



## wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 01:24 PM JST

PDB ID : 6J3Y  
EMDB ID : EMD-9775  
Title : Structure of C2S2-type PSII-FCPII supercomplex from diatom  
Authors : Nagao, R.; Kato, K.; Shen, J.R.; Miyazaki, N.; Akita, F.  
Deposited on : 2019-01-07  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

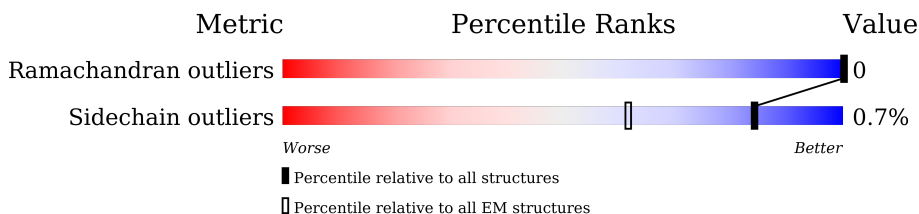
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	509	
2	b	509	
3	C	471	
3	c	471	
4	D	351	
4	d	351	
5	E	84	

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Mol	Chain	Length	Quality of chain
5	e	84	89% 11%
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	6% 98% ..
13	o	248	7% 98% ..
14	T	31	10% 94% ..
14	t	31	6% 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%

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Mol	Chain	Length	Quality of chain
18	X	38	5% 97%
18	x	38	5% 97%
19	Z	61	97%
19	z	61	97%
20	Q	155	12% 88% 12%
20	q	155	14% 88% 12%
21	W	72	8% 71% 28%
21	w	72	7% 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	5% 84% 15%
25	13	207	9% 84% 15%
25	14	207	8% 84% 15%
25	31	207	84% 15%
25	32	207	5% 84% 15%
25	33	207	10% 84% 15%
25	34	207	10% 84% 15%

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
27	CLA	11	301	X	-	-	-
27	CLA	11	302	X	-	-	-
27	CLA	11	303	X	-	-	-
27	CLA	11	304	X	-	-	-
27	CLA	11	305	X	-	-	-
27	CLA	11	306	X	-	-	-
27	CLA	11	307	X	-	-	-
27	CLA	11	309	X	-	-	-
27	CLA	11	315	X	-	-	-
27	CLA	12	303	X	-	-	-
27	CLA	12	305	X	-	-	-
27	CLA	12	306	X	-	-	-
27	CLA	12	307	X	-	-	-
27	CLA	12	308	X	-	-	-
27	CLA	12	309	X	-	-	-
27	CLA	12	310	X	-	-	-
27	CLA	12	311	X	-	-	-
27	CLA	12	313	X	-	-	-
27	CLA	13	301	X	-	-	-
27	CLA	13	303	X	-	-	-
27	CLA	13	304	X	-	-	-
27	CLA	13	305	X	-	-	-
27	CLA	13	306	X	-	-	-
27	CLA	13	307	X	-	-	-
27	CLA	13	308	X	-	-	-
27	CLA	13	309	X	-	-	-
27	CLA	13	311	X	-	-	-
27	CLA	14	302	X	-	-	-
27	CLA	14	303	X	-	-	-
27	CLA	14	304	X	-	-	-
27	CLA	14	305	X	-	-	-
27	CLA	14	306	X	-	-	-
27	CLA	14	307	X	-	-	-
27	CLA	14	308	X	-	-	-
27	CLA	14	309	X	-	-	-
27	CLA	14	311	X	-	-	-
27	CLA	31	301	X	-	-	-
27	CLA	31	302	X	-	-	-
27	CLA	31	303	X	-	-	-
27	CLA	31	304	X	-	-	-
27	CLA	31	305	X	-	-	-
27	CLA	31	306	X	-	-	-
27	CLA	31	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	31	309	X	-	-	-
27	CLA	31	315	X	-	-	-
27	CLA	32	303	X	-	-	-
27	CLA	32	305	X	-	-	-
27	CLA	32	306	X	-	-	-
27	CLA	32	307	X	-	-	-
27	CLA	32	308	X	-	-	-
27	CLA	32	309	X	-	-	-
27	CLA	32	310	X	-	-	-
27	CLA	32	311	X	-	-	-
27	CLA	32	313	X	-	-	-
27	CLA	33	301	X	-	-	-
27	CLA	33	303	X	-	-	-
27	CLA	33	304	X	-	-	-
27	CLA	33	305	X	-	-	-
27	CLA	33	306	X	-	-	-
27	CLA	33	307	X	-	-	-
27	CLA	33	308	X	-	-	-
27	CLA	33	309	X	-	-	-
27	CLA	33	311	X	-	-	-
27	CLA	34	302	X	-	-	-
27	CLA	34	304	X	-	-	-
27	CLA	34	305	X	-	-	-
27	CLA	34	306	X	-	-	-
27	CLA	34	307	X	-	-	-
27	CLA	34	308	X	-	-	-
27	CLA	34	309	X	-	-	-
27	CLA	34	310	X	-	-	-
27	CLA	34	312	X	-	-	-
27	CLA	A	402	X	-	-	-
27	CLA	A	404	X	-	-	-
27	CLA	B	601	X	-	-	-
27	CLA	B	602	X	-	-	-
27	CLA	B	603	X	-	-	-
27	CLA	B	604	X	-	-	-
27	CLA	B	605	X	-	-	-
27	CLA	B	606	X	-	-	-
27	CLA	B	607	X	-	-	-
27	CLA	B	608	X	-	-	-
27	CLA	B	609	X	-	-	-
27	CLA	B	610	X	-	-	-
27	CLA	B	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	612	X	-	-	-
27	CLA	B	613	X	-	-	-
27	CLA	B	614	X	-	-	-
27	CLA	B	615	X	-	-	-
27	CLA	B	622	X	-	-	-
27	CLA	C	502	X	-	-	-
27	CLA	C	503	X	-	-	-
27	CLA	C	504	X	-	-	-
27	CLA	C	505	X	-	-	-
27	CLA	C	506	X	-	-	-
27	CLA	C	507	X	-	-	-
27	CLA	C	508	X	-	-	-
27	CLA	C	509	X	-	-	-
27	CLA	C	510	X	-	-	-
27	CLA	C	511	X	-	-	-
27	CLA	C	512	X	-	-	-
27	CLA	C	513	X	-	-	-
27	CLA	C	514	X	-	-	-
27	CLA	D	401	X	-	-	-
27	CLA	D	402	X	-	-	-
27	CLA	D	405	X	-	-	-
27	CLA	D	406	X	-	-	-
27	CLA	M	102	X	-	-	-
27	CLA	W	102	X	-	-	-
27	CLA	a	402	X	-	-	-
27	CLA	a	404	X	-	-	-
27	CLA	b	601	X	-	-	-
27	CLA	b	602	X	-	-	-
27	CLA	b	603	X	-	-	-
27	CLA	b	604	X	-	-	-
27	CLA	b	605	X	-	-	-
27	CLA	b	606	X	-	-	-
27	CLA	b	607	X	-	-	-
27	CLA	b	608	X	-	-	-
27	CLA	b	609	X	-	-	-
27	CLA	b	610	X	-	-	-
27	CLA	b	611	X	-	-	-
27	CLA	b	612	X	-	-	-
27	CLA	b	613	X	-	-	-
27	CLA	b	614	X	-	-	-
27	CLA	b	615	X	-	-	-
27	CLA	b	622	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	c	502	X	-	-	-
27	CLA	c	503	X	-	-	-
27	CLA	c	504	X	-	-	-
27	CLA	c	505	X	-	-	-
27	CLA	c	506	X	-	-	-
27	CLA	c	507	X	-	-	-
27	CLA	c	508	X	-	-	-
27	CLA	c	509	X	-	-	-
27	CLA	c	510	X	-	-	-
27	CLA	c	511	X	-	-	-
27	CLA	c	512	X	-	-	-
27	CLA	c	513	X	-	-	-
27	CLA	c	514	X	-	-	-
27	CLA	d	401	X	-	-	-
27	CLA	d	402	X	-	-	-
27	CLA	d	405	X	-	-	-
27	CLA	d	406	X	-	-	-
27	CLA	m	101	X	-	-	-
27	CLA	w	102	X	-	-	-



## 2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 70136 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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
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
			Total	C	N	O		
10	k	37	302	212	45	45	0	0

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

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

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

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

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

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

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

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

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

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

- 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	31	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

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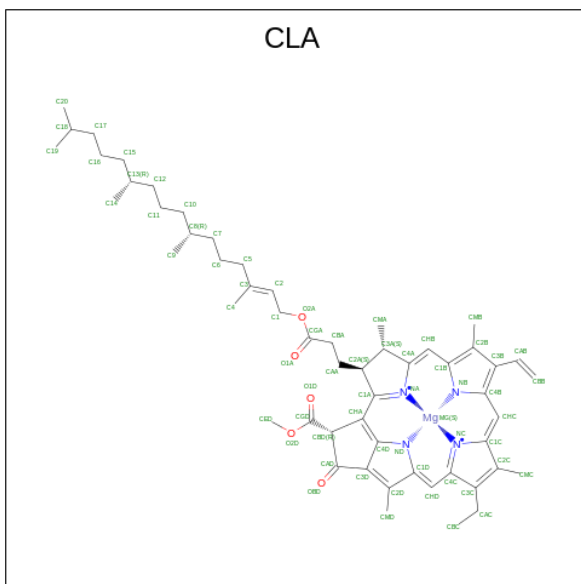
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Mol	Chain	Residues	Atoms					AltConf	Trace
25	32	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	33	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	34	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

- Molecule 26 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 27 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
27	A	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	D	1	Total 260	C 220	Mg 4	N 16	O 20	0
27	D	1	Total 260	C 220	Mg 4	N 16	O 20	0
27	D	1	Total 260	C 220	Mg 4	N 16	O 20	0
27	D	1	Total 260	C 220	Mg 4	N 16	O 20	0
27	M	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	W	1	Total 130	C 110	Mg 2	N 8	O 10	0
27	W	1	Total 130	C 110	Mg 2	N 8	O 10	0
27	a	1	Total 130	C 110	Mg 2	N 8	O 10	0
27	a	1	Total 130	C 110	Mg 2	N 8	O 10	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	c	1	Total 845	C 715	Mg 13	N 52	O 65	0
27	d	1	Total 260	C 220	Mg 4	N 16	O 20	0
27	d	1	Total 260	C 220	Mg 4	N 16	O 20	0
27	d	1	Total 260	C 220	Mg 4	N 16	O 20	0
27	d	1	Total 260	C 220	Mg 4	N 16	O 20	0
27	m	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	w	1	Total 130	C 110	Mg 2	N 8	O 10	0
27	w	1	Total 130	C 110	Mg 2	N 8	O 10	0
27	11	1	Total 530	C 430	Mg 10	N 40	O 50	0
27	11	1	Total 530	C 430	Mg 10	N 40	O 50	0
27	11	1	Total 530	C 430	Mg 10	N 40	O 50	0
27	11	1	Total 530	C 430	Mg 10	N 40	O 50	0
27	11	1	Total 530	C 430	Mg 10	N 40	O 50	0
27	11	1	Total 530	C 430	Mg 10	N 40	O 50	0
27	11	1	Total 530	C 430	Mg 10	N 40	O 50	0
27	11	1	Total 530	C 430	Mg 10	N 40	O 50	0
27	11	1	Total 530	C 430	Mg 10	N 40	O 50	0
27	11	1	Total 530	C 430	Mg 10	N 40	O 50	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	12	1	530	430	10	40	50	0
27	12	1	530	430	10	40	50	0
27	12	1	530	430	10	40	50	0
27	12	1	530	430	10	40	50	0
27	12	1	530	430	10	40	50	0
27	12	1	530	430	10	40	50	0
27	12	1	530	430	10	40	50	0
27	12	1	530	430	10	40	50	0
27	12	1	530	430	10	40	50	0
27	12	1	530	430	10	40	50	0
27	13	1	530	430	10	40	50	0
27	13	1	530	430	10	40	50	0
27	13	1	530	430	10	40	50	0
27	13	1	530	430	10	40	50	0
27	13	1	530	430	10	40	50	0
27	13	1	530	430	10	40	50	0
27	13	1	530	430	10	40	50	0
27	13	1	530	430	10	40	50	0
27	13	1	530	430	10	40	50	0
27	13	1	530	430	10	40	50	0
27	14	1	530	430	10	40	50	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	14	1	530	430	10	40	50	0
27	14	1	530	430	10	40	50	0
27	14	1	530	430	10	40	50	0
27	14	1	530	430	10	40	50	0
27	14	1	530	430	10	40	50	0
27	14	1	530	430	10	40	50	0
27	14	1	530	430	10	40	50	0
27	14	1	530	430	10	40	50	0
27	14	1	530	430	10	40	50	0
27	31	1	530	430	10	40	50	0
27	31	1	530	430	10	40	50	0
27	31	1	530	430	10	40	50	0
27	31	1	530	430	10	40	50	0
27	31	1	530	430	10	40	50	0
27	31	1	530	430	10	40	50	0
27	31	1	530	430	10	40	50	0
27	31	1	530	430	10	40	50	0
27	31	1	530	430	10	40	50	0
27	31	1	530	430	10	40	50	0
27	31	1	530	430	10	40	50	0
27	31	1	530	430	10	40	50	0
27	32	1	530	430	10	40	50	0
27	32	1	530	430	10	40	50	0

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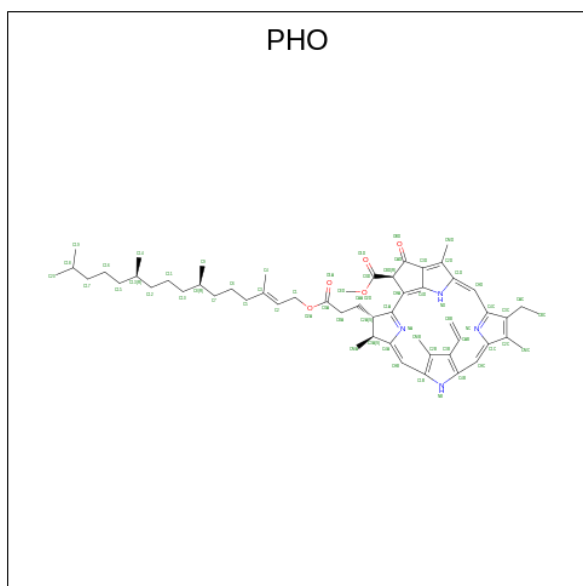
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	32	1	530	430	10	40	50	0
27	32	1	530	430	10	40	50	0
27	32	1	530	430	10	40	50	0
27	32	1	530	430	10	40	50	0
27	32	1	530	430	10	40	50	0
27	32	1	530	430	10	40	50	0
27	32	1	530	430	10	40	50	0
27	32	1	530	430	10	40	50	0
27	33	1	530	430	10	40	50	0
27	33	1	530	430	10	40	50	0
27	33	1	530	430	10	40	50	0
27	33	1	530	430	10	40	50	0
27	33	1	530	430	10	40	50	0
27	33	1	530	430	10	40	50	0
27	33	1	530	430	10	40	50	0
27	33	1	530	430	10	40	50	0
27	33	1	530	430	10	40	50	0
27	33	1	530	430	10	40	50	0
27	34	1	530	430	10	40	50	0
27	34	1	530	430	10	40	50	0
27	34	1	530	430	10	40	50	0

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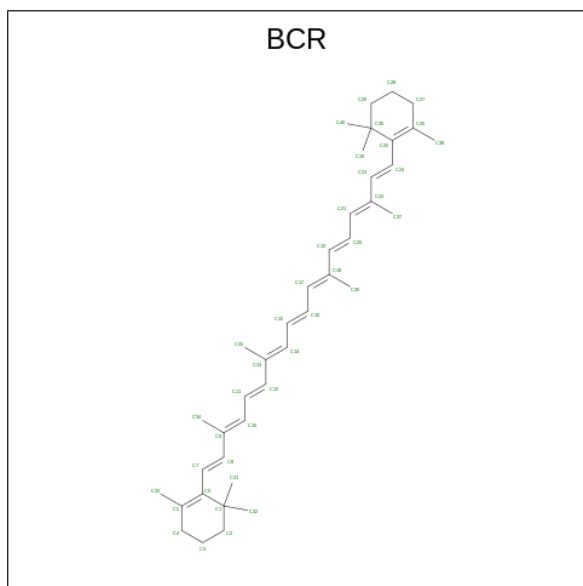
Mol	Chain	Residues	Atoms					AltConf
27	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
27	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
27	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
27	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
27	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	
27	34	1	Total	C	Mg	N	O	0
			530	430	10	40	50	

- Molecule 28 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 29 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



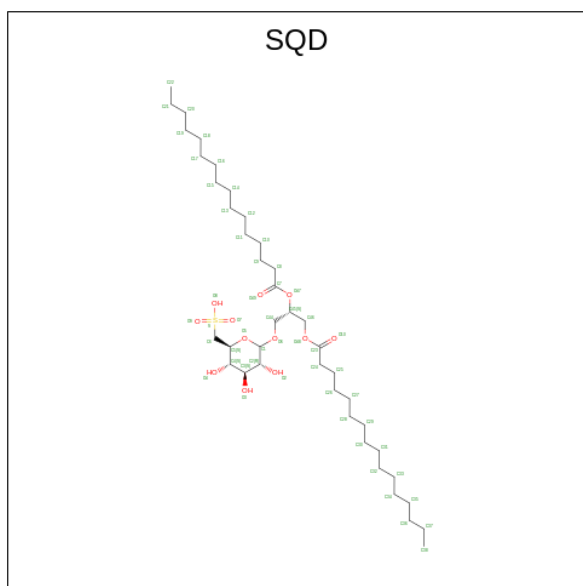
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 80 80	0
29	A	1	Total C 80 80	0
29	B	1	Total C 120 120	0
29	B	1	Total C 120 120	0
29	B	1	Total C 120 120	0
29	C	1	Total C 120 120	0
29	C	1	Total C 120 120	0
29	C	1	Total C 120 120	0
29	F	1	Total C 40 40	0
29	H	1	Total C 40 40	0
29	M	1	Total C 40 40	0
29	Z	1	Total C 40 40	0
29	a	1	Total C 80 80	0

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Mol	Chain	Residues	Atoms	AltConf
29	a	1	Total C 80 80	0
29	b	1	Total C 120 120	0
29	b	1	Total C 120 120	0
29	b	1	Total C 120 120	0
29	c	1	Total C 120 120	0
29	c	1	Total C 120 120	0
29	c	1	Total C 120 120	0
29	f	1	Total C 40 40	0
29	h	1	Total C 40 40	0
29	m	1	Total C 40 40	0
29	z	1	Total C 40 40	0

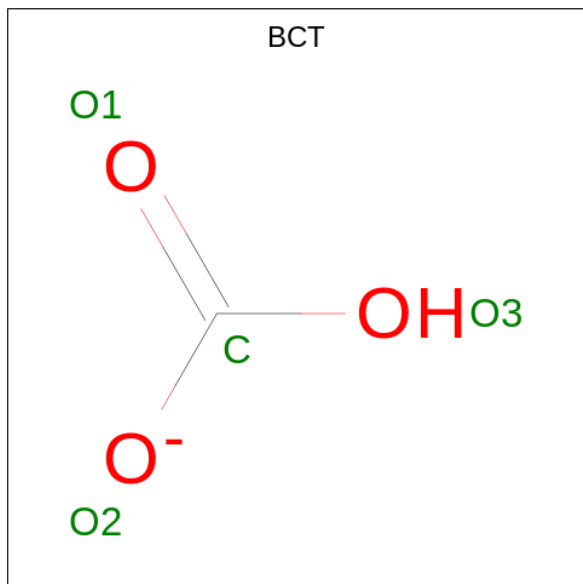
- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).





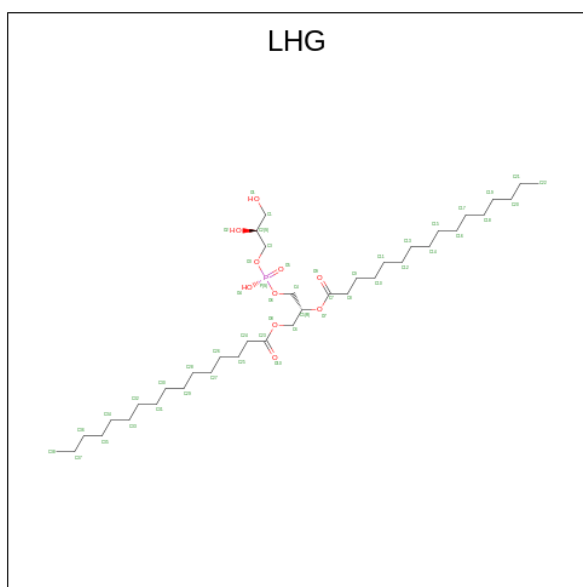
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			54	41	12	1	
30	B	1	Total	C	O	S	0
			37	24	12	1	
30	L	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			54	41	12	1	
30	b	1	Total	C	O	S	0
			37	24	12	1	
30	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



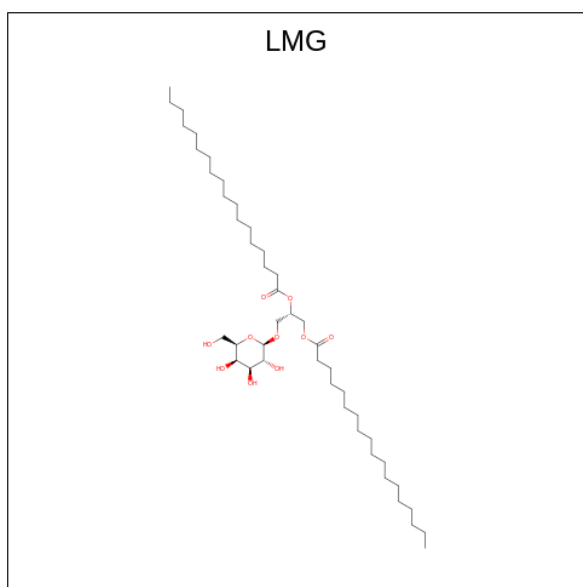
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			4	1	3	
31	a	1	Total	C	O	0
			4	1	3	

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$ ).



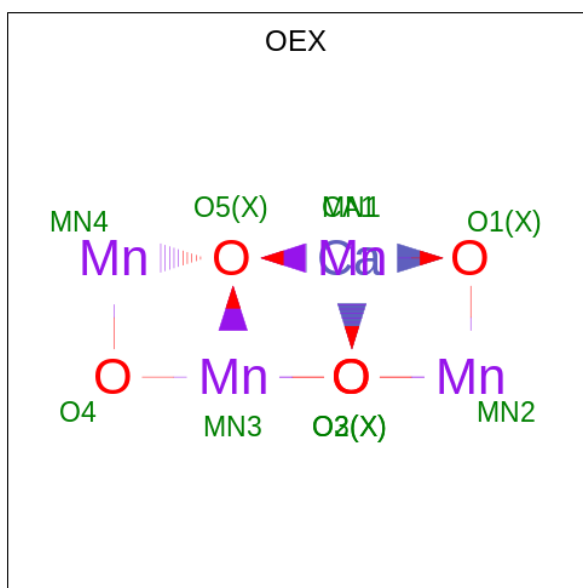
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
32	A	1	46	35	10	1	0
32	B	1	49	38	10	1	0
32	L	1	98	76	20	2	0
32	L	1	98	76	20	2	0
32	a	1	46	35	10	1	0
32	b	1	49	38	10	1	0
32	l	1	98	76	20	2	0
32	l	1	98	76	20	2	0

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



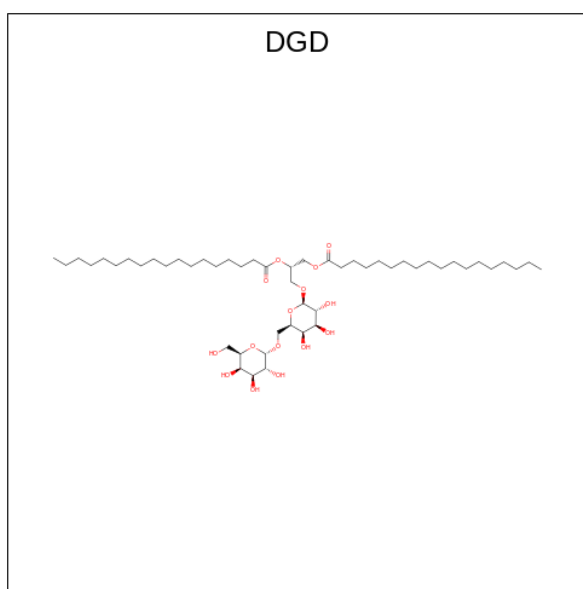
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	B	1	102	82	20	0
33	B	1	102	82	20	0
33	C	1	51	41	10	0
33	D	1	51	41	10	0
33	M	1	40	30	10	0
33	W	1	51	41	10	0
33	b	1	102	82	20	0
33	b	1	102	82	20	0
33	d	1	51	41	10	0
33	m	1	40	30	10	0
33	q	1	51	41	10	0
33	w	1	51	41	10	0
33	12	1	39	29	10	0
33	32	1	39	29	10	0

- Molecule 34 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



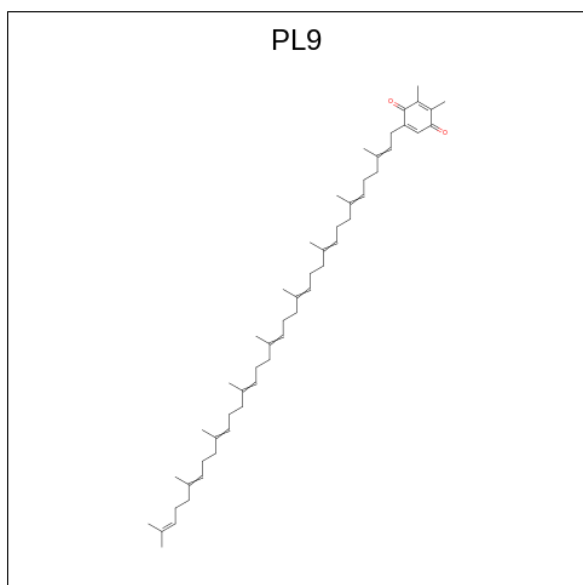
Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
34	C	1	10	1	4	5	0
34	c	1	10	1	4	5	0

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $\text{C}_{51}\text{H}_{96}\text{O}_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
35	C	1	Total	C	O	0
			124	94	30	
35	C	1	Total	C	O	0
			124	94	30	
35	H	1	Total	C	O	0
			62	47	15	
35	J	1	Total	C	O	0
			62	47	15	
35	c	1	Total	C	O	0
			124	94	30	
35	c	1	Total	C	O	0
			124	94	30	
35	h	1	Total	C	O	0
			62	47	15	
35	j	1	Total	C	O	0
			62	47	15	

- Molecule 36 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 (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



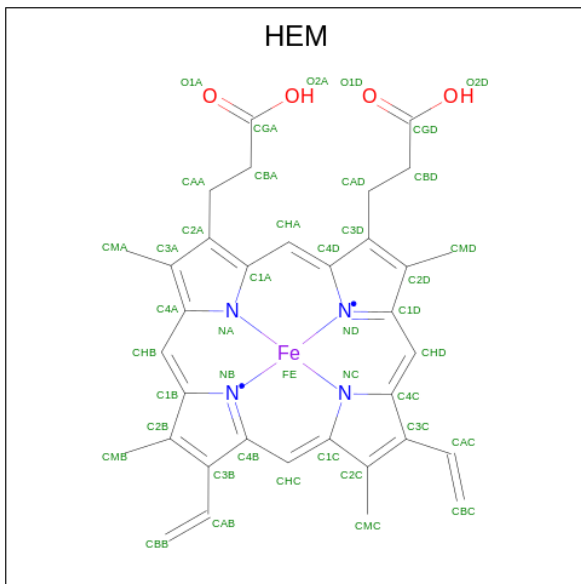
Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total	C	O	0
			110	106	4	
36	D	1	Total	C	O	0
			110	106	4	

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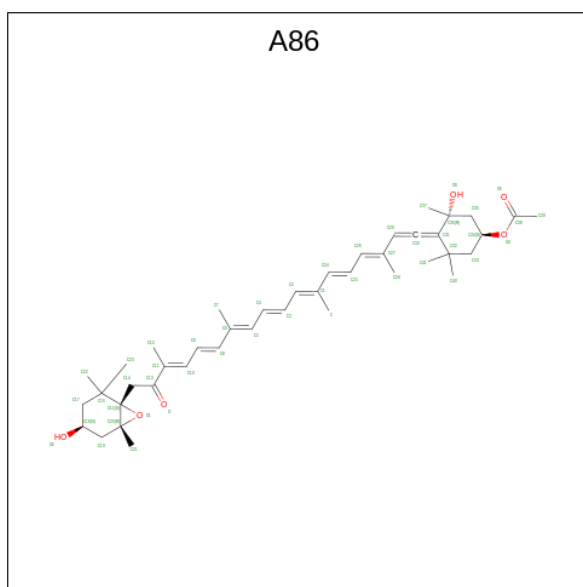
Mol	Chain	Residues	Atoms			AltConf
36	d	1	Total	C	O	0
			110	106	4	
36	d	1	Total	C	O	0
			110	106	4	

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 38 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (three-letter code: A86) (formula:  $C_{42}H_{58}O_6$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
38	11	1	288	252	36	0
38	11	1	288	252	36	0
38	11	1	288	252	36	0
38	11	1	288	252	36	0
38	11	1	288	252	36	0
38	11	1	288	252	36	0
38	11	1	288	252	36	0
38	12	1	240	210	30	0
38	12	1	240	210	30	0
38	12	1	240	210	30	0
38	12	1	240	210	30	0
38	12	1	240	210	30	0
38	12	1	240	210	30	0
38	13	1	336	294	42	0
38	13	1	336	294	42	0
38	13	1	336	294	42	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
38	13	1	336	294	42	0
38	13	1	336	294	42	0
38	13	1	336	294	42	0
38	13	1	336	294	42	0
38	14	1	288	252	36	0
38	14	1	288	252	36	0
38	14	1	288	252	36	0
38	14	1	288	252	36	0
38	14	1	288	252	36	0
38	14	1	288	252	36	0
38	14	1	288	252	36	0
38	31	1	288	252	36	0
38	31	1	288	252	36	0
38	31	1	288	252	36	0
38	31	1	288	252	36	0
38	31	1	288	252	36	0
38	31	1	288	252	36	0
38	32	1	288	252	36	0
38	32	1	288	252	36	0
38	32	1	288	252	36	0
38	32	1	288	252	36	0
38	32	1	288	252	36	0

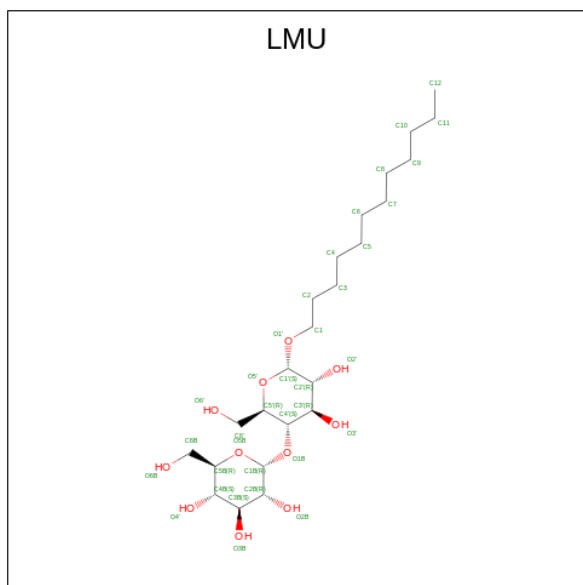
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
38	32	1	288	252	36	0
38	33	1	288	252	36	0
38	33	1	288	252	36	0
38	33	1	288	252	36	0
38	33	1	288	252	36	0
38	33	1	288	252	36	0
38	33	1	288	252	36	0
38	34	1	288	252	36	0
38	34	1	288	252	36	0
38	34	1	288	252	36	0
38	34	1	288	252	36	0
38	34	1	288	252	36	0
38	34	1	288	252	36	0
38	34	1	288	252	36	0

- Molecule 39 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).

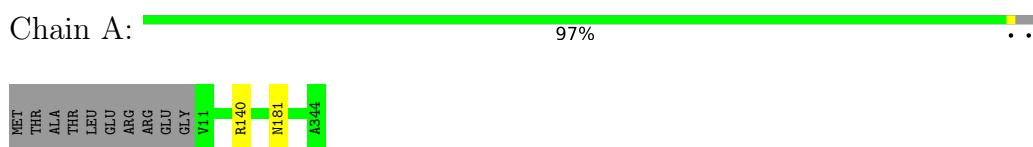


Mol	Chain	Residues	Atoms			AltConf
39	12	1	Total	C	O	0
			32	21	11	
39	32	1	Total	C	O	0
			32	21	11	

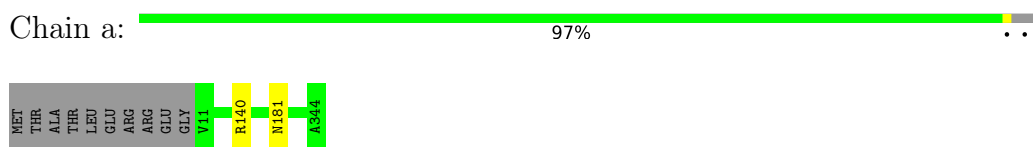
### 3 Residue-property plots [i](#)

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

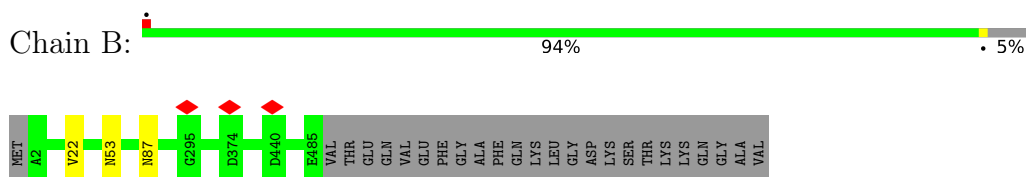
- Molecule 1: Photosystem II reaction center protein D1



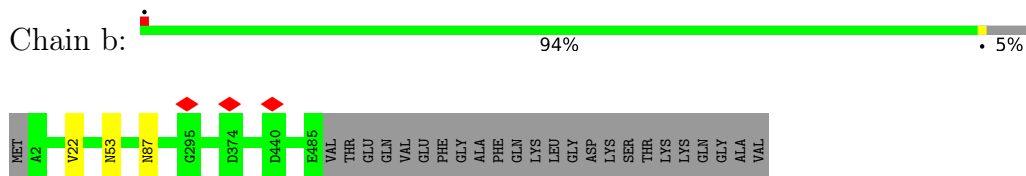
- Molecule 1: Photosystem II reaction center protein D1



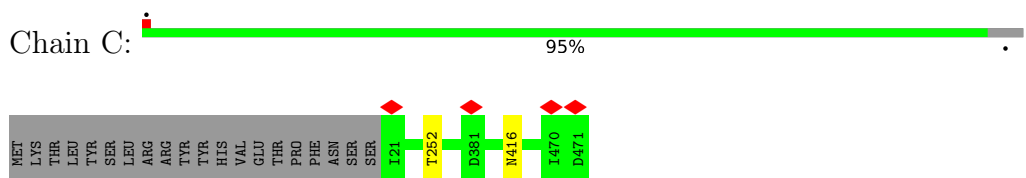
- Molecule 2: Photosystem II chlorophyll protein CP47



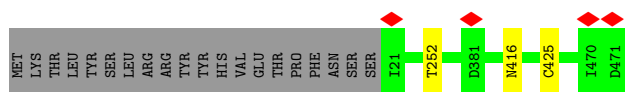
- Molecule 2: Photosystem II chlorophyll protein CP47



- Molecule 3: Photosystem II chlorophyll protein CP43



- Molecule 3: Photosystem II chlorophyll protein CP43



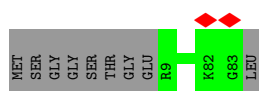
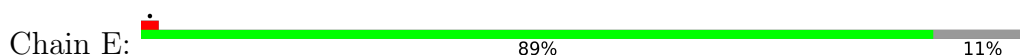
● Molecule 4: Photosystem II reaction center protein D2



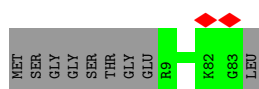
● Molecule 4: Photosystem II reaction center protein D2



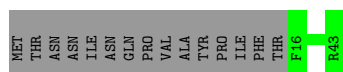
● Molecule 5: Cytochrome b559 subunit alpha



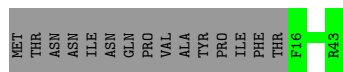
● Molecule 5: Cytochrome b559 subunit alpha



● Molecule 6: Cytochrome b559 subunit beta

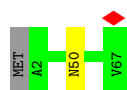


● Molecule 6: Cytochrome b559 subunit beta



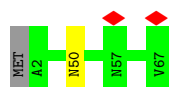
- Molecule 7: Photosystem II reaction center protein H

Chain H:  97%

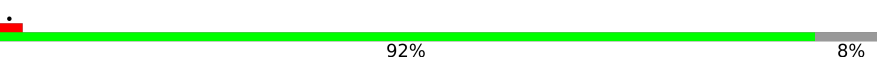


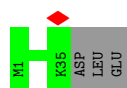
- Molecule 7: Photosystem II reaction center protein H

Chain h:  97%

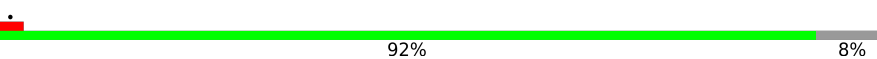


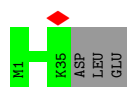
- Molecule 8: Photosystem II reaction center protein I

Chain I:  92%




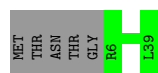
- Molecule 8: Photosystem II reaction center protein I

Chain i:  92%




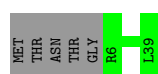
- Molecule 9: Photosystem II reaction center protein J

Chain J:  87%




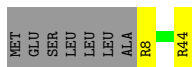
- Molecule 9: Photosystem II reaction center protein J

Chain j:  87%

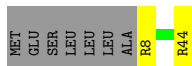
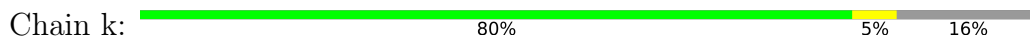


- Molecule 10: Photosystem II reaction center protein K

Chain K:  80%



- Molecule 10: Photosystem II reaction center protein K



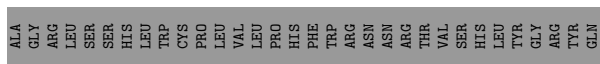
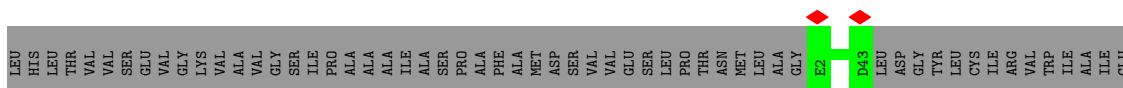
- Molecule 11: Photosystem II reaction center protein L



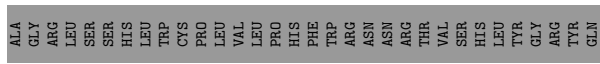
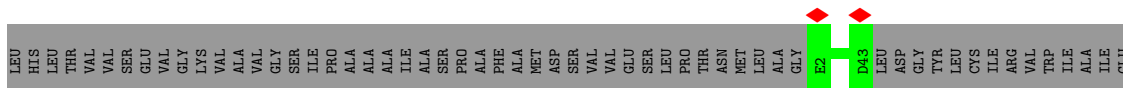
- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

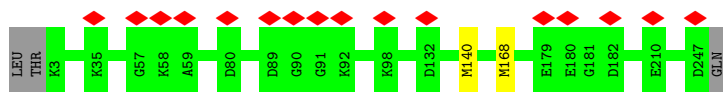


- Molecule 12: Photosystem II reaction center protein M

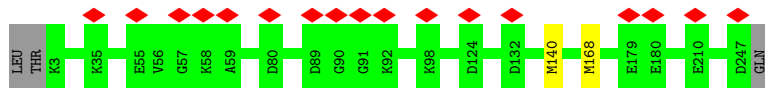


- Molecule 13: Extrinsic protein in photosystem II





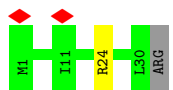
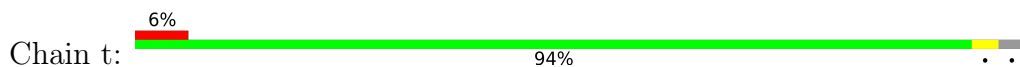
- Molecule 13: Extrinsic protein in photosystem II



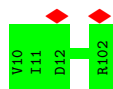
- Molecule 14: Photosystem II reaction center protein T



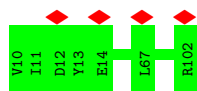
- Molecule 14: Photosystem II reaction center protein T



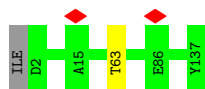
- Molecule 15: Extrinsic protein in photosystem II



- Molecule 15: Extrinsic protein in photosystem II

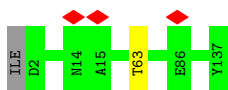


- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550

Chain v:  99%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  100%



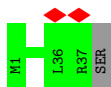
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  100%



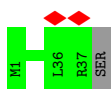
- Molecule 18: Photosystem II reaction center X protein

Chain X:  5% 97%



- Molecule 18: Photosystem II reaction center X protein

Chain x:  5% 97%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  97%



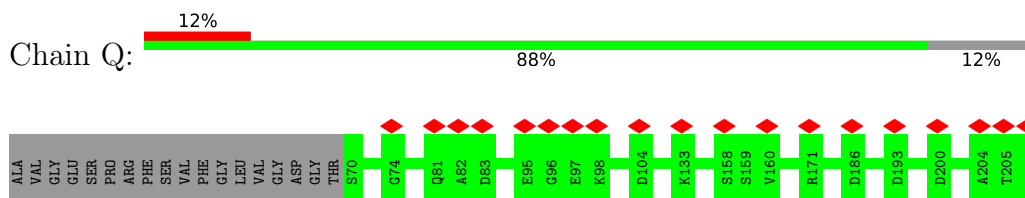
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  97%

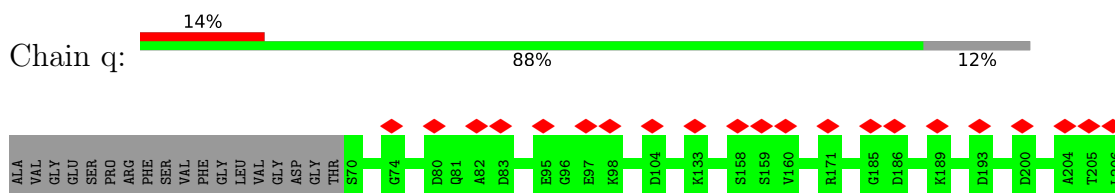




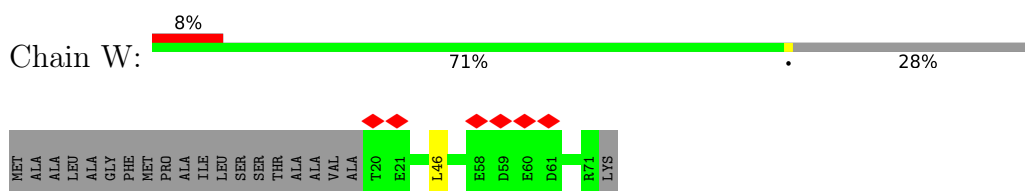
- Molecule 20: Extrinsic protein in photosystem II



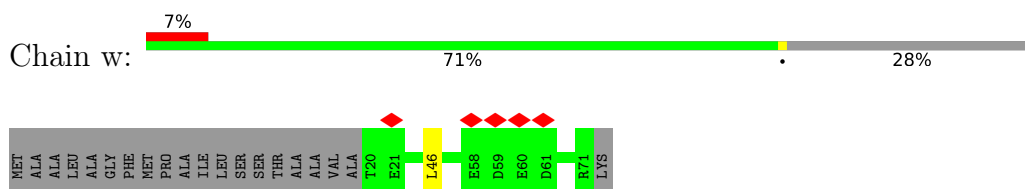
- Molecule 20: Extrinsic protein in photosystem II



- Molecule 21: Photosystem II reaction center protein W



- Molecule 21: Photosystem II reaction center protein W



- Molecule 22: Unknown protein 0



There are no outlier residues recorded for this chain.

- Molecule 22: Unknown protein 0



There are no outlier residues recorded for this chain.

- Molecule 23: Unknown protein 1



There are no outlier residues recorded for this chain.

- Molecule 23: Unknown protein 1



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.

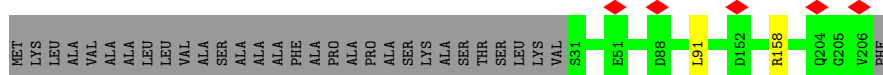
- Molecule 24: Unknown protein 2

Chain 7:  100%


There are no outlier residues recorded for this chain.

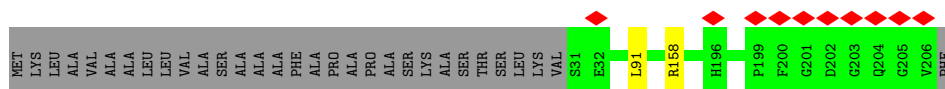
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 11:  84% 15%




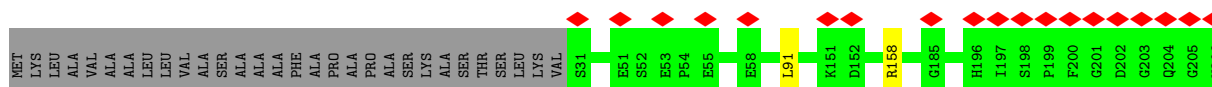
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 12:  5% 84% 15%




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

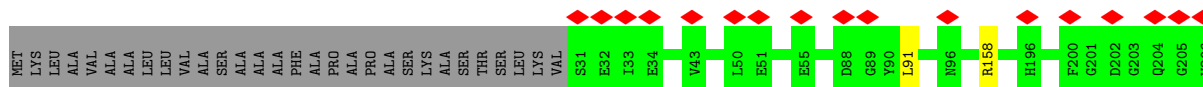
Chain 13:  9% 84% 15%



PHE

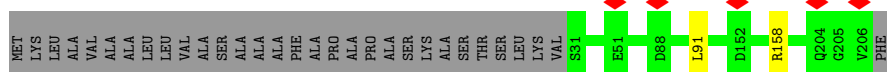
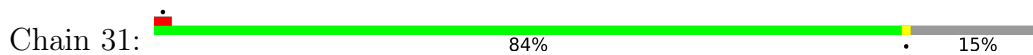
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 14:  8% 84% 15%

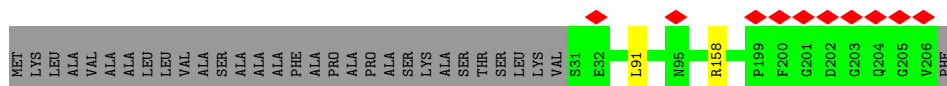
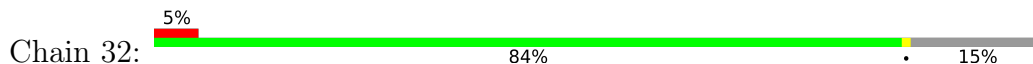


PHE

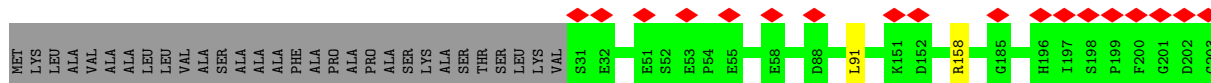
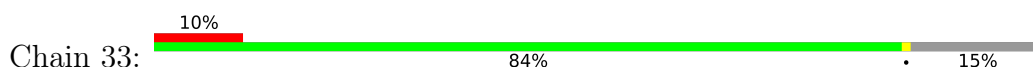
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1



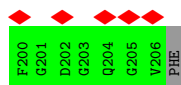
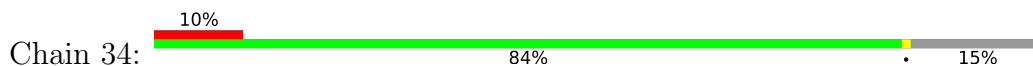
• Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	214939	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
Maximum map value	0.380	Depositor
Minimum map value	-0.155	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.06	Depositor
Map size ( $\text{\AA}$ )	573.44, 573.44, 573.44	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.12, 1.12, 1.12	Depositor

## 5 Model quality [i](#)

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

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

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	0/3620	0.60	1/4933 (0.0%)
3	c	0.58	1/3620 (0.0%)	0.60	1/4933 (0.0%)
4	D	0.58	0/2789	0.60	0/3803
4	d	0.58	0/2789	0.60	0/3803
5	E	0.44	0/634	0.52	0/864
5	e	0.44	0/634	0.53	0/864
6	F	0.45	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	0.62	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	0.56	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	0.41	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	0.53	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	0.41	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	0.42	0/1373	0.55	1/1861 (0.1%)
25	14	0.42	0/1373	0.55	1/1861 (0.1%)
25	31	0.43	0/1373	0.55	1/1861 (0.1%)
25	32	0.43	0/1373	0.55	1/1861 (0.1%)
25	33	0.43	0/1373	0.55	1/1861 (0.1%)
25	34	0.43	0/1373	0.55	1/1861 (0.1%)
All	All	0.51	3/55724 (0.0%)	0.58	12/75702 (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
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	22	VAL	CB-CG1	-7.23	1.37	1.52
2	B	22	VAL	CB-CG1	-7.23	1.37	1.52
3	c	425	CYS	CB-SG	-5.06	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	6.19	137.18	121.70
3	c	252	THR	C-N-CA	6.16	137.11	121.70
21	w	46	LEU	CB-CG-CD1	-5.35	101.90	111.00
21	W	46	LEU	CB-CG-CD1	-5.34	101.93	111.00
25	33	91	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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 [i](#)

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	322 (97%)	10 (3%)	0	100	100
1	a	332/344 (96%)	321 (97%)	11 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	167 (96%)	7 (4%)	0	100	100
25	14	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	31	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	32	174/207 (84%)	167 (96%)	7 (4%)	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
All	All	6884/7712 (89%)	6603 (96%)	281 (4%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/280 (97%)	271 (100%)	1 (0%)	91	95
1	a	272/280 (97%)	271 (100%)	1 (0%)	91	95
2	B	385/405 (95%)	383 (100%)	2 (0%)	88	93
2	b	385/405 (95%)	383 (100%)	2 (0%)	88	93
3	C	356/376 (95%)	355 (100%)	1 (0%)	92	96
3	c	356/376 (95%)	355 (100%)	1 (0%)	92	96
4	D	273/281 (97%)	268 (98%)	5 (2%)	59	78
4	d	273/281 (97%)	268 (98%)	5 (2%)	59	78
5	E	69/75 (92%)	69 (100%)	0	100	100
5	e	69/75 (92%)	69 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	59	78
7	h	55/56 (98%)	54 (98%)	1 (2%)	59	78
8	I	34/37 (92%)	34 (100%)	0	100	100
8	i	34/37 (92%)	34 (100%)	0	100	100
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%)	18	47
10	k	32/38 (84%)	30 (94%)	2 (6%)	18	47
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%)	76	86
13	o	196/201 (98%)	194 (99%)	2 (1%)	76	86
14	T	27/28 (96%)	26 (96%)	1 (4%)	34	63
14	t	27/28 (96%)	26 (96%)	1 (4%)	34	63
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	w	43/55 (78%)	43 (100%)	0	100	100
25	11	138/158 (87%)	137 (99%)	1 (1%)	84	90
25	12	138/158 (87%)	137 (99%)	1 (1%)	84	90
25	13	138/158 (87%)	137 (99%)	1 (1%)	84	90
25	14	138/158 (87%)	137 (99%)	1 (1%)	84	90
25	31	138/158 (87%)	137 (99%)	1 (1%)	84	90
25	32	138/158 (87%)	137 (99%)	1 (1%)	84	90
25	33	138/158 (87%)	137 (99%)	1 (1%)	84	90
25	34	138/158 (87%)	137 (99%)	1 (1%)	84	90
All	All	5628/6184 (91%)	5590 (99%)	38 (1%)	84	90

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	o	168	MET
25	32	158	ARG
14	t	24	ARG
25	13	158	ARG
25	34	158	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	229	ASN
25	33	161	ASN
16	v	25	GLN
25	33	82	ASN
25	31	82	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 286 ligands modelled in this entry, 2 are monoatomic - leaving 284 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
27	CLA	13	308	25	45,53,73	1.76	8 (17%)	52,89,113	1.82	8 (15%)
27	CLA	33	304	-	45,53,73	1.66	11 (24%)	52,89,113	1.79	9 (17%)
27	CLA	12	309	-	45,53,73	1.71	7 (15%)	52,89,113	1.70	7 (13%)
27	CLA	34	309	25	45,53,73	1.76	8 (17%)	52,89,113	1.81	9 (17%)
38	A86	12	314	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
27	CLA	A	404	-	65,73,73	1.47	10 (15%)	76,113,113	1.52	10 (13%)
27	CLA	D	405	-	65,73,73	1.48	10 (15%)	76,113,113	1.61	10 (13%)
38	A86	32	314	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
27	CLA	d	406	-	65,73,73	1.41	11 (16%)	76,113,113	1.60	7 (9%)
27	CLA	11	306	25	45,53,73	1.76	8 (17%)	52,89,113	1.82	8 (15%)
27	CLA	B	614	-	65,73,73	1.38	10 (15%)	76,113,113	1.58	10 (13%)
27	CLA	33	307	-	45,53,73	1.71	7 (15%)	52,89,113	1.69	7 (13%)
29	BCR	m	103	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	8 (14%)
27	CLA	32	306	39	45,53,73	1.69	11 (24%)	52,89,113	1.79	9 (17%)
27	CLA	34	302	-	65,73,73	1.46	9 (13%)	76,113,113	1.47	8 (10%)
32	LHG	l	103	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
33	LMG	D	408	-	51,51,55	0.90	3 (5%)	59,59,63	1.42	7 (11%)
38	A86	14	314	-	44,50,50	4.04	22 (50%)	51,76,76	7.81	19 (37%)
27	CLA	31	305	-	45,53,73	1.71	8 (17%)	52,89,113	1.69	7 (13%)
27	CLA	d	405	-	65,73,73	1.48	10 (15%)	76,113,113	1.61	11 (14%)
27	CLA	13	307	-	45,53,73	1.71	8 (17%)	52,89,113	1.70	7 (13%)
33	LMG	d	408	-	51,51,55	0.90	3 (5%)	59,59,63	1.43	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	DGD	J	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
27	CLA	12	307	-	65,73,73	1.42	10 (15%)	76,113,113	1.59	10 (13%)
36	PL9	d	404	4	55,55,55	1.36	6 (10%)	68,69,69	1.49	14 (20%)
37	HEM	E	101	6,5	41,50,50	1.50	4 (9%)	45,82,82	1.25	5 (11%)
38	A86	14	315	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
38	A86	12	304	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
27	CLA	b	611	-	65,73,73	1.52	12 (18%)	76,113,113	1.58	11 (14%)
27	CLA	31	308	25	45,53,73	1.75	11 (24%)	52,89,113	1.75	9 (17%)
29	BCR	A	409	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
29	BCR	b	616	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	9 (16%)
27	CLA	C	510	-	65,73,73	1.48	12 (18%)	76,113,113	1.73	10 (13%)
38	A86	31	316	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
27	CLA	11	307	25	65,73,73	1.46	10 (15%)	76,113,113	1.54	10 (13%)
27	CLA	32	311	25	65,73,73	1.47	10 (15%)	76,113,113	1.55	10 (13%)
27	CLA	B	613	-	65,73,73	1.43	11 (16%)	76,113,113	1.61	10 (13%)
27	CLA	B	608	-	65,73,73	1.50	10 (15%)	76,113,113	1.47	8 (10%)
27	CLA	13	310	25	45,53,73	1.75	11 (24%)	52,89,113	1.76	9 (17%)
27	CLA	B	604	-	65,73,73	1.45	12 (18%)	76,113,113	1.69	16 (21%)
38	A86	11	316	-	44,50,50	4.00	23 (52%)	51,76,76	7.59	20 (39%)
27	CLA	b	610	-	65,73,73	1.51	11 (16%)	76,113,113	1.51	8 (10%)
29	BCR	c	516	-	41,41,41	1.31	4 (9%)	56,56,56	1.40	9 (16%)
38	A86	31	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
27	CLA	33	301	-	65,73,73	1.47	9 (13%)	76,113,113	1.48	8 (10%)
27	CLA	14	305	-	65,73,73	1.41	10 (15%)	76,113,113	1.59	10 (13%)
27	CLA	31	309	-	45,53,73	1.75	8 (17%)	52,89,113	1.66	7 (13%)
27	CLA	33	308	25	45,53,73	1.78	7 (15%)	52,89,113	1.83	8 (15%)
27	CLA	C	513	-	65,73,73	1.44	9 (13%)	76,113,113	1.48	8 (10%)
27	CLA	11	305	-	45,53,73	1.71	8 (17%)	52,89,113	1.70	7 (13%)
29	BCR	C	516	-	41,41,41	1.31	5 (12%)	56,56,56	1.41	10 (17%)
27	CLA	32	310	25	45,53,73	1.76	7 (15%)	52,89,113	1.81	9 (17%)
29	BCR	h	101	-	41,41,41	1.28	4 (9%)	56,56,56	1.31	7 (12%)
27	CLA	c	502	-	65,73,73	1.39	11 (16%)	76,113,113	1.66	11 (14%)
27	CLA	c	513	-	65,73,73	1.45	9 (13%)	76,113,113	1.48	8 (10%)
27	CLA	32	303	-	65,73,73	1.47	9 (13%)	76,113,113	1.48	8 (10%)
38	A86	11	314	-	44,50,50	3.94	23 (52%)	51,76,76	7.97	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	A86	13	317	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
38	A86	13	315	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
29	BCR	c	519	-	41,41,41	1.27	2 (4%)	56,56,56	1.37	6 (10%)
33	LMG	M	103	27	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
33	LMG	b	619	-	51,51,55	0.98	5 (9%)	59,59,63	1.44	8 (13%)
35	DGD	c	517	-	63,63,67	1.05	8 (12%)	77,77,81	1.60	15 (19%)
27	CLA	33	311	-	45,53,73	1.74	8 (17%)	52,89,113	1.66	8 (15%)
27	CLA	31	301	25	65,73,73	1.45	9 (13%)	76,113,113	1.67	8 (10%)
35	DGD	j	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
27	CLA	C	503	-	65,73,73	1.52	12 (18%)	76,113,113	1.52	12 (15%)
27	CLA	34	311	25	45,53,73	1.74	11 (24%)	52,89,113	1.74	9 (17%)
37	HEM	V	201	16	41,50,50	1.61	5 (12%)	45,82,82	1.27	2 (4%)
27	CLA	M	102	33,12	65,73,73	1.42	10 (15%)	76,113,113	1.41	6 (7%)
27	CLA	C	509	-	65,73,73	1.48	11 (16%)	76,113,113	1.65	9 (11%)
27	CLA	14	311	-	45,53,73	1.74	9 (20%)	52,89,113	1.66	8 (15%)
27	CLA	m	101	33,12	65,73,73	1.42	10 (15%)	76,113,113	1.40	6 (7%)
38	A86	14	313	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
27	CLA	C	514	-	65,73,73	1.39	8 (12%)	76,113,113	1.63	8 (10%)
27	CLA	B	609	-	65,73,73	1.47	10 (15%)	76,113,113	1.51	9 (11%)
31	BCT	A	407	1,26	2,3,3	1.26	0	2,3,3	3.93	2 (100%)
27	CLA	12	308	33,25	45,53,73	1.71	8 (17%)	52,89,113	2.03	11 (21%)
27	CLA	34	308	-	45,53,73	1.70	7 (15%)	52,89,113	1.69	7 (13%)
27	CLA	13	301	-	65,73,73	1.47	9 (13%)	76,113,113	1.48	8 (10%)
29	BCR	B	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.42	10 (17%)
29	BCR	b	623	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
35	DGD	c	518	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	15 (19%)
27	CLA	33	309	25	65,73,73	1.50	11 (16%)	76,113,113	1.55	10 (13%)
38	A86	33	313	-	44,50,50	3.96	23 (52%)	51,76,76	7.93	18 (35%)
27	CLA	C	502	-	65,73,73	1.39	11 (16%)	76,113,113	1.66	12 (15%)
38	A86	33	314	-	44,50,50	4.04	22 (50%)	51,76,76	7.81	20 (39%)
32	LHG	B	621	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	6 (11%)
29	BCR	b	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.41	10 (17%)
38	A86	11	312	-	44,50,50	4.04	22 (50%)	51,76,76	7.82	19 (37%)
38	A86	12	315	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
27	CLA	B	602	-	65,73,73	1.47	10 (15%)	76,113,113	1.55	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	b	614	-	65,73,73	1.39	10 (15%)	76,113,113	1.59	10 (13%)
27	CLA	c	504	-	65,73,73	1.47	11 (16%)	76,113,113	1.52	10 (13%)
27	CLA	13	306	25	45,53,73	1.71	8 (17%)	52,89,113	2.02	11 (21%)
29	BCR	z	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.46	9 (16%)
27	CLA	b	606	-	65,73,73	1.58	12 (18%)	76,113,113	1.60	13 (17%)
29	BCR	C	520	-	41,41,41	1.28	2 (4%)	56,56,56	1.37	6 (10%)
32	LHG	a	408	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	7 (14%)
27	CLA	c	506	-	65,73,73	1.46	11 (16%)	76,113,113	1.56	11 (14%)
27	CLA	12	306	39	45,53,73	1.69	11 (24%)	52,89,113	1.79	9 (17%)
27	CLA	14	308	25	45,53,73	1.76	8 (17%)	52,89,113	1.81	8 (15%)
32	LHG	b	621	-	48,48,48	0.75	1 (2%)	51,54,54	1.29	6 (11%)
33	LMG	w	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.40	7 (11%)
27	CLA	32	313	-	45,53,73	1.74	8 (17%)	52,89,113	1.65	8 (15%)
27	CLA	34	306	-	65,73,73	1.41	9 (13%)	76,113,113	1.59	10 (13%)
32	LHG	L	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
34	OEX	C	501	1,3	0,15,15	-	-	-	-	-
27	CLA	c	514	-	65,73,73	1.38	8 (12%)	76,113,113	1.63	8 (10%)
27	CLA	w	102	-	65,73,73	1.44	9 (13%)	76,113,113	1.47	10 (13%)
35	DGD	C	518	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	15 (19%)
37	HEM	f	102	6,5	41,50,50	1.50	4 (9%)	45,82,82	1.25	5 (11%)
27	CLA	13	303	25	65,73,73	1.45	8 (12%)	76,113,113	1.68	8 (10%)
27	CLA	32	309	-	45,53,73	1.70	7 (15%)	52,89,113	1.69	7 (13%)
33	LMG	q	301	-	51,51,55	0.96	5 (9%)	59,59,63	1.46	9 (15%)
27	CLA	12	310	25	45,53,73	1.77	7 (15%)	52,89,113	1.81	8 (15%)
37	HEM	v	201	16	41,50,50	1.61	5 (12%)	45,82,82	1.26	2 (4%)
38	A86	11	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
27	CLA	b	613	-	65,73,73	1.43	11 (16%)	76,113,113	1.63	9 (11%)
27	CLA	C	505	-	65,73,73	1.43	12 (18%)	76,113,113	1.67	11 (14%)
38	A86	33	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.97	17 (33%)
27	CLA	11	302	-	45,53,73	1.69	11 (24%)	52,89,113	1.78	9 (17%)
27	CLA	31	303	-	65,73,73	1.42	10 (15%)	76,113,113	1.58	10 (13%)
27	CLA	34	304	25	65,73,73	1.45	9 (13%)	76,113,113	1.67	8 (10%)
27	CLA	b	602	-	65,73,73	1.47	10 (15%)	76,113,113	1.54	12 (15%)
29	BCR	c	515	-	41,41,41	1.33	3 (7%)	56,56,56	1.41	8 (14%)
39	LMU	32	302	27,25	33,33,36	1.29	3 (9%)	44,44,47	1.57	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	BCR	M	101	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	8 (14%)
27	CLA	11	309	-	45,53,73	1.74	8 (17%)	52,89,113	1.66	7 (13%)
36	PL9	D	404	4	55,55,55	1.35	6 (10%)	68,69,69	1.49	14 (20%)
27	CLA	34	305	-	45,53,73	1.69	10 (22%)	52,89,113	1.79	9 (17%)
27	CLA	B	601	-	65,73,73	1.44	11 (16%)	76,113,113	1.50	8 (10%)
27	CLA	34	307	25	45,53,73	1.71	8 (17%)	52,89,113	2.04	11 (21%)
27	CLA	B	605	-	65,73,73	1.49	10 (15%)	76,113,113	1.50	9 (11%)
33	LMG	C	519	-	51,51,55	0.96	5 (9%)	59,59,63	1.46	9 (15%)
38	A86	13	313	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
38	A86	12	317	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
29	BCR	a	409	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	5 (8%)
38	A86	32	315	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
28	PHO	a	403	-	51,69,69	1.23	9 (17%)	47,99,99	1.31	8 (17%)
30	SQD	b	620	-	36,37,54	1.20	7 (19%)	45,48,65	1.64	9 (20%)
27	CLA	a	402	-	65,73,73	1.45	8 (12%)	76,113,113	1.61	8 (10%)
30	SQD	a	406	-	53,54,54	0.96	6 (11%)	62,65,65	1.58	11 (17%)
38	A86	14	301	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	19 (37%)
33	LMG	m	102	27	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
38	A86	31	313	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
27	CLA	b	605	-	65,73,73	1.49	10 (15%)	76,113,113	1.50	9 (11%)
38	A86	33	312	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
38	A86	34	313	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
35	DGD	H	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.42	8 (10%)
29	BCR	a	405	-	41,41,41	1.29	2 (4%)	56,56,56	1.39	6 (10%)
27	CLA	d	401	-	65,73,73	1.49	12 (18%)	76,113,113	1.52	9 (11%)
29	BCR	H	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.31	6 (10%)
29	BCR	C	515	-	41,41,41	1.32	3 (7%)	56,56,56	1.41	8 (14%)
27	CLA	32	307	-	65,73,73	1.42	10 (15%)	76,113,113	1.59	10 (13%)
29	BCR	Z	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.46	10 (17%)
27	CLA	11	315	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	8 (10%)
38	A86	11	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
27	CLA	b	604	-	65,73,73	1.45	12 (18%)	76,113,113	1.69	16 (21%)
27	CLA	C	504	-	65,73,73	1.47	11 (16%)	76,113,113	1.52	11 (14%)
38	A86	32	316	-	44,50,50	4.04	22 (50%)	51,76,76	7.81	19 (37%)
27	CLA	B	615	-	65,73,73	1.53	12 (18%)	76,113,113	1.44	11 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	A86	32	318	-	44,50,50	3.94	23 (52%)	51,76,76	7.97	19 (37%)
27	CLA	D	402	-	65,73,73	1.44	11 (16%)	76,113,113	1.50	8 (10%)
35	DGD	C	517	-	63,63,67	1.05	7 (11%)	77,77,81	1.60	15 (19%)
27	CLA	12	303	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	8 (10%)
28	PHO	D	403	-	51,69,69	1.13	8 (15%)	47,99,99	1.28	6 (12%)
30	SQD	L	103	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
38	A86	14	316	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	18 (35%)
38	A86	32	317	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
27	CLA	c	512	3	65,73,73	1.51	10 (15%)	76,113,113	1.59	12 (15%)
27	CLA	31	307	25	65,73,73	1.47	10 (15%)	76,113,113	1.54	10 (13%)
27	CLA	d	402	-	65,73,73	1.45	11 (16%)	76,113,113	1.50	8 (10%)
27	CLA	b	609	-	65,73,73	1.46	10 (15%)	76,113,113	1.51	9 (11%)
33	LMG	W	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.40	7 (11%)
38	A86	33	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	20 (39%)
27	CLA	c	508	-	65,73,73	1.43	12 (18%)	76,113,113	1.67	12 (15%)
28	PHO	d	403	-	51,69,69	1.13	8 (15%)	47,99,99	1.28	6 (12%)
27	CLA	31	304	25	45,53,73	1.72	8 (17%)	52,89,113	2.04	11 (21%)
27	CLA	D	406	-	65,73,73	1.41	11 (16%)	76,113,113	1.59	7 (9%)
33	LMG	b	618	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	9 (15%)
27	CLA	11	308	25	45,53,73	1.75	11 (24%)	52,89,113	1.75	9 (17%)
32	LHG	A	408	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	6 (12%)
33	LMG	B	618	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	8 (13%)
27	CLA	33	310	25	45,53,73	1.75	11 (24%)	52,89,113	1.75	9 (17%)
32	LHG	L	101	-	48,48,48	0.81	1 (2%)	51,54,54	1.27	5 (9%)
27	CLA	c	505	-	65,73,73	1.44	12 (18%)	76,113,113	1.68	11 (14%)
27	CLA	Z	102	-	65,73,73	1.46	10 (15%)	76,113,113	1.48	7 (9%)
27	CLA	14	306	25	45,53,73	1.70	8 (17%)	52,89,113	2.04	11 (21%)
27	CLA	32	312	25	45,53,73	1.76	11 (24%)	52,89,113	1.75	9 (17%)
38	A86	34	303	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
38	A86	34	315	-	44,50,50	4.03	23 (52%)	51,76,76	7.81	19 (37%)
27	CLA	c	509	-	65,73,73	1.48	11 (16%)	76,113,113	1.65	9 (11%)
29	BCR	B	616	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	9 (16%)
30	SQD	B	620	-	36,37,54	1.20	6 (16%)	45,48,65	1.64	9 (20%)
38	A86	13	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	18 (35%)
27	CLA	33	305	-	65,73,73	1.42	10 (15%)	76,113,113	1.58	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	A	402	-	65,73,73	1.44	8 (12%)	76,113,113	1.61	9 (11%)
39	LMU	12	302	27,25	33,33,36	1.30	3 (9%)	44,44,47	1.54	7 (15%)
27	CLA	C	511	-	65,73,73	1.46	12 (18%)	76,113,113	1.59	11 (14%)
33	LMG	12	301	27	39,39,55	1.01	4 (10%)	47,47,63	1.21	5 (10%)
27	CLA	34	312	-	45,53,73	1.73	8 (17%)	52,89,113	1.66	8 (15%)
27	CLA	14	303	25	65,73,73	1.45	9 (13%)	76,113,113	1.67	8 (10%)
28	PHO	A	403	-	51,69,69	1.24	9 (17%)	47,99,99	1.31	8 (17%)
27	CLA	13	305	-	65,73,73	1.41	10 (15%)	76,113,113	1.58	10 (13%)
27	CLA	14	304	-	45,53,73	1.69	10 (22%)	52,89,113	1.80	9 (17%)
27	CLA	B	610	-	65,73,73	1.50	11 (16%)	76,113,113	1.51	8 (10%)
29	BCR	A	405	-	41,41,41	1.29	2 (4%)	56,56,56	1.39	6 (10%)
27	CLA	B	622	-	65,73,73	1.47	10 (15%)	76,113,113	1.59	14 (18%)
27	CLA	c	511	-	65,73,73	1.45	12 (18%)	76,113,113	1.58	11 (14%)
38	A86	11	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
38	A86	33	315	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
38	A86	13	314	-	44,50,50	4.05	23 (52%)	51,76,76	7.81	19 (37%)
32	LHG	l	102	-	48,48,48	0.81	1 (2%)	51,54,54	1.27	5 (9%)
38	A86	34	301	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	18 (35%)
27	CLA	C	506	-	65,73,73	1.46	11 (16%)	76,113,113	1.56	12 (15%)
33	LMG	B	619	-	51,51,55	0.98	5 (9%)	59,59,63	1.44	8 (13%)
38	A86	13	312	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
38	A86	34	314	-	44,50,50	3.96	23 (52%)	51,76,76	7.95	18 (35%)
27	CLA	W	103	-	65,73,73	1.49	6 (9%)	76,113,113	1.41	7 (9%)
27	CLA	z	102	-	65,73,73	1.46	10 (15%)	76,113,113	1.48	7 (9%)
27	CLA	b	601	-	65,73,73	1.45	11 (16%)	76,113,113	1.49	7 (9%)
27	CLA	B	606	-	65,73,73	1.58	12 (18%)	76,113,113	1.61	13 (17%)
31	BCT	a	407	1,26	2,3,3	1.27	0	2,3,3	3.95	2 (100%)
38	A86	31	312	-	44,50,50	4.03	22 (50%)	51,76,76	7.81	20 (39%)
27	CLA	14	302	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	8 (10%)
27	CLA	31	302	-	45,53,73	1.69	11 (24%)	52,89,113	1.79	9 (17%)
27	CLA	34	310	25	65,73,73	1.47	10 (15%)	76,113,113	1.54	10 (13%)
27	CLA	C	512	3	65,73,73	1.50	10 (15%)	76,113,113	1.60	13 (17%)
27	CLA	a	404	-	65,73,73	1.48	10 (15%)	76,113,113	1.52	10 (13%)
38	A86	13	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
27	CLA	w	103	-	65,73,73	1.49	6 (9%)	76,113,113	1.41	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	14	309	25	65,73,73	1.46	10 (15%)	76,113,113	1.54	10 (13%)
27	CLA	b	615	-	65,73,73	1.52	12 (18%)	76,113,113	1.44	11 (14%)
27	CLA	13	311	-	45,53,73	1.75	9 (20%)	52,89,113	1.66	7 (13%)
27	CLA	14	310	25	45,53,73	1.75	11 (24%)	52,89,113	1.75	9 (17%)
27	CLA	b	612	-	65,73,73	1.50	9 (13%)	76,113,113	1.78	10 (13%)
27	CLA	13	304	-	45,53,73	1.69	11 (24%)	52,89,113	1.80	9 (17%)
38	A86	14	312	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
27	CLA	b	603	-	65,73,73	1.43	11 (16%)	76,113,113	1.64	12 (15%)
27	CLA	b	608	-	65,73,73	1.50	10 (15%)	76,113,113	1.47	8 (10%)
27	CLA	33	306	25	45,53,73	1.72	8 (17%)	52,89,113	2.04	11 (21%)
29	BCR	f	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	9 (16%)
27	CLA	c	507	-	65,73,73	1.52	11 (16%)	76,113,113	1.55	10 (13%)
27	CLA	12	311	25	65,73,73	1.46	10 (15%)	76,113,113	1.54	10 (13%)
27	CLA	B	607	-	65,73,73	1.41	11 (16%)	76,113,113	1.55	7 (9%)
27	CLA	B	612	-	65,73,73	1.49	9 (13%)	76,113,113	1.78	10 (13%)
27	CLA	c	503	-	65,73,73	1.52	12 (18%)	76,113,113	1.52	12 (15%)
29	BCR	B	623	-	41,41,41	1.13	3 (7%)	56,56,56	1.31	7 (12%)
27	CLA	11	301	25	65,73,73	1.45	9 (13%)	76,113,113	1.68	8 (10%)
27	CLA	W	102	-	65,73,73	1.45	9 (13%)	76,113,113	1.47	10 (13%)
27	CLA	11	304	25	45,53,73	1.71	8 (17%)	52,89,113	2.03	11 (21%)
27	CLA	14	307	-	45,53,73	1.70	8 (17%)	52,89,113	1.70	7 (13%)
29	BCR	F	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
27	CLA	33	303	25	65,73,73	1.46	9 (13%)	76,113,113	1.68	8 (10%)
27	CLA	C	507	-	65,73,73	1.52	11 (16%)	76,113,113	1.54	10 (13%)
30	SQD	A	406	-	53,54,54	0.97	6 (11%)	62,65,65	1.58	11 (17%)
38	A86	32	304	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	21 (41%)
35	DGD	h	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.42	8 (10%)
38	A86	31	314	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	19 (37%)
27	CLA	D	401	-	65,73,73	1.50	12 (18%)	76,113,113	1.52	9 (11%)
27	CLA	31	306	25	45,53,73	1.77	8 (17%)	52,89,113	1.81	8 (15%)
27	CLA	c	510	-	65,73,73	1.49	12 (18%)	76,113,113	1.74	10 (13%)
36	PL9	d	407	-	55,55,55	2.32	14 (25%)	68,69,69	1.48	14 (20%)
27	CLA	B	603	-	65,73,73	1.42	11 (16%)	76,113,113	1.63	12 (15%)
33	LMG	32	301	27	39,39,55	1.00	4 (10%)	47,47,63	1.18	4 (8%)
27	CLA	12	313	-	45,53,73	1.74	8 (17%)	52,89,113	1.65	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	B	611	-	65,73,73	1.51	12 (18%)	76,113,113	1.58	11 (14%)
30	SQD	l	101	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
27	CLA	b	607	-	65,73,73	1.41	11 (16%)	76,113,113	1.55	7 (9%)
27	CLA	31	315	-	65,73,73	1.46	9 (13%)	76,113,113	1.47	8 (10%)
34	OEX	c	501	1,3	0,15,15	-	-	-	-	-
27	CLA	b	622	-	65,73,73	1.47	9 (13%)	76,113,113	1.60	14 (18%)
38	A86	12	316	-	44,50,50	4.04	22 (50%)	51,76,76	7.81	20 (39%)
27	CLA	11	303	-	65,73,73	1.41	10 (15%)	76,113,113	1.58	10 (13%)
38	A86	34	316	-	44,50,50	4.02	23 (52%)	51,76,76	8.21	20 (39%)
36	PL9	D	407	-	55,55,55	2.32	15 (27%)	68,69,69	1.48	14 (20%)
38	A86	31	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)
27	CLA	32	308	33,25	45,53,73	1.72	8 (17%)	52,89,113	2.04	11 (21%)
27	CLA	C	508	-	65,73,73	1.43	12 (18%)	76,113,113	1.68	12 (15%)
27	CLA	12	312	25	45,53,73	1.75	11 (24%)	52,89,113	1.76	9 (17%)
27	CLA	12	305	25	65,73,73	1.46	9 (13%)	76,113,113	1.68	8 (10%)
27	CLA	13	309	25	65,73,73	1.46	10 (15%)	76,113,113	1.54	10 (13%)
27	CLA	32	305	25	65,73,73	1.45	9 (13%)	76,113,113	1.68	8 (10%)

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
27	CLA	13	308	25	1/1/11/20	8/13/91/115	-
27	CLA	33	304	-	1/1/11/20	5/13/91/115	-
27	CLA	12	309	-	1/1/11/20	8/13/91/115	-
27	CLA	34	309	25	1/1/11/20	8/13/91/115	-
38	A86	12	314	-	-	8/34/90/90	0/3/3/3
27	CLA	A	404	-	1/1/15/20	10/37/115/115	-
27	CLA	D	405	-	1/1/15/20	8/37/115/115	-
38	A86	32	314	-	-	7/34/90/90	0/3/3/3
27	CLA	d	406	-	1/1/15/20	4/37/115/115	-
27	CLA	11	306	25	1/1/11/20	8/13/91/115	-
27	CLA	B	614	-	1/1/15/20	8/37/115/115	-
27	CLA	33	307	-	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	m	103	-	-	8/29/63/63	0/2/2/2
27	CLA	32	306	39	1/1/11/20	5/13/91/115	-
27	CLA	34	302	-	1/1/15/20	11/37/115/115	-
32	LHG	l	103	-	-	22/53/53/53	-
33	LMG	D	408	-	-	14/46/66/70	0/1/1/1
38	A86	14	314	-	-	8/34/90/90	0/3/3/3
27	CLA	31	305	-	1/1/11/20	8/13/91/115	-
27	CLA	d	405	-	1/1/15/20	8/37/115/115	-
27	CLA	13	307	-	1/1/11/20	8/13/91/115	-
33	LMG	d	408	-	-	14/46/66/70	0/1/1/1
35	DGD	J	101	-	-	15/51/91/95	0/2/2/2
27	CLA	12	307	-	1/1/15/20	13/37/115/115	-
36	PL9	d	404	4	-	17/53/73/73	0/1/1/1
37	HEM	E	101	6,5	-	7/12/54/54	-
38	A86	14	315	-	-	10/34/90/90	0/3/3/3
38	A86	12	304	-	-	16/34/90/90	0/3/3/3
27	CLA	b	611	-	1/1/15/20	12/37/115/115	-
27	CLA	31	308	25	-	6/13/91/115	-
29	BCR	A	409	-	-	9/29/63/63	0/2/2/2
29	BCR	b	616	-	-	9/29/63/63	0/2/2/2
27	CLA	C	510	-	1/1/15/20	12/37/115/115	-
38	A86	31	316	-	-	15/34/90/90	0/3/3/3
27	CLA	11	307	25	1/1/15/20	14/37/115/115	-
27	CLA	32	311	25	1/1/15/20	14/37/115/115	-
27	CLA	B	613	-	1/1/15/20	8/37/115/115	-
27	CLA	B	608	-	1/1/15/20	8/37/115/115	-
27	CLA	13	310	25	-	6/13/91/115	-
27	CLA	B	604	-	1/1/15/20	14/37/115/115	-
38	A86	11	316	-	-	15/34/90/90	0/3/3/3
27	CLA	b	610	-	1/1/15/20	14/37/115/115	-
29	BCR	c	516	-	-	10/29/63/63	0/2/2/2
38	A86	31	311	-	-	3/34/90/90	0/3/3/3
27	CLA	33	301	-	1/1/15/20	11/37/115/115	-
27	CLA	14	305	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	31	309	-	1/1/11/20	6/13/91/115	-
27	CLA	33	308	25	1/1/11/20	8/13/91/115	-
27	CLA	C	513	-	1/1/15/20	16/37/115/115	-
27	CLA	11	305	-	1/1/11/20	8/13/91/115	-
29	BCR	C	516	-	-	10/29/63/63	0/2/2/2
27	CLA	32	310	25	1/1/11/20	8/13/91/115	-
29	BCR	h	101	-	-	7/29/63/63	0/2/2/2
27	CLA	c	502	-	1/1/15/20	14/37/115/115	-
27	CLA	c	513	-	1/1/15/20	16/37/115/115	-
27	CLA	32	303	-	1/1/15/20	11/37/115/115	-
38	A86	11	314	-	-	7/34/90/90	0/3/3/3
38	A86	13	317	-	-	16/34/90/90	0/3/3/3
38	A86	13	315	-	-	10/34/90/90	0/3/3/3
29	BCR	c	519	-	-	8/29/63/63	0/2/2/2
33	LMG	M	103	27	-	10/35/55/70	0/1/1/1
33	LMG	b	619	-	-	20/46/66/70	0/1/1/1
35	DGD	c	517	-	-	19/51/91/95	0/2/2/2
27	CLA	33	311	-	1/1/11/20	6/13/91/115	-
27	CLA	31	301	25	1/1/15/20	12/37/115/115	-
35	DGD	j	101	-	-	15/51/91/95	0/2/2/2
27	CLA	C	503	-	1/1/15/20	11/37/115/115	-
27	CLA	34	311	25	-	6/13/91/115	-
37	HEM	V	201	16	-	0/12/54/54	-
27	CLA	M	102	33,12	1/1/15/20	19/37/115/115	-
27	CLA	C	509	-	1/1/15/20	12/37/115/115	-
27	CLA	14	311	-	1/1/11/20	6/13/91/115	-
27	CLA	m	101	33,12	1/1/15/20	19/37/115/115	-
38	A86	14	313	-	-	3/34/90/90	0/3/3/3
27	CLA	C	514	-	1/1/15/20	13/37/115/115	-
27	CLA	B	609	-	1/1/15/20	8/37/115/115	-
27	CLA	12	308	33,25	1/1/11/20	9/13/91/115	-
27	CLA	34	308	-	1/1/11/20	8/13/91/115	-
27	CLA	13	301	-	1/1/15/20	11/37/115/115	-
29	BCR	B	617	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	b	623	-	-	18/29/63/63	0/2/2/2
35	DGD	c	518	-	-	22/51/91/95	0/2/2/2
27	CLA	33	309	25	1/1/15/20	14/37/115/115	-
38	A86	33	313	-	-	3/34/90/90	0/3/3/3
27	CLA	C	502	-	1/1/15/20	14/37/115/115	-
38	A86	33	314	-	-	8/34/90/90	0/3/3/3
32	LHG	B	621	-	-	20/53/53/53	-
29	BCR	b	617	-	-	9/29/63/63	0/2/2/2
38	A86	11	312	-	-	8/34/90/90	0/3/3/3
38	A86	12	315	-	-	3/34/90/90	0/3/3/3
27	CLA	B	602	-	1/1/15/20	13/37/115/115	-
27	CLA	b	614	-	1/1/15/20	8/37/115/115	-
27	CLA	c	504	-	1/1/15/20	17/37/115/115	-
27	CLA	13	306	25	1/1/11/20	9/13/91/115	-
29	BCR	z	101	-	-	16/29/63/63	0/2/2/2
27	CLA	b	606	-	1/1/15/20	7/37/115/115	-
29	BCR	C	520	-	-	8/29/63/63	0/2/2/2
32	LHG	a	408	-	-	23/50/50/53	-
27	CLA	c	506	-	1/1/15/20	16/37/115/115	-
27	CLA	12	306	39	1/1/11/20	5/13/91/115	-
27	CLA	14	308	25	1/1/11/20	8/13/91/115	-
32	LHG	b	621	-	-	20/53/53/53	-
33	LMG	w	101	-	-	28/46/66/70	0/1/1/1
27	CLA	32	313	-	1/1/11/20	6/13/91/115	-
27	CLA	34	306	-	1/1/15/20	13/37/115/115	-
32	LHG	L	102	-	-	22/53/53/53	-
39	LMU	32	302	27,25	-	7/18/58/61	0/2/2/2
27	CLA	c	514	-	1/1/15/20	13/37/115/115	-
27	CLA	w	102	-	1/1/15/20	14/37/115/115	-
35	DGD	C	518	-	-	22/51/91/95	0/2/2/2
37	HEM	f	102	6,5	-	7/12/54/54	-
27	CLA	13	303	25	1/1/15/20	12/37/115/115	-
27	CLA	32	309	-	1/1/11/20	8/13/91/115	-
33	LMG	q	301	-	-	22/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	12	310	25	1/1/11/20	8/13/91/115	-
37	HEM	v	201	16	-	0/12/54/54	-
38	A86	11	313	-	-	10/34/90/90	0/3/3/3
27	CLA	b	613	-	1/1/15/20	8/37/115/115	-
27	CLA	C	505	-	1/1/15/20	17/37/115/115	-
38	A86	33	316	-	-	7/34/90/90	0/3/3/3
27	CLA	11	302	-	1/1/11/20	5/13/91/115	-
27	CLA	31	303	-	1/1/15/20	13/37/115/115	-
27	CLA	34	304	25	1/1/15/20	12/37/115/115	-
27	CLA	b	602	-	1/1/15/20	13/37/115/115	-
29	BCR	c	515	-	-	15/29/63/63	0/2/2/2
29	BCR	M	101	-	-	8/29/63/63	0/2/2/2
27	CLA	11	309	-	1/1/11/20	6/13/91/115	-
36	PL9	D	404	4	-	17/53/73/73	0/1/1/1
27	CLA	34	305	-	1/1/11/20	5/13/91/115	-
27	CLA	B	601	-	1/1/15/20	18/37/115/115	-
27	CLA	34	307	25	1/1/11/20	9/13/91/115	-
27	CLA	B	605	-	1/1/15/20	17/37/115/115	-
33	LMG	C	519	-	-	22/46/66/70	0/1/1/1
38	A86	13	313	-	-	3/34/90/90	0/3/3/3
38	A86	12	317	-	-	10/34/90/90	0/3/3/3
29	BCR	a	409	-	-	9/29/63/63	0/2/2/2
38	A86	32	315	-	-	3/34/90/90	0/3/3/3
28	PHO	a	403	-	-	12/37/103/103	0/5/6/6
30	SQD	b	620	-	-	9/32/52/69	0/1/1/1
27	CLA	a	402	-	1/1/15/20	7/37/115/115	-
30	SQD	a	406	-	-	14/49/69/69	0/1/1/1
38	A86	14	301	-	-	7/34/90/90	0/3/3/3
33	LMG	m	102	27	-	10/35/55/70	0/1/1/1
38	A86	31	313	-	-	10/34/90/90	0/3/3/3
27	CLA	b	605	-	1/1/15/20	17/37/115/115	-
38	A86	33	312	-	-	8/34/90/90	0/3/3/3
38	A86	34	313	-	-	8/34/90/90	0/3/3/3
35	DGD	H	102	-	-	24/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	a	405	-	-	12/29/63/63	0/2/2/2
27	CLA	d	401	-	1/1/15/20	12/37/115/115	-
29	BCR	H	101	-	-	7/29/63/63	0/2/2/2
29	BCR	C	515	-	-	15/29/63/63	0/2/2/2
27	CLA	32	307	-	1/1/15/20	13/37/115/115	-
29	BCR	Z	101	-	-	16/29/63/63	0/2/2/2
27	CLA	11	315	-	1/1/15/20	11/37/115/115	-
38	A86	11	310	-	-	8/34/90/90	0/3/3/3
27	CLA	b	604	-	1/1/15/20	14/37/115/115	-
27	CLA	C	504	-	1/1/15/20	17/37/115/115	-
38	A86	32	316	-	-	8/34/90/90	0/3/3/3
27	CLA	B	615	-	1/1/15/20	13/37/115/115	-
38	A86	32	318	-	-	7/34/90/90	0/3/3/3
27	CLA	D	402	-	1/1/15/20	13/37/115/115	-
35	DGD	C	517	-	-	19/51/91/95	0/2/2/2
27	CLA	12	303	-	1/1/15/20	11/37/115/115	-
28	PHO	D	403	-	-	8/37/103/103	0/5/6/6
30	SQD	L	103	-	-	21/49/69/69	0/1/1/1
38	A86	14	316	-	-	7/34/90/90	0/3/3/3
38	A86	32	317	-	-	10/34/90/90	0/3/3/3
27	CLA	c	512	3	1/1/15/20	8/37/115/115	-
27	CLA	31	307	25	1/1/15/20	14/37/115/115	-
27	CLA	d	402	-	1/1/15/20	13/37/115/115	-
27	CLA	b	609	-	1/1/15/20	8/37/115/115	-
33	LMG	W	101	-	-	28/46/66/70	0/1/1/1
38	A86	33	302	-	-	16/34/90/90	0/3/3/3
27	CLA	c	508	-	1/1/15/20	18/37/115/115	-
28	PHO	d	403	-	-	8/37/103/103	0/5/6/6
27	CLA	31	304	25	1/1/11/20	9/13/91/115	-
27	CLA	D	406	-	1/1/15/20	4/37/115/115	-
33	LMG	b	618	-	-	18/46/66/70	0/1/1/1
27	CLA	11	308	25	-	6/13/91/115	-
32	LHG	A	408	-	-	23/50/50/53	-
33	LMG	B	618	-	-	18/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	33	310	25	-	6/13/91/115	-
32	LHG	L	101	-	-	29/53/53/53	-
27	CLA	c	505	-	1/1/15/20	17/37/115/115	-
27	CLA	Z	102	-	-	21/37/115/115	-
27	CLA	14	306	25	1/1/11/20	9/13/91/115	-
27	CLA	32	312	25	-	6/13/91/115	-
38	A86	34	303	-	-	15/34/90/90	0/3/3/3
38	A86	34	315	-	-	9/34/90/90	0/3/3/3
27	CLA	c	509	-	1/1/15/20	12/37/115/115	-
29	BCR	B	616	-	-	9/29/63/63	0/2/2/2
30	SQD	B	620	-	-	9/32/52/69	0/1/1/1
38	A86	13	316	-	-	7/34/90/90	0/3/3/3
27	CLA	33	305	-	1/1/15/20	13/37/115/115	-
27	CLA	A	402	-	1/1/15/20	7/37/115/115	-
39	LMU	12	302	27,25	-	7/18/58/61	0/2/2/2
27	CLA	C	511	-	1/1/15/20	12/37/115/115	-
33	LMG	12	301	27	-	17/34/54/70	0/1/1/1
27	CLA	34	312	-	1/1/11/20	6/13/91/115	-
27	CLA	14	303	25	1/1/15/20	12/37/115/115	-
28	PHO	A	403	-	-	12/37/103/103	0/5/6/6
27	CLA	13	305	-	1/1/15/20	13/37/115/115	-
27	CLA	14	304	-	1/1/11/20	4/13/91/115	-
27	CLA	B	610	-	1/1/15/20	14/37/115/115	-
29	BCR	A	405	-	-	12/29/63/63	0/2/2/2
27	CLA	B	622	-	1/1/15/20	15/37/115/115	-
27	CLA	c	511	-	1/1/15/20	12/37/115/115	-
38	A86	11	311	-	-	3/34/90/90	0/3/3/3
38	A86	33	315	-	-	10/34/90/90	0/3/3/3
38	A86	13	314	-	-	9/34/90/90	0/3/3/3
32	LHG	l	102	-	-	29/53/53/53	-
38	A86	34	301	-	-	7/34/90/90	0/3/3/3
27	CLA	C	506	-	1/1/15/20	16/37/115/115	-
33	LMG	B	619	-	-	21/46/66/70	0/1/1/1
38	A86	13	312	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	A86	34	314	-	-	3/34/90/90	0/3/3/3
27	CLA	W	103	-	-	19/37/115/115	-
27	CLA	z	102	-	-	21/37/115/115	-
27	CLA	b	601	-	1/1/15/20	18/37/115/115	-
27	CLA	B	606	-	1/1/15/20	7/37/115/115	-
38	A86	31	312	-	-	8/34/90/90	0/3/3/3
27	CLA	14	302	-	1/1/15/20	11/37/115/115	-
27	CLA	31	302	-	1/1/11/20	4/13/91/115	-
27	CLA	34	310	25	1/1/15/20	14/37/115/115	-
27	CLA	C	512	3	1/1/15/20	8/37/115/115	-
27	CLA	a	404	-	1/1/15/20	10/37/115/115	-
38	A86	13	302	-	-	15/34/90/90	0/3/3/3
27	CLA	w	103	-	-	19/37/115/115	-
27	CLA	14	309	25	1/1/15/20	14/37/115/115	-
27	CLA	b	615	-	1/1/15/20	13/37/115/115	-
27	CLA	13	311	-	1/1/11/20	6/13/91/115	-
27	CLA	14	310	25	-	6/13/91/115	-
27	CLA	b	612	-	1/1/15/20	13/37/115/115	-
27	CLA	13	304	-	1/1/11/20	5/13/91/115	-
38	A86	14	312	-	-	8/34/90/90	0/3/3/3
27	CLA	b	603	-	1/1/15/20	10/37/115/115	-
27	CLA	b	608	-	1/1/15/20	8/37/115/115	-
27	CLA	33	306	25	1/1/11/20	9/13/91/115	-
29	BCR	f	101	-	-	15/29/63/63	0/2/2/2
27	CLA	c	507	-	1/1/15/20	17/37/115/115	-
27	CLA	12	311	25	1/1/15/20	14/37/115/115	-
27	CLA	B	607	-	1/1/15/20	12/37/115/115	-
27	CLA	B	612	-	1/1/15/20	13/37/115/115	-
27	CLA	c	503	-	1/1/15/20	11/37/115/115	-
29	BCR	B	623	-	-	18/29/63/63	0/2/2/2
27	CLA	11	301	25	1/1/15/20	11/37/115/115	-
27	CLA	W	102	-	1/1/15/20	14/37/115/115	-
27	CLA	11	304	25	1/1/11/20	9/13/91/115	-
27	CLA	14	307	-	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	F	101	-	-	15/29/63/63	0/2/2/2
27	CLA	33	303	25	1/1/15/20	12/37/115/115	-
27	CLA	C	507	-	1/1/15/20	17/37/115/115	-
30	SQD	A	406	-	-	14/49/69/69	0/1/1/1
38	A86	32	304	-	-	15/34/90/90	0/3/3/3
35	DGD	h	102	-	-	24/51/91/95	0/2/2/2
38	A86	31	314	-	-	7/34/90/90	0/3/3/3
27	CLA	D	401	-	1/1/15/20	12/37/115/115	-
27	CLA	31	306	25	1/1/11/20	8/13/91/115	-
27	CLA	c	510	-	1/1/15/20	12/37/115/115	-
36	PL9	d	407	-	-	13/53/73/73	0/1/1/1
27	CLA	B	603	-	1/1/15/20	10/37/115/115	-
33	LMG	32	301	27	-	14/34/54/70	0/1/1/1
27	CLA	12	313	-	1/1/11/20	6/13/91/115	-
27	CLA	B	611	-	1/1/15/20	12/37/115/115	-
30	SQD	l	101	-	-	21/49/69/69	0/1/1/1
27	CLA	b	607	-	1/1/15/20	12/37/115/115	-
27	CLA	31	315	-	1/1/15/20	11/37/115/115	-
27	CLA	b	622	-	1/1/15/20	15/37/115/115	-
38	A86	12	316	-	-	9/34/90/90	0/3/3/3
27	CLA	11	303	-	1/1/15/20	13/37/115/115	-
38	A86	34	316	-	-	10/34/90/90	0/3/3/3
36	PL9	D	407	-	-	13/53/73/73	0/1/1/1
38	A86	31	310	-	-	8/34/90/90	0/3/3/3
27	CLA	32	308	33,25	1/1/11/20	9/13/91/115	-
27	CLA	C	508	-	1/1/15/20	18/37/115/115	-
27	CLA	12	312	25	-	6/13/91/115	-
27	CLA	12	305	25	1/1/15/20	12/37/115/115	-
27	CLA	13	309	25	1/1/15/20	14/37/115/115	-
27	CLA	32	305	25	1/1/15/20	12/37/115/115	-

