



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 04:46 PM JST

PDB ID : 6J40 / pdb_00006j40
EMDB ID : EMD-9777
Title : Structure of C2S2M2-type PSII-FCPII supercomplex from diatom
Authors : Nagao, R.; Kato, K.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on : 2019-01-07
Resolution : 3.80 Å(reported)
Based on initial models : 3WU2, 3JCU

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:

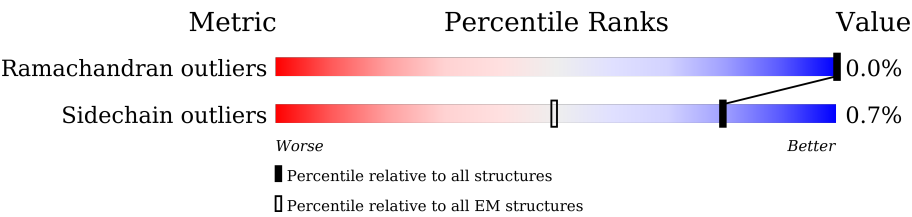
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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.





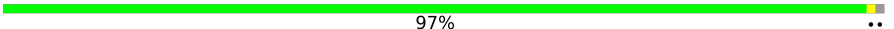
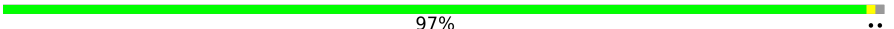






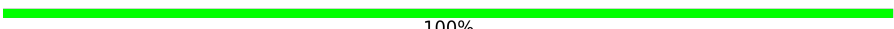
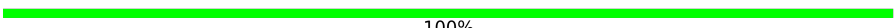


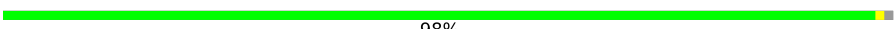
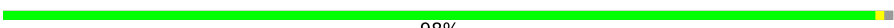


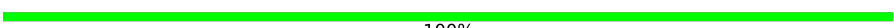
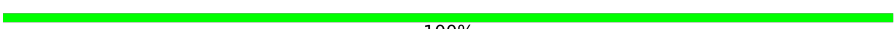
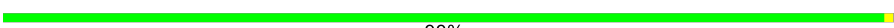

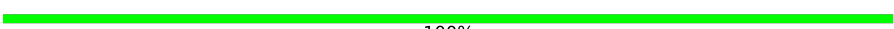


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	344	<div><div>97%</div><div><div></div><div></div><div></div><div></div></div><div>..</div></div>
1	a	344	<div><div>97%</div><div><div></div><div></div><div></div><div></div></div><div>..</div></div>
2	B	509	<div><div>94%</div><div><div></div><div></div><div></div><div></div></div><div>. 5%</div></div>
2	b	509	<div><div>94%</div><div><div></div><div></div><div></div><div></div></div><div>. 5%</div></div>
3	C	471	<div><div>95%</div><div><div></div><div></div><div></div><div></div></div><div>..</div></div>
3	c	471	<div><div>95%</div><div><div></div><div></div><div></div><div></div></div><div>..</div></div>
4	D	351	<div><div>95%</div><div><div></div><div></div><div></div><div></div></div><div>..</div></div>
4	d	351	<div><div>96%</div><div><div></div><div></div><div></div><div></div></div><div>..</div></div>
5	E	84	<div><div>89%</div><div><div></div><div></div><div></div><div></div></div><div>11%</div></div>
5	e	84	<div><div>89%</div><div><div></div><div></div><div></div><div></div></div><div>11%</div></div>

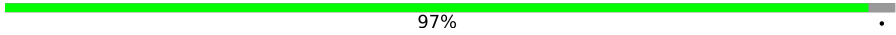
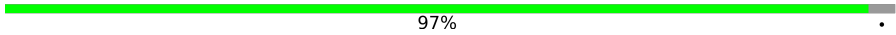
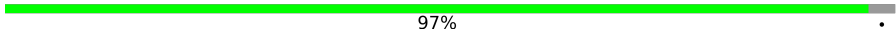




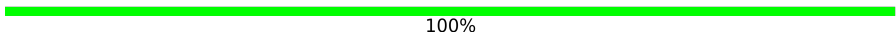
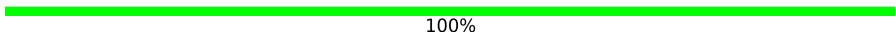
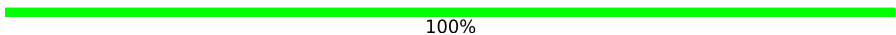
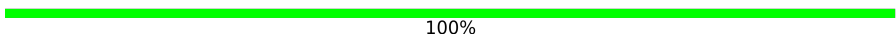














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Mol	Chain	Length	Quality of chain
6	F	43	 65%35%
6	f	43	 65%35%
7	H	67	 97%..
7	h	67	 97%..
8	I	38	 92%8%
8	i	38	 92%8%
9	J	39	 87%13%
9	j	39	 87%13%
10	K	44	 80%5%16%
10	k	44	 80%5%16%
11	L	38	 100%
11	l	38	 100%
12	M	131	 32%68%
12	m	131	 32%68%
13	O	248	 98%..
13	o	248	 98%..
14	T	31	 94%. .
14	t	31	 94%. .
15	U	93	 100%
15	u	93	 100%
16	V	137	 99%..
16	v	137	 99%..
17	Y	34	 100%
17	y	34	 100%
18	X	38	 97%.



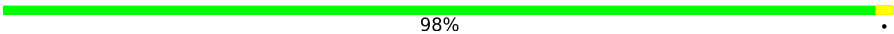
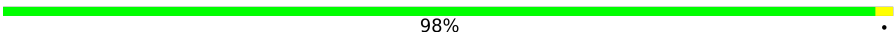
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Mol	Chain	Length	Quality of chain
18	x	38	 97% .
19	Z	61	 97% .
19	z	61	 97% .
20	Q	155	 88% 12%
20	q	155	 88% 12%
21	W	72	 71% . 28%
21	w	72	 71% . 28%
22	0	31	 100%
22	5	31	 100%
23	1	30	 100%
23	6	30	 100%
24	2	10	 100%
24	7	10	 100%
25	11	207	 84% . 15%
25	12	207	 84% . 15%
25	13	207	 84% . 15%
25	14	207	 84% . 15%
25	15	207	 85% 15%
25	16	207	 84% . 15%
25	17	207	 84% . 15%
25	18	207	 84% . 15%
25	31	207	 85% 15%
25	32	207	 85% 15%
25	33	207	 85% 15%
25	34	207	 85% 15%

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Mol	Chain	Length	Quality of chain
25	35	207	 85% 15%
25	36	207	 84% 15%
25	37	207	 84% 15%
25	38	207	 84% 15%
26	19	215	 98%
26	39	215	 98%
27	20	143	 98%
27	40	143	 98%
28	21	155	 100%
28	41	155	 100%

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
30	CLA	11	301	X	-	-	-
30	CLA	11	302	X	-	-	-
30	CLA	11	303	X	-	-	-
30	CLA	11	304	X	-	-	-
30	CLA	11	305	X	-	-	-
30	CLA	11	306	X	-	-	-
30	CLA	11	307	X	-	-	-
30	CLA	11	309	X	-	-	-
30	CLA	11	315	X	-	-	-
30	CLA	12	303	X	-	-	-
30	CLA	12	305	X	-	-	-
30	CLA	12	306	X	-	-	-
30	CLA	12	307	X	-	-	-
30	CLA	12	308	X	-	-	-
30	CLA	12	309	X	-	-	-
30	CLA	12	310	X	-	-	-
30	CLA	12	311	X	-	-	-
30	CLA	12	312	X	-	-	-
30	CLA	12	314	X	-	-	-
30	CLA	13	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	13	303	X	-	-	-
30	CLA	13	304	X	-	-	-
30	CLA	13	305	X	-	-	-
30	CLA	13	306	X	-	-	-
30	CLA	13	307	X	-	-	-
30	CLA	13	308	X	-	-	-
30	CLA	13	310	X	-	-	-
30	CLA	14	301	X	-	-	-
30	CLA	14	302	X	-	-	-
30	CLA	14	303	X	-	-	-
30	CLA	14	304	X	-	-	-
30	CLA	14	305	X	-	-	-
30	CLA	14	306	X	-	-	-
30	CLA	14	307	X	-	-	-
30	CLA	14	308	X	-	-	-
30	CLA	14	310	X	-	-	-
30	CLA	15	301	X	-	-	-
30	CLA	15	302	X	-	-	-
30	CLA	15	303	X	-	-	-
30	CLA	15	305	X	-	-	-
30	CLA	15	306	X	-	-	-
30	CLA	15	307	X	-	-	-
30	CLA	15	308	X	-	-	-
30	CLA	15	309	X	-	-	-
30	CLA	16	301	X	-	-	-
30	CLA	16	302	X	-	-	-
30	CLA	16	303	X	-	-	-
30	CLA	16	304	X	-	-	-
30	CLA	16	306	X	-	-	-
30	CLA	16	307	X	-	-	-
30	CLA	16	309	X	-	-	-
30	CLA	17	301	X	-	-	-
30	CLA	17	303	X	-	-	-
30	CLA	17	305	X	-	-	-
30	CLA	17	307	X	-	-	-
30	CLA	17	308	X	-	-	-
30	CLA	17	309	X	-	-	-
30	CLA	17	310	X	-	-	-
30	CLA	18	301	X	-	-	-
30	CLA	18	303	X	-	-	-
30	CLA	18	304	X	-	-	-
30	CLA	18	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	18	307	X	-	-	-
30	CLA	18	308	X	-	-	-
30	CLA	18	309	X	-	-	-
30	CLA	18	310	X	-	-	-
30	CLA	18	311	X	-	-	-
30	CLA	18	312	X	-	-	-
30	CLA	19	302	X	-	-	-
30	CLA	19	303	X	-	-	-
30	CLA	19	304	X	-	-	-
30	CLA	19	305	X	-	-	-
30	CLA	19	306	X	-	-	-
30	CLA	19	307	X	-	-	-
30	CLA	19	308	X	-	-	-
30	CLA	20	203	X	-	-	-
30	CLA	20	204	X	-	-	-
30	CLA	20	206	X	-	-	-
30	CLA	20	207	X	-	-	-
30	CLA	20	209	X	-	-	-
30	CLA	21	303	X	-	-	-
30	CLA	21	304	X	-	-	-
30	CLA	21	305	X	-	-	-
30	CLA	21	306	X	-	-	-
30	CLA	21	307	X	-	-	-
30	CLA	21	308	X	-	-	-
30	CLA	21	309	X	-	-	-
30	CLA	31	301	X	-	-	-
30	CLA	31	302	X	-	-	-
30	CLA	31	303	X	-	-	-
30	CLA	31	304	X	-	-	-
30	CLA	31	305	X	-	-	-
30	CLA	31	306	X	-	-	-
30	CLA	31	307	X	-	-	-
30	CLA	31	309	X	-	-	-
30	CLA	31	315	X	-	-	-
30	CLA	32	303	X	-	-	-
30	CLA	32	305	X	-	-	-
30	CLA	32	306	X	-	-	-
30	CLA	32	307	X	-	-	-
30	CLA	32	308	X	-	-	-
30	CLA	32	309	X	-	-	-
30	CLA	32	310	X	-	-	-
30	CLA	32	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	32	313	X	-	-	-
30	CLA	33	301	X	-	-	-
30	CLA	33	303	X	-	-	-
30	CLA	33	304	X	-	-	-
30	CLA	33	305	X	-	-	-
30	CLA	33	306	X	-	-	-
30	CLA	33	307	X	-	-	-
30	CLA	33	308	X	-	-	-
30	CLA	33	309	X	-	-	-
30	CLA	33	311	X	-	-	-
30	CLA	34	301	X	-	-	-
30	CLA	34	302	X	-	-	-
30	CLA	34	303	X	-	-	-
30	CLA	34	304	X	-	-	-
30	CLA	34	305	X	-	-	-
30	CLA	34	306	X	-	-	-
30	CLA	34	307	X	-	-	-
30	CLA	34	308	X	-	-	-
30	CLA	34	310	X	-	-	-
30	CLA	35	301	X	-	-	-
30	CLA	35	302	X	-	-	-
30	CLA	35	303	X	-	-	-
30	CLA	35	305	X	-	-	-
30	CLA	35	306	X	-	-	-
30	CLA	35	307	X	-	-	-
30	CLA	35	308	X	-	-	-
30	CLA	35	309	X	-	-	-
30	CLA	36	301	X	-	-	-
30	CLA	36	302	X	-	-	-
30	CLA	36	303	X	-	-	-
30	CLA	36	304	X	-	-	-
30	CLA	36	306	X	-	-	-
30	CLA	36	307	X	-	-	-
30	CLA	36	309	X	-	-	-
30	CLA	37	301	X	-	-	-
30	CLA	37	303	X	-	-	-
30	CLA	37	305	X	-	-	-
30	CLA	37	307	X	-	-	-
30	CLA	37	308	X	-	-	-
30	CLA	37	309	X	-	-	-
30	CLA	37	310	X	-	-	-
30	CLA	38	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	38	303	X	-	-	-
30	CLA	38	304	X	-	-	-
30	CLA	38	305	X	-	-	-
30	CLA	38	307	X	-	-	-
30	CLA	38	308	X	-	-	-
30	CLA	38	309	X	-	-	-
30	CLA	38	310	X	-	-	-
30	CLA	38	311	X	-	-	-
30	CLA	38	312	X	-	-	-
30	CLA	39	302	X	-	-	-
30	CLA	39	303	X	-	-	-
30	CLA	39	304	X	-	-	-
30	CLA	39	305	X	-	-	-
30	CLA	39	306	X	-	-	-
30	CLA	39	307	X	-	-	-
30	CLA	39	308	X	-	-	-
30	CLA	40	203	X	-	-	-
30	CLA	40	204	X	-	-	-
30	CLA	40	206	X	-	-	-
30	CLA	40	207	X	-	-	-
30	CLA	40	209	X	-	-	-
30	CLA	41	303	X	-	-	-
30	CLA	41	304	X	-	-	-
30	CLA	41	305	X	-	-	-
30	CLA	41	306	X	-	-	-
30	CLA	41	307	X	-	-	-
30	CLA	41	308	X	-	-	-
30	CLA	41	309	X	-	-	-
30	CLA	A	402	X	-	-	-
30	CLA	A	404	X	-	-	-
30	CLA	B	601	X	-	-	-
30	CLA	B	602	X	-	-	-
30	CLA	B	603	X	-	-	-
30	CLA	B	604	X	-	-	-
30	CLA	B	605	X	-	-	-
30	CLA	B	606	X	-	-	-
30	CLA	B	607	X	-	-	-
30	CLA	B	608	X	-	-	-
30	CLA	B	609	X	-	-	-
30	CLA	B	610	X	-	-	-
30	CLA	B	611	X	-	-	-
30	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	B	613	X	-	-	-
30	CLA	B	614	X	-	-	-
30	CLA	B	615	X	-	-	-
30	CLA	B	623	X	-	-	-
30	CLA	C	502	X	-	-	-
30	CLA	C	503	X	-	-	-
30	CLA	C	504	X	-	-	-
30	CLA	C	505	X	-	-	-
30	CLA	C	506	X	-	-	-
30	CLA	C	507	X	-	-	-
30	CLA	C	508	X	-	-	-
30	CLA	C	509	X	-	-	-
30	CLA	C	510	X	-	-	-
30	CLA	C	511	X	-	-	-
30	CLA	C	512	X	-	-	-
30	CLA	C	513	X	-	-	-
30	CLA	C	514	X	-	-	-
30	CLA	C	520	X	-	-	-
30	CLA	C	521	X	-	-	-
30	CLA	D	401	X	-	-	-
30	CLA	D	402	X	-	-	-
30	CLA	D	405	X	-	-	-
30	CLA	D	406	X	-	-	-
30	CLA	M	101	X	-	-	-
30	CLA	W	102	X	-	-	-
30	CLA	Z	102	X	-	-	-
30	CLA	a	402	X	-	-	-
30	CLA	a	403	X	-	-	-
30	CLA	b	601	X	-	-	-
30	CLA	b	602	X	-	-	-
30	CLA	b	603	X	-	-	-
30	CLA	b	604	X	-	-	-
30	CLA	b	605	X	-	-	-
30	CLA	b	606	X	-	-	-
30	CLA	b	607	X	-	-	-
30	CLA	b	608	X	-	-	-
30	CLA	b	609	X	-	-	-
30	CLA	b	610	X	-	-	-
30	CLA	b	611	X	-	-	-
30	CLA	b	612	X	-	-	-
30	CLA	b	613	X	-	-	-
30	CLA	b	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	b	615	X	-	-	-
30	CLA	b	622	X	-	-	-
30	CLA	c	502	X	-	-	-
30	CLA	c	503	X	-	-	-
30	CLA	c	504	X	-	-	-
30	CLA	c	505	X	-	-	-
30	CLA	c	506	X	-	-	-
30	CLA	c	507	X	-	-	-
30	CLA	c	508	X	-	-	-
30	CLA	c	509	X	-	-	-
30	CLA	c	510	X	-	-	-
30	CLA	c	511	X	-	-	-
30	CLA	c	512	X	-	-	-
30	CLA	c	513	X	-	-	-
30	CLA	c	514	X	-	-	-
30	CLA	c	522	X	-	-	-
30	CLA	c	523	X	-	-	-
30	CLA	c	524	X	-	-	-
30	CLA	d	401	X	-	-	-
30	CLA	d	402	X	-	-	-
30	CLA	d	406	X	-	-	-
30	CLA	d	407	X	-	-	-
30	CLA	m	101	X	-	-	-
30	CLA	w	102	X	-	-	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 96390 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 II reaction center protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2618	1712	429	462	15		
1	a	334	Total	C	N	O	S	0	0
			2618	1712	429	462	15		

- Molecule 2 is a protein called Photosystem II chlorophyll protein CP47.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3812	2494	645	660	13		
2	b	484	Total	C	N	O	S	0	0
			3812	2494	645	660	13		

- Molecule 3 is a protein called Photosystem II chlorophyll protein CP43.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	451	Total	C	N	O	S	0	0
			3504	2289	589	612	14		
3	c	451	Total	C	N	O	S	0	0
			3504	2289	589	612	14		

- Molecule 4 is a protein called Photosystem II reaction center protein D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2697	1781	441	465	10		
4	d	341	Total	C	N	O	S	0	0
			2697	1781	441	465	10		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	75	Total	C	N	O	0	0
			616	401	102	113		
5	e	75	Total	C	N	O	0	0
			616	401	102	113		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	28	Total	C	N	O	S	0	0
			228	155	39	33	1		
6	f	28	Total	C	N	O	S	0	0
			228	155	39	33	1		

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	66	Total	C	N	O	S	0	0
			513	340	83	88	2		
7	h	66	Total	C	N	O	S	0	0
			513	340	83	88	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	35	Total	C	N	O	S	0	0
			287	194	45	47	1		
8	i	35	Total	C	N	O	S	0	0
			287	194	45	47	1		

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	34	Total	C	N	O	S	0	0
			254	172	38	43	1		
9	j	34	Total	C	N	O	S	0	0
			254	172	38	43	1		

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			302	212	45	45		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	k	37	Total	C	N	O	0	0
			302	212	45	45		

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	38	Total	C	N	O	S	0	0
			310	208	48	53	1		
11	l	38	Total	C	N	O	S	0	0
			310	208	48	53	1		

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	42	Total	C	N	O	0	0
			316	207	51	58		
12	m	42	Total	C	N	O	0	0
			316	207	51	58		

- Molecule 13 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	245	Total	C	N	O	S	0	0
			1845	1166	306	365	8		
13	o	245	Total	C	N	O	S	0	0
			1845	1166	306	365	8		

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	30	Total	C	N	O	S	0	0
			250	174	36	38	2		
14	t	30	Total	C	N	O	S	0	0
			250	174	36	38	2		

- Molecule 15 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	93	Total	C	N	O	S	0	0
			713	455	119	137	2		
15	u	93	Total	C	N	O	S	0	0
			713	455	119	137	2		

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	136	Total	C	N	O	S	0	0
			1037	647	180	206	4		
16	v	136	Total	C	N	O	S	0	0
			1037	647	180	206	4		

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	34	Total	C	N	O	S	0	0
			250	166	41	40	3		
17	y	34	Total	C	N	O	S	0	0
			250	166	41	40	3		

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	37	Total	C	N	O	S	0	0
			263	171	45	46	1		
18	x	37	Total	C	N	O	S	0	0
			263	171	45	46	1		

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	59	Total	C	N	O	S	0	0
			447	305	68	73	1		
19	z	59	Total	C	N	O	S	0	0
			447	305	68	73	1		

- Molecule 20 is a protein called Extrinsic protein in photosystem II.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	137	Total	C	N	O	S	0	0
			1079	684	179	215	1		
20	q	137	Total	C	N	O	S	0	0
			1079	684	179	215	1		

- Molecule 21 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	52	Total	C	N	O	0	0
			422	273	65	84		
21	w	52	Total	C	N	O	0	0
			422	273	65	84		

- Molecule 22 is a protein called Unknown protein 0.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	0	31	Total	C	N	O	0	0
			155	93	31	31		
22	5	31	Total	C	N	O	0	0
			155	93	31	31		

- Molecule 23 is a protein called Unknown protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	1	30	Total	C	N	O	0	0
			150	90	30	30		
23	6	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 24 is a protein called Unknown protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	2	10	Total	C	N	O	0	0
			50	30	10	10		
24	7	10	Total	C	N	O	0	0
			50	30	10	10		

- Molecule 25 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	11	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	12	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	13	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	14	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	15	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
25	16	176	Total 1343	C 852	N 228	O 256	S 7	0	0
25	17	176	Total 1343	C 852	N 228	O 256	S 7	0	0
25	18	176	Total 1343	C 852	N 228	O 256	S 7	0	0
25	31	176	Total 1343	C 852	N 228	O 256	S 7	0	0
25	32	176	Total 1343	C 852	N 228	O 256	S 7	0	0
25	33	176	Total 1343	C 852	N 228	O 256	S 7	0	0
25	34	176	Total 1343	C 852	N 228	O 256	S 7	0	0
25	35	176	Total 1343	C 852	N 228	O 256	S 7	0	0
25	36	176	Total 1343	C 852	N 228	O 256	S 7	0	0
25	37	176	Total 1343	C 852	N 228	O 256	S 7	0	0
25	38	176	Total 1343	C 852	N 228	O 256	S 7	0	0

- Molecule 26 is a protein called Fucoxanthin chlorophyll a/c-binding protein monomer 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	19	215	Total 1075	C 645	N 215	O 215	0	0
26	39	215	Total 1075	C 645	N 215	O 215	0	0

- Molecule 27 is a protein called Fucoxanthin chlorophyll a/c-binding protein monomer 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	20	143	Total 715	C 429	N 143	O 143	0	0
27	40	143	Total 715	C 429	N 143	O 143	0	0

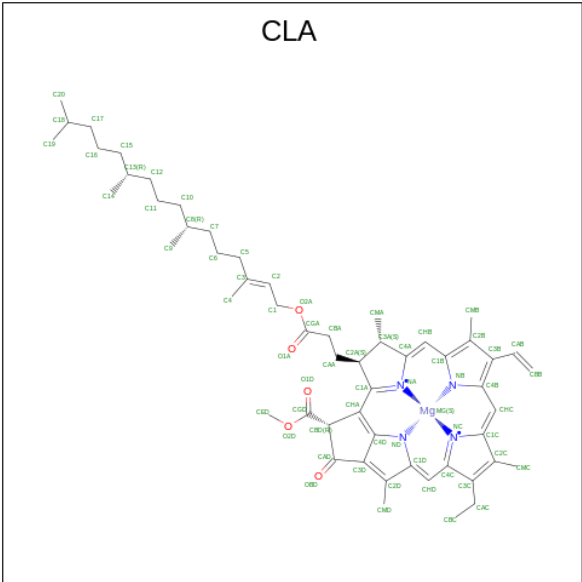
- Molecule 28 is a protein called Fucoxanthin chlorophyll a/c-binding protein monomer 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	21	155	Total	C	N	O	0	0
			775	465	155	155		
28	41	155	Total	C	N	O	0	0
			775	465	155	155		

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	Fe	0
			1	1	
29	a	1	Total	Fe	0
			1	1	

- Molecule 30 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	z	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	11	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	17	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	18	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	19	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	19	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	20	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	20	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	20	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	20	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	21	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	21	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	21	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	21	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	21	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	31	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	31	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	31	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	31	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	31	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	33	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	33	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	33	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	33	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	33	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	34	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	34	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	34	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	34	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	34	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	35	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	35	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	35	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	35	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	35	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	35	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	35	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	35	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	35	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	36	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	36	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	36	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	36	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	36	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	36	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	36	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	36	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	36	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	37	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	37	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	37	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	37	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	37	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	37	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	37	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	37	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	37	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	38	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	38	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	38	1	Total 65	C 55	Mg 1	N 4	O 5	0

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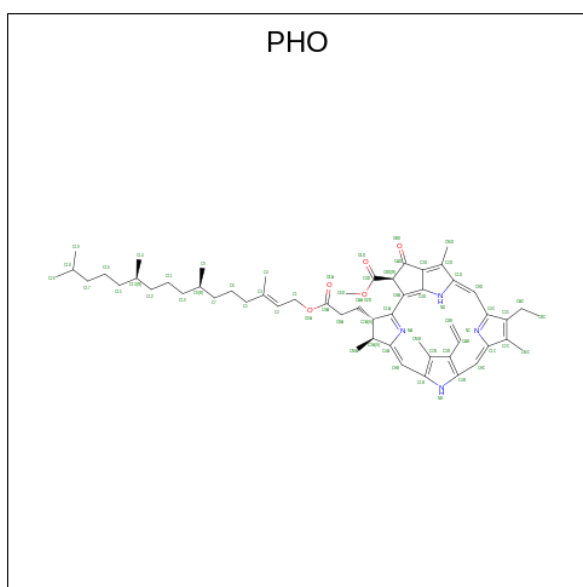
Mol	Chain	Residues	Atoms					AltConf
30	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	38	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	38	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	39	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	39	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	39	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	39	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	39	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	39	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	39	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	39	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	40	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	40	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	40	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	40	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	40	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	40	1	Total 45	C 35	Mg 1	N 4	O 5	0

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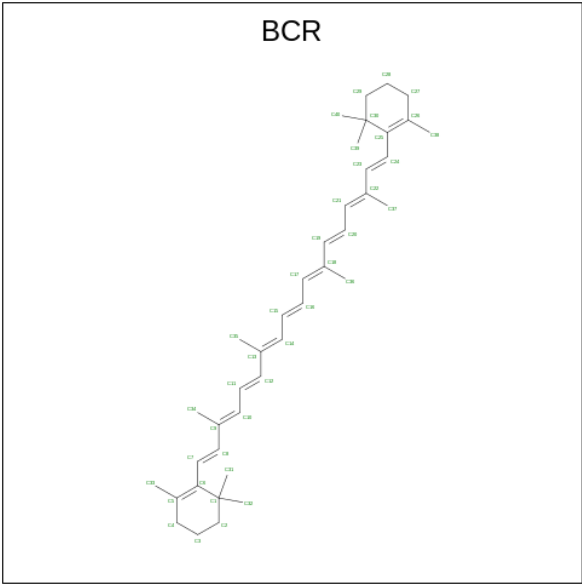
Mol	Chain	Residues	Atoms					AltConf
30	40	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	40	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 31 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	N	O	0
			64	55	4	5	
31	D	1	Total	C	N	O	0
			64	55	4	5	
31	d	1	Total	C	N	O	0
			64	55	4	5	
31	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 32 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



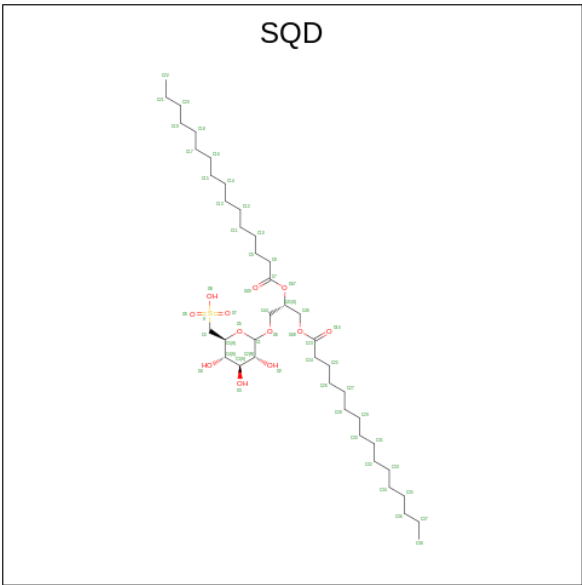
Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	C	0
			40	40	
32	A	1	Total	C	0
			40	40	
32	B	1	Total	C	0
			40	40	
32	B	1	Total	C	0
			40	40	
32	B	1	Total	C	0
			40	40	
32	B	1	Total	C	0
			40	40	
32	C	1	Total	C	0
			40	40	
32	C	1	Total	C	0
			40	40	

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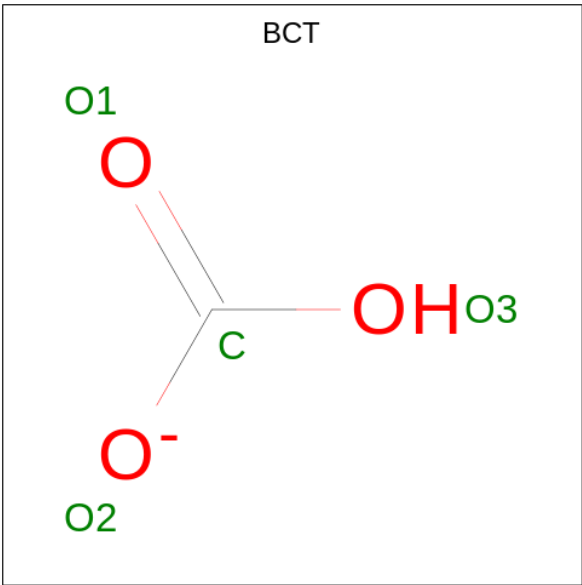
Mol	Chain	Residues	Atoms	AltConf
32	F	1	Total C 40 40	0
32	H	1	Total C 40 40	0
32	Y	1	Total C 40 40	0
32	Z	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	h	1	Total C 40 40	0
32	m	1	Total C 40 40	0

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



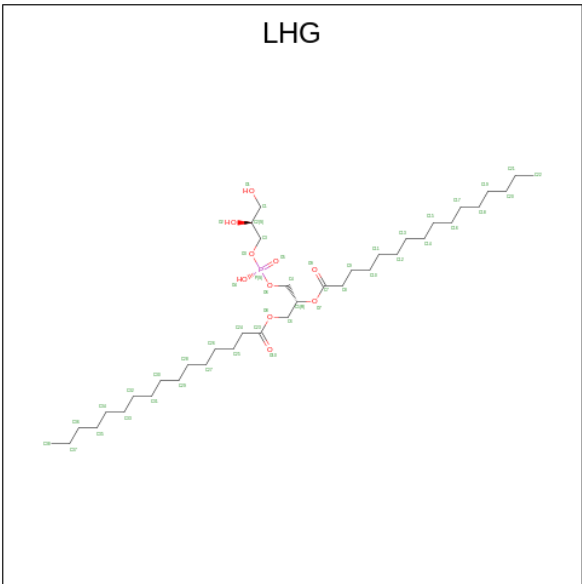
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	S	0
			54	41	12	1	
33	B	1	Total	C	O	S	0
			37	24	12	1	
33	L	1	Total	C	O	S	0
			54	41	12	1	
33	a	1	Total	C	O	S	0
			54	41	12	1	
33	b	1	Total	C	O	S	0
			37	24	12	1	
33	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			4	1	3	
34	a	1	Total	C	O	0
			4	1	3	

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



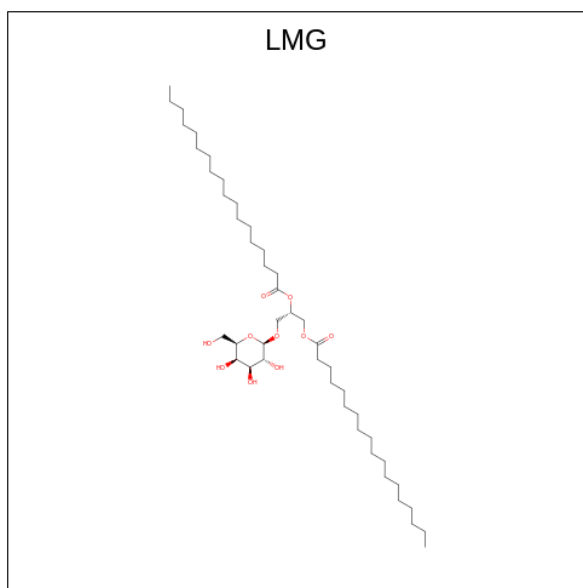
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	P	0
			46	35	10	1	

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Mol	Chain	Residues	Atoms				AltConf
35	B	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	a	1	Total	C	O	P	0
			46	35	10	1	
35	b	1	Total	C	O	P	0
			49	38	10	1	
35	d	1	Total	C	O	P	0
			49	38	10	1	
35	l	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



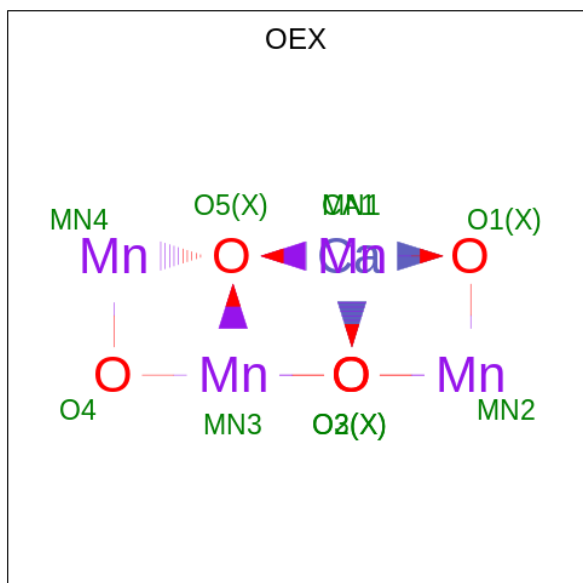
Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			51	41	10	
36	B	1	Total	C	O	0
			51	41	10	
36	D	1	Total	C	O	0
			51	41	10	
36	M	1	Total	C	O	0
			40	30	10	

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Mol	Chain	Residues	Atoms			AltConf
36	Q	1	Total	C	O	0
			51	41	10	
36	W	1	Total	C	O	0
			51	41	10	
36	b	1	Total	C	O	0
			51	41	10	
36	b	1	Total	C	O	0
			51	41	10	
36	c	1	Total	C	O	0
			51	41	10	
36	d	1	Total	C	O	0
			51	41	10	
36	m	1	Total	C	O	0
			40	30	10	
36	w	1	Total	C	O	0
			51	41	10	
36	12	1	Total	C	O	0
			39	29	10	
36	32	1	Total	C	O	0
			39	29	10	

- Molecule 37 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



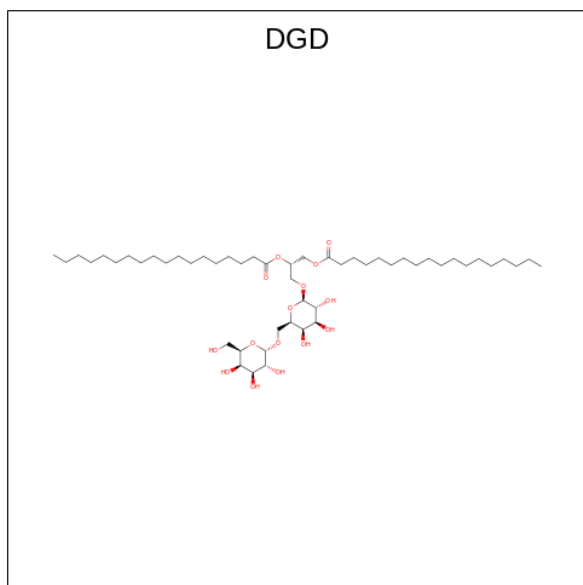
Mol	Chain	Residues	Atoms				AltConf
37	C	1	Total	Ca	Mn	O	0
			10	1	4	5	

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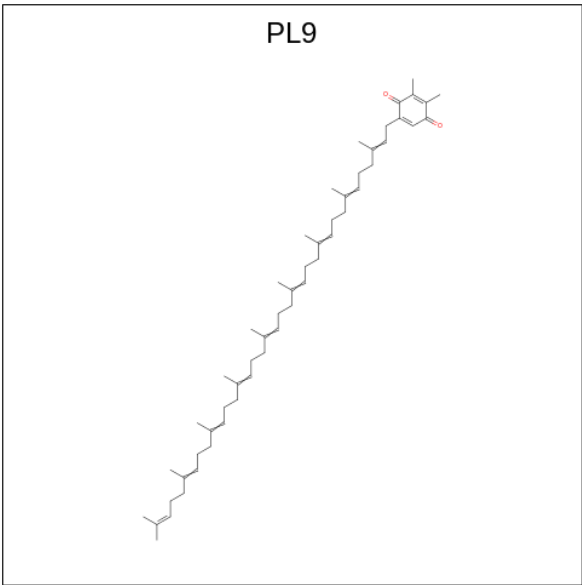
Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
37	c	1	10	1	4	5	0

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



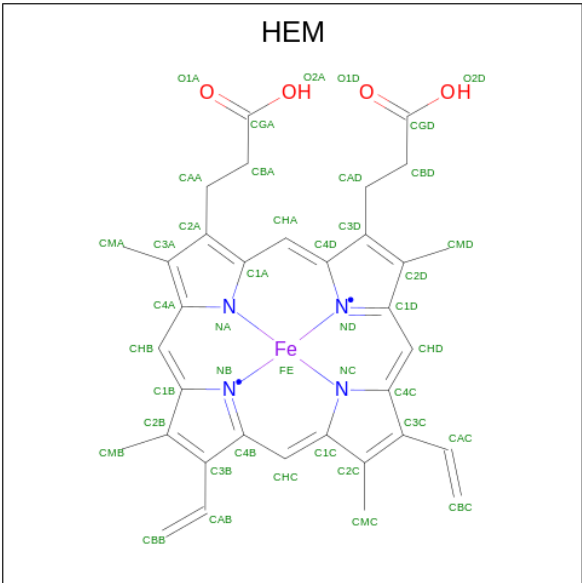
Mol	Chain	Residues	Atoms			AltConf
38	C	1	Total	C	O	0
			62	47	15	
38	C	1	Total	C	O	0
			62	47	15	
38	H	1	Total	C	O	0
			62	47	15	
38	J	1	Total	C	O	0
			62	47	15	
38	c	1	Total	C	O	0
			62	47	15	
38	c	1	Total	C	O	0
			62	47	15	
38	h	1	Total	C	O	0
			62	47	15	
38	j	1	Total	C	O	0
			62	47	15	

- Molecule 39 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



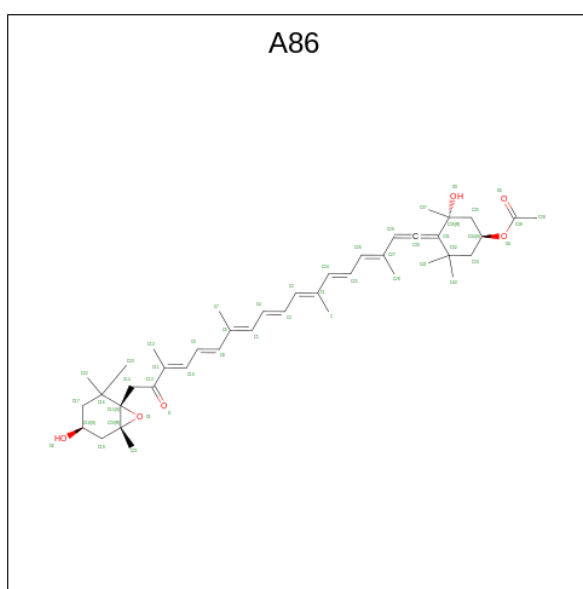
Mol	Chain	Residues	Atoms			AltConf
39	D	1	Total	C	O	0
			55	53	2	
39	D	1	Total	C	O	0
			55	53	2	
39	d	1	Total	C	O	0
			55	53	2	
39	d	1	Total	C	O	0
			55	53	2	

- Molecule 40 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
40	E	1	Total 43	C 34	Fe 1	N 4	O 4	0
40	V	1	Total 43	C 34	Fe 1	N 4	O 4	0
40	e	1	Total 43	C 34	Fe 1	N 4	O 4	0
40	v	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 41 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆).



Mol	Chain	Residues	Atoms			AltConf
41	11	1	Total	C	O	0
			48	42	6	
41	11	1	Total	C	O	0
			48	42	6	
41	11	1	Total	C	O	0
			48	42	6	
41	11	1	Total	C	O	0
			48	42	6	
41	11	1	Total	C	O	0
			48	42	6	
41	11	1	Total	C	O	0
			48	42	6	
41	12	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
41	12	1	Total	C	O	0
			48	42	6	
41	12	1	Total	C	O	0
			48	42	6	
41	12	1	Total	C	O	0
			48	42	6	
41	12	1	Total	C	O	0
			48	42	6	
41	12	1	Total	C	O	0
			48	42	6	
41	13	1	Total	C	O	0
			48	42	6	
41	13	1	Total	C	O	0
			48	42	6	
41	13	1	Total	C	O	0
			48	42	6	
41	13	1	Total	C	O	0
			48	42	6	
41	13	1	Total	C	O	0
			48	42	6	
41	13	1	Total	C	O	0
			48	42	6	
41	13	1	Total	C	O	0
			48	42	6	
41	13	1	Total	C	O	0
			48	42	6	
41	14	1	Total	C	O	0
			48	42	6	
41	14	1	Total	C	O	0
			48	42	6	
41	14	1	Total	C	O	0
			48	42	6	
41	14	1	Total	C	O	0
			48	42	6	
41	15	1	Total	C	O	0
			48	42	6	
41	15	1	Total	C	O	0
			48	42	6	
41	15	1	Total	C	O	0
			48	42	6	
41	15	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
41	15	1	Total	C	O	0
			48	42	6	
41	15	1	Total	C	O	0
			48	42	6	
41	15	1	Total	C	O	0
			48	42	6	
41	16	1	Total	C	O	0
			48	42	6	
41	16	1	Total	C	O	0
			48	42	6	
41	16	1	Total	C	O	0
			48	42	6	
41	16	1	Total	C	O	0
			48	42	6	
41	17	1	Total	C	O	0
			48	42	6	
41	17	1	Total	C	O	0
			48	42	6	
41	17	1	Total	C	O	0
			48	42	6	
41	17	1	Total	C	O	0
			48	42	6	
41	17	1	Total	C	O	0
			48	42	6	
41	17	1	Total	C	O	0
			48	42	6	
41	18	1	Total	C	O	0
			48	42	6	
41	18	1	Total	C	O	0
			48	42	6	
41	18	1	Total	C	O	0
			48	42	6	
41	18	1	Total	C	O	0
			48	42	6	
41	19	1	Total	C	O	0
			48	42	6	
41	19	1	Total	C	O	0
			48	42	6	
41	19	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
41	20	1	Total	C	O	0
			48	42	6	
41	20	1	Total	C	O	0
			48	42	6	
41	20	1	Total	C	O	0
			48	42	6	
41	20	1	Total	C	O	0
			48	42	6	
41	20	1	Total	C	O	0
			48	42	6	
41	21	1	Total	C	O	0
			48	42	6	
41	21	1	Total	C	O	0
			48	42	6	
41	21	1	Total	C	O	0
			48	42	6	
41	21	1	Total	C	O	0
			48	42	6	
41	21	1	Total	C	O	0
			48	42	6	
41	31	1	Total	C	O	0
			48	42	6	
41	31	1	Total	C	O	0
			48	42	6	
41	31	1	Total	C	O	0
			48	42	6	
41	31	1	Total	C	O	0
			48	42	6	
41	31	1	Total	C	O	0
			48	42	6	
41	31	1	Total	C	O	0
			48	42	6	
41	32	1	Total	C	O	0
			48	42	6	
41	32	1	Total	C	O	0
			48	42	6	
41	32	1	Total	C	O	0
			48	42	6	
41	32	1	Total	C	O	0
			48	42	6	
41	32	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
41	32	1	Total	C	O	0
			48	42	6	
41	32	1	Total	C	O	0
			48	42	6	
41	33	1	Total	C	O	0
			48	42	6	
41	33	1	Total	C	O	0
			48	42	6	
41	33	1	Total	C	O	0
			48	42	6	
41	33	1	Total	C	O	0
			48	42	6	
41	33	1	Total	C	O	0
			48	42	6	
41	33	1	Total	C	O	0
			48	42	6	
41	34	1	Total	C	O	0
			48	42	6	
41	34	1	Total	C	O	0
			48	42	6	
41	34	1	Total	C	O	0
			48	42	6	
41	34	1	Total	C	O	0
			48	42	6	
41	35	1	Total	C	O	0
			48	42	6	
41	35	1	Total	C	O	0
			48	42	6	
41	35	1	Total	C	O	0
			48	42	6	
41	35	1	Total	C	O	0
			48	42	6	
41	35	1	Total	C	O	0
			48	42	6	
41	35	1	Total	C	O	0
			48	42	6	
41	36	1	Total	C	O	0
			48	42	6	

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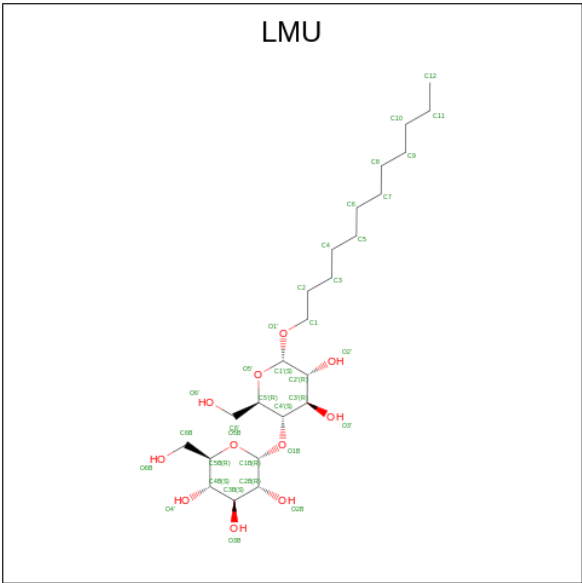
Mol	Chain	Residues	Atoms			AltConf
41	36	1	Total	C	O	0
			48	42	6	
41	36	1	Total	C	O	0
			48	42	6	
41	36	1	Total	C	O	0
			48	42	6	
41	37	1	Total	C	O	0
			48	42	6	
41	37	1	Total	C	O	0
			48	42	6	
41	37	1	Total	C	O	0
			48	42	6	
41	37	1	Total	C	O	0
			48	42	6	
41	37	1	Total	C	O	0
			48	42	6	
41	37	1	Total	C	O	0
			48	42	6	
41	38	1	Total	C	O	0
			48	42	6	
41	38	1	Total	C	O	0
			48	42	6	
41	38	1	Total	C	O	0
			48	42	6	
41	38	1	Total	C	O	0
			48	42	6	
41	39	1	Total	C	O	0
			48	42	6	
41	39	1	Total	C	O	0
			48	42	6	
41	39	1	Total	C	O	0
			48	42	6	
41	40	1	Total	C	O	0
			48	42	6	
41	40	1	Total	C	O	0
			48	42	6	
41	40	1	Total	C	O	0
			48	42	6	
41	40	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
41	40	1	Total	C	O	0
			48	42	6	
41	41	1	Total	C	O	0
			48	42	6	
41	41	1	Total	C	O	0
			48	42	6	
41	41	1	Total	C	O	0
			48	42	6	
41	41	1	Total	C	O	0
			48	42	6	
41	41	1	Total	C	O	0
			48	42	6	

- Molecule 42 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



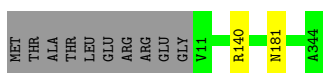
Mol	Chain	Residues	Atoms			AltConf
42	12	1	Total	C	O	0
			32	21	11	
42	32	1	Total	C	O	0
			32	21	11	

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. 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. 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.

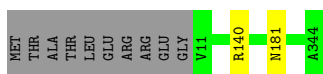
- Molecule 1: Photosystem II reaction center protein D1

Chain A:  97%



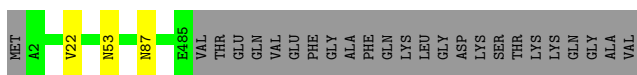
- Molecule 1: Photosystem II reaction center protein D1

Chain a:  97%



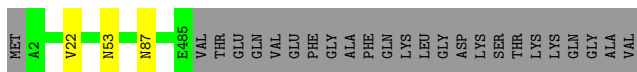
- Molecule 2: Photosystem II chlorophyll protein CP47

Chain B:  94% 5%



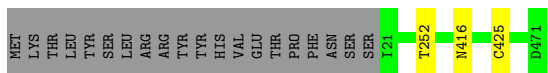
- Molecule 2: Photosystem II chlorophyll protein CP47

Chain b:  94% 5%



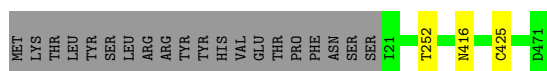
- Molecule 3: Photosystem II chlorophyll protein CP43

Chain C:  95%



- Molecule 3: Photosystem II chlorophyll protein CP43

Chain c:  95%



- Molecule 4: Photosystem II reaction center protein D2

Chain D: 95%



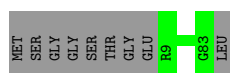
- Molecule 4: Photosystem II reaction center protein D2

Chain d: 96%



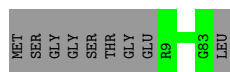
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 89%



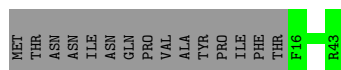
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 89%



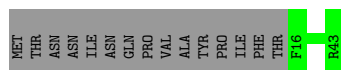
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 65%



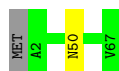
- Molecule 6: Cytochrome b559 subunit beta

Chain f: 65%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 97%



- Molecule 7: Photosystem II reaction center protein H

Chain h: 97%



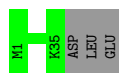
- Molecule 8: Photosystem II reaction center protein I

Chain I: 92%



- Molecule 8: Photosystem II reaction center protein I

Chain i: 92%



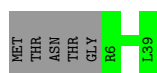
- Molecule 9: Photosystem II reaction center protein J

Chain J: 87%



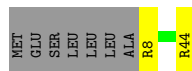
- Molecule 9: Photosystem II reaction center protein J

Chain j: 87%



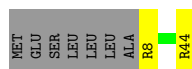
- Molecule 10: Photosystem II reaction center protein K

Chain K: 80%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 80%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 100%

There are no outlier residues recorded for this chain.

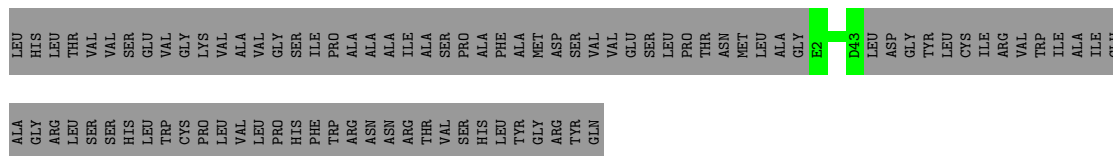
- Molecule 11: Photosystem II reaction center protein L

Chain l: 100%

There are no outlier residues recorded for this chain.

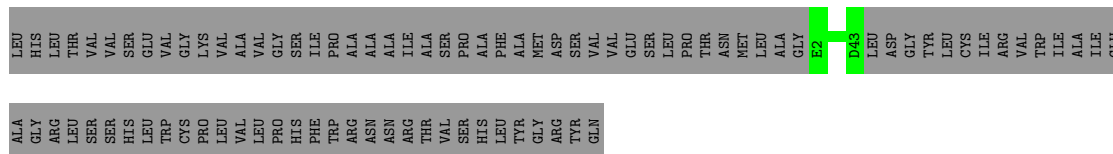
- Molecule 12: Photosystem II reaction center protein M

Chain M: 32% 68%



- Molecule 12: Photosystem II reaction center protein M

Chain m: 32% 68%



- Molecule 13: Extrinsic protein in photosystem II

Chain O: 98% ..



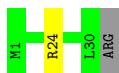
- Molecule 13: Extrinsic protein in photosystem II

Chain o: 98% ..



- Molecule 14: Photosystem II reaction center protein T

Chain T:  94% . .



- Molecule 14: Photosystem II reaction center protein T

Chain t:  94% . .



- Molecule 15: Extrinsic protein in photosystem II

Chain U:  100%

There are no outlier residues recorded for this chain.

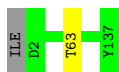
- Molecule 15: Extrinsic protein in photosystem II

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: Cytochrome c-550

Chain V:  99% ..



- Molecule 16: Cytochrome c-550

Chain v:  99% ..



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: Photosystem II reaction center X protein

Chain X:  97% .



- Molecule 18: Photosystem II reaction center X protein

Chain x:  97% .



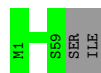
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  97% .




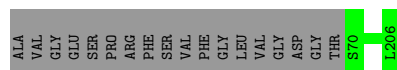
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  97% .




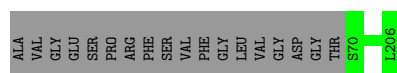
- Molecule 20: Extrinsic protein in photosystem II

Chain Q:  88% 12%



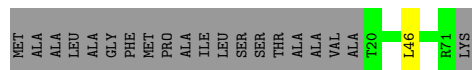
- Molecule 20: Extrinsic protein in photosystem II

Chain q:  88% 12%



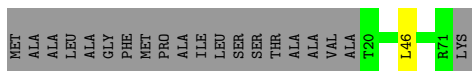
- Molecule 21: Photosystem II reaction center protein W

Chain W:  71% 28%



- Molecule 21: Photosystem II reaction center protein W

Chain w:  71% 28%



- Molecule 22: Unknown protein 0

Chain 0:  100%

There are no outlier residues recorded for this chain.

- Molecule 22: Unknown protein 0

Chain 5:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: Unknown protein 1

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: Unknown protein 1

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: Unknown protein 2

Chain 2:  100%


There are no outlier residues recorded for this chain.

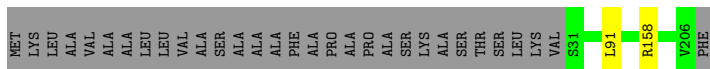
- Molecule 24: Unknown protein 2

Chain 7:  100%


There are no outlier residues recorded for this chain.

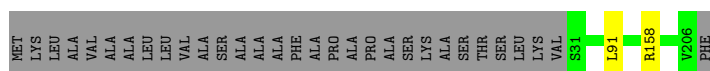
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 11:  84% 15%



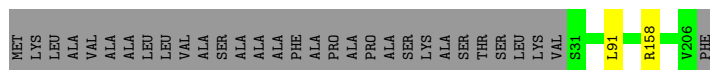
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 12:  84% 15%



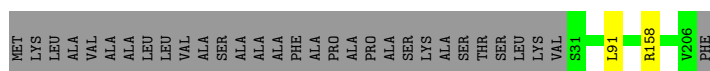
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 13: 84% 15%



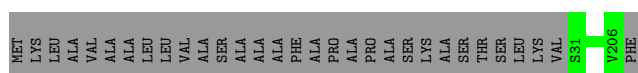
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 14: 84% 15%



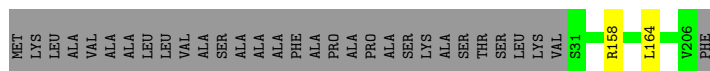
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 15: 85% 15%



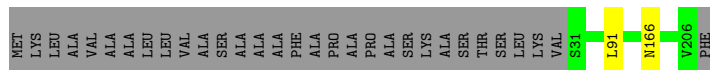
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 16: 84% 15%



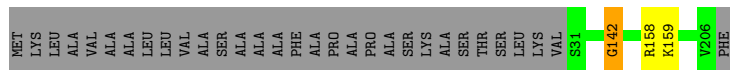
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 17: 84% 15%



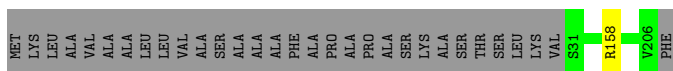
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 18: 84% 15%



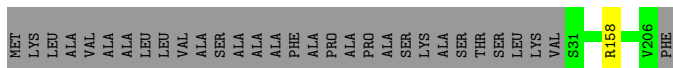
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 31: 85% 15%



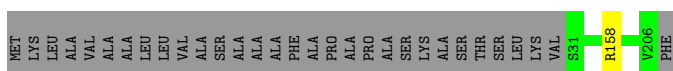
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 32: 85% 15%



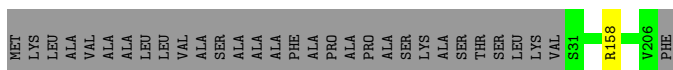
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 33: 85% 15%



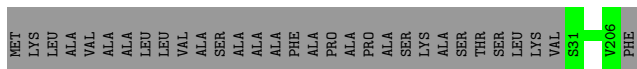
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 34: 85% 15%



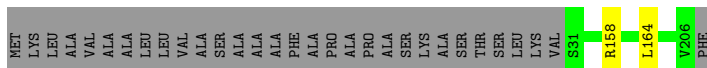
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 35: 85% 15%



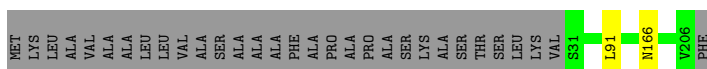
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 36: 84% 15%



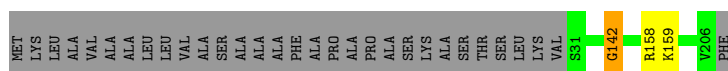
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 37: 84% 15%



- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 38: 84% 15%



- Molecule 26: Fucoxanthin chlorophyll a/c-binding protein monomer 1

Chain 19: 98%



- Molecule 26: Fucoxanthin chlorophyll a/c-binding protein monomer 1

Chain 39: 98%



- Molecule 27: Fucoxanthin chlorophyll a/c-binding protein monomer 2

Chain 20: 98%



- Molecule 27: Fucoxanthin chlorophyll a/c-binding protein monomer 2

Chain 40: 98%



- Molecule 28: Fucoxanthin chlorophyll a/c-binding protein monomer 3

Chain 21: 100%

There are no outlier residues recorded for this chain.

- Molecule 28: Fucoxanthin chlorophyll a/c-binding protein monomer 3

Chain 41: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	98936	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OEX, LHG, FE2, LMU, BCR, LMG, CLA, PHO, A86, SQD, BCT, HEM, PL9, DGD

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	0.58	0/2701	0.60	0/3682
1	a	0.58	0/2701	0.60	0/3682
2	B	0.58	1/3942 (0.0%)	0.57	0/5362
2	b	0.58	1/3942 (0.0%)	0.57	0/5362
3	C	0.58	1/3620 (0.0%)	0.60	1/4933 (0.0%)
3	c	0.58	1/3620 (0.0%)	0.60	1/4933 (0.0%)
4	D	0.58	1/2789 (0.0%)	0.60	0/3803
4	d	0.58	0/2789	0.60	0/3803
5	E	0.44	0/634	0.53	0/864
5	e	0.44	0/634	0.53	0/864
6	F	0.46	0/235	0.70	0/316
6	f	0.45	0/235	0.70	0/316
7	H	0.49	0/523	0.61	0/714
7	h	0.49	0/523	0.61	0/714
8	I	0.62	0/294	0.70	0/397
8	i	0.63	0/294	0.70	0/397
9	J	0.43	0/260	0.59	0/351
9	j	0.43	0/260	0.59	0/351
10	K	0.57	0/313	0.69	0/429
10	k	0.57	0/313	0.68	0/429
11	L	0.61	0/319	0.55	0/433
11	l	0.61	0/319	0.55	0/433
12	M	0.47	0/321	0.61	0/433
12	m	0.47	0/321	0.61	0/433
13	O	0.42	0/1875	0.58	0/2528
13	o	0.41	0/1875	0.58	0/2528
14	T	0.45	0/256	0.52	0/346
14	t	0.45	0/256	0.52	0/346
15	U	0.40	0/728	0.58	0/989
15	u	0.41	0/728	0.58	0/989
16	V	0.42	0/1056	0.56	0/1435
16	v	0.42	0/1056	0.56	0/1435

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.32	0/252	0.52	0/341
17	y	0.32	0/252	0.52	0/341
18	X	0.31	0/263	0.54	0/355
18	x	0.31	0/263	0.54	0/355
19	Z	0.41	0/456	0.58	0/624
19	z	0.41	0/456	0.58	0/624
20	Q	0.39	0/1099	0.56	0/1482
20	q	0.39	0/1099	0.56	0/1482
21	W	0.53	0/434	0.67	1/590 (0.2%)
21	w	0.53	0/434	0.67	1/590 (0.2%)
25	11	0.43	0/1373	0.55	1/1861 (0.1%)
25	12	0.43	0/1373	0.55	1/1861 (0.1%)
25	13	0.43	0/1373	0.55	1/1861 (0.1%)
25	14	0.43	0/1373	0.55	1/1861 (0.1%)
25	15	0.33	0/1373	0.52	0/1861
25	16	0.42	0/1373	0.64	1/1861 (0.1%)
25	17	0.41	0/1373	0.58	1/1861 (0.1%)
25	18	0.35	0/1373	0.54	0/1861
25	31	0.46	0/1373	0.56	0/1861
25	32	0.46	0/1373	0.56	0/1861
25	33	0.46	0/1373	0.56	0/1861
25	34	0.46	0/1373	0.56	0/1861
25	35	0.33	0/1373	0.52	0/1861
25	36	0.42	0/1373	0.64	1/1861 (0.1%)
25	37	0.41	0/1373	0.58	1/1861 (0.1%)
25	38	0.35	0/1373	0.54	0/1861
All	All	0.49	5/66708 (0.0%)	0.58	12/90590 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	a	0	1
16	V	0	1
16	v	0	1
25	18	0	1
25	38	0	1
26	19	0	4
26	39	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	20	0	3
27	40	0	3
All	All	0	20

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	22	VAL	CB-CG1	-7.25	1.37	1.52
2	B	22	VAL	CB-CG1	-7.19	1.37	1.52
3	c	425	CYS	CB-SG	-5.08	1.73	1.81
4	D	314	TYR	CD1-CE1	-5.05	1.31	1.39
3	C	425	CYS	CB-SG	-5.01	1.73	1.81

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	252	THR	C-N-CA	6.18	137.15	121.70
3	c	252	THR	C-N-CA	6.15	137.08	121.70
21	W	46	LEU	CB-CG-CD1	-5.34	101.92	111.00
21	w	46	LEU	CB-CG-CD1	-5.34	101.93	111.00
25	16	164	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	18	142	GLY	Peptide
1	A	140	ARG	Peptide
16	V	63	THR	Peptide
1	a	140	ARG	Peptide
16	v	63	THR	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	321 (97%)	11 (3%)	0	100	100
1	a	332/344 (96%)	322 (97%)	10 (3%)	0	100	100
2	B	482/509 (95%)	467 (97%)	15 (3%)	0	100	100
2	b	482/509 (95%)	466 (97%)	16 (3%)	0	100	100
3	C	449/471 (95%)	429 (96%)	20 (4%)	0	100	100
3	c	449/471 (95%)	429 (96%)	20 (4%)	0	100	100
4	D	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
4	d	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
5	E	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
5	e	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
6	F	26/43 (60%)	26 (100%)	0	0	100	100
6	f	26/43 (60%)	26 (100%)	0	0	100	100
7	H	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
7	h	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	32/39 (82%)	32 (100%)	0	0	100	100
9	j	32/39 (82%)	32 (100%)	0	0	100	100
10	K	35/44 (80%)	35 (100%)	0	0	100	100
10	k	35/44 (80%)	35 (100%)	0	0	100	100
11	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	M	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
12	m	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
13	O	243/248 (98%)	231 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	243/248 (98%)	231 (95%)	12 (5%)	0	100	100
14	T	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
14	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
15	U	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
15	u	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
16	V	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
16	v	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
17	Y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
17	y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
18	X	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
18	x	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
19	Z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
19	z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
20	Q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
20	q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
21	W	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
21	w	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
25	11	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	12	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	13	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	14	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	15	174/207 (84%)	163 (94%)	11 (6%)	0	100	100
25	16	174/207 (84%)	159 (91%)	15 (9%)	0	100	100
25	17	174/207 (84%)	162 (93%)	12 (7%)	0	100	100
25	18	174/207 (84%)	165 (95%)	8 (5%)	1 (1%)	22	55
25	31	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	32	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	33	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	34	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	35	174/207 (84%)	163 (94%)	11 (6%)	0	100	100
25	36	174/207 (84%)	159 (91%)	15 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	37	174/207 (84%)	162 (93%)	12 (7%)	0	100	100
25	38	174/207 (84%)	165 (95%)	8 (5%)	1 (1%)	22	55
All	All	8276/9368 (88%)	7903 (96%)	371 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	18	142	GLY
25	38	142	GLY

5.3.2 Protein sidechains ⓘ

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	272/280 (97%)	271 (100%)	1 (0%)	89	91
1	a	272/280 (97%)	271 (100%)	1 (0%)	89	91
2	B	385/405 (95%)	383 (100%)	2 (0%)	86	90
2	b	385/405 (95%)	383 (100%)	2 (0%)	86	90
3	C	356/376 (95%)	355 (100%)	1 (0%)	91	92
3	c	356/376 (95%)	355 (100%)	1 (0%)	91	92
4	D	273/281 (97%)	268 (98%)	5 (2%)	54	71
4	d	273/281 (97%)	268 (98%)	5 (2%)	54	71
5	E	69/75 (92%)	69 (100%)	0	100	100
5	e	69/75 (92%)	69 (100%)	0	100	100
6	F	22/36 (61%)	22 (100%)	0	100	100
6	f	22/36 (61%)	22 (100%)	0	100	100
7	H	55/56 (98%)	54 (98%)	1 (2%)	54	71
7	h	55/56 (98%)	54 (98%)	1 (2%)	54	71
8	I	34/37 (92%)	34 (100%)	0	100	100
8	i	34/37 (92%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	27/31 (87%)	27 (100%)	0	100	100
9	j	27/31 (87%)	27 (100%)	0	100	100
10	K	32/38 (84%)	30 (94%)	2 (6%)	15	40
10	k	32/38 (84%)	30 (94%)	2 (6%)	15	40
11	L	34/34 (100%)	34 (100%)	0	100	100
11	l	34/34 (100%)	34 (100%)	0	100	100
12	M	31/104 (30%)	31 (100%)	0	100	100
12	m	31/104 (30%)	31 (100%)	0	100	100
13	O	196/201 (98%)	194 (99%)	2 (1%)	73	80
13	o	196/201 (98%)	194 (99%)	2 (1%)	73	80
14	T	27/28 (96%)	26 (96%)	1 (4%)	29	53
14	t	27/28 (96%)	26 (96%)	1 (4%)	29	53
15	U	77/77 (100%)	77 (100%)	0	100	100
15	u	77/77 (100%)	77 (100%)	0	100	100
16	V	114/115 (99%)	114 (100%)	0	100	100
16	v	114/115 (99%)	114 (100%)	0	100	100
17	Y	27/27 (100%)	27 (100%)	0	100	100
17	y	27/27 (100%)	27 (100%)	0	100	100
18	X	29/30 (97%)	29 (100%)	0	100	100
18	x	29/30 (97%)	29 (100%)	0	100	100
19	Z	48/50 (96%)	48 (100%)	0	100	100
19	z	48/50 (96%)	48 (100%)	0	100	100
20	Q	111/124 (90%)	111 (100%)	0	100	100
20	q	111/124 (90%)	111 (100%)	0	100	100
21	W	43/55 (78%)	43 (100%)	0	100	100
21	w	43/55 (78%)	43 (100%)	0	100	100
25	11	138/158 (87%)	137 (99%)	1 (1%)	81	86
25	12	138/158 (87%)	137 (99%)	1 (1%)	81	86
25	13	138/158 (87%)	137 (99%)	1 (1%)	81	86
25	14	138/158 (87%)	137 (99%)	1 (1%)	81	86
25	15	138/158 (87%)	138 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	16	138/158 (87%)	137 (99%)	1 (1%)	81	86
25	17	138/158 (87%)	137 (99%)	1 (1%)	81	86
25	18	138/158 (87%)	136 (99%)	2 (1%)	62	75
25	31	138/158 (87%)	137 (99%)	1 (1%)	81	86
25	32	138/158 (87%)	137 (99%)	1 (1%)	81	86
25	33	138/158 (87%)	137 (99%)	1 (1%)	81	86
25	34	138/158 (87%)	137 (99%)	1 (1%)	81	86
25	35	138/158 (87%)	138 (100%)	0	100	100
25	36	138/158 (87%)	137 (99%)	1 (1%)	81	86
25	37	138/158 (87%)	137 (99%)	1 (1%)	81	86
25	38	138/158 (87%)	136 (99%)	2 (1%)	62	75
All	All	6732/7448 (90%)	6686 (99%)	46 (1%)	80	86

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	168	MET
25	17	166	ASN
14	t	24	ARG
25	13	158	ARG
25	18	159	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
25	18	96	ASN
25	36	96	ASN
25	31	161	ASN
25	33	177	ASN
25	37	161	ASN

5.3.3 RNA ⓘ

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](#)

Of 488 ligands modelled in this entry, 2 are monoatomic - leaving 486 for Mogul analysis.

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	$\# Z > 2$
41	A86	13	311	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	11	309	-	45,53,73	1.74	8 (17%)	52,89,113	1.65	7 (13%)
30	CLA	C	521	-	65,73,73	1.42	9 (13%)	76,113,113	1.69	11 (14%)
41	A86	40	201	-	44,50,50	3.93	22 (50%)	51,76,76	7.88	19 (37%)
41	A86	33	317	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	18 (35%)
30	CLA	20	202	-	65,73,73	1.43	7 (10%)	76,113,113	1.44	8 (10%)
41	A86	32	315	-	44,50,50	3.98	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	18	306	25	45,53,73	1.75	7 (15%)	52,89,113	1.85	8 (15%)
41	A86	17	312	-	44,50,50	3.98	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	32	310	25	45,53,73	1.75	9 (20%)	52,89,113	1.84	9 (17%)
33	SQD	b	620	-	36,37,54	1.20	7 (19%)	45,48,65	1.64	9 (20%)
30	CLA	c	512	3	65,73,73	1.51	10 (15%)	76,113,113	1.60	12 (15%)
30	CLA	39	303	-	65,73,73	1.45	10 (15%)	76,113,113	1.55	9 (11%)
32	BCR	c	516	-	41,41,41	1.31	5 (12%)	56,56,56	1.40	7 (12%)
41	A86	15	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.93	18 (35%)
30	CLA	32	307	-	65,73,73	1.41	11 (16%)	76,113,113	1.60	10 (13%)
30	CLA	38	305	-	65,73,73	1.45	9 (13%)	76,113,113	1.49	7 (9%)
30	CLA	37	309	25	45,53,73	1.79	10 (22%)	52,89,113	2.10	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	18	304	-	45,53,73	1.71	8 (17%)	52,89,113	1.82	8 (15%)
30	CLA	14	310	-	45,53,73	1.75	9 (20%)	52,89,113	1.67	8 (15%)
30	CLA	36	307	25	45,53,73	1.76	10 (22%)	52,89,113	1.95	7 (13%)
30	CLA	40	202	-	65,73,73	1.43	7 (10%)	76,113,113	1.45	8 (10%)
30	CLA	13	310	-	45,53,73	1.75	9 (20%)	52,89,113	1.66	7 (13%)
41	A86	18	313	-	44,50,50	3.93	23 (52%)	51,76,76	8.34	17 (33%)
30	CLA	17	310	-	45,53,73	1.75	8 (17%)	52,89,113	1.68	9 (17%)
30	CLA	16	308	25	45,53,73	1.78	9 (20%)	52,89,113	1.72	11 (21%)
30	CLA	B	613	-	65,73,73	1.43	11 (16%)	76,113,113	1.61	10 (13%)
41	A86	15	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
41	A86	21	314	-	44,50,50	4.01	23 (52%)	51,76,76	7.82	18 (35%)
41	A86	38	315	-	44,50,50	4.03	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	11	303	-	65,73,73	1.41	10 (15%)	76,113,113	1.59	10 (13%)
30	CLA	36	309	-	45,53,73	1.76	10 (22%)	52,89,113	1.61	9 (17%)
41	A86	41	314	-	44,50,50	4.00	23 (52%)	51,76,76	7.82	18 (35%)
30	CLA	15	301	25	65,73,73	1.48	9 (13%)	76,113,113	1.57	10 (13%)
30	CLA	37	308	25	65,73,73	1.47	10 (15%)	76,113,113	1.52	11 (14%)
30	CLA	19	304	26	45,53,73	1.71	8 (17%)	52,89,113	1.82	11 (21%)
30	CLA	C	511	-	65,73,73	1.45	12 (18%)	76,113,113	1.57	11 (14%)
30	CLA	36	303	-	45,53,73	1.68	8 (17%)	52,89,113	2.02	11 (21%)
41	A86	35	316	-	44,50,50	3.99	23 (52%)	51,76,76	7.59	20 (39%)
41	A86	37	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	18 (35%)
30	CLA	41	301	28	65,73,73	1.48	8 (12%)	76,113,113	1.43	7 (9%)
30	CLA	B	608	-	65,73,73	1.50	10 (15%)	76,113,113	1.46	8 (10%)
42	LMU	32	302	-	33,33,36	1.28	3 (9%)	44,44,47	1.57	8 (18%)
30	CLA	20	209	30	65,73,73	1.47	8 (12%)	76,113,113	1.44	9 (11%)
41	A86	41	311	-	44,50,50	3.89	23 (52%)	51,76,76	7.51	15 (29%)
41	A86	41	313	-	44,50,50	3.90	23 (52%)	51,76,76	7.52	22 (43%)
30	CLA	39	301	-	65,73,73	1.49	10 (15%)	76,113,113	1.50	11 (14%)
30	CLA	19	306	-	45,53,73	1.72	11 (24%)	52,89,113	1.63	7 (13%)
30	CLA	C	513	-	65,73,73	1.45	9 (13%)	76,113,113	1.47	8 (10%)
30	CLA	14	305	25	45,53,73	1.70	8 (17%)	52,89,113	2.06	11 (21%)
41	A86	31	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
36	LMG	D	408	-	51,51,55	0.90	3 (5%)	59,59,63	1.42	7 (11%)
32	BCR	f	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.32	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	13	305	25	45,53,73	1.72	8 (17%)	52,89,113	2.02	11 (21%)
36	LMG	m	102	30	40,40,55	0.95	3 (7%)	48,48,63	1.34	7 (14%)
41	A86	31	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
38	DGD	C	516	-	63,63,67	1.06	7 (11%)	77,77,81	1.60	15 (19%)
41	A86	13	313	-	44,50,50	4.05	24 (54%)	51,76,76	7.81	19 (37%)
30	CLA	12	307	-	65,73,73	1.43	10 (15%)	76,113,113	1.59	10 (13%)
30	CLA	39	306	-	45,53,73	1.71	11 (24%)	52,89,113	1.61	7 (13%)
30	CLA	c	513	-	65,73,73	1.45	9 (13%)	76,113,113	1.47	8 (10%)
30	CLA	15	302	-	45,53,73	1.72	8 (17%)	52,89,113	1.88	8 (15%)
30	CLA	33	307	-	45,53,73	1.70	9 (20%)	52,89,113	1.73	7 (13%)
30	CLA	41	303	-	65,73,73	1.43	7 (10%)	76,113,113	1.42	7 (9%)
30	CLA	14	302	25	65,73,73	1.44	8 (12%)	76,113,113	1.68	9 (11%)
41	A86	37	312	-	44,50,50	3.98	23 (52%)	51,76,76	7.96	18 (35%)
36	LMG	c	519	-	51,51,55	0.97	5 (9%)	59,59,63	1.46	9 (15%)
30	CLA	37	301	-	65,73,73	1.44	10 (15%)	76,113,113	1.48	10 (13%)
30	CLA	B	606	-	65,73,73	1.59	12 (18%)	76,113,113	1.61	13 (17%)
32	BCR	Z	101	-	41,41,41	1.31	3 (7%)	56,56,56	1.41	8 (14%)
30	CLA	38	301	-	65,73,73	1.47	11 (16%)	76,113,113	1.44	11 (14%)
30	CLA	C	508	-	65,73,73	1.43	12 (18%)	76,113,113	1.68	12 (15%)
30	CLA	21	307	-	65,73,73	1.44	6 (9%)	76,113,113	1.41	7 (9%)
30	CLA	35	307	25	65,73,73	1.47	10 (15%)	76,113,113	1.63	11 (14%)
30	CLA	C	505	-	65,73,73	1.44	12 (18%)	76,113,113	1.67	11 (14%)
30	CLA	33	301	-	65,73,73	1.46	9 (13%)	76,113,113	1.50	8 (10%)
30	CLA	D	401	-	65,73,73	1.50	12 (18%)	76,113,113	1.53	10 (13%)
32	BCR	C	518	-	41,41,41	1.28	2 (4%)	56,56,56	1.36	6 (10%)
41	A86	13	316	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
38	DGD	H	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.41	8 (10%)
30	CLA	37	310	-	45,53,73	1.74	9 (20%)	52,89,113	1.68	8 (15%)
30	CLA	16	306	25	45,53,73	1.73	9 (20%)	52,89,113	1.77	8 (15%)
41	A86	21	310	-	44,50,50	3.88	22 (50%)	51,76,76	7.41	21 (41%)
30	CLA	d	401	-	65,73,73	1.49	12 (18%)	76,113,113	1.52	9 (11%)
41	A86	17	311	-	44,50,50	4.03	22 (50%)	51,76,76	8.33	19 (37%)
30	CLA	17	308	25	65,73,73	1.48	10 (15%)	76,113,113	1.53	11 (14%)
30	CLA	34	305	25	45,53,73	1.72	9 (20%)	52,89,113	2.07	14 (26%)
30	CLA	41	307	-	65,73,73	1.44	6 (9%)	76,113,113	1.40	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	BCR	A	405	-	41,41,41	1.28	2 (4%)	56,56,56	1.40	6 (10%)
42	LMU	12	302	30	33,33,36	1.30	3 (9%)	44,44,47	1.54	7 (15%)
36	LMG	12	301	30	39,39,55	1.00	4 (10%)	47,47,63	1.21	4 (8%)
30	CLA	C	509	-	65,73,73	1.48	11 (16%)	76,113,113	1.65	9 (11%)
30	CLA	31	307	25	65,73,73	1.47	10 (15%)	76,113,113	1.56	10 (13%)
41	A86	37	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	b	603	-	65,73,73	1.44	11 (16%)	76,113,113	1.64	12 (15%)
30	CLA	16	303	-	45,53,73	1.69	8 (17%)	52,89,113	2.02	11 (21%)
30	CLA	18	303	25	65,73,73	1.47	10 (15%)	76,113,113	1.47	8 (10%)
30	CLA	31	309	-	45,53,73	1.72	8 (17%)	52,89,113	1.67	7 (13%)
41	A86	31	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	c	509	-	65,73,73	1.48	11 (16%)	76,113,113	1.64	9 (11%)
34	BCT	A	407	29,1	2,3,3	1.26	0	2,3,3	3.93	2 (100%)
41	A86	21	313	-	44,50,50	3.90	23 (52%)	51,76,76	7.51	22 (43%)
30	CLA	16	304	-	65,73,73	1.42	10 (15%)	76,113,113	1.48	8 (10%)
41	A86	21	312	-	44,50,50	3.82	22 (50%)	51,76,76	7.17	21 (41%)
41	A86	35	312	-	44,50,50	4.04	24 (54%)	51,76,76	7.81	20 (39%)
30	CLA	12	306	42	45,53,73	1.69	11 (24%)	52,89,113	1.79	9 (17%)
30	CLA	13	302	25	65,73,73	1.46	10 (15%)	76,113,113	1.68	8 (10%)
38	DGD	j	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
30	CLA	17	305	-	65,73,73	1.42	10 (15%)	76,113,113	1.53	9 (11%)
30	CLA	c	505	-	65,73,73	1.44	12 (18%)	76,113,113	1.68	11 (14%)
30	CLA	32	311	25	65,73,73	1.49	10 (15%)	76,113,113	1.56	10 (13%)
32	BCR	F	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
30	CLA	B	602	-	65,73,73	1.48	10 (15%)	76,113,113	1.55	11 (14%)
30	CLA	19	307	-	45,53,73	1.69	8 (17%)	52,89,113	1.79	7 (13%)
30	CLA	D	402	-	65,73,73	1.43	10 (15%)	76,113,113	1.49	8 (10%)
37	OEX	c	501	1,3	0,15,15	-	-	-	-	-
30	CLA	40	206	27	45,53,73	1.71	9 (20%)	52,89,113	1.78	10 (19%)
32	BCR	m	103	-	41,41,41	1.30	2 (4%)	56,56,56	1.39	8 (14%)
30	CLA	11	304	25	45,53,73	1.72	8 (17%)	52,89,113	2.03	11 (21%)
41	A86	41	312	-	44,50,50	3.82	21 (47%)	51,76,76	7.17	21 (41%)
30	CLA	19	302	-	45,53,73	1.65	9 (20%)	52,89,113	1.89	10 (19%)
30	CLA	b	601	-	65,73,73	1.44	11 (16%)	76,113,113	1.50	8 (10%)
36	LMG	B	619	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	11	306	25	45,53,73	1.76	8 (17%)	52,89,113	1.82	7 (13%)
30	CLA	20	207	-	45,53,73	1.73	9 (20%)	52,89,113	1.73	10 (19%)
30	CLA	35	305	-	45,53,73	1.76	6 (13%)	52,89,113	1.67	6 (11%)
32	BCR	c	520	-	41,41,41	1.28	3 (7%)	56,56,56	1.46	10 (17%)
41	A86	14	311	-	44,50,50	3.93	23 (52%)	51,76,76	8.32	17 (33%)
33	SQD	l	101	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
30	CLA	b	606	-	65,73,73	1.58	12 (18%)	76,113,113	1.61	13 (17%)
41	A86	18	315	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	b	605	-	65,73,73	1.48	10 (15%)	76,113,113	1.50	9 (11%)
35	LHG	L	101	-	48,48,48	0.81	1 (2%)	51,54,54	1.26	5 (9%)
30	CLA	C	504	-	65,73,73	1.48	11 (16%)	76,113,113	1.53	10 (13%)
41	A86	15	312	-	44,50,50	4.05	24 (54%)	51,76,76	7.82	19 (37%)
35	LHG	b	621	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	6 (11%)
30	CLA	38	307	-	45,53,73	1.76	7 (15%)	52,89,113	1.63	8 (15%)
40	HEM	V	201	16	41,50,50	1.61	5 (12%)	45,82,82	1.28	4 (8%)
30	CLA	c	504	-	65,73,73	1.47	11 (16%)	76,113,113	1.51	10 (13%)
30	CLA	18	301	-	65,73,73	1.47	11 (16%)	76,113,113	1.45	11 (14%)
30	CLA	36	306	25	45,53,73	1.74	9 (20%)	52,89,113	1.78	8 (15%)
38	DGD	C	517	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	16 (20%)
30	CLA	40	207	-	45,53,73	1.73	9 (20%)	52,89,113	1.74	10 (19%)
41	A86	33	312	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	a	402	-	65,73,73	1.45	8 (12%)	76,113,113	1.60	8 (10%)
30	CLA	13	308	25	65,73,73	1.46	10 (15%)	76,113,113	1.55	10 (13%)
36	LMG	w	101	-	51,51,55	0.89	3 (5%)	59,59,63	1.40	7 (11%)
30	CLA	33	306	25	45,53,73	1.72	9 (20%)	52,89,113	2.09	12 (23%)
41	A86	32	304	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	21 (41%)
32	BCR	Y	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.47	9 (16%)
41	A86	19	309	-	44,50,50	3.89	23 (52%)	51,76,76	7.70	16 (31%)
30	CLA	C	503	-	65,73,73	1.52	12 (18%)	76,113,113	1.53	12 (15%)
30	CLA	A	402	-	65,73,73	1.45	8 (12%)	76,113,113	1.62	9 (11%)
41	A86	37	313	-	44,50,50	4.05	23 (52%)	51,76,76	7.81	19 (37%)
30	CLA	C	520	-	65,73,73	1.41	11 (16%)	76,113,113	1.49	8 (10%)
30	CLA	31	303	-	65,73,73	1.40	11 (16%)	76,113,113	1.58	10 (13%)
30	CLA	21	306	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	9 (11%)
38	DGD	c	517	-	63,63,67	1.06	8 (12%)	77,77,81	1.60	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	b	608	-	65,73,73	1.50	10 (15%)	76,113,113	1.47	8 (10%)
30	CLA	37	307	25	45,53,73	1.80	9 (20%)	52,89,113	1.77	13 (25%)
30	CLA	d	406	-	65,73,73	1.48	9 (13%)	76,113,113	1.61	10 (13%)
30	CLA	36	308	25	45,53,73	1.78	9 (20%)	52,89,113	1.72	11 (21%)
41	A86	18	314	-	44,50,50	3.98	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	37	303	25	65,73,73	1.49	10 (15%)	76,113,113	1.58	8 (10%)
41	A86	14	312	-	44,50,50	3.97	23 (52%)	51,76,76	7.96	18 (35%)
32	BCR	h	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.32	7 (12%)
30	CLA	b	622	-	65,73,73	1.47	9 (13%)	76,113,113	1.59	14 (18%)
30	CLA	31	301	25	65,73,73	1.46	10 (15%)	76,113,113	1.67	8 (10%)
30	CLA	14	307	25	45,53,73	1.75	8 (17%)	52,89,113	1.81	8 (15%)
30	CLA	17	301	-	65,73,73	1.44	9 (13%)	76,113,113	1.48	10 (13%)
30	CLA	C	507	-	65,73,73	1.52	11 (16%)	76,113,113	1.55	11 (14%)
30	CLA	21	309	-	45,53,73	1.82	7 (15%)	52,89,113	1.72	11 (21%)
31	PHO	d	403	-	51,69,69	1.23	8 (15%)	47,99,99	1.31	8 (17%)
41	A86	13	312	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
41	A86	12	316	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	13	307	25	45,53,73	1.75	7 (15%)	52,89,113	1.82	7 (13%)
30	CLA	B	611	-	65,73,73	1.51	12 (18%)	76,113,113	1.58	11 (14%)
41	A86	37	315	-	44,50,50	4.06	23 (52%)	51,76,76	8.44	16 (31%)
35	LHG	L	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
30	CLA	16	302	25	65,73,73	1.48	9 (13%)	76,113,113	1.86	16 (21%)
41	A86	33	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
39	PL9	D	404	4	55,55,55	1.36	6 (10%)	68,69,69	1.49	14 (20%)
30	CLA	20	208	-	45,53,73	1.70	8 (17%)	52,89,113	1.78	9 (17%)
30	CLA	21	305	28	45,53,73	1.75	6 (13%)	52,89,113	1.79	8 (15%)
30	CLA	39	304	26	45,53,73	1.70	8 (17%)	52,89,113	1.82	11 (21%)
36	LMG	B	620	-	51,51,55	0.99	5 (9%)	59,59,63	1.44	8 (13%)
30	CLA	14	304	-	65,73,73	1.41	10 (15%)	76,113,113	1.60	10 (13%)
30	CLA	b	604	-	65,73,73	1.45	12 (18%)	76,113,113	1.69	15 (19%)
30	CLA	34	302	25	65,73,73	1.46	10 (15%)	76,113,113	1.68	8 (10%)
41	A86	35	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
38	DGD	J	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
30	CLA	c	503	-	65,73,73	1.52	12 (18%)	76,113,113	1.53	12 (15%)
30	CLA	B	612	-	65,73,73	1.50	9 (13%)	76,113,113	1.78	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	z	101	-	65,73,73	1.45	9 (13%)	76,113,113	1.49	8 (10%)
30	CLA	14	306	-	45,53,73	1.72	8 (17%)	52,89,113	1.69	7 (13%)
33	SQD	L	103	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
30	CLA	C	514	30	65,73,73	1.39	8 (12%)	76,113,113	1.63	9 (11%)
32	BCR	b	623	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
34	BCT	a	406	29,1	2,3,3	1.26	0	2,3,3	3.95	2 (100%)
30	CLA	15	307	25	65,73,73	1.47	10 (15%)	76,113,113	1.63	11 (14%)
41	A86	13	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	19	305	-	45,53,73	1.72	10 (22%)	52,89,113	1.69	6 (11%)
30	CLA	c	502	-	65,73,73	1.40	11 (16%)	76,113,113	1.65	11 (14%)
41	A86	12	318	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
41	A86	20	212	-	44,50,50	4.18	23 (52%)	51,76,76	8.23	15 (29%)
30	CLA	37	304	-	45,53,73	1.70	11 (24%)	52,89,113	1.82	9 (17%)
30	CLA	c	507	-	65,73,73	1.52	11 (16%)	76,113,113	1.55	11 (14%)
41	A86	35	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.93	18 (35%)
30	CLA	36	301	-	65,73,73	1.46	9 (13%)	76,113,113	1.43	8 (10%)
30	CLA	34	309	25	45,53,73	1.75	11 (24%)	52,89,113	1.77	9 (17%)
30	CLA	41	309	-	45,53,73	1.81	6 (13%)	52,89,113	1.72	11 (21%)
41	A86	38	313	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	C	506	-	65,73,73	1.46	11 (16%)	76,113,113	1.56	12 (15%)
30	CLA	12	314	-	45,53,73	1.74	9 (20%)	52,89,113	1.66	8 (15%)
30	CLA	17	309	25	45,53,73	1.79	10 (22%)	52,89,113	2.10	13 (25%)
30	CLA	37	306	25	45,53,73	1.71	7 (15%)	52,89,113	1.97	10 (19%)
30	CLA	B	610	-	65,73,73	1.50	11 (16%)	76,113,113	1.51	8 (10%)
41	A86	11	312	-	44,50,50	4.04	23 (52%)	51,76,76	7.83	20 (39%)
41	A86	15	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
36	LMG	M	102	30	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
40	HEM	e	101	6,5	41,50,50	1.49	5 (12%)	45,82,82	1.26	5 (11%)
30	CLA	c	508	-	65,73,73	1.43	12 (18%)	76,113,113	1.66	12 (15%)
30	CLA	C	519	-	65,73,73	1.46	11 (16%)	76,113,113	1.47	7 (9%)
30	CLA	14	308	25	65,73,73	1.47	10 (15%)	76,113,113	1.55	10 (13%)
30	CLA	c	523	-	65,73,73	1.42	9 (13%)	76,113,113	1.68	11 (14%)
41	A86	11	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
41	A86	20	213	-	44,50,50	4.01	23 (52%)	51,76,76	7.82	18 (35%)
30	CLA	C	502	-	65,73,73	1.39	11 (16%)	76,113,113	1.65	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	11	315	-	65,73,73	1.45	9 (13%)	76,113,113	1.49	8 (10%)
36	LMG	b	618	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	9 (15%)
41	A86	36	313	-	44,50,50	3.94	23 (52%)	51,76,76	7.95	17 (33%)
38	DGD	c	518	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	16 (20%)
41	A86	39	311	-	44,50,50	4.00	21 (47%)	51,76,76	8.15	18 (35%)
30	CLA	17	307	25	45,53,73	1.80	9 (20%)	52,89,113	1.76	13 (25%)
30	CLA	39	308	-	45,53,73	1.69	7 (15%)	52,89,113	1.79	9 (17%)
30	CLA	15	303	-	65,73,73	1.42	7 (10%)	76,113,113	1.54	10 (13%)
30	CLA	B	609	-	65,73,73	1.47	10 (15%)	76,113,113	1.49	10 (13%)
30	CLA	b	614	-	65,73,73	1.39	10 (15%)	76,113,113	1.59	10 (13%)
30	CLA	c	514	30	65,73,73	1.40	9 (13%)	76,113,113	1.62	8 (10%)
30	CLA	B	603	-	65,73,73	1.41	11 (16%)	76,113,113	1.64	12 (15%)
30	CLA	41	302	-	45,53,73	1.73	7 (15%)	52,89,113	1.72	10 (19%)
30	CLA	32	312	25	45,53,73	1.76	11 (24%)	52,89,113	1.75	9 (17%)
30	CLA	12	311	25	65,73,73	1.48	10 (15%)	76,113,113	1.53	10 (13%)
30	CLA	B	615	-	65,73,73	1.53	12 (18%)	76,113,113	1.44	11 (14%)
30	CLA	21	301	28	65,73,73	1.48	8 (12%)	76,113,113	1.43	7 (9%)
30	CLA	31	302	-	45,53,73	1.67	11 (24%)	52,89,113	1.81	9 (17%)
31	PHO	A	403	-	51,69,69	1.24	9 (17%)	47,99,99	1.31	8 (17%)
30	CLA	b	609	-	65,73,73	1.46	10 (15%)	76,113,113	1.51	9 (11%)
39	PL9	d	405	4	55,55,55	1.36	6 (10%)	68,69,69	1.50	14 (20%)
30	CLA	18	307	-	45,53,73	1.75	6 (13%)	52,89,113	1.63	8 (15%)
41	A86	32	314	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	32	306	-	45,53,73	1.68	11 (24%)	52,89,113	1.81	9 (17%)
30	CLA	b	611	-	65,73,73	1.51	12 (18%)	76,113,113	1.58	11 (14%)
30	CLA	14	301	-	65,73,73	1.46	9 (13%)	76,113,113	1.47	8 (10%)
41	A86	12	319	-	44,50,50	3.93	23 (52%)	51,76,76	7.98	19 (37%)
30	CLA	18	309	25	65,73,73	1.52	8 (12%)	76,113,113	1.60	10 (13%)
30	CLA	D	406	-	65,73,73	1.41	11 (16%)	76,113,113	1.61	7 (9%)
41	A86	39	310	-	44,50,50	4.09	22 (50%)	51,76,76	7.17	19 (37%)
41	A86	33	314	-	44,50,50	4.05	22 (50%)	51,76,76	7.80	19 (37%)
30	CLA	33	311	-	45,53,73	1.74	9 (20%)	52,89,113	1.68	7 (13%)
41	A86	16	311	-	44,50,50	3.96	23 (52%)	51,76,76	7.93	18 (35%)
41	A86	15	316	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	12	310	25	45,53,73	1.76	8 (17%)	52,89,113	1.82	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	BCR	H	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.31	7 (12%)
30	CLA	c	510	-	65,73,73	1.49	12 (18%)	76,113,113	1.73	10 (13%)
30	CLA	b	615	-	65,73,73	1.52	12 (18%)	76,113,113	1.44	11 (14%)
33	SQD	a	405	-	53,54,54	0.96	5 (9%)	62,65,65	1.58	11 (17%)
41	A86	20	211	-	44,50,50	3.89	23 (52%)	51,76,76	7.49	15 (29%)
30	CLA	14	309	25	45,53,73	1.76	11 (24%)	52,89,113	1.75	9 (17%)
32	BCR	B	624	-	41,41,41	1.13	3 (7%)	56,56,56	1.31	7 (12%)
30	CLA	B	604	-	65,73,73	1.44	12 (18%)	76,113,113	1.67	15 (19%)
41	A86	33	316	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
39	PL9	d	408	-	55,55,55	2.33	14 (25%)	68,69,69	1.49	15 (22%)
30	CLA	35	301	25	65,73,73	1.48	9 (13%)	76,113,113	1.56	10 (13%)
41	A86	13	301	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	38	312	-	45,53,73	1.74	9 (20%)	52,89,113	1.61	7 (13%)
30	CLA	35	304	25	45,53,73	1.79	7 (15%)	52,89,113	1.78	9 (17%)
30	CLA	32	305	25	65,73,73	1.47	10 (15%)	76,113,113	1.68	8 (10%)
30	CLA	13	306	-	45,53,73	1.70	8 (17%)	52,89,113	1.70	7 (13%)
41	A86	11	314	-	44,50,50	3.92	23 (52%)	51,76,76	7.97	19 (37%)
36	LMG	32	301	30	39,39,55	1.00	4 (10%)	47,47,63	1.18	4 (8%)
41	A86	21	311	-	44,50,50	3.90	23 (52%)	51,76,76	7.51	15 (29%)
30	CLA	13	309	25	45,53,73	1.75	11 (24%)	52,89,113	1.75	9 (17%)
30	CLA	32	308	25,36	45,53,73	1.72	8 (17%)	52,89,113	2.06	14 (26%)
30	CLA	36	304	-	65,73,73	1.43	10 (15%)	76,113,113	1.48	8 (10%)
30	CLA	20	203	30	45,53,73	1.78	9 (20%)	52,89,113	1.72	8 (15%)
30	CLA	34	310	-	45,53,73	1.74	8 (17%)	52,89,113	1.67	7 (13%)
30	CLA	20	204	-	65,73,73	1.41	10 (15%)	76,113,113	1.53	10 (13%)
40	HEM	v	201	16	41,50,50	1.60	5 (12%)	45,82,82	1.27	2 (4%)
30	CLA	12	313	25	45,53,73	1.75	11 (24%)	52,89,113	1.76	9 (17%)
30	CLA	B	605	-	65,73,73	1.49	10 (15%)	76,113,113	1.50	9 (11%)
30	CLA	34	303	-	45,53,73	1.66	11 (24%)	52,89,113	1.81	9 (17%)
30	CLA	39	302	-	45,53,73	1.67	9 (20%)	52,89,113	1.89	10 (19%)
30	CLA	B	607	-	65,73,73	1.42	11 (16%)	76,113,113	1.57	7 (9%)
30	CLA	13	303	-	45,53,73	1.69	10 (22%)	52,89,113	1.80	9 (17%)
32	BCR	B	616	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	7 (12%)
41	A86	40	211	-	44,50,50	3.89	23 (52%)	51,76,76	7.50	15 (29%)
41	A86	32	316	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A86	32	317	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	15	306	25	45,53,73	1.77	8 (17%)	52,89,113	1.79	9 (17%)
30	CLA	d	402	-	65,73,73	1.45	11 (16%)	76,113,113	1.50	8 (10%)
30	CLA	11	305	-	45,53,73	1.72	8 (17%)	52,89,113	1.72	7 (13%)
41	A86	20	201	-	44,50,50	3.93	22 (50%)	51,76,76	7.88	19 (37%)
30	CLA	B	601	-	65,73,73	1.44	11 (16%)	76,113,113	1.49	8 (10%)
36	LMG	Q	301	-	51,51,55	0.97	4 (7%)	59,59,63	1.46	9 (15%)
30	CLA	34	301	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	8 (10%)
32	BCR	b	616	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	9 (16%)
32	BCR	B	617	-	41,41,41	1.20	2 (4%)	56,56,56	1.36	9 (16%)
30	CLA	c	522	-	65,73,73	1.42	11 (16%)	76,113,113	1.48	8 (10%)
30	CLA	39	305	-	45,53,73	1.72	10 (22%)	52,89,113	1.69	6 (11%)
30	CLA	14	303	-	45,53,73	1.69	10 (22%)	52,89,113	1.81	9 (17%)
30	CLA	32	303	-	65,73,73	1.45	9 (13%)	76,113,113	1.49	8 (10%)
30	CLA	40	203	30	45,53,73	1.78	9 (20%)	52,89,113	1.71	9 (17%)
30	CLA	12	309	-	45,53,73	1.69	7 (15%)	52,89,113	1.70	7 (13%)
30	CLA	33	308	25	45,53,73	1.76	8 (17%)	52,89,113	1.84	8 (15%)
35	LHG	d	409	-	48,48,48	0.81	1 (2%)	51,54,54	1.26	5 (9%)
41	A86	16	312	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
30	CLA	21	304	-	45,53,73	1.69	8 (17%)	52,89,113	1.64	6 (11%)
41	A86	36	310	-	44,50,50	3.97	23 (52%)	51,76,76	8.08	20 (39%)
30	CLA	b	612	-	65,73,73	1.50	10 (15%)	76,113,113	1.77	10 (13%)
30	CLA	40	205	-	45,53,73	1.73	10 (22%)	52,89,113	1.79	9 (17%)
41	A86	34	312	-	44,50,50	3.96	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	c	524	30	65,73,73	1.45	6 (9%)	76,113,113	1.41	8 (10%)
30	CLA	12	303	-	65,73,73	1.45	9 (13%)	76,113,113	1.49	8 (10%)
30	CLA	17	303	25	65,73,73	1.48	10 (15%)	76,113,113	1.58	8 (10%)
30	CLA	38	311	25	45,53,73	1.82	9 (20%)	52,89,113	1.80	11 (21%)
30	CLA	38	308	25	45,53,73	1.78	7 (15%)	52,89,113	1.72	8 (15%)
41	A86	34	313	-	44,50,50	4.05	22 (50%)	51,76,76	7.80	19 (37%)
36	LMG	d	410	-	51,51,55	0.89	3 (5%)	59,59,63	1.43	7 (11%)
30	CLA	C	512	3	65,73,73	1.50	10 (15%)	76,113,113	1.62	12 (15%)
41	A86	11	316	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	20 (39%)
30	CLA	41	304	-	45,53,73	1.68	8 (17%)	52,89,113	1.65	6 (11%)
36	LMG	W	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.40	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A86	40	213	-	44,50,50	4.02	23 (52%)	51,76,76	7.83	18 (35%)
30	CLA	11	308	25	45,53,73	1.75	11 (24%)	52,89,113	1.76	10 (19%)
41	A86	32	318	-	44,50,50	3.93	23 (52%)	51,76,76	7.98	19 (37%)
41	A86	13	315	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	31	304	25	45,53,73	1.72	7 (15%)	52,89,113	2.08	13 (25%)
31	PHO	d	404	-	51,69,69	1.13	8 (15%)	47,99,99	1.28	6 (12%)
30	CLA	17	304	-	45,53,73	1.70	11 (24%)	52,89,113	1.83	9 (17%)
30	CLA	13	304	-	65,73,73	1.41	10 (15%)	76,113,113	1.58	10 (13%)
30	CLA	12	308	25,36	45,53,73	1.71	8 (17%)	52,89,113	2.04	12 (23%)
30	CLA	38	310	25	65,73,73	1.47	8 (12%)	76,113,113	1.37	8 (10%)
30	CLA	16	305	25	45,53,73	1.69	8 (17%)	52,89,113	1.92	10 (19%)
41	A86	17	315	-	44,50,50	4.06	23 (52%)	51,76,76	8.44	16 (31%)
41	A86	16	313	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	18 (35%)
41	A86	31	312	-	44,50,50	4.04	23 (52%)	51,76,76	7.82	20 (39%)
30	CLA	41	306	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	9 (11%)
41	A86	19	311	-	44,50,50	4.00	21 (47%)	51,76,76	8.15	18 (35%)
33	SQD	A	406	-	53,54,54	0.97	6 (11%)	62,65,65	1.58	11 (17%)
30	CLA	12	305	25	65,73,73	1.46	9 (13%)	76,113,113	1.68	8 (10%)
41	A86	34	311	-	44,50,50	3.93	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	31	306	25	45,53,73	1.74	10 (22%)	52,89,113	1.84	9 (17%)
30	CLA	17	306	25	45,53,73	1.71	7 (15%)	52,89,113	1.96	10 (19%)
30	CLA	A	404	-	65,73,73	1.48	10 (15%)	76,113,113	1.52	10 (13%)
35	LHG	A	408	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	7 (14%)
41	A86	17	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	18 (35%)
30	CLA	B	623	-	65,73,73	1.46	10 (15%)	76,113,113	1.58	14 (18%)
41	A86	11	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
41	A86	34	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
41	A86	13	317	-	44,50,50	3.94	23 (52%)	51,76,76	7.97	18 (35%)
35	LHG	B	622	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	6 (11%)
32	BCR	a	408	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
30	CLA	20	205	-	45,53,73	1.74	10 (22%)	52,89,113	1.80	9 (17%)
30	CLA	38	304	-	45,53,73	1.72	8 (17%)	52,89,113	1.84	8 (15%)
30	CLA	37	305	-	65,73,73	1.41	10 (15%)	76,113,113	1.53	9 (11%)
30	CLA	d	407	-	65,73,73	1.40	11 (16%)	76,113,113	1.60	7 (9%)
32	BCR	b	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.41	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A86	12	315	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)
32	BCR	C	515	-	41,41,41	1.30	4 (9%)	56,56,56	1.40	9 (16%)
41	A86	15	314	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	19 (37%)
32	BCR	c	521	-	41,41,41	1.27	2 (4%)	56,56,56	1.37	6 (10%)
30	CLA	40	209	30	65,73,73	1.47	10 (15%)	76,113,113	1.44	9 (11%)
41	A86	14	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	35	309	-	45,53,73	1.75	8 (17%)	52,89,113	1.61	7 (13%)
36	LMG	b	619	-	51,51,55	0.99	5 (9%)	59,59,63	1.44	8 (13%)
38	DGD	h	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.42	7 (9%)
30	CLA	19	301	-	65,73,73	1.49	10 (15%)	76,113,113	1.49	11 (14%)
30	CLA	36	305	25	45,53,73	1.69	9 (20%)	52,89,113	1.91	10 (19%)
30	CLA	41	308	-	45,53,73	1.75	6 (13%)	52,89,113	1.64	7 (13%)
37	OEX	C	501	1,3	0,15,15	-	-	-	-	-
30	CLA	38	306	25	45,53,73	1.74	7 (15%)	52,89,113	1.85	8 (15%)
41	A86	17	302	-	44,50,50	3.94	23 (52%)	51,76,76	8.11	21 (41%)
30	CLA	m	101	12,36	65,73,73	1.42	11 (16%)	76,113,113	1.41	6 (7%)
41	A86	31	314	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	18 (35%)
41	A86	14	313	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
30	CLA	a	403	-	65,73,73	1.48	11 (16%)	76,113,113	1.52	10 (13%)
30	CLA	b	610	-	65,73,73	1.51	11 (16%)	76,113,113	1.50	8 (10%)
30	CLA	21	303	-	65,73,73	1.43	8 (12%)	76,113,113	1.41	7 (9%)
32	BCR	c	515	-	41,41,41	1.34	3 (7%)	56,56,56	1.41	8 (14%)
30	CLA	35	303	-	65,73,73	1.42	7 (10%)	76,113,113	1.54	10 (13%)
30	CLA	33	310	25	45,53,73	1.74	11 (24%)	52,89,113	1.77	9 (17%)
30	CLA	34	308	25	65,73,73	1.48	10 (15%)	76,113,113	1.57	10 (13%)
30	CLA	36	302	25	65,73,73	1.49	10 (15%)	76,113,113	1.87	16 (21%)
30	CLA	b	613	-	65,73,73	1.42	11 (16%)	76,113,113	1.64	9 (11%)
35	LHG	l	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
41	A86	37	302	-	44,50,50	3.95	23 (52%)	51,76,76	8.11	21 (41%)
30	CLA	33	309	25	65,73,73	1.48	10 (15%)	76,113,113	1.54	10 (13%)
30	CLA	31	315	-	65,73,73	1.47	9 (13%)	76,113,113	1.50	8 (10%)
41	A86	32	319	-	44,50,50	3.93	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	c	506	-	65,73,73	1.46	11 (16%)	76,113,113	1.56	12 (15%)
41	A86	38	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	20 (39%)
41	A86	35	314	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A86	41	310	-	44,50,50	3.88	22 (50%)	51,76,76	7.41	21 (41%)
30	CLA	34	307	25	45,53,73	1.77	9 (20%)	52,89,113	1.84	9 (17%)
30	CLA	21	308	-	45,53,73	1.75	6 (13%)	52,89,113	1.64	7 (13%)
30	CLA	35	308	25	45,53,73	1.77	10 (22%)	52,89,113	1.75	10 (19%)
30	CLA	12	312	-	65,73,73	1.47	9 (13%)	76,113,113	1.48	8 (10%)
41	A86	40	212	-	44,50,50	4.18	23 (52%)	51,76,76	8.23	15 (29%)
30	CLA	M	101	12,36	65,73,73	1.42	10 (15%)	76,113,113	1.41	6 (7%)
41	A86	38	314	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
30	CLA	15	305	-	45,53,73	1.76	6 (13%)	52,89,113	1.67	6 (11%)
30	CLA	D	405	-	65,73,73	1.48	10 (15%)	76,113,113	1.61	11 (14%)
30	CLA	18	312	-	45,53,73	1.75	8 (17%)	52,89,113	1.61	7 (13%)
30	CLA	w	102	-	65,73,73	1.44	9 (13%)	76,113,113	1.47	10 (13%)
30	CLA	15	309	-	45,53,73	1.75	9 (20%)	52,89,113	1.60	7 (13%)
30	CLA	C	510	-	65,73,73	1.48	12 (18%)	76,113,113	1.72	10 (13%)
30	CLA	B	614	-	65,73,73	1.39	10 (15%)	76,113,113	1.58	10 (13%)
30	CLA	Z	102	30,19	65,73,73	1.45	6 (9%)	76,113,113	1.41	8 (10%)
41	A86	12	304	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	20 (39%)
41	A86	17	314	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	21	302	-	45,53,73	1.74	7 (15%)	52,89,113	1.73	10 (19%)
30	CLA	35	302	-	45,53,73	1.72	8 (17%)	52,89,113	1.88	9 (17%)
30	CLA	40	204	-	65,73,73	1.41	10 (15%)	76,113,113	1.52	9 (11%)
30	CLA	c	511	-	65,73,73	1.45	12 (18%)	76,113,113	1.58	12 (15%)
30	CLA	W	103	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	7 (9%)
30	CLA	33	305	-	65,73,73	1.41	11 (16%)	76,113,113	1.61	10 (13%)
30	CLA	18	305	-	65,73,73	1.44	8 (12%)	76,113,113	1.47	7 (9%)
41	A86	35	315	-	44,50,50	4.00	23 (52%)	51,76,76	7.59	20 (39%)
30	CLA	32	313	-	45,53,73	1.72	9 (20%)	52,89,113	1.67	7 (13%)
41	A86	33	313	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
41	A86	17	313	-	44,50,50	4.06	23 (52%)	51,76,76	7.82	19 (37%)
30	CLA	20	206	27	45,53,73	1.71	9 (20%)	52,89,113	1.80	10 (19%)
30	CLA	16	309	-	45,53,73	1.75	10 (22%)	52,89,113	1.61	9 (17%)
41	A86	37	311	-	44,50,50	4.02	22 (50%)	51,76,76	8.33	19 (37%)
30	CLA	b	602	-	65,73,73	1.47	10 (15%)	76,113,113	1.54	12 (15%)
30	CLA	15	308	25	45,53,73	1.75	10 (22%)	52,89,113	1.74	10 (19%)
30	CLA	b	607	-	65,73,73	1.41	11 (16%)	76,113,113	1.55	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	SQD	B	621	-	36,37,54	1.20	6 (16%)	45,48,65	1.64	9 (20%)
41	A86	33	315	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	19	303	-	65,73,73	1.45	8 (12%)	76,113,113	1.55	9 (11%)
41	A86	36	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
41	A86	12	317	-	44,50,50	4.04	22 (50%)	51,76,76	7.80	19 (37%)
31	PHO	D	403	-	51,69,69	1.13	8 (15%)	47,99,99	1.29	6 (12%)
41	A86	20	210	-	44,50,50	4.07	23 (52%)	51,76,76	8.31	17 (33%)
30	CLA	32	309	-	45,53,73	1.70	8 (17%)	52,89,113	1.69	7 (13%)
30	CLA	W	102	-	65,73,73	1.45	9 (13%)	76,113,113	1.48	10 (13%)
30	CLA	11	307	25	65,73,73	1.47	10 (15%)	76,113,113	1.55	10 (13%)
30	CLA	31	308	25	45,53,73	1.75	11 (24%)	52,89,113	1.77	9 (17%)
40	HEM	E	101	6,5	41,50,50	1.51	4 (9%)	45,82,82	1.24	5 (11%)
30	CLA	18	311	25	45,53,73	1.83	9 (20%)	52,89,113	1.81	11 (21%)
30	CLA	19	308	-	45,53,73	1.70	7 (15%)	52,89,113	1.80	9 (17%)
30	CLA	18	308	25	45,53,73	1.78	7 (15%)	52,89,113	1.72	8 (15%)
30	CLA	41	305	28	45,53,73	1.76	6 (13%)	52,89,113	1.79	8 (15%)
32	BCR	a	404	-	41,41,41	1.29	2 (4%)	56,56,56	1.40	6 (10%)
30	CLA	39	307	-	45,53,73	1.68	9 (20%)	52,89,113	1.79	7 (13%)
30	CLA	31	305	-	45,53,73	1.69	8 (17%)	52,89,113	1.70	7 (13%)
30	CLA	40	208	-	45,53,73	1.70	7 (15%)	52,89,113	1.78	9 (17%)
41	A86	15	315	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	35	306	25	45,53,73	1.77	7 (15%)	52,89,113	1.79	9 (17%)
39	PL9	D	407	-	55,55,55	2.32	15 (27%)	68,69,69	1.48	14 (20%)
30	CLA	18	310	25	65,73,73	1.46	10 (15%)	76,113,113	1.38	8 (10%)
32	BCR	A	409	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	4 (7%)
30	CLA	w	103	-	65,73,73	1.49	6 (9%)	76,113,113	1.41	7 (9%)
41	A86	16	310	-	44,50,50	3.97	23 (52%)	51,76,76	8.08	20 (39%)
30	CLA	11	301	25	65,73,73	1.45	8 (12%)	76,113,113	1.67	9 (11%)
30	CLA	15	304	25	45,53,73	1.79	7 (15%)	52,89,113	1.80	9 (17%)
41	A86	40	210	-	44,50,50	4.07	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	33	303	25	65,73,73	1.47	10 (15%)	76,113,113	1.69	8 (10%)
41	A86	35	313	-	44,50,50	4.03	23 (52%)	51,76,76	8.22	20 (39%)
41	A86	39	309	-	44,50,50	3.88	23 (52%)	51,76,76	7.69	16 (31%)
41	A86	19	310	-	44,50,50	4.09	21 (47%)	51,76,76	7.18	19 (37%)
32	BCR	B	618	-	41,41,41	1.24	2 (4%)	56,56,56	1.41	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	34	304	-	65,73,73	1.42	11 (16%)	76,113,113	1.59	10 (13%)
30	CLA	16	301	-	65,73,73	1.46	9 (13%)	76,113,113	1.43	8 (10%)
41	A86	36	312	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
30	CLA	33	304	-	45,53,73	1.67	11 (24%)	52,89,113	1.81	9 (17%)
41	A86	18	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	38	309	25	65,73,73	1.52	8 (12%)	76,113,113	1.61	10 (13%)
30	CLA	11	302	-	45,53,73	1.69	11 (24%)	52,89,113	1.80	9 (17%)
41	A86	31	316	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
35	LHG	a	407	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	8 (16%)
30	CLA	38	303	25	65,73,73	1.47	10 (15%)	76,113,113	1.47	8 (10%)
30	CLA	16	307	25	45,53,73	1.76	10 (22%)	52,89,113	1.96	7 (13%)
30	CLA	34	306	-	45,53,73	1.70	9 (20%)	52,89,113	1.69	7 (13%)
41	A86	11	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)

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
41	A86	13	311	-	-	8/34/90/90	0/3/3/3
30	CLA	11	309	-	1/1/11/20	6/13/91/115	-
30	CLA	C	521	-	1/1/15/20	14/37/115/115	-
41	A86	40	201	-	-	12/34/90/90	0/3/3/3
41	A86	33	317	-	-	7/34/90/90	0/3/3/3
30	CLA	20	202	-	-	19/37/115/115	-
41	A86	32	315	-	-	3/34/90/90	0/3/3/3
30	CLA	18	306	25	-	9/13/91/115	-
41	A86	17	312	-	-	3/34/90/90	0/3/3/3
30	CLA	32	310	25	1/1/11/20	8/13/91/115	-
33	SQD	b	620	-	-	9/32/52/69	0/1/1/1
30	CLA	c	512	3	1/1/15/20	8/37/115/115	-
30	CLA	39	303	-	1/1/15/20	15/37/115/115	-
32	BCR	c	516	-	-	10/29/63/63	0/2/2/2
41	A86	15	311	-	-	3/34/90/90	0/3/3/3
30	CLA	32	307	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	38	305	-	1/1/15/20	19/37/115/115	-
30	CLA	37	309	25	1/1/11/20	4/13/91/115	-
30	CLA	18	304	-	1/1/11/20	5/13/91/115	-
30	CLA	14	310	-	1/1/11/20	6/13/91/115	-
30	CLA	36	307	25	1/1/11/20	9/13/91/115	-
30	CLA	40	202	-	-	19/37/115/115	-
30	CLA	13	310	-	1/1/11/20	6/13/91/115	-
41	A86	18	313	-	-	8/34/90/90	0/3/3/3
30	CLA	17	310	-	1/1/11/20	7/13/91/115	-
30	CLA	16	308	25	-	7/13/91/115	-
30	CLA	B	613	-	1/1/15/20	8/37/115/115	-
41	A86	15	310	-	-	8/34/90/90	0/3/3/3
41	A86	21	314	-	-	12/34/90/90	0/3/3/3
41	A86	38	315	-	-	10/34/90/90	0/3/3/3
30	CLA	11	303	-	1/1/15/20	13/37/115/115	-
30	CLA	36	309	-	1/1/11/20	5/13/91/115	-
41	A86	41	314	-	-	12/34/90/90	0/3/3/3
30	CLA	15	301	25	1/1/15/20	10/37/115/115	-
30	CLA	37	308	25	1/1/15/20	17/37/115/115	-
30	CLA	19	304	26	1/1/11/20	9/13/91/115	-
30	CLA	C	511	-	1/1/15/20	12/37/115/115	-
30	CLA	36	303	-	1/1/11/20	6/13/91/115	-
41	A86	35	316	-	-	16/34/90/90	0/3/3/3
41	A86	37	316	-	-	7/34/90/90	0/3/3/3
30	CLA	41	301	28	-	14/37/115/115	-
30	CLA	B	608	-	1/1/15/20	8/37/115/115	-
42	LMU	32	302	-	-	7/18/58/61	0/2/2/2
30	CLA	20	209	30	1/1/15/20	11/37/115/115	-
41	A86	41	311	-	-	8/34/90/90	0/3/3/3
41	A86	41	313	-	-	16/34/90/90	0/3/3/3
30	CLA	39	301	-	-	12/37/115/115	-
30	CLA	19	306	-	1/1/11/20	8/13/91/115	-
30	CLA	C	513	-	1/1/15/20	16/37/115/115	-
30	CLA	14	305	25	1/1/11/20	9/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	31	311	-	-	3/34/90/90	0/3/3/3
36	LMG	D	408	-	-	14/46/66/70	0/1/1/1
32	BCR	f	101	-	-	15/29/63/63	0/2/2/2
30	CLA	13	305	25	1/1/11/20	9/13/91/115	-
36	LMG	m	102	30	-	10/35/55/70	0/1/1/1
41	A86	31	313	-	-	10/34/90/90	0/3/3/3
38	DGD	C	516	-	-	19/51/91/95	0/2/2/2
41	A86	13	313	-	-	8/34/90/90	0/3/3/3
30	CLA	12	307	-	1/1/15/20	13/37/115/115	-
30	CLA	39	306	-	1/1/11/20	8/13/91/115	-
30	CLA	c	513	-	1/1/15/20	16/37/115/115	-
30	CLA	15	302	-	1/1/11/20	8/13/91/115	-
30	CLA	33	307	-	1/1/11/20	8/13/91/115	-
30	CLA	41	303	-	1/1/15/20	17/37/115/115	-
30	CLA	14	302	25	1/1/15/20	11/37/115/115	-
41	A86	37	312	-	-	3/34/90/90	0/3/3/3
36	LMG	c	519	-	-	22/46/66/70	0/1/1/1
30	CLA	37	301	-	1/1/15/20	14/37/115/115	-
30	CLA	B	606	-	1/1/15/20	7/37/115/115	-
32	BCR	Z	101	-	-	15/29/63/63	0/2/2/2
30	CLA	38	301	-	1/1/15/20	11/37/115/115	-
30	CLA	C	508	-	1/1/15/20	18/37/115/115	-
30	CLA	21	307	-	1/1/15/20	11/37/115/115	-
30	CLA	35	307	25	1/1/15/20	11/37/115/115	-
30	CLA	C	505	-	1/1/15/20	17/37/115/115	-
30	CLA	33	301	-	1/1/15/20	10/37/115/115	-
30	CLA	D	401	-	1/1/15/20	12/37/115/115	-
32	BCR	C	518	-	-	8/29/63/63	0/2/2/2
41	A86	13	316	-	-	16/34/90/90	0/3/3/3
38	DGD	H	102	-	-	24/51/91/95	0/2/2/2
30	CLA	37	310	-	1/1/11/20	7/13/91/115	-
30	CLA	16	306	25	1/1/11/20	7/13/91/115	-
41	A86	21	310	-	-	9/34/90/90	0/3/3/3
30	CLA	d	401	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	17	311	-	-	13/34/90/90	0/3/3/3
30	CLA	17	308	25	1/1/15/20	17/37/115/115	-
30	CLA	34	305	25	1/1/11/20	9/13/91/115	-
30	CLA	41	307	-	1/1/15/20	11/37/115/115	-
32	BCR	A	405	-	-	12/29/63/63	0/2/2/2
42	LMU	12	302	30	-	7/18/58/61	0/2/2/2
36	LMG	12	301	30	-	17/34/54/70	0/1/1/1
30	CLA	C	509	-	1/1/15/20	12/37/115/115	-
30	CLA	31	307	25	1/1/15/20	14/37/115/115	-
41	A86	37	314	-	-	10/34/90/90	0/3/3/3
30	CLA	b	603	-	1/1/15/20	10/37/115/115	-
30	CLA	16	303	-	1/1/11/20	6/13/91/115	-
30	CLA	18	303	25	1/1/15/20	14/37/115/115	-
30	CLA	31	309	-	1/1/11/20	5/13/91/115	-
41	A86	31	310	-	-	8/34/90/90	0/3/3/3
30	CLA	c	509	-	1/1/15/20	12/37/115/115	-
41	A86	21	313	-	-	16/34/90/90	0/3/3/3
30	CLA	16	304	-	1/1/15/20	15/37/115/115	-
41	A86	21	312	-	-	7/34/90/90	0/3/3/3
41	A86	35	312	-	-	9/34/90/90	0/3/3/3
30	CLA	12	306	42	1/1/11/20	4/13/91/115	-
30	CLA	13	302	25	1/1/15/20	11/37/115/115	-
38	DGD	j	101	-	-	15/51/91/95	0/2/2/2
30	CLA	17	305	-	1/1/15/20	19/37/115/115	-
30	CLA	c	505	-	1/1/15/20	17/37/115/115	-
30	CLA	32	311	25	1/1/15/20	14/37/115/115	-
32	BCR	F	101	-	-	15/29/63/63	0/2/2/2
30	CLA	B	602	-	1/1/15/20	13/37/115/115	-
30	CLA	19	307	-	1/1/11/20	3/13/91/115	-
30	CLA	D	402	-	1/1/15/20	13/37/115/115	-
30	CLA	40	206	27	1/1/11/20	7/13/91/115	-
32	BCR	m	103	-	-	8/29/63/63	0/2/2/2
30	CLA	11	304	25	1/1/11/20	9/13/91/115	-
41	A86	41	312	-	-	7/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	19	302	-	1/1/11/20	4/13/91/115	-
30	CLA	b	601	-	1/1/15/20	18/37/115/115	-
36	LMG	B	619	-	-	18/46/66/70	0/1/1/1
30	CLA	11	306	25	1/1/11/20	8/13/91/115	-
30	CLA	20	207	-	1/1/11/20	7/13/91/115	-
30	CLA	35	305	-	1/1/11/20	8/13/91/115	-
32	BCR	c	520	-	-	16/29/63/63	0/2/2/2
41	A86	14	311	-	-	8/34/90/90	0/3/3/3
33	SQD	l	101	-	-	21/49/69/69	0/1/1/1
30	CLA	b	606	-	1/1/15/20	7/37/115/115	-
41	A86	18	315	-	-	10/34/90/90	0/3/3/3
30	CLA	b	605	-	1/1/15/20	17/37/115/115	-
35	LHG	L	101	-	-	29/53/53/53	-
30	CLA	C	504	-	1/1/15/20	17/37/115/115	-
41	A86	15	312	-	-	8/34/90/90	0/3/3/3
35	LHG	b	621	-	-	20/53/53/53	-
30	CLA	38	307	-	1/1/11/20	6/13/91/115	-
40	HEM	V	201	16	-	0/12/54/54	-
30	CLA	c	504	-	1/1/15/20	17/37/115/115	-
30	CLA	18	301	-	1/1/15/20	11/37/115/115	-
30	CLA	36	306	25	1/1/11/20	7/13/91/115	-
38	DGD	C	517	-	-	22/51/91/95	0/2/2/2
30	CLA	40	207	-	1/1/11/20	7/13/91/115	-
41	A86	33	312	-	-	8/34/90/90	0/3/3/3
30	CLA	a	402	-	1/1/15/20	7/37/115/115	-
30	CLA	13	308	25	1/1/15/20	14/37/115/115	-
36	LMG	w	101	-	-	28/46/66/70	0/1/1/1
30	CLA	33	306	25	1/1/11/20	10/13/91/115	-
41	A86	32	304	-	-	16/34/90/90	0/3/3/3
32	BCR	Y	101	-	-	16/29/63/63	0/2/2/2
41	A86	19	309	-	-	11/34/90/90	0/3/3/3
30	CLA	C	503	-	1/1/15/20	11/37/115/115	-
30	CLA	A	402	-	1/1/15/20	7/37/115/115	-
41	A86	37	313	-	-	9/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	C	520	-	1/1/15/20	15/37/115/115	-
30	CLA	31	303	-	1/1/15/20	13/37/115/115	-
30	CLA	21	306	-	1/1/15/20	14/37/115/115	-
38	DGD	c	517	-	-	19/51/91/95	0/2/2/2
30	CLA	b	608	-	1/1/15/20	8/37/115/115	-
30	CLA	37	307	25	1/1/11/20	7/13/91/115	-
30	CLA	d	406	-	1/1/15/20	8/37/115/115	-
30	CLA	36	308	25	-	7/13/91/115	-
41	A86	18	314	-	-	3/34/90/90	0/3/3/3
30	CLA	37	303	25	1/1/15/20	13/37/115/115	-
41	A86	14	312	-	-	3/34/90/90	0/3/3/3
32	BCR	h	101	-	-	7/29/63/63	0/2/2/2
30	CLA	b	622	-	1/1/15/20	15/37/115/115	-
30	CLA	31	301	25	1/1/15/20	12/37/115/115	-
30	CLA	14	307	25	1/1/11/20	8/13/91/115	-
30	CLA	17	301	-	1/1/15/20	14/37/115/115	-
30	CLA	C	507	-	1/1/15/20	17/37/115/115	-
30	CLA	21	309	-	1/1/11/20	6/13/91/115	-
31	PHO	d	403	-	-	12/37/103/103	0/5/6/6
41	A86	13	312	-	-	3/34/90/90	0/3/3/3
41	A86	12	316	-	-	3/34/90/90	0/3/3/3
30	CLA	13	307	25	1/1/11/20	8/13/91/115	-
30	CLA	B	611	-	1/1/15/20	12/37/115/115	-
41	A86	37	315	-	-	13/34/90/90	0/3/3/3
35	LHG	L	102	-	-	22/53/53/53	-
30	CLA	16	302	25	1/1/15/20	15/37/115/115	-
41	A86	33	302	-	-	15/34/90/90	0/3/3/3
39	PL9	D	404	4	-	17/53/73/73	0/1/1/1
30	CLA	20	208	-	-	8/13/91/115	-
30	CLA	21	305	28	1/1/11/20	9/13/91/115	-
30	CLA	39	304	26	1/1/11/20	9/13/91/115	-
36	LMG	B	620	-	-	20/46/66/70	0/1/1/1
30	CLA	14	304	-	1/1/15/20	13/37/115/115	-
30	CLA	b	604	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	34	302	25	1/1/15/20	12/37/115/115	-
41	A86	35	310	-	-	8/34/90/90	0/3/3/3
38	DGD	J	101	-	-	15/51/91/95	0/2/2/2
30	CLA	c	503	-	1/1/15/20	11/37/115/115	-
30	CLA	B	612	-	1/1/15/20	13/37/115/115	-
30	CLA	z	101	-	-	21/37/115/115	-
30	CLA	14	306	-	1/1/11/20	8/13/91/115	-
33	SQD	L	103	-	-	21/49/69/69	0/1/1/1
30	CLA	C	514	30	1/1/15/20	13/37/115/115	-
32	BCR	b	623	-	-	18/29/63/63	0/2/2/2
30	CLA	15	307	25	1/1/15/20	11/37/115/115	-
41	A86	13	314	-	-	10/34/90/90	0/3/3/3
30	CLA	19	305	-	1/1/11/20	7/13/91/115	-
30	CLA	c	502	-	1/1/15/20	14/37/115/115	-
41	A86	12	318	-	-	10/34/90/90	0/3/3/3
41	A86	20	212	-	-	11/34/90/90	0/3/3/3
30	CLA	37	304	-	-	6/13/91/115	-
30	CLA	c	507	-	1/1/15/20	17/37/115/115	-
41	A86	35	311	-	-	3/34/90/90	0/3/3/3
30	CLA	36	301	-	1/1/15/20	10/37/115/115	-
30	CLA	41	309	-	1/1/11/20	6/13/91/115	-
30	CLA	34	309	25	-	6/13/91/115	-
41	A86	38	313	-	-	8/34/90/90	0/3/3/3
30	CLA	C	506	-	1/1/15/20	16/37/115/115	-
30	CLA	12	314	-	1/1/11/20	6/13/91/115	-
30	CLA	17	309	25	1/1/11/20	4/13/91/115	-
30	CLA	37	306	25	-	8/13/91/115	-
30	CLA	B	610	-	1/1/15/20	14/37/115/115	-
41	A86	11	312	-	-	8/34/90/90	0/3/3/3
41	A86	15	313	-	-	10/34/90/90	0/3/3/3
36	LMG	M	102	30	-	10/35/55/70	0/1/1/1
40	HEM	e	101	6,5	-	7/12/54/54	-
30	CLA	c	508	-	1/1/15/20	18/37/115/115	-
30	CLA	C	519	-	-	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	14	308	25	1/1/15/20	14/37/115/115	-
30	CLA	c	523	-	1/1/15/20	14/37/115/115	-
41	A86	11	311	-	-	3/34/90/90	0/3/3/3
41	A86	20	213	-	-	12/34/90/90	0/3/3/3
30	CLA	C	502	-	1/1/15/20	14/37/115/115	-
30	CLA	11	315	-	1/1/15/20	11/37/115/115	-
36	LMG	b	618	-	-	18/46/66/70	0/1/1/1
41	A86	36	313	-	-	7/34/90/90	0/3/3/3
38	DGD	c	518	-	-	22/51/91/95	0/2/2/2
41	A86	39	311	-	-	8/34/90/90	0/3/3/3
30	CLA	17	307	25	1/1/11/20	8/13/91/115	-
30	CLA	39	308	-	1/1/11/20	8/13/91/115	-
30	CLA	15	303	-	1/1/15/20	15/37/115/115	-
30	CLA	B	609	-	1/1/15/20	8/37/115/115	-
30	CLA	b	614	-	1/1/15/20	8/37/115/115	-
30	CLA	c	514	30	1/1/15/20	13/37/115/115	-
30	CLA	B	603	-	1/1/15/20	10/37/115/115	-
30	CLA	41	302	-	-	7/13/91/115	-
30	CLA	32	312	25	-	6/13/91/115	-
30	CLA	12	311	25	1/1/15/20	14/37/115/115	-
30	CLA	B	615	-	1/1/15/20	13/37/115/115	-
30	CLA	21	301	28	-	14/37/115/115	-
30	CLA	31	302	-	1/1/11/20	4/13/91/115	-
31	PHO	A	403	-	-	12/37/103/103	0/5/6/6
30	CLA	b	609	-	1/1/15/20	8/37/115/115	-
39	PL9	d	405	4	-	17/53/73/73	0/1/1/1
30	CLA	18	307	-	1/1/11/20	6/13/91/115	-
41	A86	32	314	-	-	8/34/90/90	0/3/3/3
30	CLA	32	306	-	1/1/11/20	4/13/91/115	-
30	CLA	b	611	-	1/1/15/20	12/37/115/115	-
30	CLA	14	301	-	1/1/15/20	11/37/115/115	-
41	A86	12	319	-	-	7/34/90/90	0/3/3/3
30	CLA	18	309	25	1/1/15/20	16/37/115/115	-
30	CLA	D	406	-	1/1/15/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	39	310	-	-	17/34/90/90	0/3/3/3
41	A86	33	314	-	-	9/34/90/90	0/3/3/3
30	CLA	33	311	-	1/1/11/20	5/13/91/115	-
41	A86	16	311	-	-	3/34/90/90	0/3/3/3
41	A86	15	316	-	-	16/34/90/90	0/3/3/3
30	CLA	12	310	25	1/1/11/20	8/13/91/115	-
32	BCR	H	101	-	-	7/29/63/63	0/2/2/2
30	CLA	c	510	-	1/1/15/20	12/37/115/115	-
30	CLA	b	615	-	1/1/15/20	13/37/115/115	-
33	SQD	a	405	-	-	14/49/69/69	0/1/1/1
41	A86	20	211	-	-	8/34/90/90	0/3/3/3
30	CLA	14	309	25	-	6/13/91/115	-
32	BCR	B	624	-	-	18/29/63/63	0/2/2/2
30	CLA	B	604	-	1/1/15/20	14/37/115/115	-
41	A86	33	316	-	-	16/34/90/90	0/3/3/3
39	PL9	d	408	-	-	13/53/73/73	0/1/1/1
30	CLA	35	301	25	1/1/15/20	10/37/115/115	-
41	A86	13	301	-	-	15/34/90/90	0/3/3/3
30	CLA	38	312	-	1/1/11/20	4/13/91/115	-
30	CLA	35	304	25	-	7/13/91/115	-
30	CLA	32	305	25	1/1/15/20	12/37/115/115	-
30	CLA	13	306	-	1/1/11/20	8/13/91/115	-
41	A86	11	314	-	-	7/34/90/90	0/3/3/3
36	LMG	32	301	30	-	14/34/54/70	0/1/1/1
41	A86	21	311	-	-	8/34/90/90	0/3/3/3
30	CLA	13	309	25	-	6/13/91/115	-
30	CLA	32	308	25,36	1/1/11/20	10/13/91/115	-
30	CLA	36	304	-	1/1/15/20	15/37/115/115	-
30	CLA	20	203	30	1/1/11/20	5/13/91/115	-
30	CLA	34	310	-	1/1/11/20	5/13/91/115	-
30	CLA	20	204	-	1/1/15/20	13/37/115/115	-
40	HEM	v	201	16	-	0/12/54/54	-
30	CLA	12	313	25	-	6/13/91/115	-
30	CLA	B	605	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	34	303	-	1/1/11/20	4/13/91/115	-
30	CLA	39	302	-	1/1/11/20	4/13/91/115	-
30	CLA	B	607	-	1/1/15/20	12/37/115/115	-
30	CLA	13	303	-	1/1/11/20	5/13/91/115	-
32	BCR	B	616	-	-	8/29/63/63	0/2/2/2
41	A86	40	211	-	-	8/34/90/90	0/3/3/3
41	A86	32	316	-	-	9/34/90/90	0/3/3/3
41	A86	32	317	-	-	10/34/90/90	0/3/3/3
30	CLA	15	306	25	1/1/11/20	8/13/91/115	-
30	CLA	d	402	-	1/1/15/20	13/37/115/115	-
30	CLA	11	305	-	1/1/11/20	8/13/91/115	-
41	A86	20	201	-	-	12/34/90/90	0/3/3/3
30	CLA	B	601	-	1/1/15/20	18/37/115/115	-
36	LMG	Q	301	-	-	22/46/66/70	0/1/1/1
30	CLA	34	301	-	1/1/15/20	10/37/115/115	-
32	BCR	b	616	-	-	9/29/63/63	0/2/2/2
32	BCR	B	617	-	-	9/29/63/63	0/2/2/2
30	CLA	c	522	-	1/1/15/20	15/37/115/115	-
30	CLA	39	305	-	1/1/11/20	7/13/91/115	-
30	CLA	14	303	-	1/1/11/20	5/13/91/115	-
30	CLA	32	303	-	1/1/15/20	10/37/115/115	-
30	CLA	40	203	30	1/1/11/20	5/13/91/115	-
30	CLA	12	309	-	1/1/11/20	8/13/91/115	-
30	CLA	33	308	25	1/1/11/20	8/13/91/115	-
35	LHG	d	409	-	-	29/53/53/53	-
41	A86	16	312	-	-	8/34/90/90	0/3/3/3
30	CLA	21	304	-	1/1/11/20	8/13/91/115	-
41	A86	36	310	-	-	12/34/90/90	0/3/3/3
30	CLA	b	612	-	1/1/15/20	13/37/115/115	-
30	CLA	40	205	-	-	9/13/91/115	-
41	A86	34	312	-	-	3/34/90/90	0/3/3/3
30	CLA	c	524	30	1/1/15/20	15/37/115/115	-
30	CLA	12	303	-	1/1/15/20	11/37/115/115	-
30	CLA	17	303	25	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	38	311	25	1/1/11/20	8/13/91/115	-
30	CLA	38	308	25	1/1/11/20	8/13/91/115	-
41	A86	34	313	-	-	9/34/90/90	0/3/3/3
36	LMG	d	410	-	-	14/46/66/70	0/1/1/1
30	CLA	C	512	3	1/1/15/20	8/37/115/115	-
41	A86	11	316	-	-	15/34/90/90	0/3/3/3
30	CLA	41	304	-	1/1/11/20	8/13/91/115	-
36	LMG	W	101	-	-	28/46/66/70	0/1/1/1
41	A86	40	213	-	-	12/34/90/90	0/3/3/3
30	CLA	11	308	25	-	6/13/91/115	-
41	A86	32	318	-	-	7/34/90/90	0/3/3/3
41	A86	13	315	-	-	7/34/90/90	0/3/3/3
30	CLA	31	304	25	1/1/11/20	10/13/91/115	-
31	PHO	d	404	-	-	8/37/103/103	0/5/6/6
30	CLA	17	304	-	-	6/13/91/115	-
30	CLA	13	304	-	1/1/15/20	13/37/115/115	-
30	CLA	12	308	25,36	1/1/11/20	9/13/91/115	-
30	CLA	38	310	25	1/1/15/20	10/37/115/115	-
30	CLA	16	305	25	-	8/13/91/115	-
41	A86	17	315	-	-	13/34/90/90	0/3/3/3
41	A86	16	313	-	-	7/34/90/90	0/3/3/3
41	A86	31	312	-	-	8/34/90/90	0/3/3/3
30	CLA	41	306	-	1/1/15/20	14/37/115/115	-
41	A86	19	311	-	-	8/34/90/90	0/3/3/3
33	SQD	A	406	-	-	14/49/69/69	0/1/1/1
30	CLA	12	305	25	1/1/15/20	11/37/115/115	-
41	A86	34	311	-	-	8/34/90/90	0/3/3/3
30	CLA	31	306	25	1/1/11/20	8/13/91/115	-
30	CLA	17	306	25	-	8/13/91/115	-
30	CLA	A	404	-	1/1/15/20	10/37/115/115	-
35	LHG	A	408	-	-	23/50/50/53	-
41	A86	17	316	-	-	7/34/90/90	0/3/3/3
30	CLA	B	623	-	1/1/15/20	15/37/115/115	-
41	A86	11	310	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	34	314	-	-	10/34/90/90	0/3/3/3
41	A86	13	317	-	-	7/34/90/90	0/3/3/3
35	LHG	B	622	-	-	20/53/53/53	-
32	BCR	a	408	-	-	9/29/63/63	0/2/2/2
30	CLA	20	205	-	-	9/13/91/115	-
30	CLA	38	304	-	1/1/11/20	5/13/91/115	-
30	CLA	37	305	-	1/1/15/20	19/37/115/115	-
30	CLA	d	407	-	1/1/15/20	4/37/115/115	-
32	BCR	b	617	-	-	9/29/63/63	0/2/2/2
41	A86	12	315	-	-	8/34/90/90	0/3/3/3
32	BCR	C	515	-	-	10/29/63/63	0/2/2/2
41	A86	15	314	-	-	7/34/90/90	0/3/3/3
32	BCR	c	521	-	-	8/29/63/63	0/2/2/2
30	CLA	40	209	30	1/1/15/20	11/37/115/115	-
41	A86	14	314	-	-	10/34/90/90	0/3/3/3
30	CLA	35	309	-	1/1/11/20	4/13/91/115	-
36	LMG	b	619	-	-	20/46/66/70	0/1/1/1
38	DGD	h	102	-	-	24/51/91/95	0/2/2/2
30	CLA	41	308	-	1/1/11/20	8/13/91/115	-
30	CLA	19	301	-	-	12/37/115/115	-
30	CLA	36	305	25	-	8/13/91/115	-
30	CLA	38	306	25	-	9/13/91/115	-
41	A86	17	302	-	-	16/34/90/90	1/3/3/3
30	CLA	m	101	12,36	1/1/15/20	19/37/115/115	-
41	A86	31	314	-	-	7/34/90/90	0/3/3/3
41	A86	14	313	-	-	8/34/90/90	0/3/3/3
30	CLA	a	403	-	1/1/15/20	10/37/115/115	-
30	CLA	b	610	-	1/1/15/20	14/37/115/115	-
30	CLA	21	303	-	1/1/15/20	17/37/115/115	-
32	BCR	c	515	-	-	15/29/63/63	0/2/2/2
30	CLA	35	303	-	1/1/15/20	15/37/115/115	-
30	CLA	33	310	25	-	6/13/91/115	-
30	CLA	34	308	25	1/1/15/20	14/37/115/115	-
30	CLA	36	302	25	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	613	-	1/1/15/20	8/37/115/115	-
35	LHG	l	102	-	-	22/53/53/53	-
41	A86	37	302	-	-	16/34/90/90	1/3/3/3
30	CLA	33	309	25	1/1/15/20	14/37/115/115	-
30	CLA	31	315	-	1/1/15/20	10/37/115/115	-
41	A86	32	319	-	-	7/34/90/90	0/3/3/3
30	CLA	c	506	-	1/1/15/20	16/37/115/115	-
41	A86	38	302	-	-	15/34/90/90	0/3/3/3
41	A86	35	314	-	-	7/34/90/90	0/3/3/3
41	A86	41	310	-	-	9/34/90/90	0/3/3/3
30	CLA	34	307	25	1/1/11/20	8/13/91/115	-
30	CLA	21	308	-	1/1/11/20	8/13/91/115	-
30	CLA	35	308	25	1/1/11/20	6/13/91/115	-
30	CLA	12	312	-	1/1/15/20	11/37/115/115	-
41	A86	40	212	-	-	11/34/90/90	0/3/3/3
30	CLA	M	101	12,36	1/1/15/20	19/37/115/115	-
41	A86	38	314	-	-	3/34/90/90	0/3/3/3
30	CLA	15	305	-	1/1/11/20	8/13/91/115	-
30	CLA	D	405	-	1/1/15/20	8/37/115/115	-
30	CLA	18	312	-	1/1/11/20	4/13/91/115	-
30	CLA	w	102	-	1/1/15/20	14/37/115/115	-
30	CLA	15	309	-	1/1/11/20	4/13/91/115	-
30	CLA	C	510	-	1/1/15/20	12/37/115/115	-
30	CLA	B	614	-	1/1/15/20	8/37/115/115	-
30	CLA	Z	102	30,19	1/1/15/20	16/37/115/115	-
41	A86	12	304	-	-	16/34/90/90	0/3/3/3
41	A86	17	314	-	-	10/34/90/90	0/3/3/3
30	CLA	21	302	-	-	7/13/91/115	-
30	CLA	35	302	-	1/1/11/20	8/13/91/115	-
30	CLA	40	204	-	1/1/15/20	13/37/115/115	-
30	CLA	c	511	-	1/1/15/20	12/37/115/115	-
30	CLA	W	103	-	-	19/37/115/115	-
30	CLA	33	305	-	1/1/15/20	13/37/115/115	-
30	CLA	18	305	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	35	315	-	-	15/34/90/90	0/3/3/3
30	CLA	32	313	-	1/1/11/20	5/13/91/115	-
41	A86	33	313	-	-	3/34/90/90	0/3/3/3
41	A86	17	313	-	-	8/34/90/90	0/3/3/3
30	CLA	20	206	27	1/1/11/20	7/13/91/115	-
30	CLA	16	309	-	1/1/11/20	5/13/91/115	-
41	A86	37	311	-	-	13/34/90/90	0/3/3/3
30	CLA	b	602	-	1/1/15/20	13/37/115/115	-
30	CLA	15	308	25	1/1/11/20	6/13/91/115	-
30	CLA	b	607	-	1/1/15/20	12/37/115/115	-
33	SQD	B	621	-	-	9/32/52/69	0/1/1/1
41	A86	33	315	-	-	10/34/90/90	0/3/3/3
30	CLA	19	303	-	1/1/15/20	15/37/115/115	-
41	A86	36	311	-	-	3/34/90/90	0/3/3/3
41	A86	12	317	-	-	9/34/90/90	0/3/3/3
31	PHO	D	403	-	-	8/37/103/103	0/5/6/6
41	A86	20	210	-	-	14/34/90/90	0/3/3/3
30	CLA	32	309	-	1/1/11/20	8/13/91/115	-
30	CLA	W	102	-	1/1/15/20	14/37/115/115	-
30	CLA	11	307	25	1/1/15/20	14/37/115/115	-
30	CLA	31	308	25	-	6/13/91/115	-
40	HEM	E	101	6,5	-	7/12/54/54	-
30	CLA	18	311	25	1/1/11/20	8/13/91/115	-
30	CLA	19	308	-	1/1/11/20	8/13/91/115	-
30	CLA	18	308	25	1/1/11/20	8/13/91/115	-
30	CLA	41	305	28	1/1/11/20	9/13/91/115	-
32	BCR	a	404	-	-	12/29/63/63	0/2/2/2
30	CLA	39	307	-	1/1/11/20	3/13/91/115	-
30	CLA	31	305	-	1/1/11/20	8/13/91/115	-
30	CLA	40	208	-	-	8/13/91/115	-
41	A86	15	315	-	-	15/34/90/90	0/3/3/3
30	CLA	35	306	25	1/1/11/20	8/13/91/115	-
39	PL9	D	407	-	-	13/53/73/73	0/1/1/1
30	CLA	18	310	25	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	BCR	A	409	-	-	9/29/63/63	0/2/2/2
30	CLA	w	103	-	-	19/37/115/115	-
41	A86	16	310	-	-	12/34/90/90	0/3/3/3
30	CLA	11	301	25	1/1/15/20	11/37/115/115	-
30	CLA	15	304	25	-	7/13/91/115	-
41	A86	40	210	-	-	14/34/90/90	0/3/3/3
30	CLA	33	303	25	1/1/15/20	12/37/115/115	-
41	A86	35	313	-	-	10/34/90/90	0/3/3/3
41	A86	39	309	-	-	11/34/90/90	0/3/3/3
41	A86	19	310	-	-	17/34/90/90	0/3/3/3
32	BCR	B	618	-	-	9/29/63/63	0/2/2/2
30	CLA	34	304	-	1/1/15/20	13/37/115/115	-
30	CLA	16	301	-	1/1/15/20	10/37/115/115	-
41	A86	36	312	-	-	8/34/90/90	0/3/3/3
30	CLA	33	304	-	1/1/11/20	4/13/91/115	-
41	A86	18	302	-	-	15/34/90/90	0/3/3/3
30	CLA	38	309	25	1/1/15/20	16/37/115/115	-
30	CLA	11	302	-	1/1/11/20	5/13/91/115	-
41	A86	31	316	-	-	16/34/90/90	0/3/3/3
35	LHG	a	407	-	-	23/50/50/53	-
30	CLA	38	303	25	1/1/15/20	14/37/115/115	-
30	CLA	16	307	25	1/1/11/20	9/13/91/115	-
30	CLA	34	306	-	1/1/11/20	8/13/91/115	-
41	A86	11	313	-	-	10/34/90/90	0/3/3/3

The worst 5 of 5718 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	39	310	A86	C14-C13	14.36	1.68	1.51
41	19	310	A86	C14-C13	14.29	1.68	1.51
41	11	313	A86	C14-C13	14.11	1.68	1.51
41	12	318	A86	C14-C13	14.10	1.68	1.51
41	33	315	A86	C14-C13	14.10	1.68	1.51

The worst 5 of 5504 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	37	315	A86	O1-C20-C19	55.34	154.96	113.38
41	17	311	A86	O1-C20-C19	55.33	154.95	113.38
41	17	315	A86	O1-C20-C19	55.33	154.95	113.38
41	37	311	A86	O1-C20-C19	55.30	154.93	113.38
41	18	313	A86	O1-C20-C19	55.09	154.76	113.38

5 of 254 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	A	402	CLA	ND
30	A	404	CLA	ND
30	B	601	CLA	ND
30	B	602	CLA	ND
30	B	603	CLA	ND

5 of 5224 torsion outliers are listed below:

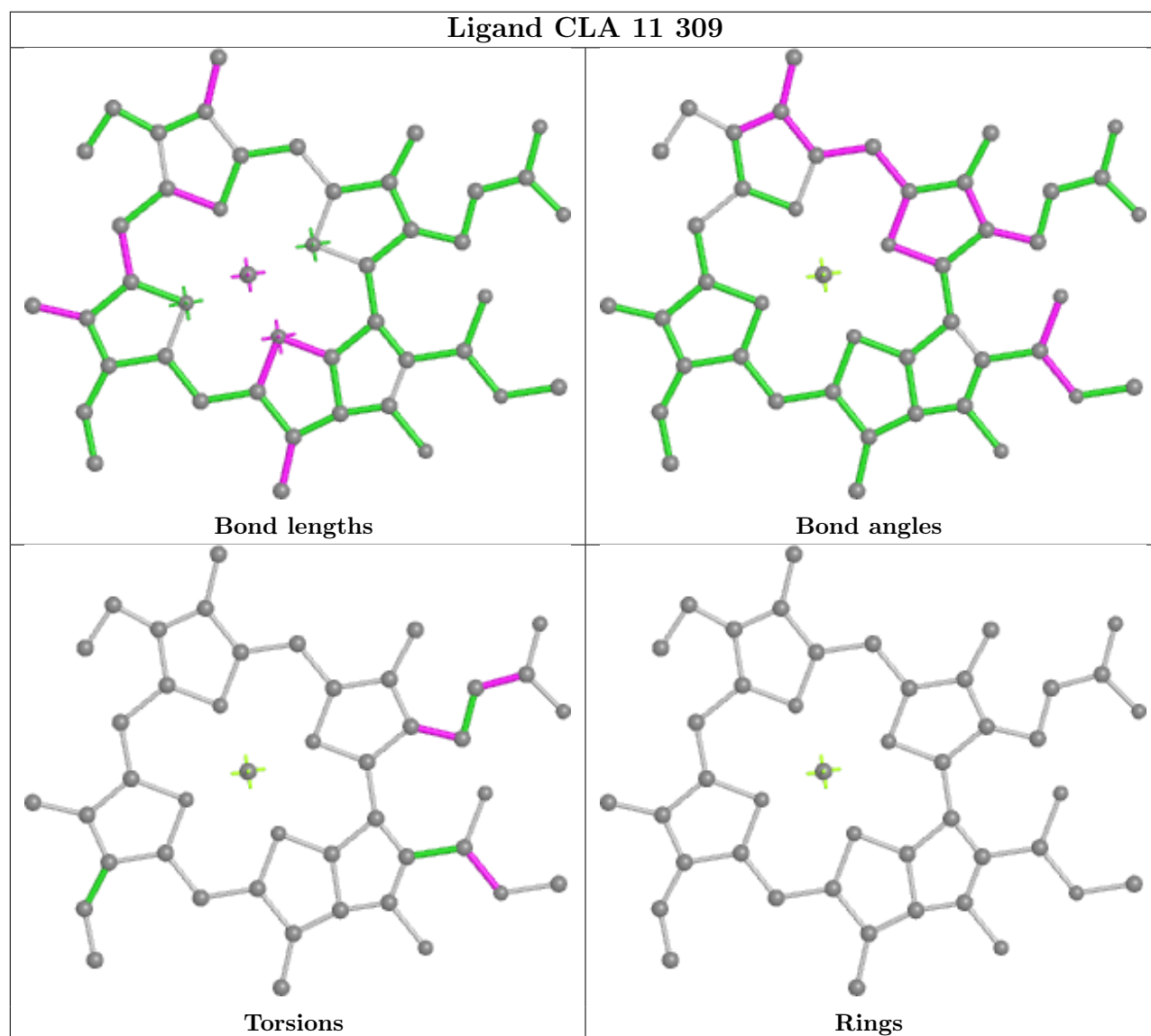
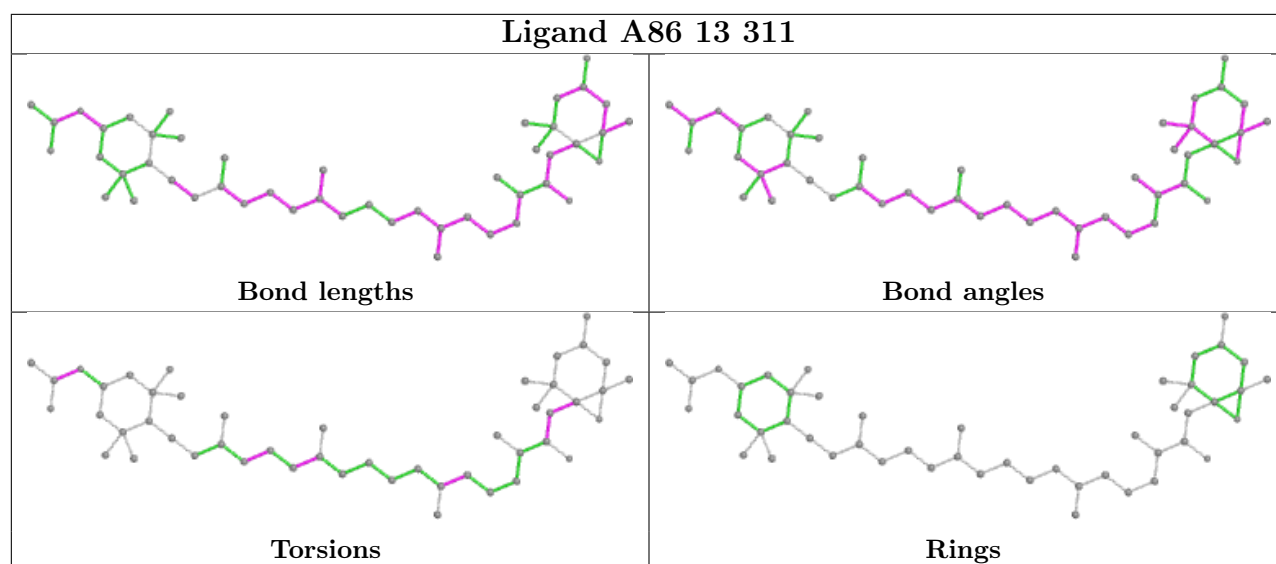
Mol	Chain	Res	Type	Atoms
30	A	402	CLA	CBD-CGD-O2D-CED
30	B	601	CLA	C1A-C2A-CAA-CBA
30	B	601	CLA	CHA-CBD-CGD-O1D
30	B	601	CLA	CHA-CBD-CGD-O2D
30	B	601	CLA	CAD-CBD-CGD-O1D

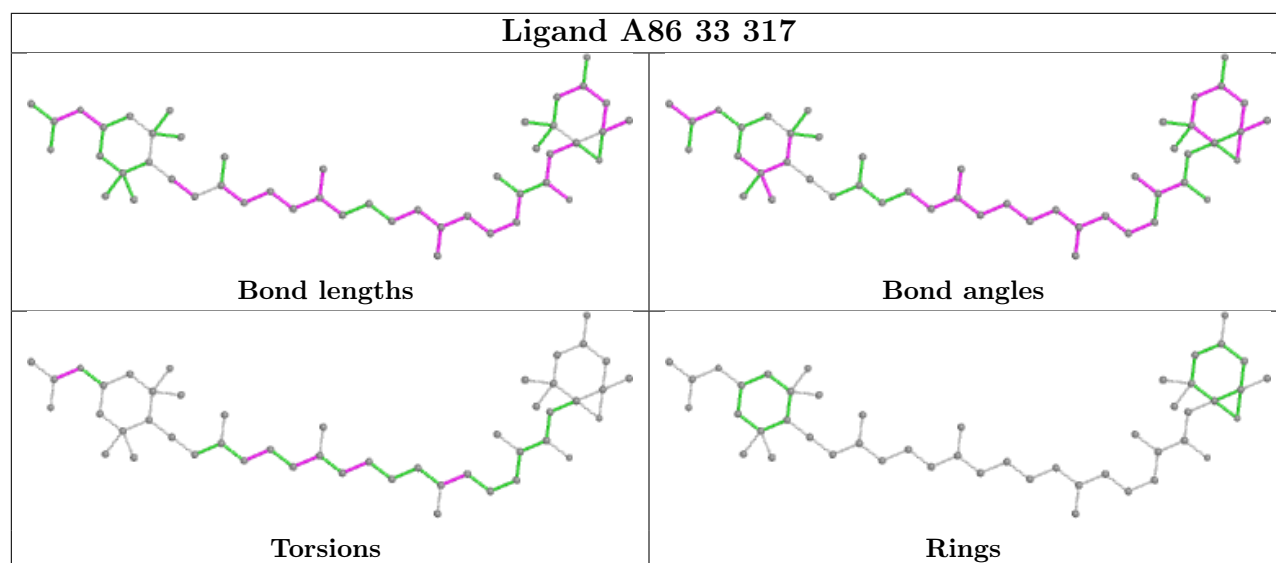
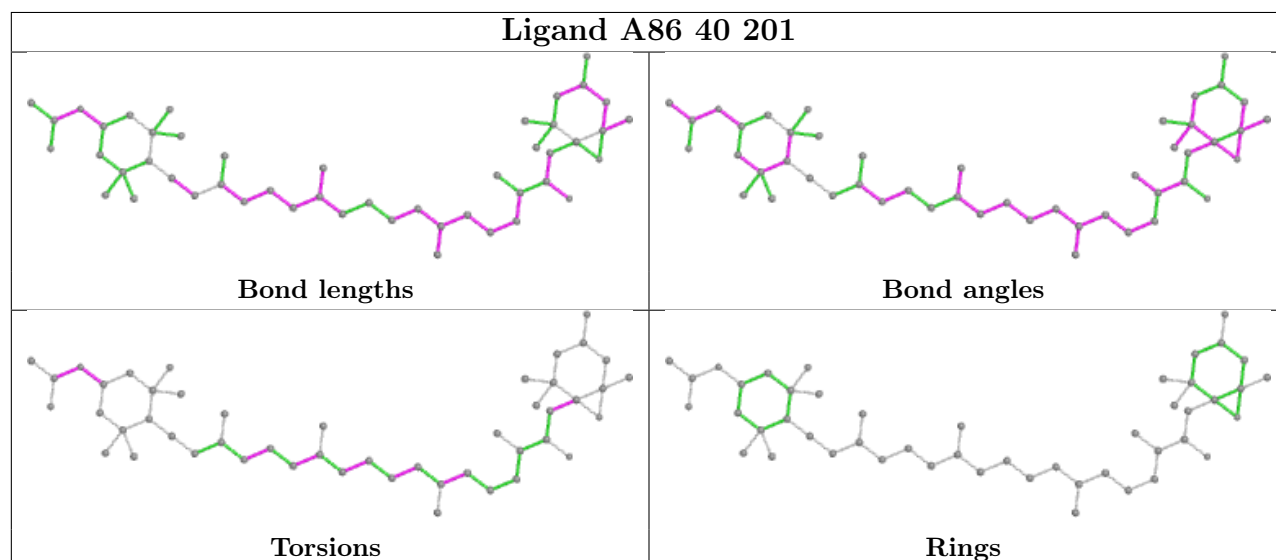
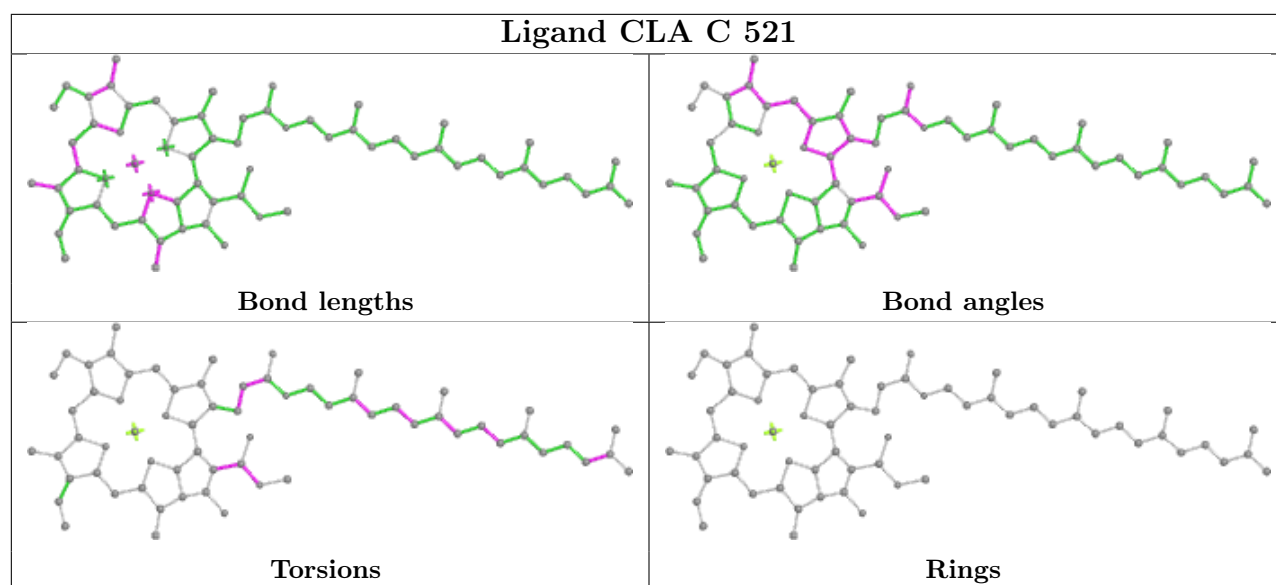
All (2) ring outliers are listed below:

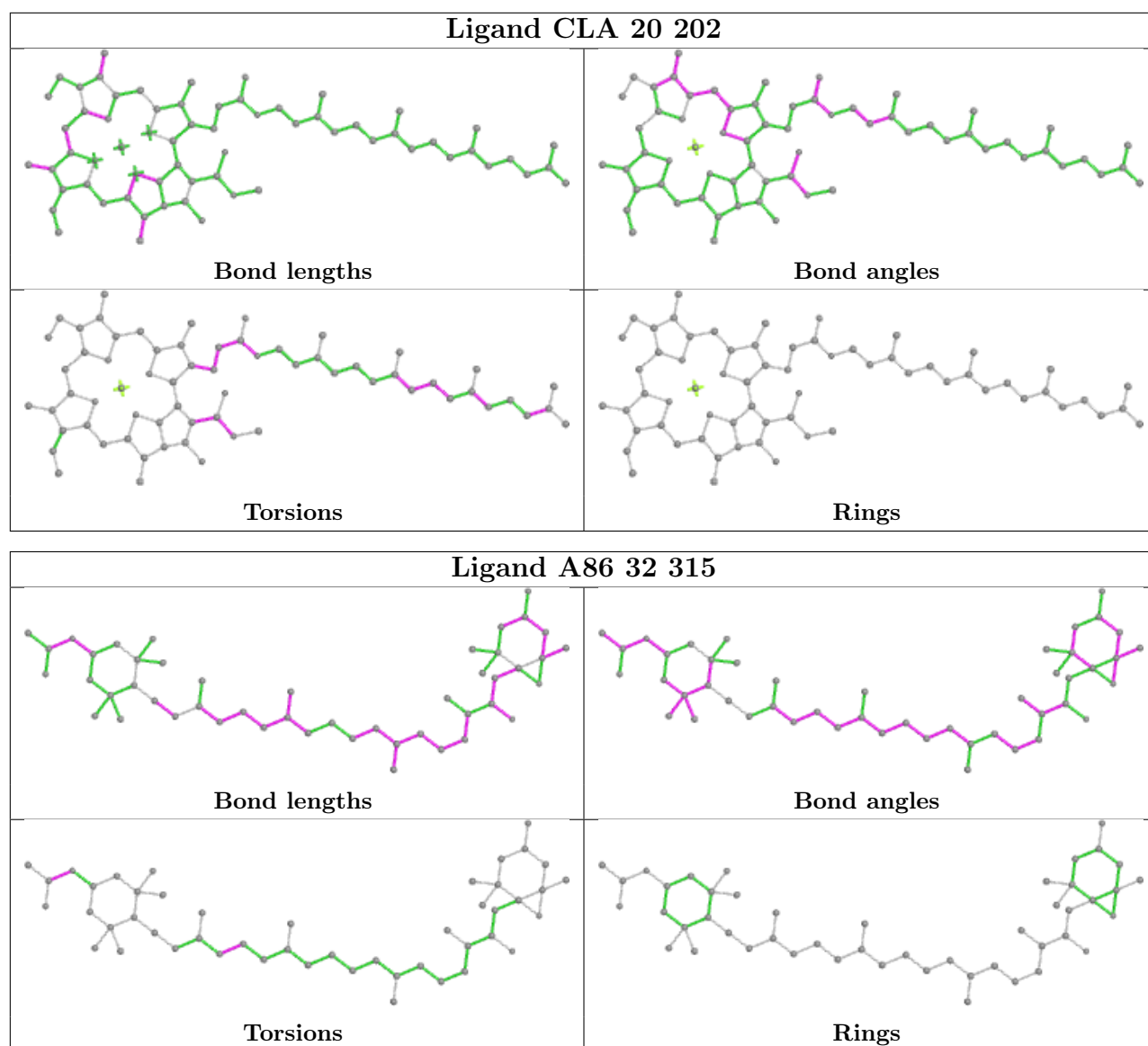
Mol	Chain	Res	Type	Atoms
41	17	302	A86	C31-C32-C33-C34-C35-C36
41	37	302	A86	C31-C32-C33-C34-C35-C36

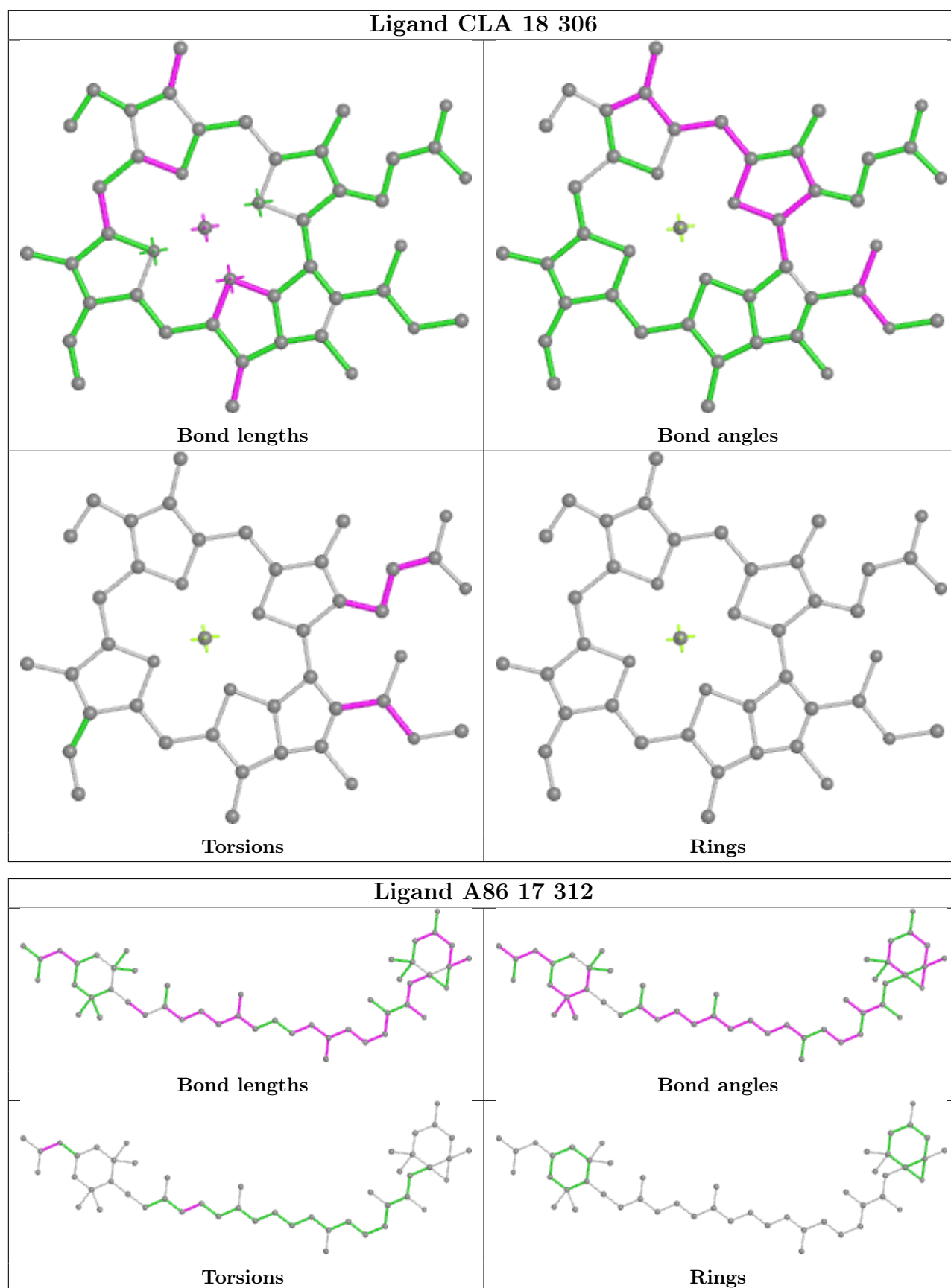
No monomer is involved in short contacts.

