



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 04:38 PM JST

PDB ID : 6J3Z / pdb_00006j3z
EMDB ID : EMD-9776
Title : Structure of C2S1M1-type PSII-FCPII supercomplex from diatom
Authors : Nagao, R.; Kato, K.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on : 2019-01-07
Resolution : 3.60 Å (reported)
Based on initial models : 3JCU, 3WU2

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

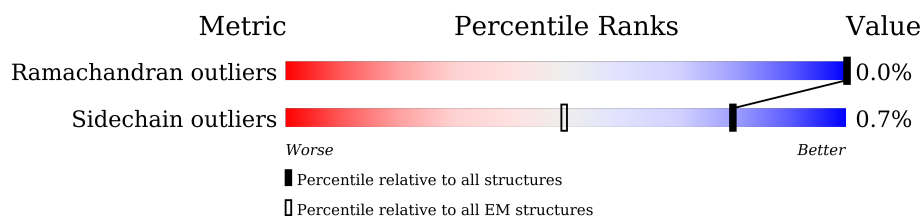
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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





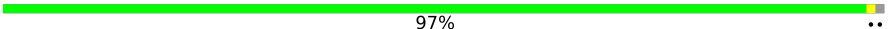
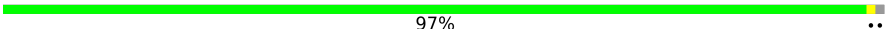






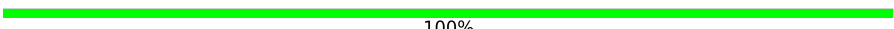
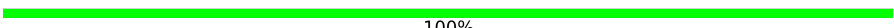


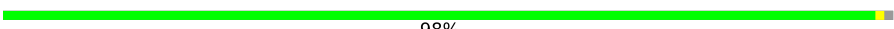
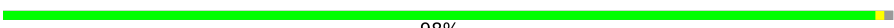


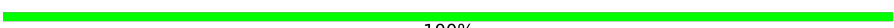
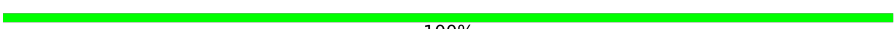
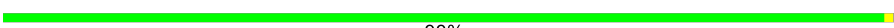

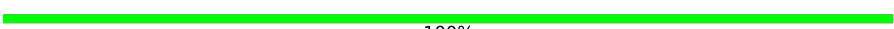


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

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

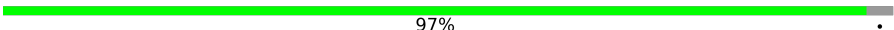
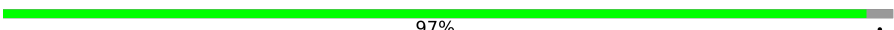
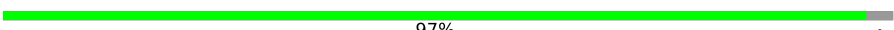









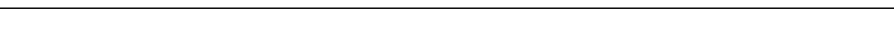
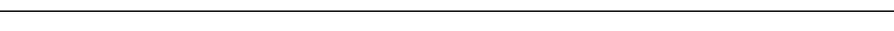
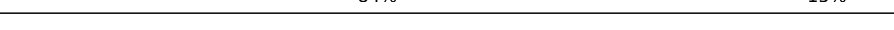







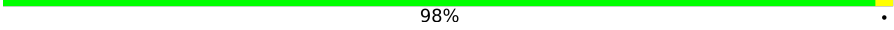
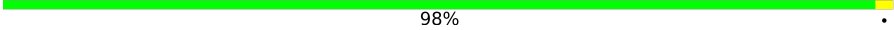
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Mol	Chain	Length	Quality of chain
6	F	43	 65%35%
6	f	43	 65%35%
7	H	67	 97%..
7	h	67	 97%..
8	I	38	 92%8%
8	i	38	 92%8%
9	J	39	 87%13%
9	j	39	 87%13%
10	K	44	 80%5%16%
10	k	44	 80%5%16%
11	L	38	 100%
11	l	38	 100%
12	M	131	 32%68%
12	m	131	 32%68%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

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Mol	Chain	Length	Quality of chain
18	x	38	 97% .
19	Z	61	 97% .
19	z	61	 97% .
20	Q	155	 88% 12%
20	q	155	 88% 12%
21	W	72	 71% . 28%
21	w	72	 71% . 28%
22	0	31	 100%
22	5	31	 100%
23	1	30	 100%
23	6	30	 100%
24	2	10	 100%
24	7	10	 100%
25	11	207	 84% . 15%
25	12	207	 84% . 15%
25	13	207	 84% . 15%
25	14	207	 84% . 15%
25	15	207	 85% 15%
25	16	207	 84% . 15%
25	17	207	 84% . 15%
25	18	207	 84% . 15%
26	19	215	 98% .
27	20	143	 98% .
28	21	155	 100%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	11	301	X	-	-	-
30	CLA	11	302	X	-	-	-
30	CLA	11	303	X	-	-	-
30	CLA	11	304	X	-	-	-
30	CLA	11	305	X	-	-	-
30	CLA	11	306	X	-	-	-
30	CLA	11	307	X	-	-	-
30	CLA	11	309	X	-	-	-
30	CLA	11	315	X	-	-	-
30	CLA	12	303	X	-	-	-
30	CLA	12	305	X	-	-	-
30	CLA	12	306	X	-	-	-
30	CLA	12	307	X	-	-	-
30	CLA	12	308	X	-	-	-
30	CLA	12	309	X	-	-	-
30	CLA	12	310	X	-	-	-
30	CLA	12	311	X	-	-	-
30	CLA	12	312	X	-	-	-
30	CLA	12	314	X	-	-	-
30	CLA	13	302	X	-	-	-
30	CLA	13	303	X	-	-	-
30	CLA	13	304	X	-	-	-
30	CLA	13	305	X	-	-	-
30	CLA	13	306	X	-	-	-
30	CLA	13	307	X	-	-	-
30	CLA	13	308	X	-	-	-
30	CLA	13	310	X	-	-	-
30	CLA	14	302	X	-	-	-
30	CLA	14	303	X	-	-	-
30	CLA	14	304	X	-	-	-
30	CLA	14	305	X	-	-	-
30	CLA	14	306	X	-	-	-
30	CLA	14	307	X	-	-	-
30	CLA	14	308	X	-	-	-
30	CLA	14	309	X	-	-	-
30	CLA	14	311	X	-	-	-
30	CLA	15	301	X	-	-	-
30	CLA	15	302	X	-	-	-
30	CLA	15	303	X	-	-	-
30	CLA	15	305	X	-	-	-
30	CLA	15	306	X	-	-	-
30	CLA	15	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	15	308	X	-	-	-
30	CLA	15	309	X	-	-	-
30	CLA	16	301	X	-	-	-
30	CLA	16	302	X	-	-	-
30	CLA	16	303	X	-	-	-
30	CLA	16	304	X	-	-	-
30	CLA	16	306	X	-	-	-
30	CLA	16	307	X	-	-	-
30	CLA	16	309	X	-	-	-
30	CLA	17	301	X	-	-	-
30	CLA	17	303	X	-	-	-
30	CLA	17	305	X	-	-	-
30	CLA	17	307	X	-	-	-
30	CLA	17	308	X	-	-	-
30	CLA	17	309	X	-	-	-
30	CLA	17	310	X	-	-	-
30	CLA	18	301	X	-	-	-
30	CLA	18	303	X	-	-	-
30	CLA	18	304	X	-	-	-
30	CLA	18	305	X	-	-	-
30	CLA	18	307	X	-	-	-
30	CLA	18	308	X	-	-	-
30	CLA	18	309	X	-	-	-
30	CLA	18	310	X	-	-	-
30	CLA	18	311	X	-	-	-
30	CLA	18	312	X	-	-	-
30	CLA	19	302	X	-	-	-
30	CLA	19	303	X	-	-	-
30	CLA	19	304	X	-	-	-
30	CLA	19	305	X	-	-	-
30	CLA	19	306	X	-	-	-
30	CLA	19	307	X	-	-	-
30	CLA	19	308	X	-	-	-
30	CLA	19	309	X	-	-	-
30	CLA	20	203	X	-	-	-
30	CLA	20	204	X	-	-	-
30	CLA	20	206	X	-	-	-
30	CLA	20	207	X	-	-	-
30	CLA	20	209	X	-	-	-
30	CLA	21	303	X	-	-	-
30	CLA	21	304	X	-	-	-
30	CLA	21	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	21	306	X	-	-	-
30	CLA	21	307	X	-	-	-
30	CLA	21	308	X	-	-	-
30	CLA	21	309	X	-	-	-
30	CLA	A	402	X	-	-	-
30	CLA	A	404	X	-	-	-
30	CLA	B	601	X	-	-	-
30	CLA	B	602	X	-	-	-
30	CLA	B	603	X	-	-	-
30	CLA	B	604	X	-	-	-
30	CLA	B	605	X	-	-	-
30	CLA	B	606	X	-	-	-
30	CLA	B	607	X	-	-	-
30	CLA	B	608	X	-	-	-
30	CLA	B	609	X	-	-	-
30	CLA	B	610	X	-	-	-
30	CLA	B	611	X	-	-	-
30	CLA	B	612	X	-	-	-
30	CLA	B	613	X	-	-	-
30	CLA	B	614	X	-	-	-
30	CLA	B	615	X	-	-	-
30	CLA	B	623	X	-	-	-
30	CLA	C	502	X	-	-	-
30	CLA	C	503	X	-	-	-
30	CLA	C	504	X	-	-	-
30	CLA	C	505	X	-	-	-
30	CLA	C	506	X	-	-	-
30	CLA	C	507	X	-	-	-
30	CLA	C	508	X	-	-	-
30	CLA	C	509	X	-	-	-
30	CLA	C	510	X	-	-	-
30	CLA	C	511	X	-	-	-
30	CLA	C	512	X	-	-	-
30	CLA	C	513	X	-	-	-
30	CLA	C	514	X	-	-	-
30	CLA	C	520	X	-	-	-
30	CLA	D	401	X	-	-	-
30	CLA	D	402	X	-	-	-
30	CLA	D	405	X	-	-	-
30	CLA	D	406	X	-	-	-
30	CLA	M	101	X	-	-	-
30	CLA	W	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	Z	102	X	-	-	-
30	CLA	a	402	X	-	-	-
30	CLA	a	403	X	-	-	-
30	CLA	b	601	X	-	-	-
30	CLA	b	602	X	-	-	-
30	CLA	b	603	X	-	-	-
30	CLA	b	604	X	-	-	-
30	CLA	b	605	X	-	-	-
30	CLA	b	606	X	-	-	-
30	CLA	b	607	X	-	-	-
30	CLA	b	608	X	-	-	-
30	CLA	b	609	X	-	-	-
30	CLA	b	610	X	-	-	-
30	CLA	b	611	X	-	-	-
30	CLA	b	612	X	-	-	-
30	CLA	b	613	X	-	-	-
30	CLA	b	614	X	-	-	-
30	CLA	b	615	X	-	-	-
30	CLA	b	622	X	-	-	-
30	CLA	c	502	X	-	-	-
30	CLA	c	503	X	-	-	-
30	CLA	c	504	X	-	-	-
30	CLA	c	505	X	-	-	-
30	CLA	c	506	X	-	-	-
30	CLA	c	507	X	-	-	-
30	CLA	c	508	X	-	-	-
30	CLA	c	509	X	-	-	-
30	CLA	c	510	X	-	-	-
30	CLA	c	511	X	-	-	-
30	CLA	c	512	X	-	-	-
30	CLA	c	513	X	-	-	-
30	CLA	c	514	X	-	-	-
30	CLA	d	401	X	-	-	-
30	CLA	d	402	X	-	-	-
30	CLA	d	406	X	-	-	-
30	CLA	d	407	X	-	-	-
30	CLA	m	101	X	-	-	-
30	CLA	w	102	X	-	-	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 74619 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II reaction center protein D1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 22 is a protein called Unknown protein 0.

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

- Molecule 23 is a protein called Unknown protein 1.

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

- Molecule 24 is a protein called Unknown protein 2.

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

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
25	16	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	17	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
25	18	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

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

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

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

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

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

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

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

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

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



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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	17	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	19	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	19	1	Total 65	C 55	Mg 1	N 4	O 5	0

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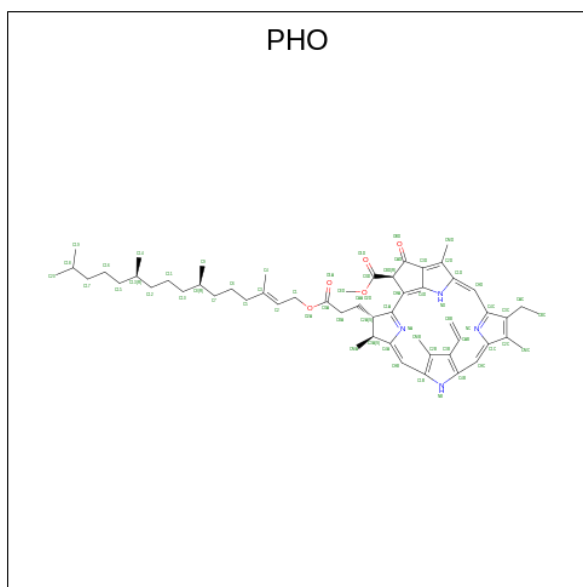
Mol	Chain	Residues	Atoms					AltConf
30	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	19	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	20	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	20	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	20	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	20	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	21	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	21	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	21	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	21	1	Total 65	C 55	Mg 1	N 4	O 5	0

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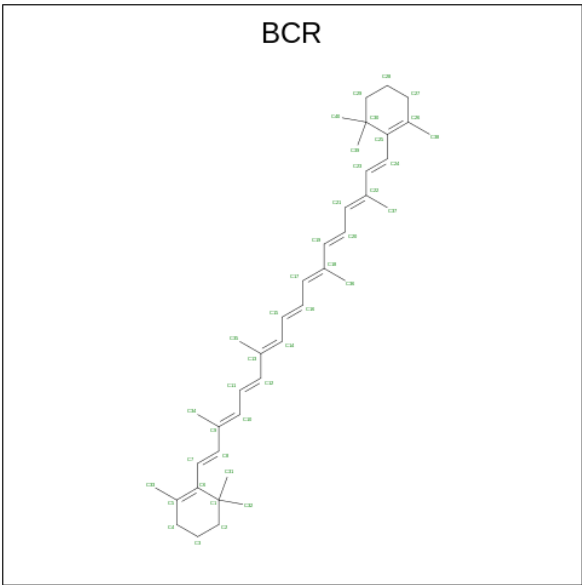
Mol	Chain	Residues	Atoms					AltConf
30	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	21	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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



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

- Molecule 32 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



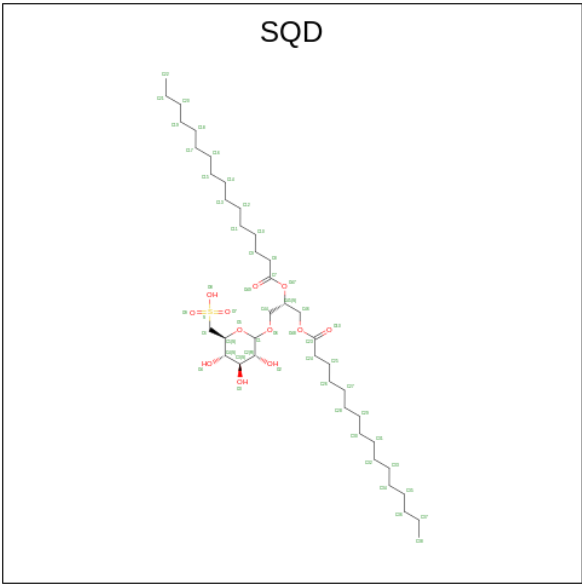
Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	C	0
			40	40	
32	A	1	Total	C	0
			40	40	
32	B	1	Total	C	0
			40	40	
32	B	1	Total	C	0
			40	40	
32	B	1	Total	C	0
			40	40	
32	B	1	Total	C	0
			40	40	
32	C	1	Total	C	0
			40	40	
32	C	1	Total	C	0
			40	40	
32	F	1	Total	C	0
			40	40	
32	H	1	Total	C	0
			40	40	
32	Y	1	Total	C	0
			40	40	
32	Z	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	
32	a	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	h	1	Total C 40 40	0
32	m	1	Total C 40 40	0

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



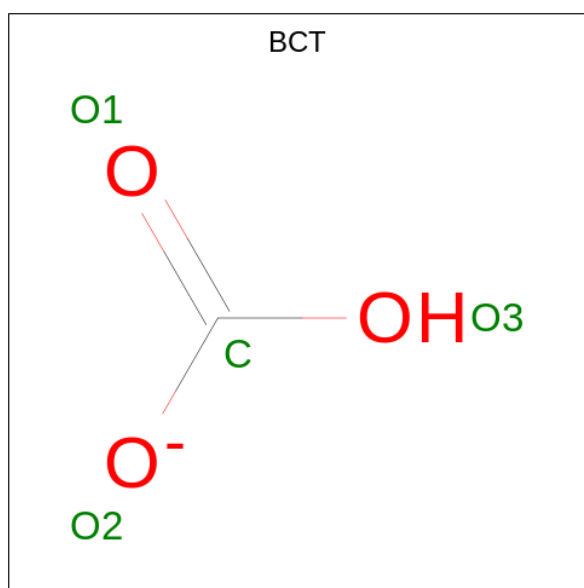
Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C O S 54 41 12 1	0

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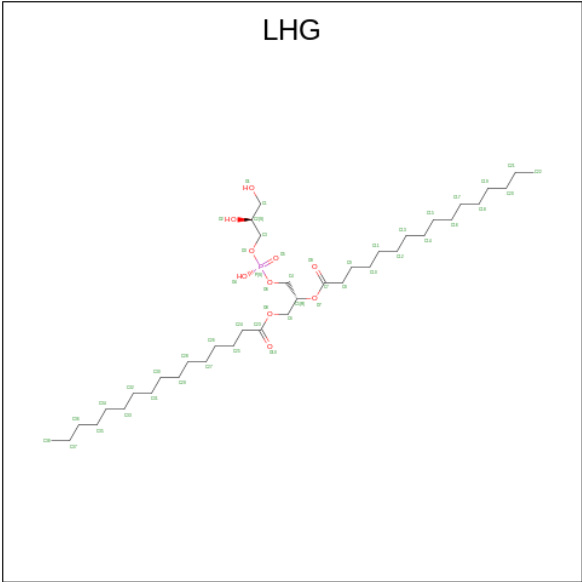
Mol	Chain	Residues	Atoms				AltConf
33	B	1	Total	C	O	S	0
			37	24	12	1	
33	L	1	Total	C	O	S	0
			54	41	12	1	
33	a	1	Total	C	O	S	0
			54	41	12	1	
33	b	1	Total	C	O	S	0
			37	24	12	1	
33	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



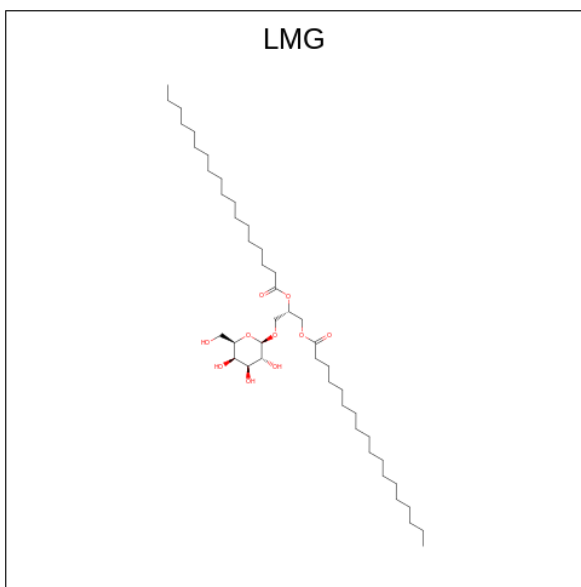
Mol	Chain	Residues	Atoms			AltConf
34	A	1	Total	C	O	0
			4	1	3	
34	a	1	Total	C	O	0
			4	1	3	

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



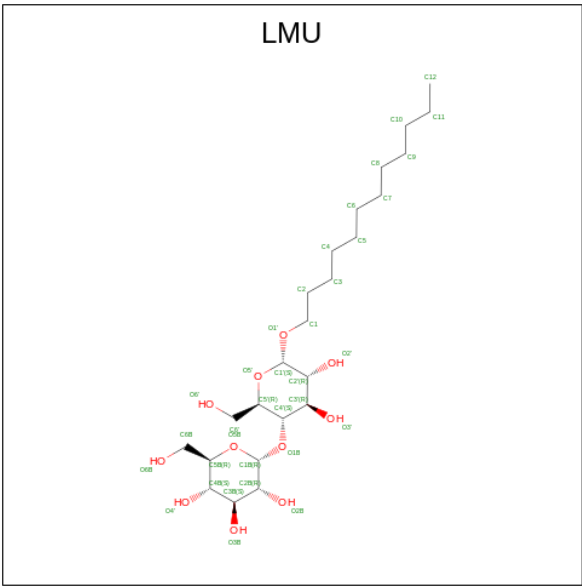
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	P	0
			46	35	10	1	
35	B	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	a	1	Total	C	O	P	0
			46	35	10	1	
35	b	1	Total	C	O	P	0
			49	38	10	1	
35	d	1	Total	C	O	P	0
			49	38	10	1	
35	l	1	Total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

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



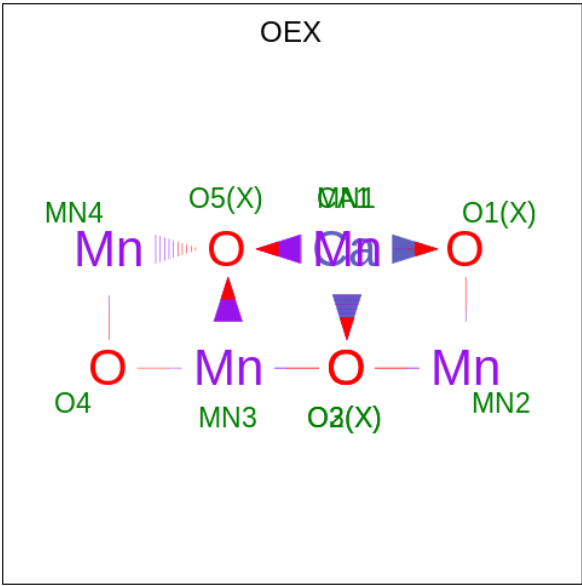
Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			51	41	10	
36	B	1	Total	C	O	0
			51	41	10	
36	D	1	Total	C	O	0
			51	41	10	
36	M	1	Total	C	O	0
			40	30	10	
36	Q	1	Total	C	O	0
			51	41	10	
36	W	1	Total	C	O	0
			51	41	10	
36	1	1	Total	C	O	0
			39	29	10	
36	b	1	Total	C	O	0
			51	41	10	
36	b	1	Total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

- Molecule 37 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			32	21	11	
37	12	1	Total	C	O	0
			32	21	11	

- Molecule 38 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn₄O₅).



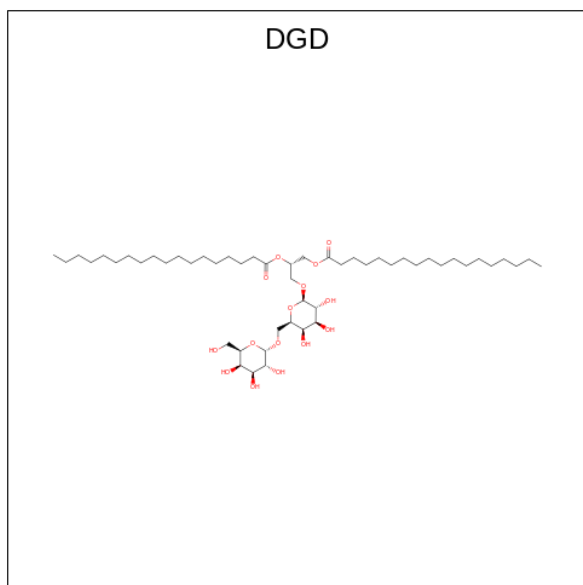
Mol	Chain	Residues	Atoms				AltConf
38	C	1	Total	Ca	Mn	O	0
			10	1	4	5	

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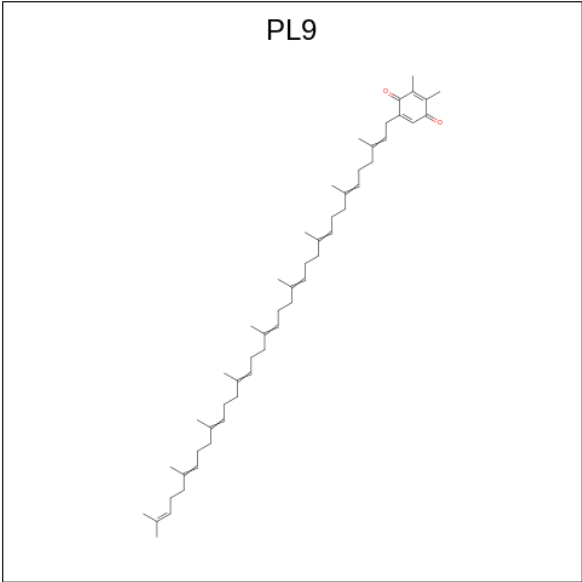
Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
38	c	1	10	1	4	5	0

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



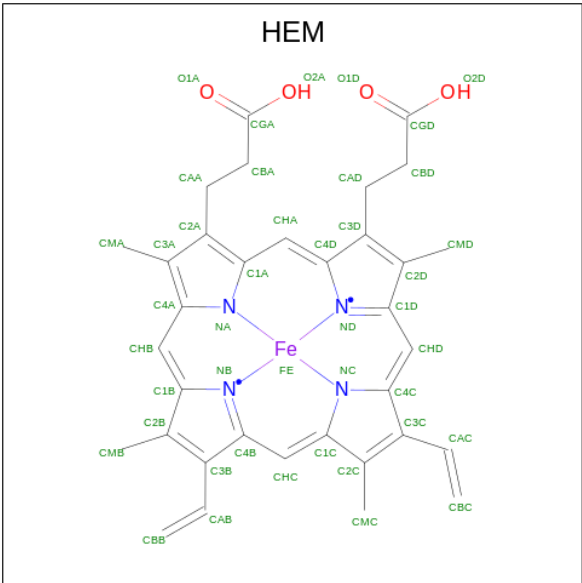
Mol	Chain	Residues	Atoms			AltConf
39	C	1	Total	C	O	0
			62	47	15	
39	C	1	Total	C	O	0
			62	47	15	
39	H	1	Total	C	O	0
			62	47	15	
39	J	1	Total	C	O	0
			62	47	15	
39	c	1	Total	C	O	0
			62	47	15	
39	c	1	Total	C	O	0
			62	47	15	
39	h	1	Total	C	O	0
			62	47	15	
39	j	1	Total	C	O	0
			62	47	15	

- Molecule 40 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



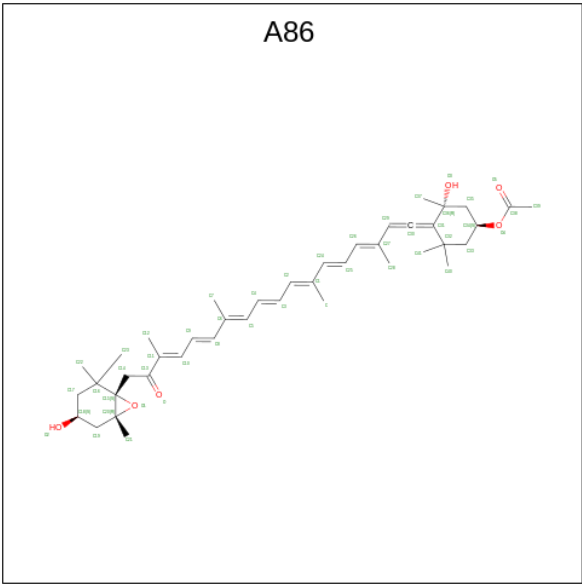
Mol	Chain	Residues	Atoms			AltConf
40	D	1	Total	C	O	0
			55	53	2	
40	D	1	Total	C	O	0
			55	53	2	
40	d	1	Total	C	O	0
			55	53	2	
40	d	1	Total	C	O	0
			55	53	2	

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 42 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆).



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

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

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

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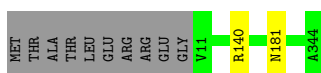
Mol	Chain	Residues	Atoms			AltConf
42	20	1	Total	C	O	0
			48	42	6	
42	20	1	Total	C	O	0
			48	42	6	
42	20	1	Total	C	O	0
			48	42	6	
42	20	1	Total	C	O	0
			48	42	6	
42	20	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	
42	21	1	Total	C	O	0
			48	42	6	
42	21	1	Total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

3 Residue-property plots [i](#)

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

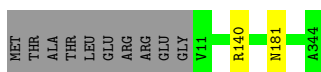
- Molecule 1: Photosystem II reaction center protein D1

Chain A:  97%



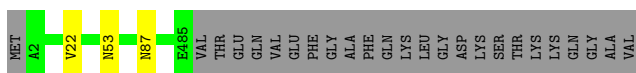
- Molecule 1: Photosystem II reaction center protein D1

Chain a:  97%



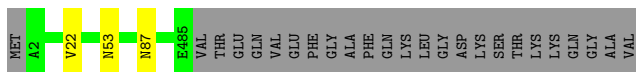
- Molecule 2: Photosystem II chlorophyll protein CP47

Chain B:  94% 5%



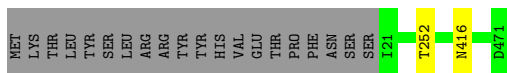
- Molecule 2: Photosystem II chlorophyll protein CP47

Chain b:  94% 5%



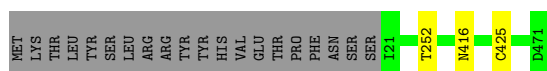
- Molecule 3: Photosystem II chlorophyll protein CP43

Chain C:  95%



- Molecule 3: Photosystem II chlorophyll protein CP43

Chain c:  95%



- Molecule 4: Photosystem II reaction center protein D2

Chain D: 95%



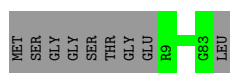
- Molecule 4: Photosystem II reaction center protein D2

Chain d: 96%



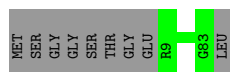
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 89%



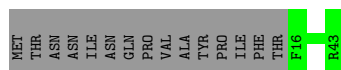
- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 89%



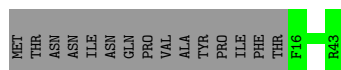
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 65%



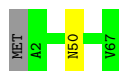
- Molecule 6: Cytochrome b559 subunit beta

Chain f: 65%



- Molecule 7: Photosystem II reaction center protein H

Chain H: 97%



- Molecule 7: Photosystem II reaction center protein H

Chain h: 97% ..



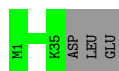
- Molecule 8: Photosystem II reaction center protein I

Chain I: 92% 8%



- Molecule 8: Photosystem II reaction center protein I

Chain i: 92% 8%



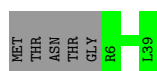
- Molecule 9: Photosystem II reaction center protein J

Chain J: 87% 13%



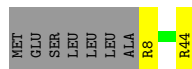
- Molecule 9: Photosystem II reaction center protein J

Chain j: 87% 13%



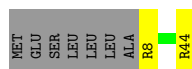
- Molecule 10: Photosystem II reaction center protein K

Chain K: 80% 5% 16%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 80% 5% 16%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 100%

There are no outlier residues recorded for this chain.

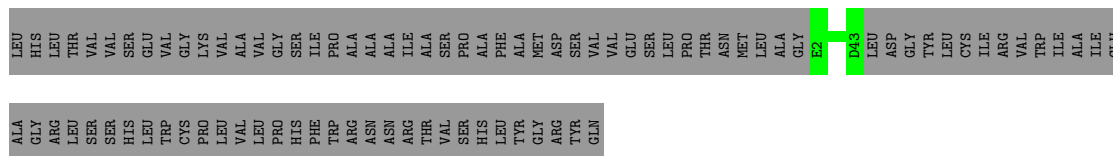
- Molecule 11: Photosystem II reaction center protein L

Chain l: 100%

There are no outlier residues recorded for this chain.

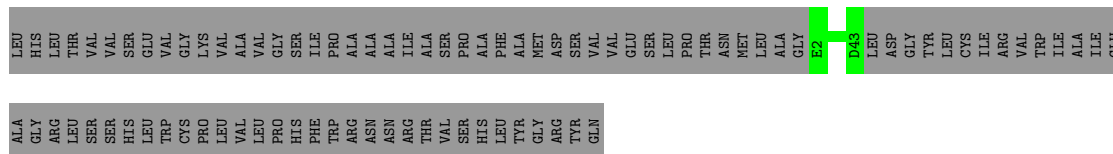
- Molecule 12: Photosystem II reaction center protein M

Chain M: 32% 68%



- Molecule 12: Photosystem II reaction center protein M

Chain m: 32% 68%



- Molecule 13: Extrinsic protein in photosystem II

Chain O: 98% ..



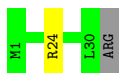
- Molecule 13: Extrinsic protein in photosystem II

Chain o: 98% ..



- Molecule 14: Photosystem II reaction center protein T

Chain T:  94% . .



- Molecule 14: Photosystem II reaction center protein T

Chain t:  94% . .



- Molecule 15: Extrinsic protein in photosystem II

Chain U:  100%

There are no outlier residues recorded for this chain.

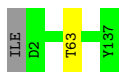
- Molecule 15: Extrinsic protein in photosystem II

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 16: Cytochrome c-550

Chain V:  99% ..



- Molecule 16: Cytochrome c-550

Chain v:  99% ..



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: Photosystem II reaction center X protein

Chain X:  97% .



- Molecule 18: Photosystem II reaction center X protein

Chain x:  97% .



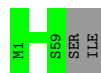
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  97% .




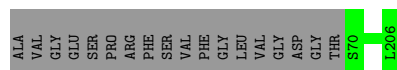
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  97% .




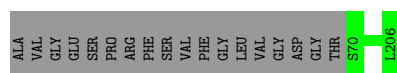
- Molecule 20: Extrinsic protein in photosystem II

Chain Q:  88% 12%



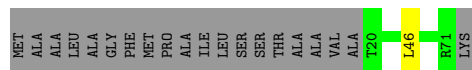
- Molecule 20: Extrinsic protein in photosystem II

Chain q:  88% 12%



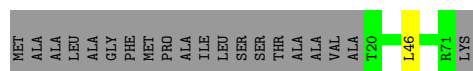
- Molecule 21: Photosystem II reaction center protein W

Chain W:  71% . 28%



- Molecule 21: Photosystem II reaction center protein W

Chain w:  71% 28%



- Molecule 22: Unknown protein 0

Chain 0:  100%

There are no outlier residues recorded for this chain.

- Molecule 22: Unknown protein 0

Chain 5:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: Unknown protein 1

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: Unknown protein 1

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: Unknown protein 2

Chain 2:  100%


There are no outlier residues recorded for this chain.

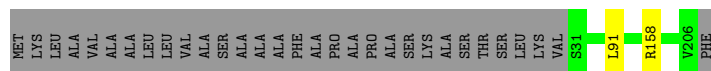
- Molecule 24: Unknown protein 2

Chain 7:  100%

There are no outlier residues recorded for this chain.

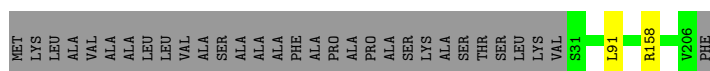
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 11:  84% 15%



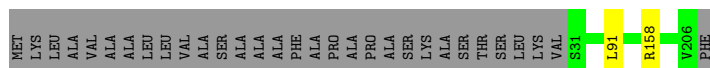
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 12:  84% 15%



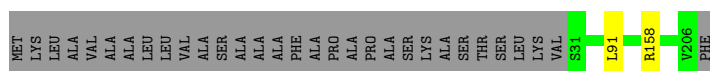
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 13: 84% 15%



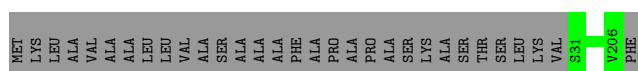
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 14: 84% 15%



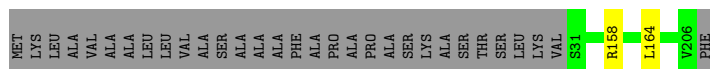
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 15: 85% 15%



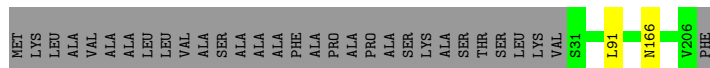
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 16: 84% 15%



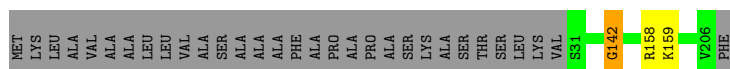
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 17: 84% 15%



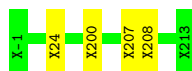
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 18: 84% 15%



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

Chain 19: 98% 2%



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

Chain 20:  98%



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

Chain 21:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	147981	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1/2789 (0.0%)	0.60	0/3803
4	d	0.58	0/2789	0.60	0/3803
5	E	0.44	0/634	0.52	0/864
5	e	0.44	0/634	0.53	0/864
6	F	0.45	0/235	0.70	0/316
6	f	0.46	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	0.57	0/313	0.68	0/429
10	k	0.56	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	0.53	0/346
14	t	0.45	0/256	0.52	0/346
15	U	0.40	0/728	0.58	0/989
15	u	0.41	0/728	0.58	0/989
16	V	0.42	0/1056	0.56	0/1435
16	v	0.42	0/1056	0.56	0/1435

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.32	0/252	0.52	0/341
17	y	0.32	0/252	0.52	0/341
18	X	0.31	0/263	0.54	0/355
18	x	0.31	0/263	0.54	0/355
19	Z	0.41	0/456	0.58	0/624
19	z	0.41	0/456	0.58	0/624
20	Q	0.39	0/1099	0.56	0/1482
20	q	0.39	0/1099	0.56	0/1482
21	W	0.53	0/434	0.67	1/590 (0.2%)
21	w	0.53	0/434	0.67	1/590 (0.2%)
25	11	0.43	0/1373	0.55	1/1861 (0.1%)
25	12	0.43	0/1373	0.55	1/1861 (0.1%)
25	13	0.43	0/1373	0.55	1/1861 (0.1%)
25	14	0.43	0/1373	0.55	1/1861 (0.1%)
25	15	0.33	0/1373	0.52	0/1861
25	16	0.42	0/1373	0.64	1/1861 (0.1%)
25	17	0.41	0/1373	0.58	1/1861 (0.1%)
25	18	0.35	0/1373	0.54	0/1861
All	All	0.51	4/55724 (0.0%)	0.58	10/75702 (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
25	18	0	1
26	19	0	4
27	20	0	3
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	22	VAL	CB-CG1	-7.21	1.37	1.52
2	B	22	VAL	CB-CG1	-7.19	1.37	1.52
3	c	425	CYS	CB-SG	-5.11	1.73	1.81
4	D	314	TYR	CD1-CE1	-5.01	1.31	1.39

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	252	THR	C-N-CA	6.19	137.17	121.70
3	c	252	THR	C-N-CA	6.15	137.08	121.70
21	w	46	LEU	CB-CG-CD1	-5.36	101.90	111.00
21	W	46	LEU	CB-CG-CD1	-5.33	101.94	111.00
25	16	164	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

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

5.2 Too-close contacts [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%)	322 (97%)	10 (3%)	0	100	100
2	B	482/509 (95%)	466 (97%)	16 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
4	d	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
5	E	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
5	e	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
6	F	26/43 (60%)	26 (100%)	0	0	100	100
6	f	26/43 (60%)	26 (100%)	0	0	100	100
7	H	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
7	h	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	32/39 (82%)	32 (100%)	0	0	100	100
9	j	32/39 (82%)	32 (100%)	0	0	100	100
10	K	35/44 (80%)	35 (100%)	0	0	100	100
10	k	35/44 (80%)	35 (100%)	0	0	100	100
11	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	M	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
12	m	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
13	O	243/248 (98%)	231 (95%)	12 (5%)	0	100	100
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%)	86 (94%)	5 (6%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
20	Q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
20	q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
21	W	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
21	w	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
25	11	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	12	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	13	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	14	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	15	174/207 (84%)	163 (94%)	11 (6%)	0	100	100
25	16	174/207 (84%)	159 (91%)	15 (9%)	0	100	100
25	17	174/207 (84%)	162 (93%)	12 (7%)	0	100	100
25	18	174/207 (84%)	165 (95%)	8 (5%)	1 (1%)	22	55
All	All	6884/7712 (89%)	6586 (96%)	297 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	18	142	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/280 (97%)	271 (100%)	1 (0%)	89	95
1	a	272/280 (97%)	271 (100%)	1 (0%)	89	95
2	B	385/405 (95%)	383 (100%)	2 (0%)	86	93
2	b	385/405 (95%)	383 (100%)	2 (0%)	86	93
3	C	356/376 (95%)	355 (100%)	1 (0%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	356/376 (95%)	355 (100%)	1 (0%)	91	96
4	D	273/281 (97%)	268 (98%)	5 (2%)	54	74
4	d	273/281 (97%)	268 (98%)	5 (2%)	54	74
5	E	69/75 (92%)	69 (100%)	0	100	100
5	e	69/75 (92%)	69 (100%)	0	100	100
6	F	22/36 (61%)	22 (100%)	0	100	100
6	f	22/36 (61%)	22 (100%)	0	100	100
7	H	55/56 (98%)	54 (98%)	1 (2%)	54	74
7	h	55/56 (98%)	54 (98%)	1 (2%)	54	74
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%)	15	44
10	k	32/38 (84%)	30 (94%)	2 (6%)	15	44
11	L	34/34 (100%)	34 (100%)	0	100	100
11	l	34/34 (100%)	34 (100%)	0	100	100
12	M	31/104 (30%)	31 (100%)	0	100	100
12	m	31/104 (30%)	31 (100%)	0	100	100
13	O	196/201 (98%)	194 (99%)	2 (1%)	73	85
13	o	196/201 (98%)	194 (99%)	2 (1%)	73	85
14	T	27/28 (96%)	26 (96%)	1 (4%)	29	58
14	t	27/28 (96%)	26 (96%)	1 (4%)	29	58
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	Z	48/50 (96%)	48 (100%)	0	100	100
19	z	48/50 (96%)	48 (100%)	0	100	100
20	Q	111/124 (90%)	111 (100%)	0	100	100
20	q	111/124 (90%)	111 (100%)	0	100	100
21	W	43/55 (78%)	43 (100%)	0	100	100
21	w	43/55 (78%)	43 (100%)	0	100	100
25	11	138/158 (87%)	137 (99%)	1 (1%)	81	90
25	12	138/158 (87%)	137 (99%)	1 (1%)	81	90
25	13	138/158 (87%)	137 (99%)	1 (1%)	81	90
25	14	138/158 (87%)	137 (99%)	1 (1%)	81	90
25	15	138/158 (87%)	138 (100%)	0	100	100
25	16	138/158 (87%)	137 (99%)	1 (1%)	81	90
25	17	138/158 (87%)	137 (99%)	1 (1%)	81	90
25	18	138/158 (87%)	136 (99%)	2 (1%)	62	79
All	All	5628/6184 (91%)	5590 (99%)	38 (1%)	80	90

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

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	229	ASN
25	17	96	ASN
16	v	68	ASN
25	17	82	ASN
25	14	177	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 323 ligands modelled in this entry, 2 are monoatomic - leaving 321 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	$\# Z > 2$
42	A86	17	311	-	44,50,50	4.03	22 (50%)	51,76,76	8.34	19 (37%)
30	CLA	16	307	25	45,53,73	1.76	10 (22%)	52,89,113	1.96	7 (13%)
36	LMG	B	620	-	51,51,55	0.98	5 (9%)	59,59,63	1.44	8 (13%)
30	CLA	14	302	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	8 (10%)
41	HEM	v	201	16	41,50,50	1.60	5 (12%)	45,82,82	1.27	2 (4%)
30	CLA	12	310	25	45,53,73	1.77	8 (17%)	52,89,113	1.82	8 (15%)
30	CLA	D	406	-	65,73,73	1.40	10 (15%)	76,113,113	1.60	7 (9%)
30	CLA	11	304	25	45,53,73	1.72	8 (17%)	52,89,113	2.02	11 (21%)
36	LMG	w	101	-	51,51,55	0.89	4 (7%)	59,59,63	1.40	7 (11%)
30	CLA	w	102	-	65,73,73	1.43	9 (13%)	76,113,113	1.47	10 (13%)
30	CLA	c	512	3	65,73,73	1.50	10 (15%)	76,113,113	1.61	13 (17%)
36	LMG	b	619	-	51,51,55	0.99	5 (9%)	59,59,63	1.44	8 (13%)
42	A86	15	312	-	44,50,50	4.04	23 (52%)	51,76,76	7.82	20 (39%)
30	CLA	20	204	-	65,73,73	1.41	10 (15%)	76,113,113	1.52	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	A86	14	315	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	b	601	-	65,73,73	1.44	11 (16%)	76,113,113	1.50	7 (9%)
32	BCR	A	409	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	5 (8%)
35	LHG	L	101	-	48,48,48	0.81	1 (2%)	51,54,54	1.27	5 (9%)
36	LMG	12	301	-	39,39,55	1.00	4 (10%)	47,47,63	1.21	5 (10%)
42	A86	12	318	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	13	304	-	65,73,73	1.41	10 (15%)	76,113,113	1.59	10 (13%)
32	BCR	m	103	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	8 (14%)
31	PHO	D	403	-	51,69,69	1.14	8 (15%)	47,99,99	1.28	6 (12%)
30	CLA	17	310	-	45,53,73	1.75	9 (20%)	52,89,113	1.67	8 (15%)
30	CLA	21	303	-	65,73,73	1.44	8 (12%)	76,113,113	1.41	7 (9%)
30	CLA	B	607	-	65,73,73	1.41	11 (16%)	76,113,113	1.56	7 (9%)
30	CLA	19	309	-	45,53,73	1.69	7 (15%)	52,89,113	1.79	9 (17%)
42	A86	12	319	-	44,50,50	3.93	23 (52%)	51,76,76	7.96	18 (35%)
42	A86	15	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
42	A86	11	312	-	44,50,50	4.04	23 (52%)	51,76,76	7.82	20 (39%)
39	DGD	C	517	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	16 (20%)
34	BCT	A	407	29,1	2,3,3	1.26	0	2,3,3	3.94	2 (100%)
35	LHG	l	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
30	CLA	20	209	30	65,73,73	1.47	9 (13%)	76,113,113	1.44	9 (11%)
42	A86	18	313	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	c	506	-	65,73,73	1.45	11 (16%)	76,113,113	1.56	11 (14%)
38	OEX	C	501	3,1	0,15,15	-	-	-	-	-
30	CLA	20	205	-	45,53,73	1.73	10 (22%)	52,89,113	1.80	9 (17%)
39	DGD	C	516	-	63,63,67	1.05	7 (11%)	77,77,81	1.60	15 (19%)
30	CLA	19	306	-	45,53,73	1.72	11 (24%)	52,89,113	1.62	7 (13%)
30	CLA	12	313	25	45,53,73	1.75	11 (24%)	52,89,113	1.76	9 (17%)
30	CLA	18	309	25	65,73,73	1.51	8 (12%)	76,113,113	1.60	10 (13%)
30	CLA	15	307	25	65,73,73	1.47	10 (15%)	76,113,113	1.63	11 (14%)
30	CLA	B	613	-	65,73,73	1.43	11 (16%)	76,113,113	1.61	10 (13%)
32	BCR	f	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
40	PL9	D	404	4	55,55,55	1.35	6 (10%)	68,69,69	1.49	15 (22%)
30	CLA	16	309	-	45,53,73	1.74	10 (22%)	52,89,113	1.61	9 (17%)
42	A86	17	315	-	44,50,50	4.06	23 (52%)	51,76,76	8.44	16 (31%)
30	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
32	BCR	A	405	-	41,41,41	1.28	2 (4%)	56,56,56	1.40	6 (10%)
30	CLA	11	305	-	45,53,73	1.71	8 (17%)	52,89,113	1.71	7 (13%)
40	PL9	d	405	4	55,55,55	1.36	6 (10%)	68,69,69	1.50	14 (20%)
30	CLA	c	510	-	65,73,73	1.49	12 (18%)	76,113,113	1.73	10 (13%)
32	BCR	C	515	-	41,41,41	1.30	4 (9%)	56,56,56	1.40	9 (16%)
30	CLA	B	614	-	65,73,73	1.38	10 (15%)	76,113,113	1.58	10 (13%)
39	DGD	H	102	-	63,63,67	0.93	3 (4%)	77,77,81	1.42	8 (10%)
42	A86	14	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.97	18 (35%)
36	LMG	D	408	-	51,51,55	0.90	3 (5%)	59,59,63	1.42	7 (11%)
30	CLA	18	306	25	45,53,73	1.74	7 (15%)	52,89,113	1.85	8 (15%)
30	CLA	c	508	-	65,73,73	1.43	12 (18%)	76,113,113	1.67	12 (15%)
39	DGD	c	517	-	63,63,67	1.06	8 (12%)	77,77,81	1.60	15 (19%)
42	A86	21	310	-	44,50,50	3.88	22 (50%)	51,76,76	7.42	21 (41%)
30	CLA	12	308	25	45,53,73	1.71	8 (17%)	52,89,113	2.04	11 (21%)
30	CLA	12	311	25	65,73,73	1.47	10 (15%)	76,113,113	1.54	10 (13%)
42	A86	16	310	-	44,50,50	3.97	23 (52%)	51,76,76	8.08	20 (39%)
42	A86	21	314	-	44,50,50	4.01	23 (52%)	51,76,76	7.82	18 (35%)
32	BCR	B	618	-	41,41,41	1.24	2 (4%)	56,56,56	1.41	10 (17%)
30	CLA	C	507	-	65,73,73	1.51	11 (16%)	76,113,113	1.55	10 (13%)
30	CLA	B	608	-	65,73,73	1.50	10 (15%)	76,113,113	1.47	8 (10%)
30	CLA	d	402	-	65,73,73	1.45	11 (16%)	76,113,113	1.50	8 (10%)
36	LMG	M	102	30	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
30	CLA	21	308	-	45,53,73	1.75	6 (13%)	52,89,113	1.65	7 (13%)
30	CLA	b	602	-	65,73,73	1.48	10 (15%)	76,113,113	1.54	12 (15%)
32	BCR	H	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.31	7 (12%)
42	A86	11	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	14	310	25	45,53,73	1.76	11 (24%)	52,89,113	1.75	9 (17%)
30	CLA	14	304	-	45,53,73	1.70	10 (22%)	52,89,113	1.80	9 (17%)
32	BCR	B	624	-	41,41,41	1.13	3 (7%)	56,56,56	1.30	7 (12%)
30	CLA	w	103	-	65,73,73	1.50	6 (9%)	76,113,113	1.41	7 (9%)
42	A86	18	314	-	44,50,50	3.98	23 (52%)	51,76,76	7.94	18 (35%)
30	CLA	B	611	-	65,73,73	1.51	12 (18%)	76,113,113	1.59	11 (14%)
30	CLA	B	623	-	65,73,73	1.46	10 (15%)	76,113,113	1.58	14 (18%)
30	CLA	C	503	-	65,73,73	1.52	12 (18%)	76,113,113	1.53	12 (15%)
32	BCR	c	520	-	41,41,41	1.27	3 (7%)	56,56,56	1.47	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	c	514	-	65,73,73	1.40	9 (13%)	76,113,113	1.62	8 (10%)
30	CLA	21	301	28	65,73,73	1.48	8 (12%)	76,113,113	1.43	7 (9%)
30	CLA	13	306	-	45,53,73	1.70	8 (17%)	52,89,113	1.70	7 (13%)
42	A86	20	211	-	44,50,50	3.89	23 (52%)	51,76,76	7.50	15 (29%)
32	BCR	b	623	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
30	CLA	B	609	-	65,73,73	1.47	10 (15%)	76,113,113	1.51	9 (11%)
30	CLA	C	509	-	65,73,73	1.48	11 (16%)	76,113,113	1.64	9 (11%)
30	CLA	C	502	-	65,73,73	1.39	11 (16%)	76,113,113	1.66	11 (14%)
35	LHG	B	622	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	6 (11%)
30	CLA	C	519	-	65,73,73	1.47	11 (16%)	76,113,113	1.47	7 (9%)
35	LHG	L	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
42	A86	11	311	-	44,50,50	3.96	23 (52%)	51,76,76	7.93	18 (35%)
33	SQD	B	621	-	36,37,54	1.20	6 (16%)	45,48,65	1.64	9 (20%)
32	BCR	b	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.41	10 (17%)
42	A86	16	313	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	16	303	-	45,53,73	1.69	9 (20%)	52,89,113	2.01	11 (21%)
30	CLA	b	608	-	65,73,73	1.50	10 (15%)	76,113,113	1.47	8 (10%)
30	CLA	b	614	-	65,73,73	1.39	10 (15%)	76,113,113	1.59	10 (13%)
32	BCR	a	408	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
42	A86	14	313	-	44,50,50	3.96	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	11	302	-	45,53,73	1.69	11 (24%)	52,89,113	1.78	9 (17%)
36	LMG	W	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.40	7 (11%)
30	CLA	14	305	-	65,73,73	1.40	10 (15%)	76,113,113	1.62	11 (14%)
30	CLA	C	520	-	65,73,73	1.41	9 (13%)	76,113,113	1.69	11 (14%)
36	LMG	b	618	-	51,51,55	0.88	4 (7%)	59,59,63	1.43	9 (15%)
30	CLA	20	206	27	45,53,73	1.70	9 (20%)	52,89,113	1.80	10 (19%)
30	CLA	17	306	25	45,53,73	1.70	7 (15%)	52,89,113	1.97	10 (19%)
30	CLA	11	301	25	65,73,73	1.45	9 (13%)	76,113,113	1.68	8 (10%)
30	CLA	a	403	-	65,73,73	1.48	10 (15%)	76,113,113	1.52	9 (11%)
35	LHG	d	409	-	48,48,48	0.81	1 (2%)	51,54,54	1.26	5 (9%)
30	CLA	19	308	-	45,53,73	1.69	8 (17%)	52,89,113	1.79	7 (13%)
30	CLA	11	308	25	45,53,73	1.75	11 (24%)	52,89,113	1.75	9 (17%)
36	LMG	m	102	30	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
42	A86	13	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	14	309	25	65,73,73	1.49	11 (16%)	76,113,113	1.55	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	14	307	-	45,53,73	1.72	8 (17%)	52,89,113	1.69	7 (13%)
39	DGD	h	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.42	8 (10%)
42	A86	21	311	-	44,50,50	3.89	23 (52%)	51,76,76	7.50	15 (29%)
30	CLA	18	304	-	45,53,73	1.72	7 (15%)	52,89,113	1.83	7 (13%)
42	A86	13	315	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
42	A86	15	315	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	b	606	-	65,73,73	1.58	12 (18%)	76,113,113	1.60	13 (17%)
30	CLA	C	504	-	65,73,73	1.47	11 (16%)	76,113,113	1.53	11 (14%)
34	BCT	a	406	29,1	2,3,3	1.27	0	2,3,3	3.96	2 (100%)
41	HEM	F	102	5,6	41,50,50	1.51	4 (9%)	45,82,82	1.24	5 (11%)
30	CLA	14	308	25	45,53,73	1.75	8 (17%)	52,89,113	1.81	8 (15%)
30	CLA	12	306	37	45,53,73	1.68	11 (24%)	52,89,113	1.78	9 (17%)
30	CLA	13	307	25	45,53,73	1.76	7 (15%)	52,89,113	1.83	7 (13%)
30	CLA	c	505	-	65,73,73	1.44	12 (18%)	76,113,113	1.68	11 (14%)
30	CLA	19	301	-	65,73,73	1.48	10 (15%)	76,113,113	1.49	11 (14%)
30	CLA	21	302	-	45,53,73	1.75	7 (15%)	52,89,113	1.73	10 (19%)
30	CLA	B	615	-	65,73,73	1.53	12 (18%)	76,113,113	1.44	11 (14%)
30	CLA	D	405	-	65,73,73	1.48	10 (15%)	76,113,113	1.61	10 (13%)
30	CLA	18	305	-	65,73,73	1.44	8 (12%)	76,113,113	1.48	7 (9%)
32	BCR	C	518	-	41,41,41	1.28	2 (4%)	56,56,56	1.37	6 (10%)
30	CLA	20	207	-	45,53,73	1.73	9 (20%)	52,89,113	1.74	10 (19%)
42	A86	20	213	-	44,50,50	4.01	23 (52%)	51,76,76	7.82	18 (35%)
30	CLA	A	404	-	65,73,73	1.48	10 (15%)	76,113,113	1.52	10 (13%)
42	A86	17	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	17	304	-	45,53,73	1.69	11 (24%)	52,89,113	1.83	9 (17%)
30	CLA	18	311	25	45,53,73	1.82	9 (20%)	52,89,113	1.81	11 (21%)
40	PL9	d	408	-	55,55,55	2.32	14 (25%)	68,69,69	1.48	14 (20%)
30	CLA	b	609	-	65,73,73	1.47	10 (15%)	76,113,113	1.52	9 (11%)
42	A86	19	312	-	44,50,50	4.00	21 (47%)	51,76,76	8.15	18 (35%)
30	CLA	16	306	25	45,53,73	1.74	9 (20%)	52,89,113	1.78	8 (15%)
30	CLA	c	511	-	65,73,73	1.45	12 (18%)	76,113,113	1.59	11 (14%)
30	CLA	11	309	-	45,53,73	1.75	8 (17%)	52,89,113	1.66	7 (13%)
40	PL9	D	407	-	55,55,55	2.32	15 (27%)	68,69,69	1.48	14 (20%)
42	A86	13	301	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
42	A86	12	304	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	17	305	-	65,73,73	1.42	10 (15%)	76,113,113	1.53	10 (13%)
30	CLA	20	208	-	45,53,73	1.70	7 (15%)	52,89,113	1.78	9 (17%)
42	A86	11	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	b	612	-	65,73,73	1.50	9 (13%)	76,113,113	1.77	10 (13%)
30	CLA	b	607	-	65,73,73	1.41	11 (16%)	76,113,113	1.55	7 (9%)
30	CLA	D	401	-	65,73,73	1.50	12 (18%)	76,113,113	1.52	9 (11%)
32	BCR	B	616	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	8 (14%)
30	CLA	11	306	25	45,53,73	1.75	8 (17%)	52,89,113	1.82	7 (13%)
42	A86	20	212	-	44,50,50	4.17	23 (52%)	51,76,76	8.24	15 (29%)
41	HEM	f	102	5,6	41,50,50	1.49	4 (9%)	45,82,82	1.26	5 (11%)
42	A86	19	310	-	44,50,50	3.88	23 (52%)	51,76,76	7.70	16 (31%)
30	CLA	m	101	36,12	65,73,73	1.42	10 (15%)	76,113,113	1.41	6 (7%)
30	CLA	Z	102	19,30	65,73,73	1.45	6 (9%)	76,113,113	1.41	8 (10%)
30	CLA	17	307	25	45,53,73	1.80	9 (20%)	52,89,113	1.77	13 (25%)
30	CLA	12	305	25	65,73,73	1.46	9 (13%)	76,113,113	1.67	8 (10%)
30	CLA	20	203	30	45,53,73	1.77	9 (20%)	52,89,113	1.72	8 (15%)
42	A86	18	315	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	c	509	-	65,73,73	1.47	11 (16%)	76,113,113	1.64	9 (11%)
30	CLA	17	308	25	65,73,73	1.49	10 (15%)	76,113,113	1.51	11 (14%)
30	CLA	13	305	25	45,53,73	1.72	8 (17%)	52,89,113	2.03	11 (21%)
42	A86	15	316	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	11	303	-	65,73,73	1.41	10 (15%)	76,113,113	1.58	9 (11%)
31	PHO	A	403	-	51,69,69	1.24	8 (15%)	47,99,99	1.31	8 (17%)
33	SQD	a	405	-	53,54,54	0.96	5 (9%)	62,65,65	1.59	11 (17%)
30	CLA	18	312	-	45,53,73	1.74	9 (20%)	52,89,113	1.61	7 (13%)
30	CLA	b	611	-	65,73,73	1.51	12 (18%)	76,113,113	1.58	11 (14%)
30	CLA	b	615	-	65,73,73	1.52	12 (18%)	76,113,113	1.44	11 (14%)
42	A86	12	316	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
39	DGD	c	518	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	16 (20%)
42	A86	17	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	18 (35%)
30	CLA	b	610	-	65,73,73	1.51	11 (16%)	76,113,113	1.51	8 (10%)
31	PHO	d	404	-	51,69,69	1.13	8 (15%)	47,99,99	1.28	6 (12%)
32	BCR	c	515	-	41,41,41	1.34	3 (7%)	56,56,56	1.41	8 (14%)
30	CLA	14	303	25	65,73,73	1.44	8 (12%)	76,113,113	1.67	8 (10%)
30	CLA	c	507	-	65,73,73	1.53	11 (16%)	76,113,113	1.55	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	BCR	a	404	-	41,41,41	1.29	2 (4%)	56,56,56	1.39	6 (10%)
30	CLA	B	603	-	65,73,73	1.42	11 (16%)	76,113,113	1.64	12 (15%)
30	CLA	A	402	-	65,73,73	1.45	8 (12%)	76,113,113	1.62	9 (11%)
36	LMG	d	410	-	51,51,55	0.90	3 (5%)	59,59,63	1.42	7 (11%)
30	CLA	21	307	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
42	A86	13	312	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
35	LHG	b	621	-	48,48,48	0.75	1 (2%)	51,54,54	1.29	6 (11%)
30	CLA	19	305	-	45,53,73	1.72	10 (22%)	52,89,113	1.69	6 (11%)
31	PHO	d	403	-	51,69,69	1.24	9 (17%)	47,99,99	1.31	8 (17%)
30	CLA	B	604	-	65,73,73	1.45	12 (18%)	76,113,113	1.68	16 (21%)
30	CLA	16	308	25	45,53,73	1.78	9 (20%)	52,89,113	1.71	11 (21%)
30	CLA	B	605	-	65,73,73	1.49	10 (15%)	76,113,113	1.50	9 (11%)
30	CLA	17	303	25	65,73,73	1.48	10 (15%)	76,113,113	1.58	8 (10%)
42	A86	20	201	-	44,50,50	3.93	22 (50%)	51,76,76	7.88	19 (37%)
30	CLA	c	503	-	65,73,73	1.51	12 (18%)	76,113,113	1.52	12 (15%)
30	CLA	20	202	-	65,73,73	1.43	7 (10%)	76,113,113	1.45	8 (10%)
30	CLA	d	406	-	65,73,73	1.48	10 (15%)	76,113,113	1.61	11 (14%)
42	A86	16	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
42	A86	14	312	-	44,50,50	3.93	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	C	512	3	65,73,73	1.51	10 (15%)	76,113,113	1.61	12 (15%)
42	A86	14	301	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	19 (37%)
30	CLA	C	505	-	65,73,73	1.44	12 (18%)	76,113,113	1.67	11 (14%)
30	CLA	18	303	25	65,73,73	1.47	10 (15%)	76,113,113	1.48	8 (10%)
42	A86	11	314	-	44,50,50	3.93	23 (52%)	51,76,76	7.98	19 (37%)
30	CLA	19	302	-	45,53,73	1.67	9 (20%)	52,89,113	1.89	10 (19%)
42	A86	21	313	-	44,50,50	3.90	23 (52%)	51,76,76	7.52	22 (43%)
30	CLA	16	302	25	65,73,73	1.49	10 (15%)	76,113,113	1.87	16 (21%)
37	LMU	12	302	30,25	33,33,36	1.30	3 (9%)	44,44,47	1.54	7 (15%)
30	CLA	B	612	-	65,73,73	1.50	9 (13%)	76,113,113	1.78	10 (13%)
42	A86	20	210	-	44,50,50	4.07	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	b	613	-	65,73,73	1.43	11 (16%)	76,113,113	1.63	9 (11%)
30	CLA	12	314	-	45,53,73	1.74	8 (17%)	52,89,113	1.67	7 (13%)
32	BCR	c	521	-	41,41,41	1.27	2 (4%)	56,56,56	1.37	6 (10%)
30	CLA	14	311	-	45,53,73	1.75	9 (20%)	52,89,113	1.67	8 (15%)
30	CLA	18	307	-	45,53,73	1.75	7 (15%)	52,89,113	1.63	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	BCR	c	516	-	41,41,41	1.31	4 (9%)	56,56,56	1.40	9 (16%)
30	CLA	b	622	-	65,73,73	1.47	9 (13%)	76,113,113	1.59	14 (18%)
30	CLA	13	310	-	45,53,73	1.75	9 (20%)	52,89,113	1.67	7 (13%)
30	CLA	11	307	25	65,73,73	1.47	10 (15%)	76,113,113	1.55	10 (13%)
32	BCR	F	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
30	CLA	M	101	36,12	65,73,73	1.42	10 (15%)	76,113,113	1.41	6 (7%)
30	CLA	C	511	-	65,73,73	1.45	12 (18%)	76,113,113	1.57	11 (14%)
30	CLA	B	610	-	65,73,73	1.50	11 (16%)	76,113,113	1.51	8 (10%)
30	CLA	B	602	-	65,73,73	1.47	10 (15%)	76,113,113	1.55	11 (14%)
42	A86	19	311	-	44,50,50	4.09	21 (47%)	51,76,76	7.17	19 (37%)
42	A86	17	302	-	44,50,50	3.94	23 (52%)	51,76,76	8.13	21 (41%)
33	SQD	b	620	-	36,37,54	1.20	6 (16%)	45,48,65	1.64	9 (20%)
42	A86	12	317	-	44,50,50	4.05	22 (50%)	51,76,76	7.80	19 (37%)
42	A86	17	312	-	44,50,50	3.97	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	13	302	25	65,73,73	1.46	9 (13%)	76,113,113	1.68	8 (10%)
42	A86	18	302	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
42	A86	15	314	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	19 (37%)
30	CLA	C	513	-	65,73,73	1.44	9 (13%)	76,113,113	1.48	8 (10%)
36	LMG	1	101	-	39,39,55	1.01	4 (10%)	47,47,63	1.18	4 (8%)
30	CLA	21	304	-	45,53,73	1.68	8 (17%)	52,89,113	1.65	6 (11%)
30	CLA	a	402	-	65,73,73	1.45	8 (12%)	76,113,113	1.61	9 (11%)
30	CLA	D	402	-	65,73,73	1.44	11 (16%)	76,113,113	1.50	8 (10%)
35	LHG	a	407	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	7 (14%)
30	CLA	16	301	-	65,73,73	1.45	9 (13%)	76,113,113	1.44	8 (10%)
30	CLA	18	301	-	65,73,73	1.47	11 (16%)	76,113,113	1.45	11 (14%)
30	CLA	18	310	25	65,73,73	1.47	9 (13%)	76,113,113	1.37	8 (10%)
30	CLA	14	306	25	45,53,73	1.70	8 (17%)	52,89,113	2.05	11 (21%)
30	CLA	c	502	-	65,73,73	1.39	11 (16%)	76,113,113	1.65	12 (15%)
30	CLA	21	309	-	45,53,73	1.82	7 (15%)	52,89,113	1.72	11 (21%)
30	CLA	b	604	-	65,73,73	1.45	12 (18%)	76,113,113	1.69	15 (19%)
30	CLA	C	508	-	65,73,73	1.43	12 (18%)	76,113,113	1.68	12 (15%)
30	CLA	13	308	25	65,73,73	1.46	10 (15%)	76,113,113	1.55	10 (13%)
30	CLA	c	513	-	65,73,73	1.45	10 (15%)	76,113,113	1.48	8 (10%)
30	CLA	15	308	25	45,53,73	1.76	10 (22%)	52,89,113	1.75	10 (19%)
30	CLA	12	307	-	65,73,73	1.43	10 (15%)	76,113,113	1.59	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	HEM	V	201	16	41,50,50	1.61	5 (12%)	45,82,82	1.27	4 (8%)
30	CLA	15	304	25	45,53,73	1.79	7 (15%)	52,89,113	1.79	9 (17%)
30	CLA	b	605	-	65,73,73	1.48	10 (15%)	76,113,113	1.50	9 (11%)
32	BCR	b	616	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	9 (16%)
30	CLA	C	510	-	65,73,73	1.48	12 (18%)	76,113,113	1.73	10 (13%)
30	CLA	z	101	-	65,73,73	1.45	9 (13%)	76,113,113	1.49	7 (9%)
30	CLA	15	302	-	45,53,73	1.71	7 (15%)	52,89,113	1.88	9 (17%)
30	CLA	21	306	-	65,73,73	1.48	9 (13%)	76,113,113	1.44	9 (11%)
39	DGD	j	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
36	LMG	c	519	-	51,51,55	0.96	5 (9%)	59,59,63	1.46	9 (15%)
42	A86	13	313	-	44,50,50	4.05	23 (52%)	51,76,76	7.81	19 (37%)
42	A86	21	312	-	44,50,50	3.82	21 (47%)	51,76,76	7.17	21 (41%)
30	CLA	b	603	-	65,73,73	1.43	11 (16%)	76,113,113	1.64	13 (17%)
30	CLA	c	504	-	65,73,73	1.47	11 (16%)	76,113,113	1.51	11 (14%)
39	DGD	J	101	-	63,63,67	1.11	10 (15%)	77,77,81	1.56	15 (19%)
30	CLA	15	301	25	65,73,73	1.48	9 (13%)	76,113,113	1.57	10 (13%)
42	A86	12	315	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	18	308	25	45,53,73	1.78	7 (15%)	52,89,113	1.72	8 (15%)
42	A86	16	312	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
33	SQD	A	406	-	53,54,54	0.97	6 (11%)	62,65,65	1.58	11 (17%)
30	CLA	d	401	-	65,73,73	1.50	12 (18%)	76,113,113	1.53	9 (11%)
30	CLA	19	304	26	45,53,73	1.71	8 (17%)	52,89,113	1.82	11 (21%)
32	BCR	B	617	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	9 (16%)
38	OEX	c	501	3,1	0,15,15	-	-	-	-	-
30	CLA	B	606	-	65,73,73	1.58	12 (18%)	76,113,113	1.61	13 (17%)
42	A86	14	314	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
30	CLA	19	303	-	65,73,73	1.46	10 (15%)	76,113,113	1.55	9 (11%)
36	LMG	Q	301	-	51,51,55	0.96	5 (9%)	59,59,63	1.46	9 (15%)
37	LMU	B	625	-	33,33,36	1.28	3 (9%)	44,44,47	1.57	8 (18%)
30	CLA	13	309	25	45,53,73	1.76	11 (24%)	52,89,113	1.76	9 (17%)
36	LMG	B	619	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	8 (13%)
32	BCR	Z	101	-	41,41,41	1.32	3 (7%)	56,56,56	1.41	8 (14%)
30	CLA	W	102	-	65,73,73	1.45	9 (13%)	76,113,113	1.47	10 (13%)
42	A86	17	313	-	44,50,50	4.05	24 (54%)	51,76,76	7.82	19 (37%)
30	CLA	17	301	-	65,73,73	1.44	10 (15%)	76,113,113	1.48	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	15	305	-	45,53,73	1.76	6 (13%)	52,89,113	1.66	6 (11%)
30	CLA	B	601	-	65,73,73	1.44	10 (15%)	76,113,113	1.50	8 (10%)
42	A86	13	311	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	d	407	-	65,73,73	1.40	11 (16%)	76,113,113	1.60	7 (9%)
42	A86	15	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
35	LHG	A	408	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	7 (14%)
30	CLA	12	303	-	65,73,73	1.45	9 (13%)	76,113,113	1.49	8 (10%)
30	CLA	12	309	-	45,53,73	1.70	8 (17%)	52,89,113	1.71	7 (13%)
33	SQD	l	101	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
32	BCR	Y	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.47	9 (16%)
42	A86	15	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	C	514	30	65,73,73	1.39	8 (12%)	76,113,113	1.63	9 (11%)
30	CLA	21	305	28	45,53,73	1.75	6 (13%)	52,89,113	1.79	9 (17%)
30	CLA	13	303	-	45,53,73	1.68	10 (22%)	52,89,113	1.81	9 (17%)
30	CLA	15	306	25	45,53,73	1.77	7 (15%)	52,89,113	1.79	9 (17%)
30	CLA	15	309	-	45,53,73	1.75	9 (20%)	52,89,113	1.61	7 (13%)
30	CLA	16	304	-	65,73,73	1.44	10 (15%)	76,113,113	1.48	8 (10%)
30	CLA	19	307	-	65,73,73	1.41	11 (16%)	76,113,113	1.48	8 (10%)
30	CLA	12	312	-	65,73,73	1.46	9 (13%)	76,113,113	1.49	8 (10%)
30	CLA	17	309	25	45,53,73	1.78	10 (22%)	52,89,113	2.10	13 (25%)
30	CLA	C	506	-	65,73,73	1.45	11 (16%)	76,113,113	1.56	12 (15%)
32	BCR	h	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.32	8 (14%)
33	SQD	L	103	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
42	A86	11	316	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	15	303	-	65,73,73	1.42	7 (10%)	76,113,113	1.54	10 (13%)
30	CLA	11	315	-	65,73,73	1.45	9 (13%)	76,113,113	1.48	8 (10%)
30	CLA	16	305	25	45,53,73	1.70	8 (17%)	52,89,113	1.90	10 (19%)

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
42	A86	17	311	-	-	13/34/90/90	0/3/3/3
30	CLA	16	307	25	1/1/11/20	9/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMG	B	620	-	-	20/46/66/70	0/1/1/1
30	CLA	14	302	-	1/1/15/20	11/37/115/115	-
41	HEM	v	201	16	-	0/12/54/54	-
30	CLA	12	310	25	1/1/11/20	8/13/91/115	-
30	CLA	D	406	-	1/1/15/20	4/37/115/115	-
30	CLA	11	304	25	1/1/11/20	9/13/91/115	-
36	LMG	w	101	-	-	28/46/66/70	0/1/1/1
30	CLA	w	102	-	1/1/15/20	14/37/115/115	-
30	CLA	c	512	3	1/1/15/20	8/37/115/115	-
36	LMG	b	619	-	-	20/46/66/70	0/1/1/1
42	A86	15	312	-	-	8/34/90/90	0/3/3/3
30	CLA	20	204	-	1/1/15/20	13/37/115/115	-
42	A86	14	315	-	-	10/34/90/90	0/3/3/3
30	CLA	b	601	-	1/1/15/20	18/37/115/115	-
32	BCR	A	409	-	-	9/29/63/63	0/2/2/2
35	LHG	L	101	-	-	29/53/53/53	-
36	LMG	12	301	-	-	17/34/54/70	0/1/1/1
42	A86	12	318	-	-	10/34/90/90	0/3/3/3
30	CLA	13	304	-	1/1/15/20	13/37/115/115	-
32	BCR	m	103	-	-	8/29/63/63	0/2/2/2
31	PHO	D	403	-	-	8/37/103/103	0/5/6/6
30	CLA	17	310	-	1/1/11/20	7/13/91/115	-
30	CLA	21	303	-	1/1/15/20	17/37/115/115	-
30	CLA	B	607	-	1/1/15/20	12/37/115/115	-
30	CLA	19	309	-	1/1/11/20	8/13/91/115	-
42	A86	12	319	-	-	7/34/90/90	0/3/3/3
42	A86	15	310	-	-	8/34/90/90	0/3/3/3
42	A86	11	312	-	-	8/34/90/90	0/3/3/3
39	DGD	C	517	-	-	22/51/91/95	0/2/2/2
35	LHG	l	102	-	-	22/53/53/53	-
30	CLA	20	209	30	1/1/15/20	11/37/115/115	-
42	A86	18	313	-	-	8/34/90/90	0/3/3/3
30	CLA	c	506	-	1/1/15/20	16/37/115/115	-
30	CLA	20	205	-	-	9/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	DGD	C	516	-	-	19/51/91/95	0/2/2/2
30	CLA	19	306	-	1/1/11/20	8/13/91/115	-
30	CLA	12	313	25	-	6/13/91/115	-
30	CLA	18	309	25	1/1/15/20	16/37/115/115	-
30	CLA	15	307	25	1/1/15/20	11/37/115/115	-
30	CLA	B	613	-	1/1/15/20	8/37/115/115	-
32	BCR	f	101	-	-	15/29/63/63	0/2/2/2
40	PL9	D	404	4	-	17/53/73/73	0/1/1/1
30	CLA	16	309	-	1/1/11/20	5/13/91/115	-
42	A86	17	315	-	-	13/34/90/90	0/3/3/3
30	CLA	W	103	-	-	19/37/115/115	-
32	BCR	A	405	-	-	12/29/63/63	0/2/2/2
30	CLA	11	305	-	1/1/11/20	8/13/91/115	-
40	PL9	d	405	4	-	17/53/73/73	0/1/1/1
30	CLA	c	510	-	1/1/15/20	12/37/115/115	-
32	BCR	C	515	-	-	10/29/63/63	0/2/2/2
30	CLA	B	614	-	1/1/15/20	8/37/115/115	-
39	DGD	H	102	-	-	24/51/91/95	0/2/2/2
42	A86	14	316	-	-	7/34/90/90	0/3/3/3
36	LMG	D	408	-	-	14/46/66/70	0/1/1/1
30	CLA	18	306	25	-	9/13/91/115	-
30	CLA	c	508	-	1/1/15/20	18/37/115/115	-
39	DGD	c	517	-	-	19/51/91/95	0/2/2/2
42	A86	21	310	-	-	9/34/90/90	0/3/3/3
30	CLA	12	308	25	1/1/11/20	9/13/91/115	-
30	CLA	12	311	25	1/1/15/20	14/37/115/115	-
42	A86	16	310	-	-	12/34/90/90	0/3/3/3
42	A86	21	314	-	-	12/34/90/90	0/3/3/3
32	BCR	B	618	-	-	9/29/63/63	0/2/2/2
30	CLA	C	507	-	1/1/15/20	17/37/115/115	-
30	CLA	B	608	-	1/1/15/20	8/37/115/115	-
30	CLA	d	402	-	1/1/15/20	13/37/115/115	-
36	LMG	M	102	30	-	10/35/55/70	0/1/1/1
30	CLA	21	308	-	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	b	602	-	1/1/15/20	13/37/115/115	-
32	BCR	H	101	-	-	7/29/63/63	0/2/2/2
42	A86	11	313	-	-	10/34/90/90	0/3/3/3
30	CLA	14	310	25	-	6/13/91/115	-
30	CLA	14	304	-	1/1/11/20	4/13/91/115	-
32	BCR	B	624	-	-	18/29/63/63	0/2/2/2
30	CLA	w	103	-	-	19/37/115/115	-
42	A86	18	314	-	-	3/34/90/90	0/3/3/3
30	CLA	B	611	-	1/1/15/20	12/37/115/115	-
30	CLA	B	623	-	1/1/15/20	15/37/115/115	-
30	CLA	C	503	-	1/1/15/20	11/37/115/115	-
32	BCR	c	520	-	-	16/29/63/63	0/2/2/2
30	CLA	c	514	-	1/1/15/20	13/37/115/115	-
30	CLA	21	301	28	-	14/37/115/115	-
30	CLA	13	306	-	1/1/11/20	8/13/91/115	-
42	A86	20	211	-	-	8/34/90/90	0/3/3/3
32	BCR	b	623	-	-	18/29/63/63	0/2/2/2
30	CLA	B	609	-	1/1/15/20	8/37/115/115	-
30	CLA	C	509	-	1/1/15/20	12/37/115/115	-
30	CLA	C	502	-	1/1/15/20	14/37/115/115	-
35	LHG	B	622	-	-	20/53/53/53	-
30	CLA	C	519	-	-	21/37/115/115	-
35	LHG	L	102	-	-	22/53/53/53	-
42	A86	11	311	-	-	3/34/90/90	0/3/3/3
33	SQD	B	621	-	-	9/32/52/69	0/1/1/1
32	BCR	b	617	-	-	9/29/63/63	0/2/2/2
42	A86	16	313	-	-	7/34/90/90	0/3/3/3
30	CLA	16	303	-	1/1/11/20	6/13/91/115	-
30	CLA	b	608	-	1/1/15/20	8/37/115/115	-
30	CLA	b	614	-	1/1/15/20	8/37/115/115	-
32	BCR	a	408	-	-	9/29/63/63	0/2/2/2
42	A86	14	313	-	-	3/34/90/90	0/3/3/3
30	CLA	11	302	-	1/1/11/20	5/13/91/115	-
36	LMG	W	101	-	-	28/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	14	305	-	1/1/15/20	13/37/115/115	-
30	CLA	C	520	-	1/1/15/20	14/37/115/115	-
36	LMG	b	618	-	-	18/46/66/70	0/1/1/1
30	CLA	20	206	27	1/1/11/20	7/13/91/115	-
30	CLA	17	306	25	-	8/13/91/115	-
30	CLA	11	301	25	1/1/15/20	11/37/115/115	-
30	CLA	a	403	-	1/1/15/20	10/37/115/115	-
35	LHG	d	409	-	-	29/53/53/53	-
30	CLA	19	308	-	1/1/11/20	3/13/91/115	-
30	CLA	11	308	25	-	6/13/91/115	-
36	LMG	m	102	30	-	10/35/55/70	0/1/1/1
42	A86	13	314	-	-	10/34/90/90	0/3/3/3
30	CLA	14	309	25	1/1/15/20	14/37/115/115	-
30	CLA	14	307	-	1/1/11/20	8/13/91/115	-
39	DGD	h	102	-	-	24/51/91/95	0/2/2/2
42	A86	21	311	-	-	8/34/90/90	0/3/3/3
30	CLA	18	304	-	1/1/11/20	5/13/91/115	-
42	A86	13	315	-	-	16/34/90/90	0/3/3/3
42	A86	15	315	-	-	15/34/90/90	0/3/3/3
30	CLA	b	606	-	1/1/15/20	7/37/115/115	-
30	CLA	C	504	-	1/1/15/20	17/37/115/115	-
41	HEM	F	102	5,6	-	7/12/54/54	-
30	CLA	14	308	25	1/1/11/20	8/13/91/115	-
30	CLA	12	306	37	1/1/11/20	4/13/91/115	-
30	CLA	13	307	25	1/1/11/20	8/13/91/115	-
30	CLA	c	505	-	1/1/15/20	17/37/115/115	-
30	CLA	19	301	-	-	12/37/115/115	-
30	CLA	21	302	-	-	7/13/91/115	-
30	CLA	B	615	-	1/1/15/20	13/37/115/115	-
30	CLA	D	405	-	1/1/15/20	8/37/115/115	-
30	CLA	18	305	-	1/1/15/20	19/37/115/115	-
32	BCR	C	518	-	-	8/29/63/63	0/2/2/2
30	CLA	20	207	-	1/1/11/20	7/13/91/115	-
42	A86	20	213	-	-	12/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	A	404	-	1/1/15/20	10/37/115/115	-
42	A86	17	314	-	-	10/34/90/90	0/3/3/3
30	CLA	17	304	-	-	6/13/91/115	-
30	CLA	18	311	25	1/1/11/20	8/13/91/115	-
40	PL9	d	408	-	-	13/53/73/73	0/1/1/1
30	CLA	b	609	-	1/1/15/20	8/37/115/115	-
42	A86	19	312	-	-	8/34/90/90	0/3/3/3
30	CLA	16	306	25	1/1/11/20	7/13/91/115	-
30	CLA	c	511	-	1/1/15/20	12/37/115/115	-
30	CLA	11	309	-	1/1/11/20	6/13/91/115	-
40	PL9	D	407	-	-	13/53/73/73	0/1/1/1
42	A86	13	301	-	-	15/34/90/90	0/3/3/3
42	A86	12	304	-	-	16/34/90/90	0/3/3/3
30	CLA	17	305	-	1/1/15/20	19/37/115/115	-
30	CLA	20	208	-	-	8/13/91/115	-
42	A86	11	310	-	-	8/34/90/90	0/3/3/3
30	CLA	b	612	-	1/1/15/20	13/37/115/115	-
30	CLA	b	607	-	1/1/15/20	12/37/115/115	-
30	CLA	D	401	-	1/1/15/20	12/37/115/115	-
32	BCR	B	616	-	-	8/29/63/63	0/2/2/2
30	CLA	11	306	25	1/1/11/20	8/13/91/115	-
42	A86	20	212	-	-	11/34/90/90	0/3/3/3
41	HEM	f	102	5,6	-	7/12/54/54	-
42	A86	19	310	-	-	11/34/90/90	0/3/3/3
30	CLA	m	101	36,12	1/1/15/20	19/37/115/115	-
30	CLA	Z	102	19,30	1/1/15/20	15/37/115/115	-
30	CLA	17	307	25	1/1/11/20	7/13/91/115	-
30	CLA	12	305	25	1/1/15/20	11/37/115/115	-
30	CLA	20	203	30	1/1/11/20	5/13/91/115	-
42	A86	18	315	-	-	10/34/90/90	0/3/3/3
30	CLA	c	509	-	1/1/15/20	12/37/115/115	-
30	CLA	17	308	25	1/1/15/20	17/37/115/115	-
30	CLA	13	305	25	1/1/11/20	9/13/91/115	-
42	A86	15	316	-	-	16/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	11	303	-	1/1/15/20	13/37/115/115	-
31	PHO	A	403	-	-	12/37/103/103	0/5/6/6
33	SQD	a	405	-	-	14/49/69/69	0/1/1/1
30	CLA	18	312	-	1/1/11/20	4/13/91/115	-
30	CLA	b	611	-	1/1/15/20	12/37/115/115	-
30	CLA	b	615	-	1/1/15/20	13/37/115/115	-
42	A86	12	316	-	-	3/34/90/90	0/3/3/3
39	DGD	c	518	-	-	22/51/91/95	0/2/2/2
42	A86	17	316	-	-	7/34/90/90	0/3/3/3
30	CLA	b	610	-	1/1/15/20	14/37/115/115	-
31	PHO	d	404	-	-	8/37/103/103	0/5/6/6
32	BCR	c	515	-	-	15/29/63/63	0/2/2/2
30	CLA	14	303	25	1/1/15/20	12/37/115/115	-
30	CLA	c	507	-	1/1/15/20	17/37/115/115	-
32	BCR	a	404	-	-	12/29/63/63	0/2/2/2
30	CLA	B	603	-	1/1/15/20	10/37/115/115	-
30	CLA	A	402	-	1/1/15/20	7/37/115/115	-
36	LMG	d	410	-	-	14/46/66/70	0/1/1/1
30	CLA	21	307	-	1/1/15/20	11/37/115/115	-
42	A86	13	312	-	-	3/34/90/90	0/3/3/3
35	LHG	b	621	-	-	20/53/53/53	-
30	CLA	19	305	-	1/1/11/20	7/13/91/115	-
31	PHO	d	403	-	-	12/37/103/103	0/5/6/6
30	CLA	B	604	-	1/1/15/20	14/37/115/115	-
30	CLA	16	308	25	-	7/13/91/115	-
30	CLA	B	605	-	1/1/15/20	17/37/115/115	-
30	CLA	17	303	25	1/1/15/20	13/37/115/115	-
42	A86	20	201	-	-	12/34/90/90	0/3/3/3
30	CLA	c	503	-	1/1/15/20	11/37/115/115	-
30	CLA	20	202	-	-	19/37/115/115	-
30	CLA	d	406	-	1/1/15/20	8/37/115/115	-
42	A86	16	311	-	-	3/34/90/90	0/3/3/3
42	A86	14	312	-	-	8/34/90/90	0/3/3/3
30	CLA	C	512	3	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	A86	14	301	-	-	7/34/90/90	0/3/3/3
30	CLA	C	505	-	1/1/15/20	17/37/115/115	-
30	CLA	18	303	25	1/1/15/20	14/37/115/115	-
42	A86	11	314	-	-	7/34/90/90	0/3/3/3
30	CLA	19	302	-	1/1/11/20	4/13/91/115	-
42	A86	21	313	-	-	16/34/90/90	0/3/3/3
30	CLA	16	302	25	1/1/15/20	15/37/115/115	-
37	LMU	12	302	30,25	-	7/18/58/61	0/2/2/2
30	CLA	B	612	-	1/1/15/20	13/37/115/115	-
42	A86	20	210	-	-	14/34/90/90	0/3/3/3
30	CLA	b	613	-	1/1/15/20	8/37/115/115	-
30	CLA	12	314	-	1/1/11/20	6/13/91/115	-
32	BCR	c	521	-	-	8/29/63/63	0/2/2/2
30	CLA	14	311	-	1/1/11/20	6/13/91/115	-
30	CLA	18	307	-	1/1/11/20	6/13/91/115	-
32	BCR	c	516	-	-	10/29/63/63	0/2/2/2
30	CLA	b	622	-	1/1/15/20	15/37/115/115	-
30	CLA	13	310	-	1/1/11/20	6/13/91/115	-
30	CLA	11	307	25	1/1/15/20	14/37/115/115	-
32	BCR	F	101	-	-	15/29/63/63	0/2/2/2
30	CLA	M	101	36,12	1/1/15/20	19/37/115/115	-
30	CLA	C	511	-	1/1/15/20	12/37/115/115	-
30	CLA	B	610	-	1/1/15/20	14/37/115/115	-
30	CLA	B	602	-	1/1/15/20	13/37/115/115	-
42	A86	19	311	-	-	17/34/90/90	0/3/3/3
42	A86	17	302	-	-	16/34/90/90	1/3/3/3
33	SQD	b	620	-	-	9/32/52/69	0/1/1/1
42	A86	12	317	-	-	9/34/90/90	0/3/3/3
42	A86	17	312	-	-	3/34/90/90	0/3/3/3
30	CLA	13	302	25	1/1/15/20	12/37/115/115	-
42	A86	18	302	-	-	15/34/90/90	0/3/3/3
42	A86	15	314	-	-	7/34/90/90	0/3/3/3
30	CLA	C	513	-	1/1/15/20	16/37/115/115	-
36	LMG	1	101	-	-	14/34/54/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	21	304	-	1/1/11/20	8/13/91/115	-
30	CLA	a	402	-	1/1/15/20	7/37/115/115	-
30	CLA	D	402	-	1/1/15/20	13/37/115/115	-
35	LHG	a	407	-	-	23/50/50/53	-
30	CLA	16	301	-	1/1/15/20	10/37/115/115	-
30	CLA	18	301	-	1/1/15/20	11/37/115/115	-
30	CLA	18	310	25	1/1/15/20	10/37/115/115	-
30	CLA	14	306	25	1/1/11/20	9/13/91/115	-
30	CLA	c	502	-	1/1/15/20	14/37/115/115	-
30	CLA	21	309	-	1/1/11/20	6/13/91/115	-
30	CLA	b	604	-	1/1/15/20	14/37/115/115	-
30	CLA	C	508	-	1/1/15/20	18/37/115/115	-
30	CLA	13	308	25	1/1/15/20	14/37/115/115	-
30	CLA	c	513	-	1/1/15/20	16/37/115/115	-
30	CLA	15	308	25	1/1/11/20	6/13/91/115	-
30	CLA	12	307	-	1/1/15/20	13/37/115/115	-
41	HEM	V	201	16	-	0/12/54/54	-
30	CLA	15	304	25	-	7/13/91/115	-
30	CLA	b	605	-	1/1/15/20	17/37/115/115	-
32	BCR	b	616	-	-	9/29/63/63	0/2/2/2
30	CLA	C	510	-	1/1/15/20	12/37/115/115	-
30	CLA	z	101	-	-	21/37/115/115	-
30	CLA	15	302	-	1/1/11/20	8/13/91/115	-
30	CLA	21	306	-	1/1/15/20	14/37/115/115	-
39	DGD	j	101	-	-	15/51/91/95	0/2/2/2
36	LMG	c	519	-	-	22/46/66/70	0/1/1/1
42	A86	13	313	-	-	9/34/90/90	0/3/3/3
42	A86	21	312	-	-	7/34/90/90	0/3/3/3
30	CLA	b	603	-	1/1/15/20	10/37/115/115	-
30	CLA	c	504	-	1/1/15/20	17/37/115/115	-
39	DGD	J	101	-	-	15/51/91/95	0/2/2/2
30	CLA	15	301	25	1/1/15/20	10/37/115/115	-
42	A86	12	315	-	-	8/34/90/90	0/3/3/3
30	CLA	18	308	25	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	A86	16	312	-	-	8/34/90/90	0/3/3/3
33	SQD	A	406	-	-	14/49/69/69	0/1/1/1
30	CLA	d	401	-	1/1/15/20	12/37/115/115	-
30	CLA	19	304	26	1/1/11/20	9/13/91/115	-
32	BCR	B	617	-	-	9/29/63/63	0/2/2/2
30	CLA	B	606	-	1/1/15/20	7/37/115/115	-
42	A86	14	314	-	-	8/34/90/90	0/3/3/3
30	CLA	19	303	-	1/1/15/20	15/37/115/115	-
36	LMG	Q	301	-	-	22/46/66/70	0/1/1/1
37	LMU	B	625	-	-	7/18/58/61	0/2/2/2
30	CLA	13	309	25	-	6/13/91/115	-
36	LMG	B	619	-	-	18/46/66/70	0/1/1/1
32	BCR	Z	101	-	-	15/29/63/63	0/2/2/2
30	CLA	W	102	-	1/1/15/20	14/37/115/115	-
42	A86	17	313	-	-	9/34/90/90	0/3/3/3
30	CLA	17	301	-	1/1/15/20	14/37/115/115	-
30	CLA	15	305	-	1/1/11/20	8/13/91/115	-
30	CLA	B	601	-	1/1/15/20	18/37/115/115	-
42	A86	13	311	-	-	8/34/90/90	0/3/3/3
30	CLA	d	407	-	1/1/15/20	4/37/115/115	-
42	A86	15	311	-	-	3/34/90/90	0/3/3/3
35	LHG	A	408	-	-	23/50/50/53	-
30	CLA	12	303	-	1/1/15/20	11/37/115/115	-
30	CLA	12	309	-	1/1/11/20	8/13/91/115	-
33	SQD	l	101	-	-	21/49/69/69	0/1/1/1
32	BCR	Y	101	-	-	16/29/63/63	0/2/2/2
42	A86	15	313	-	-	10/34/90/90	0/3/3/3
30	CLA	C	514	30	1/1/15/20	13/37/115/115	-
30	CLA	21	305	28	1/1/11/20	9/13/91/115	-
30	CLA	13	303	-	1/1/11/20	5/13/91/115	-
30	CLA	15	306	25	1/1/11/20	8/13/91/115	-
30	CLA	15	309	-	1/1/11/20	4/13/91/115	-
30	CLA	16	304	-	1/1/15/20	15/37/115/115	-
30	CLA	19	307	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	12	312	-	1/1/15/20	11/37/115/115	-
30	CLA	17	309	25	1/1/11/20	4/13/91/115	-
30	CLA	C	506	-	1/1/15/20	16/37/115/115	-
32	BCR	h	101	-	-	7/29/63/63	0/2/2/2
33	SQD	L	103	-	-	21/49/69/69	0/1/1/1
42	A86	11	316	-	-	16/34/90/90	0/3/3/3
30	CLA	15	303	-	1/1/15/20	15/37/115/115	-
30	CLA	11	315	-	1/1/15/20	11/37/115/115	-
30	CLA	16	305	25	-	8/13/91/115	-

The worst 5 of 3422 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	19	311	A86	C14-C13	14.34	1.68	1.51
42	11	313	A86	C14-C13	14.10	1.68	1.51
42	12	318	A86	C14-C13	14.06	1.68	1.51
42	13	314	A86	C14-C13	14.04	1.68	1.51
42	18	315	A86	C14-C13	14.01	1.68	1.51

The worst 5 of 3449 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	17	311	A86	O1-C20-C19	55.34	154.95	113.38
42	17	315	A86	O1-C20-C19	55.32	154.94	113.38
42	18	313	A86	O1-C20-C19	55.08	154.75	113.38
42	20	210	A86	O1-C20-C19	55.05	154.74	113.38
42	11	310	A86	O1-C20-C19	55.03	154.72	113.38

5 of 164 chirality outliers are listed below:

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

5 of 3660 torsion outliers are listed below:

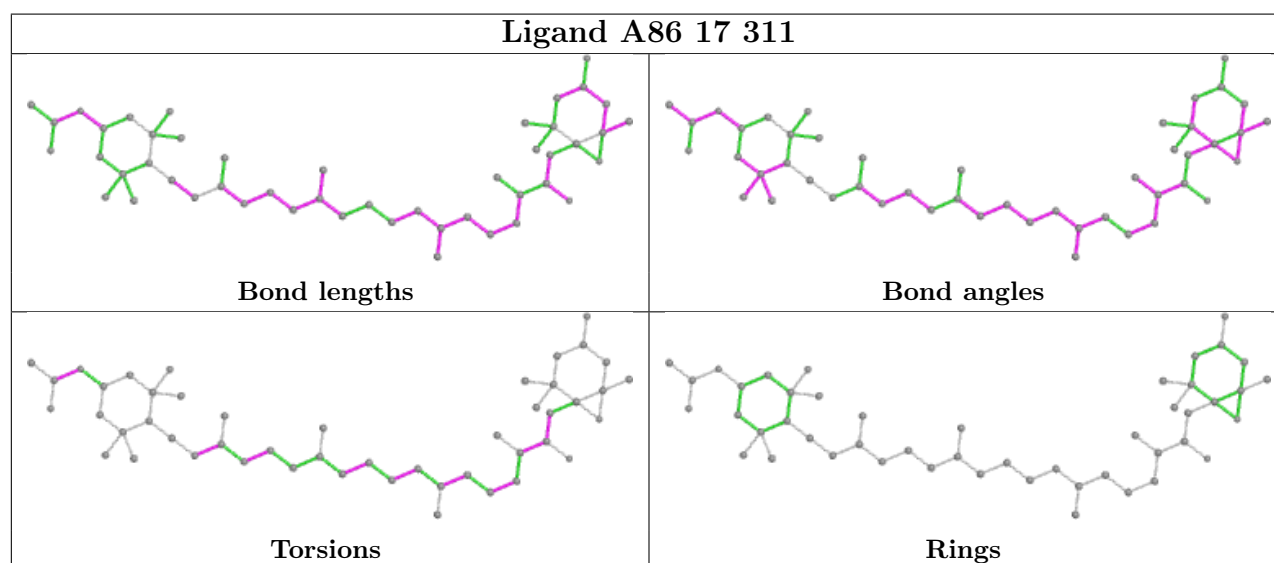
Mol	Chain	Res	Type	Atoms
30	A	402	CLA	CBD-CGD-O2D-CED
30	B	601	CLA	C1A-C2A-CAA-CBA
30	B	601	CLA	CHA-CBD-CGD-O1D
30	B	601	CLA	CHA-CBD-CGD-O2D
30	B	601	CLA	CAD-CBD-CGD-O1D

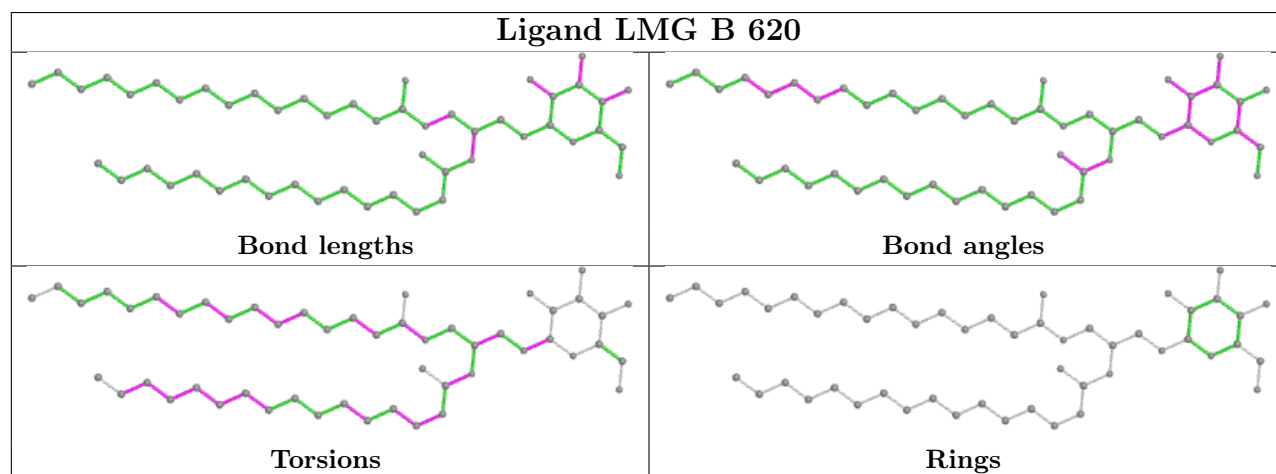
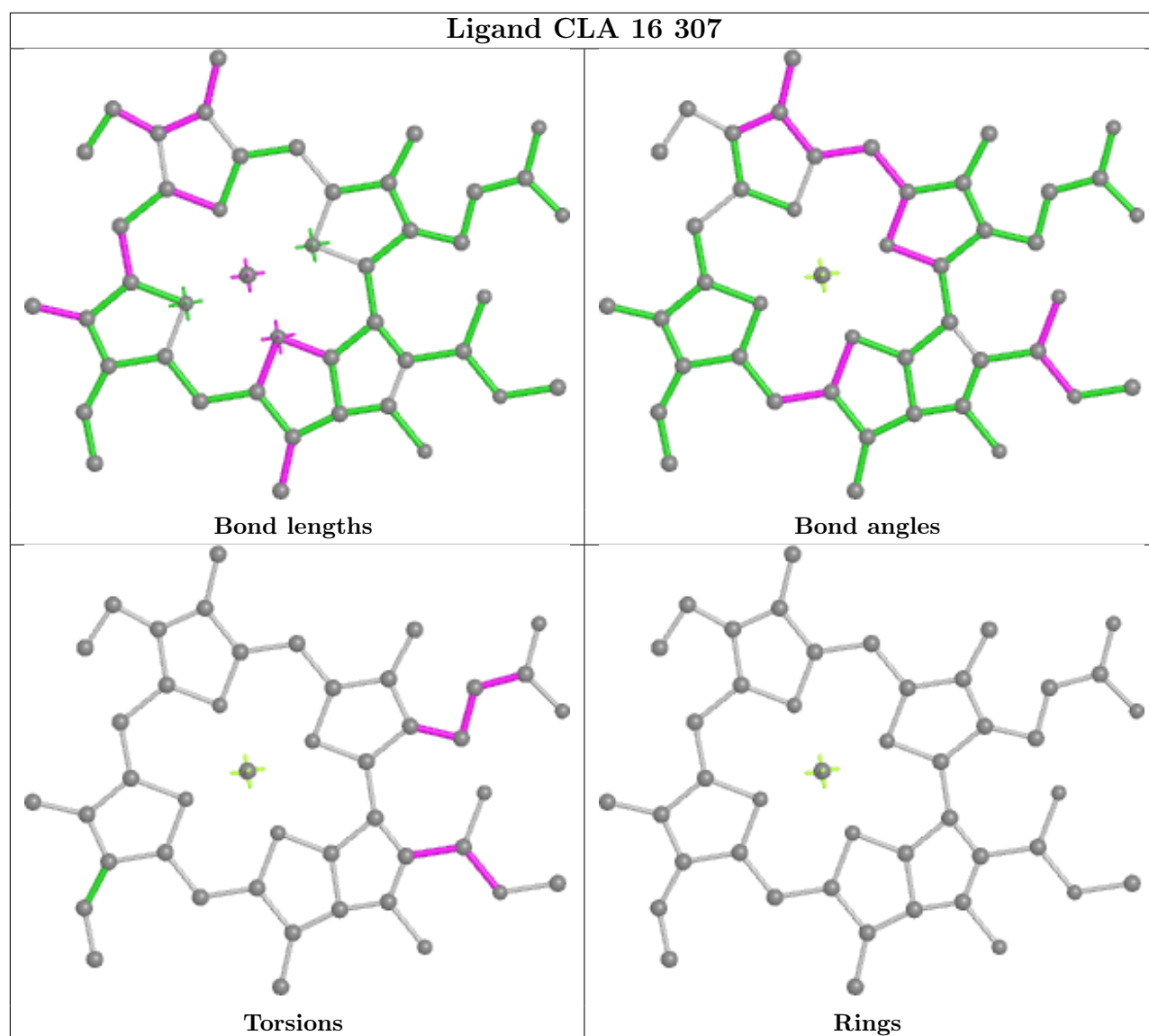
All (1) ring outliers are listed below:

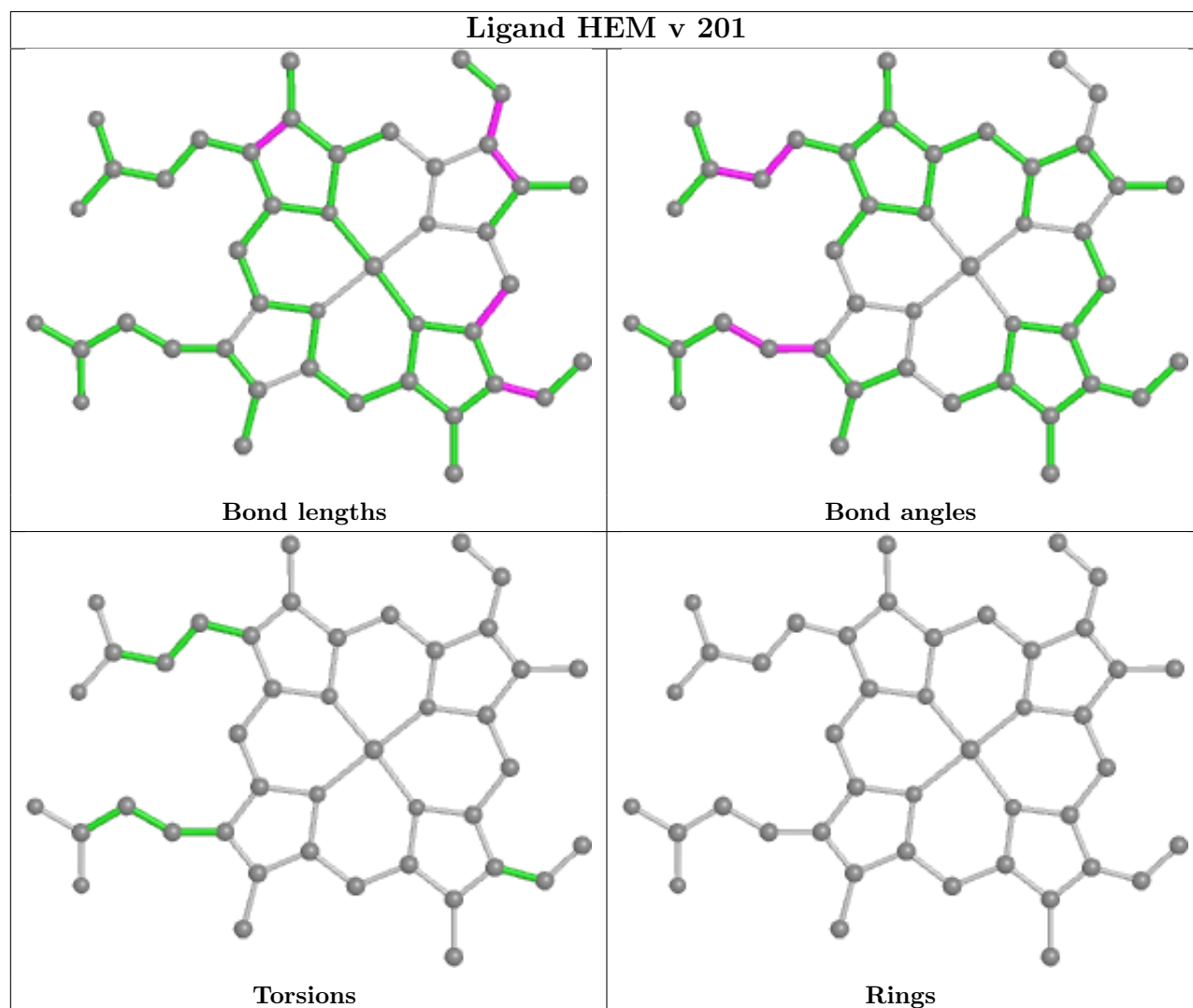
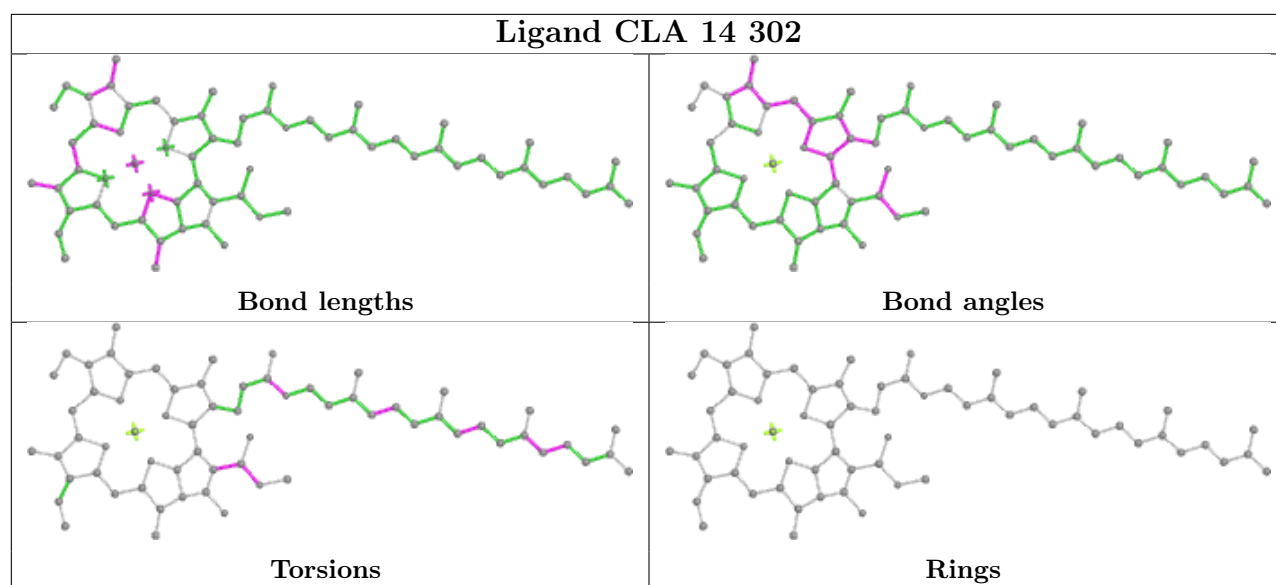
Mol	Chain	Res	Type	Atoms
42	17	302	A86	C31-C32-C33-C34-C35-C36

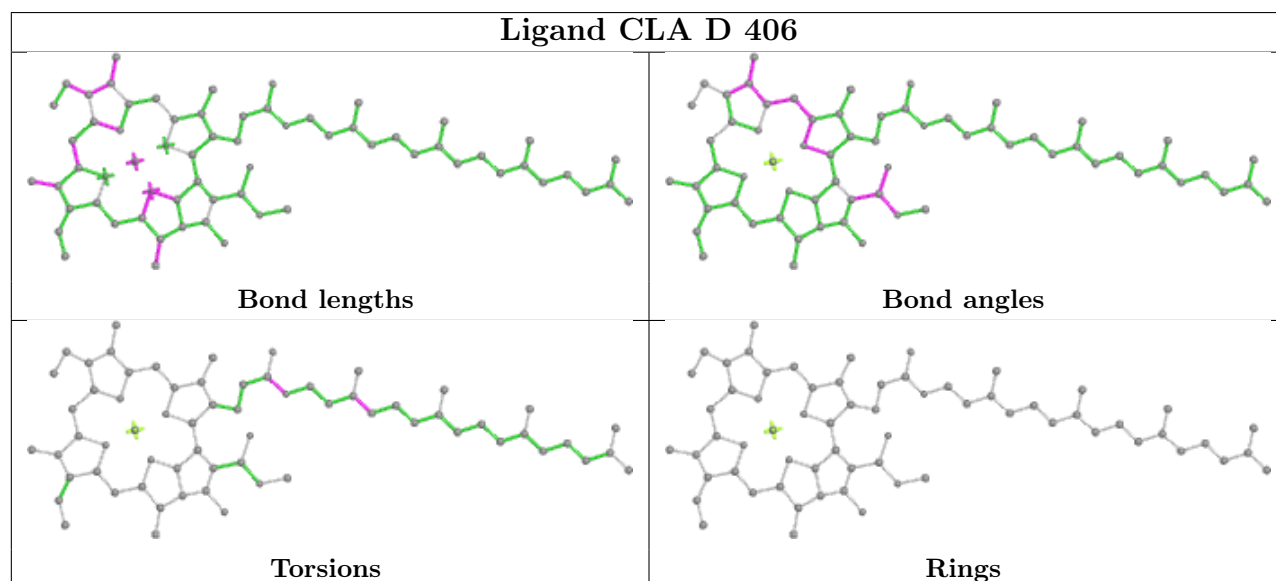
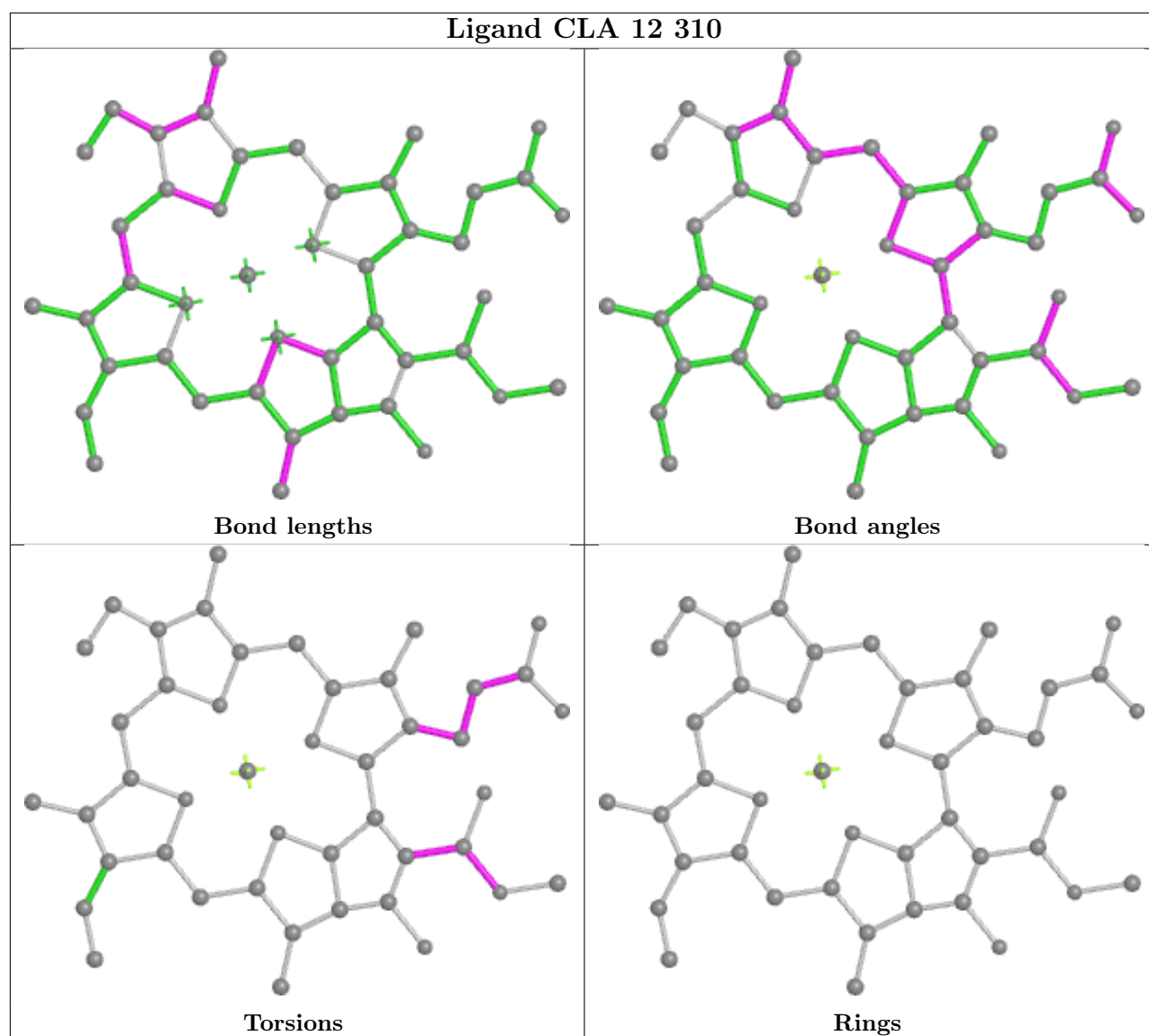
No monomer is involved in short contacts.