The worst 5 of 2970 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	34	316	A86	C14-C13	14.10	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	11	313	A86	C14-C13	14.03	1.68	1.51
38	13	315	A86	C14-C13	14.01	1.68	1.51
38	12	317	A86	C14-C13	14.01	1.68	1.51
38	31	313	A86	C14-C13	14.00	1.68	1.51

The worst 5 of 3001 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	33	312	A86	O1-C20-C19	55.03	154.72	113.38
38	34	313	A86	O1-C20-C19	55.03	154.72	113.38
38	12	314	A86	O1-C20-C19	55.02	154.72	113.38
38	14	312	A86	O1-C20-C19	55.01	154.71	113.38
38	13	312	A86	O1-C20-C19	55.01	154.71	113.38

5 of 146 chirality outliers are listed below:

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

5 of 3238 torsion outliers are listed below:

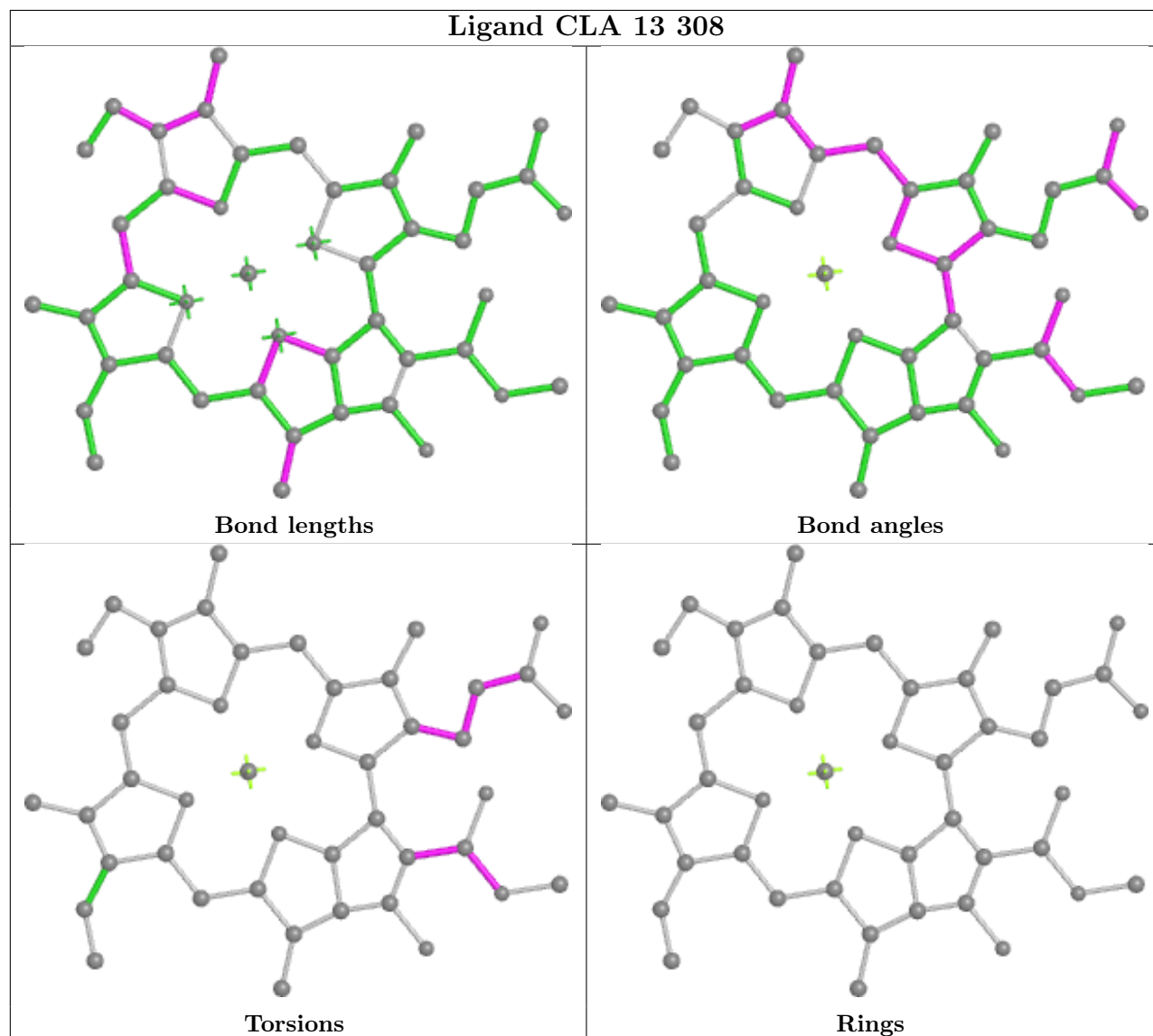
Mol	Chain	Res	Type	Atoms
27	A	402	CLA	CBD-CGD-O2D-CED
27	B	601	CLA	C1A-C2A-CAA-CBA
27	B	601	CLA	CHA-CBD-CGD-O1D
27	B	601	CLA	CHA-CBD-CGD-O2D
27	B	601	CLA	CAD-CBD-CGD-O1D

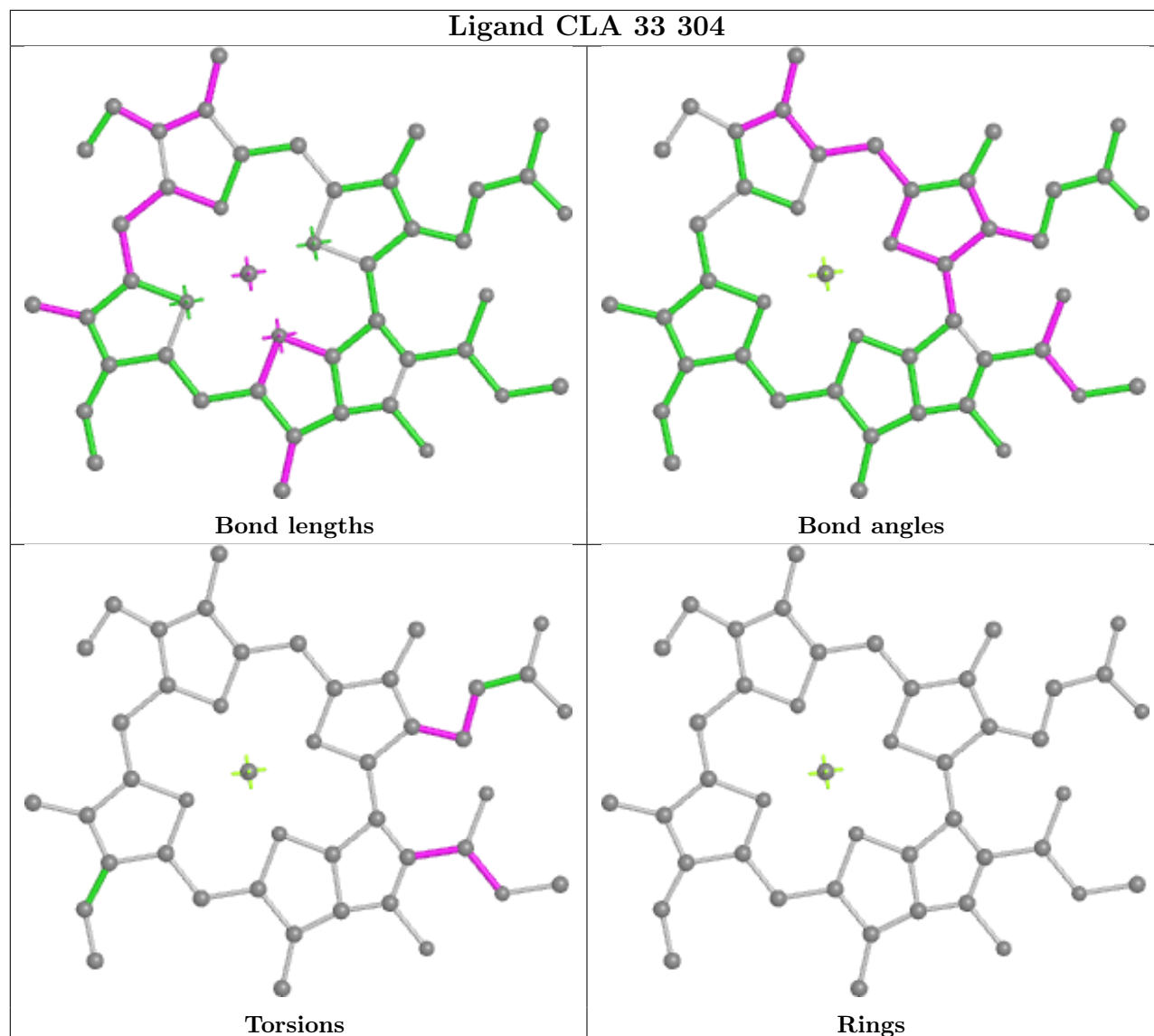
There are no ring outliers.

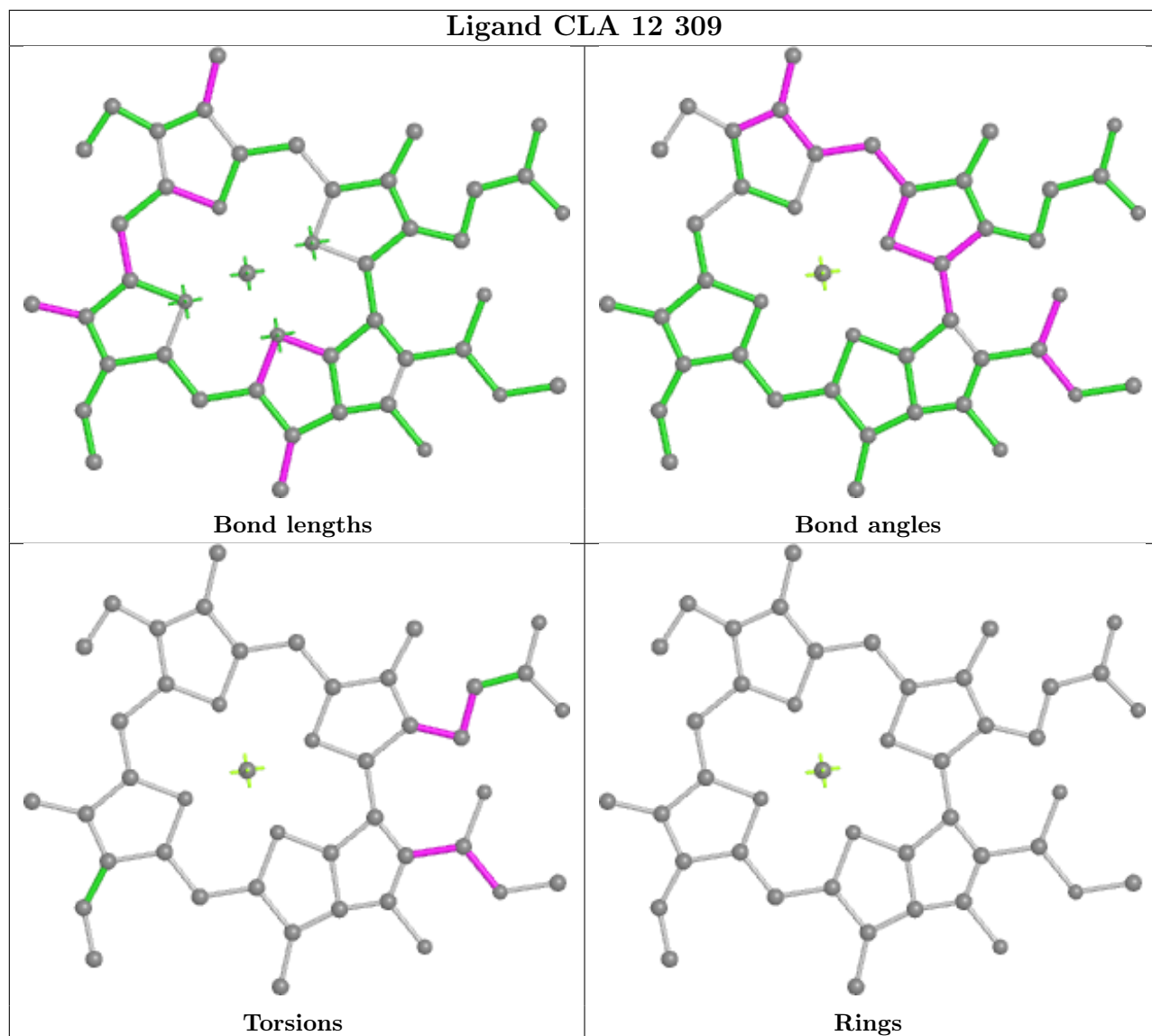
No monomer is involved in short contacts.

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

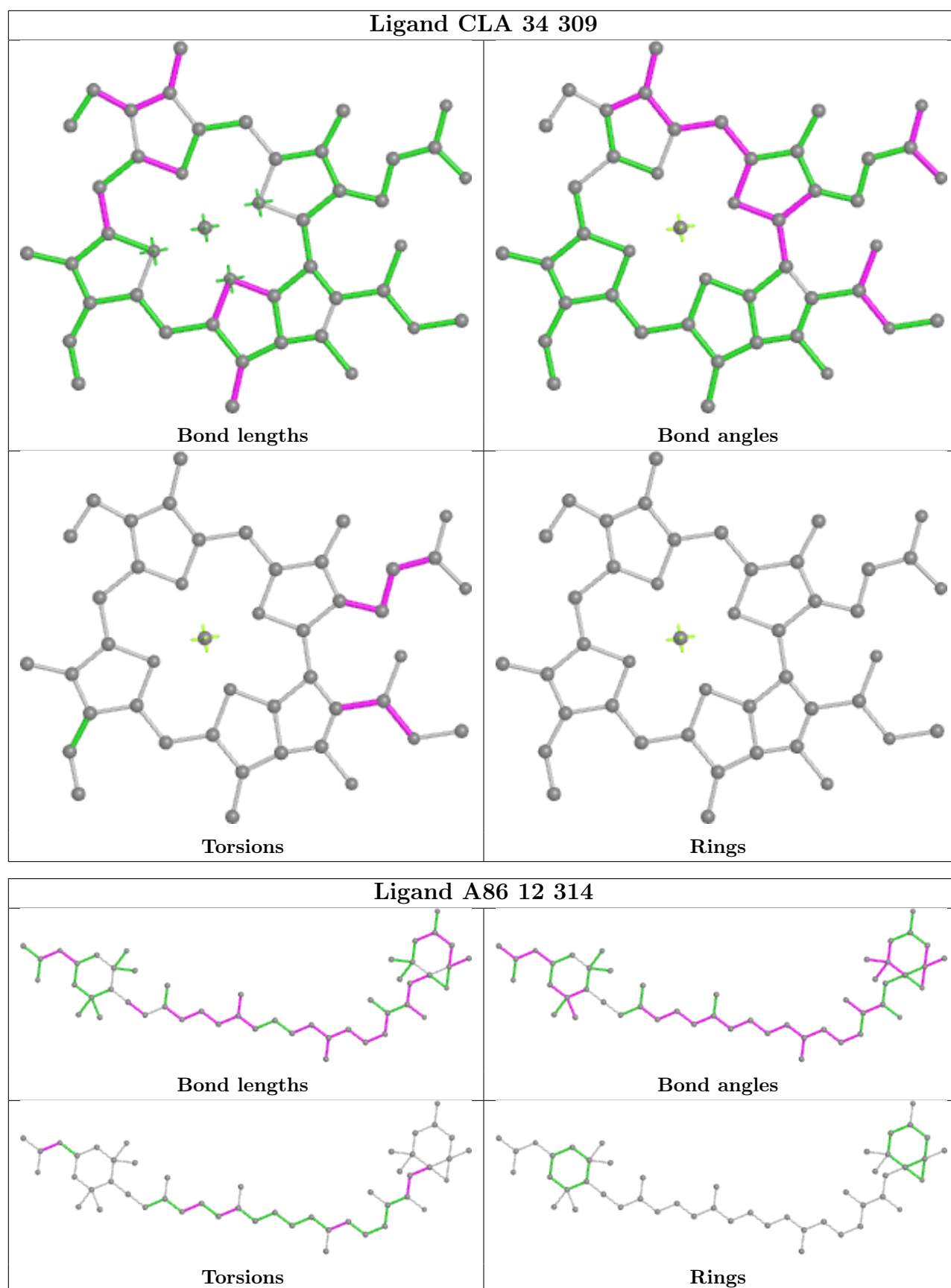
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

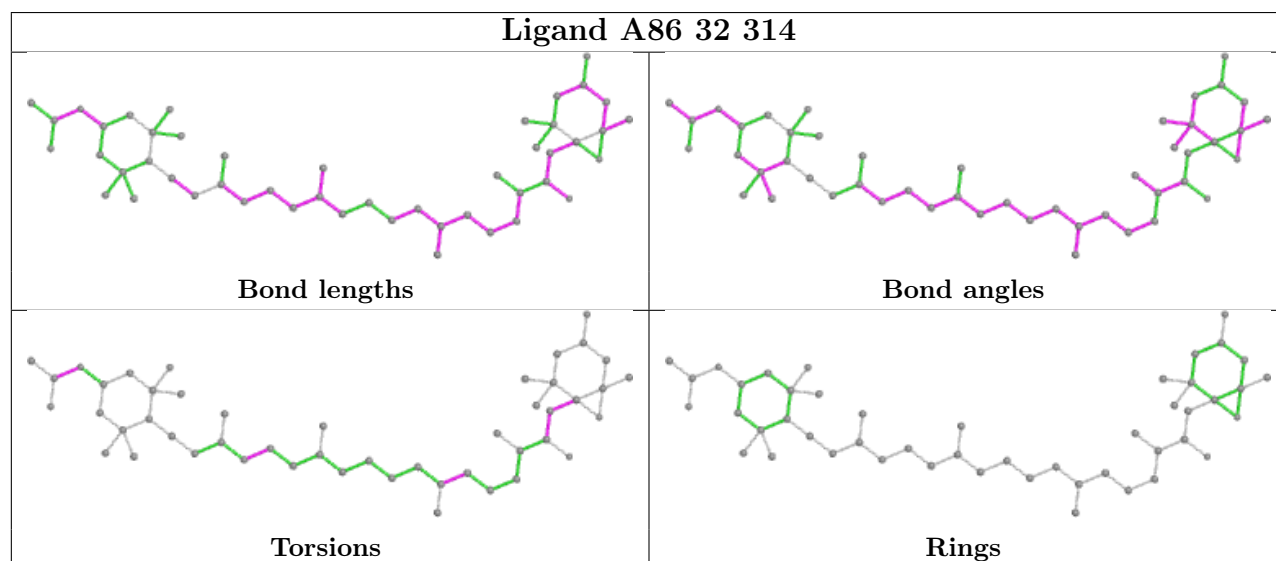
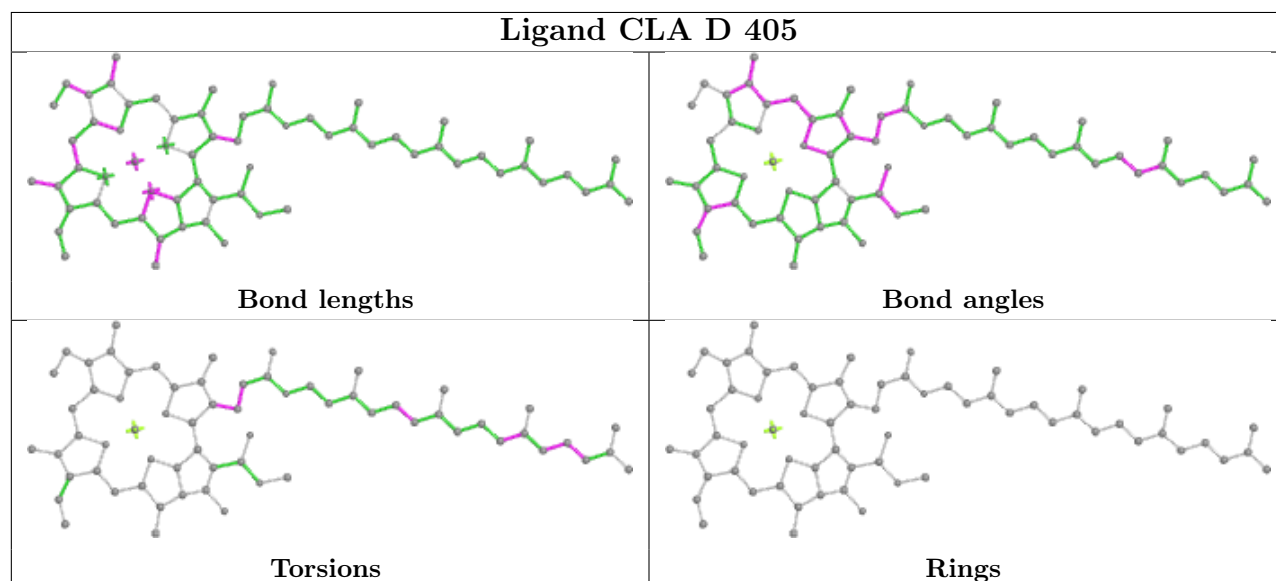
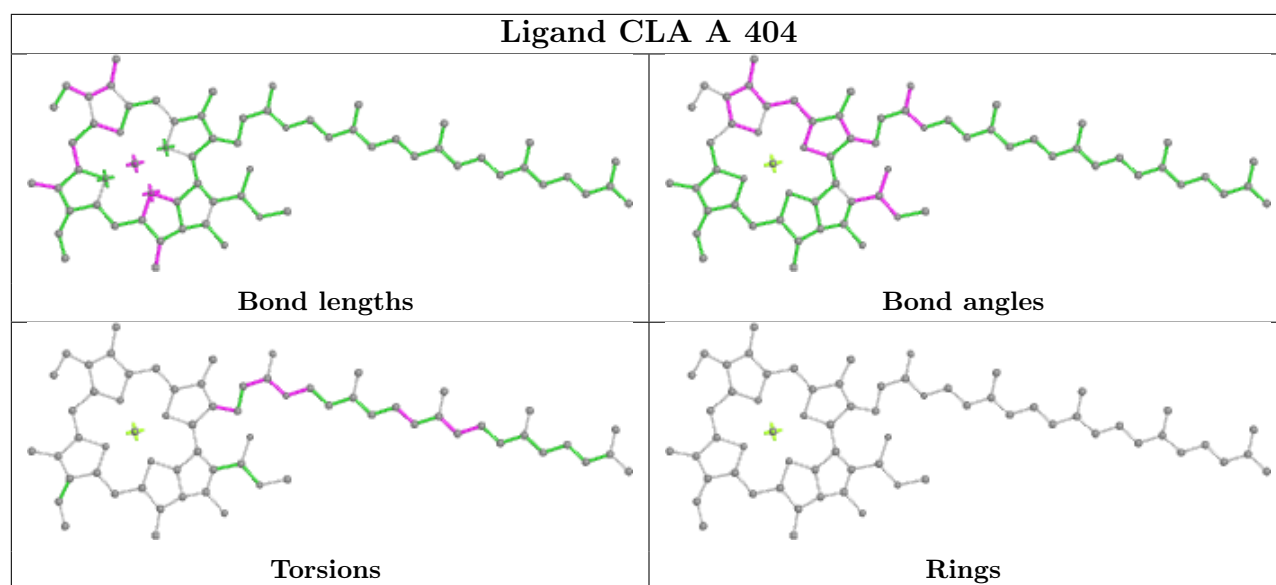


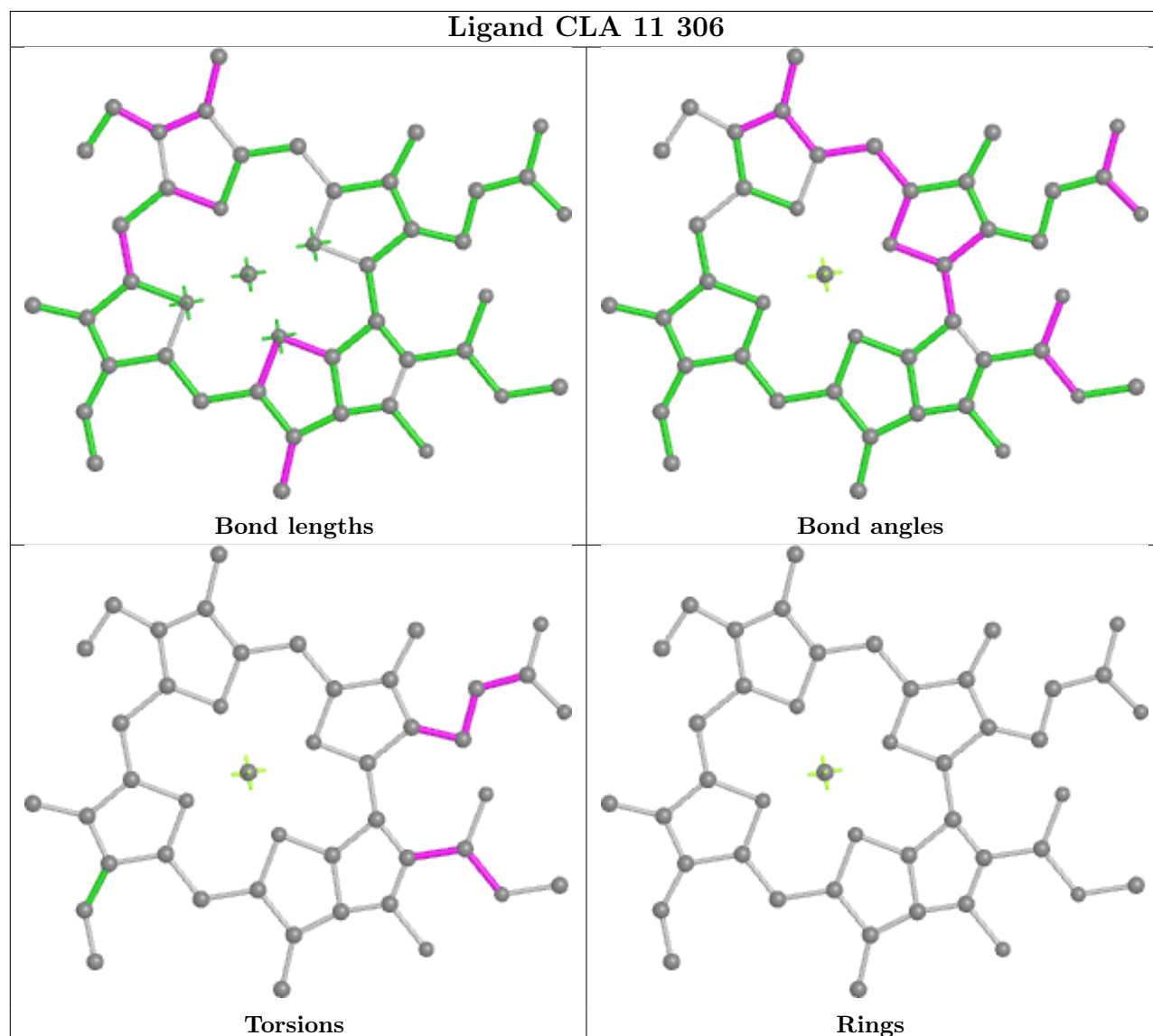
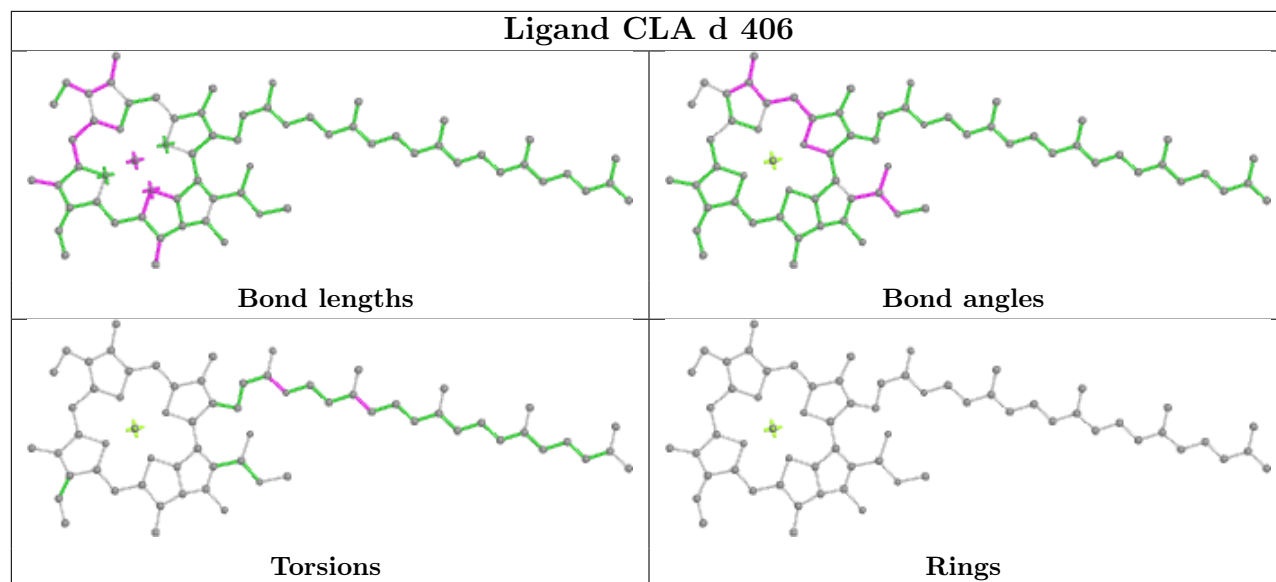


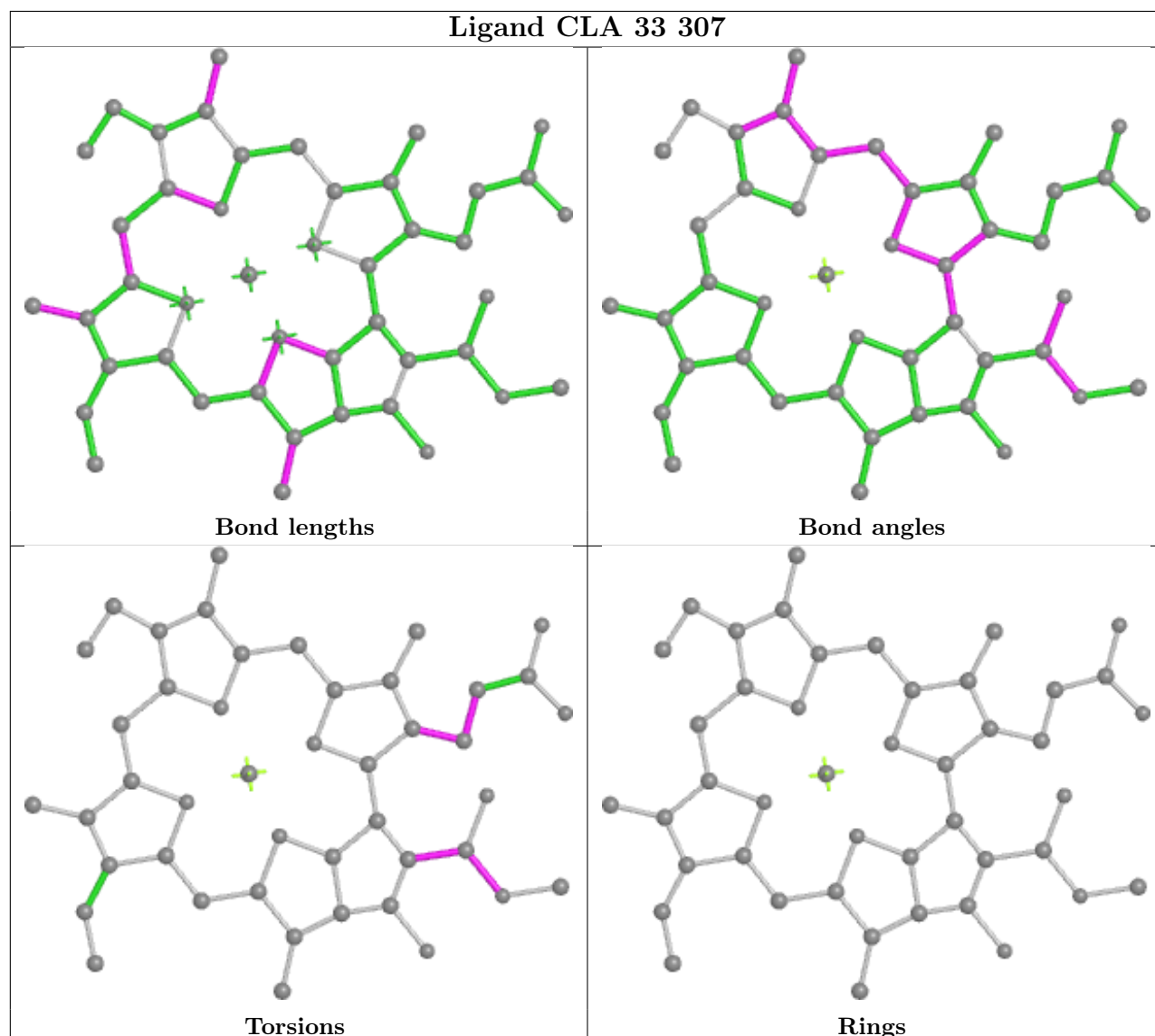
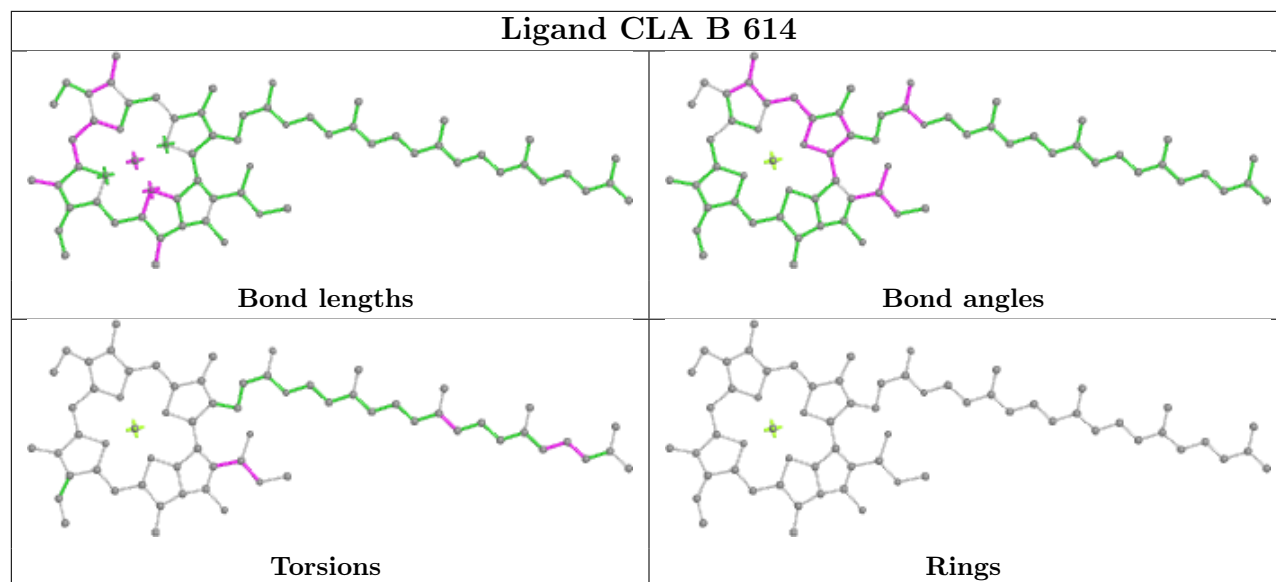


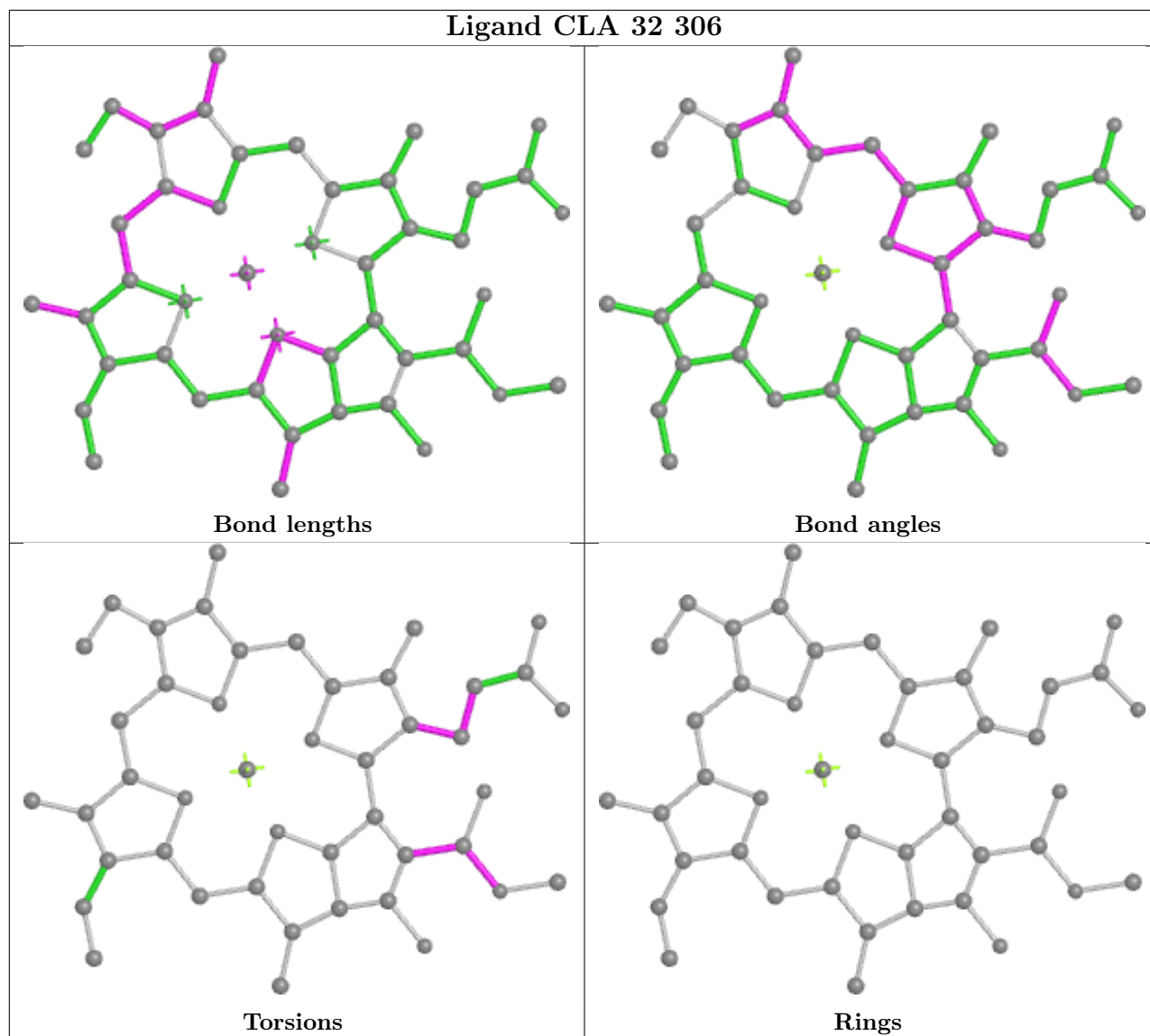
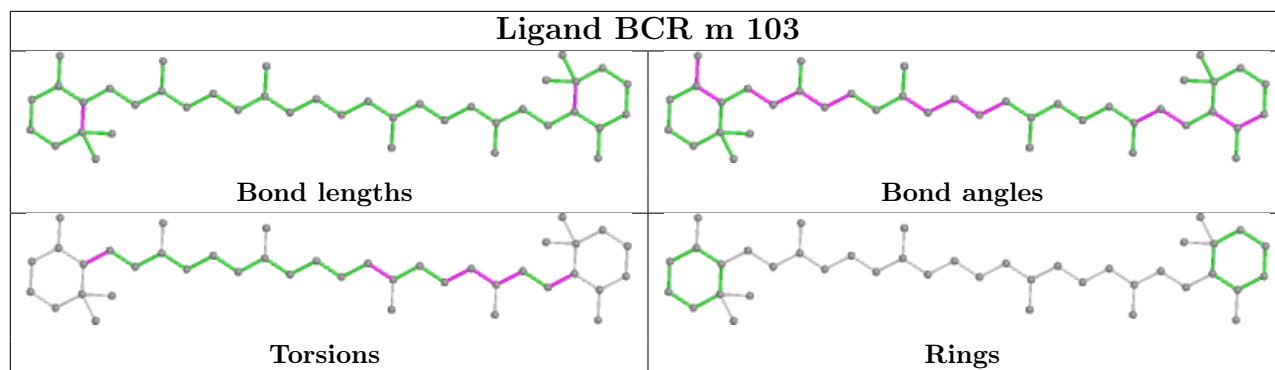


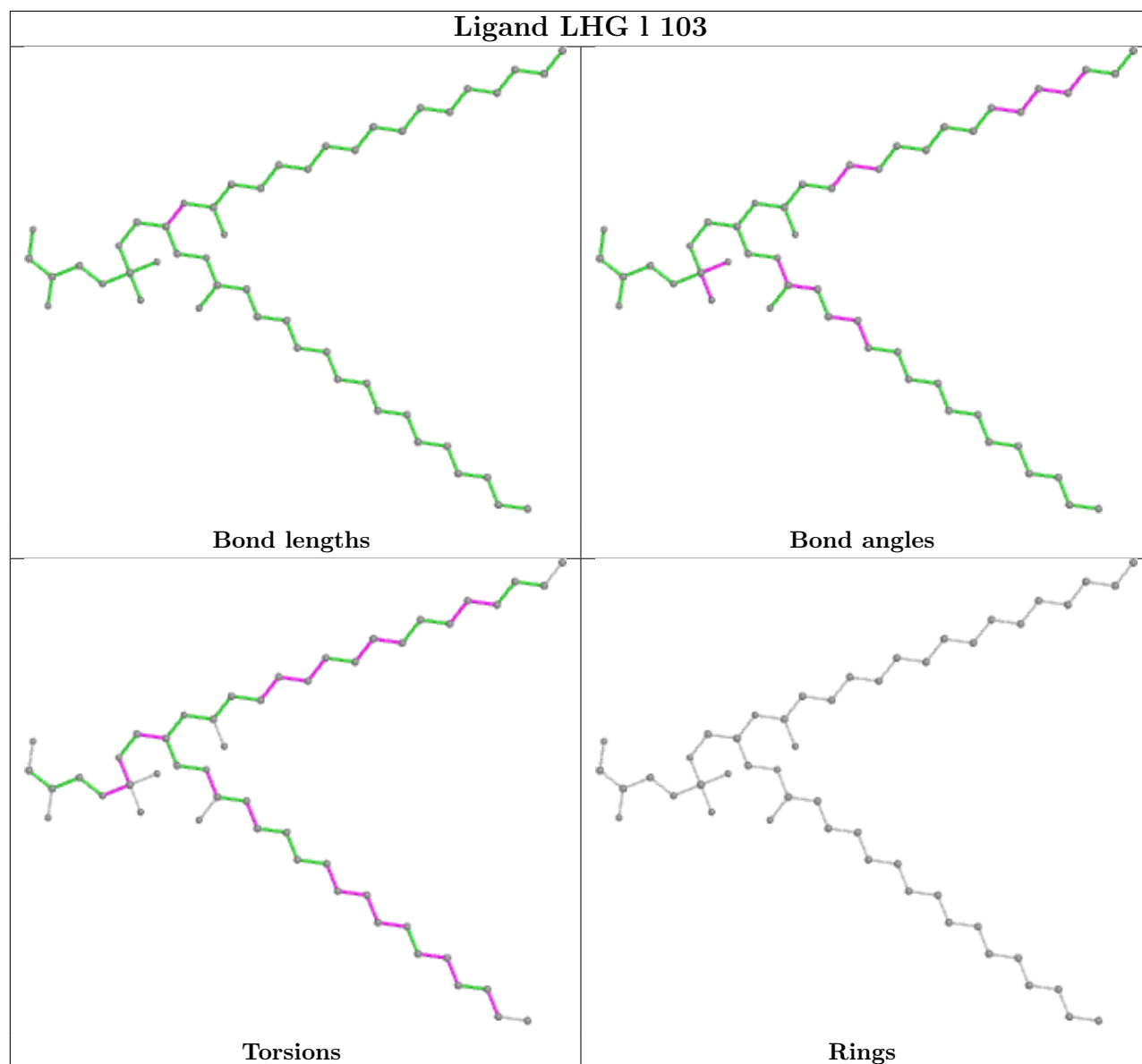
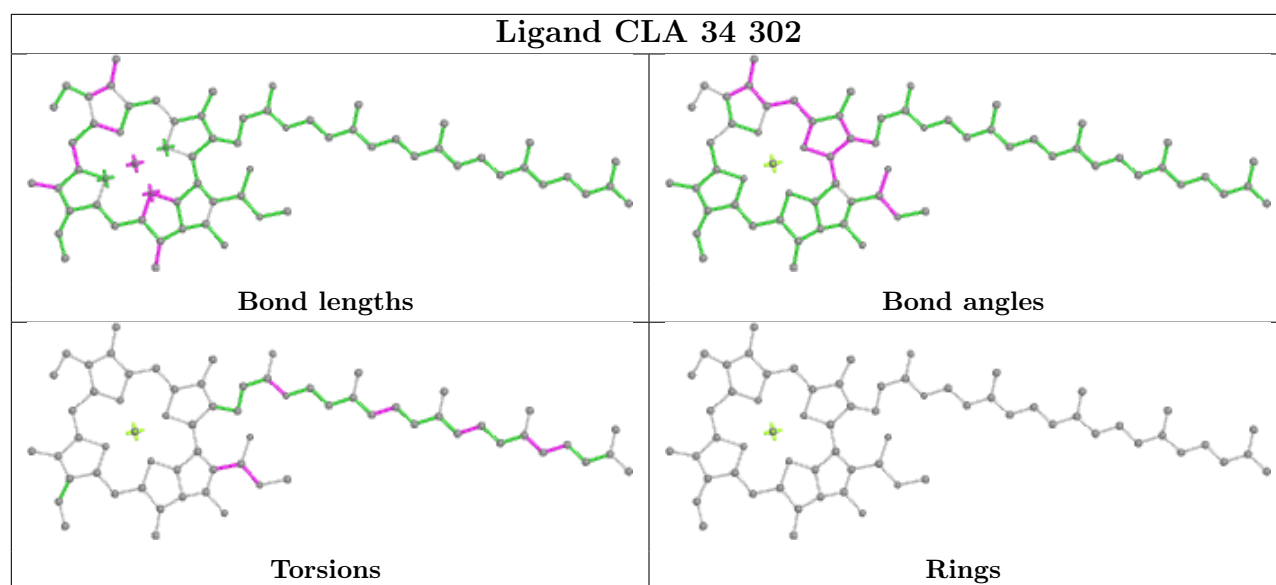


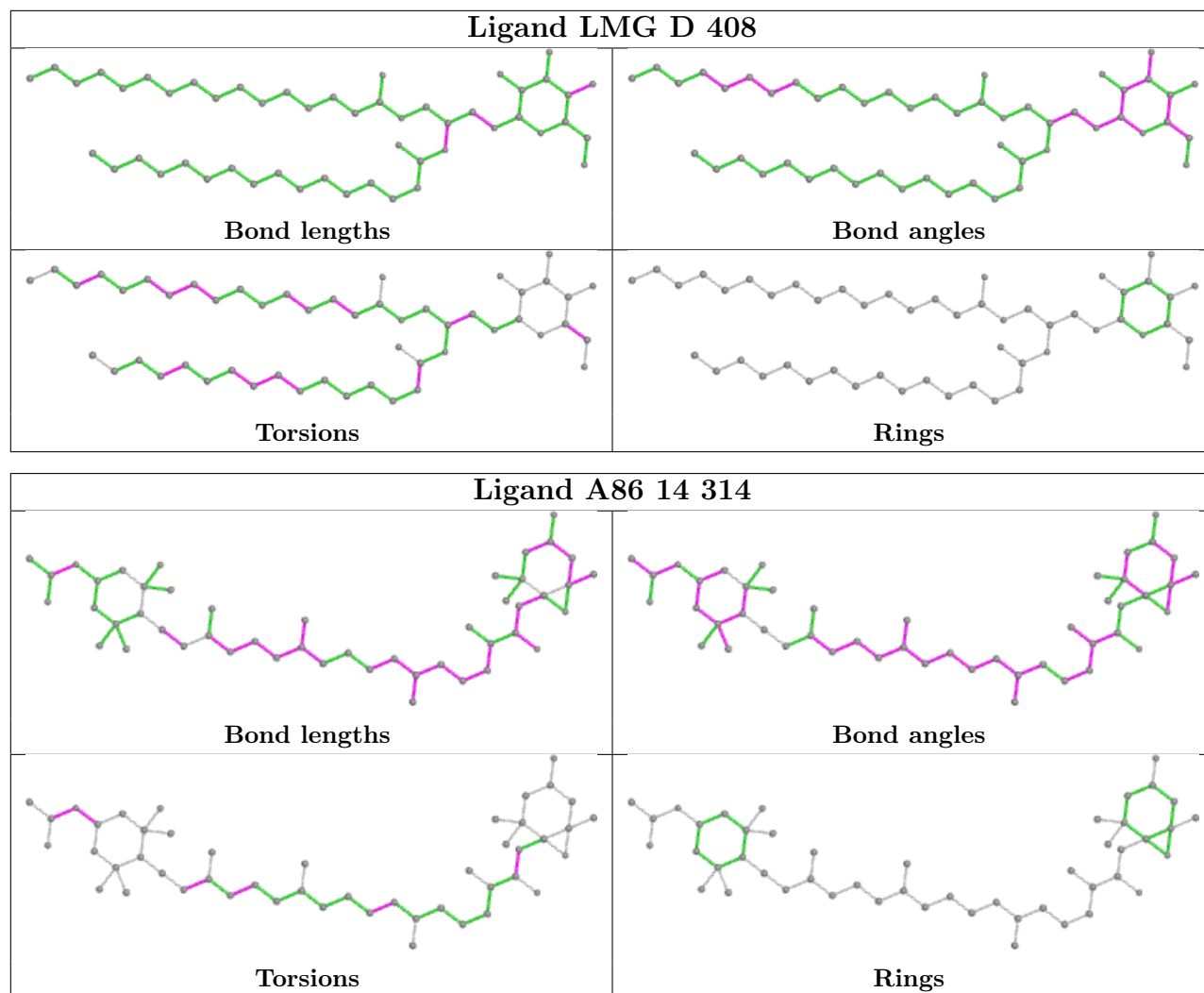


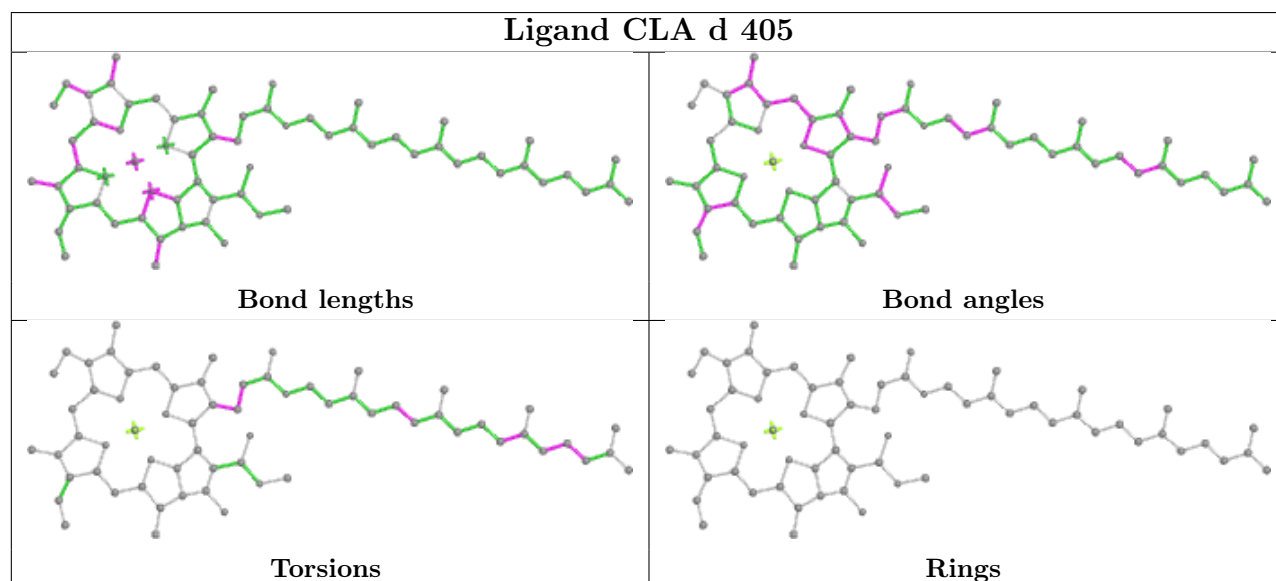
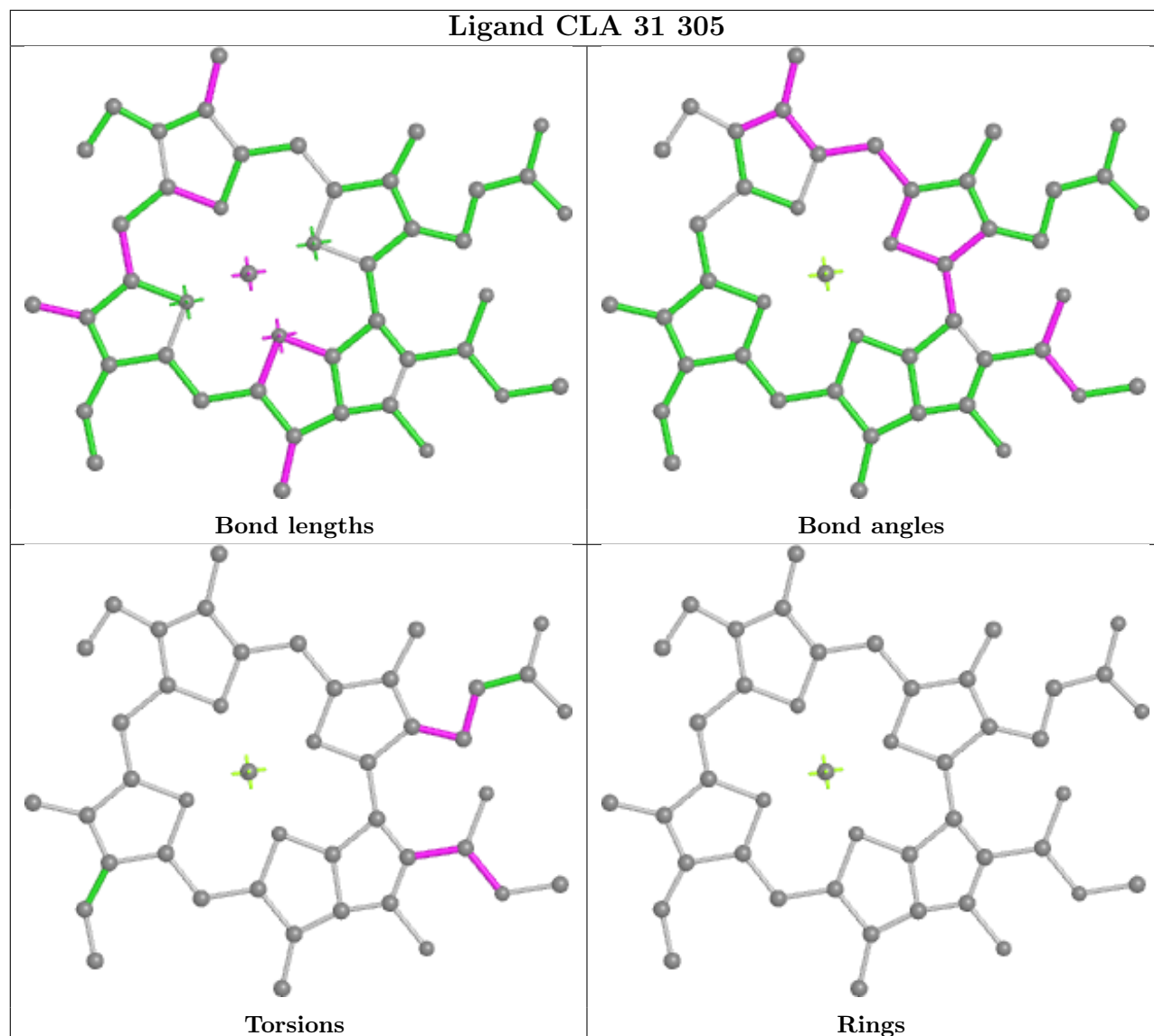




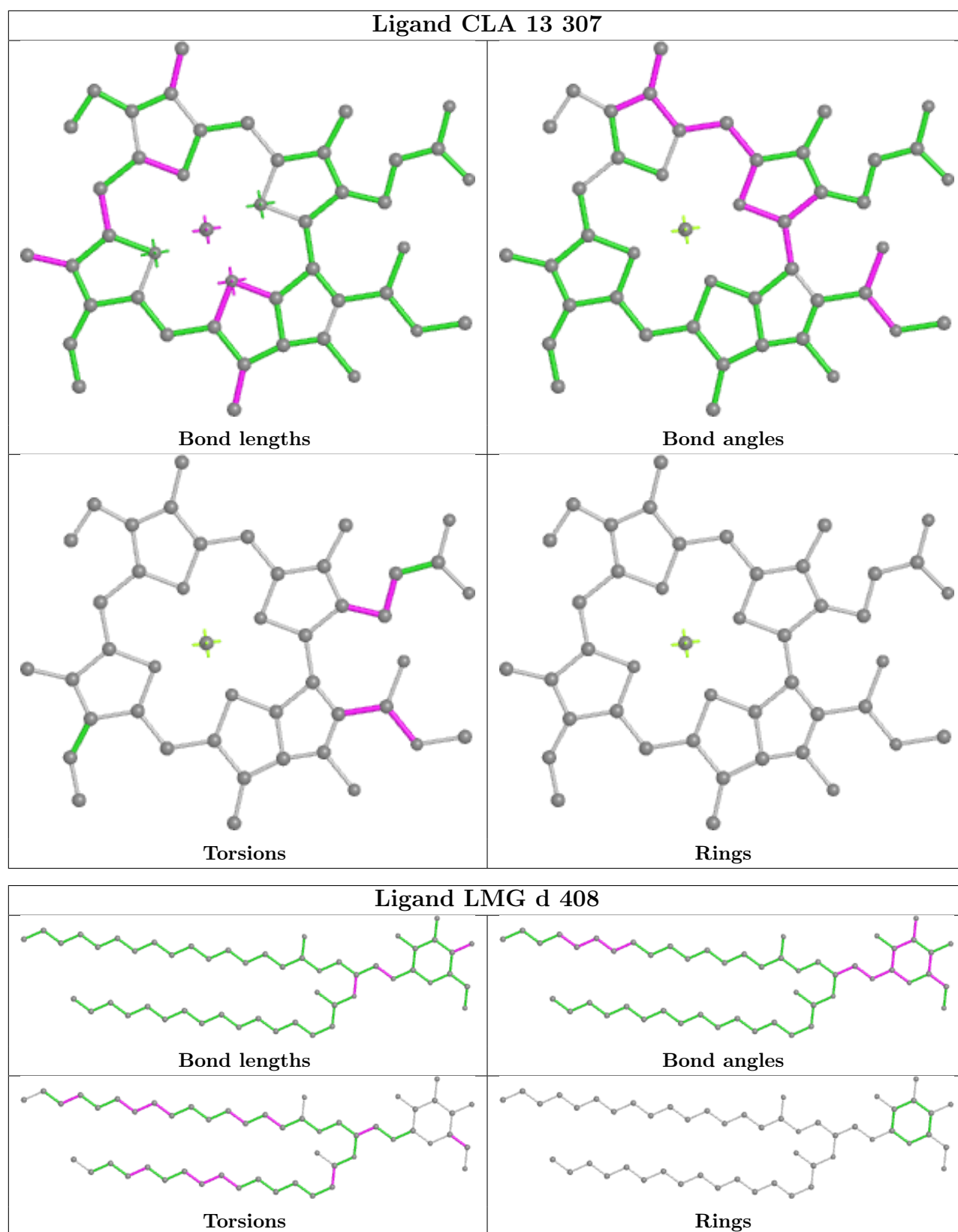


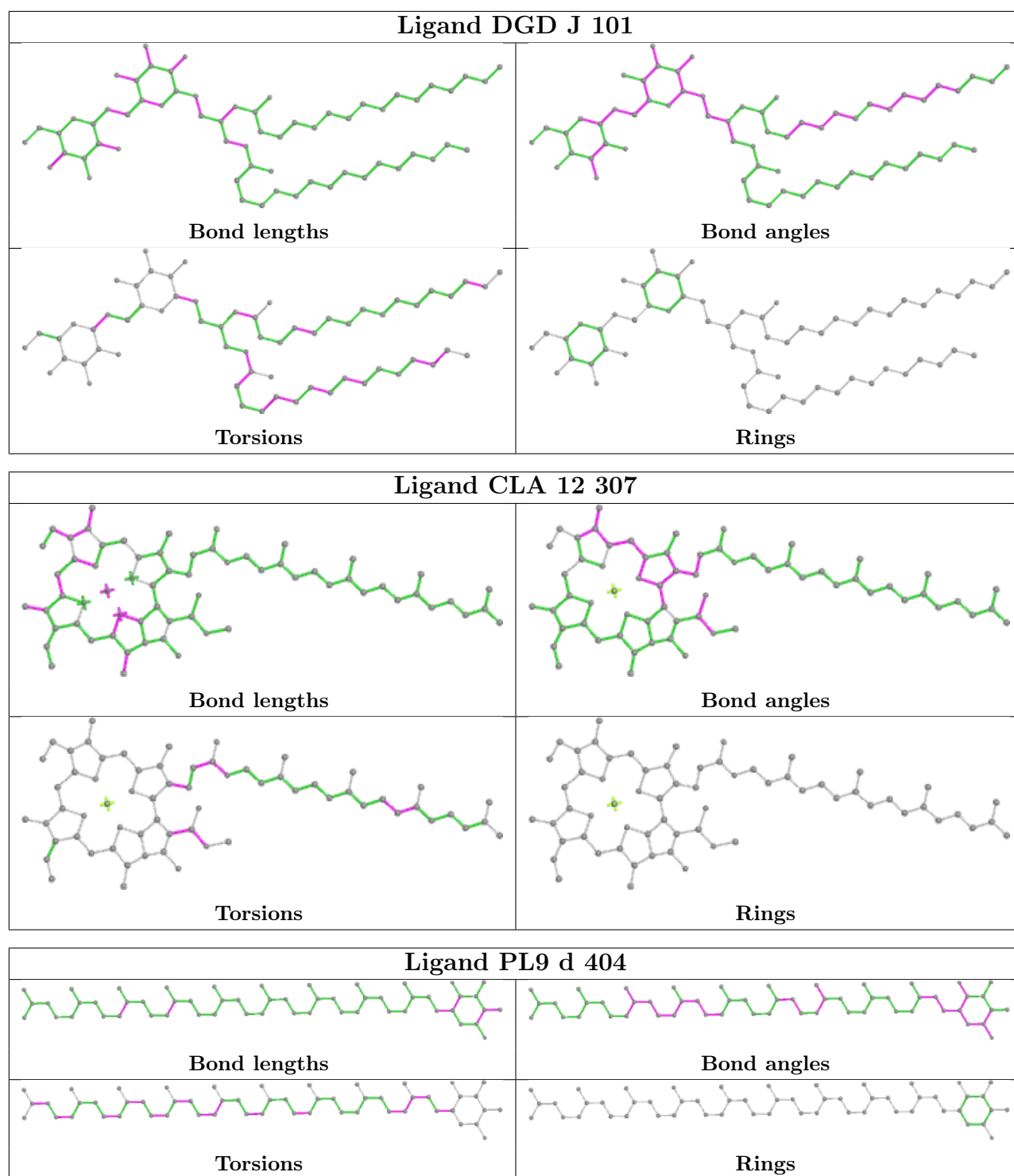


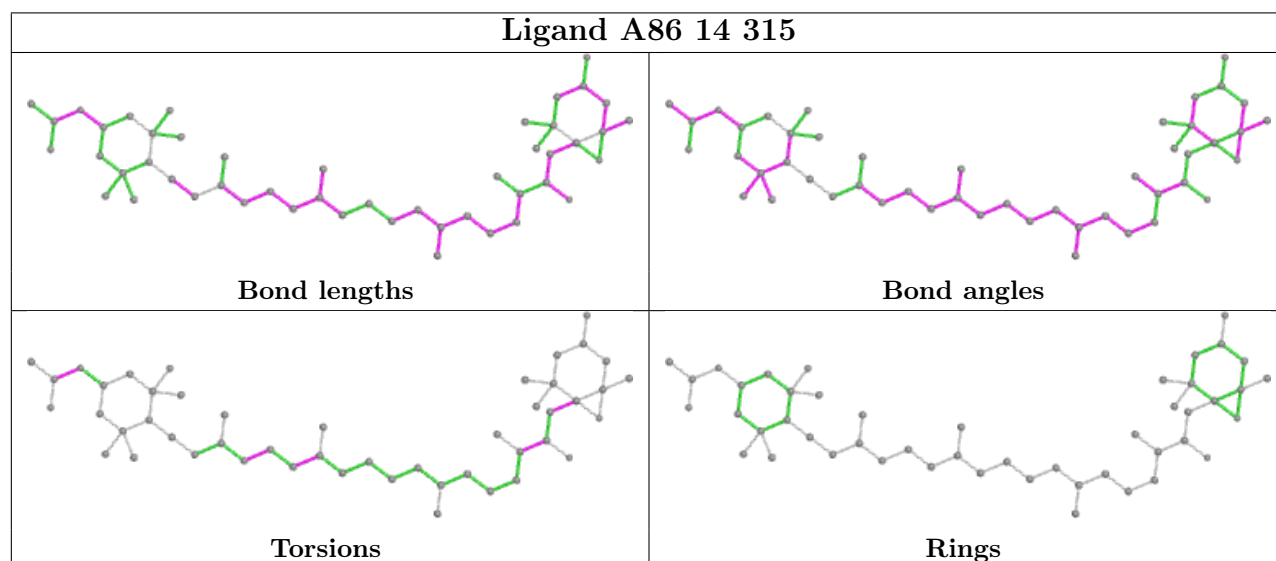
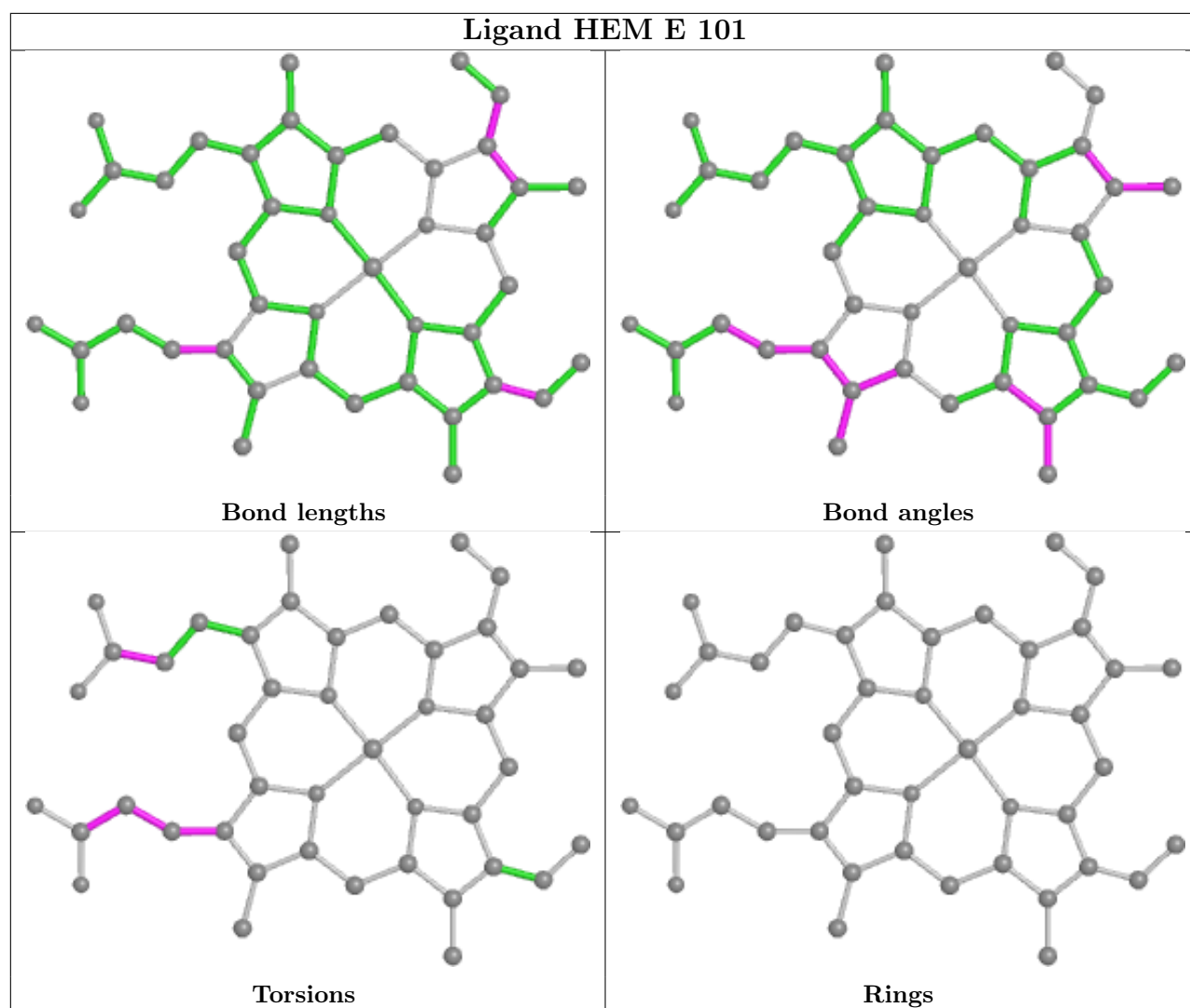


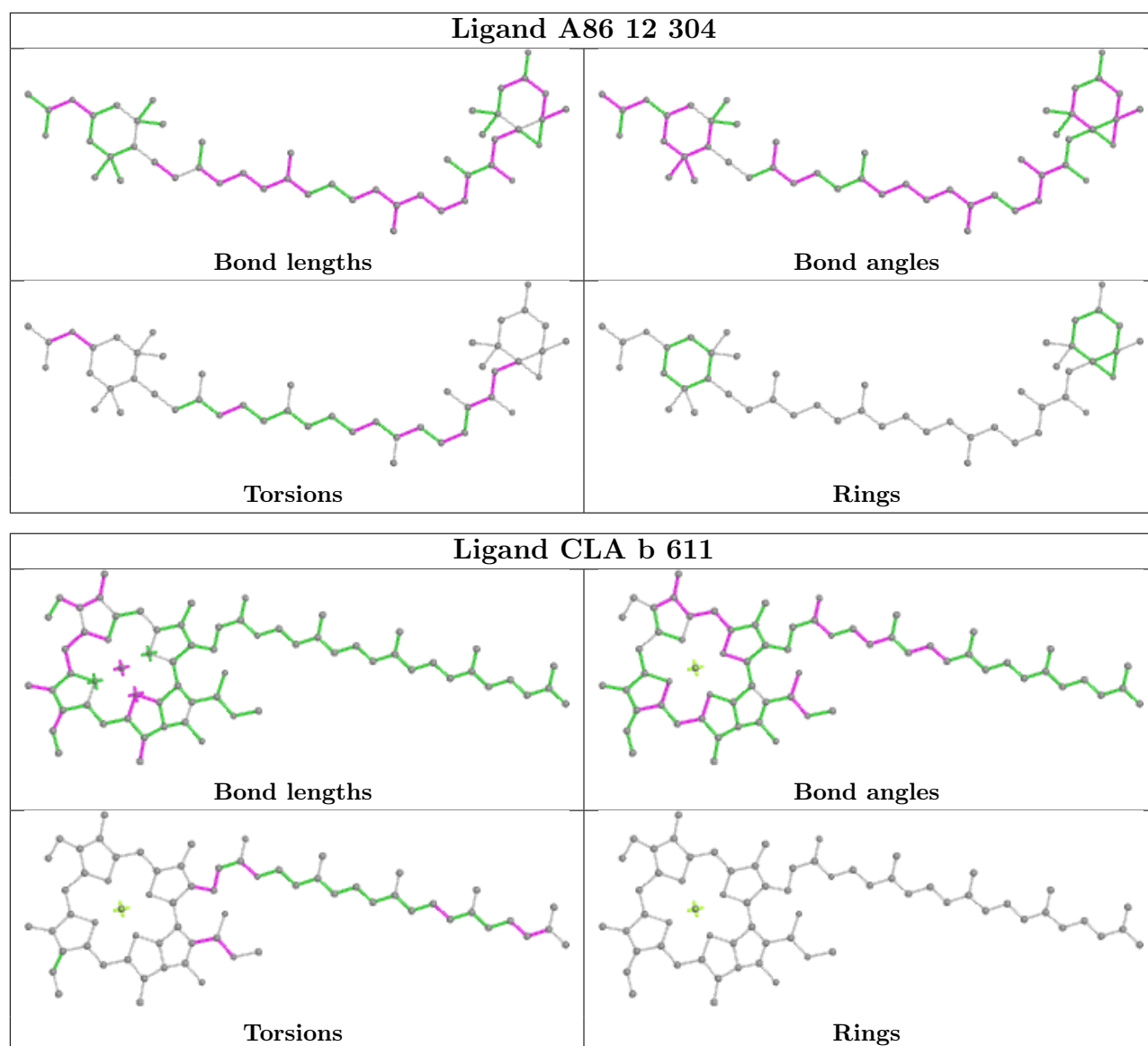


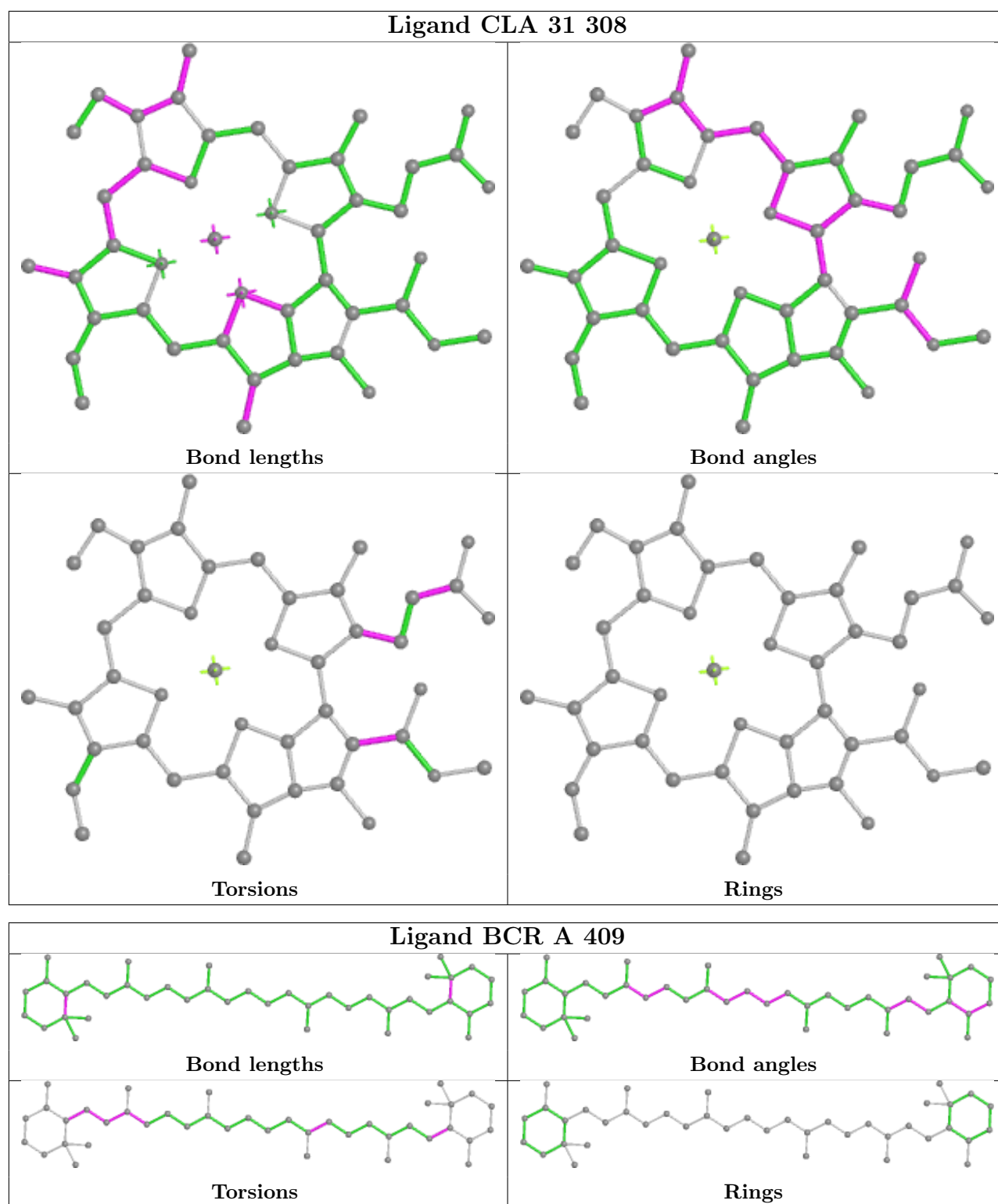


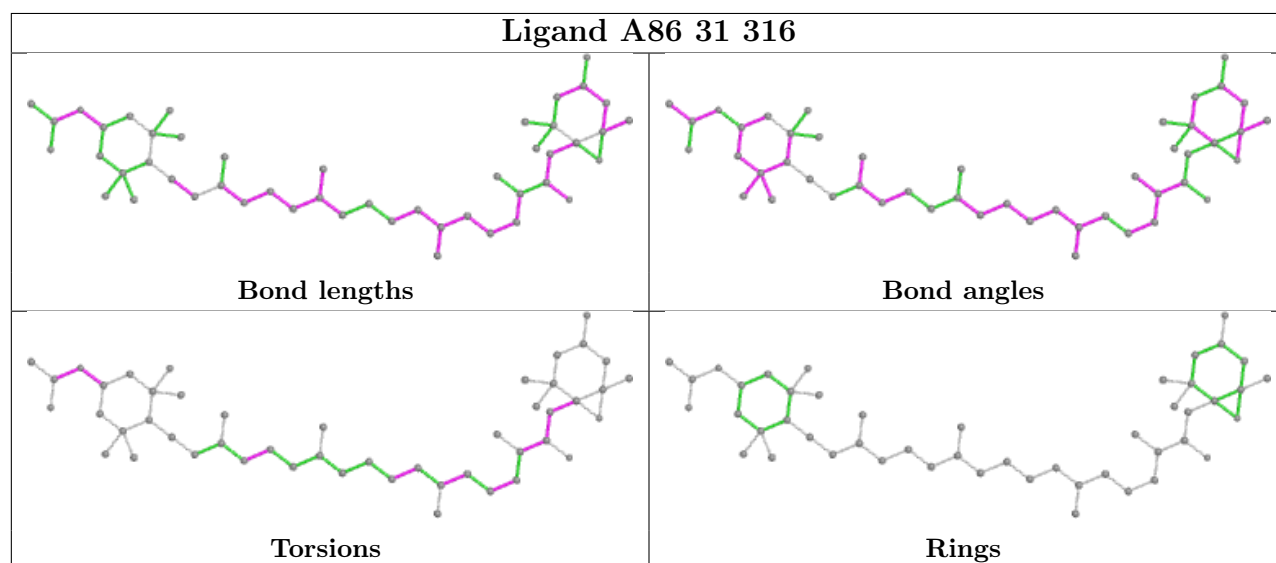
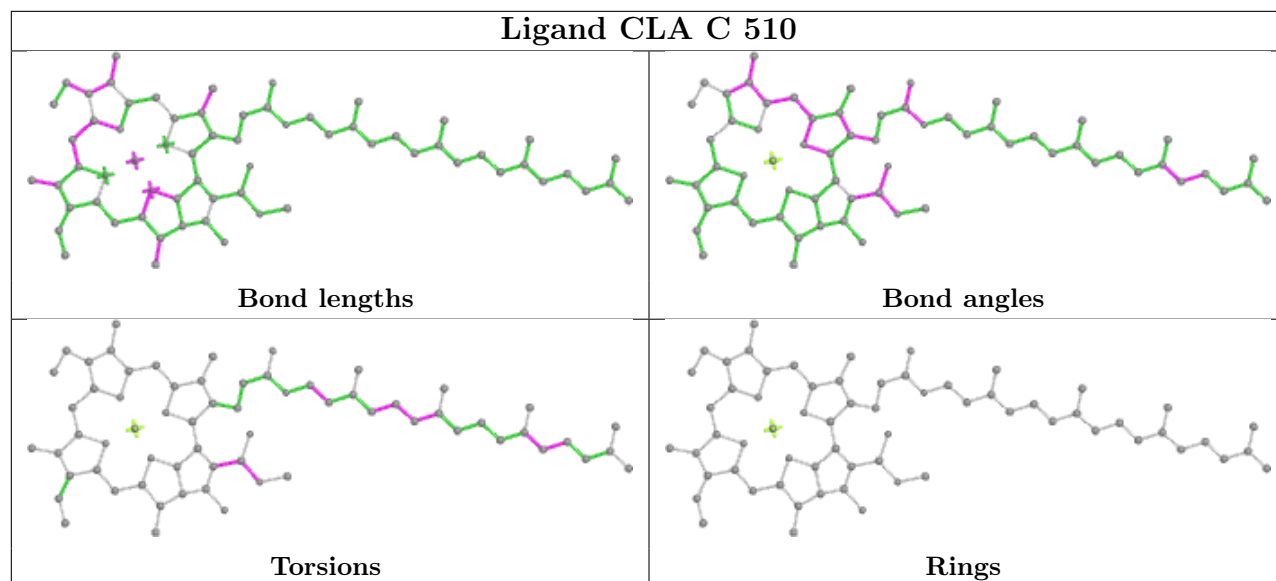
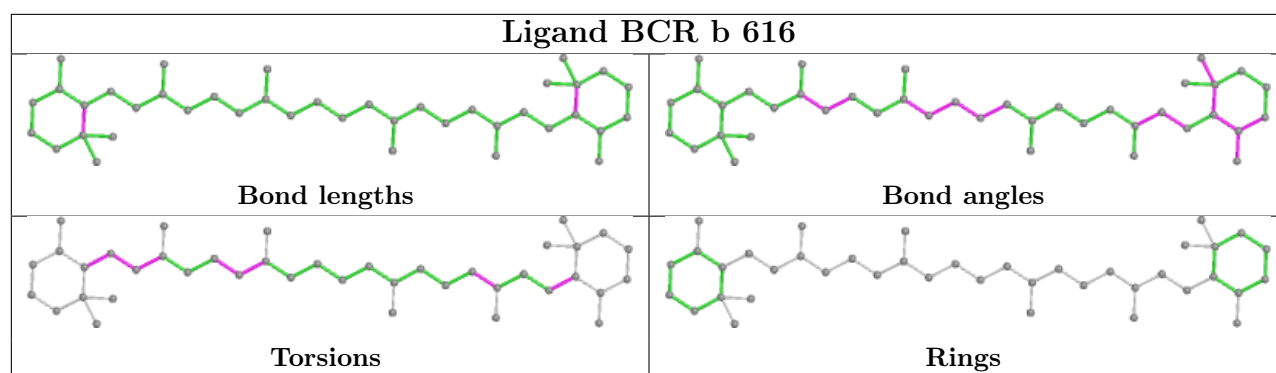