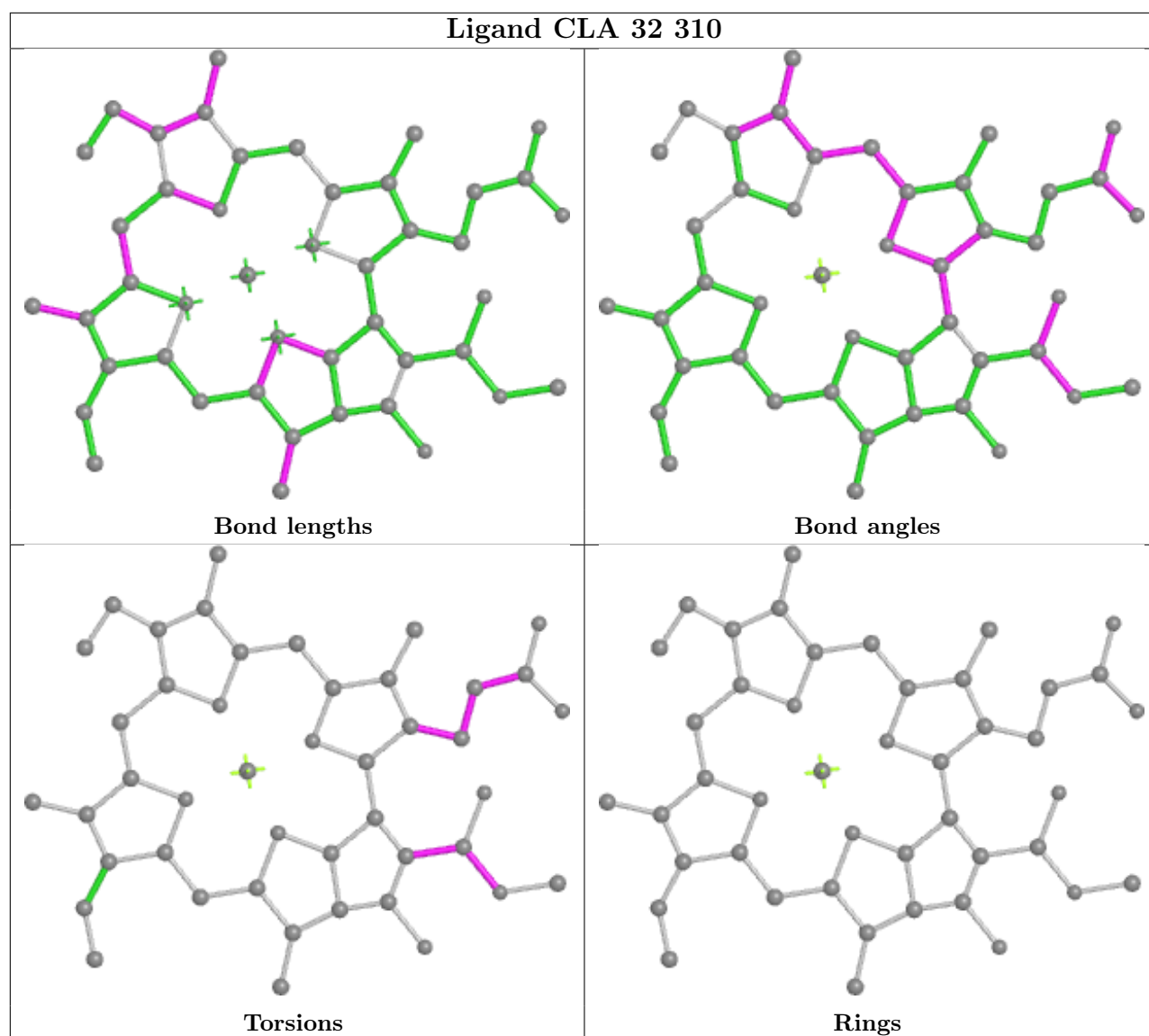
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

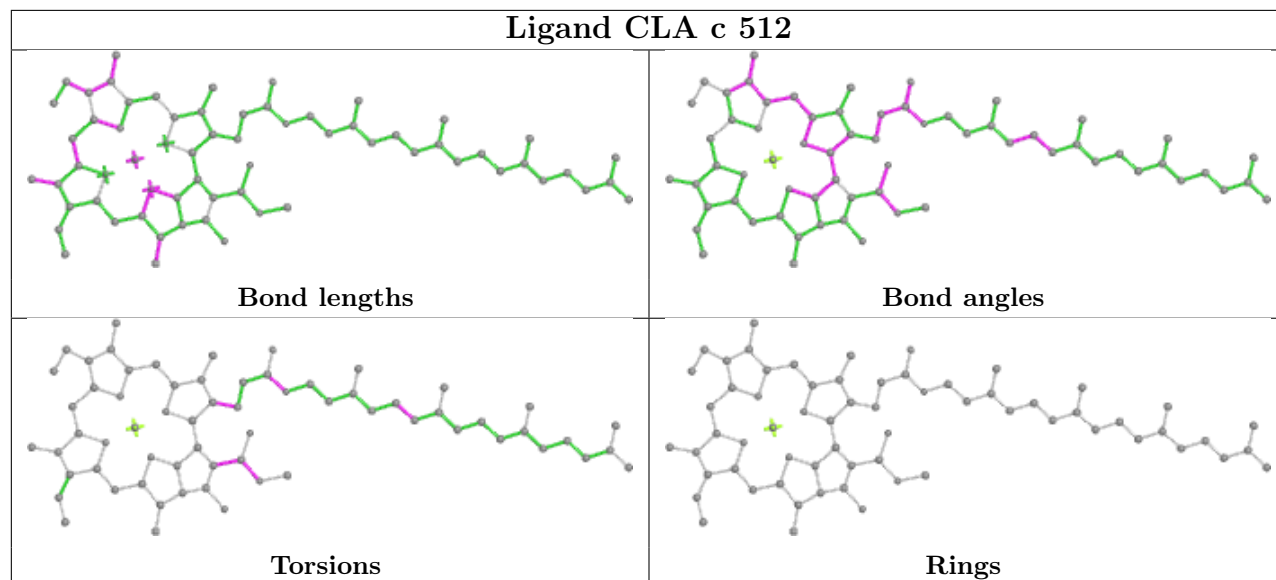
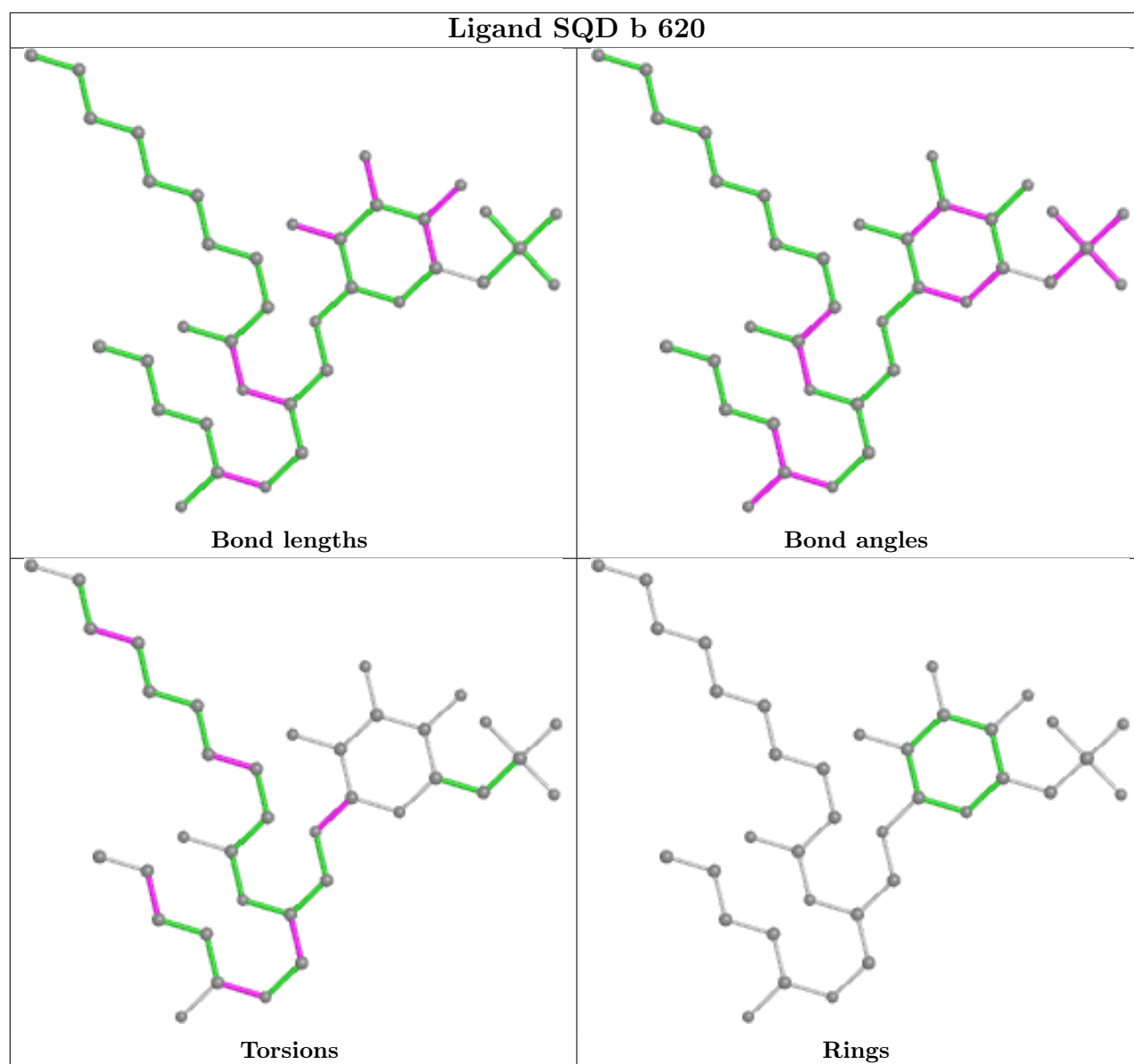


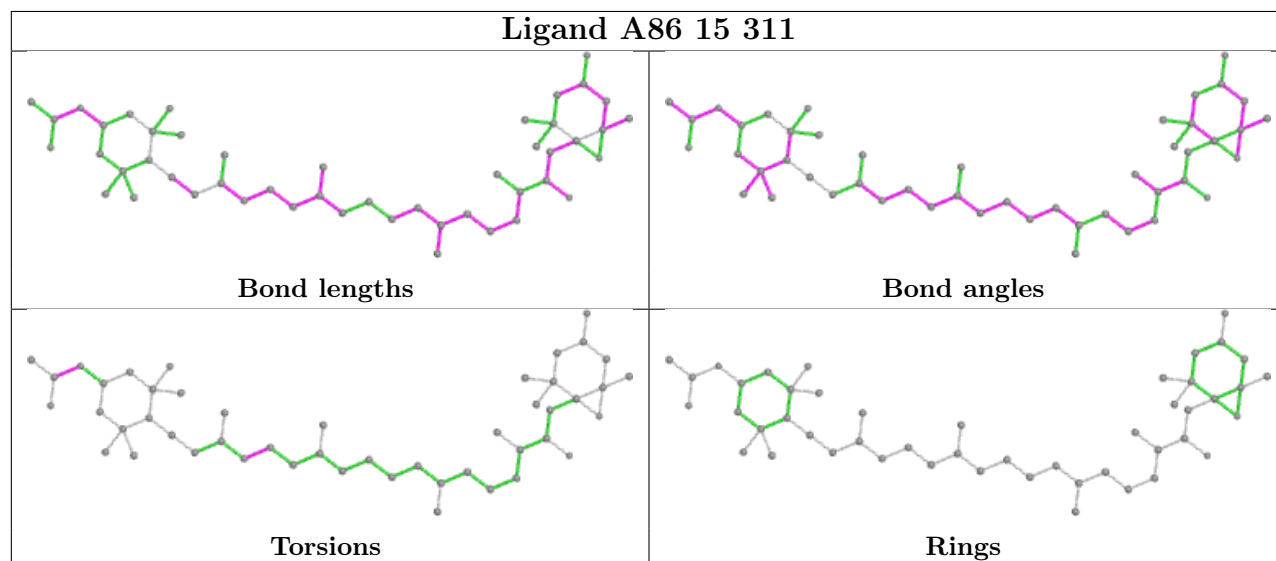
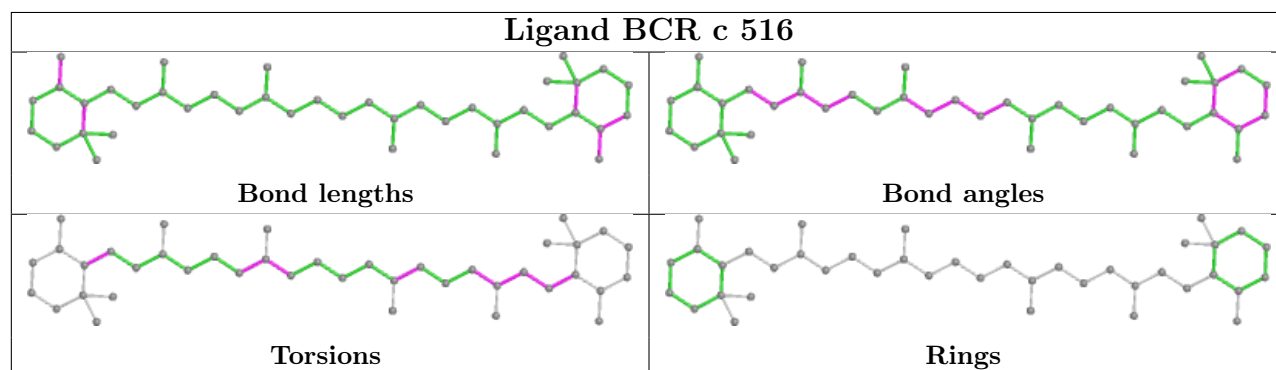
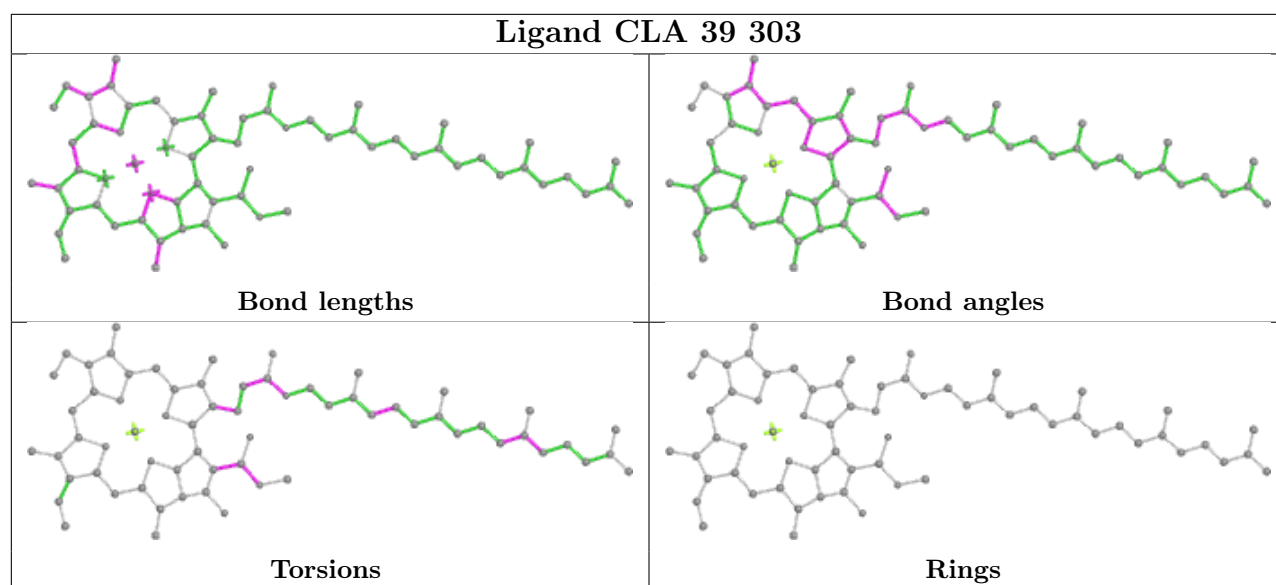


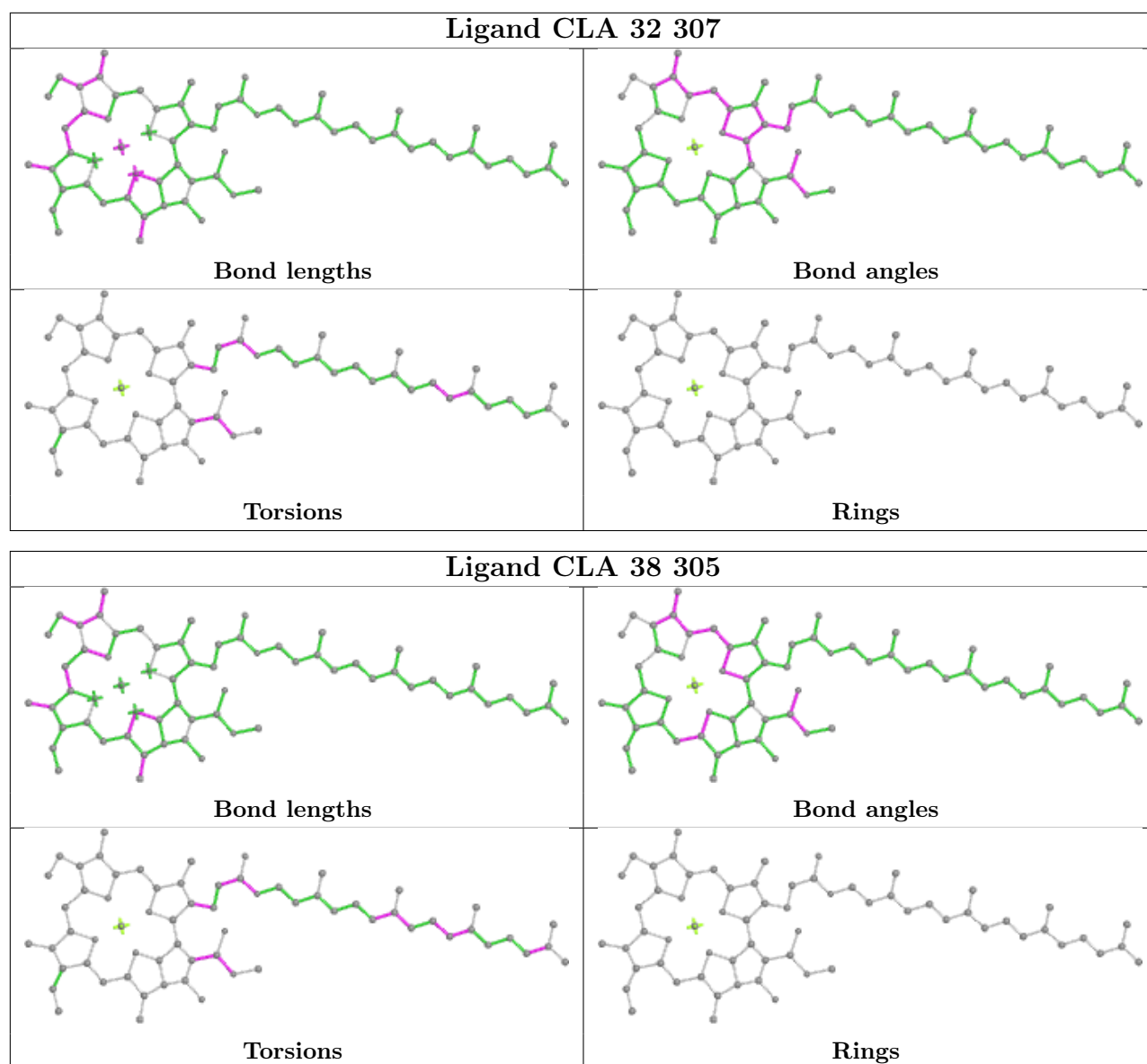


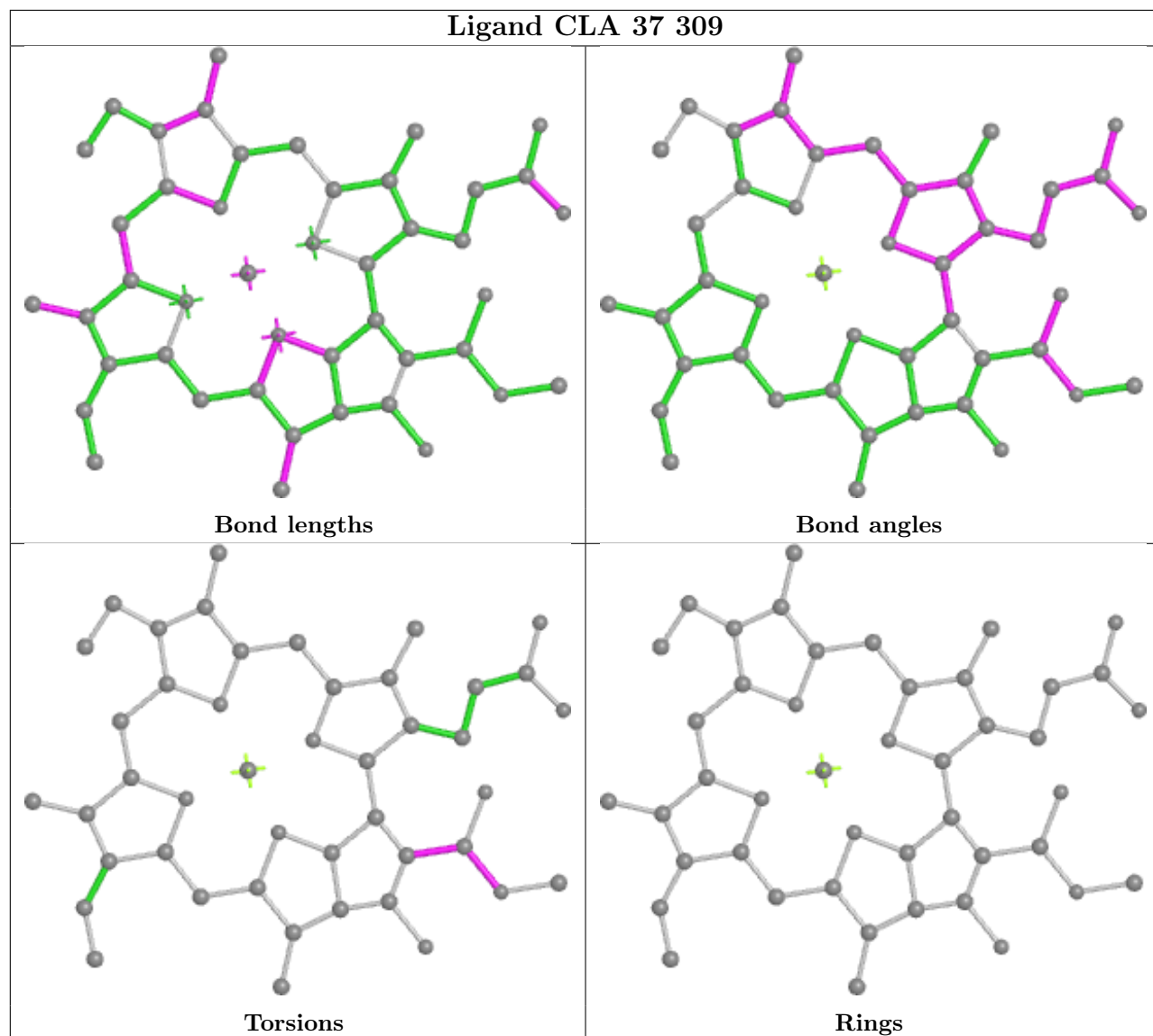


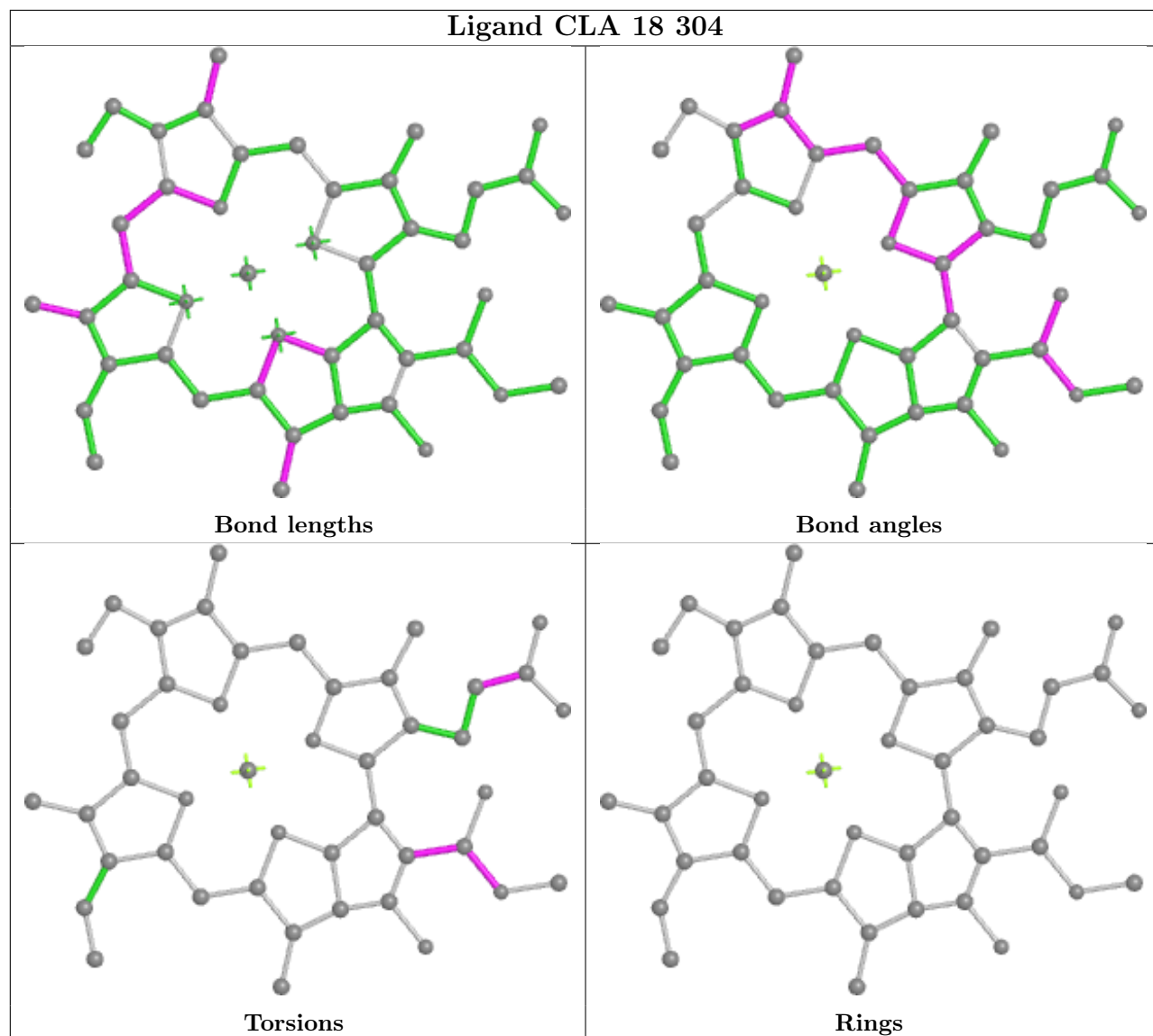


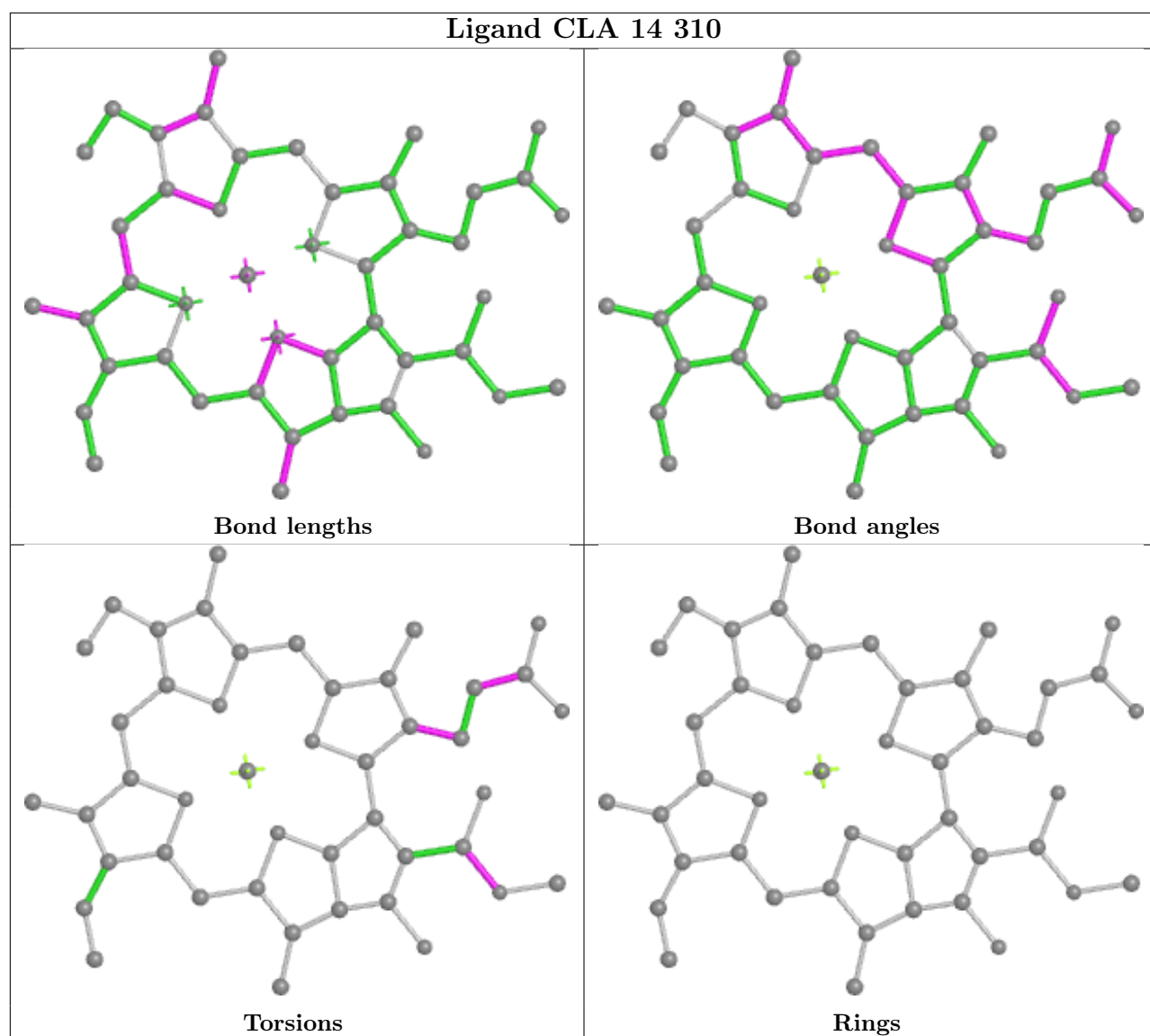




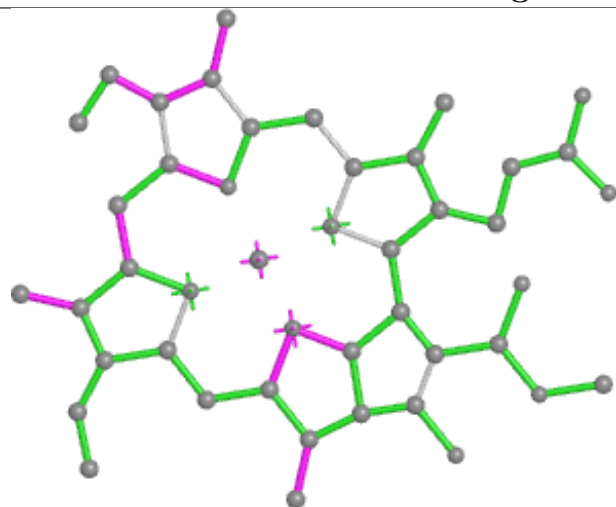




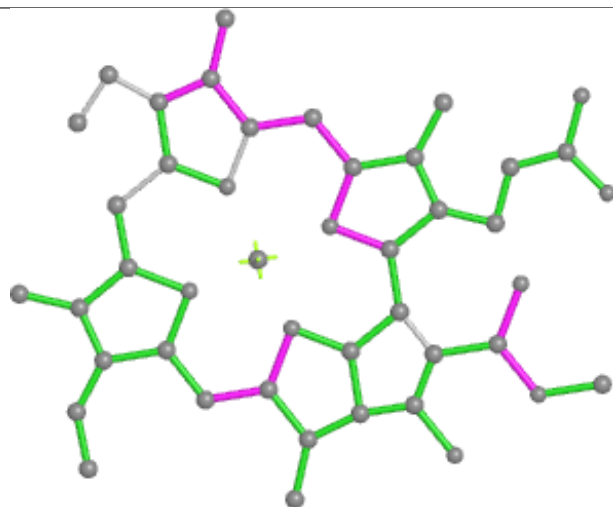




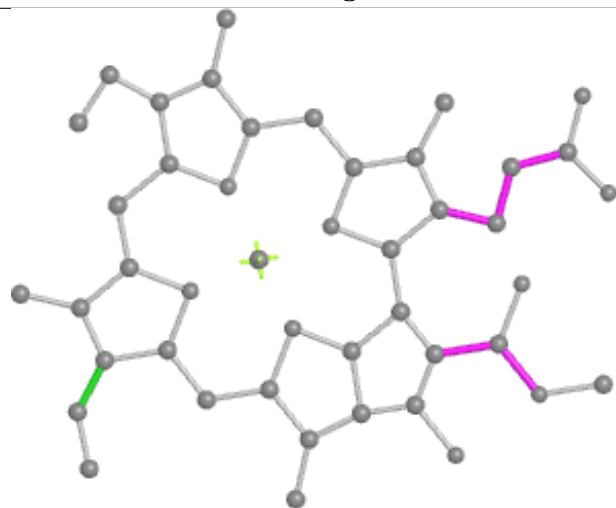
Ligand CLA 36 307



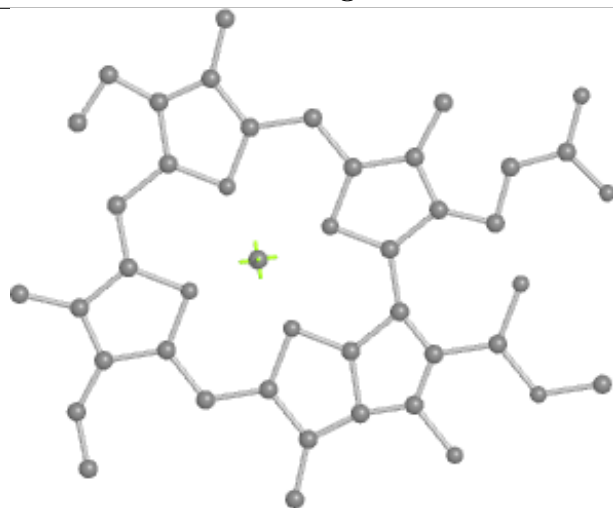
Bond lengths



Bond angles

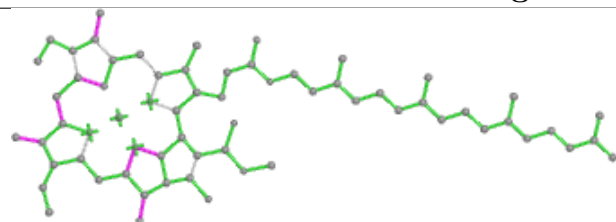


Torsions

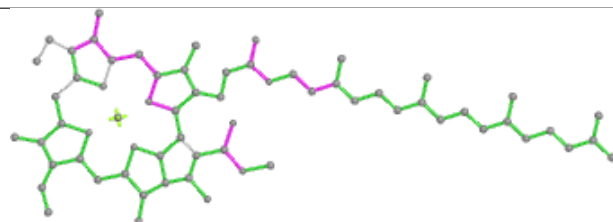


Rings

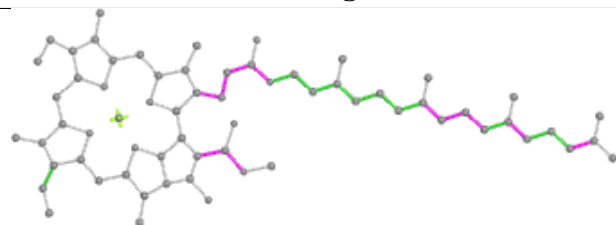
Ligand CLA 40 202



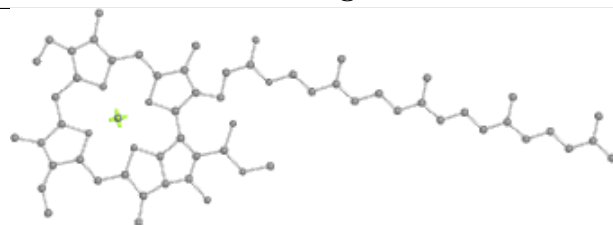
Bond lengths



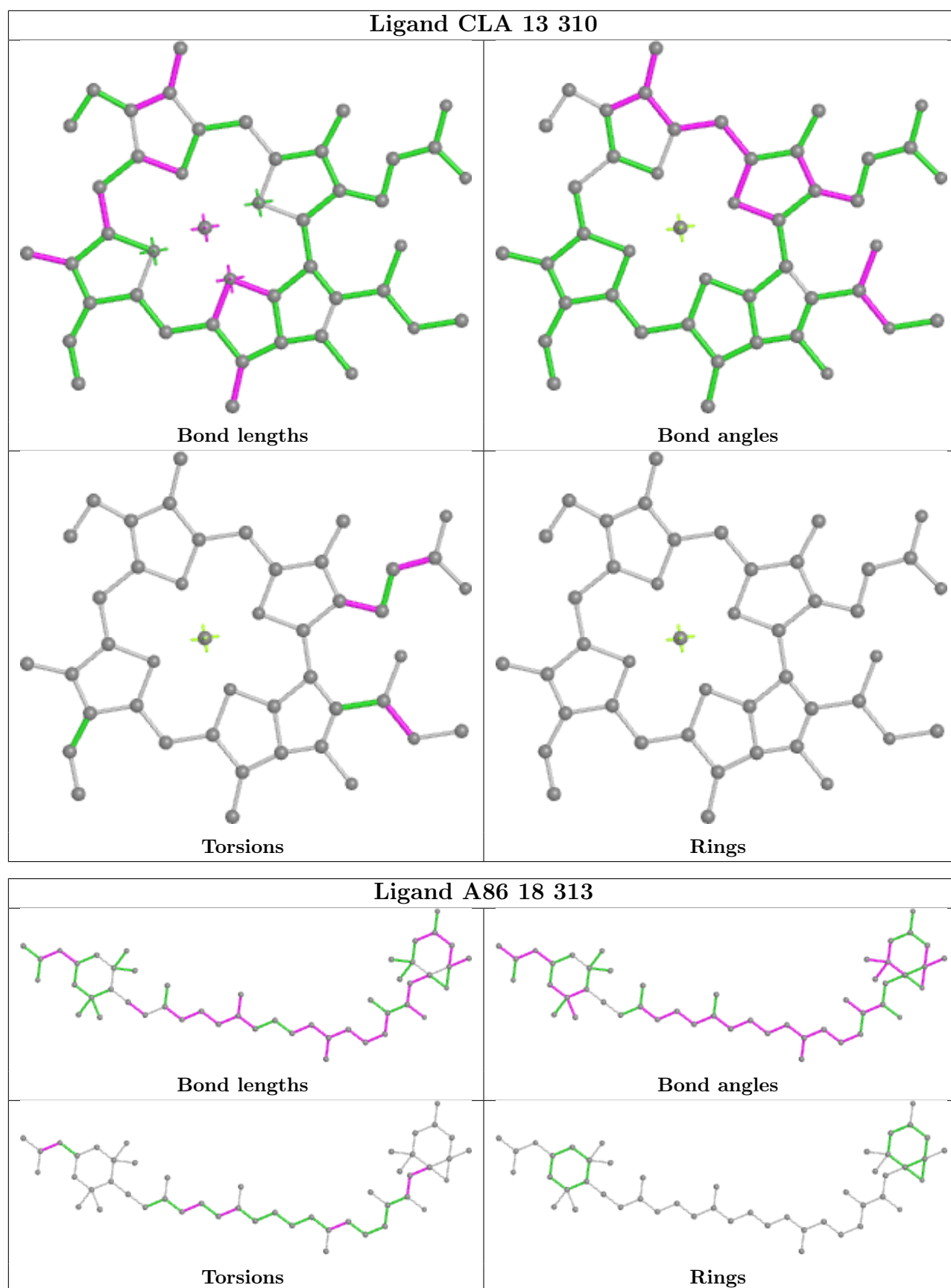
Bond angles

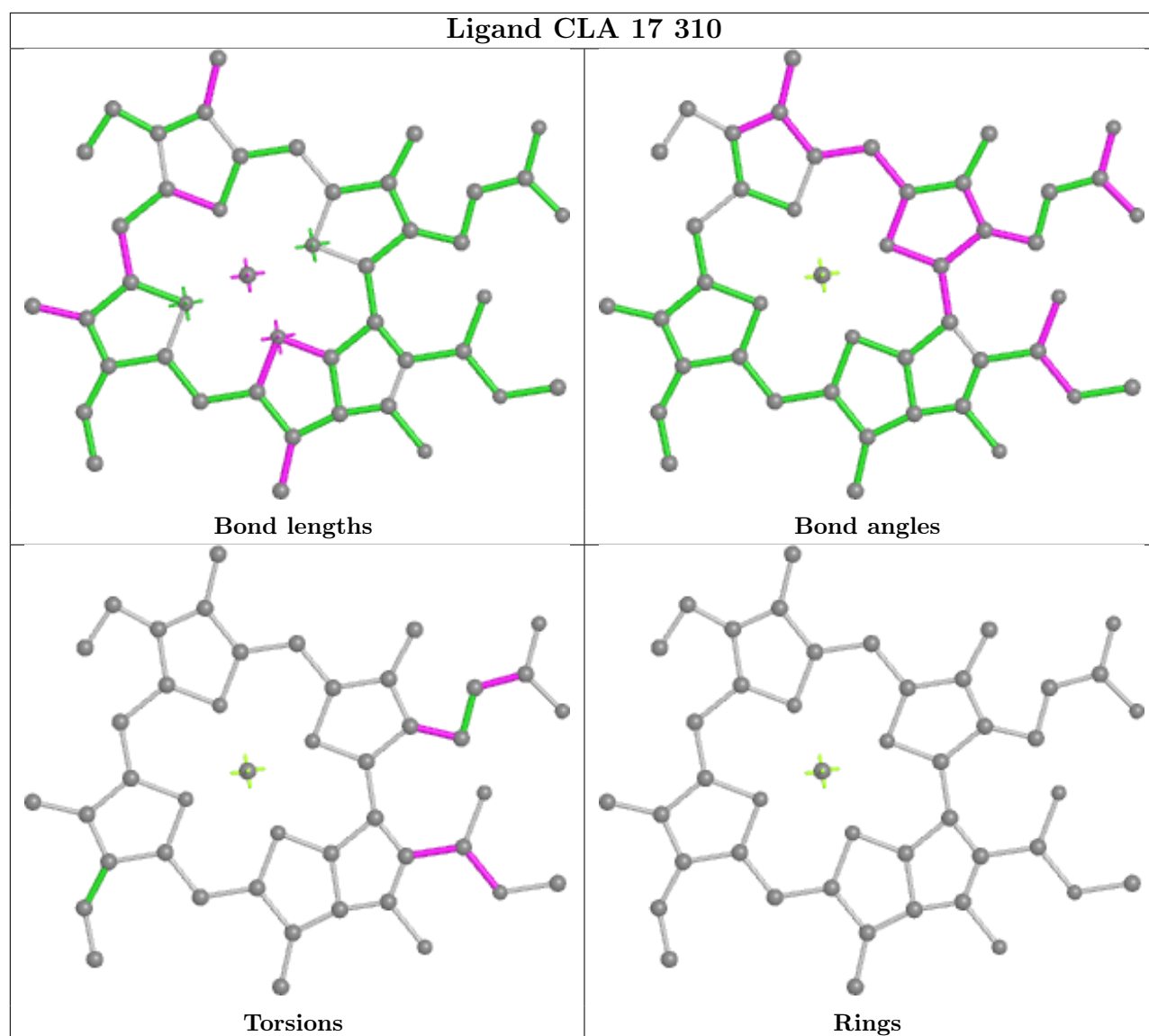


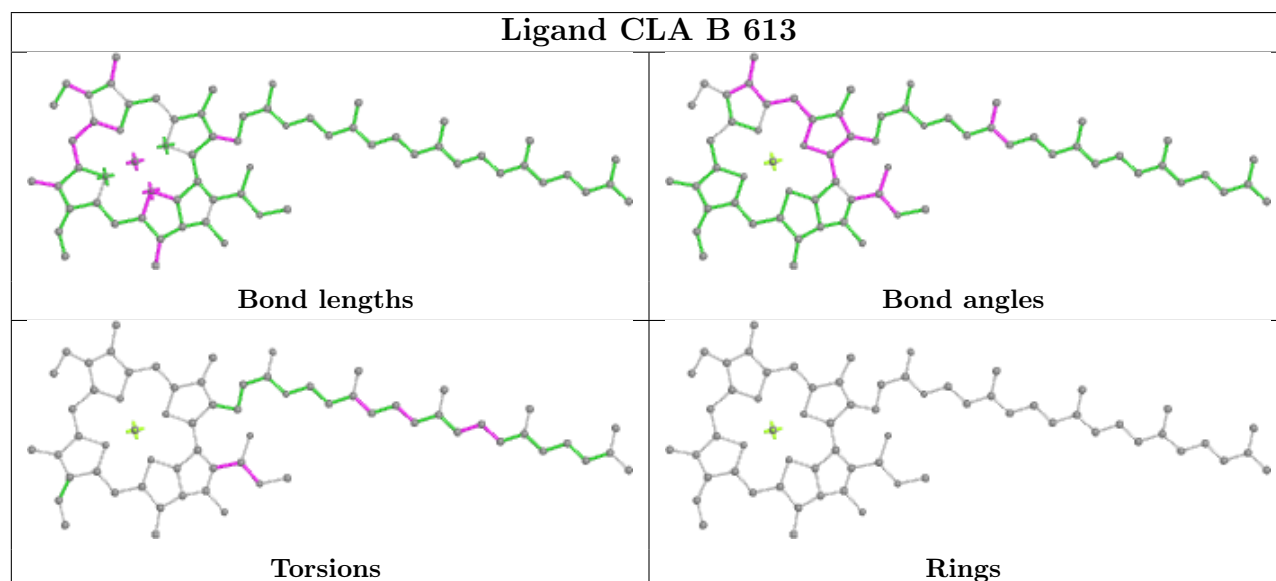
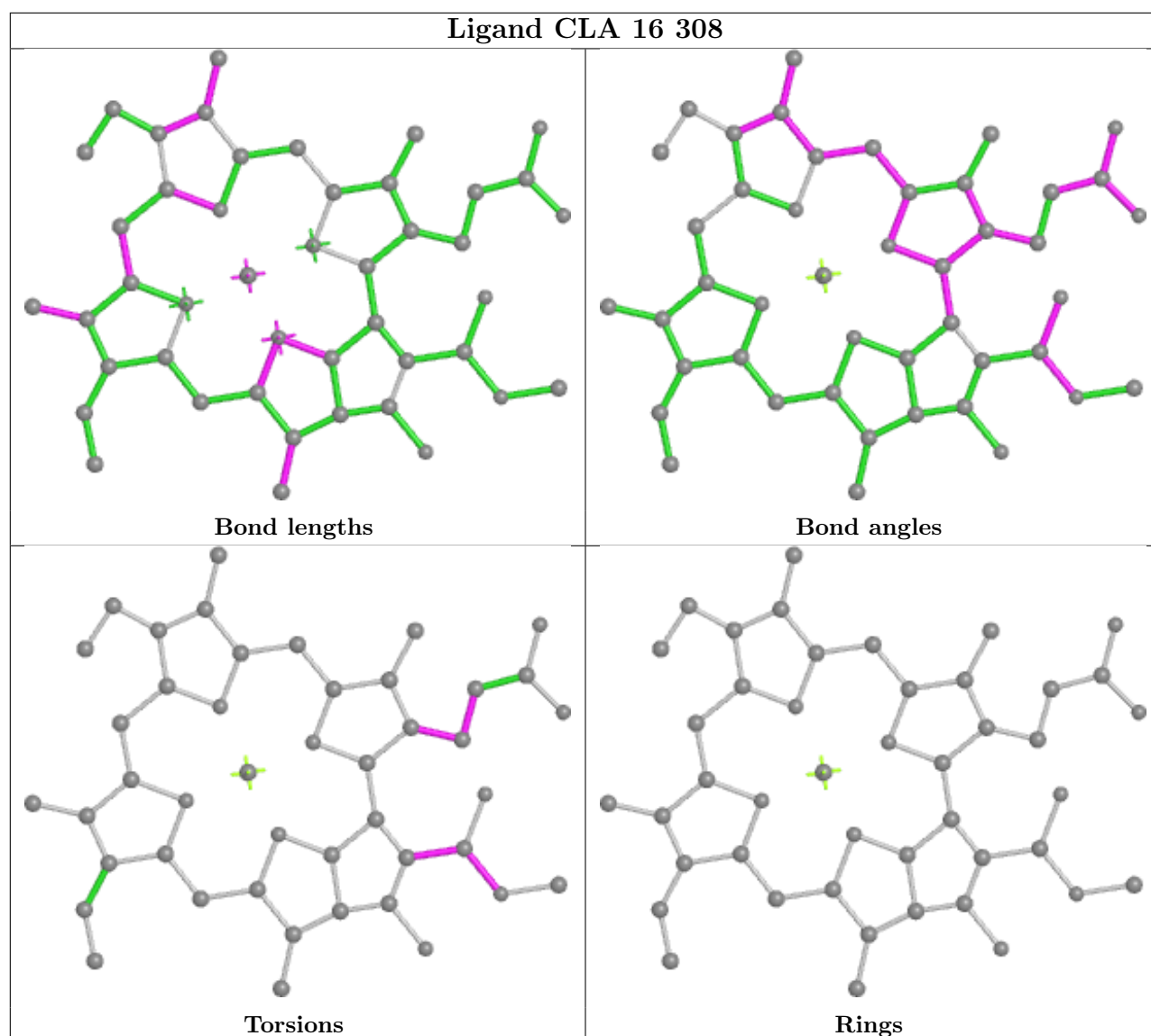
Torsions

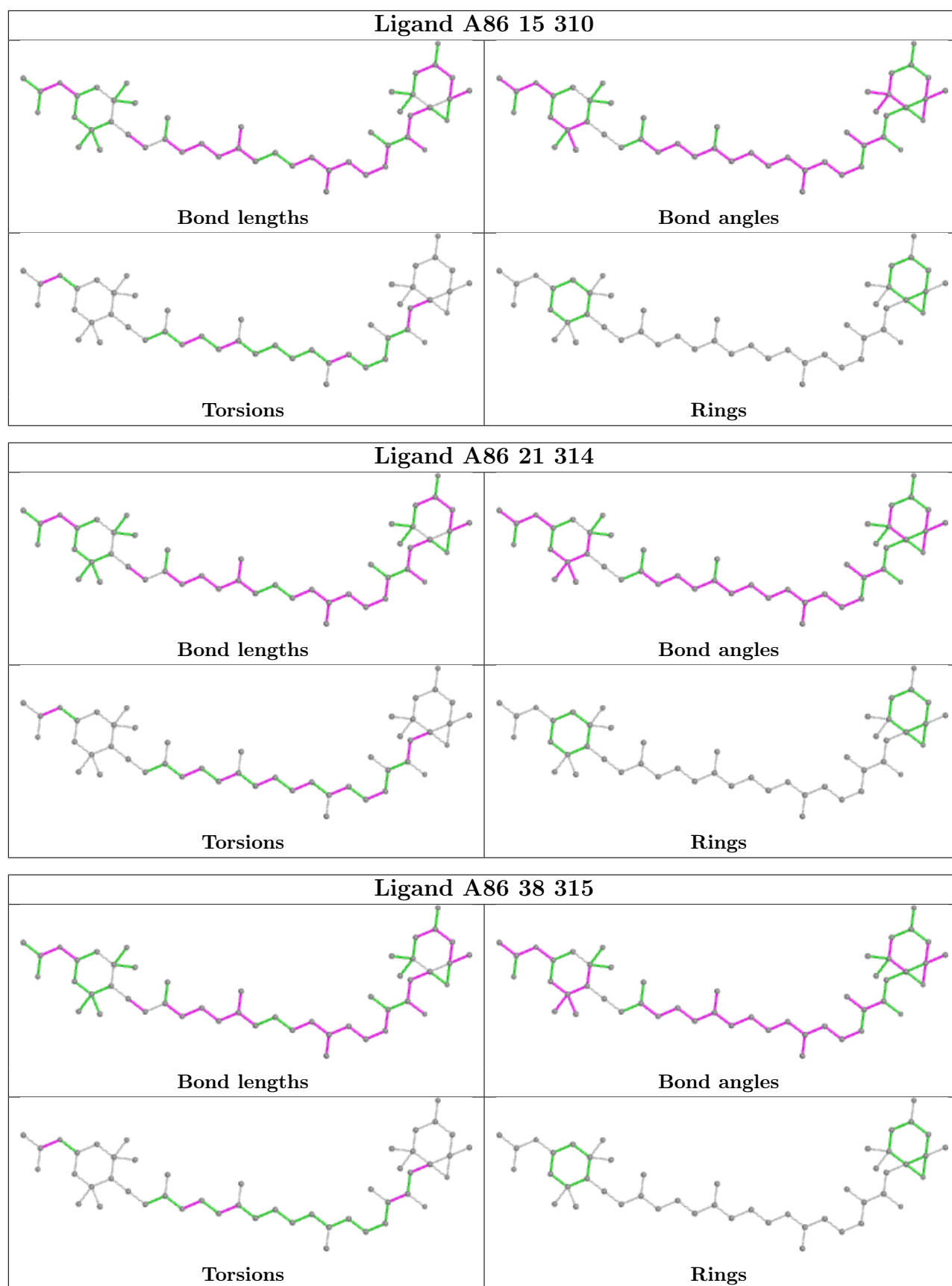


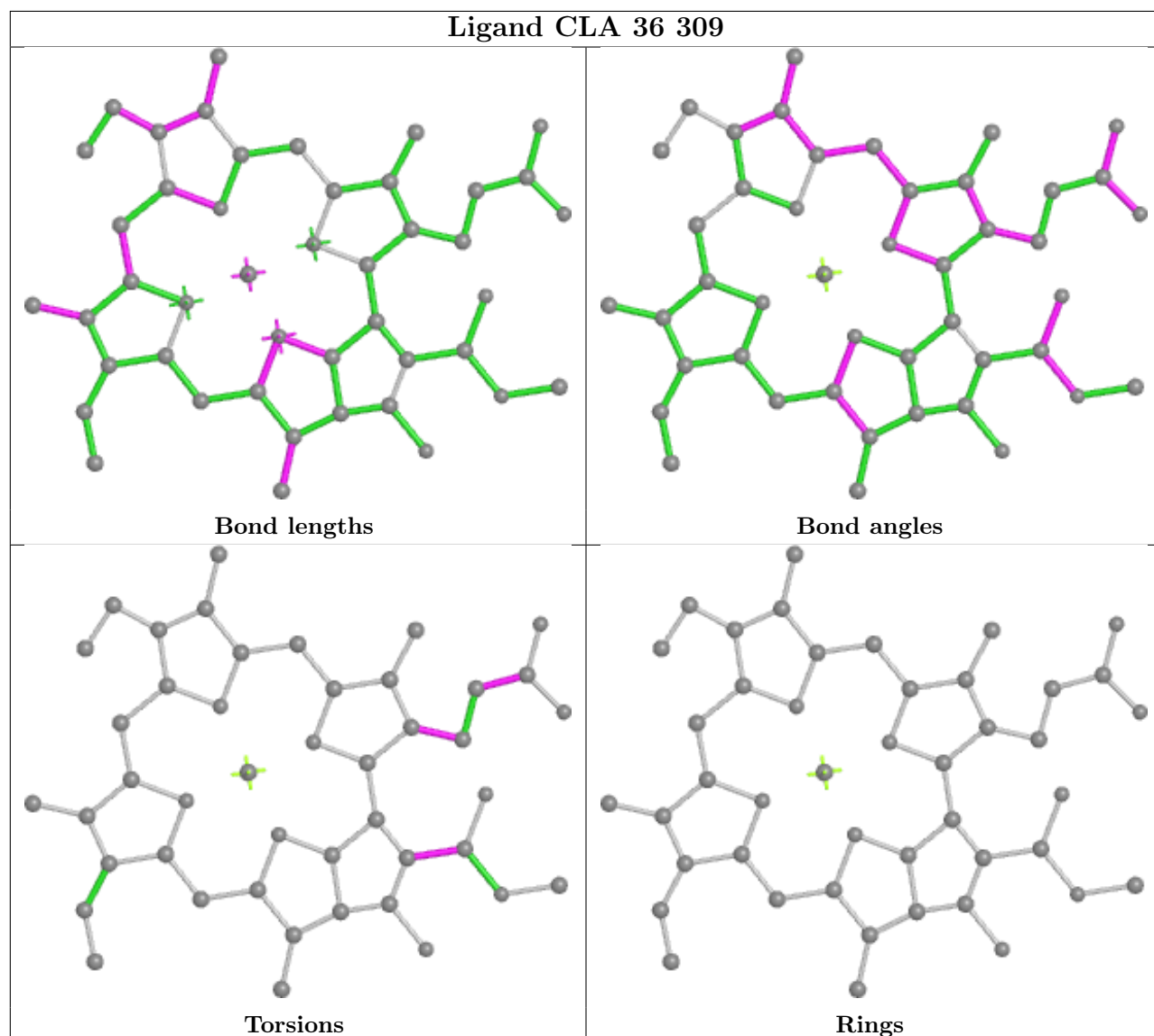
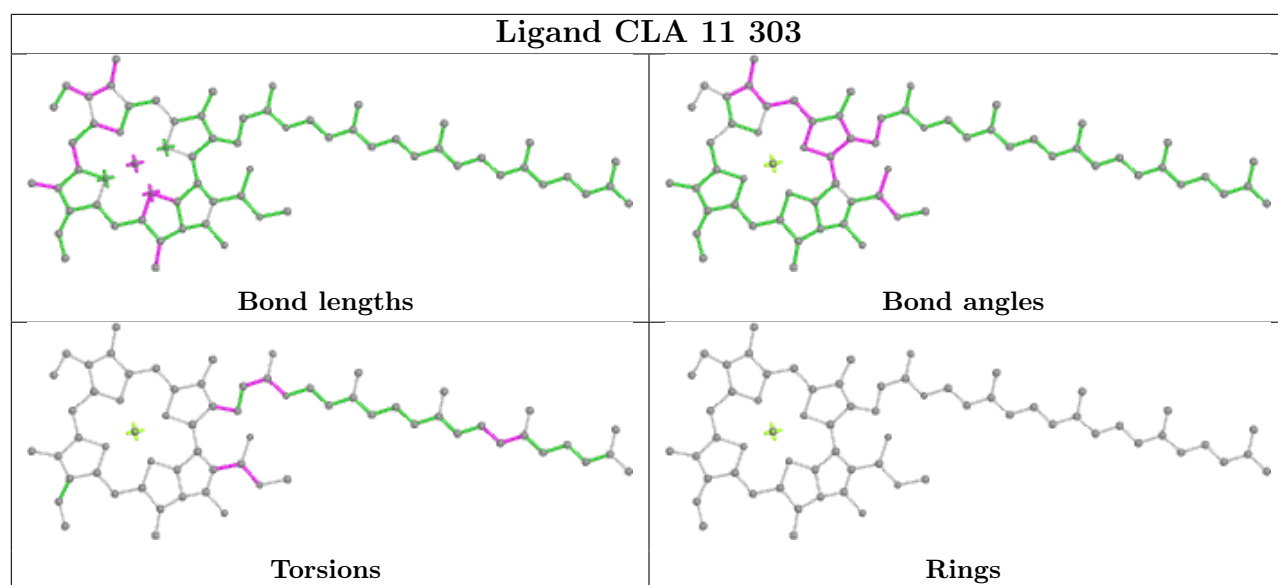
Rings

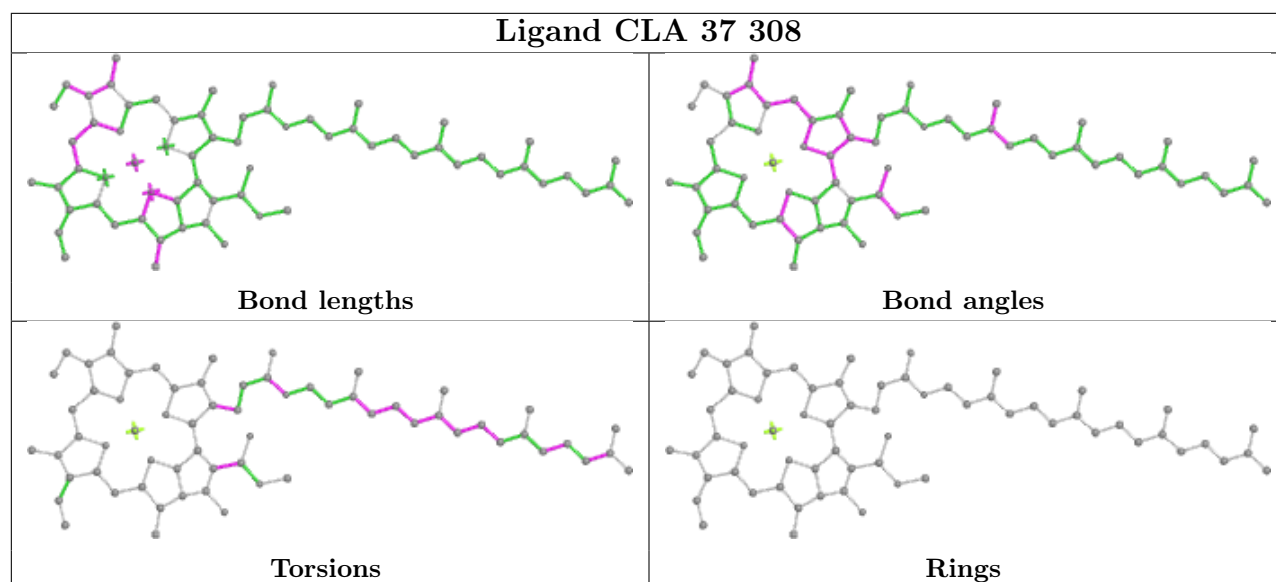
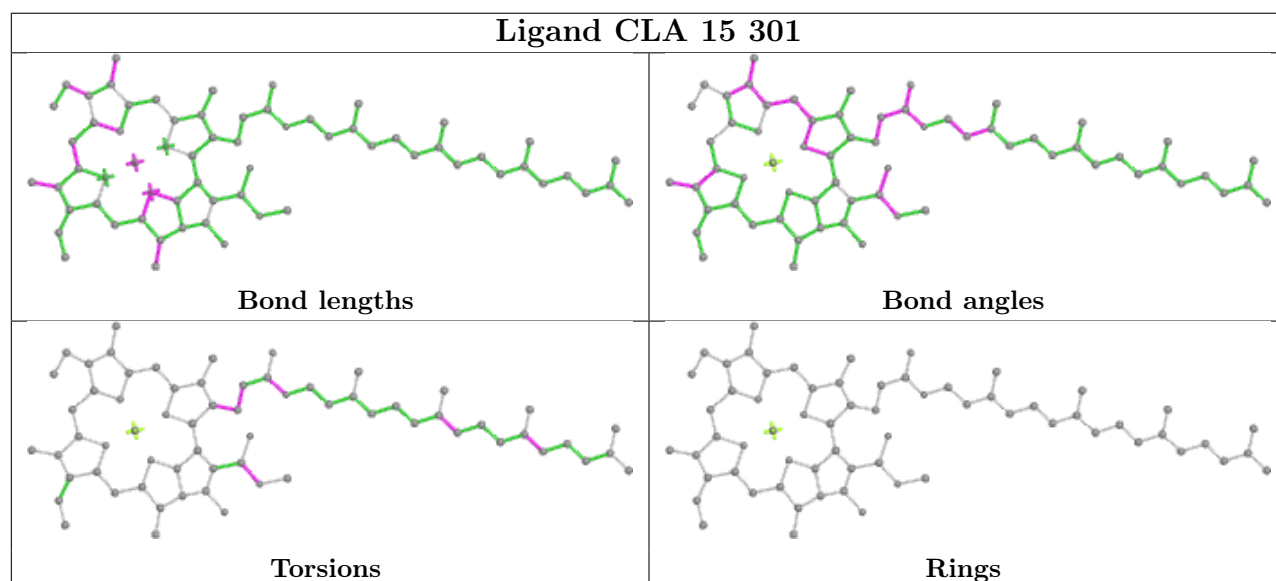
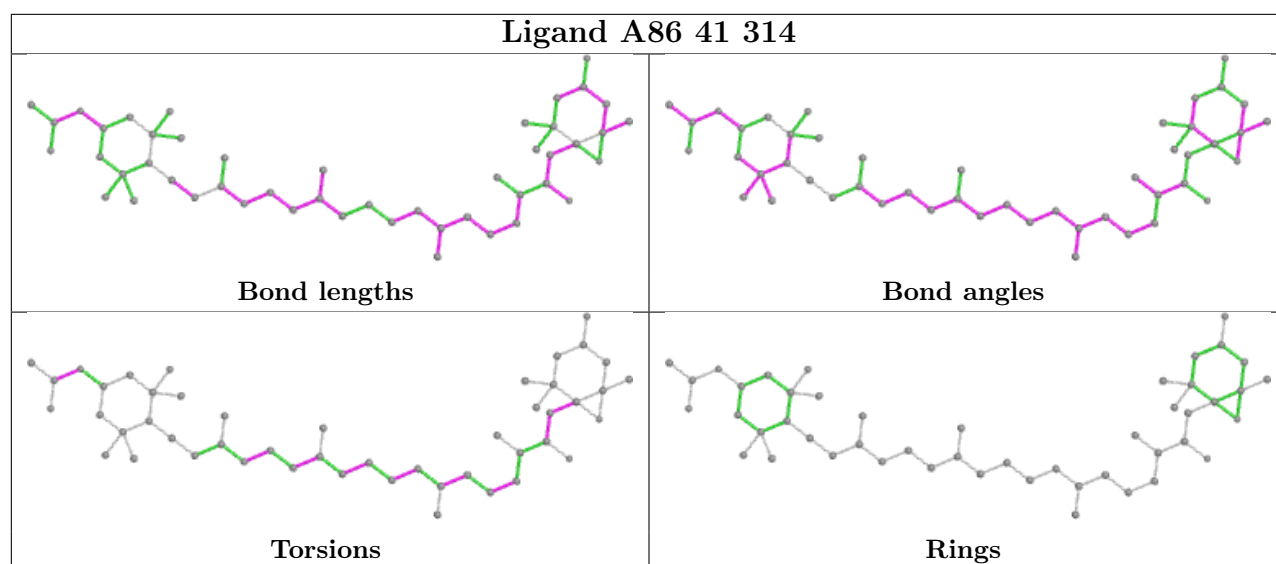


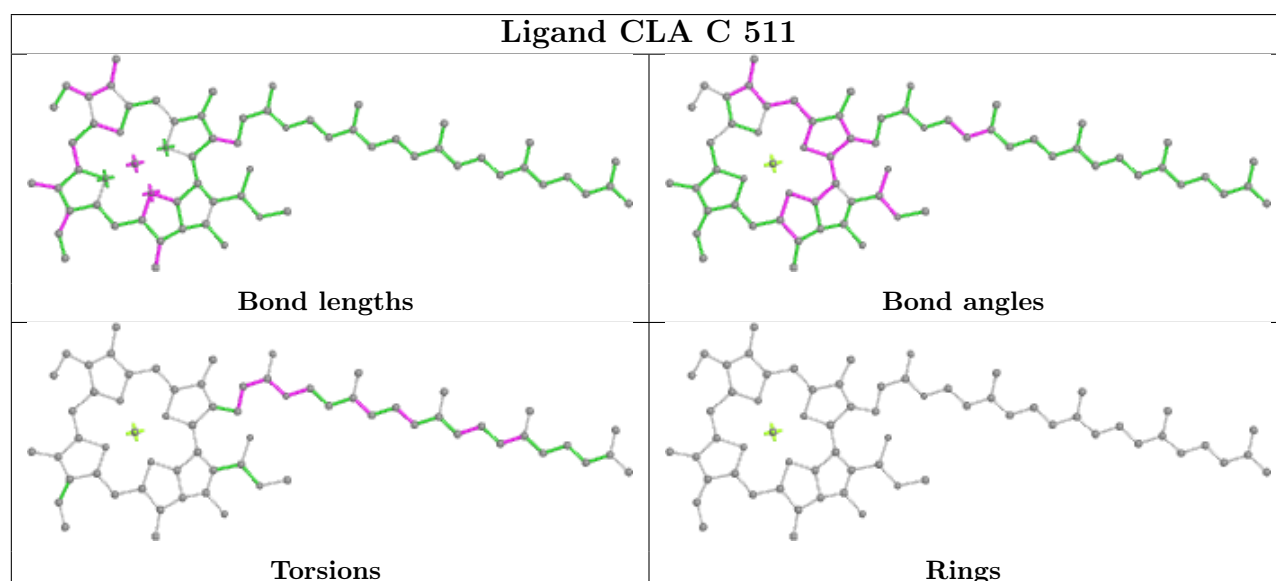
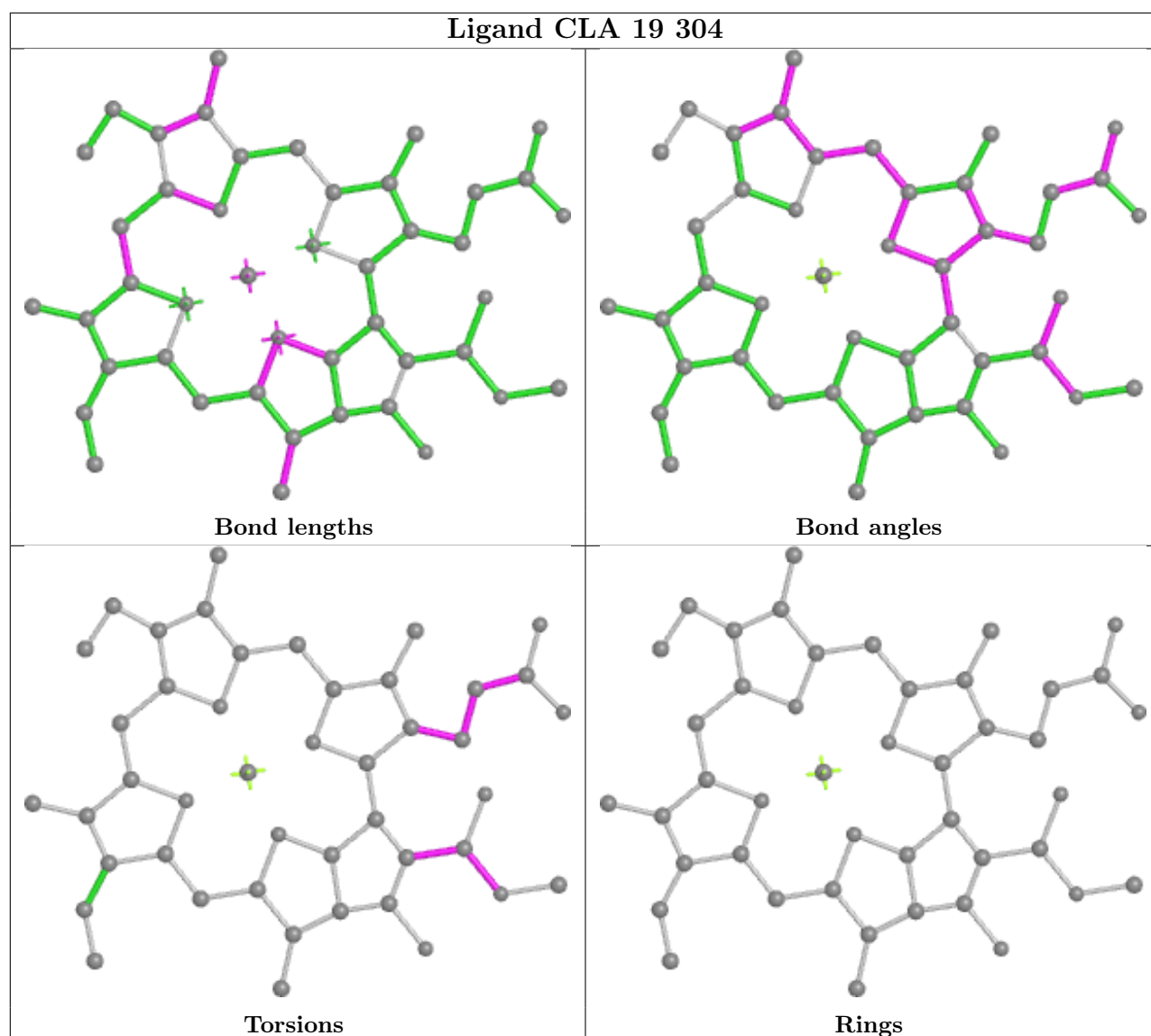


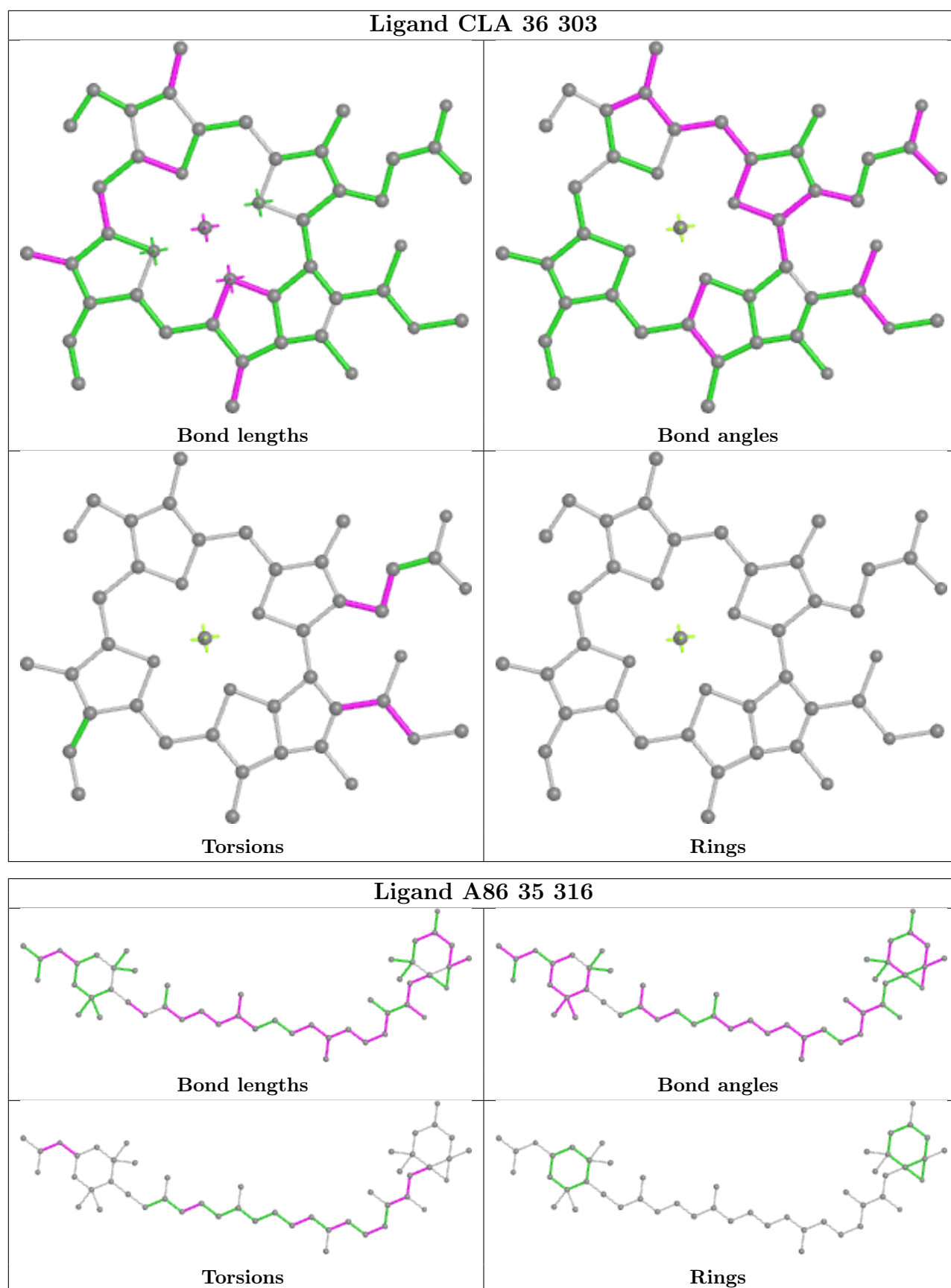


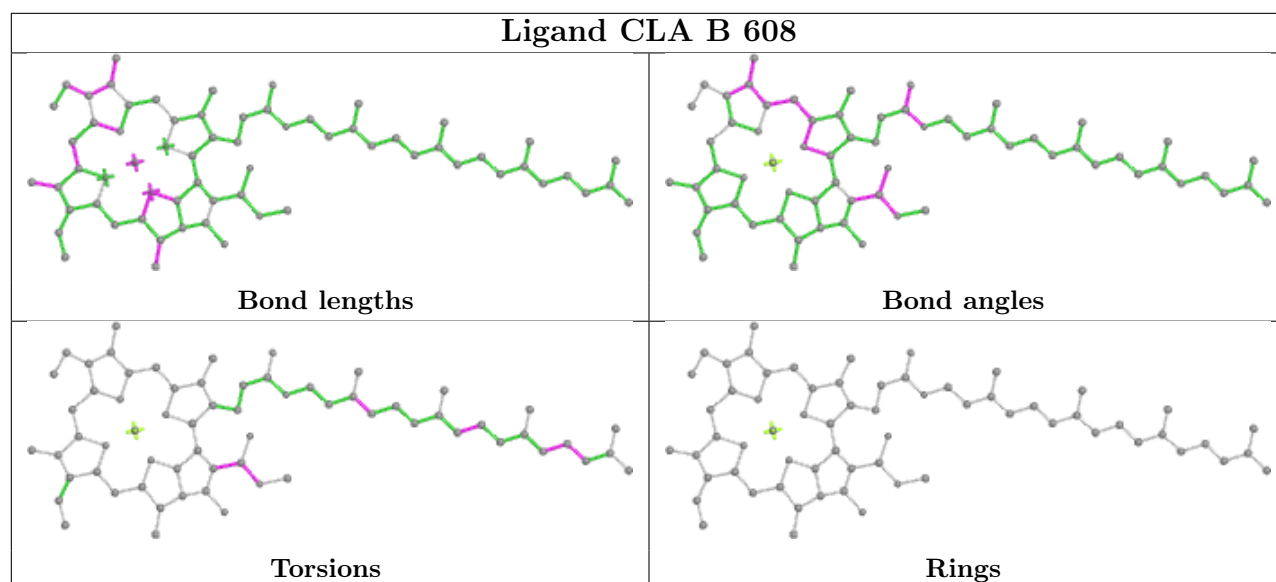
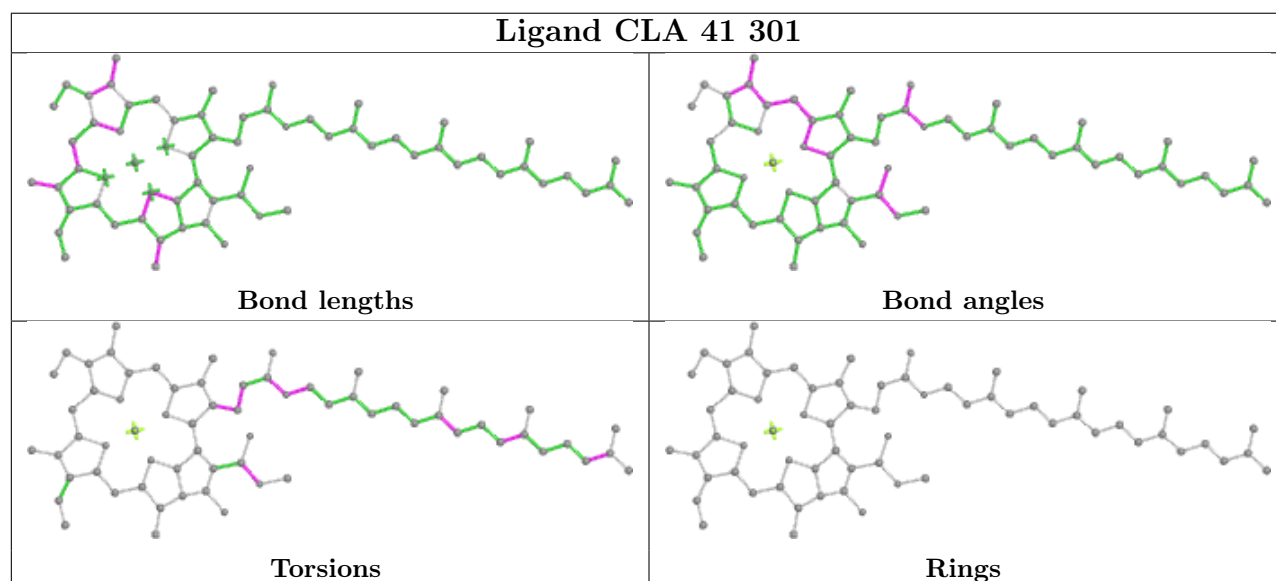
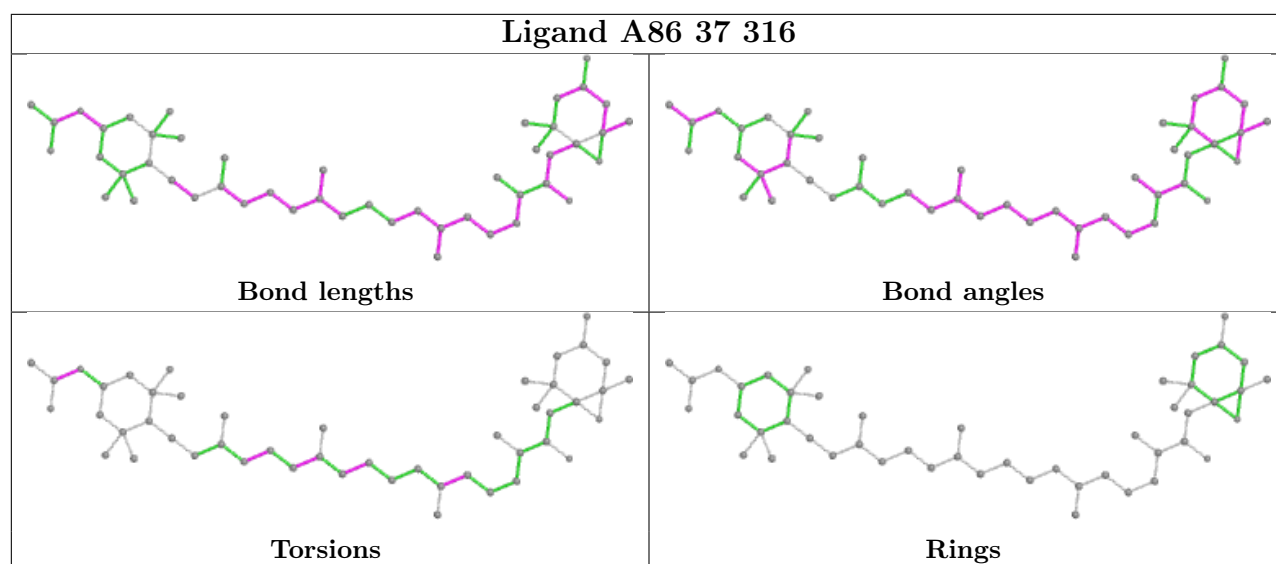


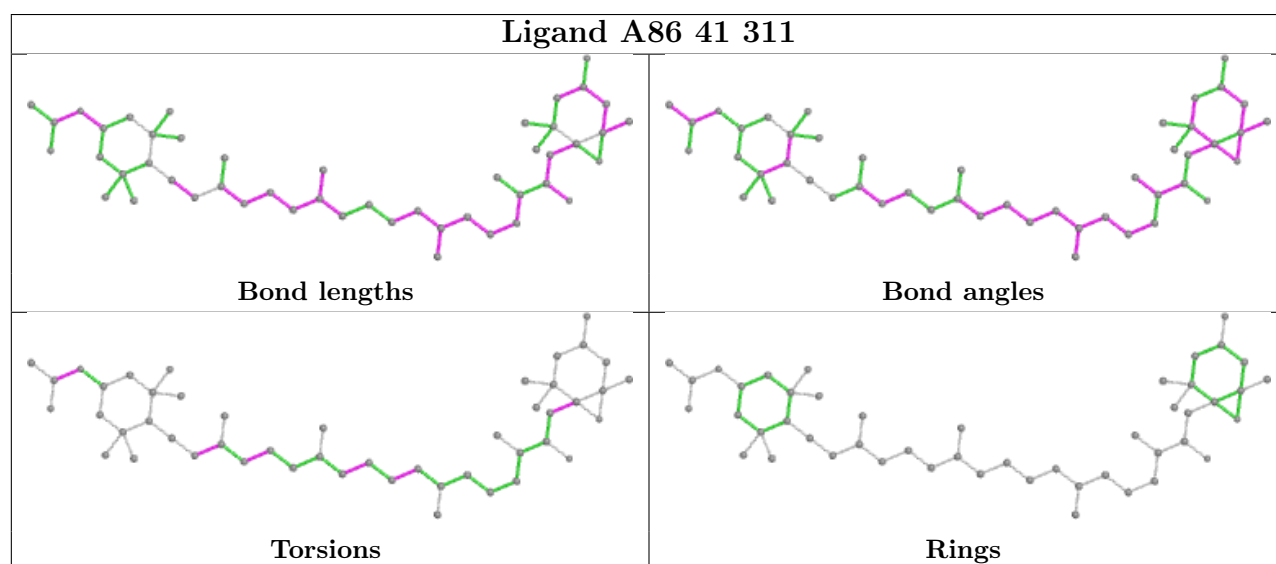
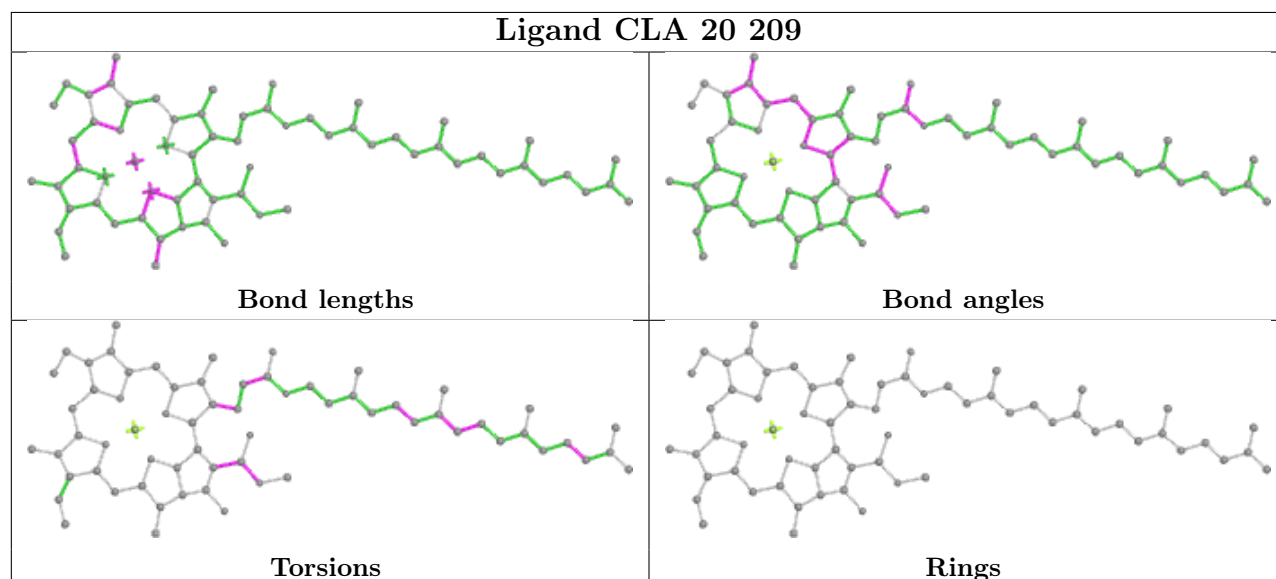
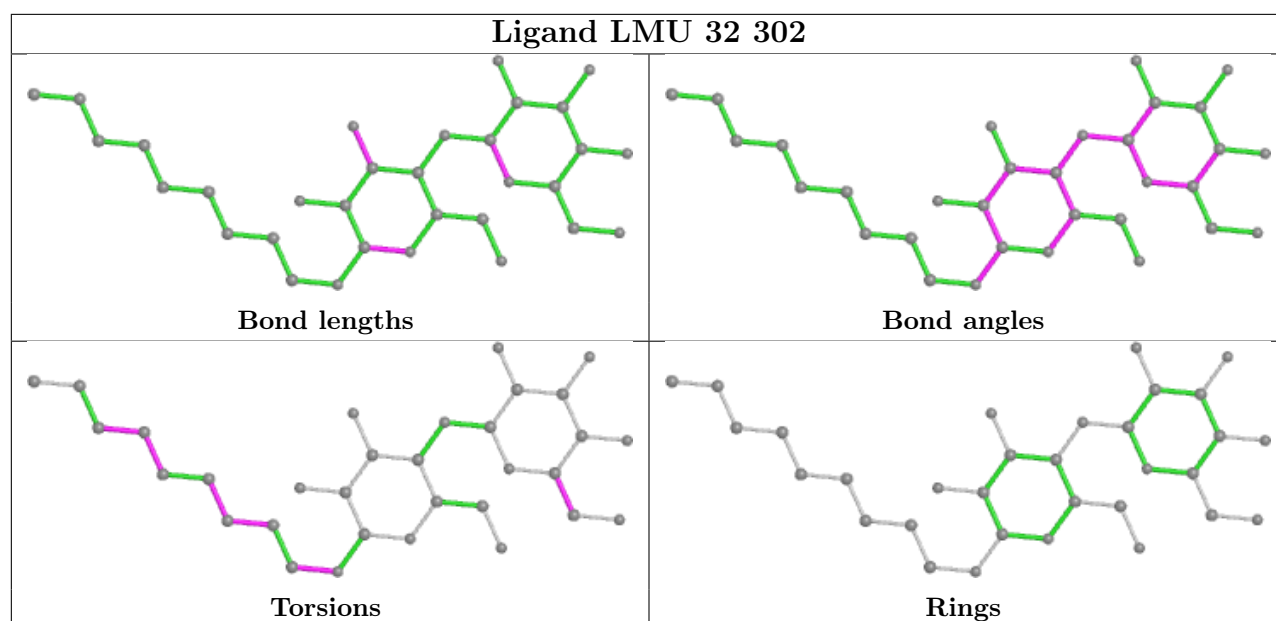


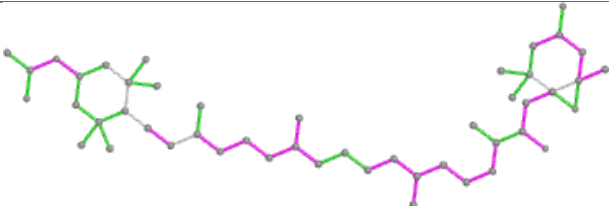
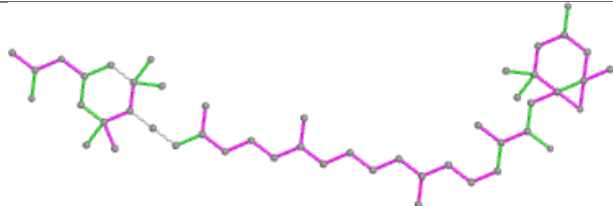
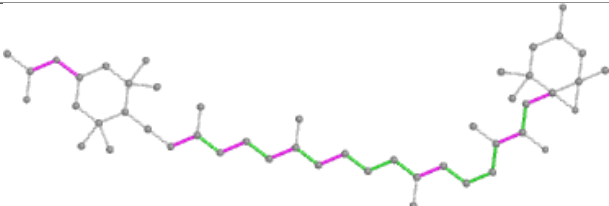
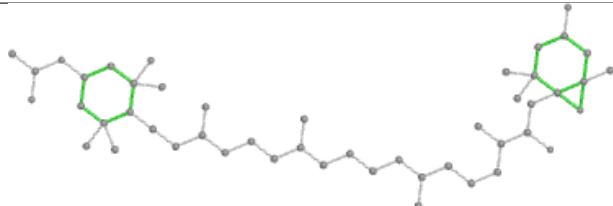


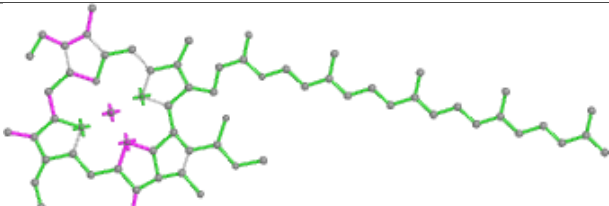
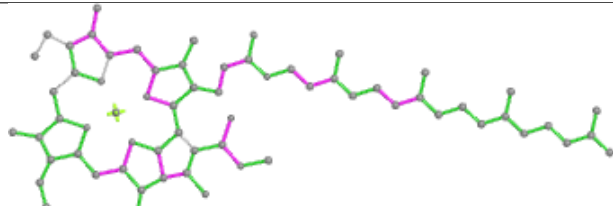
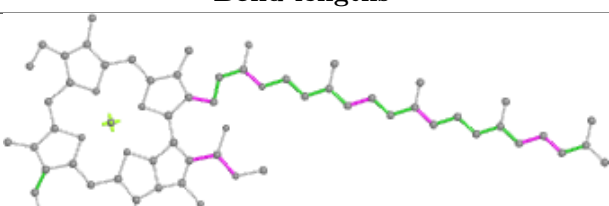
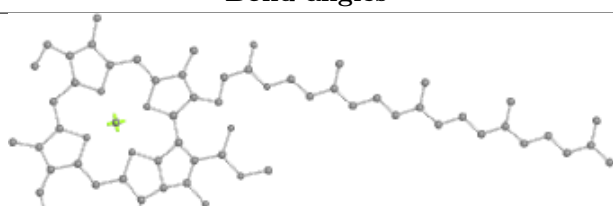


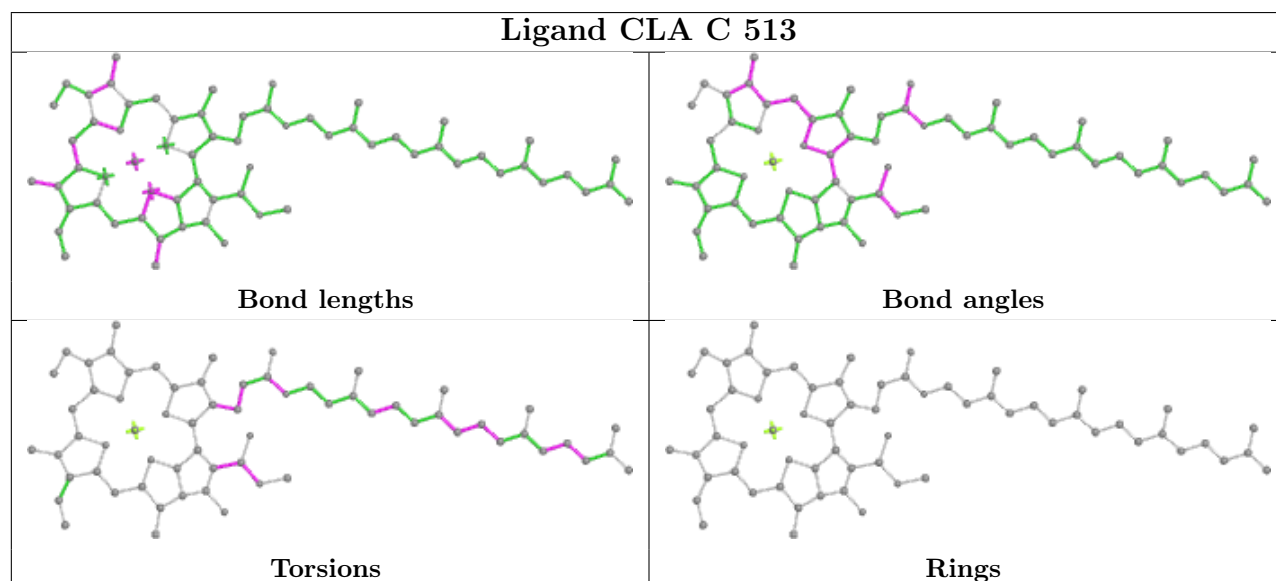
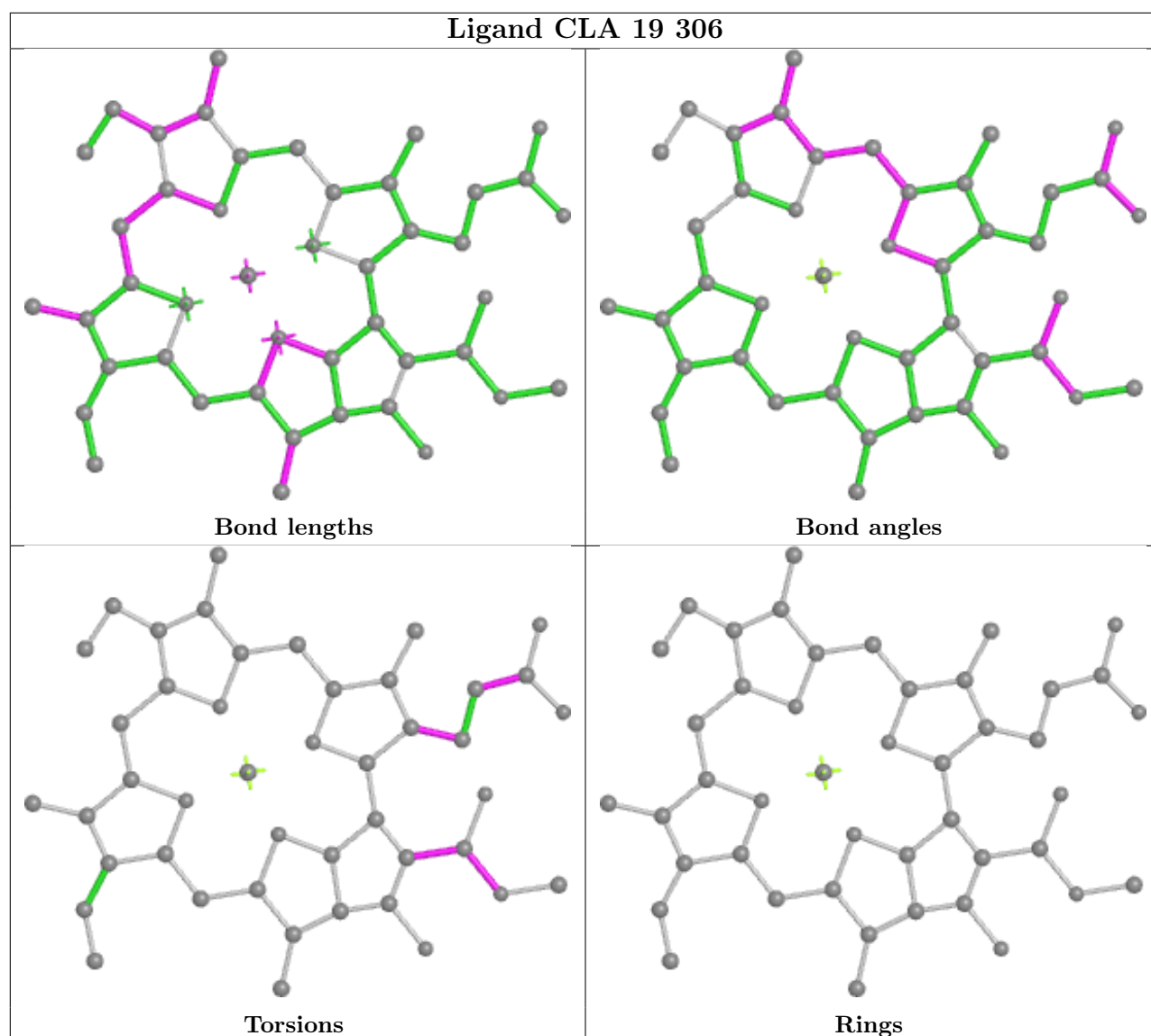


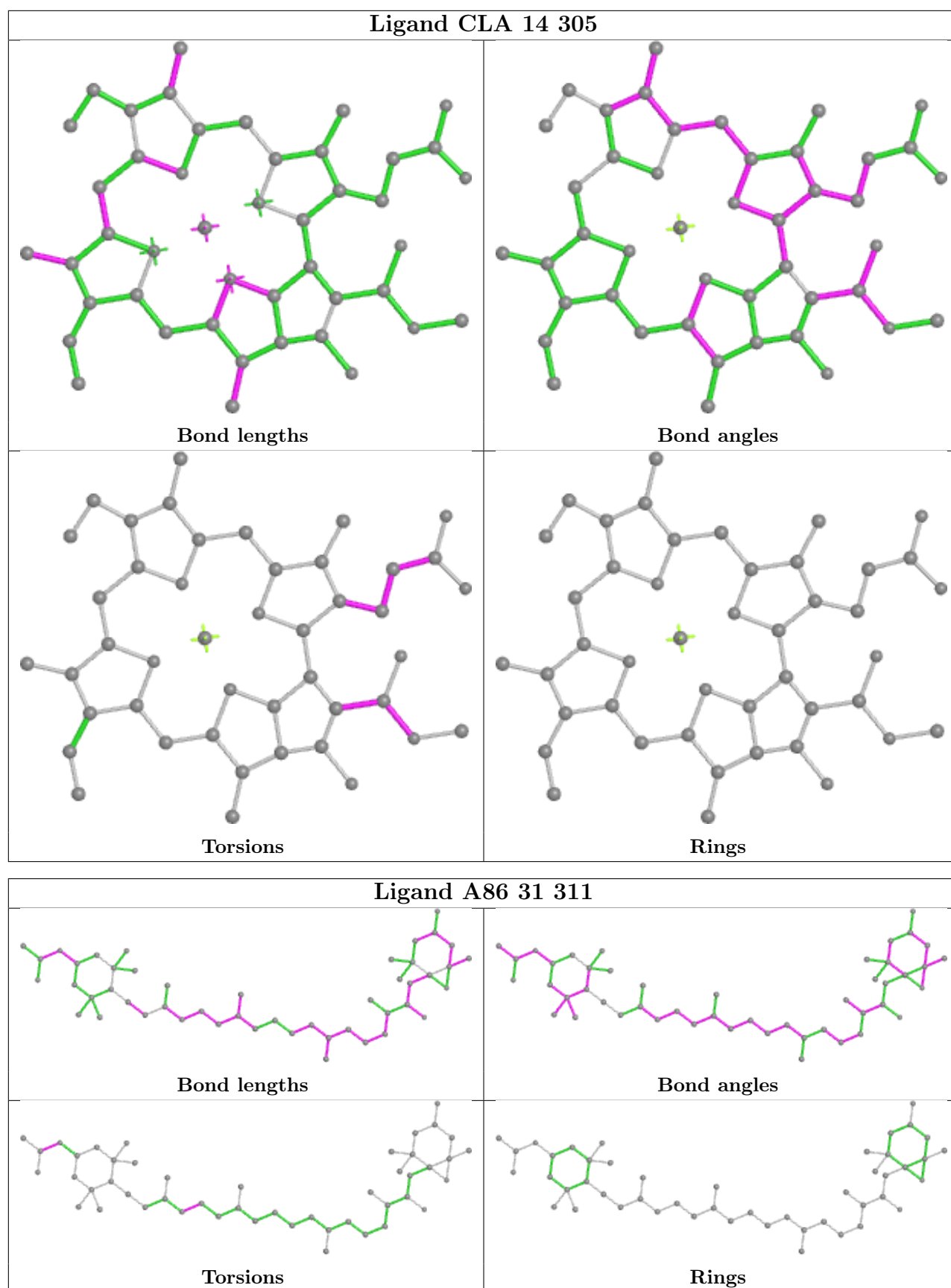


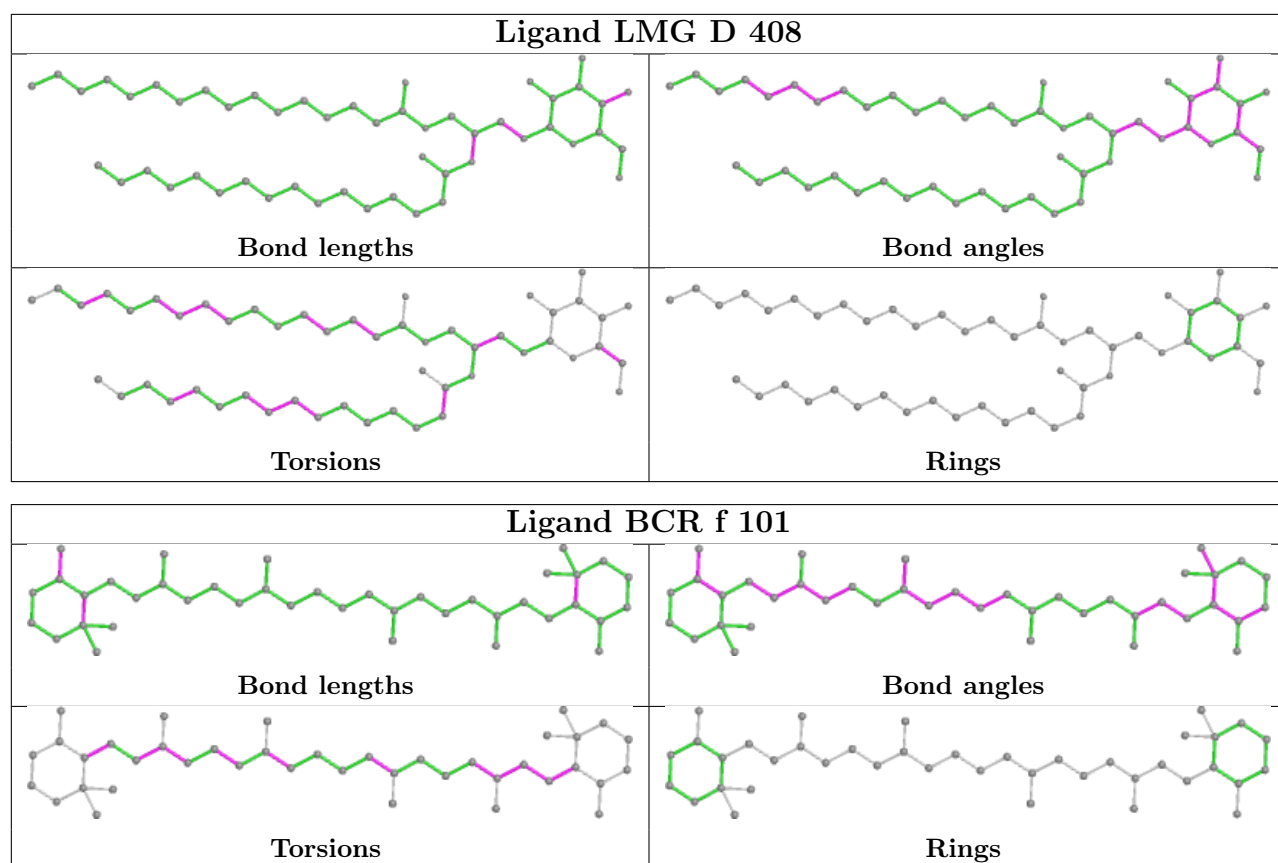


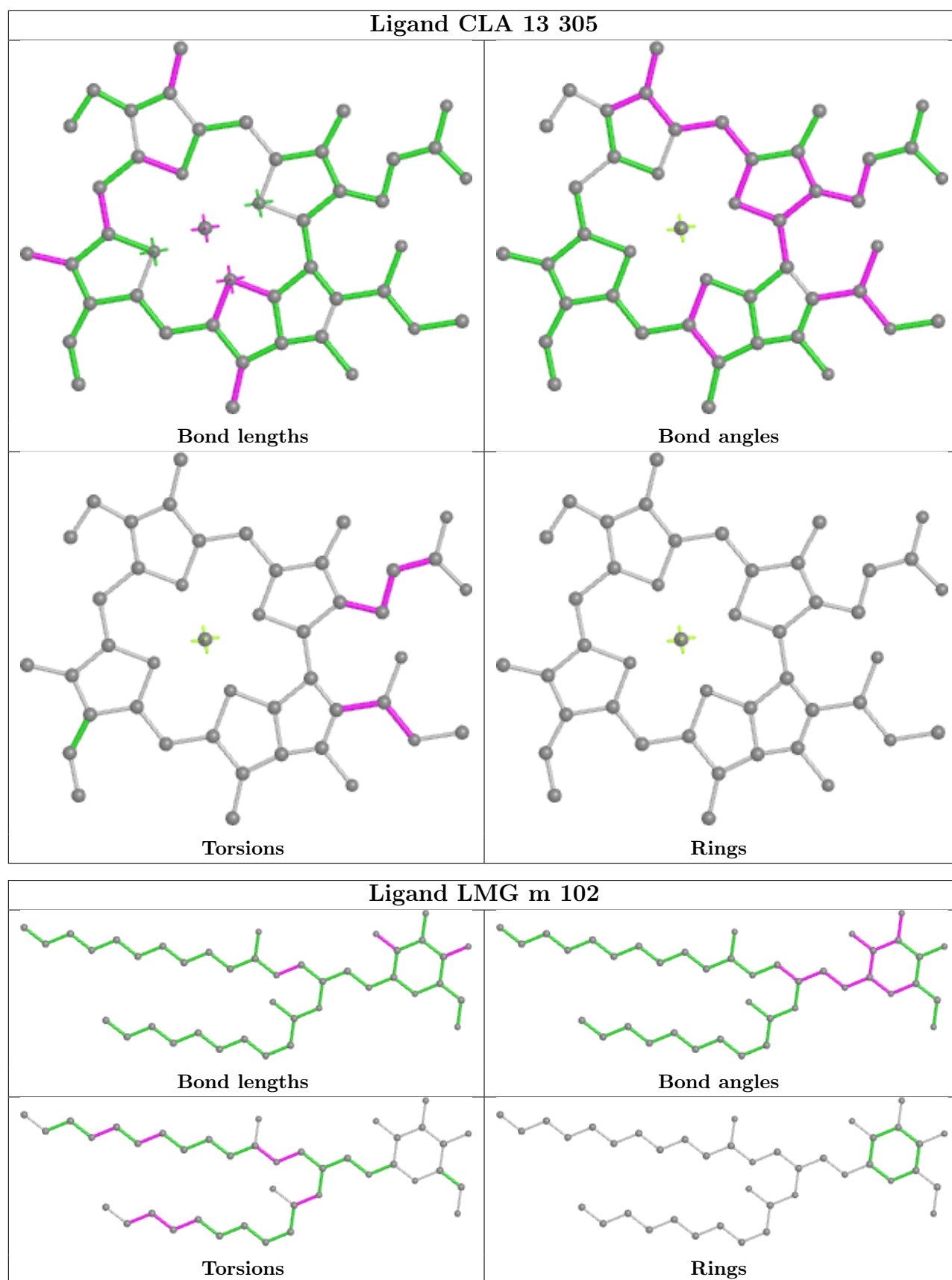
Ligand A86 41 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

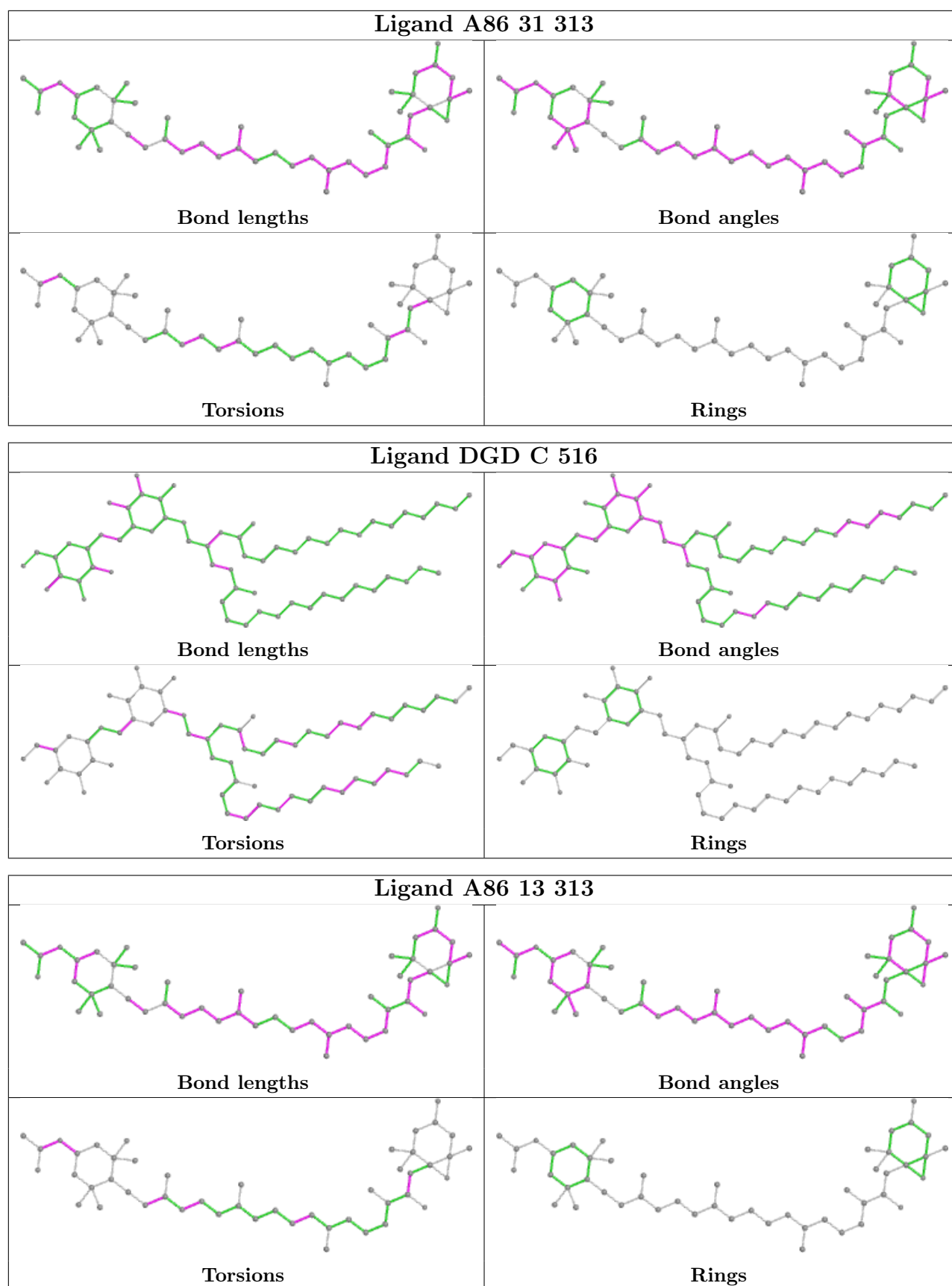
Ligand CLA 39 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

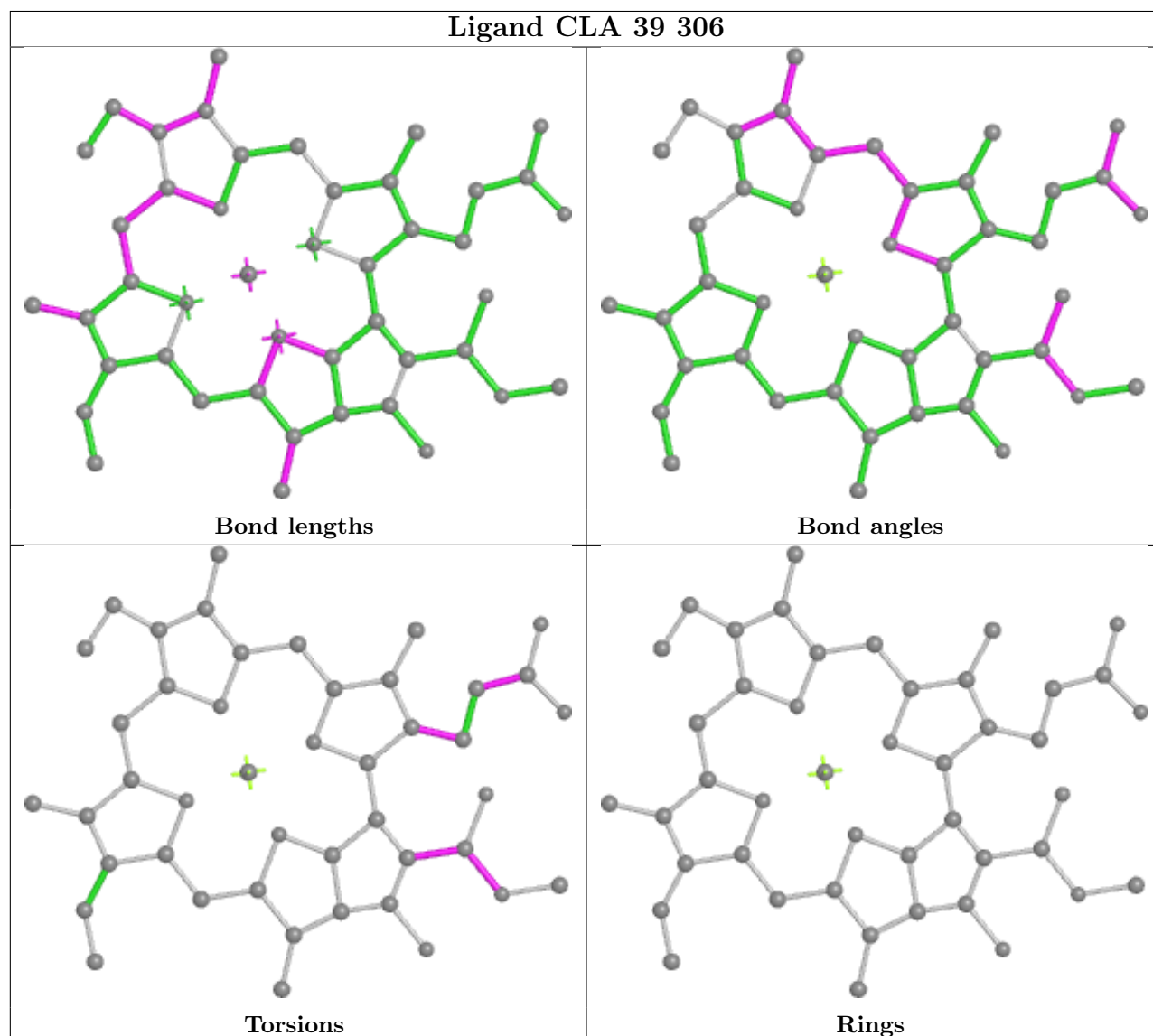
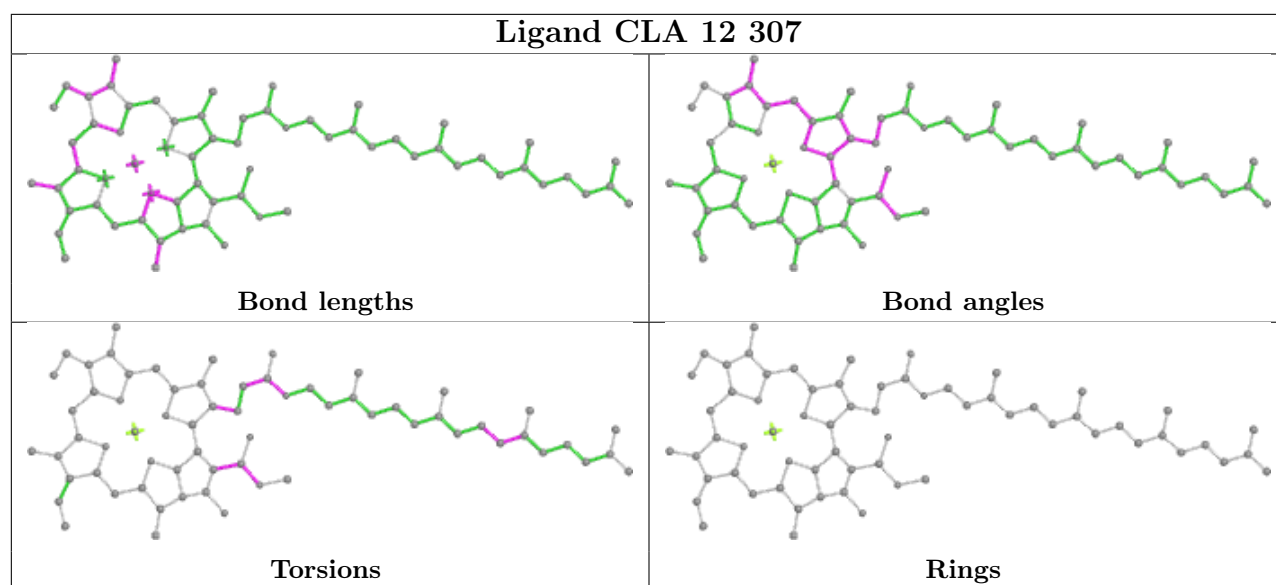




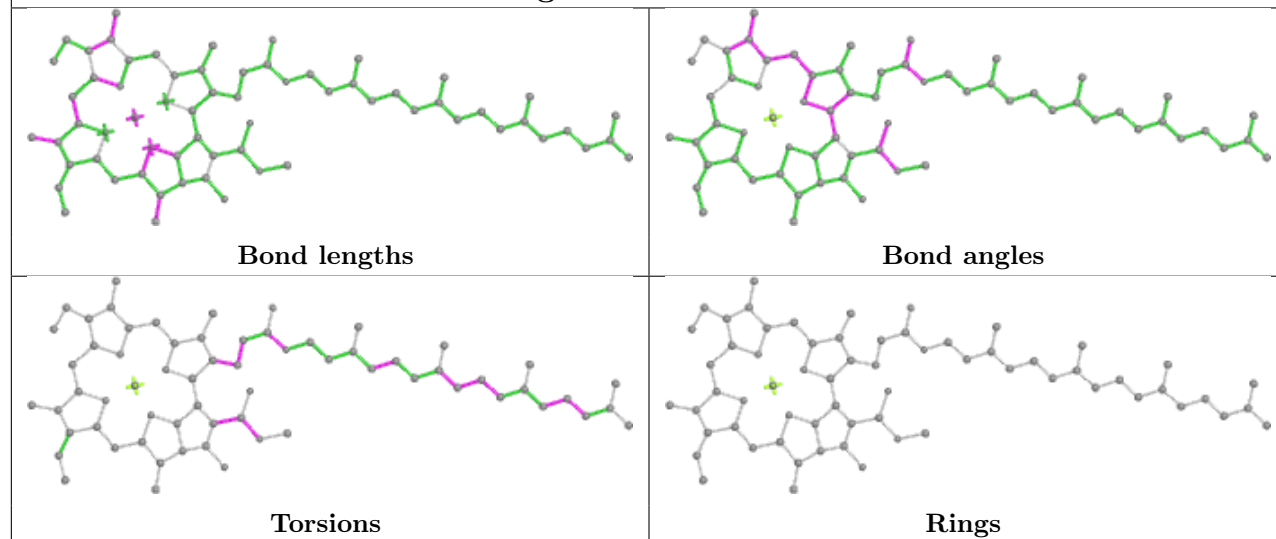




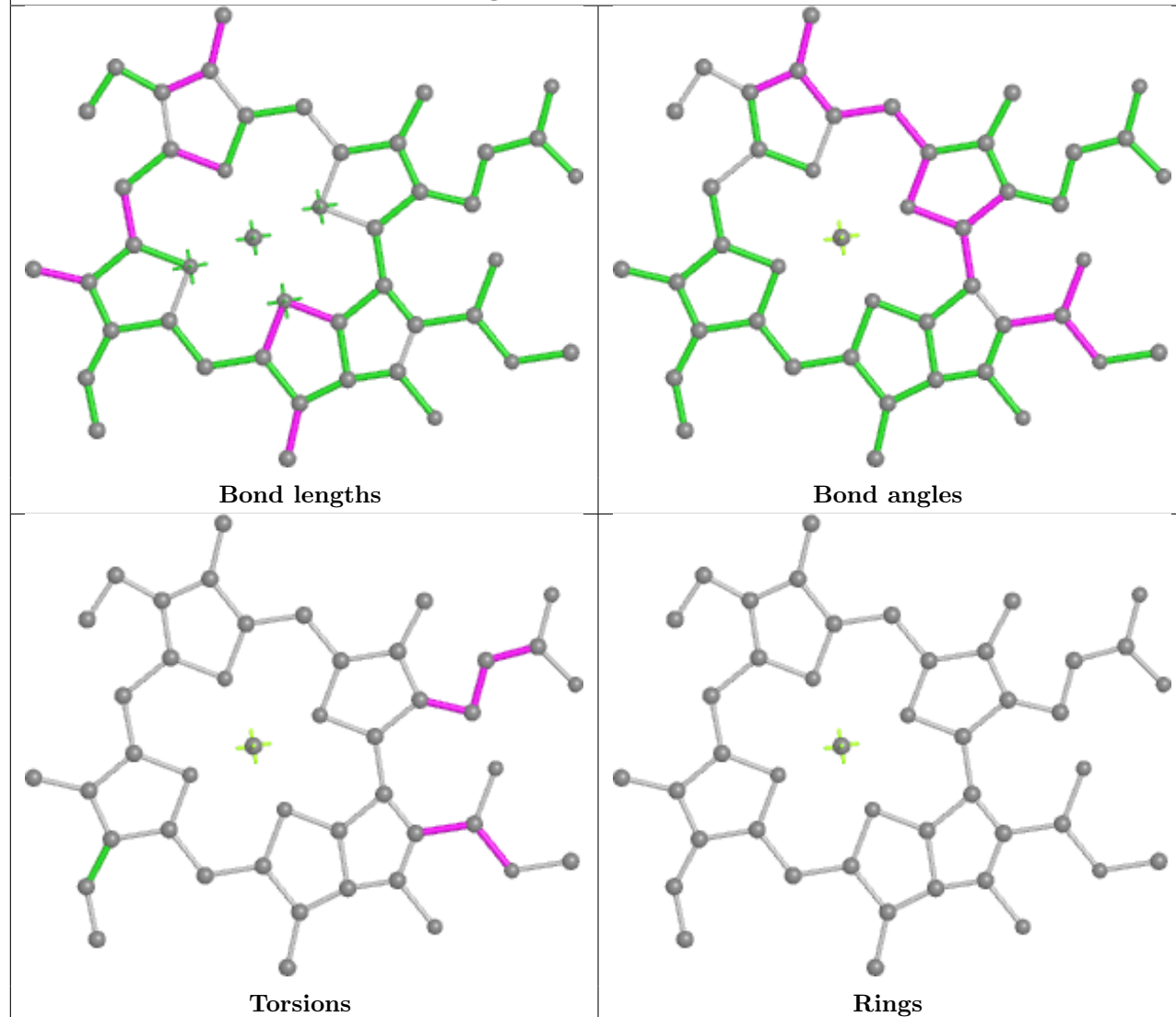


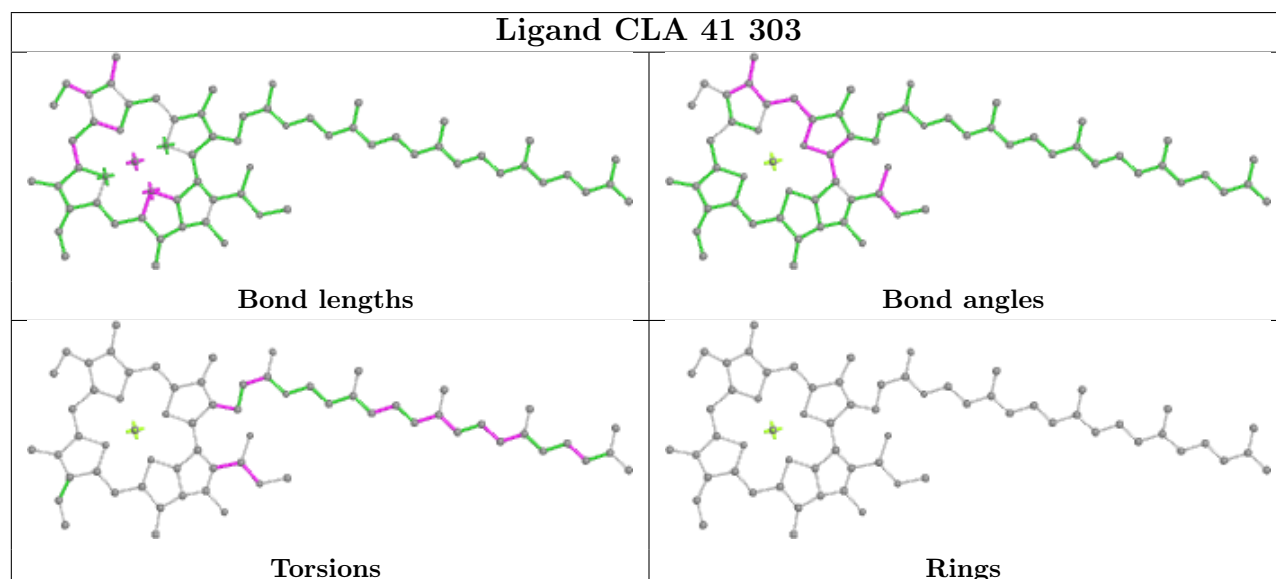
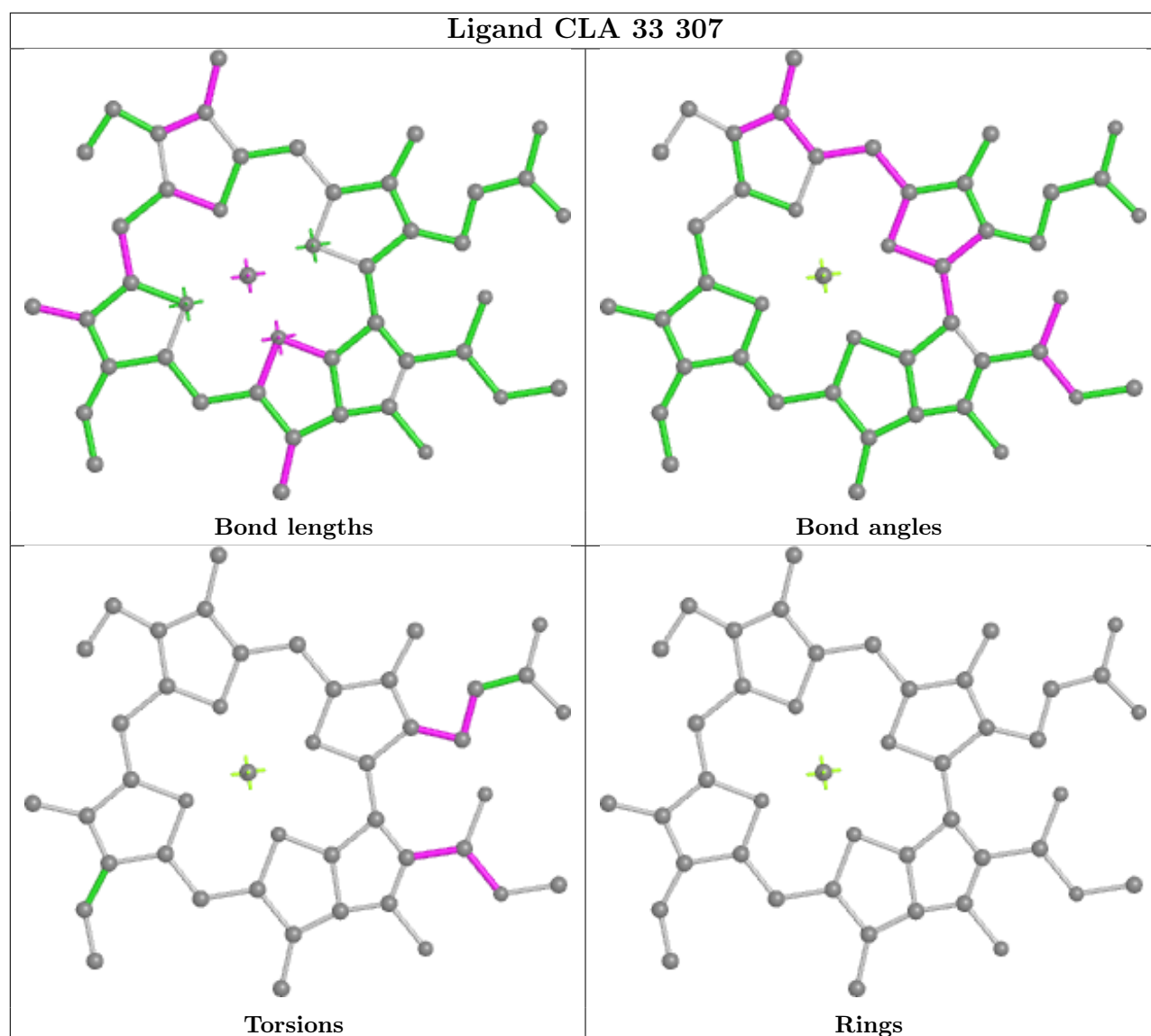


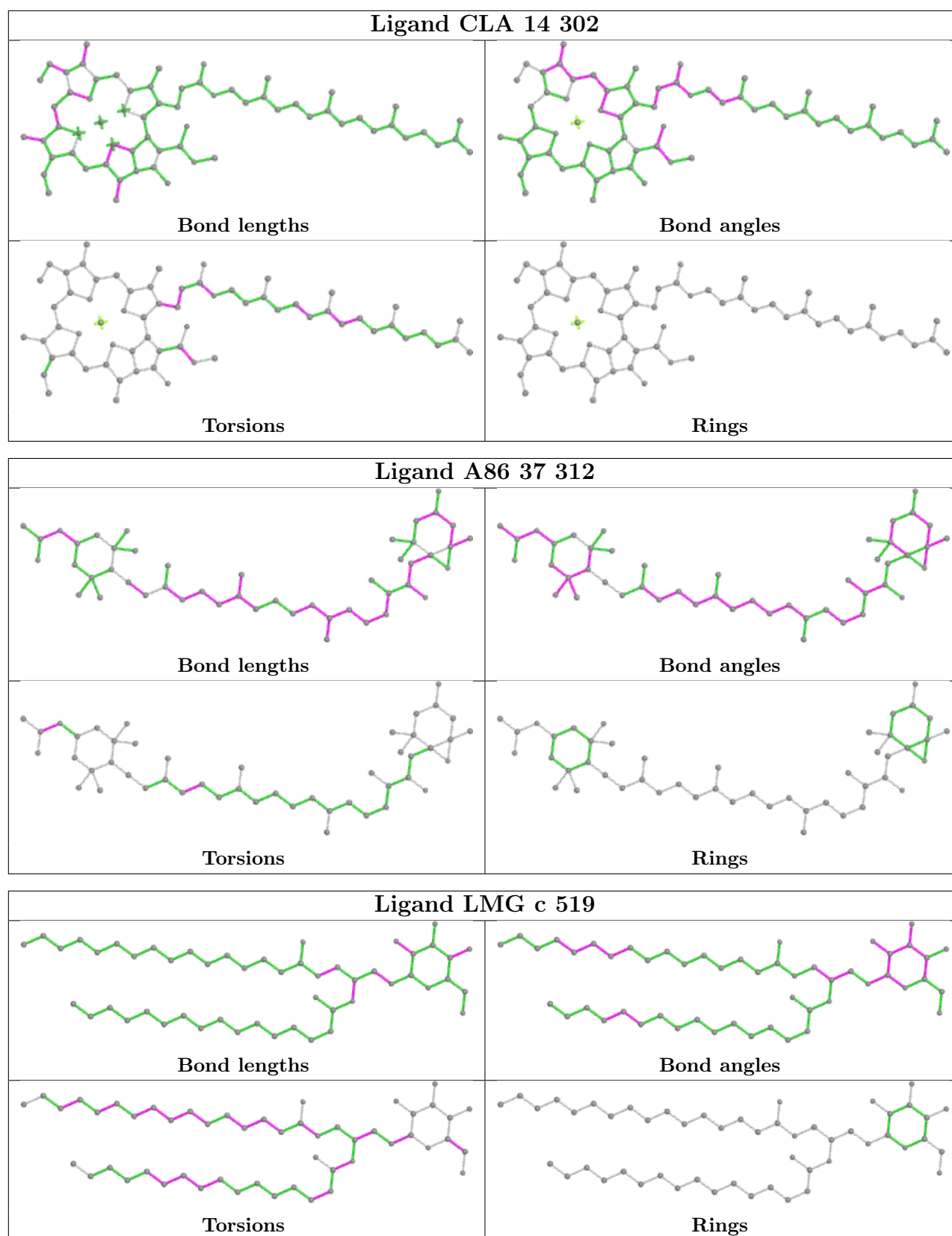
Ligand CLA c 513

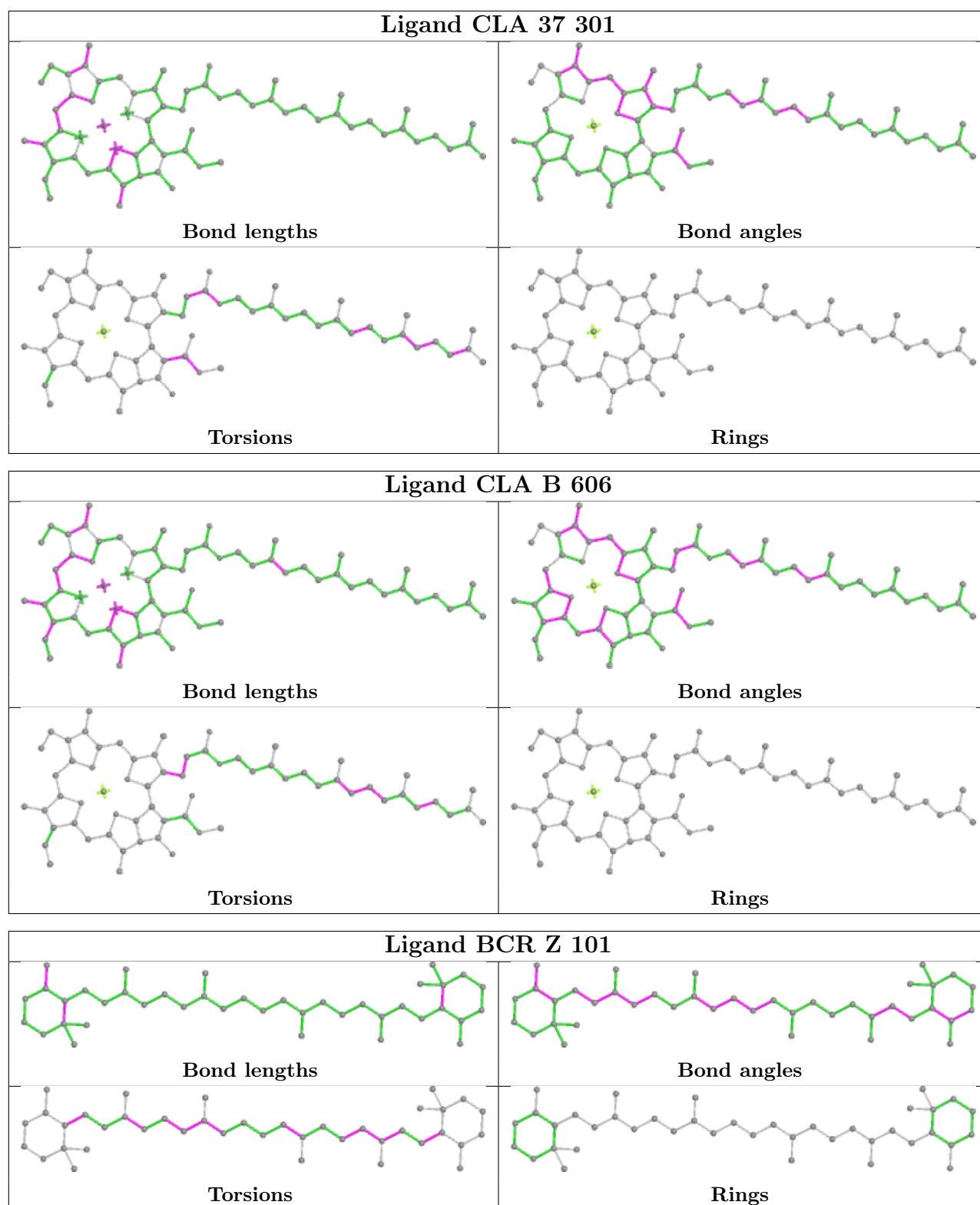


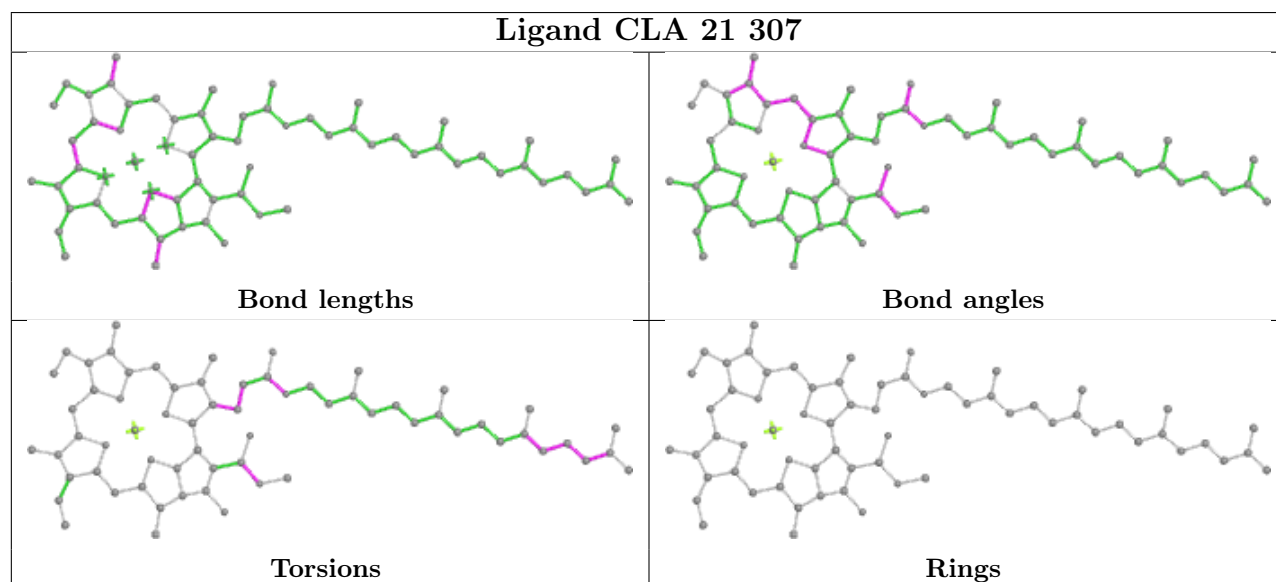
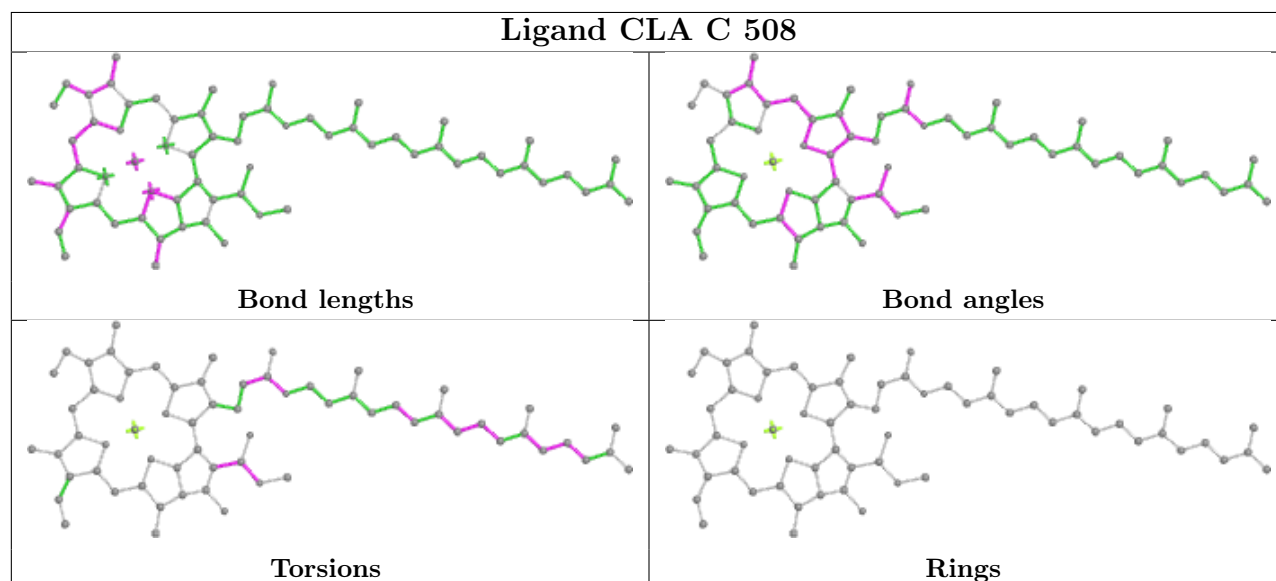
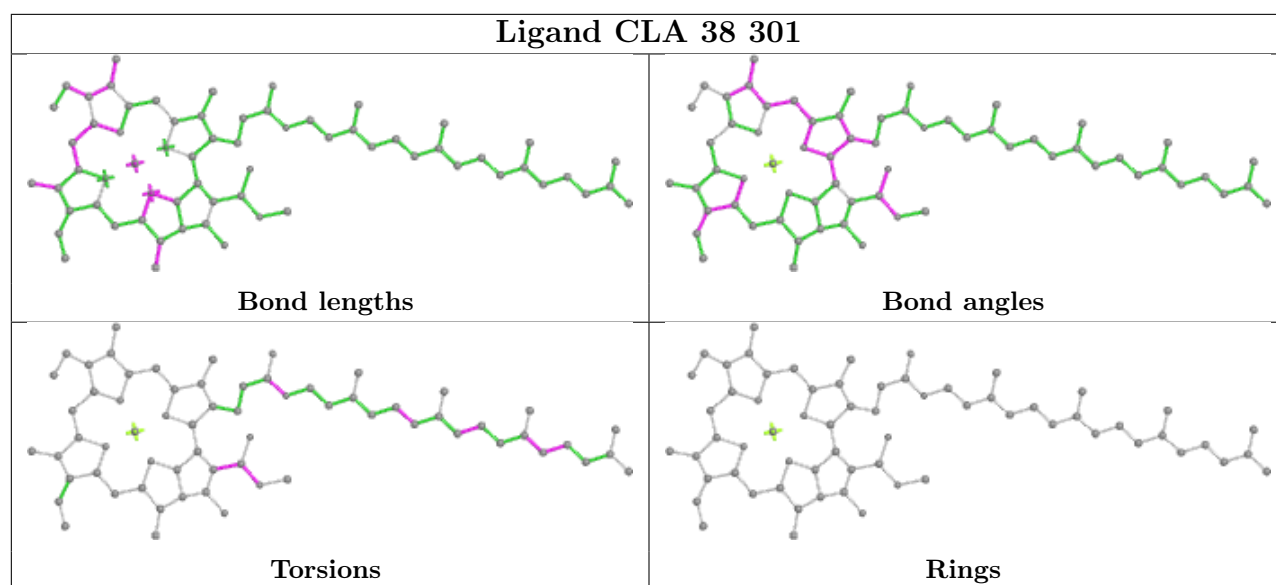
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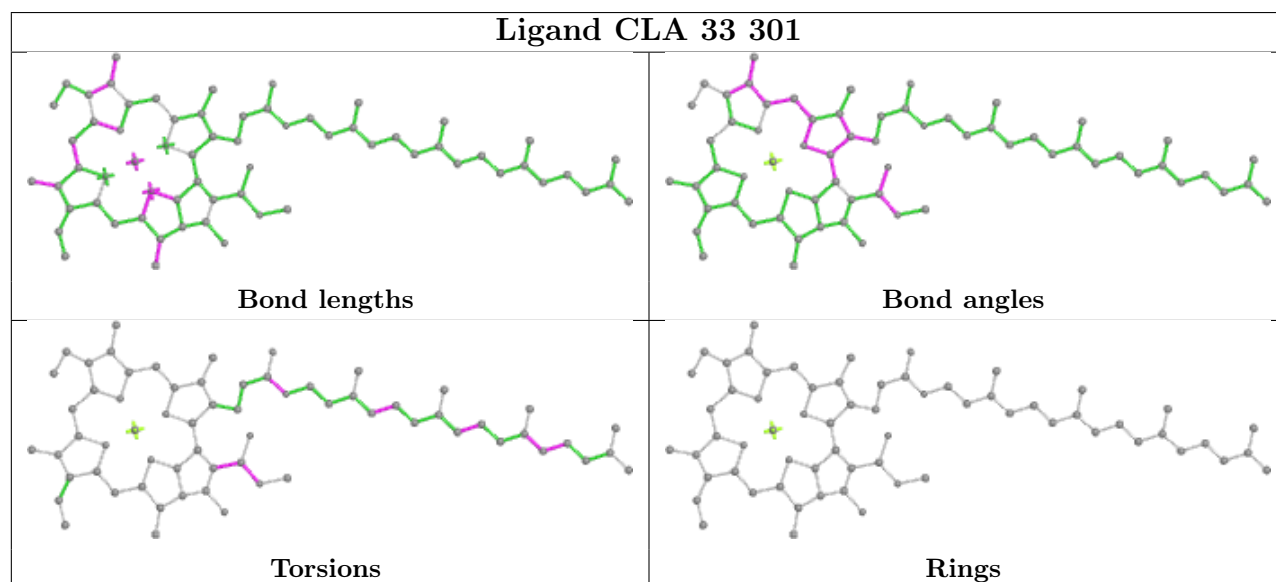
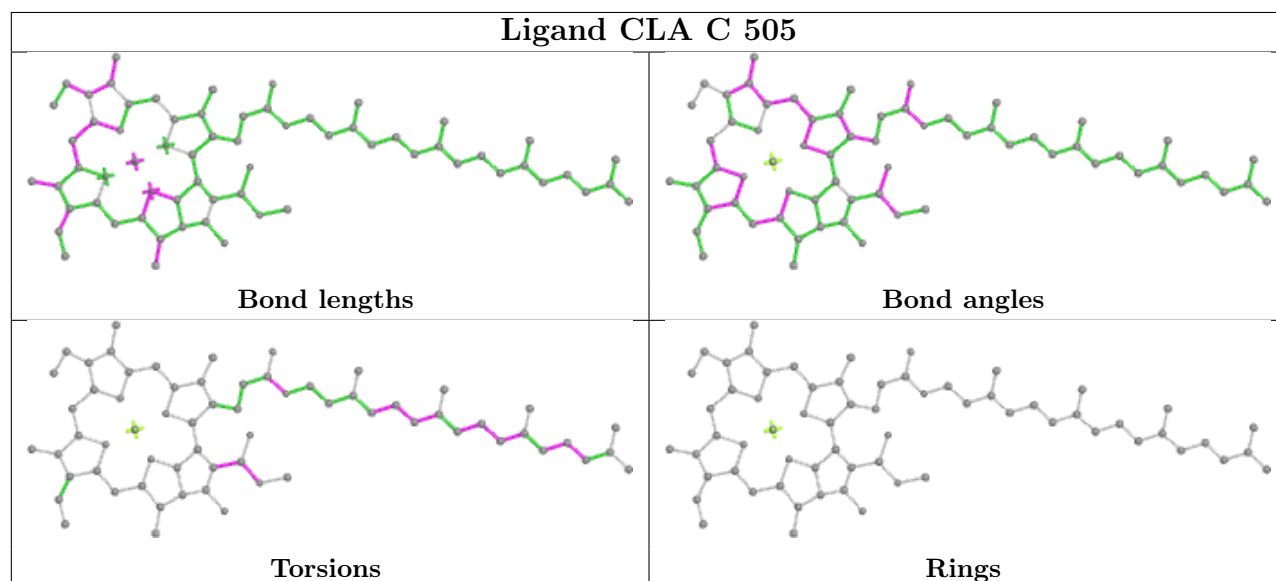
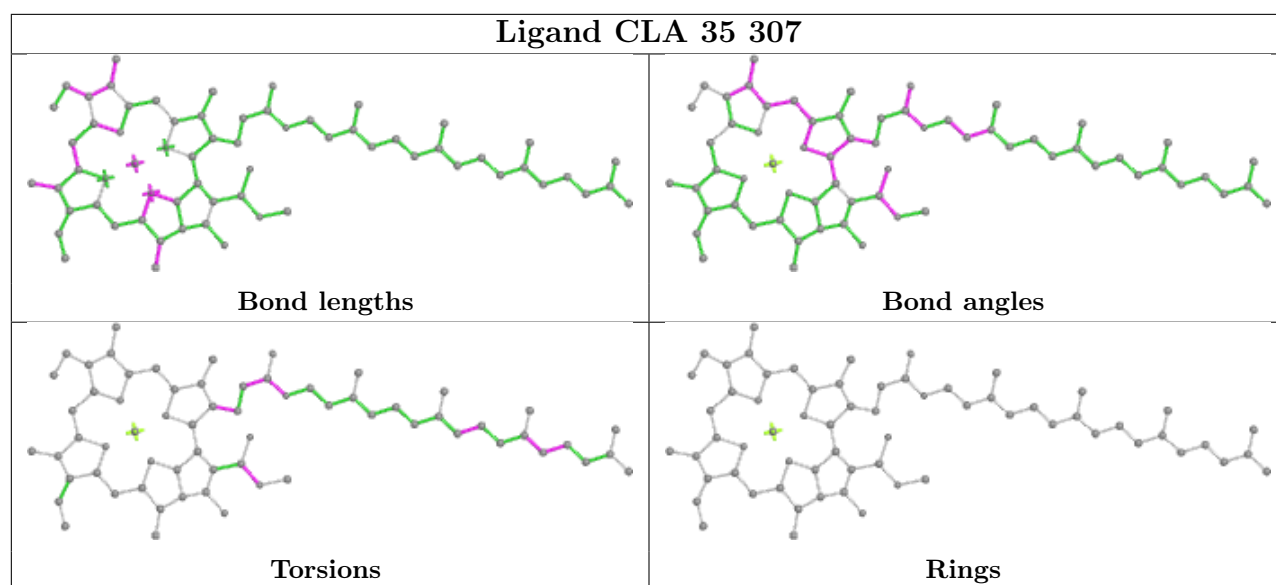