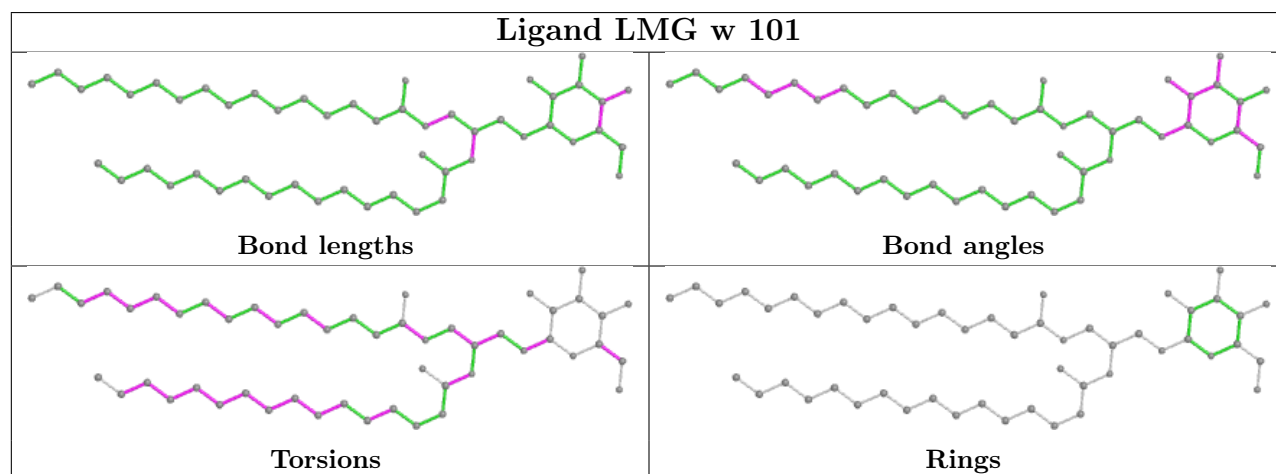
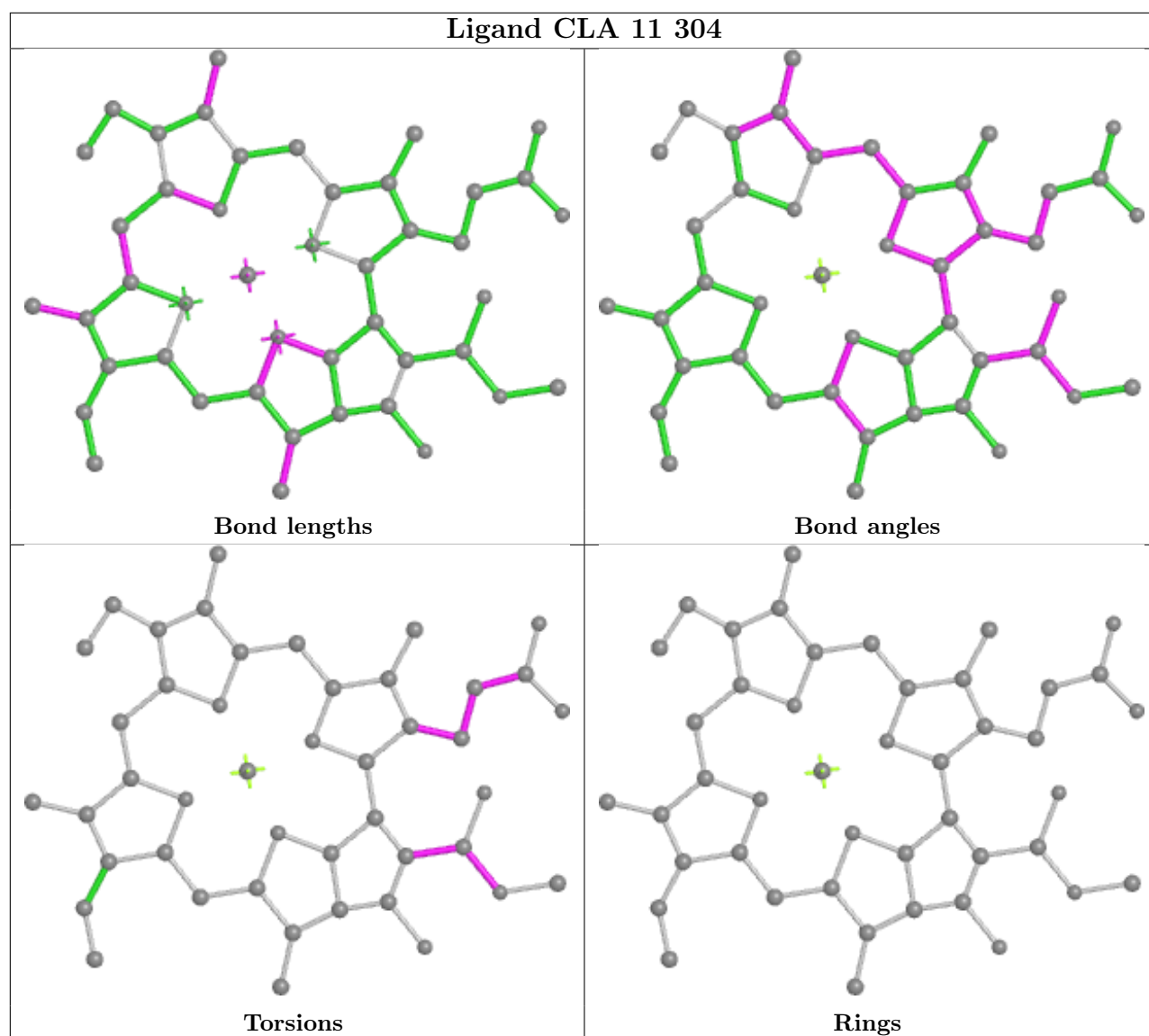
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

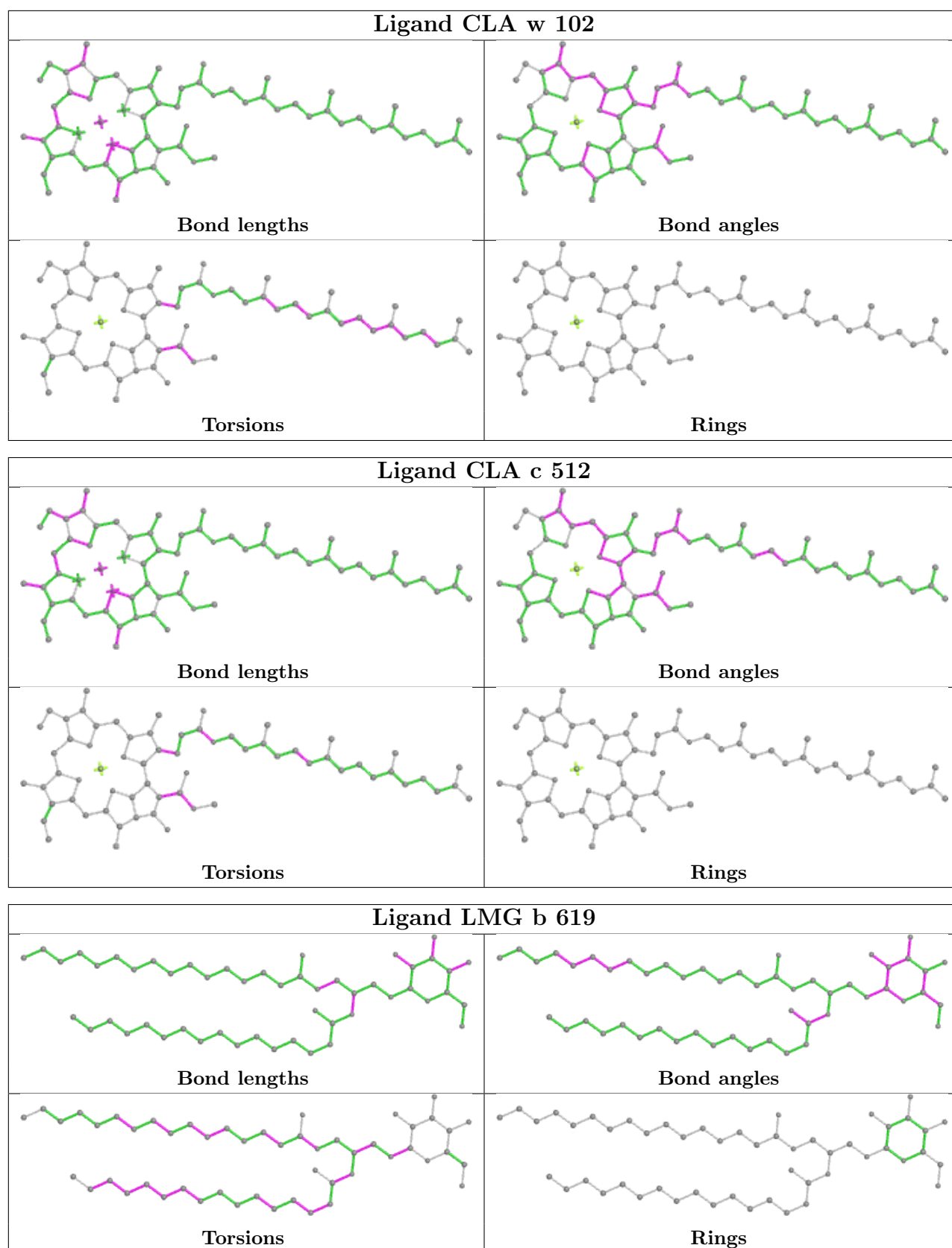


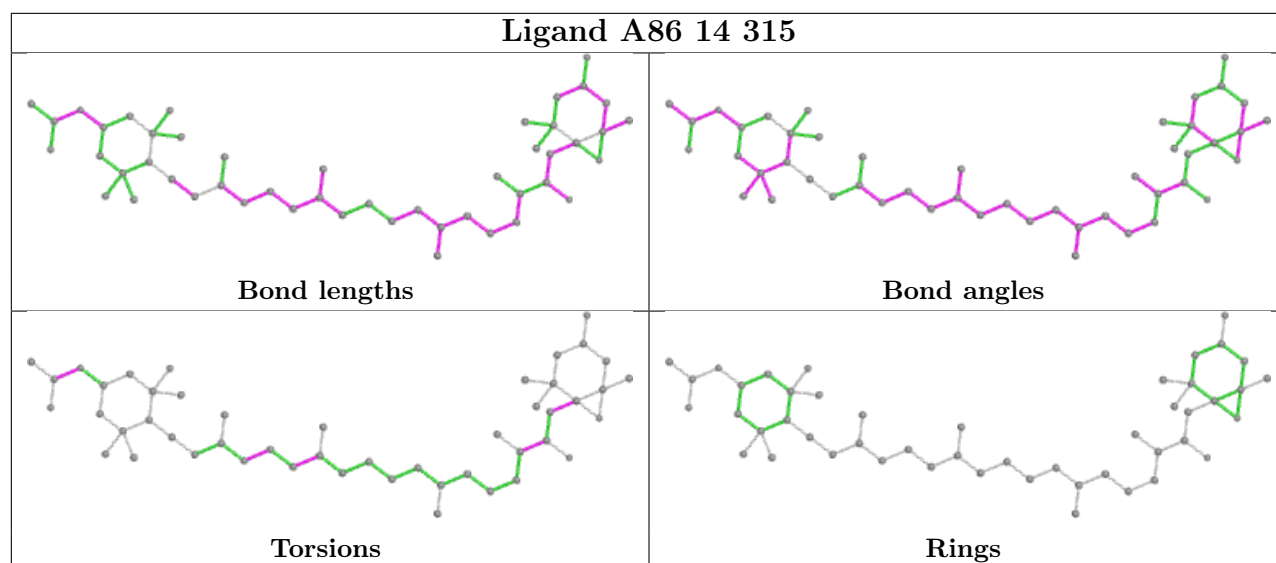
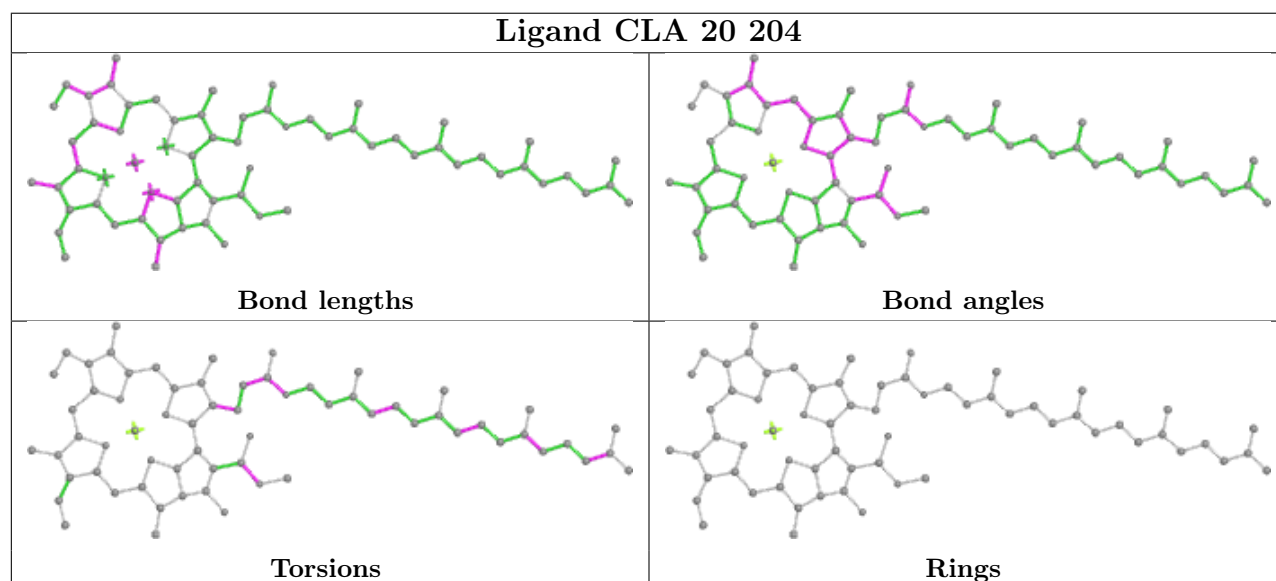
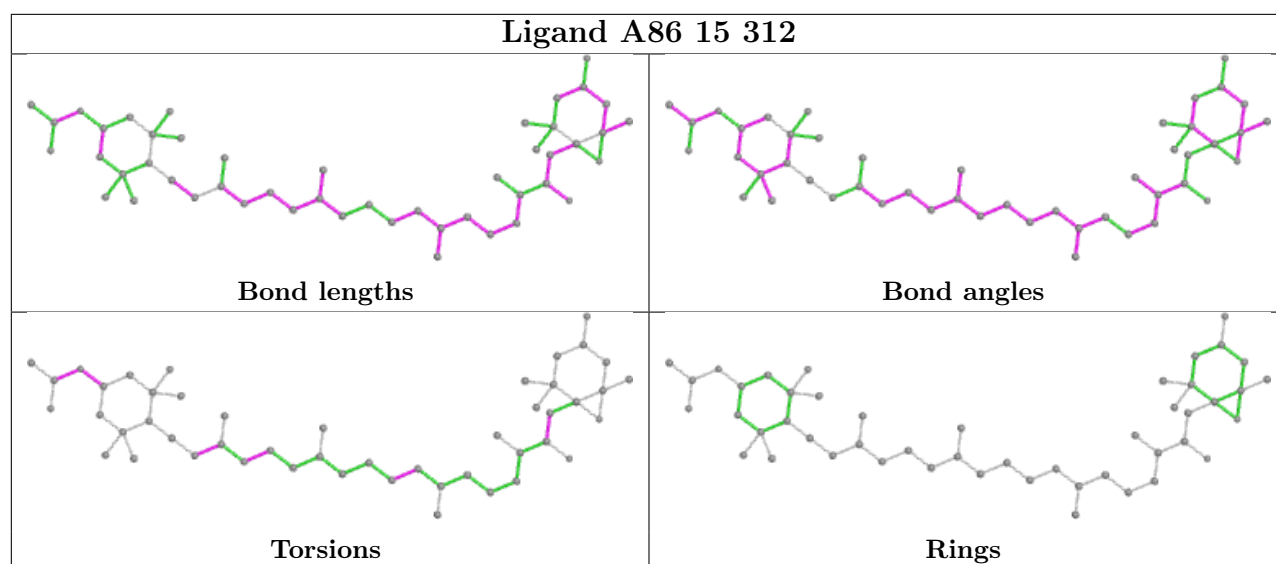


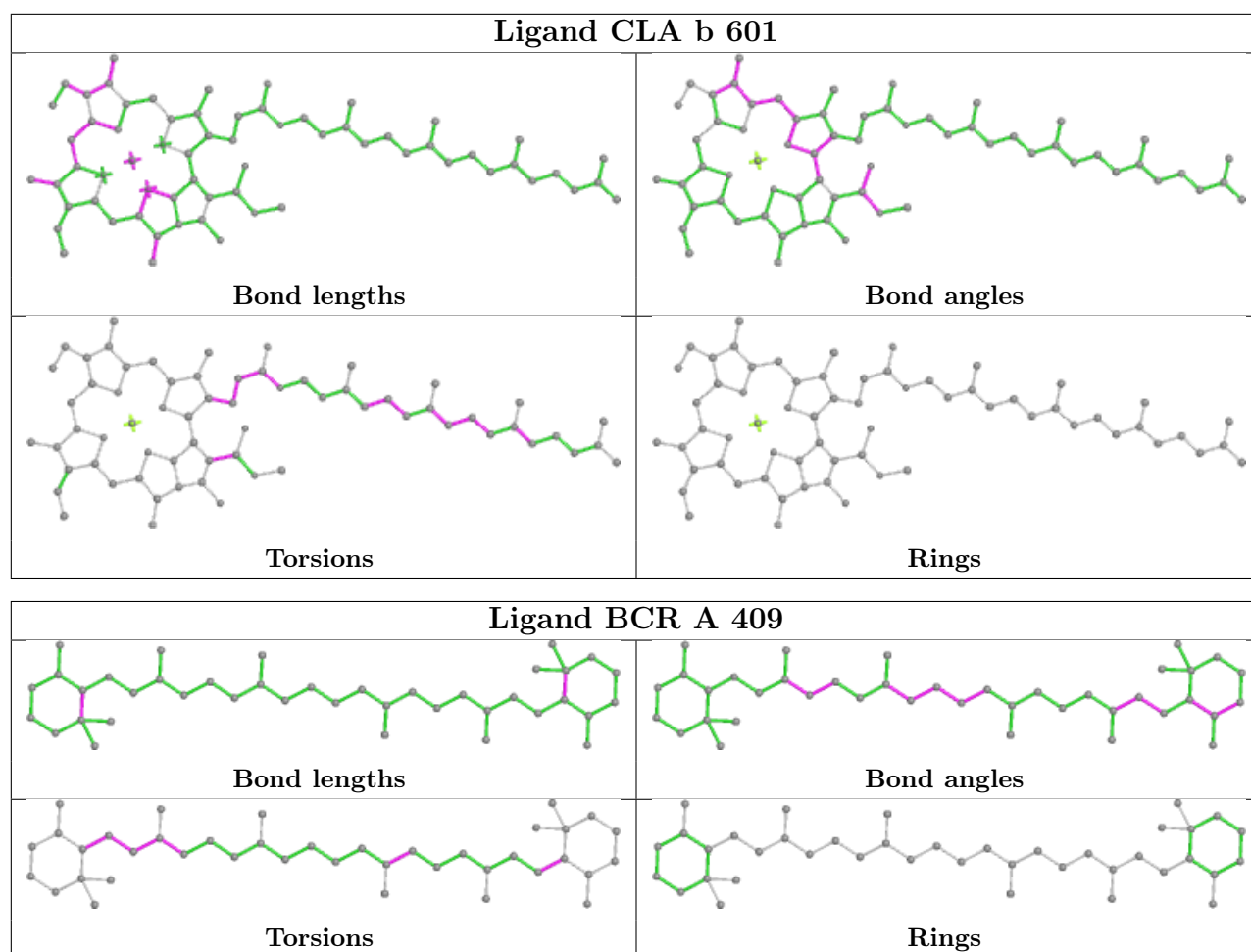


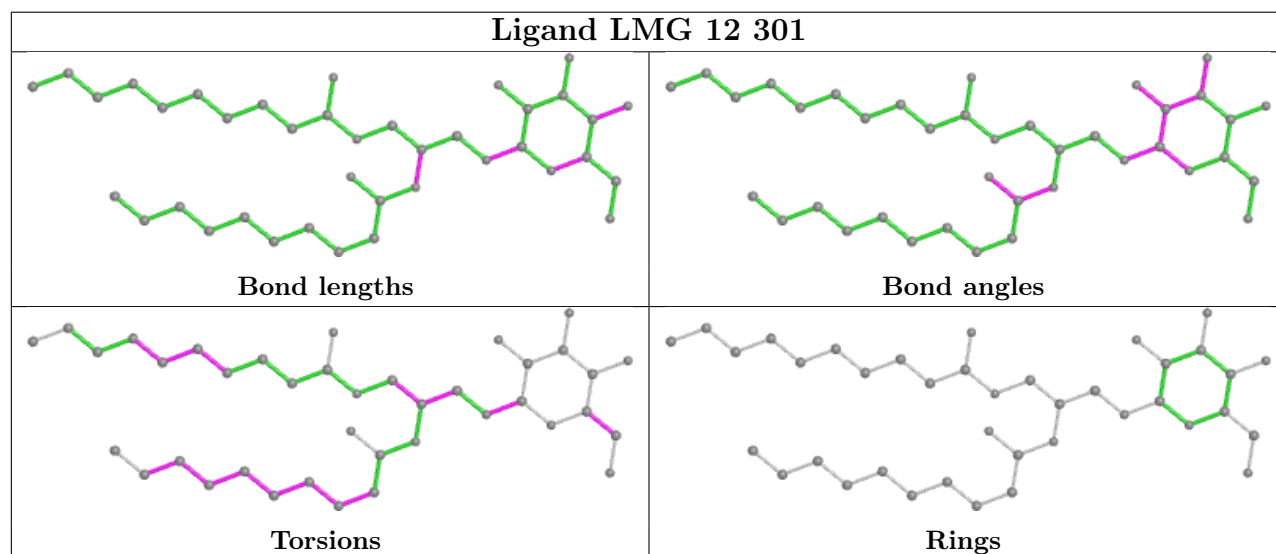
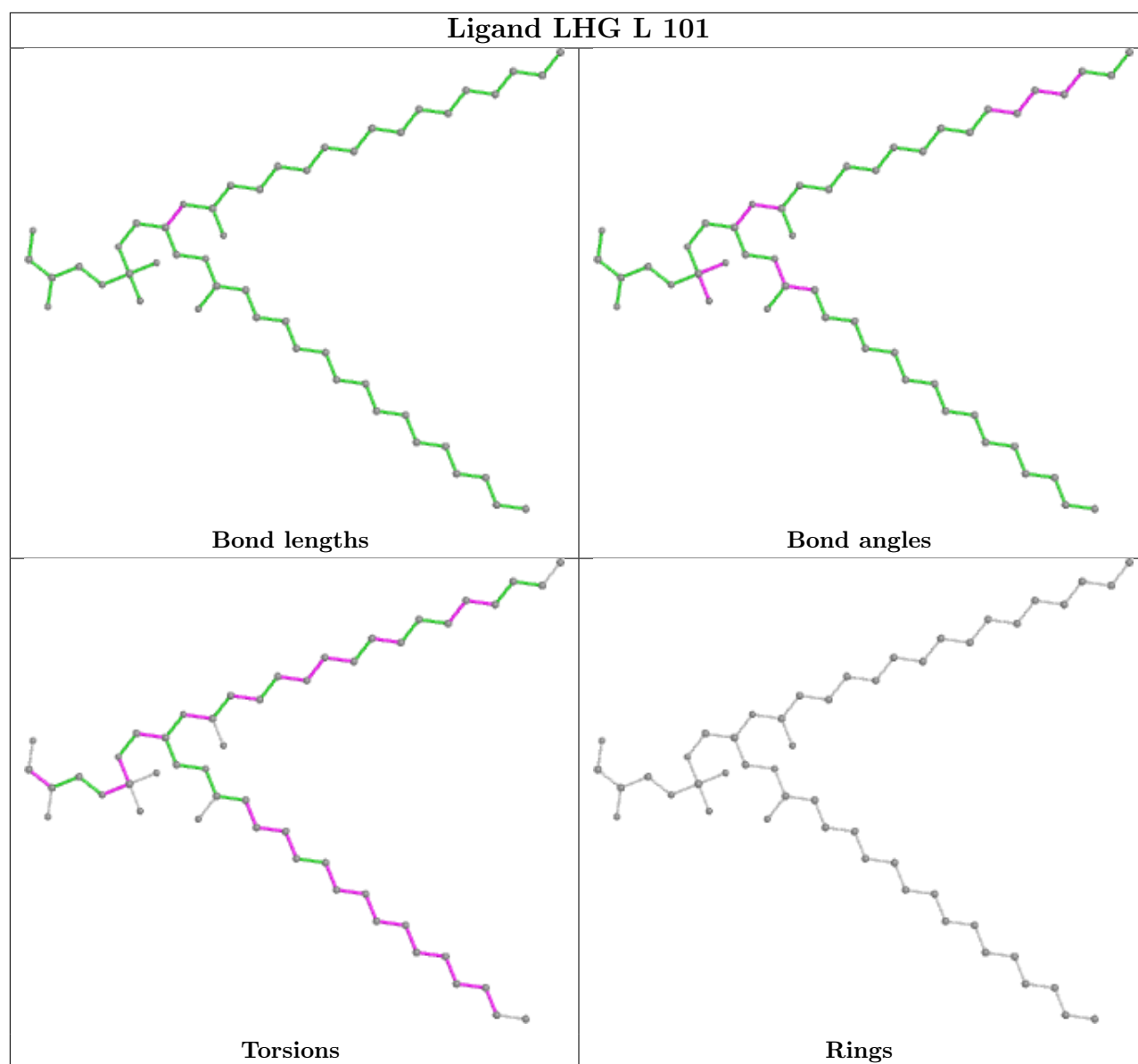


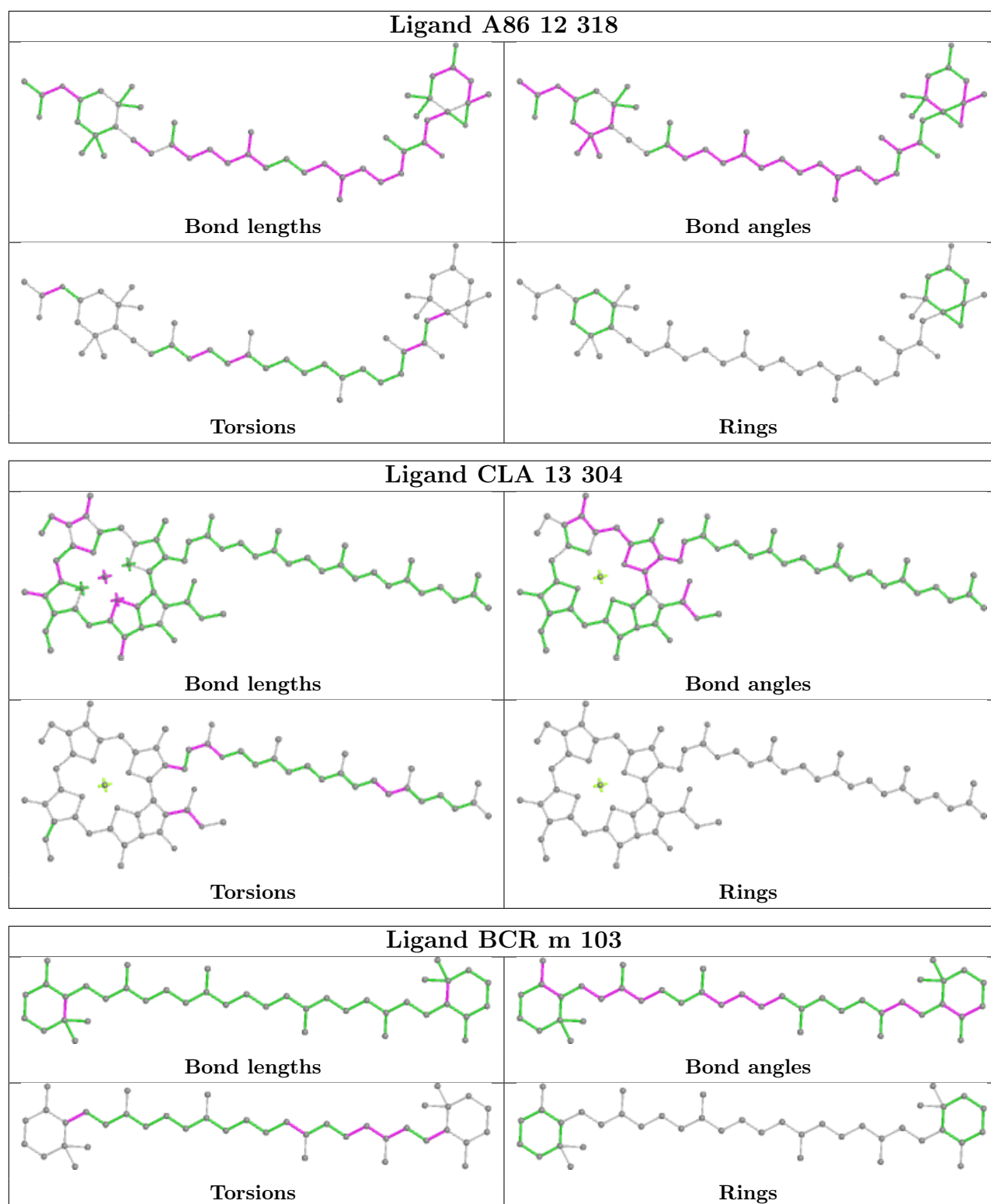


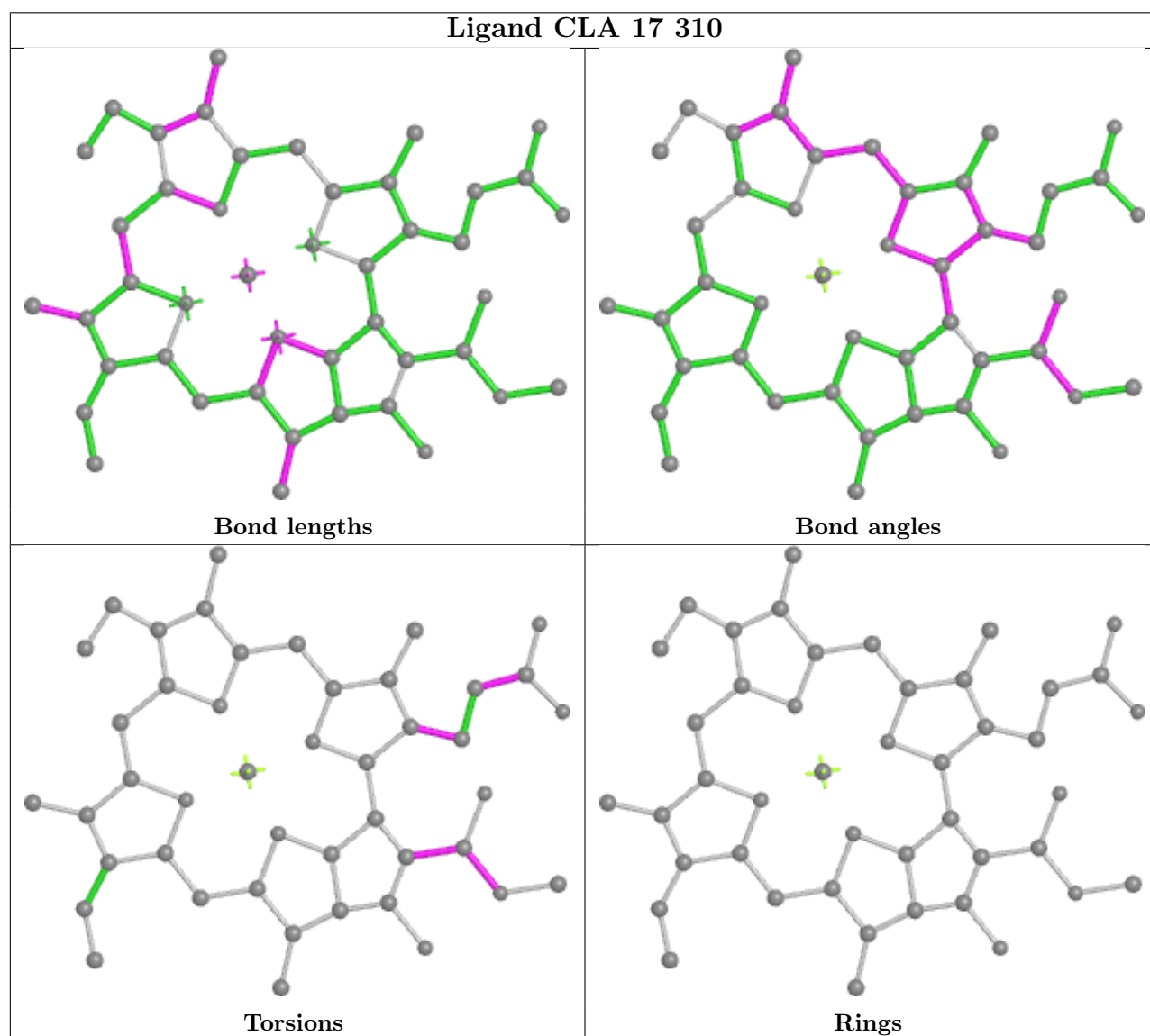
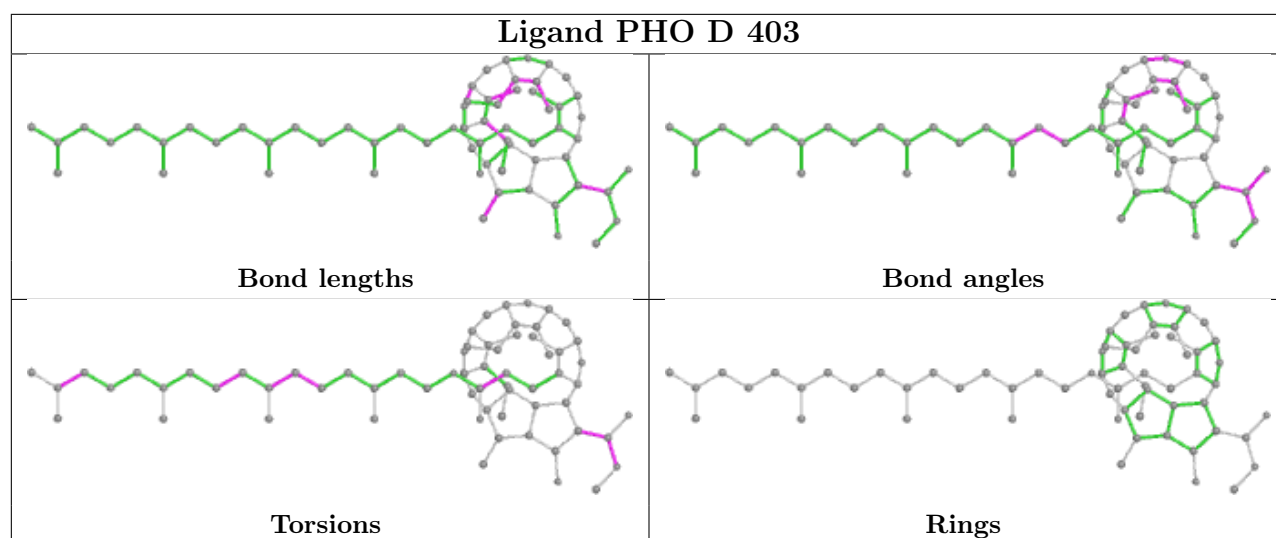


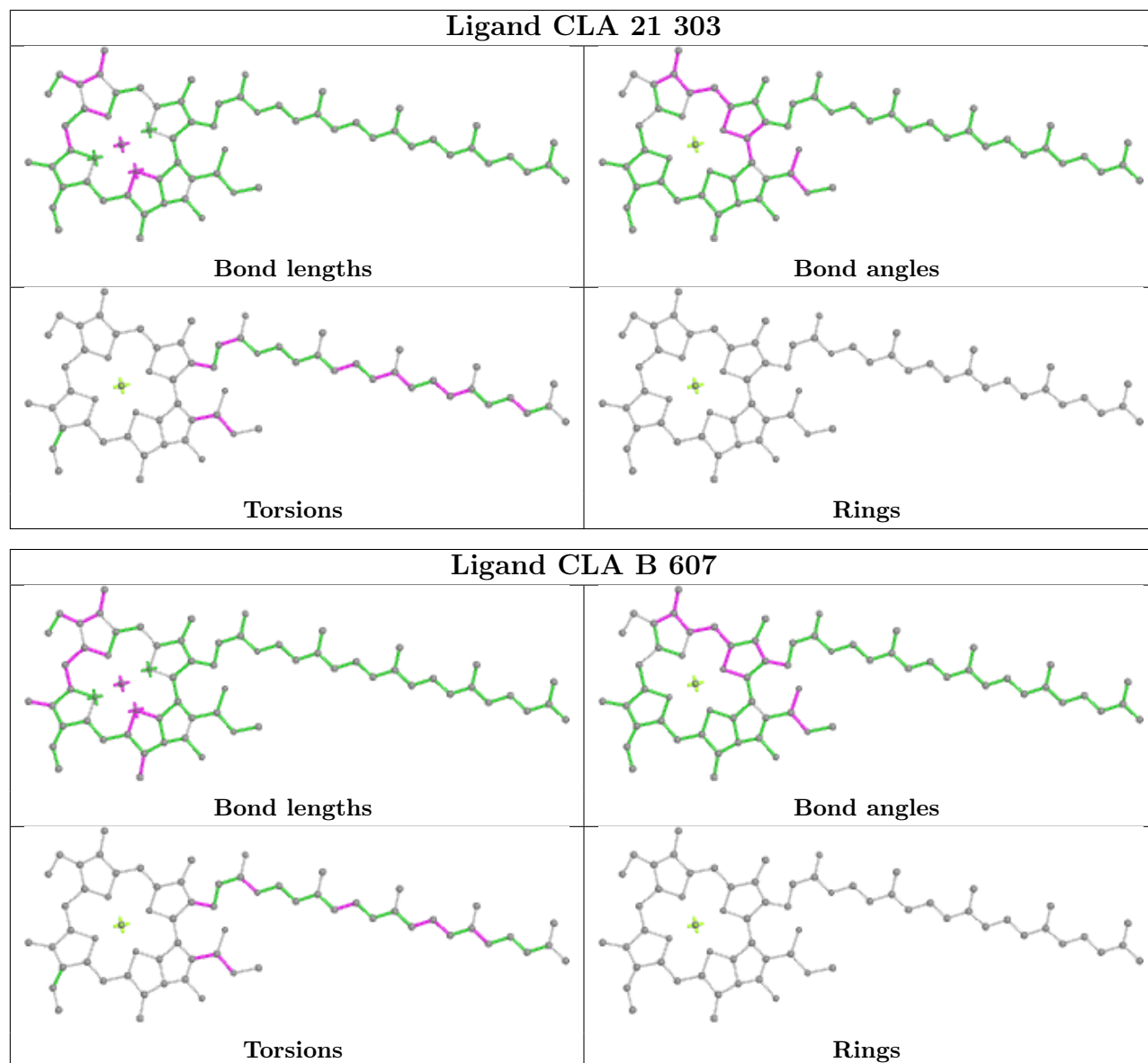


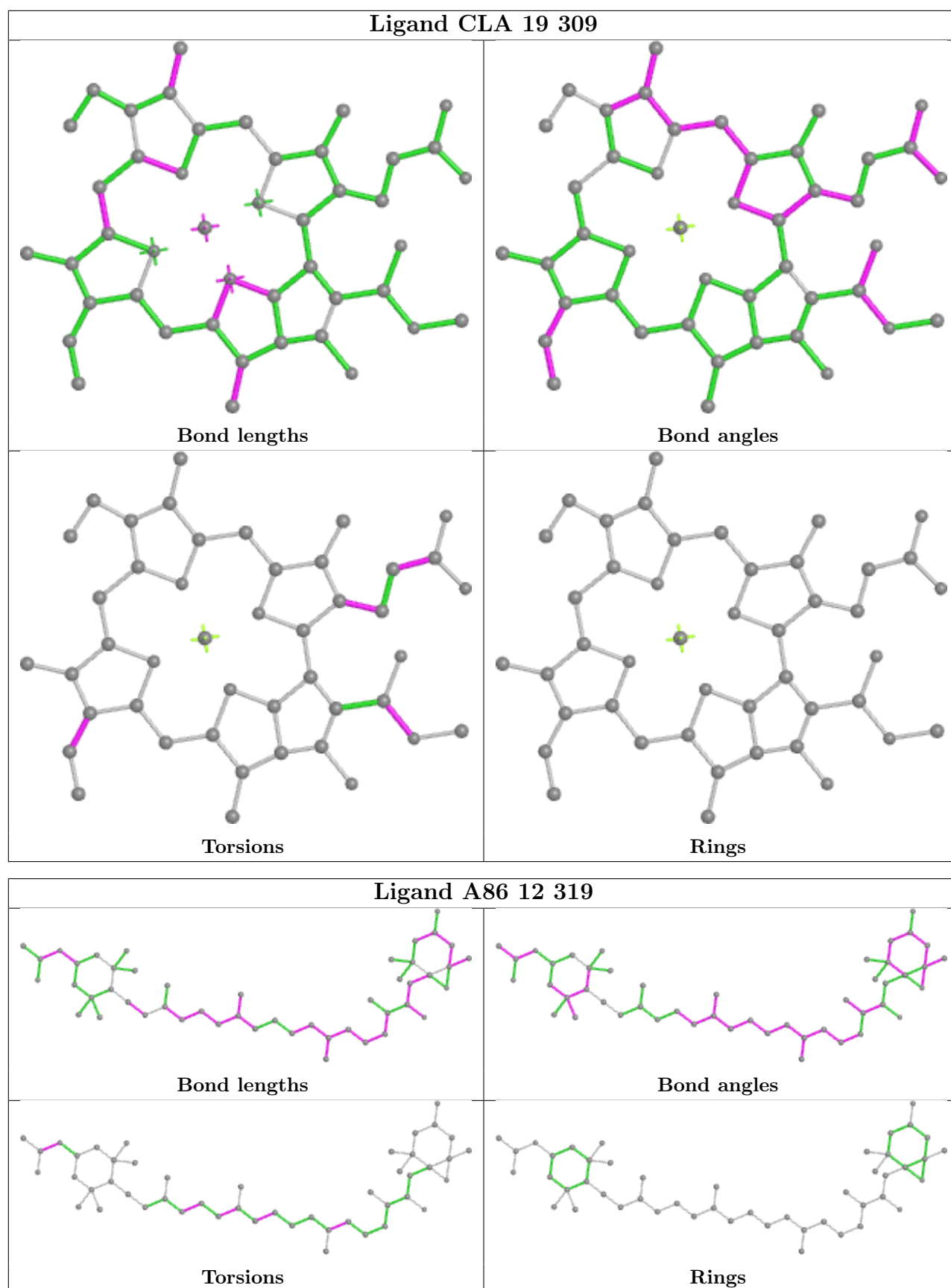


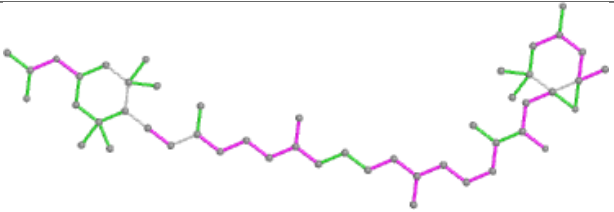
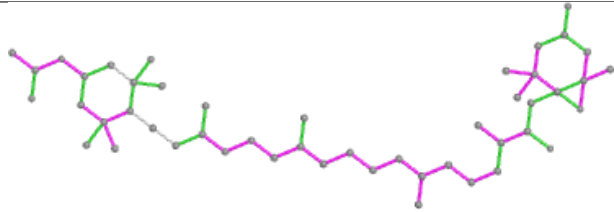
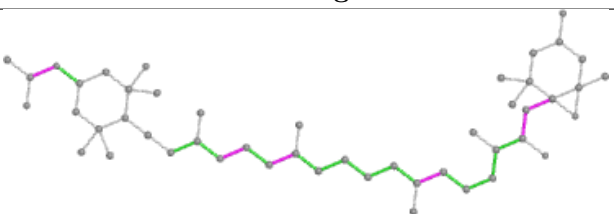
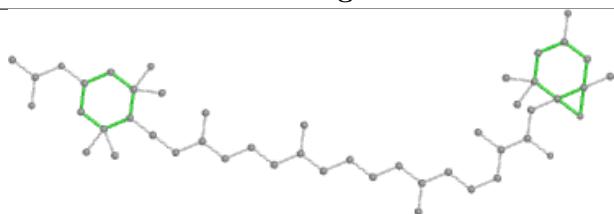


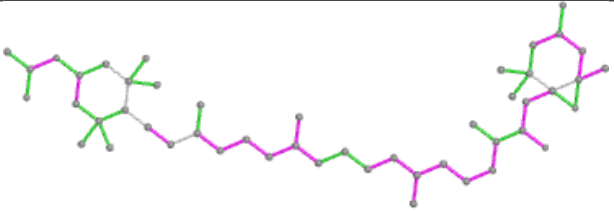
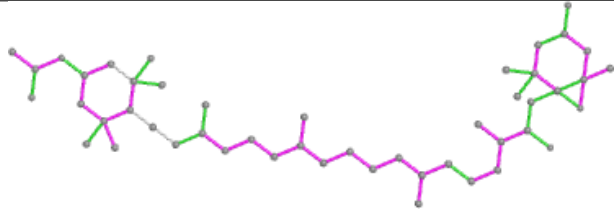
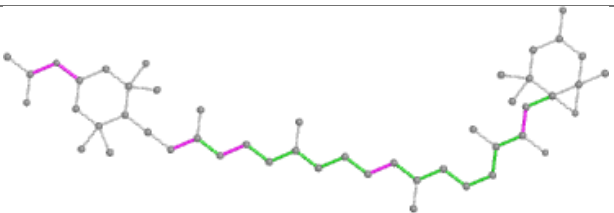
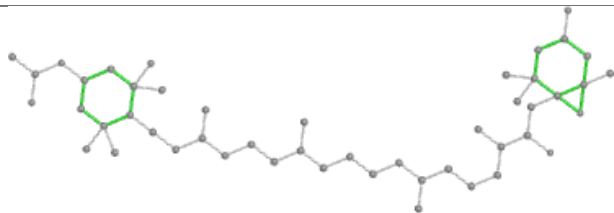


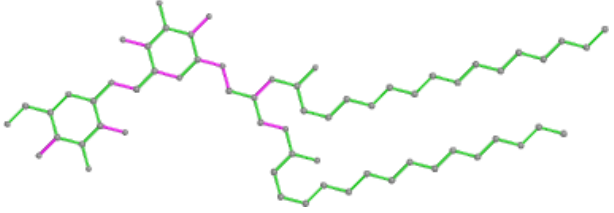
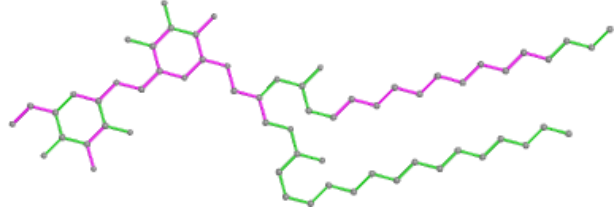
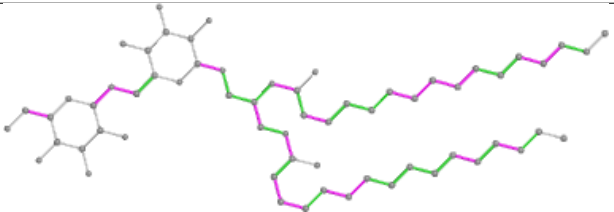
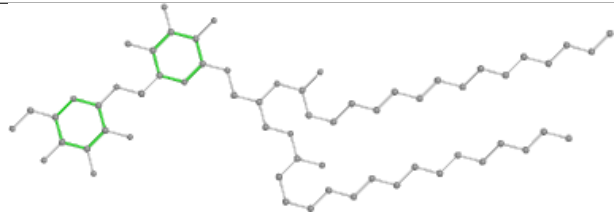


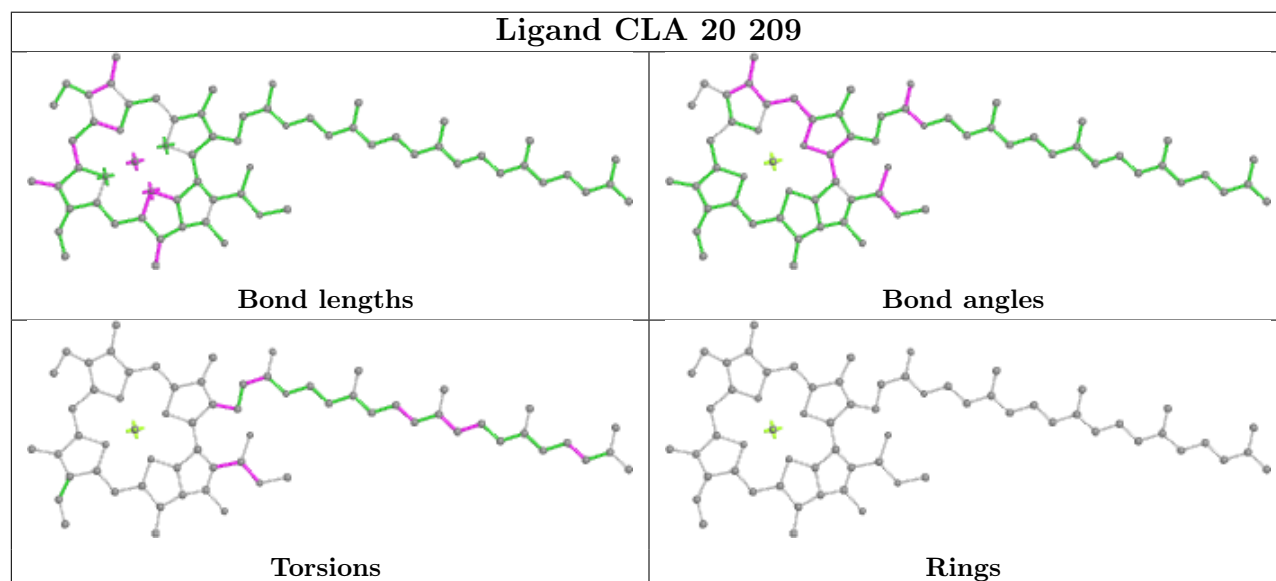
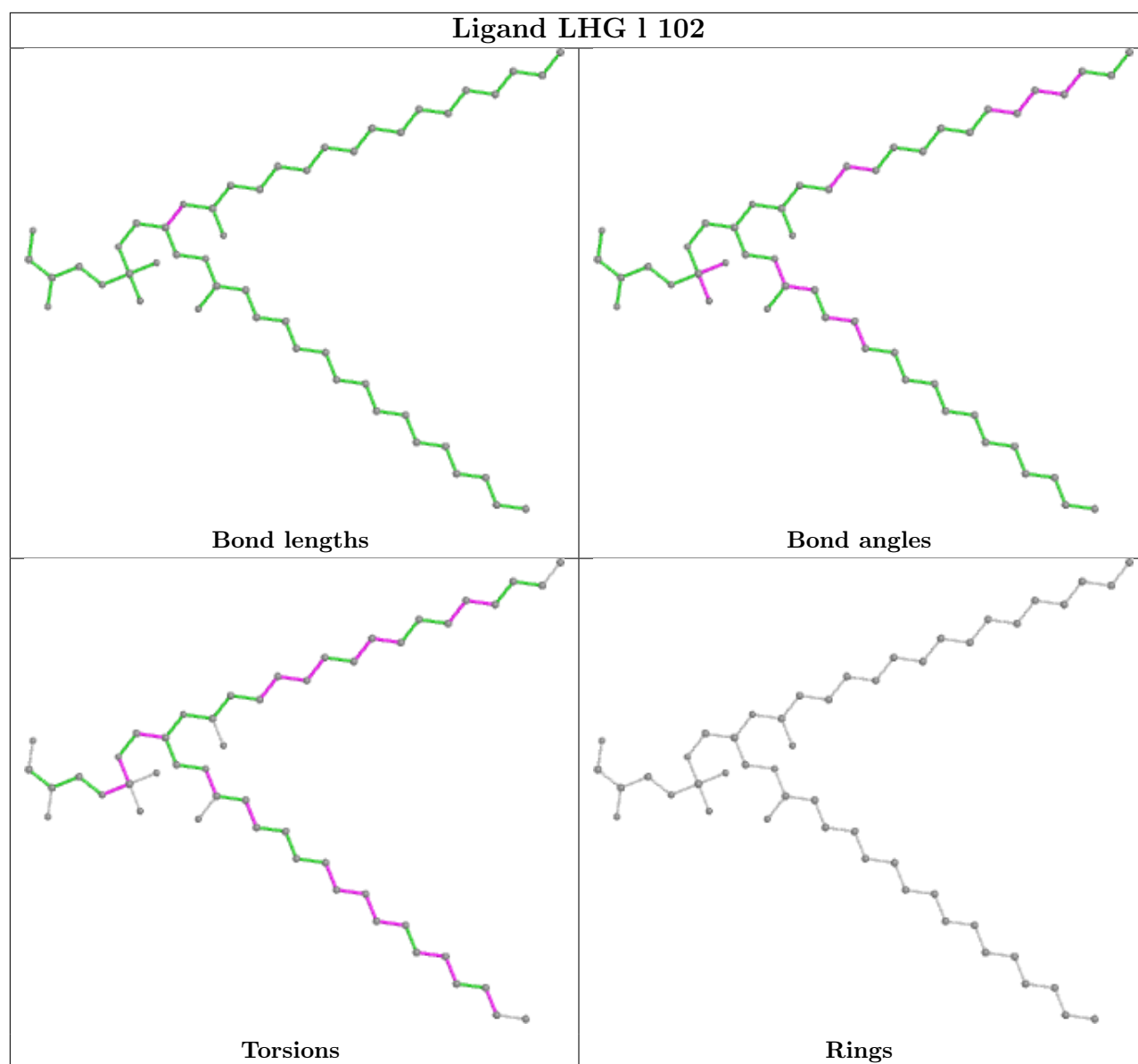


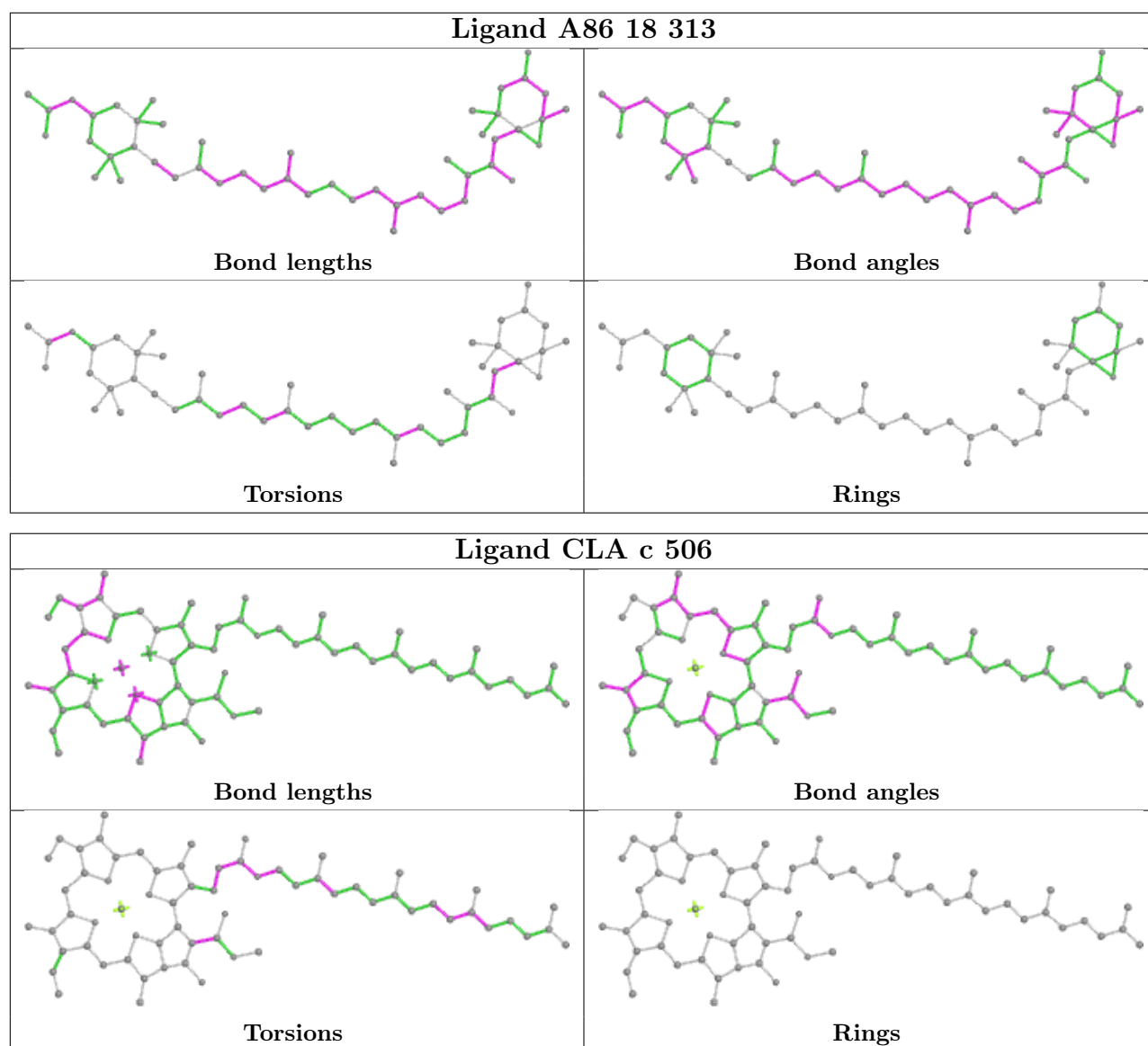


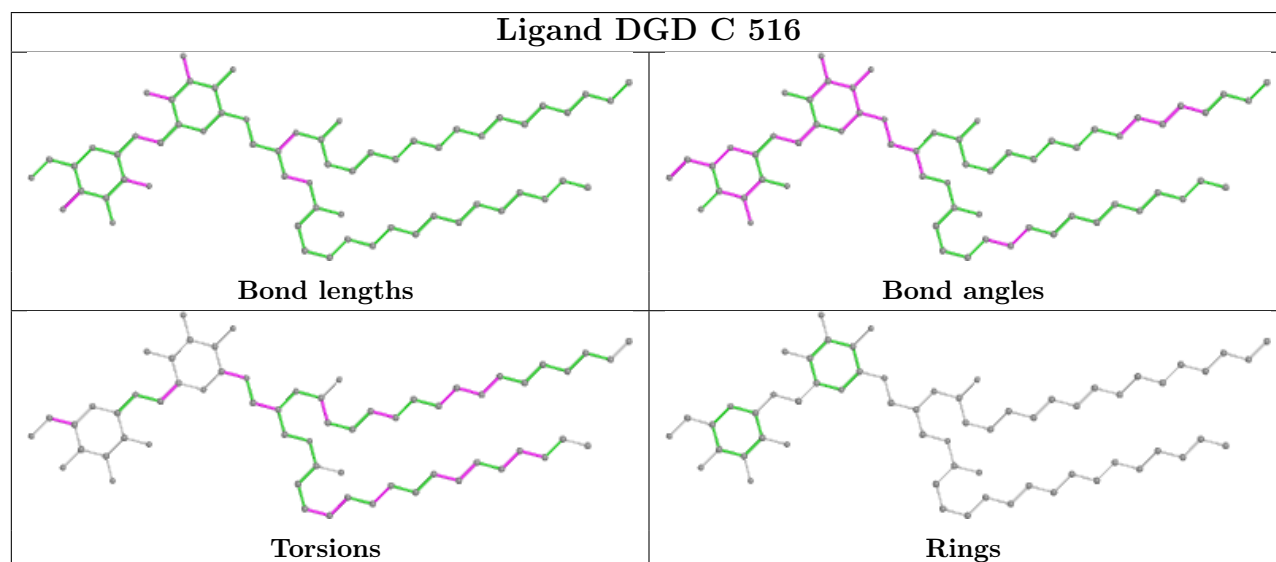
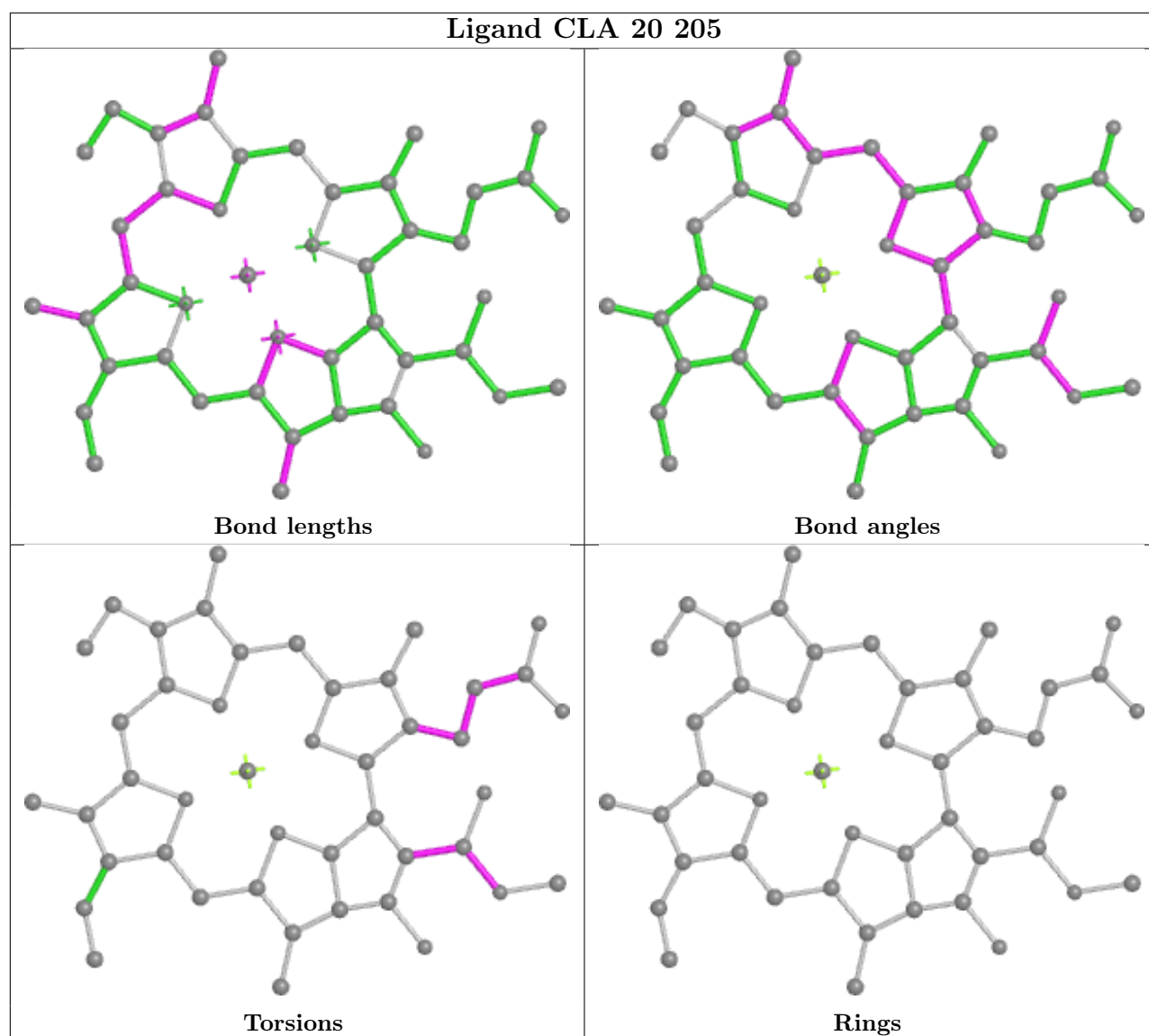
Ligand A86 15 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

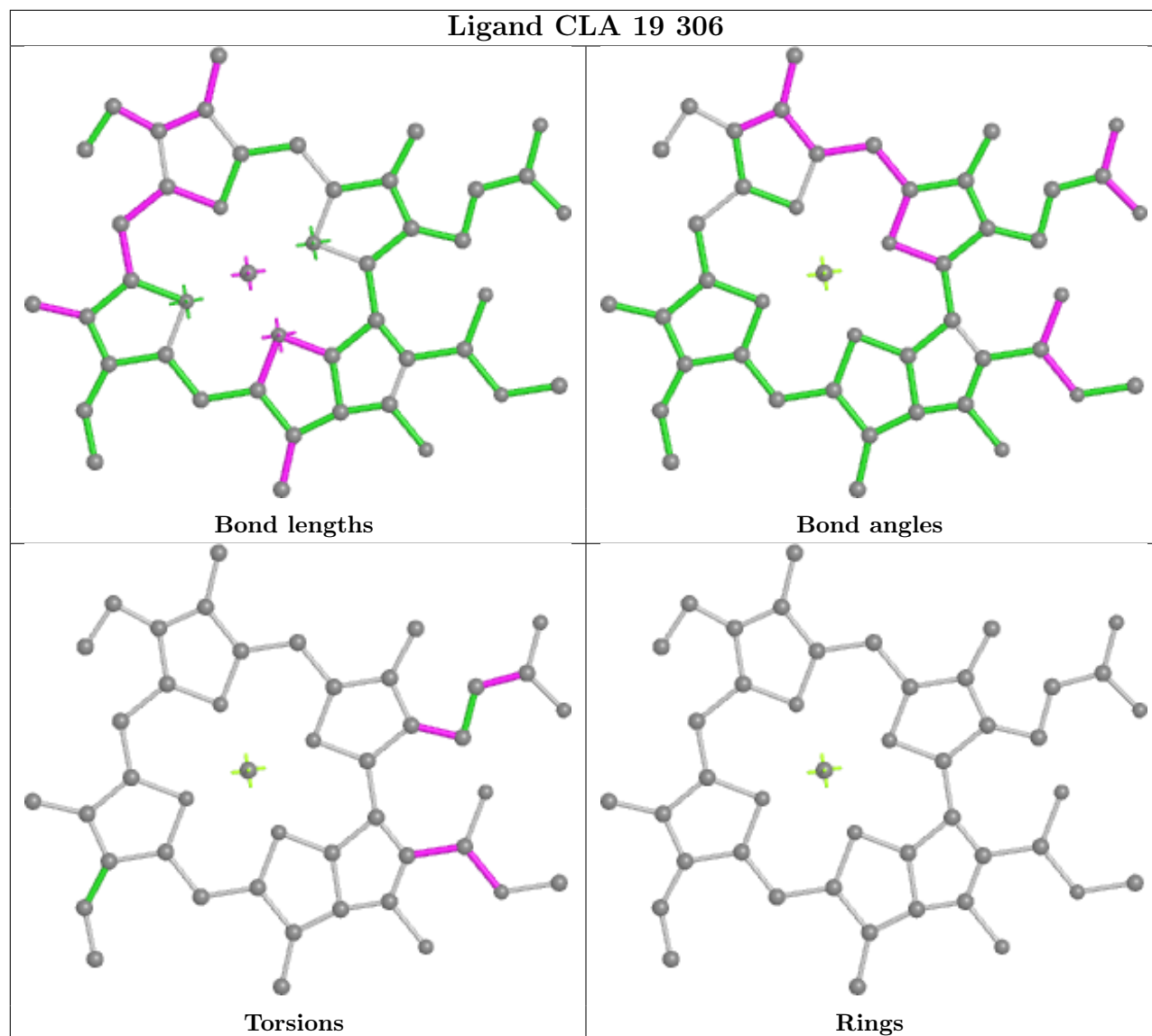
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Bond lengths	Bond angles
	
Torsions	Rings

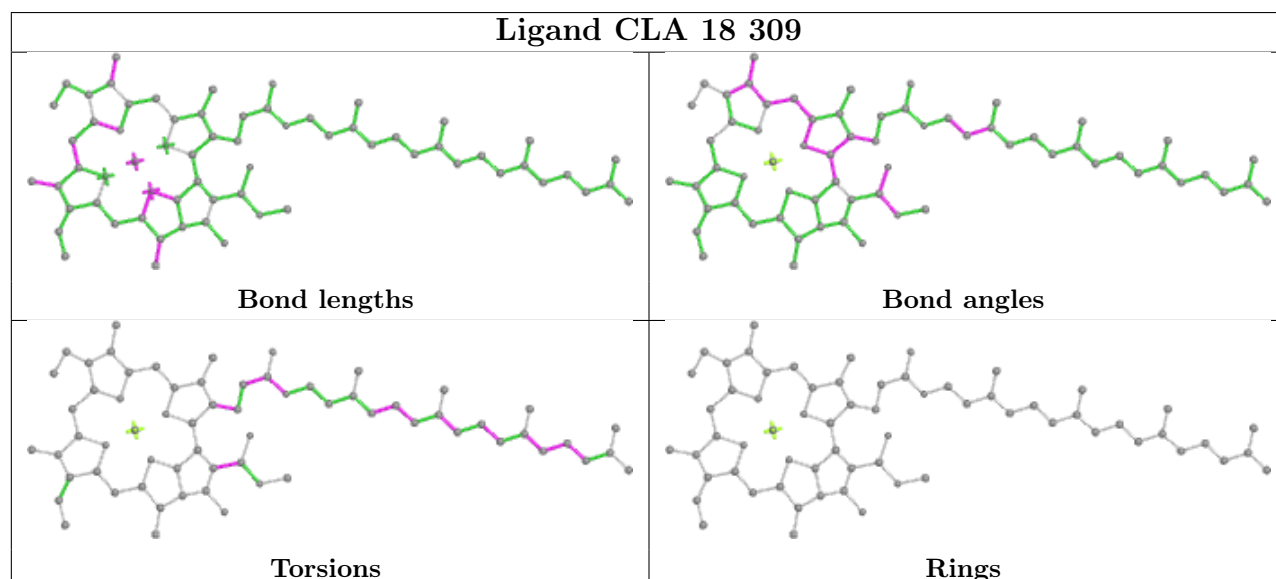
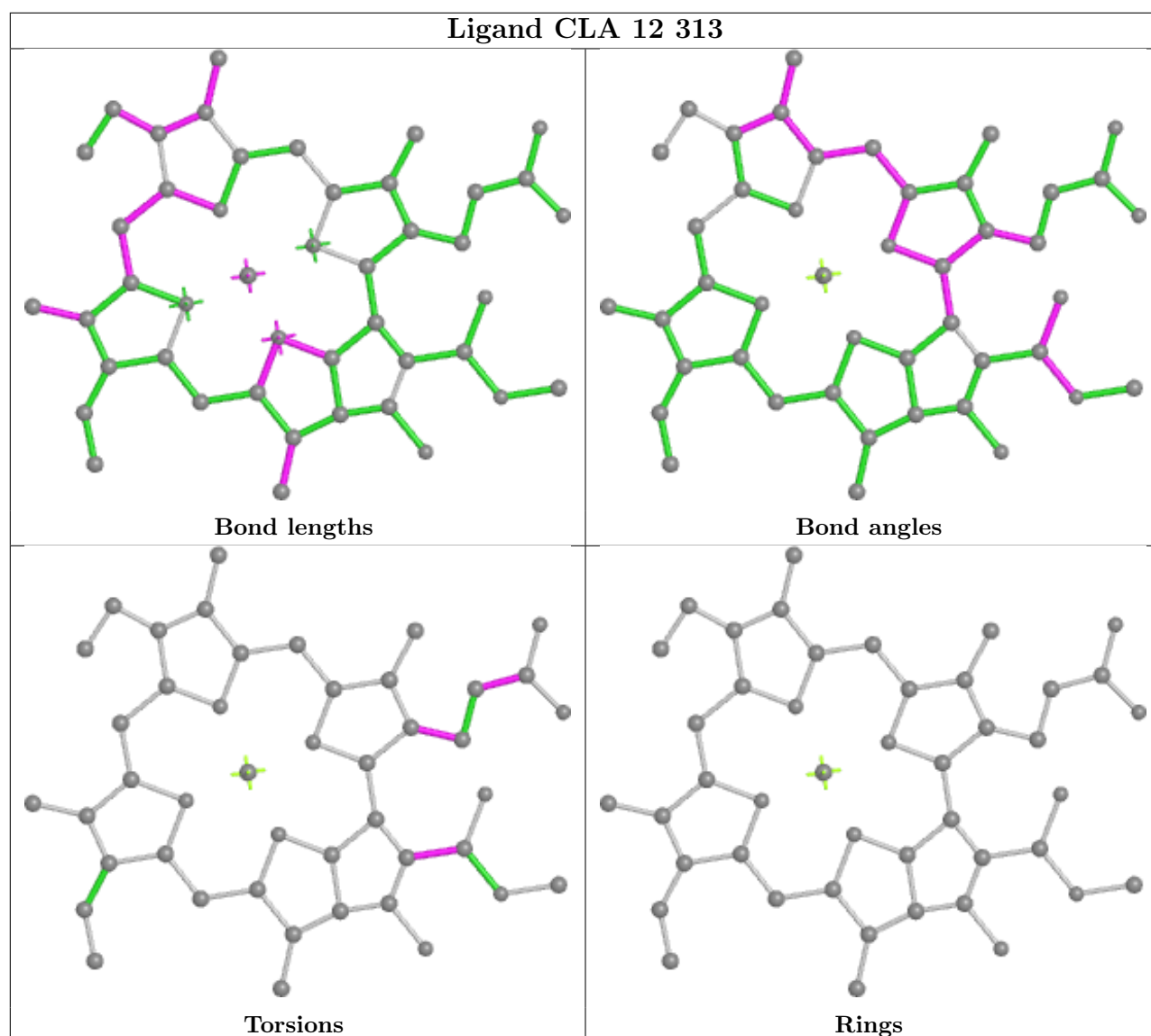
Ligand DGD C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

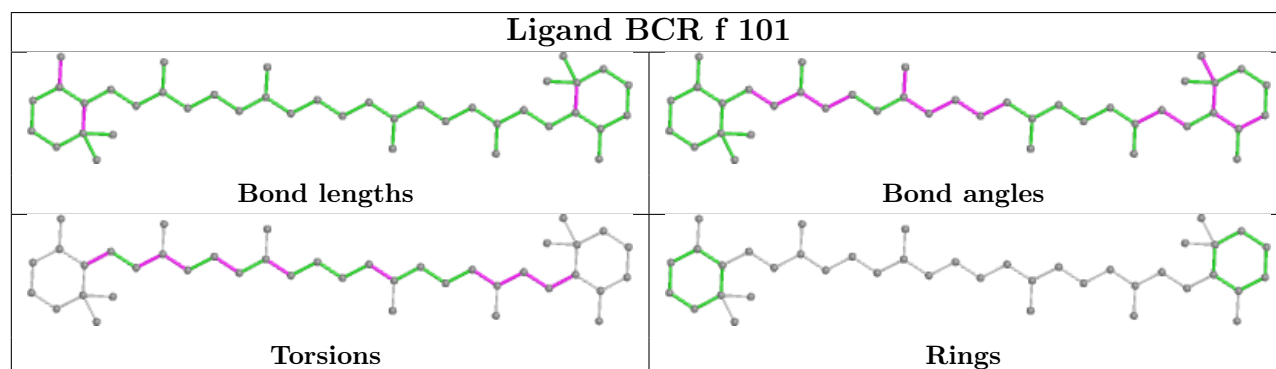
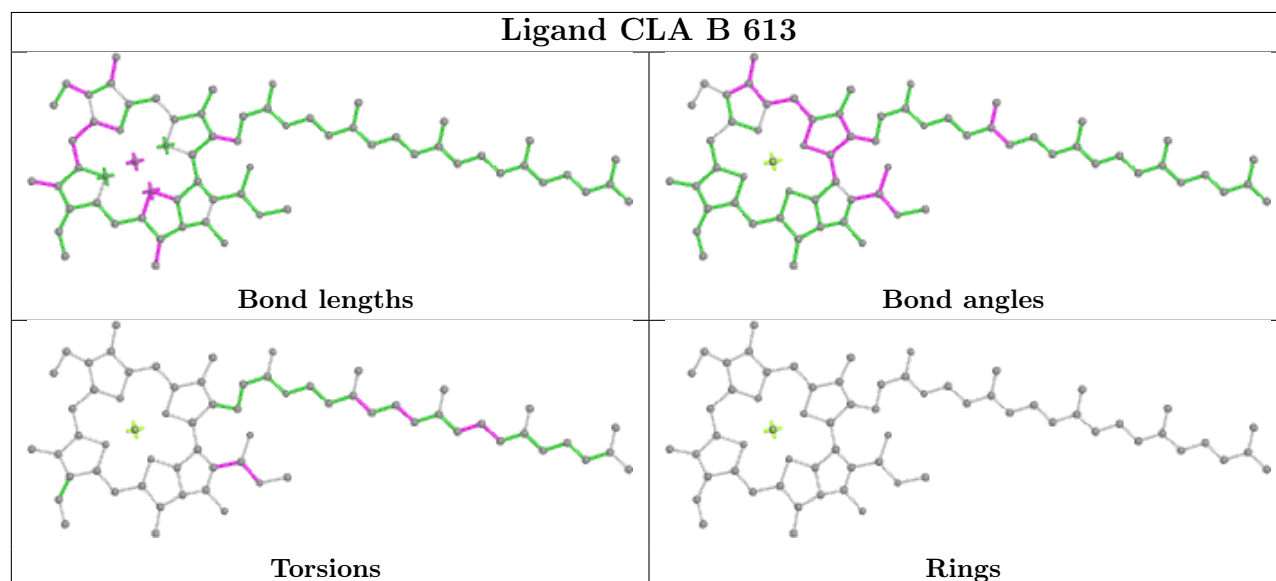
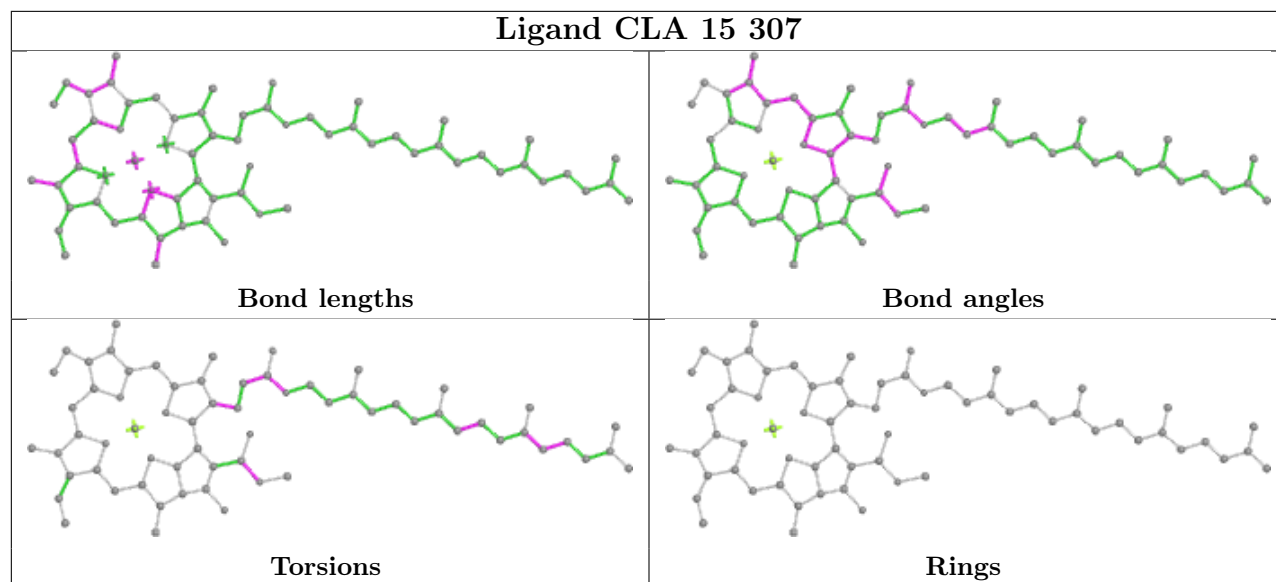


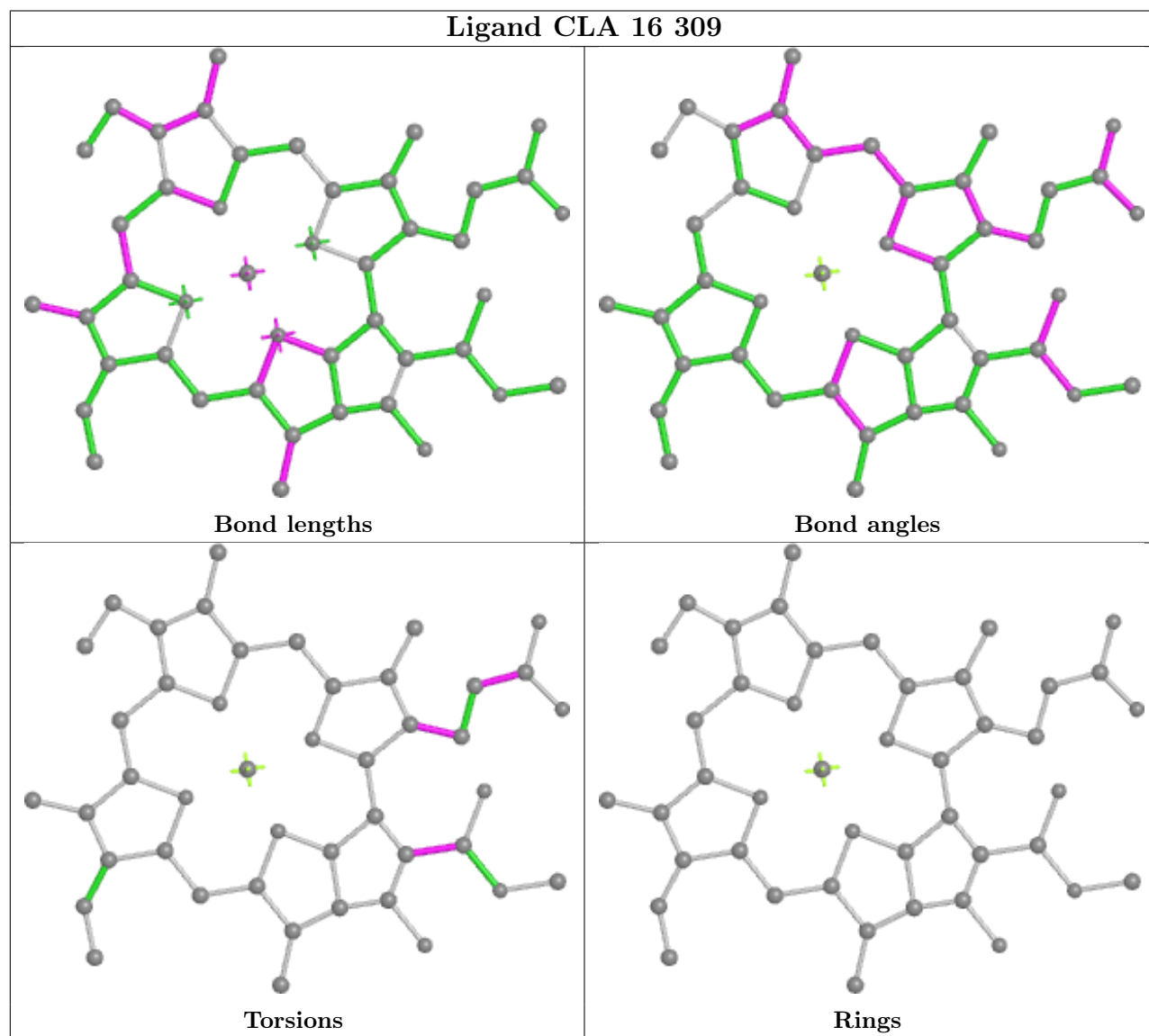
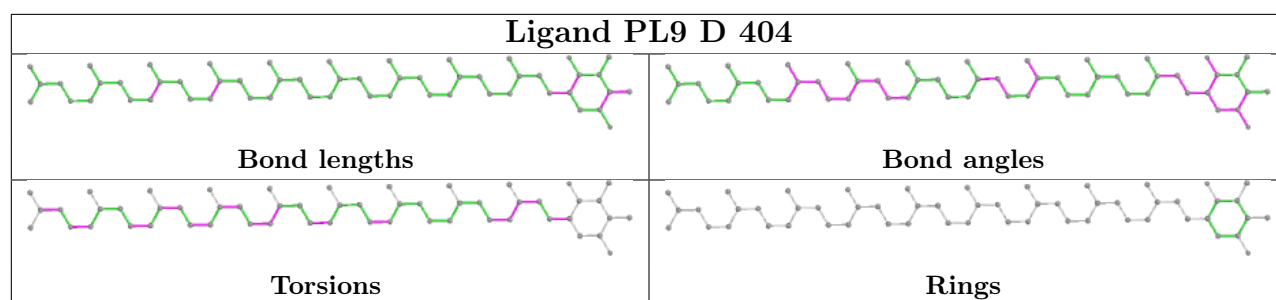


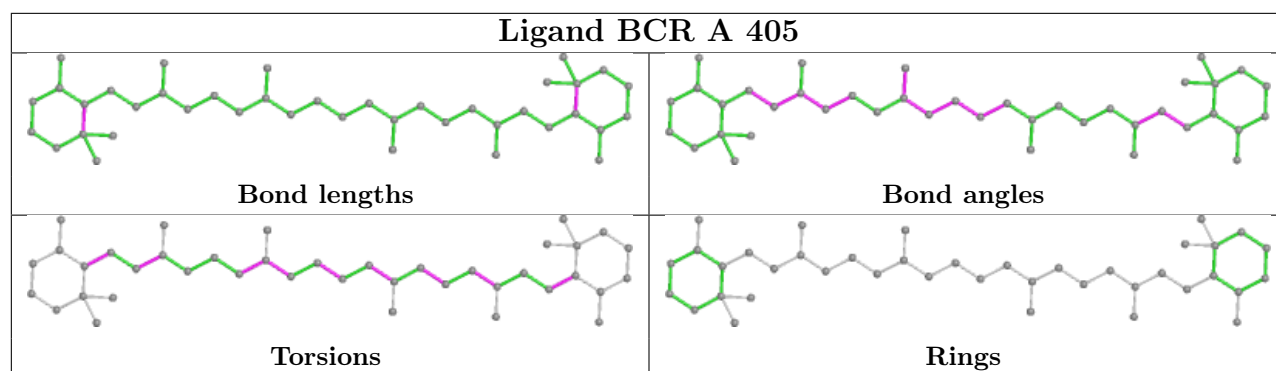
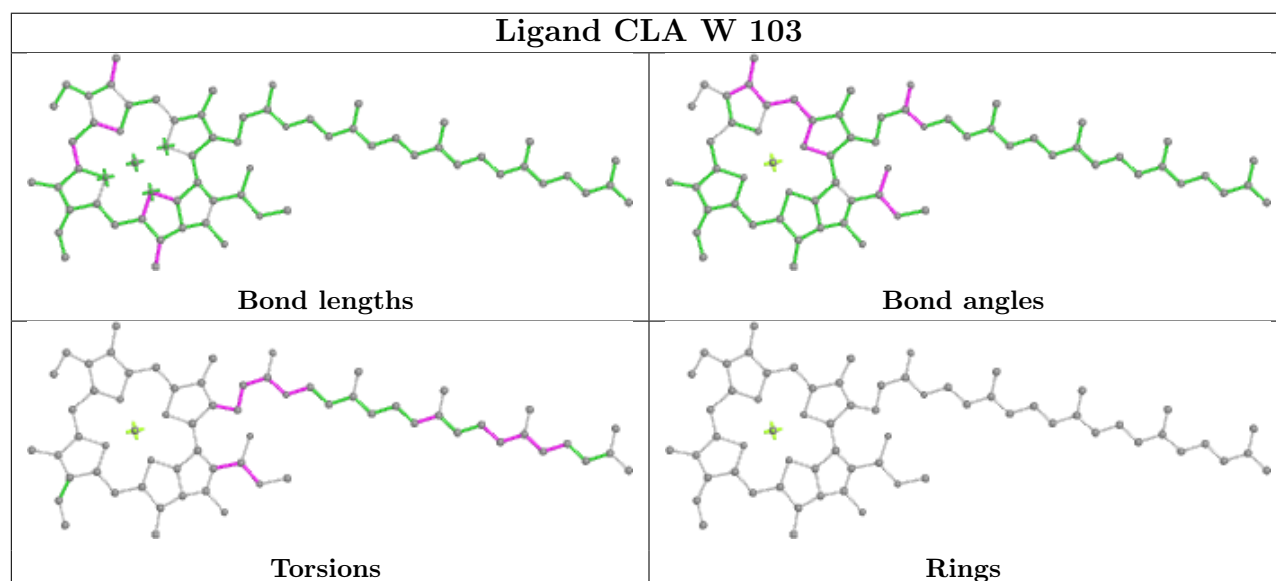
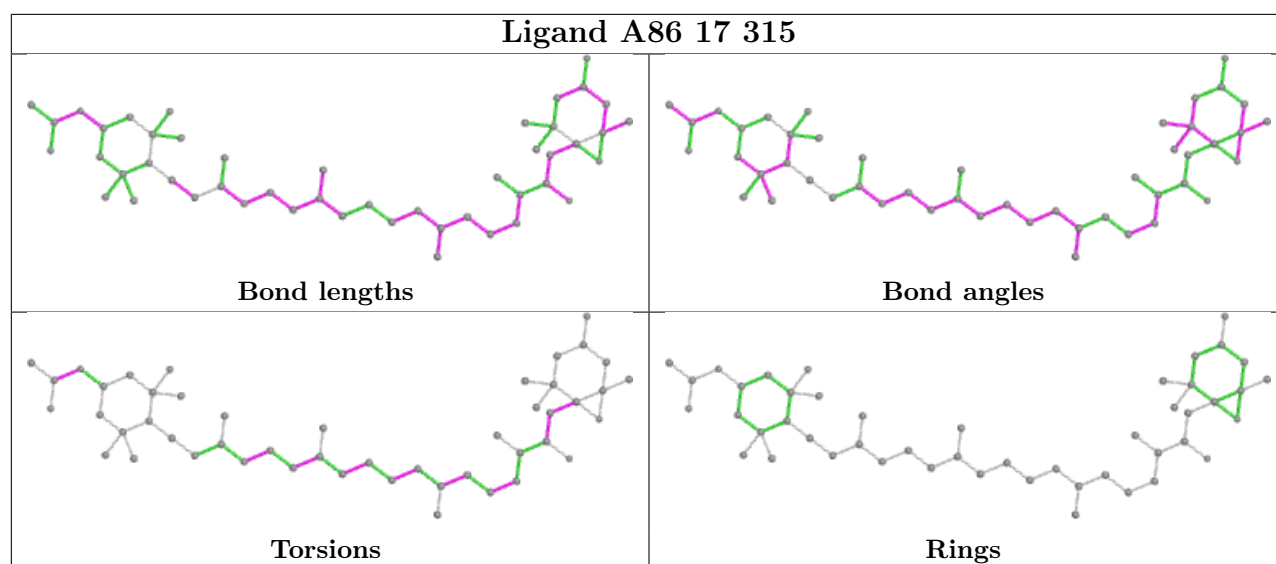