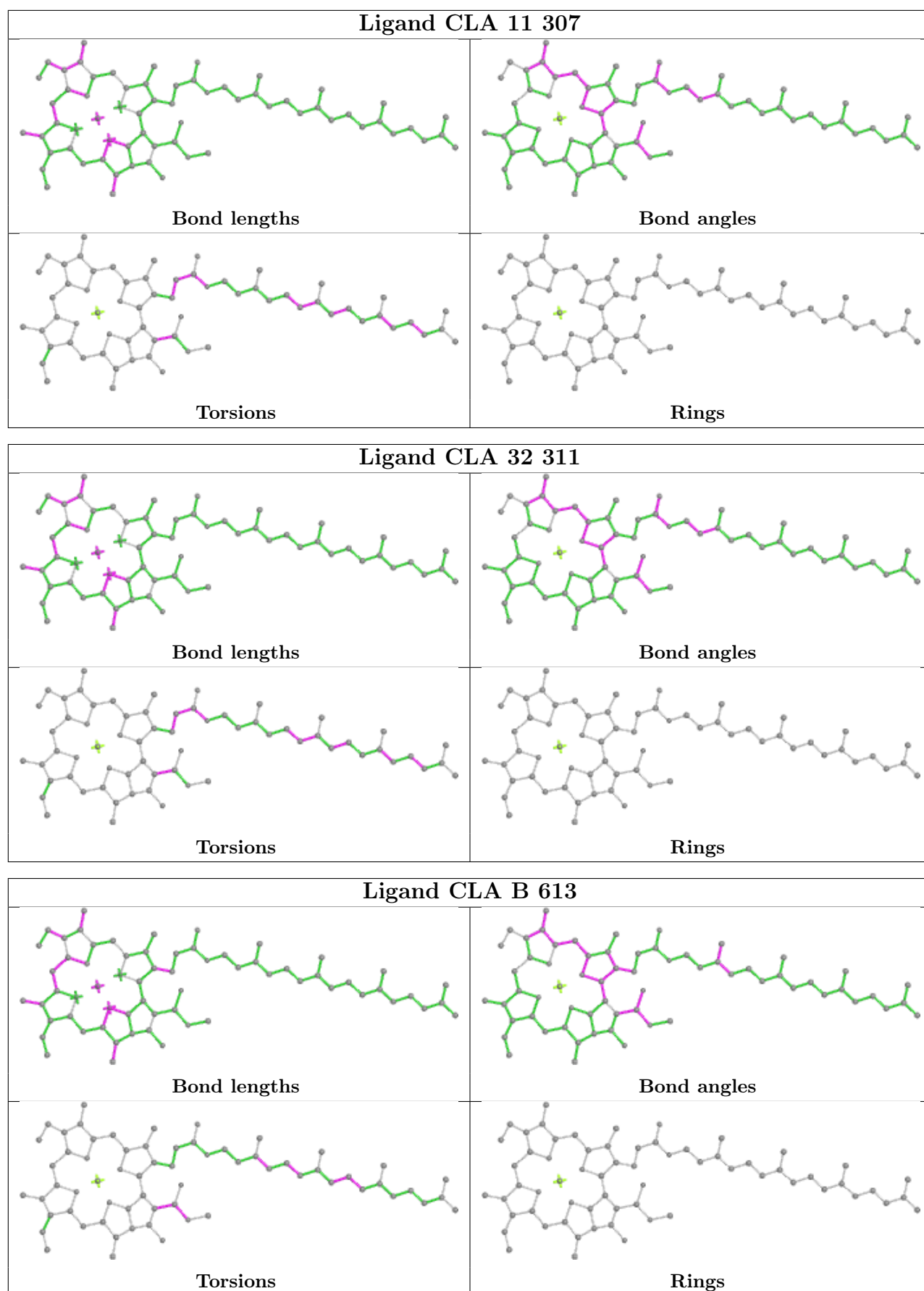


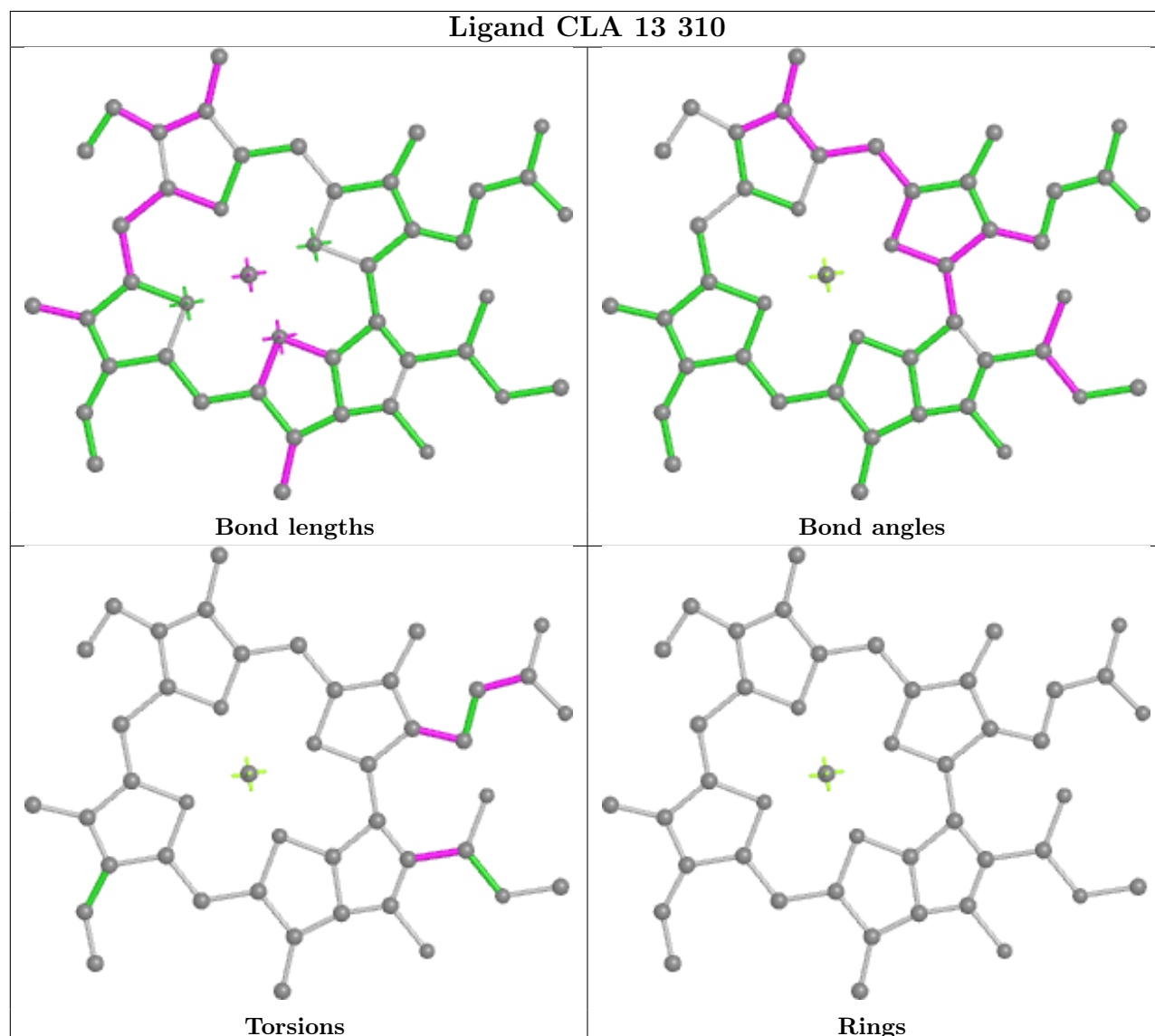
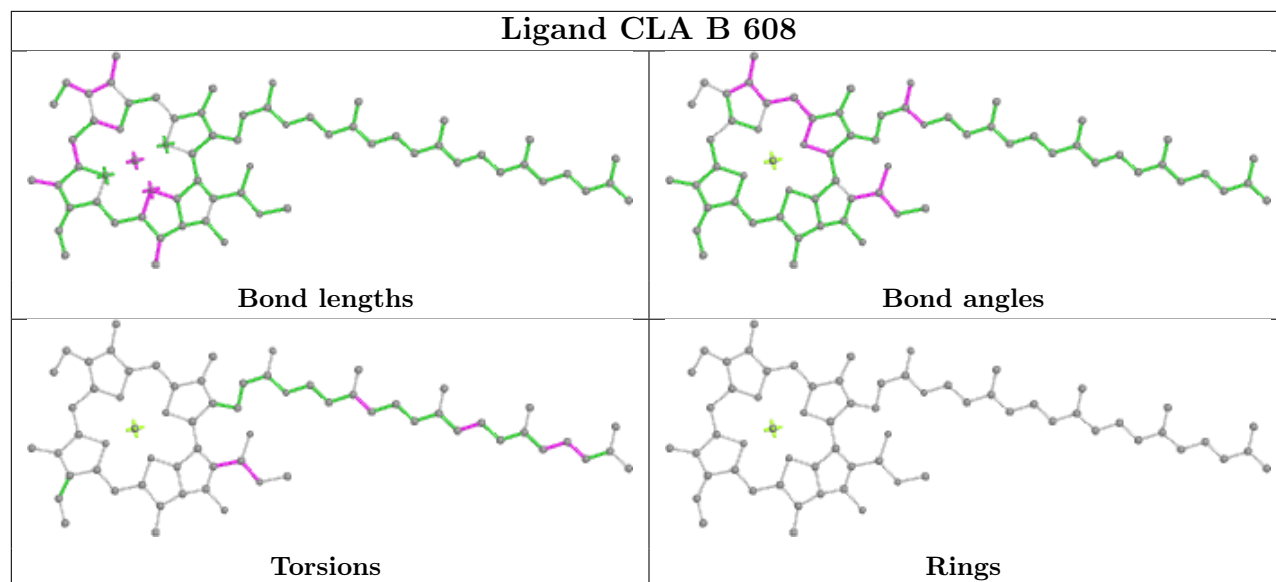




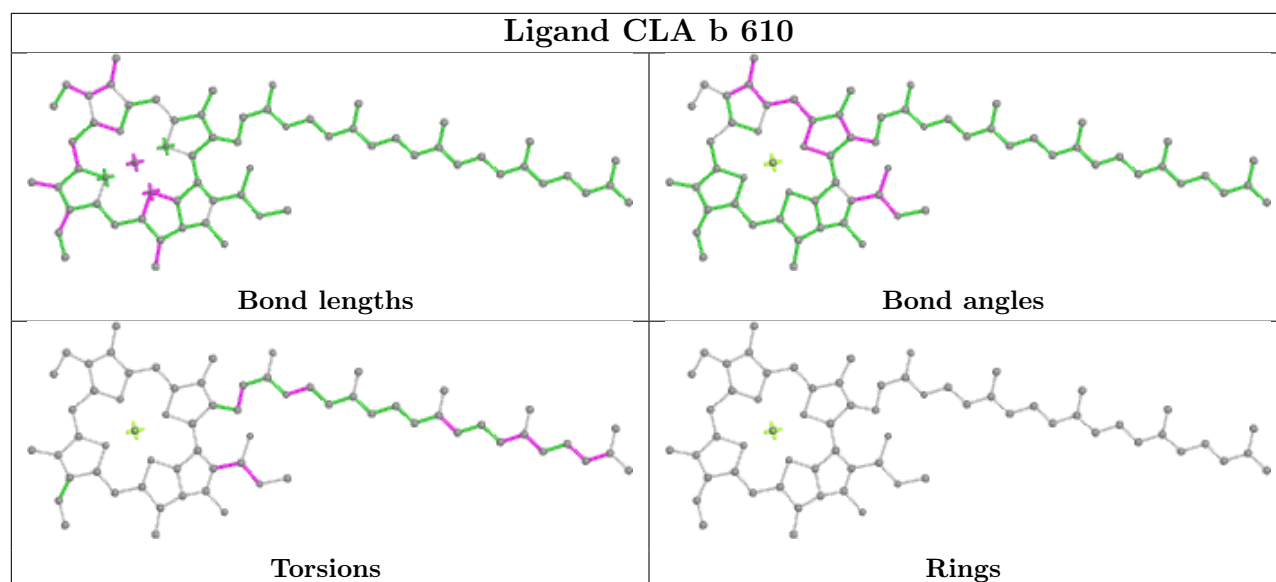
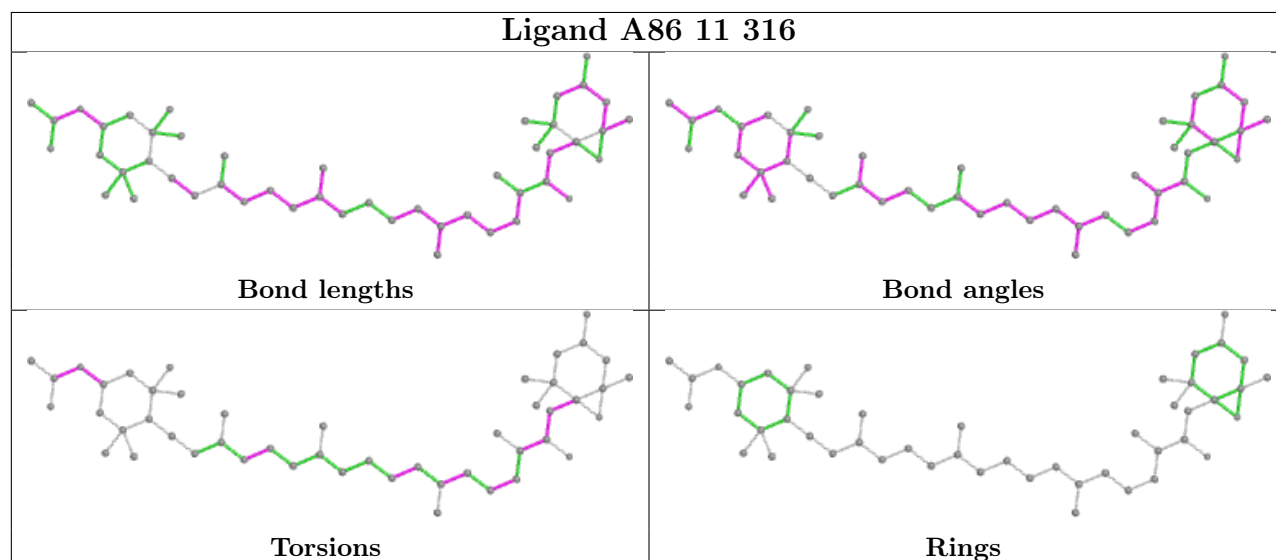
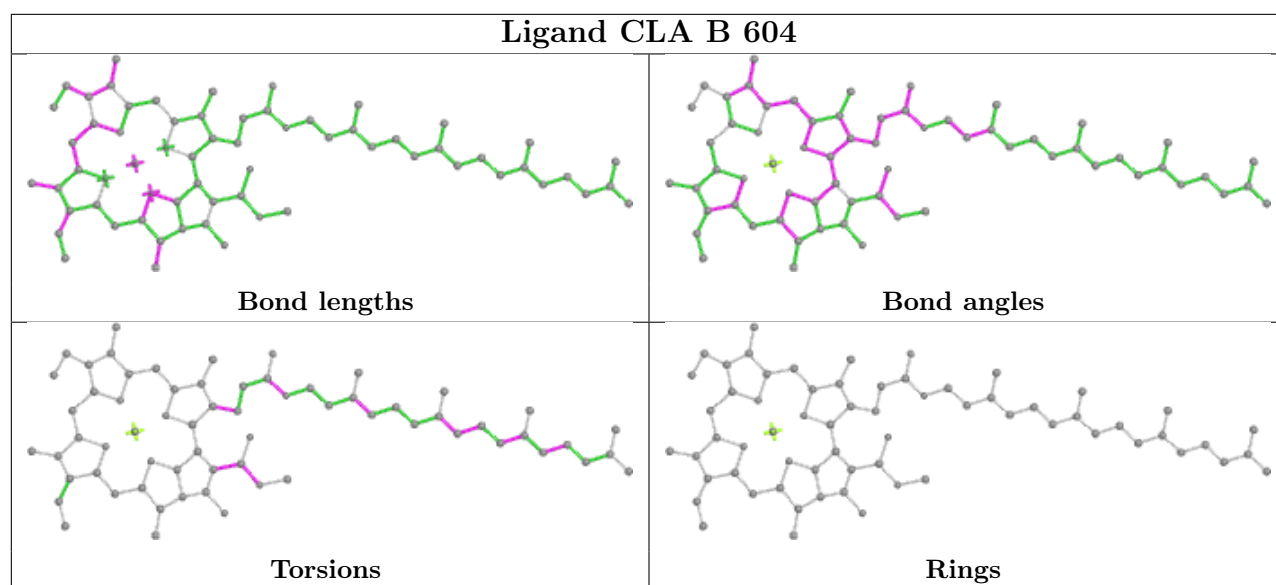


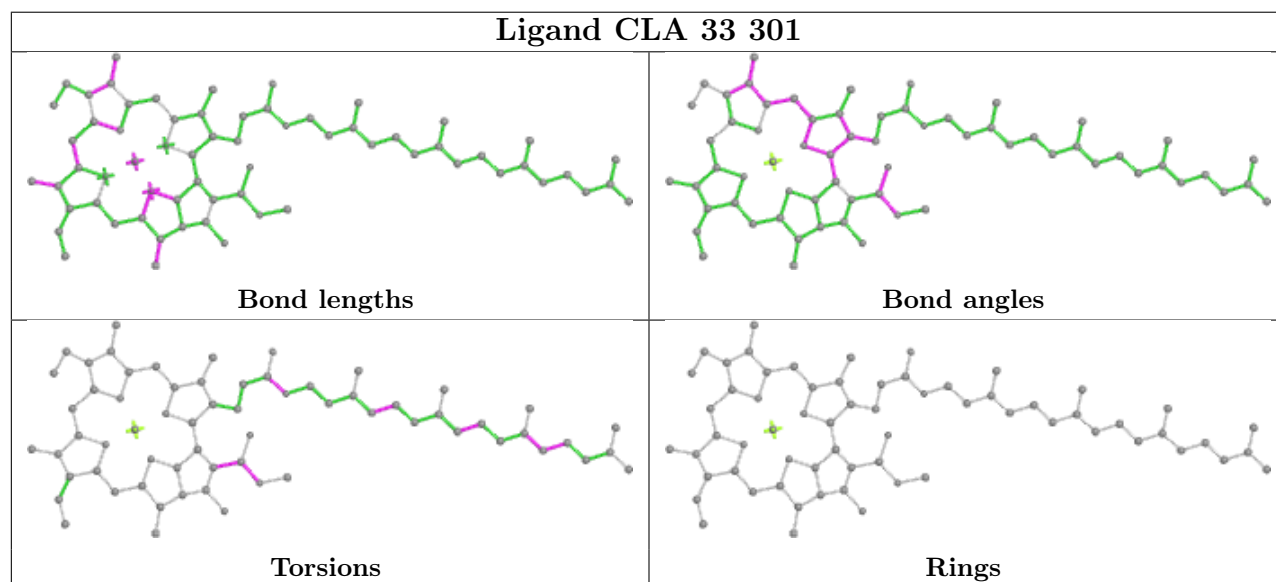
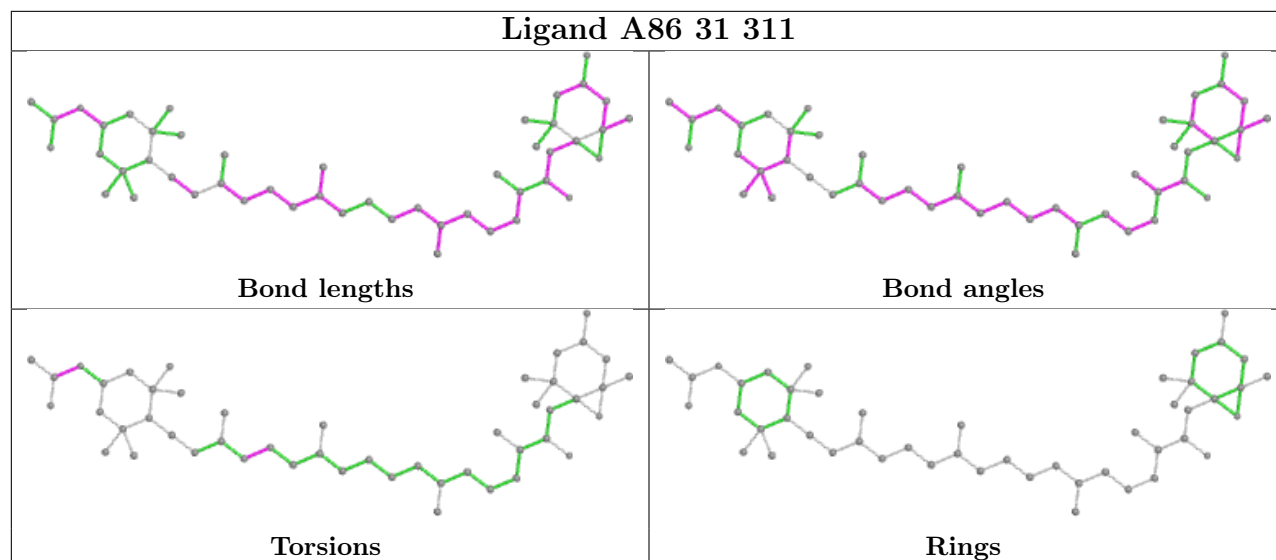
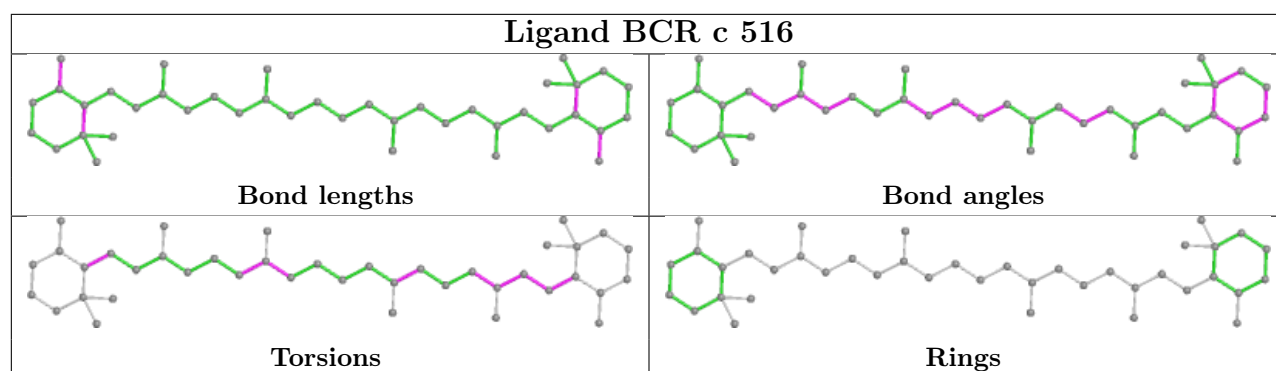


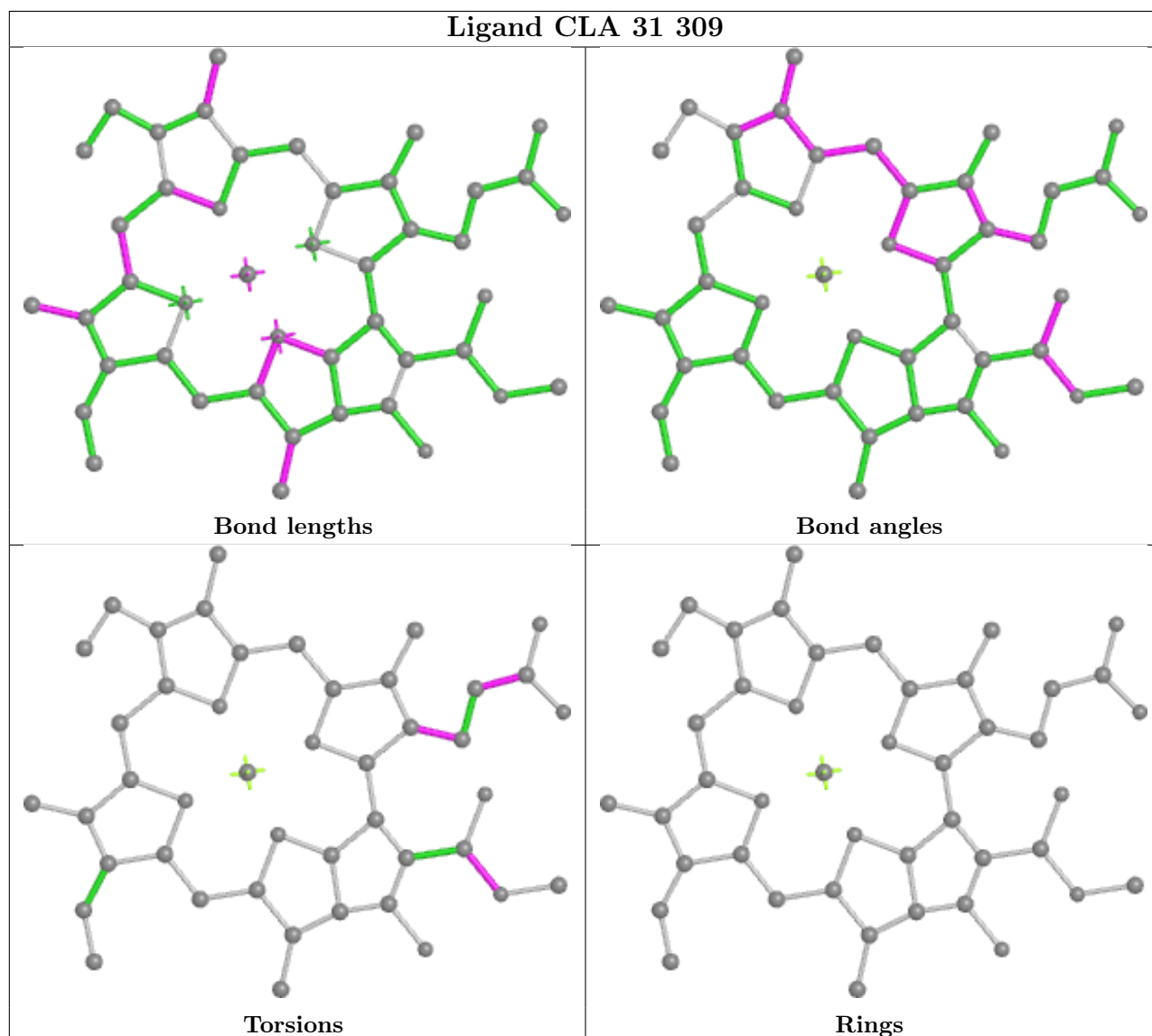
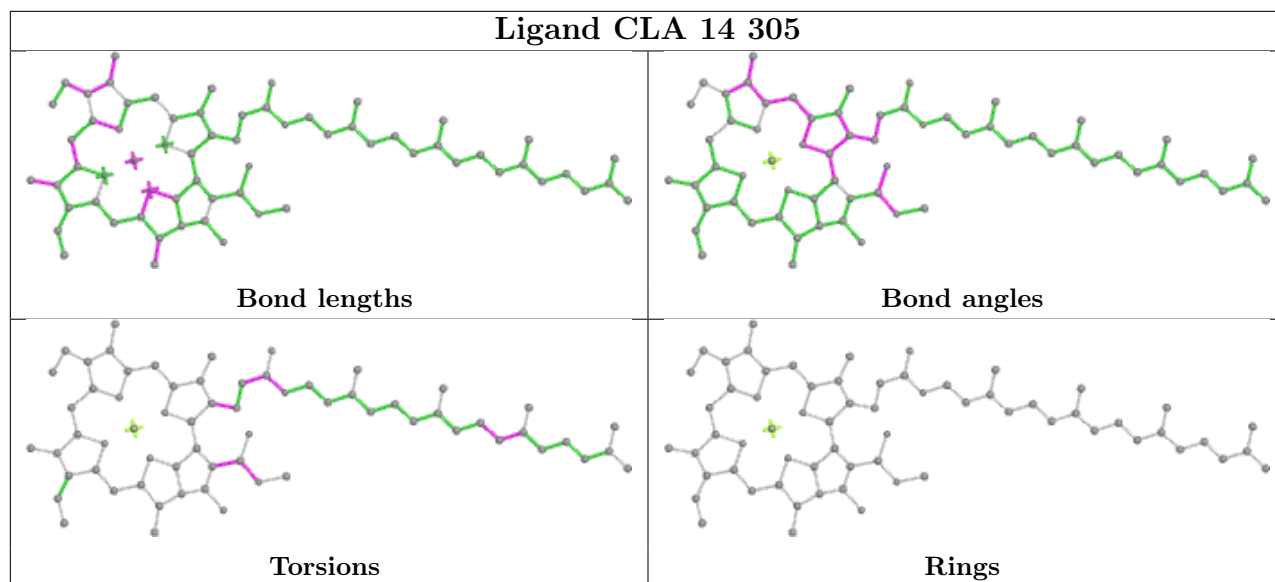


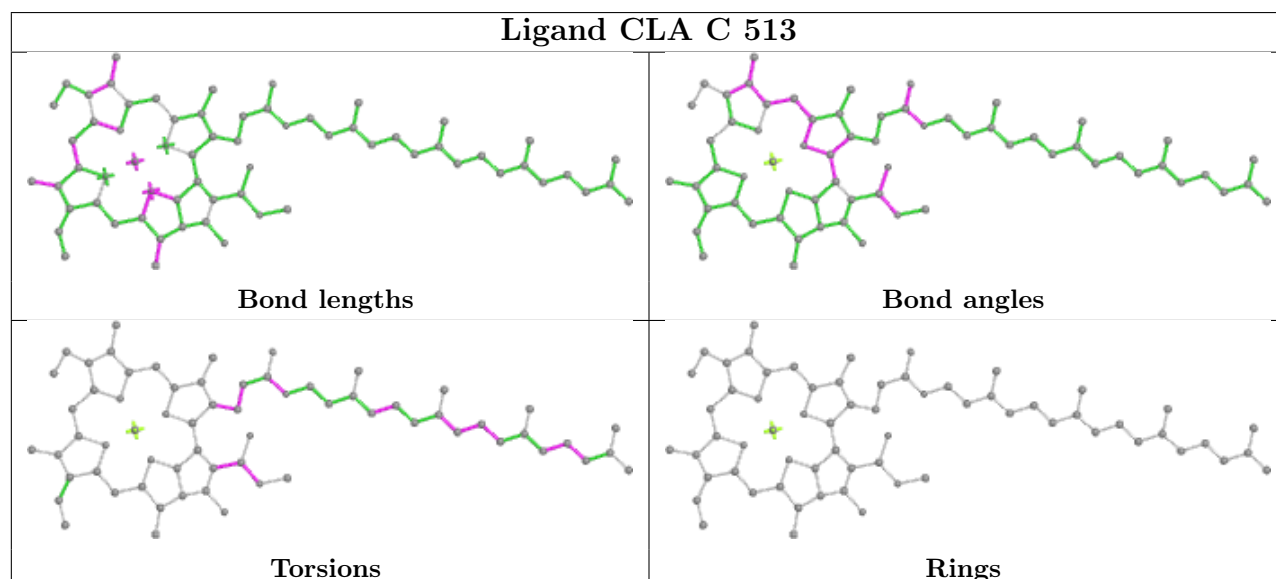
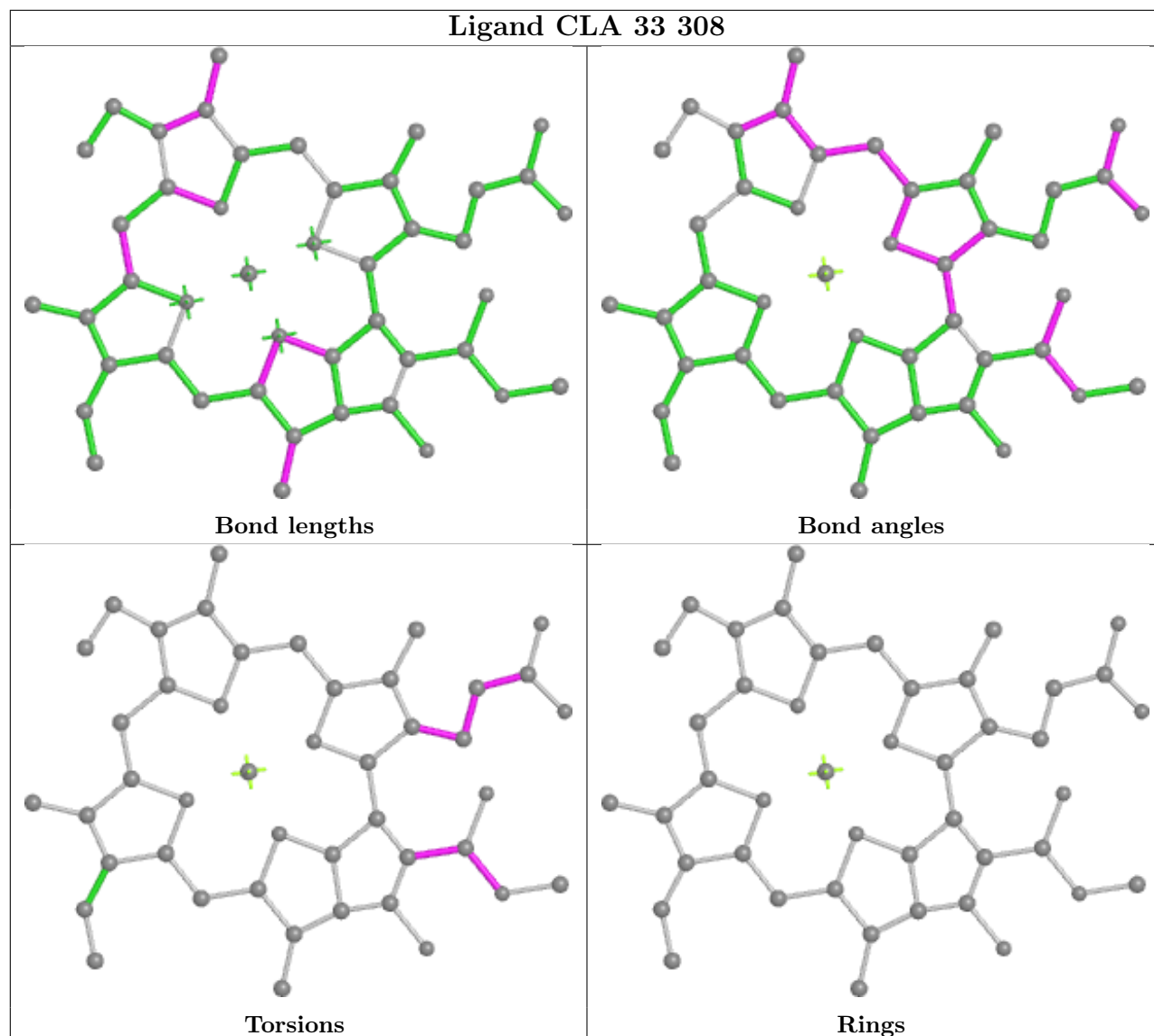


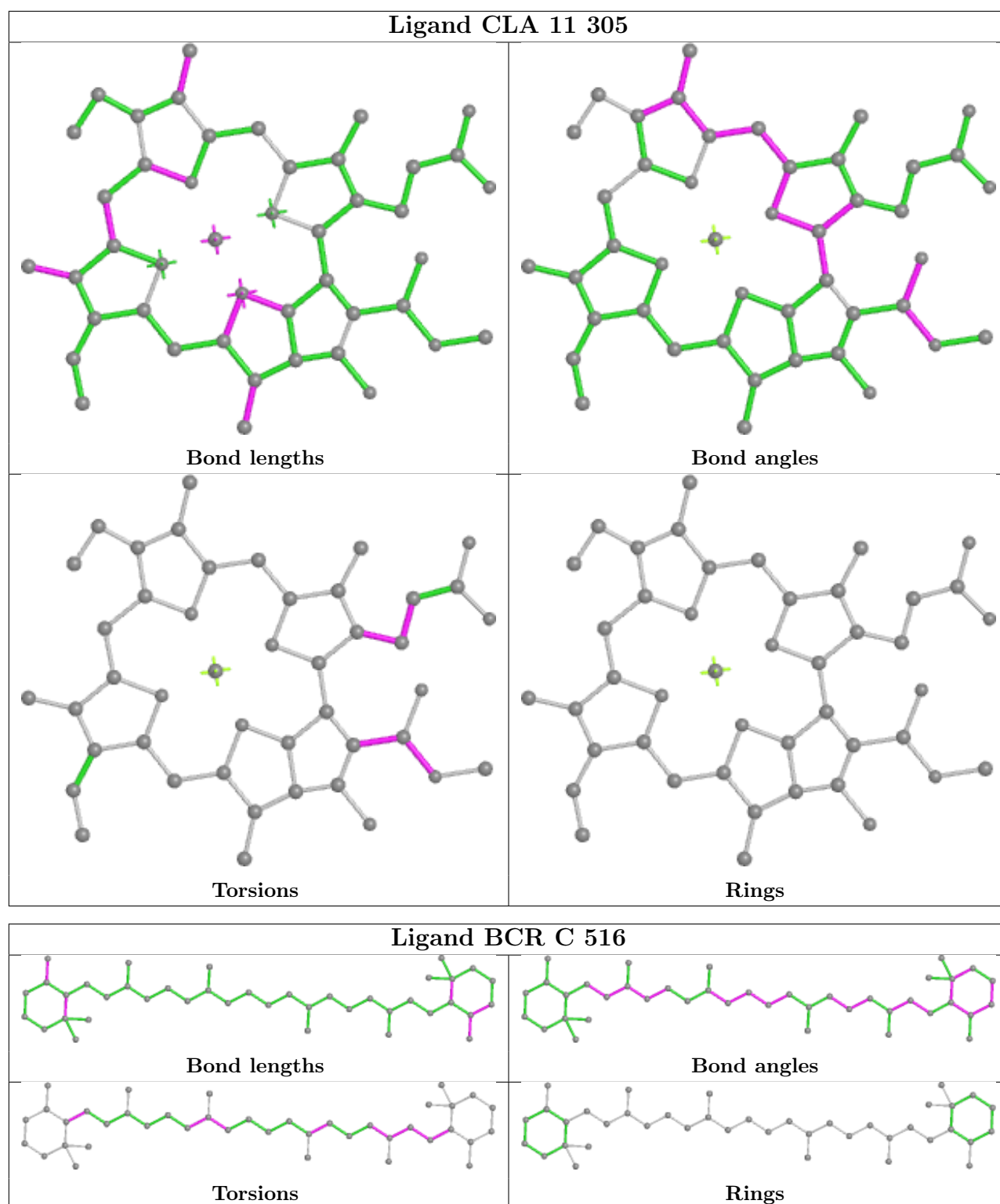


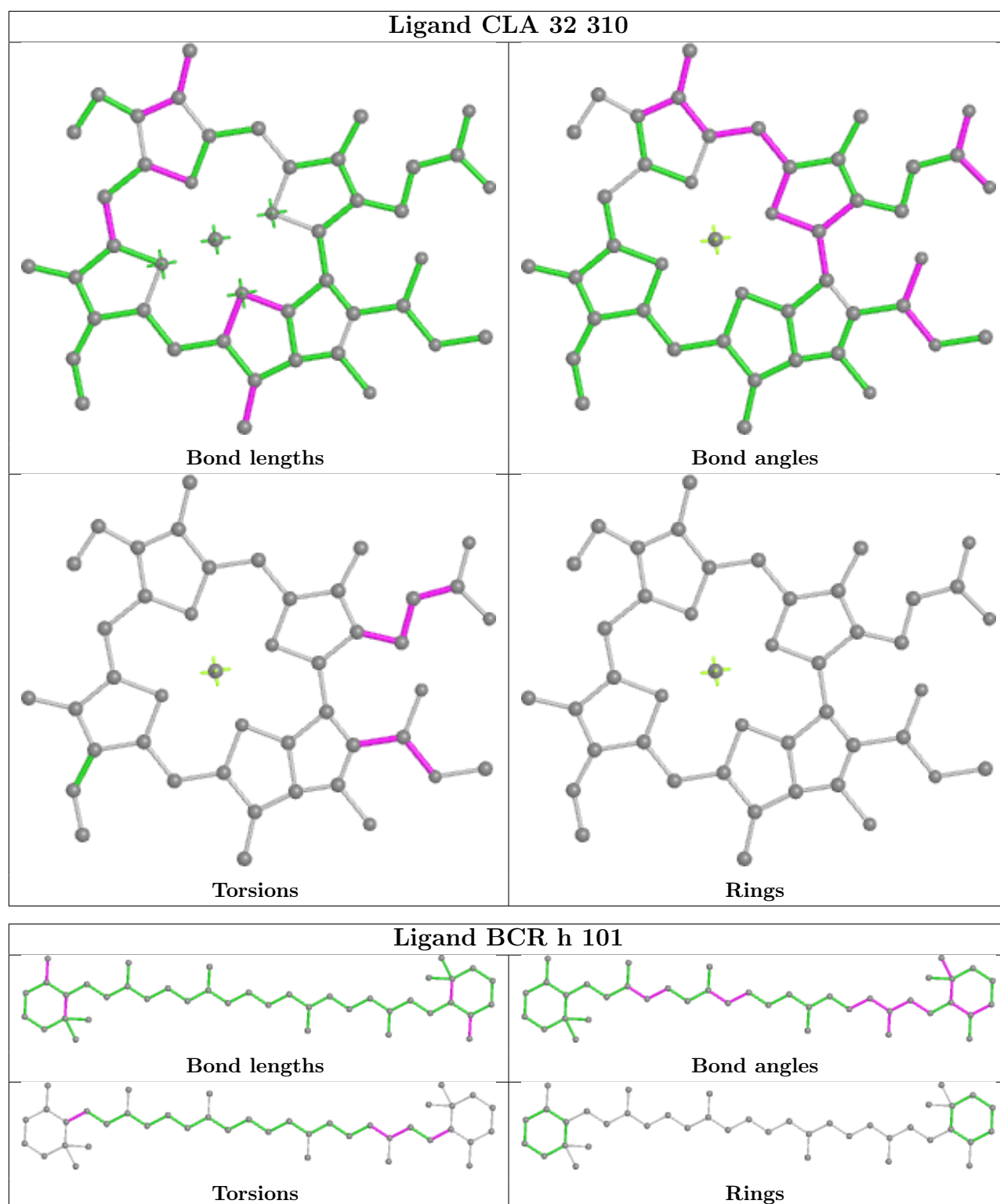


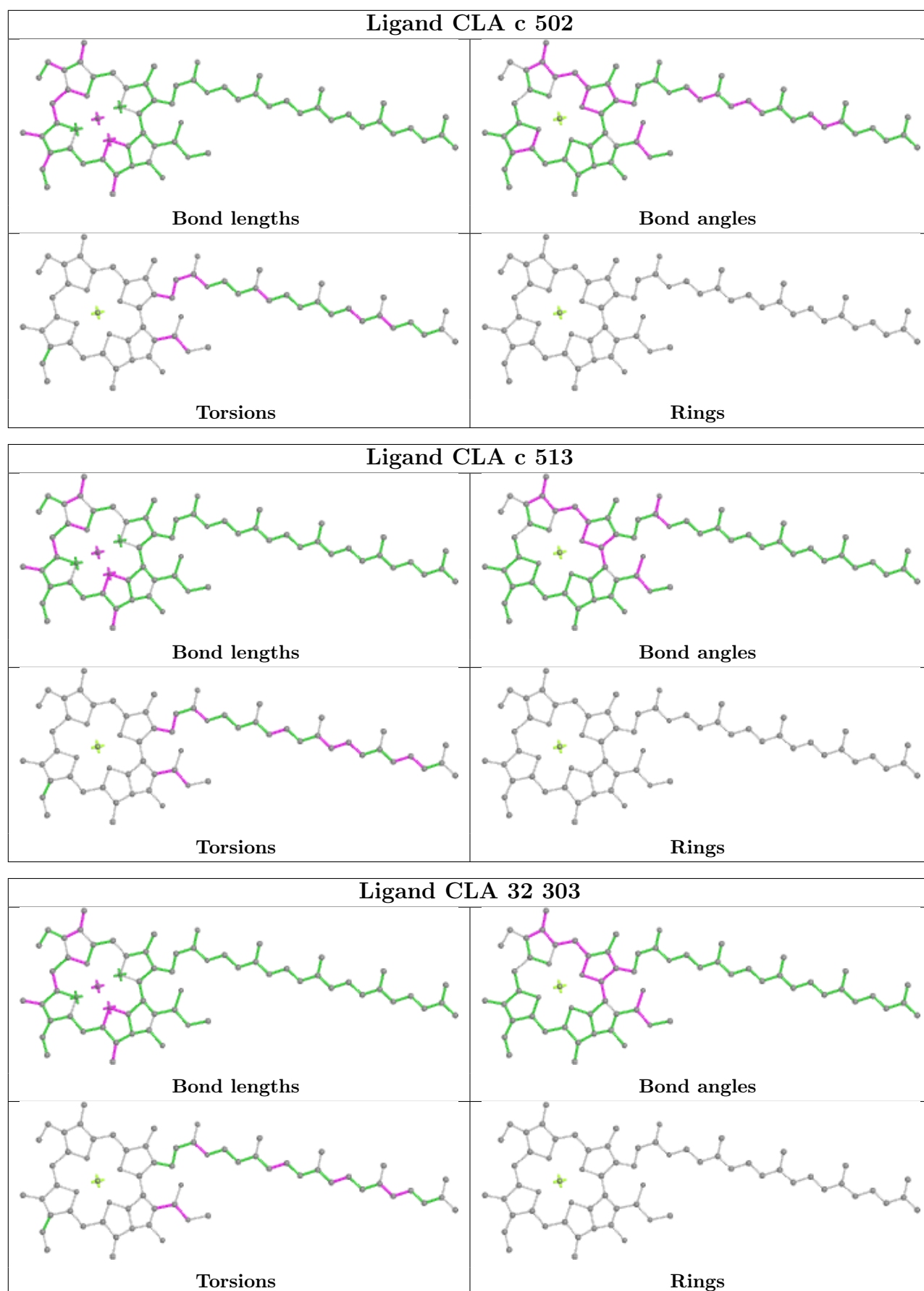


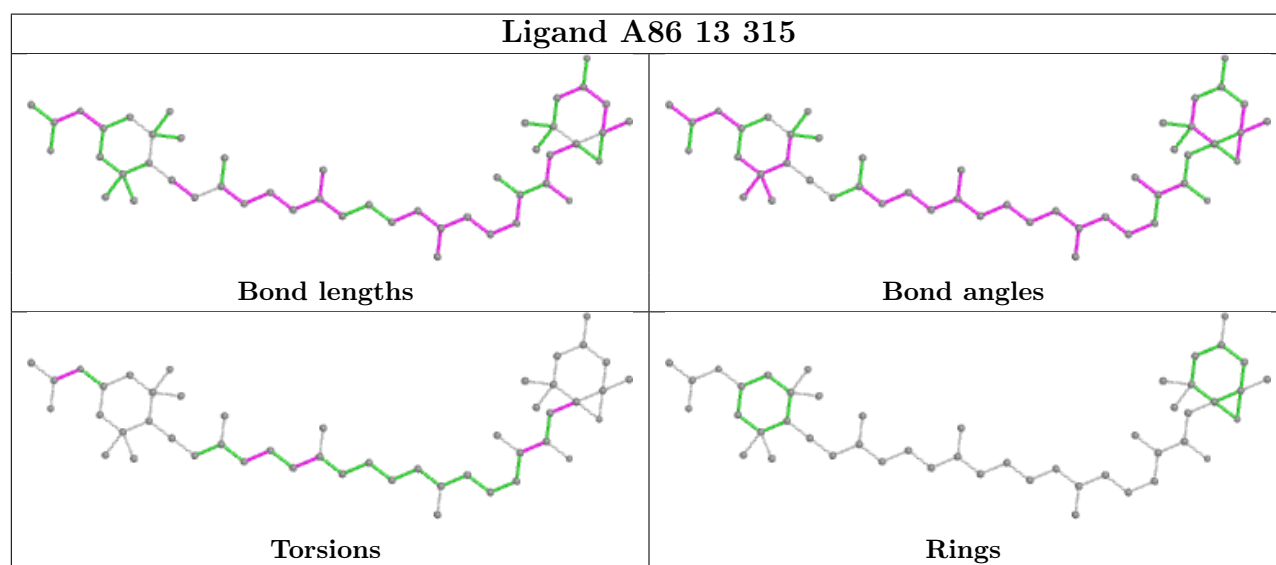
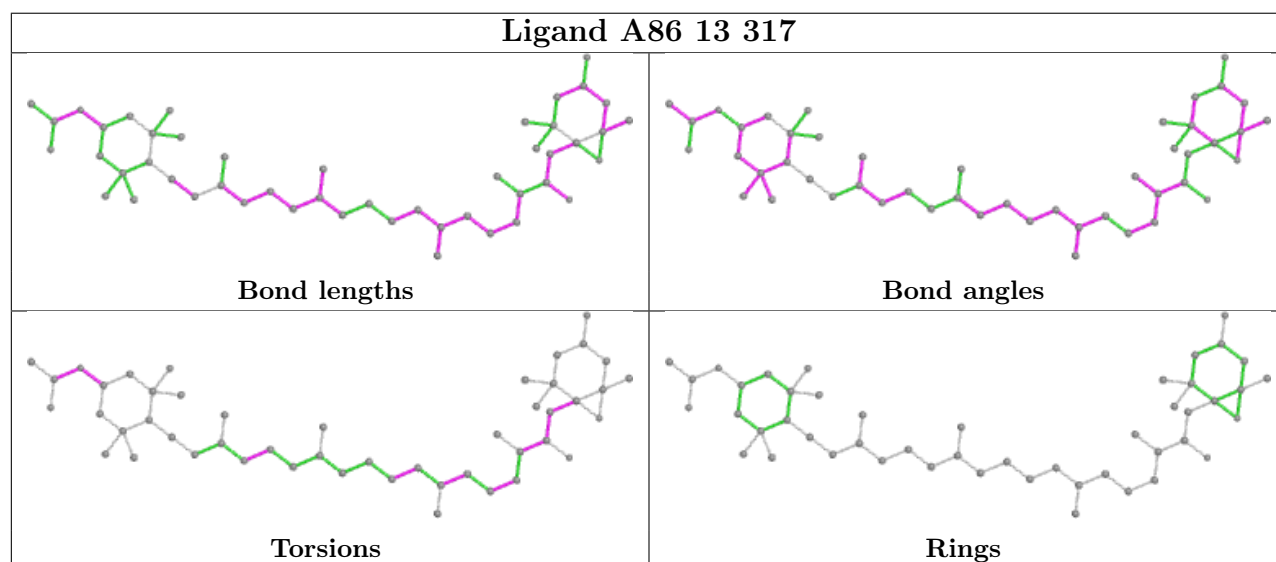
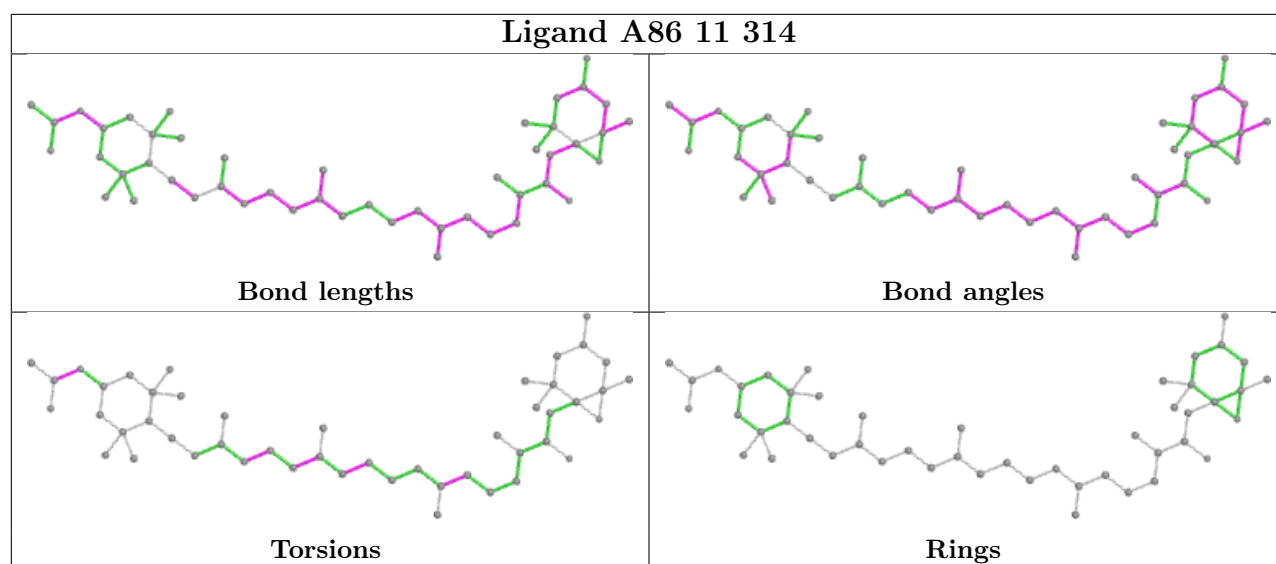




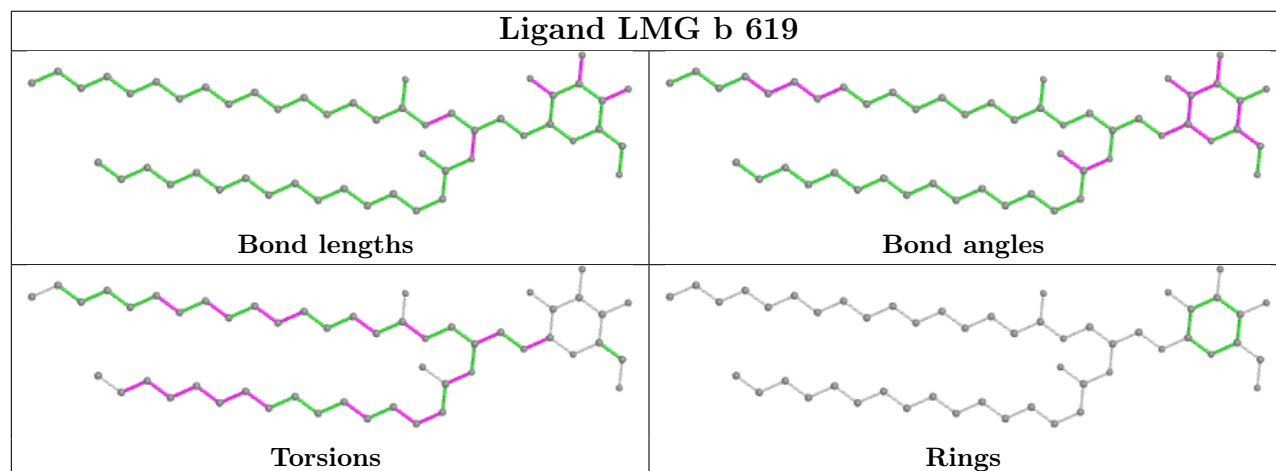
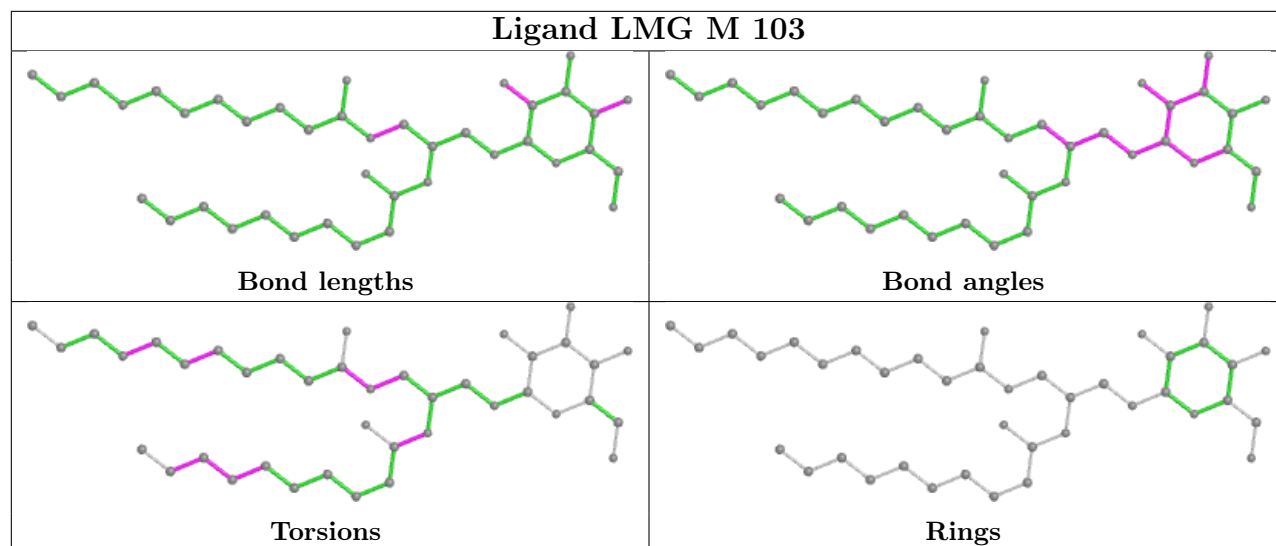
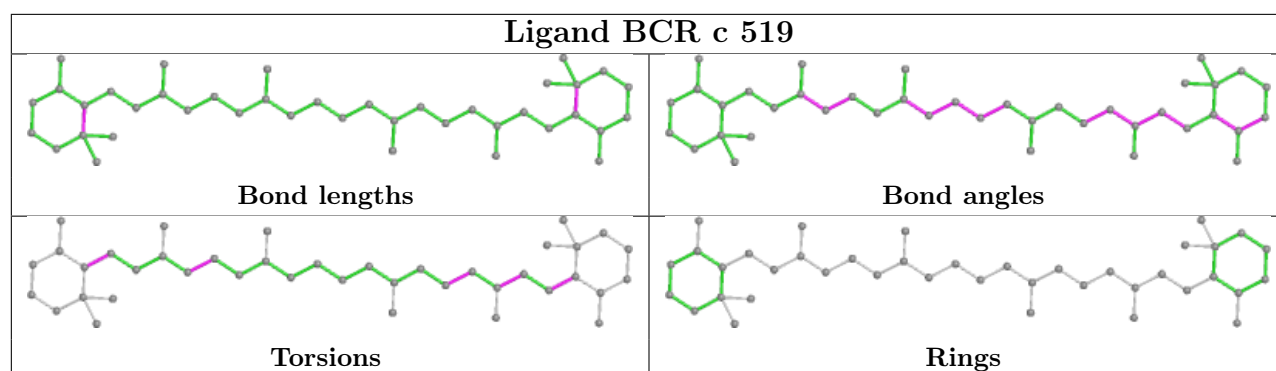


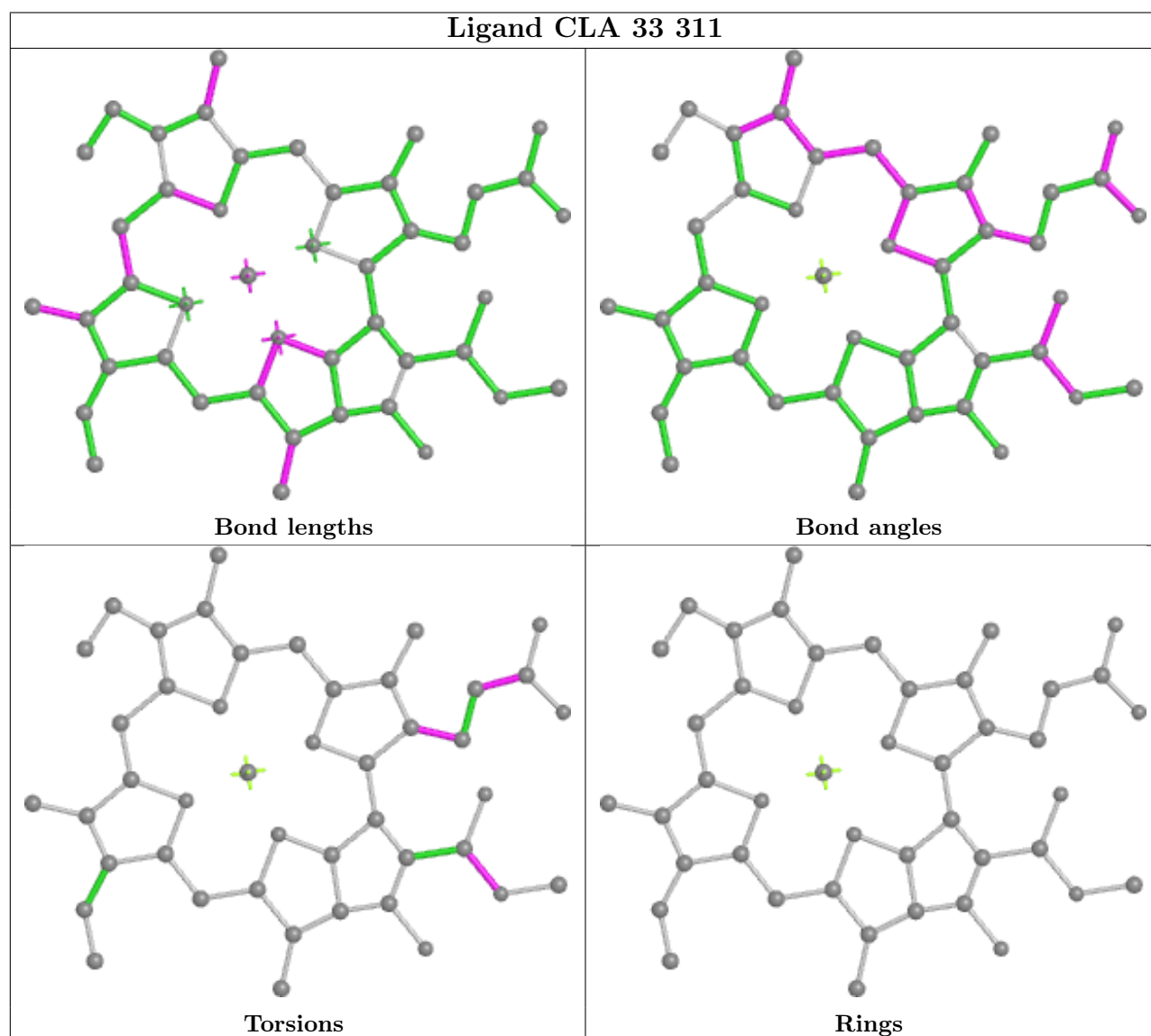
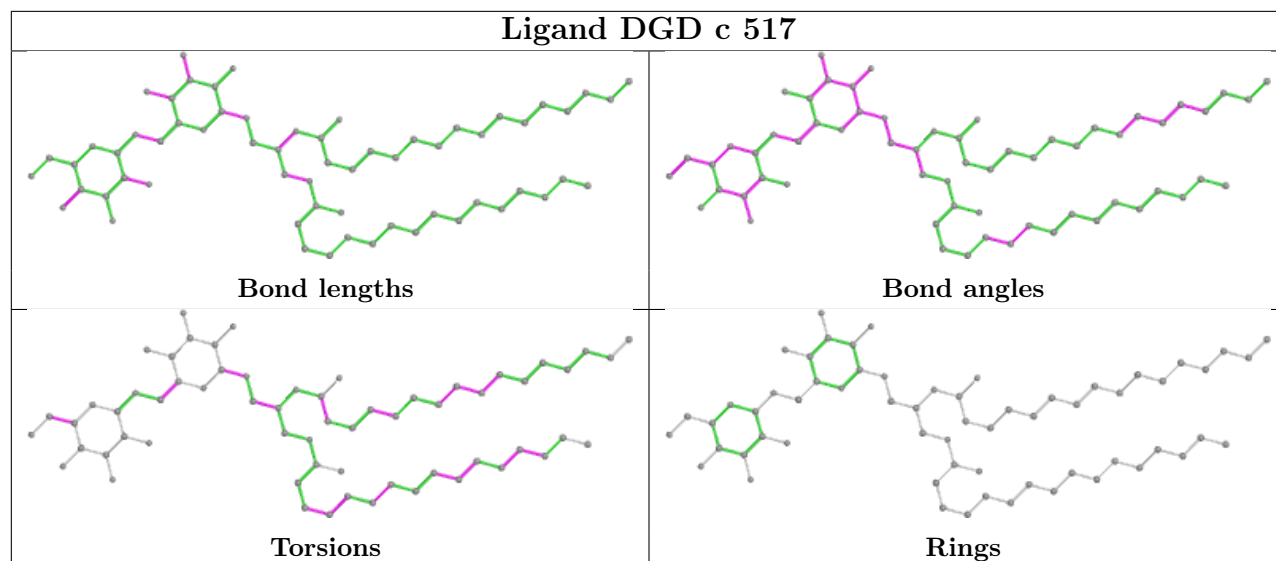


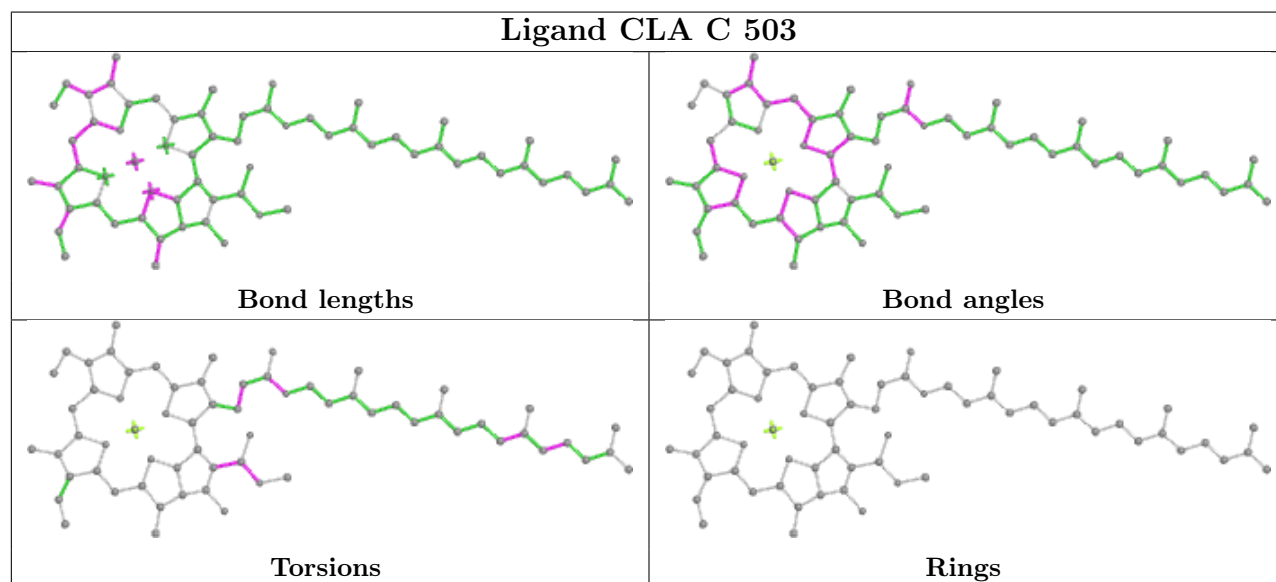
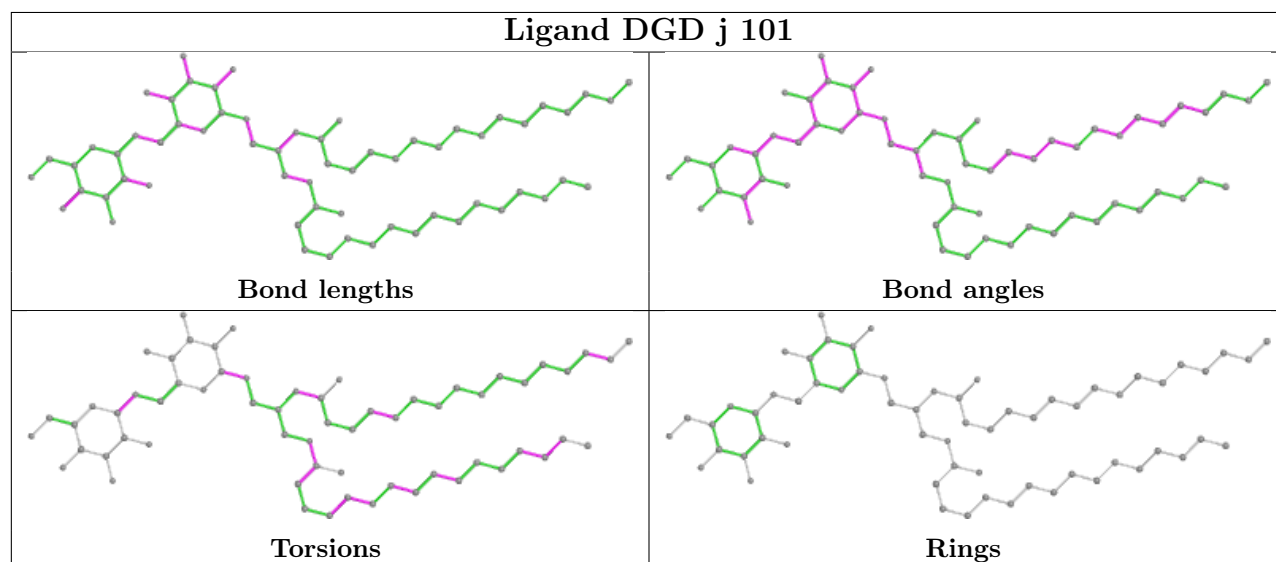
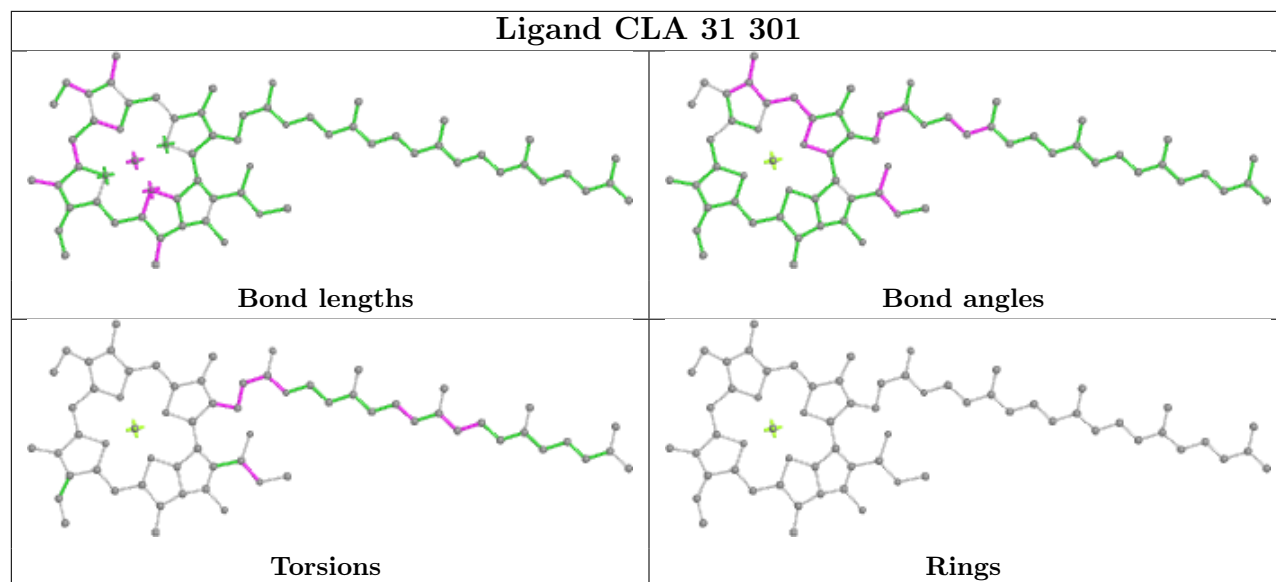


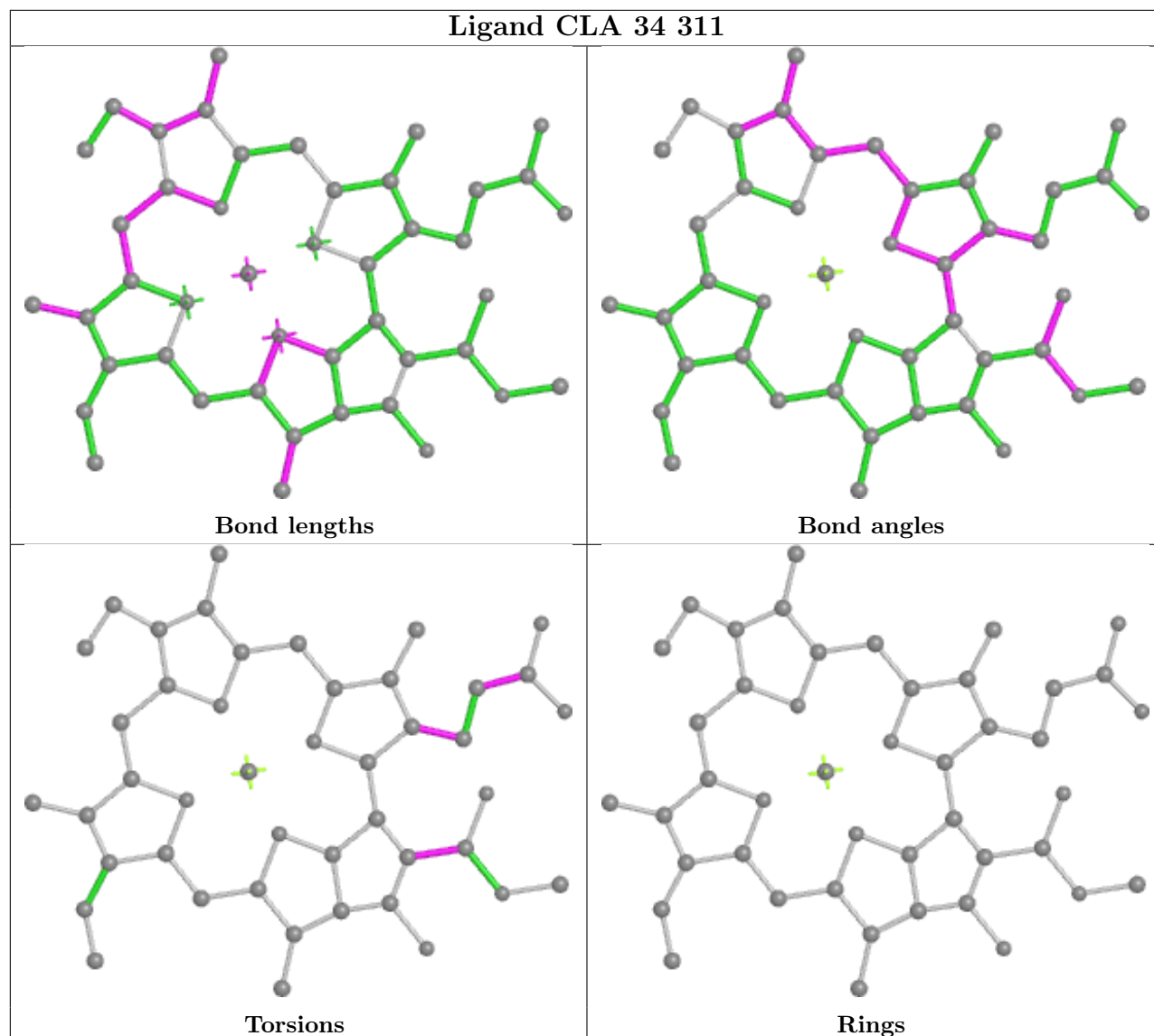


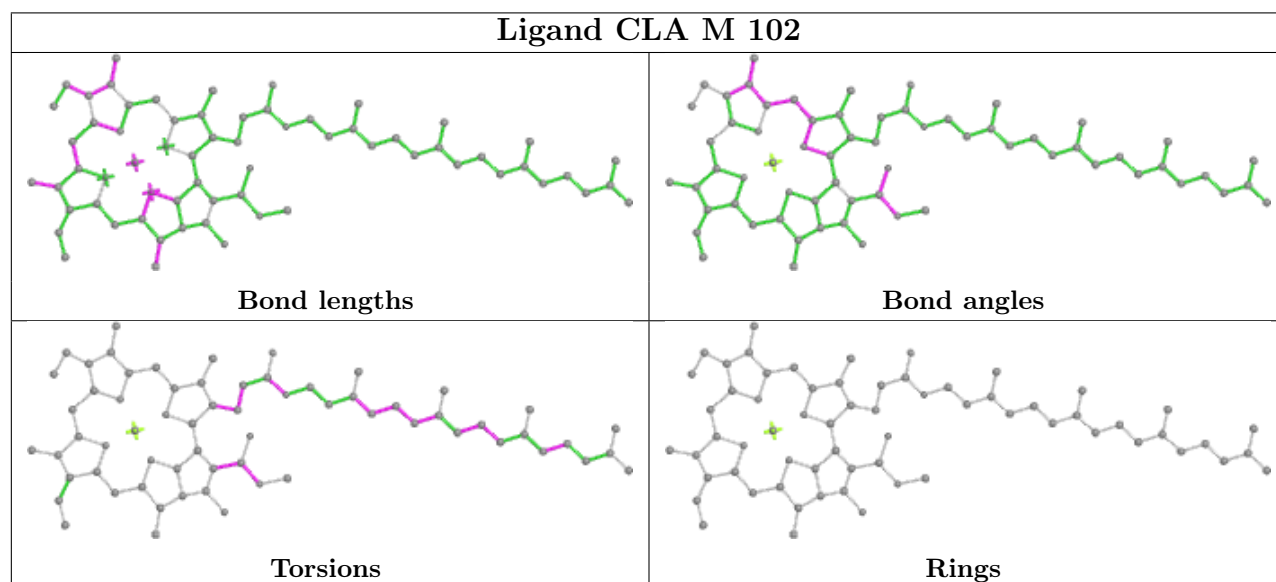
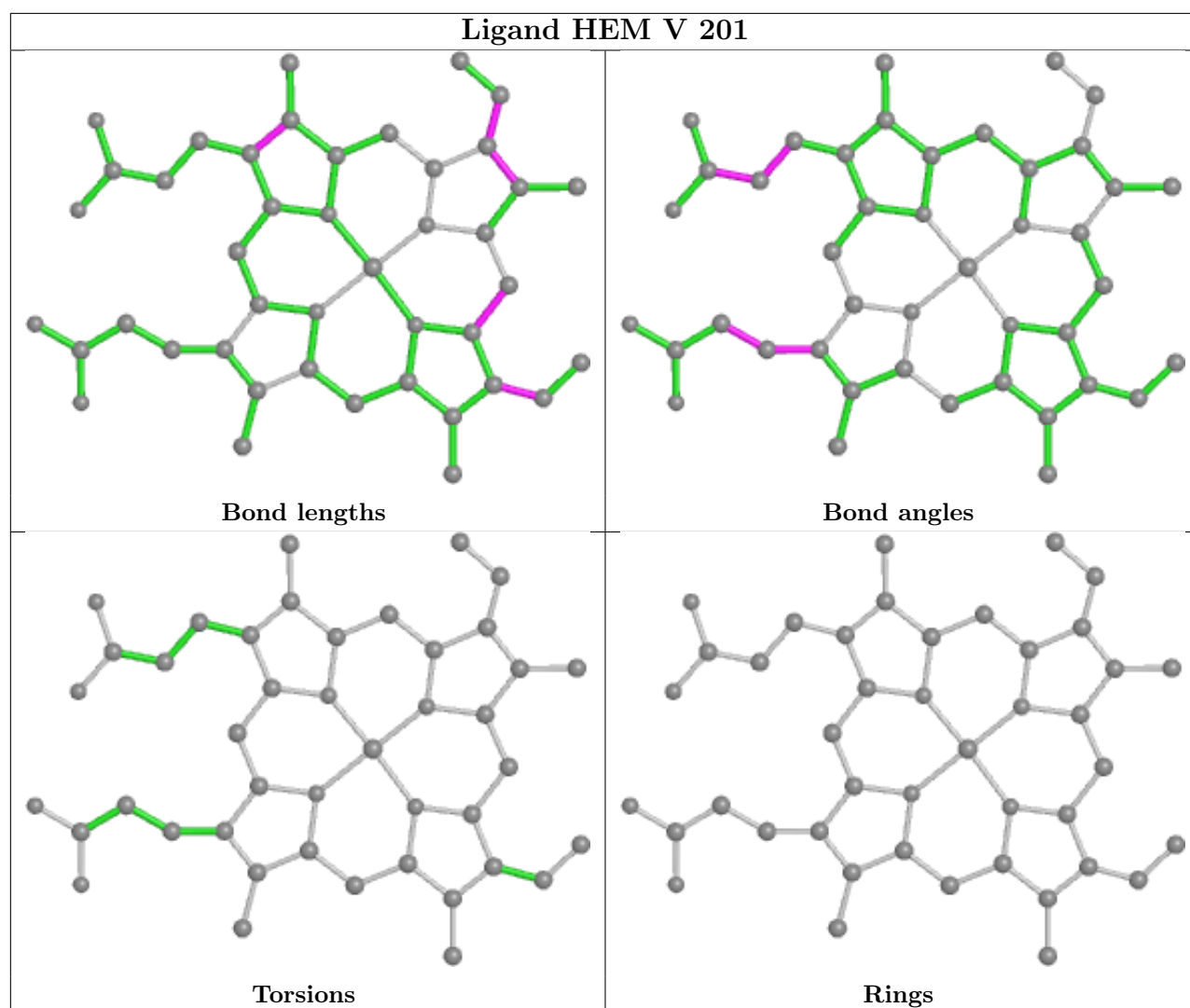


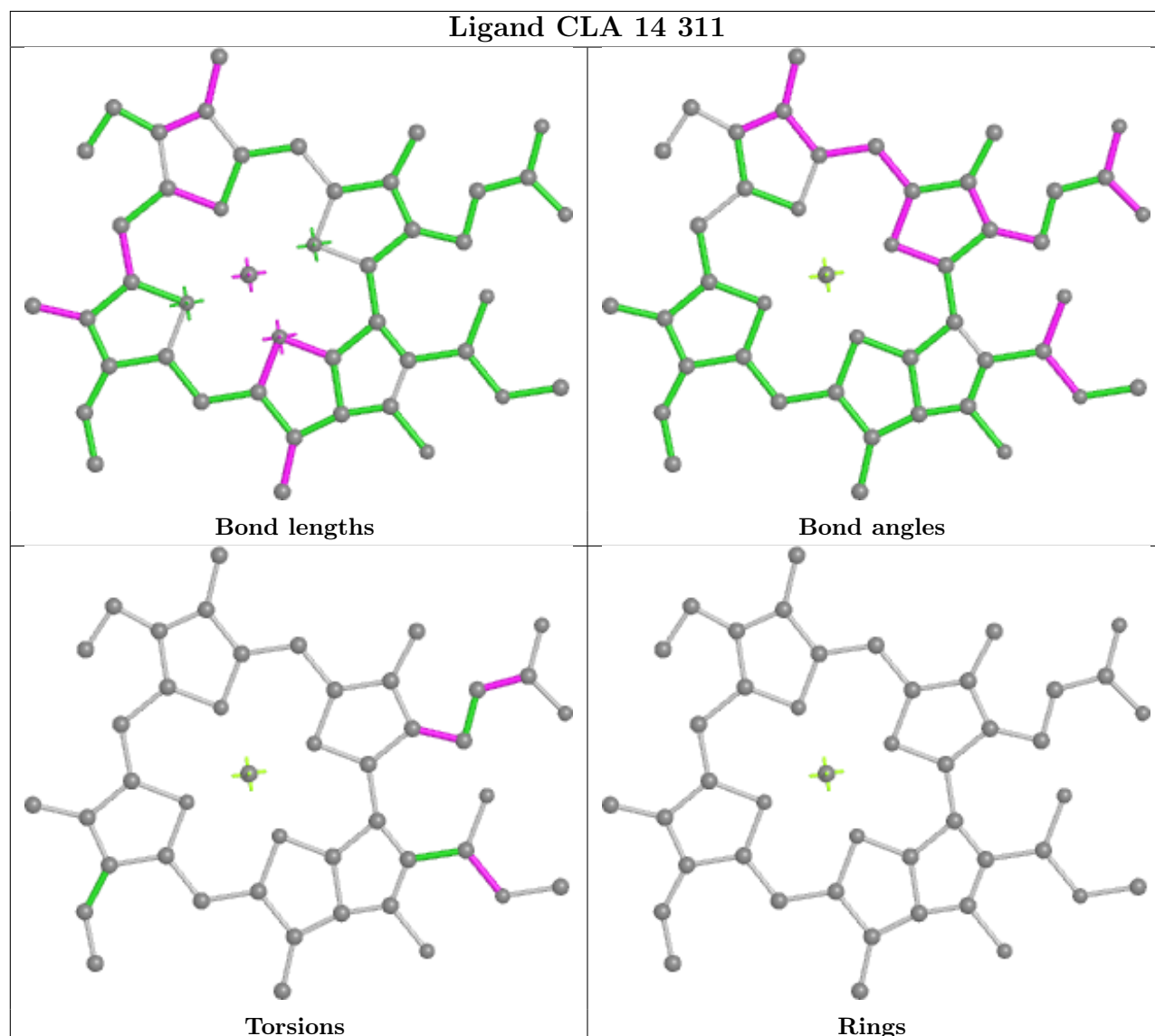
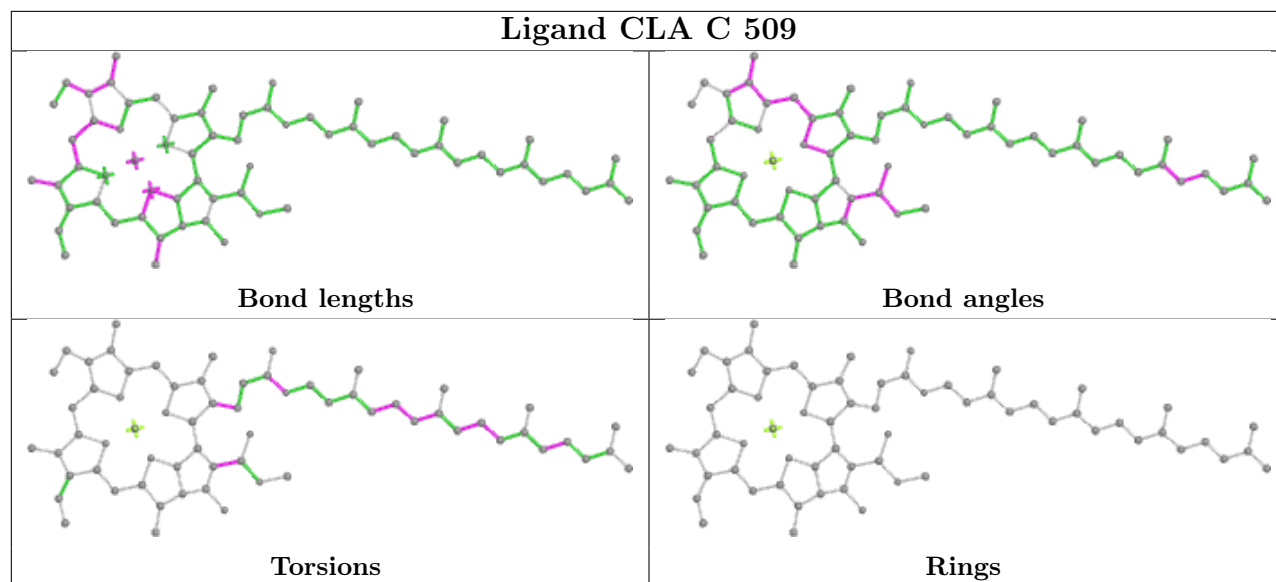


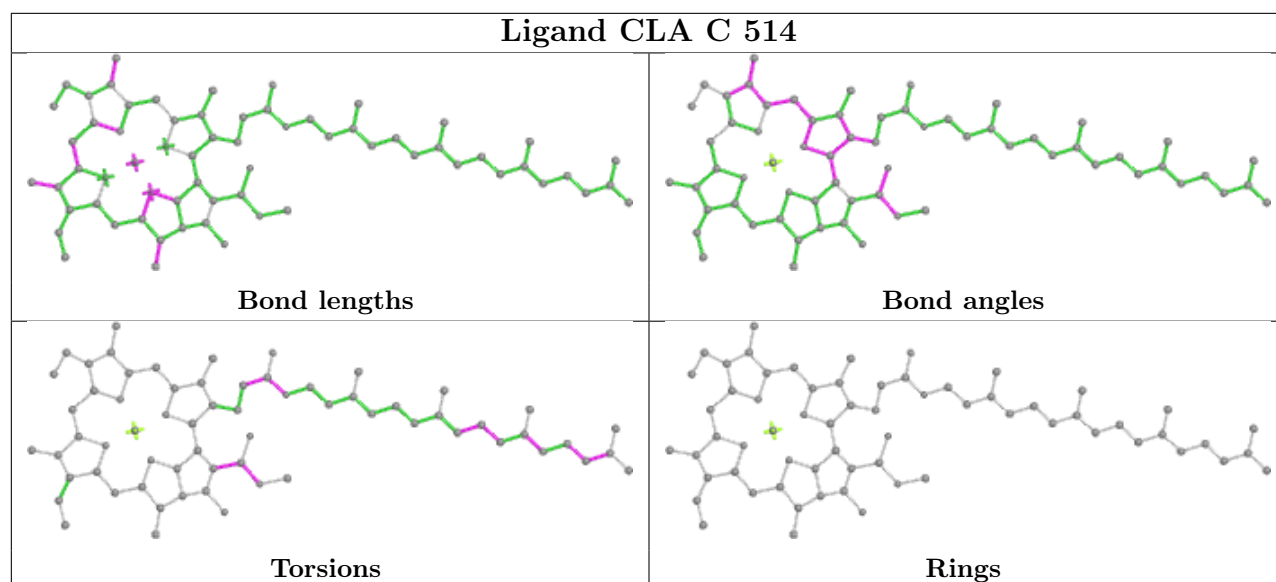
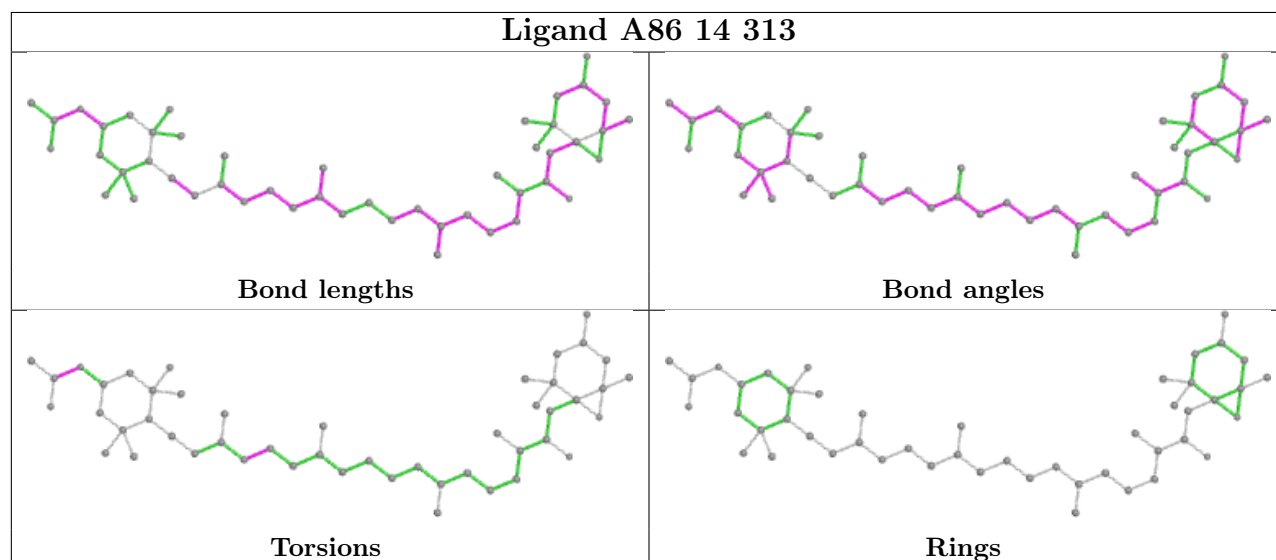
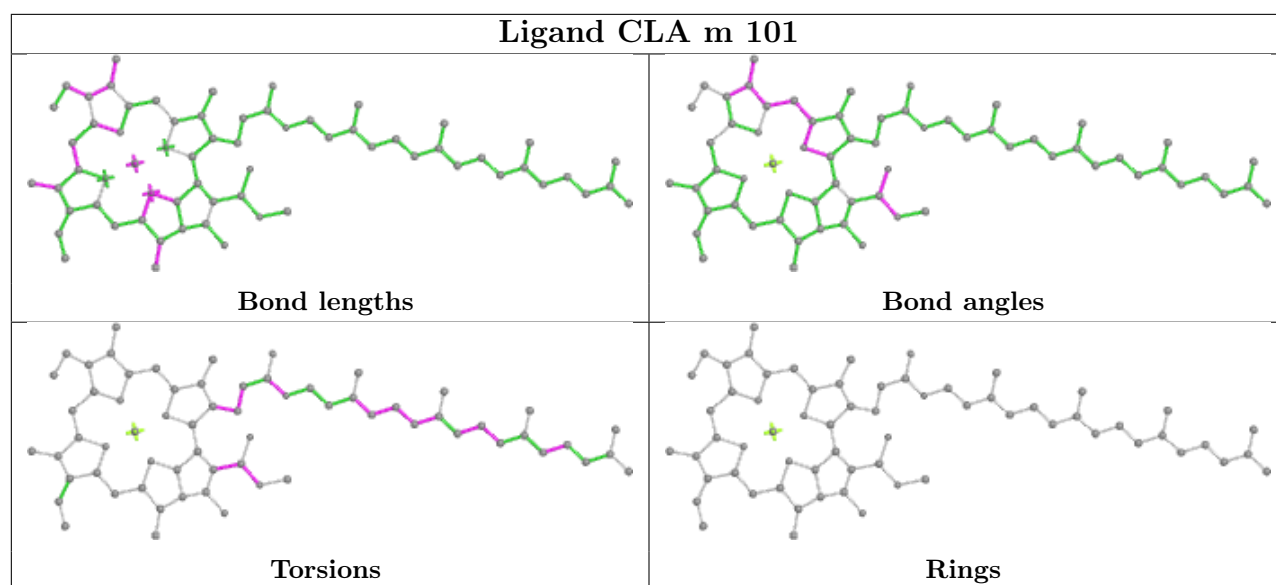


