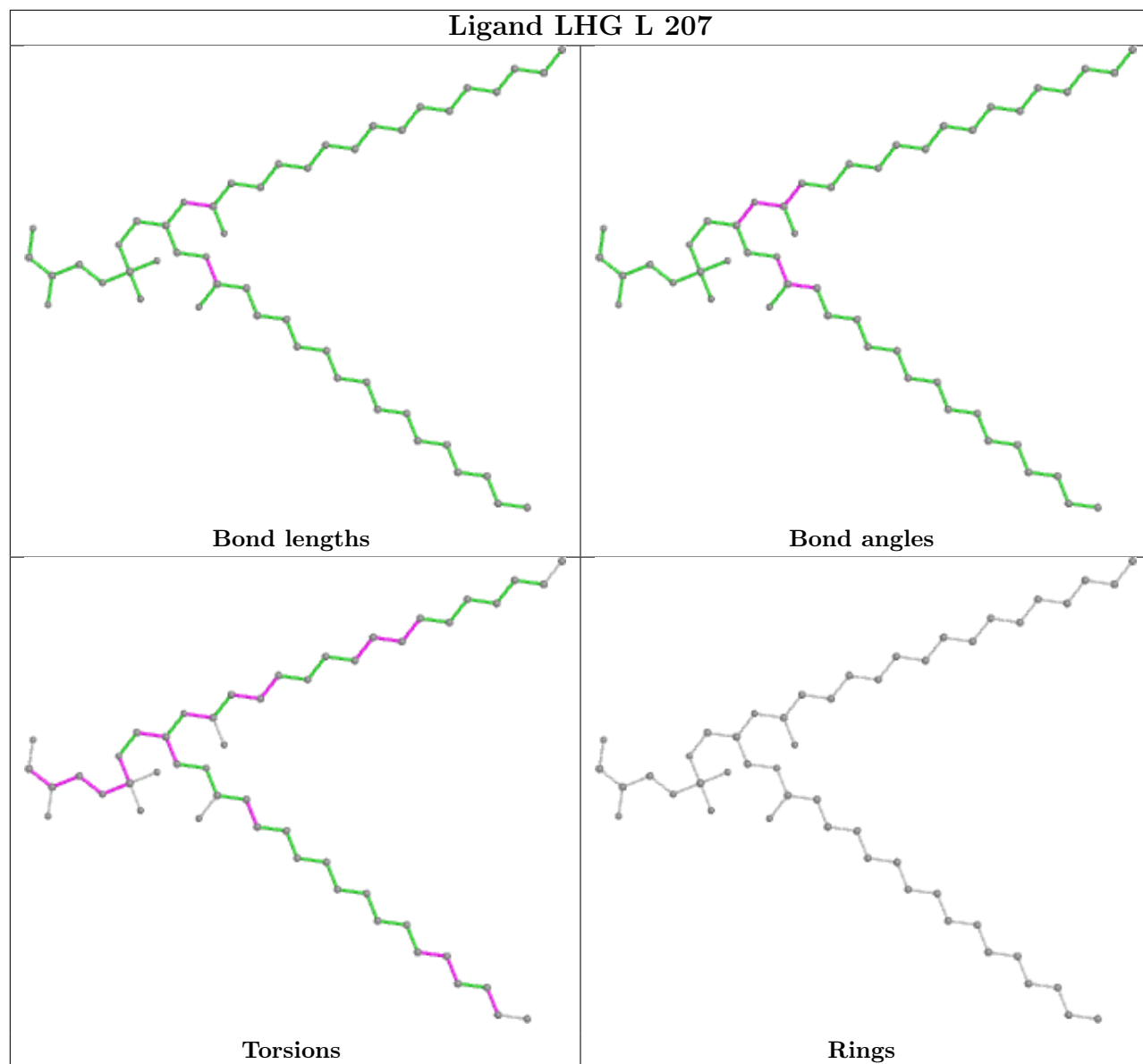


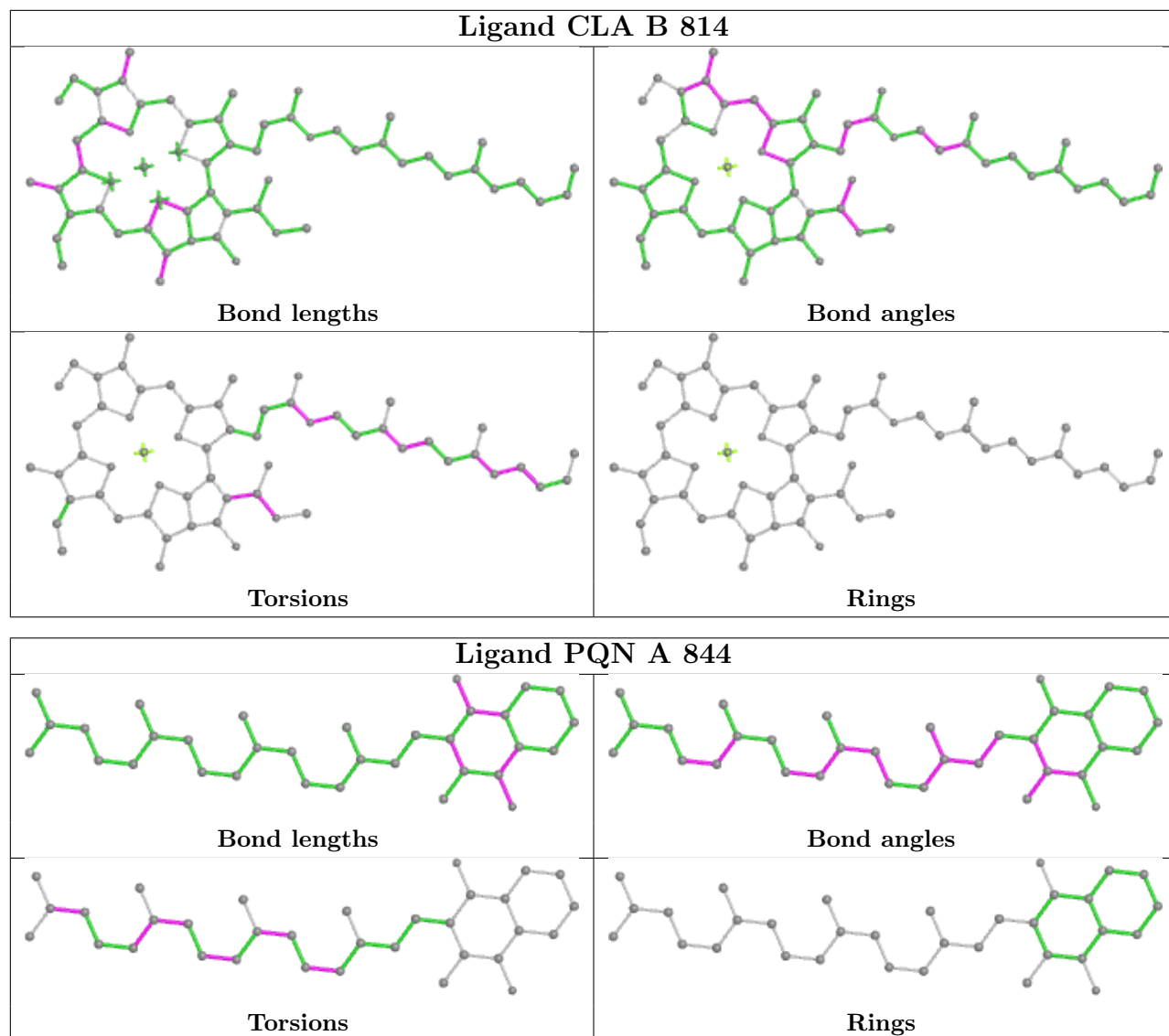


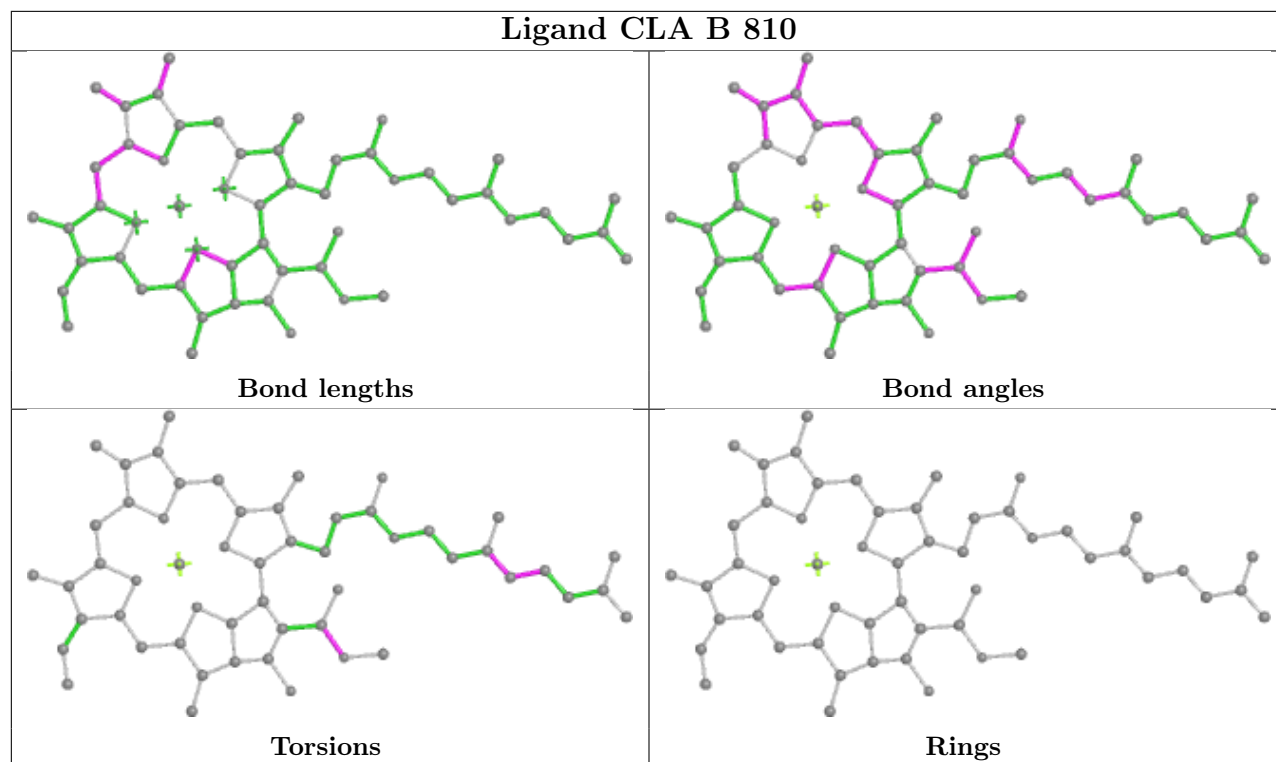


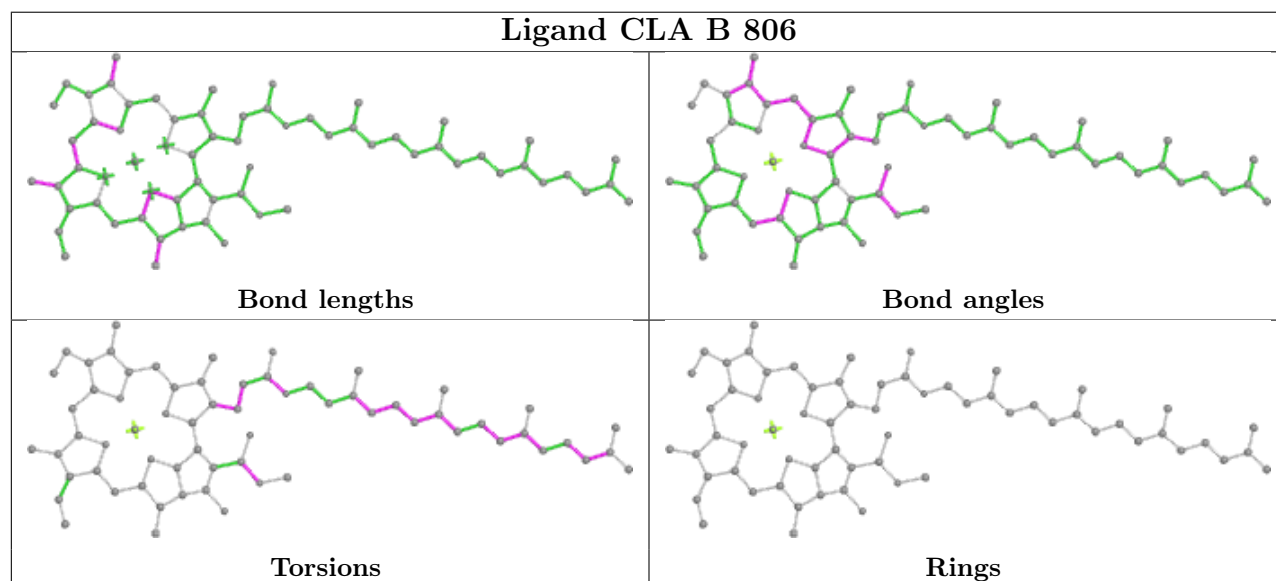
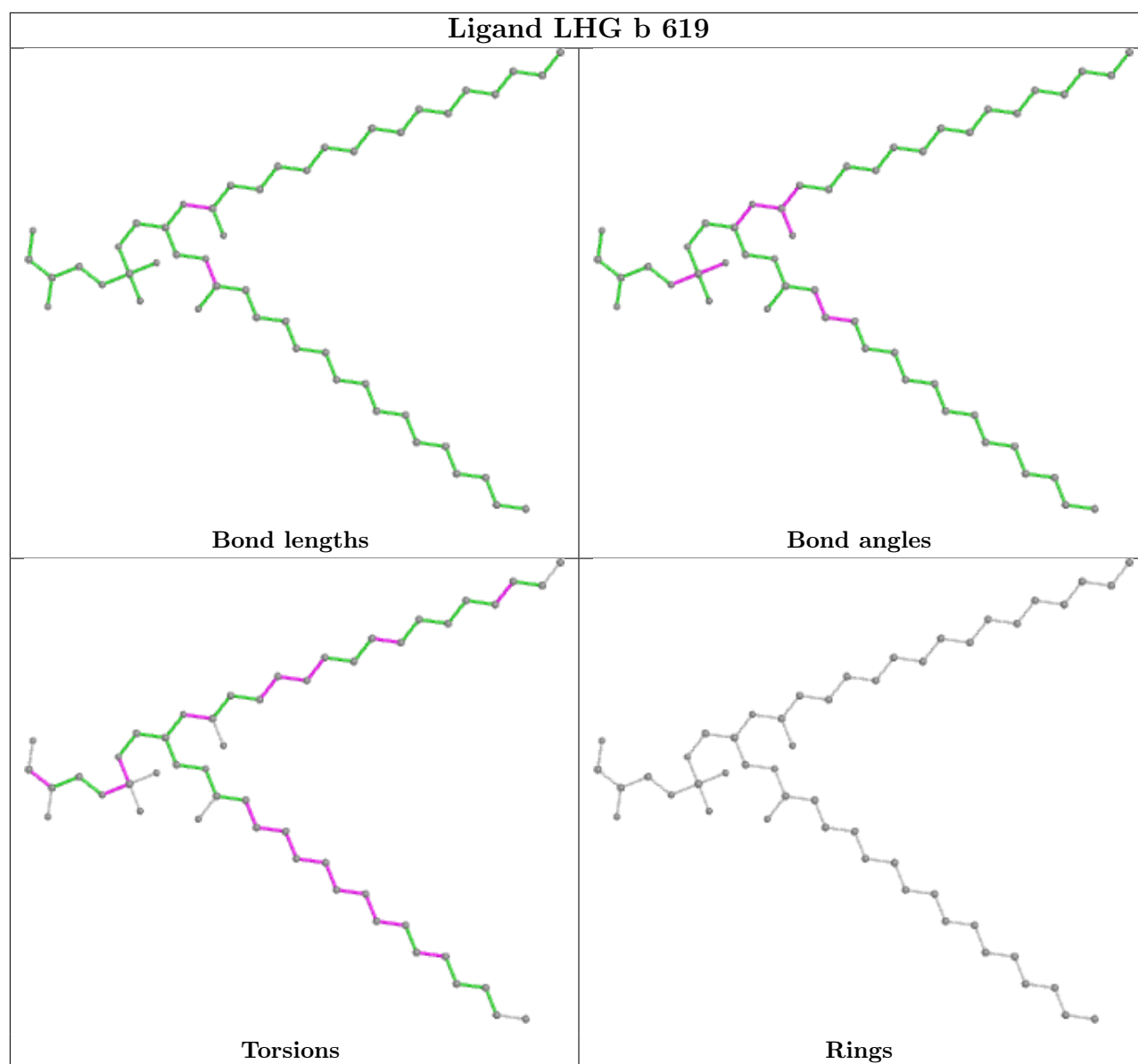


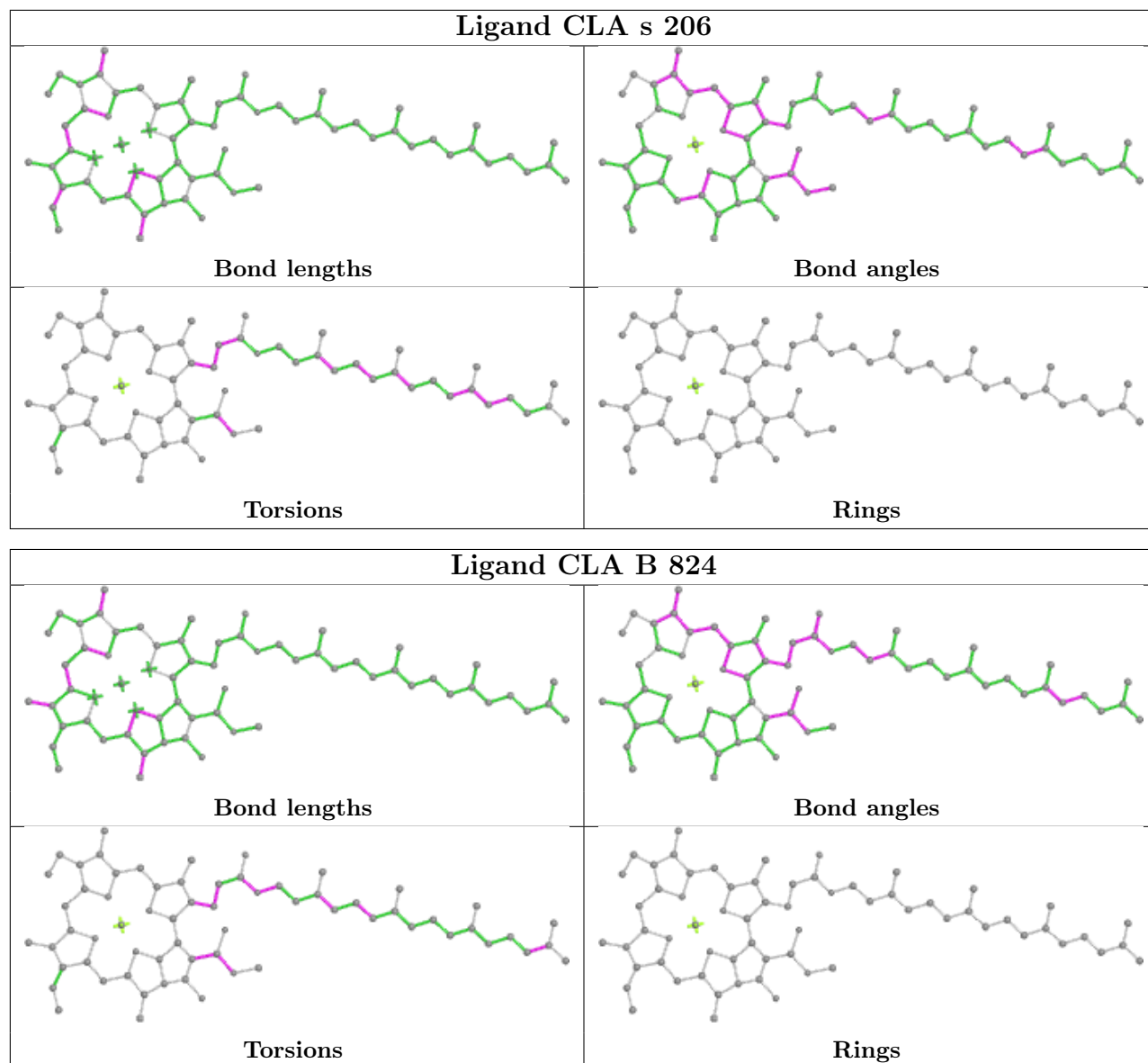


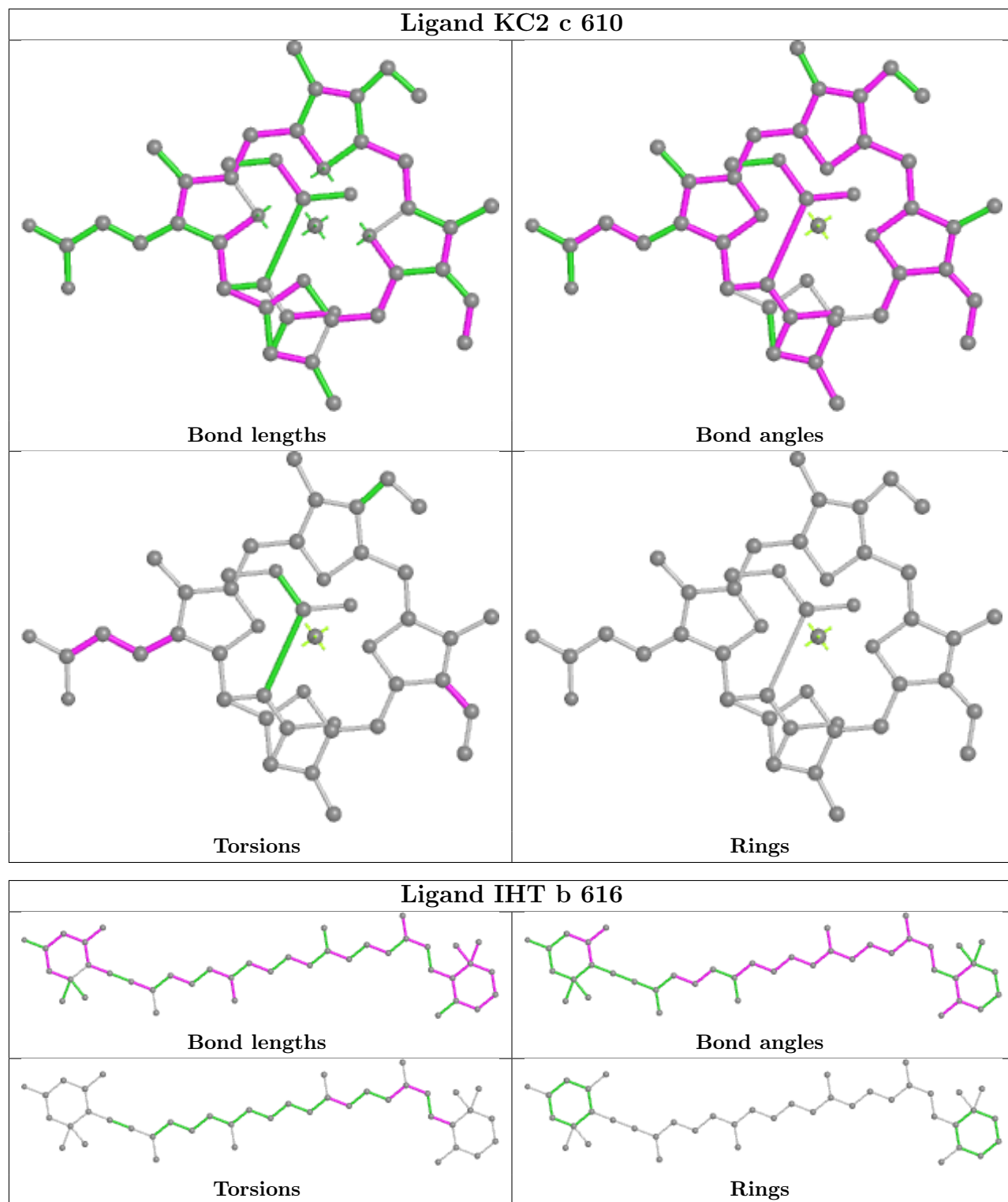


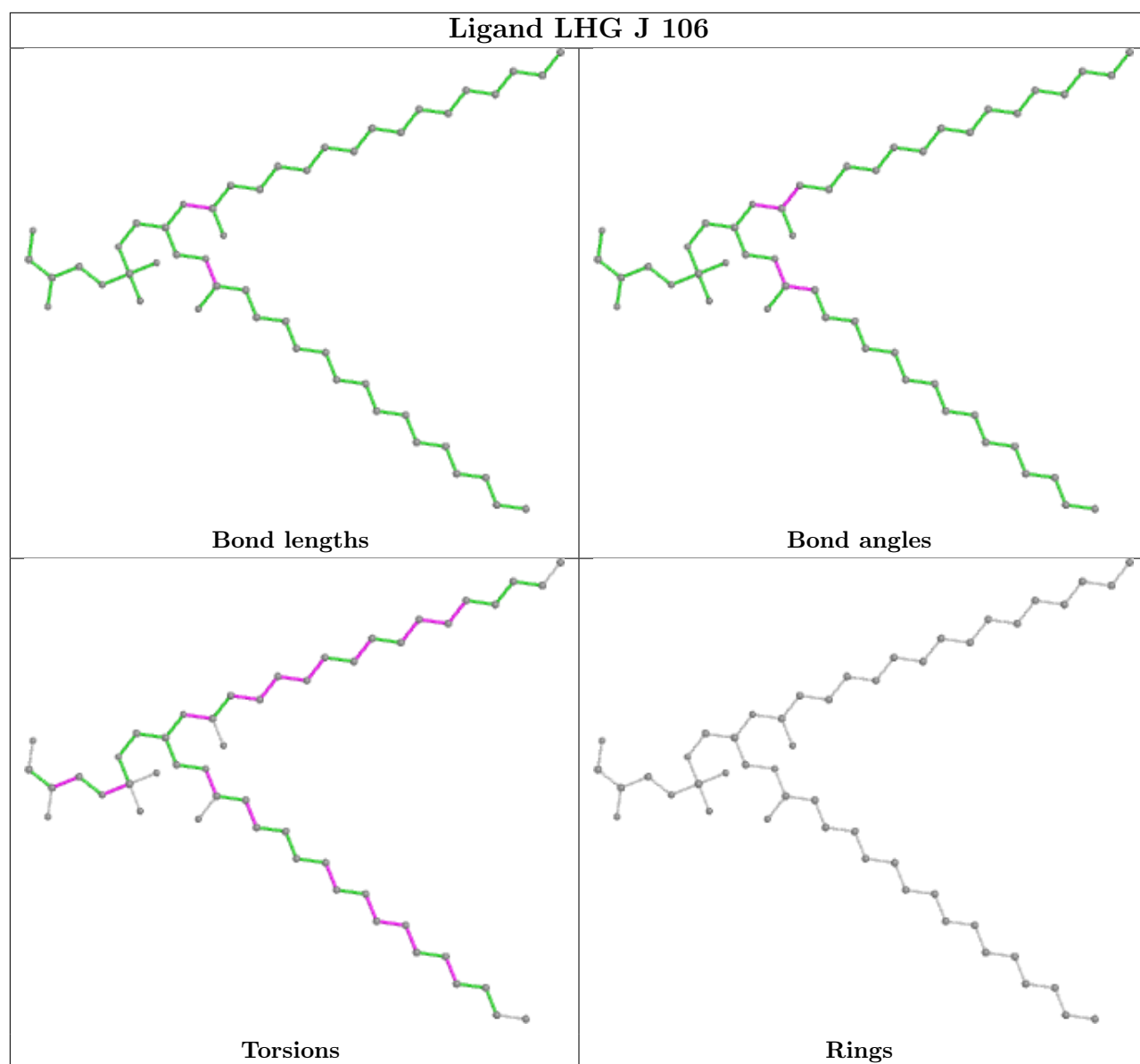


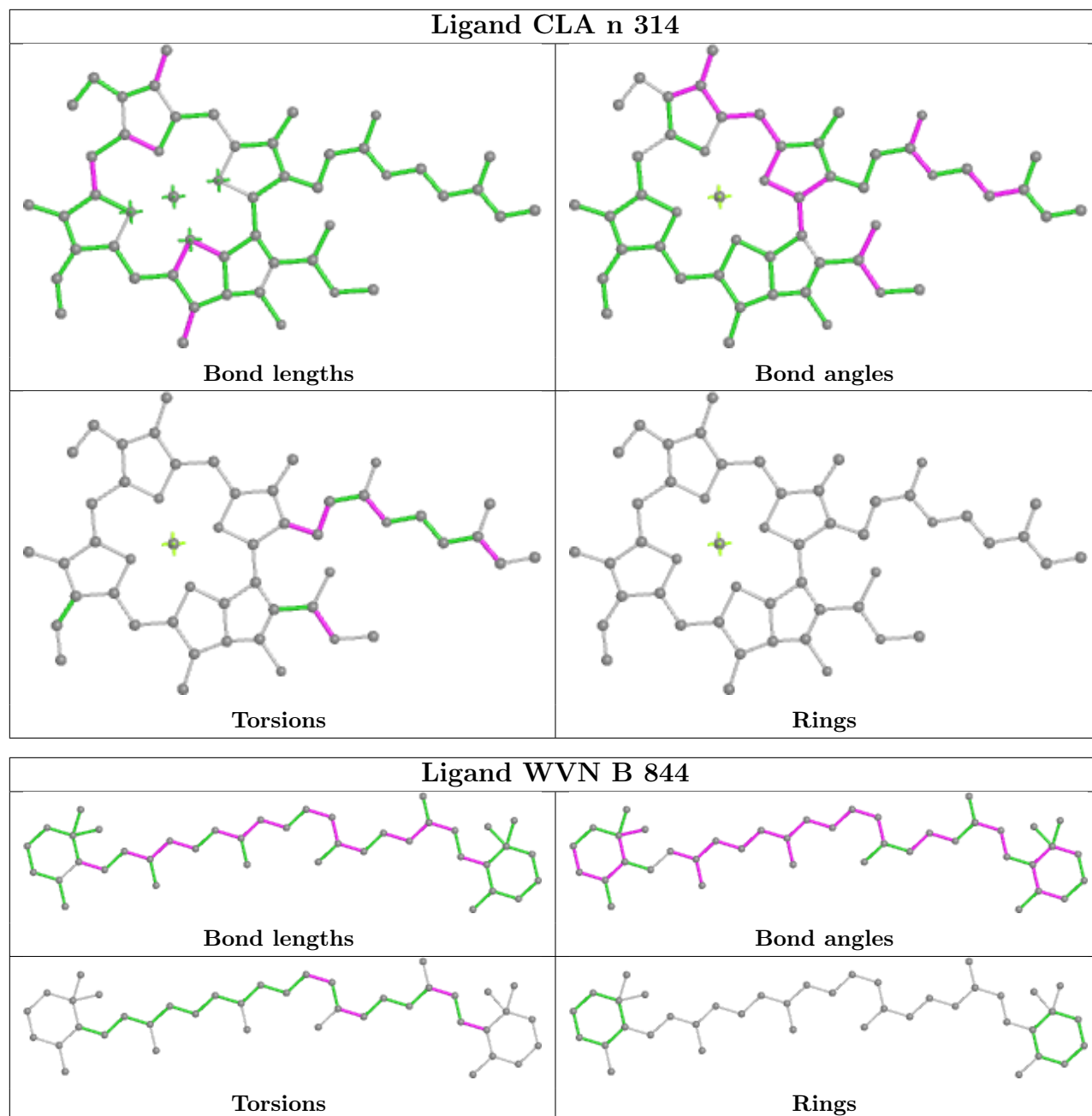


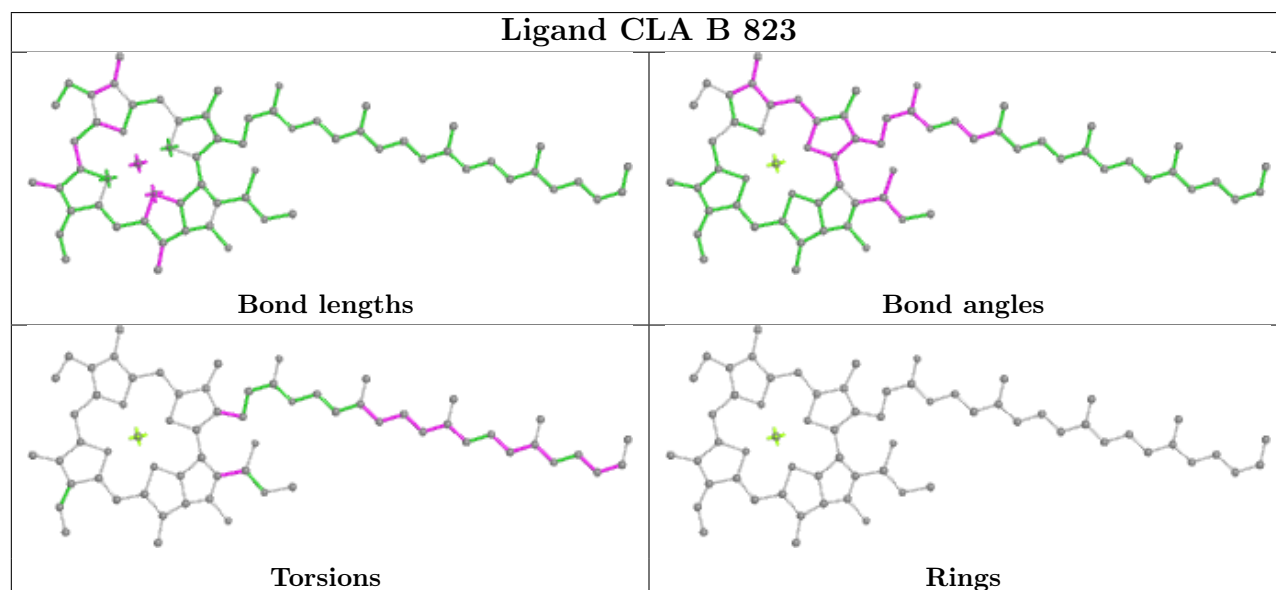
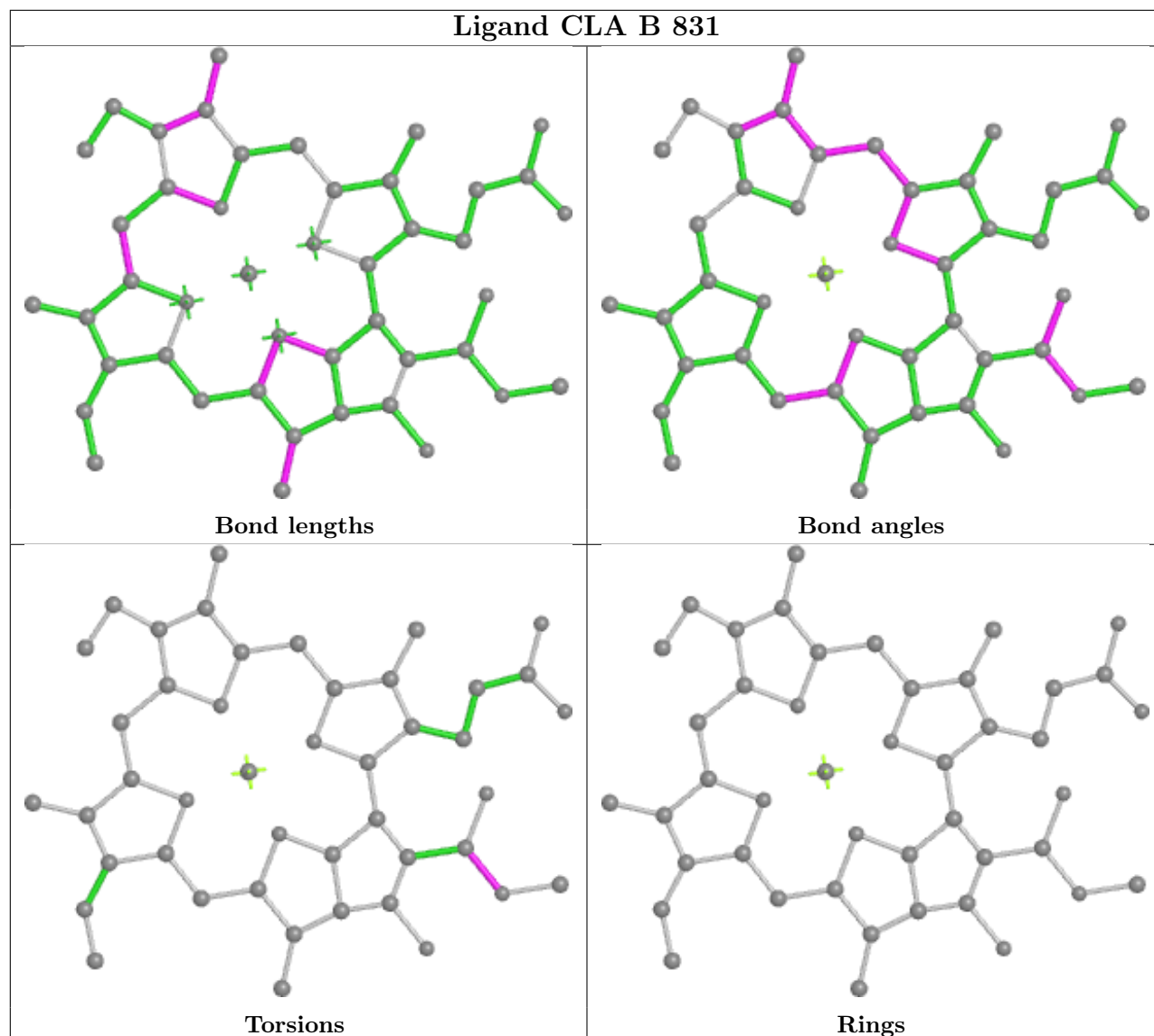