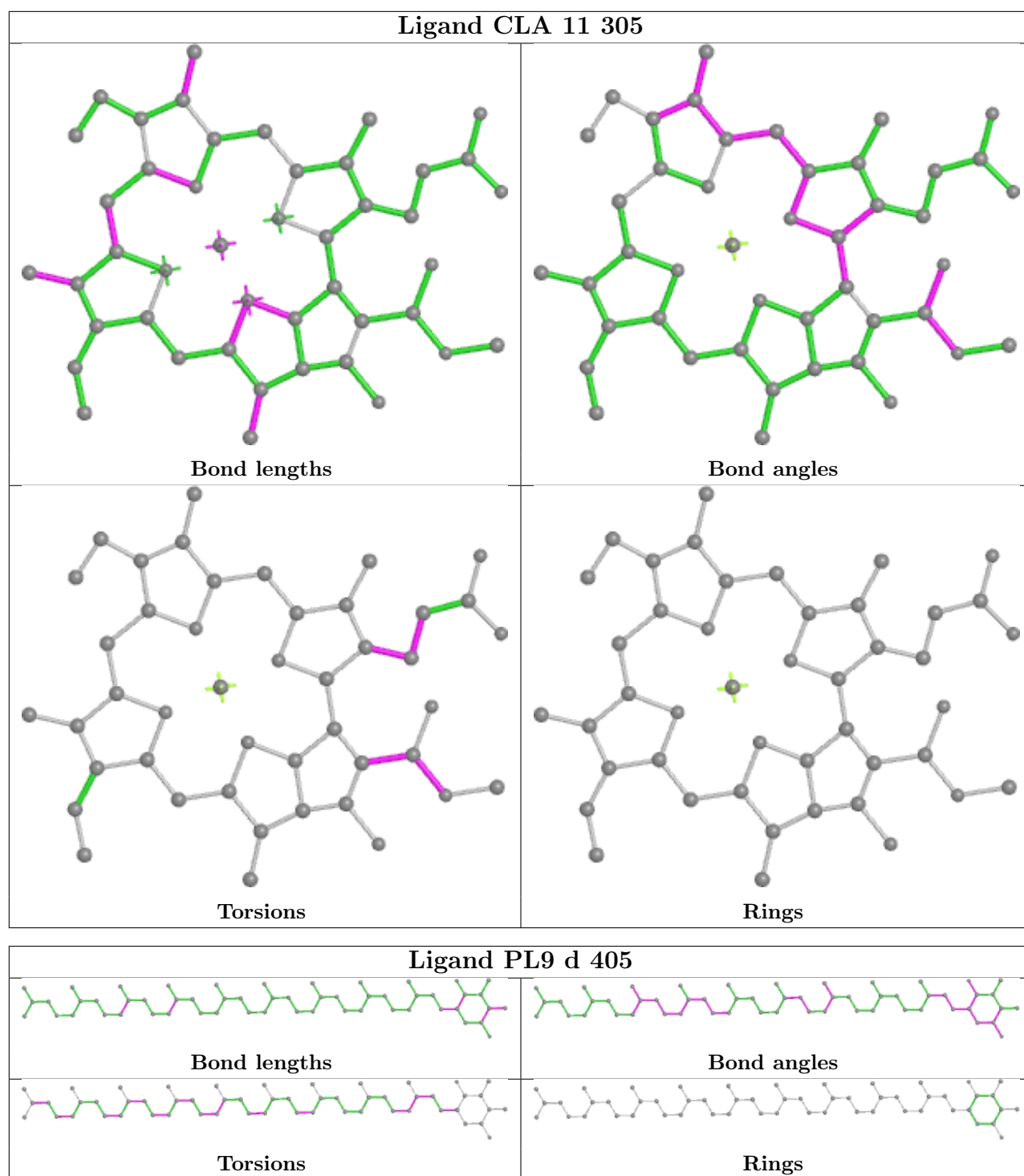


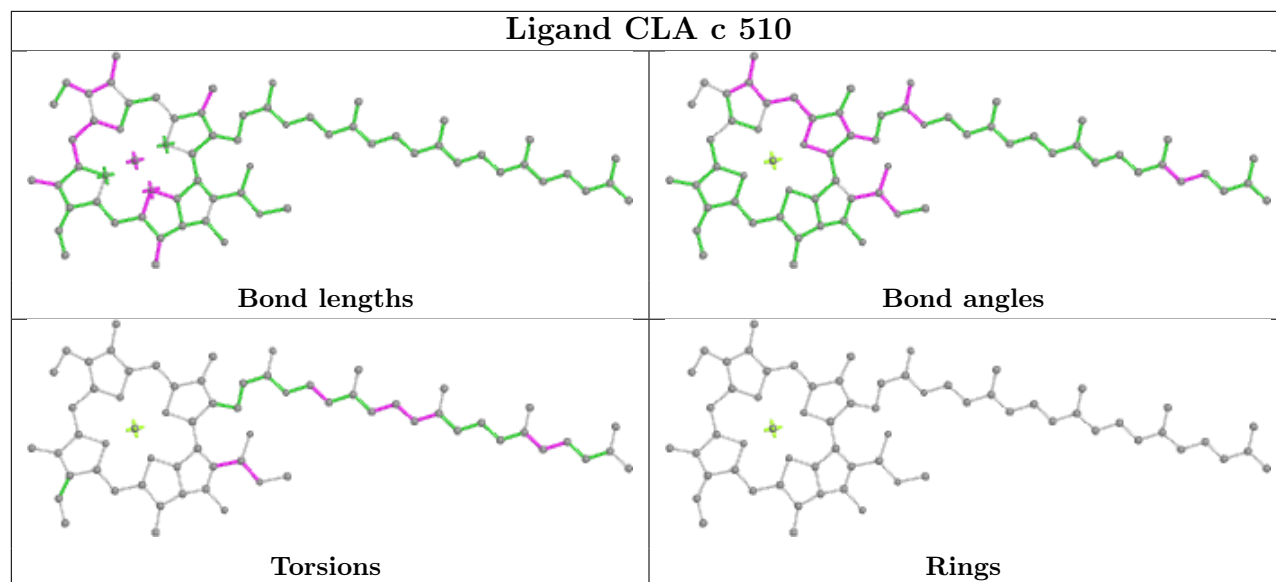
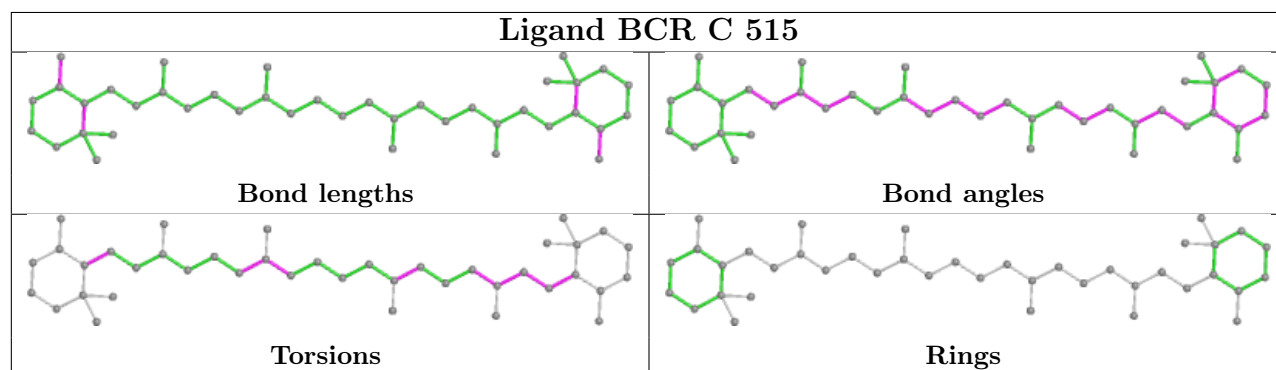
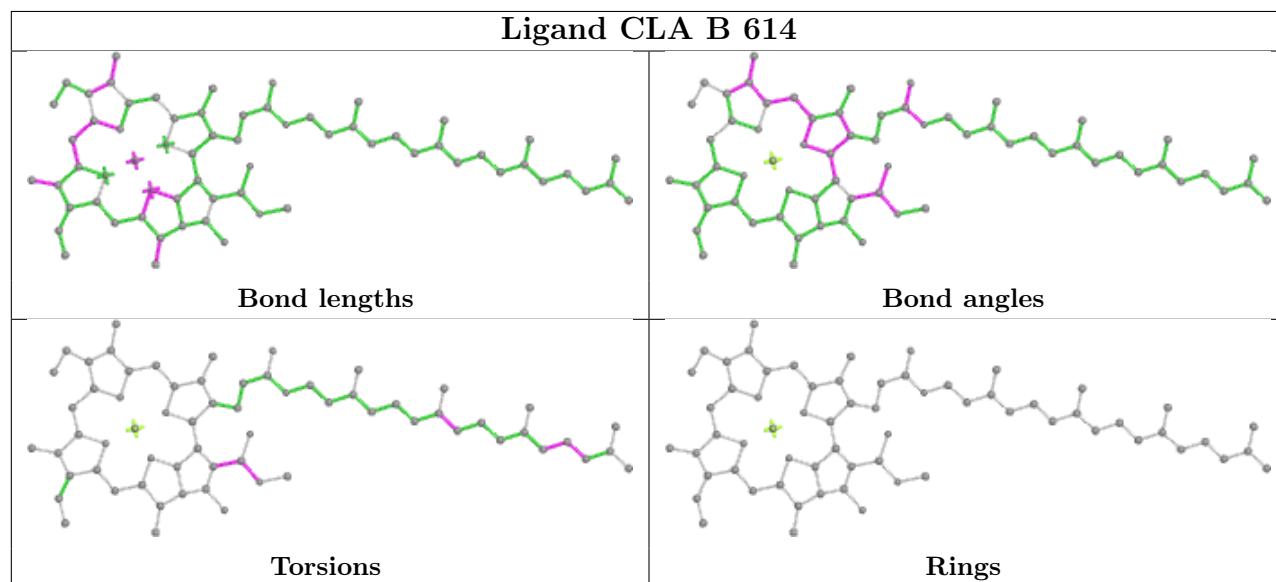


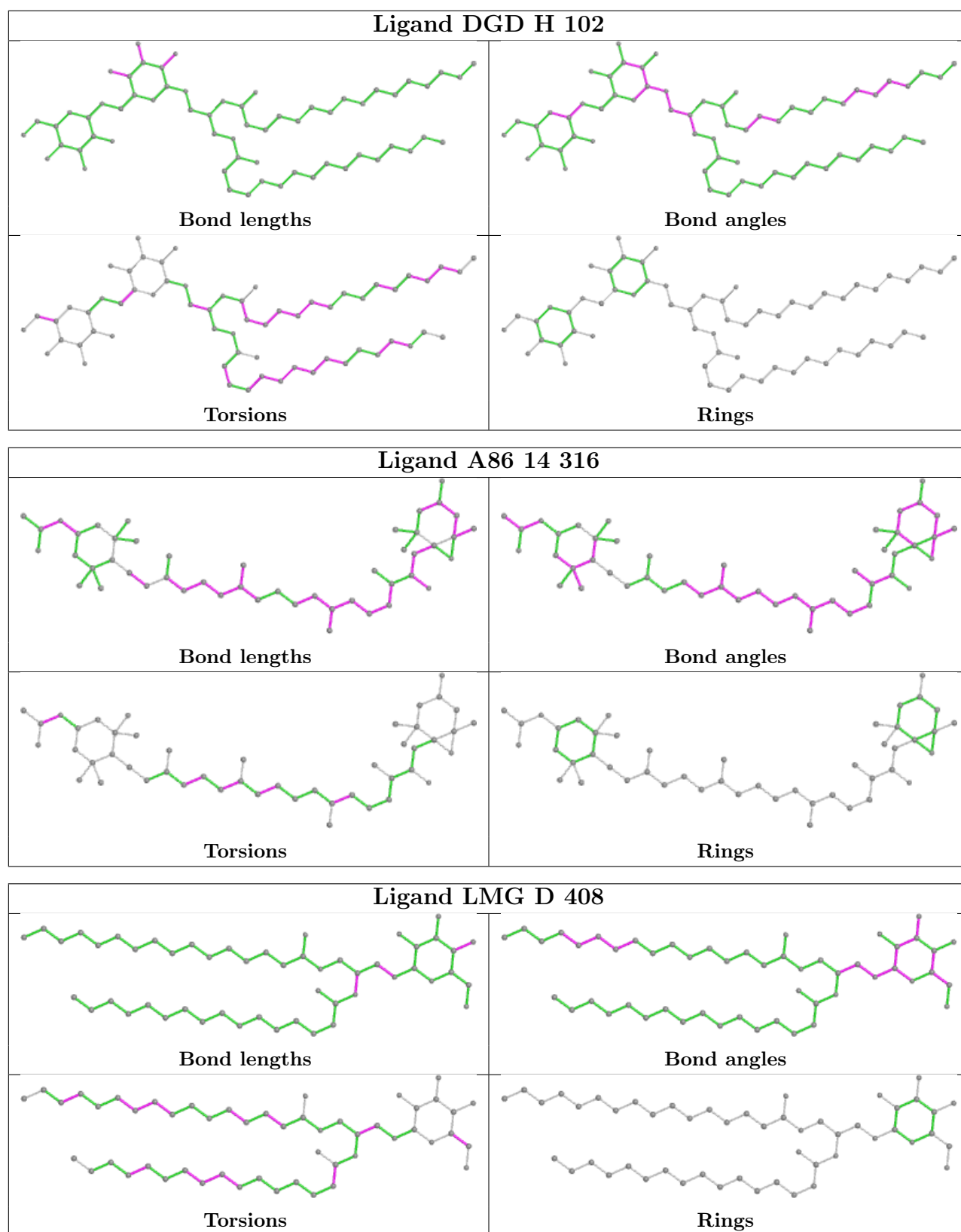




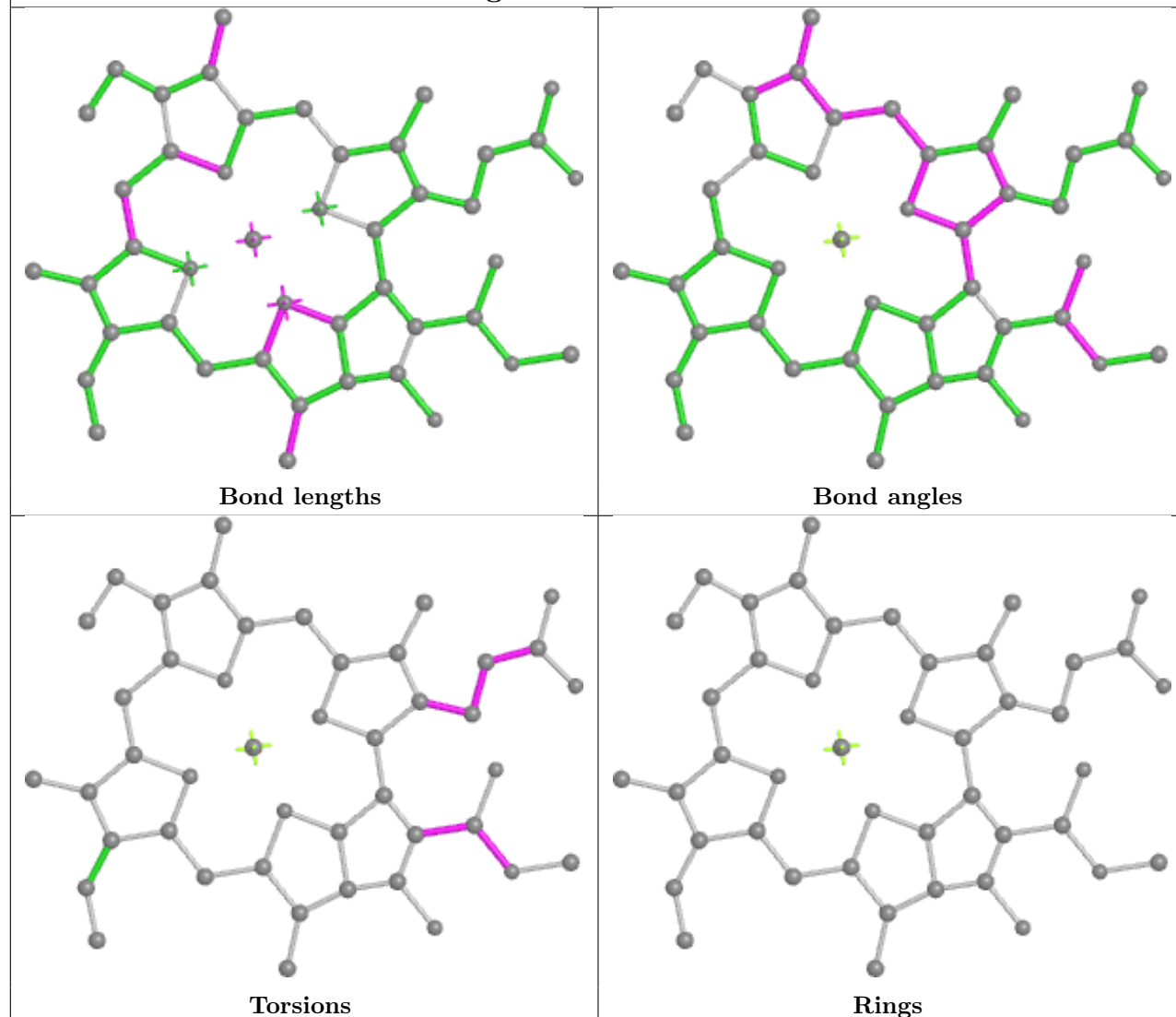




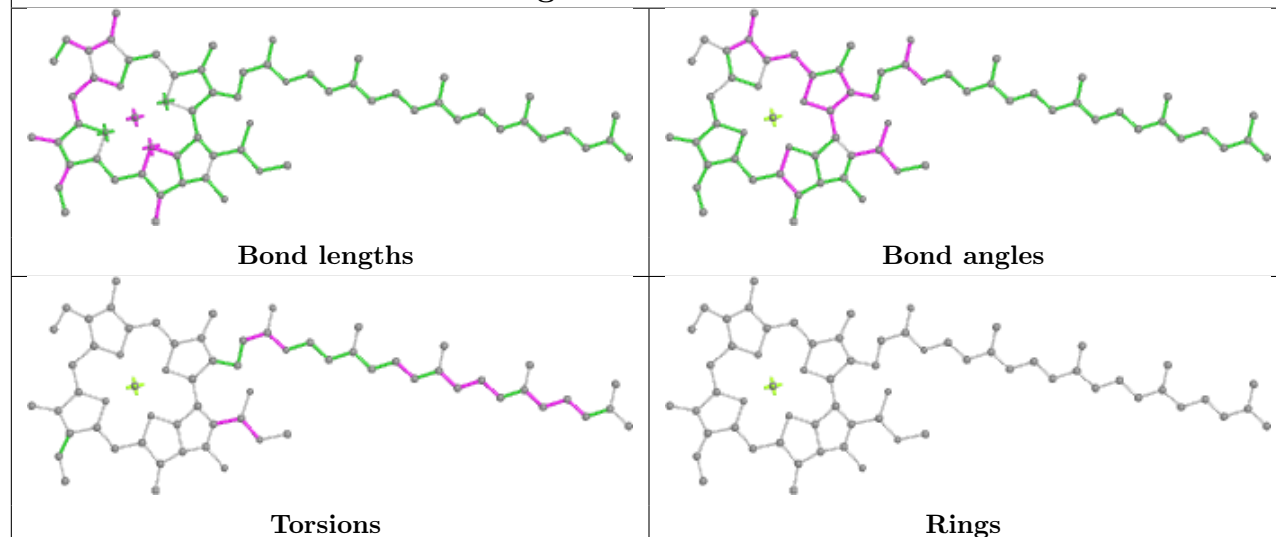
Ligand CLA c 510**Ligand BCR C 515****Ligand CLA B 614**

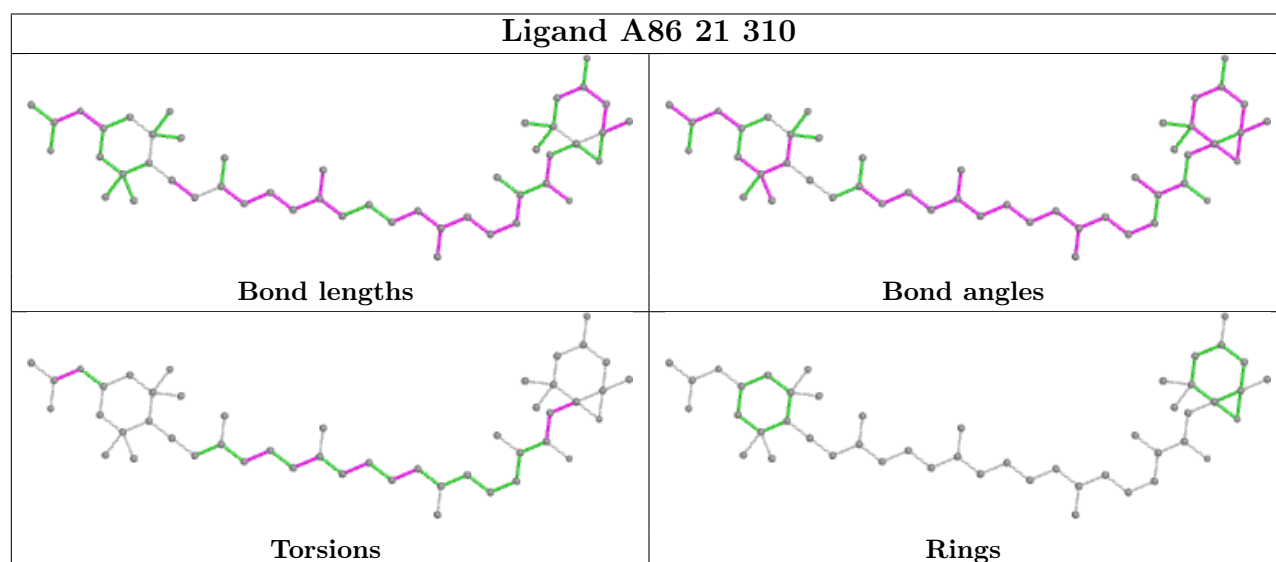
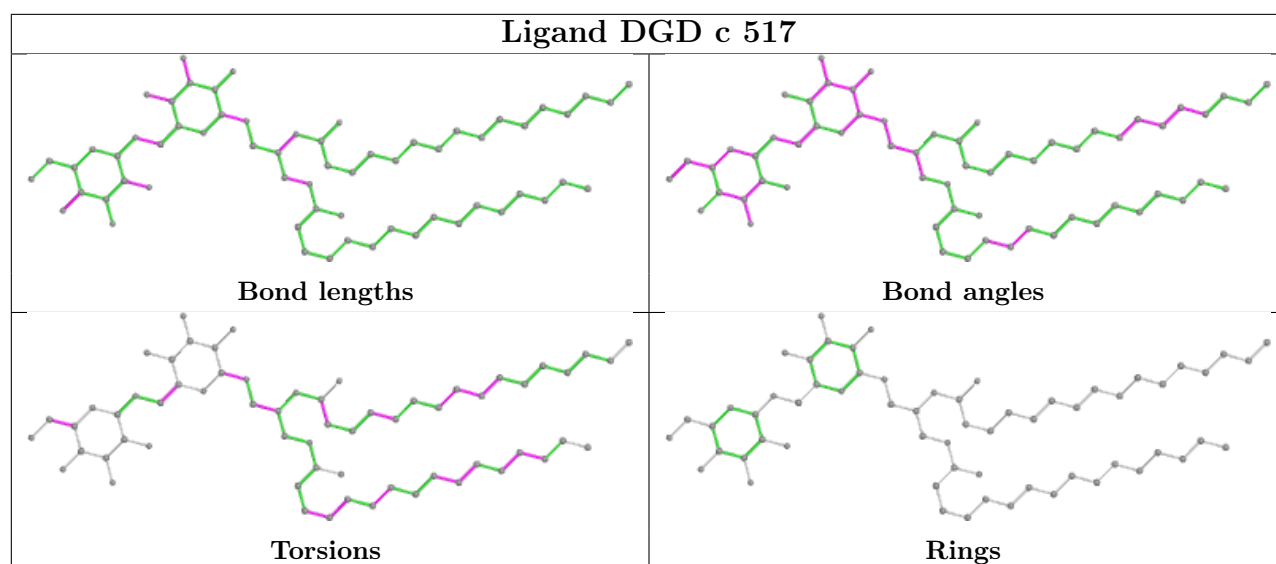


Ligand CLA 18 306

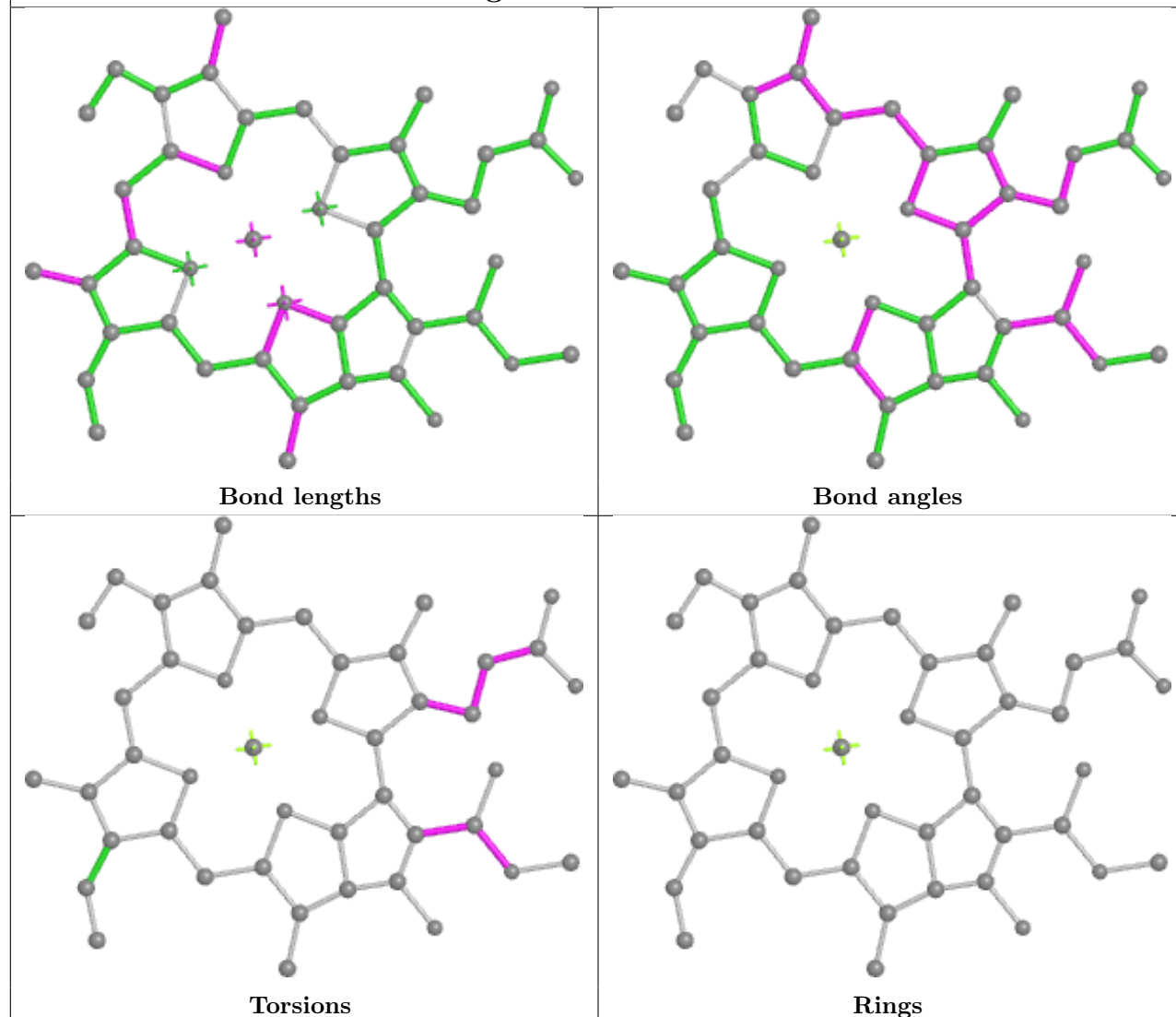


Ligand CLA c 508

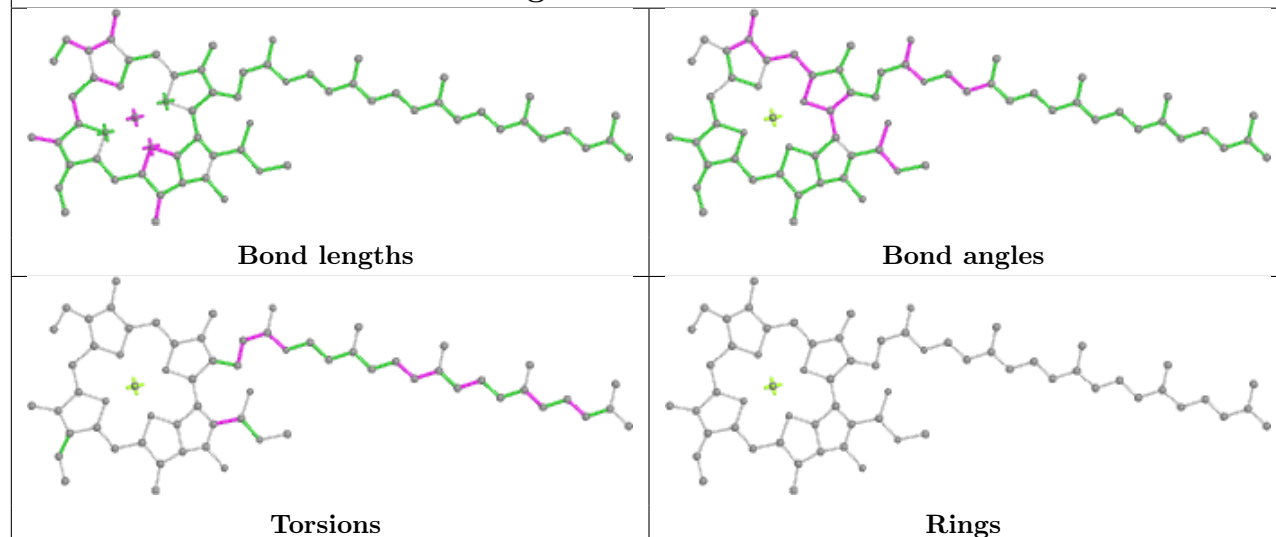


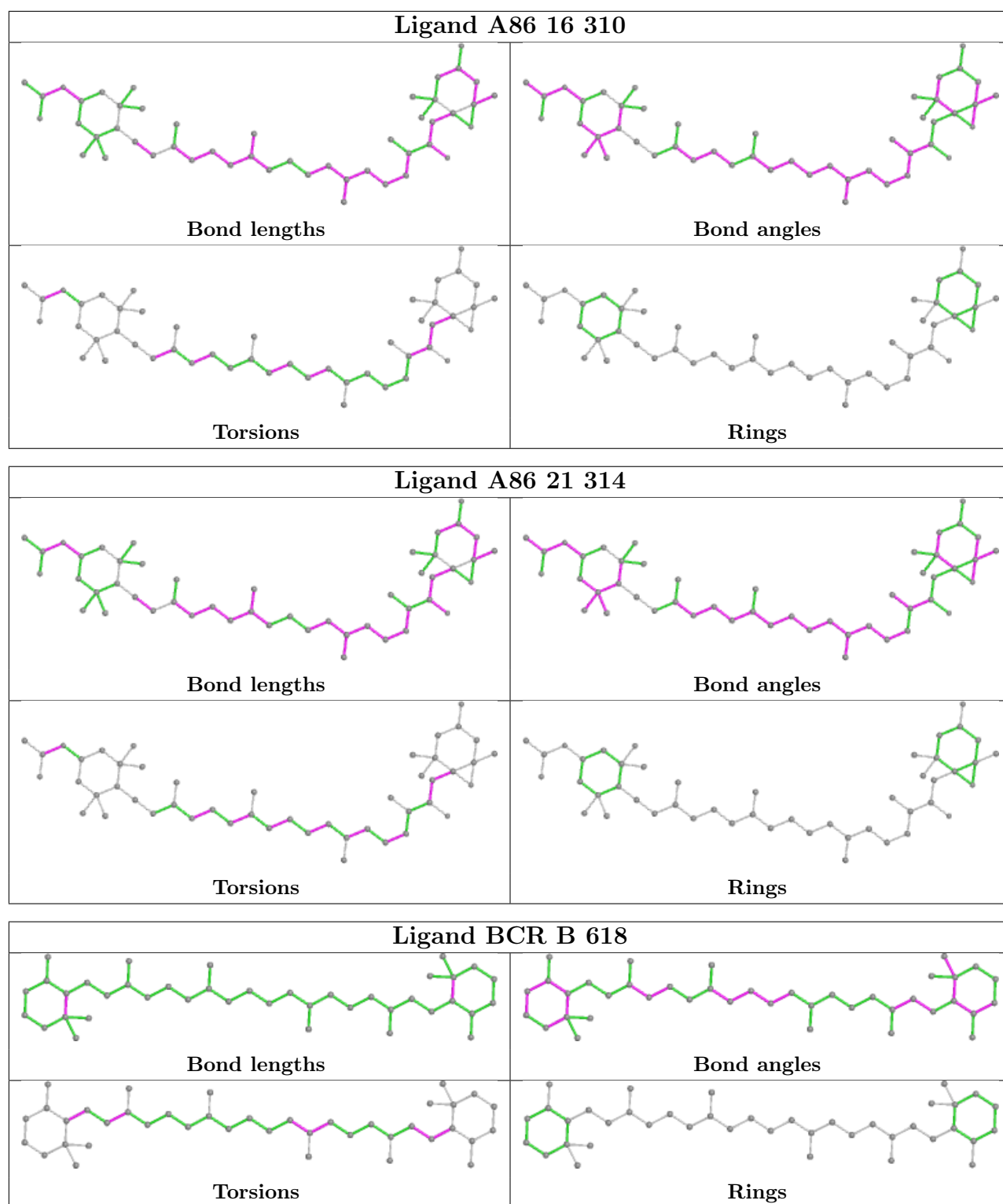


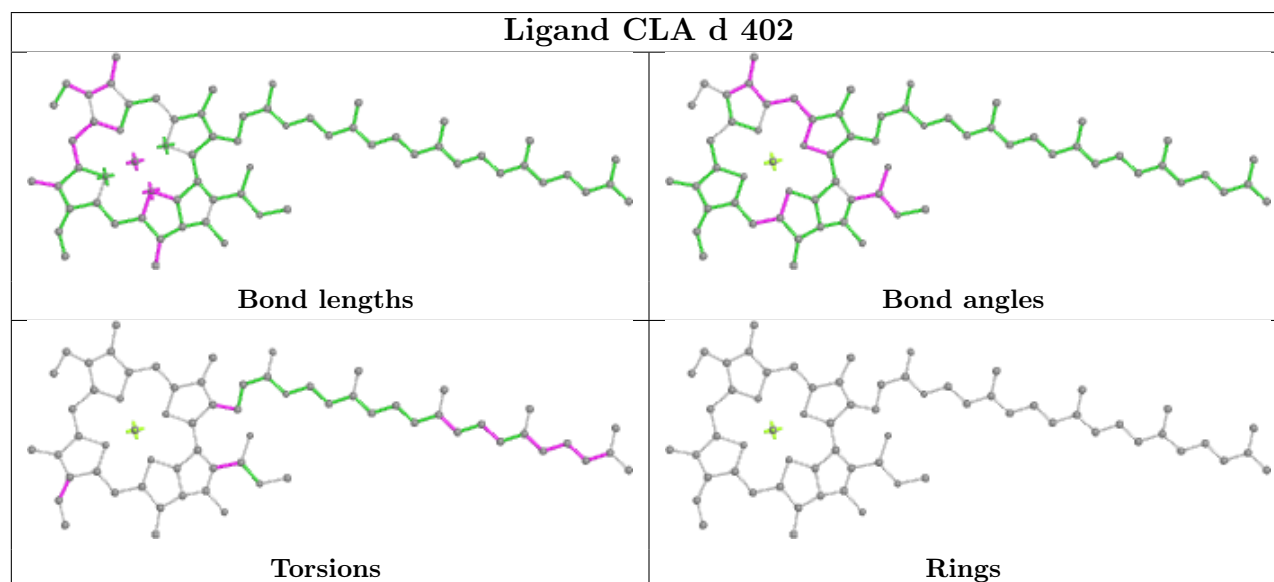
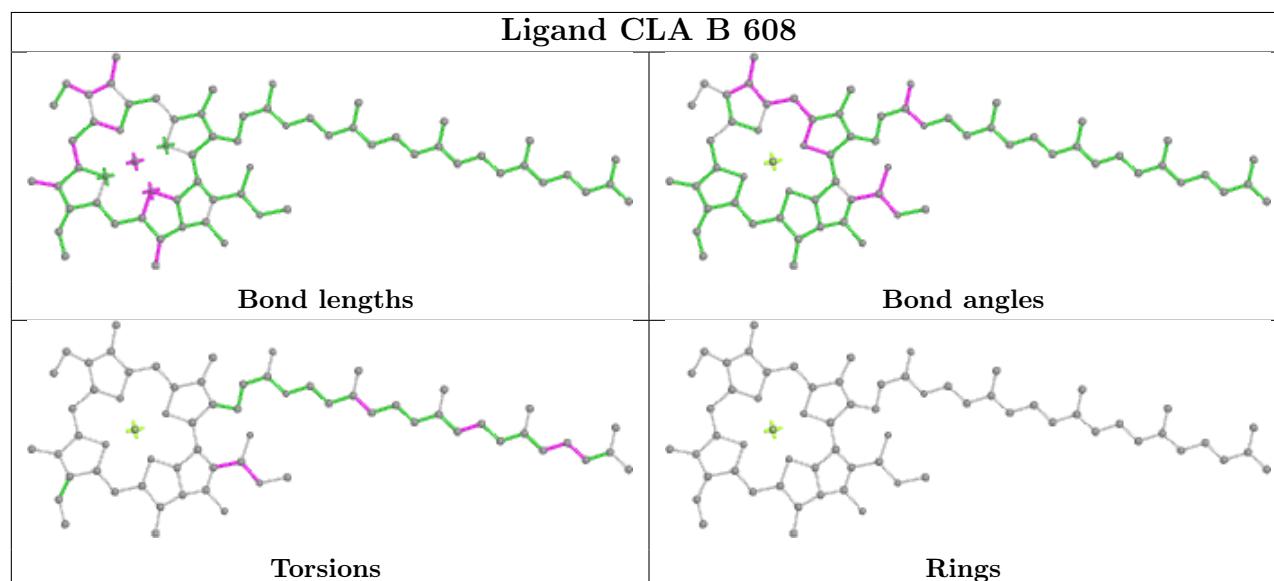
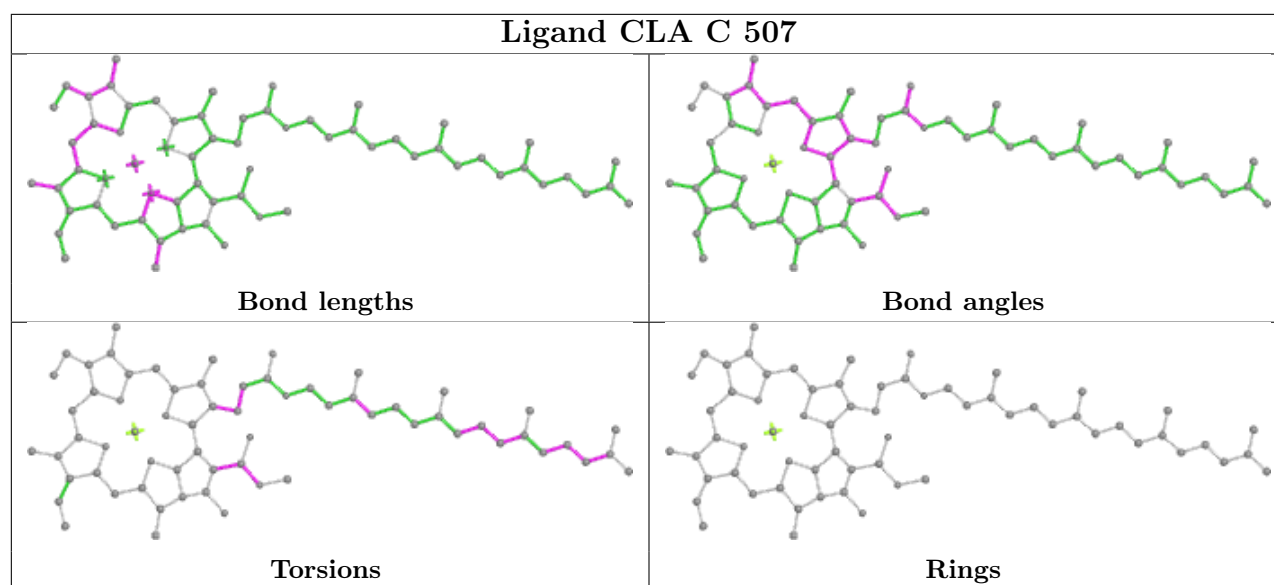
Ligand CLA 12 308

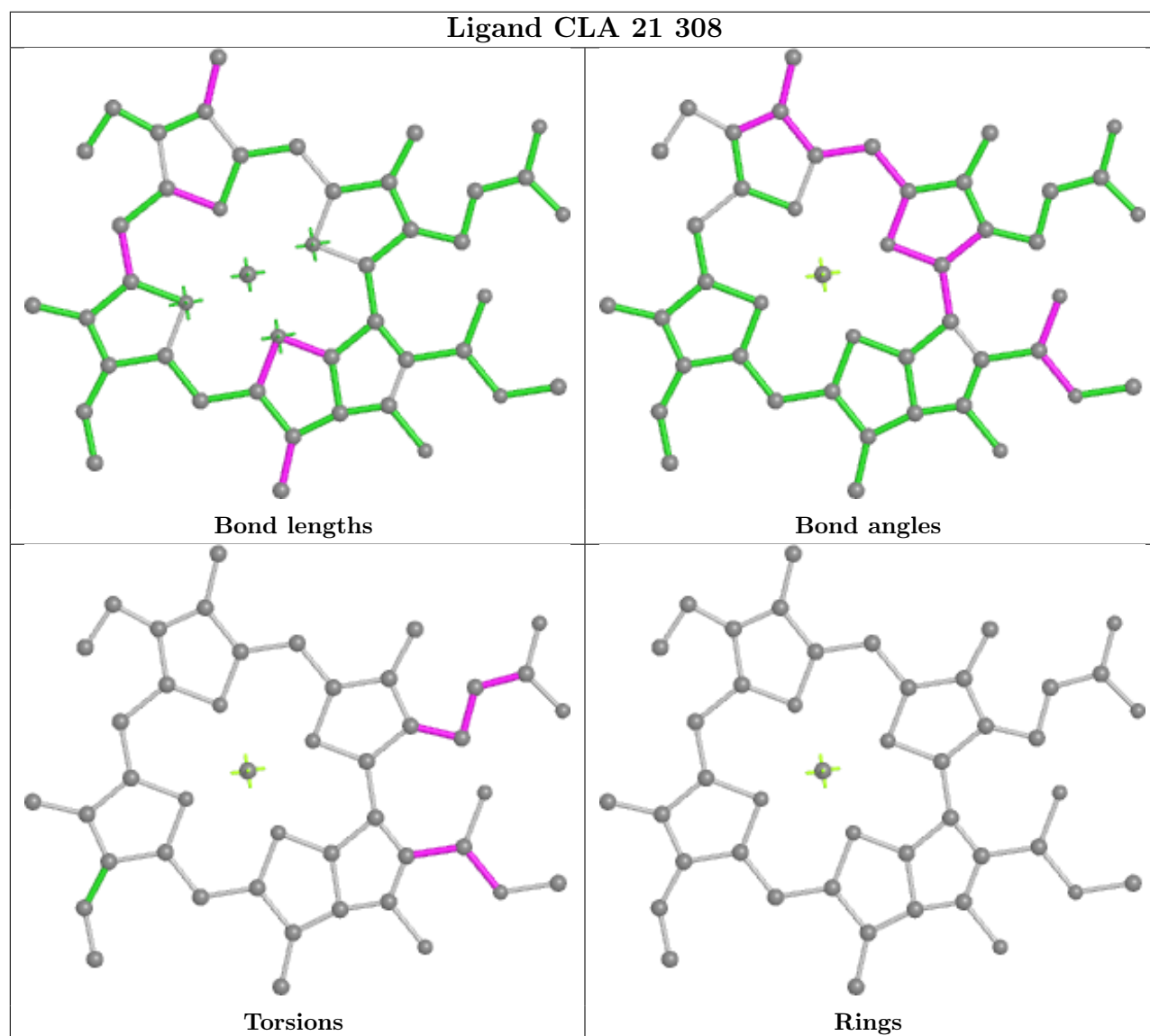
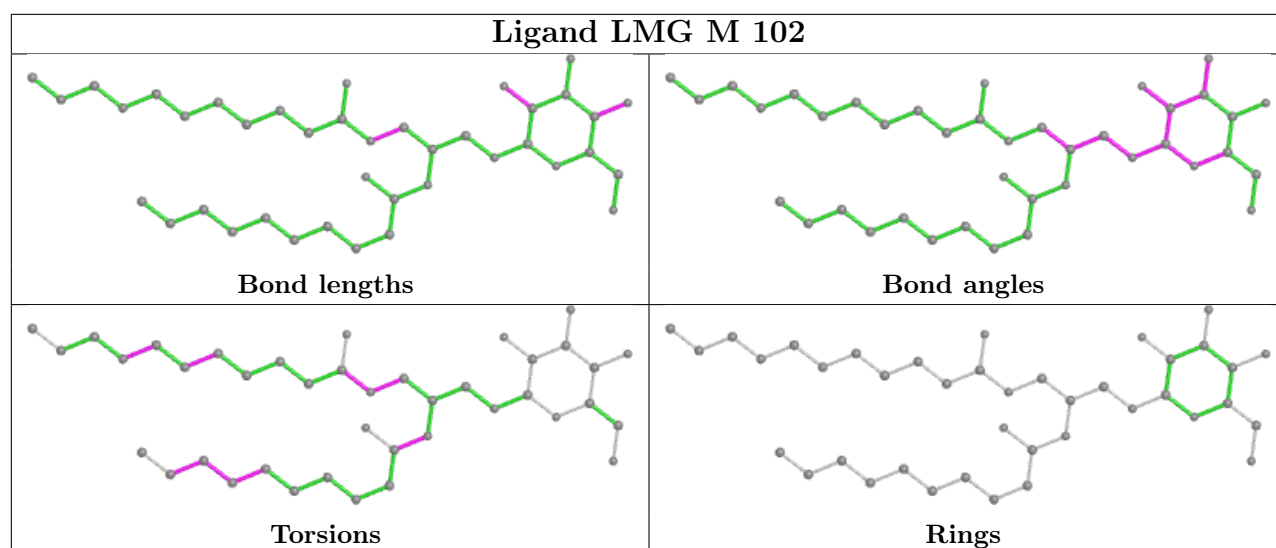


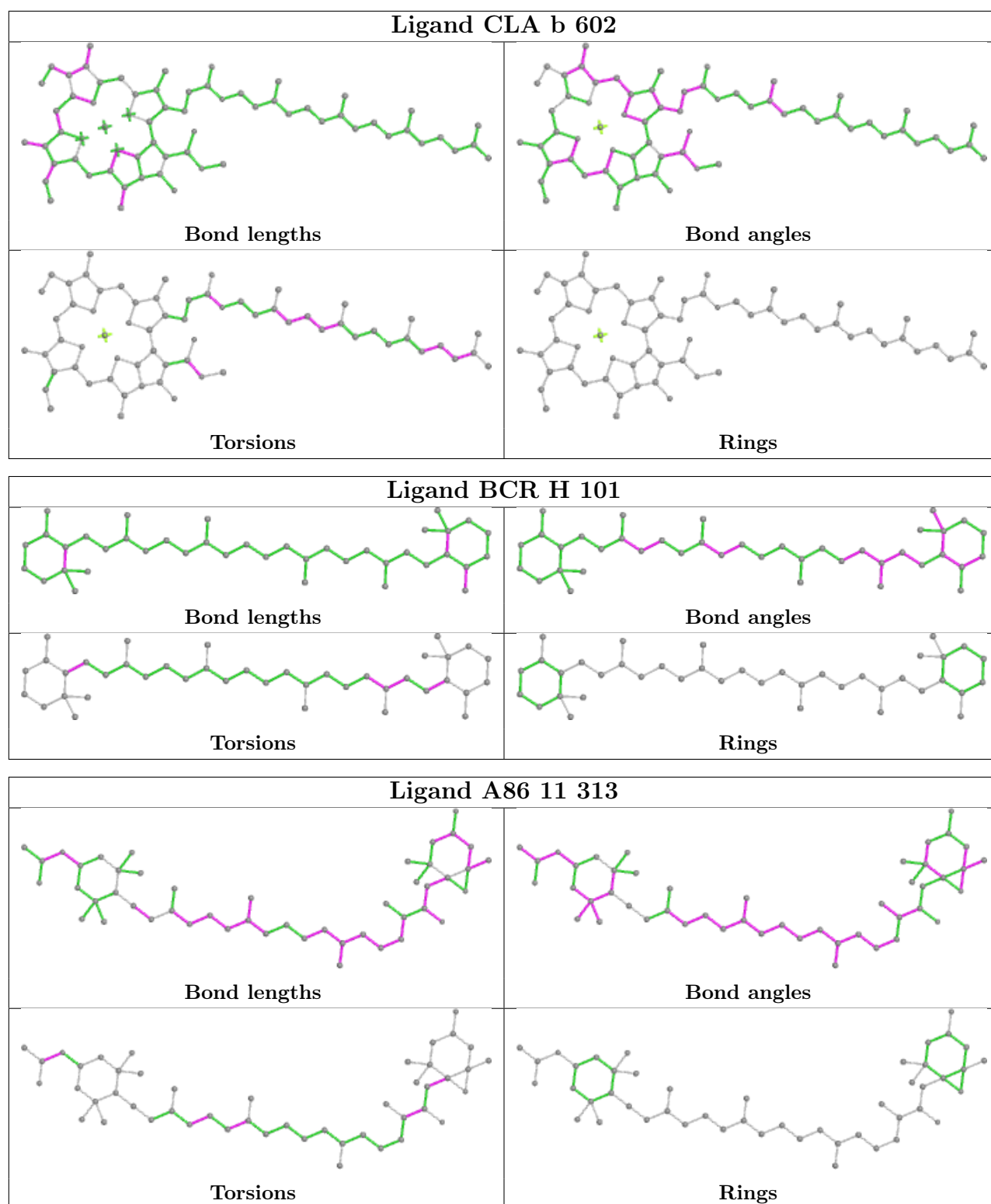
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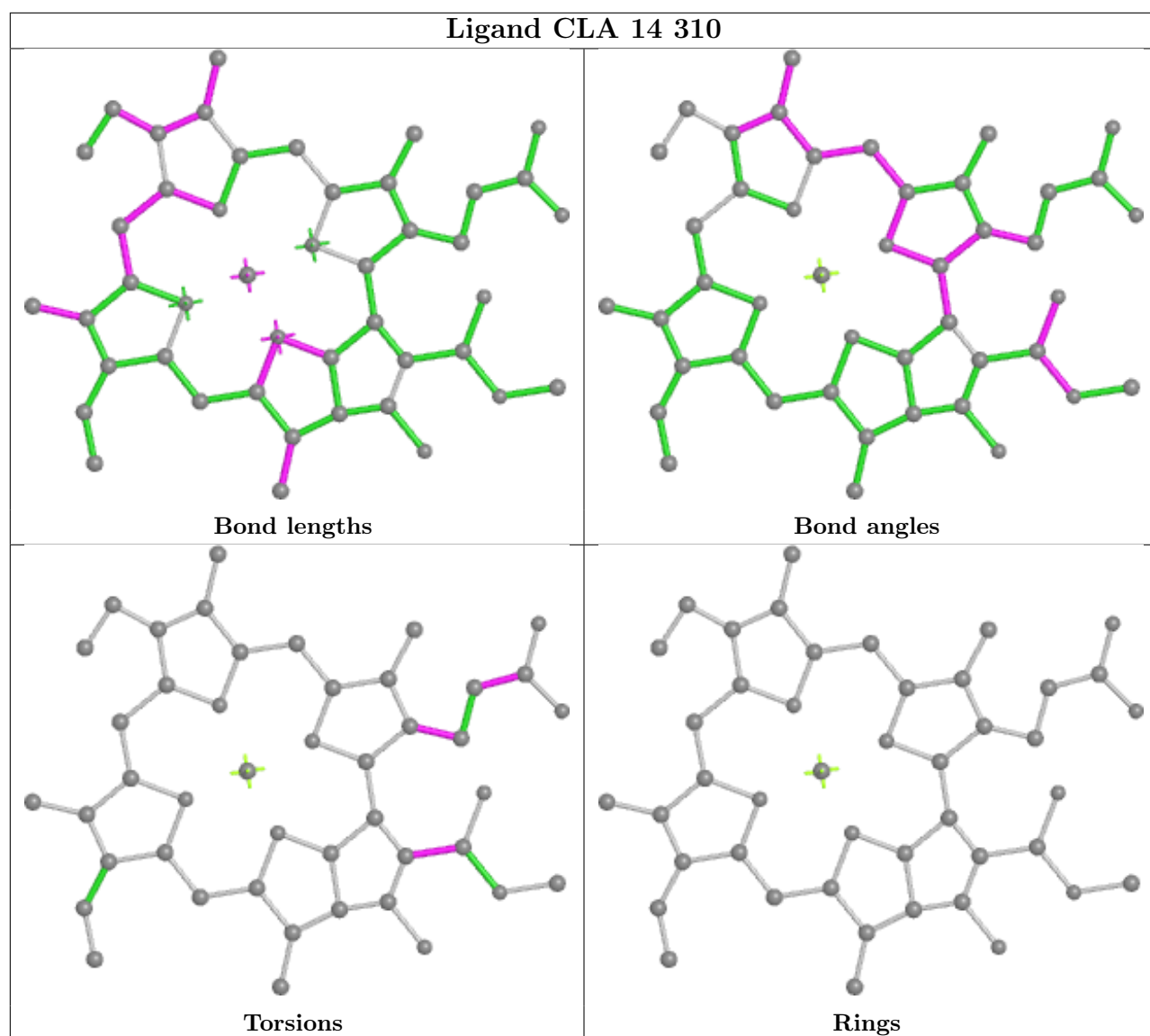


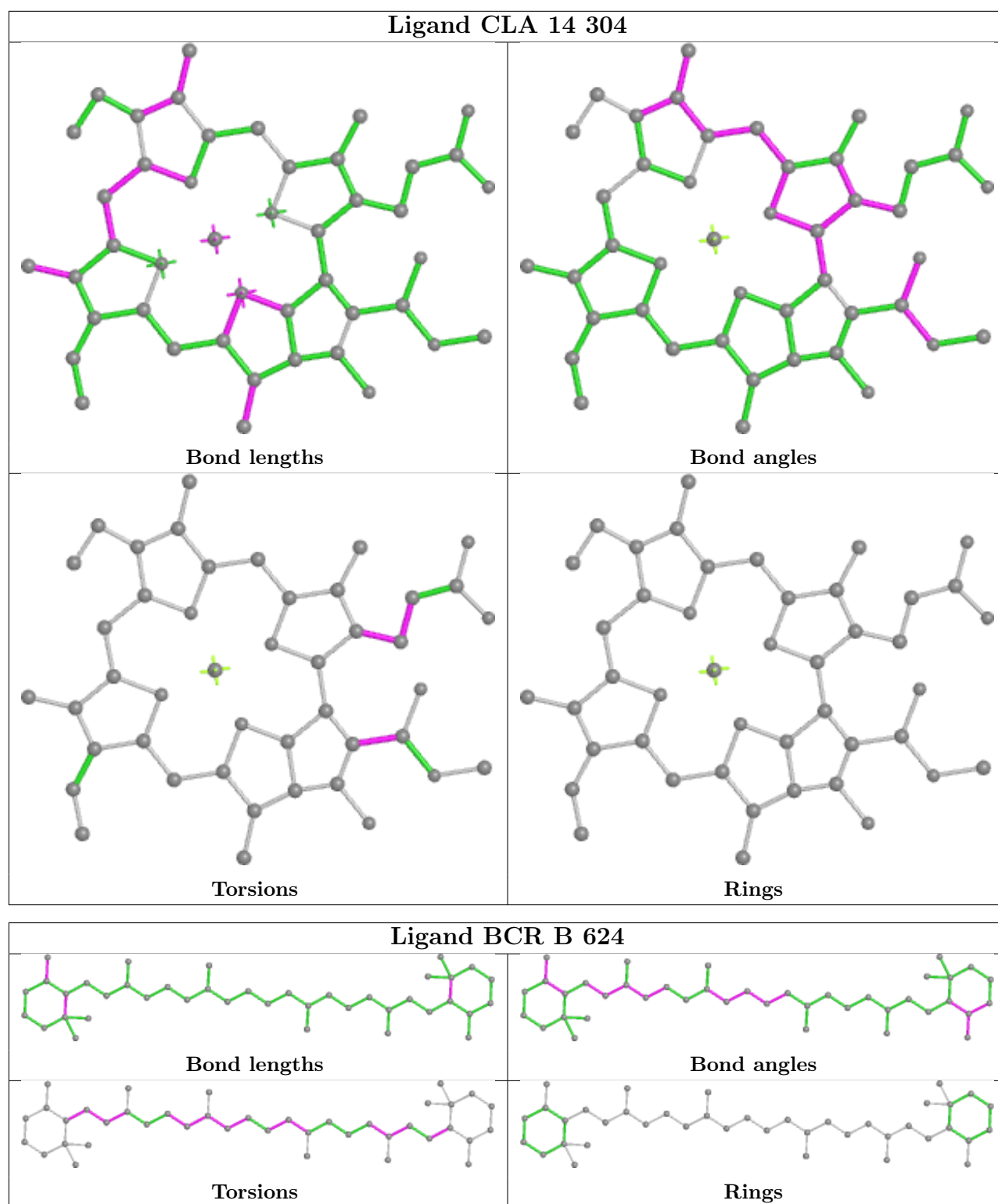


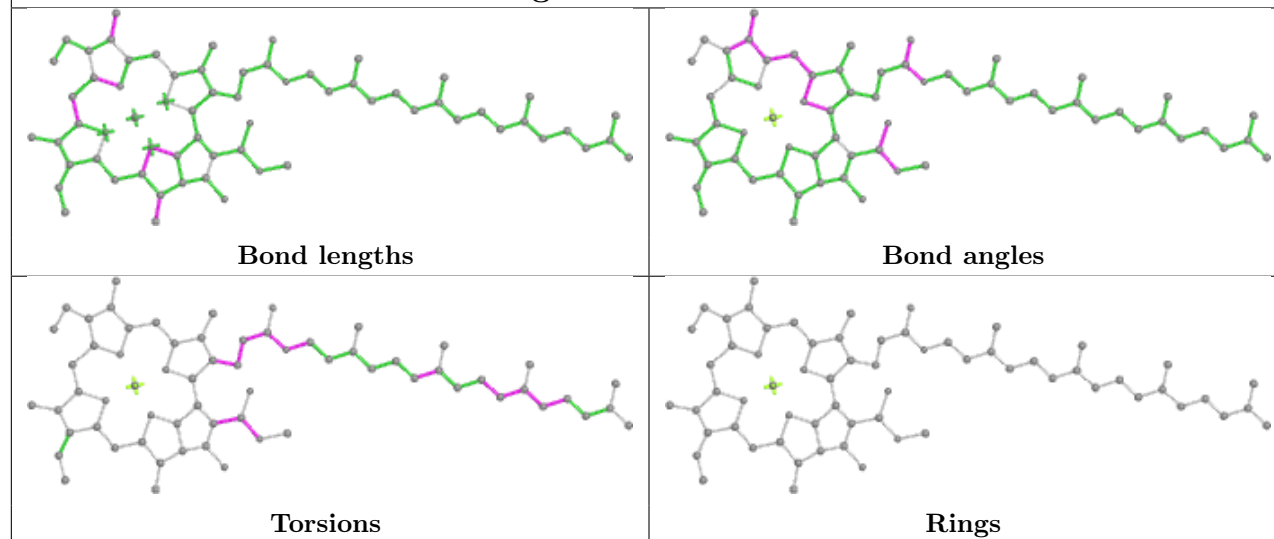
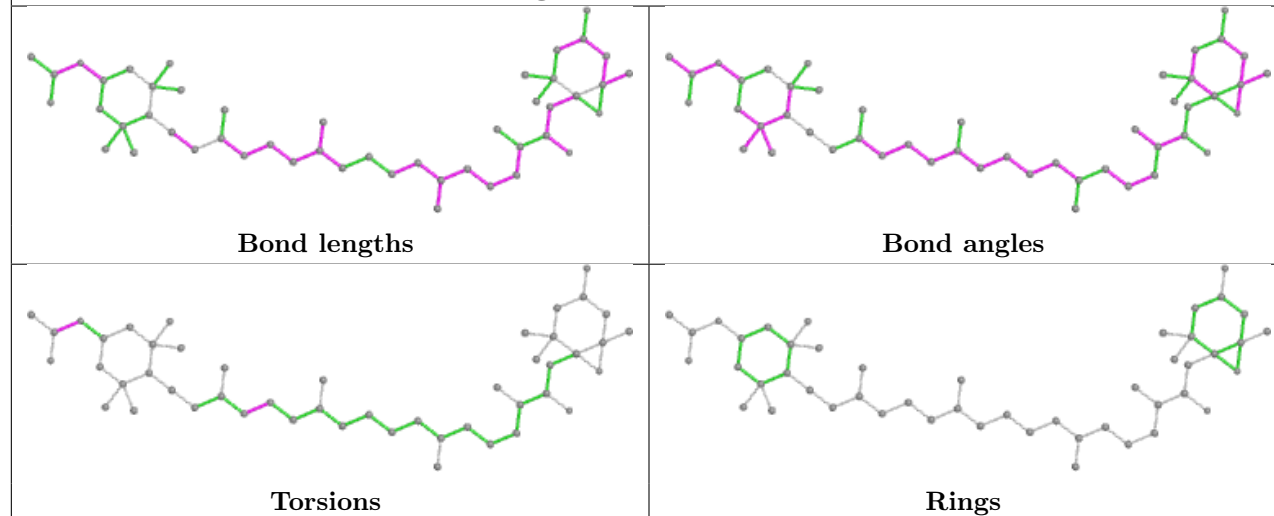
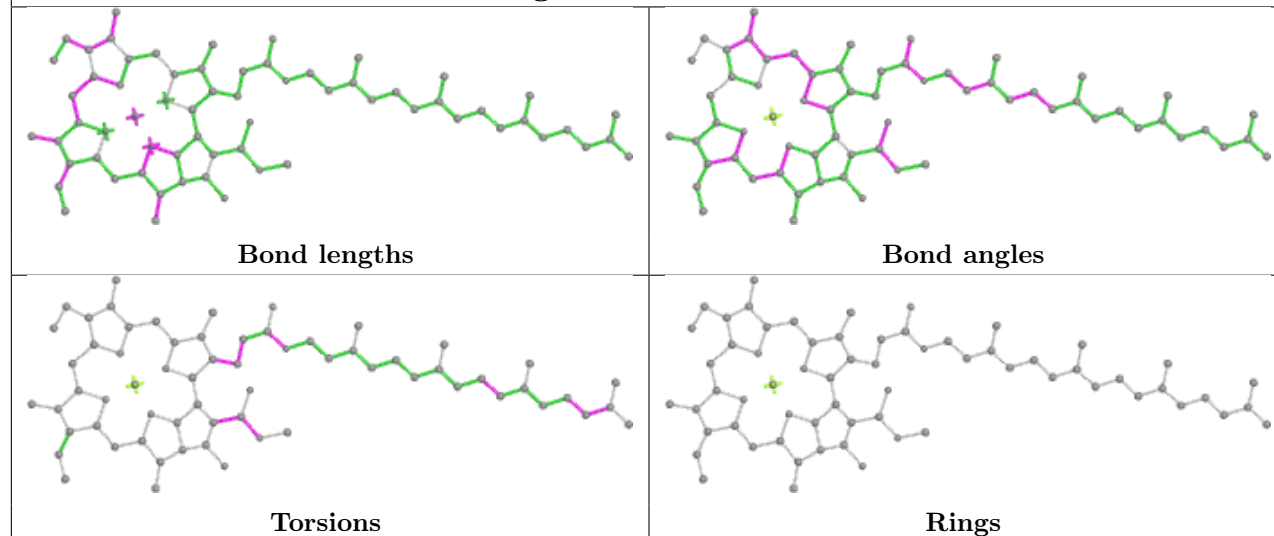


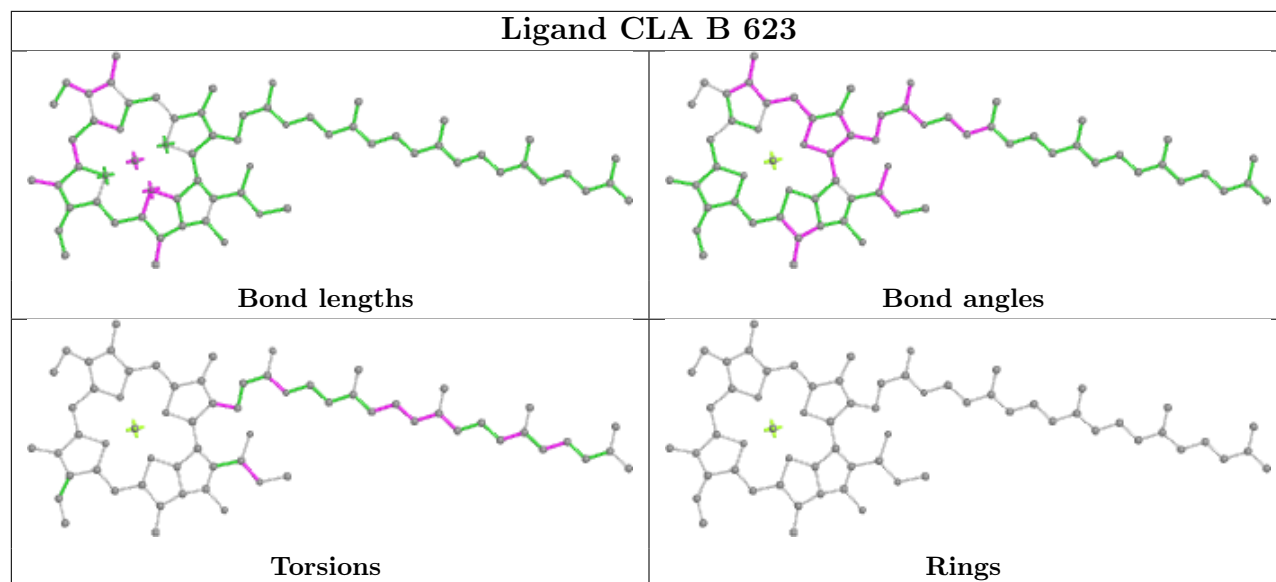
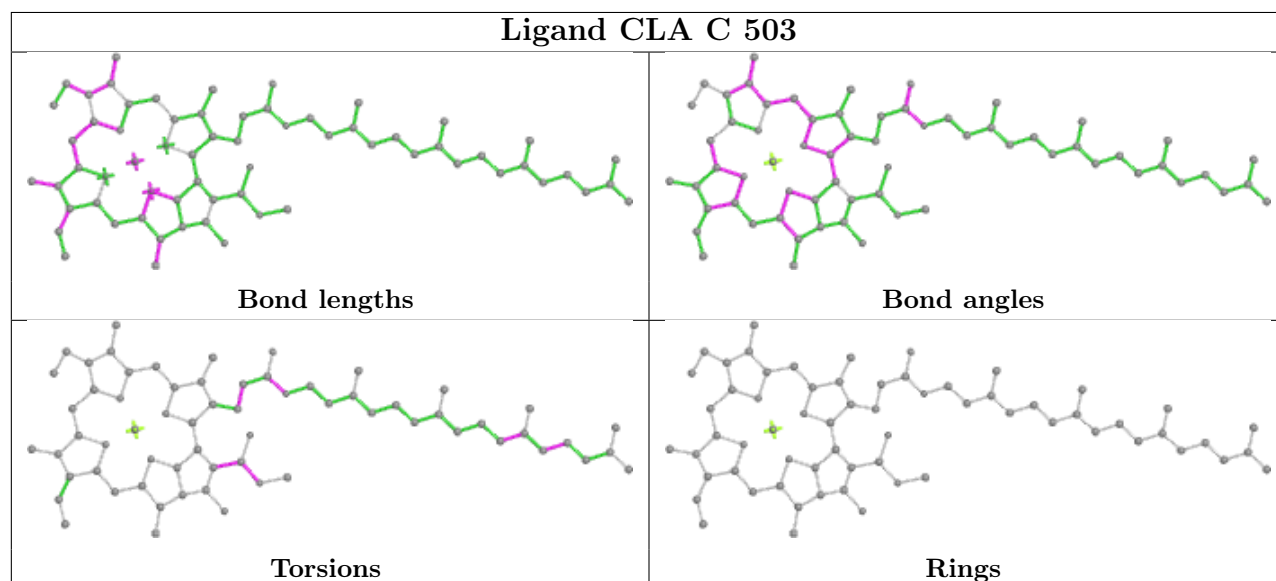
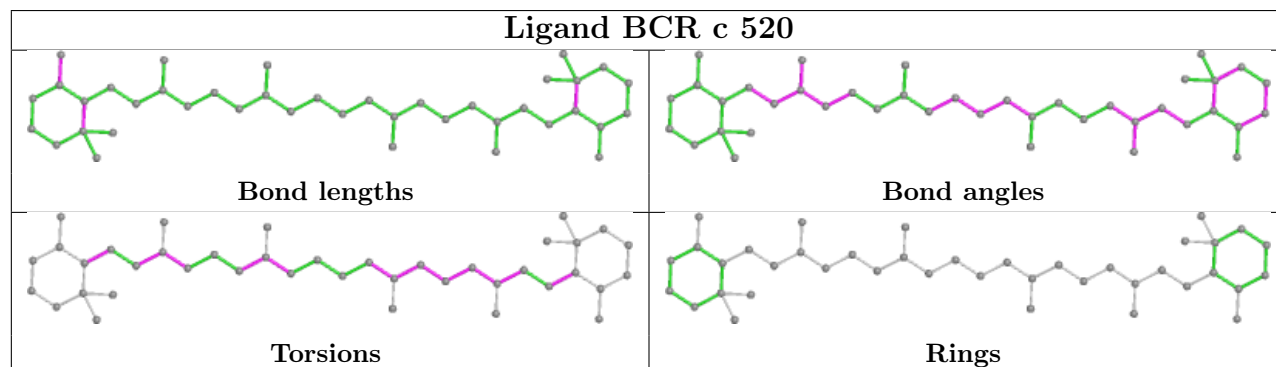




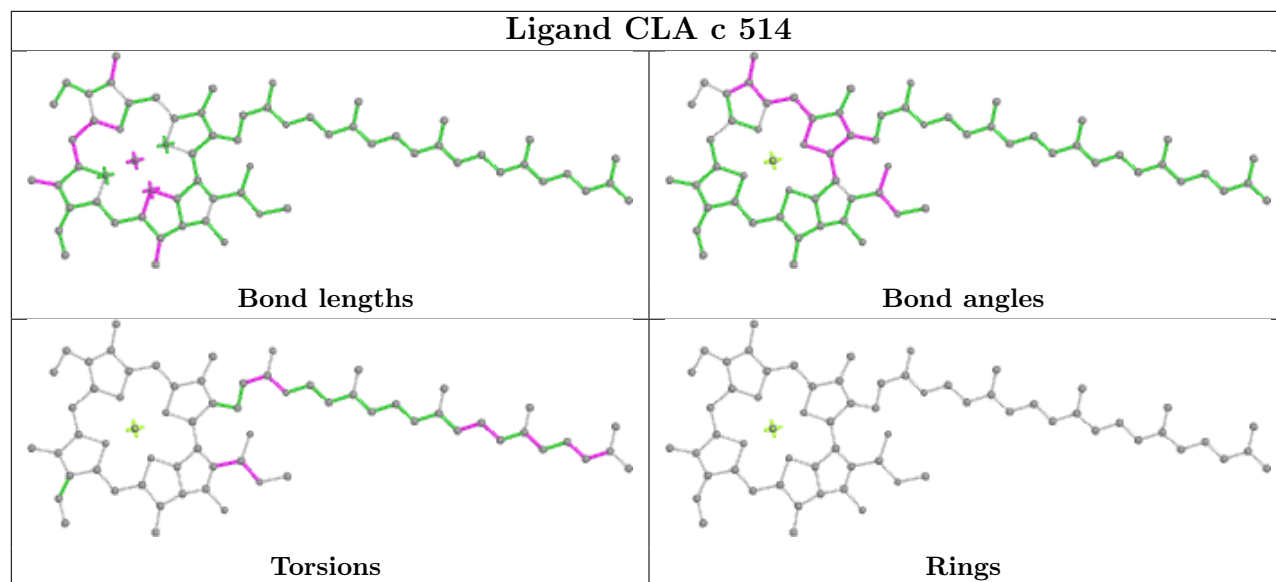




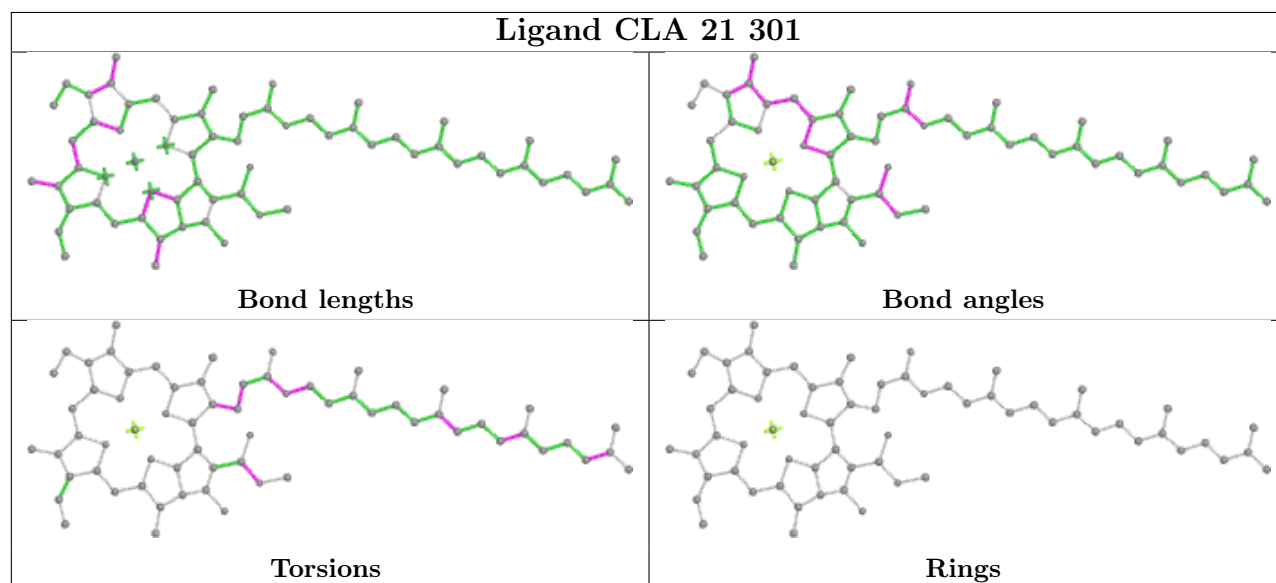
Ligand CLA w 103**Ligand A86 18 314****Ligand CLA B 611**

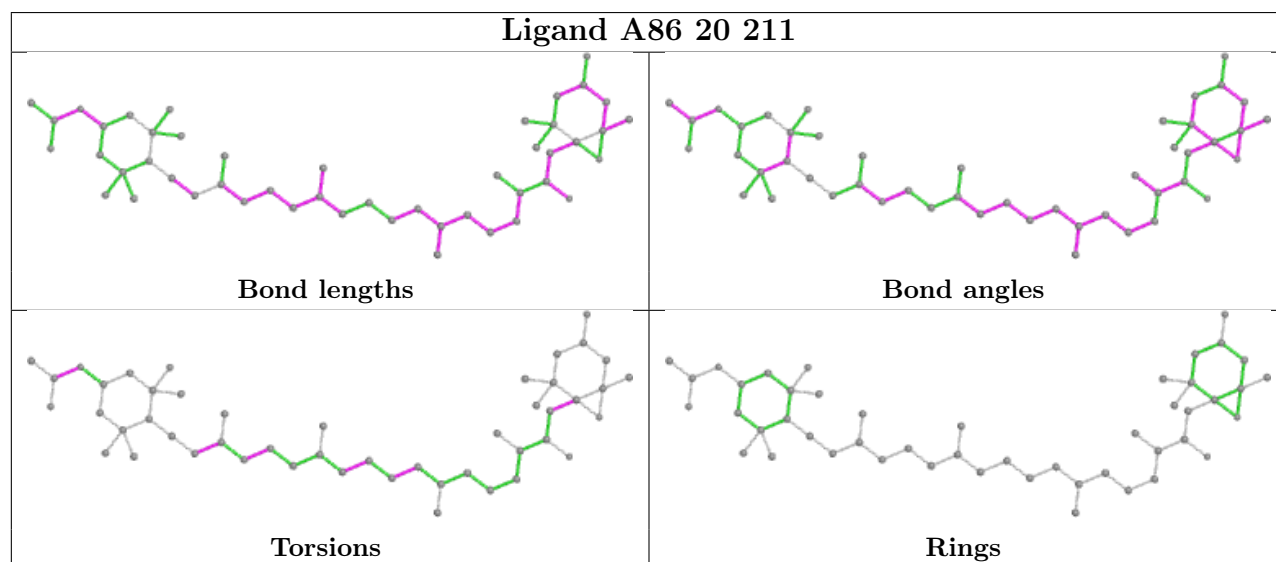
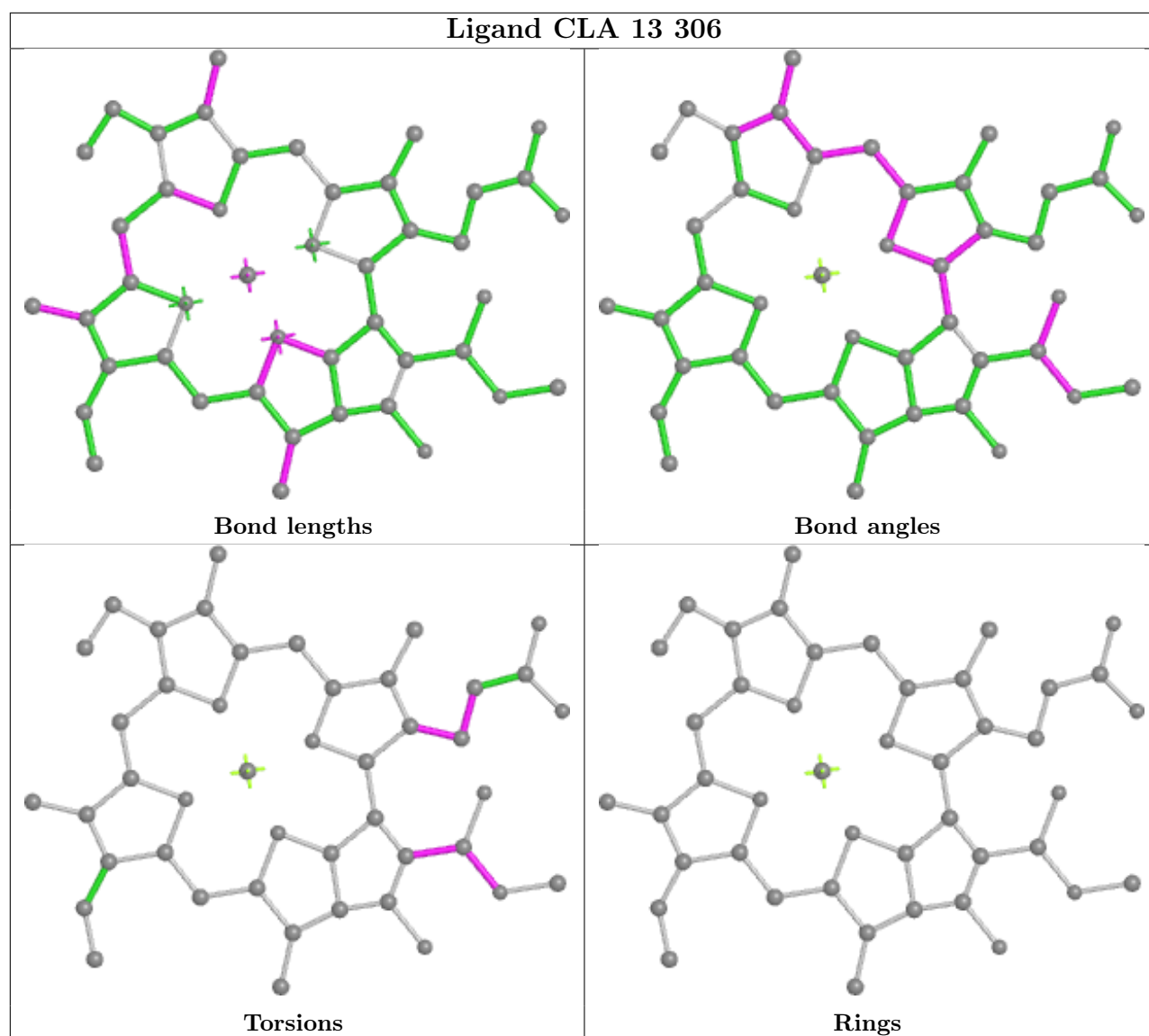
Ligand CLA B 623**Ligand CLA C 503****Ligand BCR c 520**

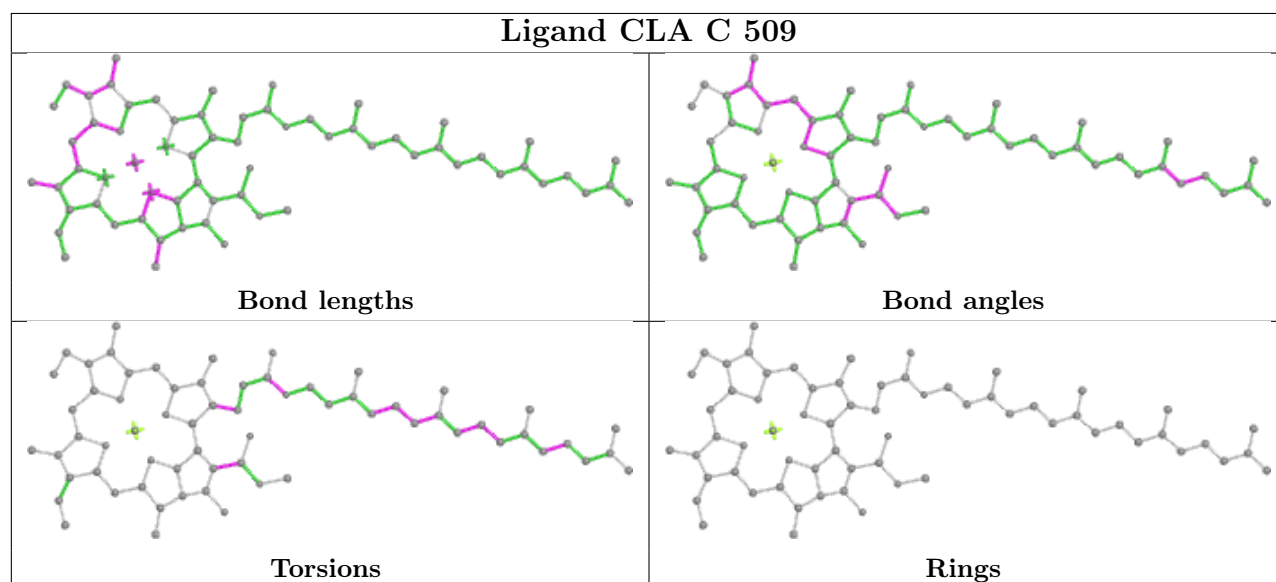
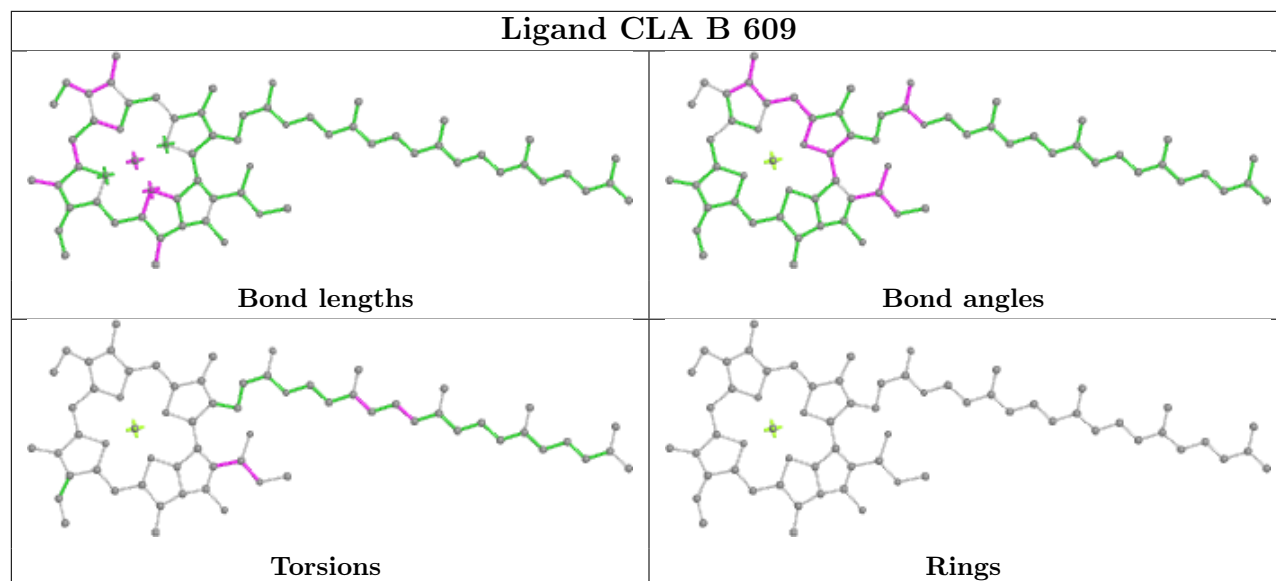
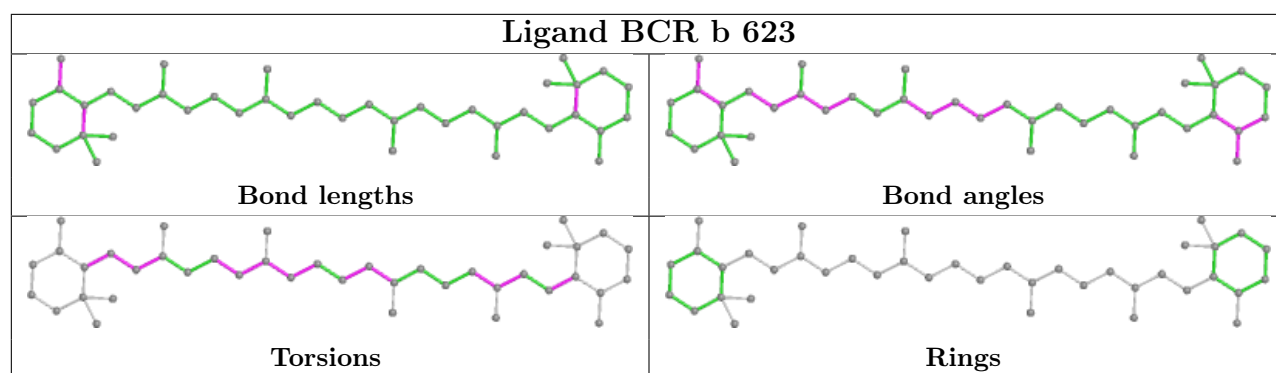
Ligand CLA c 514

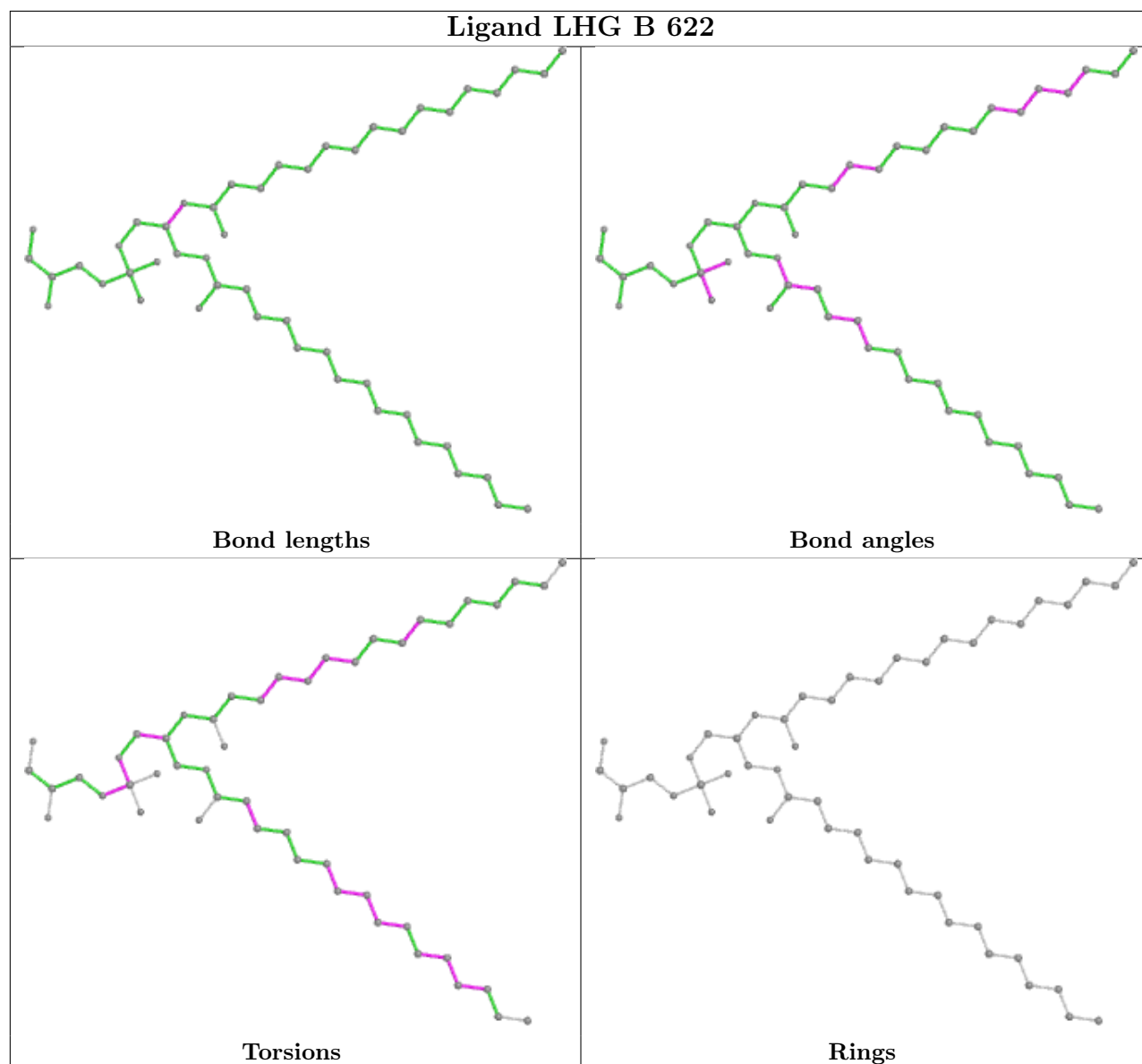
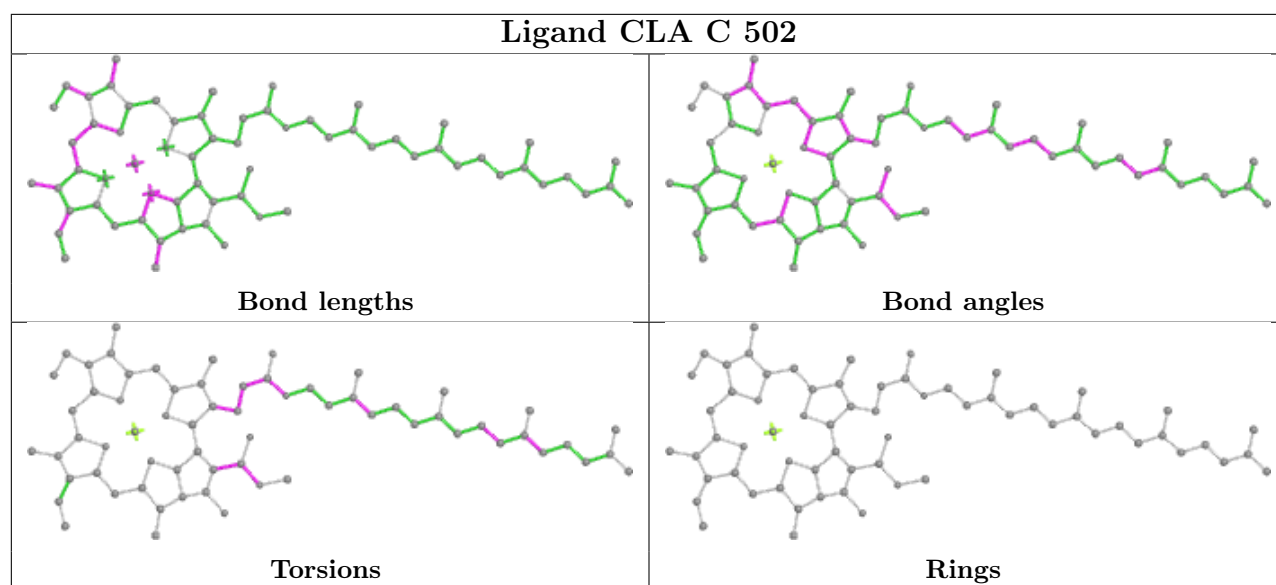


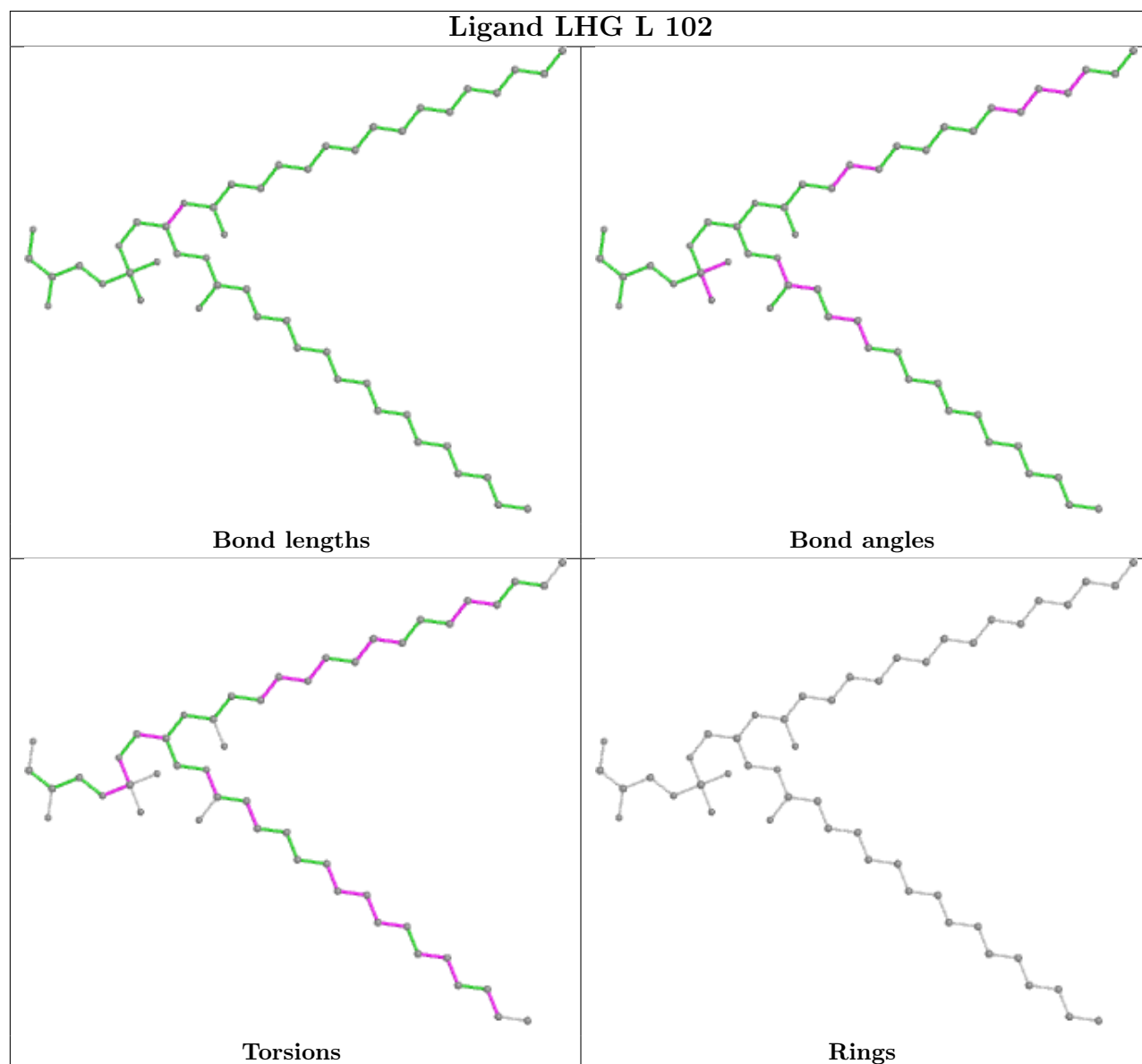
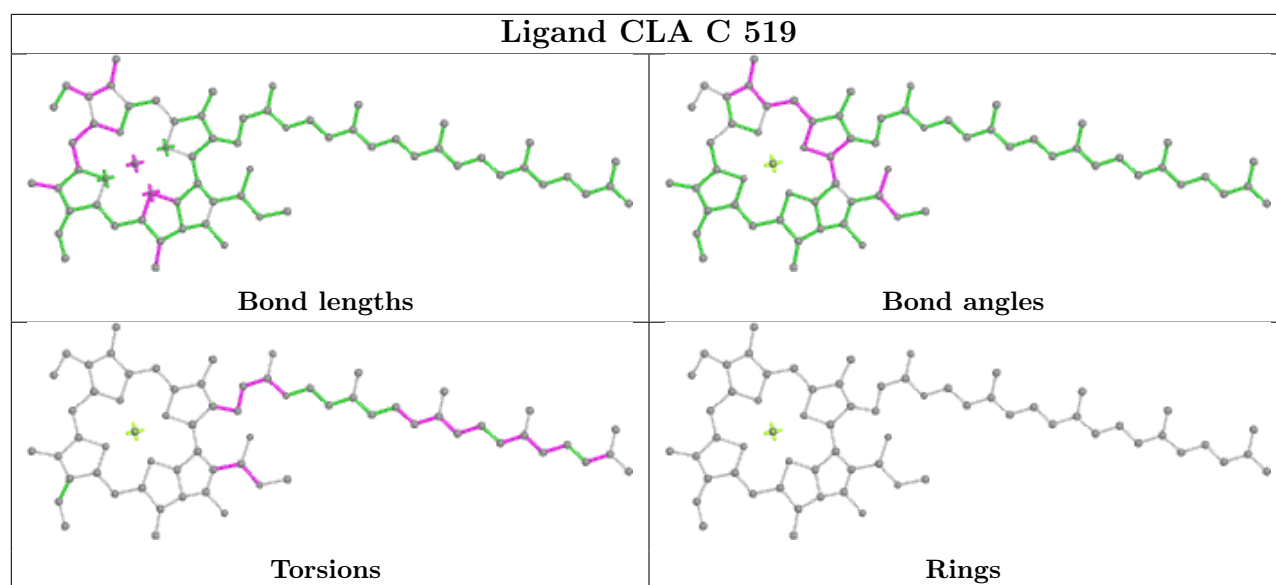
Ligand CLA 21 301