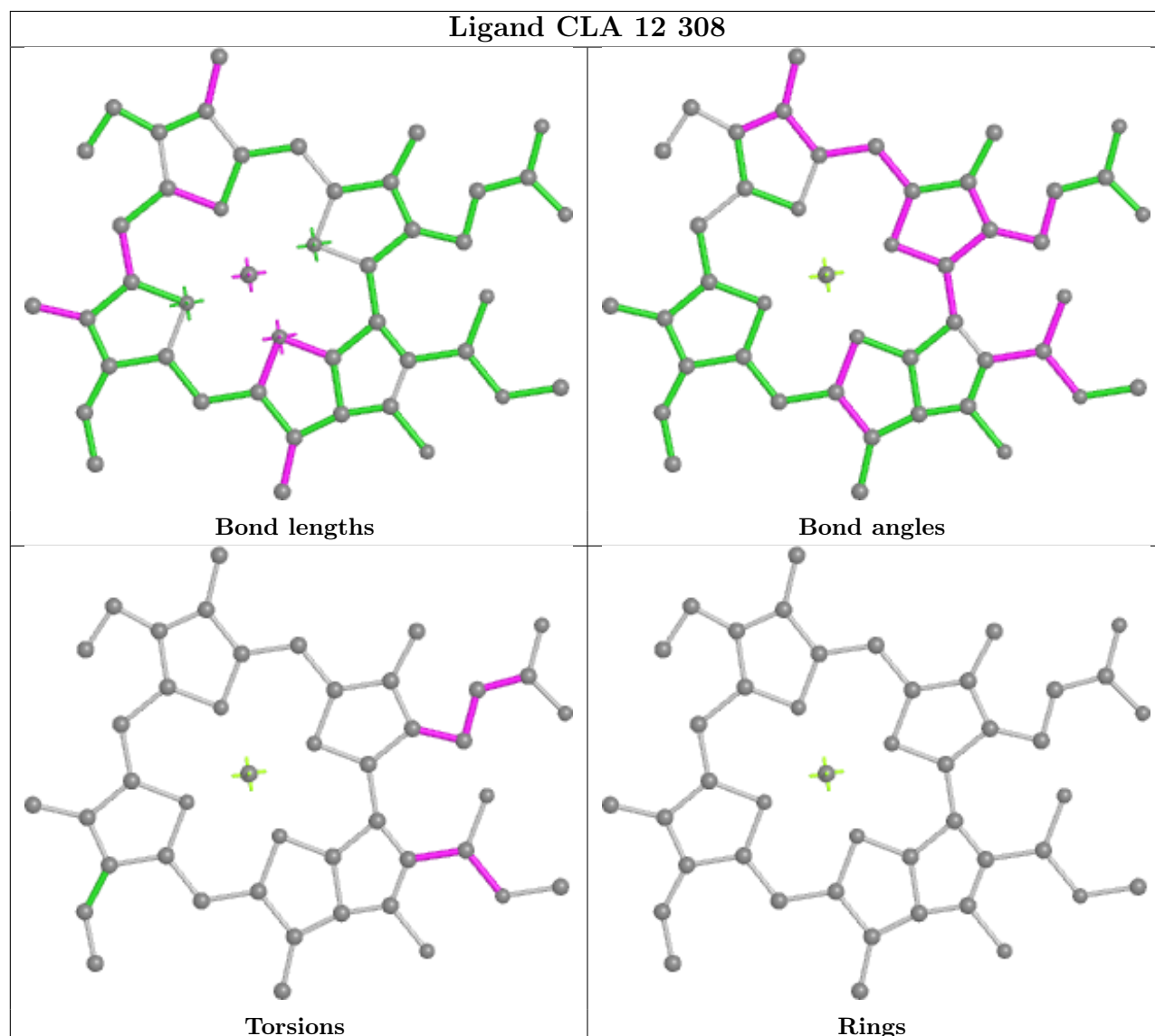
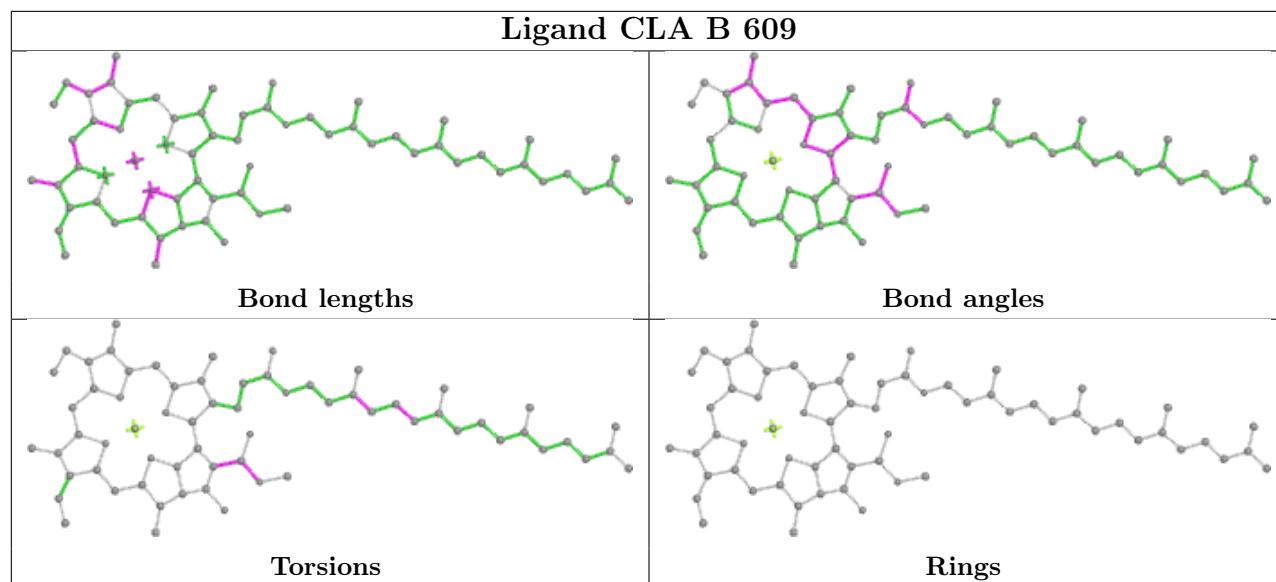




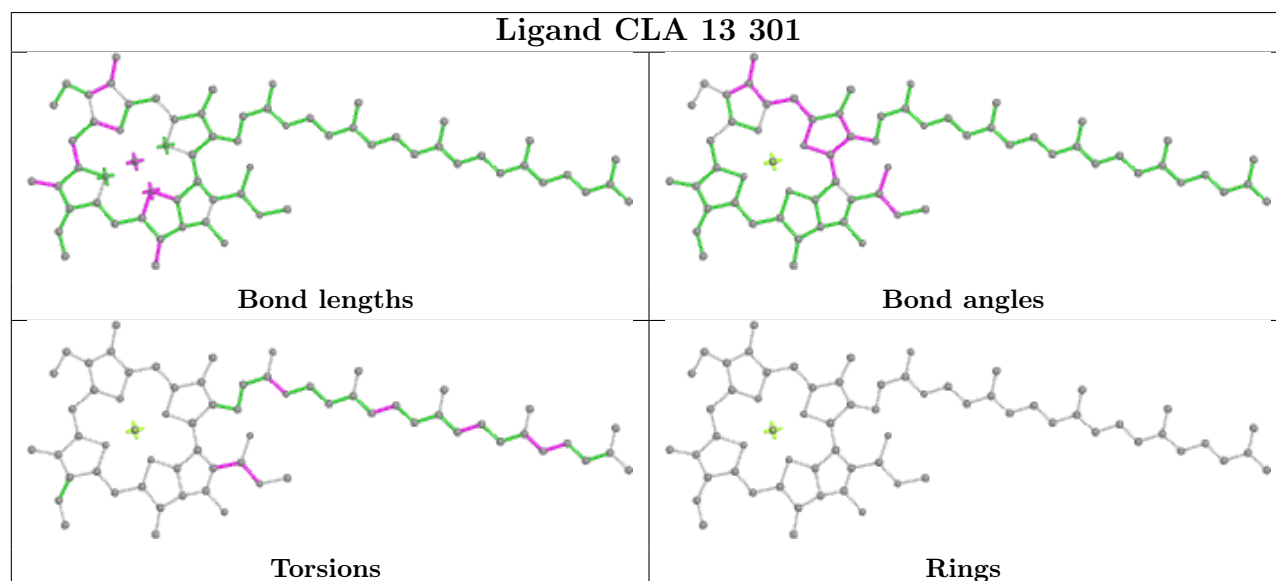
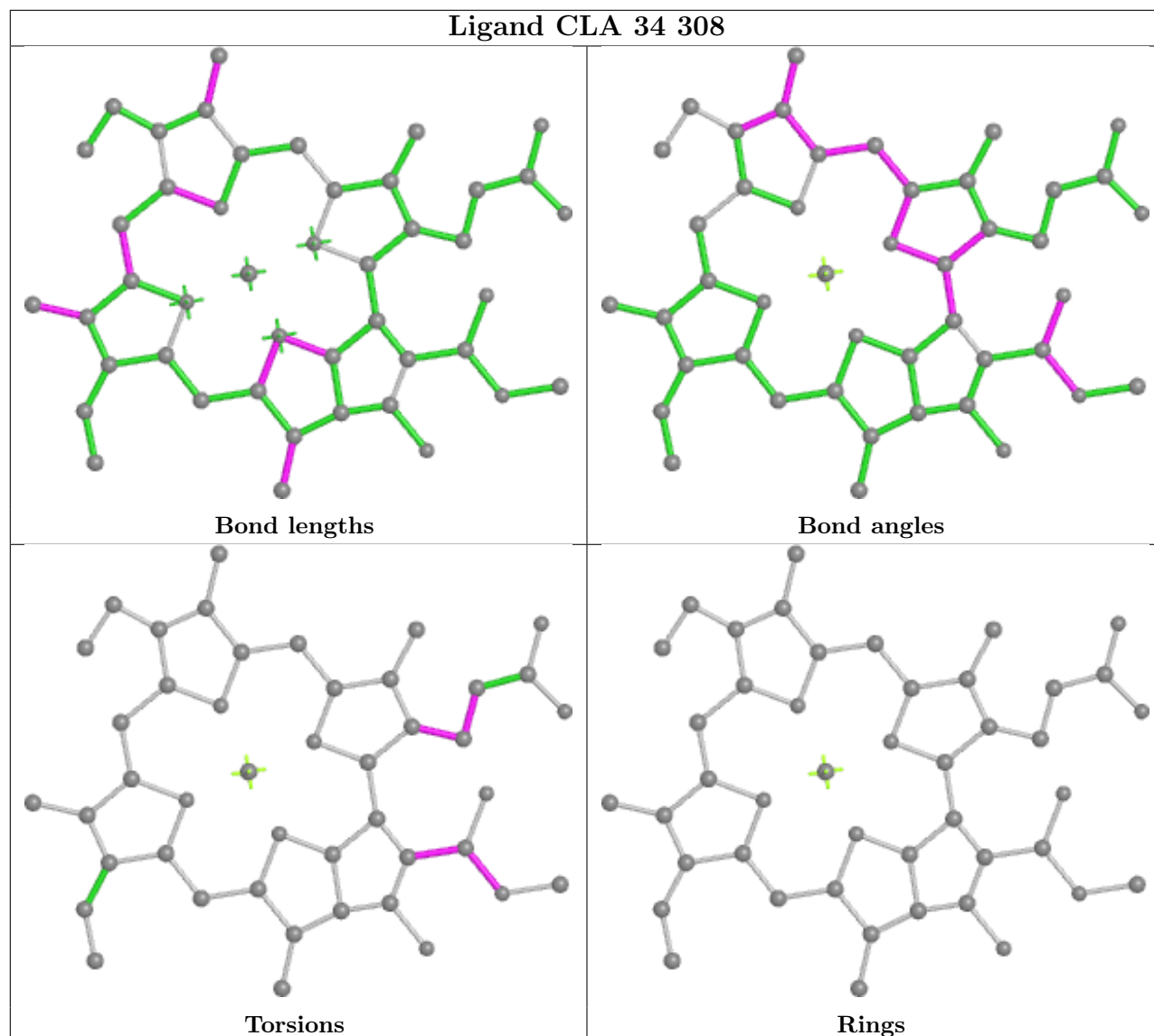


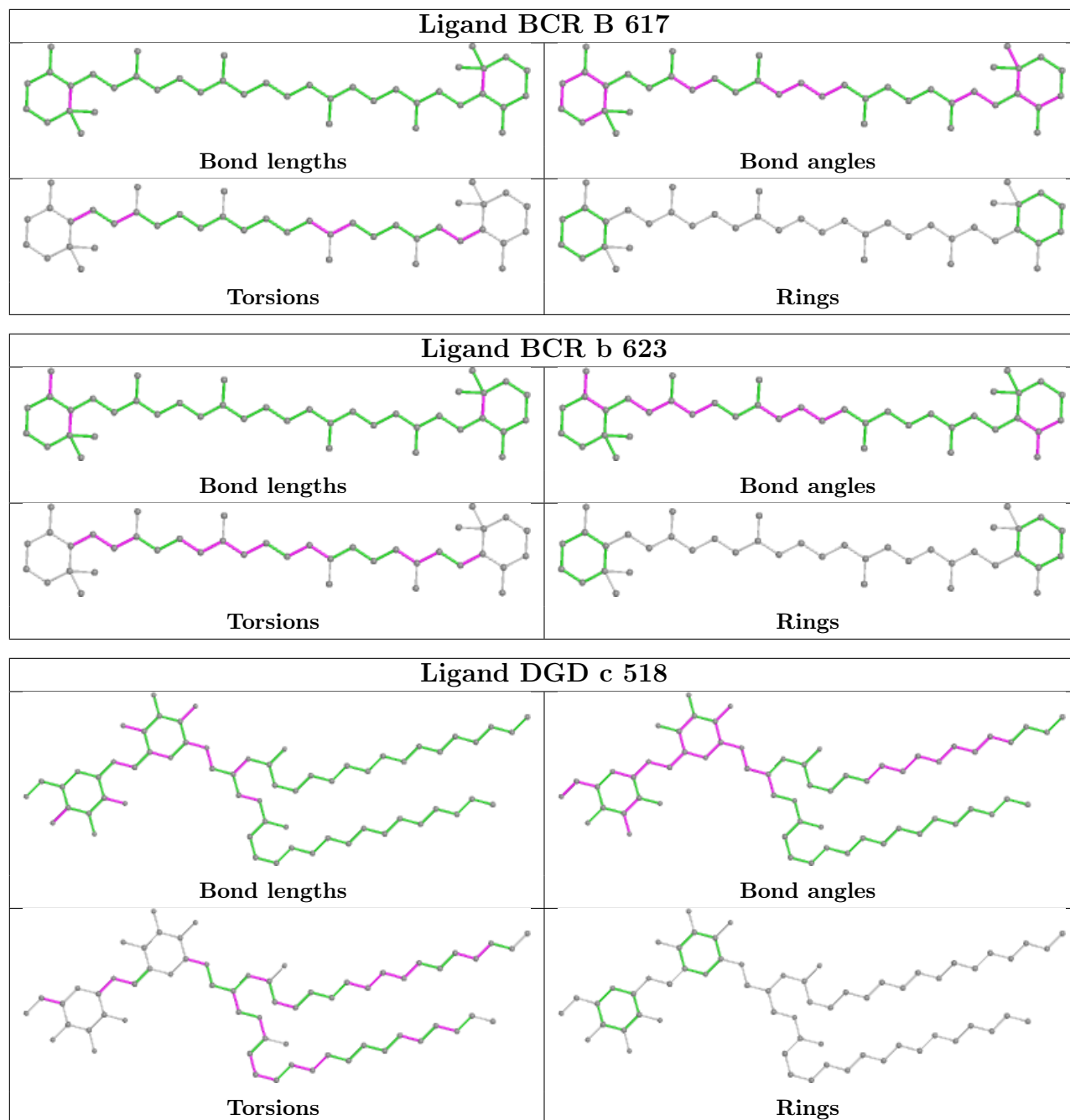


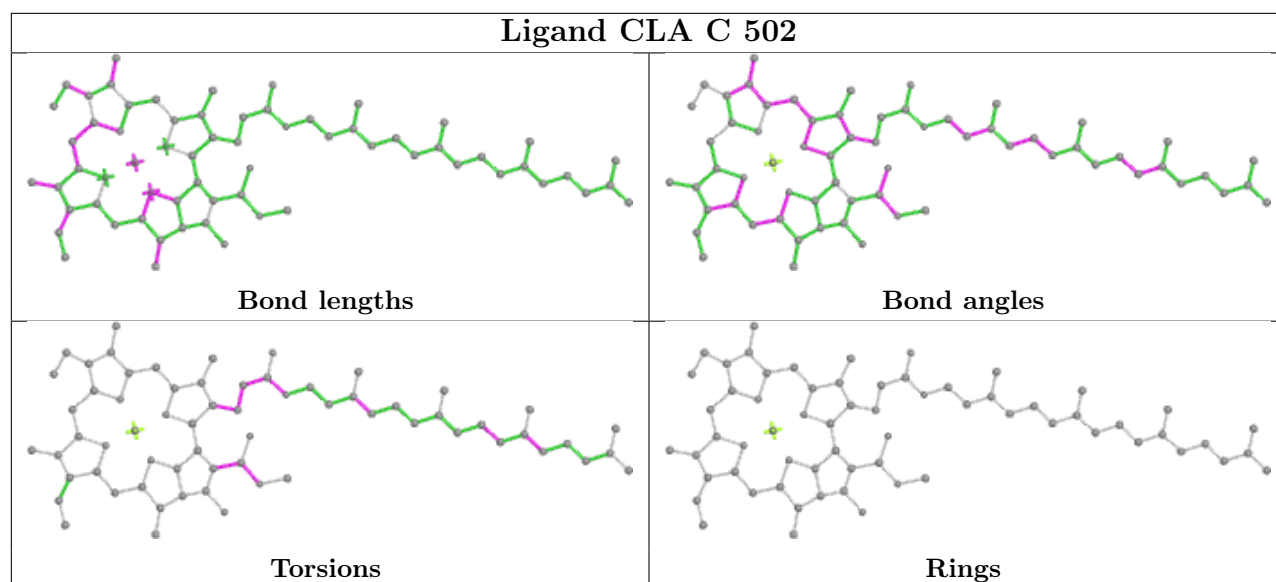
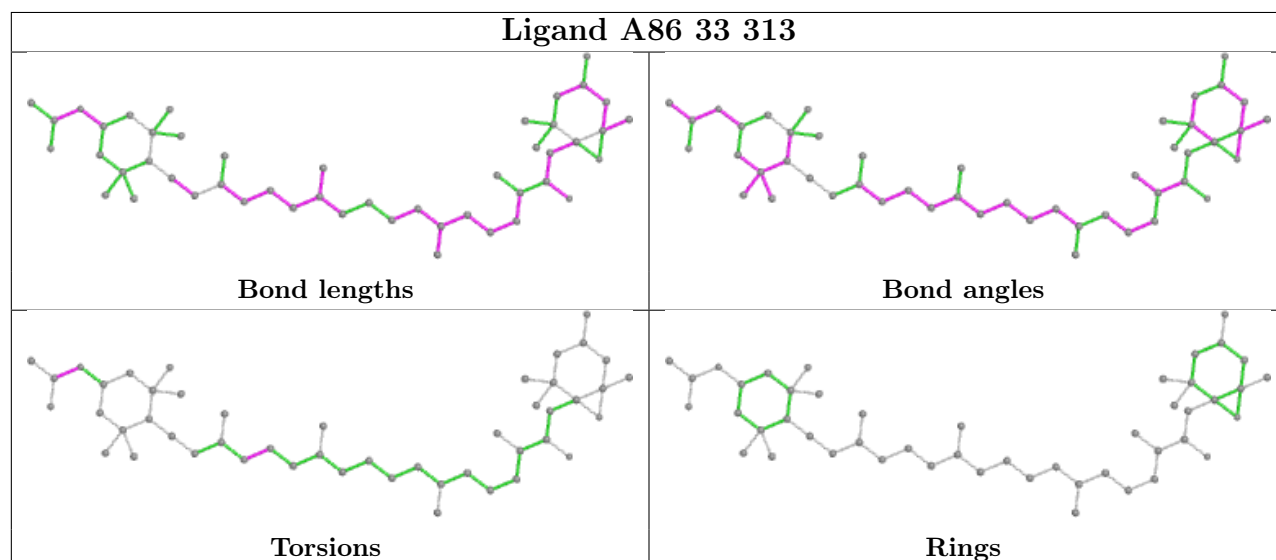
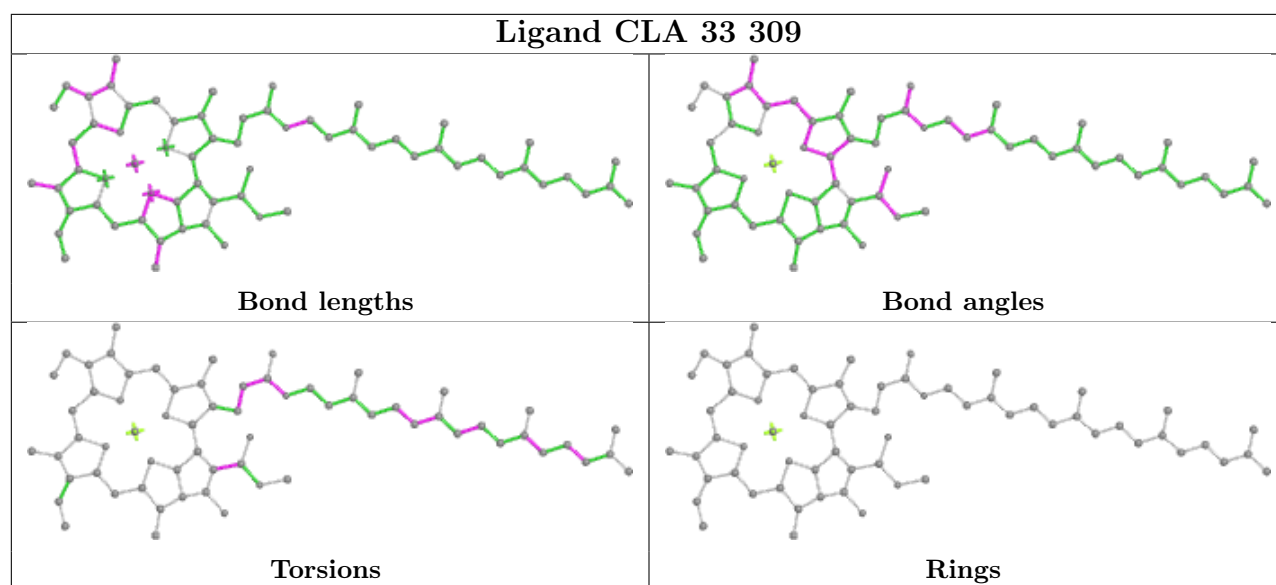


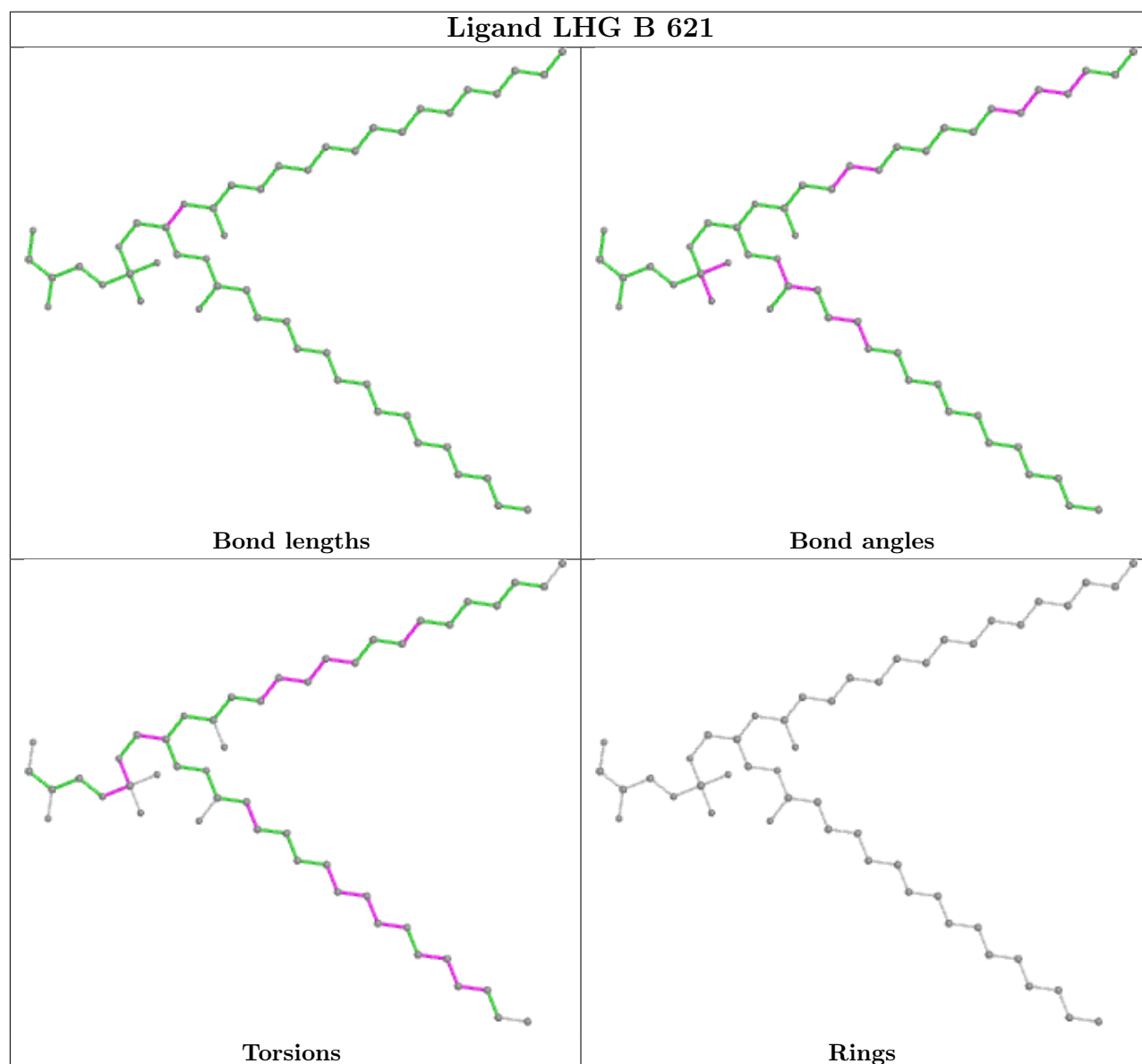
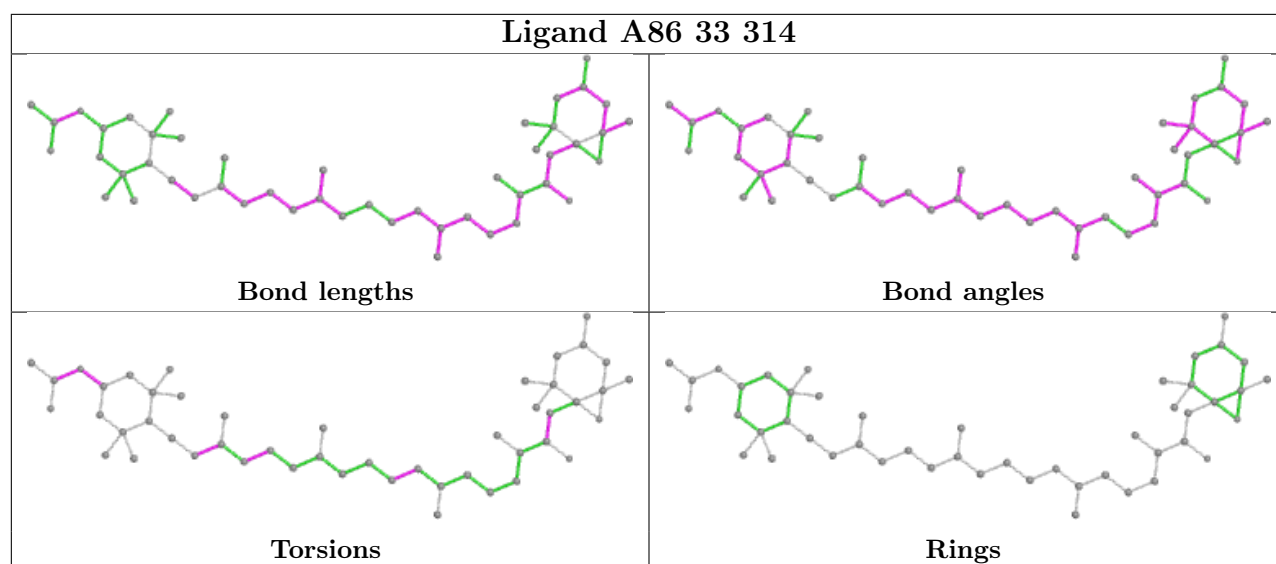


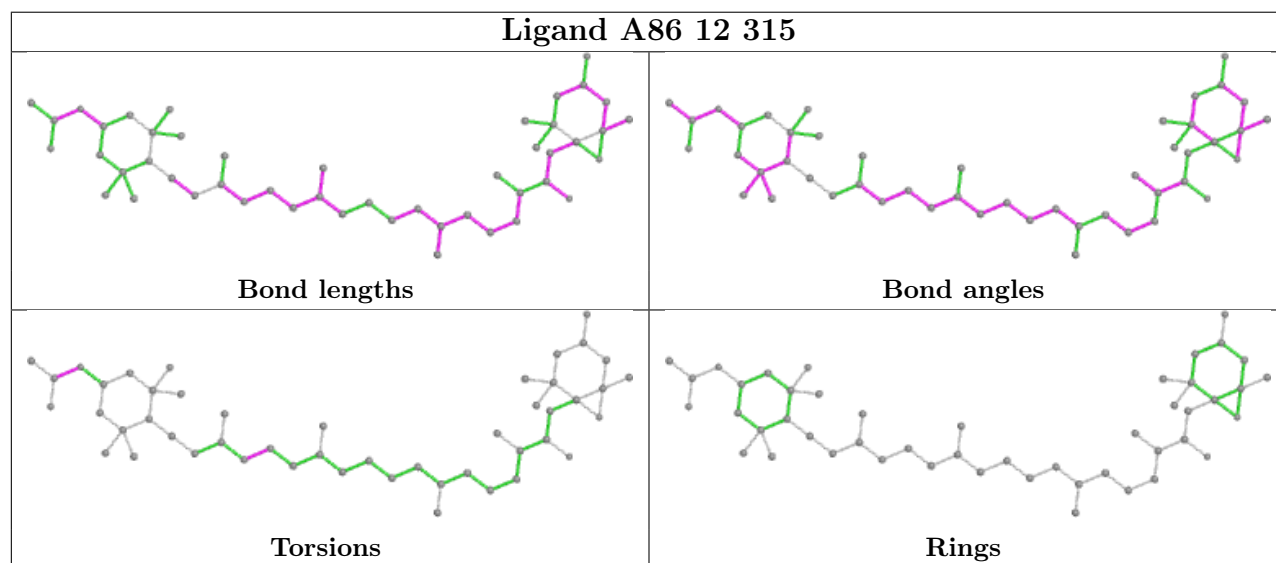
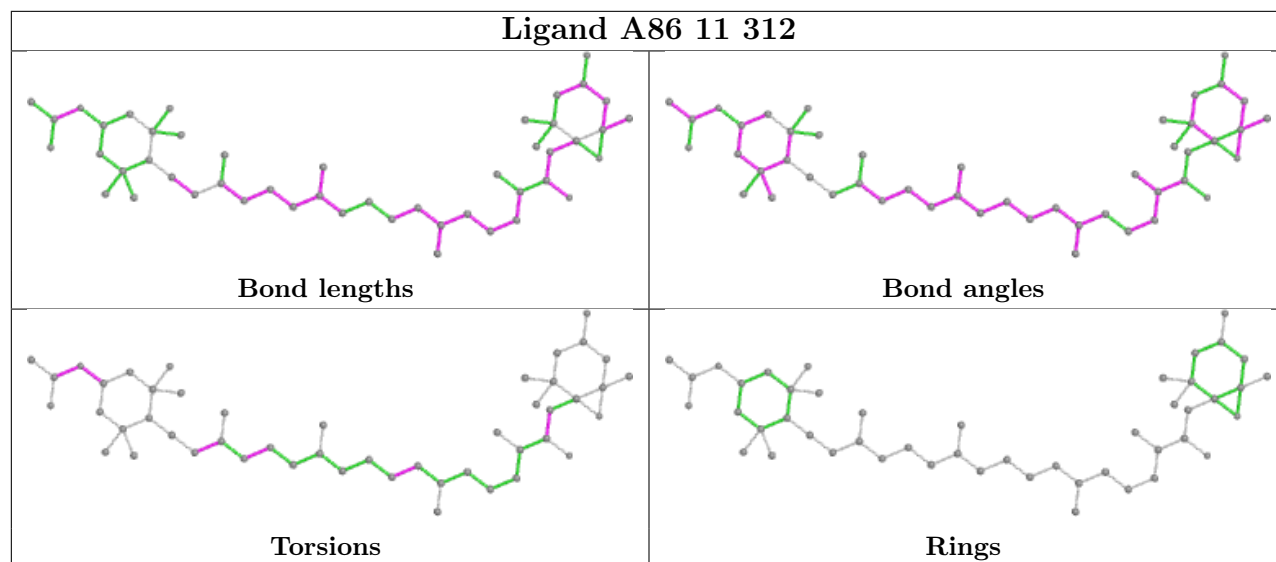
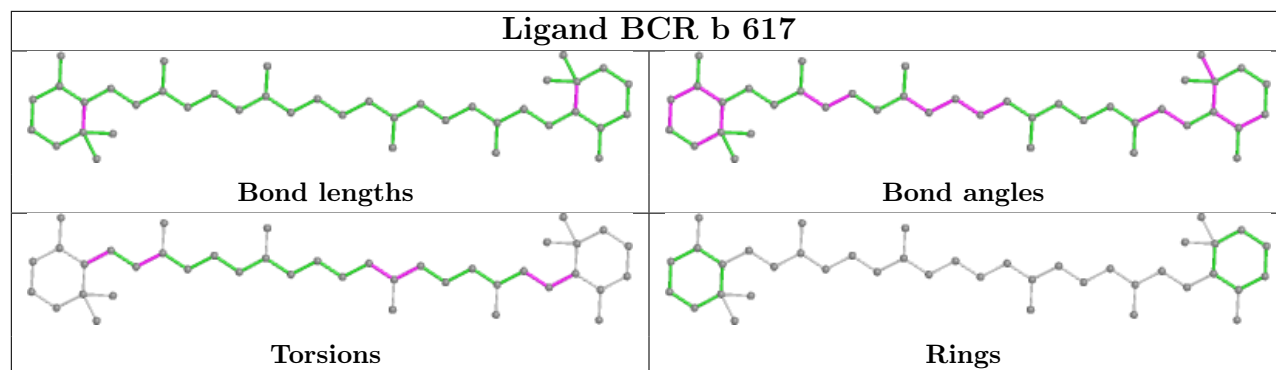


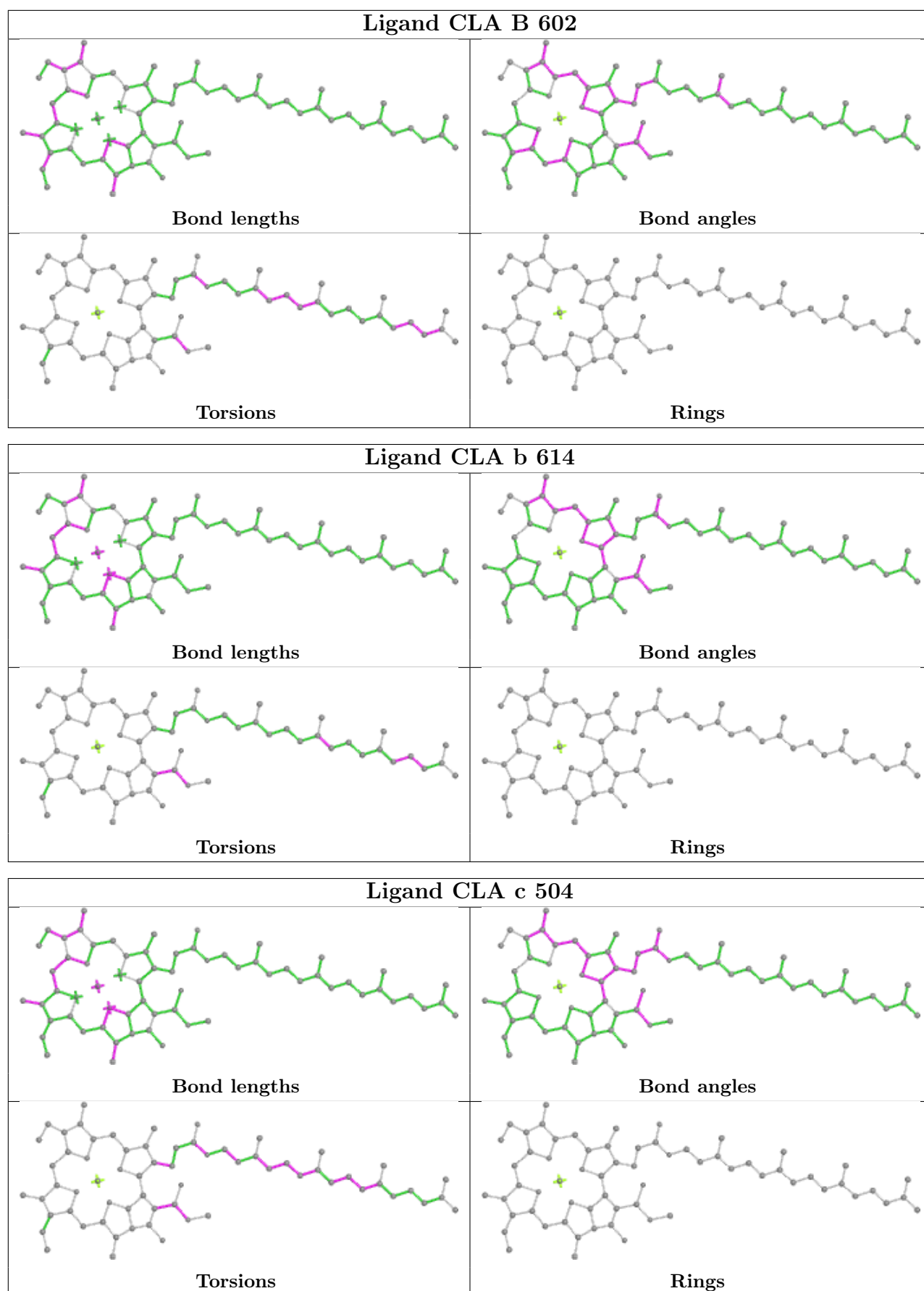


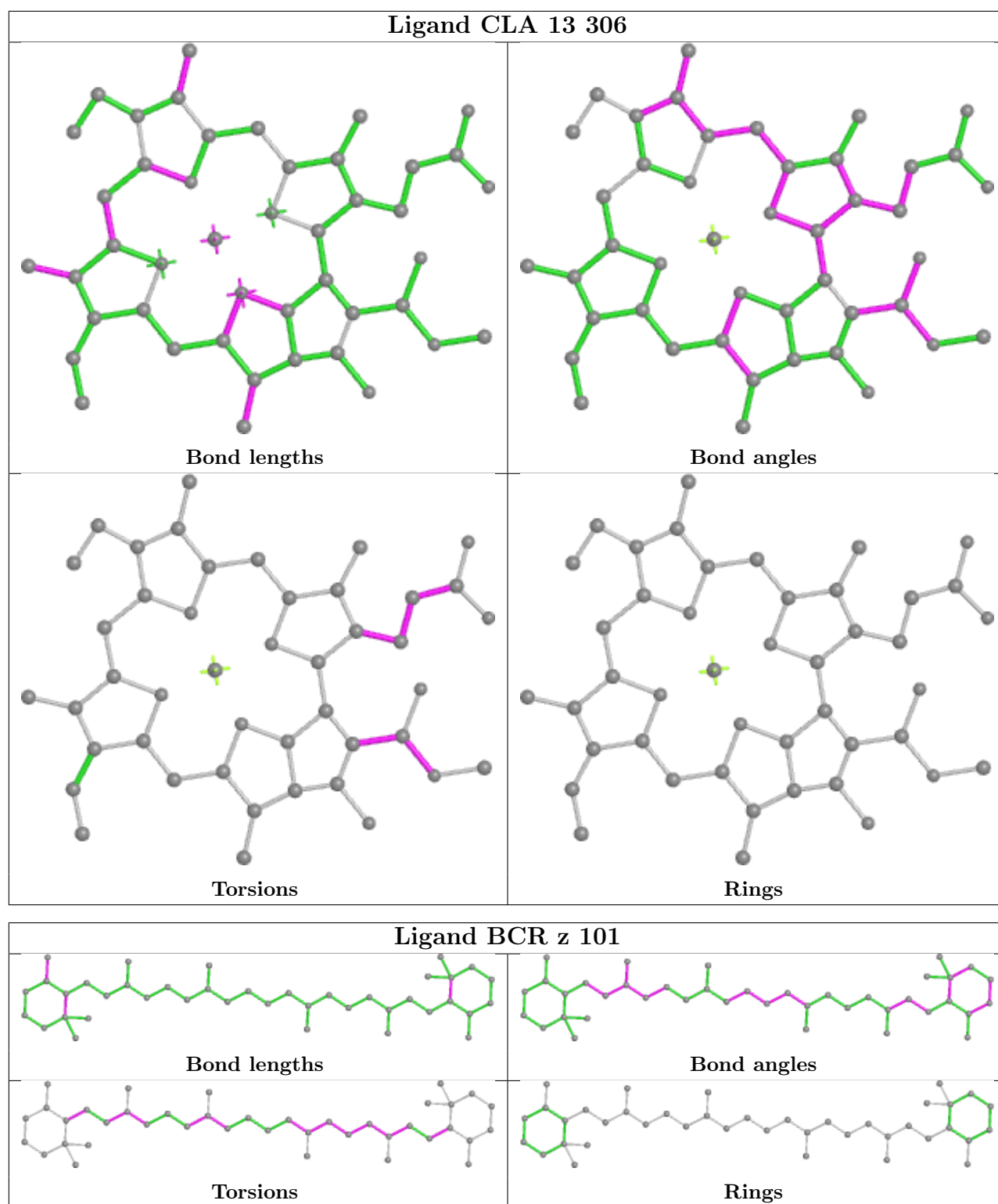


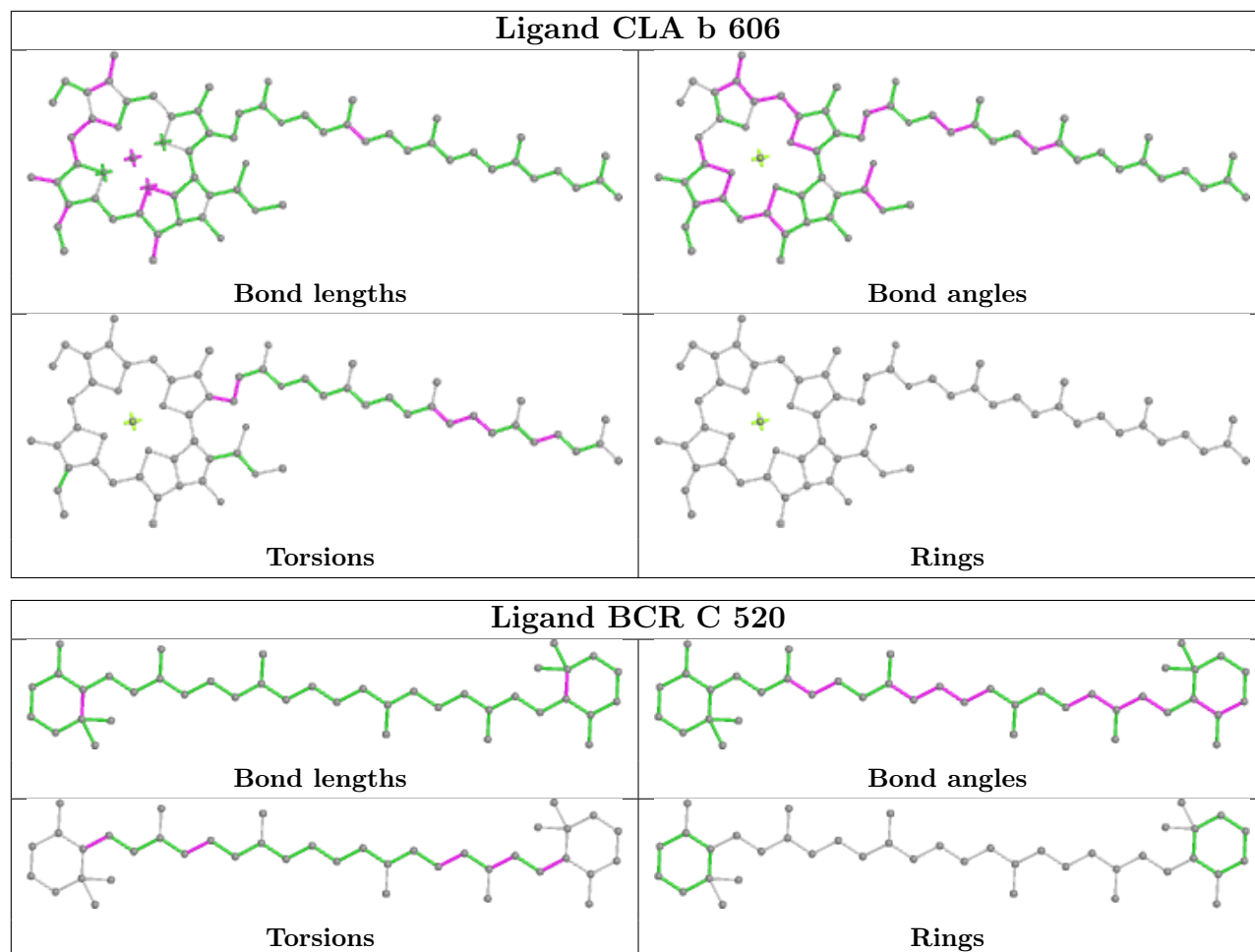




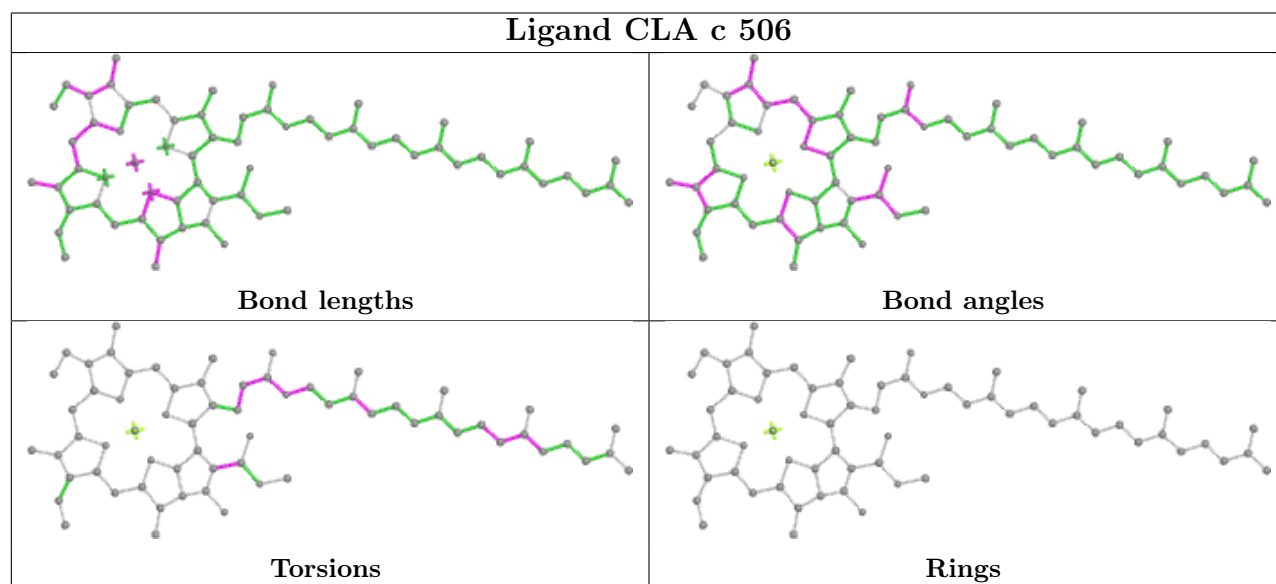
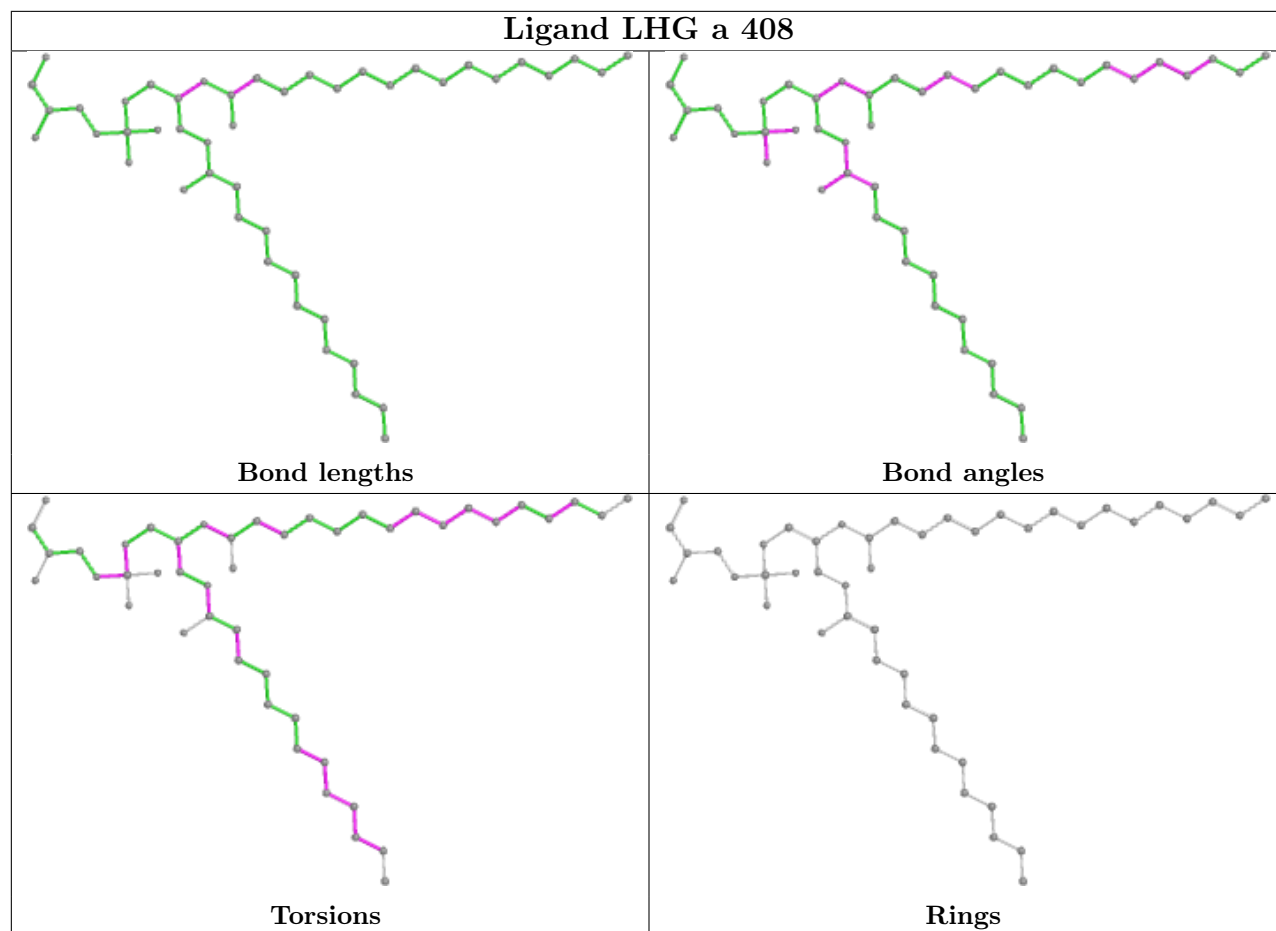


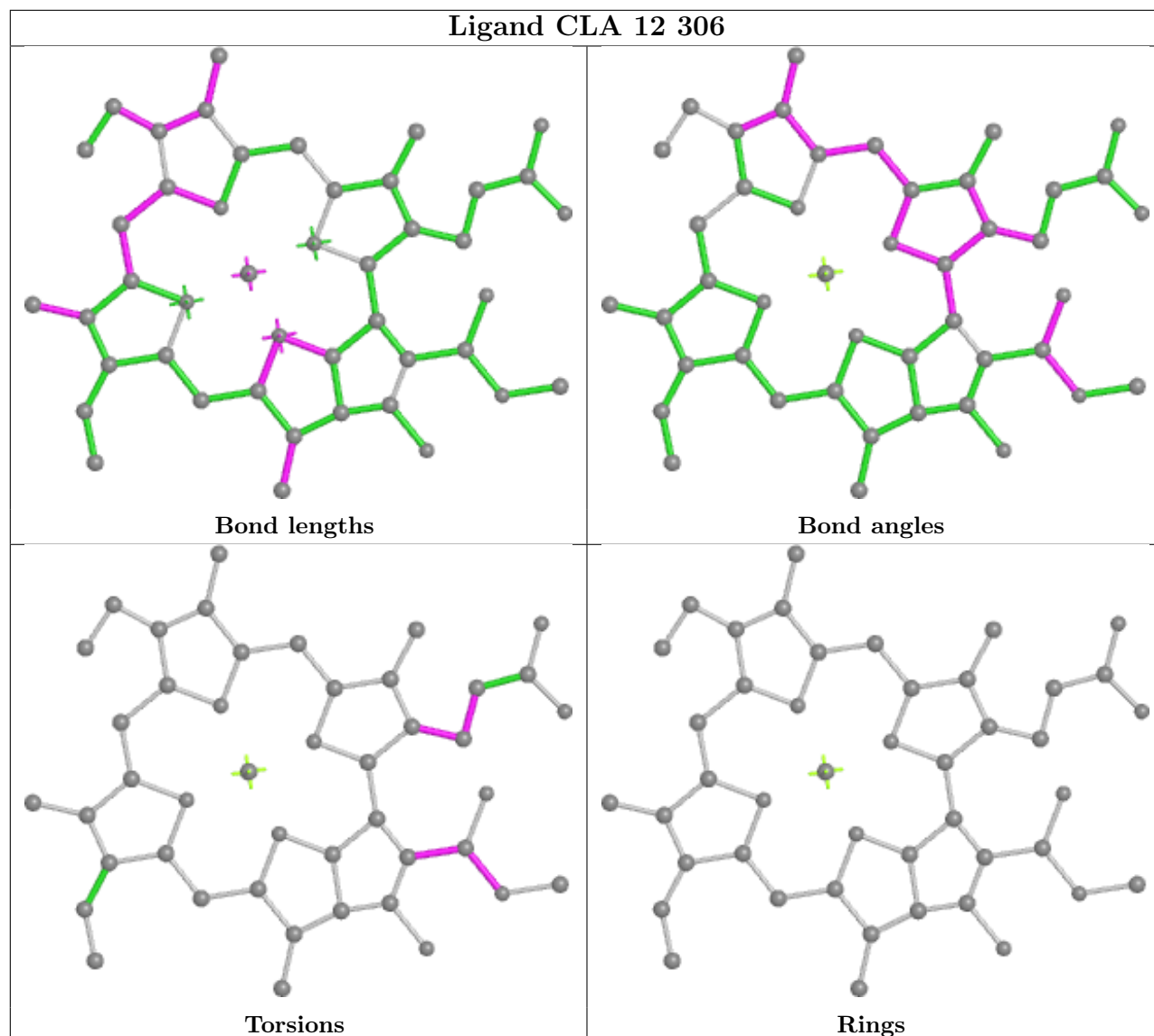


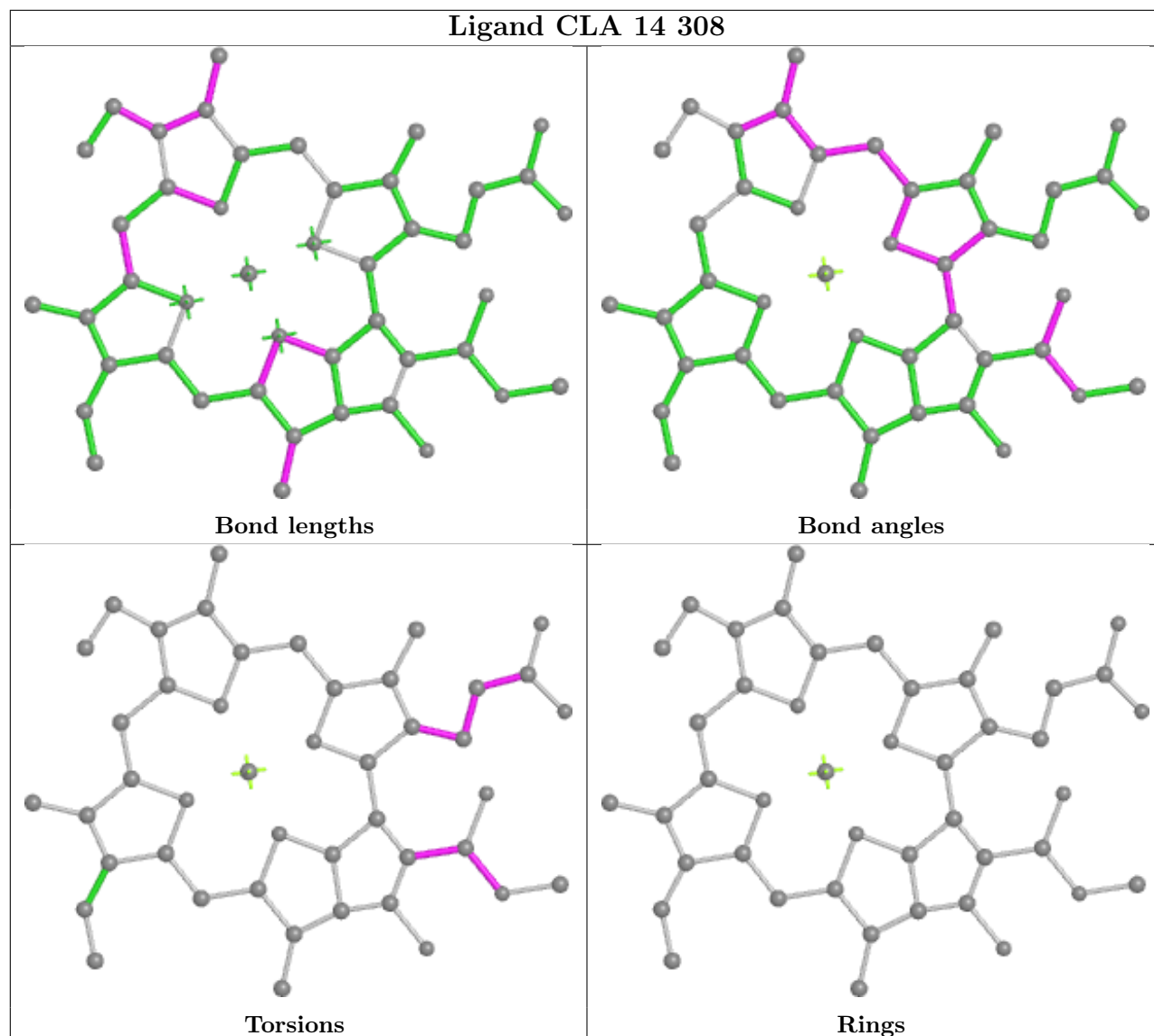


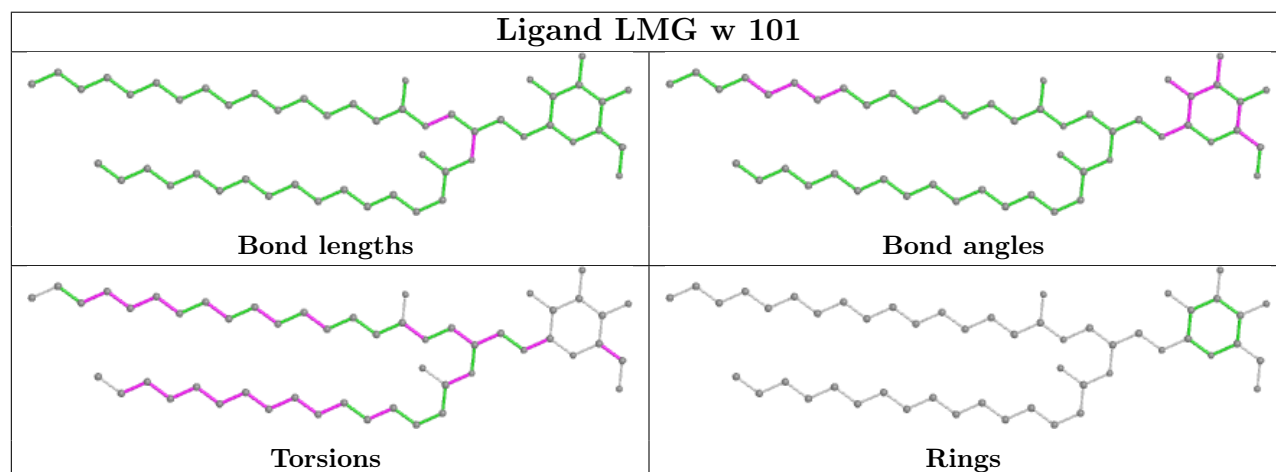
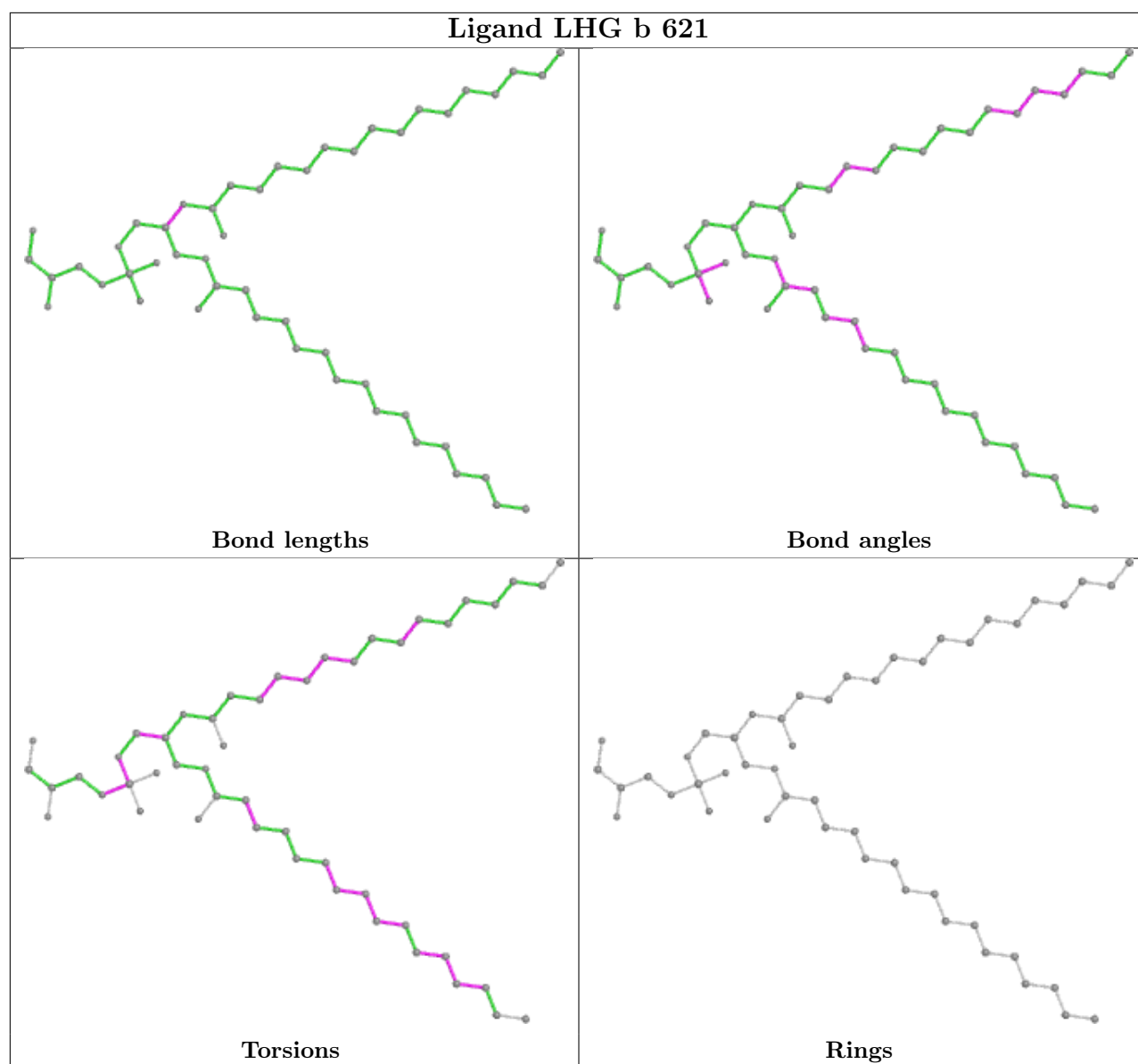


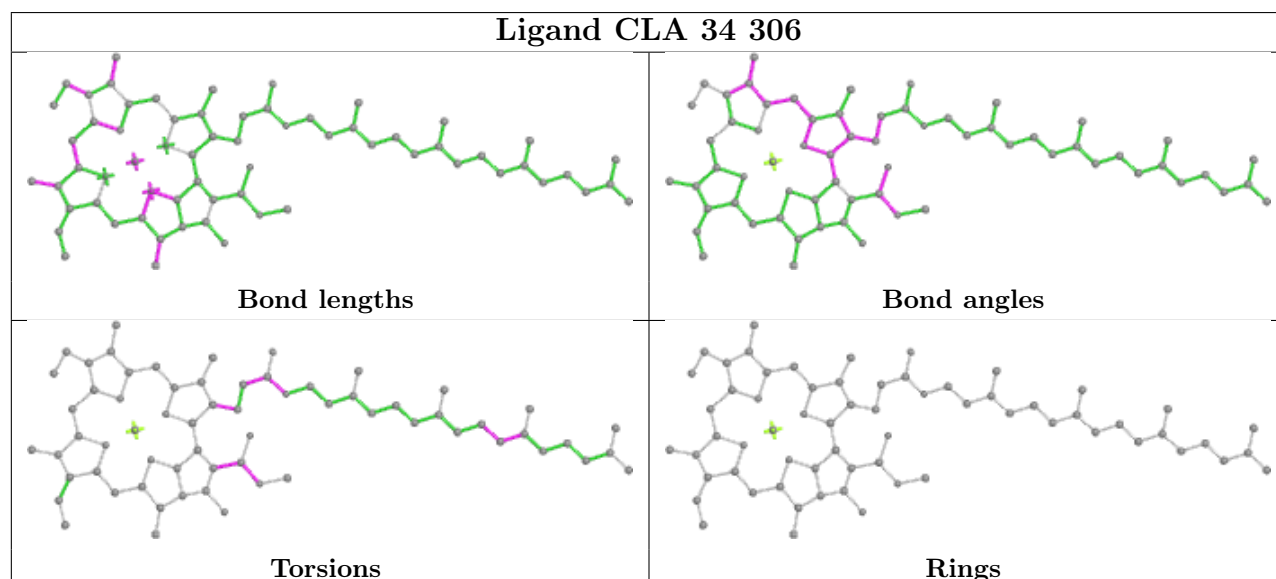
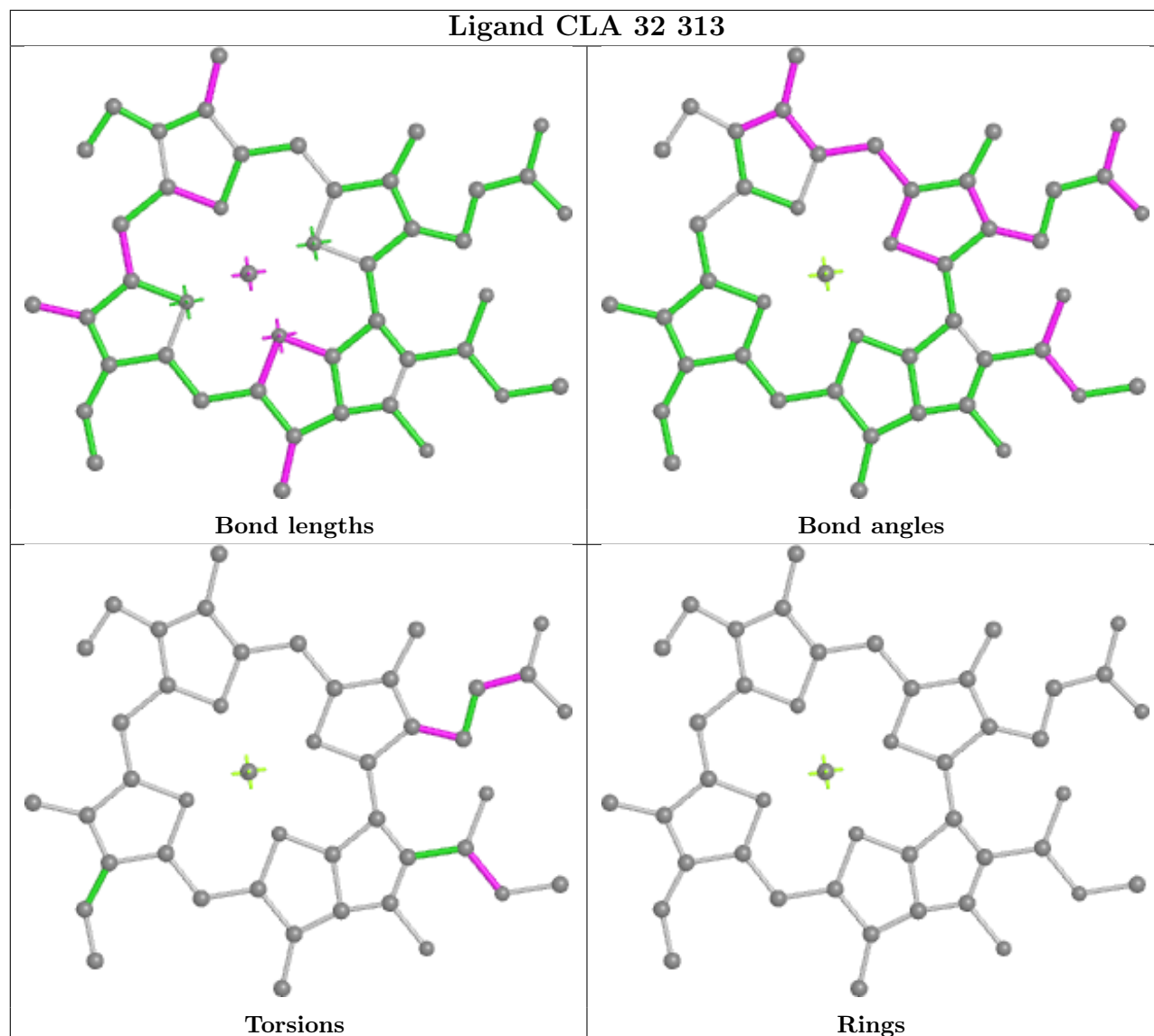


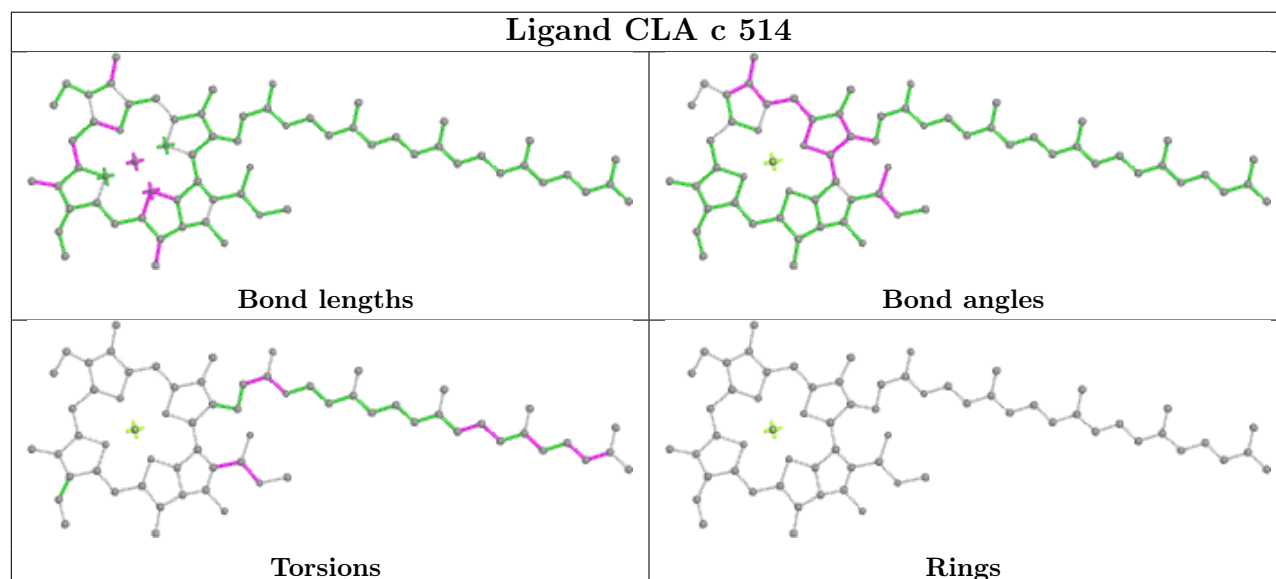
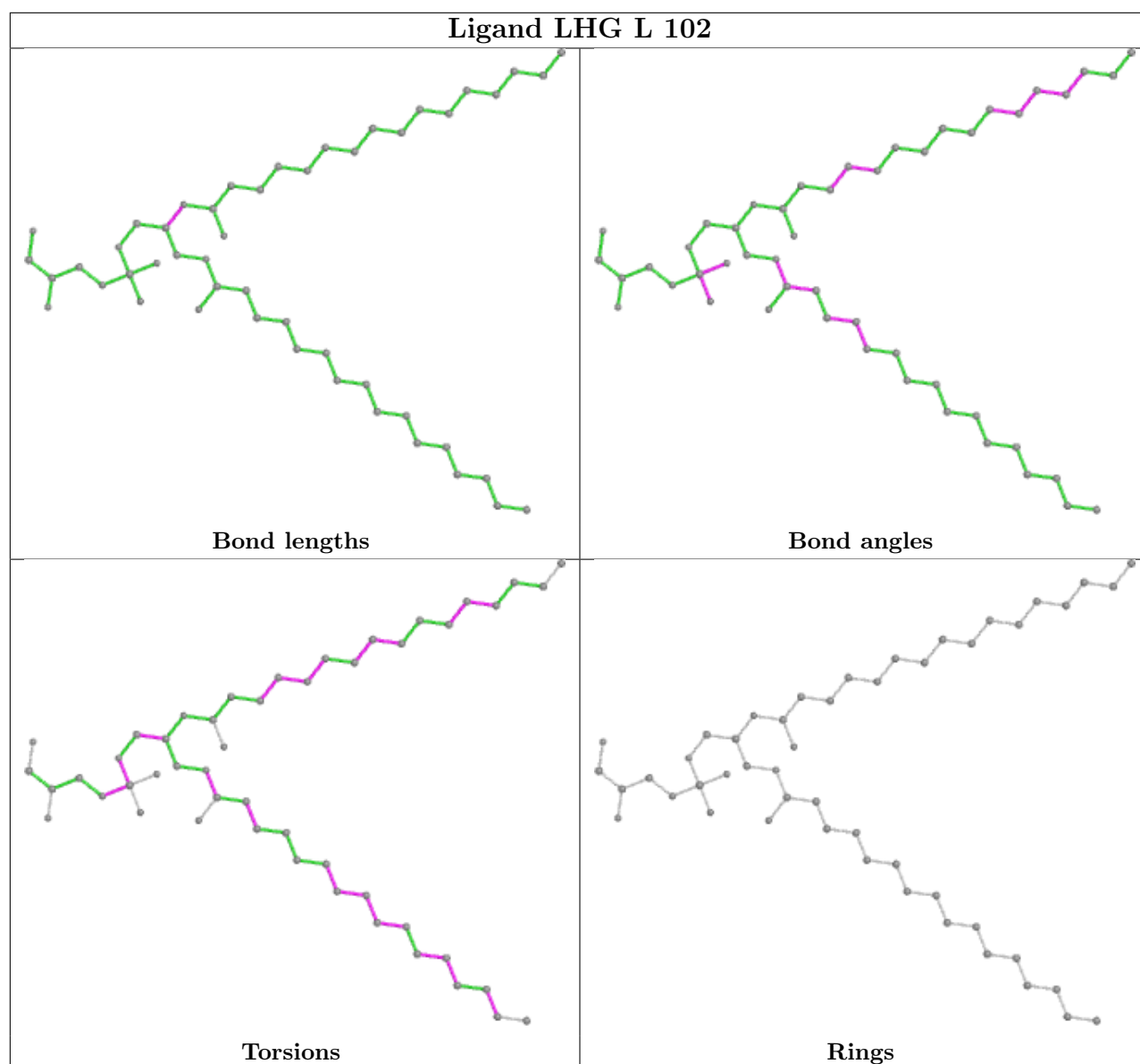


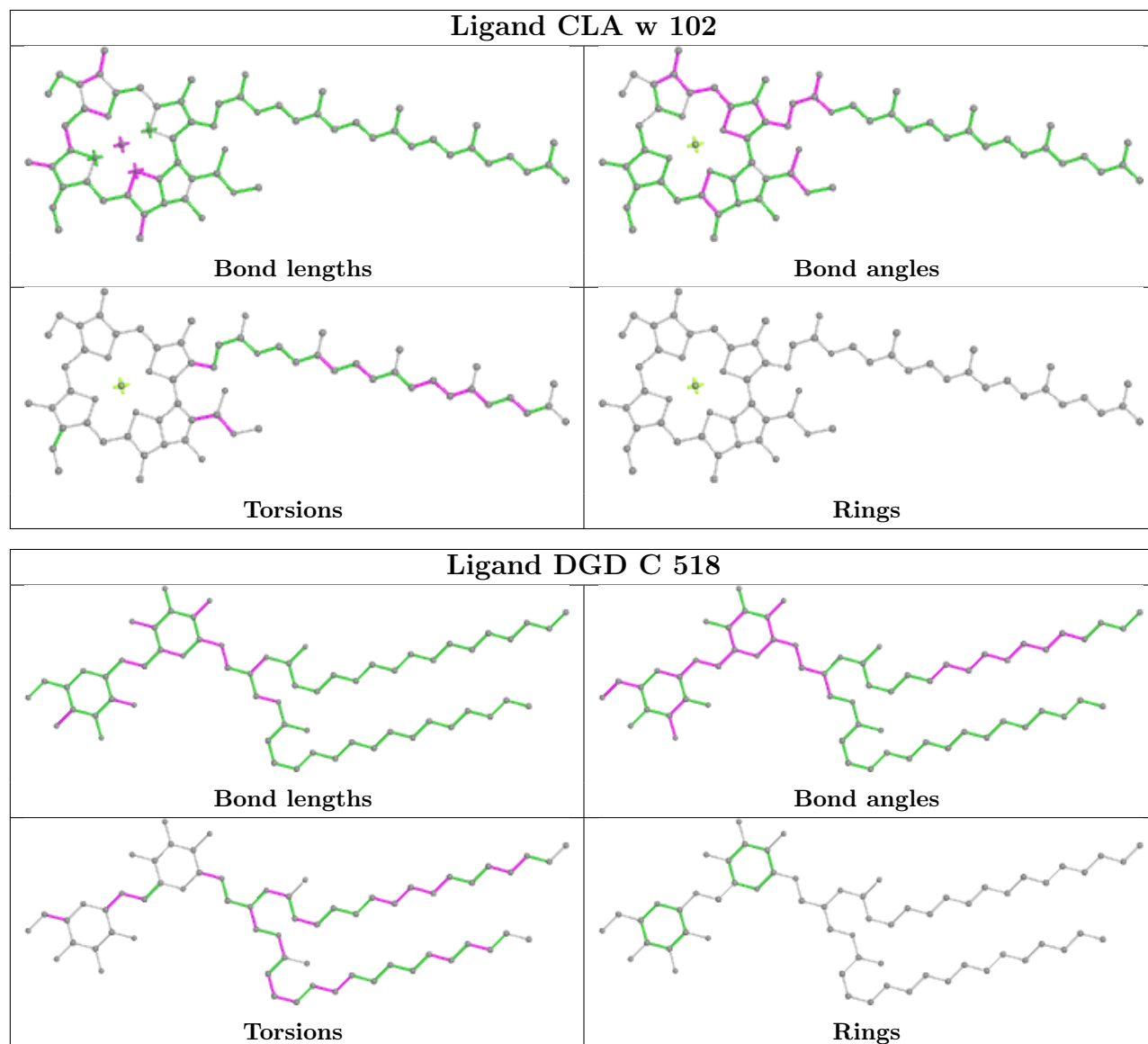


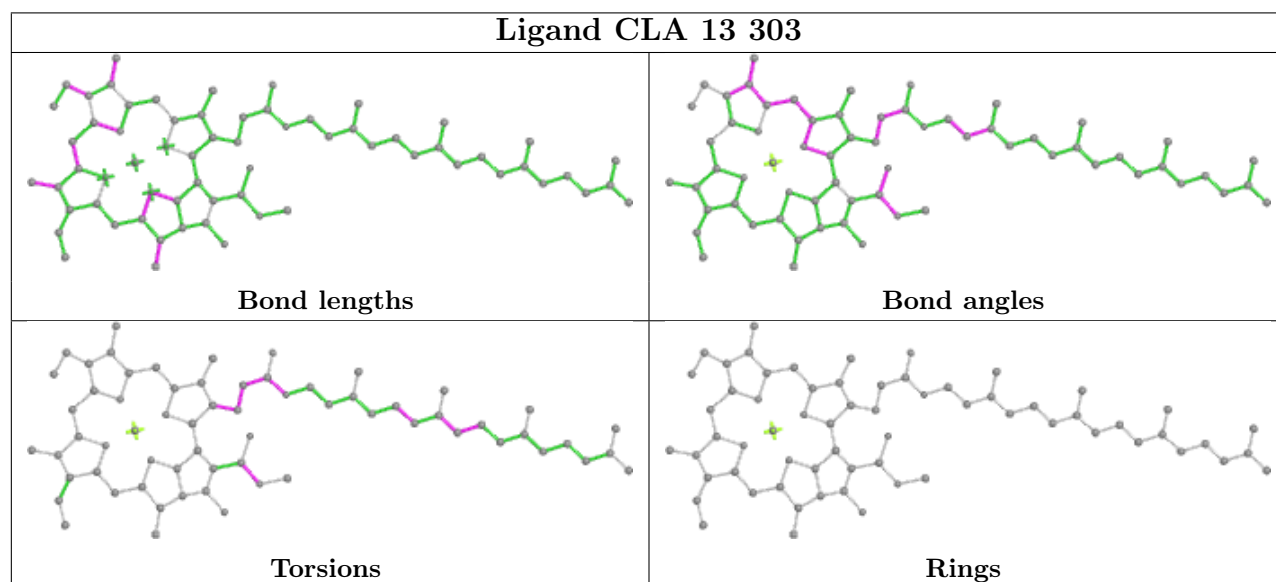
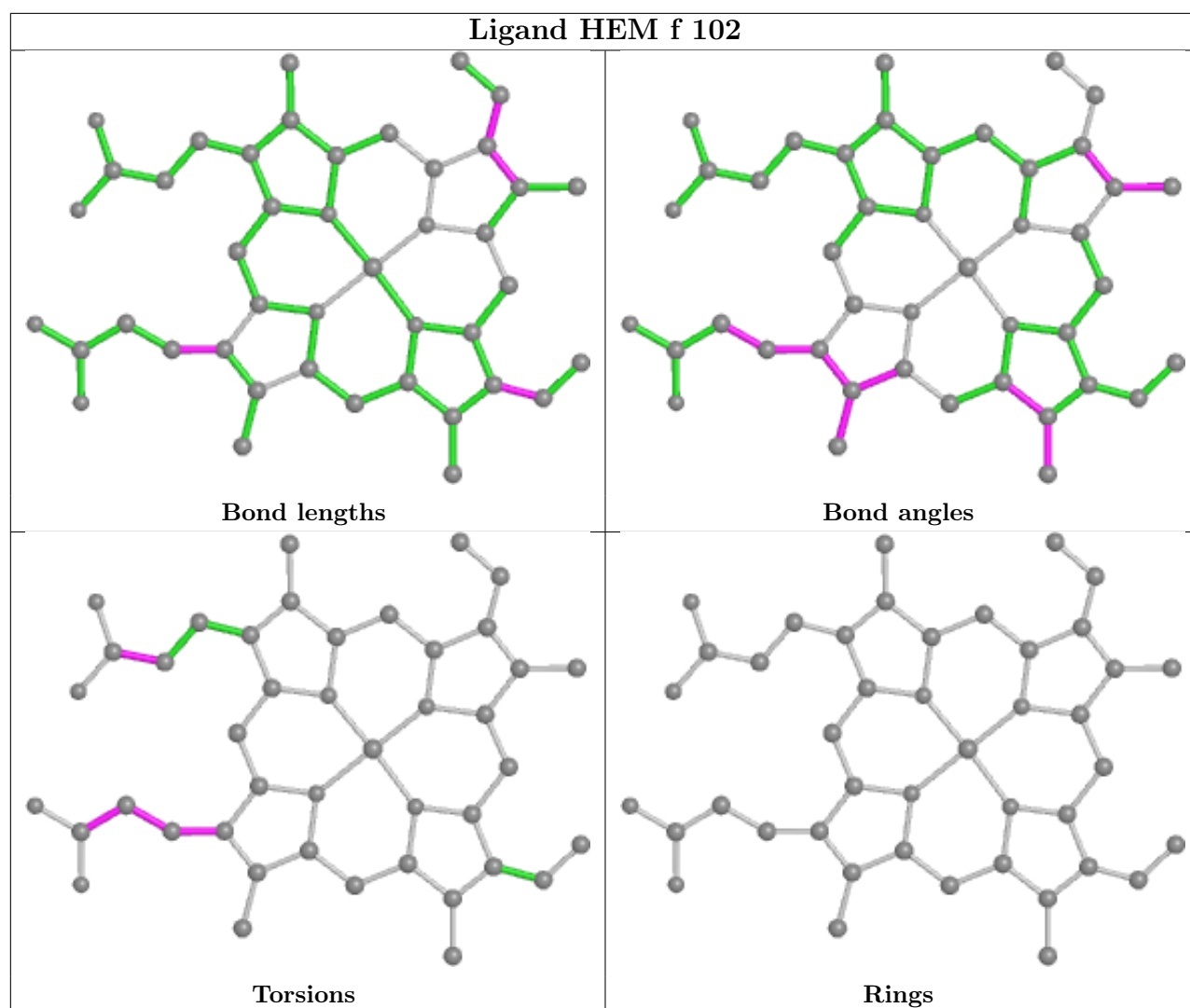




