



wwPDB EM Validation Summary Report ⓘ

Sep 10, 2026 – 01:13 AM JST

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

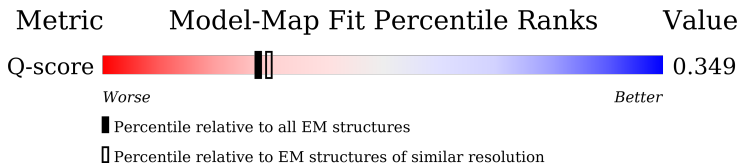
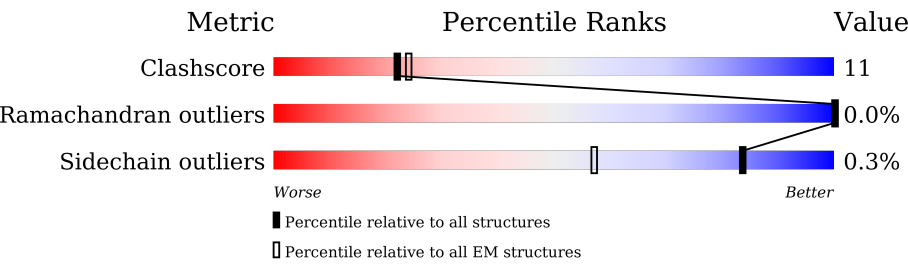
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 Å.

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



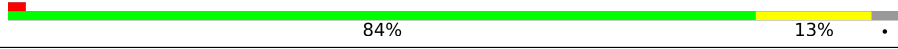
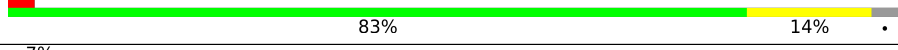
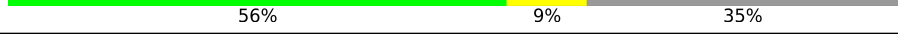
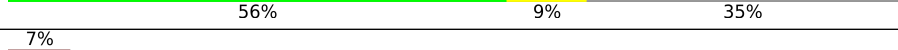
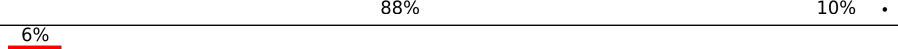
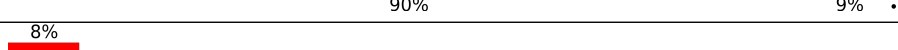
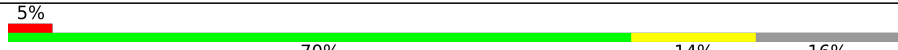
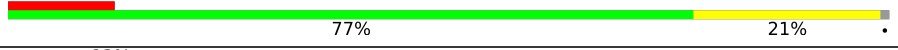
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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

Mol	Chain	Length	Quality of chain
1	A	344	84% 13%
1	a	344	83% 14%
2	B	509	82% 13% 5%
2	b	509	82% 14% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	471	
3	c	471	
4	D	351	
4	d	351	
5	E	84	
5	e	84	
6	F	43	
6	f	43	
7	H	67	
7	h	67	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	44	
10	k	44	
11	L	38	
11	l	38	
12	M	131	
12	m	131	
13	O	248	
13	o	248	
14	T	31	
14	t	31	
15	U	93	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	u	93	
16	V	137	
16	v	137	
17	Y	34	
17	y	34	
18	X	38	
18	x	38	
19	Z	61	
19	z	61	
20	Q	155	
20	q	155	
21	W	72	
21	w	72	
22	0	31	
22	5	31	
23	1	30	
23	6	30	
24	2	10	
24	7	10	
25	11	207	
25	12	207	
25	13	207	
25	14	207	
25	15	207	
25	16	207	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
25	17	207	
25	18	207	
25	31	207	
25	32	207	
25	33	207	
25	34	207	
25	35	207	
25	36	207	
25	37	207	
25	38	207	
26	19	215	
26	39	215	
27	20	143	
27	40	143	
28	21	155	
28	41	155	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	BCT	a	406	-	-	X	-
41	A86	13	312	-	-	X	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 96390 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

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

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

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

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

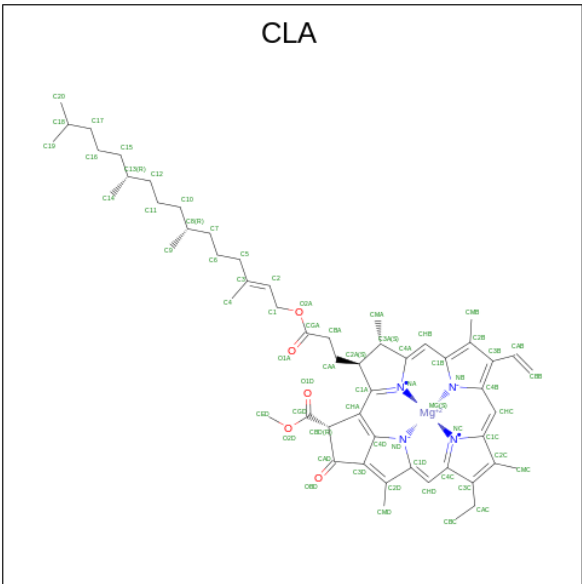
- Molecule 28 is a protein called Fucoxanthin chlorophyll a/c-binding protein monomer 3.

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

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

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

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

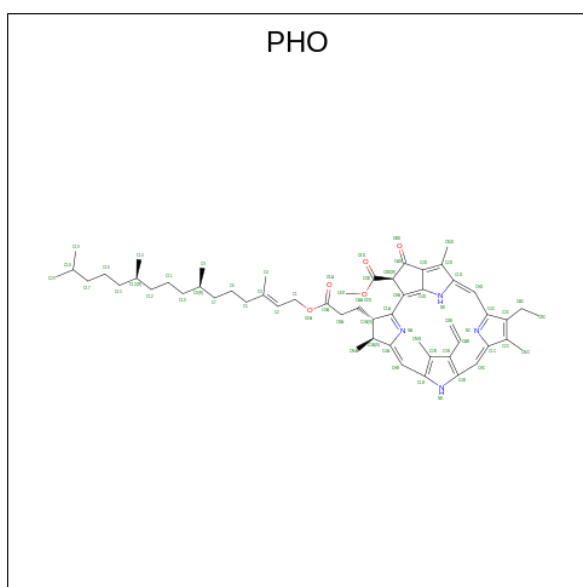
Mol	Chain	Residues	Atoms					AltConf
30	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	38	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	38	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	39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

Continued on next page...

Continued from previous page...

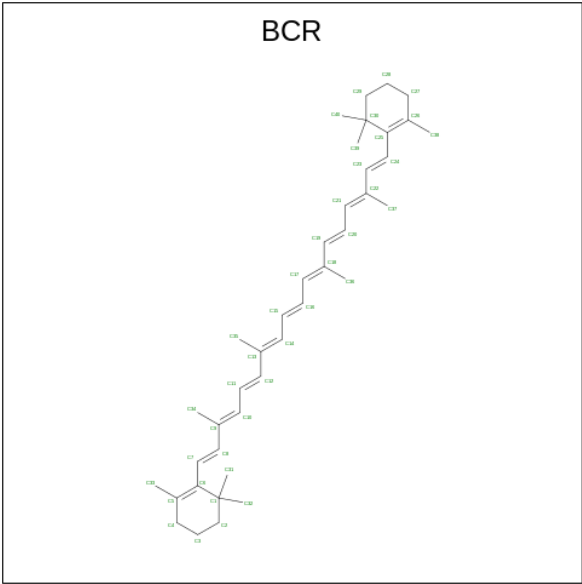
Mol	Chain	Residues	Atoms					AltConf
30	40	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	40	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	41	1	Total	C	Mg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

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



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

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



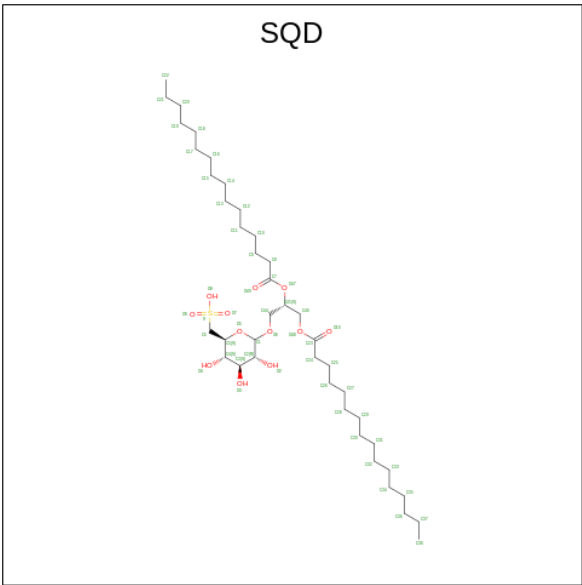
Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	C	0
			40	40	
32	A	1	Total	C	0
			40	40	
32	B	1	Total	C	0
			40	40	
32	B	1	Total	C	0
			40	40	
32	B	1	Total	C	0
			40	40	
32	B	1	Total	C	0
			40	40	
32	C	1	Total	C	0
			40	40	
32	C	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

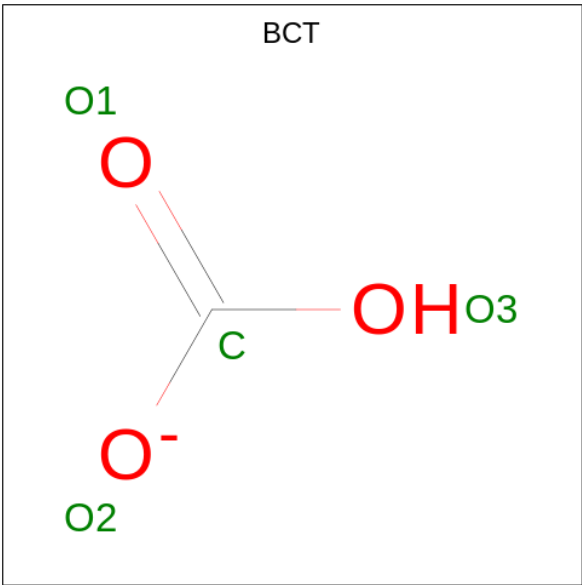
Mol	Chain	Residues	Atoms	AltConf
32	F	1	Total C 40 40	0
32	H	1	Total C 40 40	0
32	Y	1	Total C 40 40	0
32	Z	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C 40 40	0
32	c	1	Total C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

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



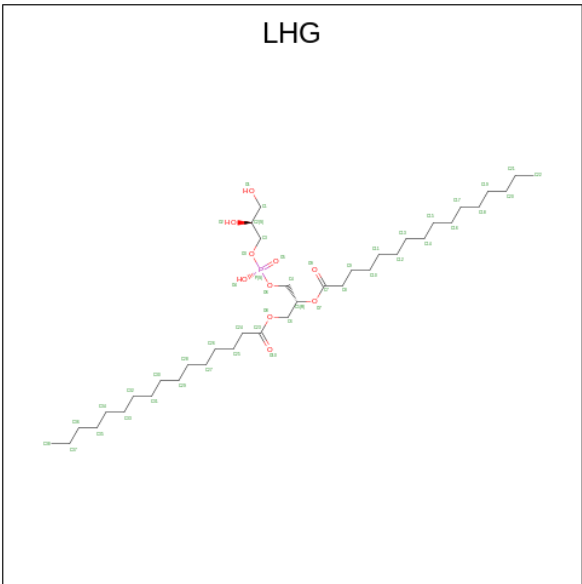
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O	S	0
			54	41	12	1	
33	B	1	Total	C	O	S	0
			37	24	12	1	
33	L	1	Total	C	O	S	0
			54	41	12	1	
33	a	1	Total	C	O	S	0
			54	41	12	1	
33	b	1	Total	C	O	S	0
			37	24	12	1	
33	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: 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: C₃₈H₇₅O₁₀P).



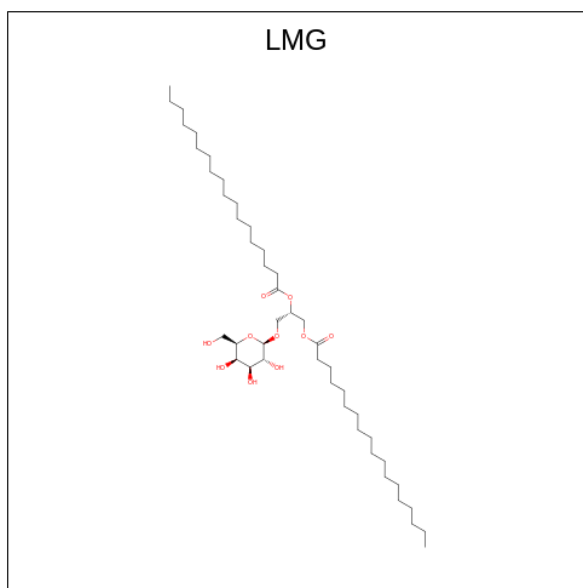
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	P	0
			46	35	10	1	

Continued on next page...

Continued from previous page...

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

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



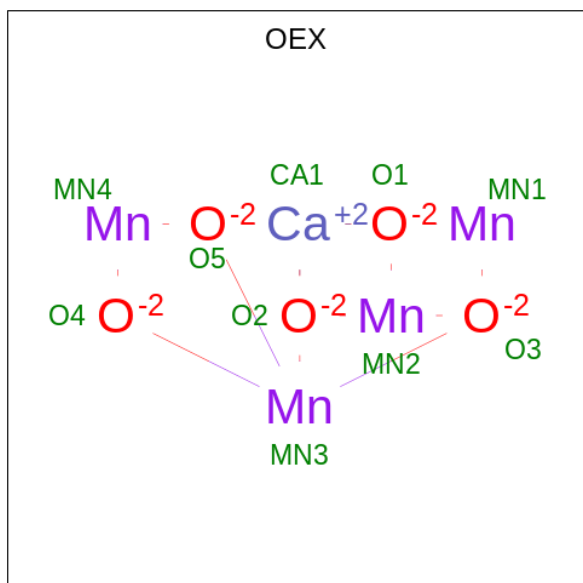
Mol	Chain	Residues	Atoms			AltConf
36	B	1	Total	C	O	0
			51	41	10	
36	B	1	Total	C	O	0
			51	41	10	
36	D	1	Total	C	O	0
			51	41	10	
36	M	1	Total	C	O	0
			40	30	10	

Continued on next page...

Continued from previous page...

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

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



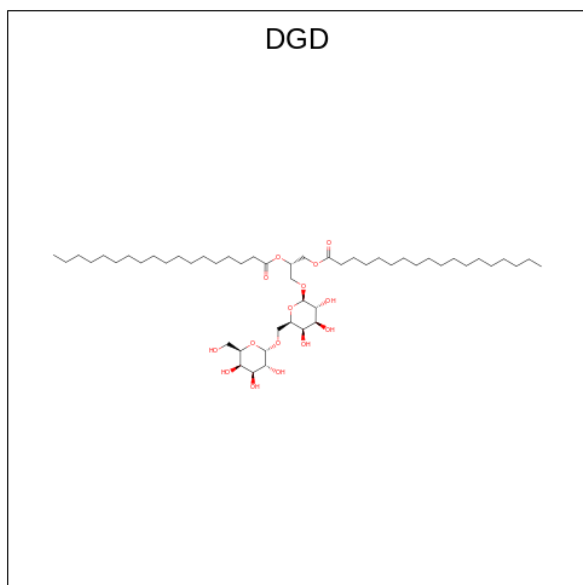
Mol	Chain	Residues	Atoms				AltConf
37	C	1	Total	Ca	Mn	O	0
			10	1	4	5	

Continued on next page...

Continued from previous page...

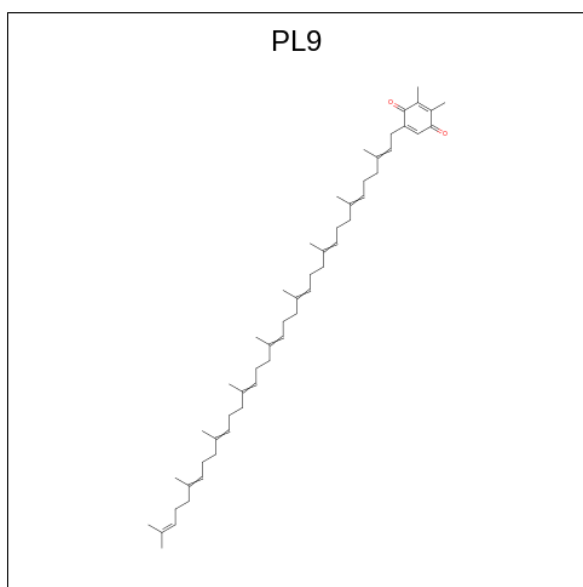
Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
37	c	1	10	1	4	5	0

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



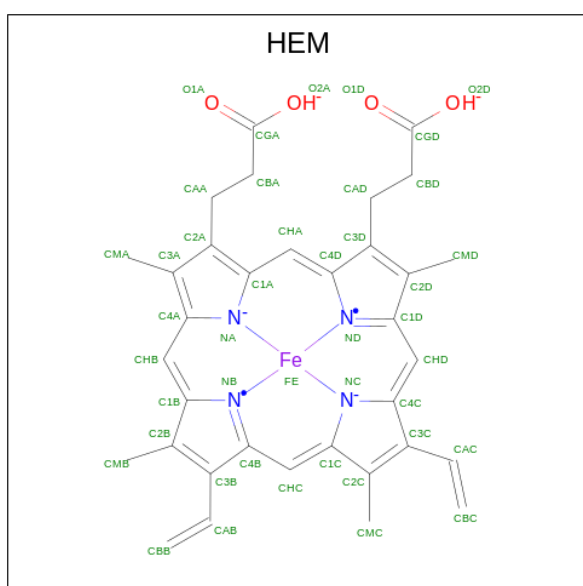
Mol	Chain	Residues	Atoms			AltConf
38	C	1	Total	C	O	0
			62	47	15	
38	C	1	Total	C	O	0
			62	47	15	
38	H	1	Total	C	O	0
			62	47	15	
38	J	1	Total	C	O	0
			62	47	15	
38	c	1	Total	C	O	0
			62	47	15	
38	c	1	Total	C	O	0
			62	47	15	
38	h	1	Total	C	O	0
			62	47	15	
38	j	1	Total	C	O	0
			62	47	15	

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



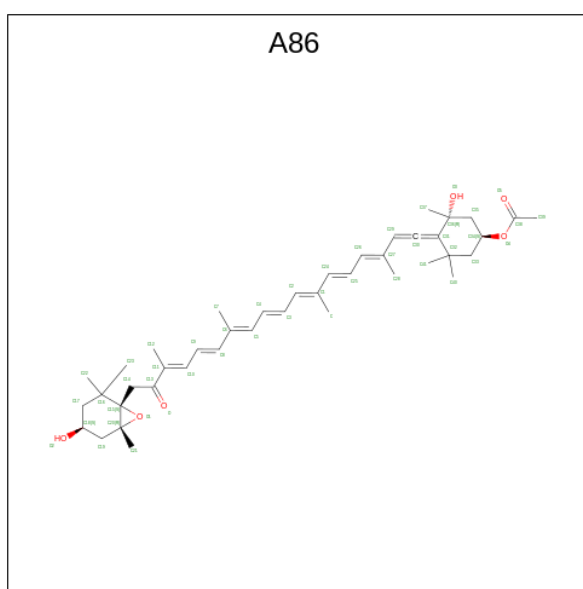
Mol	Chain	Residues	Atoms			AltConf
39	D	1	Total	C	O	0
			55	53	2	
39	D	1	Total	C	O	0
			55	53	2	
39	d	1	Total	C	O	0
			55	53	2	
39	d	1	Total	C	O	0
			55	53	2	

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



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

- Molecule 41 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

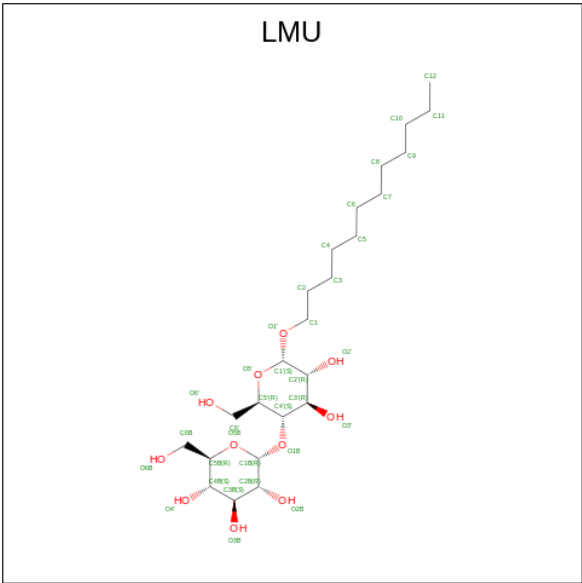
Mol	Chain	Residues	Atoms			AltConf
41	36	1	Total	C	O	0
			48	42	6	
41	36	1	Total	C	O	0
			48	42	6	
41	36	1	Total	C	O	0
			48	42	6	
41	37	1	Total	C	O	0
			48	42	6	
41	37	1	Total	C	O	0
			48	42	6	
41	37	1	Total	C	O	0
			48	42	6	
41	37	1	Total	C	O	0
			48	42	6	
41	37	1	Total	C	O	0
			48	42	6	
41	37	1	Total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

Continued on next page...

Continued from previous page...

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

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

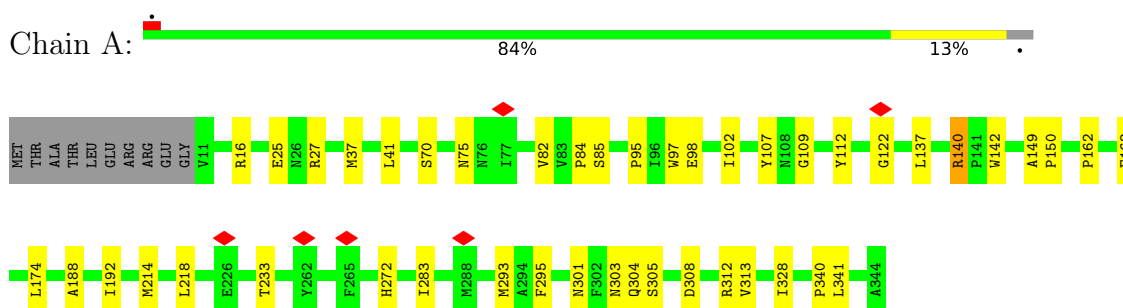


Mol	Chain	Residues	Atoms			AltConf
42	12	1	Total	C	O	0
			32	21	11	
42	32	1	Total	C	O	0
			32	21	11	

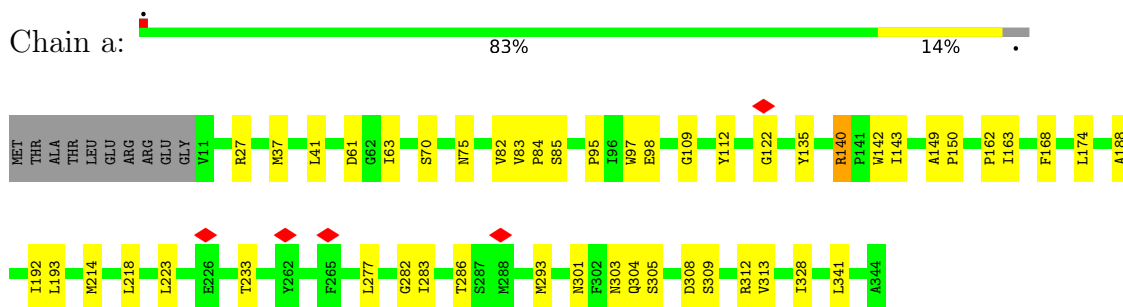
3 Residue-property plots [i](#)

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

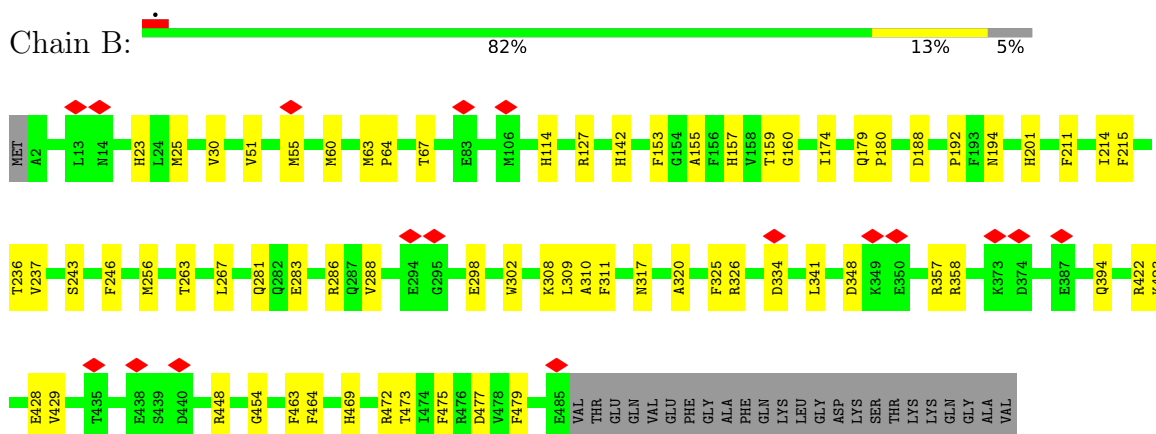
- Molecule 1: Photosystem II reaction center protein D1



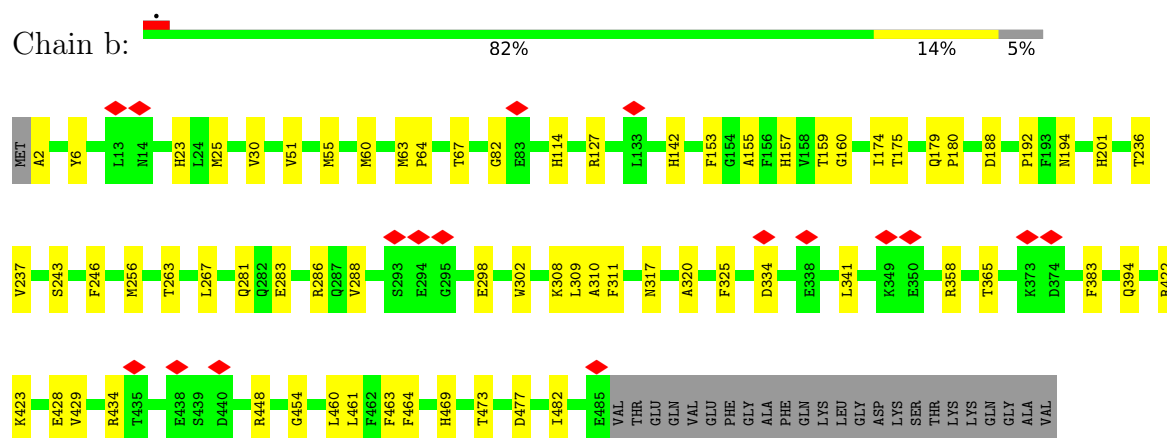
- Molecule 1: Photosystem II reaction center protein D1



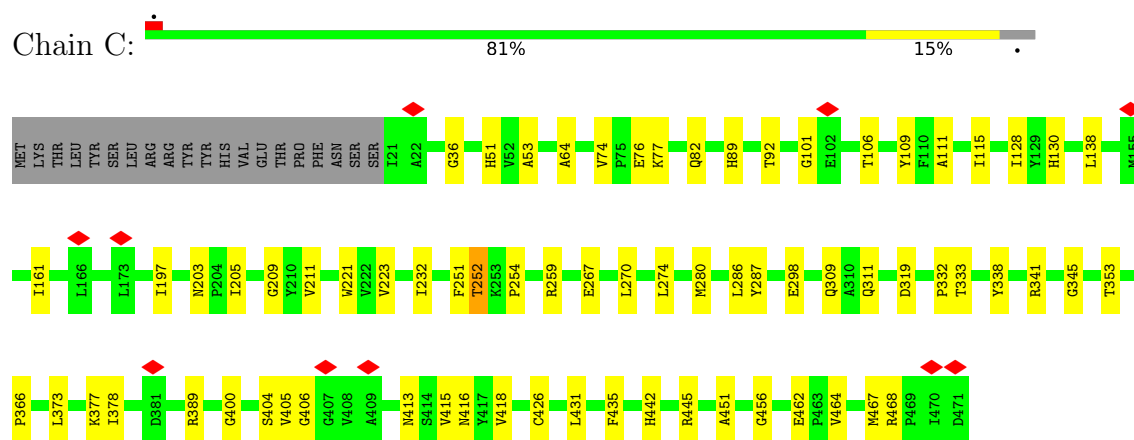
- Molecule 2: Photosystem II chlorophyll protein CP47



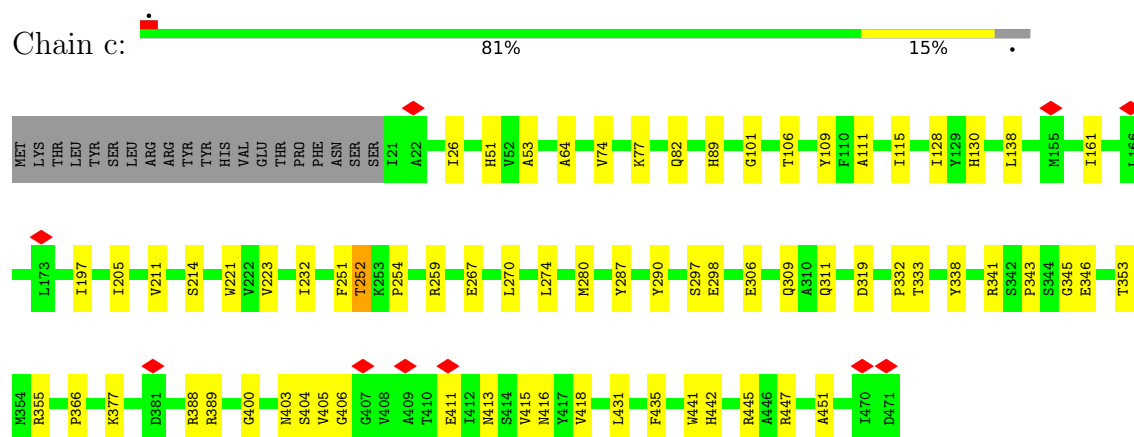
- Molecule 2: Photosystem II chlorophyll protein CP47



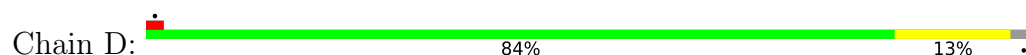
- Molecule 3: Photosystem II chlorophyll protein CP43

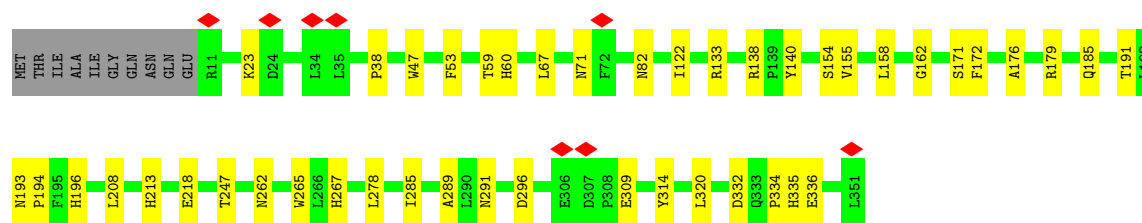


- Molecule 3: Photosystem II chlorophyll protein CP43

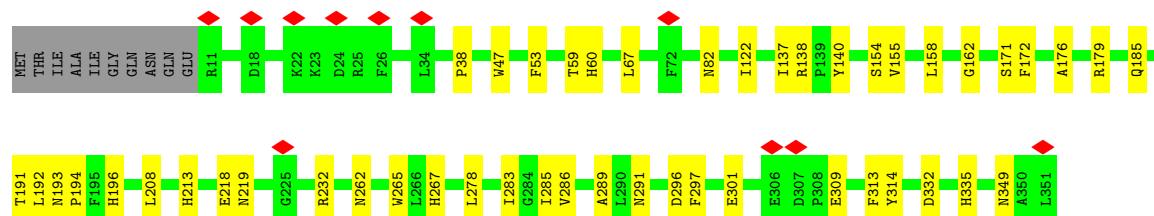
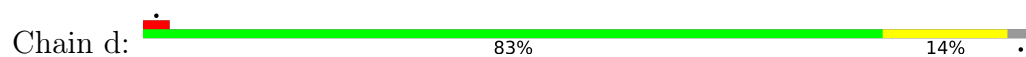


- Molecule 4: Photosystem II reaction center protein D2

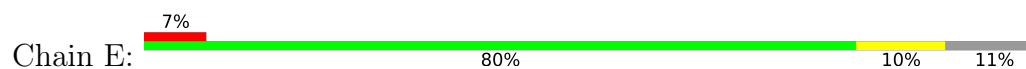




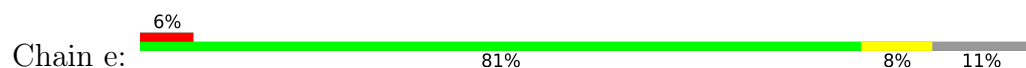
• Molecule 4: Photosystem II reaction center protein D2



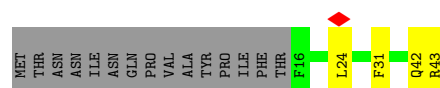
• Molecule 5: Cytochrome b559 subunit alpha



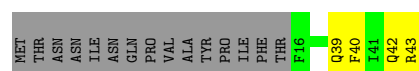
• Molecule 5: Cytochrome b559 subunit alpha



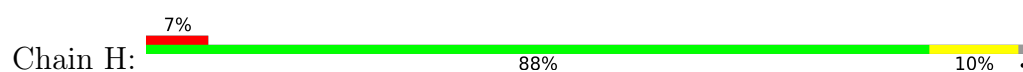
• Molecule 6: Cytochrome b559 subunit beta



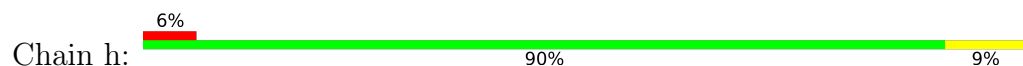
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 7: Photosystem II reaction center protein H



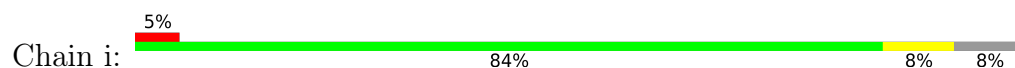
- Molecule 7: Photosystem II reaction center protein H



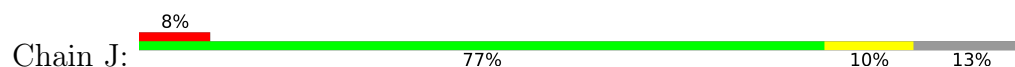
- Molecule 8: Photosystem II reaction center protein I



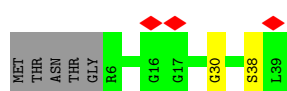
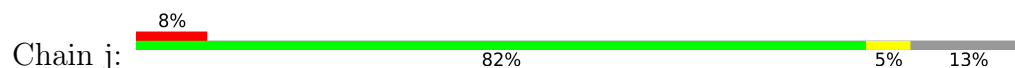
- Molecule 8: Photosystem II reaction center protein I



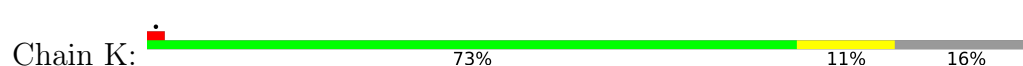
- Molecule 9: Photosystem II reaction center protein J



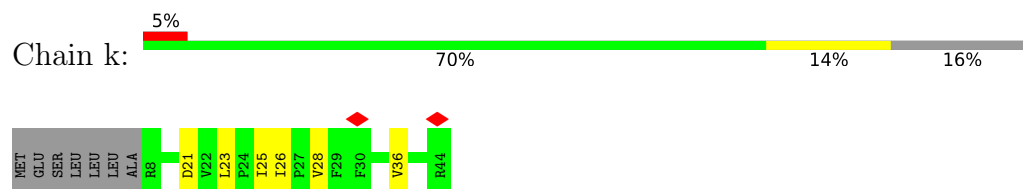
- Molecule 9: Photosystem II reaction center protein J



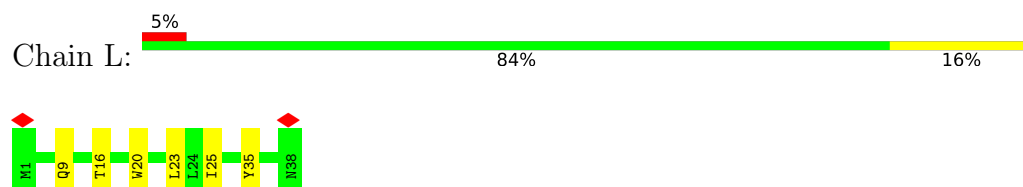
- Molecule 10: Photosystem II reaction center protein K



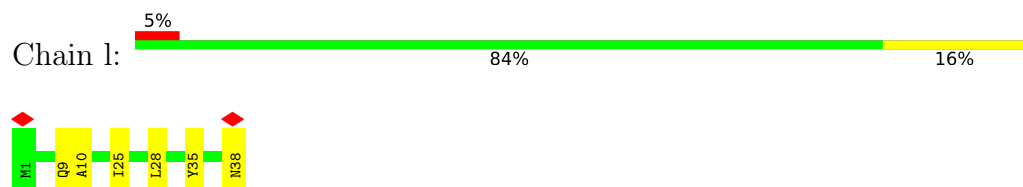
- Molecule 10: Photosystem II reaction center protein K



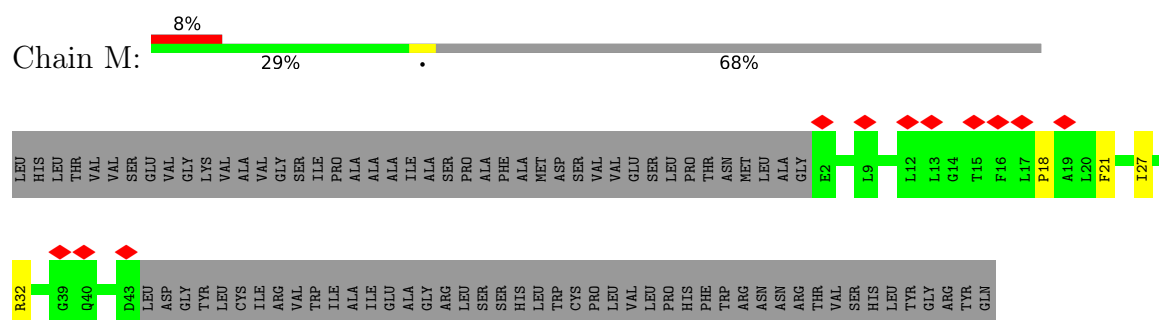
- Molecule 11: Photosystem II reaction center protein L



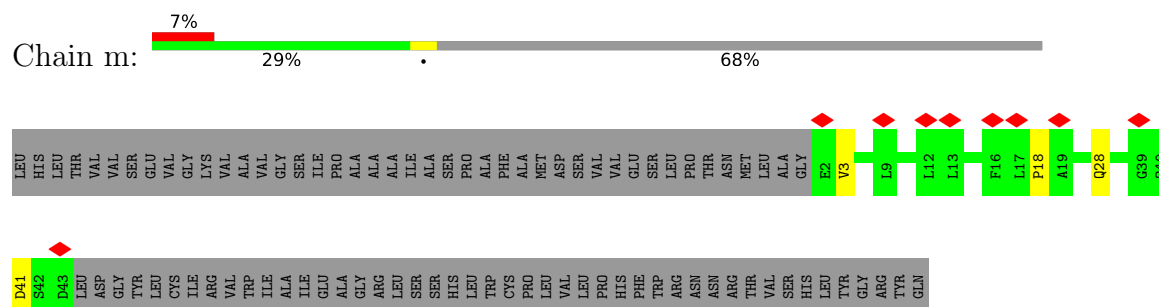
- Molecule 11: Photosystem II reaction center protein L



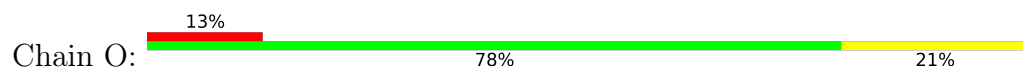
- Molecule 12: Photosystem II reaction center protein M

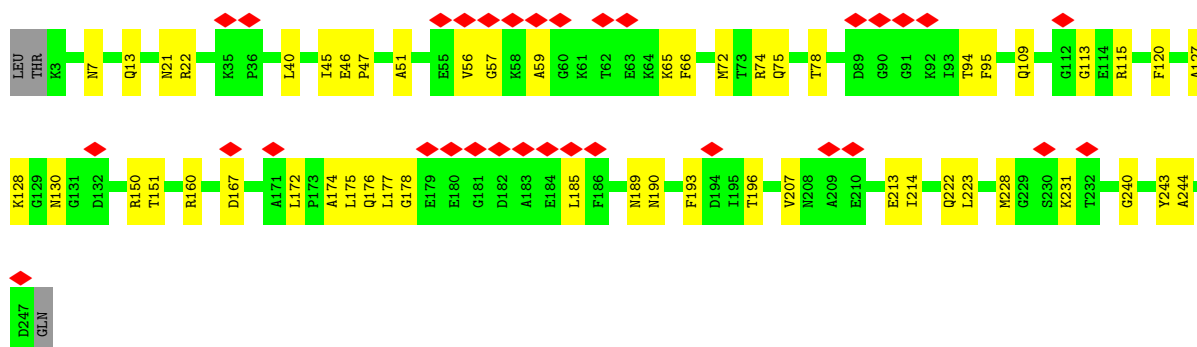


- Molecule 12: Photosystem II reaction center protein M



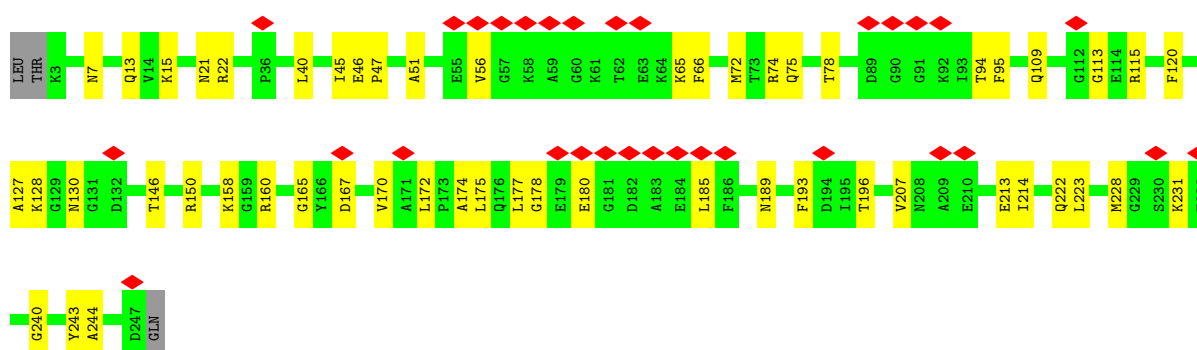
- Molecule 13: Extrinsic protein in photosystem II





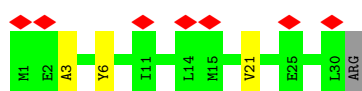
- Molecule 13: Extrinsic protein in photosystem II

Chain o: 12% 77% 21%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 23% 87% 10%



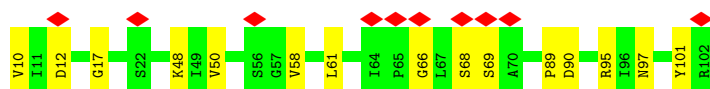
- Molecule 14: Photosystem II reaction center protein T

Chain t: 23% 81% 16%

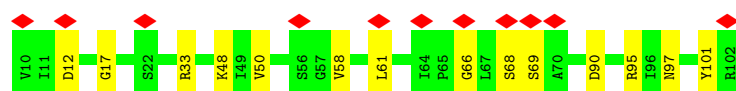
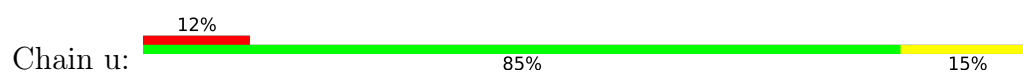


- Molecule 15: Extrinsic protein in photosystem II

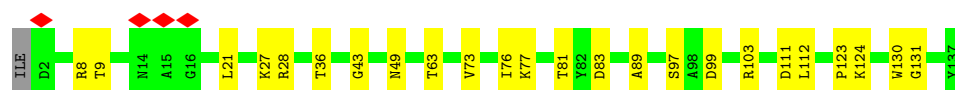
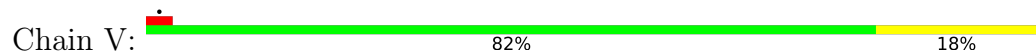
Chain U: 11% 84% 16%



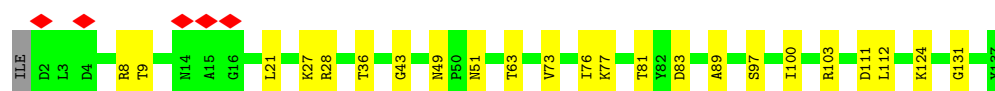
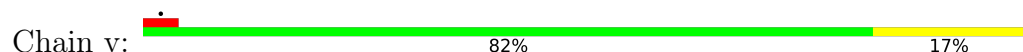
- Molecule 15: Extrinsic protein in photosystem II



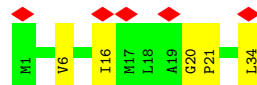
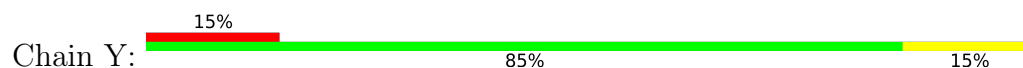
- Molecule 16: Cytochrome c-550



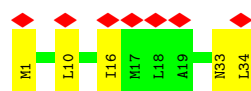
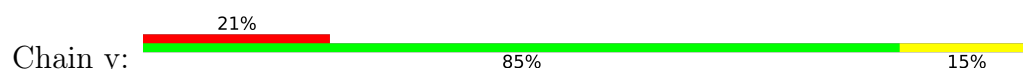
- Molecule 16: Cytochrome c-550



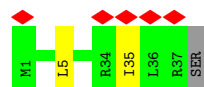
- Molecule 17: Photosystem II reaction center protein Ycf12



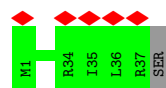
- Molecule 17: Photosystem II reaction center protein Ycf12



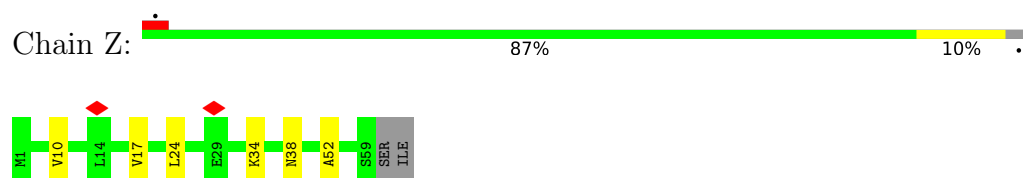
- Molecule 18: Photosystem II reaction center X protein



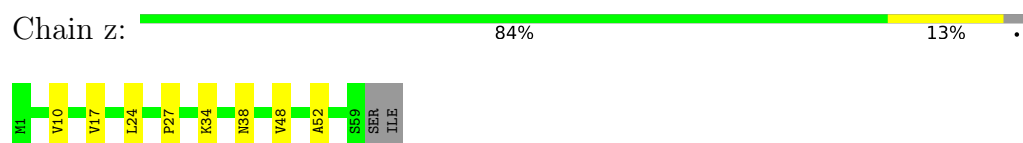
- Molecule 18: Photosystem II reaction center X protein



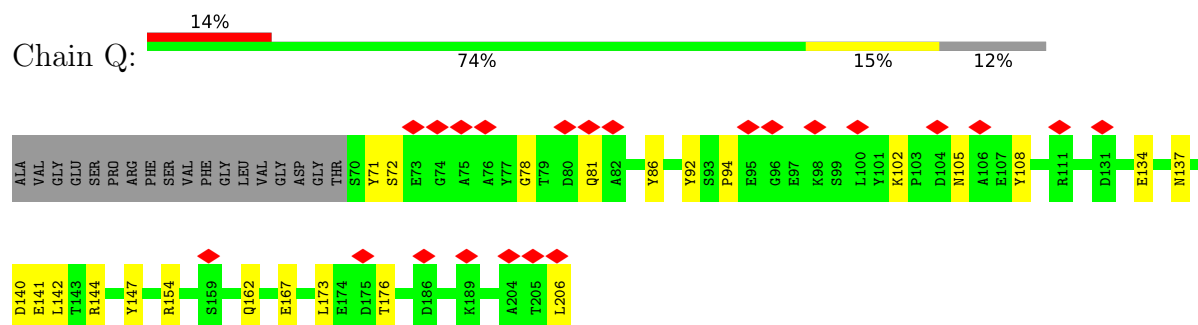
- Molecule 19: Photosystem II reaction center protein Z



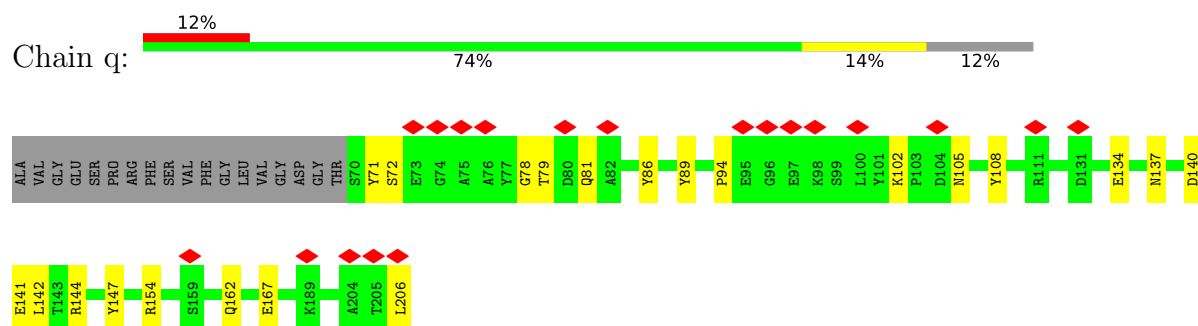
- Molecule 19: Photosystem II reaction center protein Z



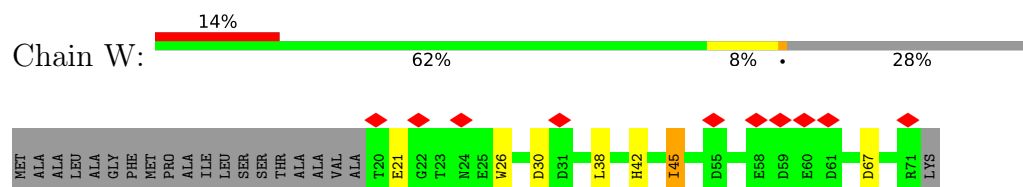
- Molecule 20: Extrinsic protein in photosystem II



- Molecule 20: Extrinsic protein in photosystem II

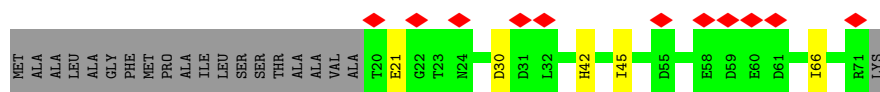


- Molecule 21: Photosystem II reaction center protein W

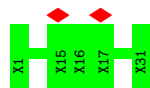


- Molecule 21: Photosystem II reaction center protein W

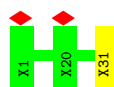




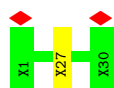
- Molecule 22: Unknown protein 0



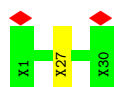
- Molecule 22: Unknown protein 0



- Molecule 23: Unknown protein 1



- Molecule 23: Unknown protein 1



- Molecule 24: Unknown protein 2

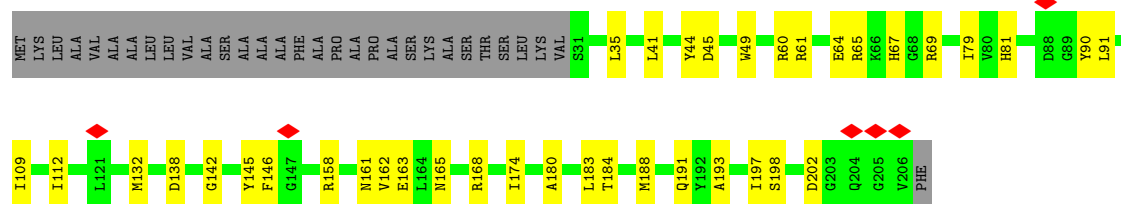


- Molecule 24: Unknown protein 2



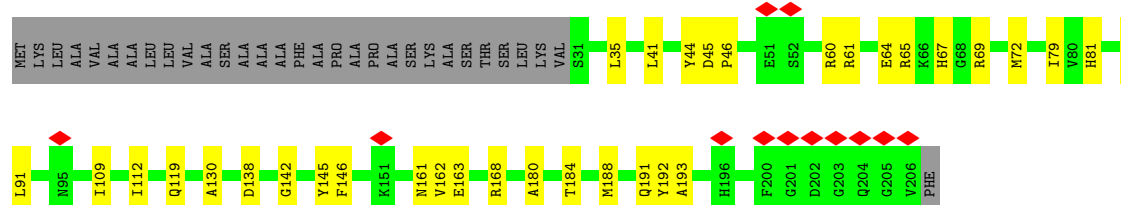
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 11: 



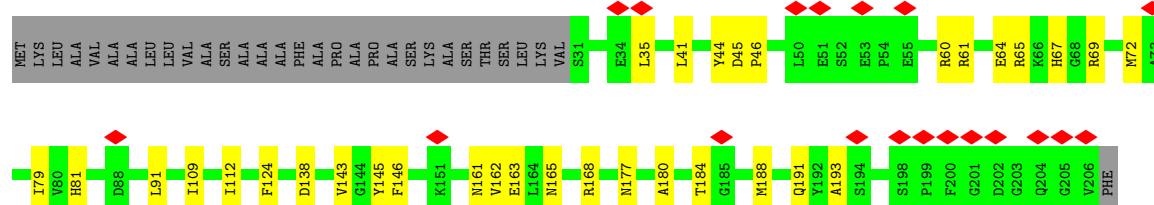
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 12: 



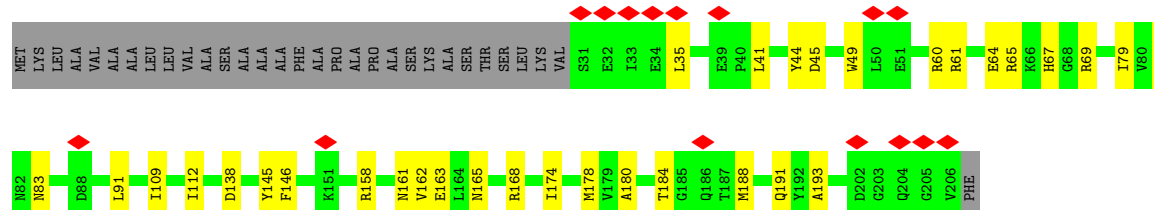
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 13: 



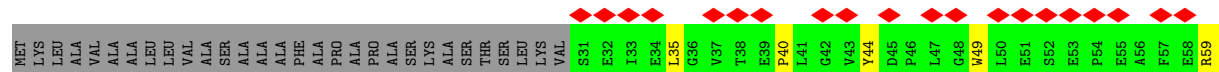
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

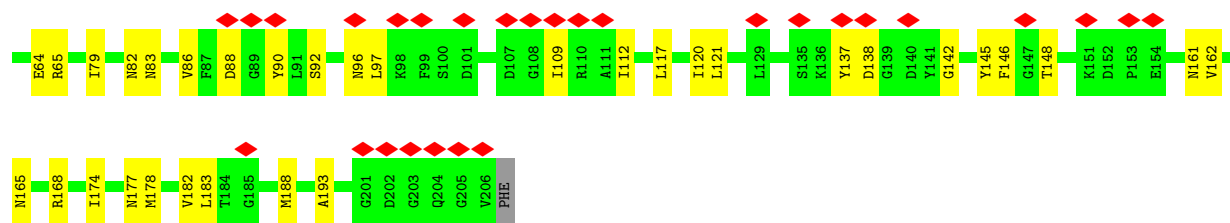
Chain 14: 



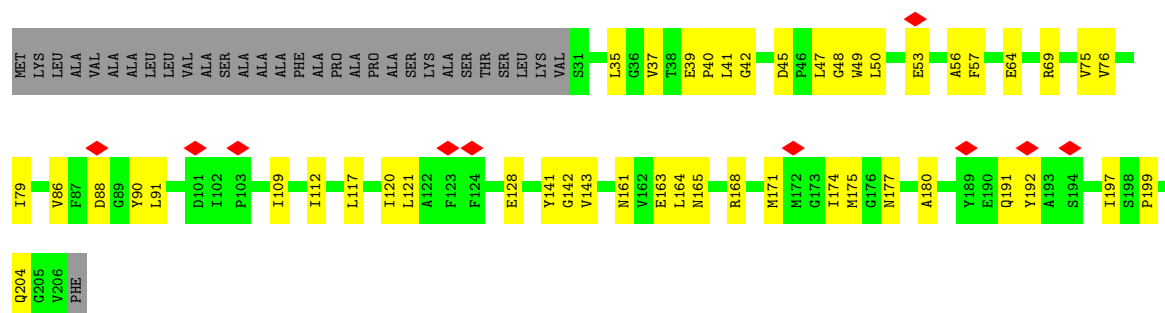
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 15: 

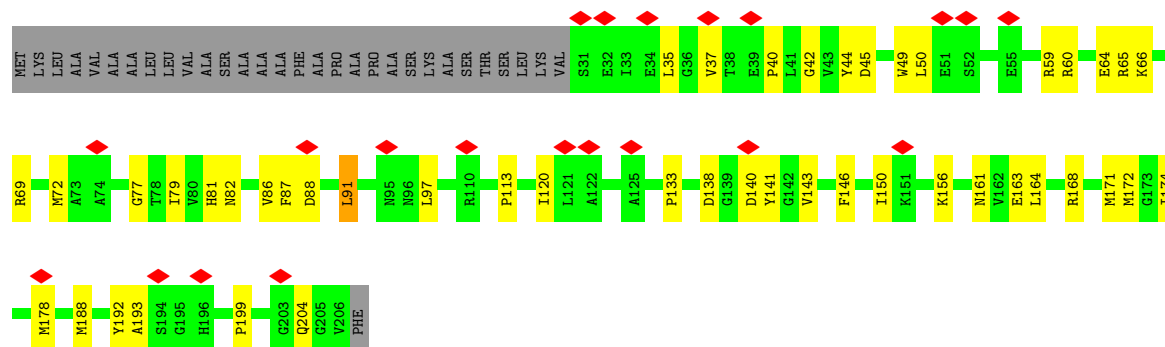




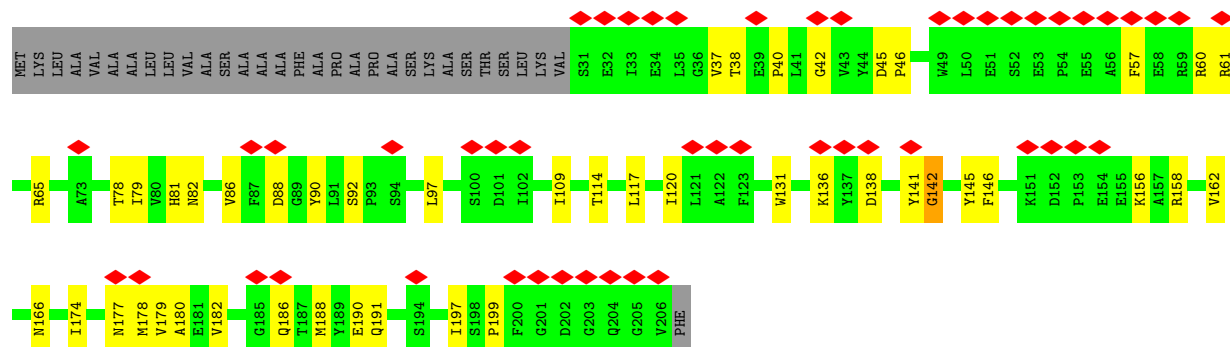
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1