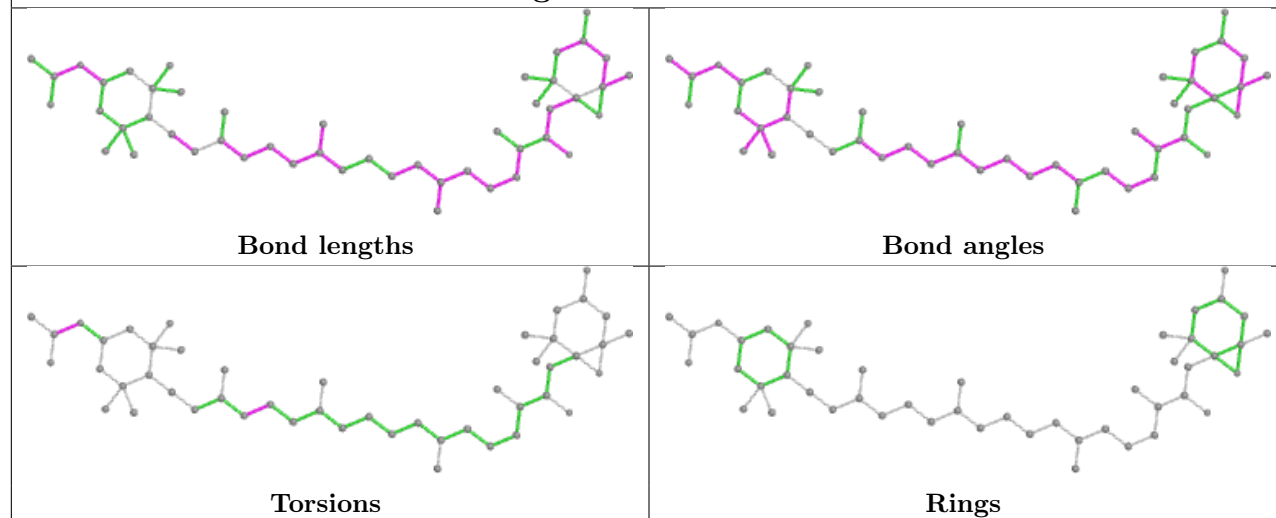




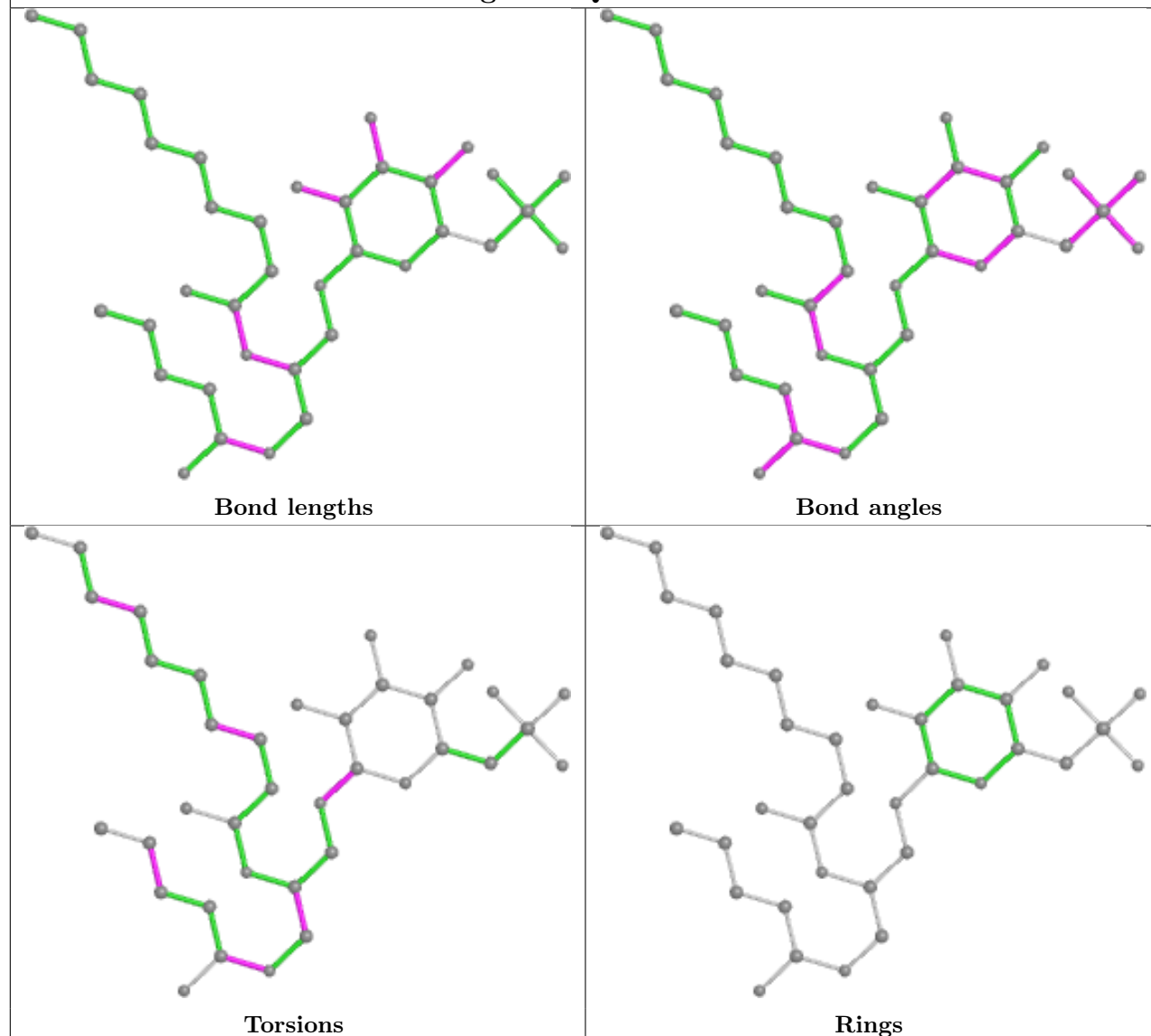


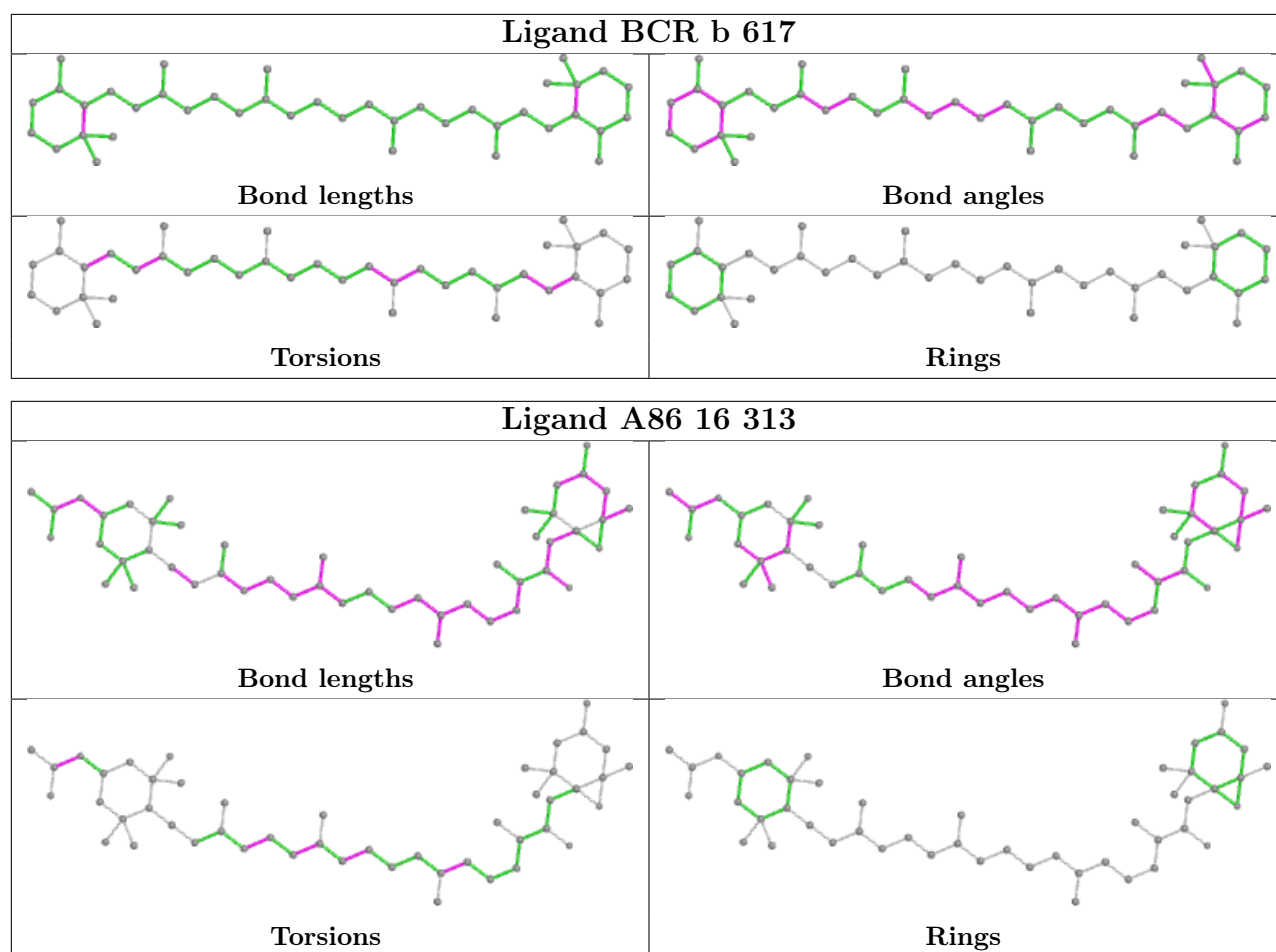


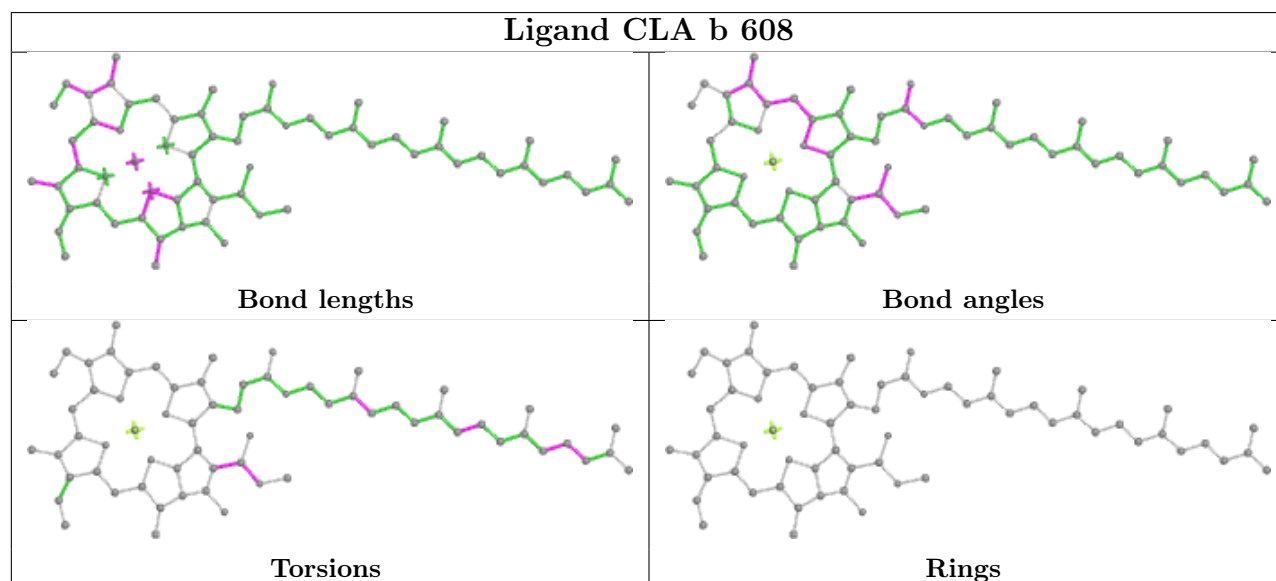
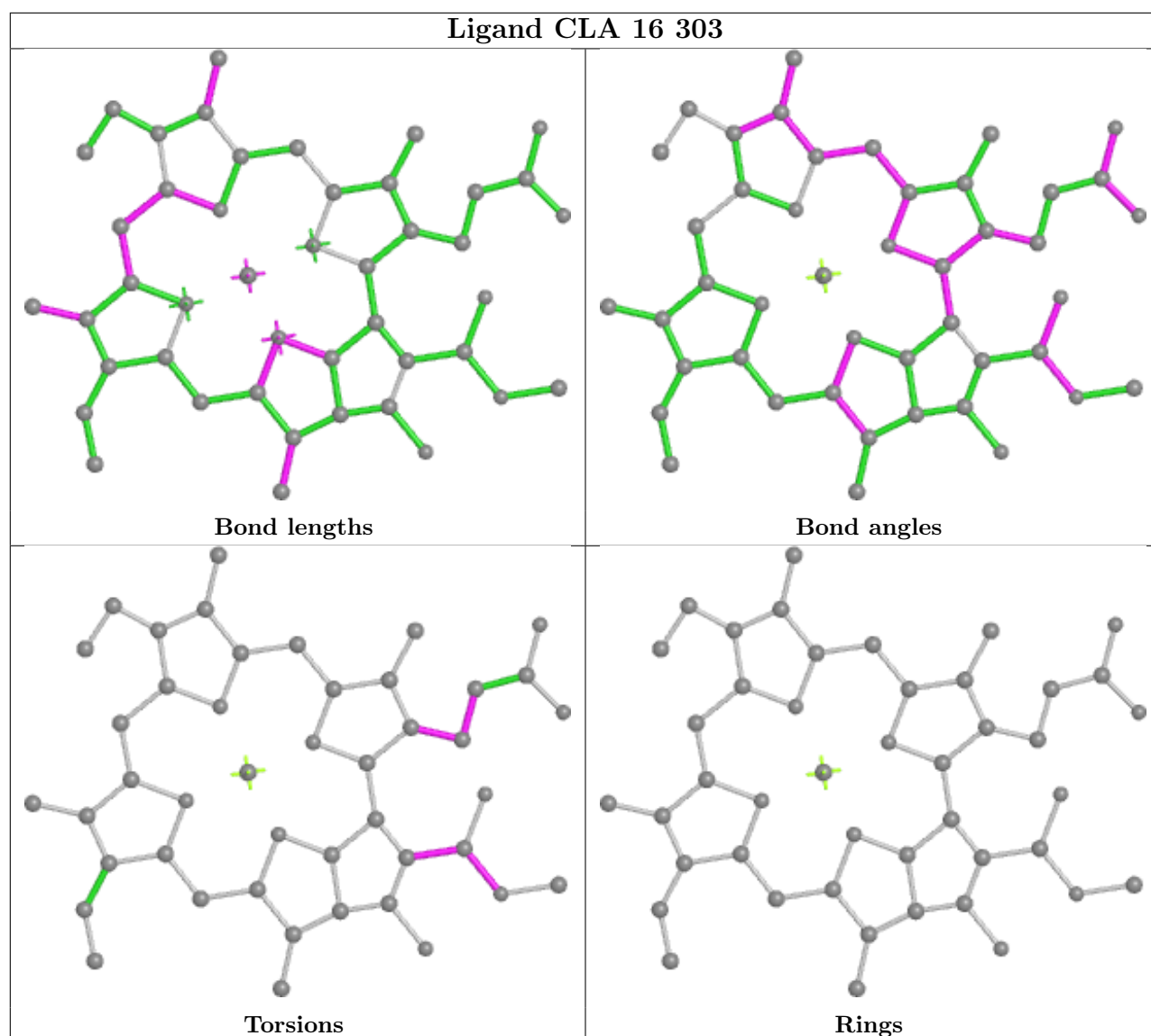
Ligand A86 11 311

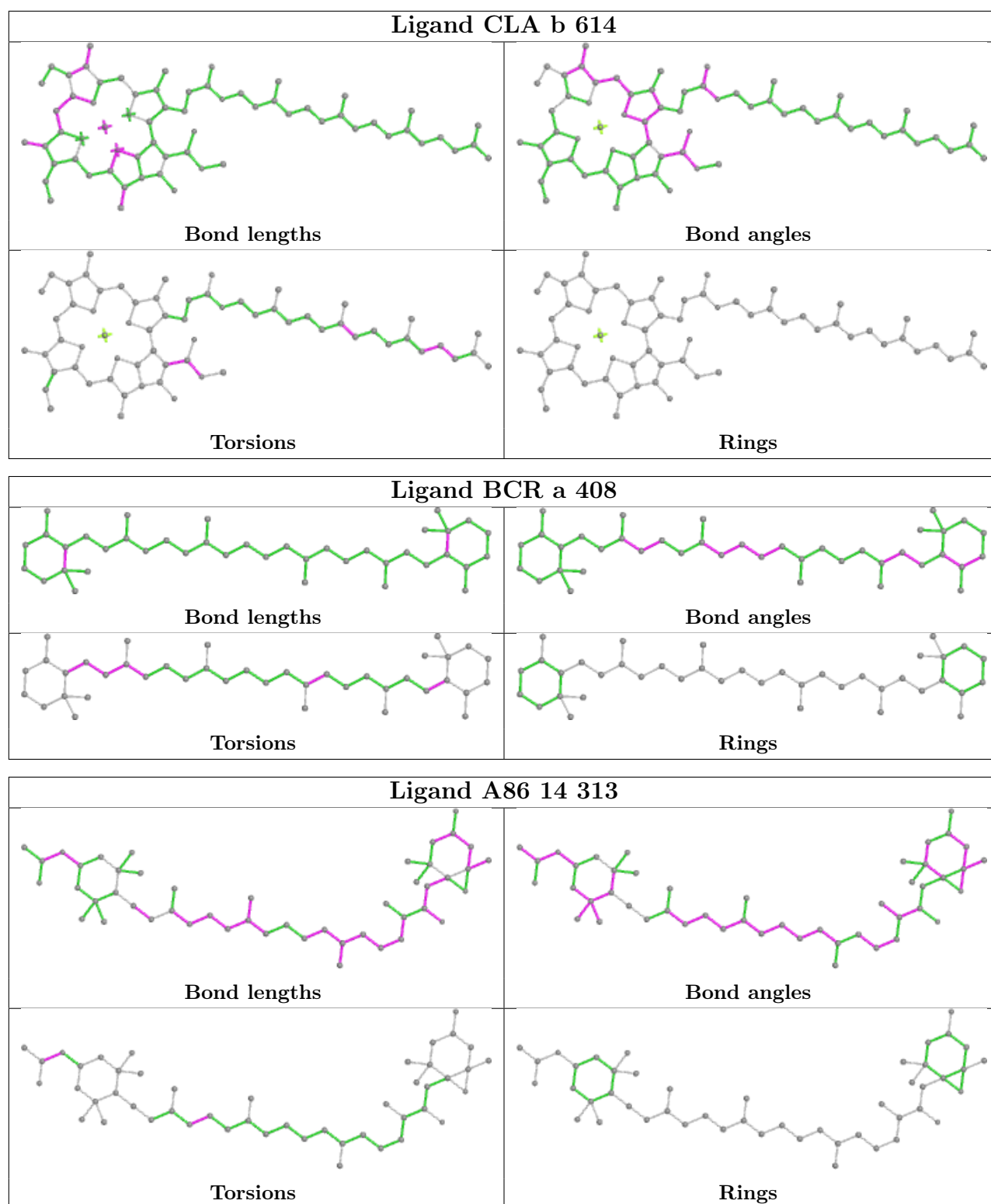


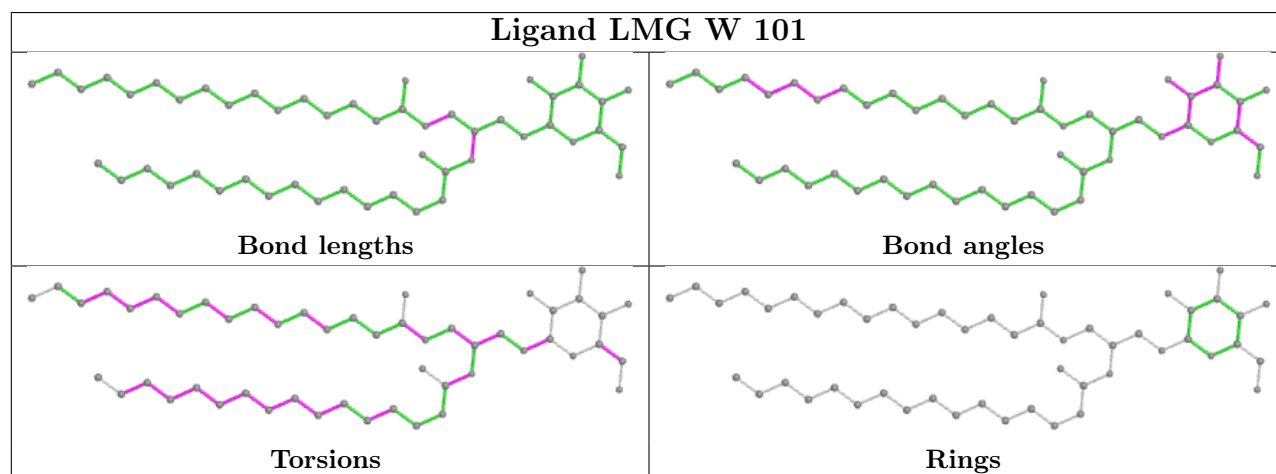
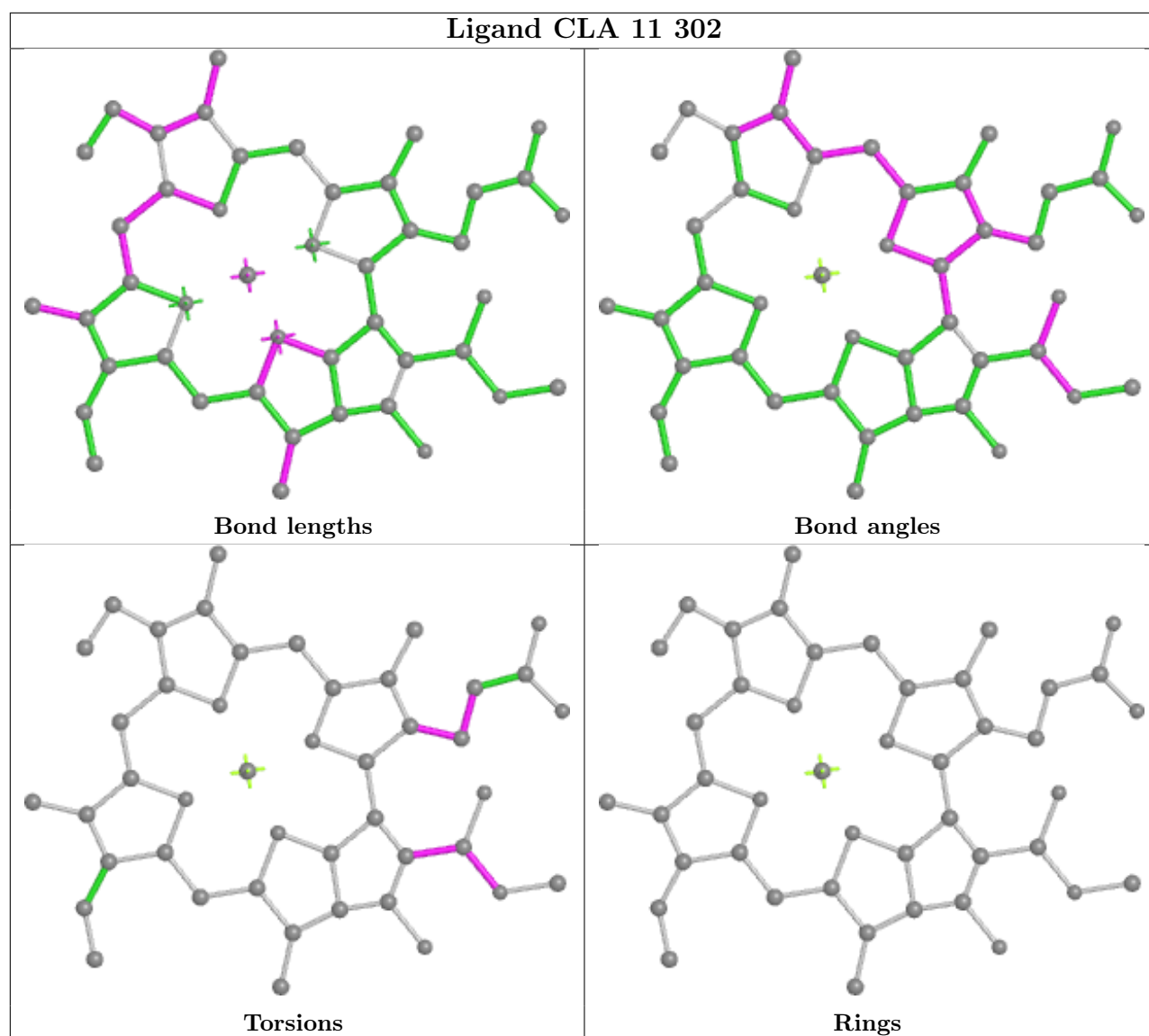
Ligand SQD B 621

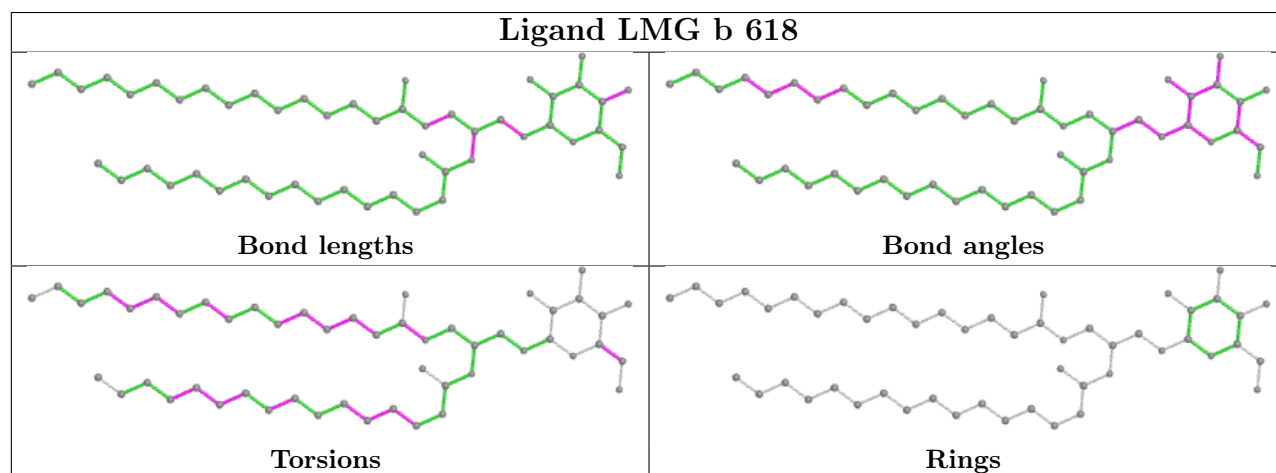
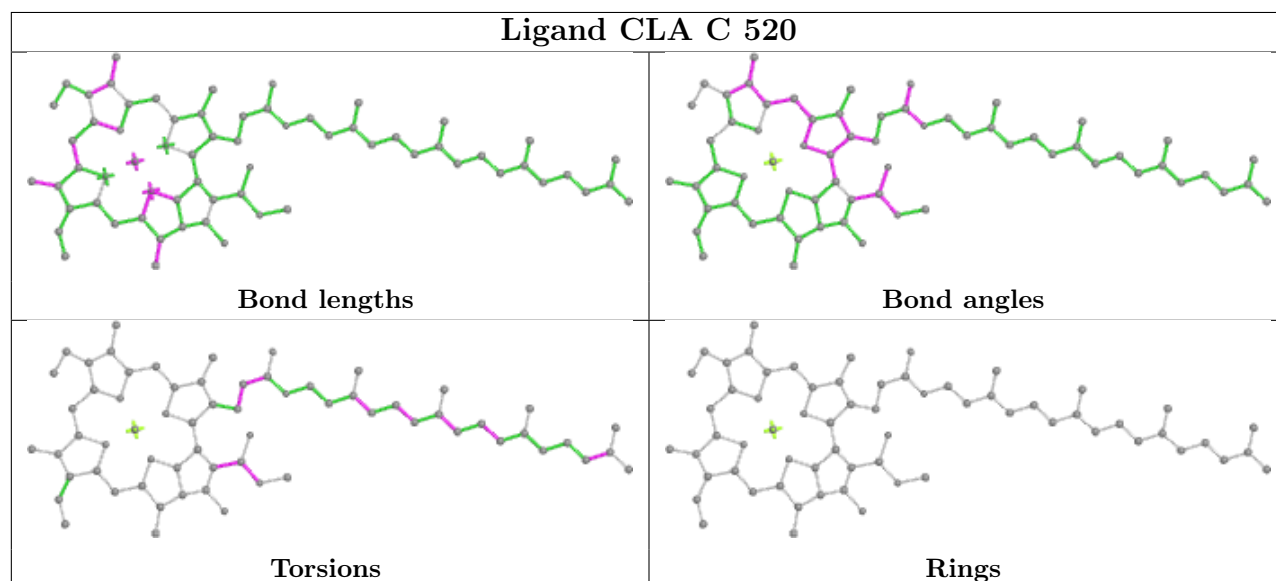
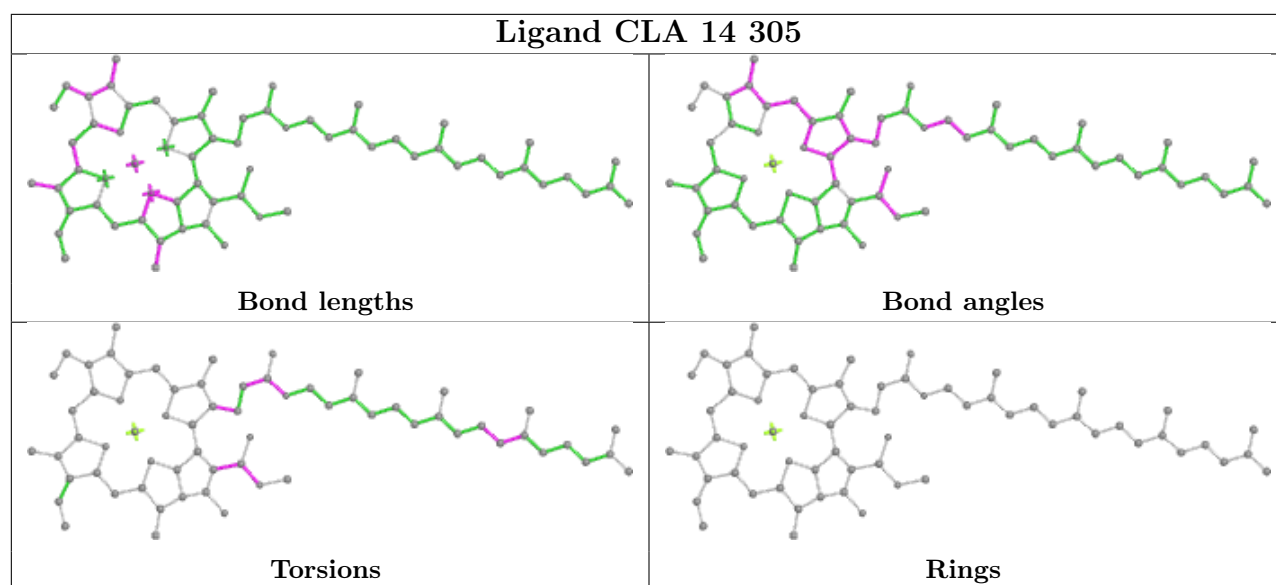


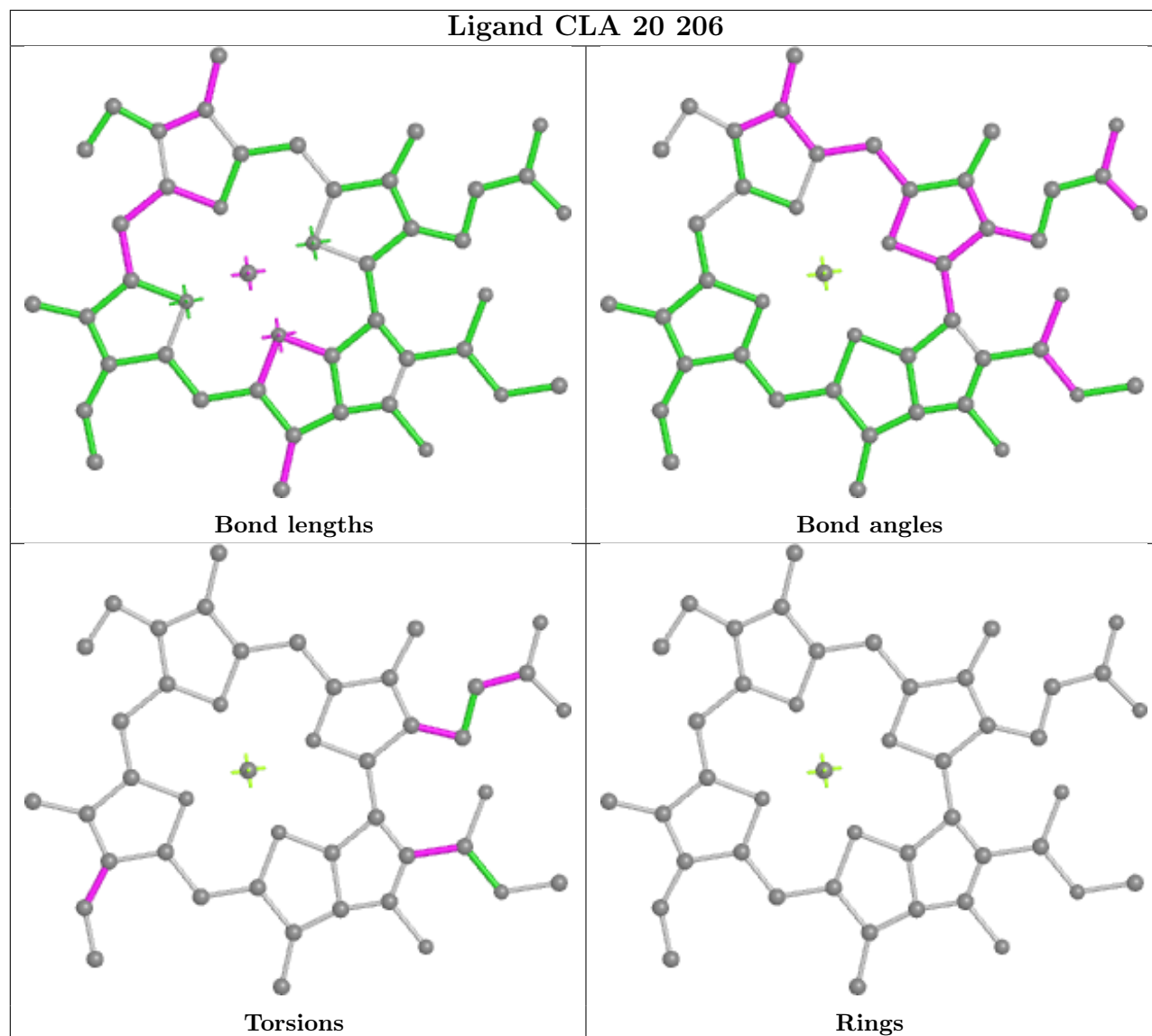


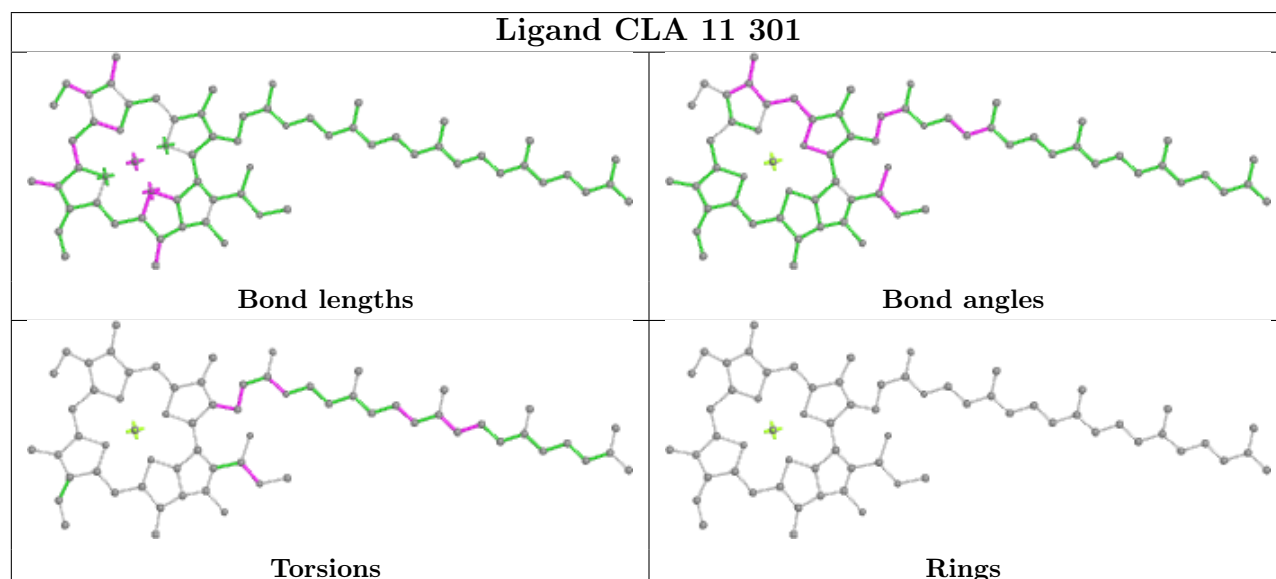
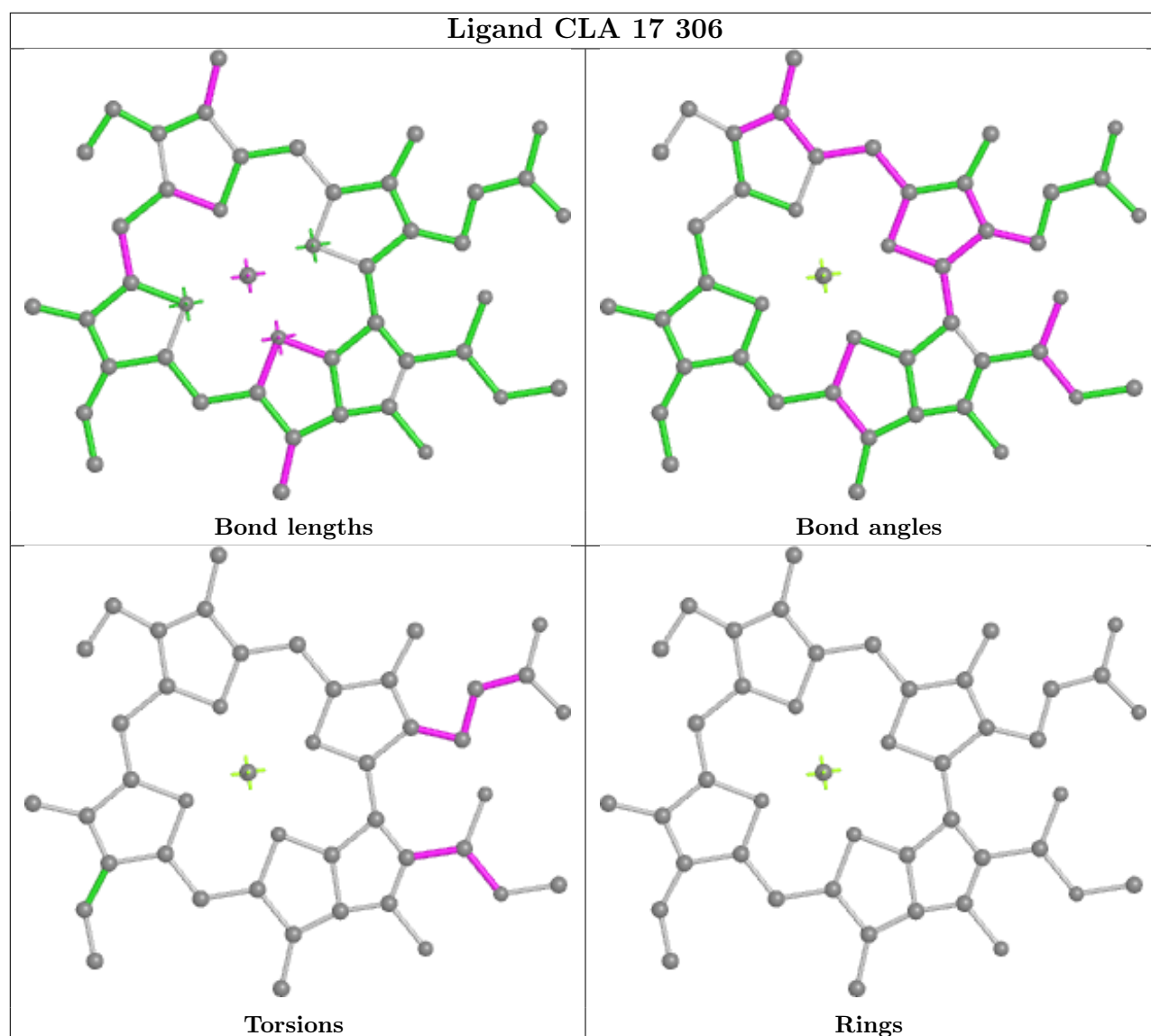


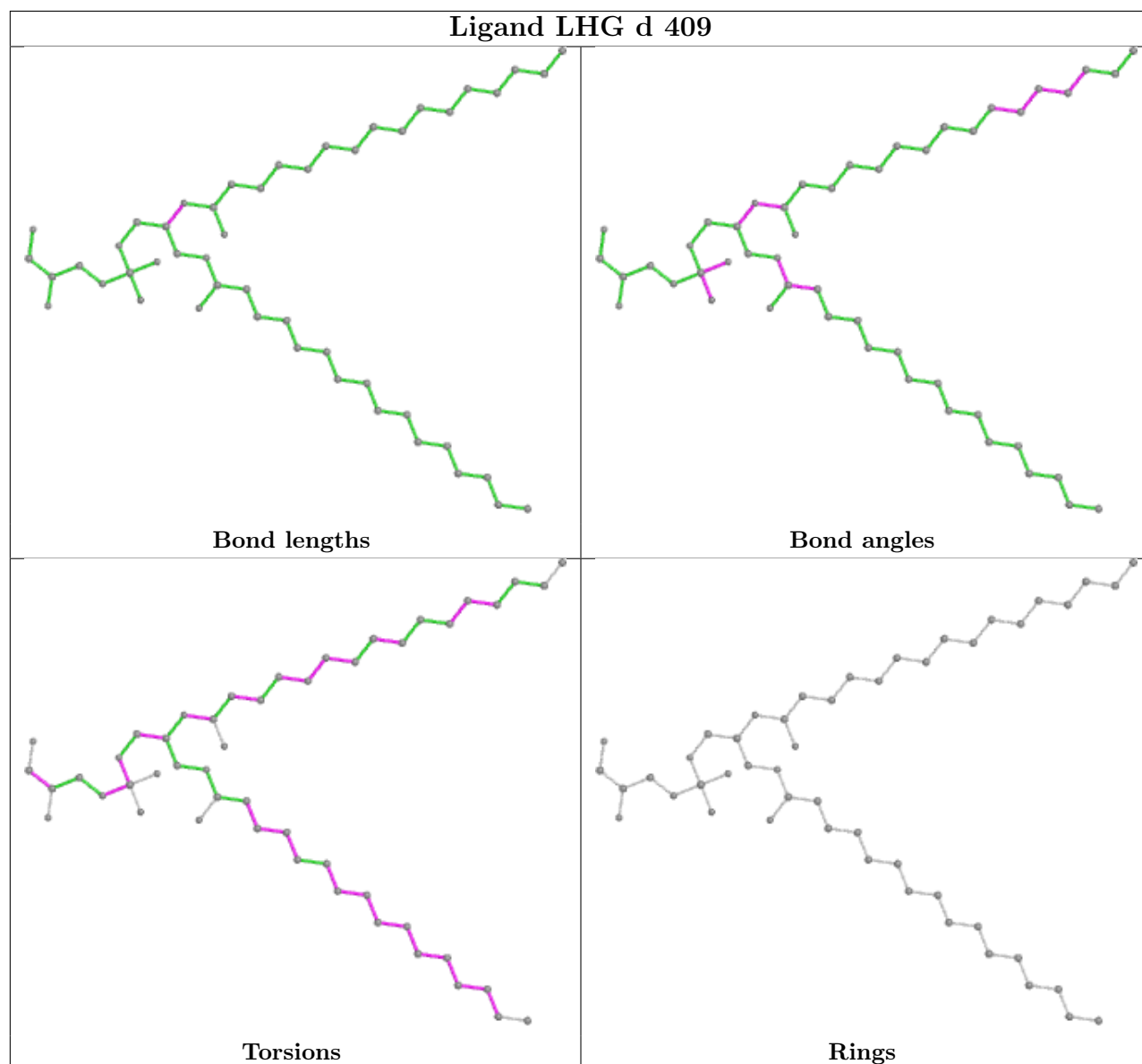
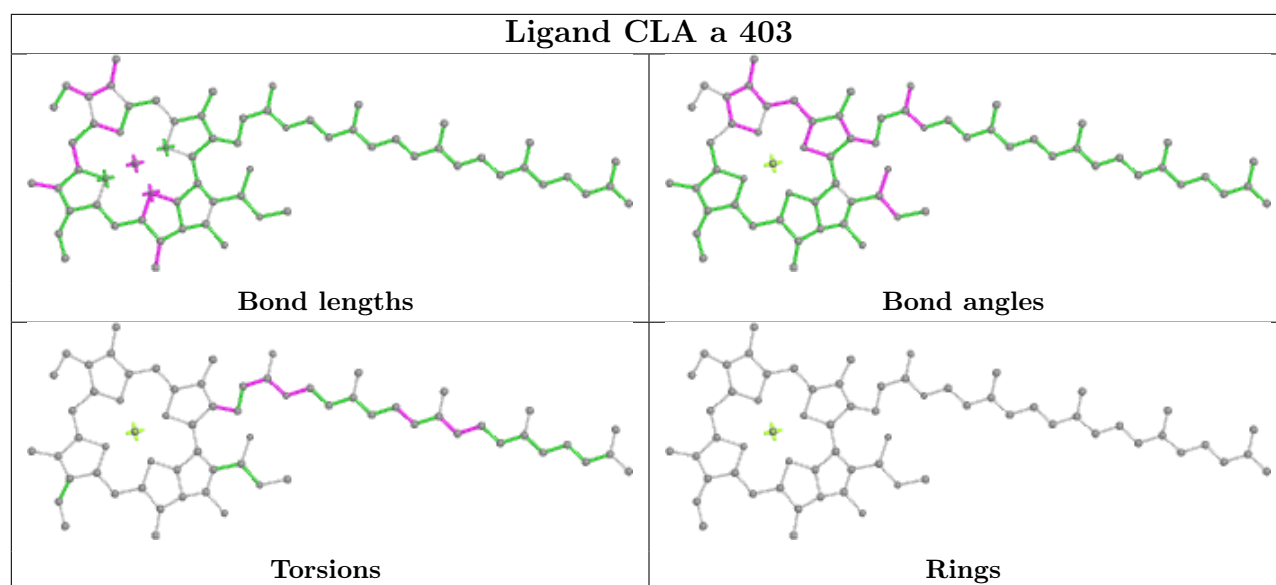


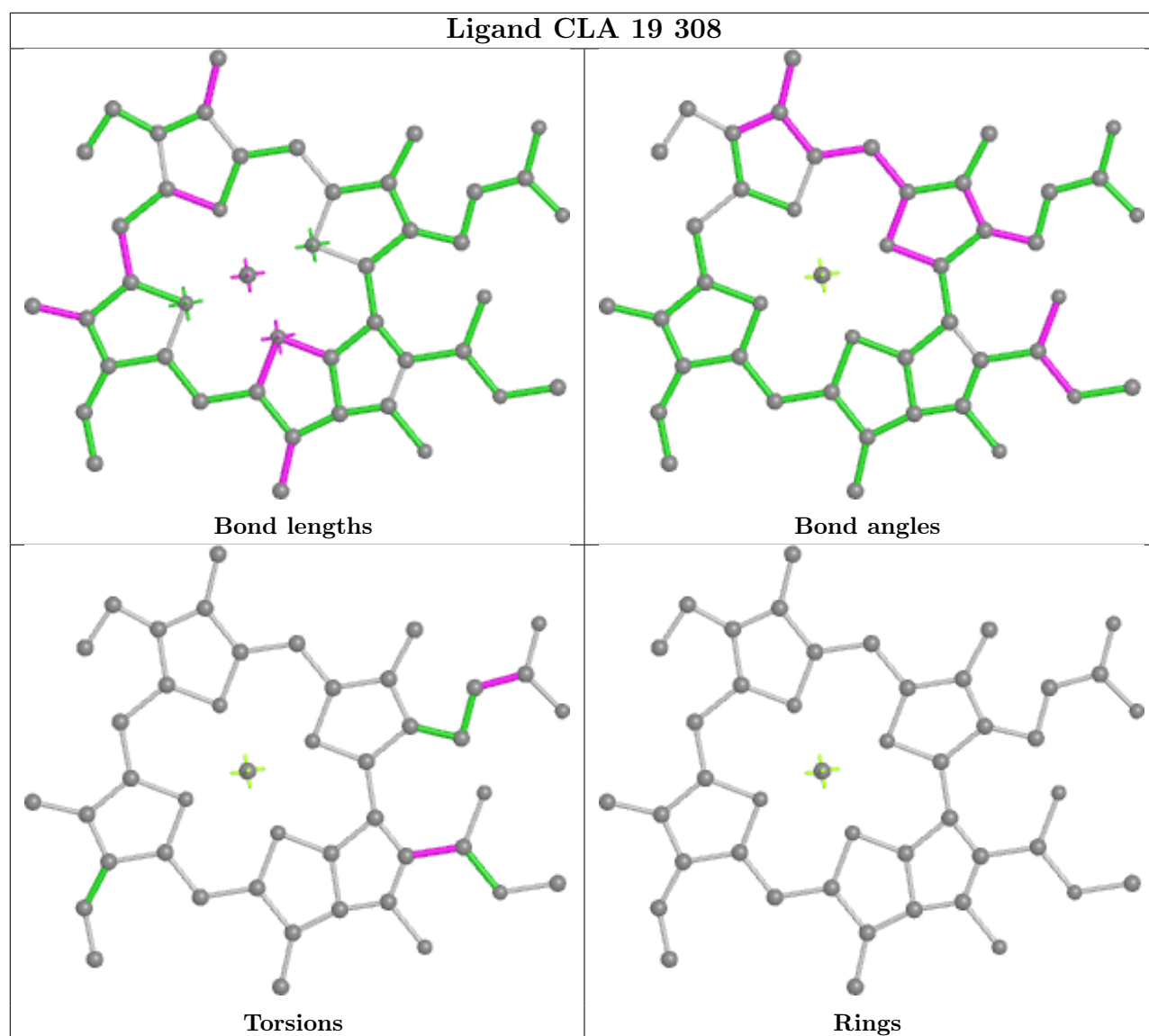


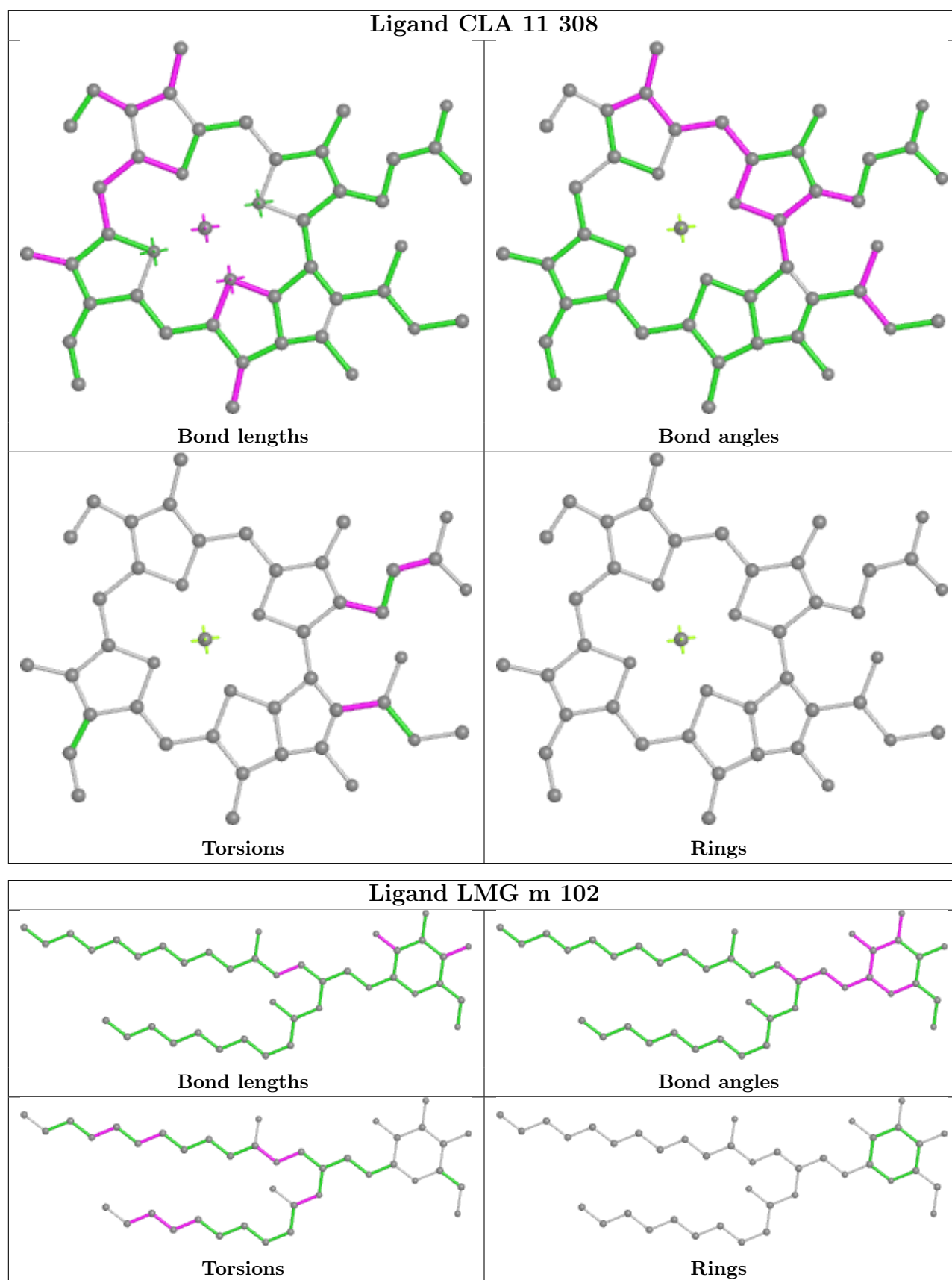


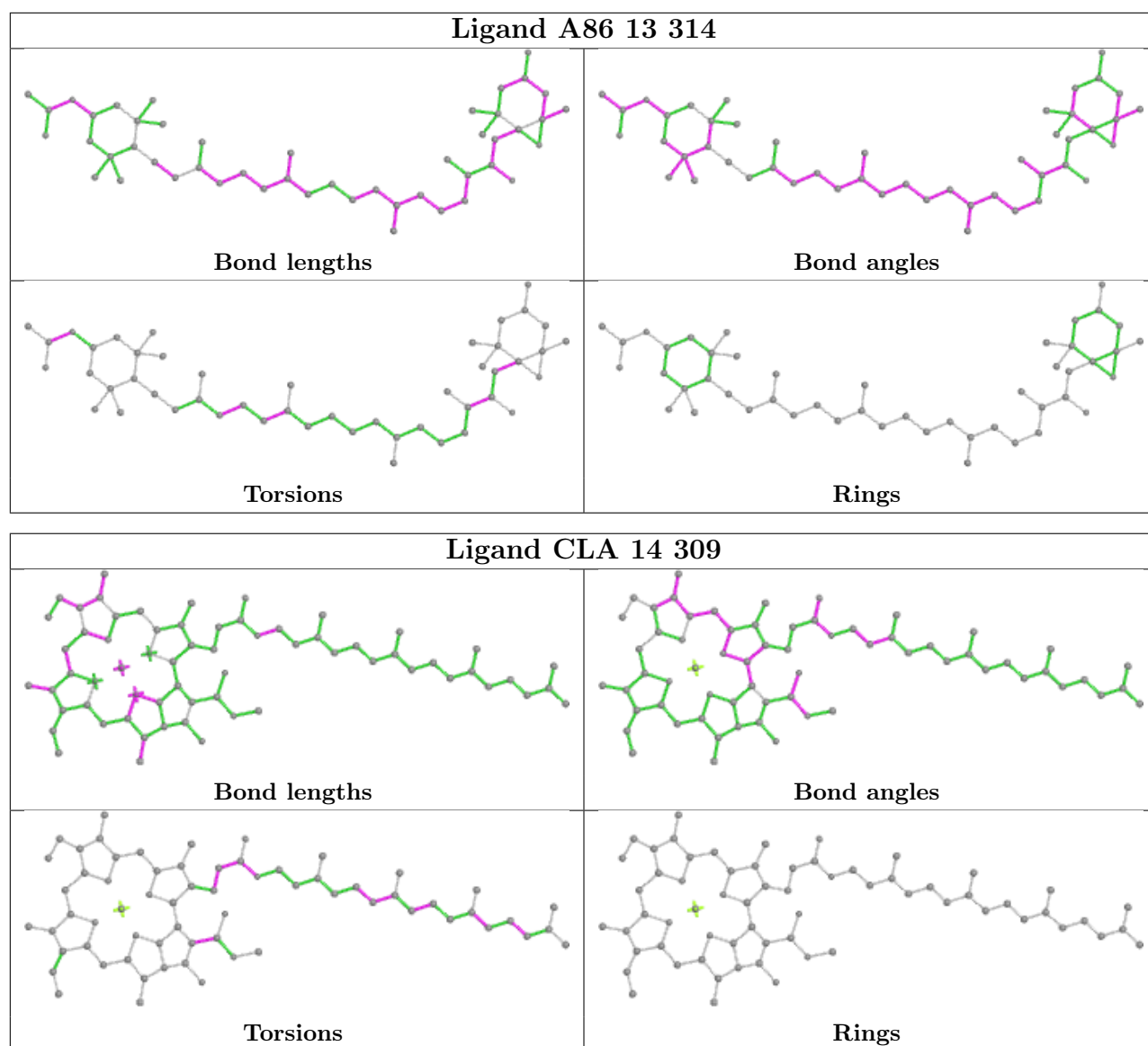


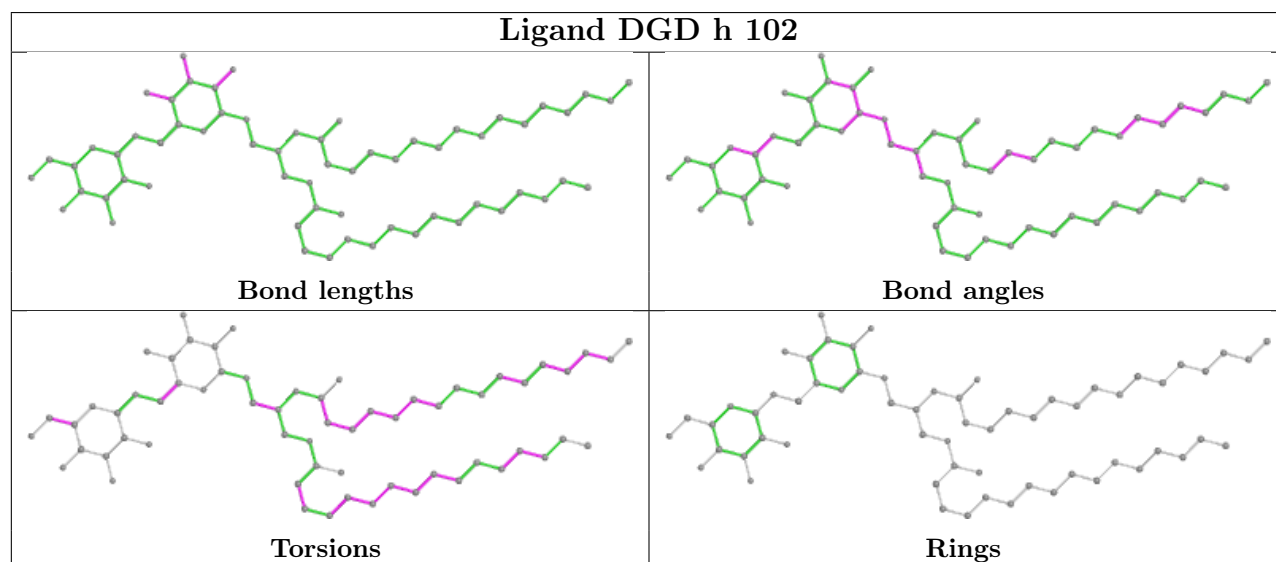
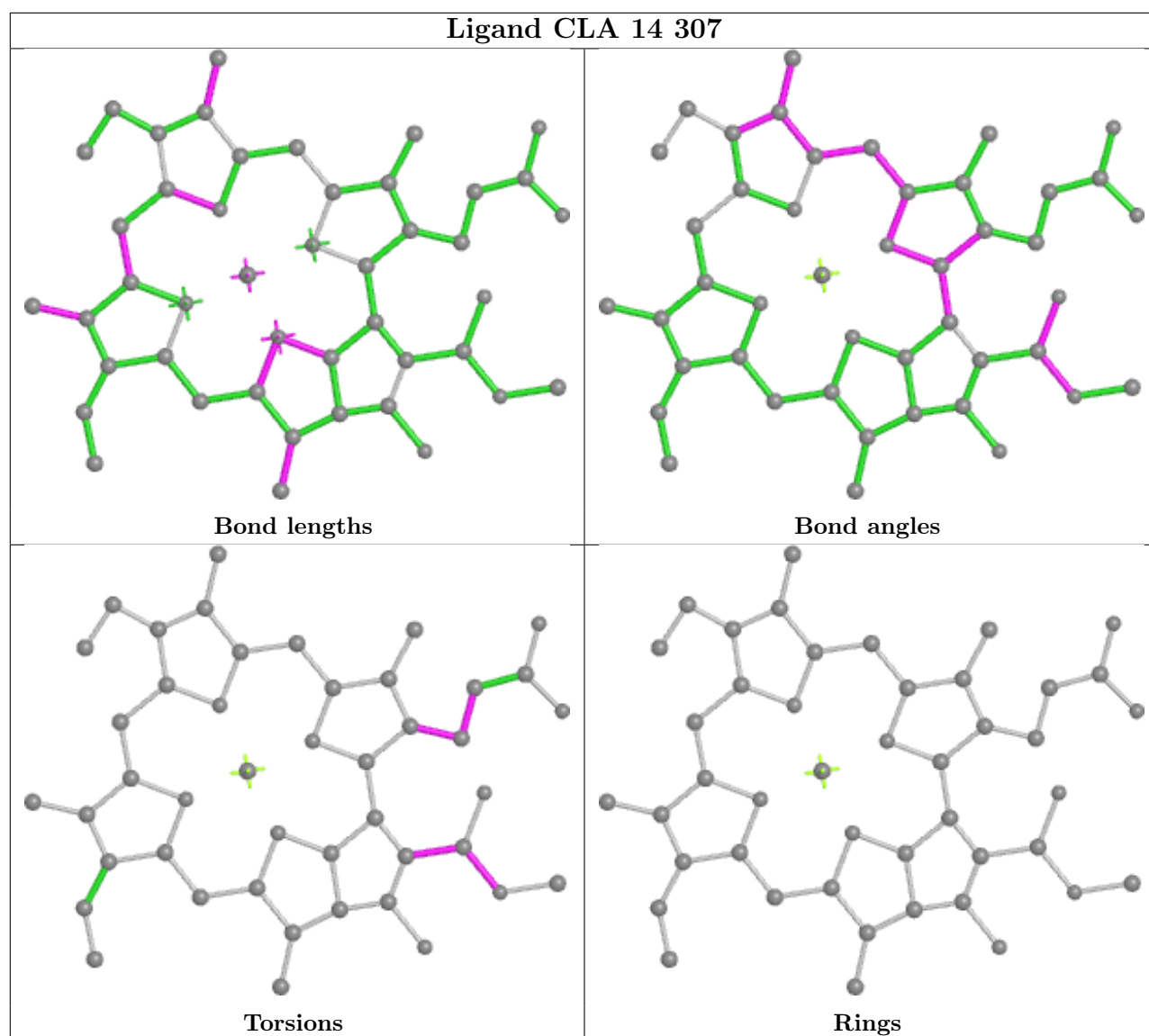




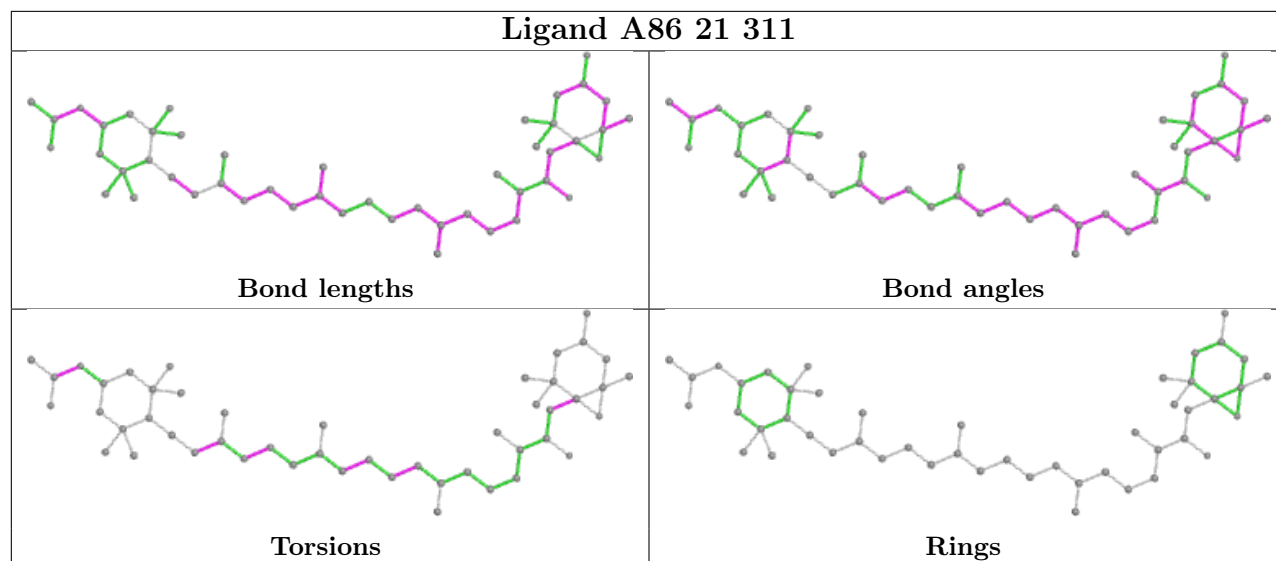




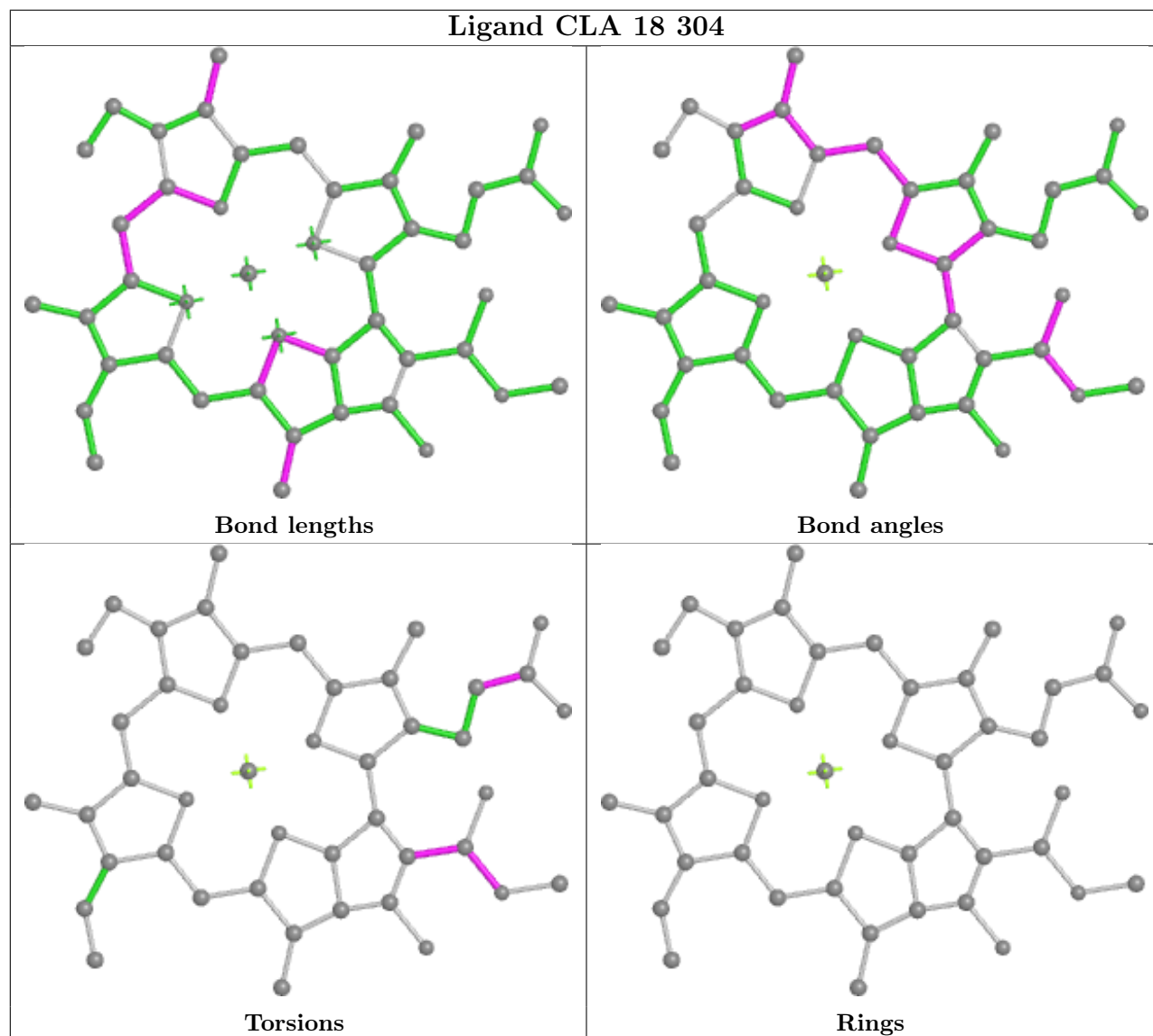


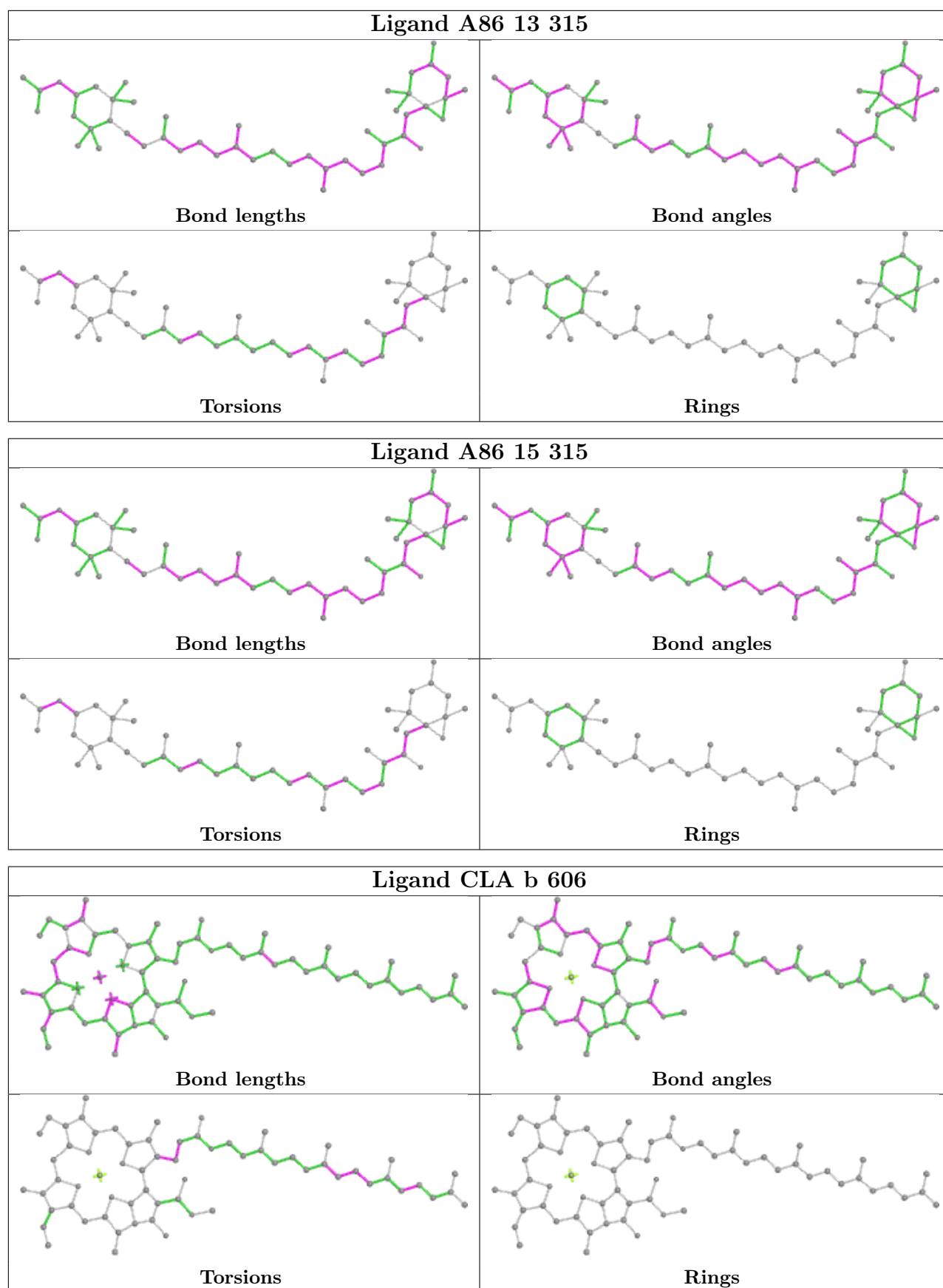


Ligand A86 21 311

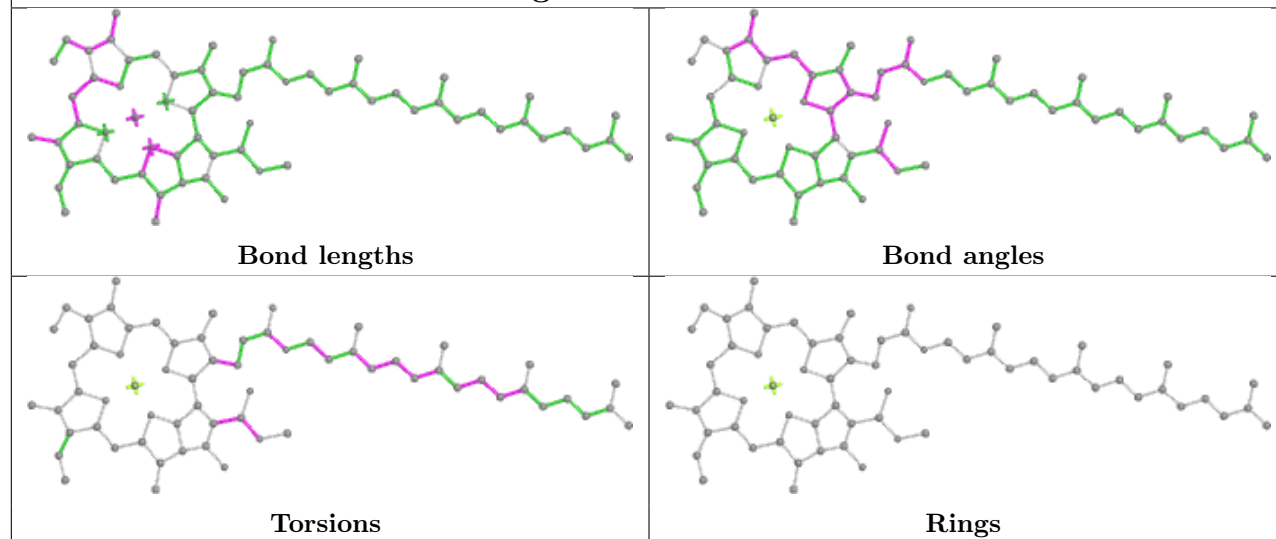


Ligand CLA 18 304

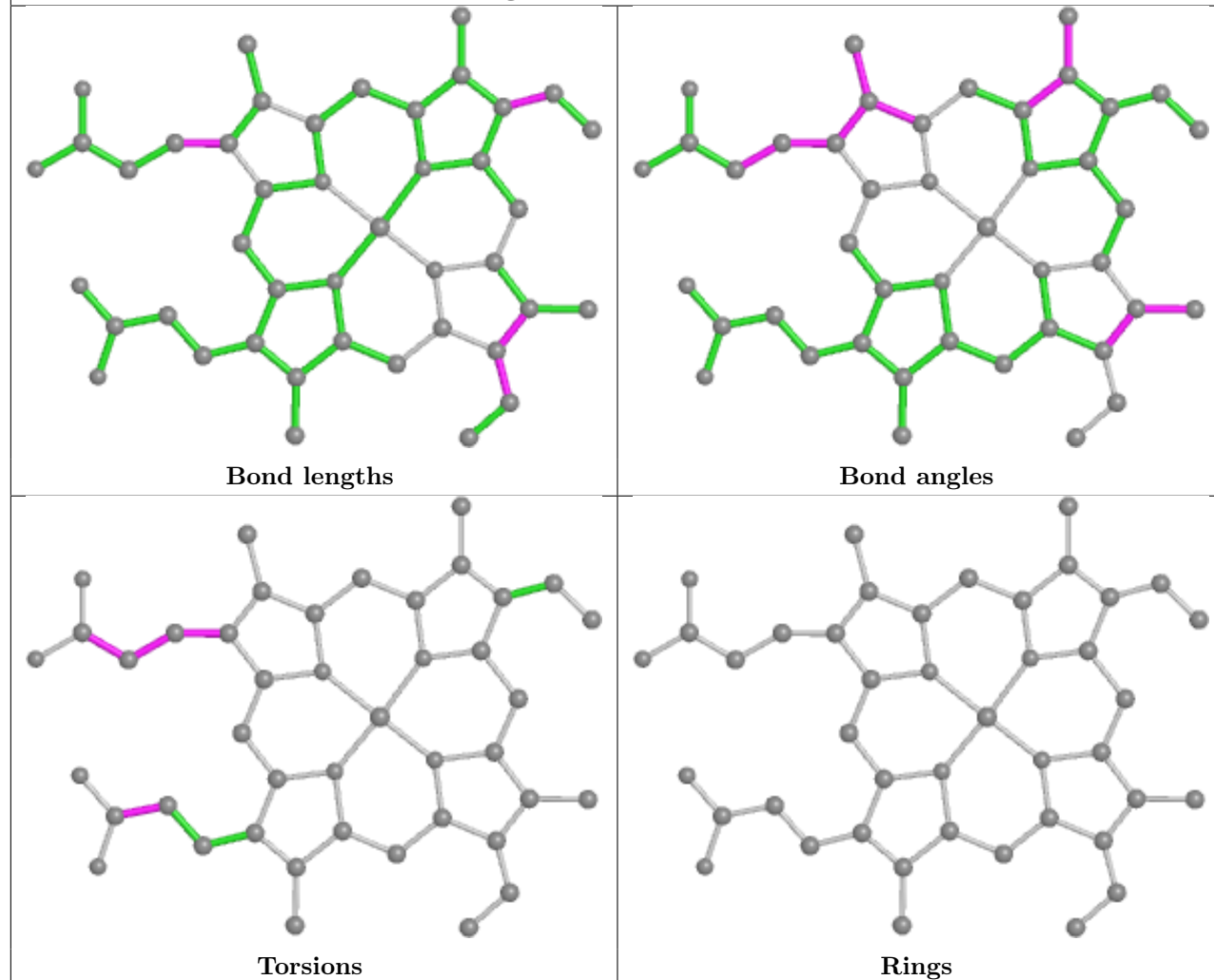


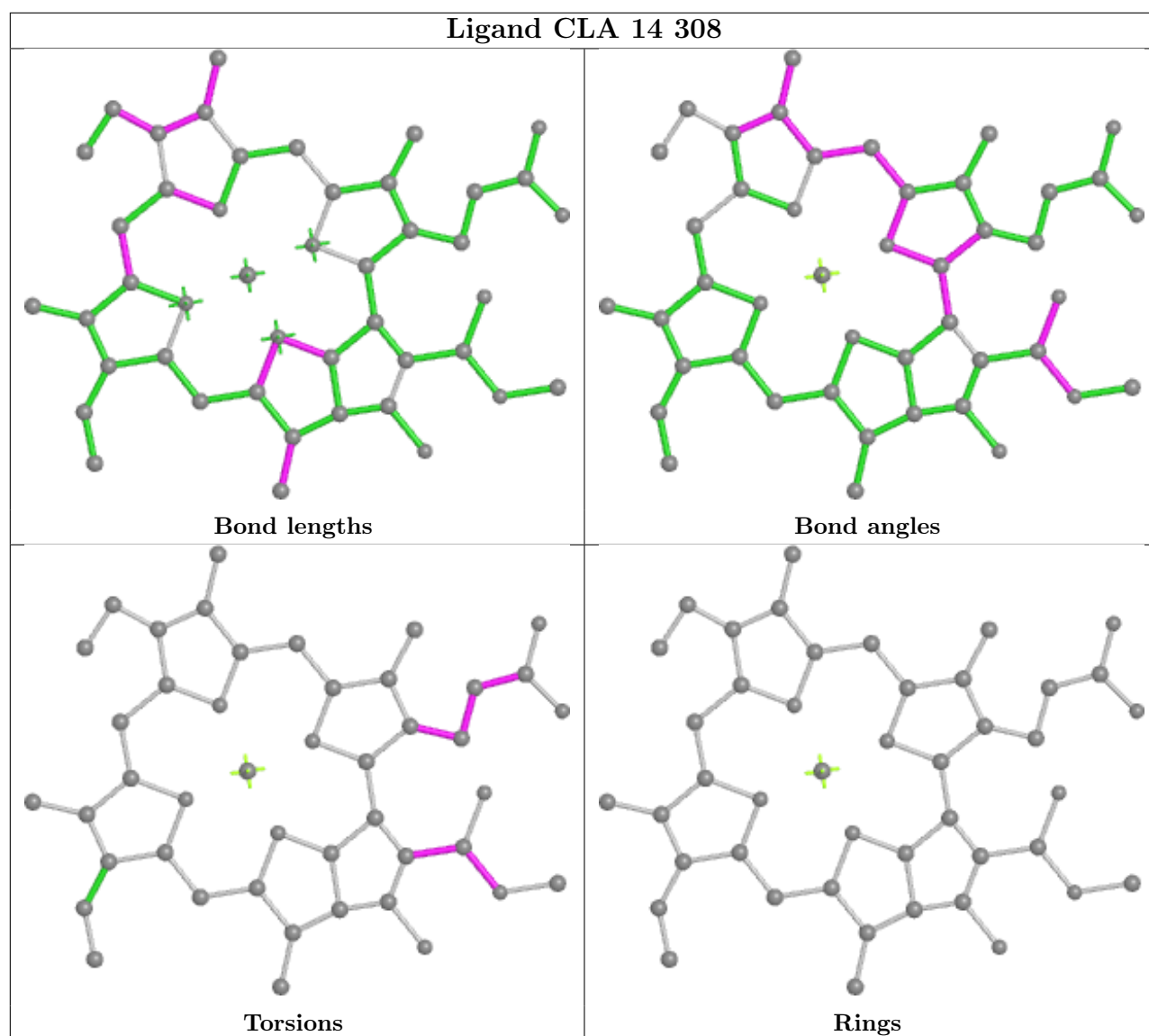


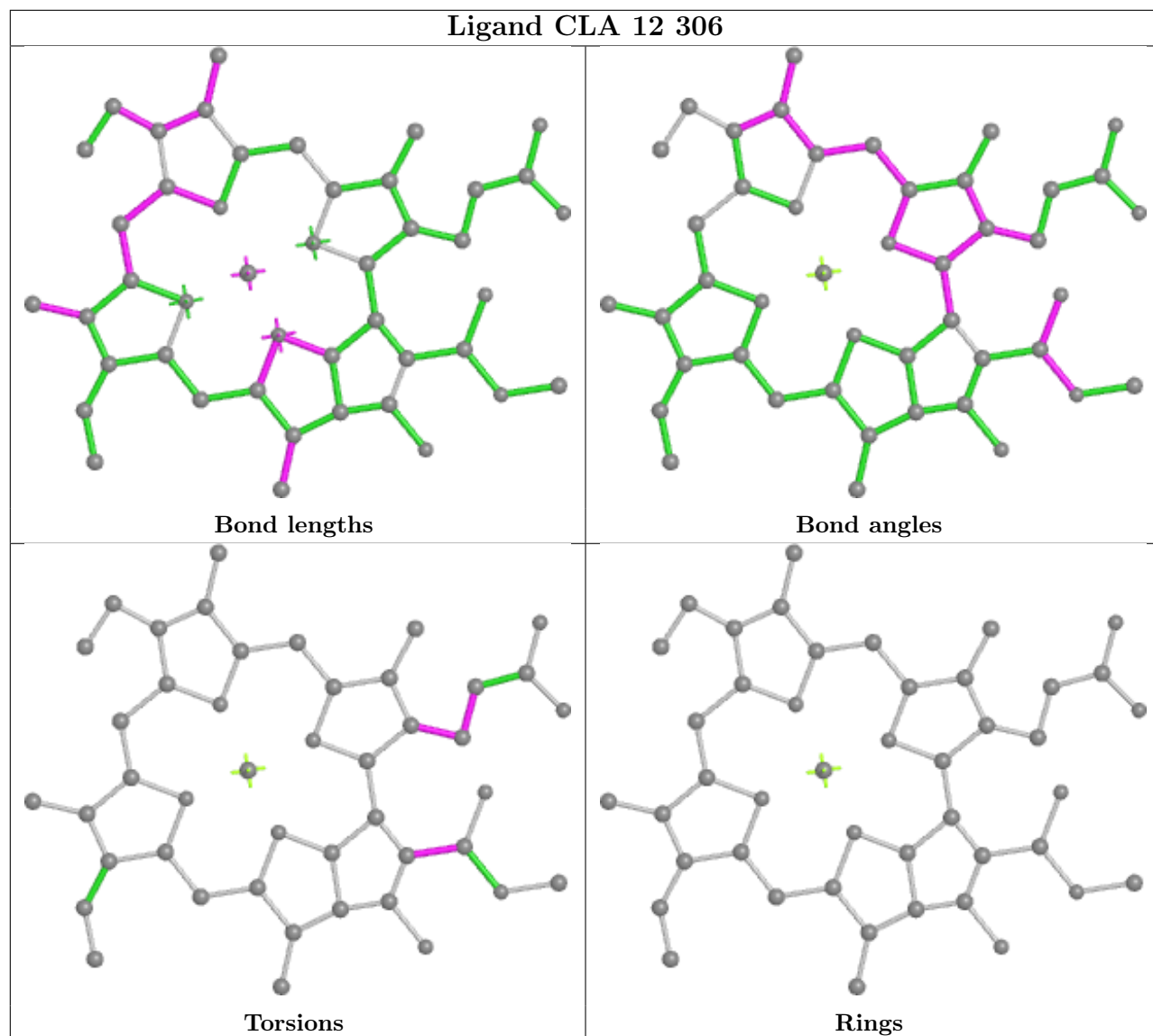
Ligand CLA C 504

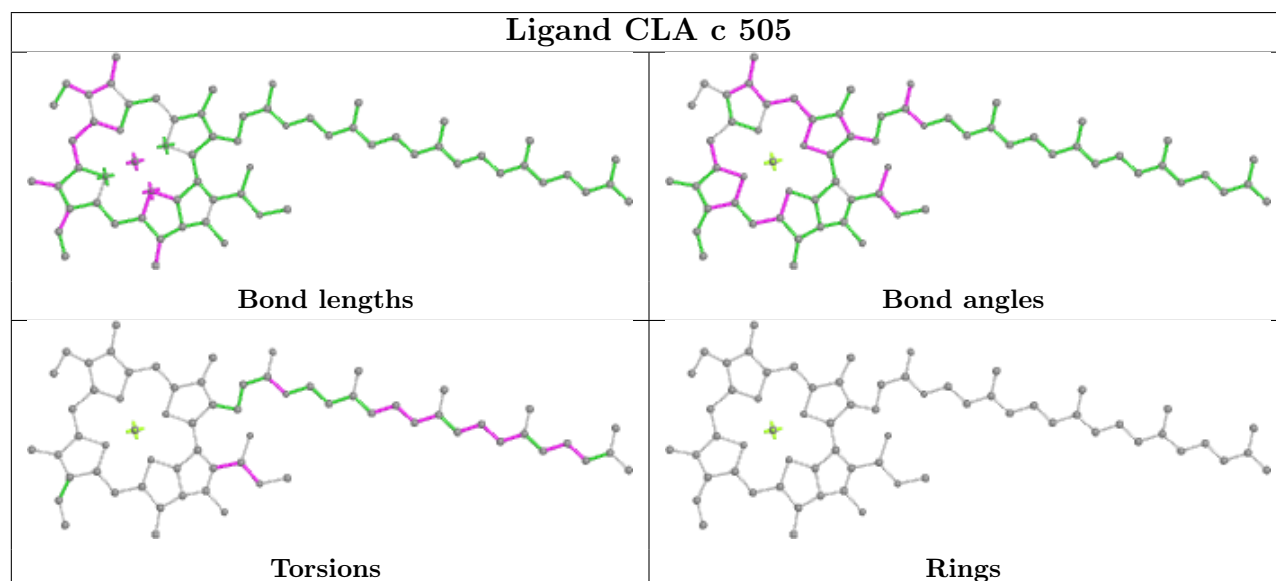
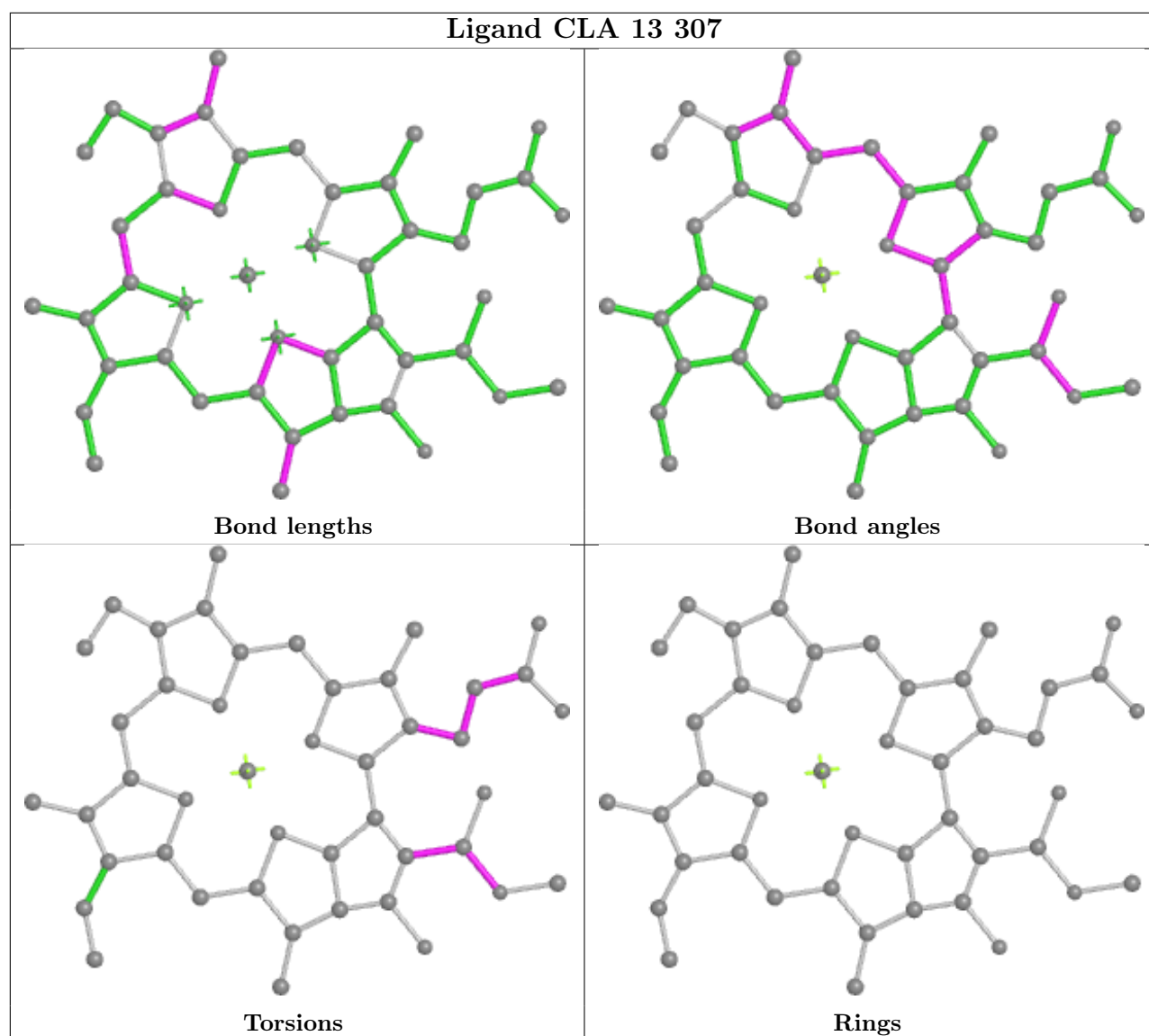


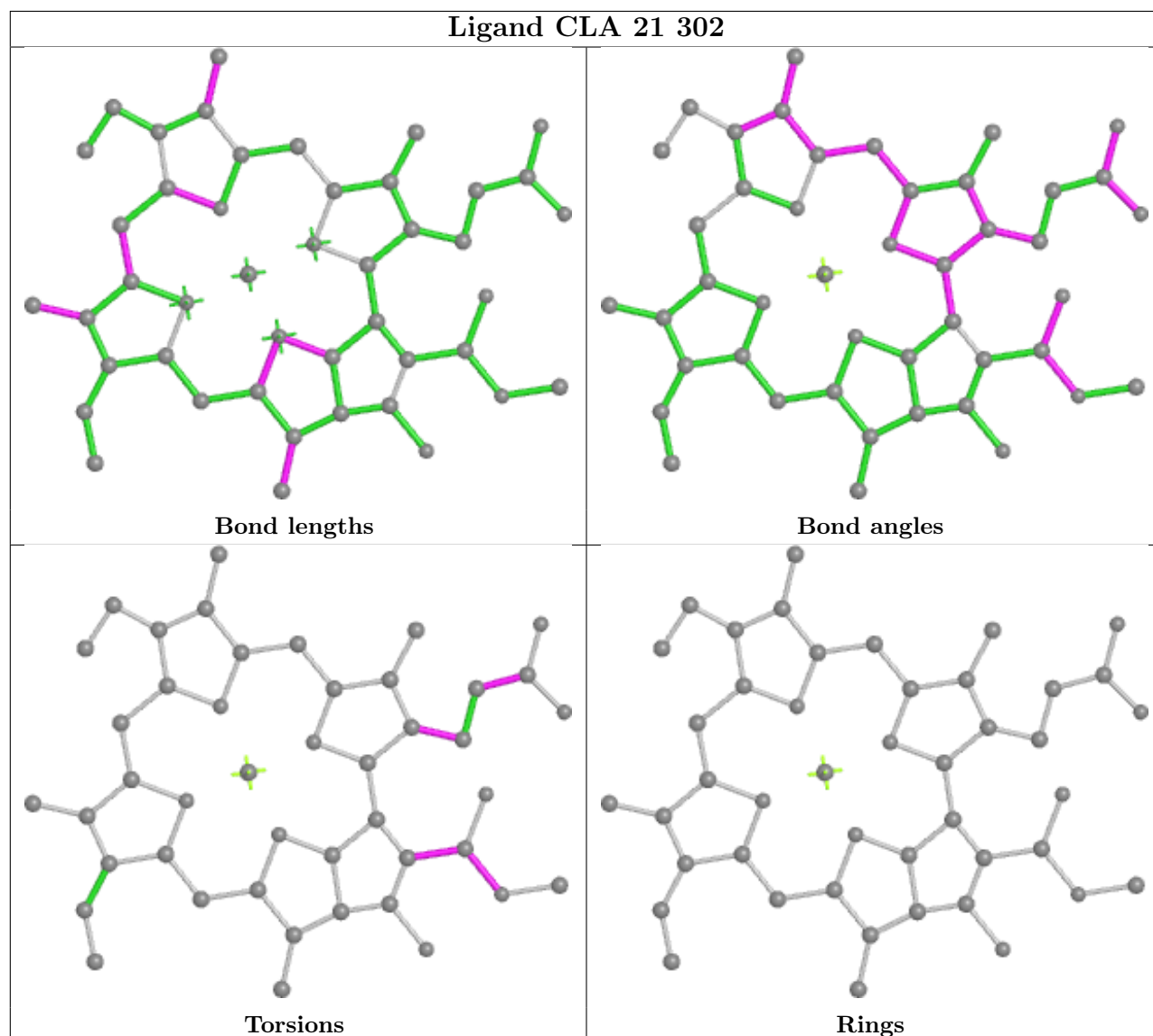
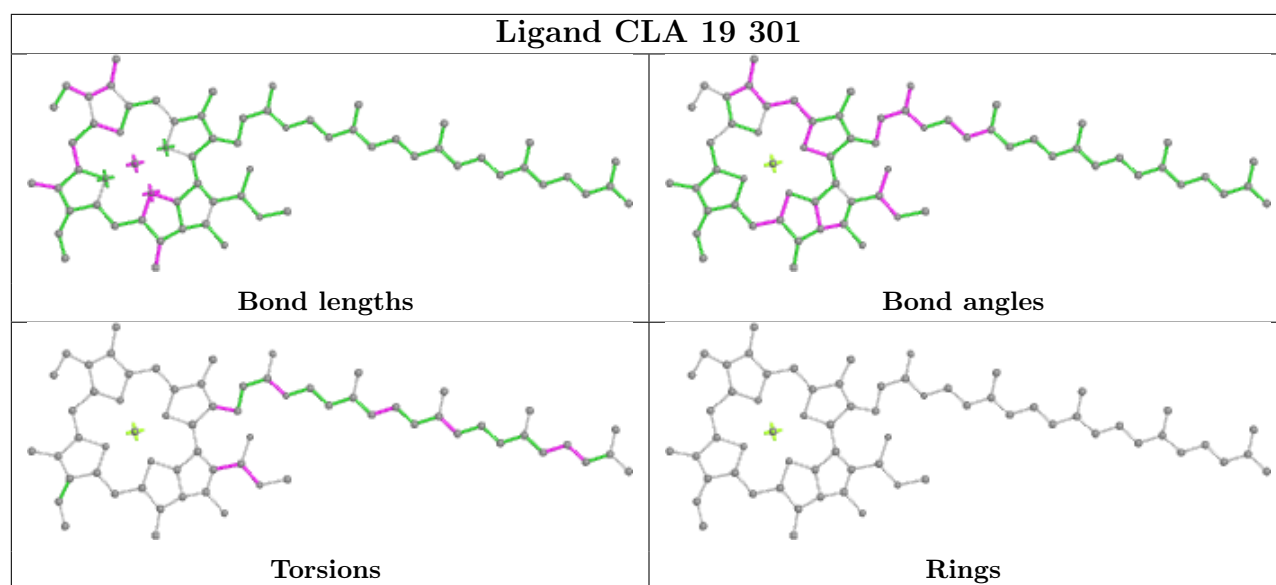
Ligand HEM F 102

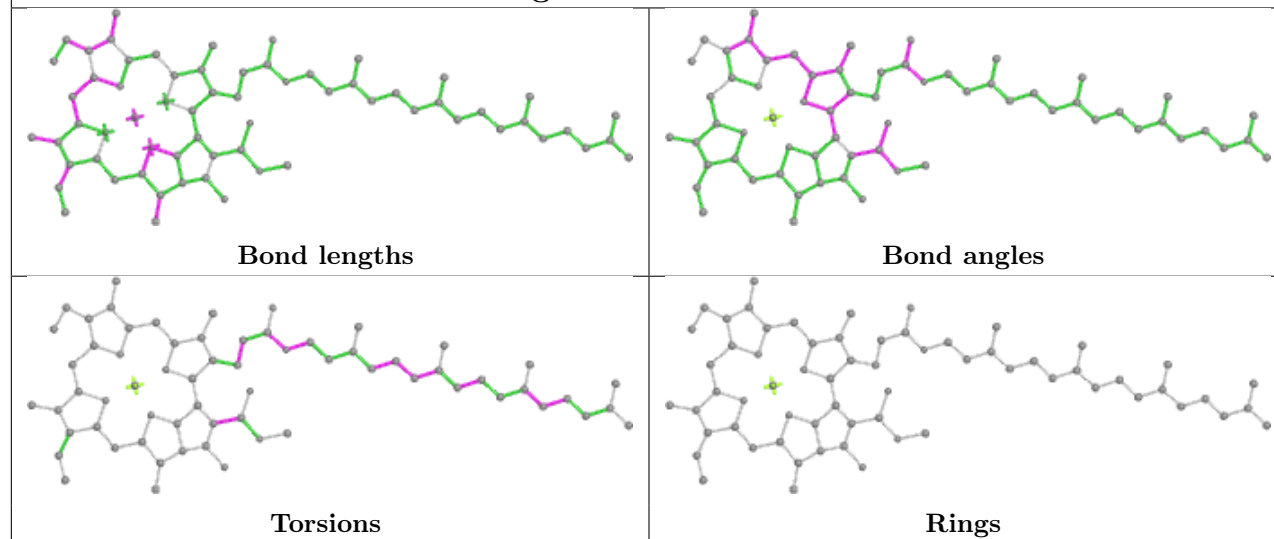
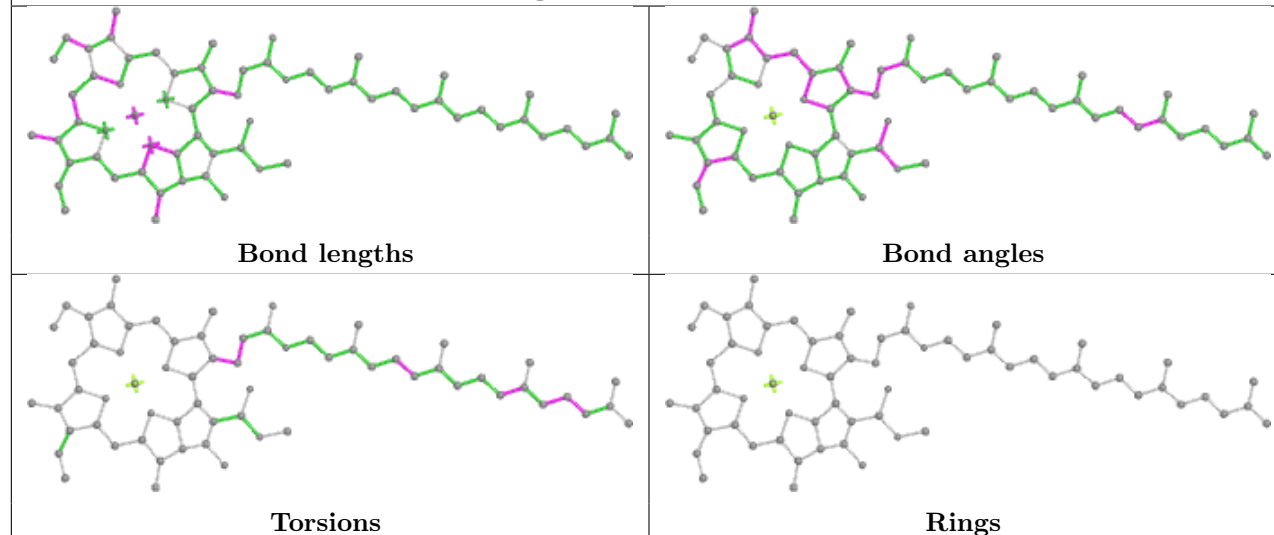
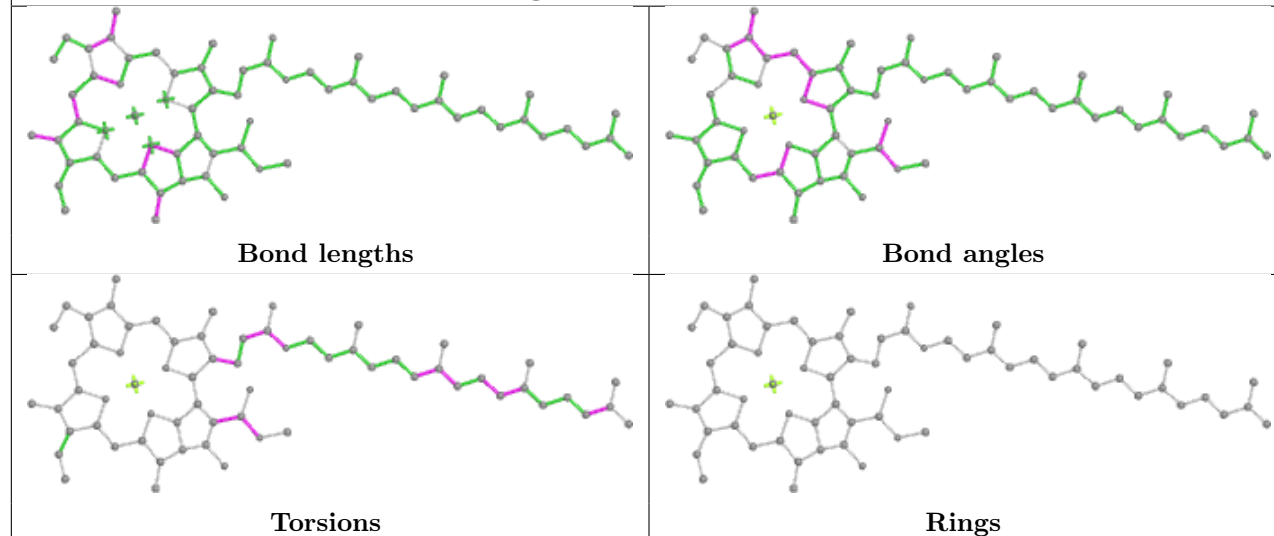


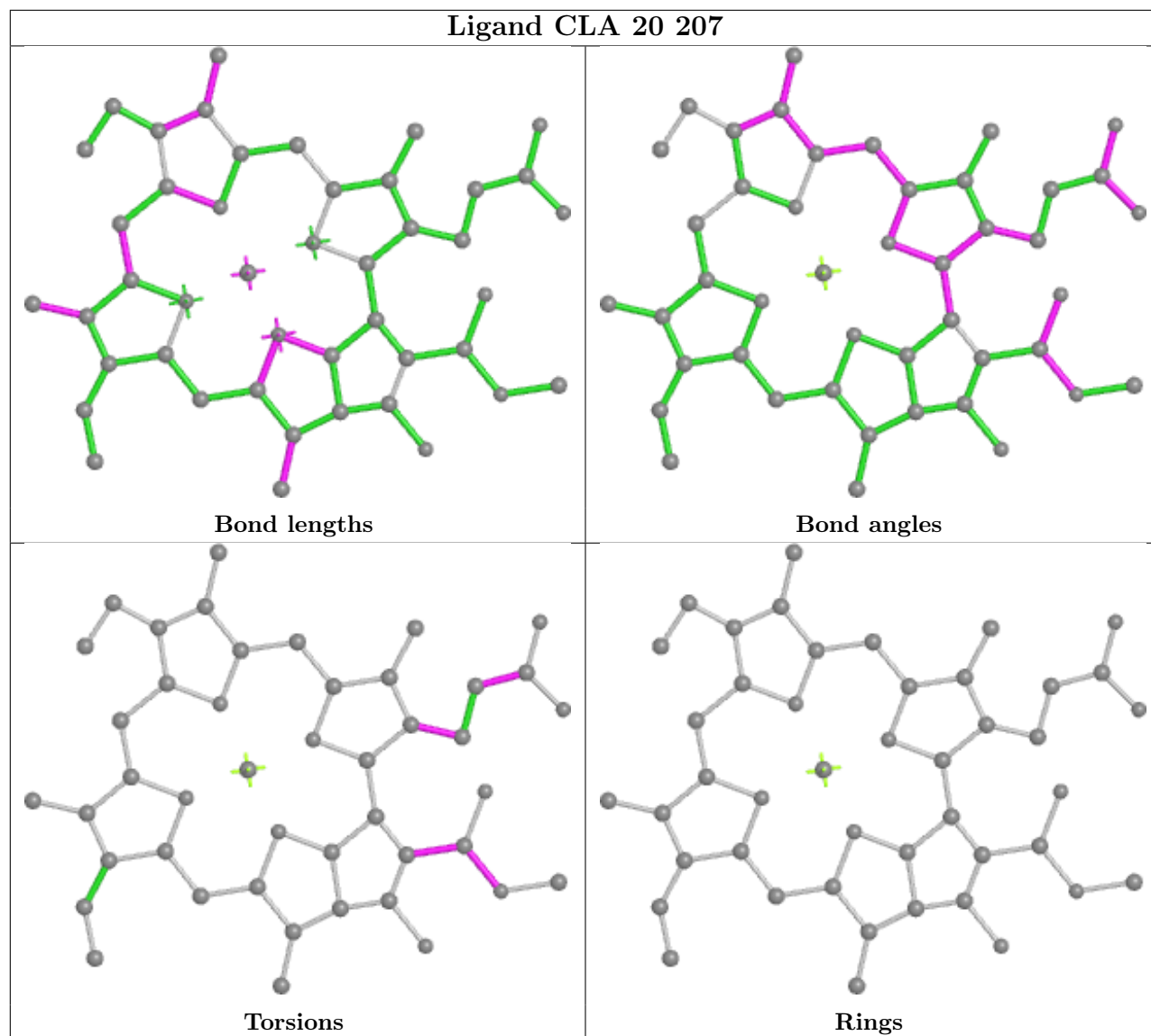
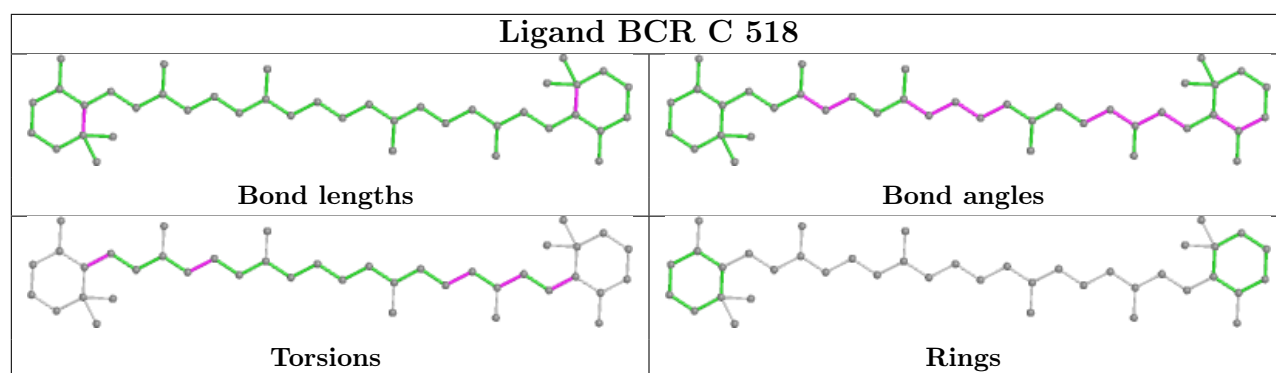