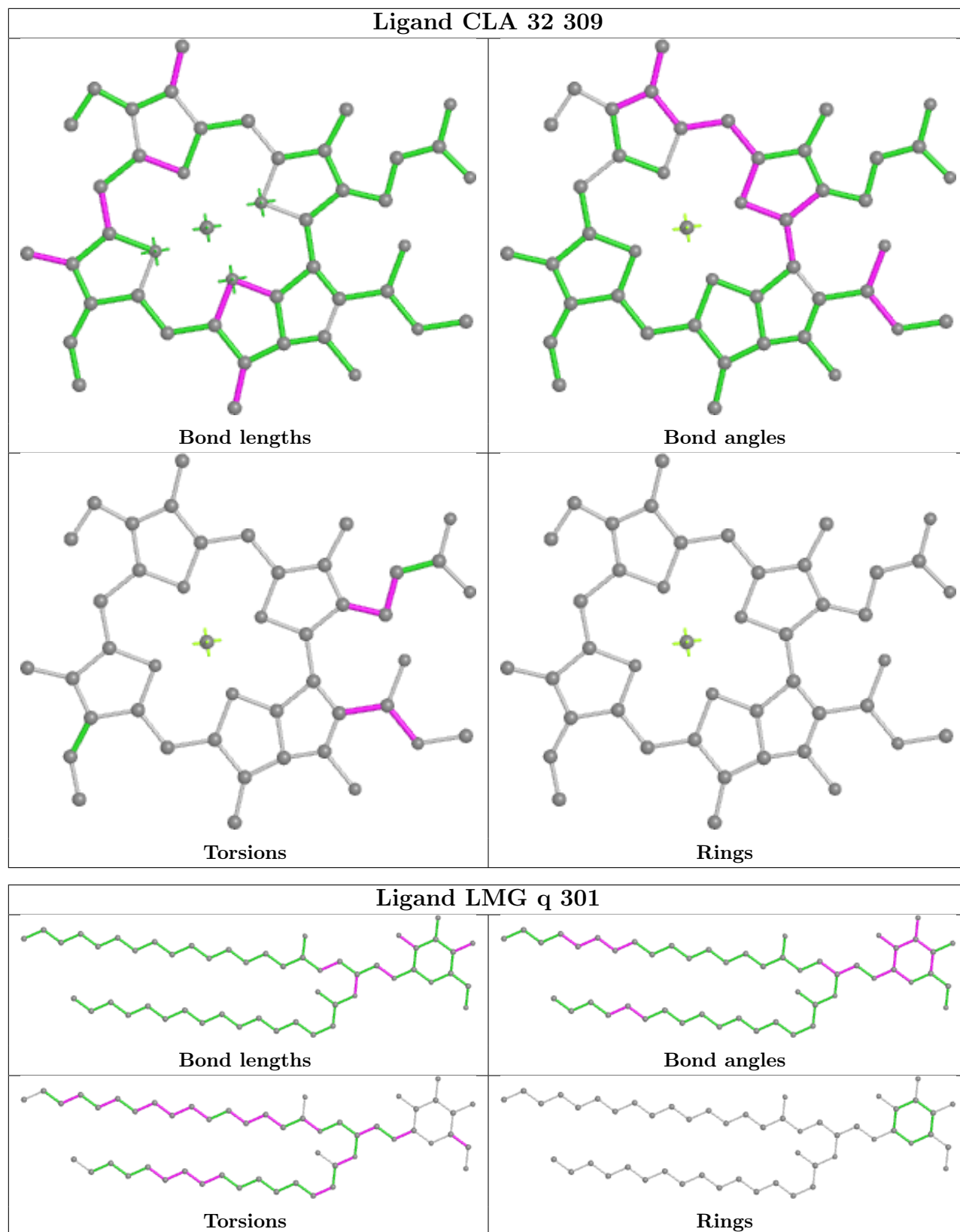


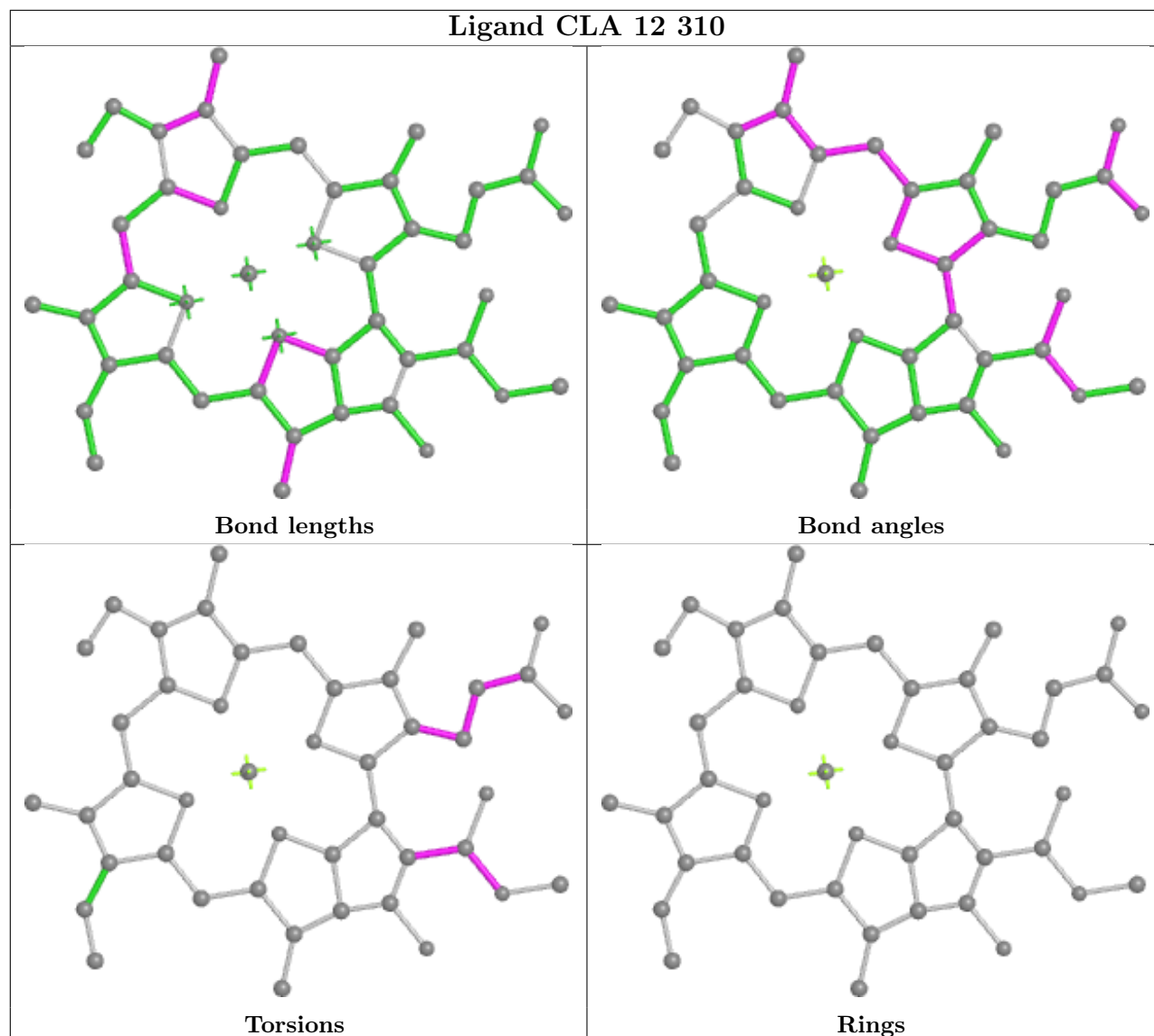


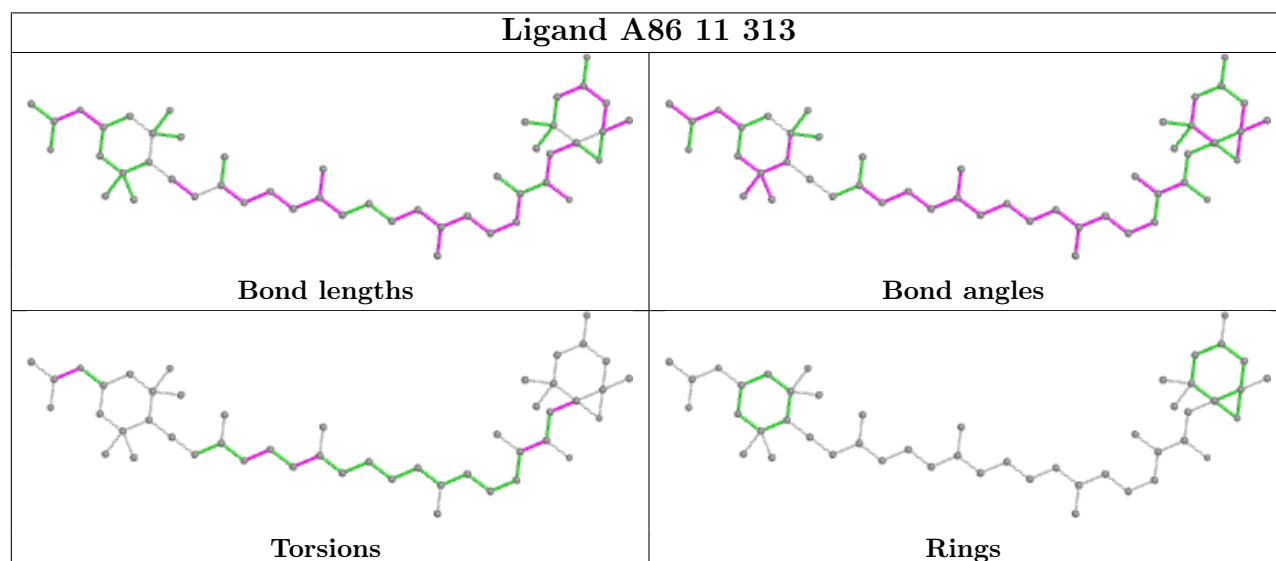
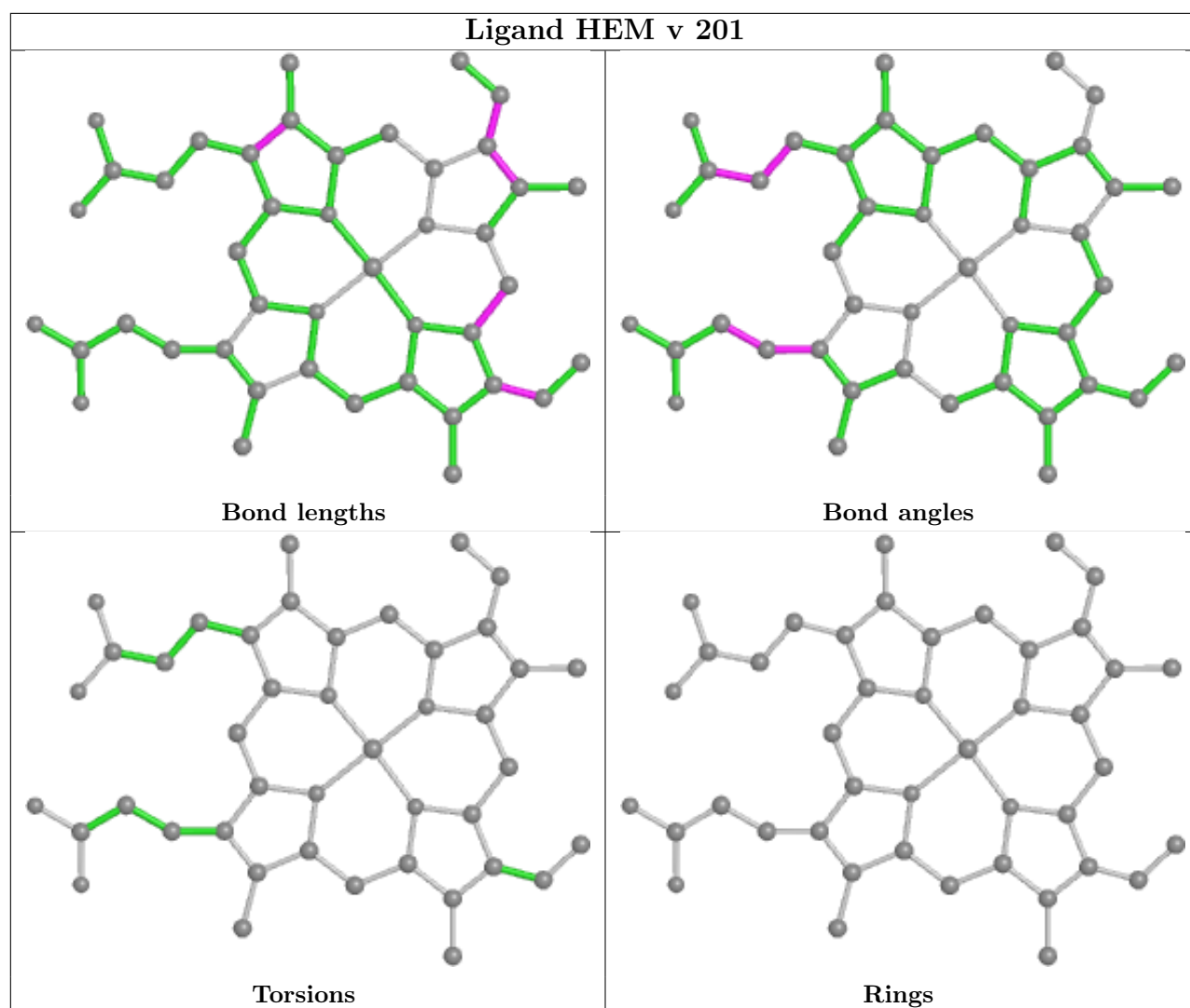


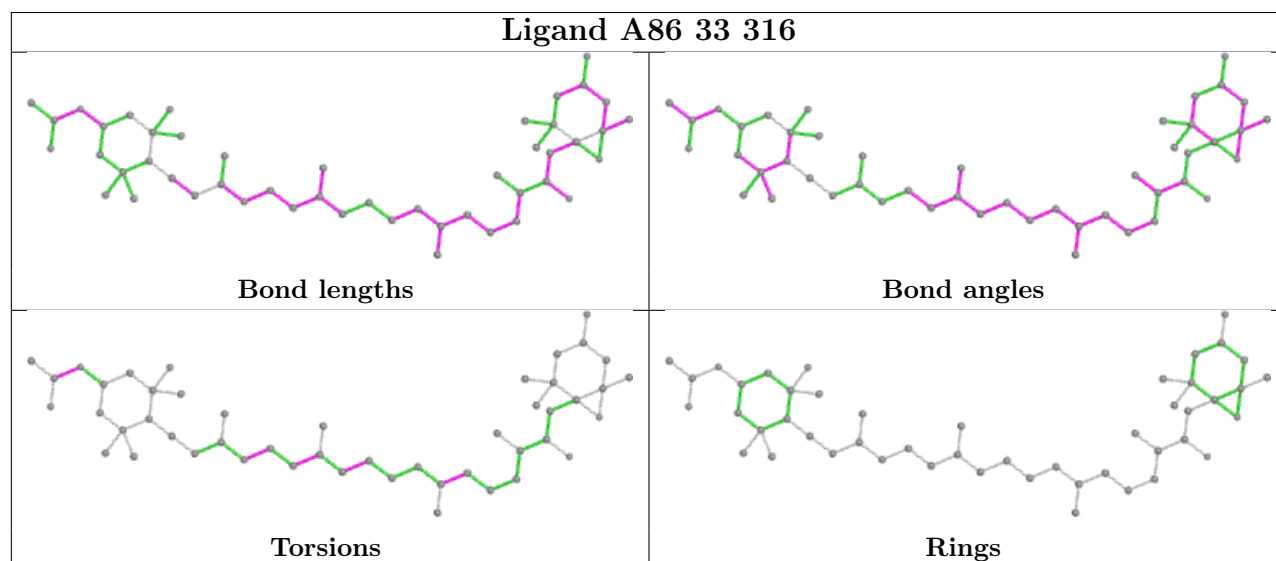
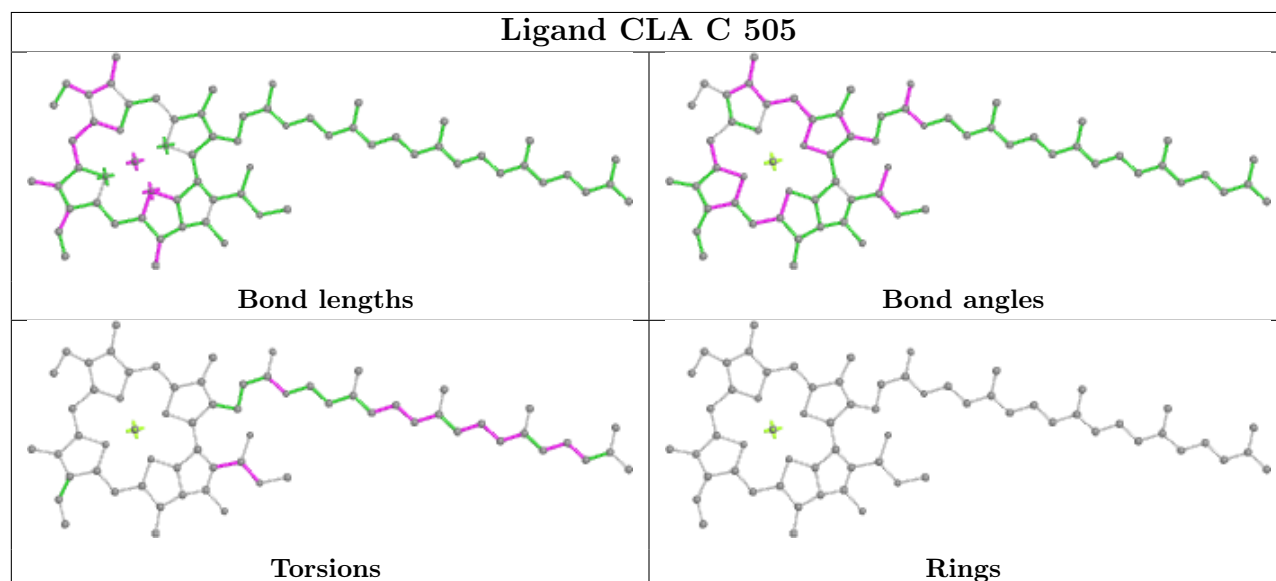
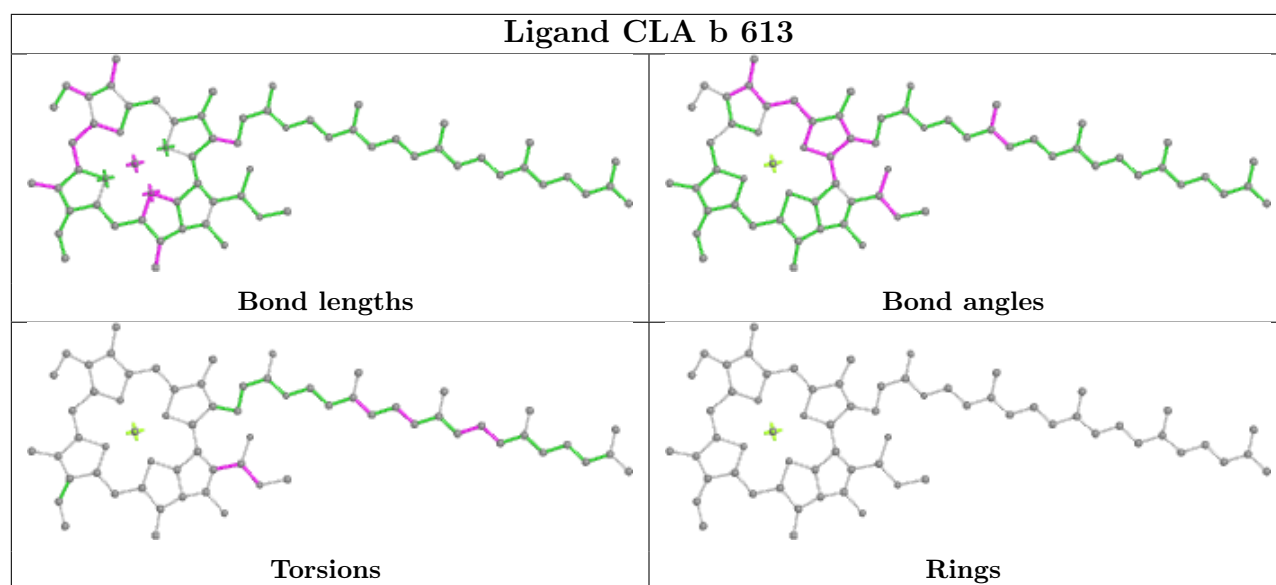


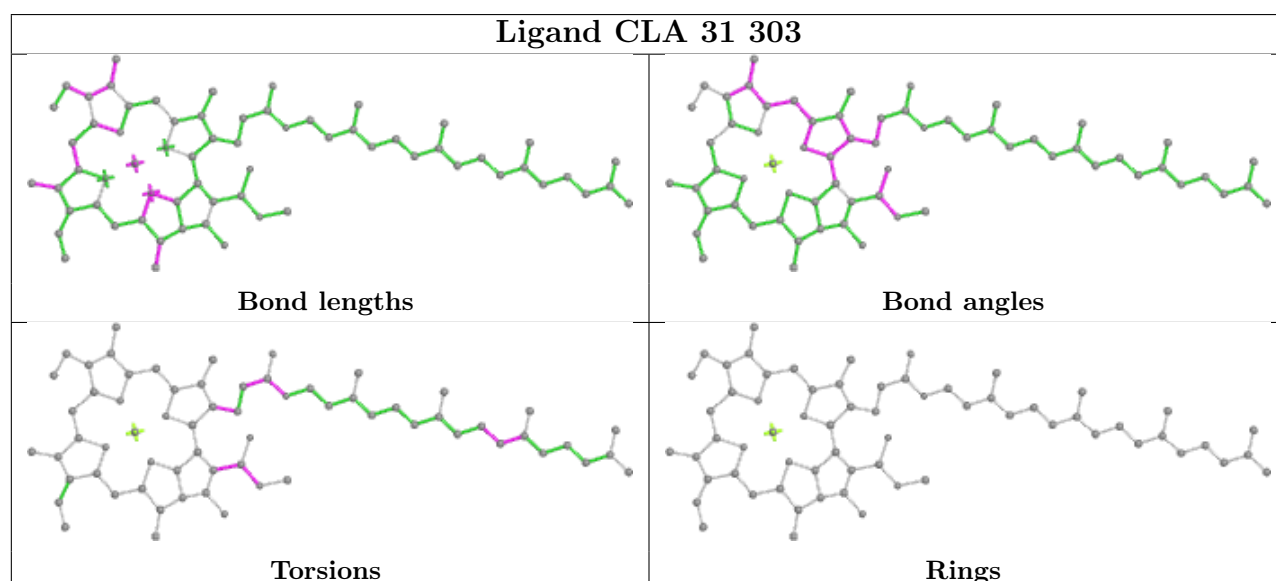
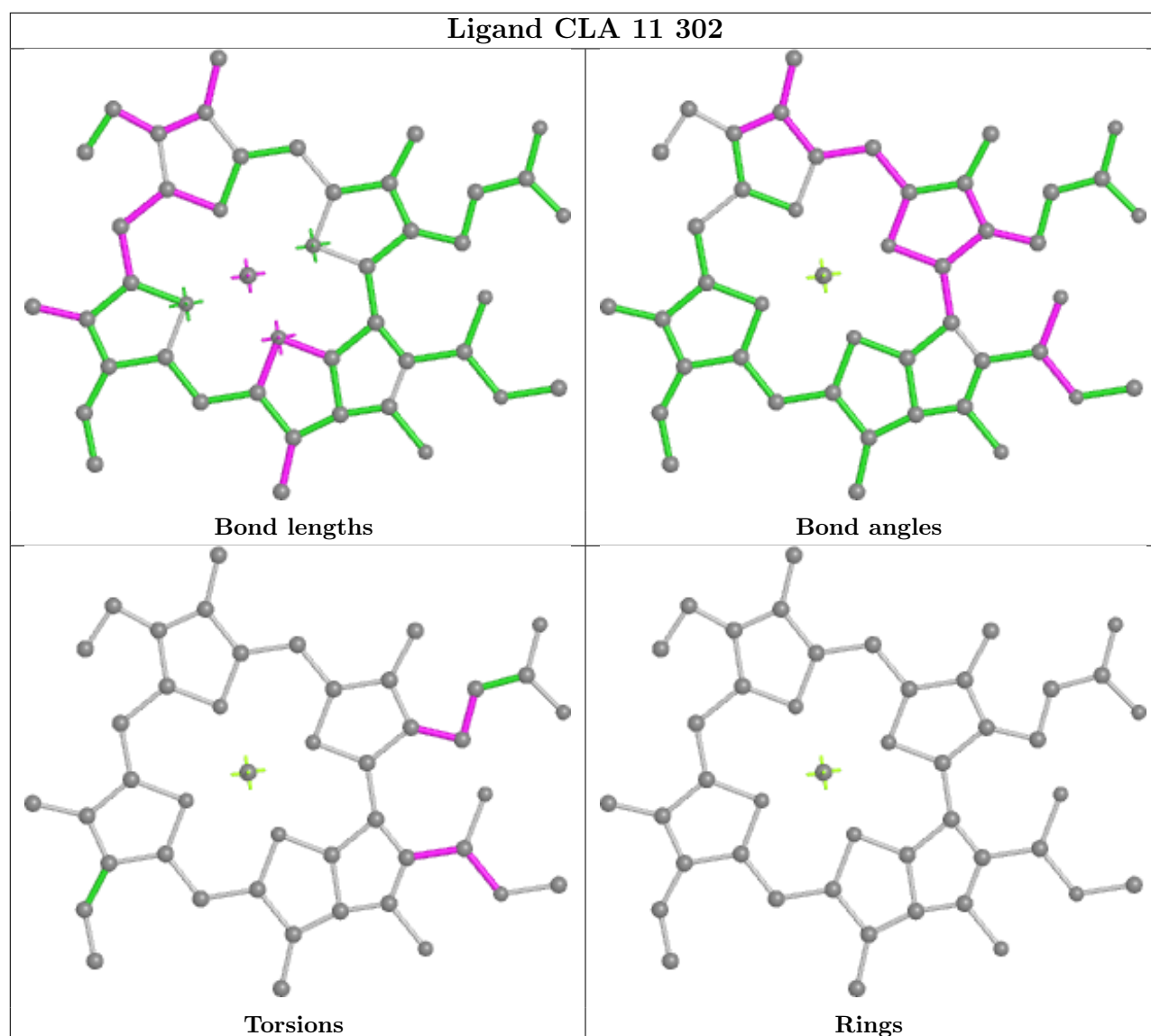


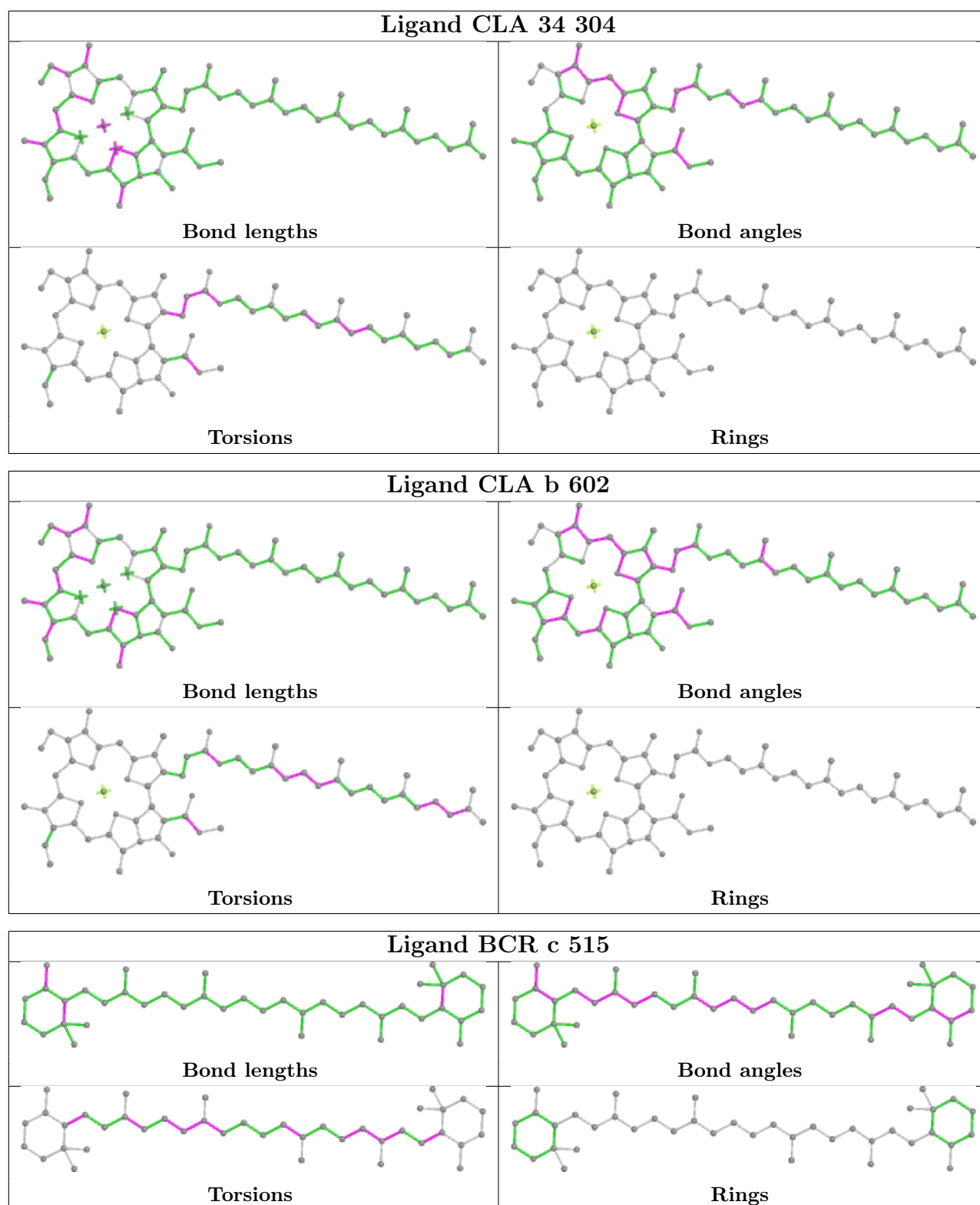


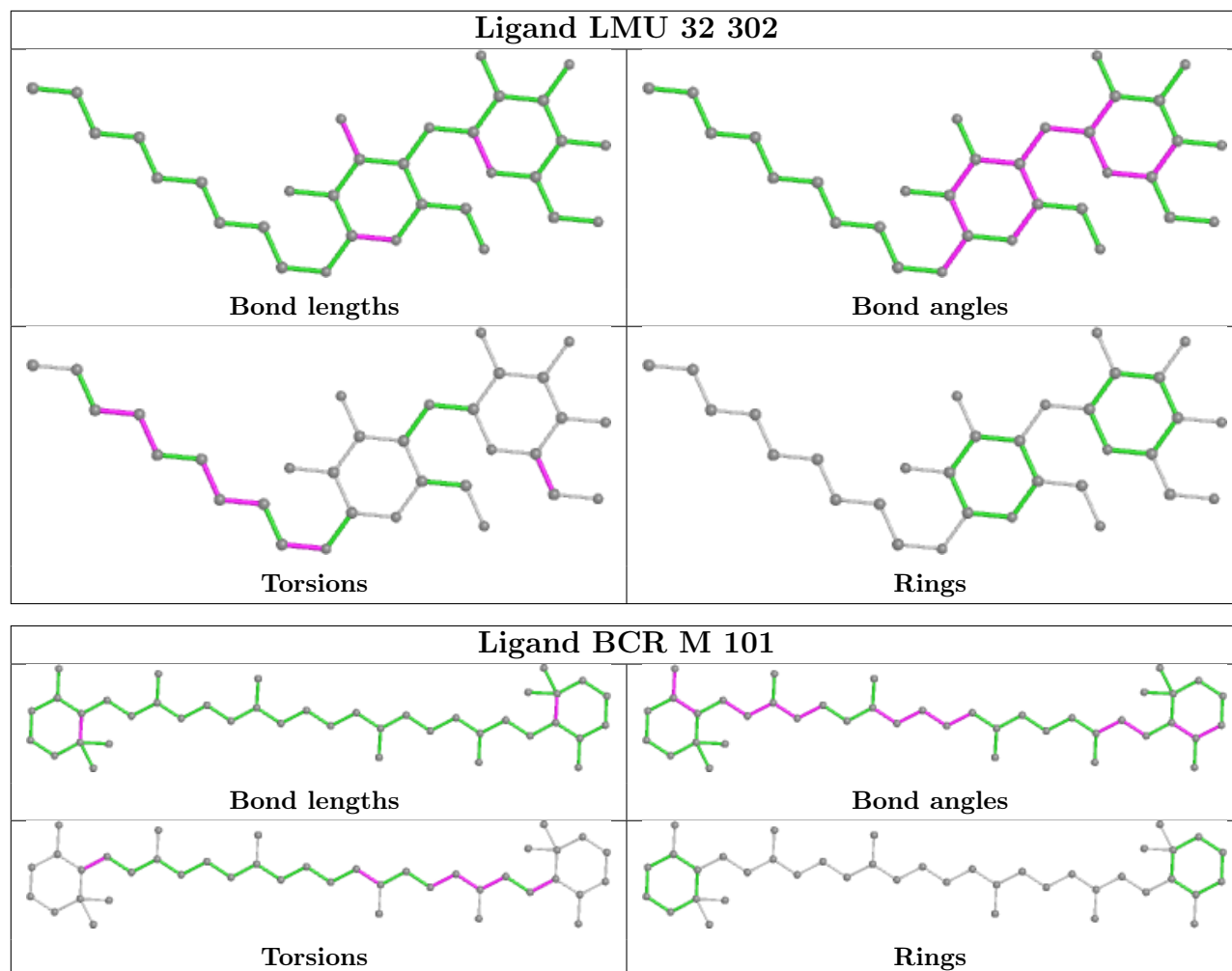


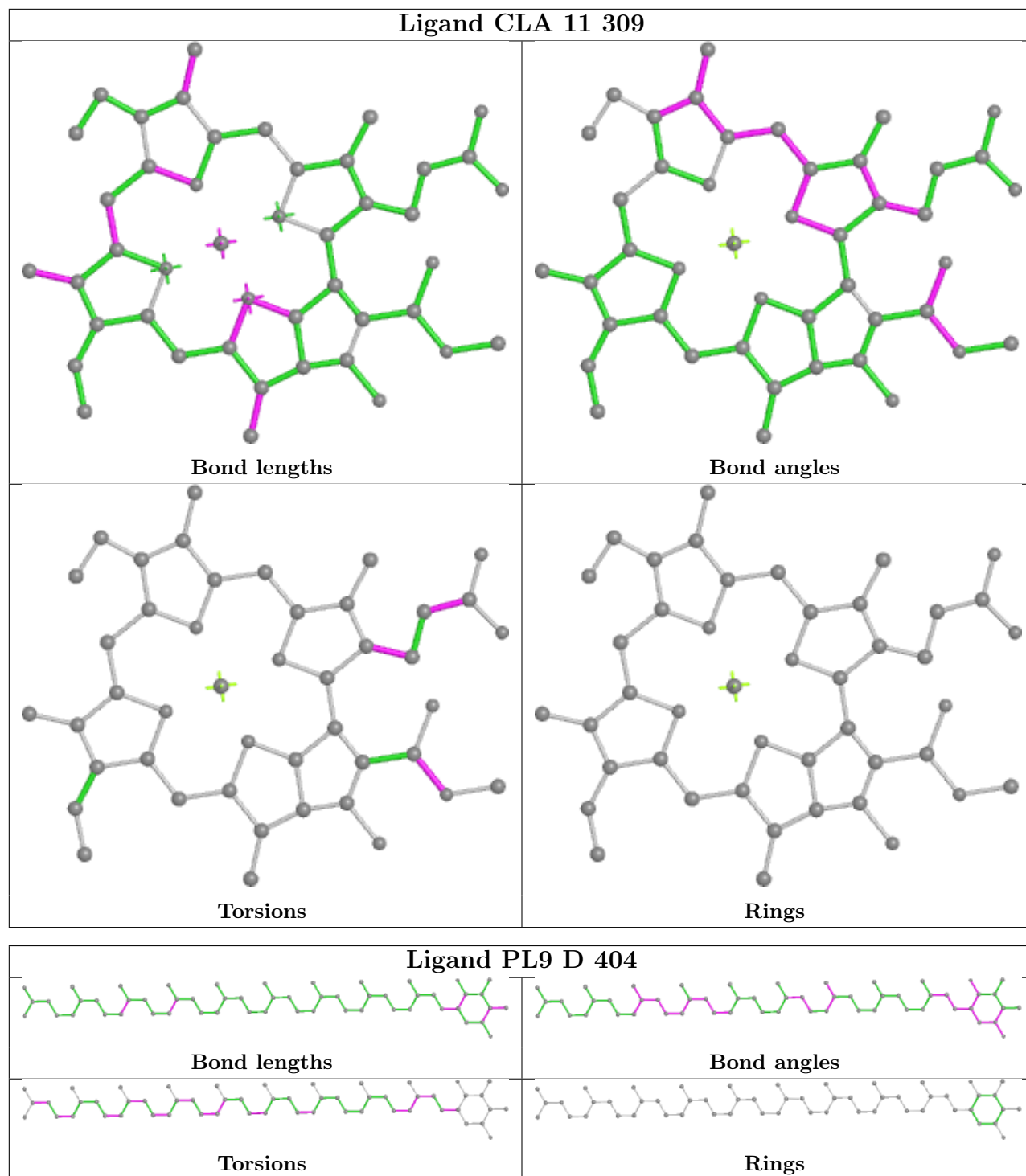




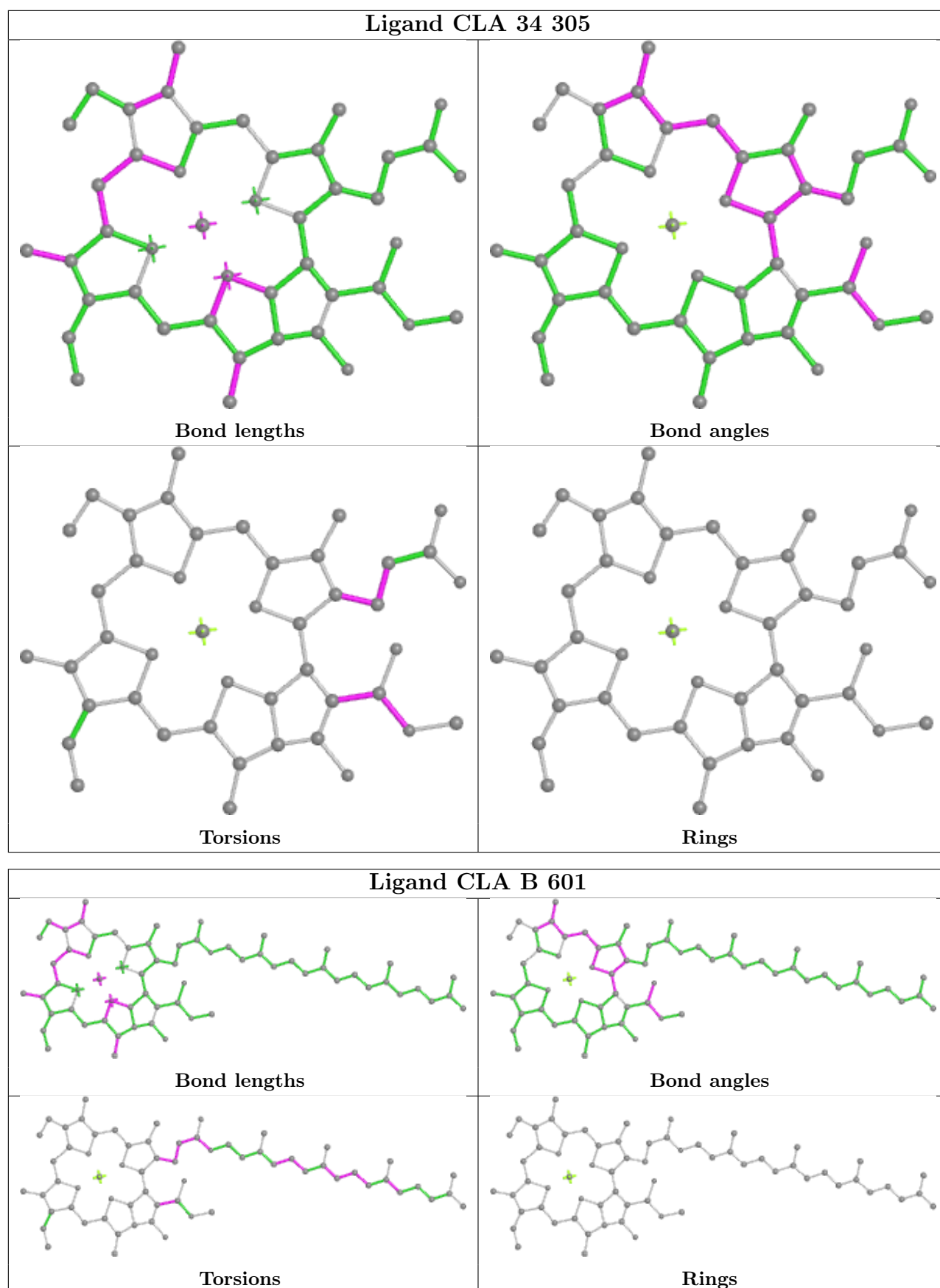


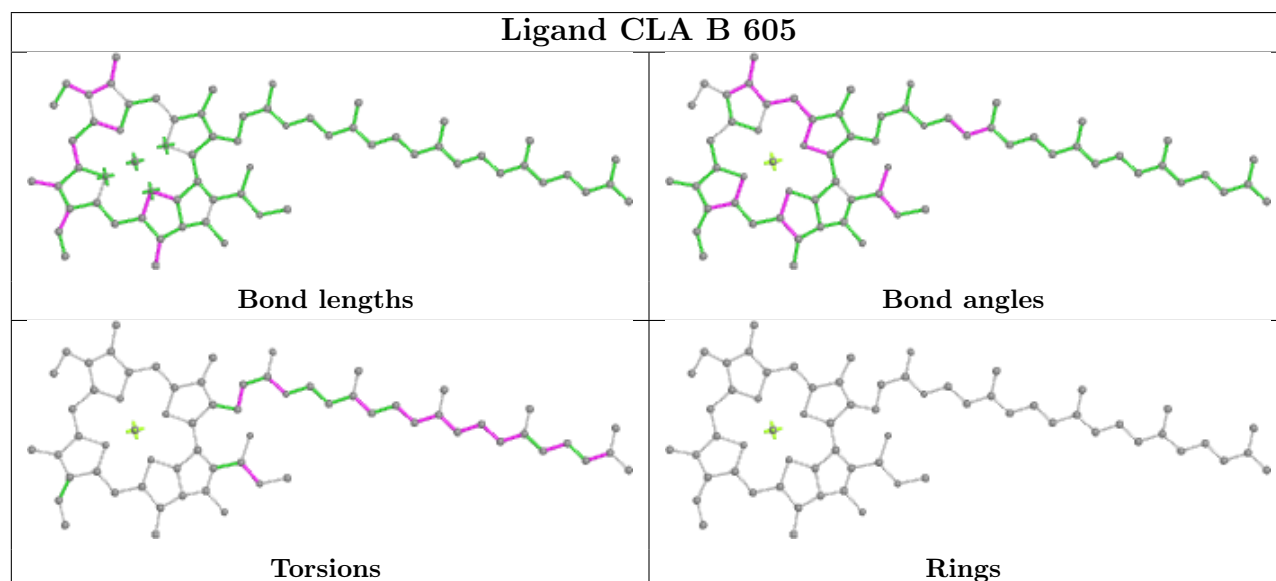
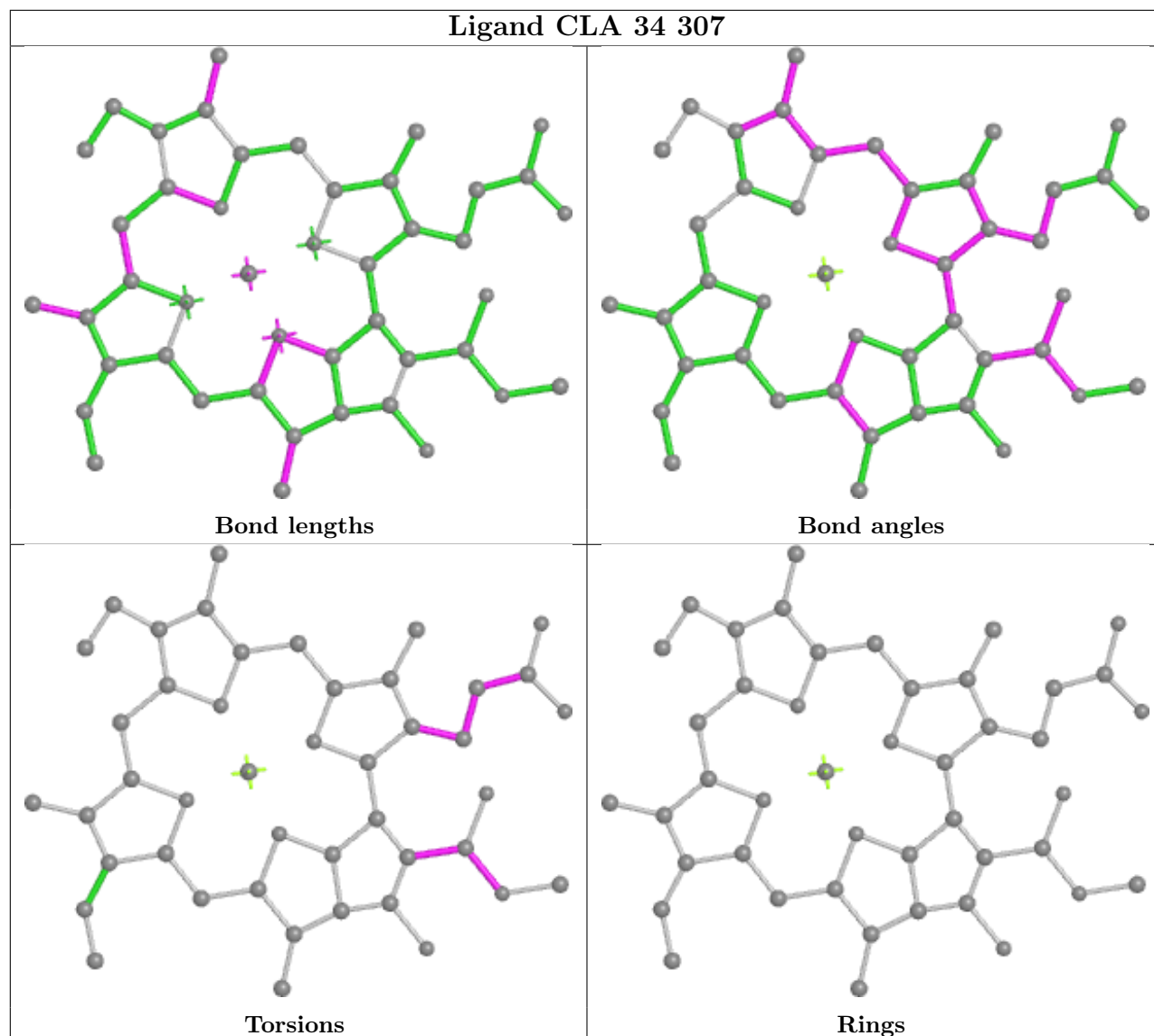


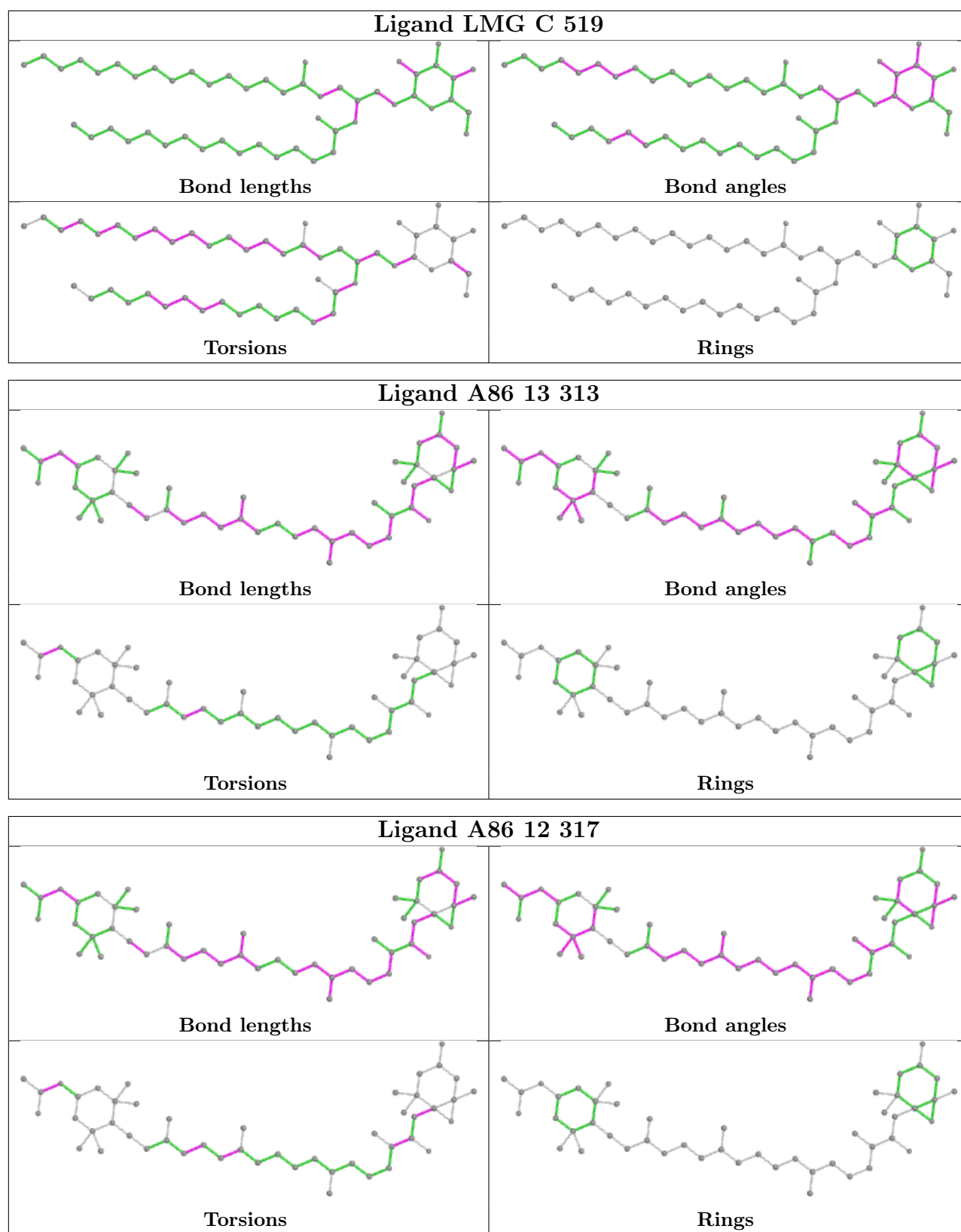


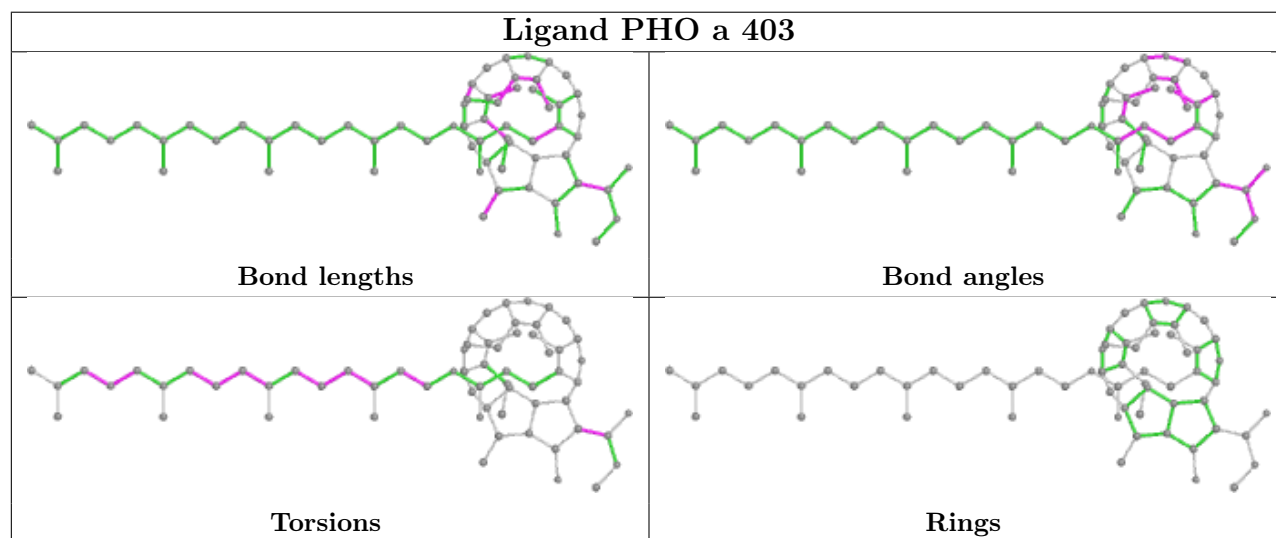
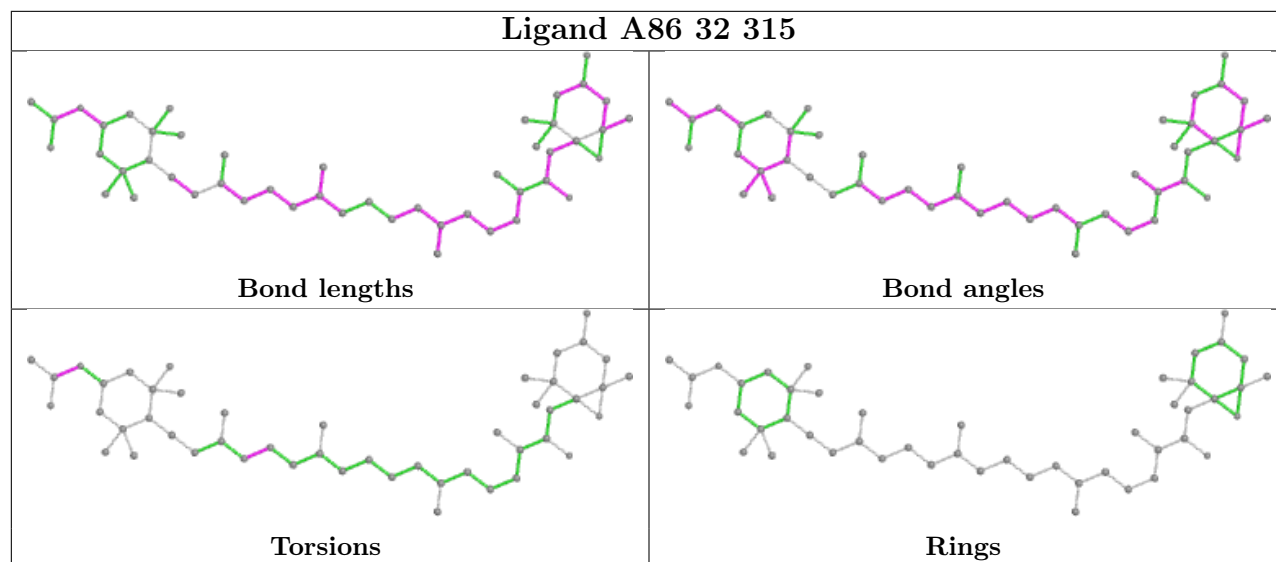
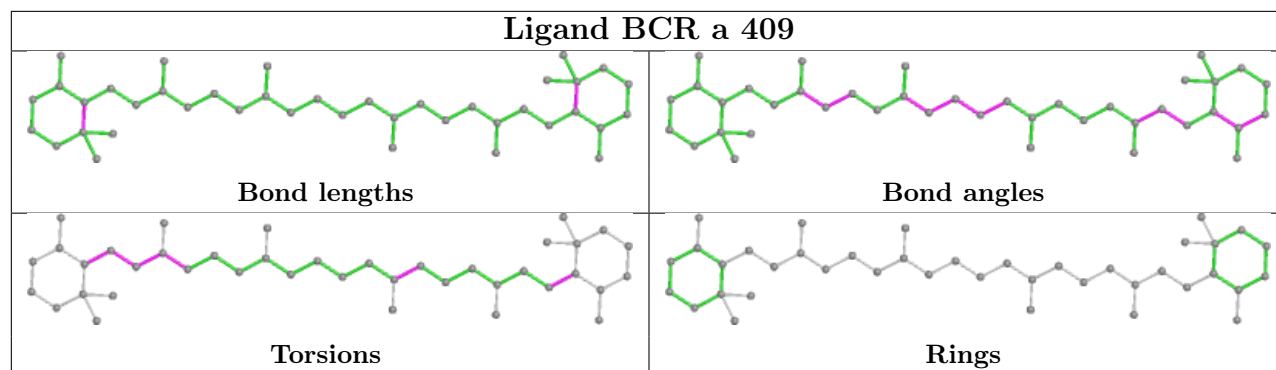


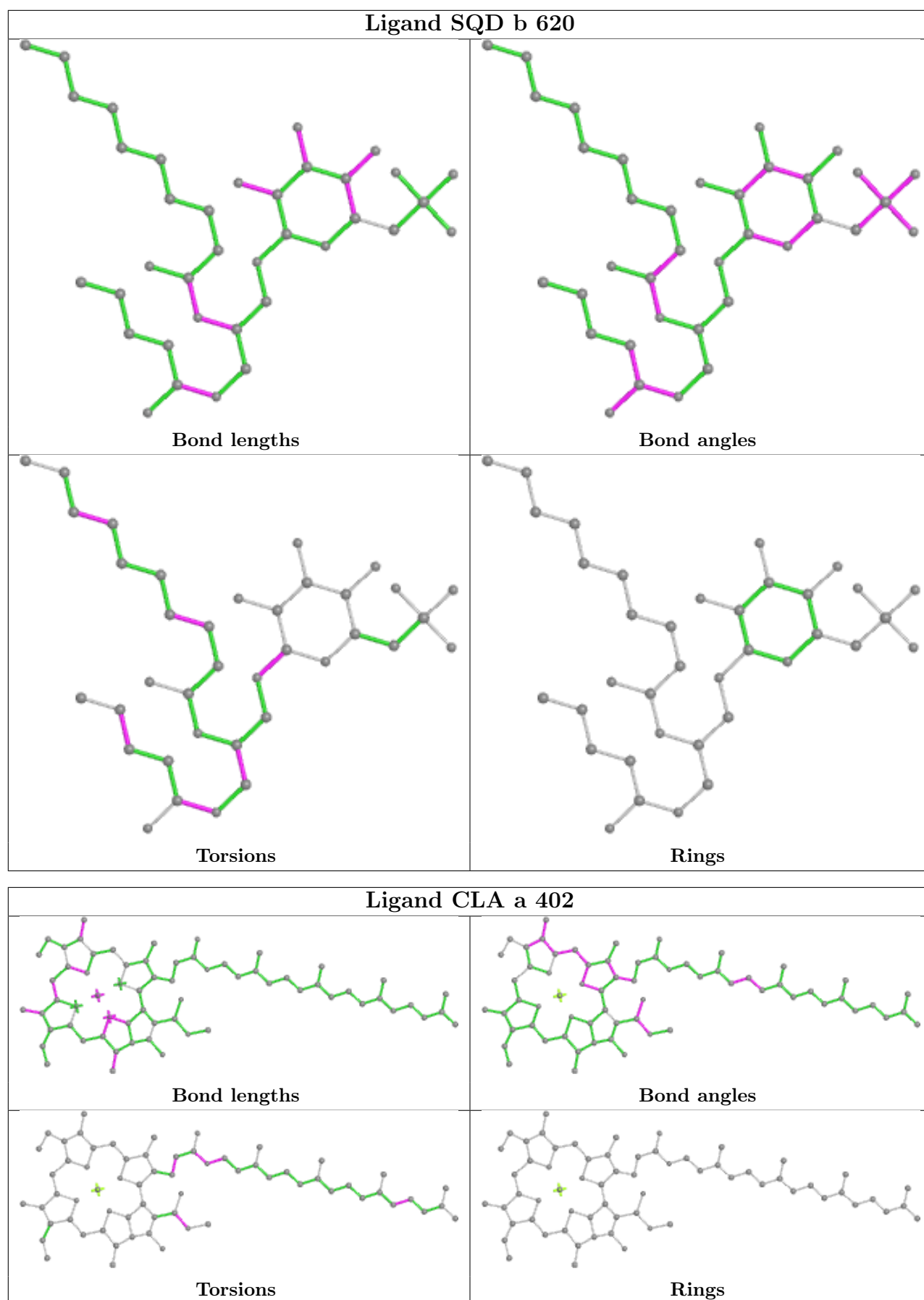


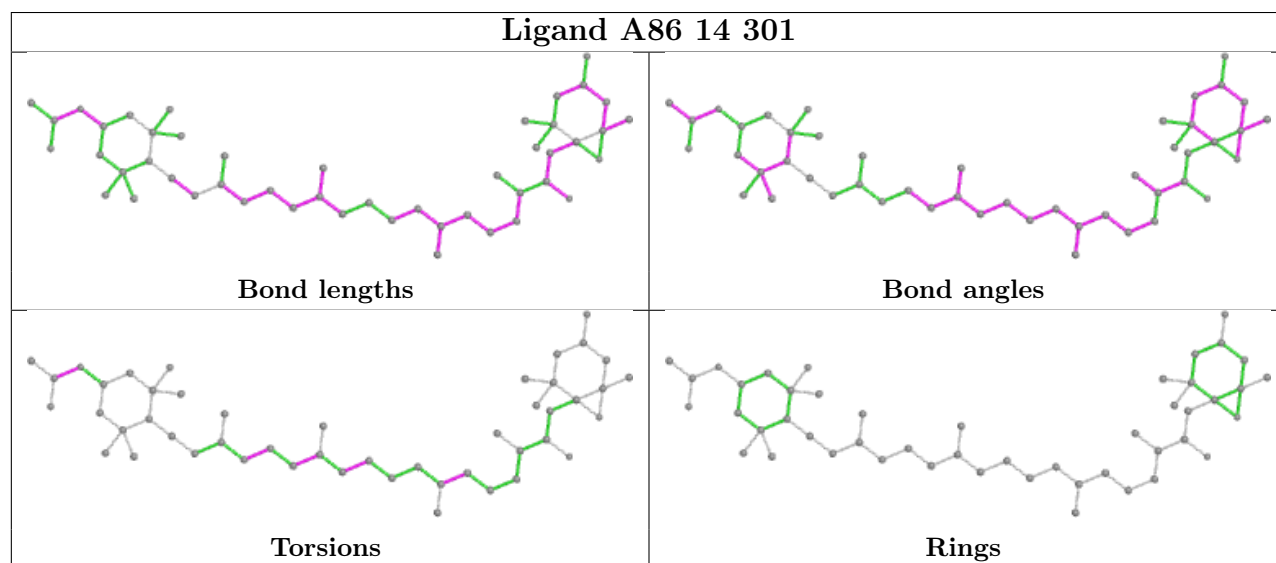
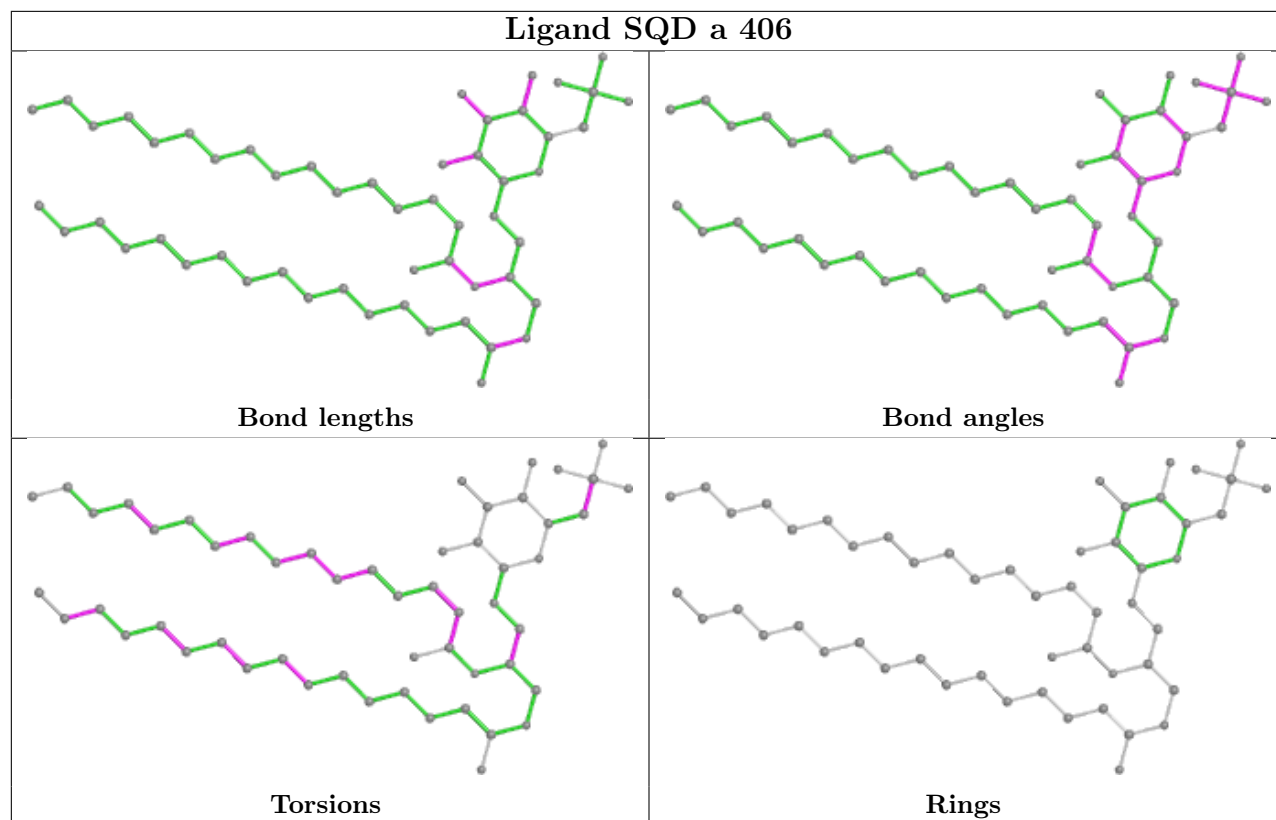


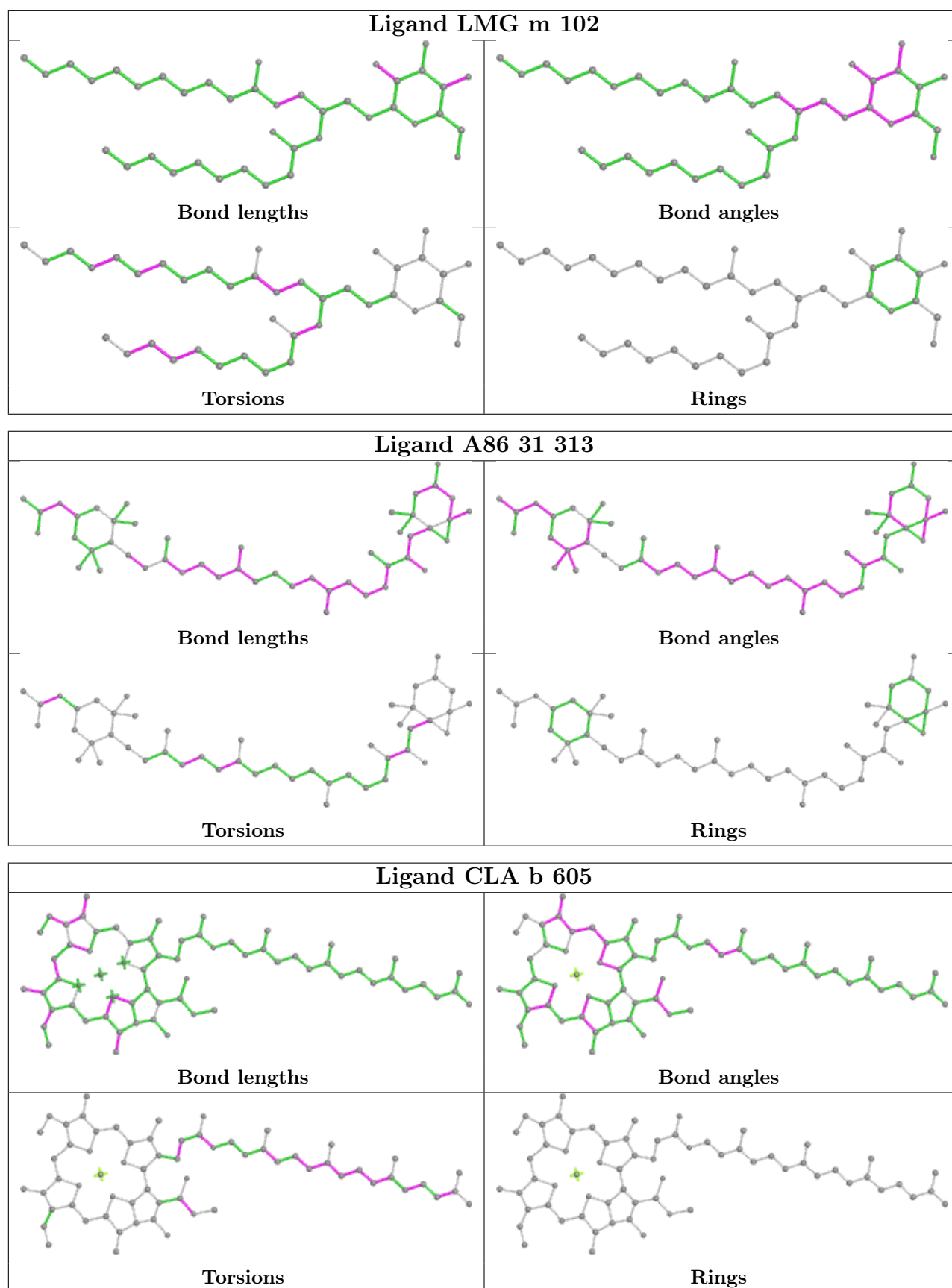


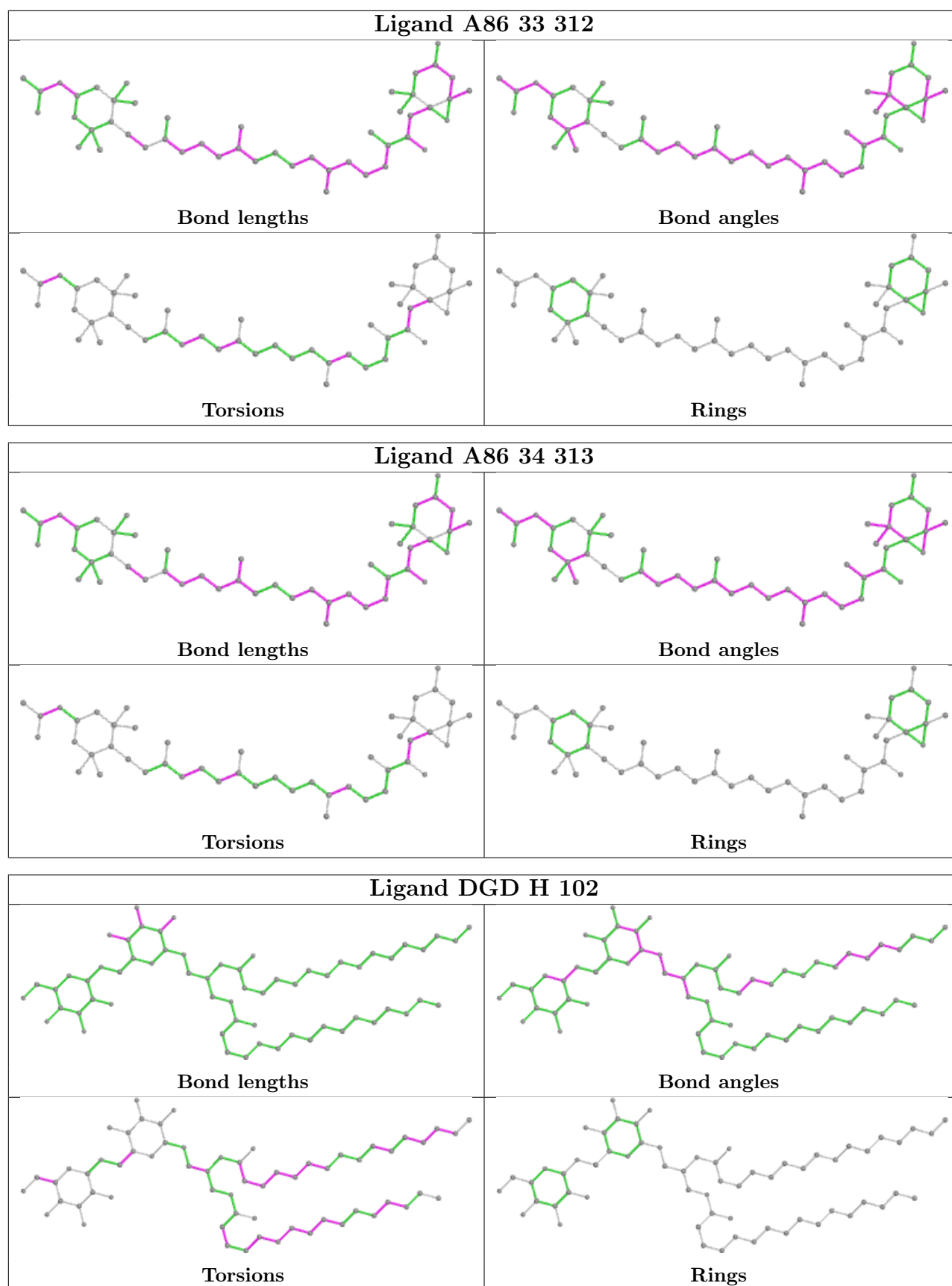




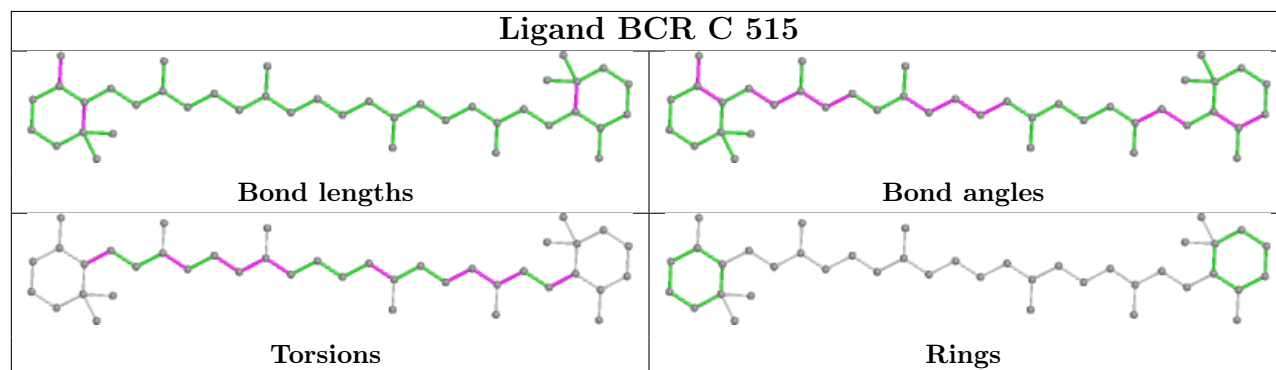
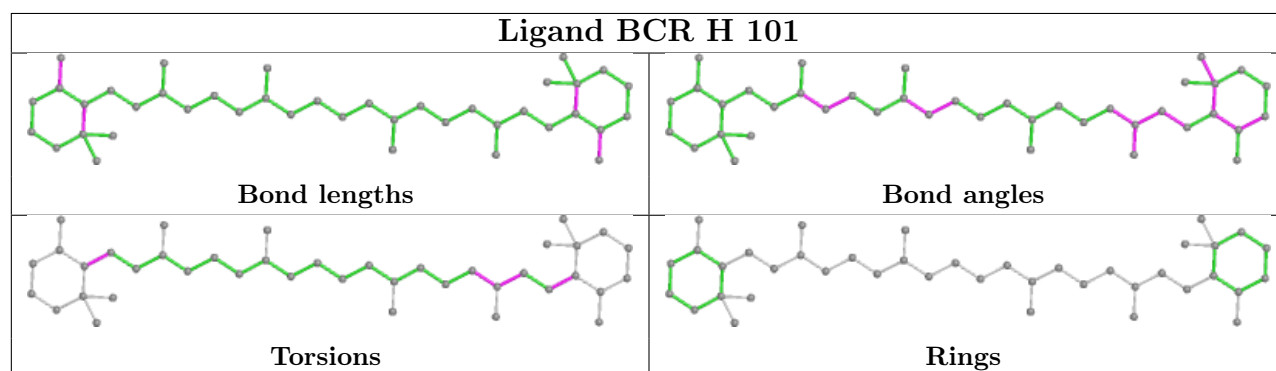
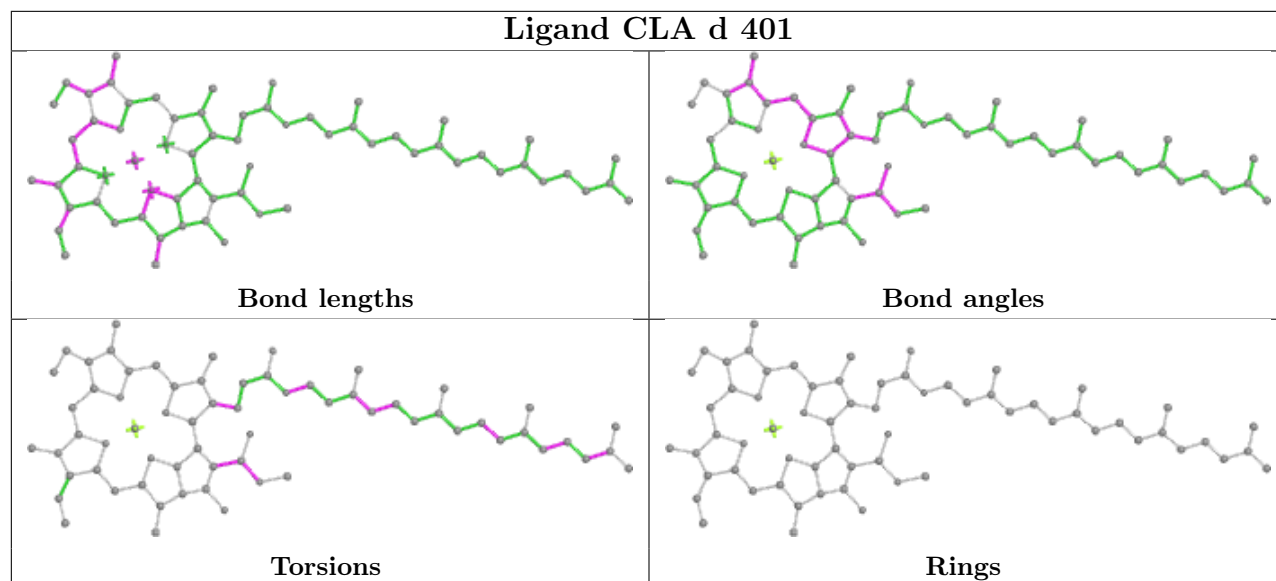
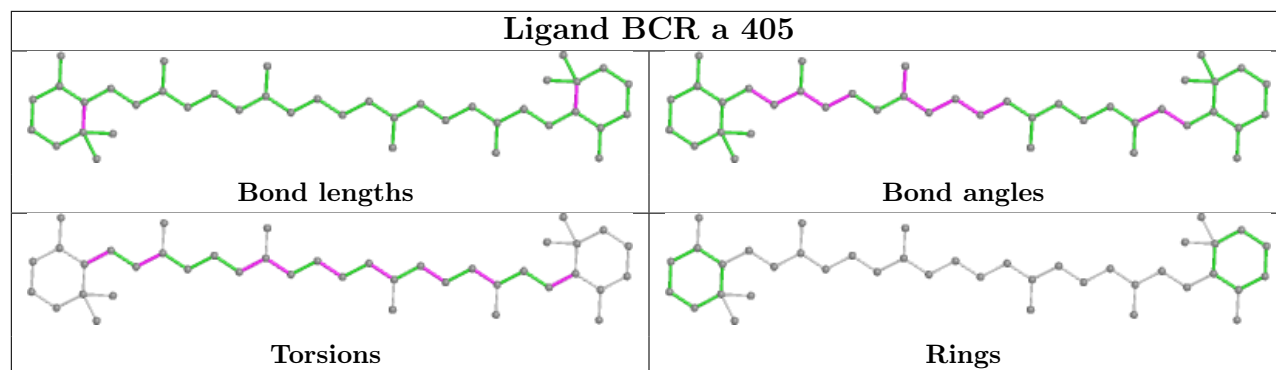


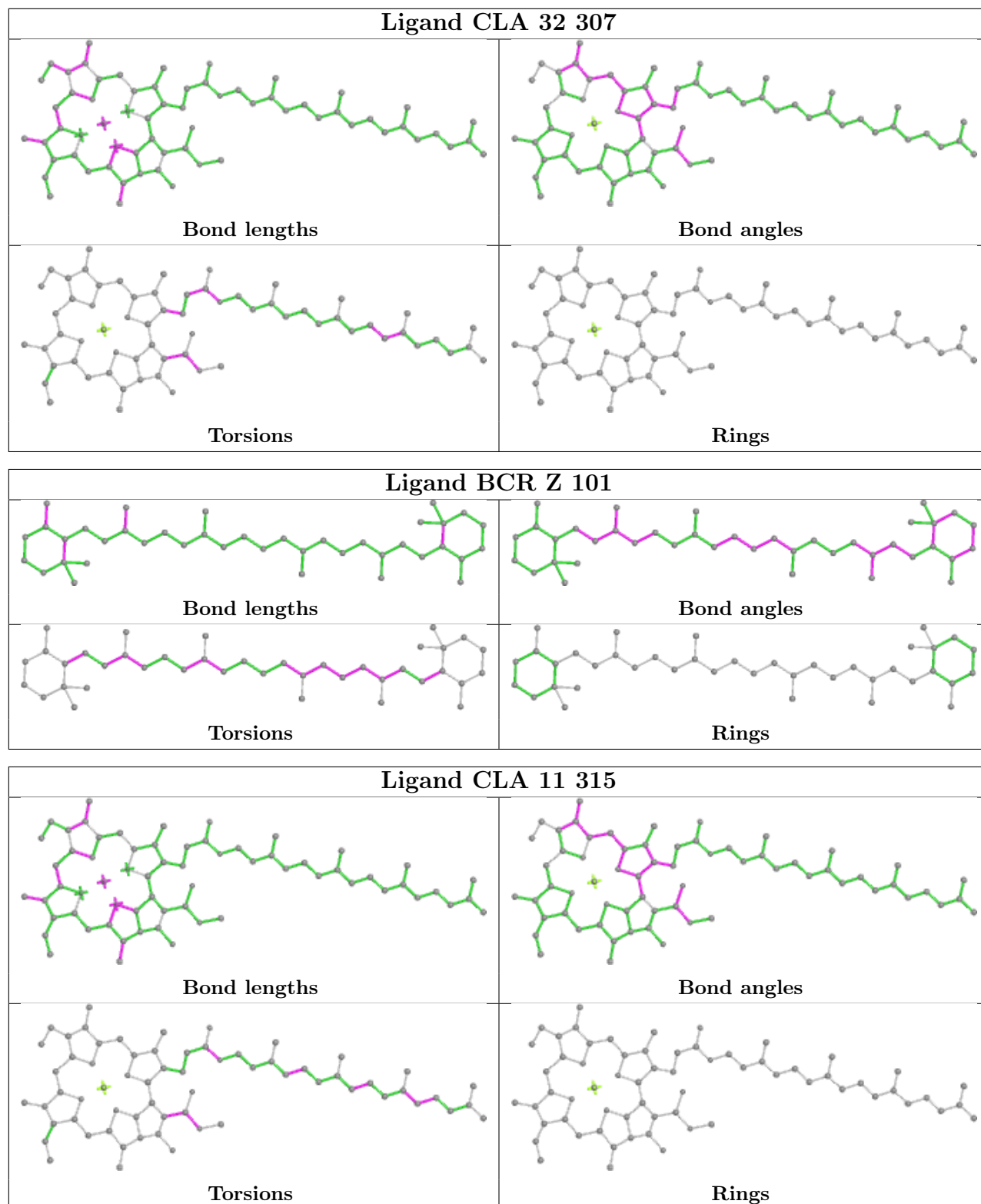


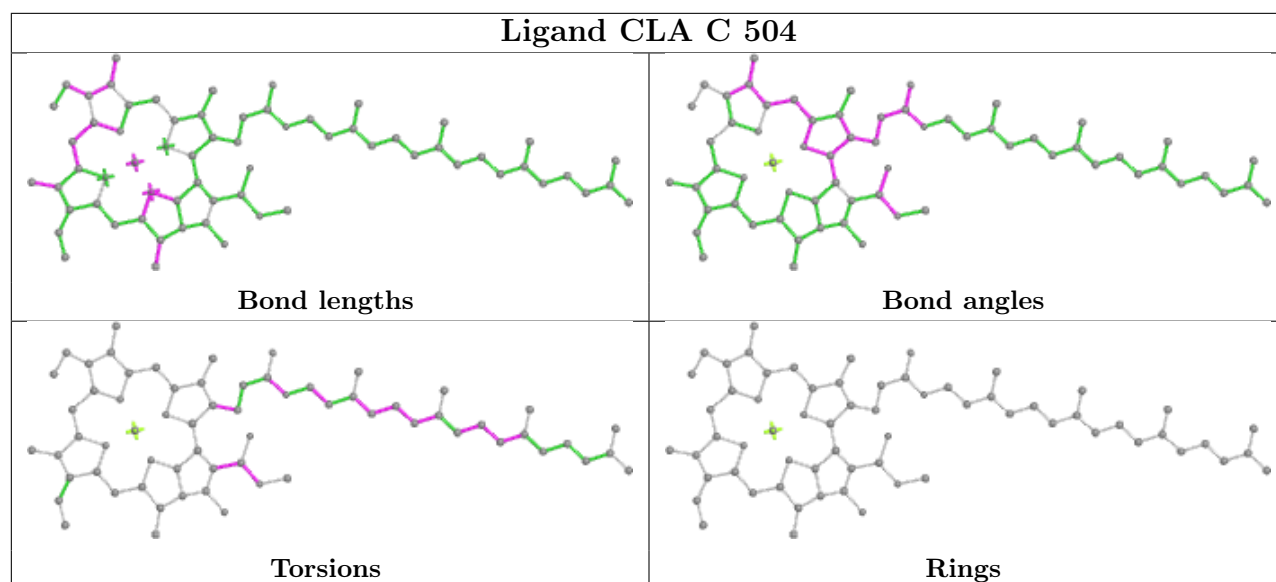
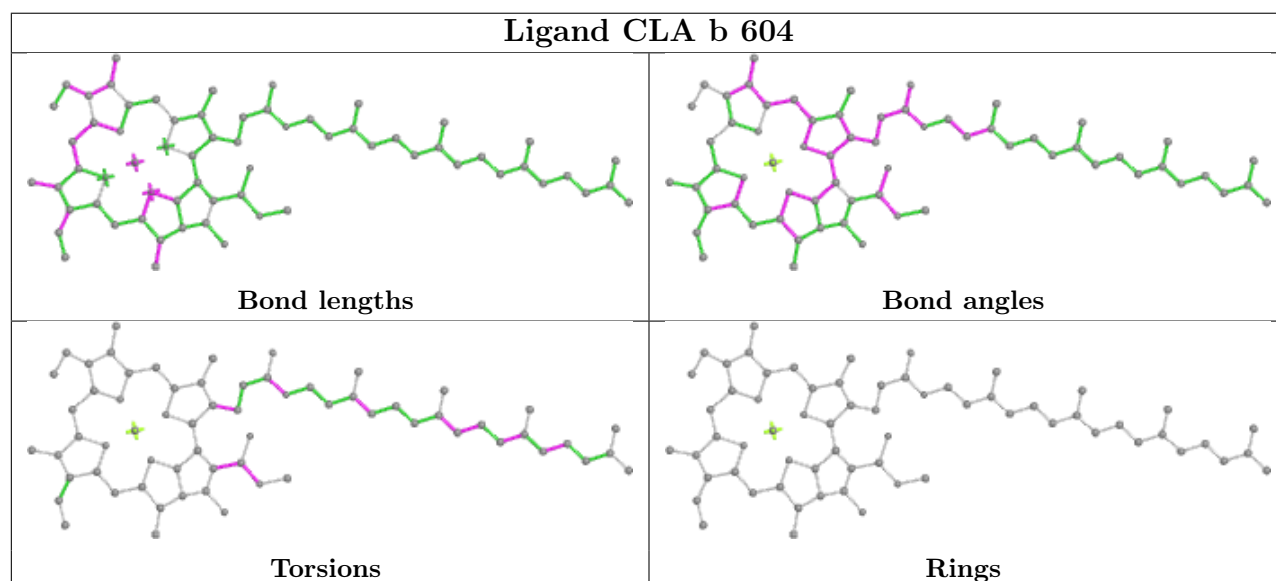
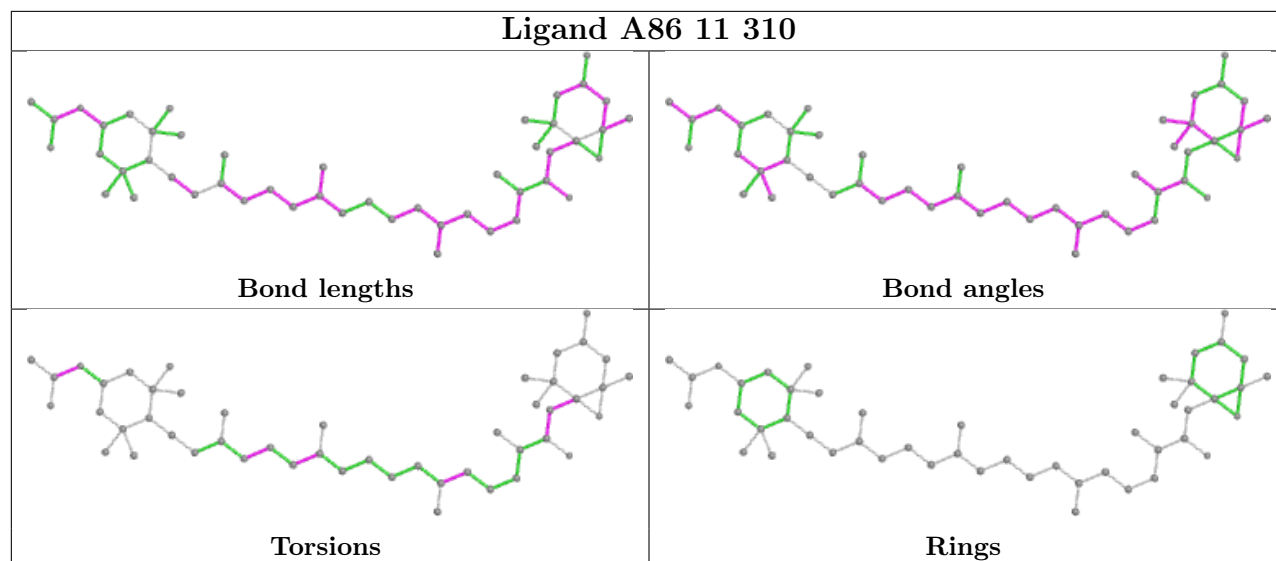


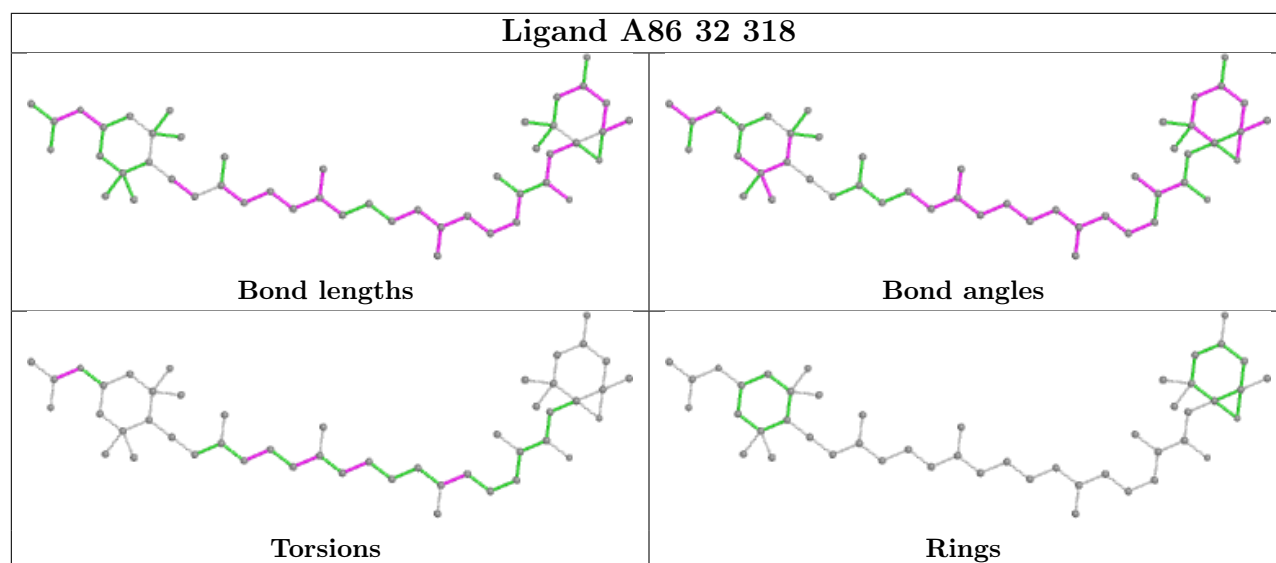
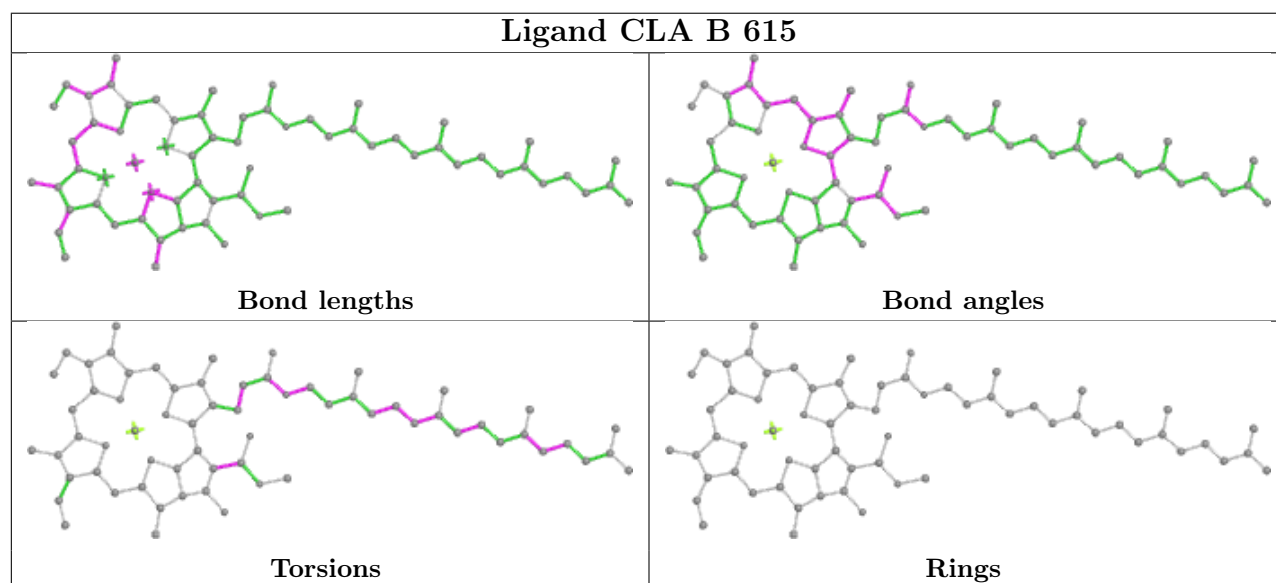
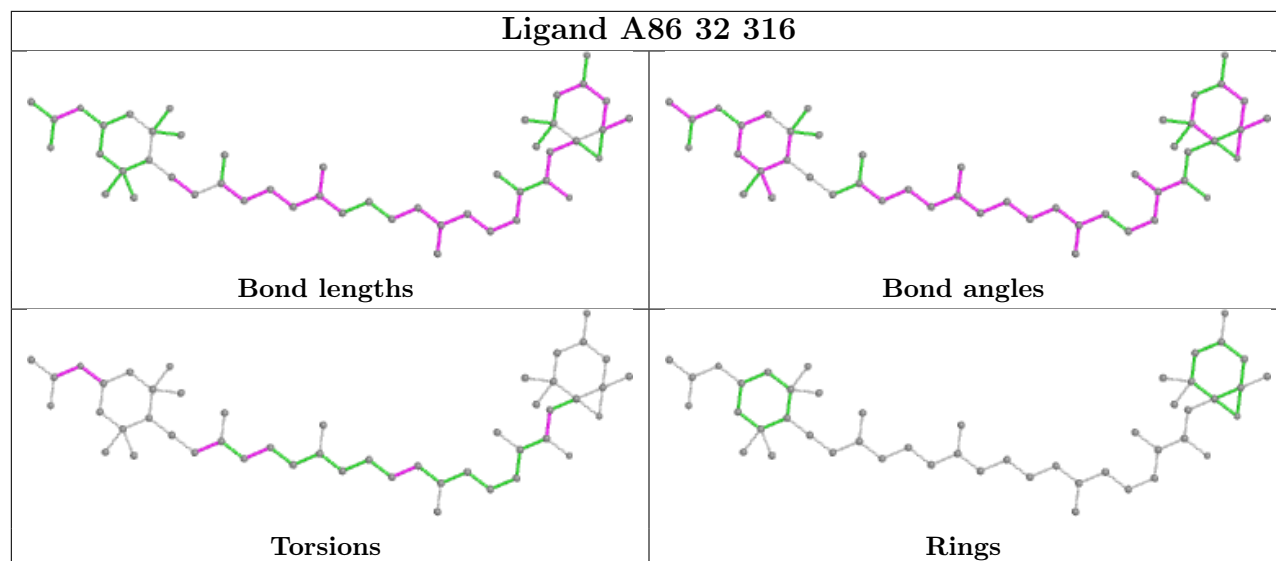