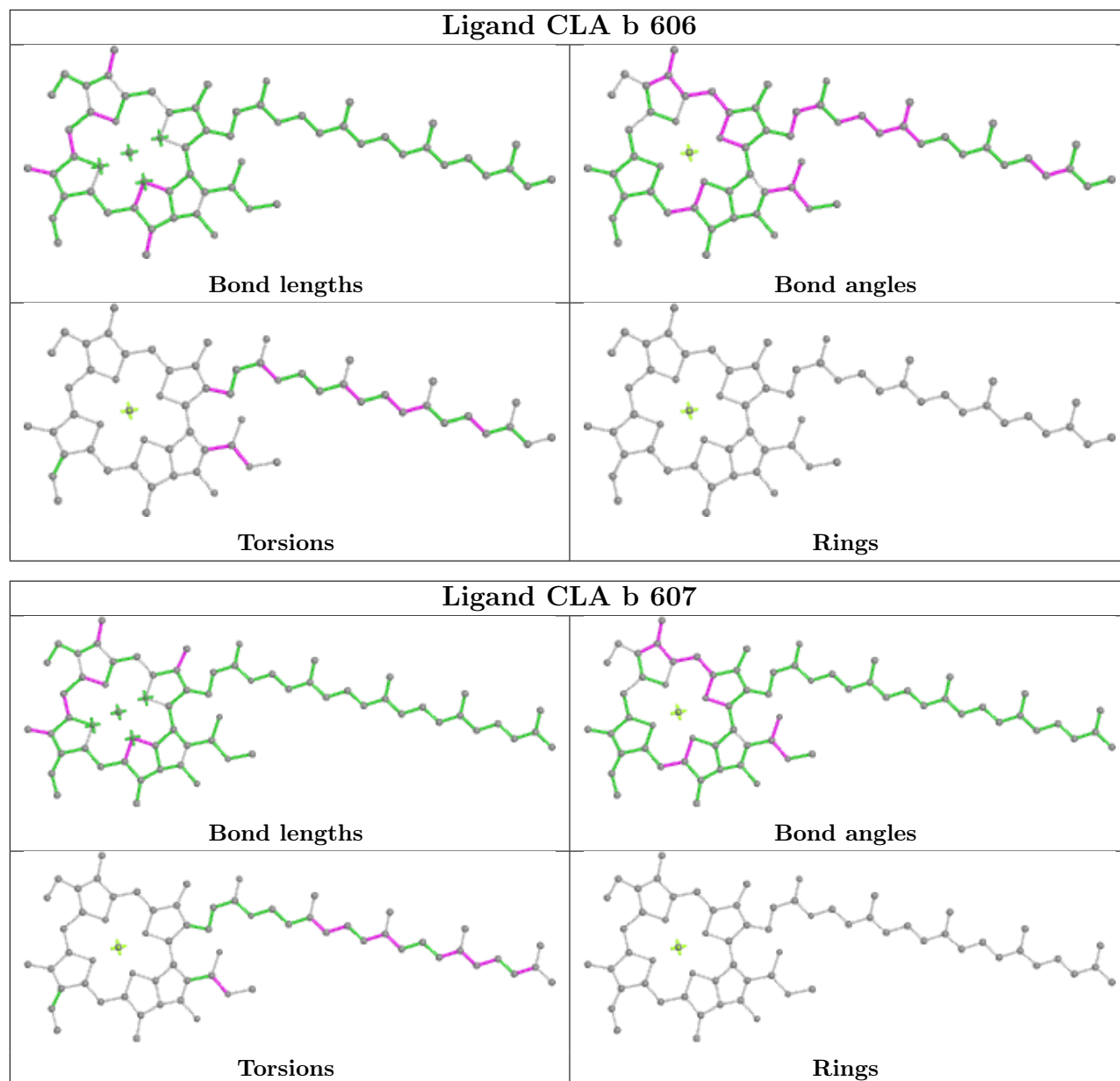


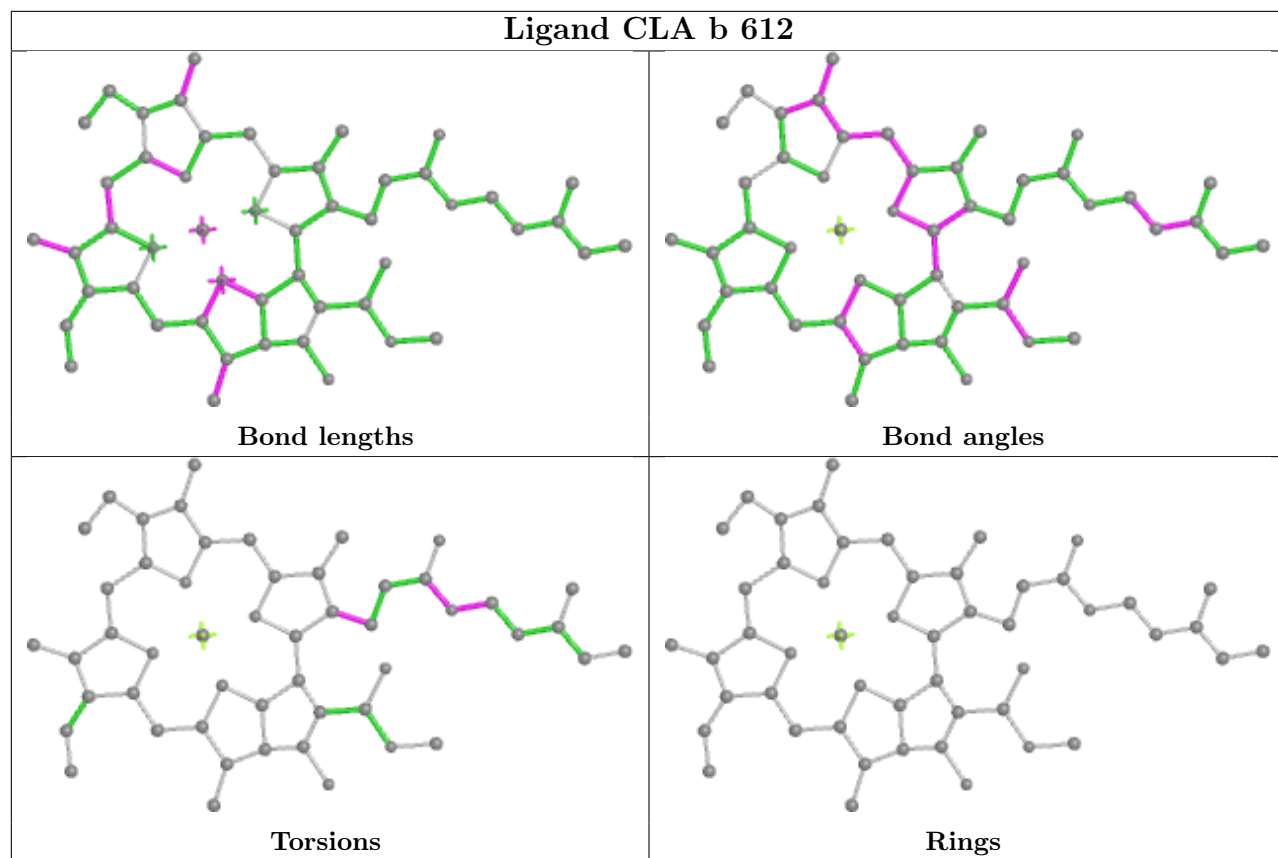


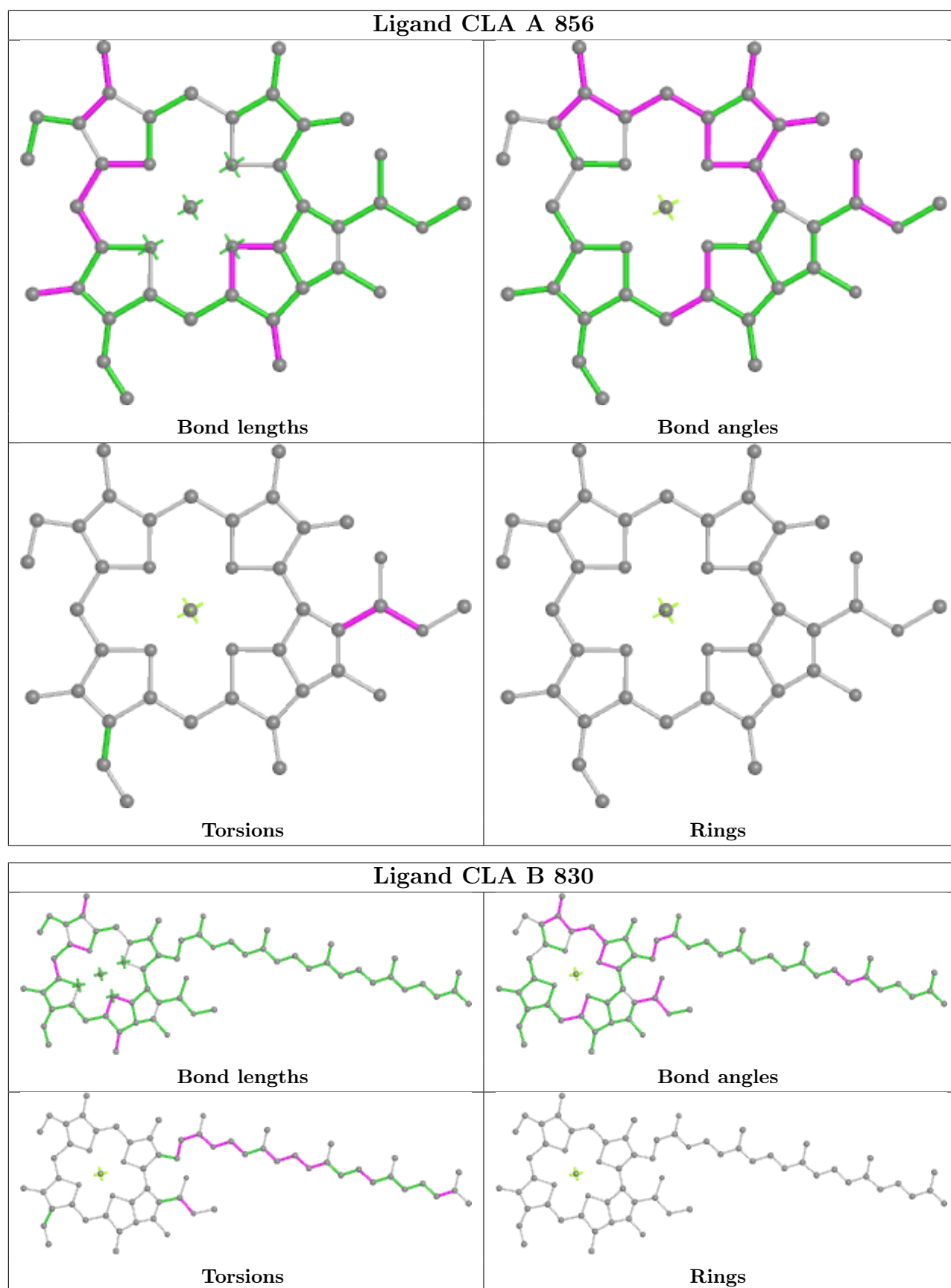


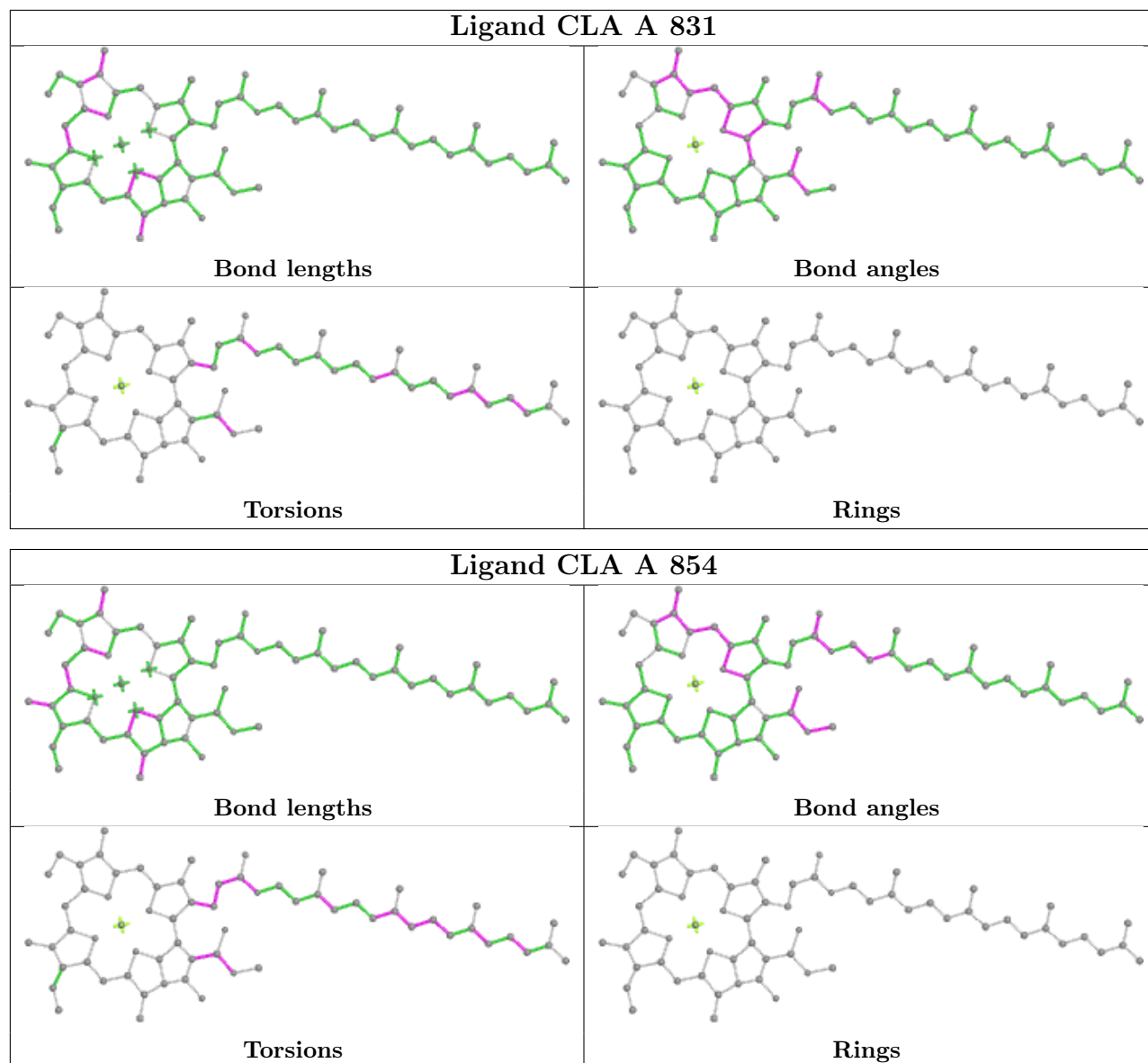


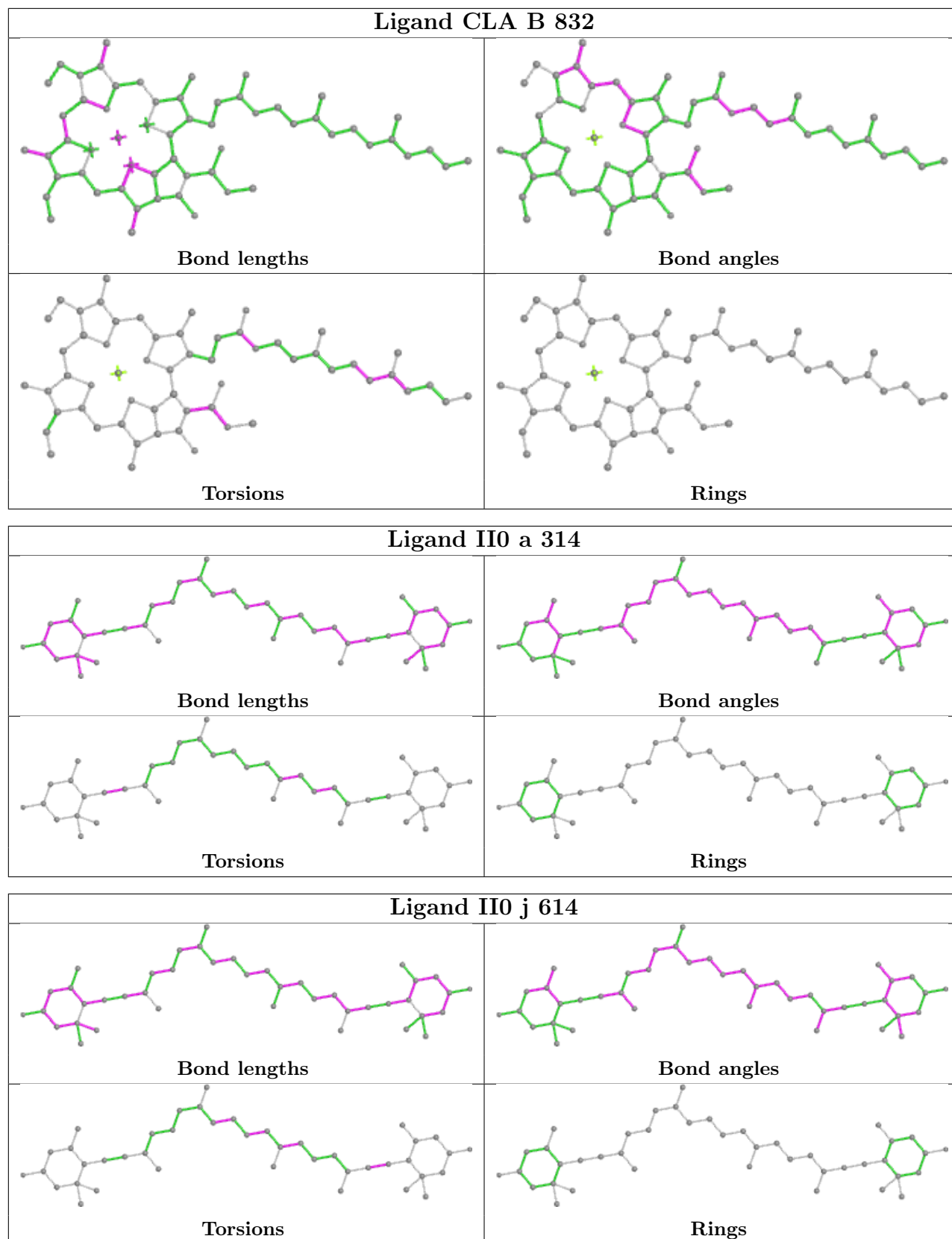


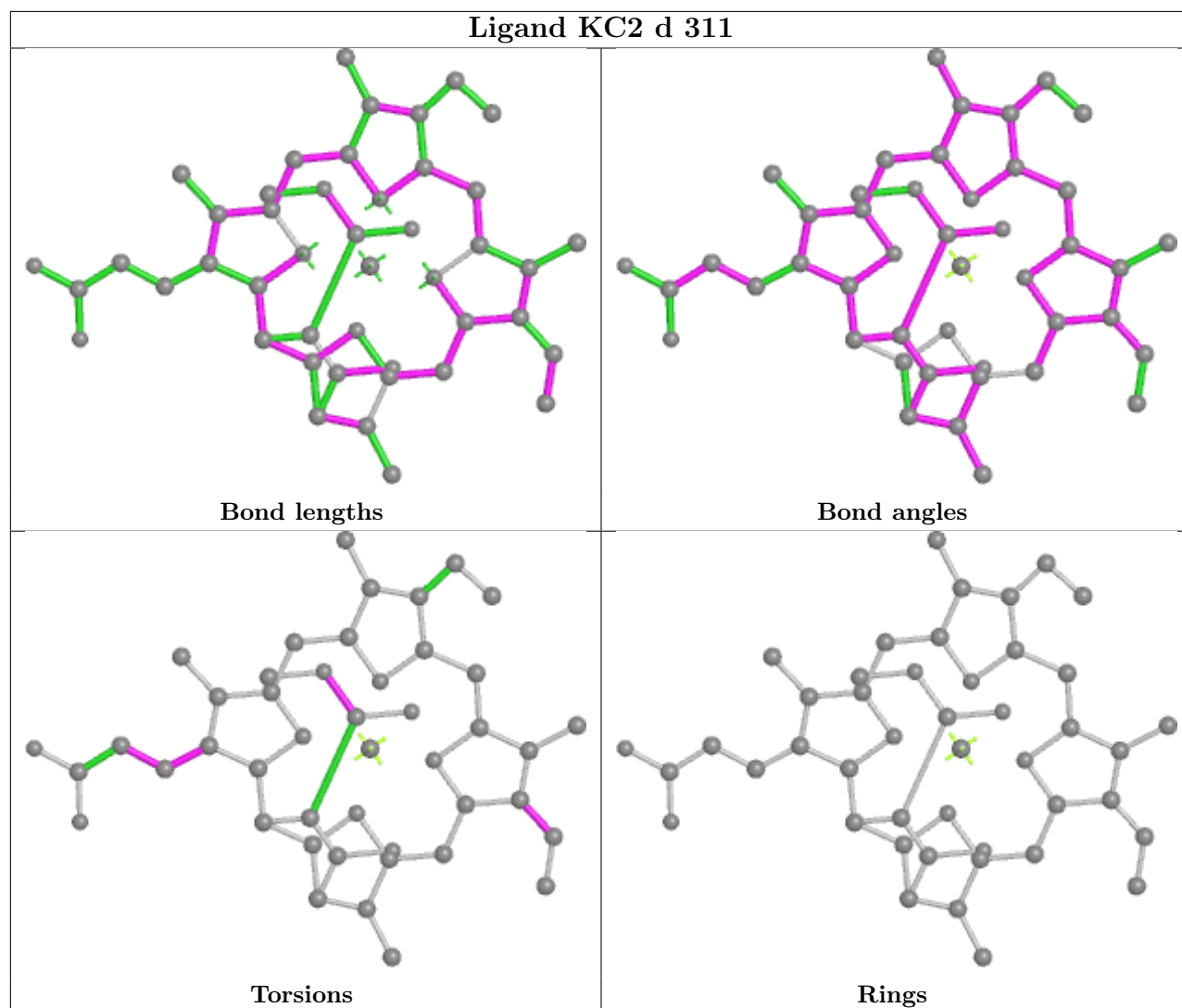
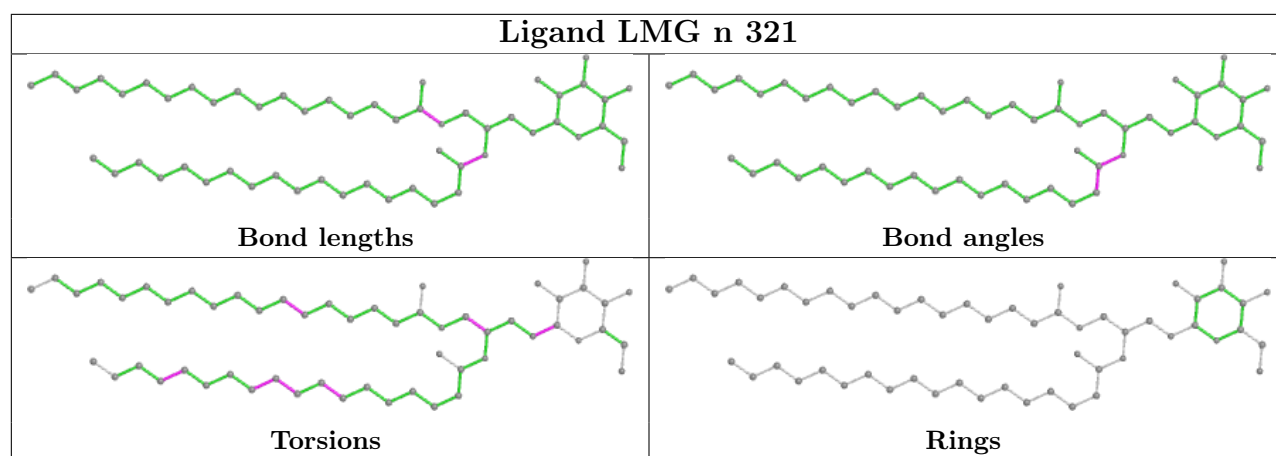


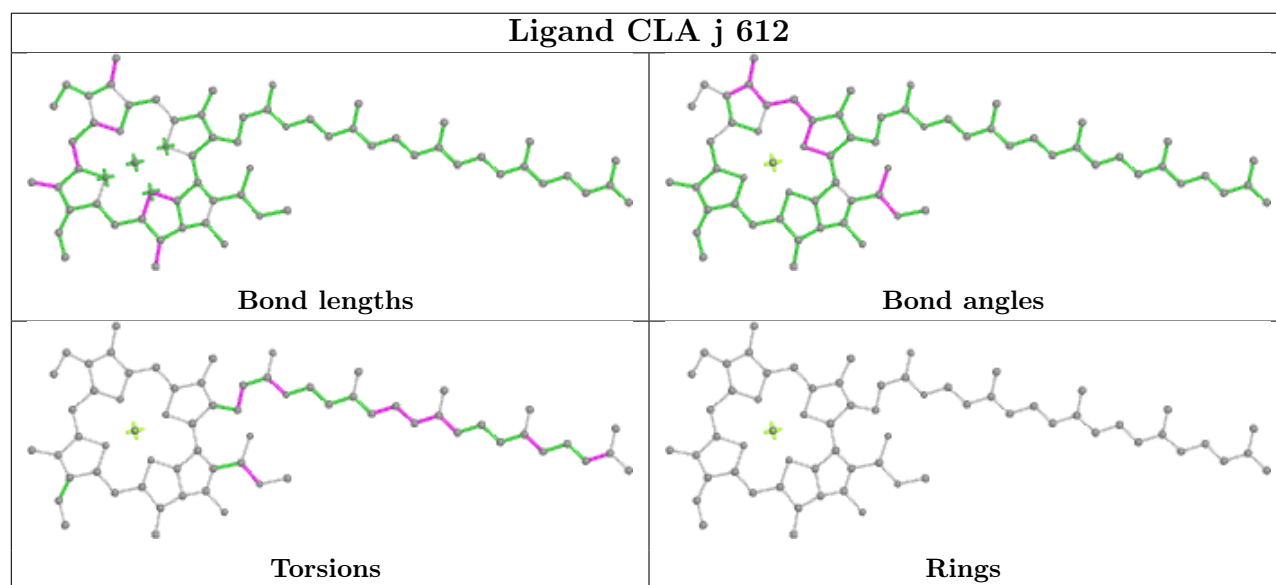
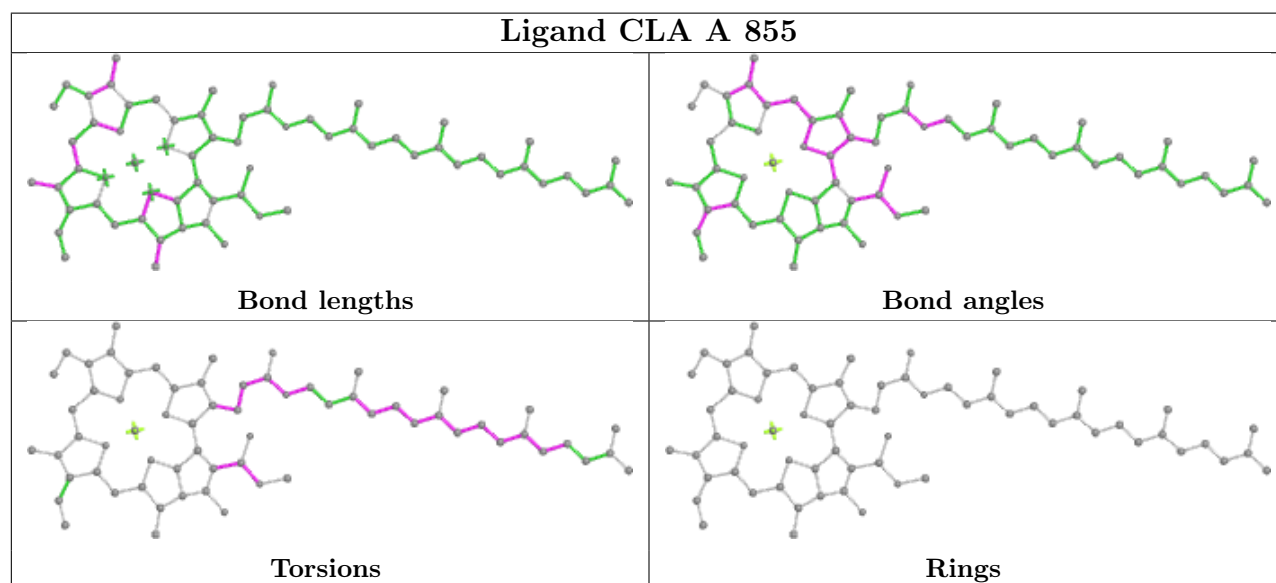
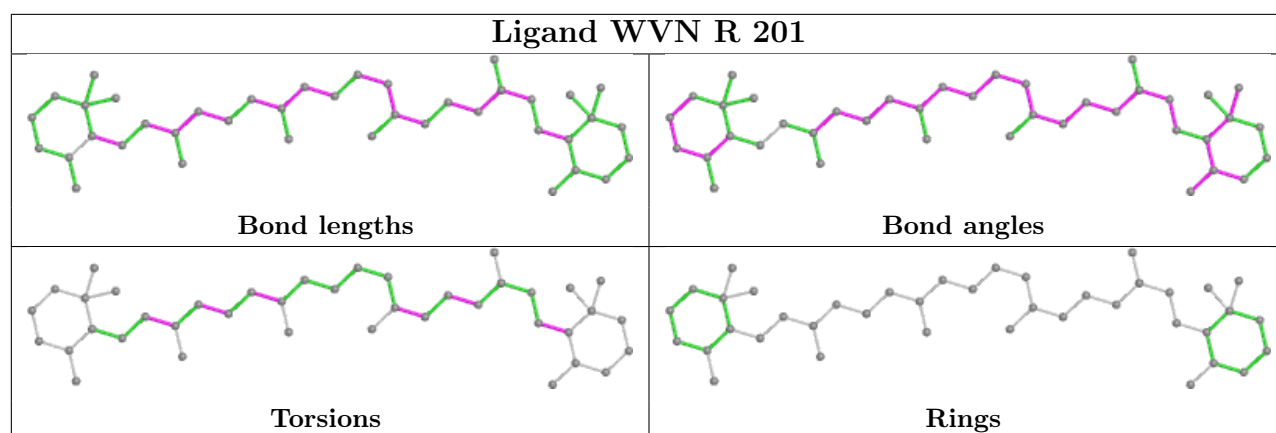


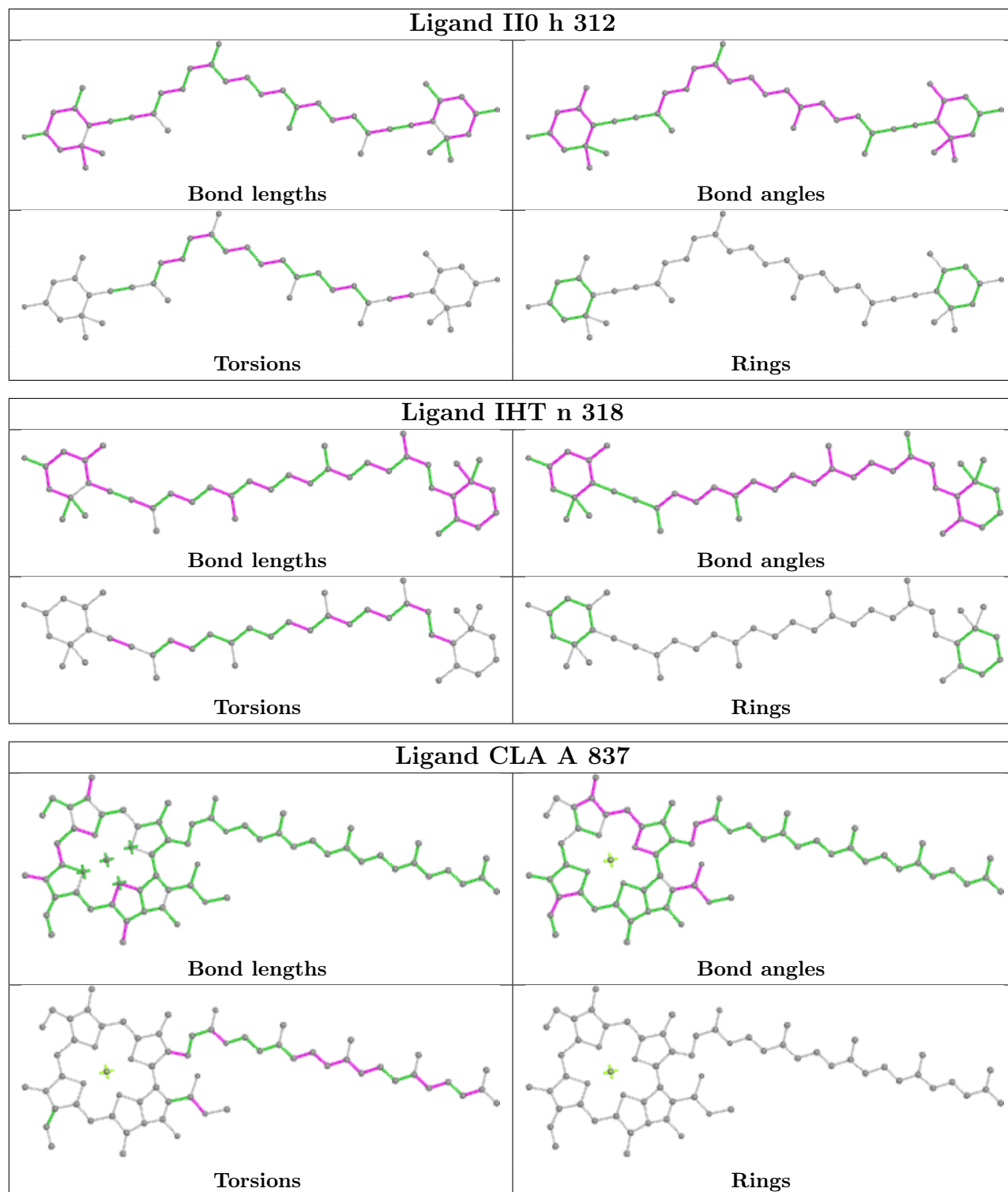


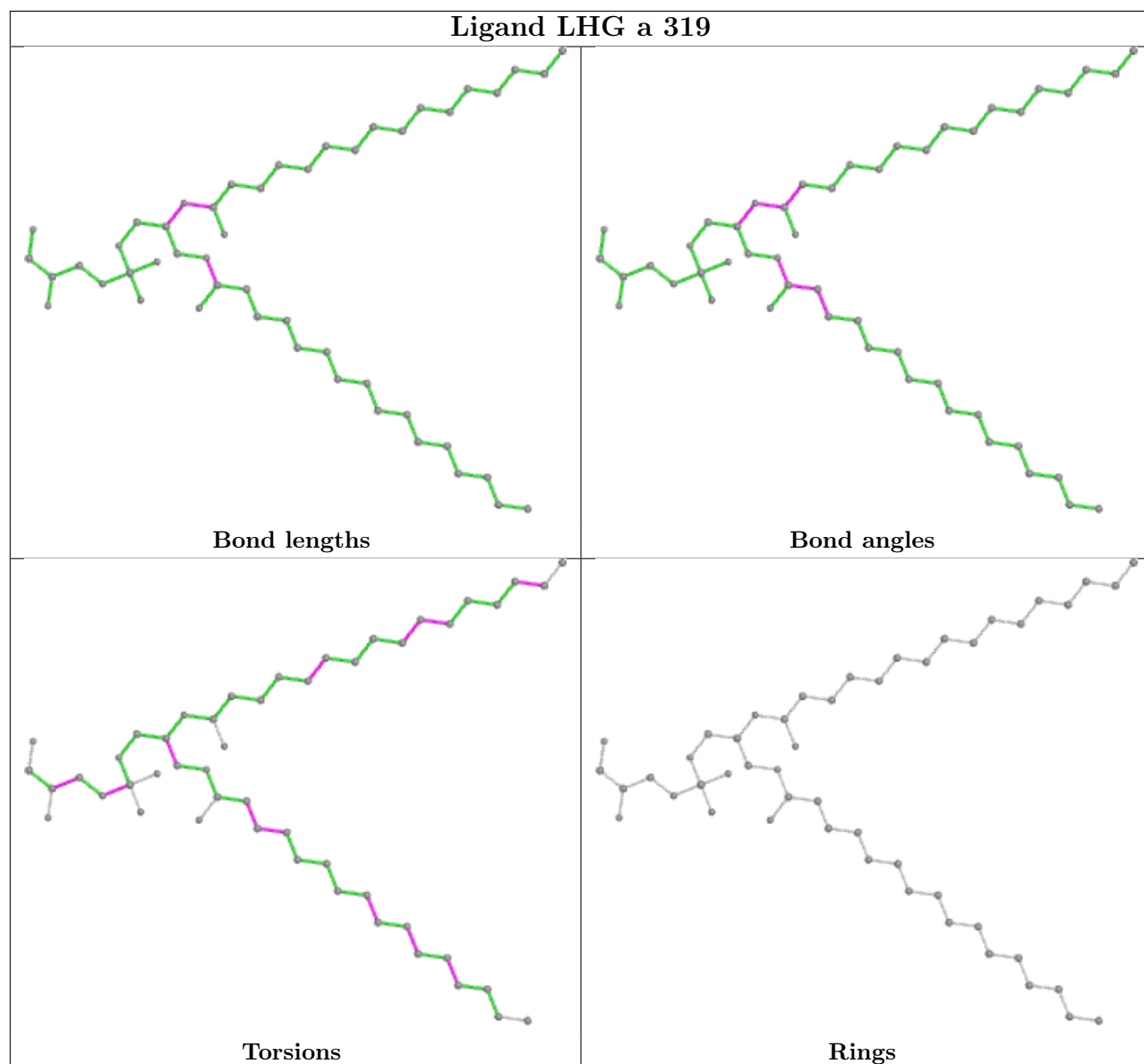
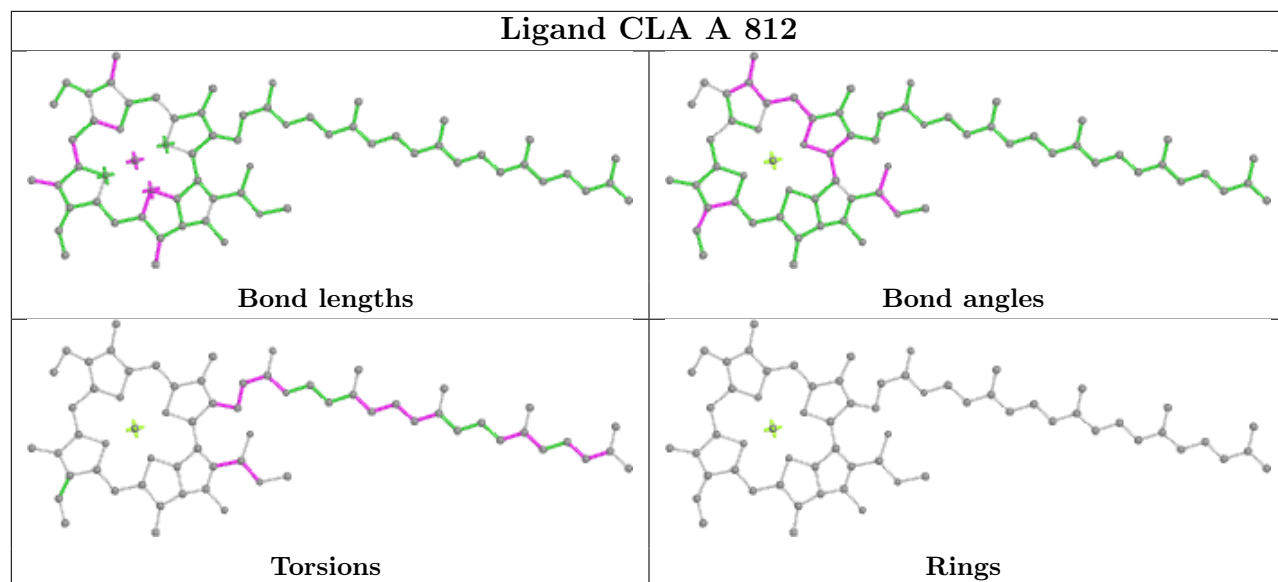