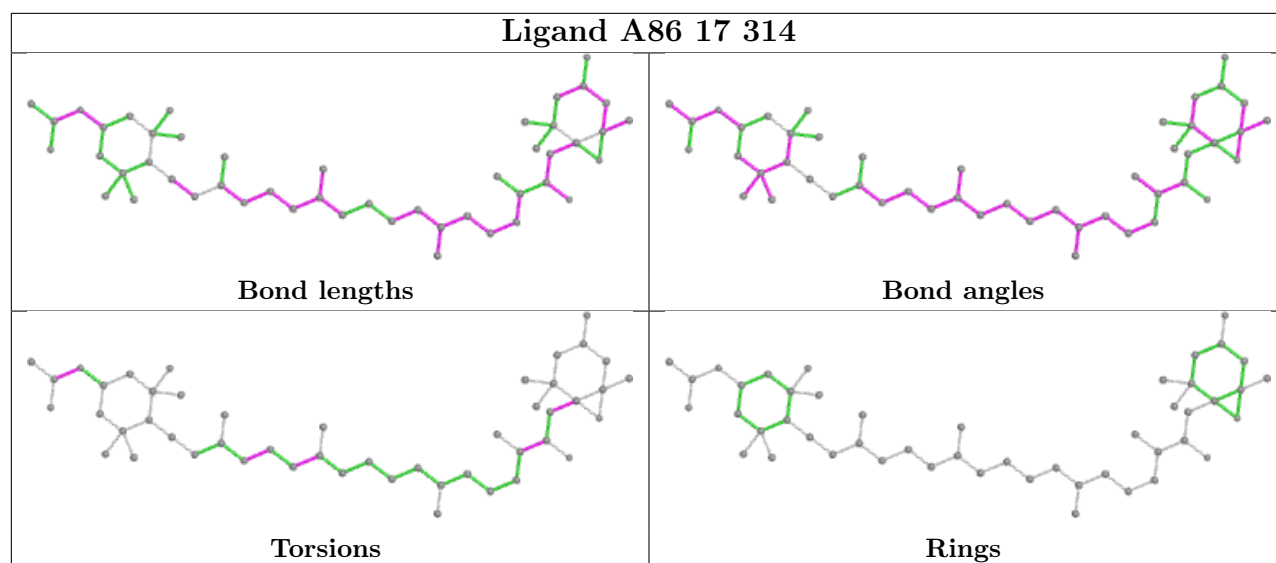
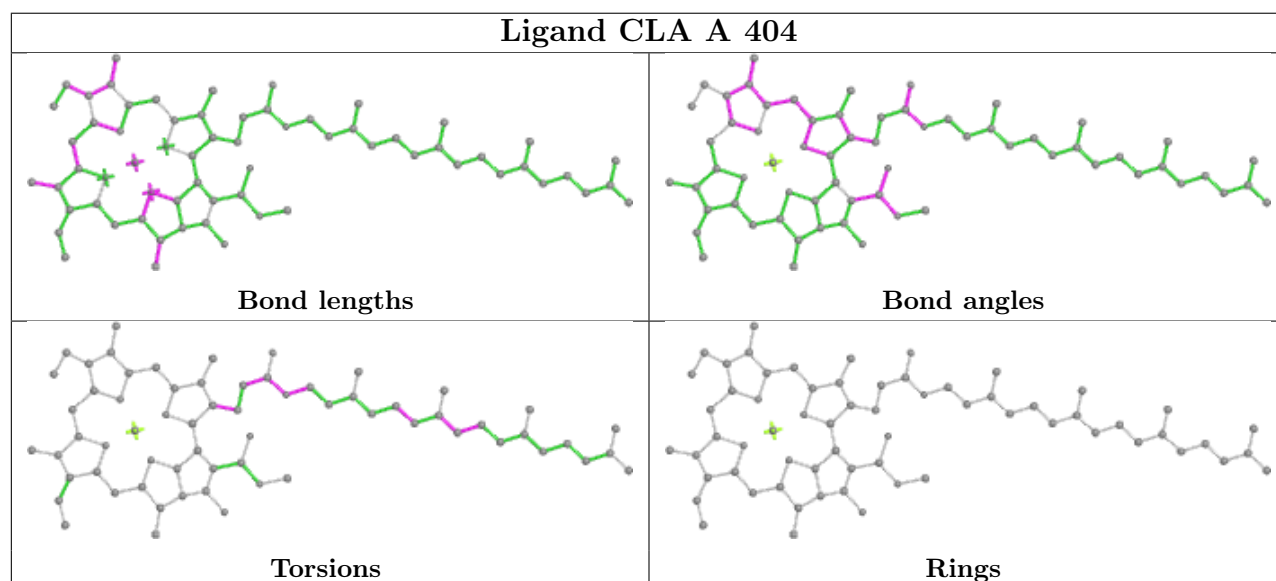
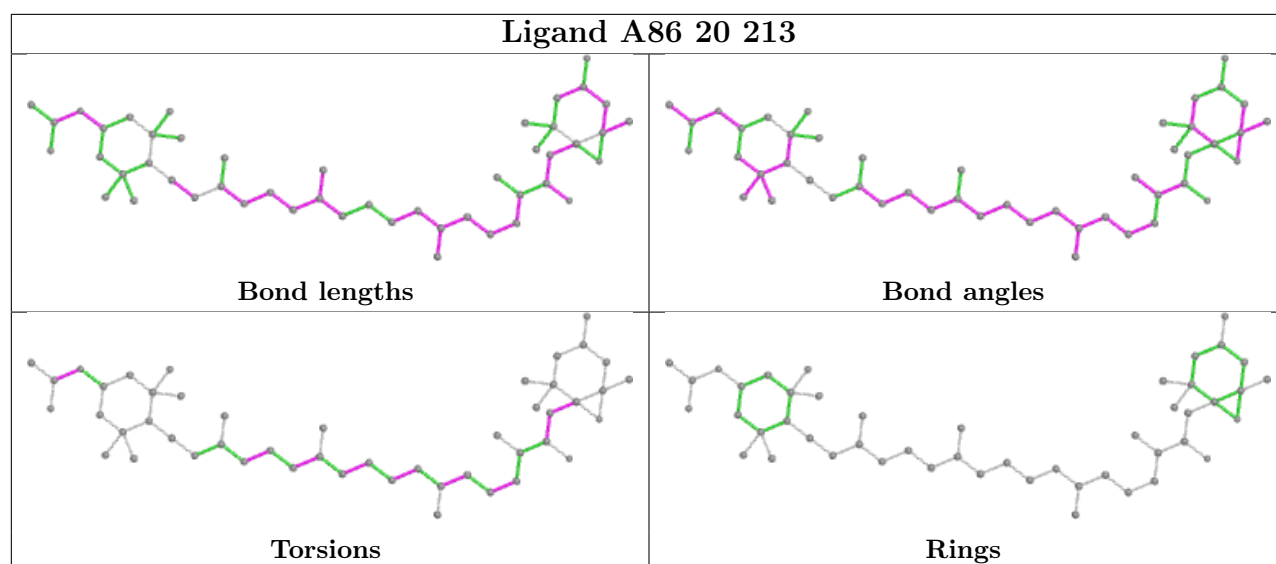


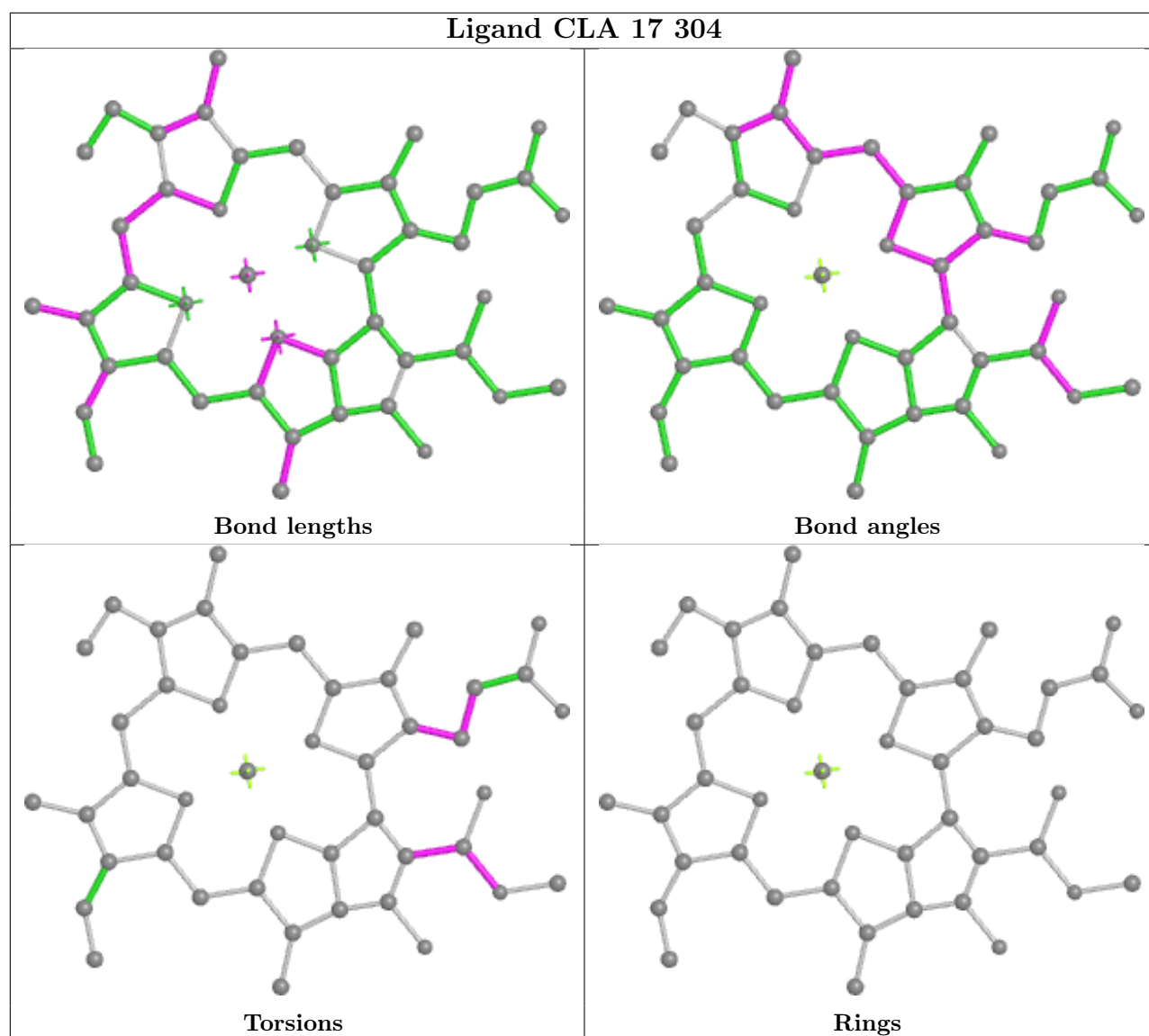


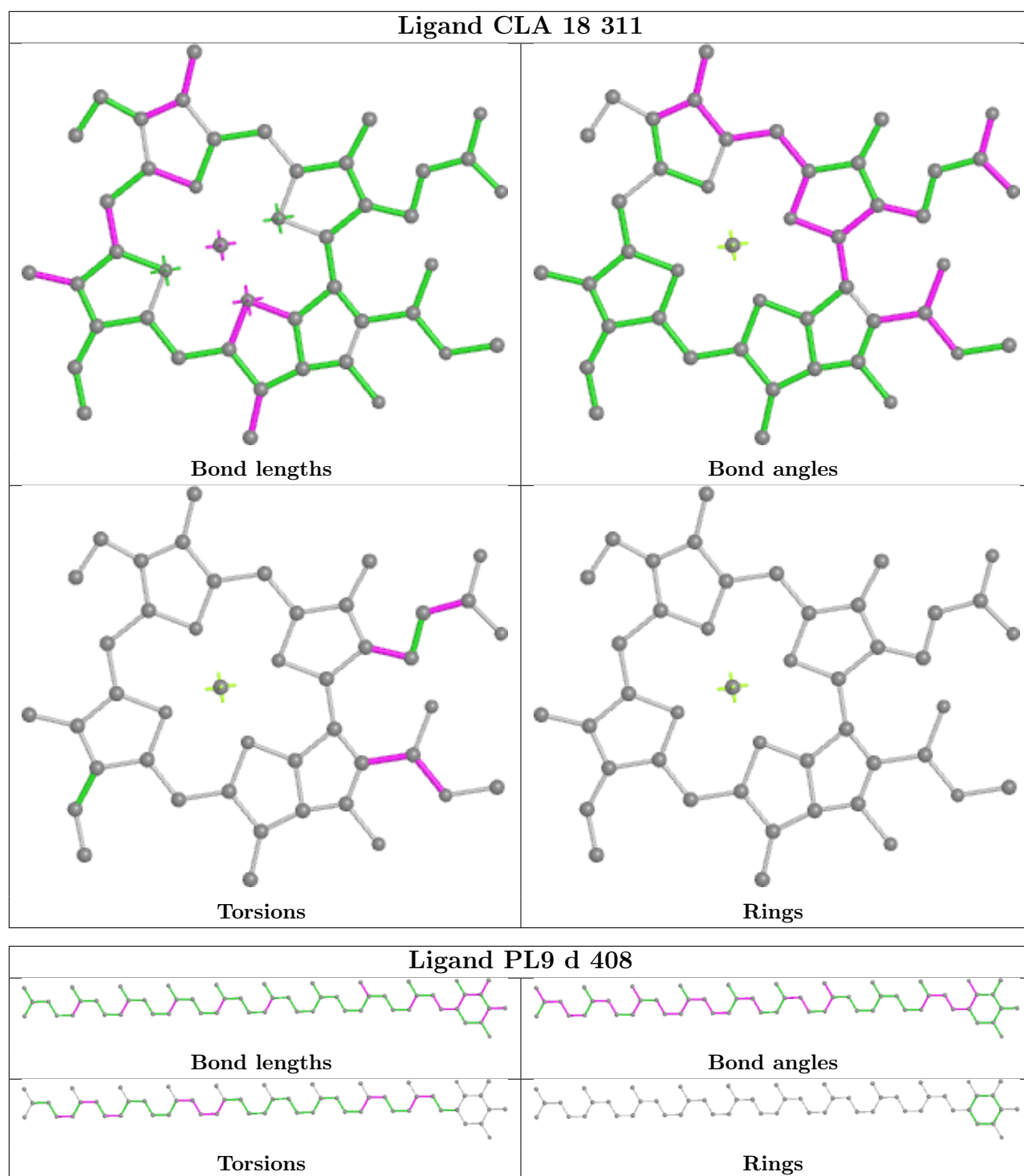


Ligand CLA B 615**Ligand CLA D 405****Ligand CLA 18 305**

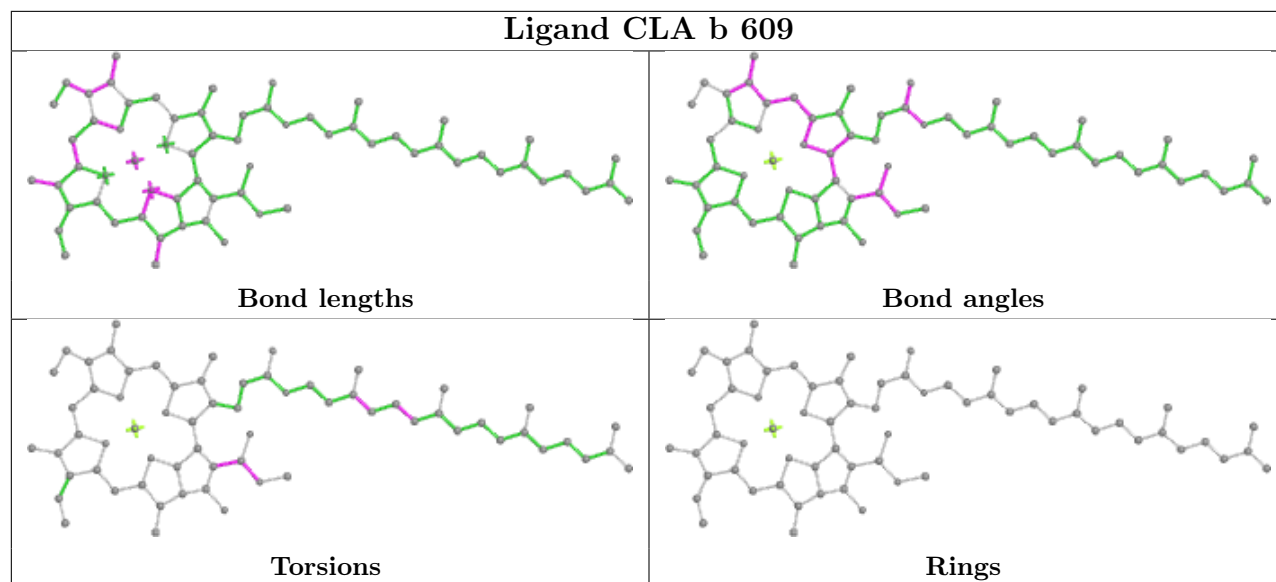




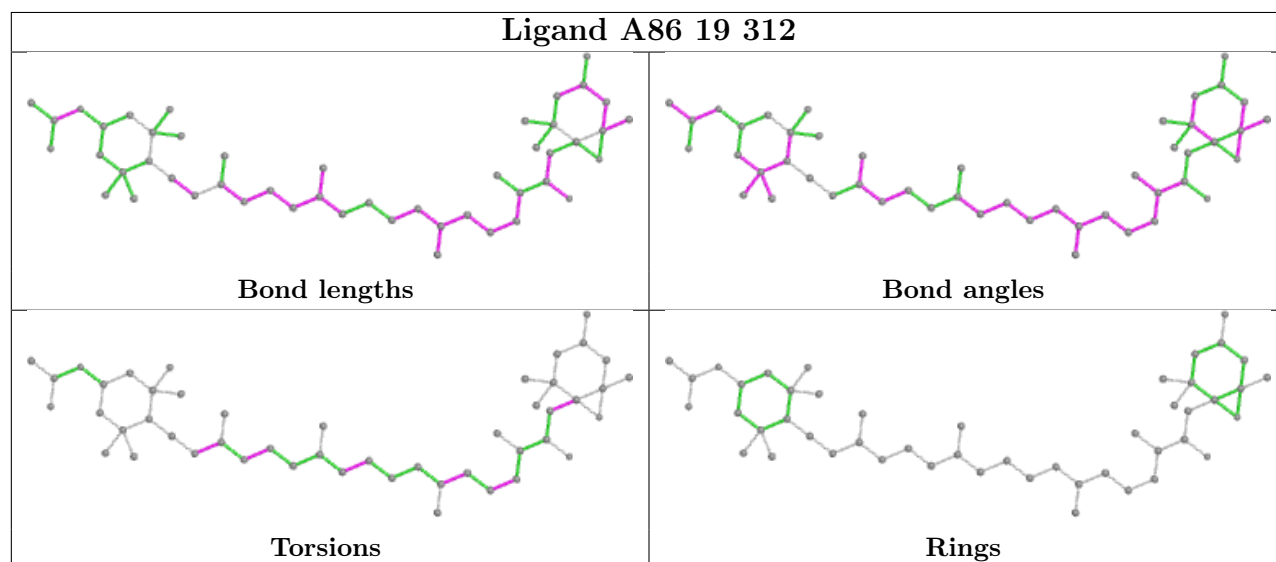


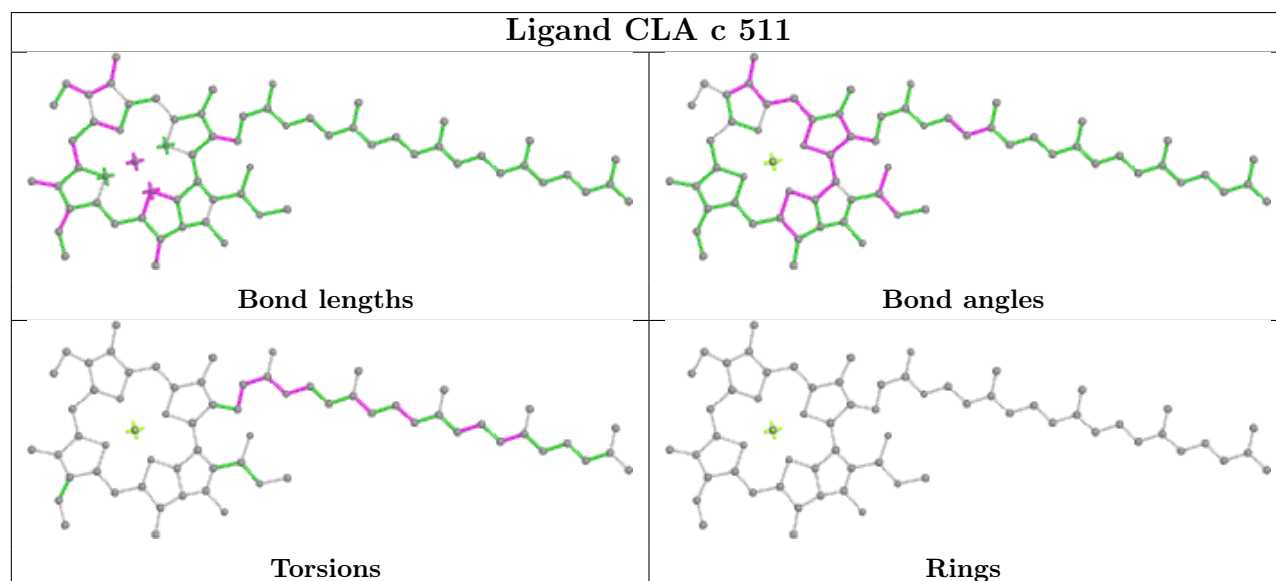
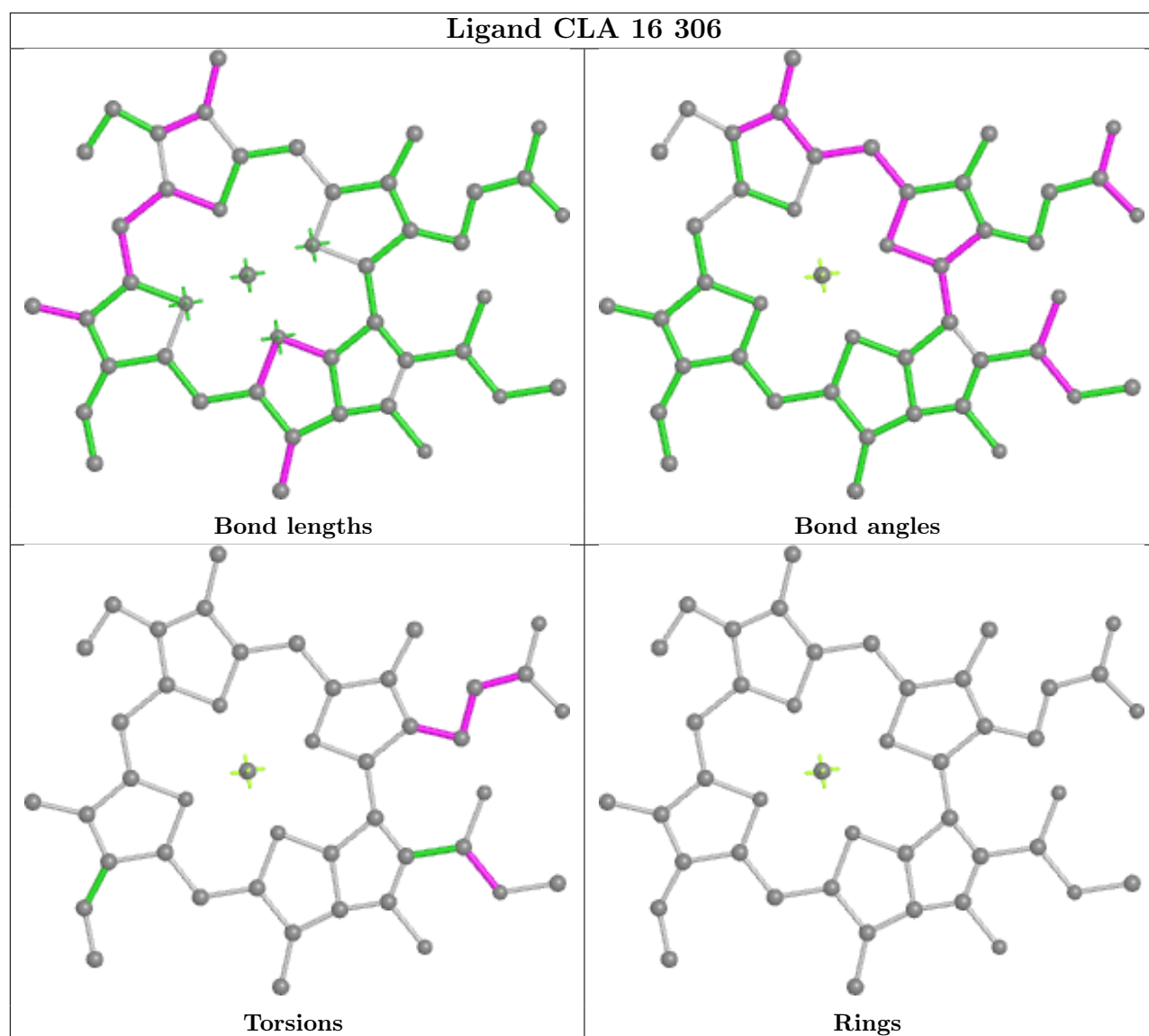


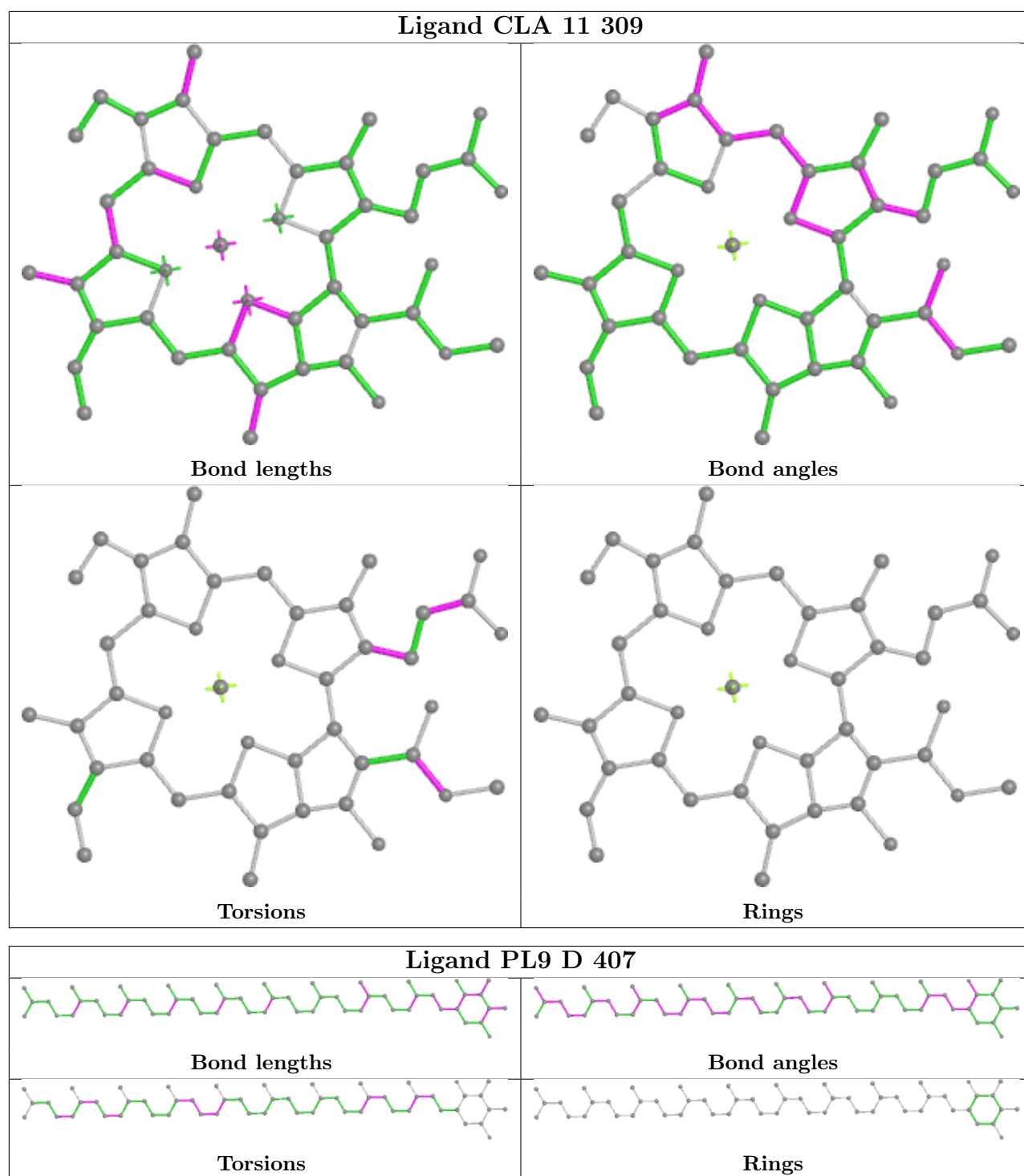
Ligand CLA b 609

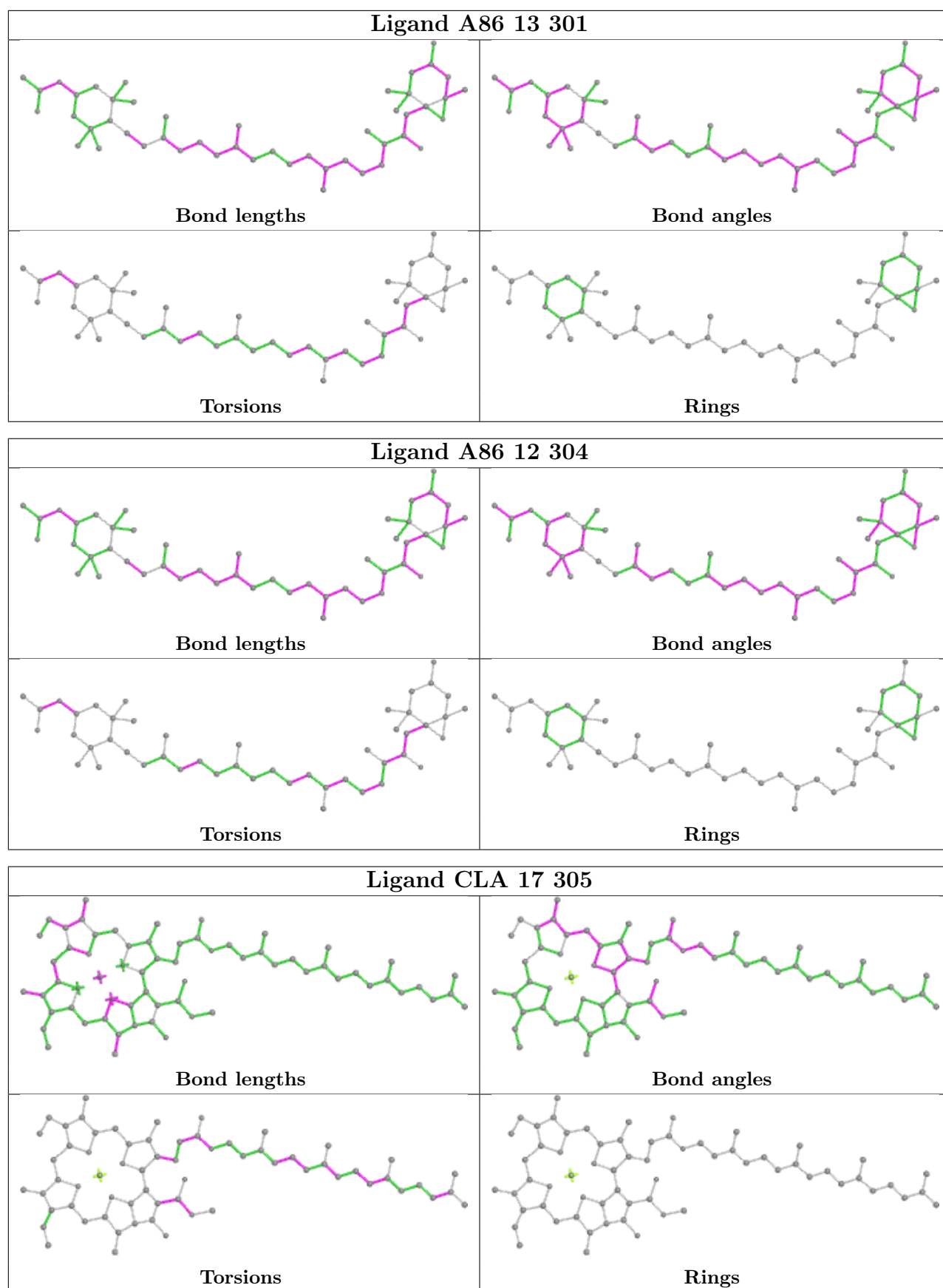


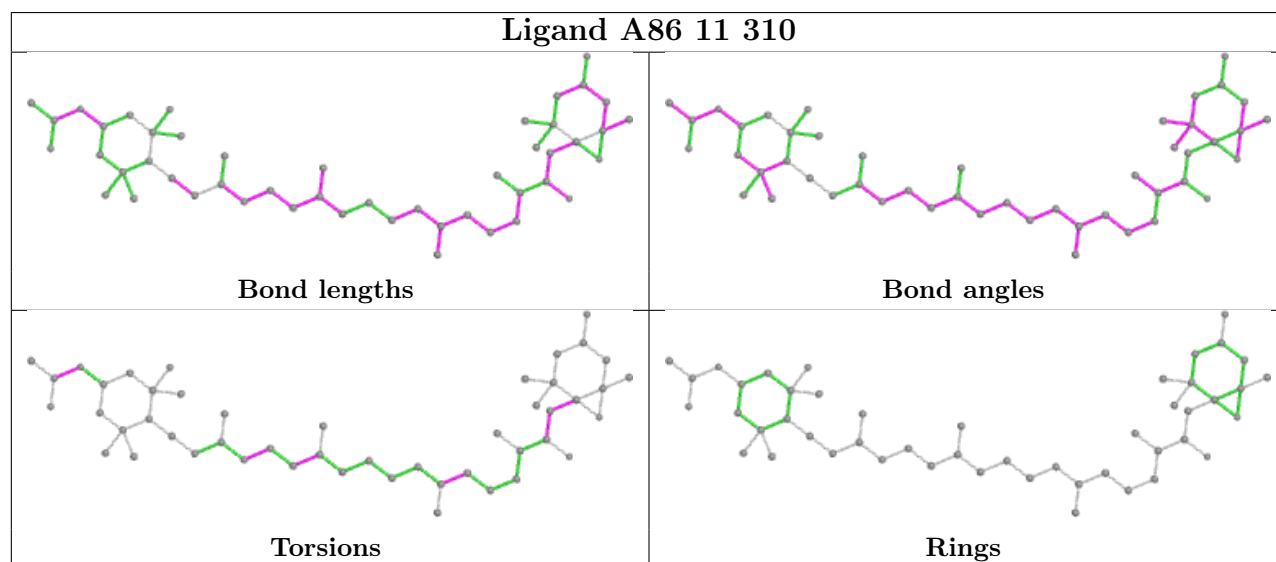
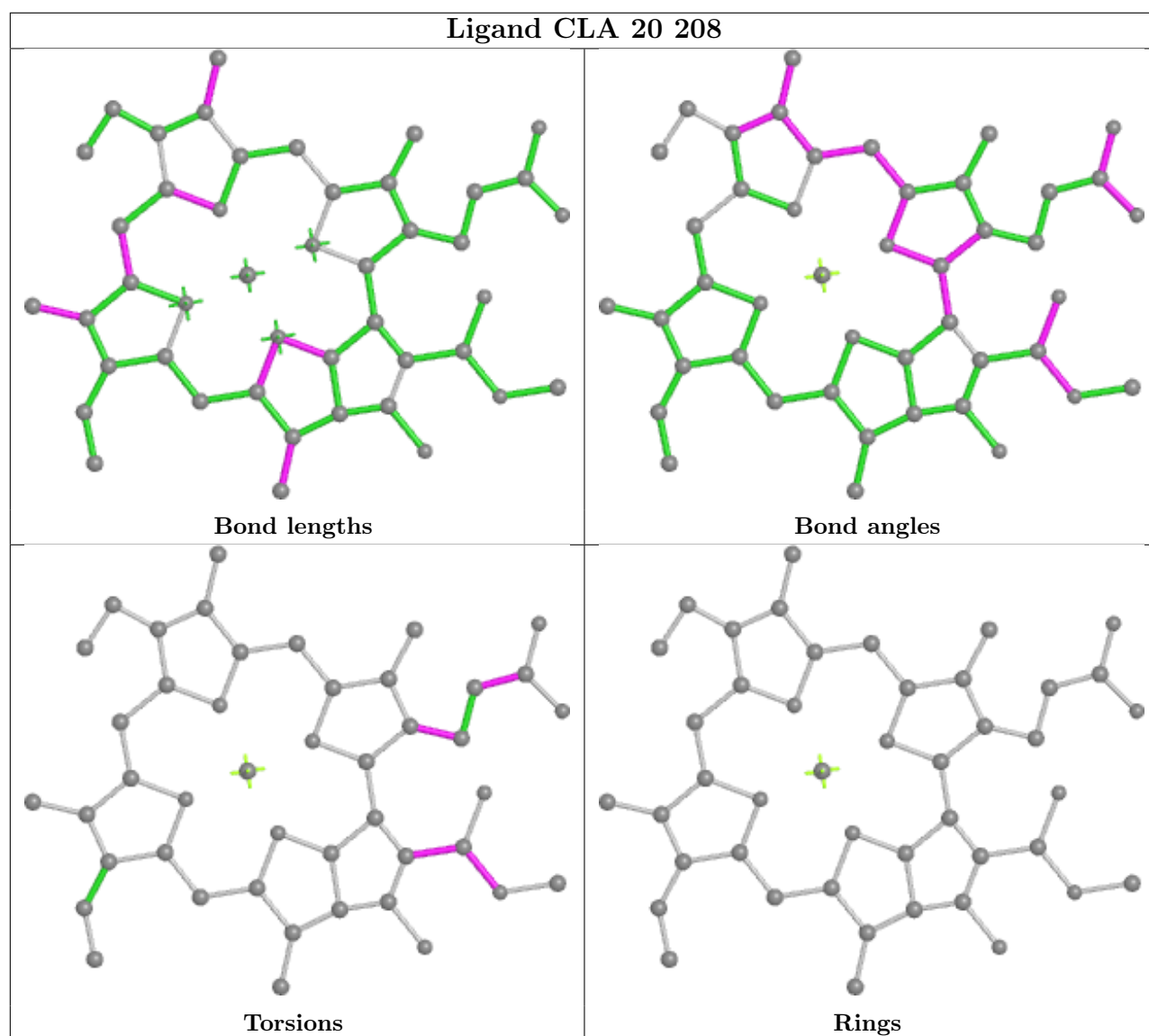
Ligand A86 19 312



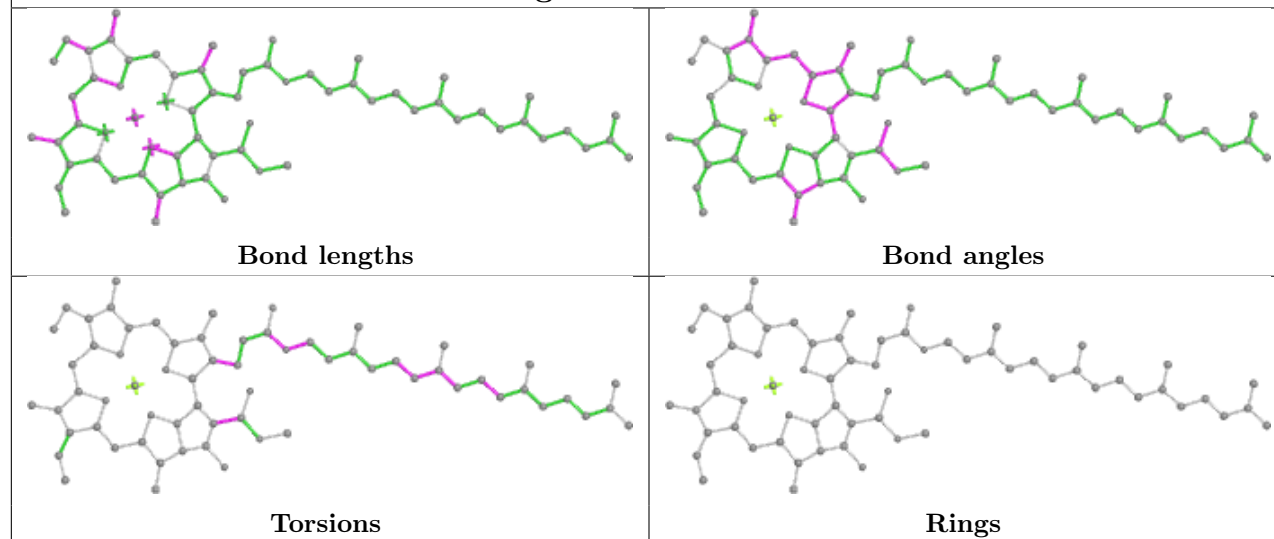




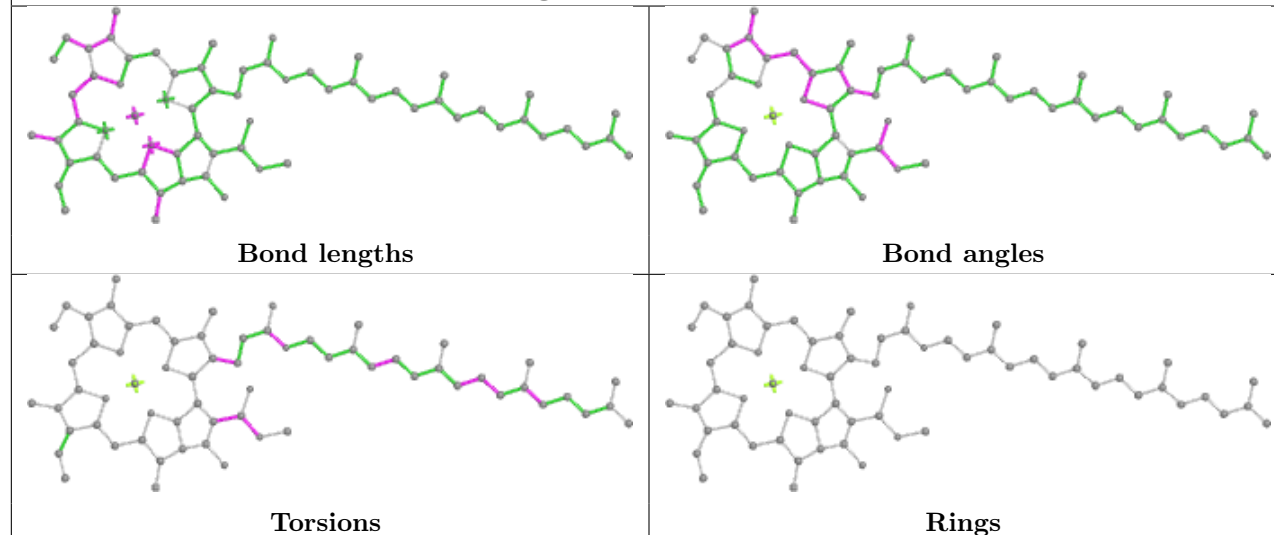




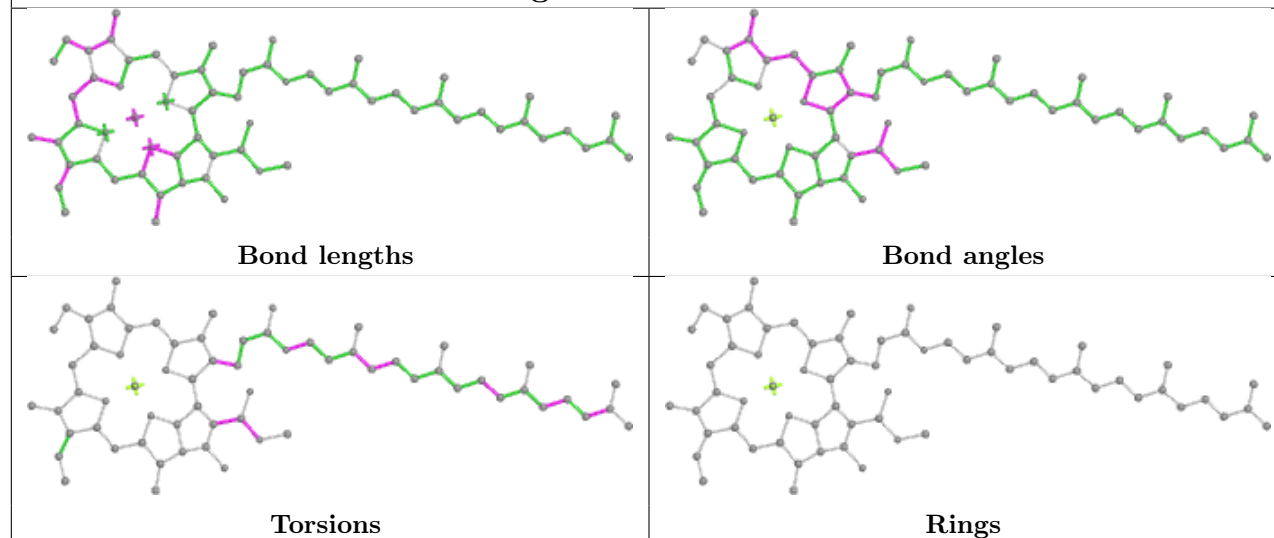
Ligand CLA b 612

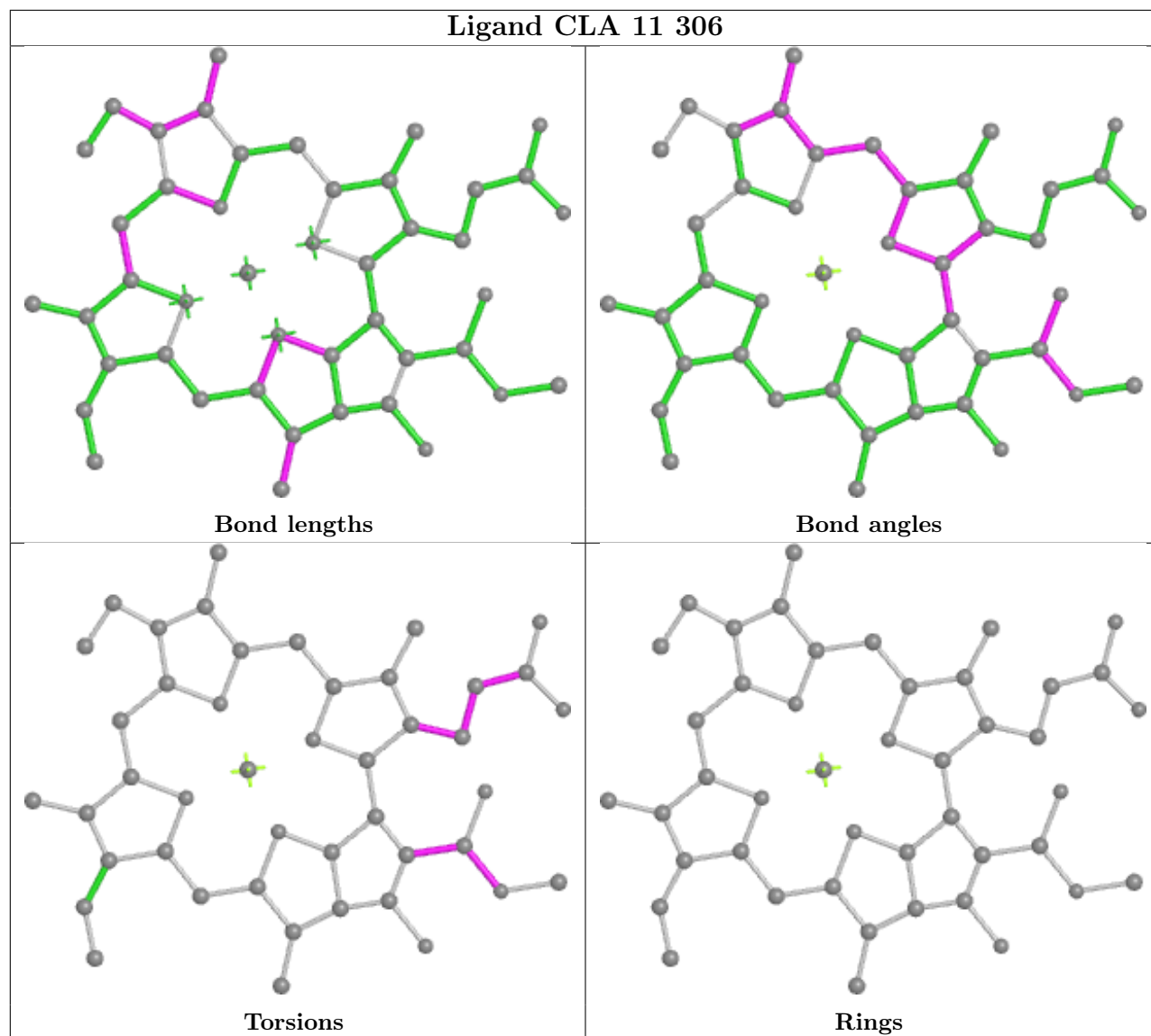
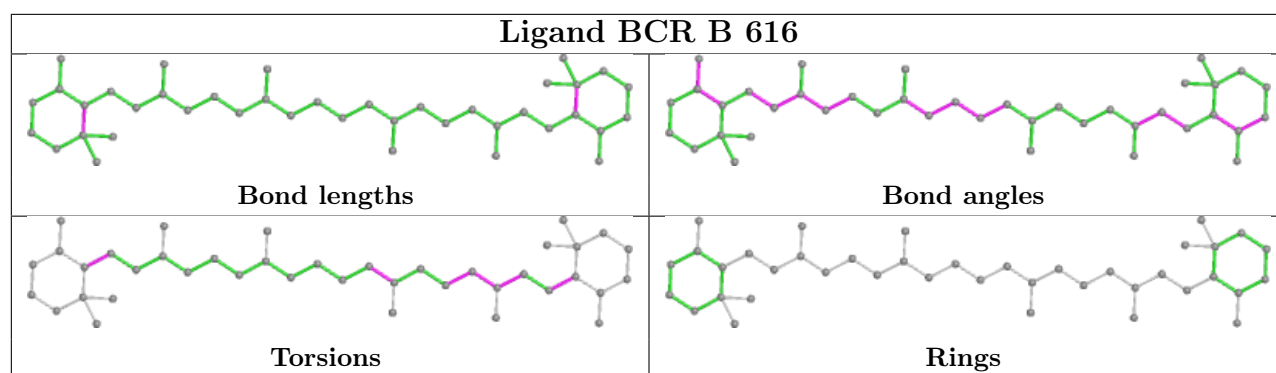


Ligand CLA b 607

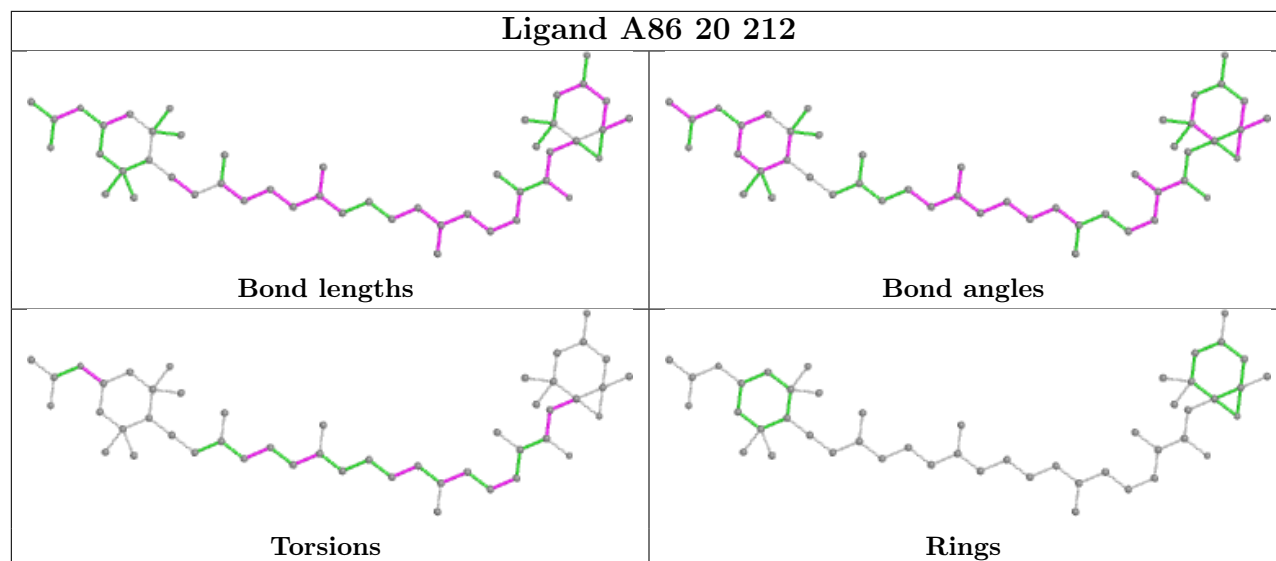


Ligand CLA D 401

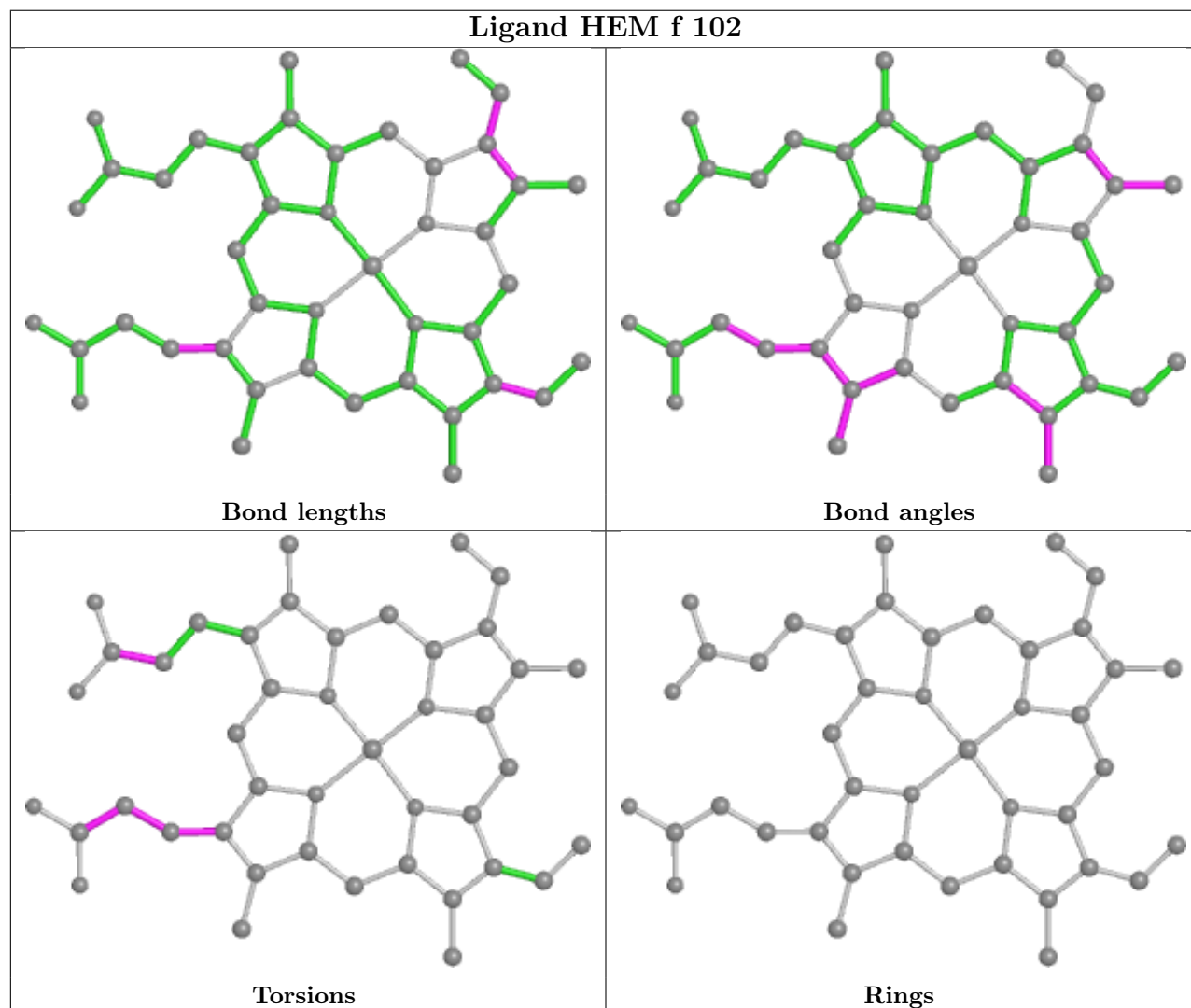


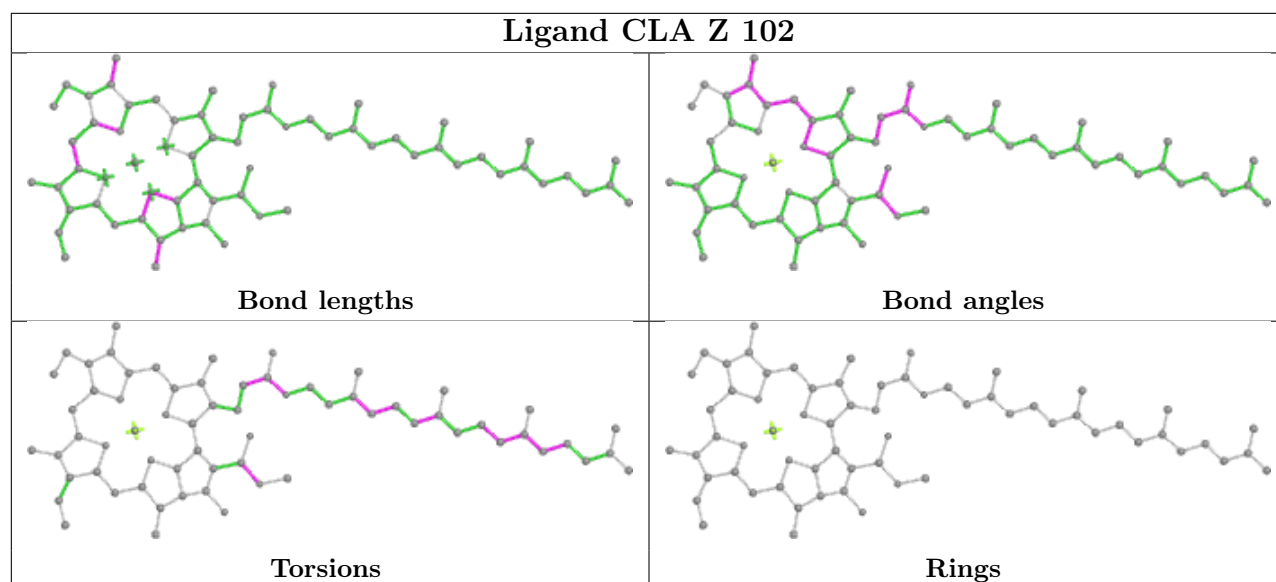
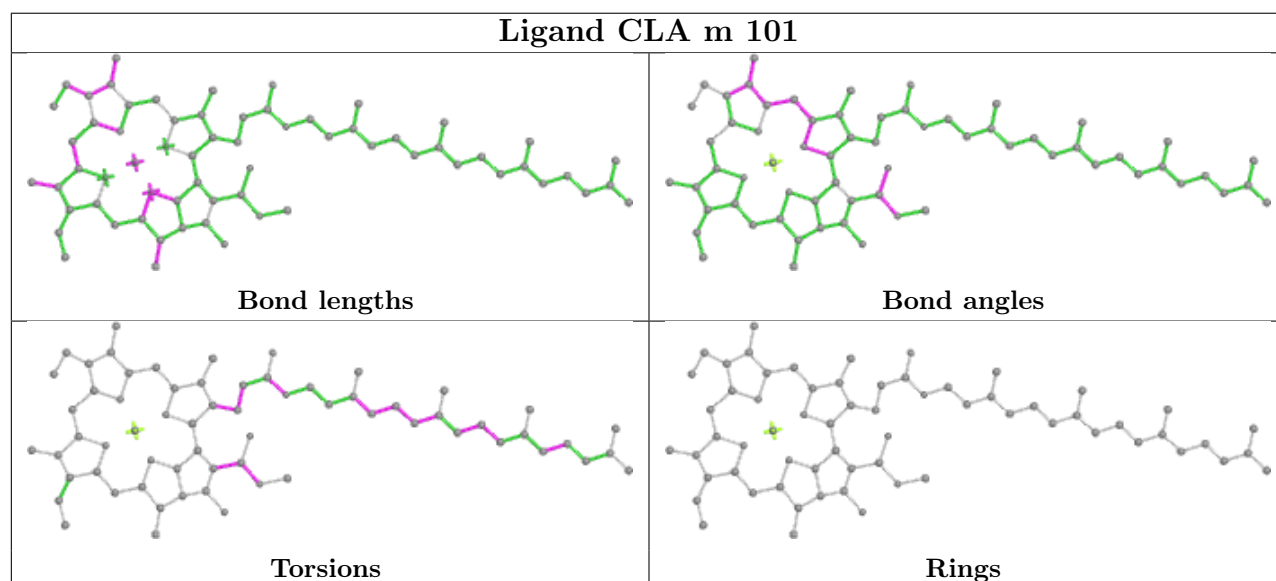
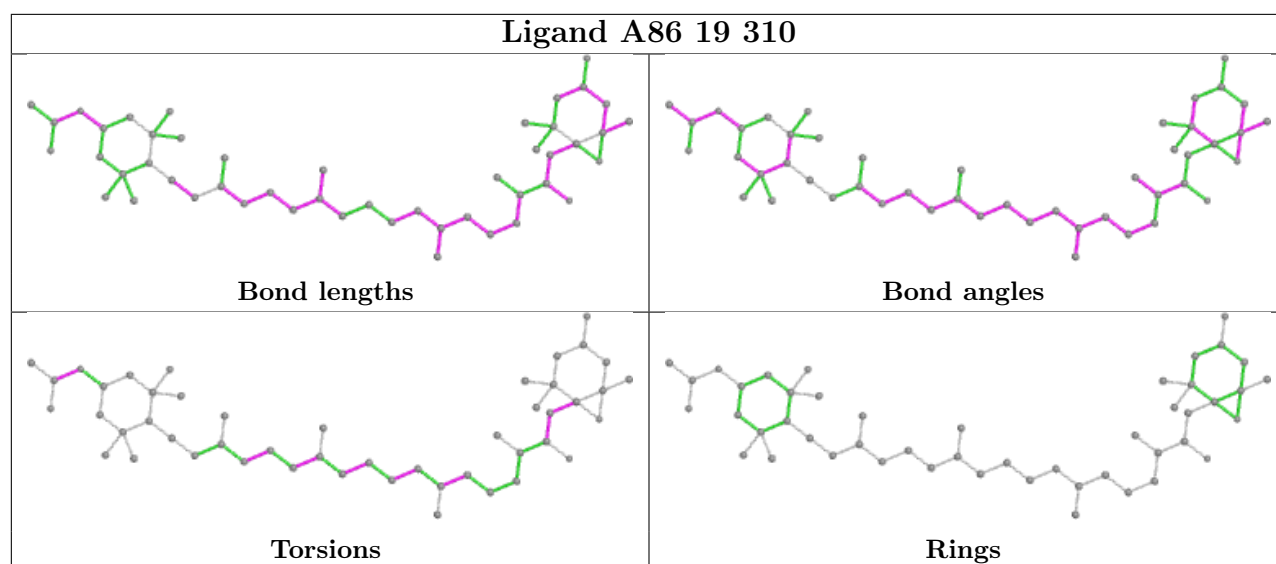


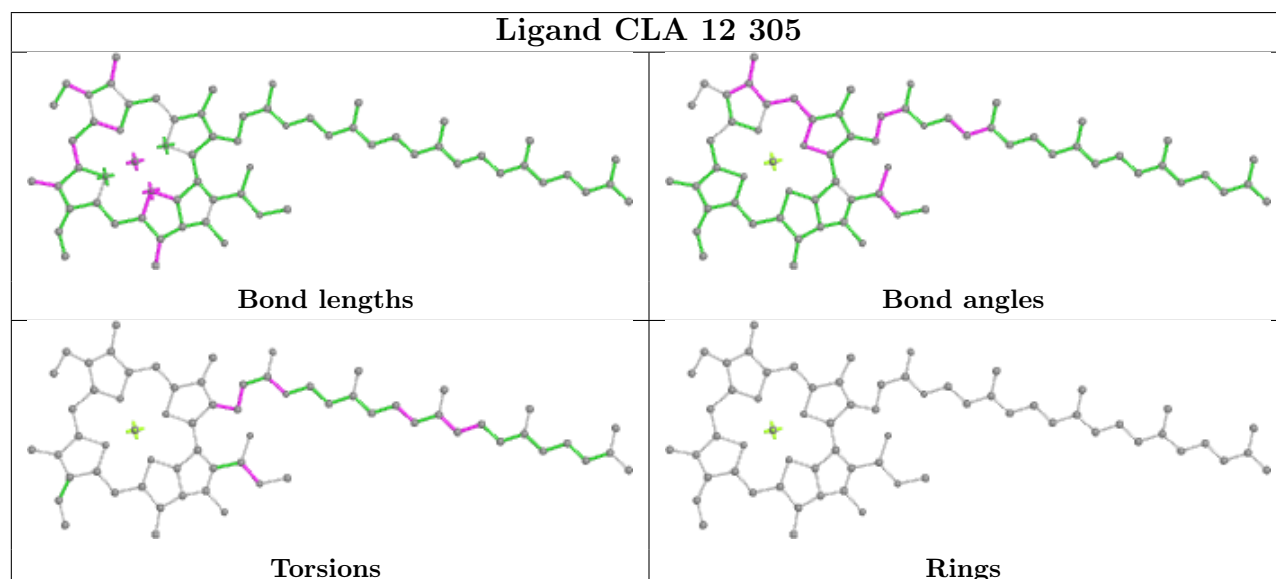
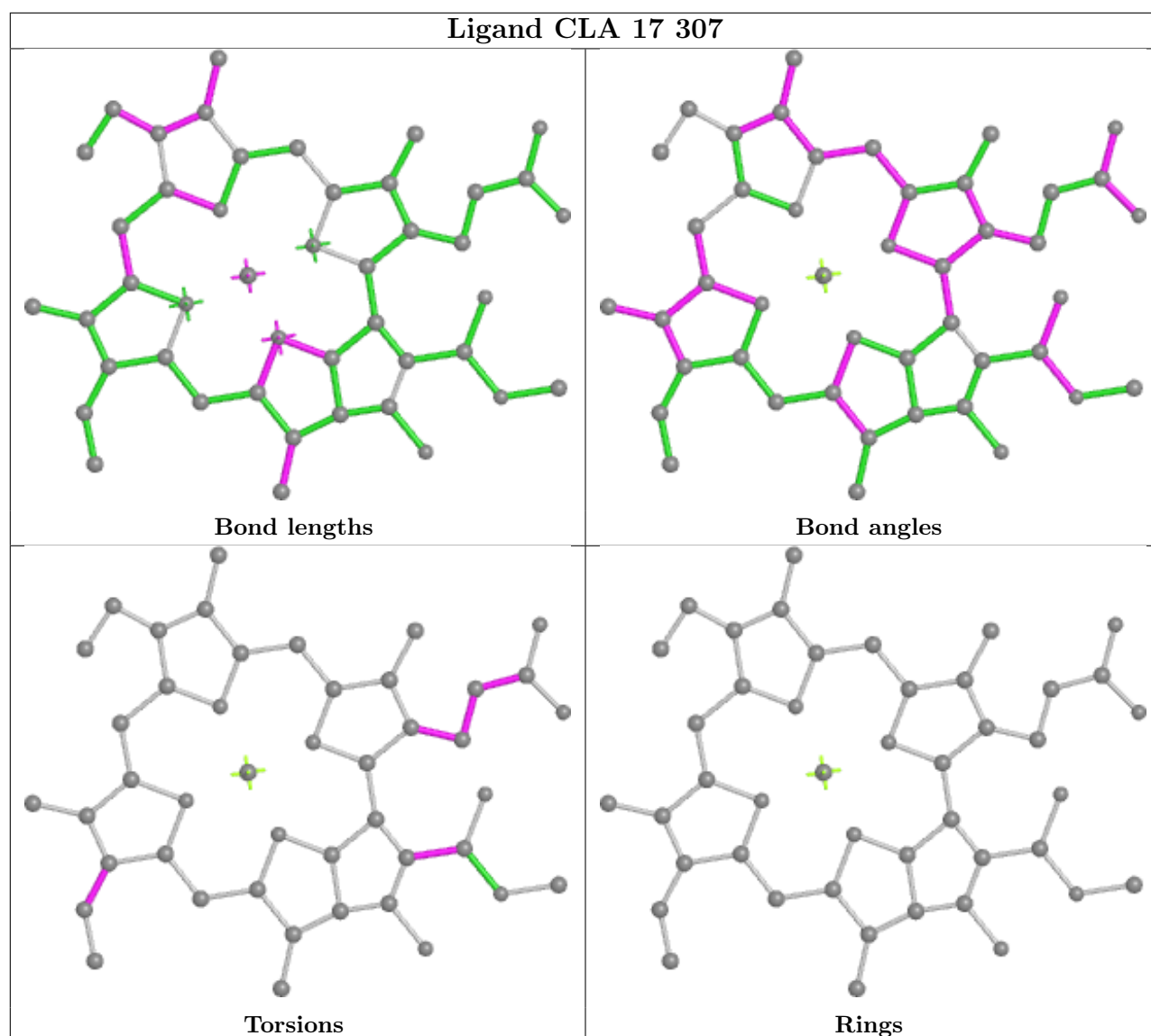
Ligand A86 20 212

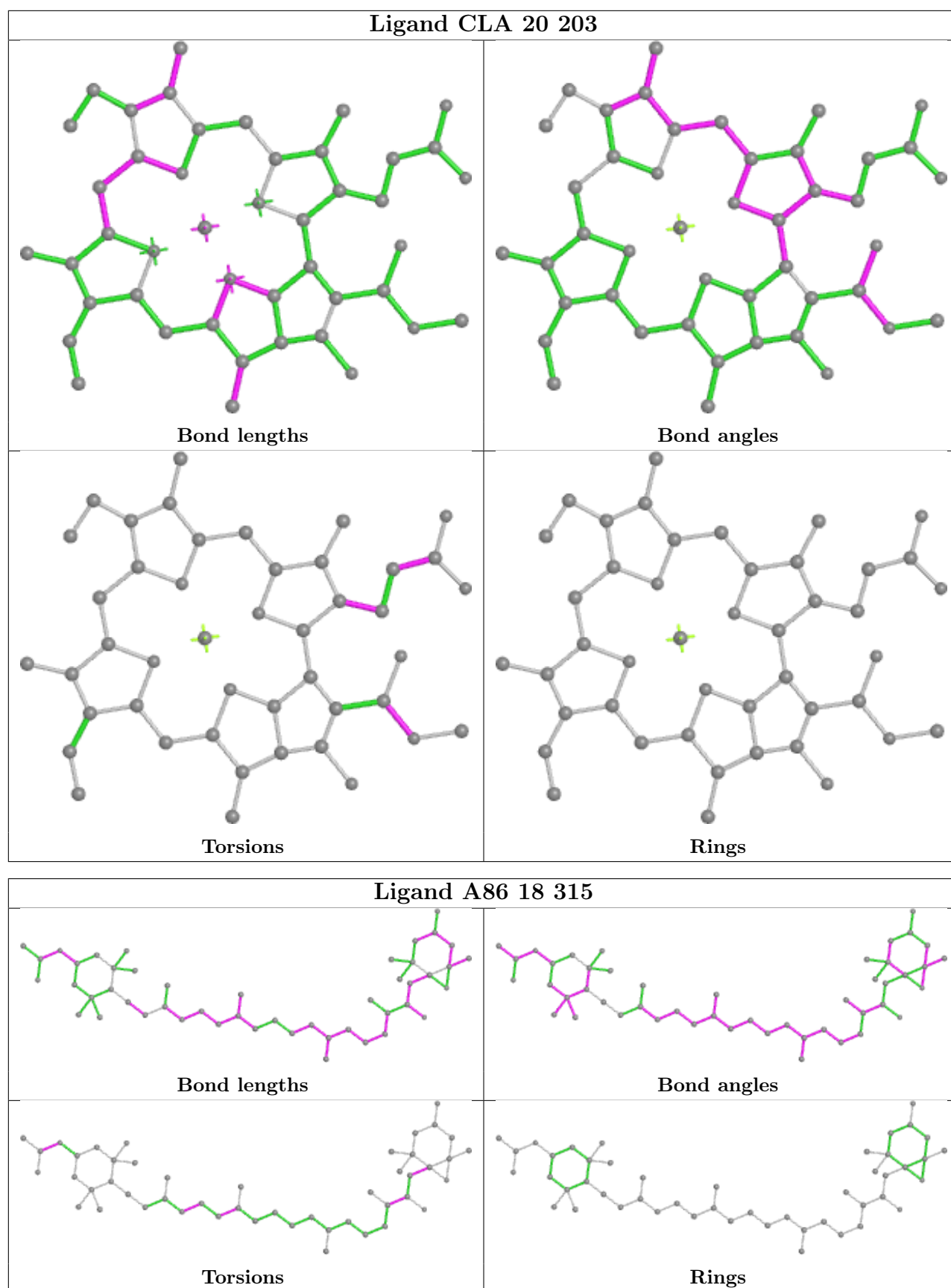


Ligand HEM f 102

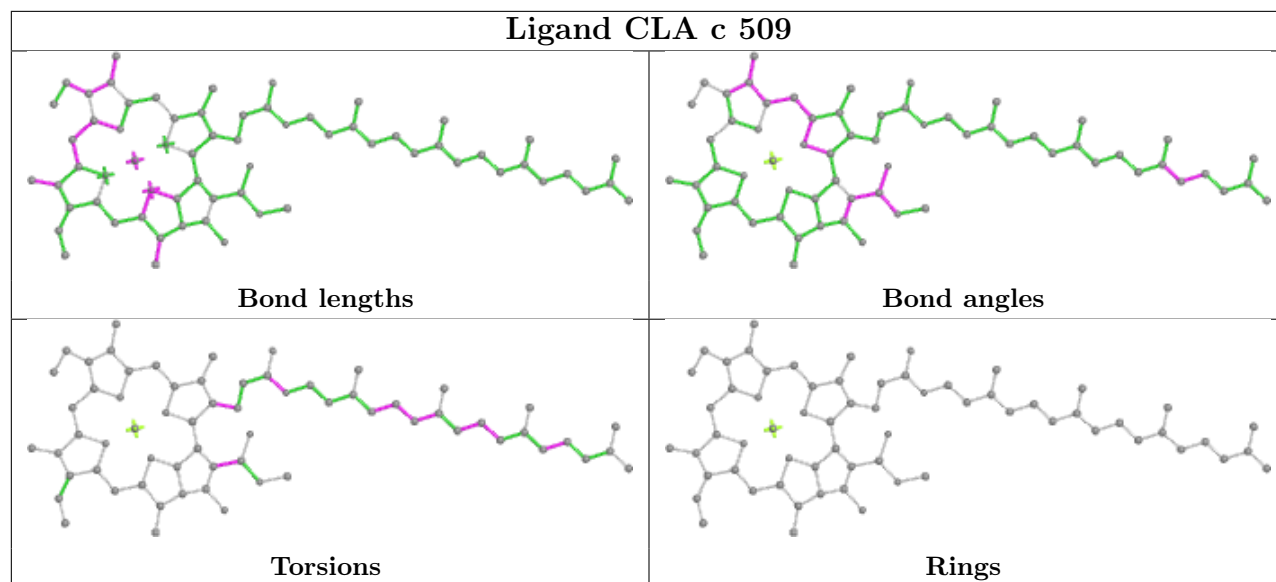




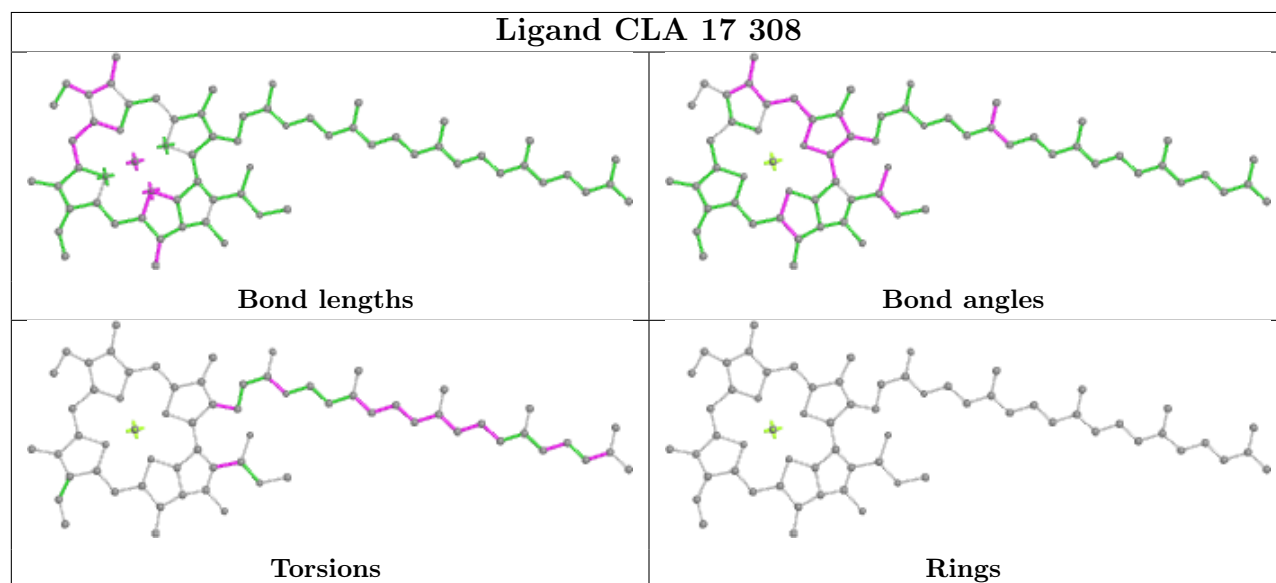


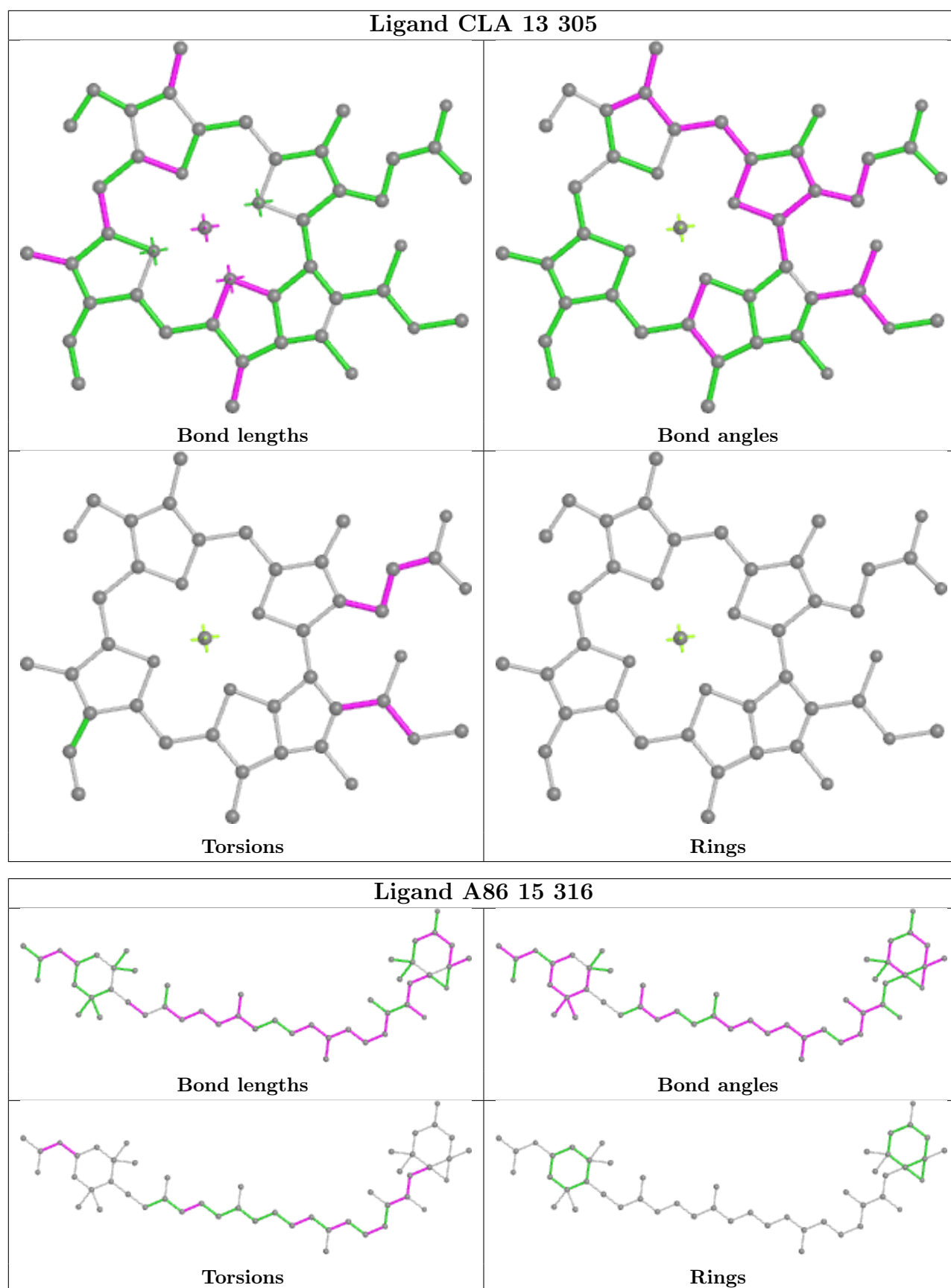


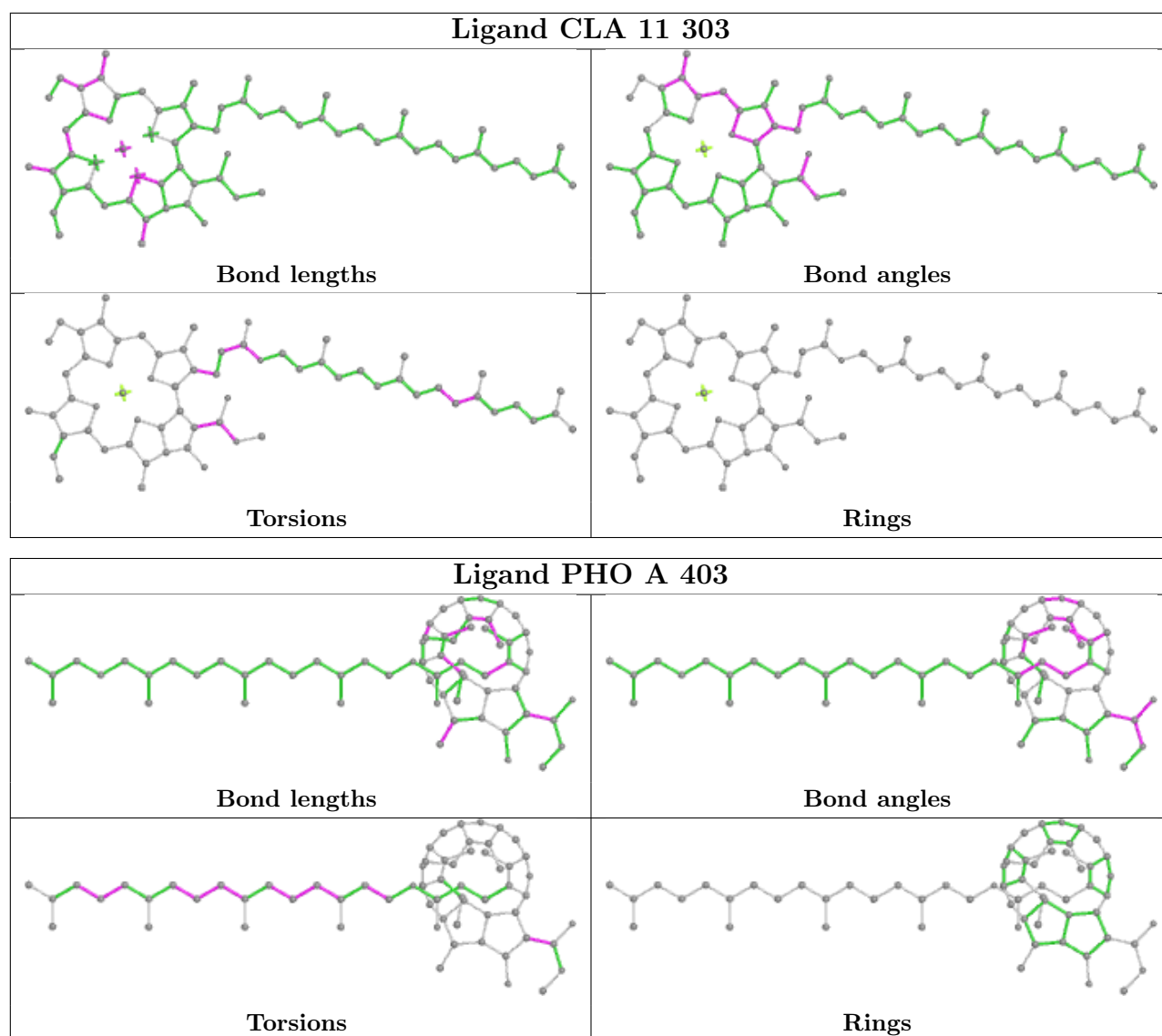
Ligand CLA c 509

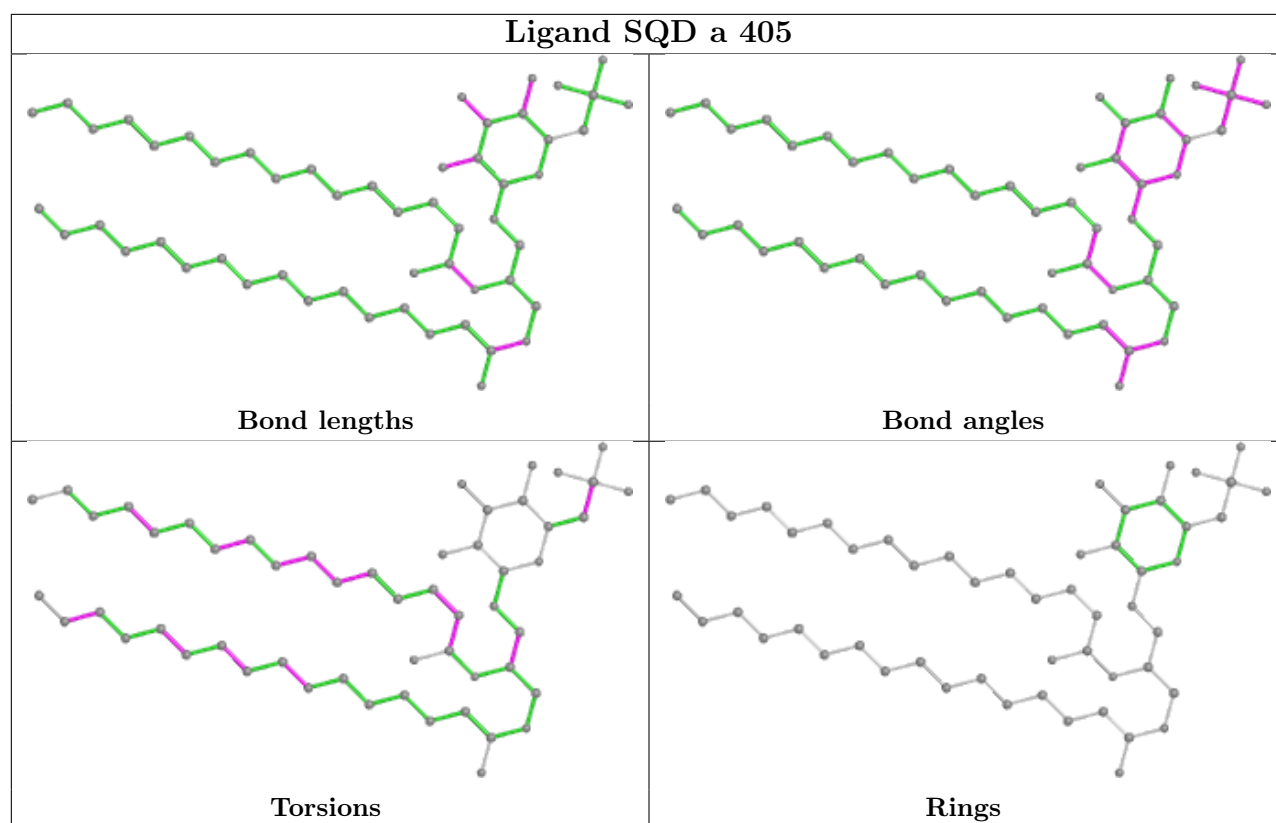


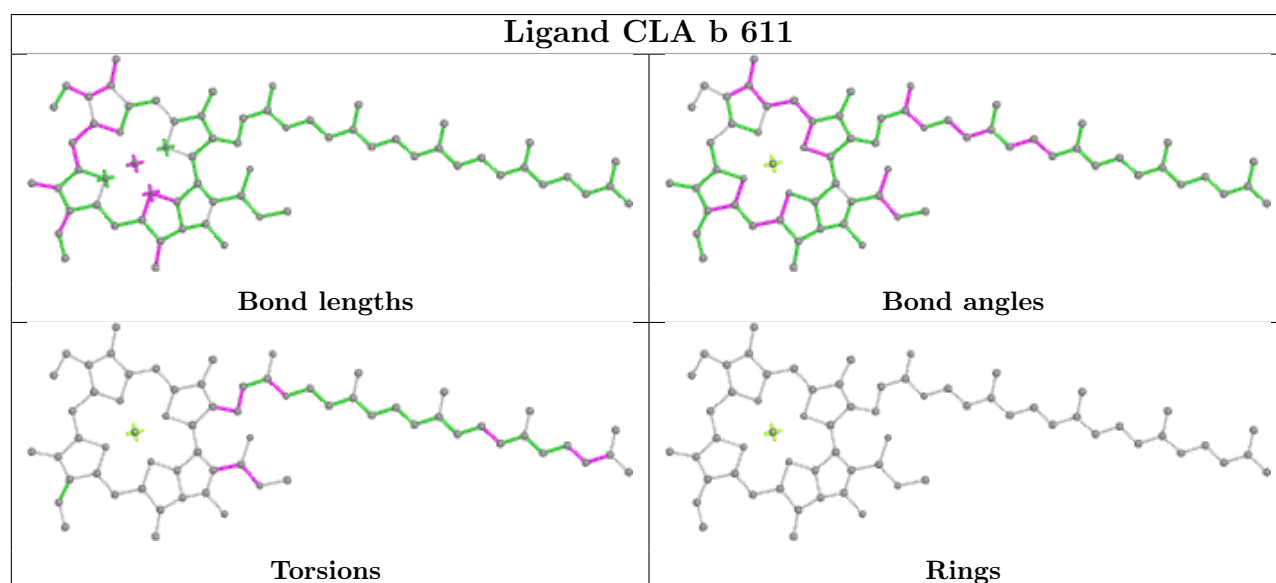
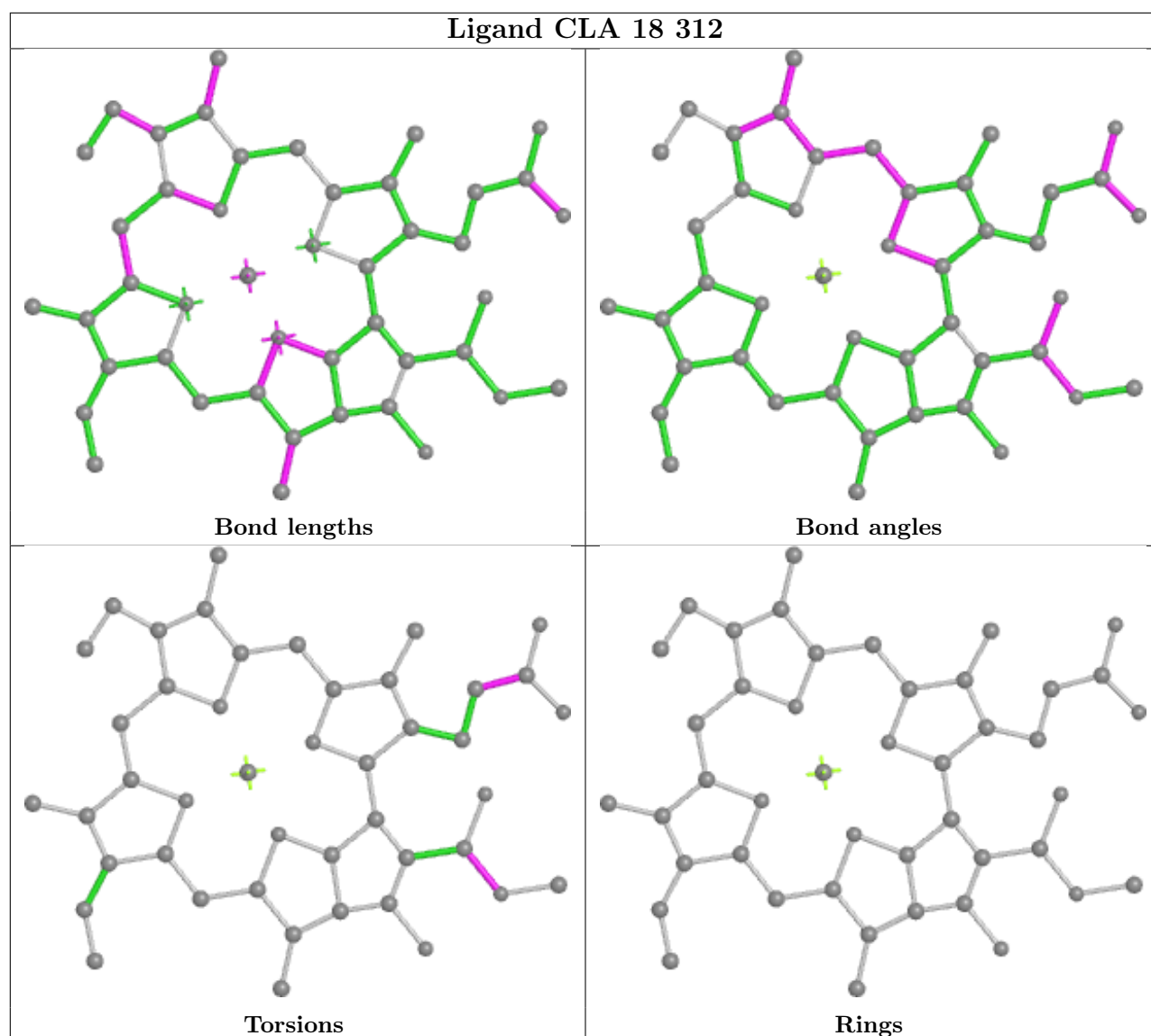
Ligand CLA 17 308



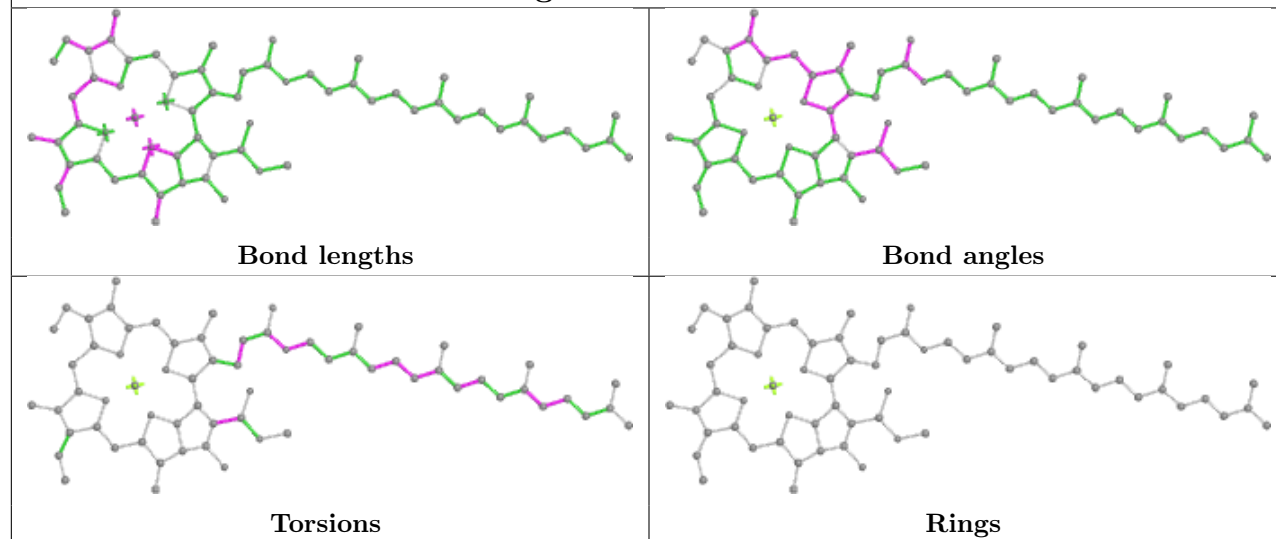




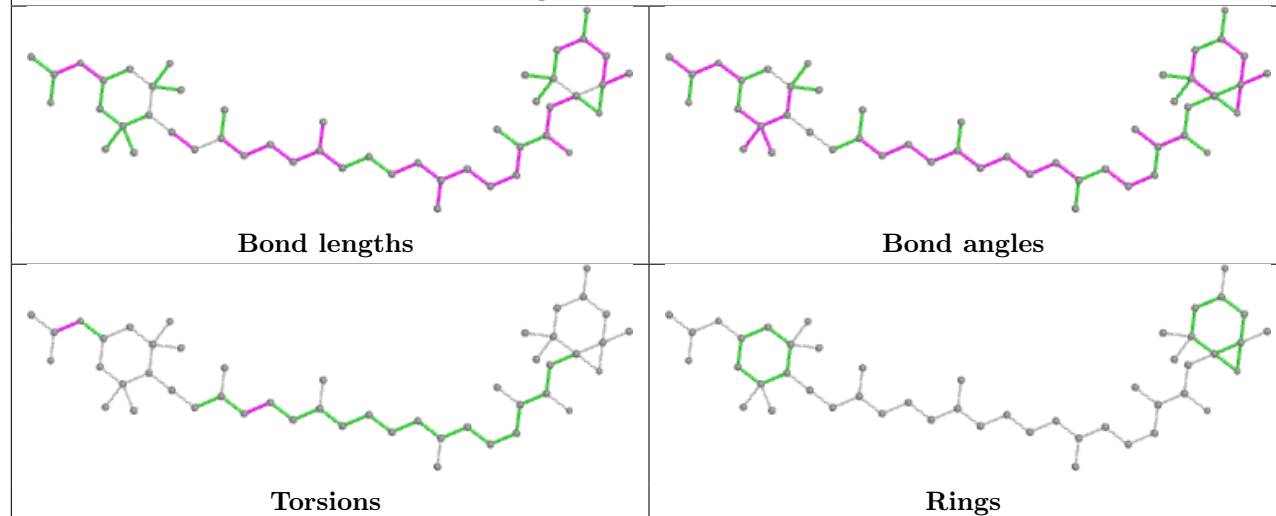




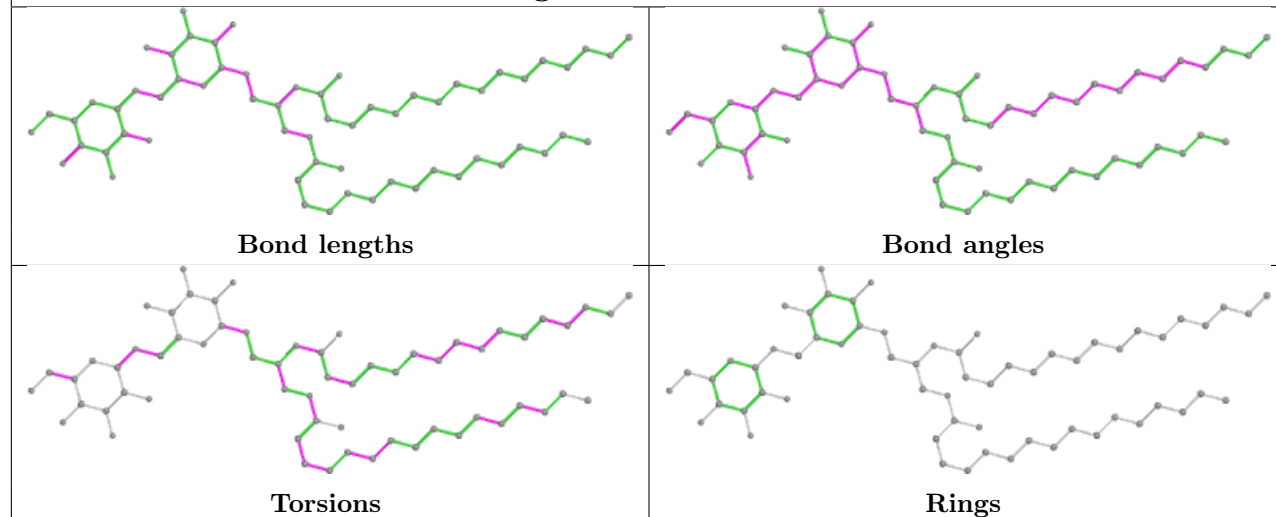
Ligand CLA b 615

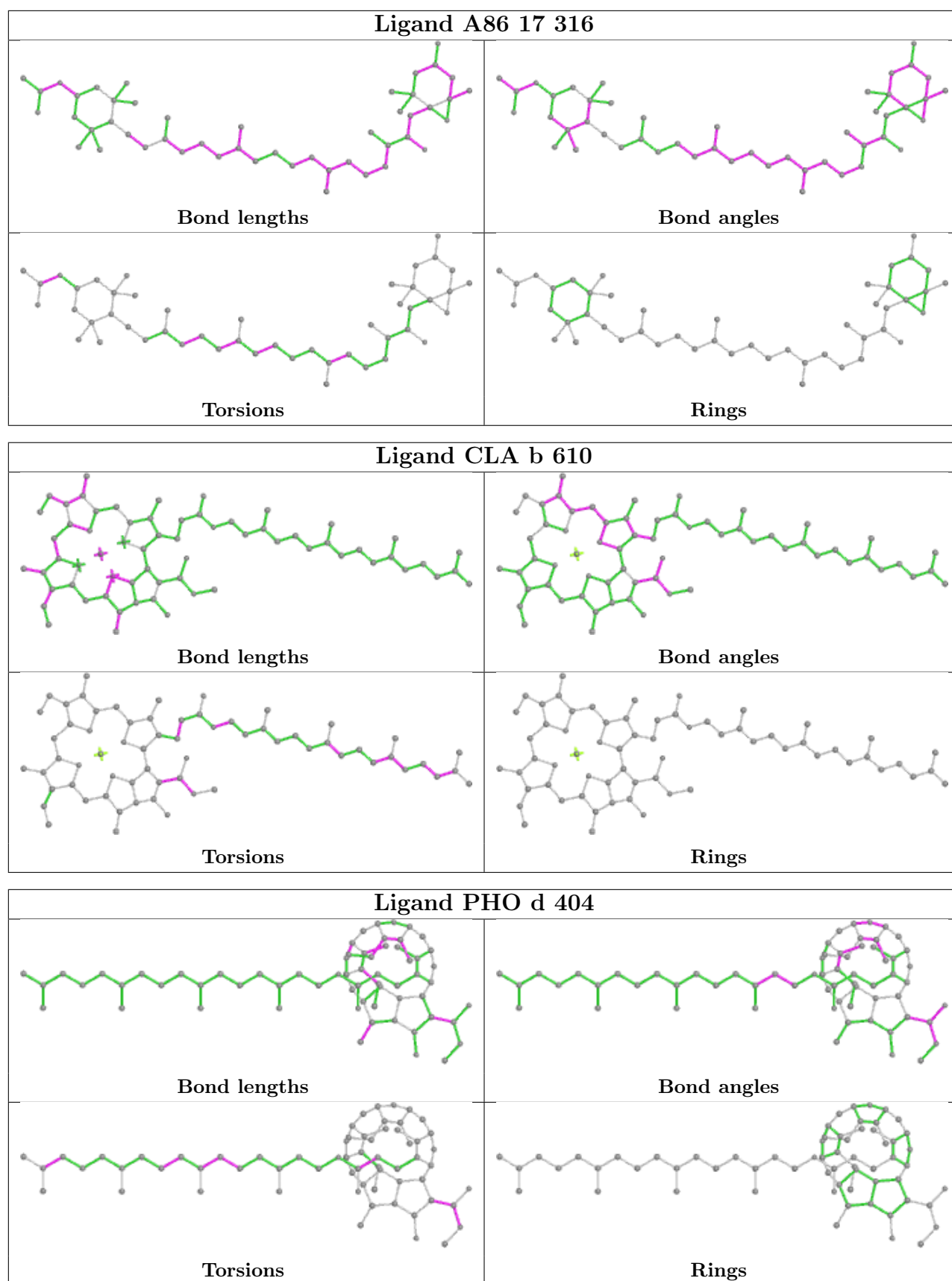


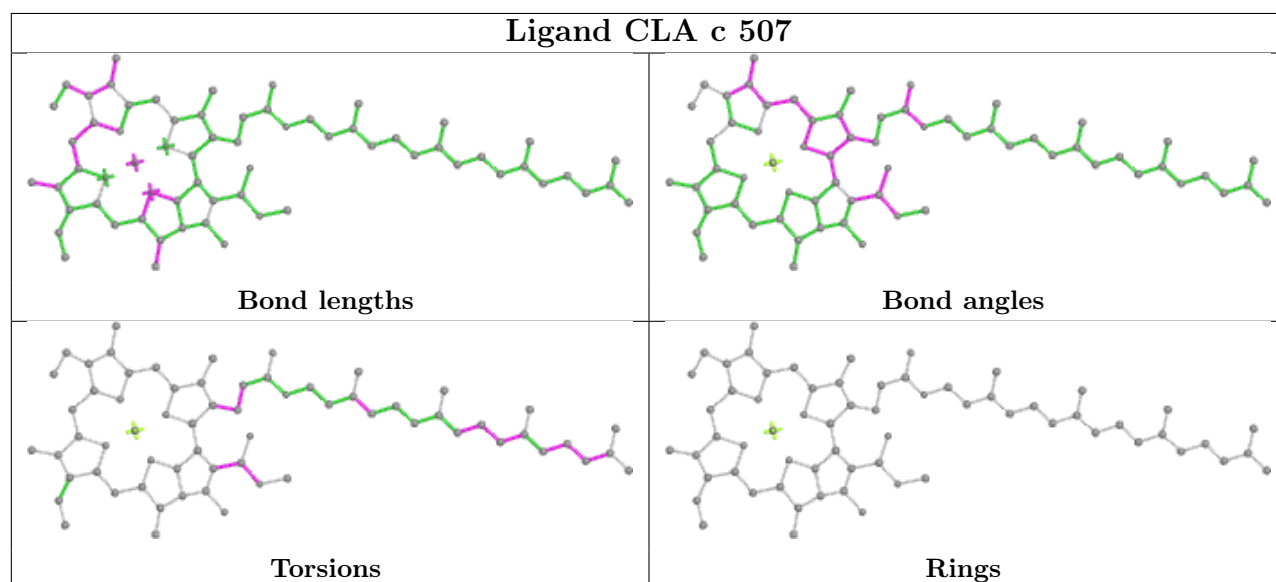
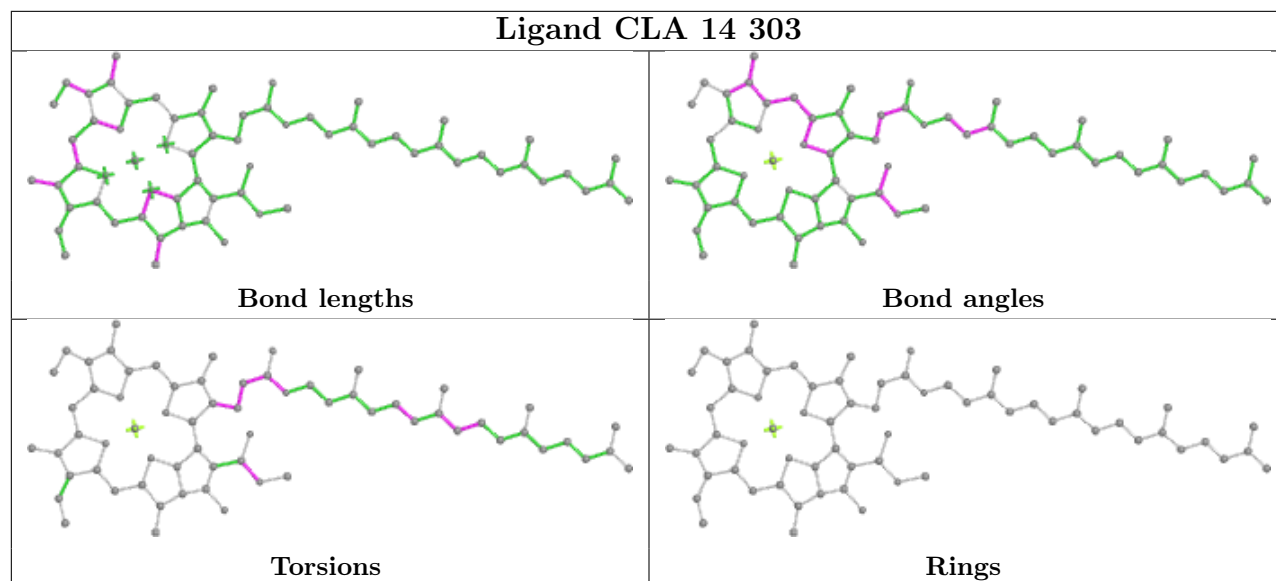
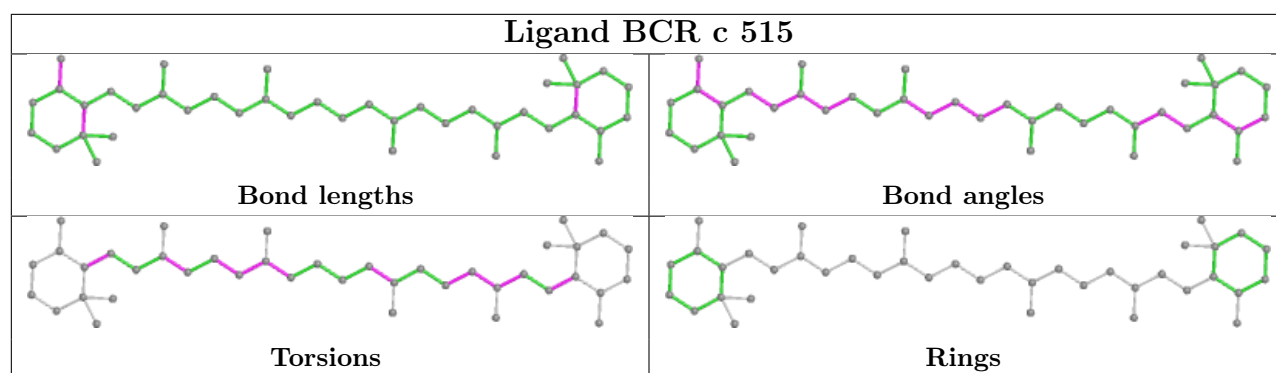
Ligand A86 12 316