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

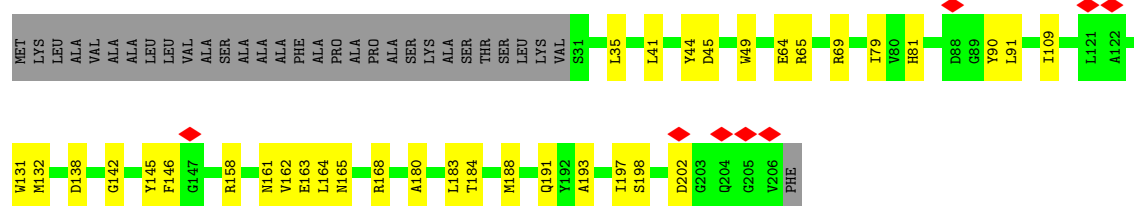


- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1



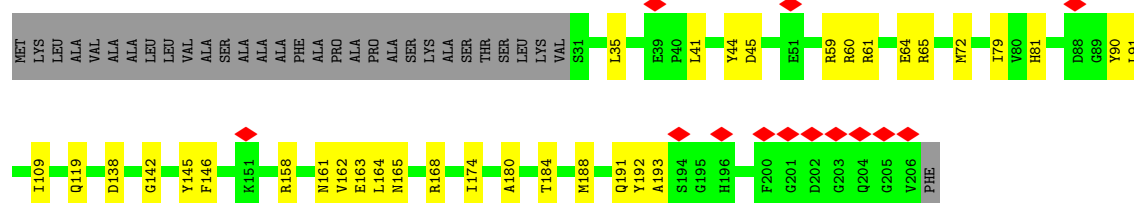
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 31:  68% 17% 15%



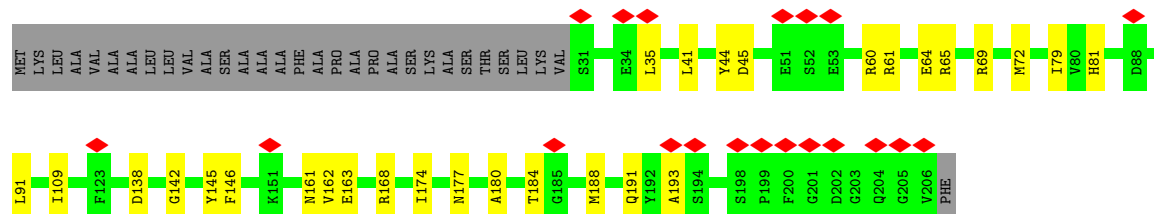
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 32:  6% 69% 16% 15%



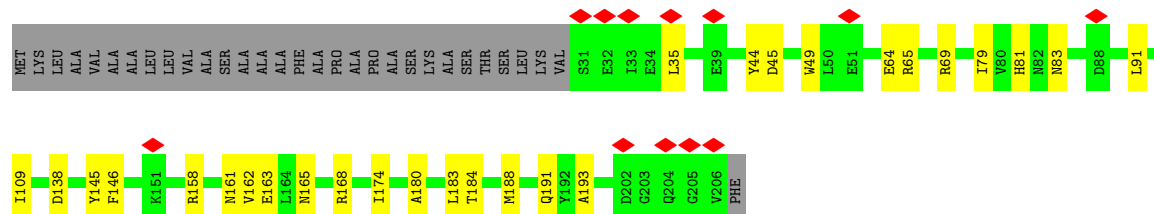
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 33:  10% 71% 14% 15%



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

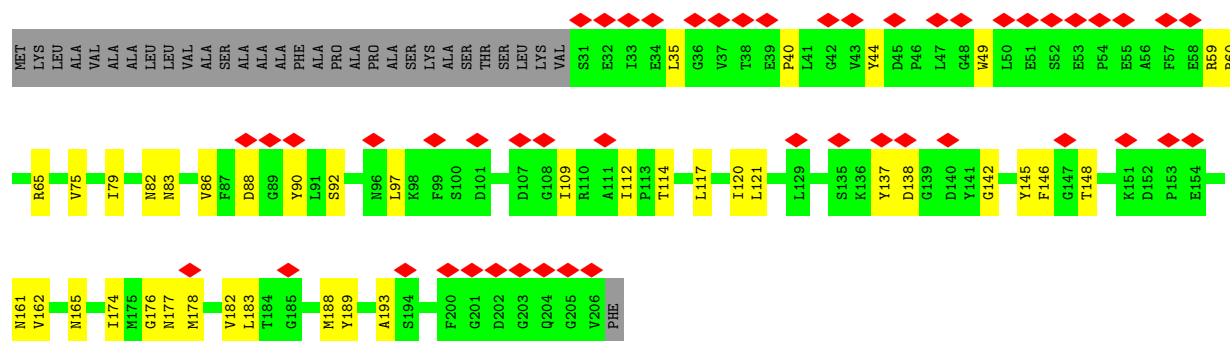
Chain 34:  6% 71% 14% 15%



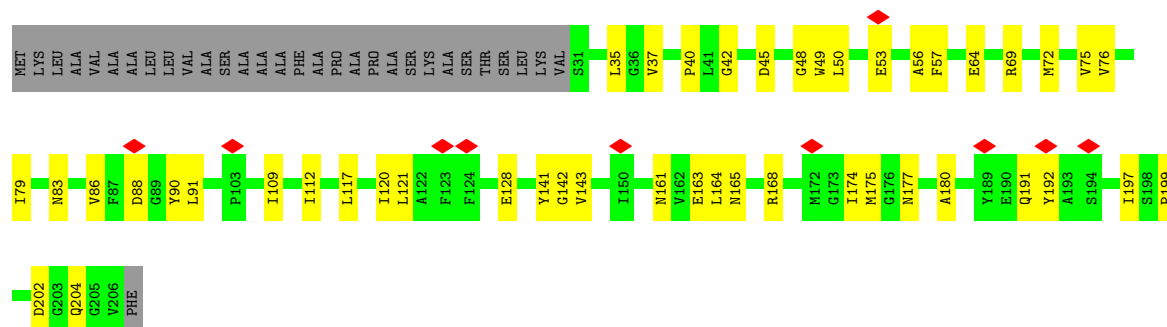
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

Chain 35:  24% 66% 19% 15%

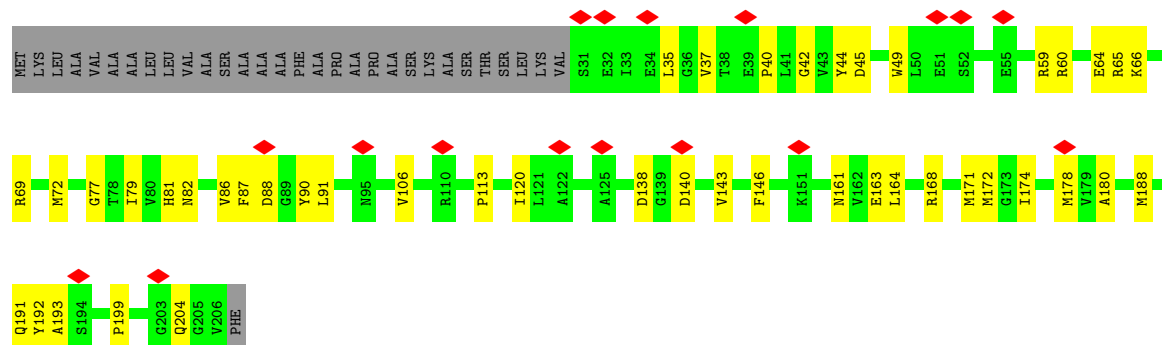




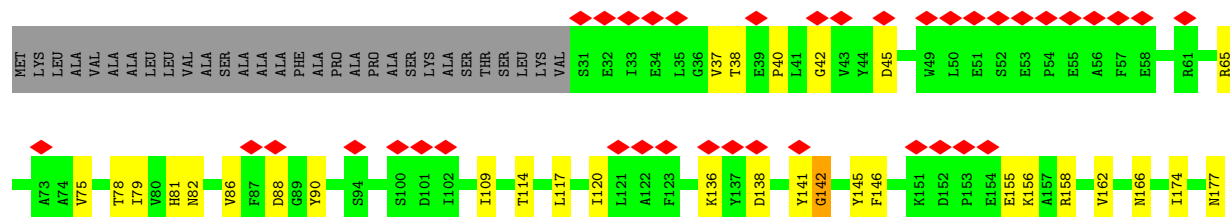
- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1



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

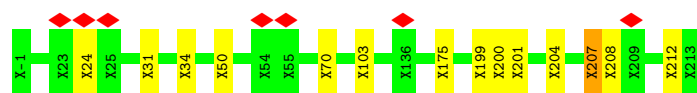


- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcf1, FCP1

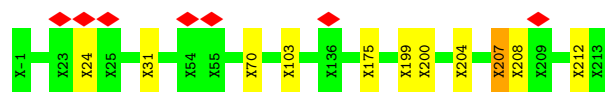




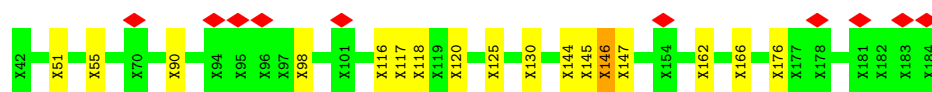
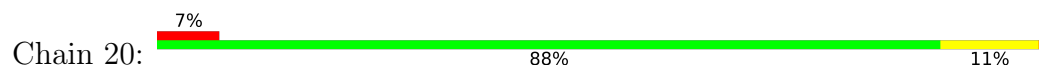
- Molecule 26: Fucoxanthin chlorophyll a/c-binding protein monomer 1



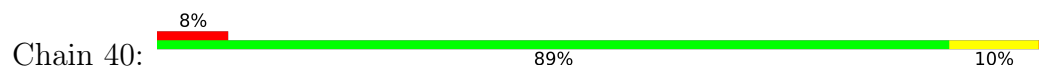
- Molecule 26: Fucoxanthin chlorophyll a/c-binding protein monomer 1



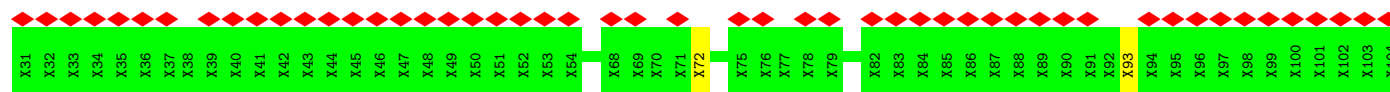
- Molecule 27: Fucoxanthin chlorophyll a/c-binding protein monomer 2



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

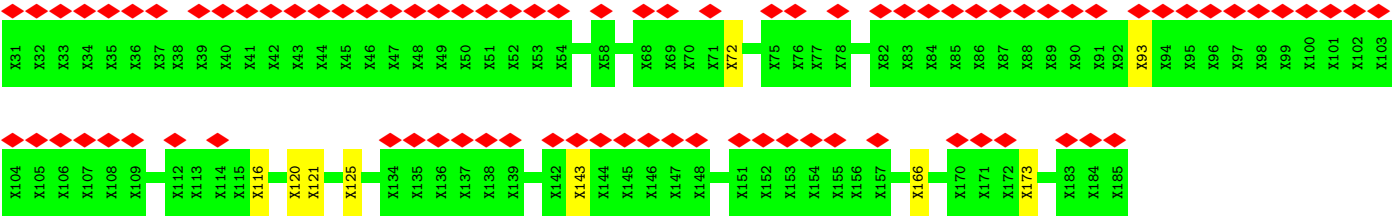


- Molecule 28: Fucoxanthin chlorophyll a/c-binding protein monomer 3



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	98936	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.218	Depositor
Minimum map value	-0.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	573.44, 573.44, 573.44	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.53	0/2701	0.61	0/3682
1	a	0.53	0/2701	0.61	0/3682
2	B	0.52	0/3942	0.60	1/5362 (0.0%)
2	b	0.52	0/3942	0.60	1/5362 (0.0%)
3	C	0.52	0/3620	0.63	2/4933 (0.0%)
3	c	0.52	0/3620	0.63	2/4933 (0.0%)
4	D	0.53	0/2789	0.61	0/3803
4	d	0.52	0/2789	0.61	0/3803
5	E	0.36	0/634	0.55	0/864
5	e	0.36	0/634	0.55	0/864
6	F	0.45	0/235	0.80	0/316
6	f	0.45	0/235	0.80	0/316
7	H	0.44	0/523	0.60	0/714
7	h	0.43	0/523	0.60	0/714
8	I	0.55	0/294	0.78	0/397
8	i	0.55	0/294	0.77	0/397
9	J	0.35	0/260	0.52	0/351
9	j	0.35	0/260	0.53	0/351
10	K	0.49	0/313	1.00	2/429 (0.5%)
10	k	0.49	0/313	1.00	2/429 (0.5%)
11	L	0.52	0/319	0.53	0/433
11	l	0.52	0/319	0.53	0/433
12	M	0.46	0/321	0.67	0/433
12	m	0.46	0/321	0.67	0/433
13	O	0.37	0/1875	0.61	2/2528 (0.1%)
13	o	0.37	0/1875	0.61	2/2528 (0.1%)
14	T	0.38	0/256	0.54	0/346
14	t	0.38	0/256	0.54	0/346
15	U	0.32	0/728	0.62	0/989
15	u	0.32	0/728	0.62	0/989
16	V	0.39	0/1056	0.57	0/1435
16	v	0.39	0/1056	0.57	0/1435

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.29	0/252	0.53	0/341
17	y	0.29	0/252	0.54	0/341
18	X	0.29	0/263	0.52	0/355
18	x	0.29	0/263	0.51	0/355
19	Z	0.35	0/456	0.55	0/624
19	z	0.35	0/456	0.56	0/624
20	Q	0.31	0/1099	0.56	0/1482
20	q	0.30	0/1099	0.56	0/1482
21	W	0.50	0/434	0.66	0/590
21	w	0.50	0/434	0.66	0/590
25	11	0.36	0/1373	0.58	0/1861
25	12	0.36	0/1373	0.58	0/1861
25	13	0.36	0/1373	0.58	0/1861
25	14	0.36	0/1373	0.59	0/1861
25	15	0.24	0/1373	0.50	0/1861
25	16	0.36	0/1373	0.66	0/1861
25	17	0.34	0/1373	0.59	0/1861
25	18	0.26	0/1373	0.53	0/1861
25	31	0.40	0/1373	0.60	0/1861
25	32	0.40	0/1373	0.60	0/1861
25	33	0.40	0/1373	0.60	0/1861
25	34	0.40	0/1373	0.60	0/1861
25	35	0.24	0/1373	0.50	0/1861
25	36	0.36	0/1373	0.66	0/1861
25	37	0.34	0/1373	0.59	0/1861
25	38	0.26	0/1373	0.53	0/1861
All	All	0.43	0/66708	0.60	14/90590 (0.0%)

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

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

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	k	25	ILE	CA-C-N	8.78	125.77	120.24
10	k	25	ILE	C-N-CA	8.78	125.77	120.24
10	K	25	ILE	CA-C-N	8.70	125.72	120.24
10	K	25	ILE	C-N-CA	8.70	125.72	120.24
3	C	252	THR	CA-C-N	6.61	137.15	122.67

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2618	0	2520	37	0
1	a	2618	0	2520	39	0
2	B	3812	0	3690	55	0
2	b	3812	0	3690	56	0
3	C	3504	0	3409	62	0
3	c	3504	0	3409	66	0
4	D	2697	0	2596	42	0
4	d	2697	0	2596	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	616	0	602	5	0
5	e	616	0	602	4	0
6	F	228	0	234	5	0
6	f	228	0	234	6	0
7	H	513	0	541	7	0
7	h	513	0	541	6	0
8	I	287	0	306	9	0
8	i	287	0	306	3	0
9	J	254	0	266	4	0
9	j	254	0	266	2	0
10	K	302	0	316	4	0
10	k	302	0	316	5	0
11	L	310	0	313	7	0
11	l	310	0	313	8	0
12	M	316	0	319	6	0
12	m	316	0	319	5	0
13	O	1845	0	1841	40	0
13	o	1845	0	1841	41	0
14	T	250	0	268	2	0
14	t	250	0	268	4	0
15	U	713	0	715	11	0
15	u	713	0	715	9	0
16	V	1037	0	1033	14	0
16	v	1037	0	1033	13	0
17	Y	250	0	287	8	0
17	y	250	0	287	6	0
18	X	263	0	301	3	0
18	x	263	0	301	0	0
19	Z	447	0	489	6	0
19	z	447	0	489	8	0
20	Q	1079	0	1068	17	0
20	q	1079	0	1068	17	0
21	W	422	0	377	8	0
21	w	422	0	377	6	0
22	0	155	0	34	0	0
22	5	155	0	34	1	0
23	1	150	0	34	1	0
23	6	150	0	34	1	0
24	2	50	0	12	4	0
24	7	50	0	12	4	0
25	11	1343	0	1306	40	0
25	12	1343	0	1304	43	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	13	1343	0	1306	47	0
25	14	1343	0	1306	35	0
25	15	1343	0	1306	41	0
25	16	1343	0	1306	43	0
25	17	1343	0	1306	52	0
25	18	1343	0	1305	58	0
25	31	1343	0	1306	38	0
25	32	1343	0	1306	45	0
25	33	1343	0	1306	35	0
25	34	1343	0	1306	26	0
25	35	1343	0	1306	44	0
25	36	1343	0	1306	41	0
25	37	1343	0	1306	47	0
25	38	1343	0	1305	60	0
26	19	1075	0	223	20	0
26	39	1075	0	224	20	0
27	20	715	0	148	14	0
27	40	715	0	148	14	0
28	21	775	0	158	11	0
28	41	775	0	158	11	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	11	530	0	486	24	0
30	12	595	0	555	37	0
30	13	465	0	414	31	0
30	14	530	0	486	25	0
30	15	465	0	414	22	0
30	16	465	0	412	34	0
30	17	485	0	451	40	0
30	18	595	0	558	52	0
30	19	400	0	341	14	0
30	20	420	0	378	16	0
30	21	485	0	452	32	0
30	31	530	0	486	20	0
30	32	530	0	484	37	0
30	33	530	0	486	25	0
30	34	530	0	486	20	0
30	35	465	0	414	20	0
30	36	465	0	412	36	0
30	37	485	0	451	38	0
30	38	595	0	558	53	0
30	39	400	0	341	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	40	420	0	378	21	0
30	41	485	0	452	31	0
30	A	130	0	144	11	0
30	B	1040	0	1152	49	0
30	C	1040	0	1152	55	0
30	D	260	0	288	10	0
30	M	65	0	67	1	0
30	W	130	0	144	10	0
30	Z	65	0	68	10	0
30	a	130	0	144	8	0
30	b	1040	0	1152	49	0
30	c	1040	0	1149	55	0
30	d	260	0	288	9	0
30	m	65	0	67	5	0
30	w	130	0	144	7	0
30	z	65	0	72	3	0
31	A	64	0	74	1	0
31	D	64	0	74	2	0
31	d	128	0	148	3	0
32	A	80	0	112	2	0
32	B	160	0	224	14	0
32	C	80	0	112	4	0
32	F	40	0	56	2	0
32	H	40	0	56	3	0
32	Y	40	0	56	4	0
32	Z	40	0	56	1	0
32	a	80	0	112	3	0
32	b	120	0	168	7	0
32	c	160	0	224	11	0
32	f	40	0	56	2	0
32	h	40	0	56	4	0
32	m	40	0	56	2	0
33	A	54	0	77	0	0
33	B	37	0	37	0	0
33	L	54	0	77	3	0
33	a	54	0	77	0	0
33	b	37	0	37	1	0
33	l	54	0	77	3	0
34	A	4	0	0	1	0
34	a	4	0	0	2	0
35	A	46	0	65	5	0
35	B	49	0	74	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	L	98	0	148	7	0
35	a	46	0	65	7	0
35	b	49	0	74	2	0
35	d	49	0	74	2	0
35	l	49	0	74	3	0
36	12	39	0	46	2	0
36	32	39	0	46	7	0
36	B	102	0	143	6	0
36	D	51	0	72	2	0
36	M	40	0	50	6	0
36	Q	51	0	72	1	0
36	W	51	0	72	5	0
36	b	102	0	143	3	0
36	c	51	0	72	1	0
36	d	51	0	72	1	0
36	m	40	0	50	1	0
36	w	51	0	72	4	0
37	C	10	0	0	0	0
37	c	10	0	0	1	0
38	C	124	0	162	1	0
38	H	62	0	82	3	0
38	J	62	0	82	2	0
38	c	124	0	162	0	0
38	h	62	0	82	3	0
38	j	62	0	82	1	0
39	D	110	0	157	6	0
39	d	110	0	157	7	0
40	E	43	0	30	1	0
40	V	43	0	30	2	0
40	e	43	0	30	2	0
40	v	43	0	30	2	0
41	11	288	0	0	30	0
41	12	288	0	0	33	0
41	13	384	0	0	68	0
41	14	192	0	0	21	0
41	15	336	0	0	39	0
41	16	192	0	0	25	0
41	17	336	0	0	60	0
41	18	192	0	0	32	0
41	19	144	0	0	23	0
41	20	240	0	0	41	0
41	21	240	0	0	46	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	31	288	0	0	32	0
41	32	336	0	0	30	0
41	33	336	0	0	42	0
41	34	192	0	0	16	0
41	35	336	0	0	41	0
41	36	192	0	0	24	0
41	37	336	0	0	57	0
41	38	192	0	0	33	0
41	39	144	0	0	23	0
41	40	240	0	0	44	0
41	41	240	0	0	45	0
42	12	32	0	34	0	0
42	32	32	0	37	15	0
All	All	96390	0	85682	2088	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 2088 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:21:303:CLA:H11	41:21:314:A86:C4	1.30	1.61
30:41:303:CLA:H11	41:41:314:A86:C4	1.21	1.60
30:18:303:CLA:H61	41:18:314:A86:C29	1.29	1.60
42:32:302:LMU:H6D	30:32:306:CLA:CED	1.24	1.58
30:36:308:CLA:HAB	41:37:302:A86:C3	1.12	1.57

There are no symmetry-related clashes.

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%)	321 (97%)	11 (3%)	0	100	100
1	a	332/344 (96%)	322 (97%)	10 (3%)	0	100	100
2	B	482/509 (95%)	467 (97%)	15 (3%)	0	100	100
2	b	482/509 (95%)	466 (97%)	16 (3%)	0	100	100
3	C	449/471 (95%)	429 (96%)	20 (4%)	0	100	100
3	c	449/471 (95%)	429 (96%)	20 (4%)	0	100	100
4	D	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
4	d	339/351 (97%)	324 (96%)	15 (4%)	0	100	100
5	E	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
5	e	73/84 (87%)	72 (99%)	1 (1%)	0	100	100
6	F	26/43 (60%)	26 (100%)	0	0	100	100
6	f	26/43 (60%)	26 (100%)	0	0	100	100
7	H	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
7	h	64/67 (96%)	62 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
9	J	32/39 (82%)	32 (100%)	0	0	100	100
9	j	32/39 (82%)	32 (100%)	0	0	100	100
10	K	35/44 (80%)	35 (100%)	0	0	100	100
10	k	35/44 (80%)	35 (100%)	0	0	100	100
11	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	l	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	M	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
12	m	40/131 (30%)	37 (92%)	3 (8%)	0	100	100
13	O	243/248 (98%)	231 (95%)	12 (5%)	0	100	100
13	o	243/248 (98%)	231 (95%)	12 (5%)	0	100	100
14	T	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
14	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
15	U	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
15	u	91/93 (98%)	85 (93%)	6 (7%)	0	100	100
16	V	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
16	v	134/137 (98%)	126 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
17	y	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
18	X	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
18	x	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
19	Z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
19	z	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
20	Q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
20	q	135/155 (87%)	126 (93%)	9 (7%)	0	100	100
21	W	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
21	w	50/72 (69%)	46 (92%)	4 (8%)	0	100	100
25	11	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	12	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	13	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	14	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	15	174/207 (84%)	163 (94%)	11 (6%)	0	100	100
25	16	174/207 (84%)	159 (91%)	15 (9%)	0	100	100
25	17	174/207 (84%)	162 (93%)	12 (7%)	0	100	100
25	18	174/207 (84%)	165 (95%)	8 (5%)	1 (1%)	21	54
25	31	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	32	174/207 (84%)	168 (97%)	6 (3%)	0	100	100
25	33	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	34	174/207 (84%)	167 (96%)	7 (4%)	0	100	100
25	35	174/207 (84%)	163 (94%)	11 (6%)	0	100	100
25	36	174/207 (84%)	159 (91%)	15 (9%)	0	100	100
25	37	174/207 (84%)	162 (93%)	12 (7%)	0	100	100
25	38	174/207 (84%)	165 (95%)	8 (5%)	1 (1%)	21	54
All	All	8276/9368 (88%)	7903 (96%)	371 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/280 (97%)	272 (100%)	0	100	100
1	a	272/280 (97%)	272 (100%)	0	100	100
2	B	385/405 (95%)	385 (100%)	0	100	100
2	b	385/405 (95%)	385 (100%)	0	100	100
3	C	356/376 (95%)	354 (99%)	2 (1%)	78	79
3	c	356/376 (95%)	354 (99%)	2 (1%)	78	79
4	D	273/281 (97%)	273 (100%)	0	100	100
4	d	273/281 (97%)	273 (100%)	0	100	100
5	E	69/75 (92%)	68 (99%)	1 (1%)	59	70
5	e	69/75 (92%)	68 (99%)	1 (1%)	59	70
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%)	55 (100%)	0	100	100
7	h	55/56 (98%)	55 (100%)	0	100	100
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%)	32 (100%)	0	100	100
10	k	32/38 (84%)	32 (100%)	0	100	100
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%)	196 (100%)	0	100	100
13	o	196/201 (98%)	196 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	27 (100%)	0	100	100
15	U	77/77 (100%)	77 (100%)	0	100	100
15	u	77/77 (100%)	77 (100%)	0	100	100
16	V	114/115 (99%)	114 (100%)	0	100	100
16	v	114/115 (99%)	114 (100%)	0	100	100
17	Y	27/27 (100%)	27 (100%)	0	100	100
17	y	27/27 (100%)	27 (100%)	0	100	100
18	X	29/30 (97%)	29 (100%)	0	100	100
18	x	29/30 (97%)	29 (100%)	0	100	100
19	Z	48/50 (96%)	48 (100%)	0	100	100
19	z	48/50 (96%)	48 (100%)	0	100	100
20	Q	111/124 (90%)	110 (99%)	1 (1%)	70	74
20	q	111/124 (90%)	110 (99%)	1 (1%)	70	74
21	W	43/55 (78%)	42 (98%)	1 (2%)	44	63
21	w	43/55 (78%)	42 (98%)	1 (2%)	44	63
25	11	138/158 (87%)	137 (99%)	1 (1%)	76	77
25	12	138/158 (87%)	137 (99%)	1 (1%)	76	77
25	13	138/158 (87%)	137 (99%)	1 (1%)	76	77
25	14	138/158 (87%)	137 (99%)	1 (1%)	76	77
25	15	138/158 (87%)	138 (100%)	0	100	100
25	16	138/158 (87%)	137 (99%)	1 (1%)	76	77
25	17	138/158 (87%)	137 (99%)	1 (1%)	76	77
25	18	138/158 (87%)	138 (100%)	0	100	100
25	31	138/158 (87%)	137 (99%)	1 (1%)	76	77
25	32	138/158 (87%)	137 (99%)	1 (1%)	76	77
25	33	138/158 (87%)	137 (99%)	1 (1%)	76	77
25	34	138/158 (87%)	137 (99%)	1 (1%)	76	77
25	35	138/158 (87%)	138 (100%)	0	100	100
25	36	138/158 (87%)	137 (99%)	1 (1%)	76	77
25	37	138/158 (87%)	137 (99%)	1 (1%)	76	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	38	138/158 (87%)	138 (100%)	0	100	100
All	All	6732/7448 (90%)	6710 (100%)	22 (0%)	84	84