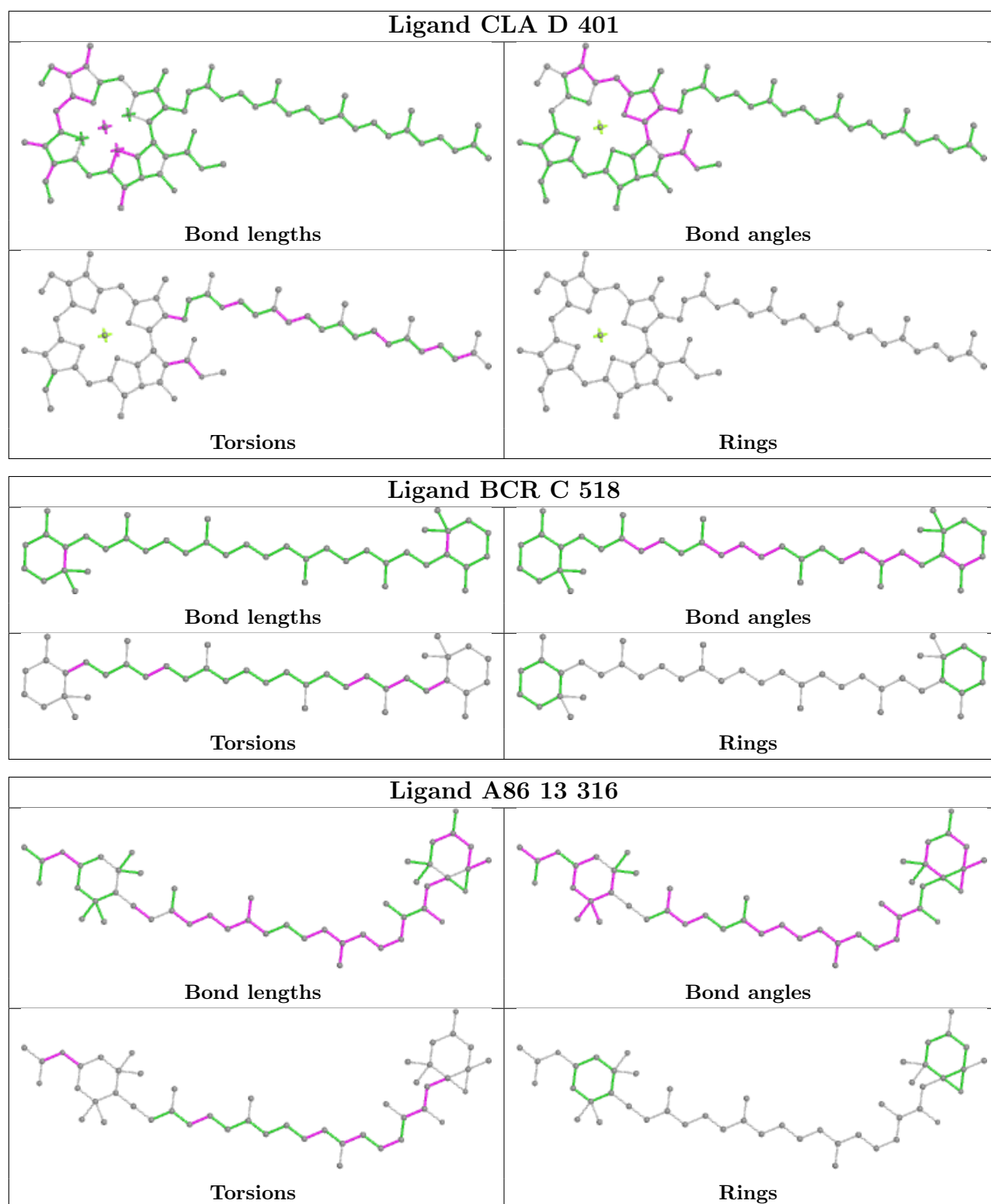


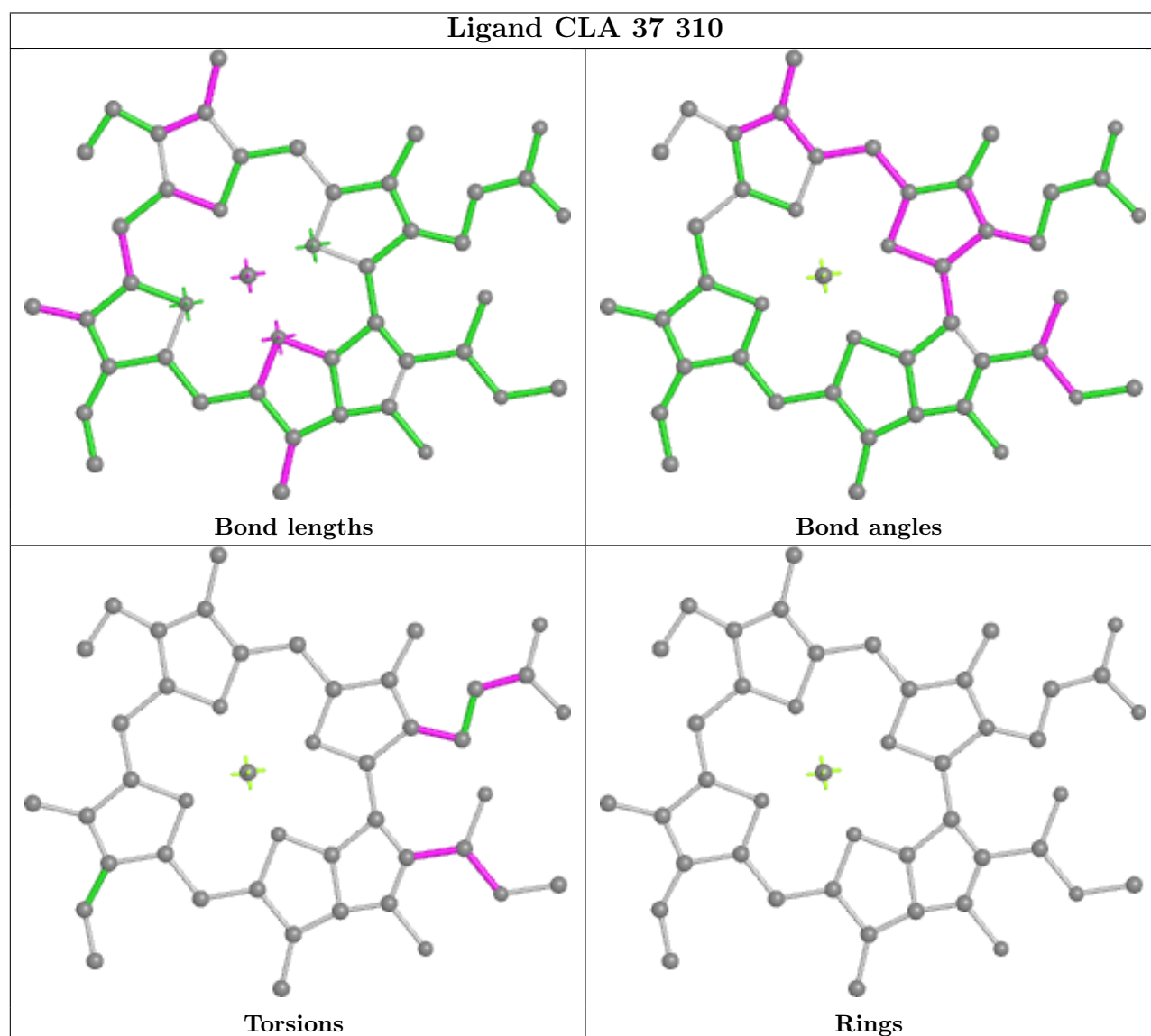
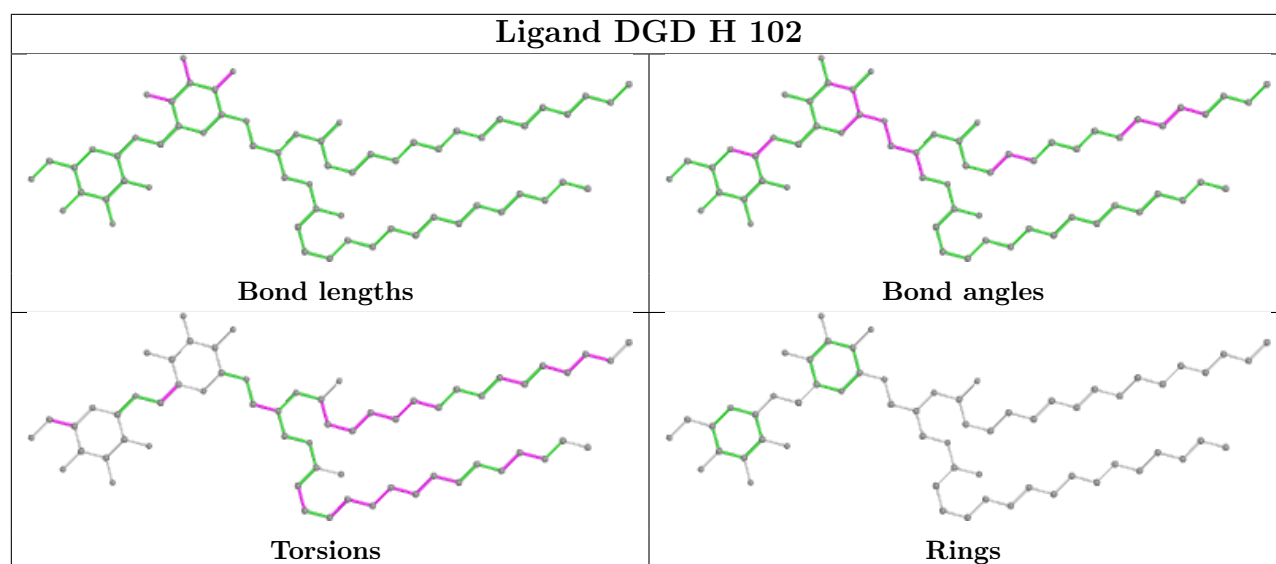


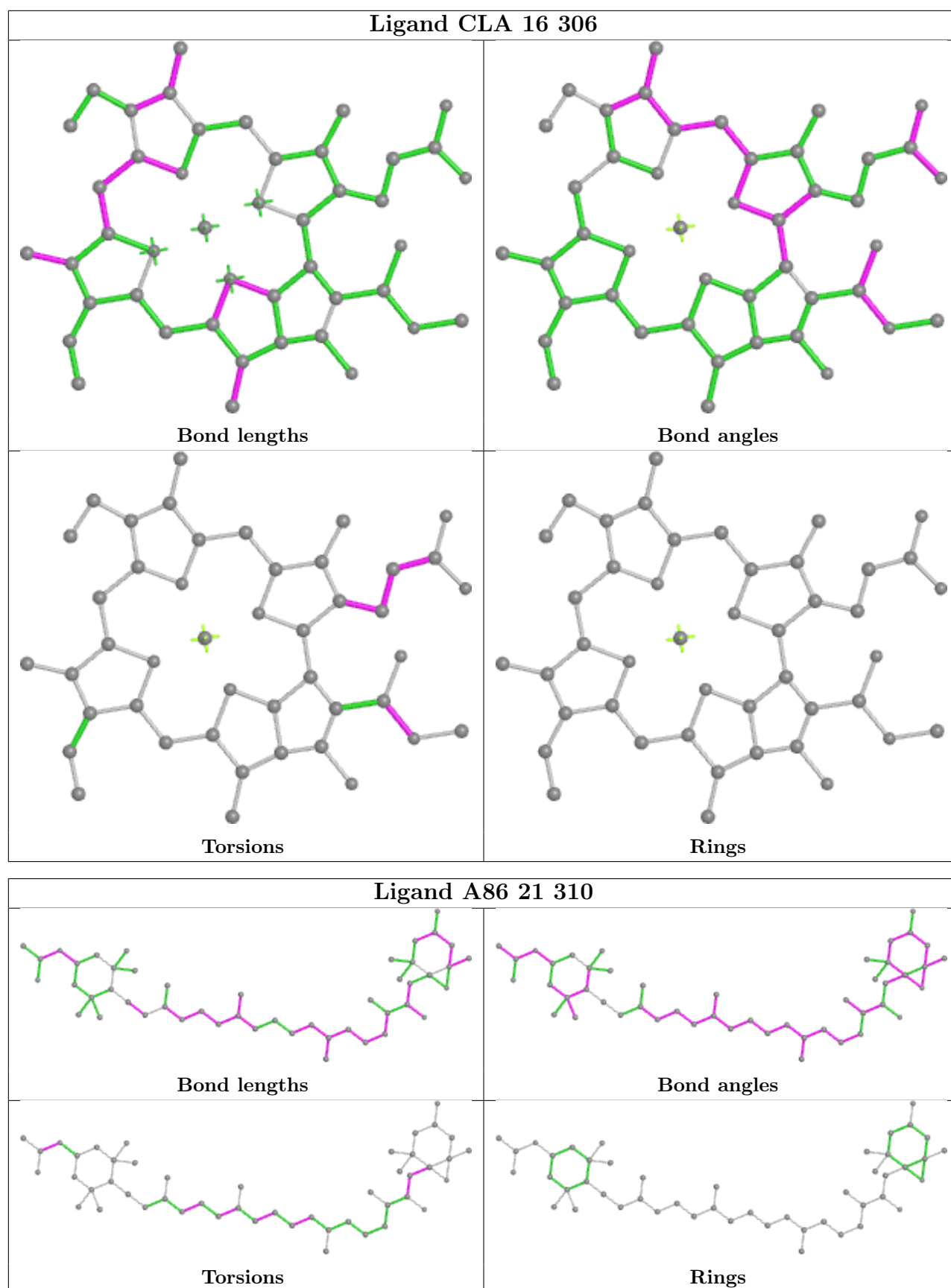




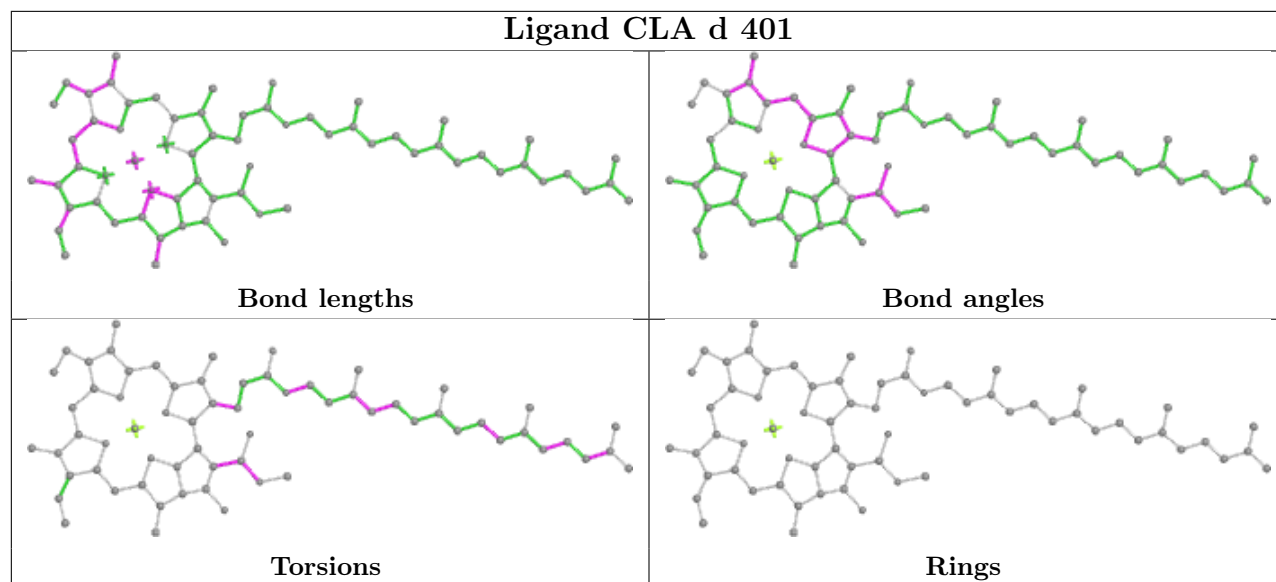




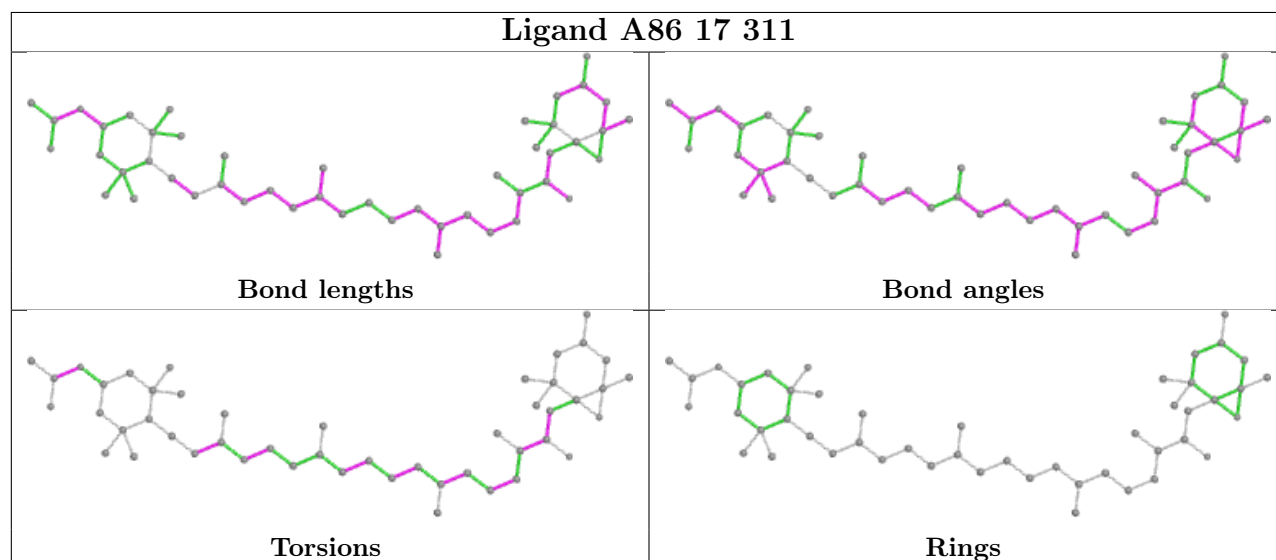




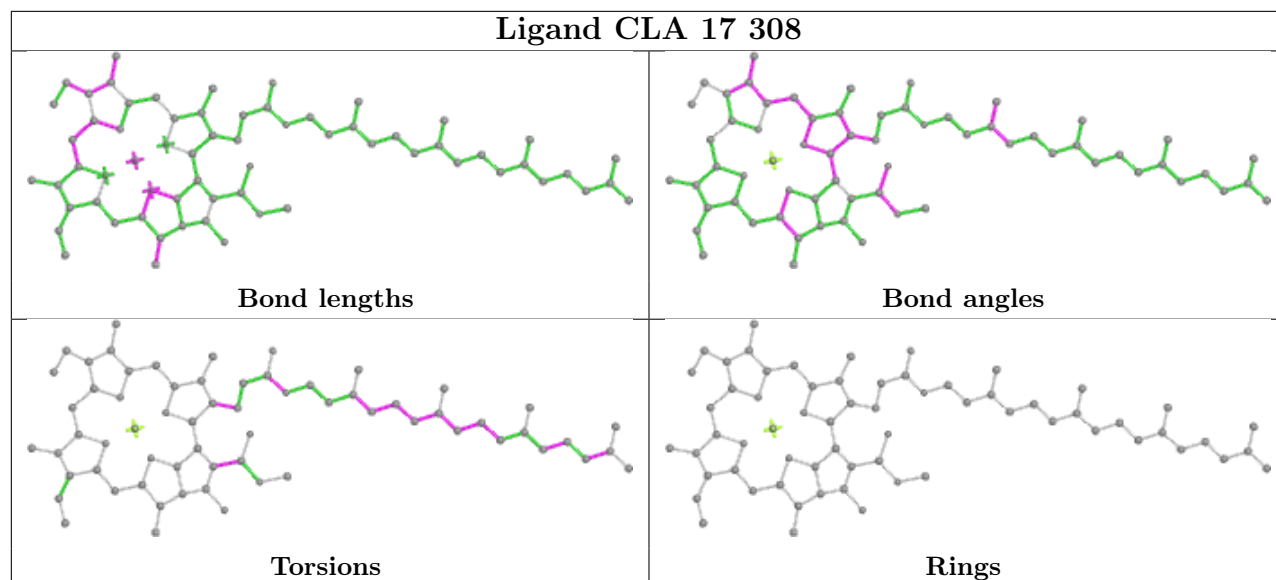
Ligand CLA d 401



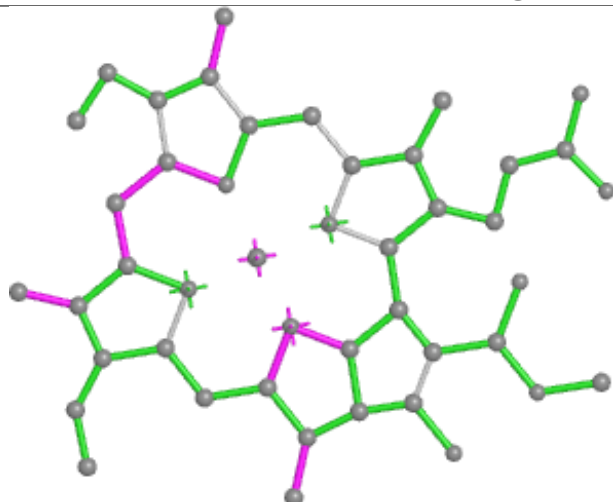
Ligand A86 17 311



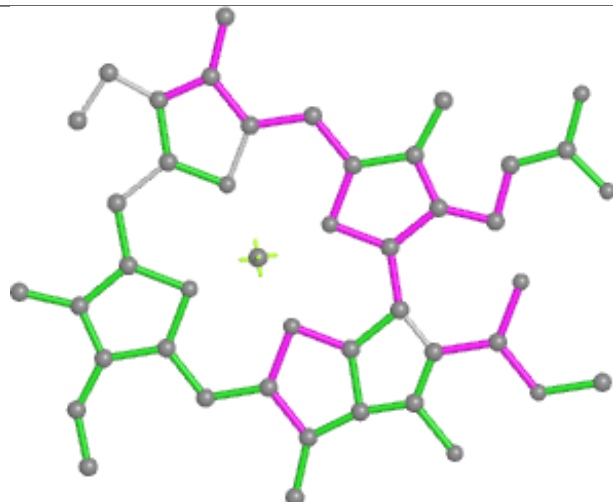
Ligand CLA 17 308



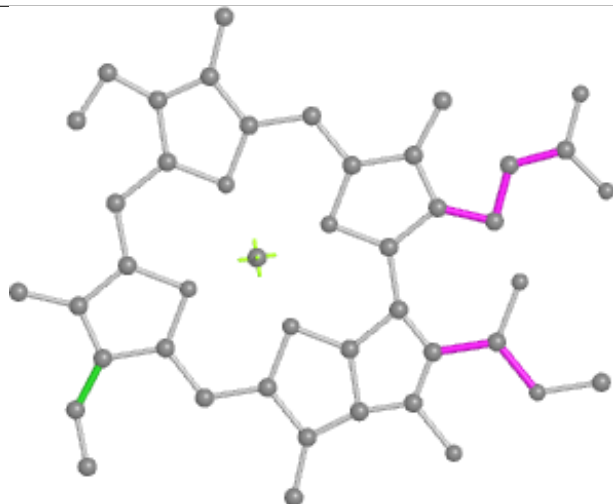
Ligand CLA 34 305



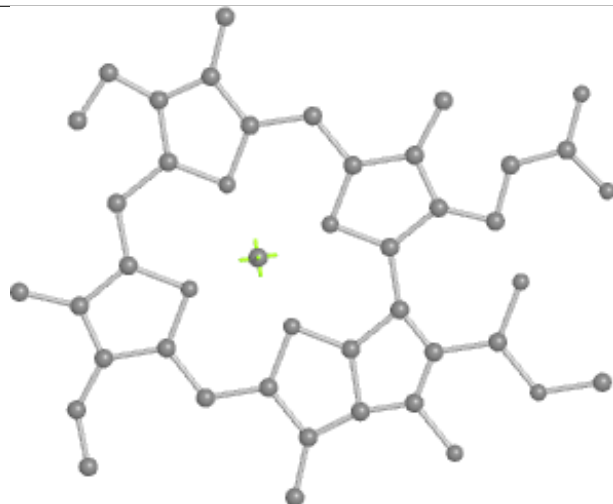
Bond lengths



Bond angles

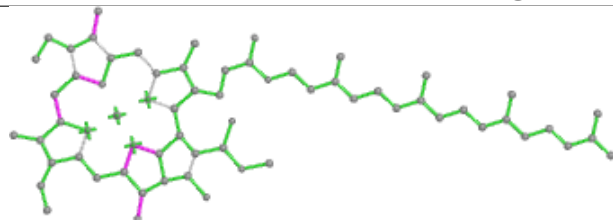


Torsions

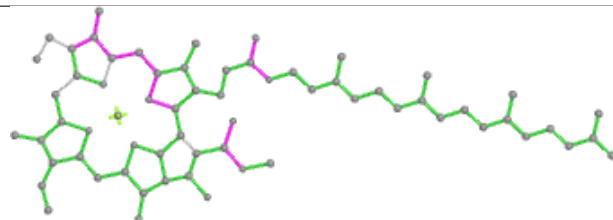


Rings

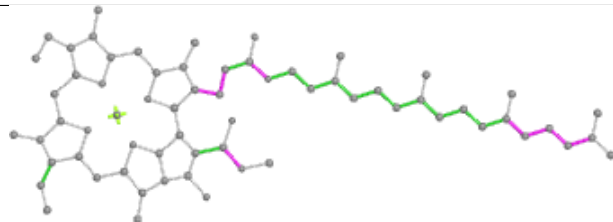
Ligand CLA 41 307



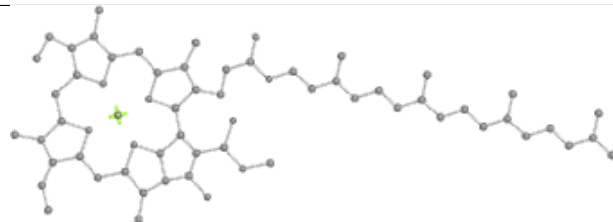
Bond lengths



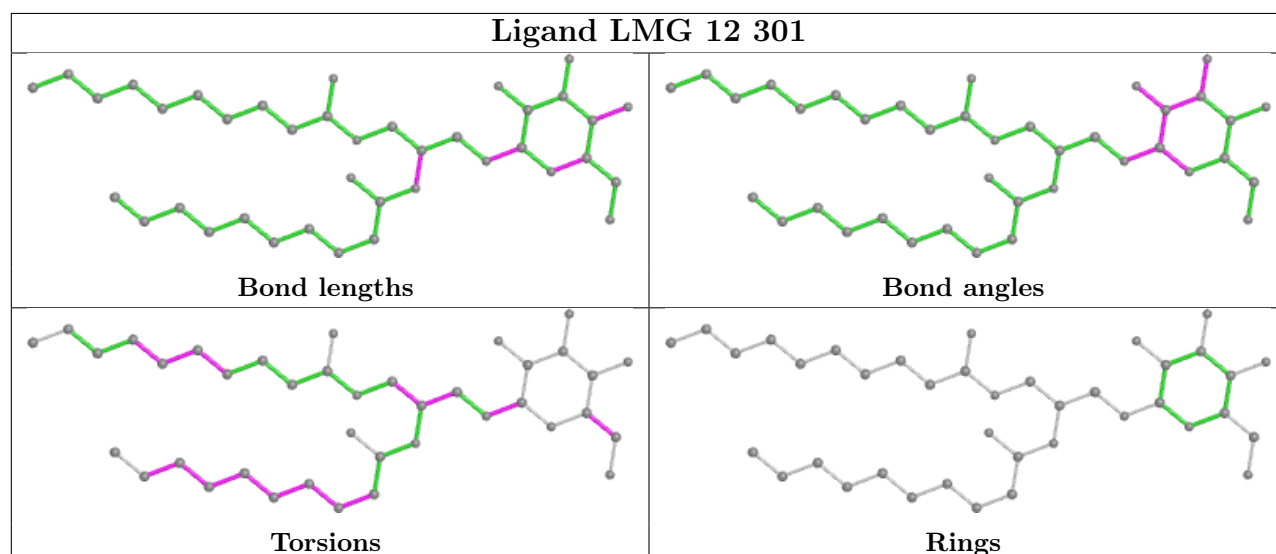
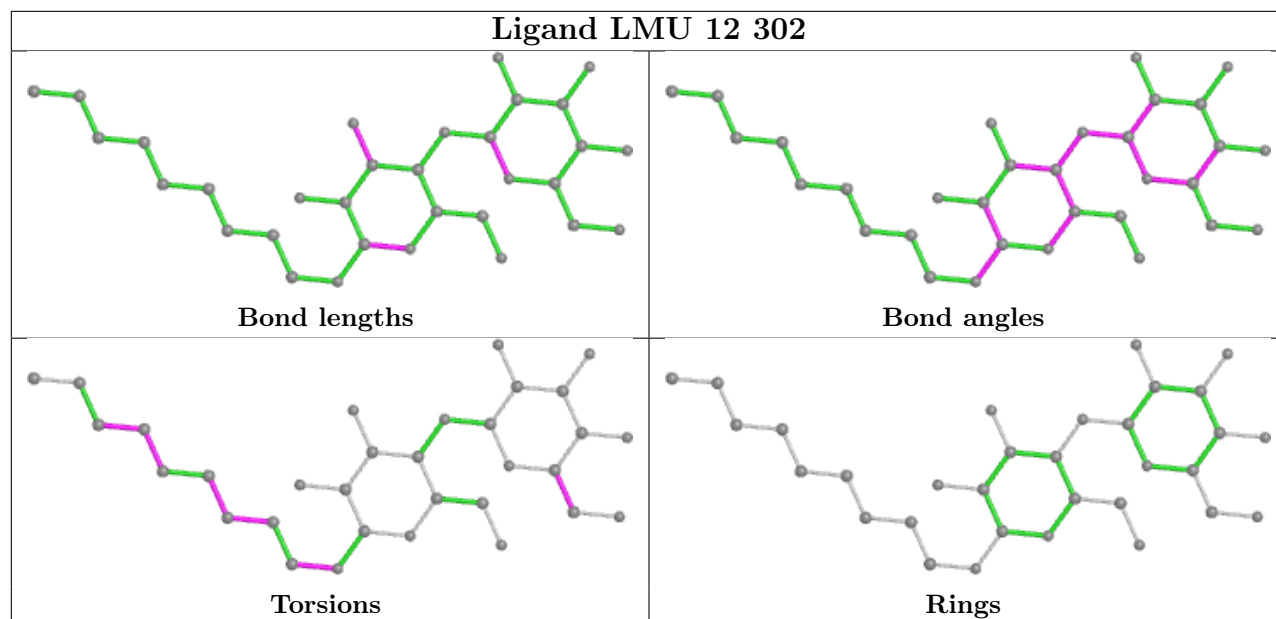
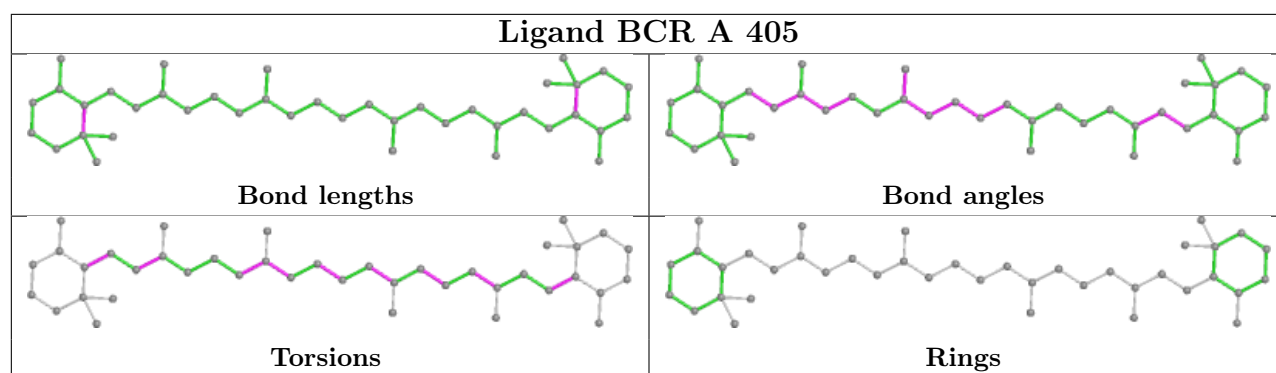
Bond angles

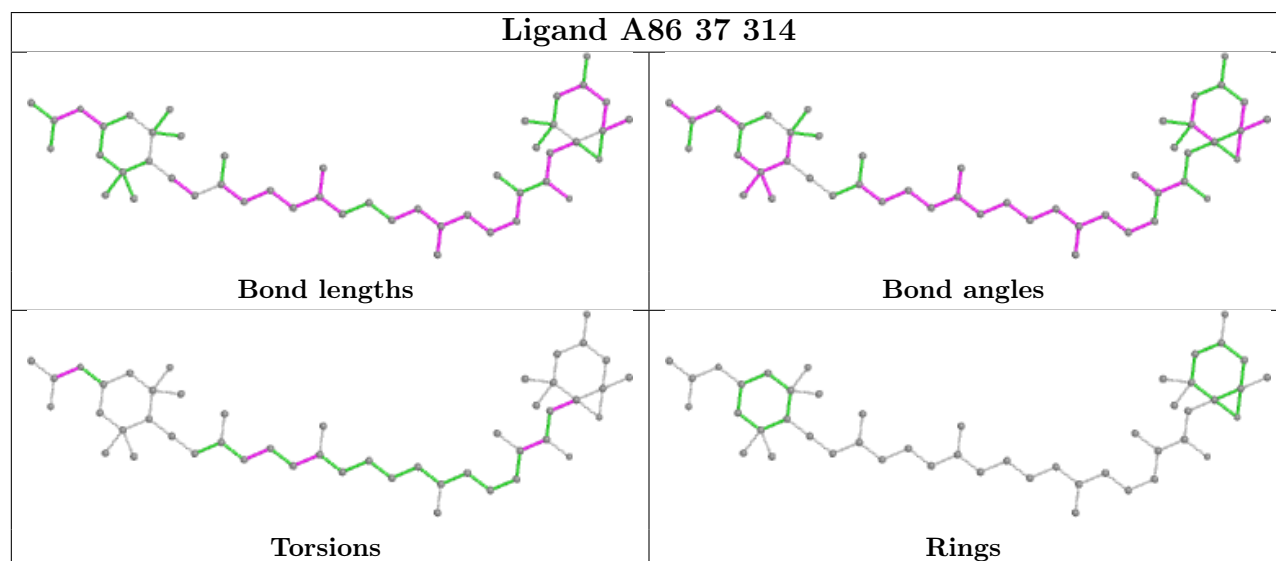
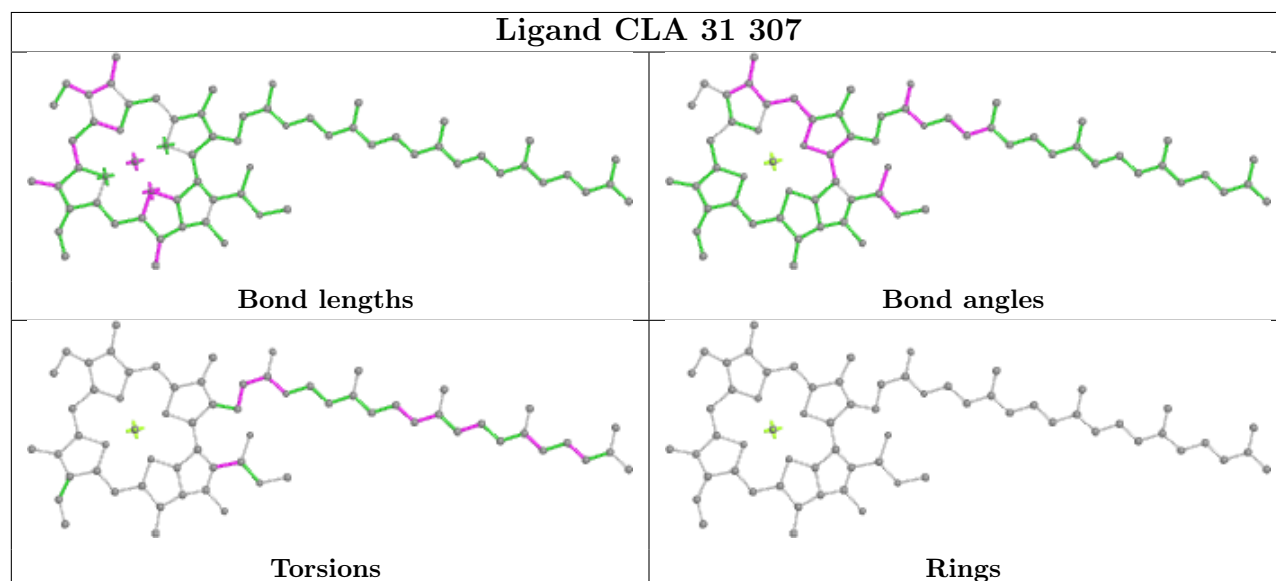
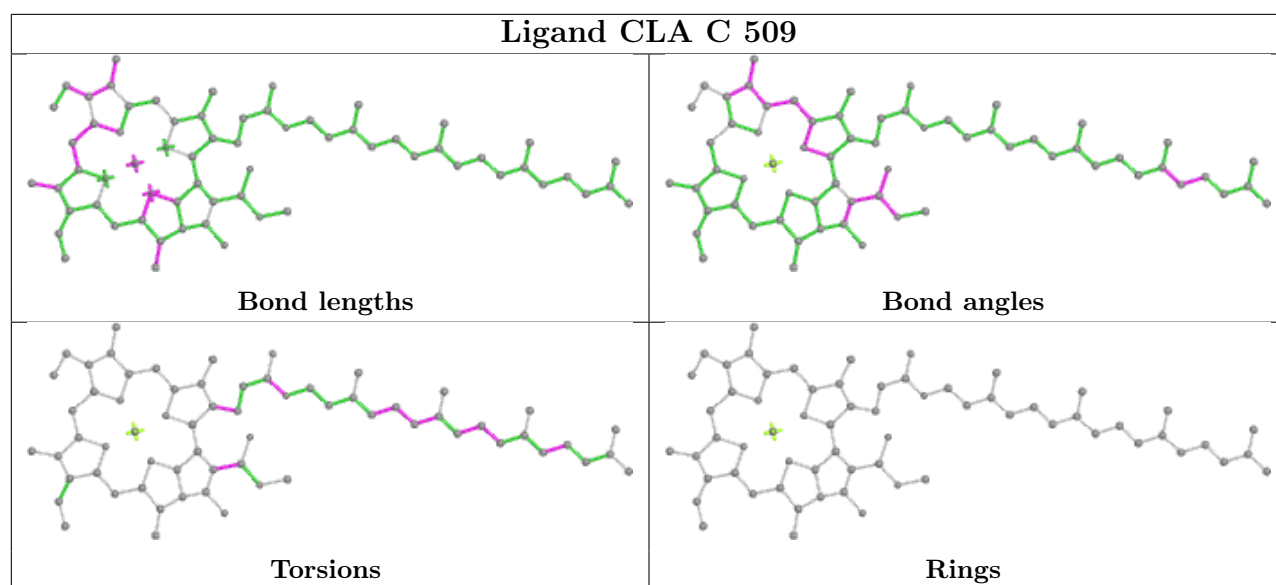


Torsions

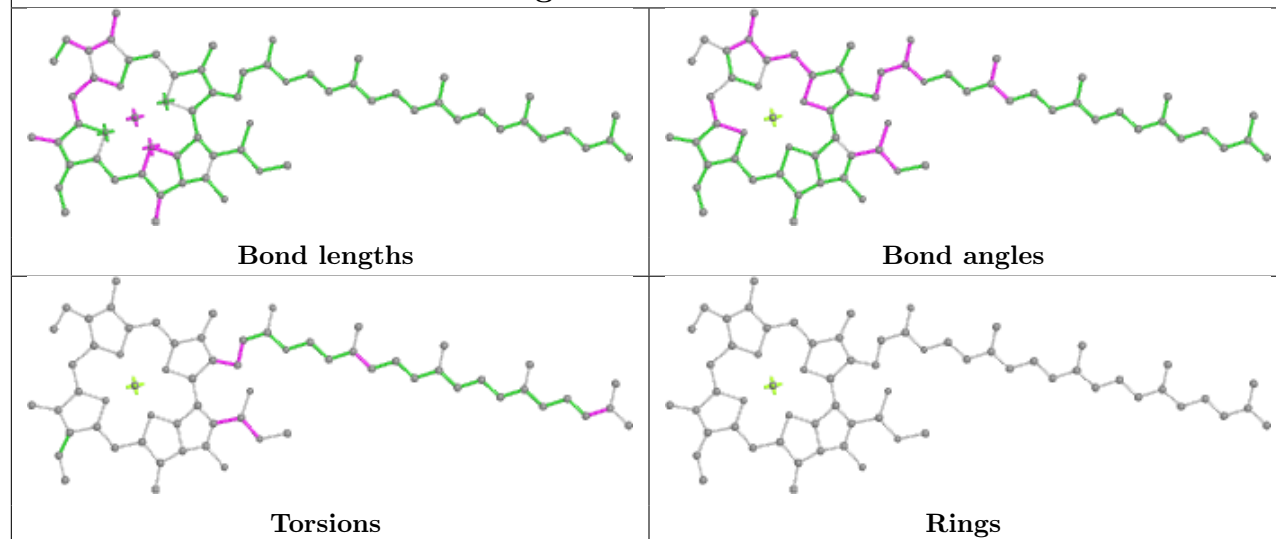


Rings

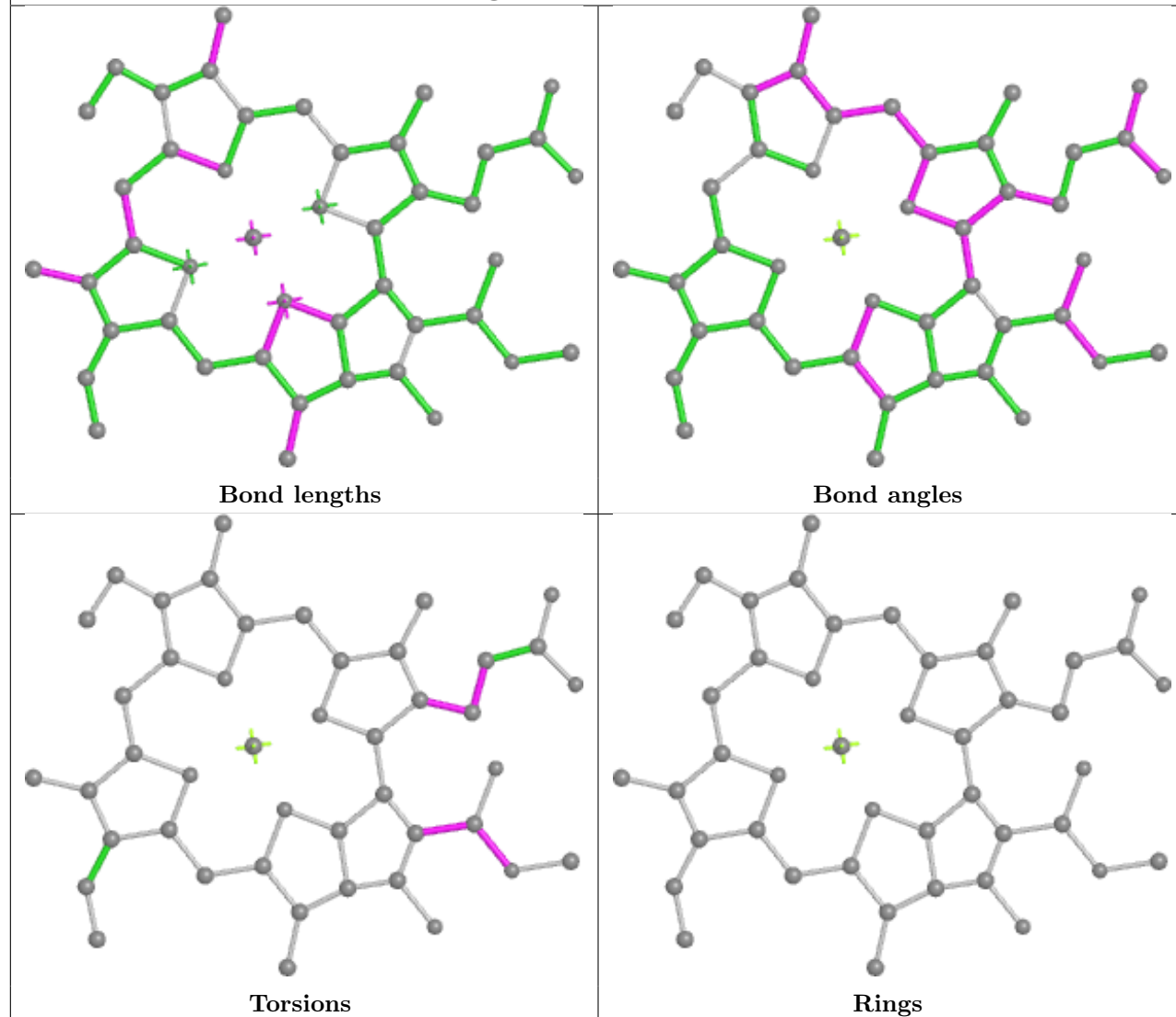


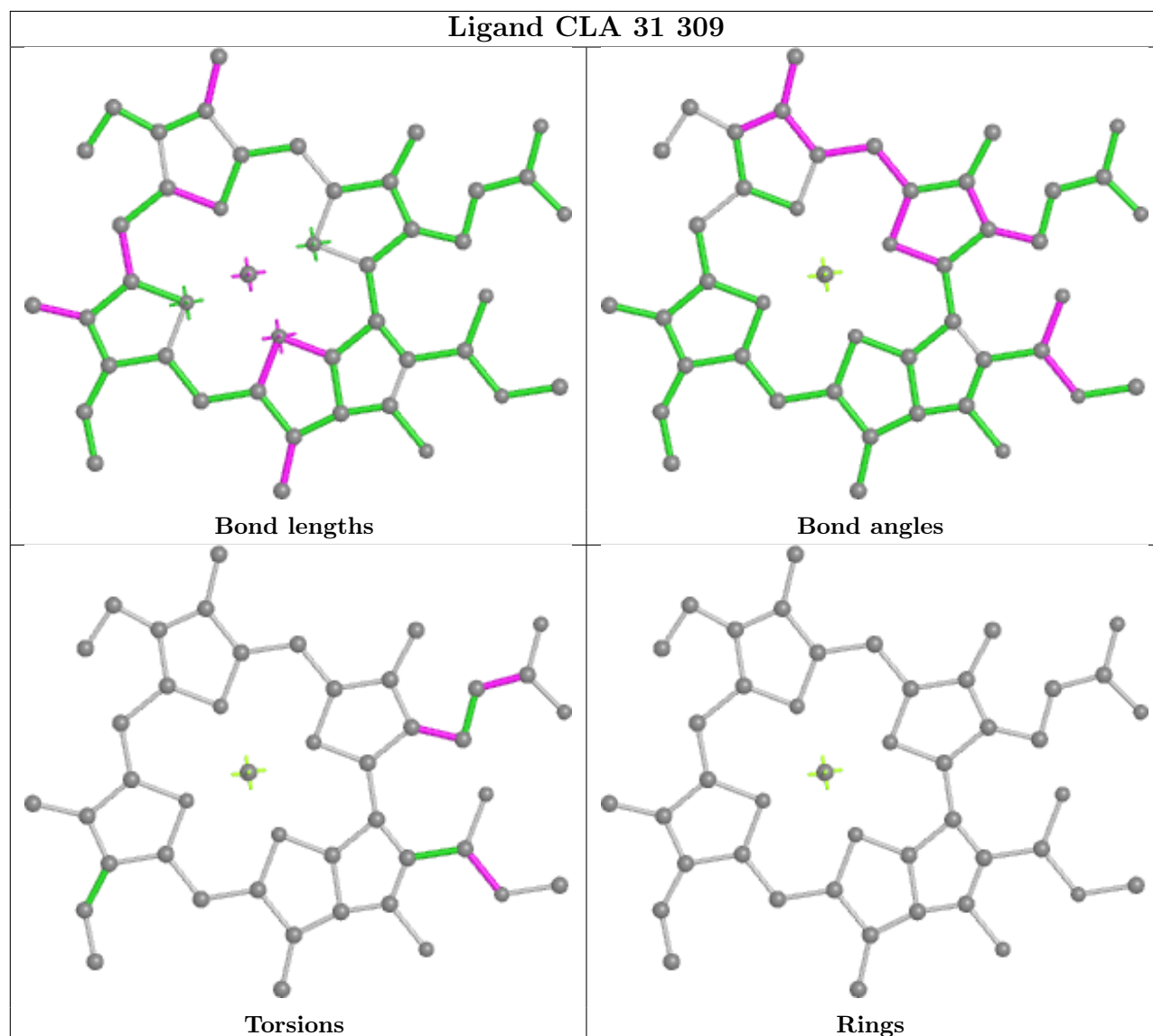
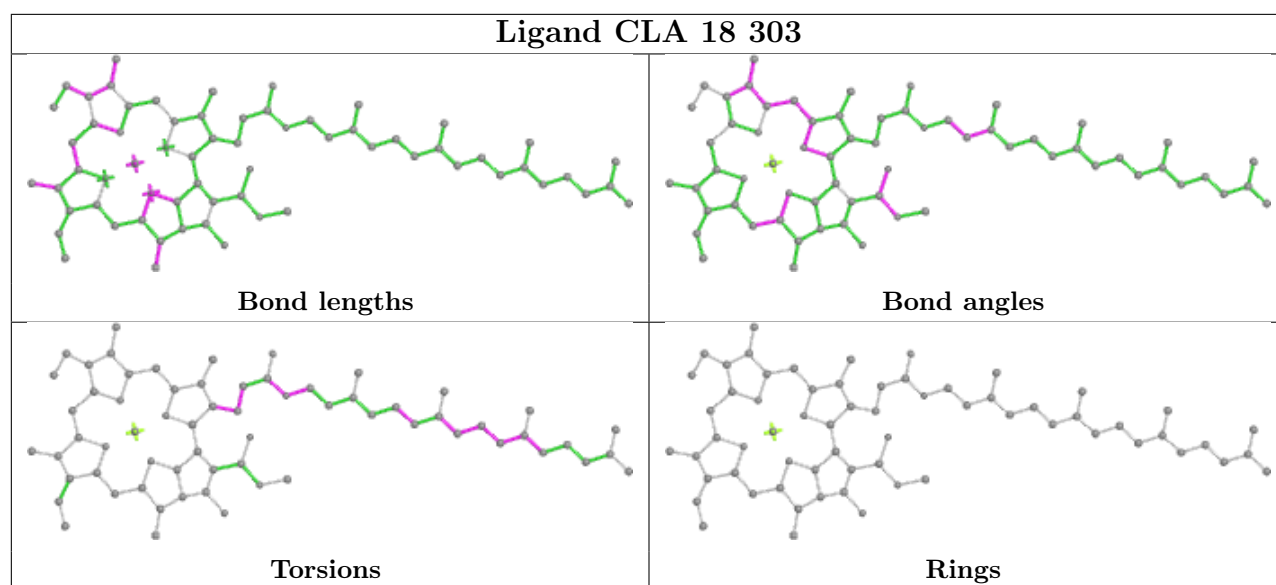


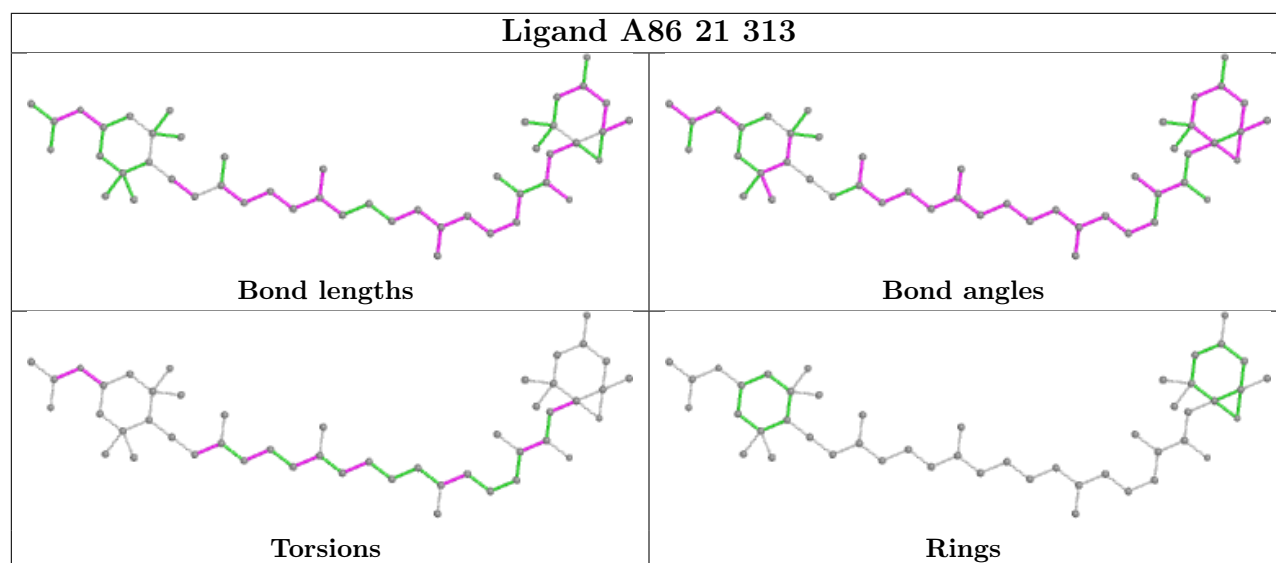
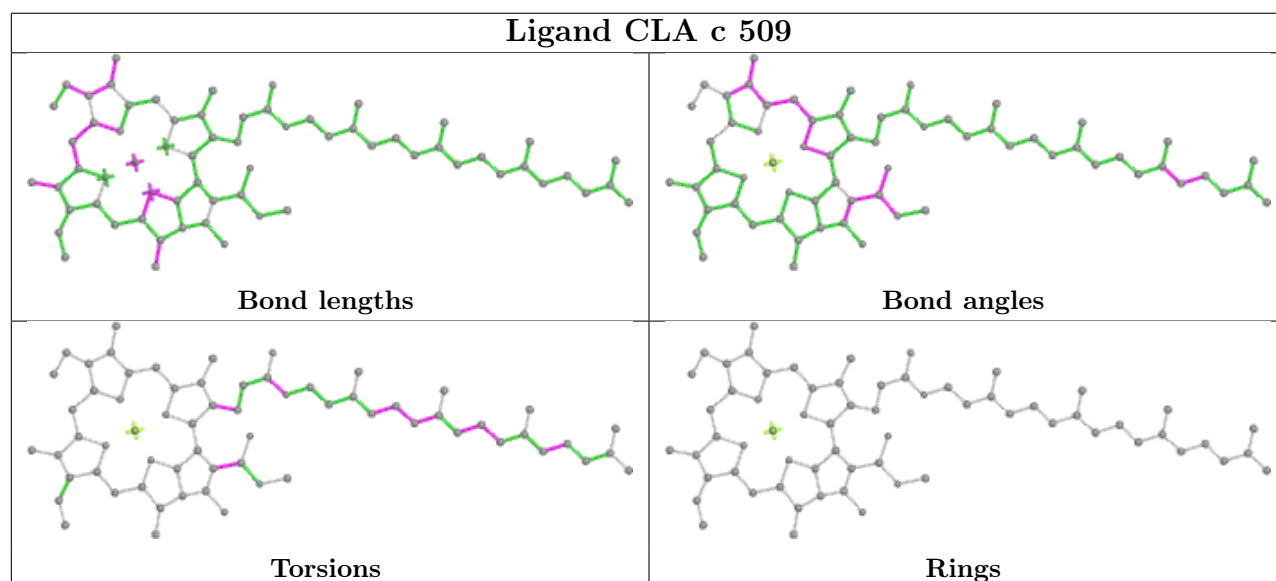
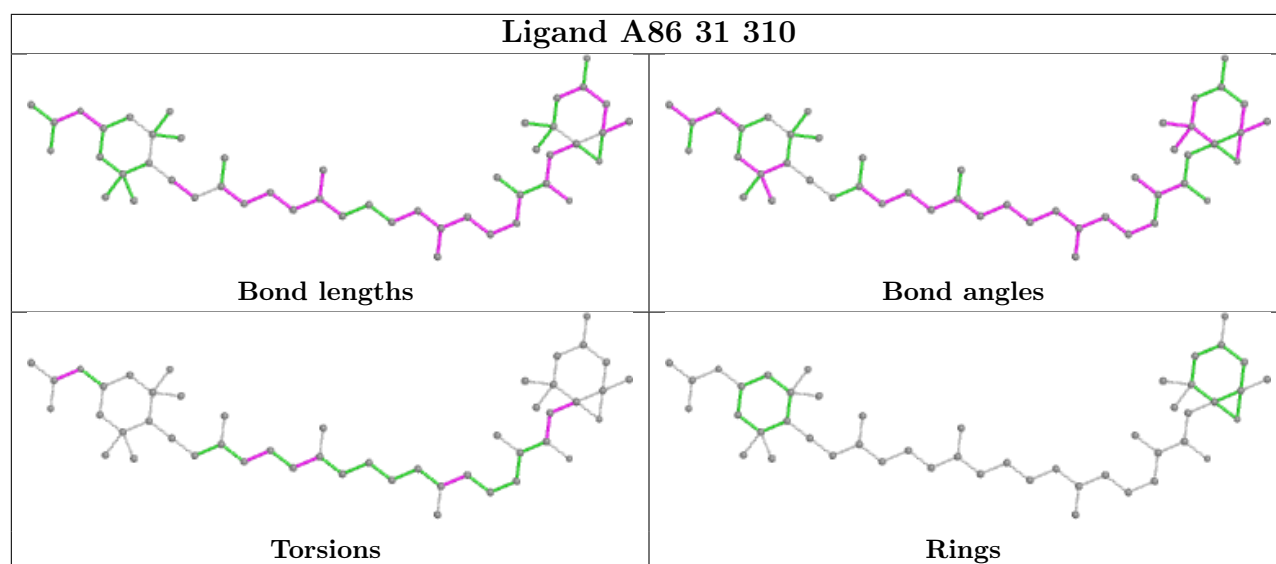
Ligand CLA b 603

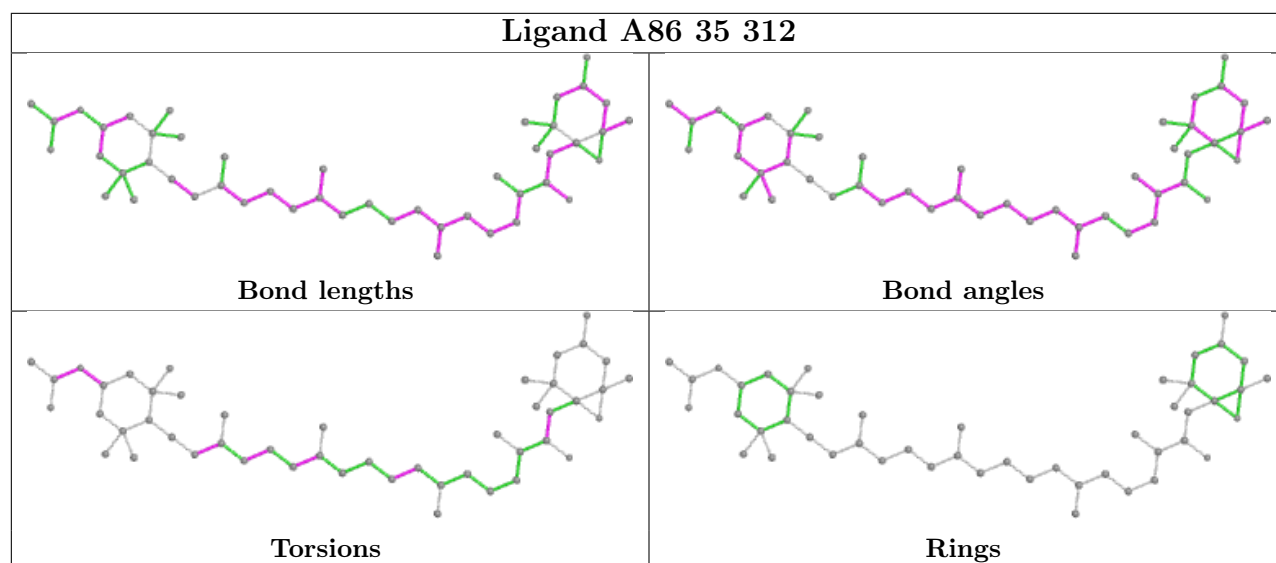
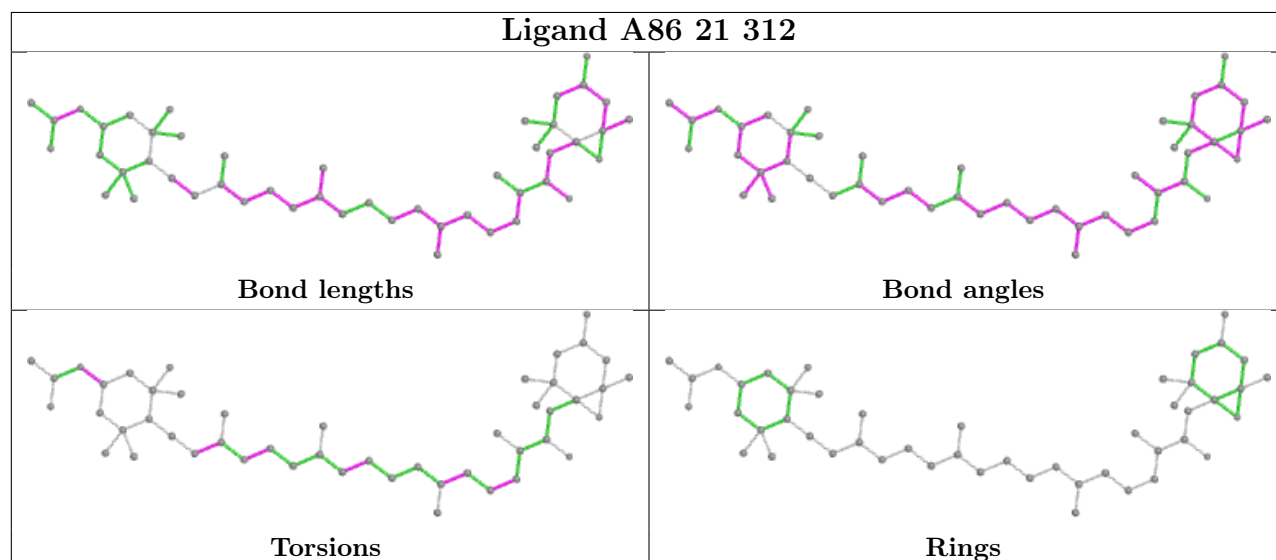
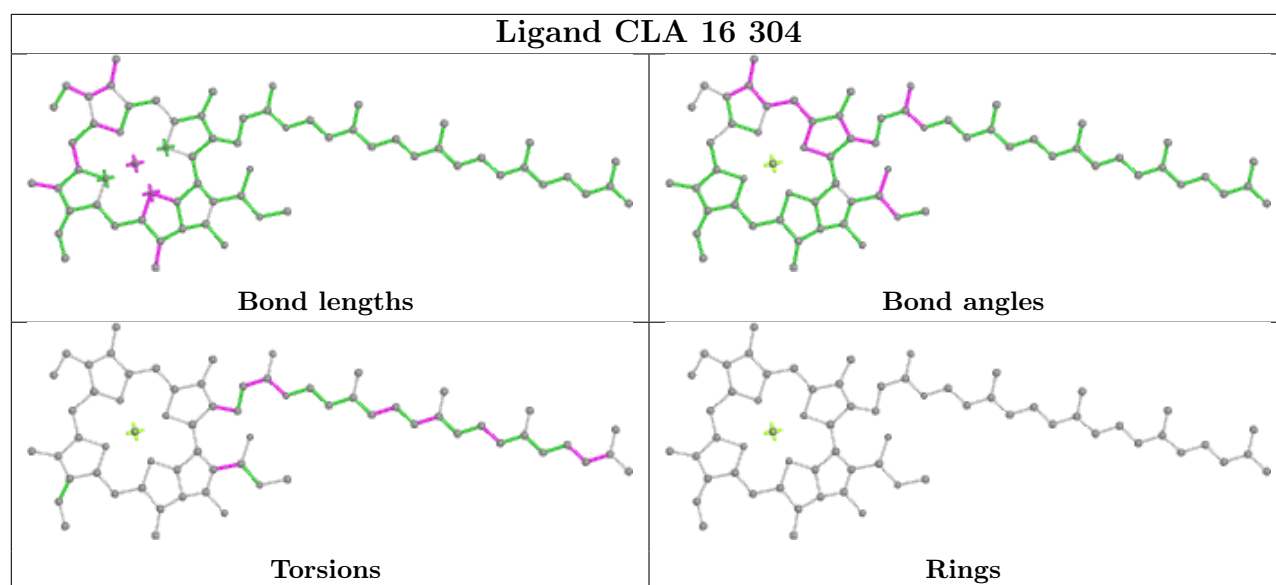


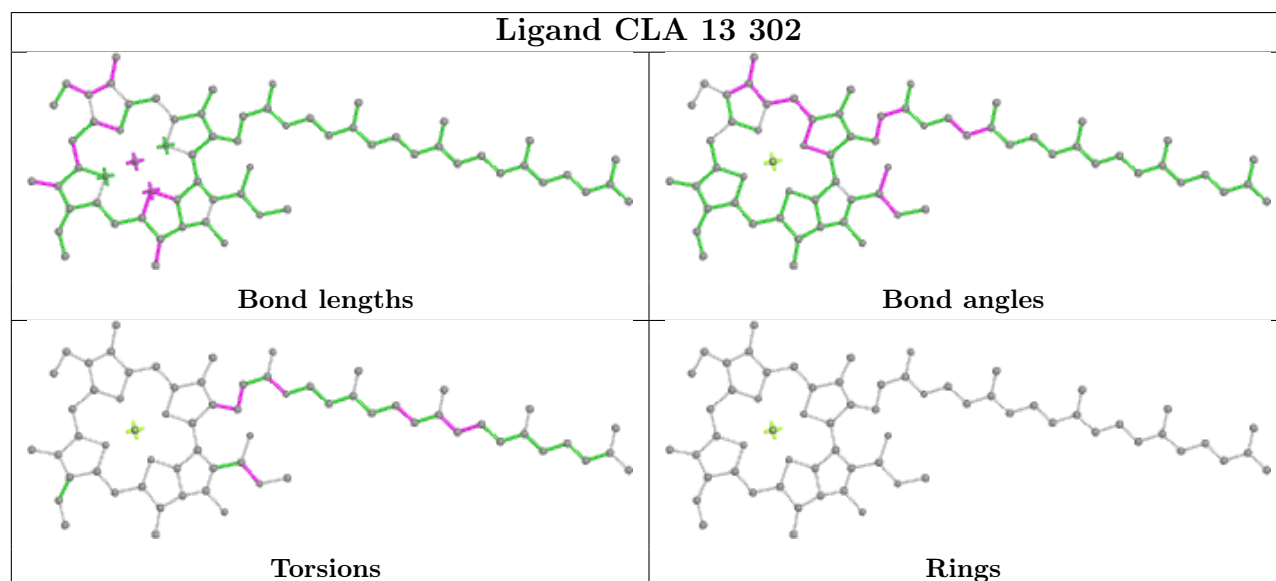
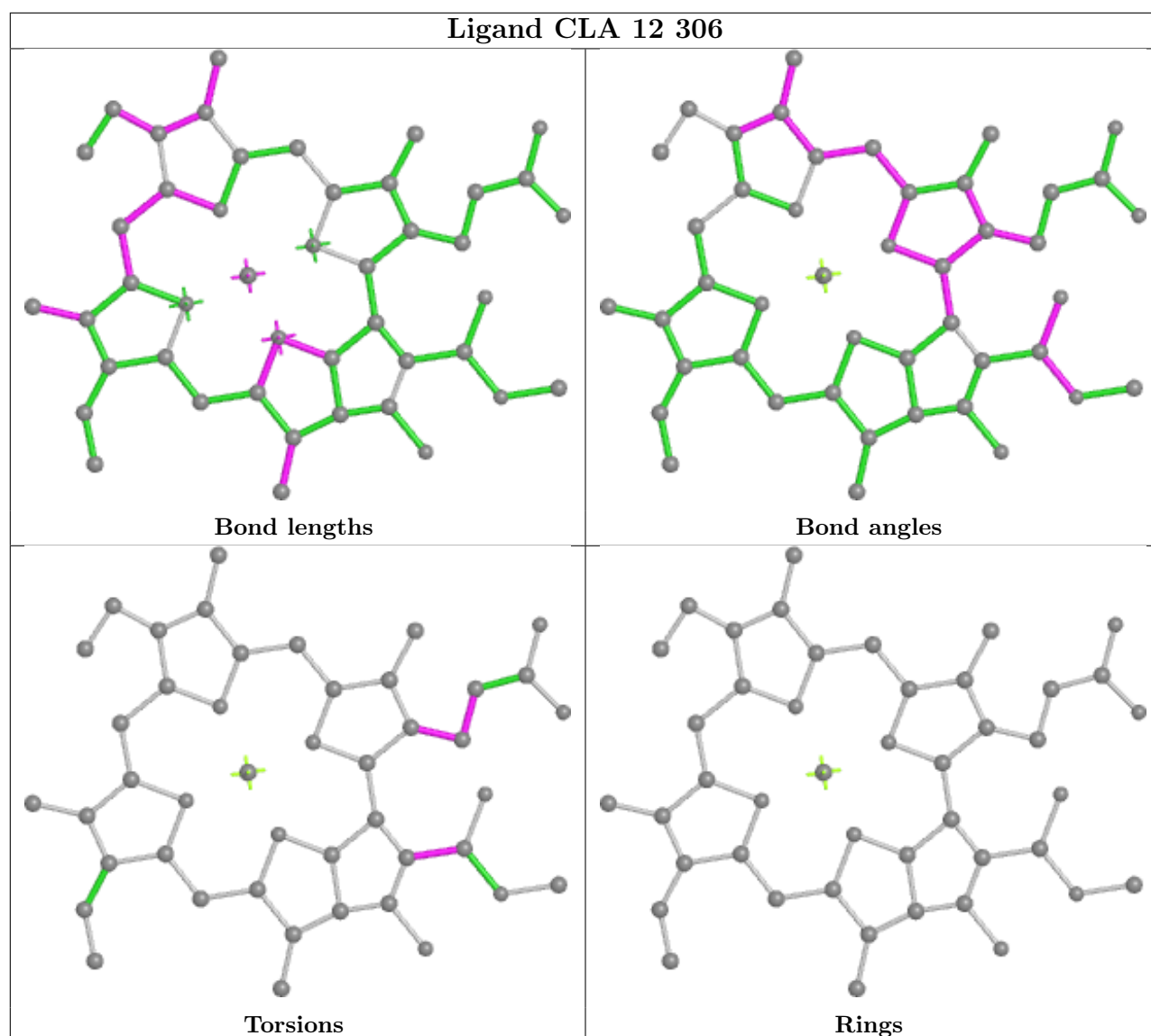
Ligand CLA 16 303

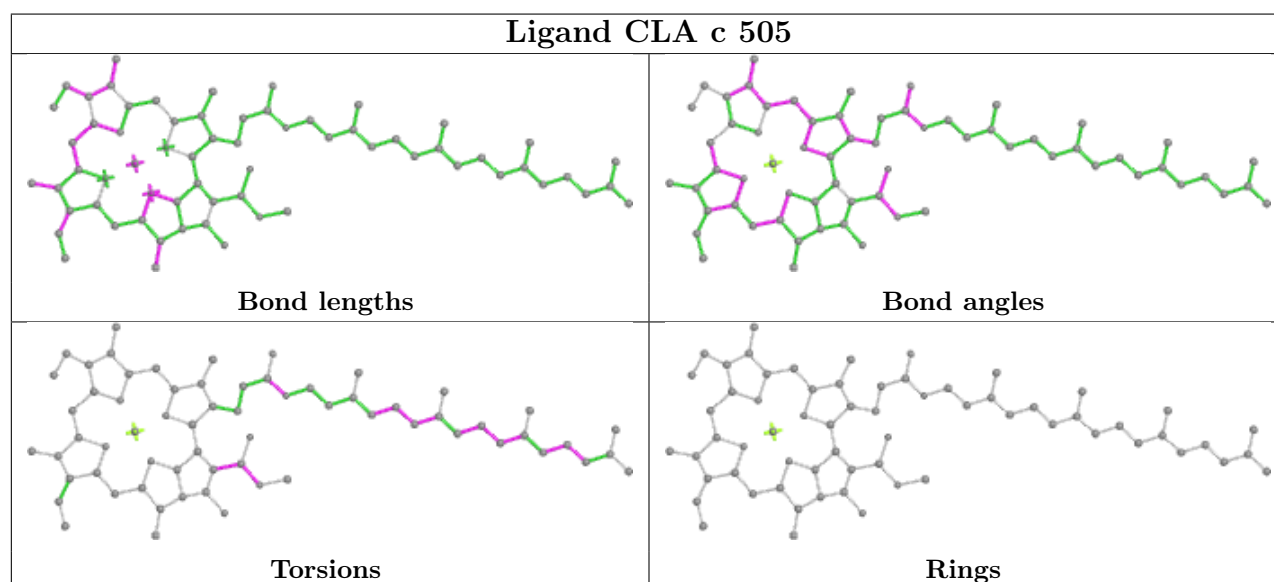
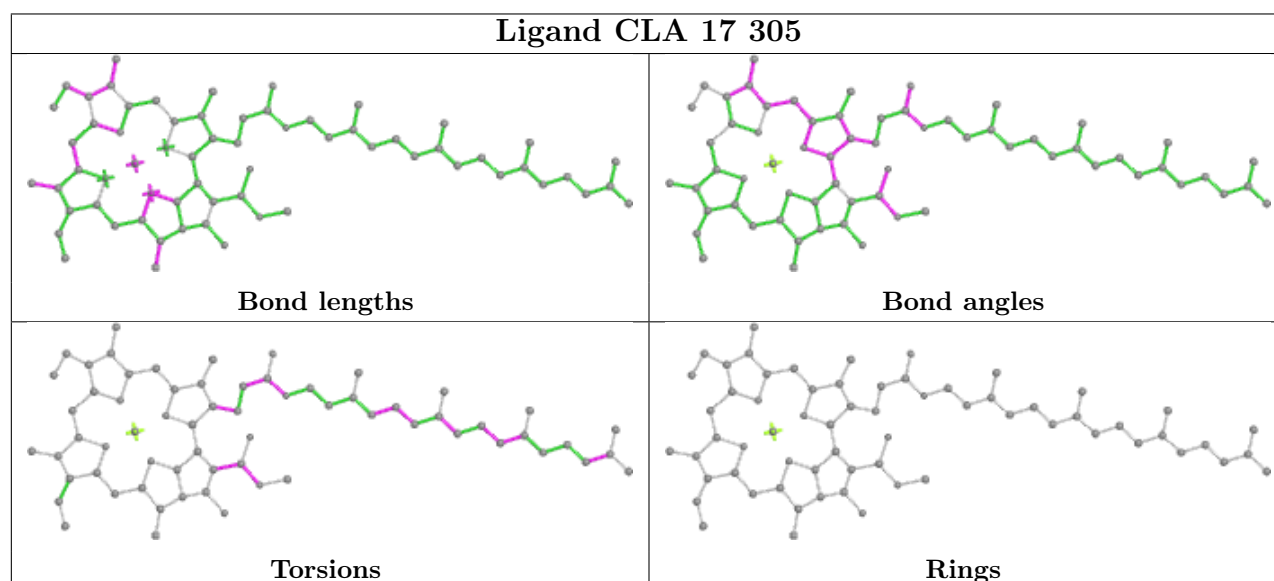
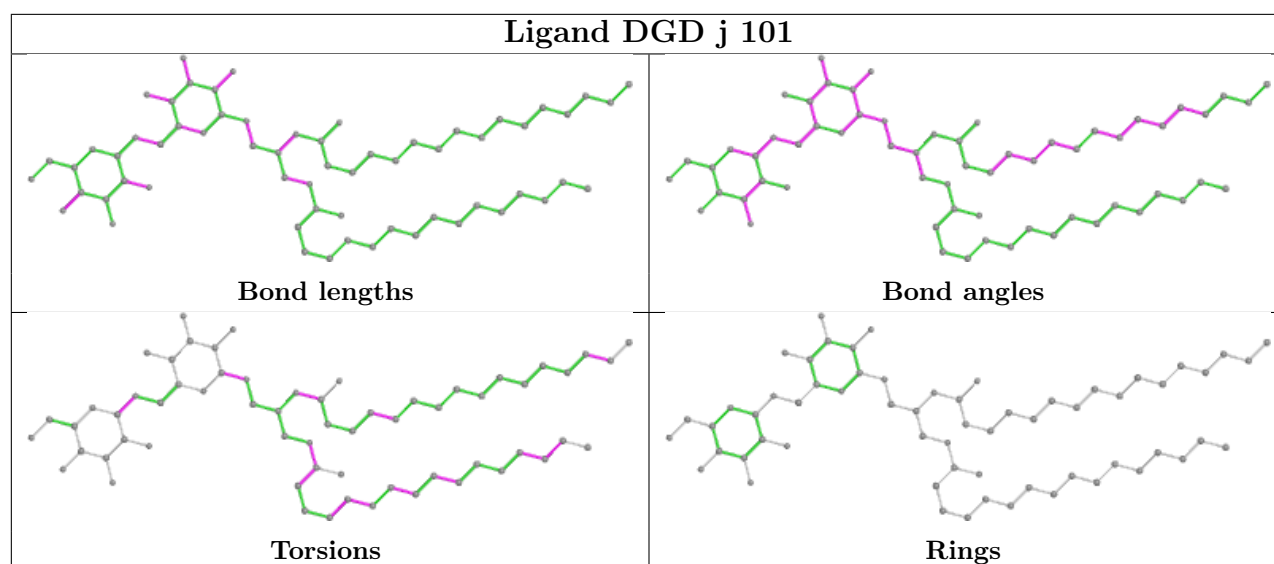


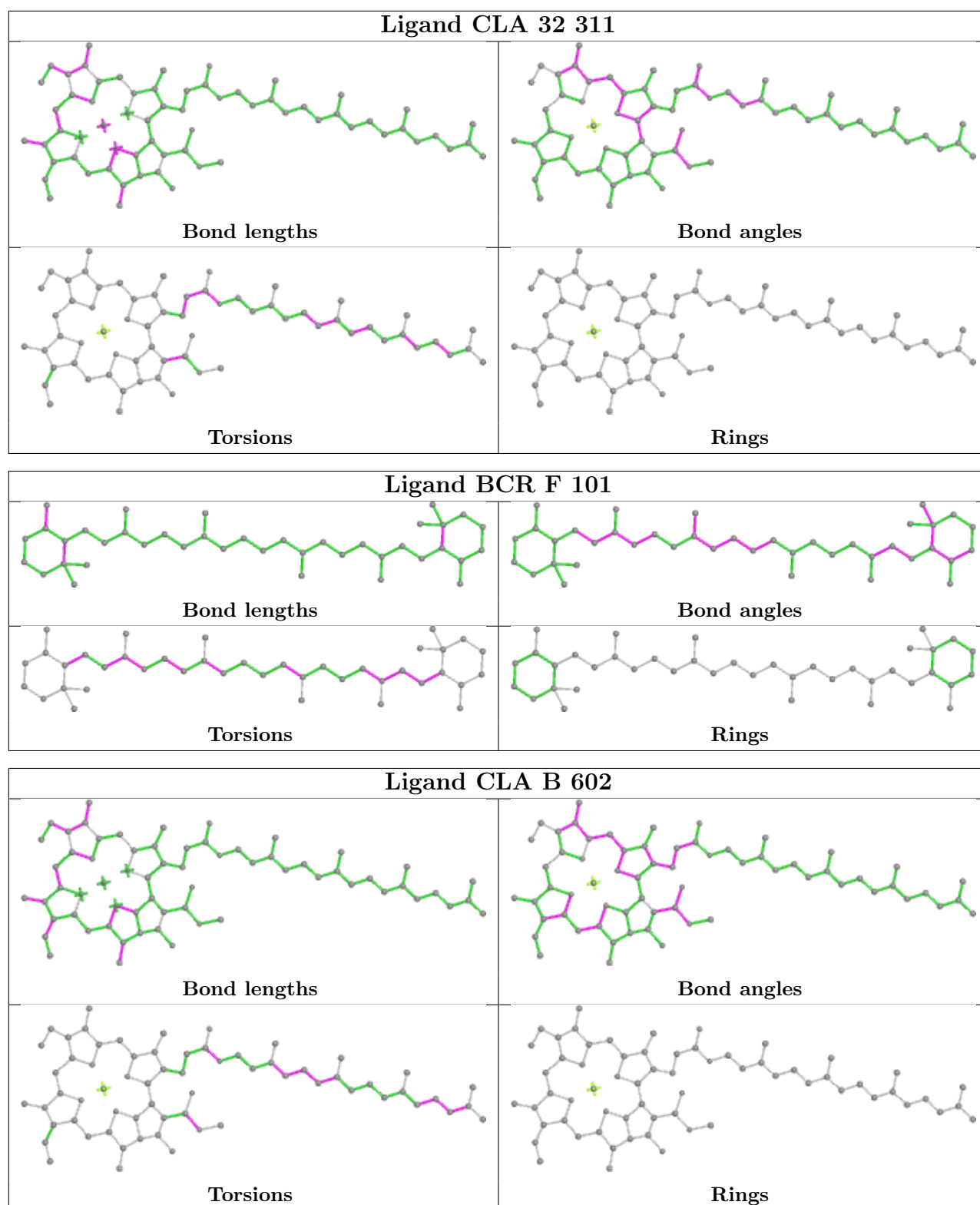




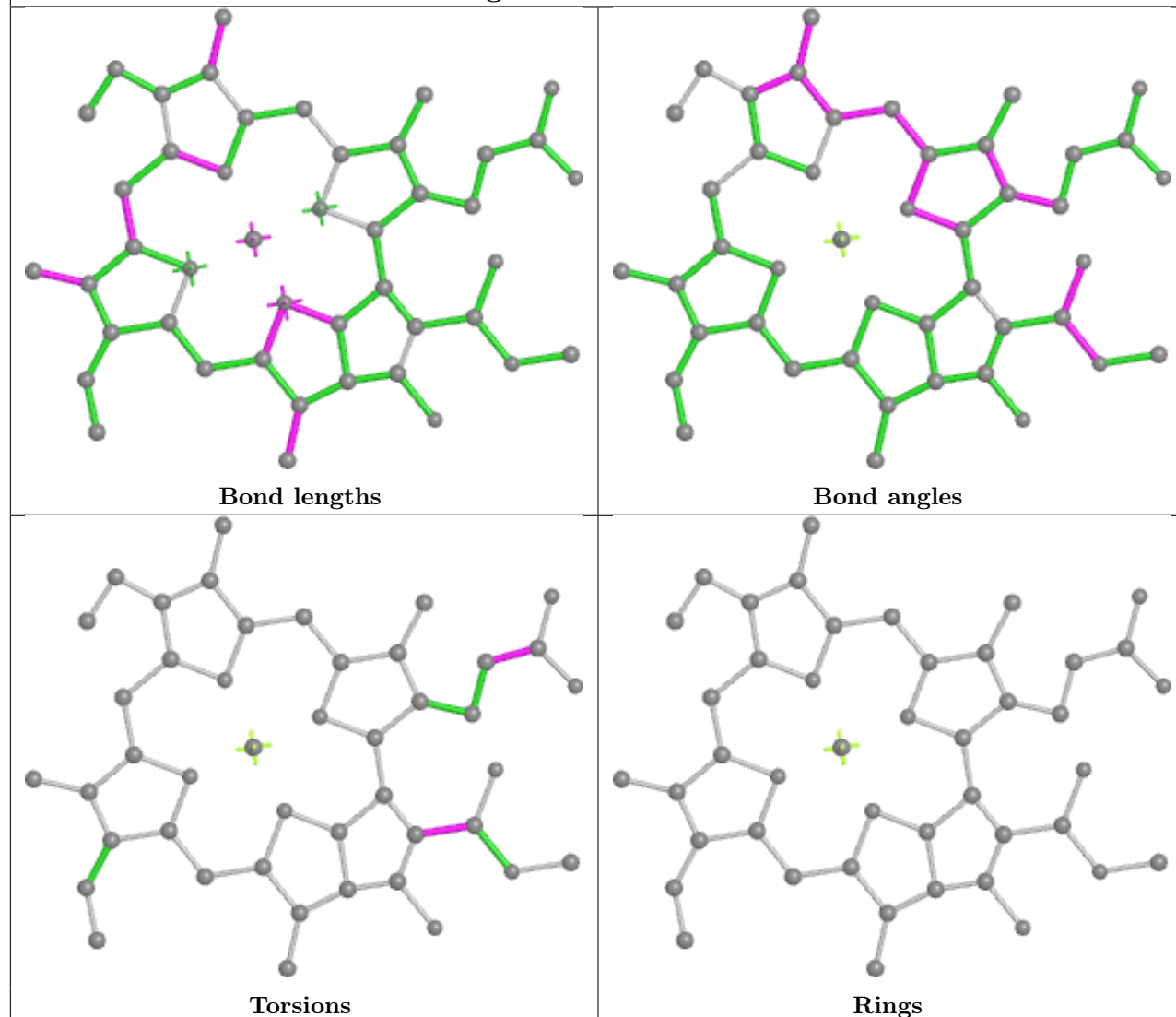




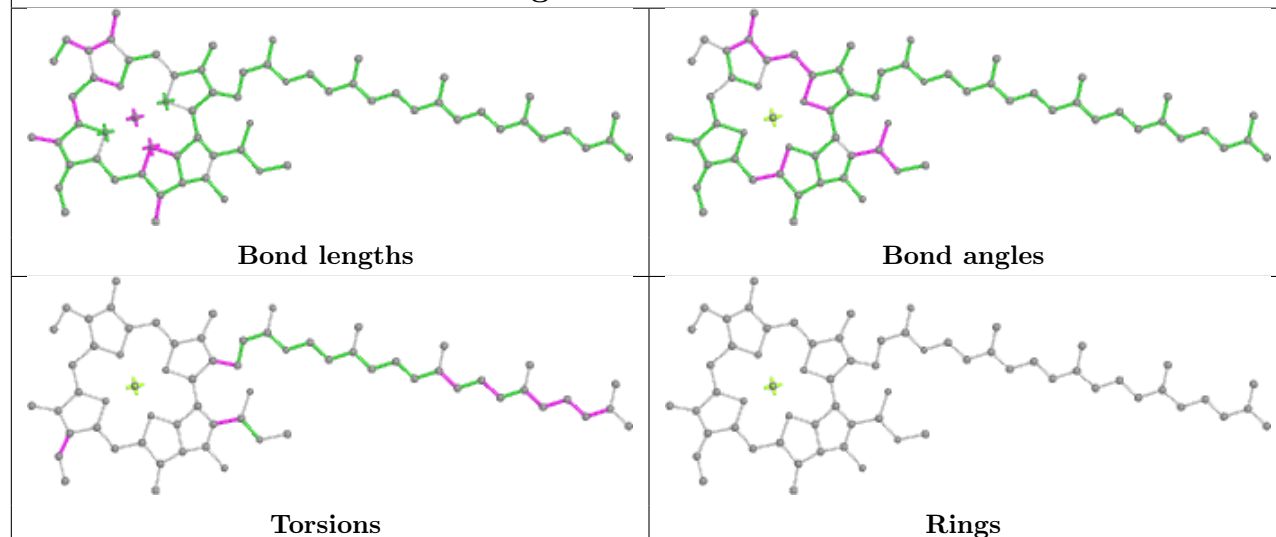


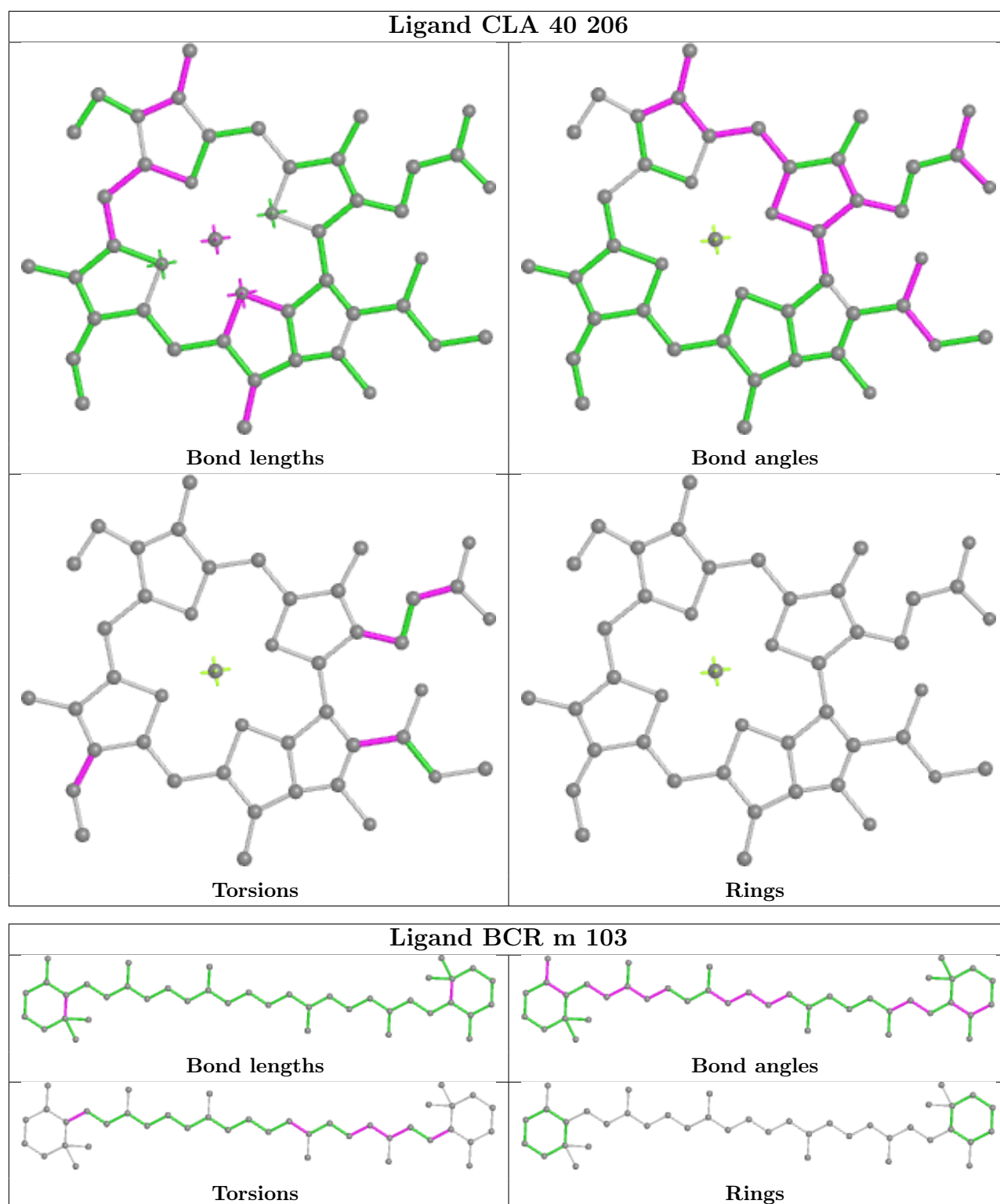


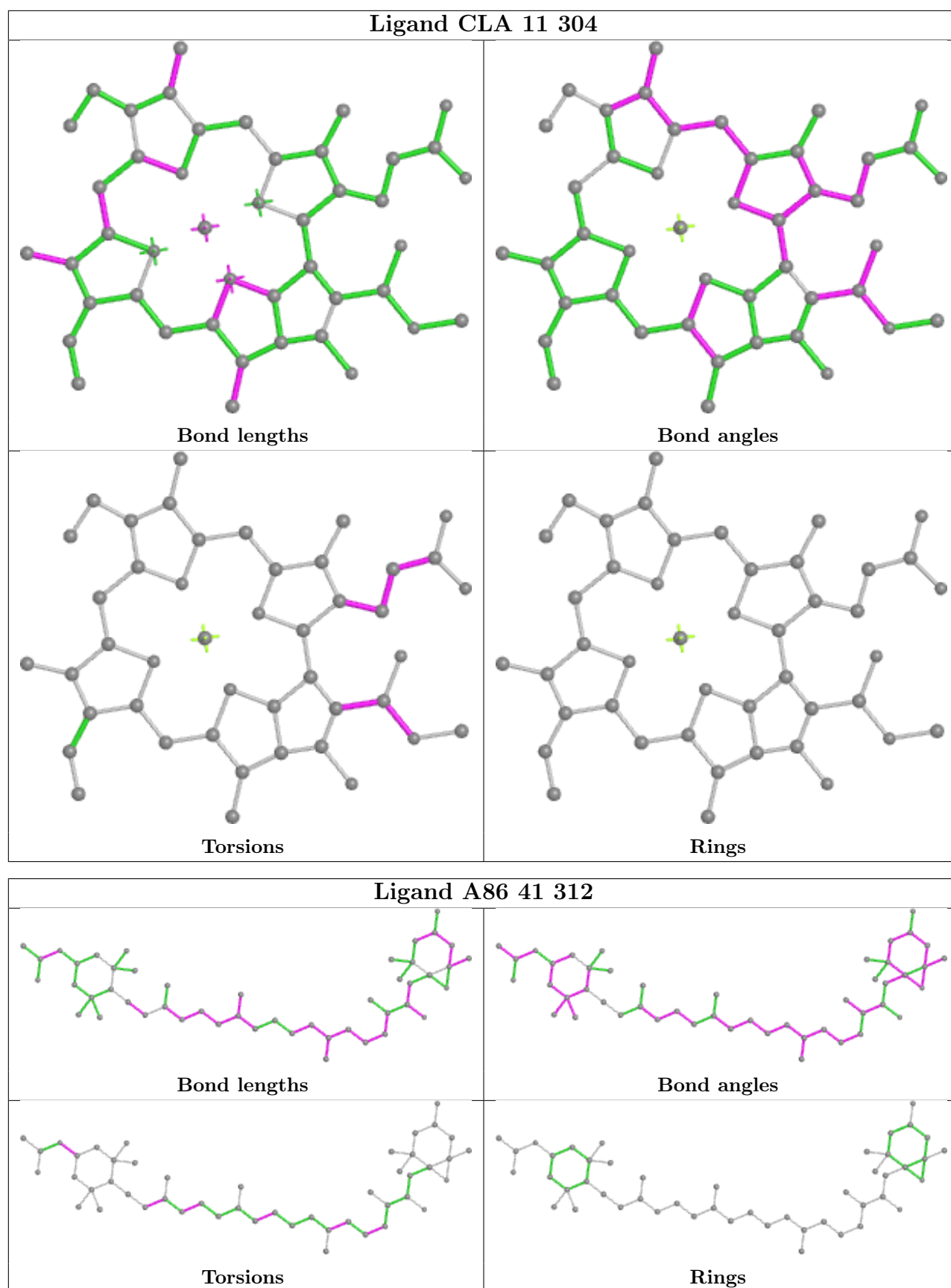
Ligand CLA 19 307

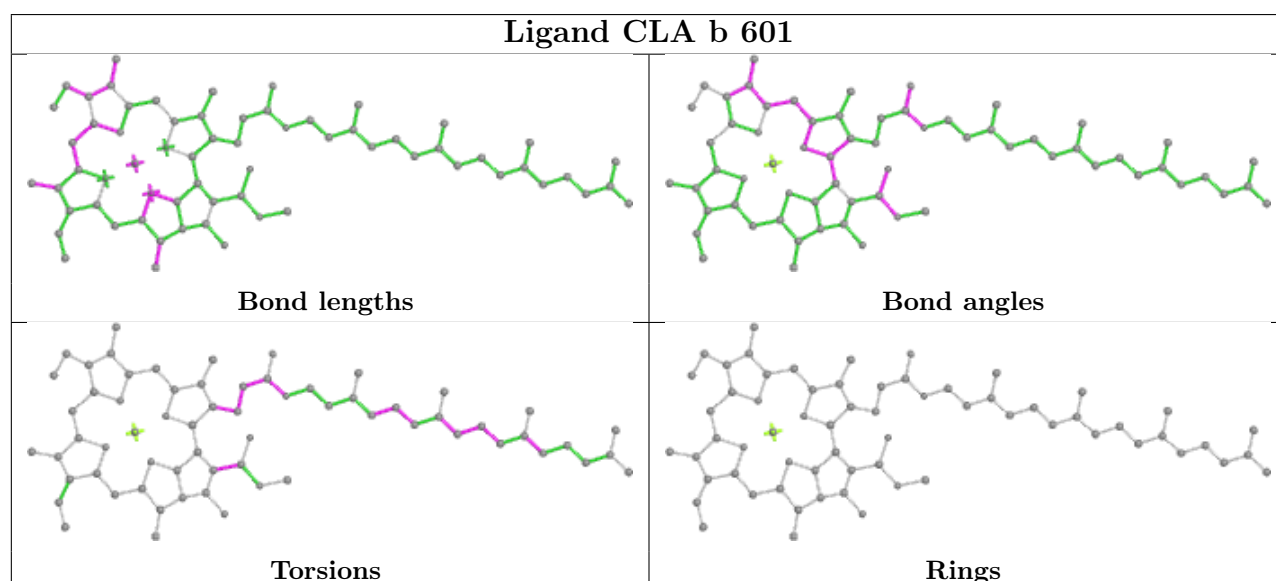
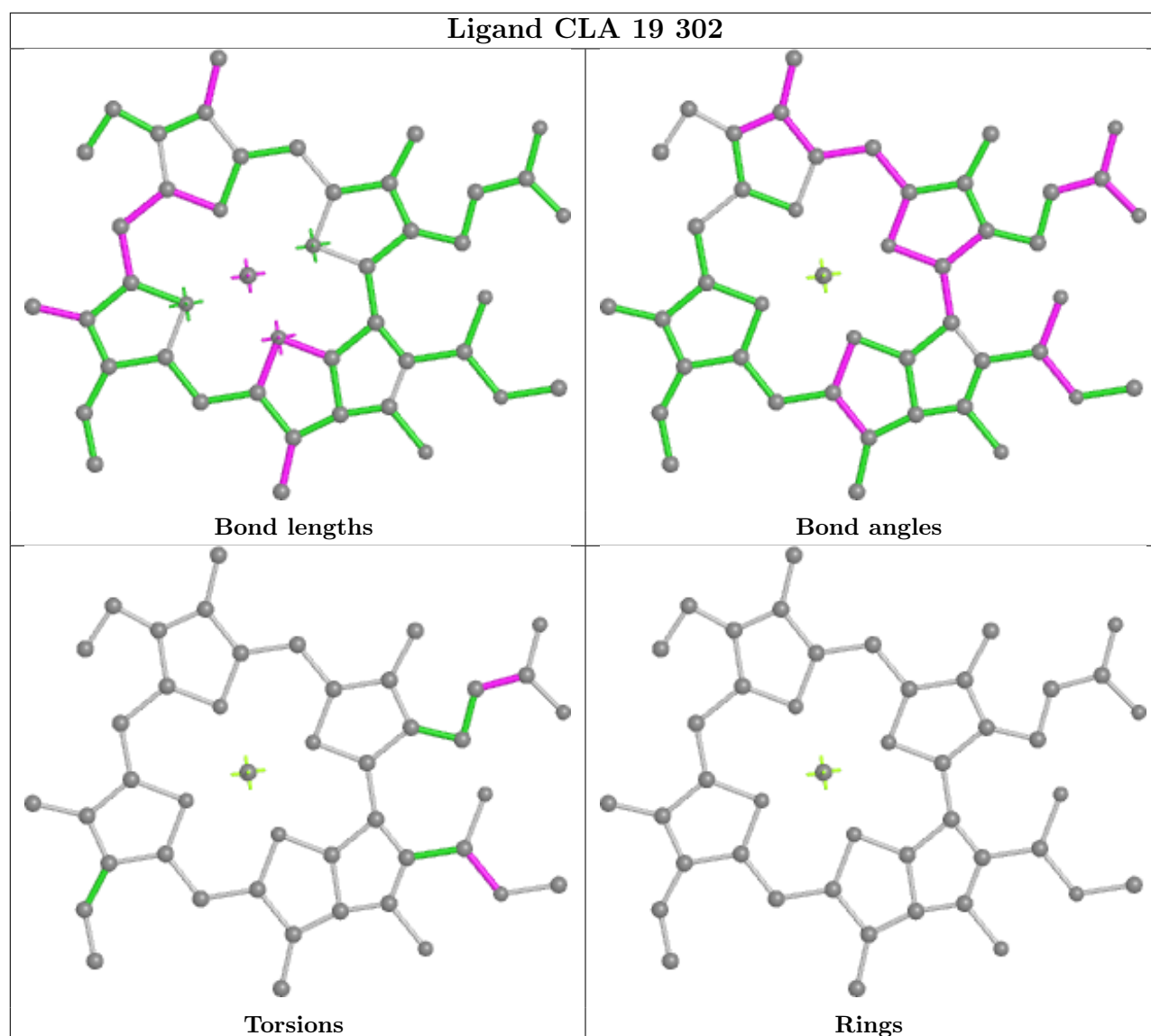


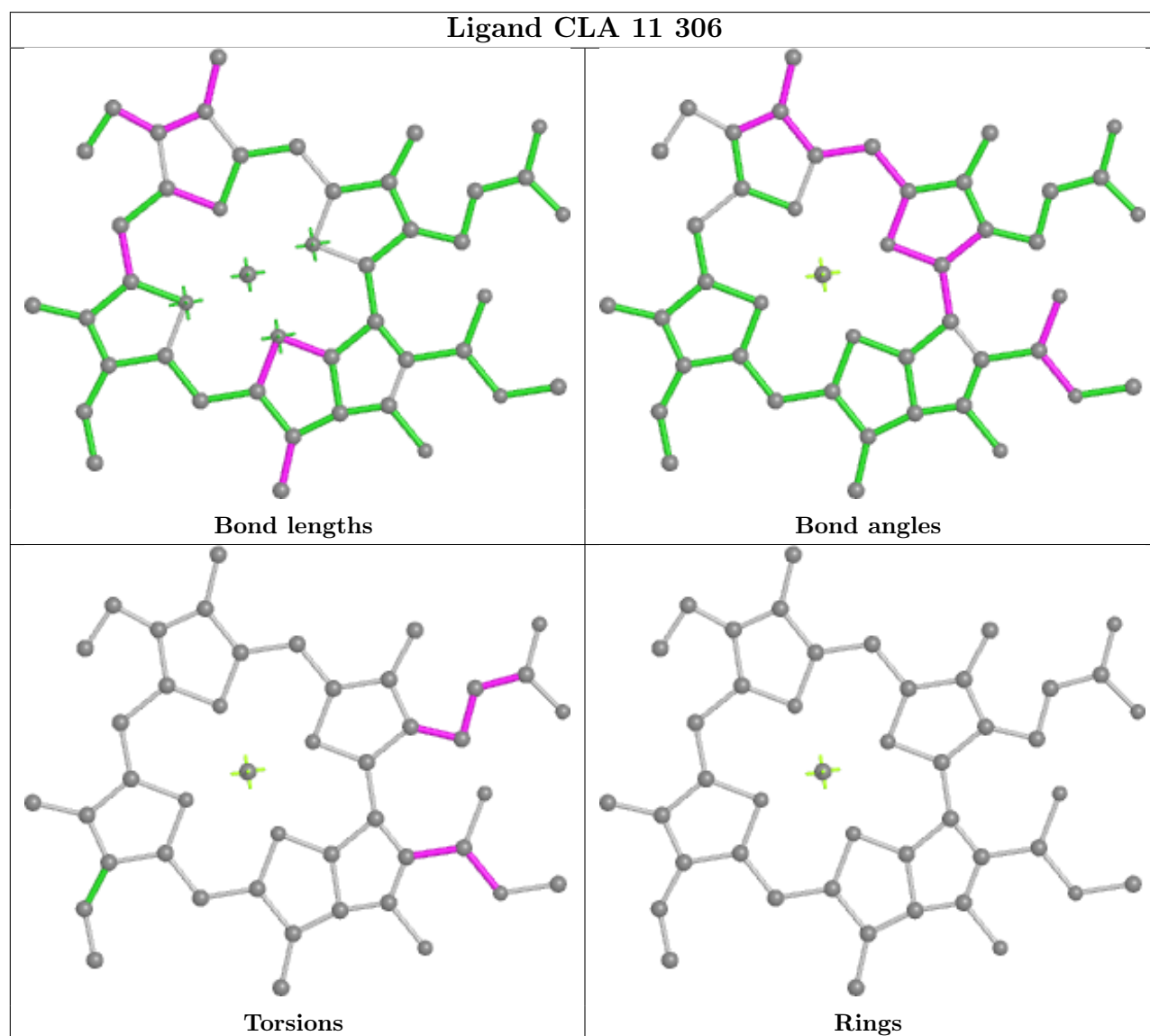
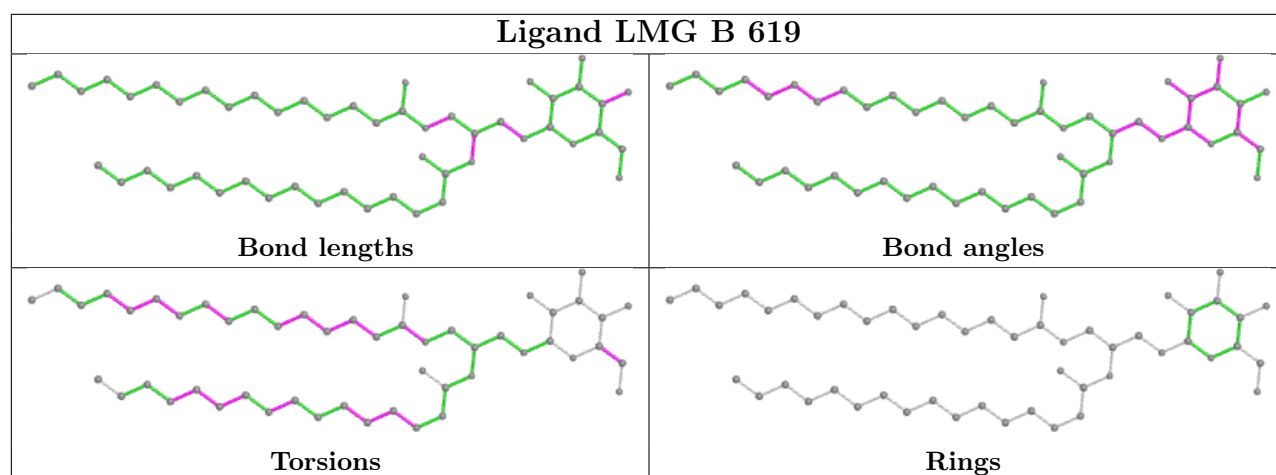
Ligand CLA D 402

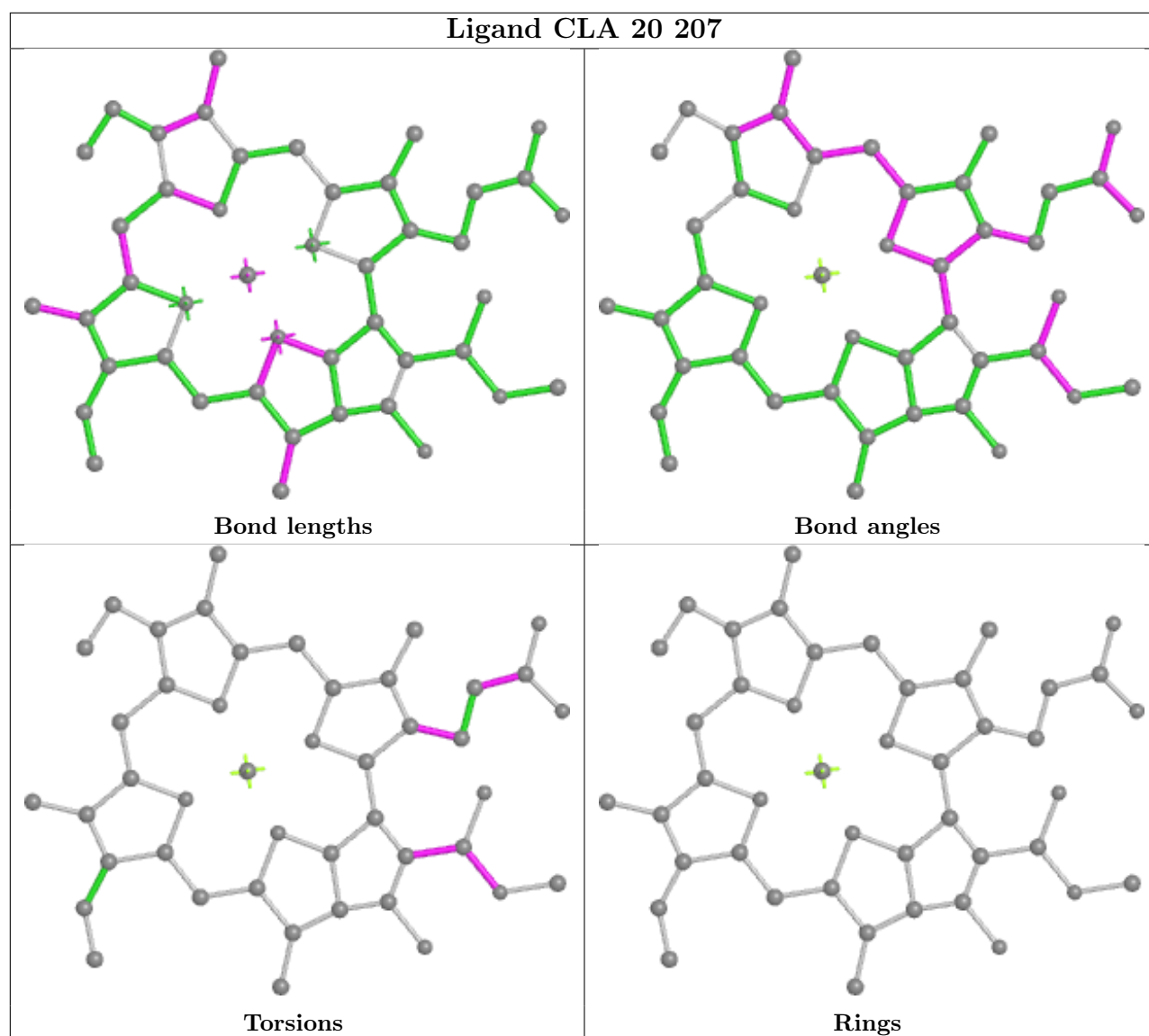


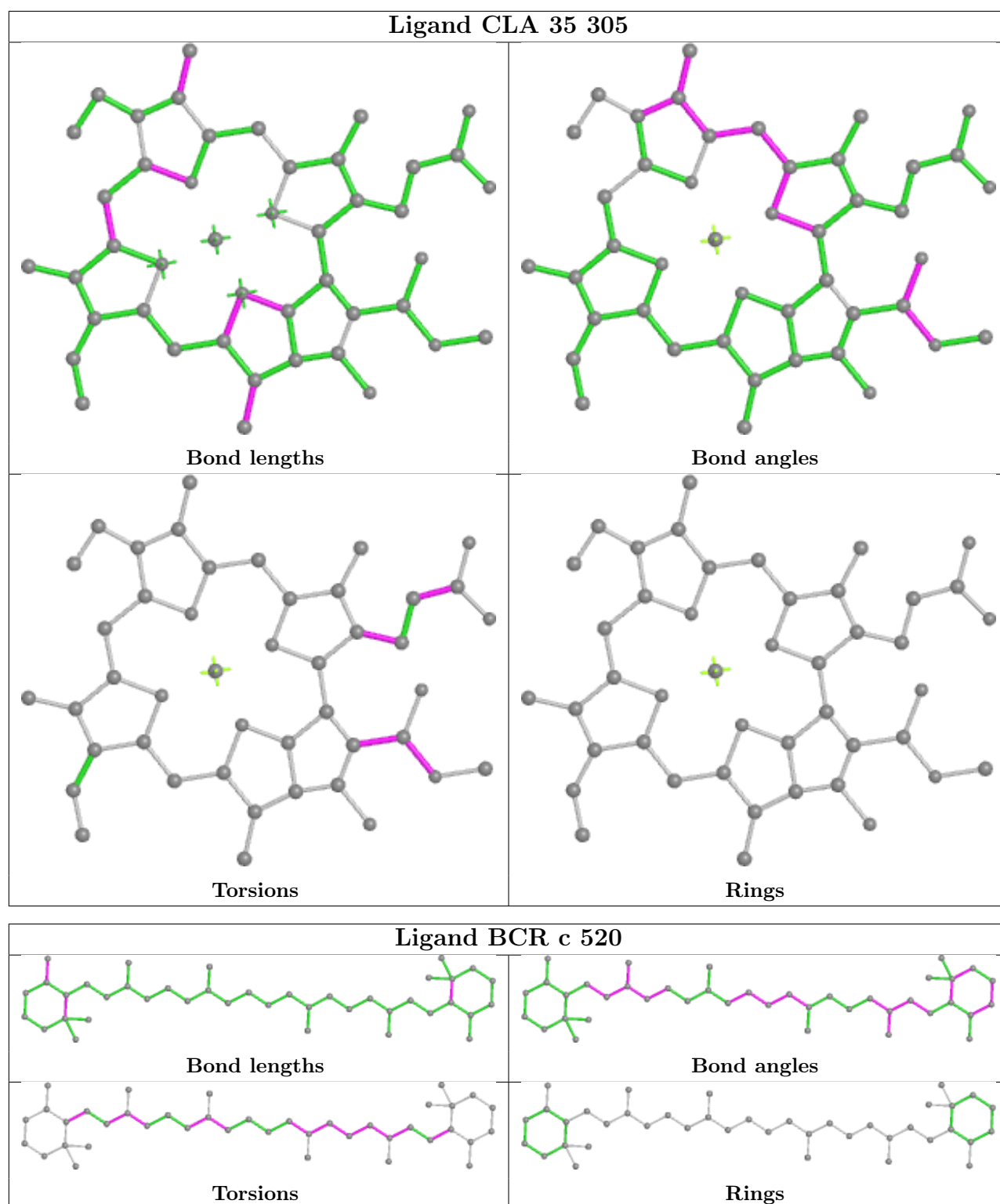


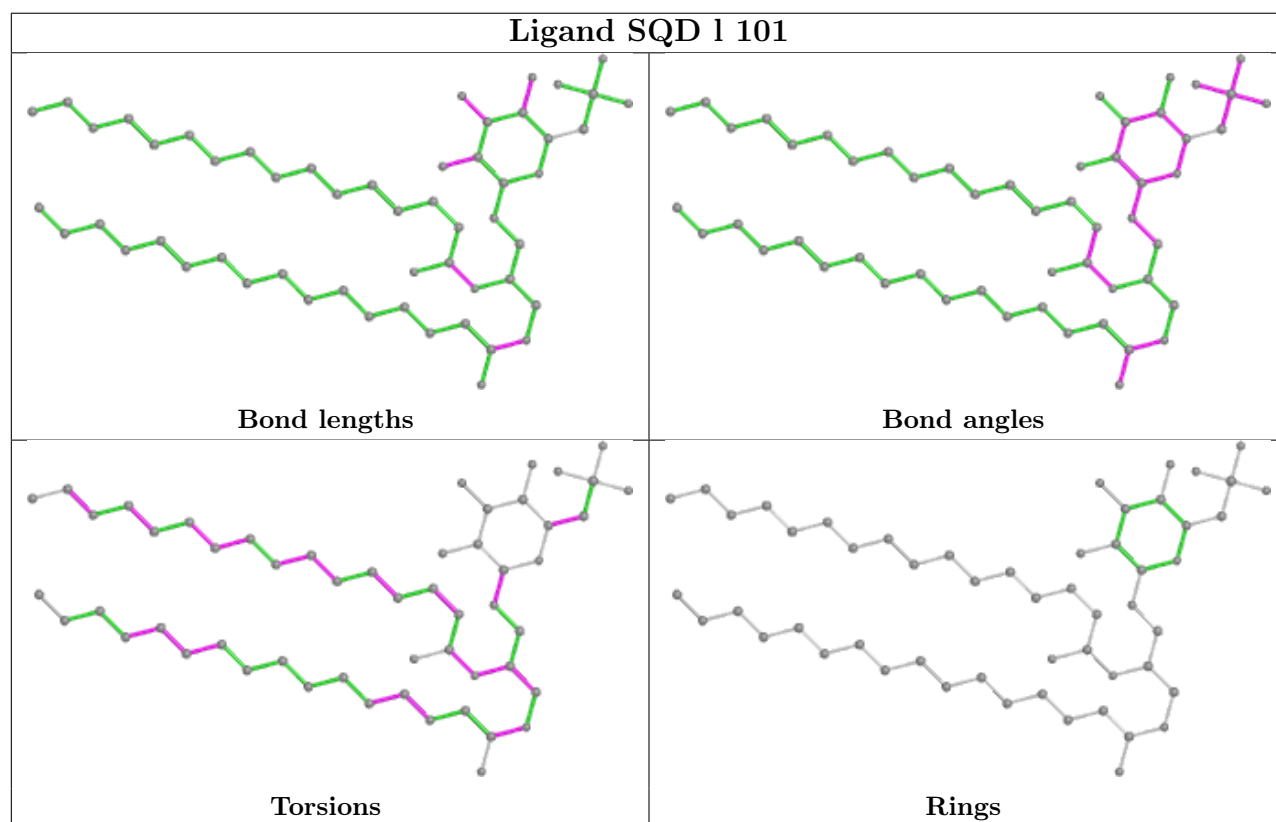
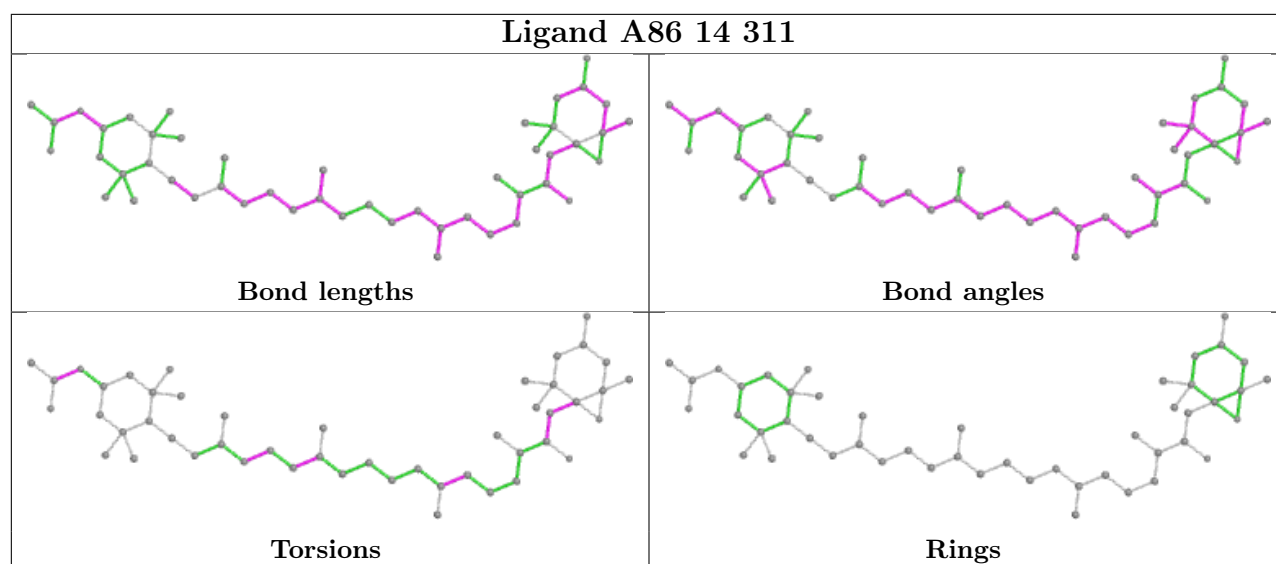




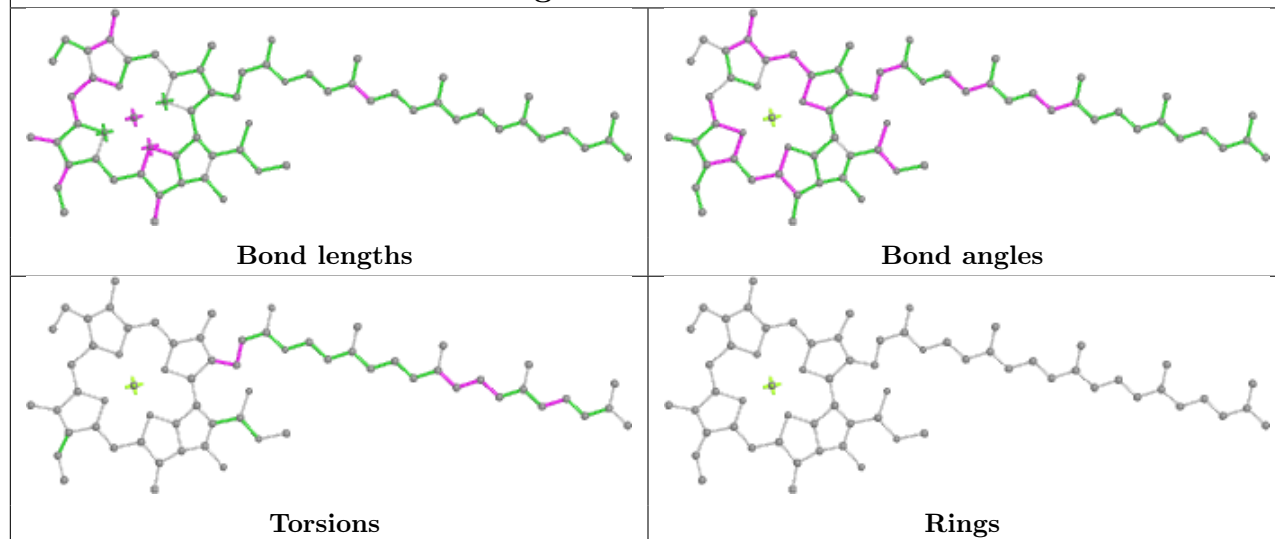




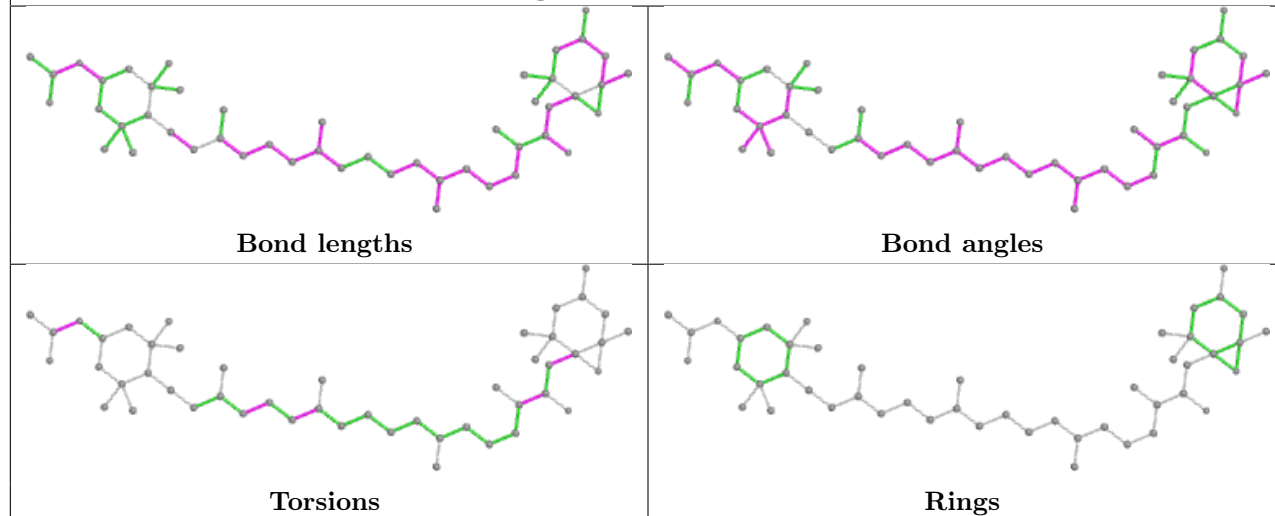




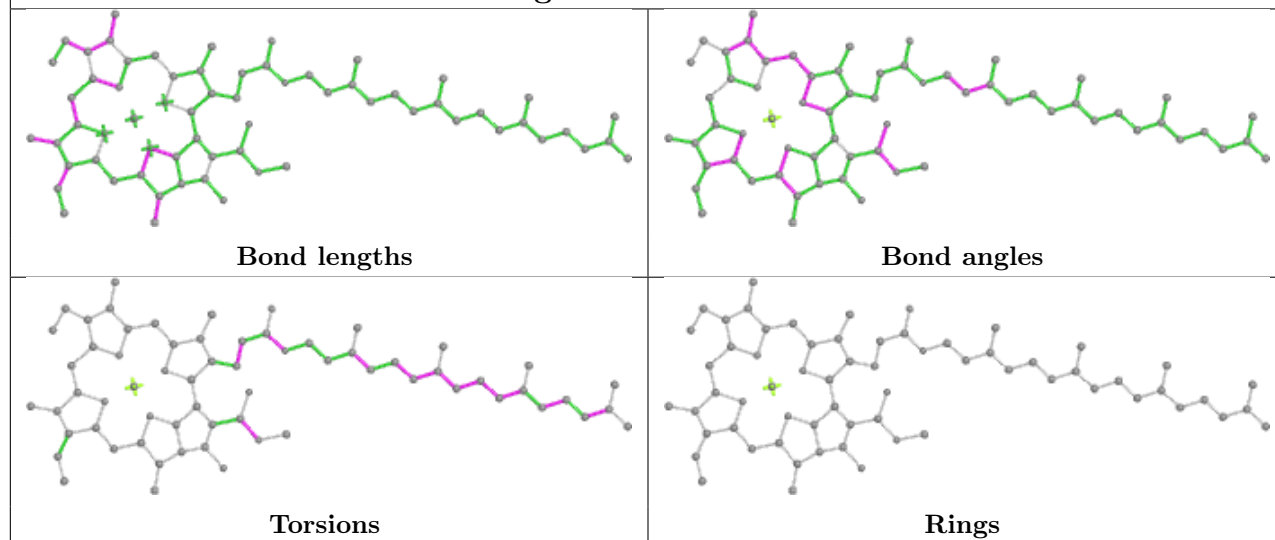
Ligand CLA b 606

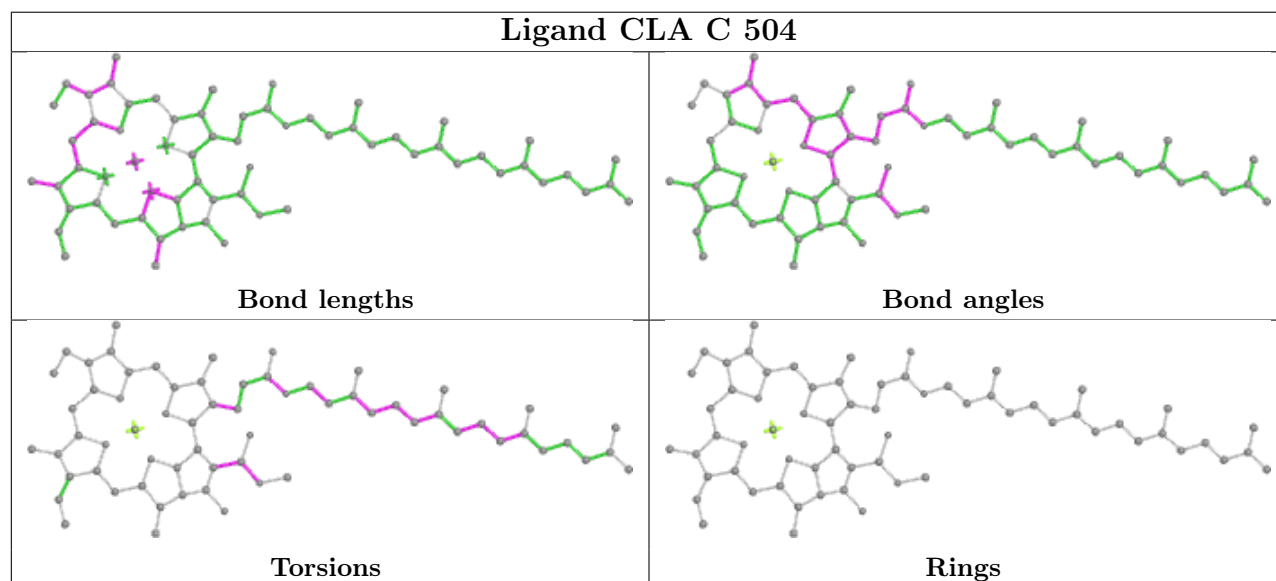
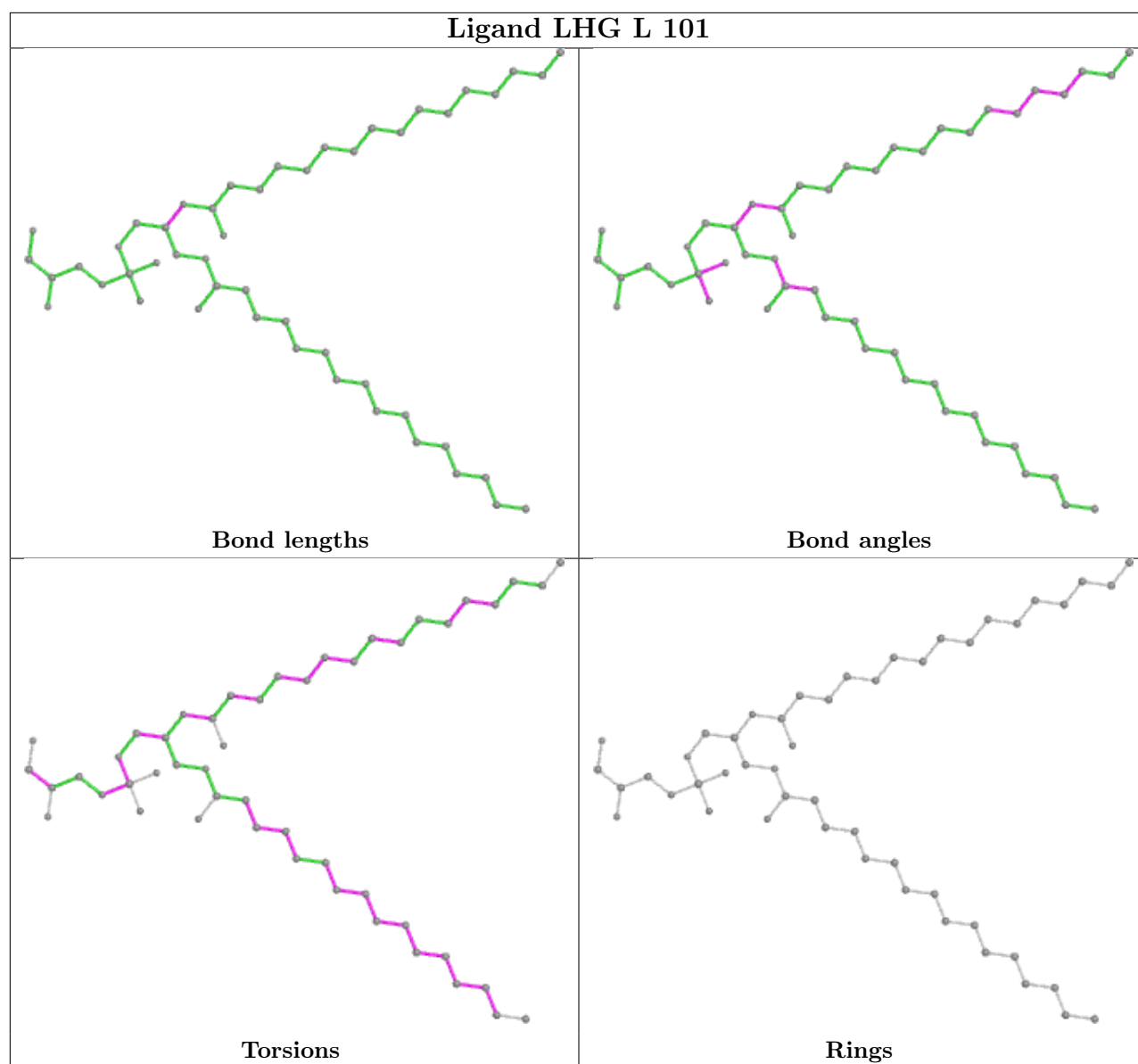


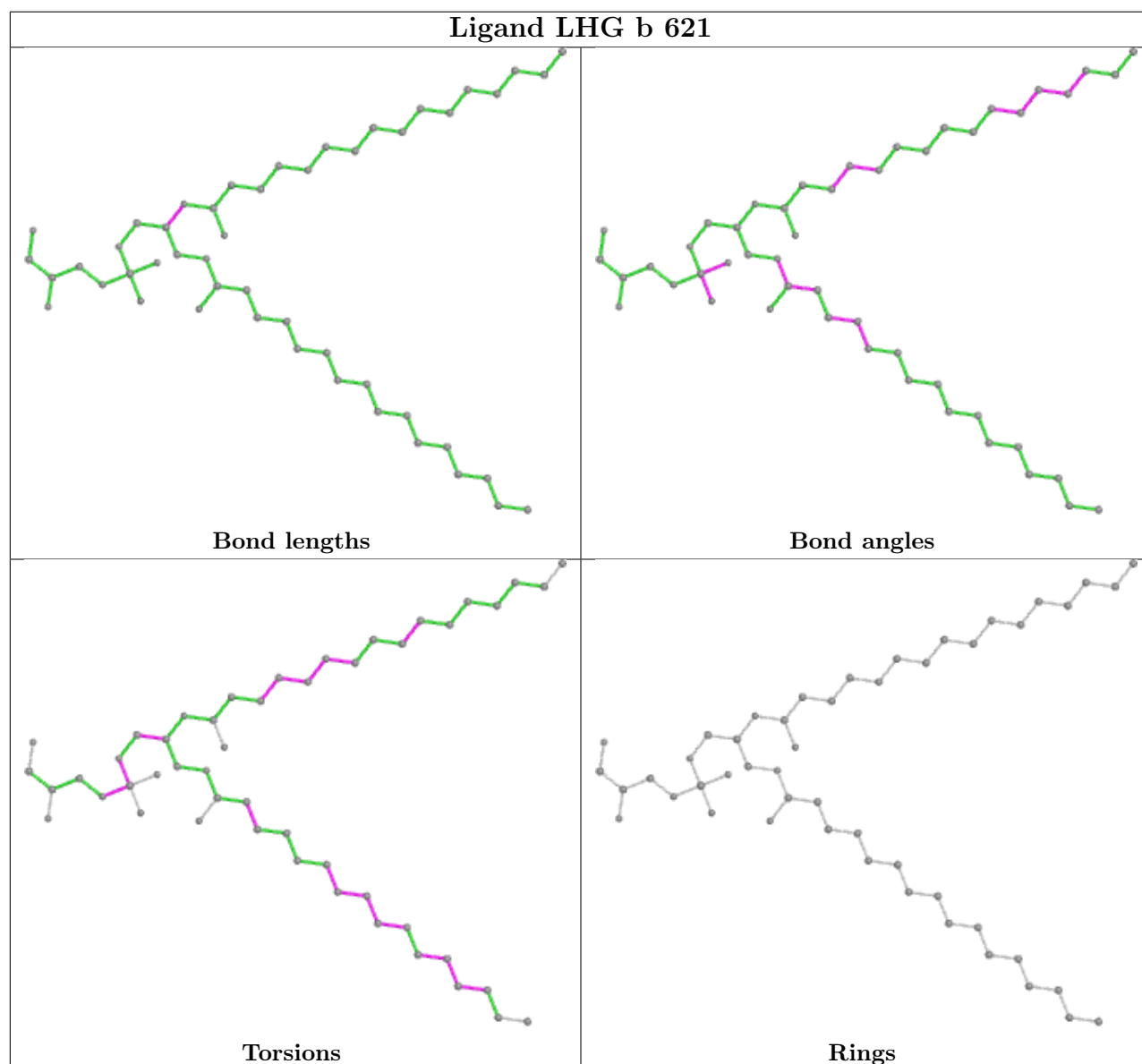
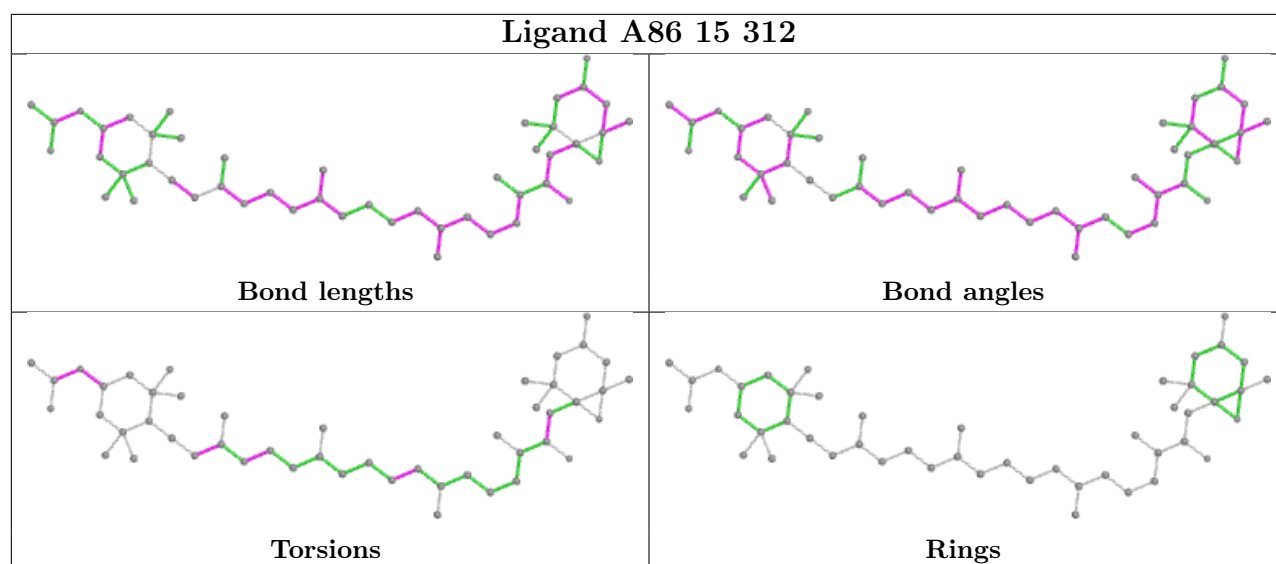
Ligand A86 18 315

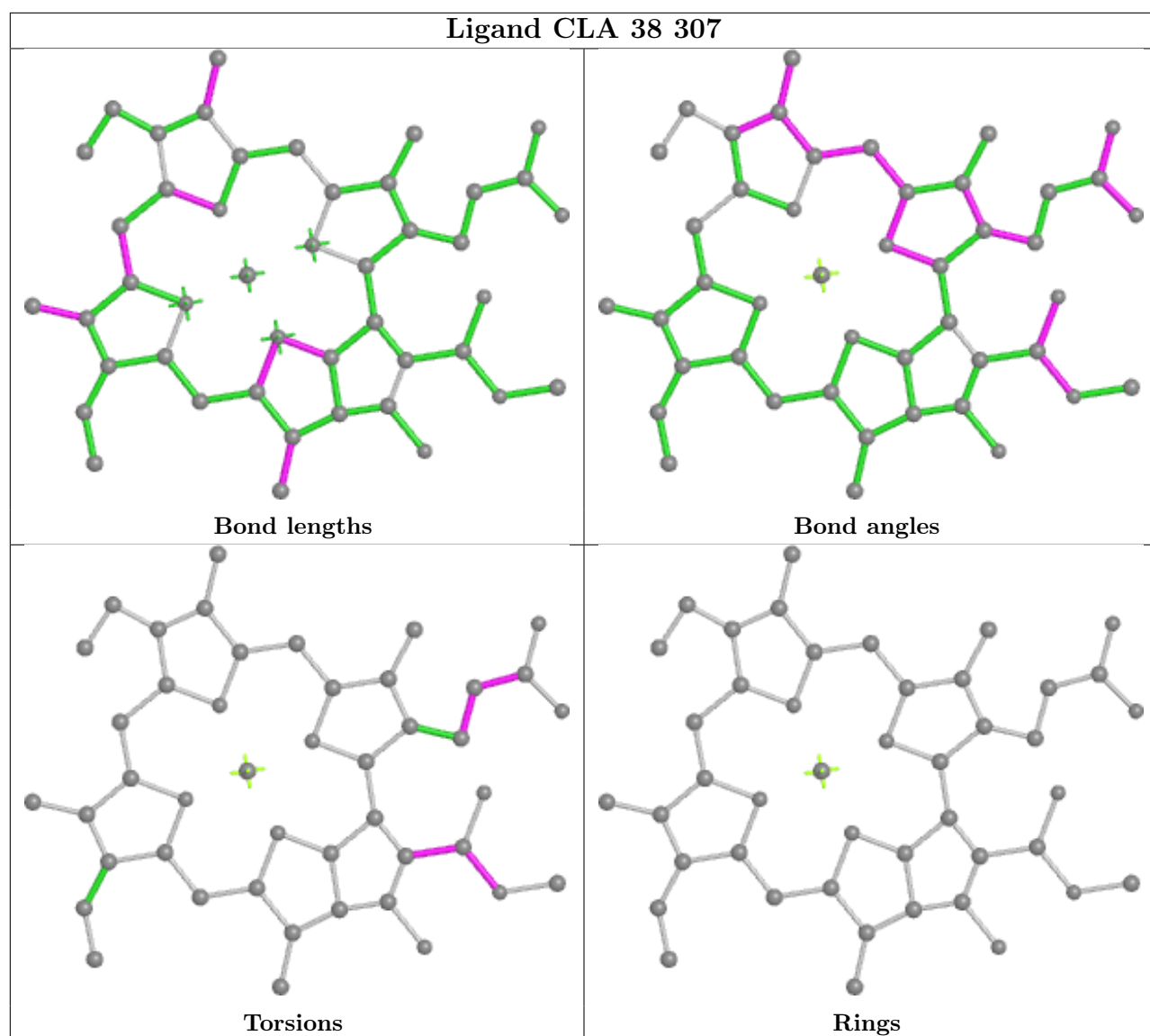


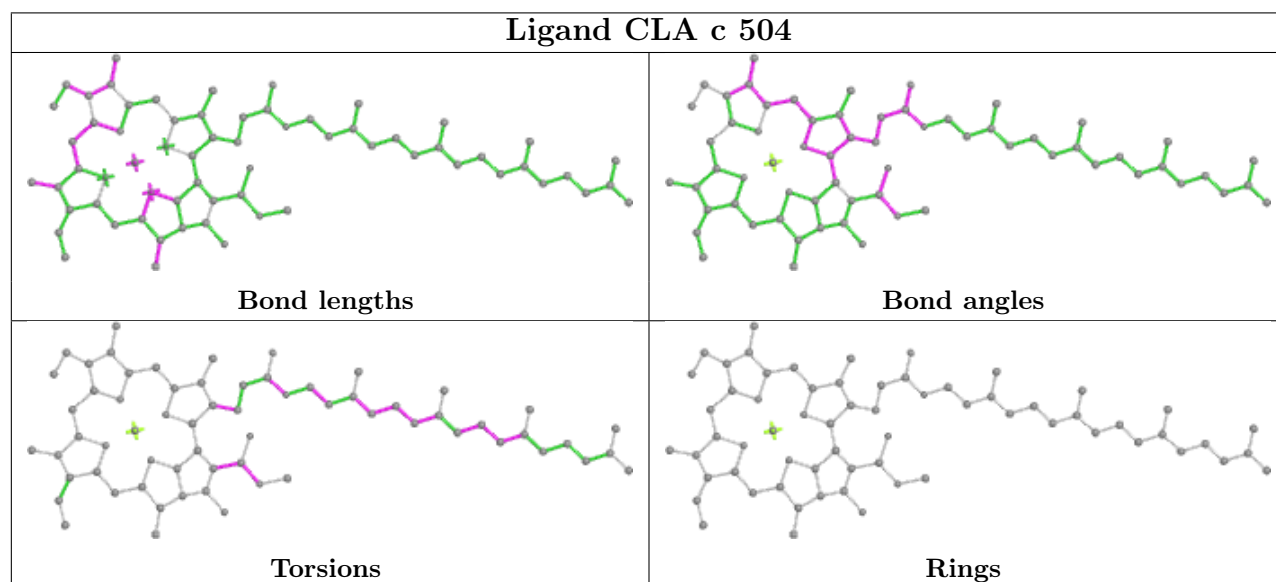
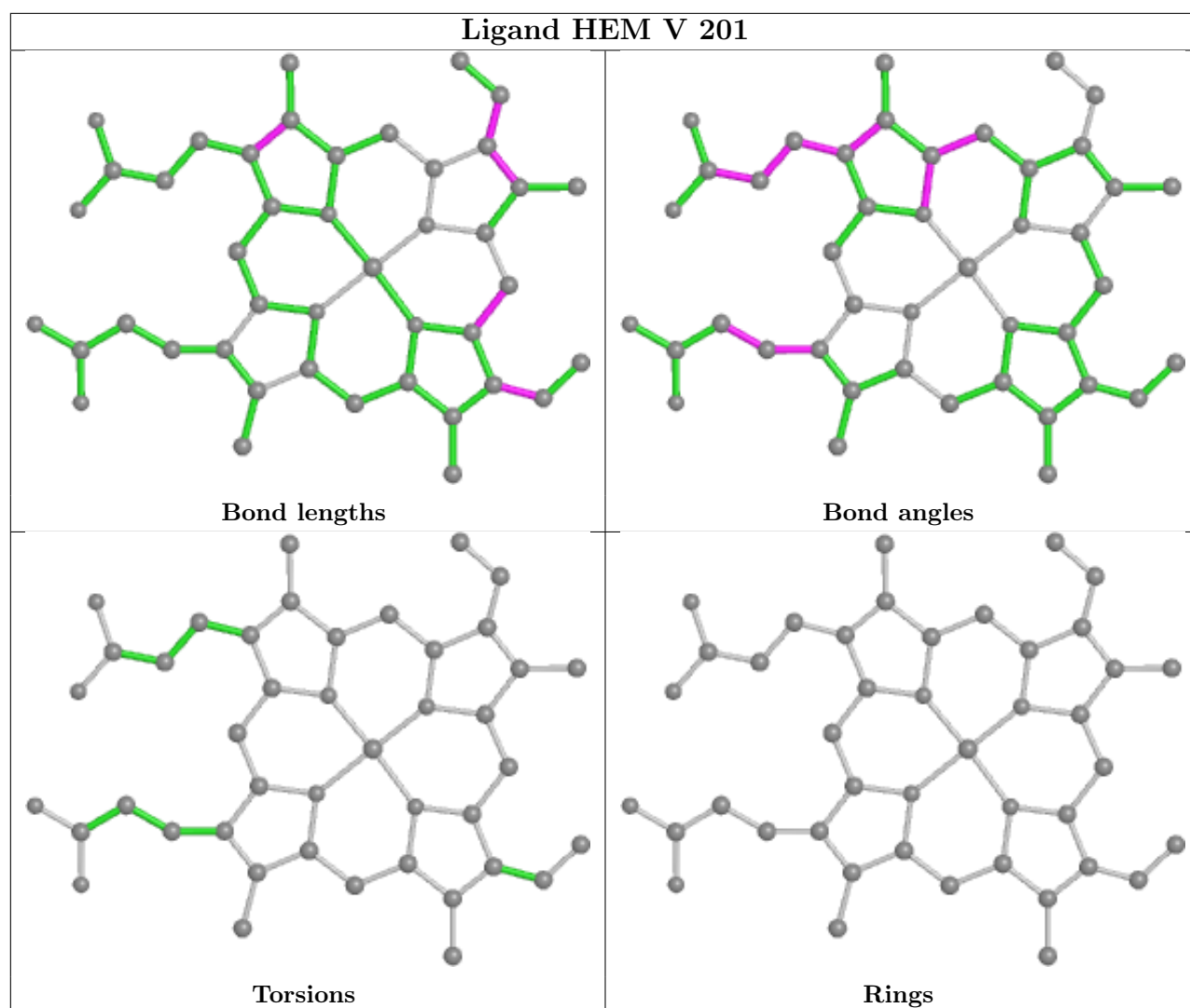
Ligand CLA b 605

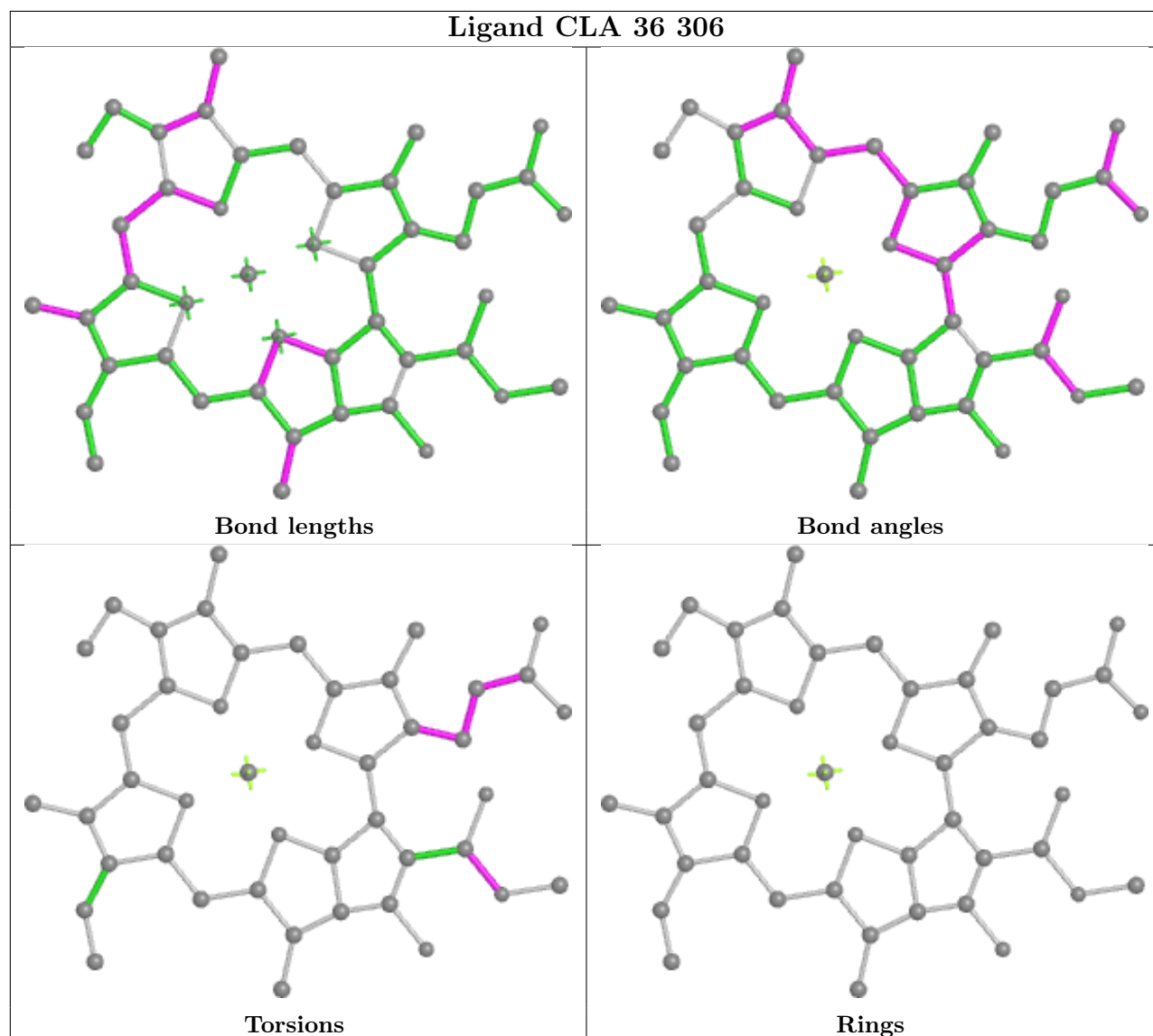
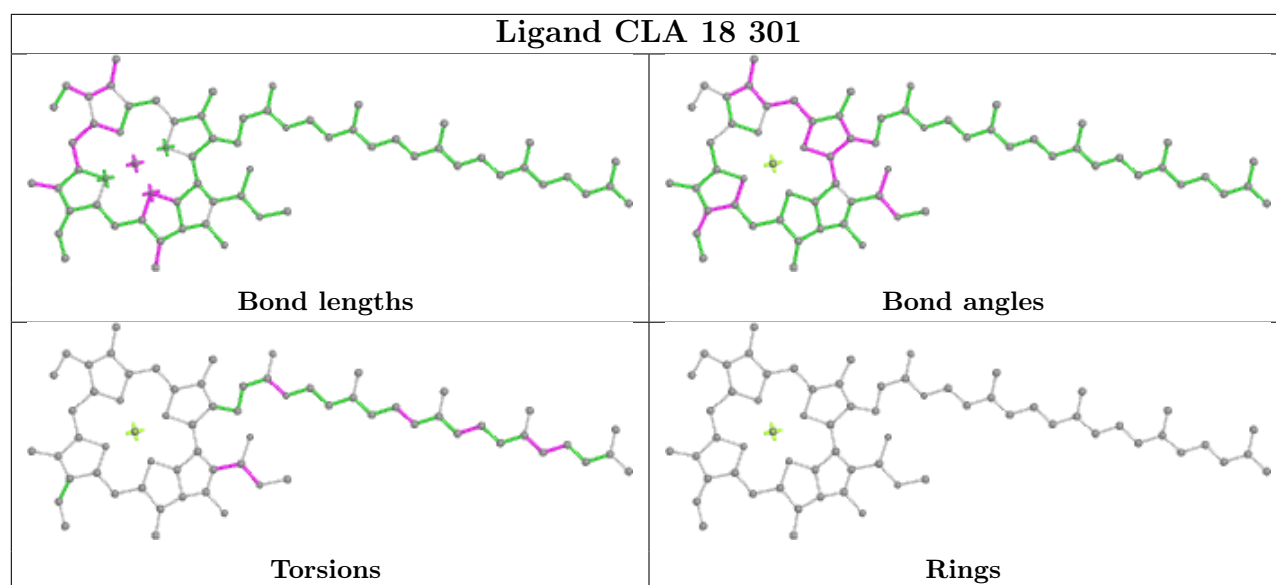