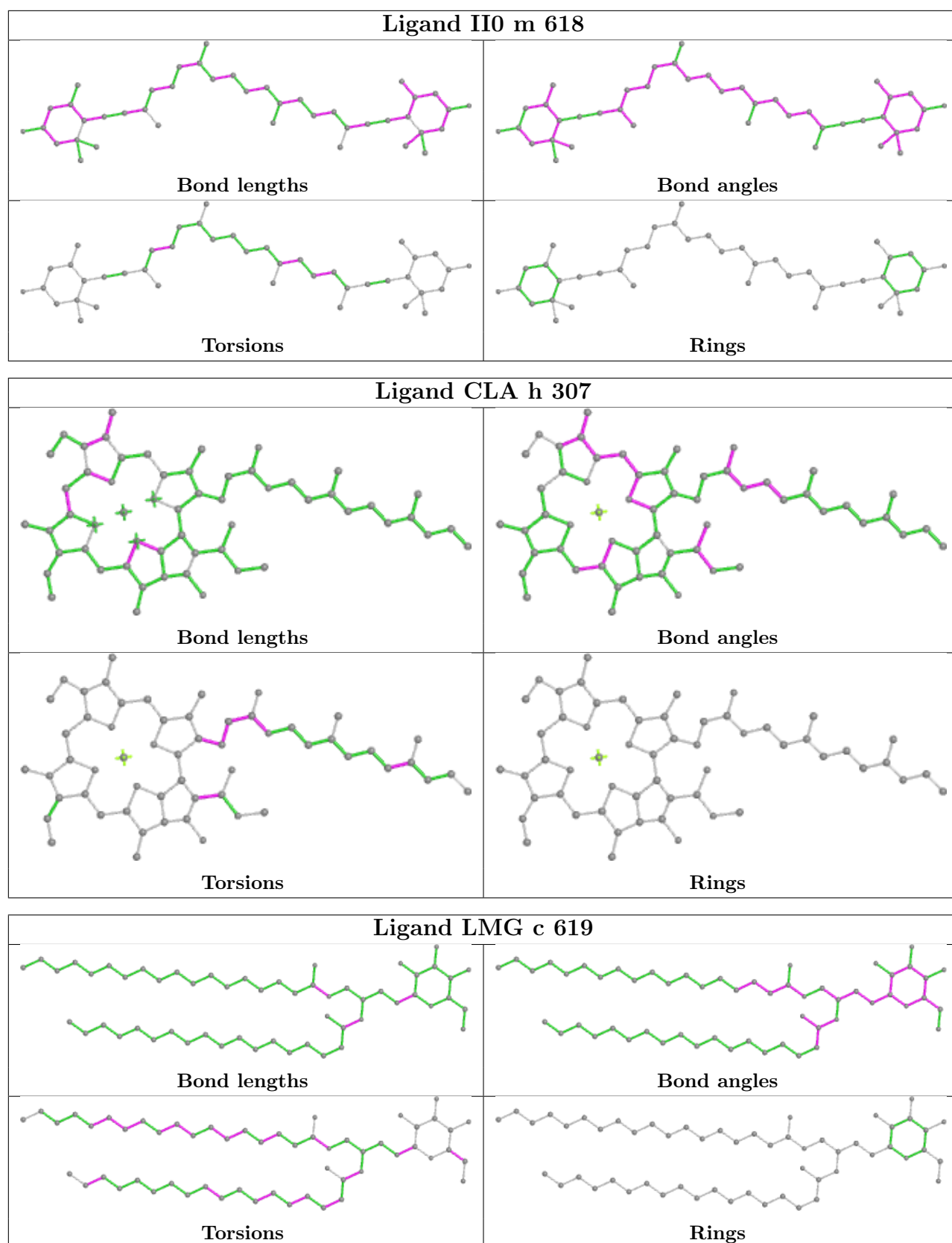


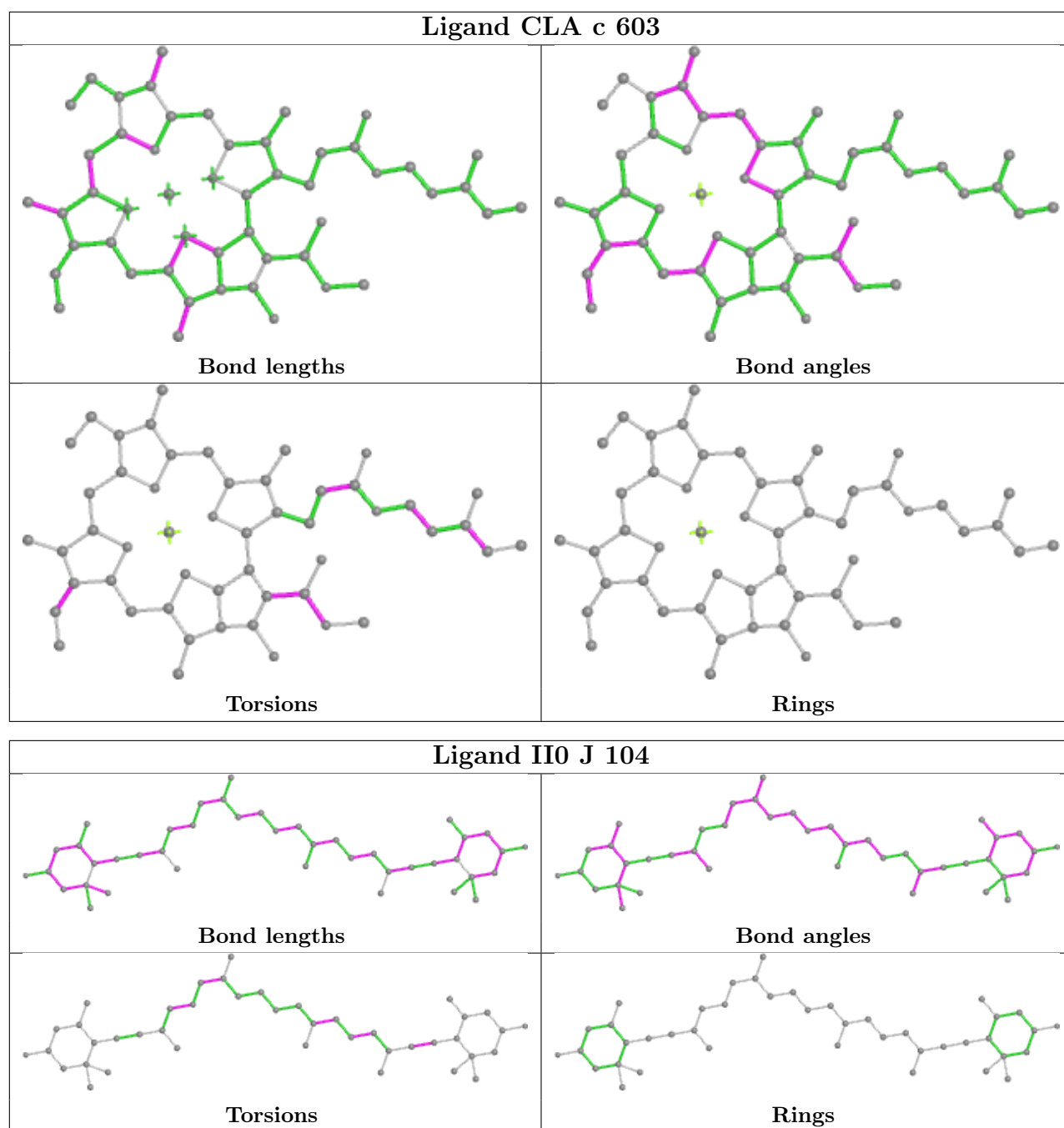


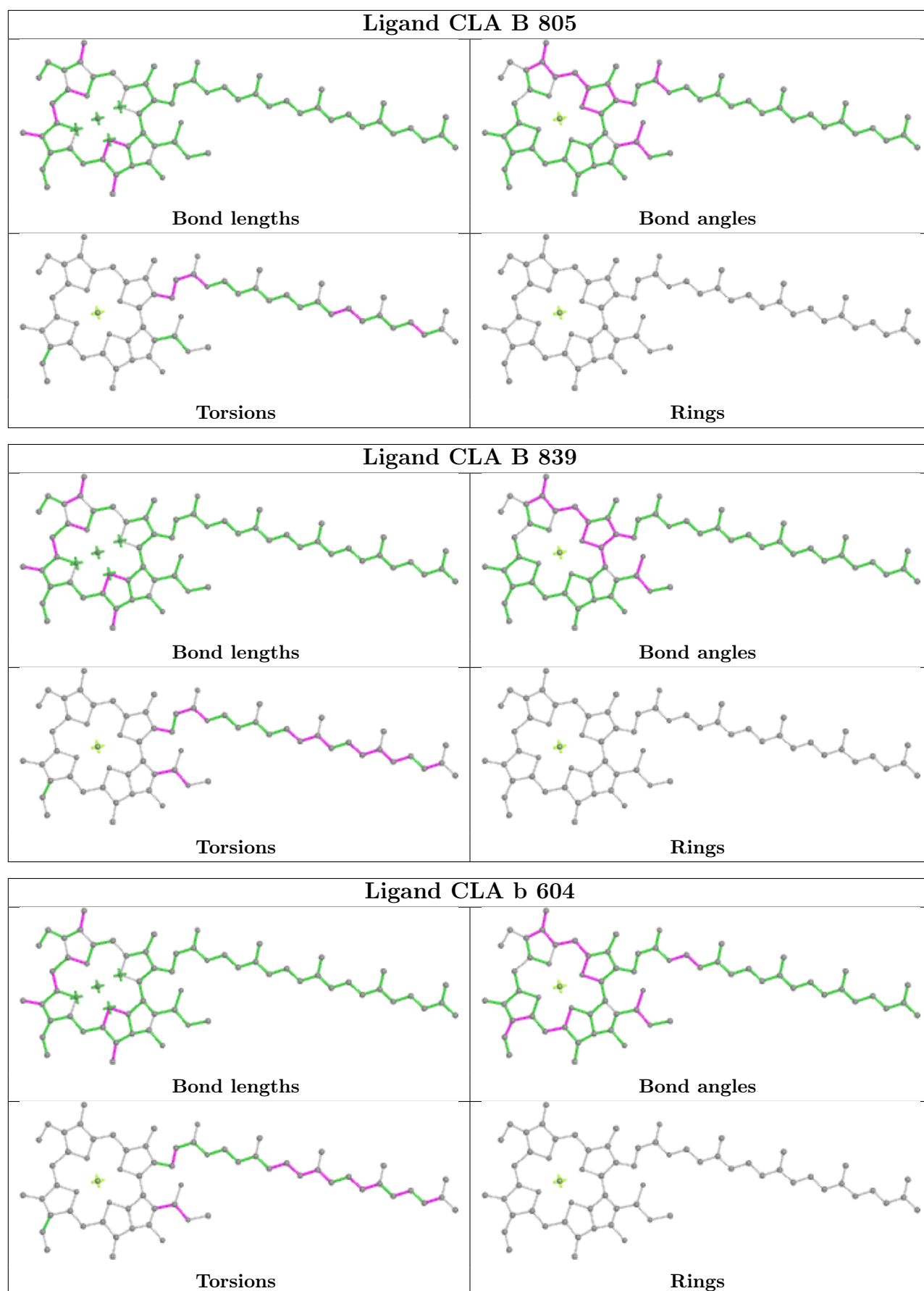


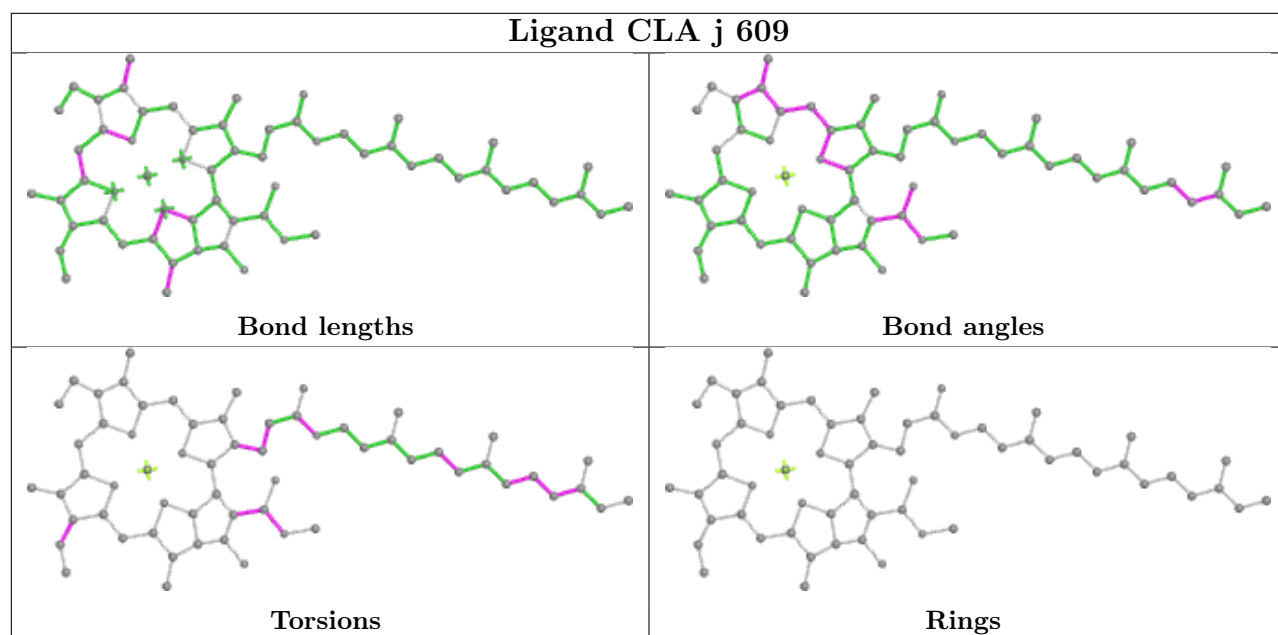
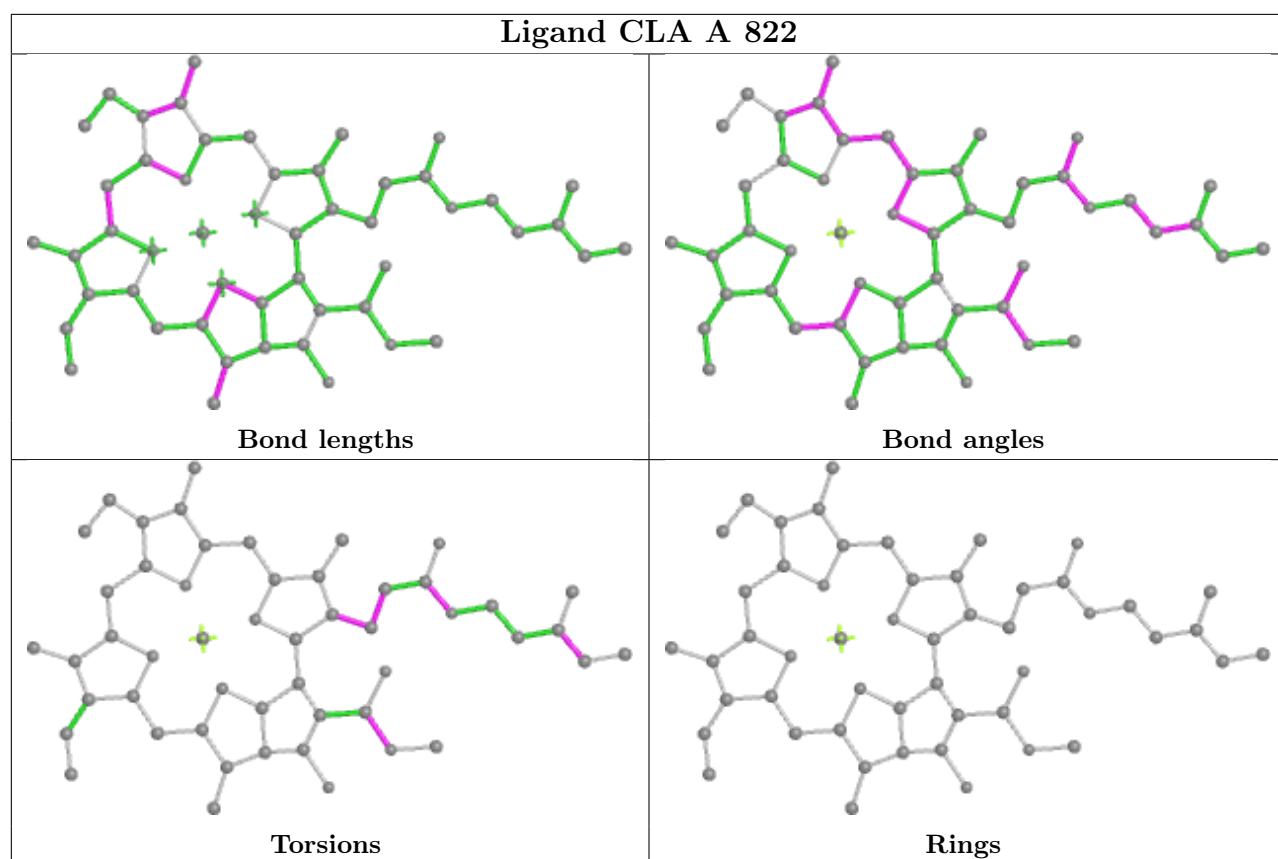


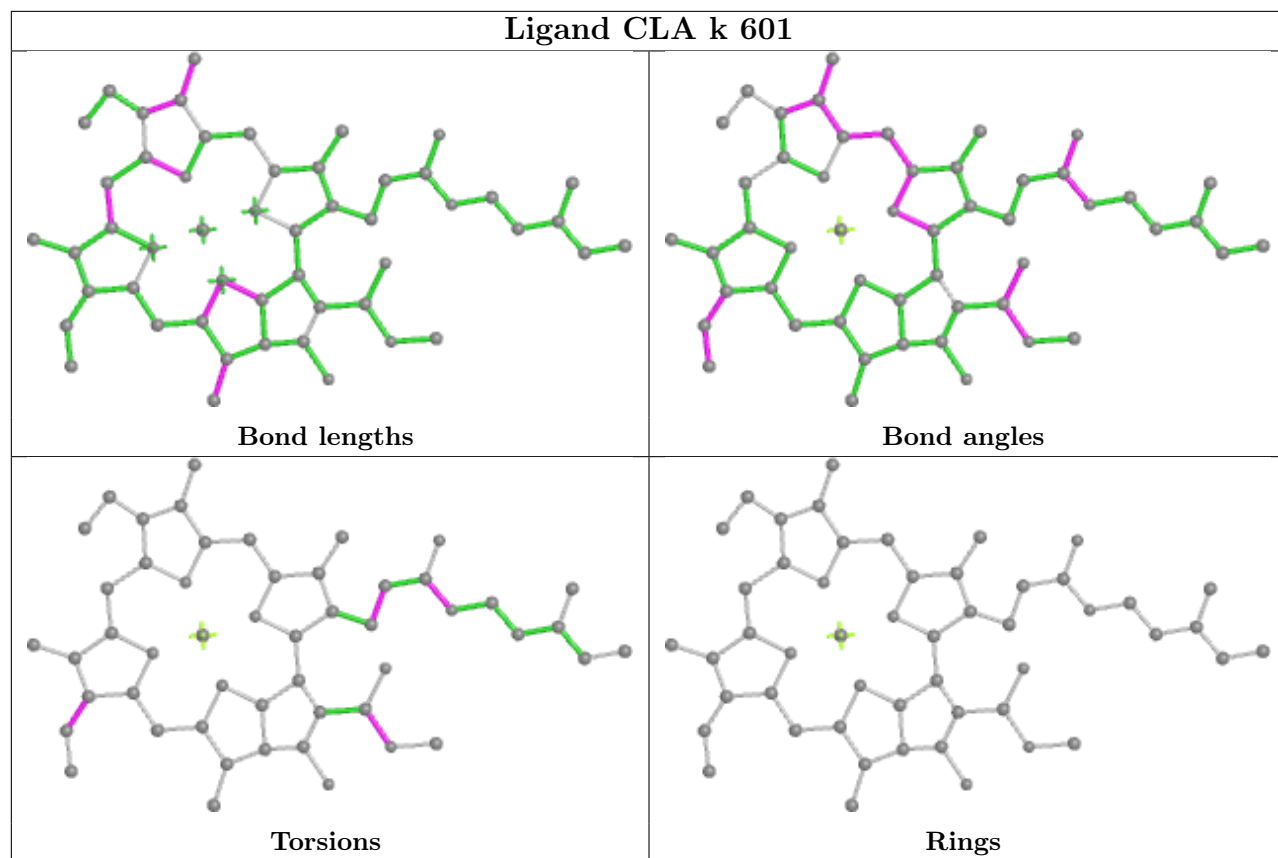


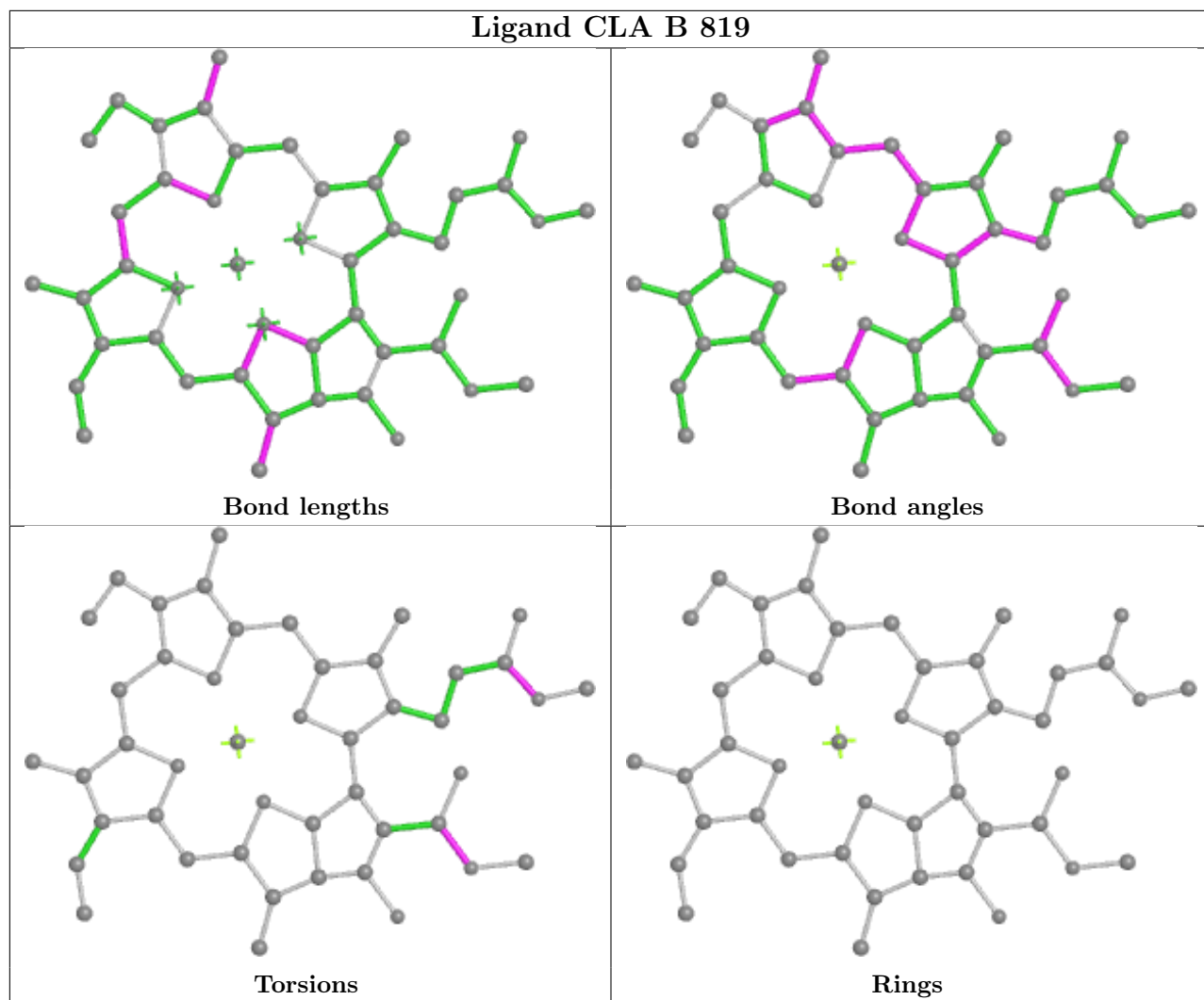


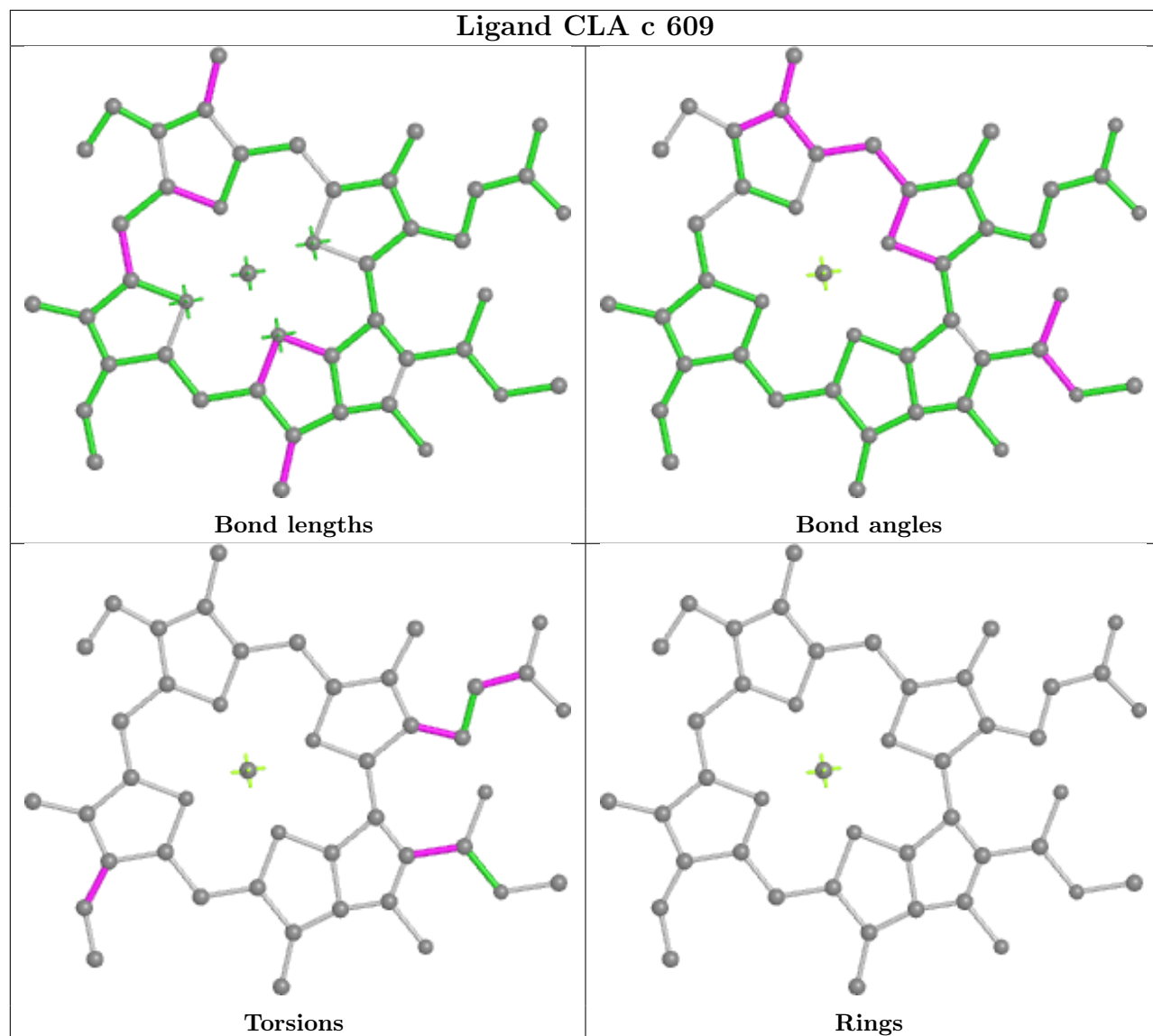


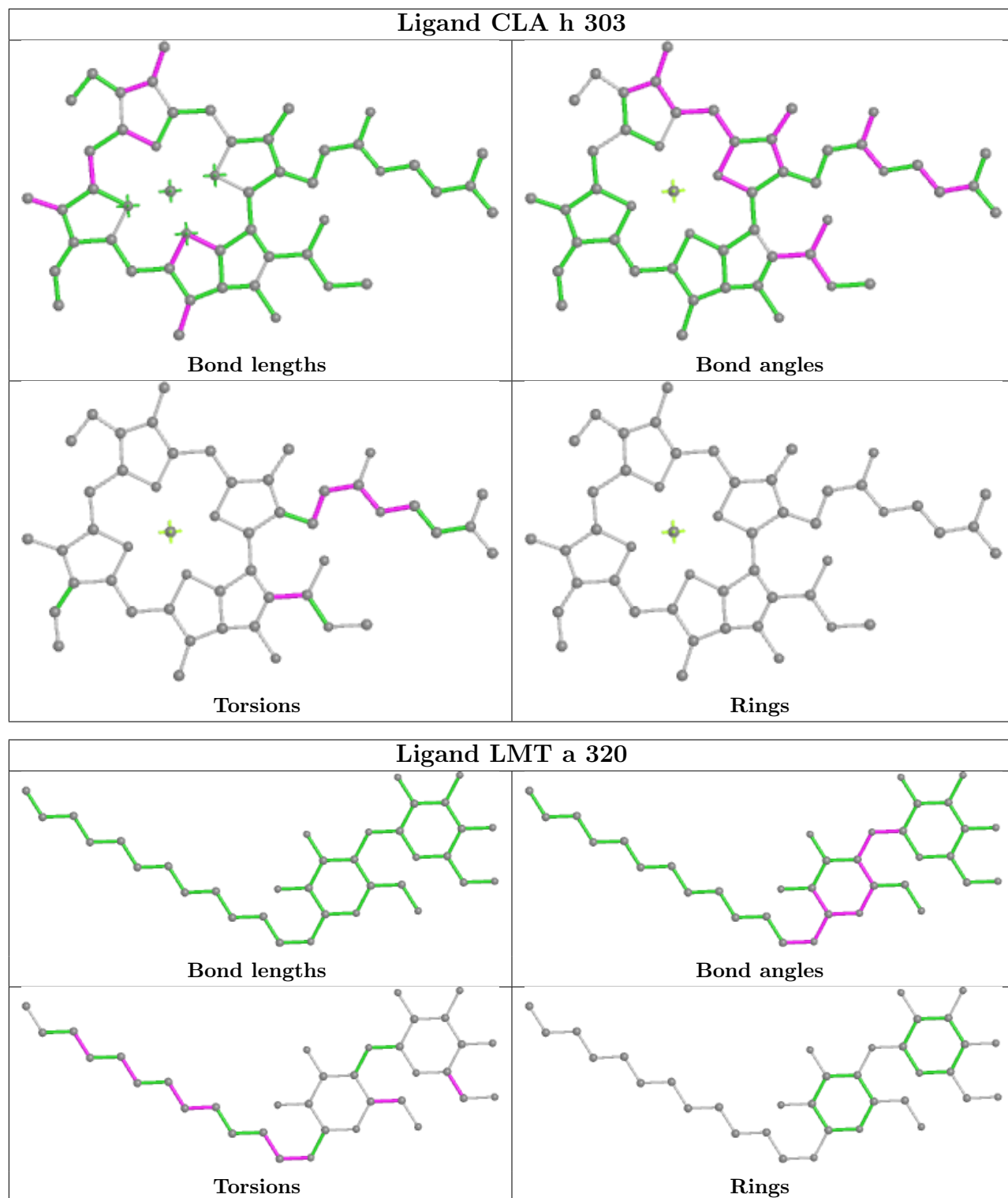


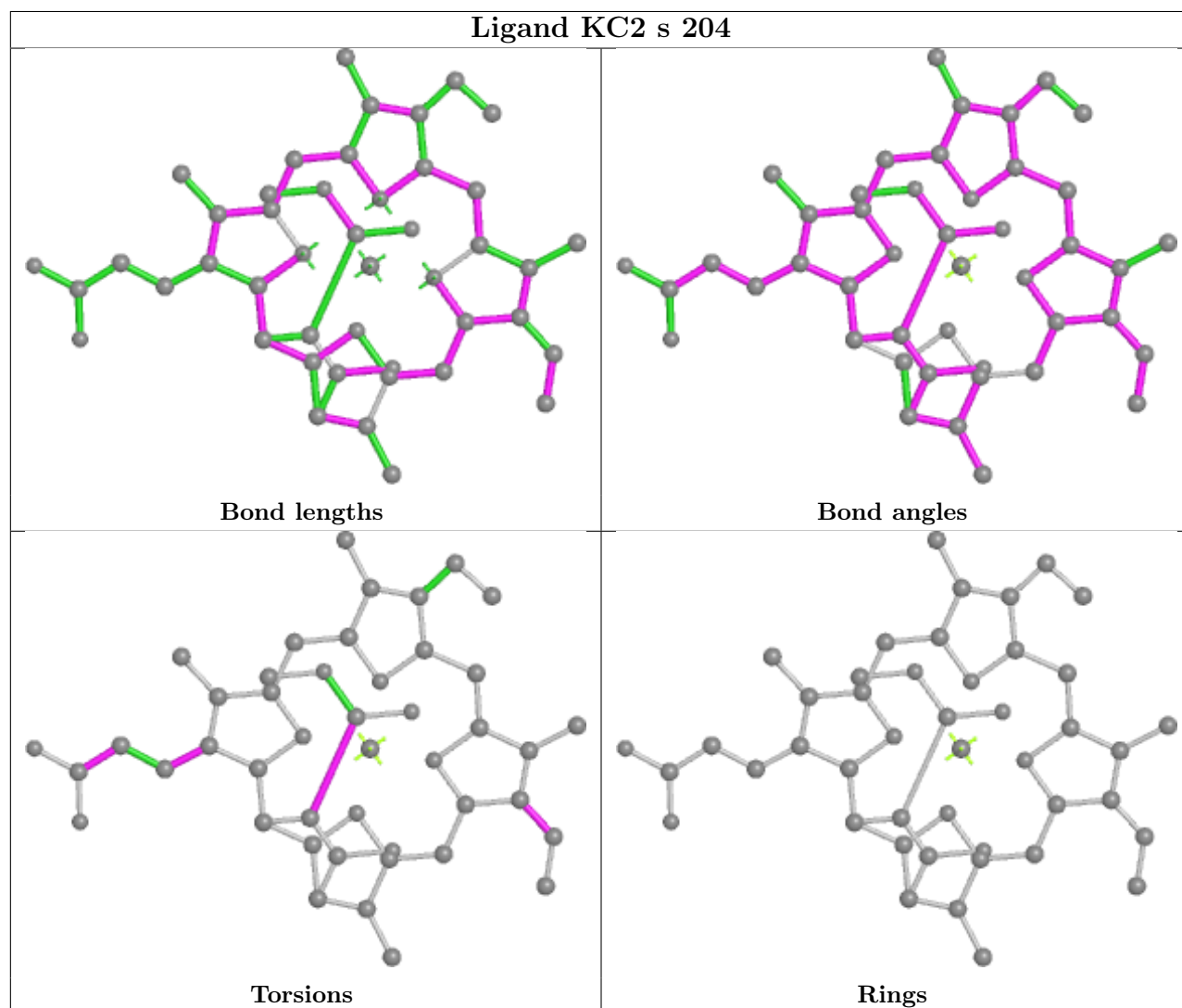
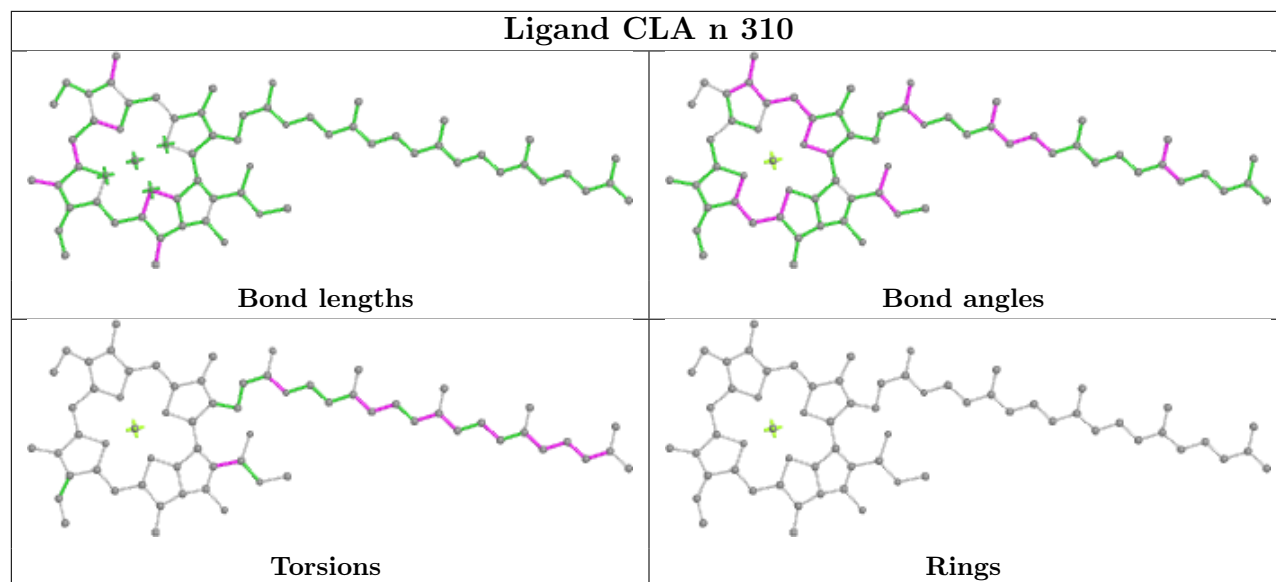


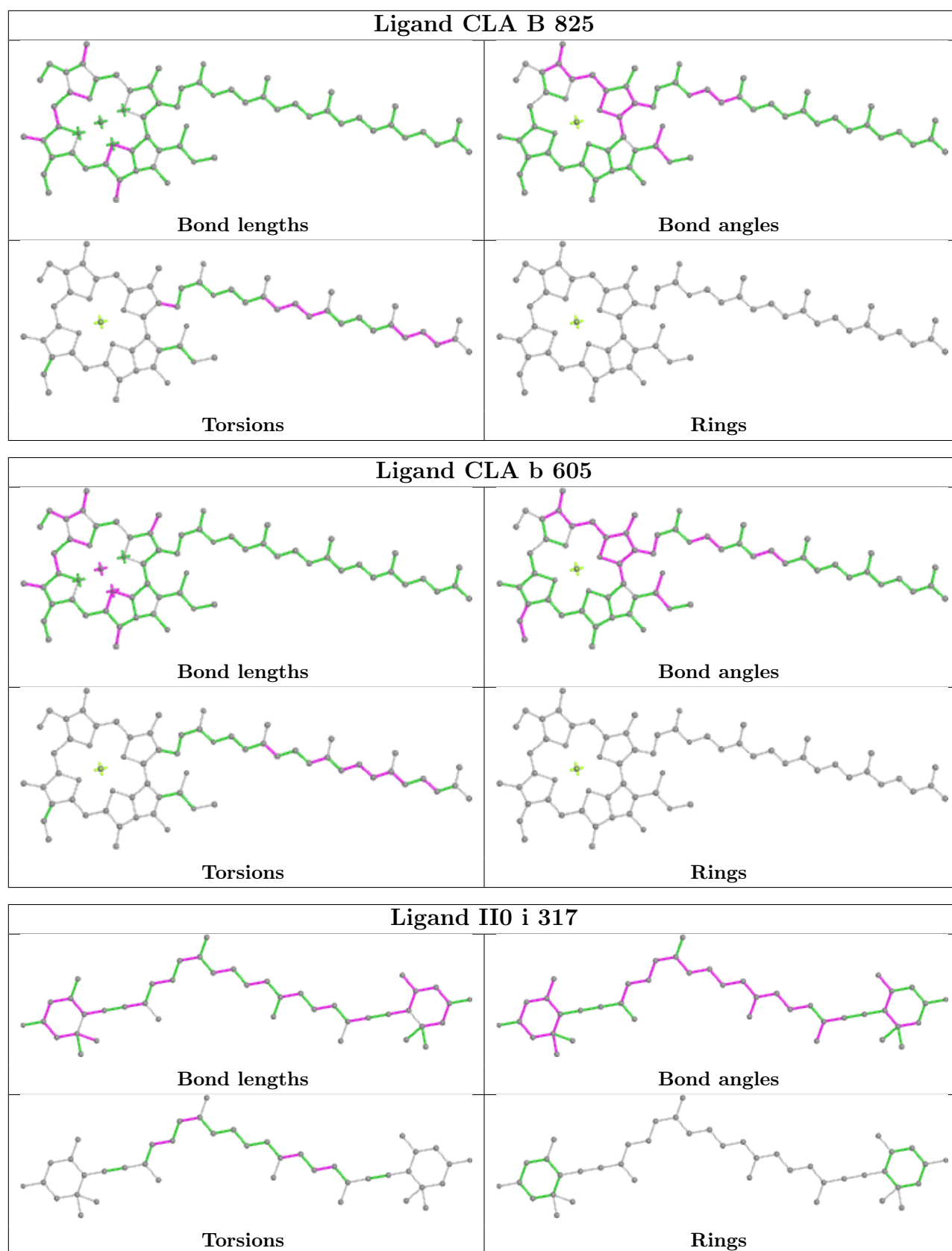


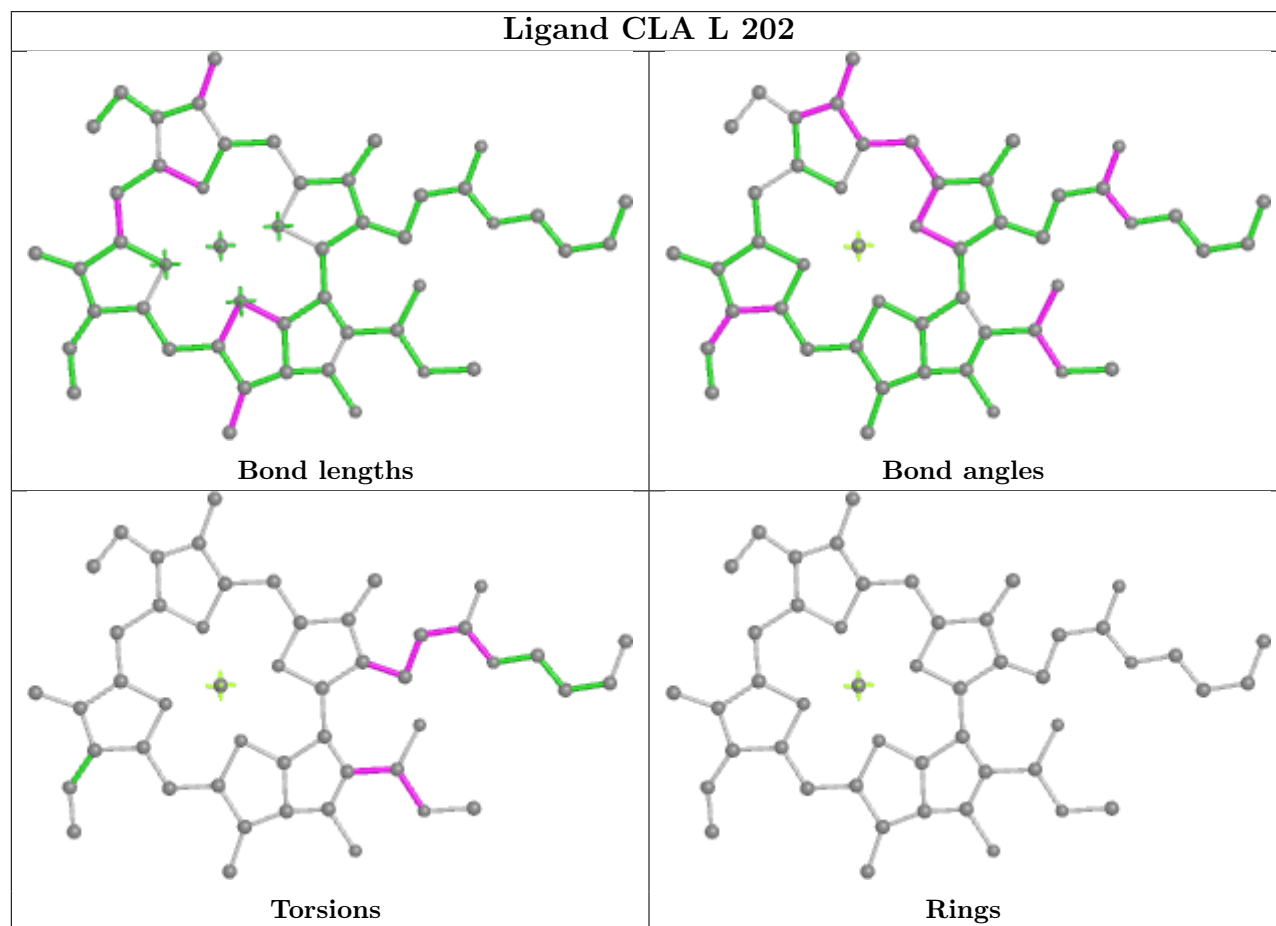
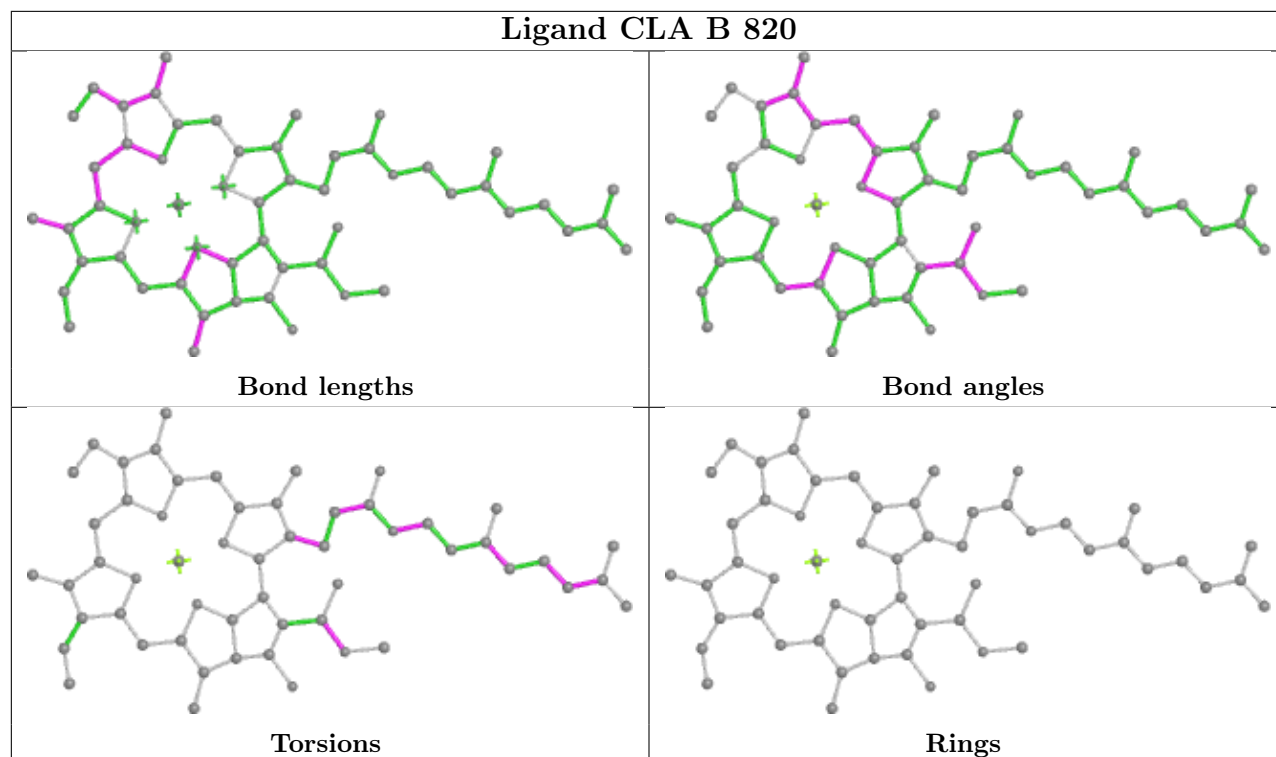