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	16	128	GLU
25	32	91	LEU
25	31	91	LEU
25	33	91	LEU
3	c	270	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
25	15	82	ASN
25	31	82	ASN
25	15	161	ASN
25	17	161	ASN
25	33	82	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	BCR	a	404	-	41,41,41	1.29	2 (4%)	56,56,56	1.40	6 (10%)
30	CLA	B	610	-	69,73,73	1.33	11 (15%)	83,113,113	1.43	7 (8%)
30	CLA	B	609	2	69,73,73	1.24	10 (14%)	83,113,113	1.42	9 (10%)
41	A86	12	316	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
32	BCR	Y	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.47	9 (16%)
30	CLA	39	307	-	49,53,73	1.47	11 (22%)	59,89,113	1.60	7 (11%)
30	CLA	15	309	-	49,53,73	1.48	10 (20%)	59,89,113	1.47	6 (10%)
30	CLA	11	301	25	69,73,73	1.28	9 (13%)	83,113,113	1.57	9 (10%)
30	CLA	12	312	25	69,73,73	1.28	11 (15%)	83,113,113	1.38	6 (7%)
30	CLA	17	303	25	69,73,73	1.27	10 (14%)	83,113,113	1.53	8 (9%)
30	CLA	35	307	25	69,73,73	1.27	11 (15%)	83,113,113	1.51	12 (14%)
35	LHG	L	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
30	CLA	34	310	-	49,53,73	1.47	10 (20%)	59,89,113	1.53	6 (10%)
30	CLA	35	304	25	49,53,73	1.48	8 (16%)	59,89,113	1.60	10 (16%)
30	CLA	41	308	-	49,53,73	1.48	8 (16%)	59,89,113	1.51	6 (10%)
30	CLA	18	304	25	49,53,73	1.45	9 (18%)	59,89,113	1.65	7 (11%)
41	A86	38	314	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
40	HEM	V	201	16	50,50,50	1.32	5 (10%)	66,82,82	1.30	9 (13%)
31	PHO	d	404	-	58,69,69	1.91	12 (20%)	56,99,99	1.78	8 (14%)
32	BCR	H	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.31	7 (12%)
41	A86	37	315	-	44,50,50	4.06	23 (52%)	51,76,76	8.44	16 (31%)
32	BCR	c	520	-	41,41,41	1.28	3 (7%)	56,56,56	1.46	10 (17%)
30	CLA	19	304	26	49,53,73	1.47	9 (18%)	59,89,113	1.67	12 (20%)
30	CLA	40	207	-	49,53,73	1.49	11 (22%)	59,89,113	1.59	8 (13%)
30	CLA	D	405	4	69,73,73	1.33	12 (17%)	83,113,113	1.46	12 (14%)
36	LMG	c	519	-	51,51,55	0.97	5 (9%)	59,59,63	1.46	9 (15%)
30	CLA	13	310	-	49,53,73	1.48	10 (20%)	59,89,113	1.53	5 (8%)
30	CLA	35	303	25	69,73,73	1.22	9 (13%)	83,113,113	1.42	10 (12%)
32	BCR	c	521	-	41,41,41	1.27	2 (4%)	56,56,56	1.37	6 (10%)
30	CLA	20	206	27	49,53,73	1.48	10 (20%)	59,89,113	1.64	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	33	301	25	69,73,73	1.28	11 (15%)	83,113,113	1.40	6 (7%)
41	A86	13	313	-	44,50,50	4.05	24 (54%)	51,76,76	7.81	19 (37%)
36	LMG	m	102	30	40,40,55	0.95	3 (7%)	48,48,63	1.34	7 (14%)
36	LMG	w	101	-	51,51,55	0.89	3 (5%)	59,59,63	1.40	7 (11%)
30	CLA	14	310	-	49,53,73	1.48	10 (20%)	59,89,113	1.53	6 (10%)
41	A86	32	316	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
41	A86	32	319	-	44,50,50	3.93	23 (52%)	51,76,76	7.95	18 (35%)
38	DGD	c	518	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	16 (20%)
30	CLA	35	301	25	69,73,73	1.26	11 (15%)	83,113,113	1.51	10 (12%)
30	CLA	41	303	-	69,73,73	1.22	8 (11%)	83,113,113	1.33	6 (7%)
36	LMG	Q	301	-	51,51,55	0.97	4 (7%)	59,59,63	1.46	9 (15%)
41	A86	38	315	-	44,50,50	4.03	23 (52%)	51,76,76	8.23	20 (39%)
41	A86	33	312	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	21	304	-	49,53,73	1.45	9 (18%)	59,89,113	1.43	6 (10%)
32	BCR	c	516	-	41,41,41	1.31	5 (12%)	56,56,56	1.40	7 (12%)
30	CLA	c	522	-	69,73,73	1.25	11 (15%)	83,113,113	1.39	8 (9%)
41	A86	17	315	-	44,50,50	4.06	23 (52%)	51,76,76	8.44	16 (31%)
41	A86	35	312	-	44,50,50	4.04	24 (54%)	51,76,76	7.81	20 (39%)
30	CLA	32	310	25	49,53,73	1.46	10 (20%)	59,89,113	1.73	8 (13%)
41	A86	21	311	-	44,50,50	3.90	23 (52%)	51,76,76	7.51	15 (29%)
30	CLA	11	308	25	49,53,73	1.49	11 (22%)	59,89,113	1.60	7 (11%)
41	A86	35	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.93	18 (35%)
30	CLA	C	503	3	69,73,73	1.38	11 (15%)	83,113,113	1.46	12 (14%)
41	A86	19	311	-	44,50,50	4.00	21 (47%)	51,76,76	8.15	18 (35%)
30	CLA	32	309	-	49,53,73	1.45	10 (20%)	59,89,113	1.53	7 (11%)
30	CLA	20	208	-	49,53,73	1.48	9 (18%)	59,89,113	1.56	8 (13%)
41	A86	11	314	-	44,50,50	3.92	23 (52%)	51,76,76	7.97	19 (37%)
30	CLA	20	204	-	69,73,73	1.23	10 (14%)	83,113,113	1.43	9 (10%)
30	CLA	33	311	-	49,53,73	1.47	10 (20%)	59,89,113	1.53	5 (8%)
30	CLA	41	301	28	69,73,73	1.25	10 (14%)	83,113,113	1.32	4 (4%)
30	CLA	b	608	2	69,73,73	1.24	9 (13%)	83,113,113	1.38	7 (8%)
30	CLA	38	312	-	49,53,73	1.47	9 (18%)	59,89,113	1.47	6 (10%)
36	LMG	B	619	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	9 (15%)
30	CLA	20	207	-	49,53,73	1.49	11 (22%)	59,89,113	1.58	8 (13%)
30	CLA	21	306	-	69,73,73	1.25	8 (11%)	83,113,113	1.35	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	DGD	H	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.41	8 (10%)
41	A86	37	312	-	44,50,50	3.98	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	38	301	25	69,73,73	1.25	10 (14%)	83,113,113	1.35	9 (10%)
41	A86	36	310	-	44,50,50	3.97	23 (52%)	51,76,76	8.08	20 (39%)
30	CLA	Z	102	30,19	69,73,73	1.26	8 (11%)	83,113,113	1.33	8 (9%)
30	CLA	11	305	-	49,53,73	1.46	10 (20%)	59,89,113	1.55	7 (11%)
30	CLA	17	309	25	49,53,73	1.51	11 (22%)	59,89,113	1.90	11 (18%)
30	CLA	34	302	25	69,73,73	1.28	10 (14%)	83,113,113	1.58	9 (10%)
30	CLA	31	305	-	49,53,73	1.45	10 (20%)	59,89,113	1.54	7 (11%)
30	CLA	32	306	25	49,53,73	1.46	11 (22%)	59,89,113	1.62	9 (15%)
30	CLA	39	304	26	49,53,73	1.46	9 (18%)	59,89,113	1.67	11 (18%)
41	A86	12	315	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)
41	A86	21	314	-	44,50,50	4.01	23 (52%)	51,76,76	7.82	18 (35%)
30	CLA	38	308	25	49,53,73	1.50	9 (18%)	59,89,113	1.56	6 (10%)
37	OEX	C	501	1,3	0,14,14	-	-	-	-	-
38	DGD	C	517	-	63,63,67	1.25	10 (15%)	77,77,81	1.52	16 (20%)
36	LMG	M	102	30	40,40,55	0.96	3 (7%)	48,48,63	1.34	7 (14%)
41	A86	13	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
41	A86	18	314	-	44,50,50	3.98	23 (52%)	51,76,76	7.95	18 (35%)
35	LHG	b	621	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	6 (11%)
30	CLA	37	301	25	69,73,73	1.30	11 (15%)	83,113,113	1.43	9 (10%)
30	CLA	38	309	25	69,73,73	1.32	10 (14%)	83,113,113	1.50	11 (13%)
41	A86	21	310	-	44,50,50	3.88	22 (50%)	51,76,76	7.41	21 (41%)
30	CLA	37	308	25	69,73,73	1.31	8 (11%)	83,113,113	1.46	10 (12%)
41	A86	13	311	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)
41	A86	16	311	-	44,50,50	3.96	23 (52%)	51,76,76	7.93	18 (35%)
41	A86	16	313	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	B	608	2	69,73,73	1.24	9 (13%)	83,113,113	1.38	7 (8%)
30	CLA	34	307	25	49,53,73	1.46	10 (20%)	59,89,113	1.71	8 (13%)
41	A86	15	316	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	b	613	2	69,73,73	1.33	10 (14%)	83,113,113	1.49	9 (10%)
30	CLA	15	307	25	69,73,73	1.27	10 (14%)	83,113,113	1.51	12 (14%)
38	DGD	j	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
30	CLA	15	304	25	49,53,73	1.48	8 (16%)	59,89,113	1.61	10 (16%)
36	LMG	b	618	-	51,51,55	0.89	4 (7%)	59,59,63	1.43	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A86	35	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	33	310	25	49,53,73	1.49	11 (22%)	59,89,113	1.61	8 (13%)
30	CLA	b	610	-	69,73,73	1.33	11 (15%)	83,113,113	1.42	7 (8%)
30	CLA	19	303	-	69,73,73	1.24	9 (13%)	83,113,113	1.46	8 (9%)
30	CLA	d	406	4	69,73,73	1.33	12 (17%)	83,113,113	1.46	11 (13%)
41	A86	32	315	-	44,50,50	3.98	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	b	603	2	69,73,73	1.27	11 (15%)	83,113,113	1.51	11 (13%)
30	CLA	34	301	25	69,73,73	1.29	11 (15%)	83,113,113	1.38	7 (8%)
30	CLA	A	404	1	69,73,73	1.27	11 (15%)	83,113,113	1.50	9 (10%)
30	CLA	c	513	3	69,73,73	1.27	11 (15%)	83,113,113	1.38	7 (8%)
30	CLA	16	303	25	49,53,73	1.46	11 (22%)	59,89,113	1.79	10 (16%)
41	A86	17	312	-	44,50,50	3.98	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	41	305	28	49,53,73	1.53	8 (16%)	59,89,113	1.62	10 (16%)
41	A86	39	310	-	44,50,50	4.09	22 (50%)	51,76,76	7.17	19 (37%)
42	LMU	32	302	-	33,33,36	1.28	3 (9%)	44,44,47	1.57	8 (18%)
30	CLA	b	614	2	69,73,73	1.24	12 (17%)	83,113,113	1.47	8 (9%)
30	CLA	36	305	25	49,53,73	1.45	10 (20%)	59,89,113	1.70	11 (18%)
30	CLA	B	623	-	69,73,73	1.29	11 (15%)	83,113,113	1.50	13 (15%)
30	CLA	a	402	1	69,73,73	1.30	11 (15%)	83,113,113	1.45	8 (9%)
30	CLA	d	407	4	69,73,73	1.25	11 (15%)	83,113,113	1.52	7 (8%)
30	CLA	18	312	-	49,53,73	1.47	9 (18%)	59,89,113	1.47	6 (10%)
32	BCR	b	617	-	41,41,41	1.23	2 (4%)	56,56,56	1.41	10 (17%)
30	CLA	B	613	2	69,73,73	1.33	10 (14%)	83,113,113	1.46	11 (13%)
30	CLA	c	523	-	69,73,73	1.25	10 (14%)	83,113,113	1.56	12 (14%)
30	CLA	31	315	25	69,73,73	1.29	11 (15%)	83,113,113	1.40	6 (7%)
38	DGD	J	101	-	63,63,67	1.10	10 (15%)	77,77,81	1.55	15 (19%)
30	CLA	16	309	-	49,53,73	1.49	11 (22%)	59,89,113	1.48	8 (13%)
35	LHG	l	102	-	48,48,48	0.76	1 (2%)	51,54,54	1.31	6 (11%)
30	CLA	18	301	25	69,73,73	1.25	10 (14%)	83,113,113	1.36	9 (10%)
41	A86	31	314	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	18 (35%)
30	CLA	36	301	25	69,73,73	1.25	9 (13%)	83,113,113	1.36	8 (9%)
30	CLA	17	308	25	69,73,73	1.32	8 (11%)	83,113,113	1.46	10 (12%)
30	CLA	c	504	3	69,73,73	1.28	11 (15%)	83,113,113	1.44	9 (10%)
30	CLA	C	511	3	69,73,73	1.36	12 (17%)	83,113,113	1.44	12 (14%)
32	BCR	B	618	-	41,41,41	1.24	2 (4%)	56,56,56	1.41	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	33	307	-	49,53,73	1.46	10 (20%)	59,89,113	1.57	7 (11%)
30	CLA	40	206	27	49,53,73	1.48	10 (20%)	59,89,113	1.63	8 (13%)
30	CLA	21	305	28	49,53,73	1.52	8 (16%)	59,89,113	1.61	10 (16%)
30	CLA	B	604	2	69,73,73	1.34	10 (14%)	83,113,113	1.55	15 (18%)
30	CLA	40	202	-	69,73,73	1.24	9 (13%)	83,113,113	1.33	9 (10%)
30	CLA	b	604	2	69,73,73	1.34	10 (14%)	83,113,113	1.57	15 (18%)
30	CLA	19	308	-	49,53,73	1.45	9 (18%)	59,89,113	1.63	10 (16%)
41	A86	15	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	c	524	30	69,73,73	1.26	8 (11%)	83,113,113	1.33	8 (9%)
30	CLA	12	314	-	49,53,73	1.48	10 (20%)	59,89,113	1.52	6 (10%)
41	A86	32	304	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	21 (41%)
33	SQD	b	620	-	36,37,54	1.20	7 (19%)	45,48,65	1.64	9 (20%)
41	A86	14	313	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
30	CLA	C	513	3	69,73,73	1.26	10 (14%)	83,113,113	1.37	7 (8%)
30	CLA	21	302	-	49,53,73	1.49	10 (20%)	59,89,113	1.57	9 (15%)
30	CLA	w	103	-	69,73,73	1.26	8 (11%)	83,113,113	1.30	7 (8%)
30	CLA	B	614	2	69,73,73	1.24	12 (17%)	83,113,113	1.46	8 (9%)
30	CLA	19	305	-	49,53,73	1.47	11 (22%)	59,89,113	1.55	5 (8%)
30	CLA	36	309	-	49,53,73	1.50	11 (22%)	59,89,113	1.48	8 (13%)
30	CLA	20	209	30	69,73,73	1.26	9 (13%)	83,113,113	1.35	10 (12%)
41	A86	37	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	18 (35%)
40	HEM	e	101	6,5	50,50,50	1.35	5 (10%)	66,82,82	1.16	4 (6%)
41	A86	34	311	-	44,50,50	3.93	23 (52%)	51,76,76	8.32	17 (33%)
32	BCR	B	617	-	41,41,41	1.20	2 (4%)	56,56,56	1.36	9 (16%)
30	CLA	c	507	3	69,73,73	1.30	10 (14%)	83,113,113	1.45	12 (14%)
30	CLA	B	606	2	69,73,73	1.37	13 (18%)	83,113,113	1.50	13 (15%)
30	CLA	C	520	-	69,73,73	1.24	11 (15%)	83,113,113	1.40	8 (9%)
30	CLA	C	509	3	69,73,73	1.33	10 (14%)	83,113,113	1.53	10 (12%)
41	A86	40	210	-	44,50,50	4.07	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	12	310	25	49,53,73	1.46	8 (16%)	59,89,113	1.70	9 (15%)
41	A86	31	312	-	44,50,50	4.04	23 (52%)	51,76,76	7.82	20 (39%)
30	CLA	41	306	-	69,73,73	1.24	8 (11%)	83,113,113	1.36	8 (9%)
30	CLA	C	521	-	69,73,73	1.25	10 (14%)	83,113,113	1.57	12 (14%)
30	CLA	36	306	25	49,53,73	1.48	9 (18%)	59,89,113	1.62	6 (10%)
30	CLA	C	519	-	69,73,73	1.28	11 (15%)	83,113,113	1.41	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	c	509	3	69,73,73	1.33	10 (14%)	83,113,113	1.53	11 (13%)
31	PHO	d	403	-	58,69,69	1.97	13 (22%)	56,99,99	1.84	9 (16%)
30	CLA	c	508	-	69,73,73	1.30	11 (15%)	83,113,113	1.54	13 (15%)
41	A86	39	311	-	44,50,50	4.00	21 (47%)	51,76,76	8.15	18 (35%)
30	CLA	36	303	25	49,53,73	1.46	11 (22%)	59,89,113	1.79	10 (16%)
30	CLA	35	305	-	49,53,73	1.48	9 (18%)	59,89,113	1.52	5 (8%)
30	CLA	C	508	-	69,73,73	1.30	10 (14%)	83,113,113	1.56	13 (15%)
30	CLA	18	310	25	69,73,73	1.27	10 (14%)	83,113,113	1.34	7 (8%)
41	A86	35	313	-	44,50,50	4.03	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	b	602	2	69,73,73	1.27	9 (13%)	83,113,113	1.41	10 (12%)
30	CLA	16	307	25	49,53,73	1.51	11 (22%)	59,89,113	1.75	9 (15%)
36	LMG	B	620	-	51,51,55	0.99	5 (9%)	59,59,63	1.44	8 (13%)
41	A86	36	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	15	303	25	69,73,73	1.22	9 (13%)	83,113,113	1.42	9 (10%)
30	CLA	C	504	3	69,73,73	1.29	11 (15%)	83,113,113	1.45	9 (10%)
30	CLA	31	308	25	49,53,73	1.50	11 (22%)	59,89,113	1.62	8 (13%)
33	SQD	l	101	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
30	CLA	13	309	25	49,53,73	1.49	11 (22%)	59,89,113	1.60	7 (11%)
30	CLA	18	309	25	69,73,73	1.32	10 (14%)	83,113,113	1.49	11 (13%)
30	CLA	12	306	42,25	49,53,73	1.45	11 (22%)	59,89,113	1.61	7 (11%)
30	CLA	16	305	25	49,53,73	1.45	9 (18%)	59,89,113	1.71	11 (18%)
30	CLA	m	101	12,2,36	69,73,73	1.25	11 (15%)	83,113,113	1.29	6 (7%)
30	CLA	D	402	-	69,73,73	1.27	9 (13%)	83,113,113	1.41	7 (8%)
30	CLA	37	307	25	49,53,73	1.49	9 (18%)	59,89,113	1.65	13 (22%)
41	A86	32	318	-	44,50,50	3.93	23 (52%)	51,76,76	7.98	19 (37%)
41	A86	15	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.93	18 (35%)
30	CLA	36	302	25	69,73,73	1.30	9 (13%)	83,113,113	1.78	16 (19%)
30	CLA	21	303	-	69,73,73	1.22	8 (11%)	83,113,113	1.33	6 (7%)
30	CLA	40	203	30	49,53,73	1.48	9 (18%)	59,89,113	1.59	8 (13%)
41	A86	13	316	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	b	612	2	69,73,73	1.39	9 (13%)	83,113,113	1.66	11 (13%)
30	CLA	32	303	25	69,73,73	1.28	11 (15%)	83,113,113	1.38	7 (8%)
30	CLA	34	308	25	69,73,73	1.30	10 (14%)	83,113,113	1.47	12 (14%)
32	BCR	A	405	-	41,41,41	1.28	2 (4%)	56,56,56	1.40	6 (10%)
30	CLA	14	309	25	49,53,73	1.49	10 (20%)	59,89,113	1.59	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	15	302	25	49,53,73	1.46	8 (16%)	59,89,113	1.70	5 (8%)
30	CLA	16	301	25	69,73,73	1.25	9 (13%)	83,113,113	1.35	7 (8%)
41	A86	41	312	-	44,50,50	3.82	21 (47%)	51,76,76	7.17	21 (41%)
30	CLA	32	305	25	69,73,73	1.29	10 (14%)	83,113,113	1.58	9 (10%)
41	A86	16	312	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
30	CLA	38	307	-	49,53,73	1.48	10 (20%)	59,89,113	1.50	7 (11%)
42	LMU	12	302	30	33,33,36	1.30	3 (9%)	44,44,47	1.54	7 (15%)
30	CLA	18	308	25	49,53,73	1.51	9 (18%)	59,89,113	1.57	6 (10%)
30	CLA	c	512	3	69,73,73	1.32	11 (15%)	83,113,113	1.51	11 (13%)
30	CLA	b	611	2	69,73,73	1.34	11 (15%)	83,113,113	1.50	11 (13%)
32	BCR	B	624	-	41,41,41	1.13	3 (7%)	56,56,56	1.31	7 (12%)
41	A86	11	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
30	CLA	21	309	-	49,53,73	1.49	10 (20%)	59,89,113	1.54	9 (15%)
30	CLA	41	304	-	49,53,73	1.44	9 (18%)	59,89,113	1.44	6 (10%)
41	A86	11	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	16	304	25	69,73,73	1.23	10 (14%)	83,113,113	1.39	8 (9%)
30	CLA	39	301	-	69,73,73	1.31	11 (15%)	83,113,113	1.39	10 (12%)
30	CLA	31	303	25	69,73,73	1.23	11 (15%)	83,113,113	1.48	9 (10%)
30	CLA	W	103	-	69,73,73	1.26	9 (13%)	83,113,113	1.30	7 (8%)
30	CLA	15	306	25	49,53,73	1.47	9 (18%)	59,89,113	1.61	7 (11%)
30	CLA	41	307	-	69,73,73	1.23	8 (11%)	83,113,113	1.31	6 (7%)
41	A86	35	315	-	44,50,50	4.00	23 (52%)	51,76,76	7.59	20 (39%)
32	BCR	b	616	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	9 (16%)
41	A86	17	311	-	44,50,50	4.03	22 (50%)	51,76,76	8.33	19 (37%)
30	CLA	14	308	25	69,73,73	1.28	11 (15%)	83,113,113	1.45	12 (14%)
41	A86	17	313	-	44,50,50	4.06	23 (52%)	51,76,76	7.82	19 (37%)
30	CLA	21	301	28	69,73,73	1.25	10 (14%)	83,113,113	1.32	4 (4%)
30	CLA	c	503	3	69,73,73	1.38	11 (15%)	83,113,113	1.46	12 (14%)
30	CLA	38	306	25	49,53,73	1.47	7 (14%)	59,89,113	1.66	10 (16%)
41	A86	32	317	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
41	A86	11	316	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	20 (39%)
41	A86	14	311	-	44,50,50	3.93	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	17	301	25	69,73,73	1.30	11 (15%)	83,113,113	1.43	9 (10%)
30	CLA	31	309	-	49,53,73	1.47	10 (20%)	59,89,113	1.53	5 (8%)
30	CLA	31	302	25	49,53,73	1.44	11 (22%)	59,89,113	1.63	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A86	36	312	-	44,50,50	4.05	22 (50%)	51,76,76	7.81	19 (37%)
41	A86	34	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
30	CLA	12	307	25	69,73,73	1.25	11 (15%)	83,113,113	1.48	9 (10%)
30	CLA	16	306	25	49,53,73	1.48	9 (18%)	59,89,113	1.62	6 (10%)
35	LHG	A	408	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	7 (14%)
41	A86	20	213	-	44,50,50	4.01	23 (52%)	51,76,76	7.82	18 (35%)
30	CLA	c	502	3	69,73,73	1.26	11 (15%)	83,113,113	1.52	12 (14%)
30	CLA	40	208	-	49,53,73	1.48	8 (16%)	59,89,113	1.56	8 (13%)
30	CLA	12	305	25	69,73,73	1.27	10 (14%)	83,113,113	1.58	8 (9%)
41	A86	17	316	-	44,50,50	3.94	23 (52%)	51,76,76	7.98	18 (35%)
30	CLA	32	311	25	69,73,73	1.30	10 (14%)	83,113,113	1.46	12 (14%)
30	CLA	34	304	25	69,73,73	1.25	11 (15%)	83,113,113	1.49	9 (10%)
39	PL9	D	404	4	55,55,55	1.36	6 (10%)	68,69,69	1.49	14 (20%)
30	CLA	37	306	25	49,53,73	1.49	9 (18%)	59,89,113	1.77	13 (22%)
39	PL9	d	408	-	55,55,55	2.33	14 (25%)	68,69,69	1.49	15 (22%)
30	CLA	11	309	-	49,53,73	1.48	10 (20%)	59,89,113	1.51	5 (8%)
30	CLA	c	511	3	69,73,73	1.36	12 (17%)	83,113,113	1.45	13 (15%)
32	BCR	B	616	-	41,41,41	1.31	2 (4%)	56,56,56	1.39	7 (12%)
41	A86	12	319	-	44,50,50	3.93	23 (52%)	51,76,76	7.98	19 (37%)
30	CLA	40	204	-	69,73,73	1.23	11 (15%)	83,113,113	1.43	8 (9%)
41	A86	41	313	-	44,50,50	3.90	23 (52%)	51,76,76	7.52	22 (43%)
38	DGD	h	102	-	63,63,67	0.94	3 (4%)	77,77,81	1.42	7 (9%)
30	CLA	M	101	12,2,36	69,73,73	1.25	10 (14%)	83,113,113	1.29	6 (7%)
30	CLA	36	308	25	49,53,73	1.48	10 (20%)	59,89,113	1.57	10 (16%)
30	CLA	13	307	25	49,53,73	1.45	9 (18%)	59,89,113	1.71	7 (11%)
30	CLA	C	510	3	69,73,73	1.35	10 (14%)	83,113,113	1.60	12 (14%)
30	CLA	C	505	-	69,73,73	1.27	11 (15%)	83,113,113	1.57	10 (12%)
30	CLA	39	308	-	49,53,73	1.45	9 (18%)	59,89,113	1.62	10 (16%)
41	A86	12	304	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	20 (39%)
41	A86	40	213	-	44,50,50	4.02	23 (52%)	51,76,76	7.83	18 (35%)
30	CLA	34	306	-	49,53,73	1.46	11 (22%)	59,89,113	1.54	7 (11%)
30	CLA	32	307	25	69,73,73	1.24	11 (15%)	83,113,113	1.50	9 (10%)
41	A86	16	310	-	44,50,50	3.97	23 (52%)	51,76,76	8.08	20 (39%)
30	CLA	32	312	25	49,53,73	1.50	11 (22%)	59,89,113	1.60	8 (13%)
41	A86	15	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A86	13	301	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	A	402	1	69,73,73	1.30	11 (15%)	83,113,113	1.48	9 (10%)
38	DGD	c	517	-	63,63,67	1.06	8 (12%)	77,77,81	1.60	15 (19%)
30	CLA	W	102	21	69,73,73	1.26	10 (14%)	83,113,113	1.36	9 (10%)
30	CLA	11	315	25	69,73,73	1.27	11 (15%)	83,113,113	1.38	6 (7%)
30	CLA	12	309	-	49,53,73	1.44	9 (18%)	59,89,113	1.54	7 (11%)
30	CLA	35	309	-	49,53,73	1.48	9 (18%)	59,89,113	1.47	6 (10%)
30	CLA	14	303	25	49,53,73	1.44	11 (22%)	59,89,113	1.62	7 (11%)
30	CLA	21	308	-	49,53,73	1.48	8 (16%)	59,89,113	1.51	6 (10%)
41	A86	18	313	-	44,50,50	3.93	23 (52%)	51,76,76	8.34	17 (33%)
30	CLA	35	302	25	49,53,73	1.46	9 (18%)	59,89,113	1.71	6 (10%)
41	A86	34	313	-	44,50,50	4.05	22 (50%)	51,76,76	7.80	19 (37%)
30	CLA	13	303	25	49,53,73	1.46	11 (22%)	59,89,113	1.62	7 (11%)
30	CLA	35	308	25	49,53,73	1.48	10 (20%)	59,89,113	1.61	9 (15%)
30	CLA	b	609	2	69,73,73	1.24	10 (14%)	83,113,113	1.44	8 (9%)
41	A86	21	312	-	44,50,50	3.82	22 (50%)	51,76,76	7.17	21 (41%)
30	CLA	35	306	25	49,53,73	1.46	9 (18%)	59,89,113	1.61	7 (11%)
30	CLA	b	622	-	69,73,73	1.29	10 (14%)	83,113,113	1.50	13 (15%)
41	A86	39	309	-	44,50,50	3.88	23 (52%)	51,76,76	7.69	16 (31%)
33	SQD	L	103	-	53,54,54	0.93	5 (9%)	62,65,65	1.84	12 (19%)
30	CLA	33	305	25	69,73,73	1.24	11 (15%)	83,113,113	1.51	9 (10%)
30	CLA	B	603	2	69,73,73	1.25	10 (14%)	83,113,113	1.52	12 (14%)
41	A86	34	312	-	44,50,50	3.96	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	32	308	25,36	49,53,73	1.53	10 (20%)	59,89,113	1.88	16 (27%)
36	LMG	W	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.40	7 (11%)
30	CLA	14	302	25	69,73,73	1.27	10 (14%)	83,113,113	1.58	9 (10%)
30	CLA	w	102	21	69,73,73	1.25	10 (14%)	83,113,113	1.35	9 (10%)
41	A86	20	210	-	44,50,50	4.07	23 (52%)	51,76,76	8.31	17 (33%)
30	CLA	16	308	25	49,53,73	1.48	10 (20%)	59,89,113	1.57	10 (16%)
30	CLA	14	301	25	69,73,73	1.27	10 (14%)	83,113,113	1.37	6 (7%)
30	CLA	b	605	2	69,73,73	1.26	10 (14%)	83,113,113	1.41	8 (9%)
33	SQD	A	406	-	53,54,54	0.97	6 (11%)	62,65,65	1.58	11 (17%)
41	A86	33	314	-	44,50,50	4.05	22 (50%)	51,76,76	7.80	19 (37%)
30	CLA	14	306	-	49,53,73	1.46	10 (20%)	59,89,113	1.53	7 (11%)
41	A86	12	318	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	C	502	3	69,73,73	1.26	11 (15%)	83,113,113	1.52	12 (14%)
30	CLA	b	607	-	69,73,73	1.26	10 (14%)	83,113,113	1.41	9 (10%)
32	BCR	m	103	-	41,41,41	1.30	2 (4%)	56,56,56	1.39	8 (14%)
30	CLA	40	205	-	49,53,73	1.48	9 (18%)	59,89,113	1.65	12 (20%)
30	CLA	17	307	25	49,53,73	1.48	9 (18%)	59,89,113	1.63	13 (22%)
41	A86	33	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	38	311	25	49,53,73	1.49	9 (18%)	59,89,113	1.64	9 (15%)
41	A86	38	313	-	44,50,50	3.93	23 (52%)	51,76,76	8.33	17 (33%)
41	A86	31	316	-	44,50,50	3.99	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	12	303	25	69,73,73	1.27	10 (14%)	83,113,113	1.39	6 (7%)
30	CLA	31	304	25	49,53,73	1.53	9 (18%)	59,89,113	1.89	15 (25%)
41	A86	37	311	-	44,50,50	4.02	22 (50%)	51,76,76	8.33	19 (37%)
30	CLA	15	305	-	49,53,73	1.47	8 (16%)	59,89,113	1.52	5 (8%)
41	A86	20	201	-	44,50,50	3.93	22 (50%)	51,76,76	7.88	19 (37%)
30	CLA	34	303	25	49,53,73	1.44	11 (22%)	59,89,113	1.63	8 (13%)
30	CLA	33	303	25	69,73,73	1.29	11 (15%)	83,113,113	1.59	9 (10%)
30	CLA	11	306	25	49,53,73	1.45	8 (16%)	59,89,113	1.71	7 (11%)
41	A86	18	315	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	a	403	1	69,73,73	1.27	10 (14%)	83,113,113	1.50	9 (10%)
30	CLA	B	615	2	69,73,73	1.33	11 (15%)	83,113,113	1.38	11 (13%)
30	CLA	b	615	2	69,73,73	1.33	11 (15%)	83,113,113	1.38	11 (13%)
32	BCR	h	101	-	41,41,41	1.27	4 (9%)	56,56,56	1.32	7 (12%)
41	A86	31	313	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
41	A86	41	314	-	44,50,50	4.00	23 (52%)	51,76,76	7.82	18 (35%)
41	A86	32	314	-	44,50,50	3.92	23 (52%)	51,76,76	8.32	17 (33%)
30	CLA	12	311	25	69,73,73	1.28	10 (14%)	83,113,113	1.43	12 (14%)
36	LMG	32	301	30	39,39,55	1.00	4 (10%)	47,47,63	1.18	4 (8%)
30	CLA	20	203	30	49,53,73	1.48	9 (18%)	59,89,113	1.59	7 (11%)
30	CLA	13	305	25	49,53,73	1.51	10 (20%)	59,89,113	1.83	13 (22%)
41	A86	38	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.61	20 (39%)
30	CLA	17	304	25	49,53,73	1.46	12 (24%)	59,89,113	1.64	9 (15%)
41	A86	41	311	-	44,50,50	3.89	23 (52%)	51,76,76	7.51	15 (29%)
30	CLA	19	302	-	49,53,73	1.48	11 (22%)	59,89,113	1.65	10 (16%)
30	CLA	B	607	-	69,73,73	1.27	11 (15%)	83,113,113	1.43	9 (10%)
30	CLA	34	309	25	49,53,73	1.50	11 (22%)	59,89,113	1.62	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	33	309	25	69,73,73	1.30	10 (14%)	83,113,113	1.44	12 (14%)
30	CLA	11	304	25	49,53,73	1.51	10 (20%)	59,89,113	1.84	13 (22%)
30	CLA	33	306	25	49,53,73	1.54	10 (20%)	59,89,113	1.90	14 (23%)
30	CLA	39	306	-	49,53,73	1.47	11 (22%)	59,89,113	1.48	5 (8%)
41	A86	40	212	-	44,50,50	4.18	23 (52%)	51,76,76	8.23	15 (29%)
40	HEM	E	101	6,5	50,50,50	1.36	4 (8%)	66,82,82	1.15	4 (6%)
41	A86	12	317	-	44,50,50	4.04	22 (50%)	51,76,76	7.80	19 (37%)
36	LMG	b	619	-	51,51,55	0.99	5 (9%)	59,59,63	1.44	8 (13%)
30	CLA	33	308	25	49,53,73	1.46	10 (20%)	59,89,113	1.72	7 (11%)
41	A86	33	317	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	18 (35%)
41	A86	37	302	-	44,50,50	3.95	23 (52%)	51,76,76	8.11	21 (41%)
30	CLA	14	307	25	49,53,73	1.44	8 (16%)	59,89,113	1.70	8 (13%)
30	CLA	14	304	25	69,73,73	1.23	11 (15%)	83,113,113	1.49	9 (10%)
30	CLA	c	505	-	69,73,73	1.27	11 (15%)	83,113,113	1.58	10 (12%)
30	CLA	38	303	25	69,73,73	1.26	10 (14%)	83,113,113	1.41	8 (9%)
30	CLA	13	304	25	69,73,73	1.23	11 (15%)	83,113,113	1.47	9 (10%)
32	BCR	f	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.32	9 (16%)
30	CLA	14	305	25	49,53,73	1.50	10 (20%)	59,89,113	1.87	13 (22%)
30	CLA	D	406	4	69,73,73	1.25	11 (15%)	83,113,113	1.53	7 (8%)
30	CLA	19	307	-	49,53,73	1.47	11 (22%)	59,89,113	1.59	7 (11%)
30	CLA	38	305	25	69,73,73	1.22	9 (13%)	83,113,113	1.39	5 (6%)
32	BCR	C	515	-	41,41,41	1.30	4 (9%)	56,56,56	1.40	9 (16%)
39	PL9	d	405	4	55,55,55	1.36	6 (10%)	68,69,69	1.50	14 (20%)
30	CLA	36	304	25	69,73,73	1.24	10 (14%)	83,113,113	1.39	8 (9%)
41	A86	21	313	-	44,50,50	3.90	23 (52%)	51,76,76	7.51	22 (43%)
30	CLA	B	605	2	69,73,73	1.27	10 (14%)	83,113,113	1.42	8 (9%)
30	CLA	20	202	-	69,73,73	1.24	9 (13%)	83,113,113	1.32	9 (10%)
30	CLA	B	602	2	69,73,73	1.27	9 (13%)	83,113,113	1.41	9 (10%)
32	BCR	F	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
41	A86	11	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
35	LHG	B	622	-	48,48,48	0.74	1 (2%)	51,54,54	1.29	6 (11%)
41	A86	19	309	-	44,50,50	3.89	23 (52%)	51,76,76	7.70	16 (31%)
30	CLA	18	311	25	49,53,73	1.49	9 (18%)	59,89,113	1.65	9 (15%)
30	CLA	37	303	25	69,73,73	1.27	10 (14%)	83,113,113	1.53	8 (9%)
33	SQD	a	405	-	53,54,54	0.96	5 (9%)	62,65,65	1.58	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	A86	17	302	-	44,50,50	3.94	23 (52%)	51,76,76	8.11	21 (41%)
30	CLA	b	601	-	69,73,73	1.25	11 (15%)	83,113,113	1.43	8 (9%)
41	A86	15	314	-	44,50,50	3.93	23 (52%)	51,76,76	7.97	19 (37%)
30	CLA	B	612	2	69,73,73	1.38	9 (13%)	83,113,113	1.67	11 (13%)
32	BCR	c	515	-	41,41,41	1.34	3 (7%)	56,56,56	1.41	8 (14%)
36	LMG	d	410	-	51,51,55	0.89	3 (5%)	59,59,63	1.43	7 (11%)
35	LHG	a	407	-	45,45,48	0.78	2 (4%)	48,51,54	1.35	8 (16%)
30	CLA	31	307	25	69,73,73	1.29	10 (14%)	83,113,113	1.47	12 (14%)
41	A86	14	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.23	20 (39%)
31	PHO	A	403	-	58,69,69	1.98	13 (22%)	56,99,99	1.83	10 (17%)
34	BCT	A	407	1,29	2,3,3	1.26	0	2,3,3	3.93	2 (100%)
38	DGD	C	516	-	63,63,67	1.06	7 (11%)	77,77,81	1.60	15 (19%)
40	HEM	v	201	16	50,50,50	1.32	5 (10%)	66,82,82	1.29	7 (10%)
33	SQD	B	621	-	36,37,54	1.20	6 (16%)	45,48,65	1.64	9 (20%)
30	CLA	17	310	-	49,53,73	1.46	10 (20%)	59,89,113	1.49	6 (10%)
30	CLA	33	304	25	49,53,73	1.45	11 (22%)	59,89,113	1.63	9 (15%)
30	CLA	17	306	25	49,53,73	1.49	9 (18%)	59,89,113	1.77	13 (22%)
35	LHG	L	101	-	48,48,48	0.81	1 (2%)	51,54,54	1.26	5 (9%)
30	CLA	C	512	3	69,73,73	1.33	11 (15%)	83,113,113	1.53	11 (13%)
36	LMG	D	408	-	51,51,55	0.90	3 (5%)	59,59,63	1.42	7 (11%)
34	BCT	a	406	1,29	2,3,3	1.26	0	2,3,3	3.95	2 (100%)
30	CLA	34	305	25	49,53,73	1.54	10 (20%)	59,89,113	1.88	16 (27%)
30	CLA	B	611	2	69,73,73	1.34	11 (15%)	83,113,113	1.50	11 (13%)
41	A86	15	315	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	d	402	-	69,73,73	1.28	10 (14%)	83,113,113	1.42	7 (8%)
41	A86	36	313	-	44,50,50	3.94	23 (52%)	51,76,76	7.95	17 (33%)
30	CLA	b	606	2	69,73,73	1.37	12 (17%)	83,113,113	1.49	13 (15%)
30	CLA	31	301	25	69,73,73	1.28	11 (15%)	83,113,113	1.58	9 (10%)
30	CLA	41	302	-	49,53,73	1.48	9 (18%)	59,89,113	1.56	8 (13%)
30	CLA	13	302	25	69,73,73	1.27	11 (15%)	83,113,113	1.58	8 (9%)
30	CLA	16	302	25	69,73,73	1.29	9 (13%)	83,113,113	1.78	16 (19%)
39	PL9	D	407	-	55,55,55	2.32	15 (27%)	68,69,69	1.48	14 (20%)
30	CLA	18	307	-	49,53,73	1.47	9 (18%)	59,89,113	1.50	7 (11%)
30	CLA	c	506	3	69,73,73	1.26	9 (13%)	83,113,113	1.46	11 (13%)
30	CLA	13	306	-	49,53,73	1.45	10 (20%)	59,89,113	1.54	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	38	310	25	69,73,73	1.27	9 (13%)	83,113,113	1.33	7 (8%)
30	CLA	B	601	-	69,73,73	1.25	11 (15%)	83,113,113	1.41	8 (9%)
41	A86	15	312	-	44,50,50	4.05	24 (54%)	51,76,76	7.82	19 (37%)
30	CLA	18	303	25	69,73,73	1.26	10 (14%)	83,113,113	1.40	8 (9%)
30	CLA	12	308	25,36	49,53,73	1.51	10 (20%)	59,89,113	1.85	14 (23%)
41	A86	31	311	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
41	A86	40	211	-	44,50,50	3.89	23 (52%)	51,76,76	7.50	15 (29%)
30	CLA	39	305	-	49,53,73	1.47	11 (22%)	59,89,113	1.55	5 (8%)
30	CLA	c	514	3,30	69,73,73	1.27	11 (15%)	83,113,113	1.46	8 (9%)
41	A86	35	316	-	44,50,50	3.99	23 (52%)	51,76,76	7.59	20 (39%)
30	CLA	11	303	25	69,73,73	1.23	11 (15%)	83,113,113	1.48	9 (10%)
41	A86	17	314	-	44,50,50	4.02	23 (52%)	51,76,76	8.23	20 (39%)
41	A86	33	316	-	44,50,50	4.01	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	20	205	-	49,53,73	1.48	9 (18%)	59,89,113	1.66	12 (20%)
32	BCR	A	409	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	4 (7%)
41	A86	37	313	-	44,50,50	4.05	23 (52%)	51,76,76	7.81	19 (37%)
36	LMG	12	301	30	39,39,55	1.00	4 (10%)	47,47,63	1.21	4 (8%)
41	A86	20	212	-	44,50,50	4.18	23 (52%)	51,76,76	8.23	15 (29%)
30	CLA	37	310	-	49,53,73	1.46	10 (20%)	59,89,113	1.49	5 (8%)
30	CLA	15	301	25	69,73,73	1.26	11 (15%)	83,113,113	1.52	10 (12%)
31	PHO	D	403	-	58,69,69	1.91	12 (20%)	56,99,99	1.77	8 (14%)
41	A86	18	302	-	44,50,50	4.00	23 (52%)	51,76,76	7.60	20 (39%)
30	CLA	15	308	25	49,53,73	1.47	10 (20%)	59,89,113	1.60	9 (15%)
30	CLA	36	307	25	49,53,73	1.51	11 (22%)	59,89,113	1.74	9 (15%)
41	A86	11	312	-	44,50,50	4.04	23 (52%)	51,76,76	7.83	20 (39%)
41	A86	33	313	-	44,50,50	3.97	23 (52%)	51,76,76	7.94	18 (35%)
30	CLA	12	313	25	49,53,73	1.49	11 (22%)	59,89,113	1.60	6 (10%)
30	CLA	32	313	-	49,53,73	1.47	10 (20%)	59,89,113	1.53	6 (10%)
30	CLA	18	306	25	49,53,73	1.47	8 (16%)	59,89,113	1.66	10 (16%)
41	A86	13	315	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	18 (35%)
32	BCR	C	518	-	41,41,41	1.28	2 (4%)	56,56,56	1.36	6 (10%)
41	A86	13	317	-	44,50,50	3.94	23 (52%)	51,76,76	7.97	18 (35%)
30	CLA	31	306	25	49,53,73	1.46	11 (22%)	59,89,113	1.72	9 (15%)
30	CLA	19	301	-	69,73,73	1.31	11 (15%)	83,113,113	1.39	10 (12%)
41	A86	33	315	-	44,50,50	4.02	23 (52%)	51,76,76	8.22	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	37	304	25	49,53,73	1.47	12 (24%)	59,89,113	1.63	9 (15%)
30	CLA	19	306	-	49,53,73	1.48	11 (22%)	59,89,113	1.50	5 (8%)
30	CLA	d	401	-	69,73,73	1.33	9 (13%)	83,113,113	1.45	11 (13%)
30	CLA	37	305	25	69,73,73	1.22	11 (15%)	83,113,113	1.43	9 (10%)
41	A86	20	211	-	44,50,50	3.89	23 (52%)	51,76,76	7.49	15 (29%)
41	A86	14	312	-	44,50,50	3.97	23 (52%)	51,76,76	7.96	18 (35%)
30	CLA	11	302	25	49,53,73	1.46	11 (22%)	59,89,113	1.62	7 (11%)
30	CLA	D	401	-	69,73,73	1.33	9 (13%)	83,113,113	1.45	12 (14%)
41	A86	35	314	-	44,50,50	3.94	23 (52%)	51,76,76	7.96	19 (37%)
41	A86	41	310	-	44,50,50	3.88	22 (50%)	51,76,76	7.41	21 (41%)
41	A86	13	312	-	44,50,50	3.97	23 (52%)	51,76,76	7.95	18 (35%)
30	CLA	C	514	3,30	69,73,73	1.26	10 (14%)	83,113,113	1.47	8 (9%)
30	CLA	21	307	-	69,73,73	1.23	8 (11%)	83,113,113	1.32	6 (7%)
32	BCR	a	408	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
41	A86	40	201	-	44,50,50	3.93	22 (50%)	51,76,76	7.88	19 (37%)
35	LHG	d	409	-	48,48,48	0.81	1 (2%)	51,54,54	1.26	5 (9%)
30	CLA	39	302	-	49,53,73	1.50	11 (22%)	59,89,113	1.66	10 (16%)
32	BCR	b	623	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
30	CLA	37	309	25	49,53,73	1.51	11 (22%)	59,89,113	1.90	11 (18%)
30	CLA	38	304	25	49,53,73	1.46	10 (20%)	59,89,113	1.66	7 (11%)
30	CLA	11	307	25	69,73,73	1.28	10 (14%)	83,113,113	1.44	11 (13%)
41	A86	31	310	-	44,50,50	3.92	23 (52%)	51,76,76	8.33	17 (33%)
30	CLA	z	101	-	69,73,73	1.28	11 (15%)	83,113,113	1.43	8 (9%)
30	CLA	17	305	25	69,73,73	1.23	11 (15%)	83,113,113	1.43	9 (10%)
30	CLA	18	305	25	69,73,73	1.22	10 (14%)	83,113,113	1.37	5 (6%)
30	CLA	41	309	-	49,53,73	1.49	9 (18%)	59,89,113	1.55	9 (15%)
41	A86	19	310	-	44,50,50	4.09	21 (47%)	51,76,76	7.18	19 (37%)
30	CLA	C	507	3	69,73,73	1.30	10 (14%)	83,113,113	1.45	12 (14%)
32	BCR	Z	101	-	41,41,41	1.31	3 (7%)	56,56,56	1.41	8 (14%)
30	CLA	39	303	-	69,73,73	1.24	10 (14%)	83,113,113	1.46	8 (9%)
30	CLA	c	510	3	69,73,73	1.35	10 (14%)	83,113,113	1.60	12 (14%)
30	CLA	C	506	3	69,73,73	1.26	9 (13%)	83,113,113	1.46	11 (13%)
41	A86	37	314	-	44,50,50	4.01	23 (52%)	51,76,76	8.22	20 (39%)
30	CLA	40	209	30	69,73,73	1.26	10 (14%)	83,113,113	1.35	10 (12%)
30	CLA	13	308	25	69,73,73	1.27	10 (14%)	83,113,113	1.45	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	OEX	c	501	1,3	0,14,14	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	BCR	a	404	-	-	12/29/63/63	0/2/2/2
30	CLA	B	610	-	-	16/39/115/115	-
30	CLA	B	609	2	-	10/39/115/115	-
41	A86	12	316	-	-	3/34/90/90	0/3/3/3
32	BCR	Y	101	-	-	16/29/63/63	0/2/2/2
30	CLA	39	307	-	-	3/15/91/115	-
30	CLA	15	309	-	-	6/15/91/115	-
30	CLA	11	301	25	-	13/39/115/115	-
30	CLA	12	312	25	-	13/39/115/115	-
30	CLA	17	303	25	-	15/39/115/115	-
30	CLA	35	307	25	-	13/39/115/115	-
35	LHG	L	102	-	-	22/53/53/53	-
30	CLA	34	310	-	-	7/15/91/115	-
30	CLA	35	304	25	-	7/15/91/115	-
30	CLA	41	308	-	-	10/15/91/115	-
30	CLA	18	304	25	-	5/15/91/115	-
41	A86	38	314	-	-	3/34/90/90	0/3/3/3
40	HEM	V	201	16	-	1/14/54/54	-
31	PHO	d	404	-	-	8/37/103/103	0/5/6/6
32	BCR	H	101	-	-	7/29/63/63	0/2/2/2
41	A86	37	315	-	-	13/34/90/90	0/3/3/3
32	BCR	c	520	-	-	16/29/63/63	0/2/2/2
30	CLA	19	304	26	-	11/15/91/115	-
30	CLA	40	207	-	-	9/15/91/115	-
30	CLA	D	405	4	-	8/39/115/115	-
36	LMG	c	519	-	-	22/46/66/70	0/1/1/1
30	CLA	13	310	-	-	8/15/91/115	-
30	CLA	35	303	25	-	17/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	BCR	c	521	-	-	8/29/63/63	0/2/2/2
30	CLA	20	206	27	-	9/15/91/115	-
30	CLA	33	301	25	-	11/39/115/115	-
41	A86	13	313	-	-	8/34/90/90	0/3/3/3
36	LMG	m	102	30	-	10/35/55/70	0/1/1/1
36	LMG	w	101	-	-	28/46/66/70	0/1/1/1
30	CLA	14	310	-	-	8/15/91/115	-
41	A86	32	316	-	-	9/34/90/90	0/3/3/3
41	A86	32	319	-	-	7/34/90/90	0/3/3/3
38	DGD	c	518	-	-	22/51/91/95	0/2/2/2
30	CLA	35	301	25	-	12/39/115/115	-
30	CLA	41	303	-	-	19/39/115/115	-
36	LMG	Q	301	-	-	22/46/66/70	0/1/1/1
41	A86	38	315	-	-	10/34/90/90	0/3/3/3
41	A86	33	312	-	-	8/34/90/90	0/3/3/3
30	CLA	21	304	-	-	8/15/91/115	-
32	BCR	c	516	-	-	10/29/63/63	0/2/2/2
30	CLA	c	522	-	-	17/39/115/115	-
41	A86	17	315	-	-	13/34/90/90	0/3/3/3
41	A86	35	312	-	-	9/34/90/90	0/3/3/3
30	CLA	32	310	25	-	10/15/91/115	-
41	A86	21	311	-	-	8/34/90/90	0/3/3/3
30	CLA	11	308	25	-	8/15/91/115	-
41	A86	35	311	-	-	3/34/90/90	0/3/3/3
30	CLA	C	503	3	-	13/39/115/115	-
41	A86	19	311	-	-	8/34/90/90	0/3/3/3
30	CLA	32	309	-	-	10/15/91/115	-
30	CLA	20	208	-	-	8/15/91/115	-
41	A86	11	314	-	-	7/34/90/90	0/3/3/3
30	CLA	20	204	-	-	15/39/115/115	-
30	CLA	33	311	-	-	7/15/91/115	-
30	CLA	41	301	28	-	16/39/115/115	-
30	CLA	b	608	2	-	9/39/115/115	-
30	CLA	38	312	-	-	6/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMG	B	619	-	-	18/46/66/70	0/1/1/1
30	CLA	20	207	-	-	9/15/91/115	-
30	CLA	21	306	-	-	16/39/115/115	-
38	DGD	H	102	-	-	24/51/91/95	0/2/2/2
41	A86	37	312	-	-	3/34/90/90	0/3/3/3
30	CLA	38	301	25	-	13/39/115/115	-
41	A86	36	310	-	-	12/34/90/90	0/3/3/3
30	CLA	Z	102	30,19	-	18/39/115/115	-
30	CLA	11	305	-	-	10/15/91/115	-
30	CLA	17	309	25	-	4/15/91/115	-
30	CLA	34	302	25	-	14/39/115/115	-
30	CLA	31	305	-	-	10/15/91/115	-
30	CLA	32	306	25	-	4/15/91/115	-
30	CLA	39	304	26	-	11/15/91/115	-
41	A86	12	315	-	-	8/34/90/90	0/3/3/3
41	A86	21	314	-	-	12/34/90/90	0/3/3/3
30	CLA	38	308	25	-	10/15/91/115	-
38	DGD	C	517	-	-	22/51/91/95	0/2/2/2
36	LMG	M	102	30	-	10/35/55/70	0/1/1/1
41	A86	13	314	-	-	10/34/90/90	0/3/3/3
41	A86	18	314	-	-	3/34/90/90	0/3/3/3
35	LHG	b	621	-	-	20/53/53/53	-
30	CLA	37	301	25	-	16/39/115/115	-
30	CLA	38	309	25	-	17/39/115/115	-
41	A86	21	310	-	-	9/34/90/90	0/3/3/3
30	CLA	37	308	25	-	19/39/115/115	-
41	A86	13	311	-	-	8/34/90/90	0/3/3/3
41	A86	16	311	-	-	3/34/90/90	0/3/3/3
41	A86	16	313	-	-	7/34/90/90	0/3/3/3
30	CLA	B	608	2	-	9/39/115/115	-
30	CLA	34	307	25	-	10/15/91/115	-
41	A86	15	316	-	-	16/34/90/90	0/3/3/3
30	CLA	b	613	2	-	8/39/115/115	-
30	CLA	15	307	25	-	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	DGD	j	101	-	-	15/51/91/95	0/2/2/2
30	CLA	15	304	25	-	7/15/91/115	-
36	LMG	b	618	-	-	18/46/66/70	0/1/1/1
41	A86	35	310	-	-	8/34/90/90	0/3/3/3
30	CLA	33	310	25	-	8/15/91/115	-
30	CLA	b	610	-	-	16/39/115/115	-
30	CLA	19	303	-	-	17/39/115/115	-
30	CLA	d	406	4	-	8/39/115/115	-
41	A86	32	315	-	-	3/34/90/90	0/3/3/3
30	CLA	b	603	2	-	12/39/115/115	-
30	CLA	34	301	25	-	11/39/115/115	-
30	CLA	A	404	1	-	12/39/115/115	-
30	CLA	c	513	3	-	18/39/115/115	-
30	CLA	16	303	25	-	6/15/91/115	-
41	A86	17	312	-	-	3/34/90/90	0/3/3/3
30	CLA	41	305	28	-	11/15/91/115	-
41	A86	39	310	-	-	17/34/90/90	0/3/3/3
42	LMU	32	302	-	-	7/18/58/61	0/2/2/2
30	CLA	b	614	2	-	8/39/115/115	-
30	CLA	36	305	25	-	8/15/91/115	-
30	CLA	B	623	-	-	17/39/115/115	-
30	CLA	a	402	1	-	7/39/115/115	-
30	CLA	d	407	4	-	6/39/115/115	-
30	CLA	18	312	-	-	6/15/91/115	-
32	BCR	b	617	-	-	9/29/63/63	0/2/2/2
30	CLA	B	613	2	-	8/39/115/115	-
30	CLA	c	523	-	-	16/39/115/115	-
30	CLA	31	315	25	-	11/39/115/115	-
38	DGD	J	101	-	-	15/51/91/95	0/2/2/2
30	CLA	16	309	-	-	7/15/91/115	-
35	LHG	l	102	-	-	22/53/53/53	-
30	CLA	18	301	25	-	13/39/115/115	-
41	A86	31	314	-	-	7/34/90/90	0/3/3/3
30	CLA	36	301	25	-	12/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	17	308	25	-	19/39/115/115	-
30	CLA	c	504	3	-	19/39/115/115	-
30	CLA	C	511	3	-	12/39/115/115	-
32	BCR	B	618	-	-	9/29/63/63	0/2/2/2
30	CLA	33	307	-	-	10/15/91/115	-
30	CLA	40	206	27	-	9/15/91/115	-
30	CLA	21	305	28	-	11/15/91/115	-
30	CLA	B	604	2	-	14/39/115/115	-
30	CLA	40	202	-	-	19/39/115/115	-
30	CLA	b	604	2	-	14/39/115/115	-
30	CLA	19	308	-	-	10/15/91/115	-
41	A86	15	310	-	-	8/34/90/90	0/3/3/3
30	CLA	c	524	30	-	17/39/115/115	-
30	CLA	12	314	-	-	8/15/91/115	-
41	A86	32	304	-	-	16/34/90/90	0/3/3/3
33	SQD	b	620	-	-	9/32/52/69	0/1/1/1
41	A86	14	313	-	-	8/34/90/90	0/3/3/3
30	CLA	C	513	3	-	18/39/115/115	-
30	CLA	21	302	-	-	9/15/91/115	-
30	CLA	w	103	-	-	21/39/115/115	-
30	CLA	B	614	2	-	8/39/115/115	-
30	CLA	19	305	-	-	9/15/91/115	-
30	CLA	36	309	-	-	7/15/91/115	-
30	CLA	20	209	30	-	13/39/115/115	-
41	A86	37	316	-	-	7/34/90/90	0/3/3/3
40	HEM	e	101	6,5	-	7/14/54/54	-
41	A86	34	311	-	-	8/34/90/90	0/3/3/3
32	BCR	B	617	-	-	9/29/63/63	0/2/2/2
30	CLA	c	507	3	-	19/39/115/115	-
30	CLA	B	606	2	-	7/39/115/115	-
30	CLA	C	520	-	-	17/39/115/115	-
30	CLA	C	509	3	-	12/39/115/115	-
41	A86	40	210	-	-	14/34/90/90	0/3/3/3
30	CLA	12	310	25	-	10/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	31	312	-	-	8/34/90/90	0/3/3/3
30	CLA	41	306	-	-	16/39/115/115	-
30	CLA	C	521	-	-	16/39/115/115	-
30	CLA	36	306	25	-	9/15/91/115	-
30	CLA	C	519	-	-	23/39/115/115	-
30	CLA	c	509	3	-	12/39/115/115	-
31	PHO	d	403	-	-	12/37/103/103	0/5/6/6
30	CLA	c	508	-	-	18/39/115/115	-
41	A86	39	311	-	-	8/34/90/90	0/3/3/3
30	CLA	36	303	25	-	6/15/91/115	-
30	CLA	35	305	-	-	10/15/91/115	-
30	CLA	C	508	-	-	18/39/115/115	-
30	CLA	18	310	25	-	12/39/115/115	-
41	A86	35	313	-	-	10/34/90/90	0/3/3/3
30	CLA	b	602	2	-	15/39/115/115	-
30	CLA	16	307	25	-	9/15/91/115	-
36	LMG	B	620	-	-	20/46/66/70	0/1/1/1
41	A86	36	311	-	-	3/34/90/90	0/3/3/3
30	CLA	15	303	25	-	17/39/115/115	-
30	CLA	C	504	3	-	19/39/115/115	-
30	CLA	31	308	25	-	8/15/91/115	-
33	SQD	l	101	-	-	21/49/69/69	0/1/1/1
30	CLA	13	309	25	-	8/15/91/115	-
30	CLA	18	309	25	-	17/39/115/115	-
30	CLA	12	306	42,25	-	4/15/91/115	-
30	CLA	16	305	25	-	8/15/91/115	-
30	CLA	m	101	12,2,36	-	21/39/115/115	-
30	CLA	D	402	-	-	15/39/115/115	-
30	CLA	37	307	25	-	9/15/91/115	-
41	A86	32	318	-	-	7/34/90/90	0/3/3/3
41	A86	15	311	-	-	3/34/90/90	0/3/3/3
30	CLA	36	302	25	-	17/39/115/115	-
30	CLA	21	303	-	-	19/39/115/115	-
30	CLA	40	203	30	-	7/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	13	316	-	-	16/34/90/90	0/3/3/3
30	CLA	b	612	2	-	13/39/115/115	-
30	CLA	32	303	25	-	11/39/115/115	-
30	CLA	34	308	25	-	16/39/115/115	-
32	BCR	A	405	-	-	12/29/63/63	0/2/2/2
30	CLA	14	309	25	-	8/15/91/115	-
30	CLA	15	302	25	-	10/15/91/115	-
30	CLA	16	301	25	-	12/39/115/115	-
41	A86	41	312	-	-	7/34/90/90	0/3/3/3
30	CLA	32	305	25	-	14/39/115/115	-
41	A86	16	312	-	-	8/34/90/90	0/3/3/3
30	CLA	38	307	-	-	8/15/91/115	-
42	LMU	12	302	30	-	7/18/58/61	0/2/2/2
30	CLA	18	308	25	-	10/15/91/115	-
30	CLA	c	512	3	-	10/39/115/115	-
30	CLA	b	611	2	-	14/39/115/115	-
32	BCR	B	624	-	-	18/29/63/63	0/2/2/2
41	A86	11	311	-	-	3/34/90/90	0/3/3/3
30	CLA	21	309	-	-	8/15/91/115	-
30	CLA	41	304	-	-	8/15/91/115	-
41	A86	11	313	-	-	10/34/90/90	0/3/3/3
30	CLA	16	304	25	-	17/39/115/115	-
30	CLA	39	301	-	-	14/39/115/115	-
30	CLA	31	303	25	-	15/39/115/115	-
30	CLA	W	103	-	-	21/39/115/115	-
30	CLA	15	306	25	-	10/15/91/115	-
30	CLA	41	307	-	-	13/39/115/115	-
41	A86	35	315	-	-	15/34/90/90	0/3/3/3
32	BCR	b	616	-	-	9/29/63/63	0/2/2/2
41	A86	17	311	-	-	13/34/90/90	0/3/3/3
30	CLA	14	308	25	-	16/39/115/115	-
41	A86	17	313	-	-	8/34/90/90	0/3/3/3
30	CLA	21	301	28	-	16/39/115/115	-
30	CLA	c	503	3	-	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	38	306	25	-	9/15/91/115	-
41	A86	32	317	-	-	10/34/90/90	0/3/3/3
41	A86	11	316	-	-	15/34/90/90	0/3/3/3
41	A86	14	311	-	-	8/34/90/90	0/3/3/3
30	CLA	17	301	25	-	16/39/115/115	-
30	CLA	31	309	-	-	7/15/91/115	-
30	CLA	31	302	25	-	4/15/91/115	-
41	A86	36	312	-	-	8/34/90/90	0/3/3/3
41	A86	34	314	-	-	10/34/90/90	0/3/3/3
30	CLA	12	307	25	-	15/39/115/115	-
30	CLA	16	306	25	-	9/15/91/115	-
35	LHG	A	408	-	-	23/50/50/53	-
41	A86	20	213	-	-	12/34/90/90	0/3/3/3
30	CLA	c	502	3	-	14/39/115/115	-
30	CLA	40	208	-	-	8/15/91/115	-
30	CLA	12	305	25	-	13/39/115/115	-
41	A86	17	316	-	-	7/34/90/90	0/3/3/3
30	CLA	32	311	25	-	16/39/115/115	-
30	CLA	34	304	25	-	15/39/115/115	-
39	PL9	D	404	4	-	17/53/73/73	0/1/1/1
30	CLA	37	306	25	-	8/15/91/115	-
39	PL9	d	408	-	-	13/53/73/73	0/1/1/1
30	CLA	11	309	-	-	8/15/91/115	-
30	CLA	c	511	3	-	12/39/115/115	-
32	BCR	B	616	-	-	8/29/63/63	0/2/2/2
41	A86	12	319	-	-	7/34/90/90	0/3/3/3
30	CLA	40	204	-	-	15/39/115/115	-
41	A86	41	313	-	-	16/34/90/90	0/3/3/3
38	DGD	h	102	-	-	24/51/91/95	0/2/2/2
30	CLA	M	101	12,2,36	-	21/39/115/115	-
30	CLA	36	308	25	-	9/15/91/115	-
30	CLA	13	307	25	-	10/15/91/115	-
30	CLA	C	510	3	-	12/39/115/115	-
30	CLA	C	505	-	-	19/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	39	308	-	-	10/15/91/115	-
41	A86	12	304	-	-	16/34/90/90	0/3/3/3
41	A86	40	213	-	-	12/34/90/90	0/3/3/3
30	CLA	34	306	-	-	10/15/91/115	-
30	CLA	32	307	25	-	15/39/115/115	-
41	A86	16	310	-	-	12/34/90/90	0/3/3/3
30	CLA	32	312	25	-	8/15/91/115	-
41	A86	15	313	-	-	10/34/90/90	0/3/3/3
41	A86	13	301	-	-	15/34/90/90	0/3/3/3
30	CLA	A	402	1	-	7/39/115/115	-
38	DGD	c	517	-	-	19/51/91/95	0/2/2/2
30	CLA	W	102	21	-	16/39/115/115	-
30	CLA	11	315	25	-	13/39/115/115	-
30	CLA	12	309	-	-	10/15/91/115	-
30	CLA	35	309	-	-	6/15/91/115	-
30	CLA	14	303	25	-	5/15/91/115	-
30	CLA	21	308	-	-	10/15/91/115	-
41	A86	18	313	-	-	8/34/90/90	0/3/3/3
30	CLA	35	302	25	-	10/15/91/115	-
41	A86	34	313	-	-	9/34/90/90	0/3/3/3
30	CLA	13	303	25	-	5/15/91/115	-
30	CLA	35	308	25	-	8/15/91/115	-
30	CLA	b	609	2	-	10/39/115/115	-
41	A86	21	312	-	-	7/34/90/90	0/3/3/3
30	CLA	35	306	25	-	10/15/91/115	-
30	CLA	b	622	-	-	17/39/115/115	-
41	A86	39	309	-	-	11/34/90/90	0/3/3/3
33	SQD	L	103	-	-	21/49/69/69	0/1/1/1
30	CLA	33	305	25	-	15/39/115/115	-
30	CLA	B	603	2	-	12/39/115/115	-
41	A86	34	312	-	-	3/34/90/90	0/3/3/3
30	CLA	32	308	25,36	-	10/15/91/115	-
36	LMG	W	101	-	-	28/46/66/70	0/1/1/1
30	CLA	14	302	25	-	13/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	w	102	21	-	16/39/115/115	-
41	A86	20	210	-	-	14/34/90/90	0/3/3/3
30	CLA	16	308	25	-	9/15/91/115	-
30	CLA	14	301	25	-	13/39/115/115	-
30	CLA	b	605	2	-	19/39/115/115	-
33	SQD	A	406	-	-	14/49/69/69	0/1/1/1
41	A86	33	314	-	-	9/34/90/90	0/3/3/3
30	CLA	14	306	-	-	10/15/91/115	-
41	A86	12	318	-	-	10/34/90/90	0/3/3/3
30	CLA	C	502	3	-	14/39/115/115	-
30	CLA	b	607	-	-	12/39/115/115	-
32	BCR	m	103	-	-	8/29/63/63	0/2/2/2
30	CLA	40	205	-	-	11/15/91/115	-
30	CLA	17	307	25	-	10/15/91/115	-
41	A86	33	302	-	-	15/34/90/90	0/3/3/3
30	CLA	38	311	25	-	10/15/91/115	-
41	A86	38	313	-	-	8/34/90/90	0/3/3/3
41	A86	31	316	-	-	16/34/90/90	0/3/3/3
30	CLA	12	303	25	-	13/39/115/115	-
30	CLA	31	304	25	-	10/15/91/115	-
41	A86	37	311	-	-	13/34/90/90	0/3/3/3
30	CLA	15	305	-	-	10/15/91/115	-
41	A86	20	201	-	-	12/34/90/90	0/3/3/3
30	CLA	34	303	25	-	4/15/91/115	-
30	CLA	33	303	25	-	14/39/115/115	-
30	CLA	11	306	25	-	10/15/91/115	-
41	A86	18	315	-	-	10/34/90/90	0/3/3/3
30	CLA	a	403	1	-	12/39/115/115	-
30	CLA	B	615	2	-	13/39/115/115	-
30	CLA	b	615	2	-	13/39/115/115	-
32	BCR	h	101	-	-	7/29/63/63	0/2/2/2
41	A86	31	313	-	-	10/34/90/90	0/3/3/3
41	A86	41	314	-	-	12/34/90/90	0/3/3/3
41	A86	32	314	-	-	8/34/90/90	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	12	311	25	-	16/39/115/115	-
36	LMG	32	301	30	-	14/34/54/70	0/1/1/1
30	CLA	20	203	30	-	7/15/91/115	-
30	CLA	13	305	25	-	9/15/91/115	-
41	A86	38	302	-	-	15/34/90/90	0/3/3/3
30	CLA	17	304	25	-	6/15/91/115	-
41	A86	41	311	-	-	8/34/90/90	0/3/3/3
30	CLA	19	302	-	-	4/15/91/115	-
30	CLA	B	607	-	-	12/39/115/115	-
30	CLA	34	309	25	-	8/15/91/115	-
30	CLA	33	309	25	-	16/39/115/115	-
30	CLA	11	304	25	-	9/15/91/115	-
30	CLA	33	306	25	-	10/15/91/115	-
30	CLA	39	306	-	-	10/15/91/115	-
41	A86	40	212	-	-	11/34/90/90	0/3/3/3
40	HEM	E	101	6,5	-	7/14/54/54	-
41	A86	12	317	-	-	9/34/90/90	0/3/3/3
36	LMG	b	619	-	-	20/46/66/70	0/1/1/1
30	CLA	33	308	25	-	10/15/91/115	-
41	A86	33	317	-	-	7/34/90/90	0/3/3/3
41	A86	37	302	-	-	16/34/90/90	1/3/3/3
30	CLA	14	307	25	-	10/15/91/115	-
30	CLA	14	304	25	-	15/39/115/115	-
30	CLA	c	505	-	-	19/39/115/115	-
30	CLA	38	303	25	-	16/39/115/115	-
30	CLA	13	304	25	-	15/39/115/115	-
32	BCR	f	101	-	-	15/29/63/63	0/2/2/2
30	CLA	14	305	25	-	9/15/91/115	-
30	CLA	D	406	4	-	6/39/115/115	-
30	CLA	19	307	-	-	3/15/91/115	-
30	CLA	38	305	25	-	21/39/115/115	-
32	BCR	C	515	-	-	10/29/63/63	0/2/2/2
39	PL9	d	405	4	-	17/53/73/73	0/1/1/1
30	CLA	36	304	25	-	17/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	21	313	-	-	16/34/90/90	0/3/3/3
30	CLA	B	605	2	-	19/39/115/115	-
30	CLA	20	202	-	-	19/39/115/115	-
30	CLA	B	602	2	-	15/39/115/115	-
32	BCR	F	101	-	-	15/29/63/63	0/2/2/2
41	A86	11	310	-	-	8/34/90/90	0/3/3/3
35	LHG	B	622	-	-	20/53/53/53	-
41	A86	19	309	-	-	11/34/90/90	0/3/3/3
30	CLA	18	311	25	-	10/15/91/115	-
30	CLA	37	303	25	-	15/39/115/115	-
33	SQD	a	405	-	-	14/49/69/69	0/1/1/1
41	A86	17	302	-	-	16/34/90/90	1/3/3/3
30	CLA	b	601	-	-	20/39/115/115	-
41	A86	15	314	-	-	7/34/90/90	0/3/3/3
30	CLA	B	612	2	-	13/39/115/115	-
32	BCR	c	515	-	-	15/29/63/63	0/2/2/2
36	LMG	d	410	-	-	14/46/66/70	0/1/1/1
35	LHG	a	407	-	-	23/50/50/53	-
30	CLA	31	307	25	-	16/39/115/115	-
41	A86	14	314	-	-	10/34/90/90	0/3/3/3
31	PHO	A	403	-	-	12/37/103/103	0/5/6/6
38	DGD	C	516	-	-	19/51/91/95	0/2/2/2
40	HEM	v	201	16	-	1/14/54/54	-
33	SQD	B	621	-	-	9/32/52/69	0/1/1/1
30	CLA	17	310	-	-	9/15/91/115	-
30	CLA	33	304	25	-	4/15/91/115	-
30	CLA	17	306	25	-	8/15/91/115	-
35	LHG	L	101	-	-	29/53/53/53	-
30	CLA	C	512	3	-	10/39/115/115	-
36	LMG	D	408	-	-	14/46/66/70	0/1/1/1
30	CLA	34	305	25	-	9/15/91/115	-
30	CLA	B	611	2	-	14/39/115/115	-
41	A86	15	315	-	-	15/34/90/90	0/3/3/3
30	CLA	d	402	-	-	15/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	36	313	-	-	7/34/90/90	0/3/3/3
30	CLA	b	606	2	-	7/39/115/115	-
30	CLA	31	301	25	-	14/39/115/115	-
30	CLA	41	302	-	-	9/15/91/115	-
30	CLA	13	302	25	-	13/39/115/115	-
30	CLA	16	302	25	-	17/39/115/115	-
39	PL9	D	407	-	-	13/53/73/73	0/1/1/1
30	CLA	18	307	-	-	8/15/91/115	-
30	CLA	c	506	3	-	18/39/115/115	-
30	CLA	13	306	-	-	10/15/91/115	-
30	CLA	38	310	25	-	12/39/115/115	-
30	CLA	B	601	-	-	20/39/115/115	-
41	A86	15	312	-	-	8/34/90/90	0/3/3/3
30	CLA	18	303	25	-	16/39/115/115	-
30	CLA	12	308	25,36	-	9/15/91/115	-
41	A86	31	311	-	-	3/34/90/90	0/3/3/3
41	A86	40	211	-	-	8/34/90/90	0/3/3/3
30	CLA	39	305	-	-	9/15/91/115	-
30	CLA	c	514	3,30	-	13/39/115/115	-
41	A86	35	316	-	-	16/34/90/90	0/3/3/3
30	CLA	11	303	25	-	15/39/115/115	-
41	A86	17	314	-	-	10/34/90/90	0/3/3/3
41	A86	33	316	-	-	16/34/90/90	0/3/3/3
30	CLA	20	205	-	-	11/15/91/115	-
32	BCR	A	409	-	-	9/29/63/63	0/2/2/2
41	A86	37	313	-	-	9/34/90/90	0/3/3/3
36	LMG	12	301	30	-	17/34/54/70	0/1/1/1
41	A86	20	212	-	-	11/34/90/90	0/3/3/3
30	CLA	37	310	-	-	9/15/91/115	-
30	CLA	15	301	25	-	12/39/115/115	-
31	PHO	D	403	-	-	8/37/103/103	0/5/6/6
41	A86	18	302	-	-	15/34/90/90	0/3/3/3
30	CLA	15	308	25	-	8/15/91/115	-
30	CLA	36	307	25	-	9/15/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A86	11	312	-	-	8/34/90/90	0/3/3/3
41	A86	33	313	-	-	3/34/90/90	0/3/3/3
30	CLA	12	313	25	-	8/15/91/115	-
30	CLA	32	313	-	-	7/15/91/115	-
30	CLA	18	306	25	-	9/15/91/115	-
41	A86	13	315	-	-	7/34/90/90	0/3/3/3
32	BCR	C	518	-	-	8/29/63/63	0/2/2/2
41	A86	13	317	-	-	7/34/90/90	0/3/3/3
30	CLA	31	306	25	-	10/15/91/115	-
30	CLA	19	301	-	-	14/39/115/115	-
41	A86	33	315	-	-	10/34/90/90	0/3/3/3
30	CLA	37	304	25	-	6/15/91/115	-
30	CLA	19	306	-	-	10/15/91/115	-
30	CLA	d	401	-	-	14/39/115/115	-
30	CLA	37	305	25	-	21/39/115/115	-
41	A86	20	211	-	-	8/34/90/90	0/3/3/3
41	A86	14	312	-	-	3/34/90/90	0/3/3/3
30	CLA	11	302	25	-	5/15/91/115	-
30	CLA	D	401	-	-	14/39/115/115	-
41	A86	35	314	-	-	7/34/90/90	0/3/3/3
41	A86	41	310	-	-	9/34/90/90	0/3/3/3
41	A86	13	312	-	-	3/34/90/90	0/3/3/3
30	CLA	C	514	3,30	-	13/39/115/115	-
30	CLA	21	307	-	-	13/39/115/115	-
32	BCR	a	408	-	-	9/29/63/63	0/2/2/2
41	A86	40	201	-	-	12/34/90/90	0/3/3/3
35	LHG	d	409	-	-	29/53/53/53	-
30	CLA	39	302	-	-	4/15/91/115	-
32	BCR	b	623	-	-	18/29/63/63	0/2/2/2
30	CLA	37	309	25	-	4/15/91/115	-
30	CLA	38	304	25	-	5/15/91/115	-
30	CLA	11	307	25	-	16/39/115/115	-
41	A86	31	310	-	-	8/34/90/90	0/3/3/3
30	CLA	z	101	-	-	23/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	17	305	25	-	21/39/115/115	-
30	CLA	18	305	25	-	21/39/115/115	-
30	CLA	41	309	-	-	8/15/91/115	-
41	A86	19	310	-	-	17/34/90/90	0/3/3/3
30	CLA	C	507	3	-	19/39/115/115	-
32	BCR	Z	101	-	-	15/29/63/63	0/2/2/2
30	CLA	39	303	-	-	17/39/115/115	-
30	CLA	c	510	3	-	12/39/115/115	-
30	CLA	C	506	3	-	18/39/115/115	-
41	A86	37	314	-	-	10/34/90/90	0/3/3/3
30	CLA	40	209	30	-	13/39/115/115	-
30	CLA	13	308	25	-	16/39/115/115	-

The worst 5 of 5938 bond length outliers are listed below:

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

The worst 5 of 5411 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 5650 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	A	402	CLA	CBD-CGD-O2D-CED
30	A	404	CLA	C2B-C3B-CAB-CBB
30	A	404	CLA	C4B-C3B-CAB-CBB
30	B	601	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	B	601	CLA	C2B-C3B-CAB-CBB

All (2) ring outliers are listed below:

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

435 monomers are involved in 1471 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	a	404	BCR	2	0
30	B	610	CLA	3	0
30	B	609	CLA	2	0
41	12	316	A86	14	0
32	Y	101	BCR	4	0
30	15	309	CLA	1	0
30	11	301	CLA	9	0
30	17	303	CLA	14	0
30	35	307	CLA	3	0
35	L	102	LHG	1	0
30	18	304	CLA	3	0
41	38	314	A86	16	0
40	V	201	HEM	2	0
31	d	404	PHO	2	0
32	H	101	BCR	3	0
41	37	315	A86	19	0
32	c	520	BCR	2	0
30	40	207	CLA	1	0
30	D	405	CLA	5	0
36	c	519	LMG	1	0
32	c	521	BCR	4	0
30	33	301	CLA	2	0
41	13	313	A86	4	0
36	m	102	LMG	1	0
36	w	101	LMG	4	0
41	32	316	A86	3	0
41	32	319	A86	5	0
30	35	301	CLA	9	0
30	41	303	CLA	10	0
36	Q	301	LMG	1	0
41	38	315	A86	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	33	312	A86	2	0
30	21	304	CLA	5	0
32	c	516	BCR	3	0
30	c	522	CLA	2	0
41	17	315	A86	16	0
30	32	310	CLA	1	0
41	21	311	A86	10	0
30	11	308	CLA	2	0
41	35	311	A86	10	0
30	C	503	CLA	3	0
41	19	311	A86	2	0
30	32	309	CLA	2	0
41	11	314	A86	2	0
30	20	204	CLA	1	0
30	41	301	CLA	3	0
30	b	608	CLA	3	0
30	38	312	CLA	19	0
36	B	619	LMG	4	0
30	20	207	CLA	1	0
30	21	306	CLA	4	0
38	H	102	DGD	3	0
41	37	312	A86	11	0
30	38	301	CLA	2	0
41	36	310	A86	9	0
30	Z	102	CLA	10	0
30	11	305	CLA	1	0
30	17	309	CLA	1	0
30	34	302	CLA	10	0
30	31	305	CLA	1	0
30	32	306	CLA	12	0
41	12	315	A86	3	0
41	21	314	A86	19	0
30	38	308	CLA	1	0
36	M	102	LMG	6	0
41	13	314	A86	3	0
41	18	314	A86	16	0
35	b	621	LHG	2	0
30	37	301	CLA	3	0
30	38	309	CLA	5	0
41	21	310	A86	12	0
30	37	308	CLA	5	0
41	13	311	A86	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	16	311	A86	8	0
41	16	313	A86	2	0
30	B	608	CLA	2	0
30	34	307	CLA	1	0
41	15	316	A86	15	0
30	b	613	CLA	4	0
30	15	307	CLA	2	0
38	j	101	DGD	1	0
36	b	618	LMG	3	0
41	35	310	A86	4	0
30	33	310	CLA	1	0
30	b	610	CLA	2	0
30	19	303	CLA	8	0
30	d	406	CLA	4	0
41	32	315	A86	9	0
30	34	301	CLA	1	0
30	A	404	CLA	10	0
30	c	513	CLA	4	0
30	16	303	CLA	1	0
41	17	312	A86	12	0
30	41	305	CLA	1	0
41	39	310	A86	14	0
42	32	302	LMU	15	0
30	b	614	CLA	5	0
30	36	305	CLA	2	0
30	B	623	CLA	3	0
30	a	402	CLA	2	0
30	d	407	CLA	1	0
30	18	312	CLA	19	0
32	b	617	BCR	2	0
30	B	613	CLA	4	0
30	c	523	CLA	4	0
30	31	315	CLA	6	0
38	J	101	DGD	2	0
30	16	309	CLA	5	0
35	l	102	LHG	3	0
30	18	301	CLA	4	0
41	31	314	A86	2	0
30	36	301	CLA	3	0
30	17	308	CLA	5	0
30	c	504	CLA	5	0
30	C	511	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	B	618	BCR	4	0
30	33	307	CLA	2	0
30	21	305	CLA	1	0
30	B	604	CLA	6	0
30	40	202	CLA	4	0
30	b	604	CLA	6	0
30	19	308	CLA	1	0
41	15	310	A86	1	0
30	c	524	CLA	10	0
41	32	304	A86	7	0
33	b	620	SQD	1	0
41	14	313	A86	4	0
30	C	513	CLA	4	0
30	21	302	CLA	5	0
30	w	103	CLA	4	0
30	B	614	CLA	6	0
30	36	309	CLA	6	0
30	20	209	CLA	2	0
41	37	316	A86	5	0
40	e	101	HEM	2	0
32	B	617	BCR	2	0
30	c	507	CLA	4	0
30	B	606	CLA	3	0
30	C	520	CLA	1	0
30	C	509	CLA	6	0
41	40	210	A86	8	0
30	12	310	CLA	3	0
41	31	312	A86	4	0
30	41	306	CLA	3	0
30	C	521	CLA	2	0
30	36	306	CLA	1	0
30	C	519	CLA	1	0
30	c	509	CLA	6	0
31	d	403	PHO	1	0
30	c	508	CLA	1	0
41	39	311	A86	3	0
30	36	303	CLA	1	0
30	35	305	CLA	1	0
30	C	508	CLA	2	0
30	18	310	CLA	2	0
41	35	313	A86	8	0
30	b	602	CLA	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	16	307	CLA	8	0
36	B	620	LMG	2	0
41	36	311	A86	5	0
30	15	303	CLA	1	0
30	C	504	CLA	4	0
30	31	308	CLA	1	0
33	l	101	SQD	3	0
30	13	309	CLA	4	0
30	18	309	CLA	5	0
30	12	306	CLA	2	0
30	16	305	CLA	1	0
30	m	101	CLA	5	0
30	D	402	CLA	2	0
30	37	307	CLA	1	0
41	32	318	A86	2	0
41	15	311	A86	10	0
30	36	302	CLA	8	0
30	21	303	CLA	11	0
30	40	203	CLA	9	0
41	13	316	A86	12	0
30	b	612	CLA	4	0
30	32	303	CLA	4	0
30	34	308	CLA	2	0
30	14	309	CLA	1	0
30	15	302	CLA	2	0
30	16	301	CLA	3	0
41	41	312	A86	3	0
30	32	305	CLA	10	0
41	16	312	A86	7	0
30	18	308	CLA	1	0
30	c	512	CLA	2	0
30	b	611	CLA	4	0
32	B	624	BCR	5	0
41	11	311	A86	9	0
30	21	309	CLA	2	0
30	41	304	CLA	6	0
41	11	313	A86	5	0
30	16	304	CLA	1	0
30	39	301	CLA	3	0
30	31	303	CLA	1	0
30	W	103	CLA	5	0
30	15	306	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	41	307	CLA	1	0
41	35	315	A86	4	0
32	b	616	BCR	2	0
41	17	311	A86	7	0
30	14	308	CLA	2	0
41	17	313	A86	2	0
30	21	301	CLA	4	0
30	c	503	CLA	3	0
41	32	317	A86	3	0
41	11	316	A86	9	0
41	14	311	A86	1	0
30	17	301	CLA	4	0
30	31	302	CLA	1	0
41	36	312	A86	7	0
41	34	314	A86	4	0
30	12	307	CLA	4	0
30	16	306	CLA	1	0
35	A	408	LHG	5	0
41	20	213	A86	2	0
30	c	502	CLA	4	0
30	40	208	CLA	1	0
30	12	305	CLA	13	0
41	17	316	A86	6	0
30	32	311	CLA	2	0
30	34	304	CLA	2	0
39	D	404	PL9	2	0
30	37	306	CLA	4	0
39	d	408	PL9	5	0
30	c	511	CLA	5	0
32	B	616	BCR	3	0
41	12	319	A86	2	0
30	40	204	CLA	3	0
41	41	313	A86	2	0
38	h	102	DGD	3	0
30	M	101	CLA	1	0
30	36	308	CLA	10	0
30	13	307	CLA	3	0
30	C	510	CLA	2	0
30	C	505	CLA	2	0
30	39	308	CLA	1	0
41	12	304	A86	8	0
41	40	213	A86	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	34	306	CLA	2	0
30	32	307	CLA	1	0
41	16	310	A86	8	0
30	32	312	CLA	1	0
41	15	313	A86	8	0
41	13	301	A86	10	0
30	A	402	CLA	1	0
30	W	102	CLA	5	0
30	11	315	CLA	5	0
30	12	309	CLA	4	0
30	35	309	CLA	1	0
30	14	303	CLA	2	0
41	18	313	A86	1	0
30	35	302	CLA	2	0
41	34	313	A86	1	0
30	13	303	CLA	2	0
30	35	308	CLA	2	0
30	b	609	CLA	2	0
41	21	312	A86	3	0
30	35	306	CLA	3	0
30	b	622	CLA	3	0
41	39	309	A86	6	0
33	L	103	SQD	3	0
30	33	305	CLA	3	0
41	34	312	A86	11	0
30	32	308	CLA	6	0
36	W	101	LMG	5	0
30	14	302	CLA	11	0
30	w	102	CLA	3	0
41	20	210	A86	8	0
30	16	308	CLA	10	0
30	14	301	CLA	2	0
30	b	605	CLA	2	0
41	33	314	A86	3	0
30	14	306	CLA	2	0
41	12	318	A86	3	0
30	C	502	CLA	4	0
30	b	607	CLA	3	0
32	m	103	BCR	2	0
30	17	307	CLA	1	0
41	33	302	A86	10	0
30	38	311	CLA	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	38	313	A86	3	0
41	31	316	A86	12	0
30	12	303	CLA	5	0
30	31	304	CLA	2	0
41	37	311	A86	5	0
30	15	305	CLA	1	0
41	20	201	A86	11	0
30	34	303	CLA	1	0
30	33	303	CLA	13	0
30	11	306	CLA	1	0
41	18	315	A86	6	0
30	a	403	CLA	6	0
30	B	615	CLA	4	0
30	b	615	CLA	3	0
32	h	101	BCR	4	0
41	31	313	A86	5	0
41	41	314	A86	20	0
41	32	314	A86	1	0
30	12	311	CLA	2	0
36	32	301	LMG	7	0
30	20	203	CLA	8	0
30	13	305	CLA	2	0
41	38	302	A86	8	0
30	17	304	CLA	2	0
41	41	311	A86	10	0
30	19	302	CLA	1	0
30	B	607	CLA	2	0
30	34	309	CLA	2	0
30	33	309	CLA	2	0
30	11	304	CLA	2	0
41	40	212	A86	15	0
40	E	101	HEM	1	0
41	12	317	A86	3	0
30	33	308	CLA	2	0
41	33	317	A86	1	0
41	37	302	A86	15	0
30	14	307	CLA	1	0
30	14	304	CLA	5	0
30	c	505	CLA	3	0
30	38	303	CLA	15	0
30	13	304	CLA	7	0
32	f	101	BCR	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	D	406	CLA	1	0
30	38	305	CLA	2	0
32	C	515	BCR	2	0
39	d	405	PL9	2	0
30	36	304	CLA	1	0
41	21	313	A86	2	0
30	B	605	CLA	2	0
30	20	202	CLA	4	0
30	B	602	CLA	7	0
32	F	101	BCR	2	0
35	B	622	LHG	1	0
41	19	309	A86	6	0
30	18	311	CLA	5	0
30	37	303	CLA	11	0
41	17	302	A86	17	0
30	b	601	CLA	5	0
41	15	314	A86	1	0
30	B	612	CLA	4	0
32	c	515	BCR	2	0
36	d	410	LMG	1	0
35	a	407	LHG	7	0
30	31	307	CLA	2	0
41	14	314	A86	4	0
31	A	403	PHO	1	0
34	A	407	BCT	1	0
38	C	516	DGD	1	0
40	v	201	HEM	2	0
30	17	310	CLA	1	0
30	33	304	CLA	1	0
30	17	306	CLA	4	0
35	L	101	LHG	6	0
30	C	512	CLA	3	0
36	D	408	LMG	2	0
34	a	406	BCT	2	0
30	B	611	CLA	3	0
41	15	315	A86	4	0
30	d	402	CLA	1	0
41	36	313	A86	3	0
30	b	606	CLA	3	0
30	31	301	CLA	8	0
30	41	302	CLA	6	0
30	13	302	CLA	10	0

Continued on next page...

Continued from previous page...