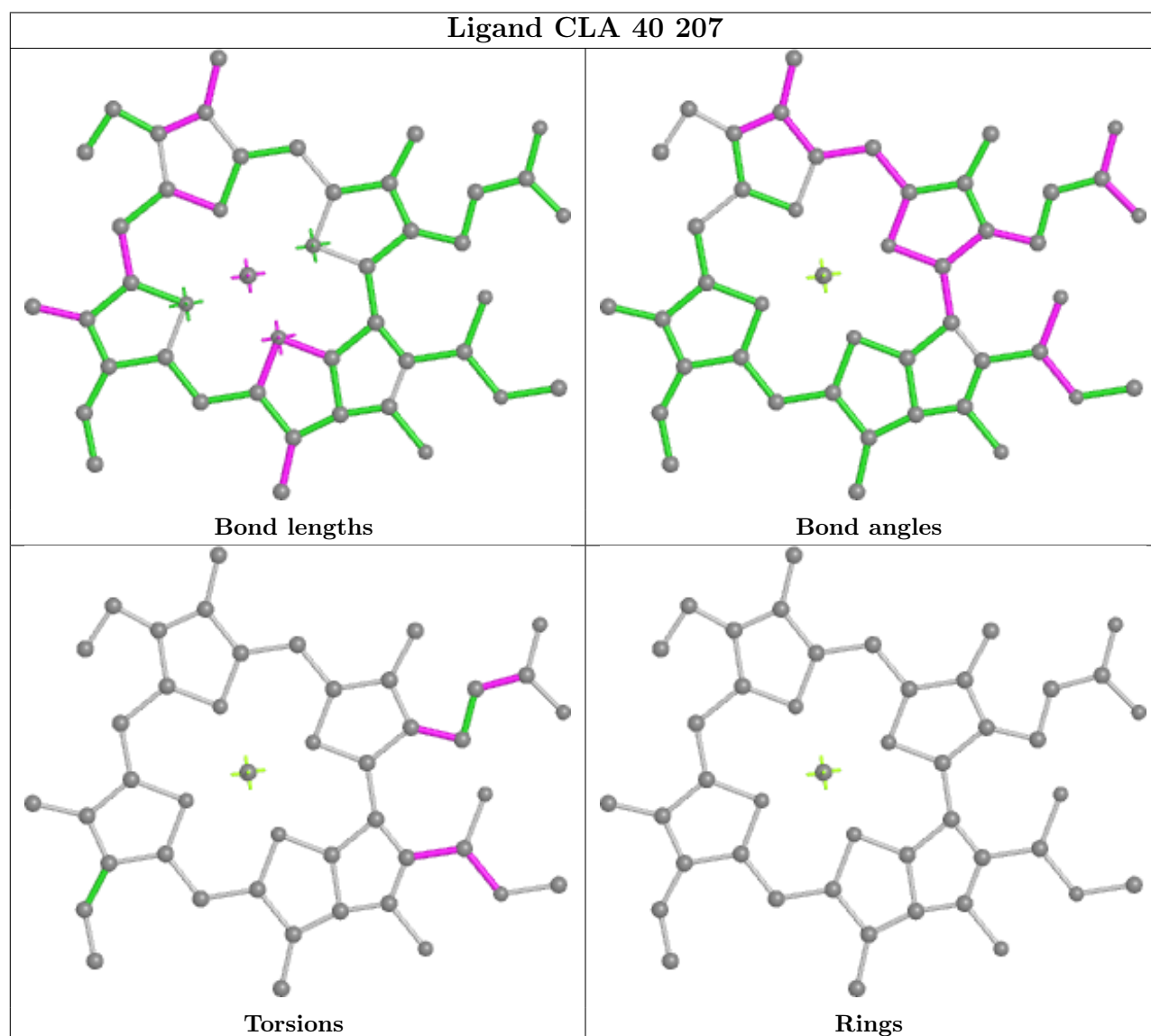
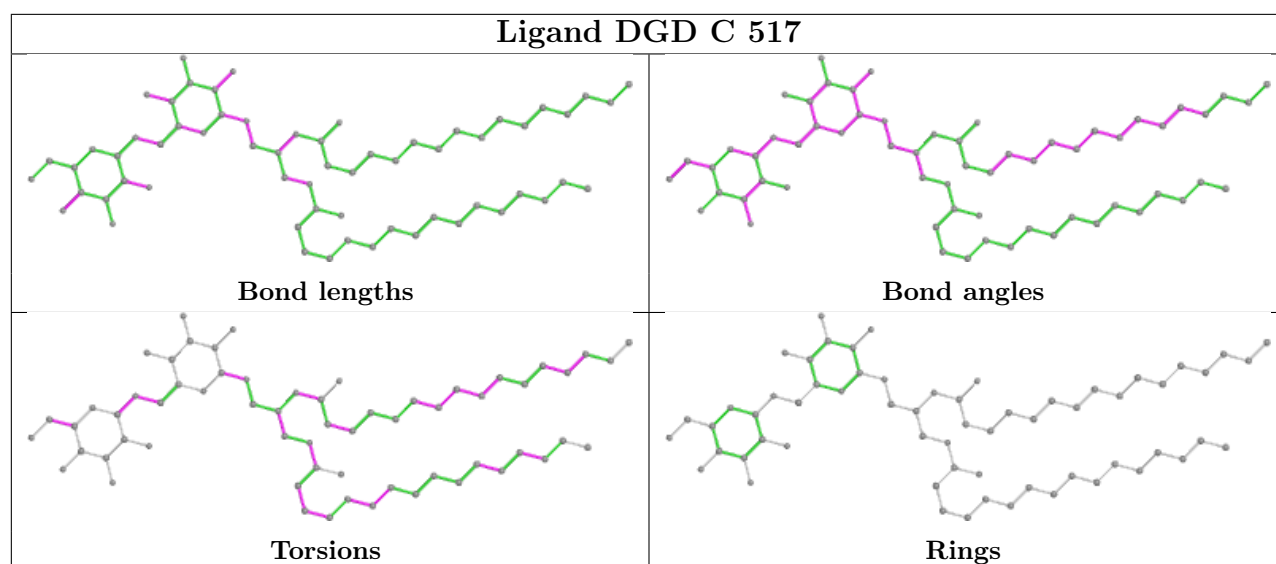


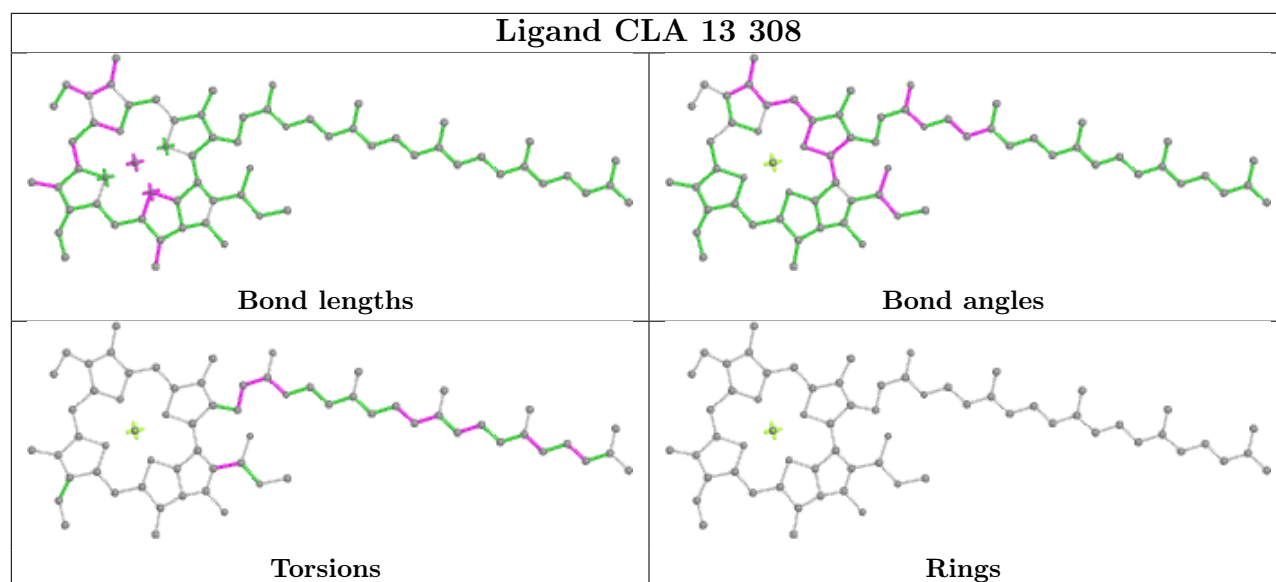
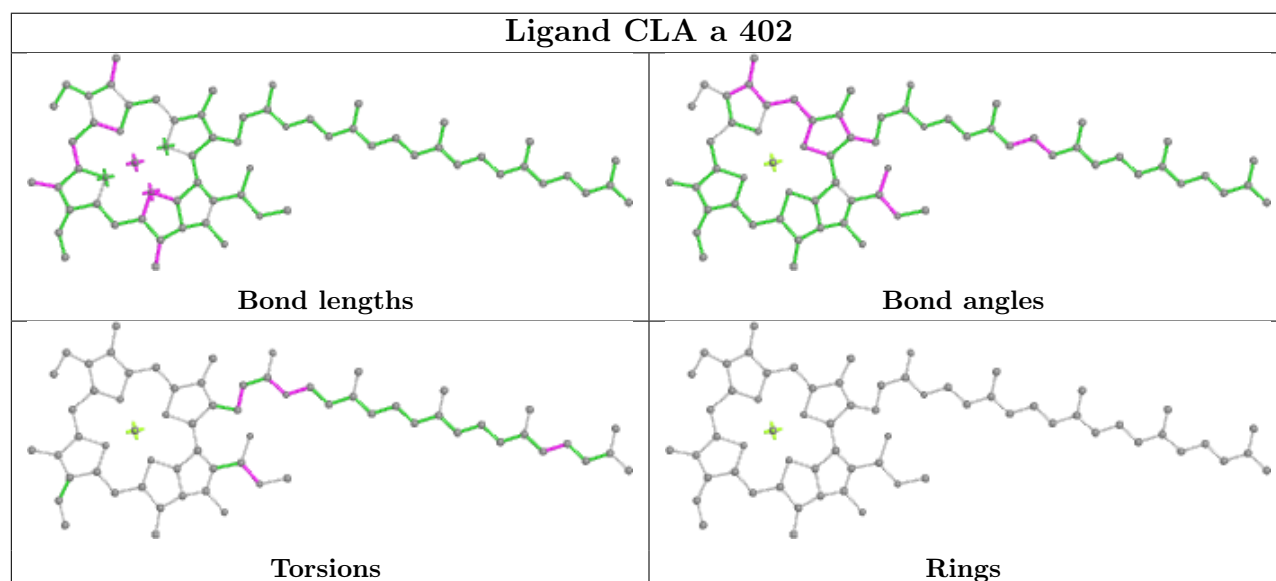
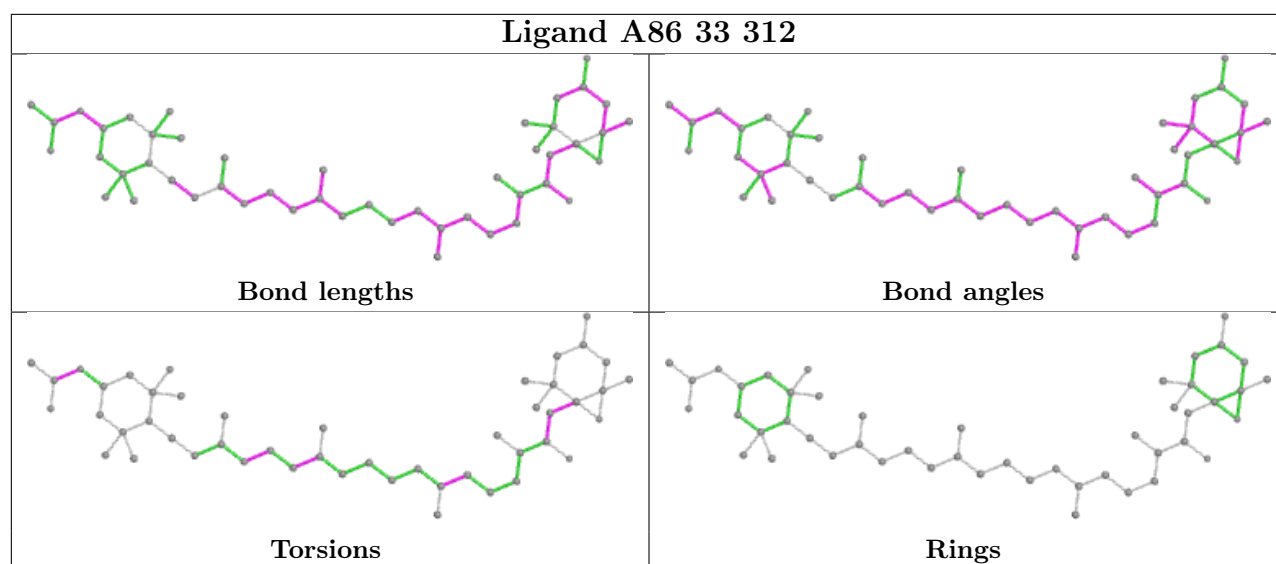


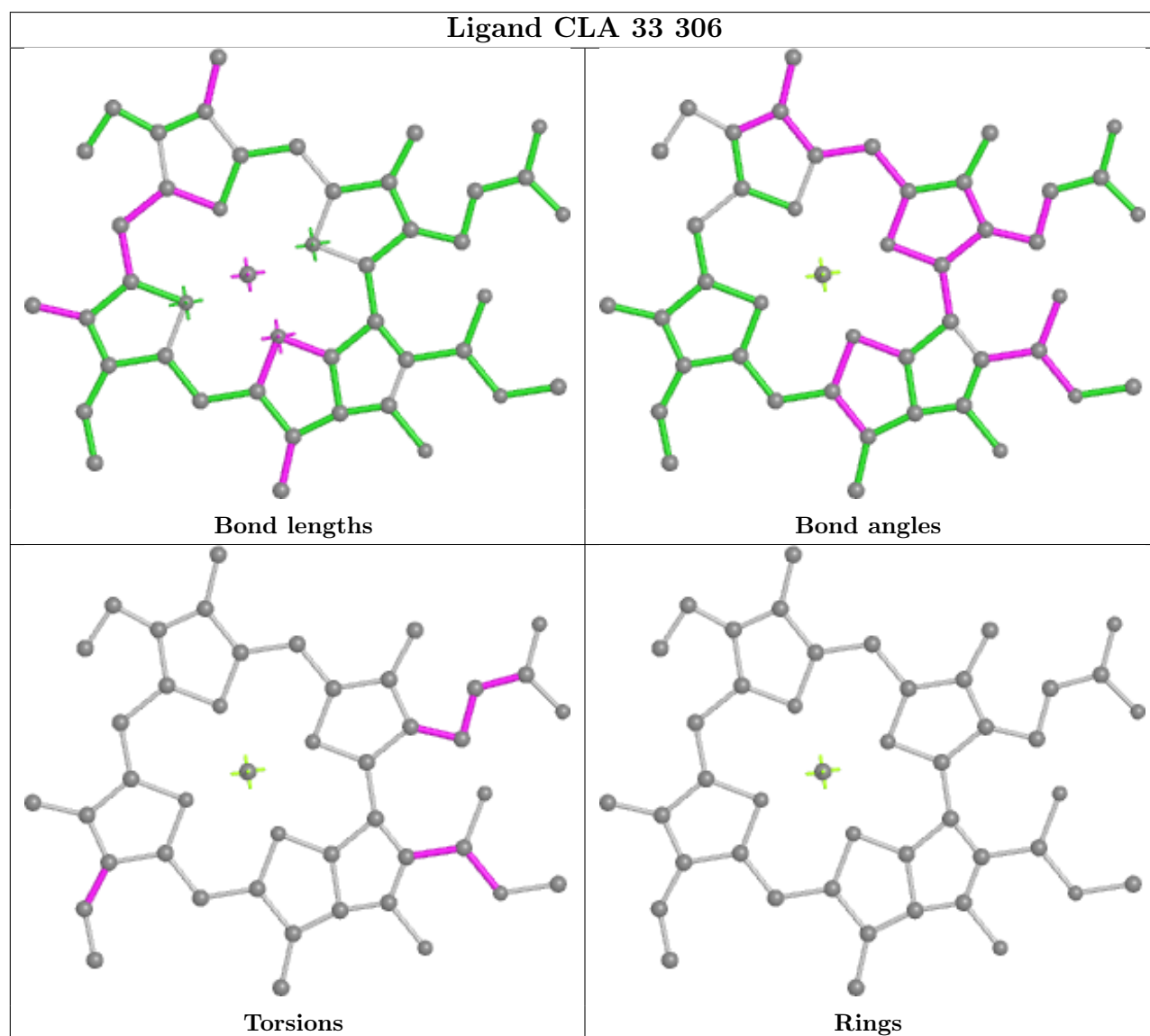
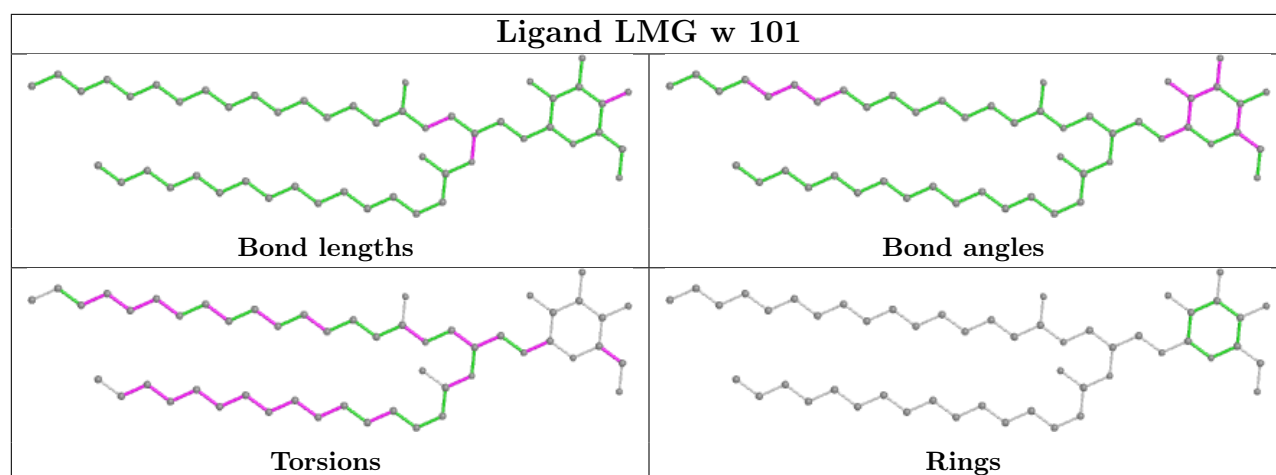


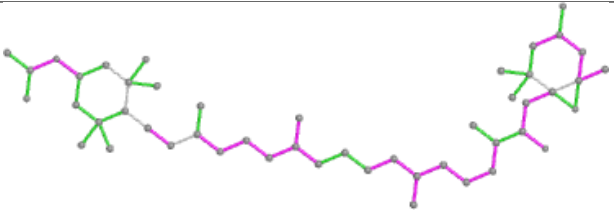
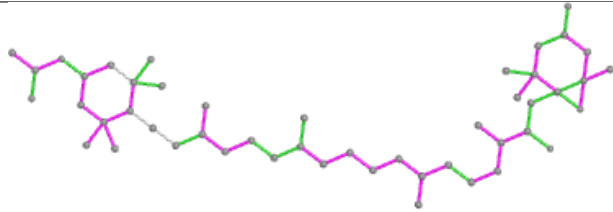
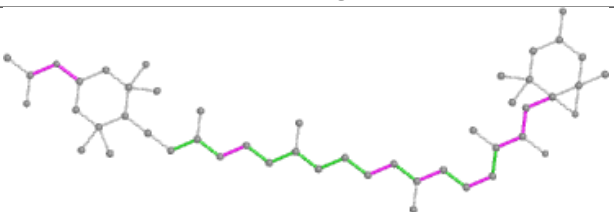
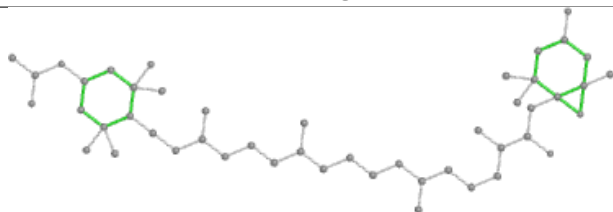


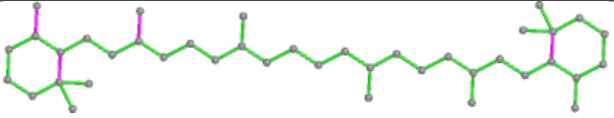
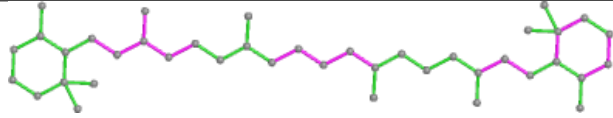
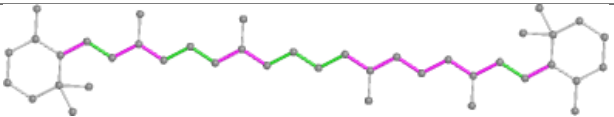
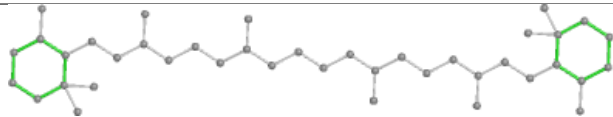


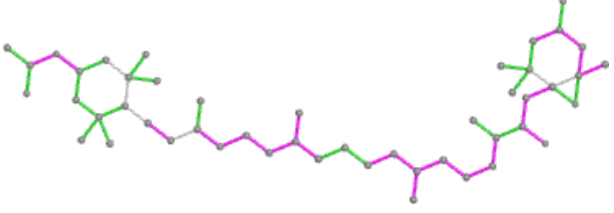
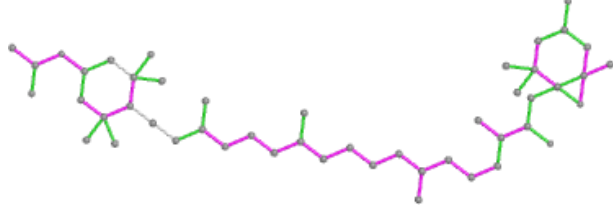
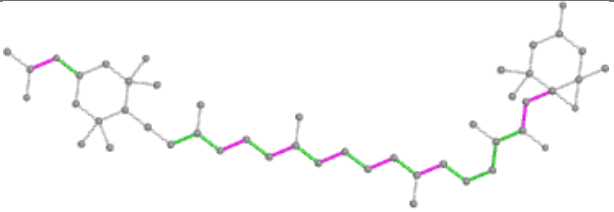
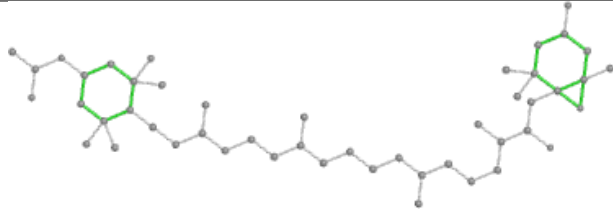


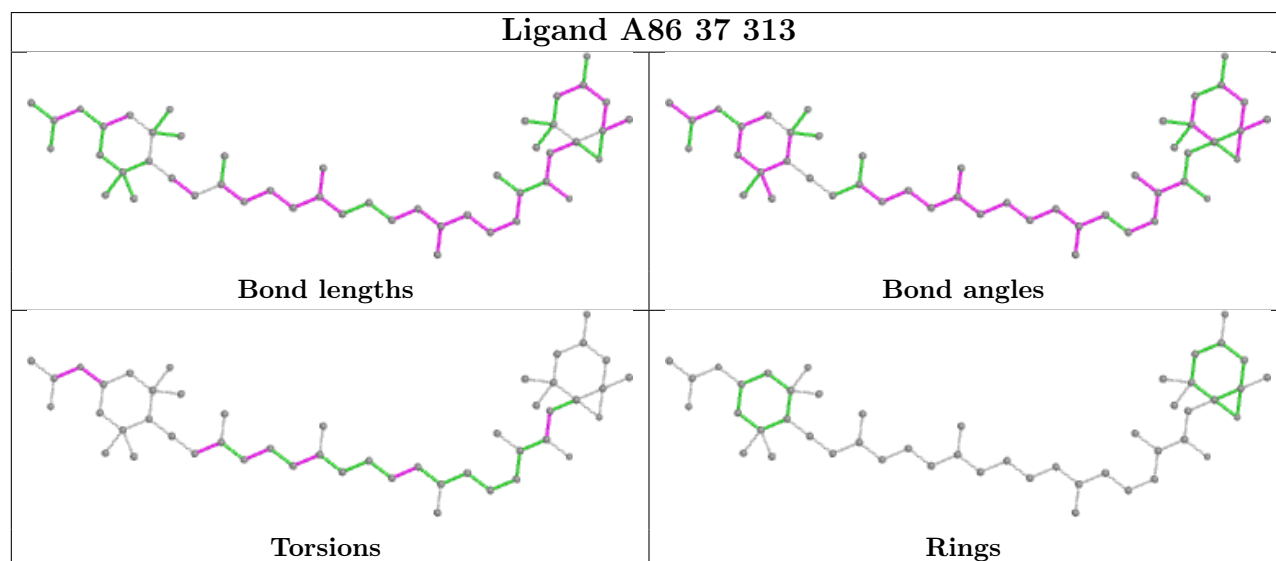
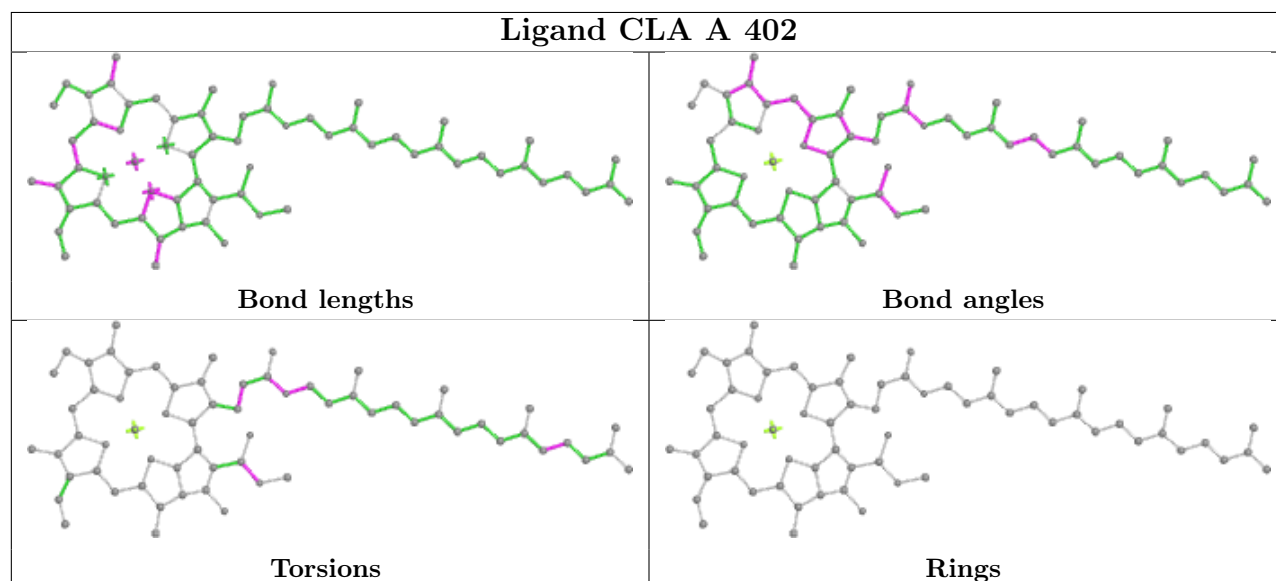
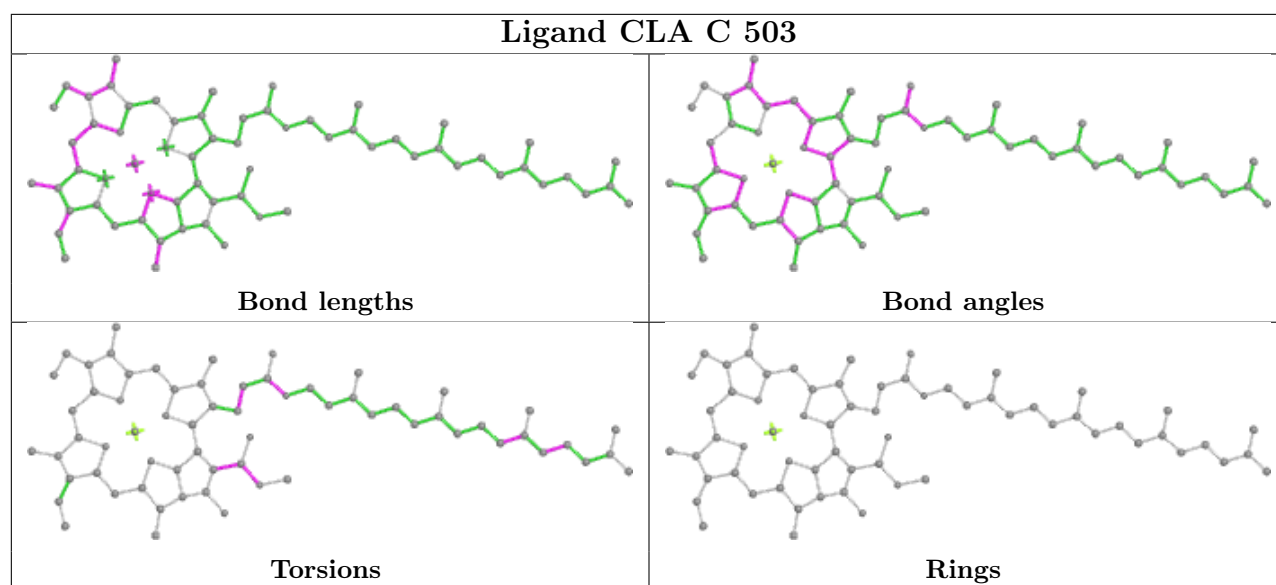


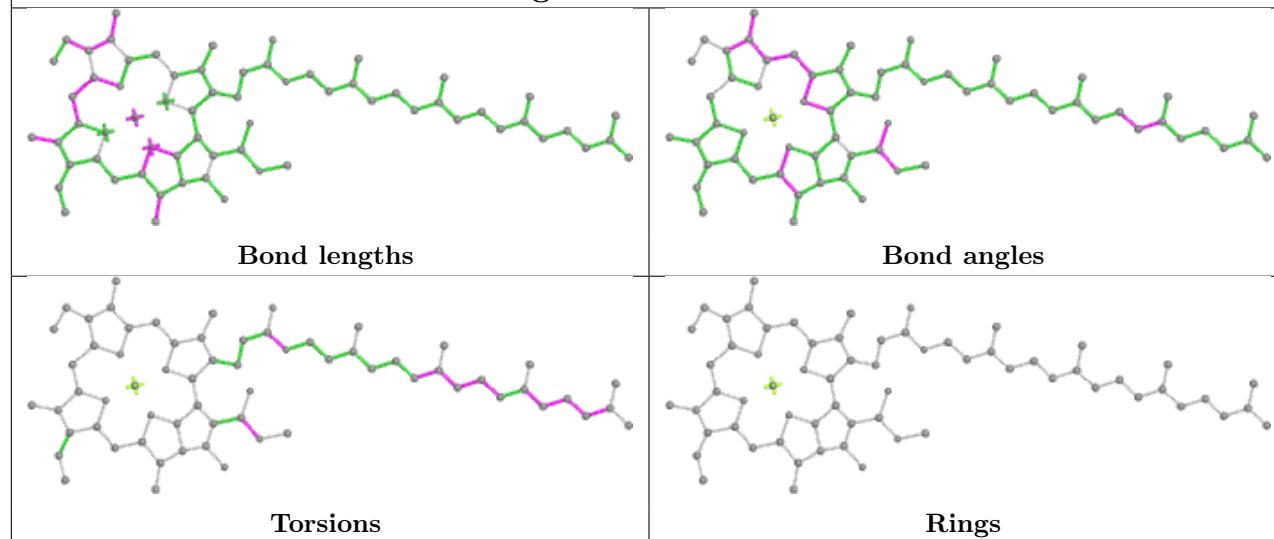
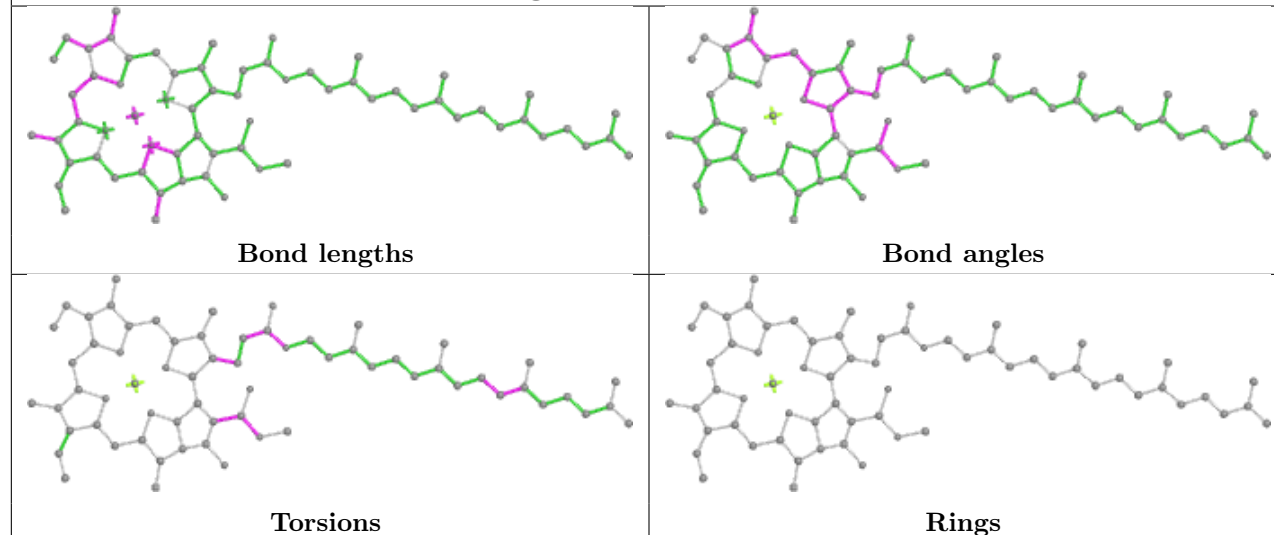
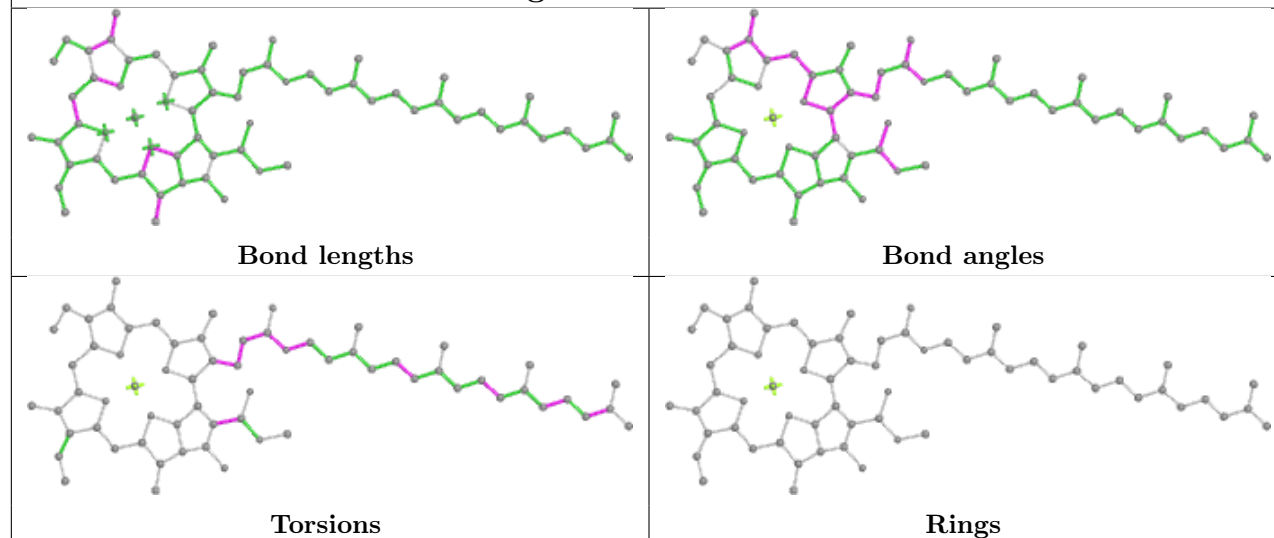


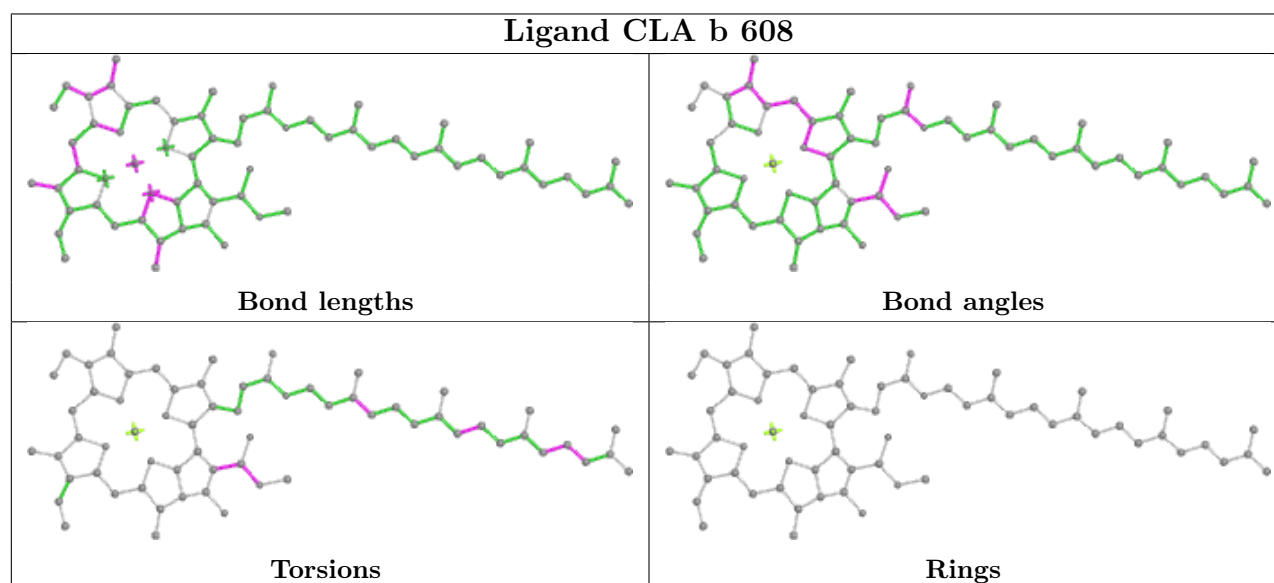
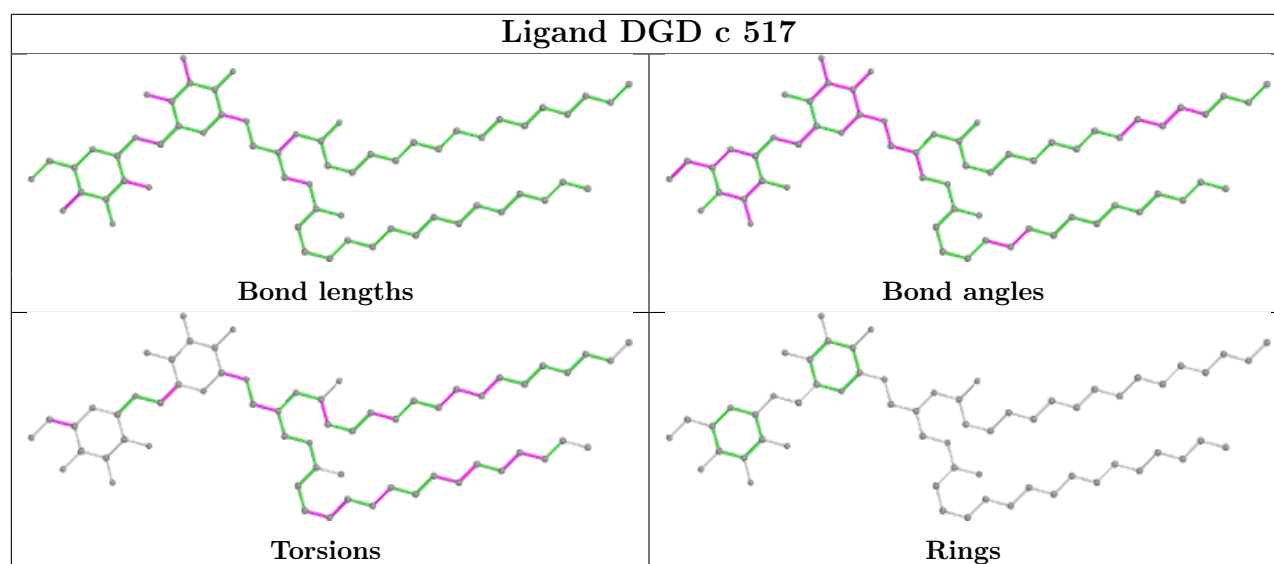
Ligand A86 32 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR Y 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

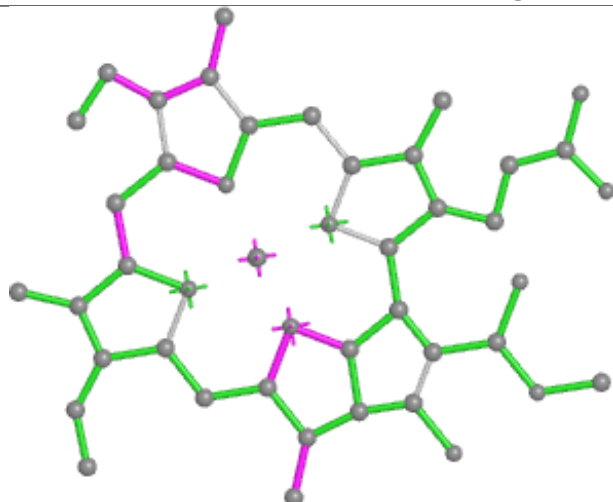
Ligand A86 19 309	
	
Bond lengths	Bond angles
	
Torsions	Rings



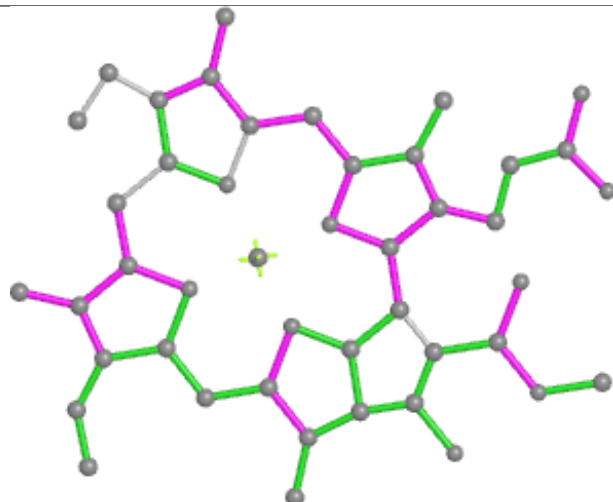
Ligand CLA C 520**Ligand CLA 31 303****Ligand CLA 21 306**



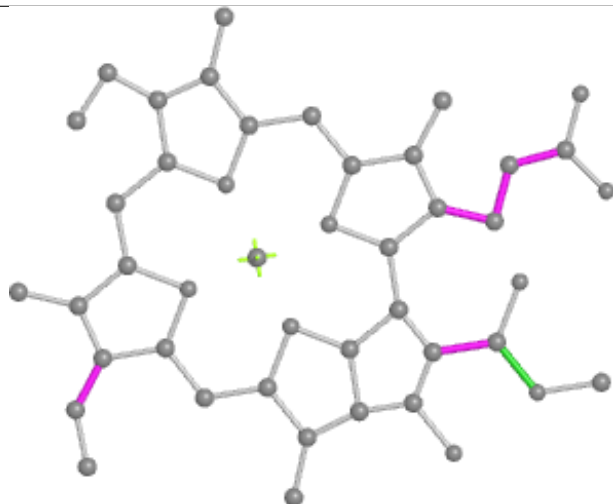
Ligand CLA 37 307



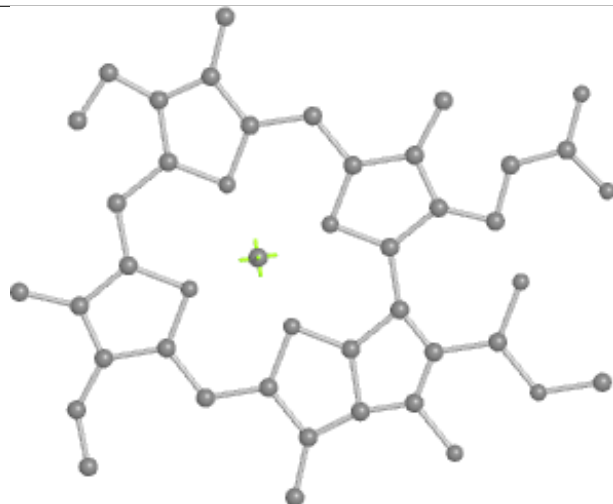
Bond lengths



Bond angles

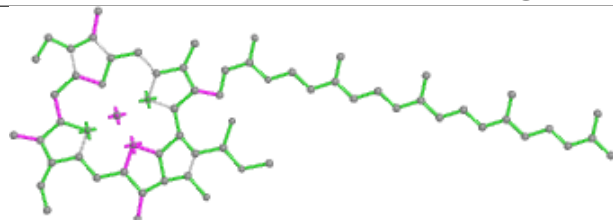


Torsions

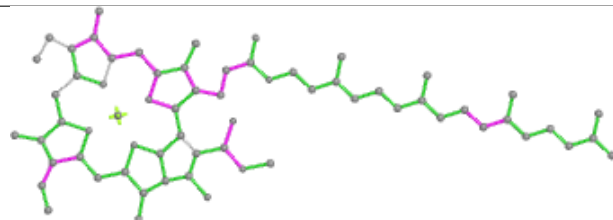


Rings

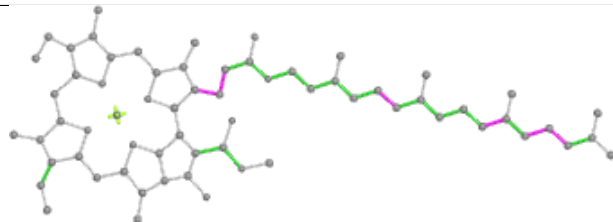
Ligand CLA d 406



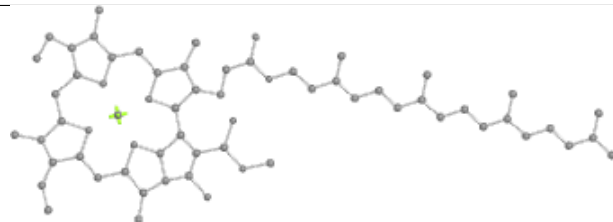
Bond lengths



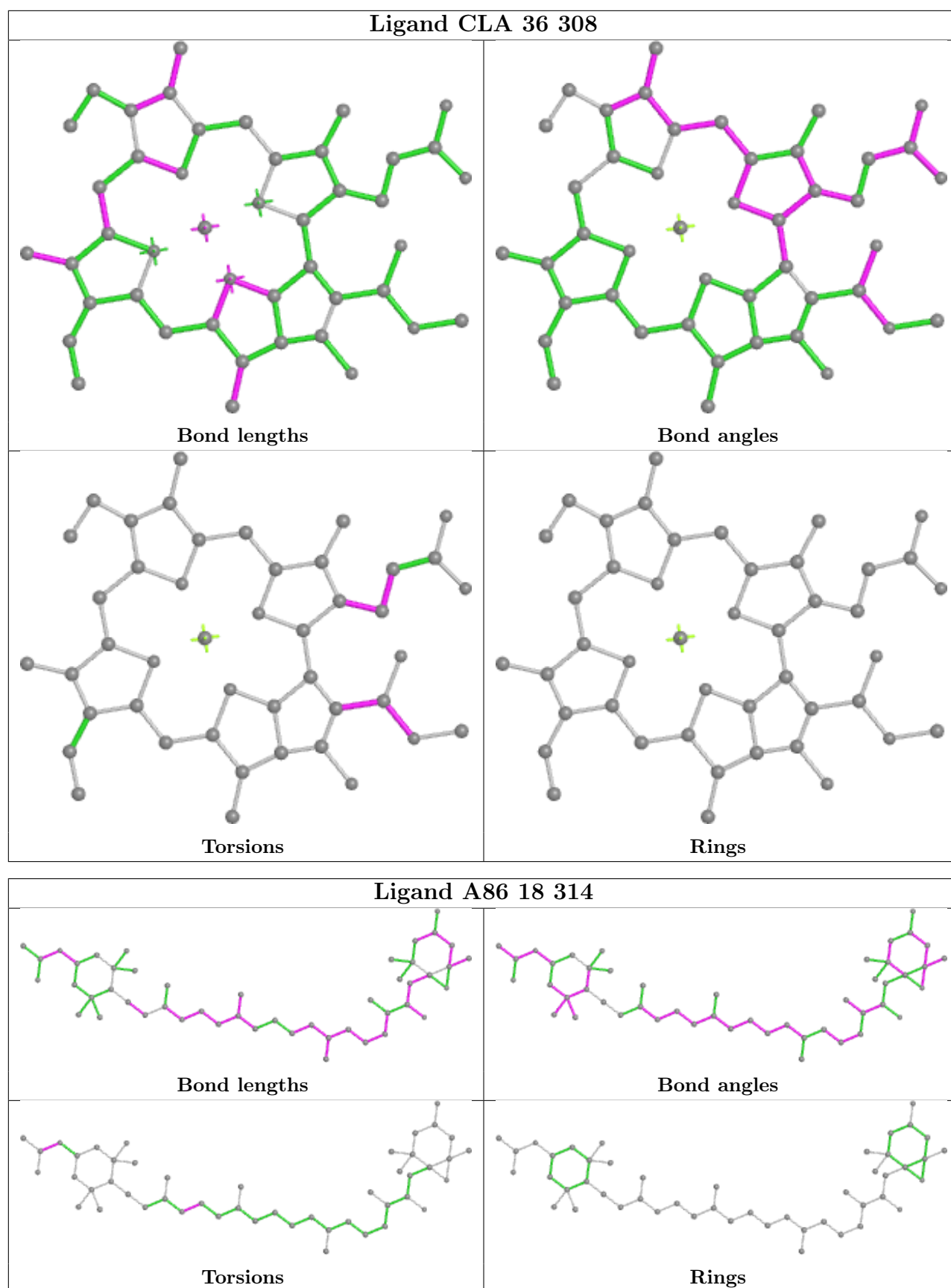
Bond angles

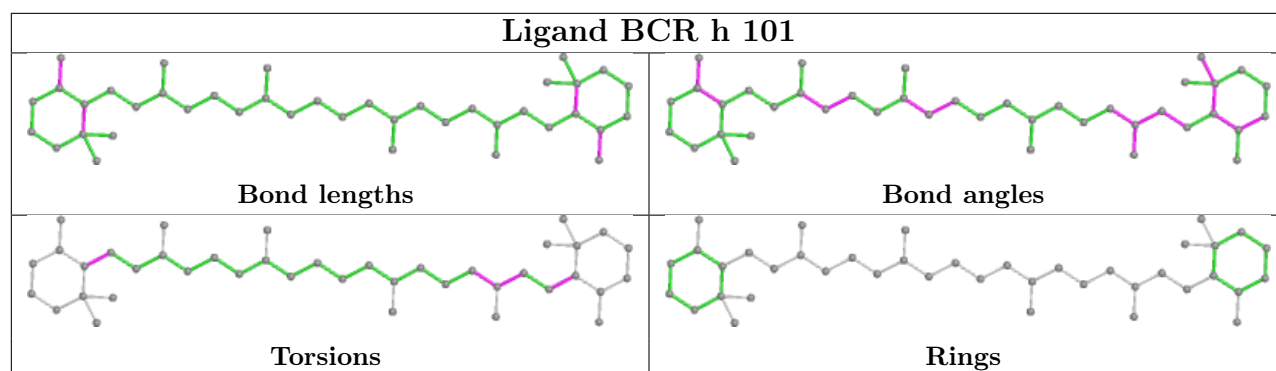
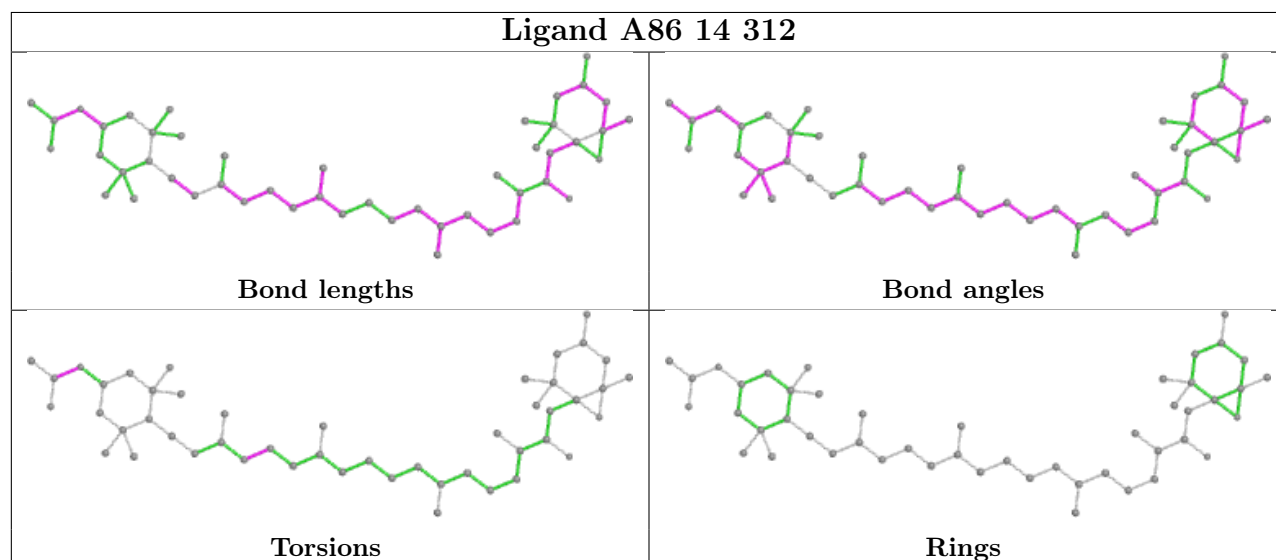
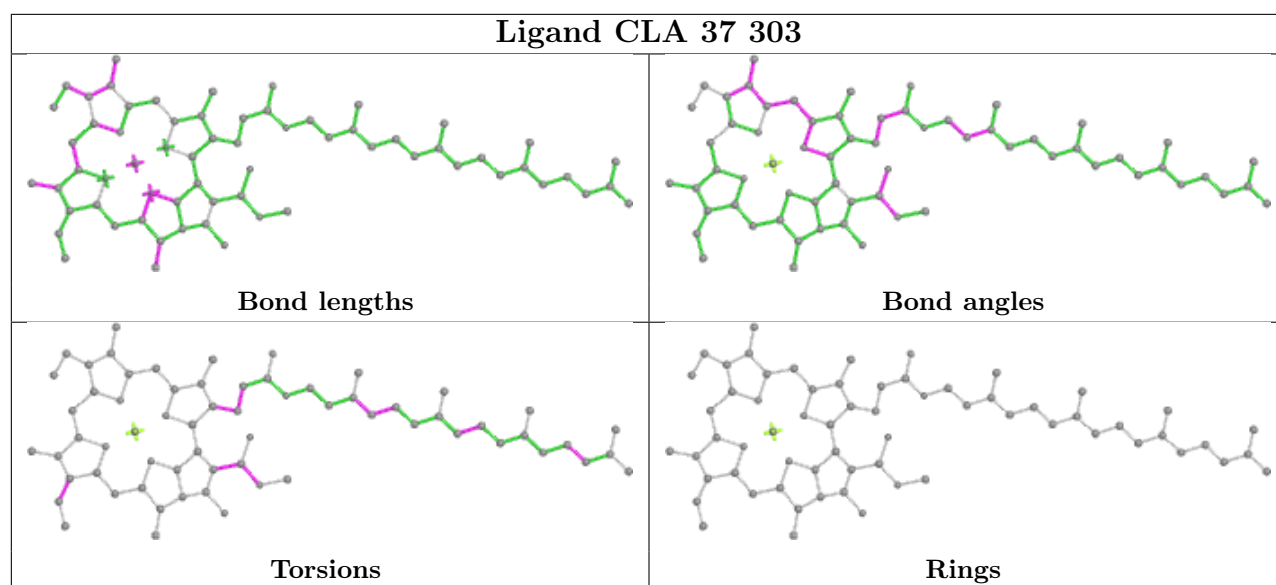


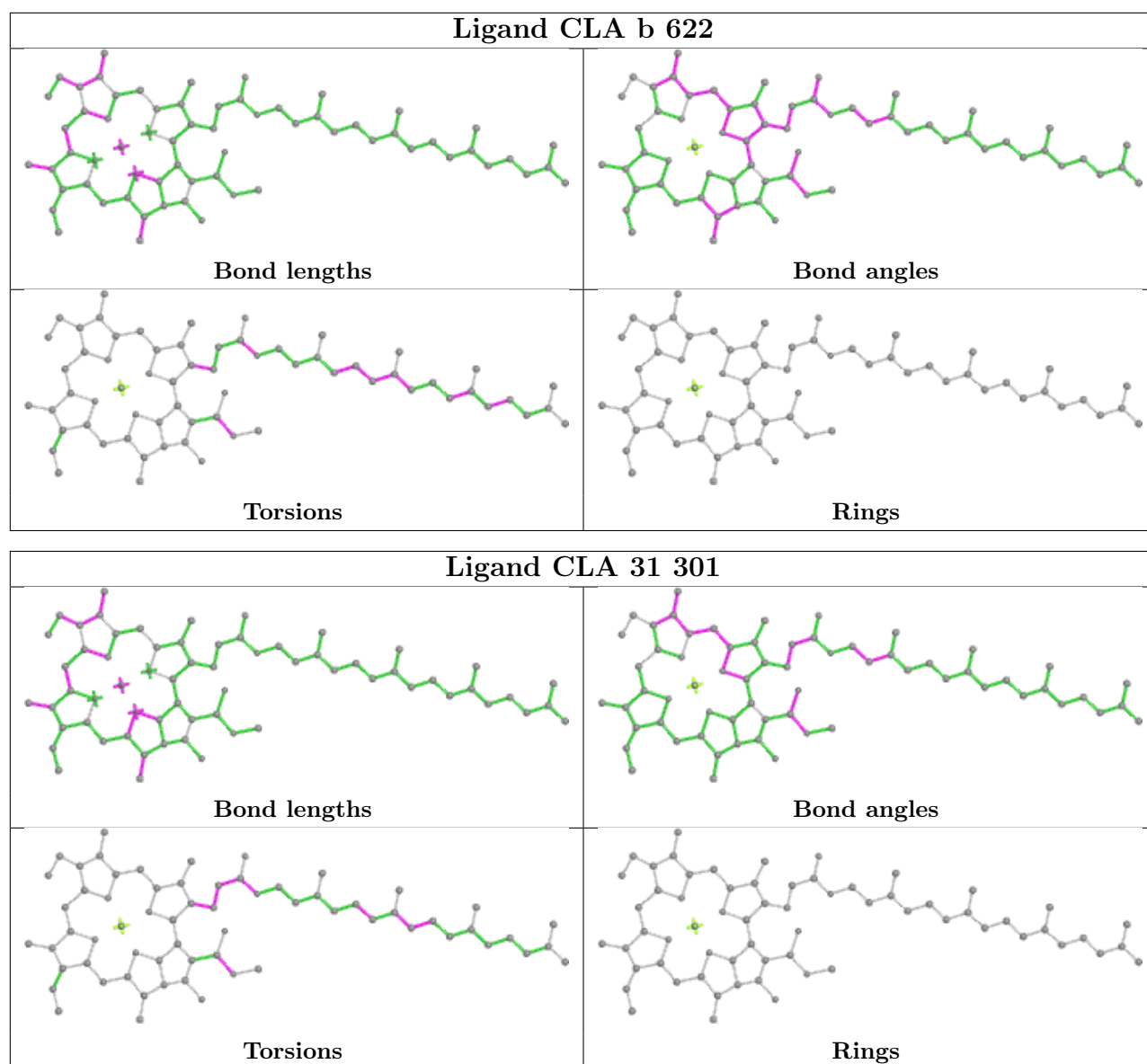
Torsions

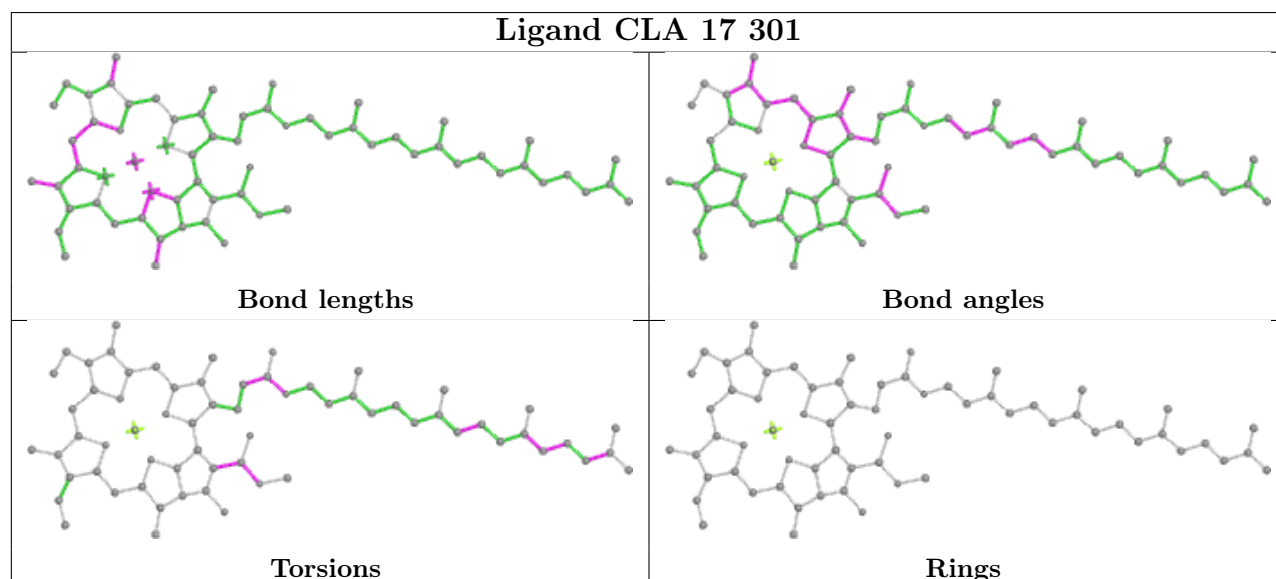
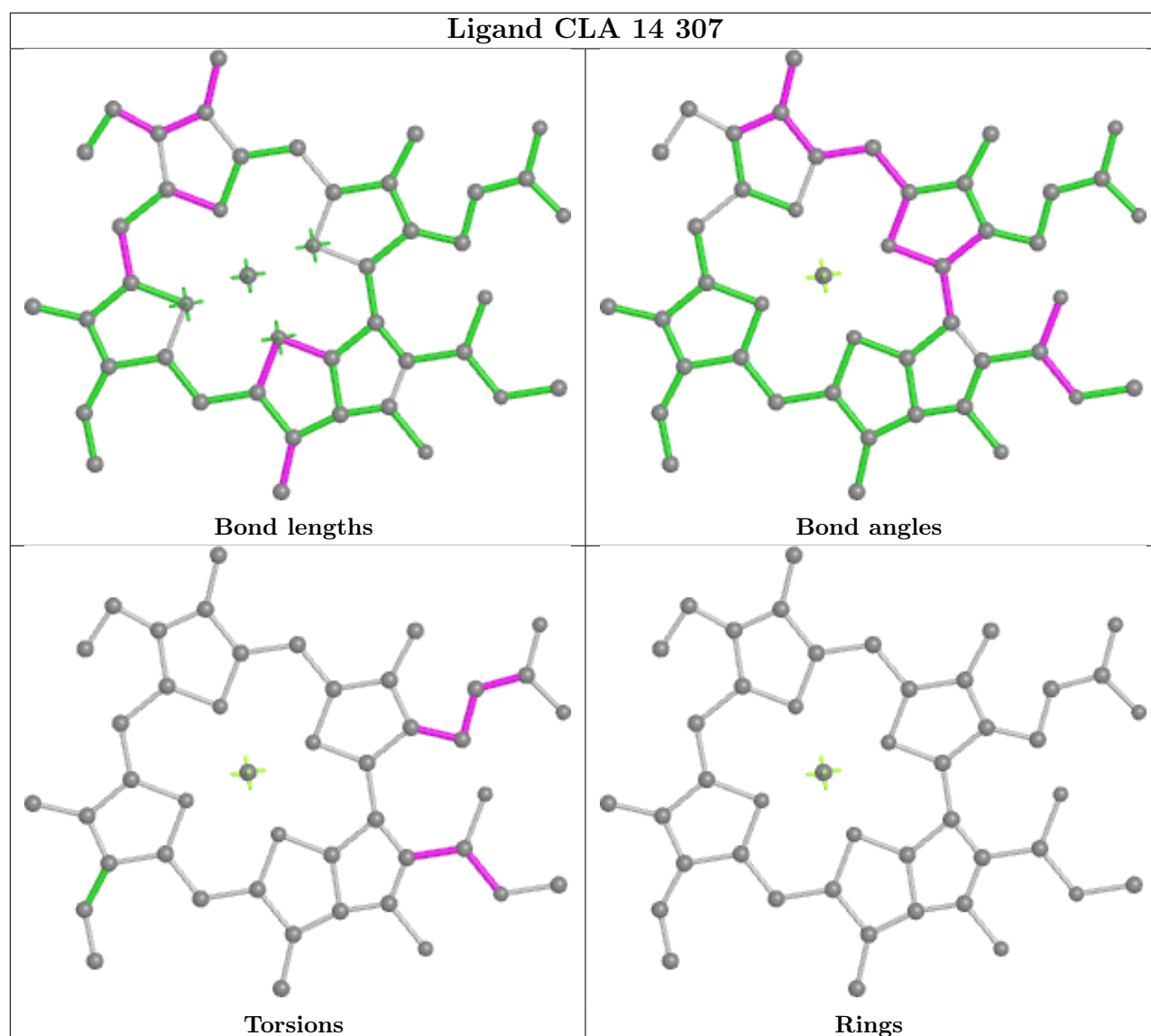


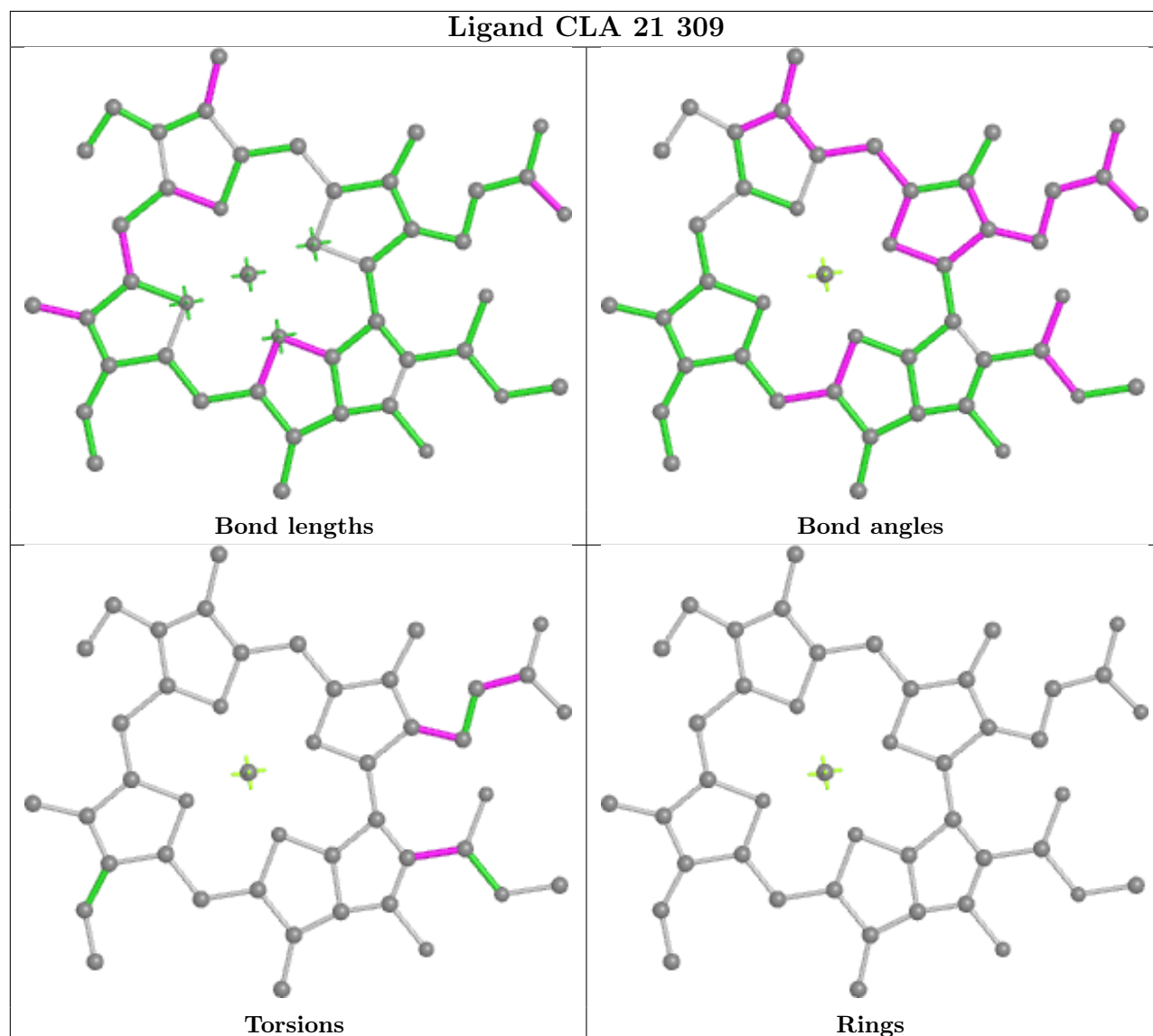
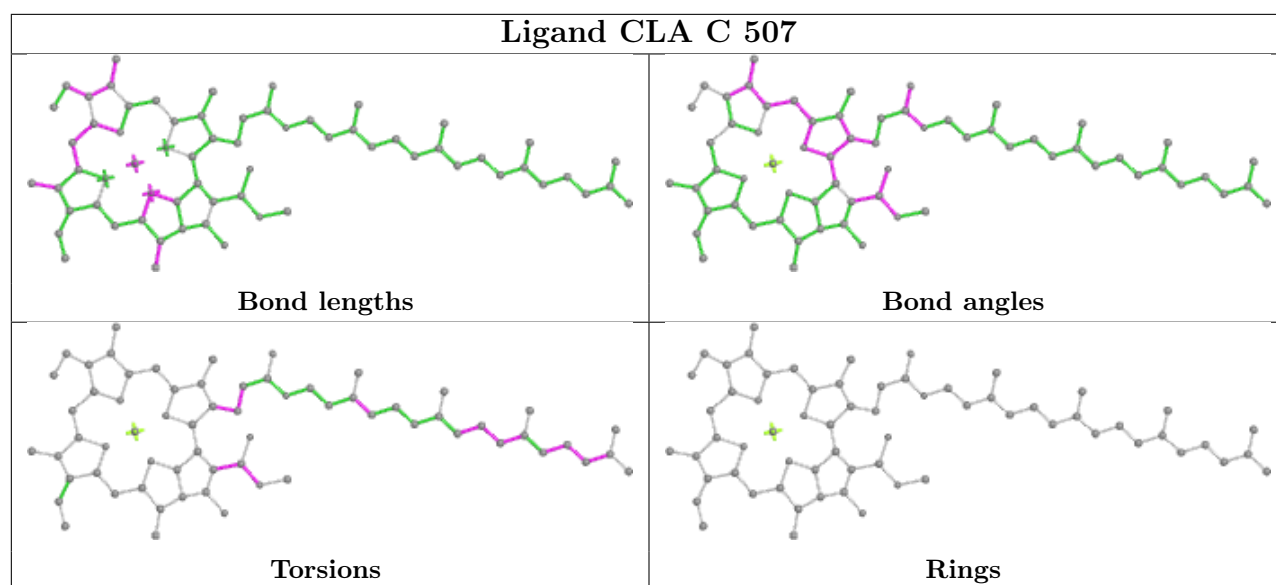
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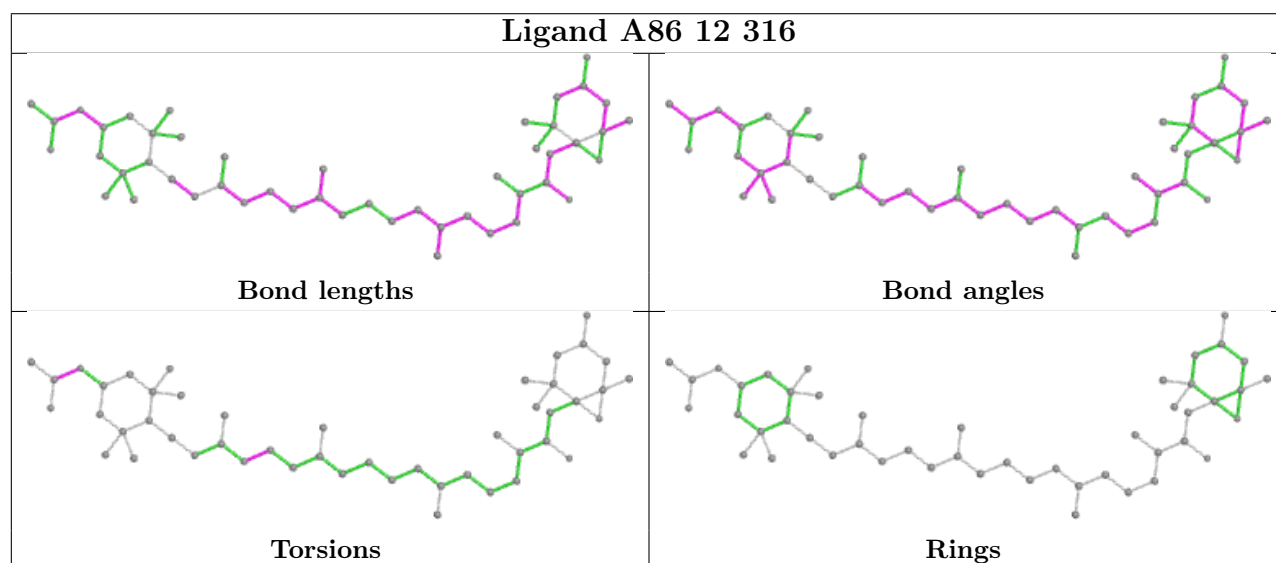
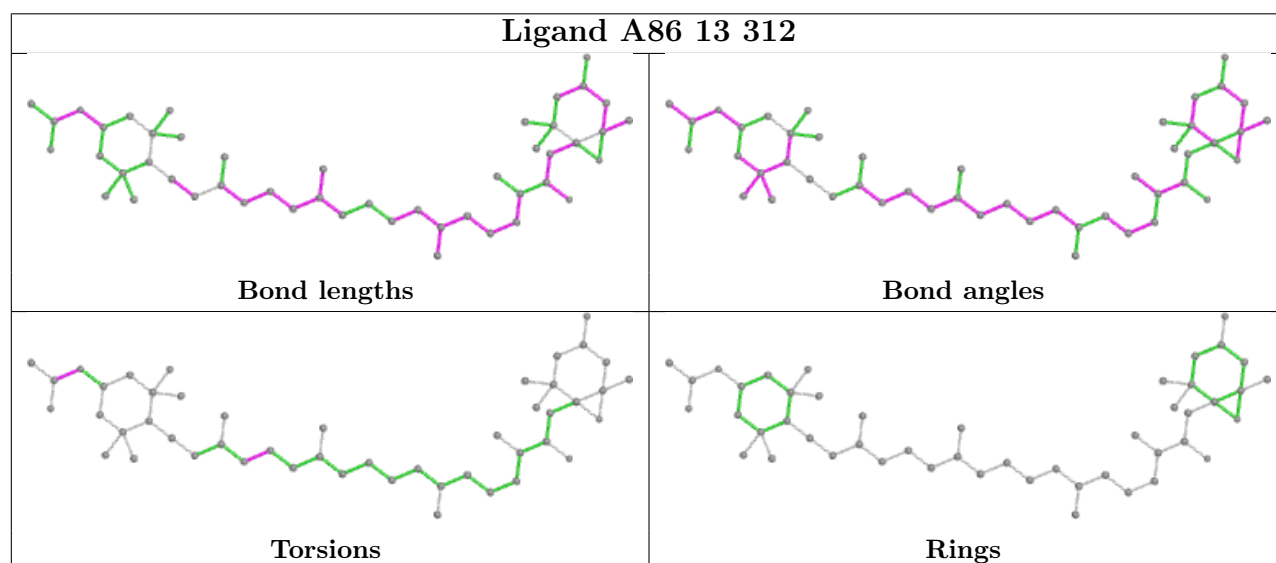
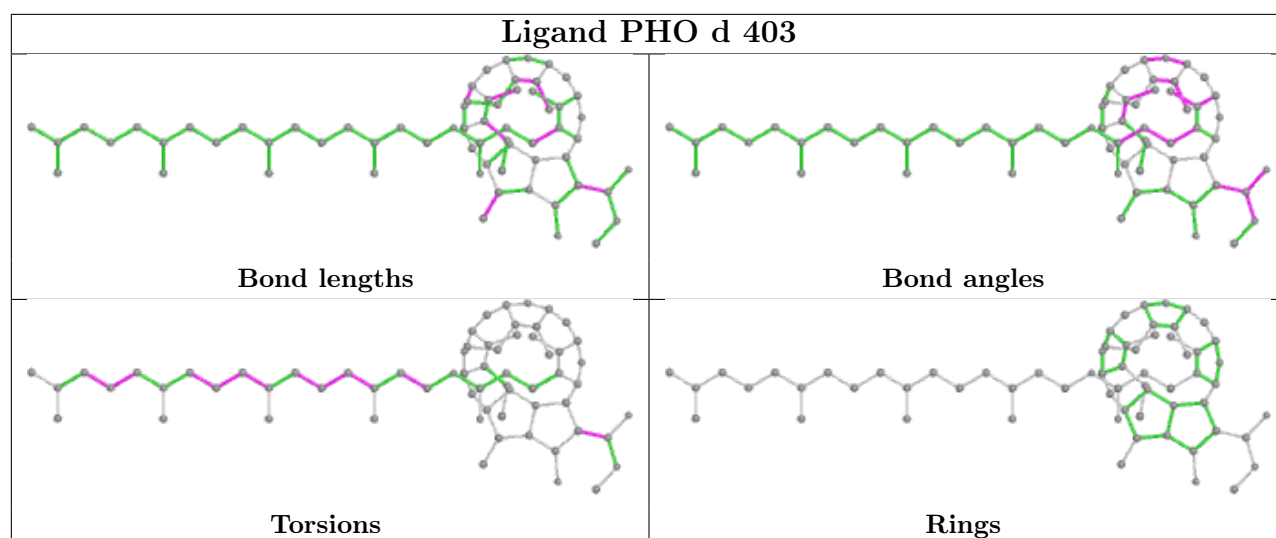


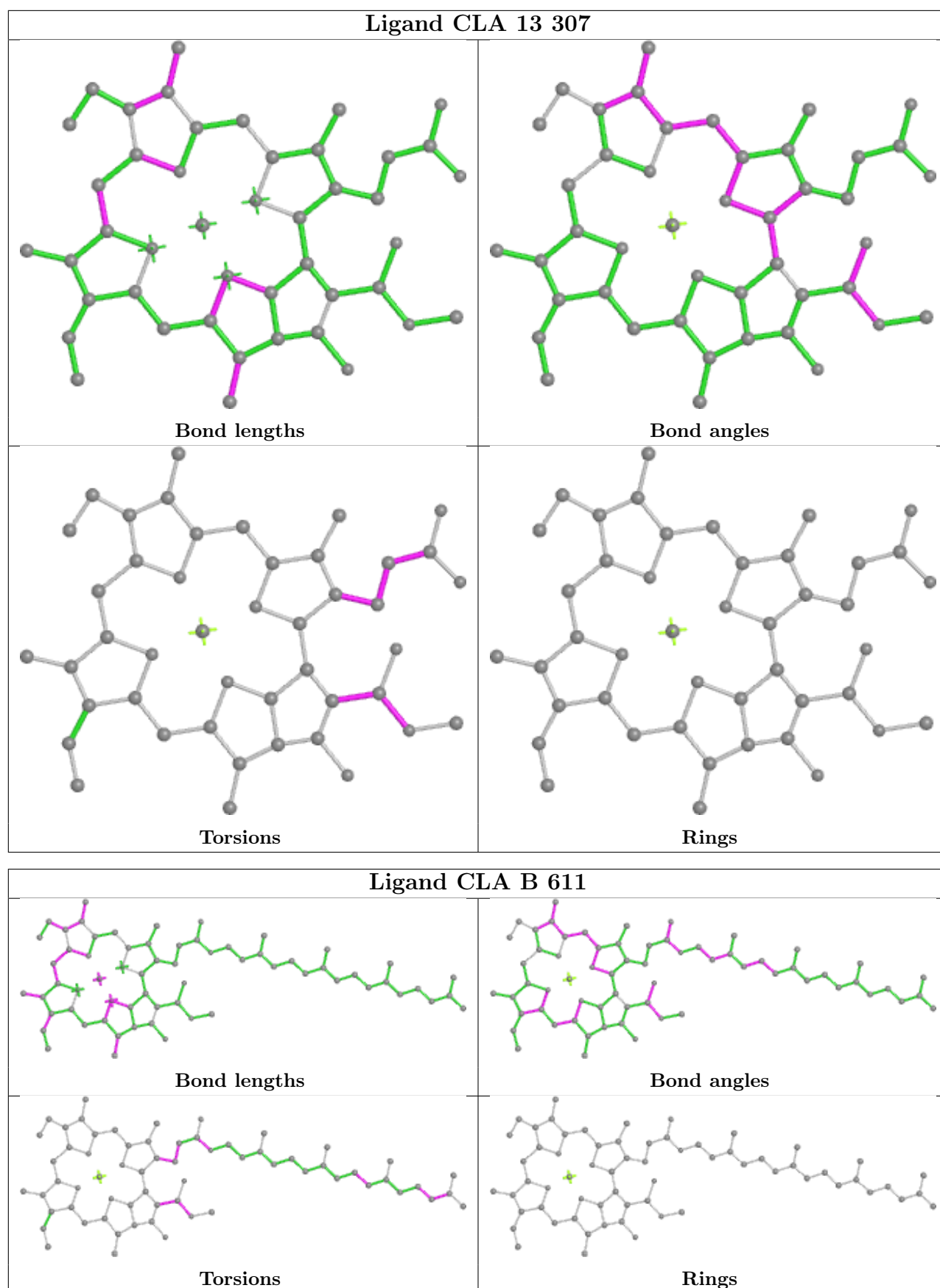


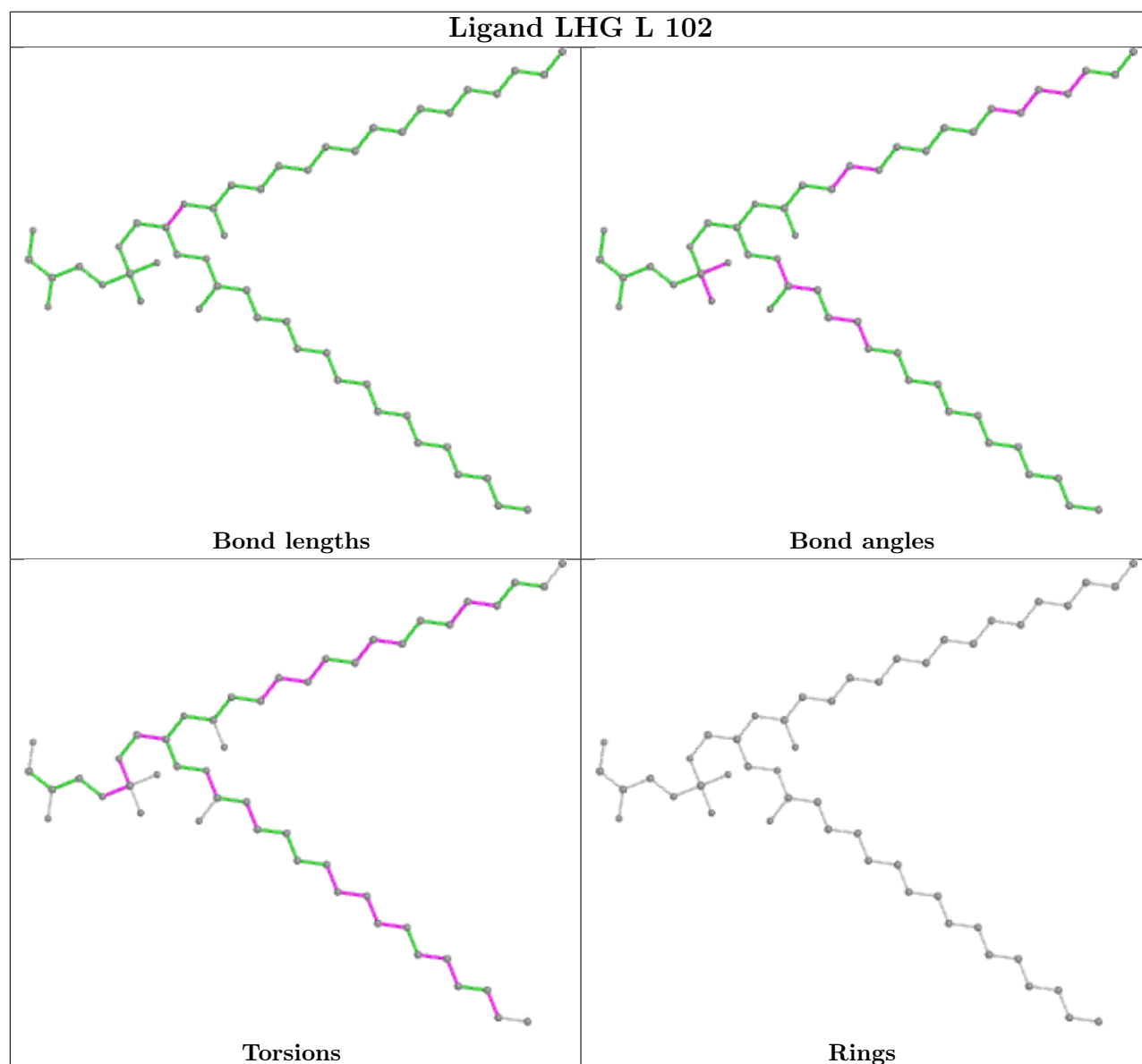
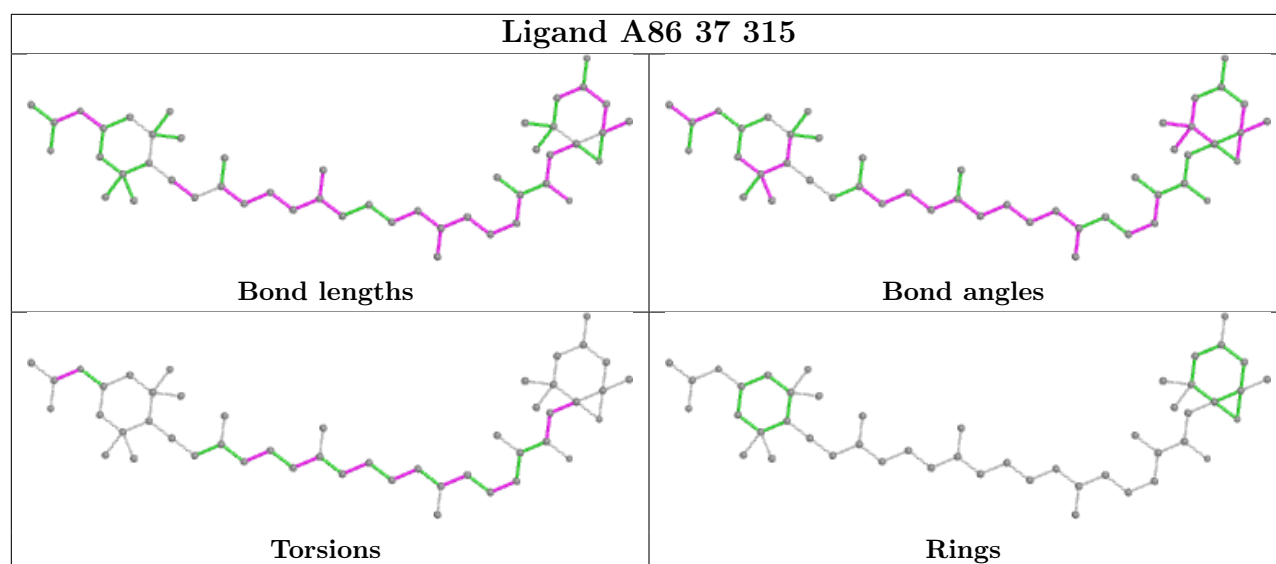


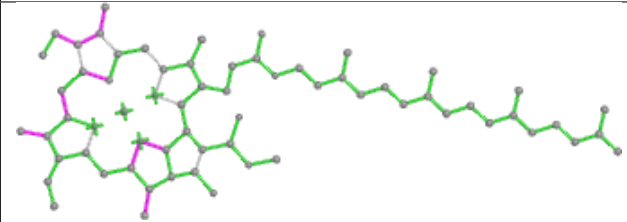
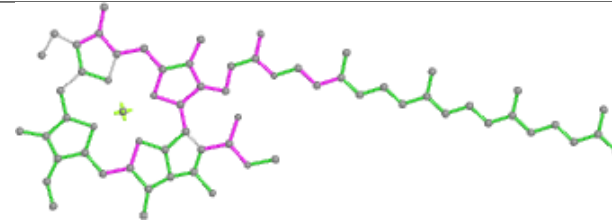
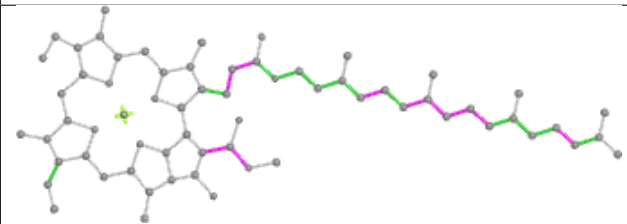
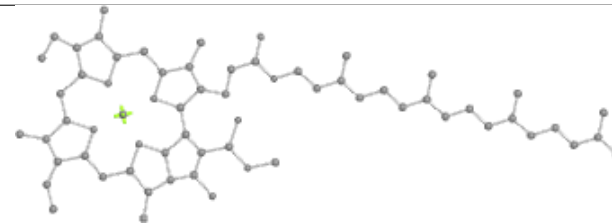


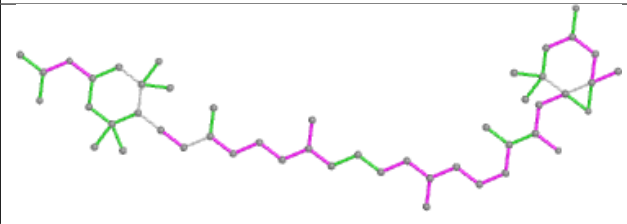
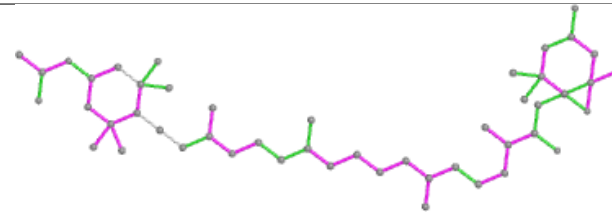
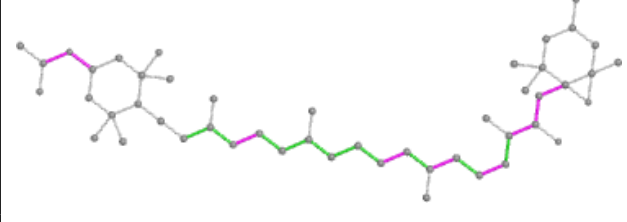
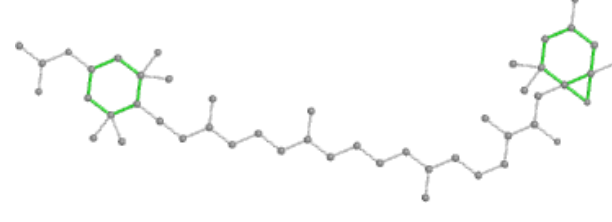


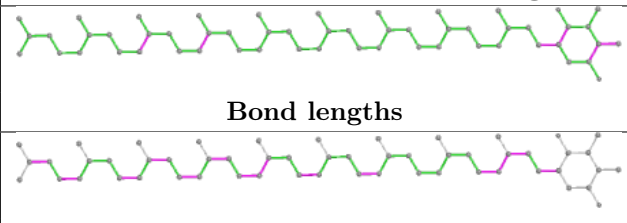
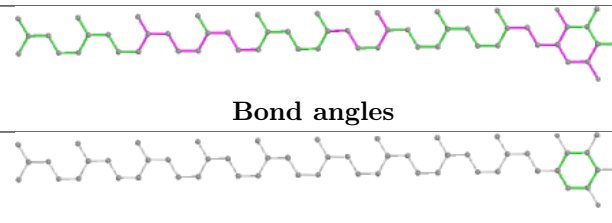
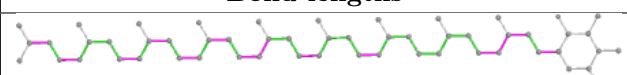
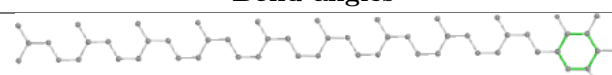


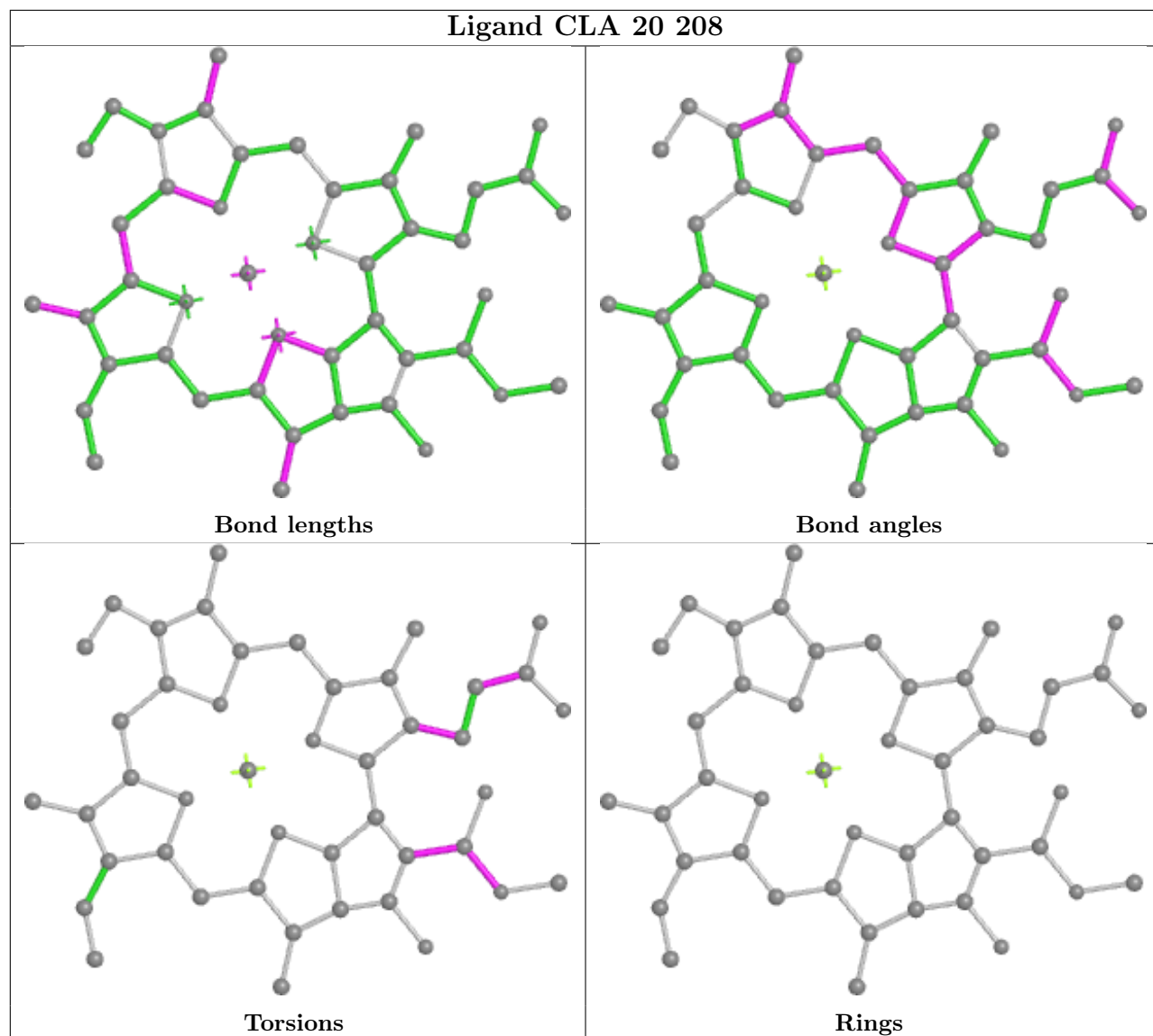


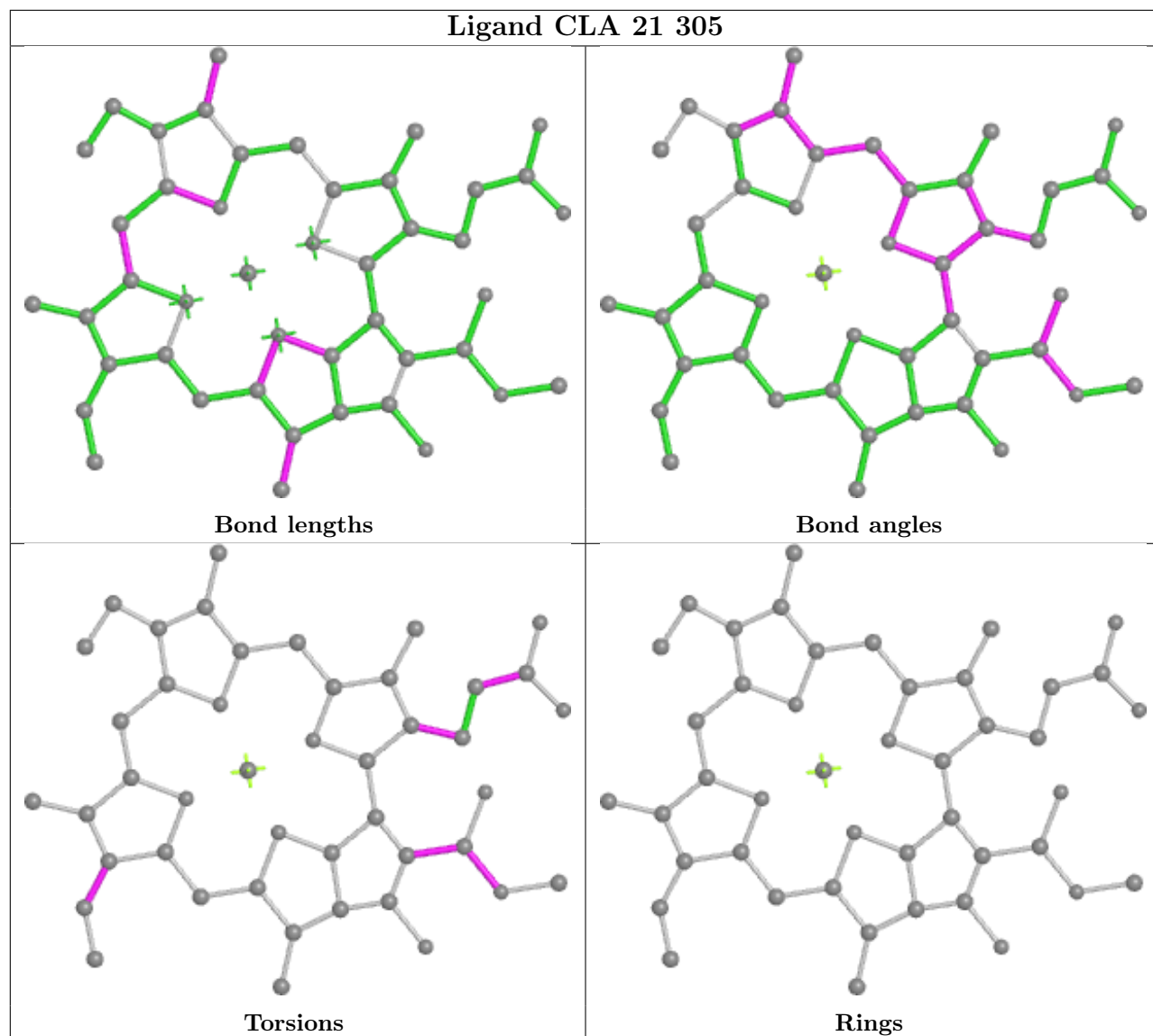


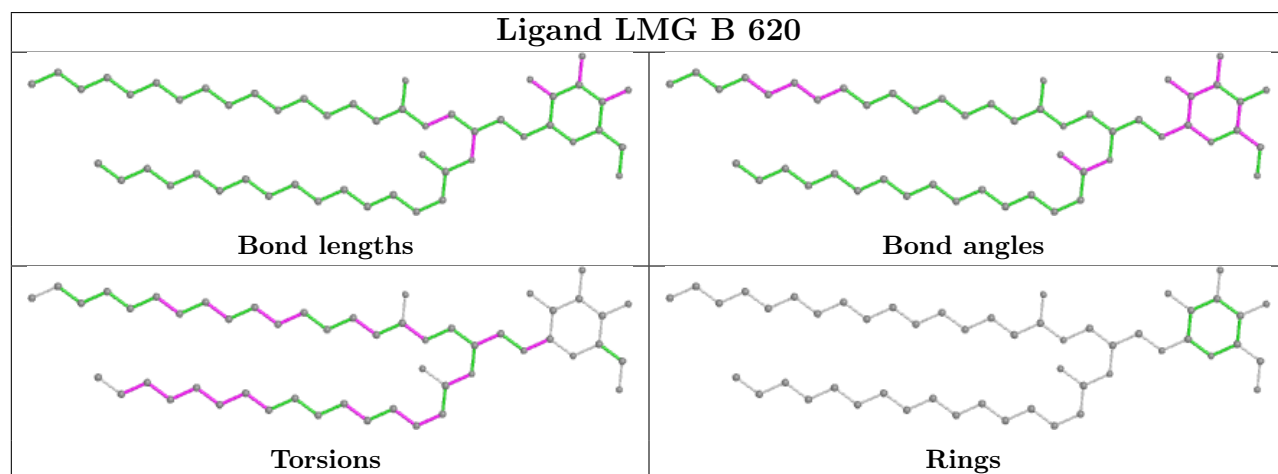
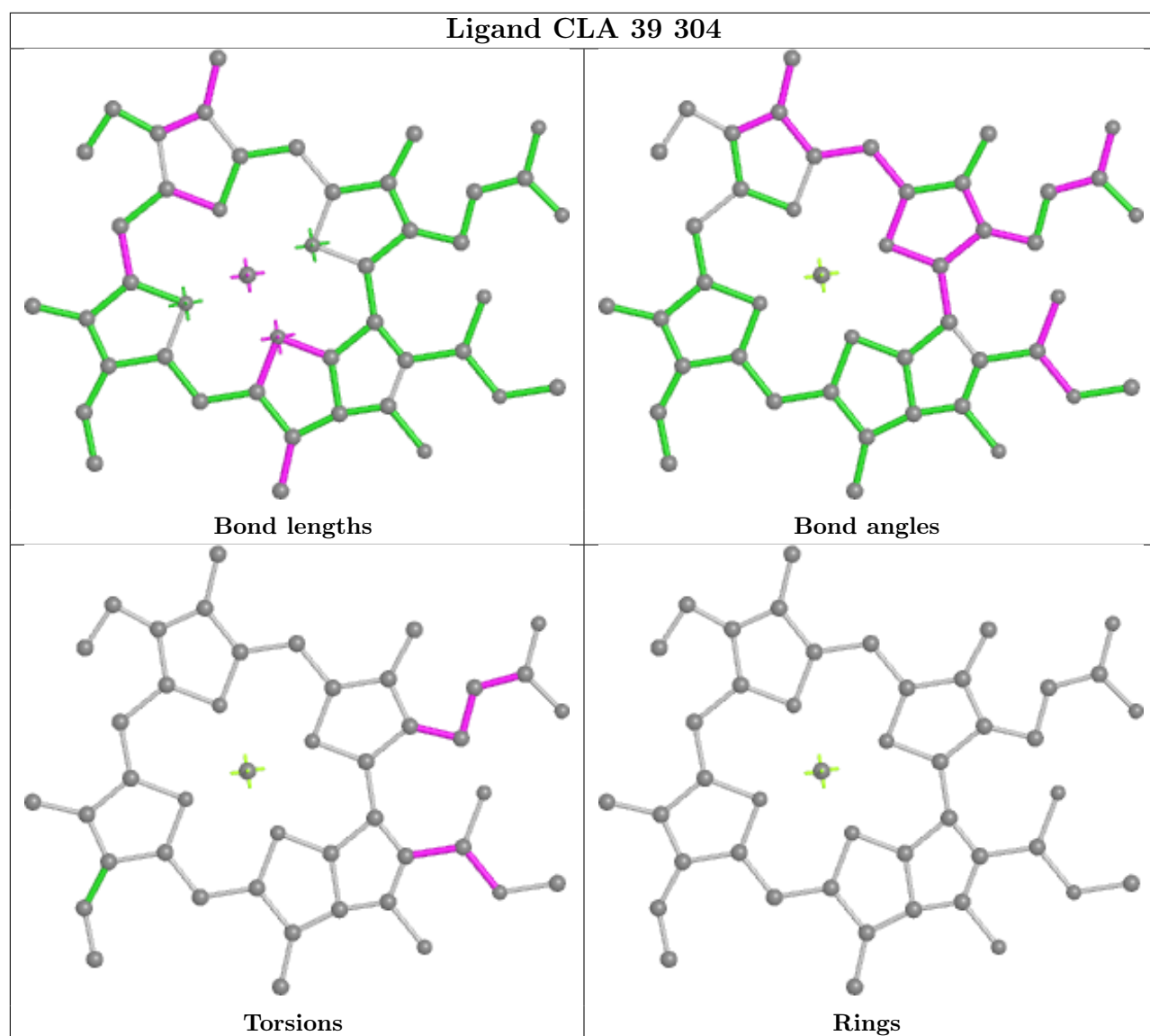
Ligand CLA 16 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

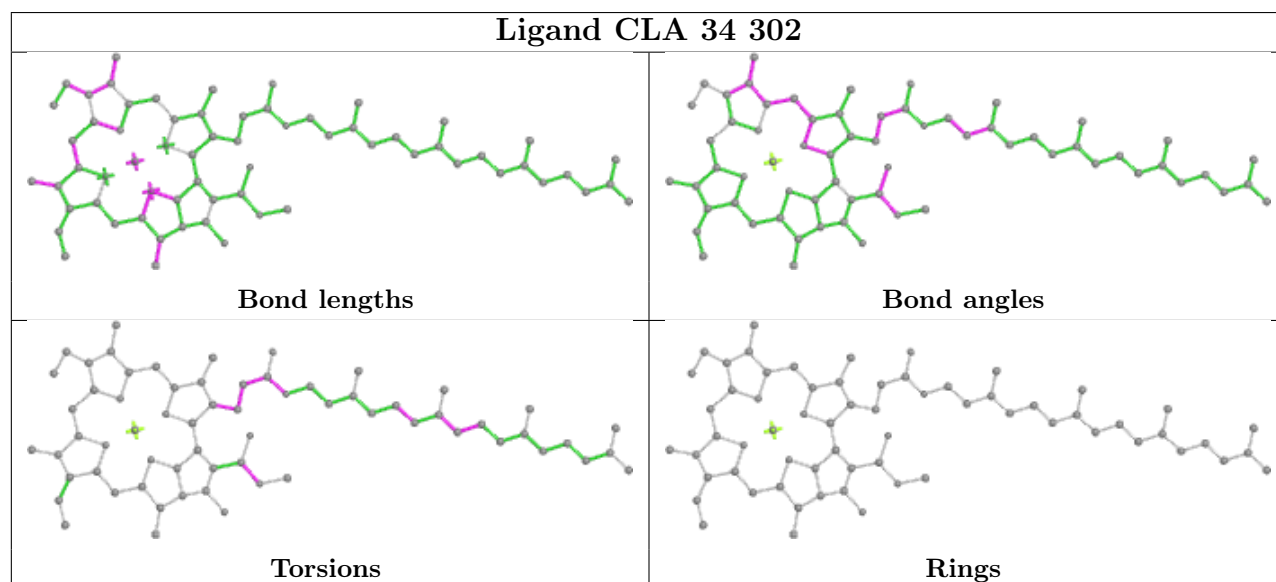
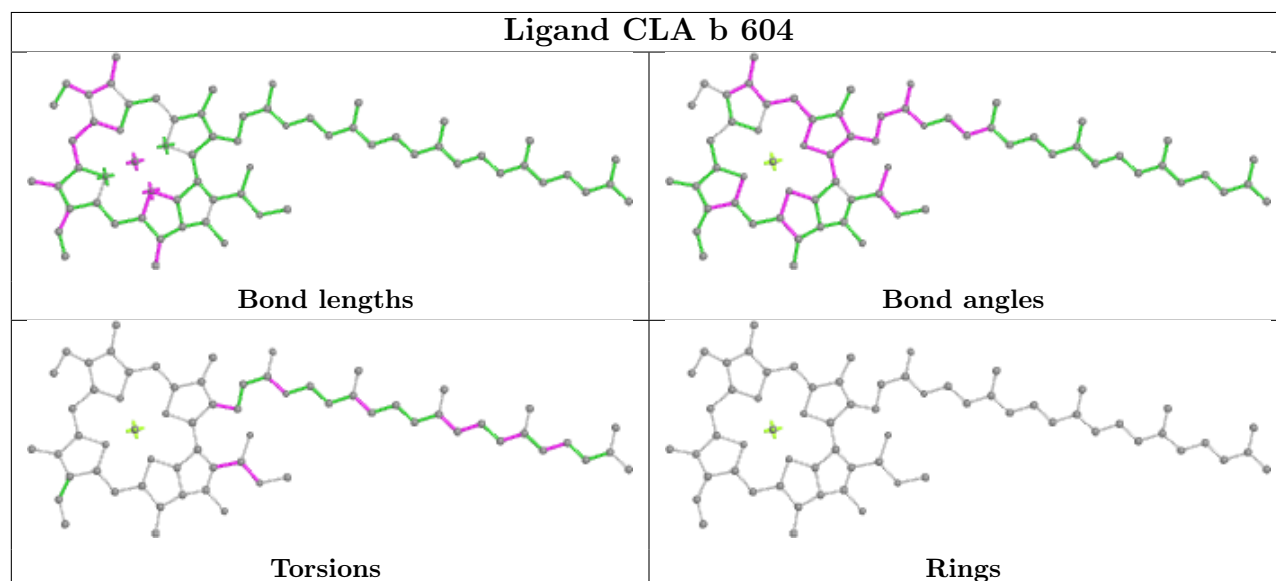
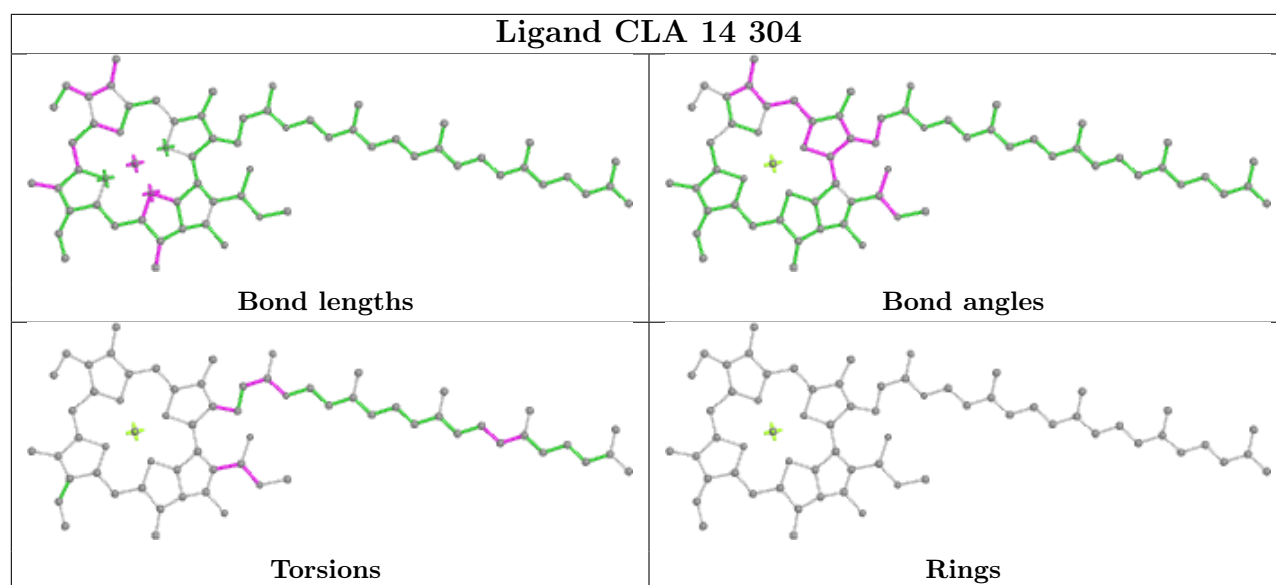
Ligand A86 33 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

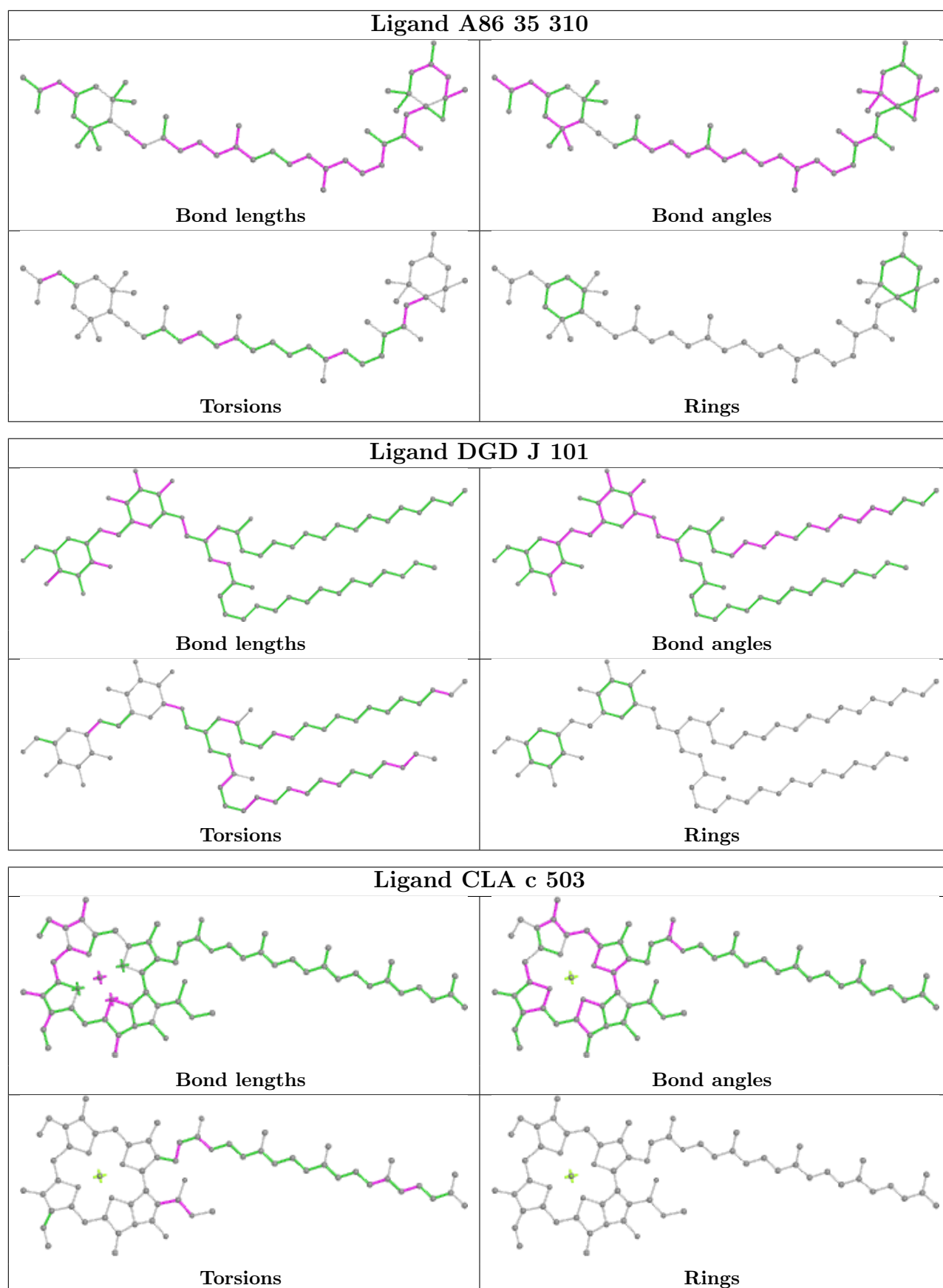
Ligand PL9 D 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

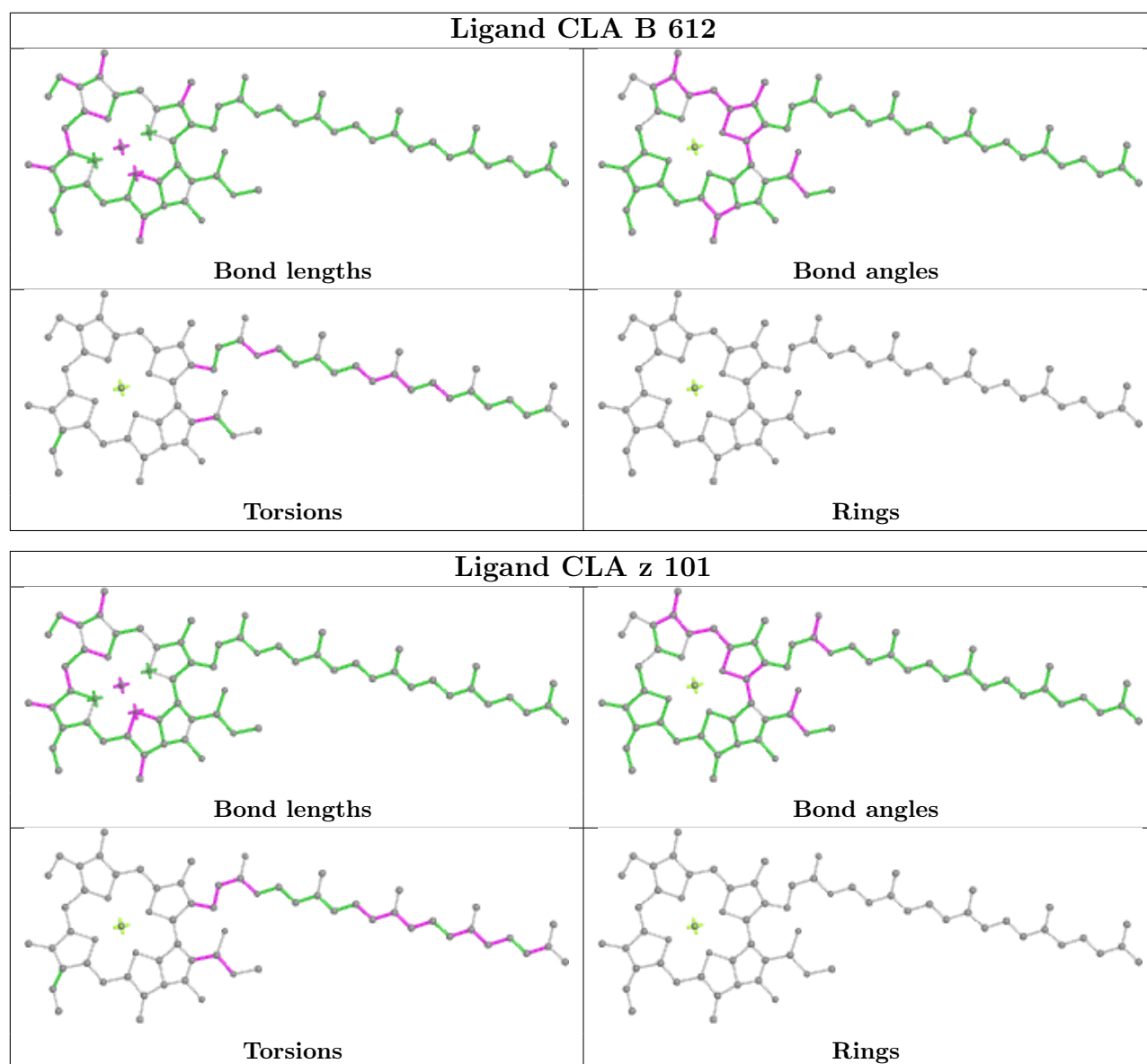


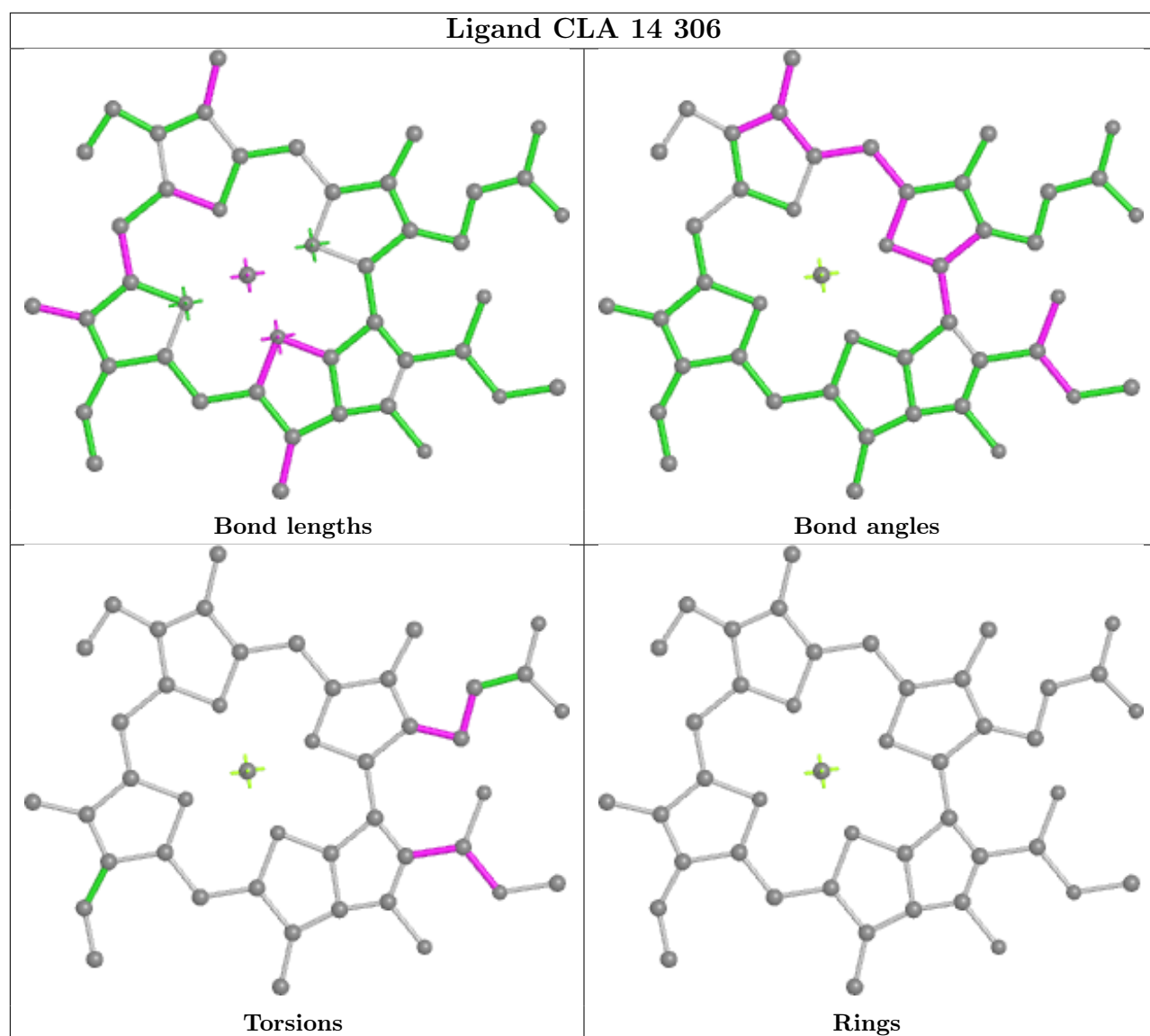


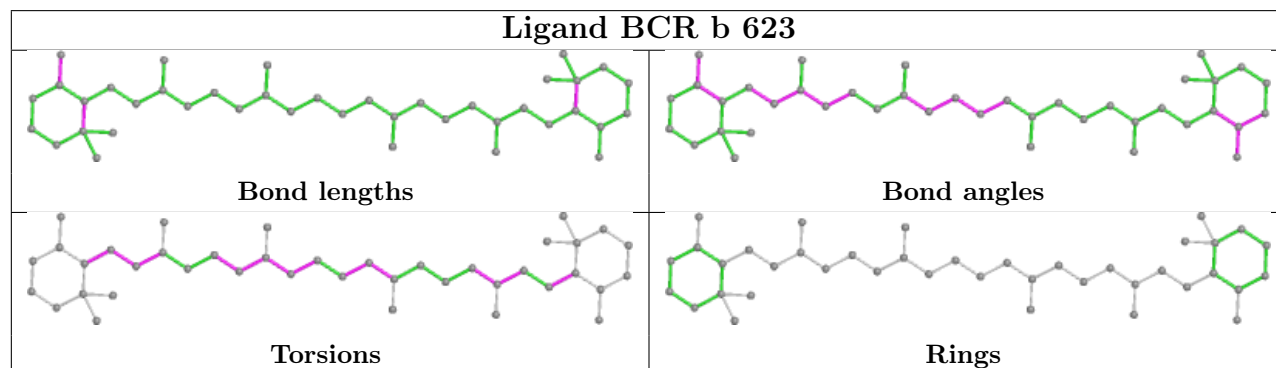
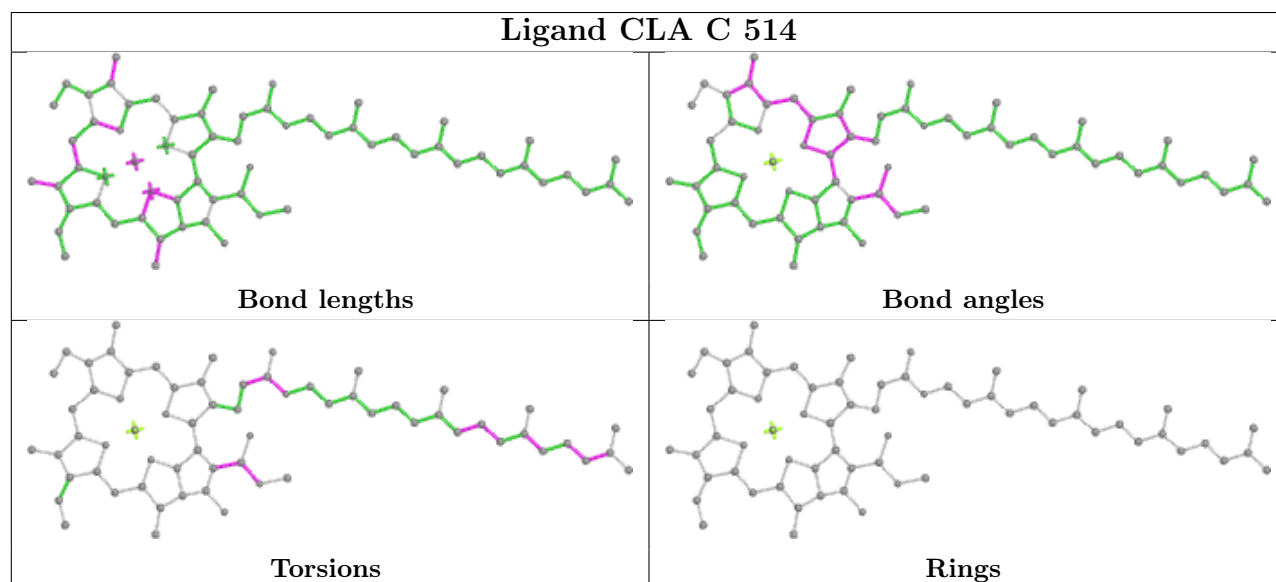
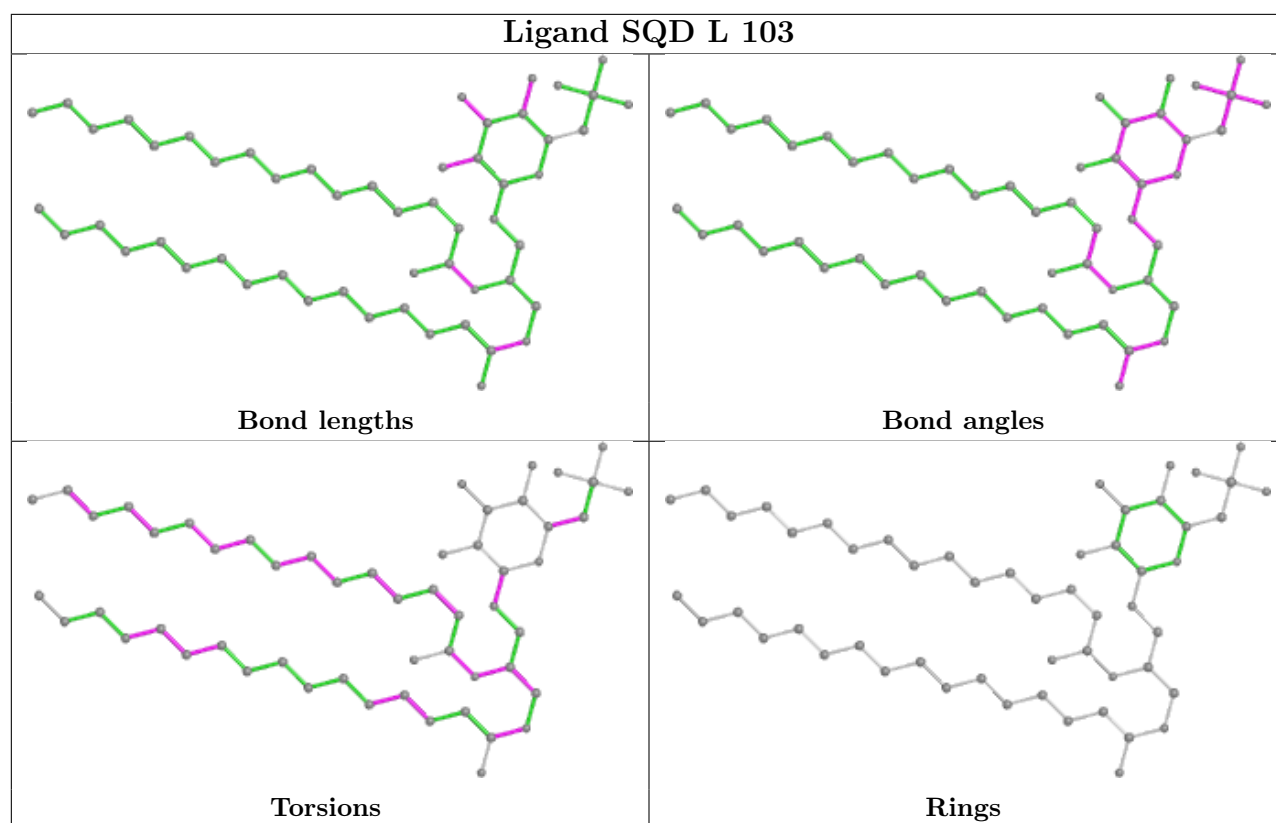


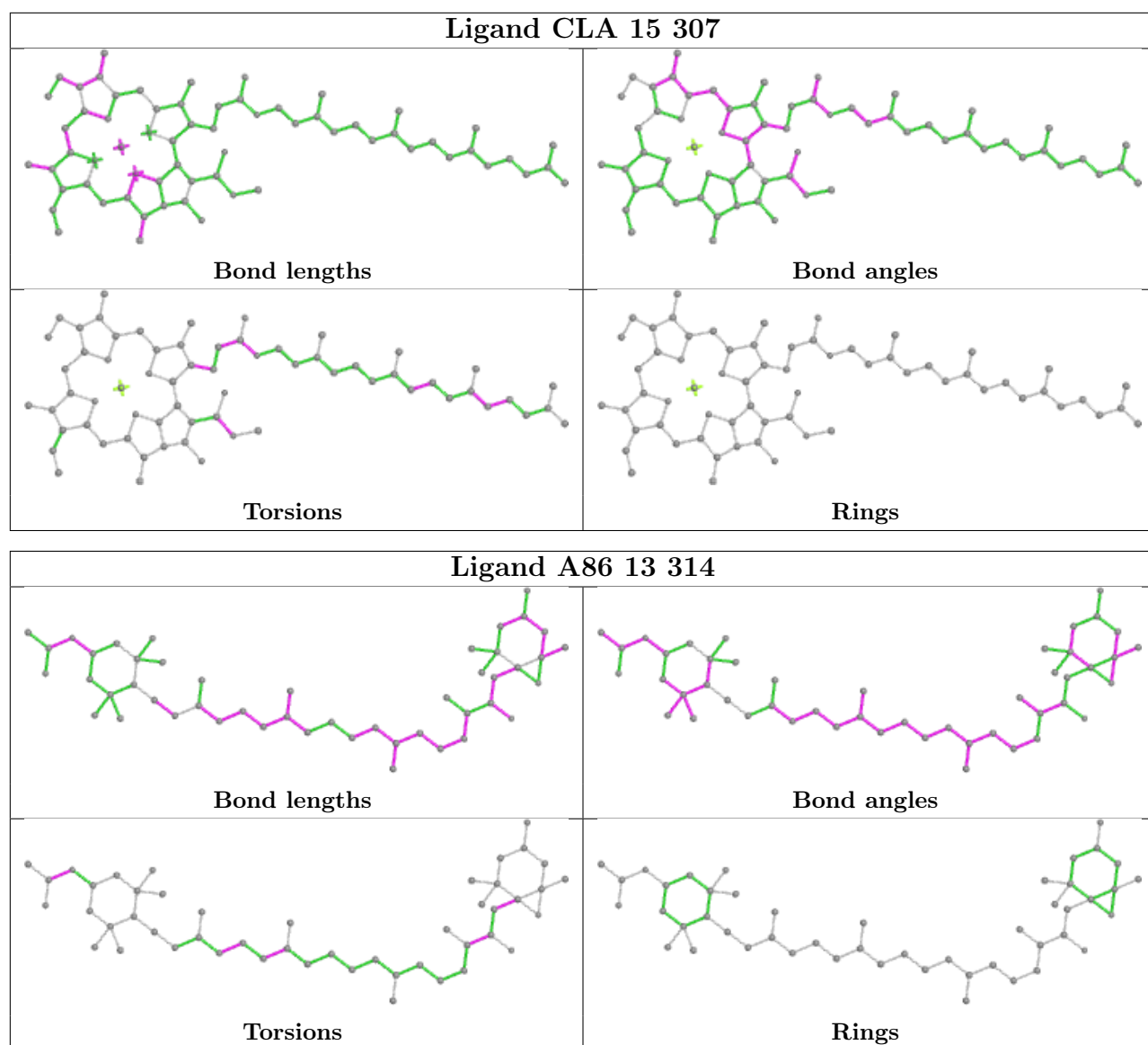


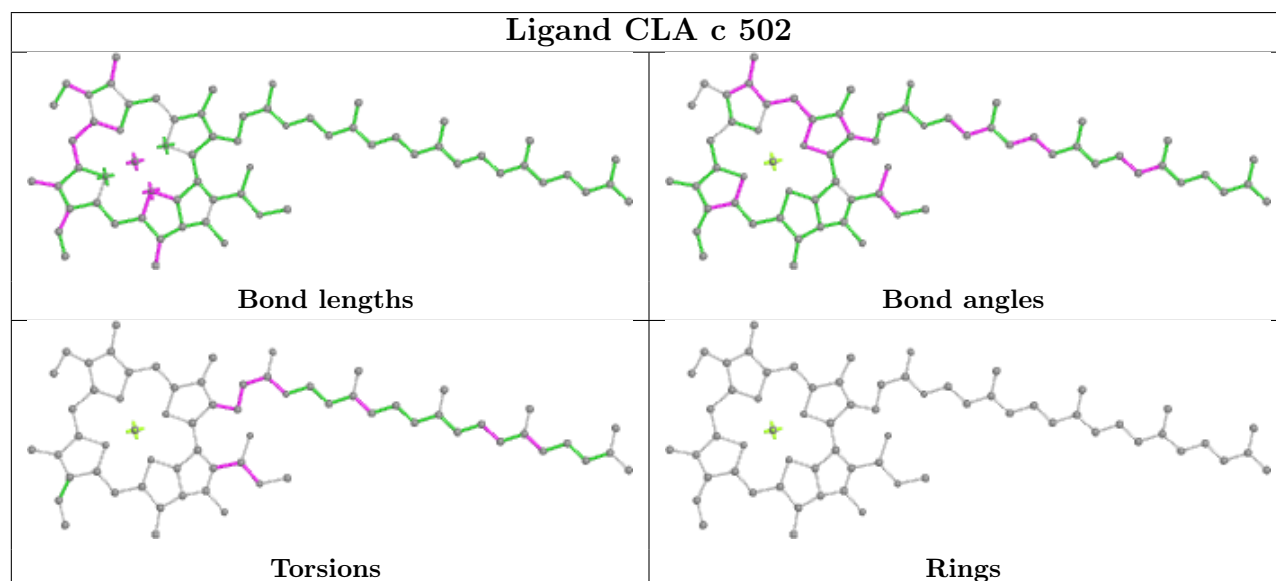
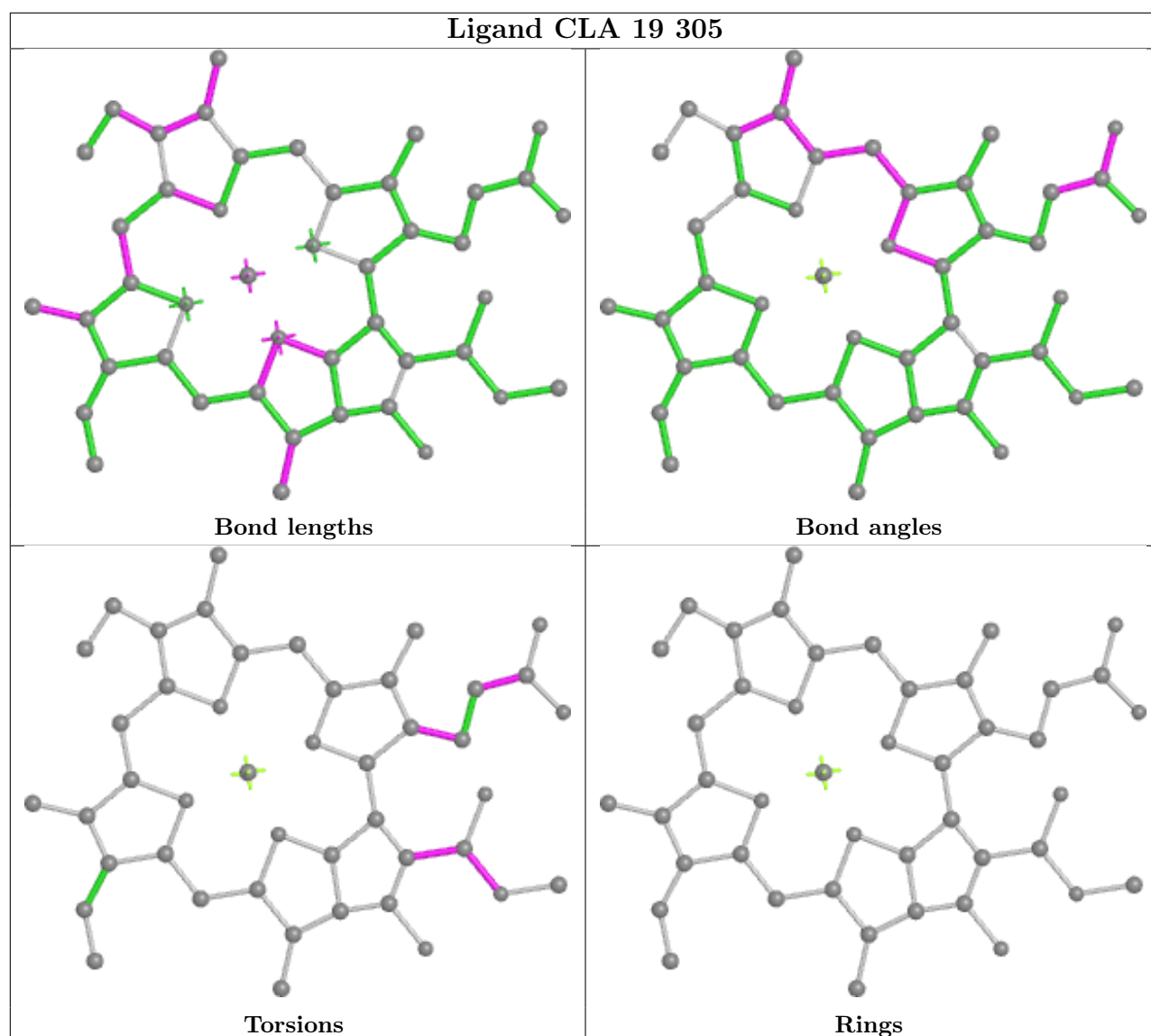


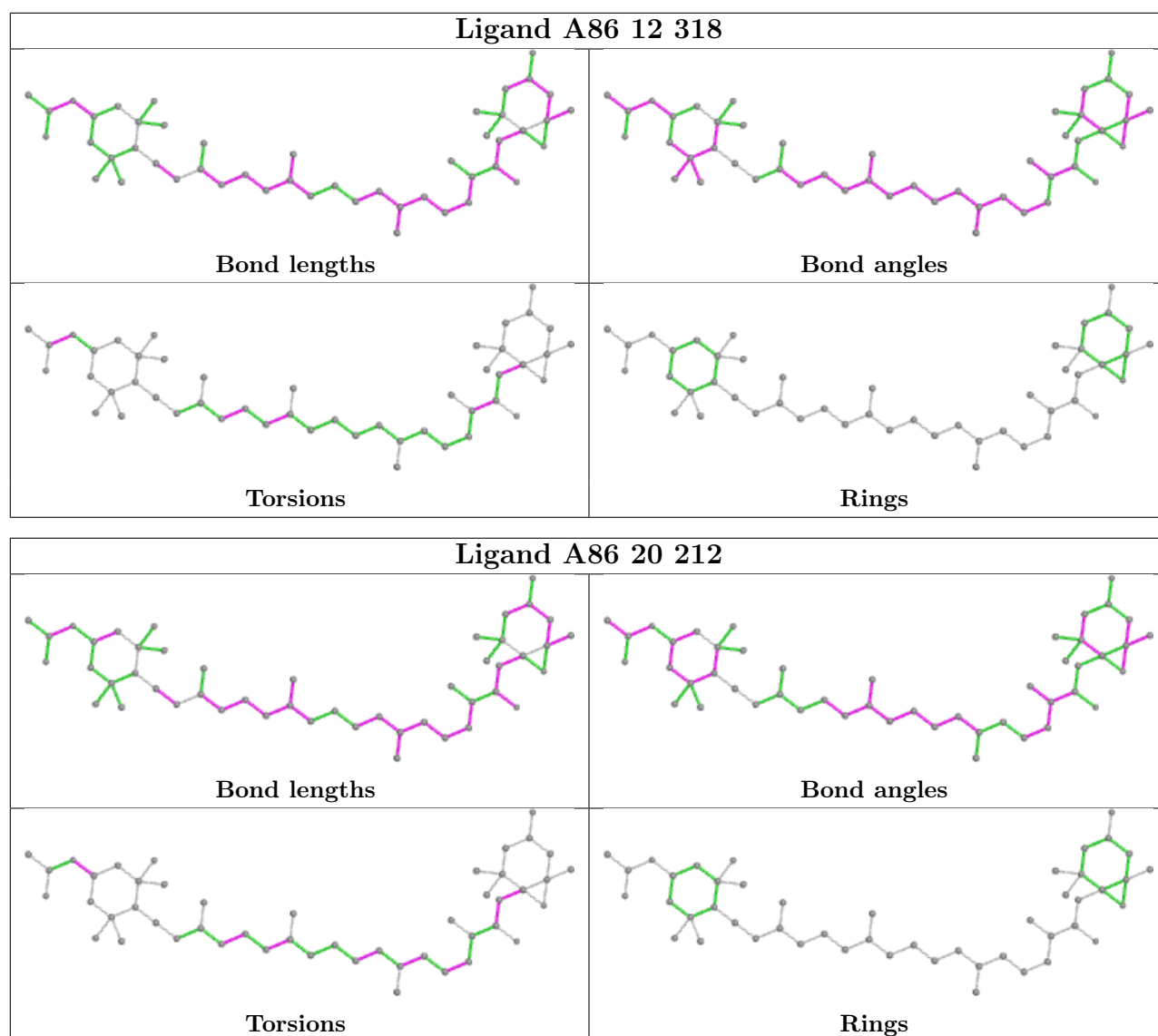


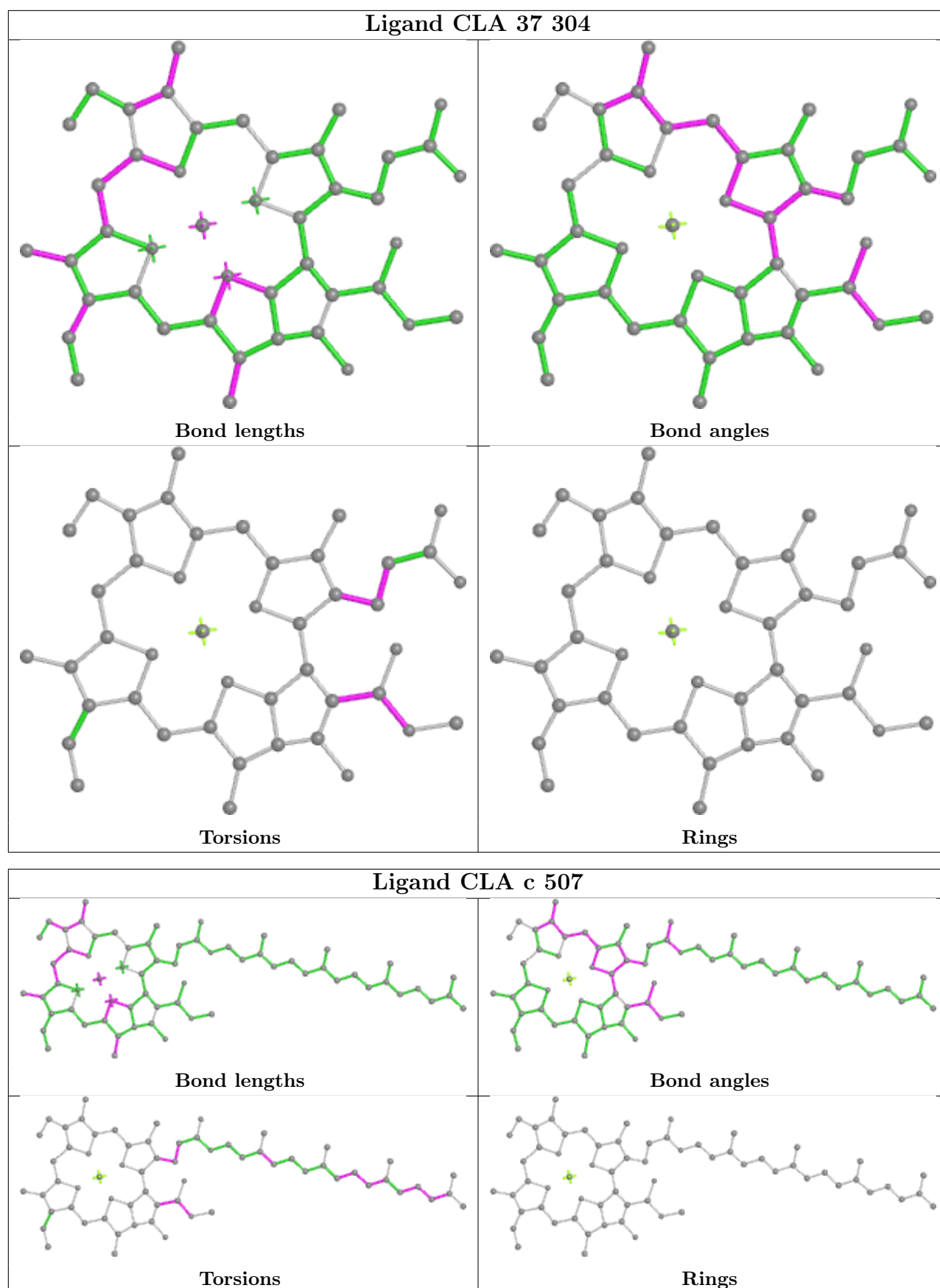


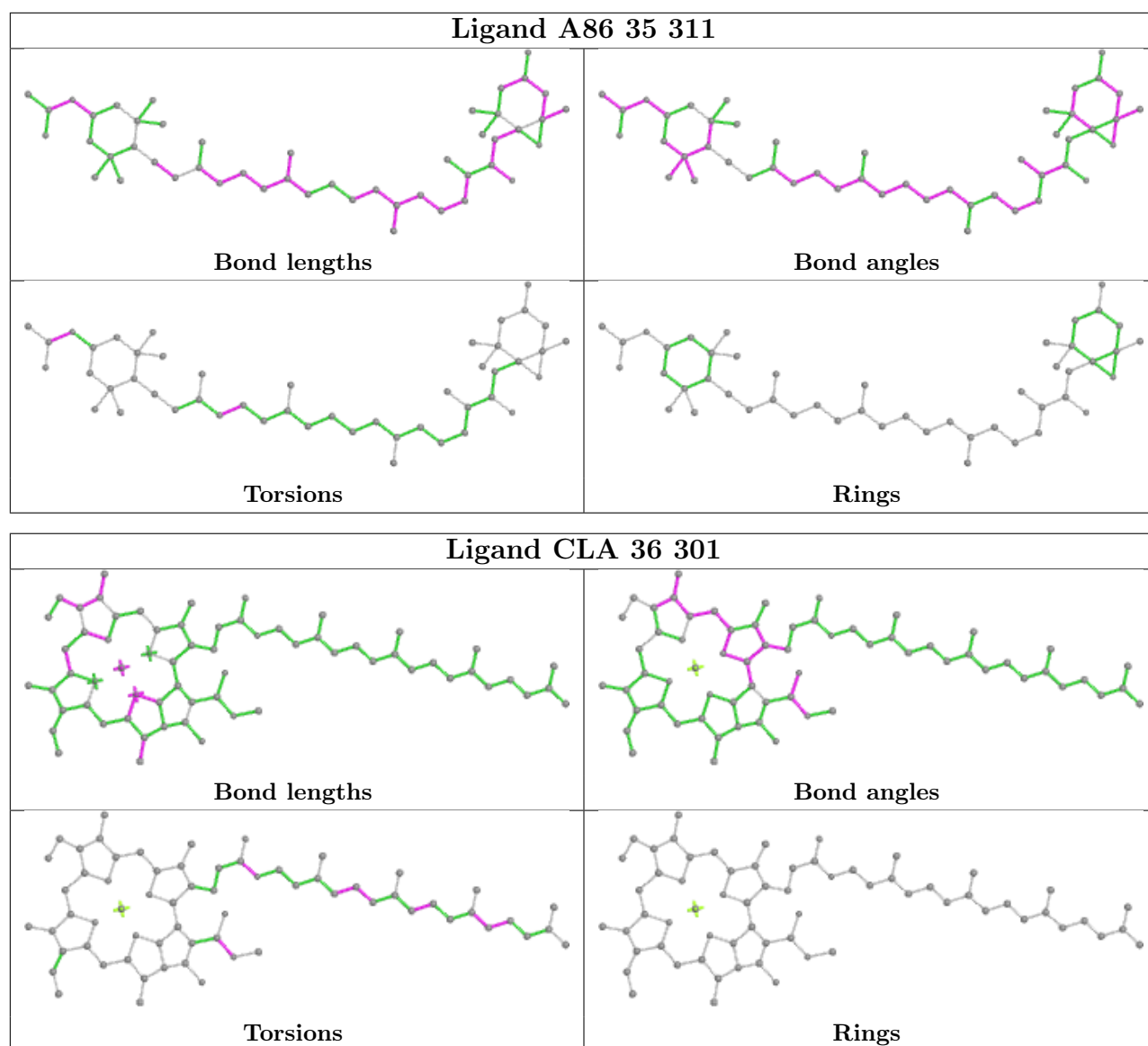


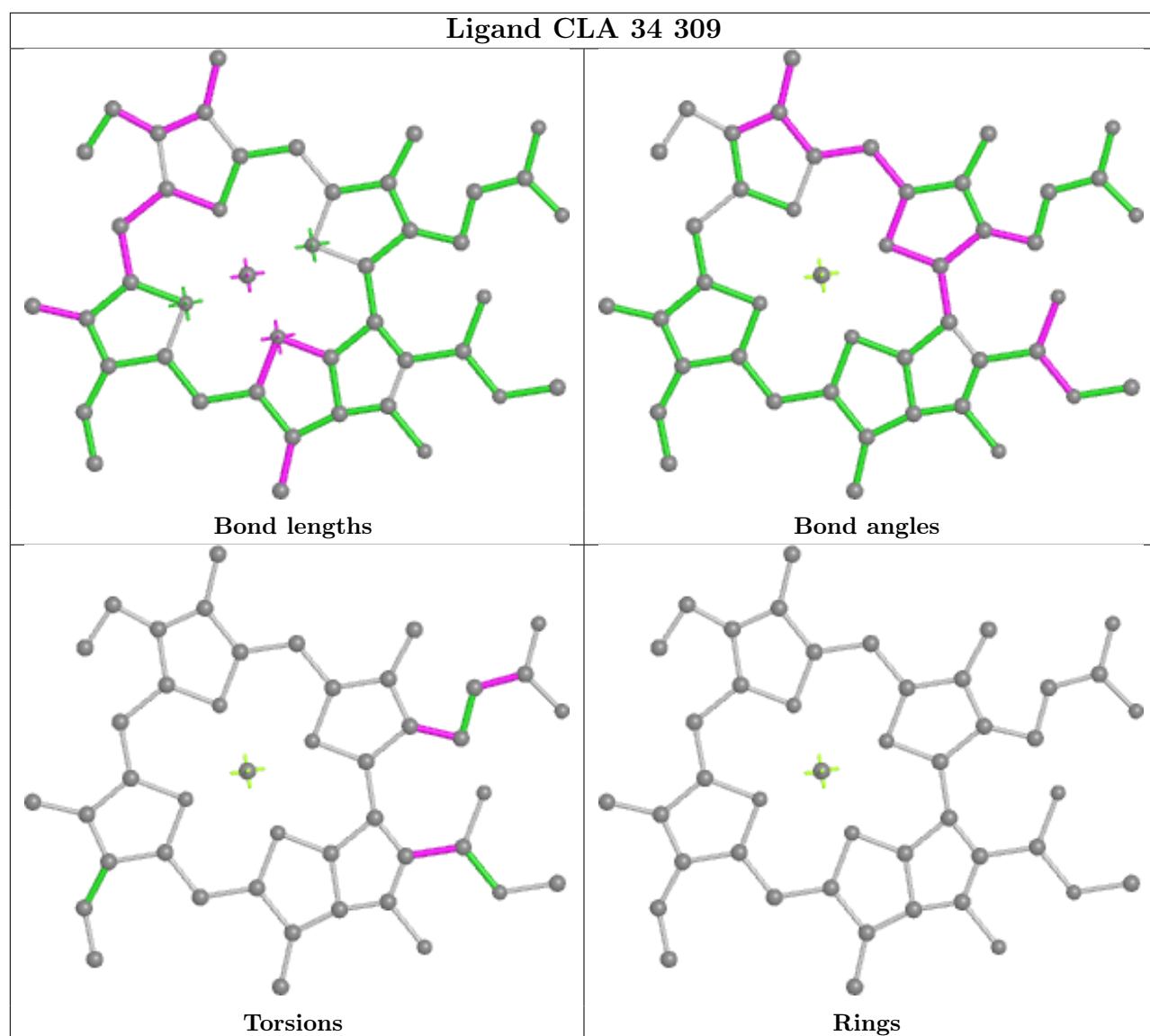


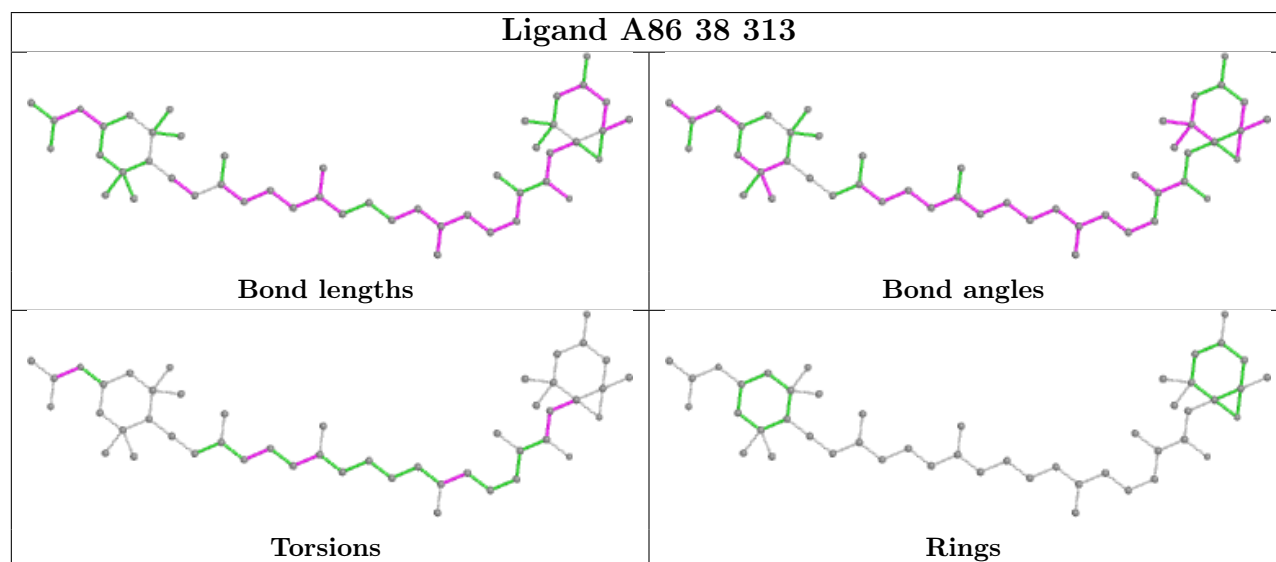
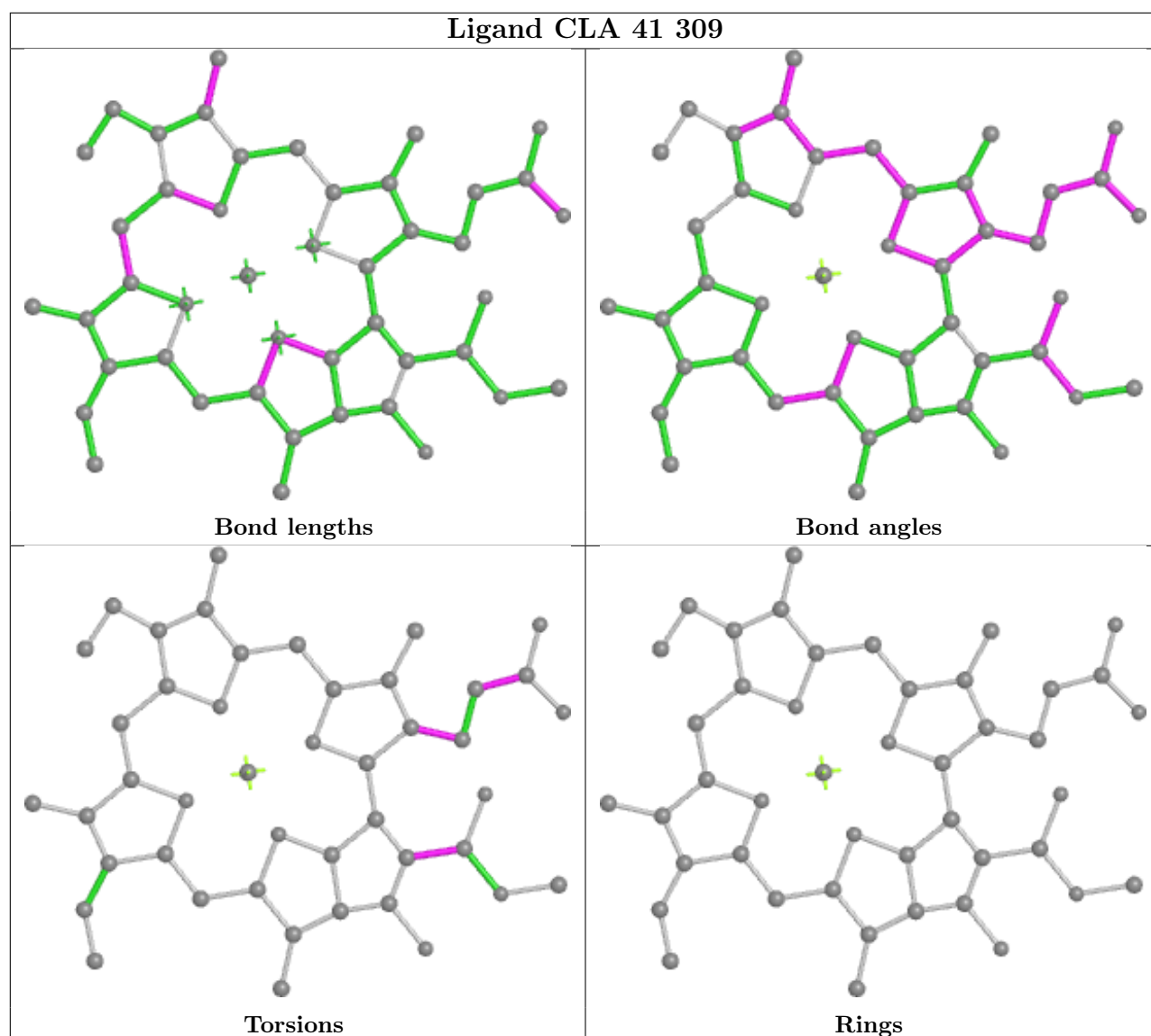