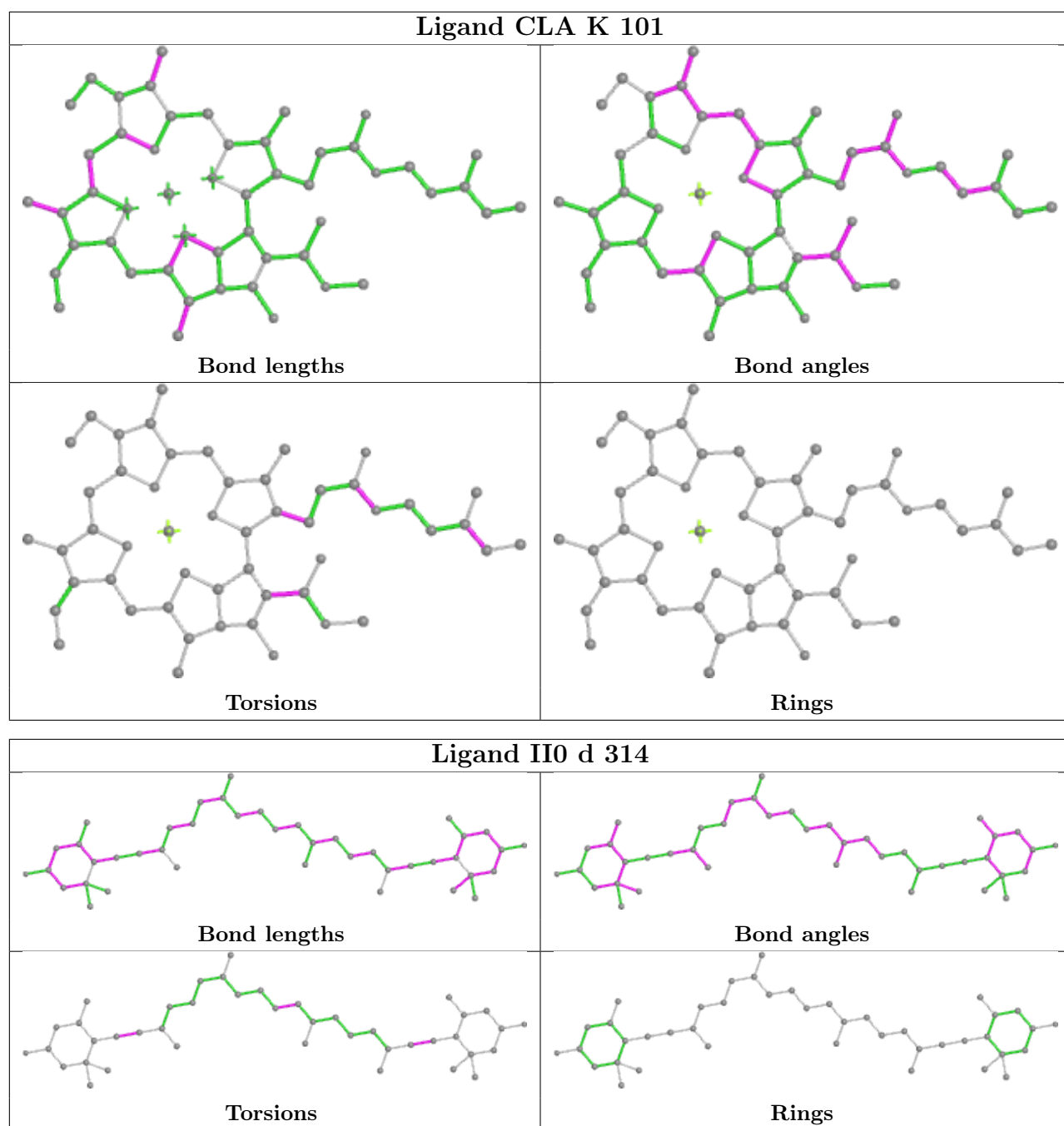


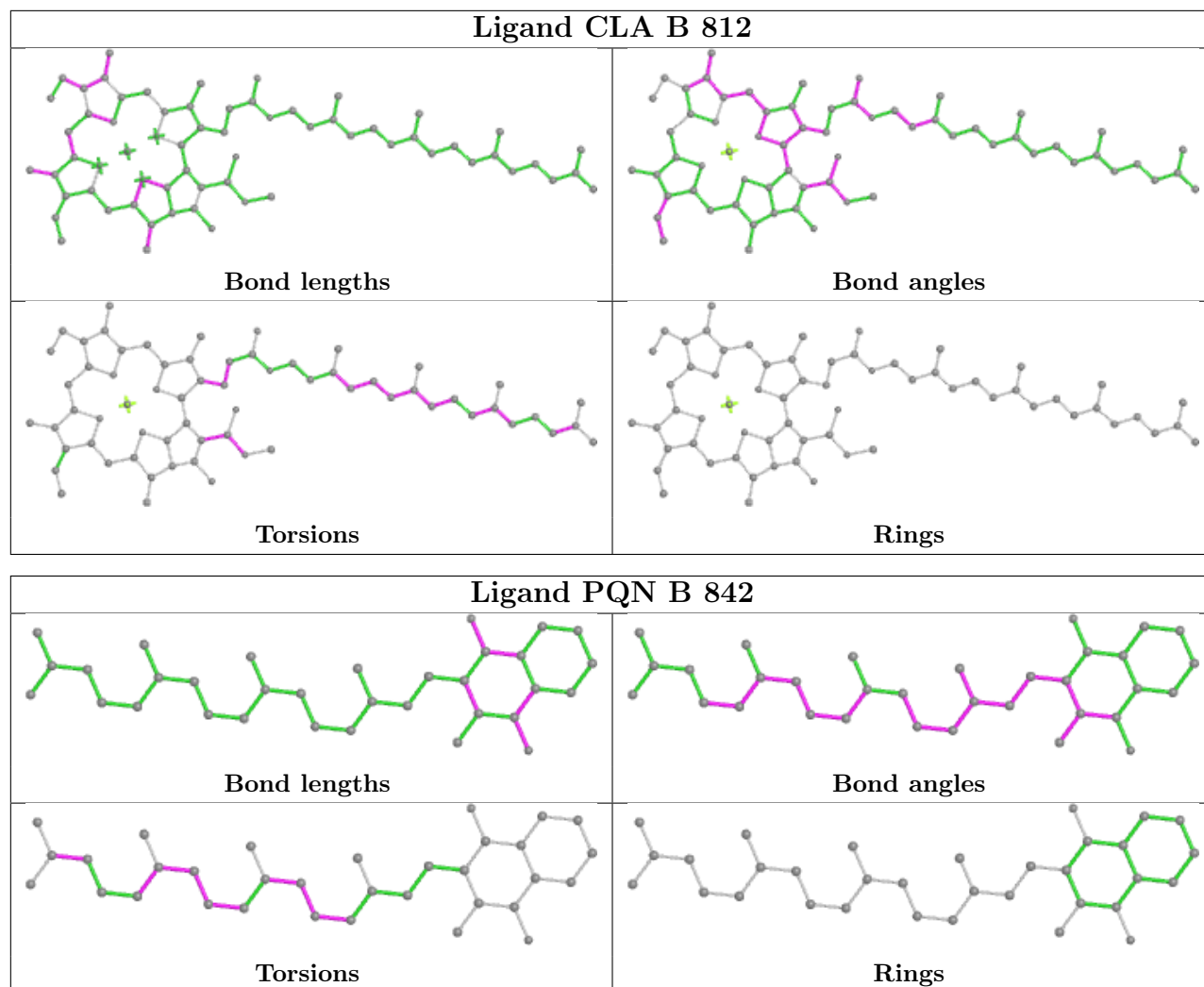


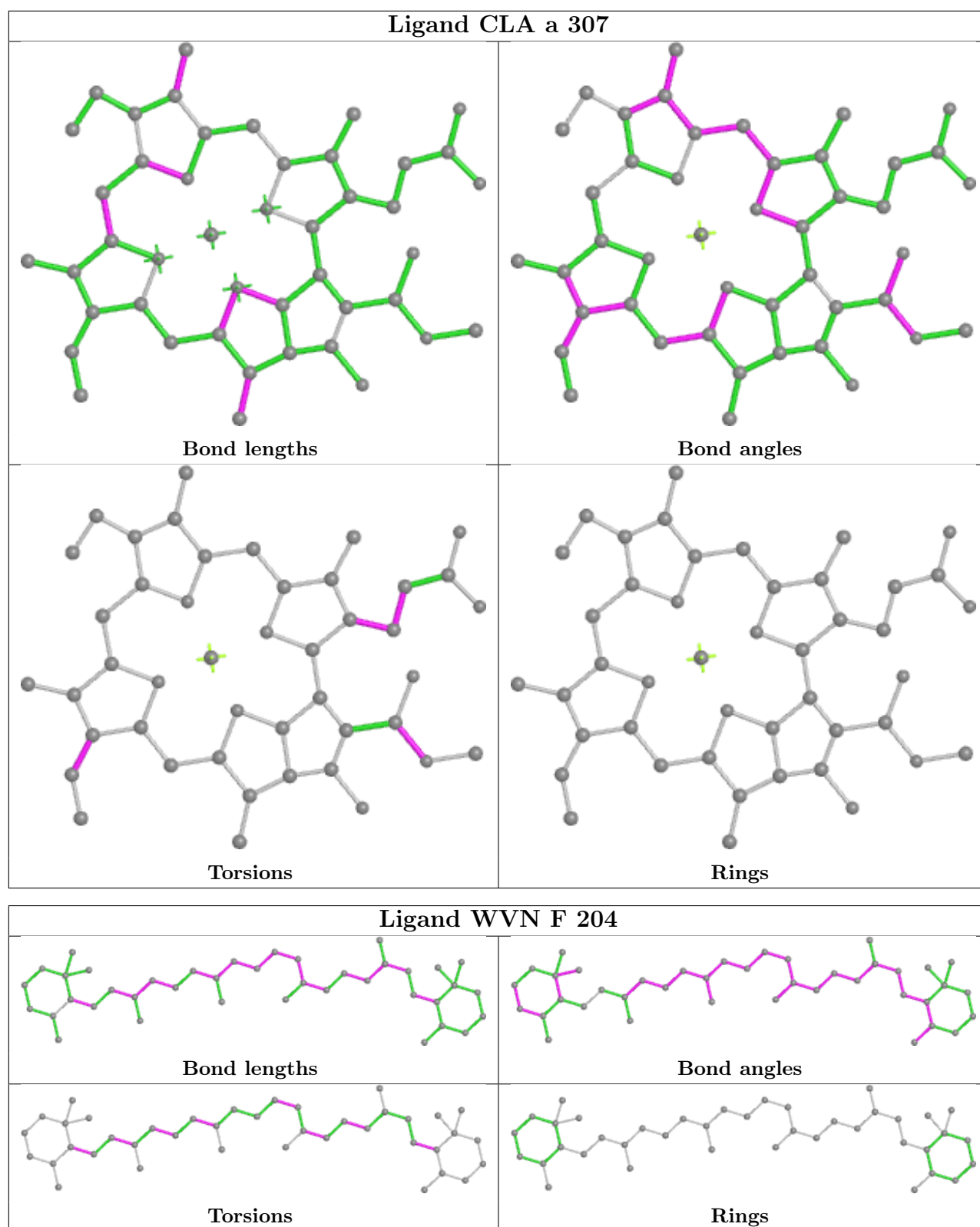


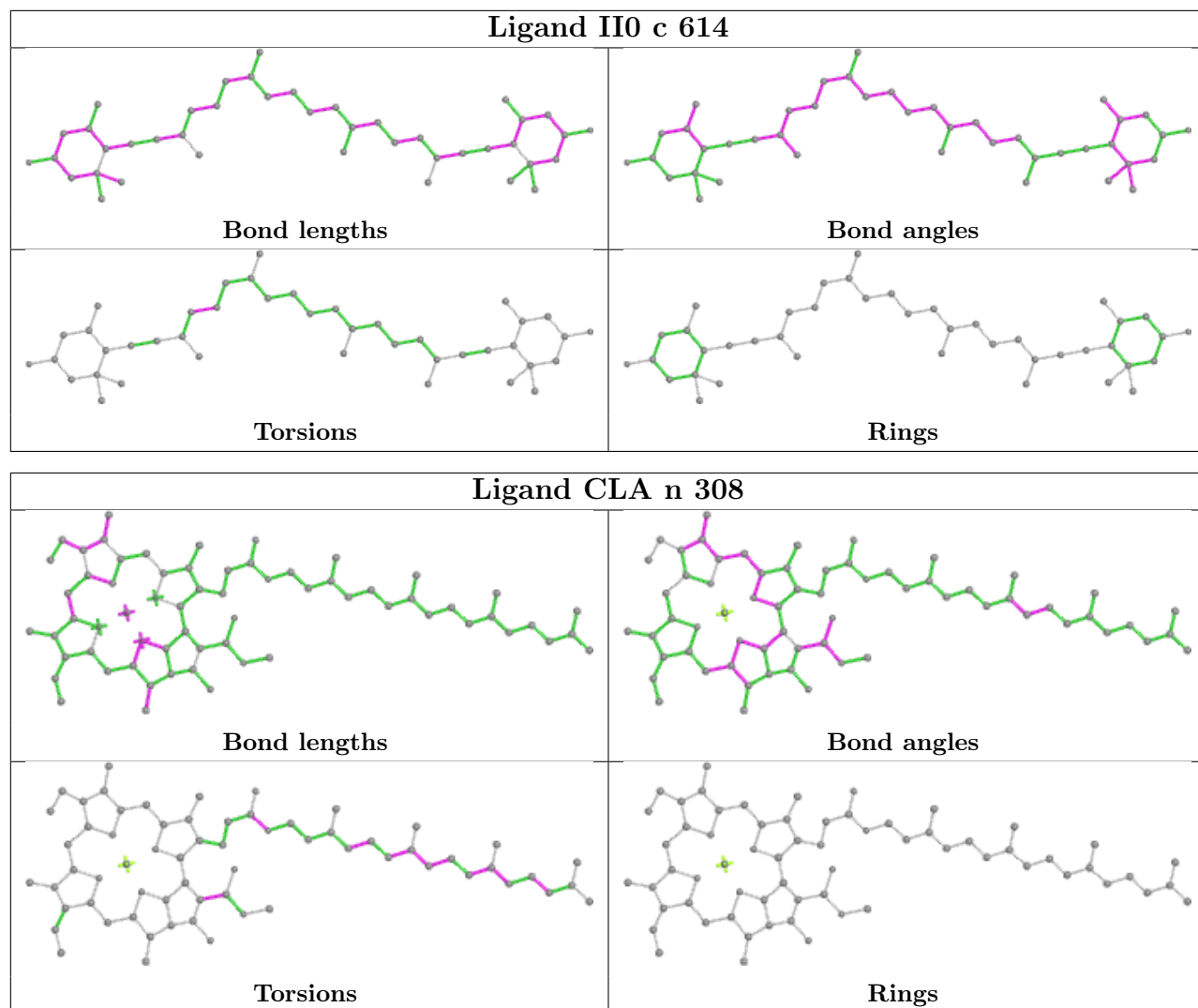


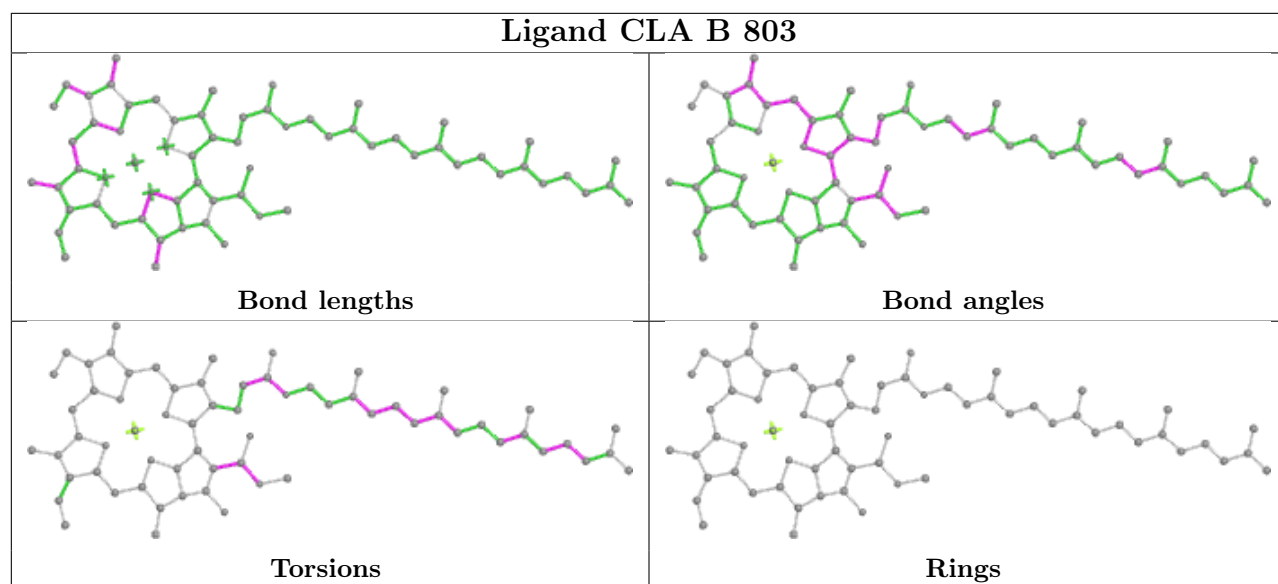
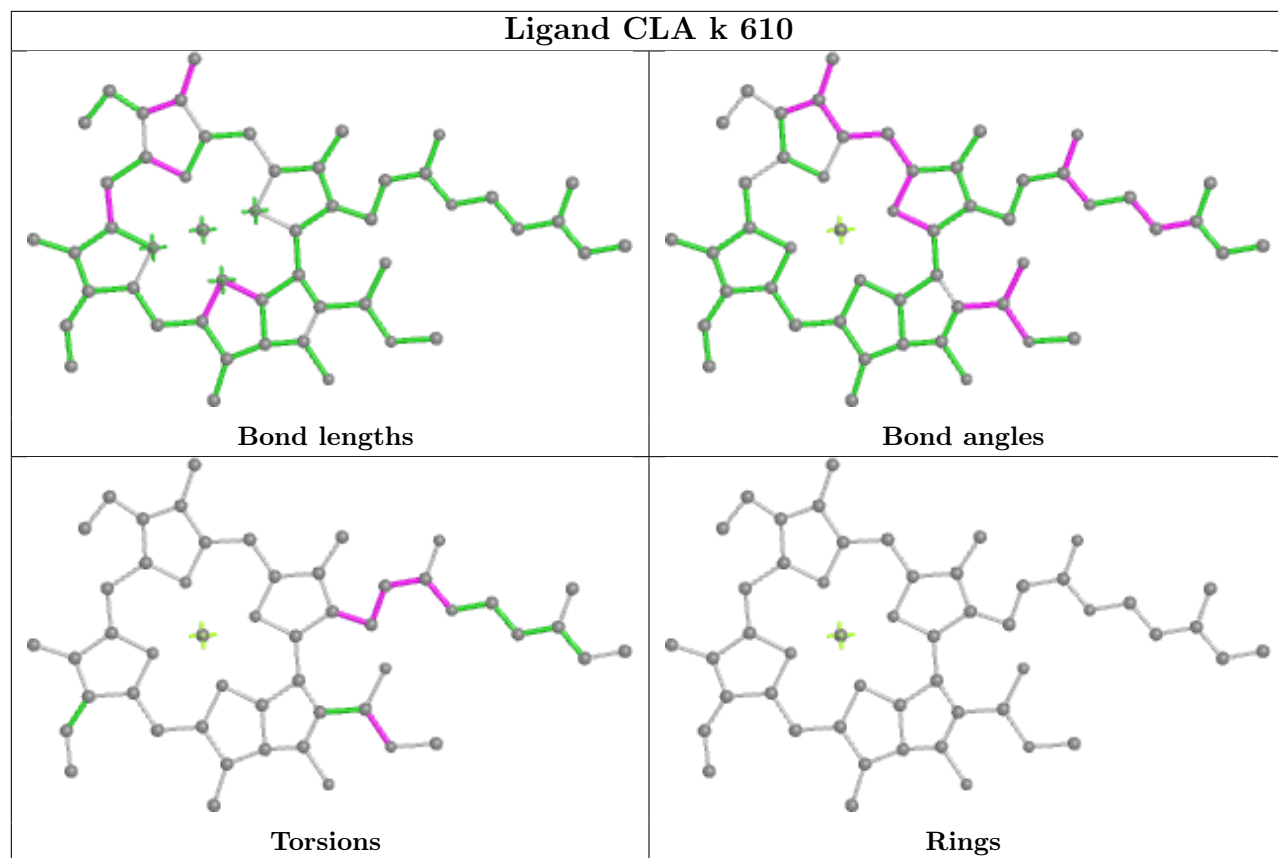


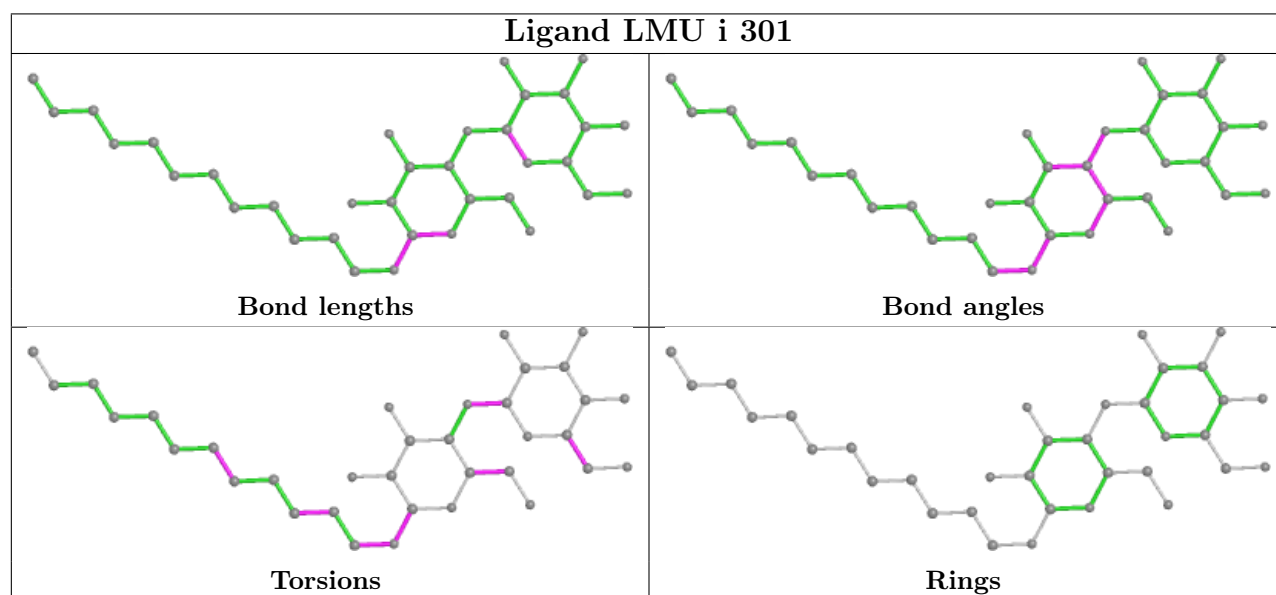
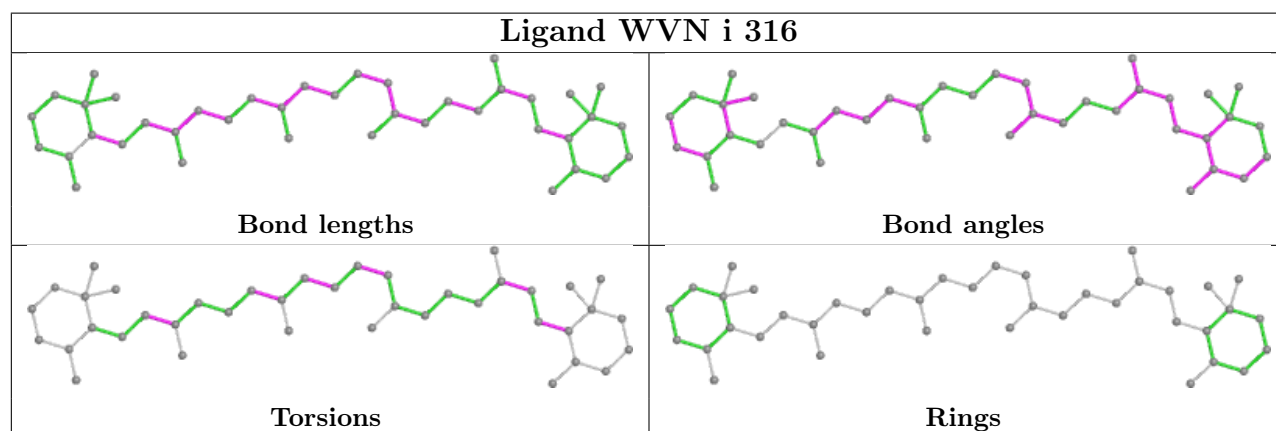
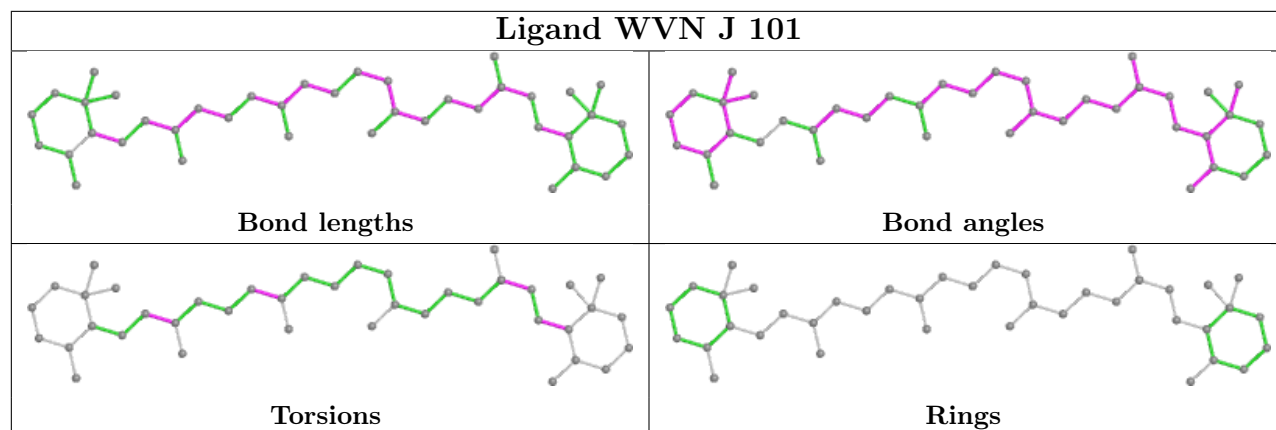


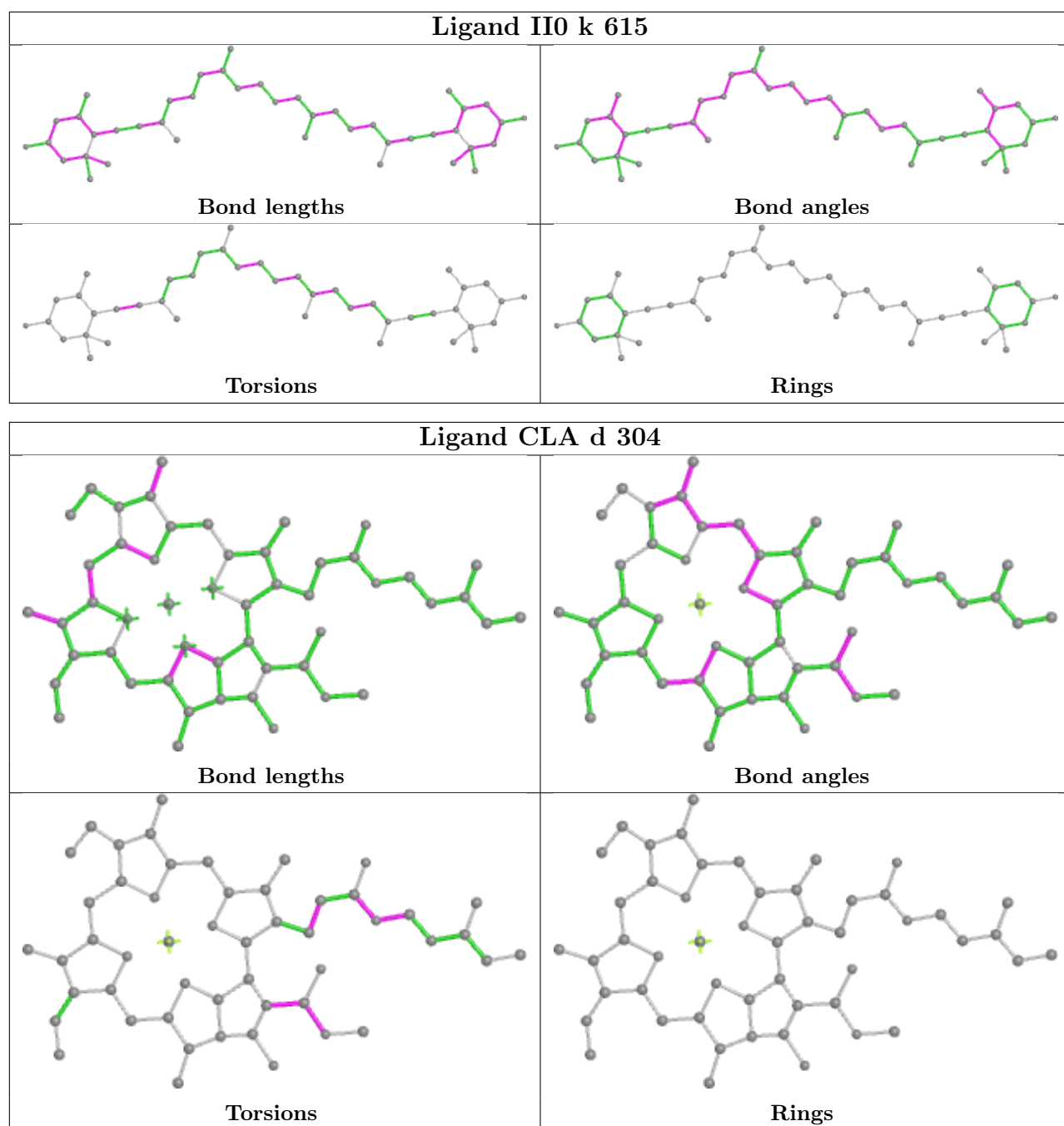


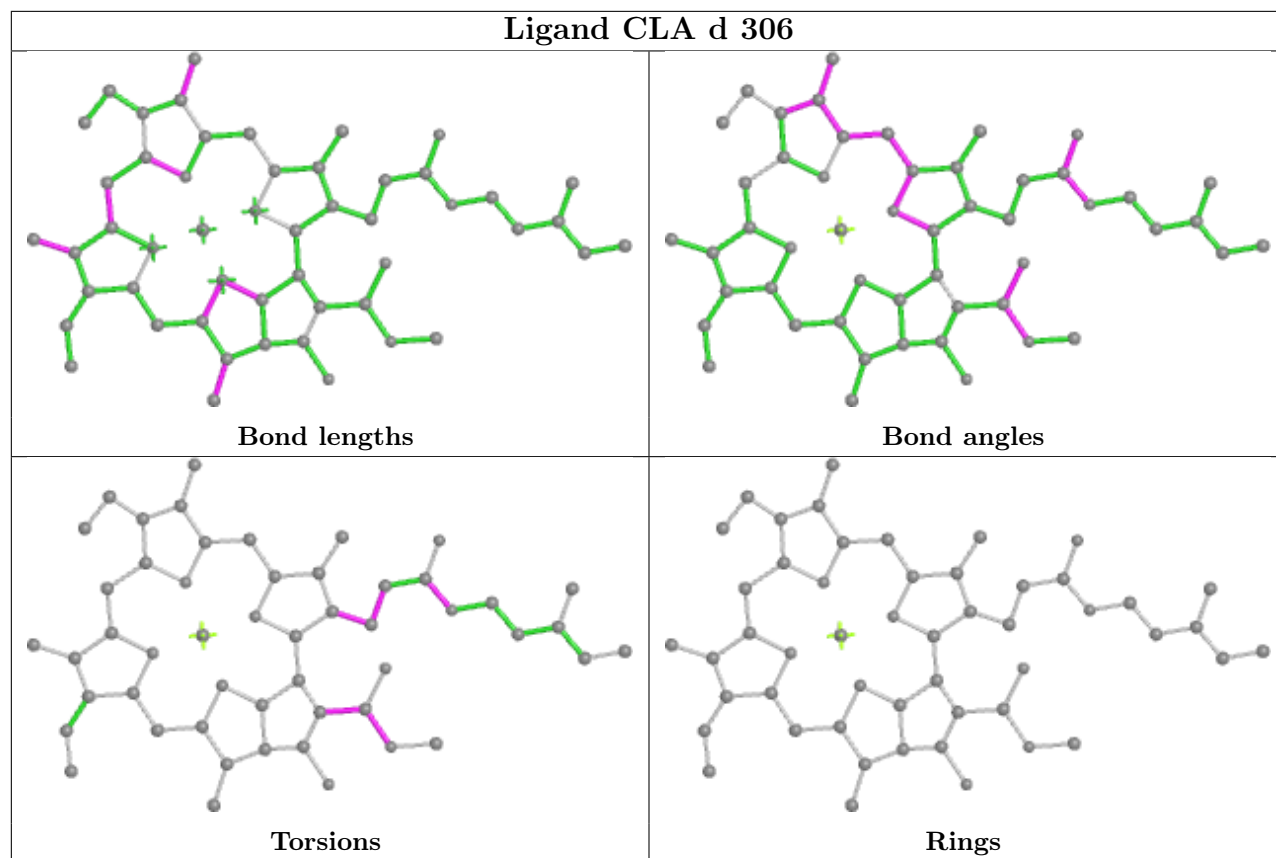


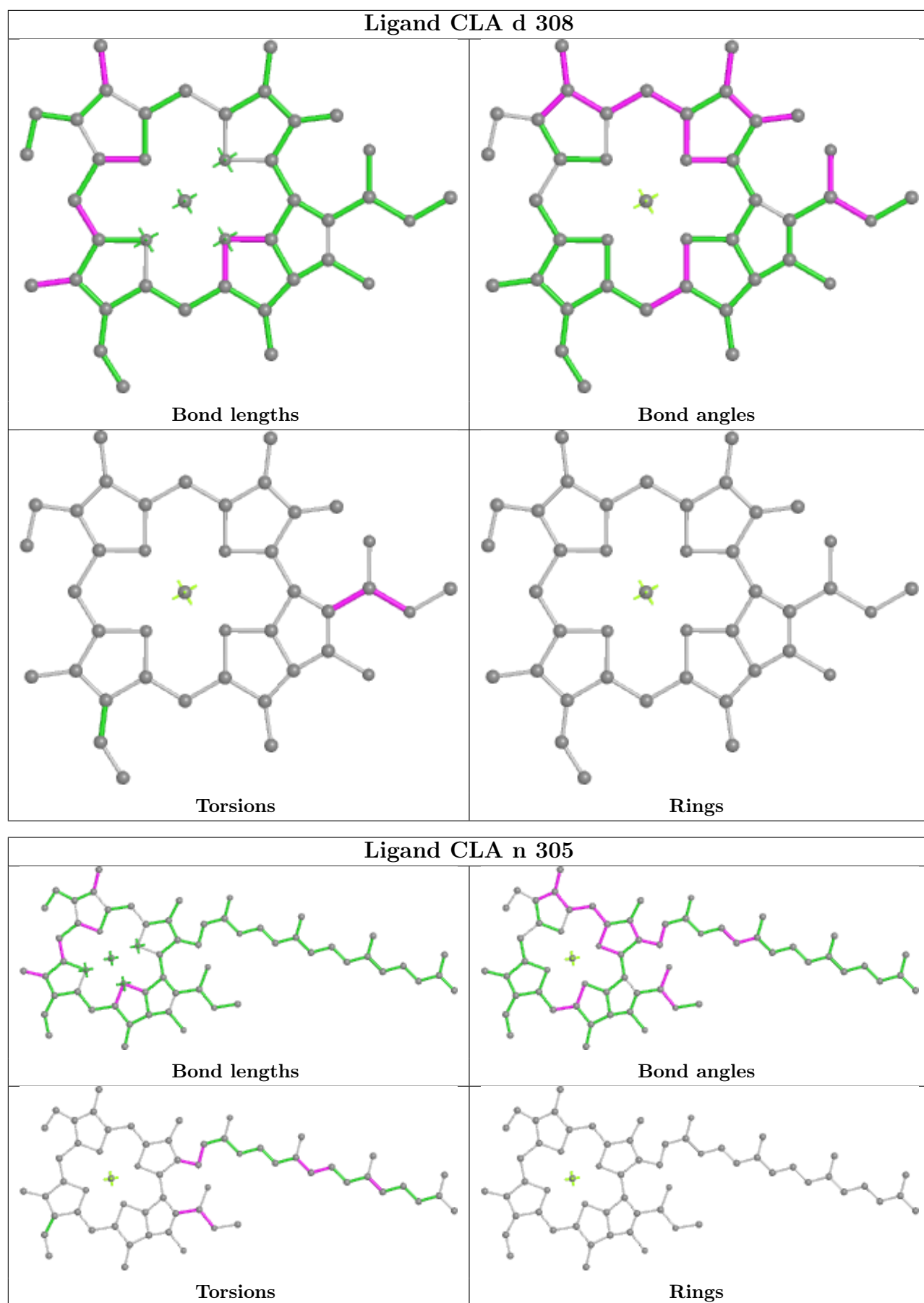


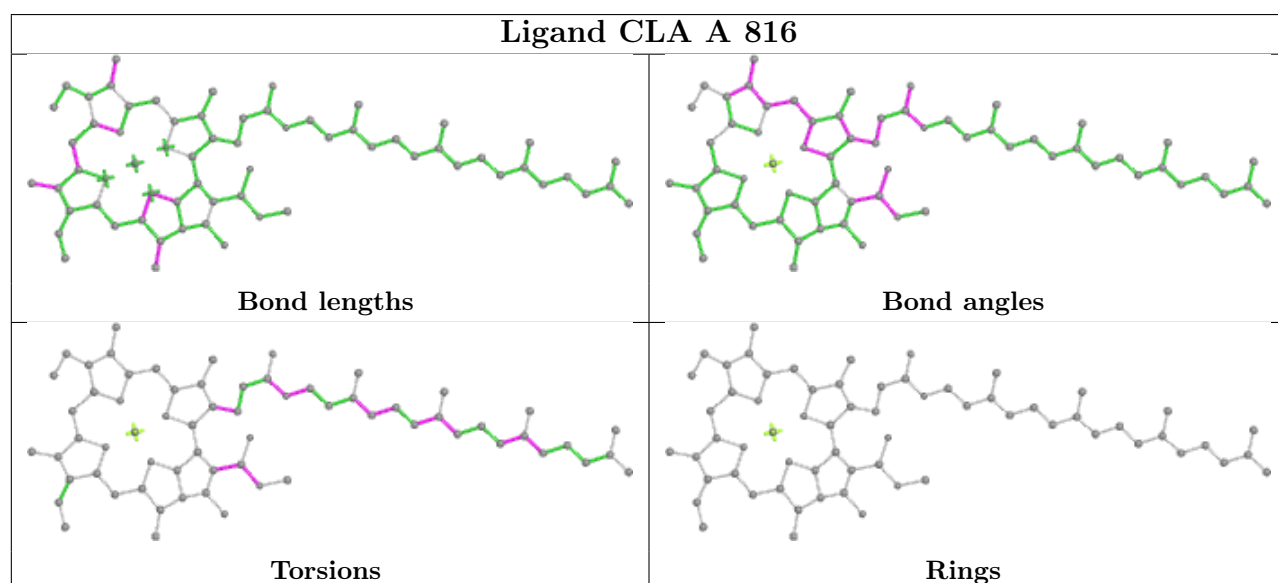
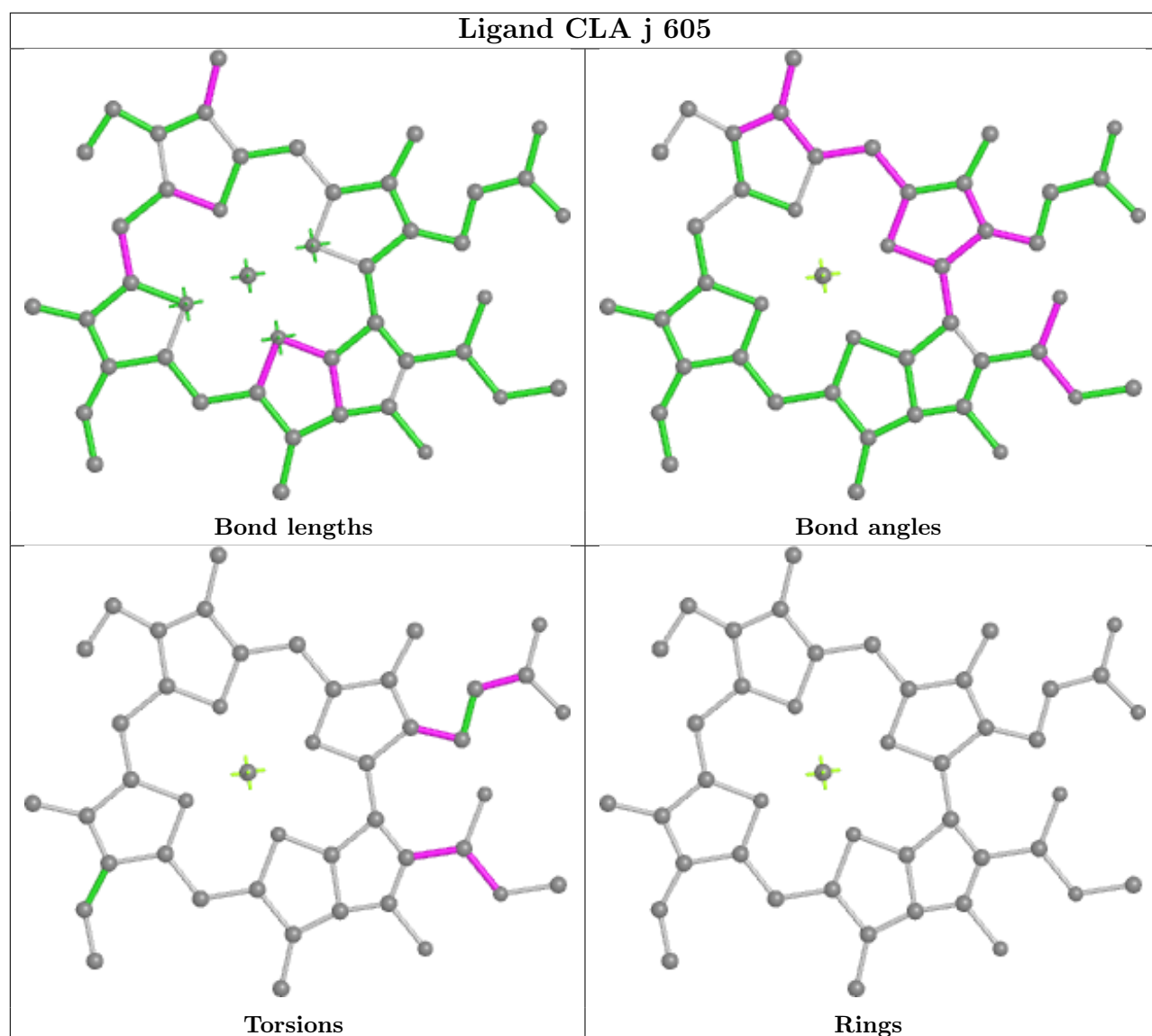