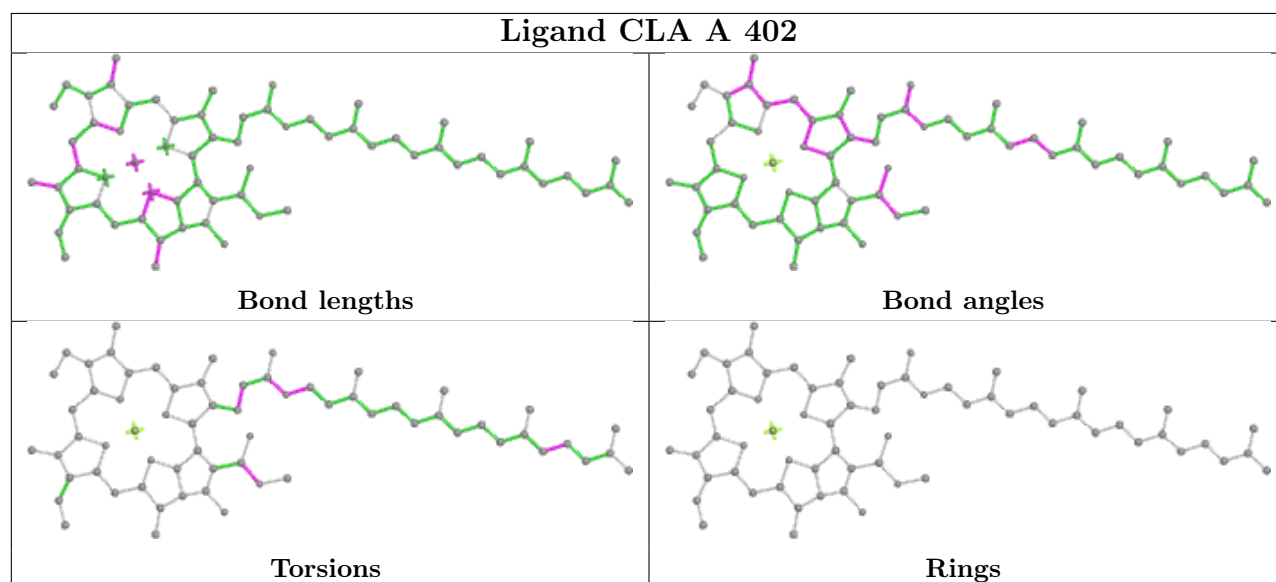
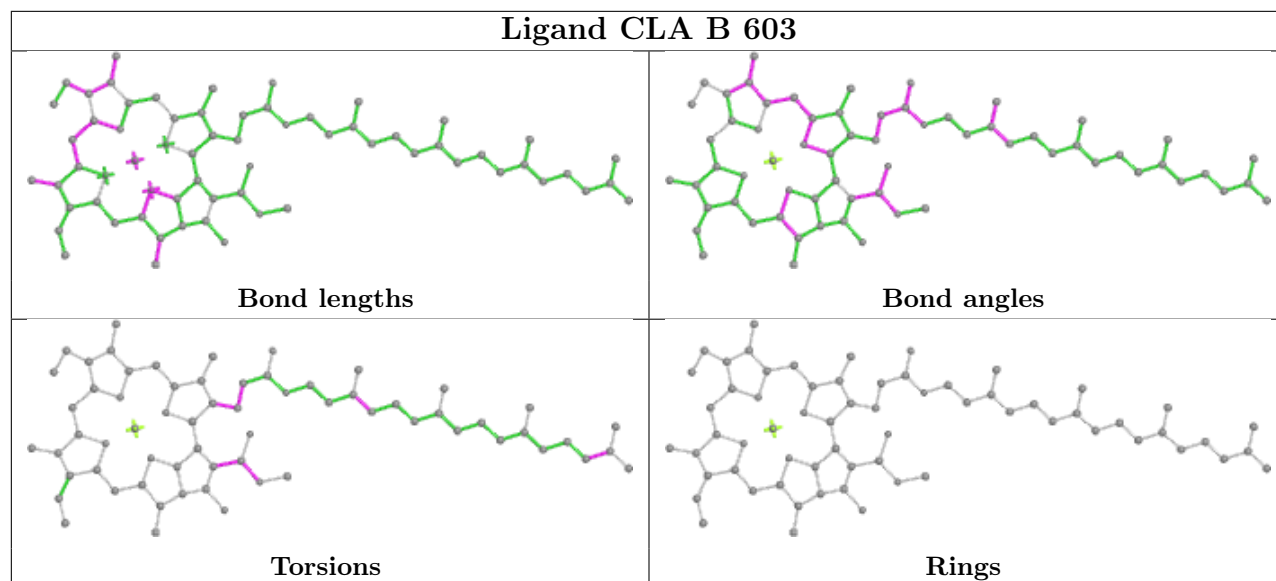
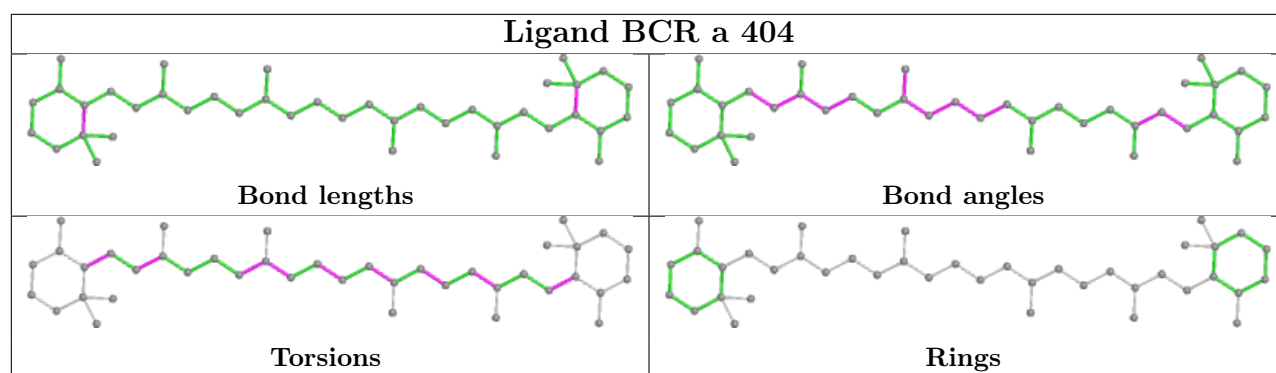


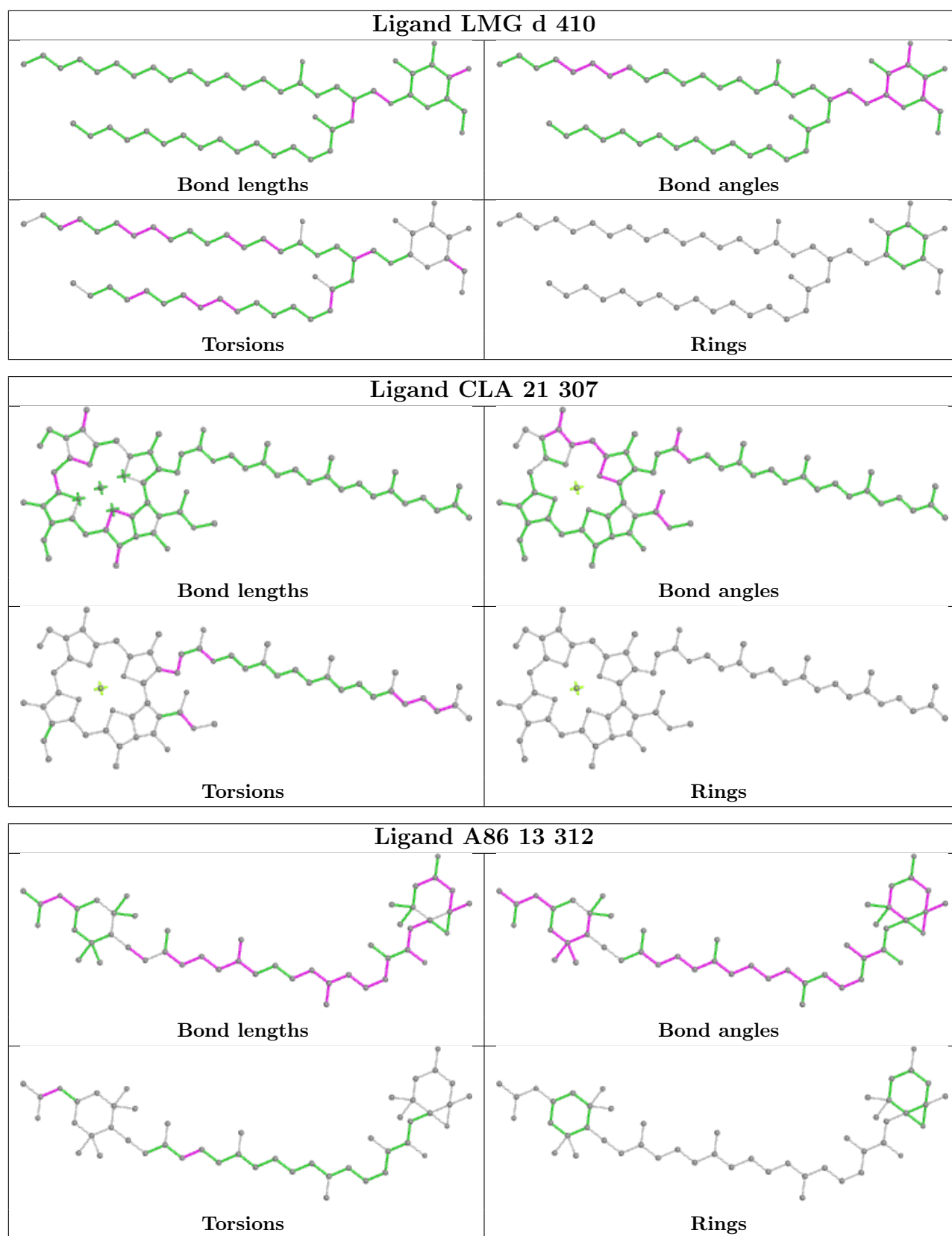
Ligand DGD c 518

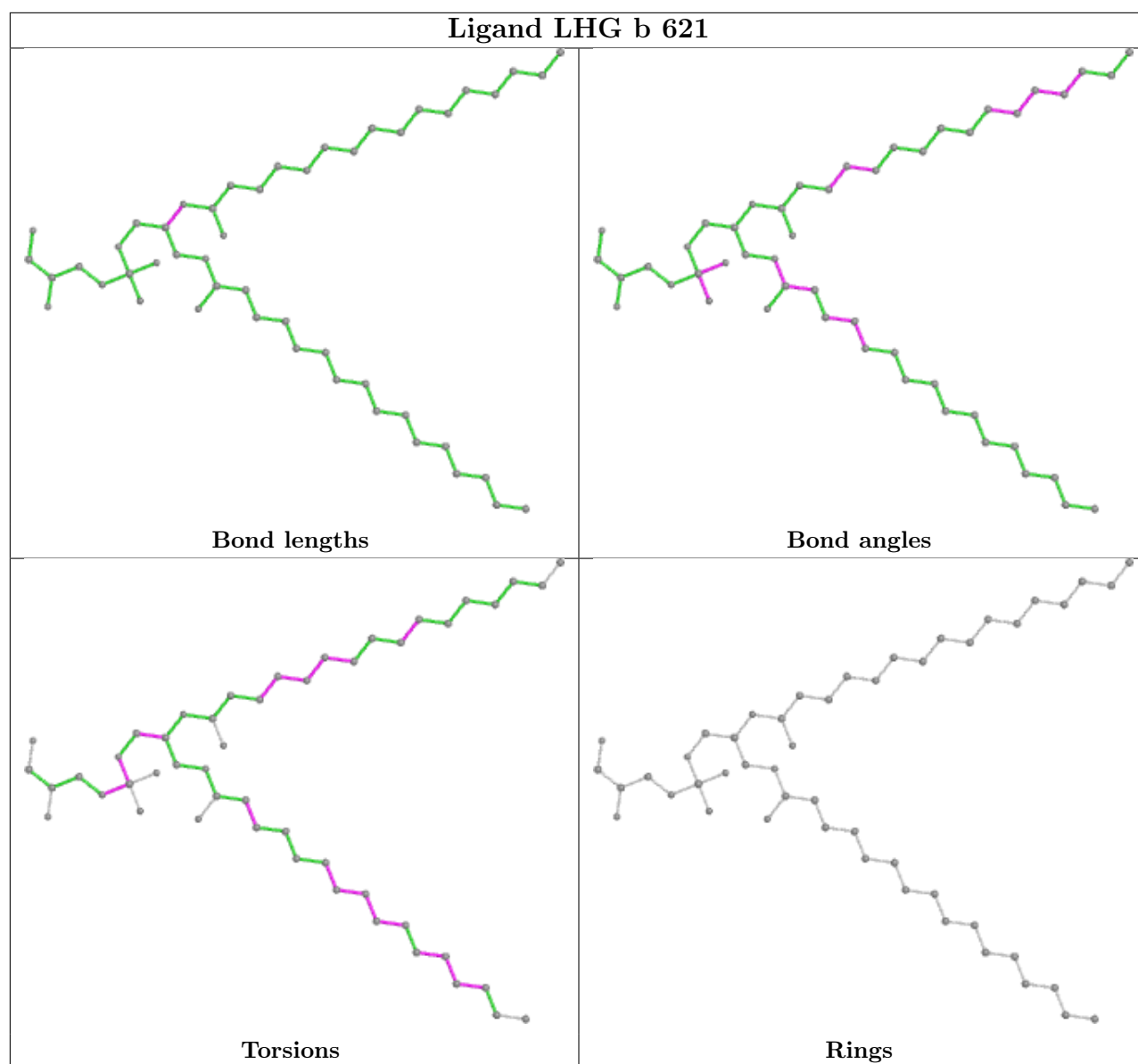


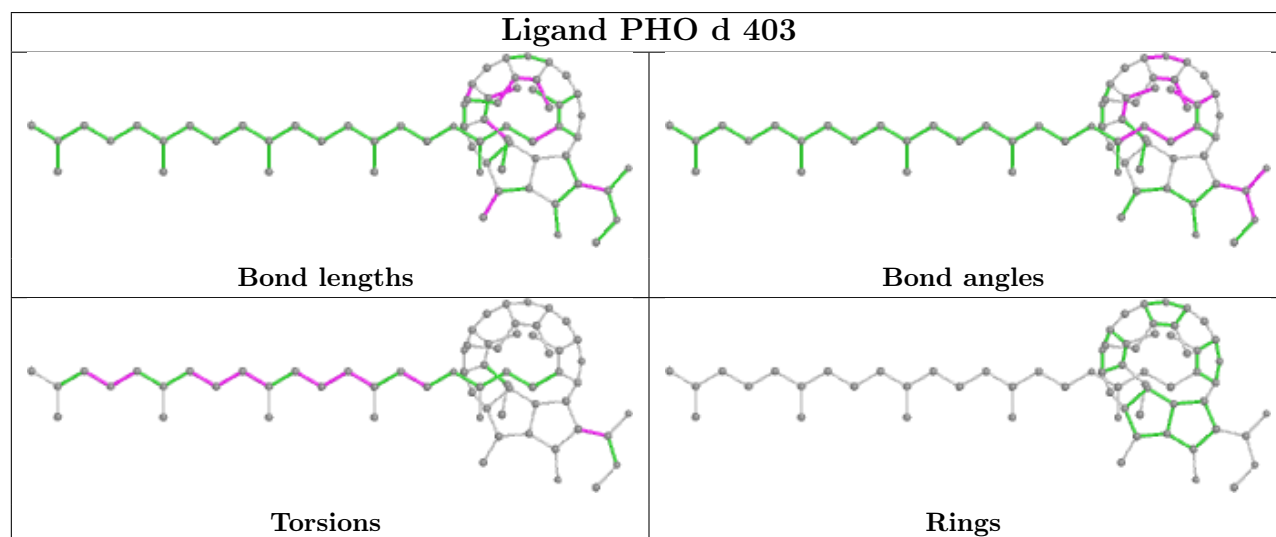
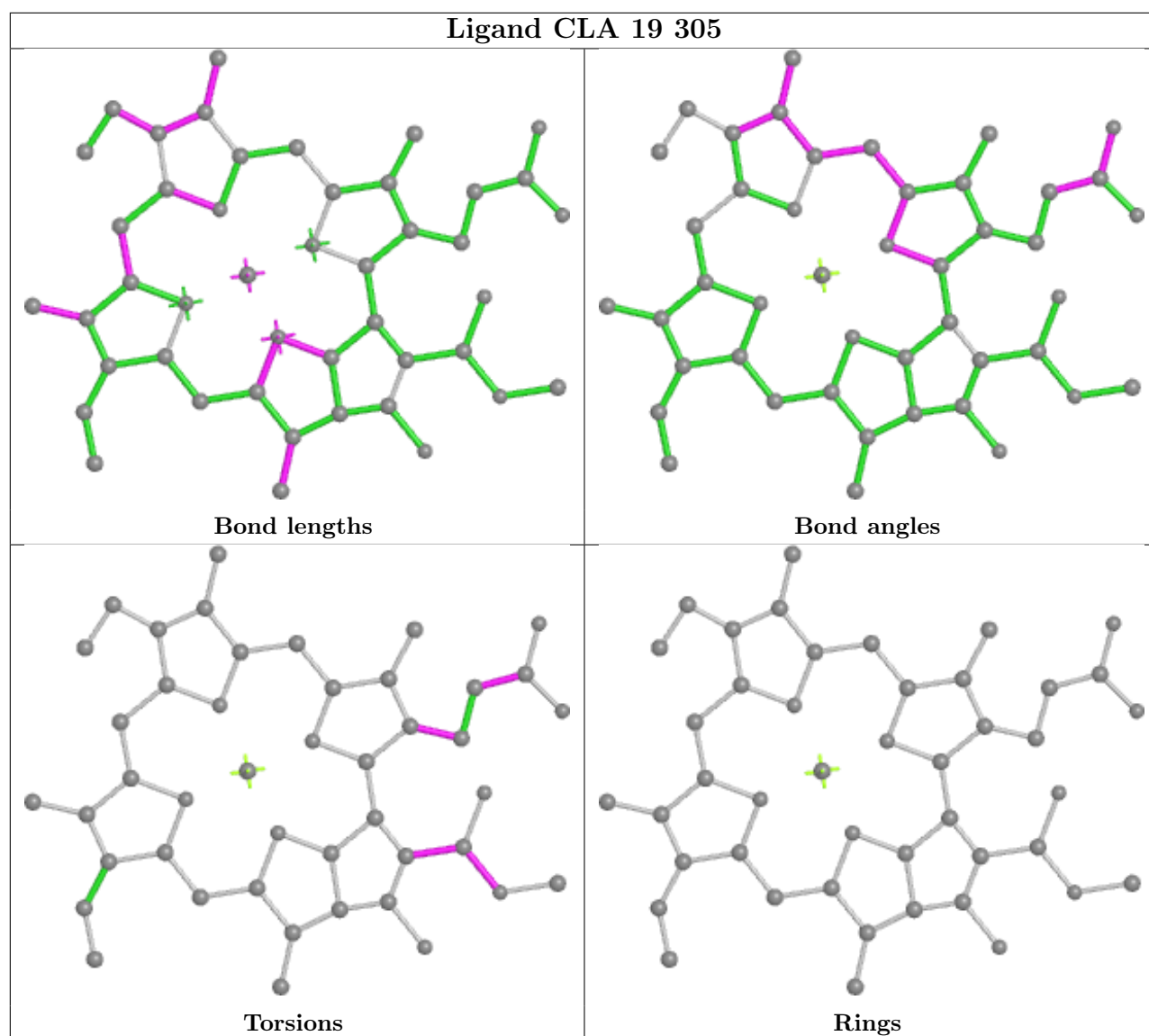




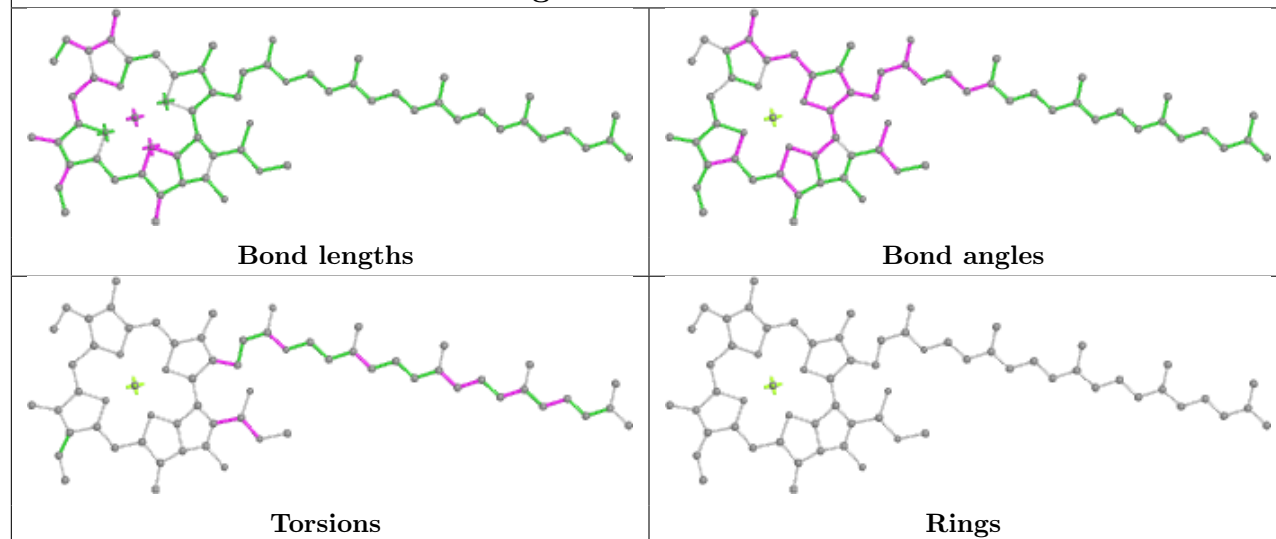




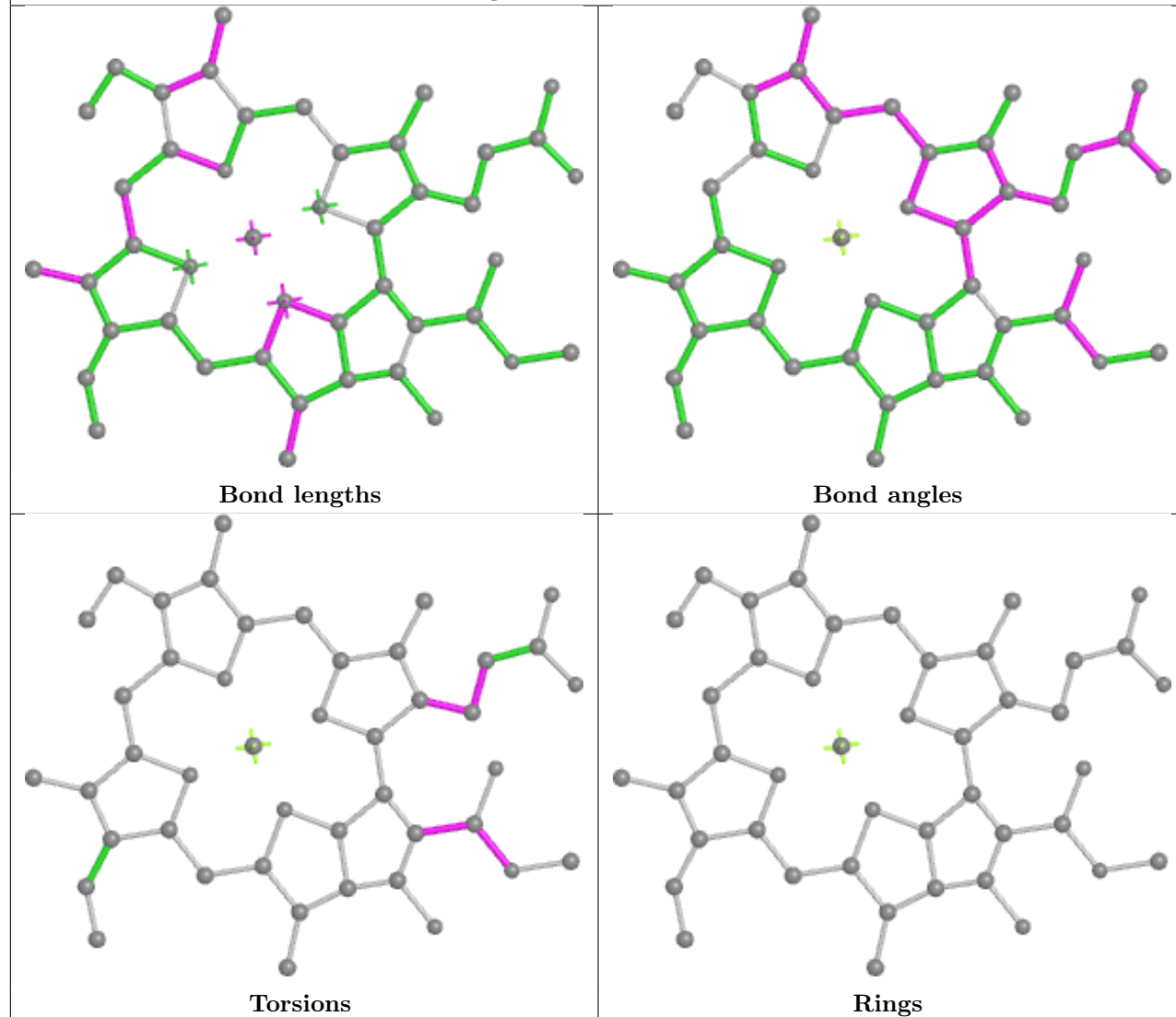




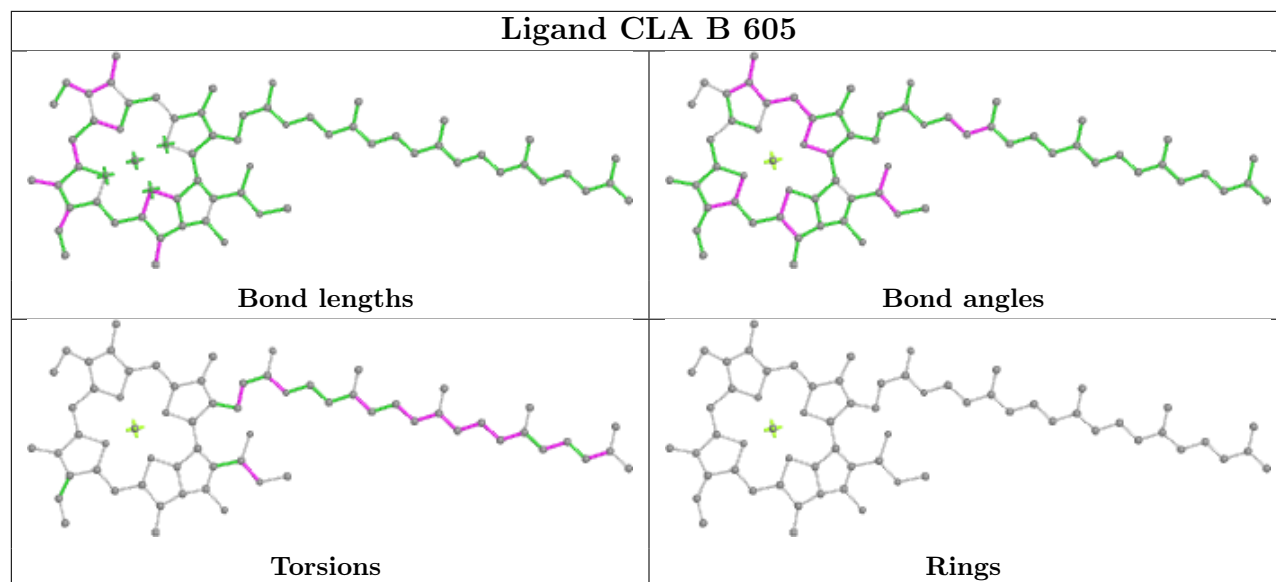
Ligand CLA B 604



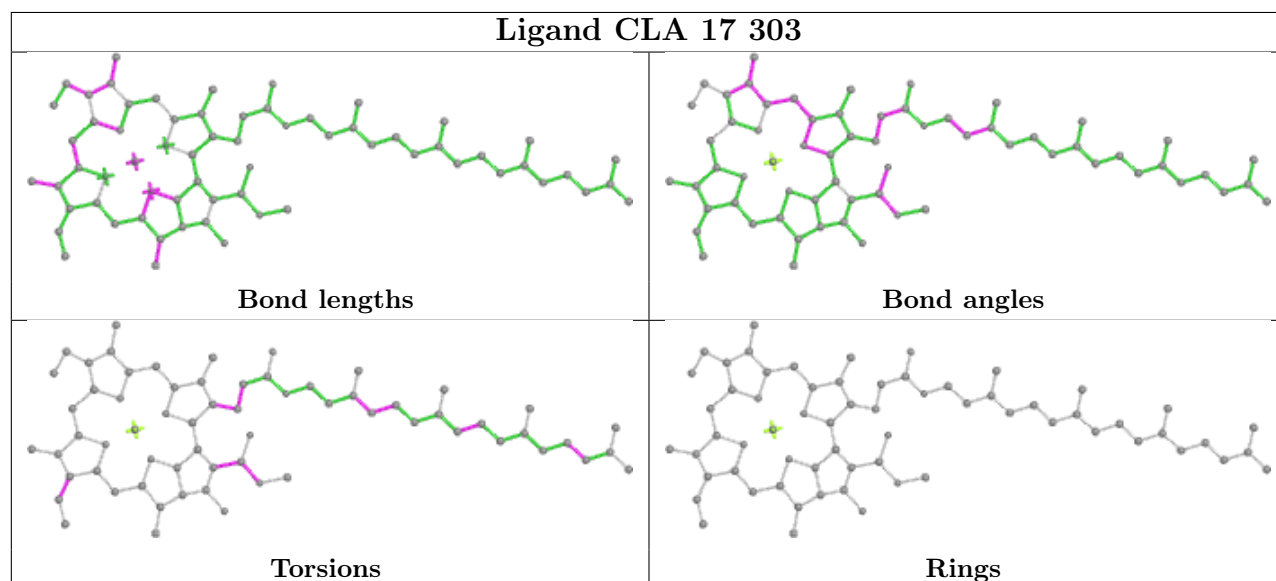
Ligand CLA 16 308



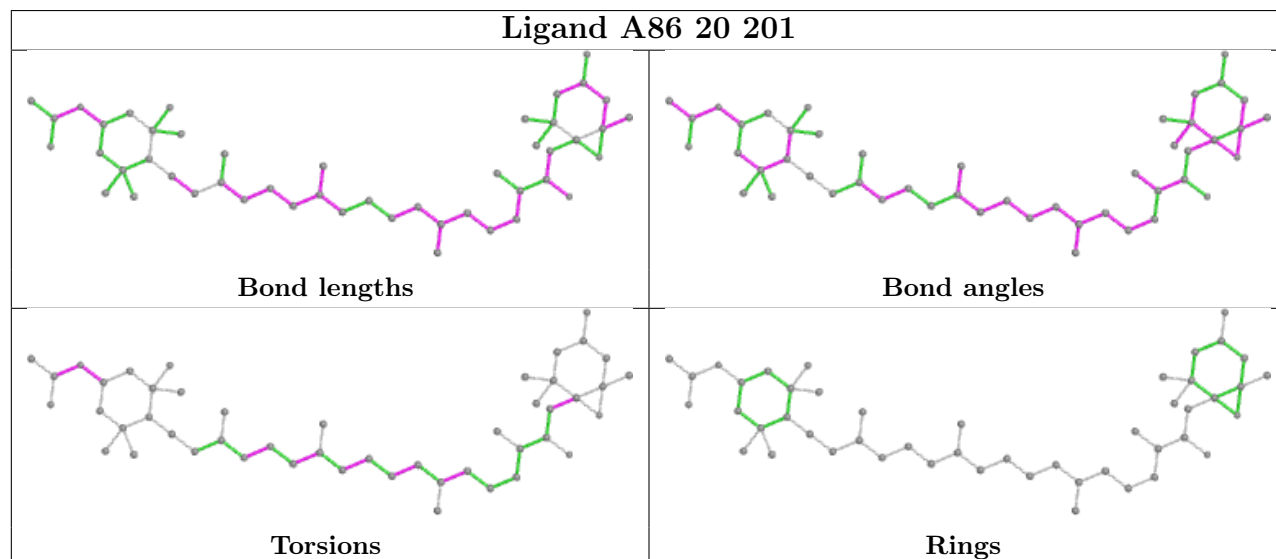
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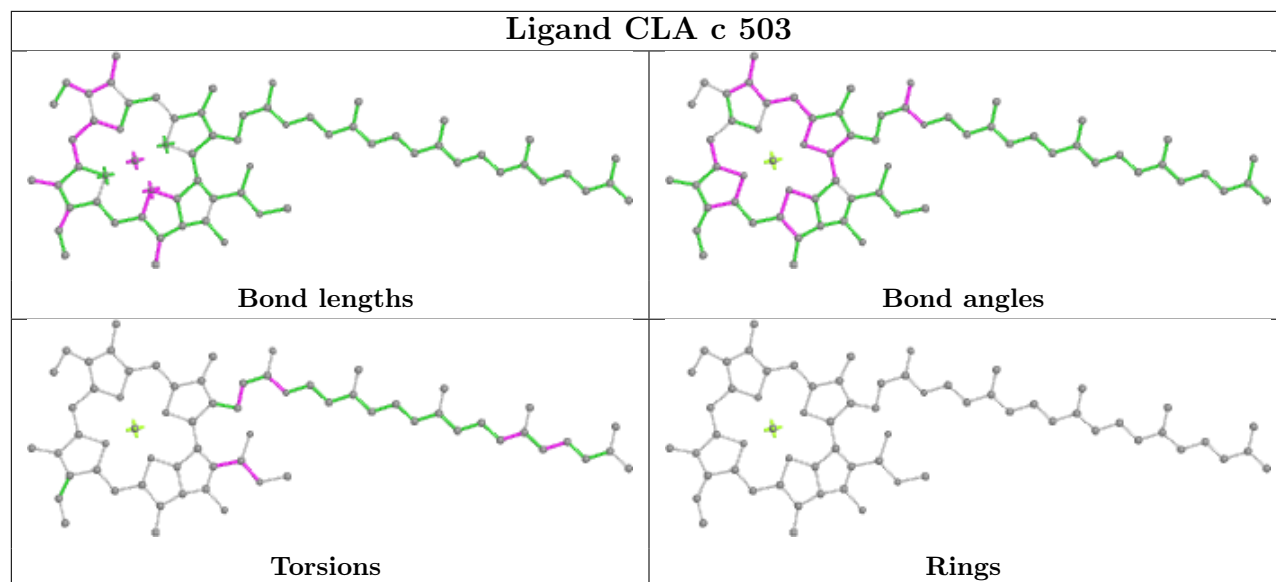
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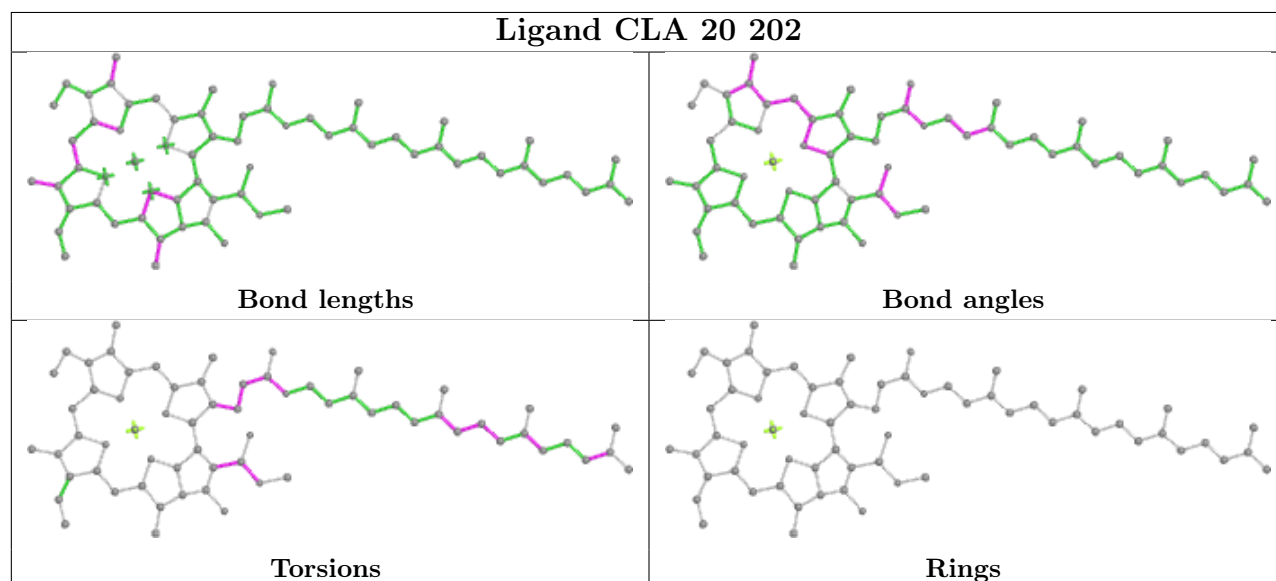
Ligand A86 20 201



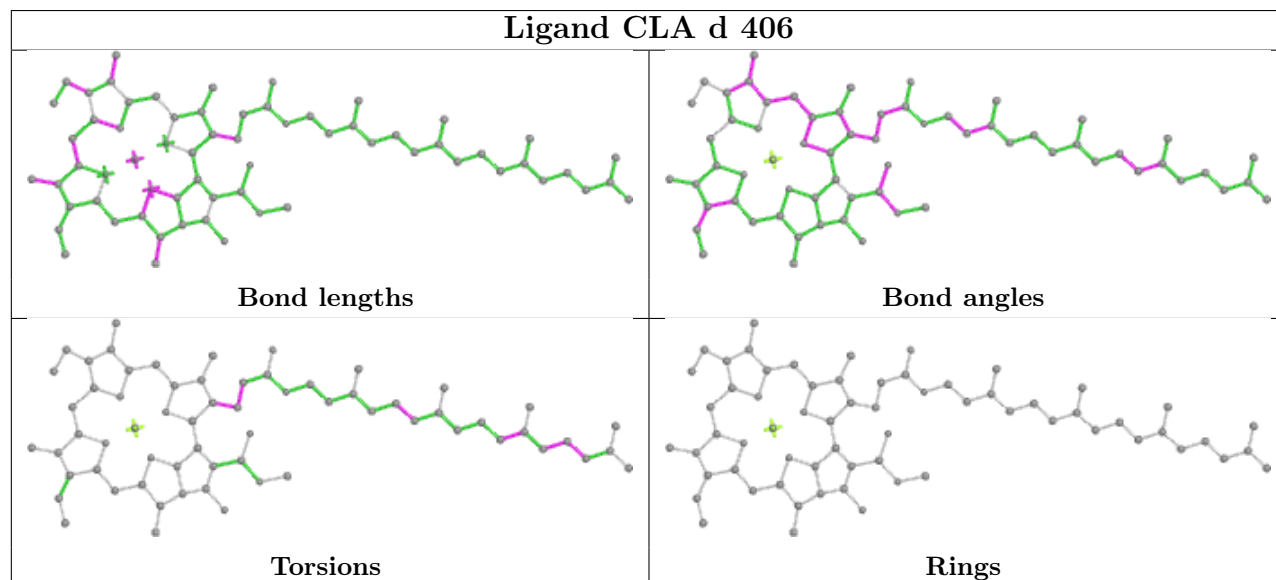
Ligand CLA c 503

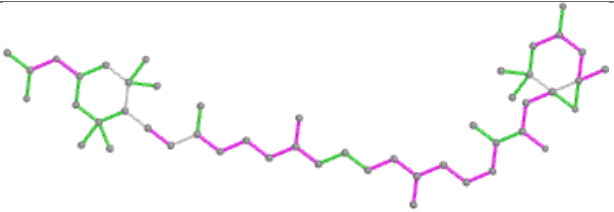
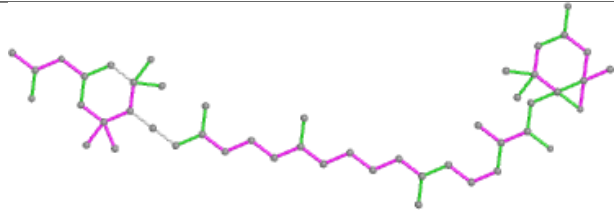
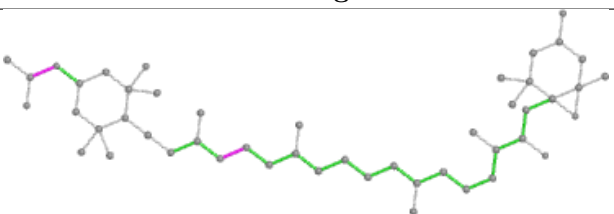
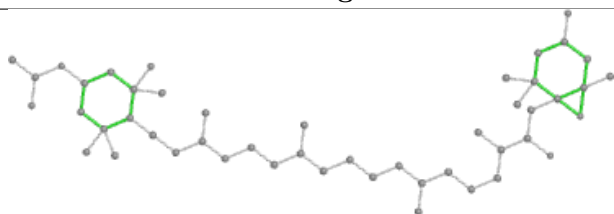


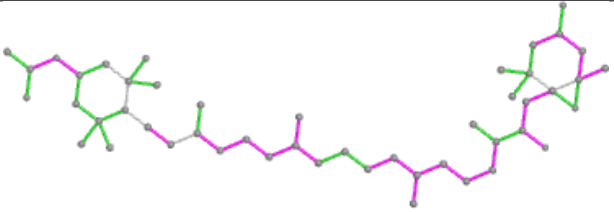
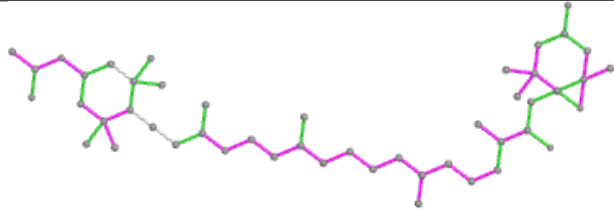
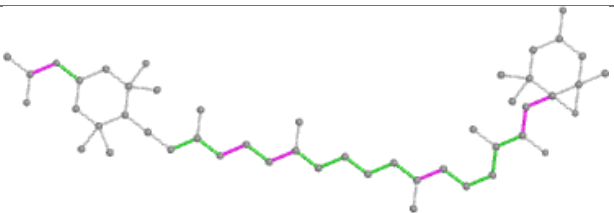
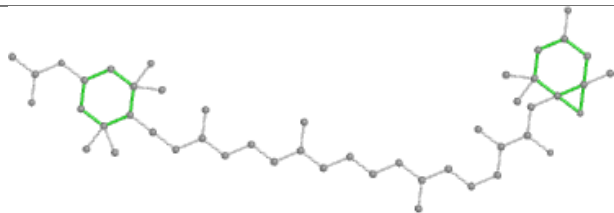
Ligand CLA 20 202

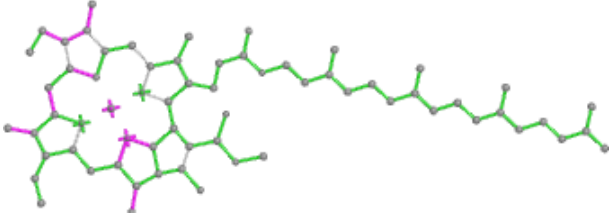
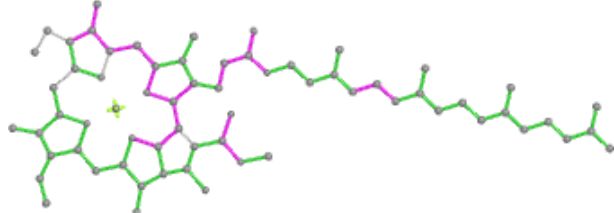
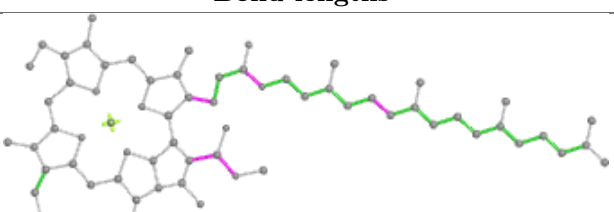
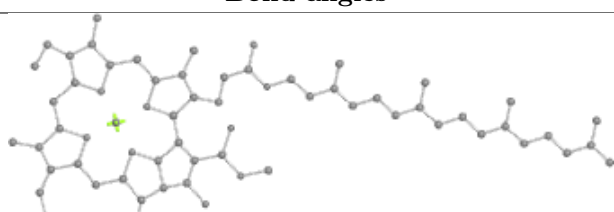


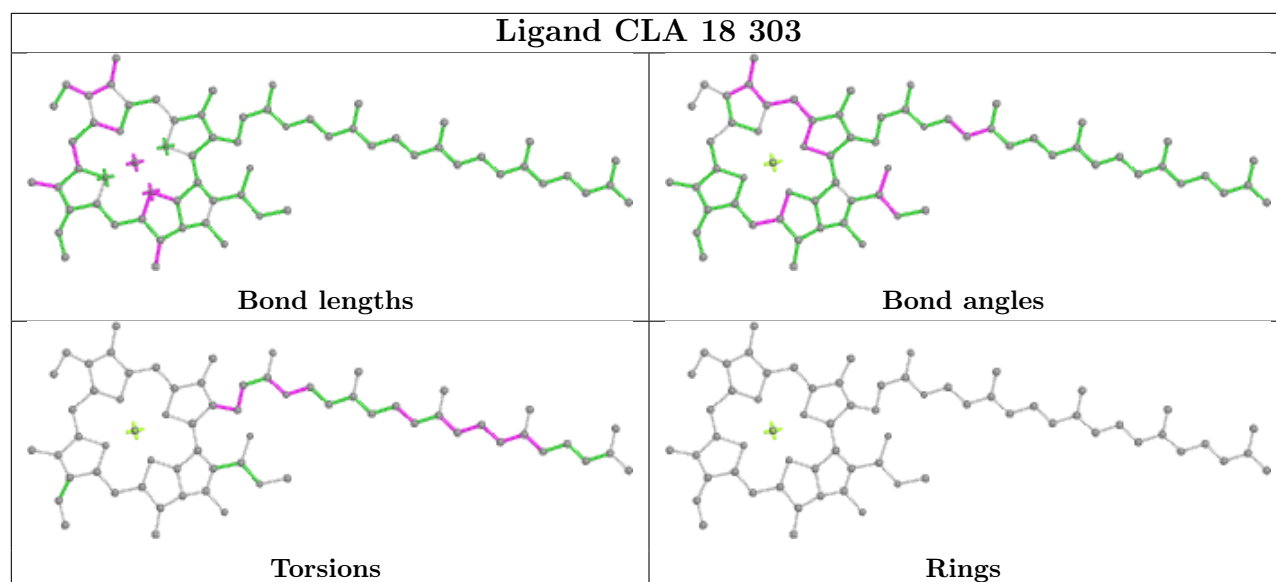
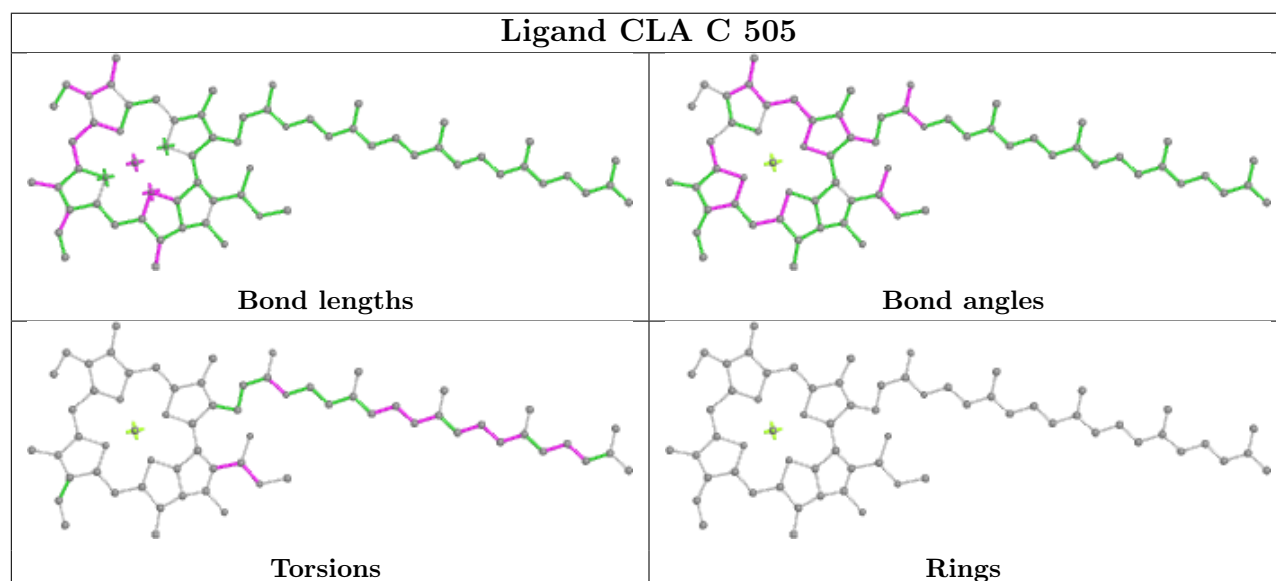
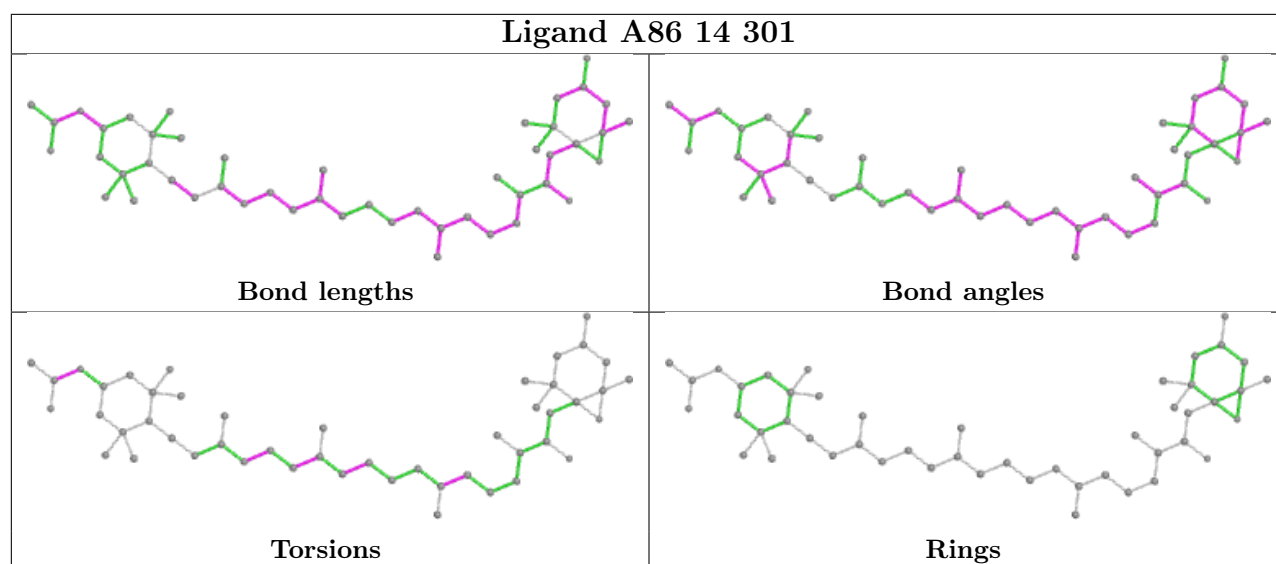
Ligand CLA d 406

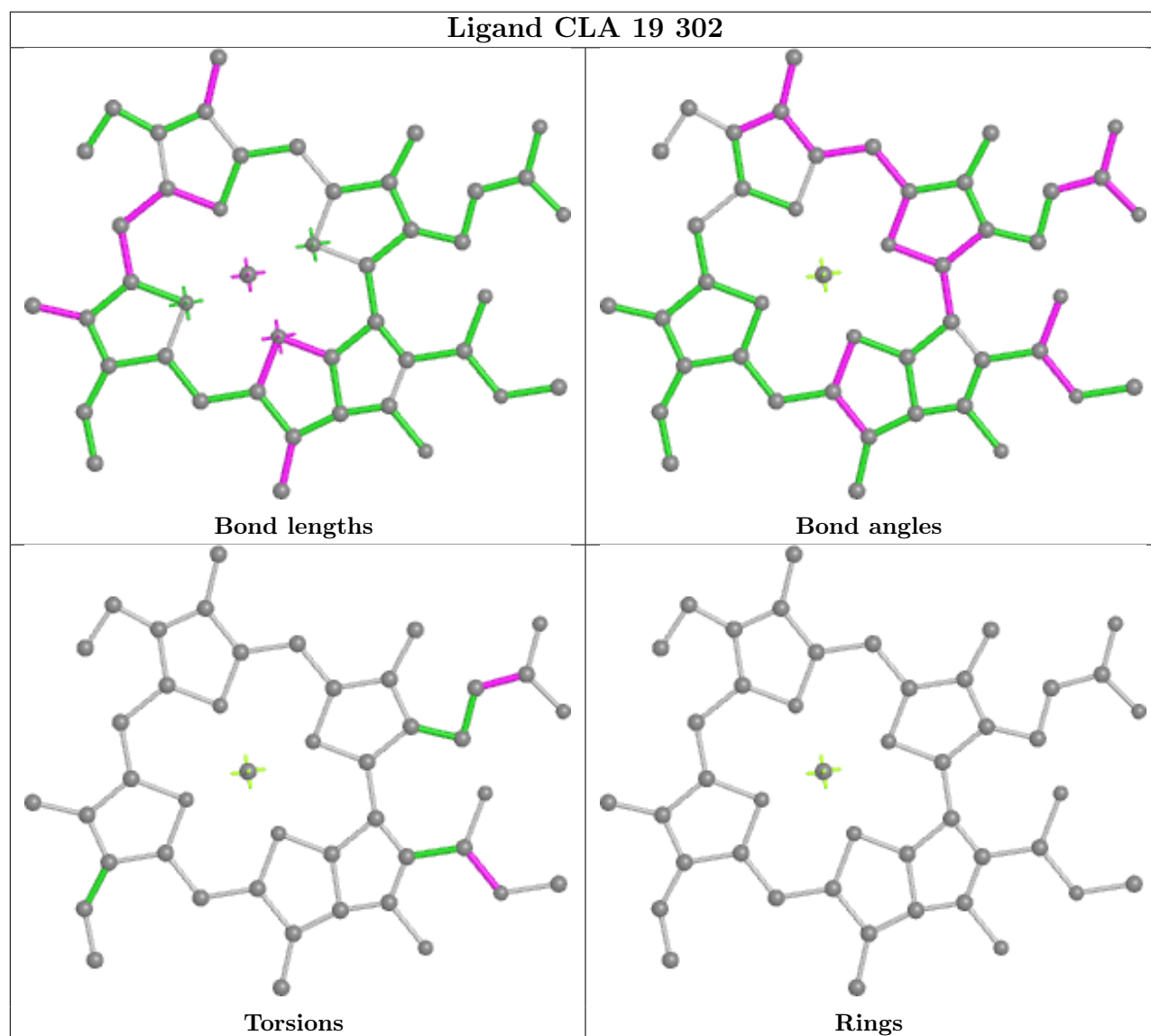
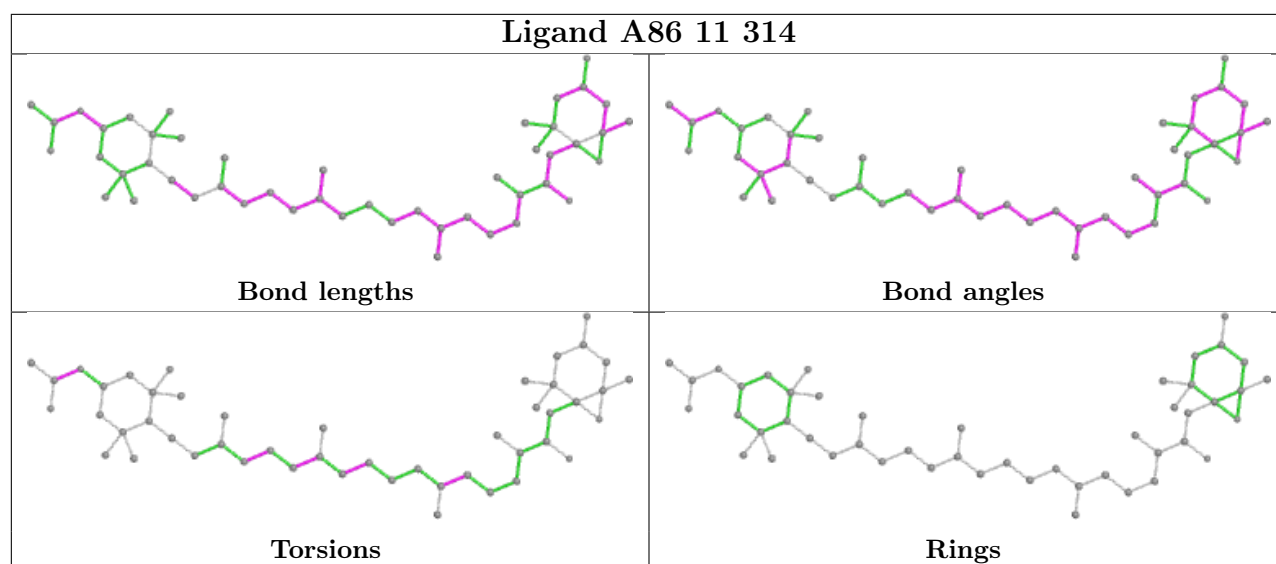


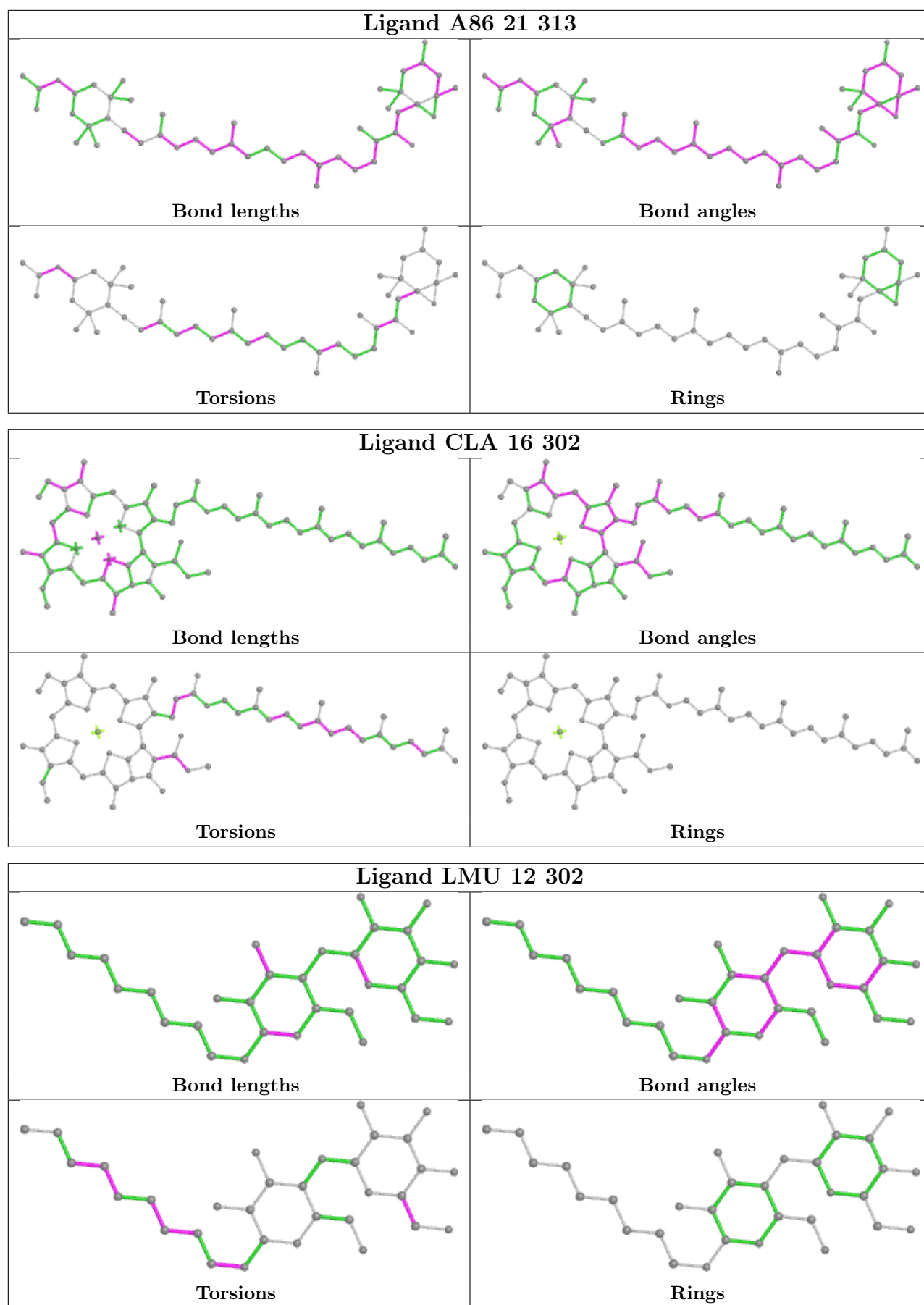
Ligand A86 16 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

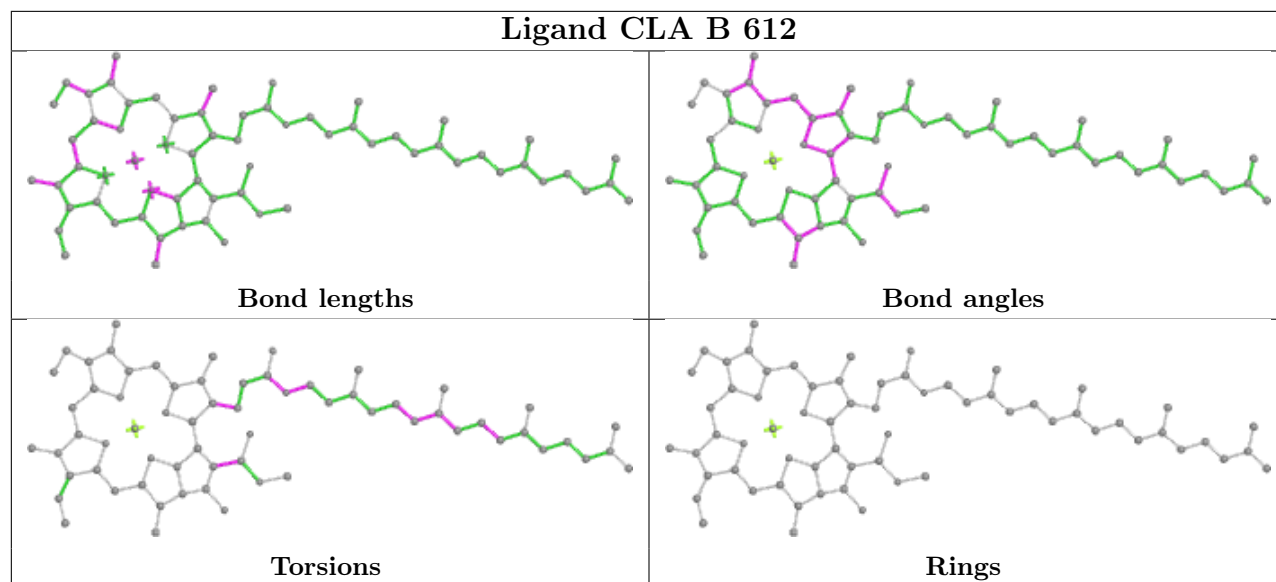
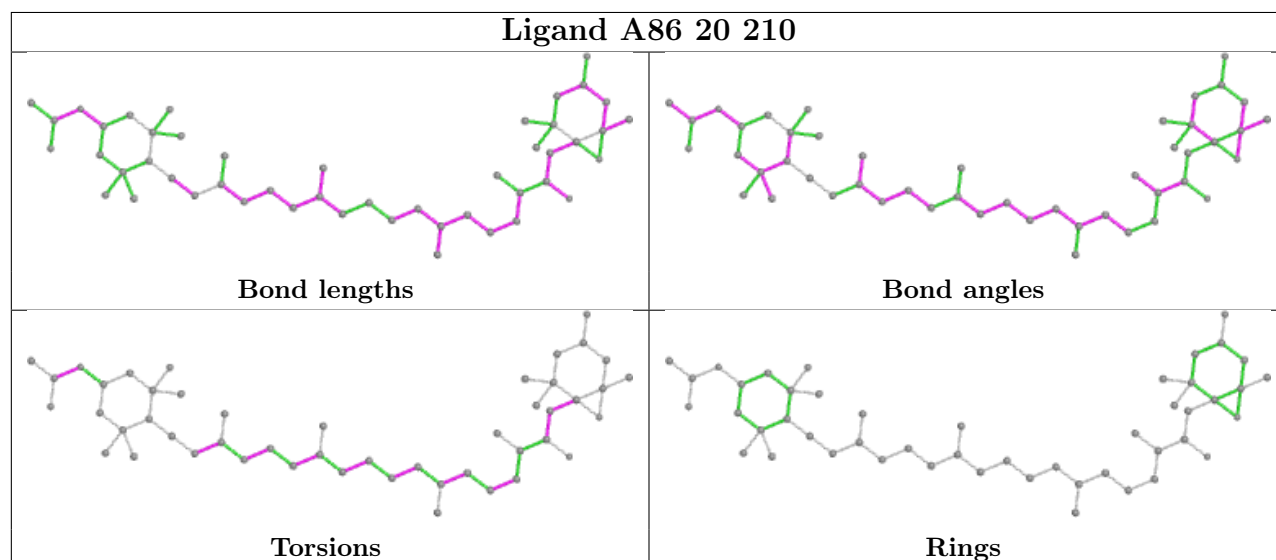
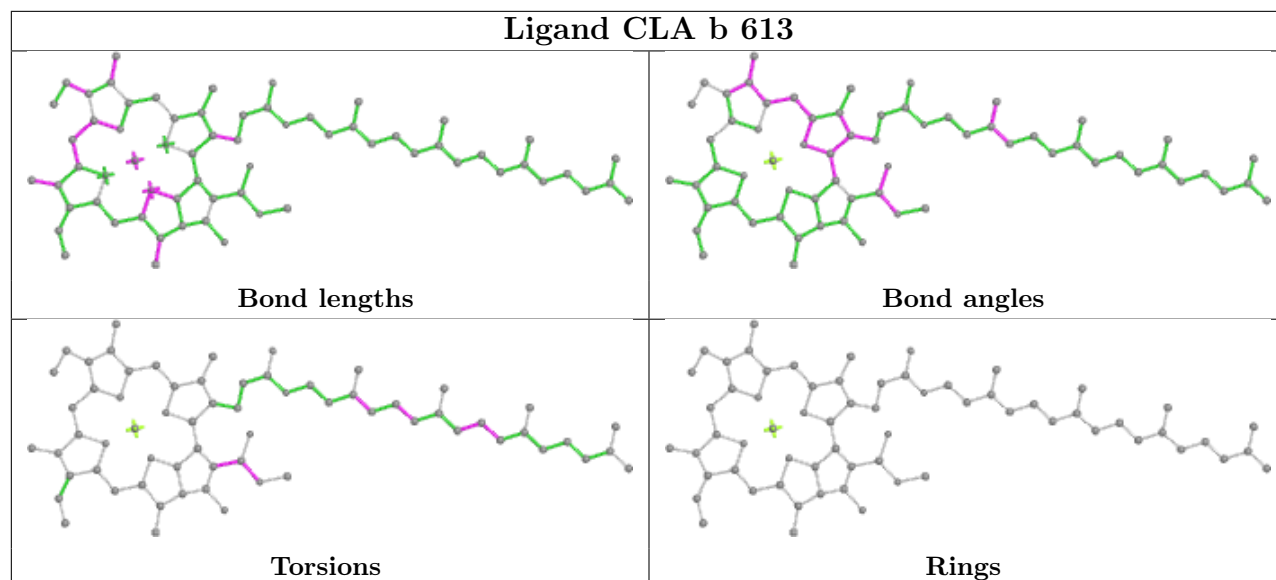
Ligand A86 14 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

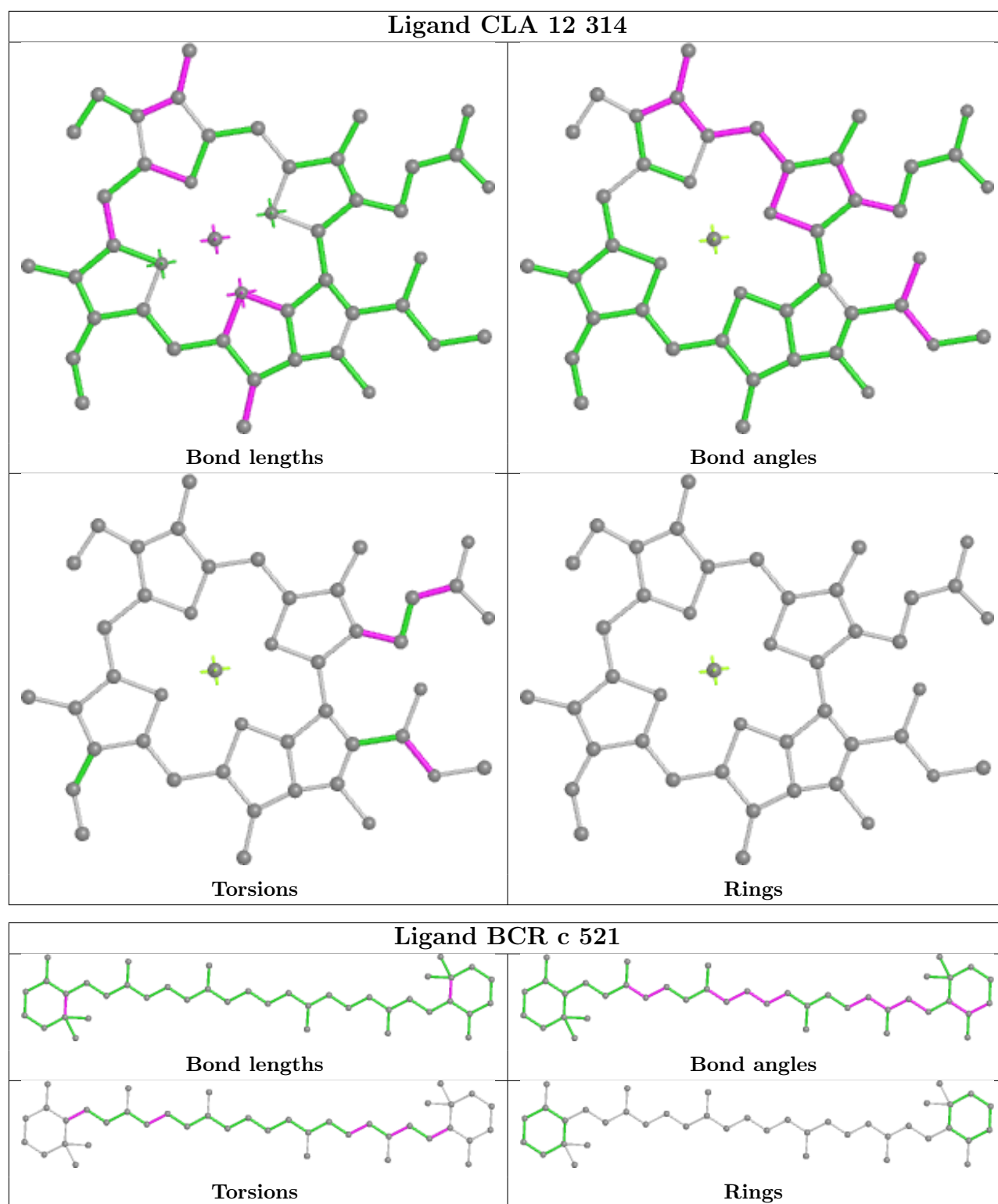
Ligand CLA C 512	
	
Bond lengths	Bond angles
	
Torsions	Rings

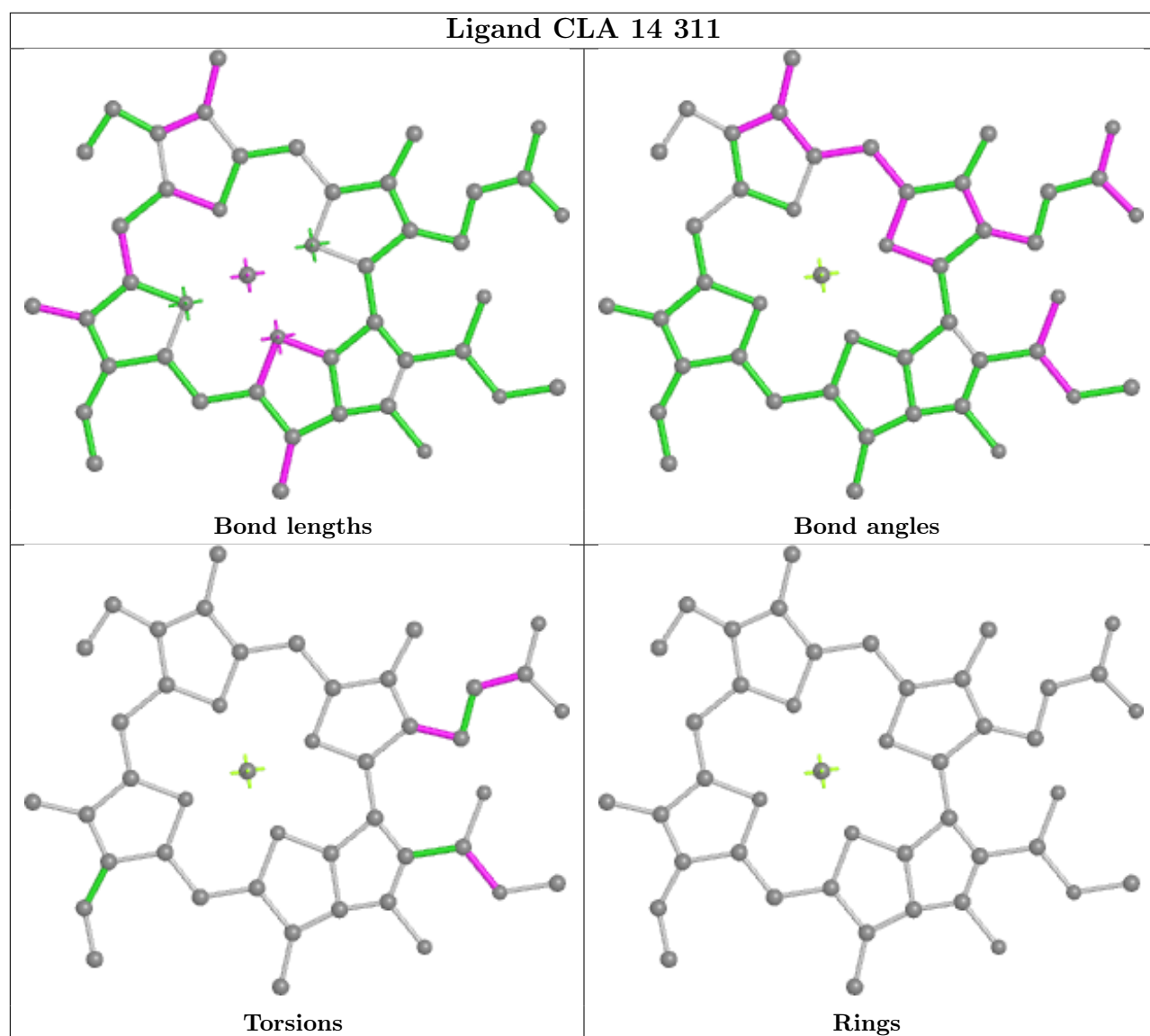


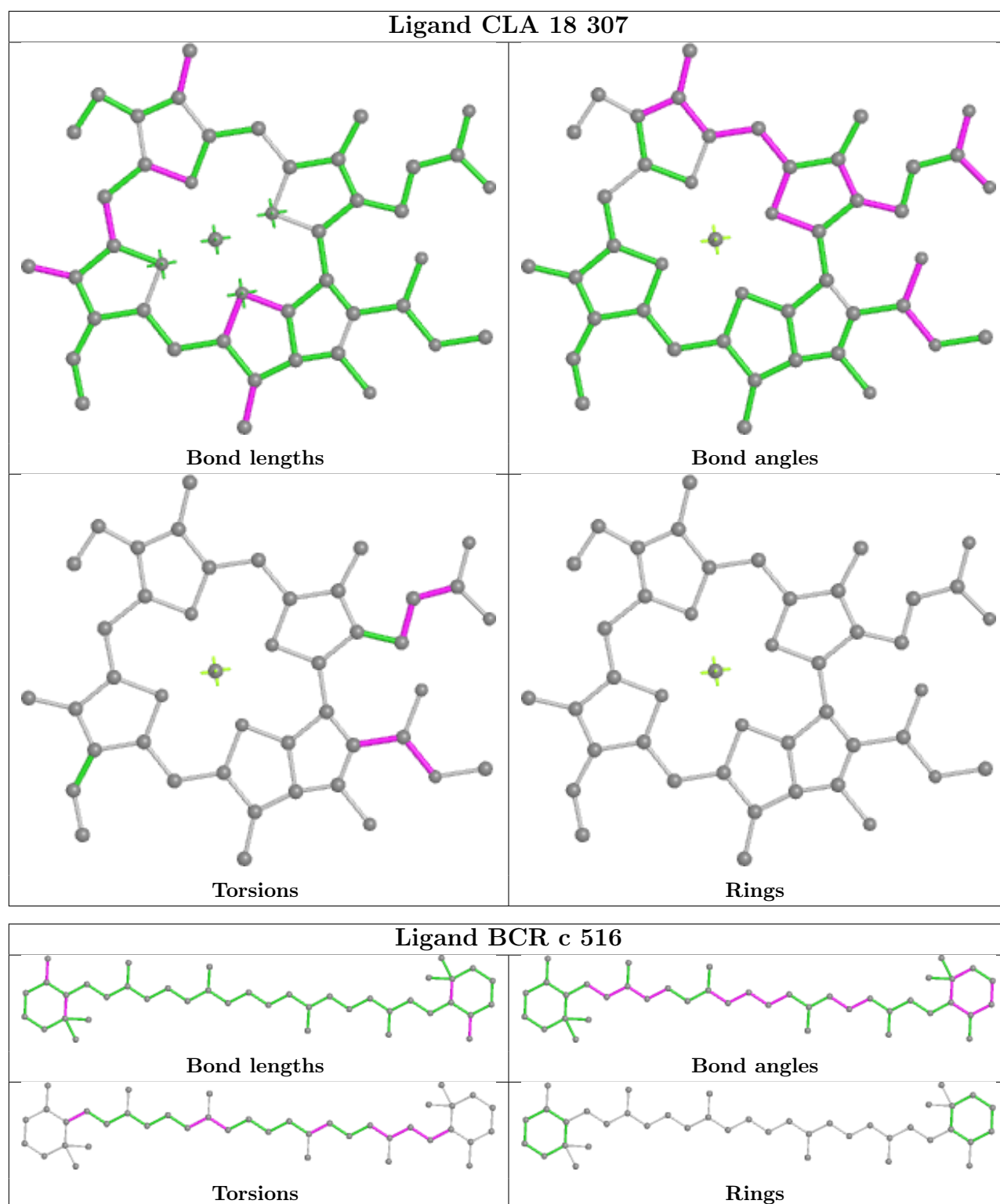




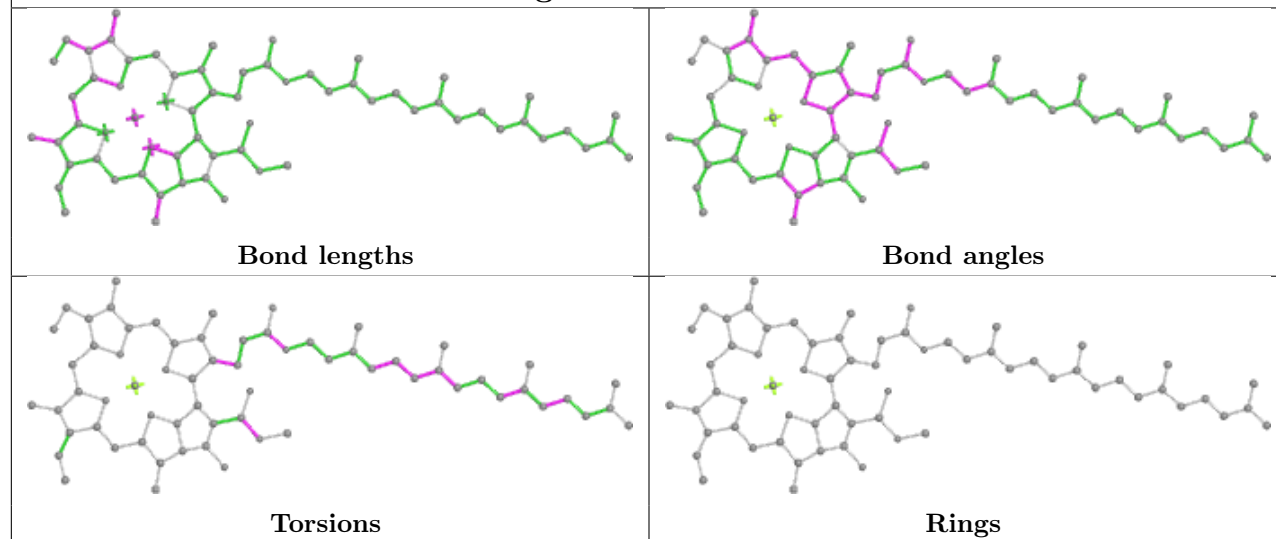
Ligand CLA B 612**Ligand A86 20 210****Ligand CLA b 613**



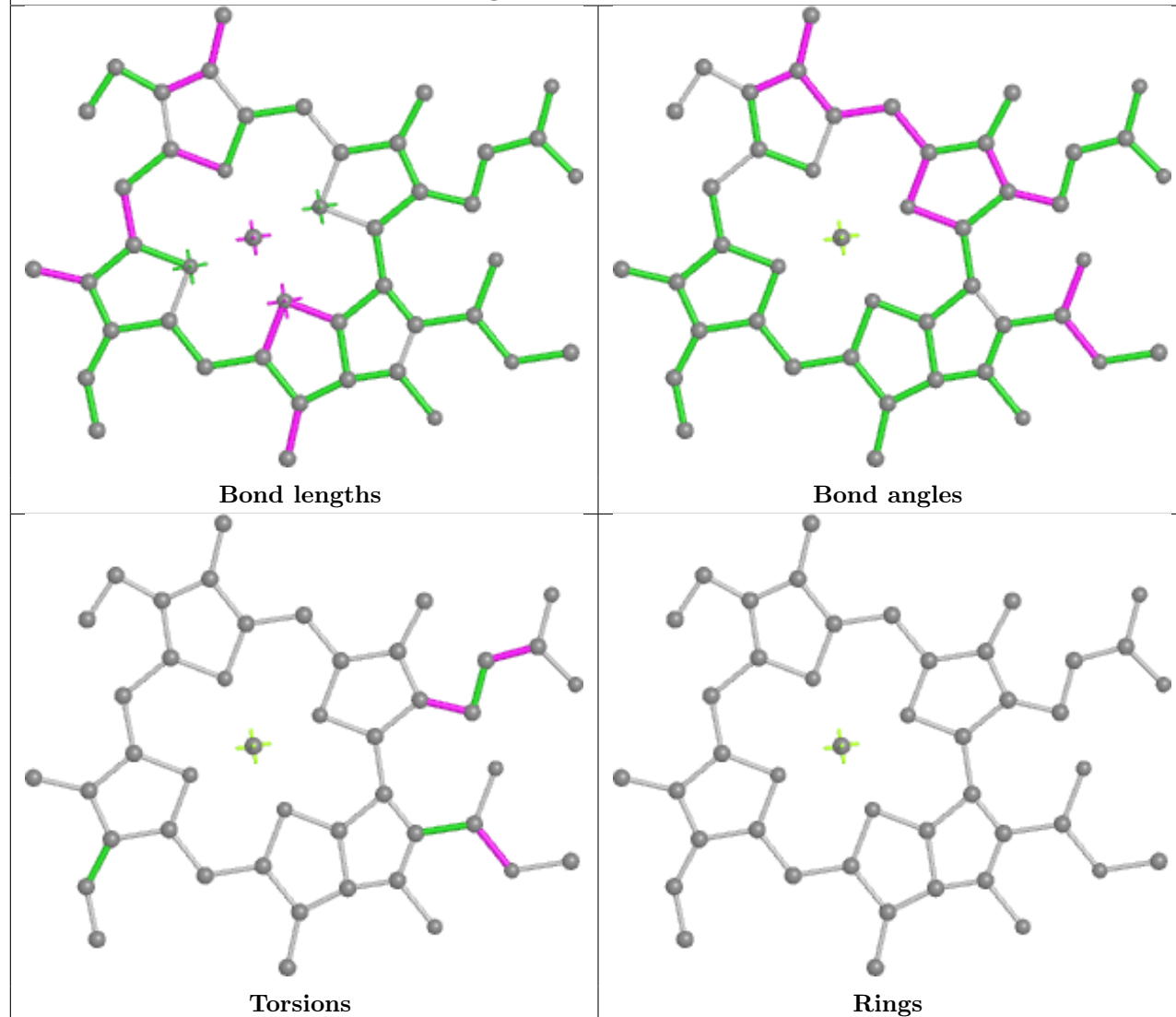


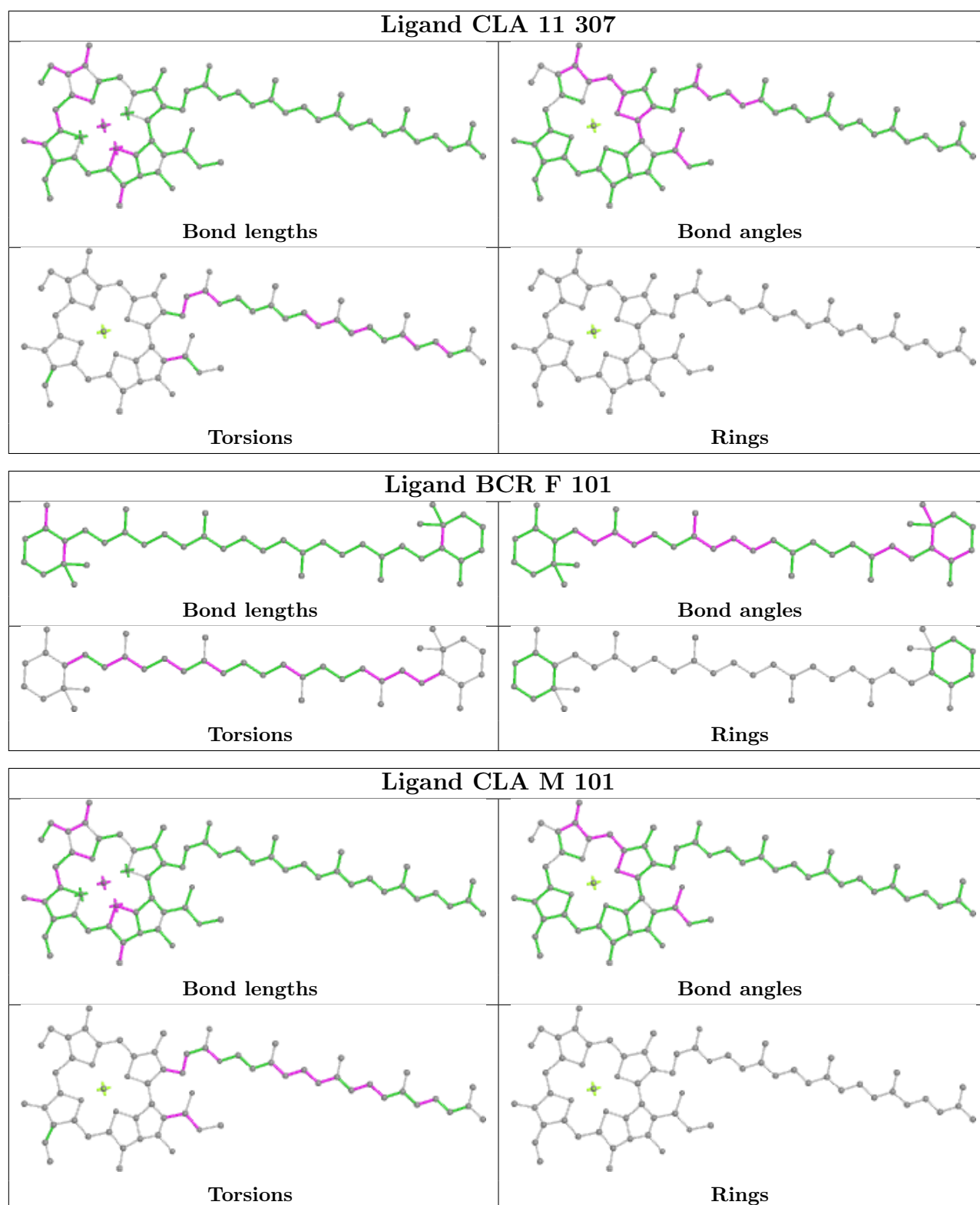


Ligand CLA b 622

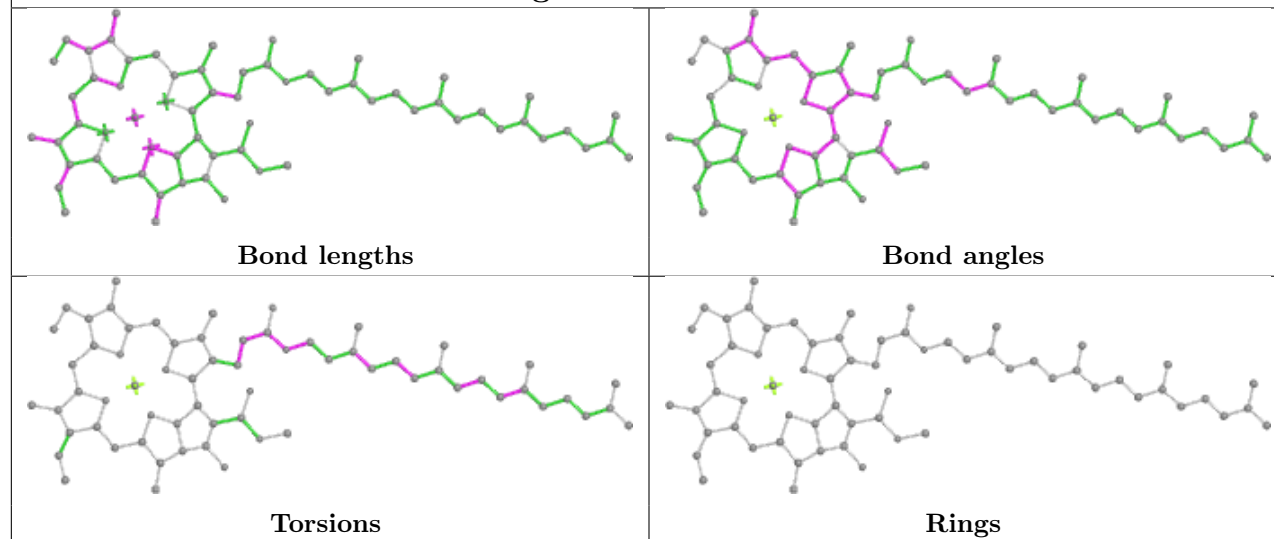


Ligand CLA 13 310

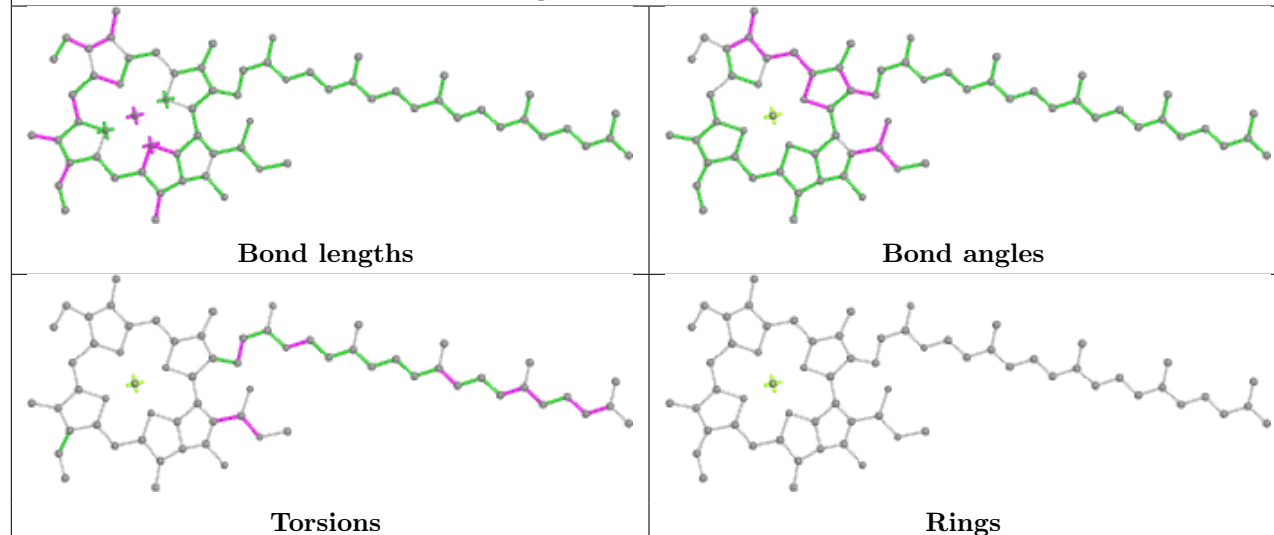




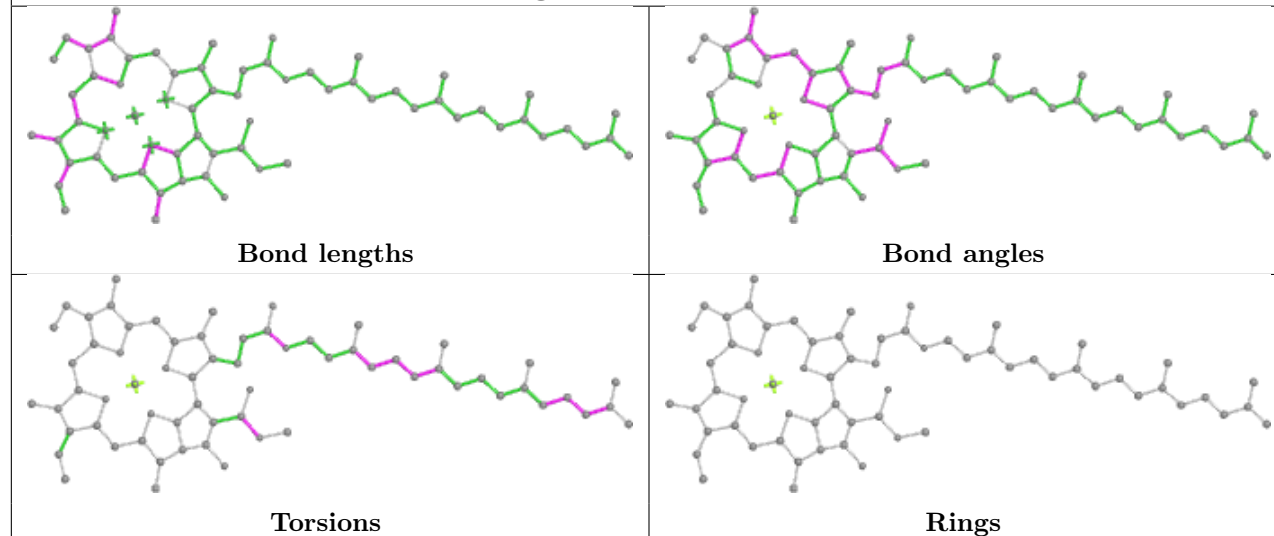
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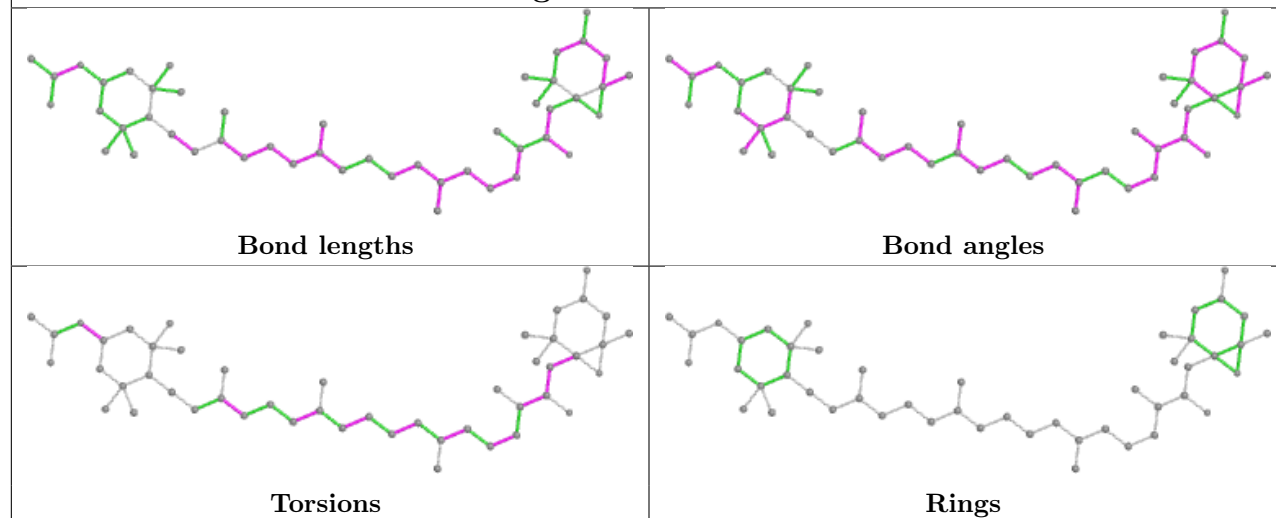
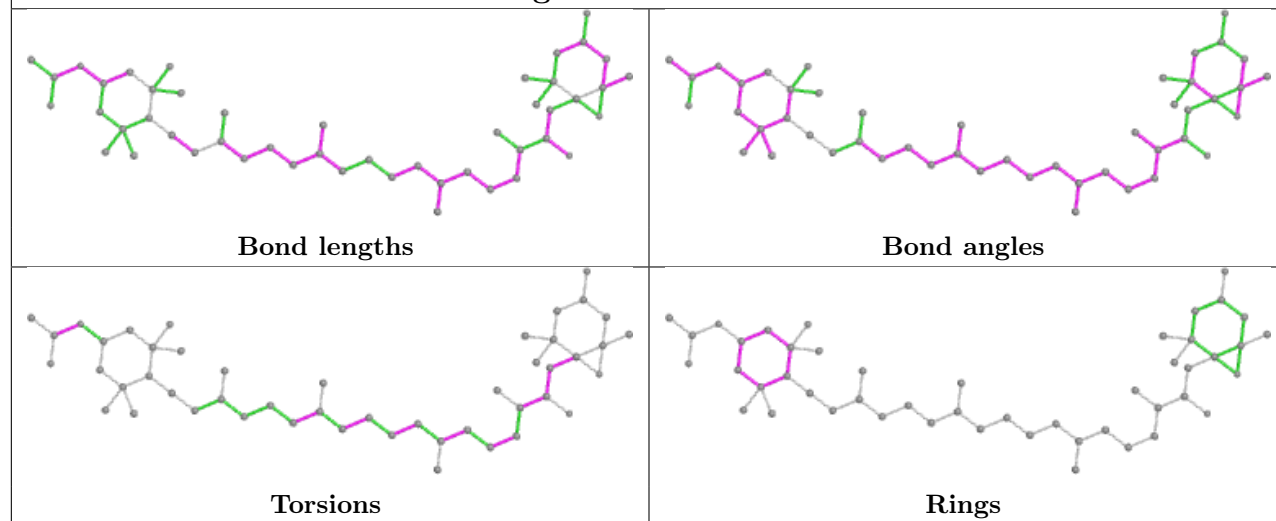