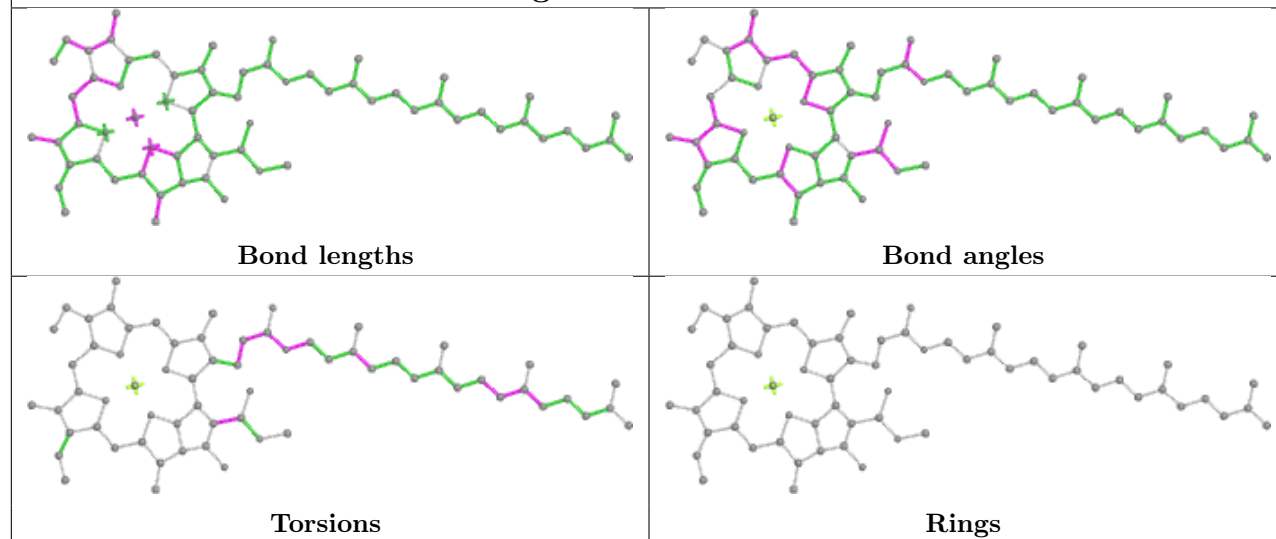




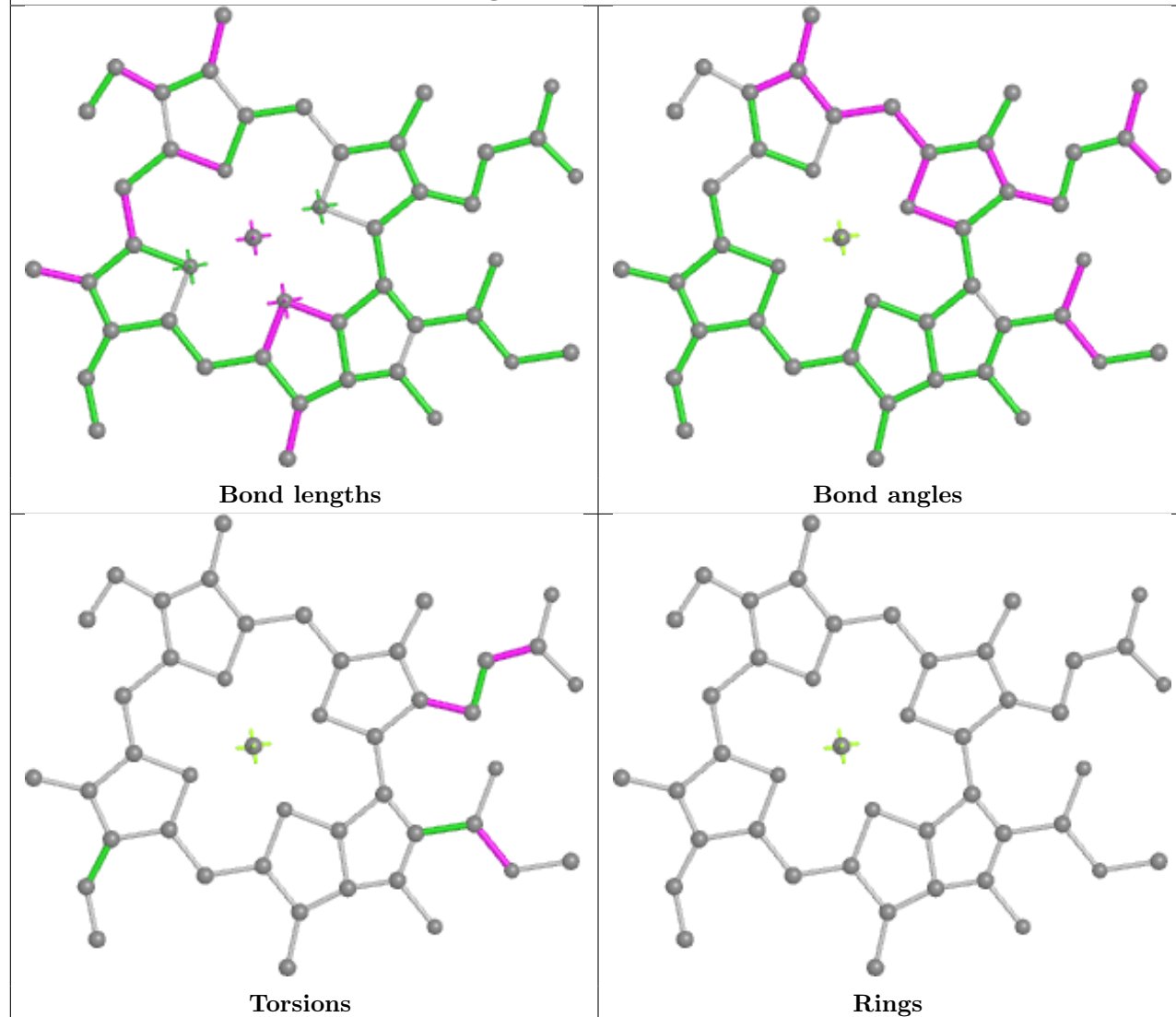


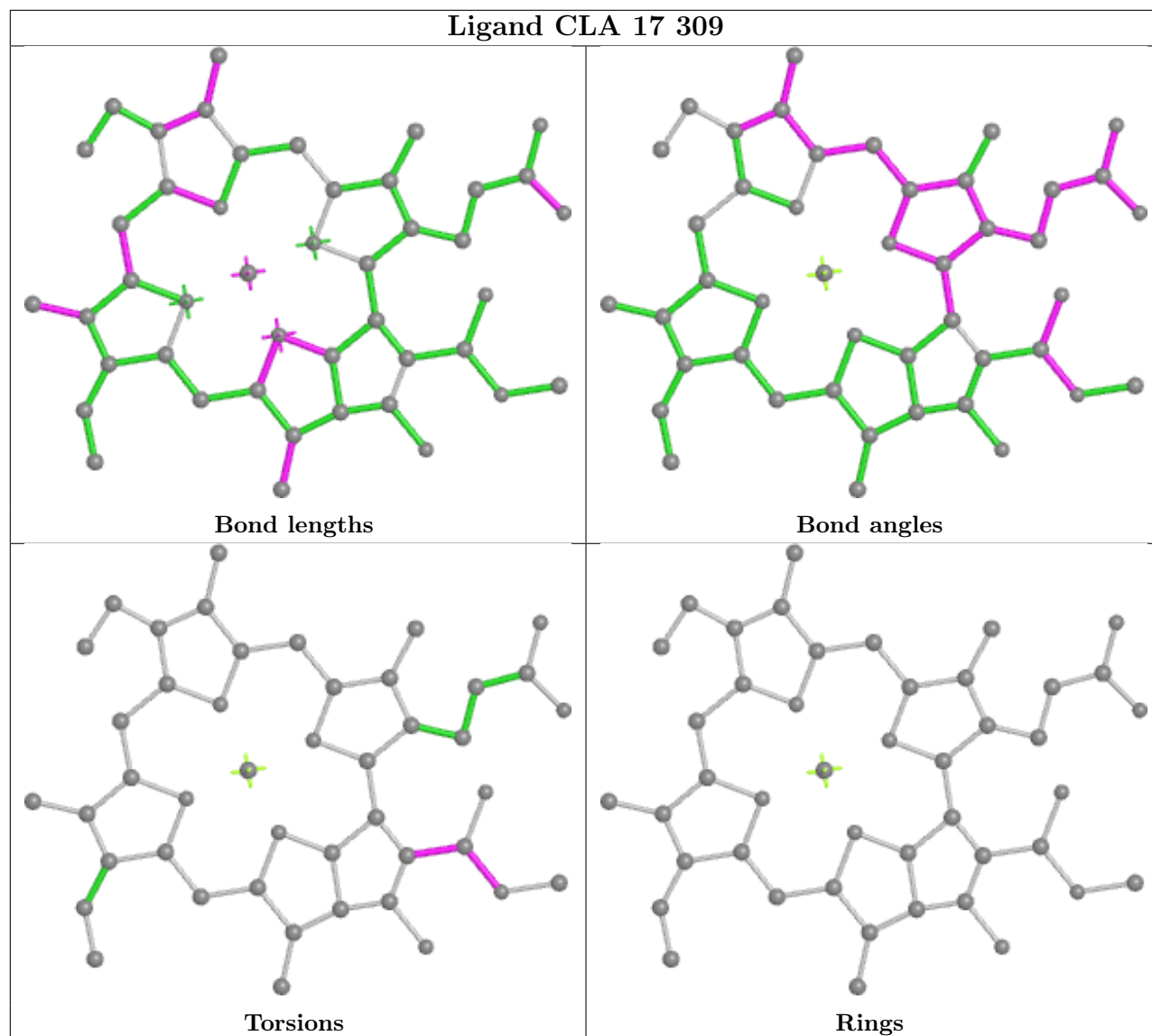


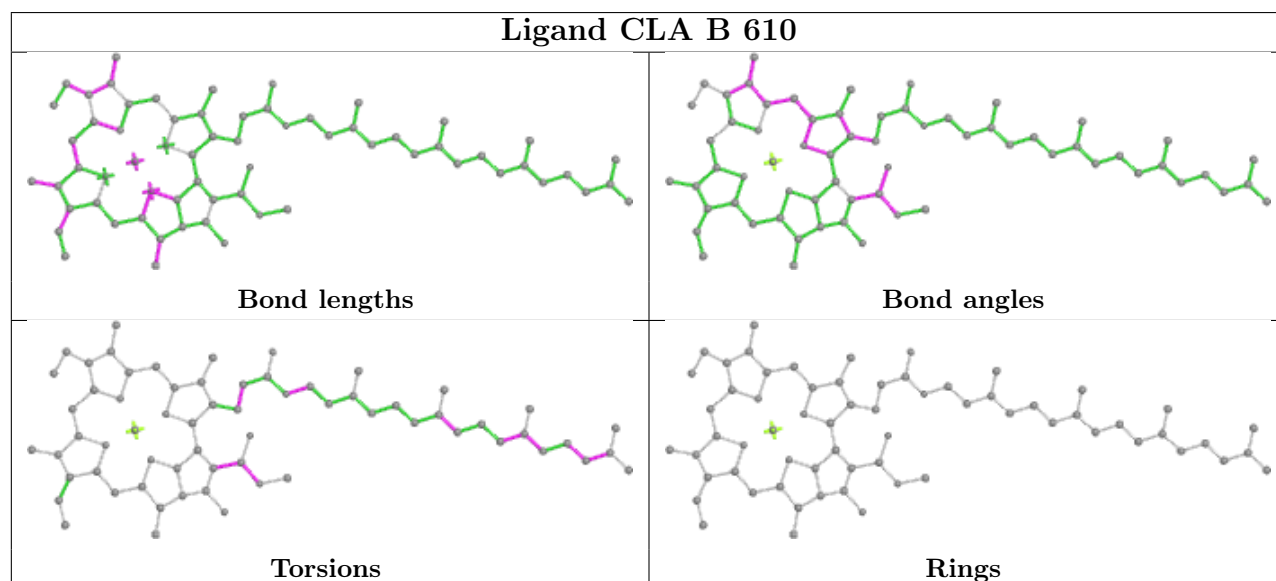
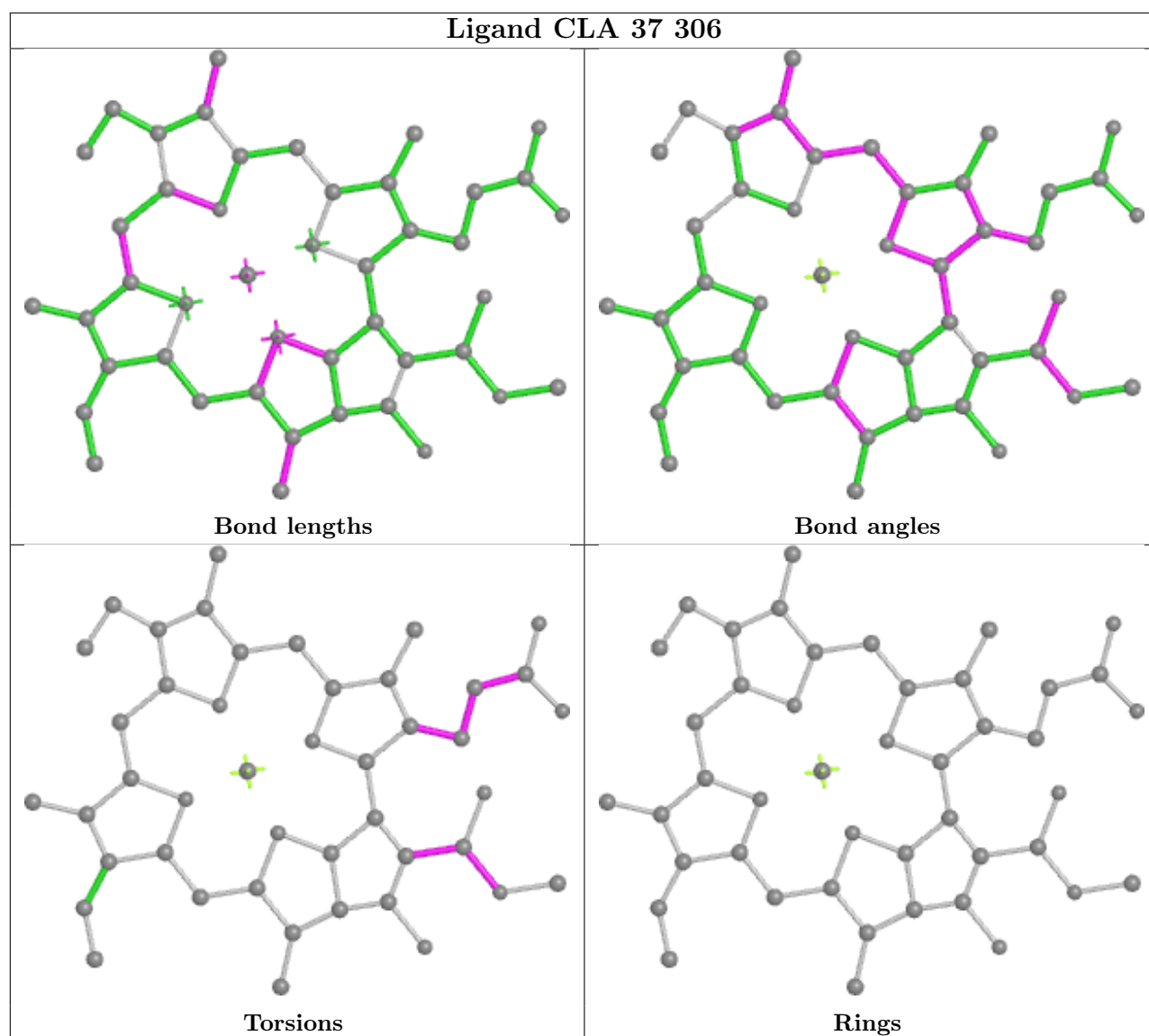
Ligand CLA C 506

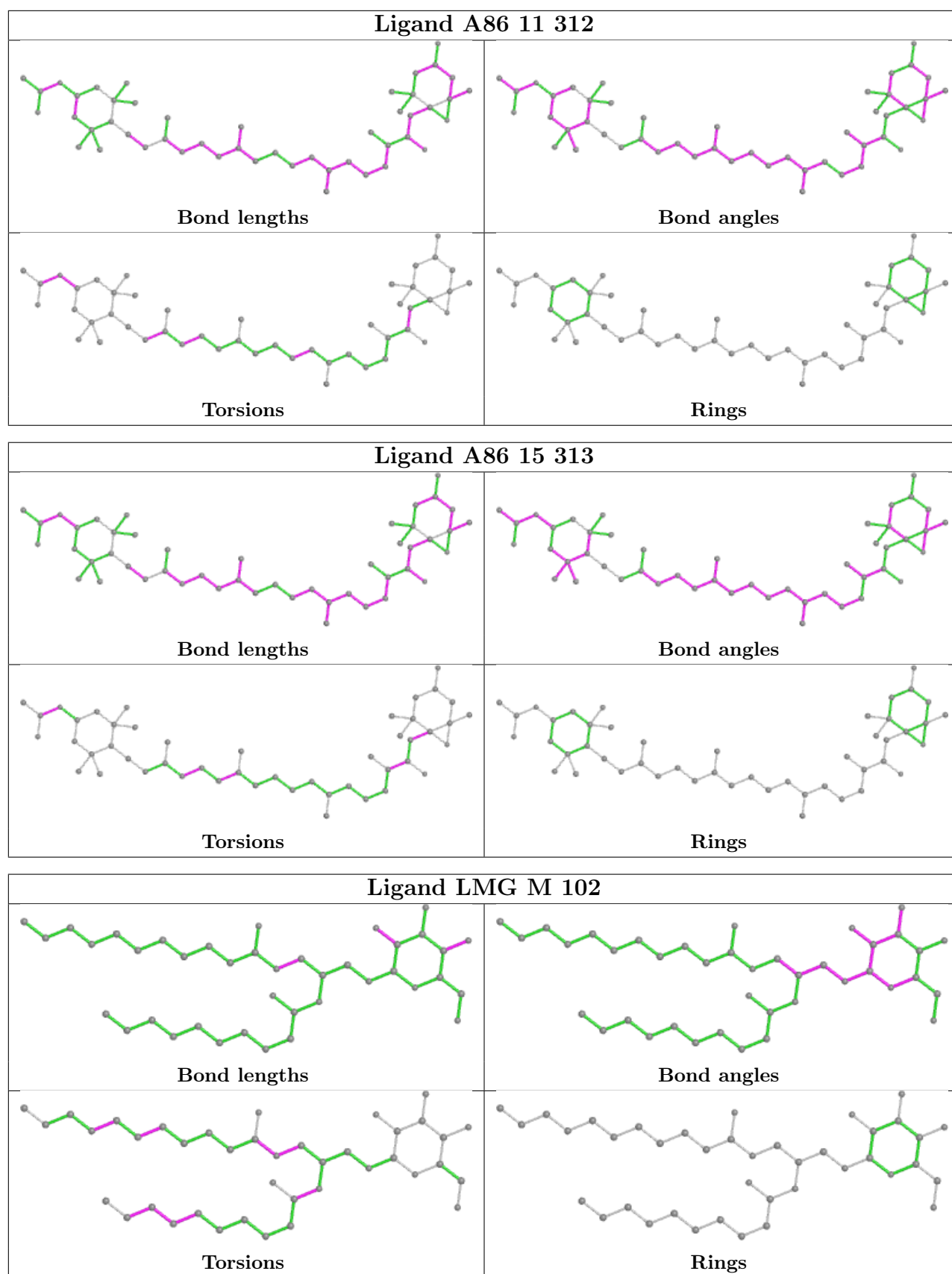


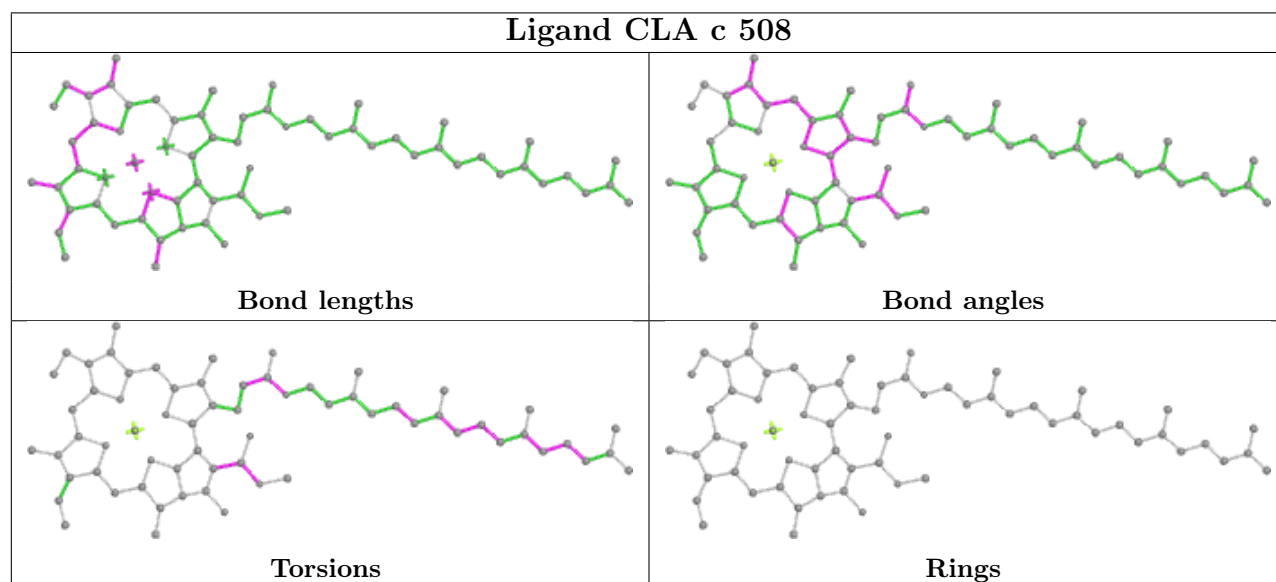
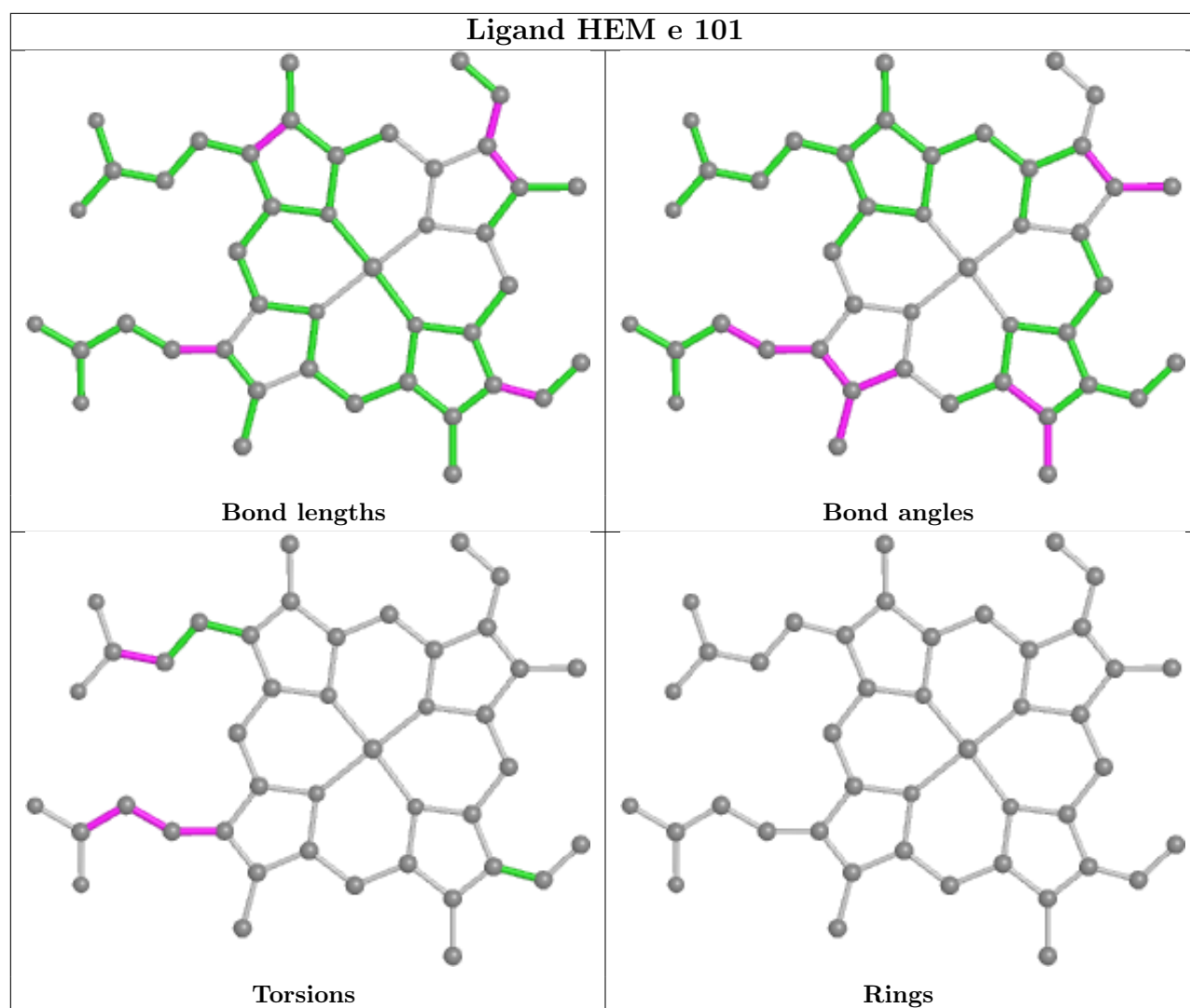
Ligand CLA 12 314



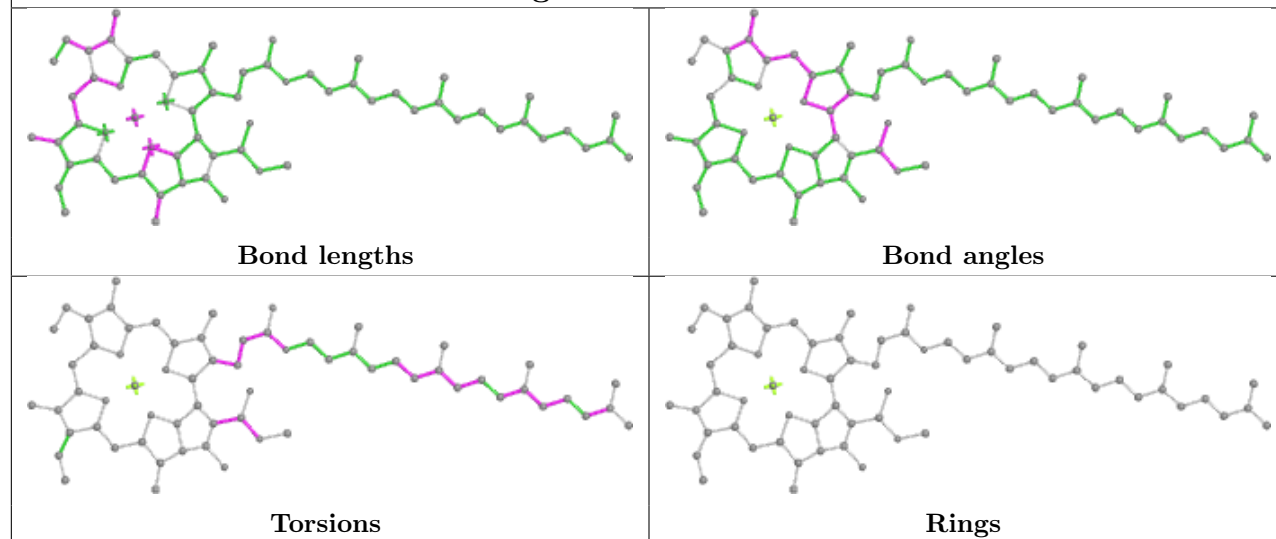




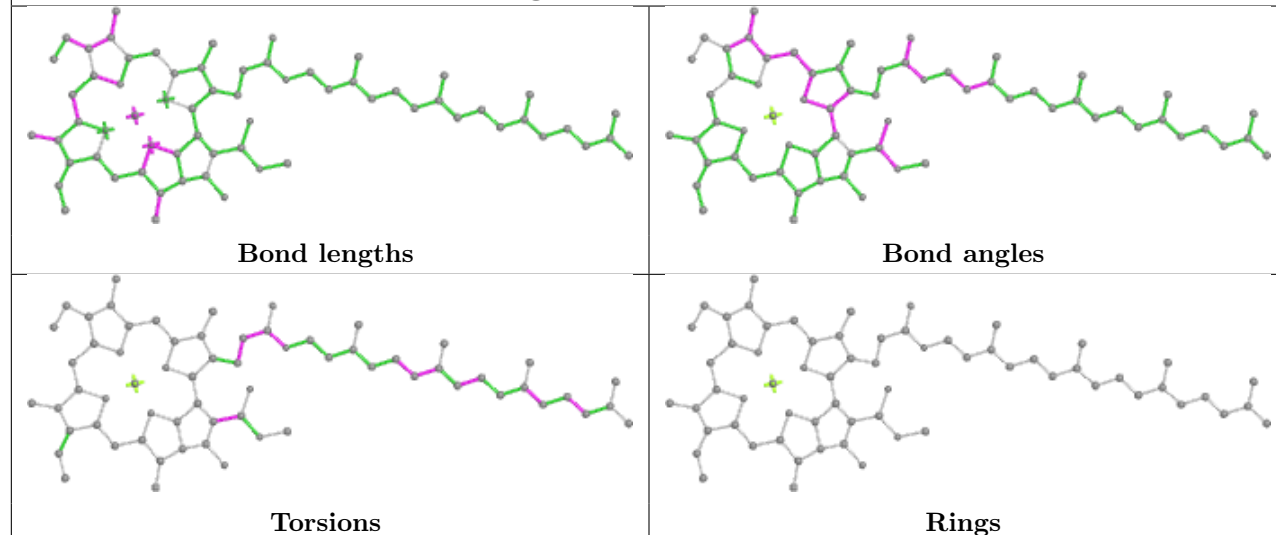




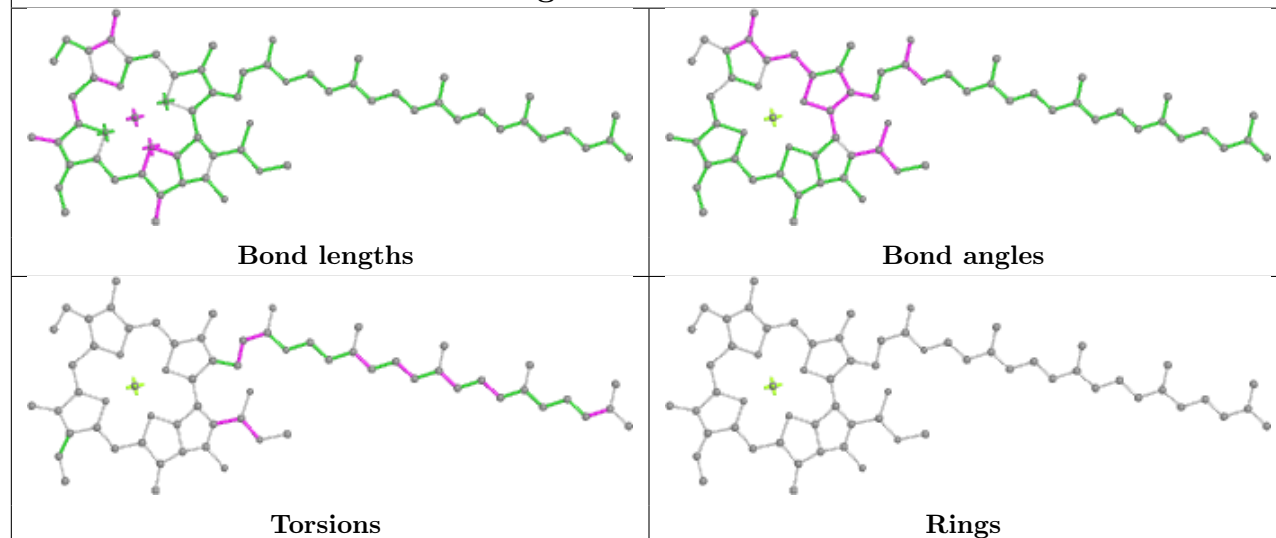
Ligand CLA C 519

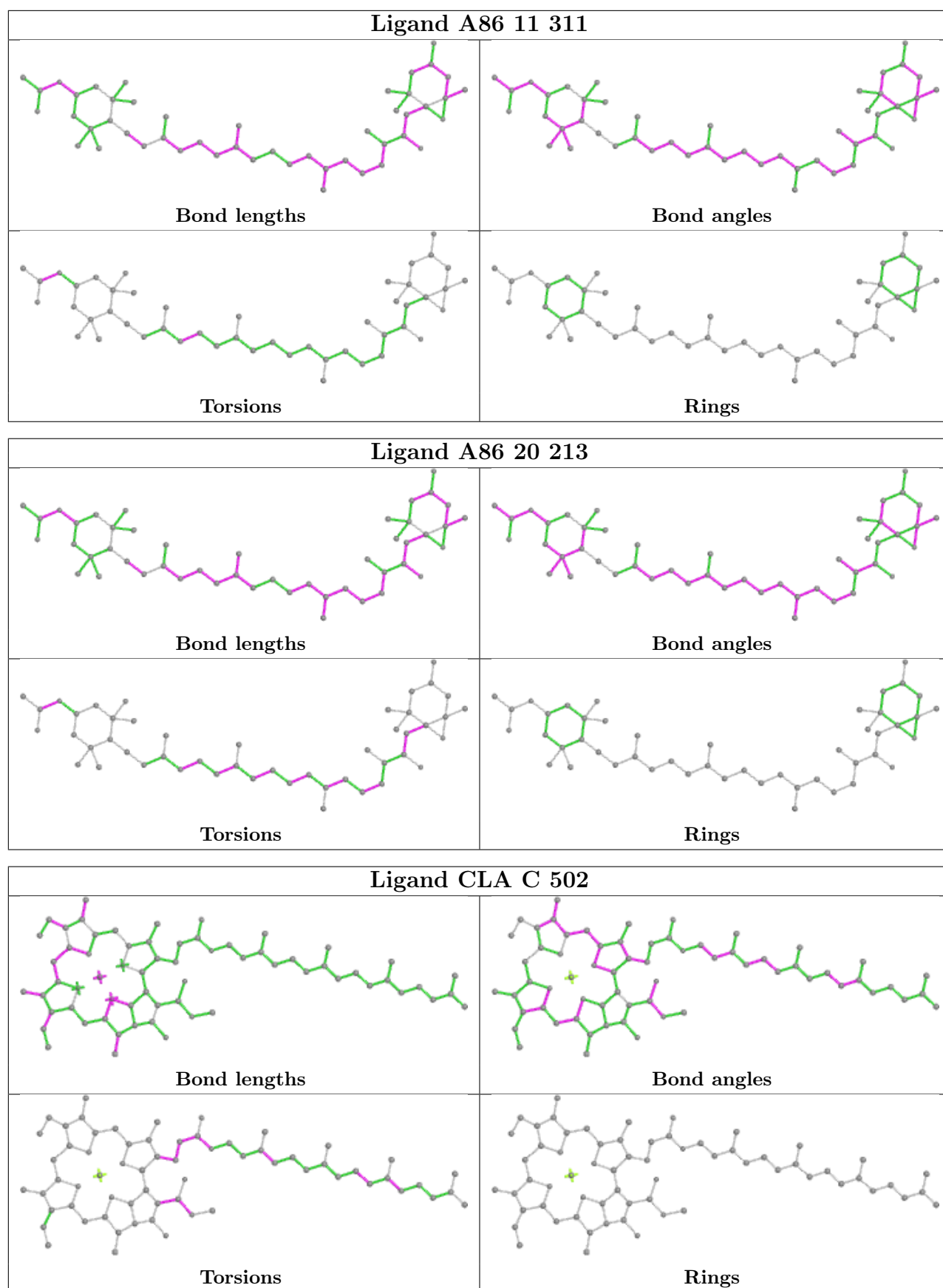


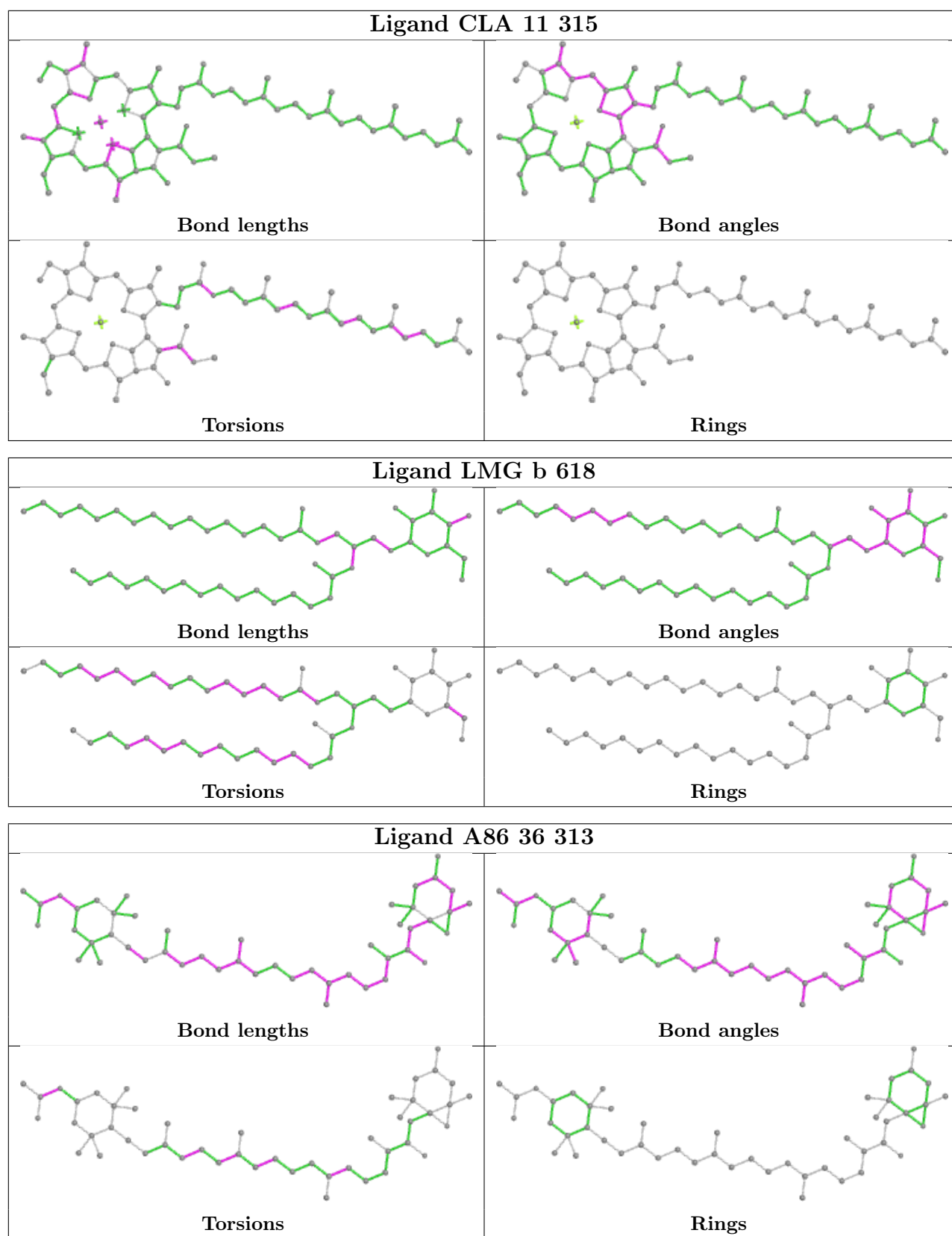
Ligand CLA 14 308

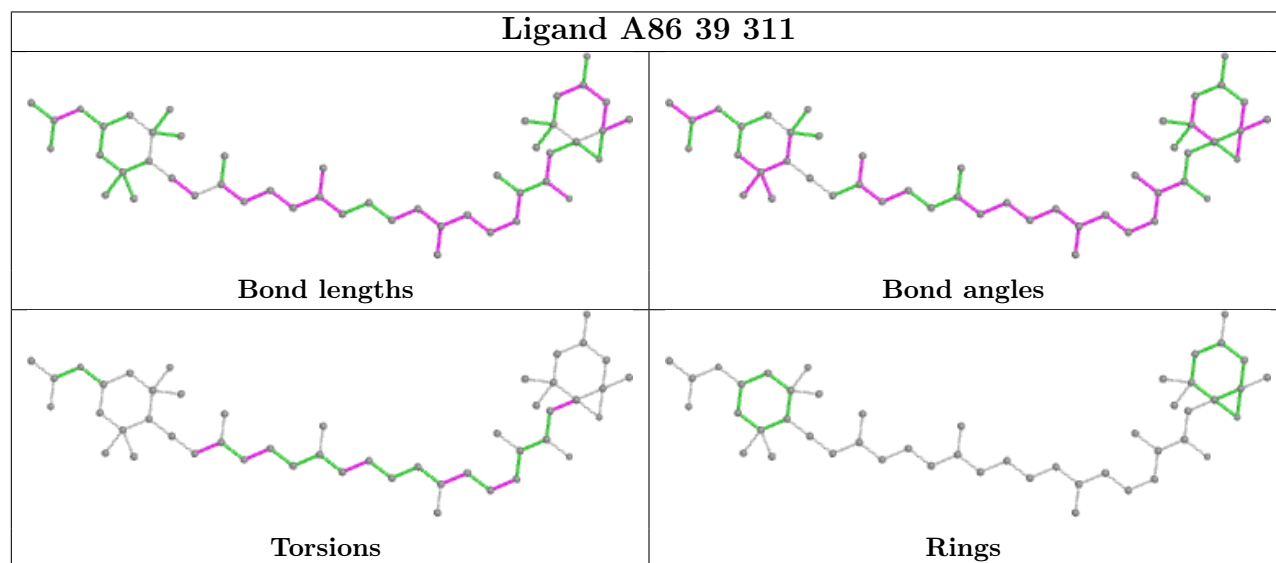
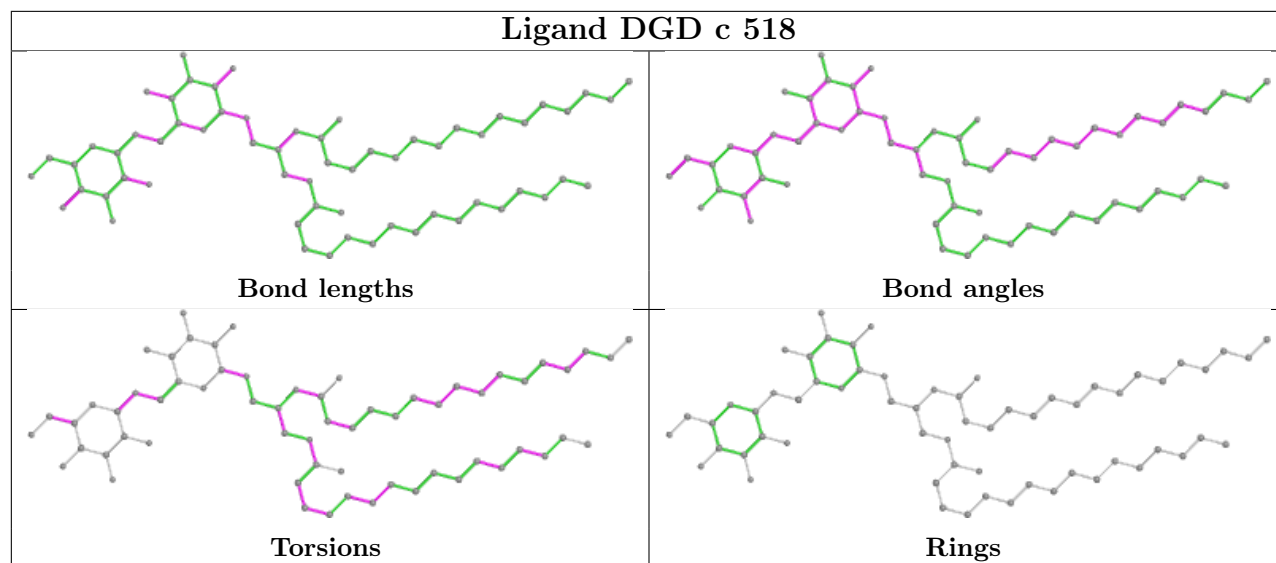


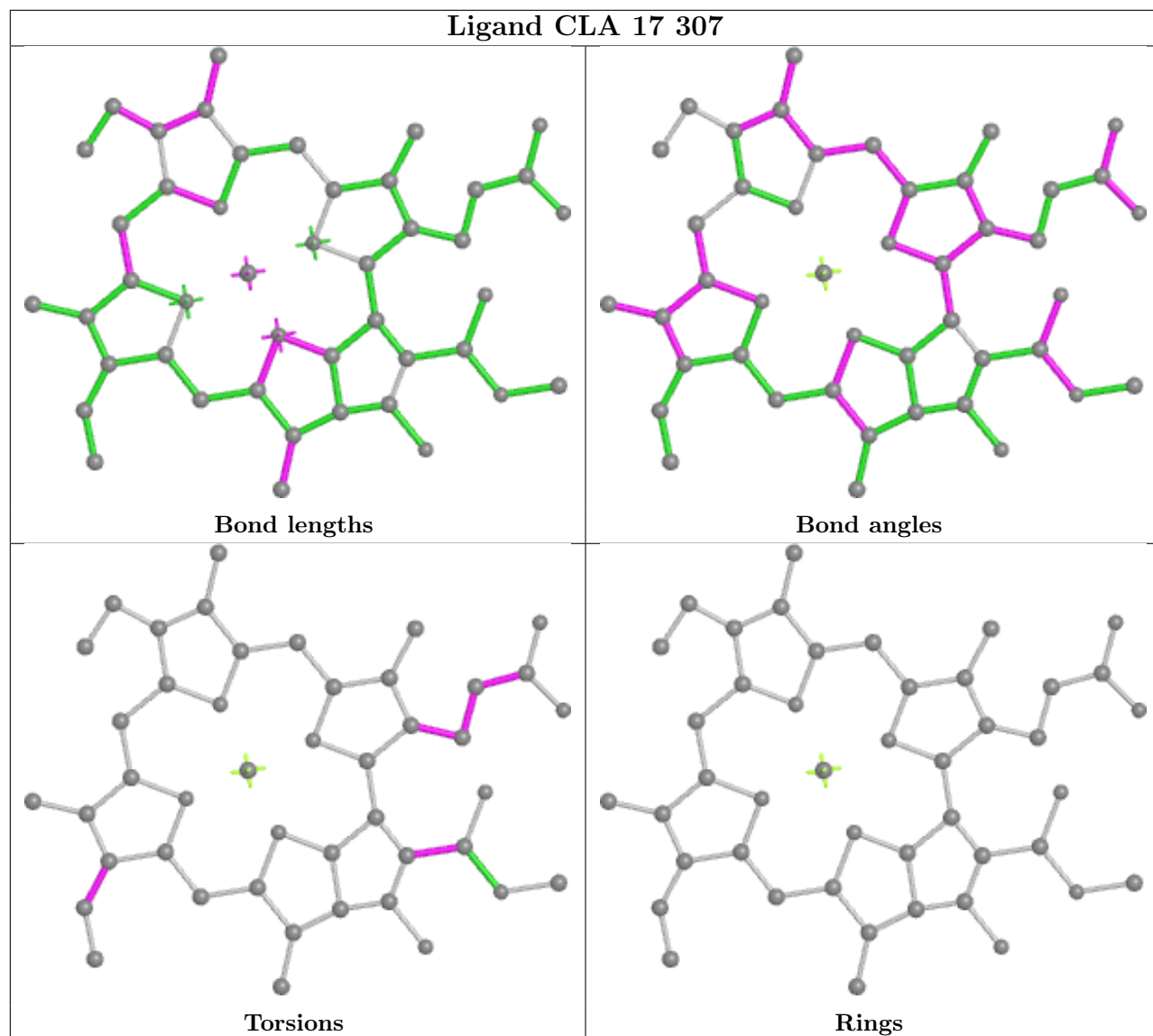
Ligand CLA c 523

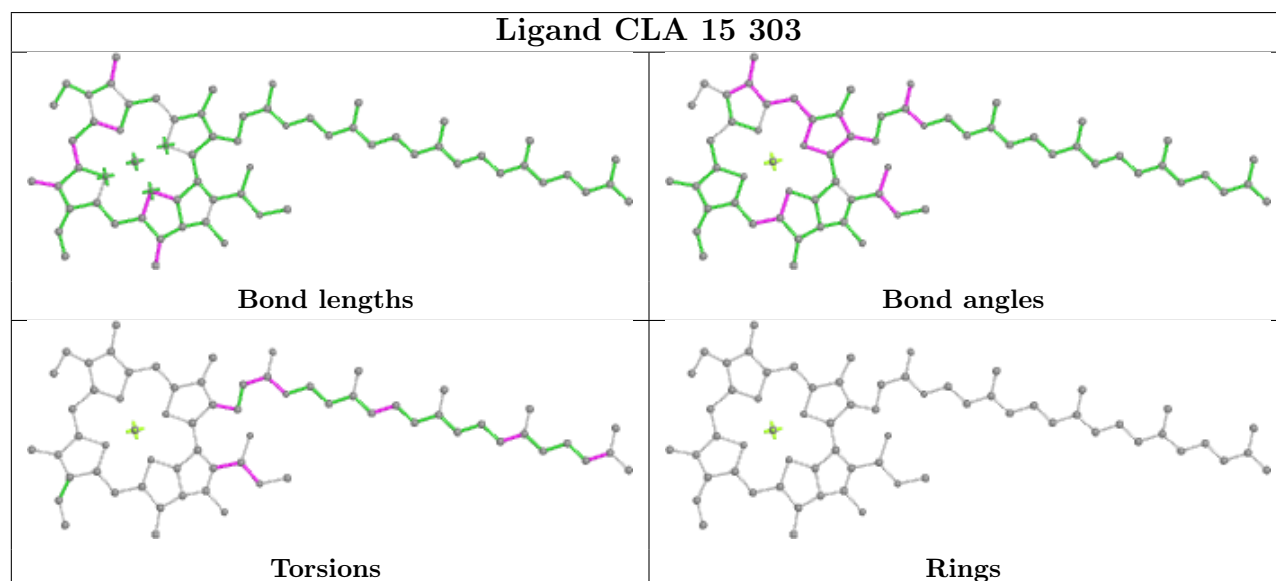
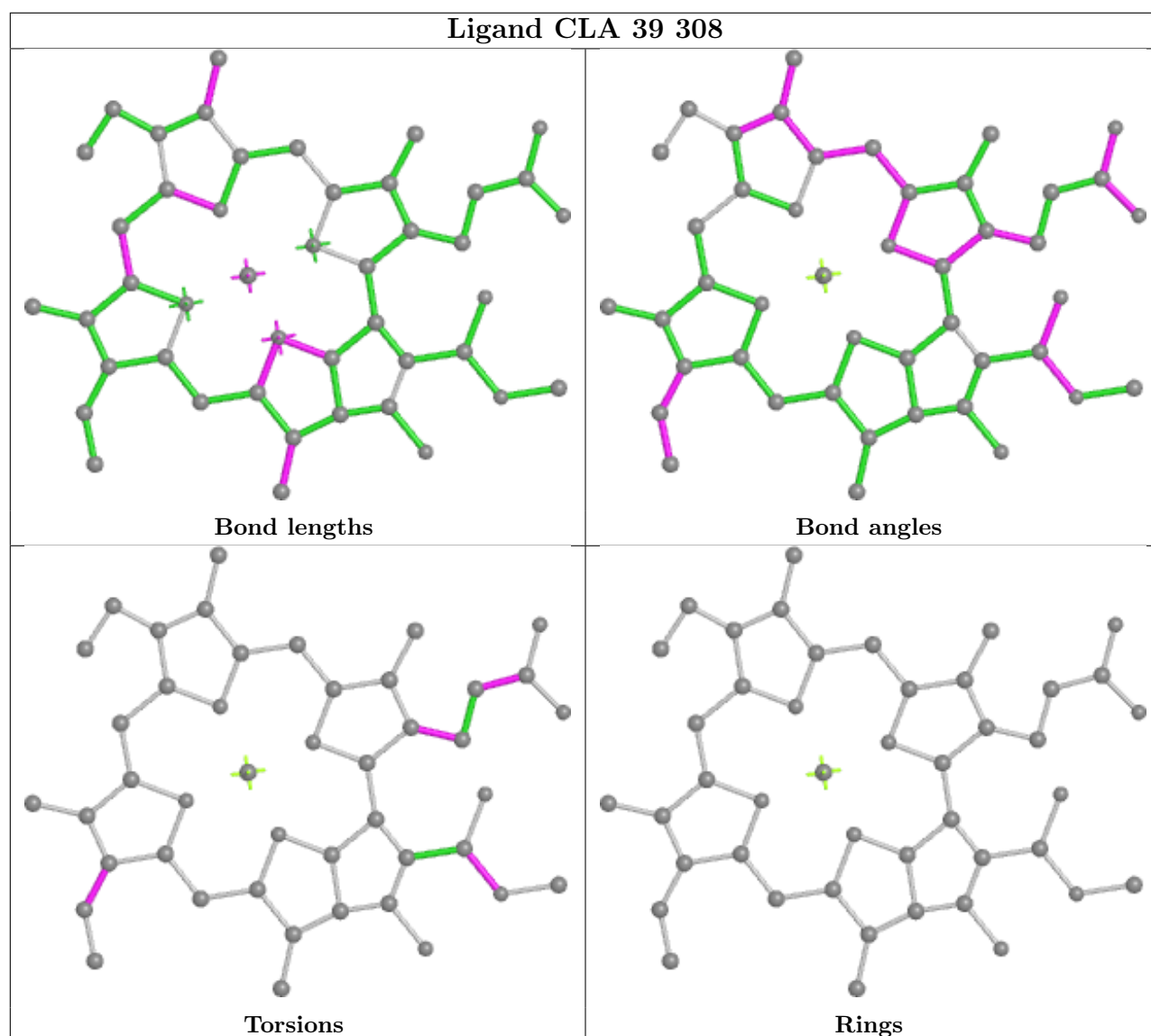


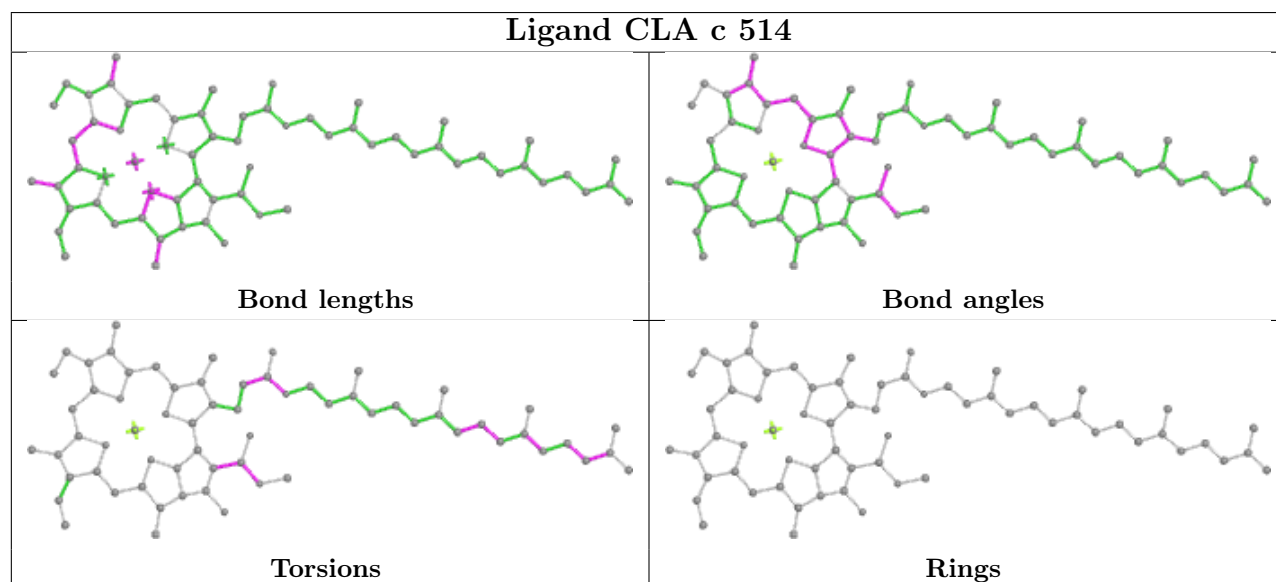
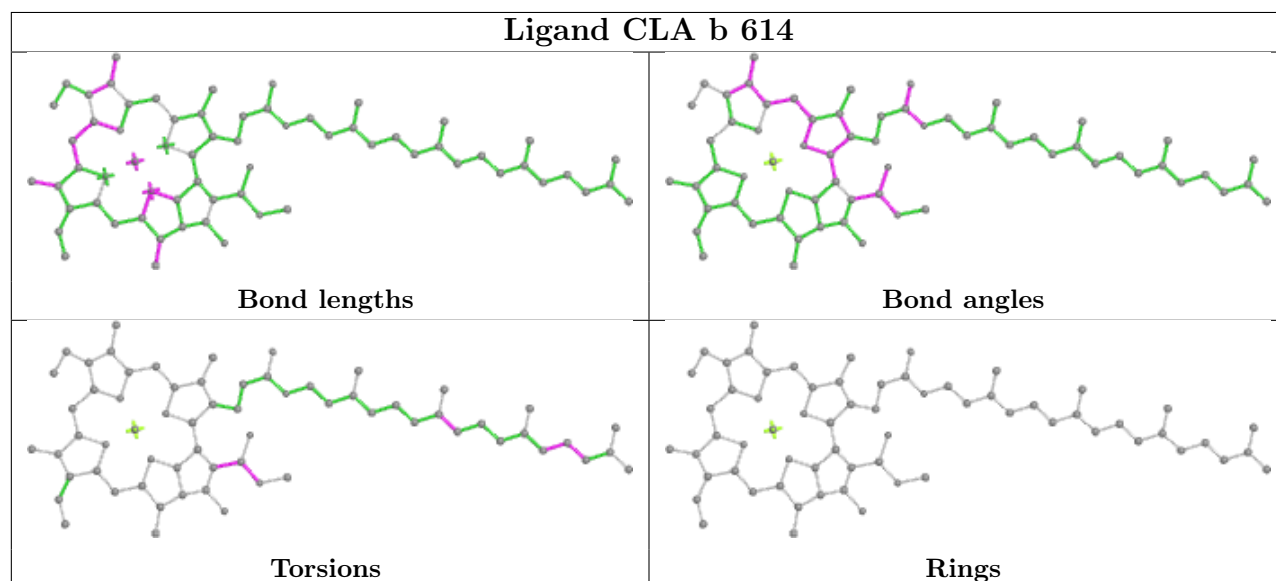
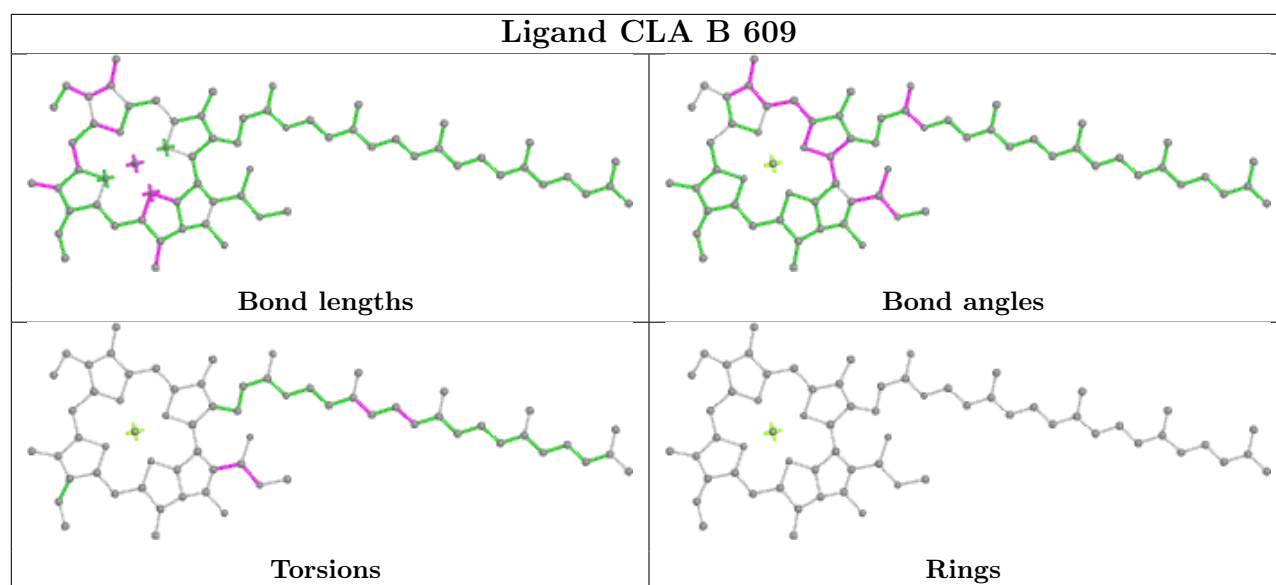


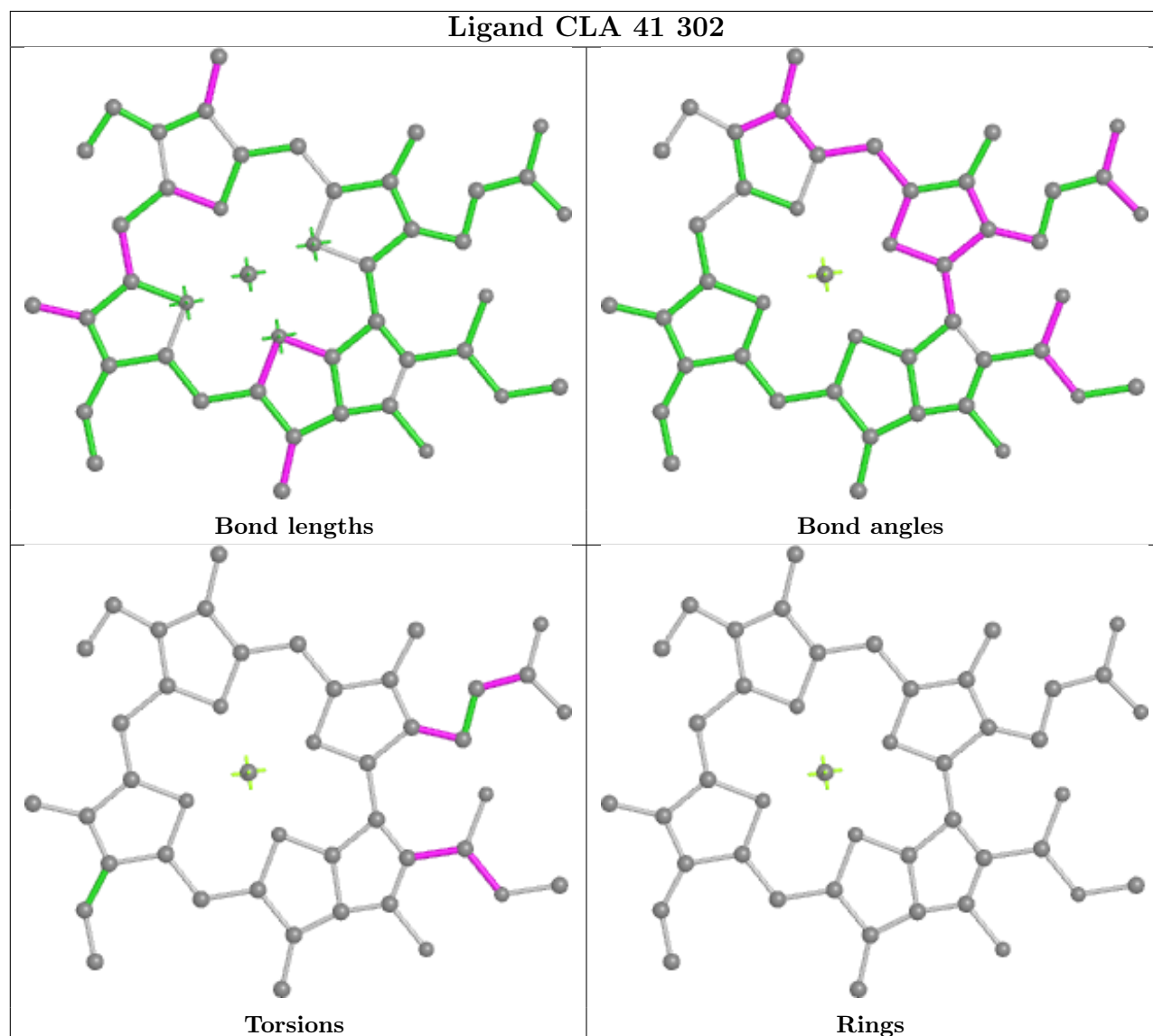
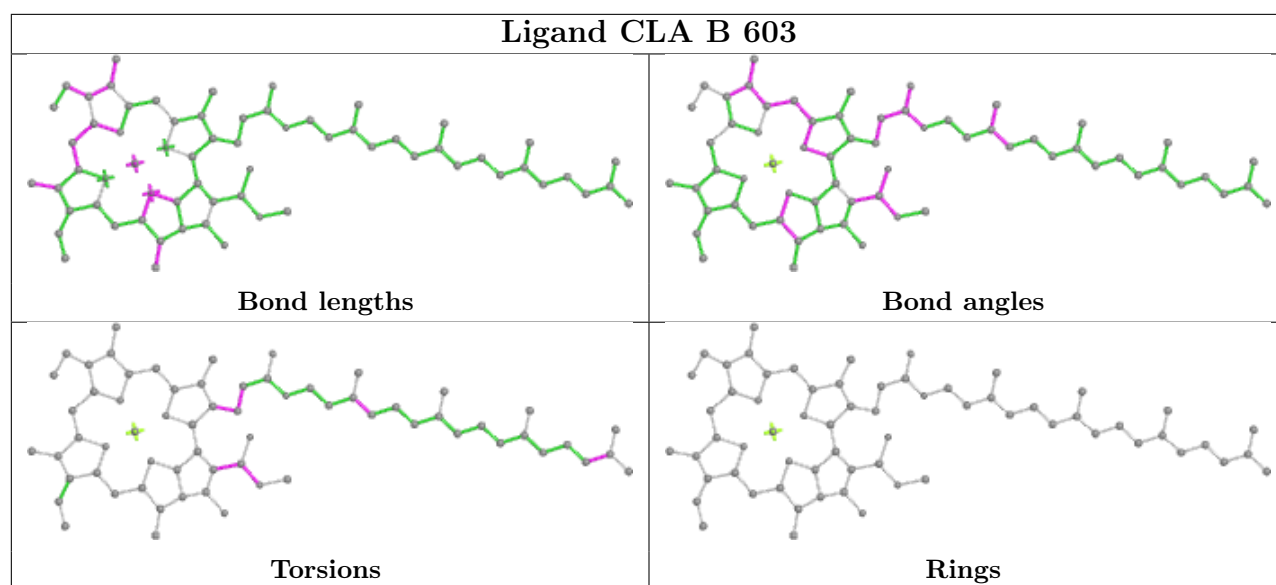


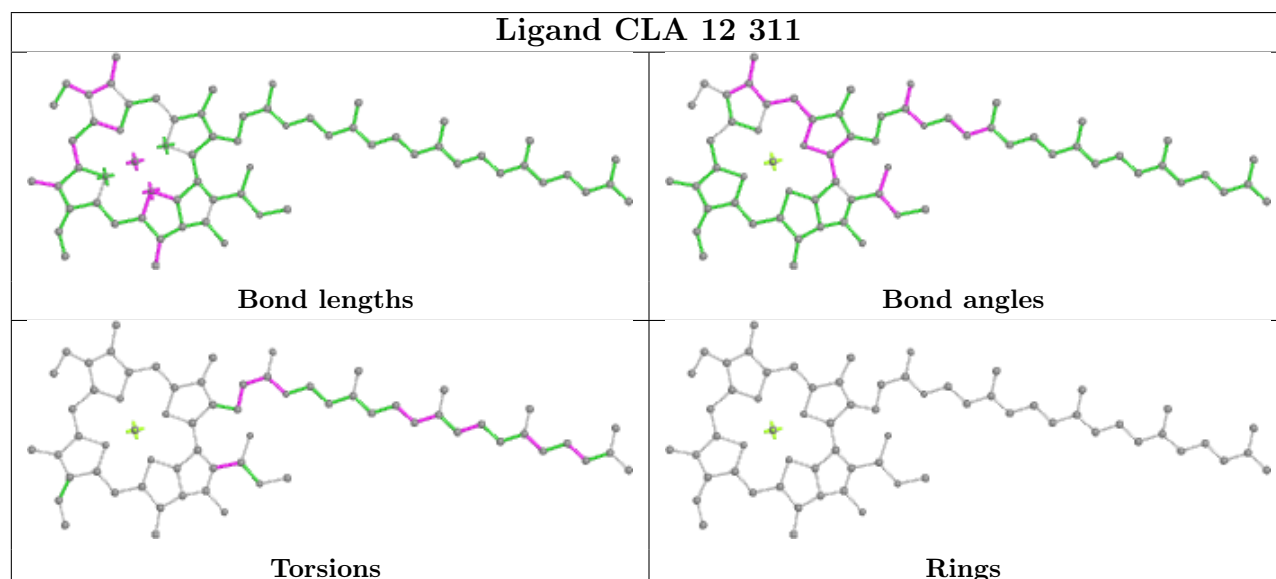
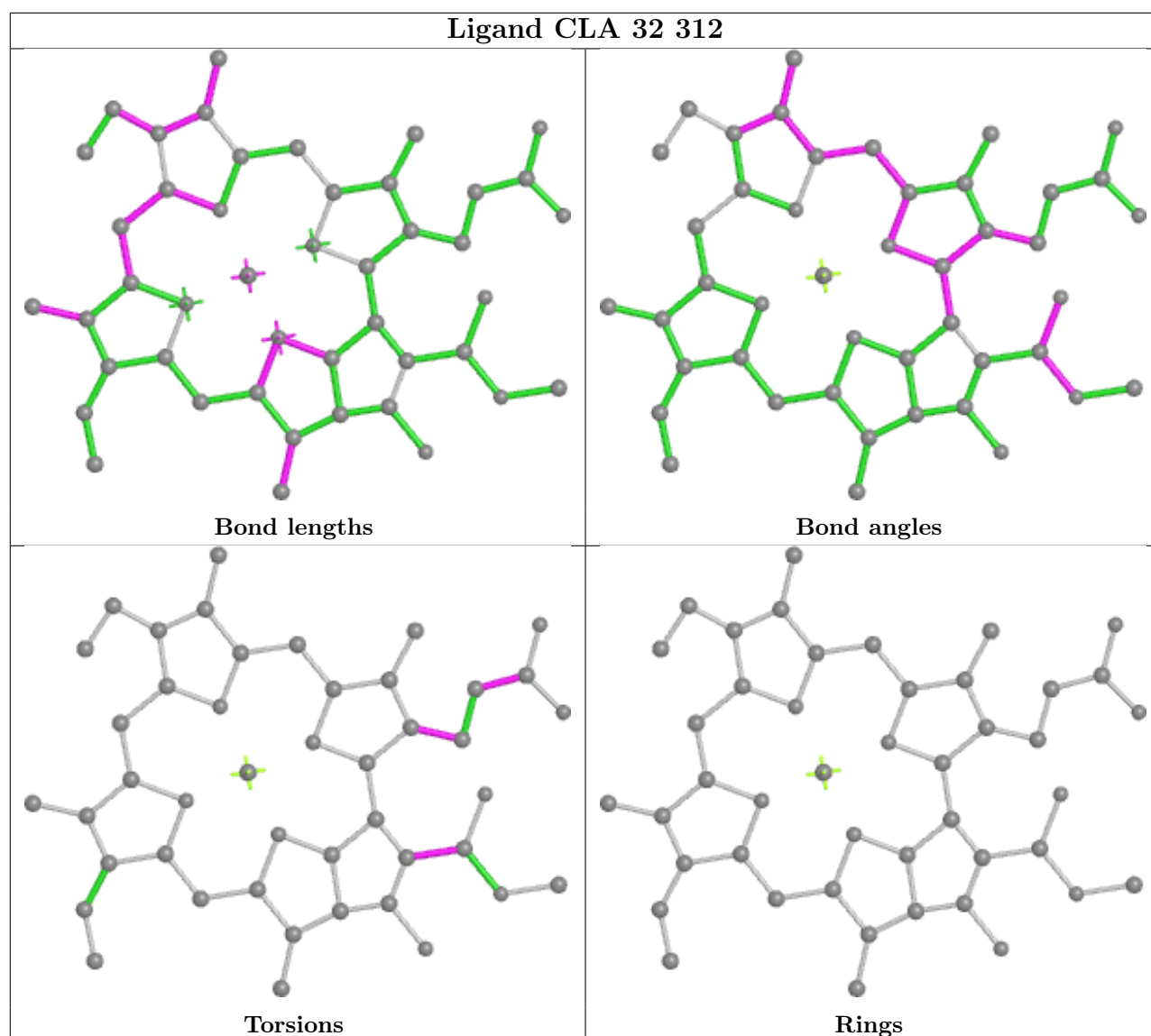


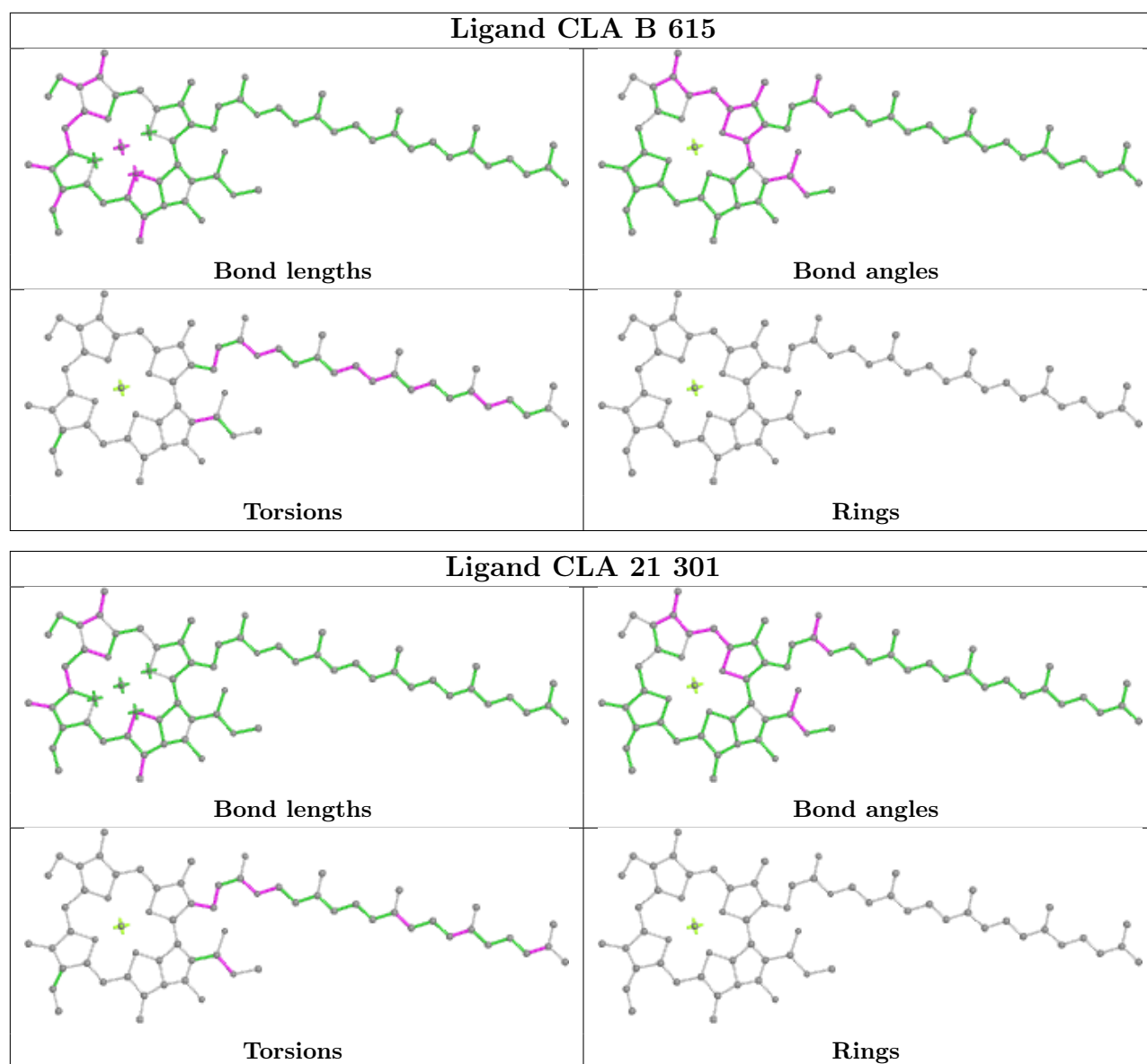


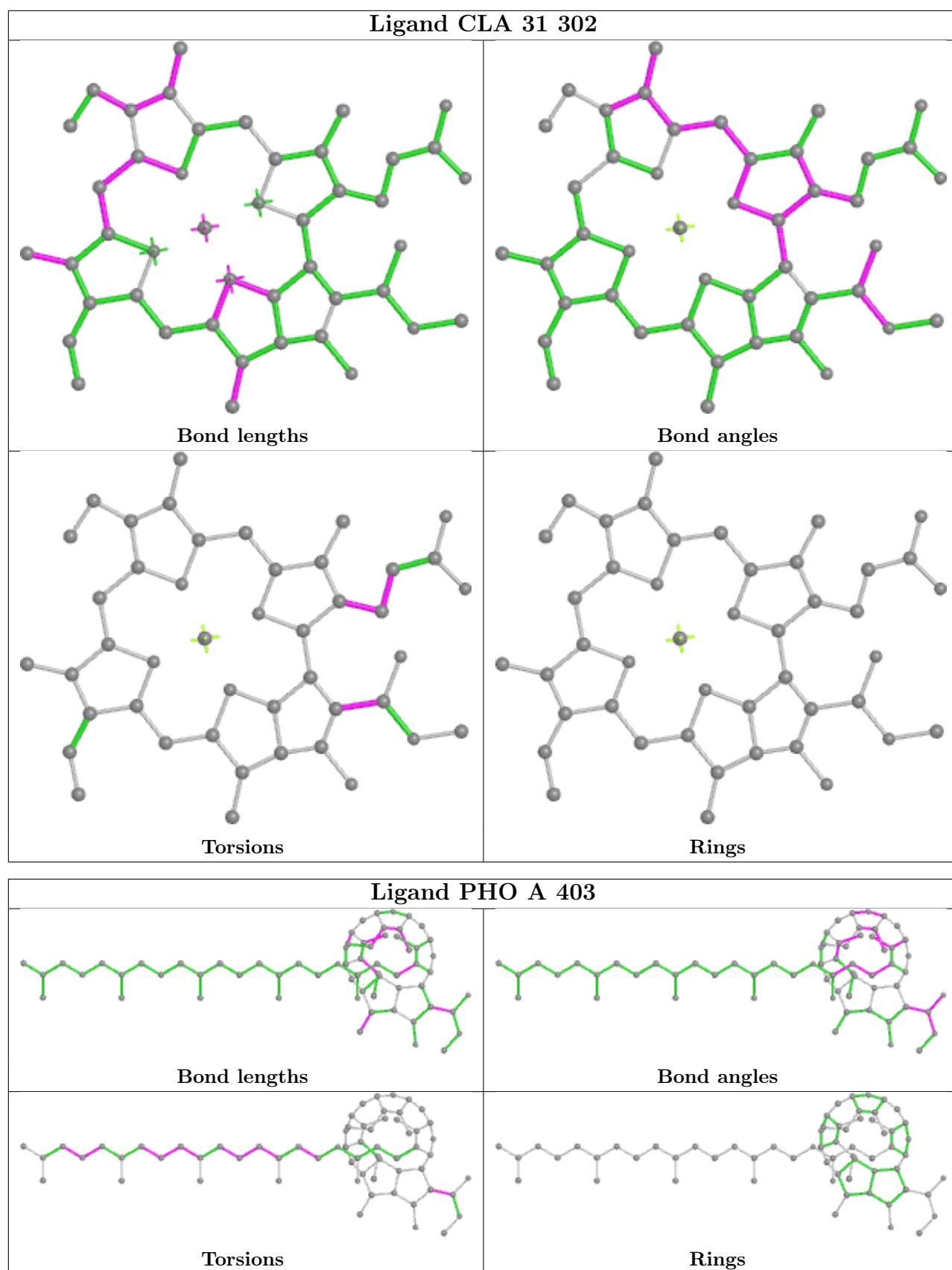


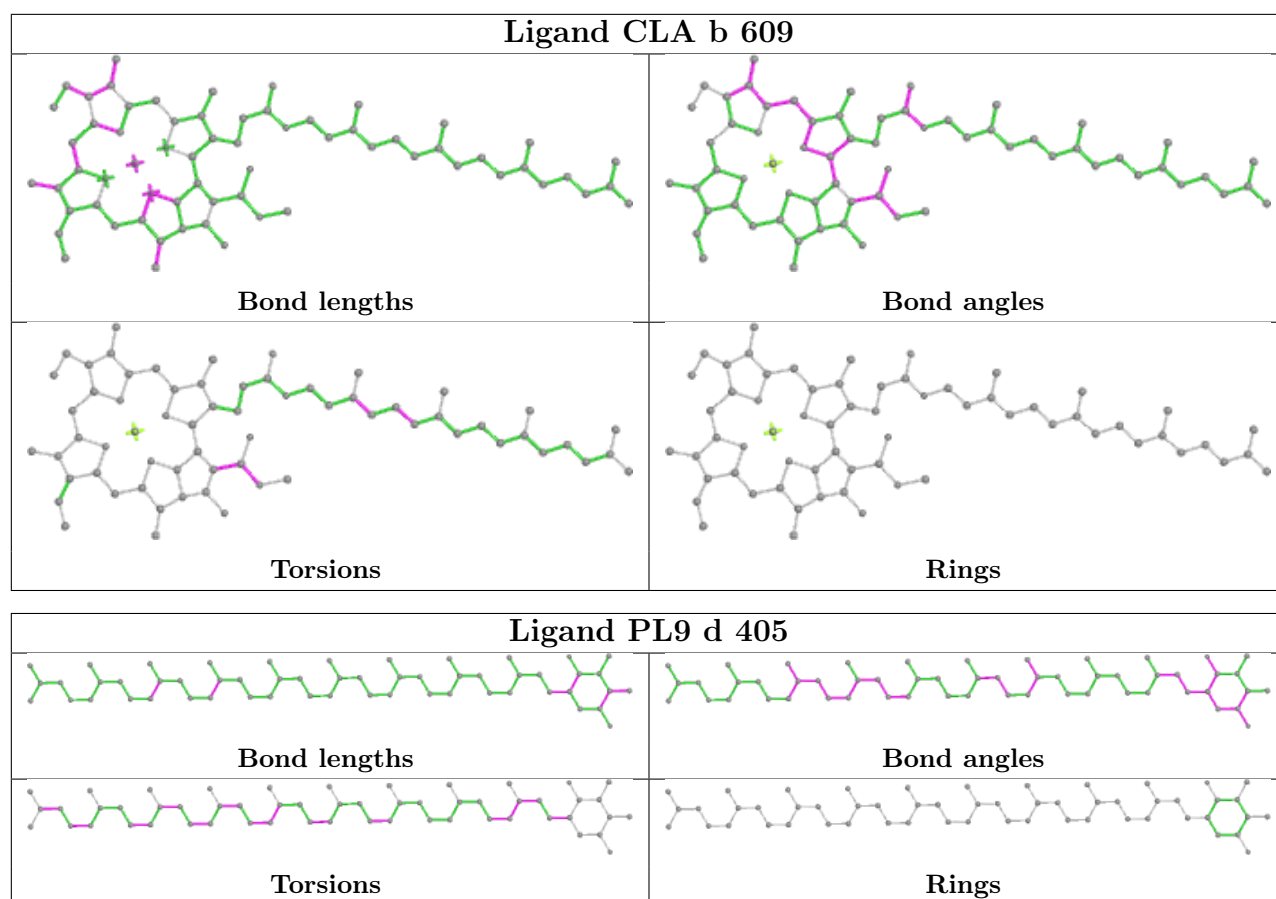


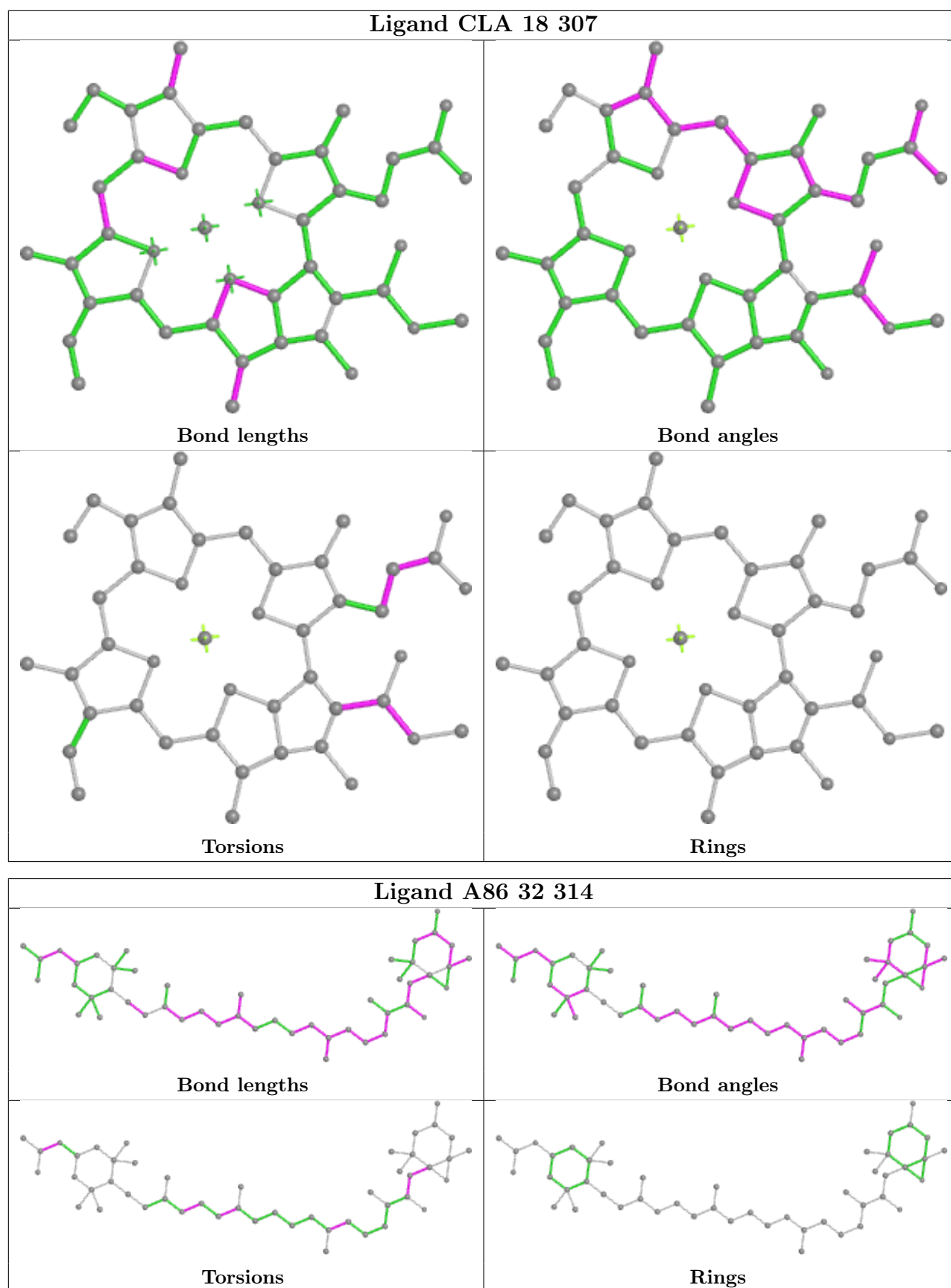


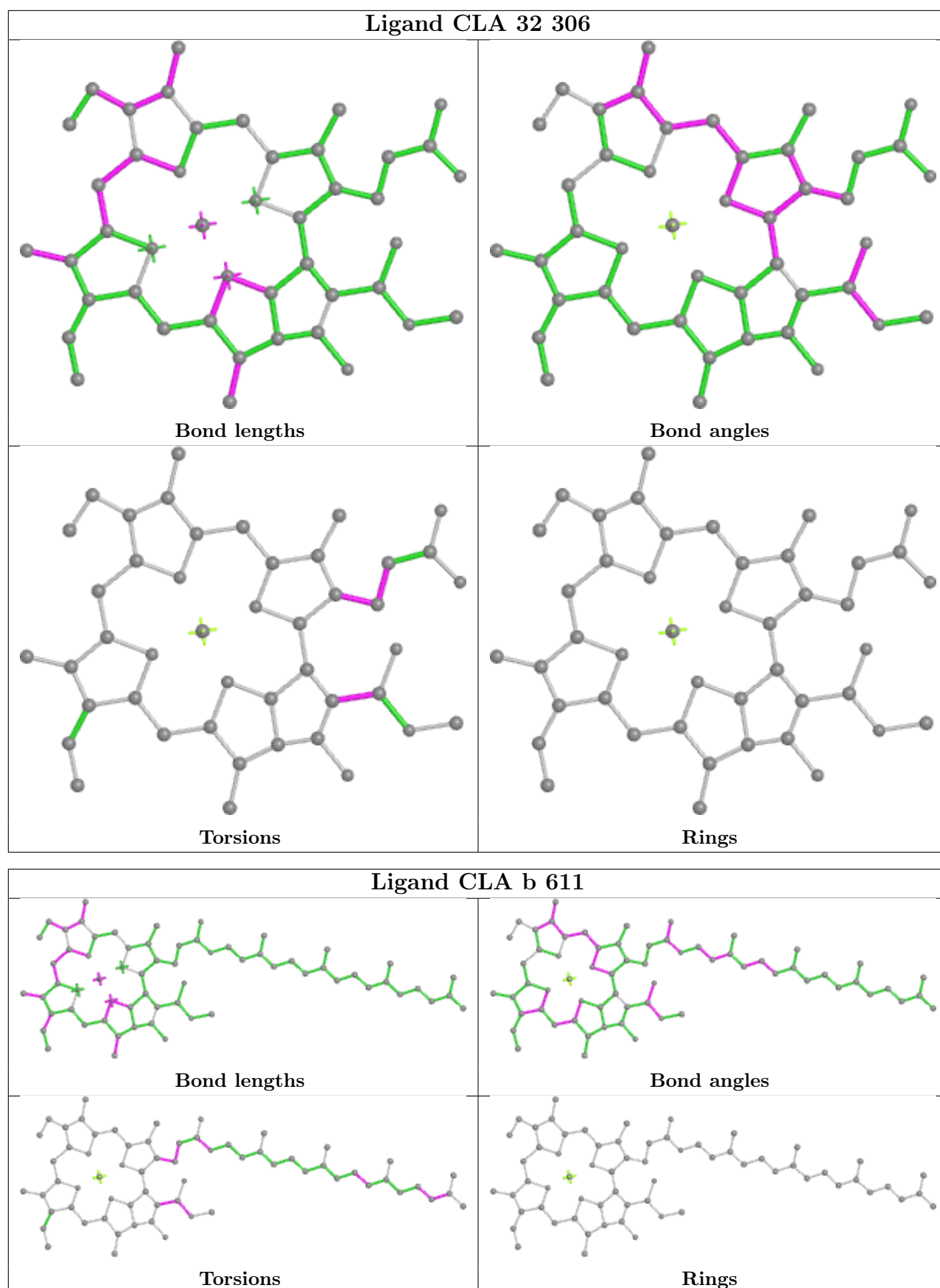


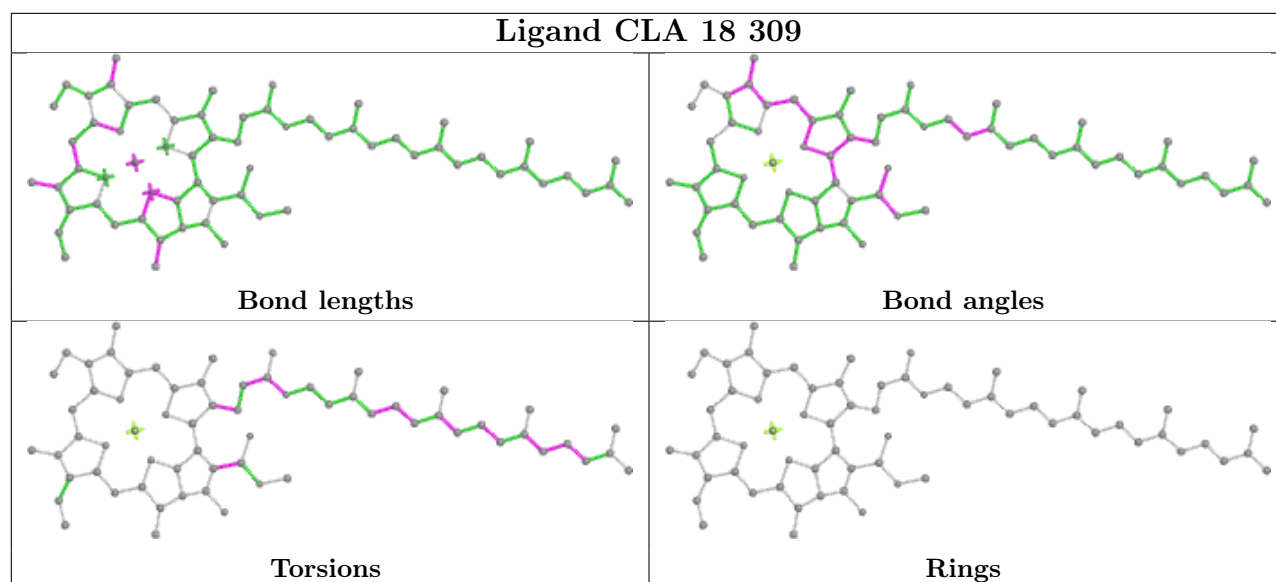
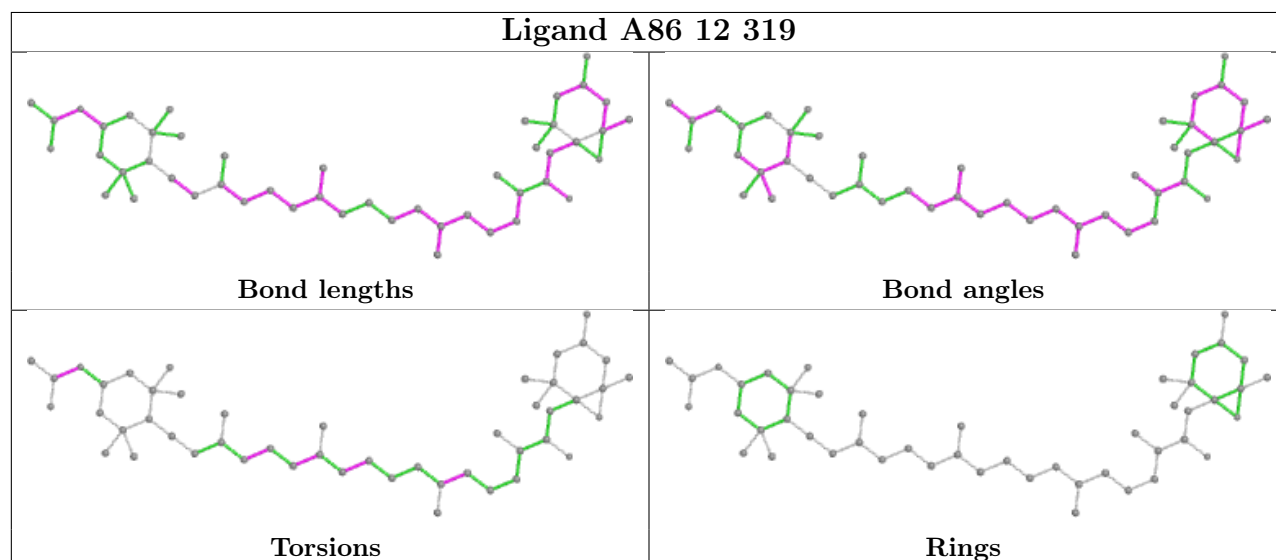
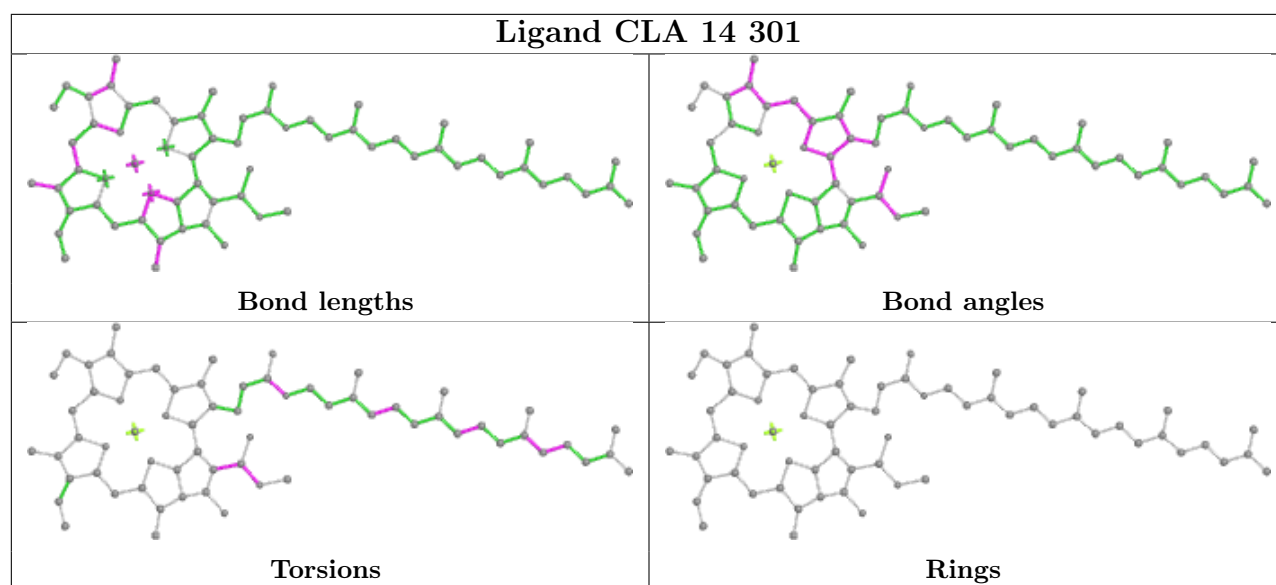


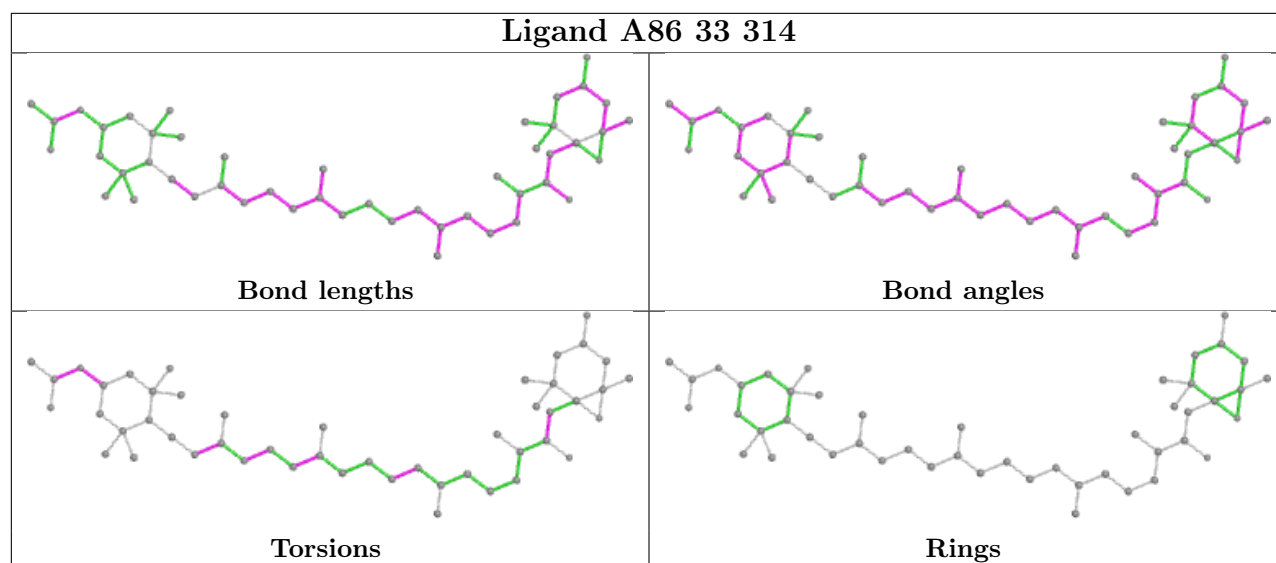
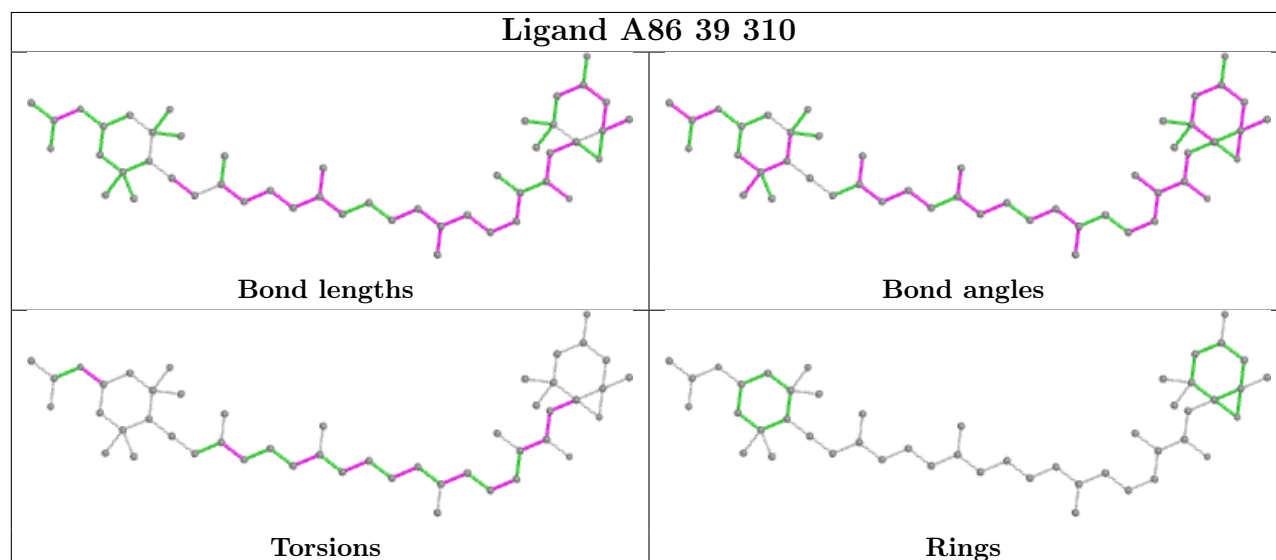
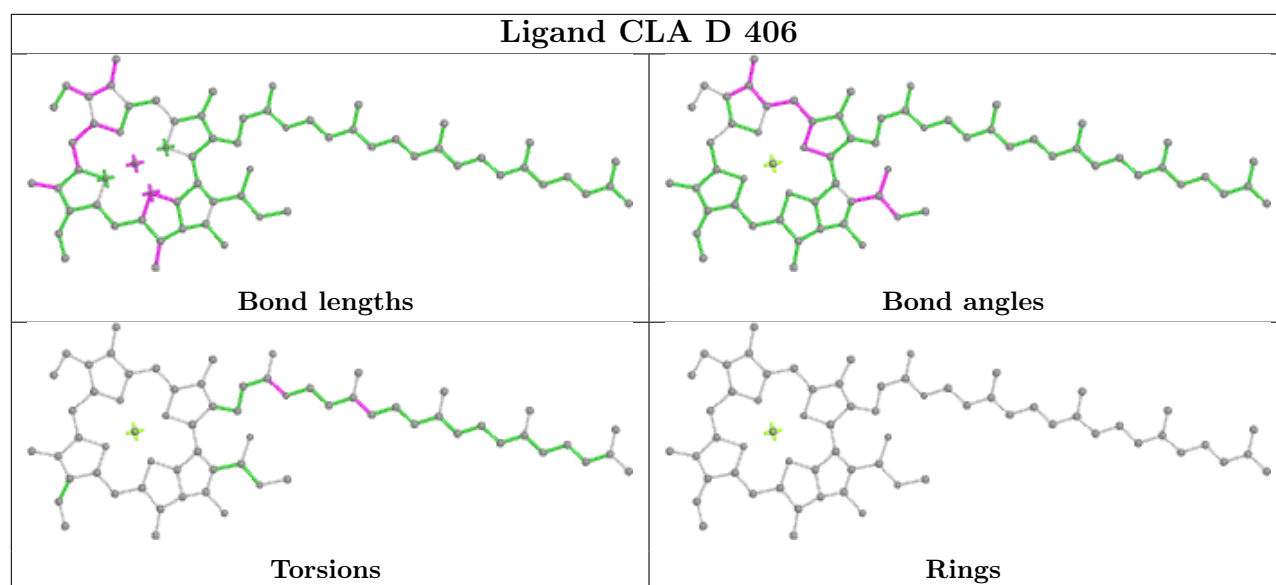


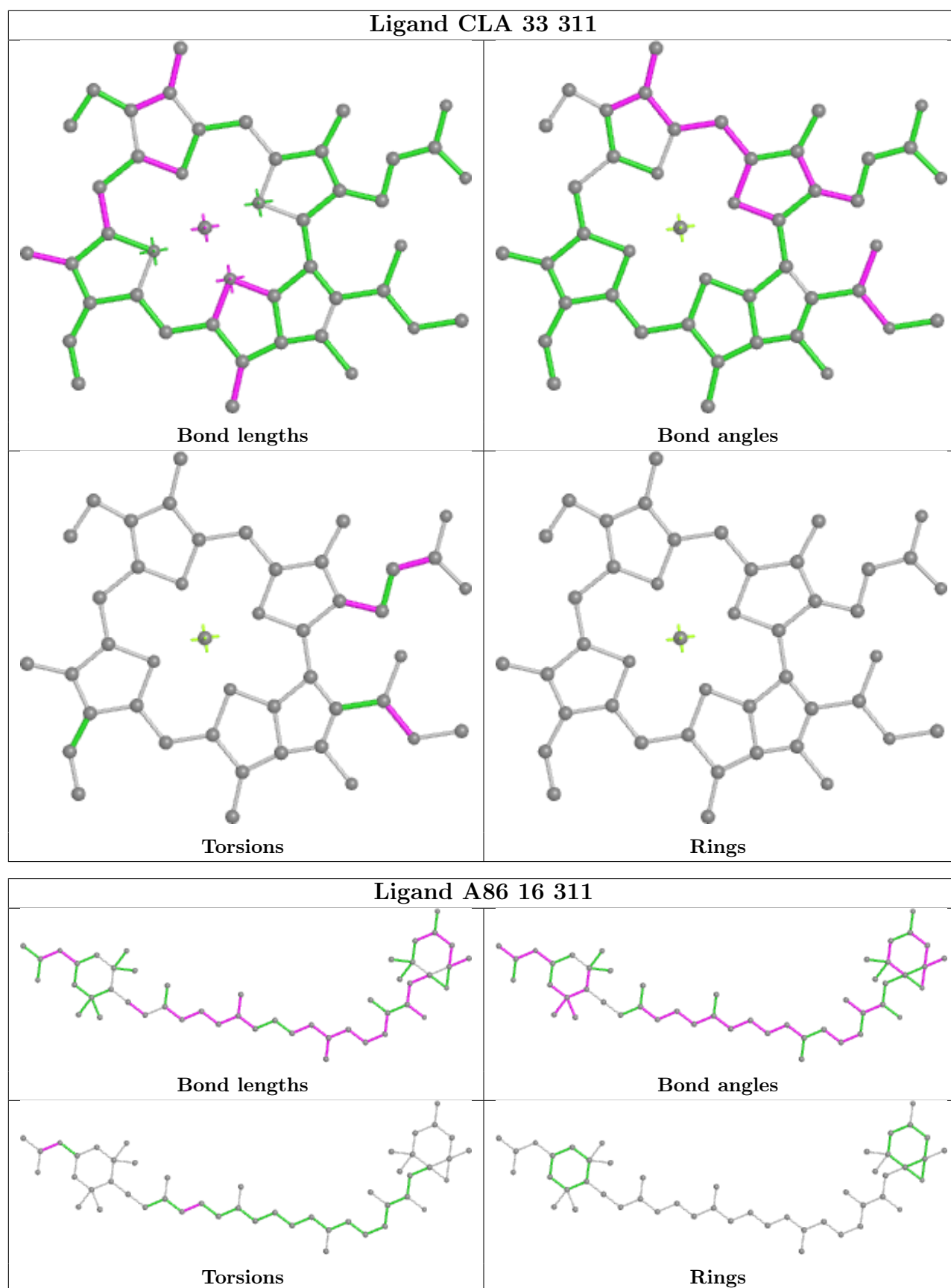


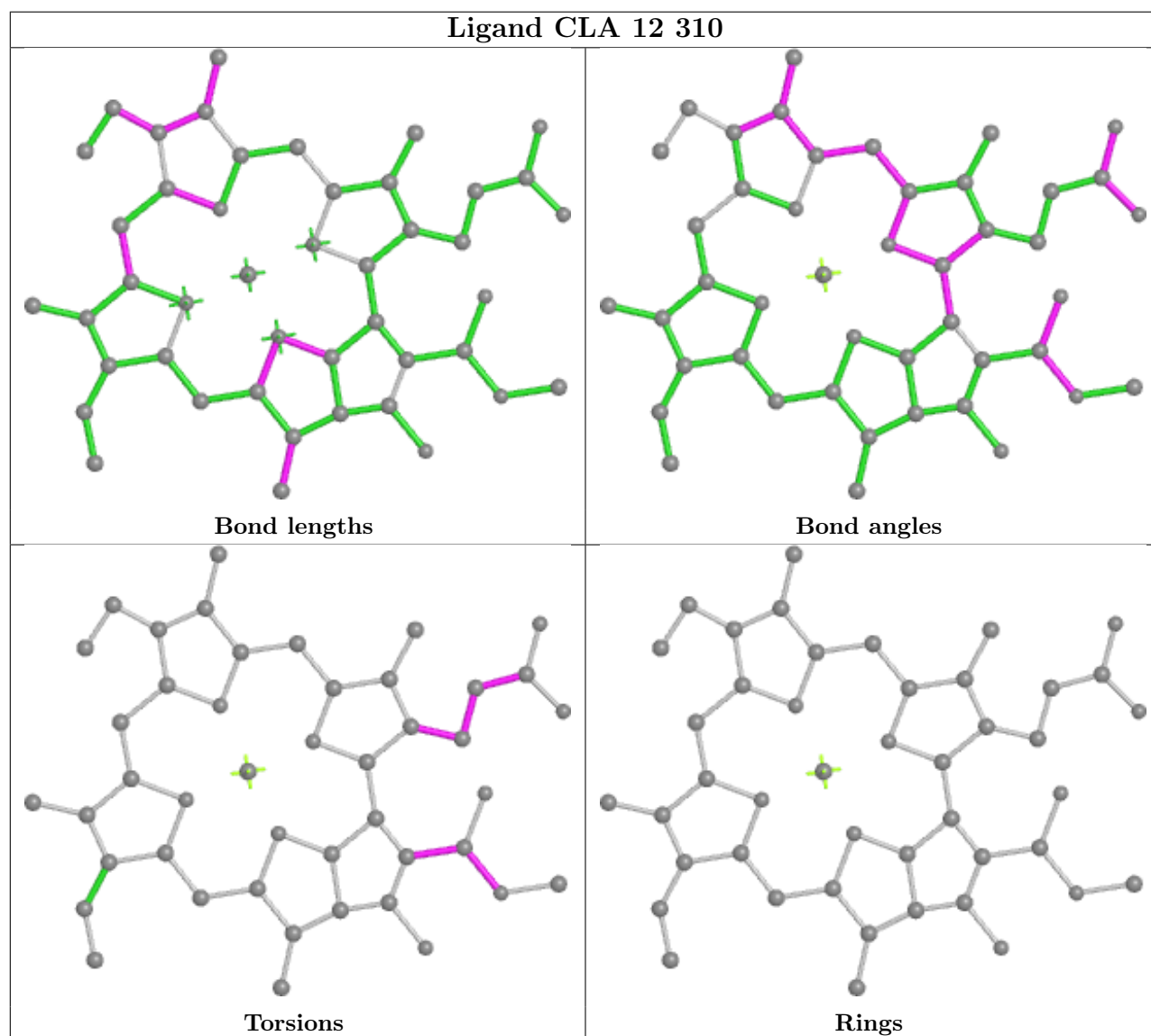
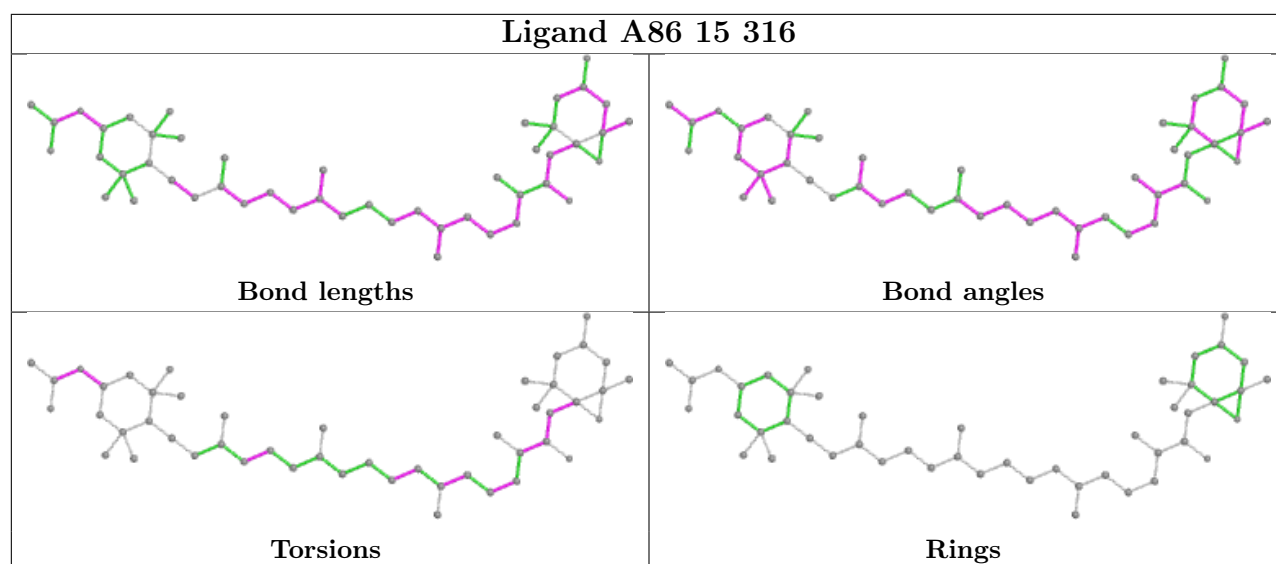


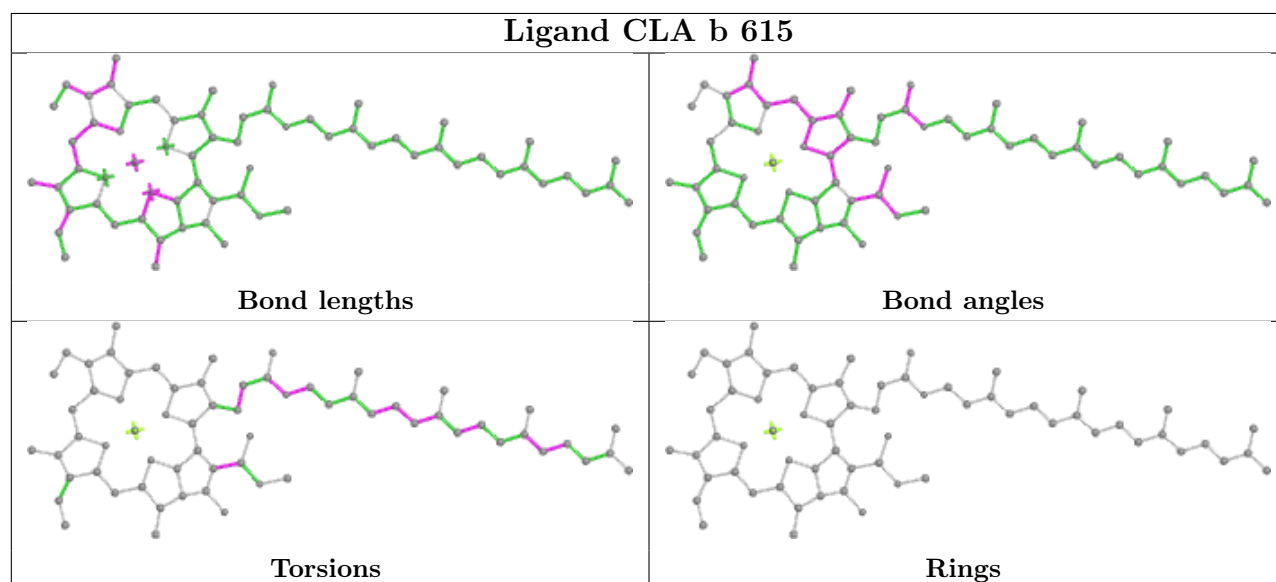
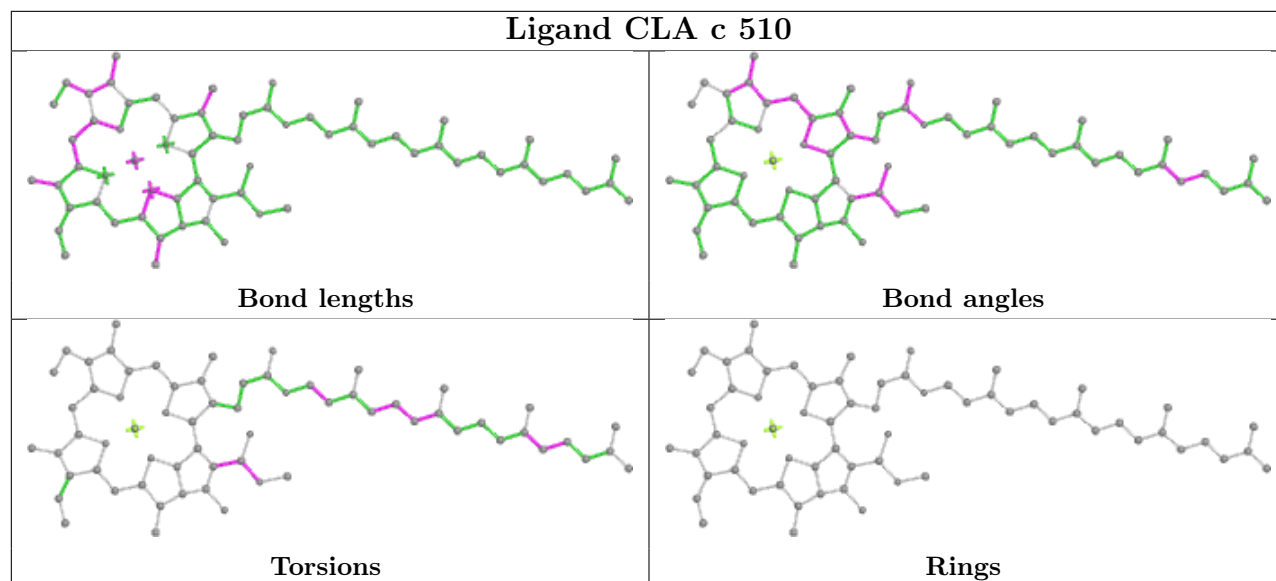
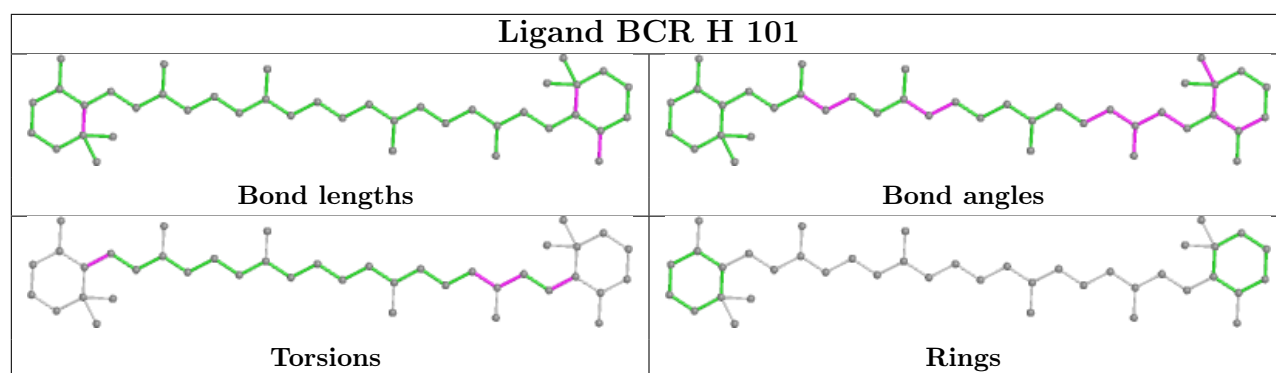


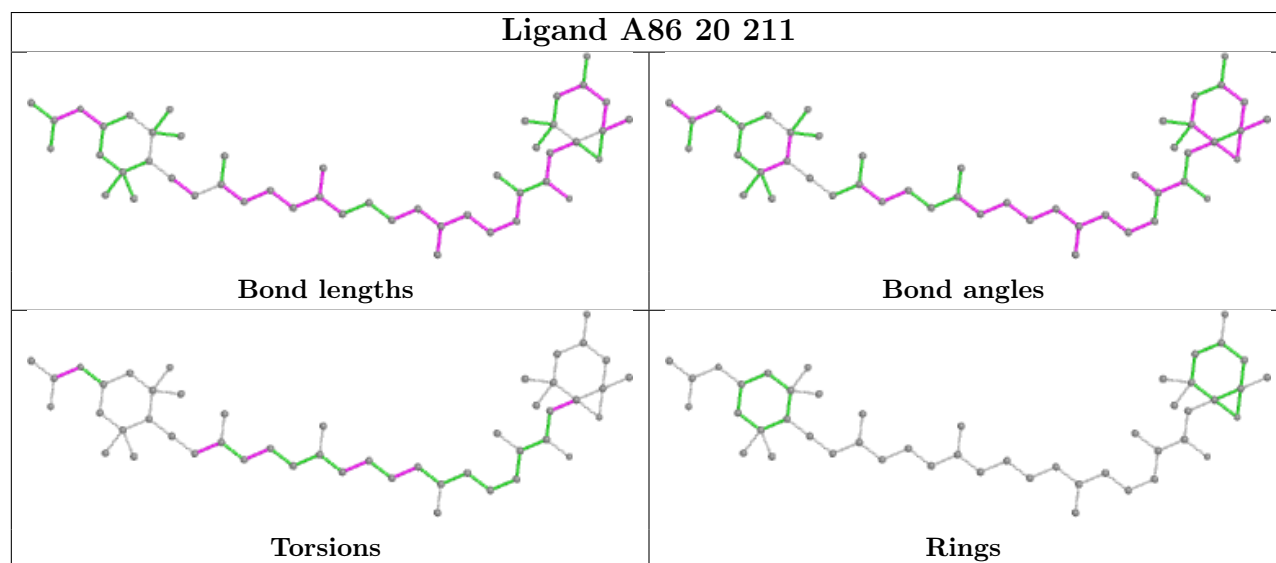
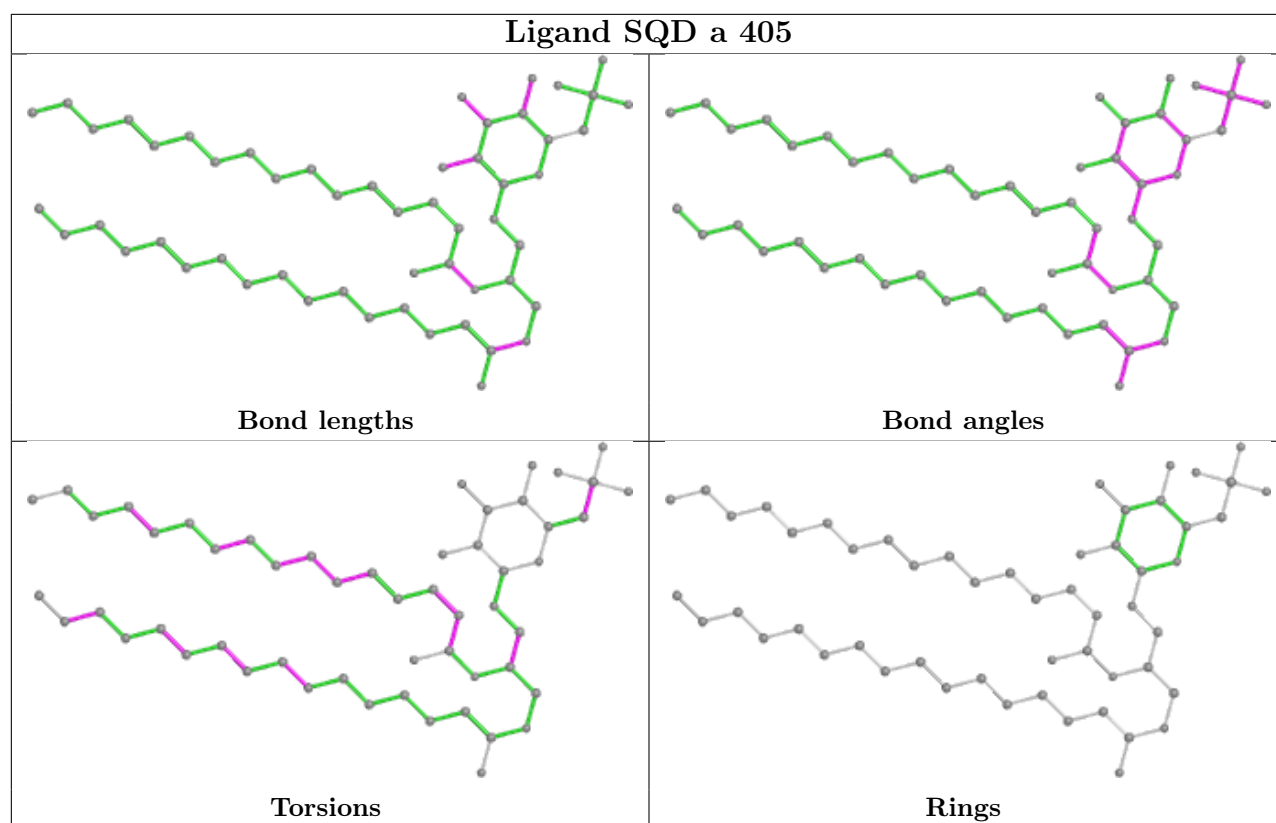


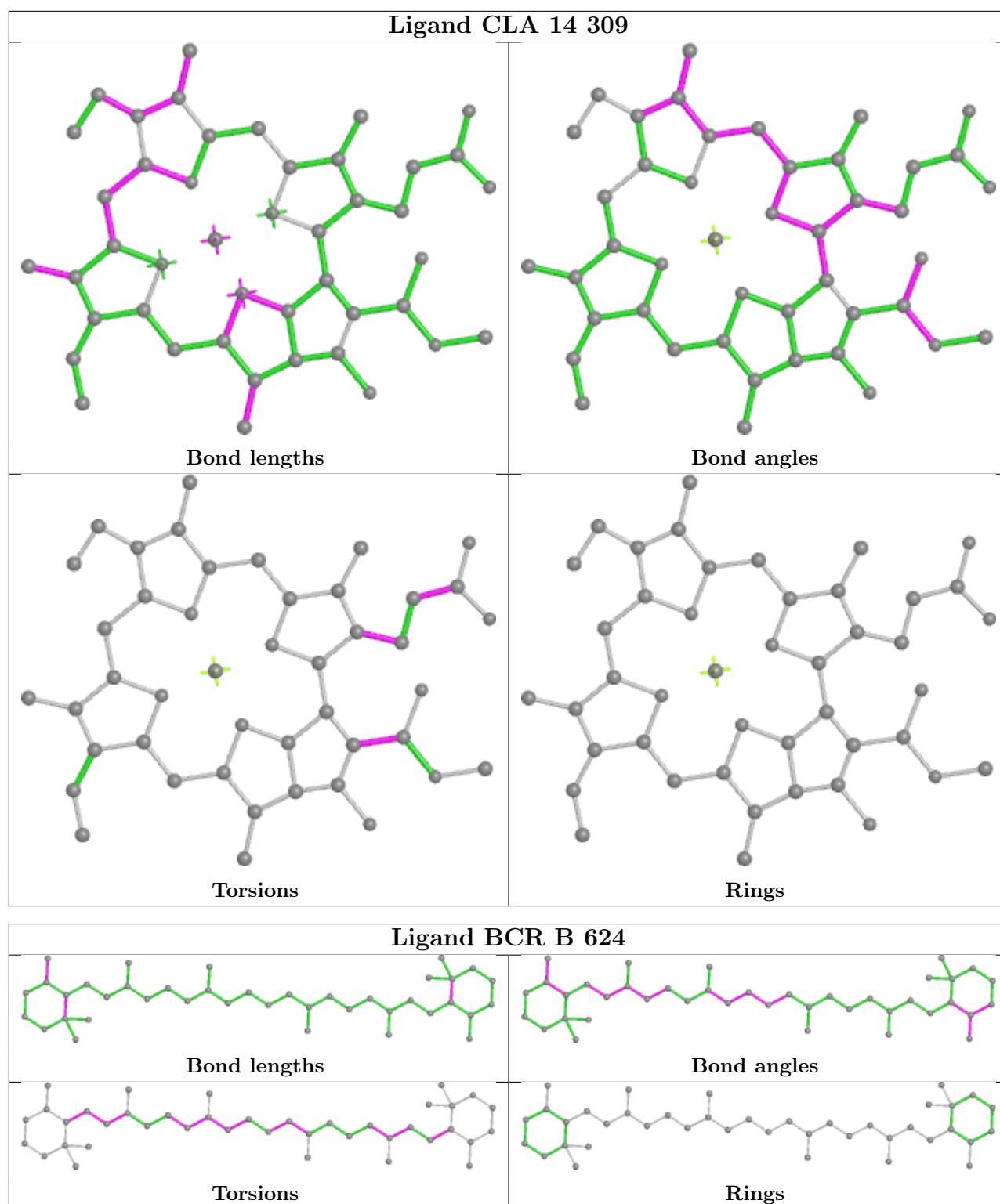


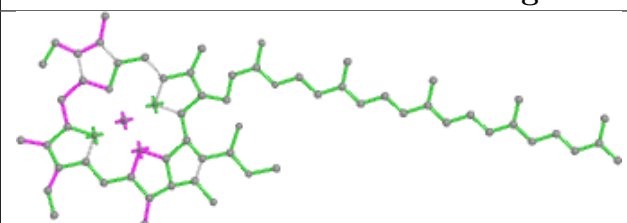
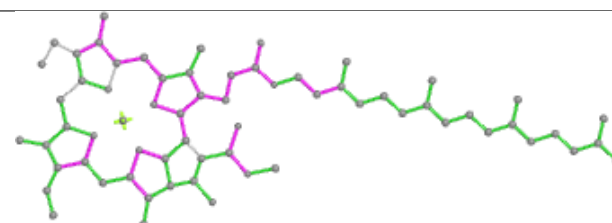
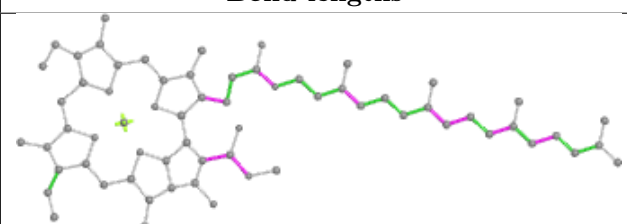
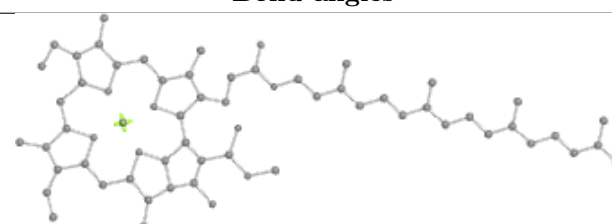


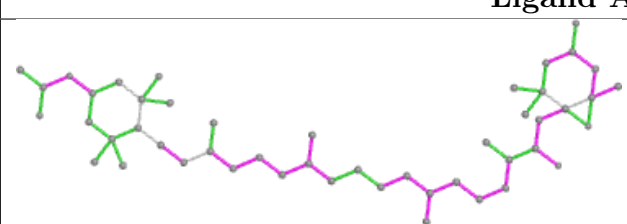
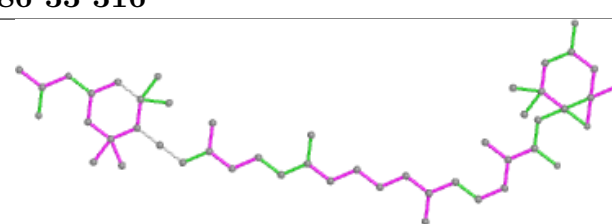
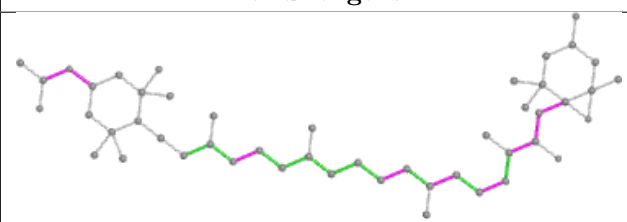
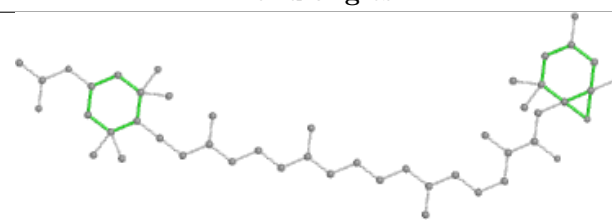


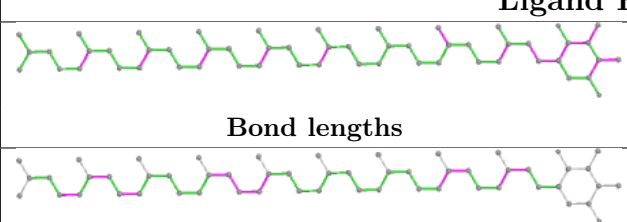
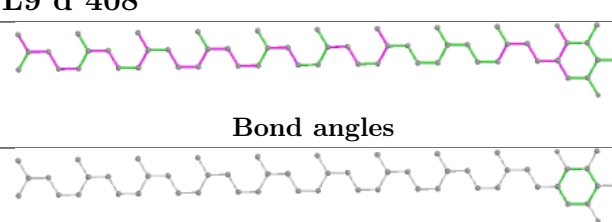
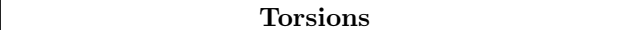



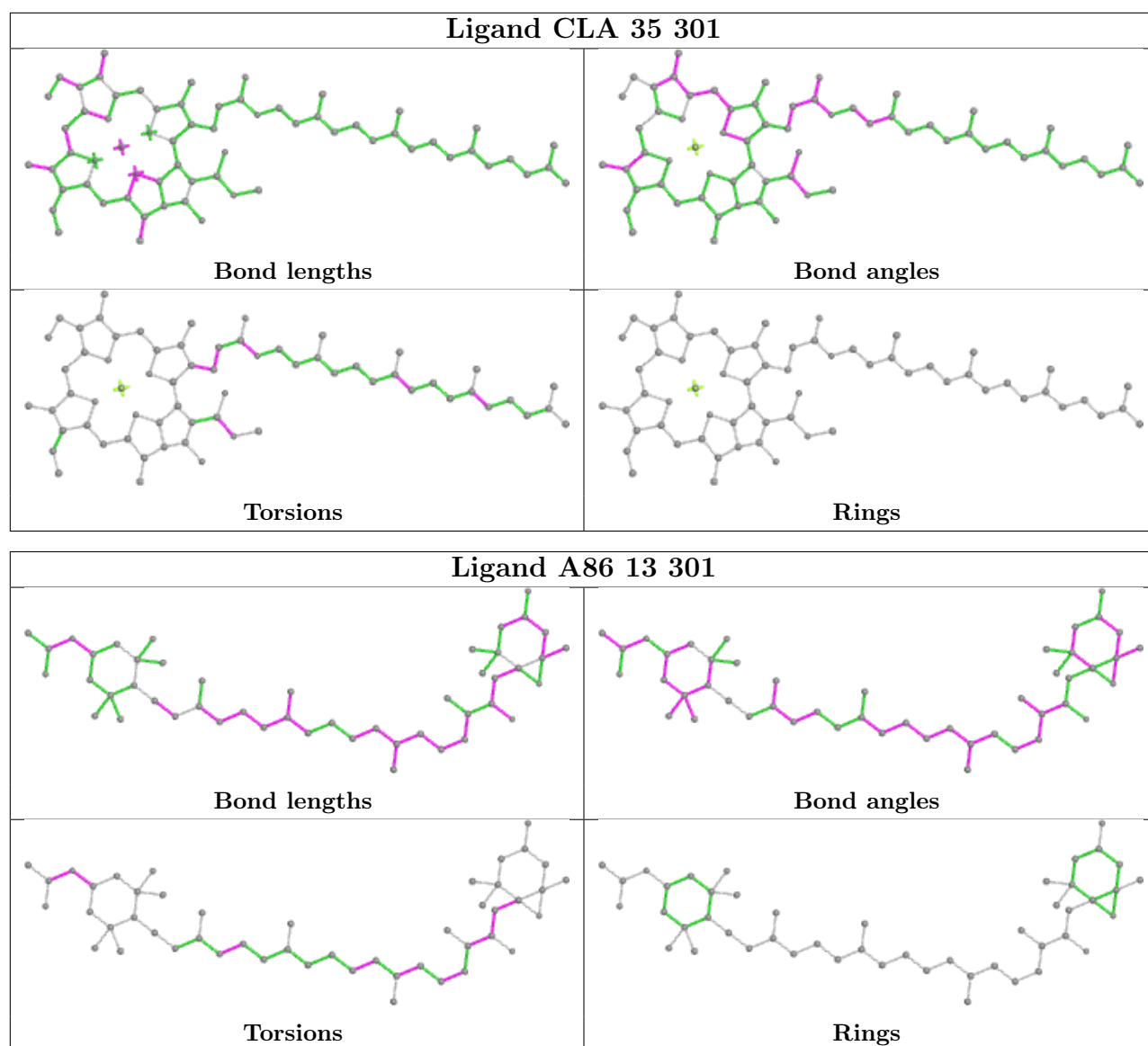


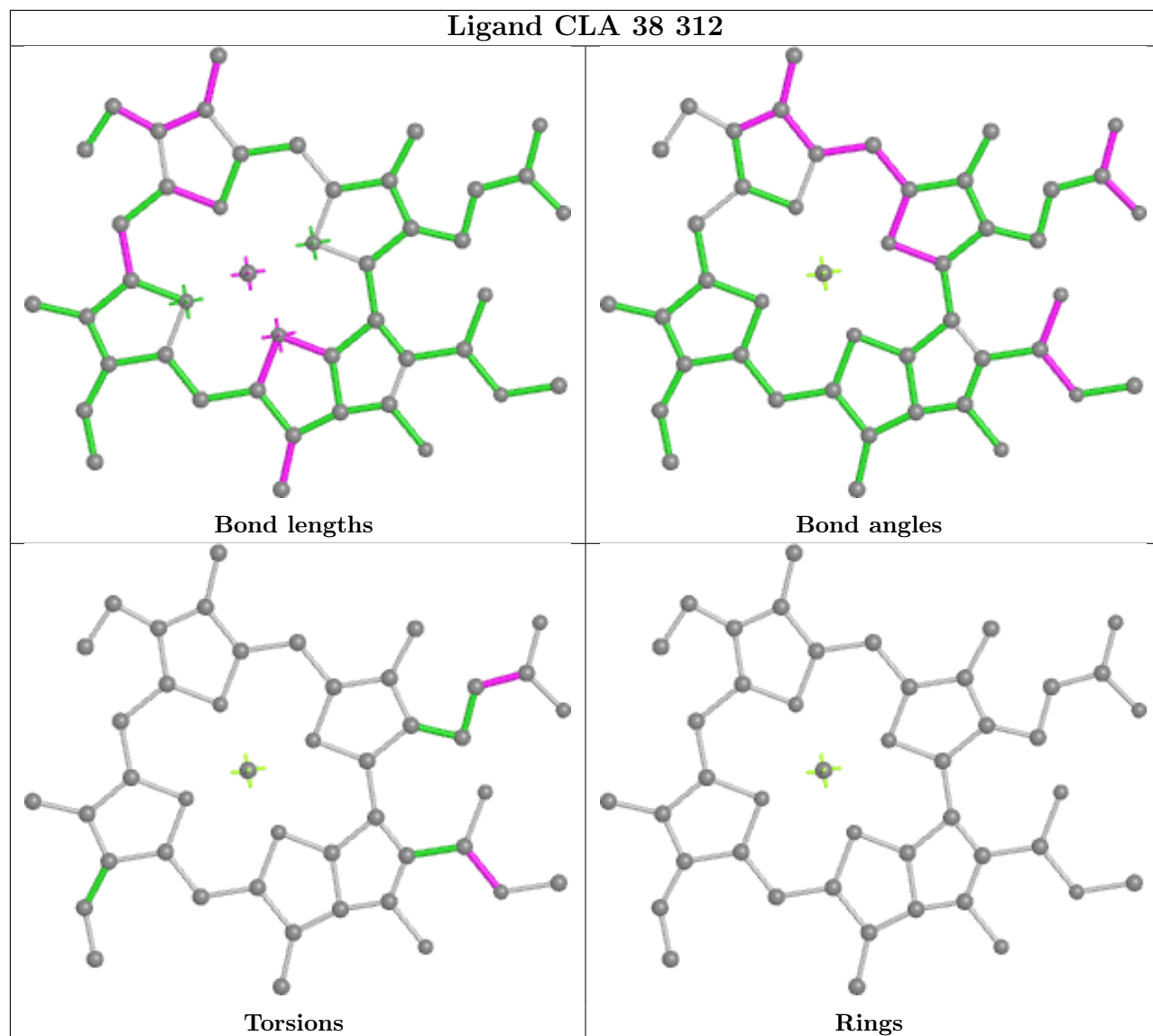


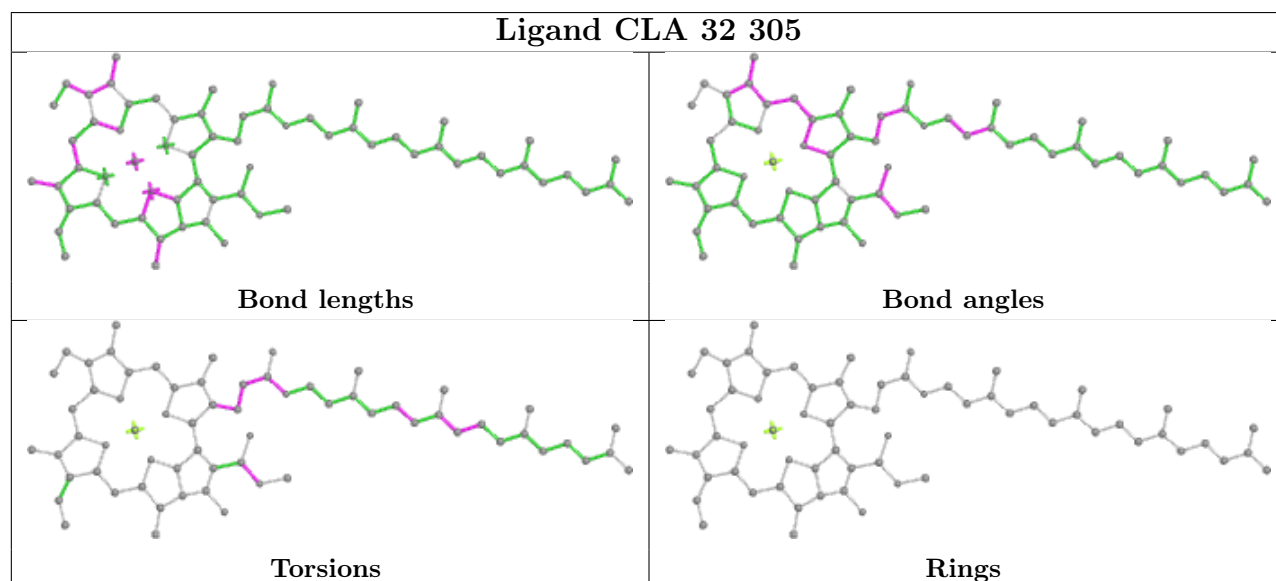
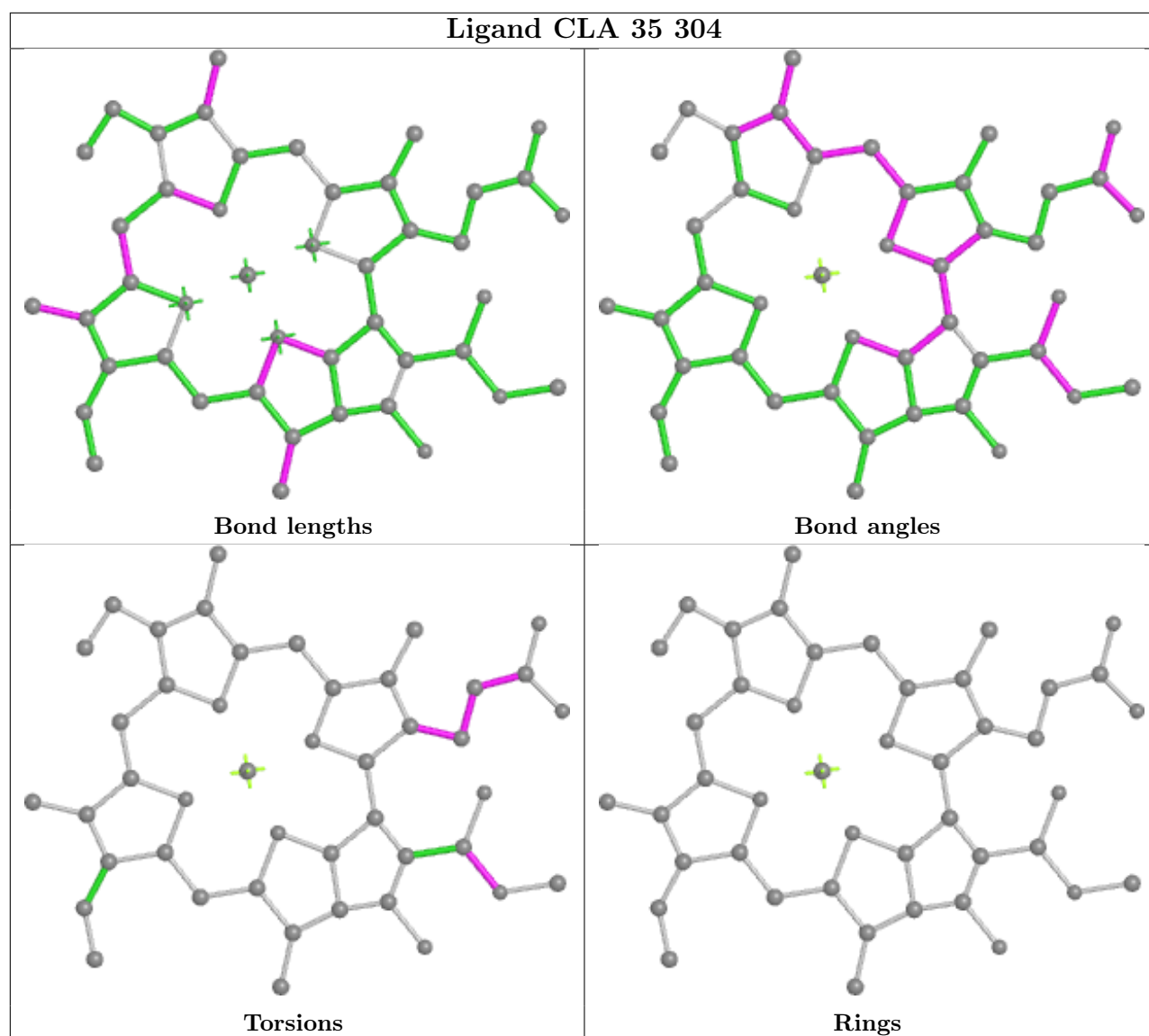
Ligand CLA B 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

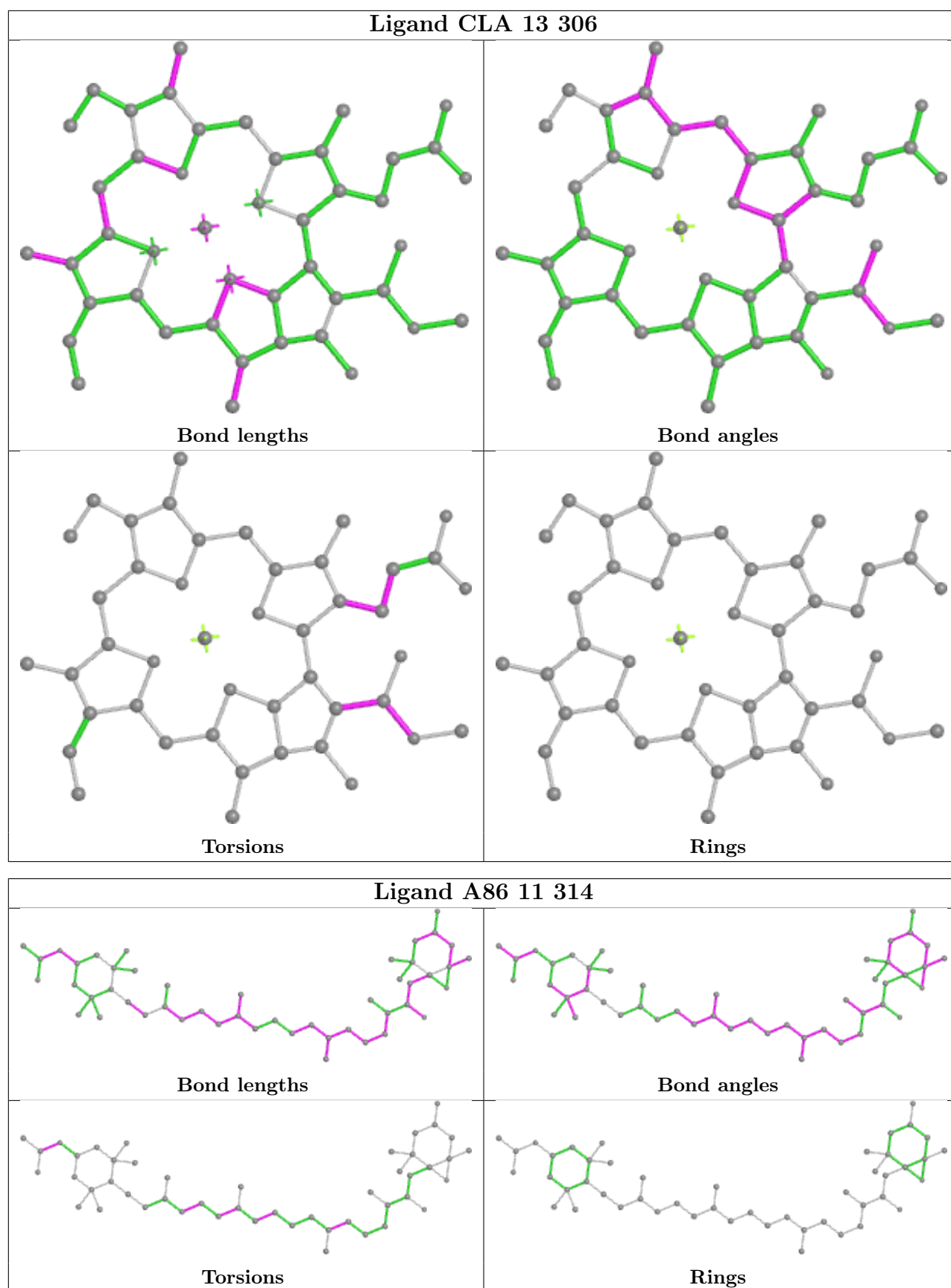
Ligand A86 33 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

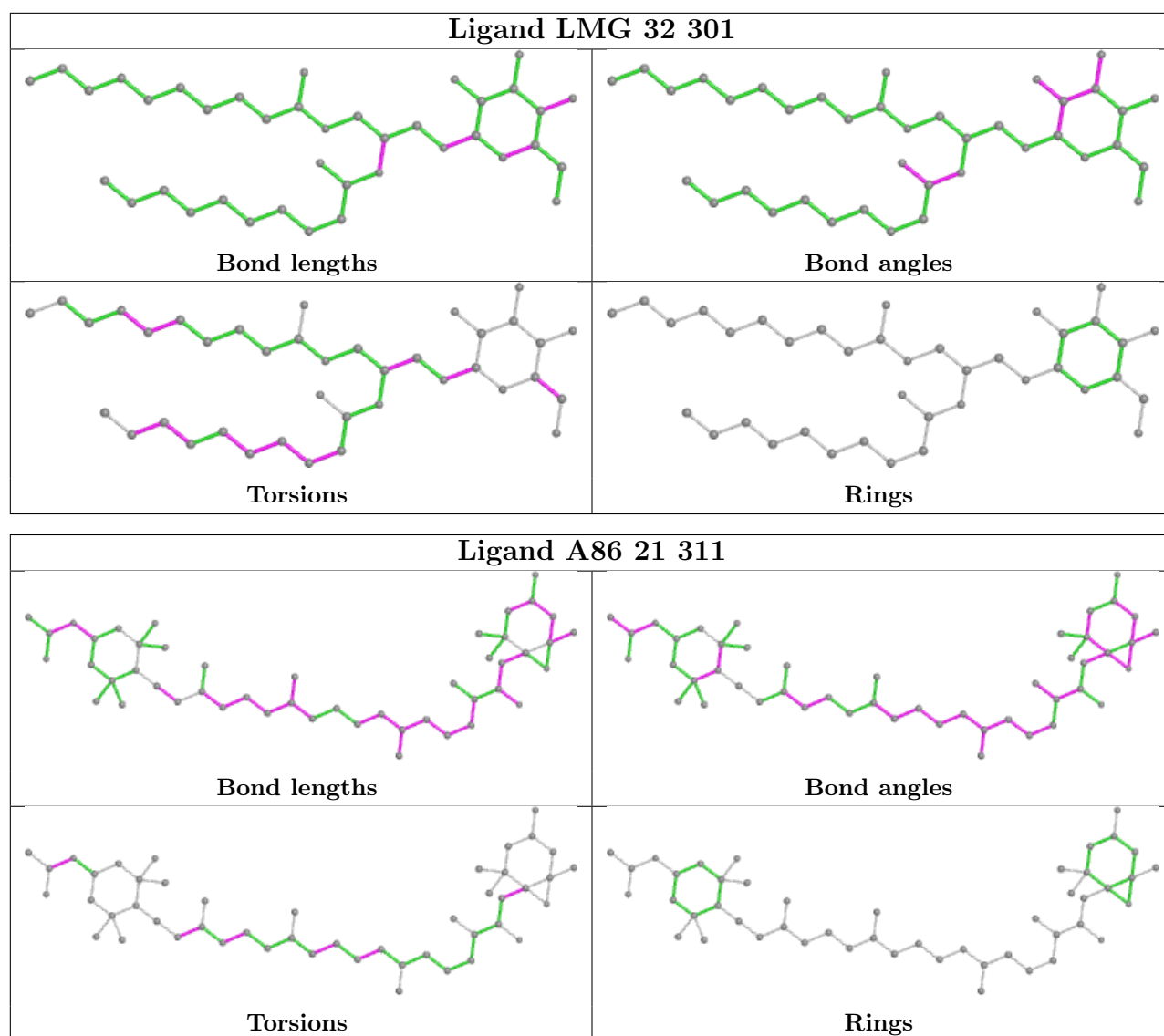
Ligand PL9 d 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