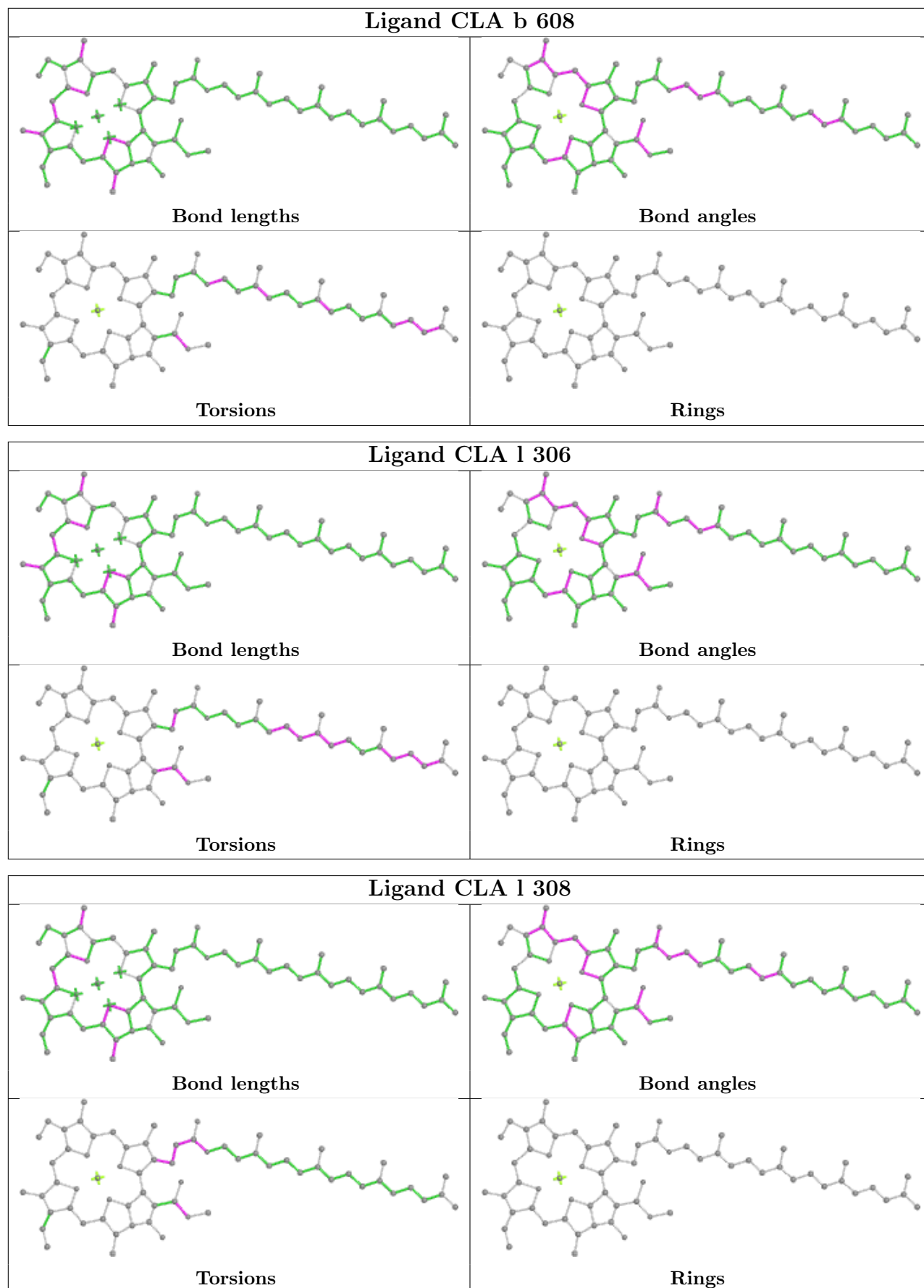


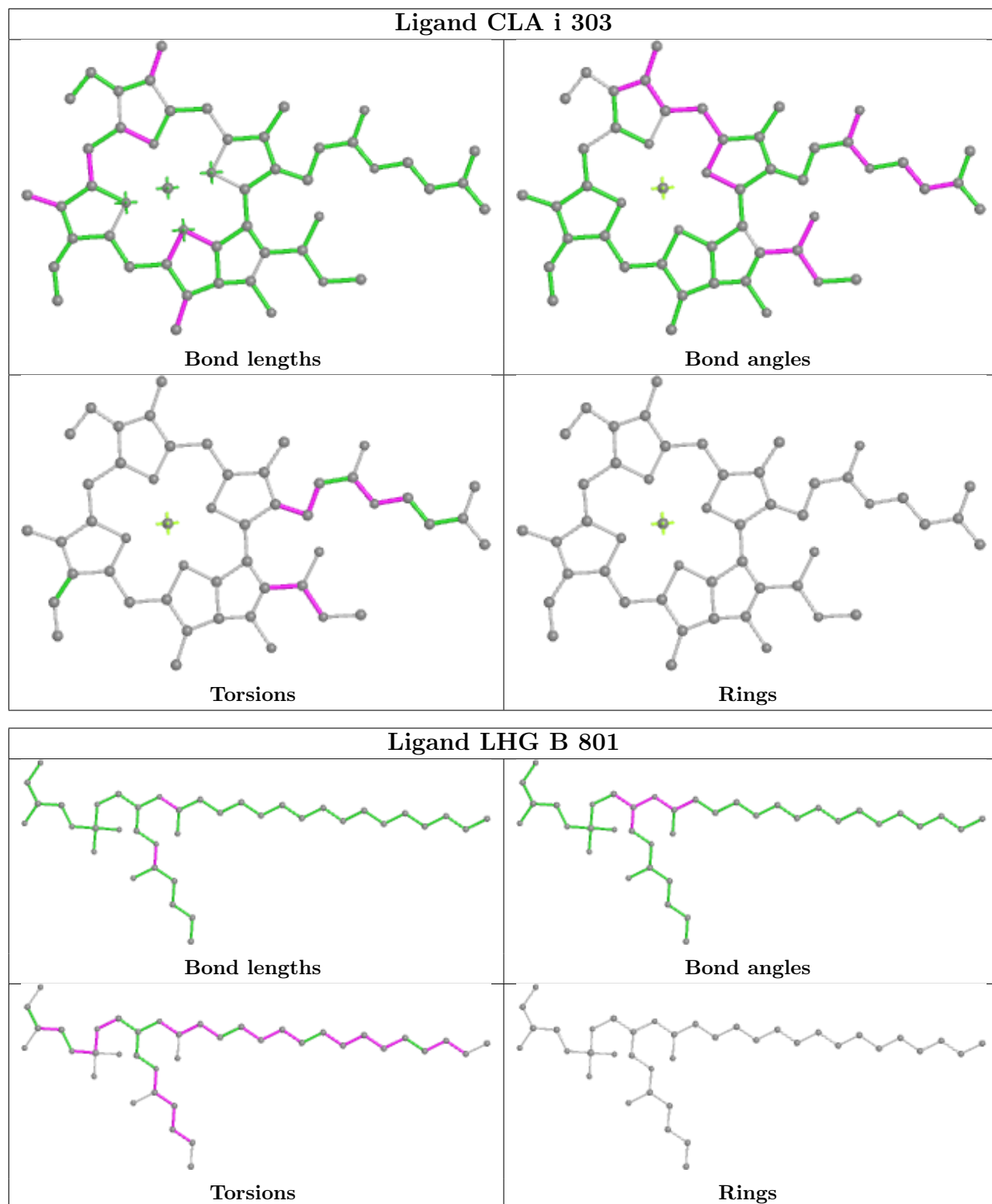


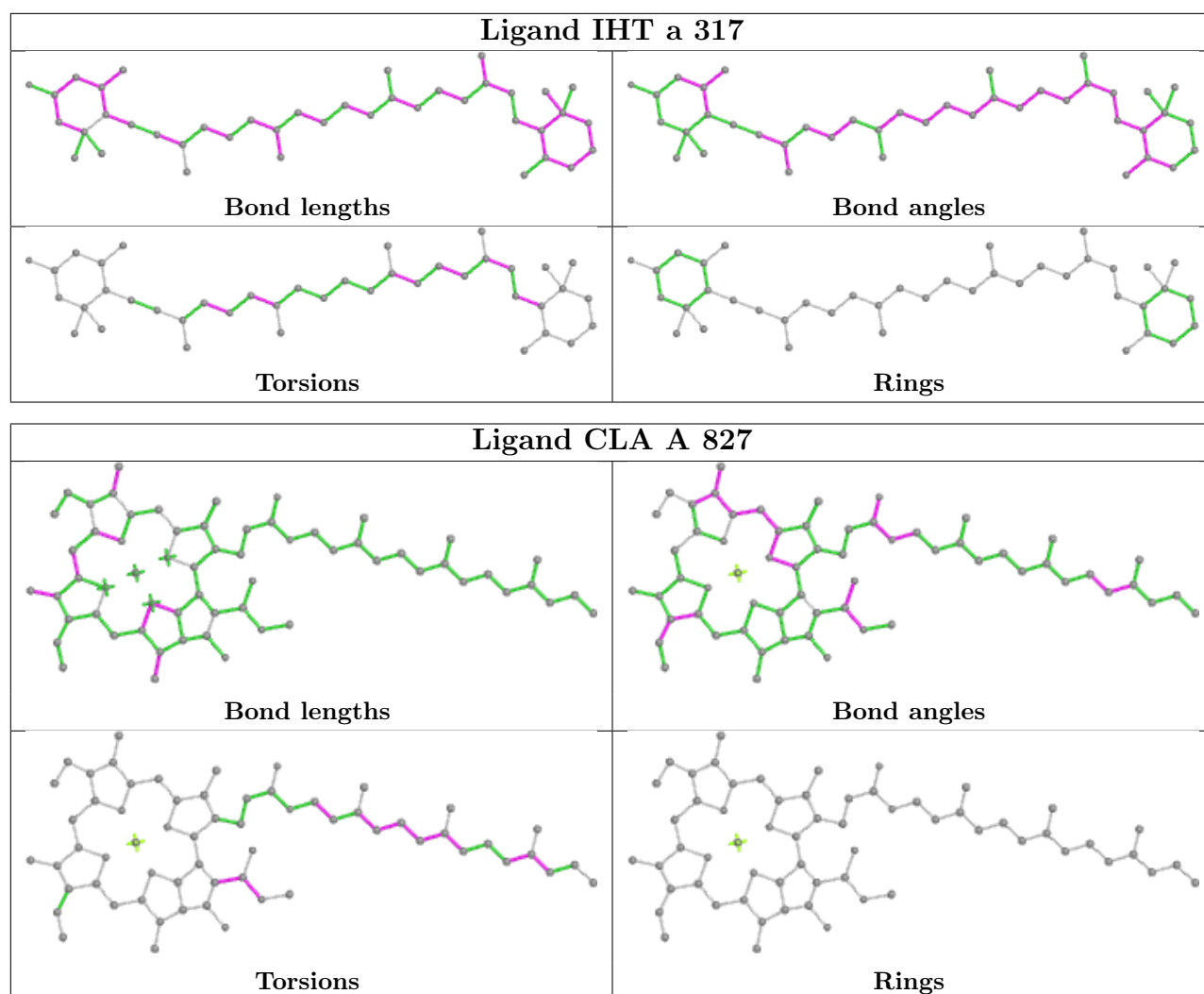


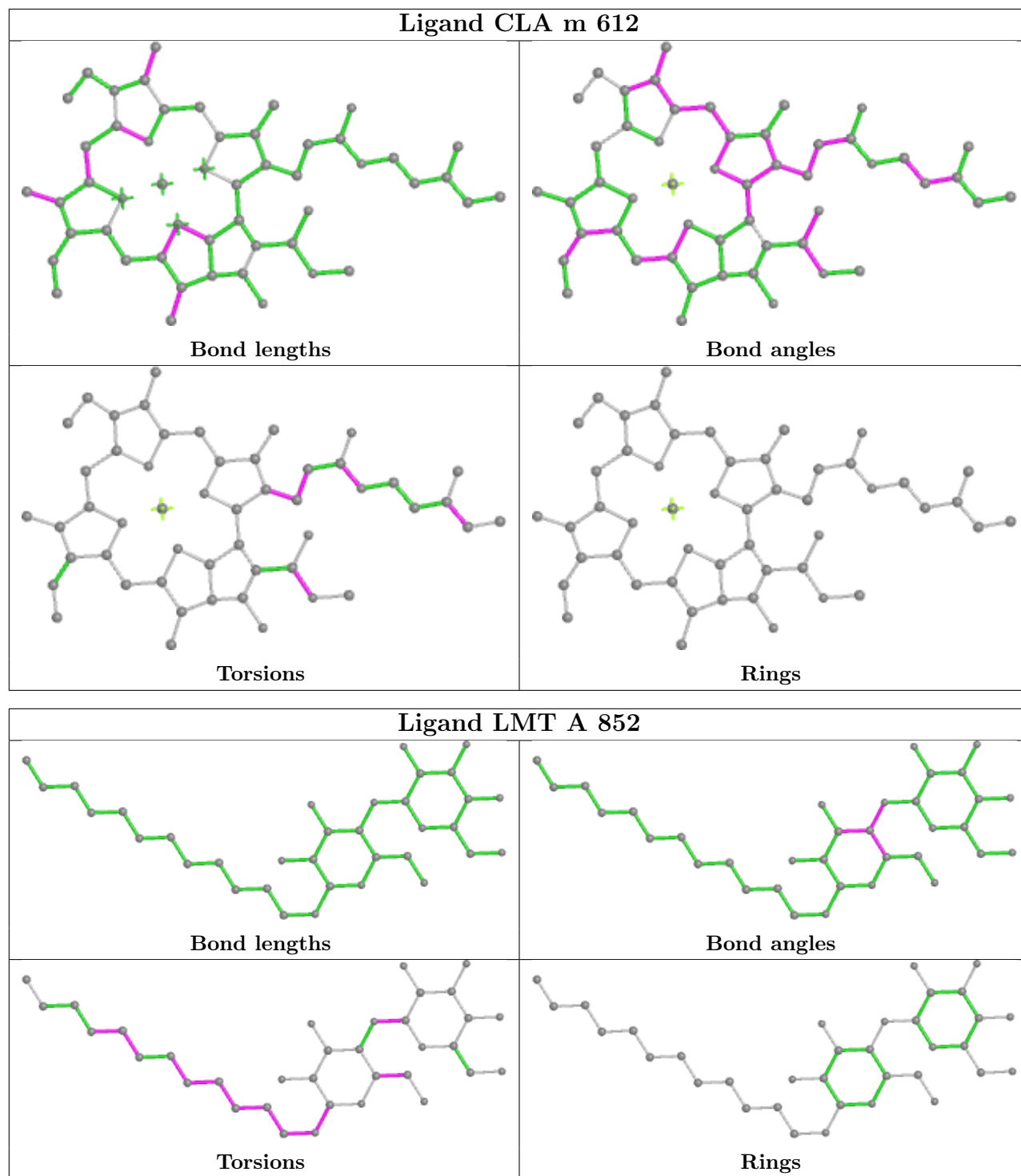


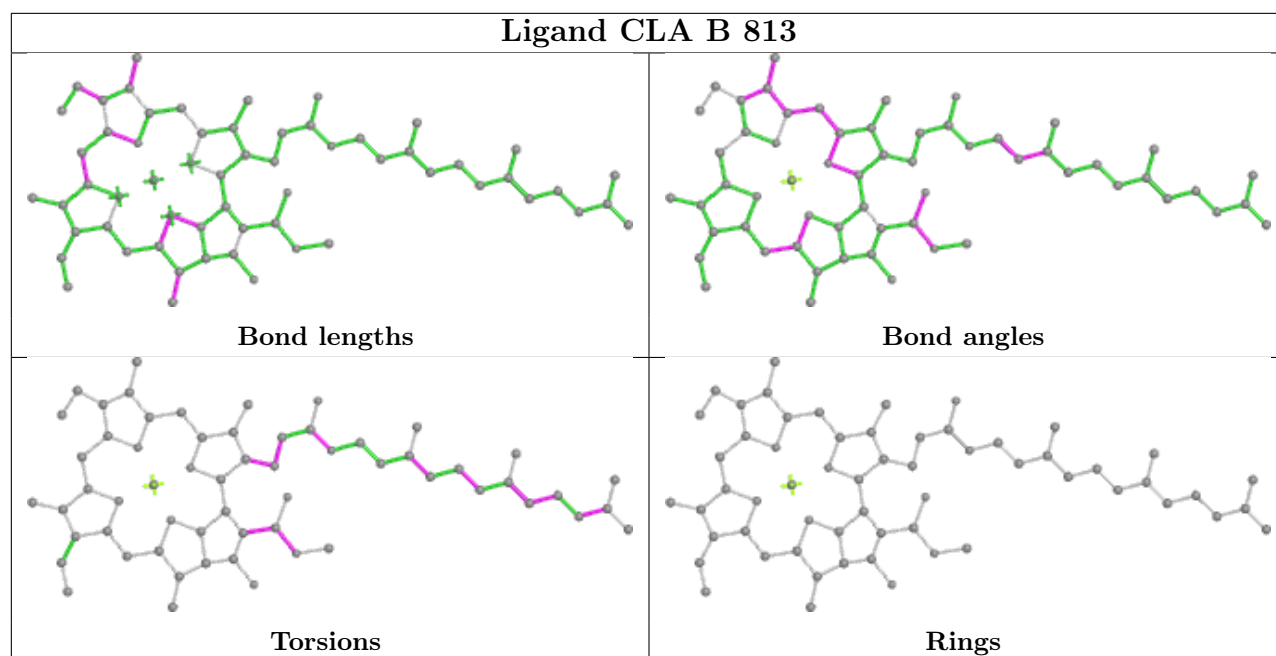
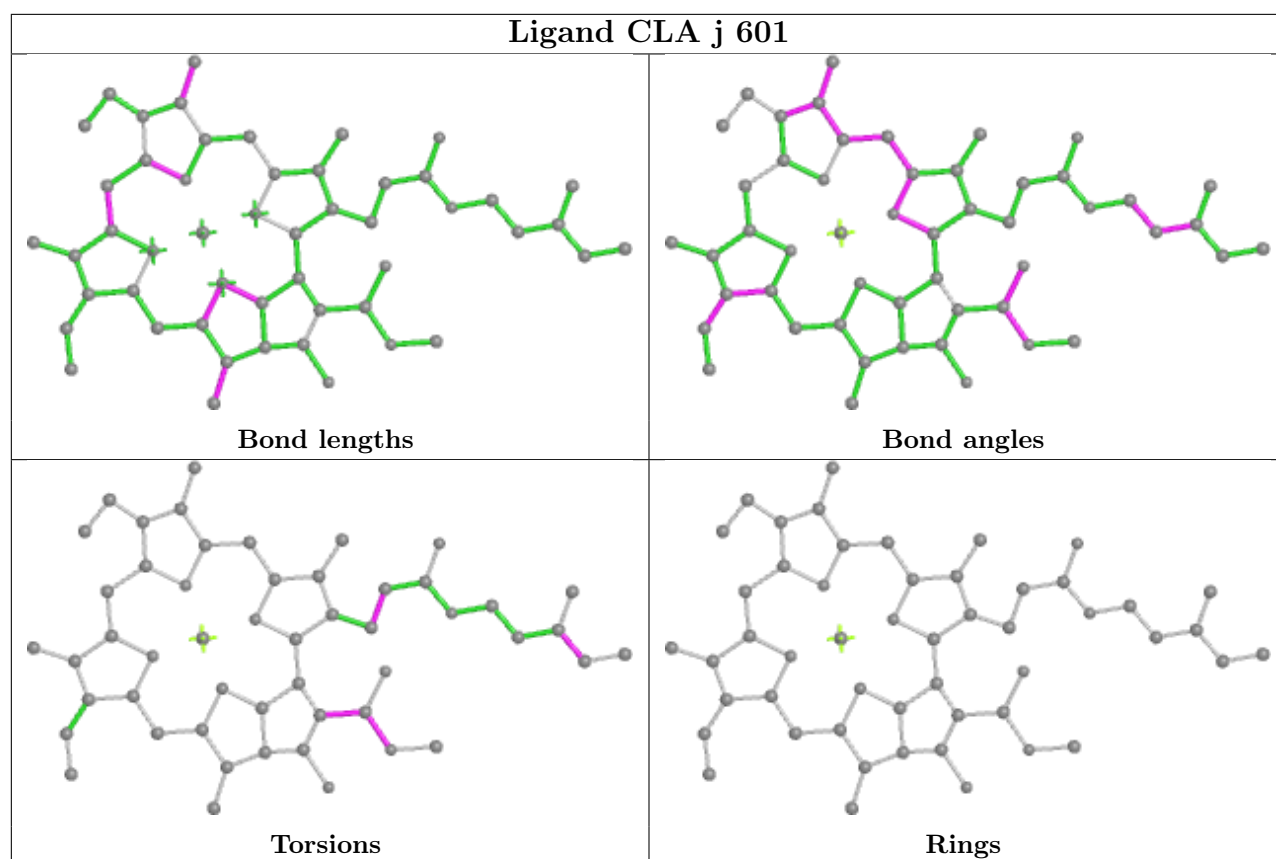


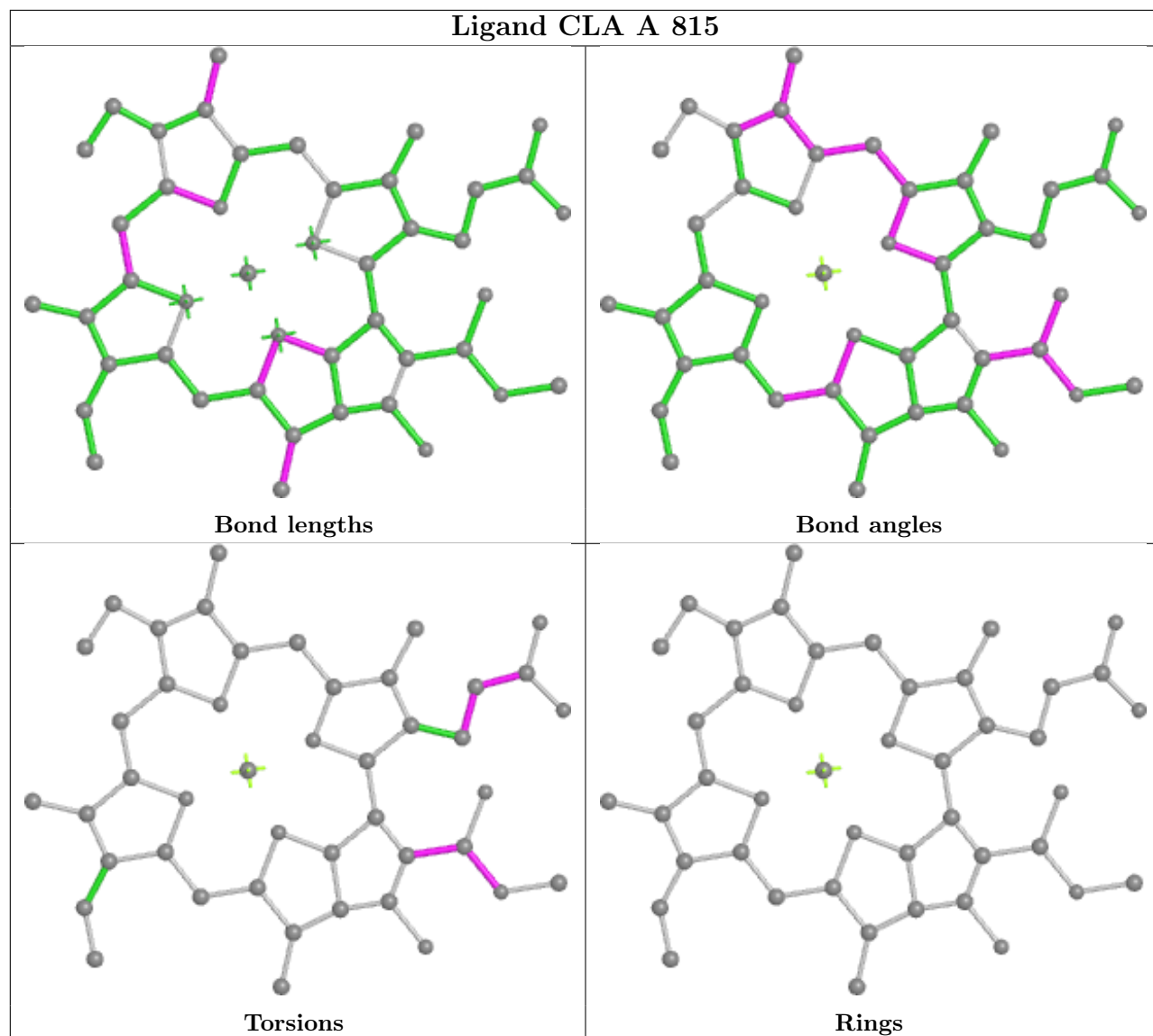


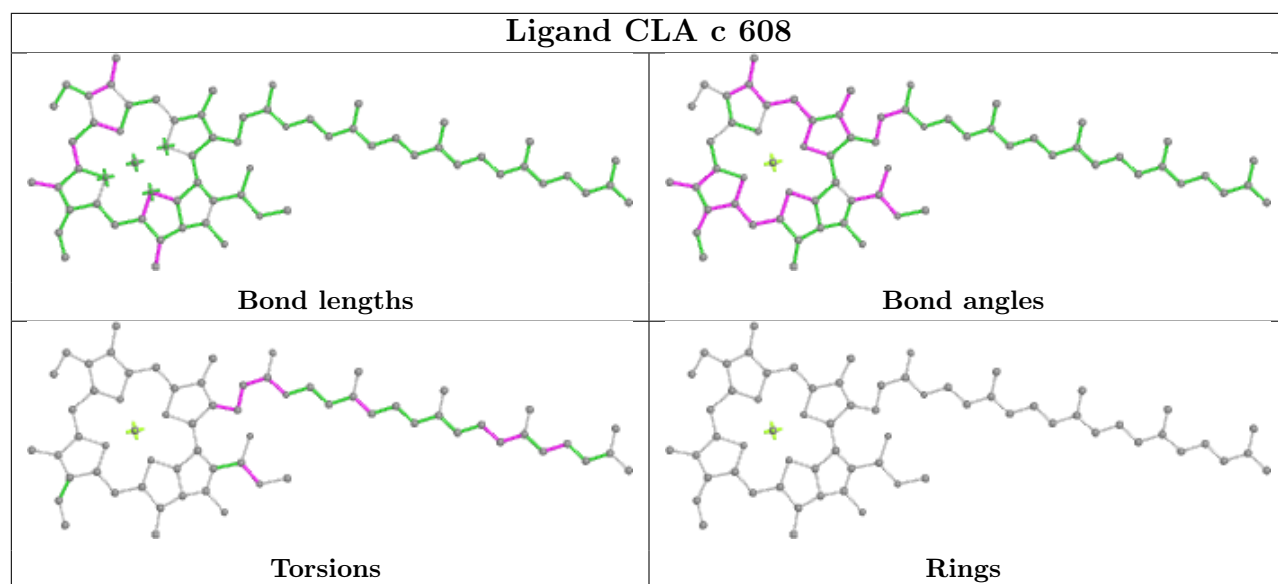
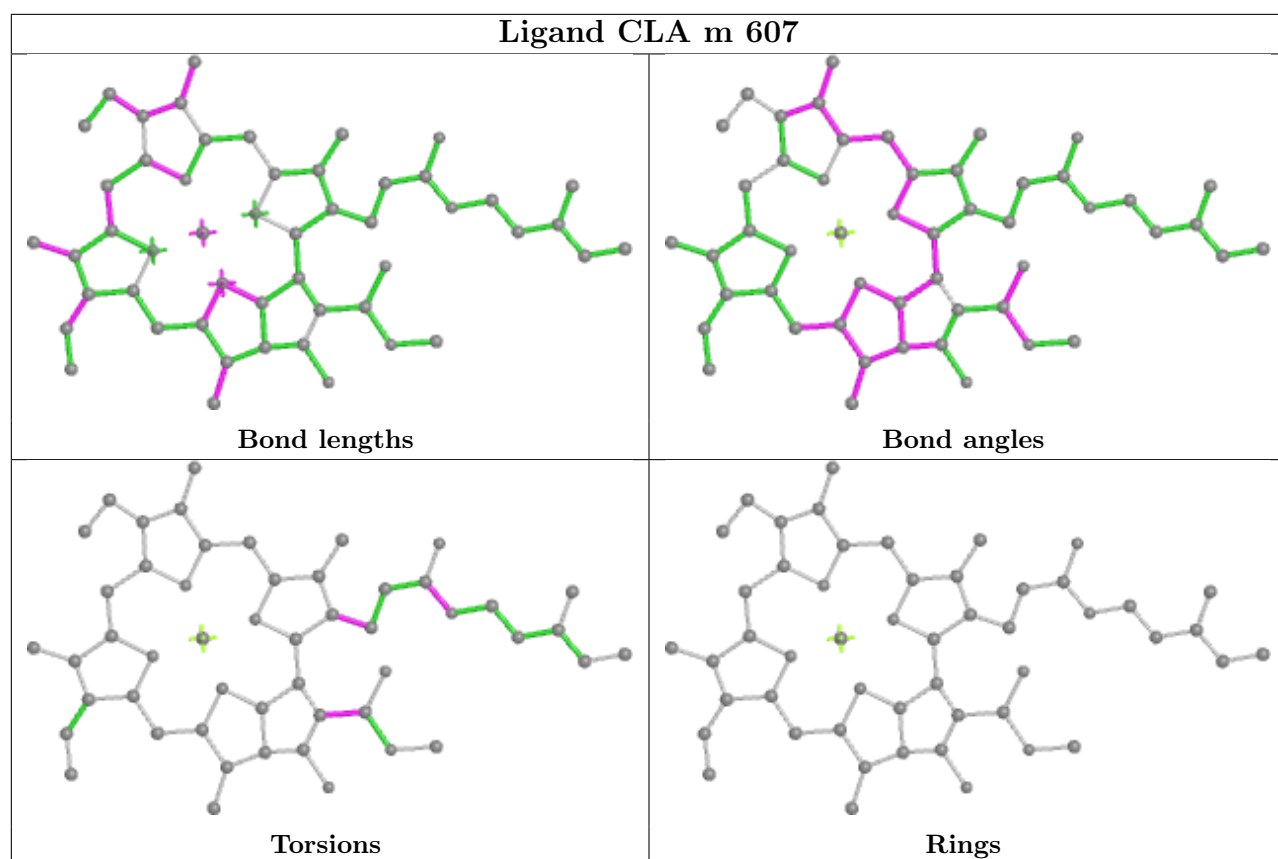


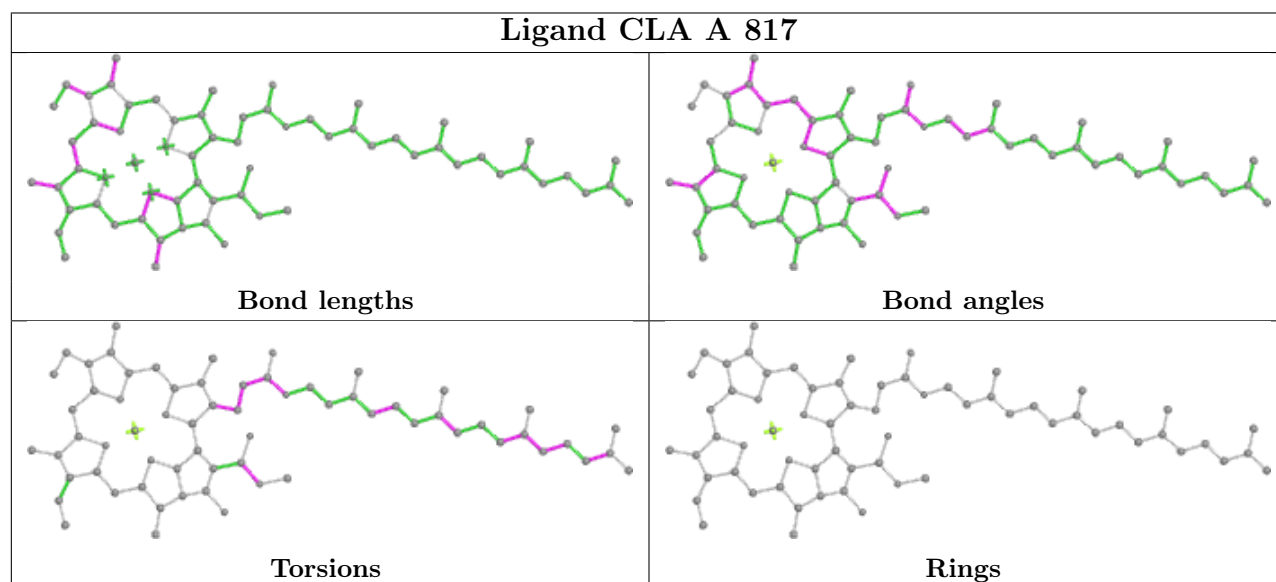
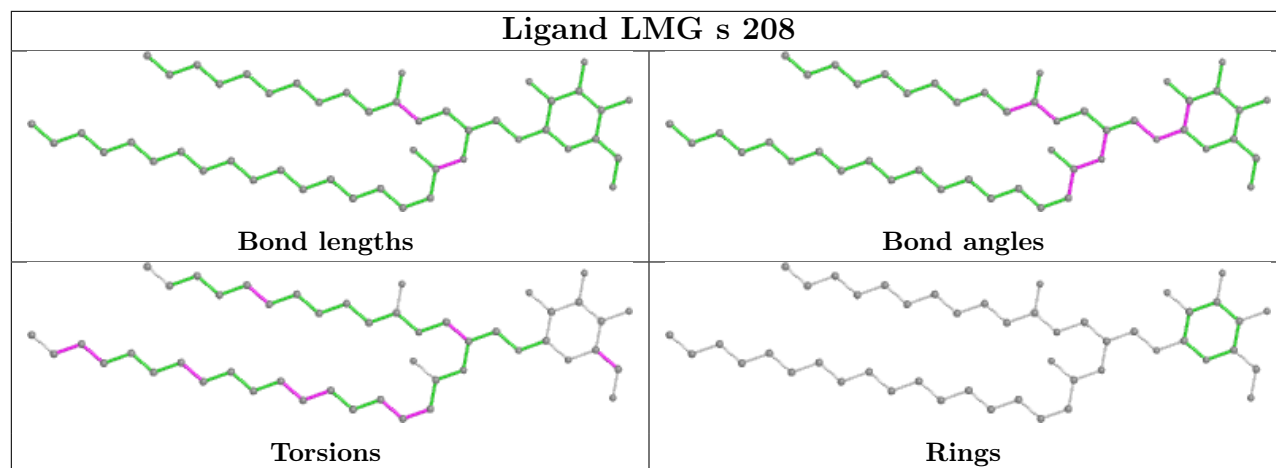


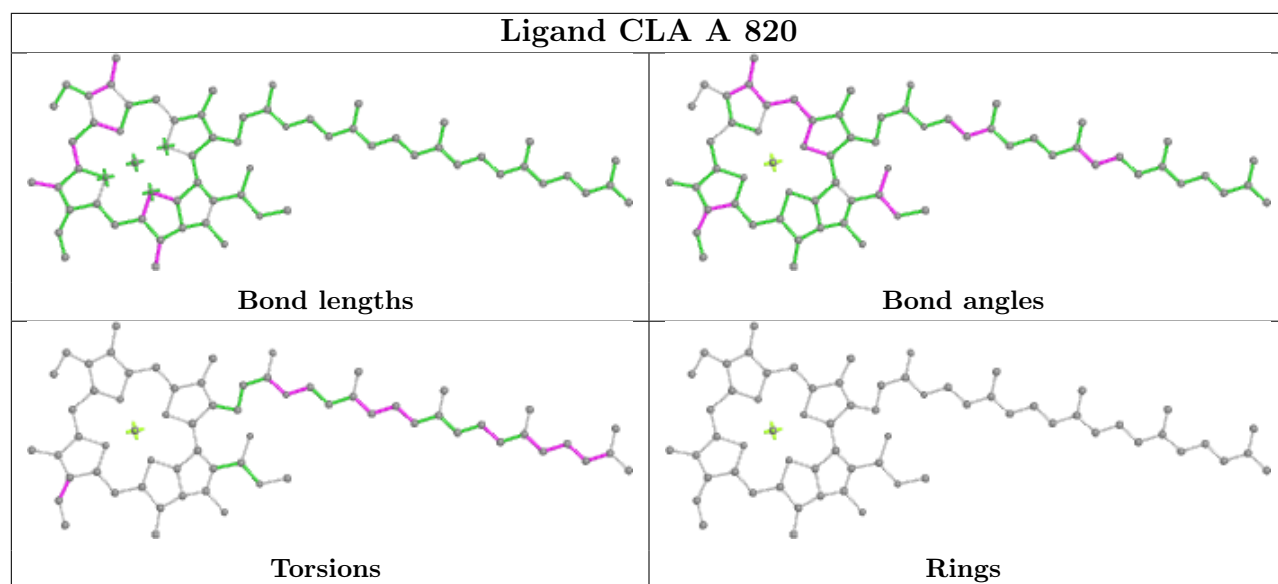
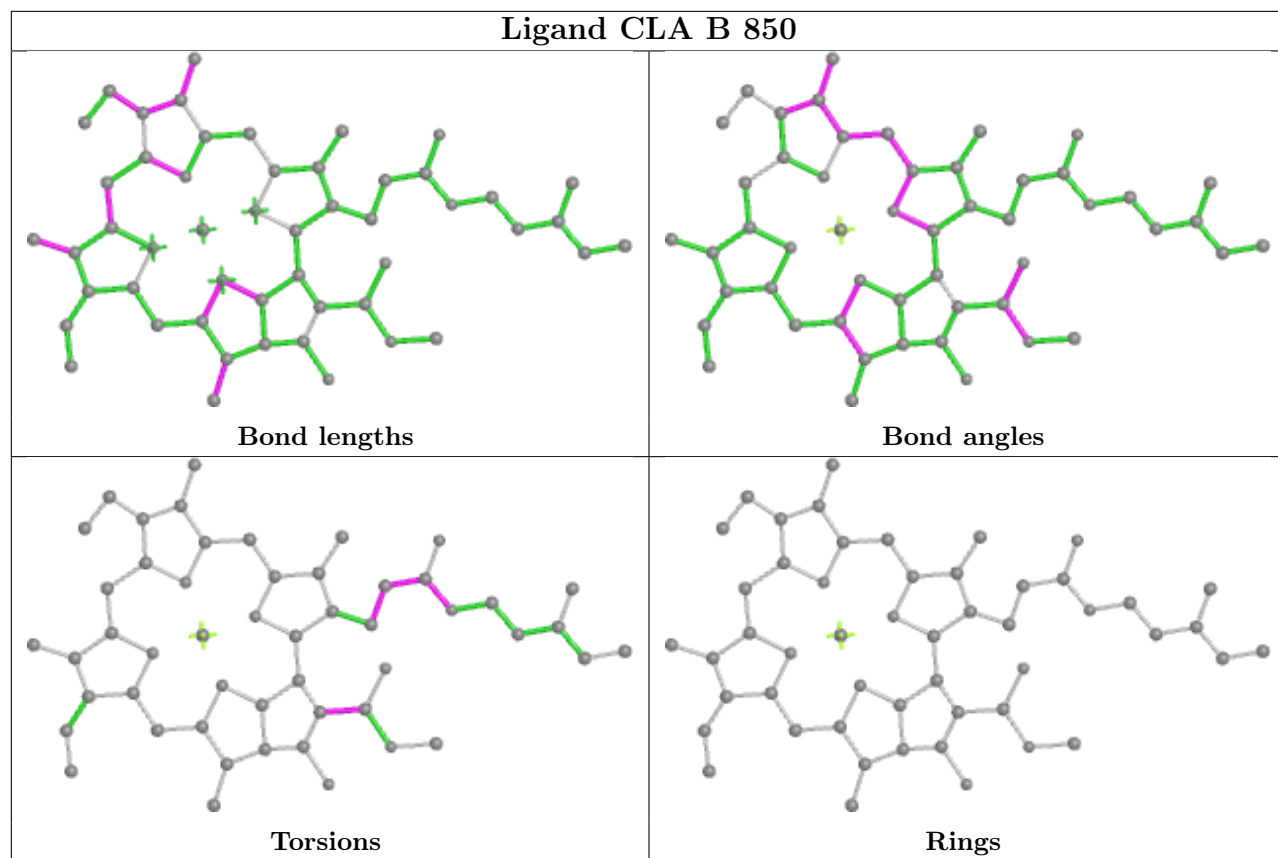


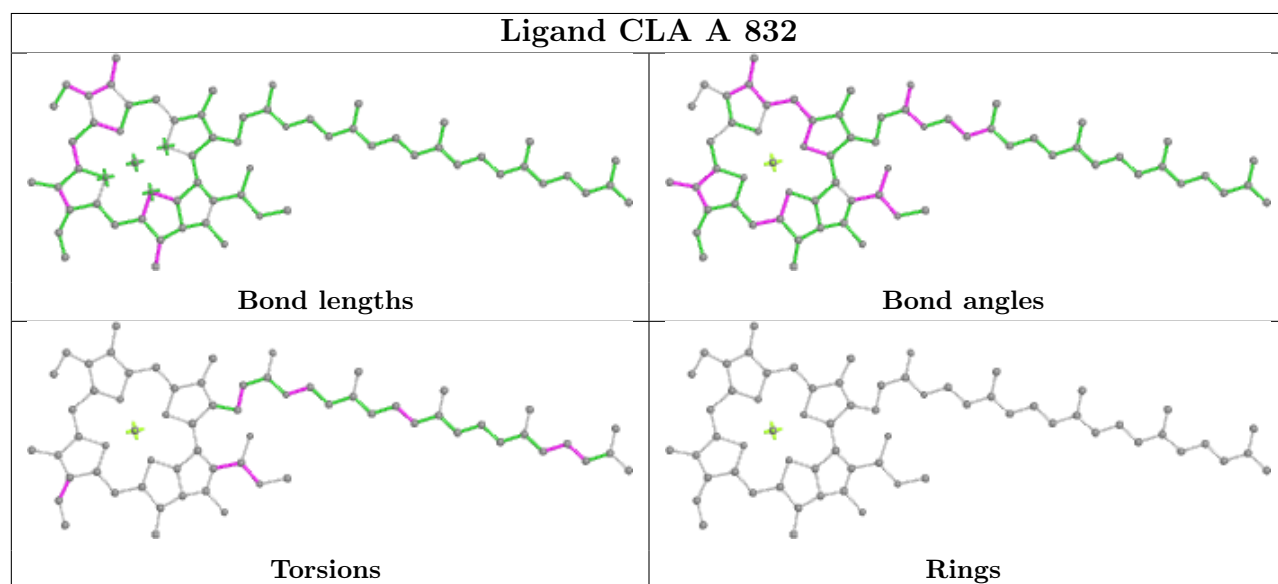
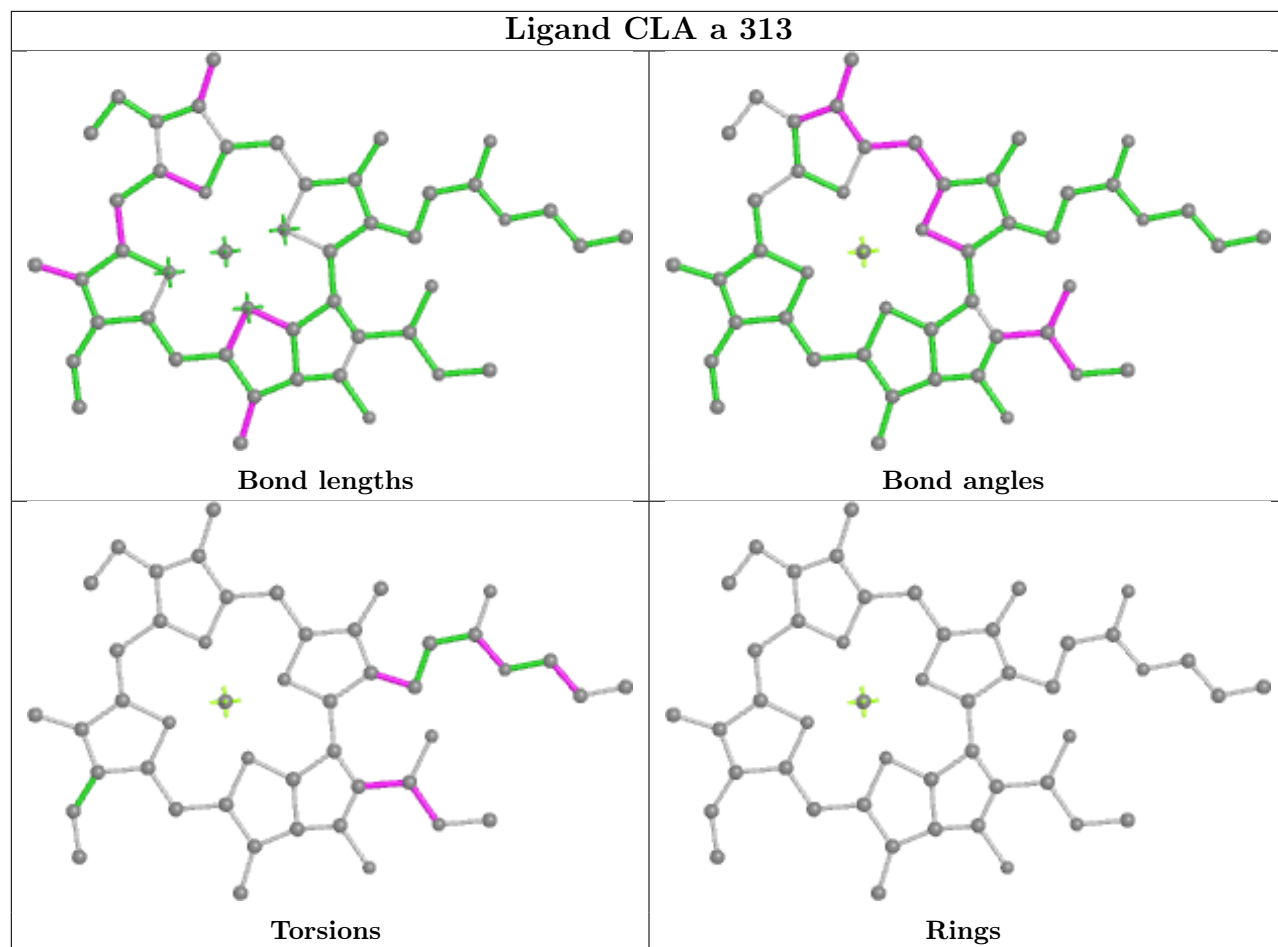