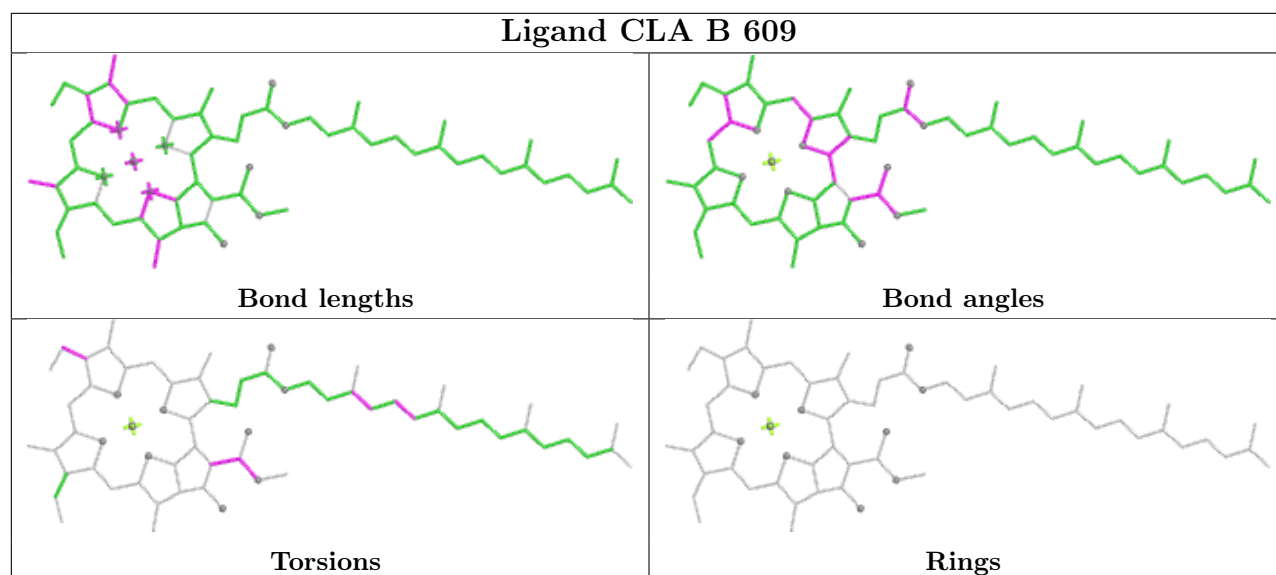
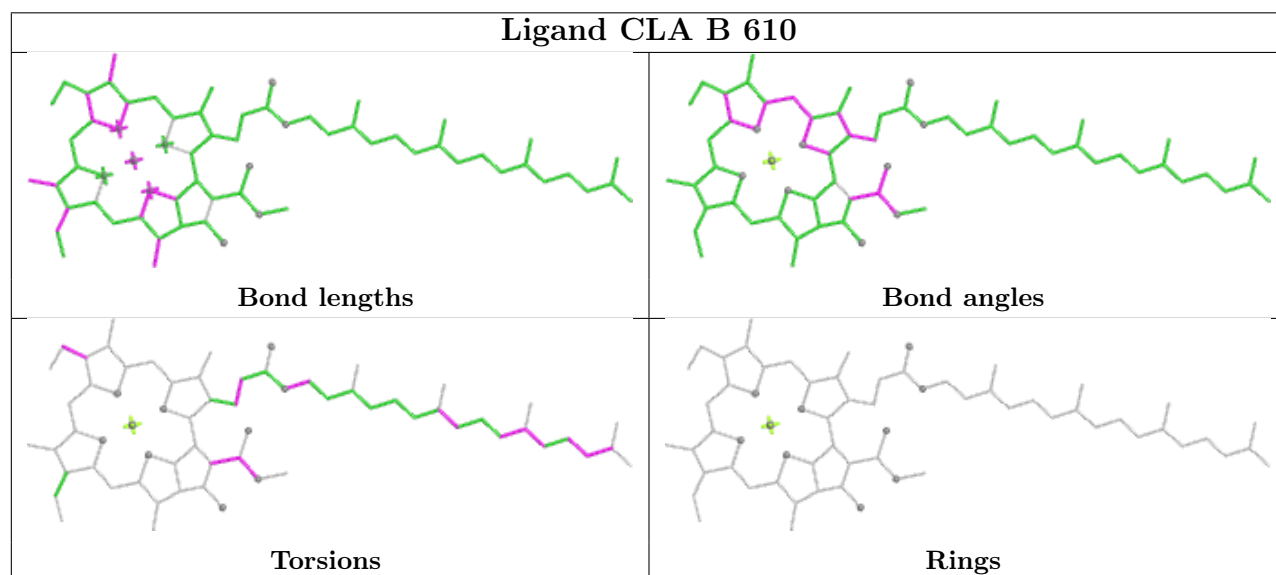
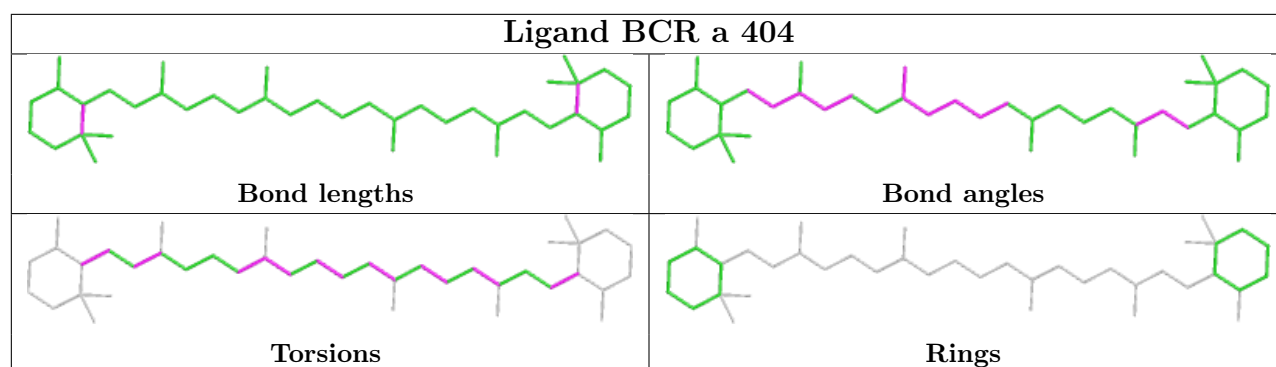
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	16	302	CLA	7	0
39	D	407	PL9	4	0
30	c	506	CLA	2	0
30	13	306	CLA	2	0
30	38	310	CLA	3	0
30	B	601	CLA	5	0
30	18	303	CLA	14	0
30	12	308	CLA	3	0
41	31	311	A86	9	0
41	40	211	A86	6	0
30	c	514	CLA	11	0
41	35	316	A86	13	0
30	11	303	CLA	3	0
41	17	314	A86	2	0
41	33	316	A86	7	0
32	A	409	BCR	2	0
41	37	313	A86	2	0
36	12	301	LMG	2	0
41	20	212	A86	14	0
30	37	310	CLA	1	0
30	15	301	CLA	10	0
31	D	403	PHO	2	0
41	18	302	A86	9	0
30	15	308	CLA	3	0
30	36	307	CLA	7	0
41	11	312	A86	5	0
41	33	313	A86	16	0
30	12	313	CLA	3	0
41	13	315	A86	11	0
32	C	518	BCR	2	0
41	13	317	A86	2	0
30	31	306	CLA	1	0
30	19	301	CLA	4	0
41	33	315	A86	3	0
30	37	304	CLA	2	0
30	d	401	CLA	3	0
30	37	305	CLA	11	0
41	20	211	A86	6	0
41	14	312	A86	12	0
30	11	302	CLA	2	0
30	D	401	CLA	3	0
41	35	314	A86	2	0

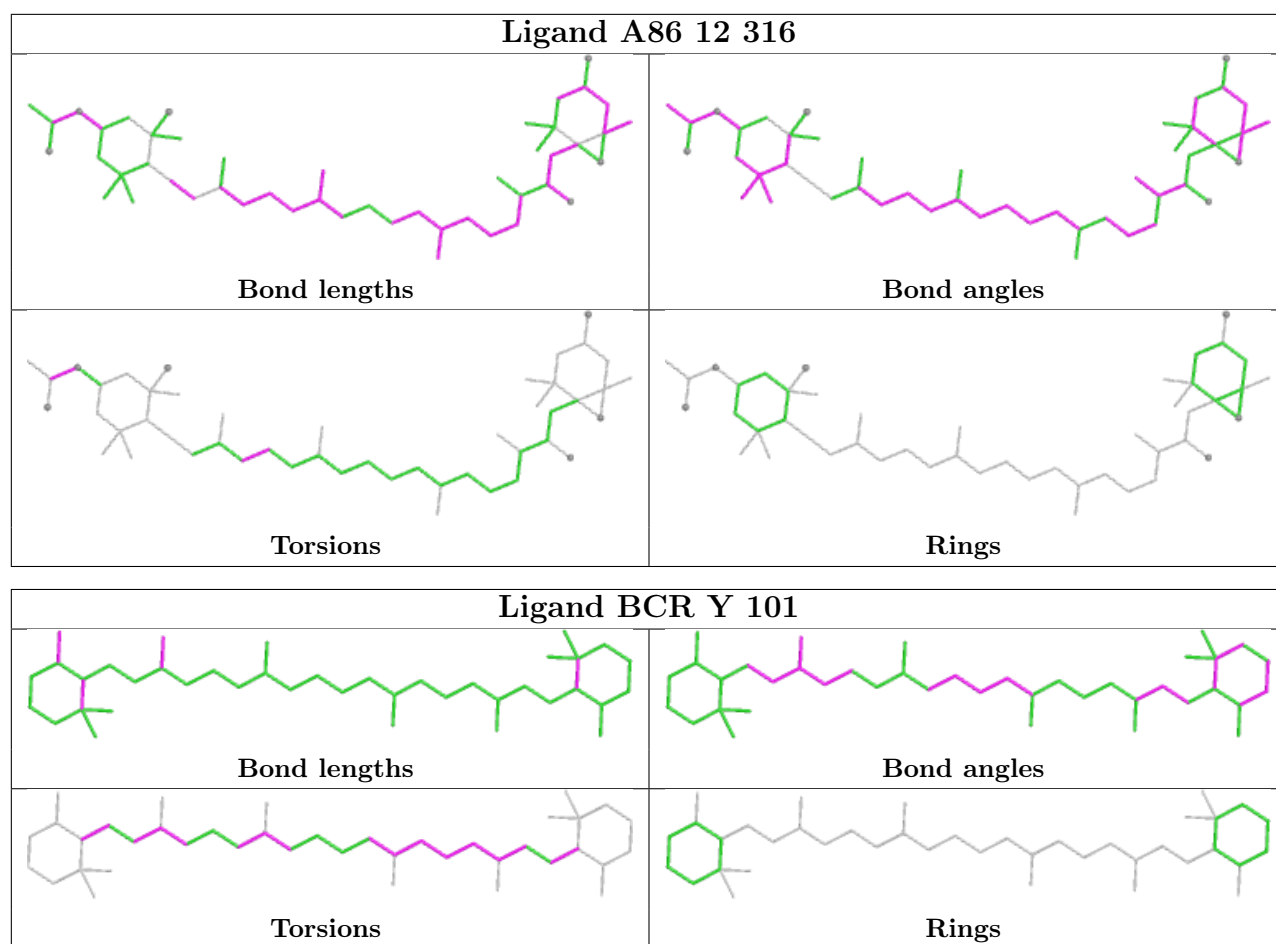
Continued on next page...

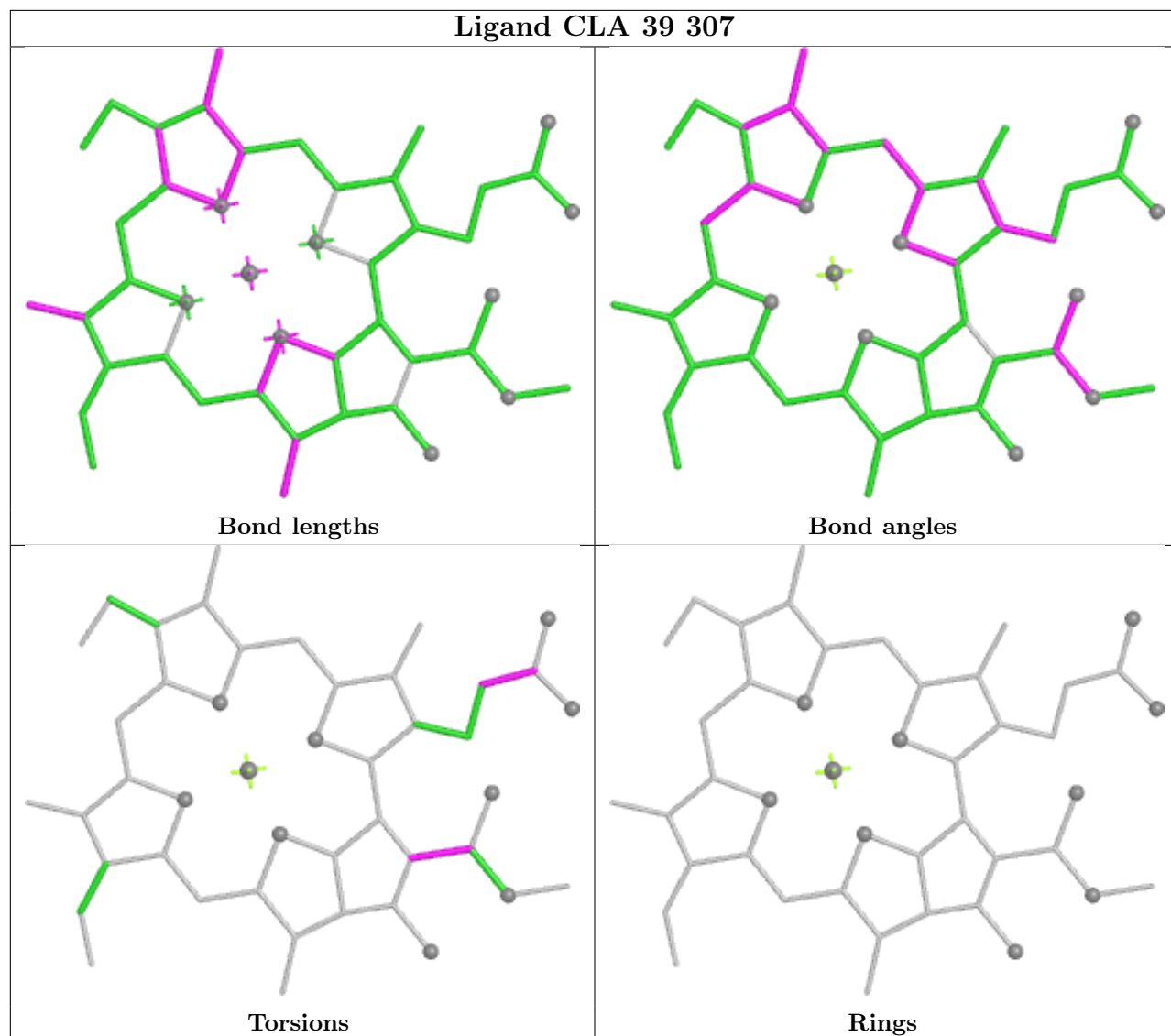
Continued from previous page...

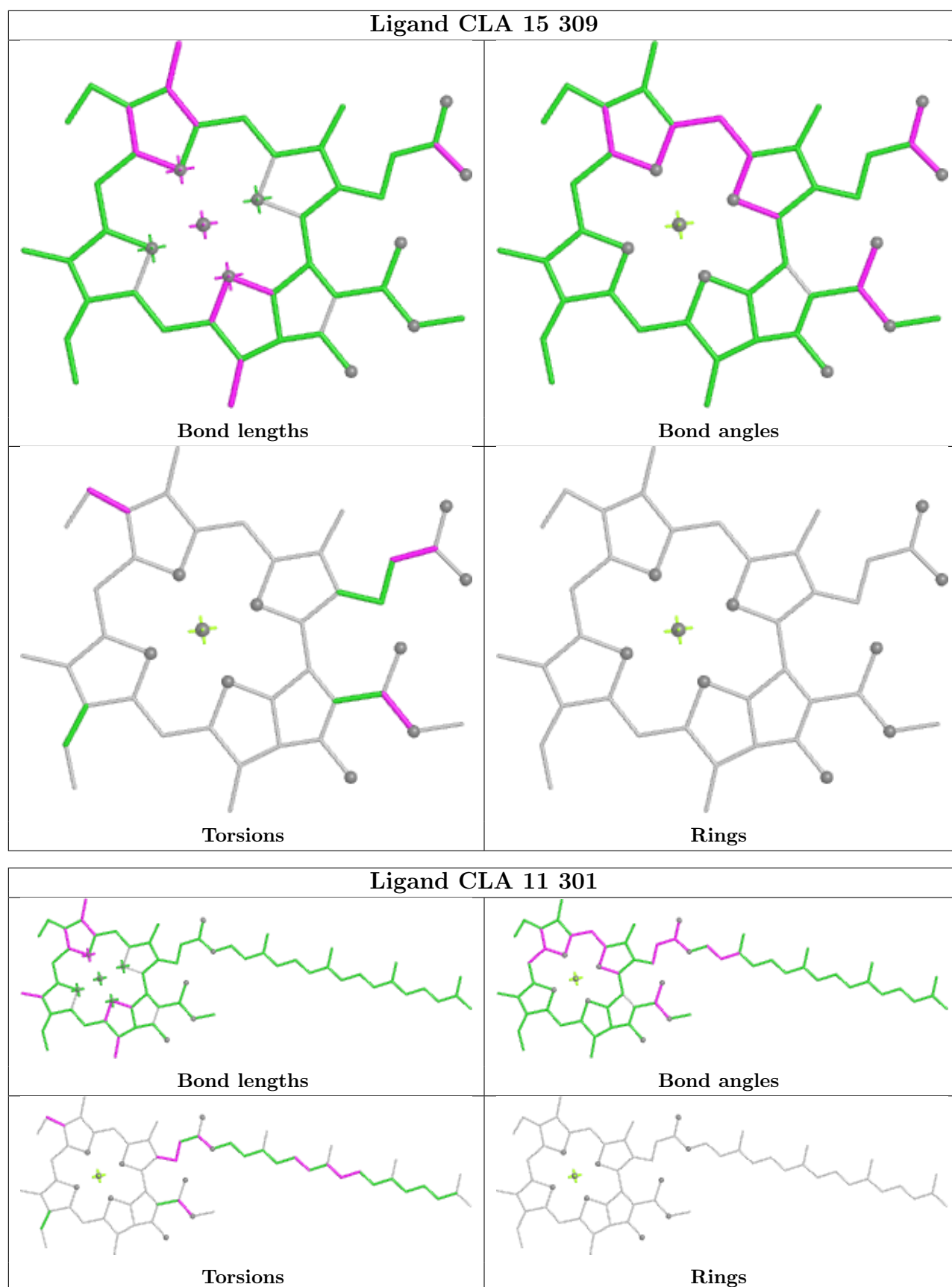
Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	41	310	A86	10	0
41	13	312	A86	22	0
30	C	514	CLA	11	0
30	21	307	CLA	1	0
32	a	408	BCR	1	0
41	40	201	A86	12	0
35	d	409	LHG	2	0
30	39	302	CLA	1	0
32	b	623	BCR	3	0
30	37	309	CLA	1	0
30	38	304	CLA	3	0
30	11	307	CLA	2	0
30	z	101	CLA	3	0
30	17	305	CLA	9	0
30	18	305	CLA	1	0
30	41	309	CLA	2	0
41	19	310	A86	15	0
30	C	507	CLA	10	0
32	Z	101	BCR	1	0
30	39	303	CLA	6	0
30	c	510	CLA	3	0
30	C	506	CLA	3	0
41	37	314	A86	2	0
30	40	209	CLA	3	0
30	13	308	CLA	2	0
37	c	501	OEX	1	0

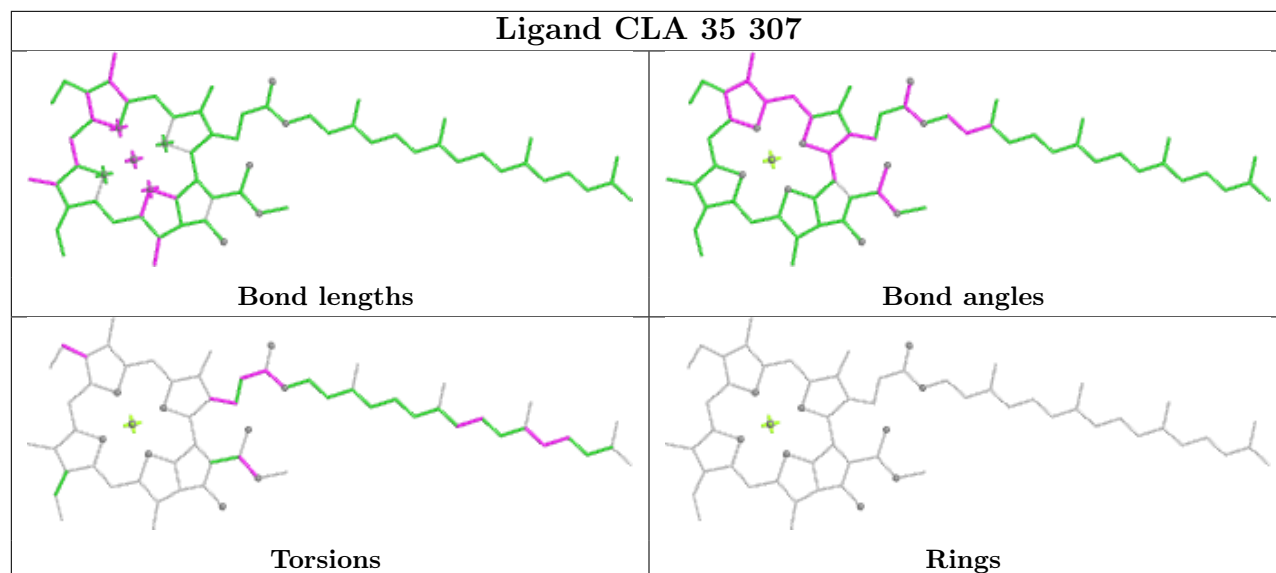
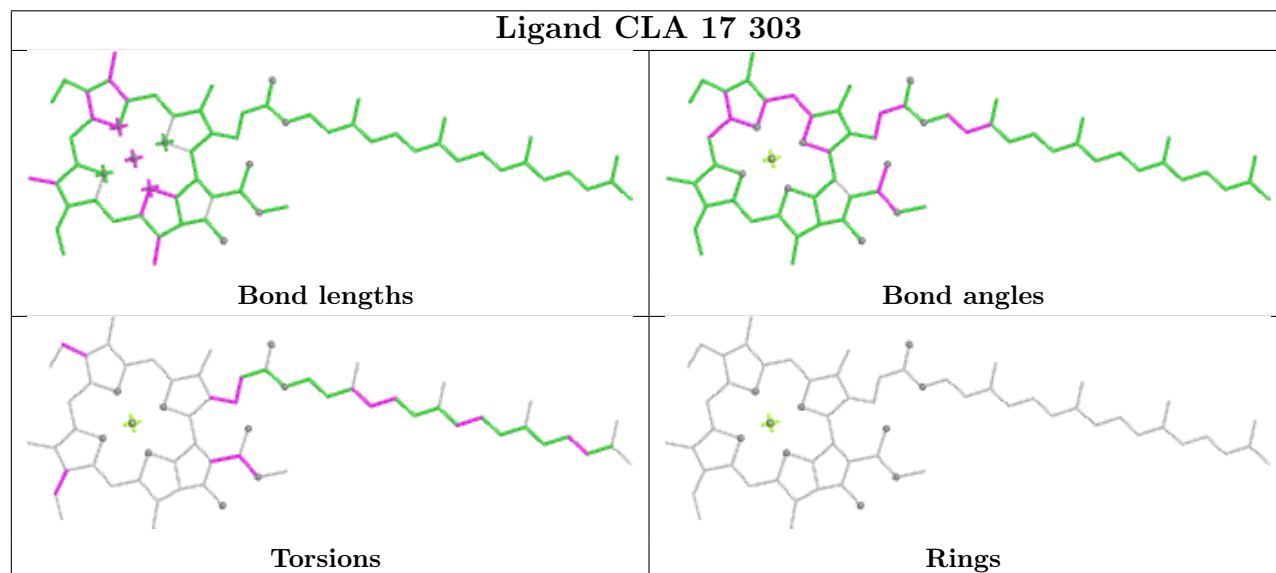
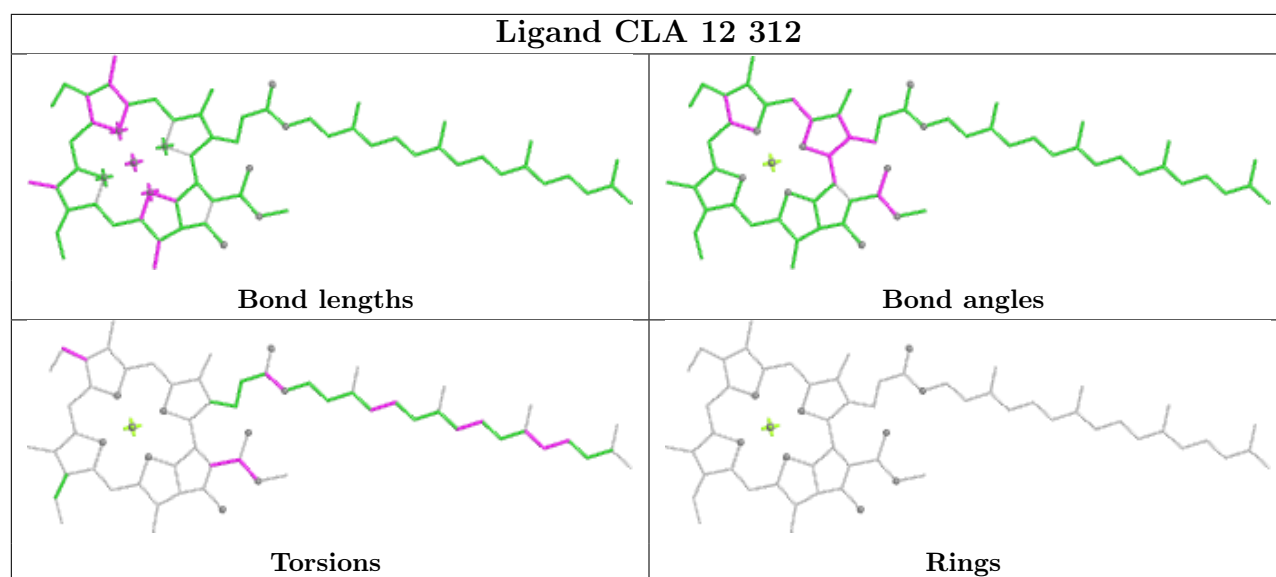
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

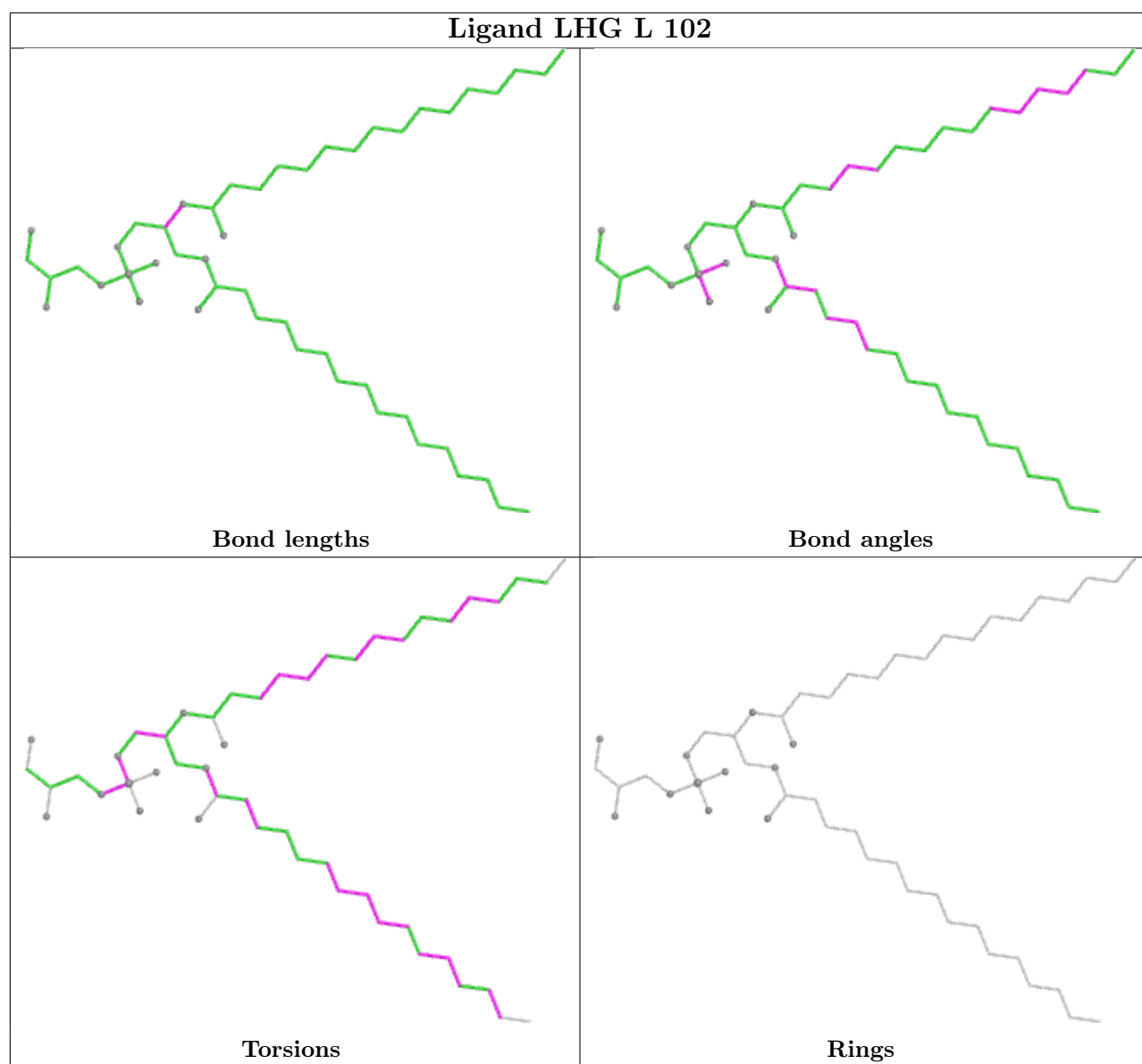


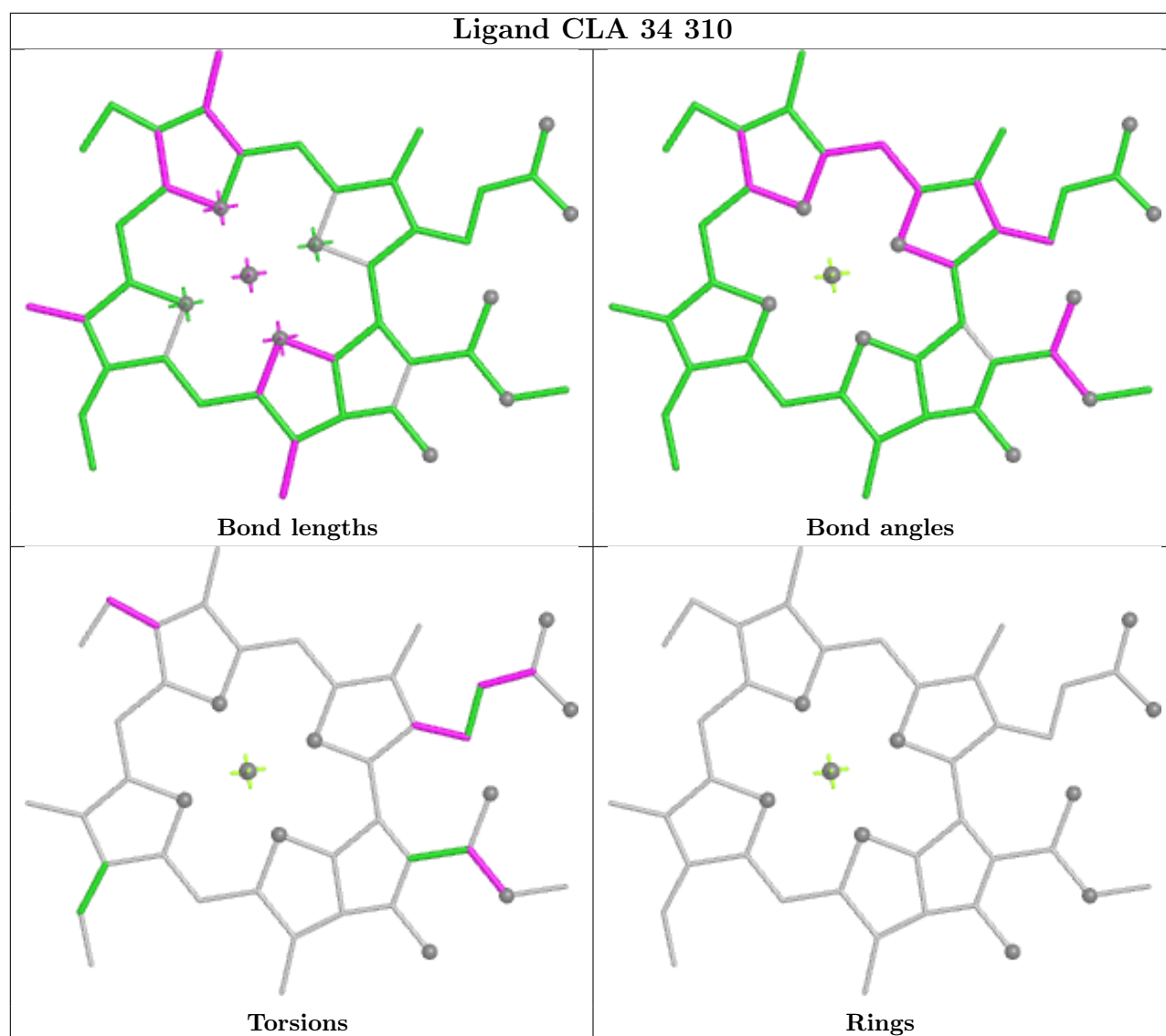


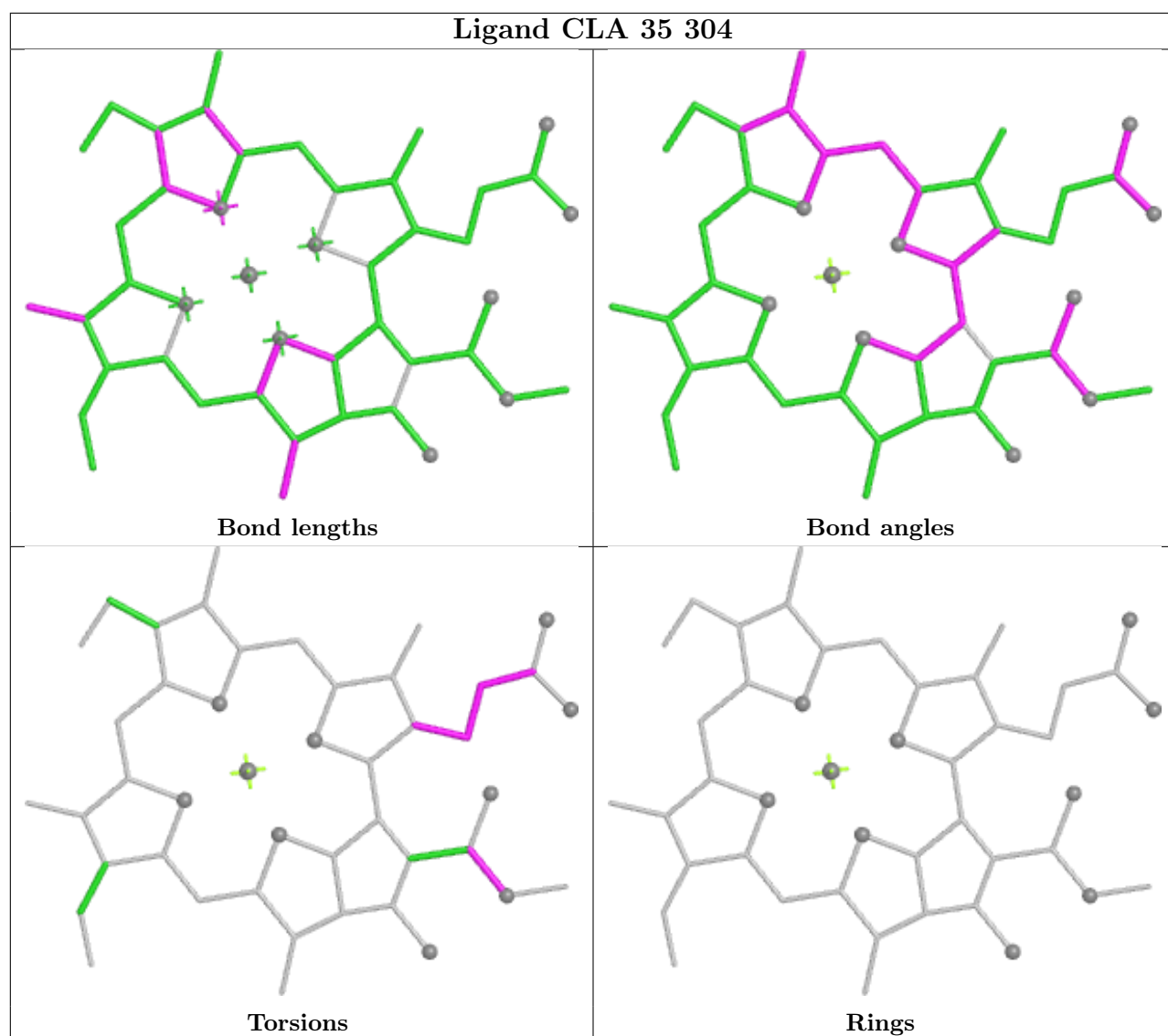


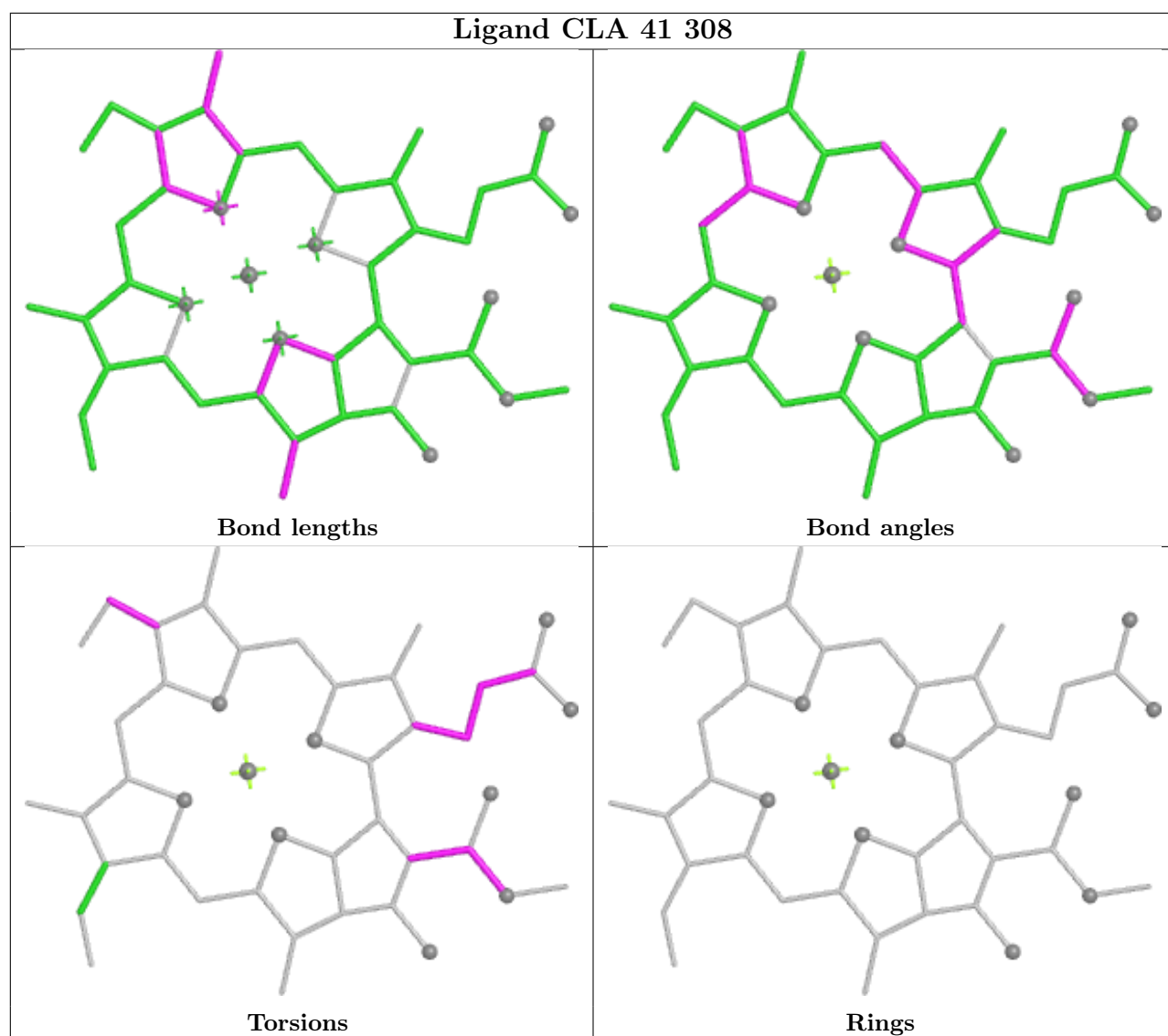


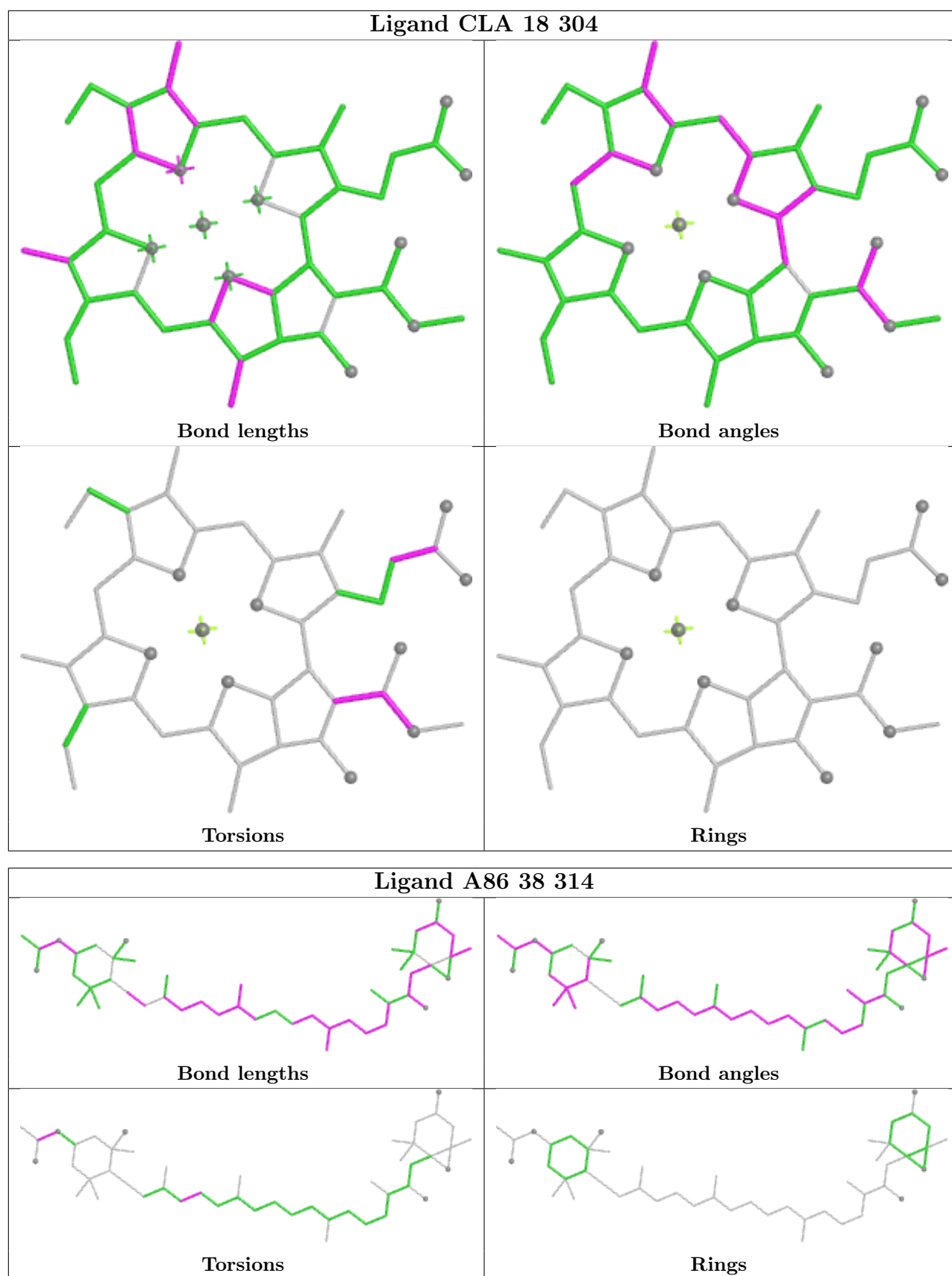


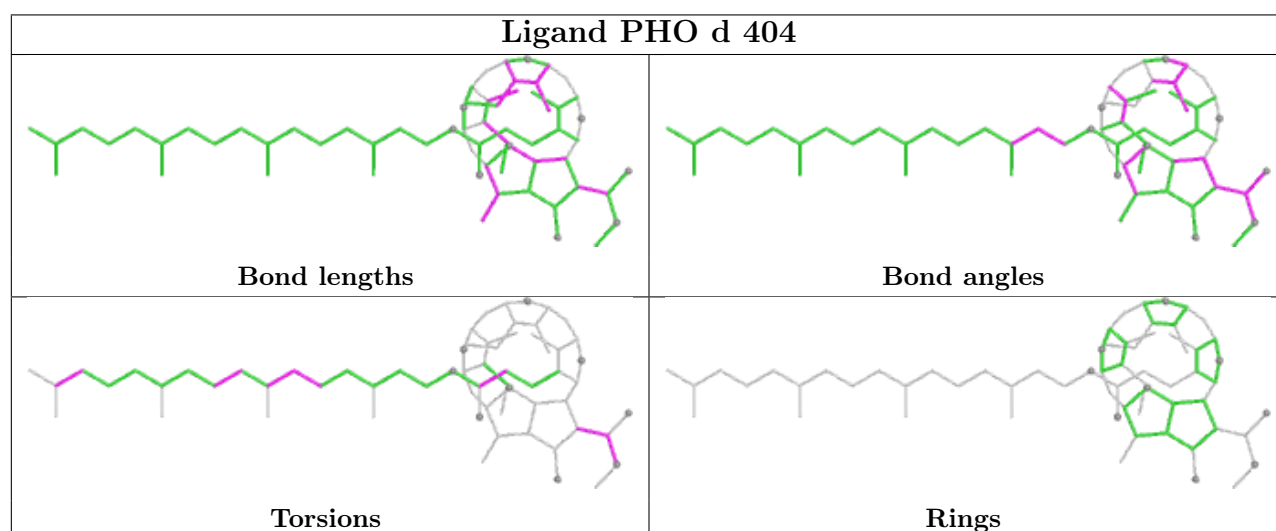
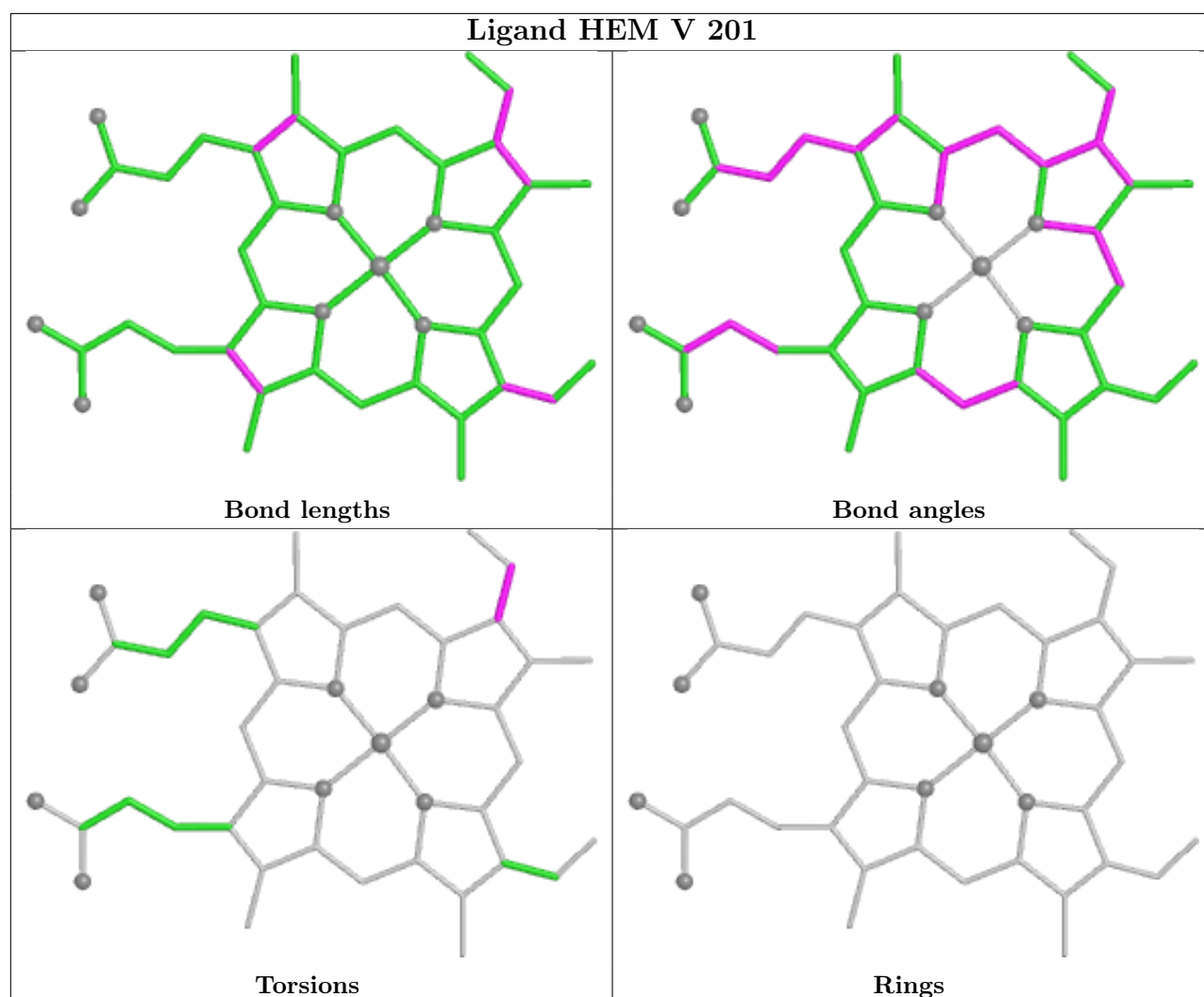


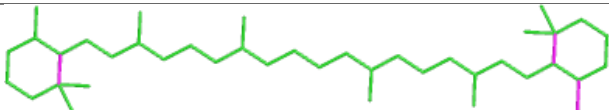
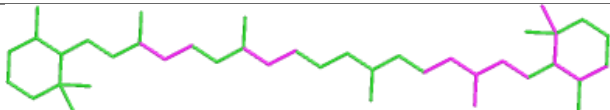
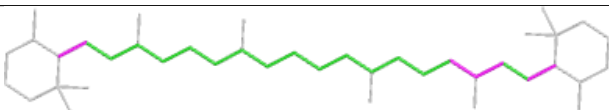
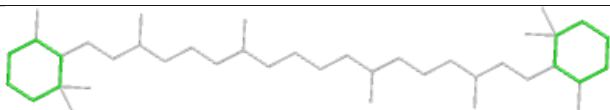


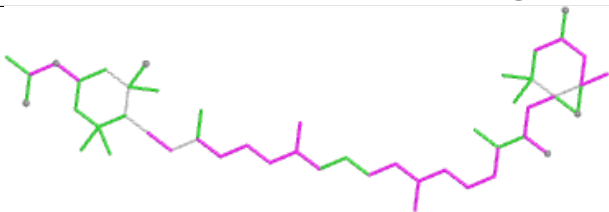
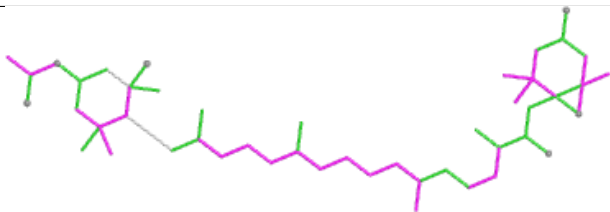
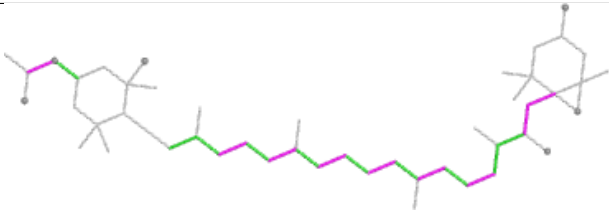
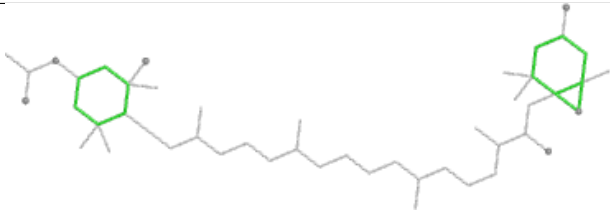


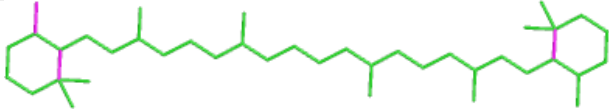
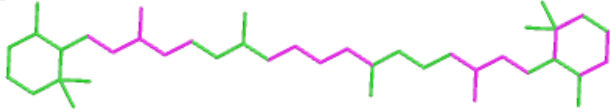
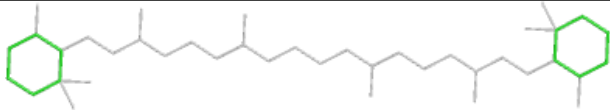