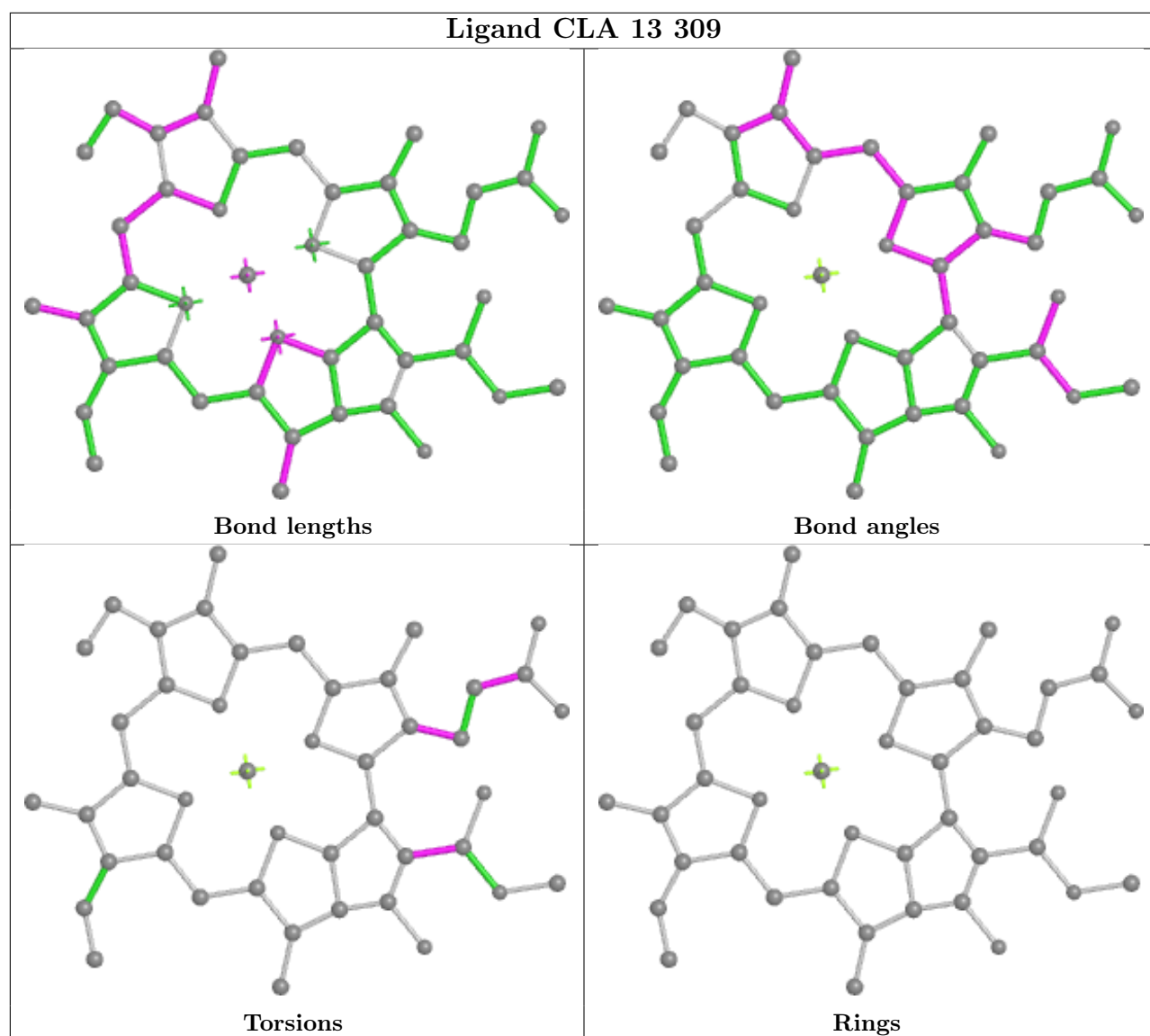


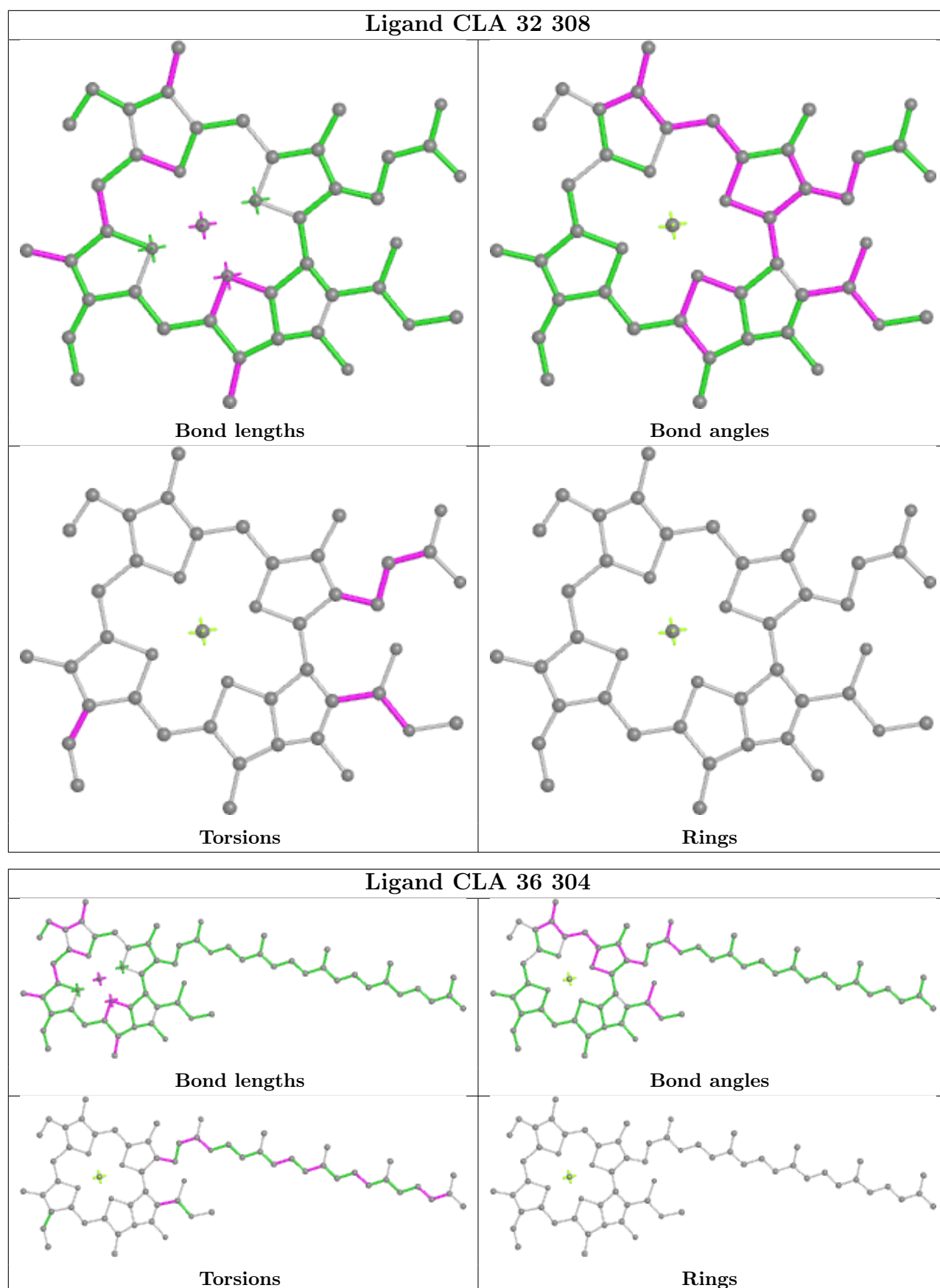


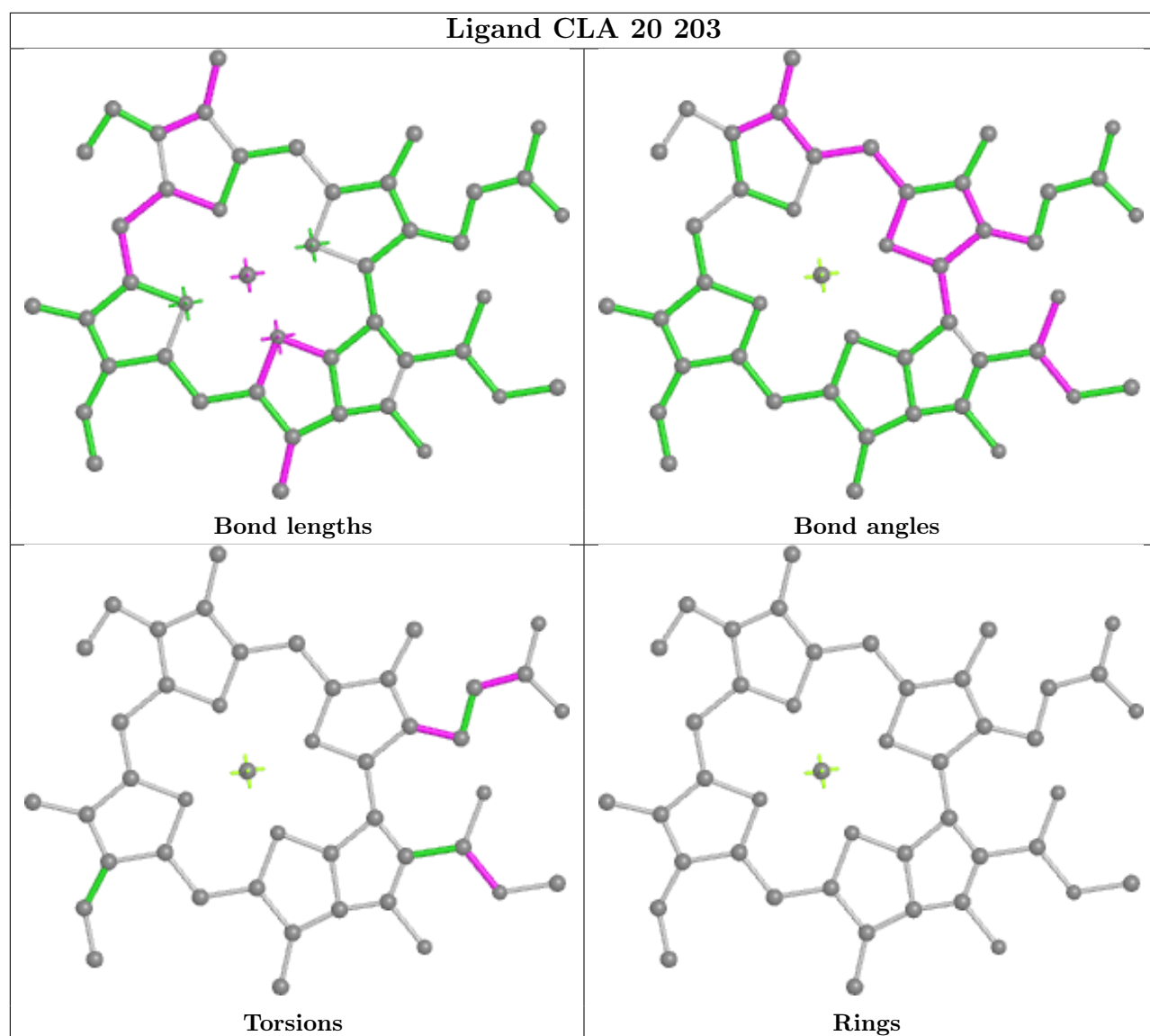


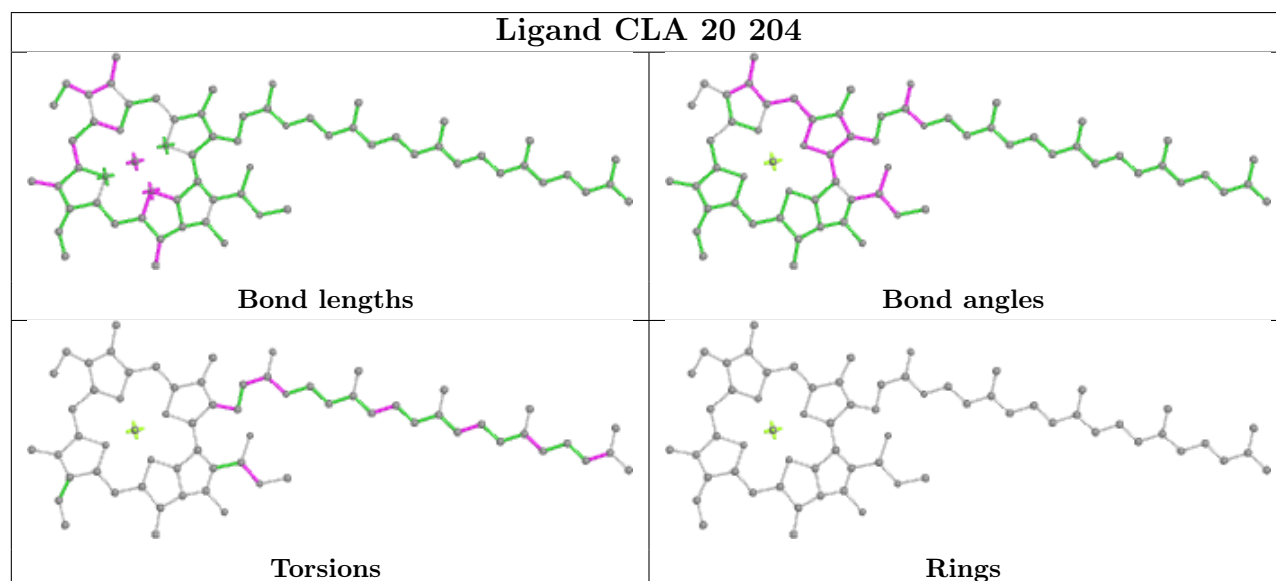
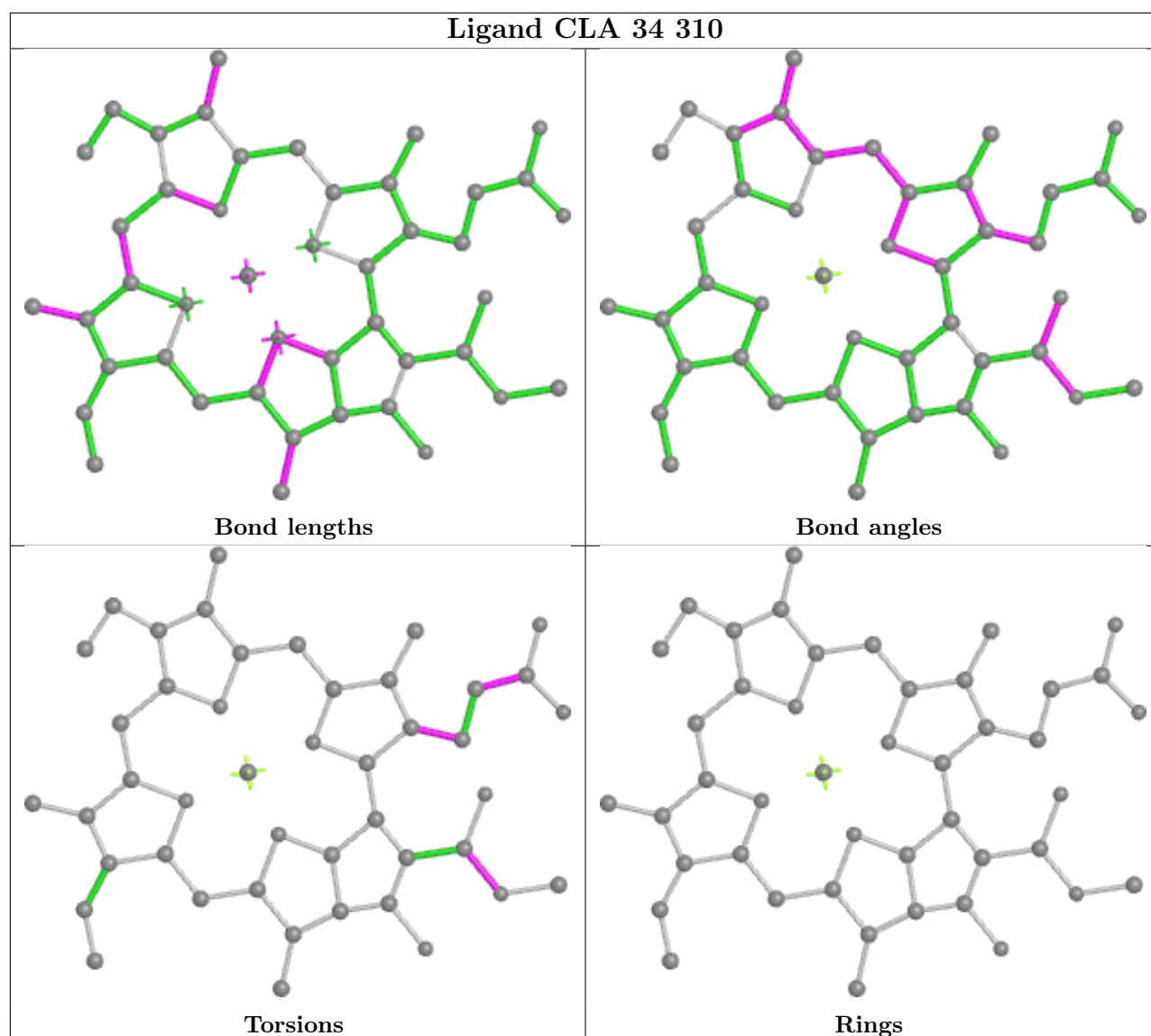


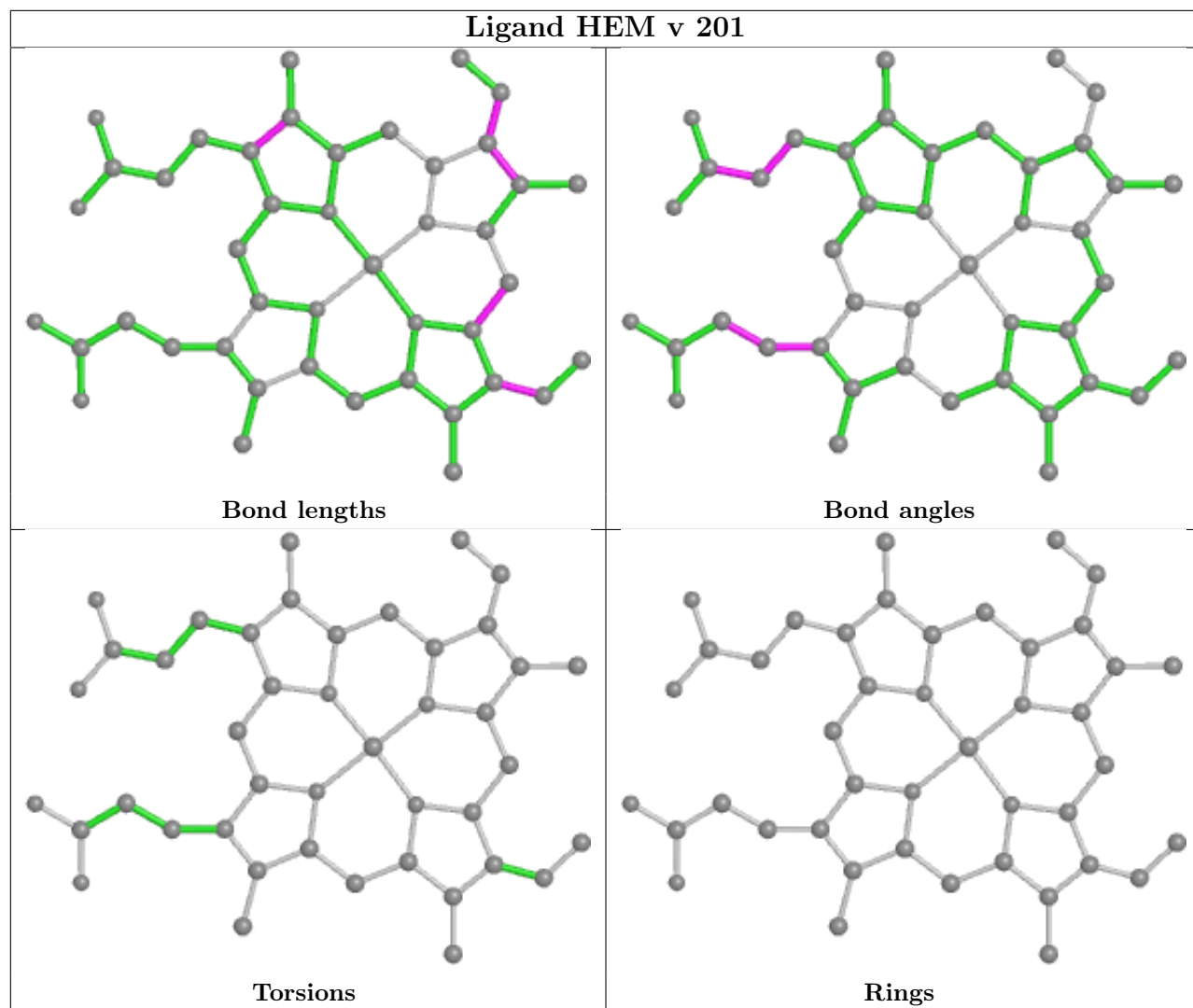


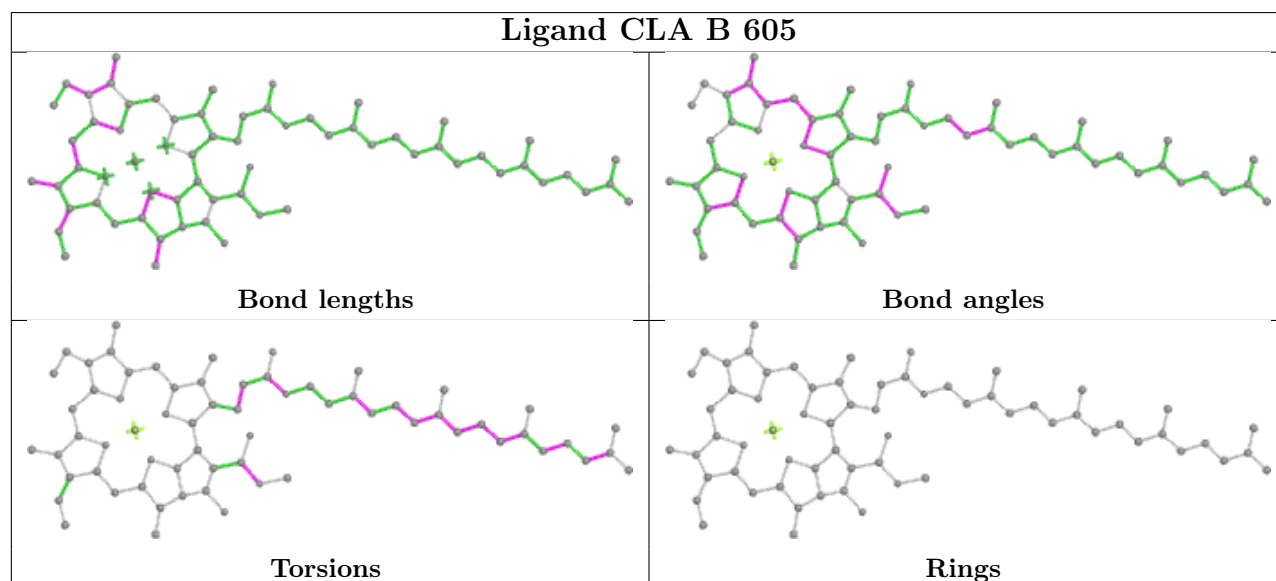
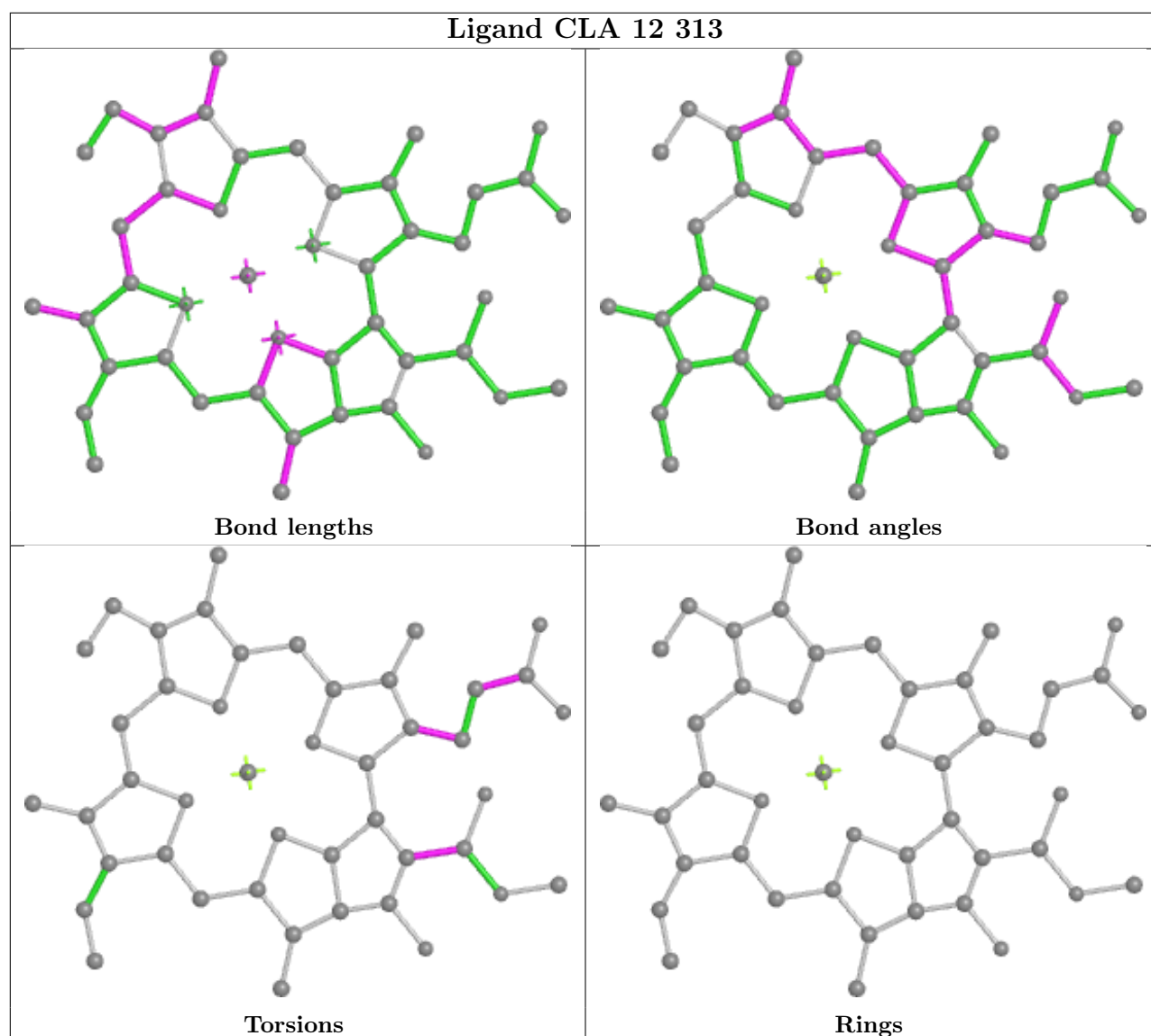


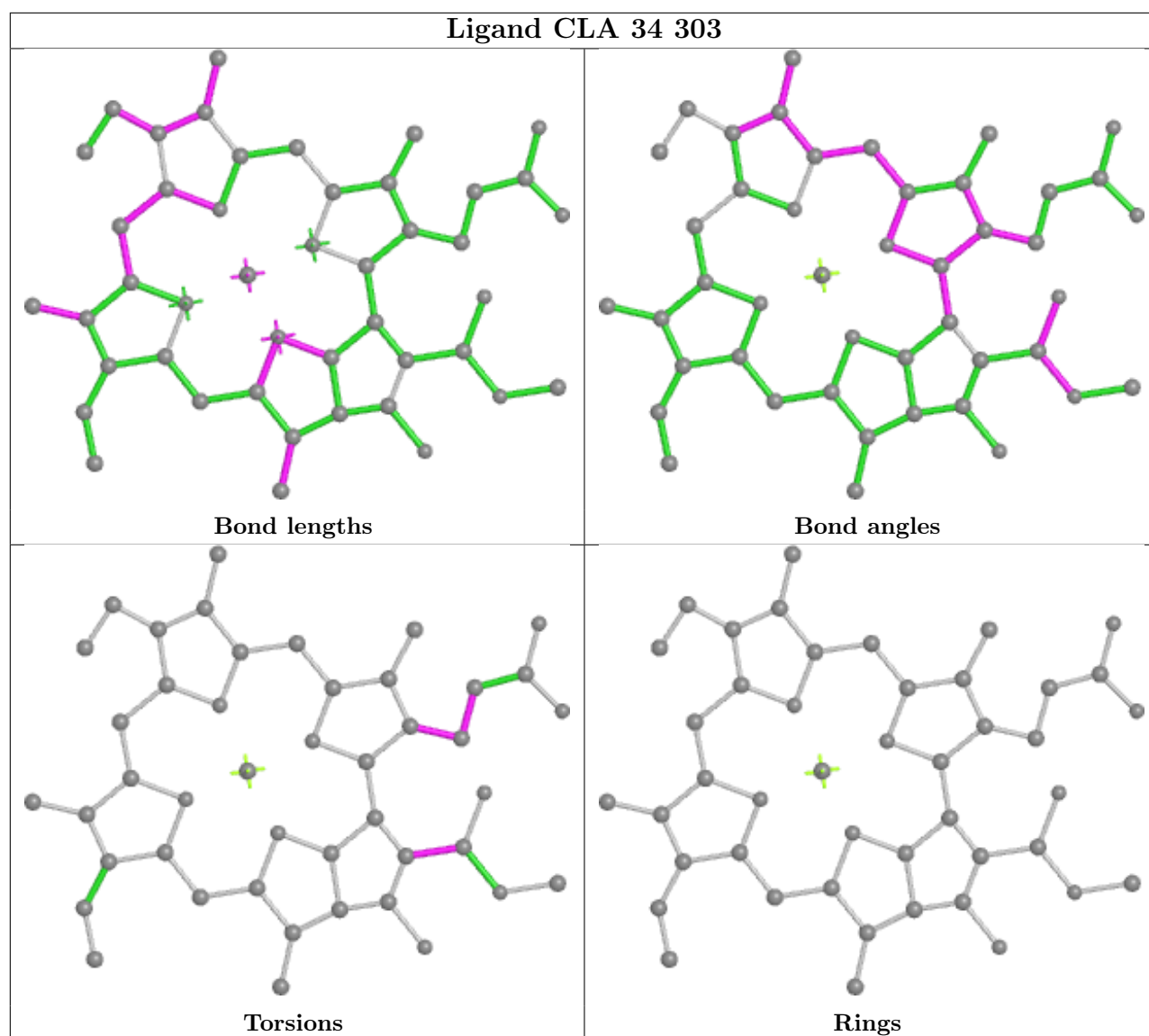


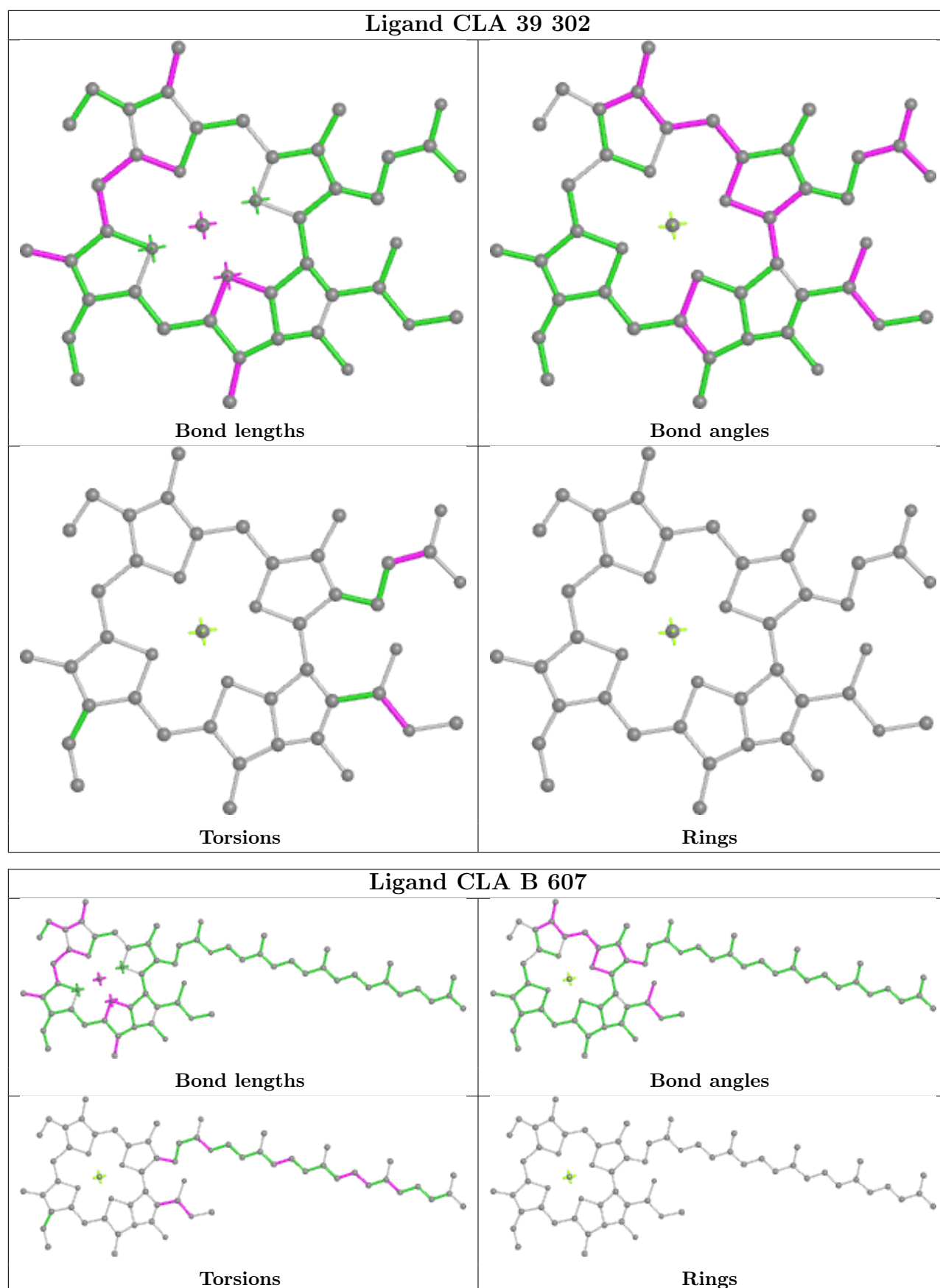


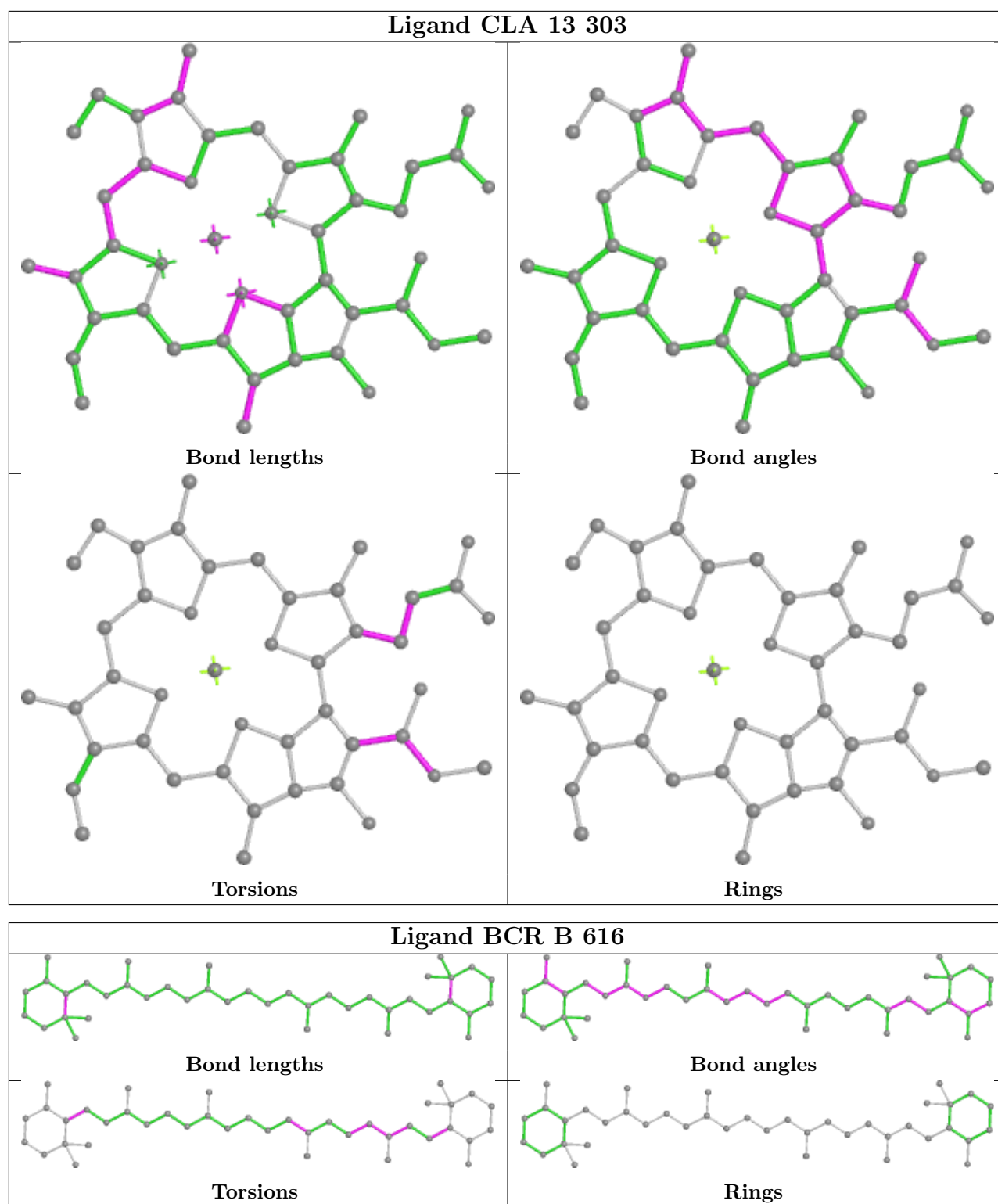


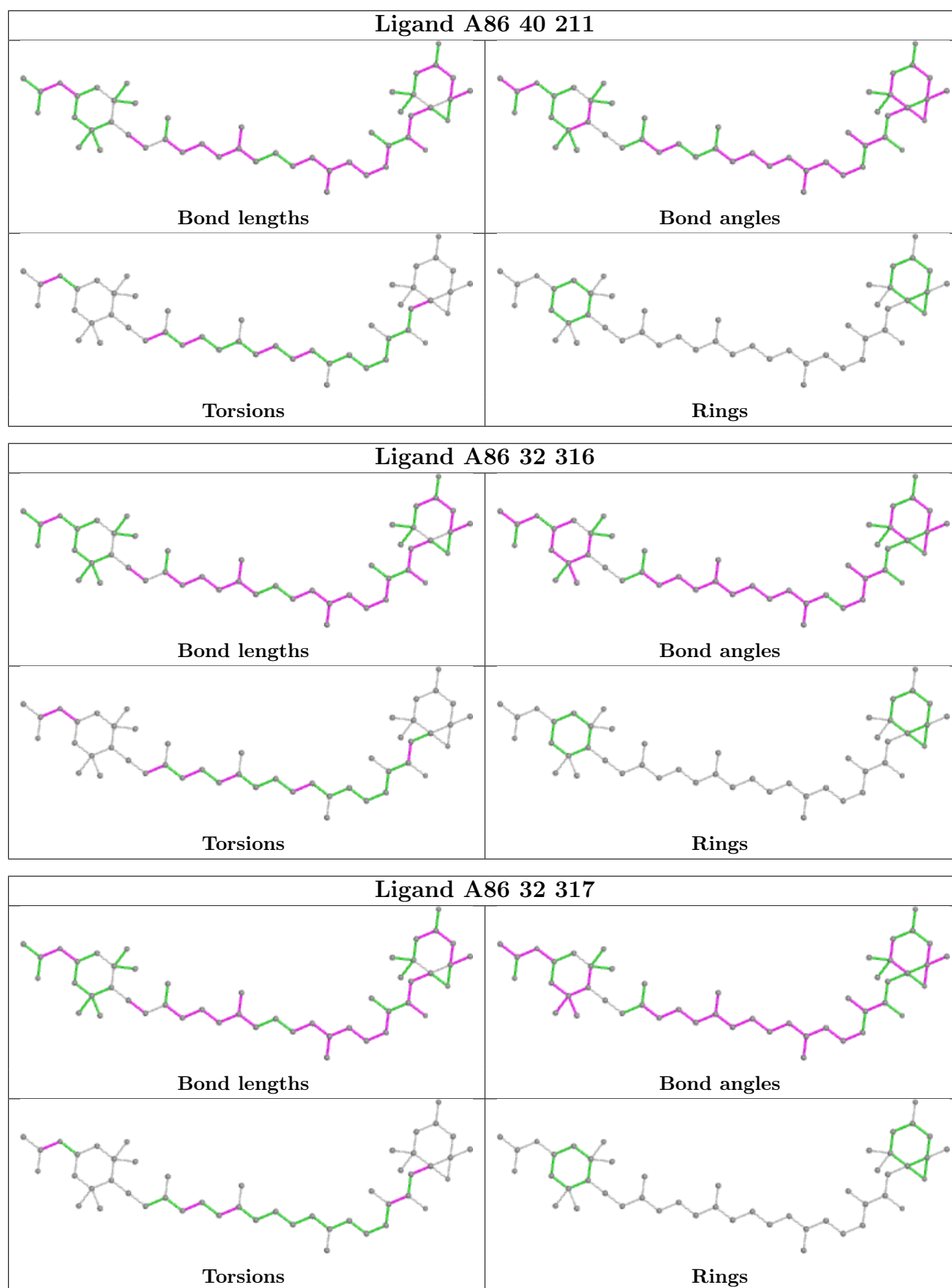


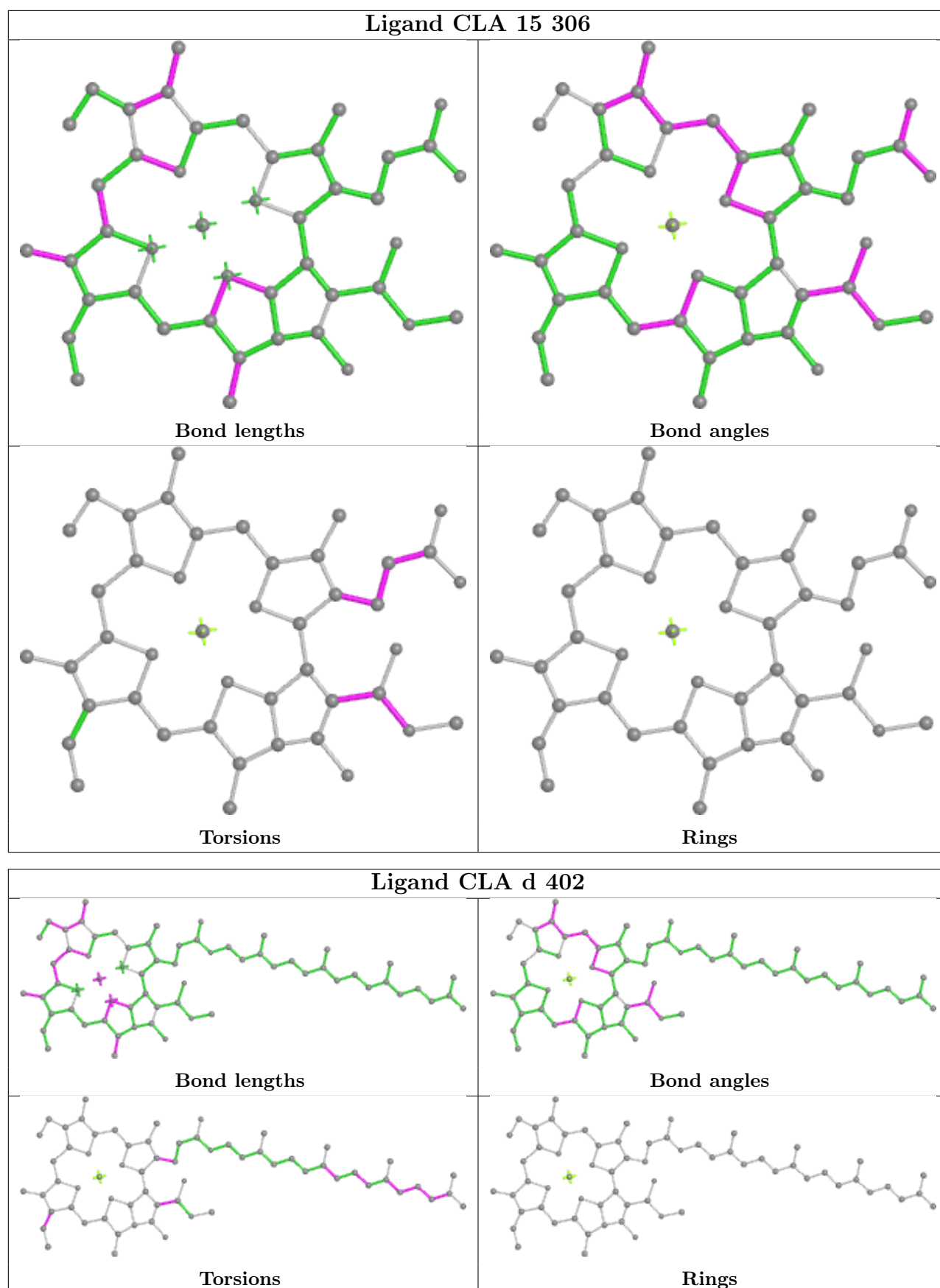


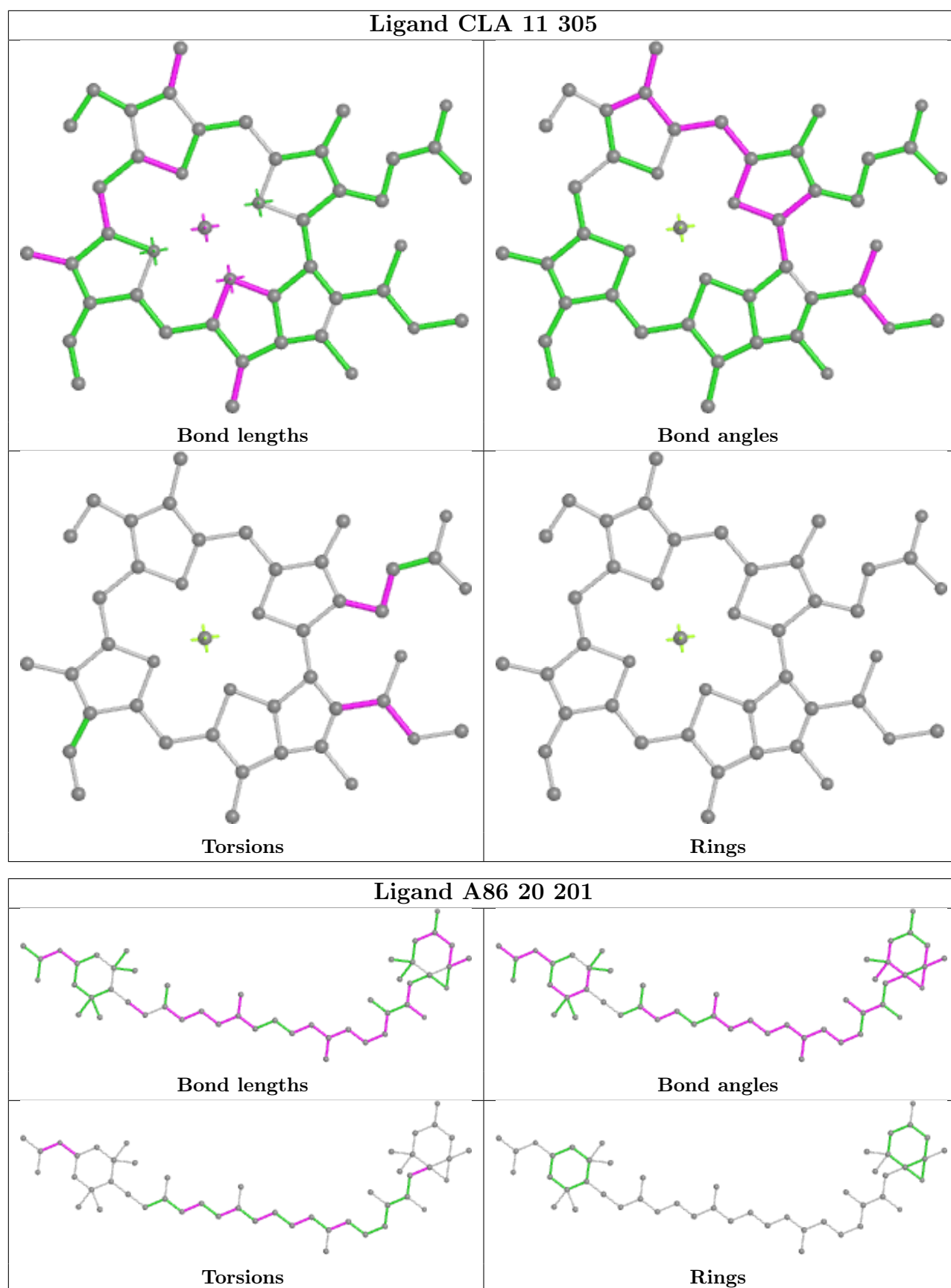




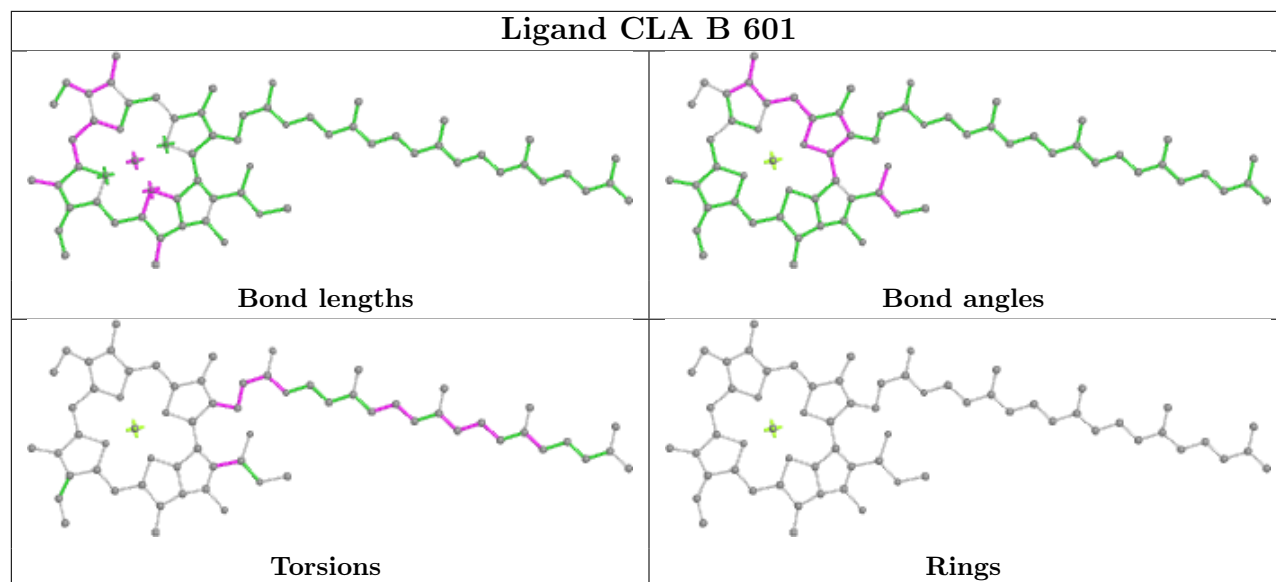




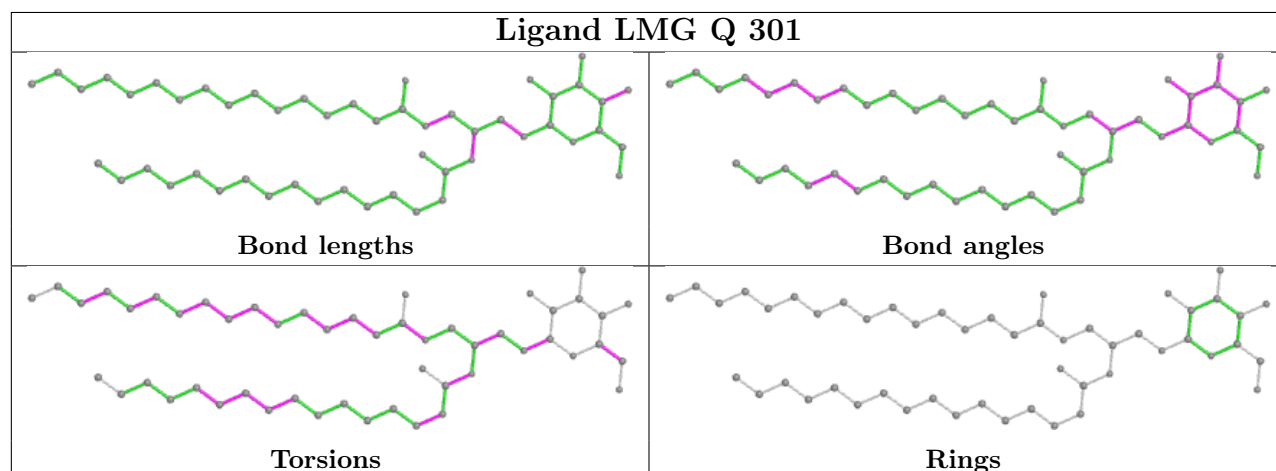




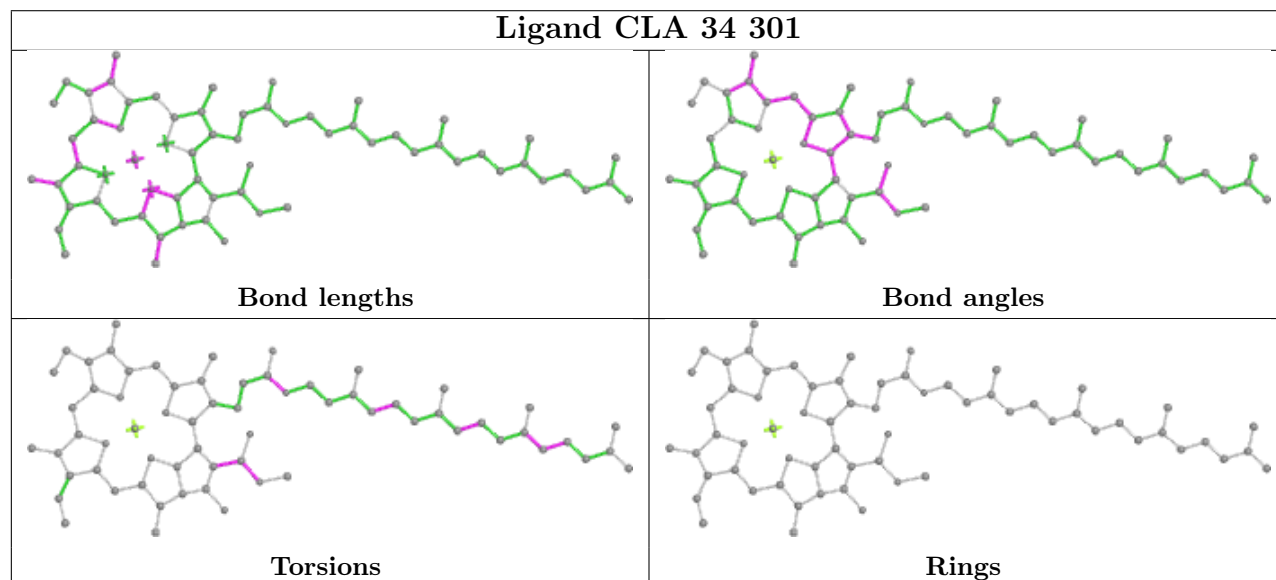
Ligand CLA B 601

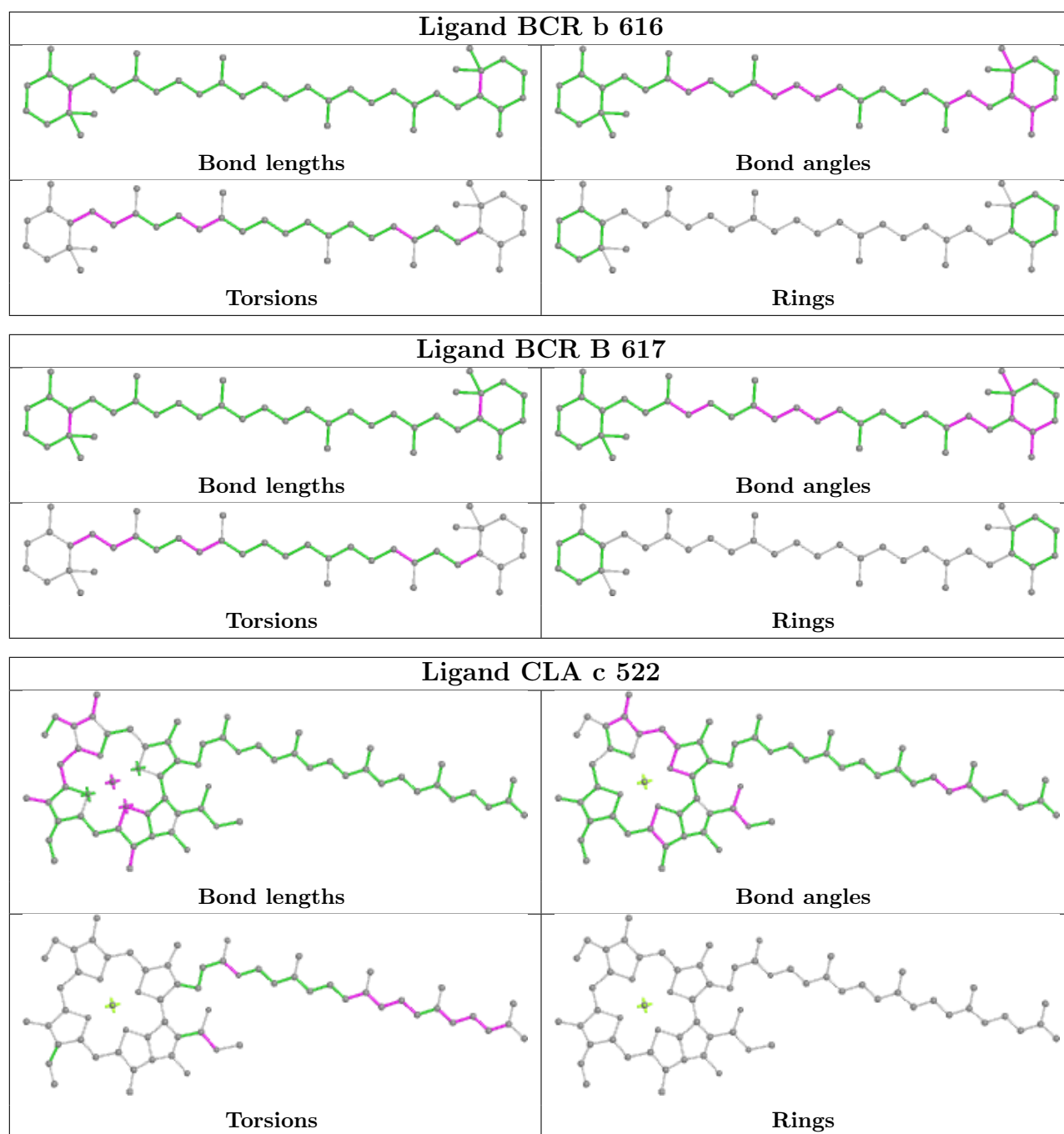


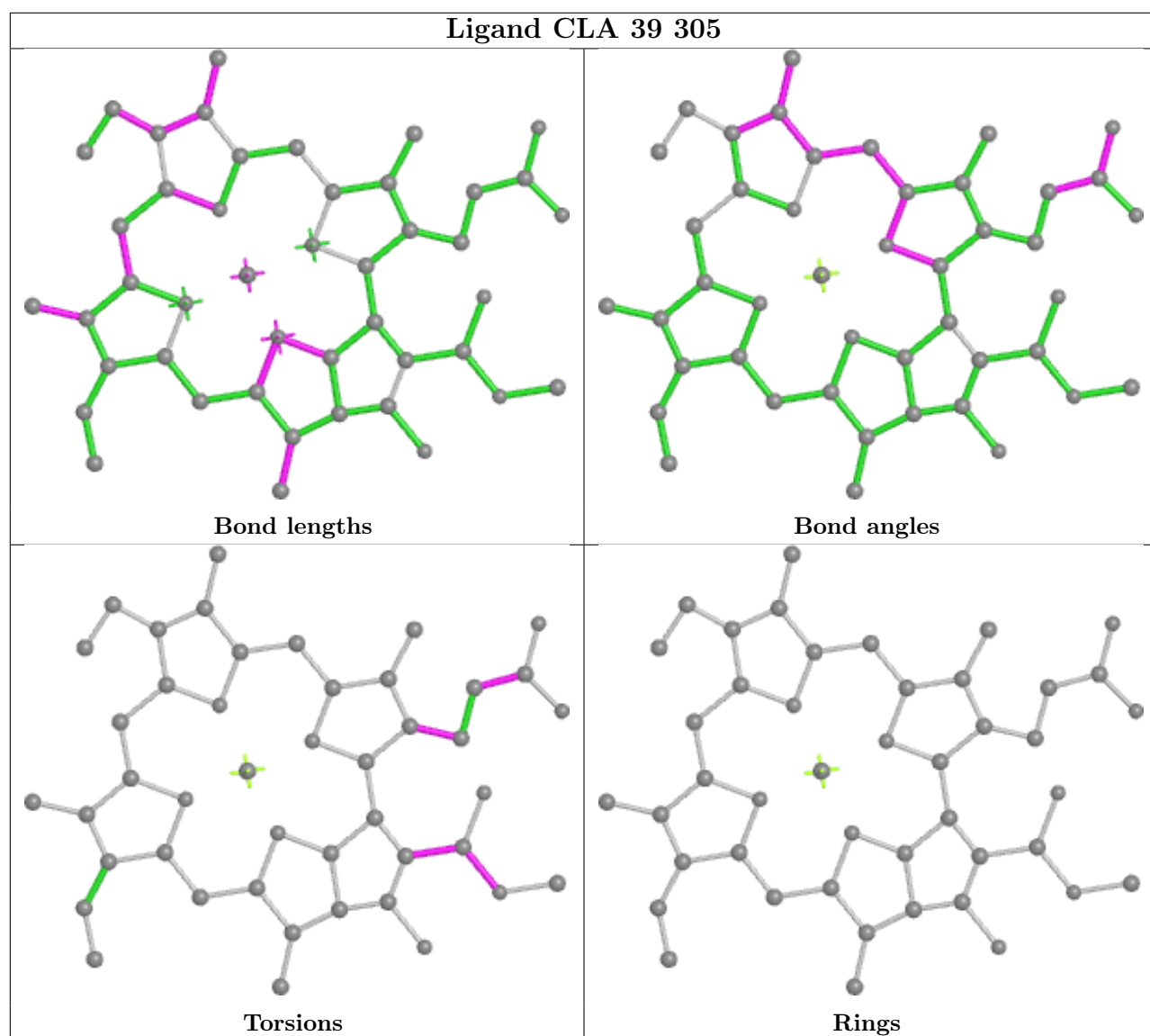
Ligand LMG Q 301

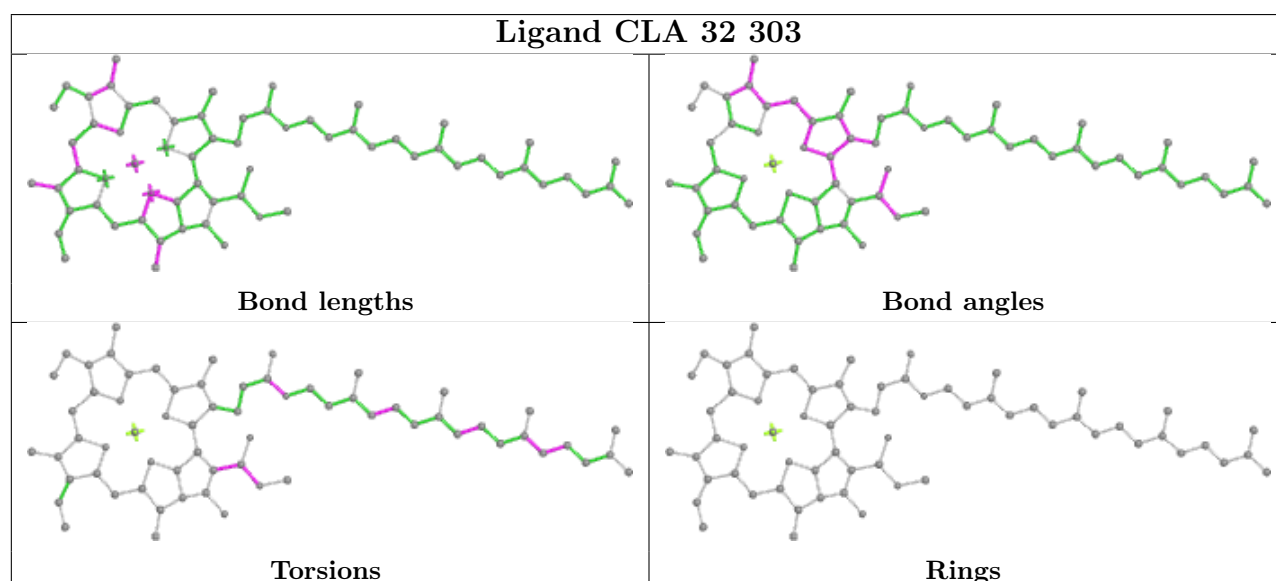
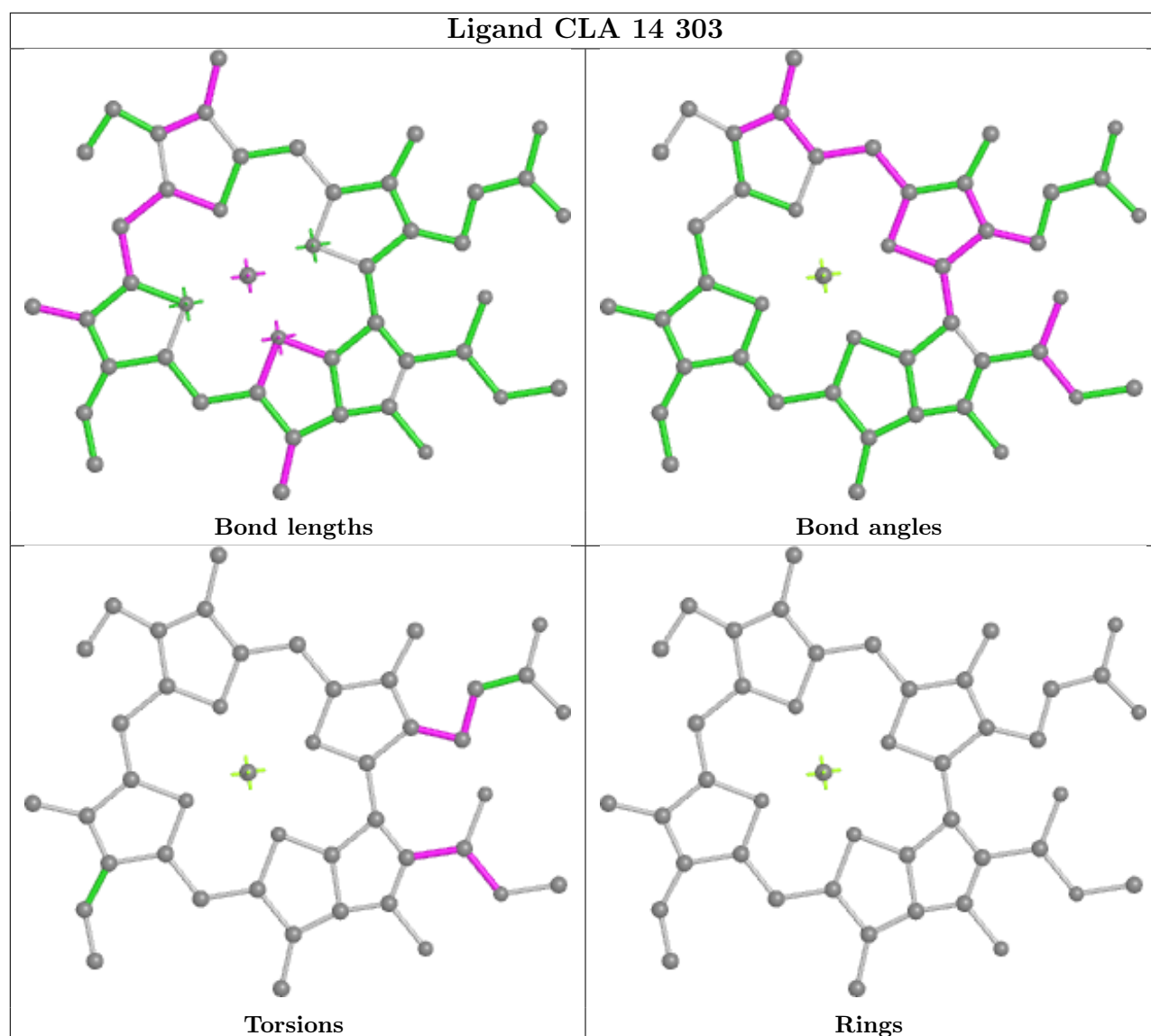


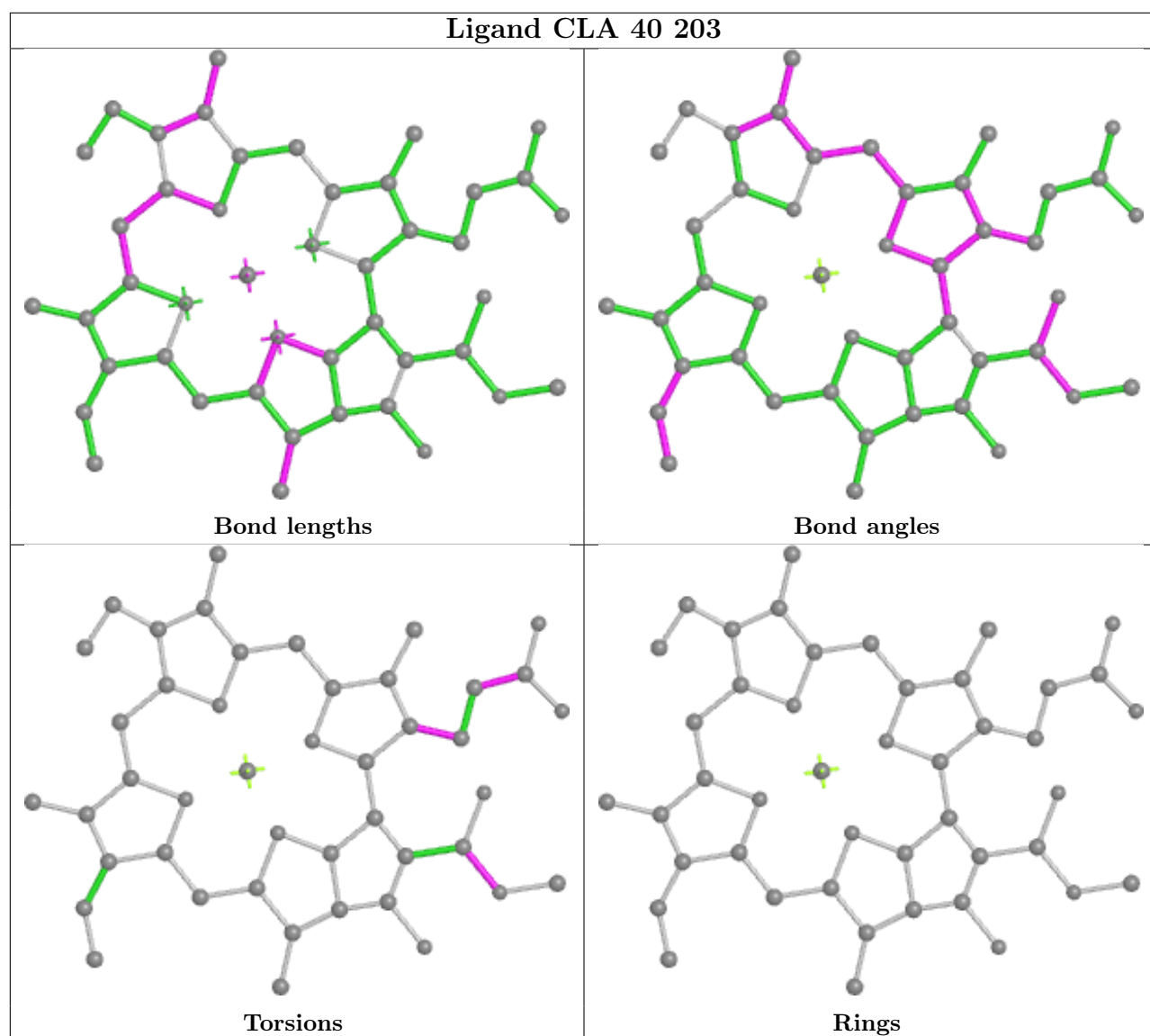
Ligand CLA 34 301

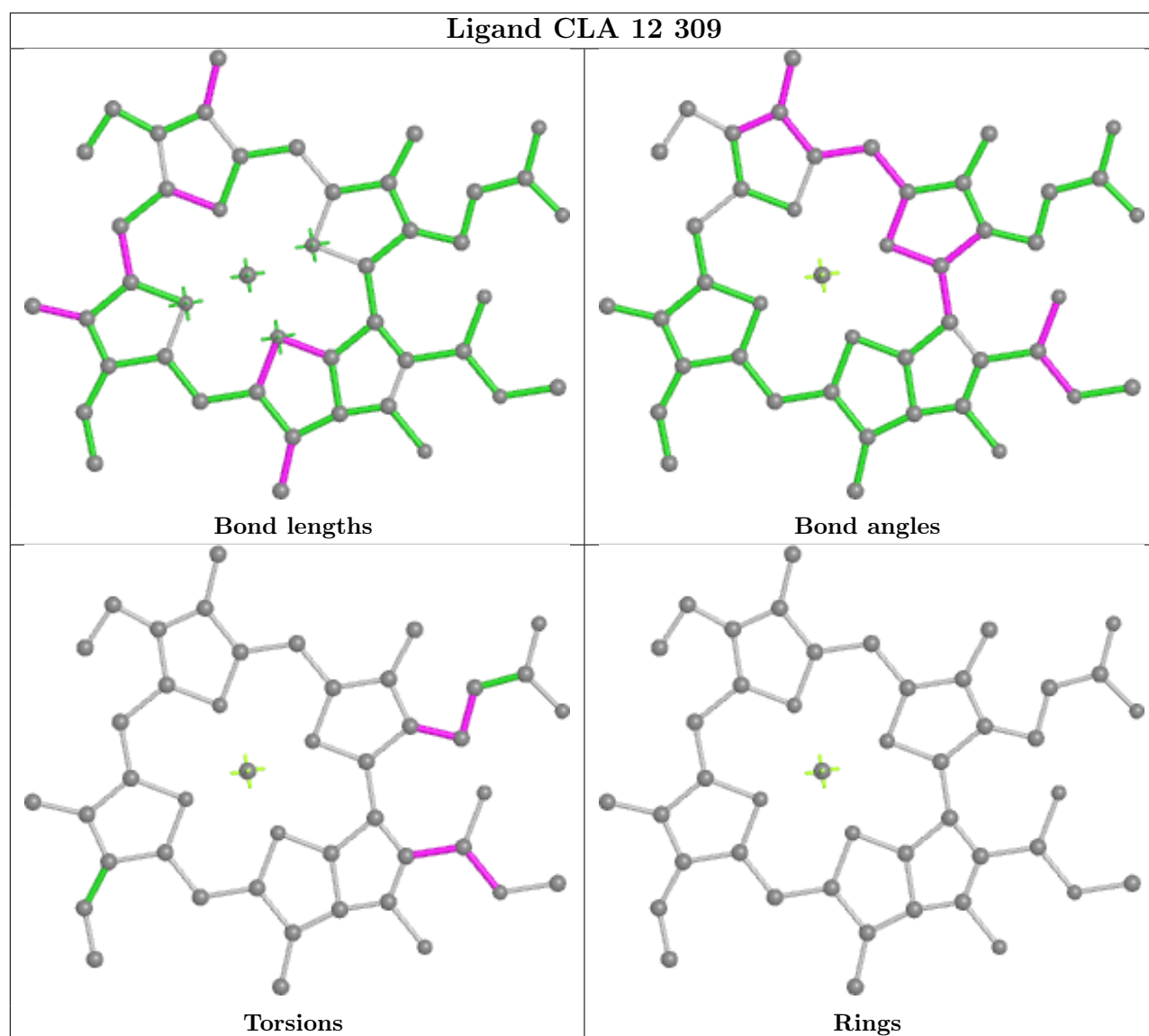


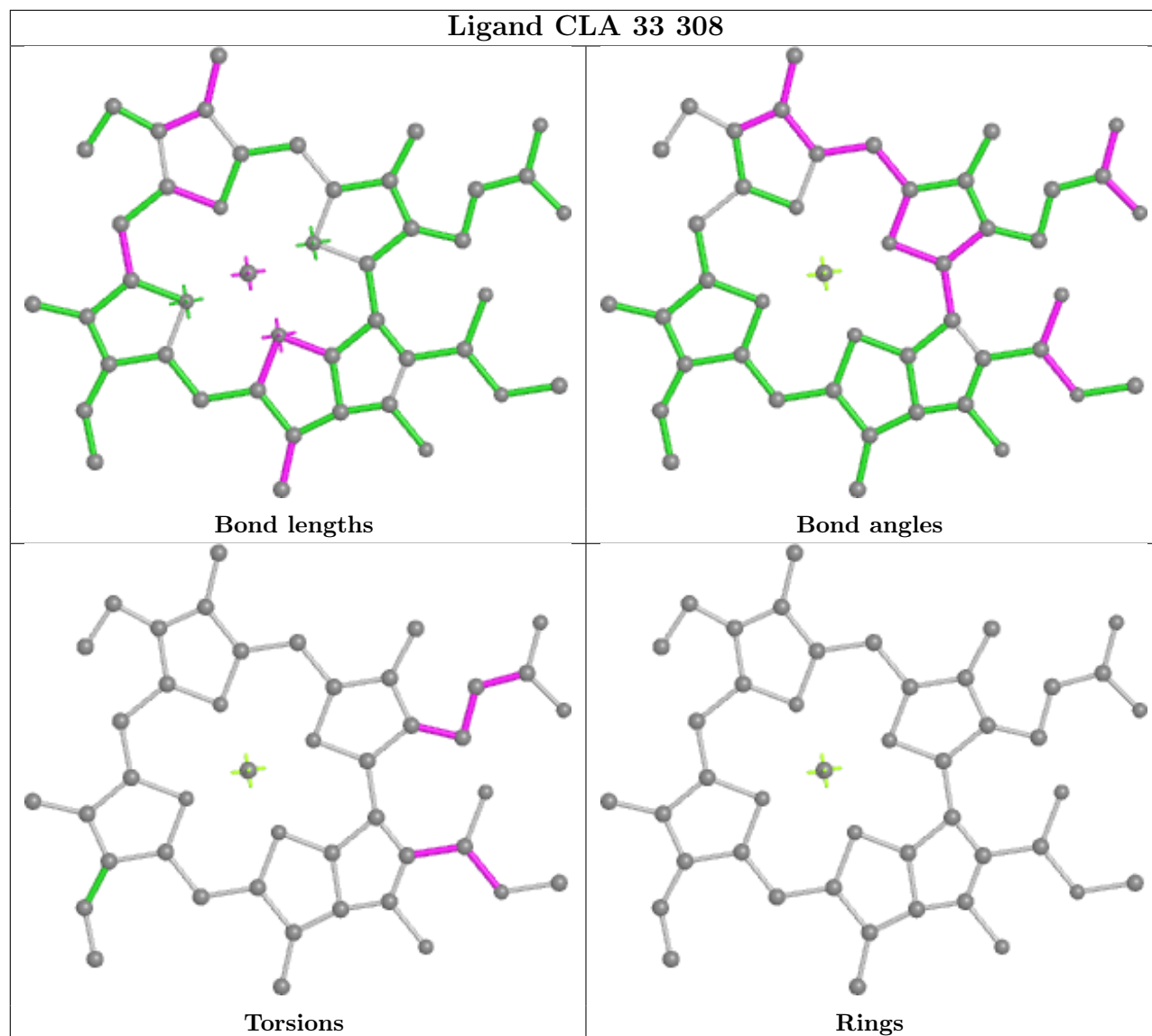


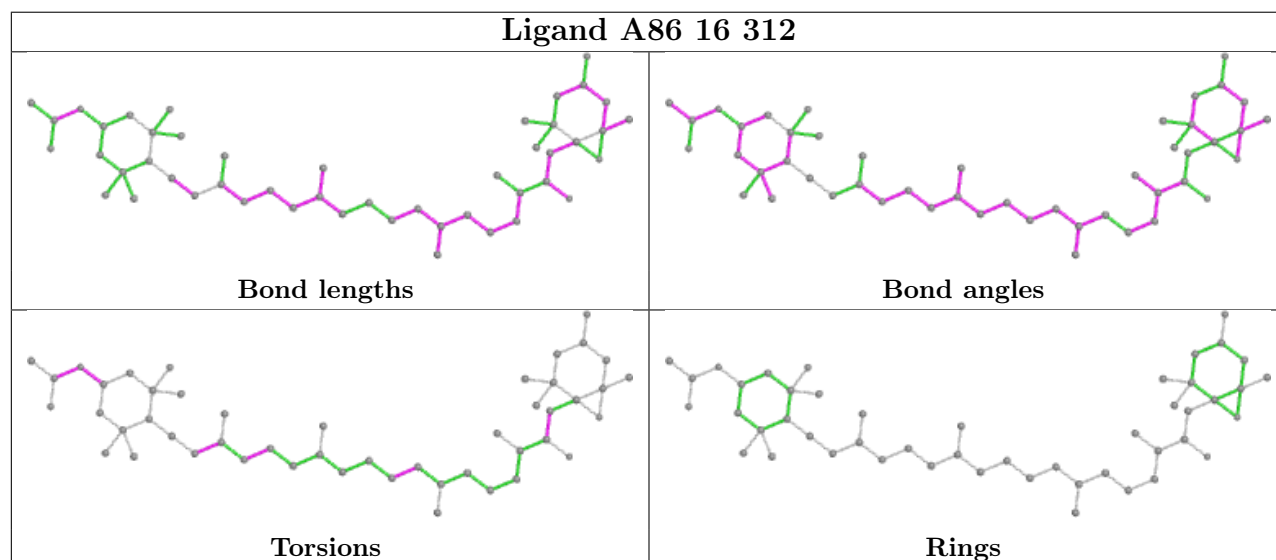
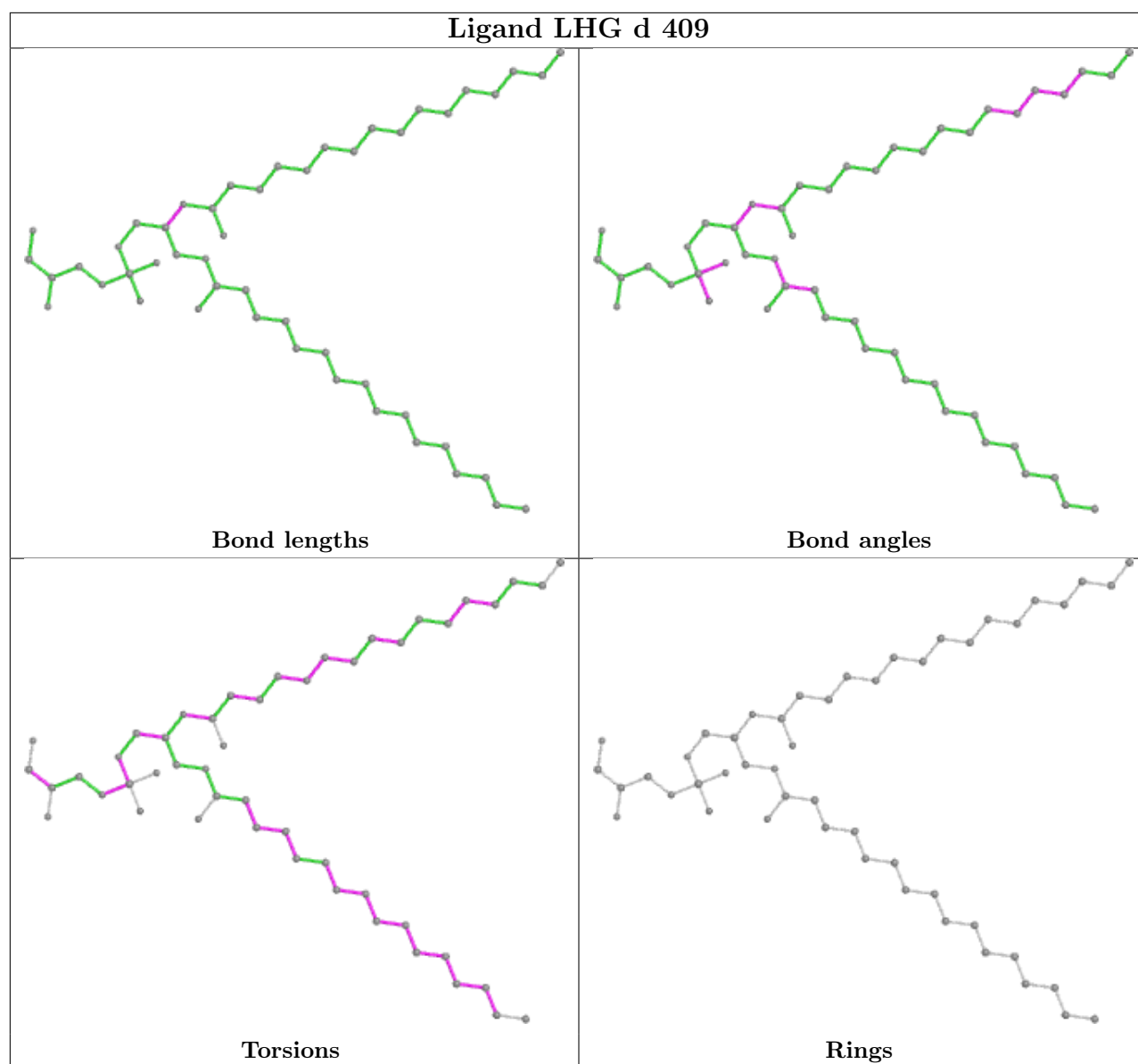


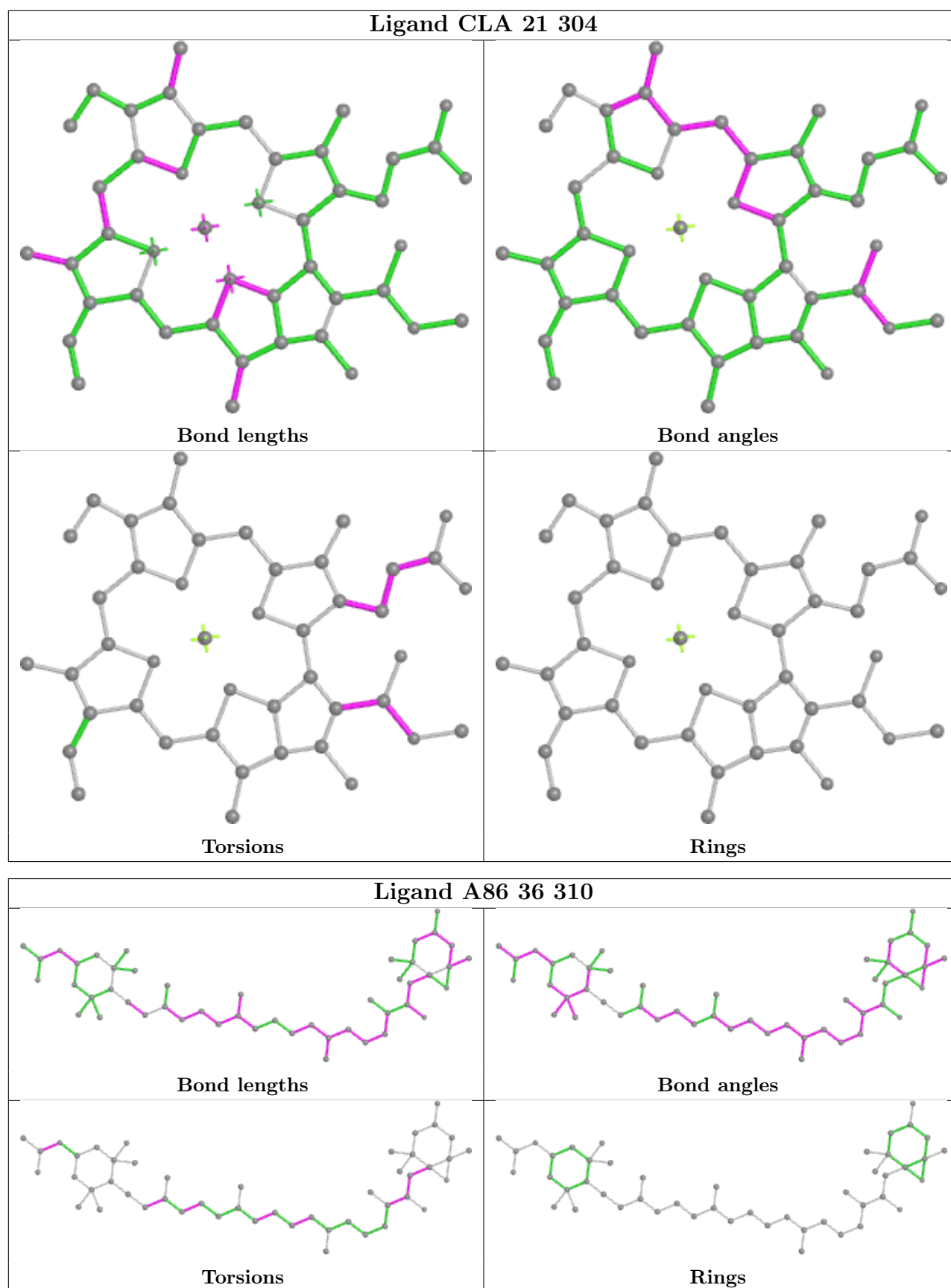




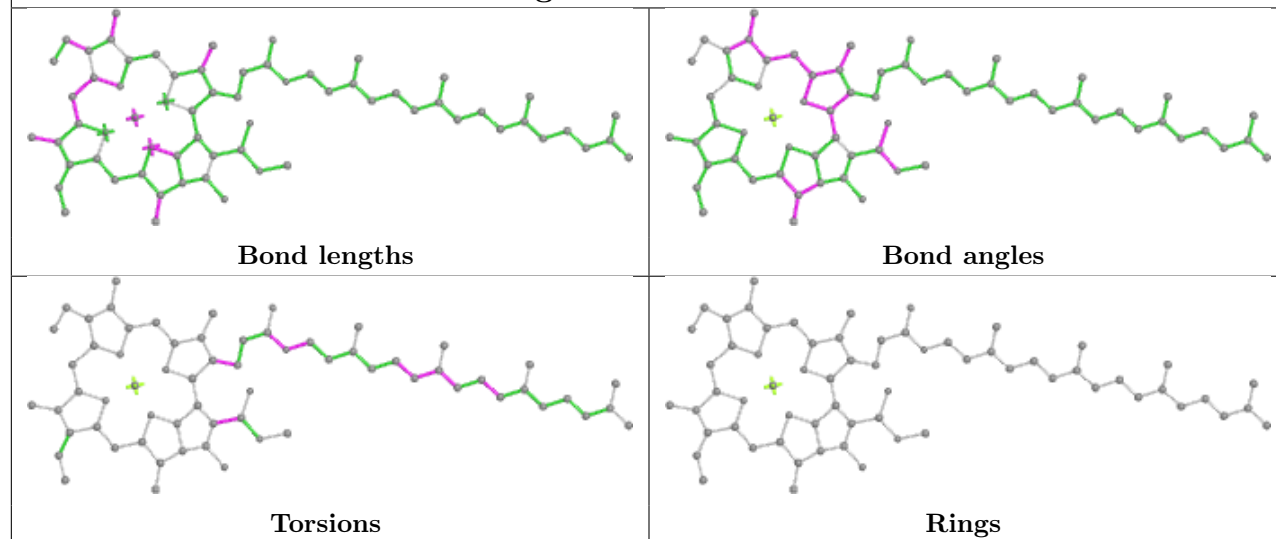




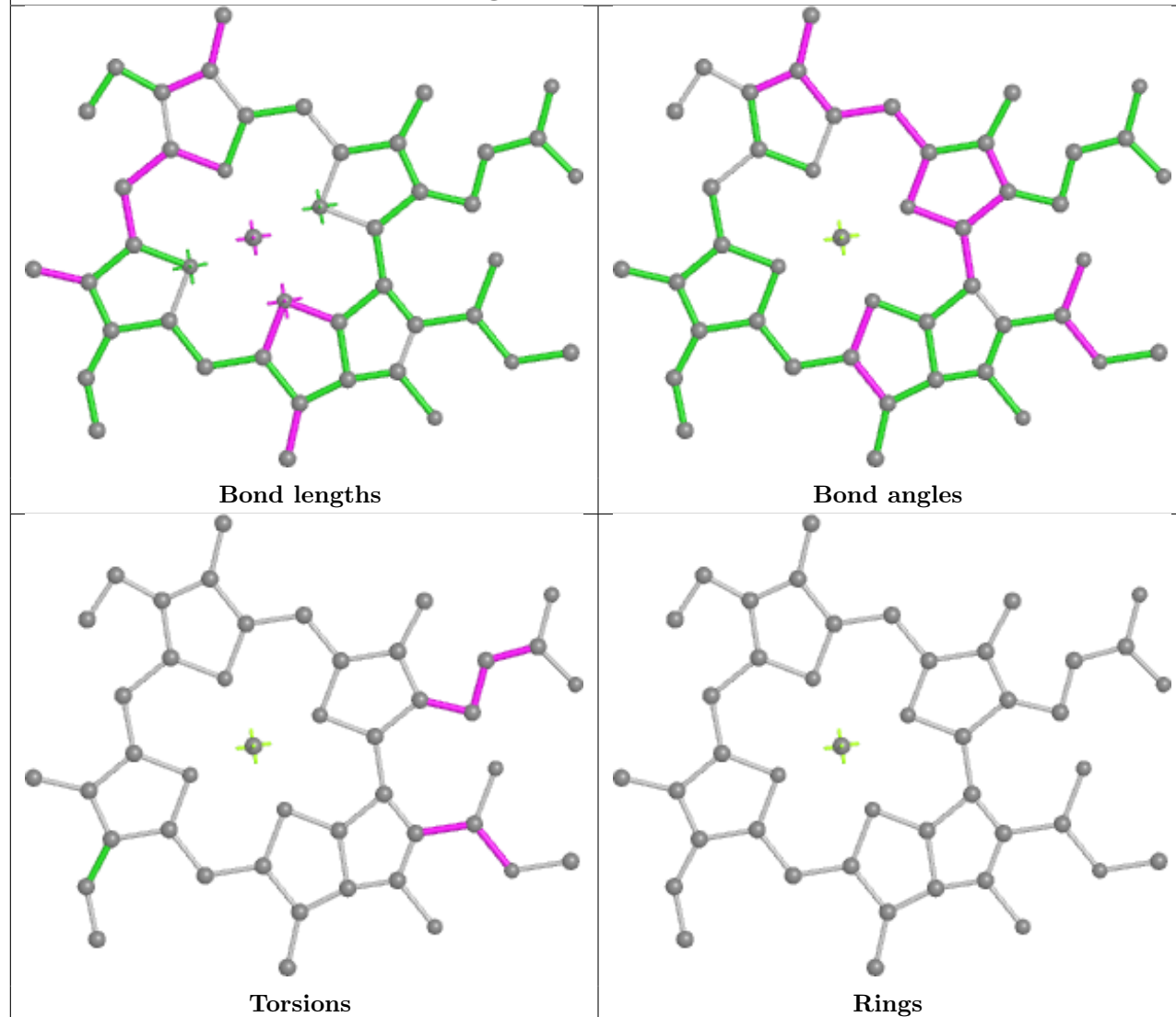


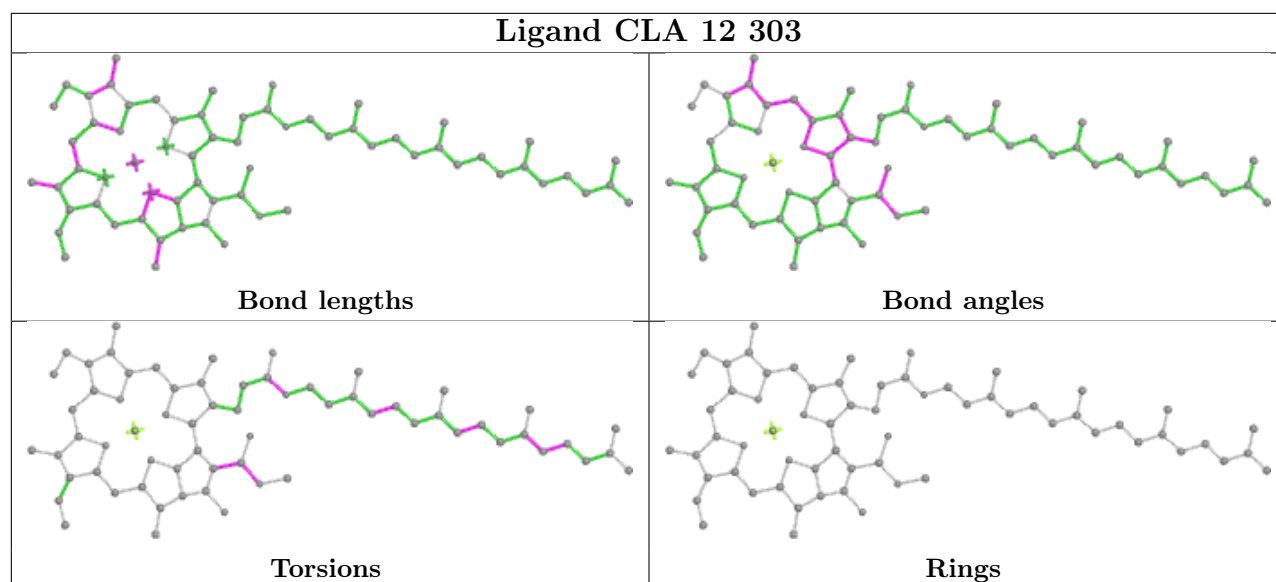
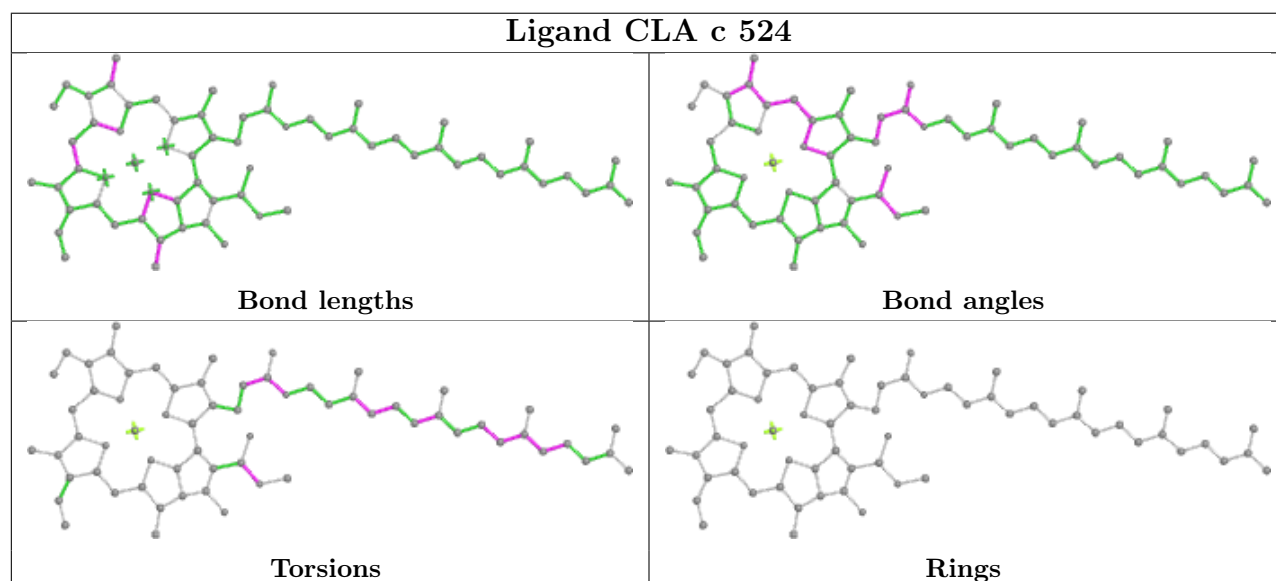
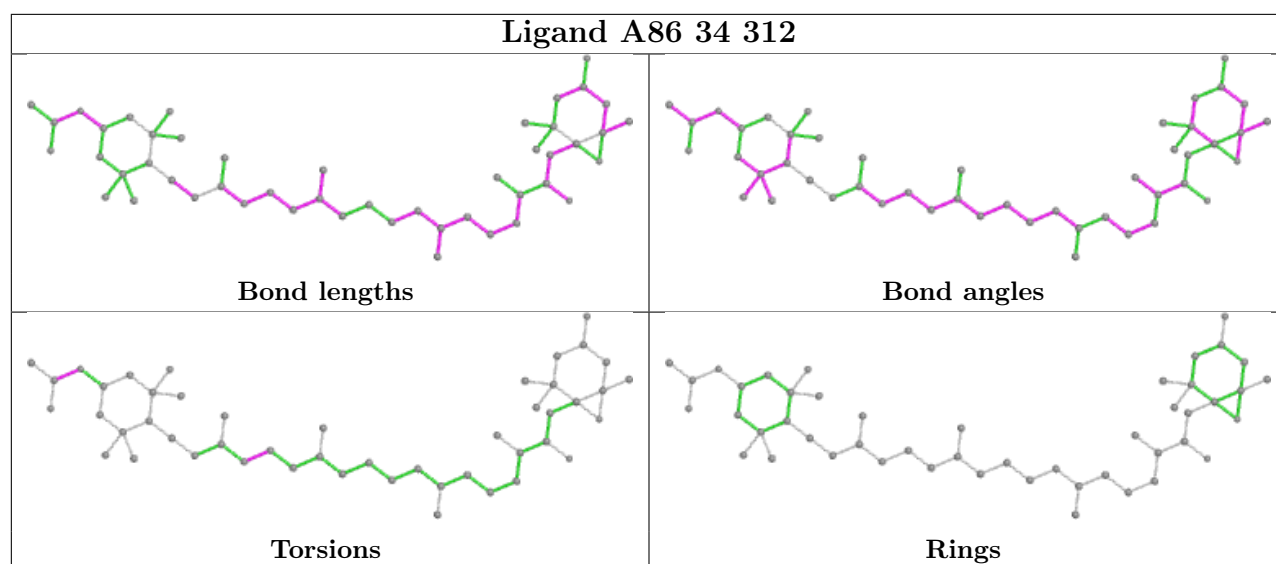


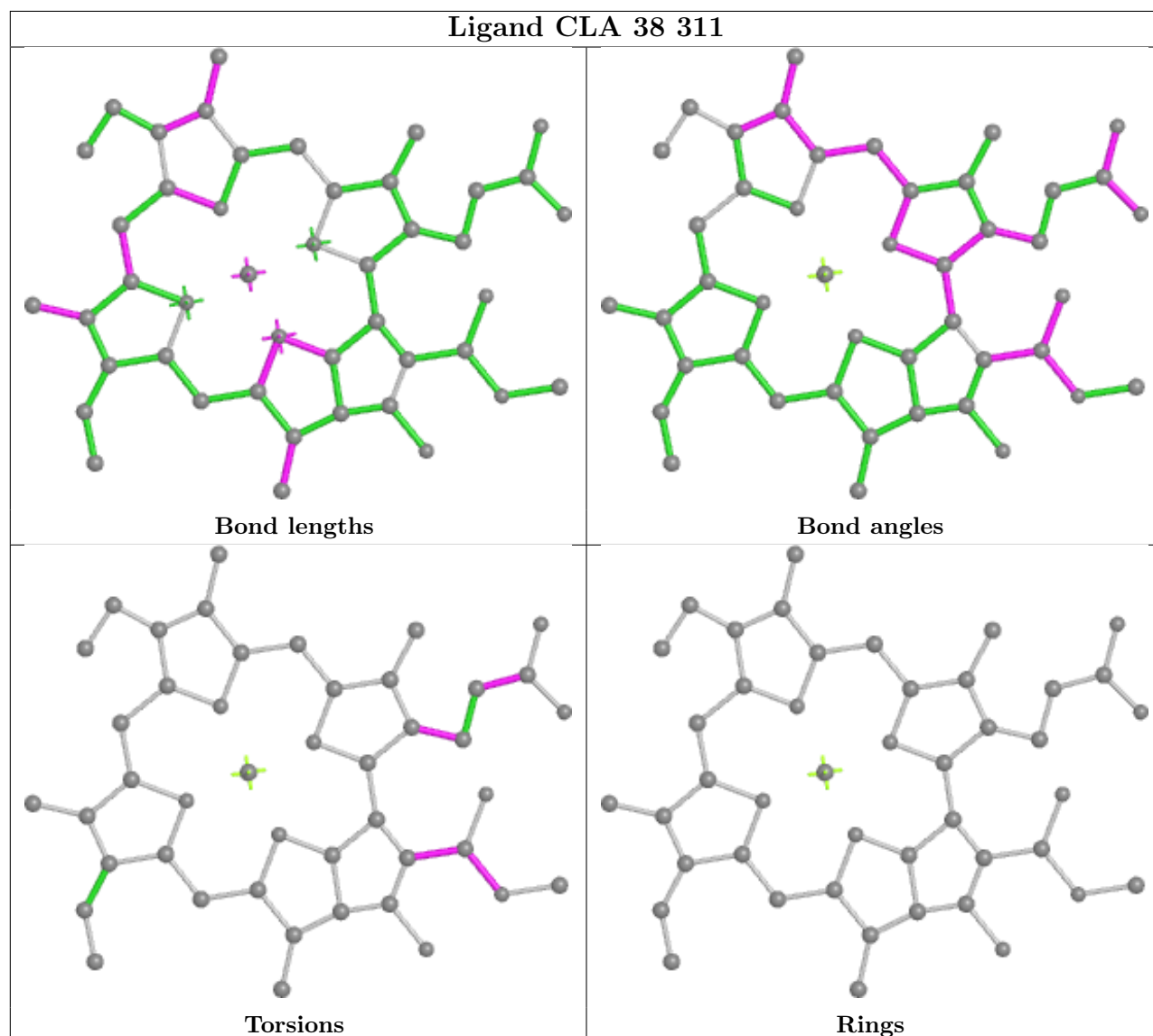
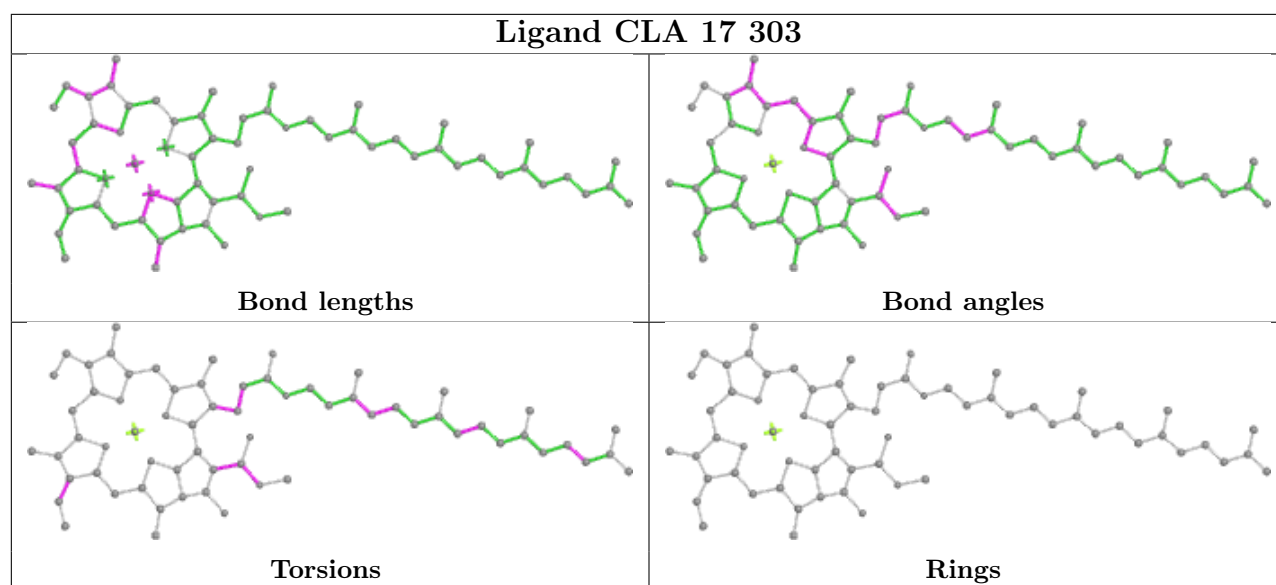
Ligand CLA b 612

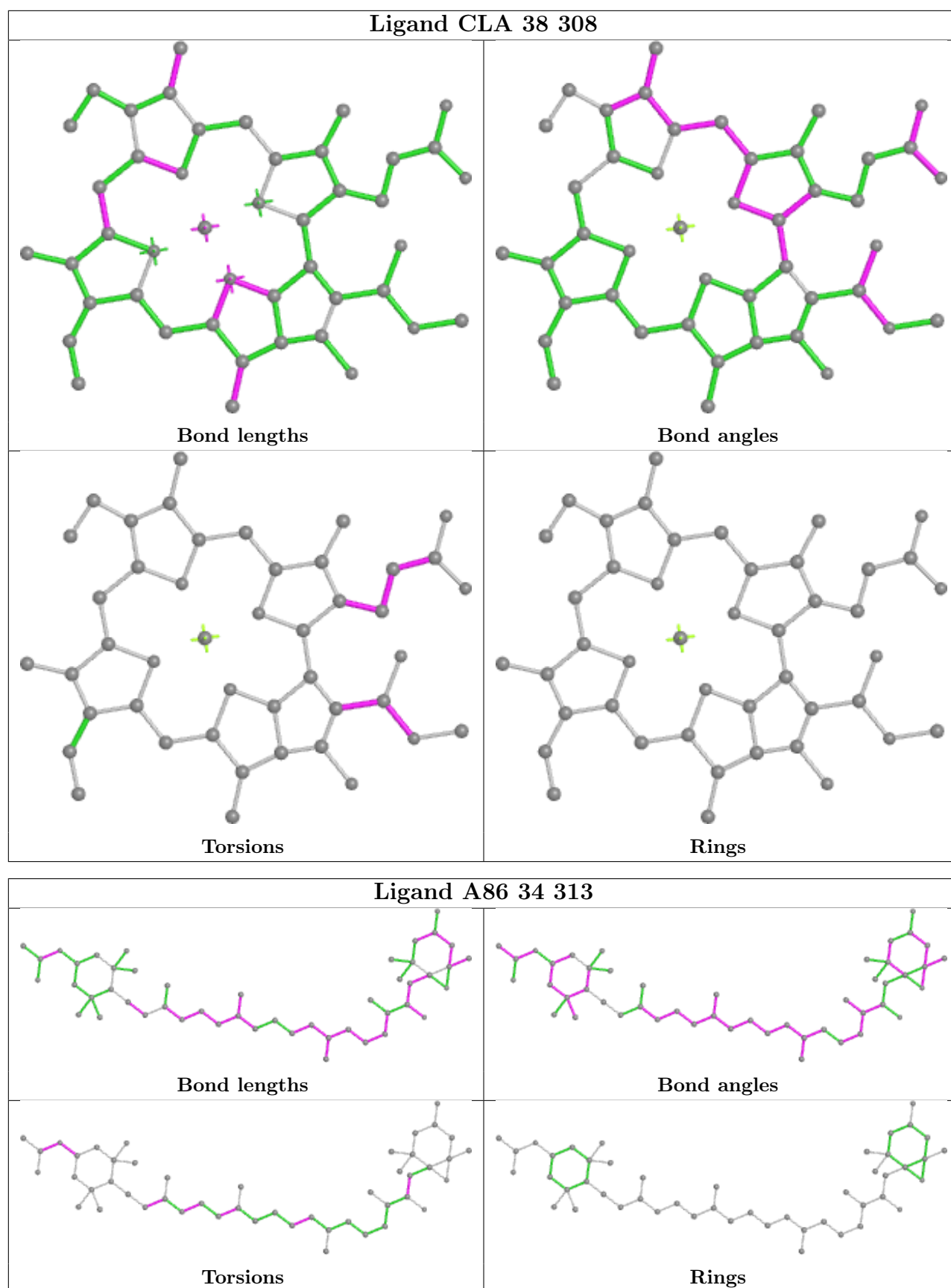


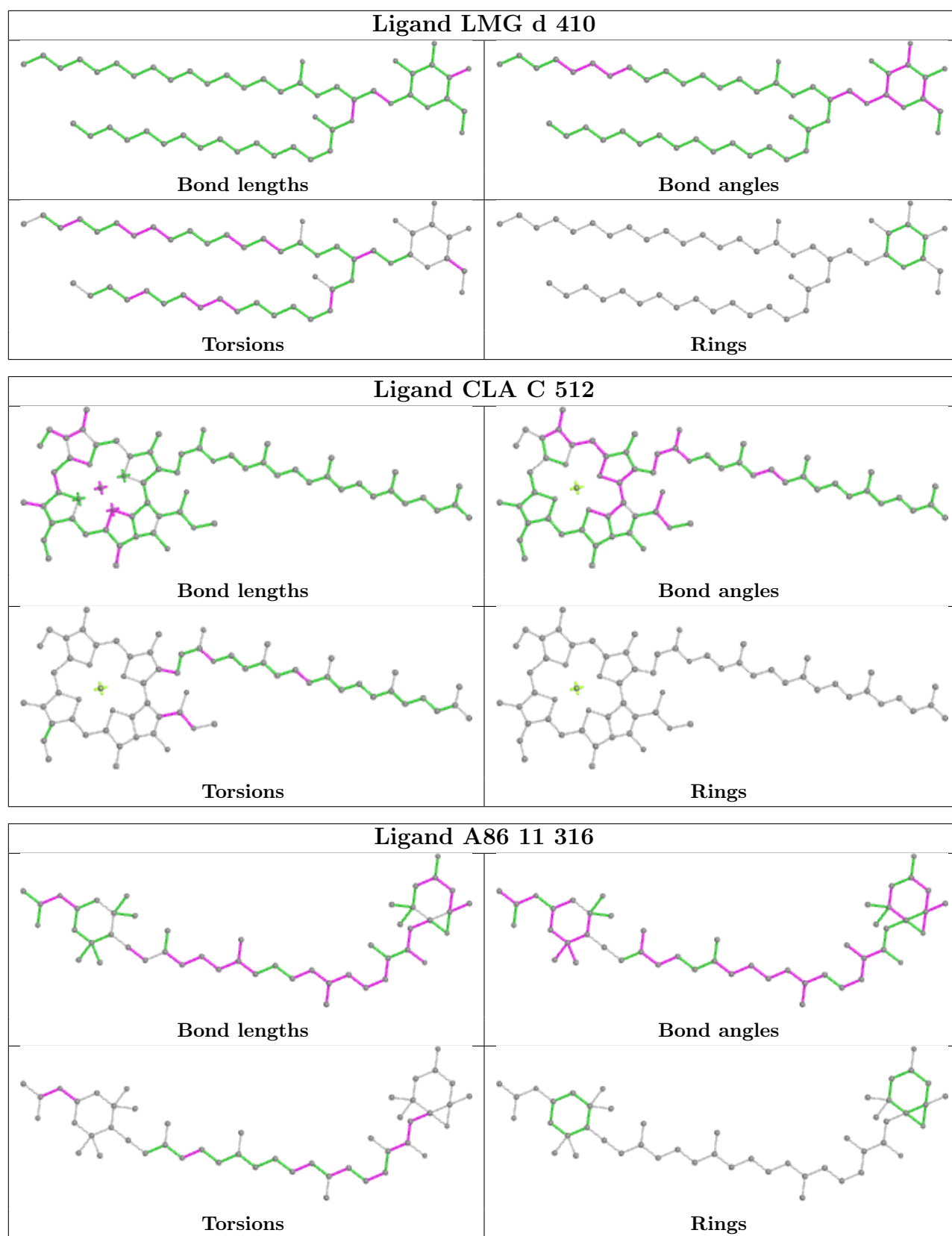
Ligand CLA 40 205

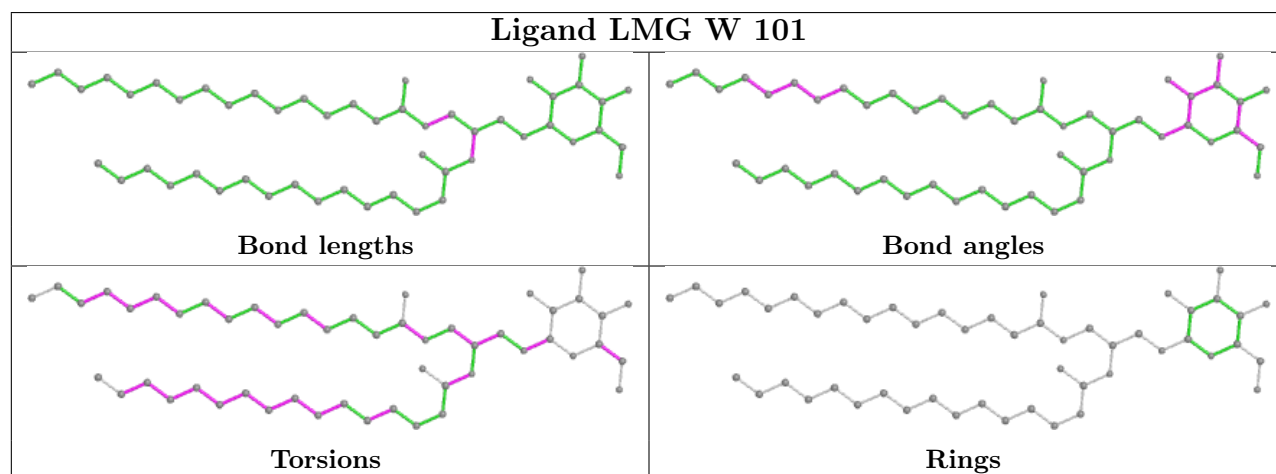
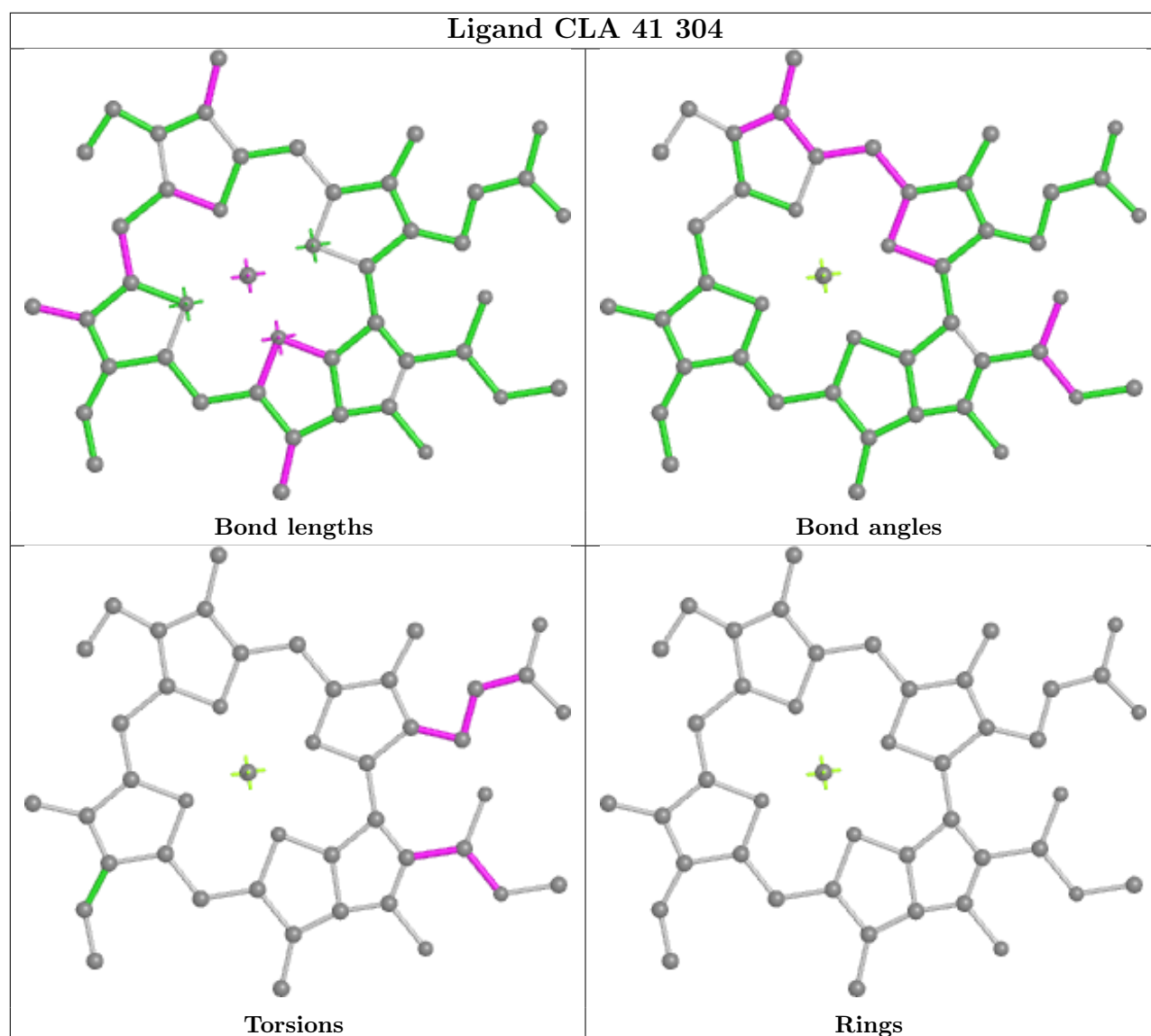




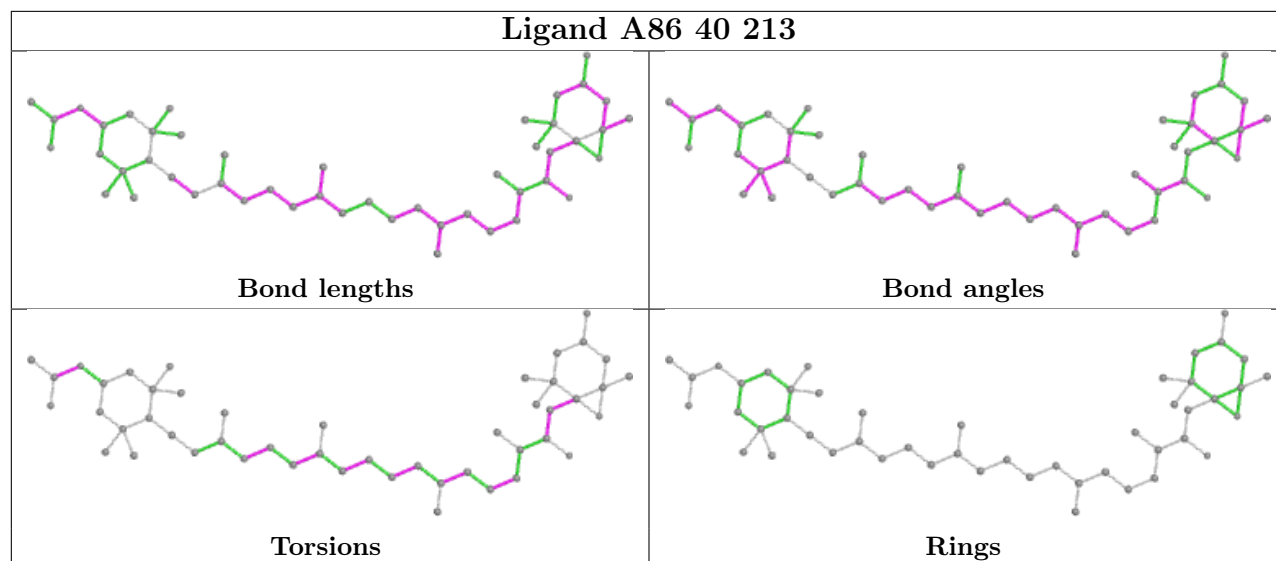




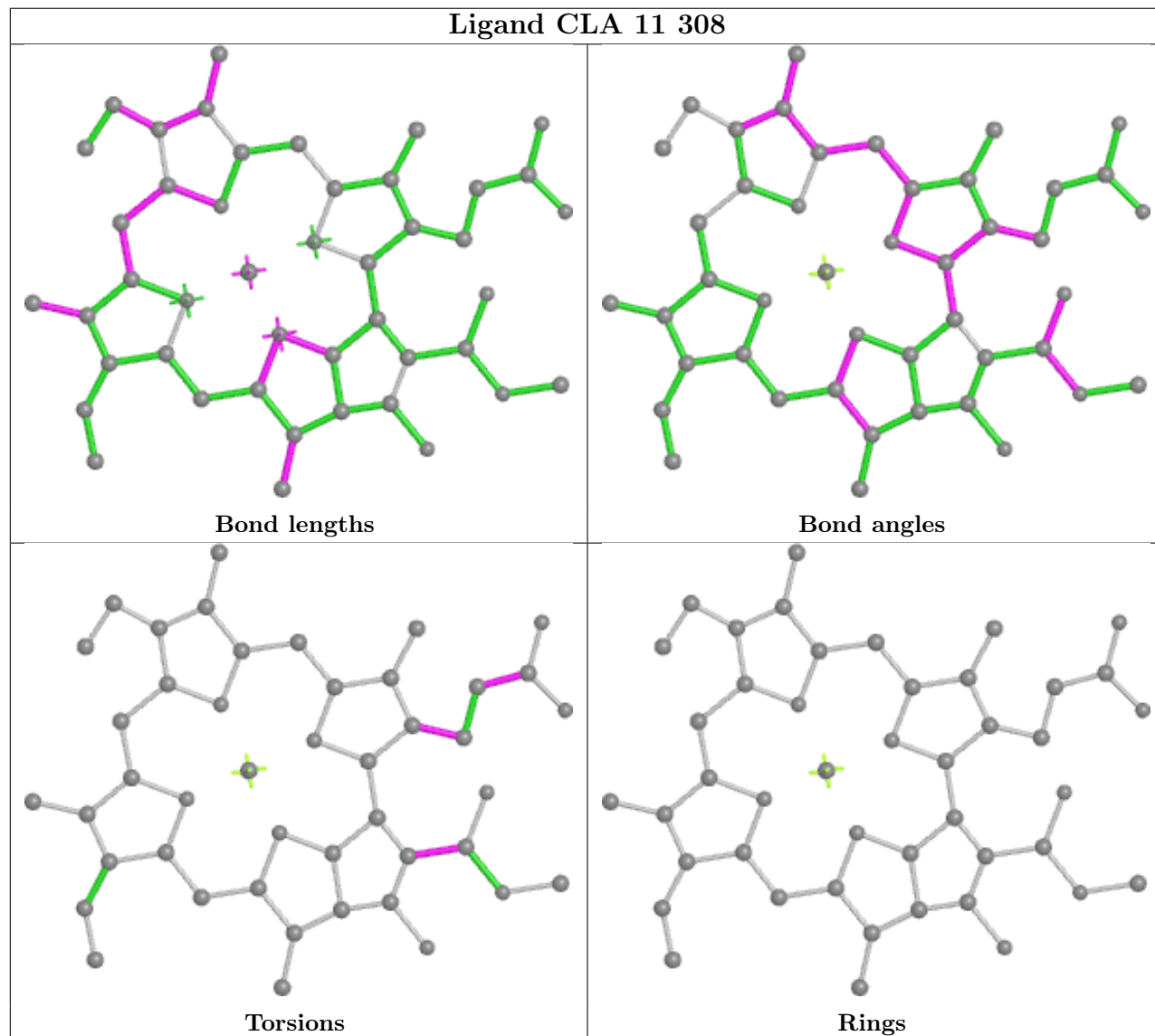


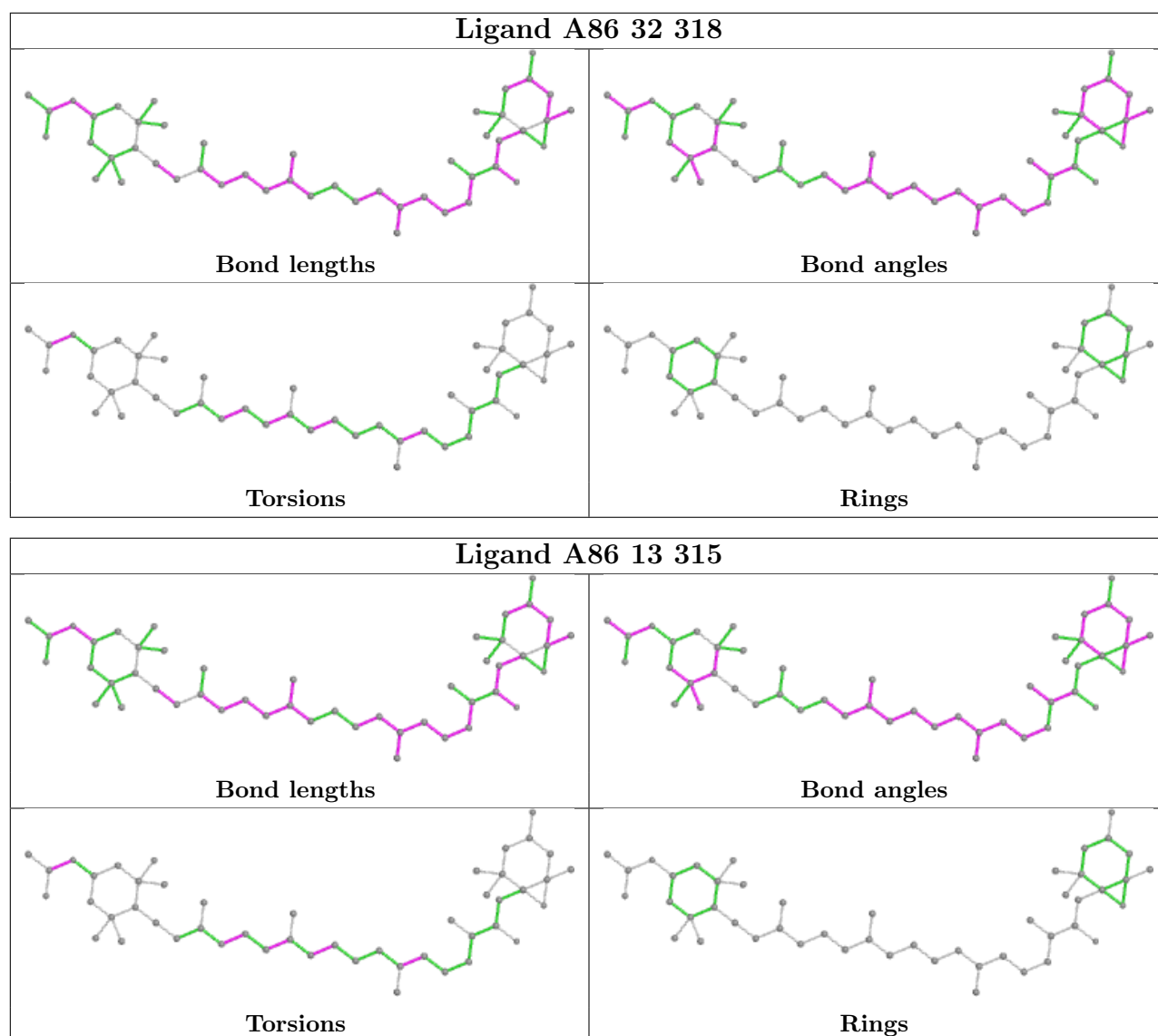


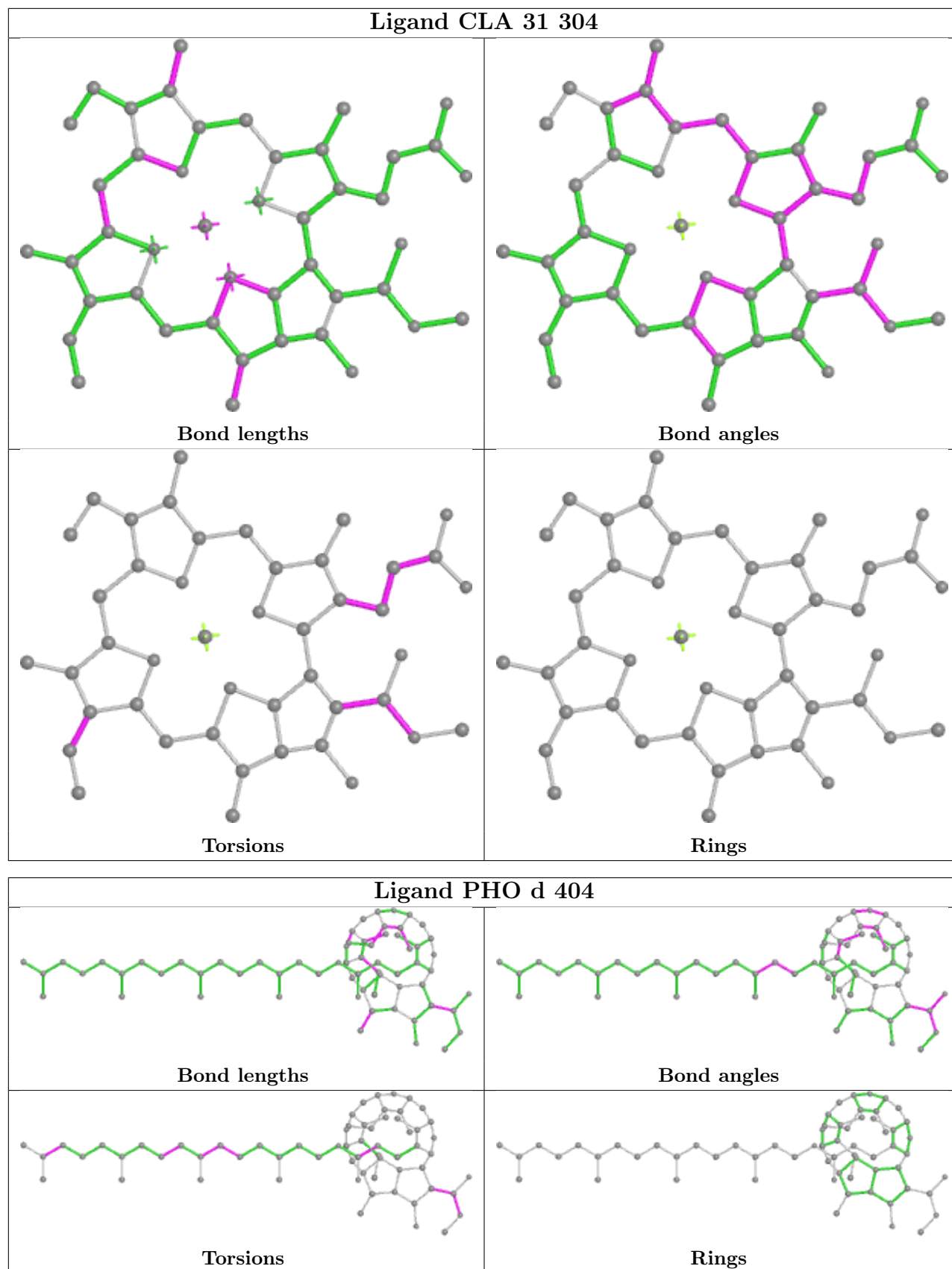
Ligand A86 40 213

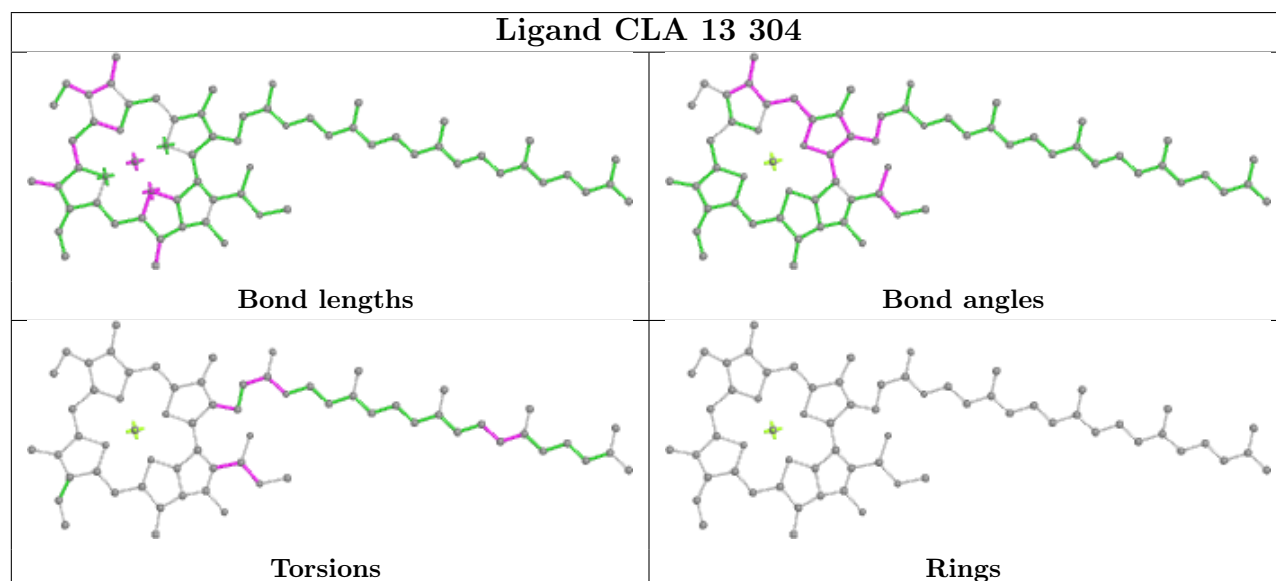
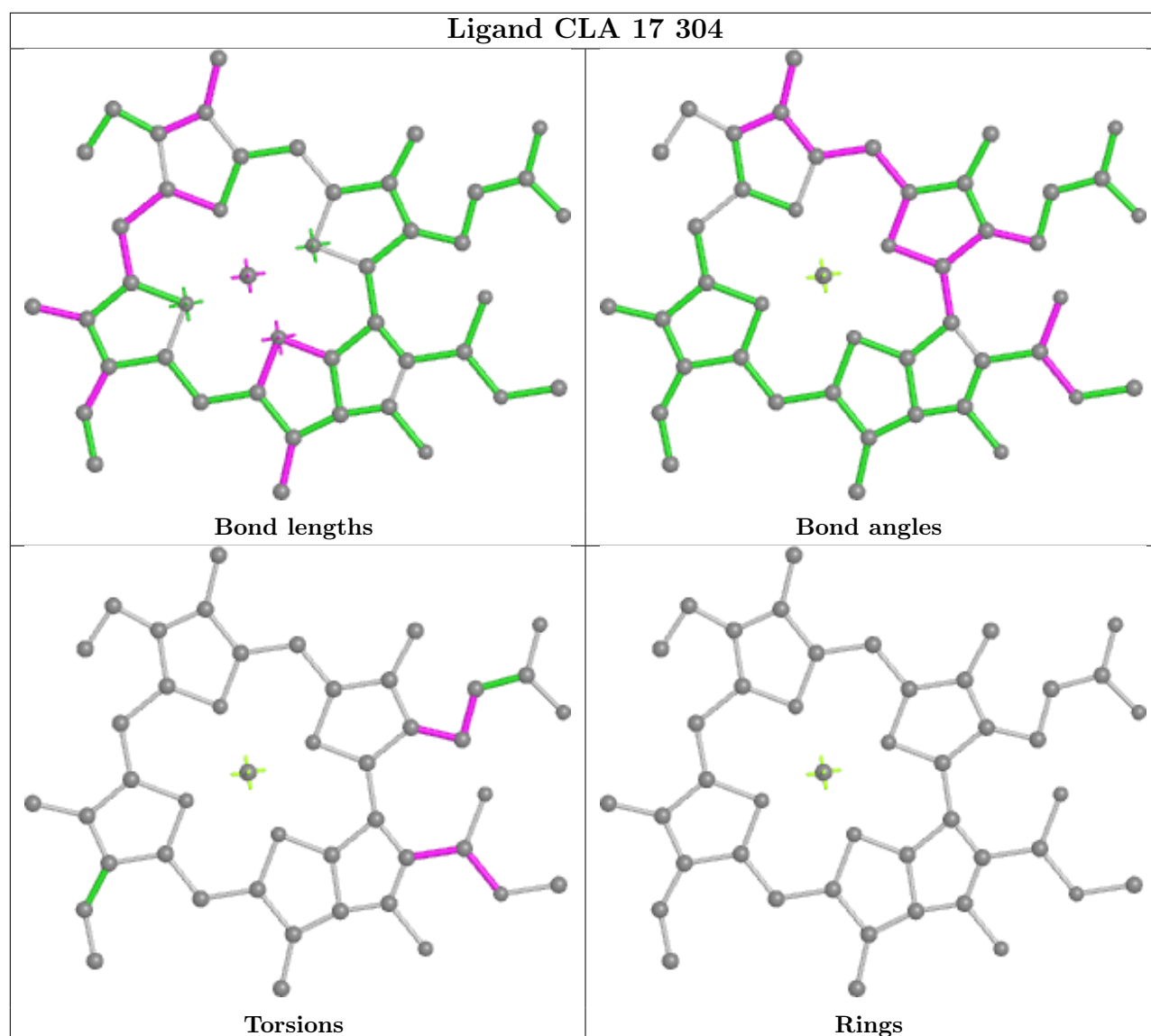


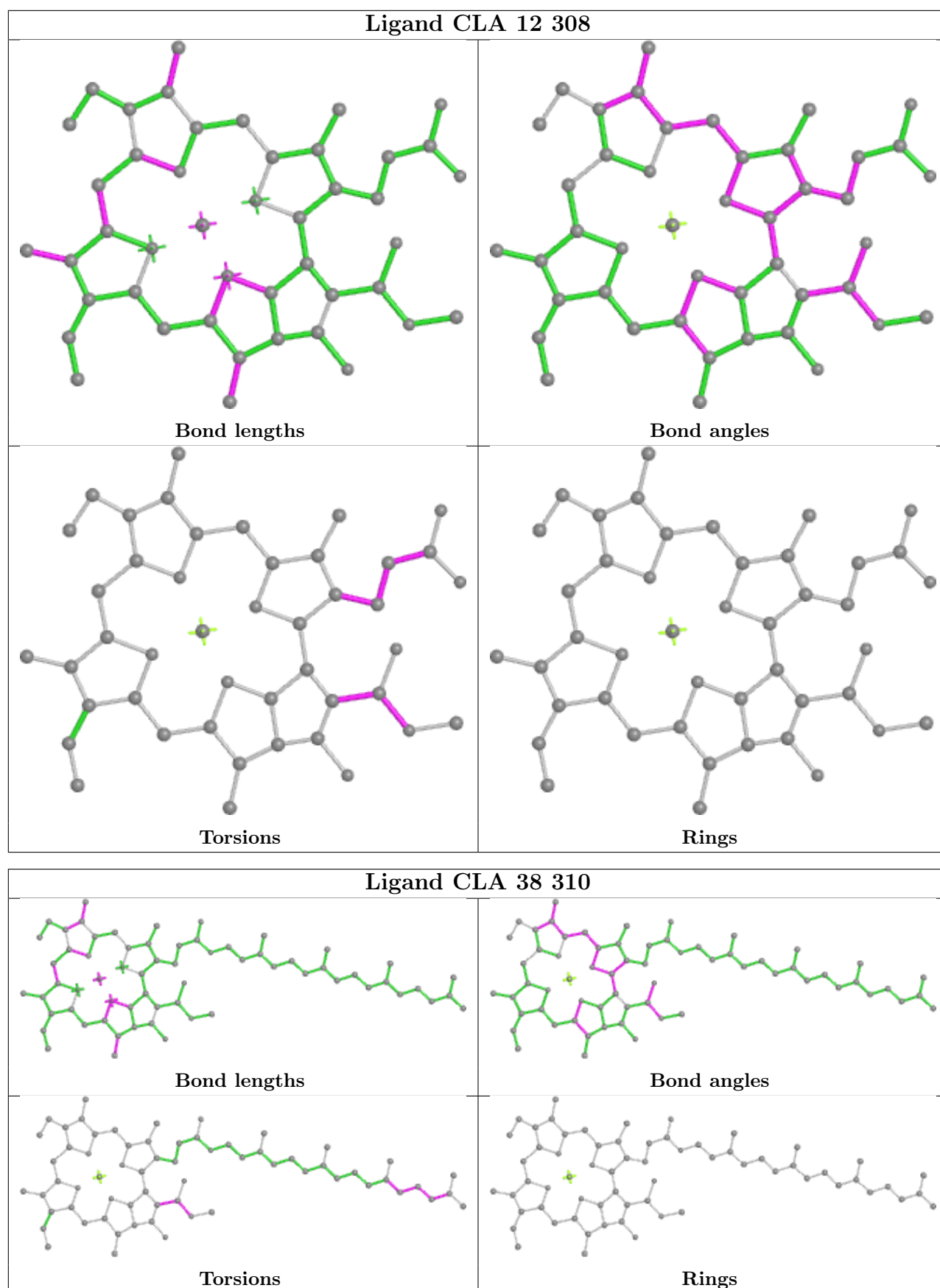
Ligand CLA 11 308

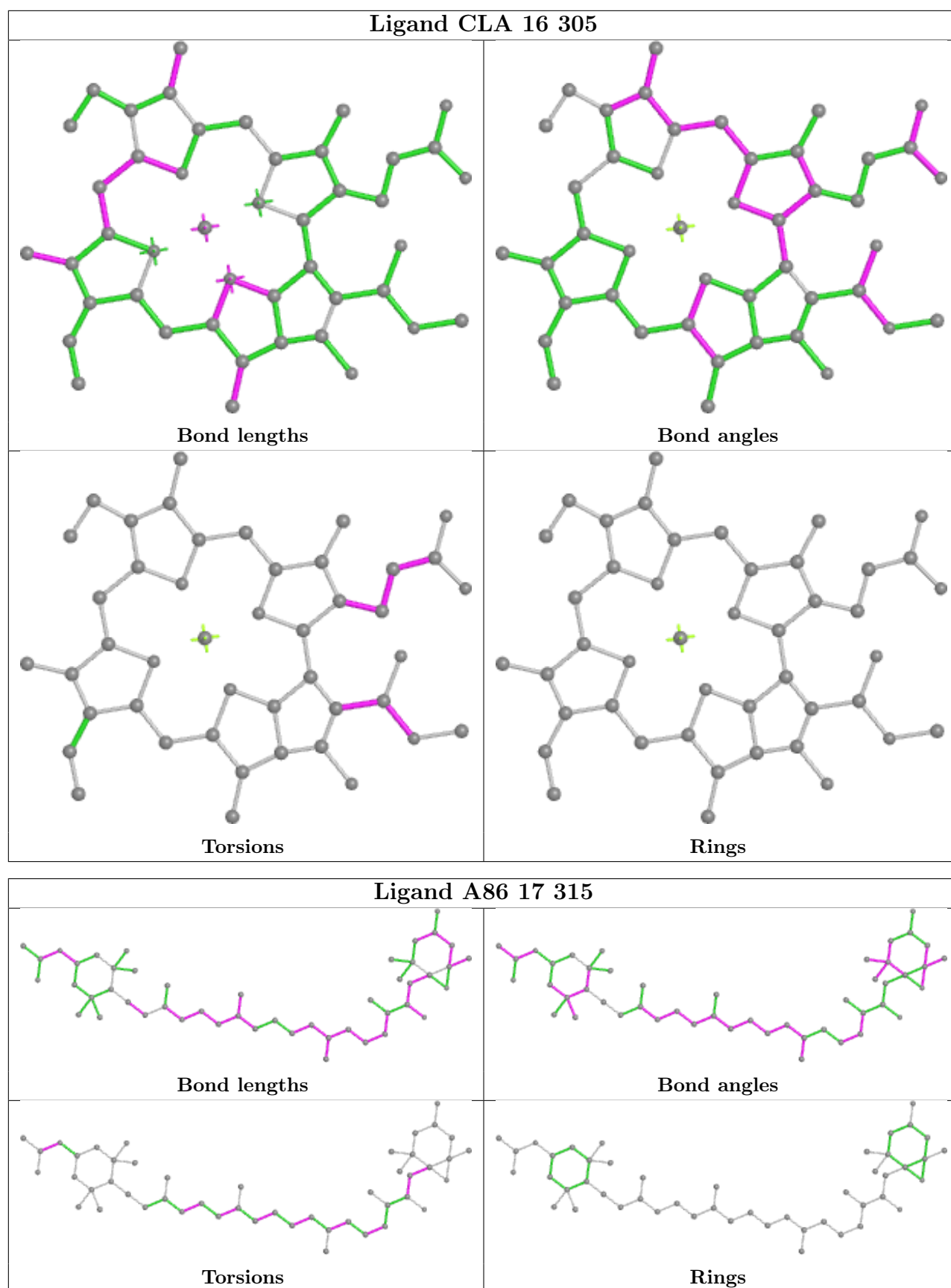


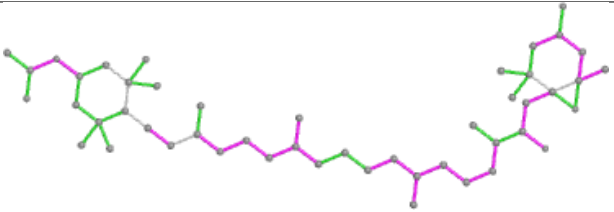
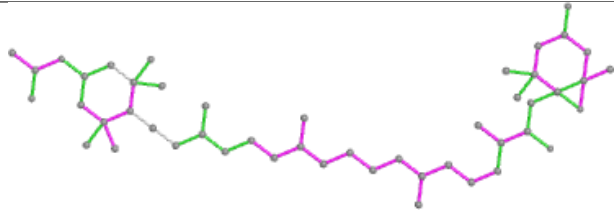
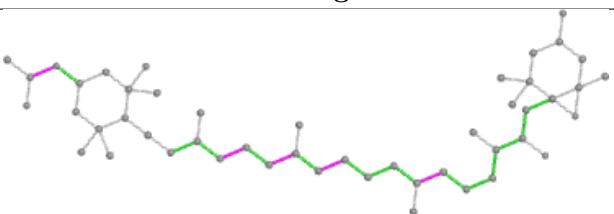
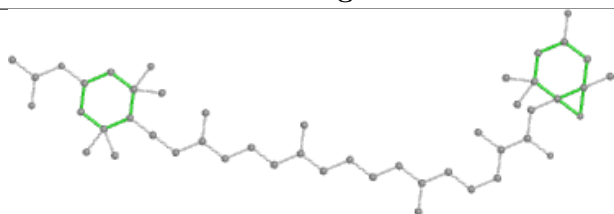


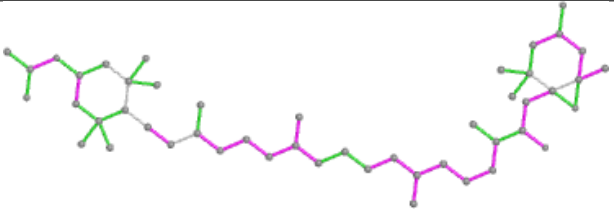
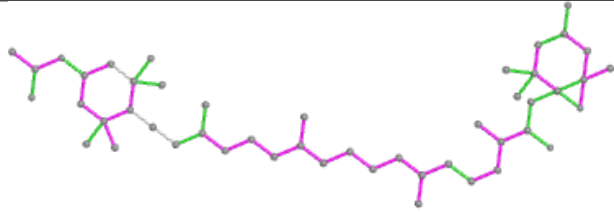
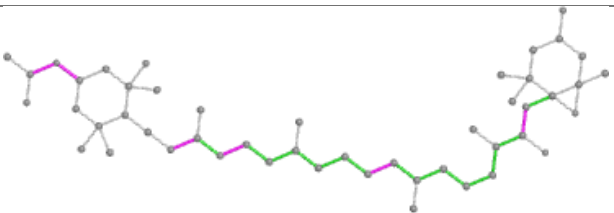
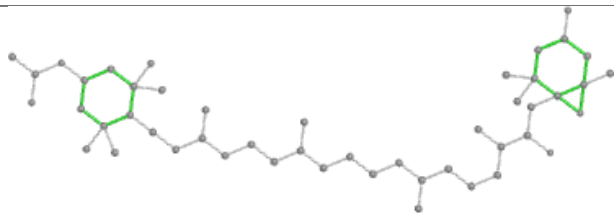


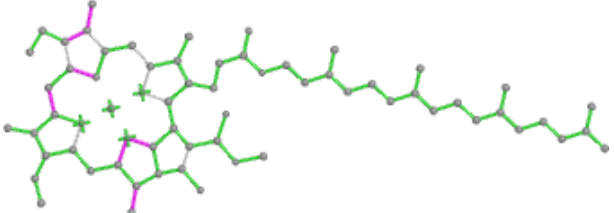
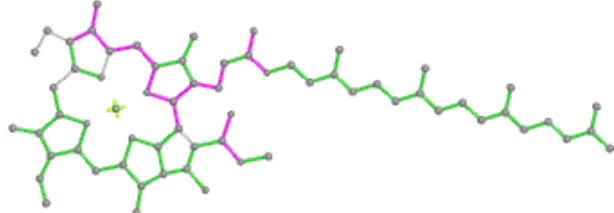
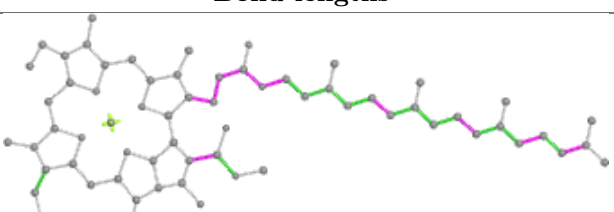
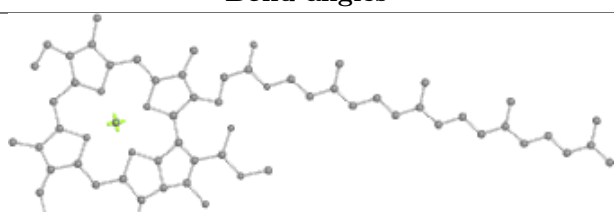


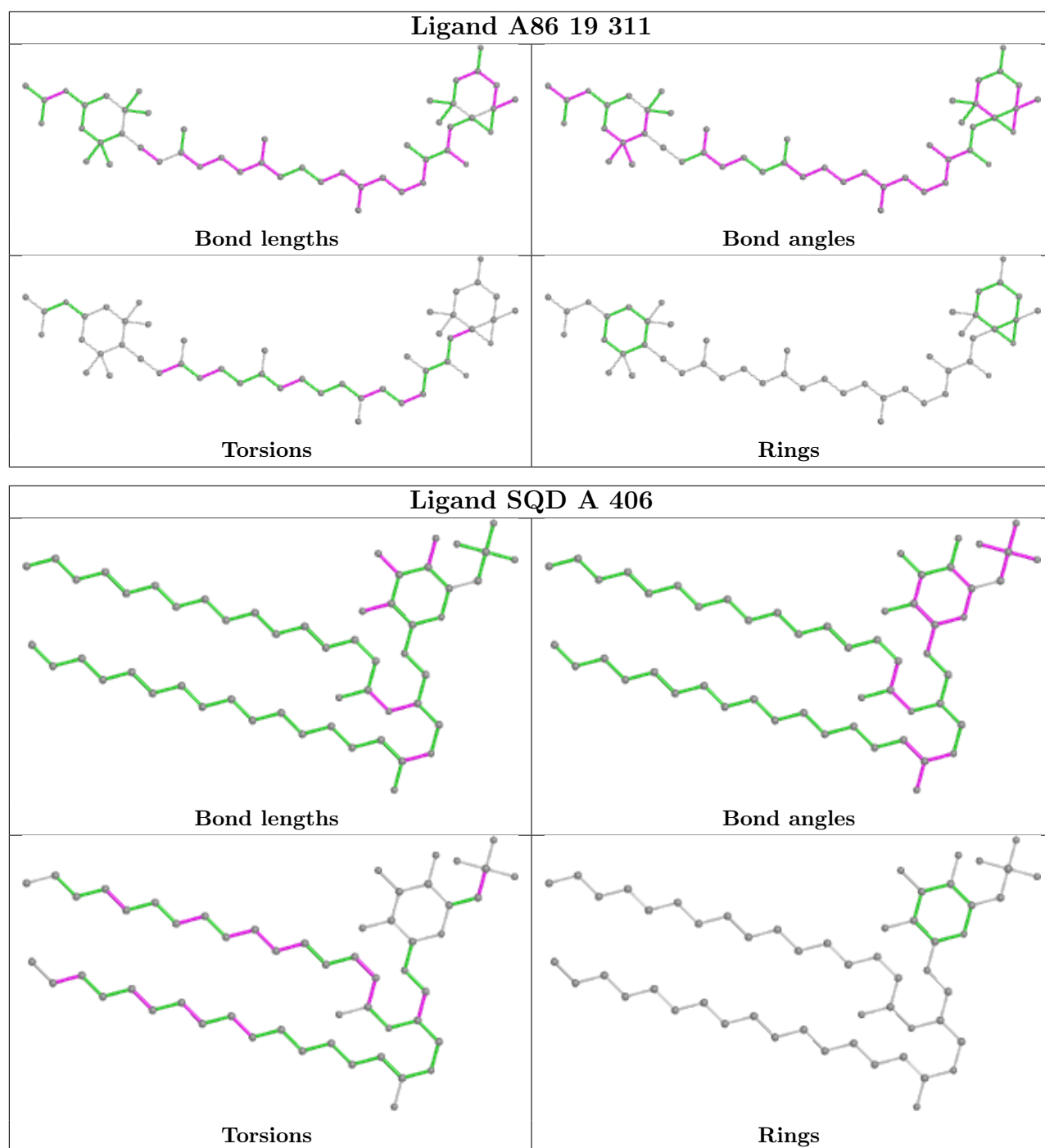


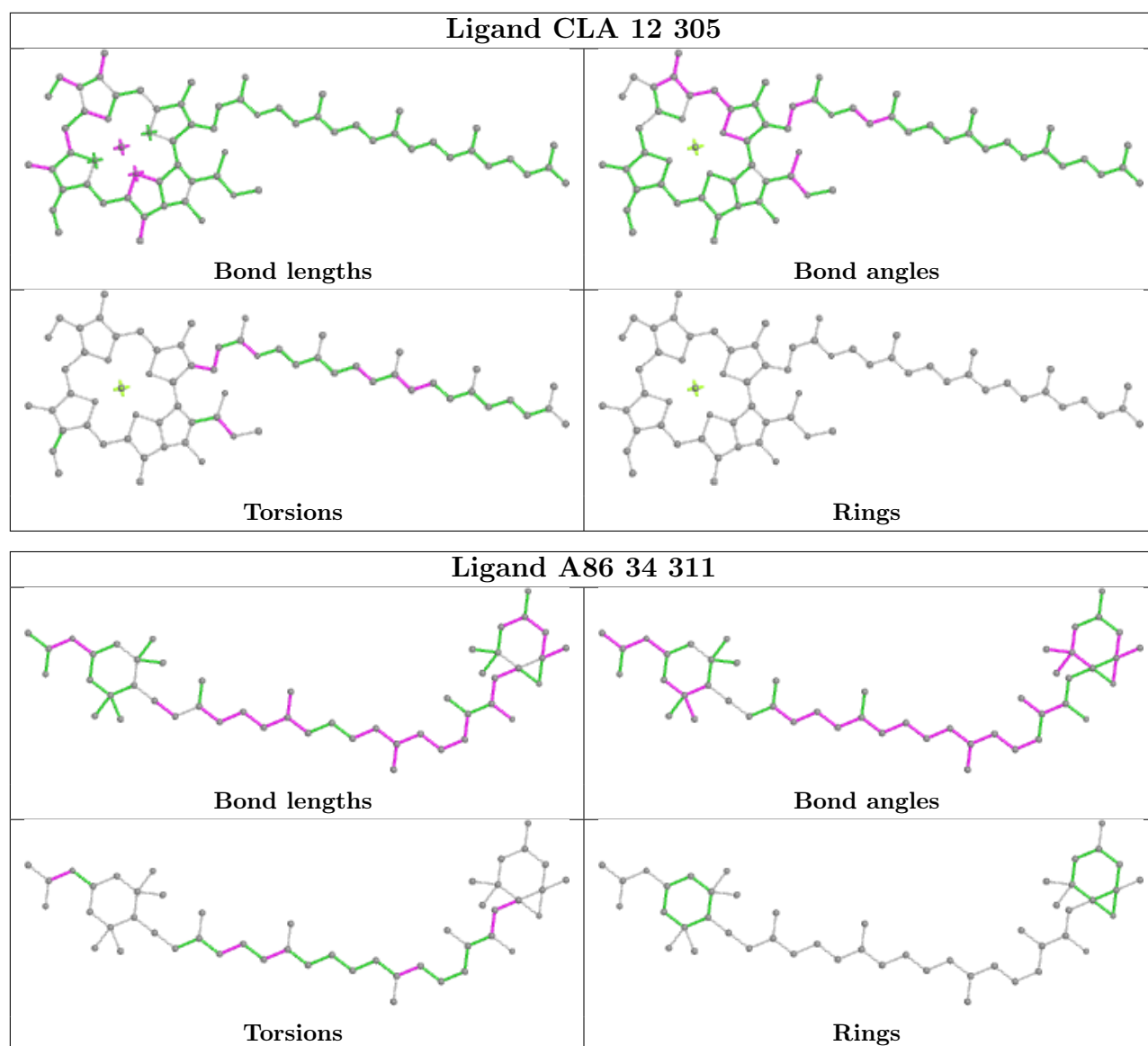


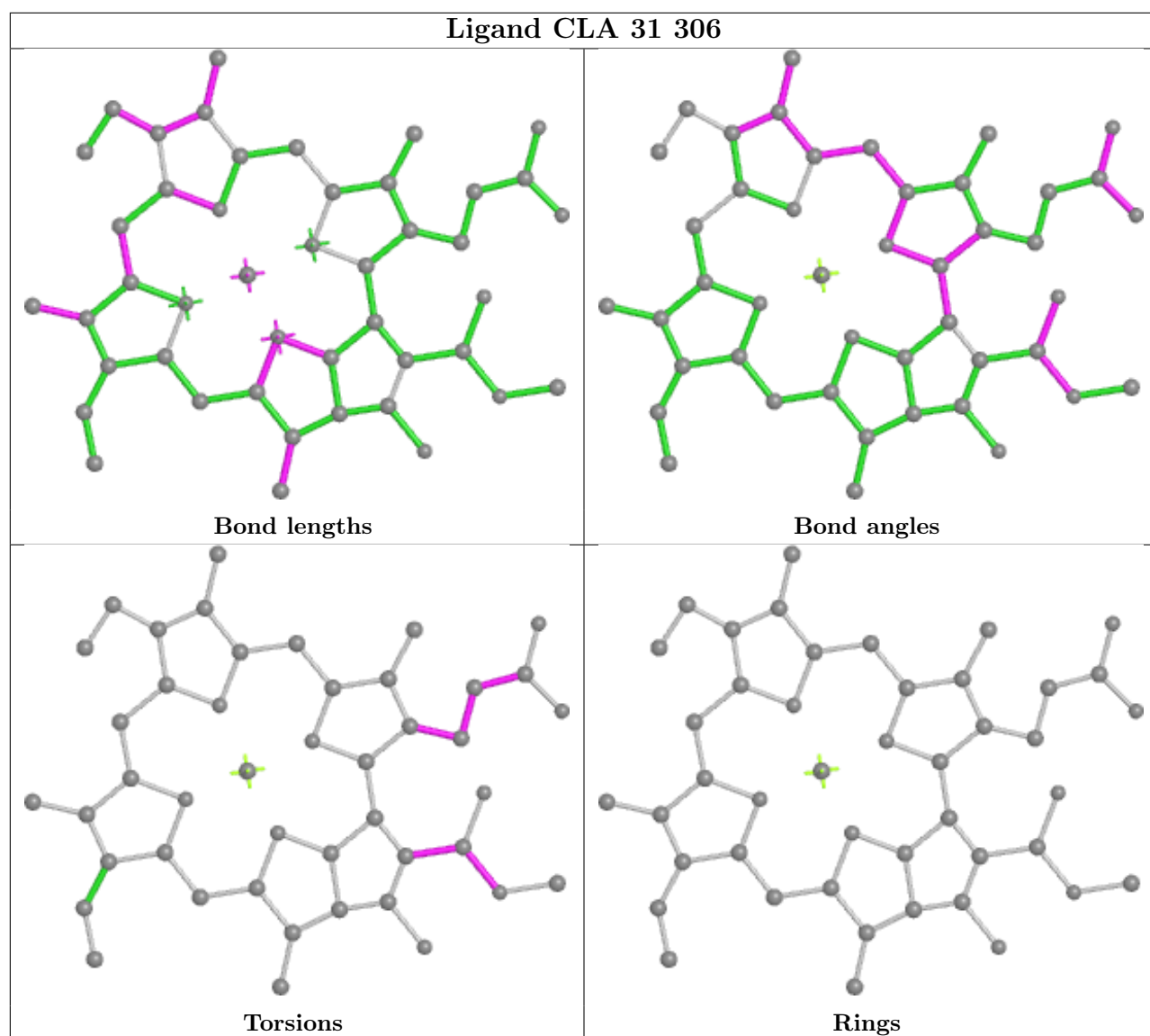
Ligand A86 16 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