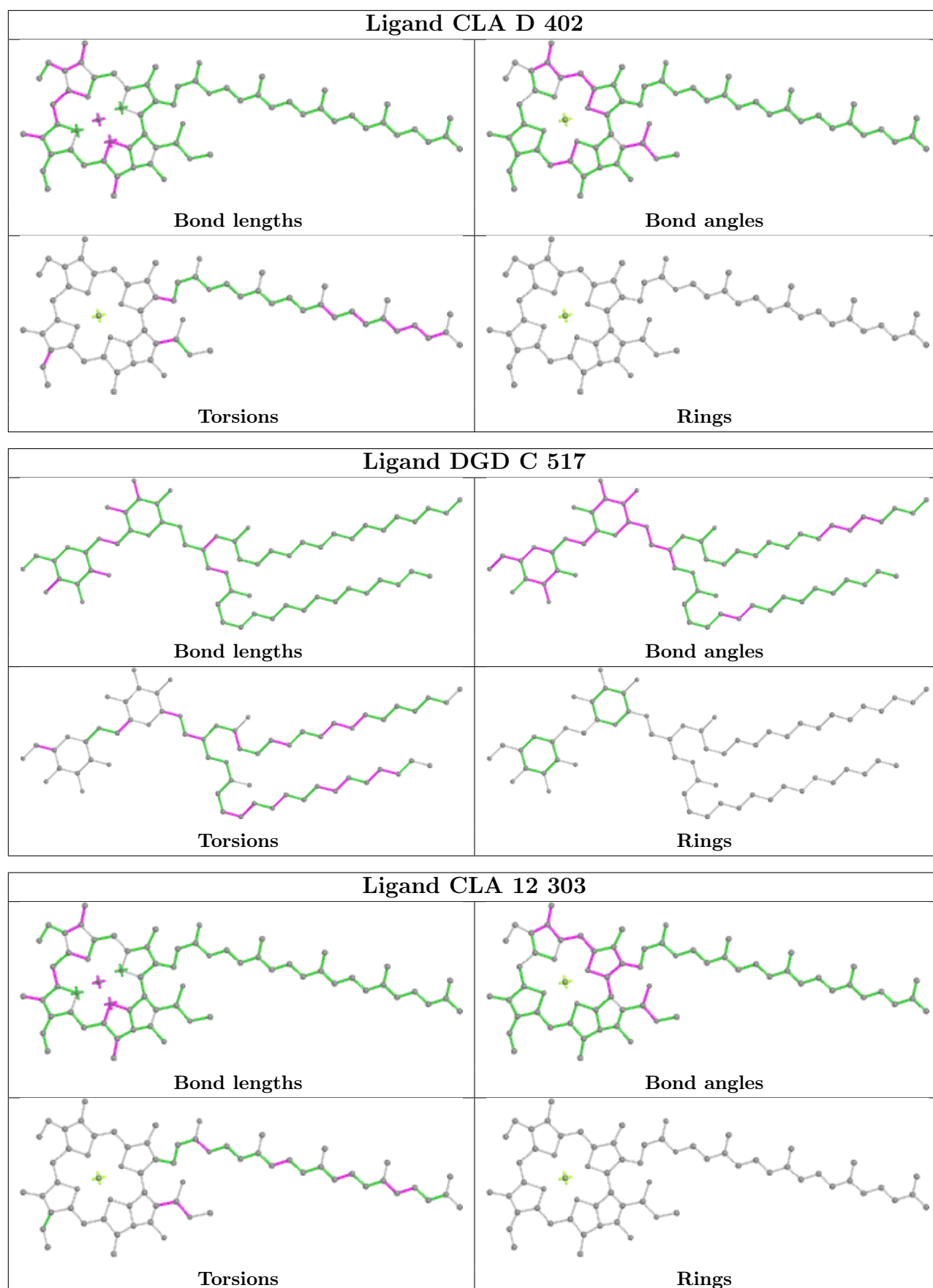


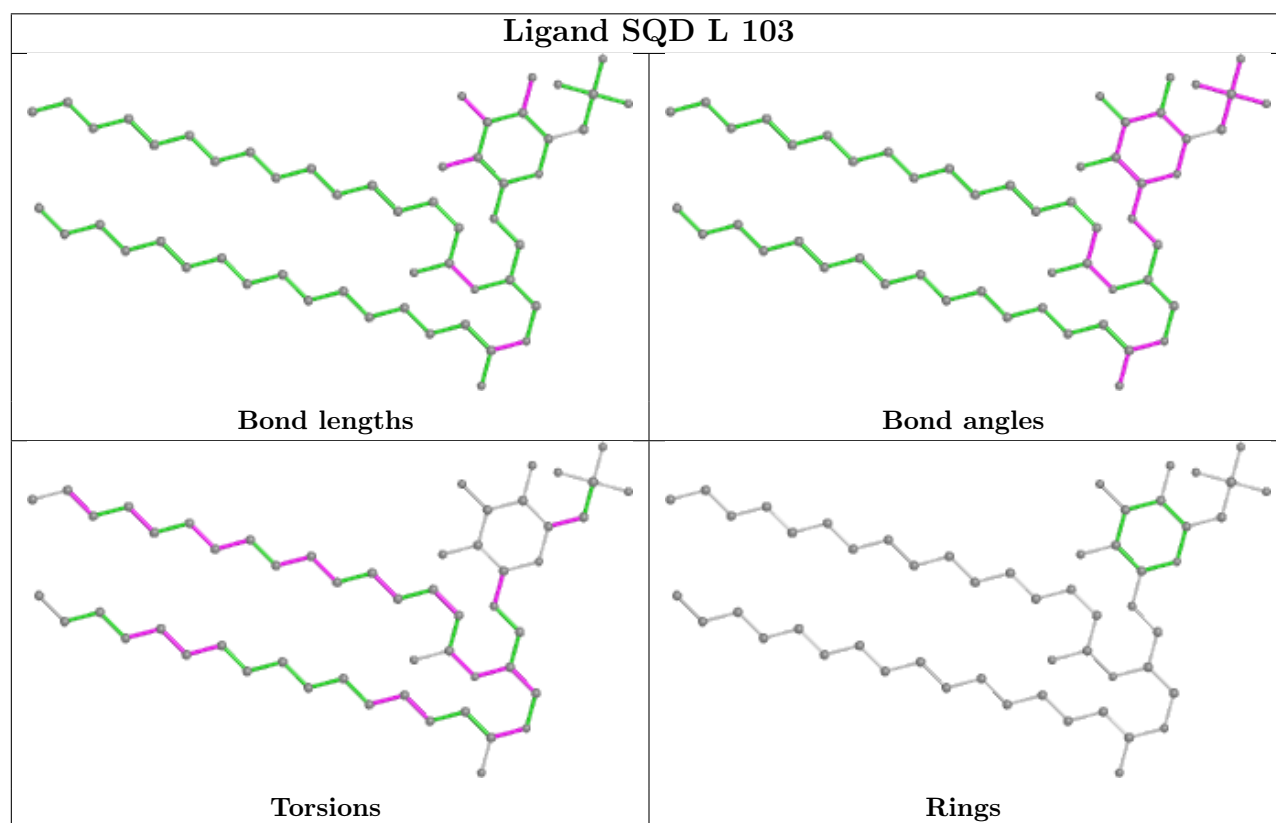
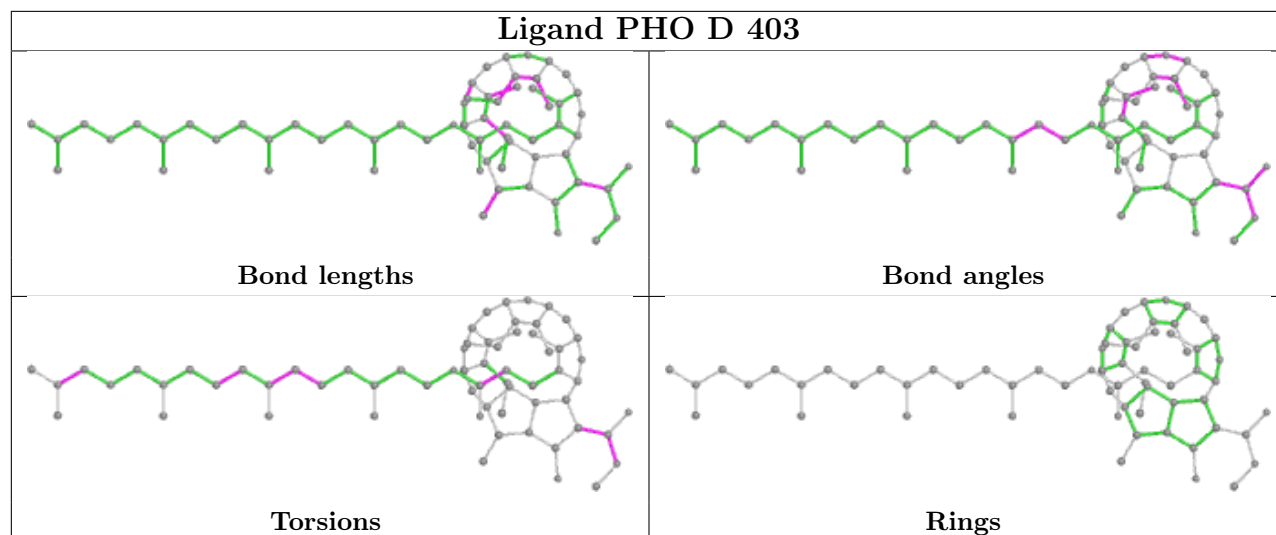


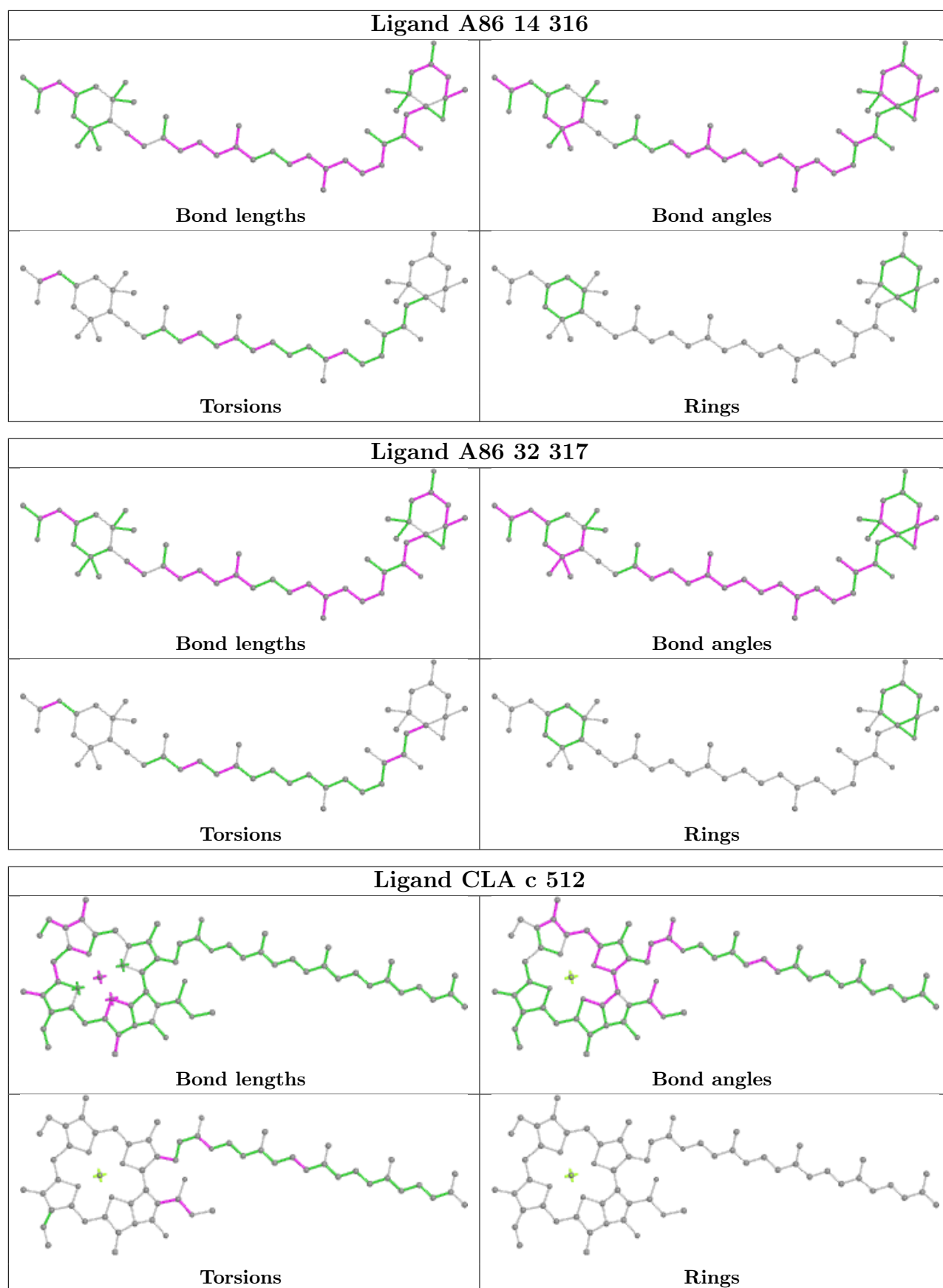


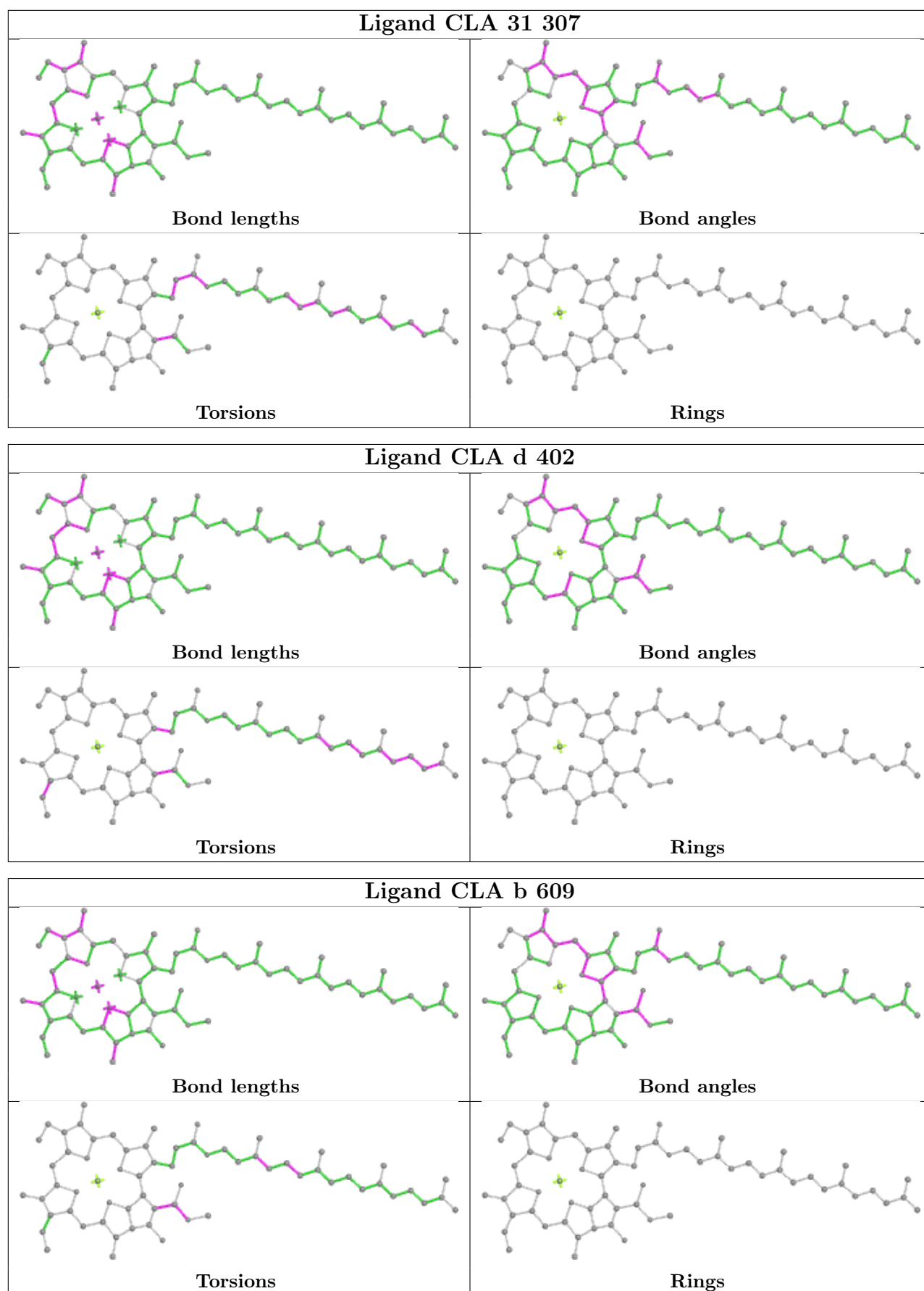




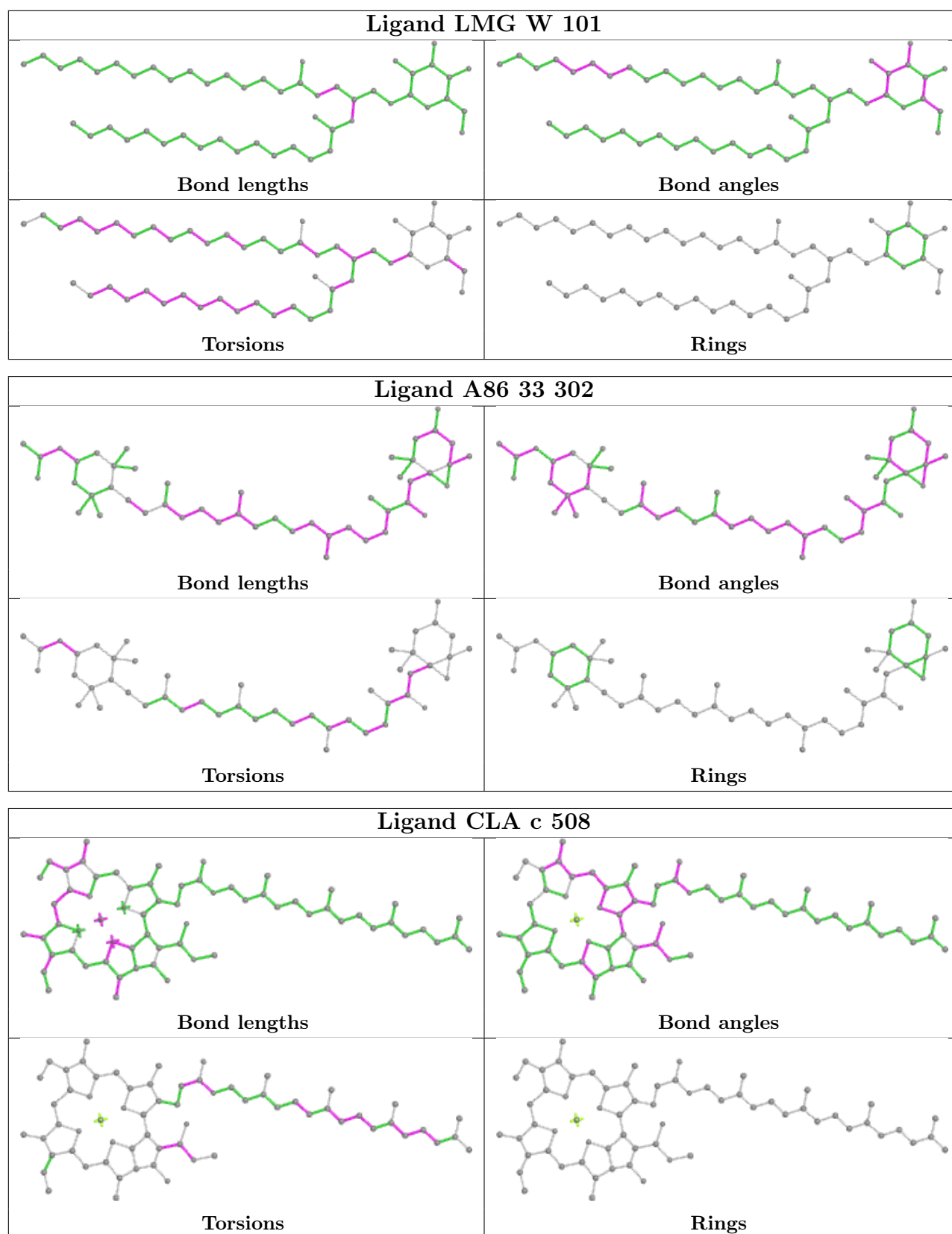


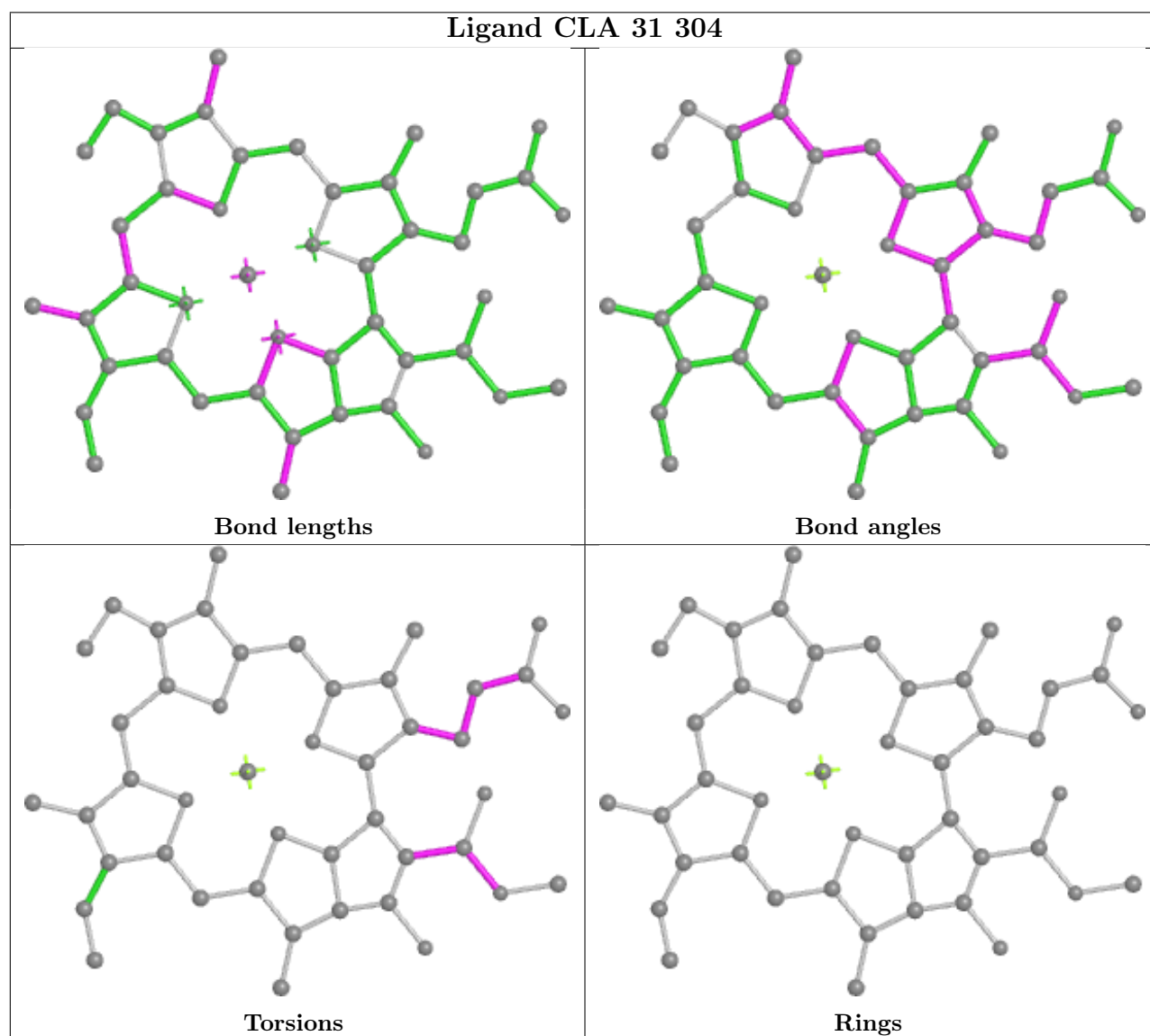
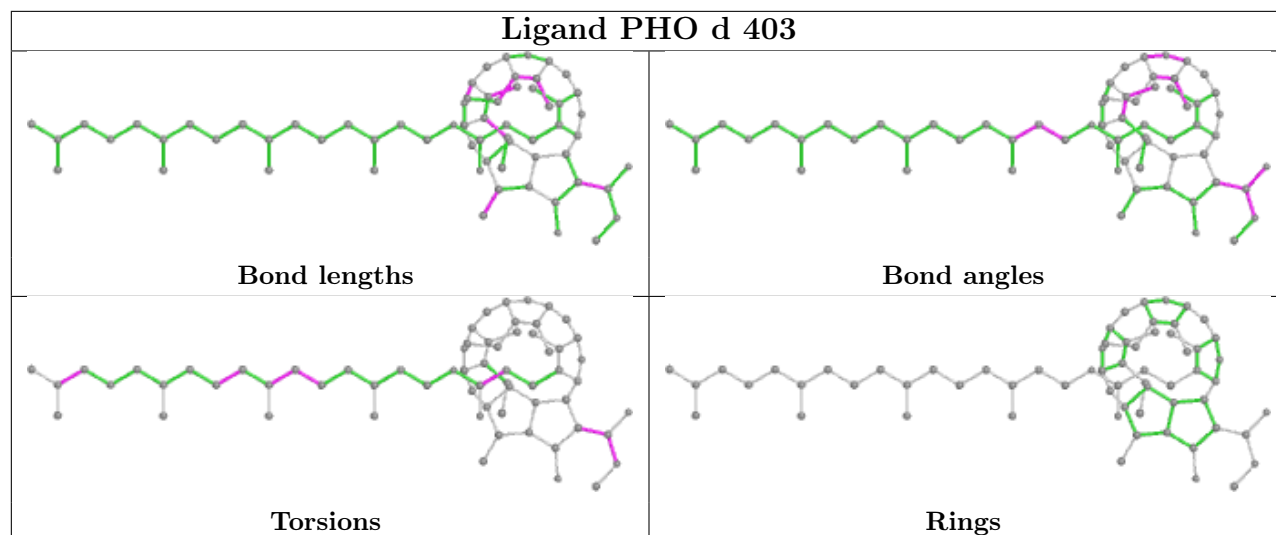


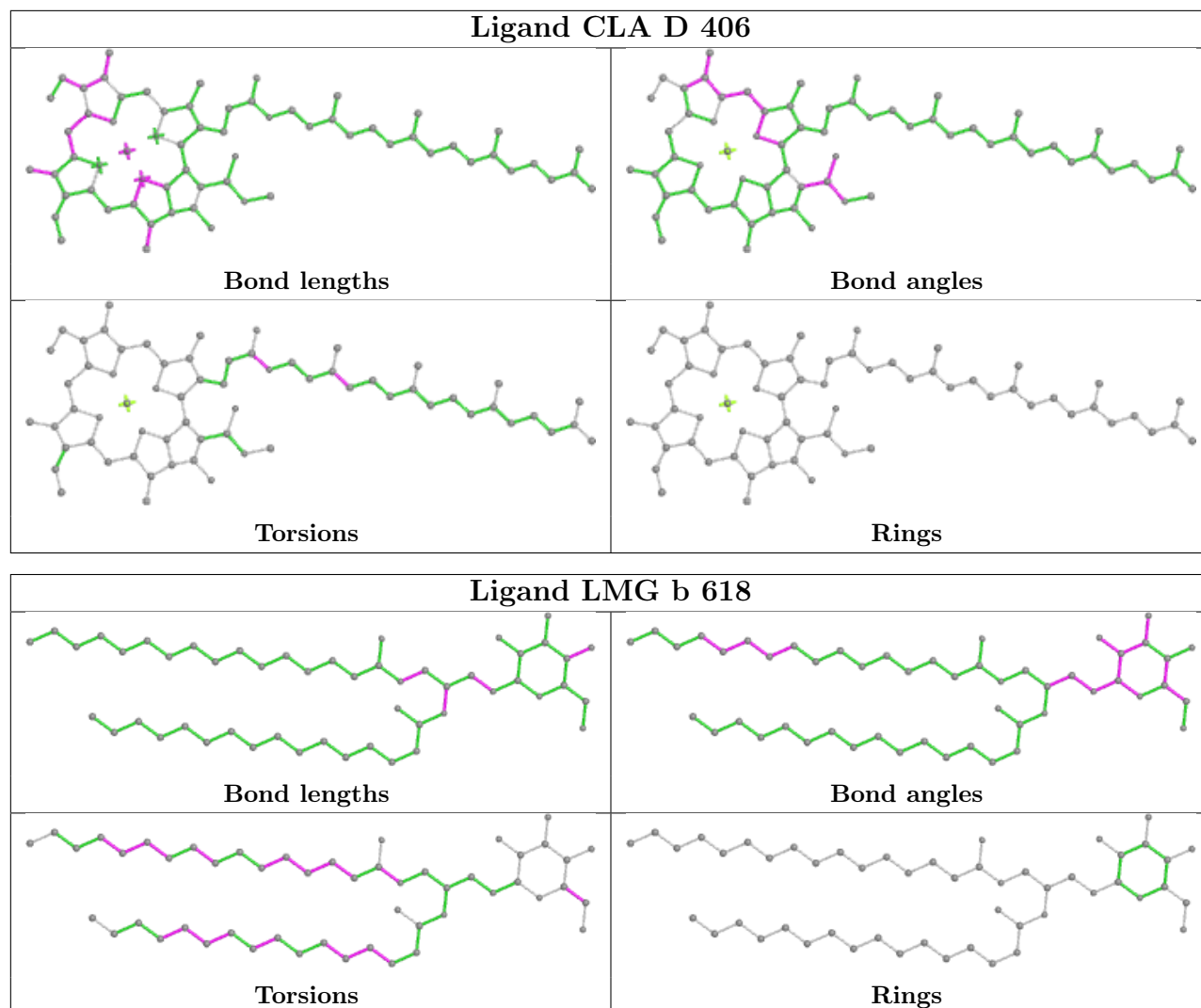


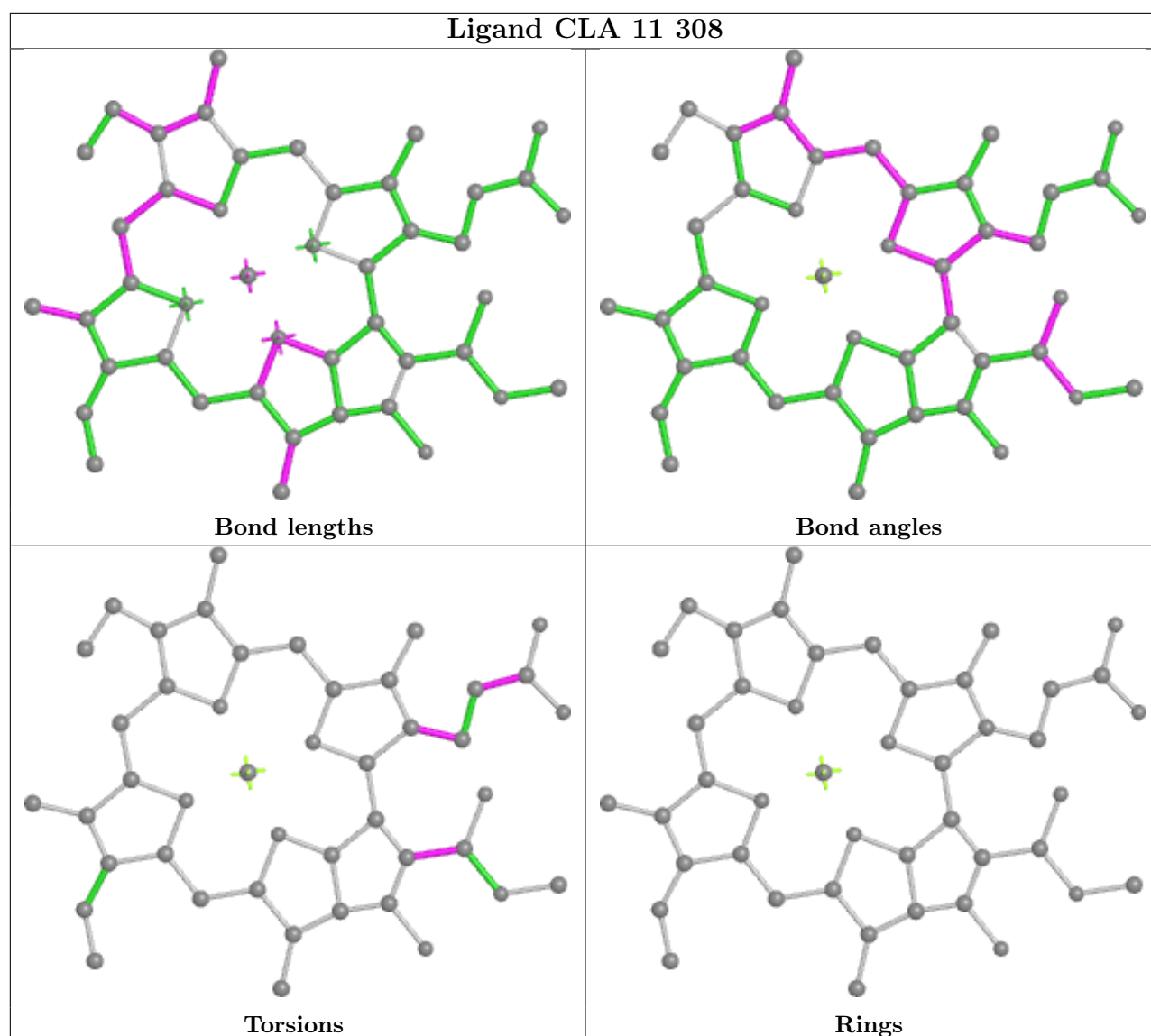


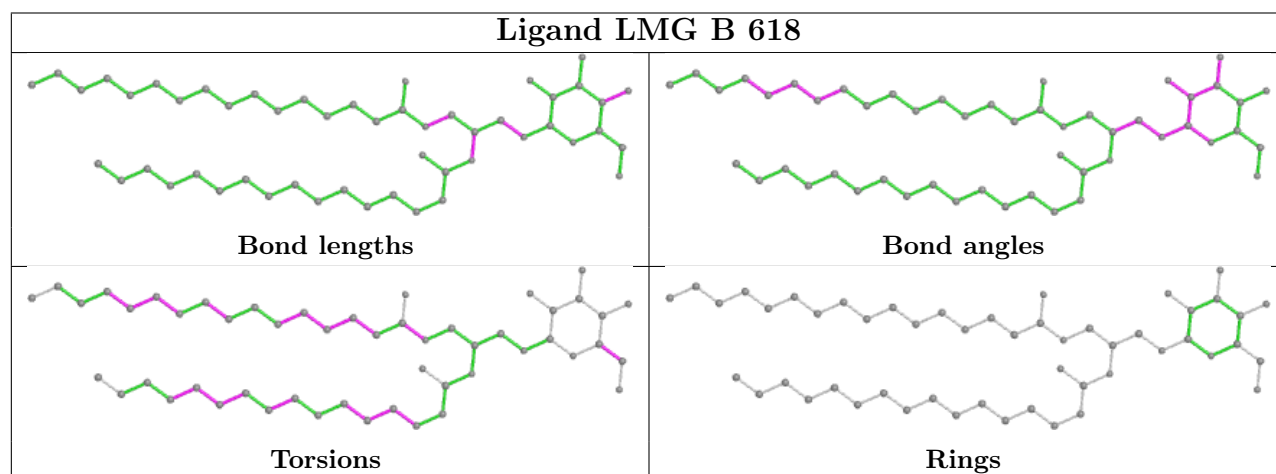
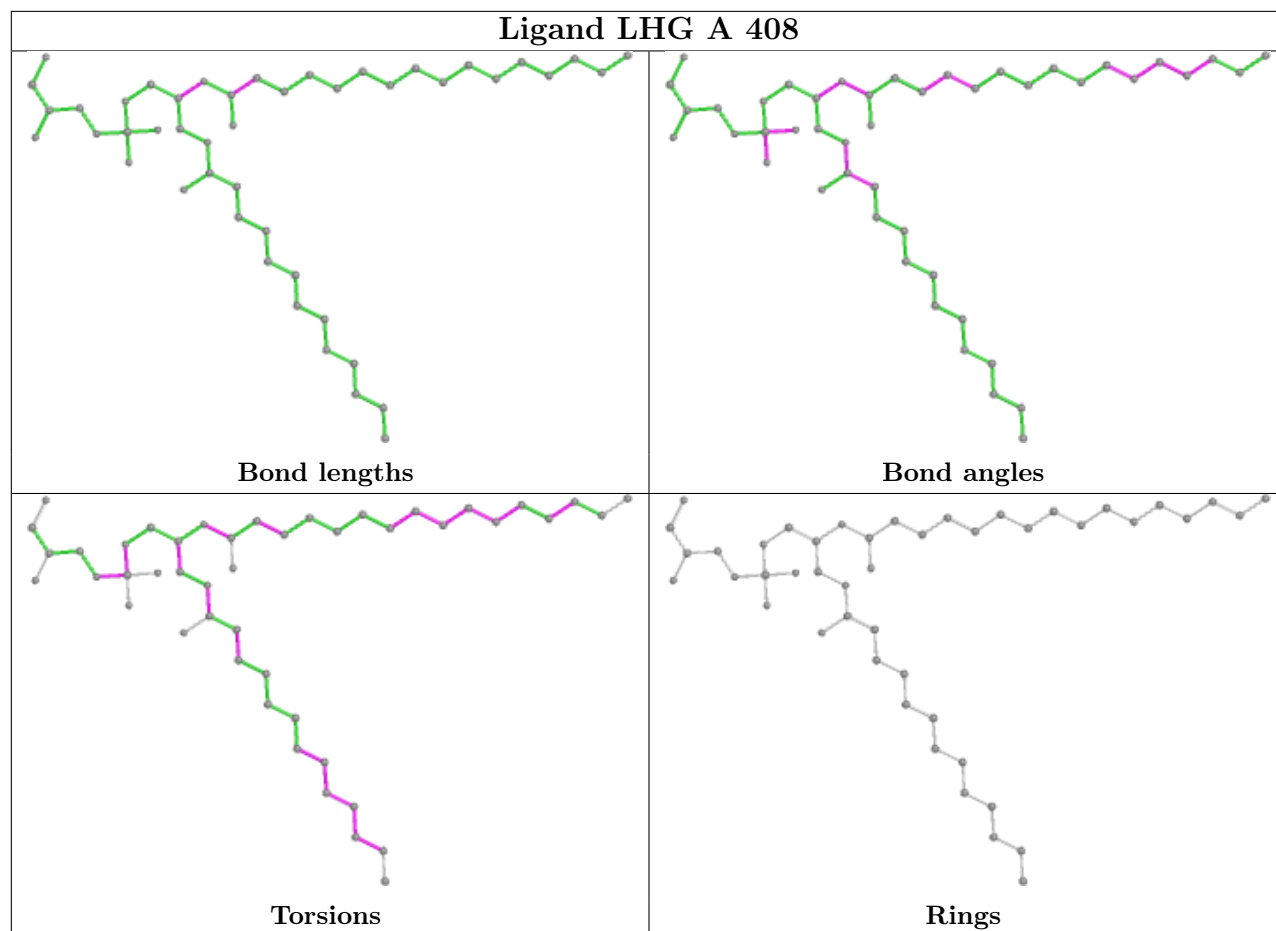


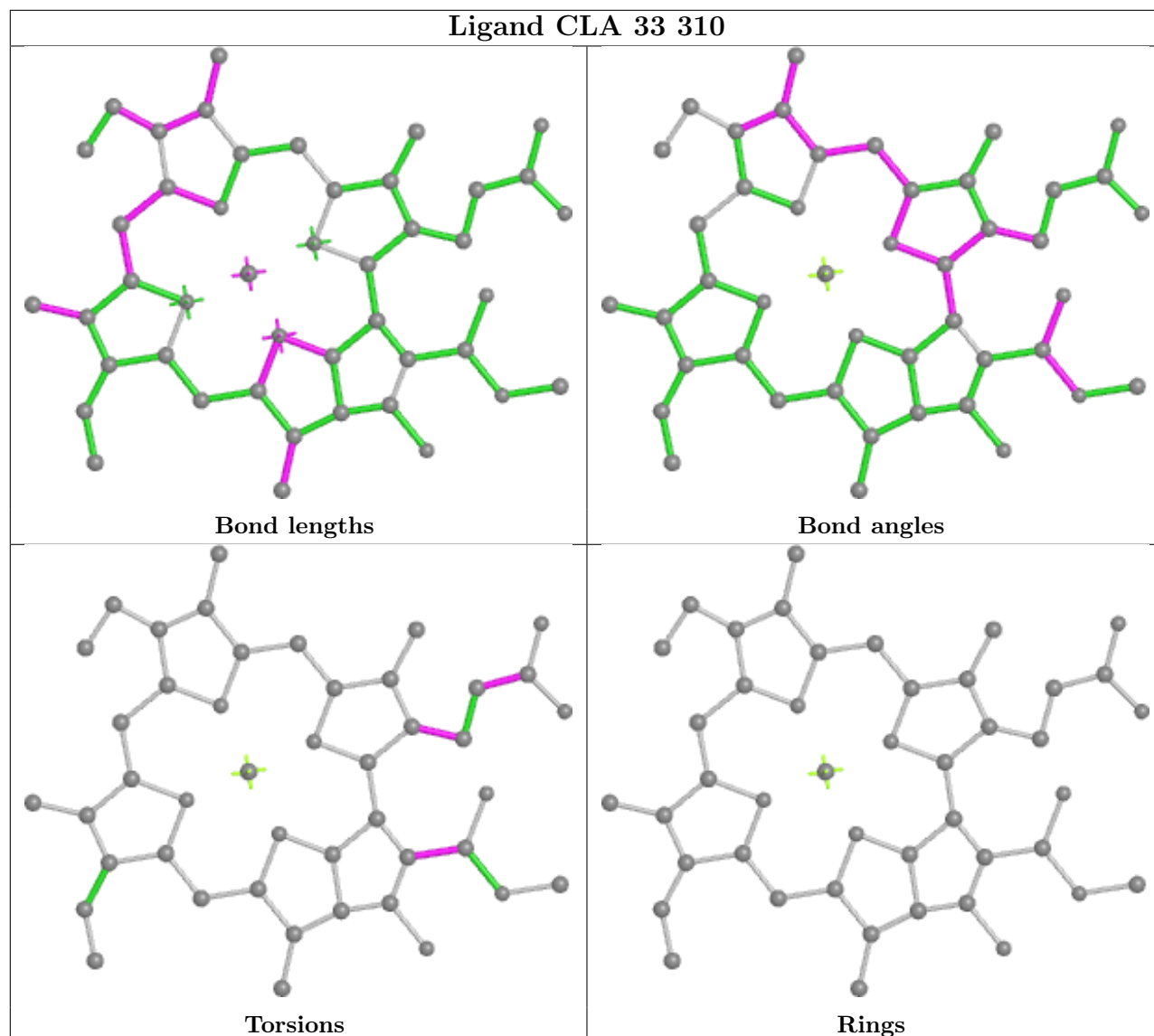


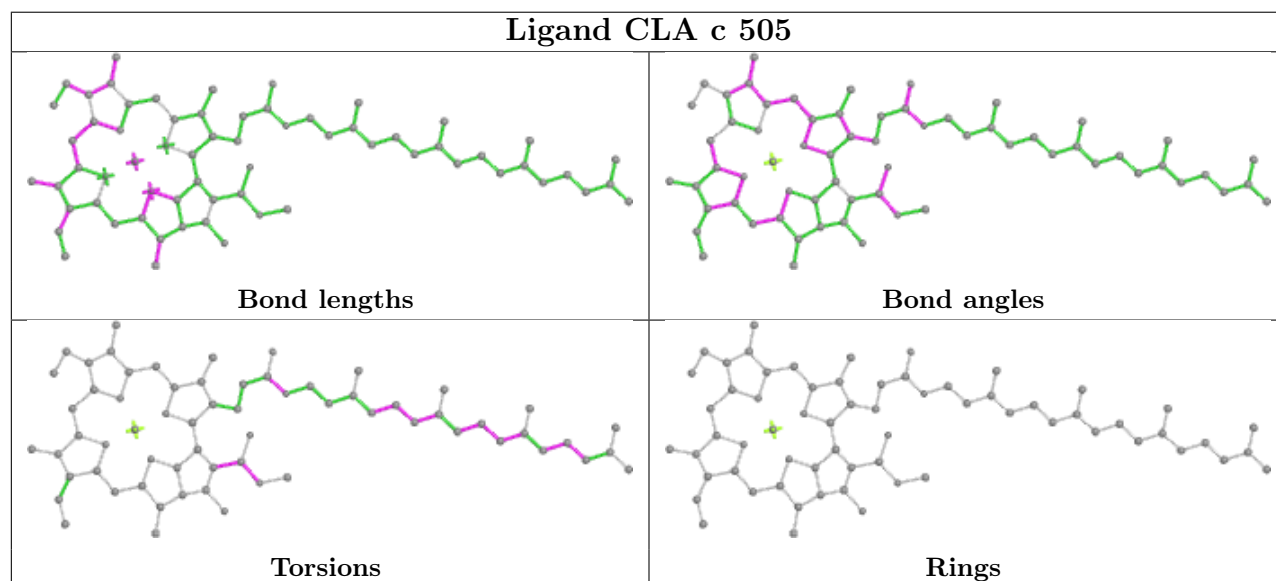
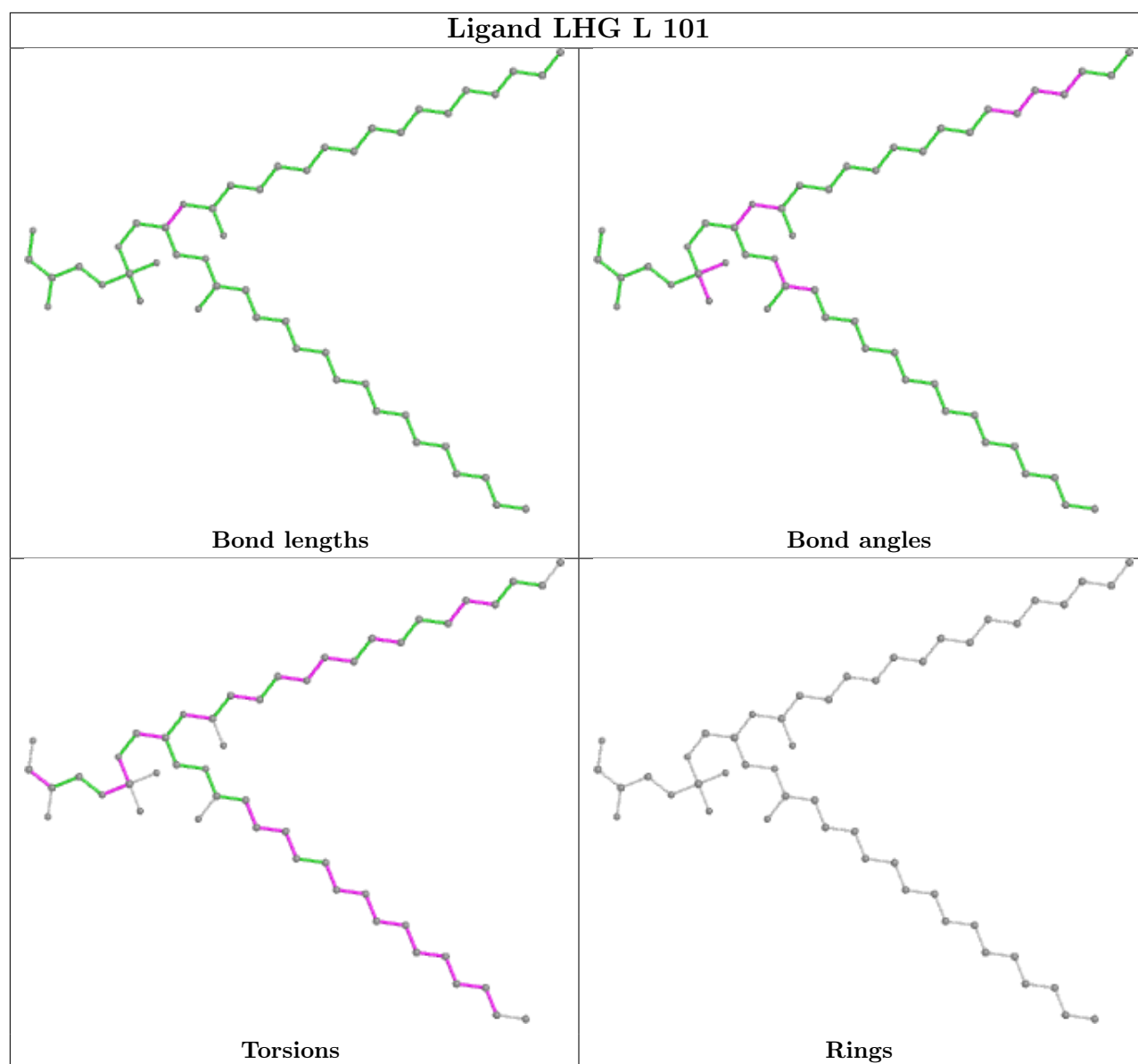


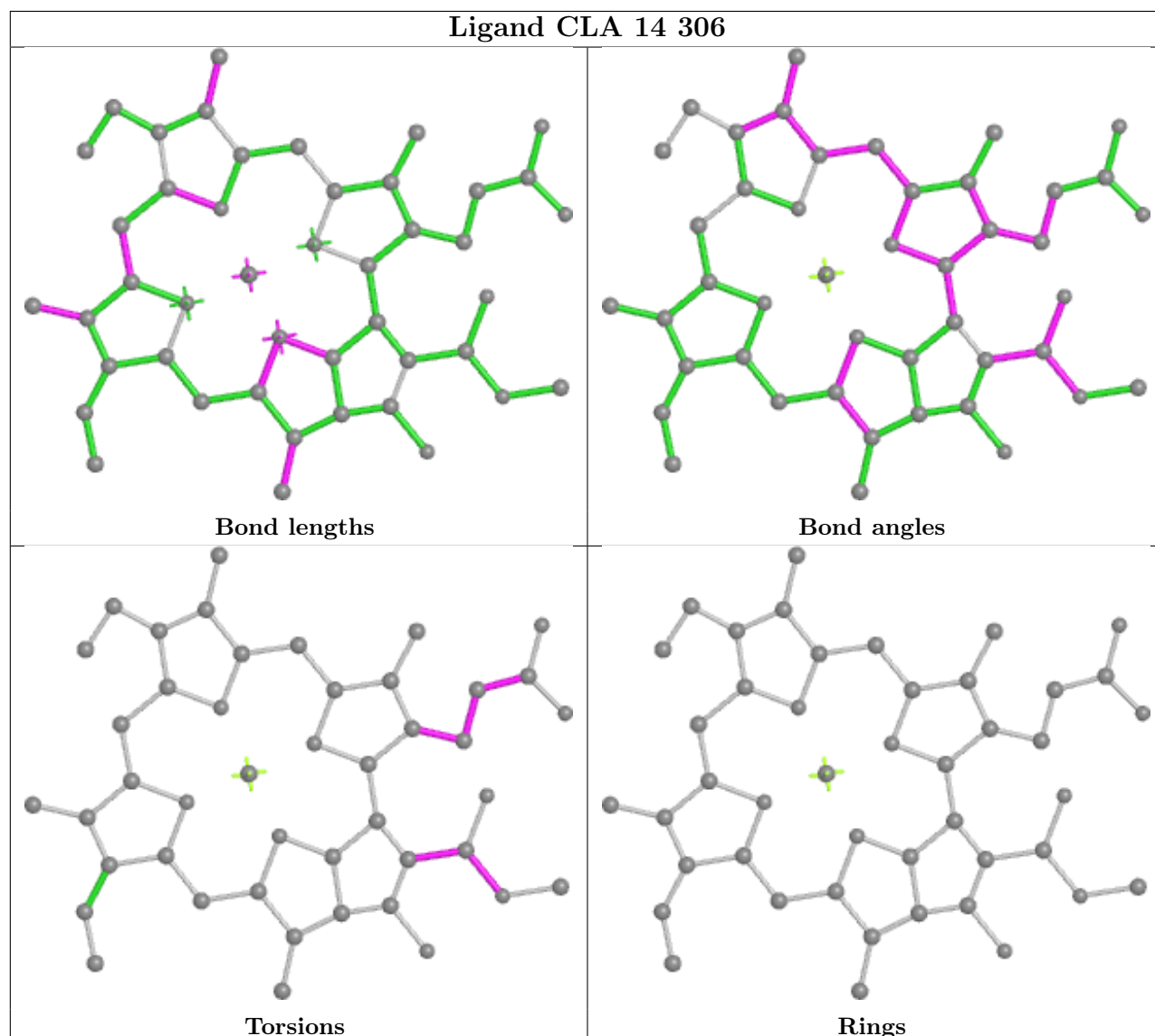
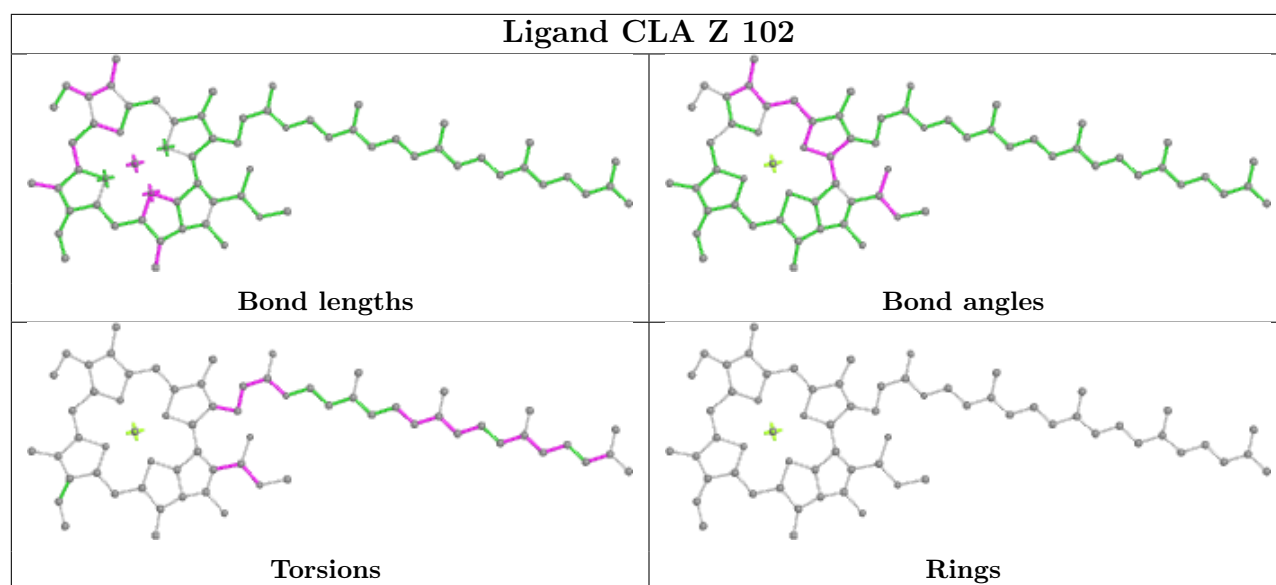




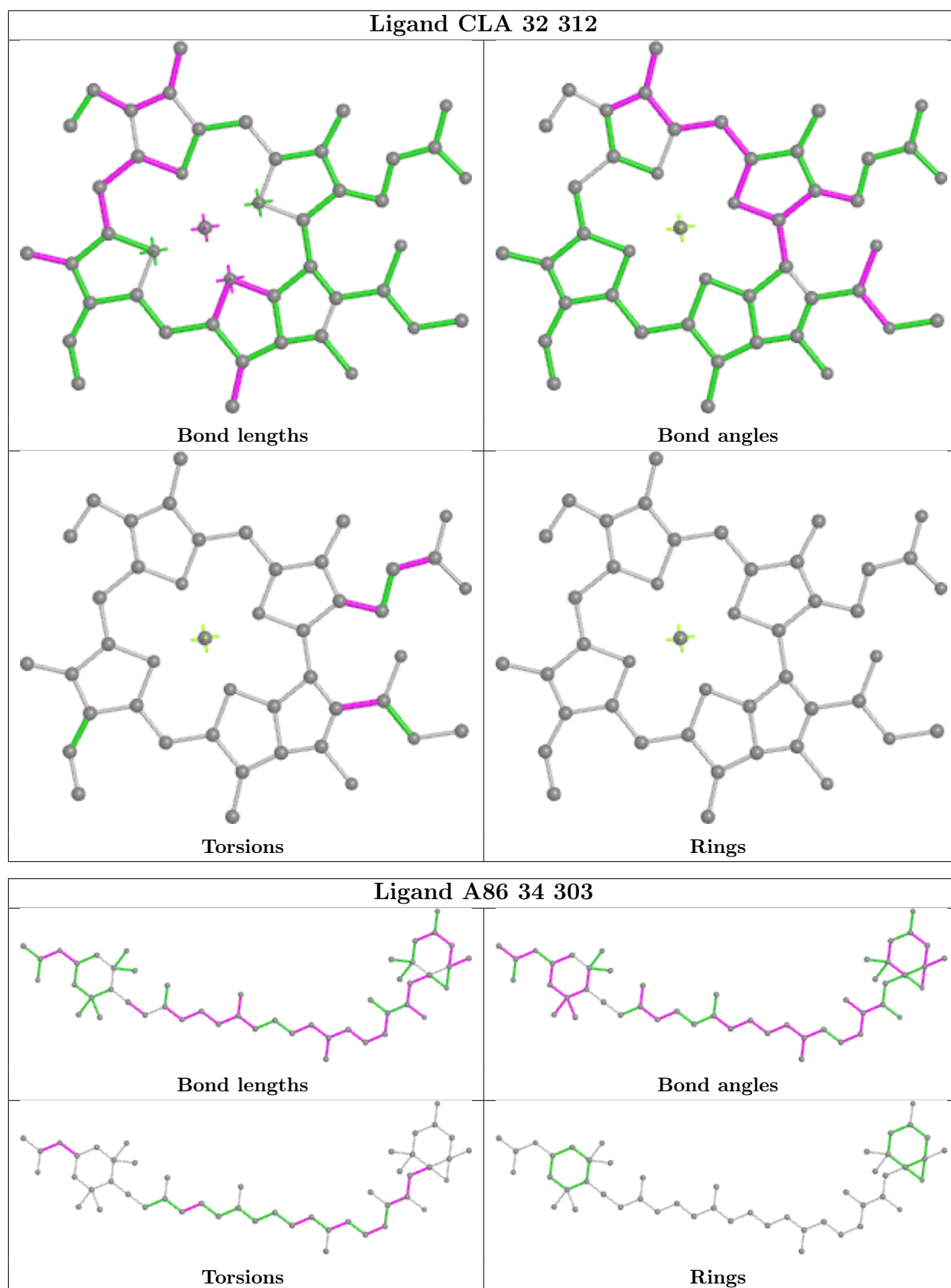


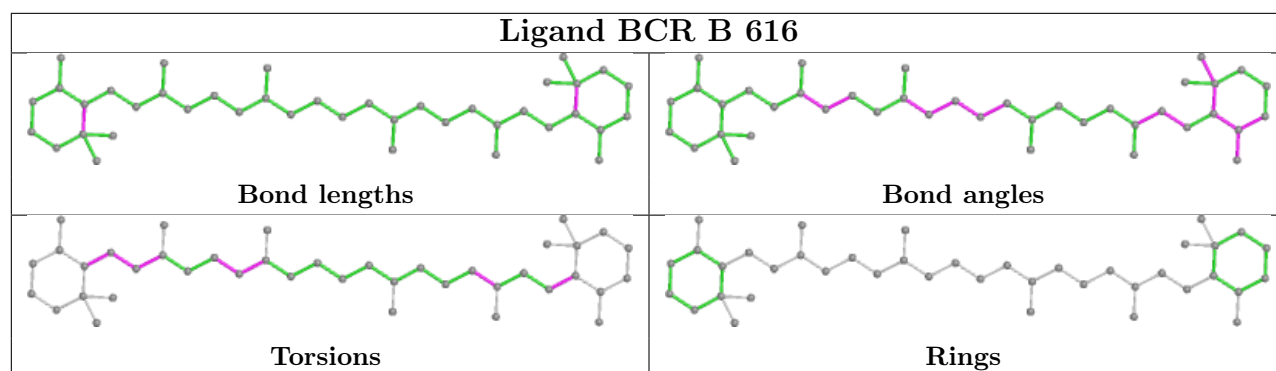
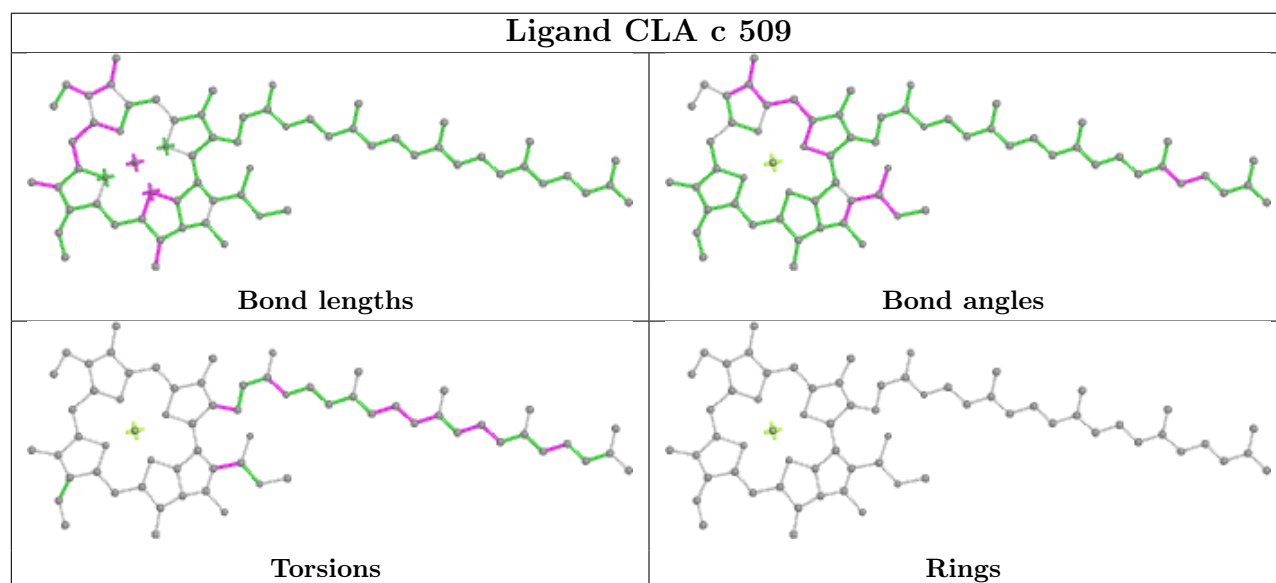
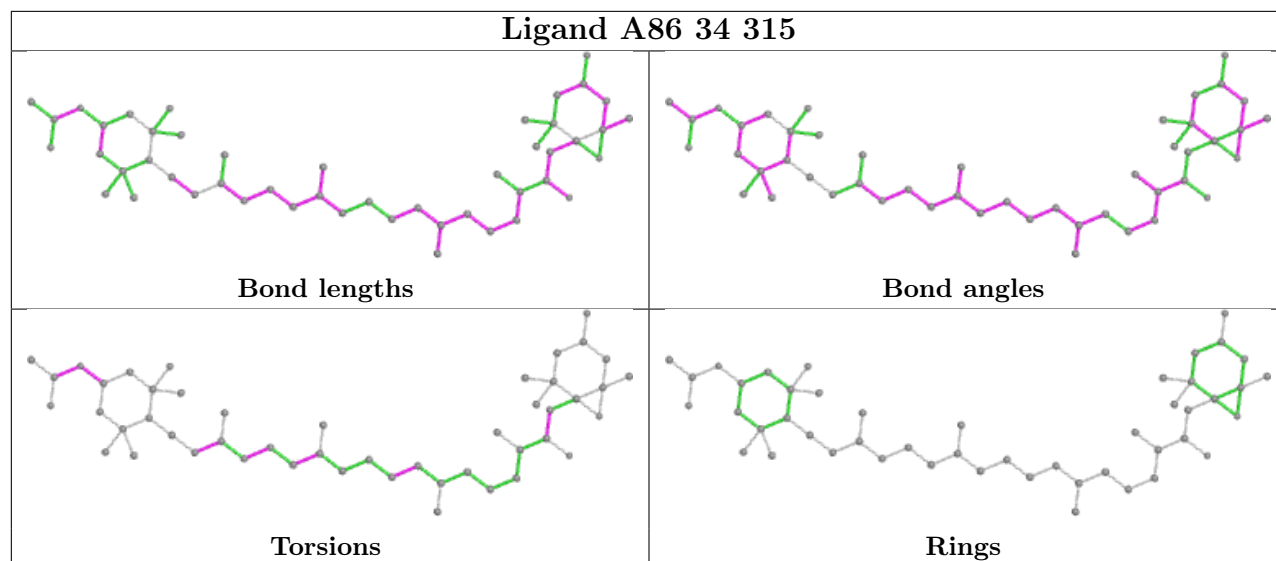


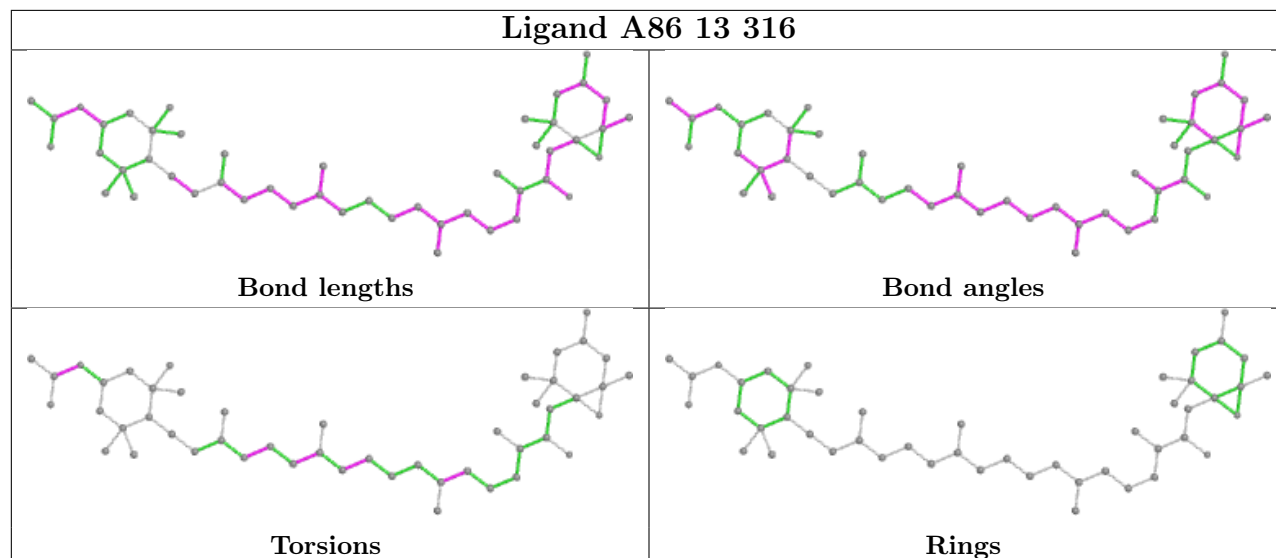
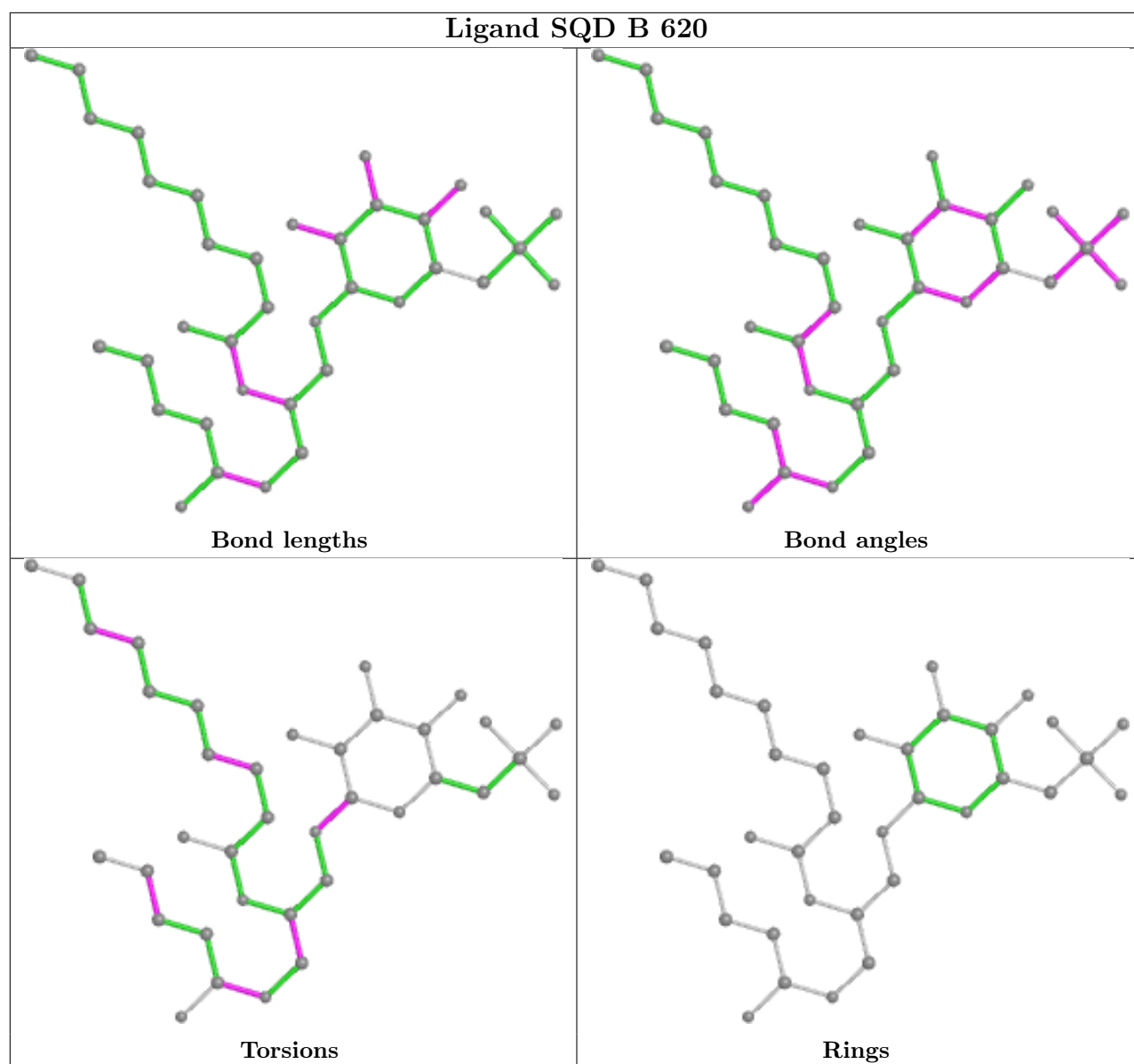


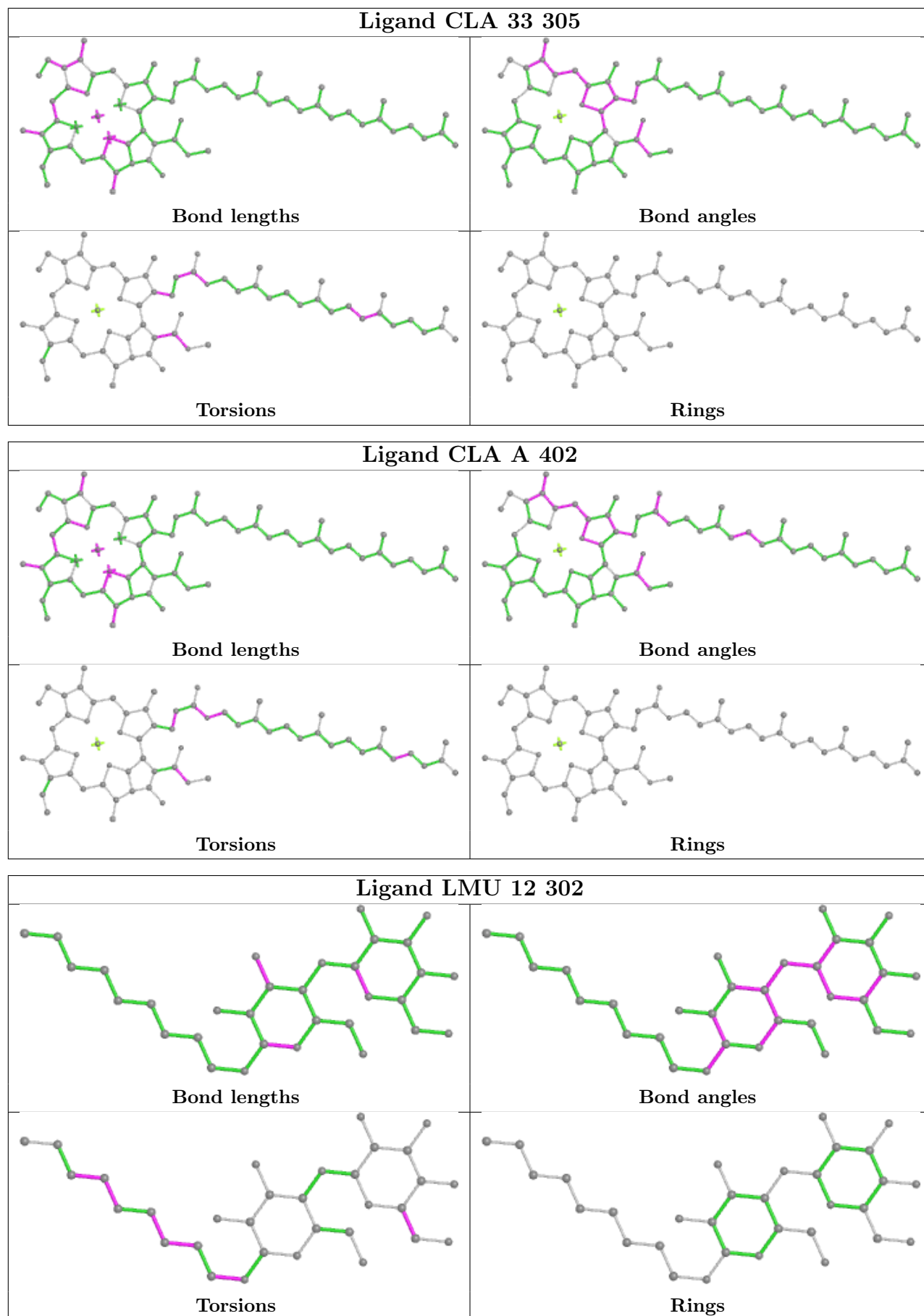


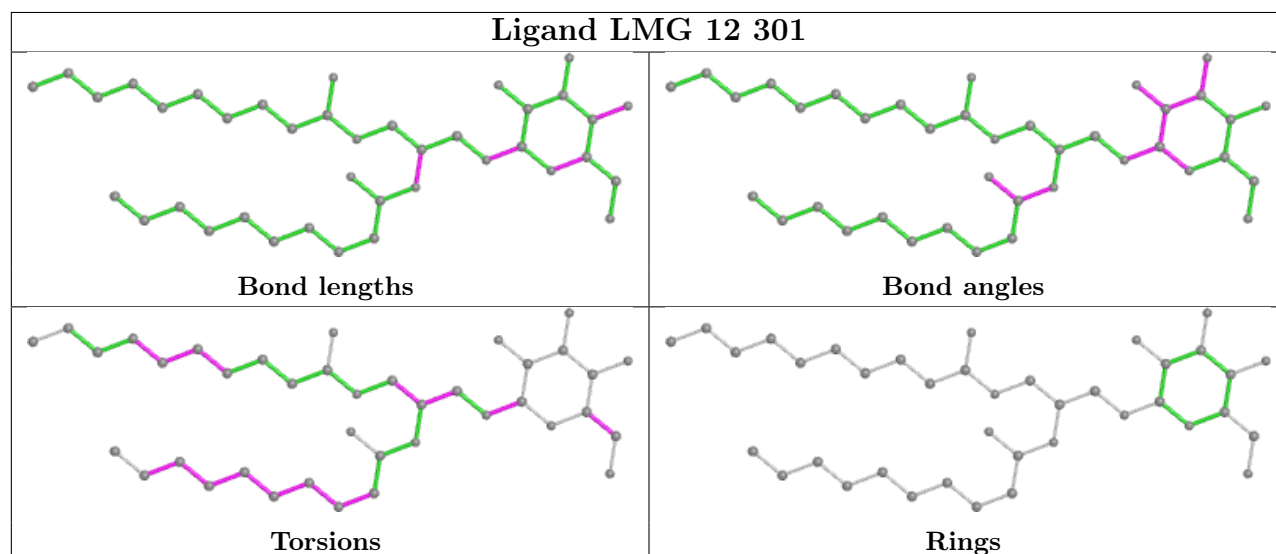
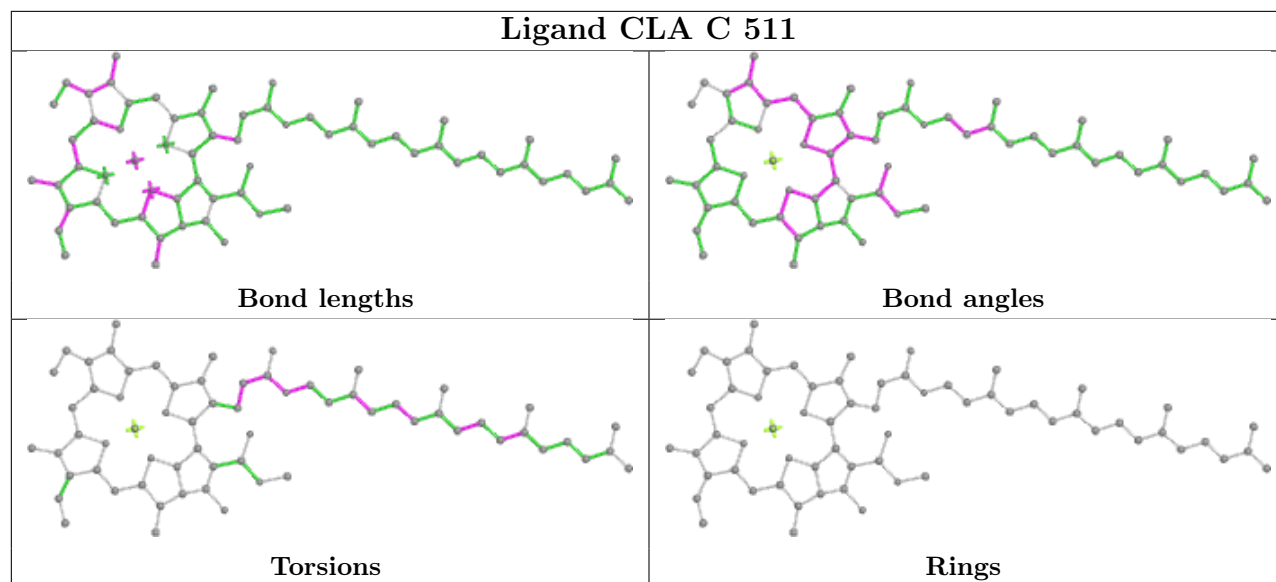


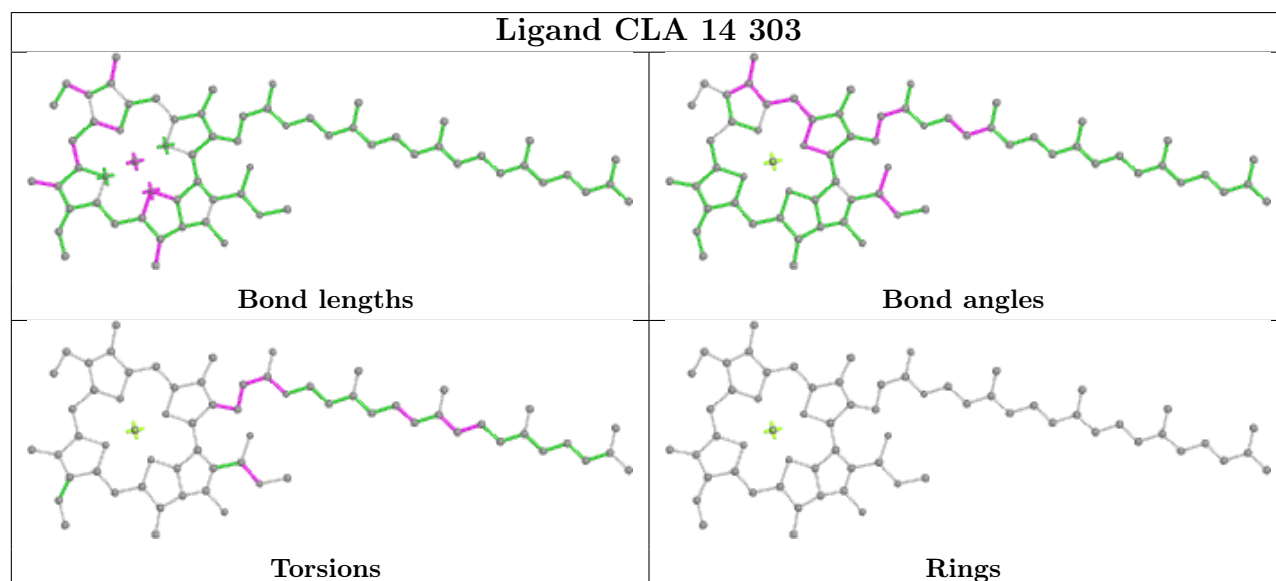
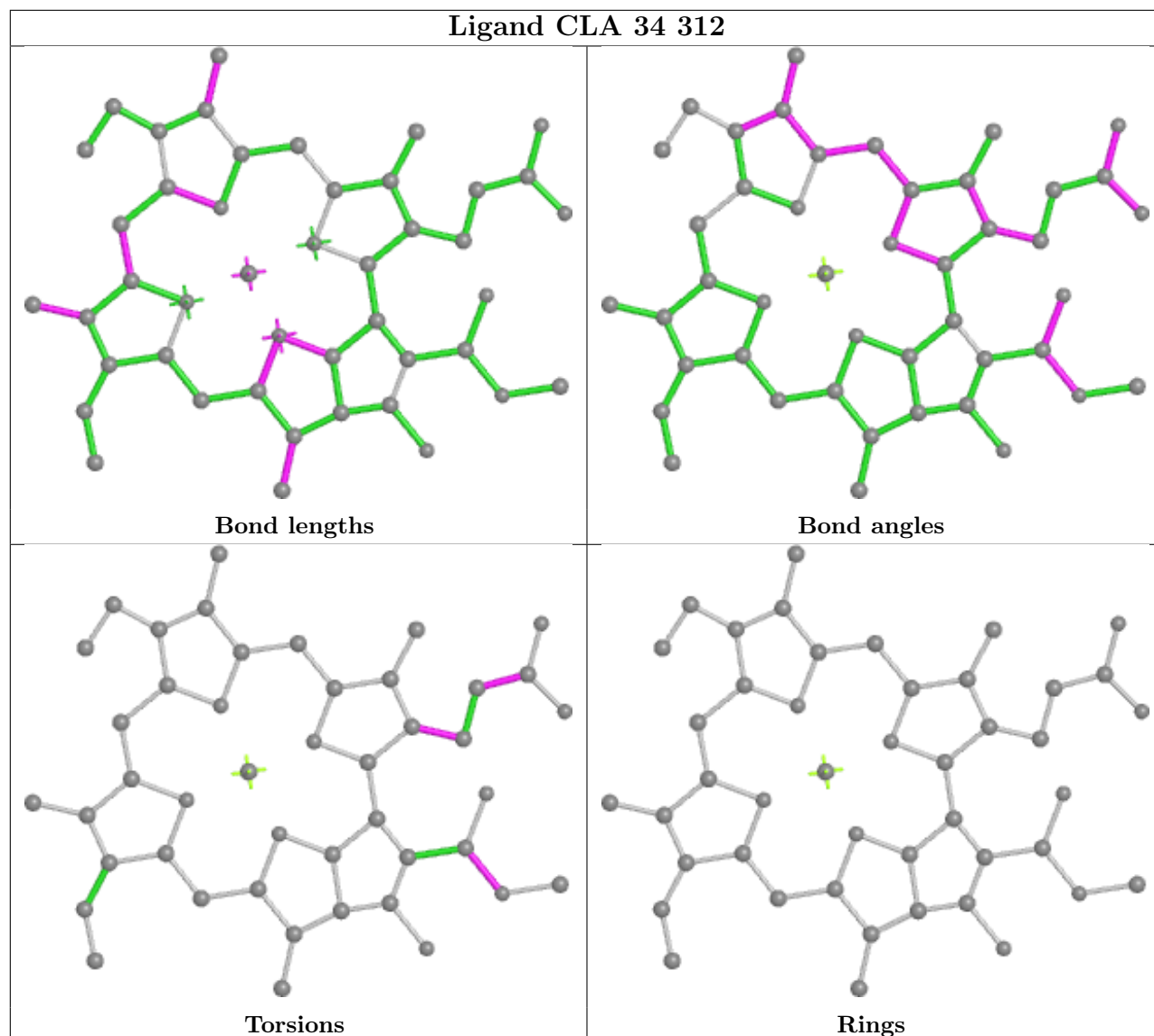


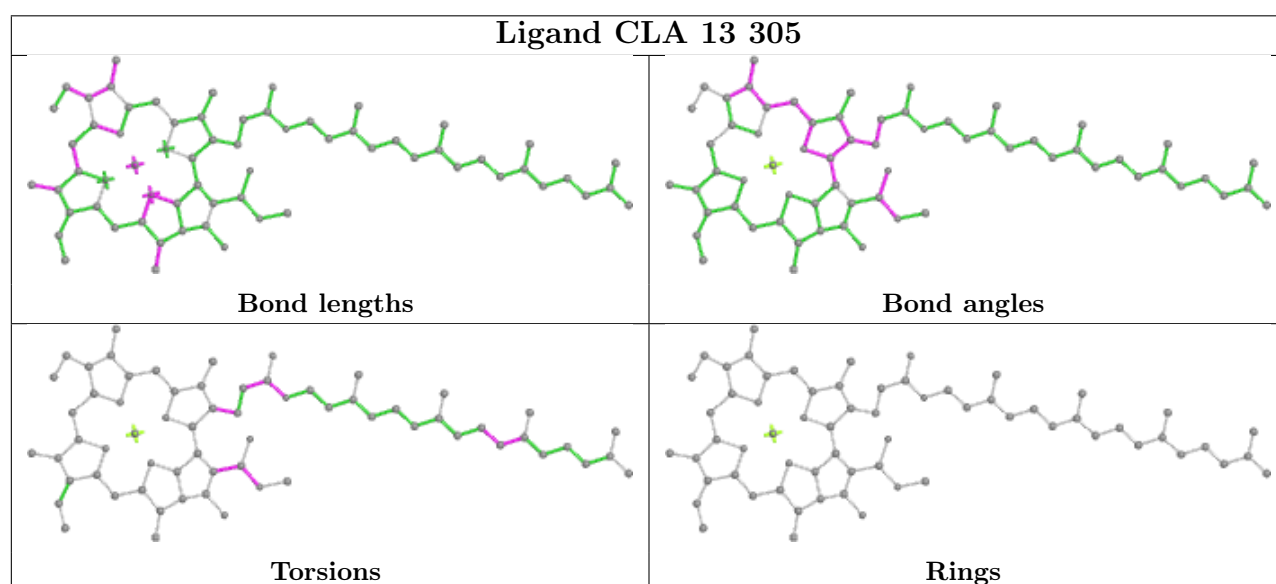
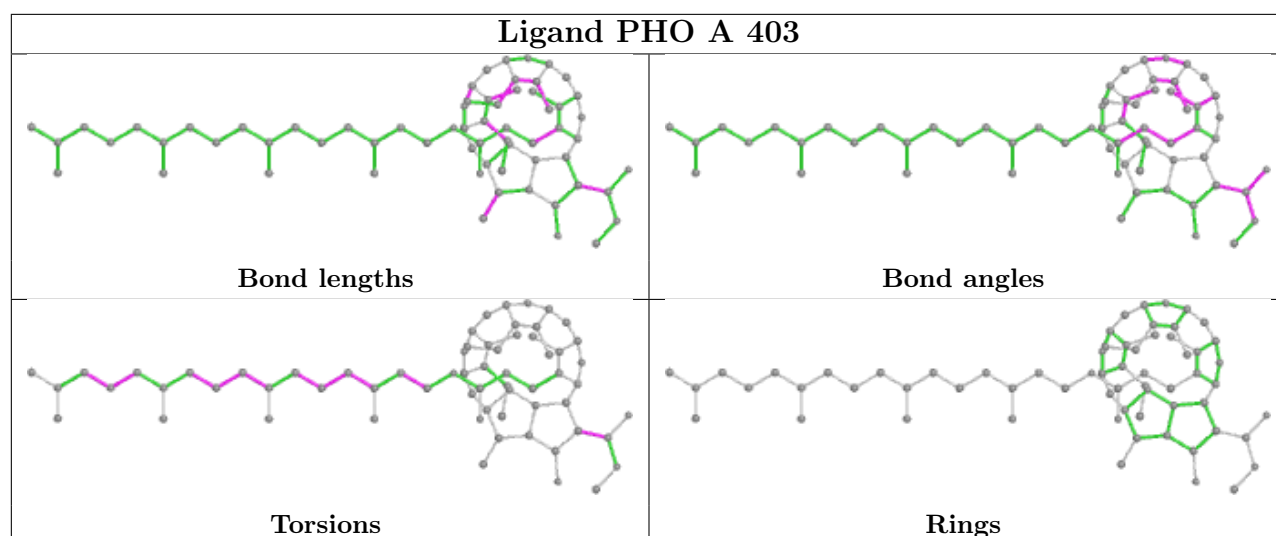