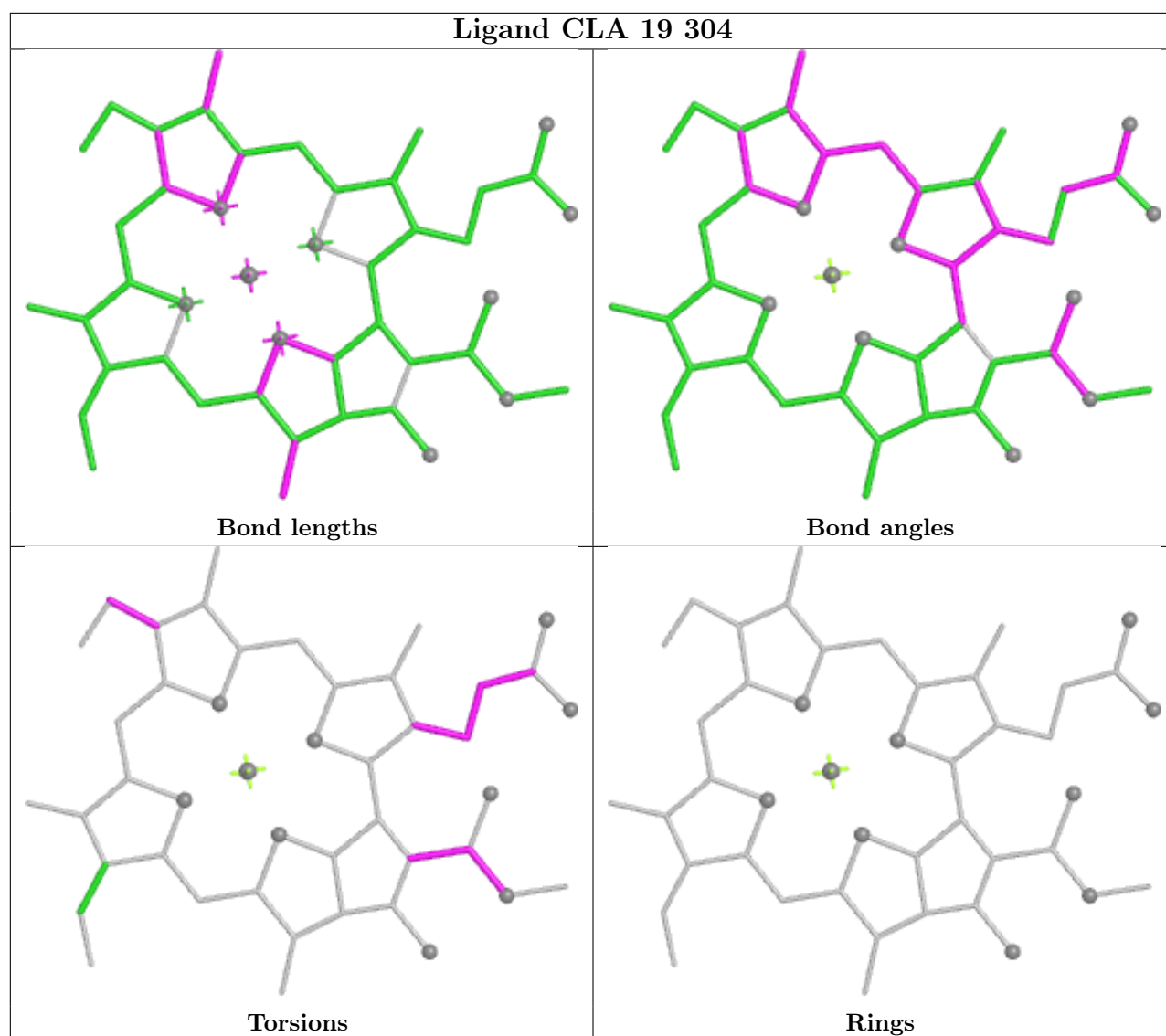


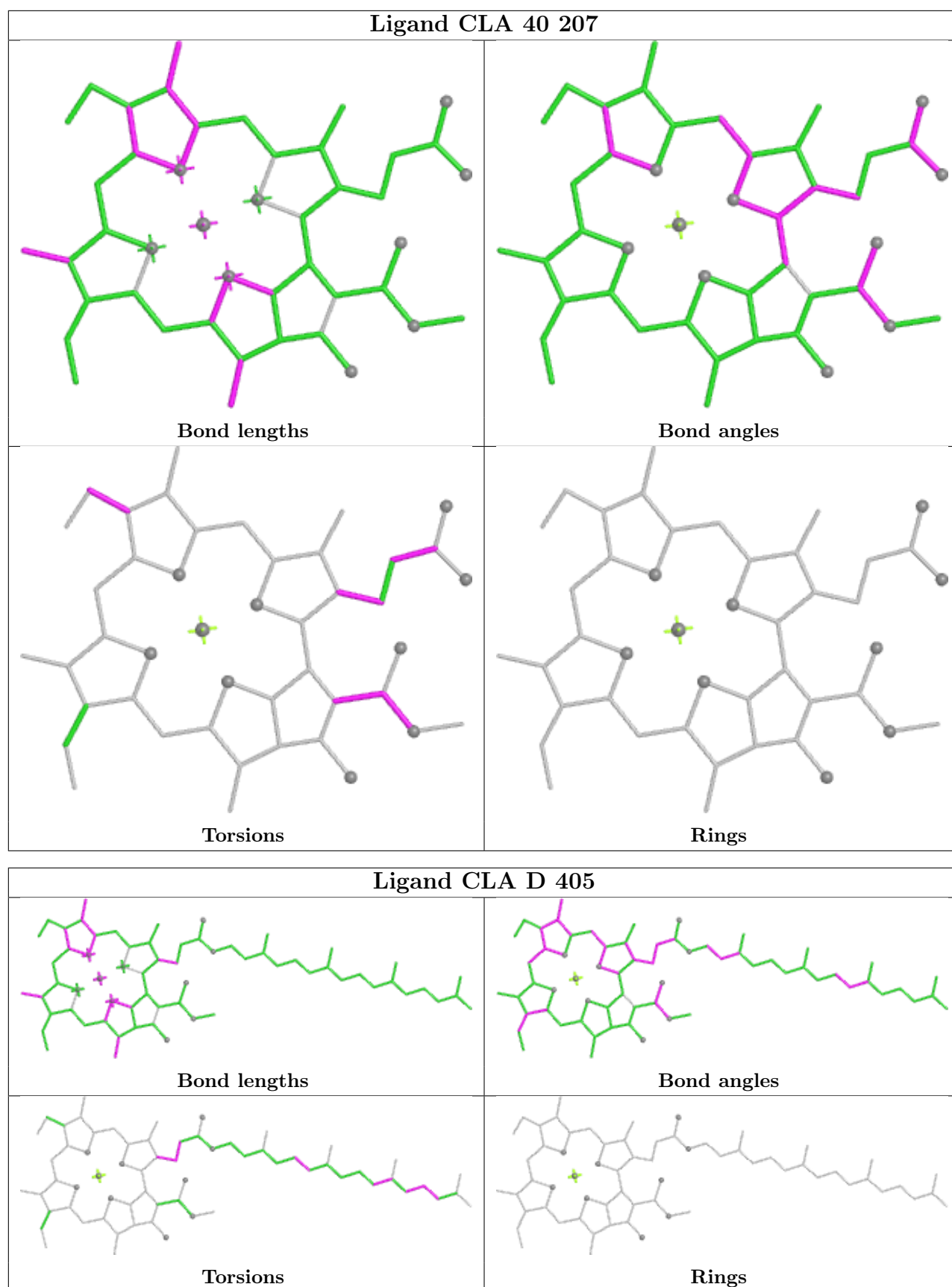


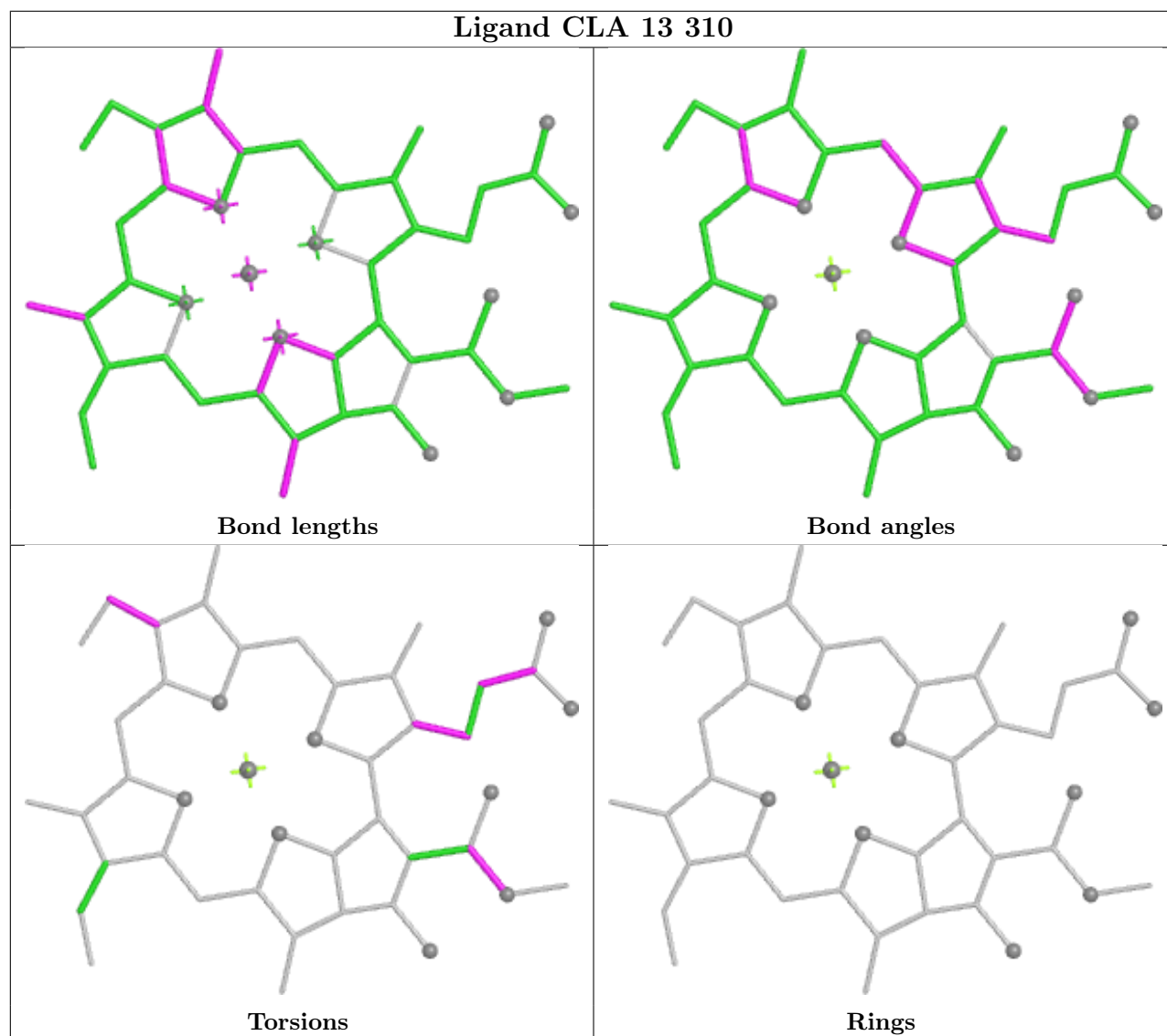
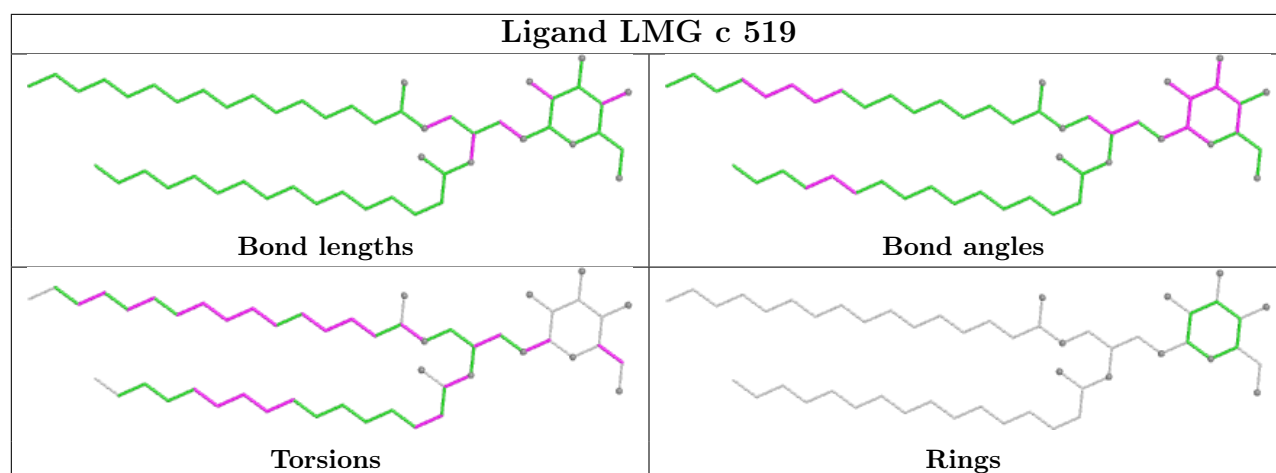
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

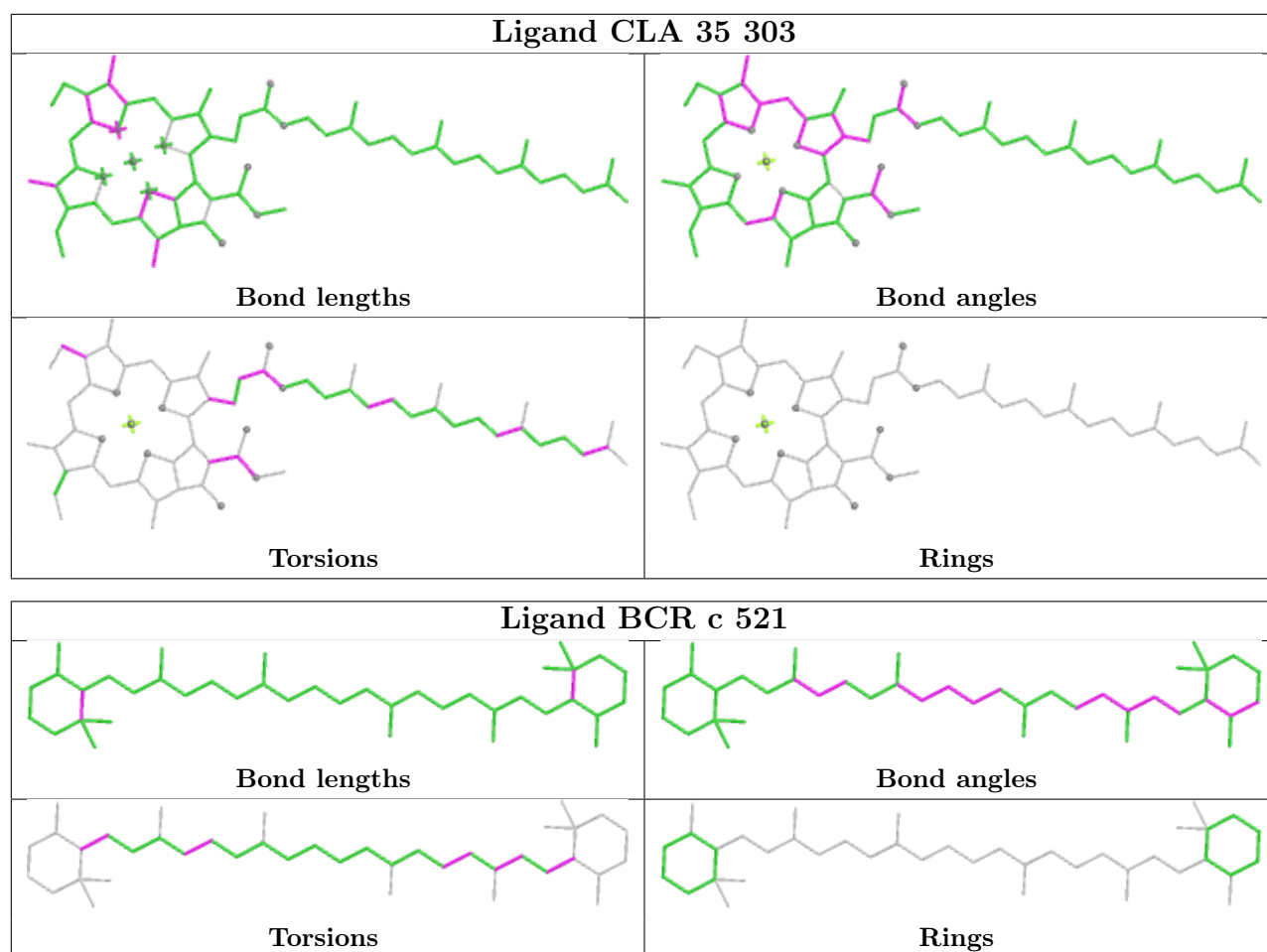
Ligand A86 37 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

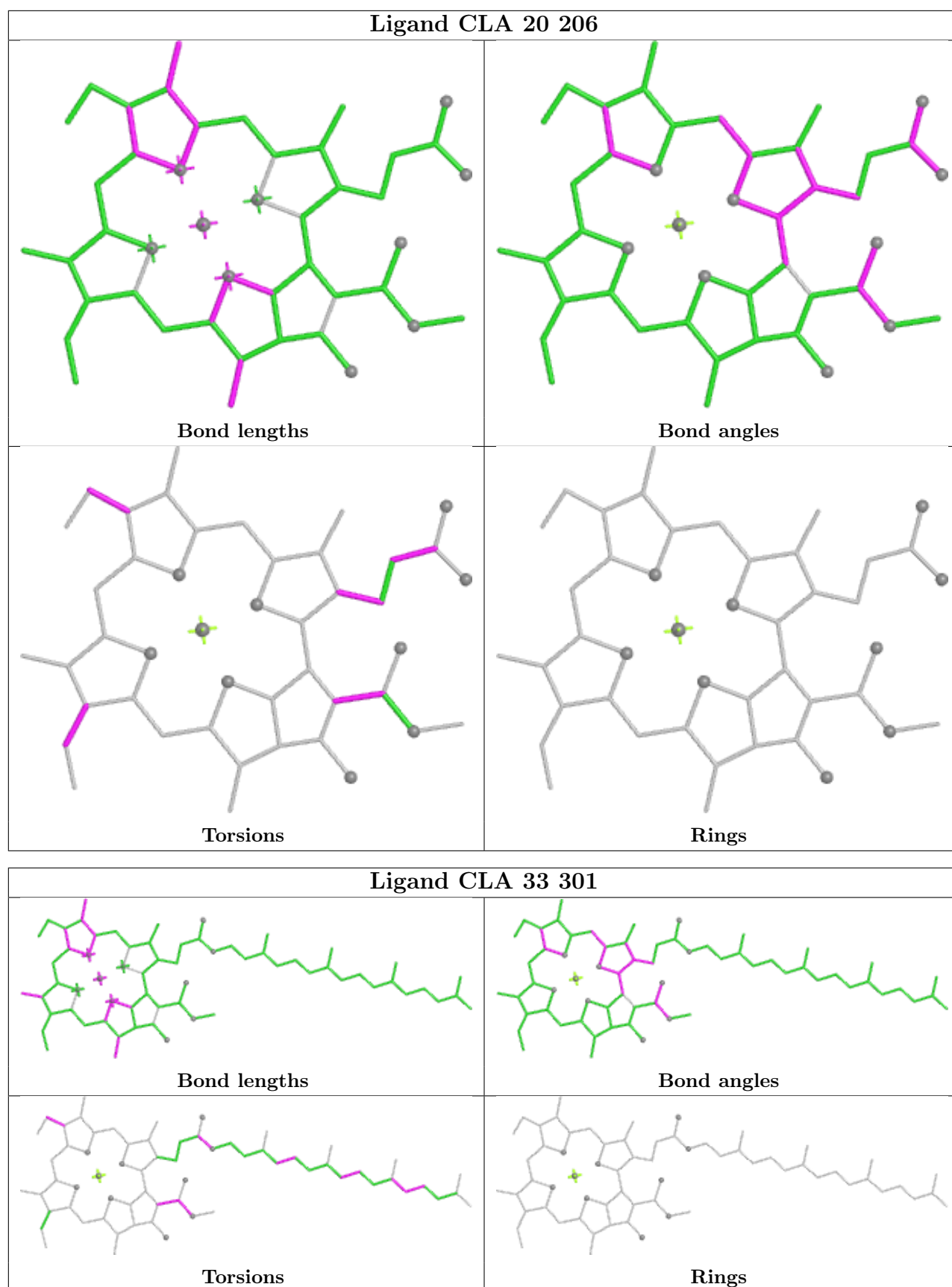
Ligand BCR c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

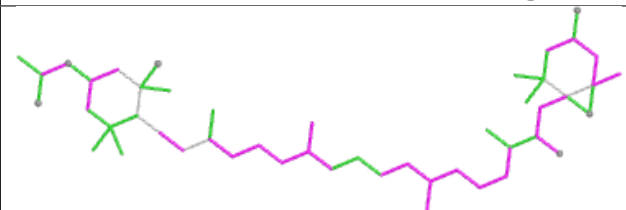
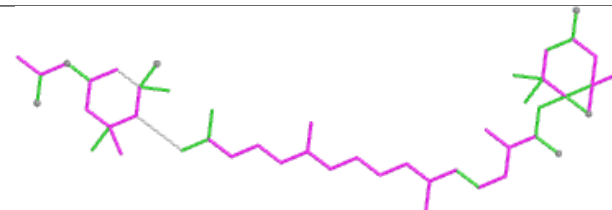
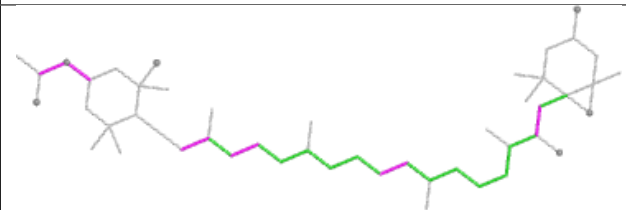
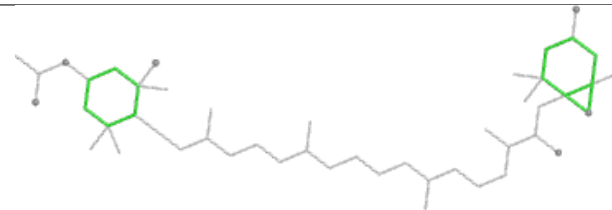


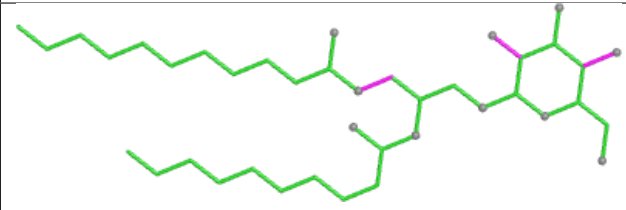
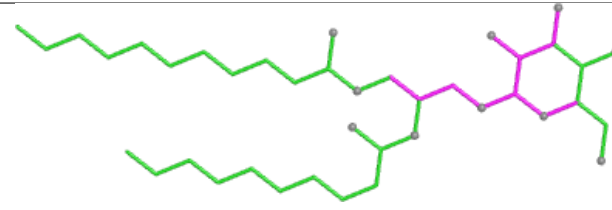
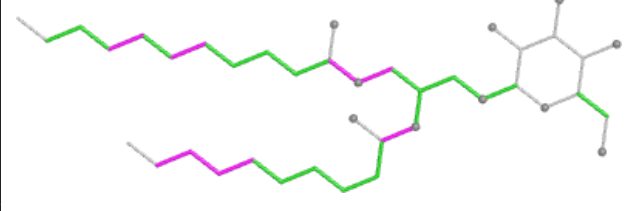
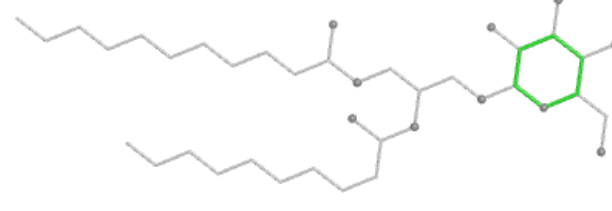


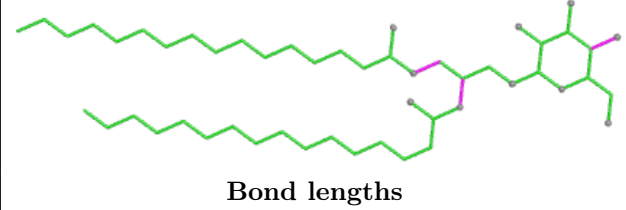
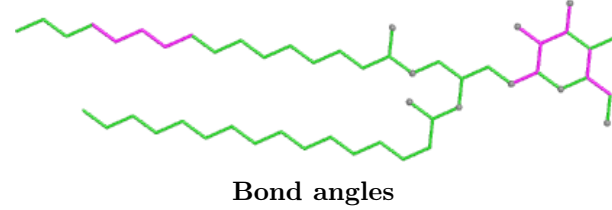
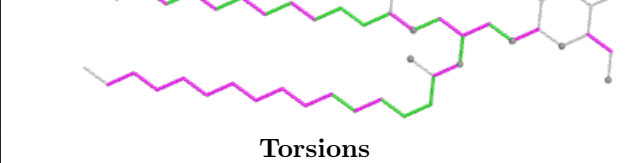


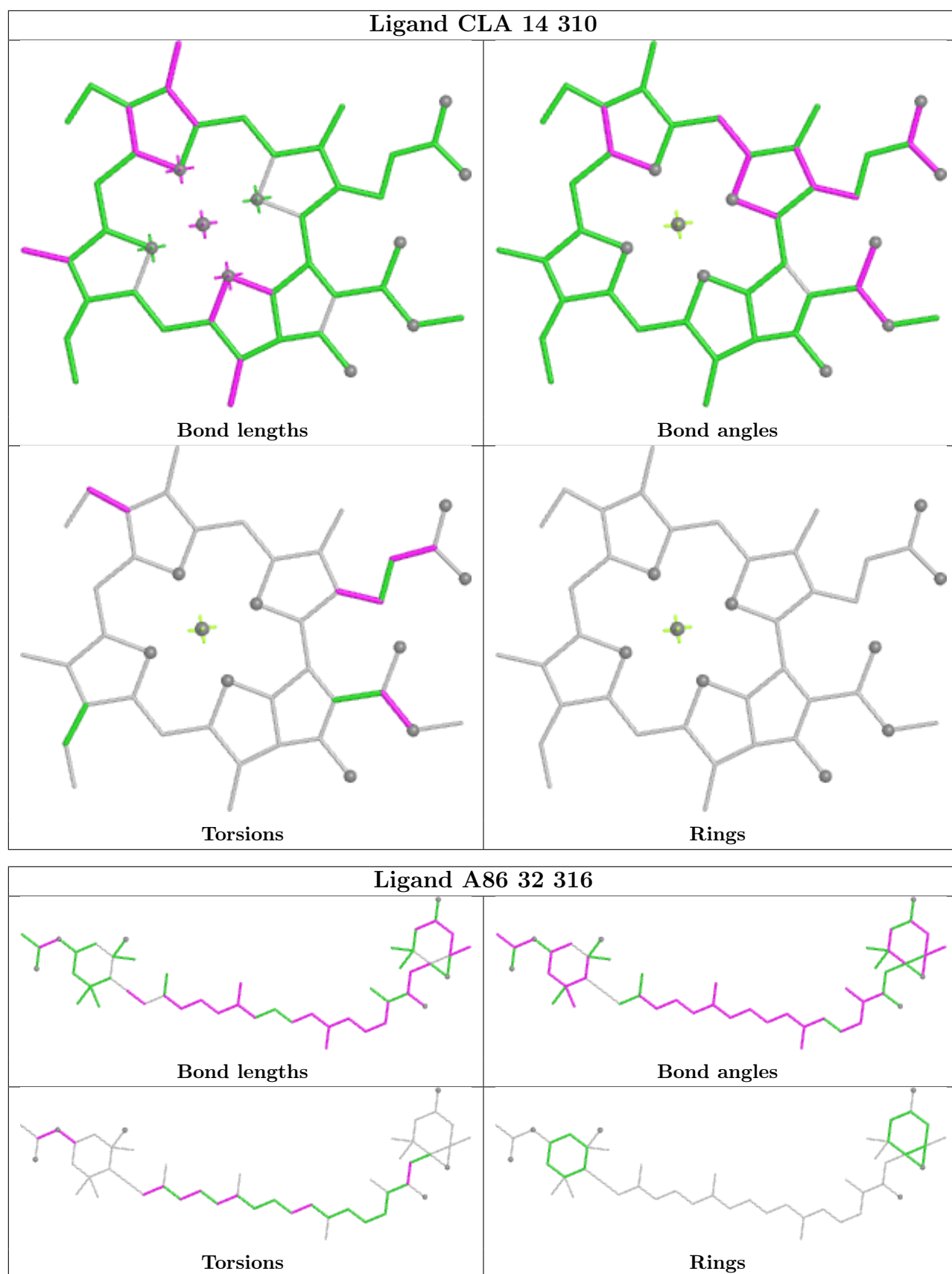


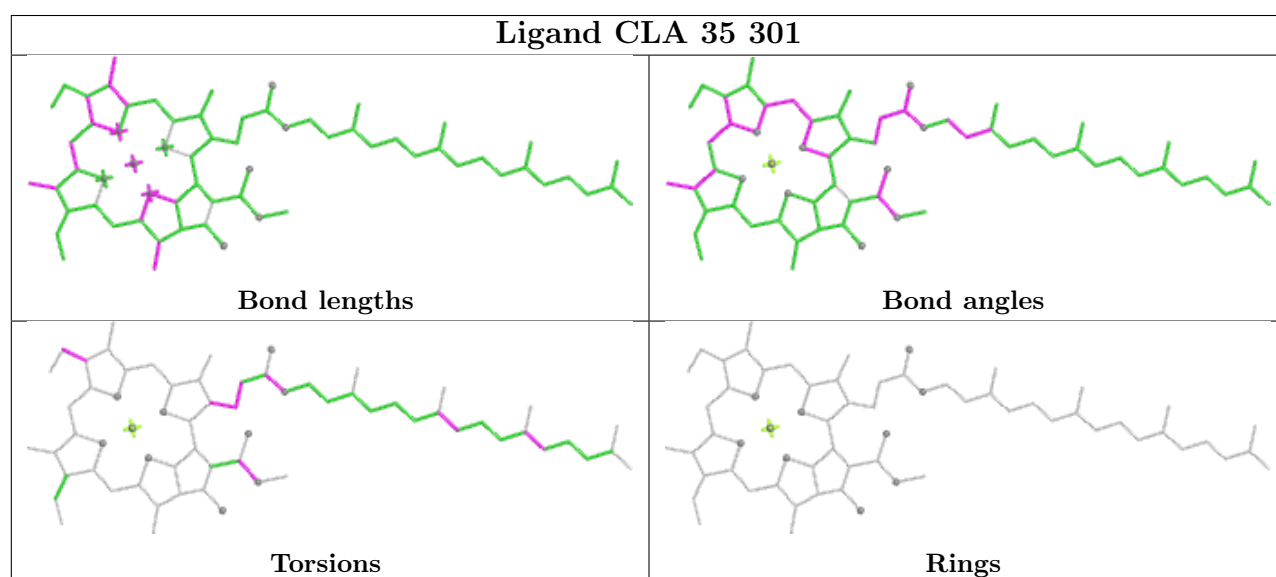
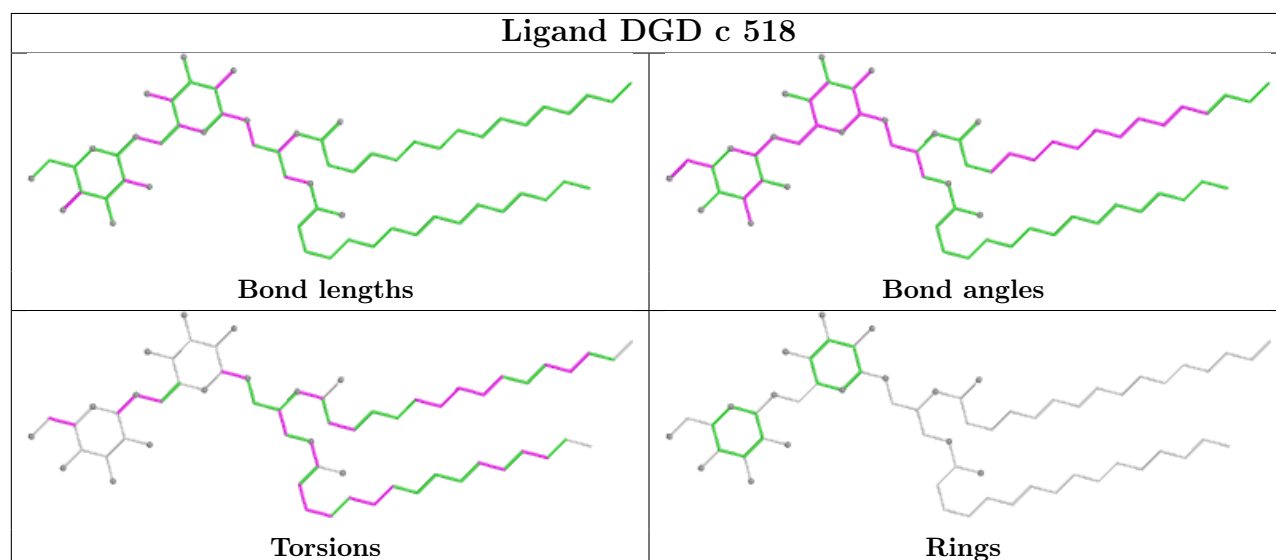
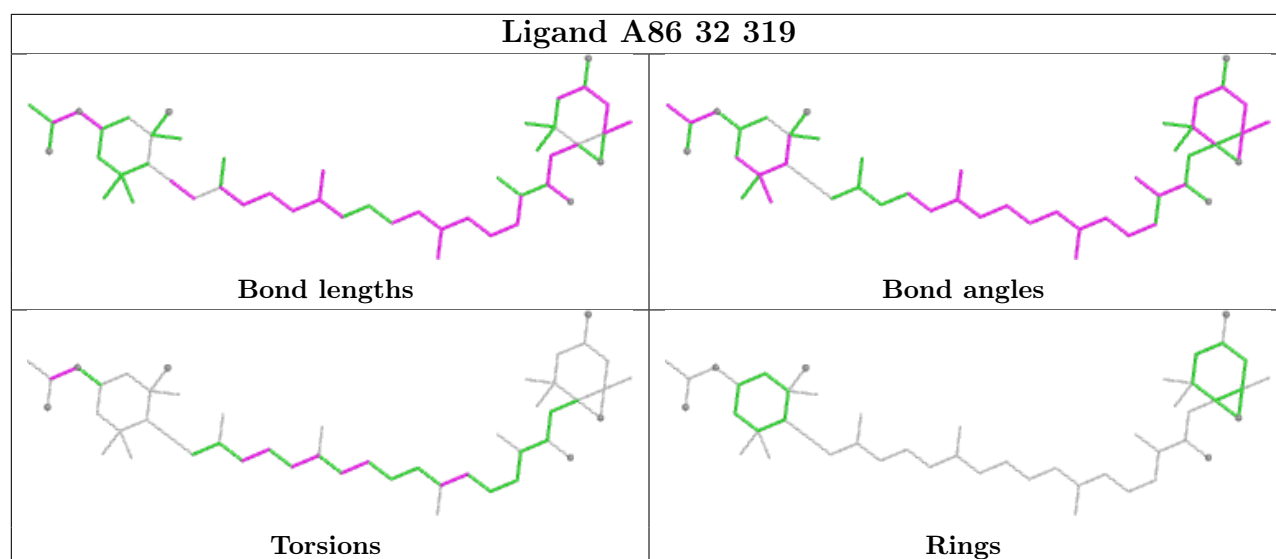


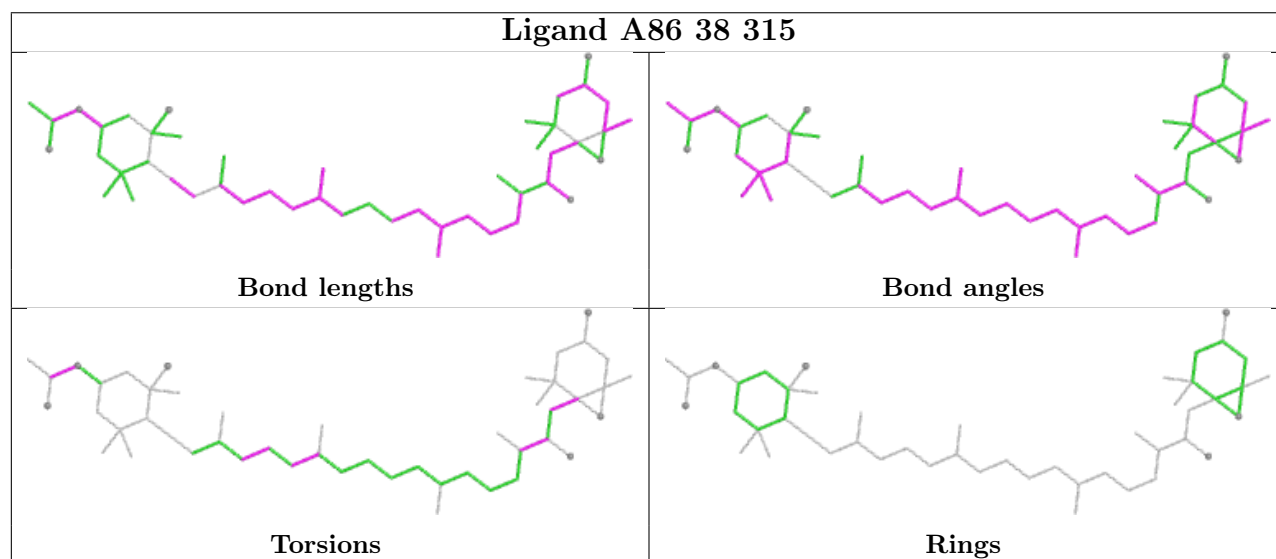
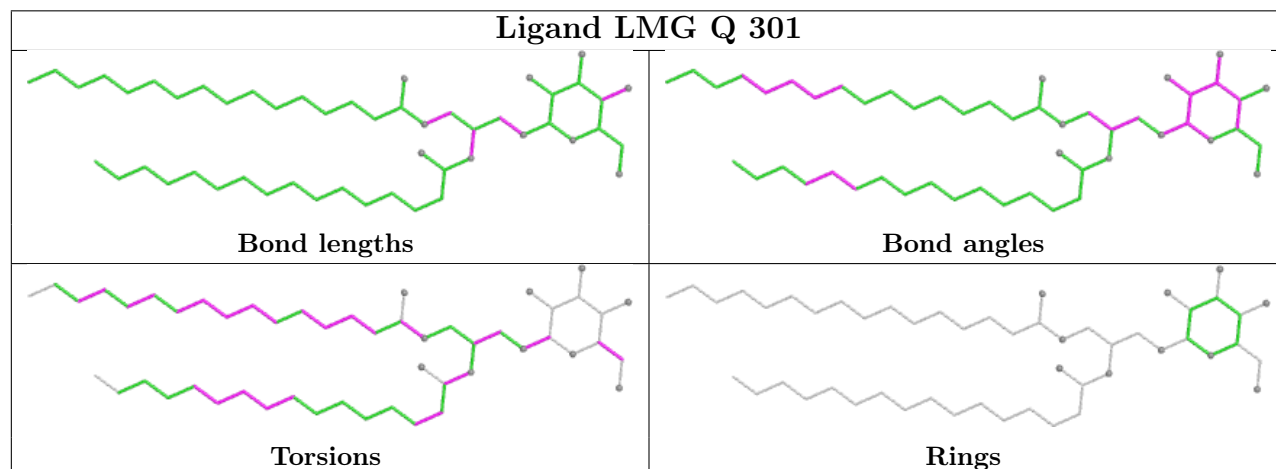
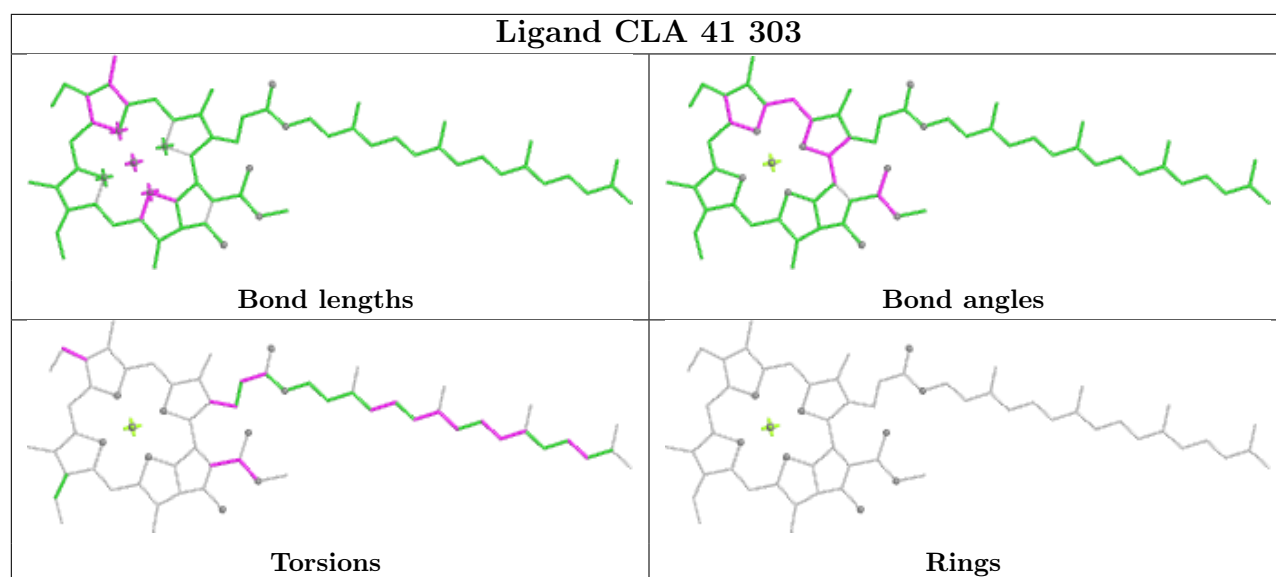
Ligand A86 13 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

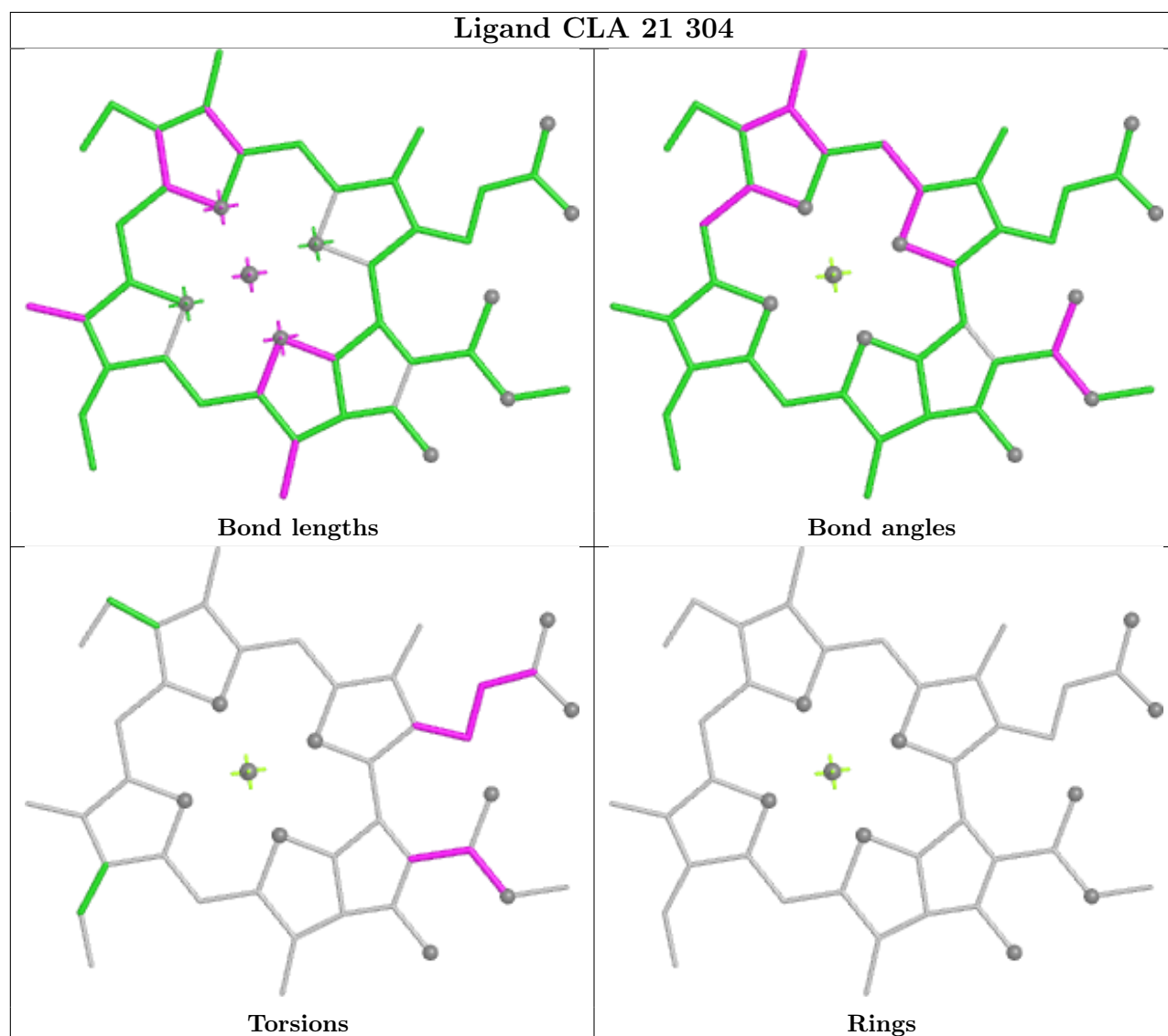
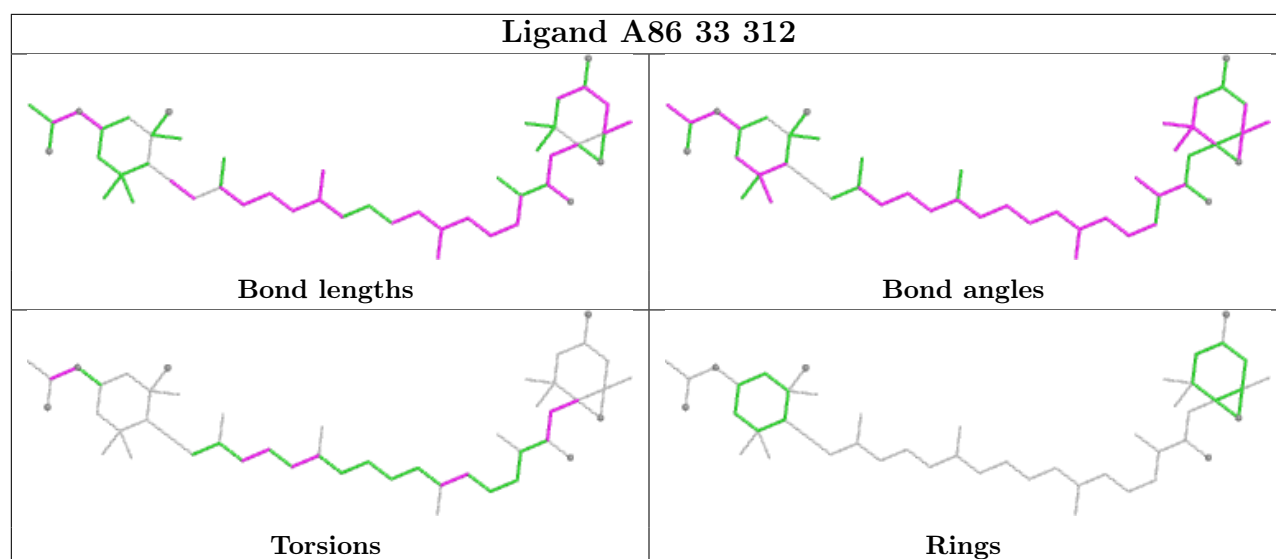
Ligand LMG m 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

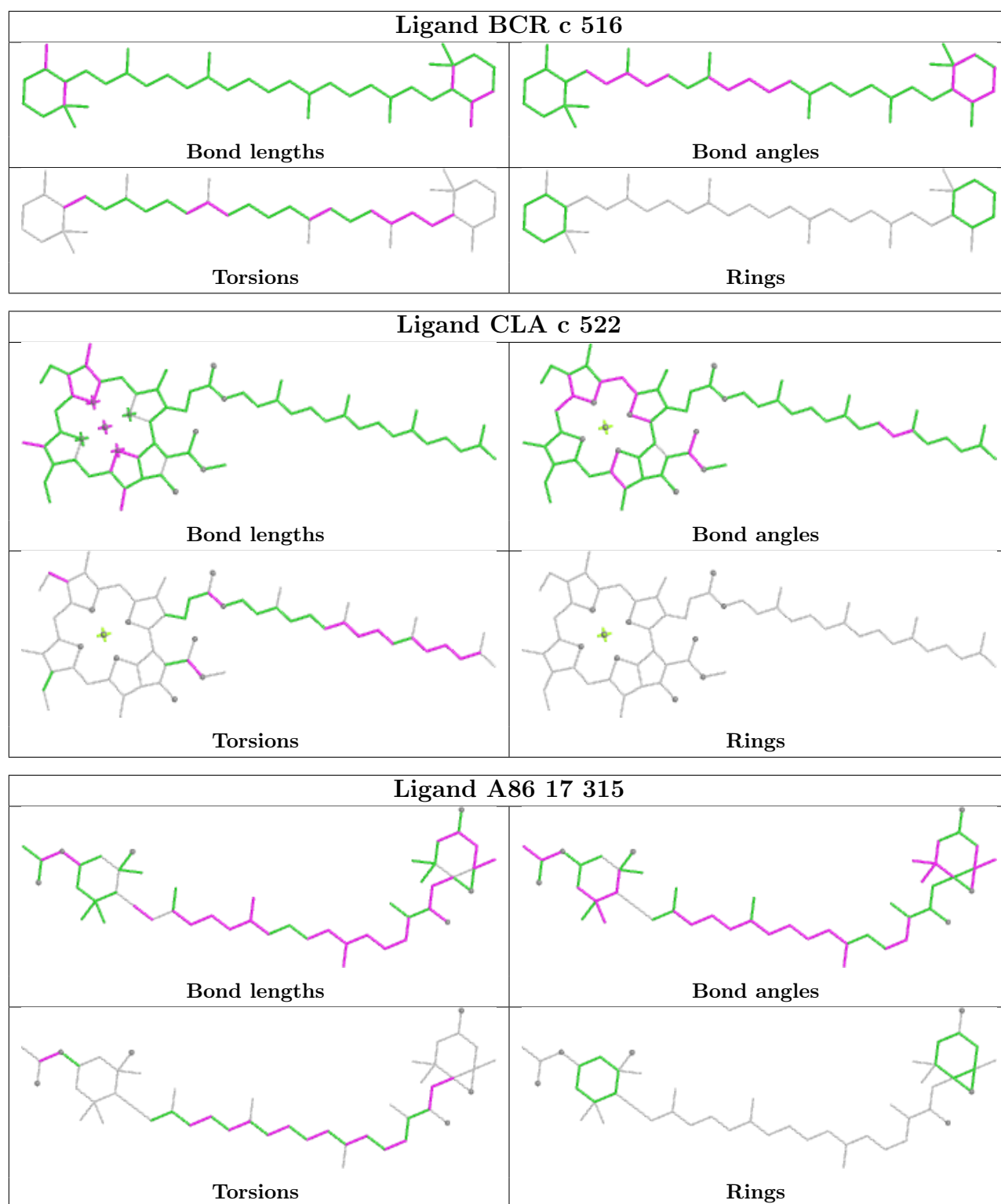
Ligand LMG w 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

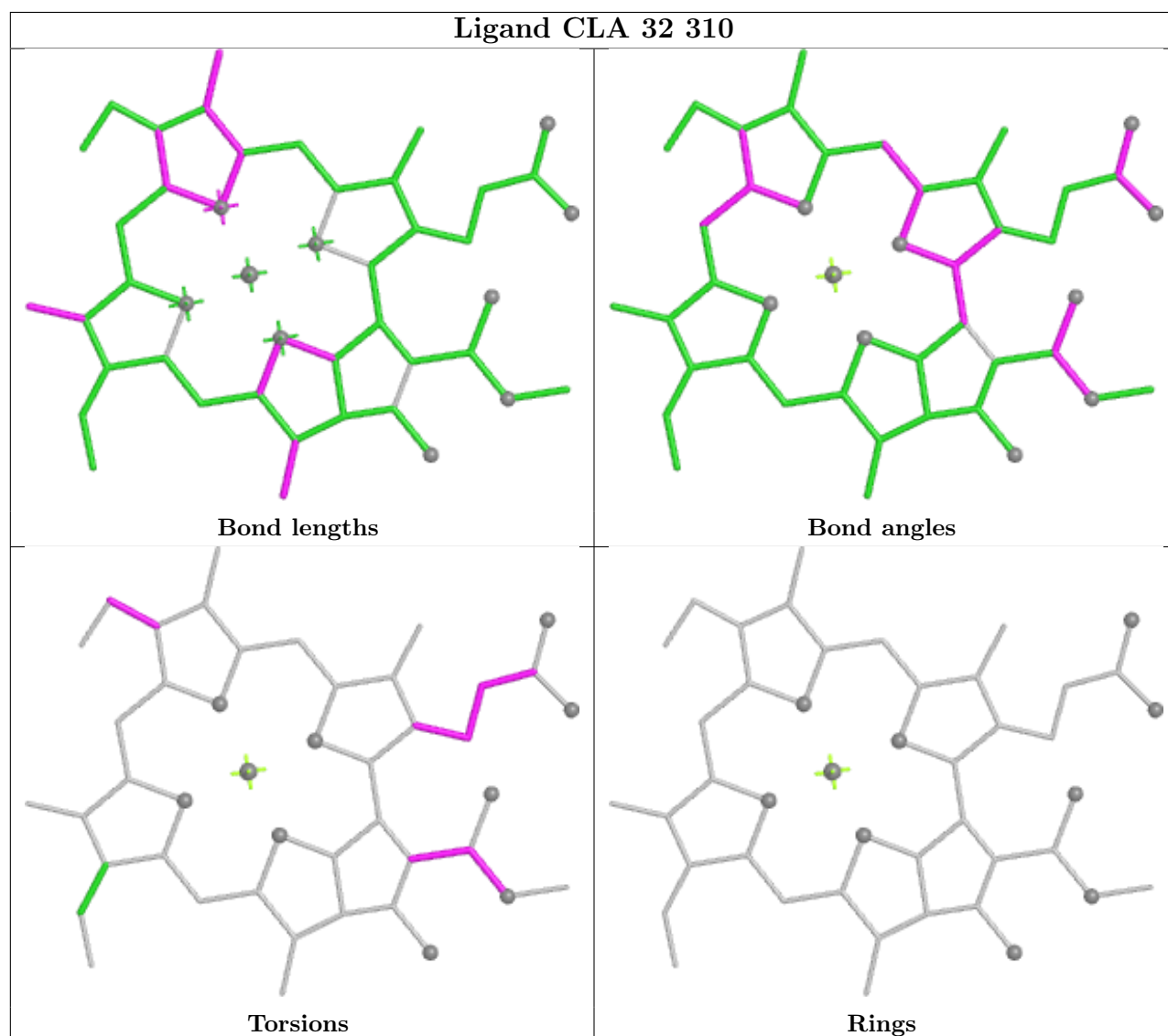
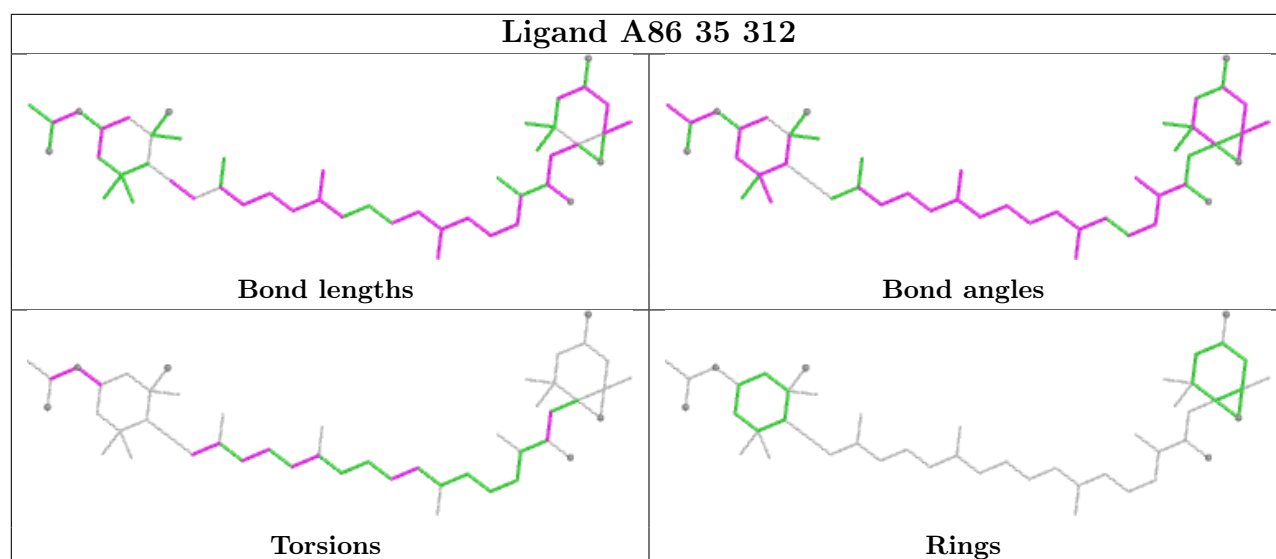


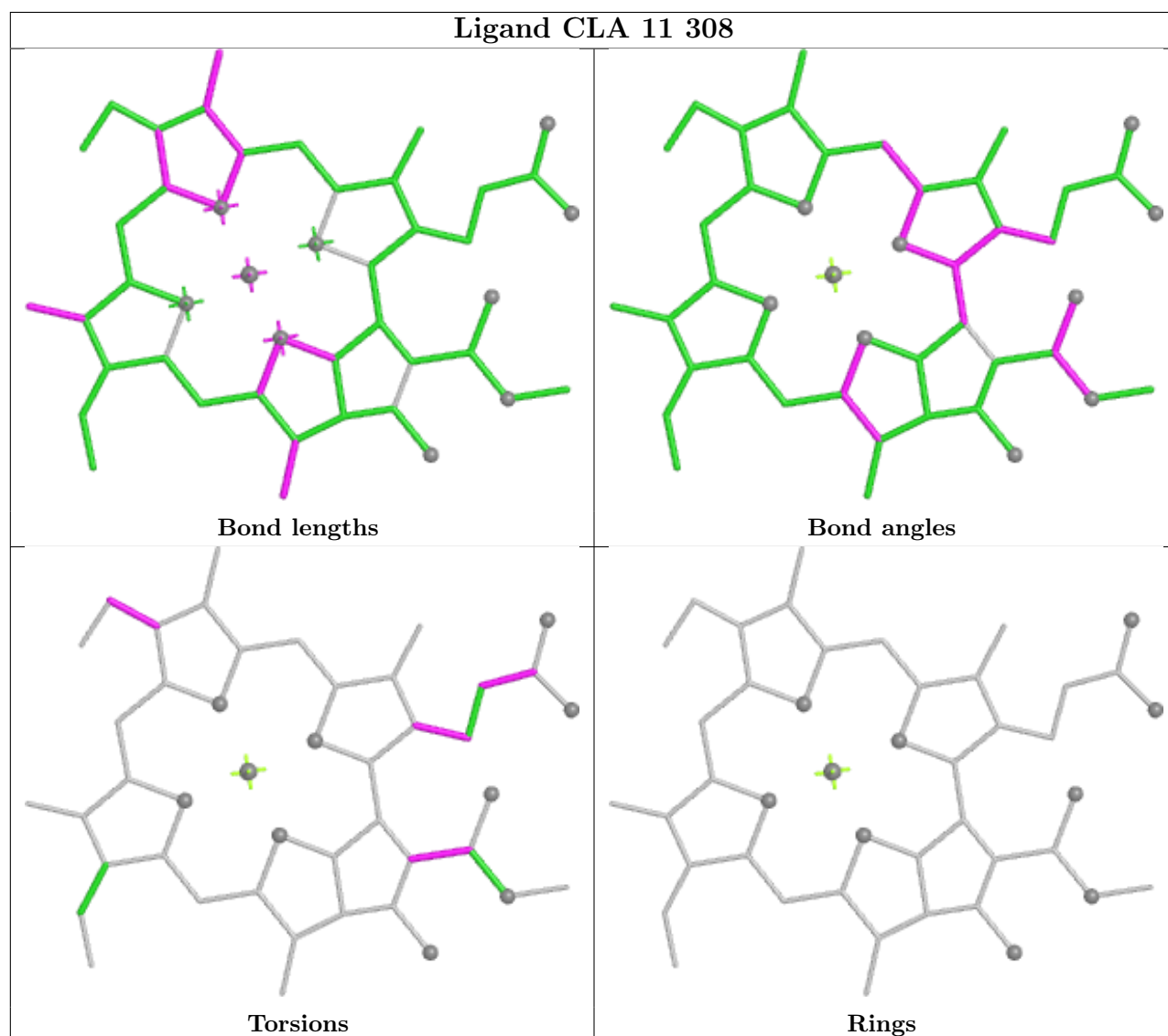
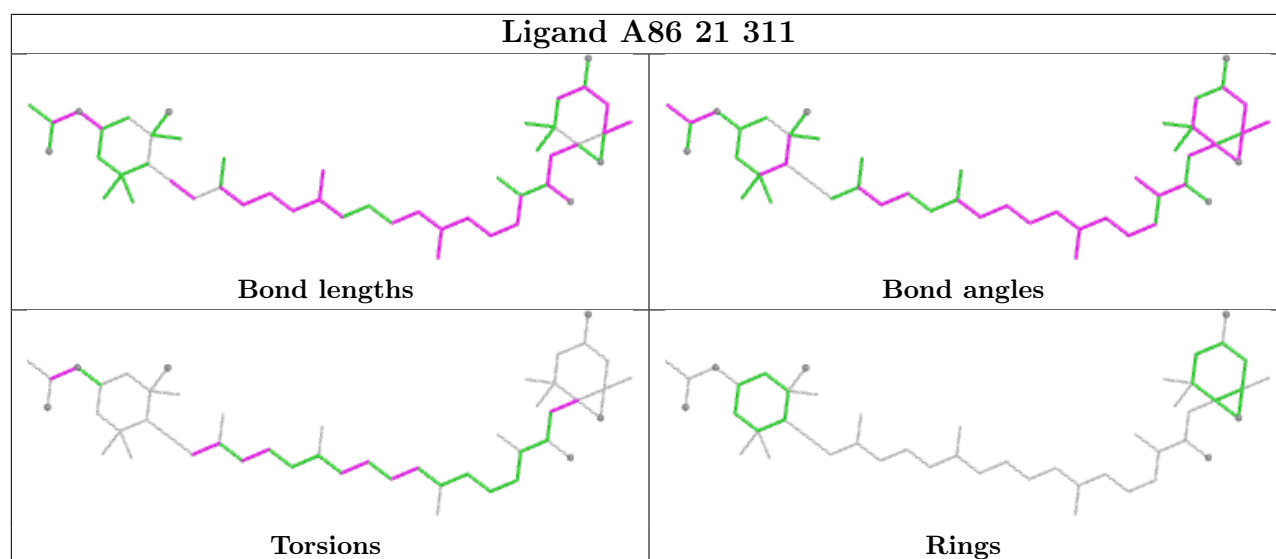