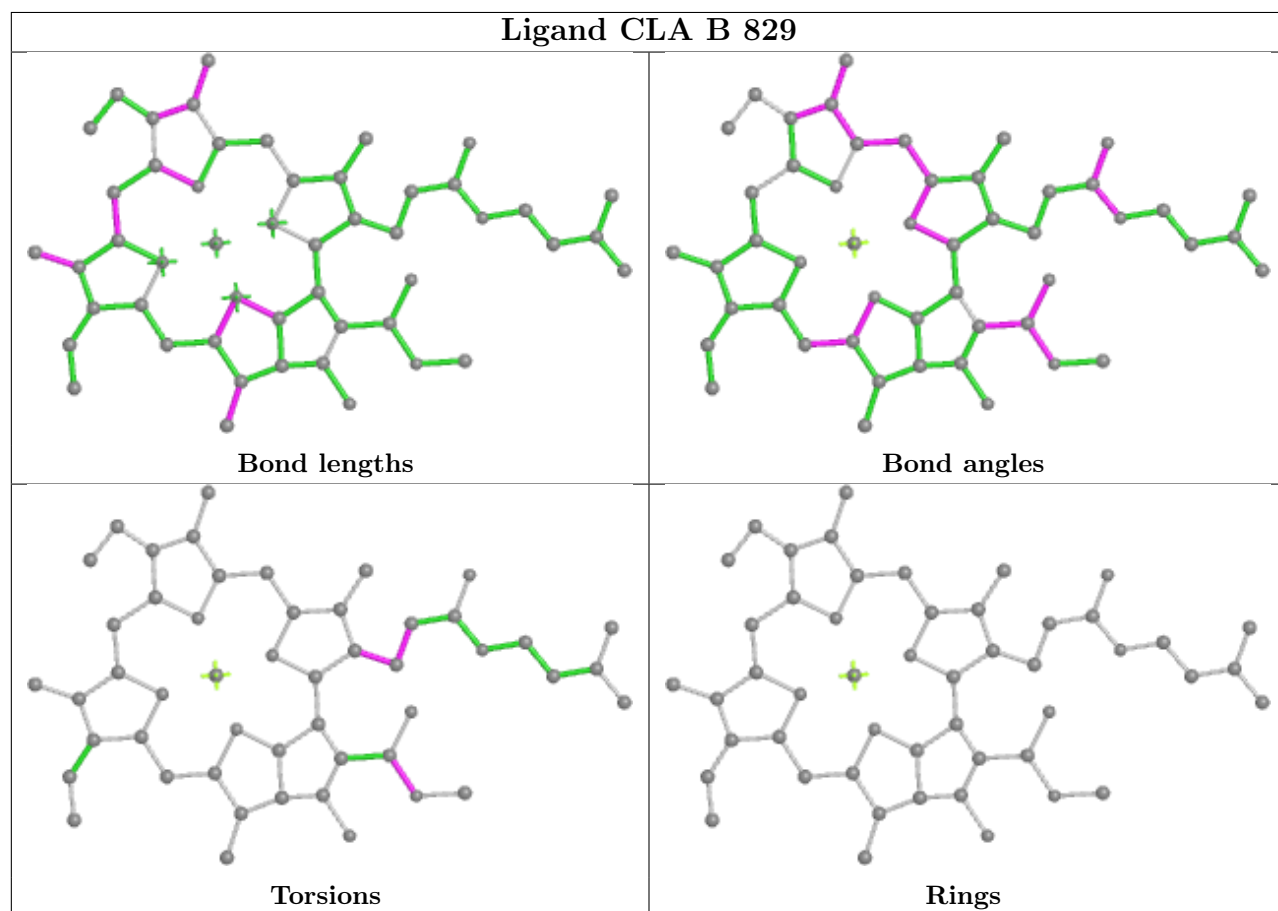
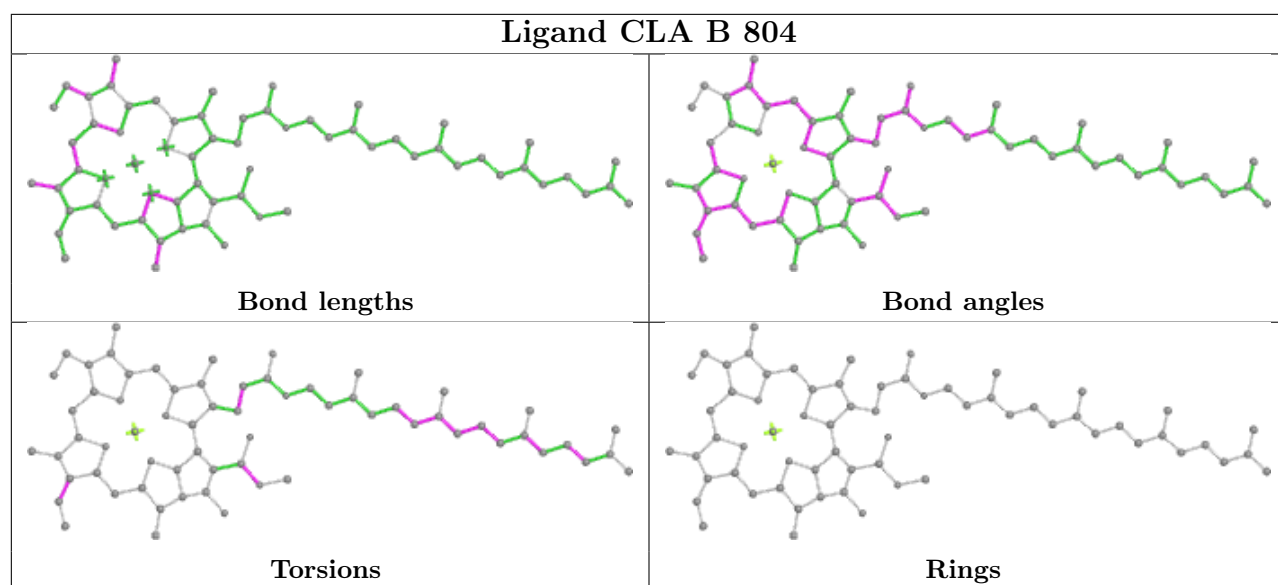


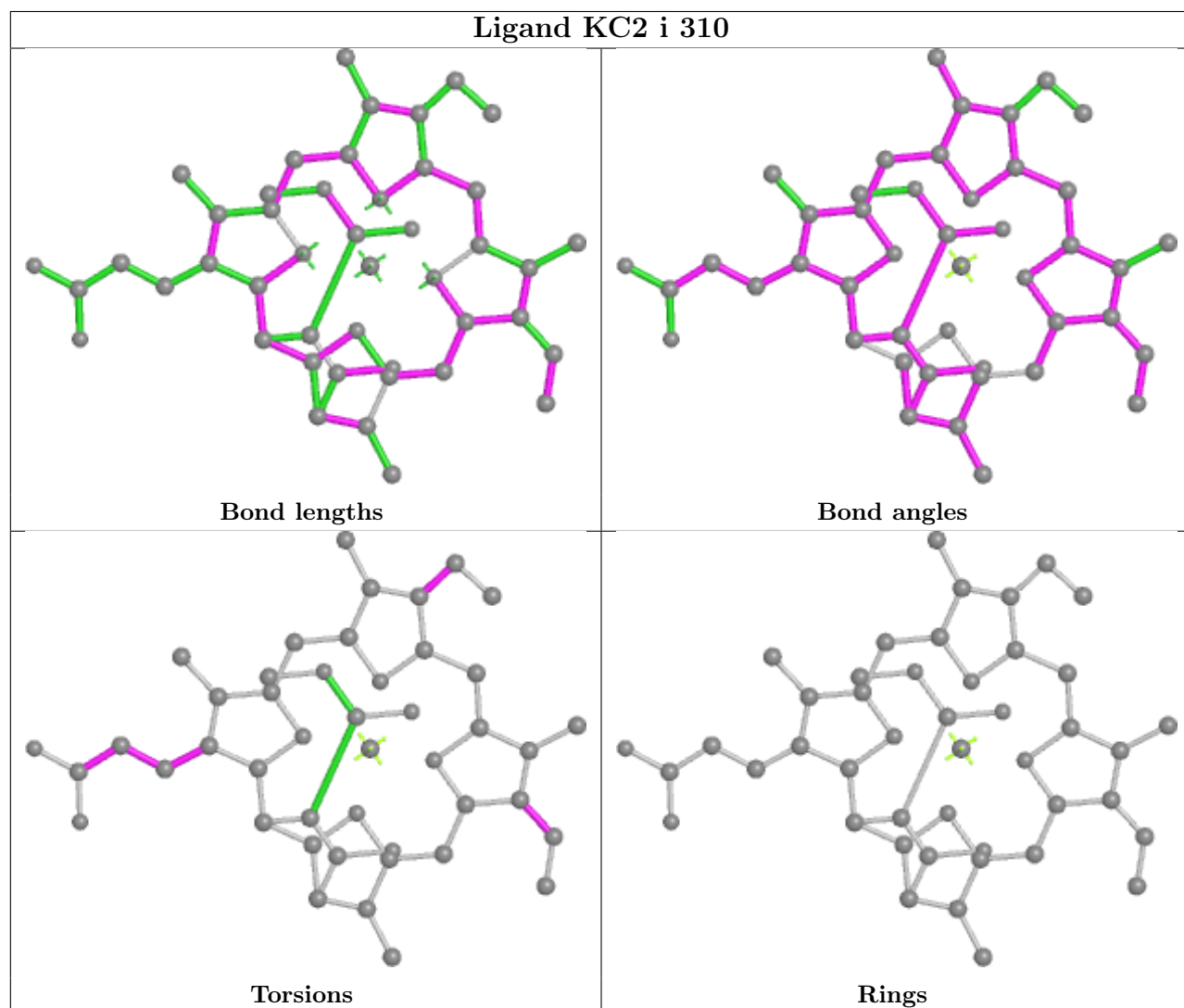
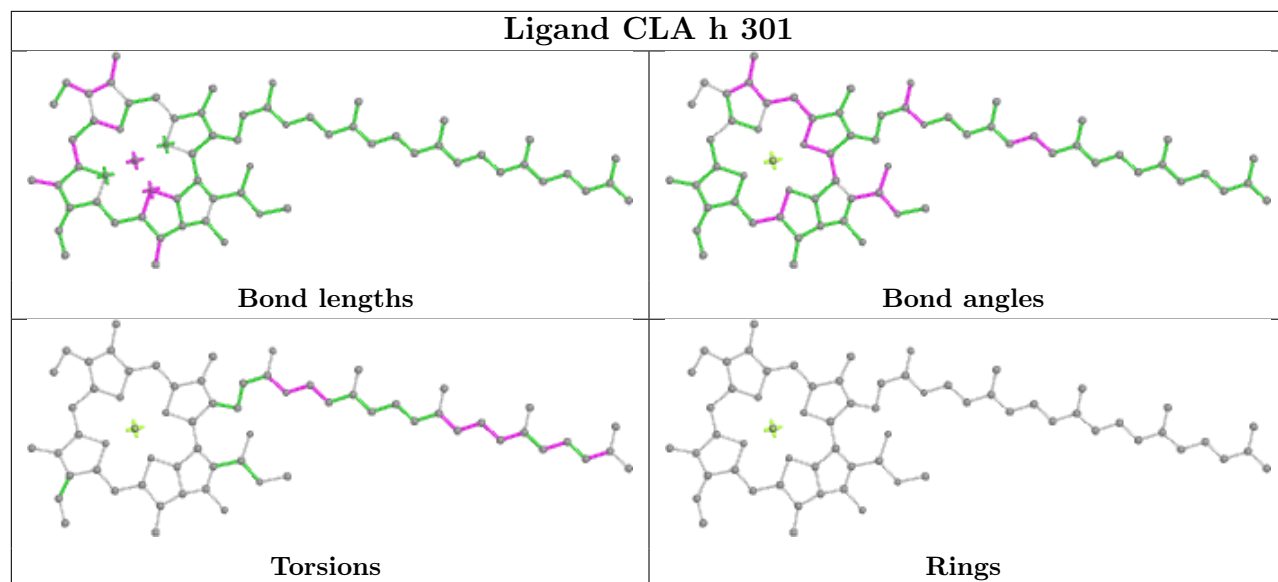


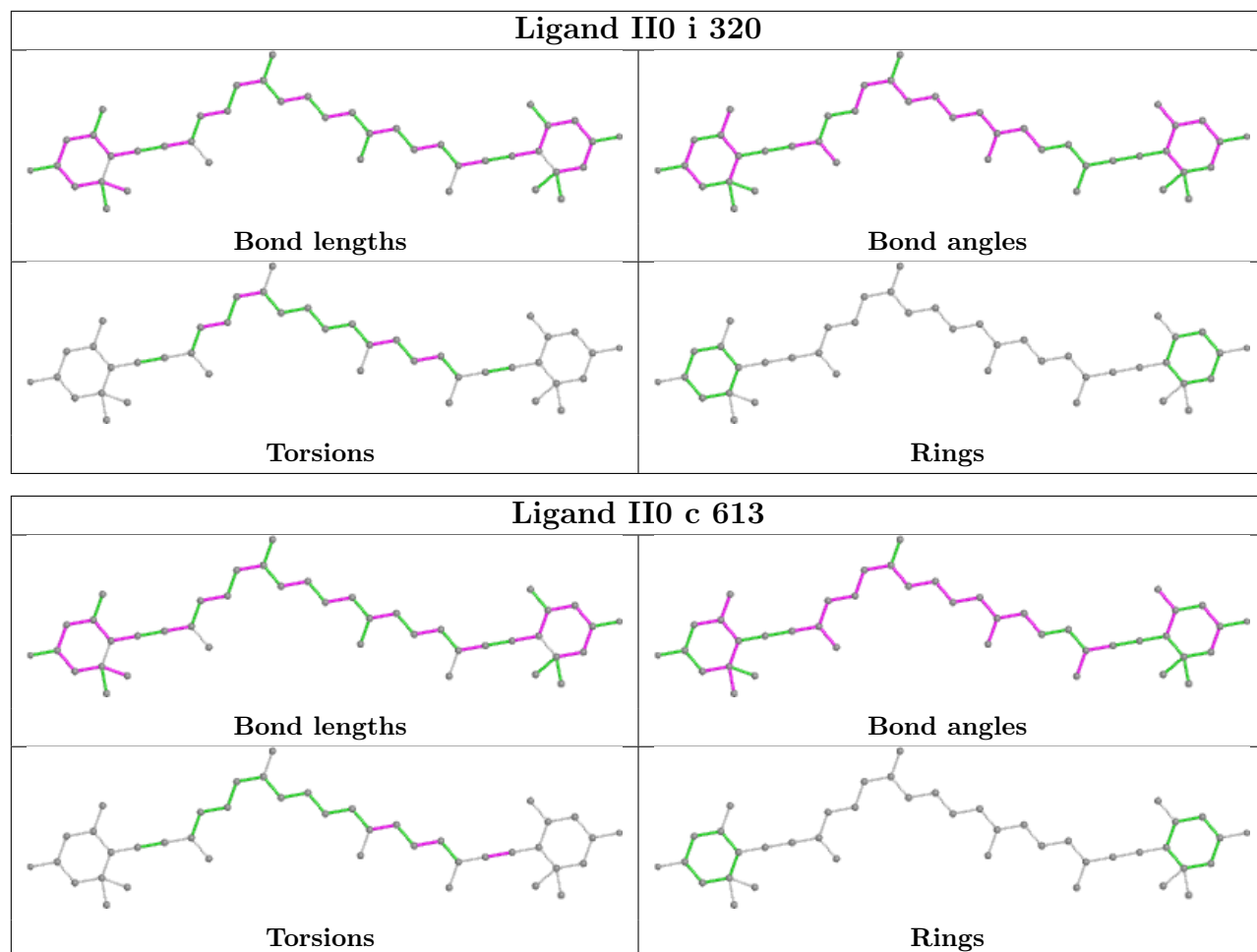


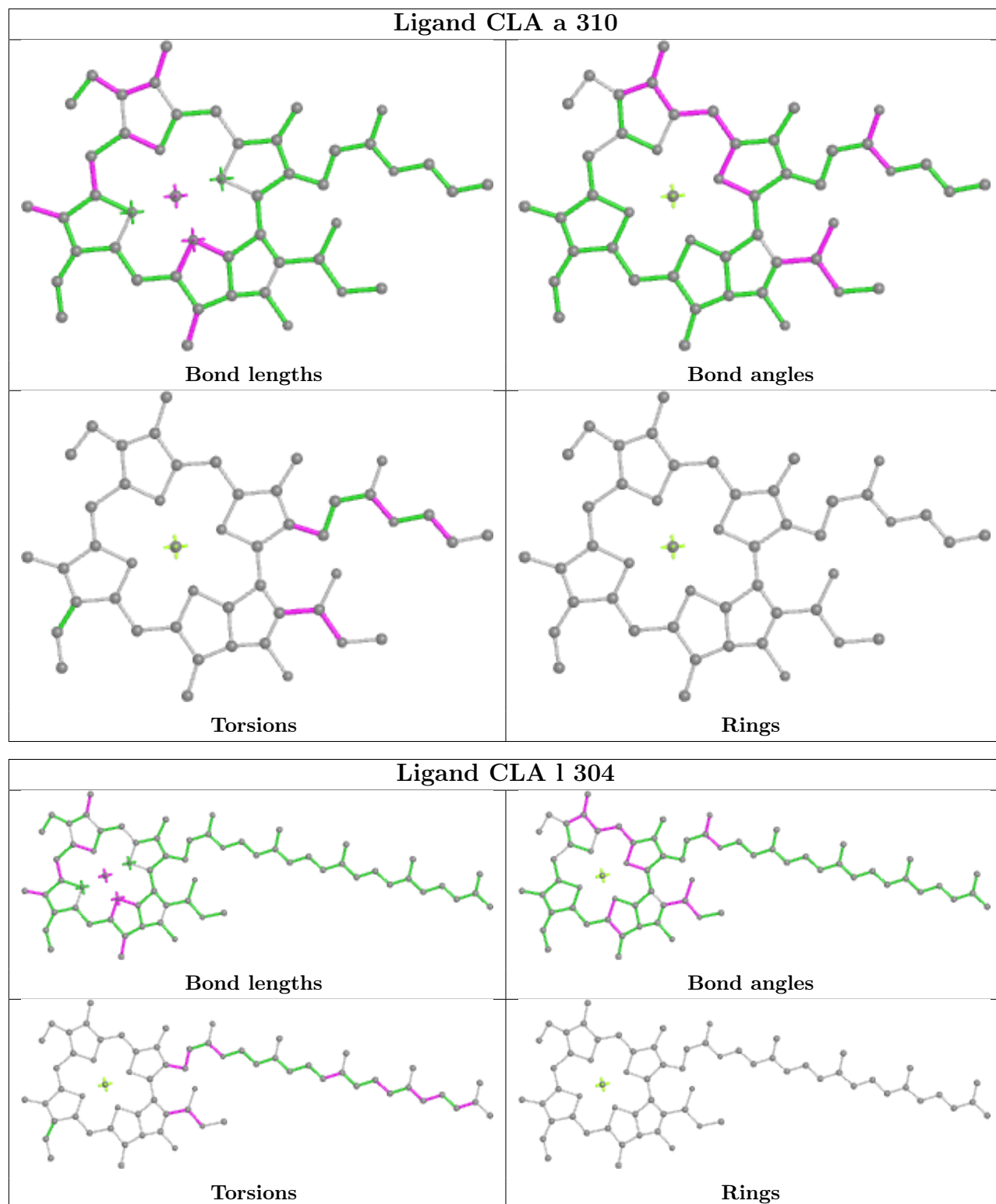


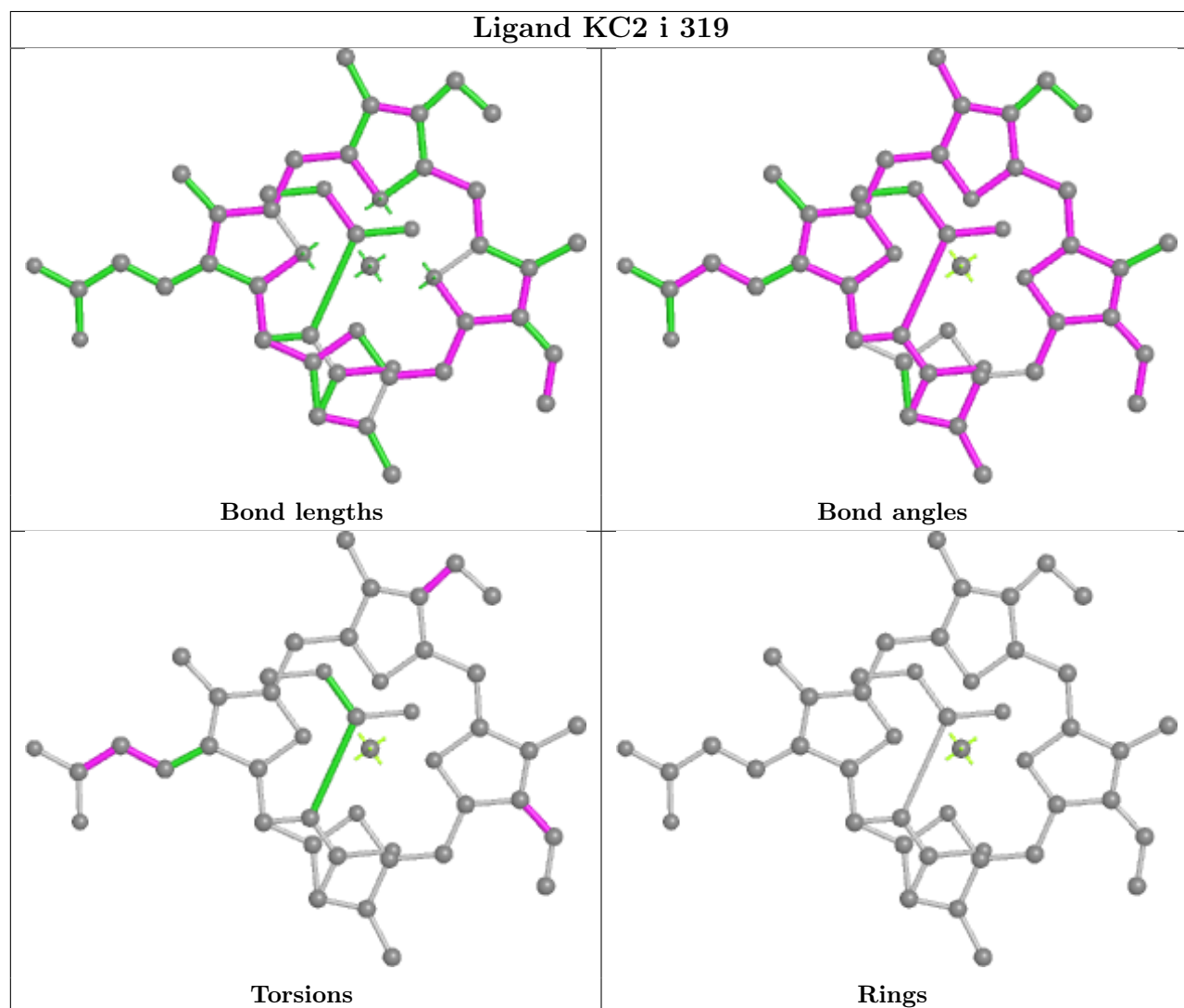
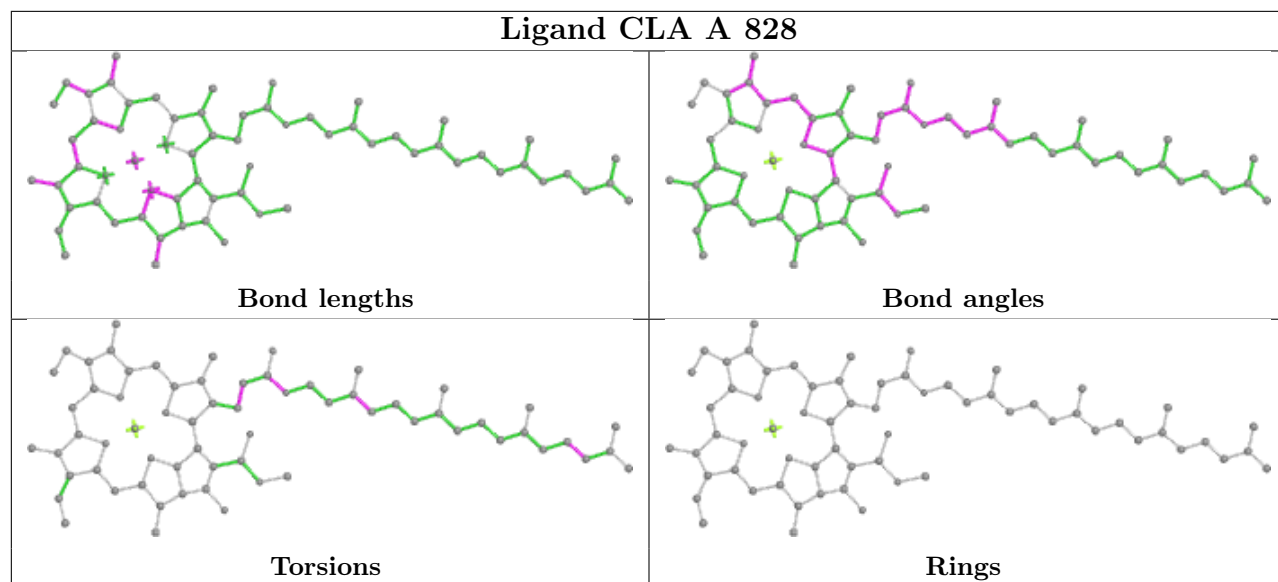


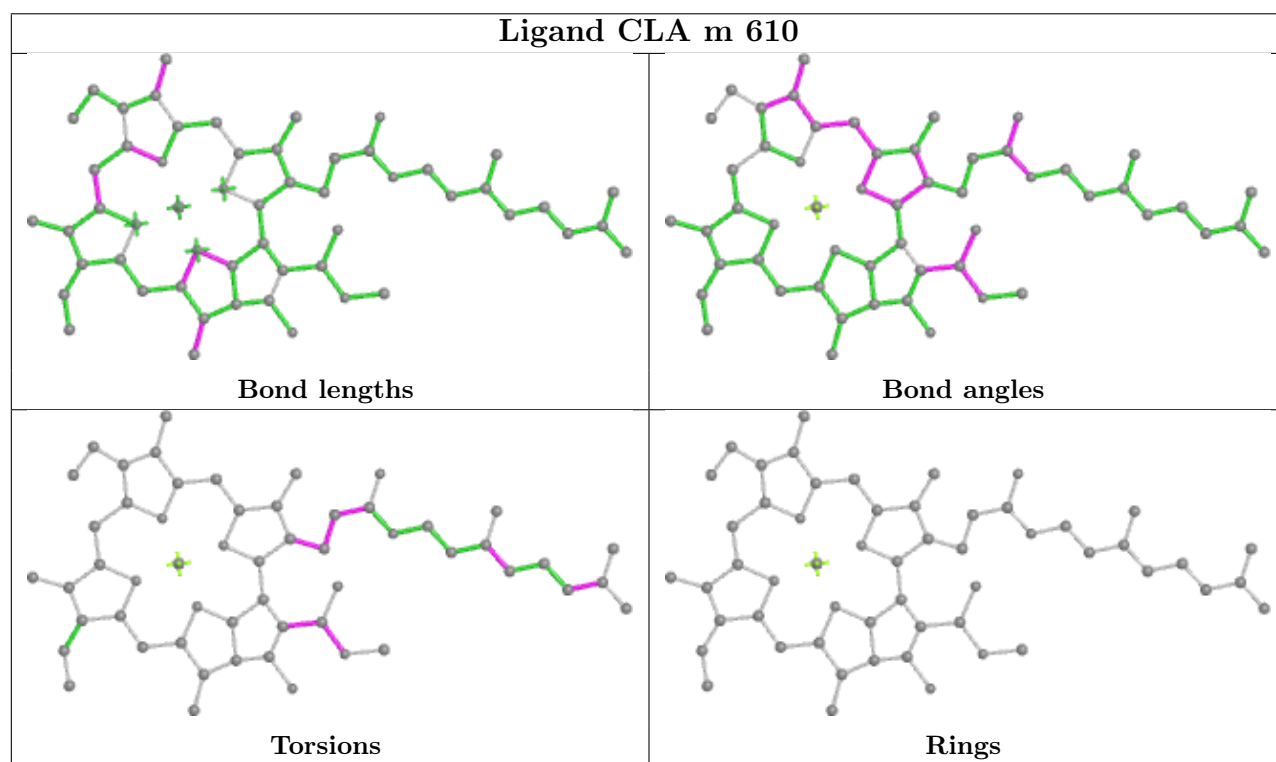
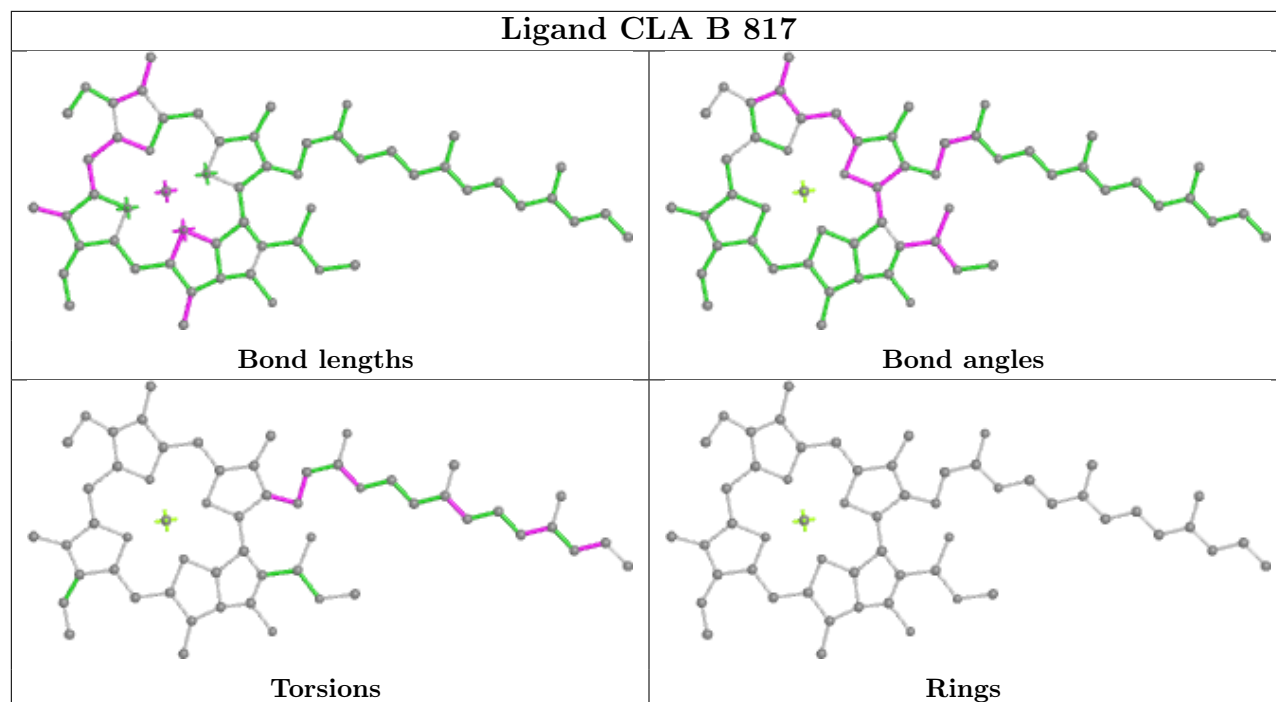


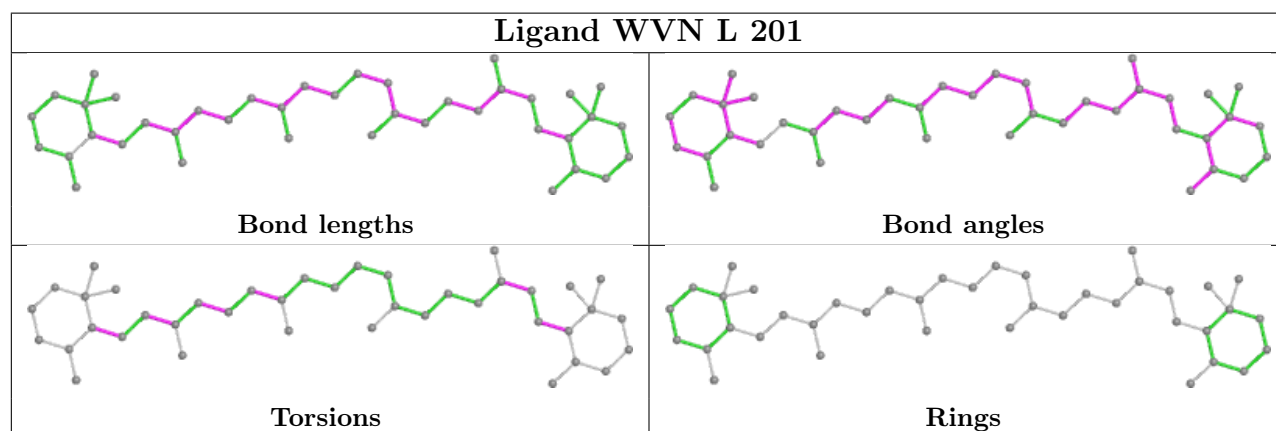
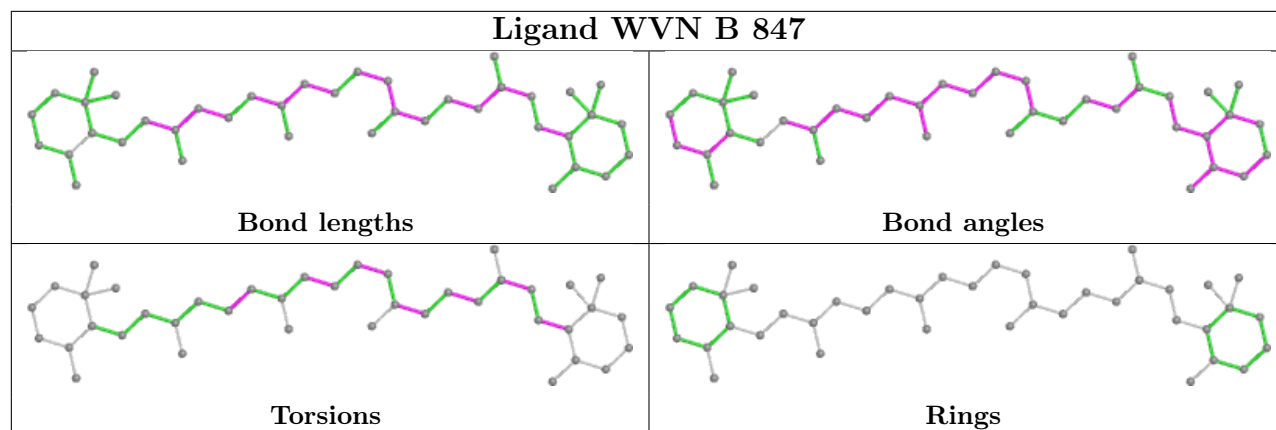


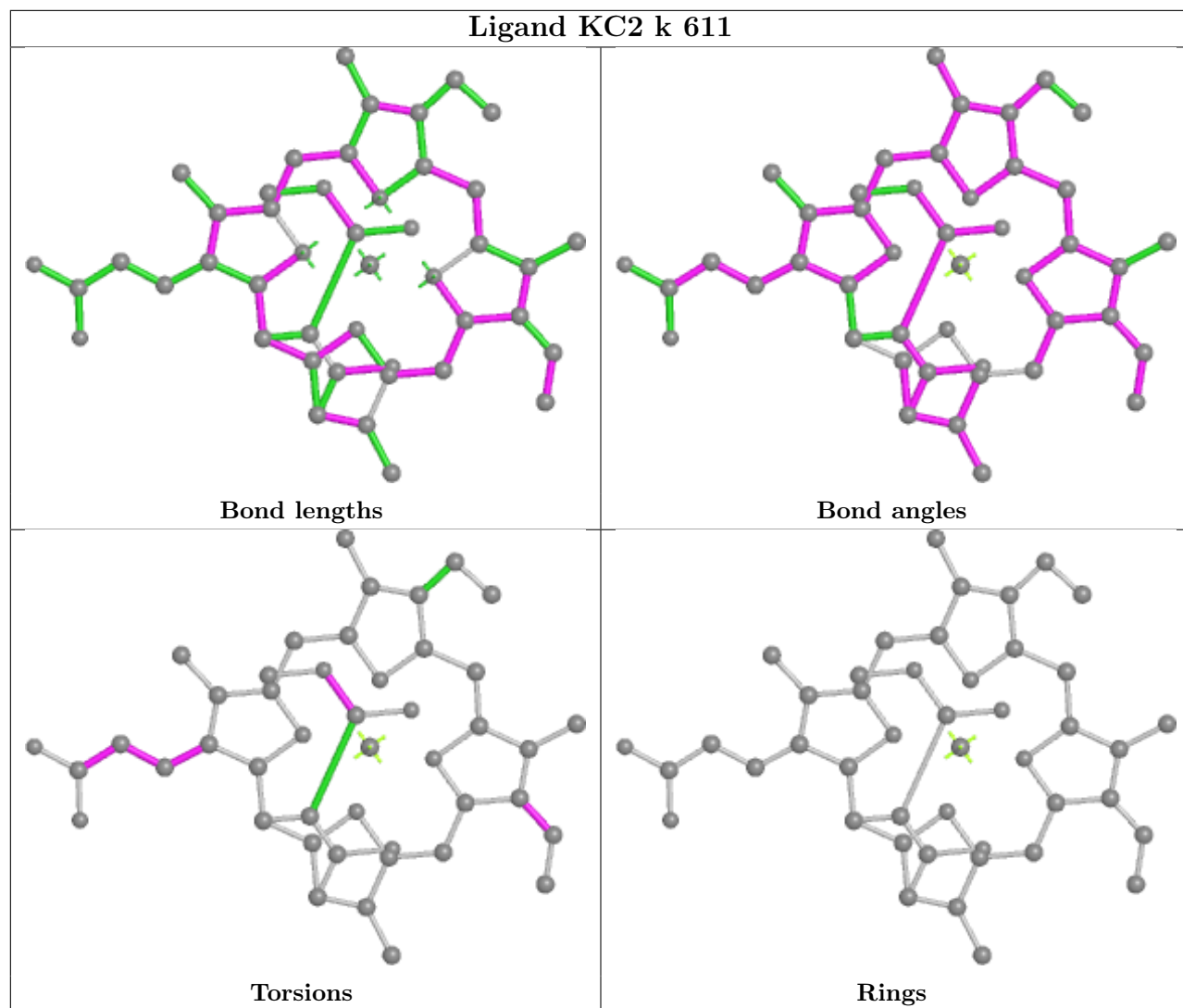


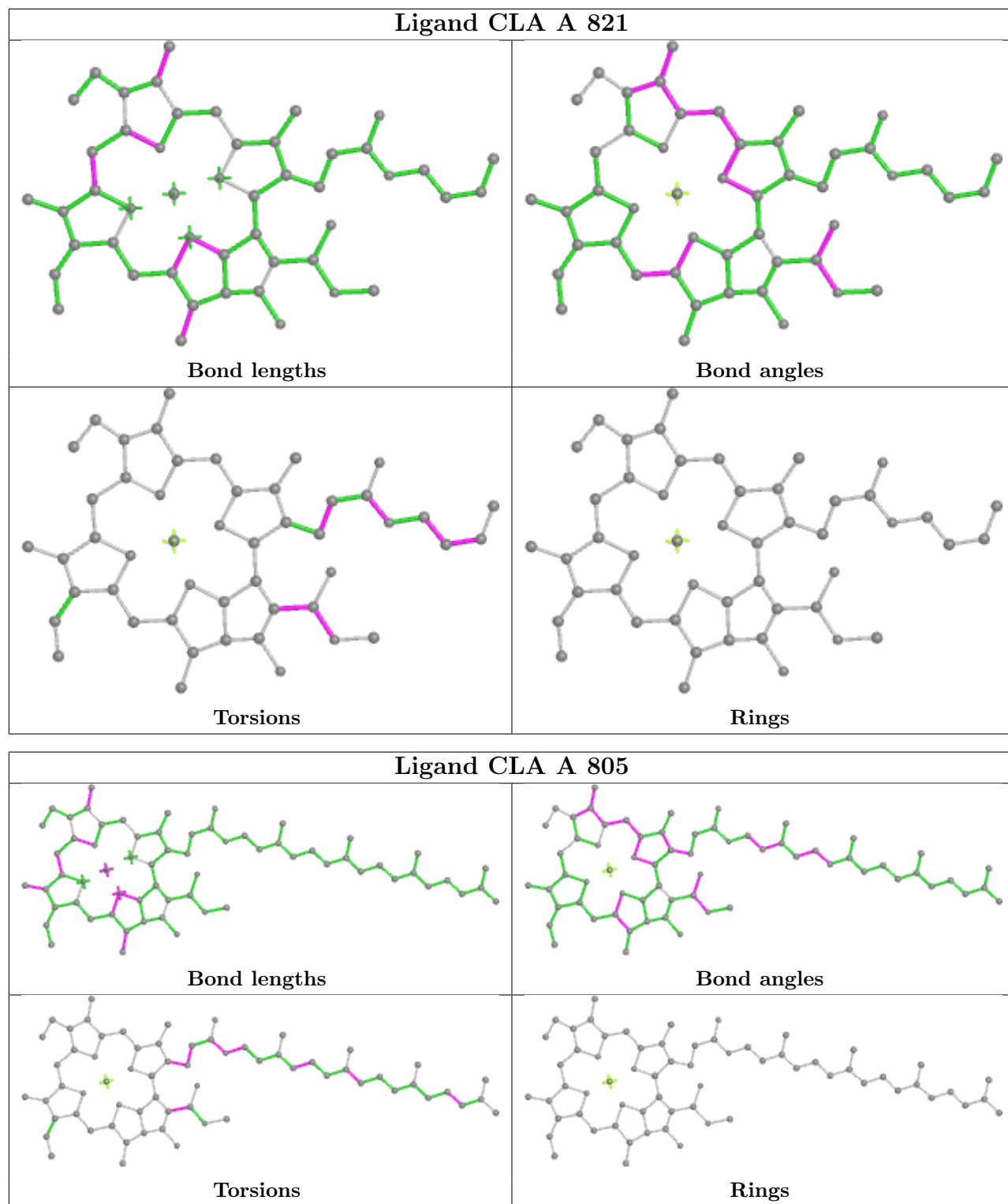


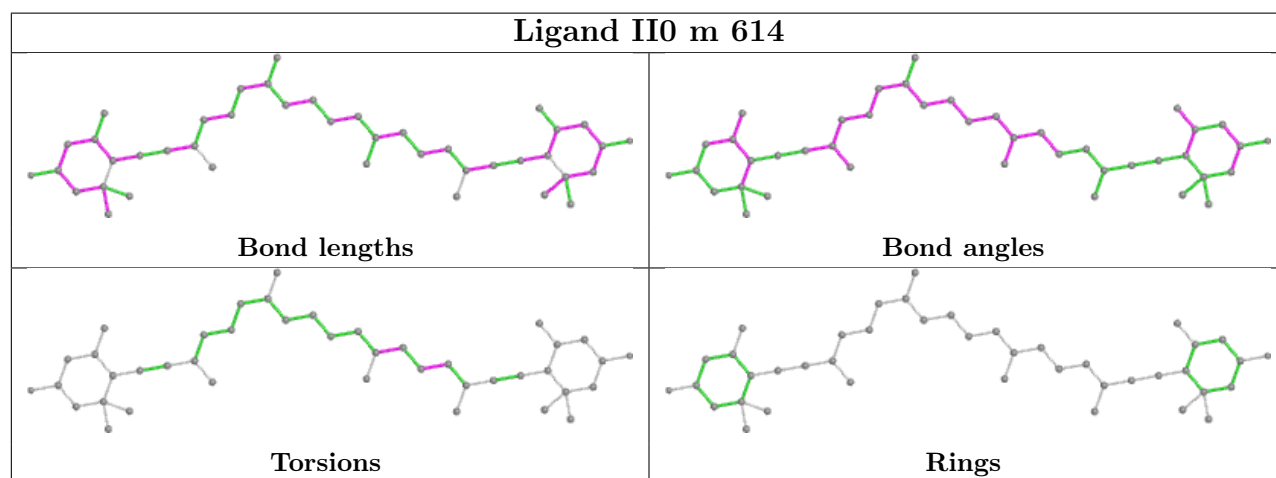
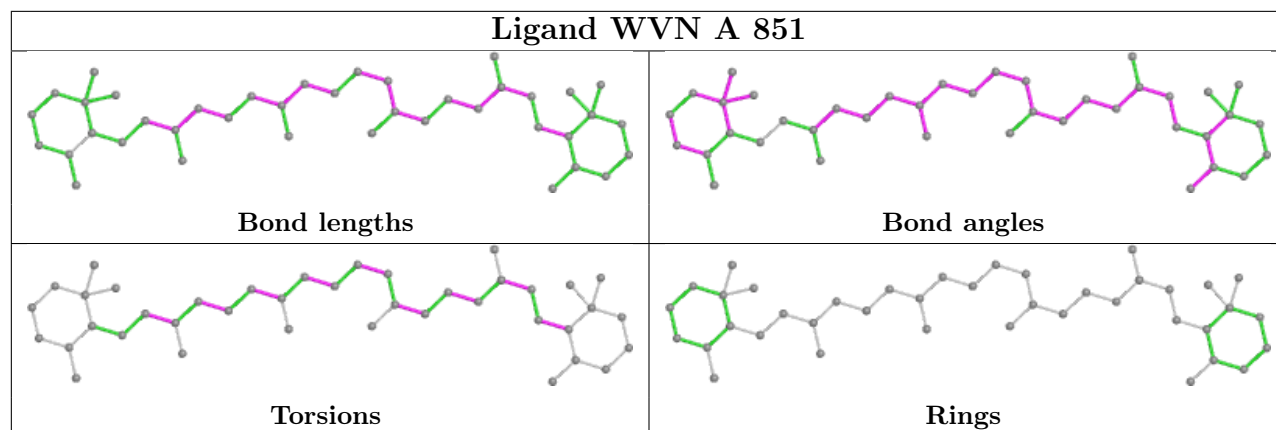