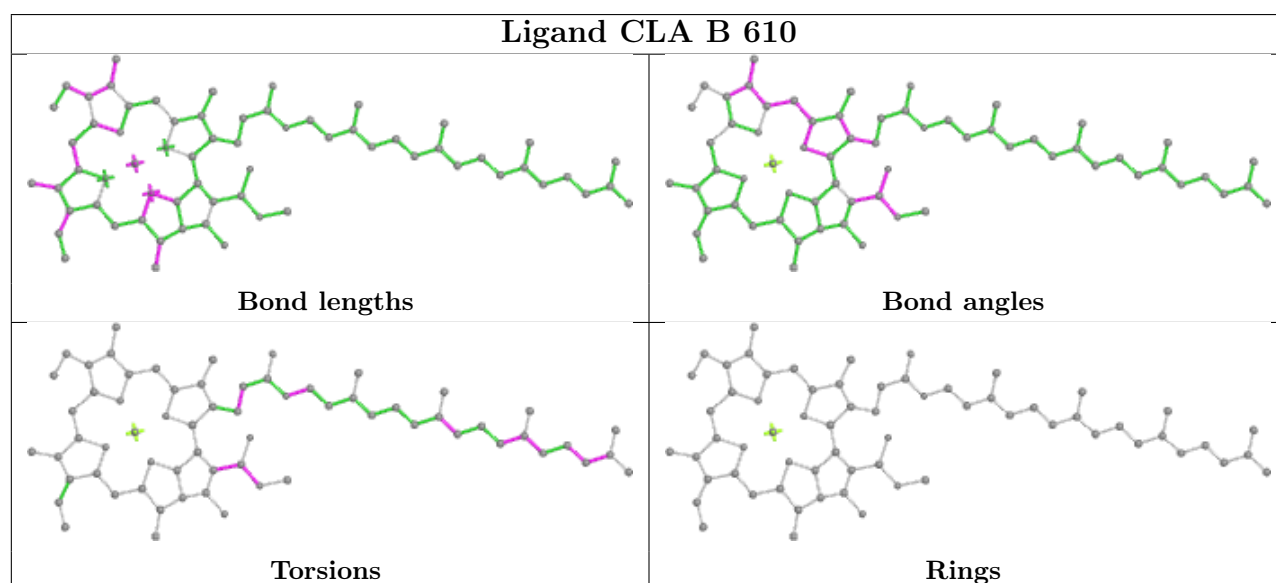
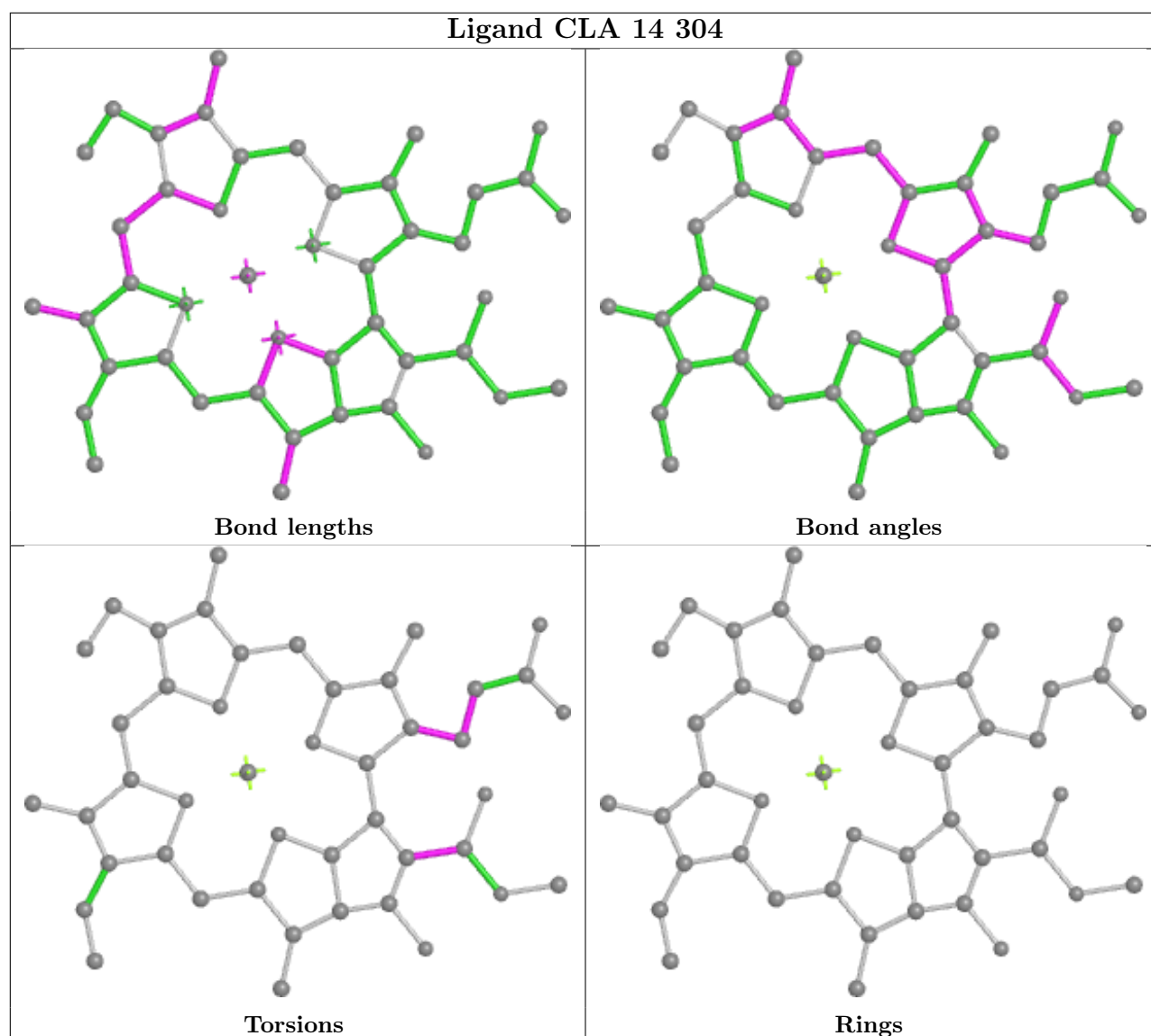




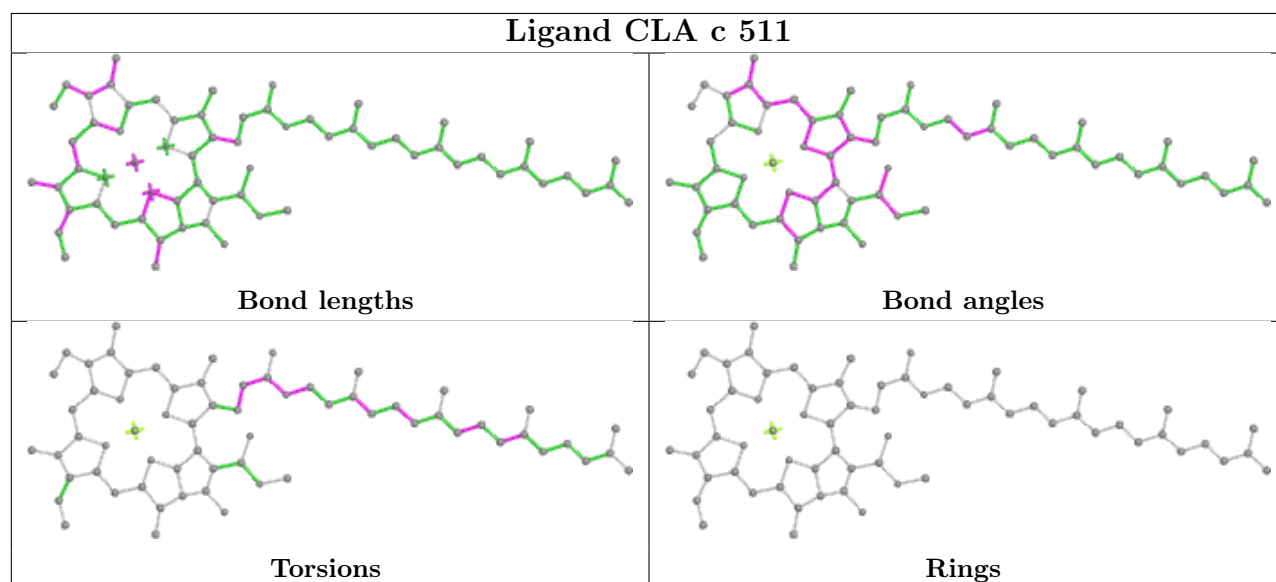
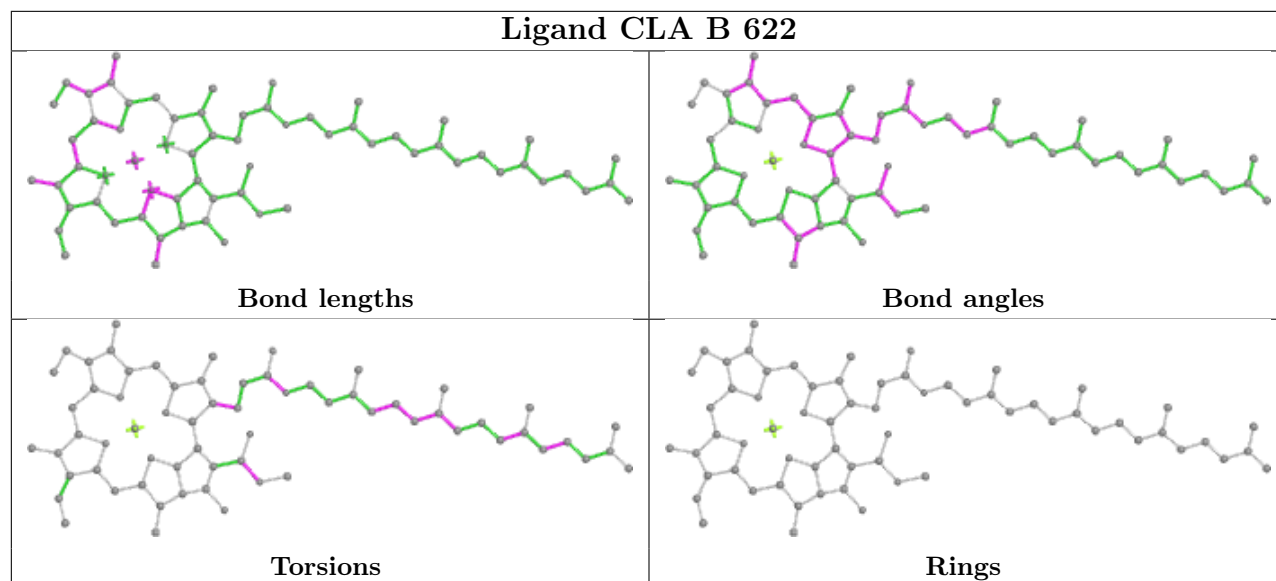
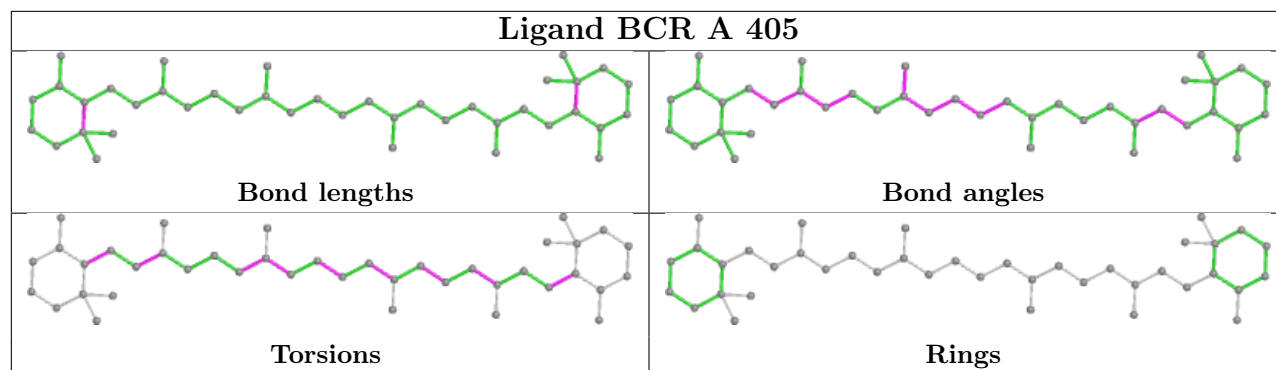


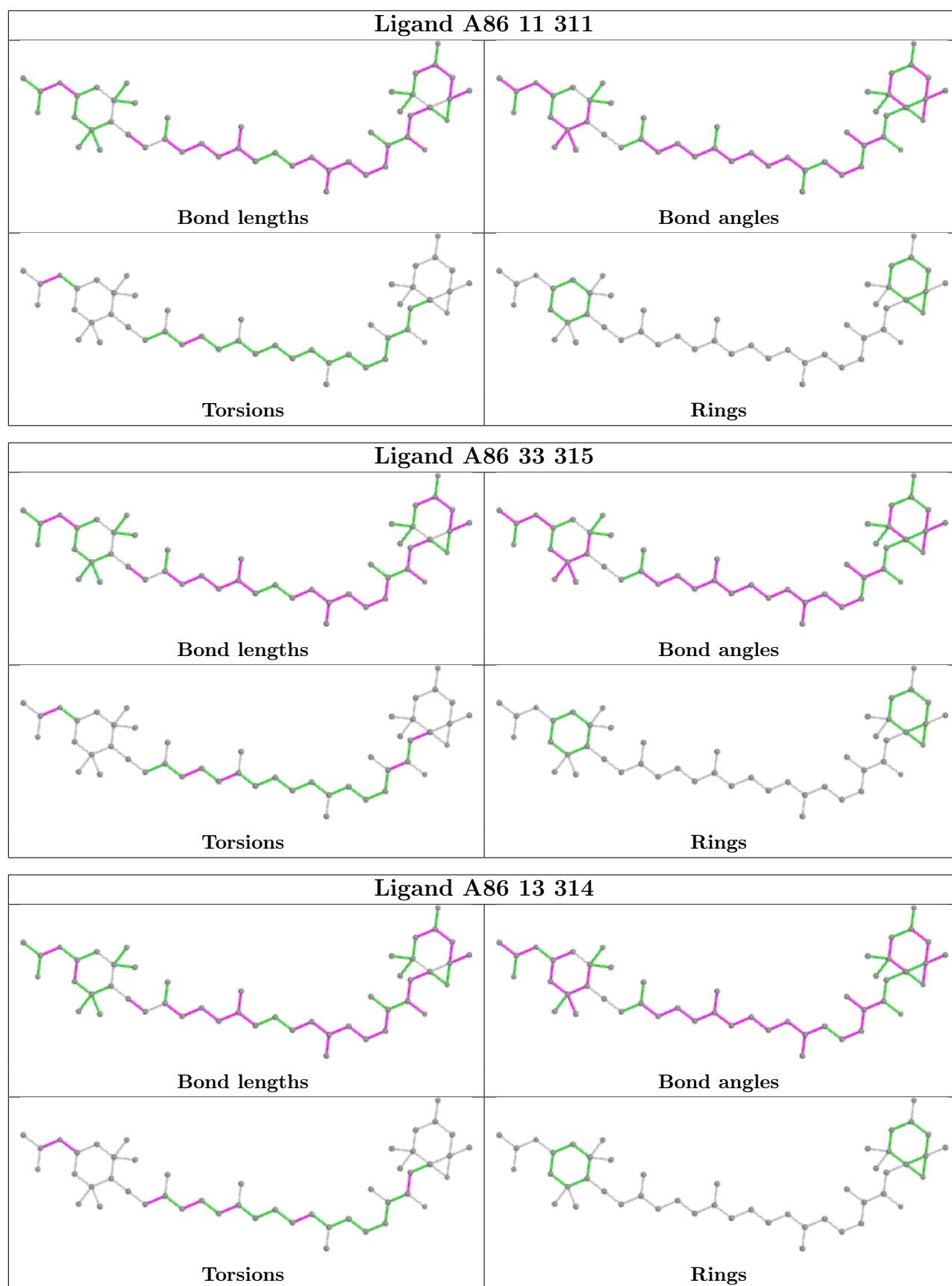


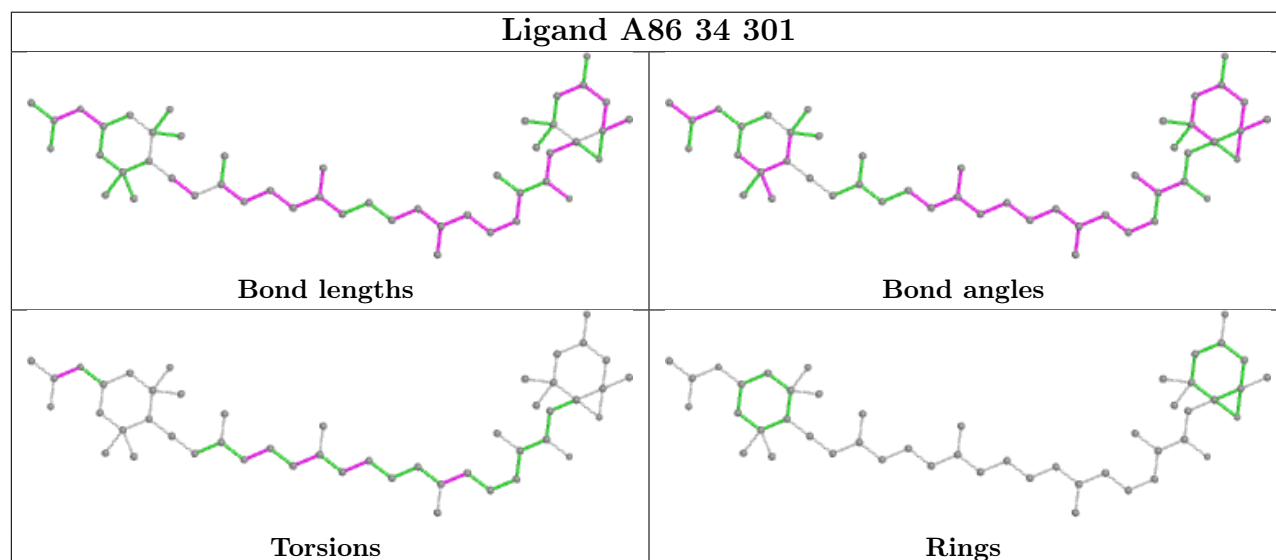
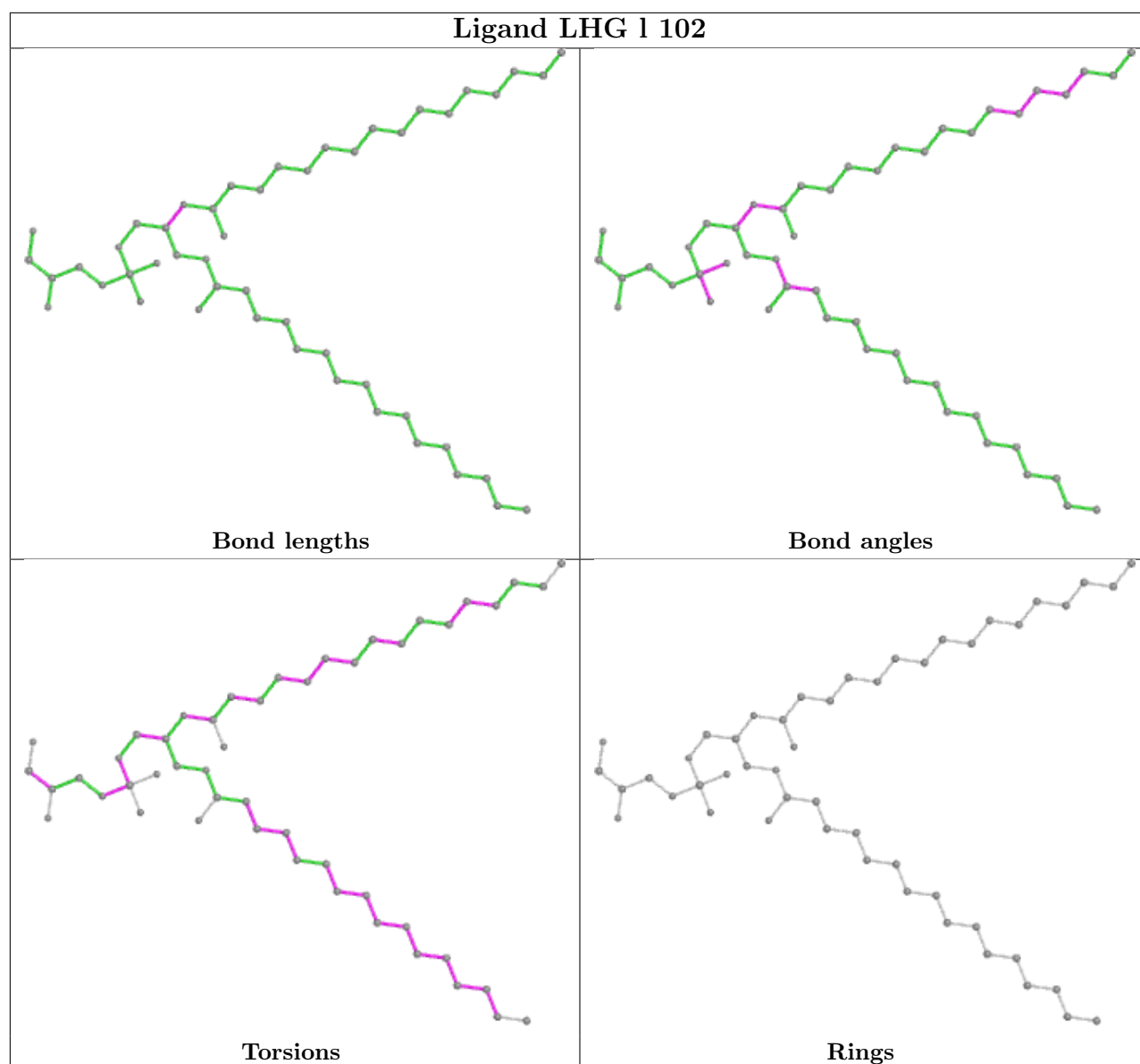


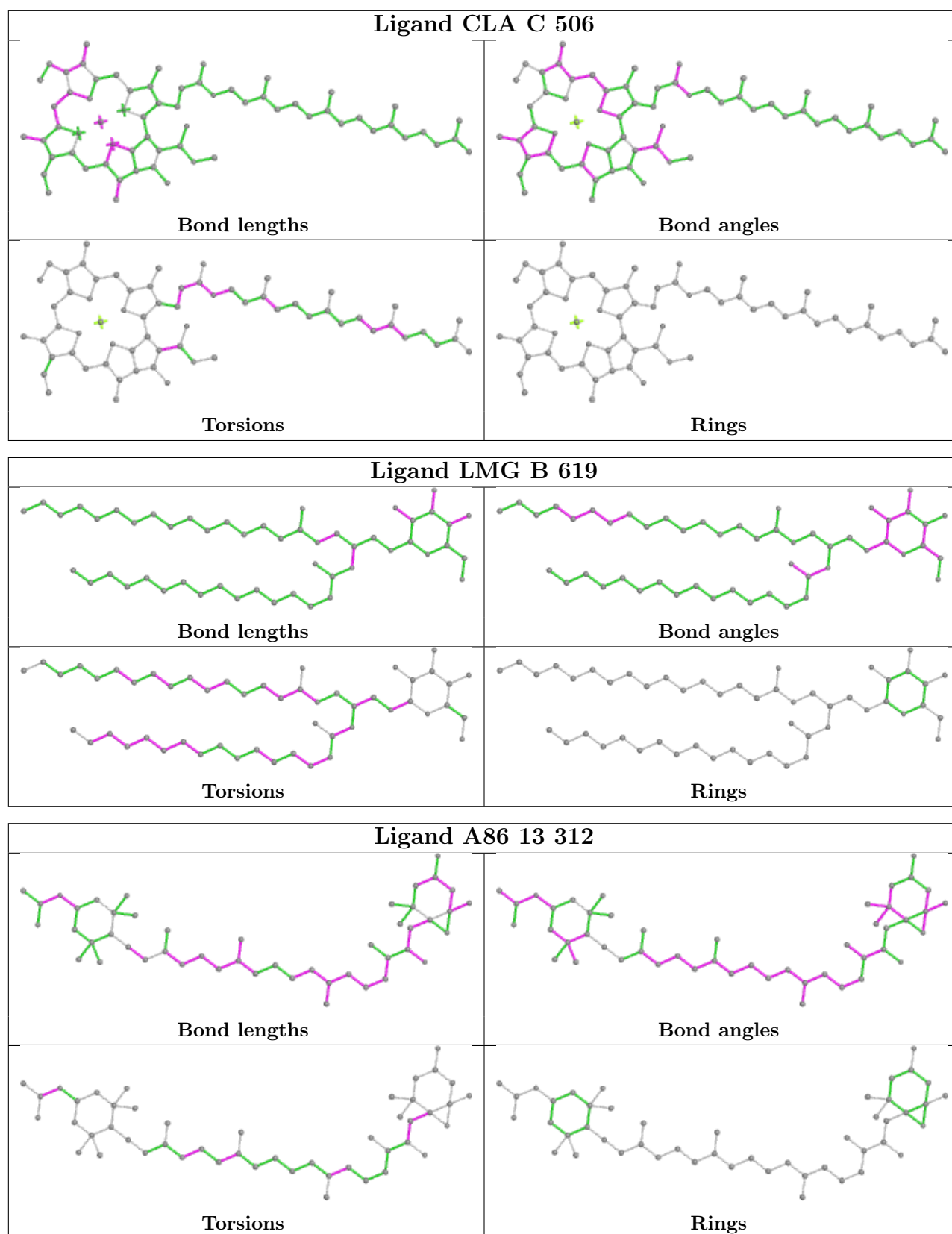


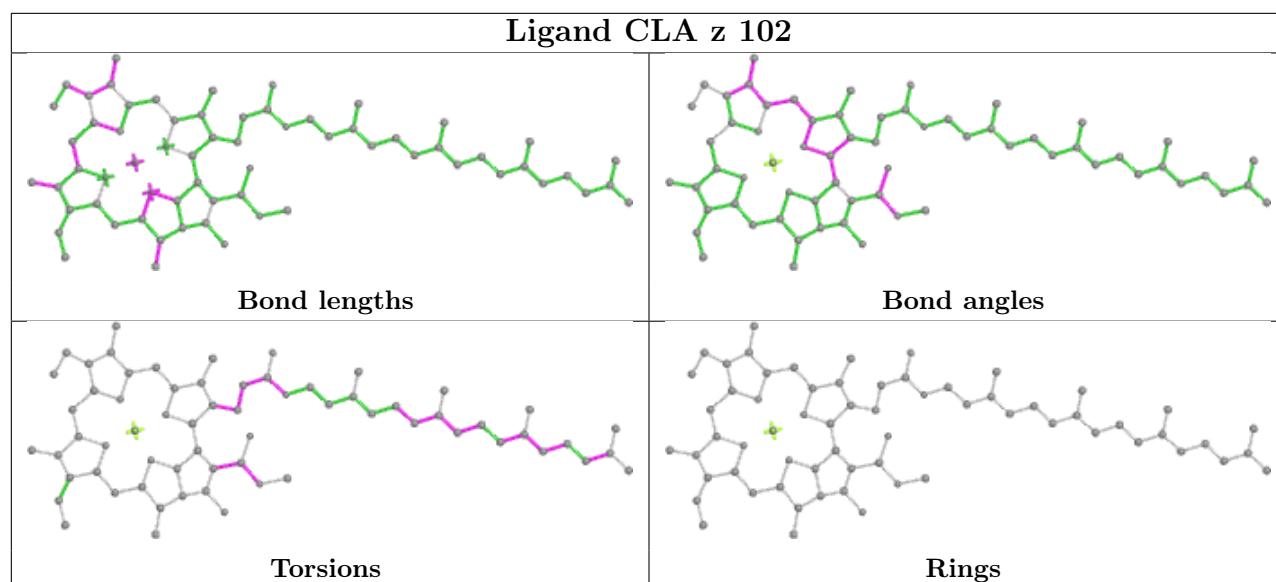
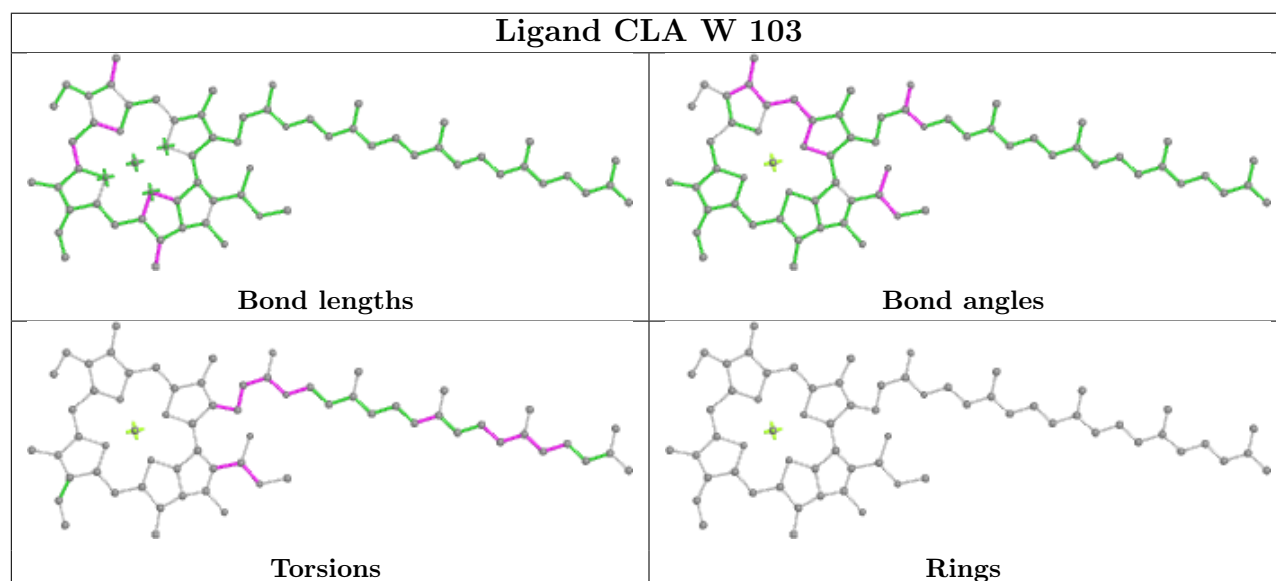
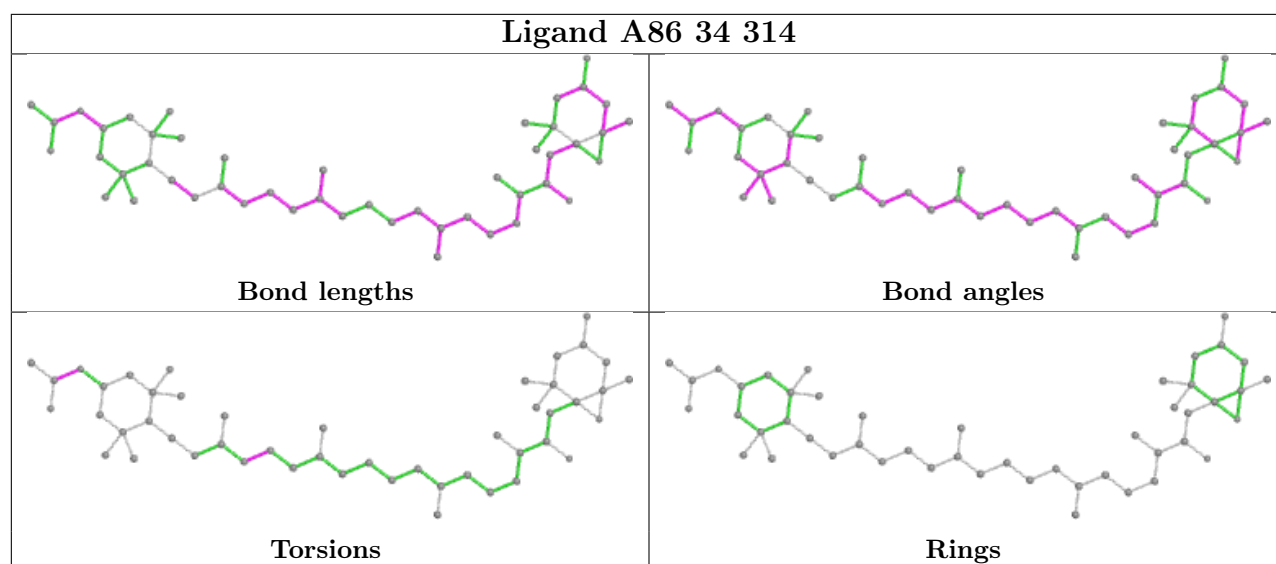


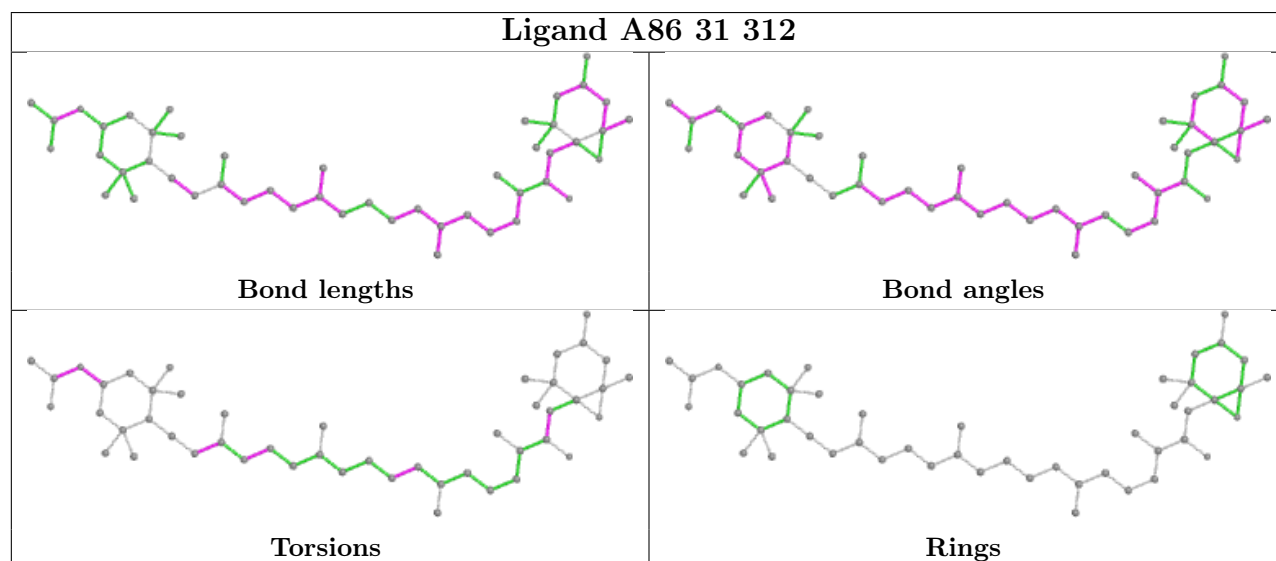
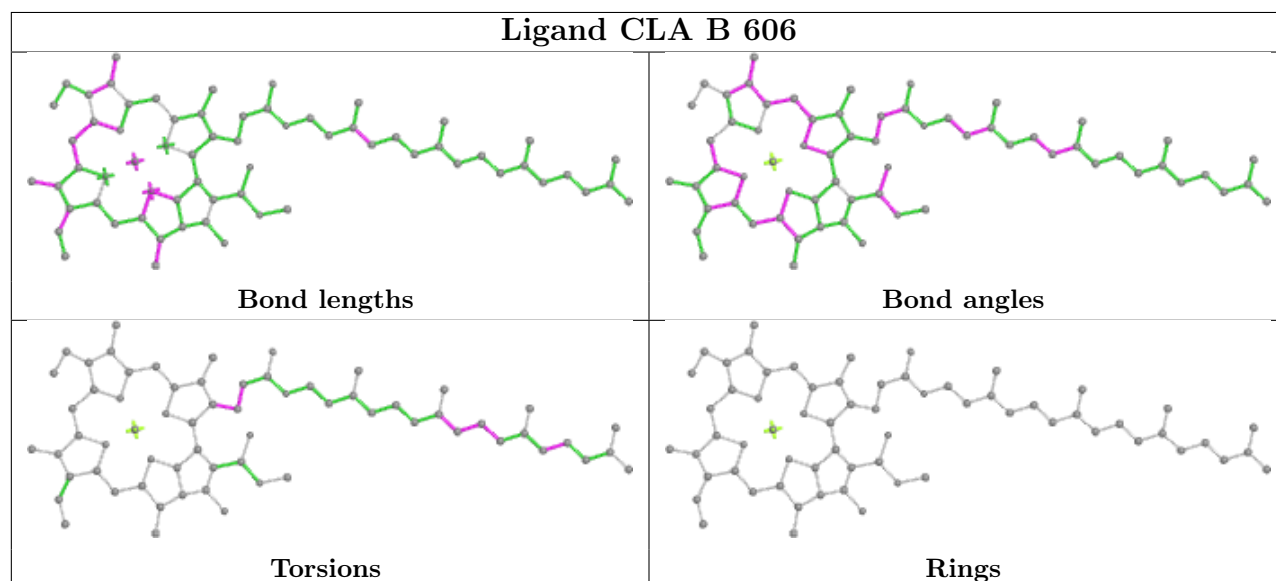
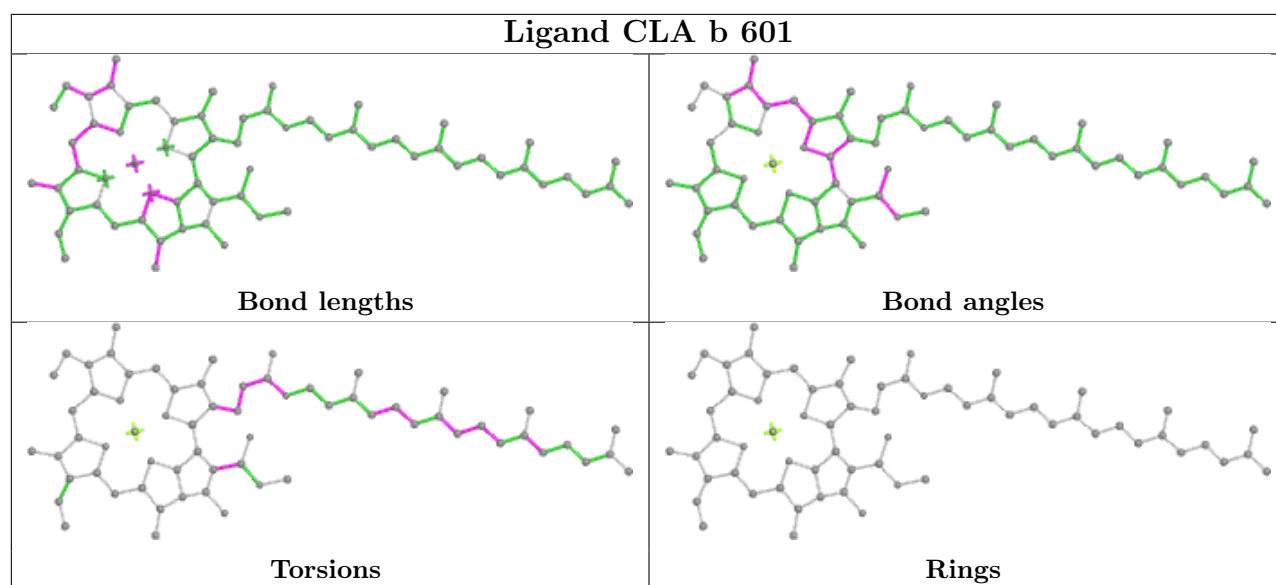


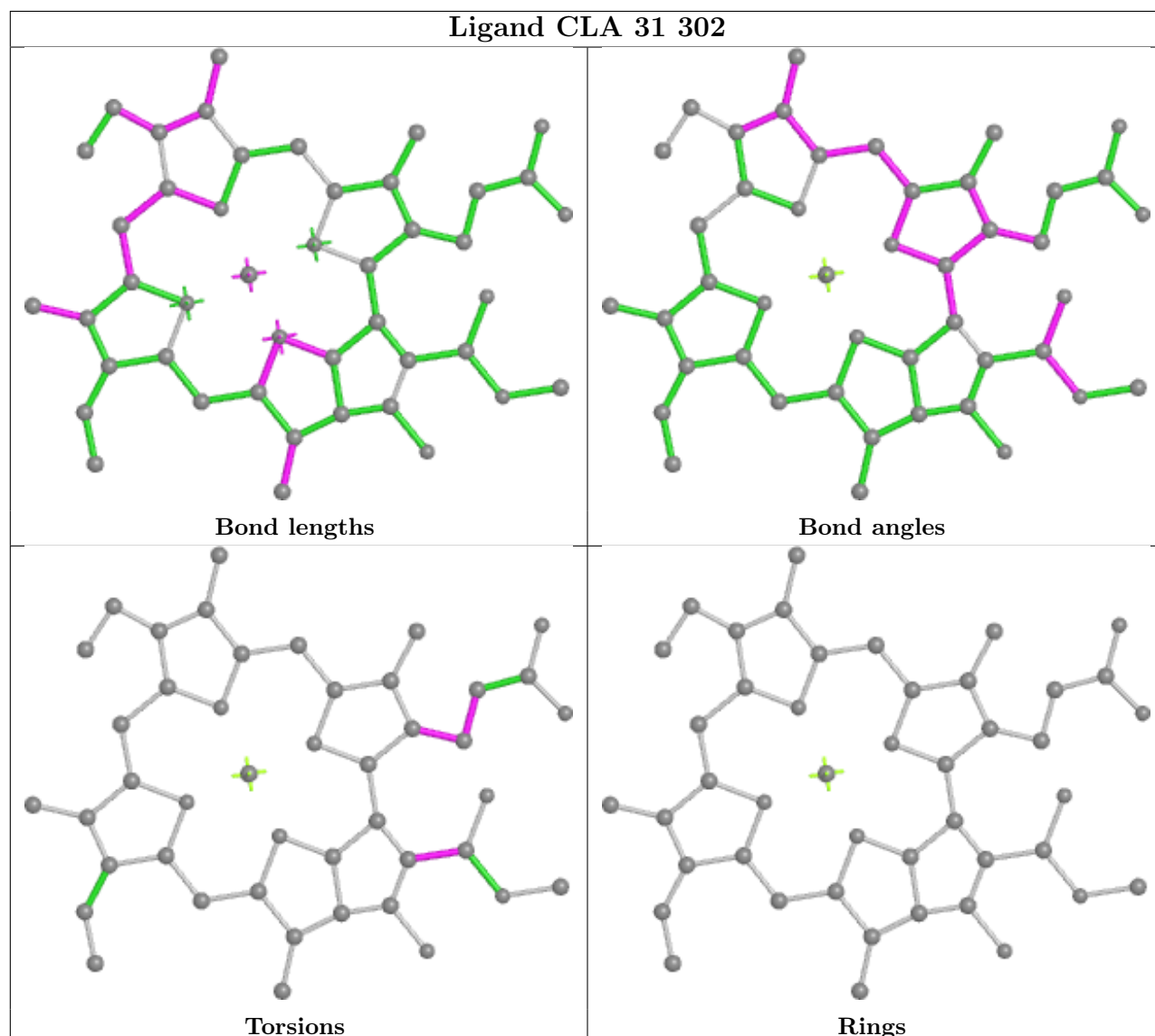
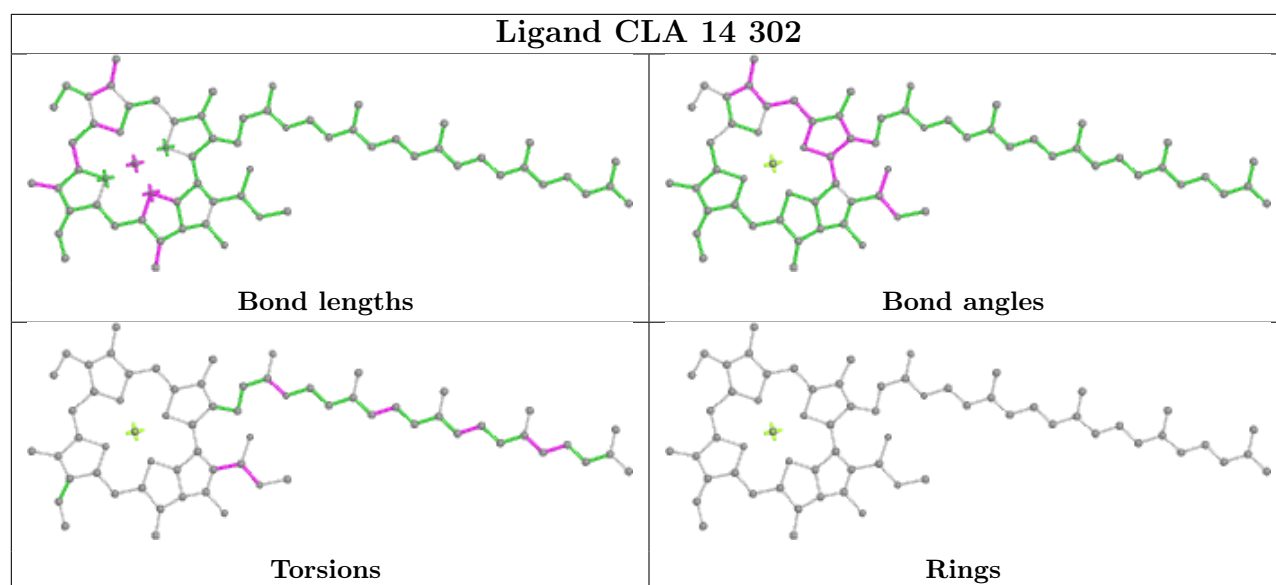


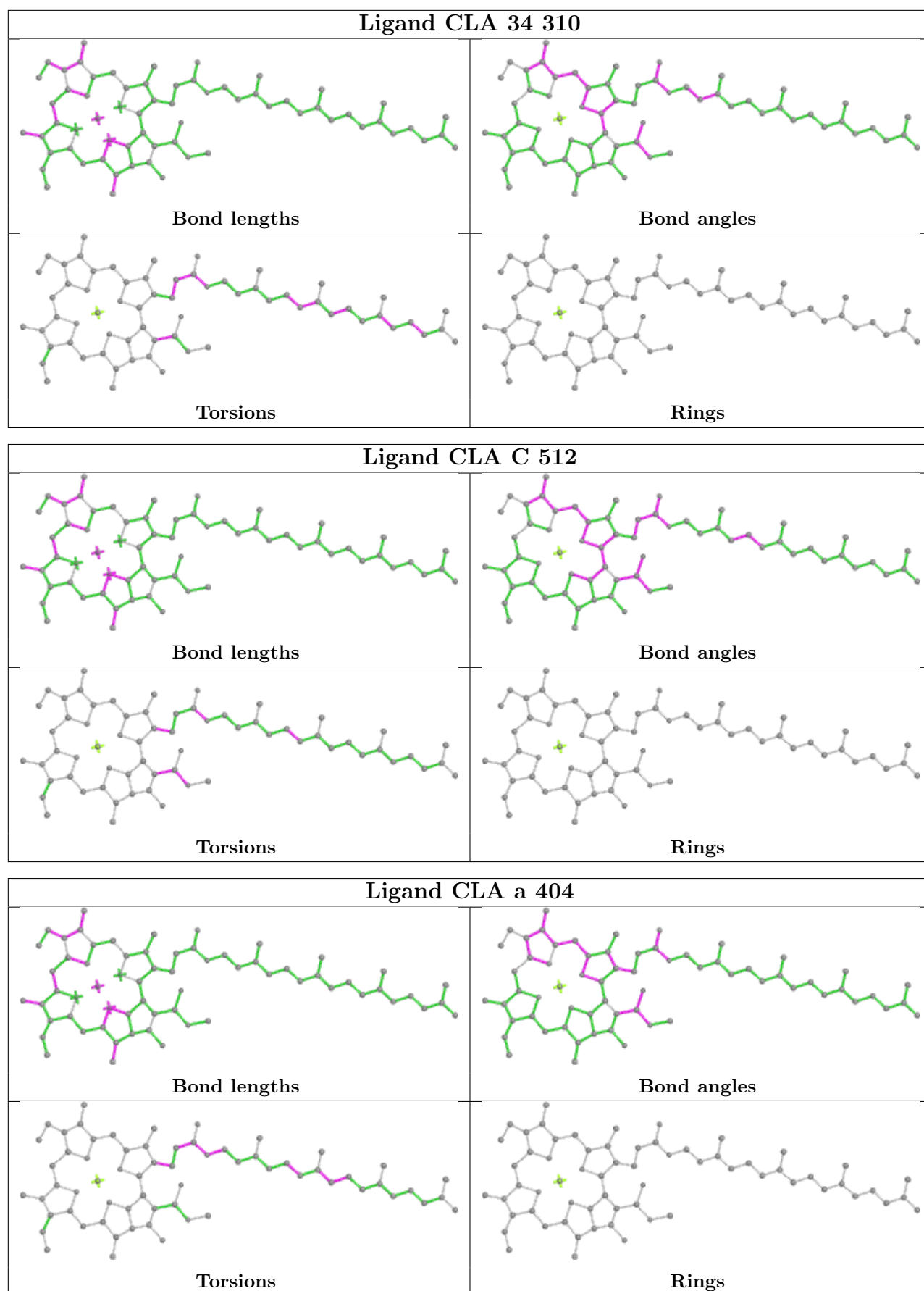




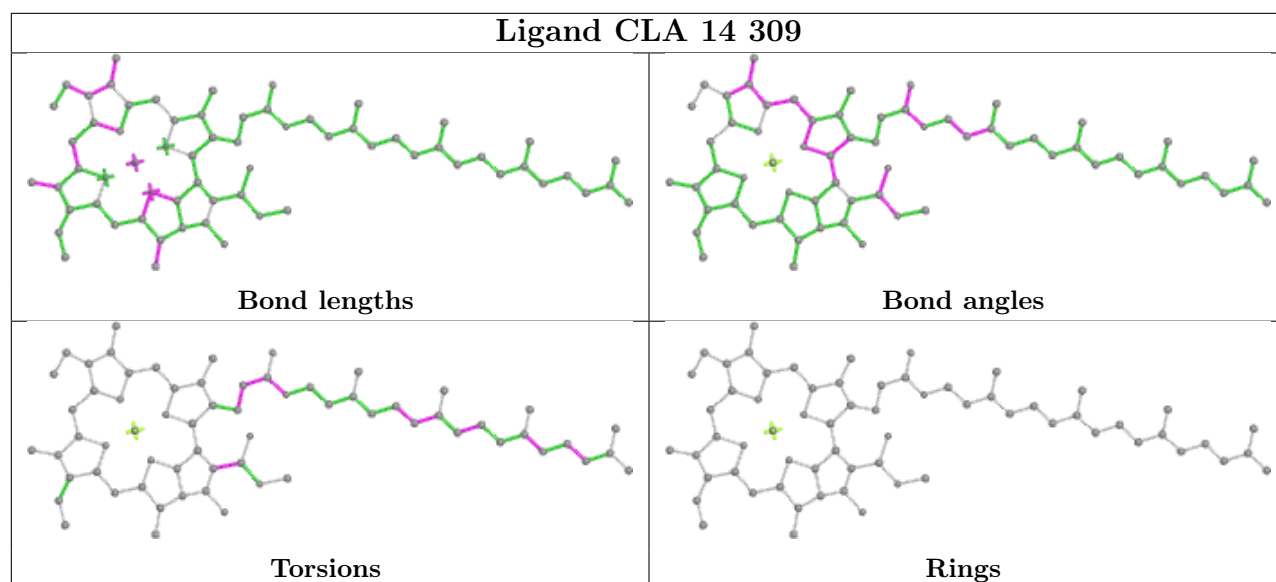
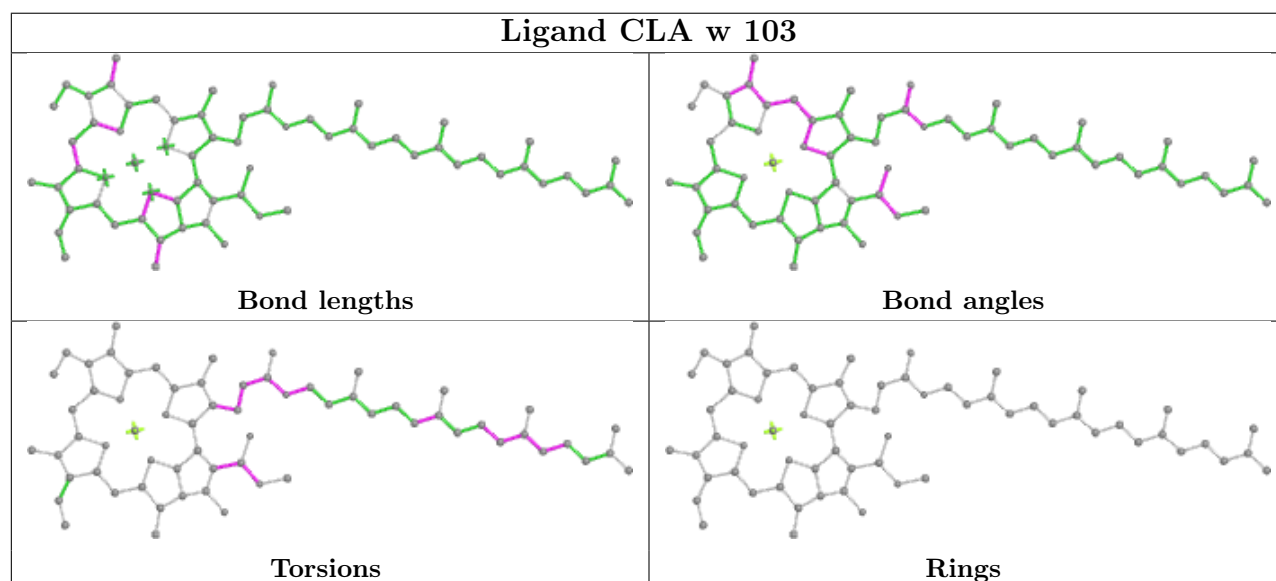
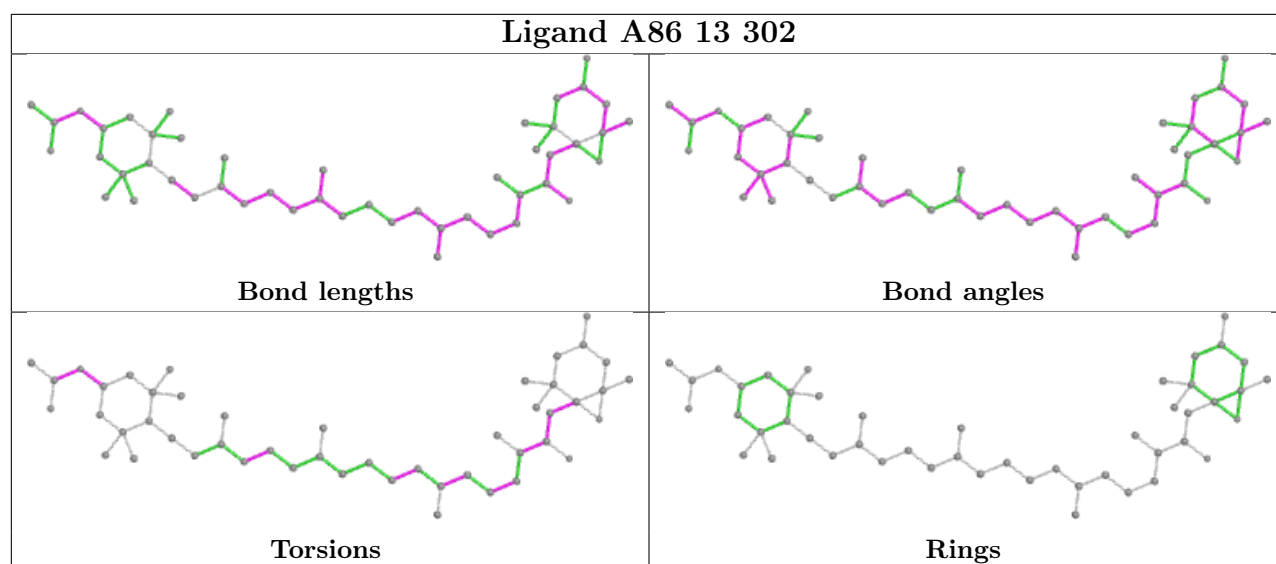


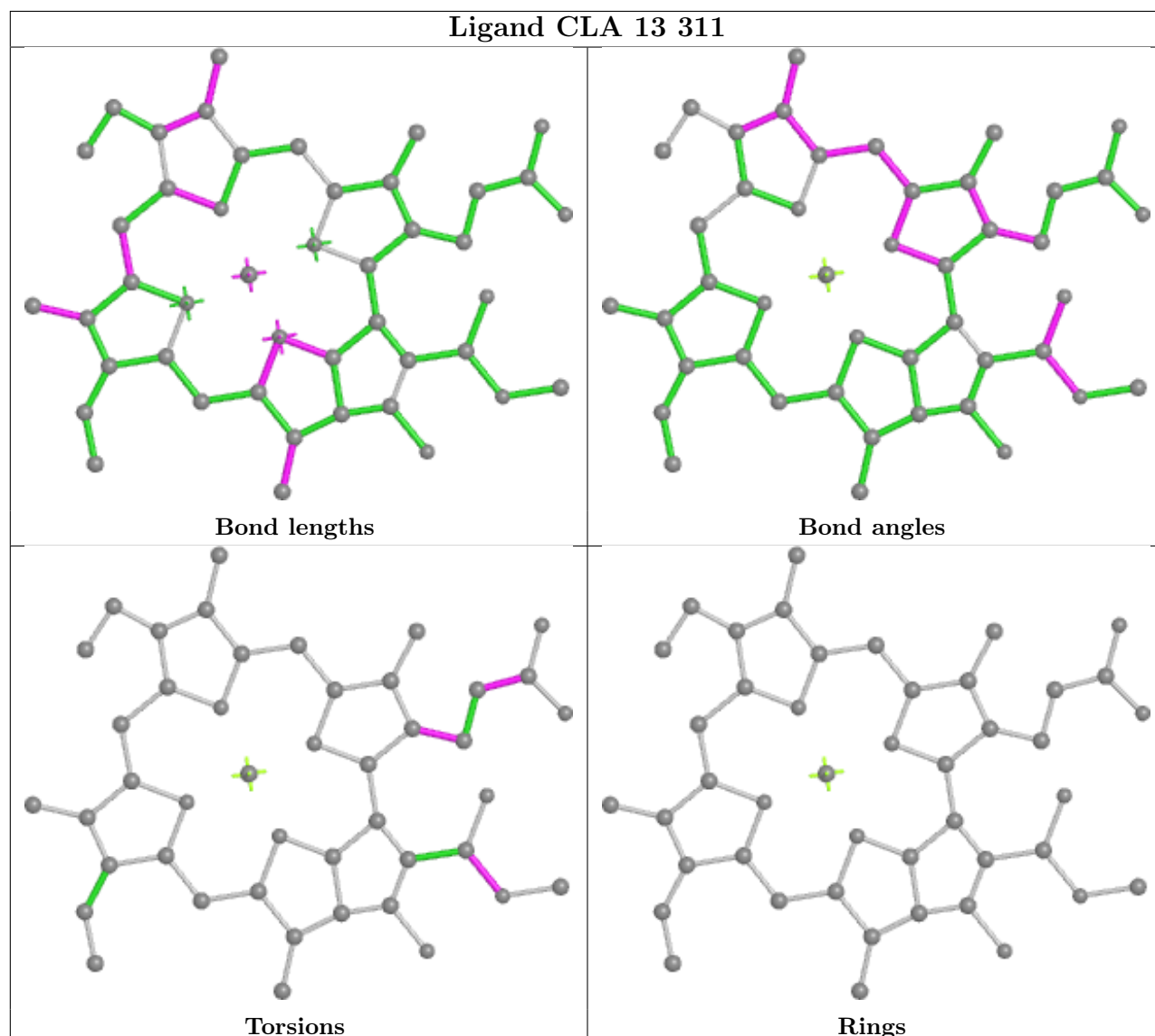
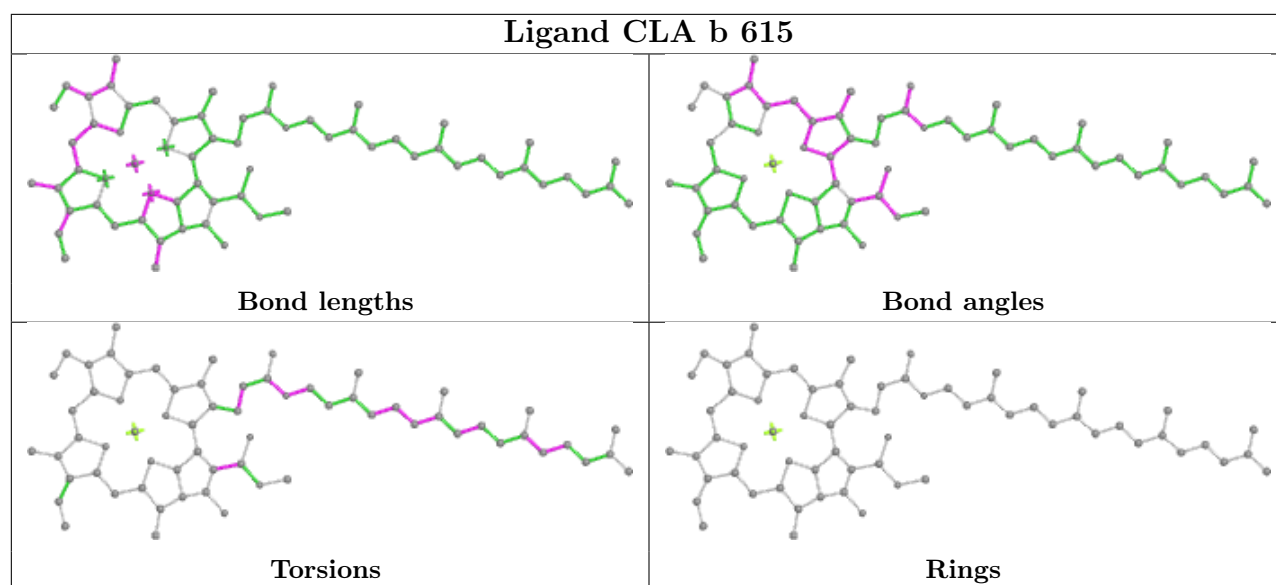


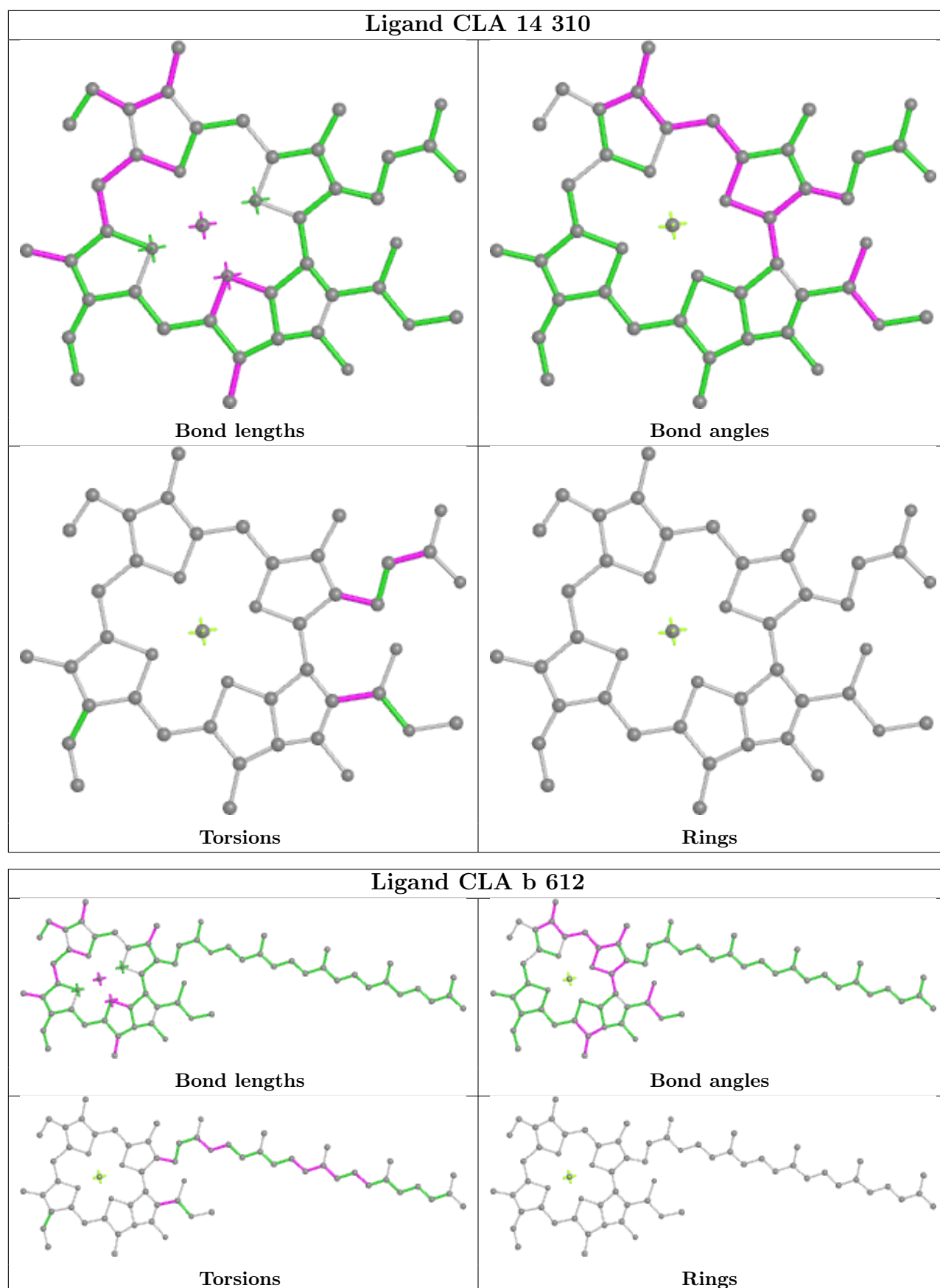


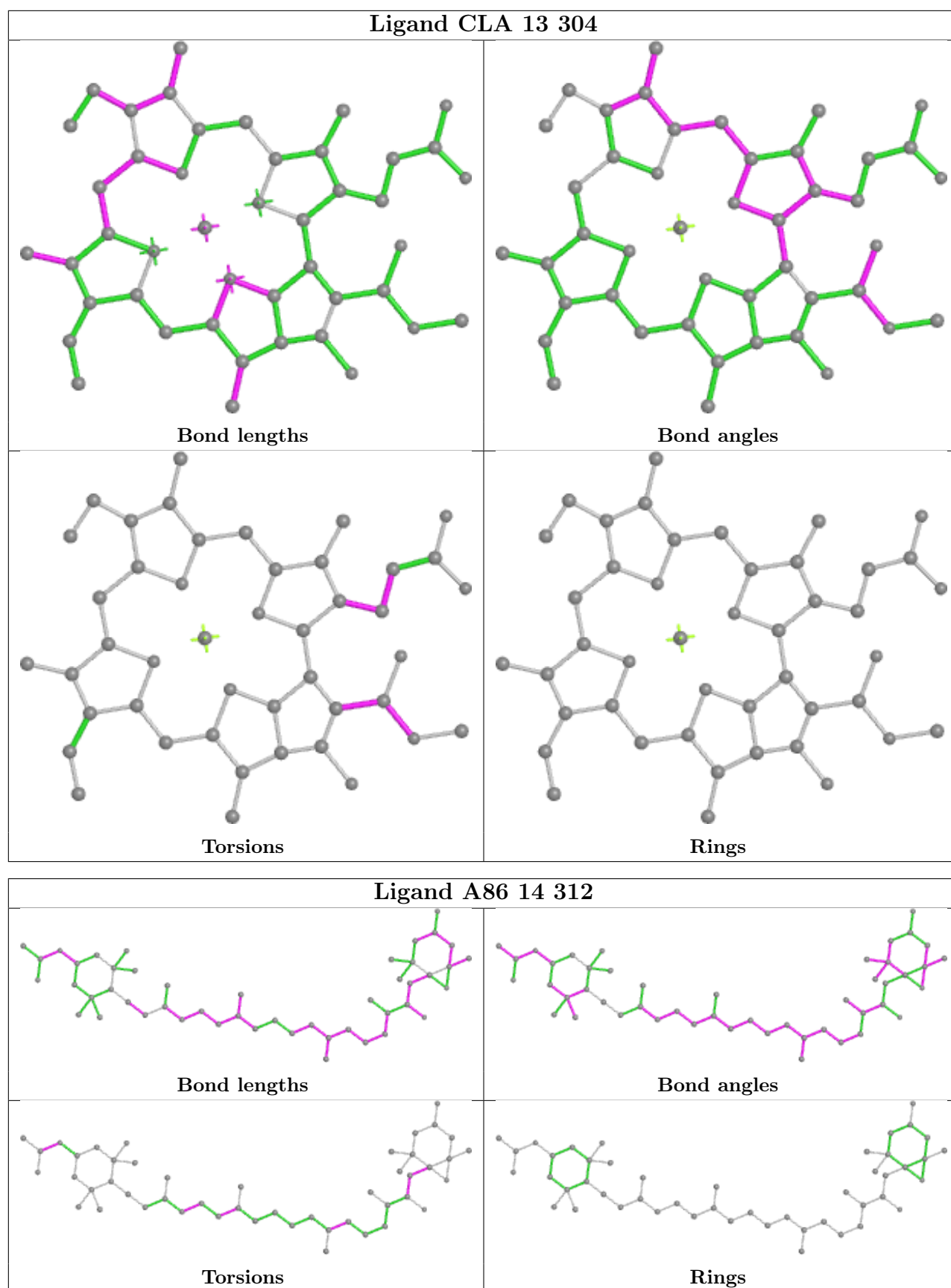


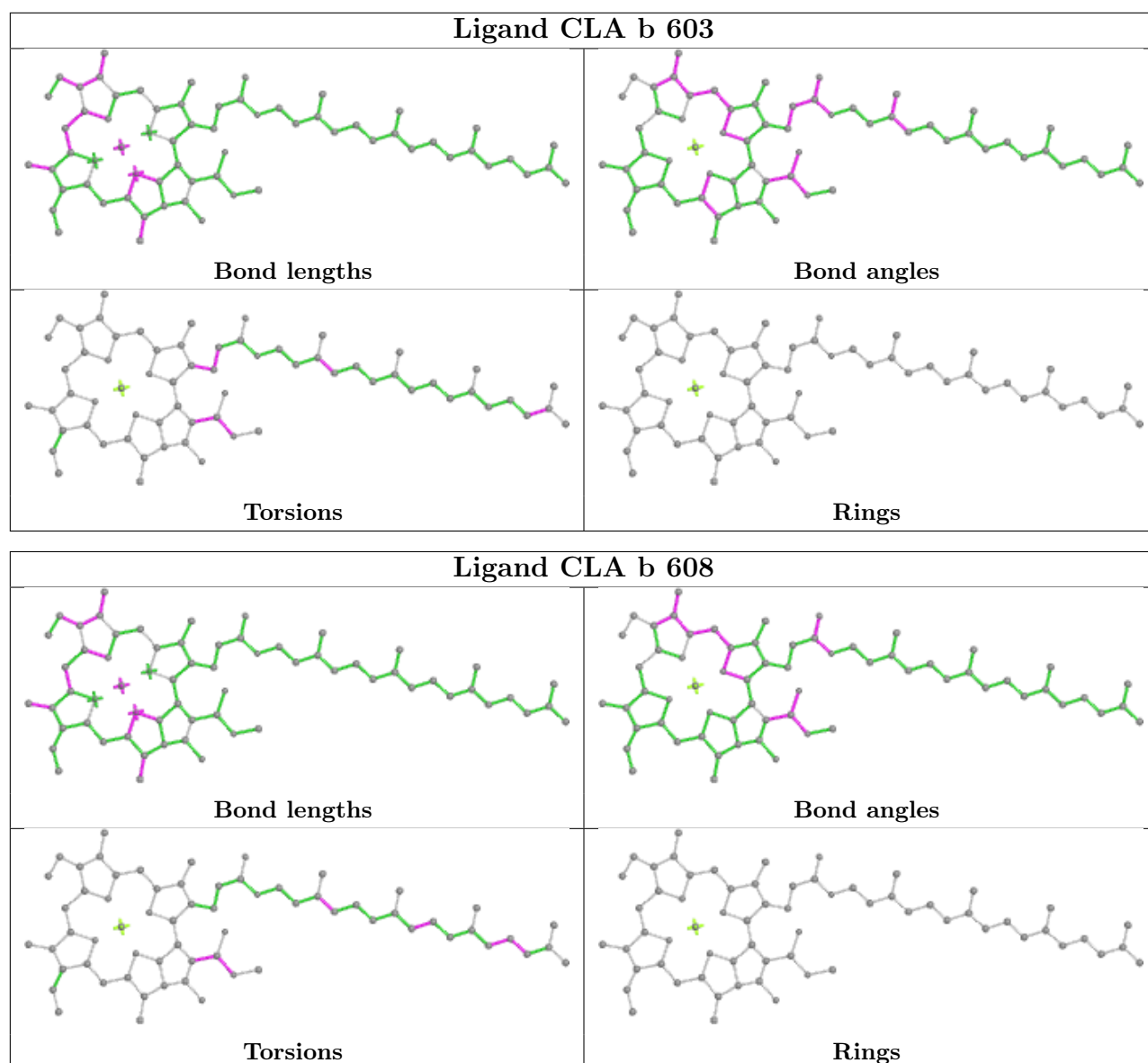


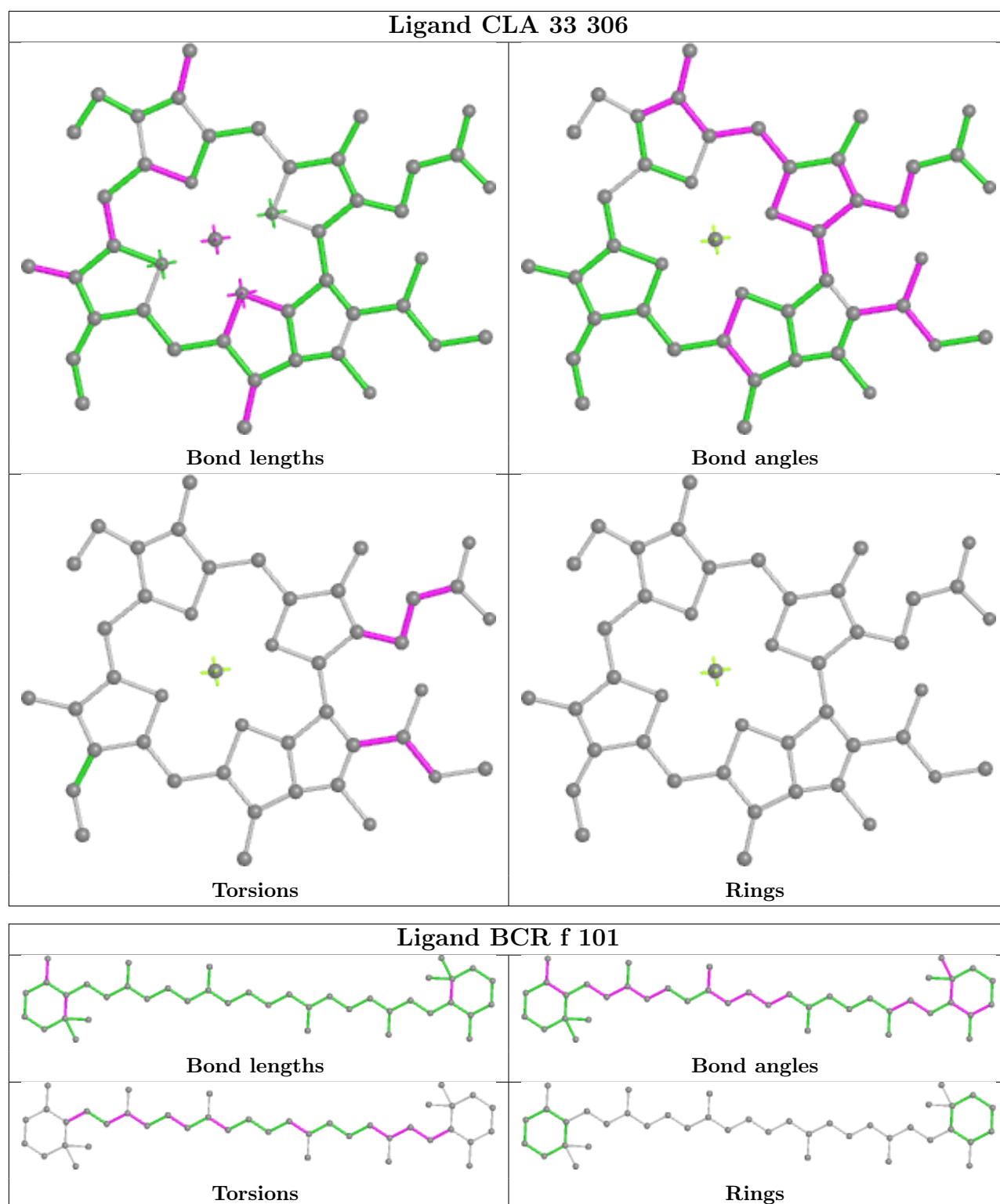


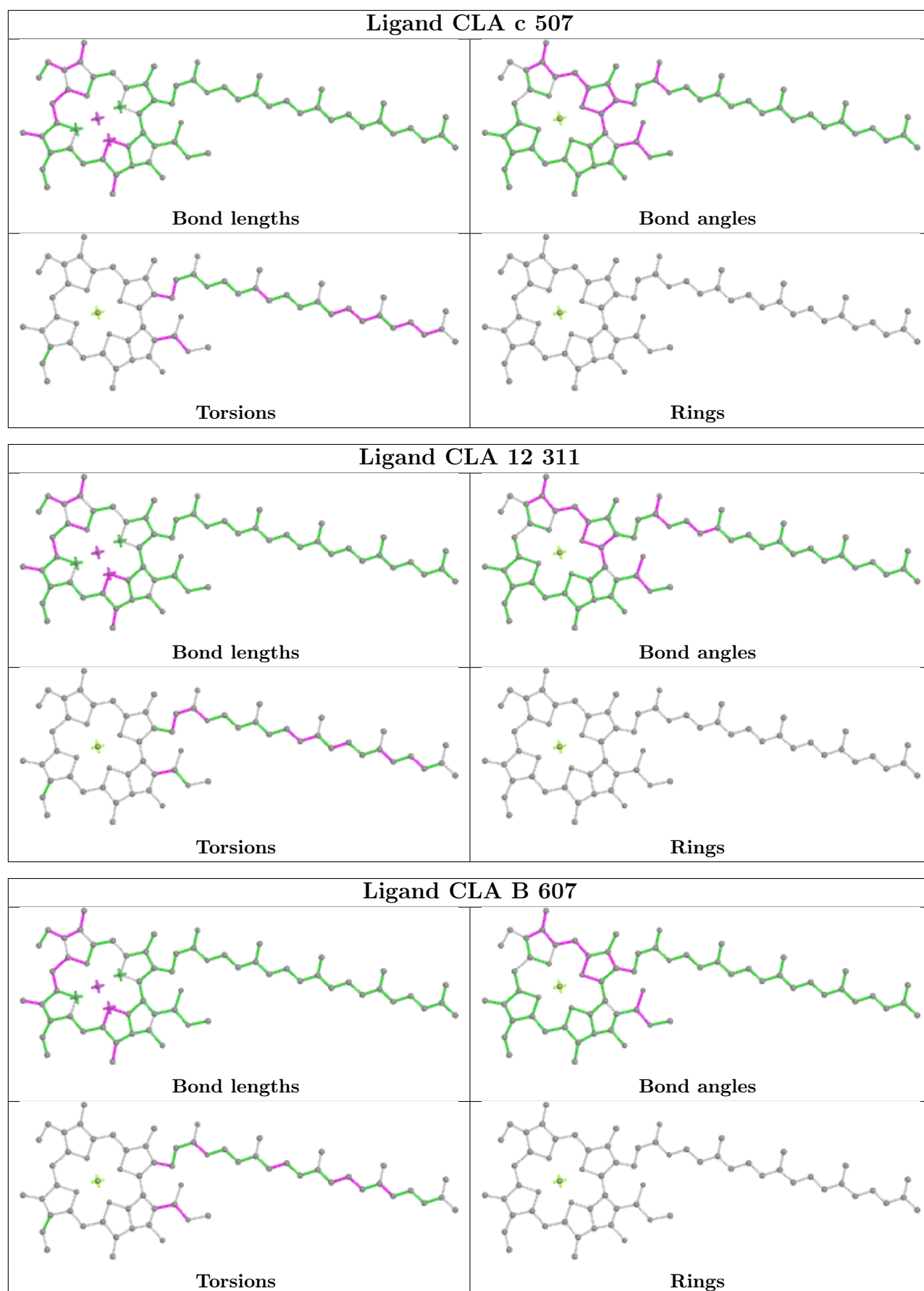


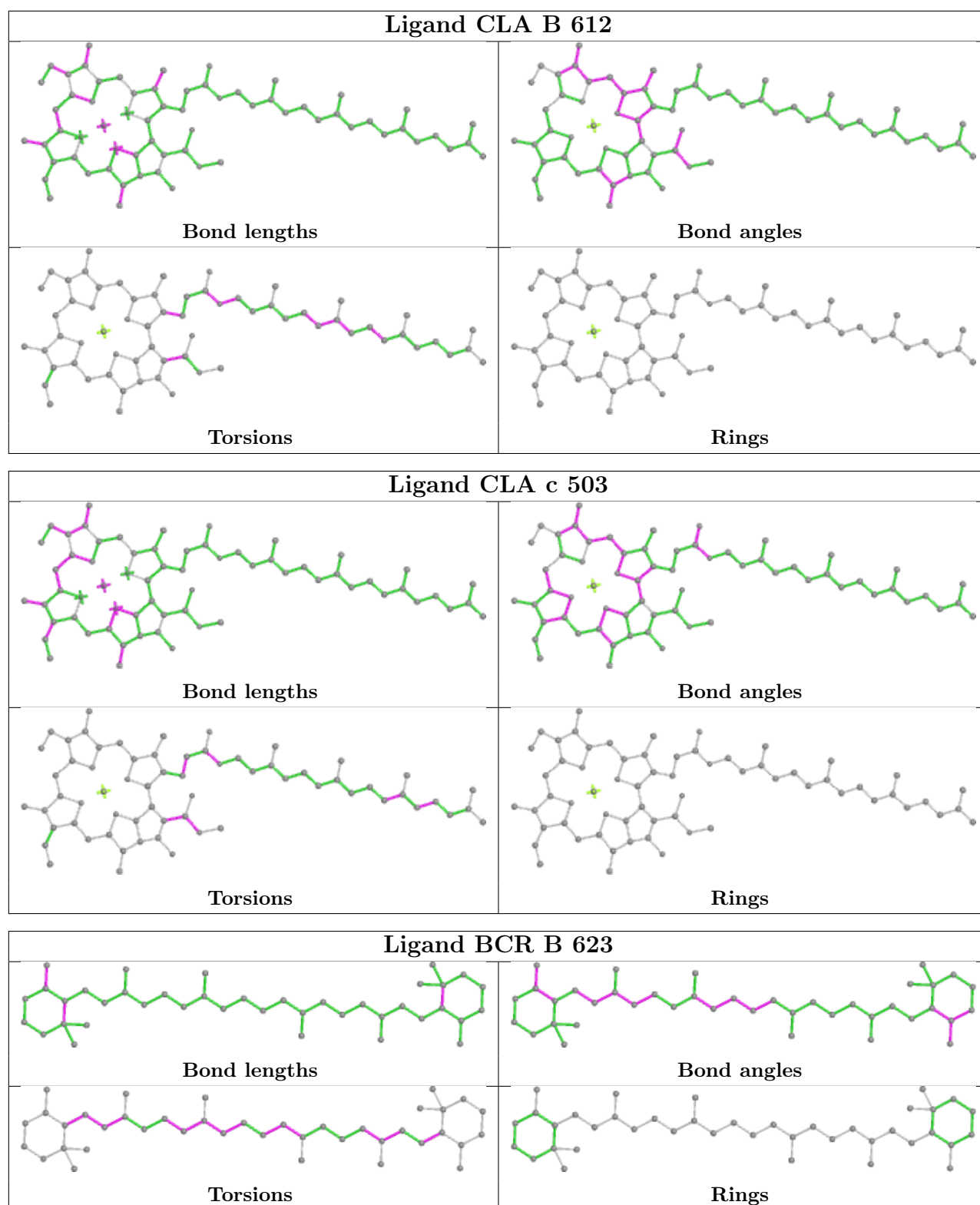




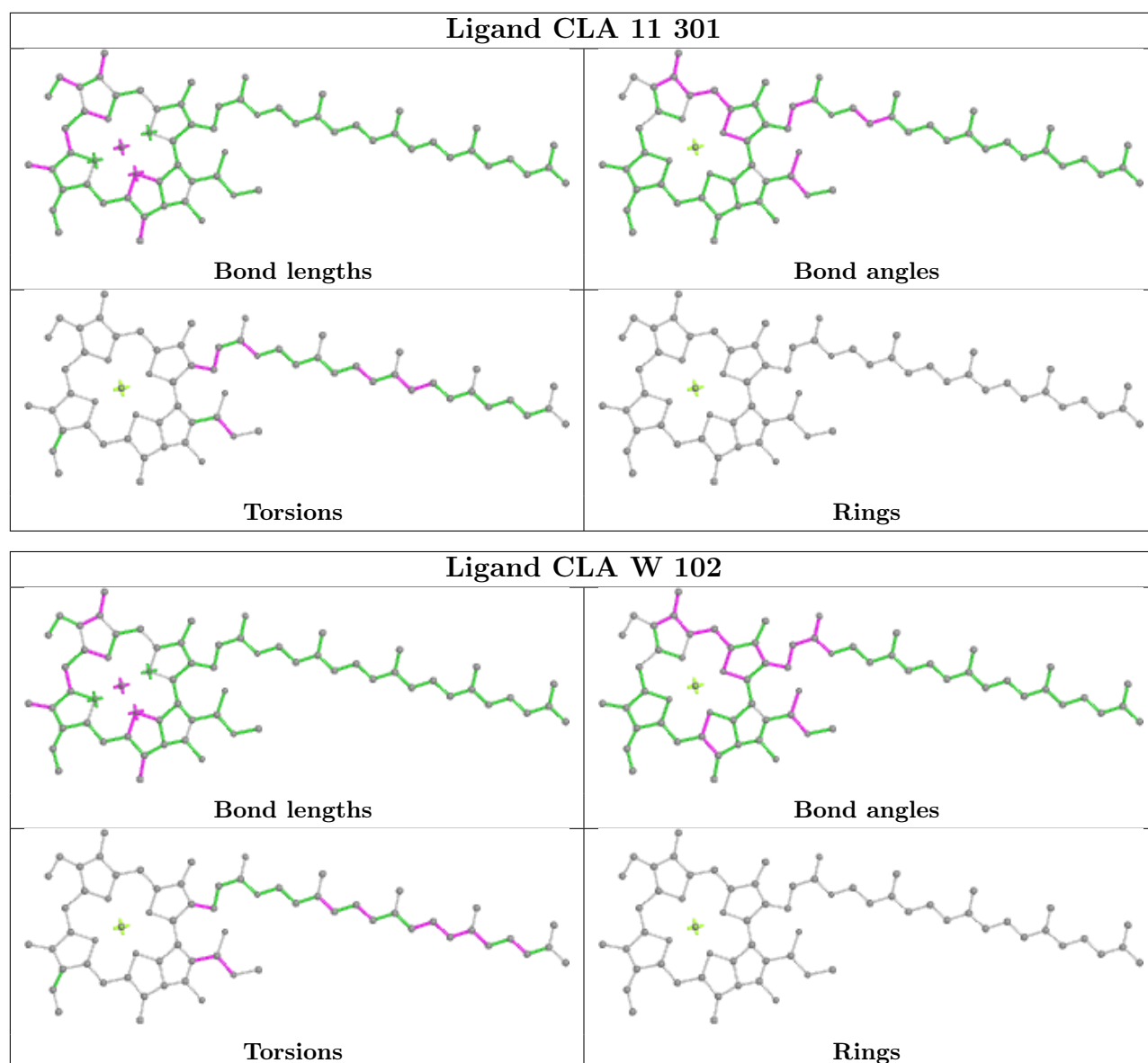


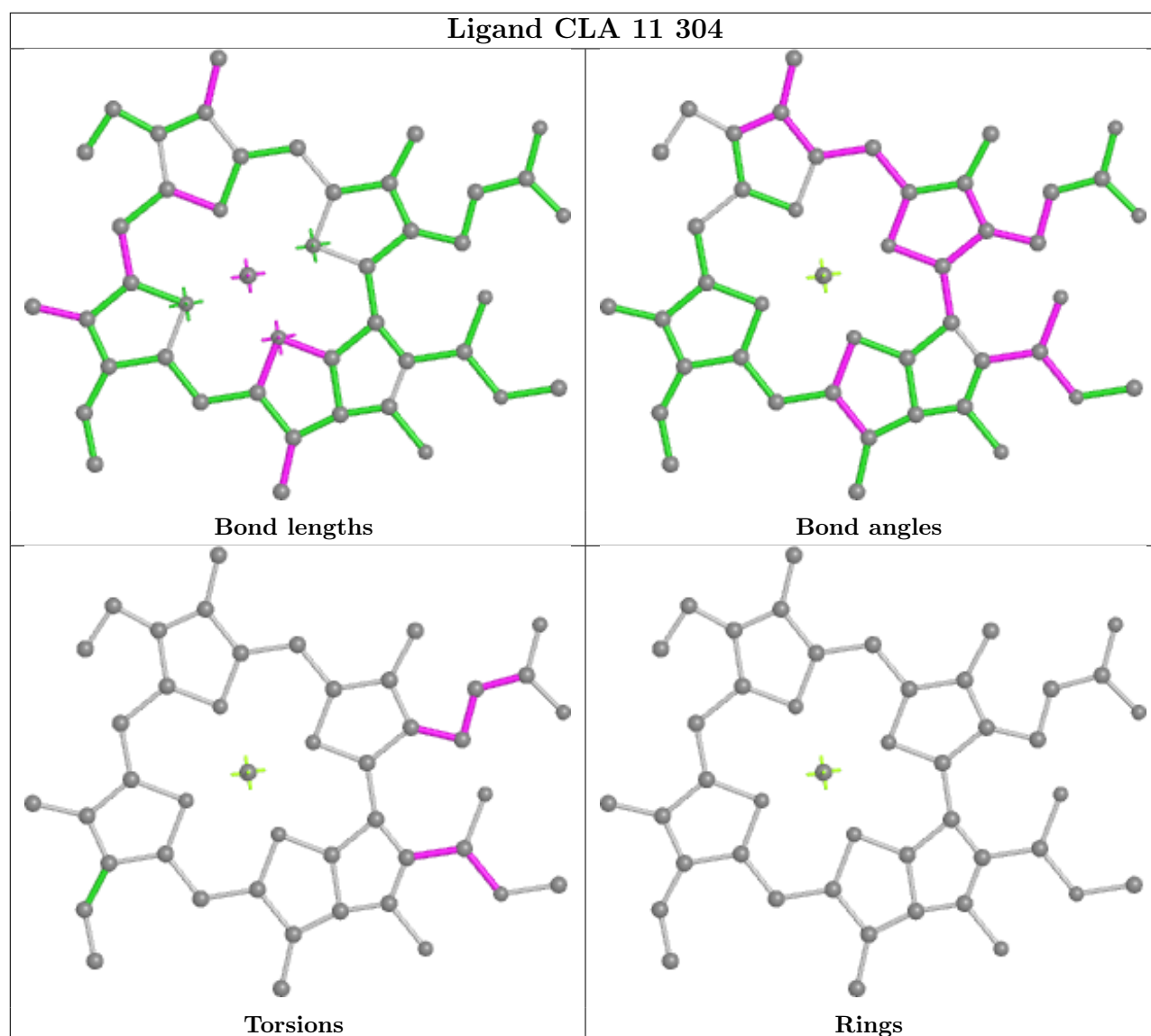


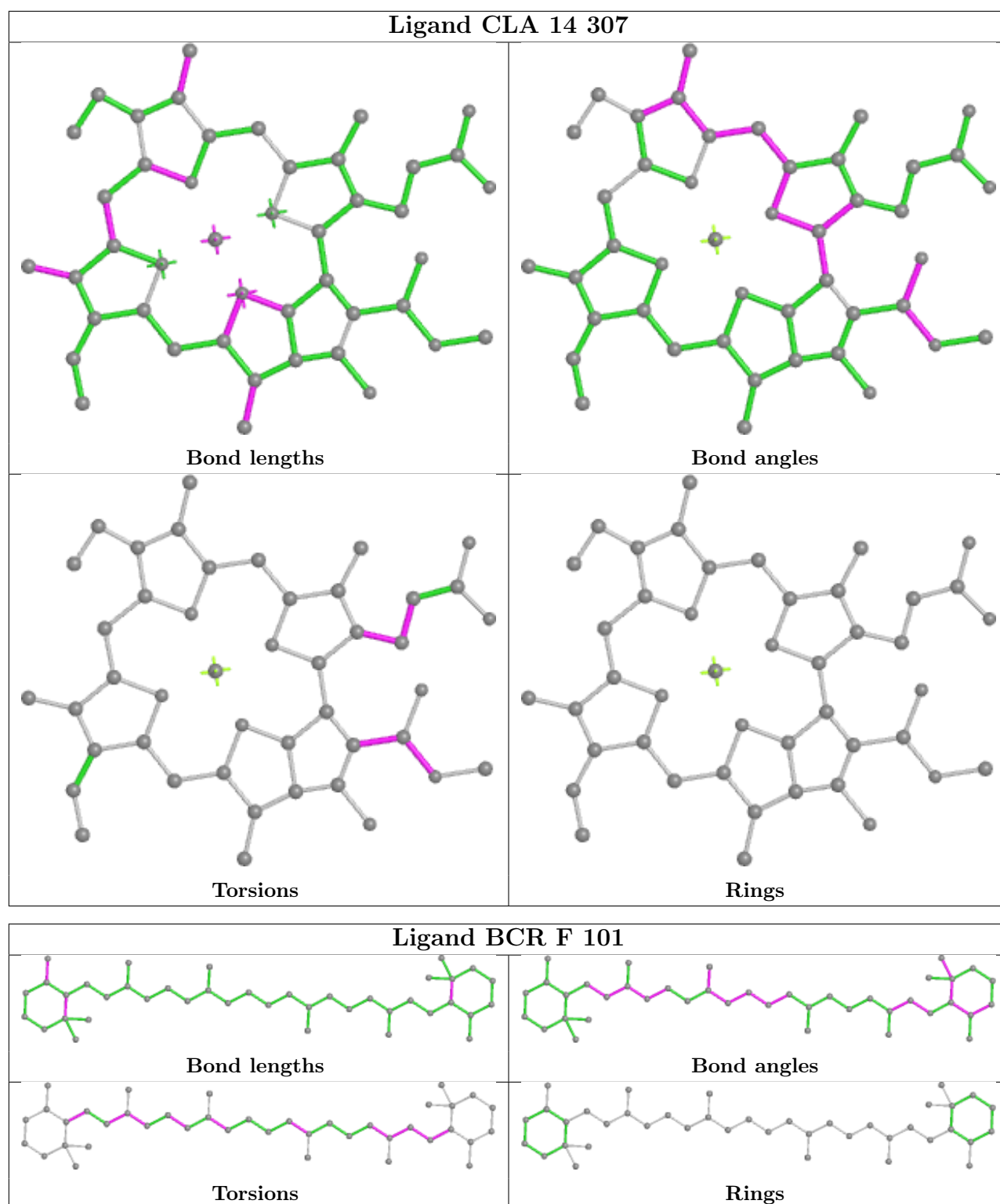


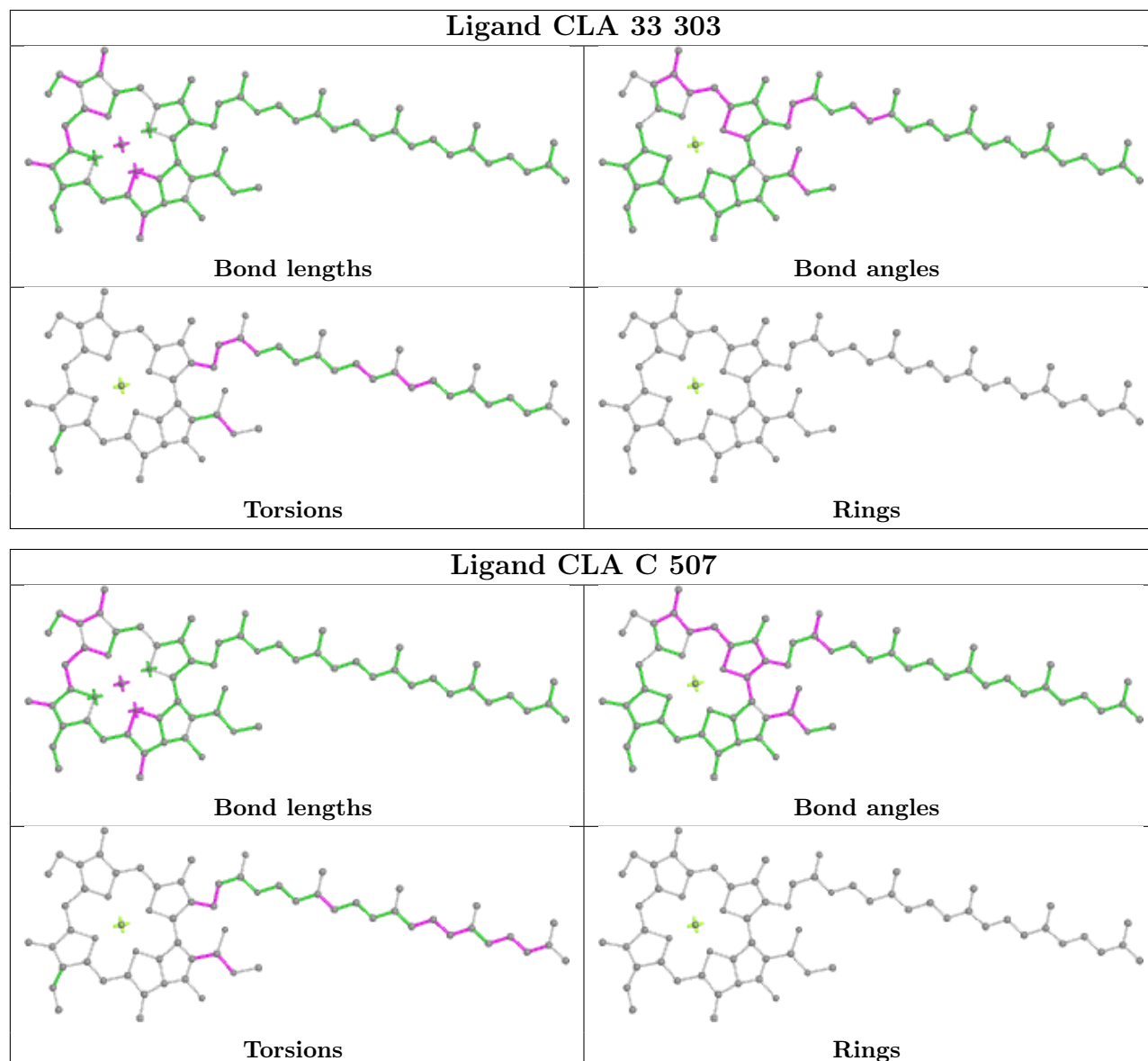


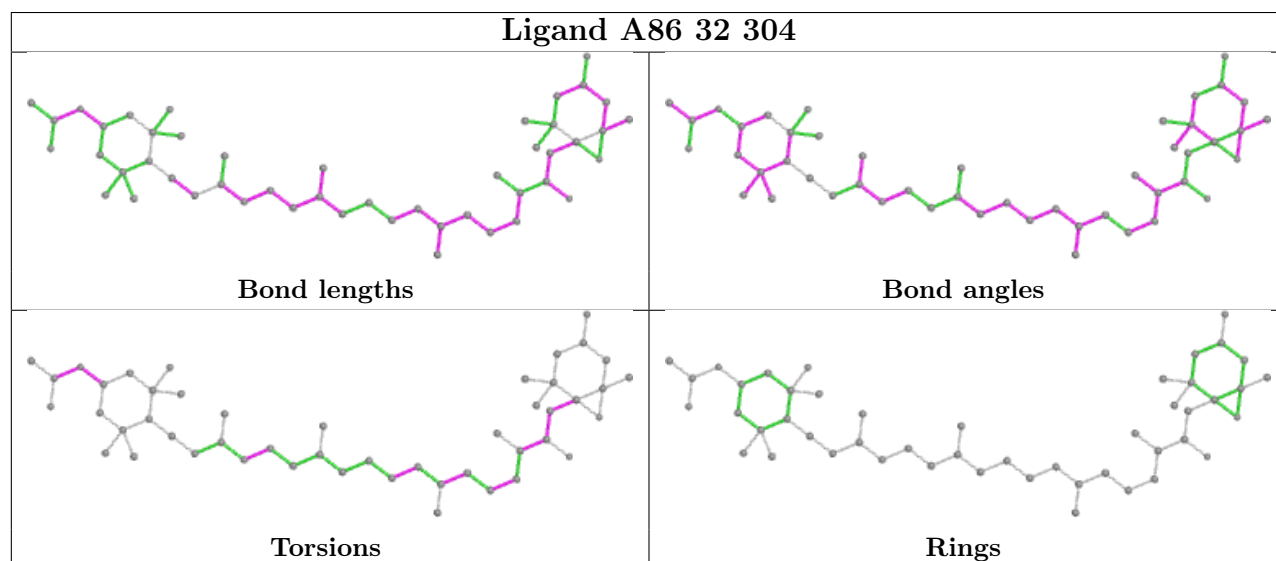
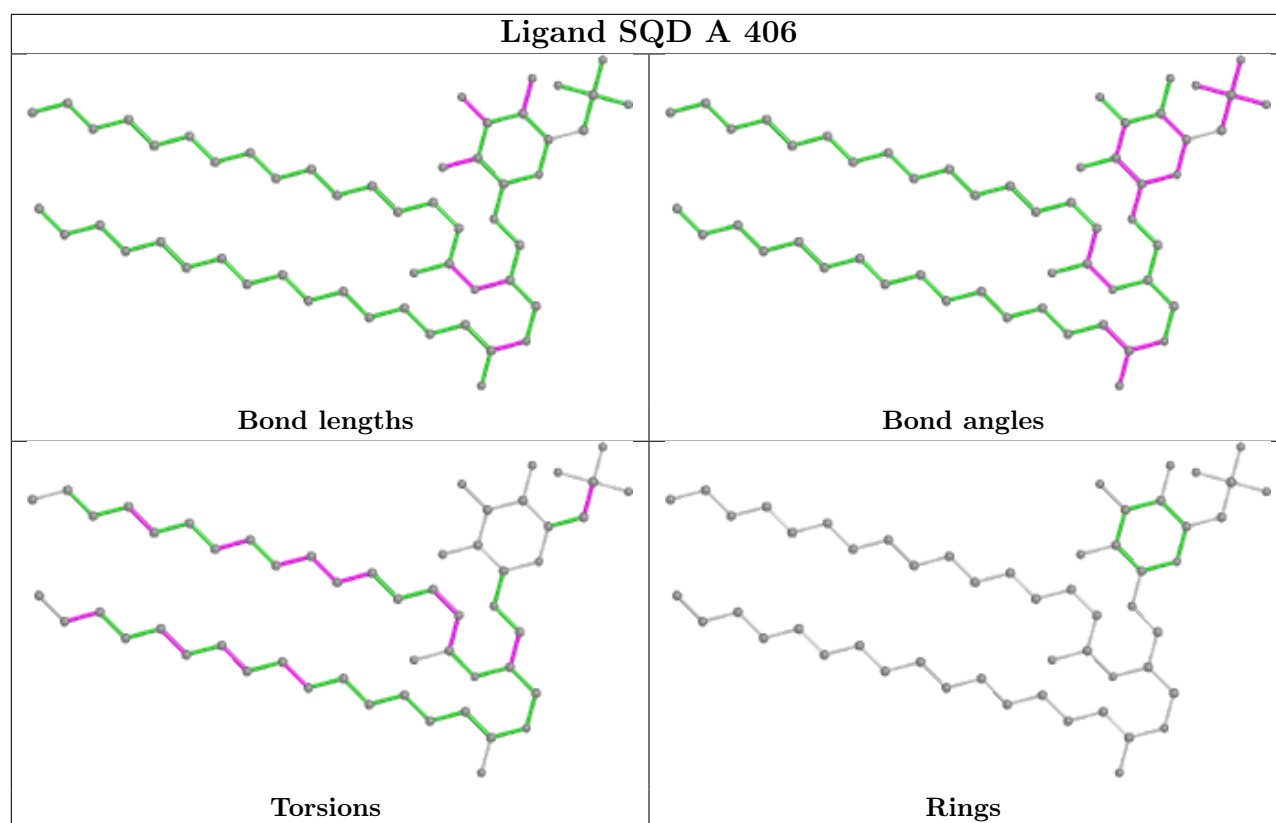