Ligand CLA B 610

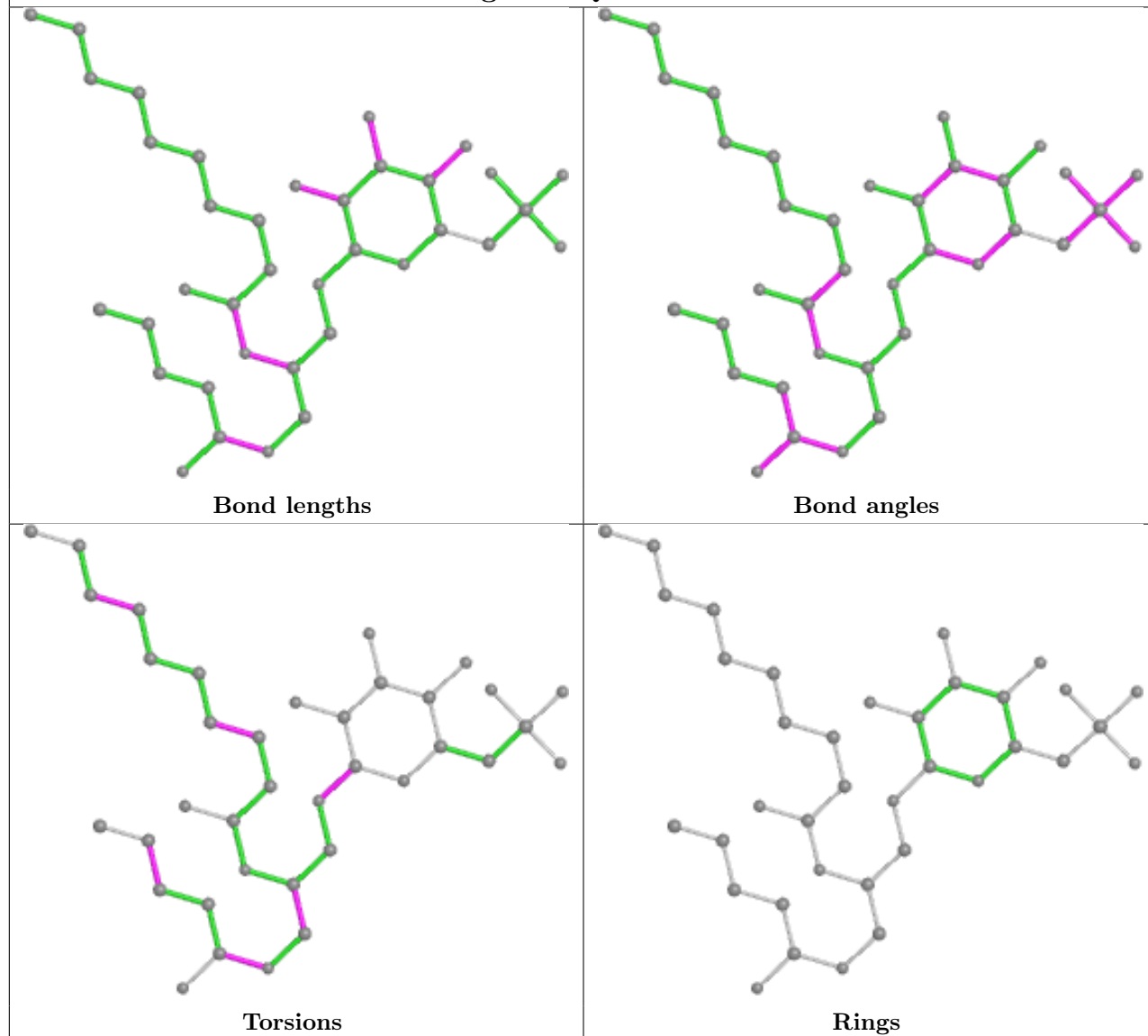


Ligand CLA B 602

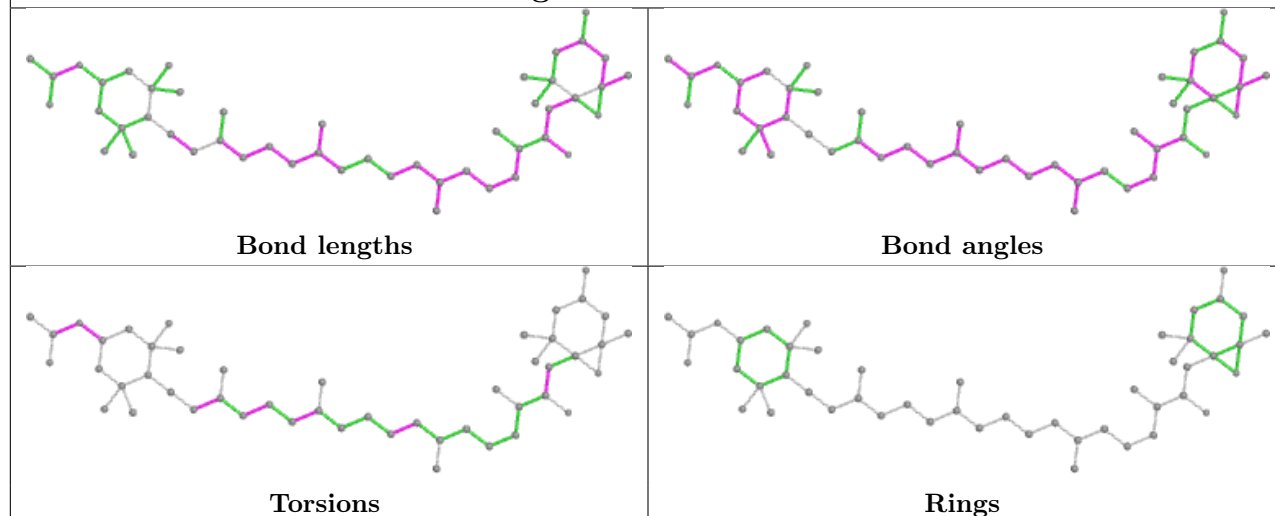


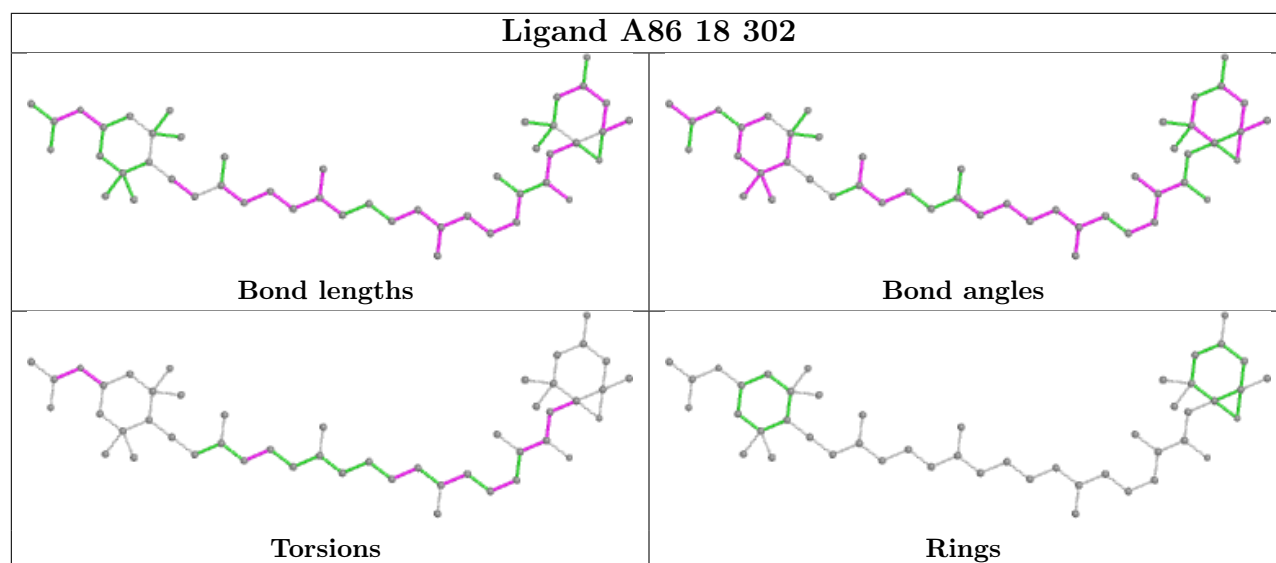
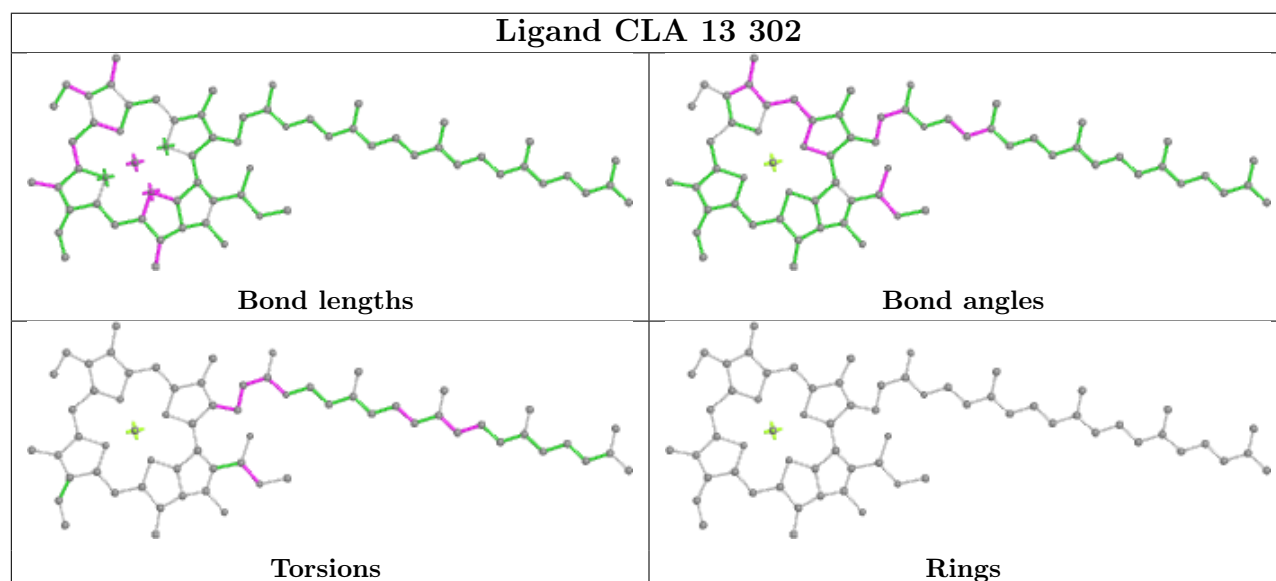
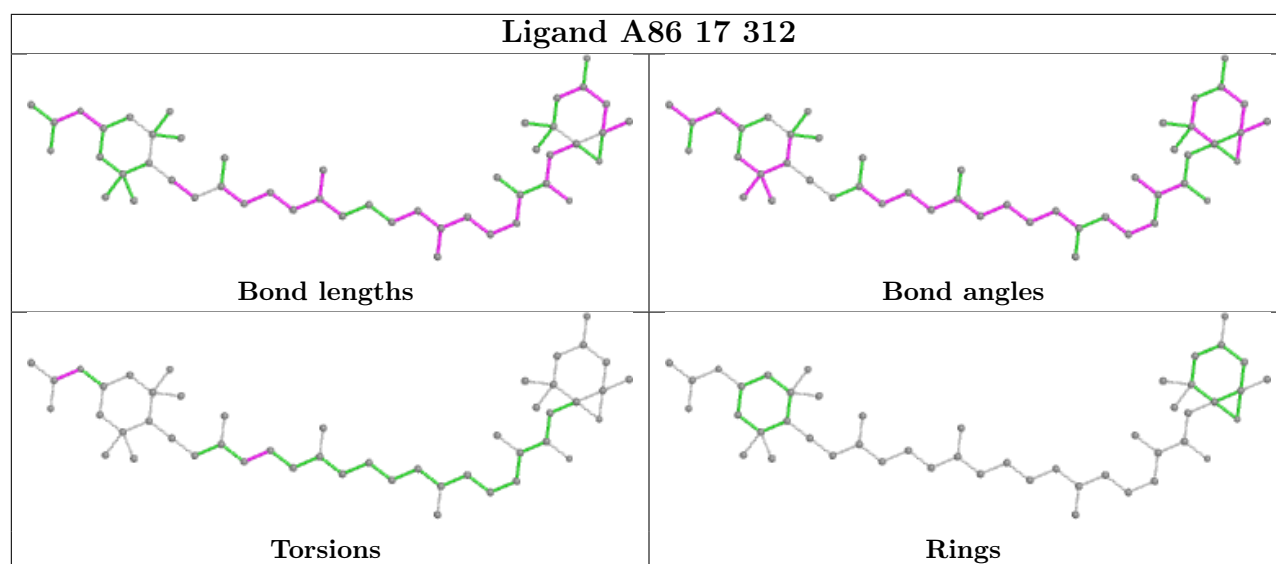
Ligand A86 19 311**Ligand A86 17 302**

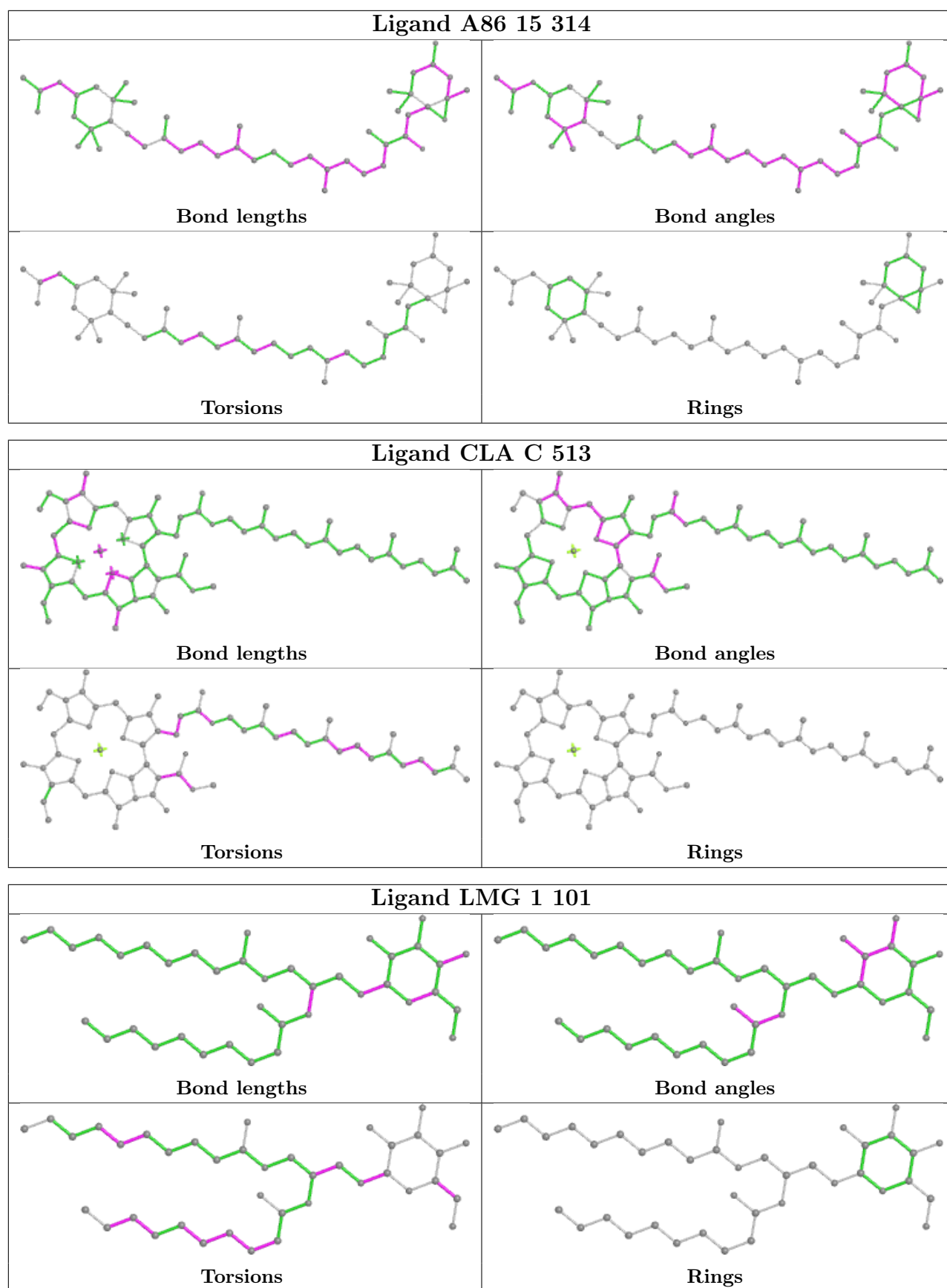
Ligand SQD b 620

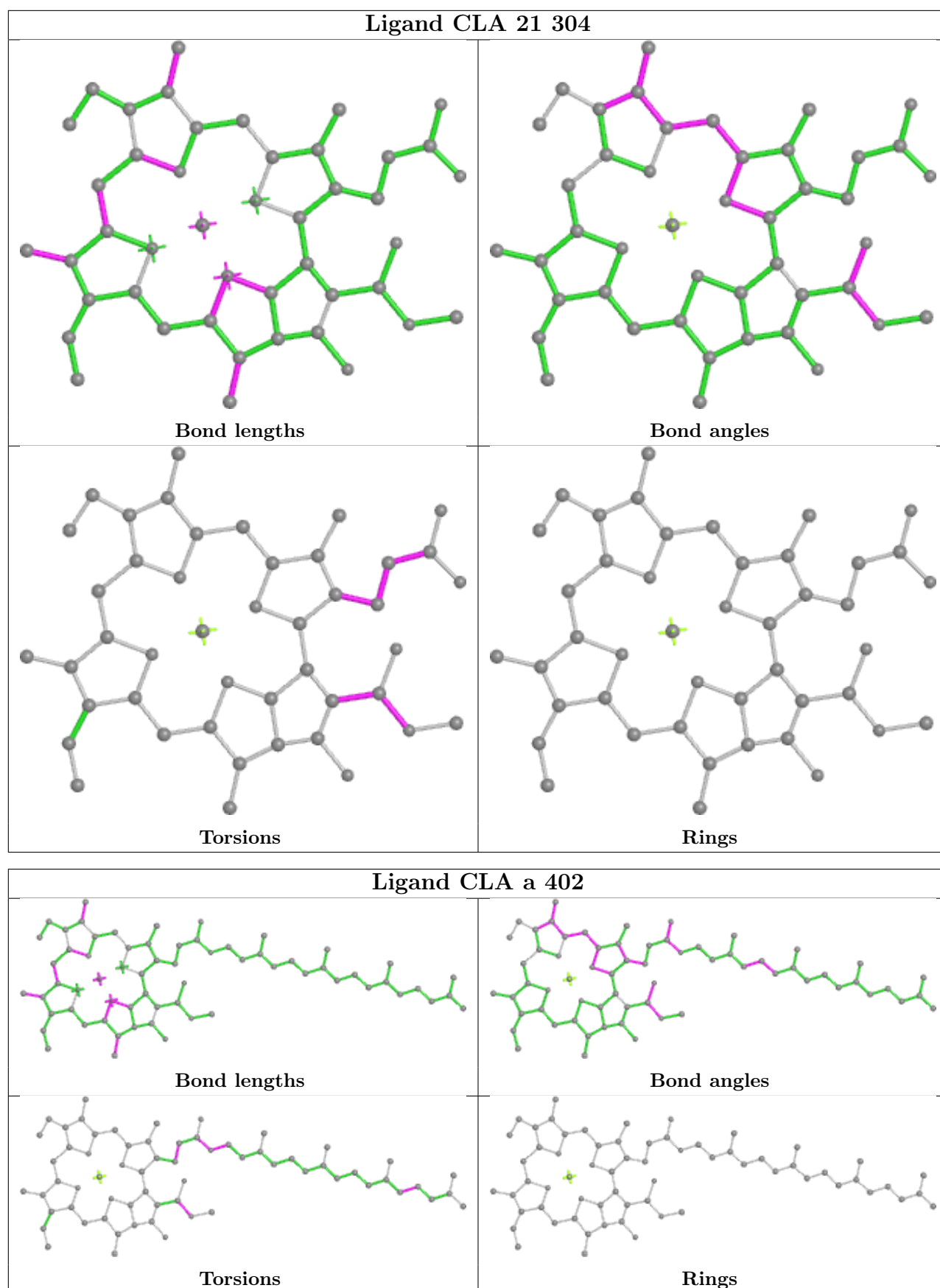


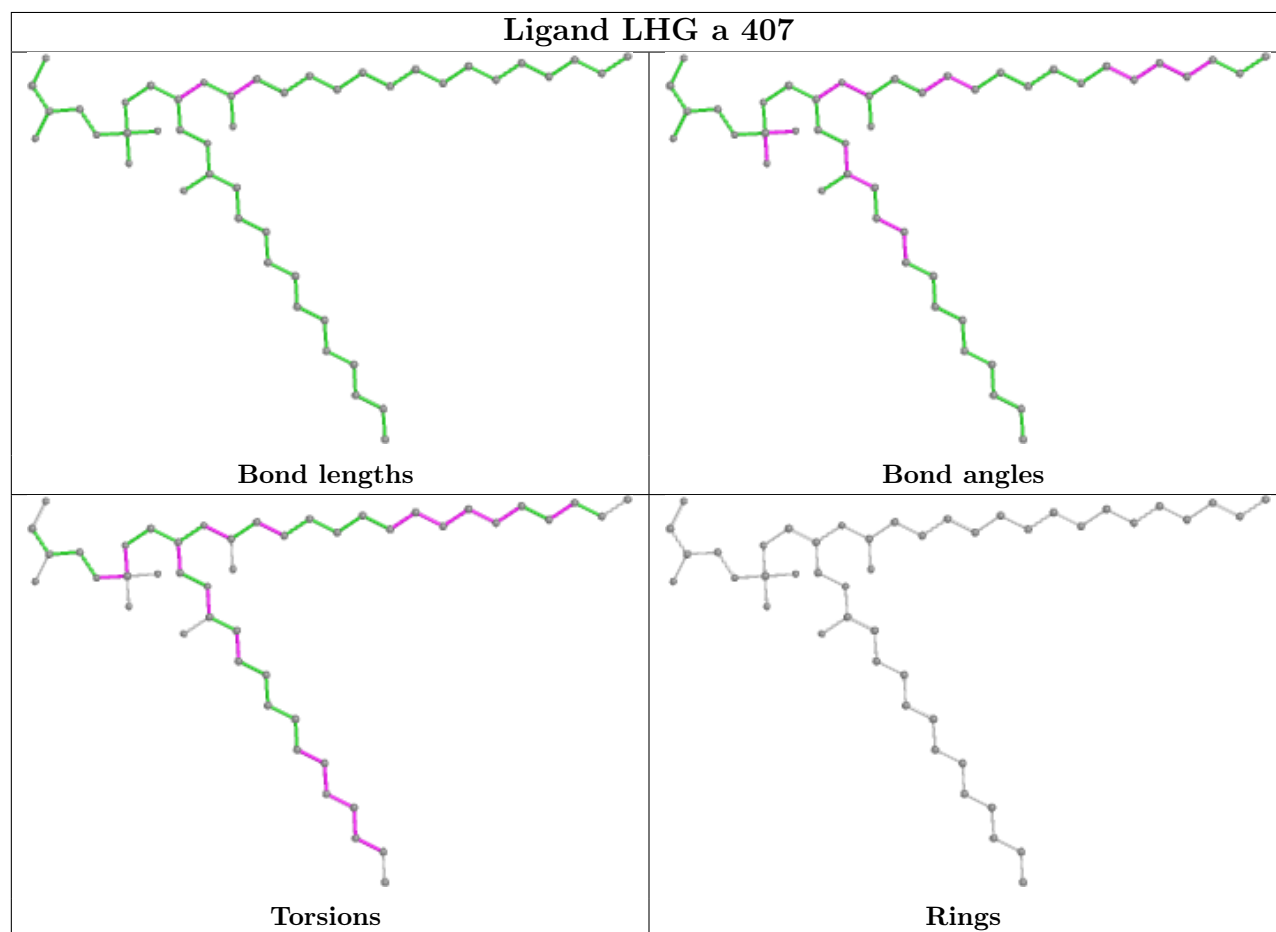
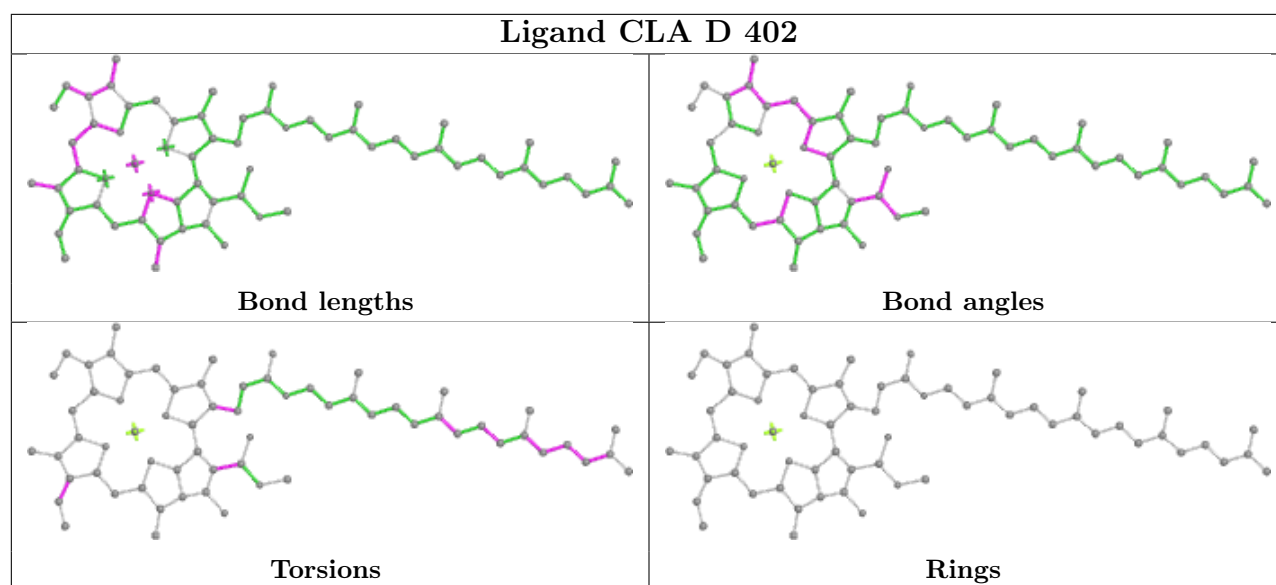
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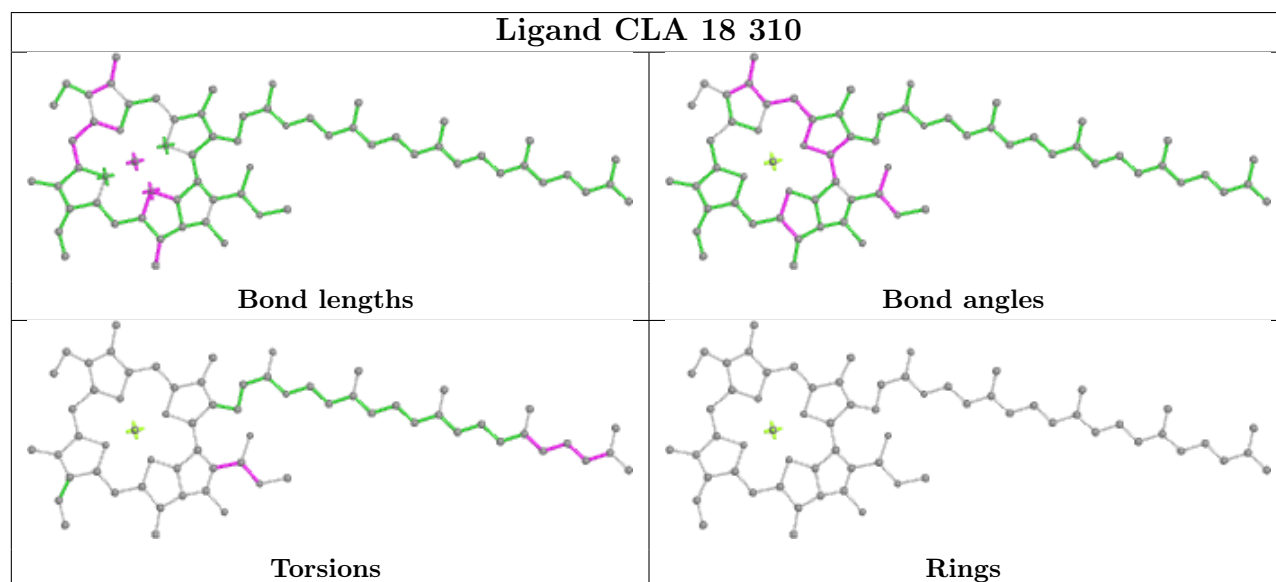
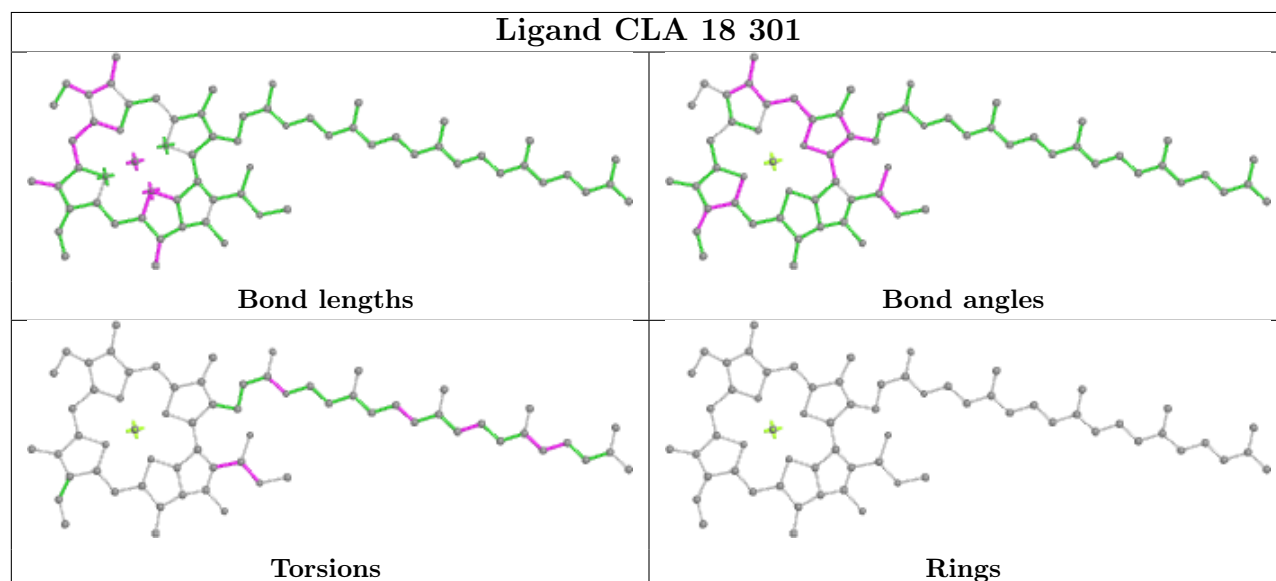
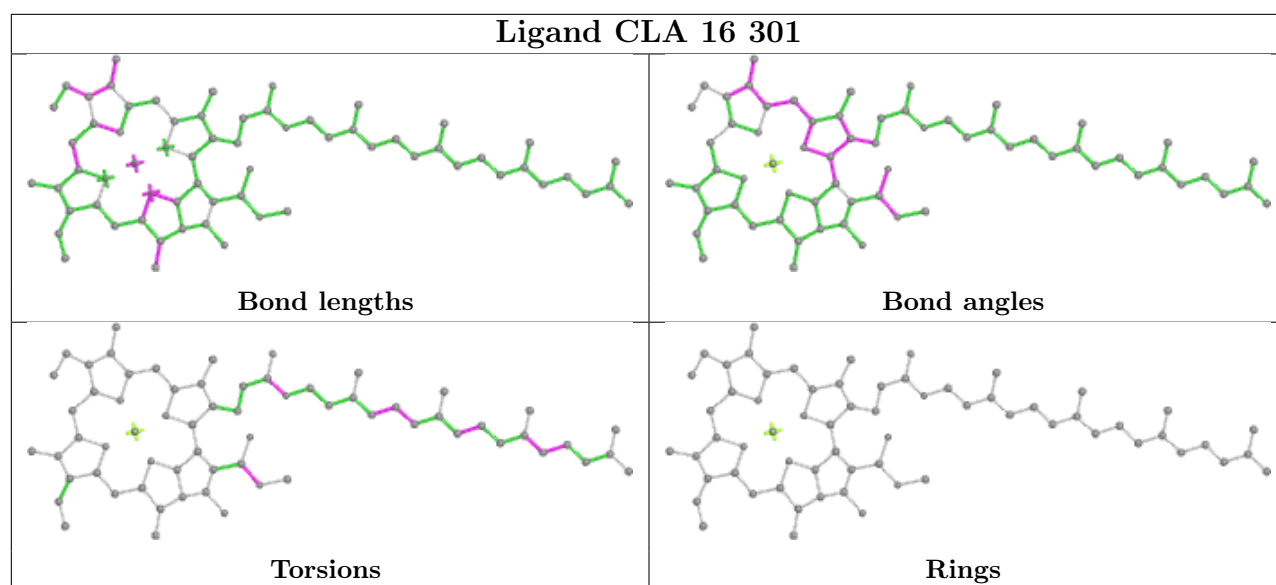




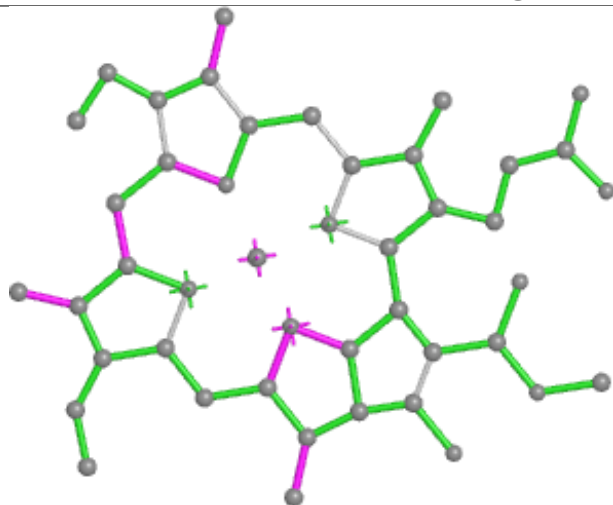




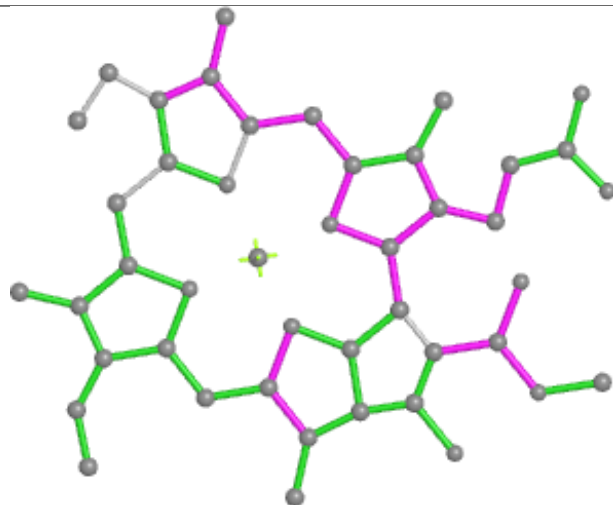




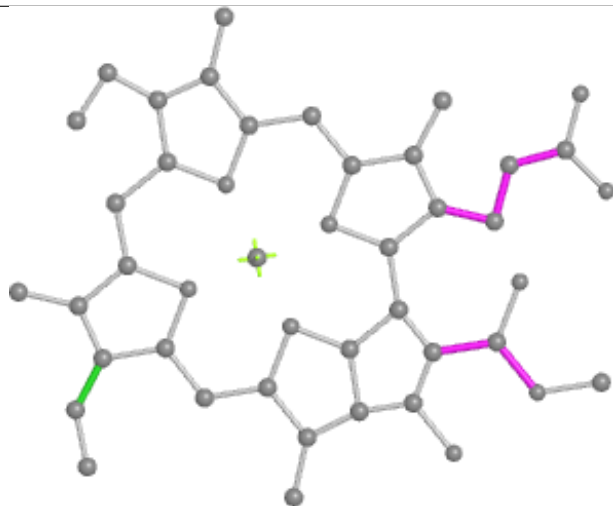
Ligand CLA 14 306



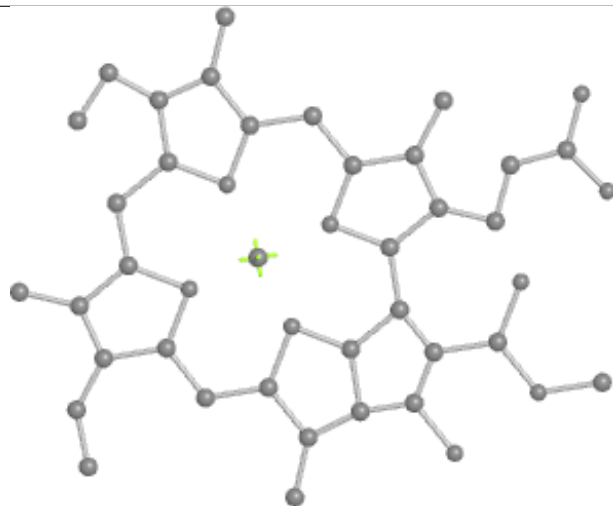
Bond lengths



Bond angles

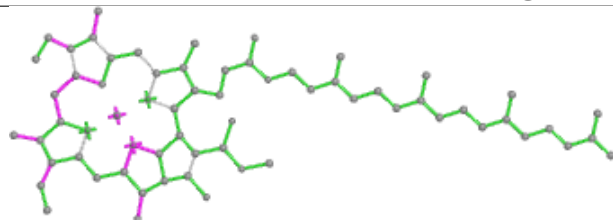


Torsions

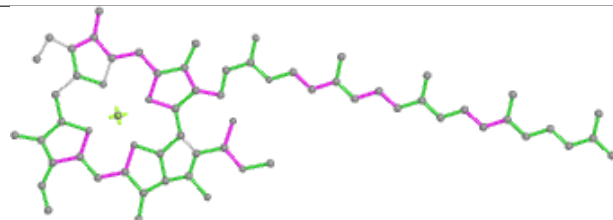


Rings

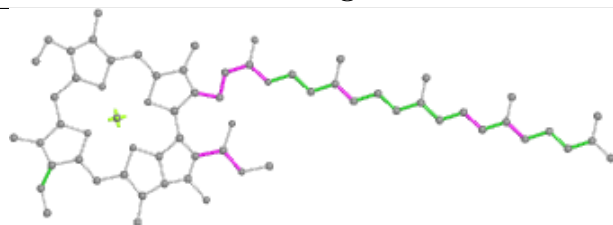
Ligand CLA c 502



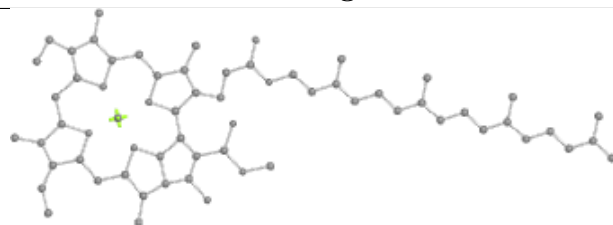
Bond lengths



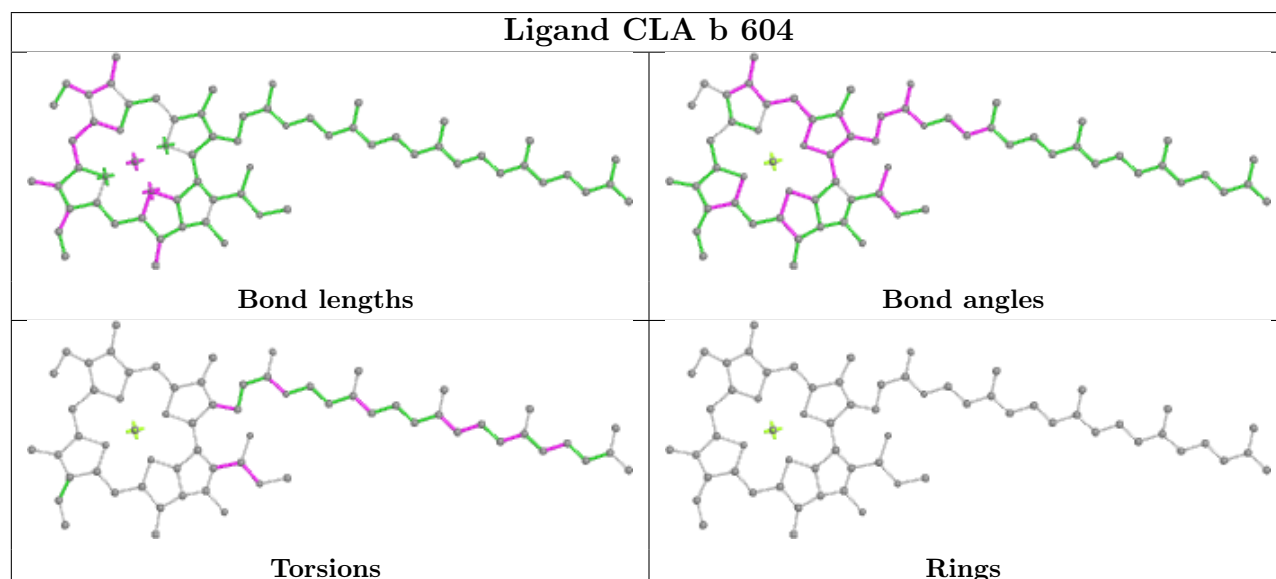
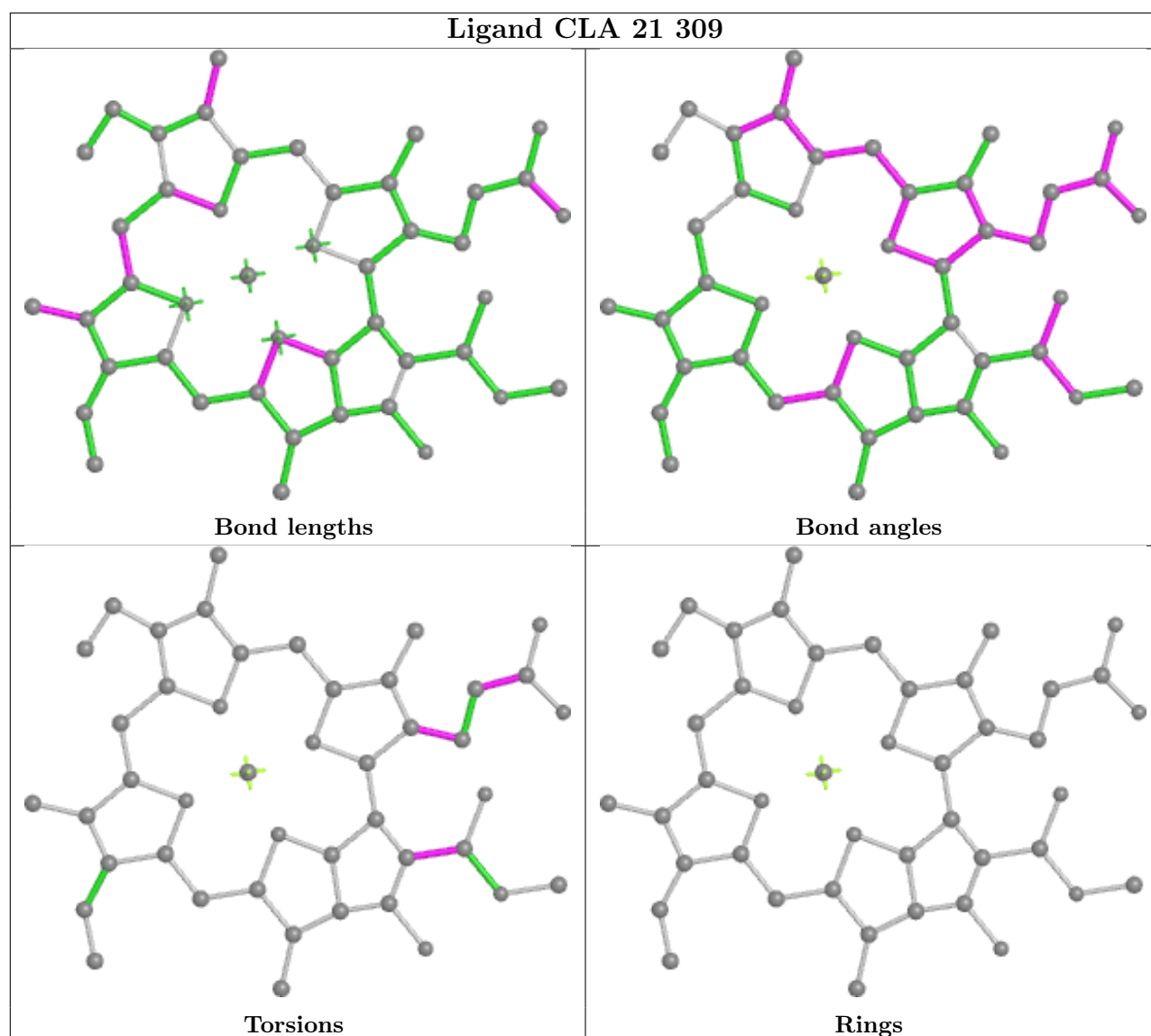
Bond angles

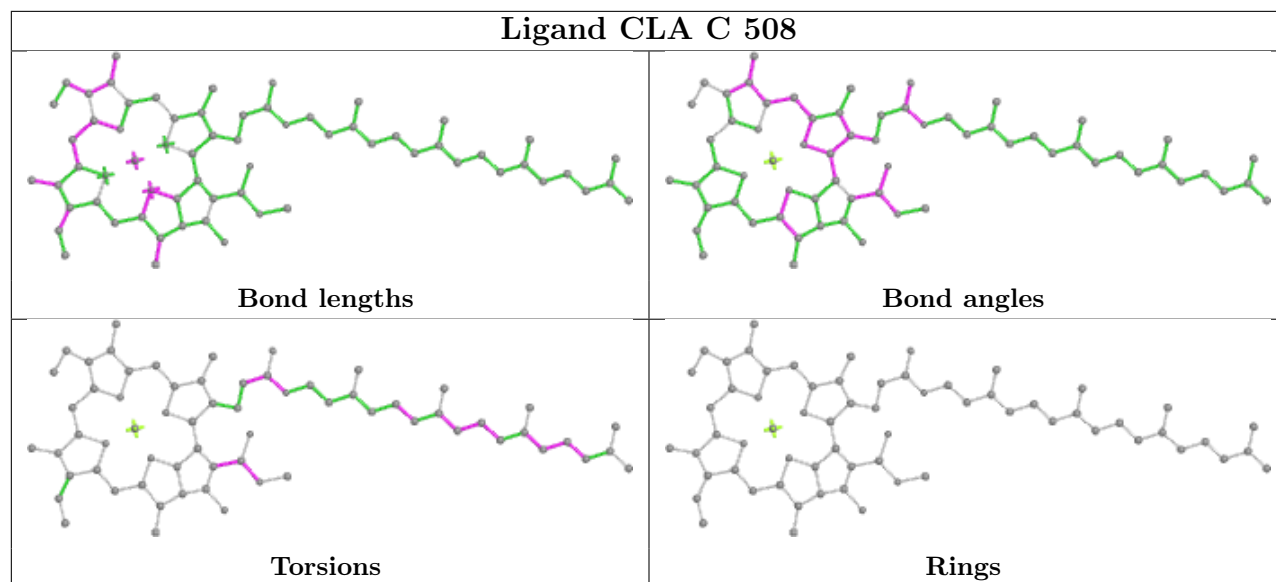
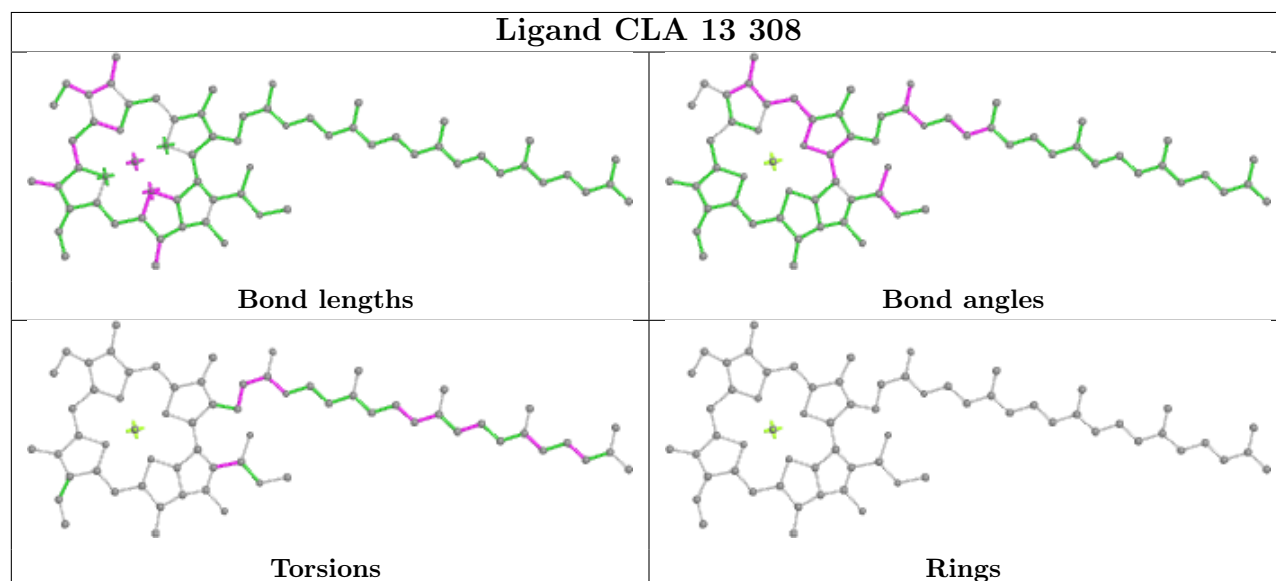
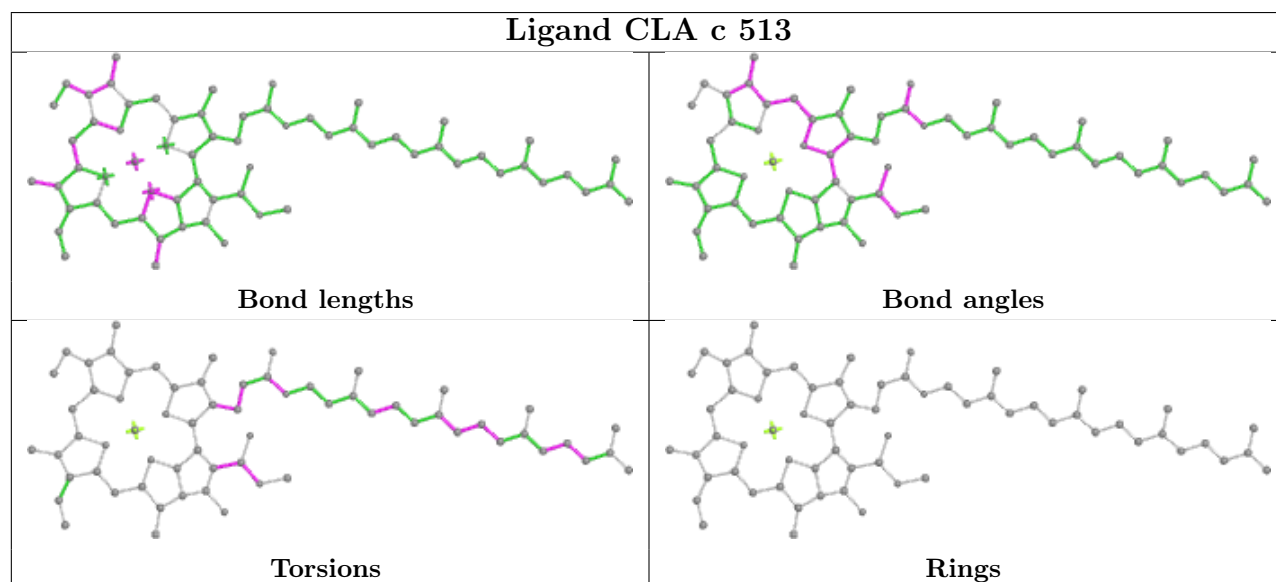


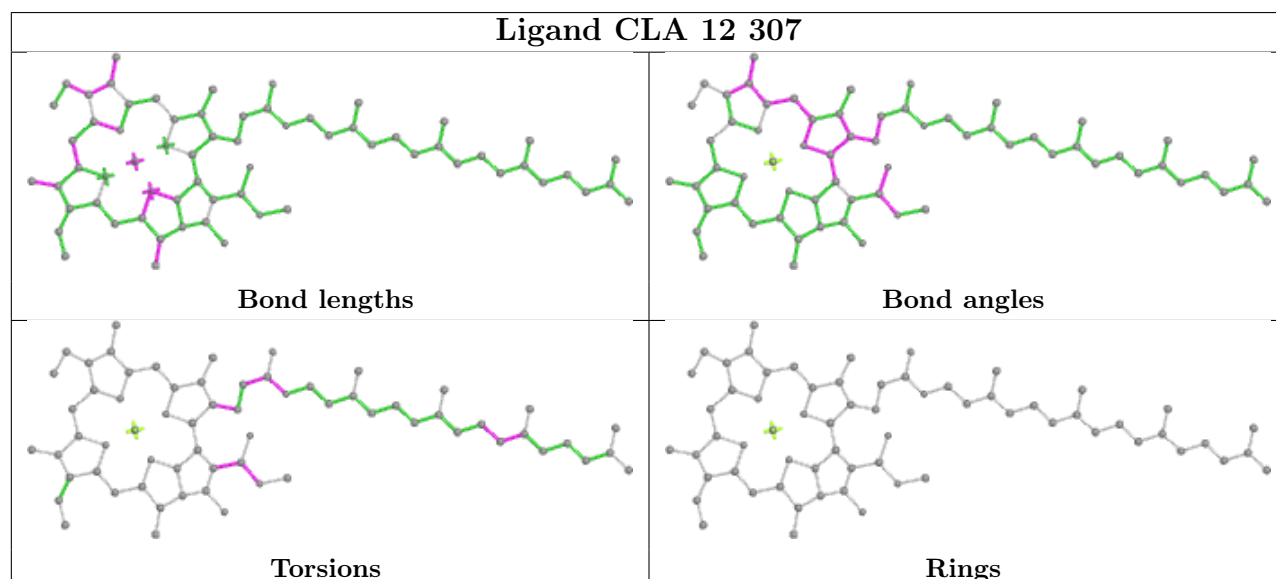
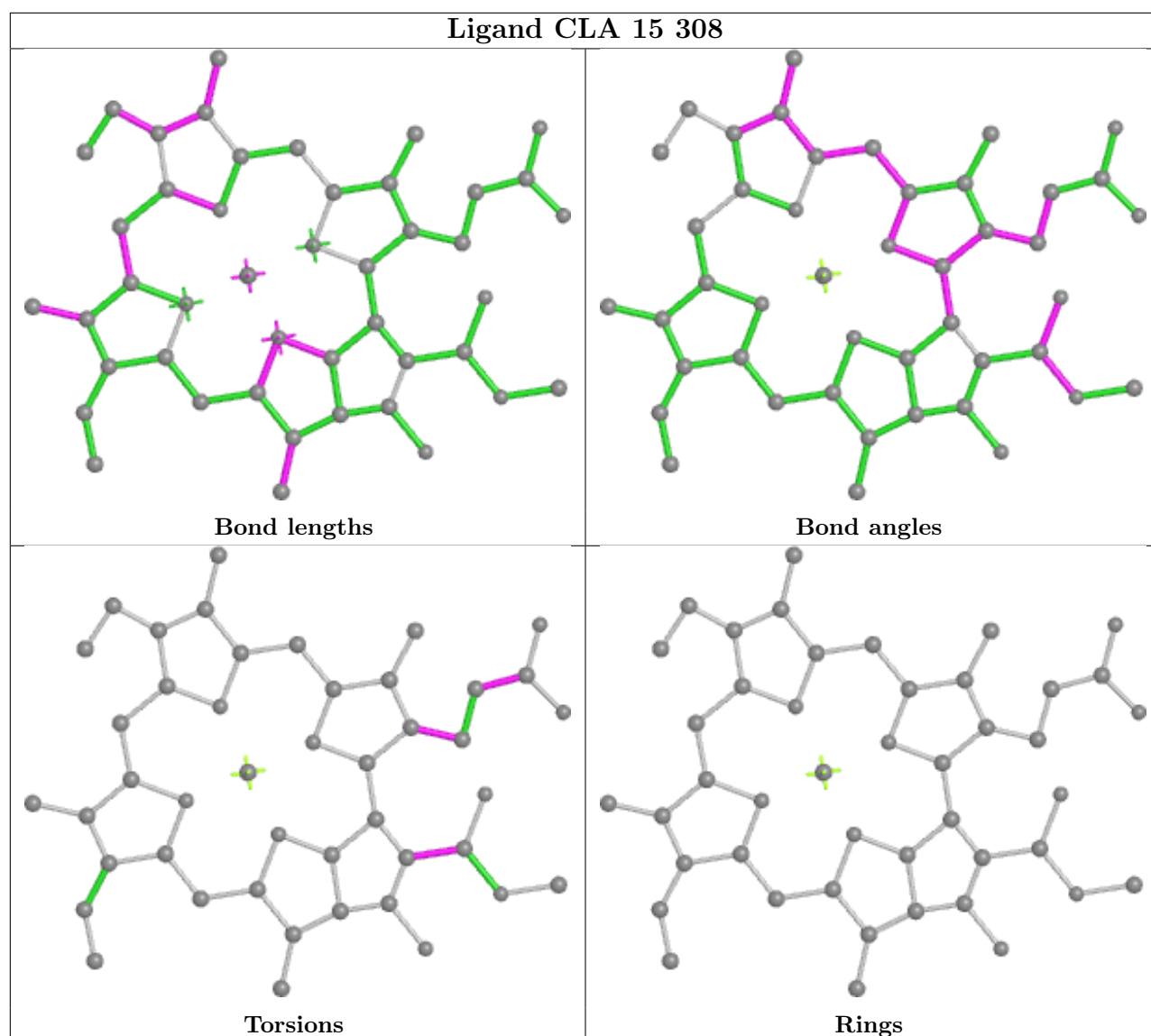
Torsions

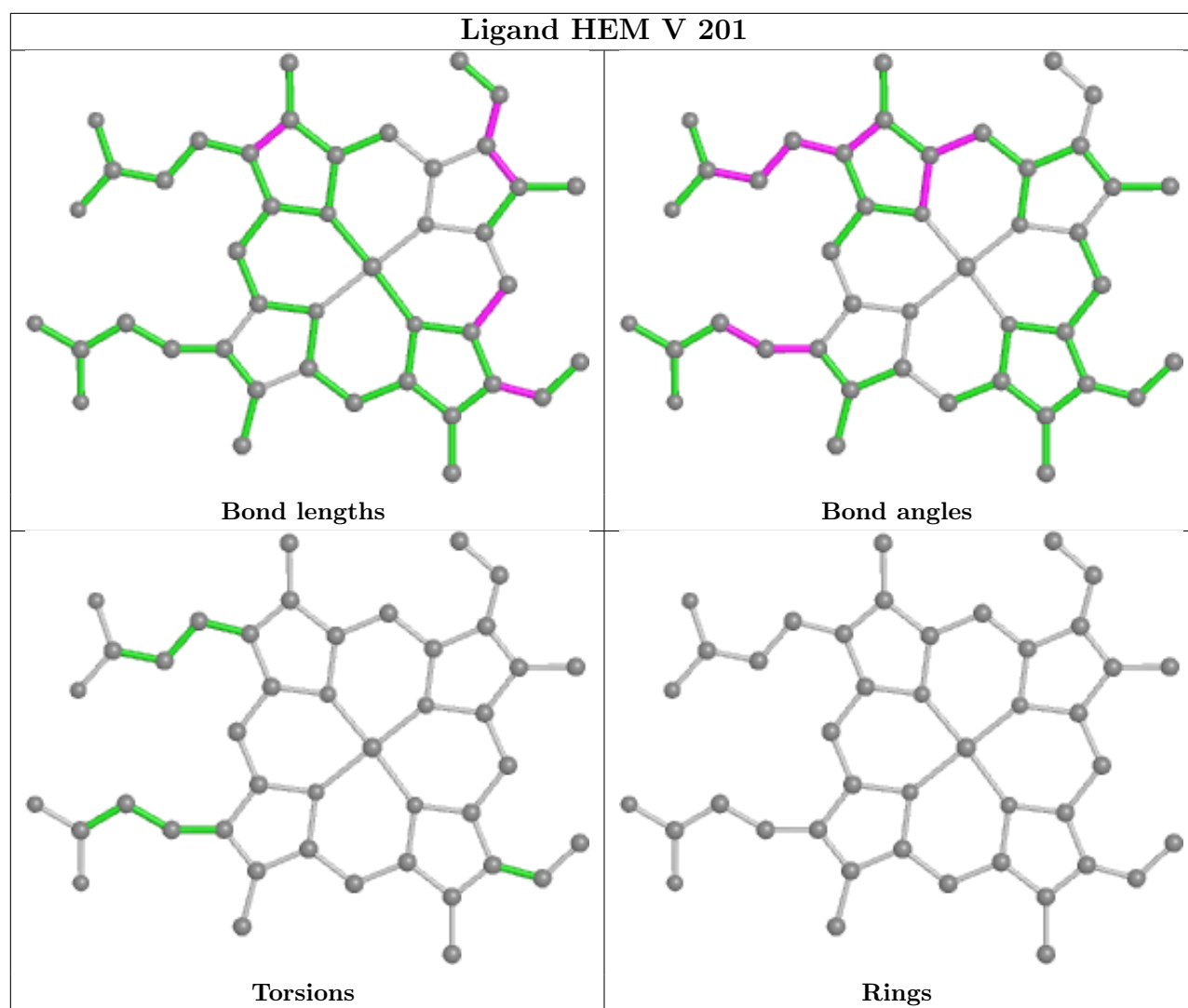


Rings

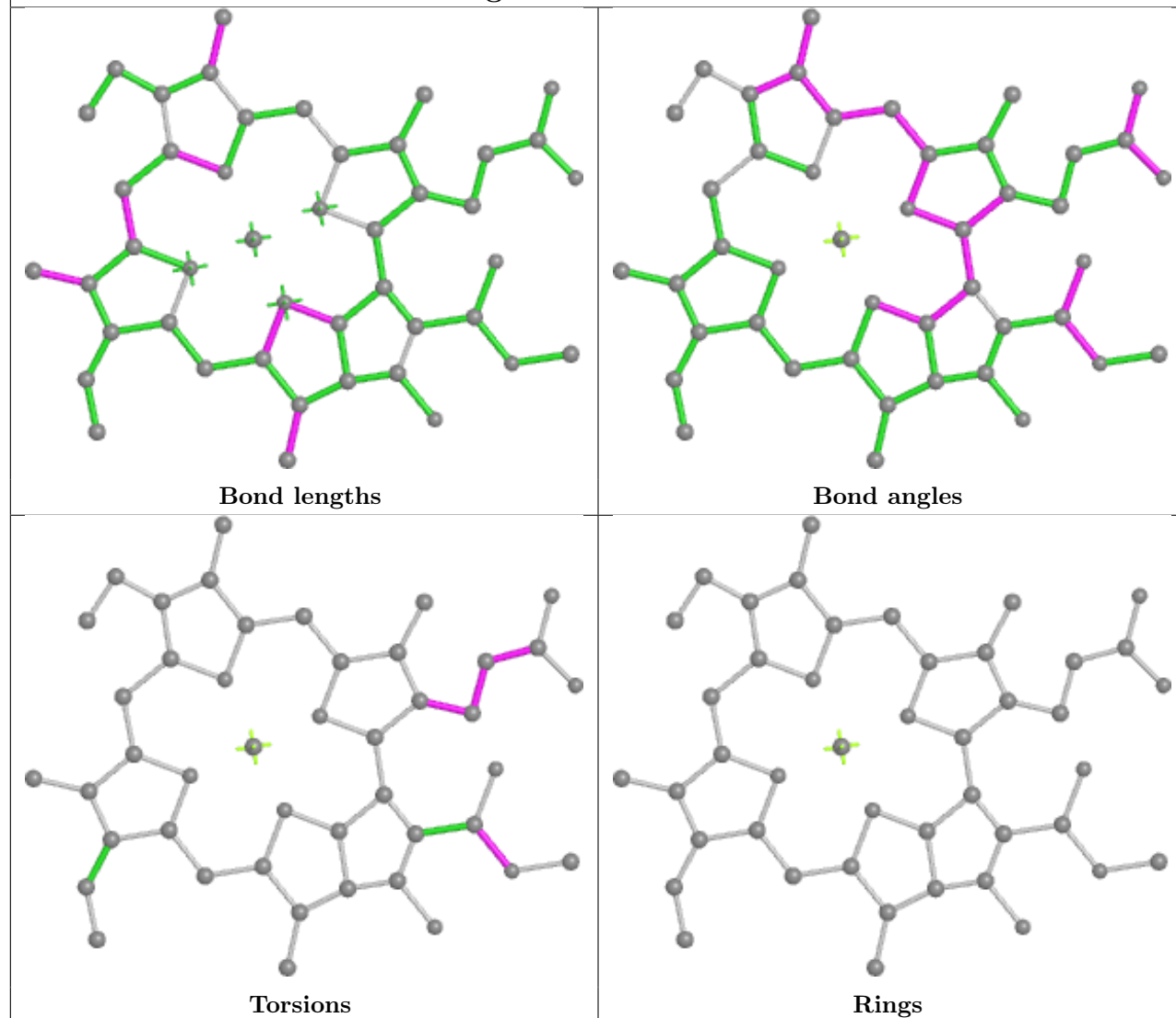


Ligand CLA C 508**Ligand CLA 13 308****Ligand CLA c 513**

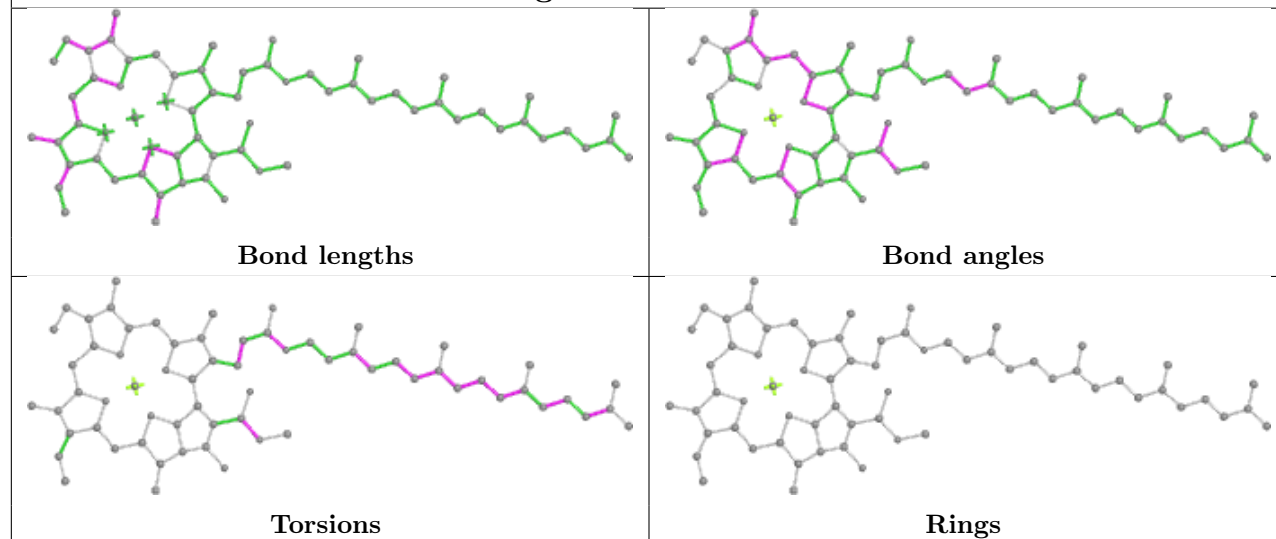


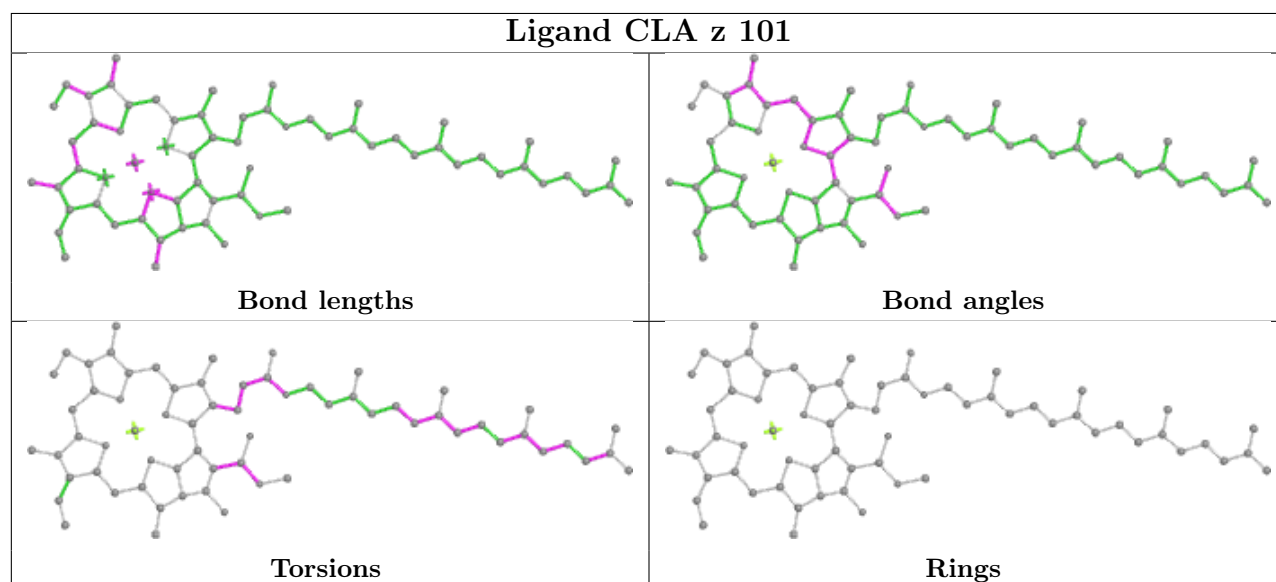
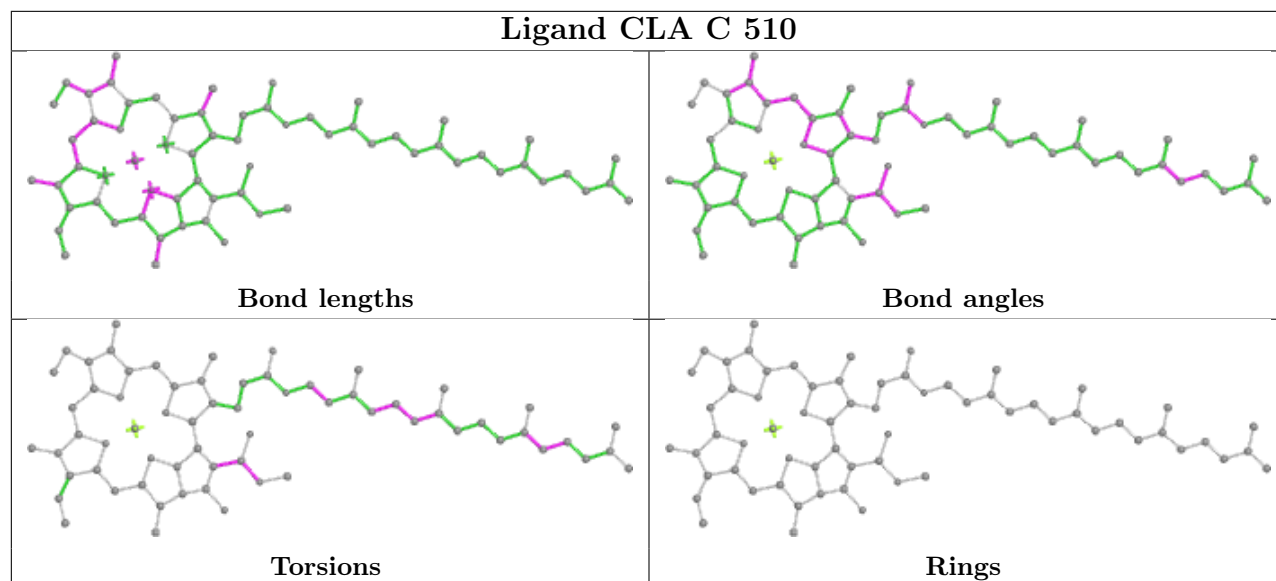
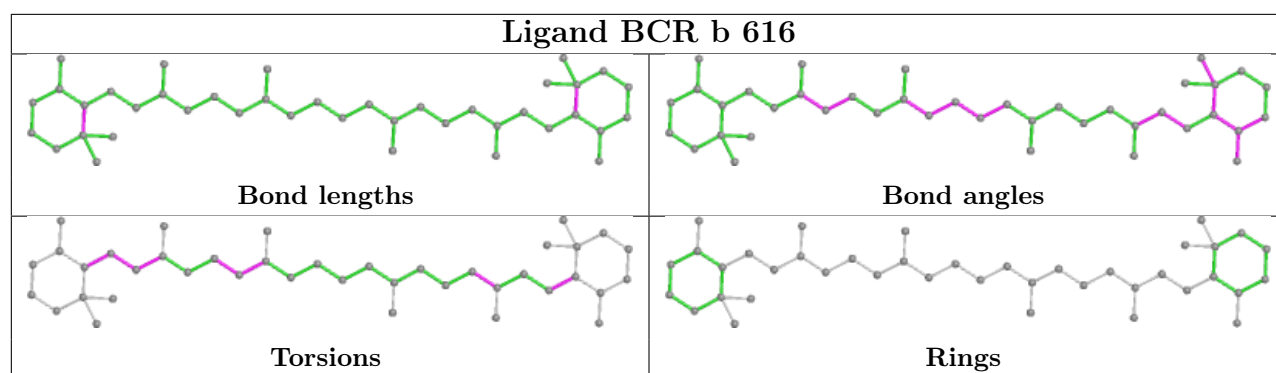


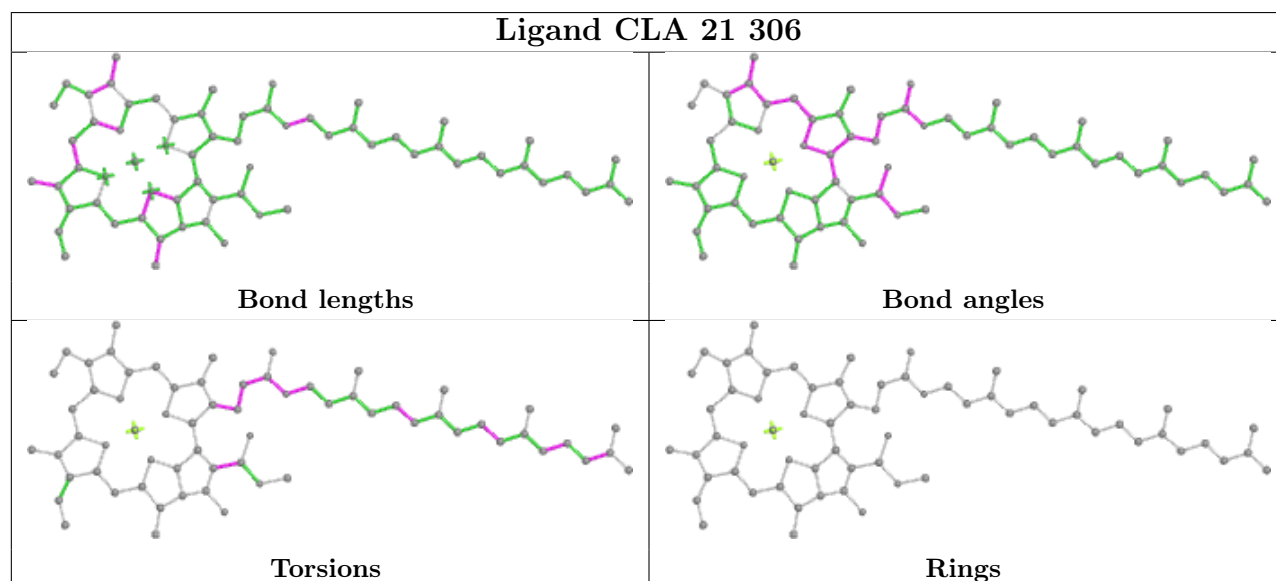
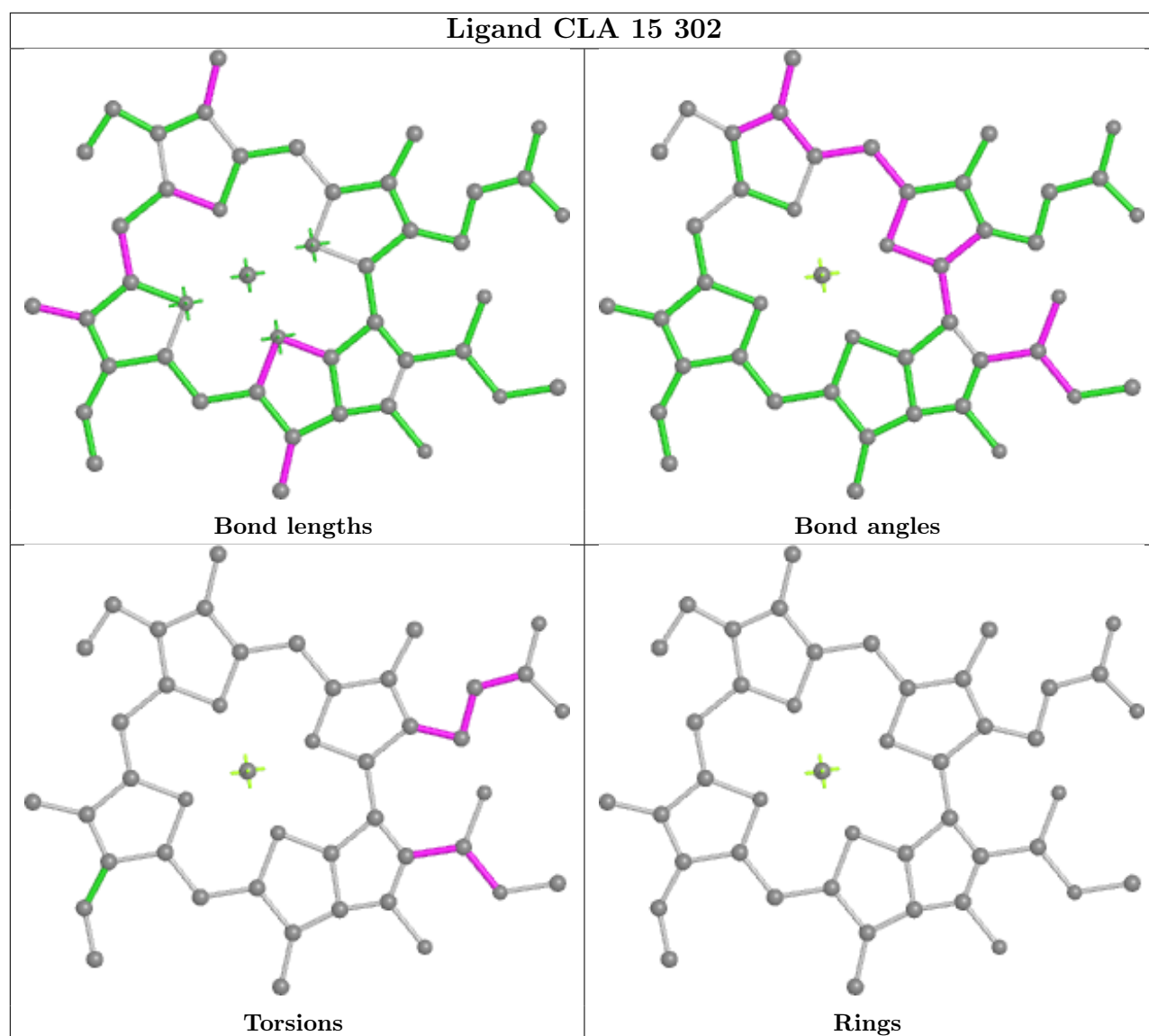
Ligand CLA 15 304

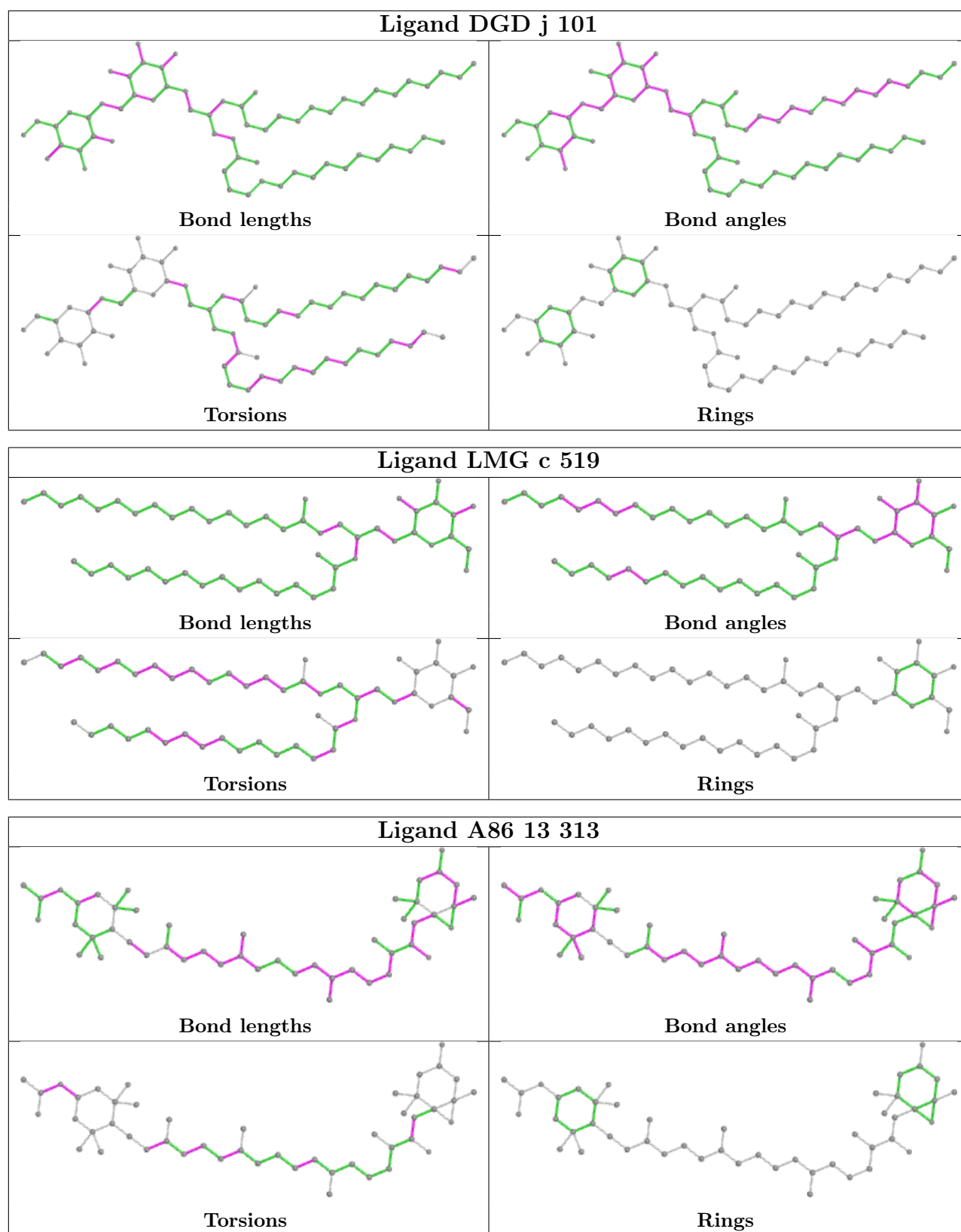


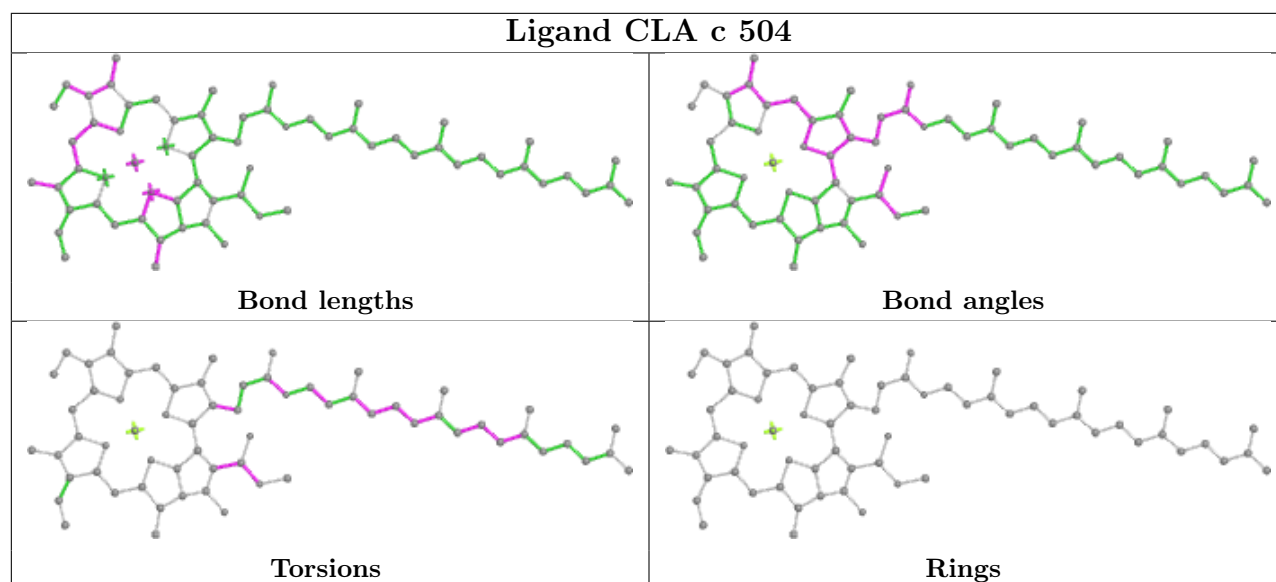
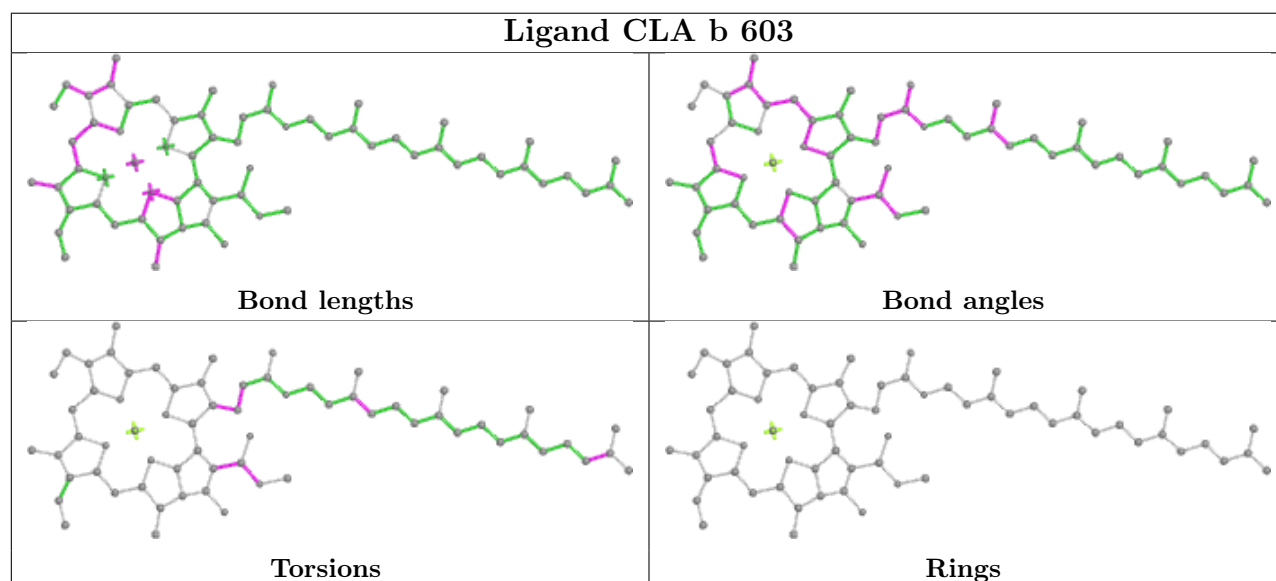
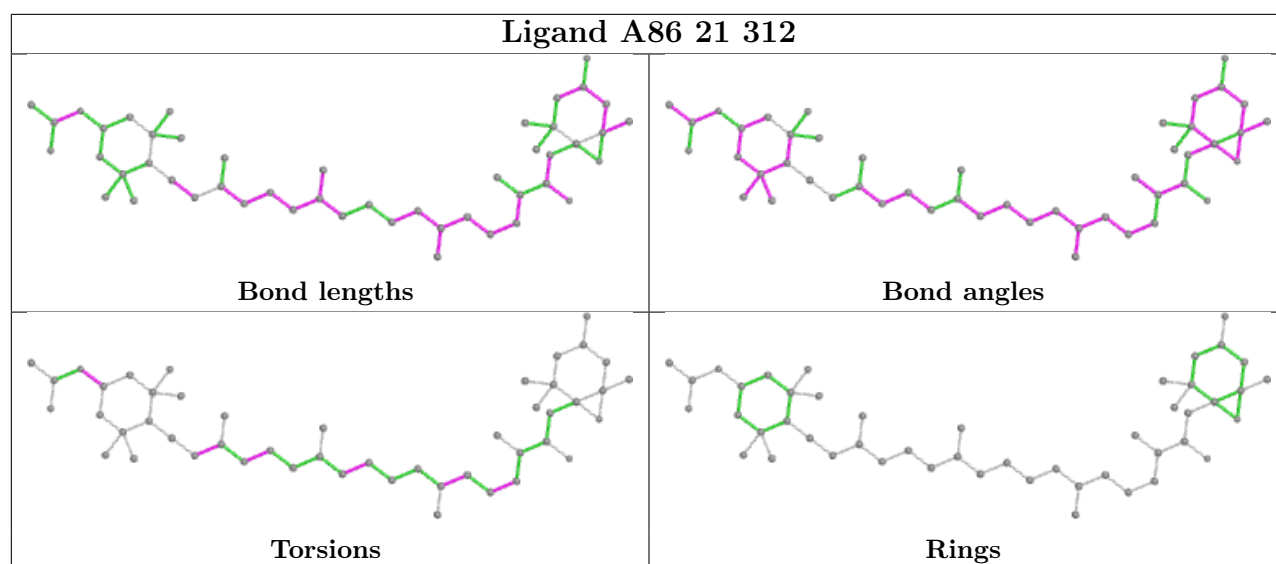
Ligand CLA b 605

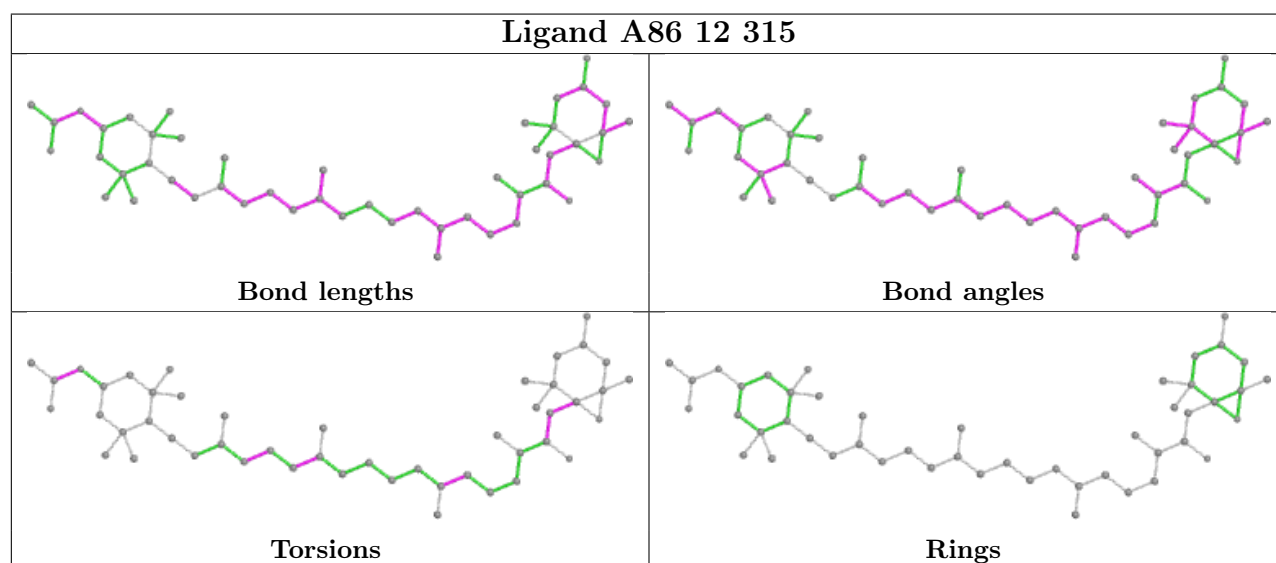
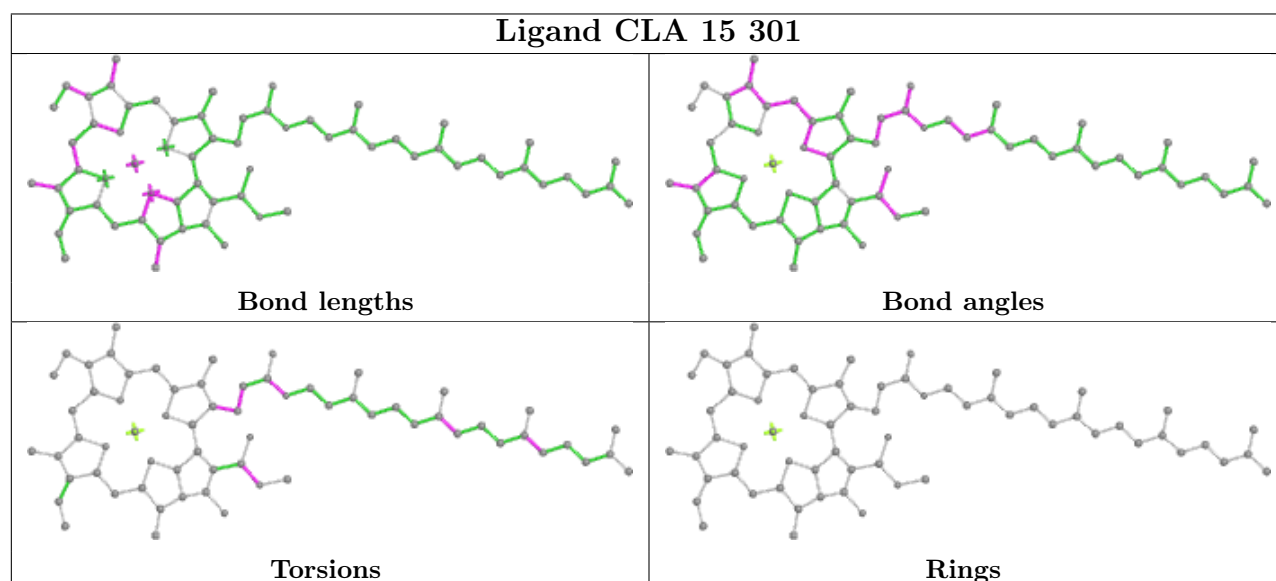
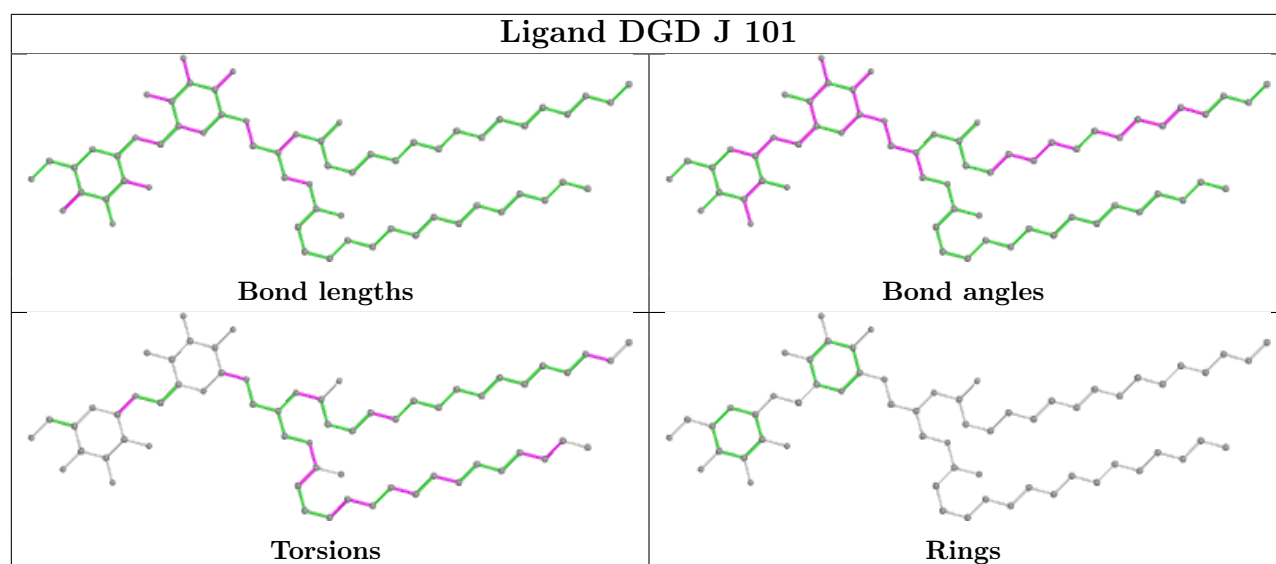