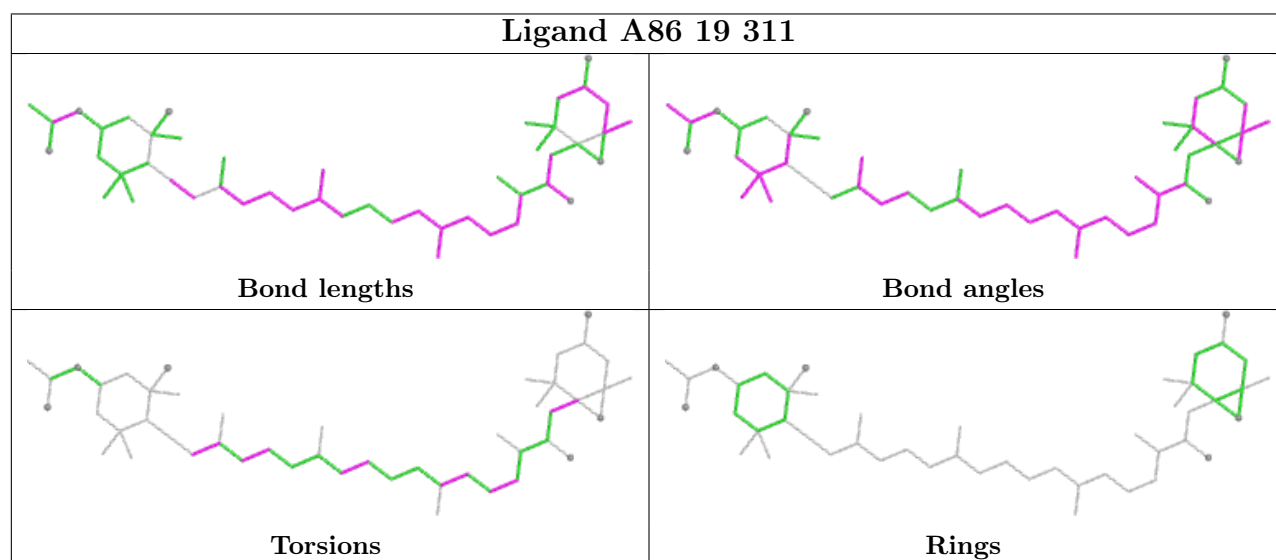
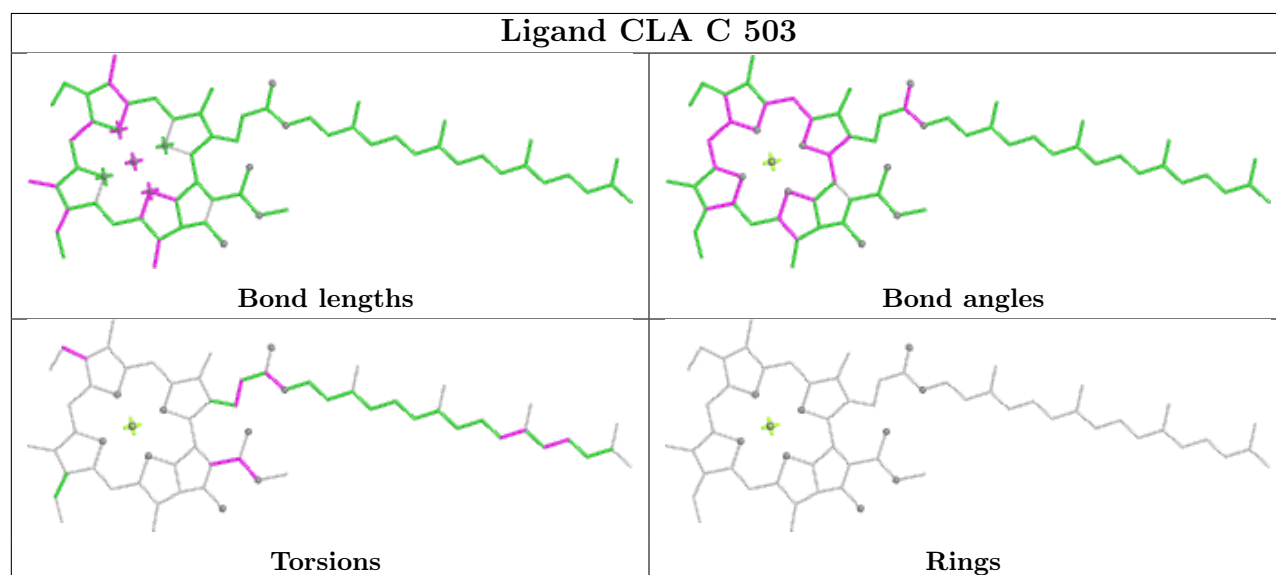
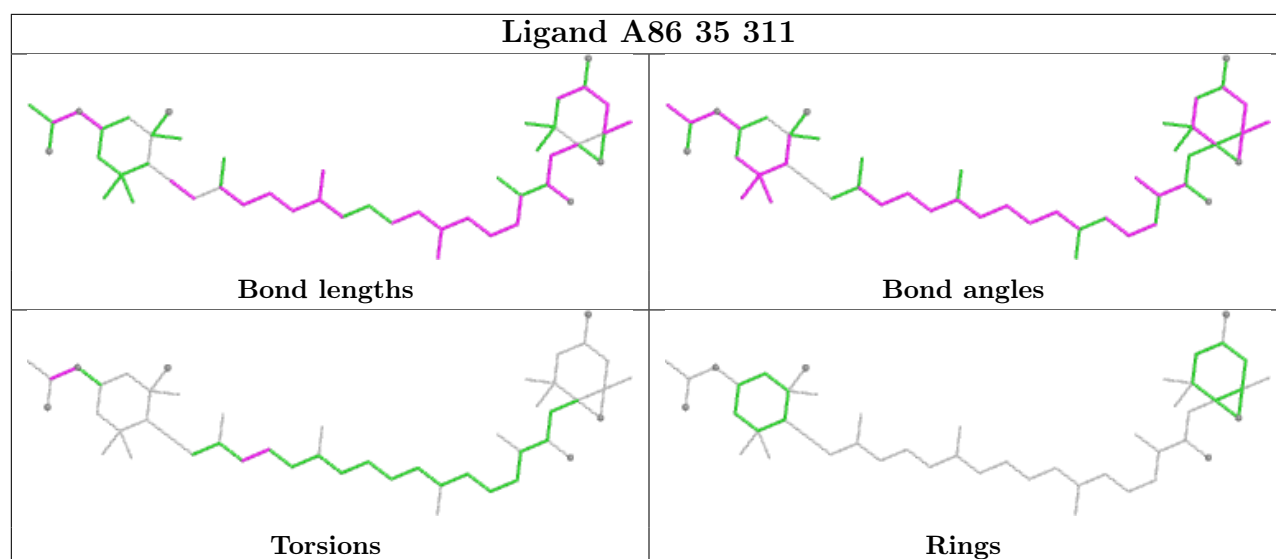


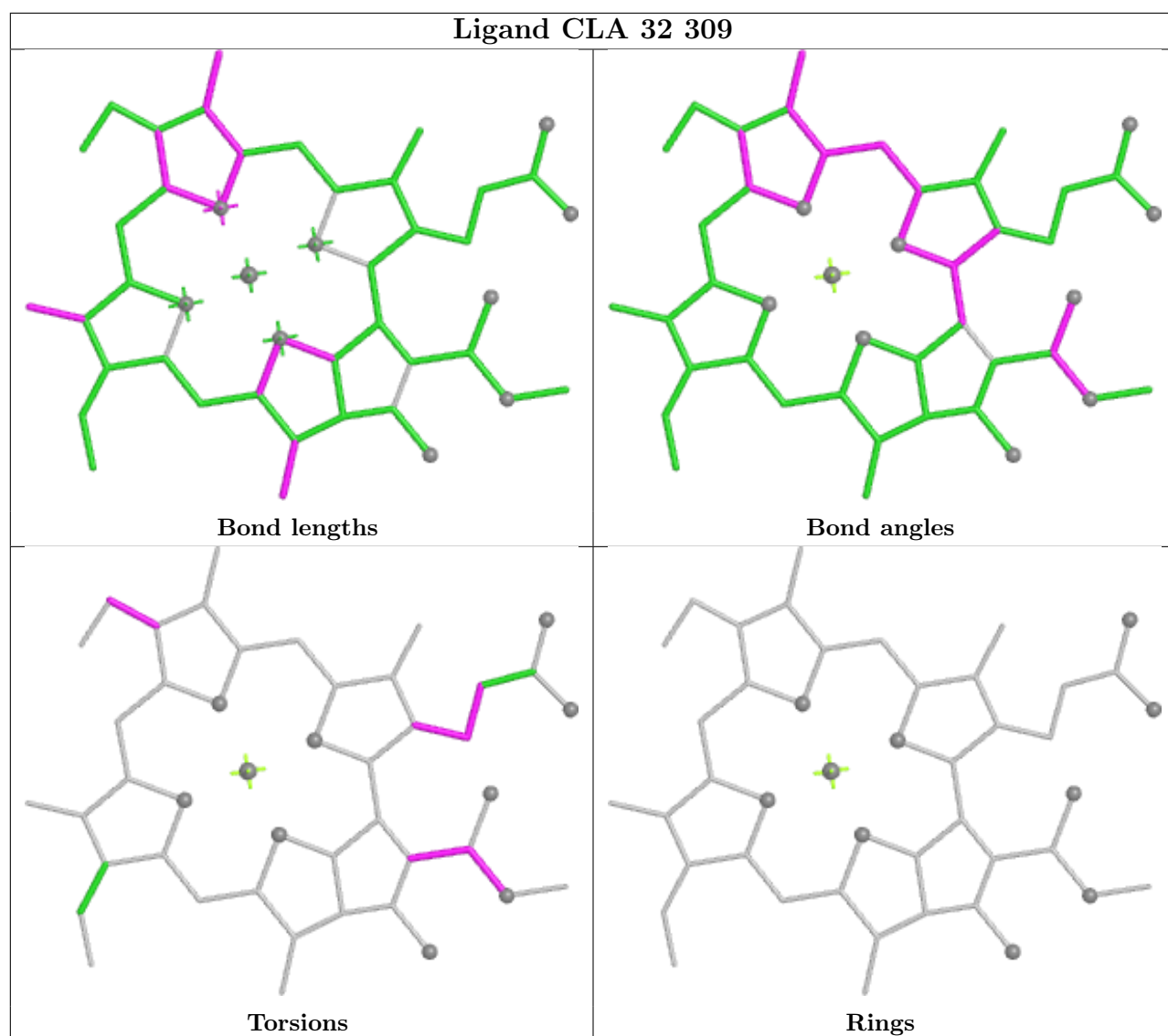


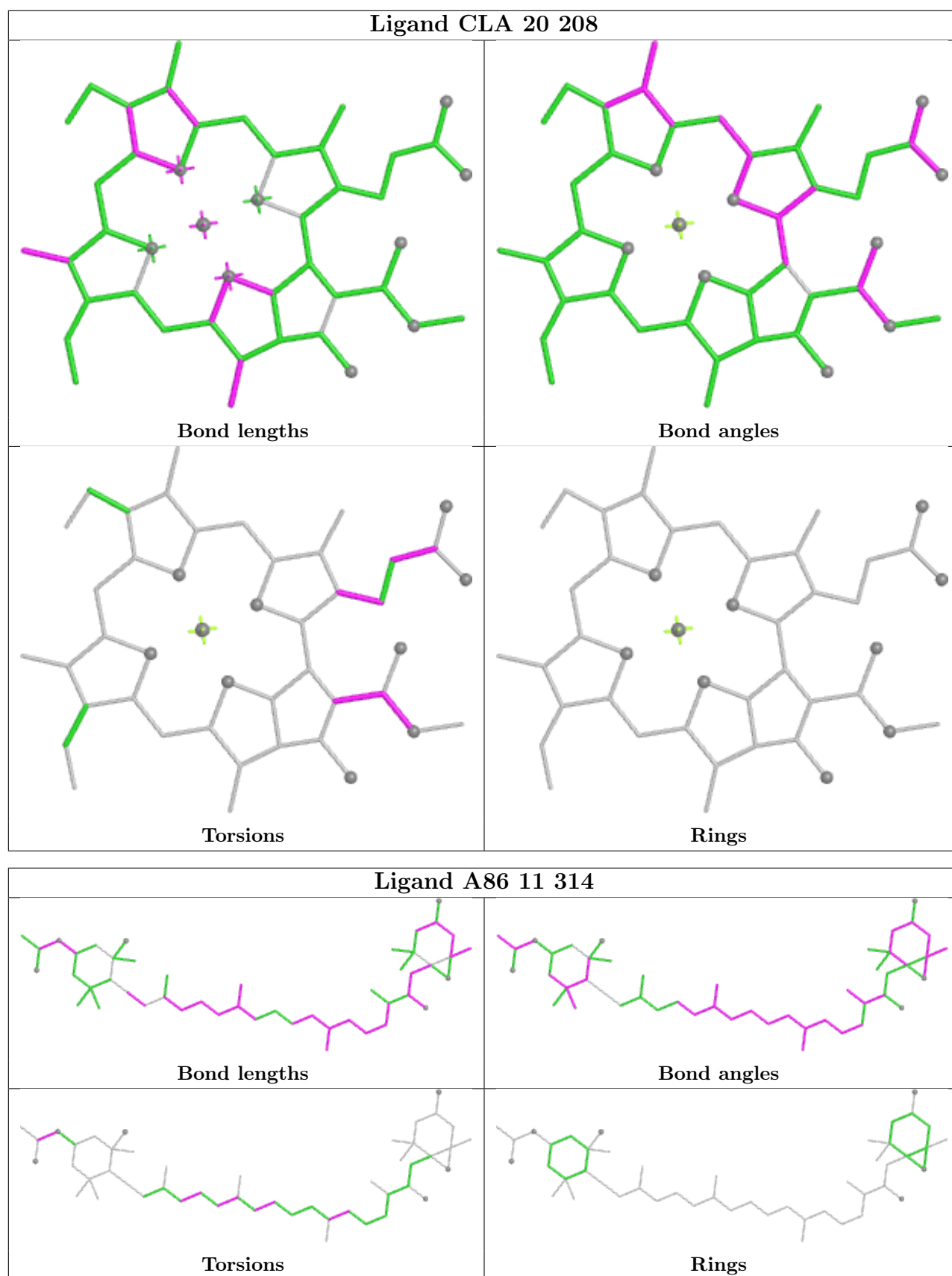


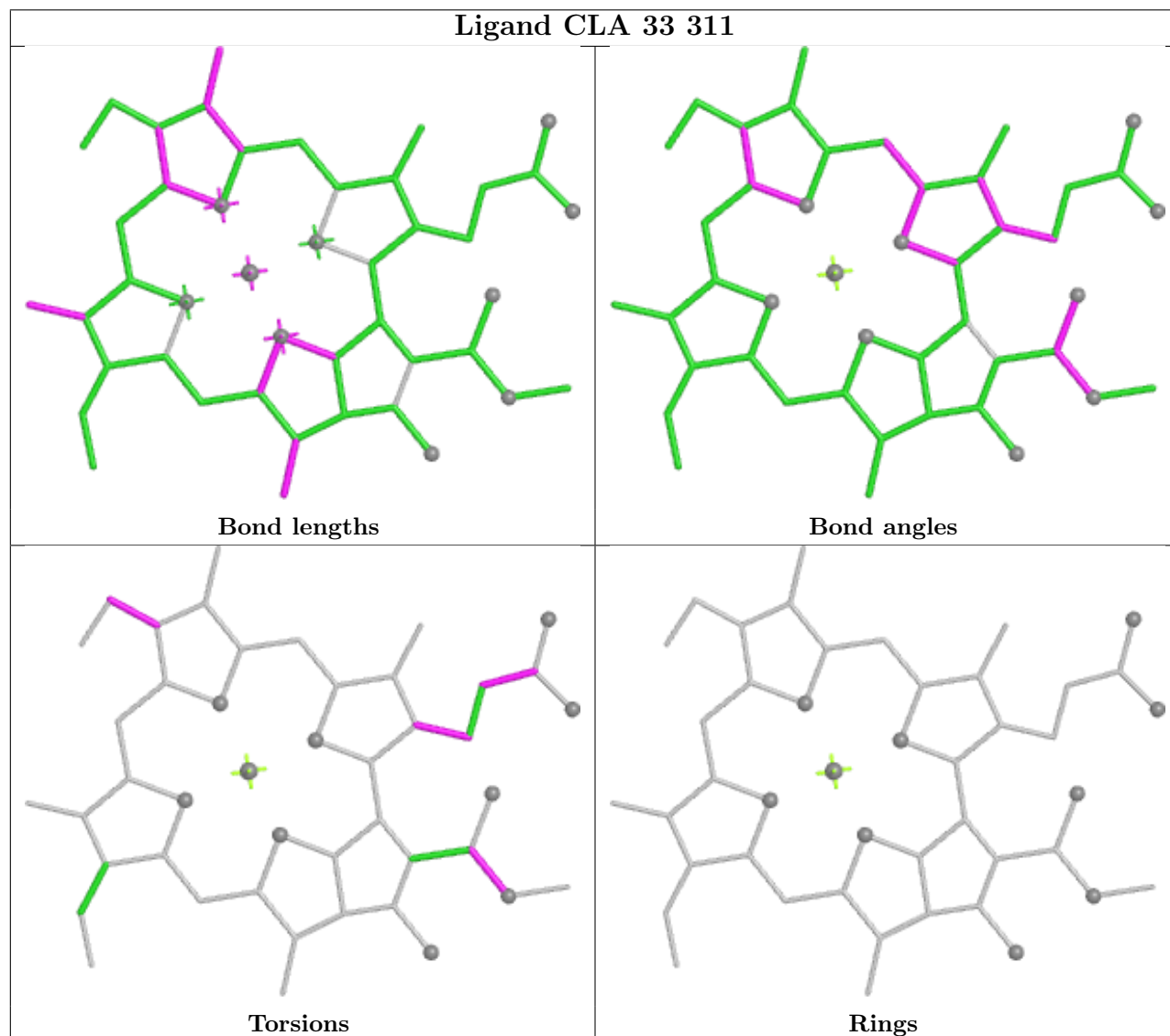
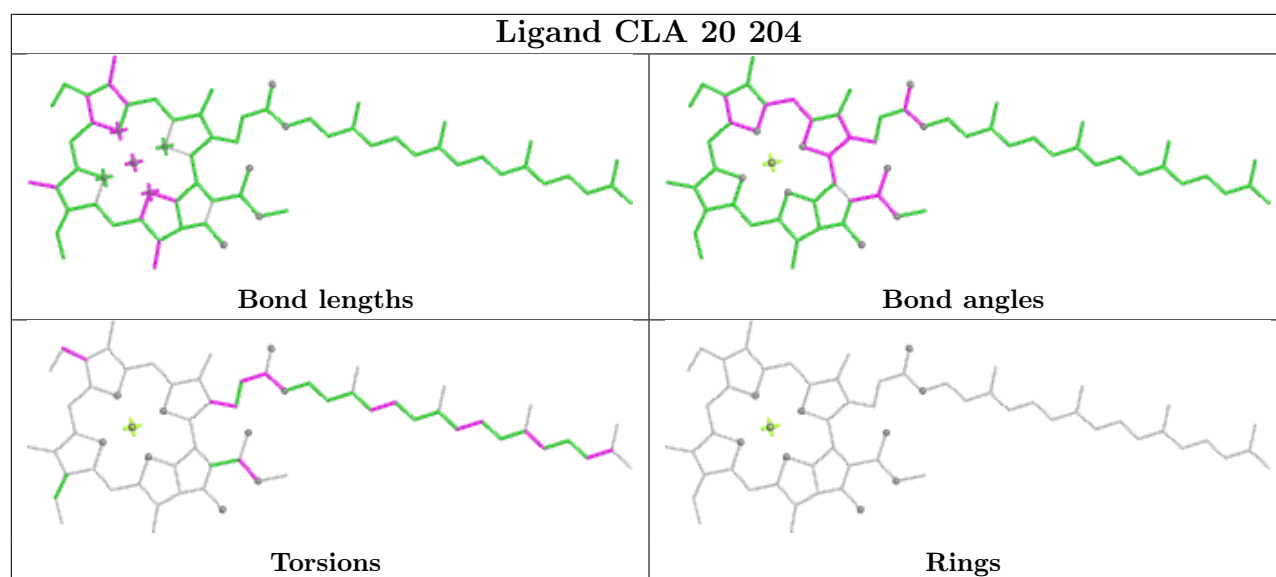


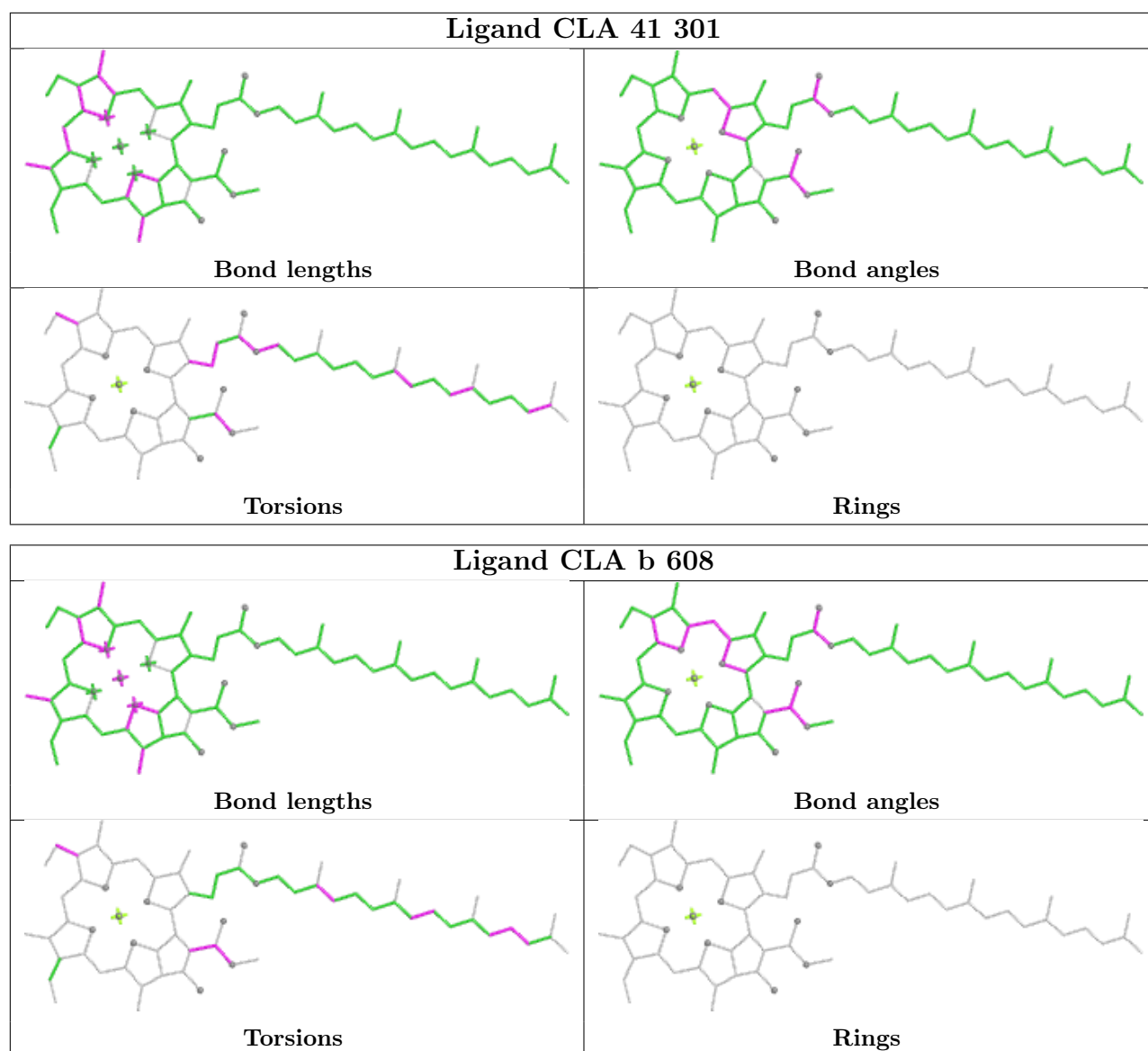


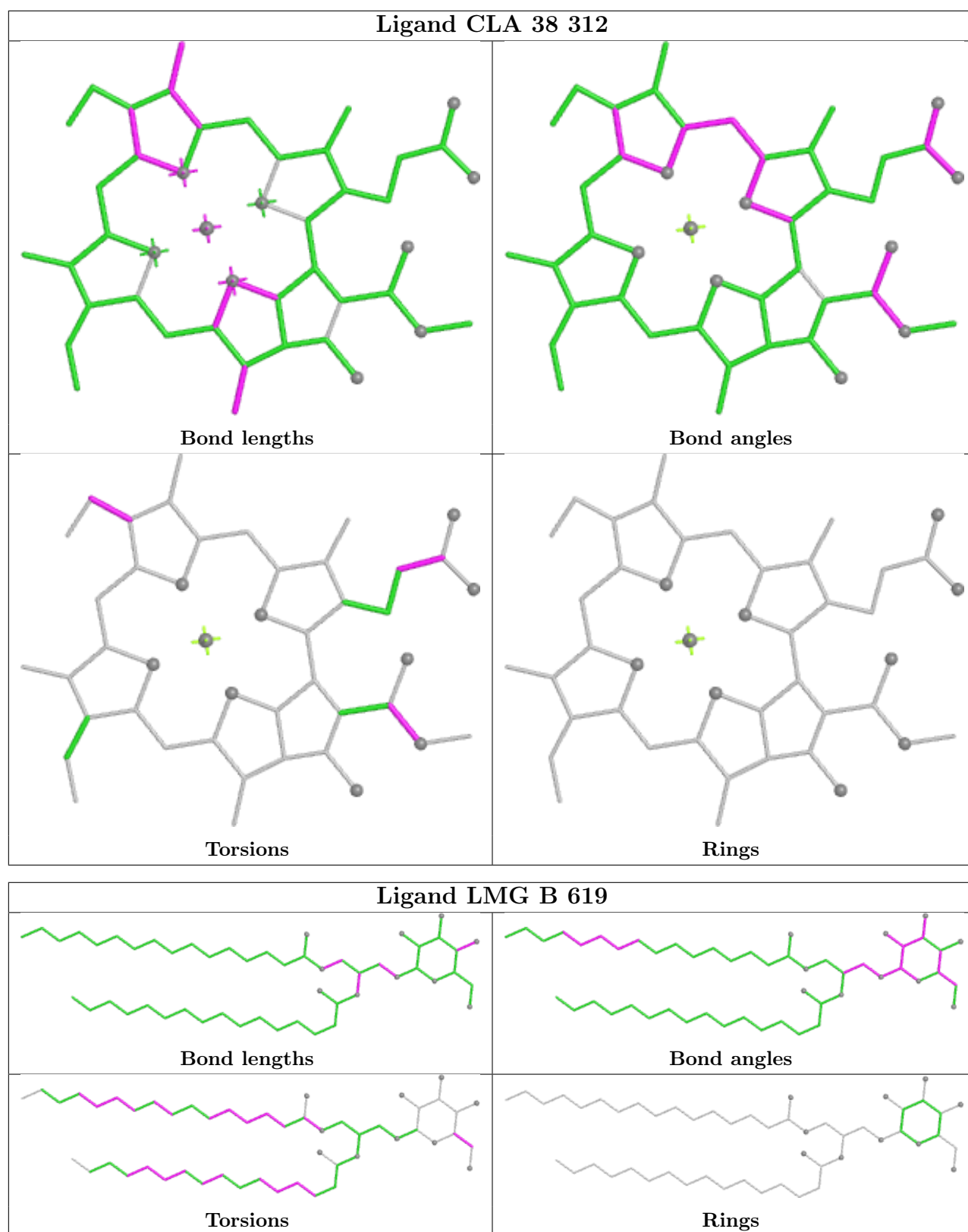


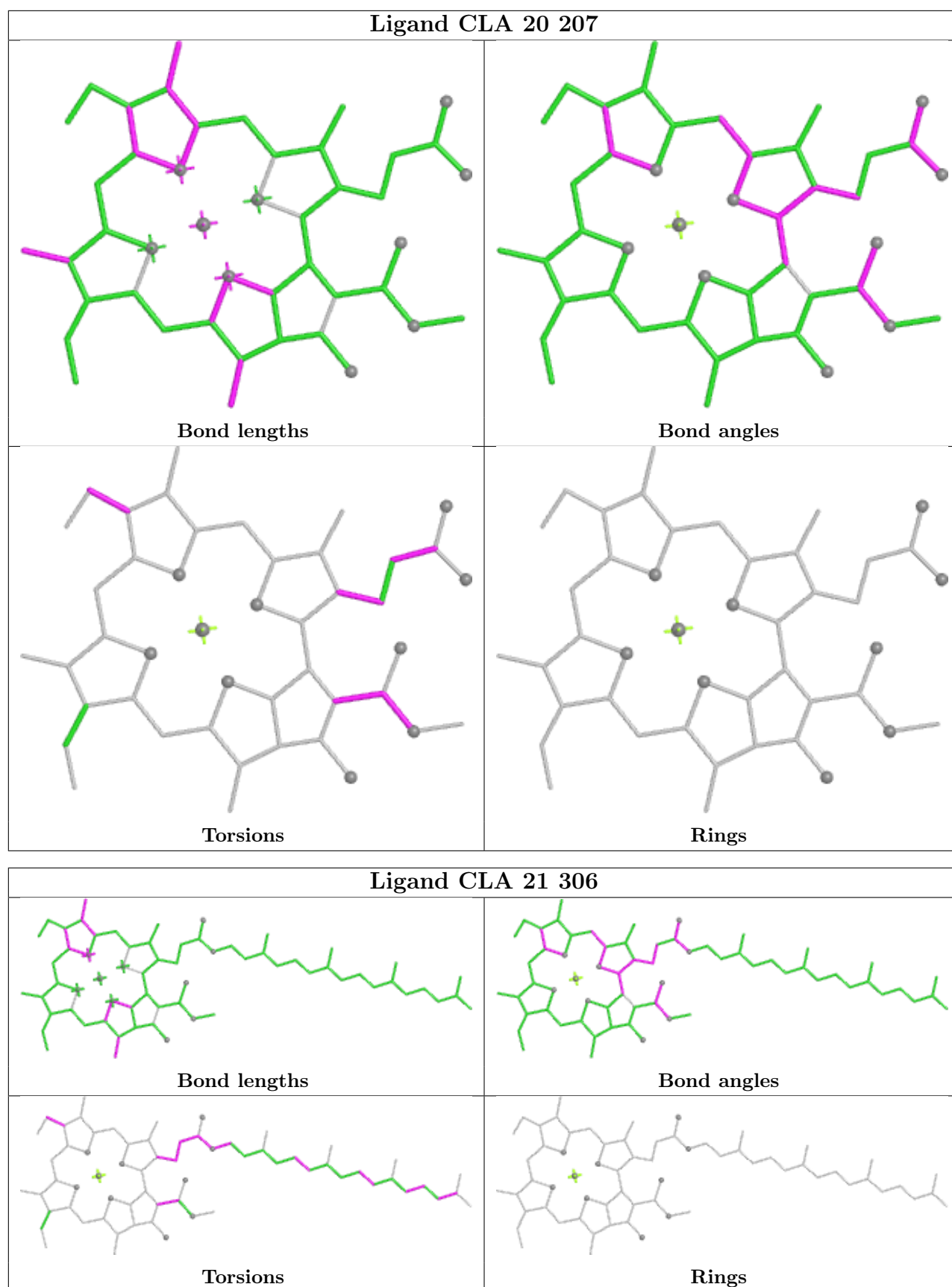


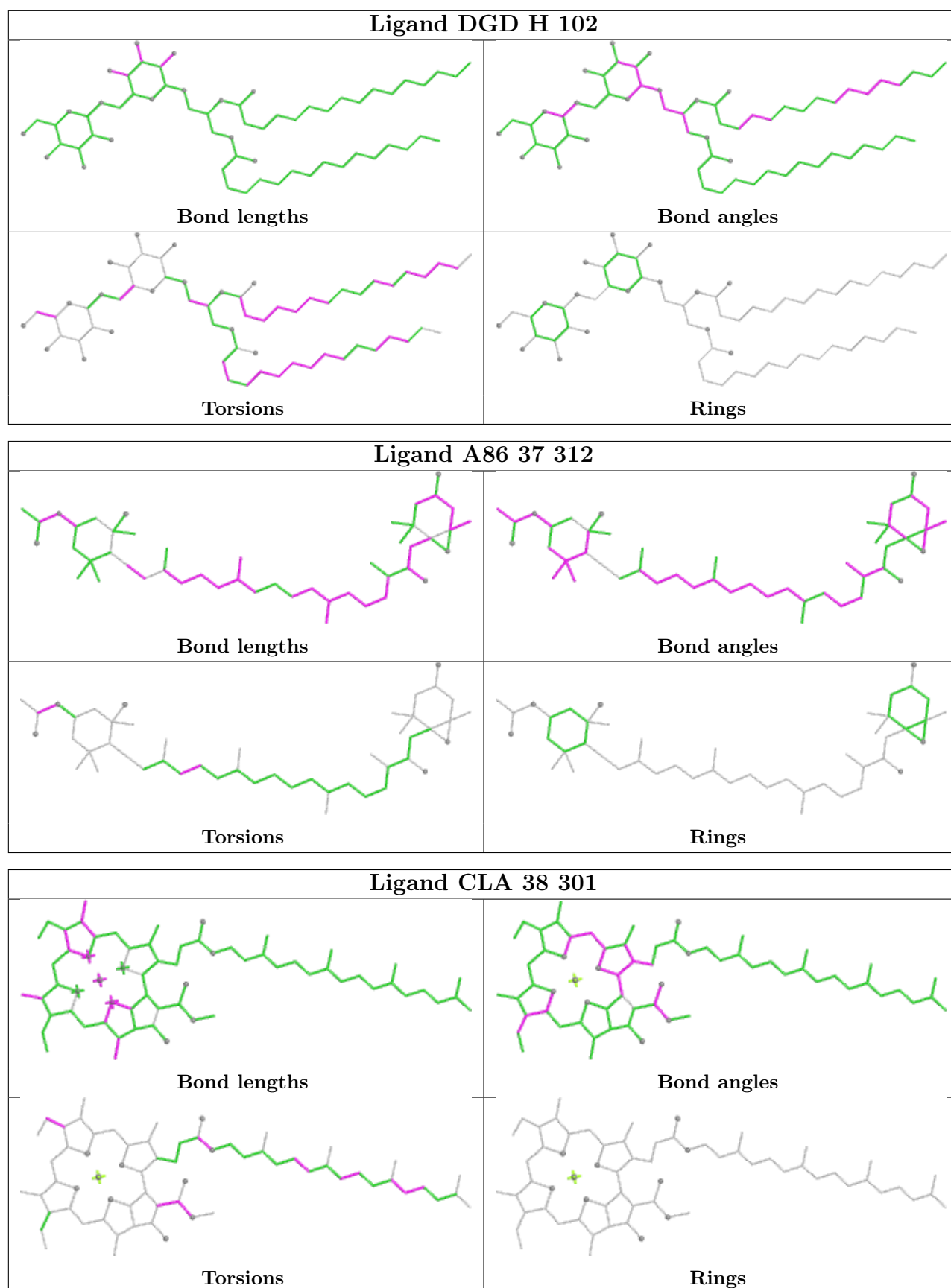


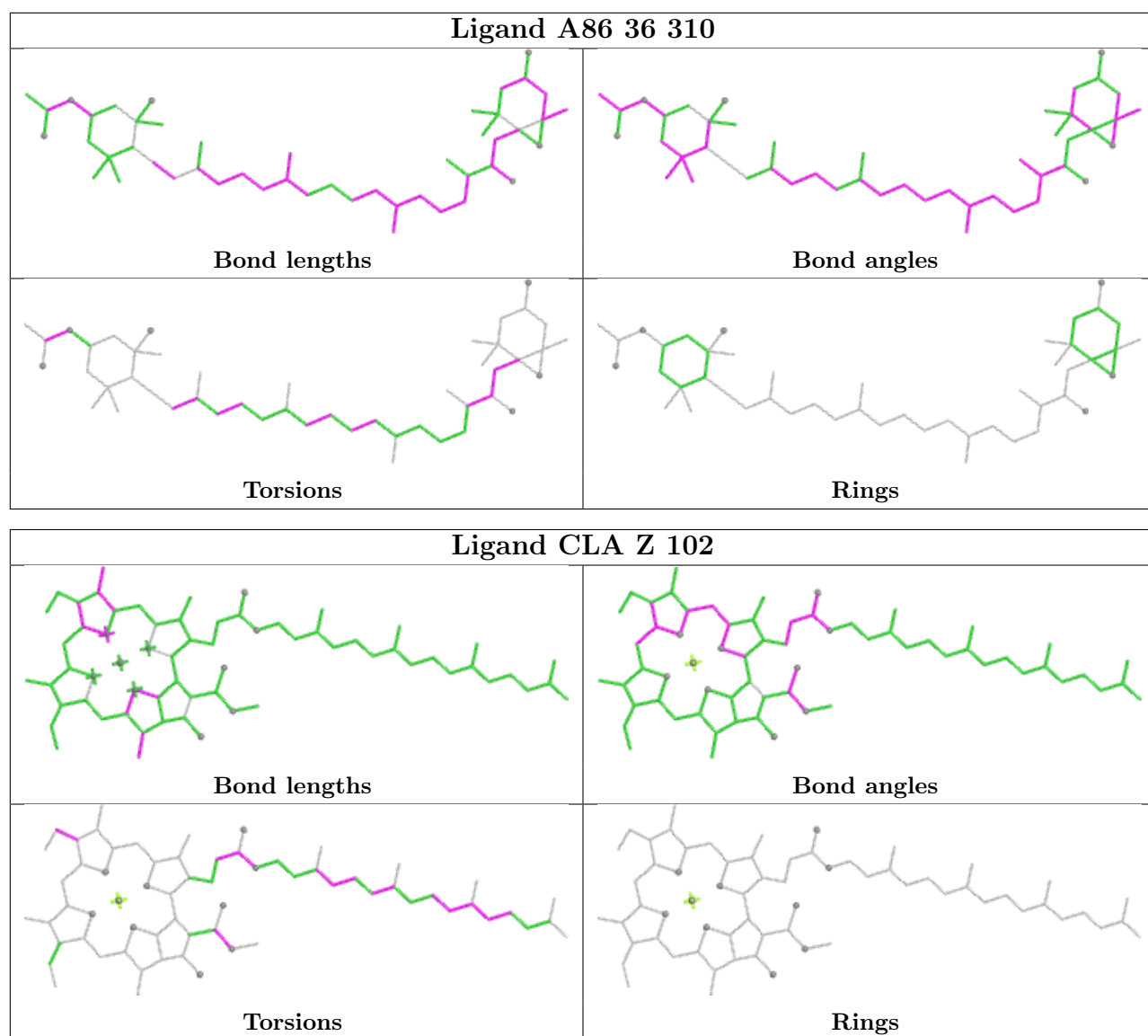


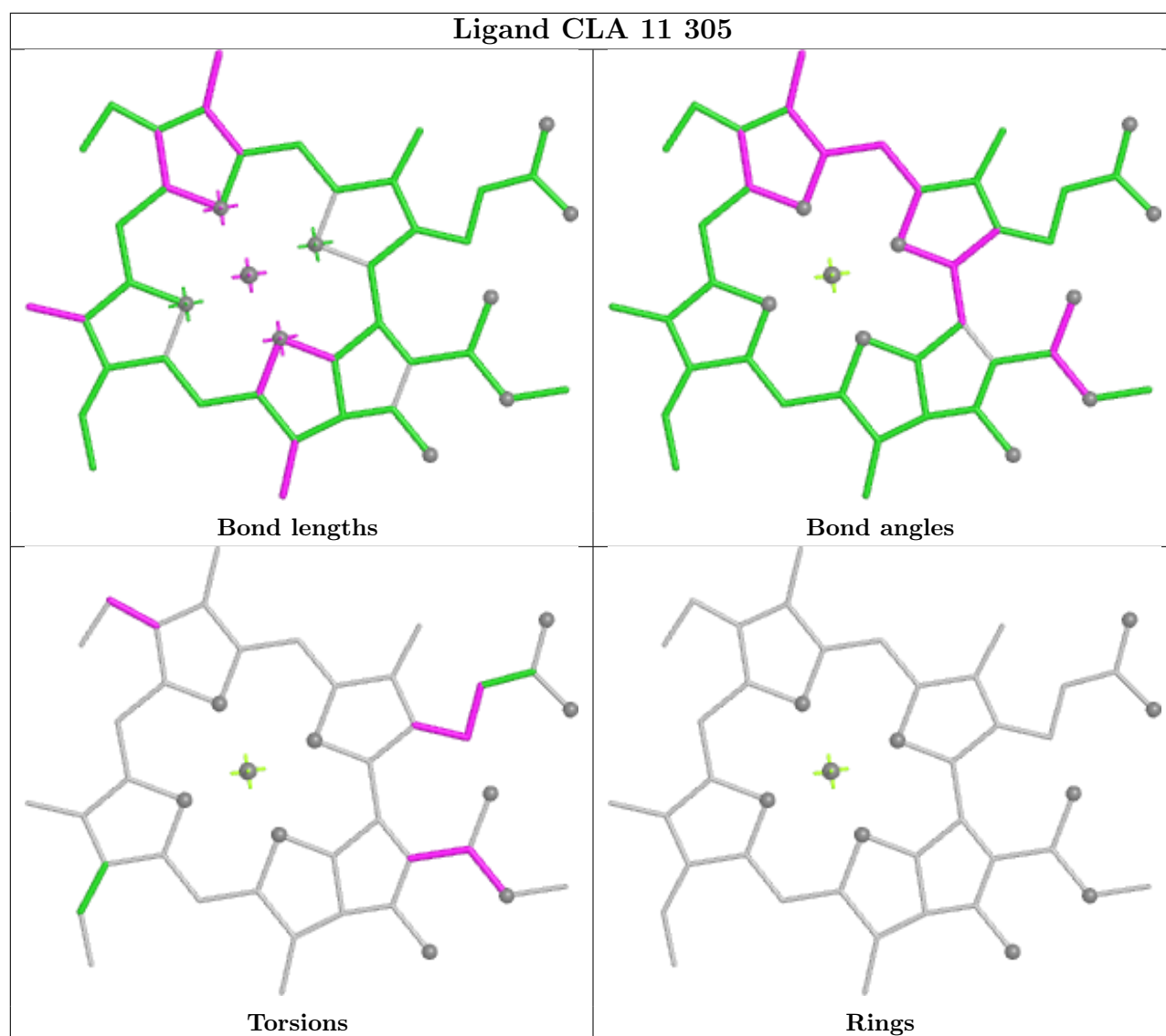


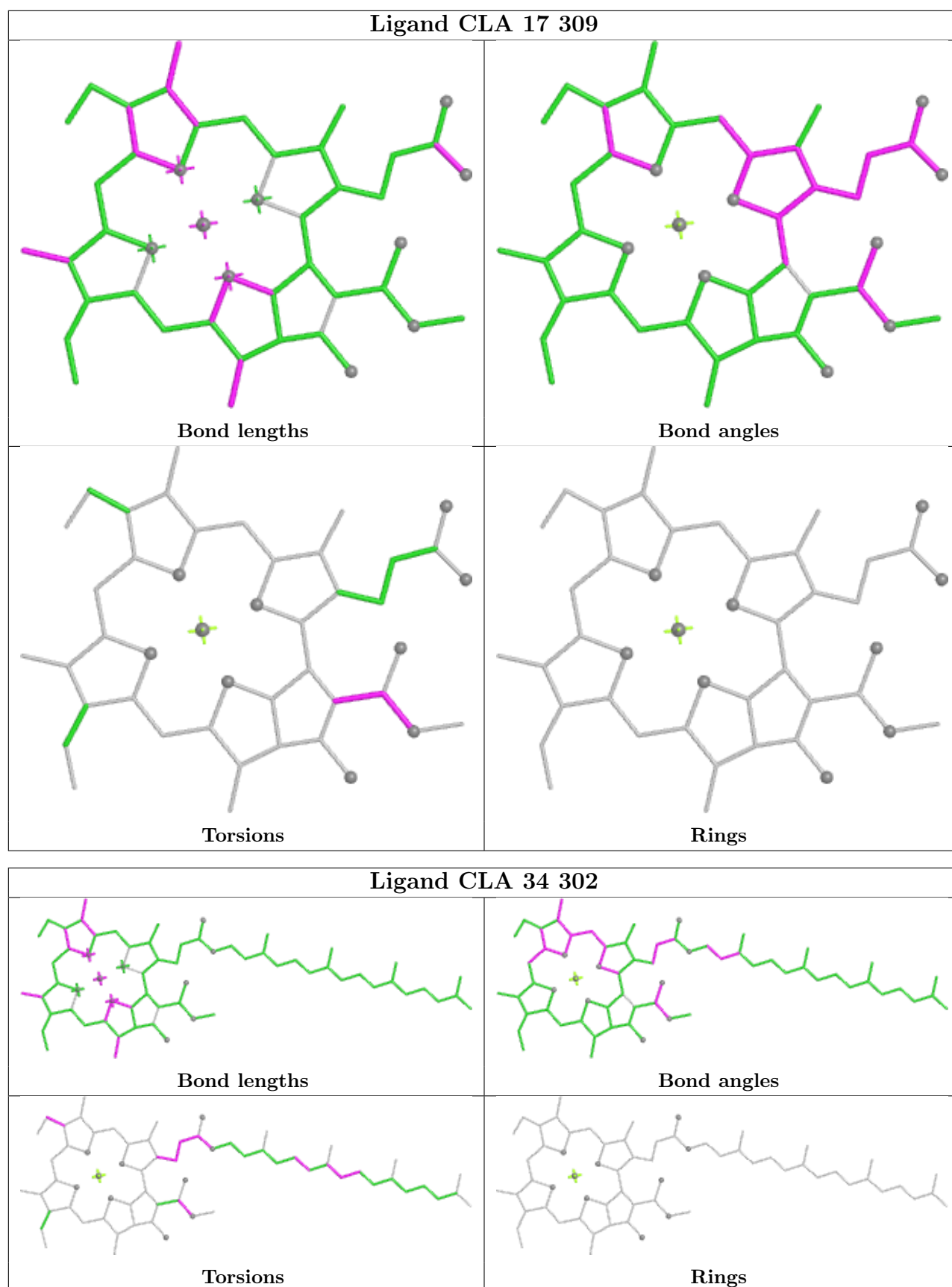


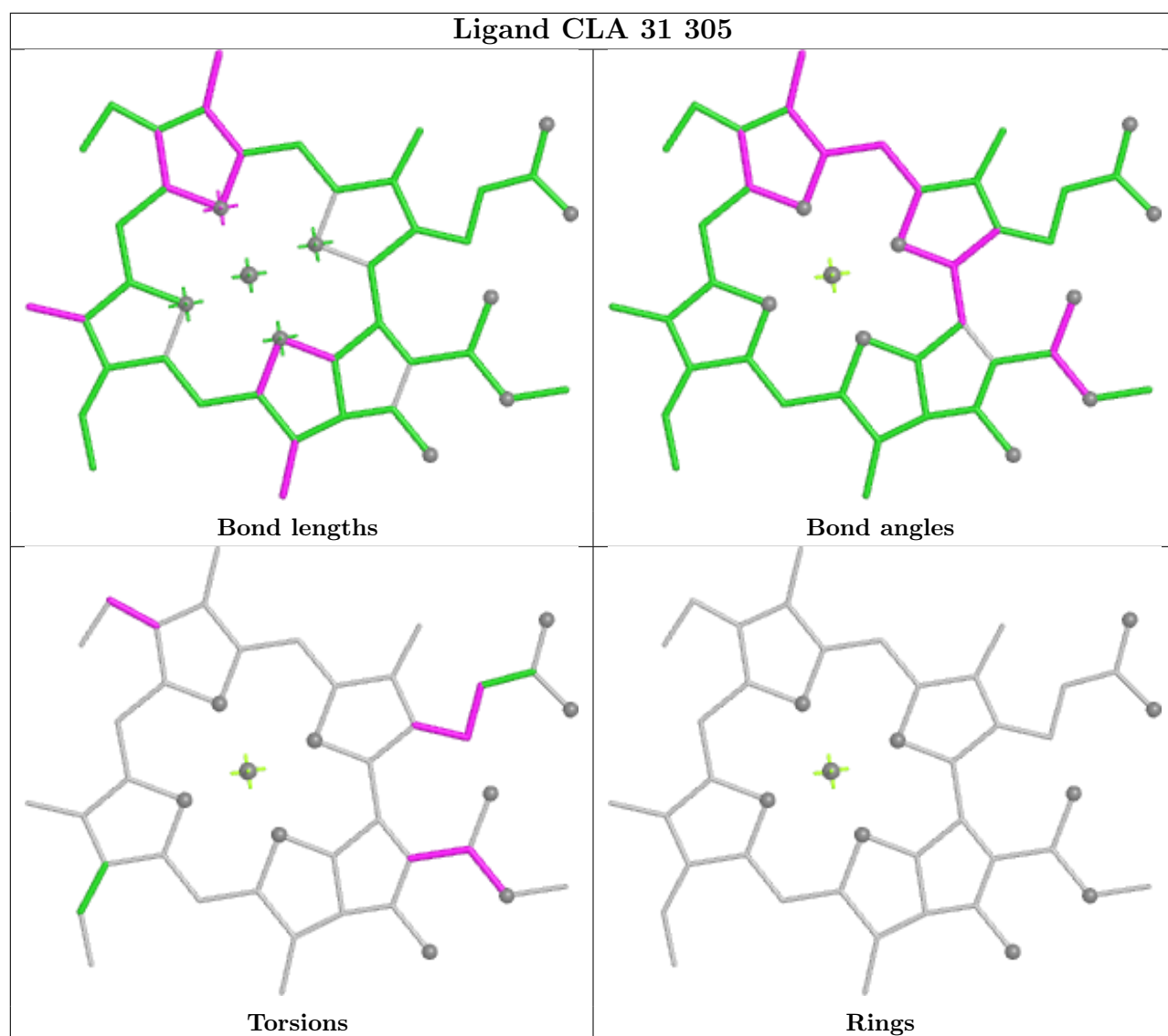


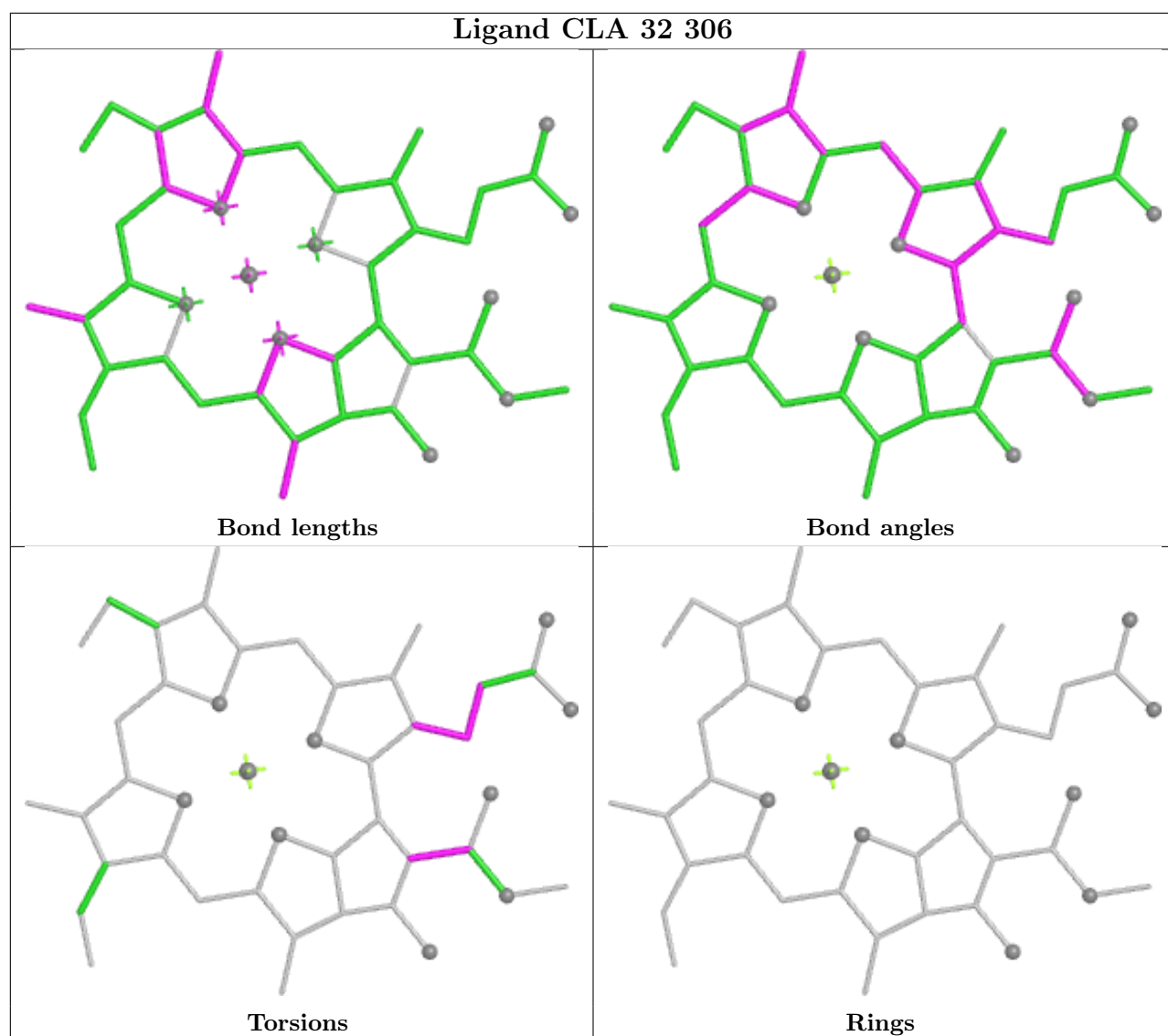


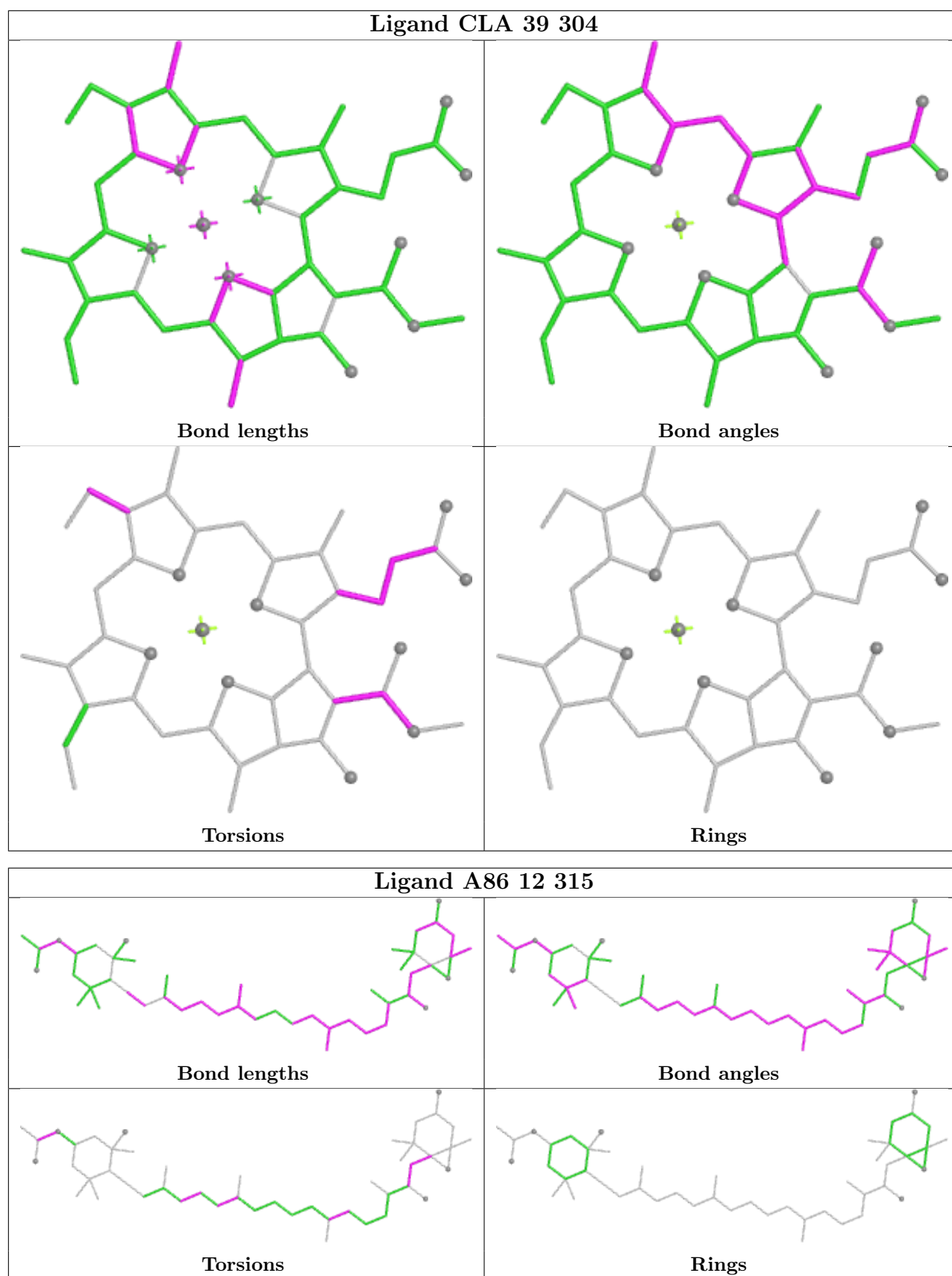


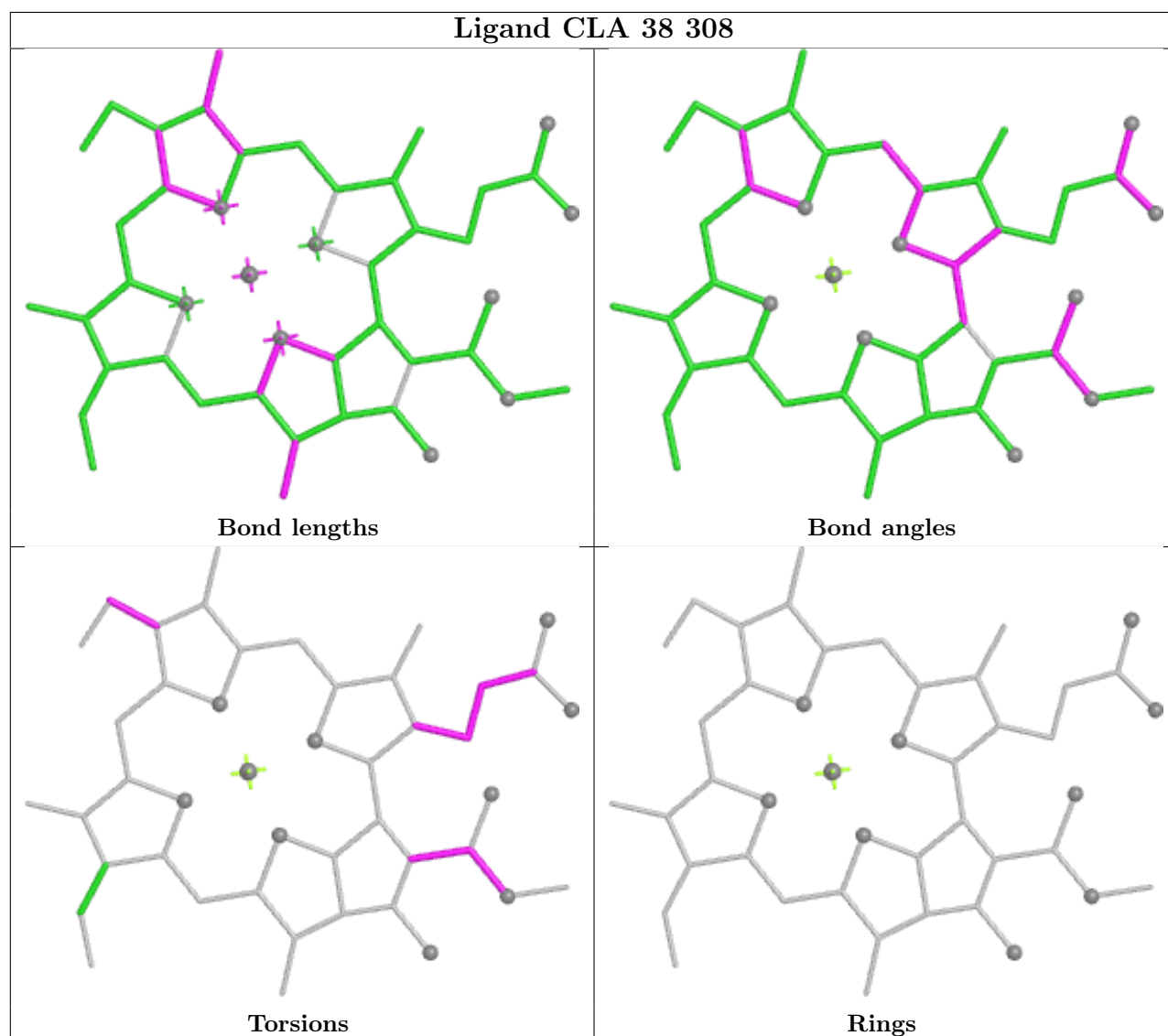
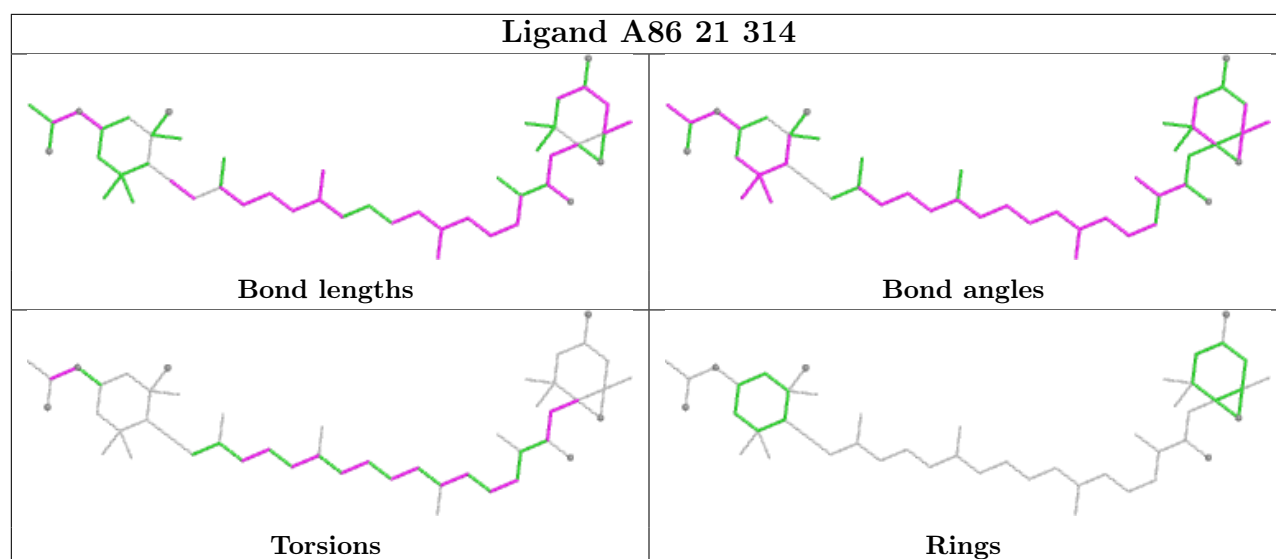