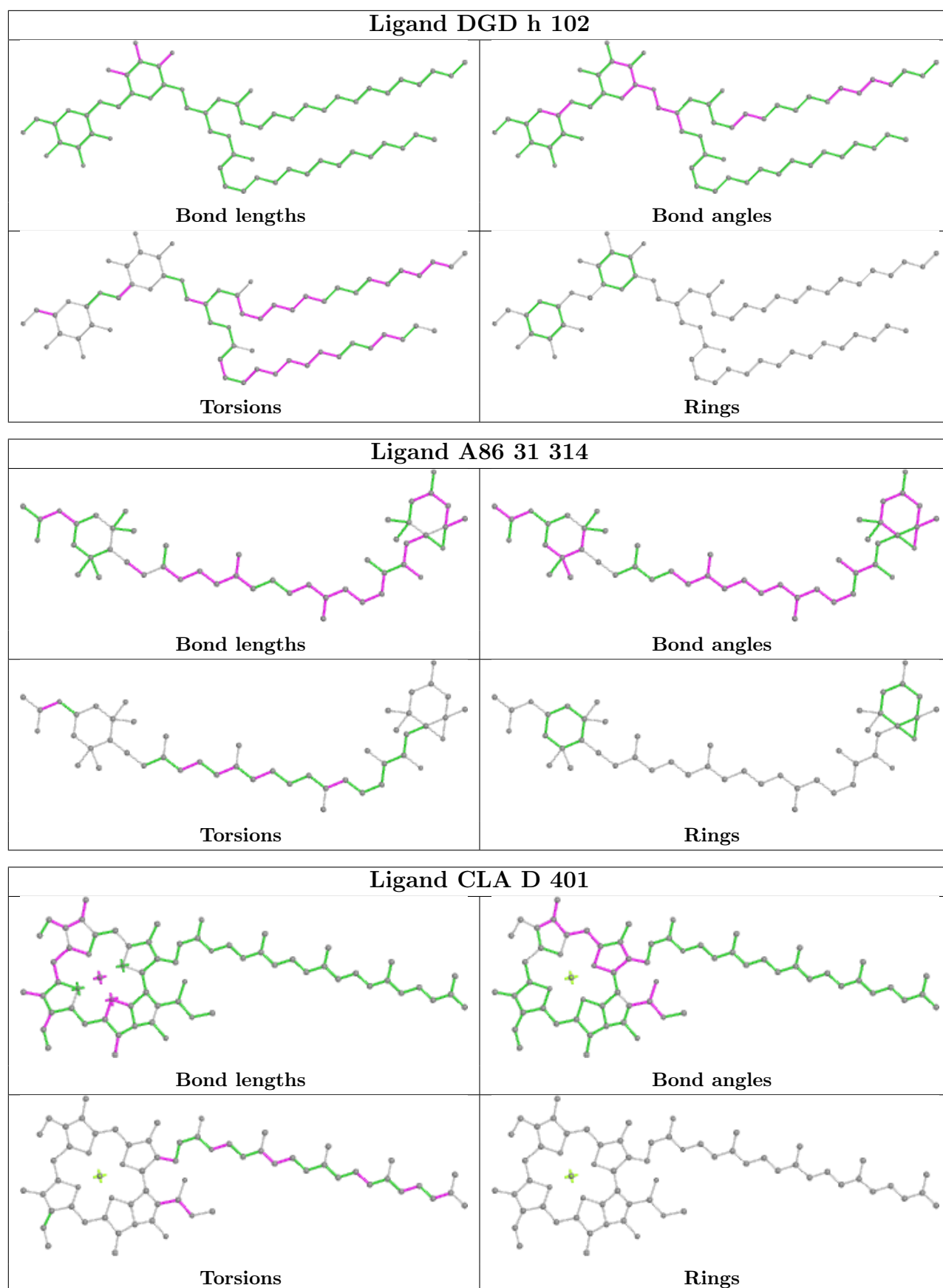


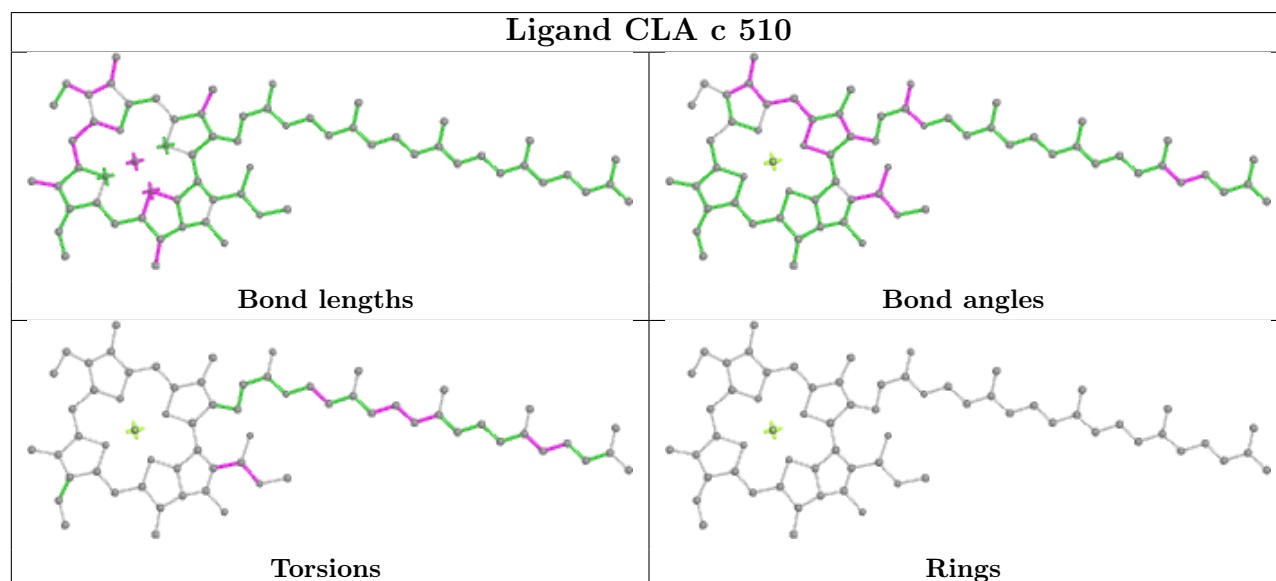
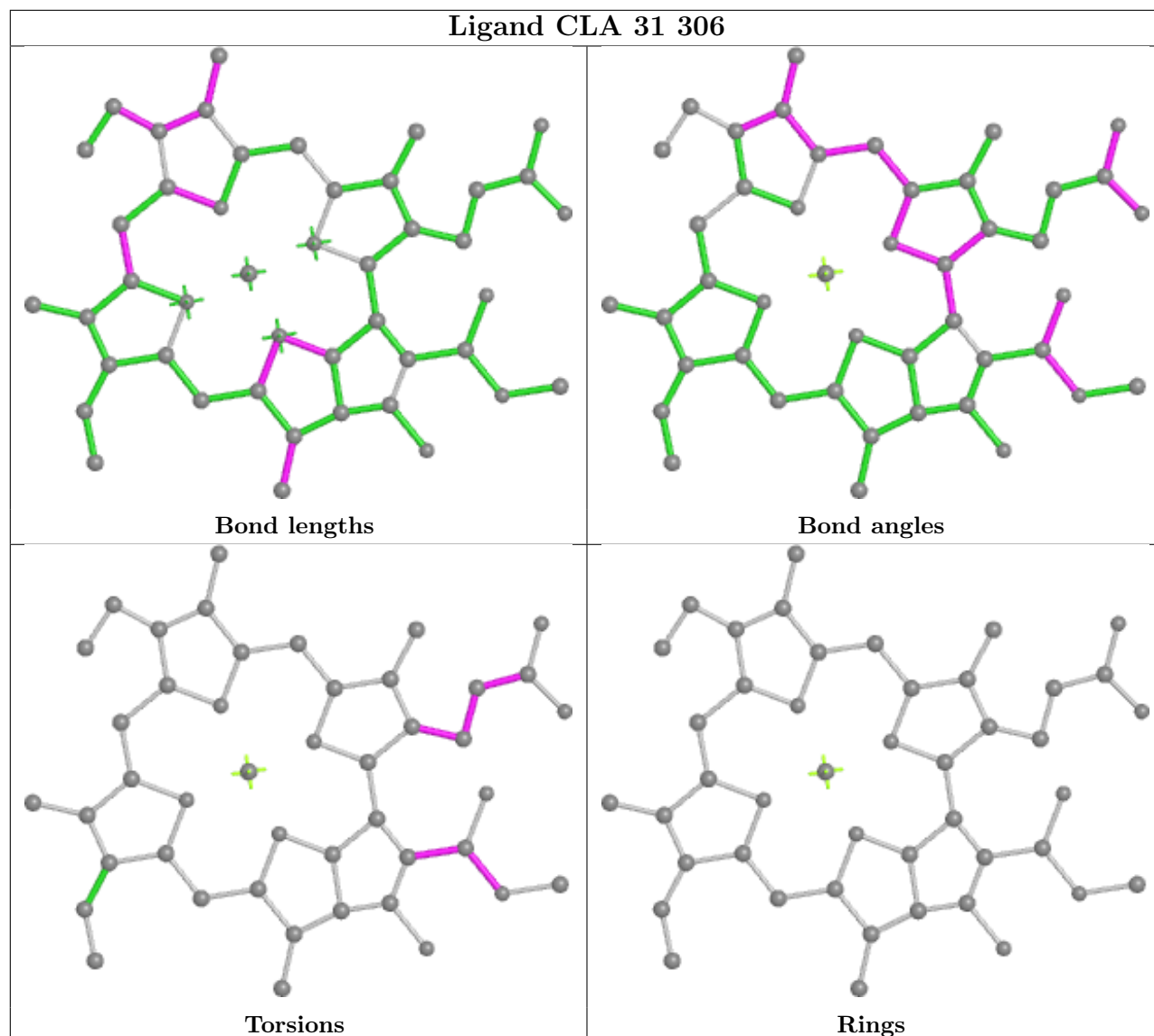


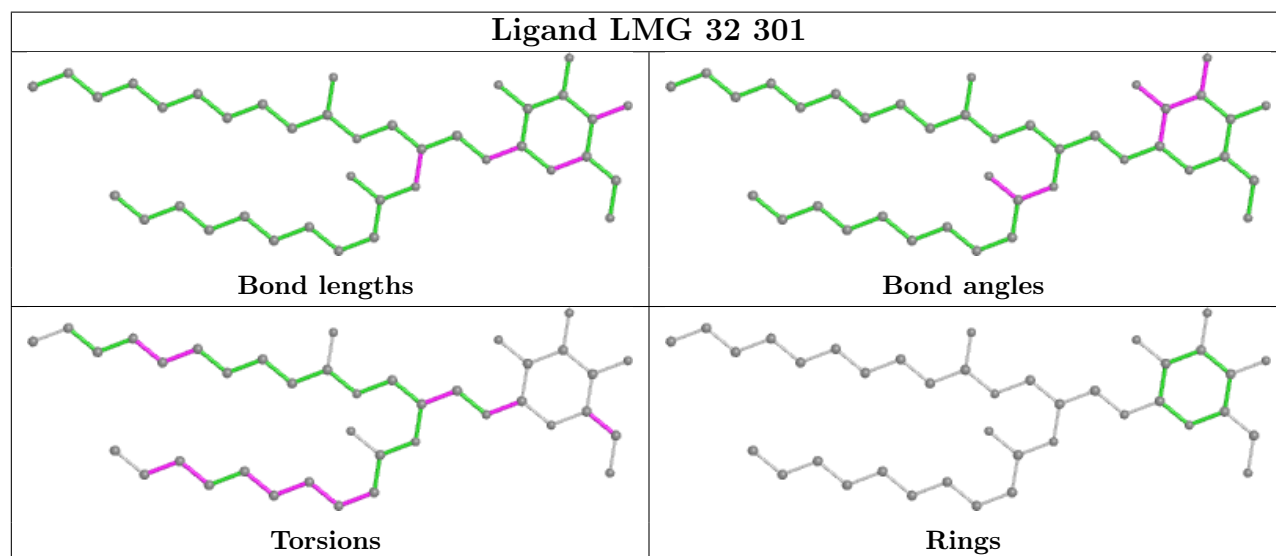
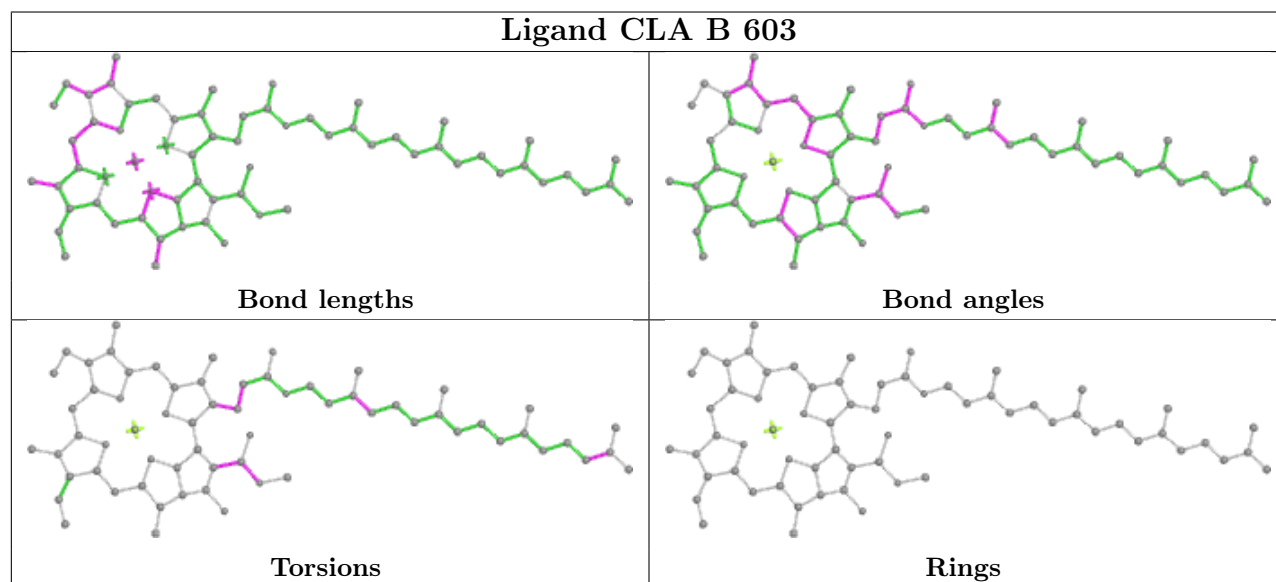
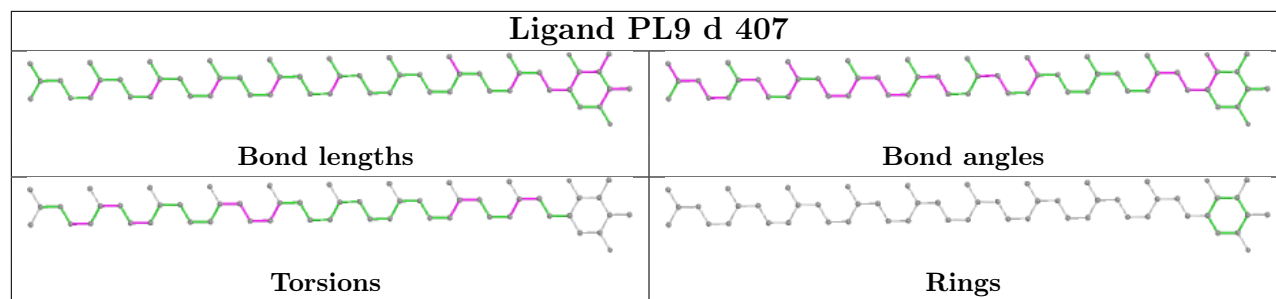




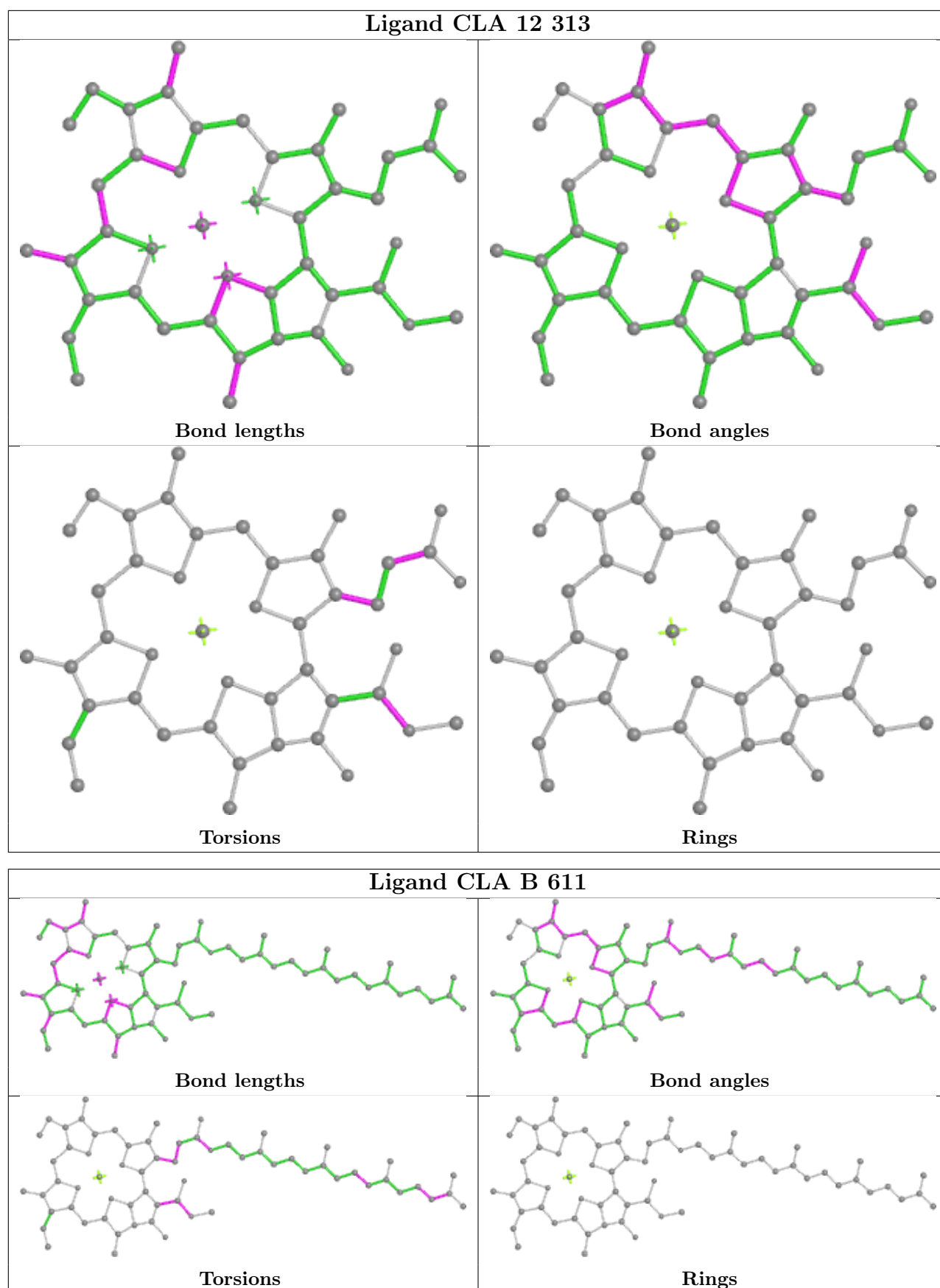


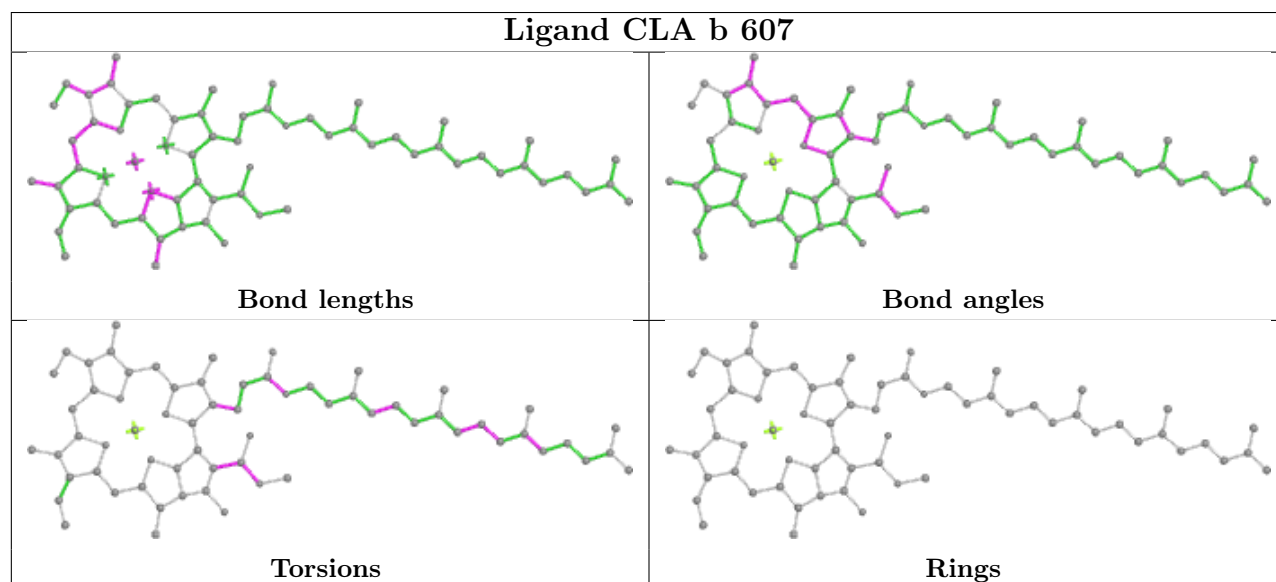
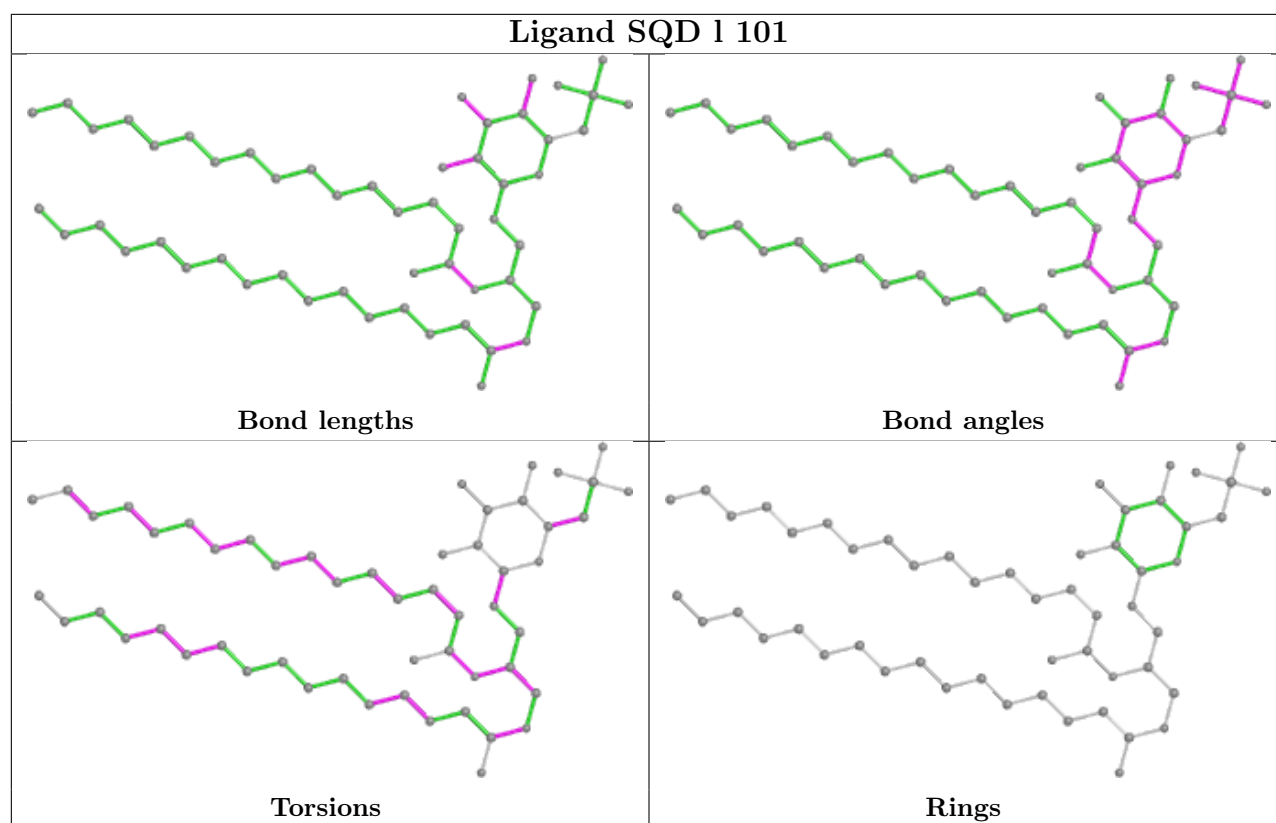


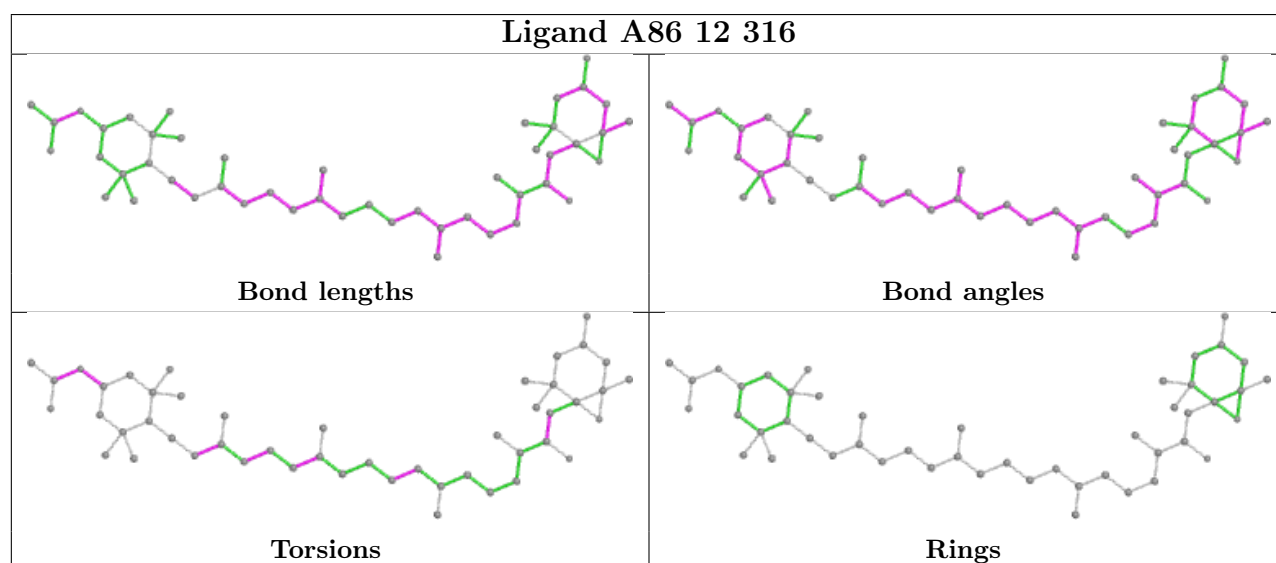
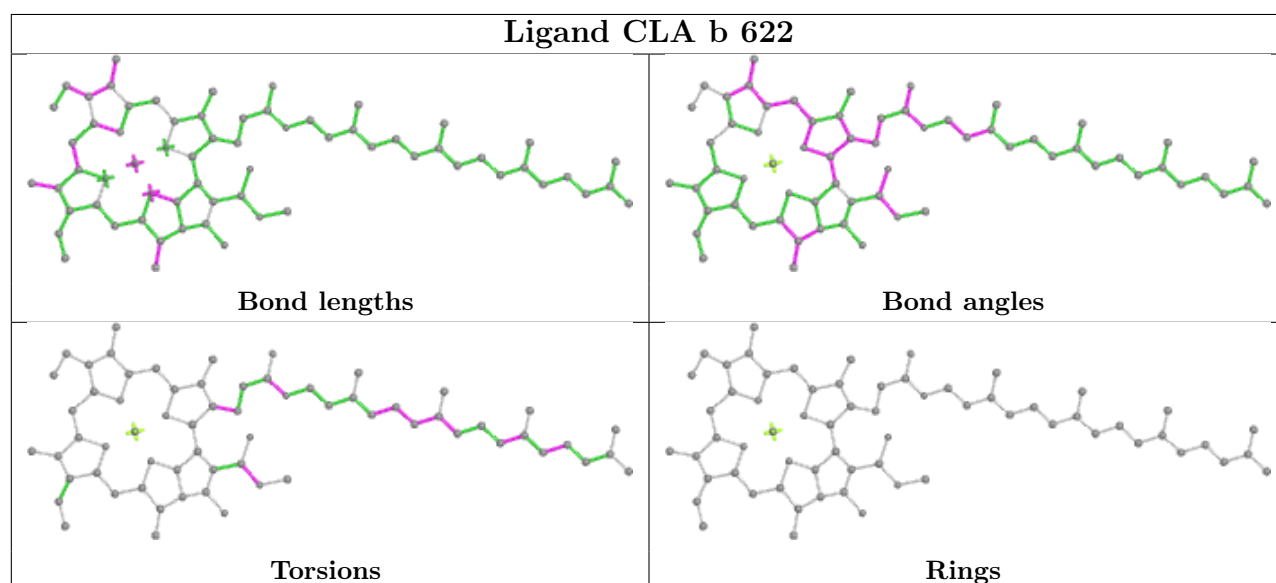
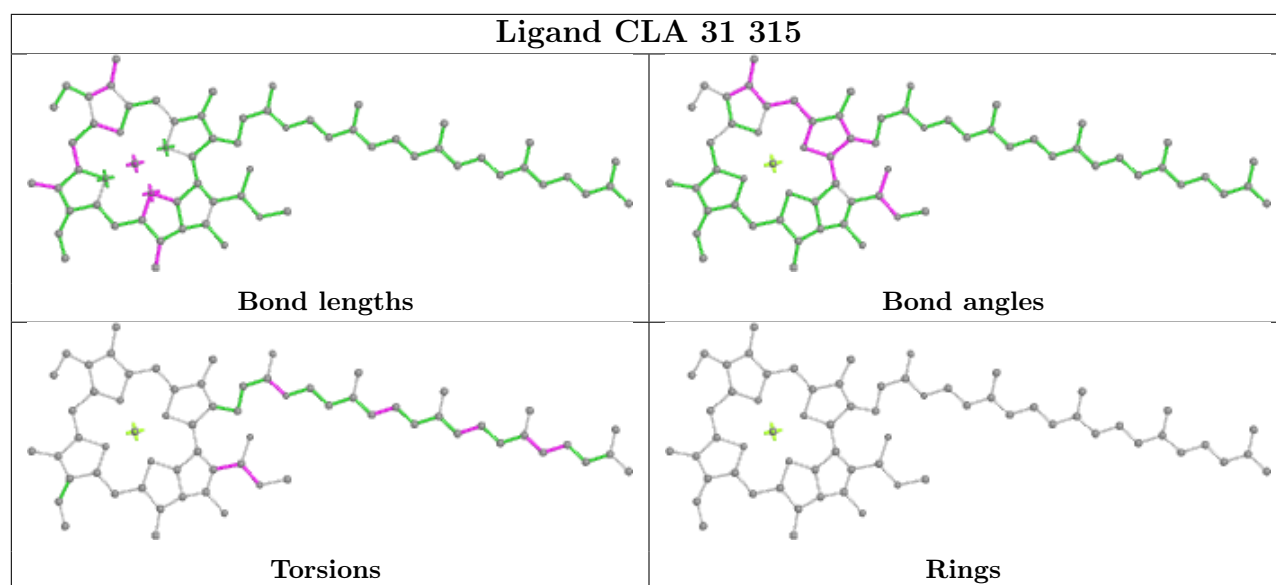


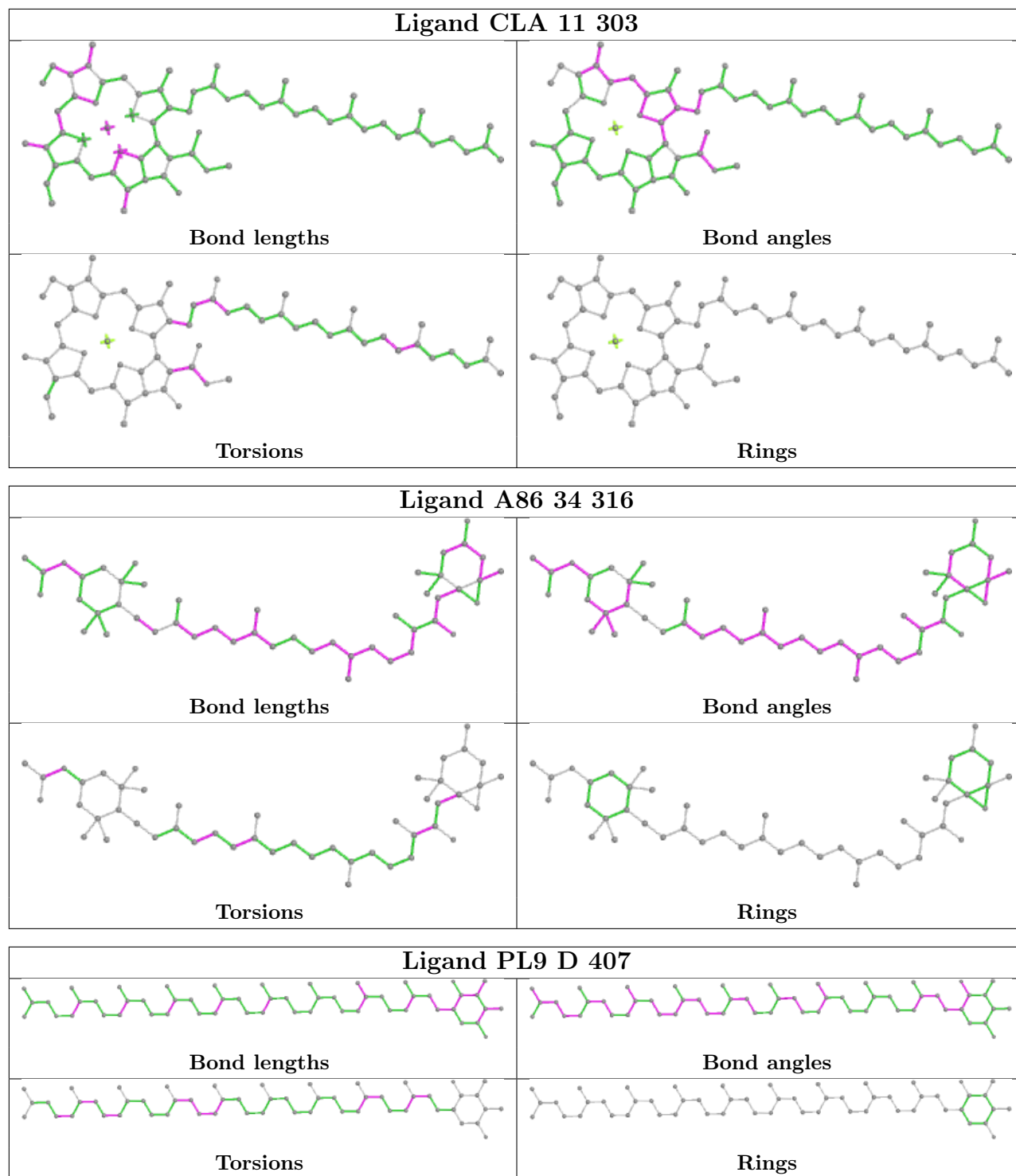


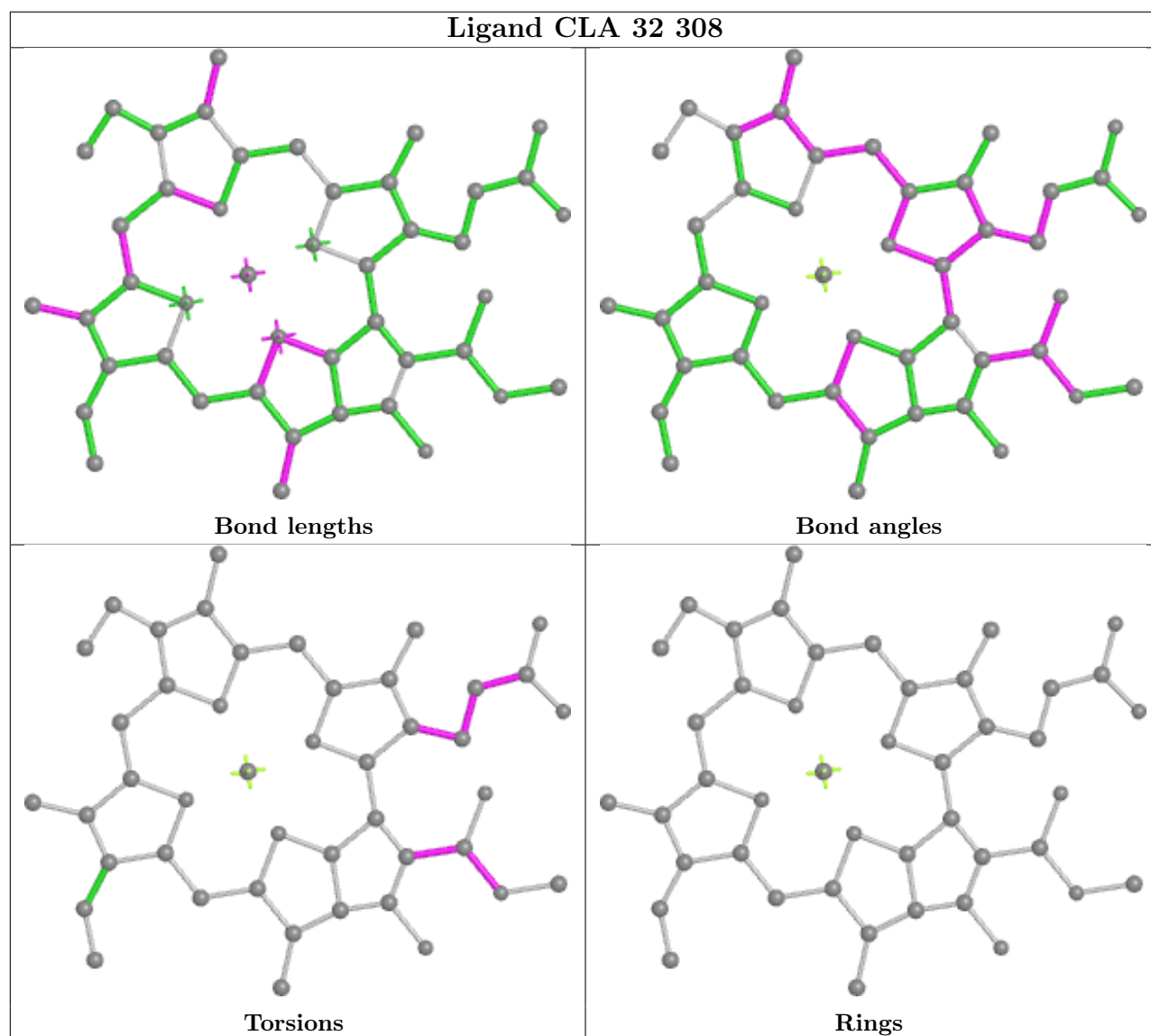
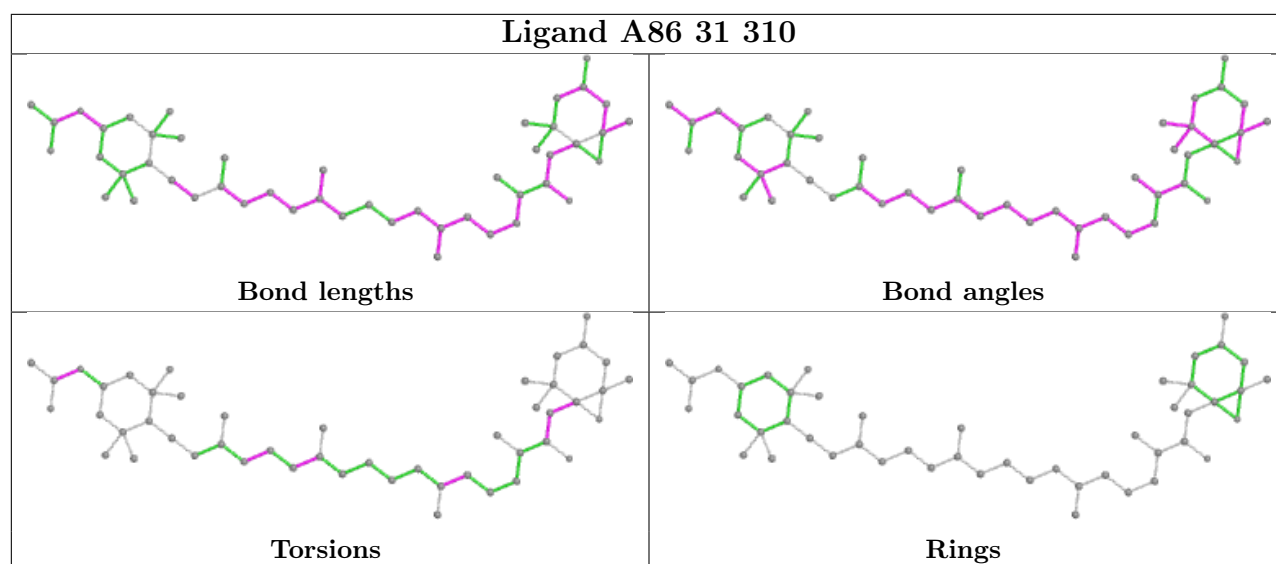


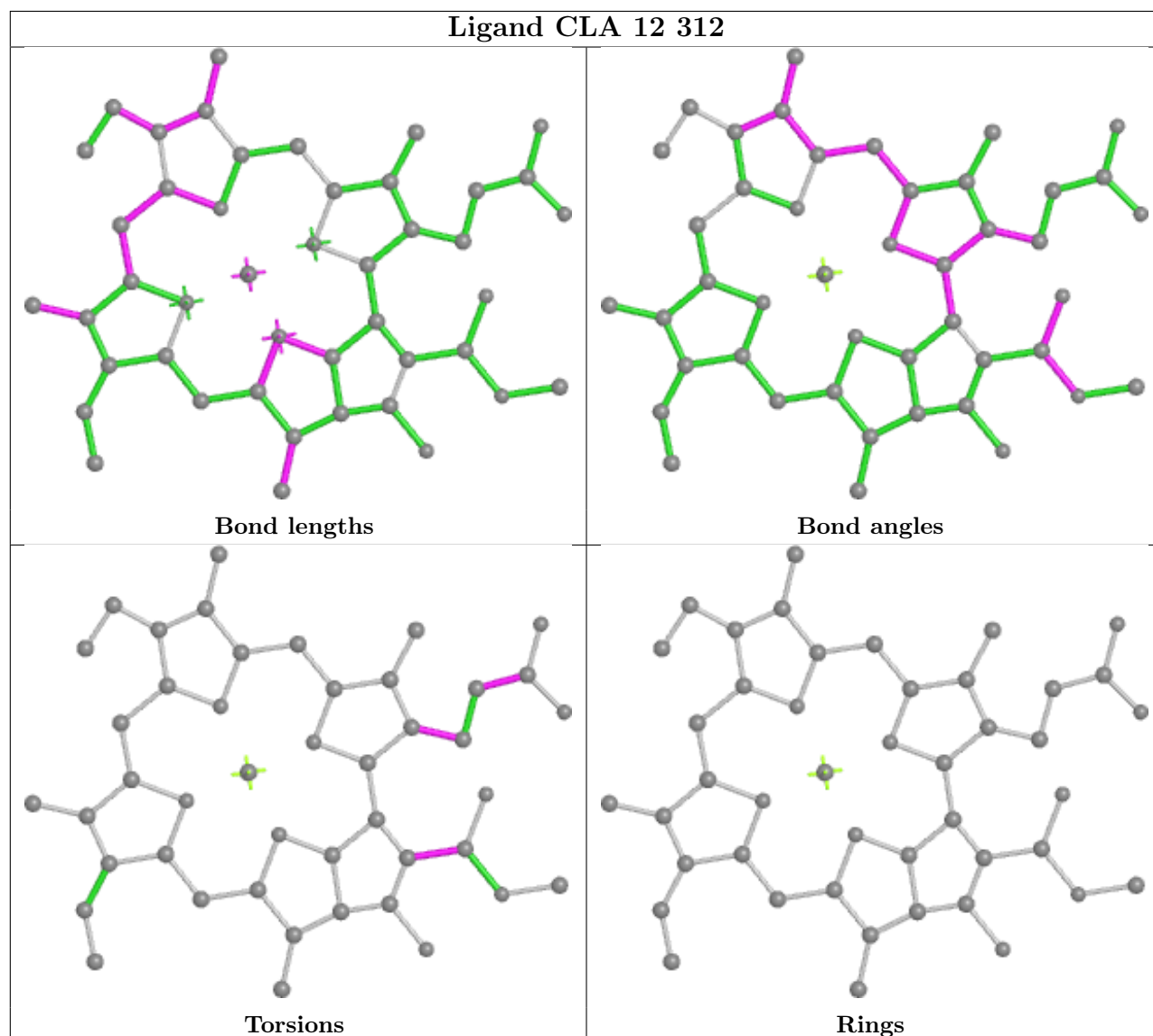
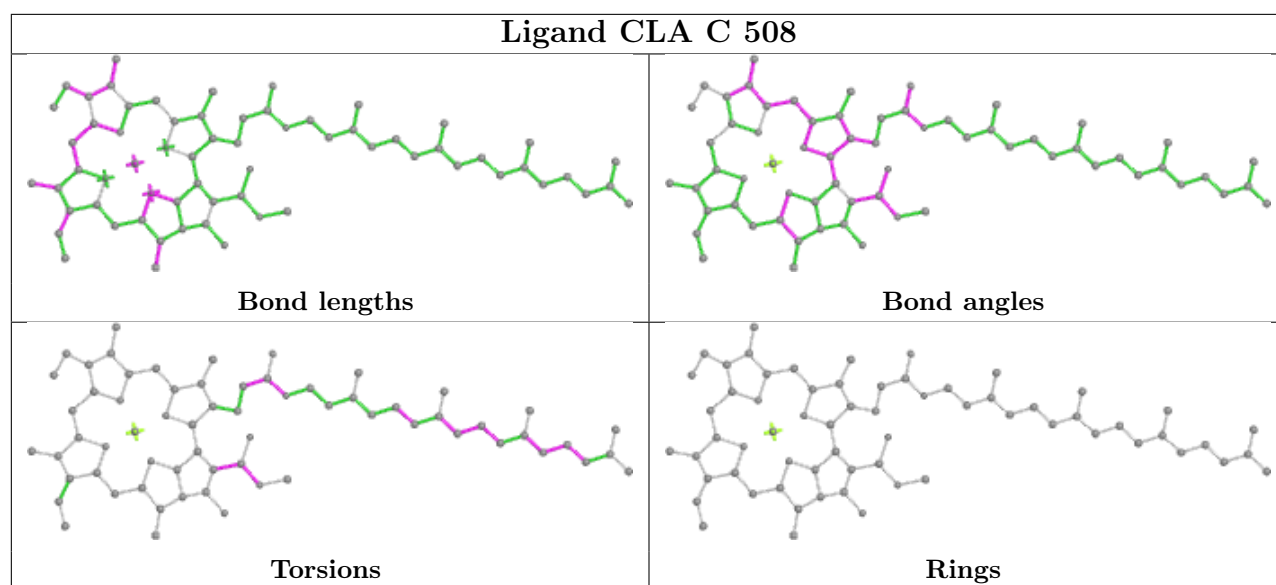


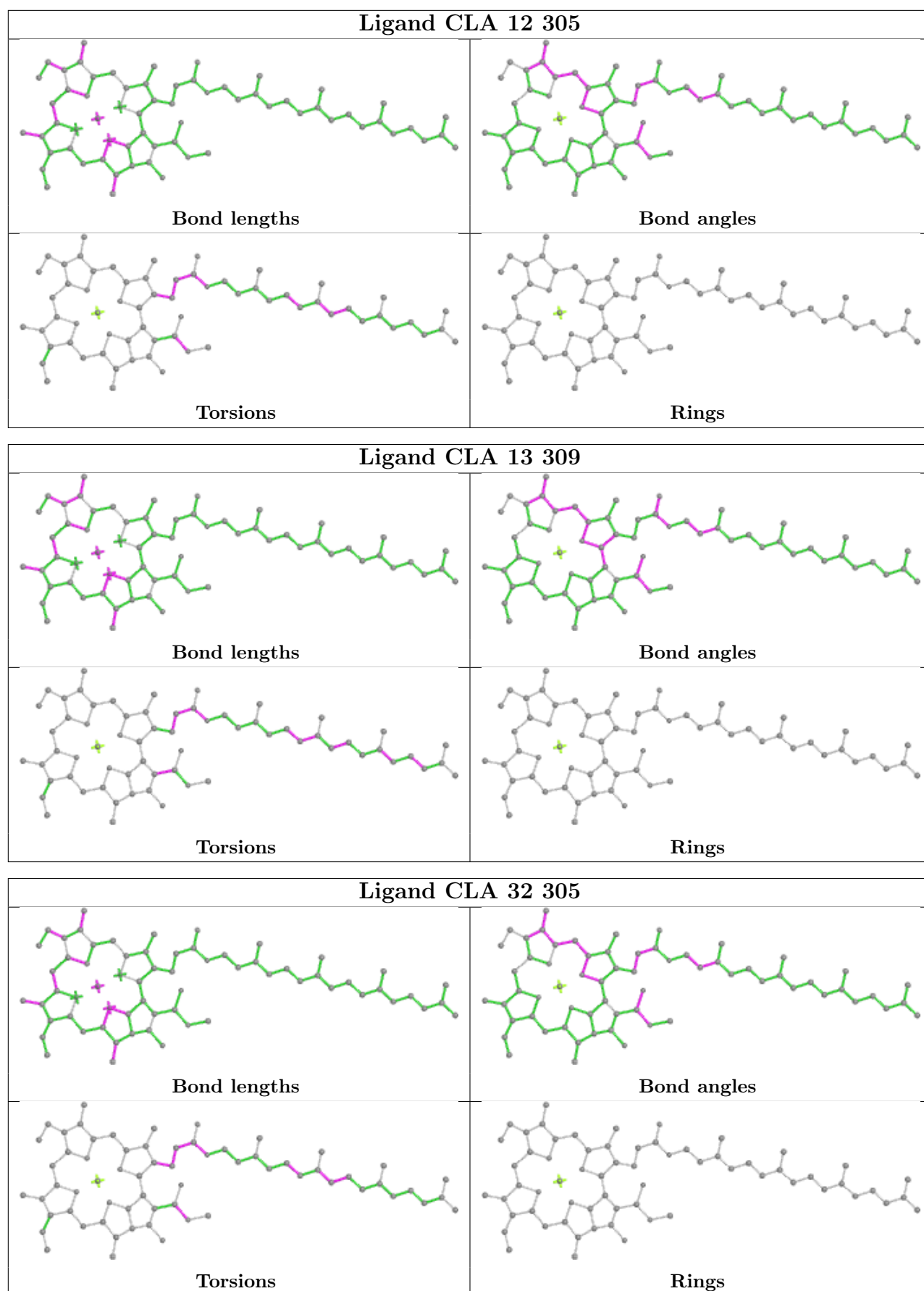












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9775. These allow visual inspection of the internal detail of the map and identification of artifacts.

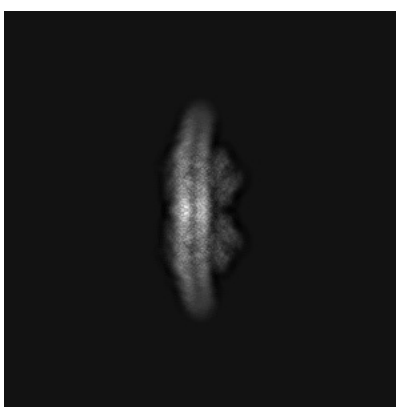
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

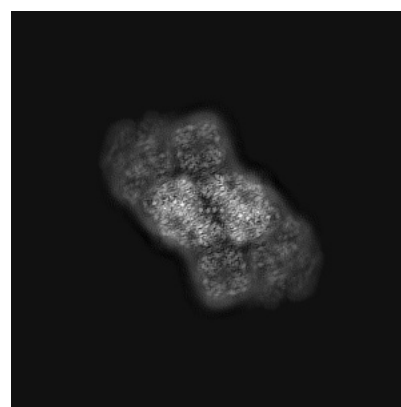
#### 6.1.1 Primary map



X



Y



Z

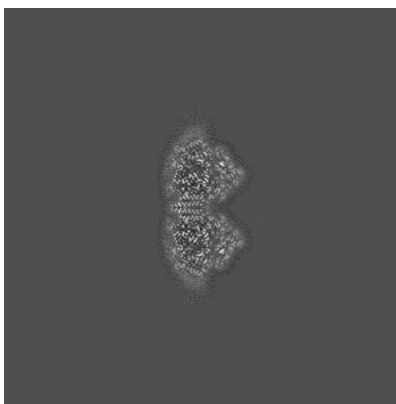
The images above show the map projected in three orthogonal directions.

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

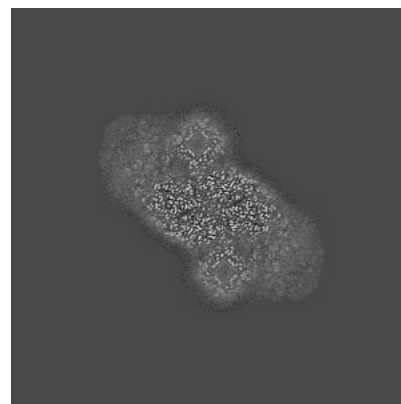
#### 6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

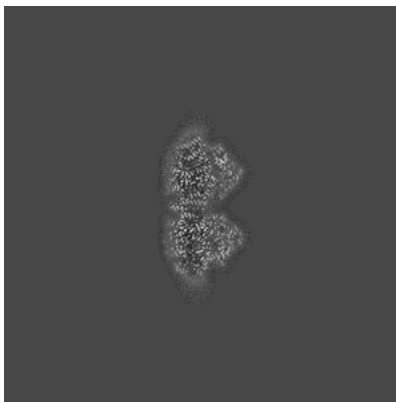
The images above show central slices of the map in three orthogonal directions.

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

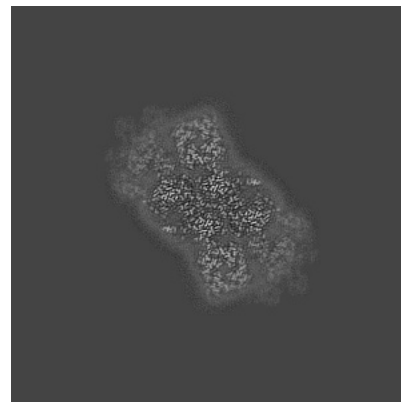
### 6.3.1 Primary map



X Index: 261



Y Index: 258



Z Index: 232

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

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

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

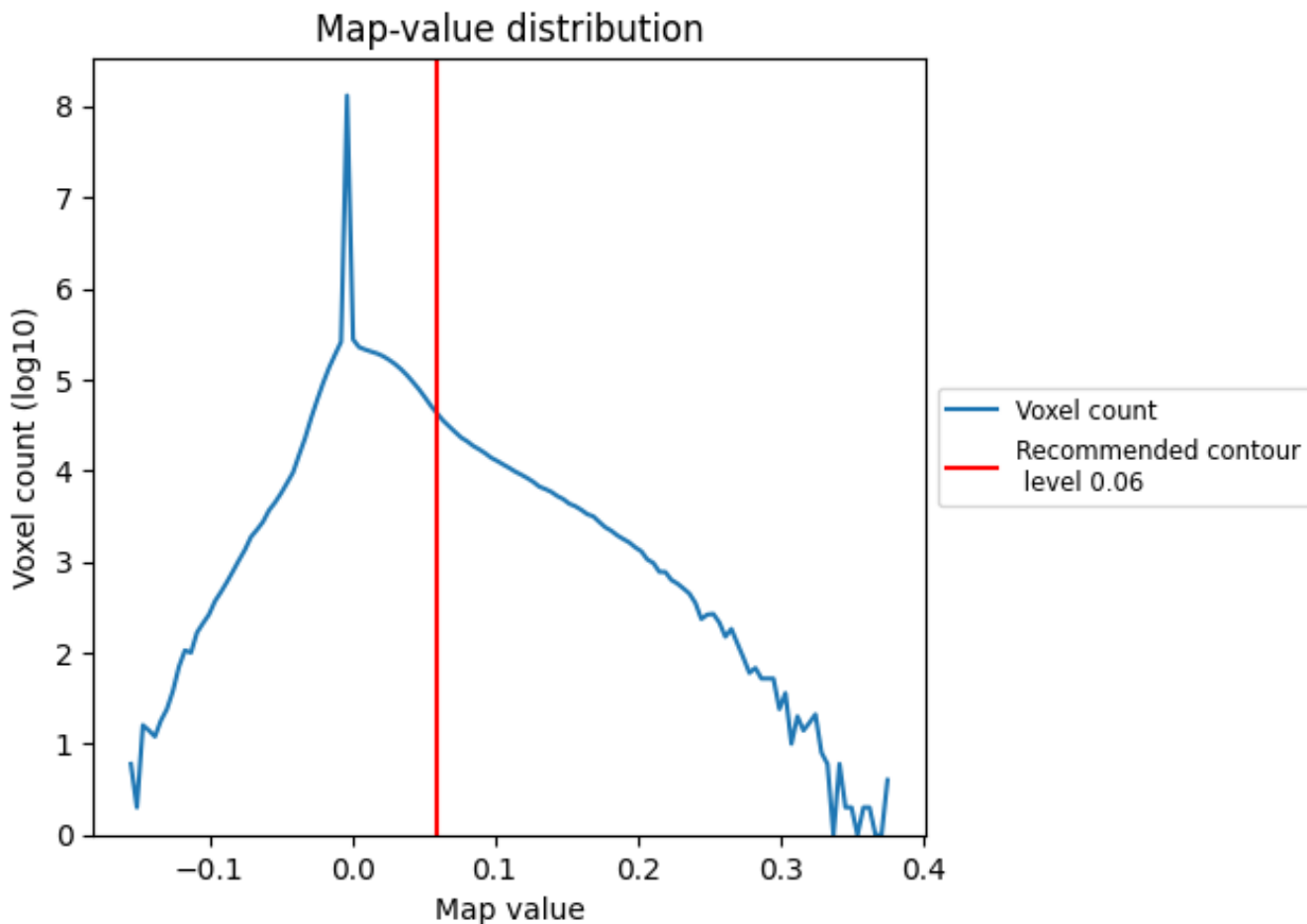
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

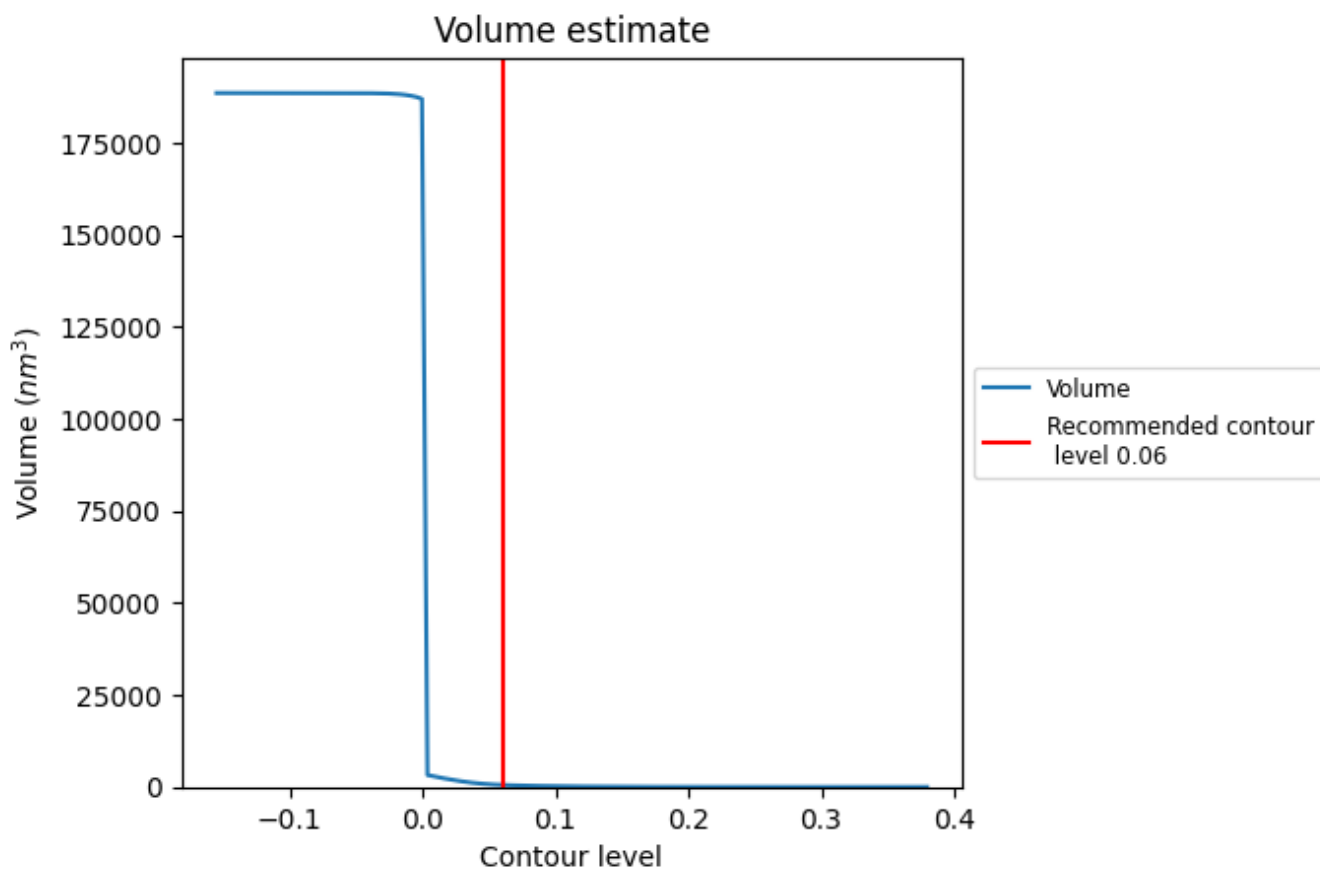
This section contains the results of statistical analysis of the map.

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



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

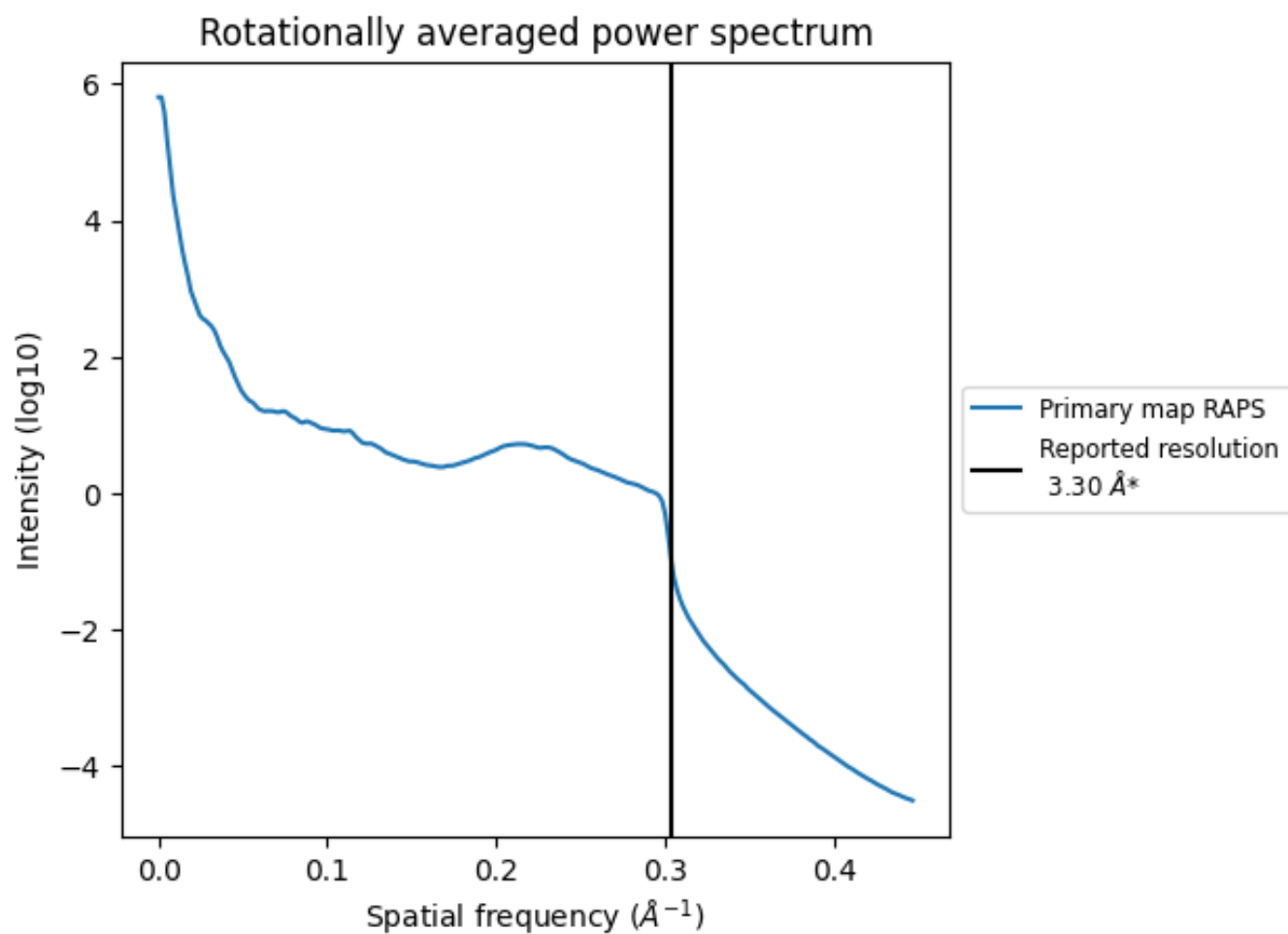
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 536 nm<sup>3</sup>; this corresponds to an approximate mass of 484 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

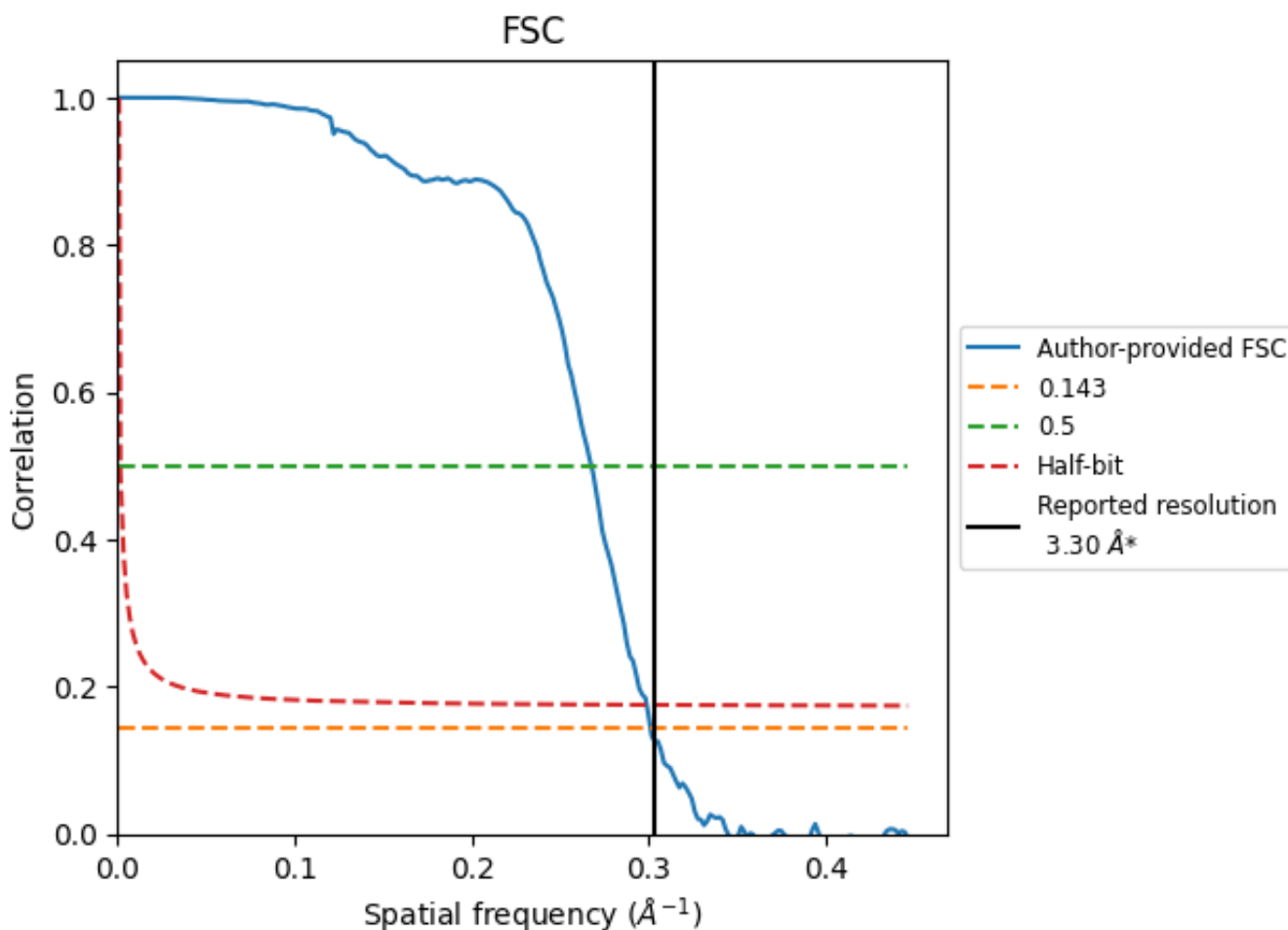


\*Reported resolution corresponds to spatial frequency of  $0.303 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.74	3.35
Unmasked-calculated*	-	-	-

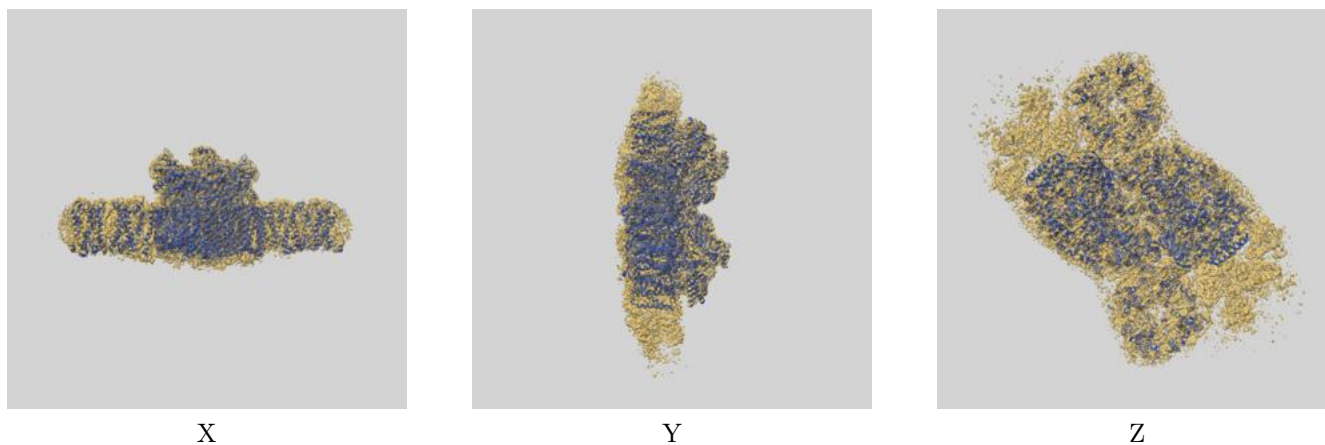
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



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

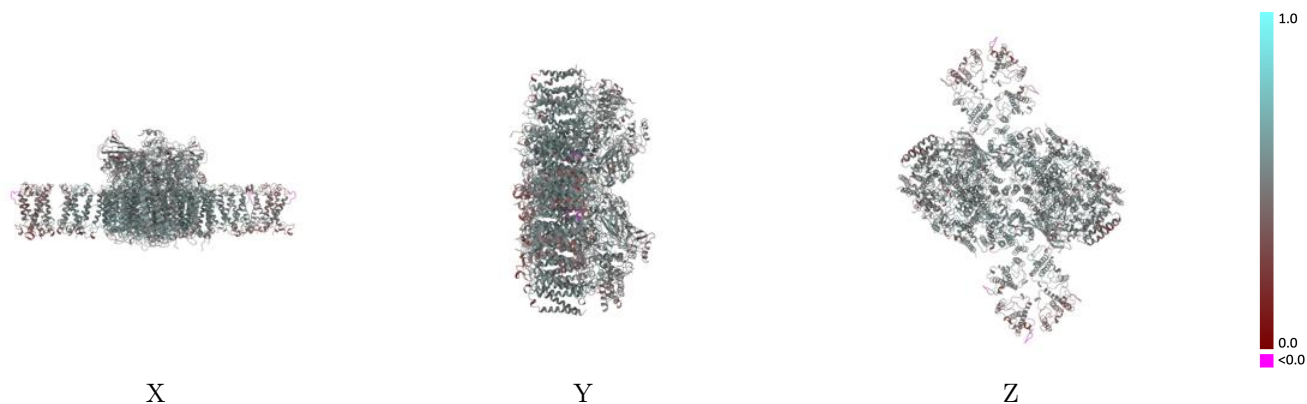
This section contains information regarding the fit between EMDB map EMD-9775 and PDB model 6J3Y. Per-residue inclusion information can be found in section 3 on page 35.

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



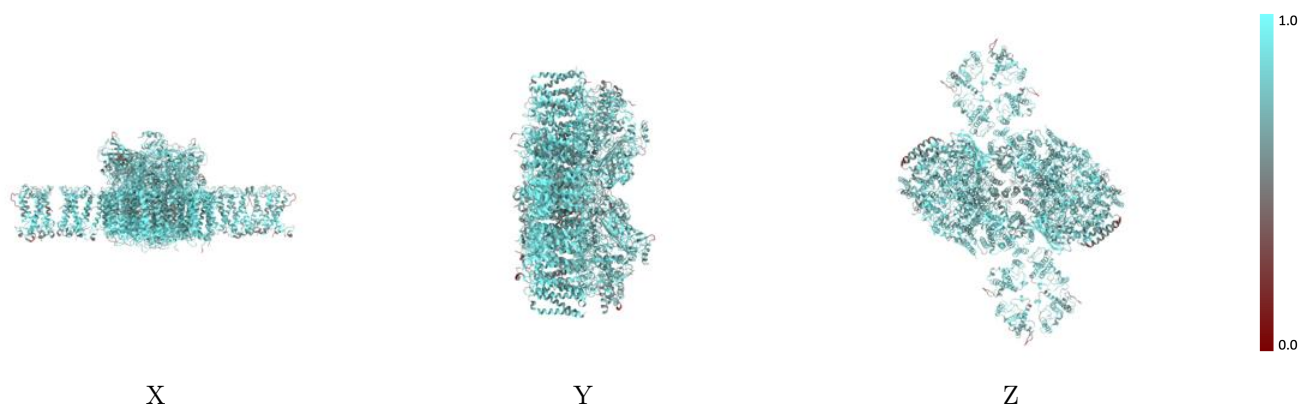
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



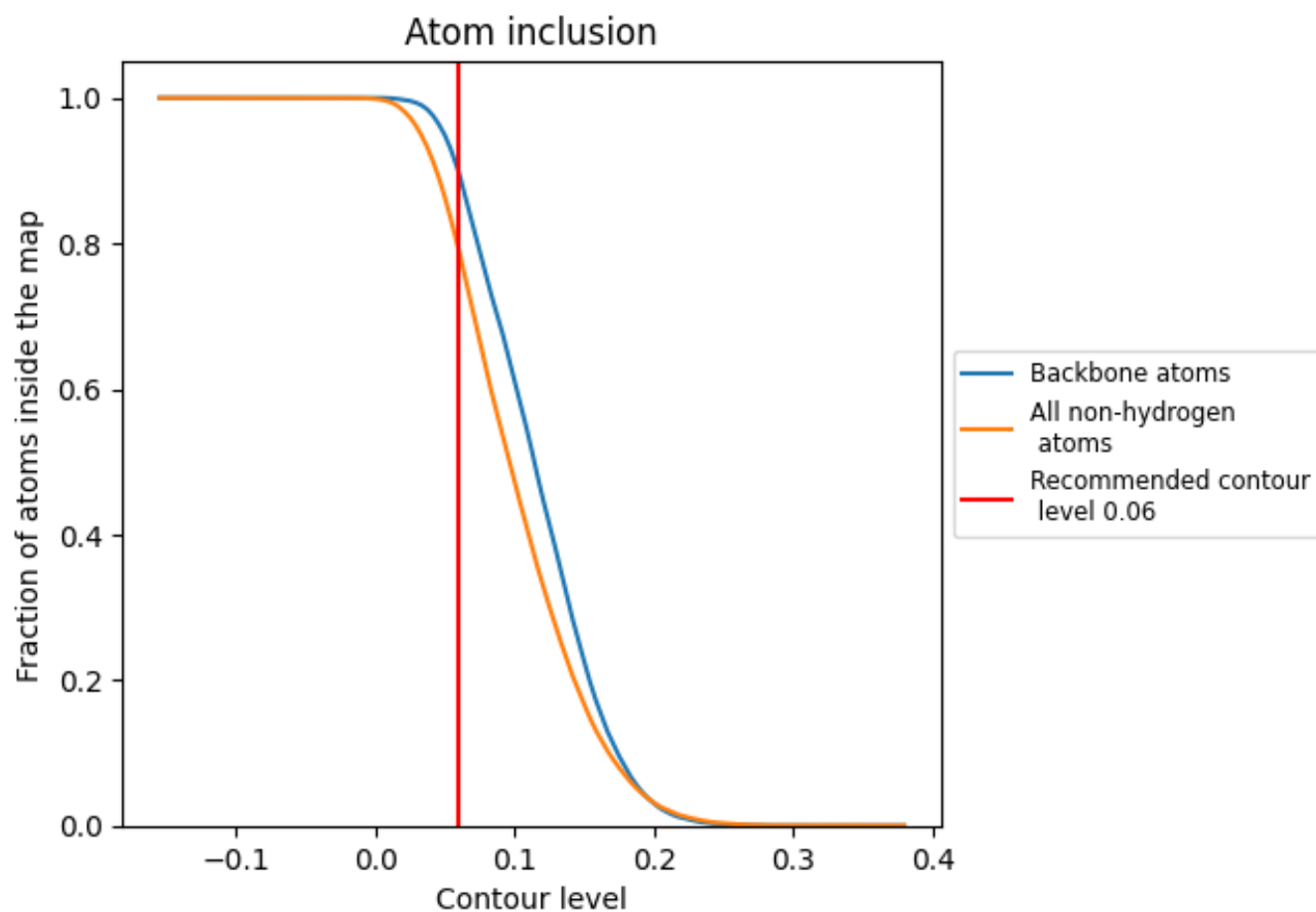
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary













































The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7896	 0.5030
0	 0.8774	 0.5350
1	 0.9000	 0.5450
11	 0.7796	 0.4900
12	 0.7730	 0.4650
13	 0.6786	 0.3890
14	 0.6827	 0.4020
2	 0.8800	 0.4930
31	 0.7781	 0.4910
32	 0.7716	 0.4620
33	 0.6818	 0.3870
34	 0.6818	 0.4030
5	 0.8710	 0.5470
6	 0.9000	 0.5440
7	 0.9000	 0.4950
A	 0.8560	 0.5520
B	 0.8406	 0.5500
C	 0.8418	 0.5410
D	 0.8281	 0.5470
E	 0.8172	 0.4860
F	 0.8137	 0.5040
H	 0.8132	 0.5260
I	 0.8262	 0.5270
J	 0.7588	 0.5270
K	 0.8311	 0.5130
L	 0.7309	 0.5450
M	 0.6850	 0.5230
O	 0.7475	 0.4760
Q	 0.6645	 0.4470
T	 0.7388	 0.5130
U	 0.7859	 0.4820
V	 0.8161	 0.4900
W	 0.6860	 0.4810
X	 0.7297	 0.4660
Y	 0.7149	 0.4790



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Chain	Atom inclusion	Q-score
Z	 0.7518	 0.4780
a	 0.8553	 0.5510
b	 0.8408	 0.5490
c	 0.8445	 0.5420
d	 0.8278	 0.5470
e	 0.8203	 0.4850
f	 0.8013	 0.5060
h	 0.8149	 0.5260
i	 0.8440	 0.5300
j	 0.7653	 0.5250
k	 0.8547	 0.5110
l	 0.7265	 0.5450
m	 0.6850	 0.5220
o	 0.7437	 0.4780
q	 0.6573	 0.4530
t	 0.7469	 0.5180
u	 0.7845	 0.4810
v	 0.8171	 0.4940
w	 0.7065	 0.4830
x	 0.7297	 0.4700
y	 0.7149	 0.4880
z	 0.7592	 0.4810