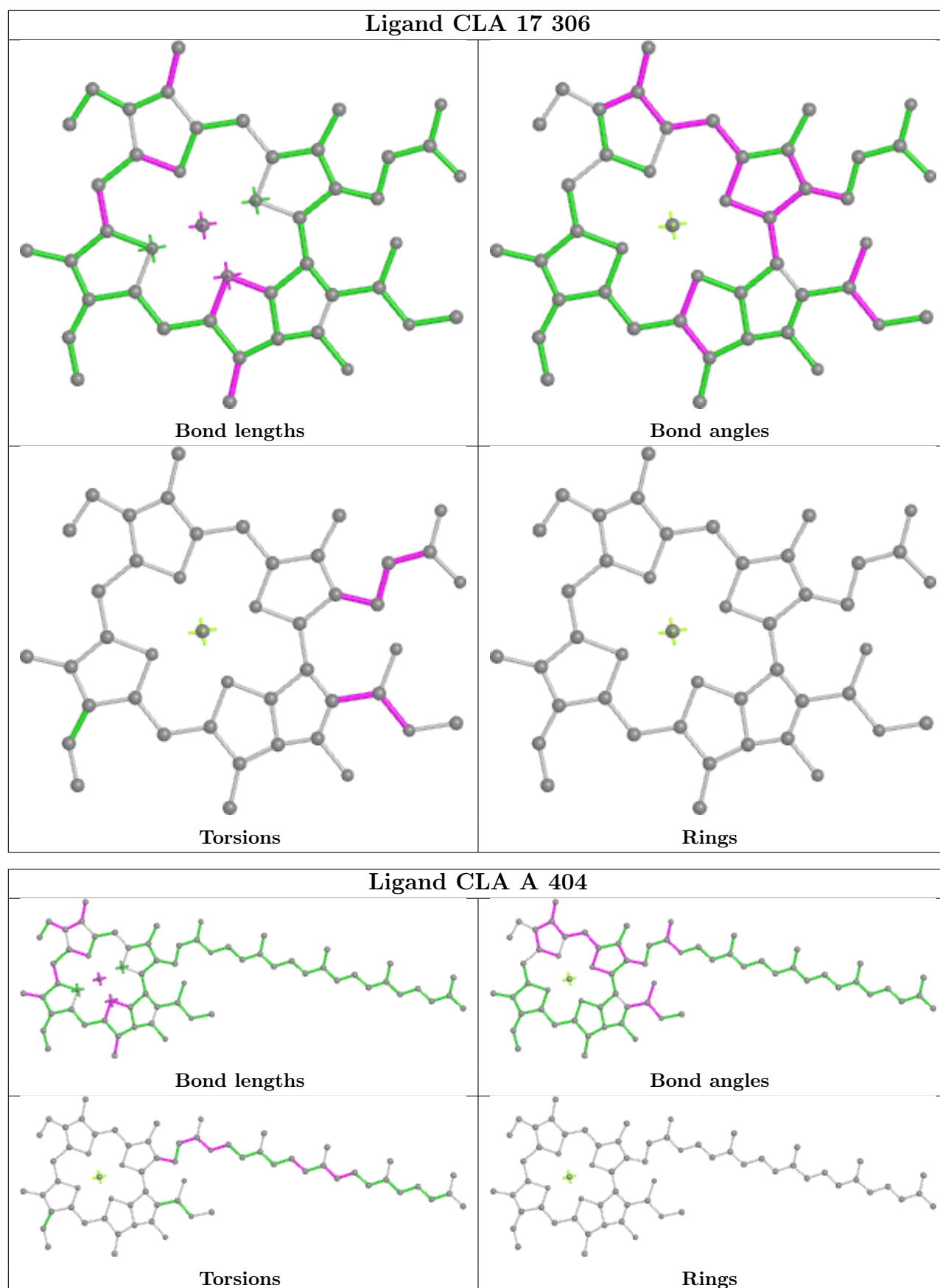
Ligand A86 31 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

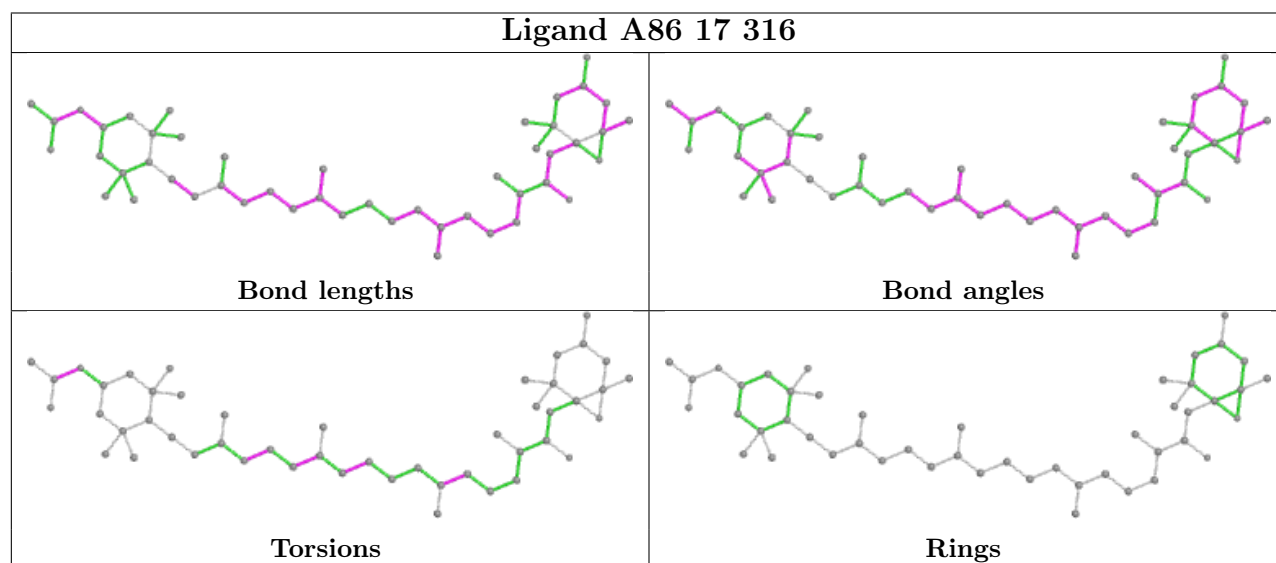
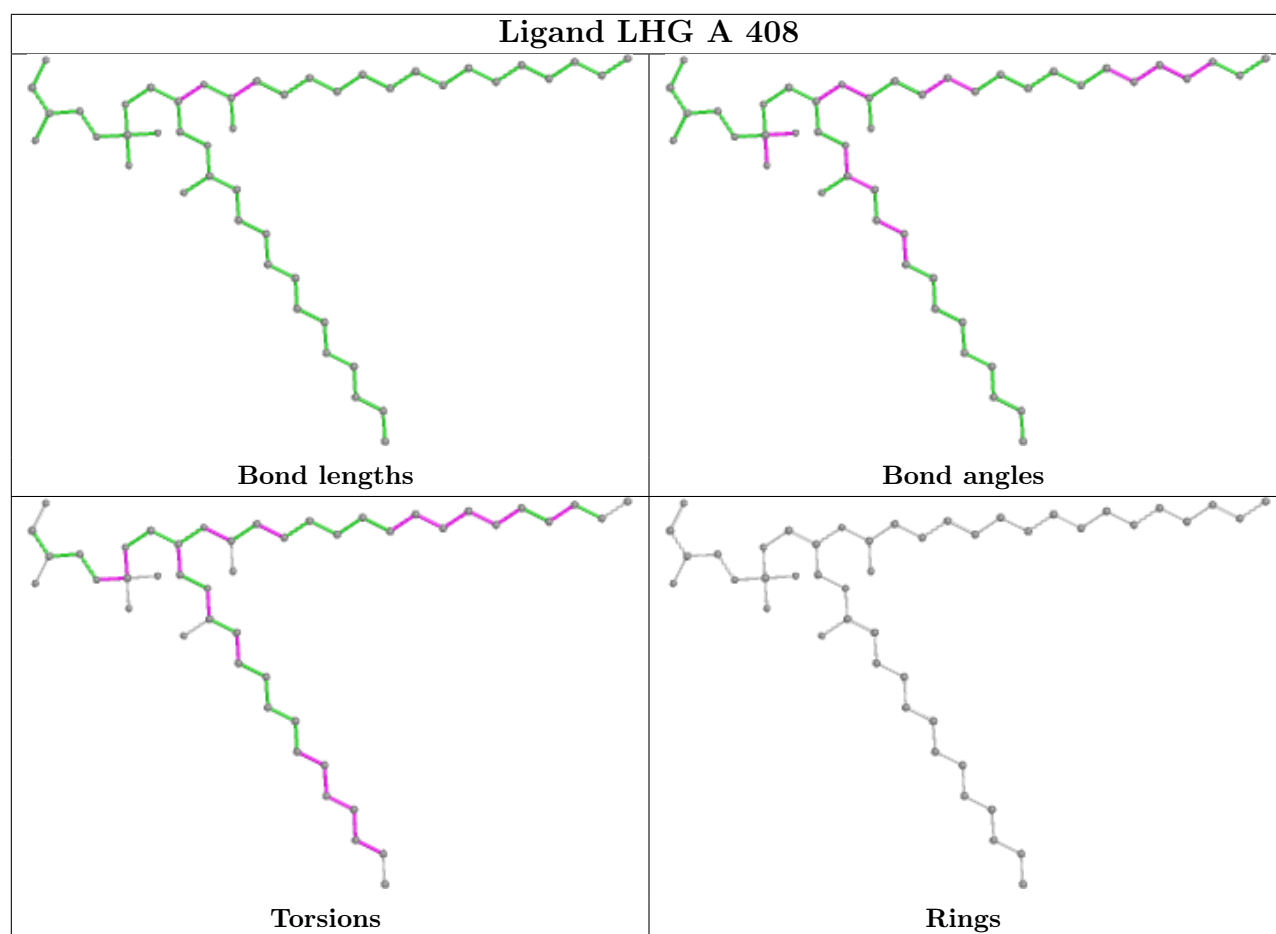
Ligand CLA 41 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

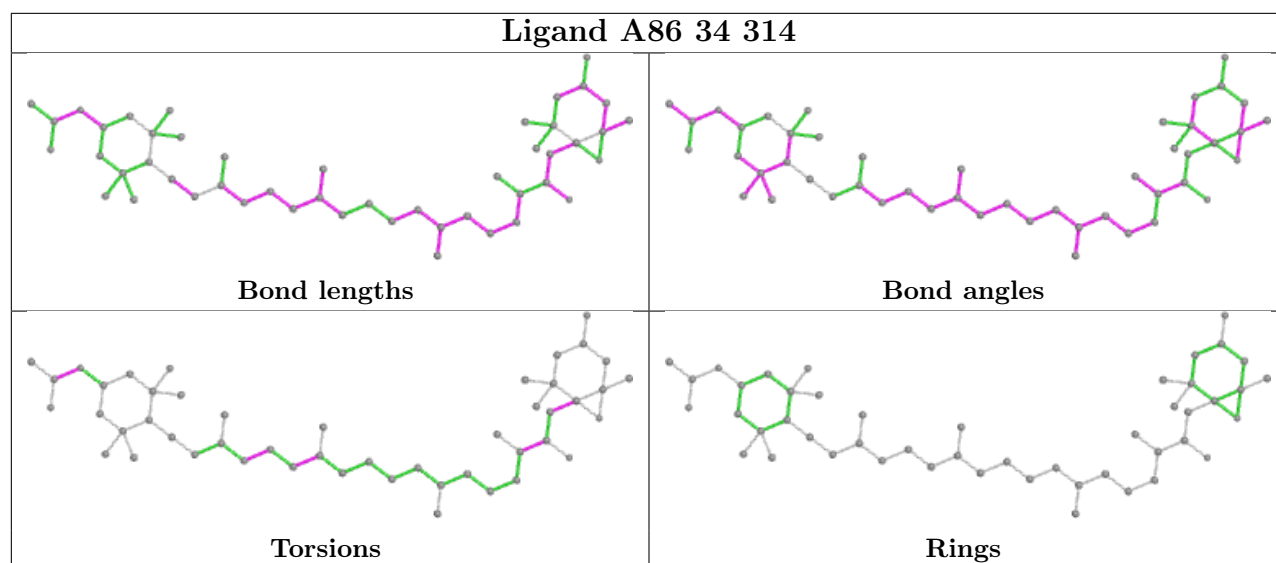
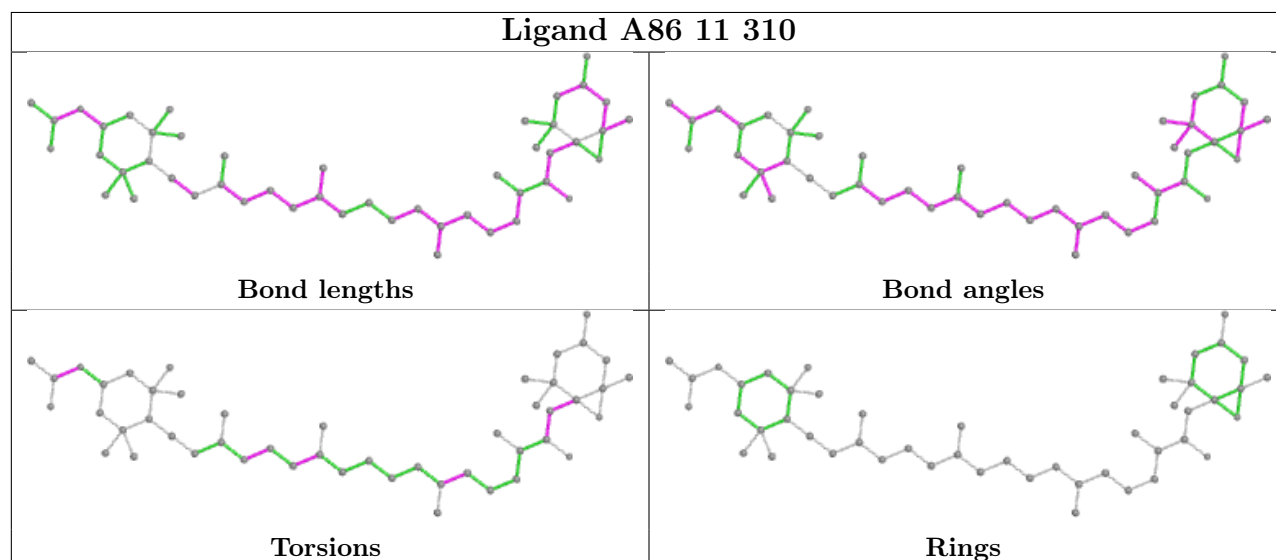
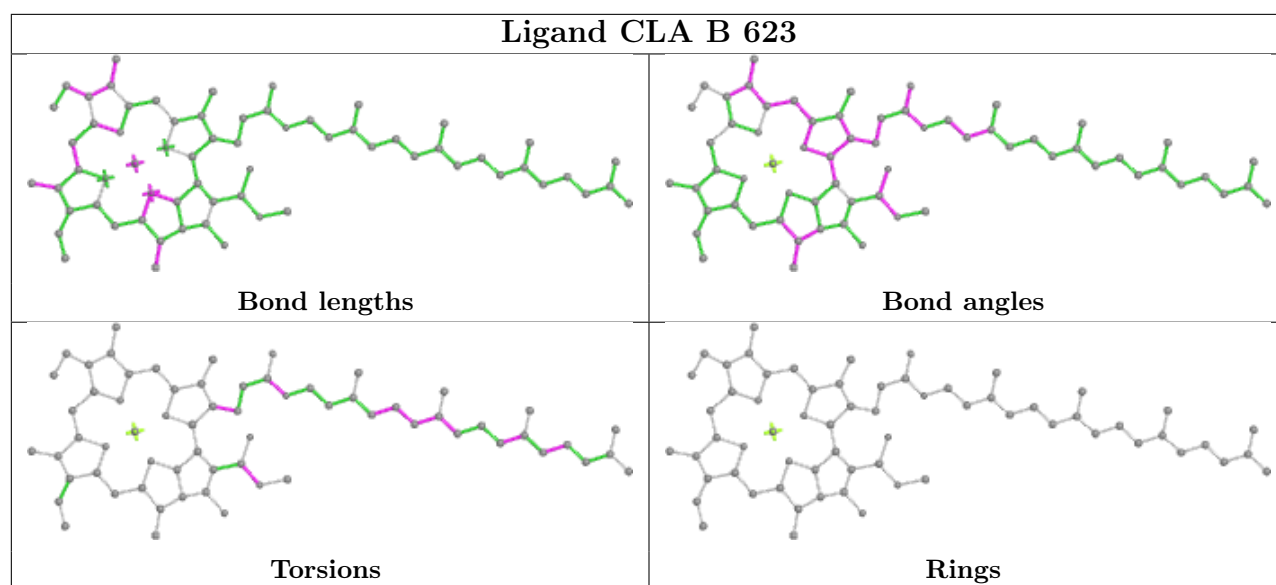


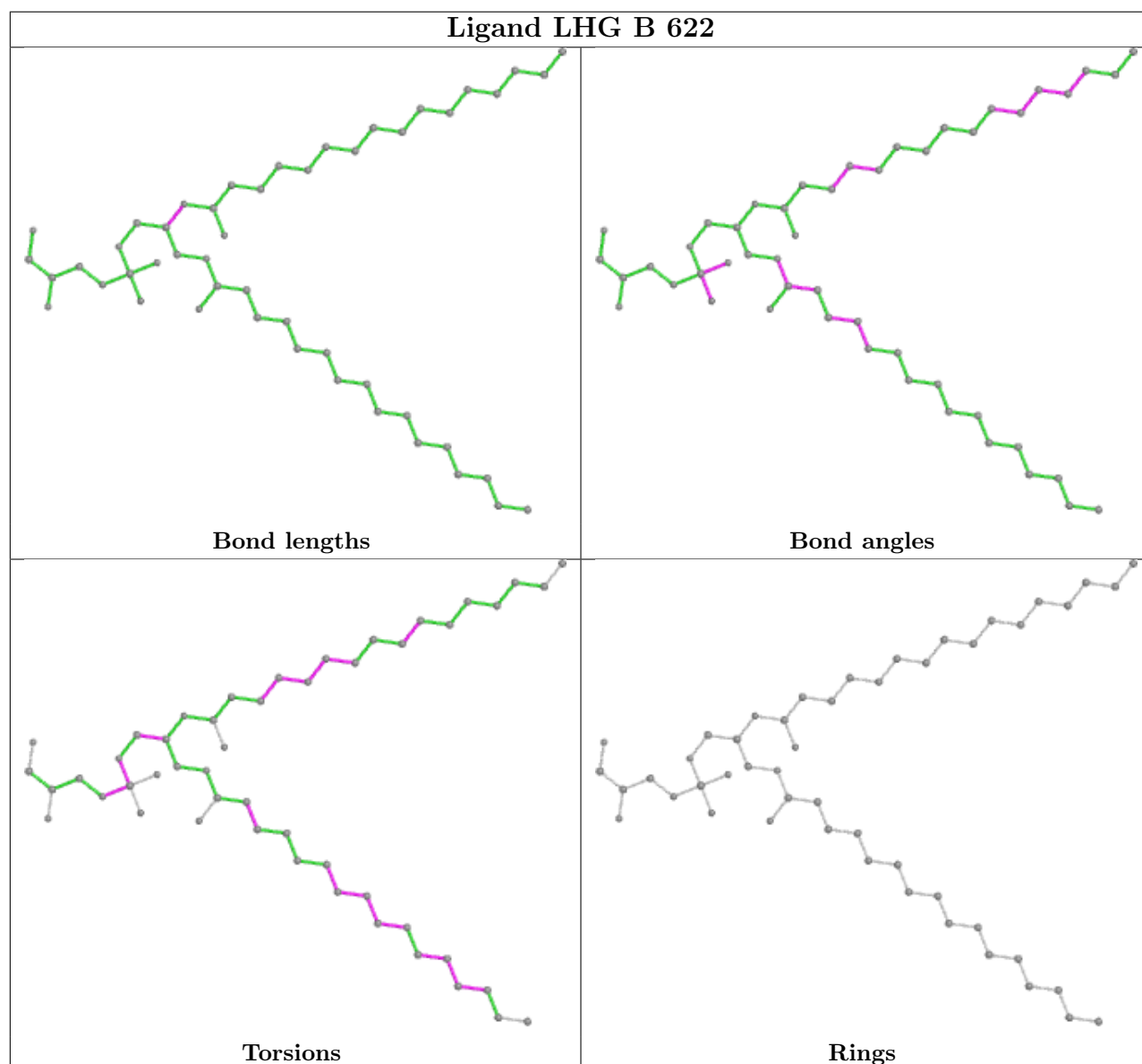
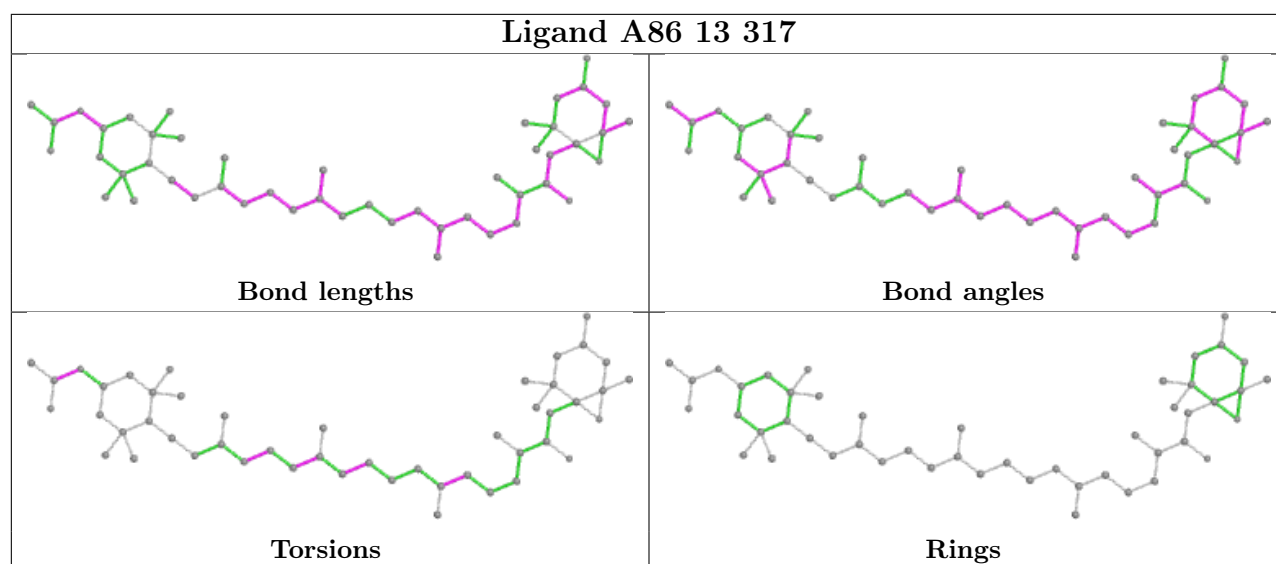


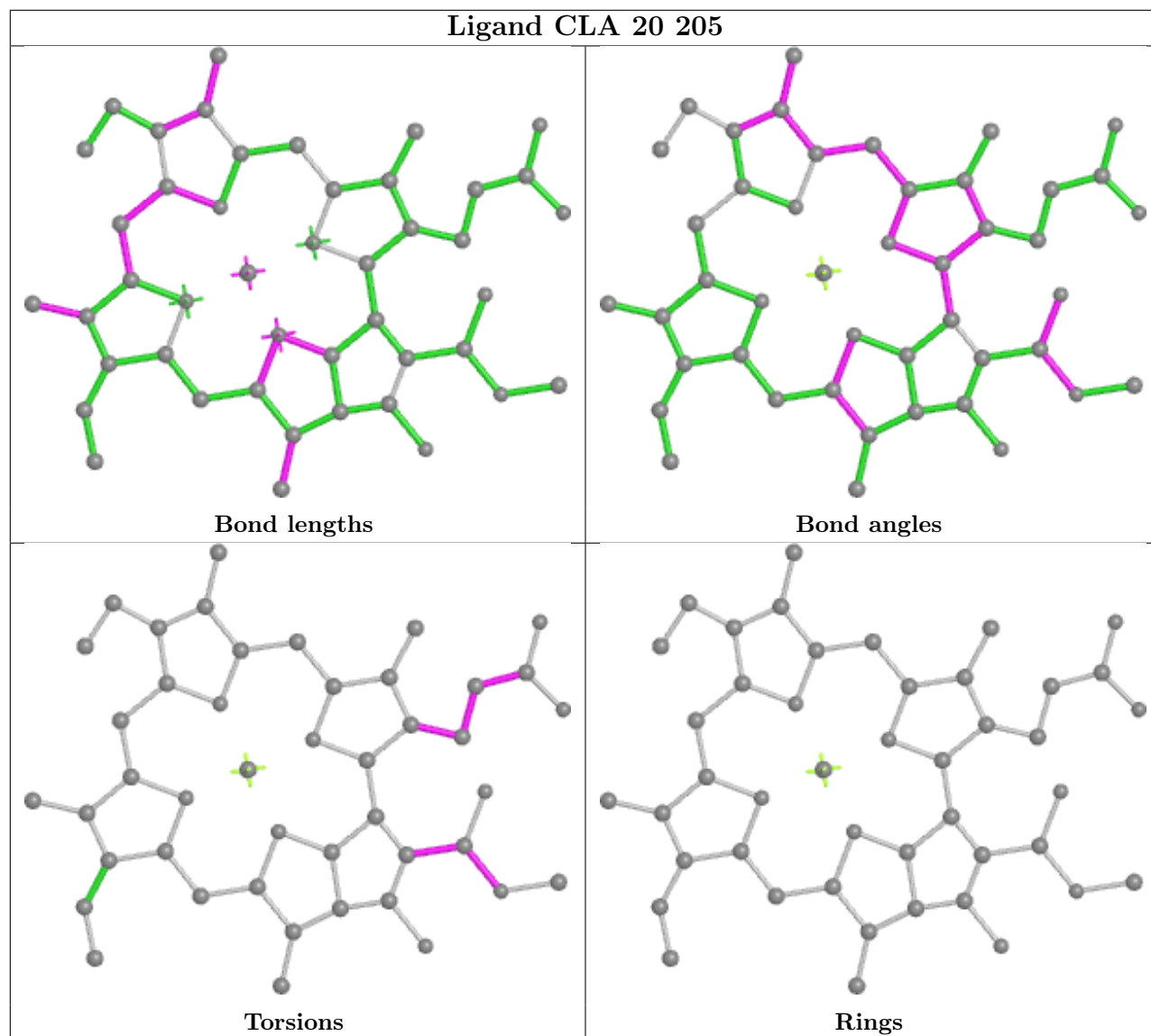
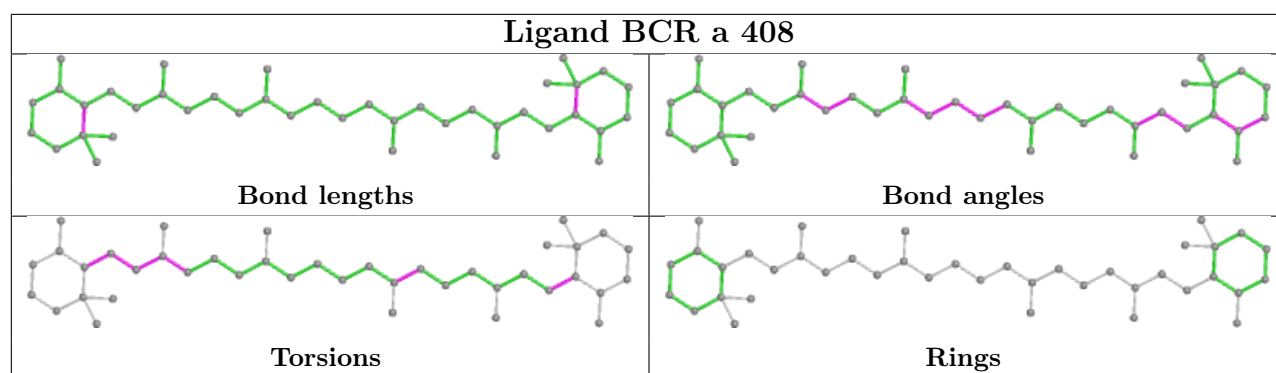


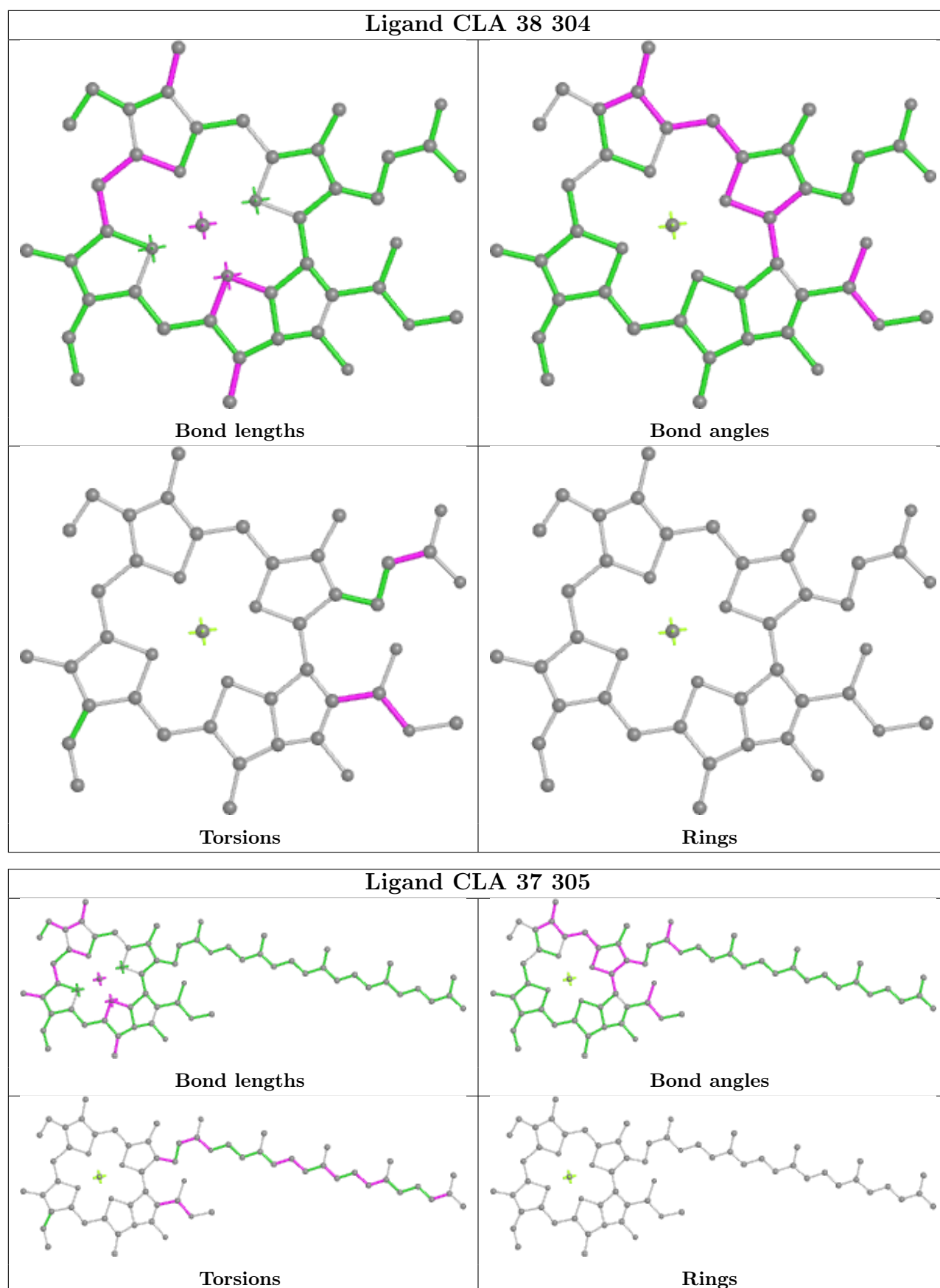


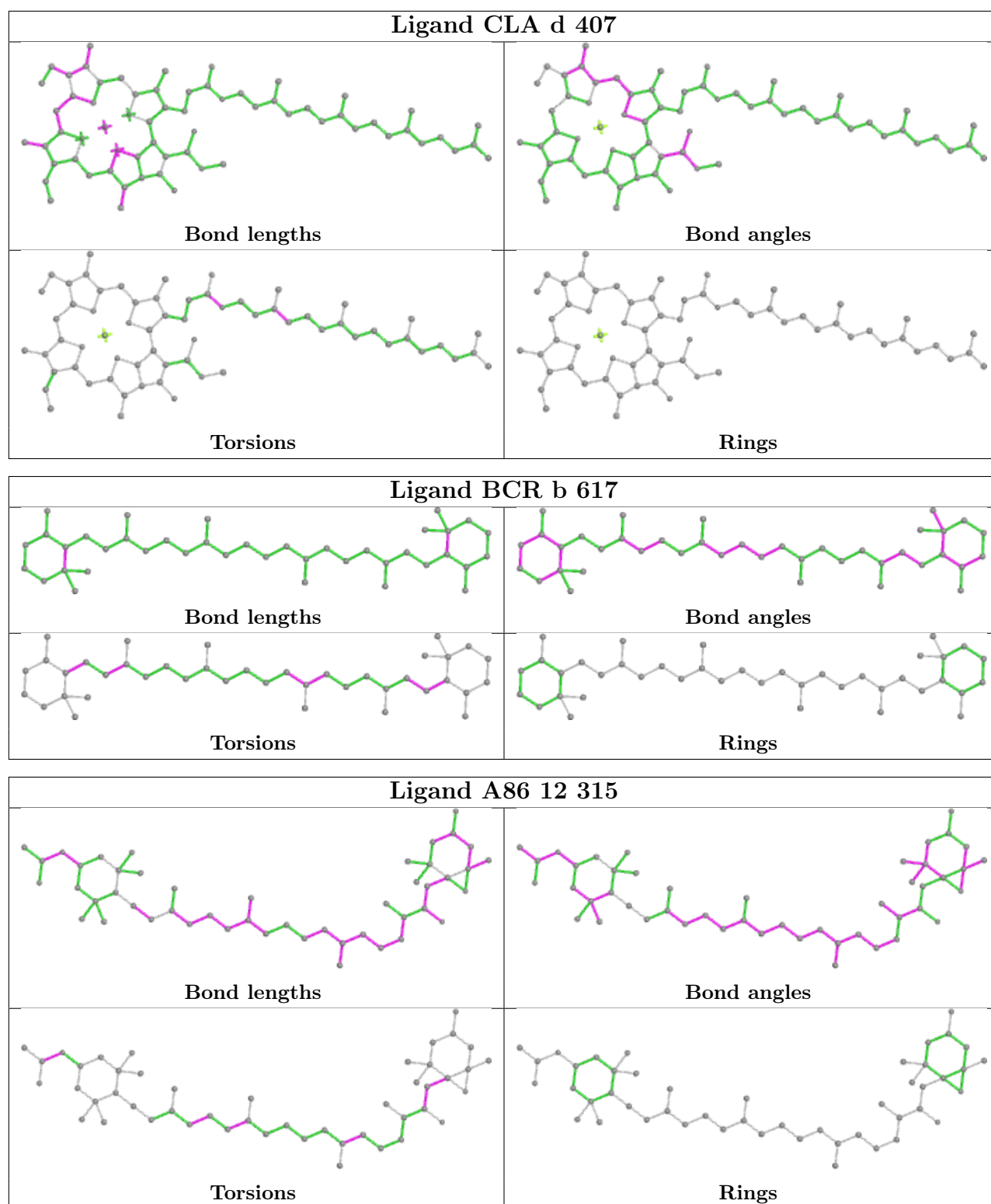


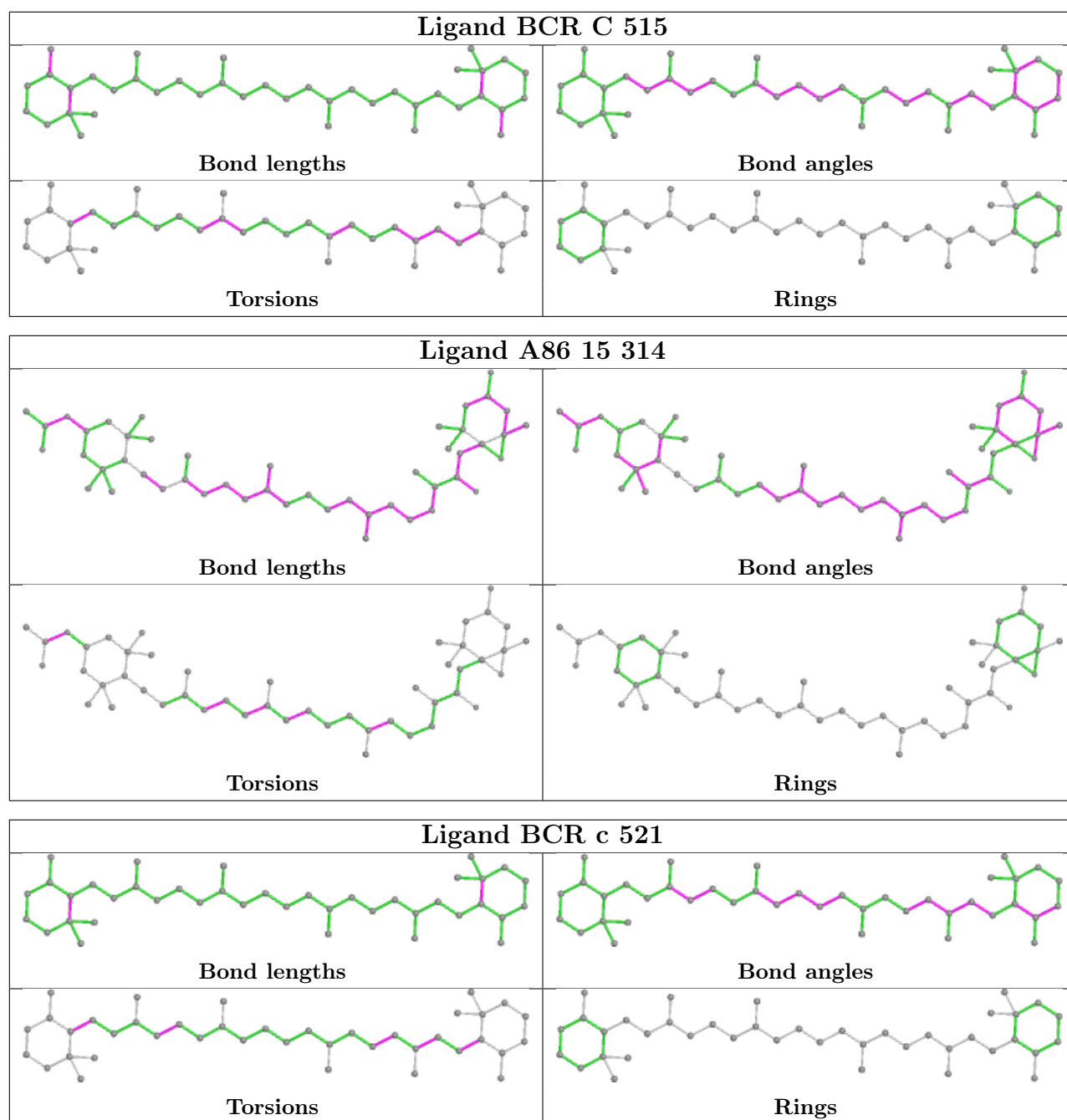


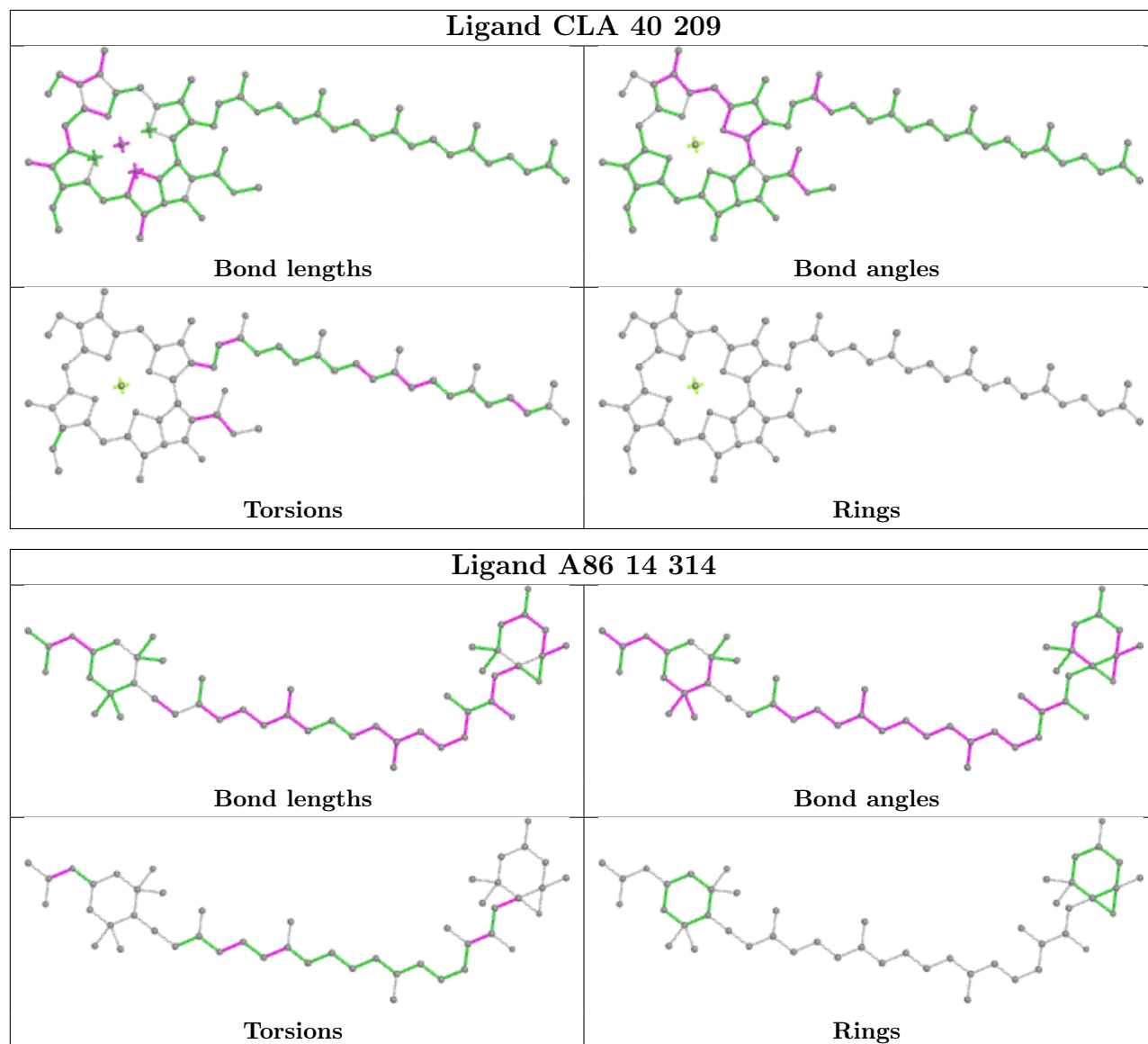


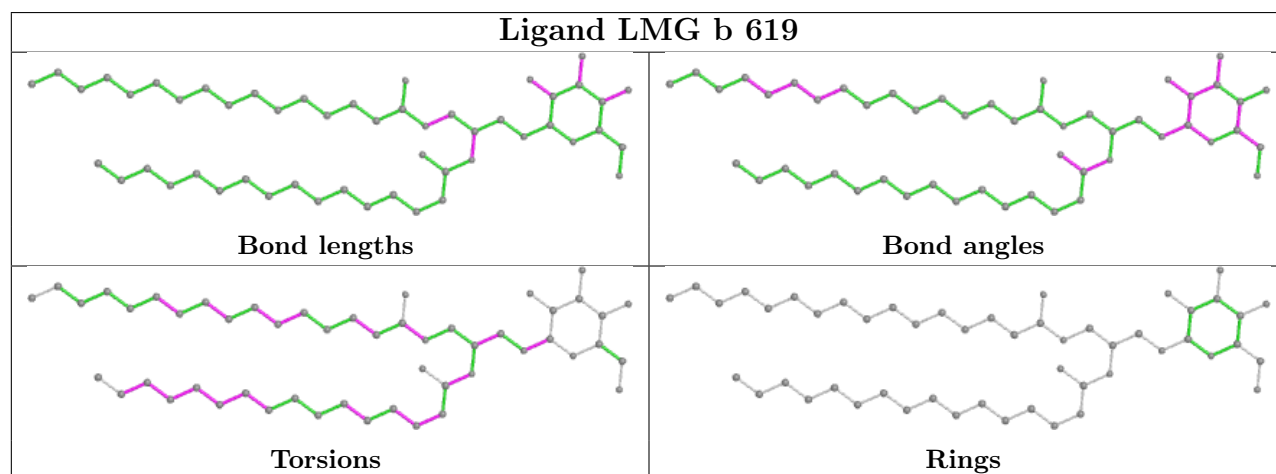
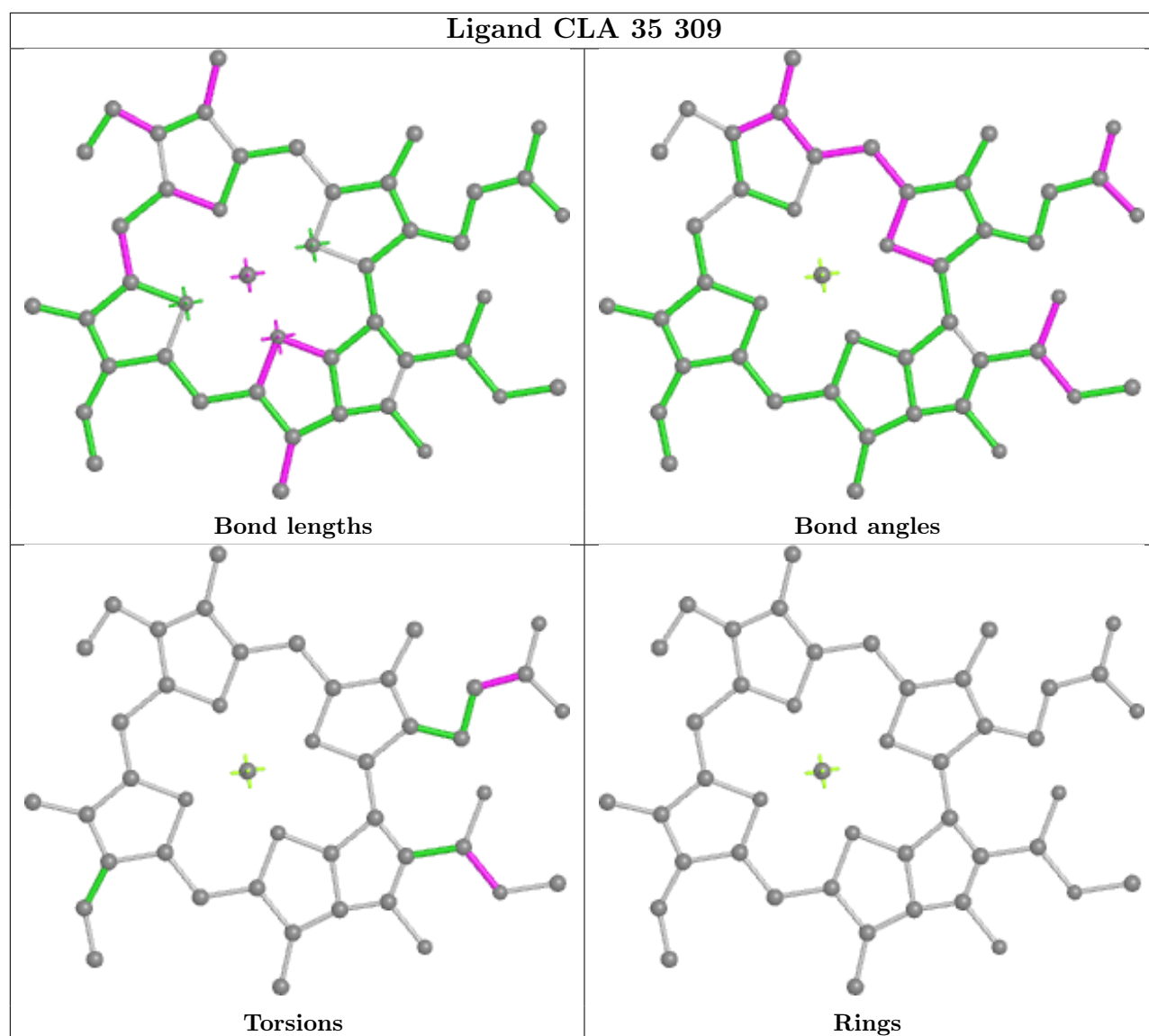


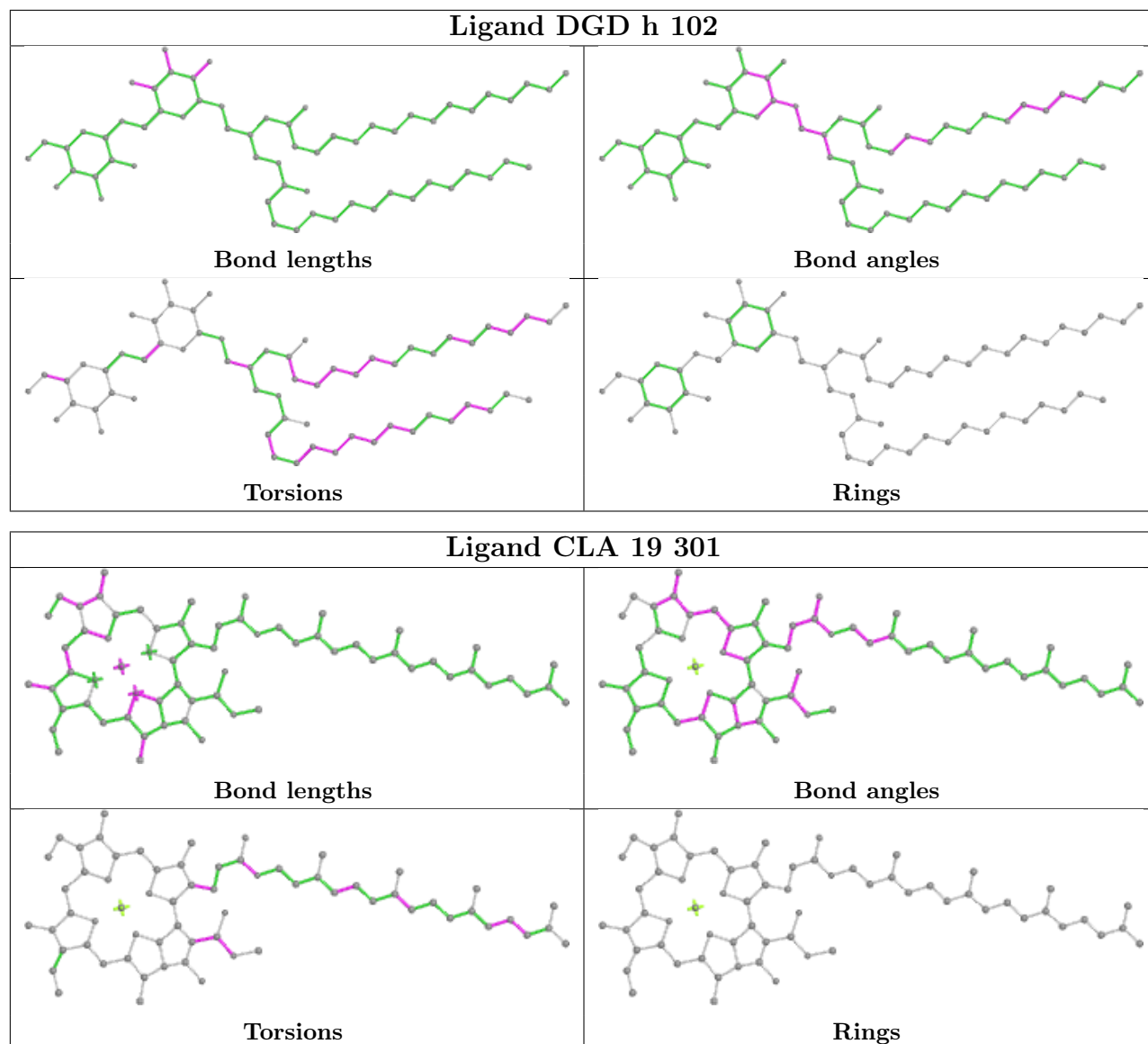


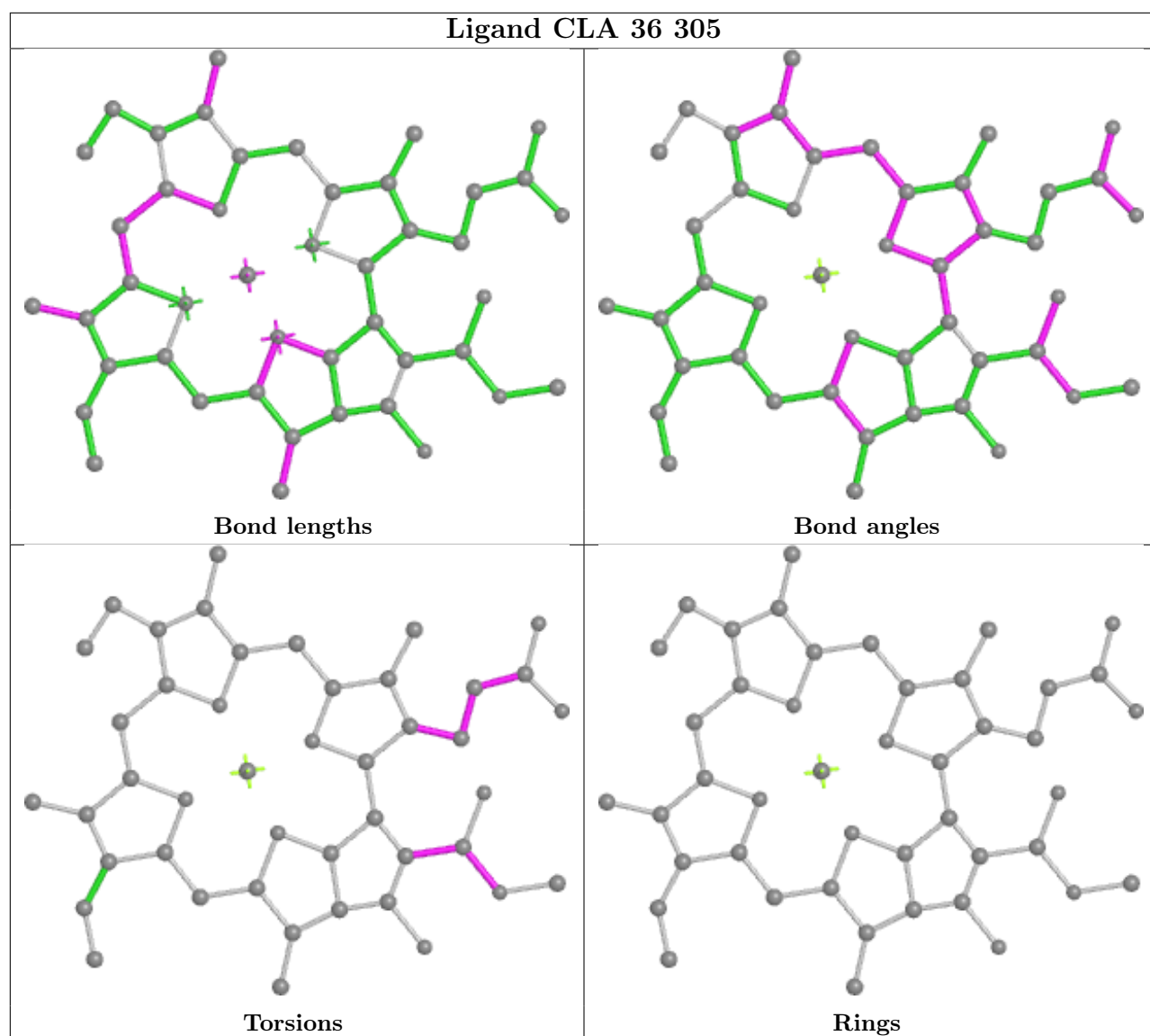


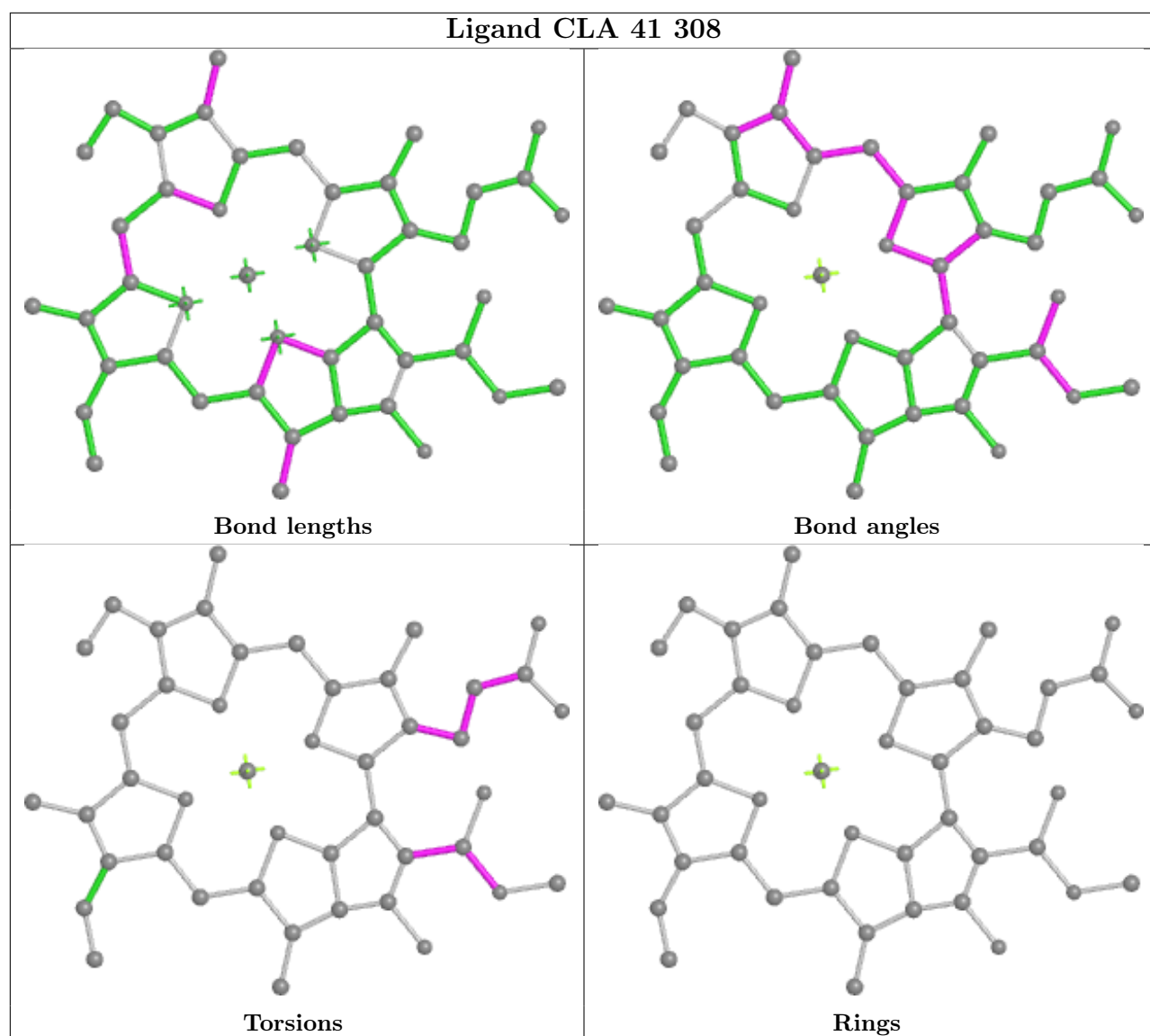


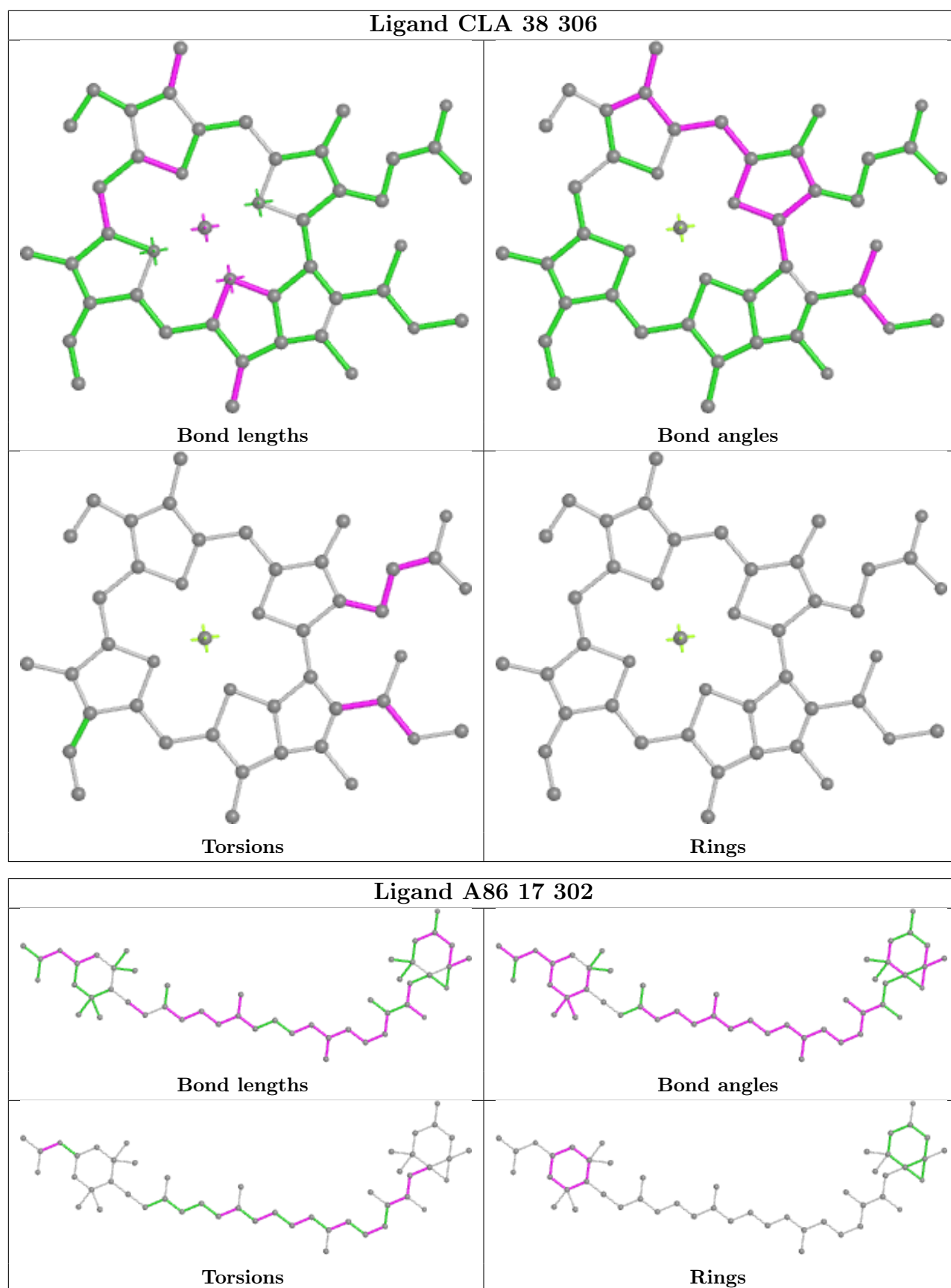


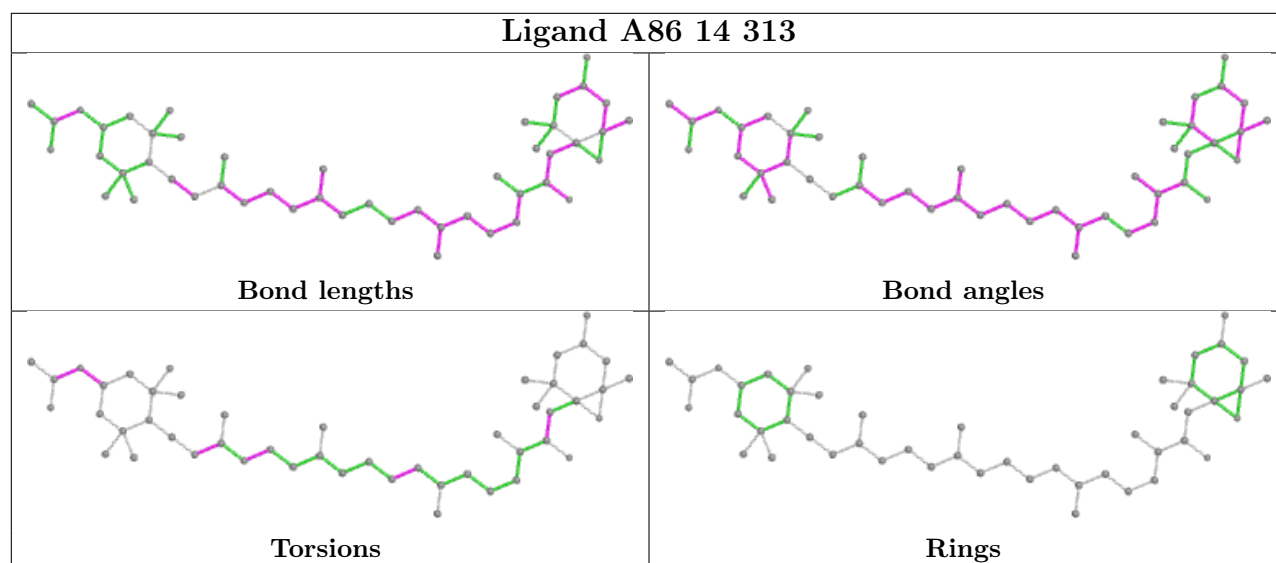
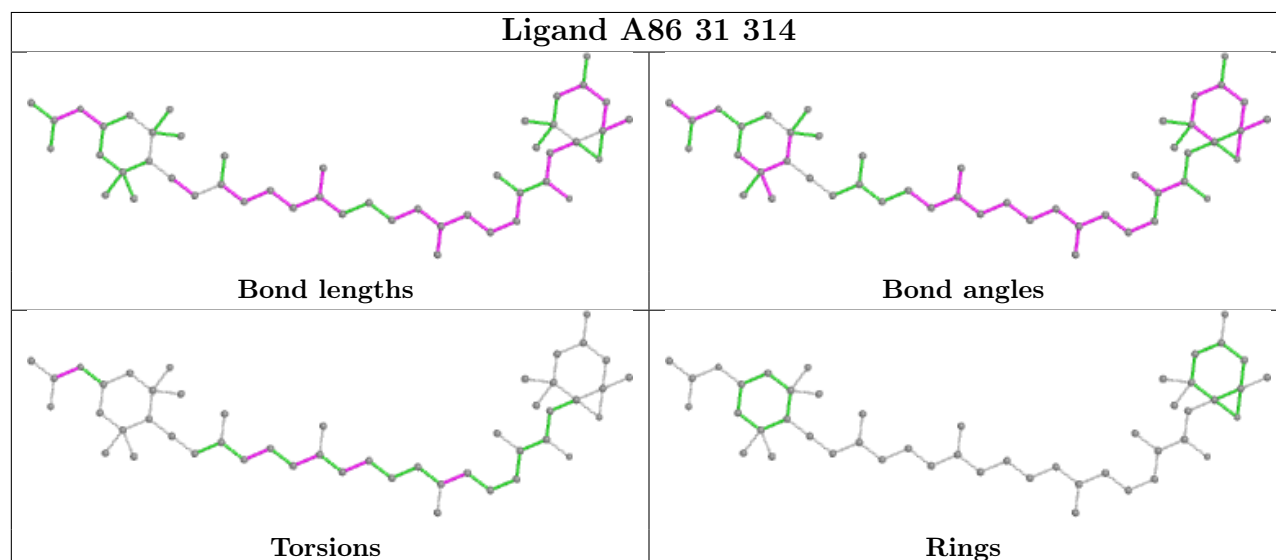
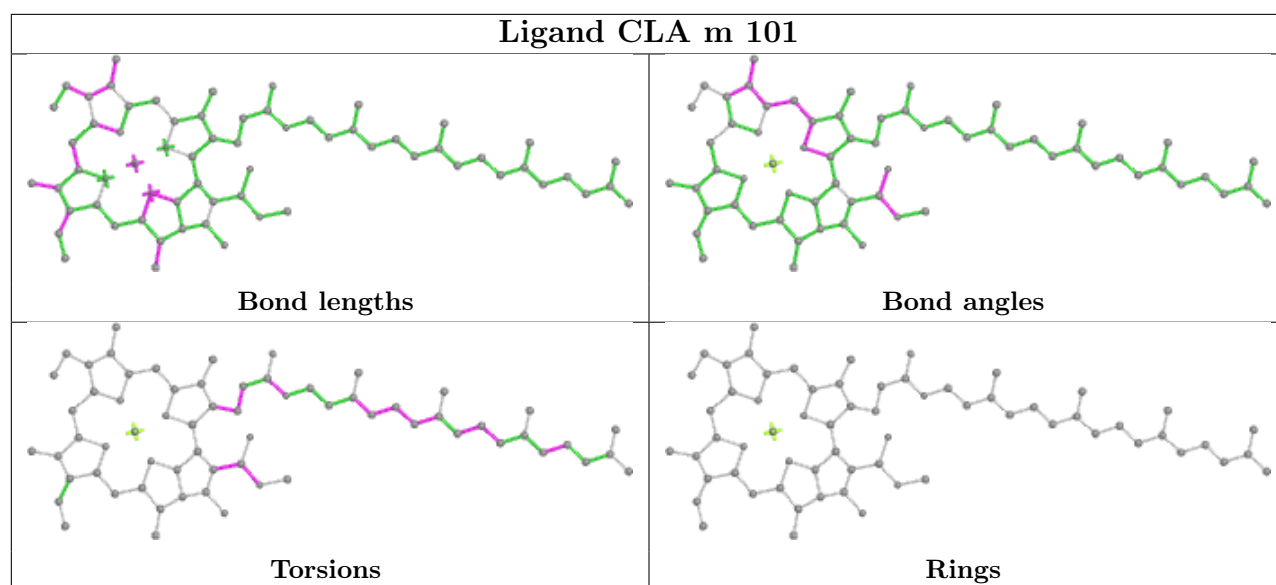


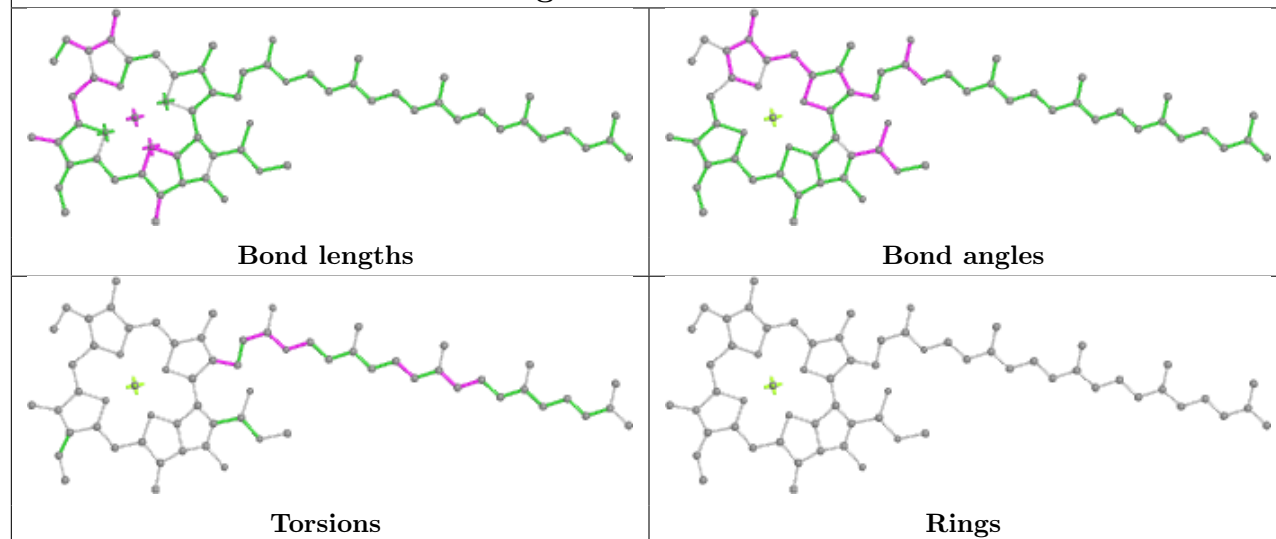
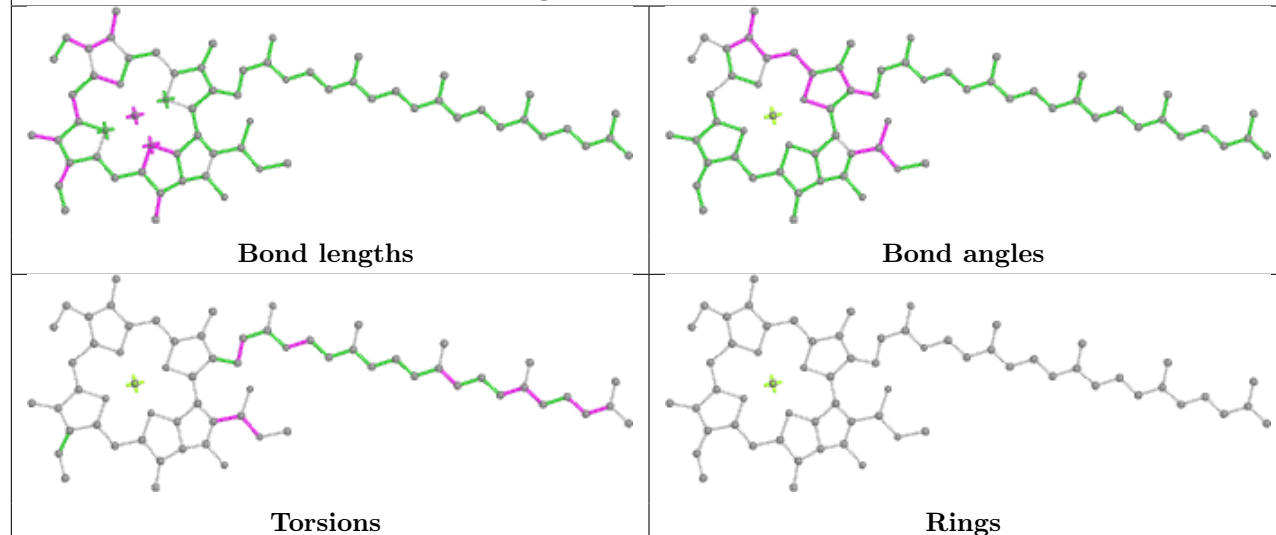
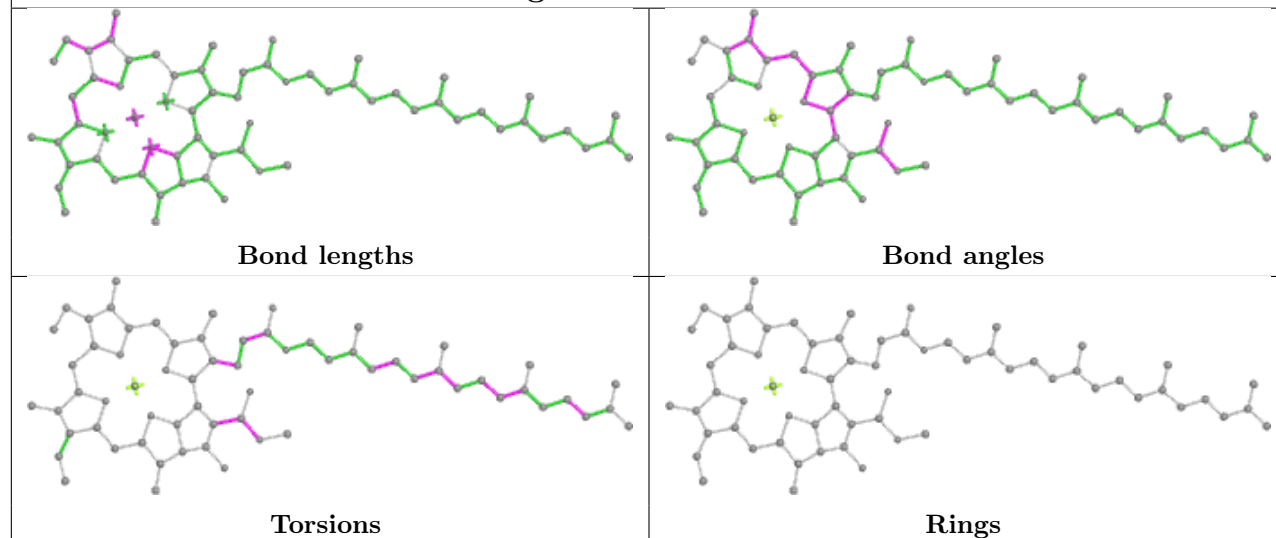


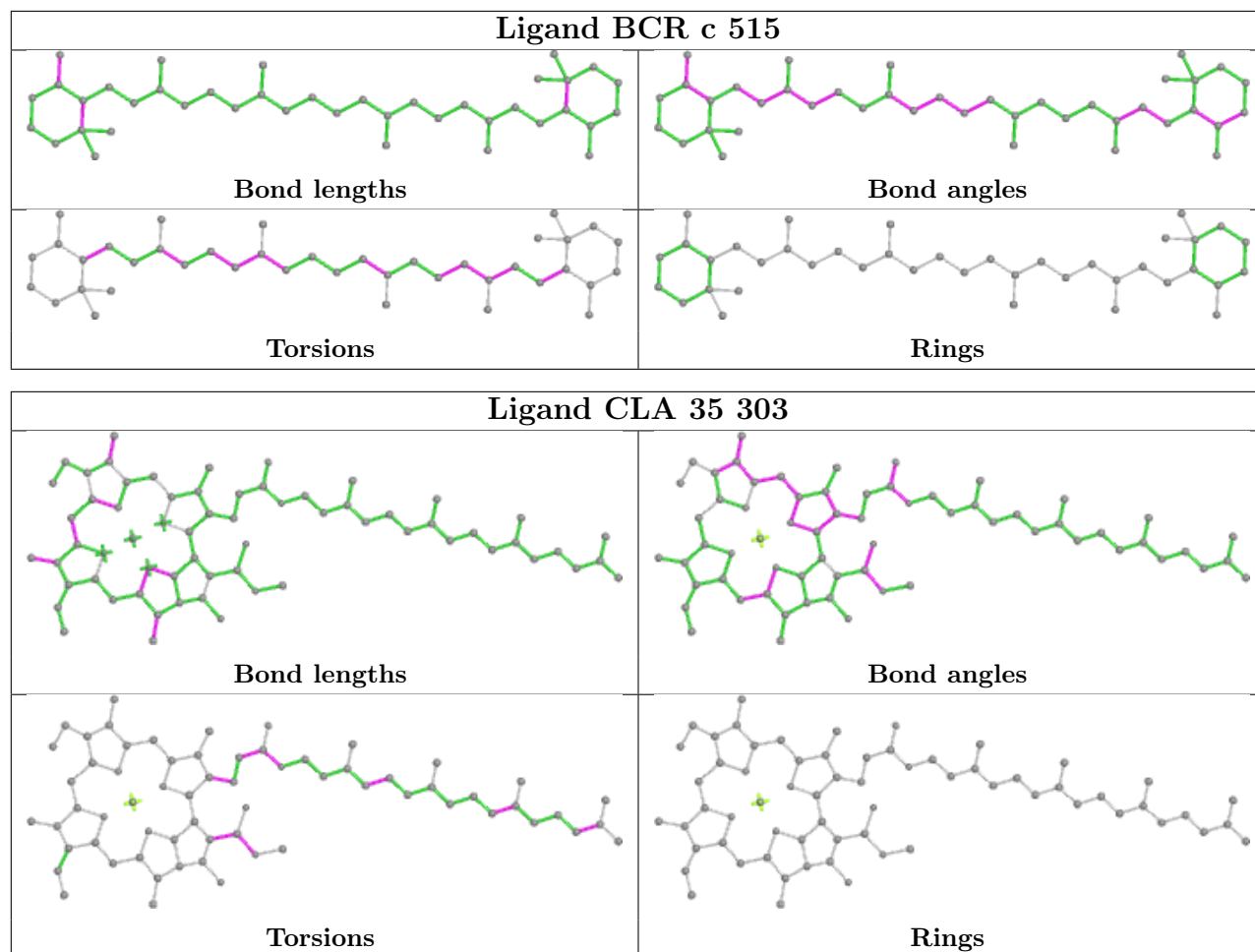


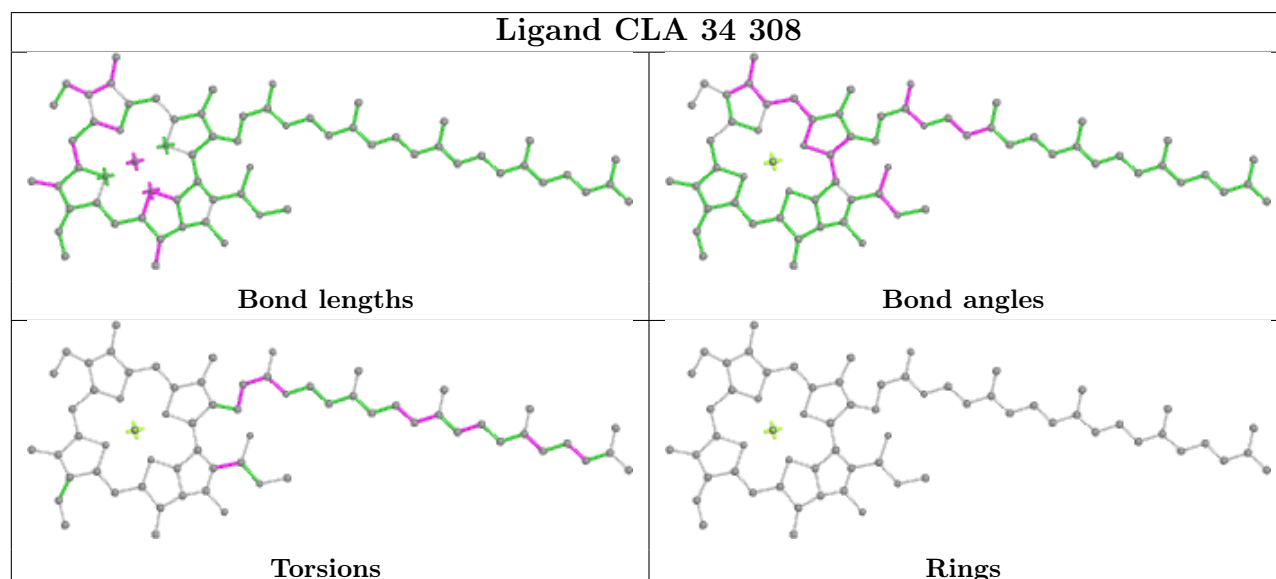
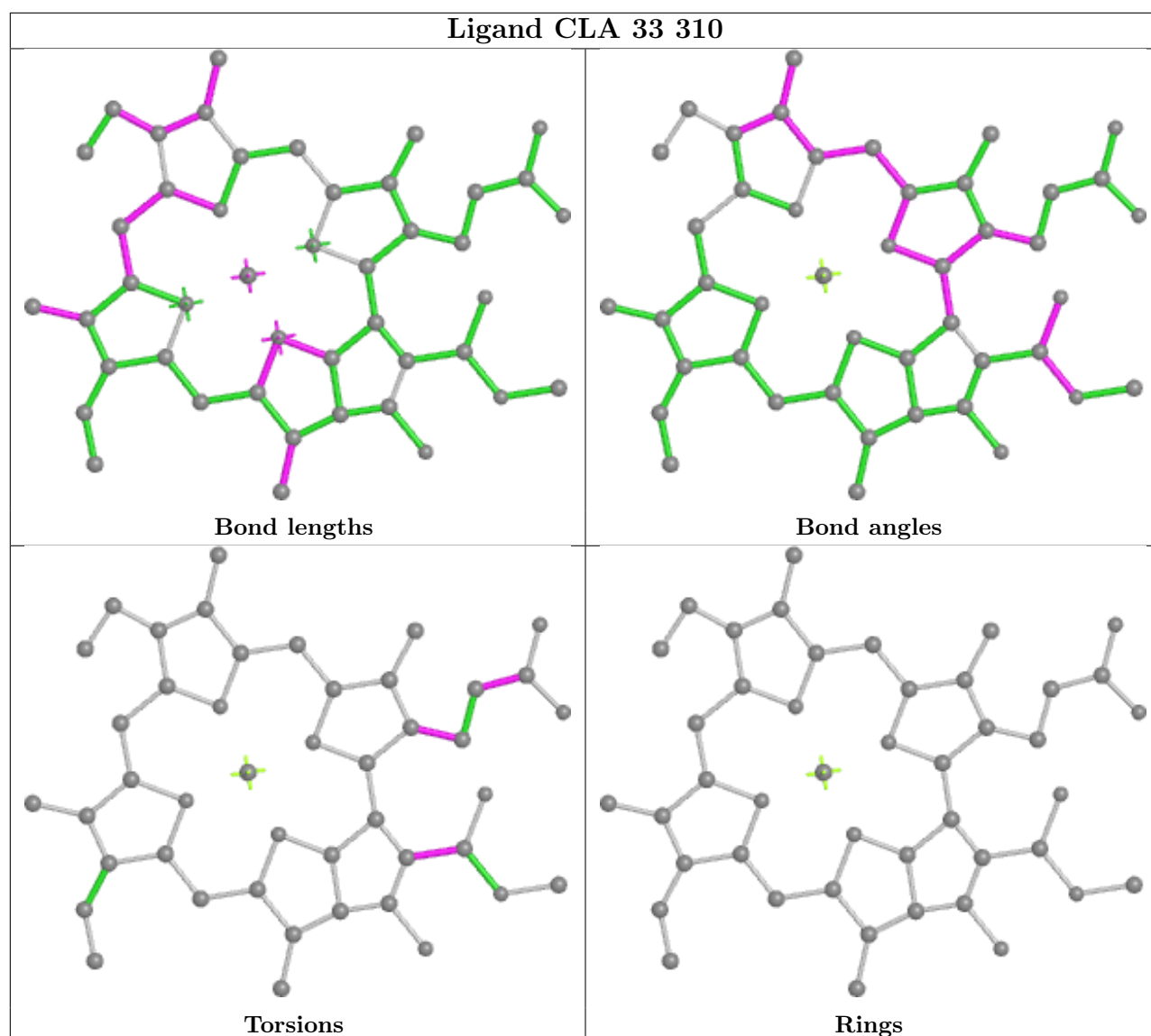


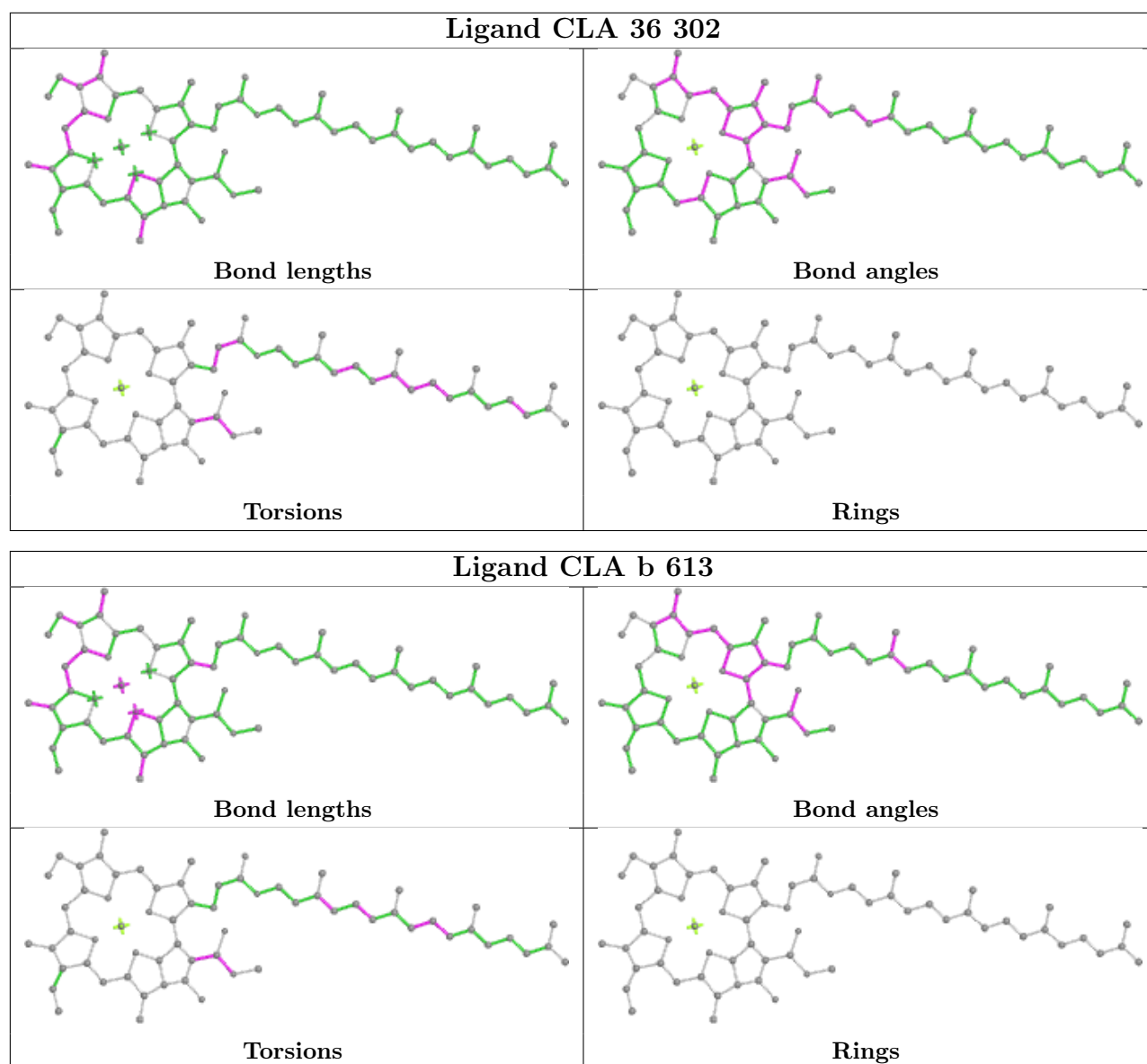


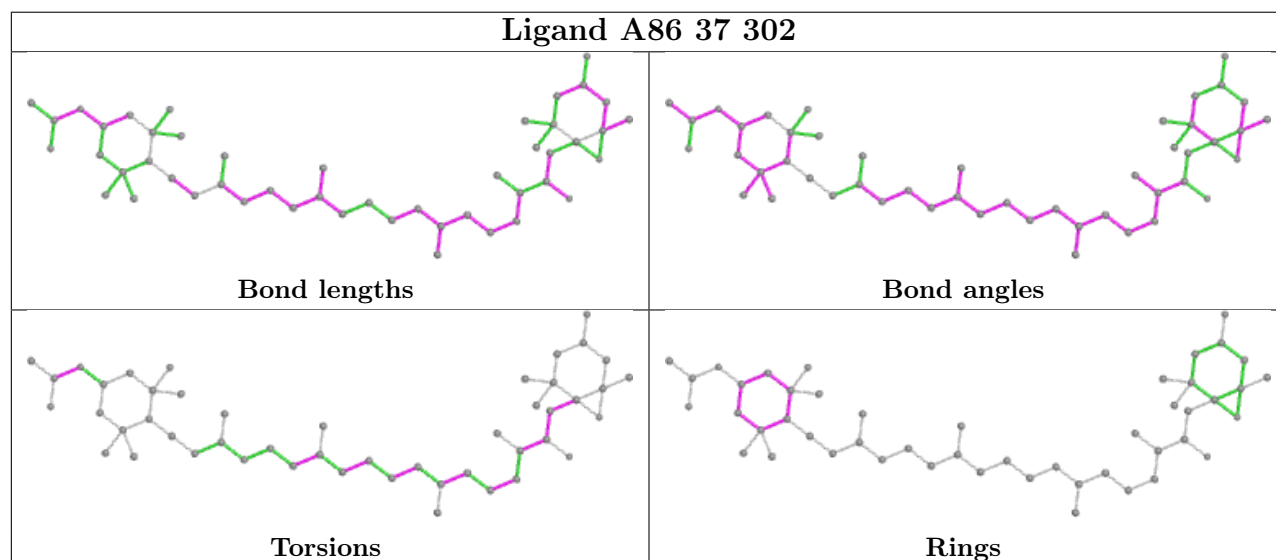
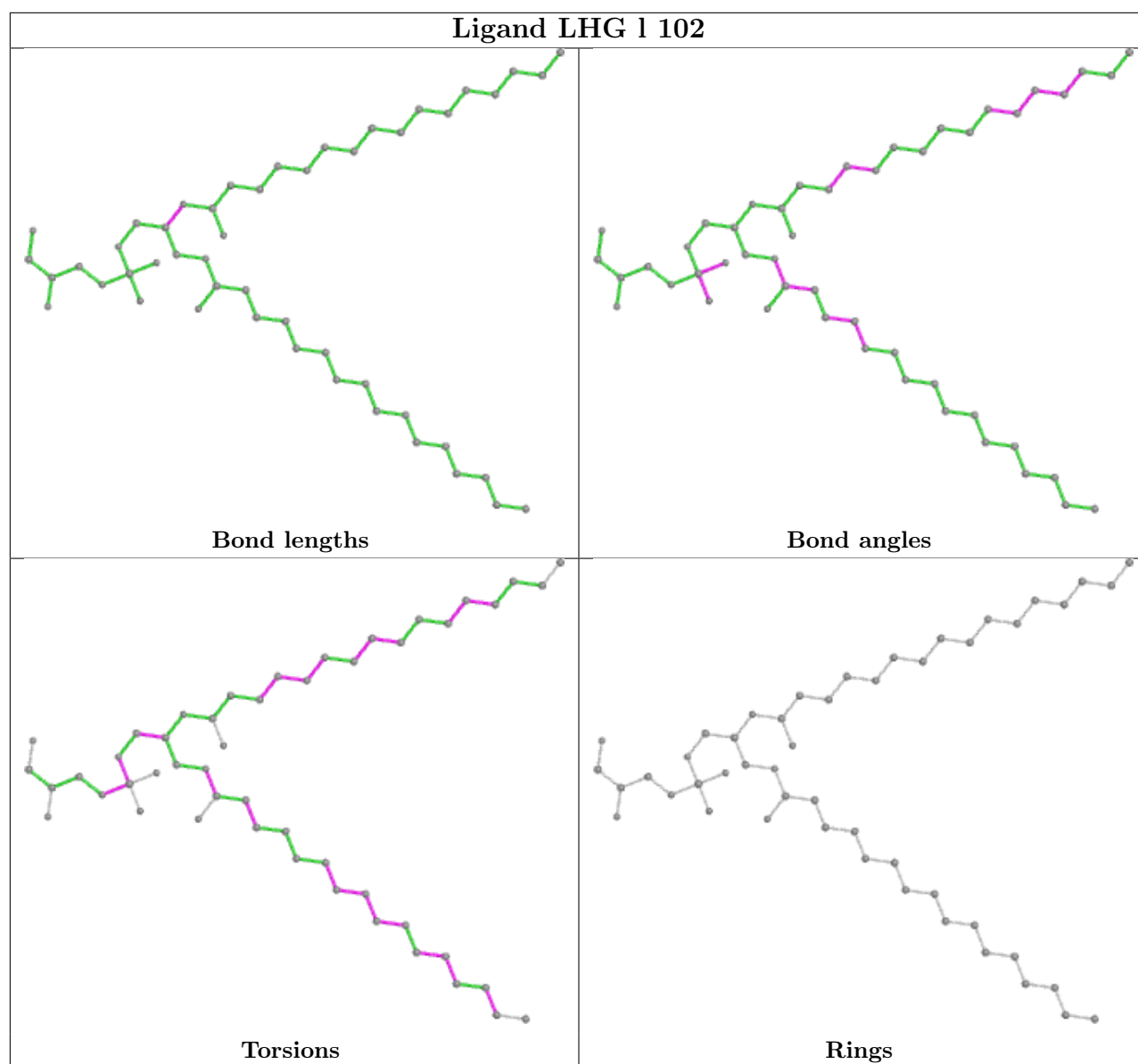


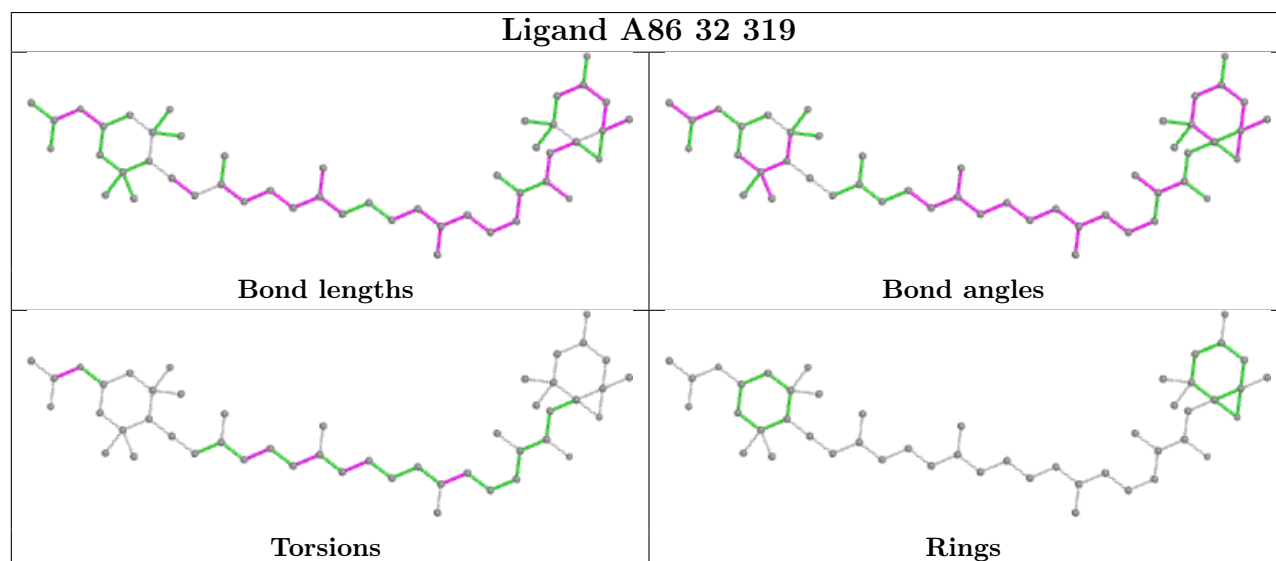
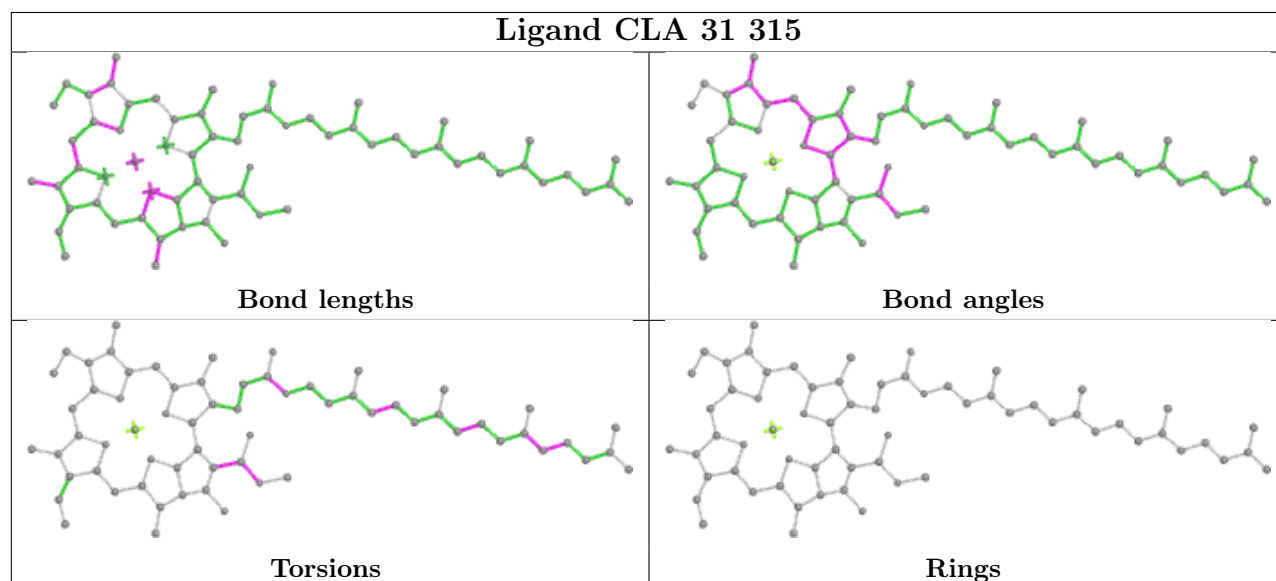
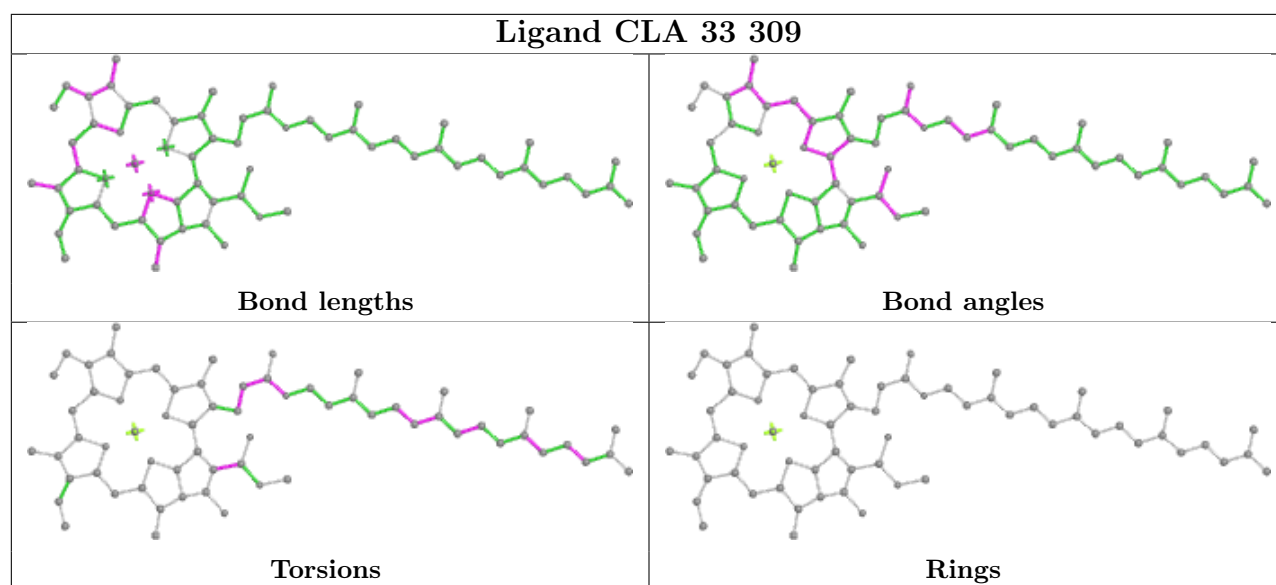
Ligand CLA a 403**Ligand CLA b 610****Ligand CLA 21 303**

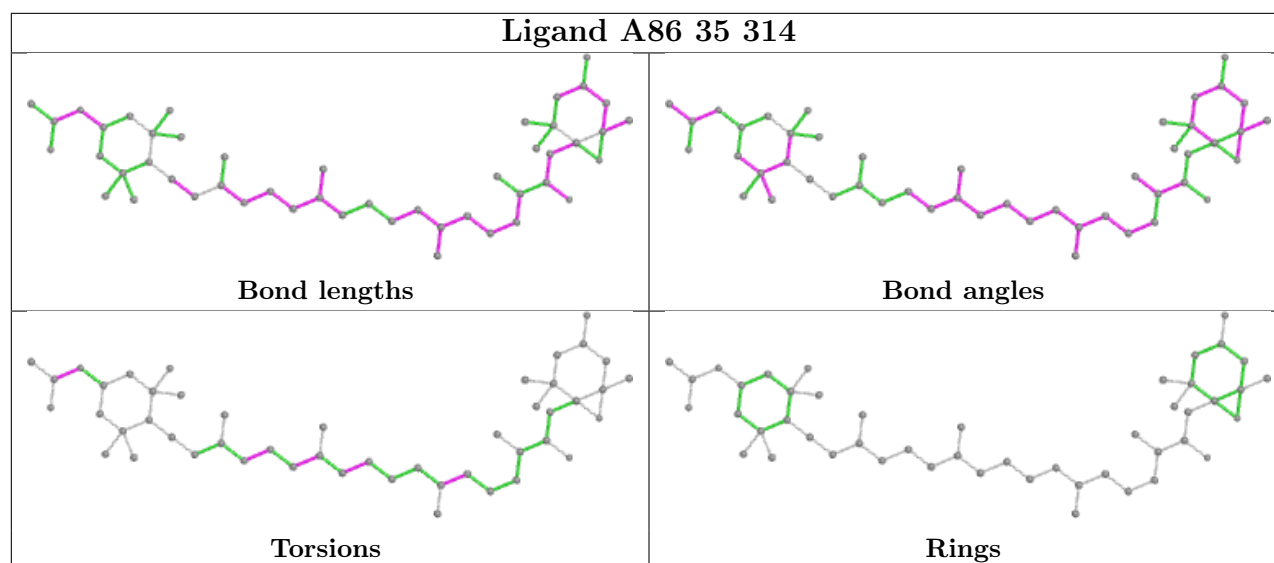
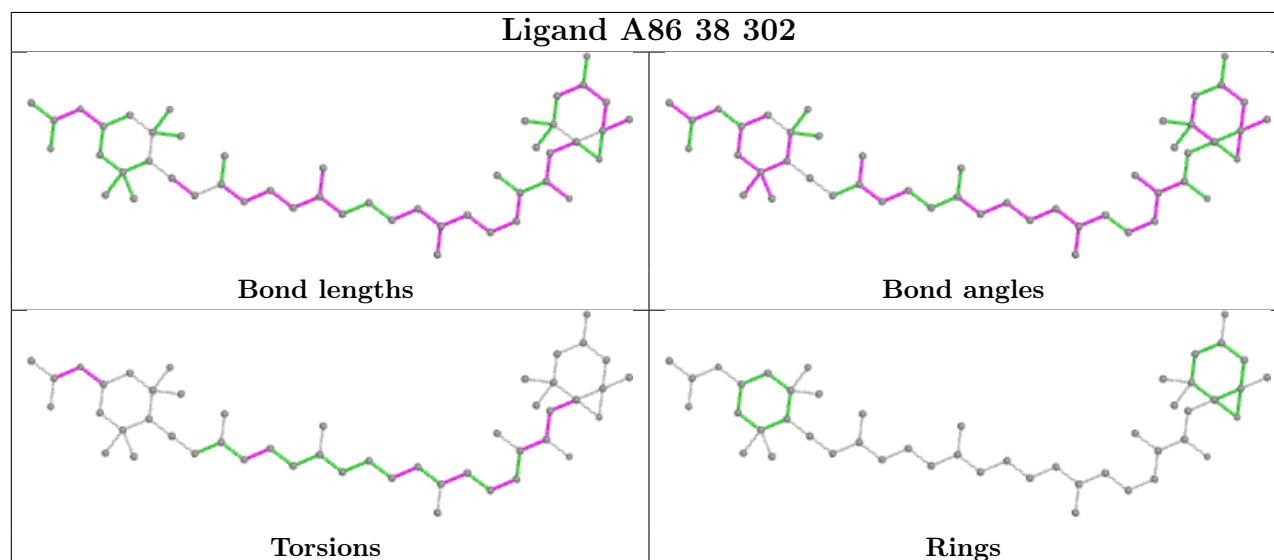
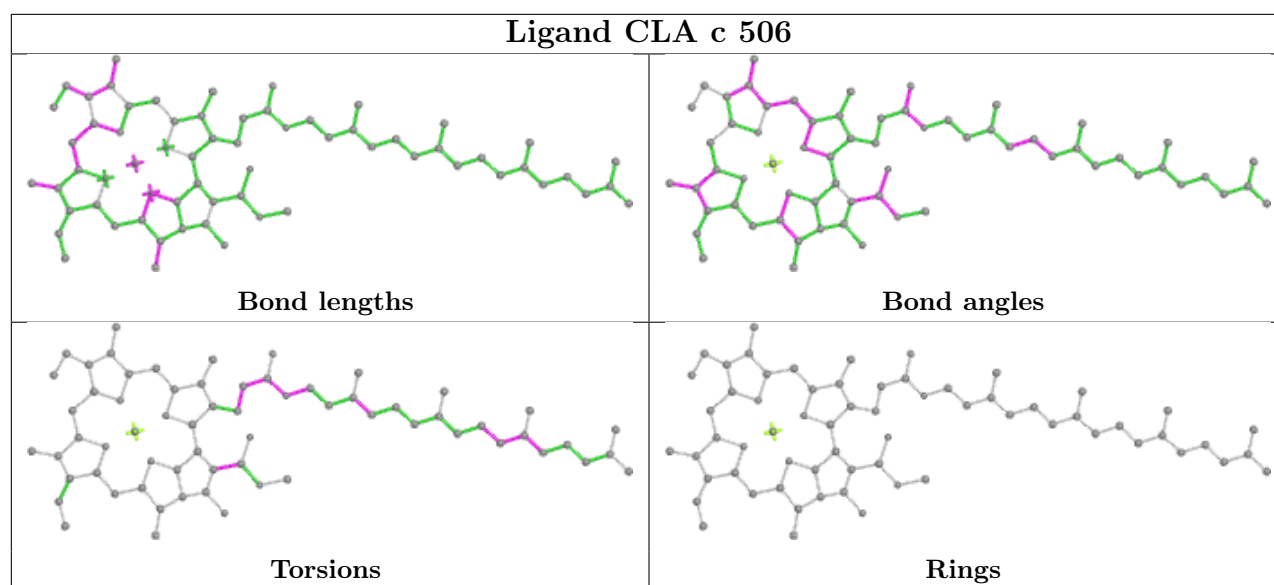


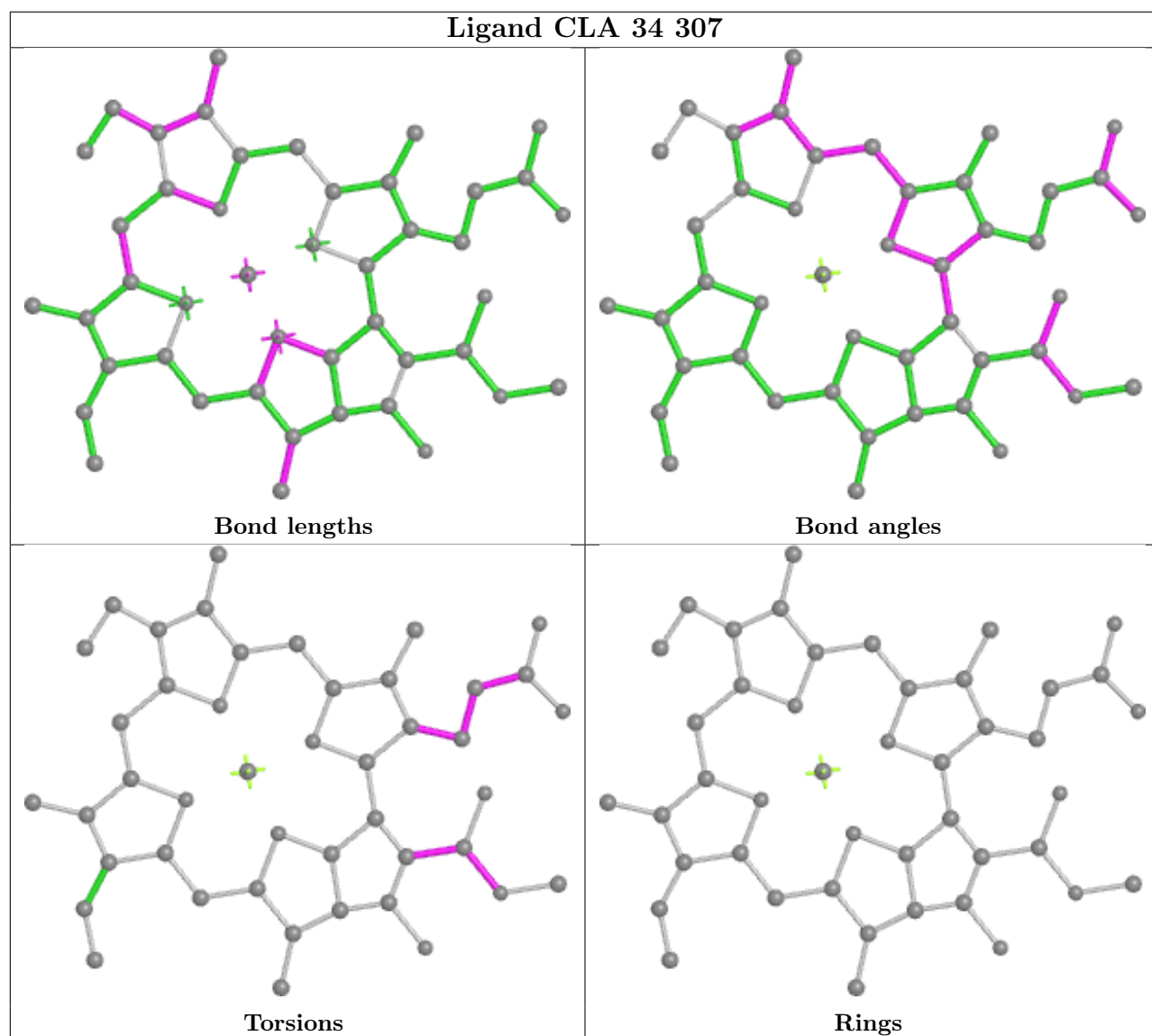
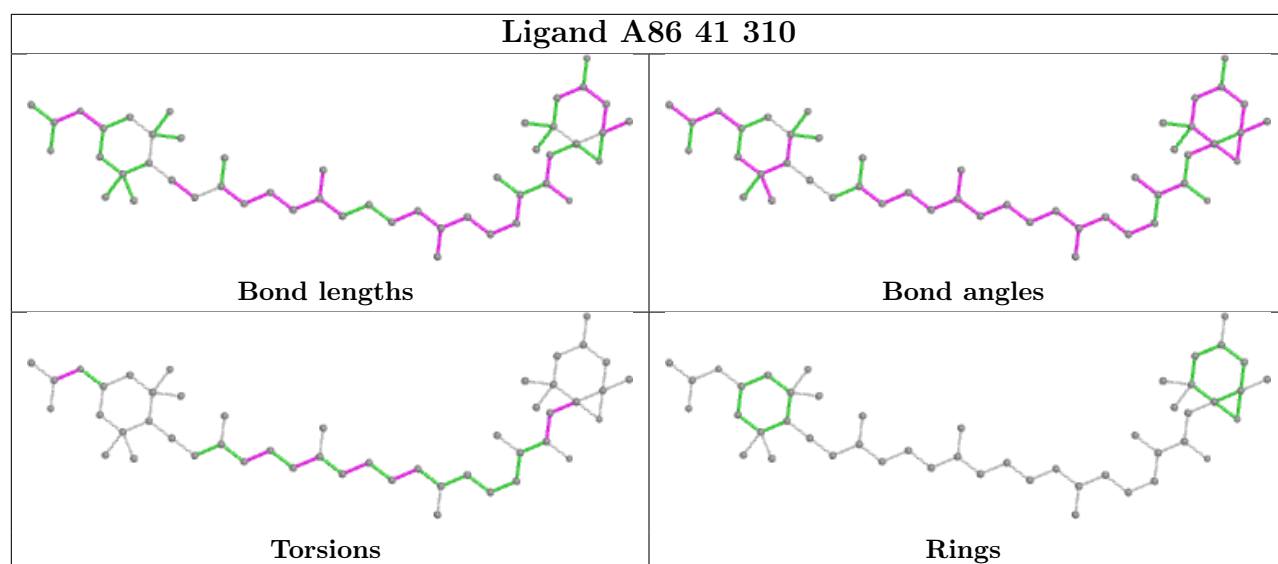


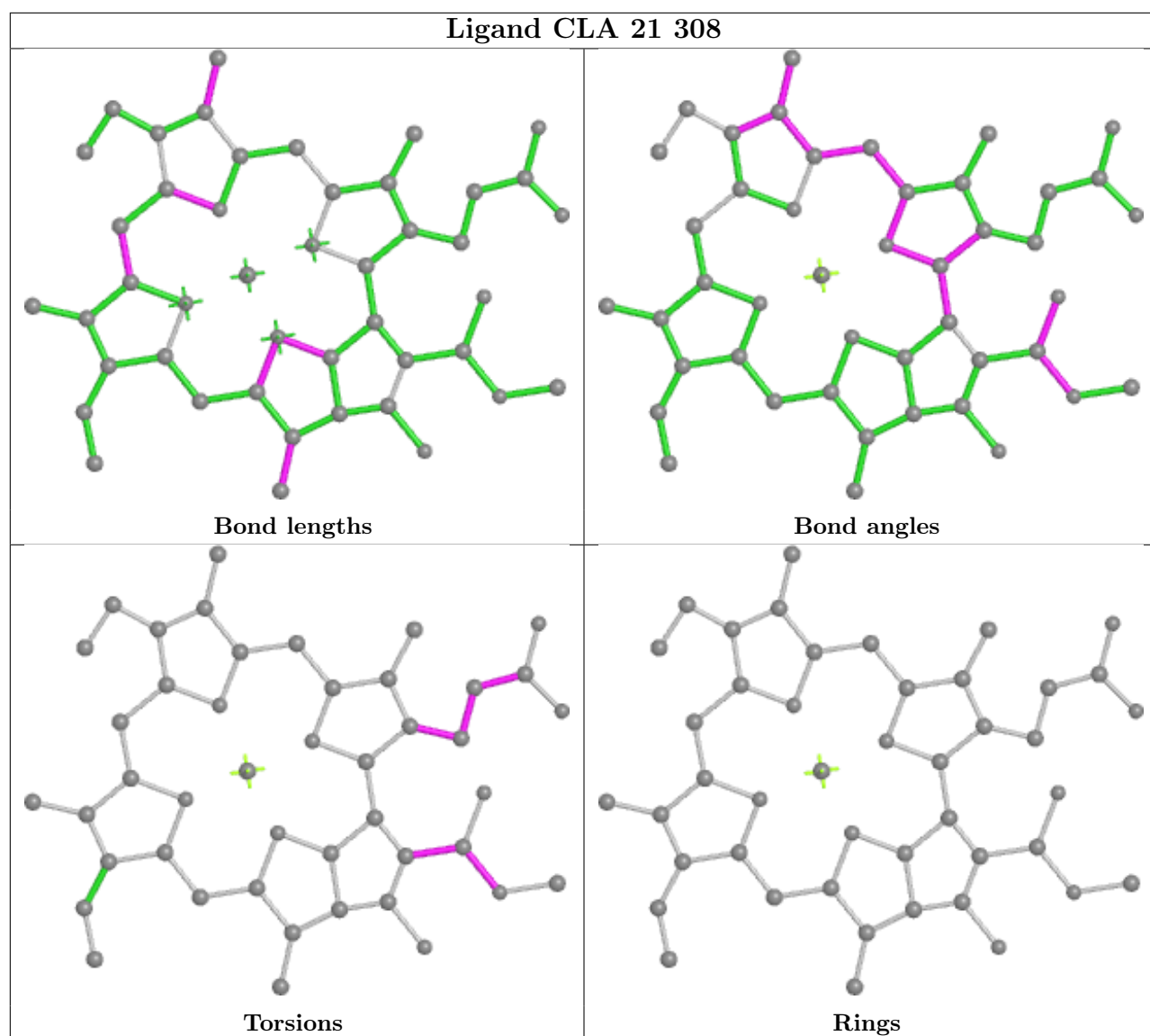


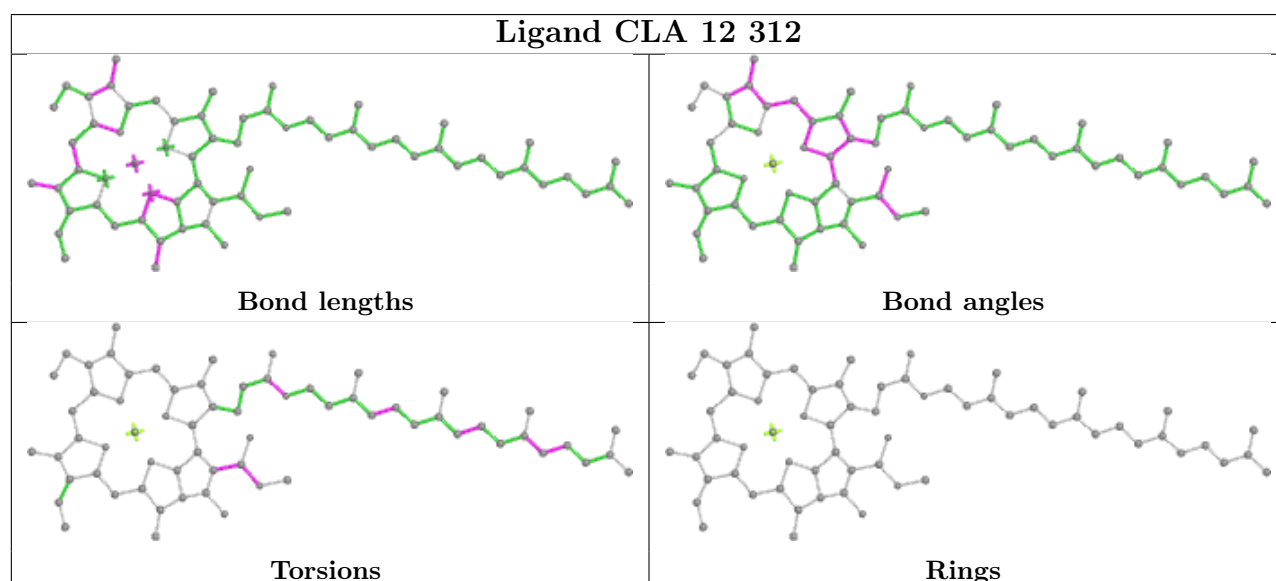
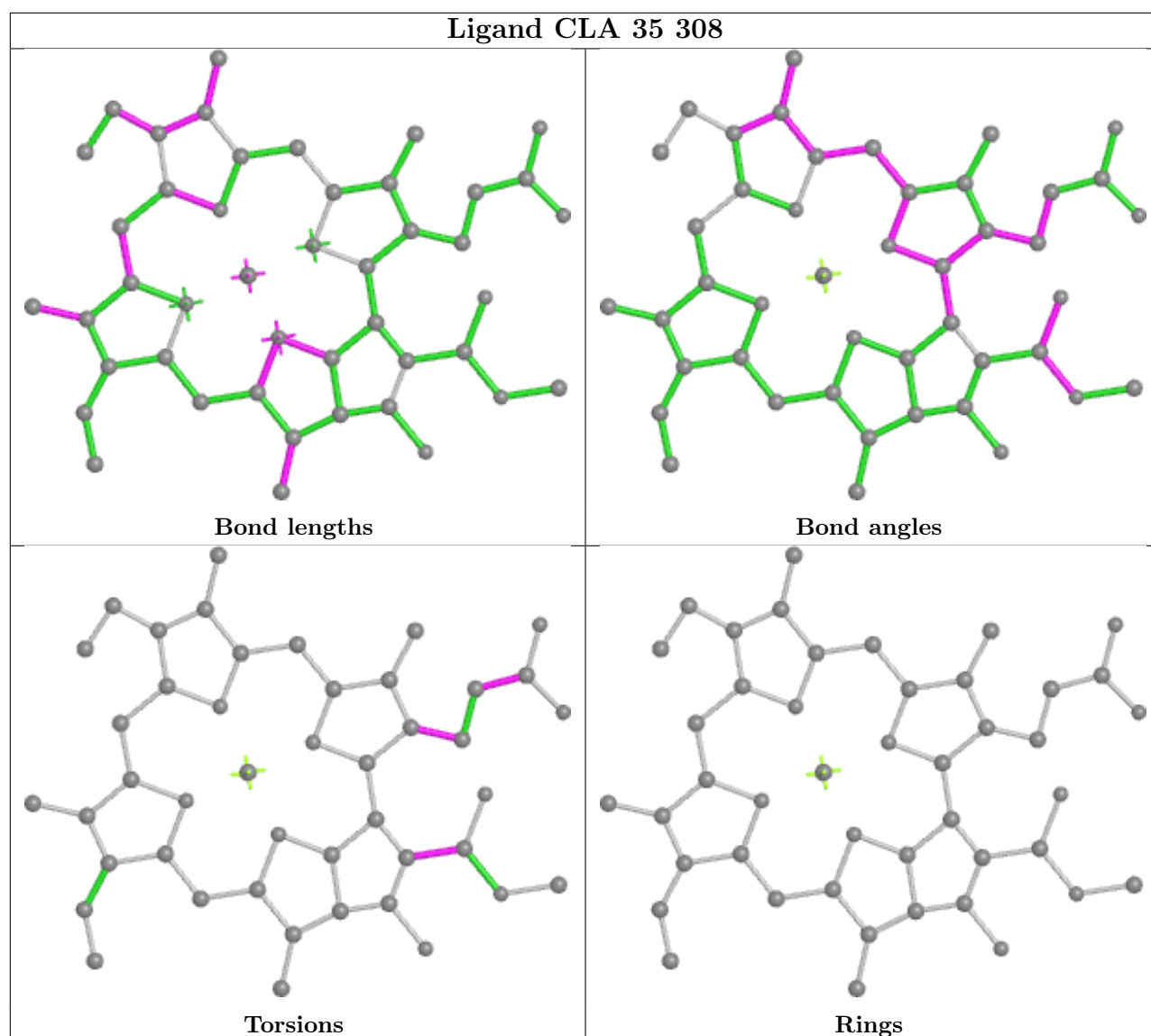


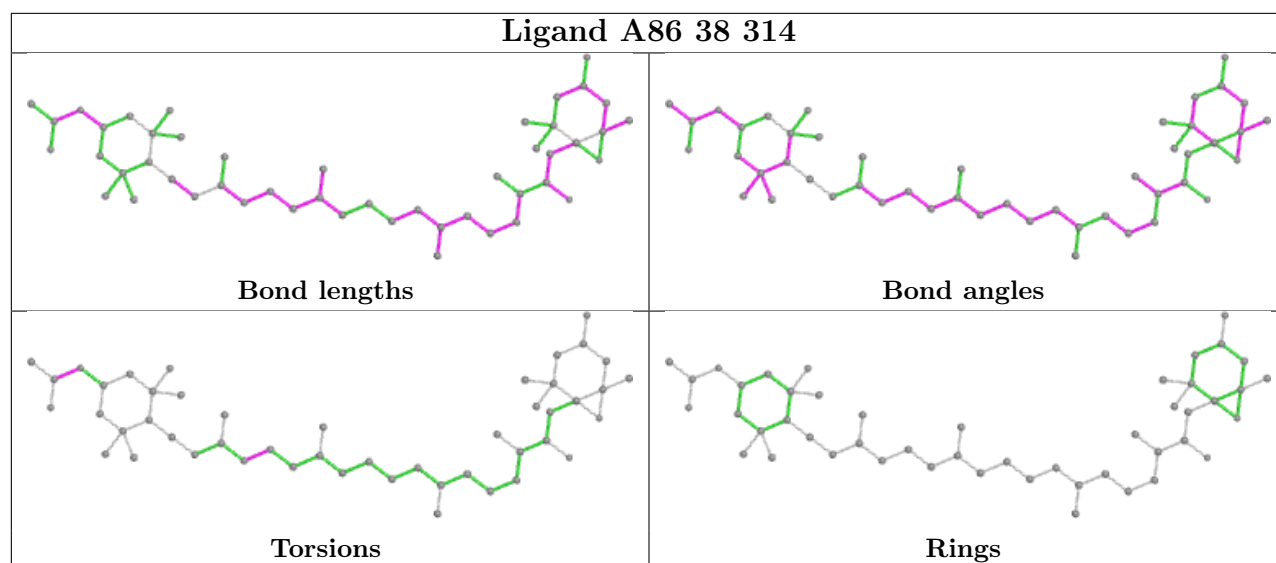
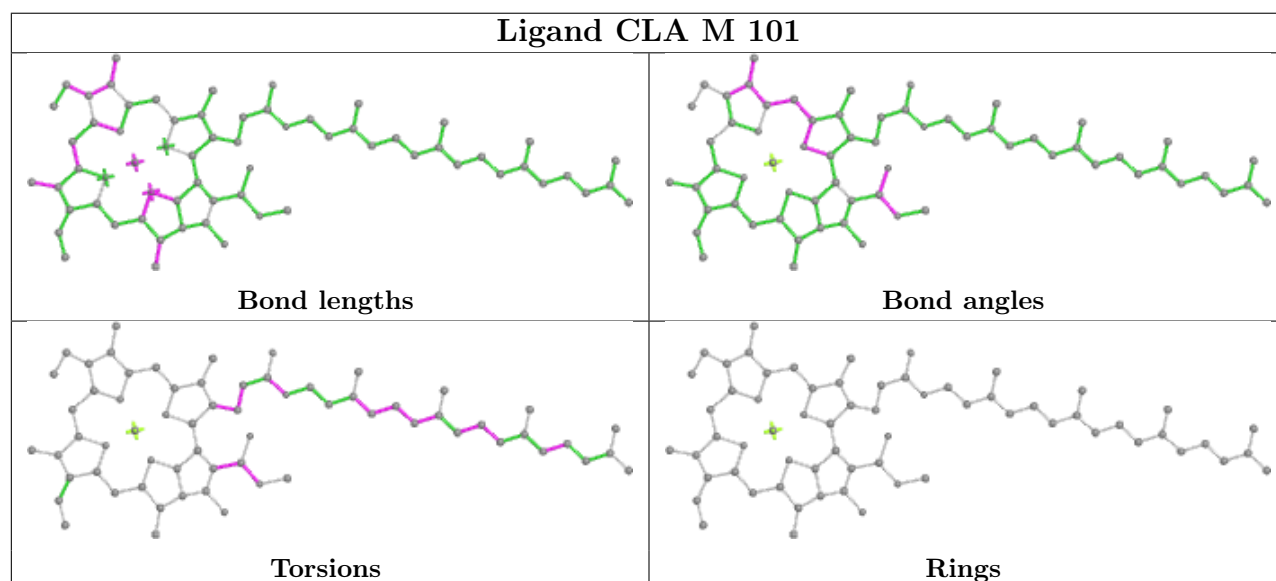
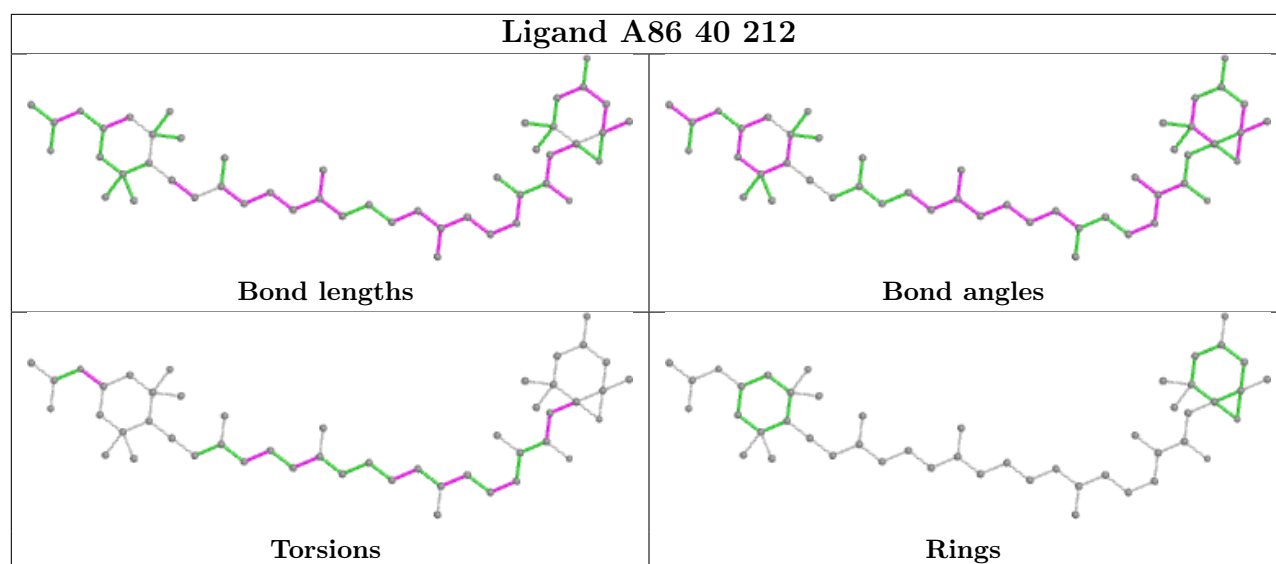


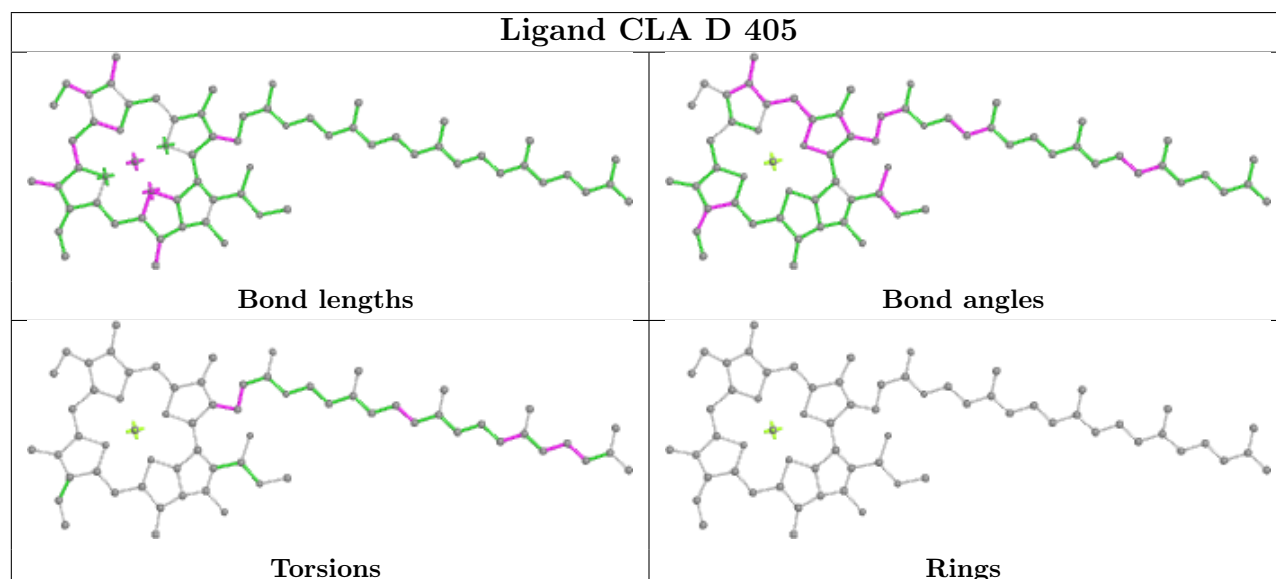
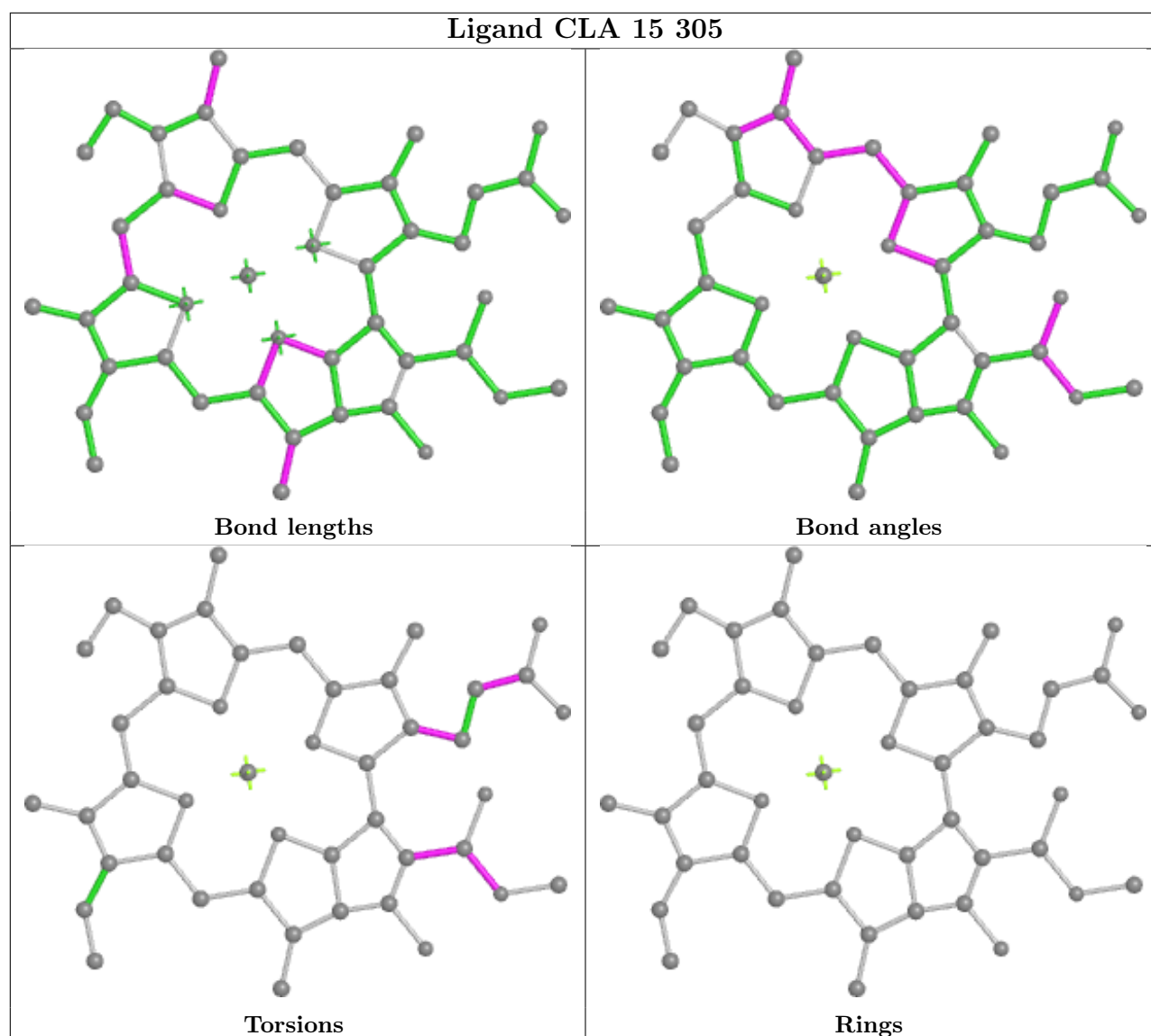


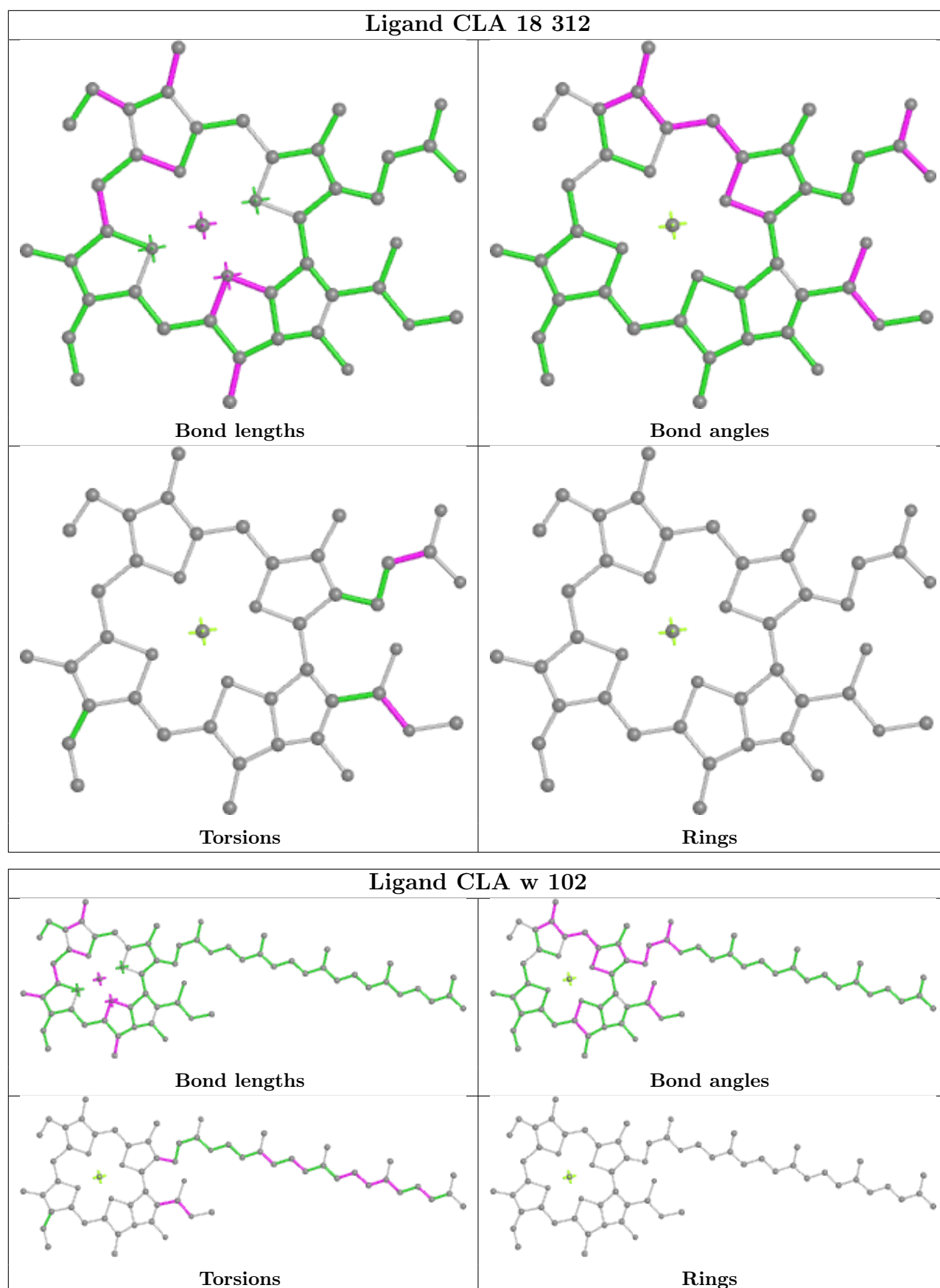


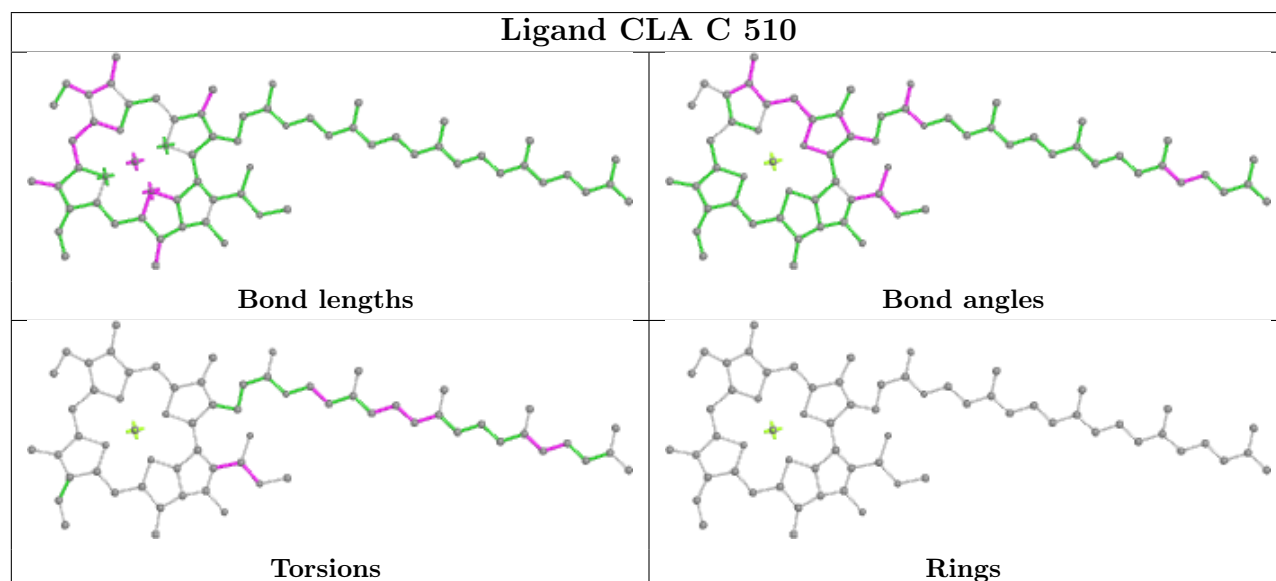
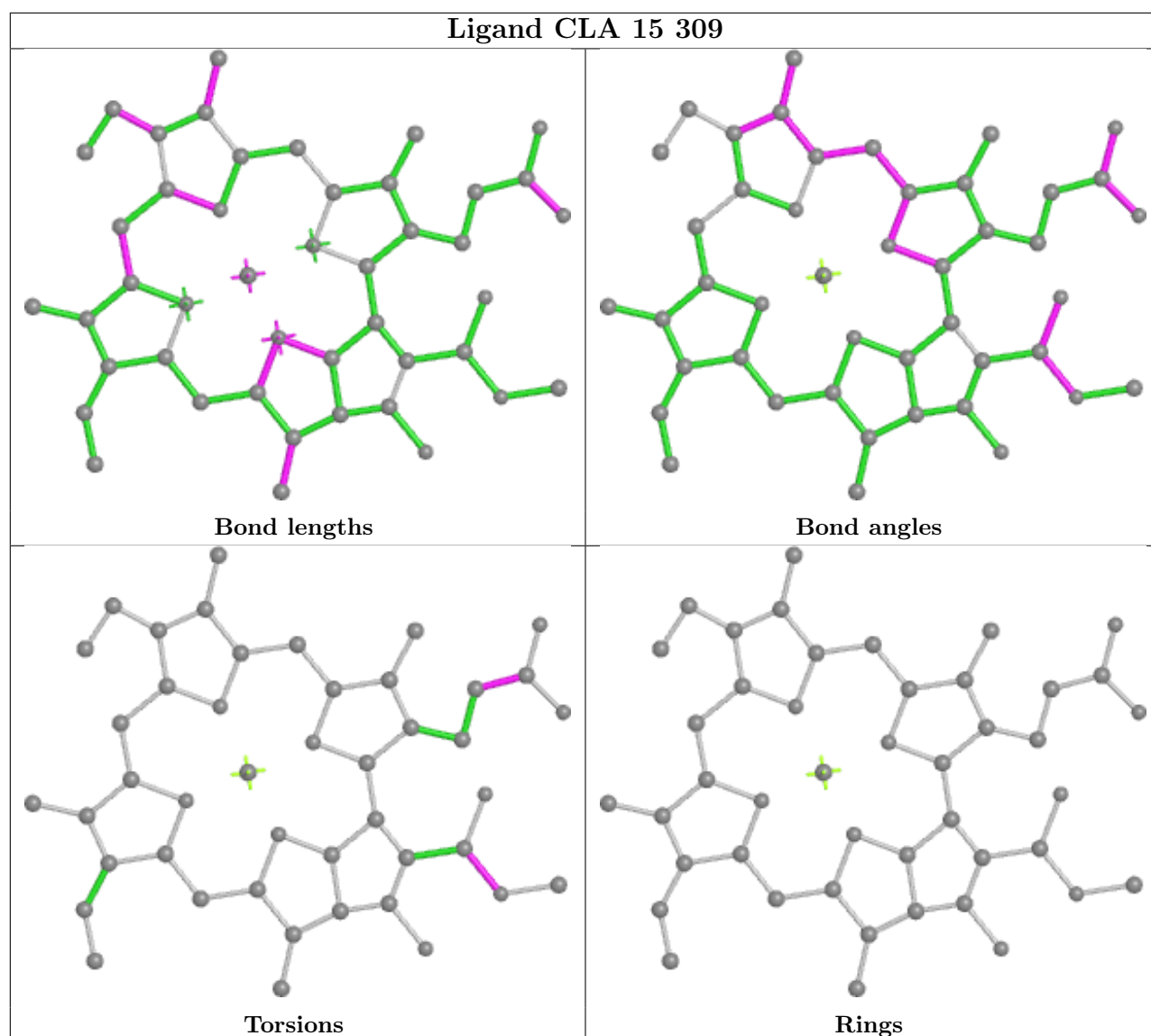


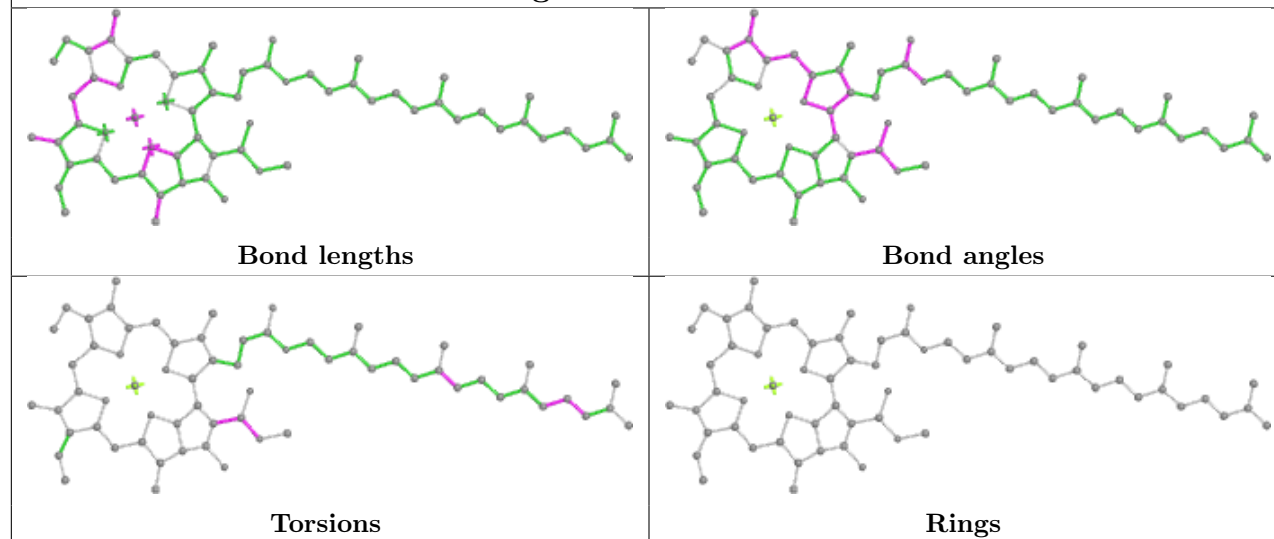
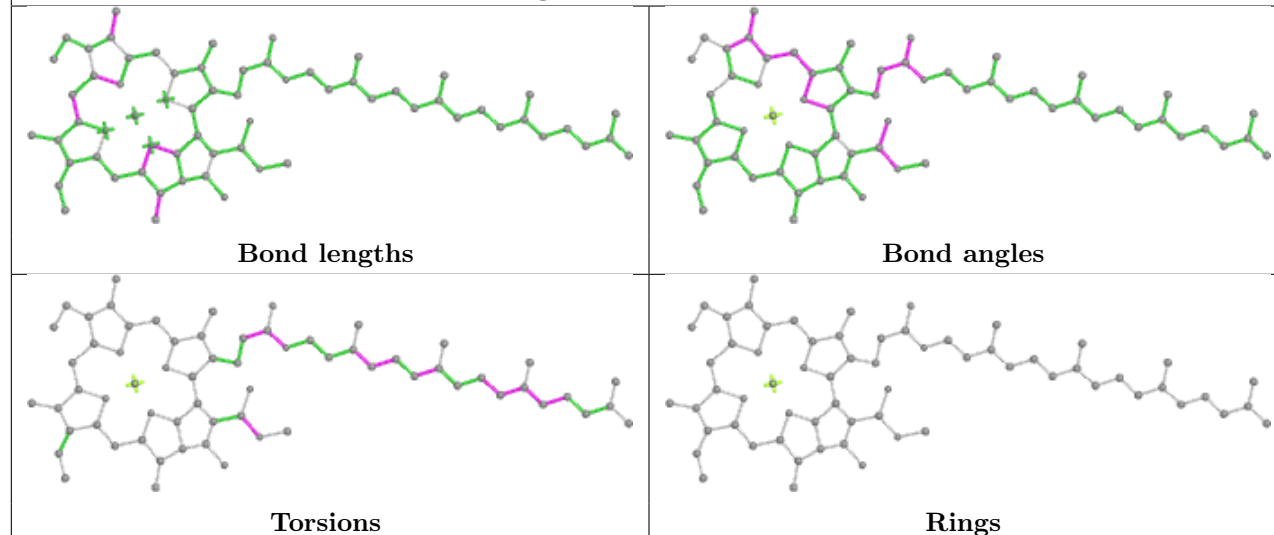
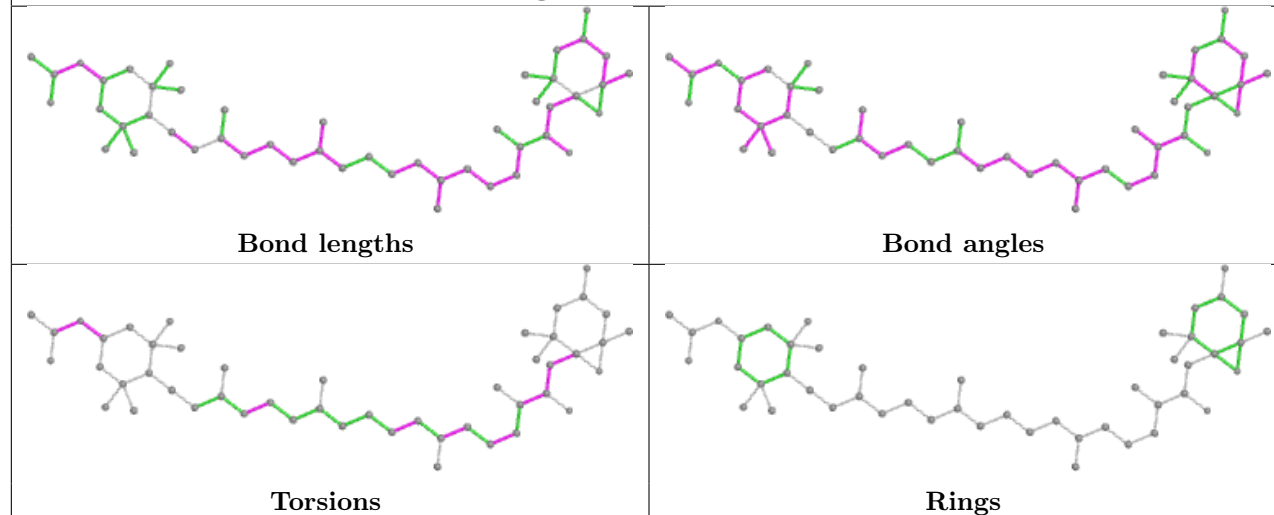