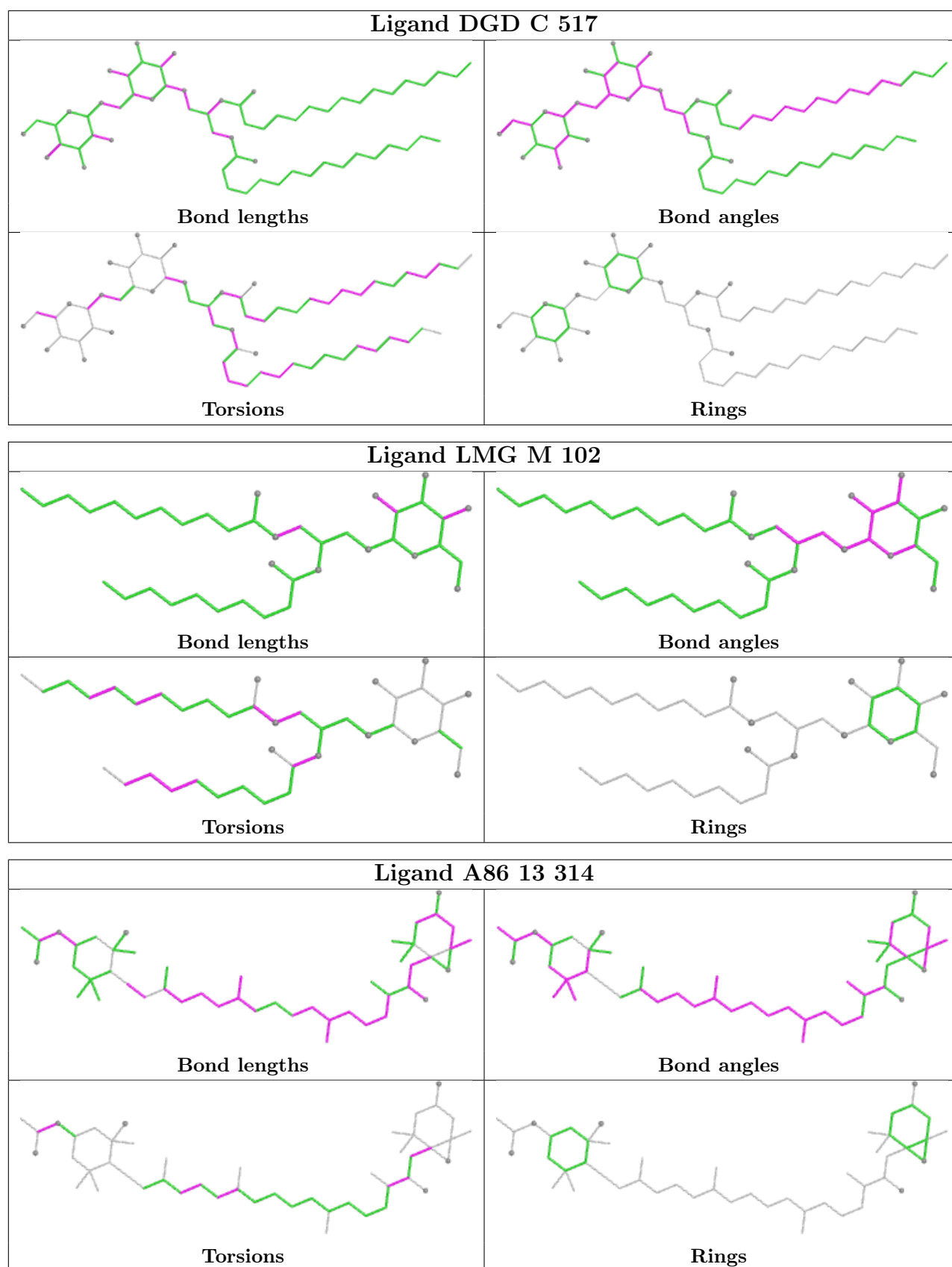


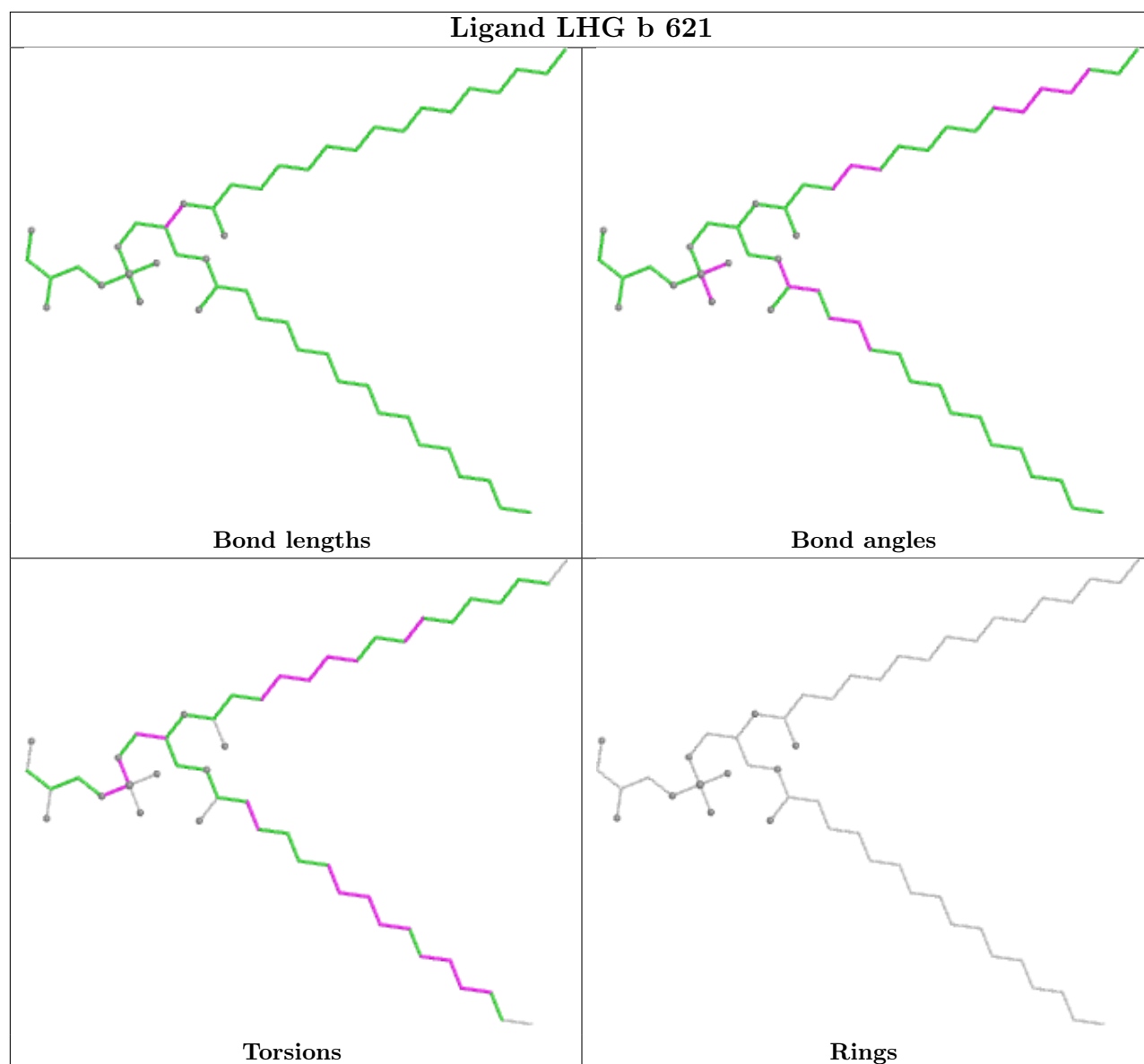
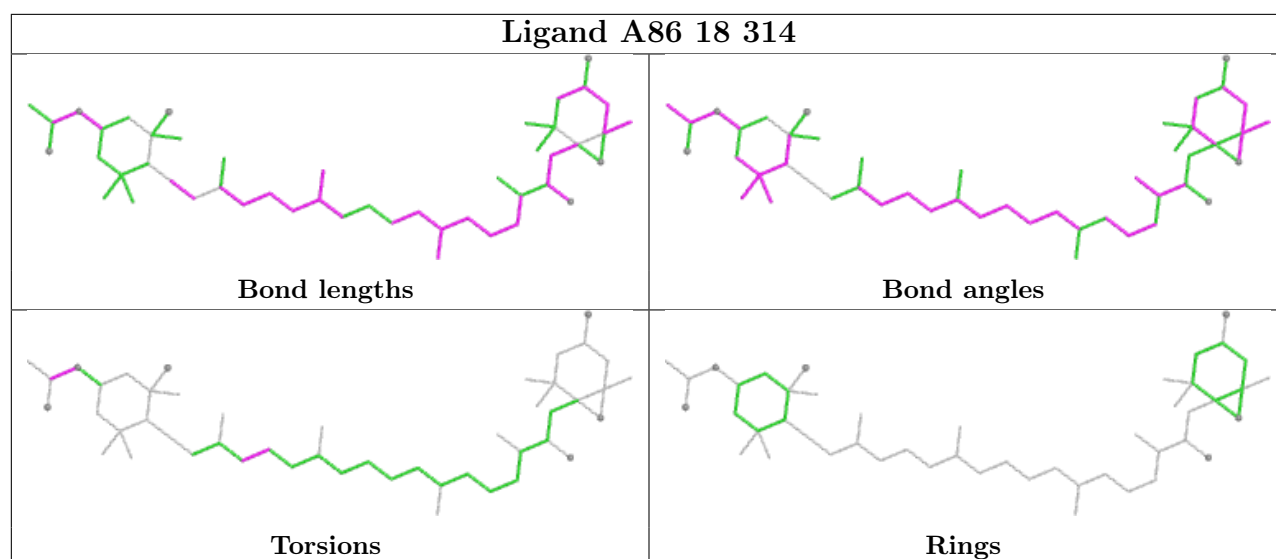


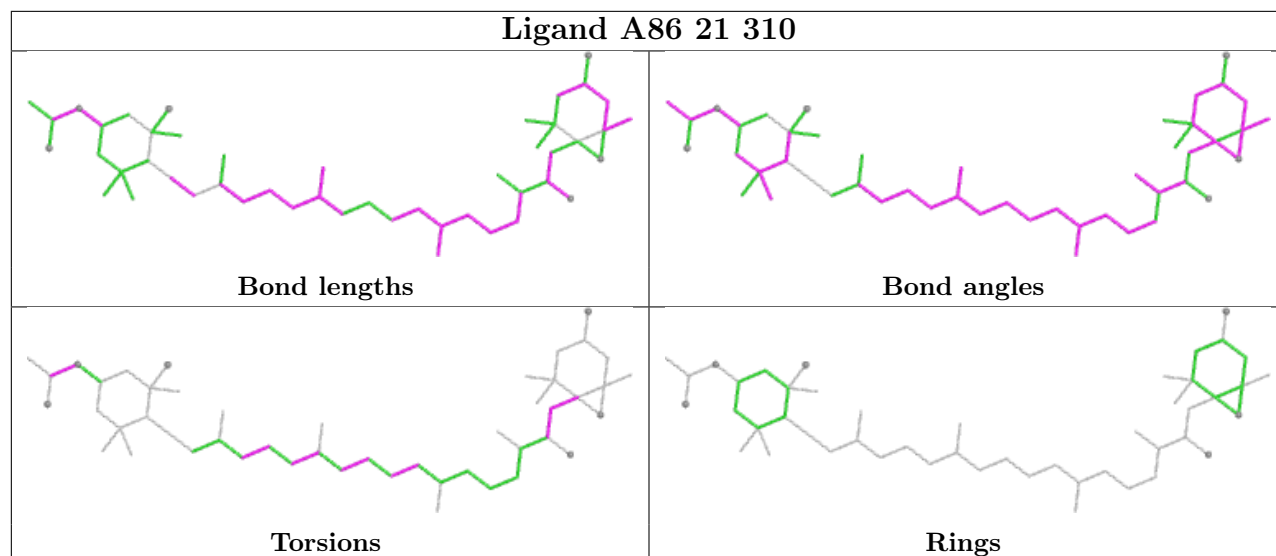
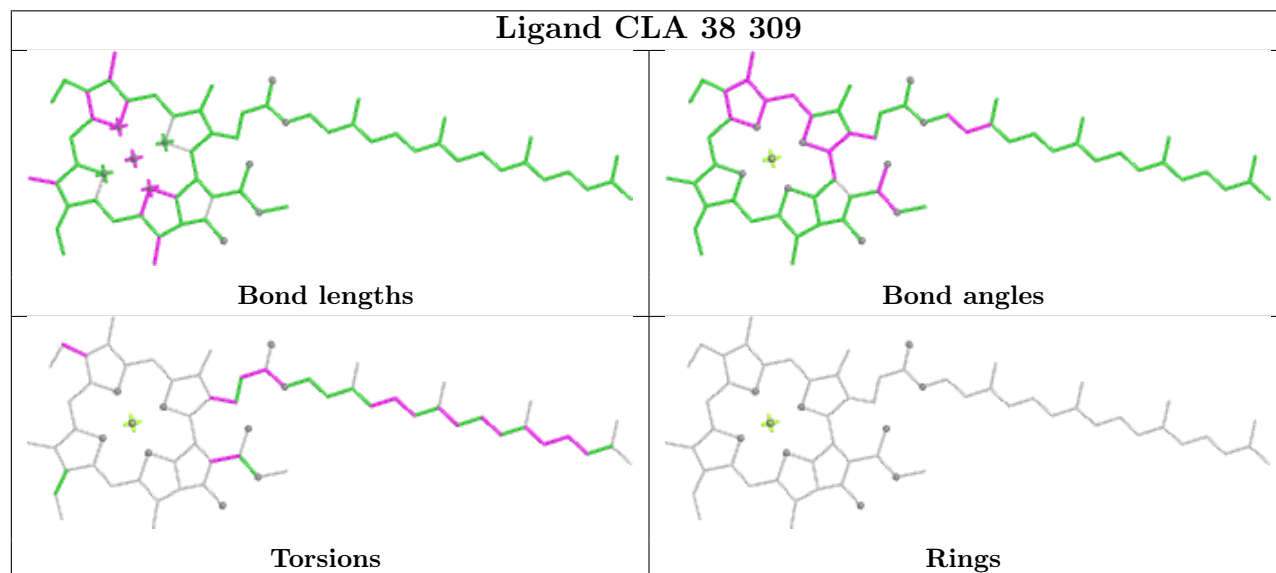
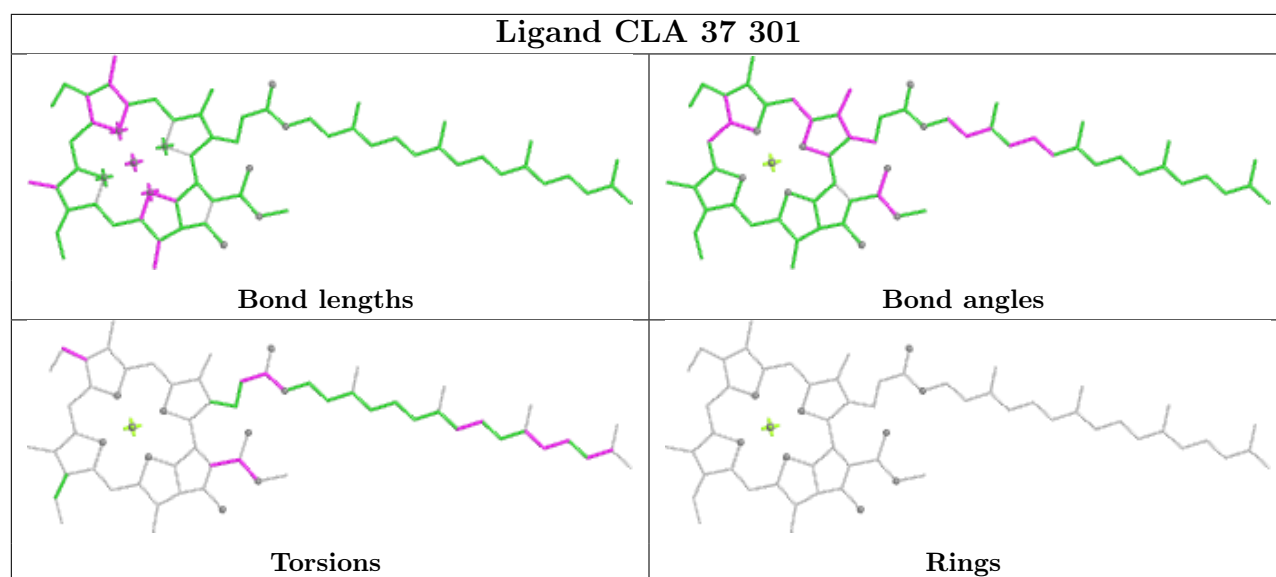


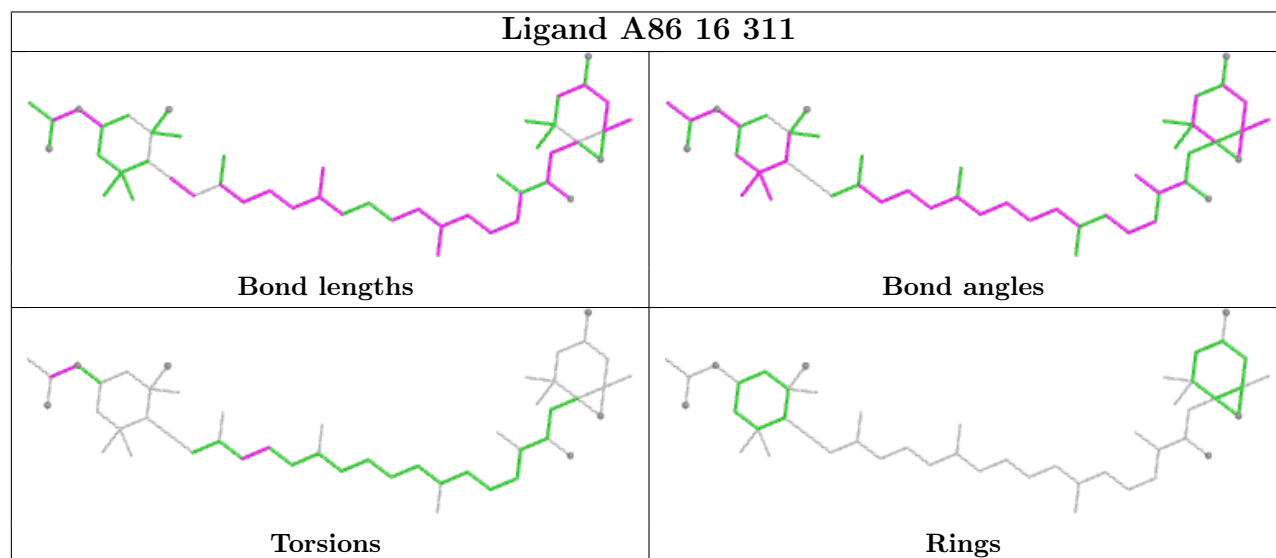
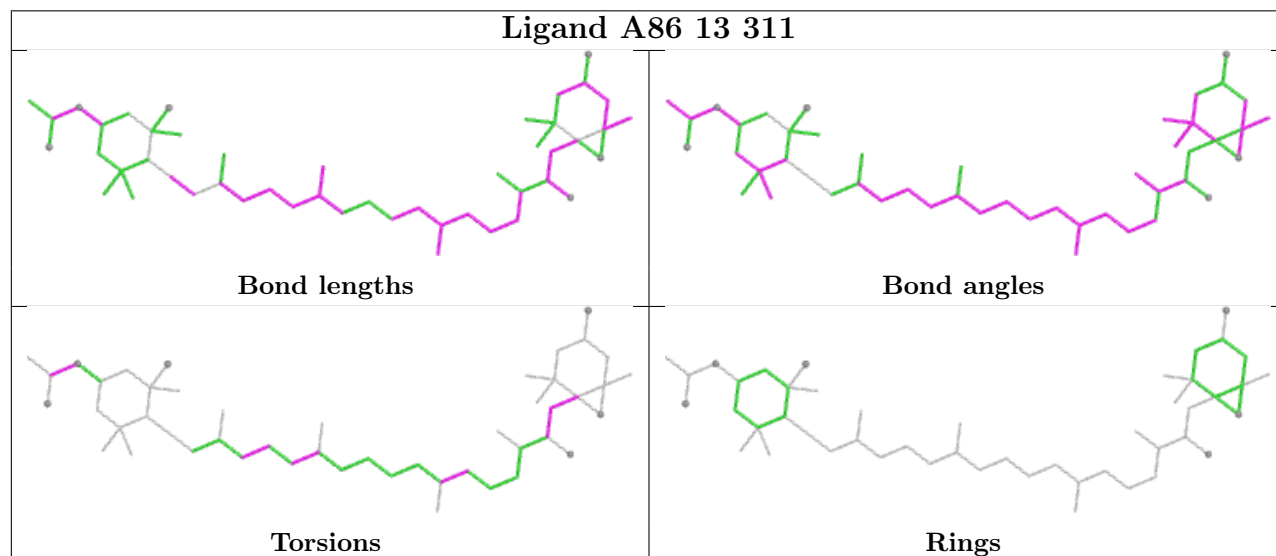
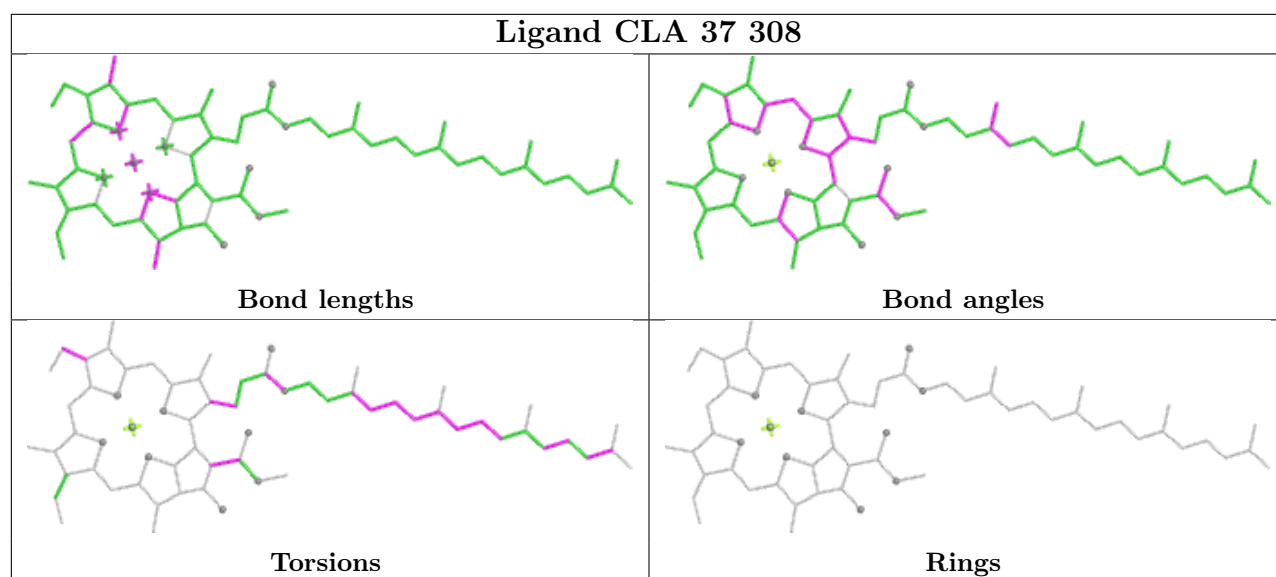


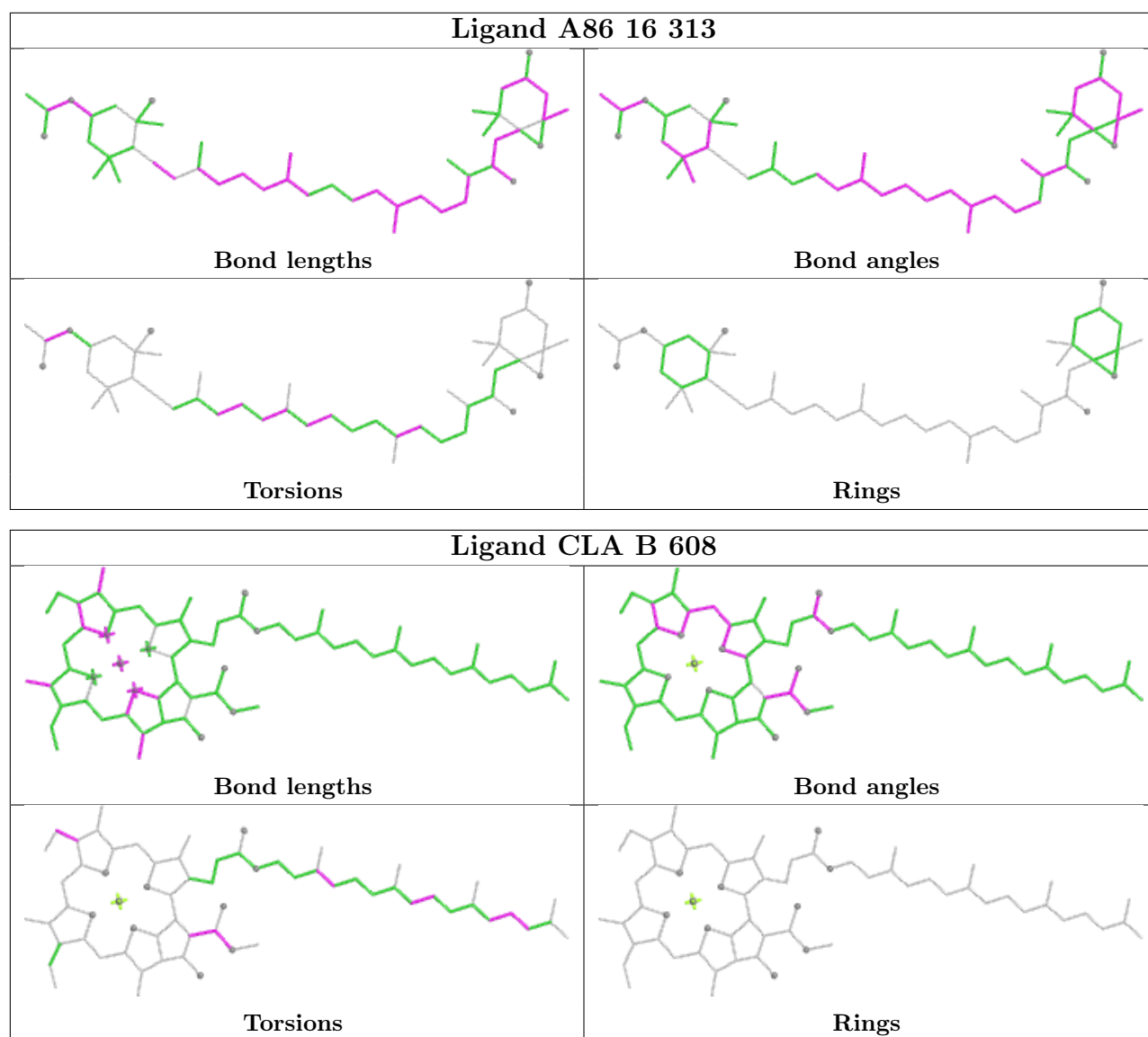


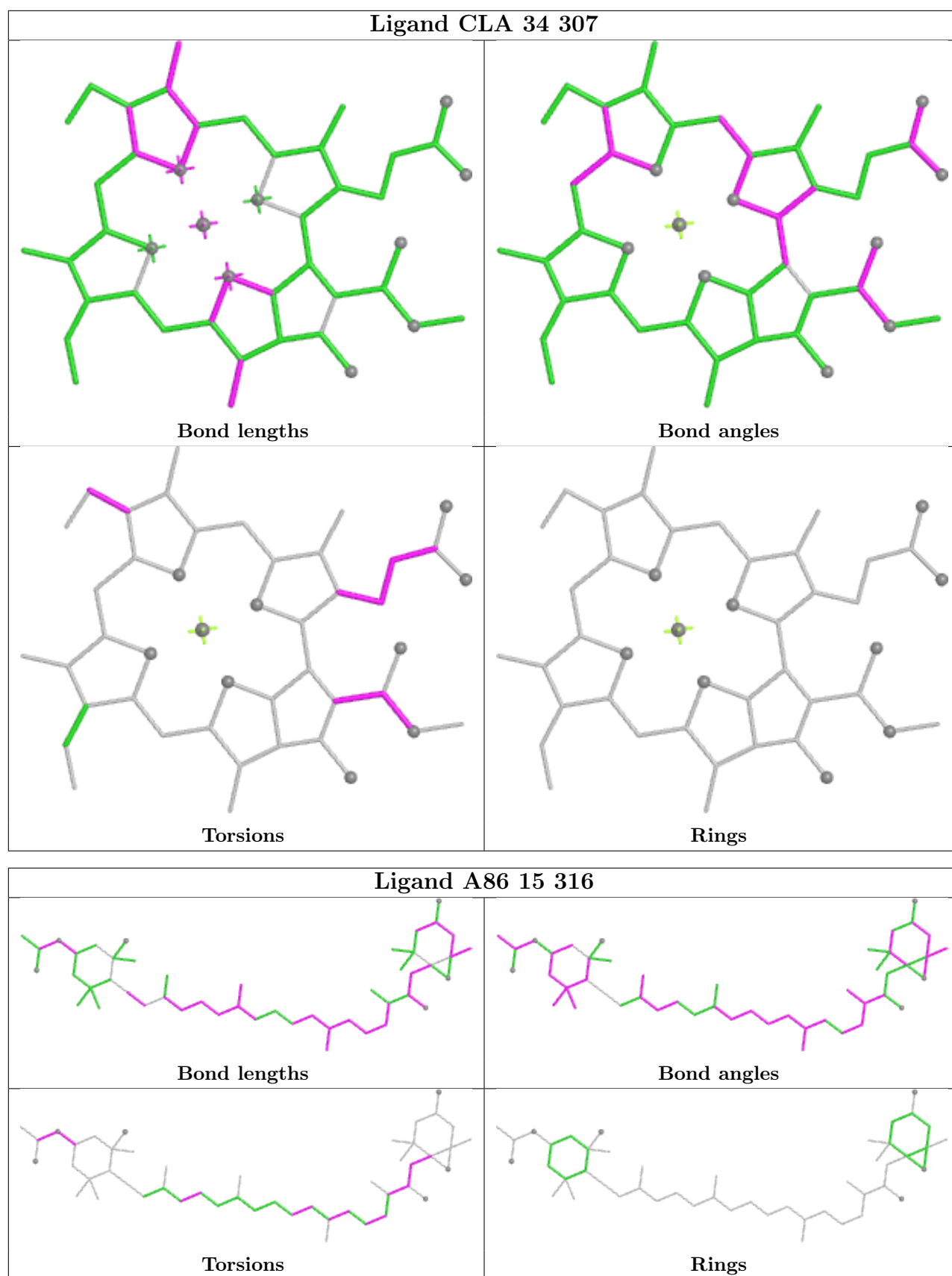


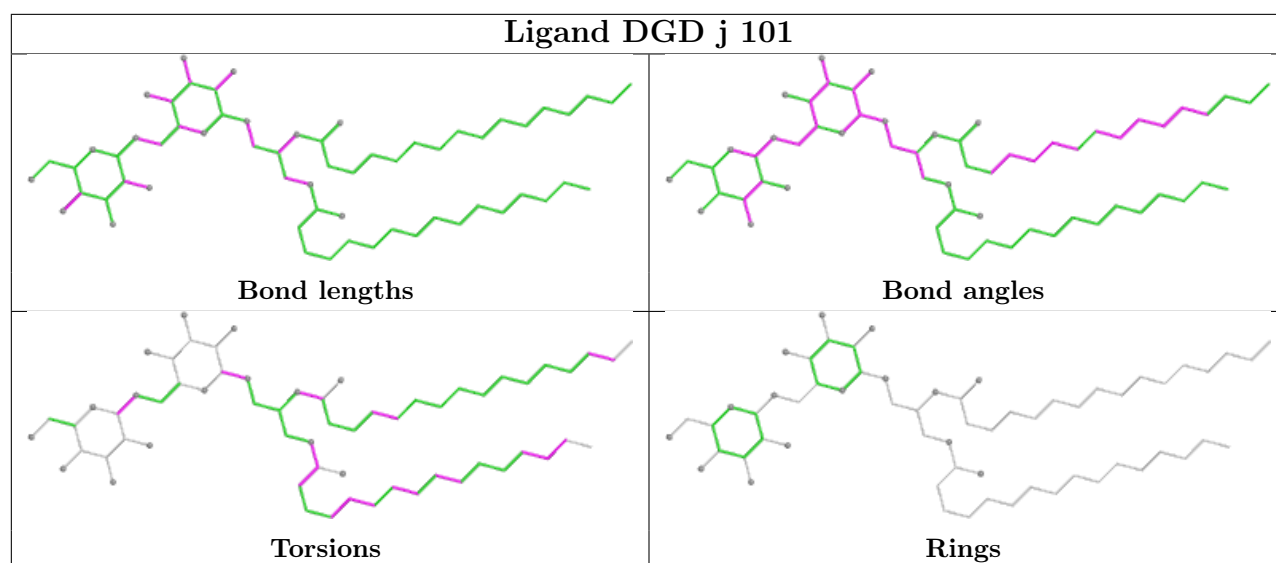
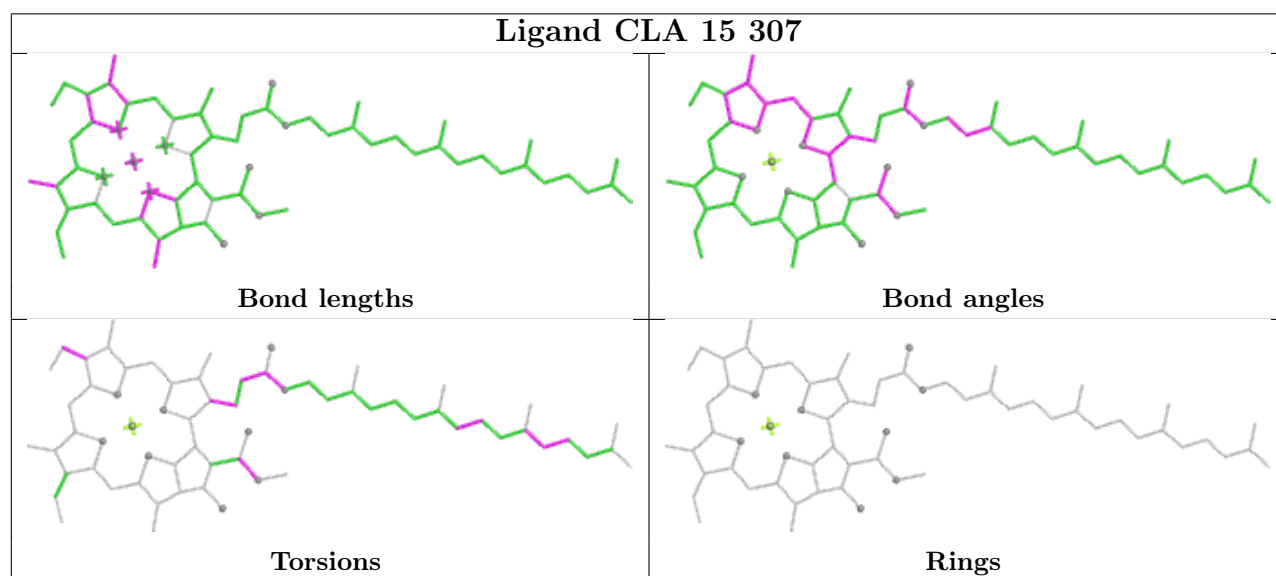
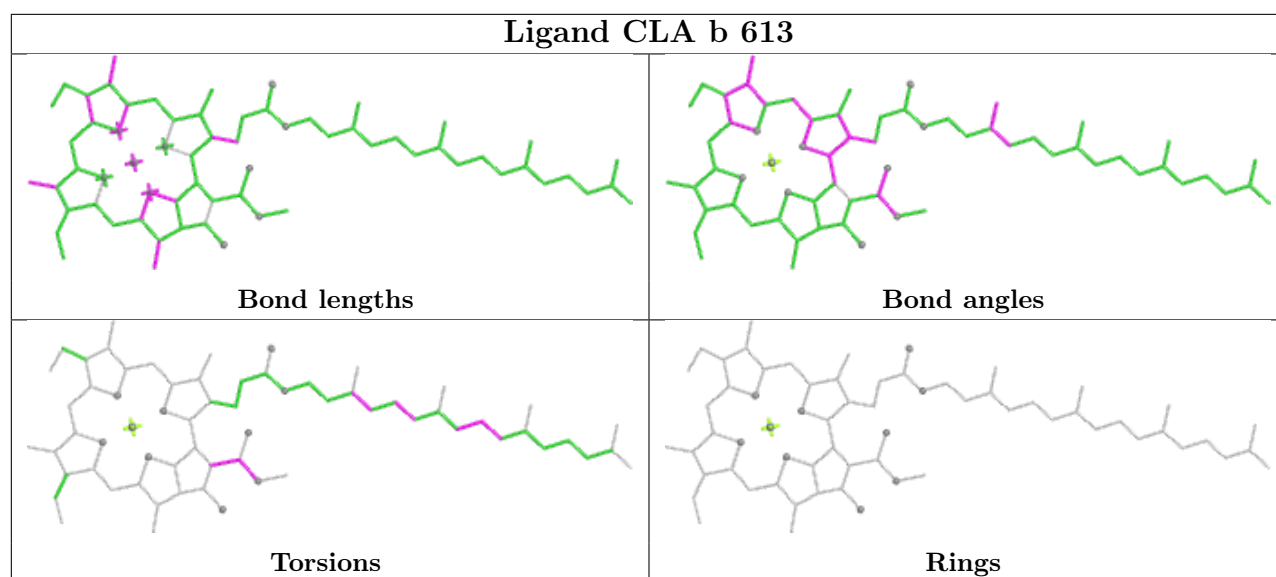


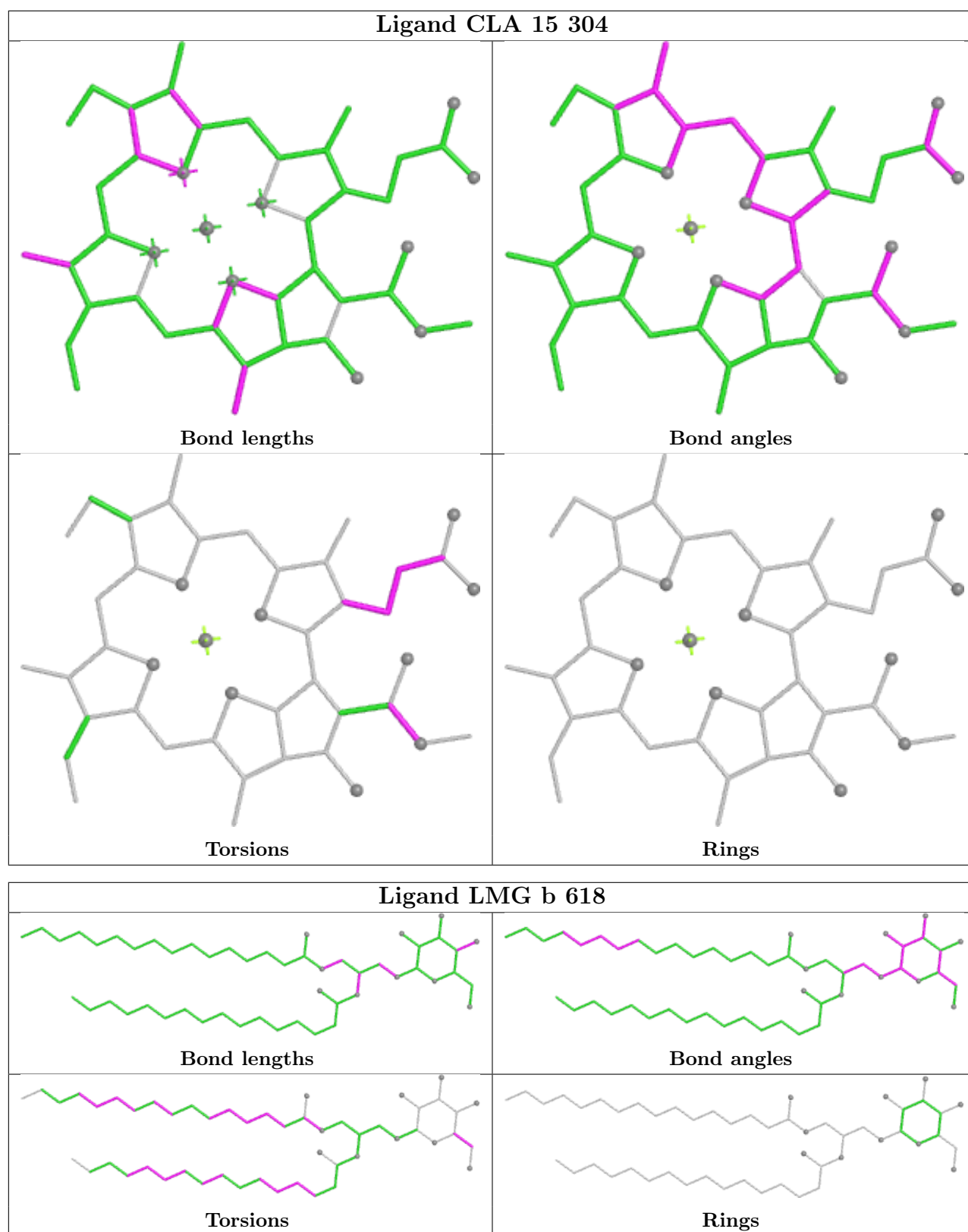


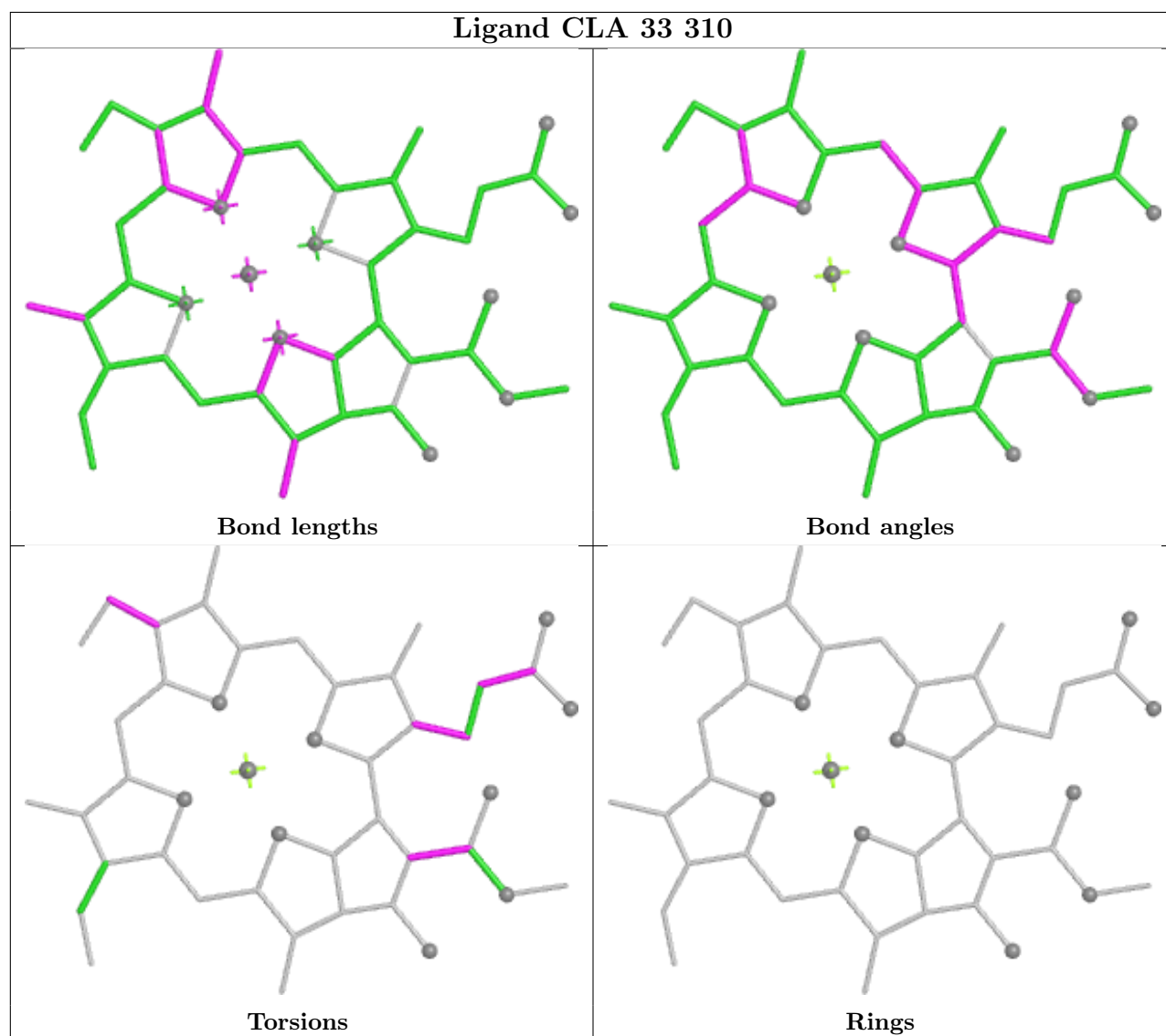
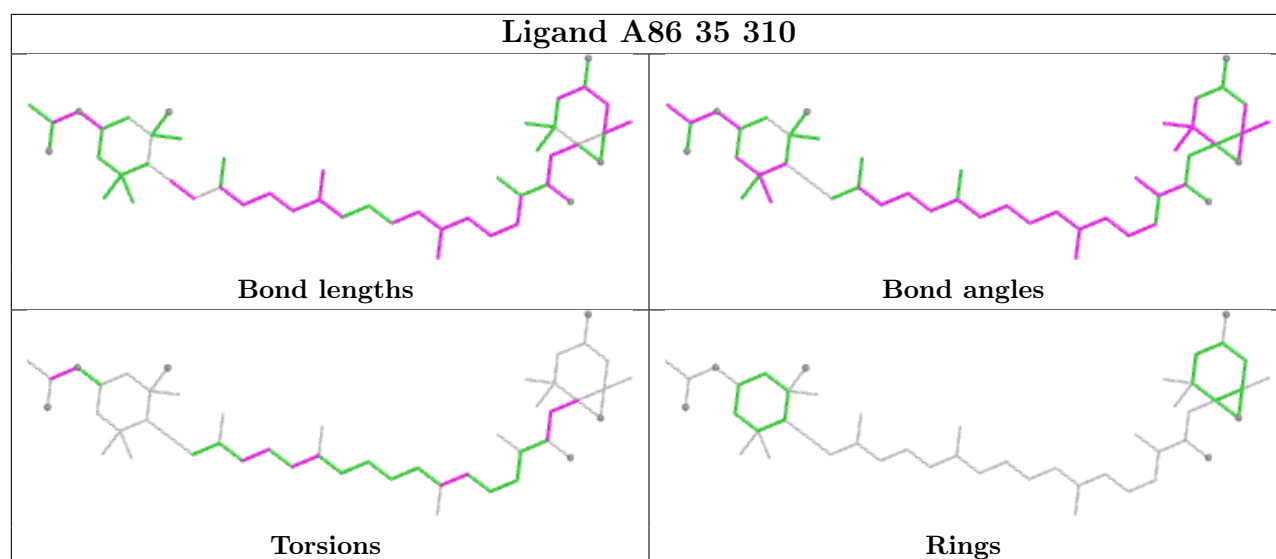


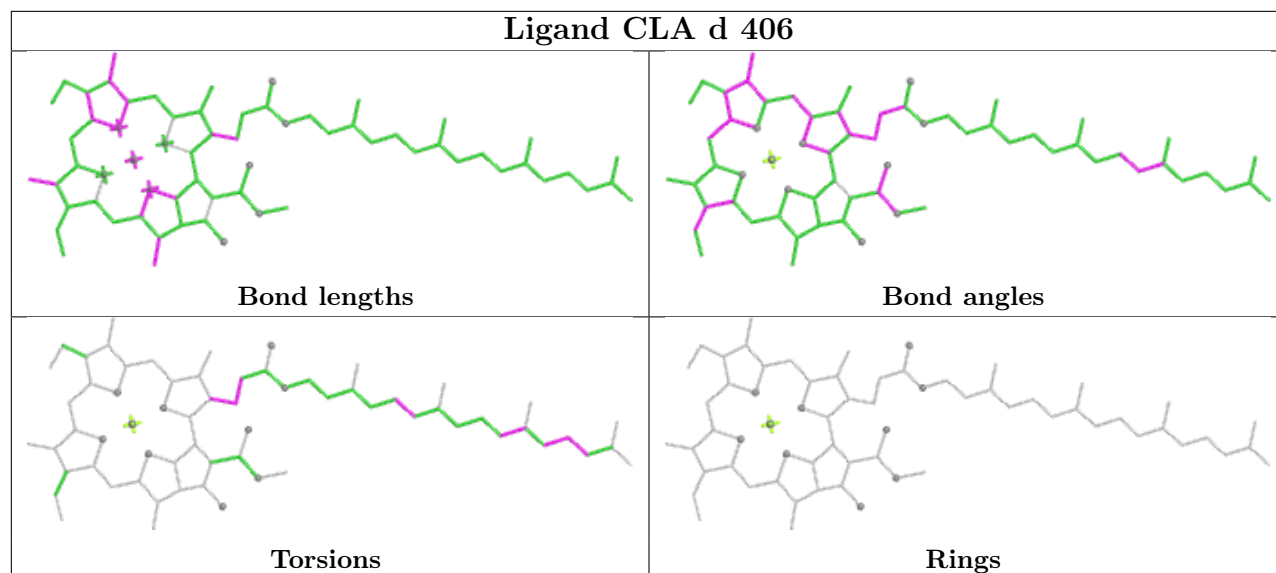
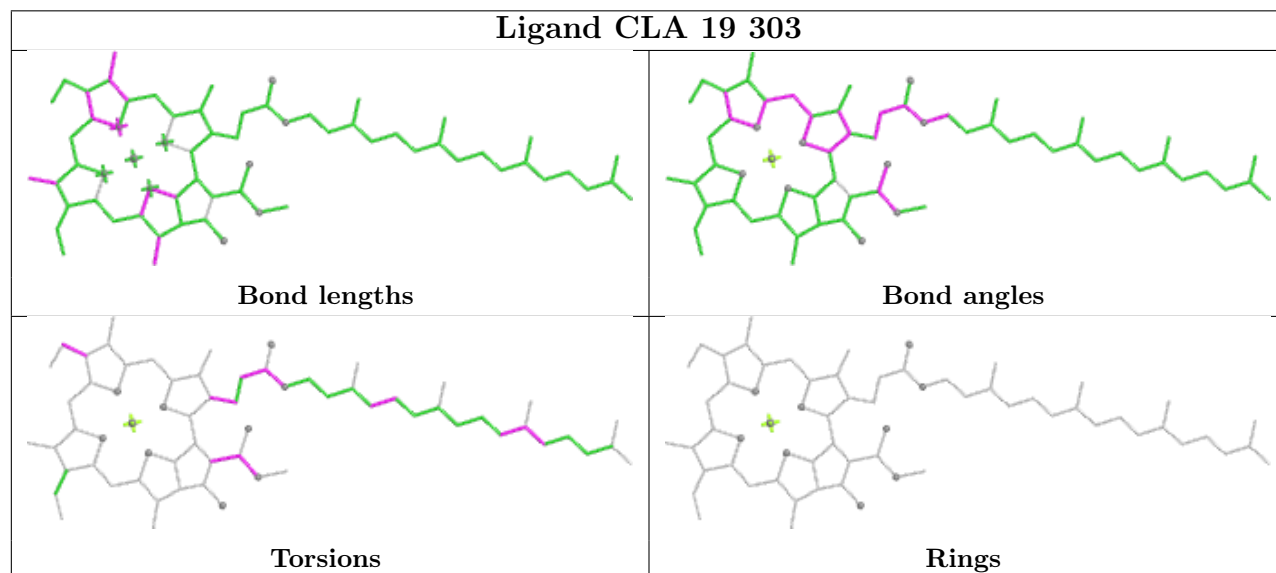
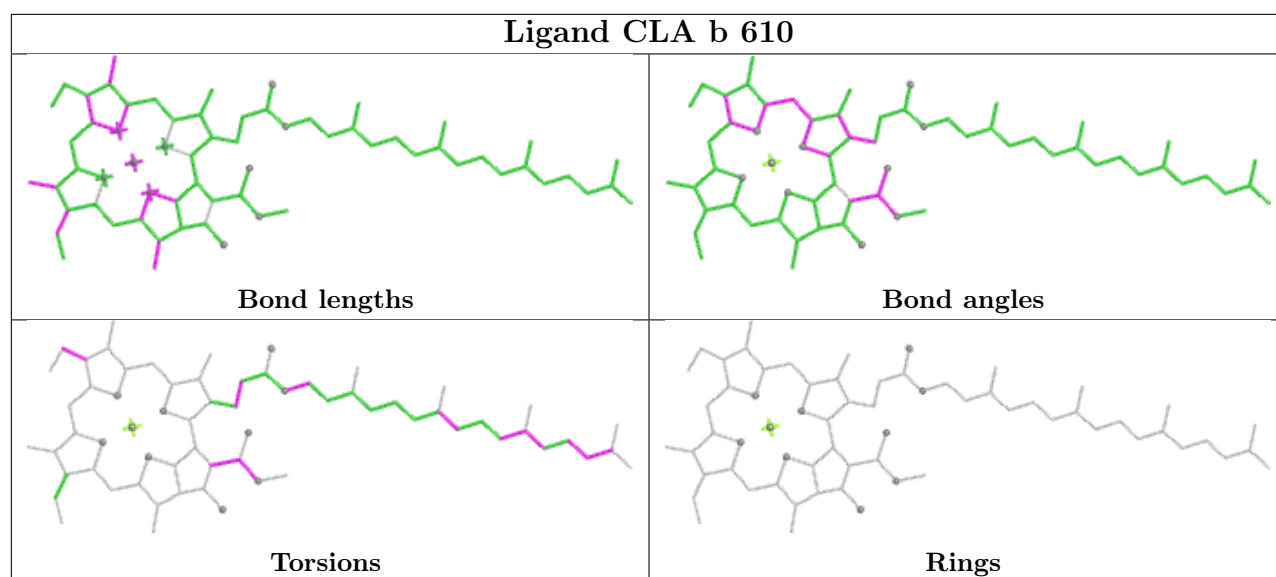