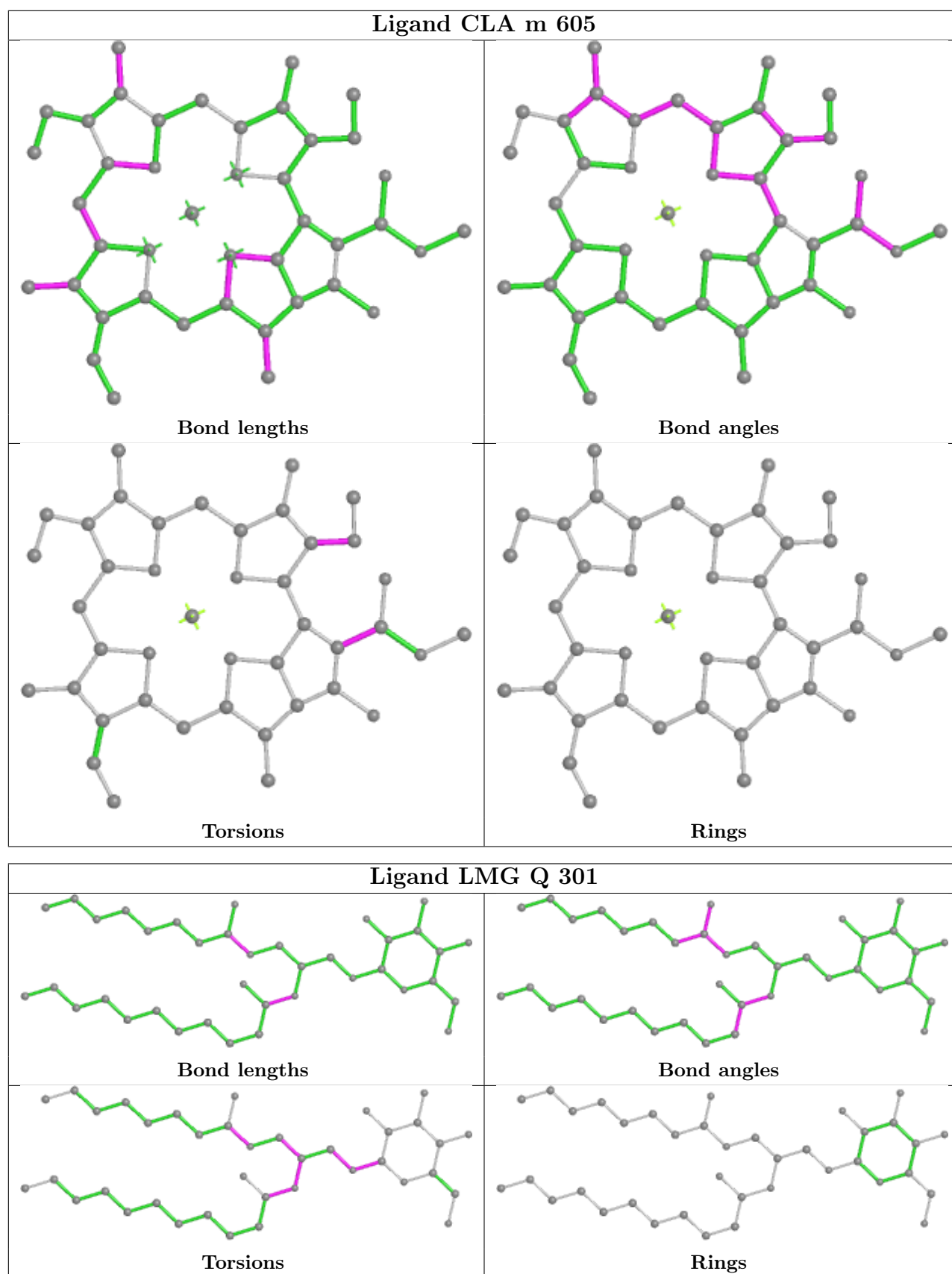


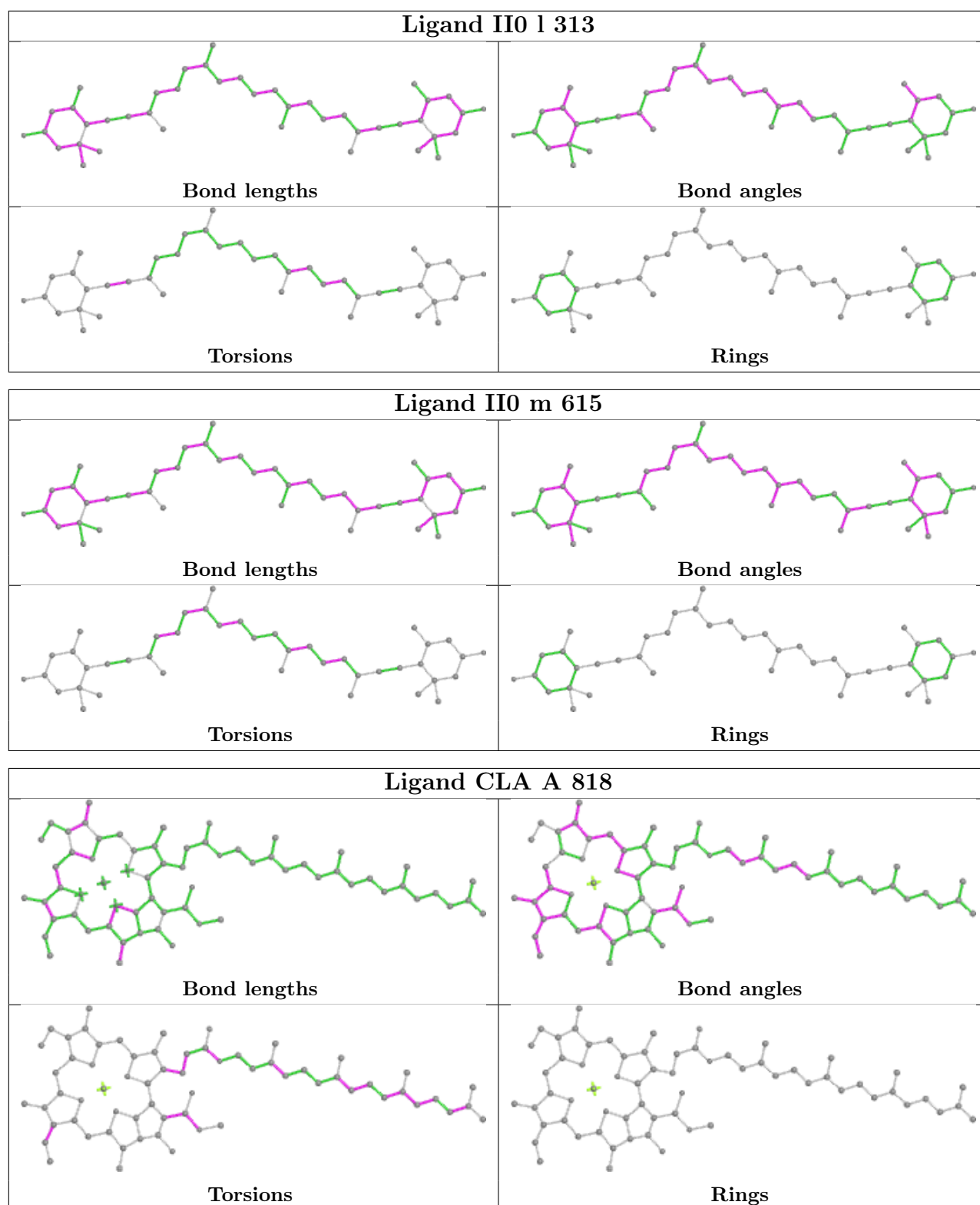


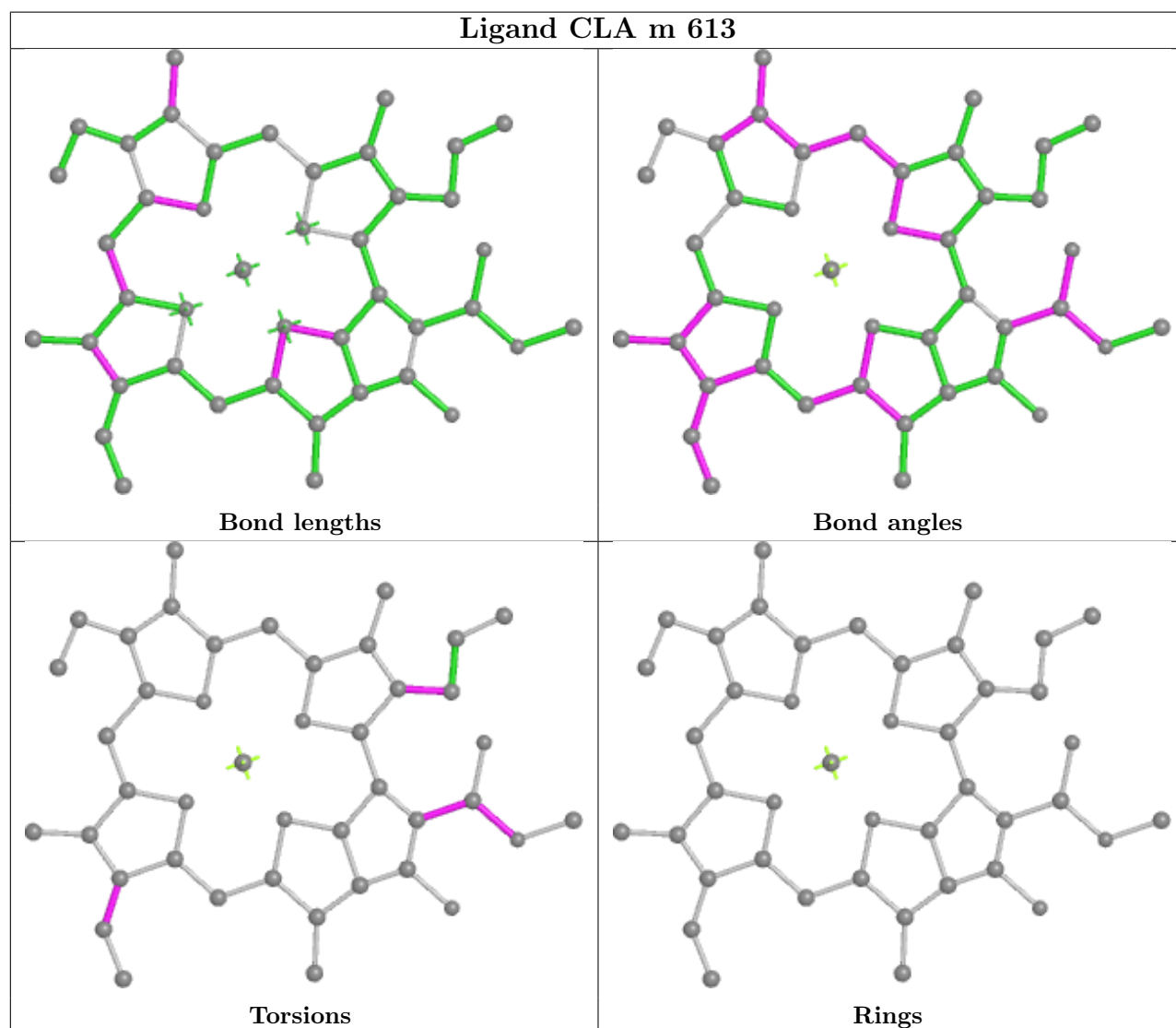
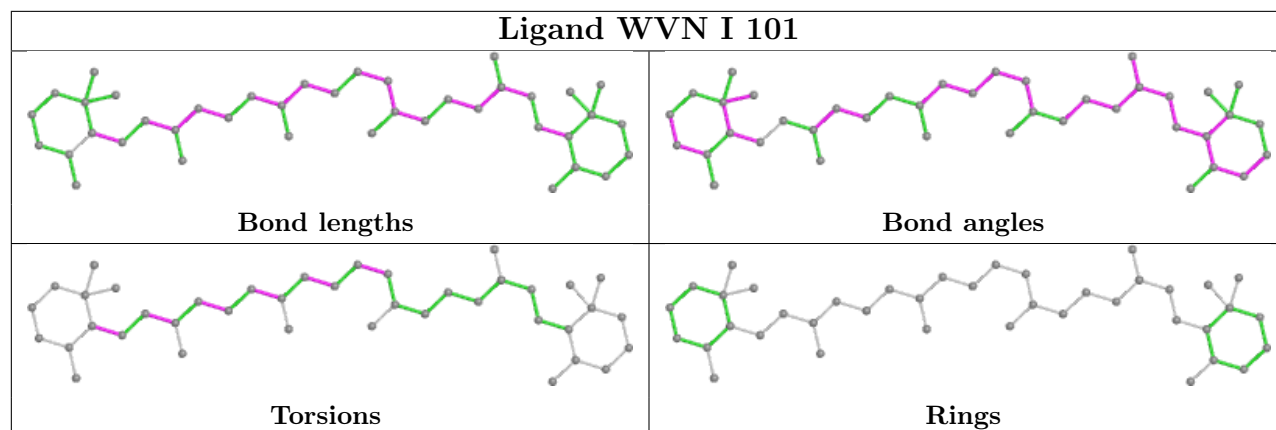


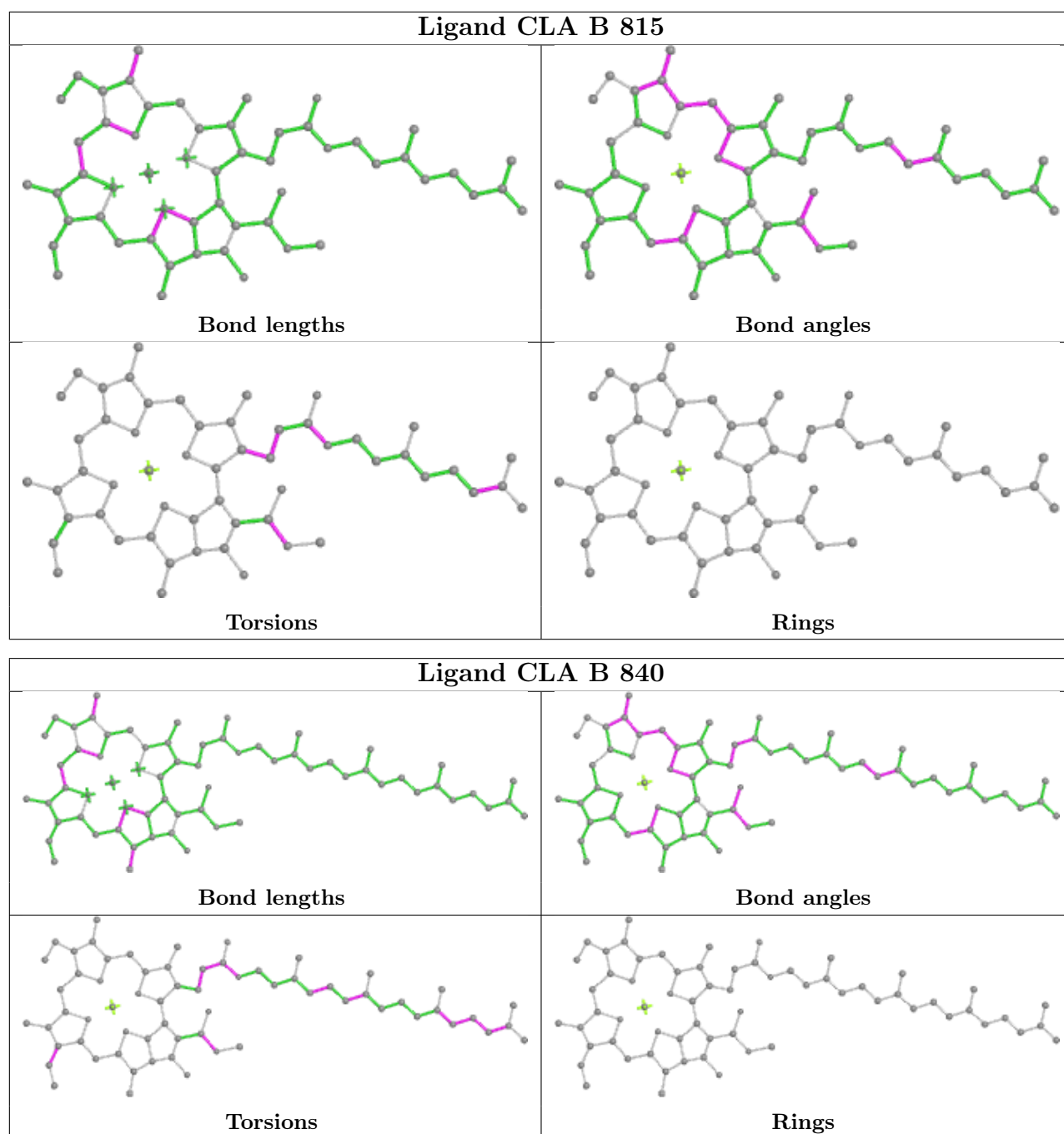


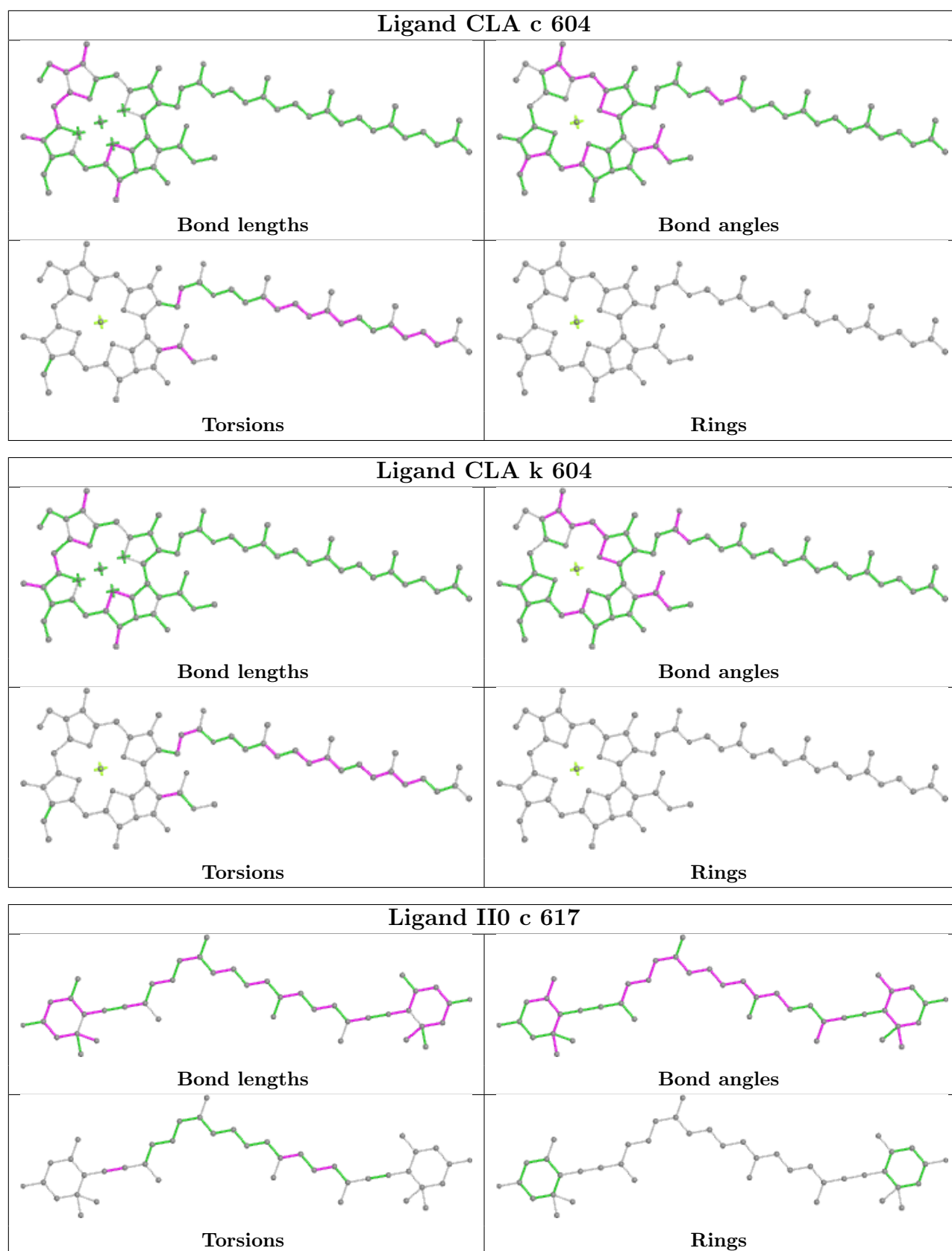


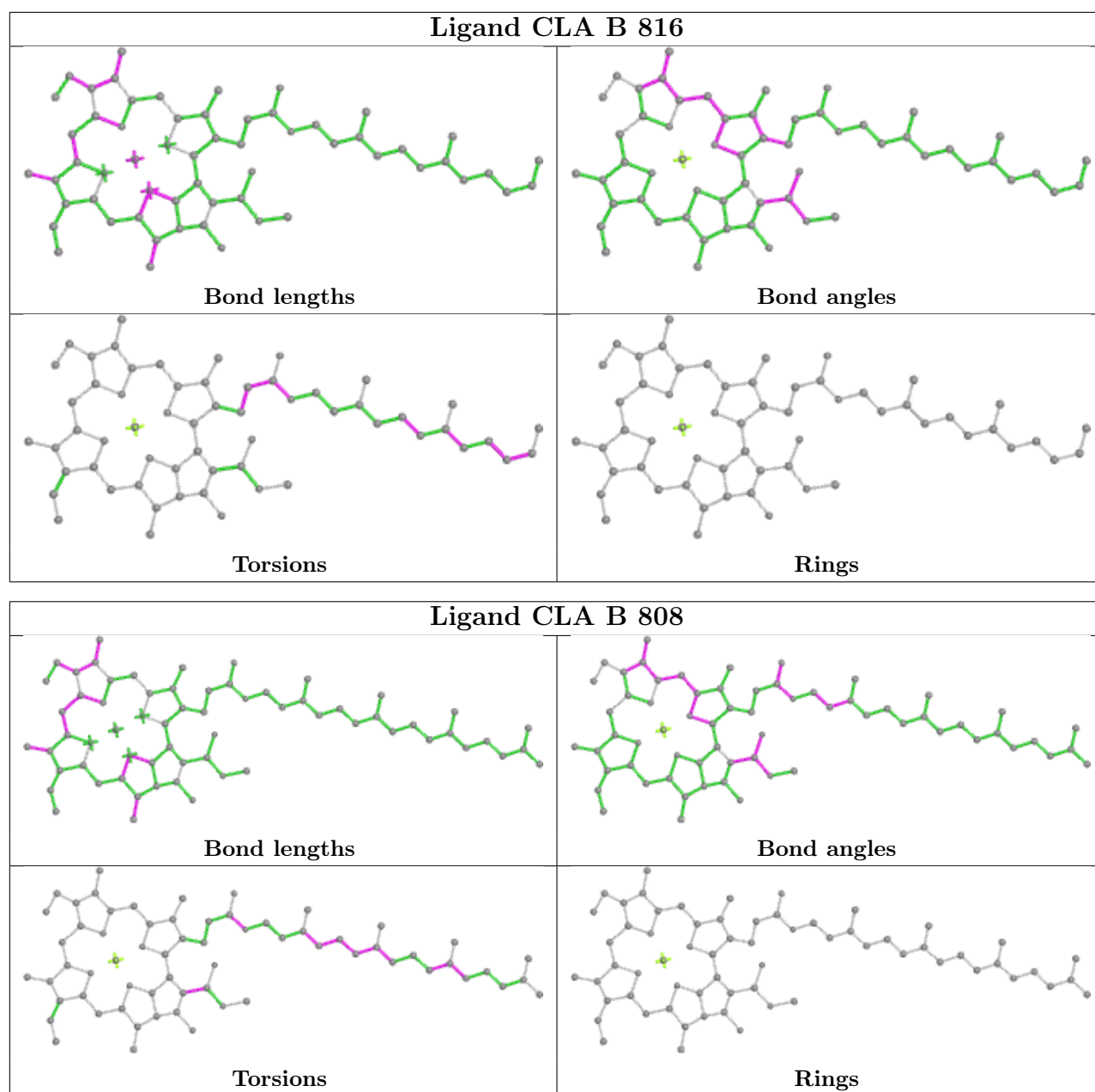


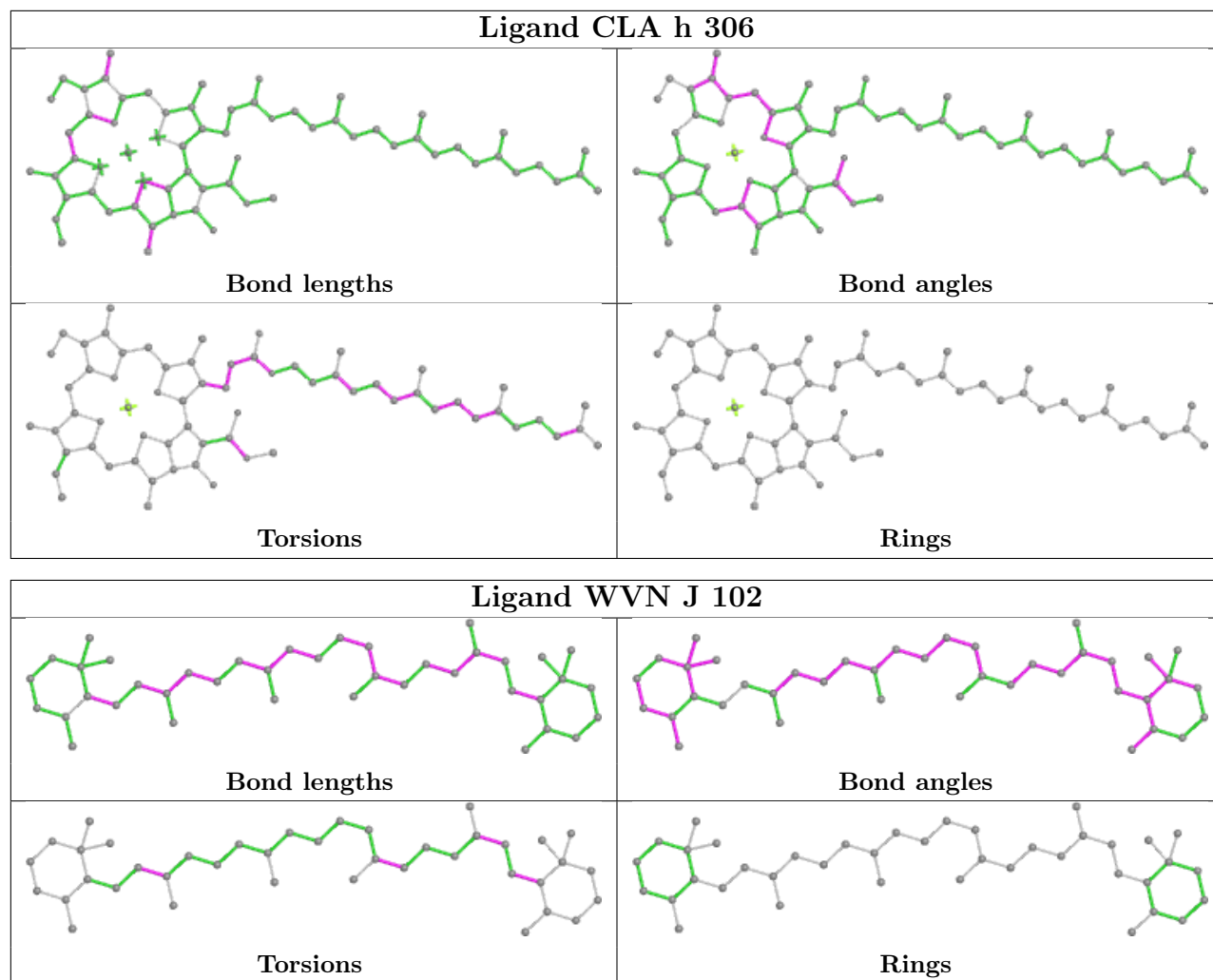


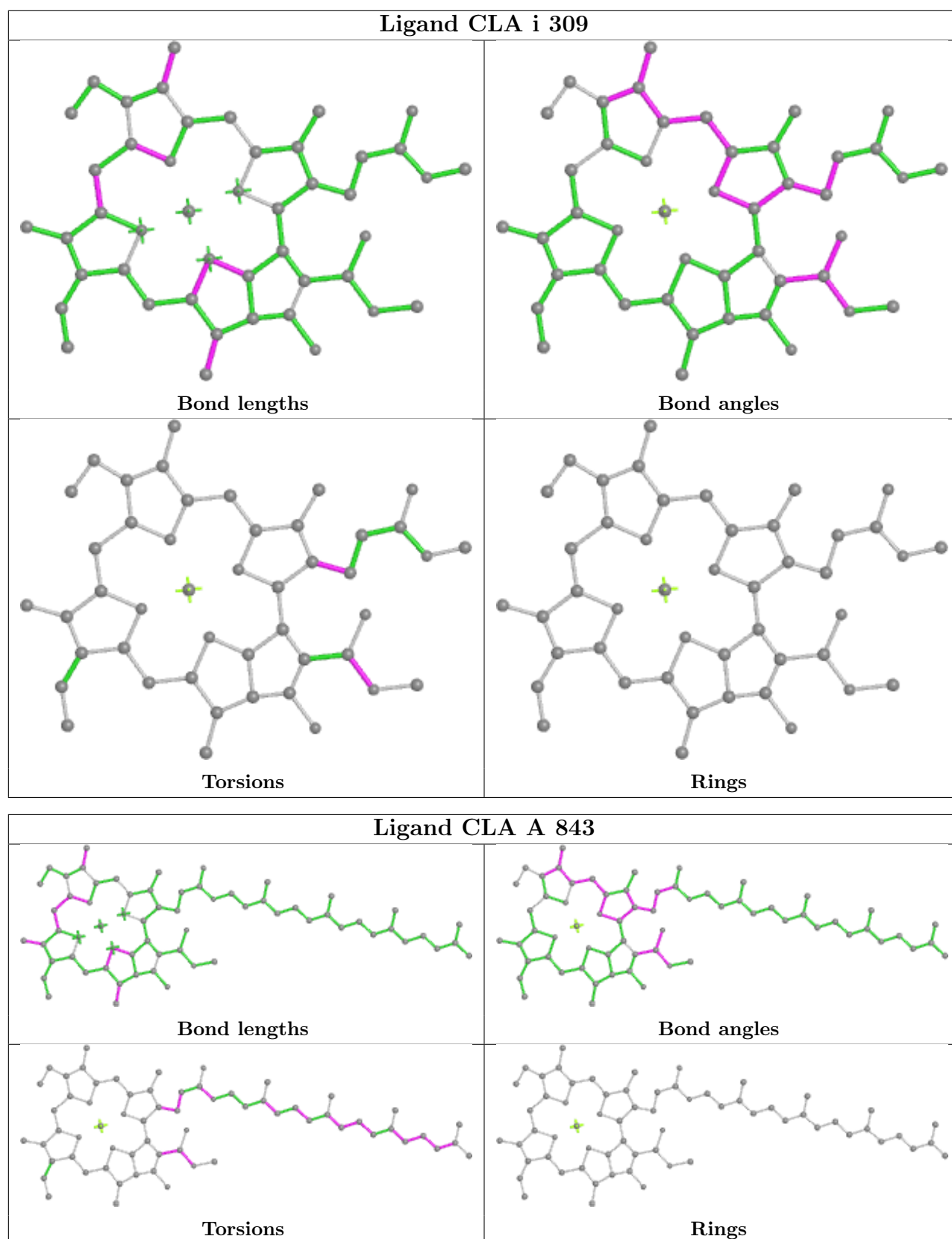


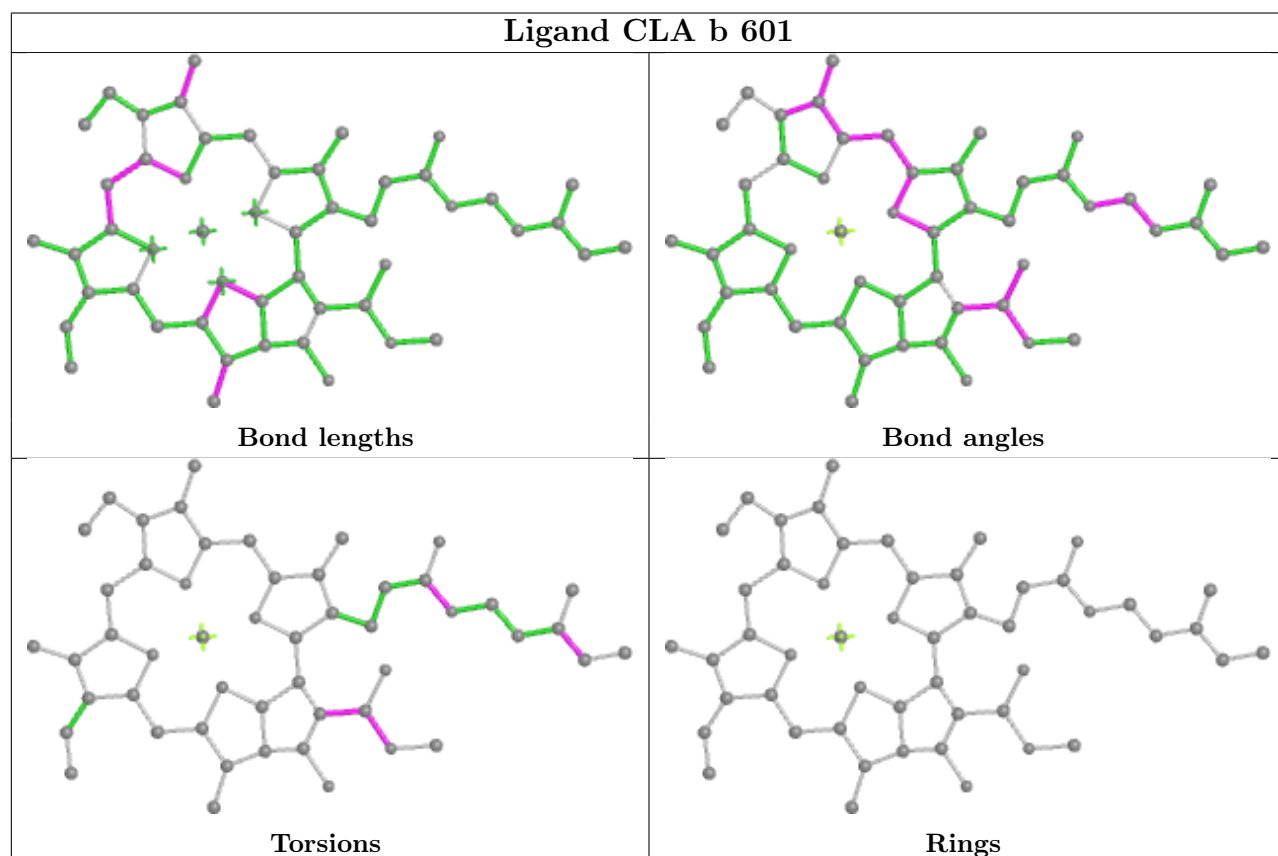
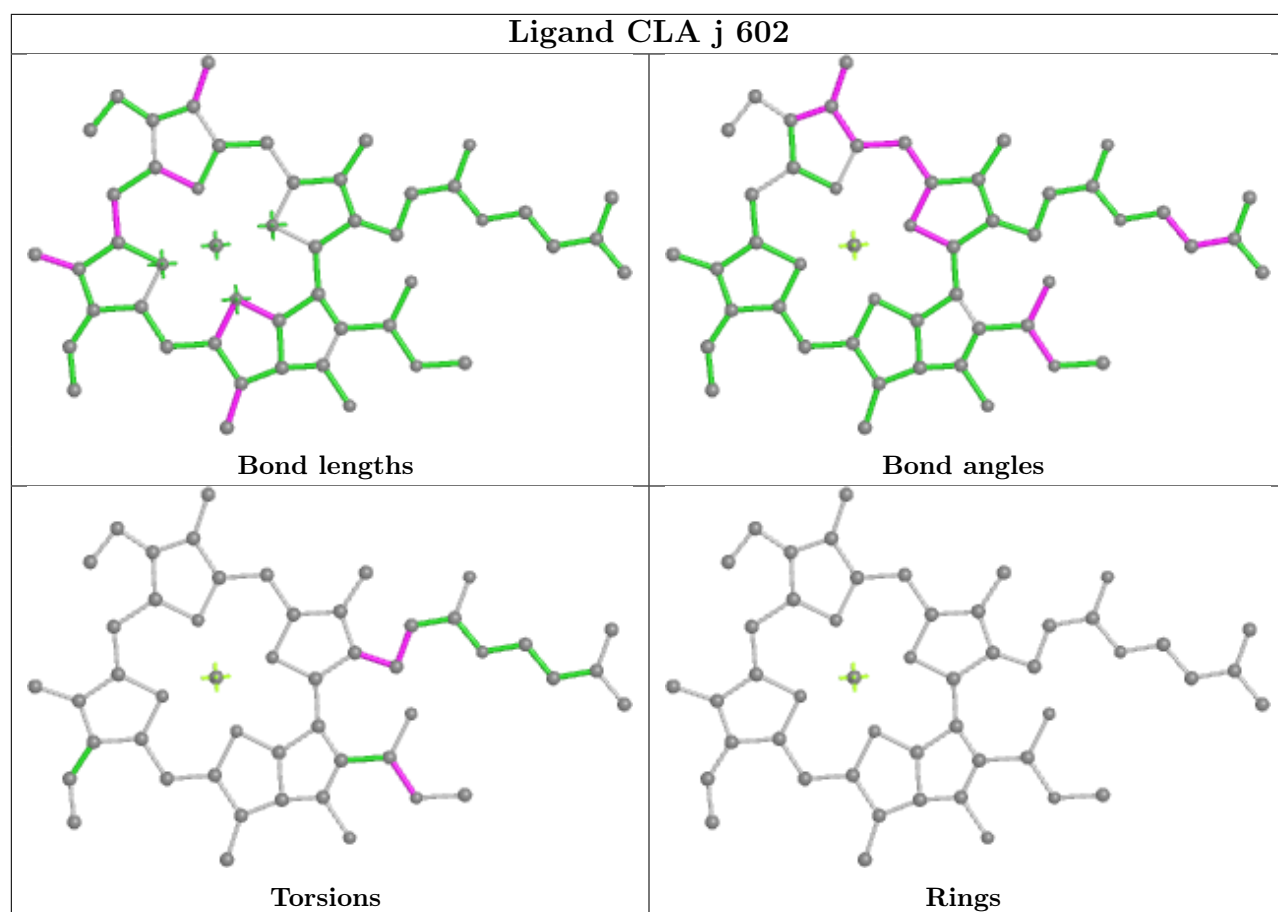


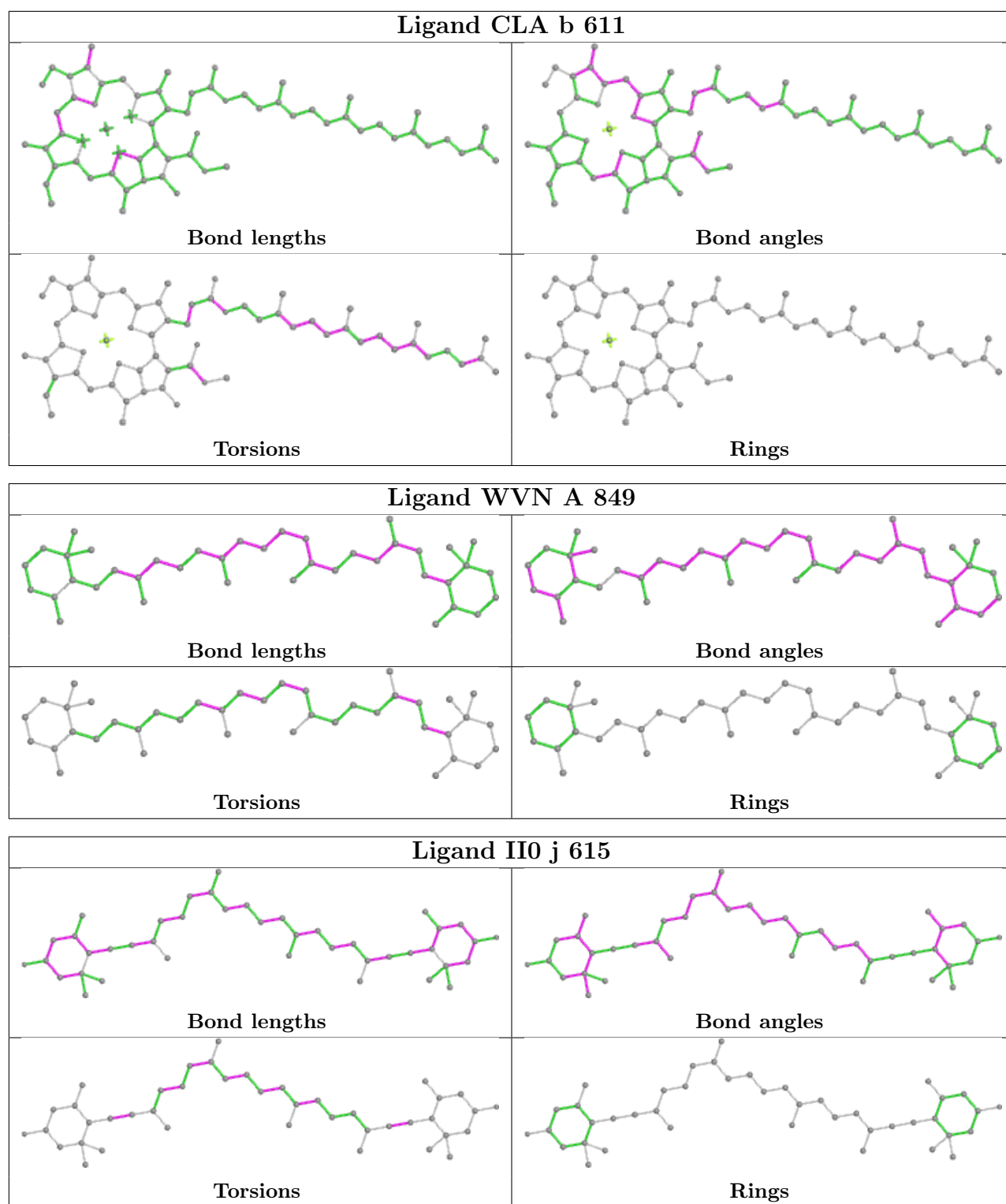


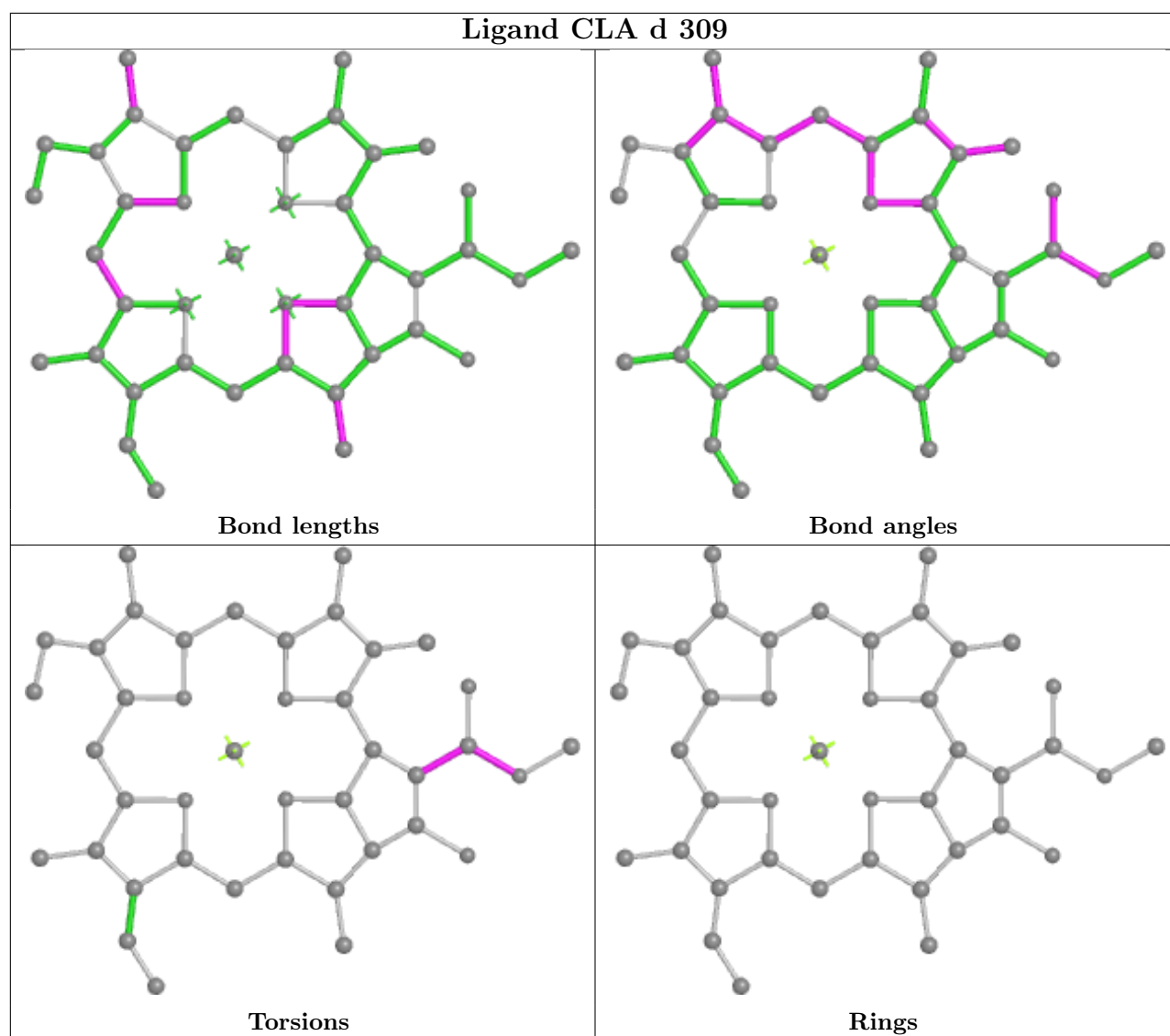












5.7 Other polymers [\(i\)](#)

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-37654. These allow visual inspection of the internal detail of the map and identification of artifacts.