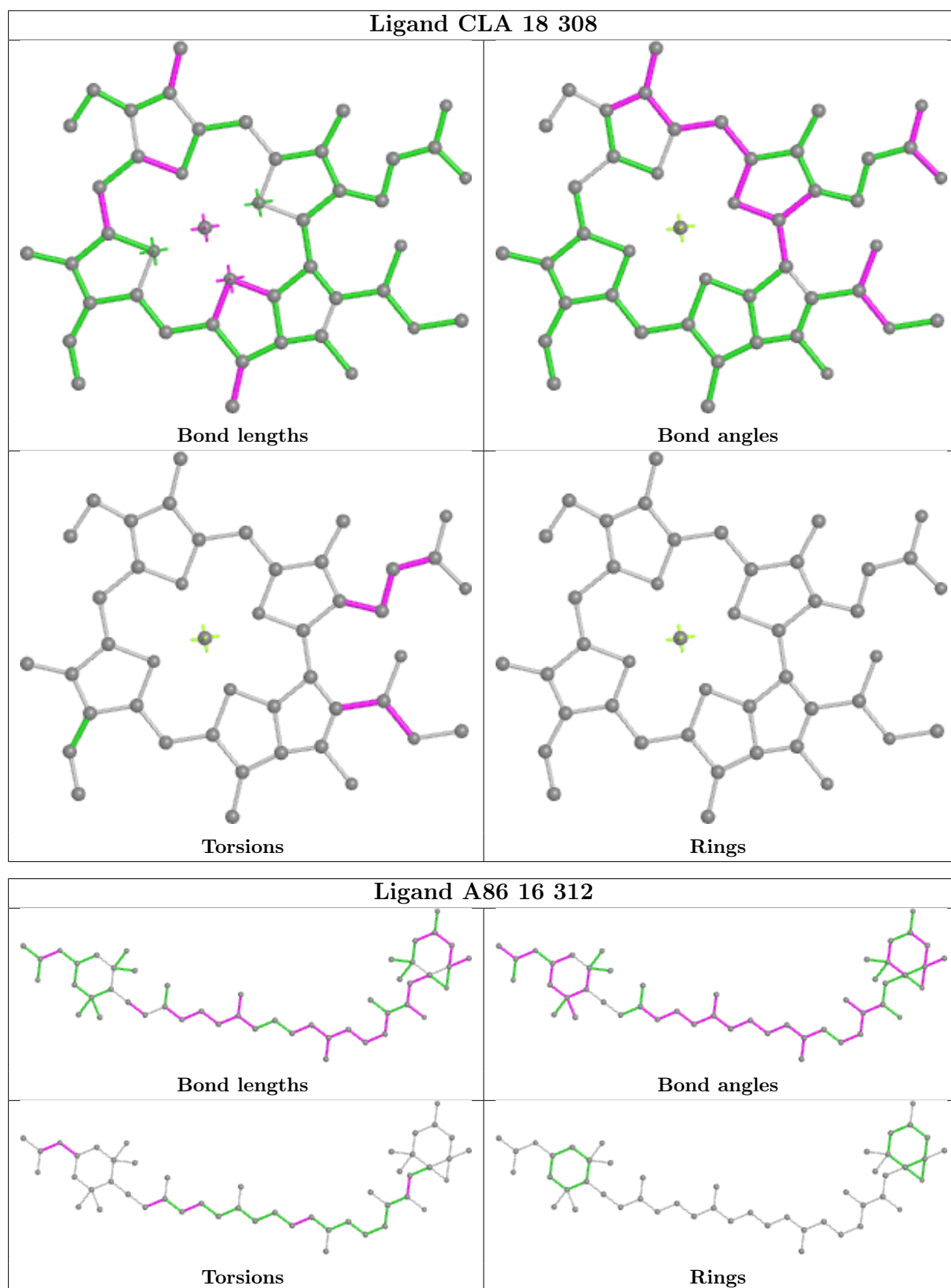


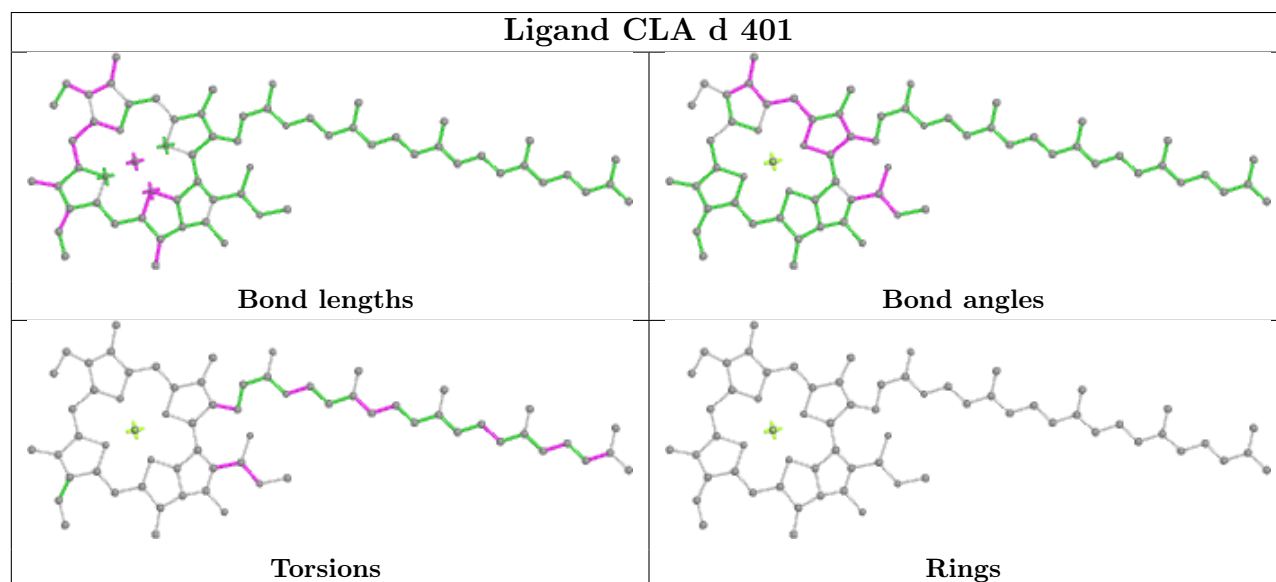
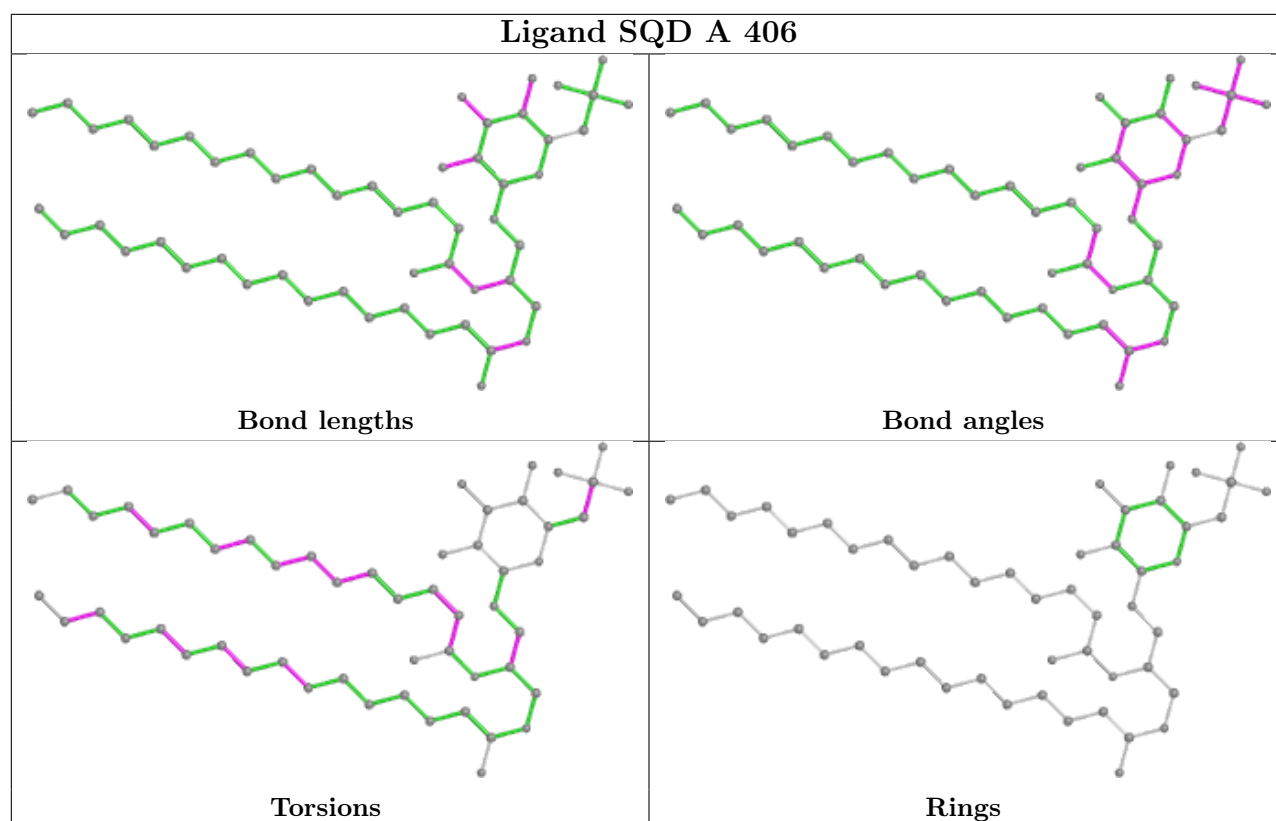


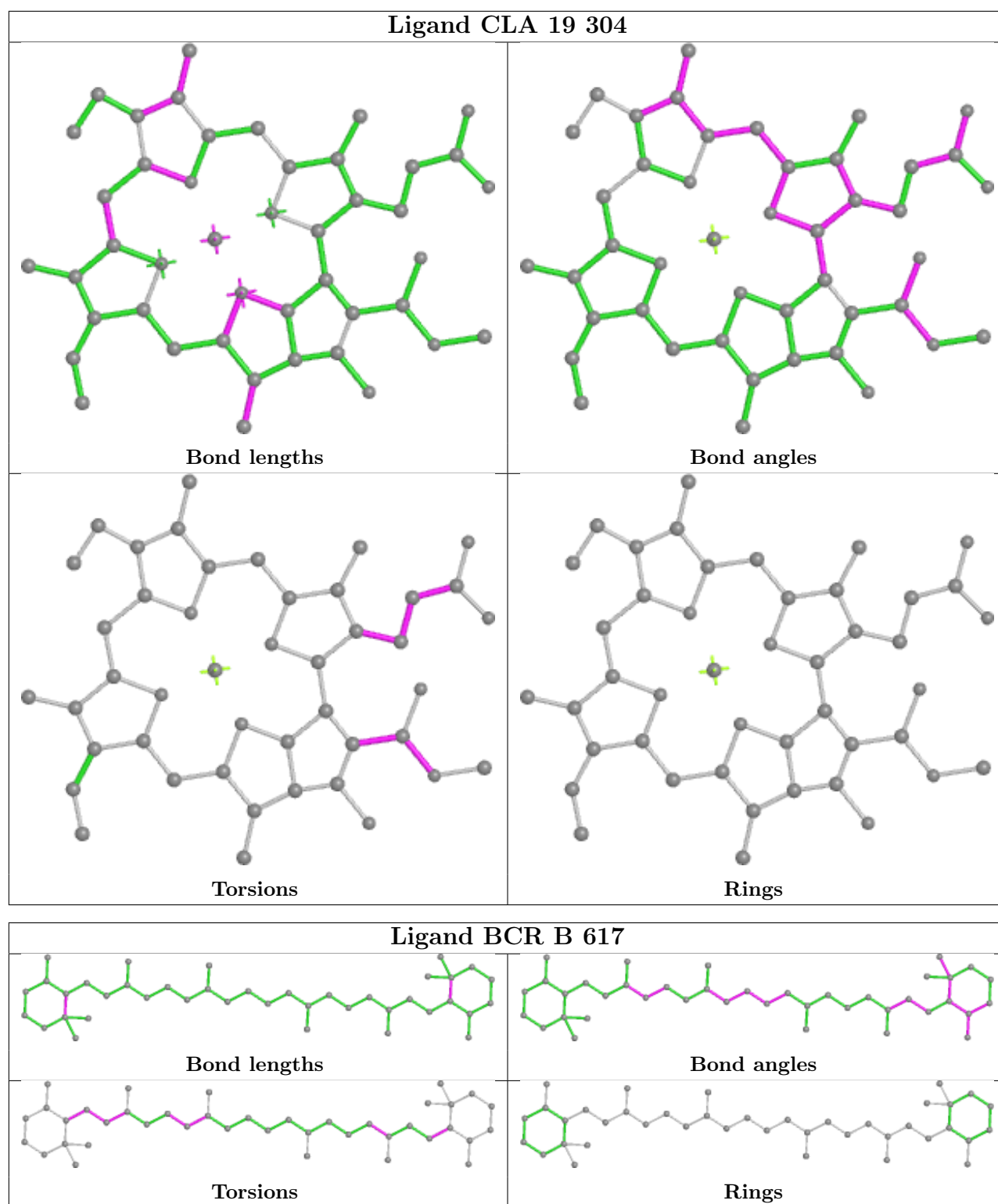


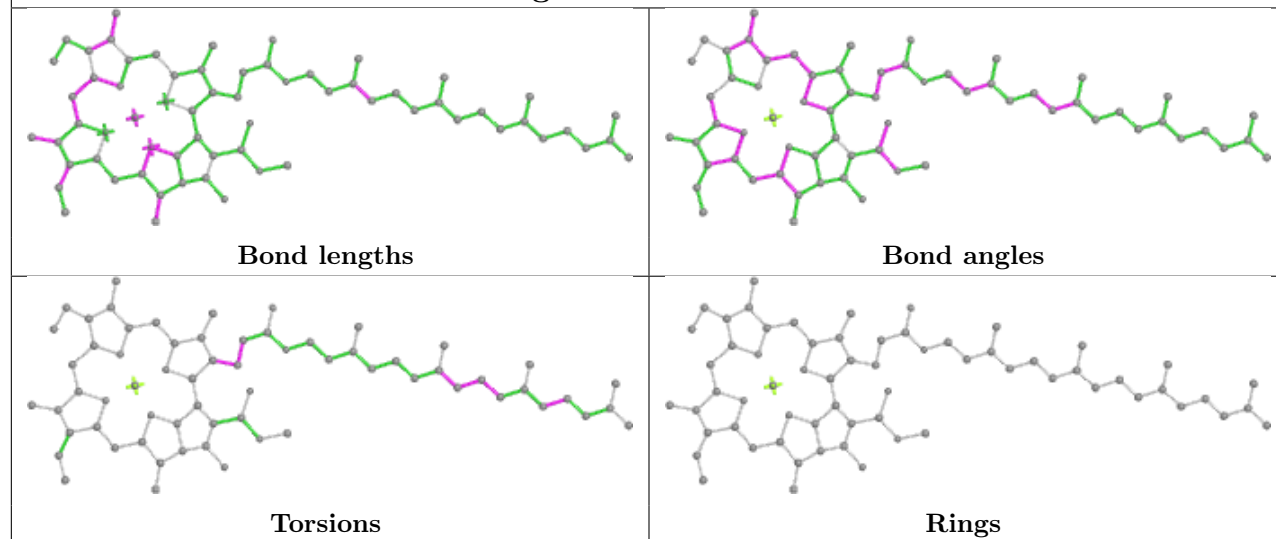
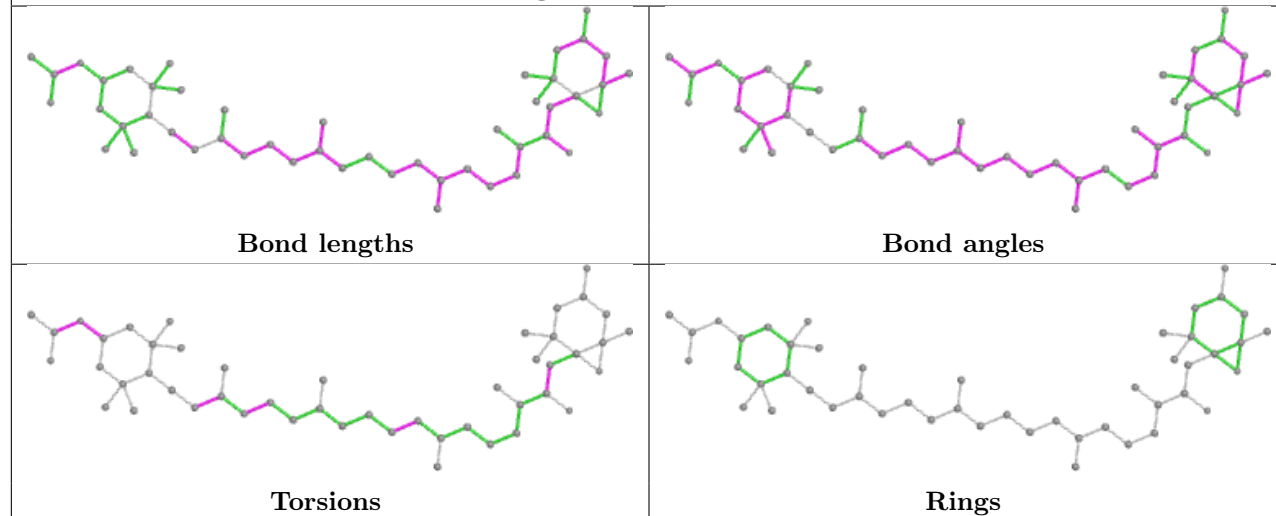
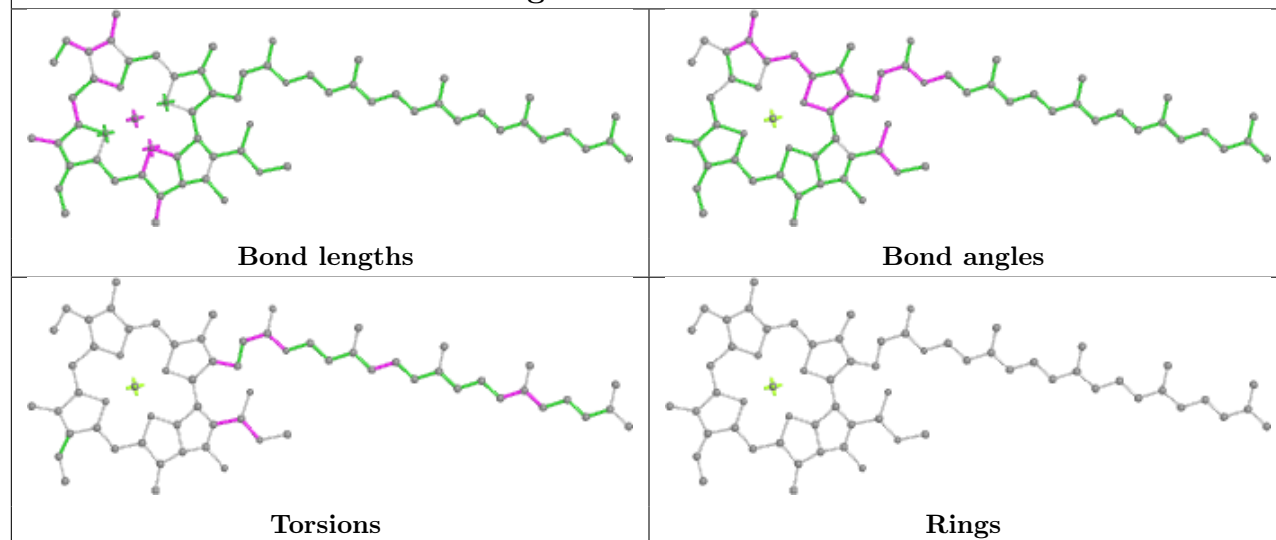


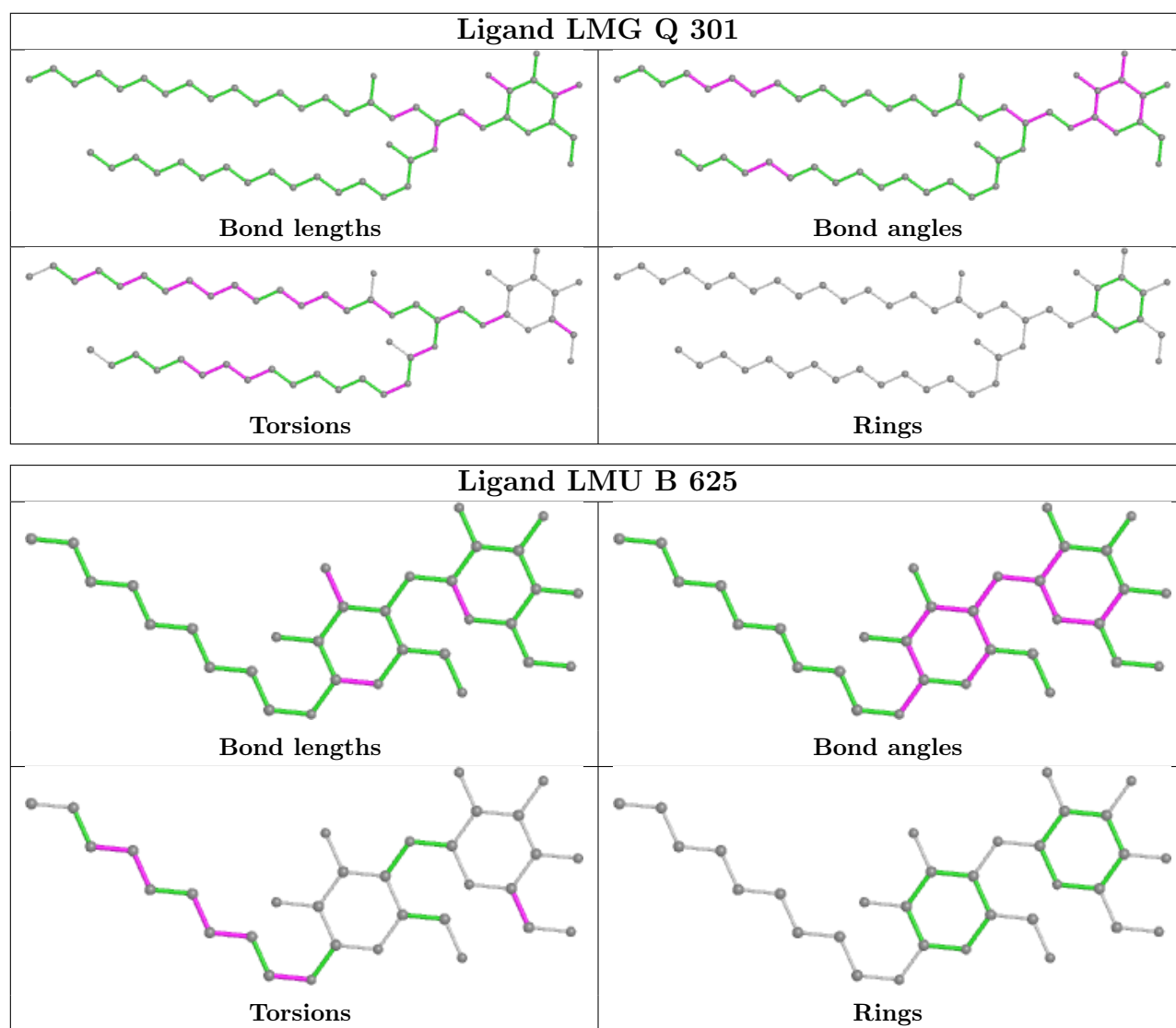


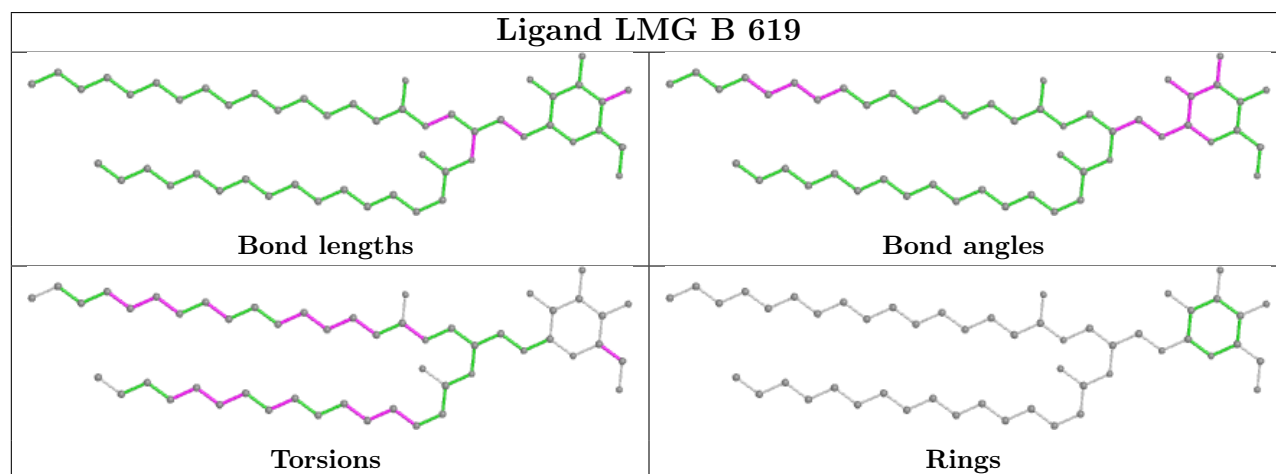
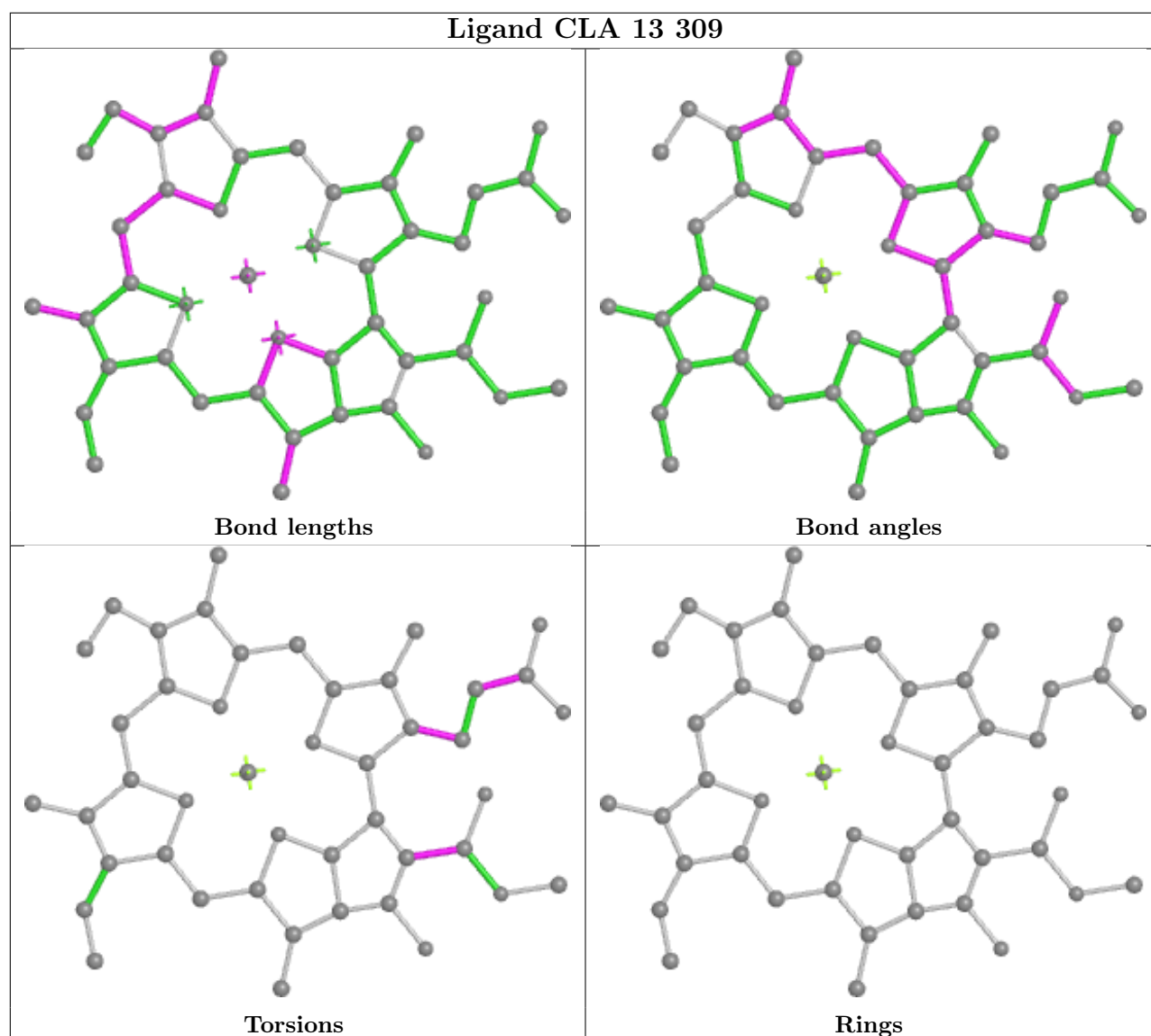


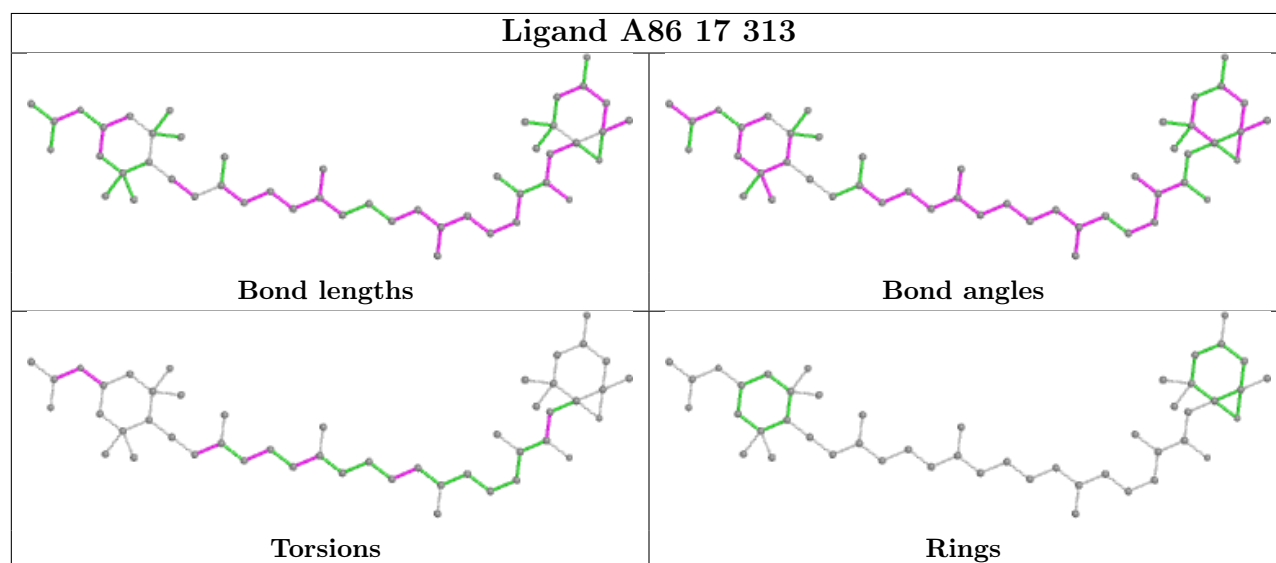
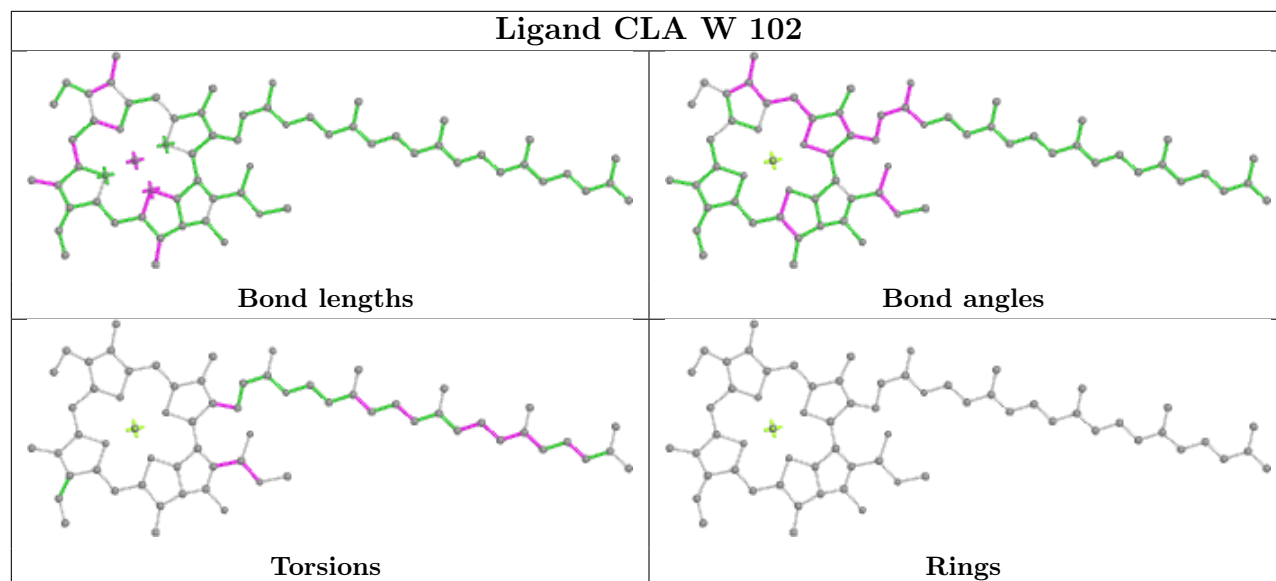
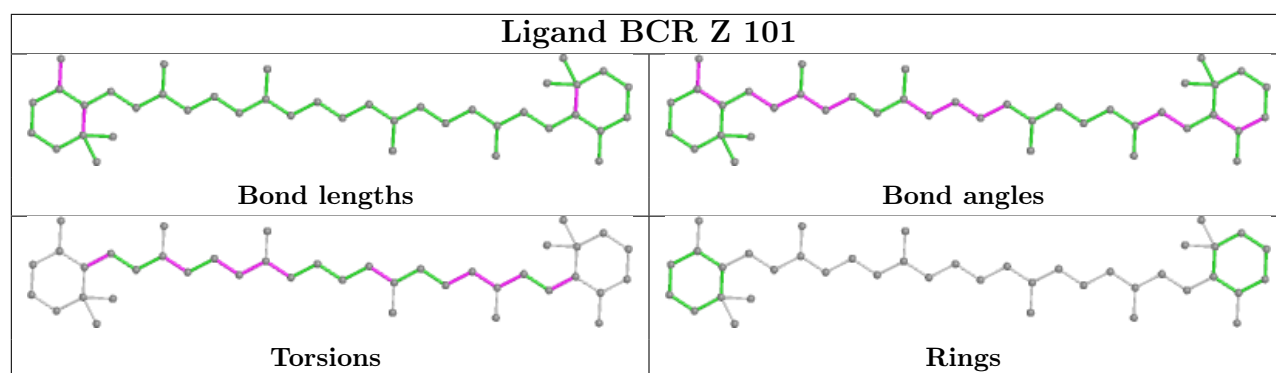


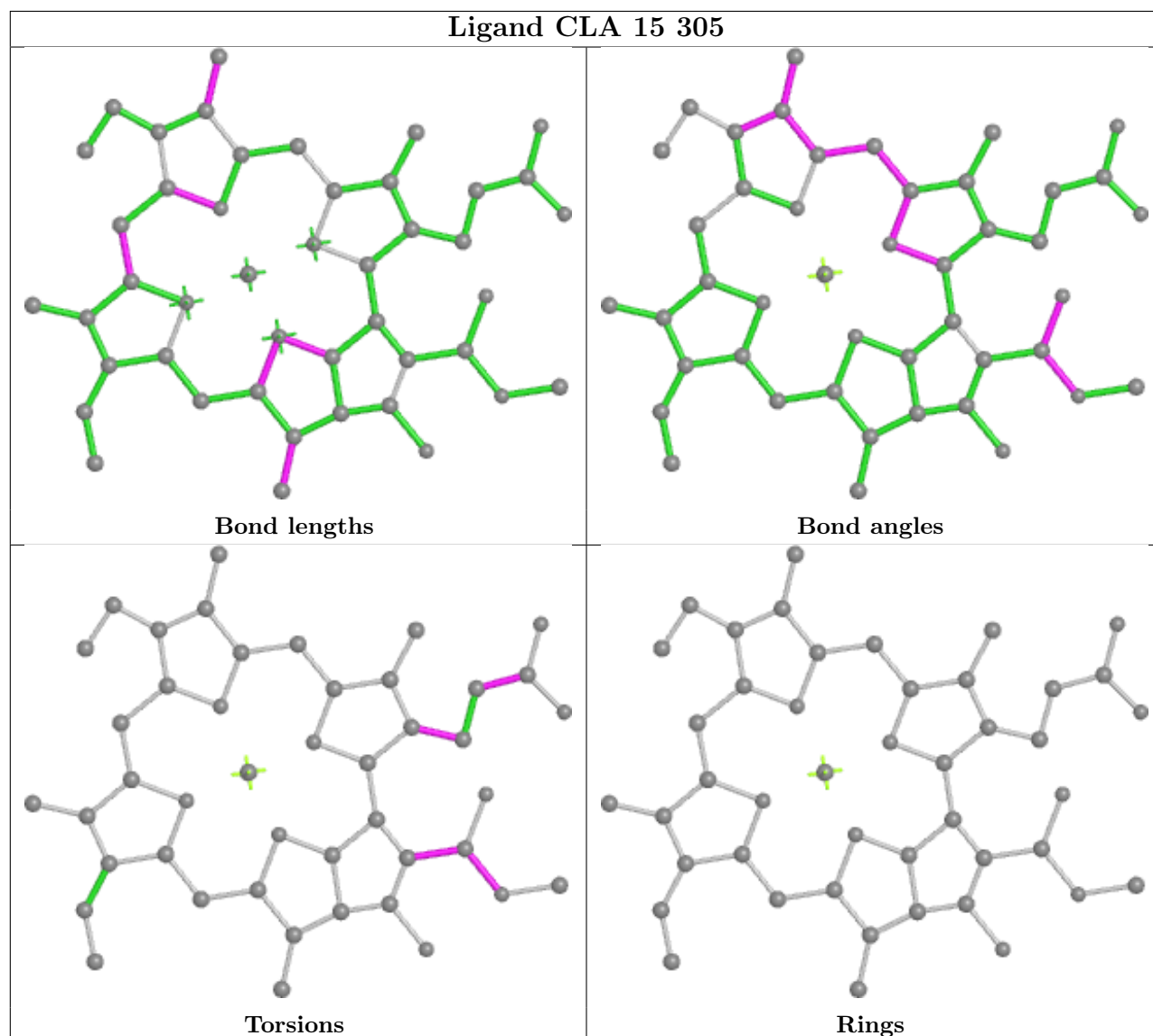
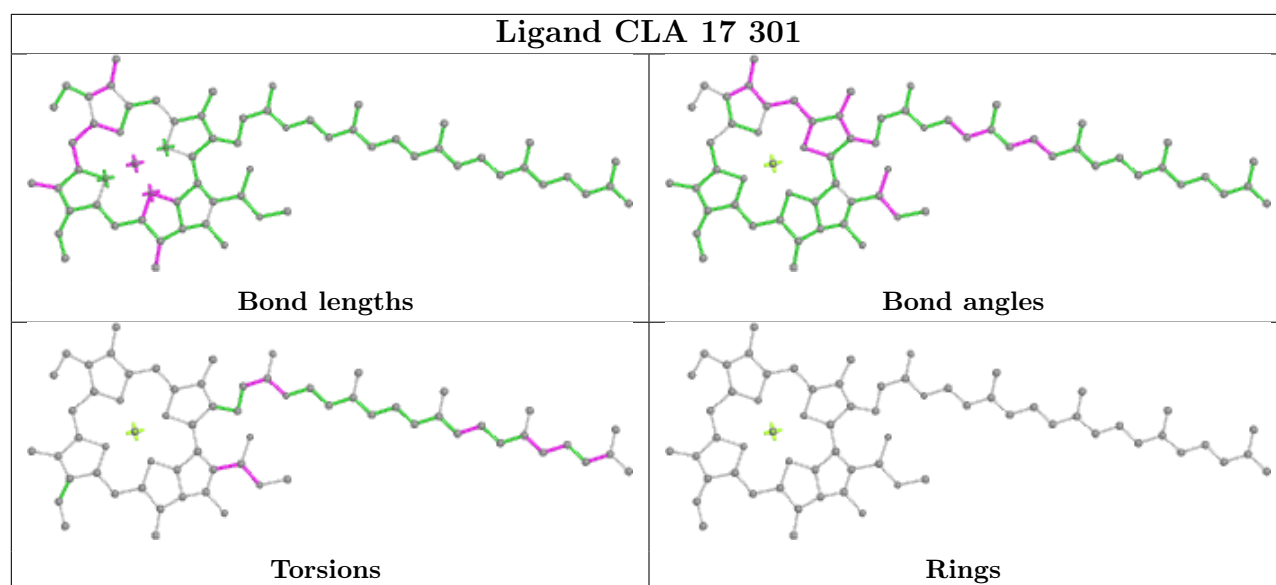


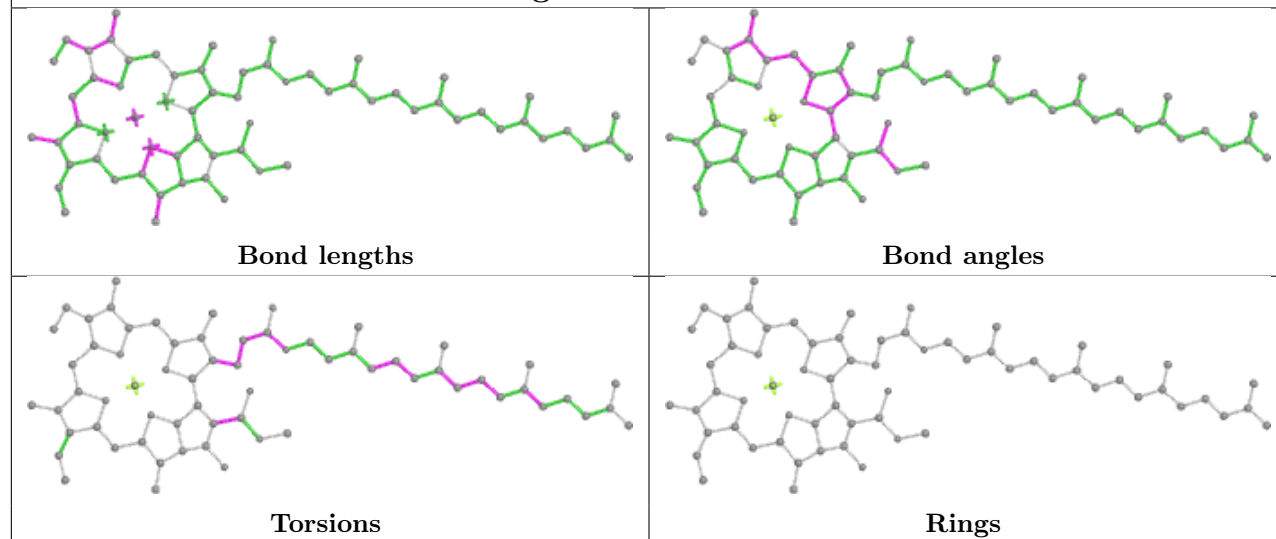
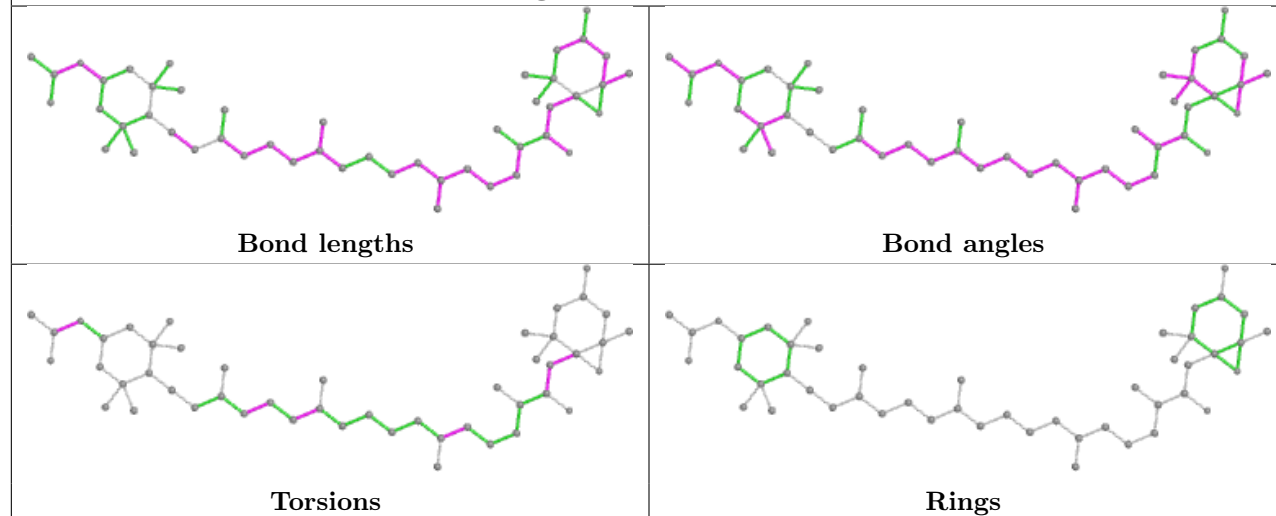
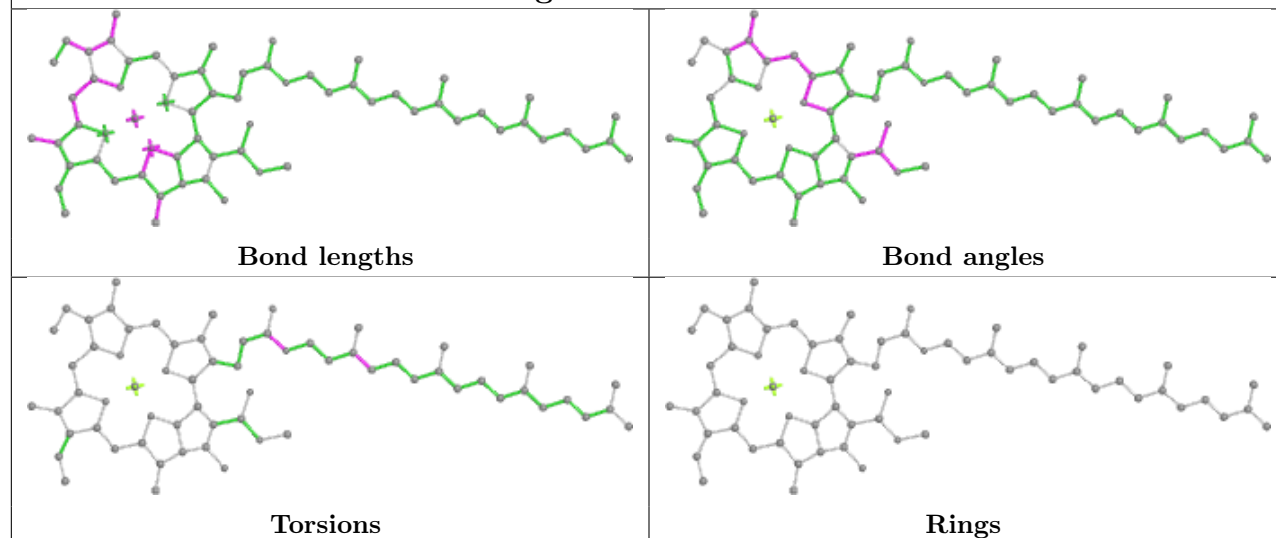
Ligand CLA B 606**Ligand A86 14 314****Ligand CLA 19 303**

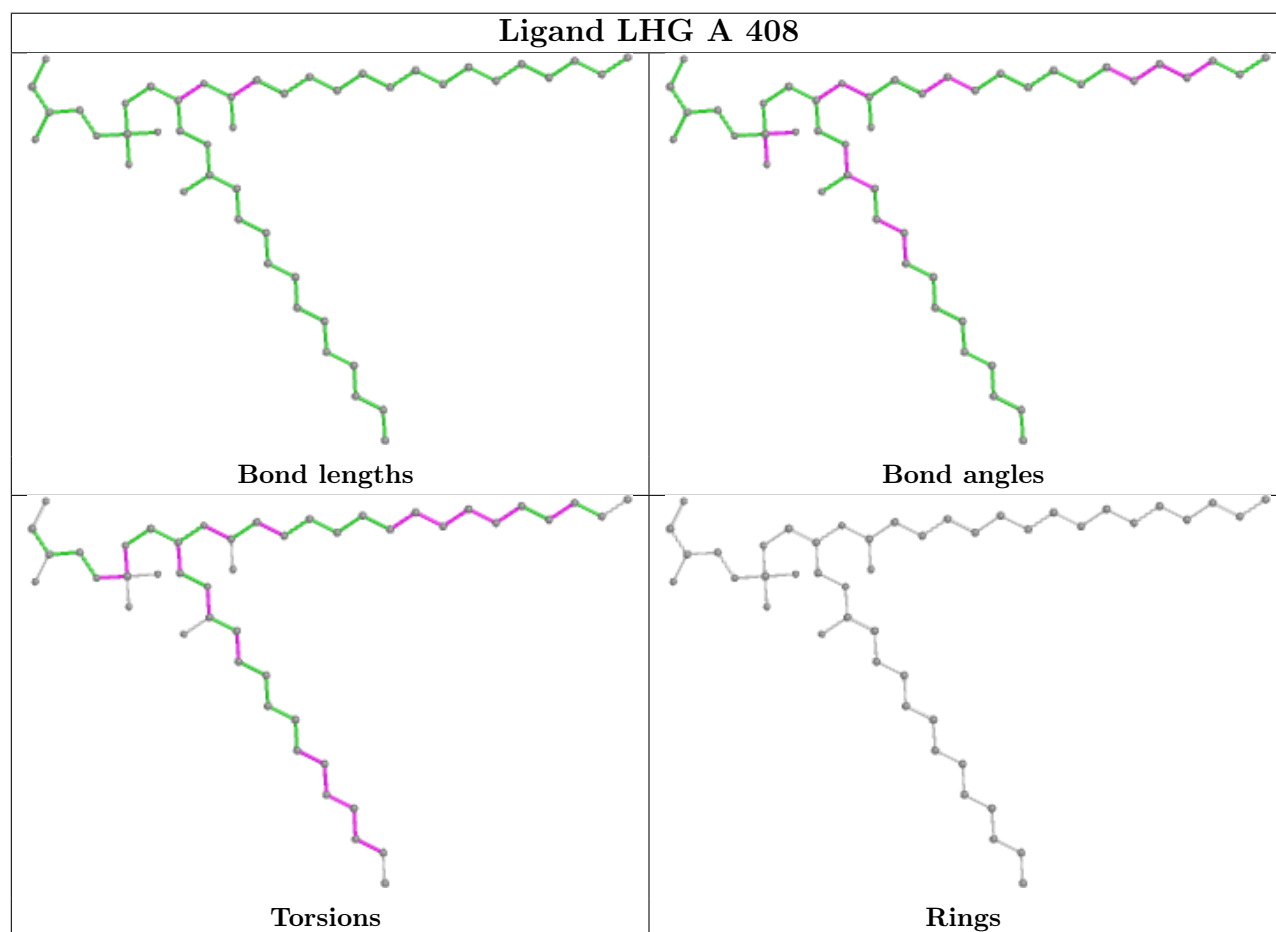
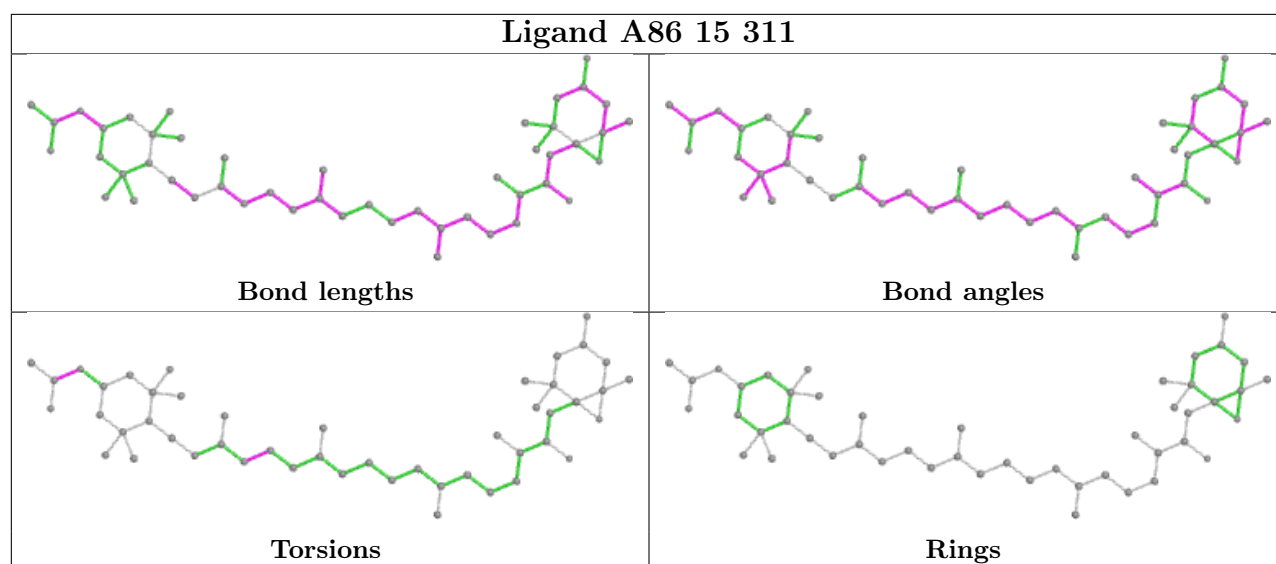


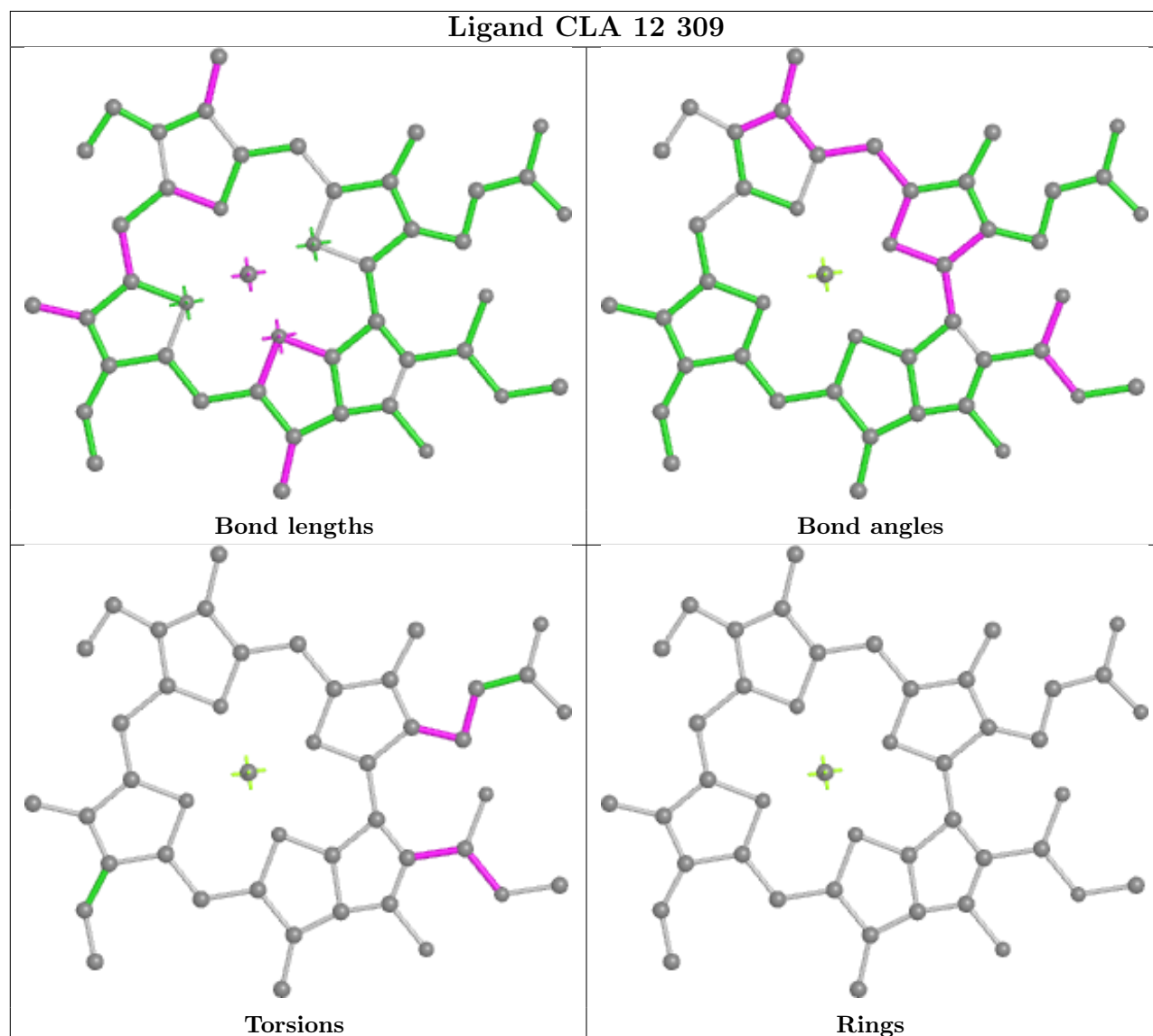
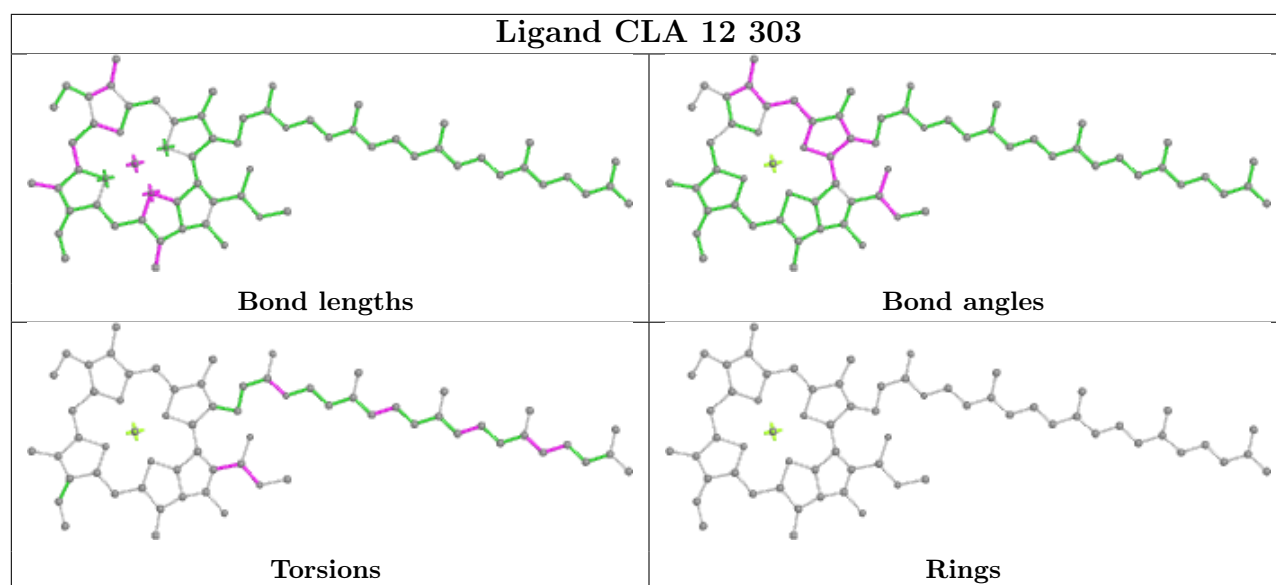


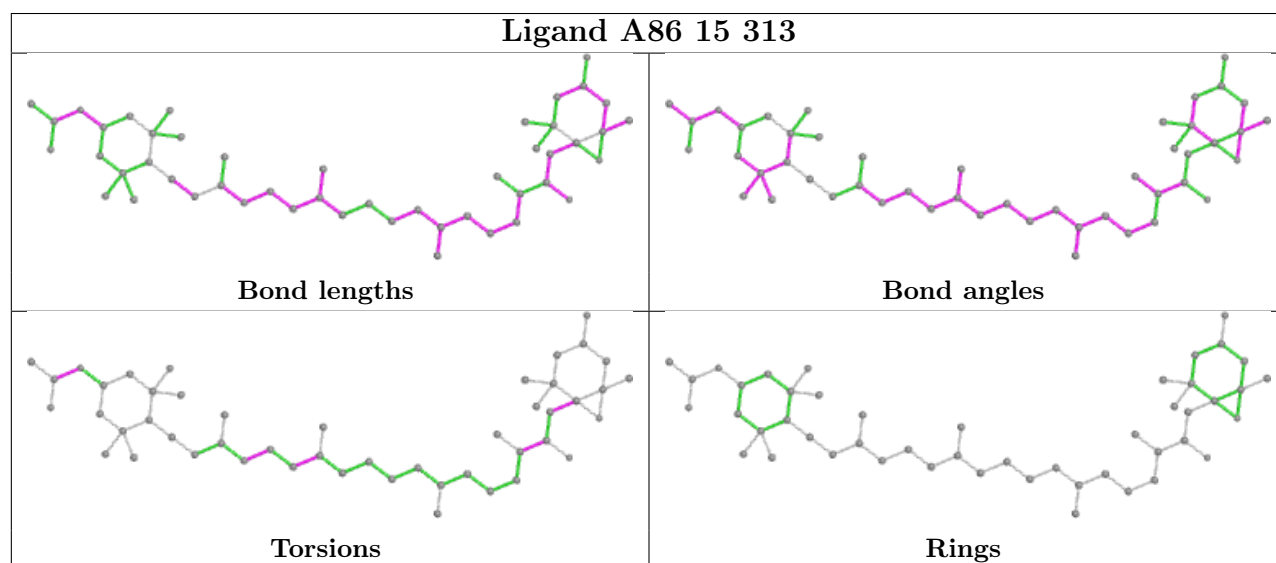
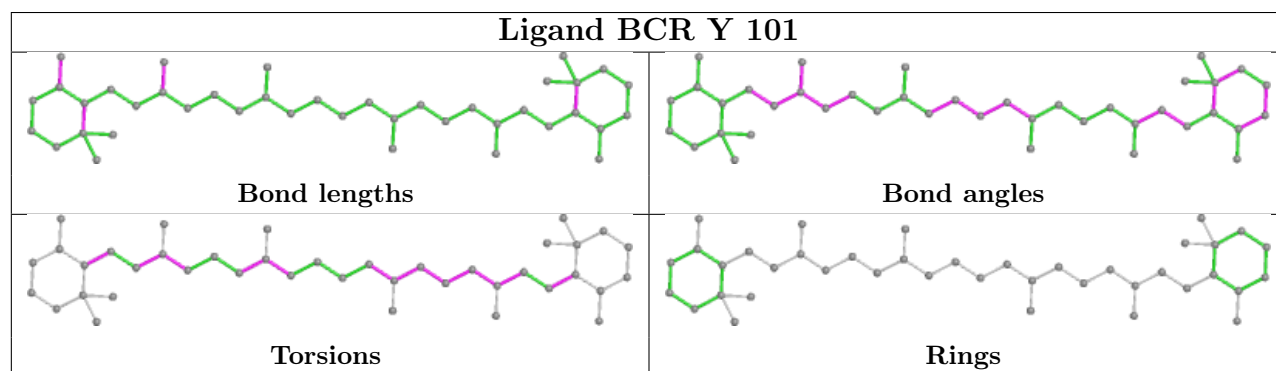
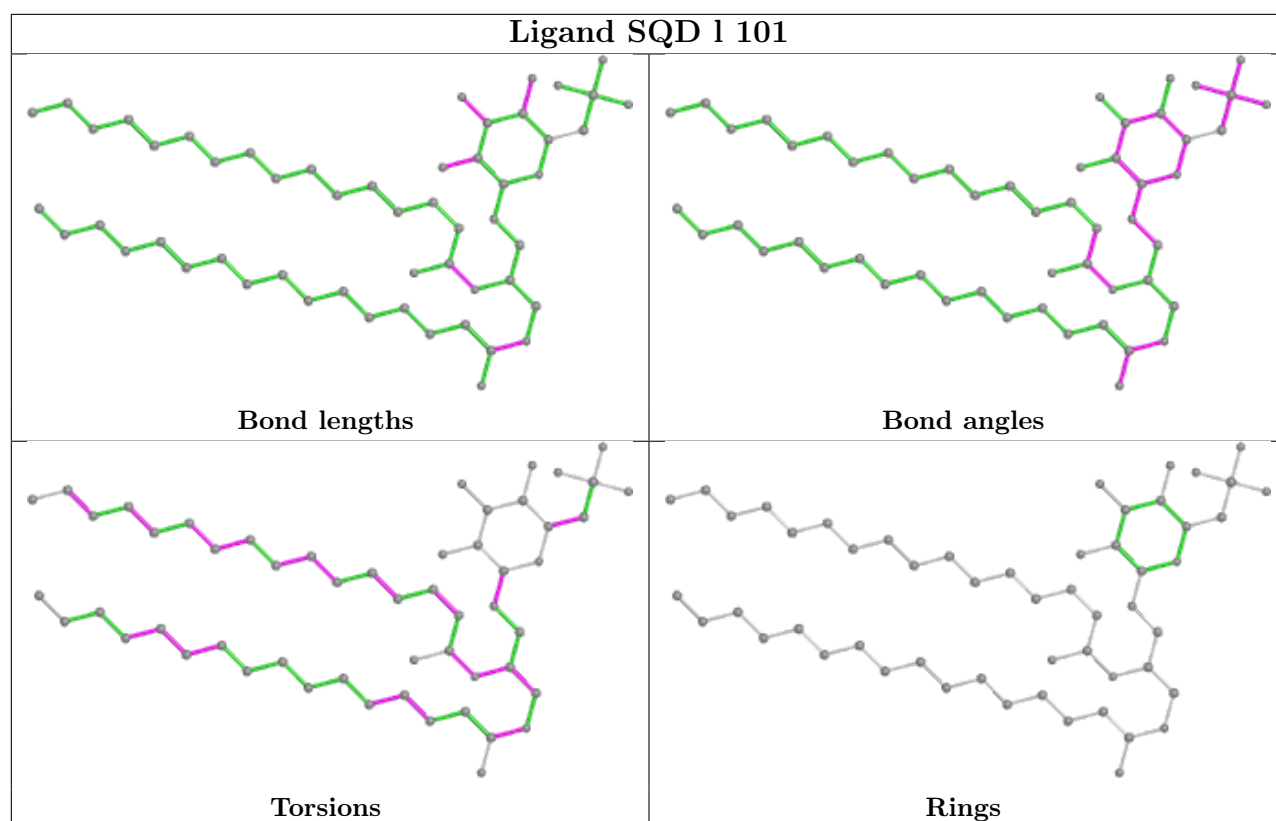




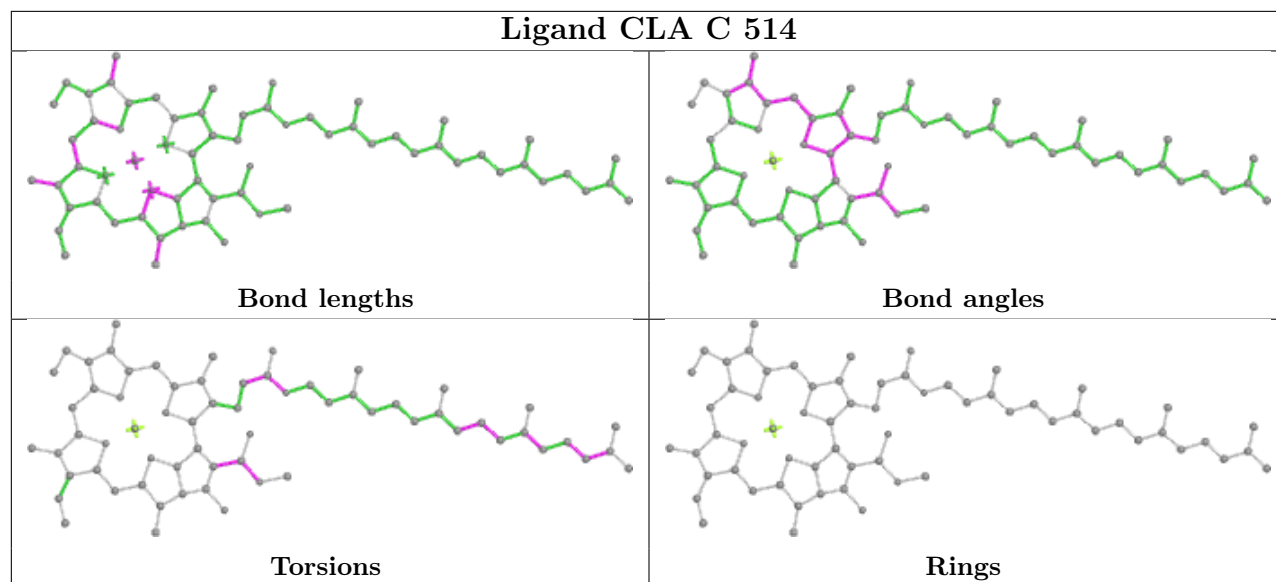
Ligand CLA B 601**Ligand A86 13 311****Ligand CLA d 407**



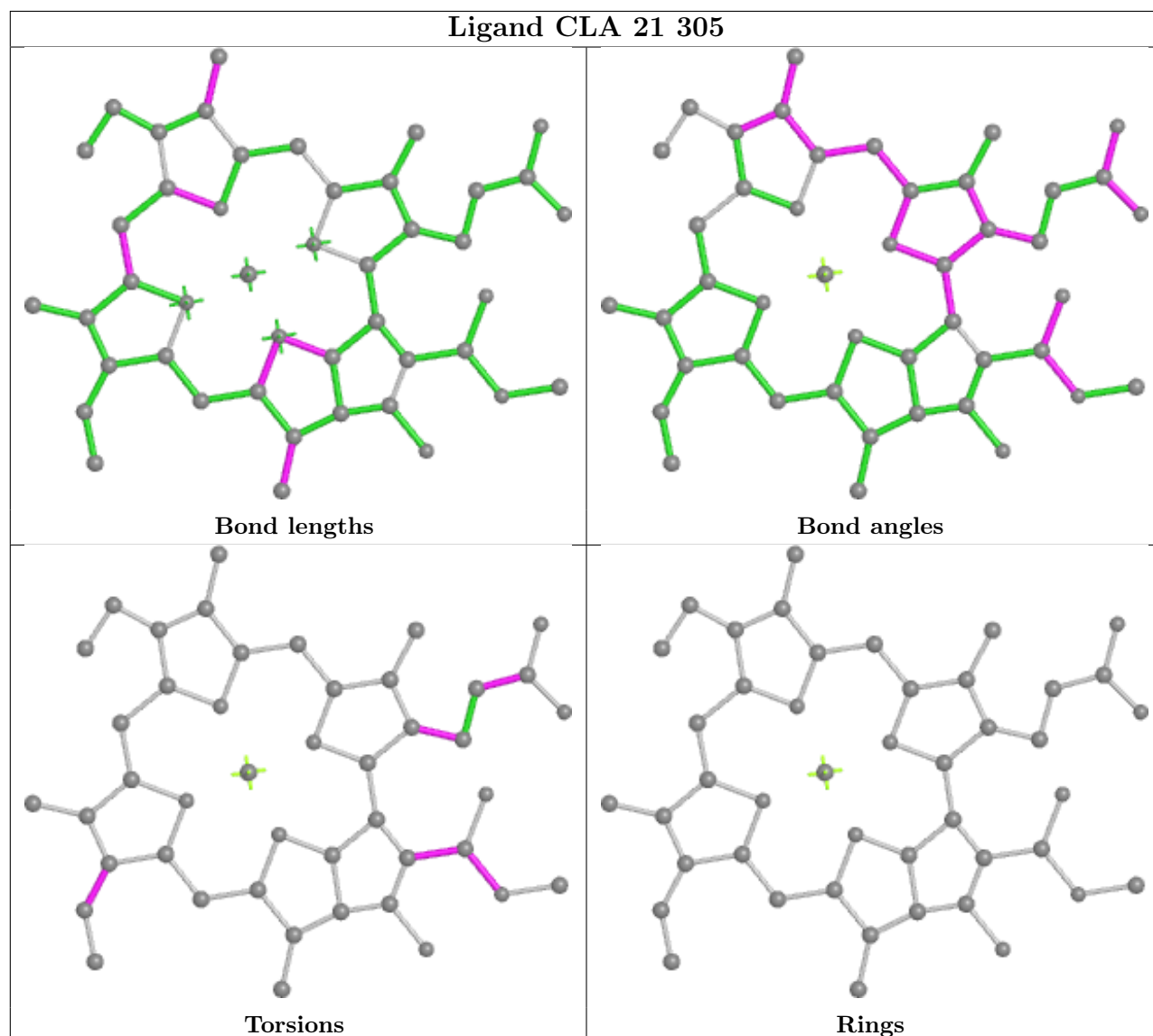


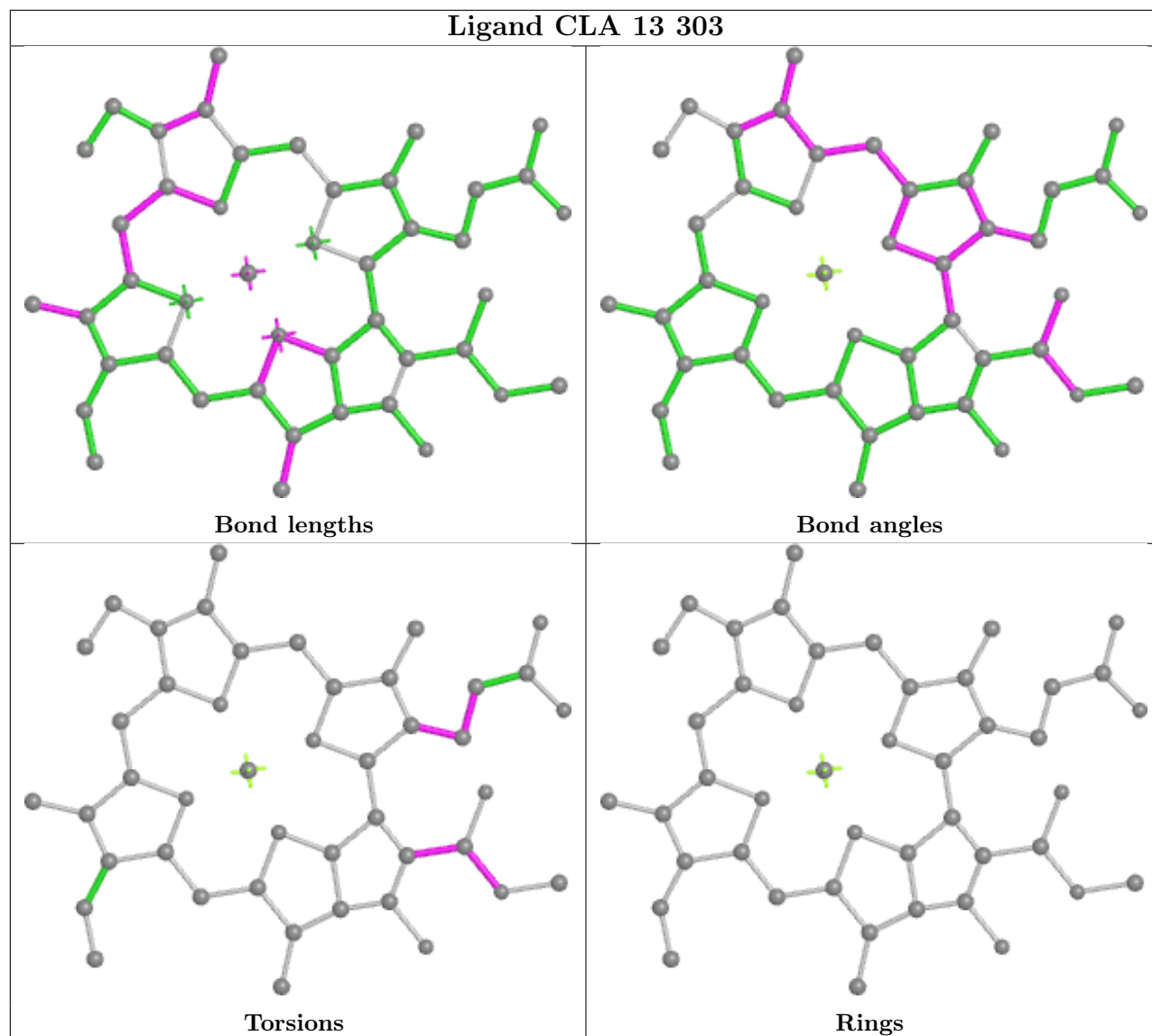


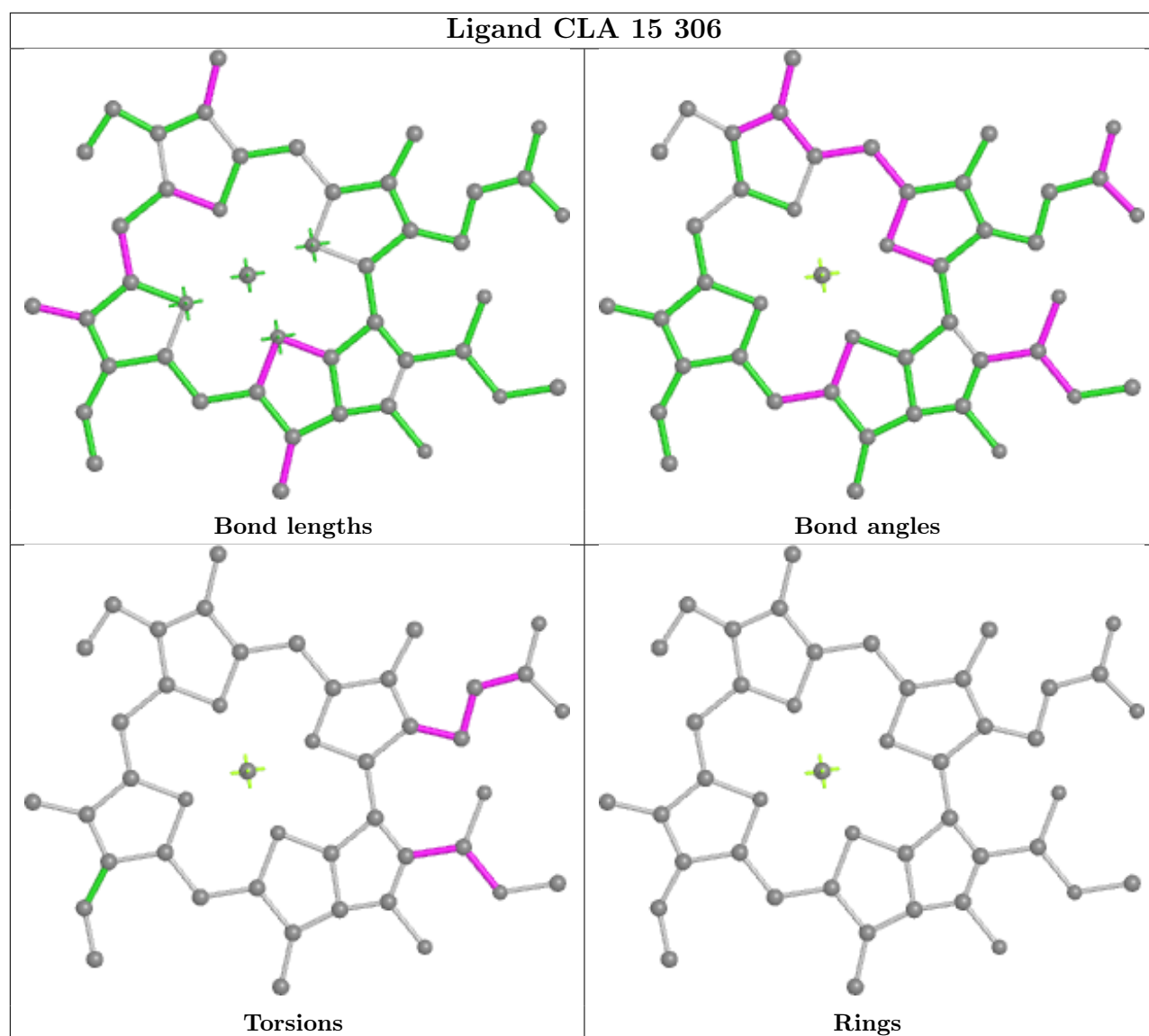
Ligand CLA C 514

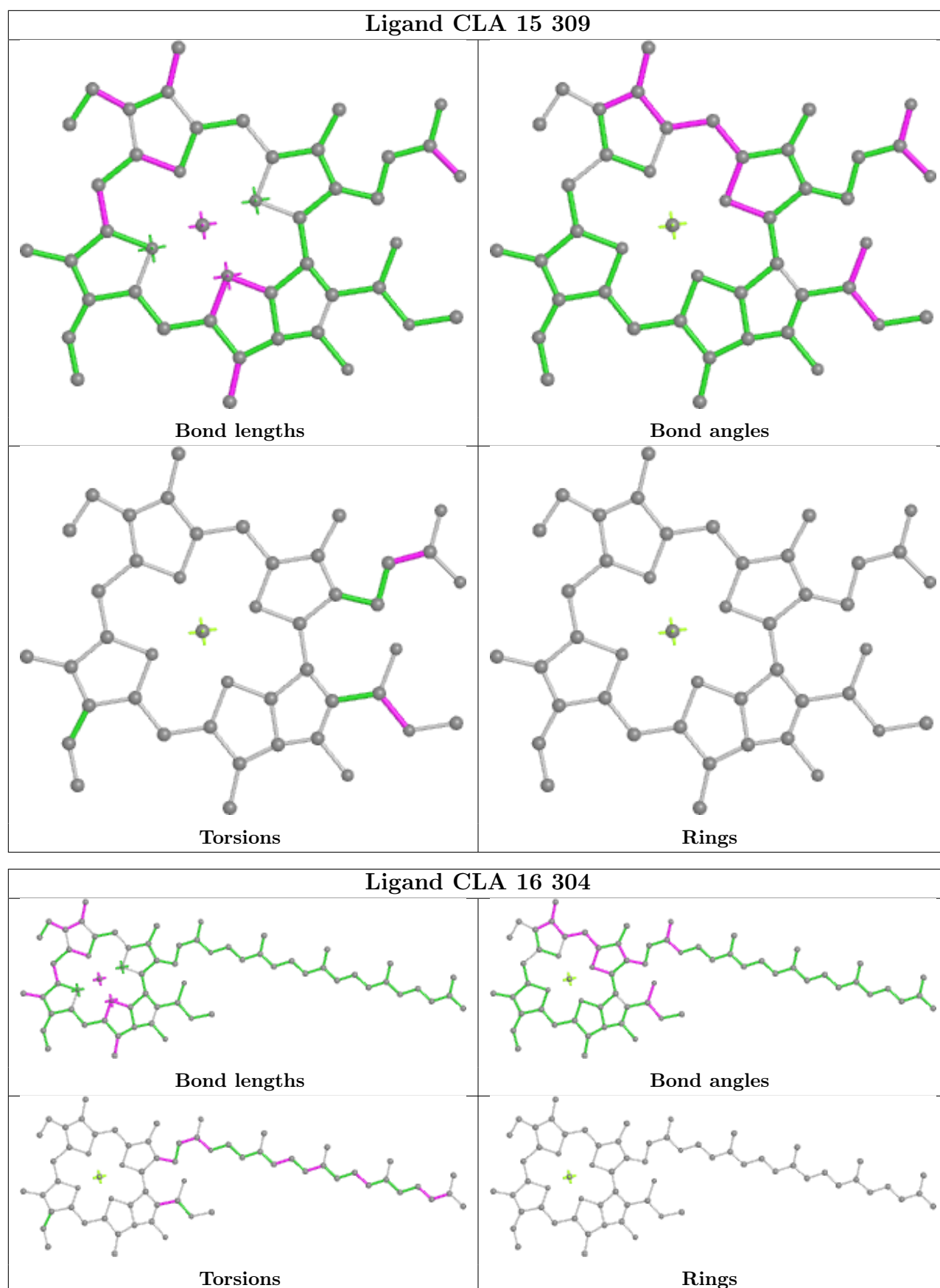


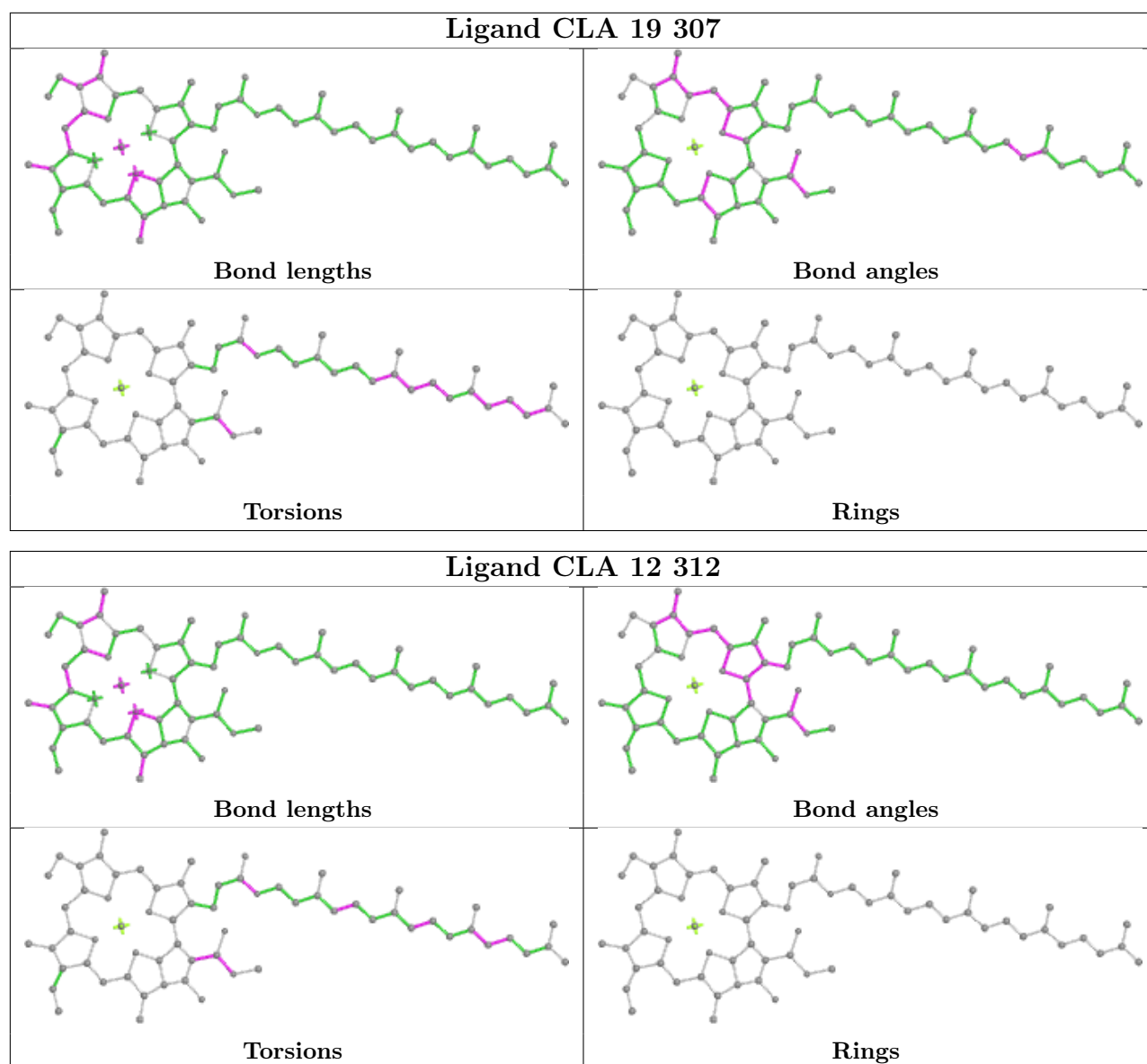
Ligand CLA 21 305



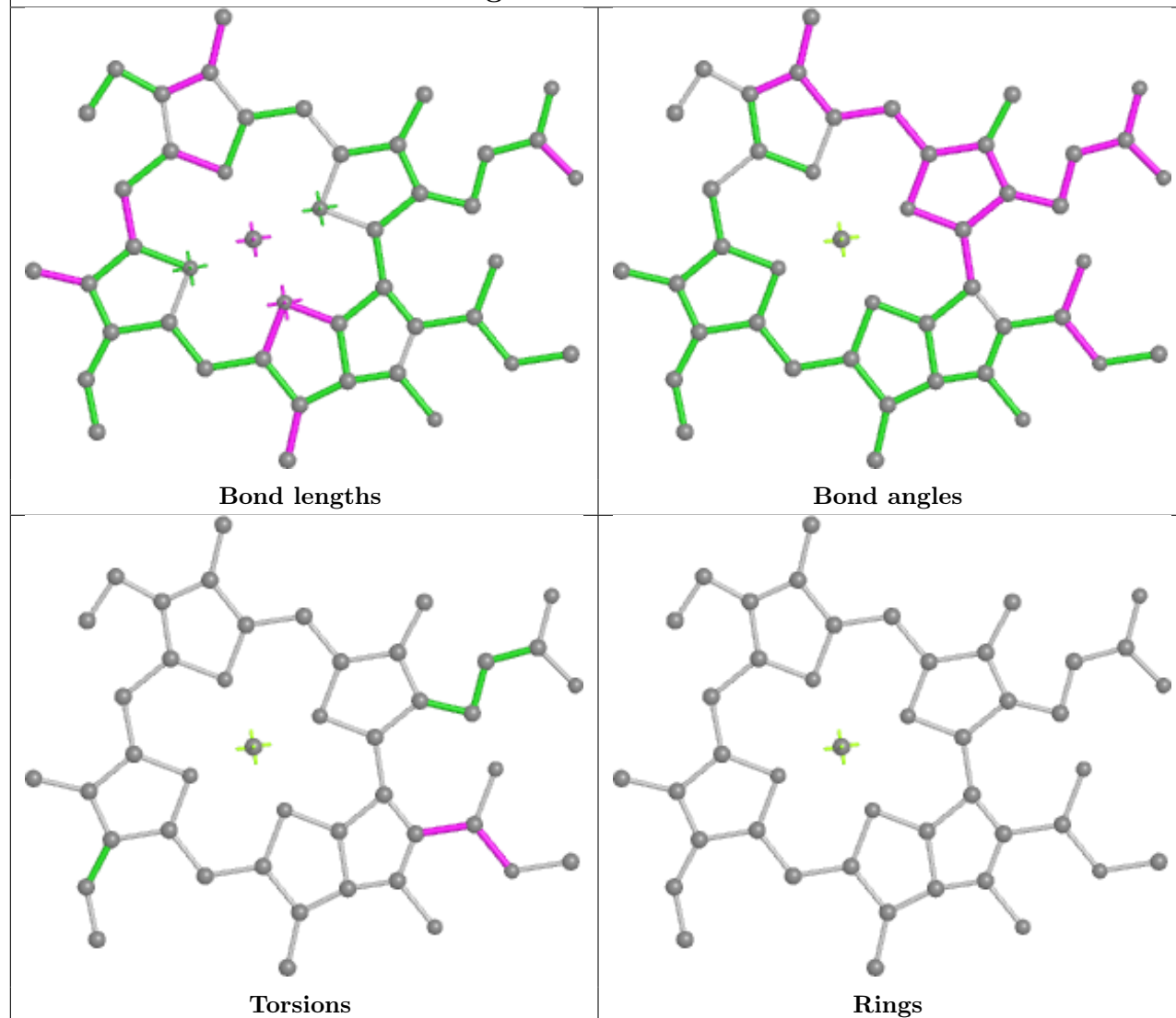




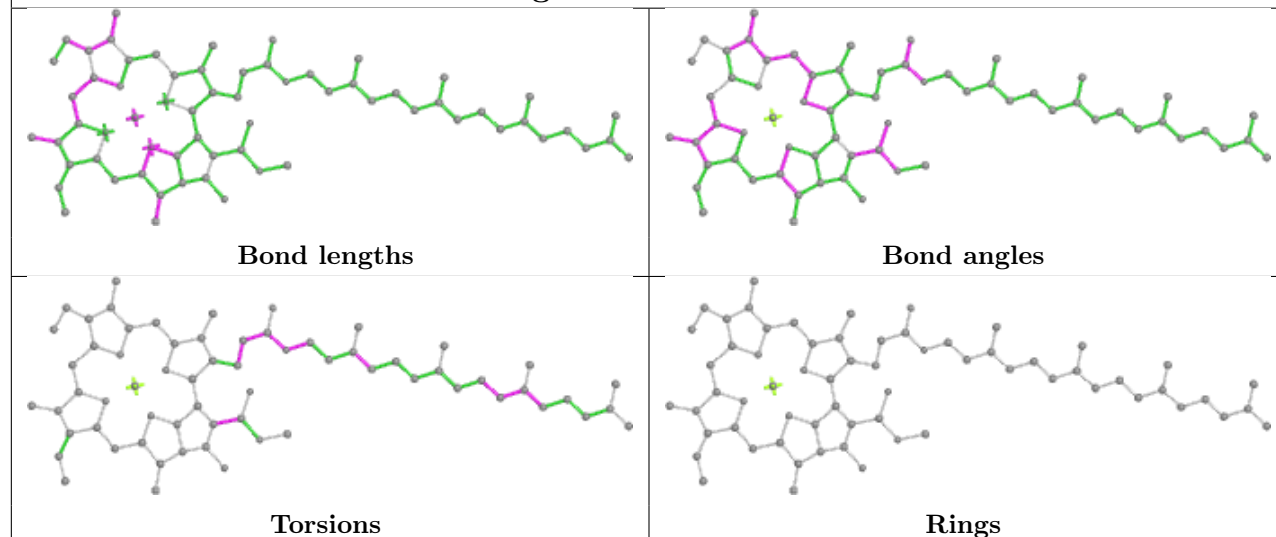


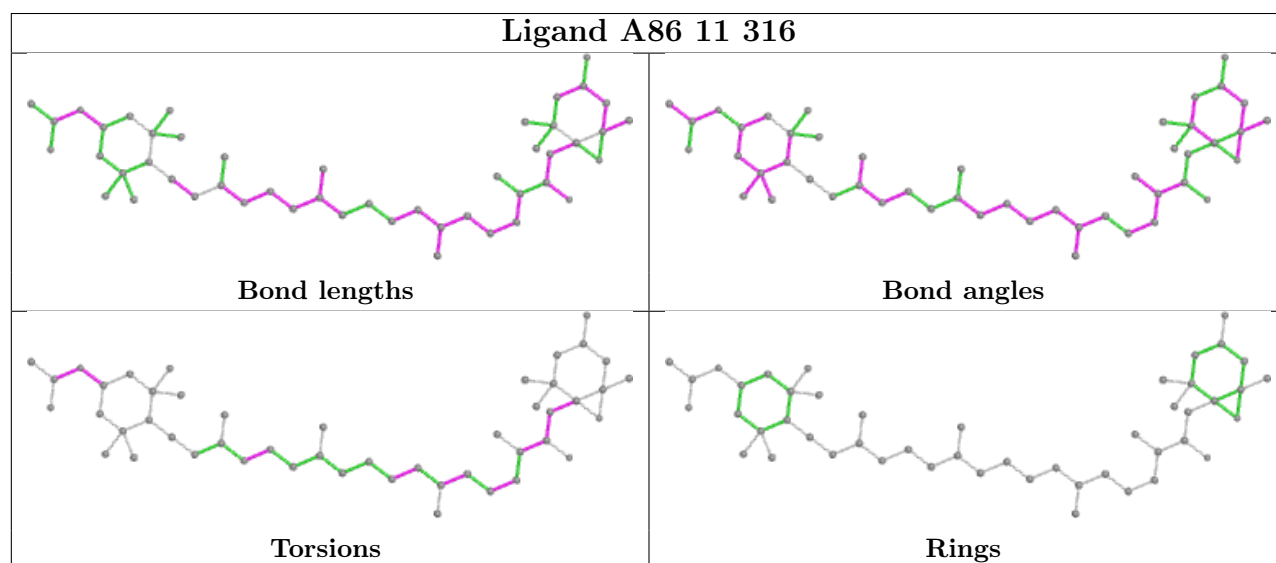
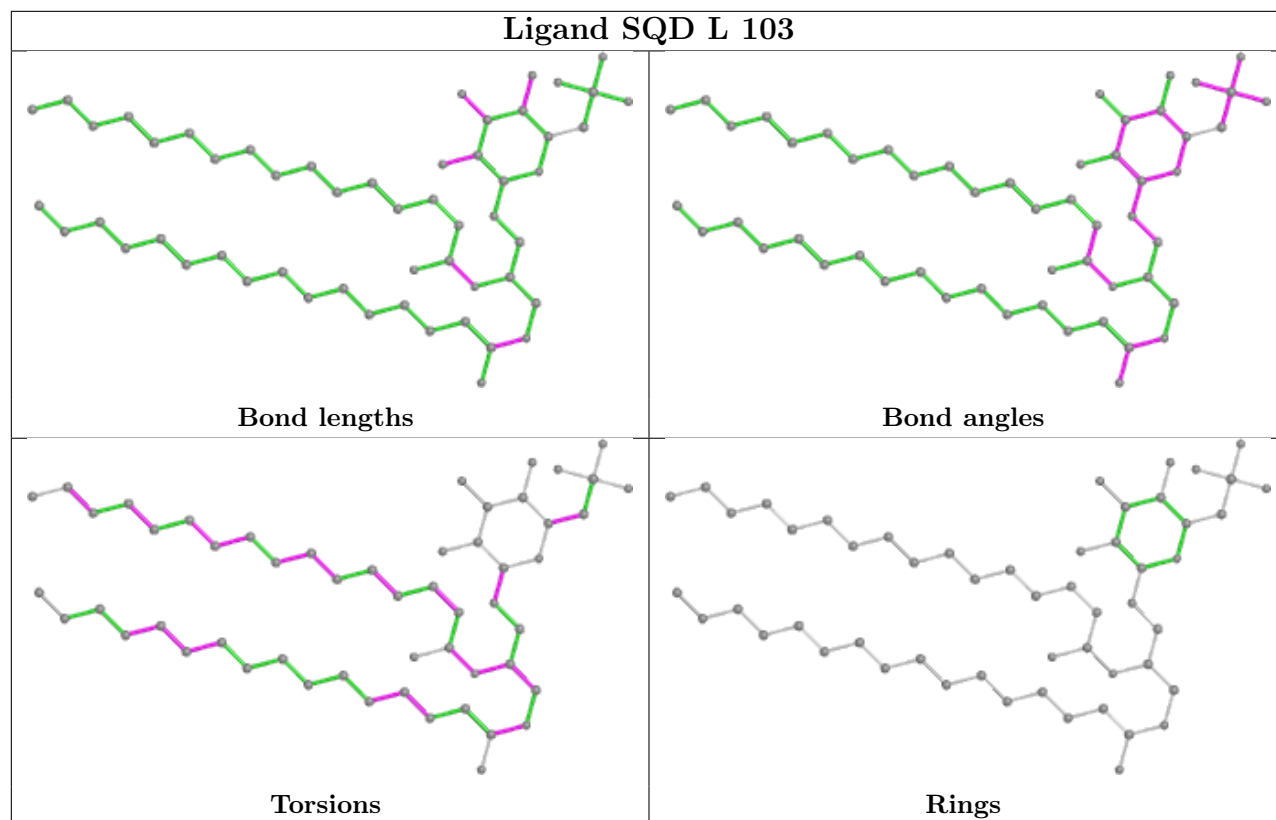
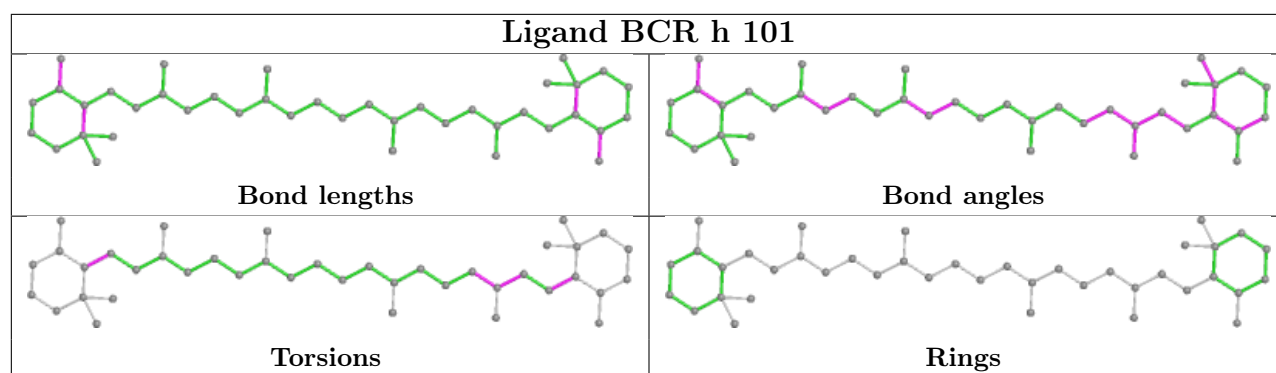


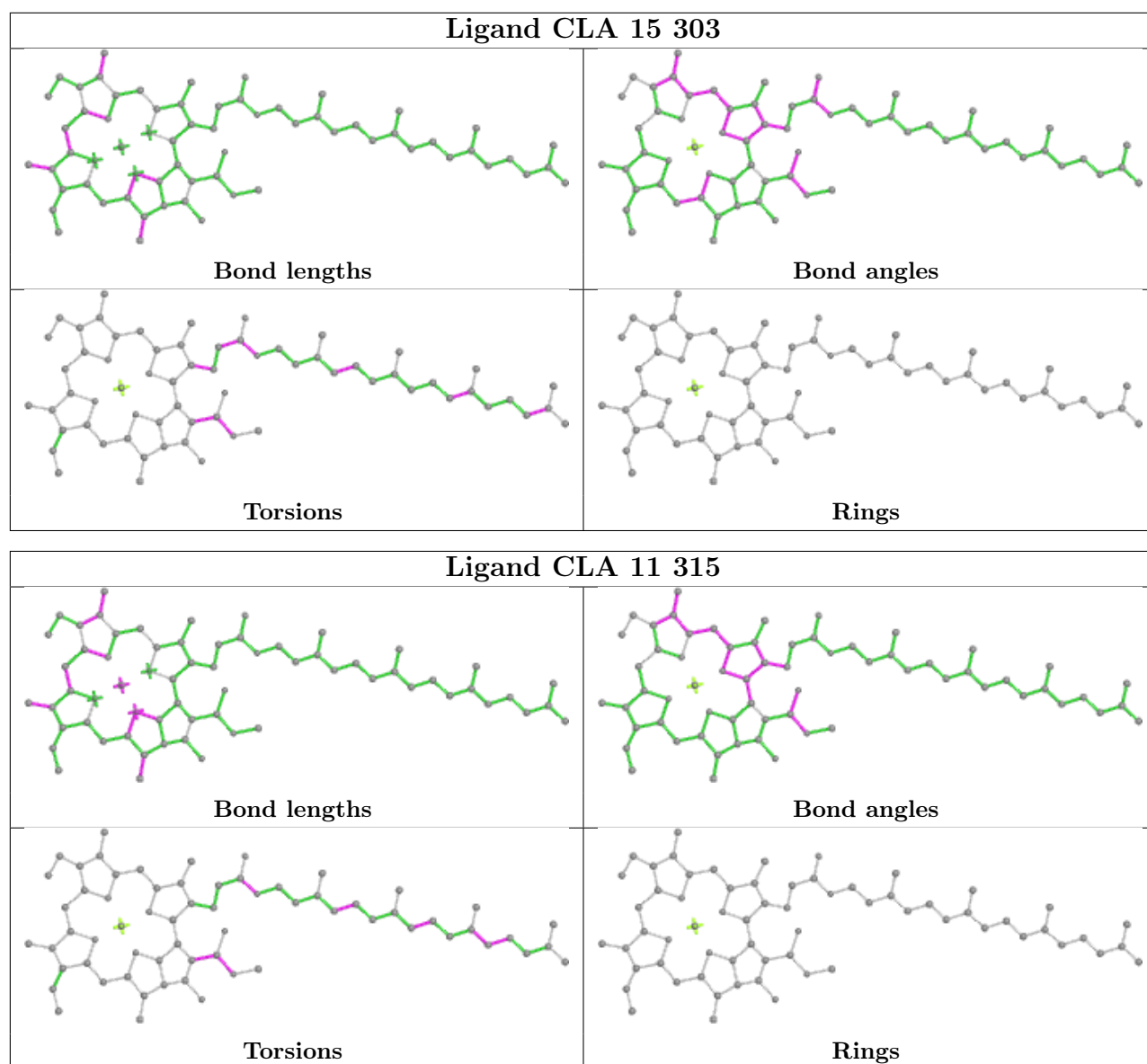
Ligand CLA 17 309

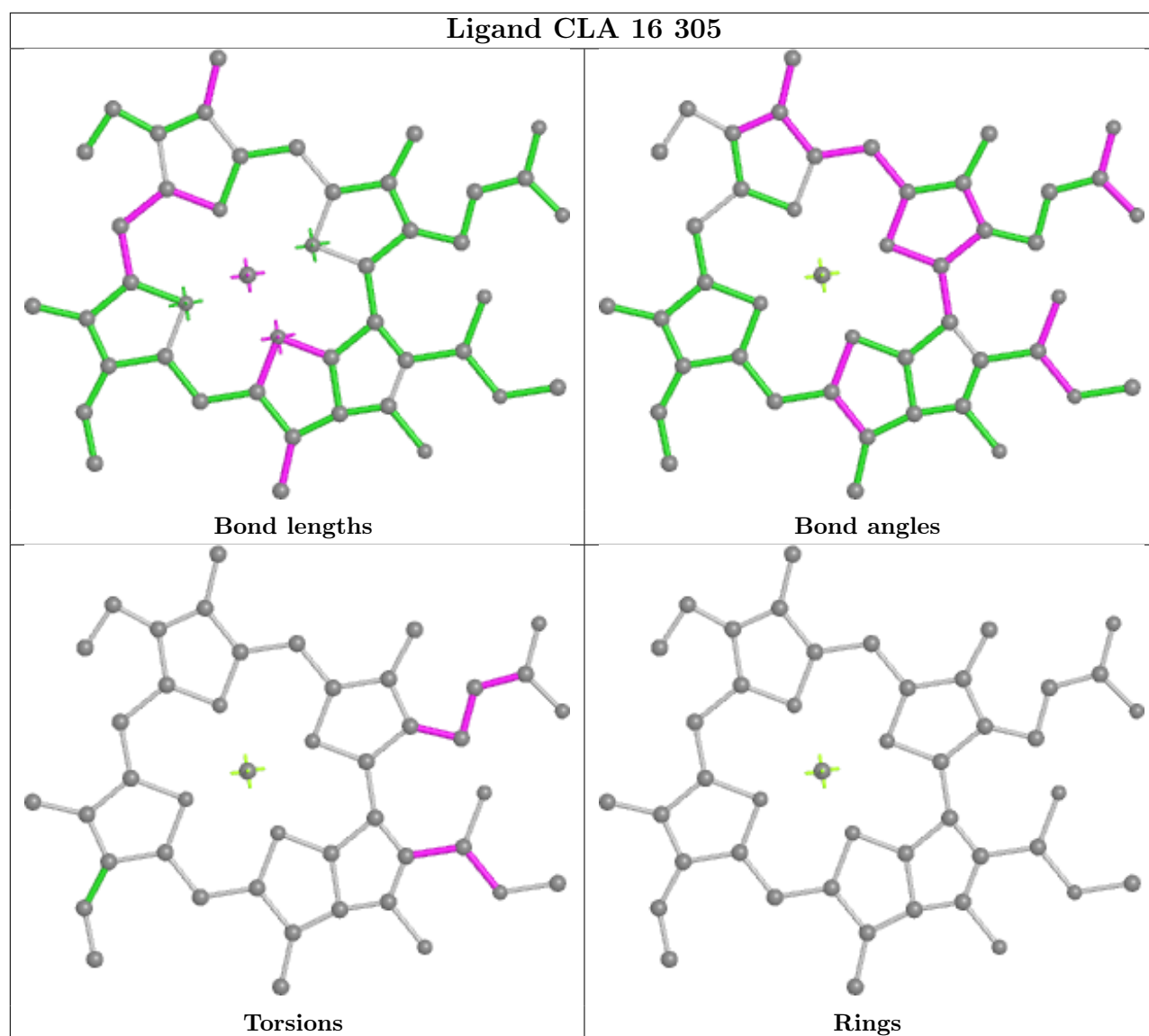


Ligand CLA C 506









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9776. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.