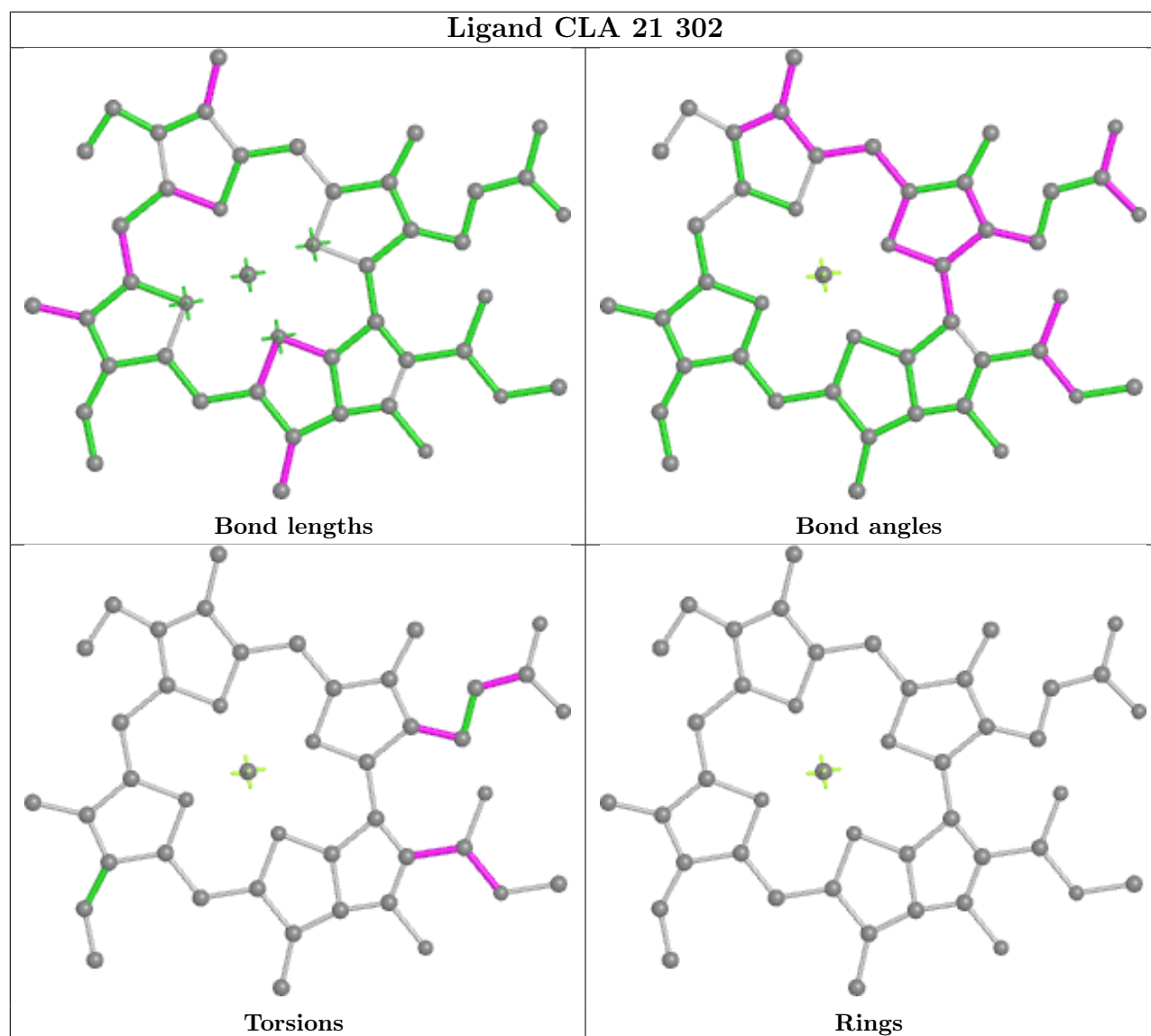
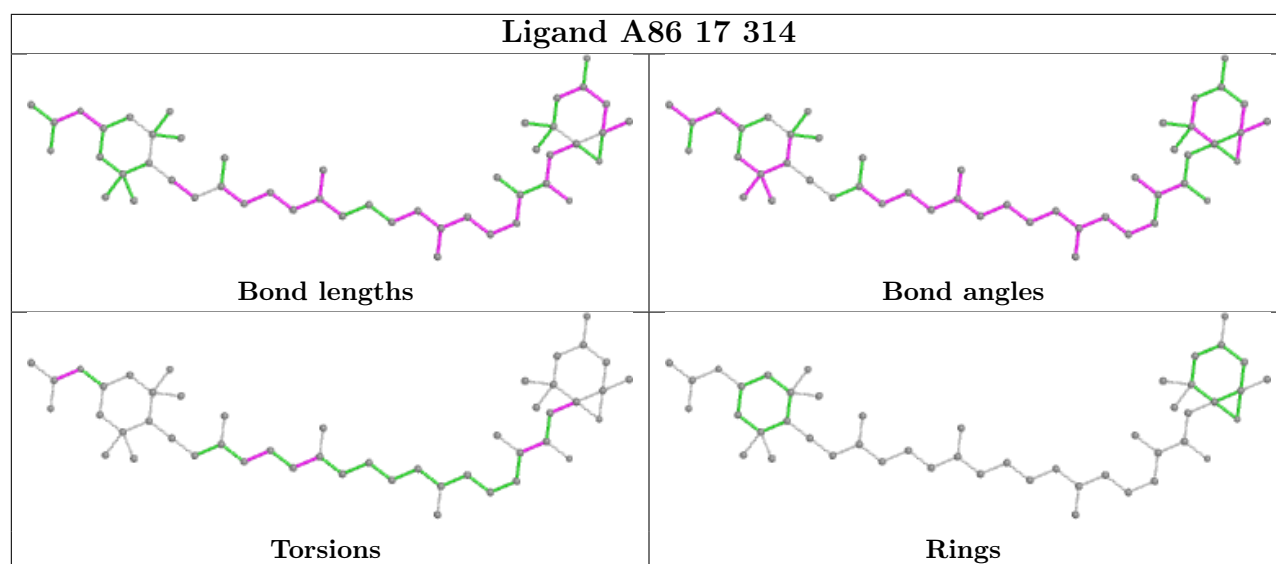


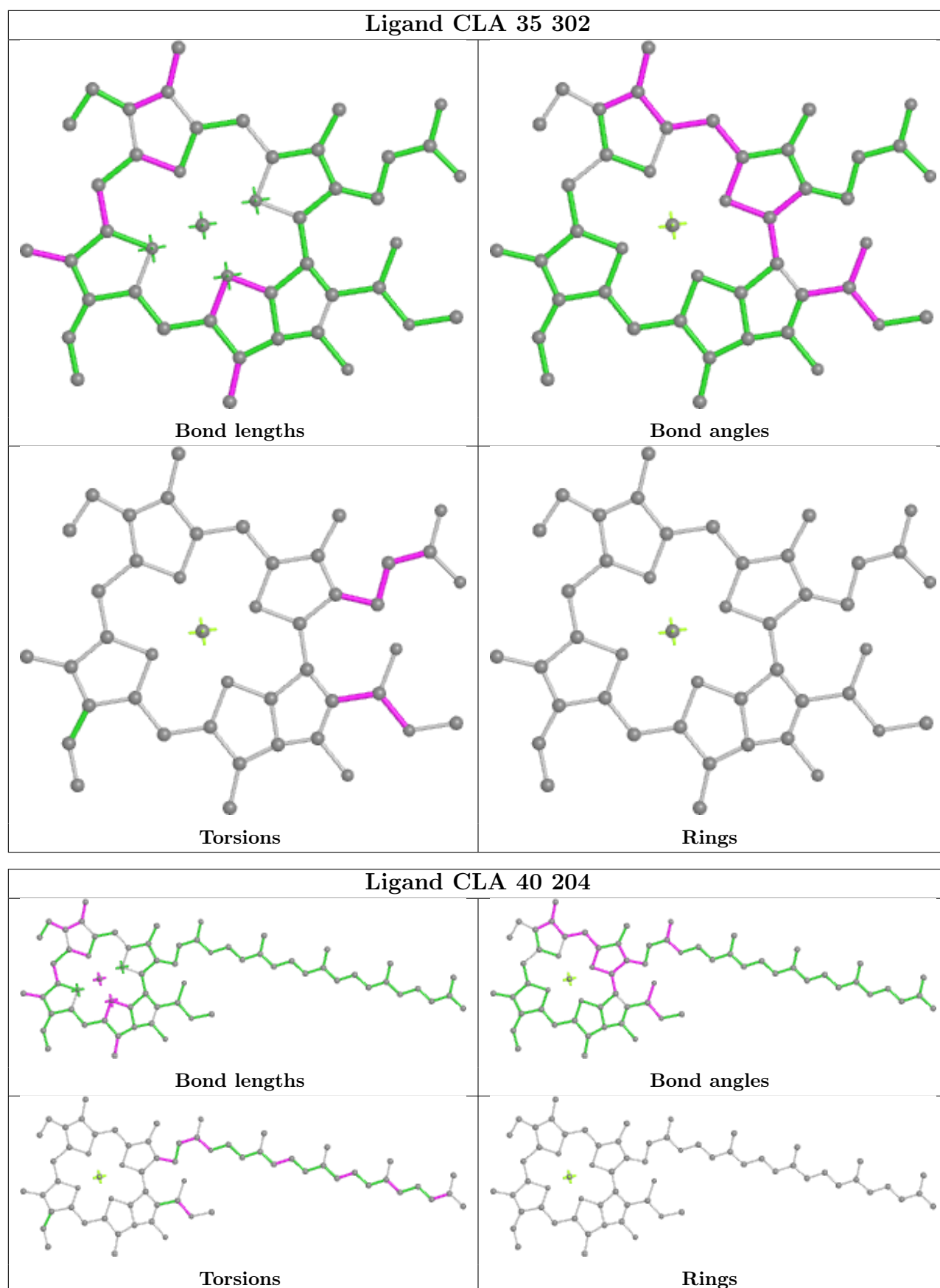




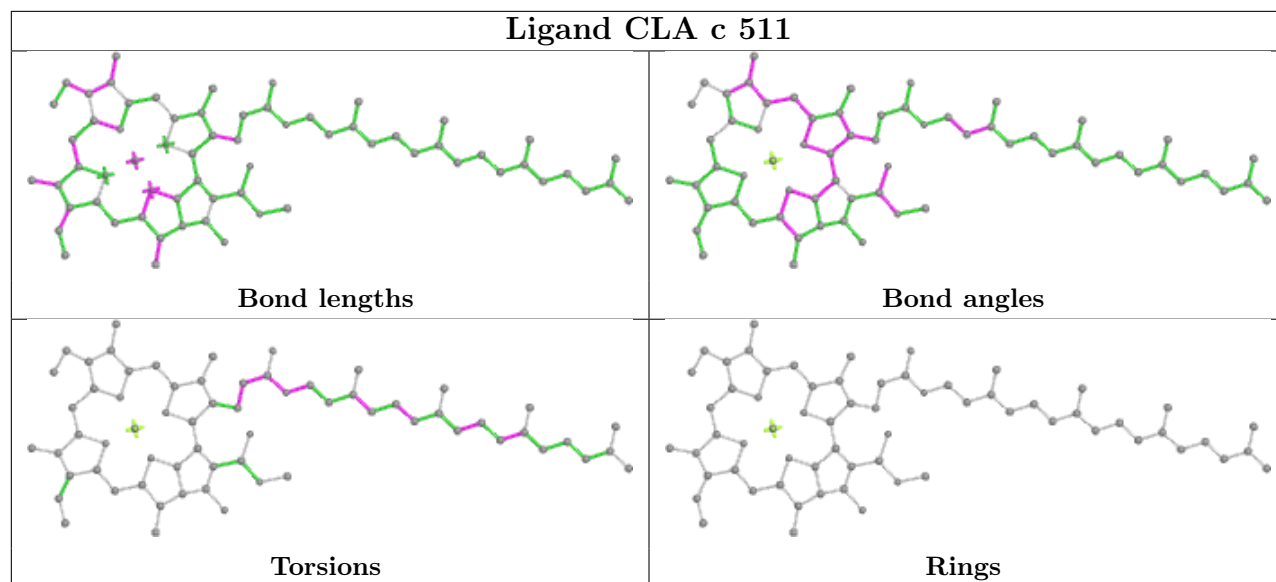


Ligand CLA B 614**Ligand CLA Z 102****Ligand A86 12 304**

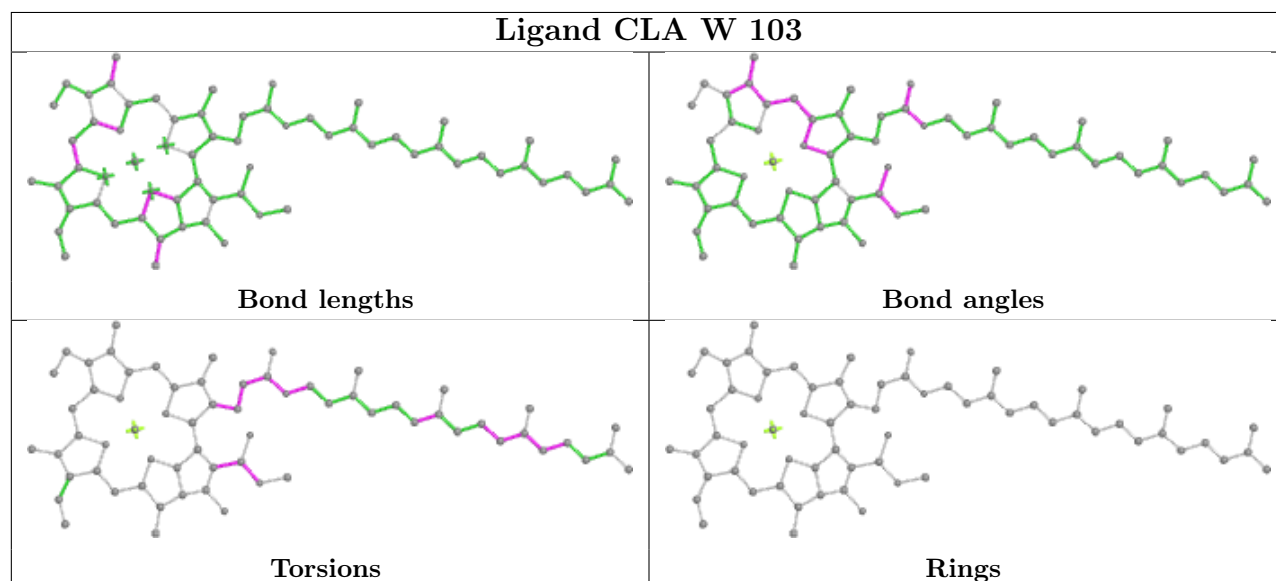




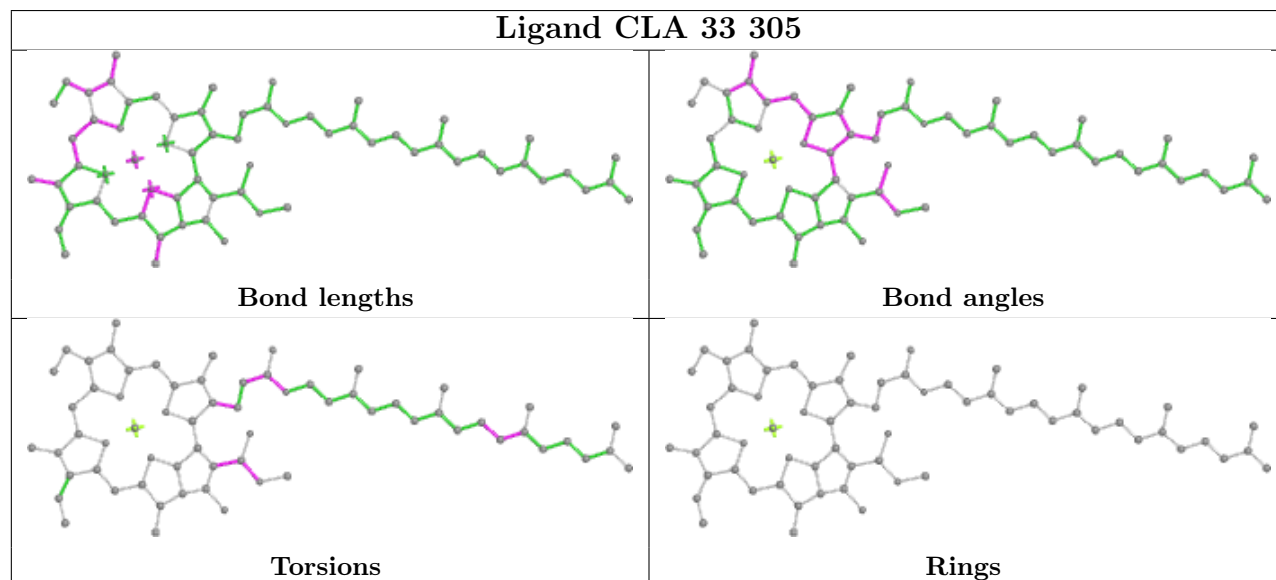
Ligand CLA c 511

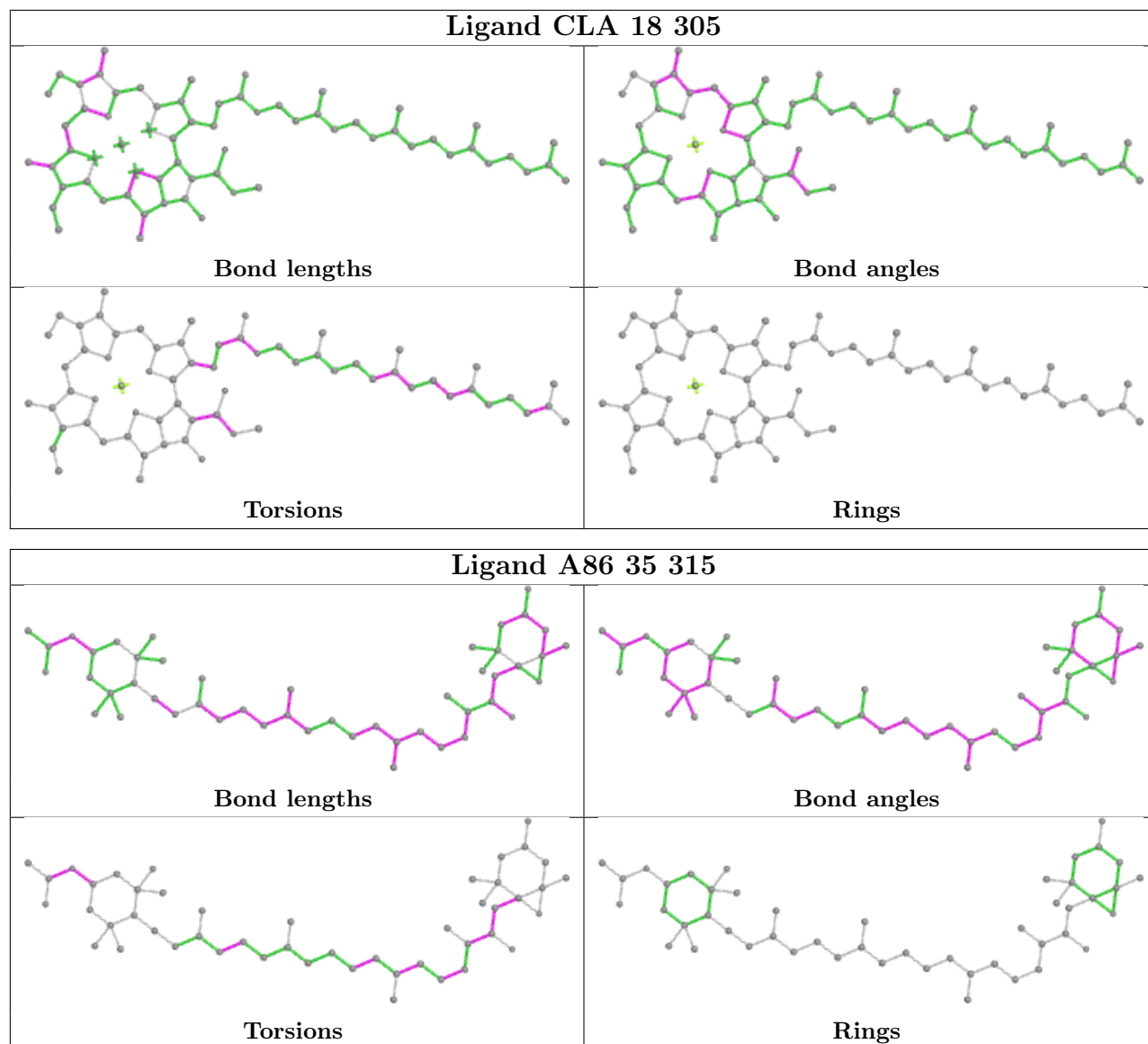


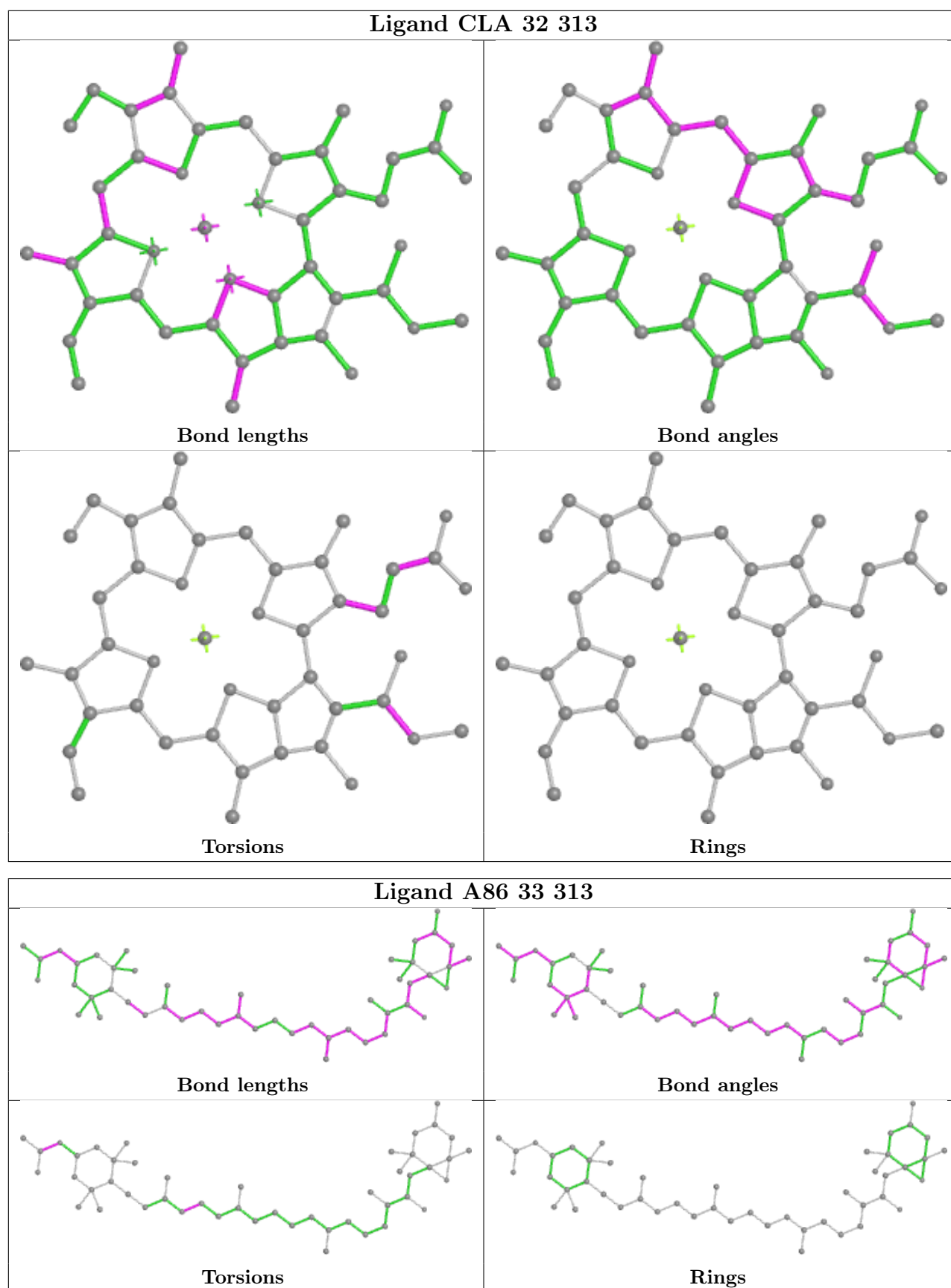
Ligand CLA W 103



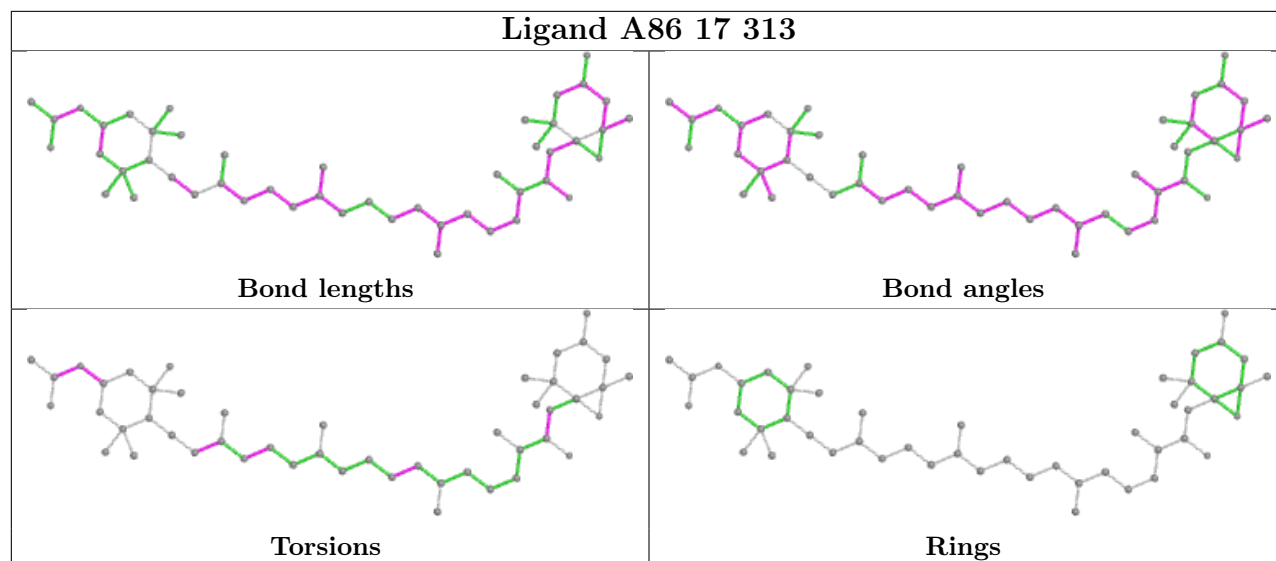
Ligand CLA 33 305



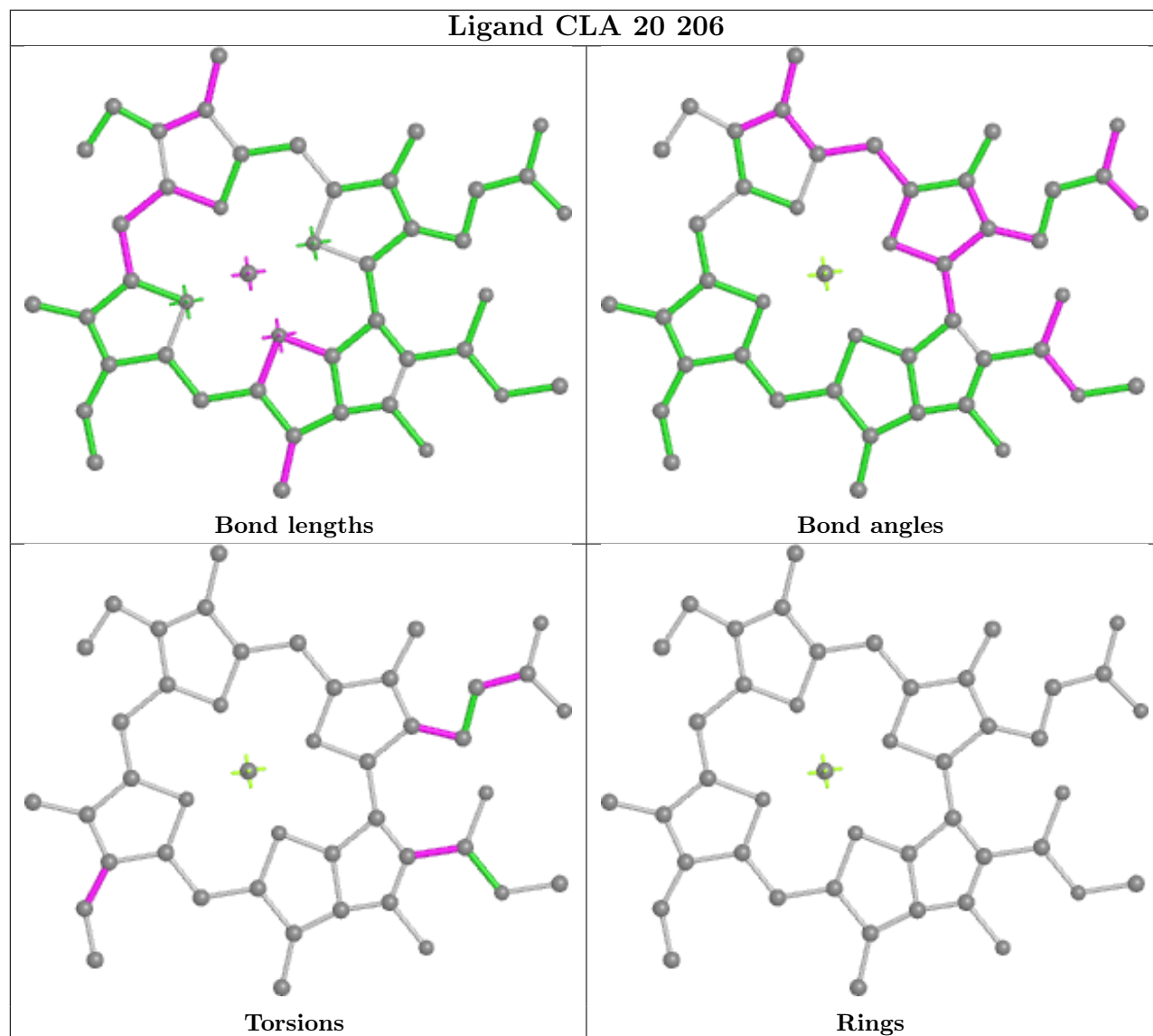


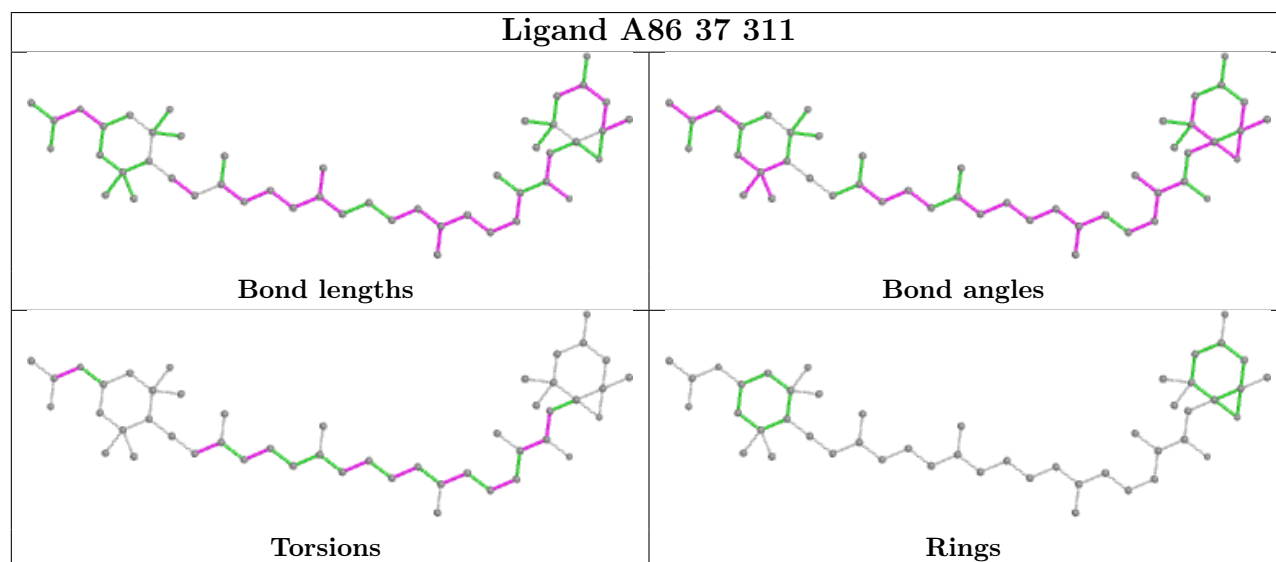
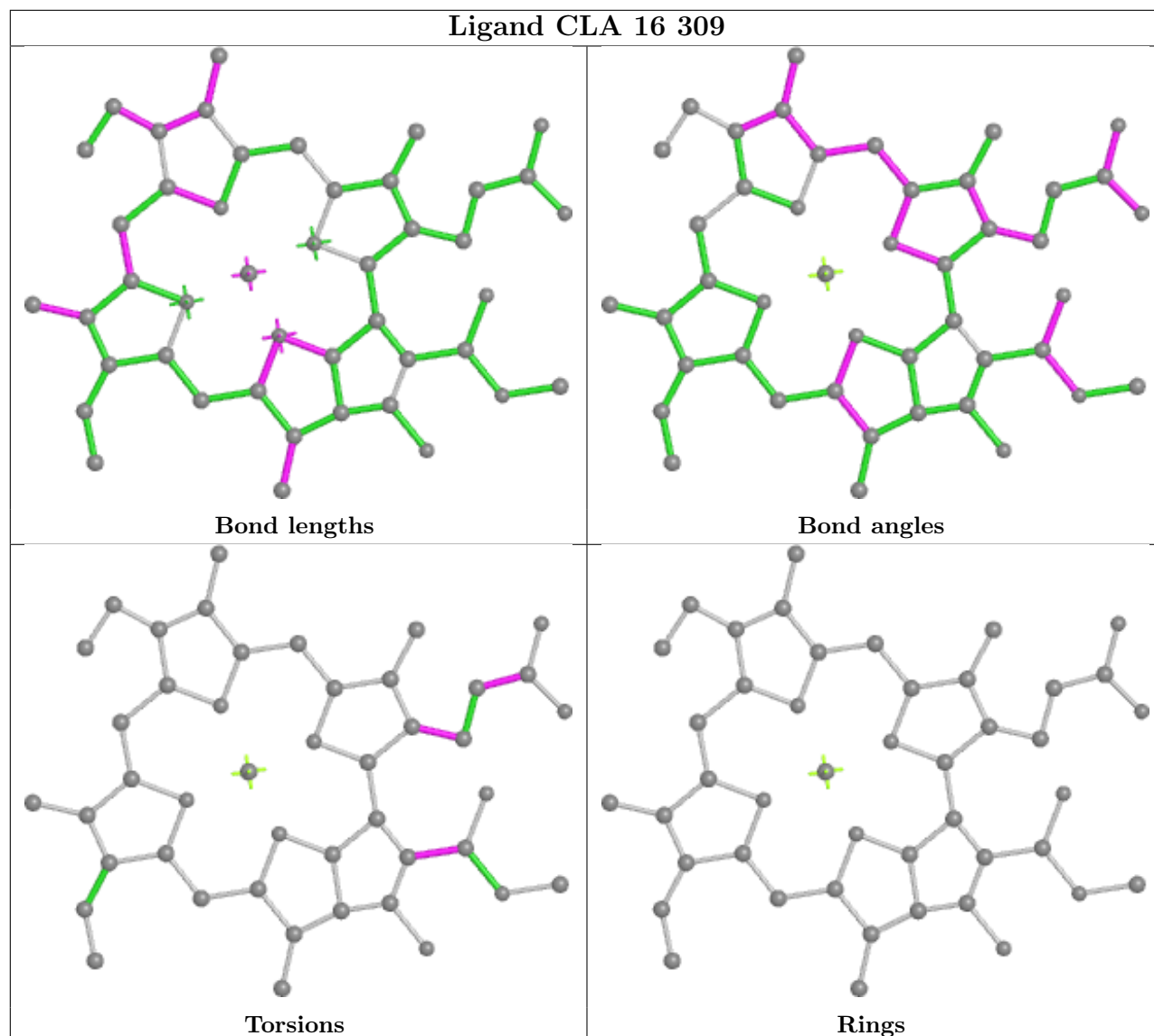


Ligand A86 17 313

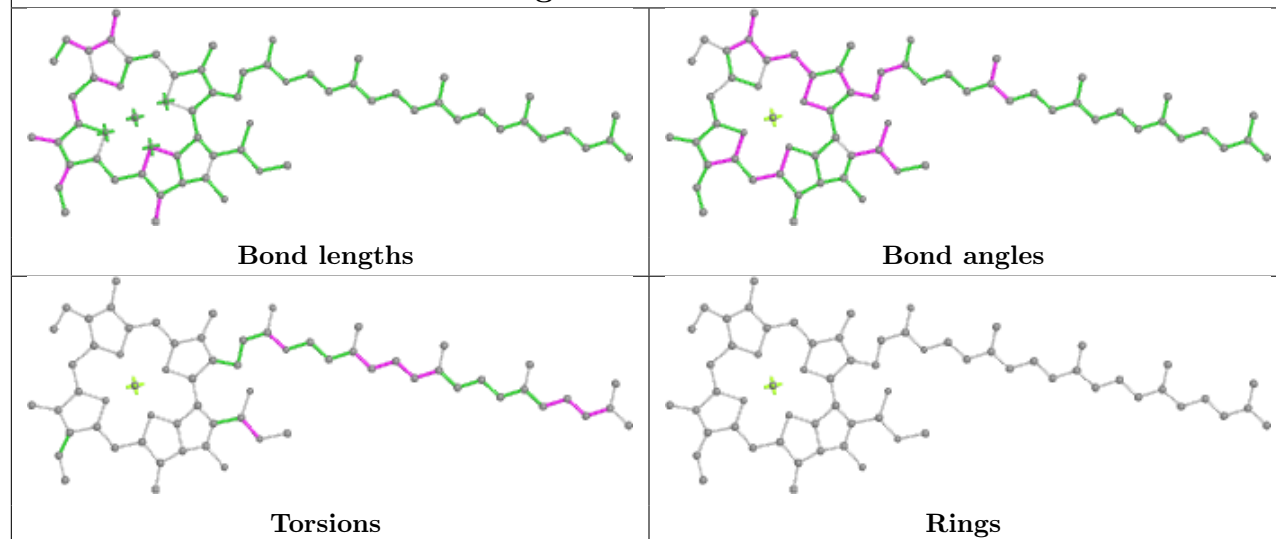


Ligand CLA 20 206

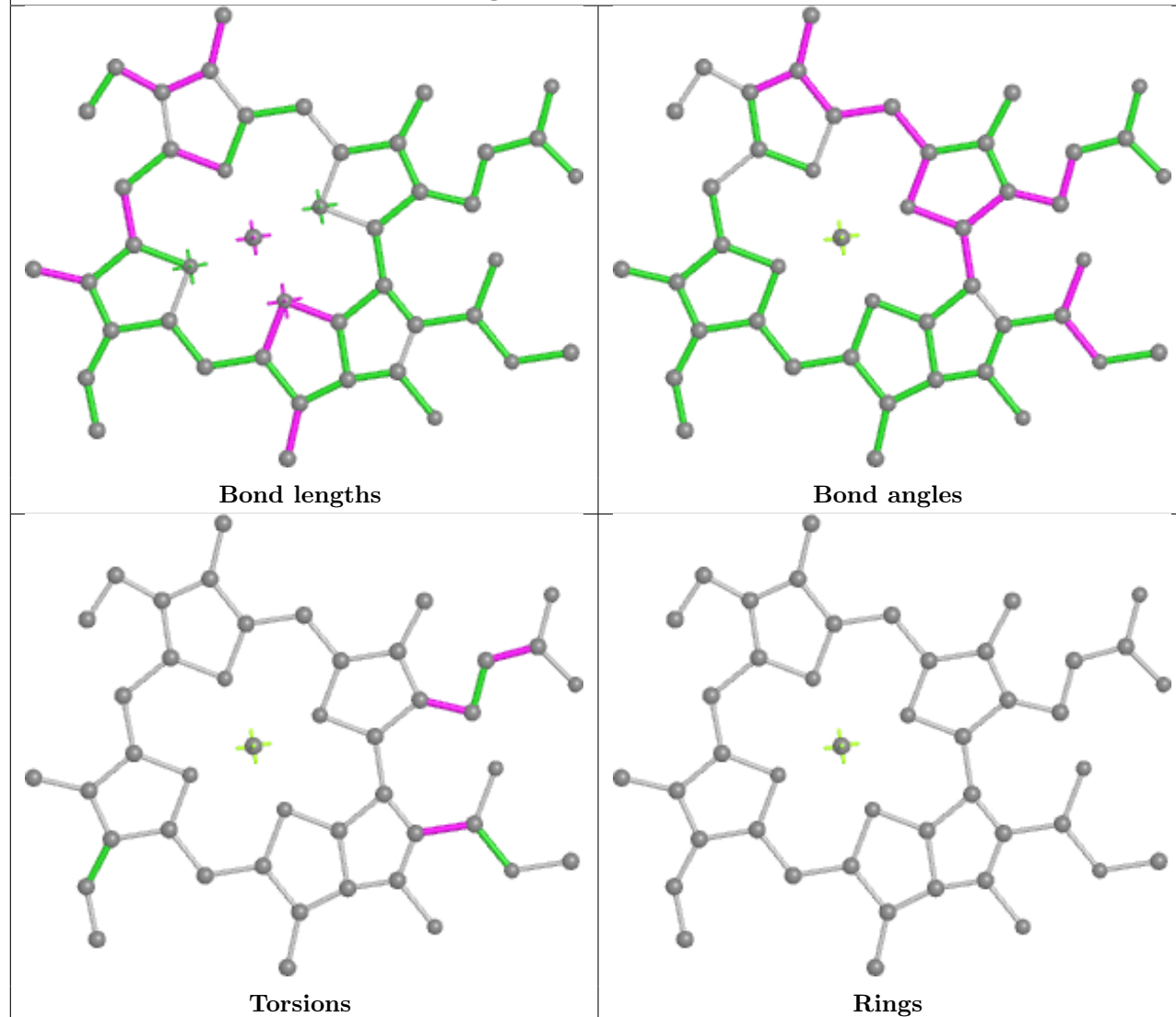




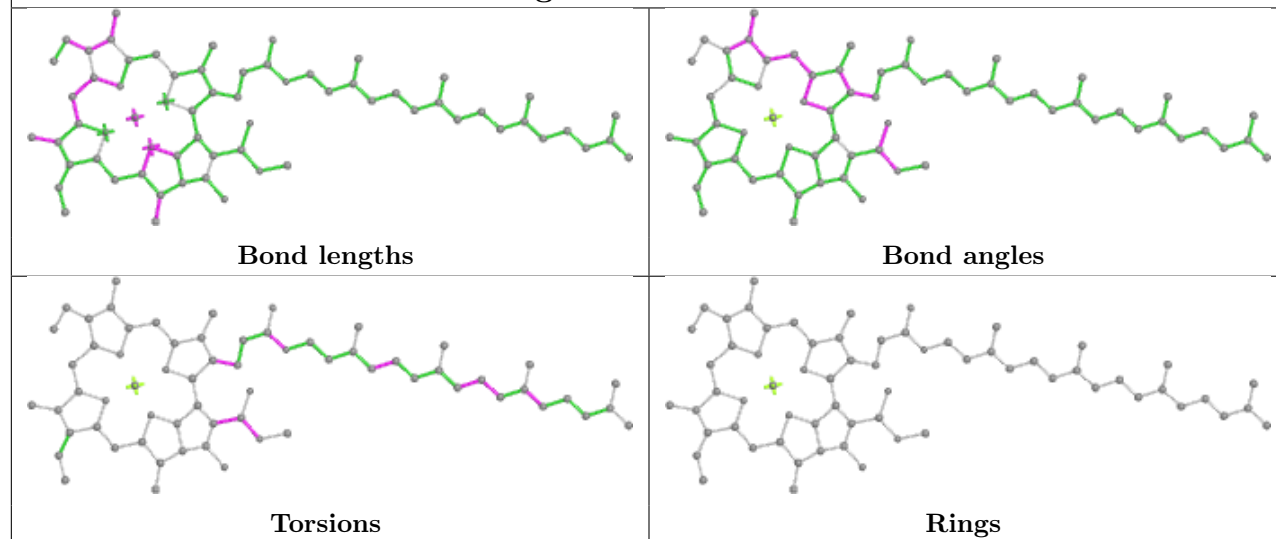
Ligand CLA b 602



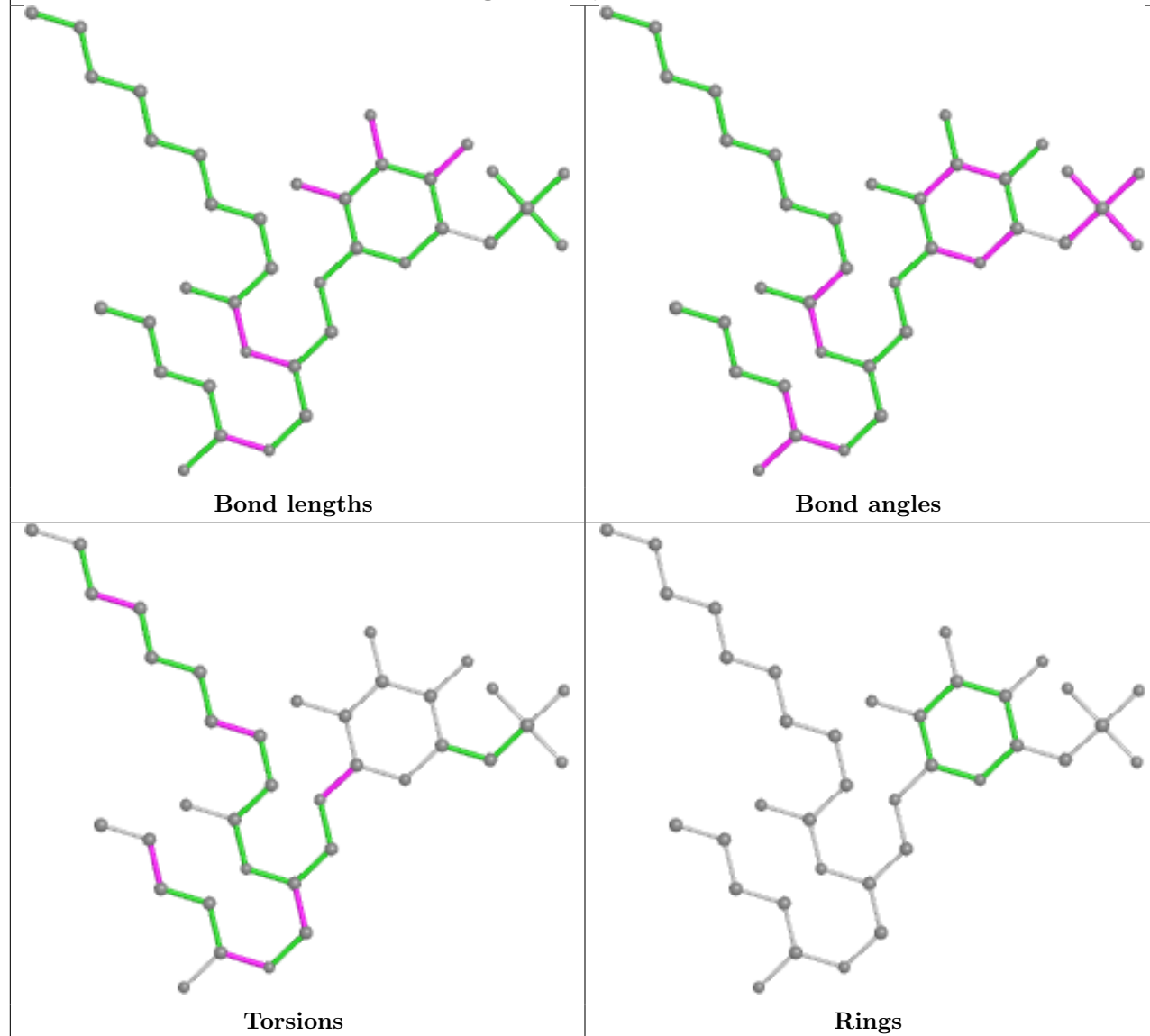
Ligand CLA 15 308

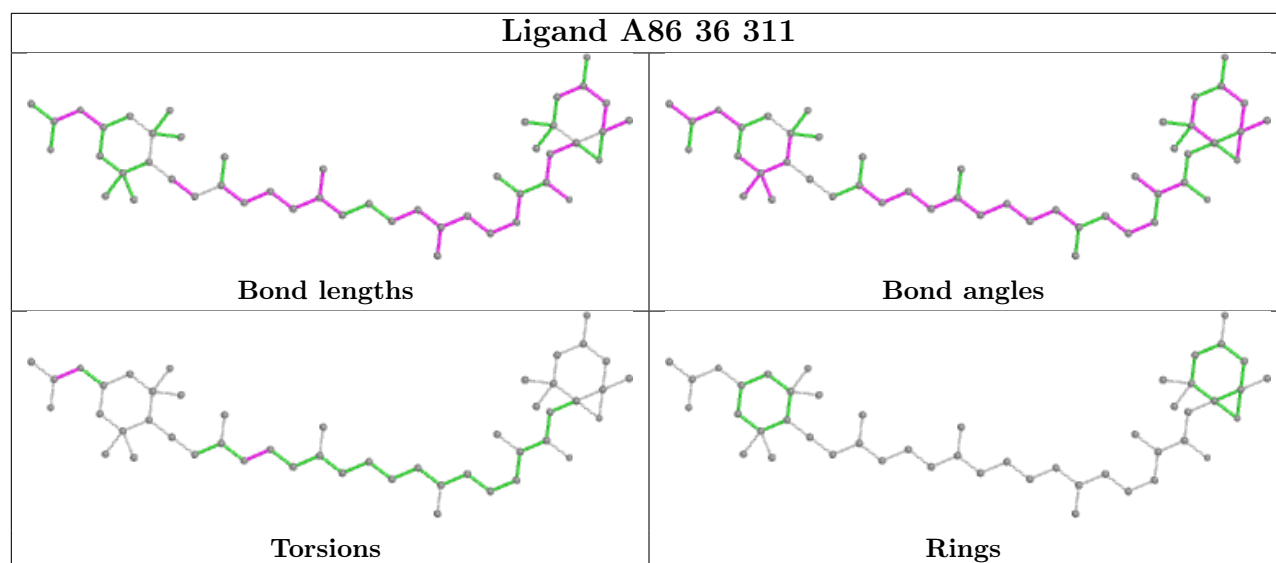
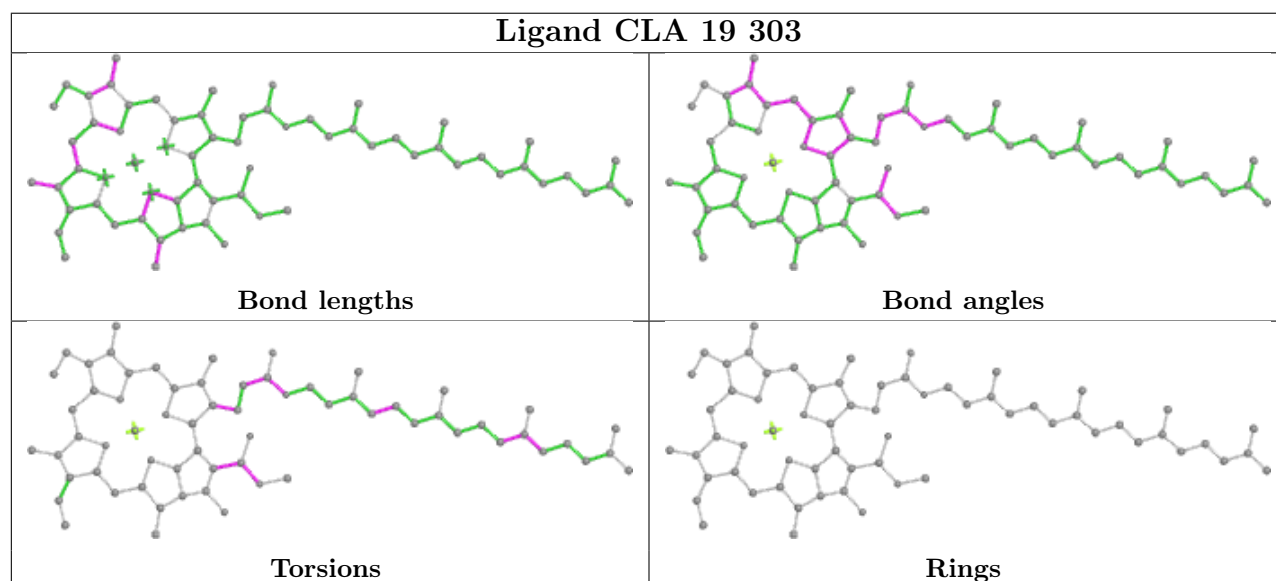
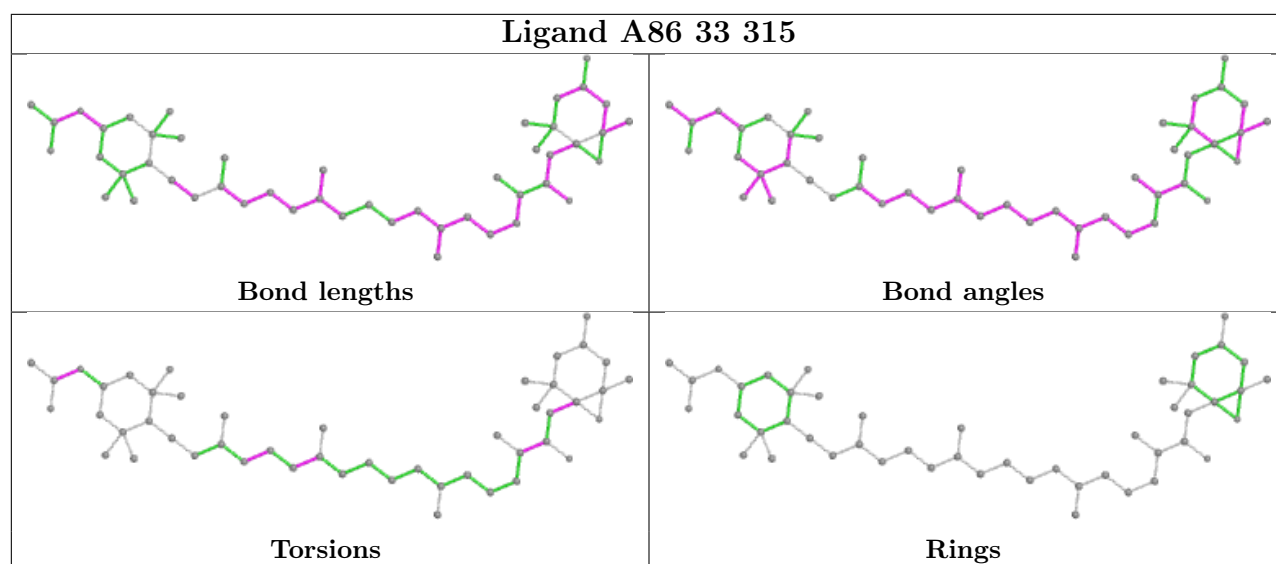


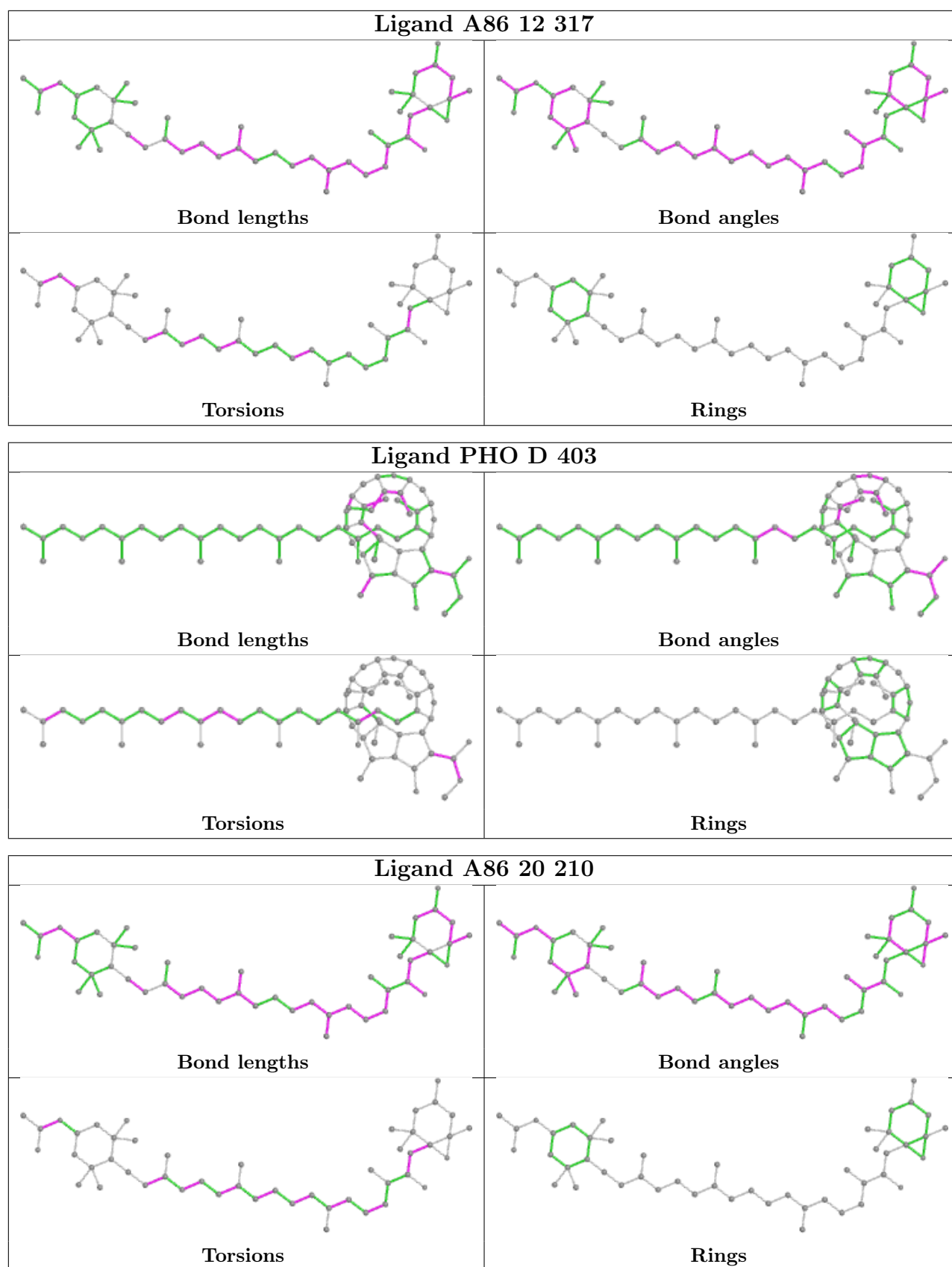
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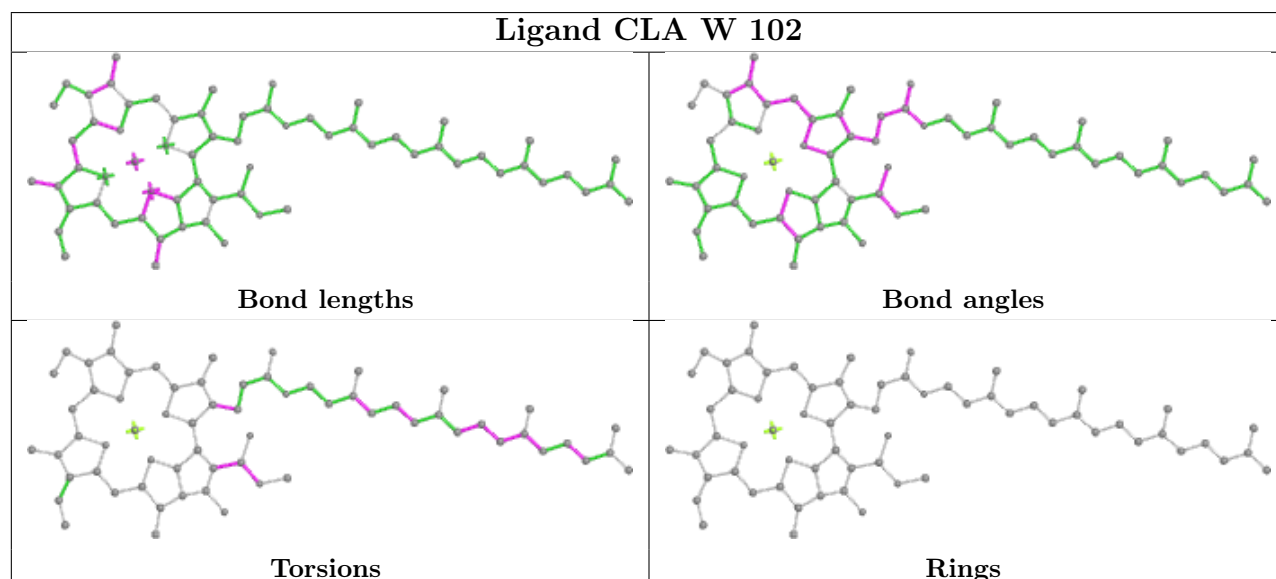
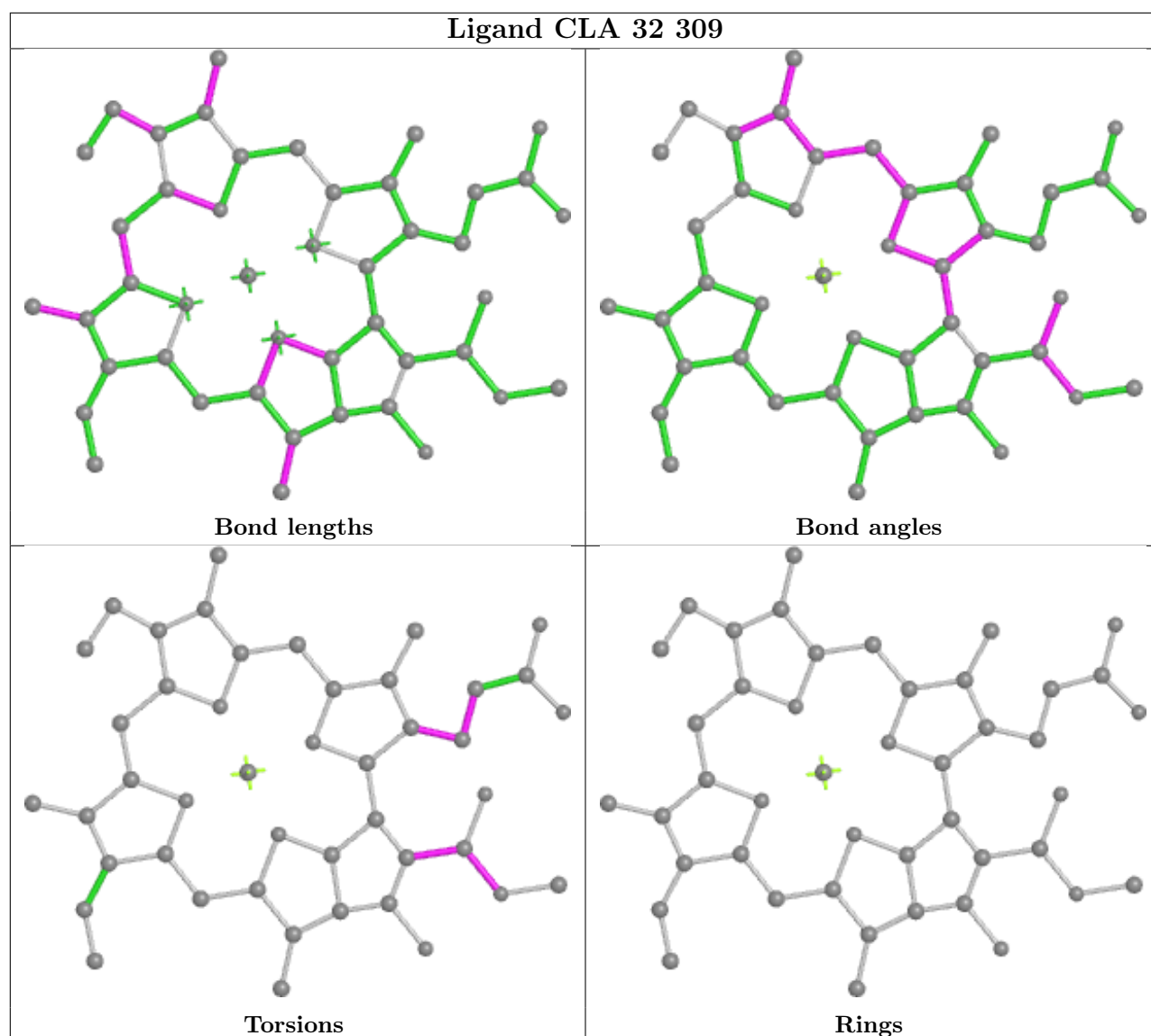


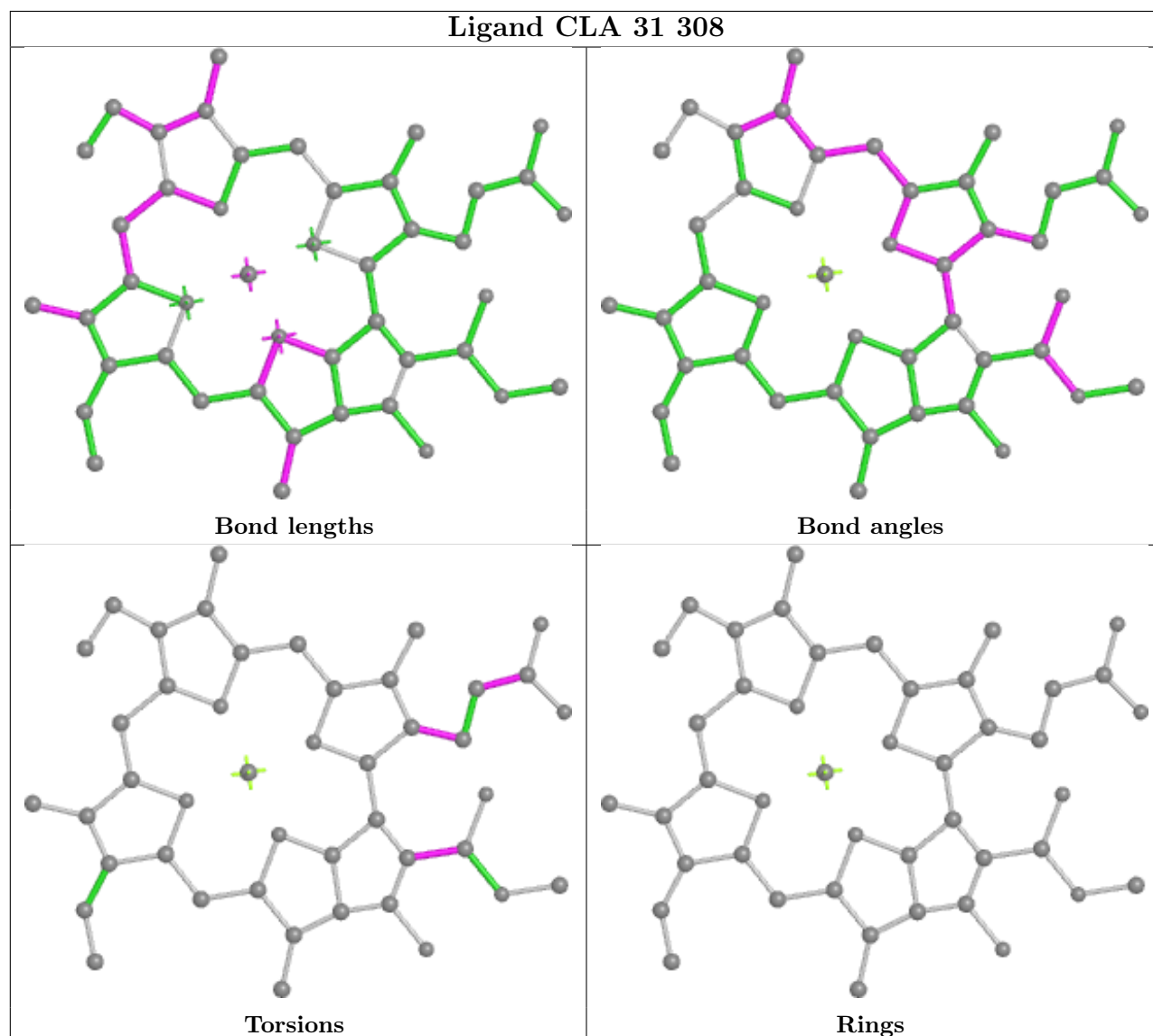
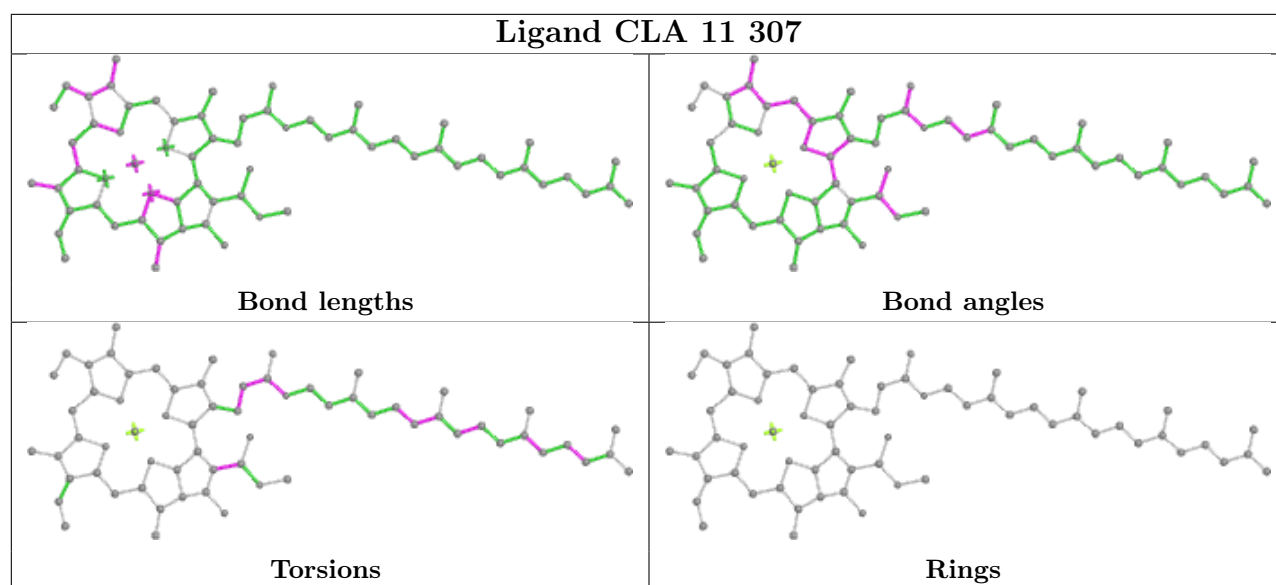
Ligand SQD B 621

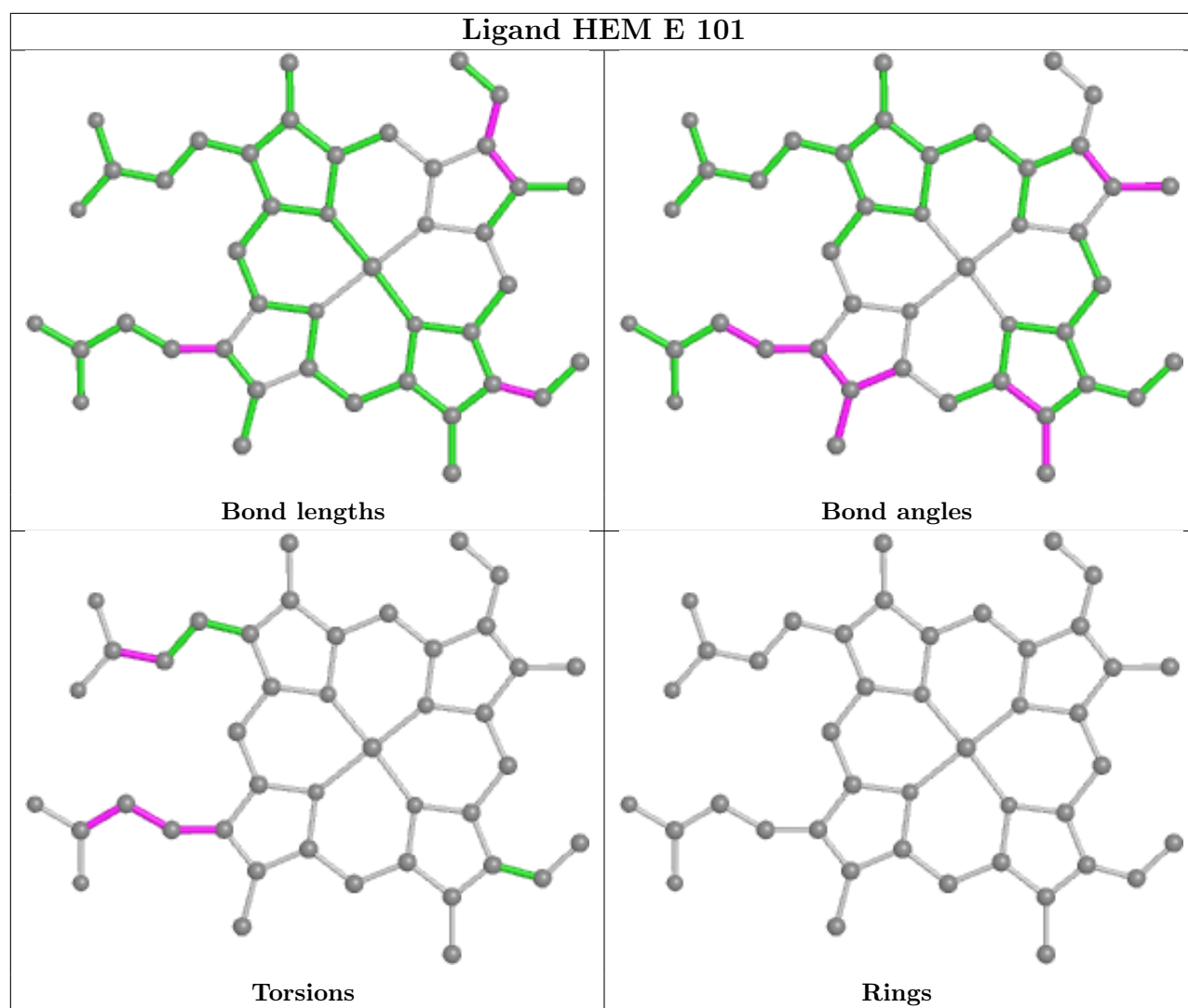


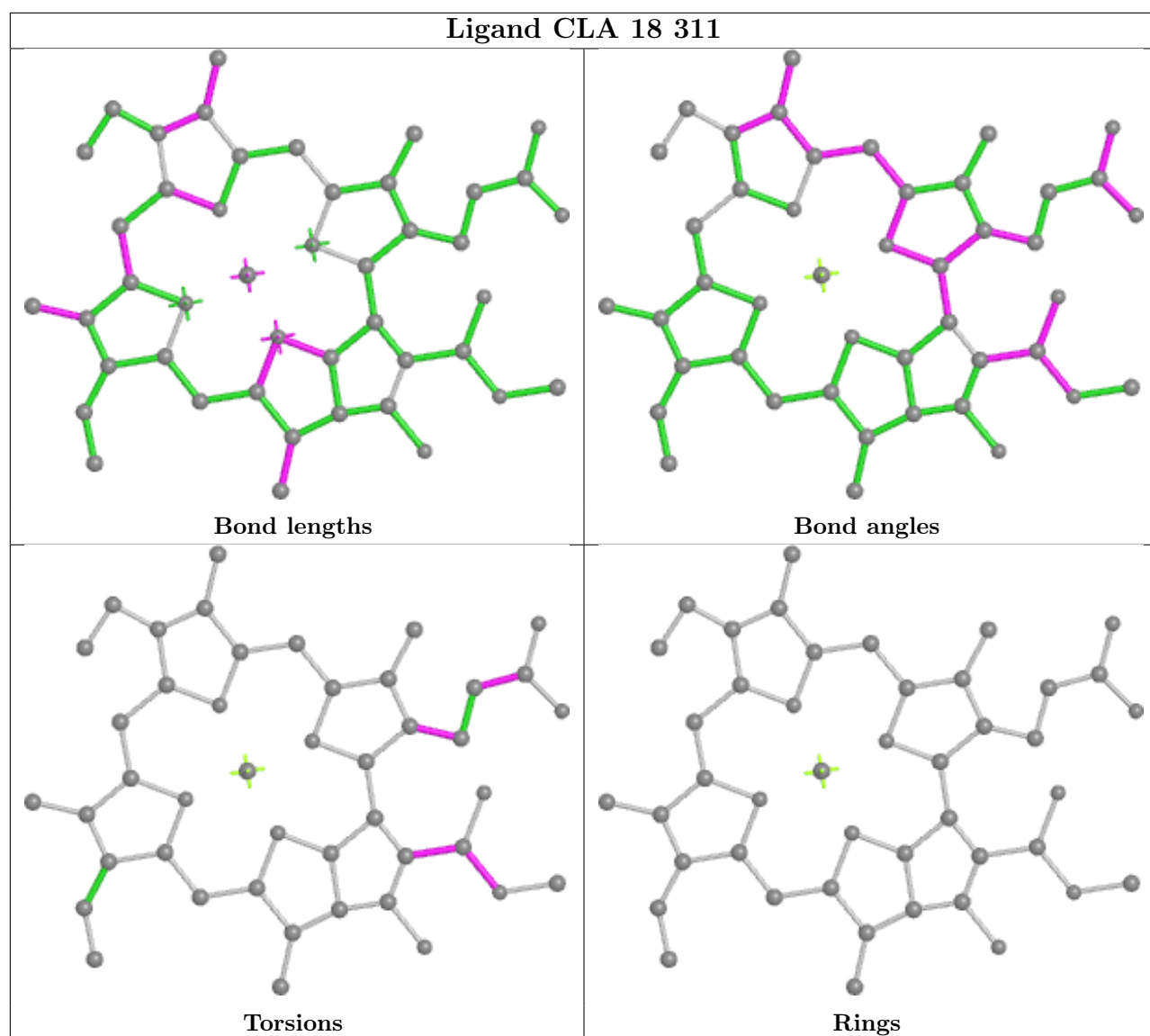


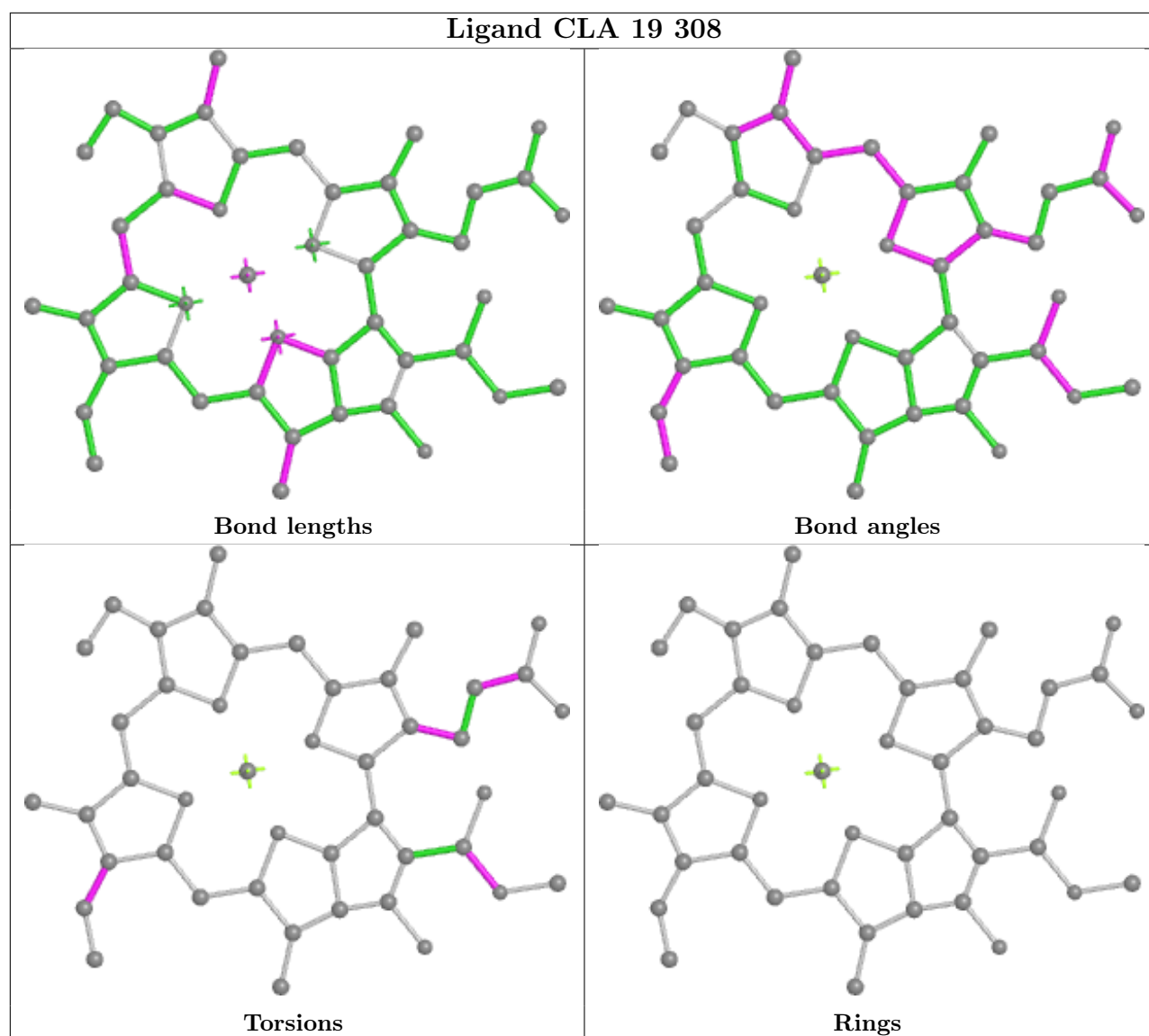


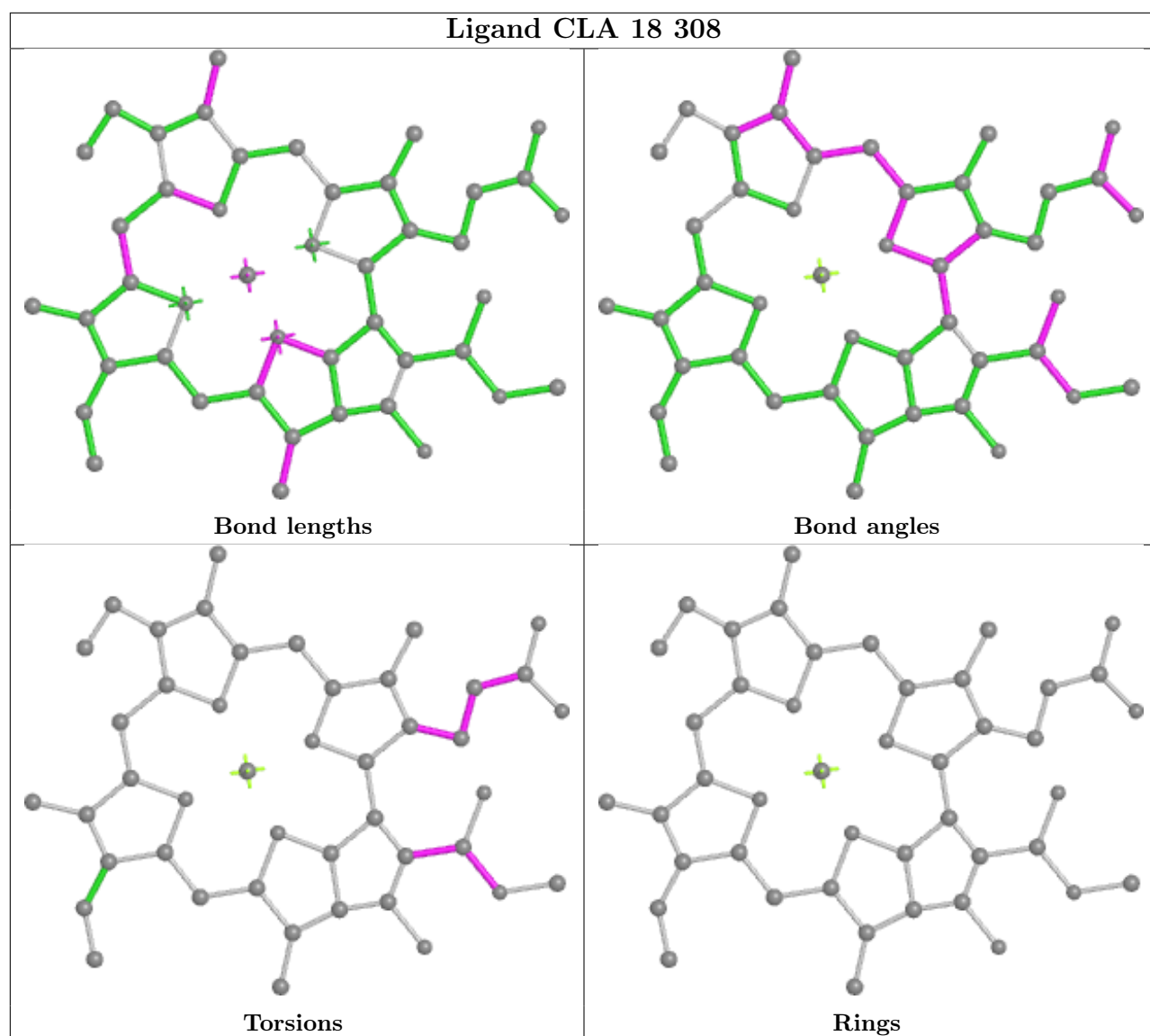


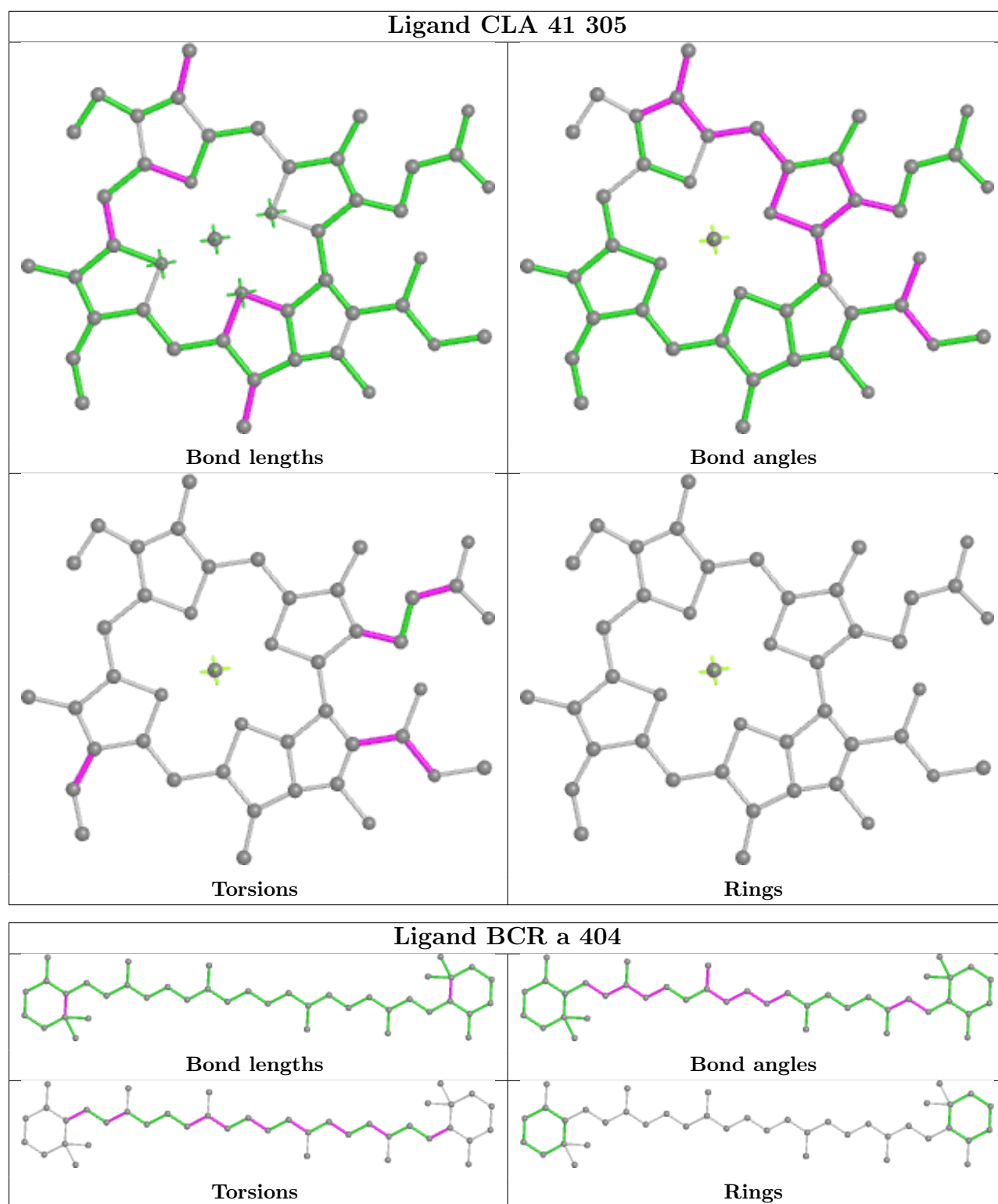


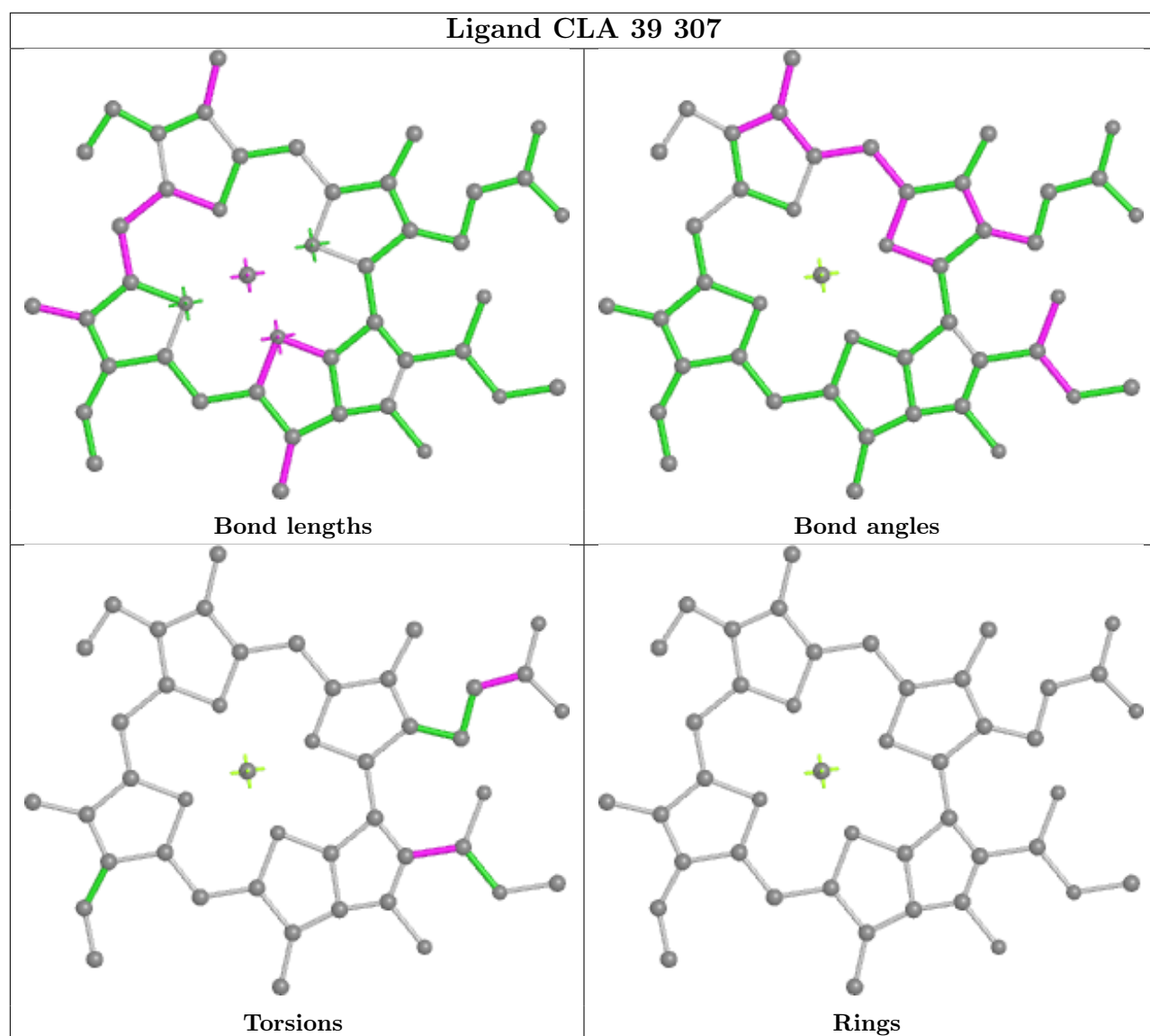


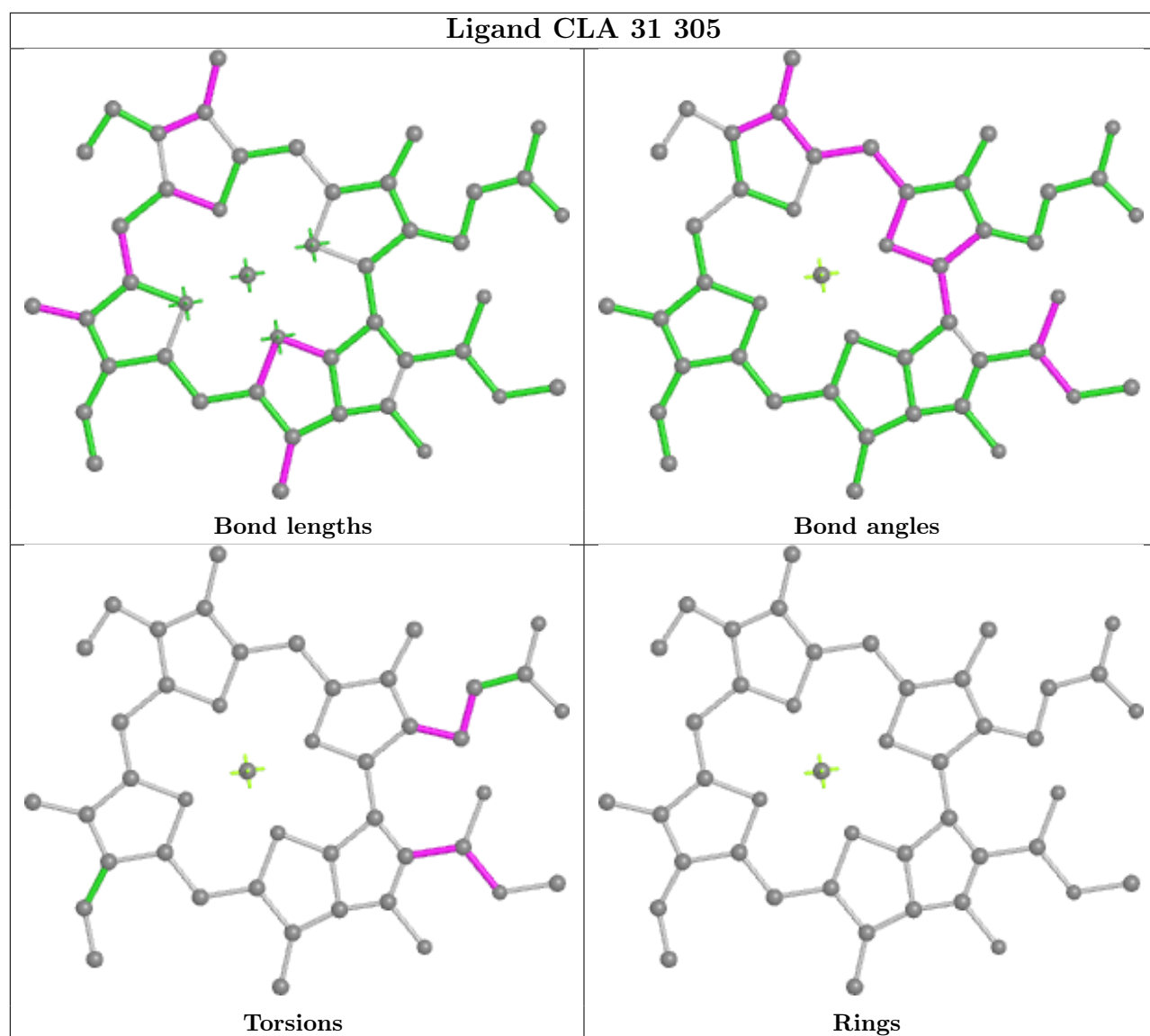


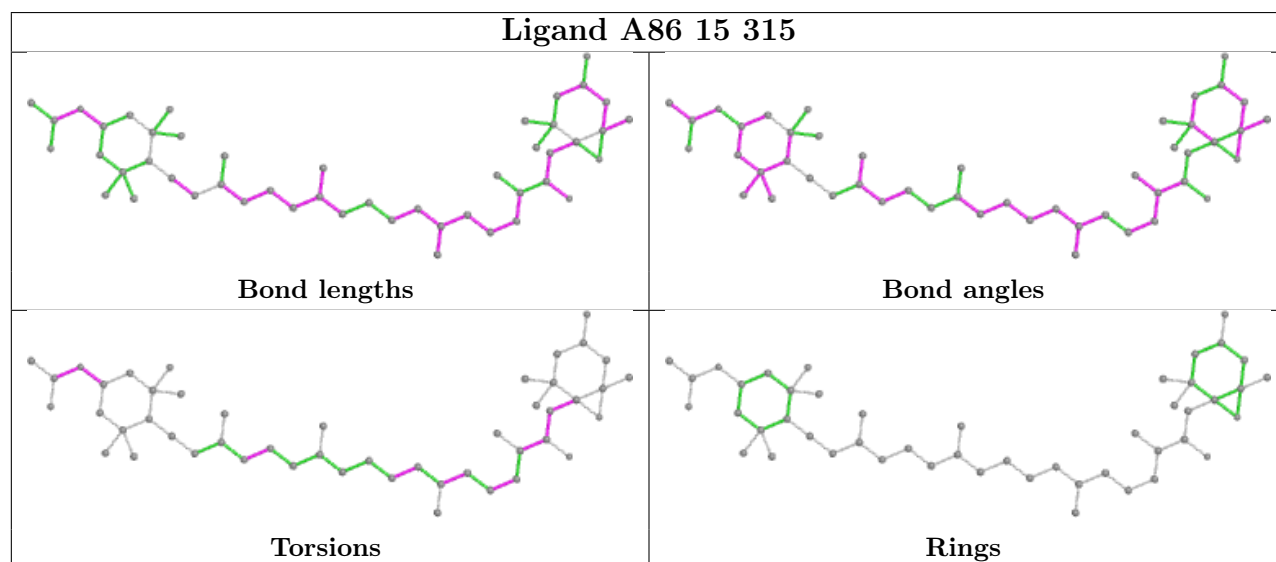
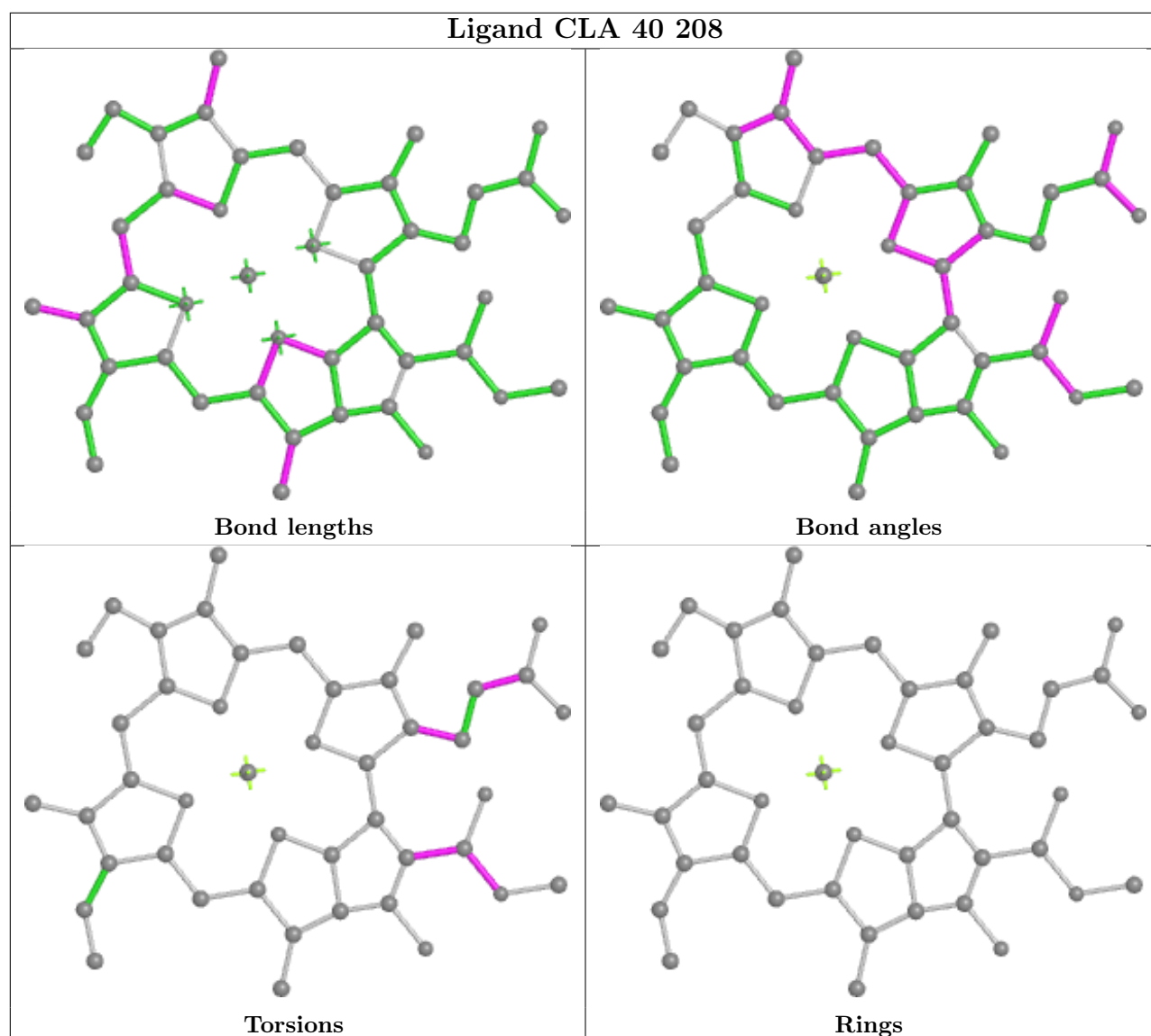


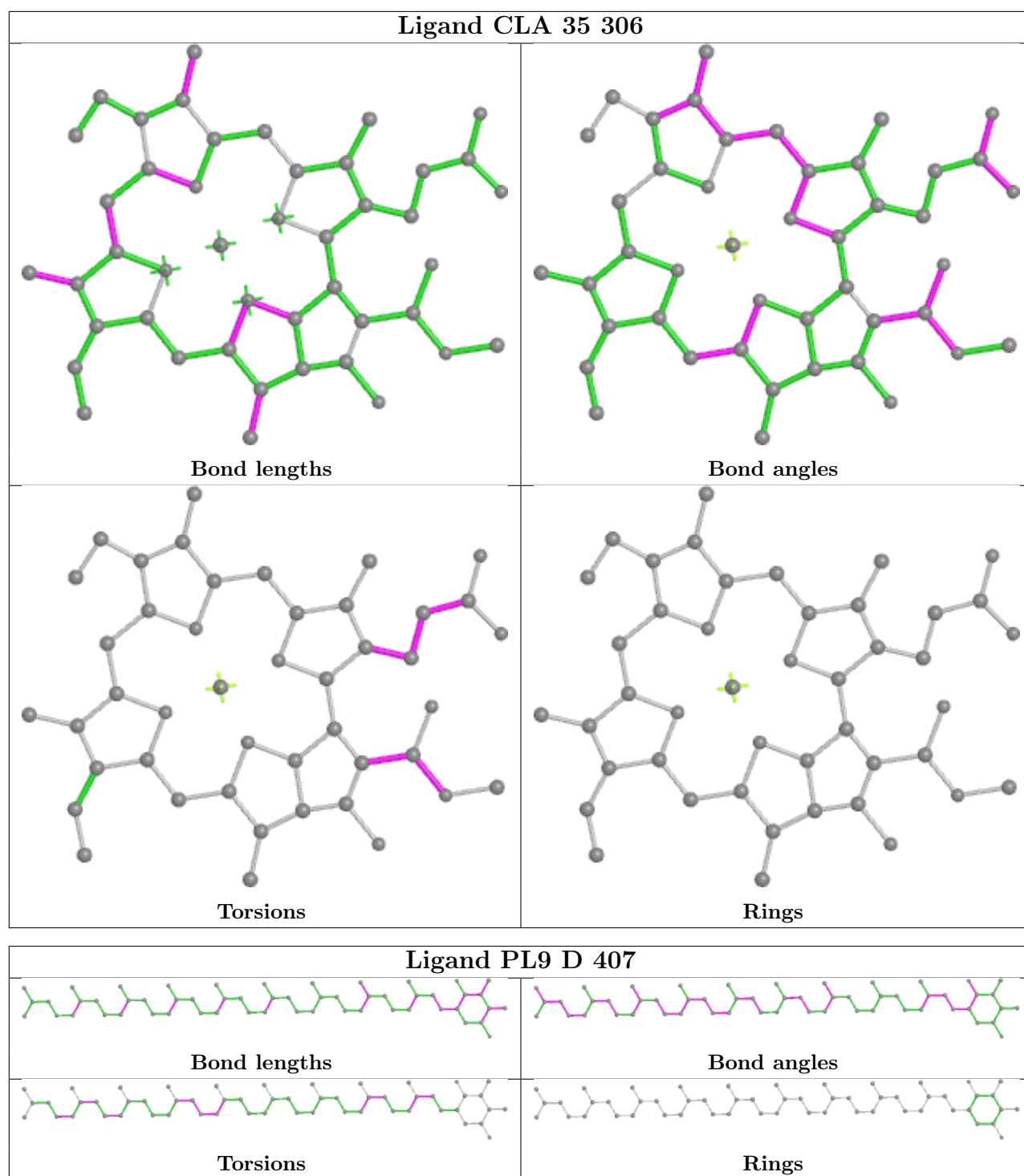


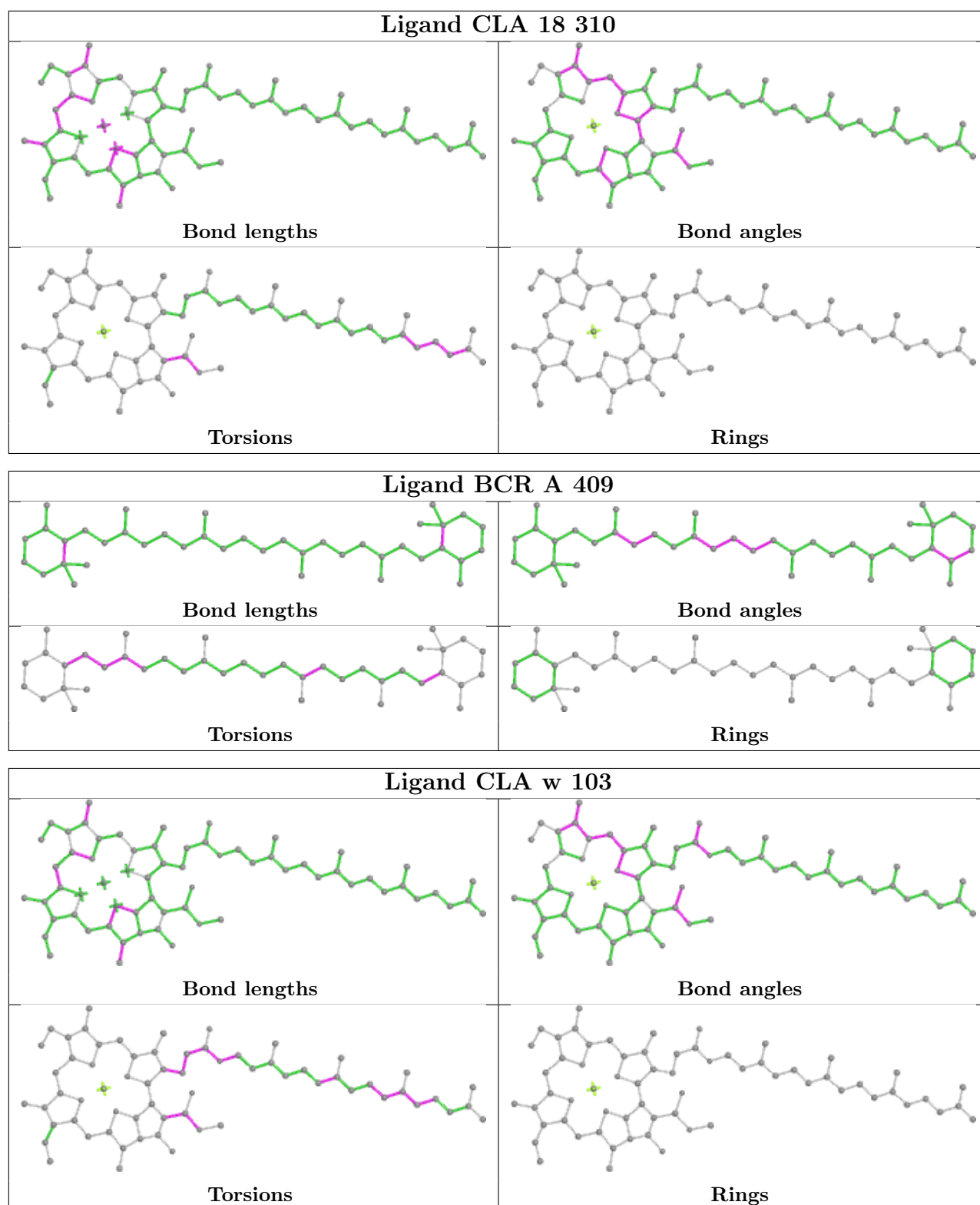


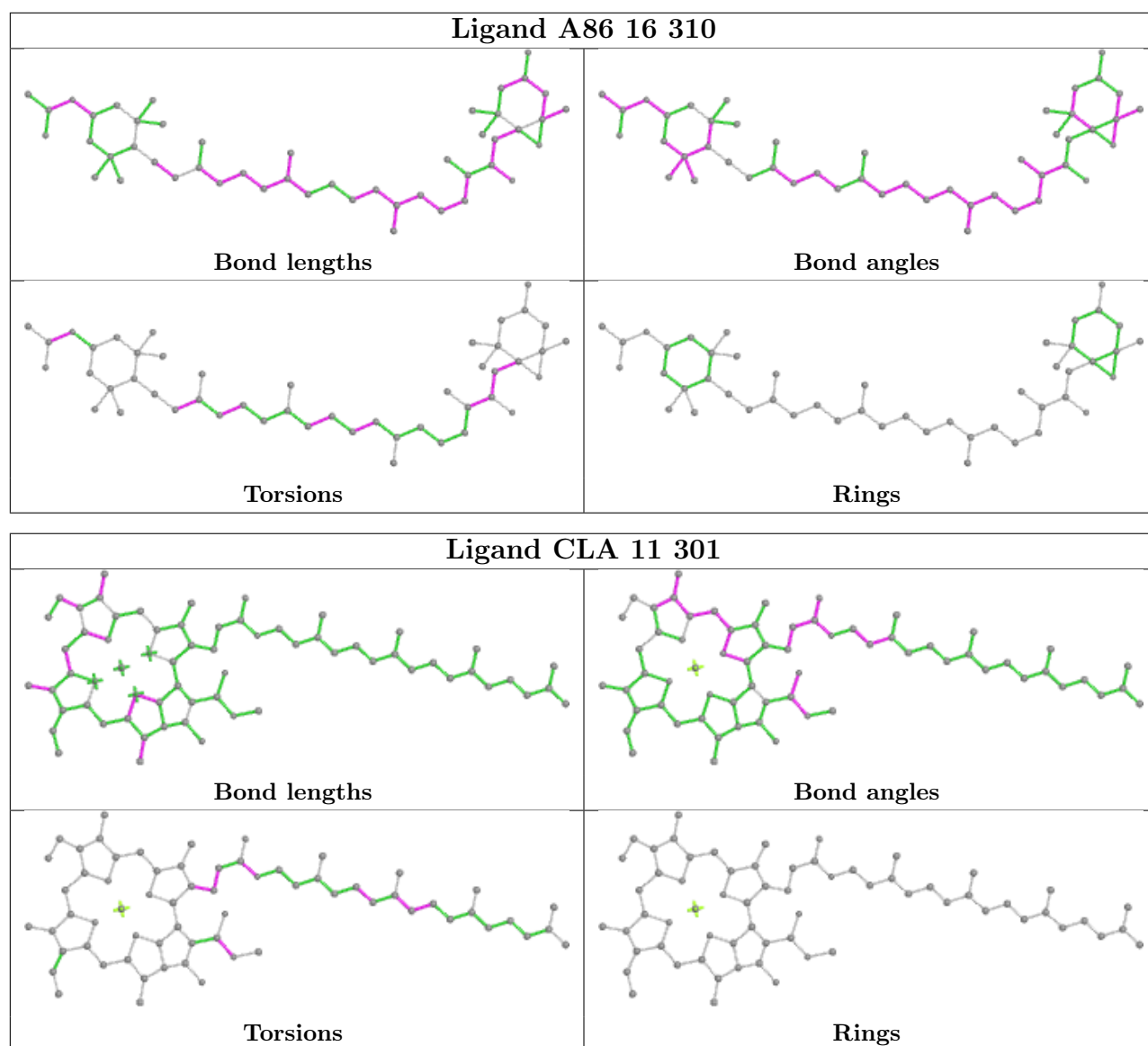


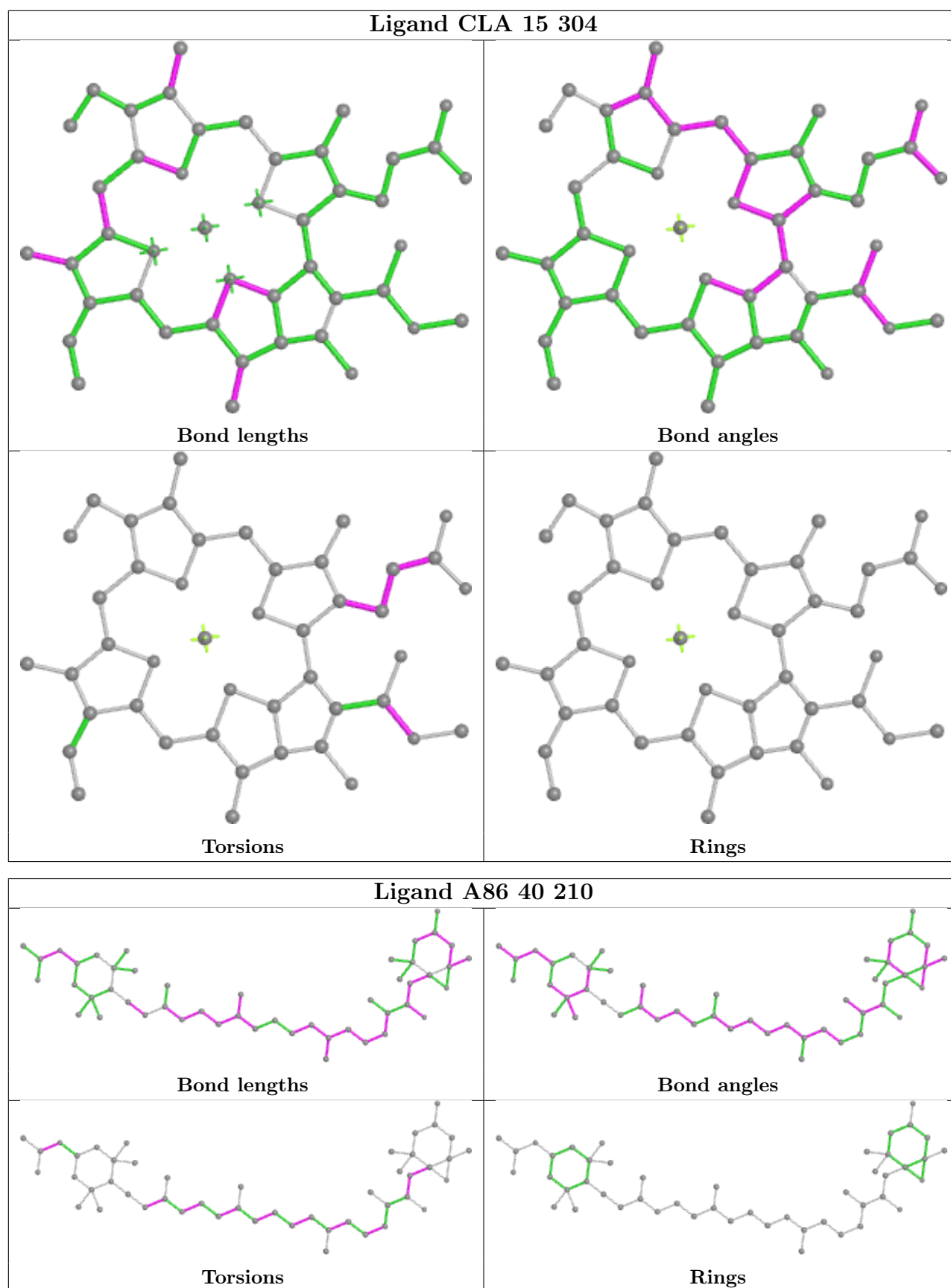


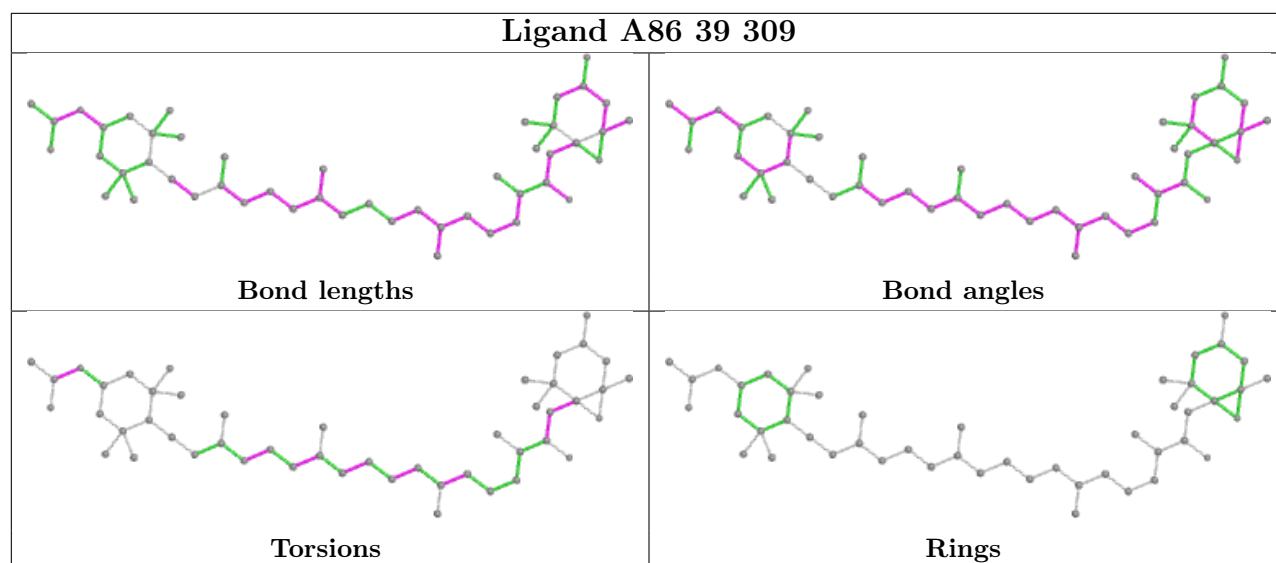
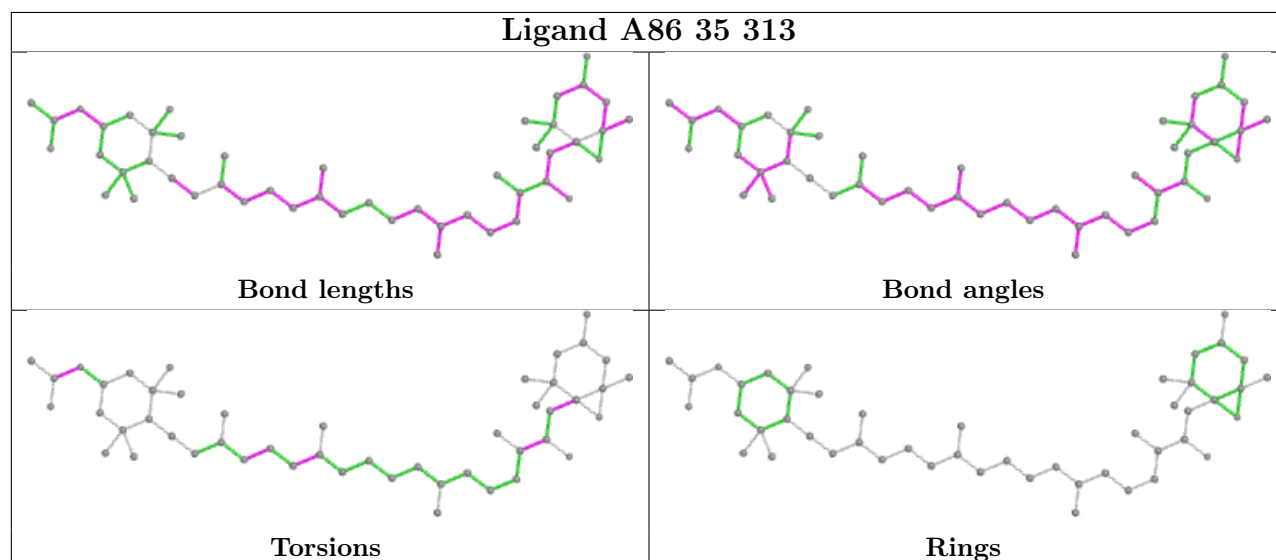
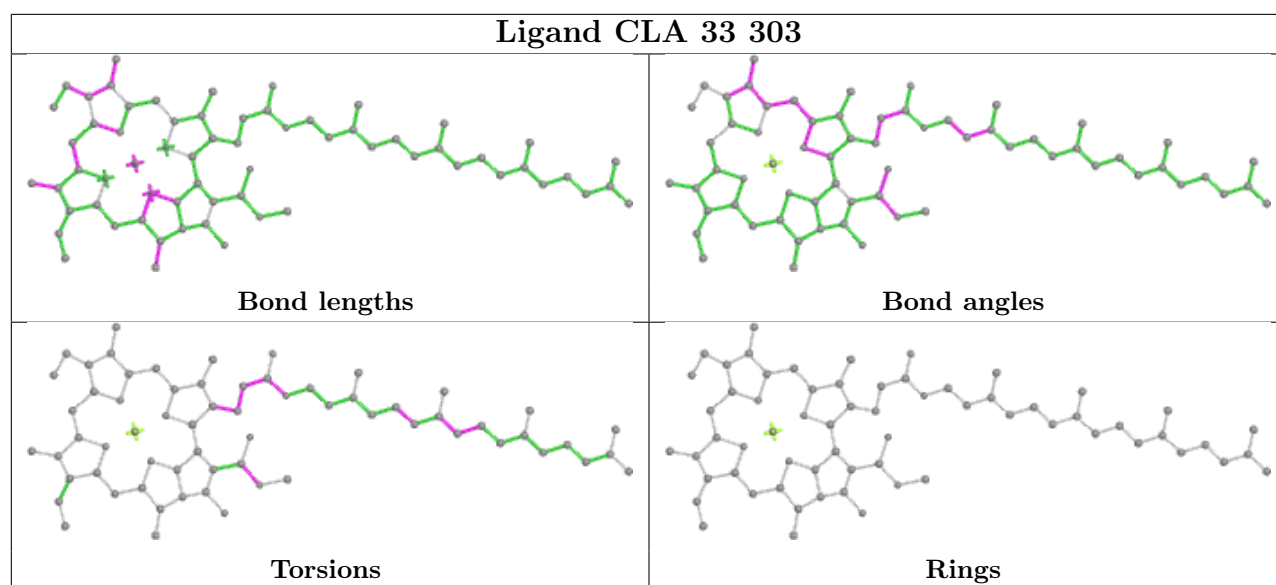


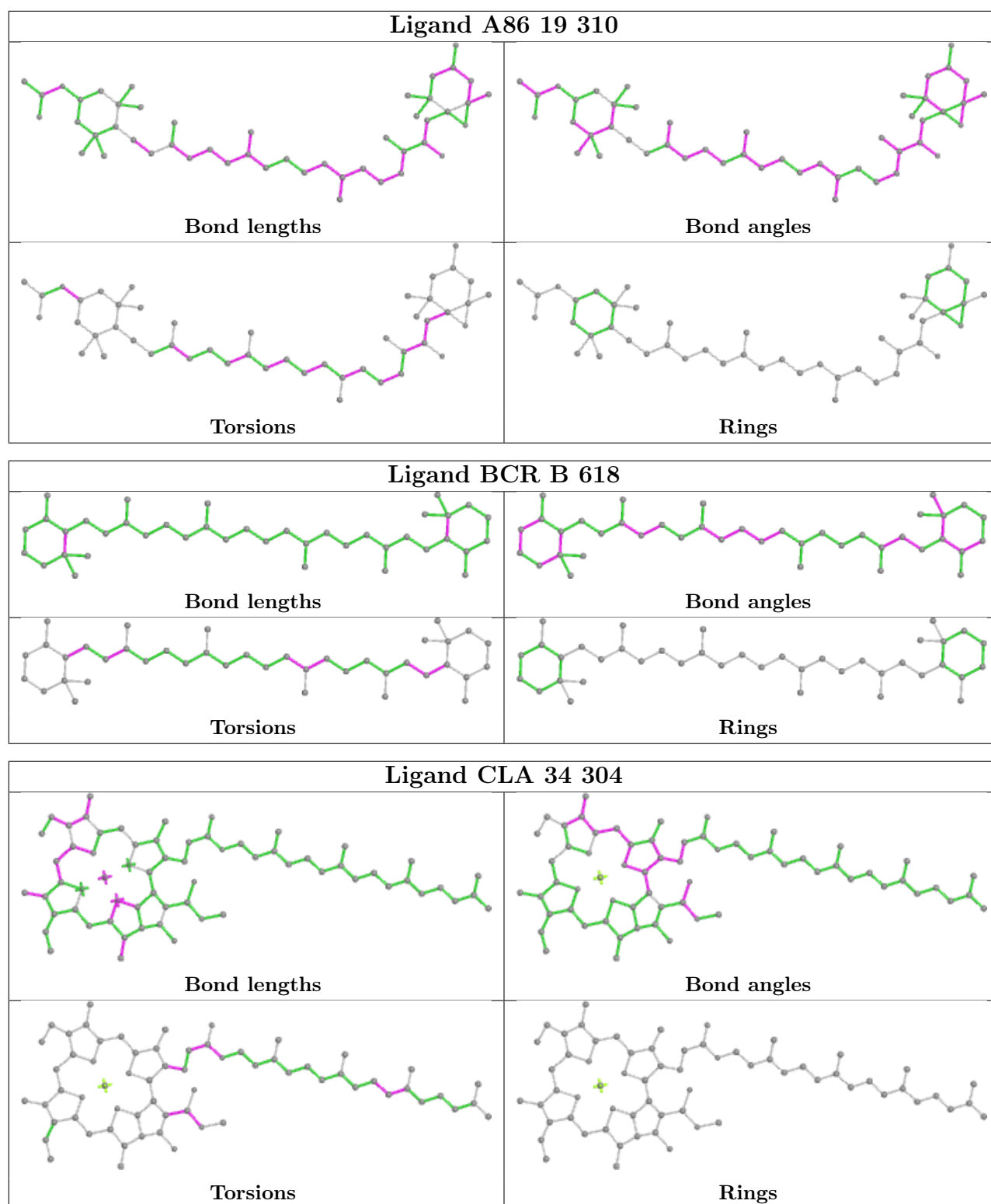


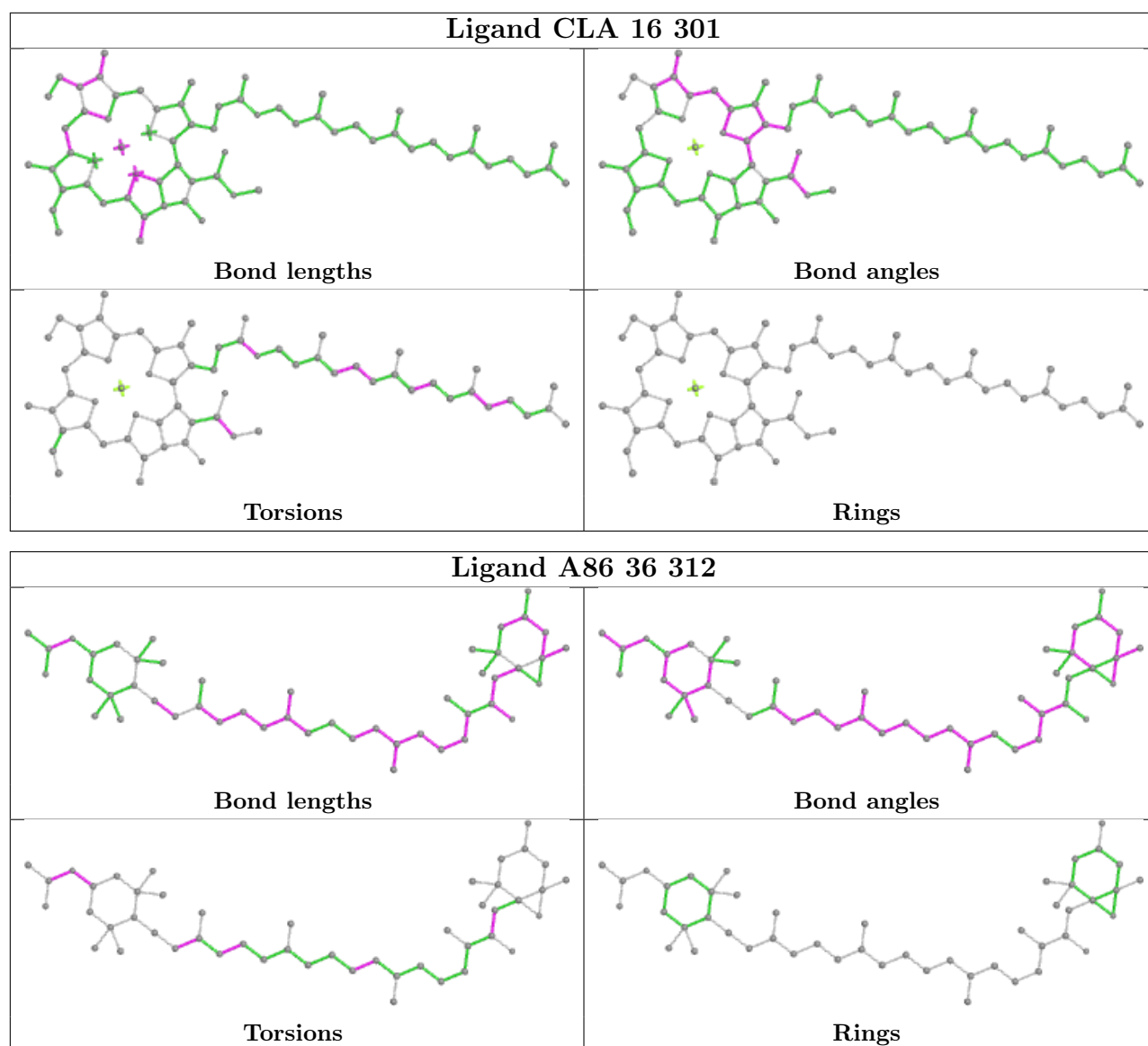


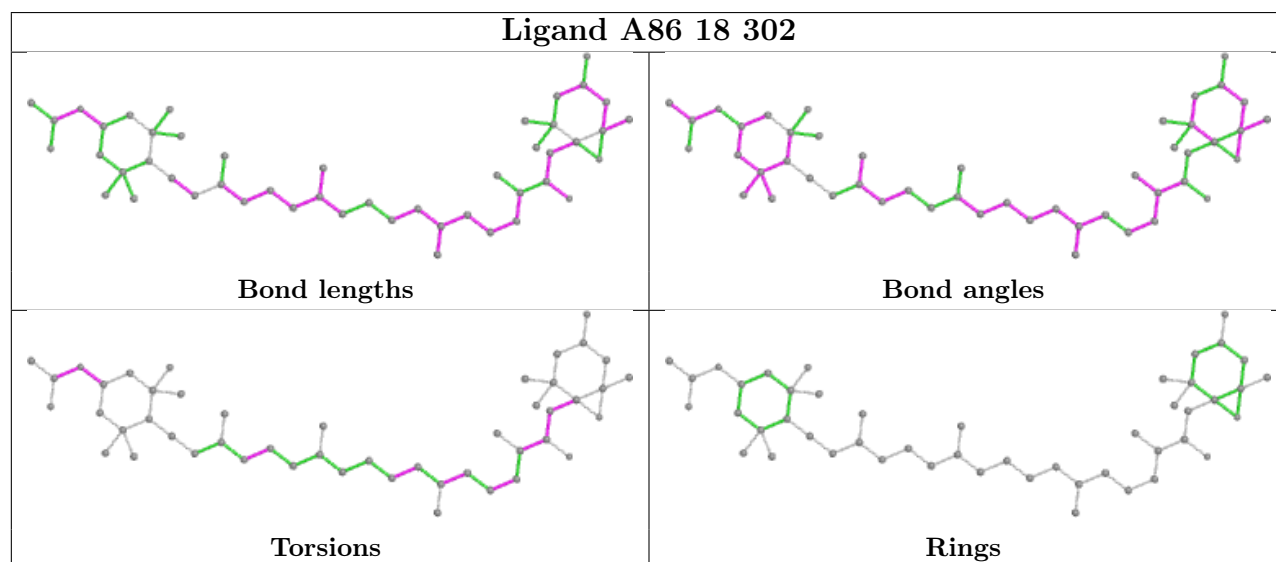
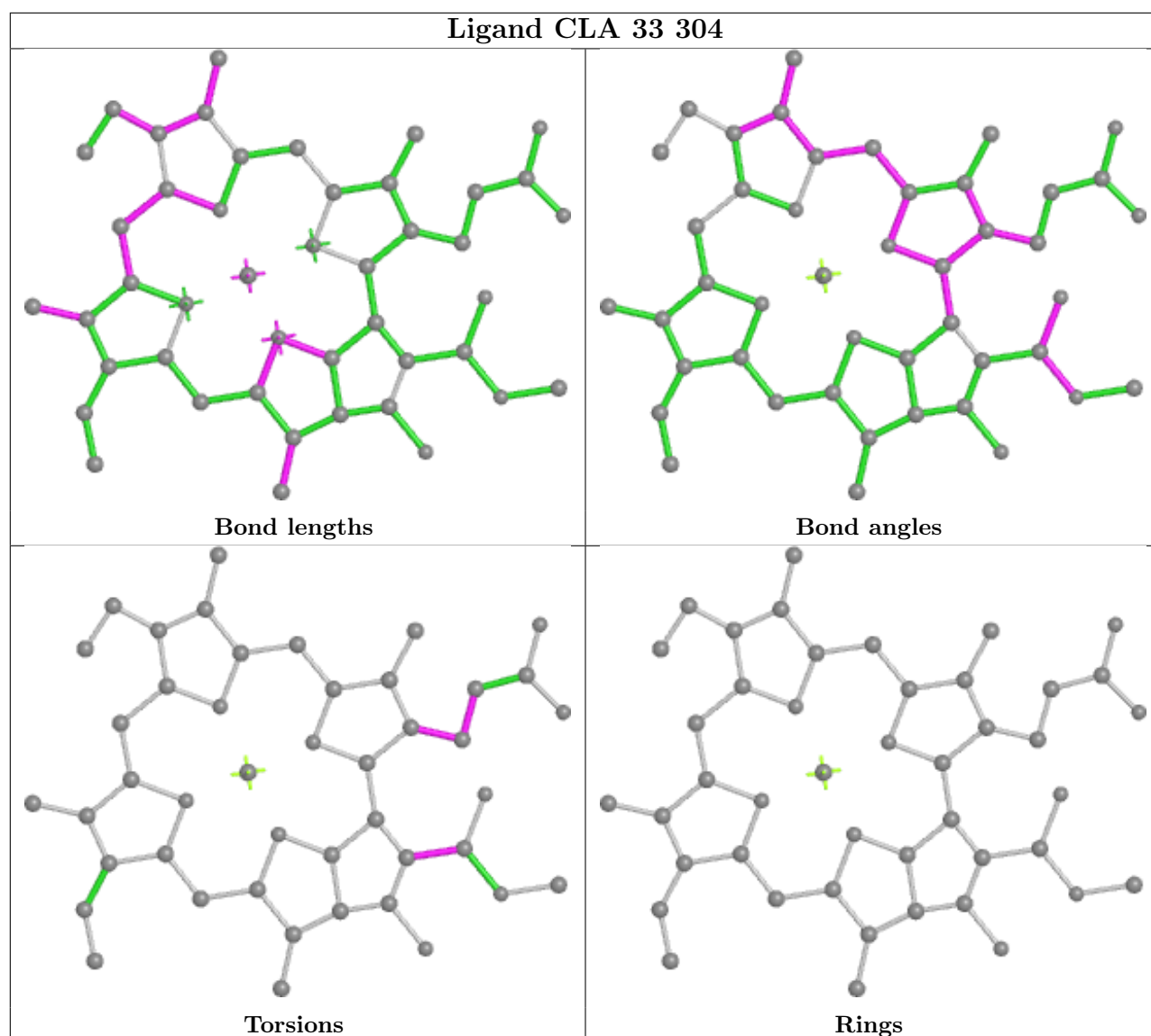


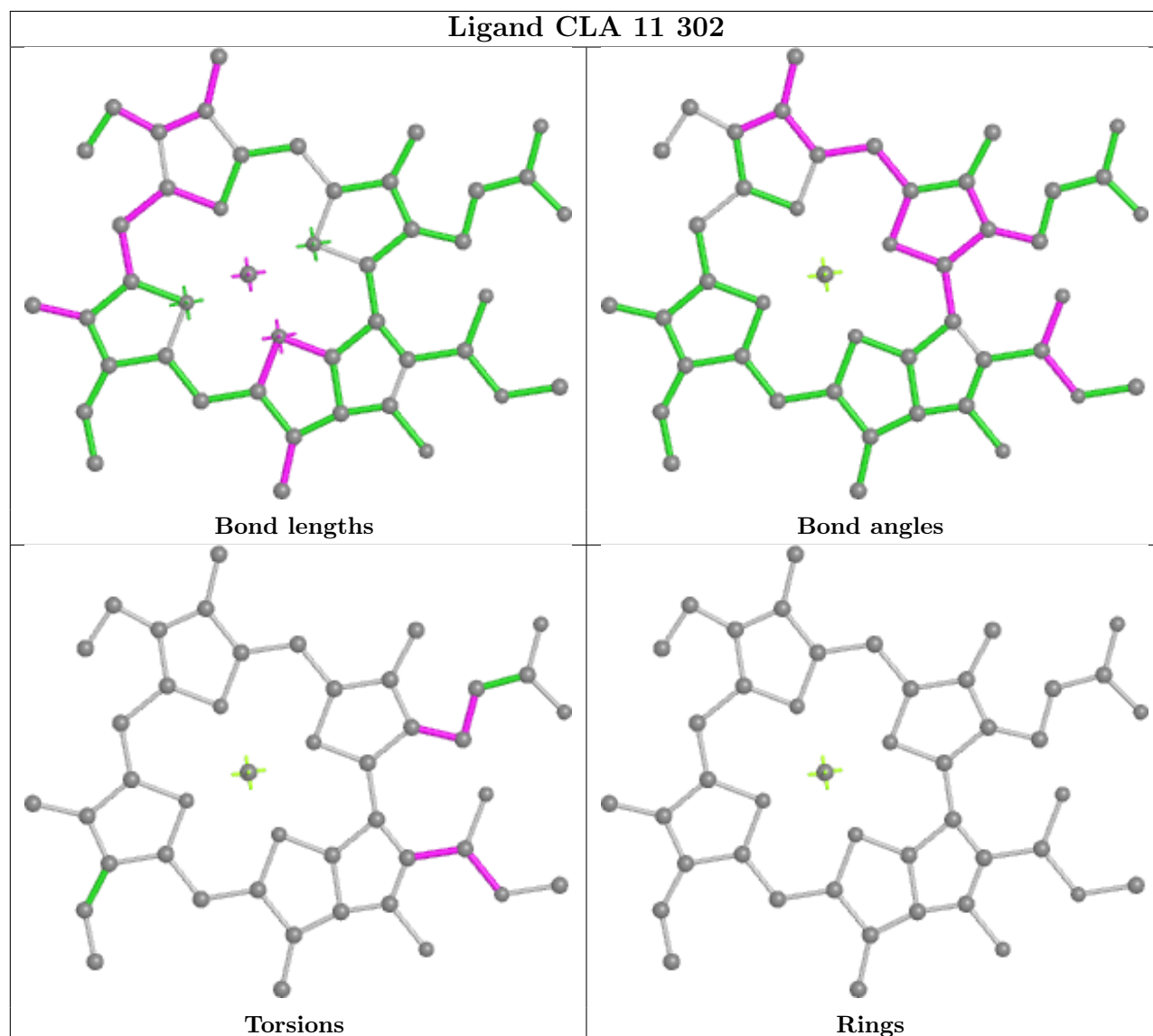
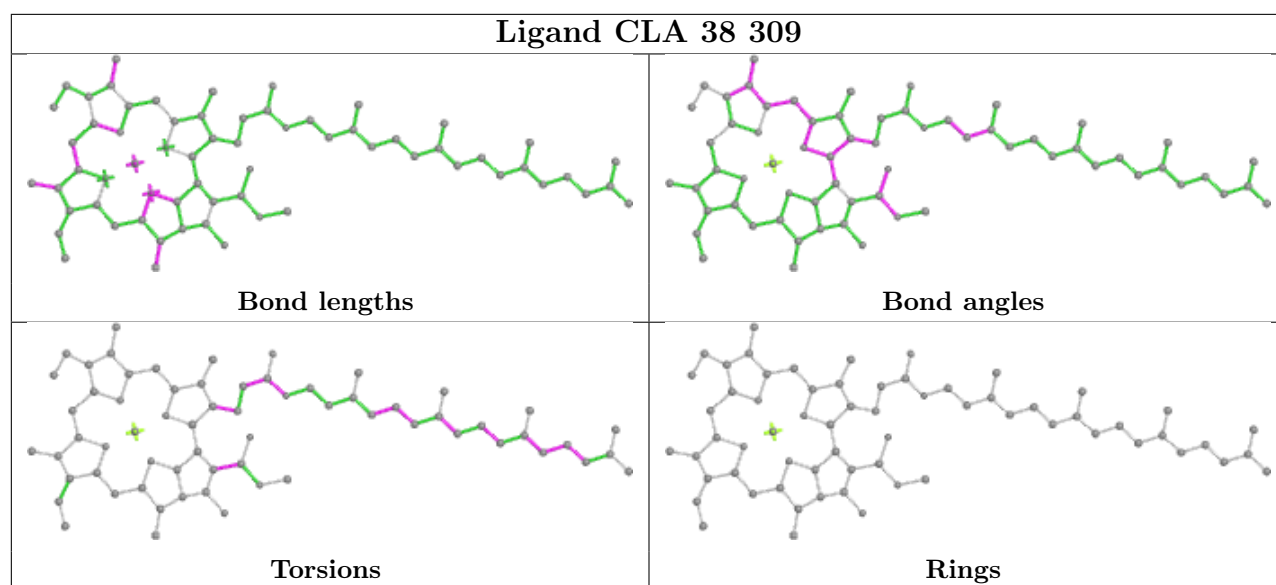


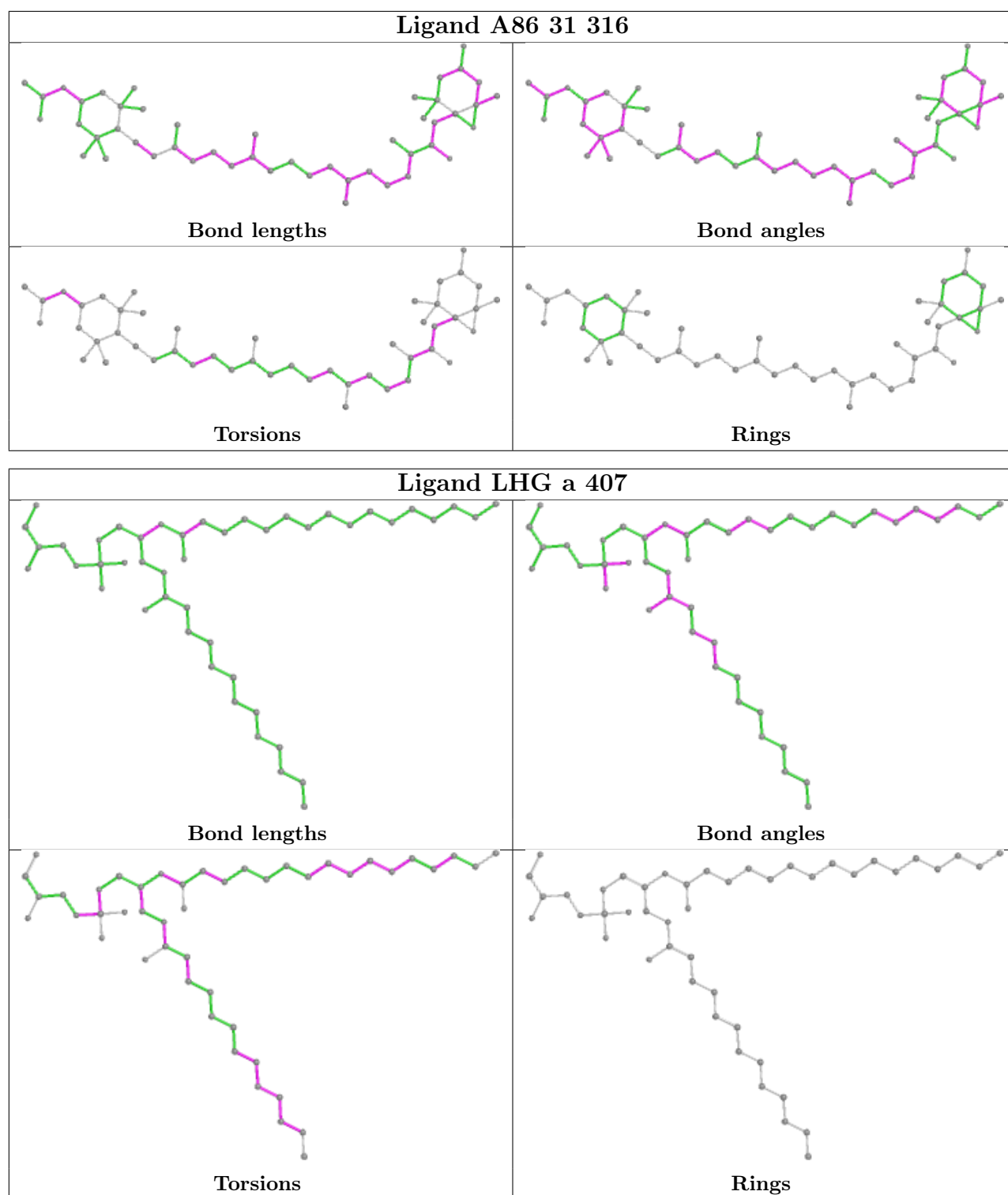


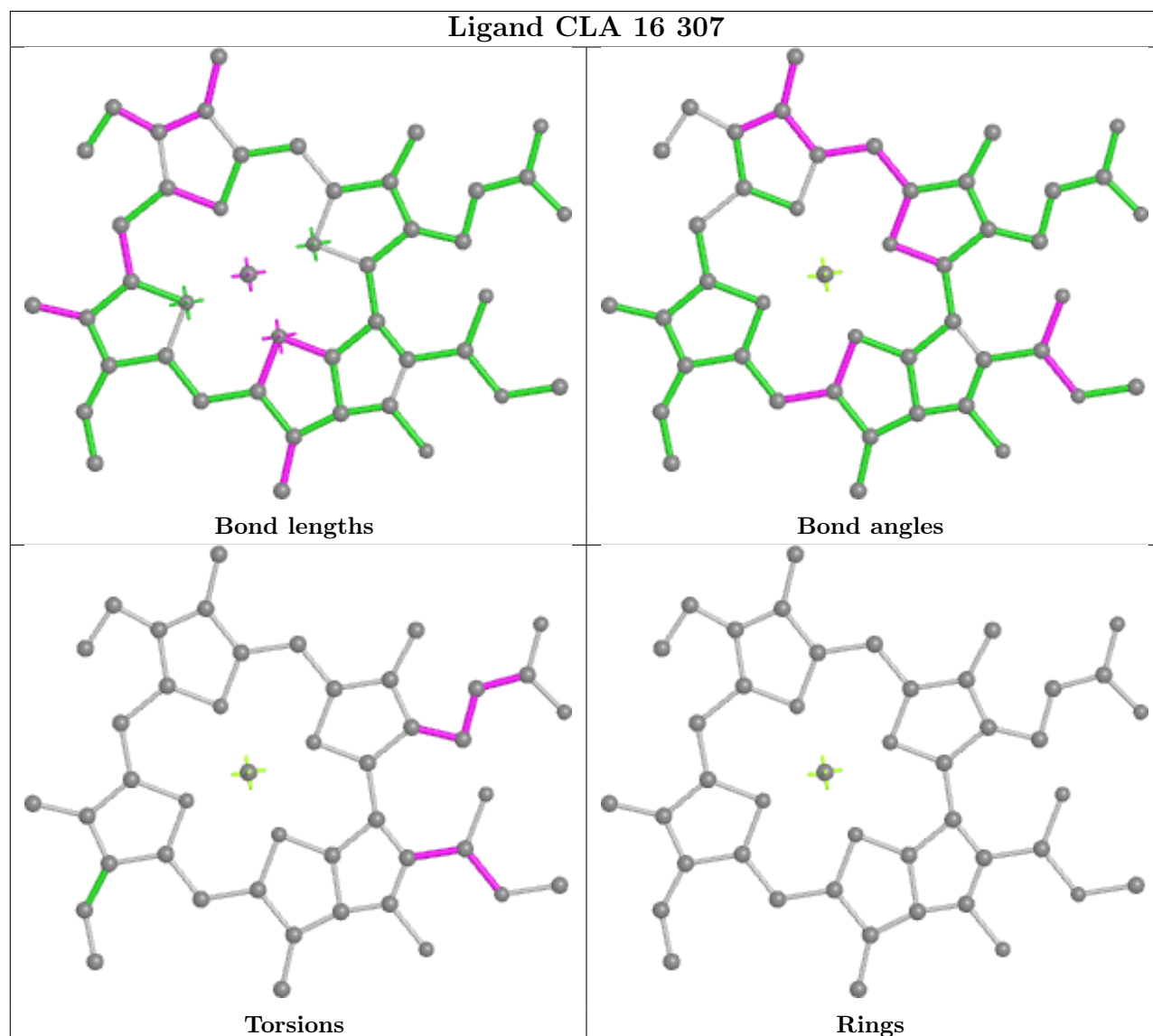
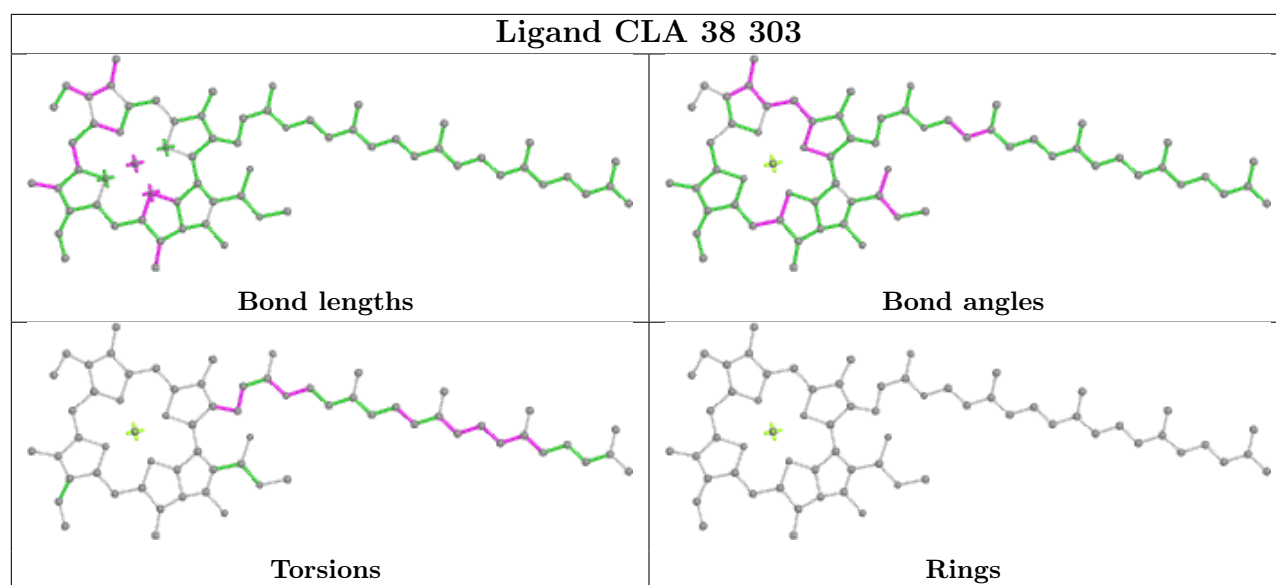


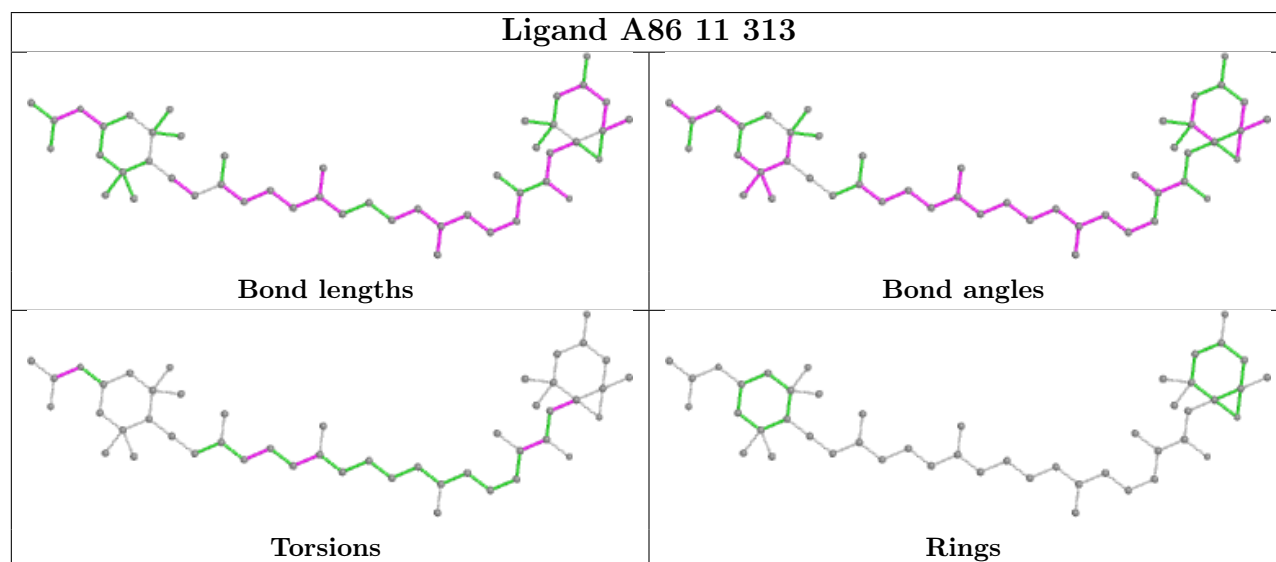
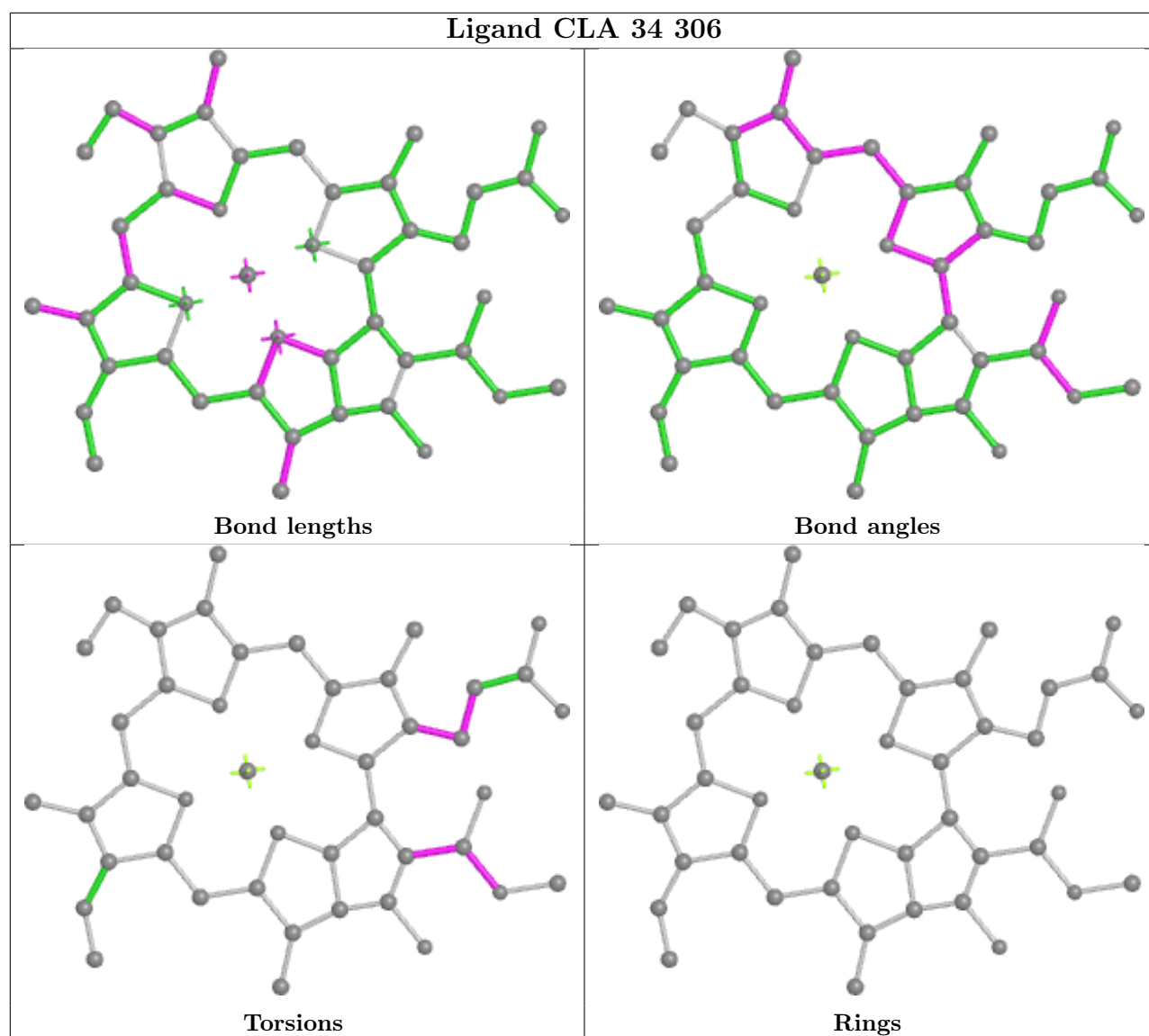












5.7 Other polymers [i](#)

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

This section contains visualisations of the EMDB entry EMD-9777. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.