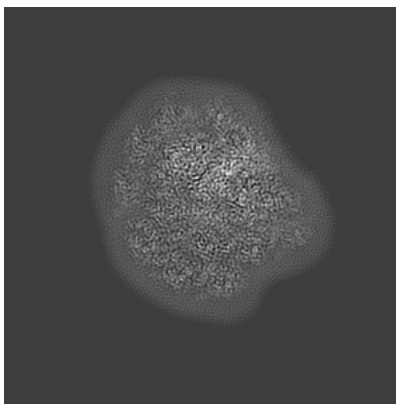
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

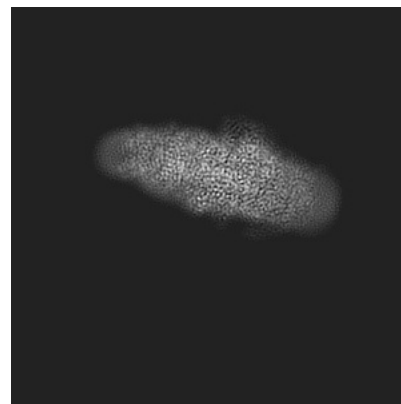
6.1.1 Primary map



X

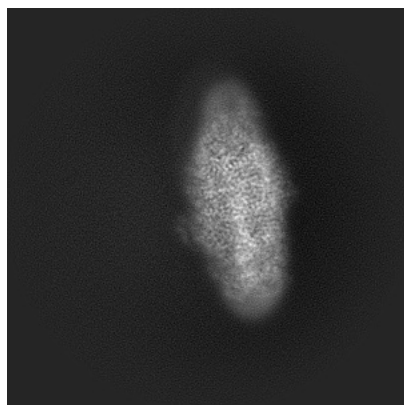


Y

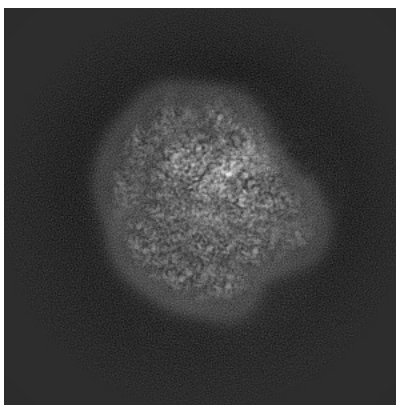


Z

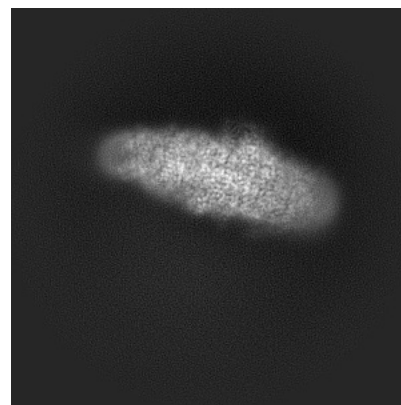
6.1.2 Raw map



X



Y

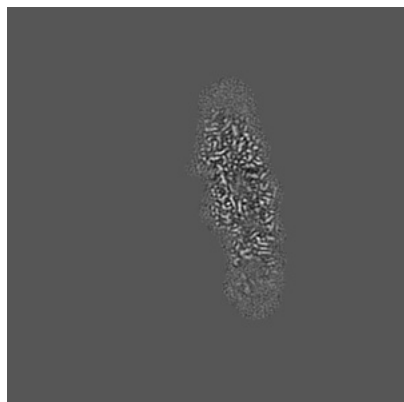


Z

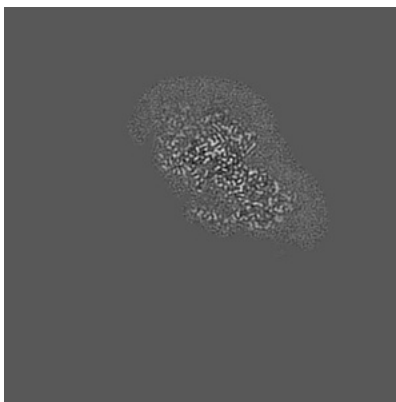
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

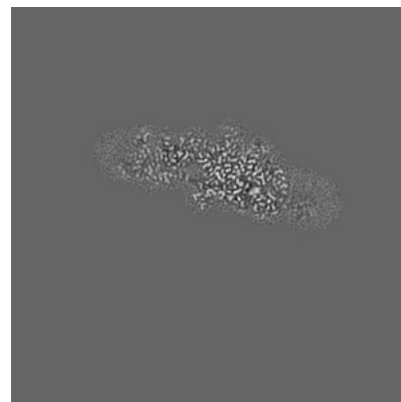
6.2.1 Primary map



X Index: 180

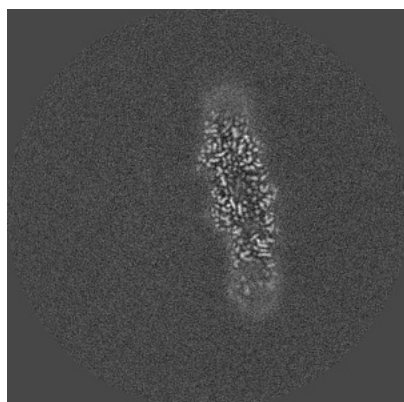


Y Index: 180

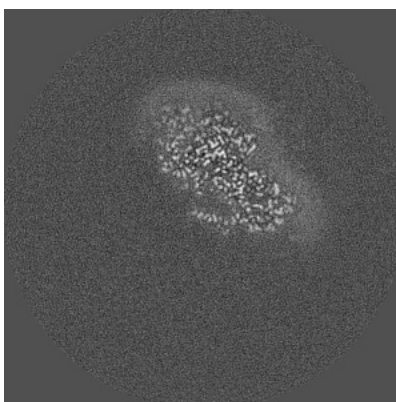


Z Index: 180

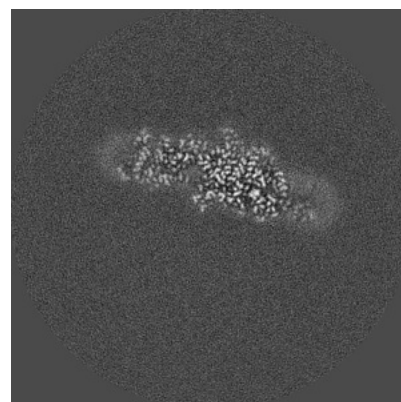
6.2.2 Raw map



X Index: 180



Y Index: 180

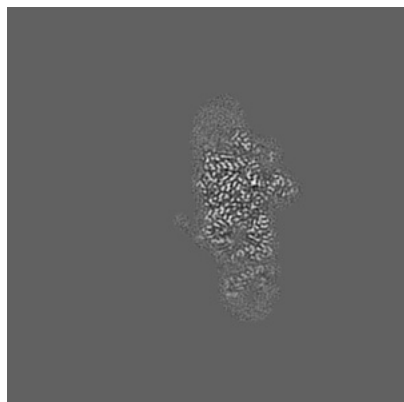


Z Index: 180

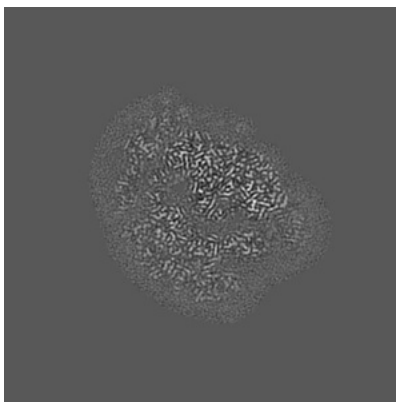
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

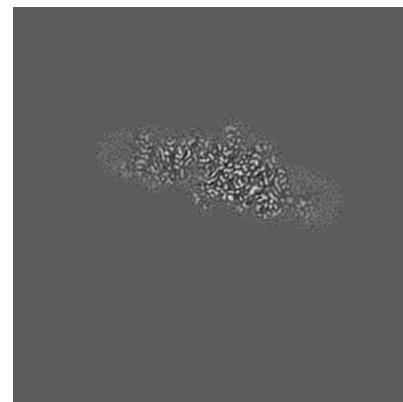
6.3.1 Primary map



X Index: 210



Y Index: 214

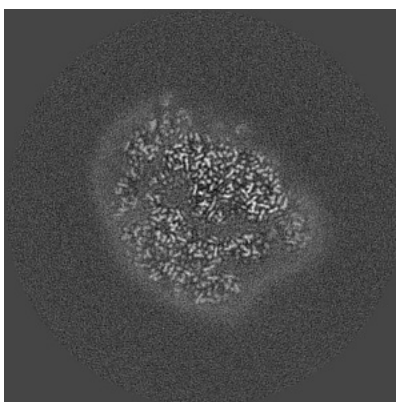


Z Index: 181

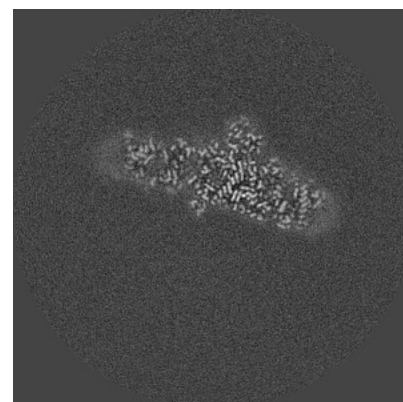
6.3.2 Raw map



X Index: 210



Y Index: 214

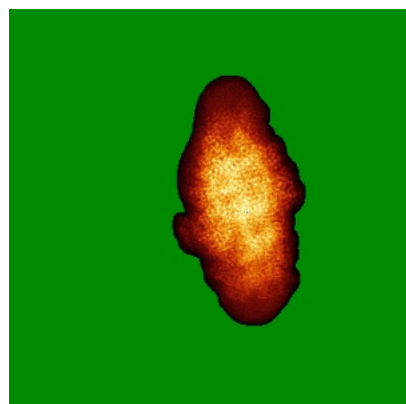


Z Index: 195

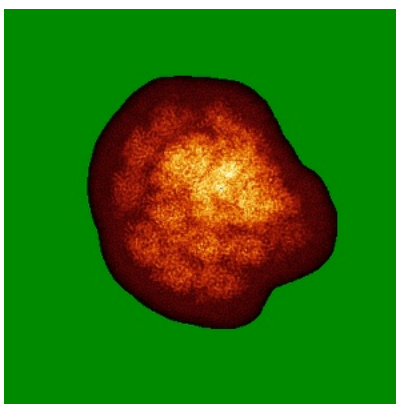
The images above show the largest variance slices of the map in three orthogonal directions.

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

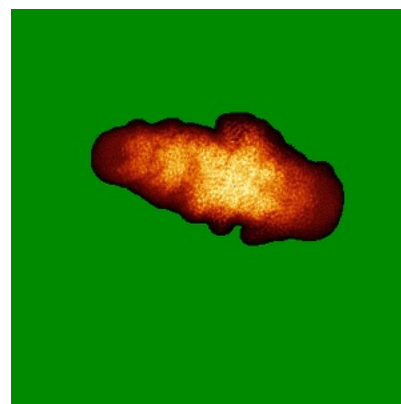
6.4.1 Primary map



X

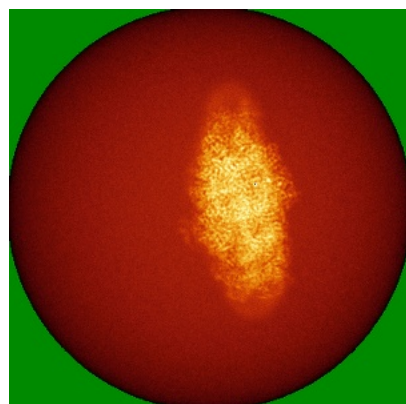


Y

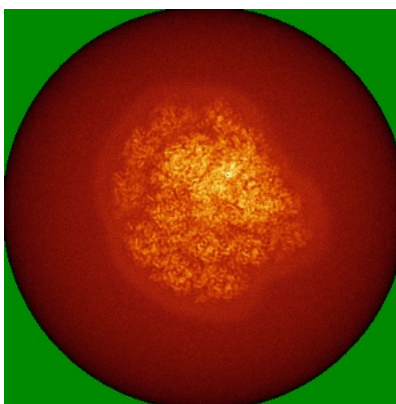


Z

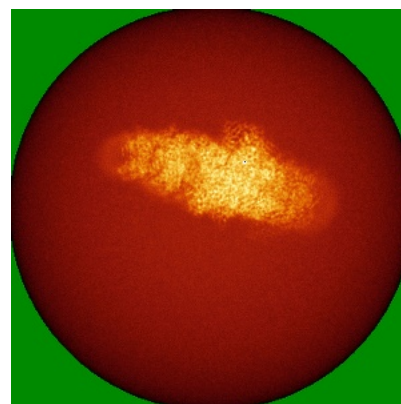
6.4.2 Raw map



X



Y

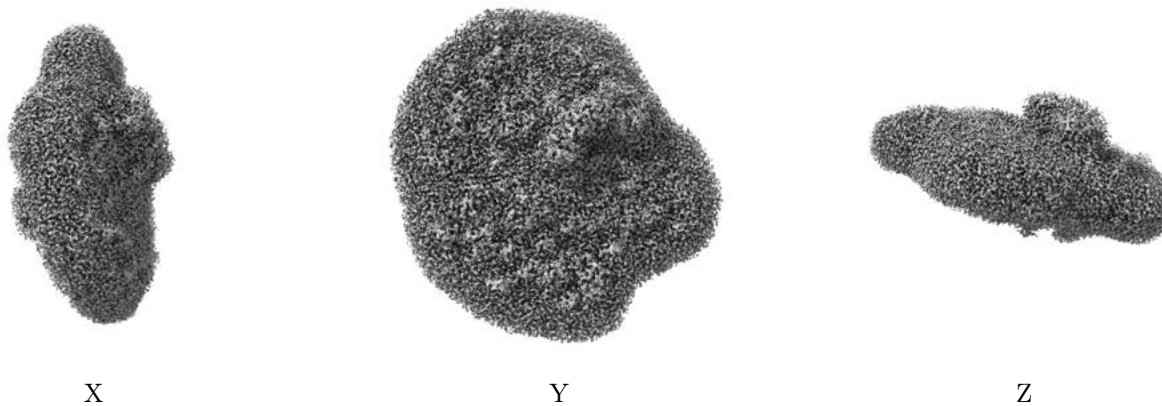


Z

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

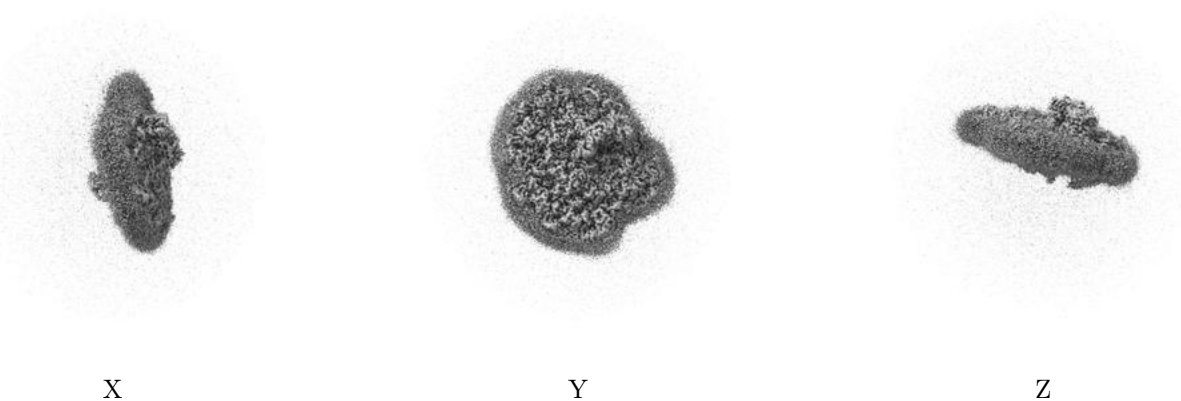
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

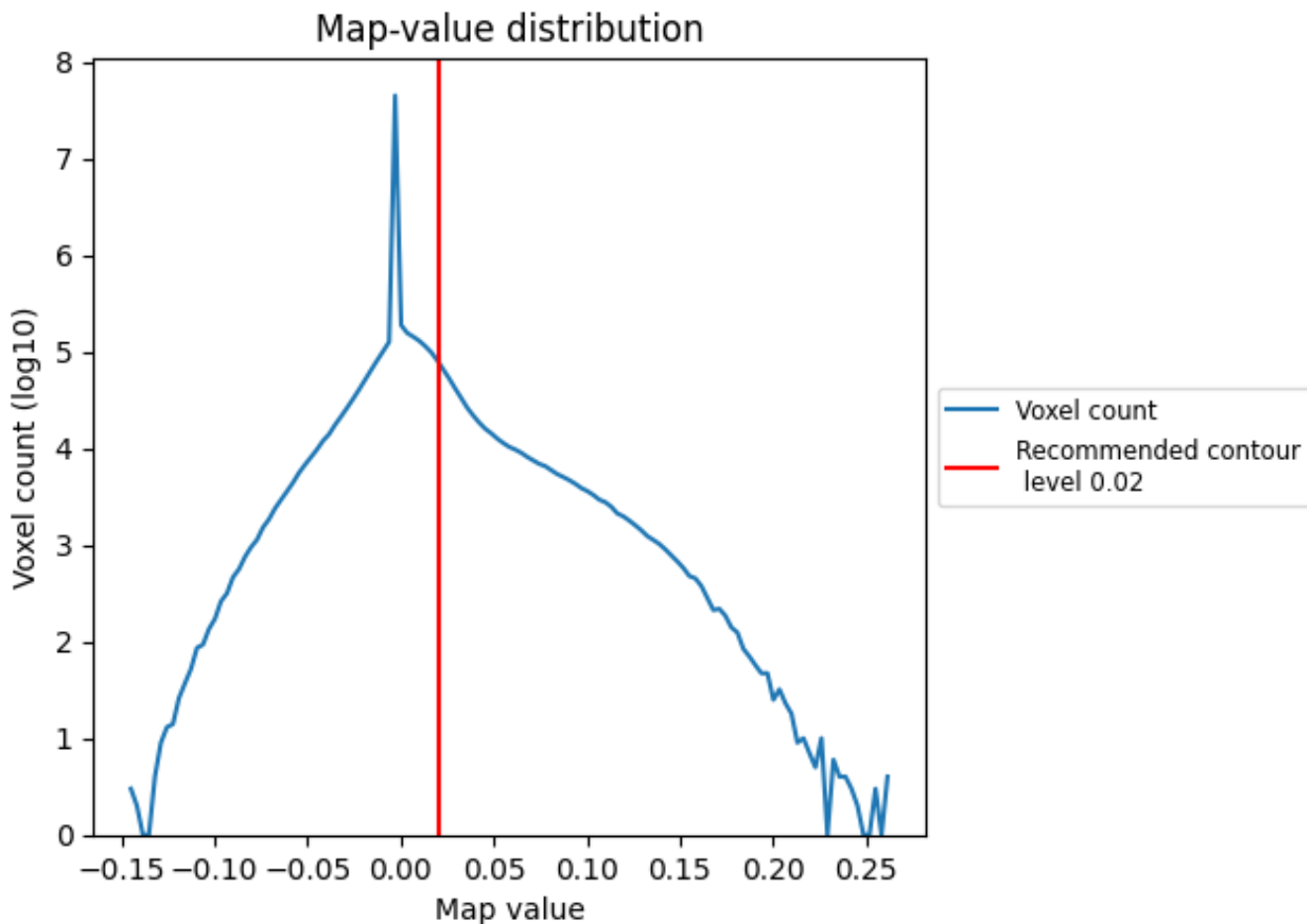
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

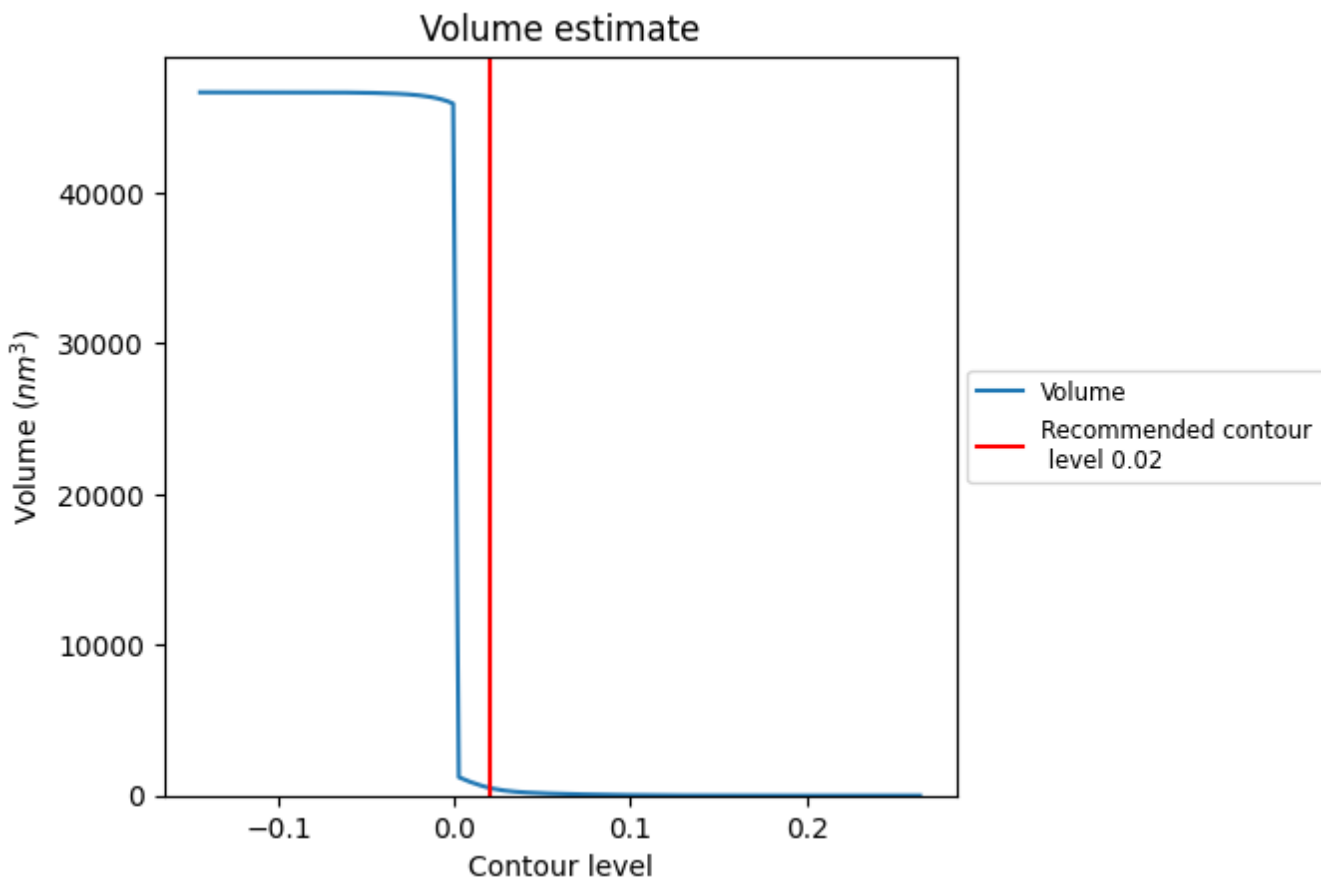
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

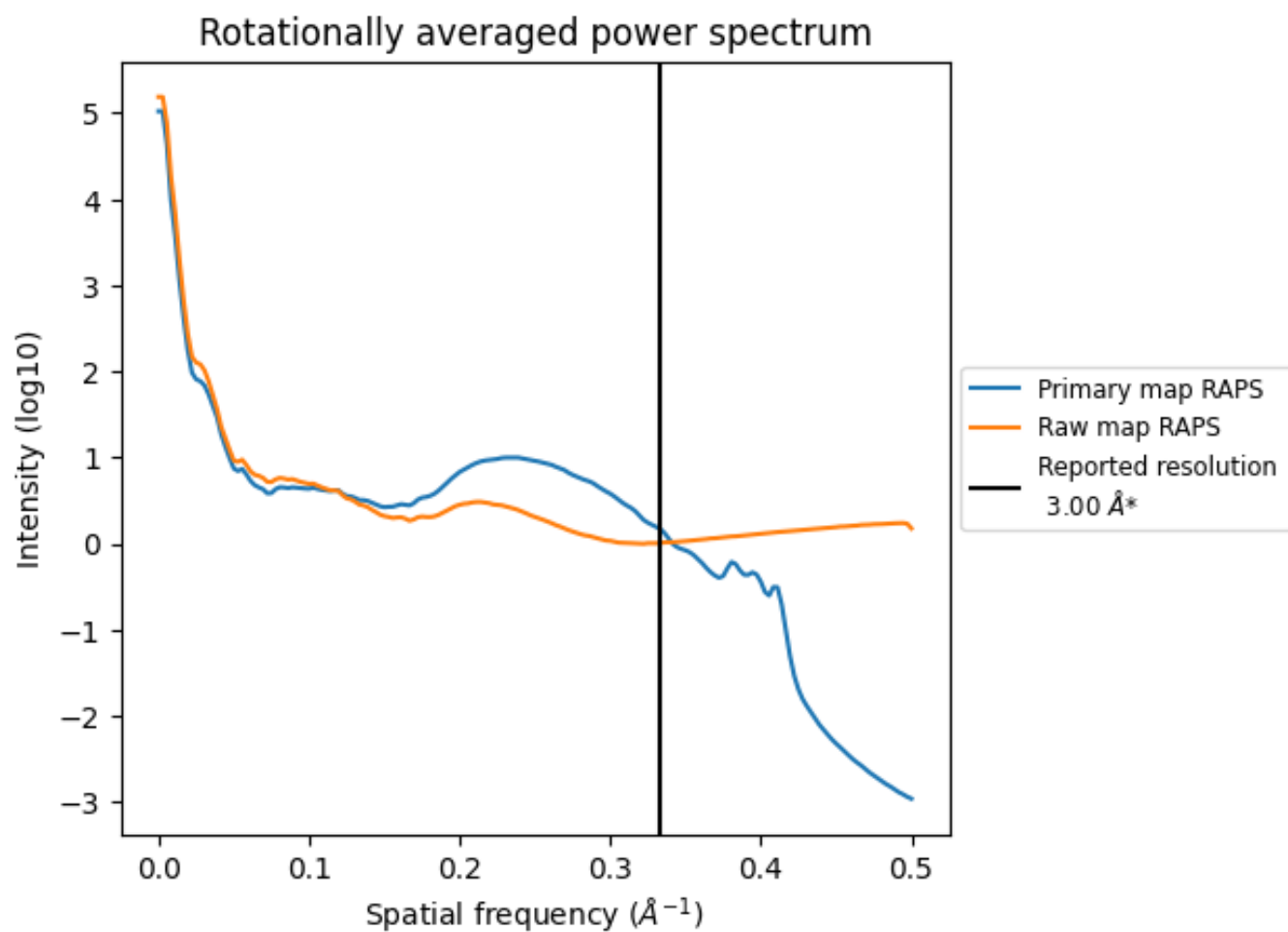
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 508 nm^3 ; this corresponds to an approximate mass of 459 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

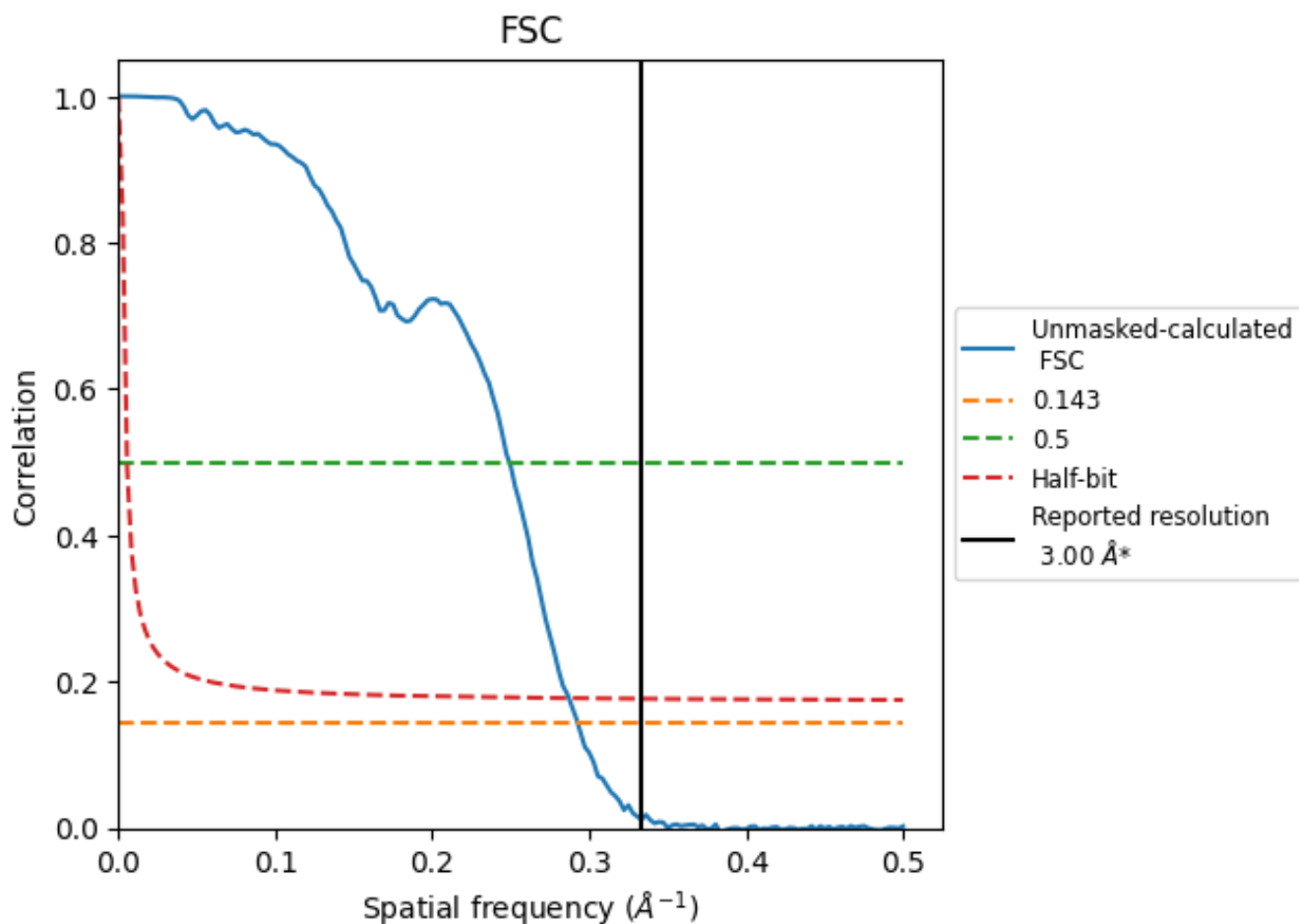


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

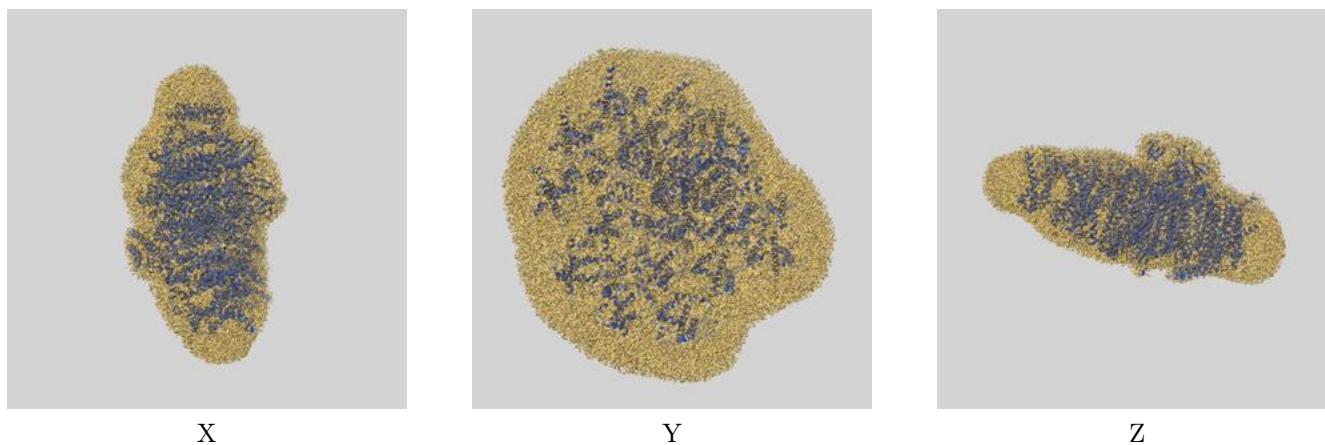
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.42	4.01	3.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

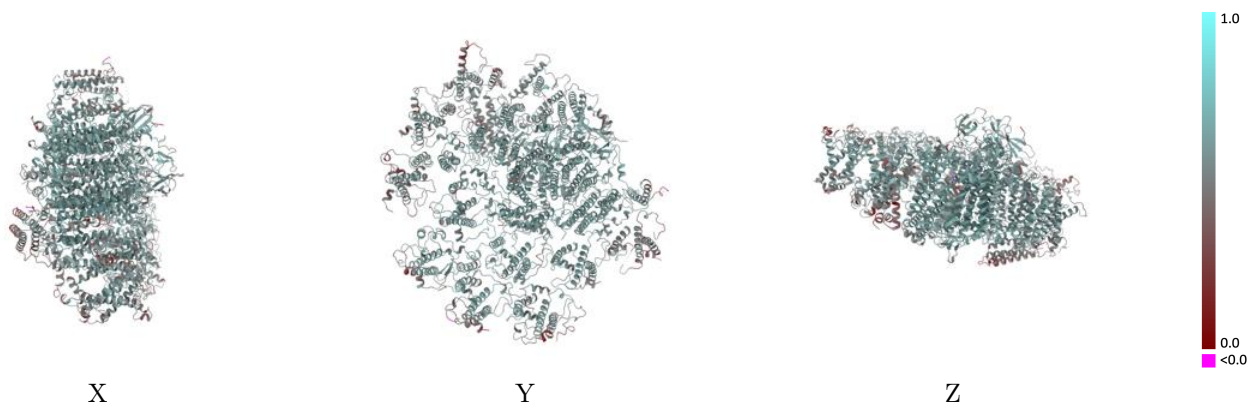
This section contains information regarding the fit between EMDB map EMD-37654 and PDB model 8WMJ. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



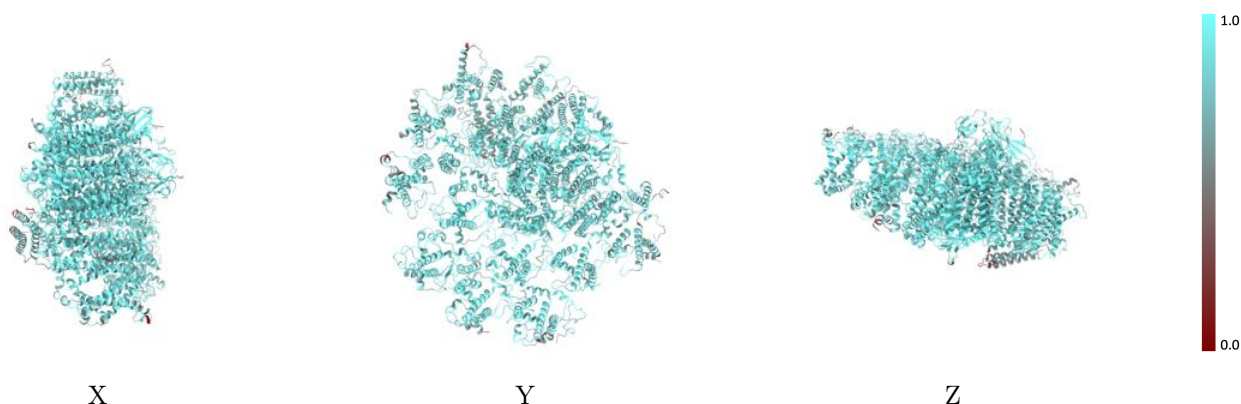
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



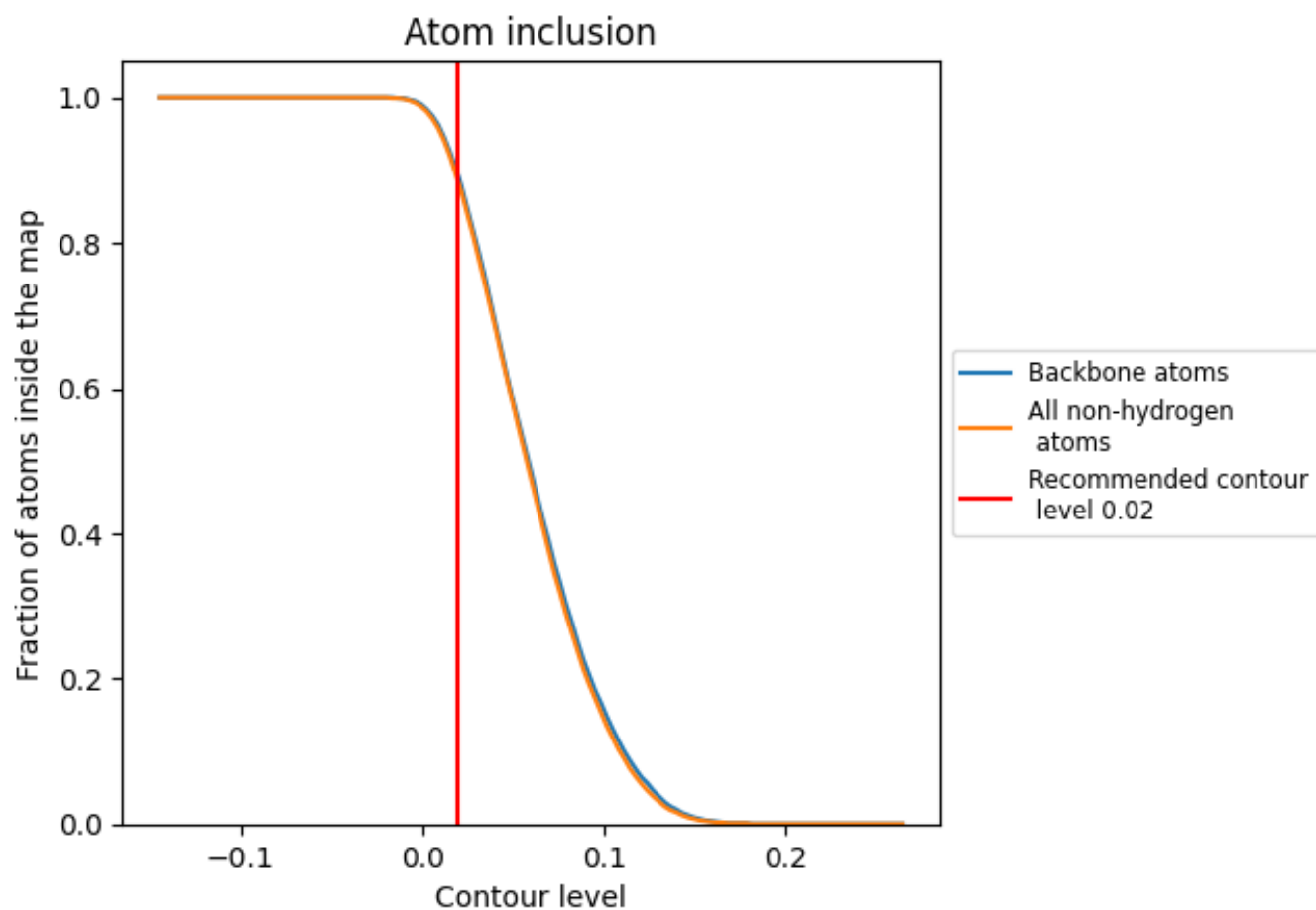
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8830	 0.5530
A	 0.9460	 0.6100
B	 0.9530	 0.6120
C	 0.9410	 0.5910
D	 0.8900	 0.5580
E	 0.8850	 0.5500
F	 0.9220	 0.5840
I	 0.8940	 0.5780
J	 0.9300	 0.5920
K	 0.8240	 0.5130
L	 0.8430	 0.5350
M	 0.8910	 0.5650
Q	 0.6840	 0.4300
R	 0.9010	 0.5660
a	 0.9300	 0.5780
b	 0.9160	 0.5800
c	 0.8770	 0.5500
d	 0.7380	 0.4250
h	 0.8570	 0.5310
i	 0.7650	 0.4540
j	 0.8170	 0.4980
k	 0.7670	 0.4580
l	 0.8590	 0.5230
m	 0.8690	 0.5300
n	 0.8230	 0.5000
s	 0.9030	 0.5690