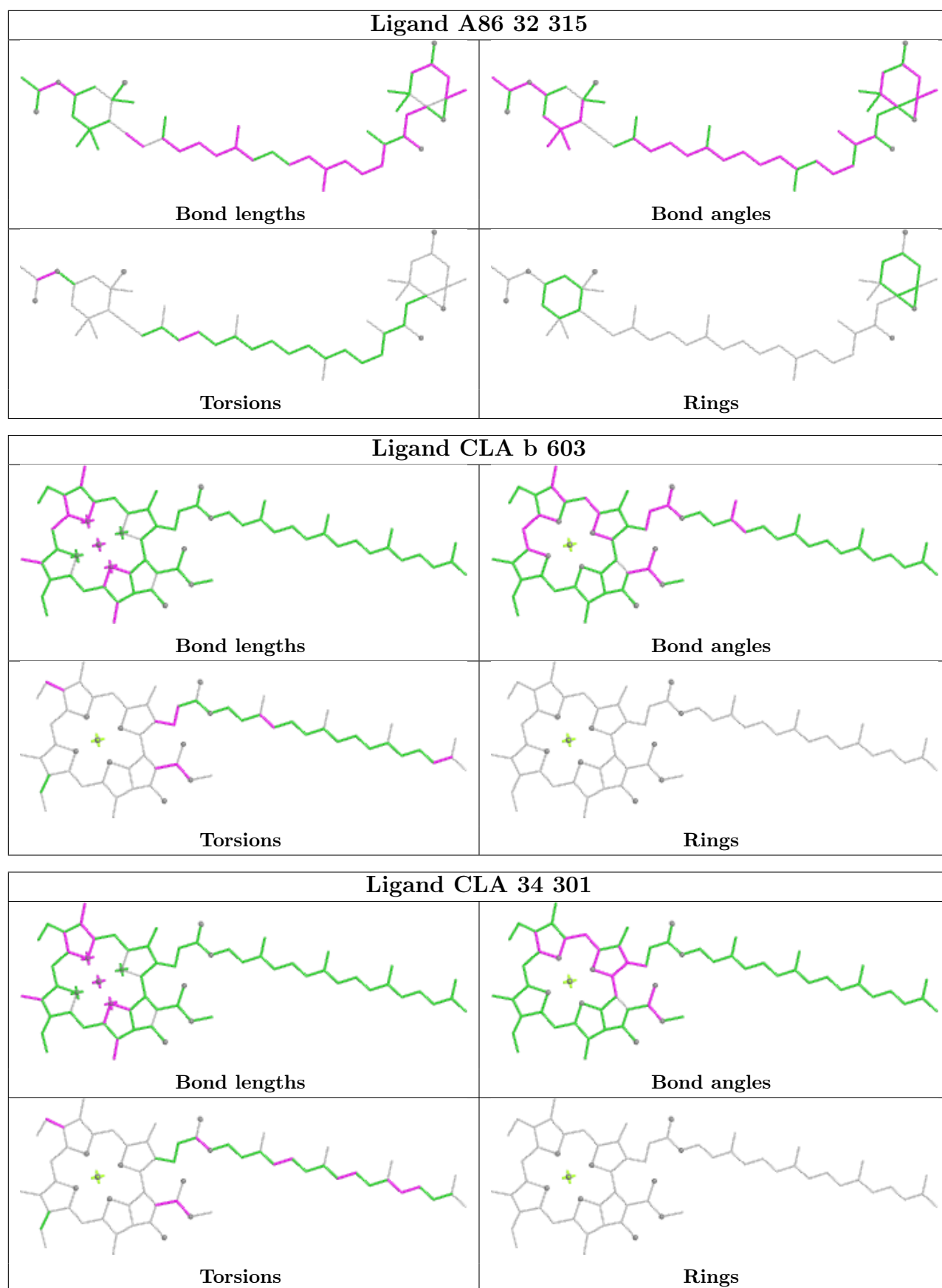


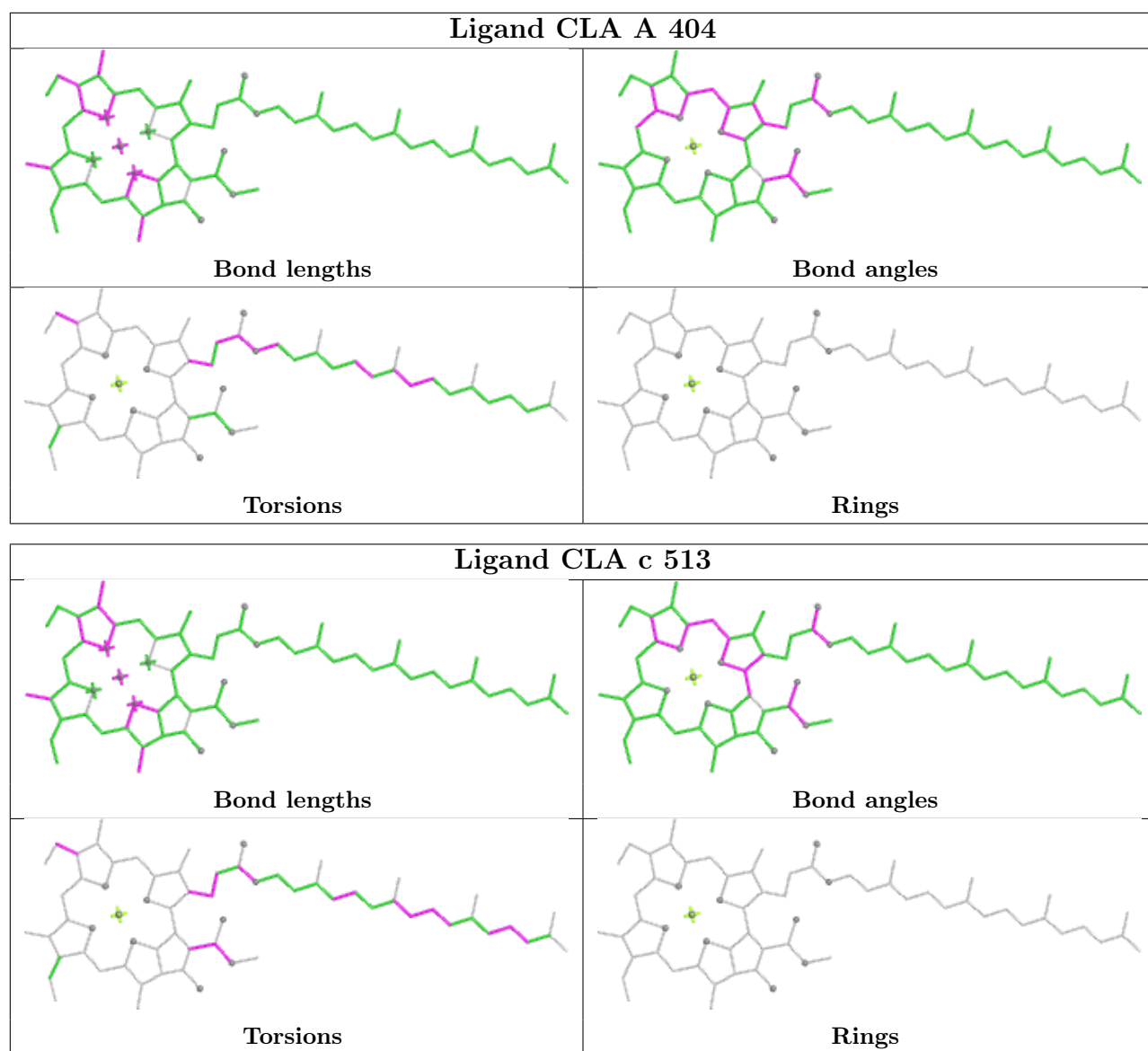


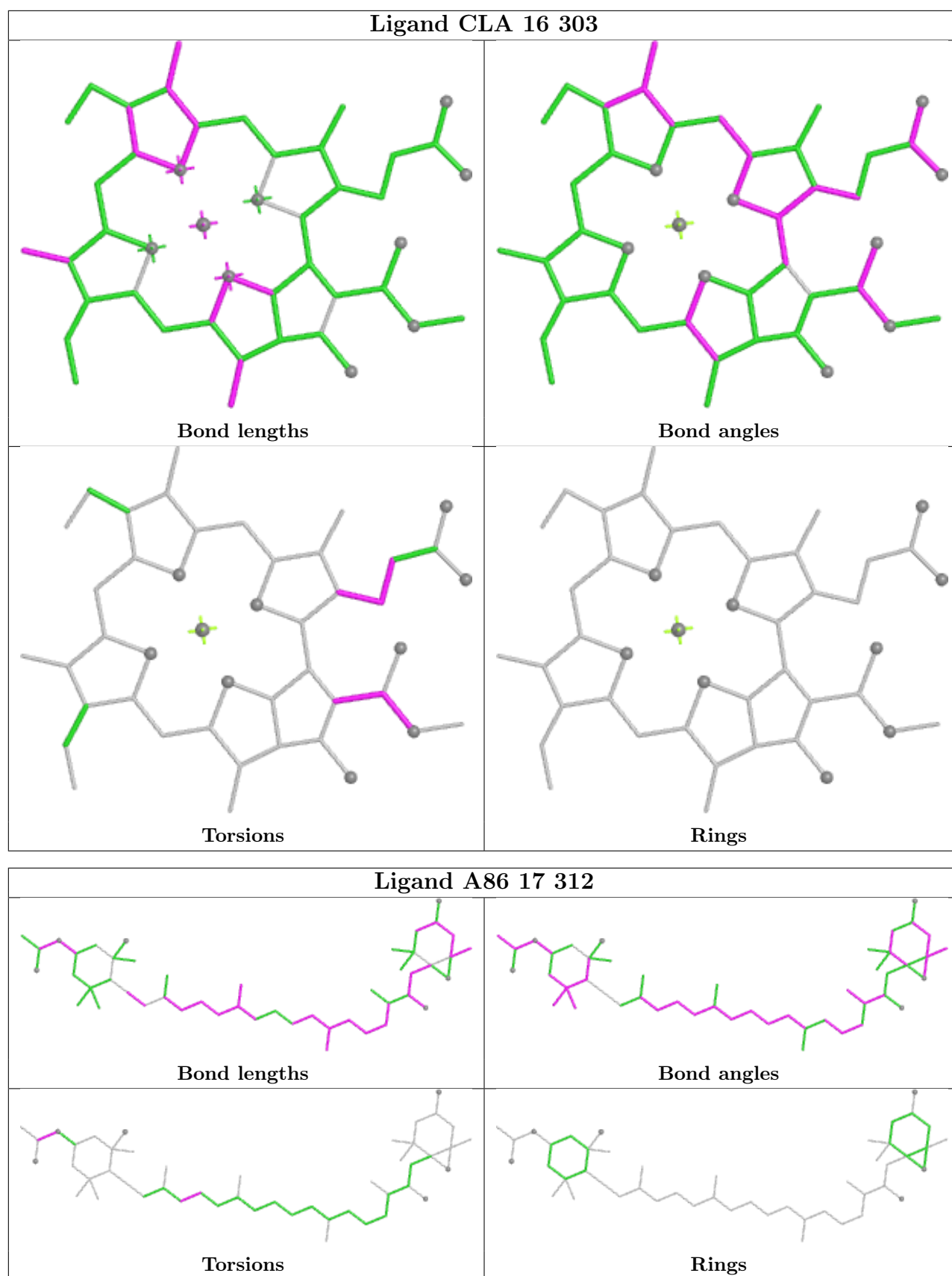


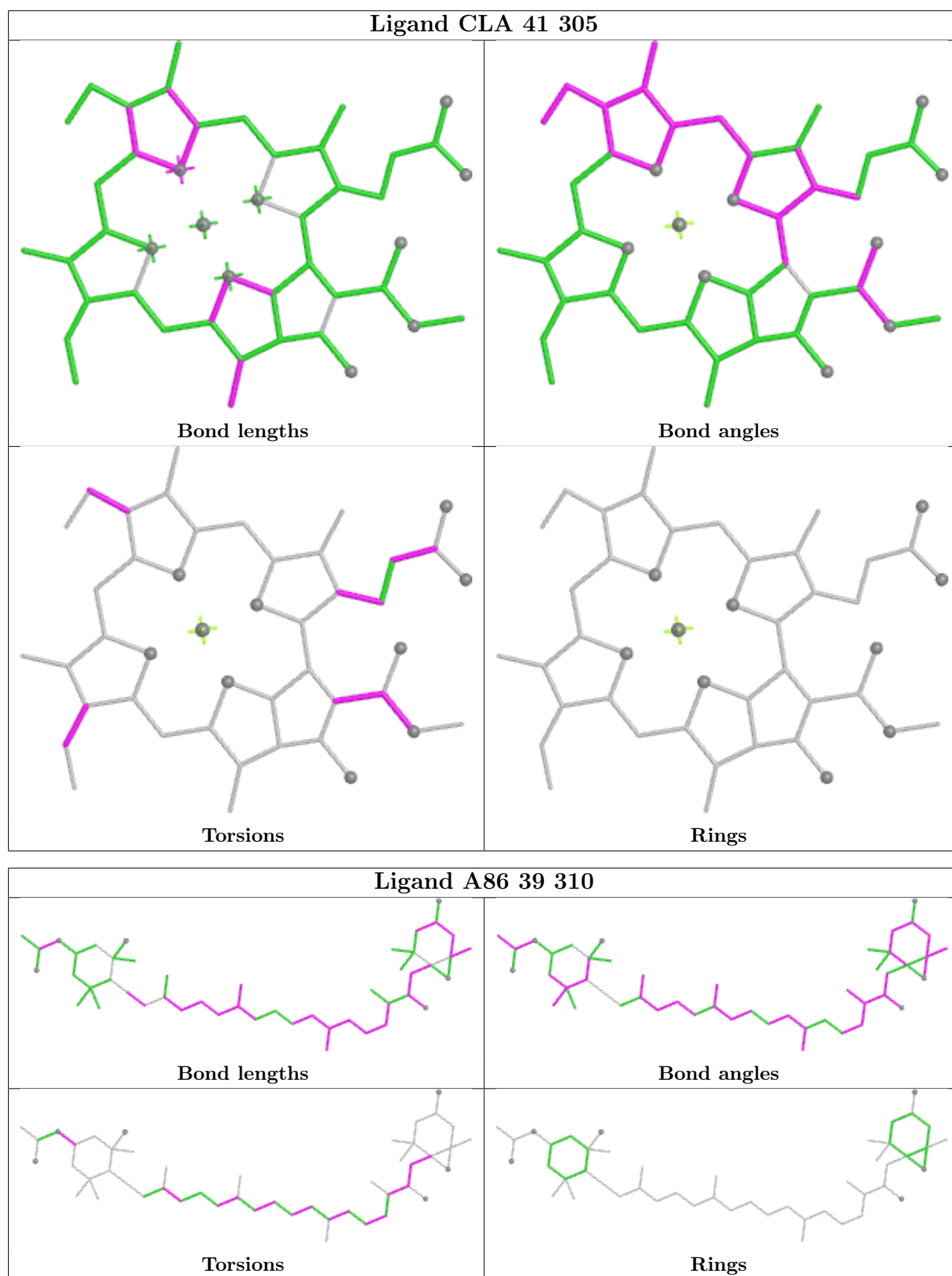


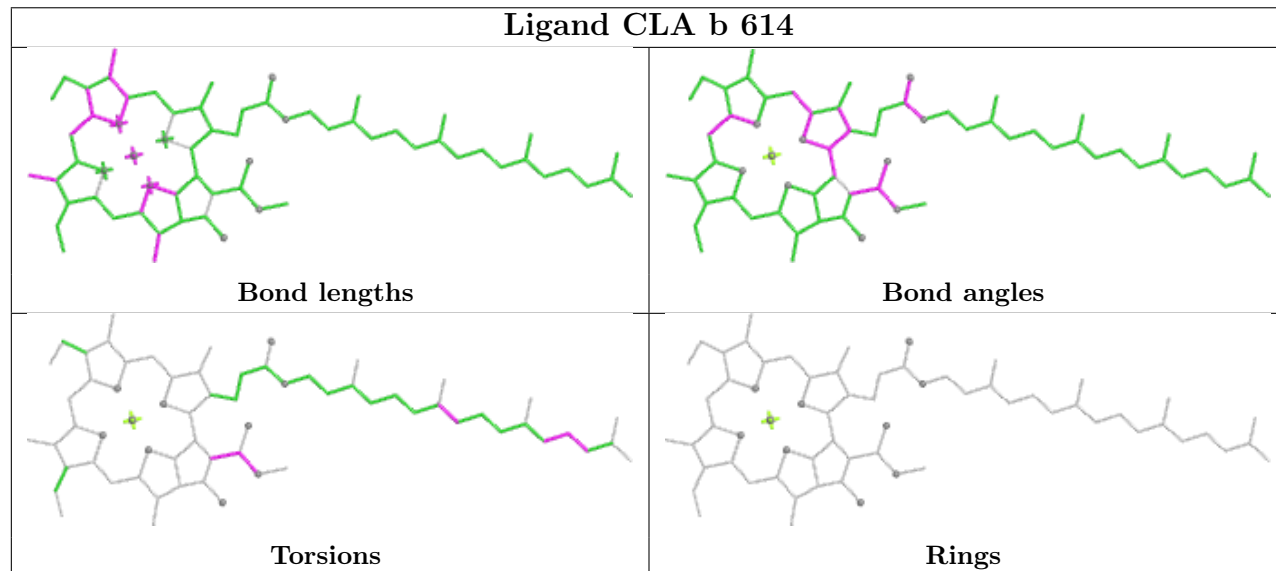
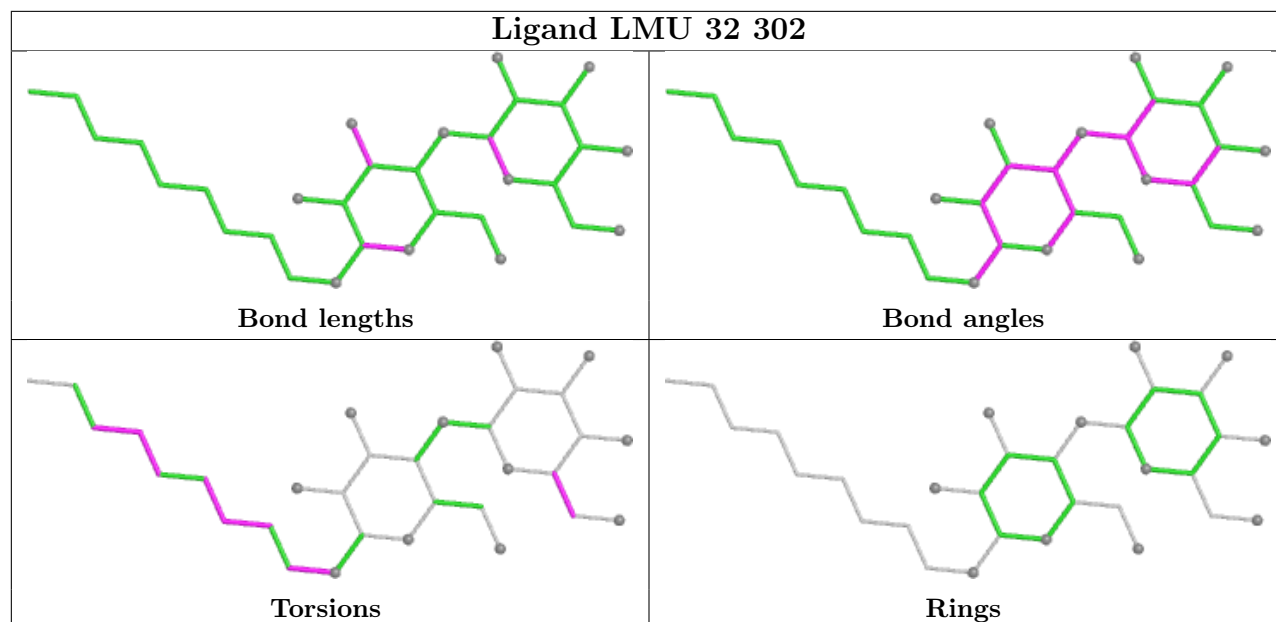


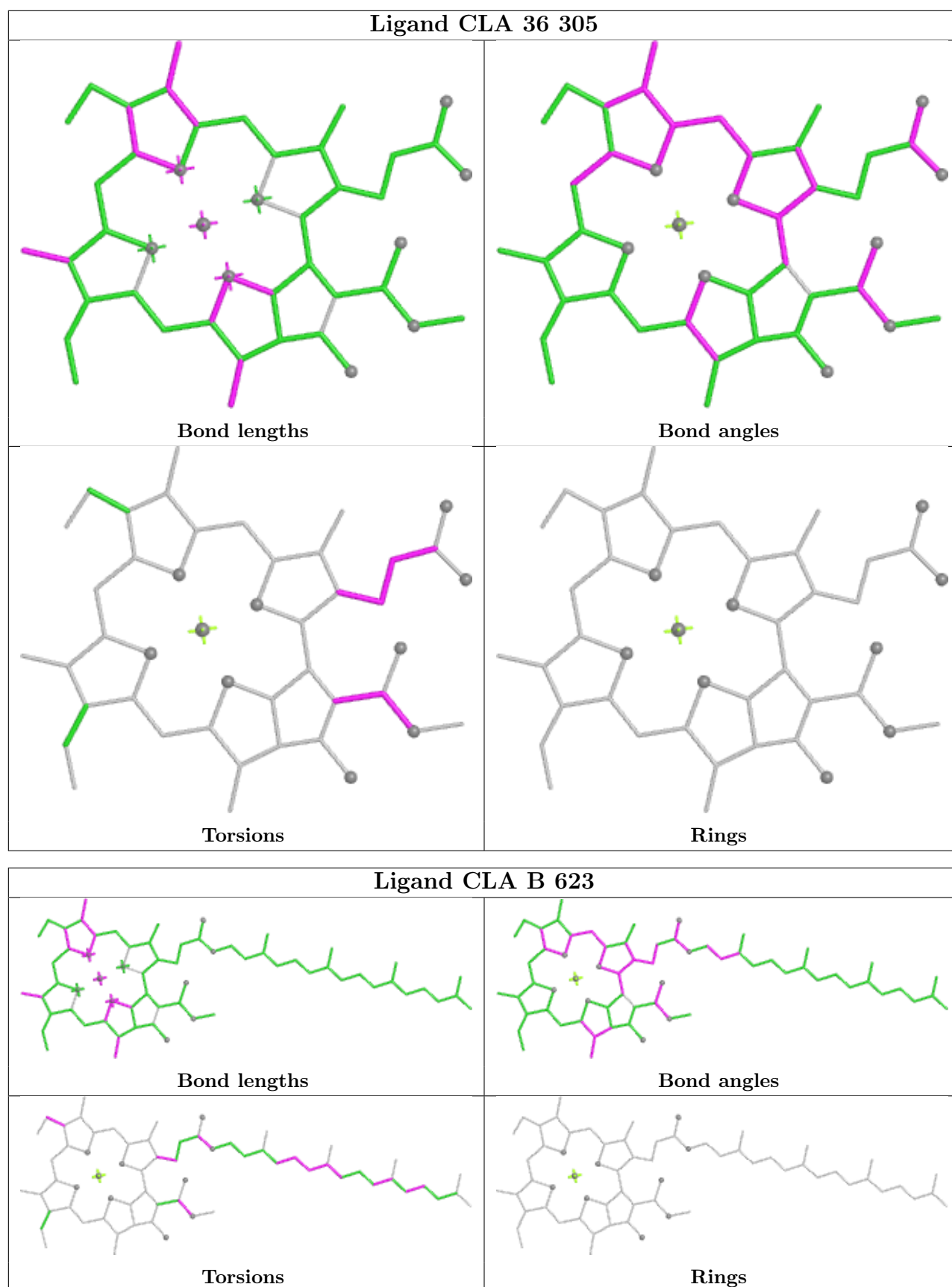


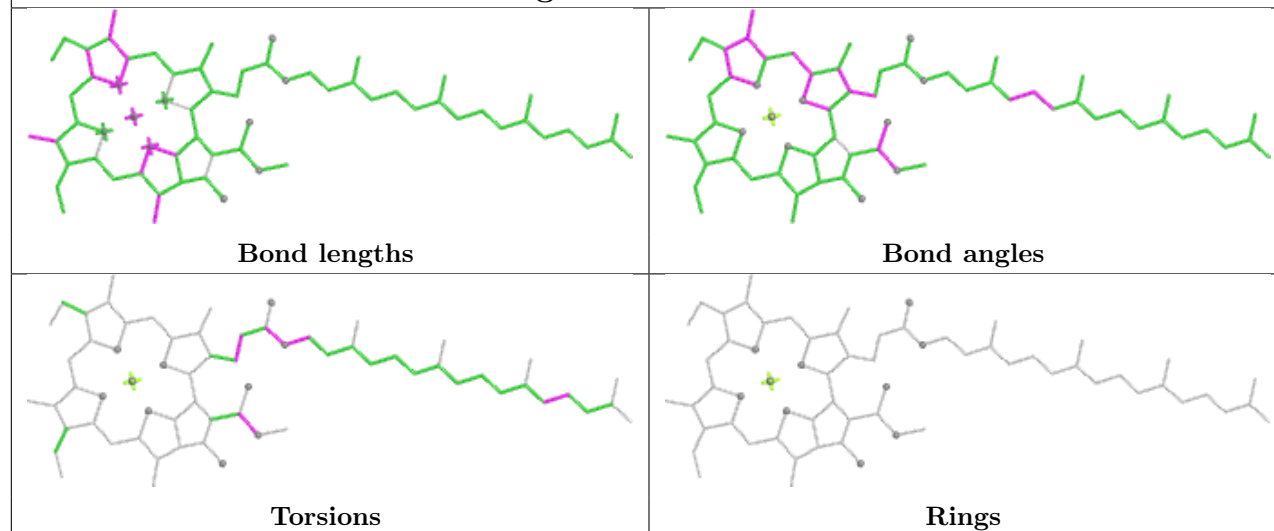
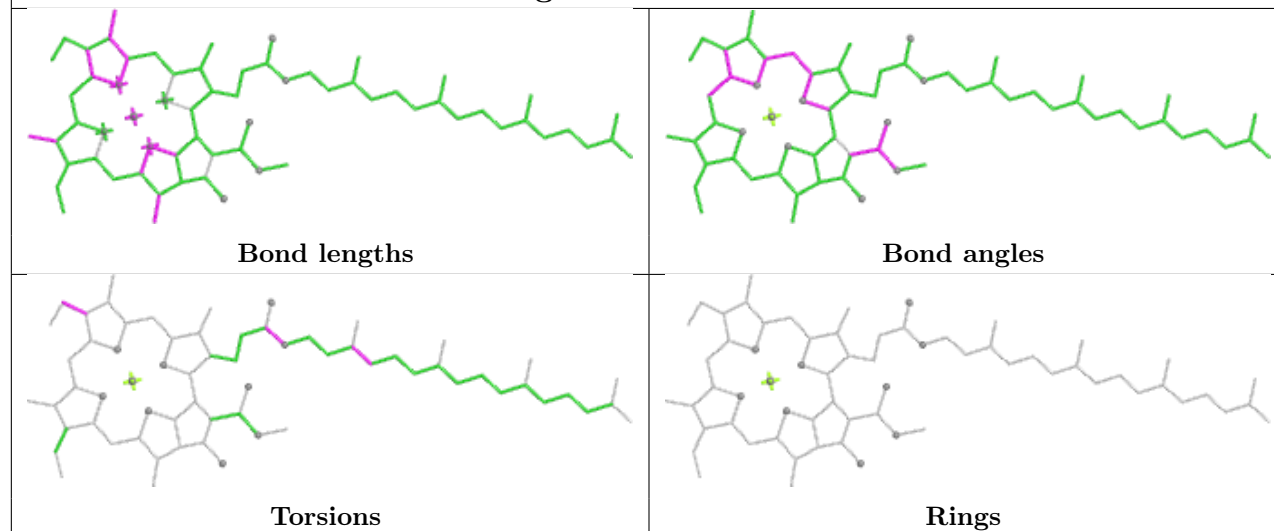


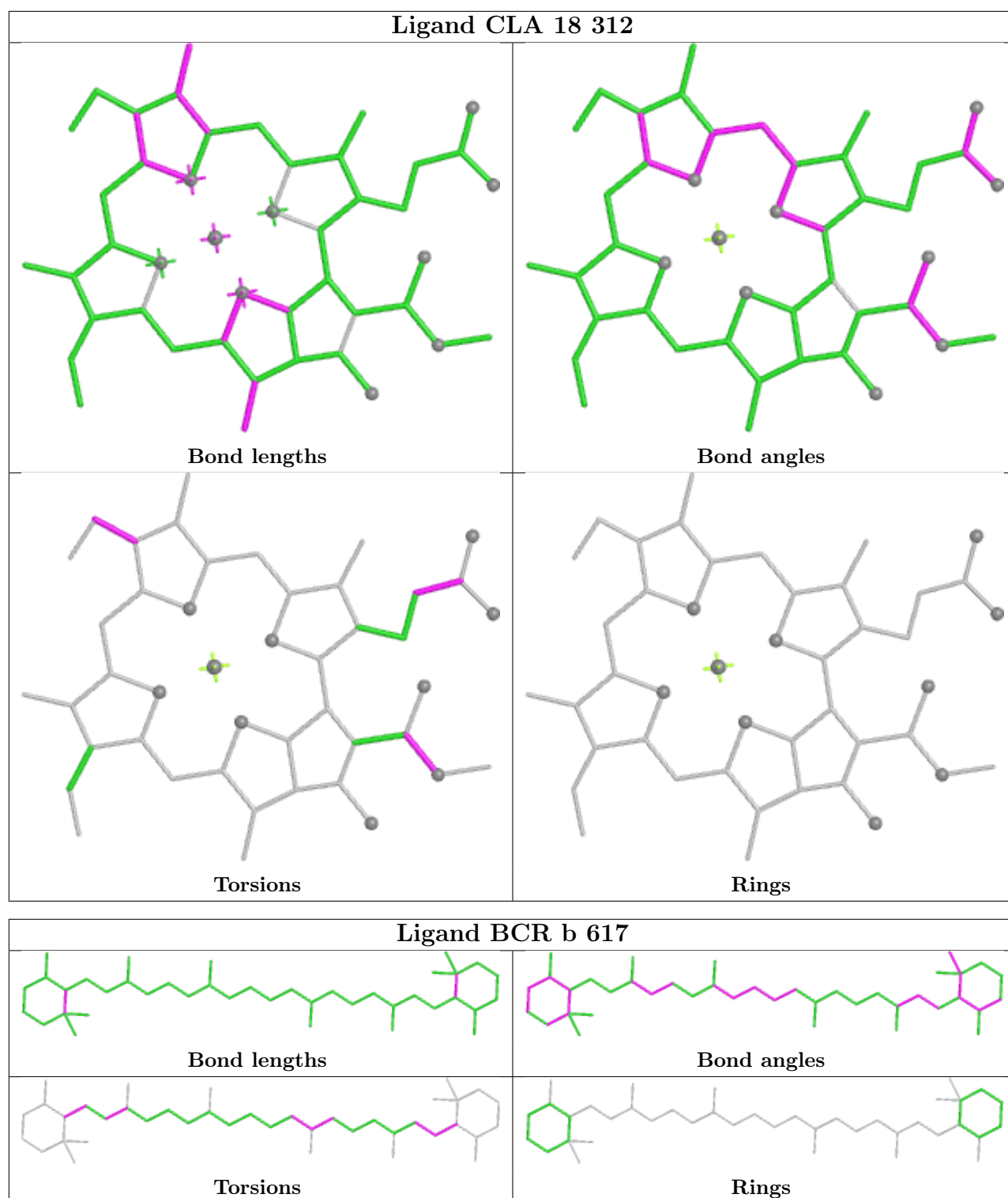


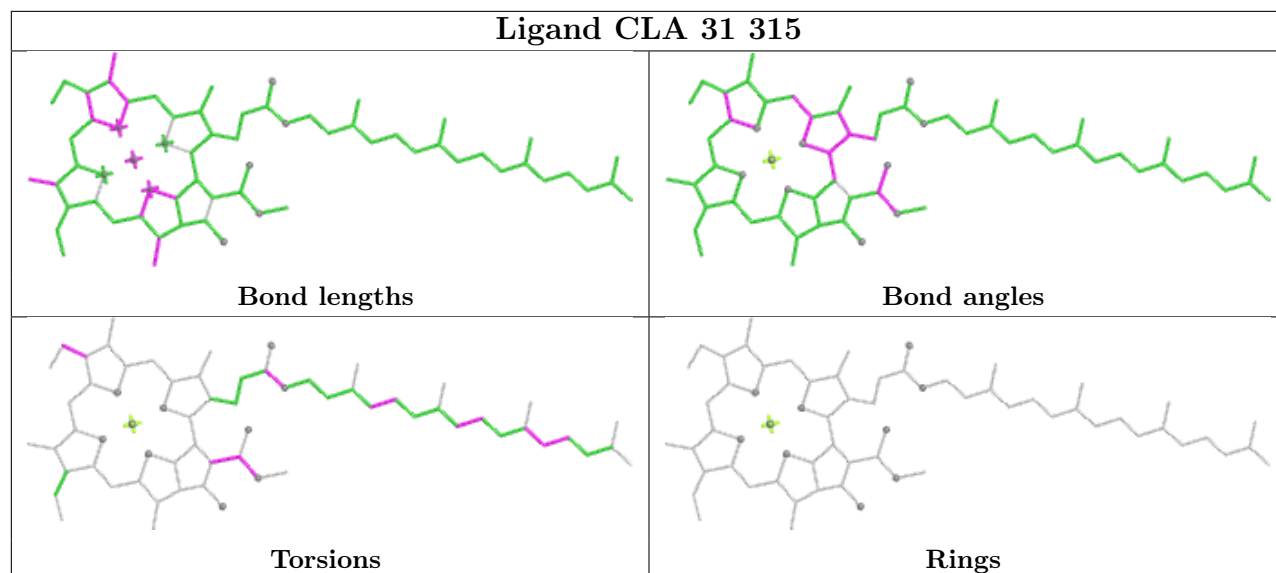
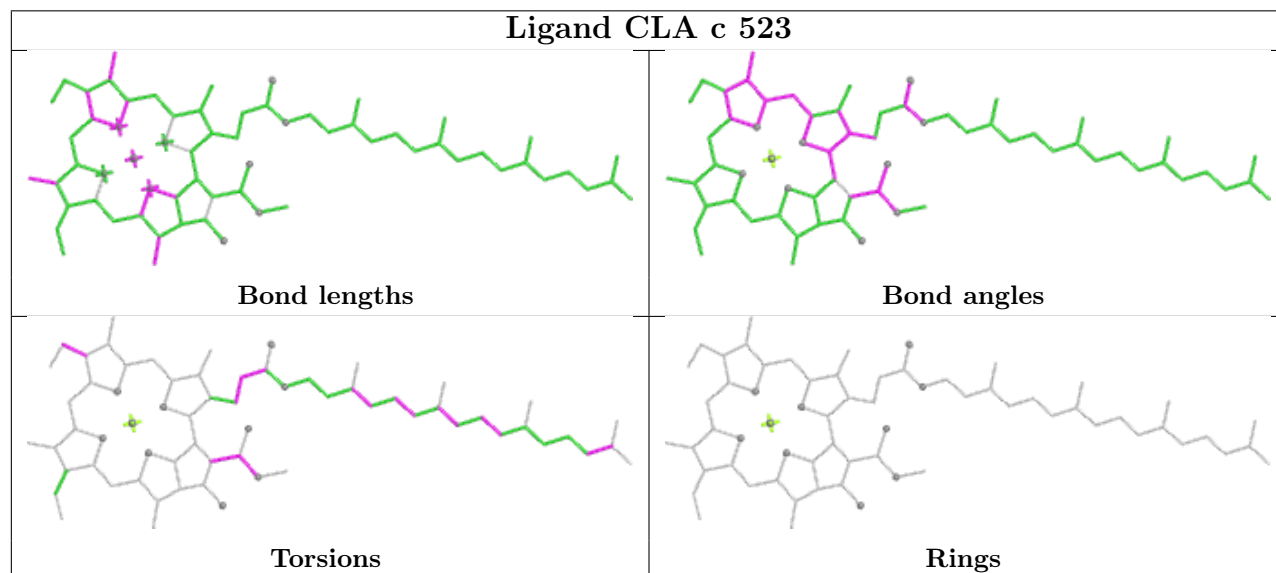
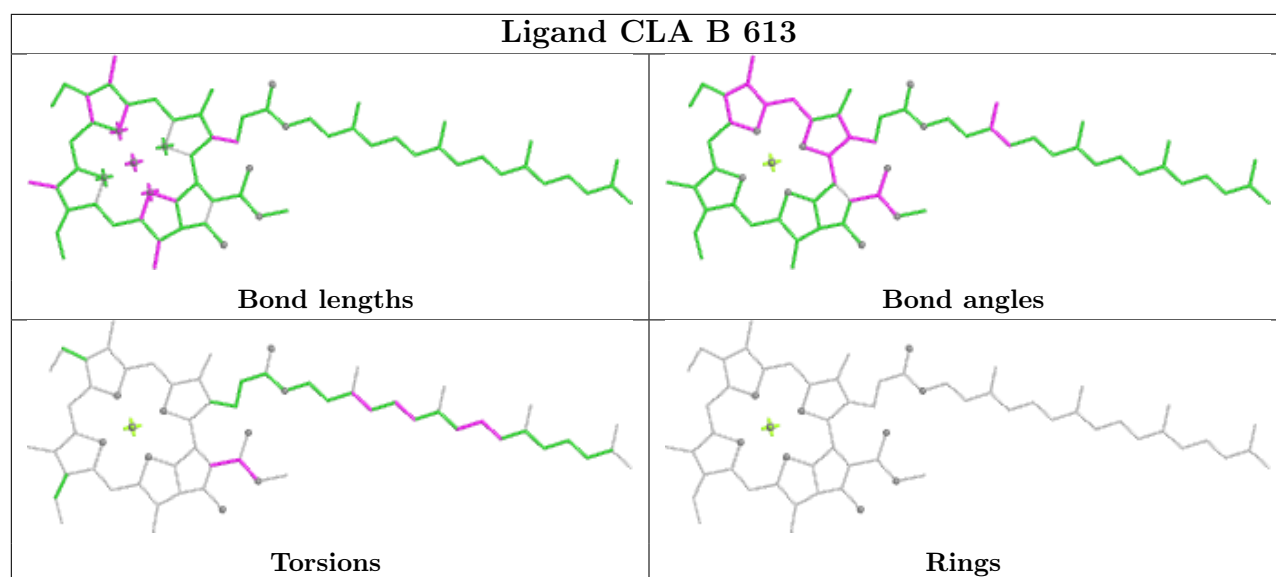


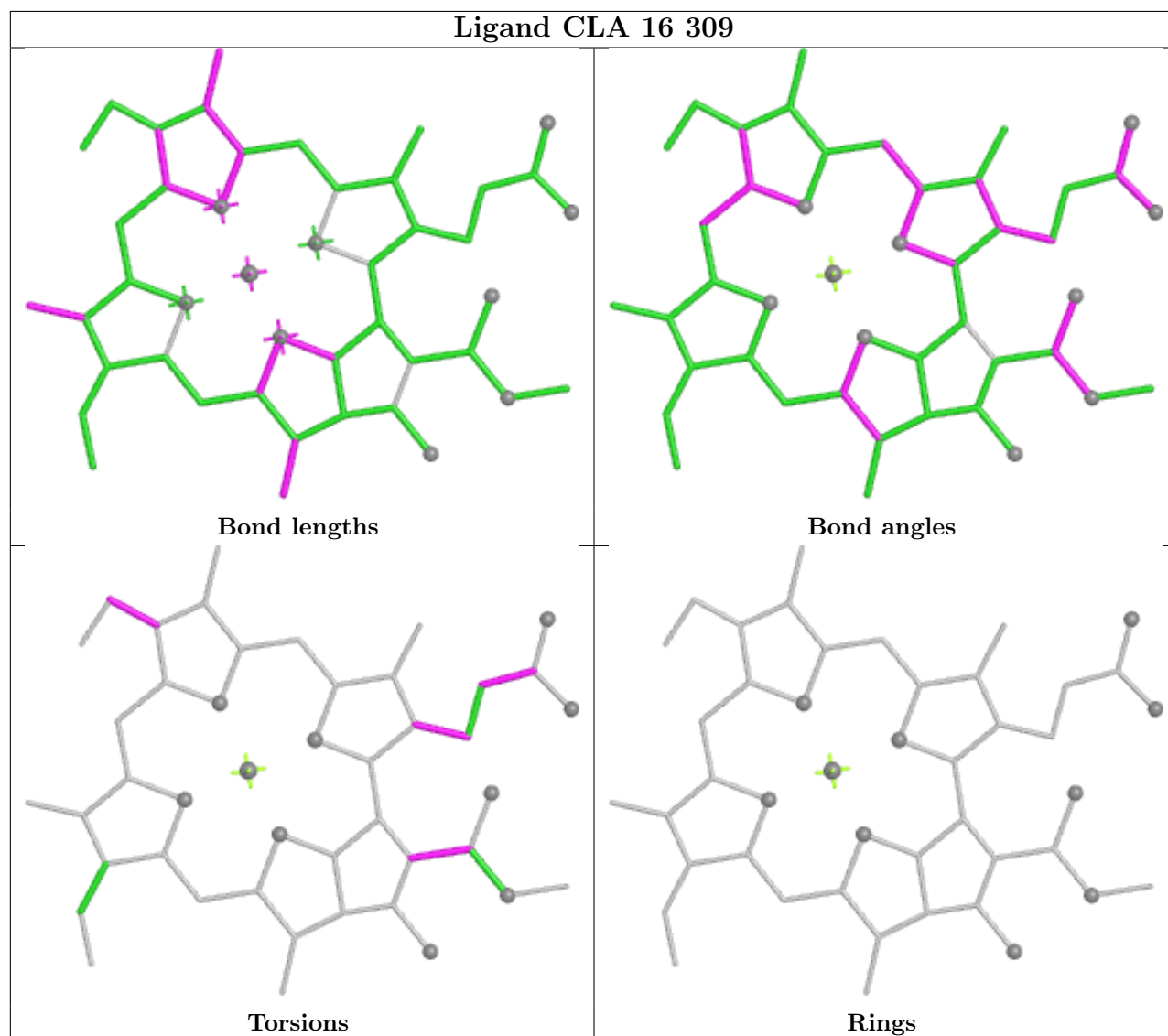
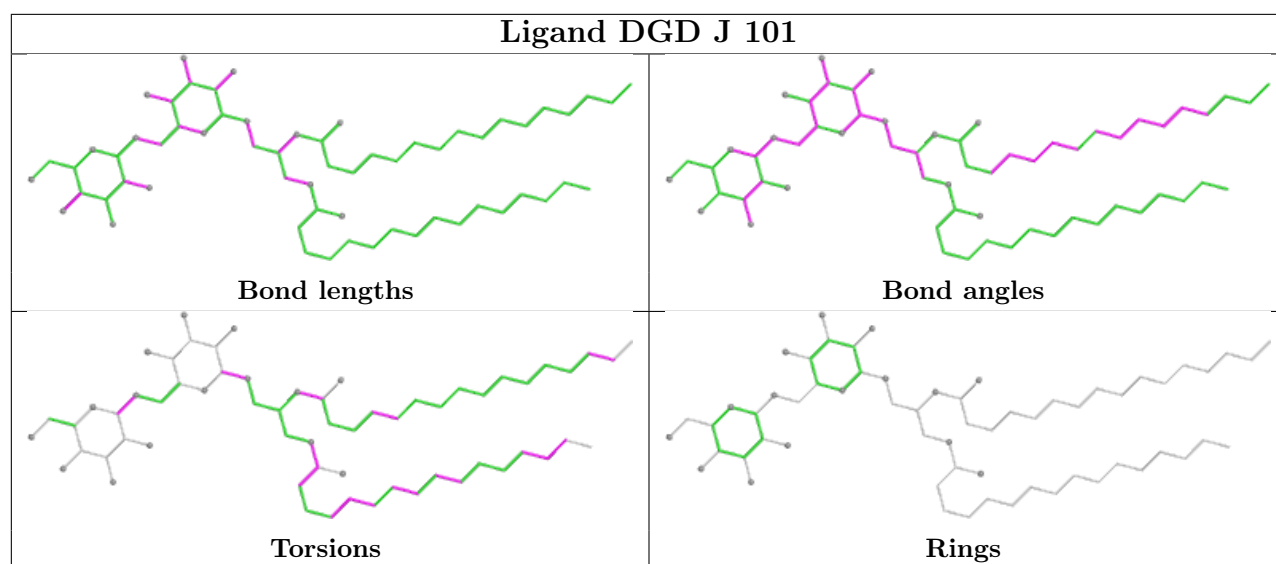


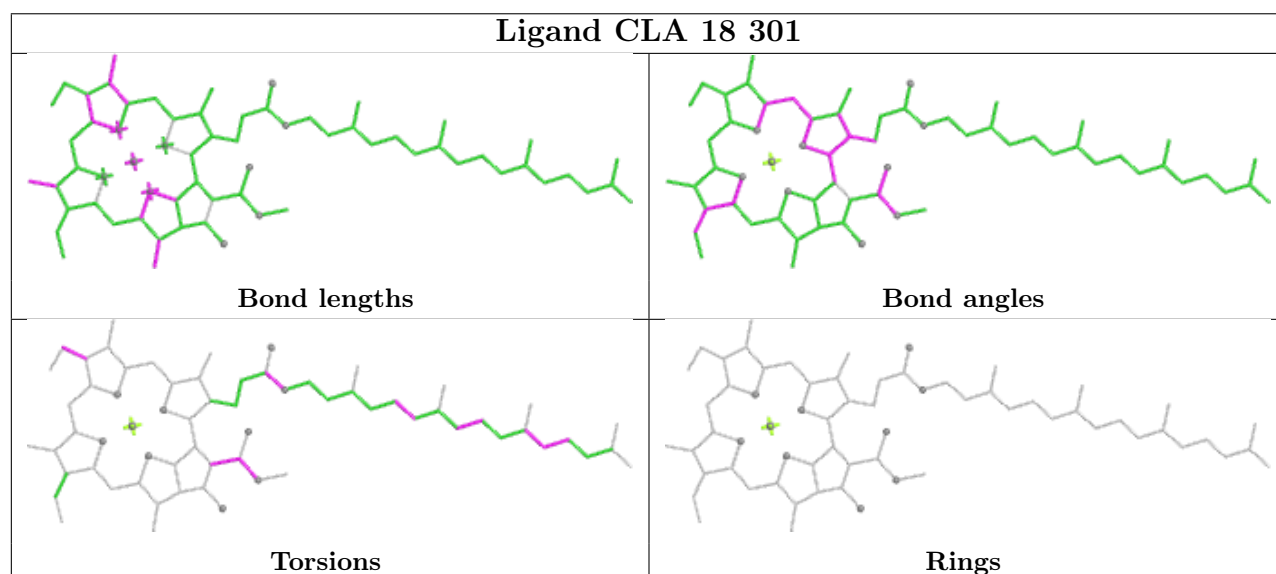
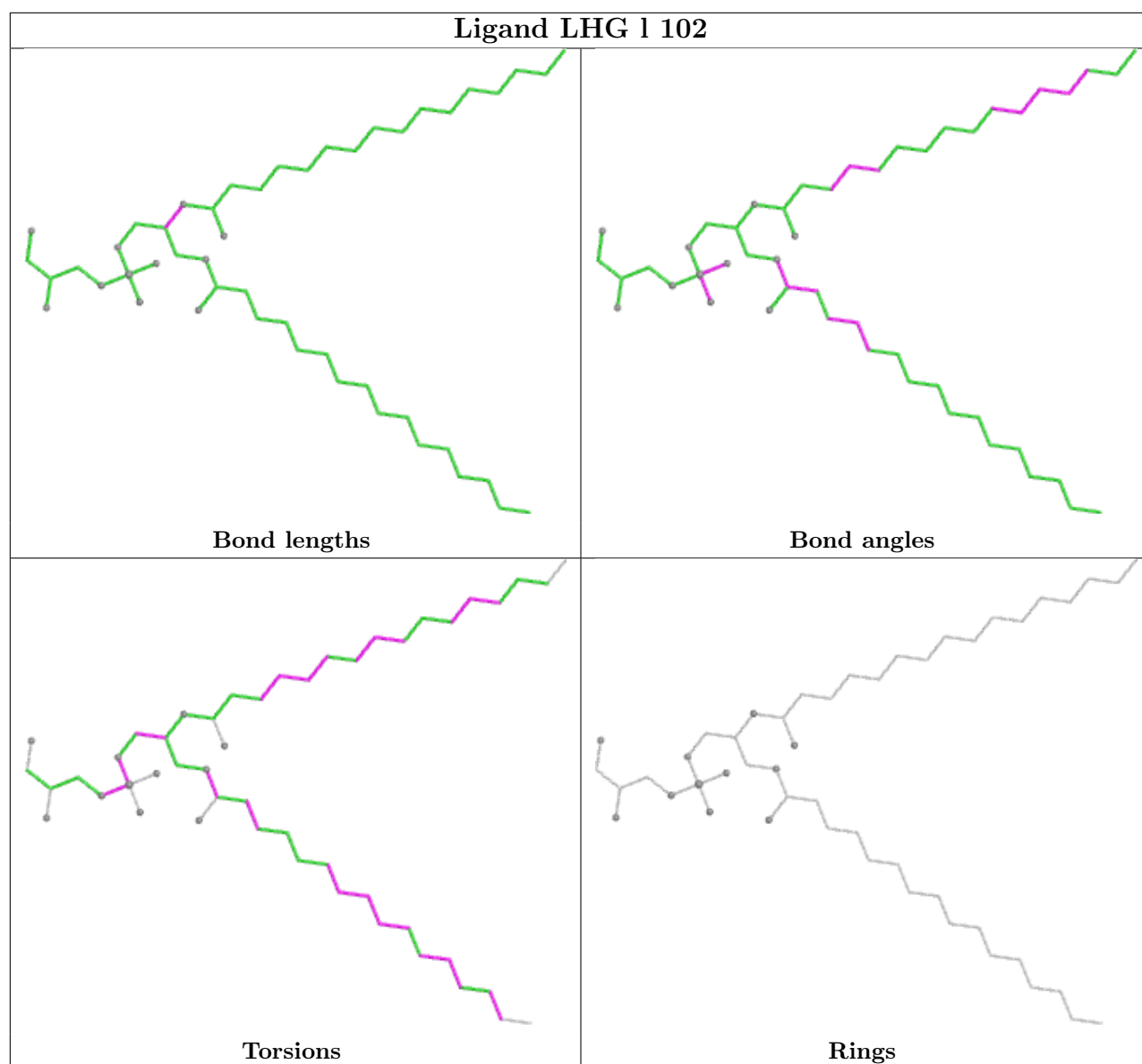


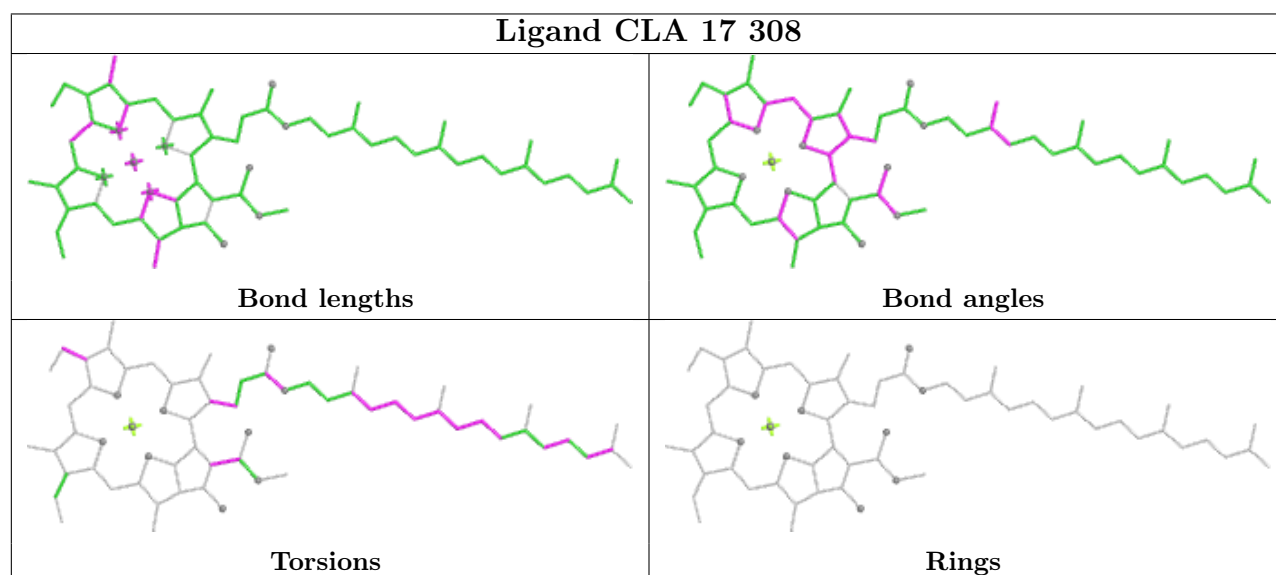
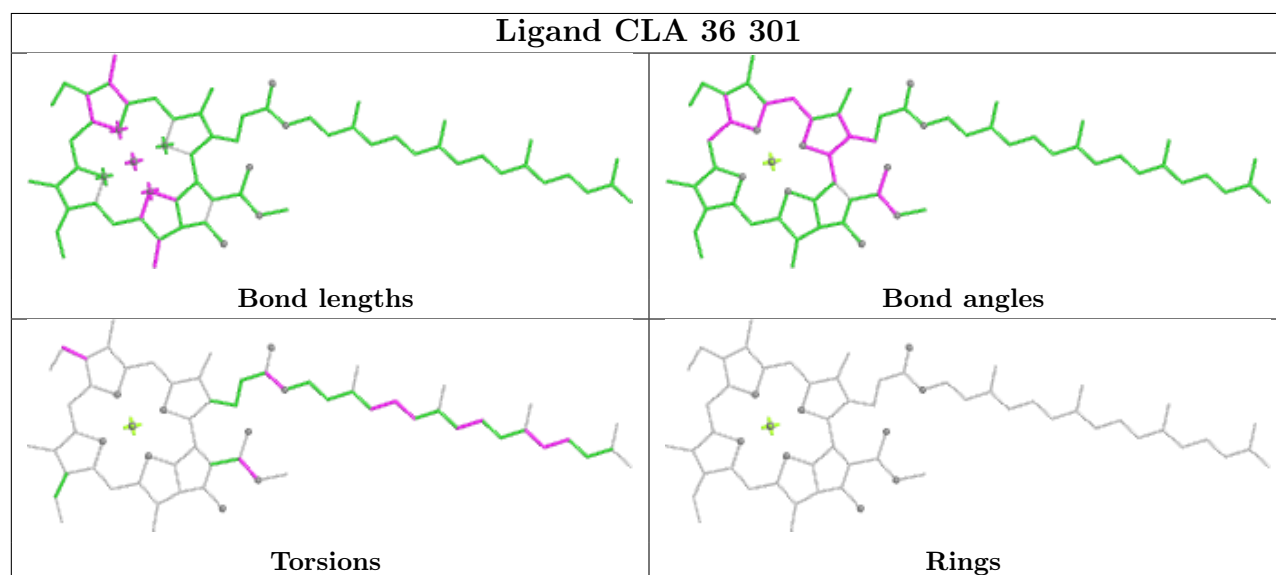
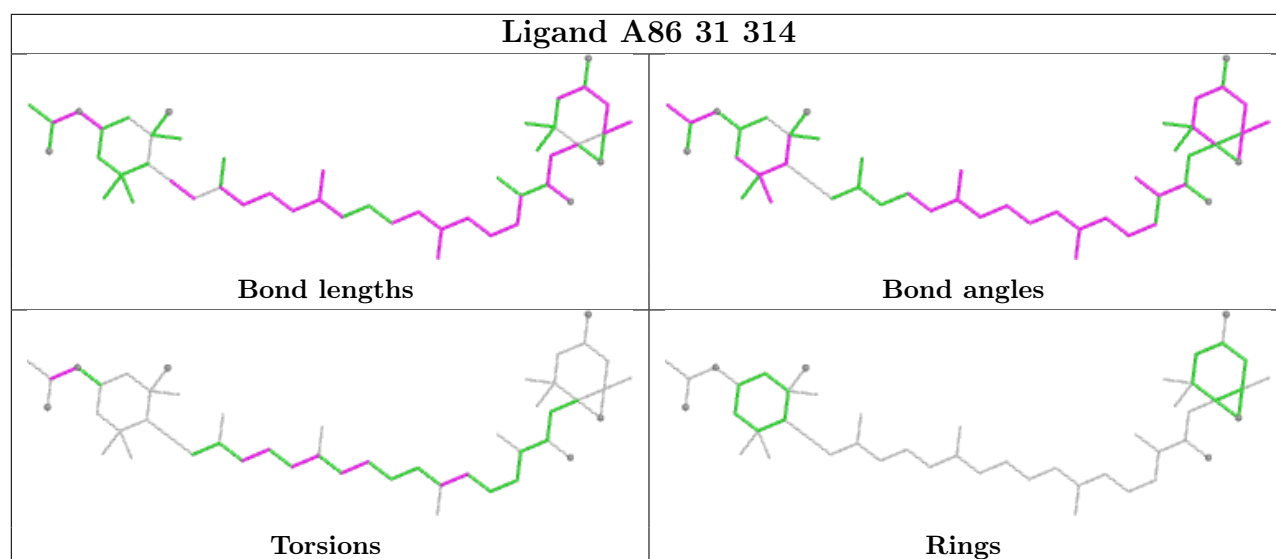
Ligand CLA a 402**Ligand CLA d 407**

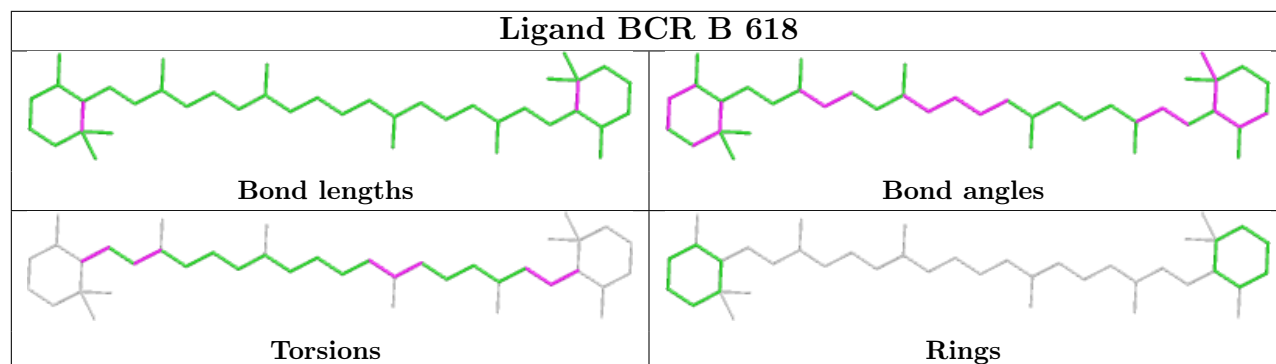
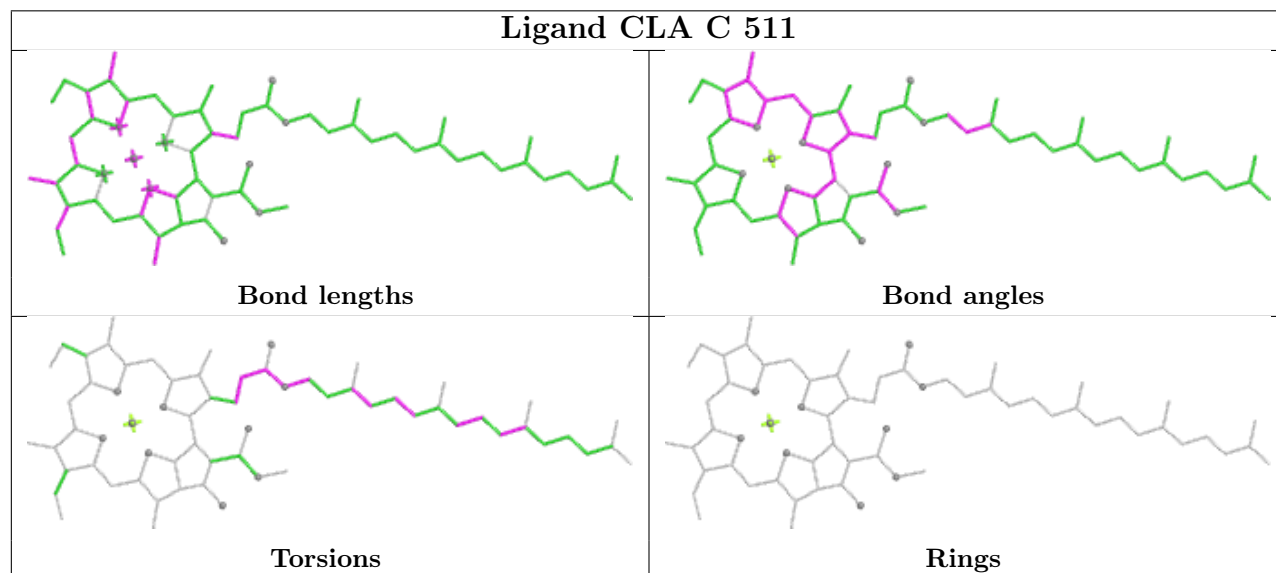
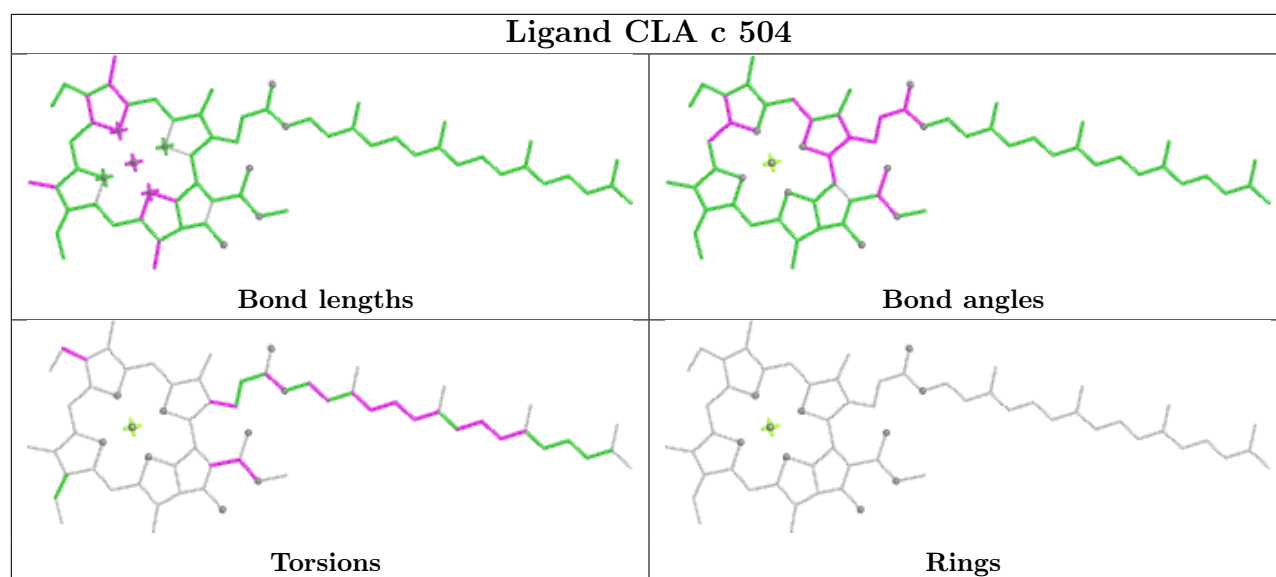


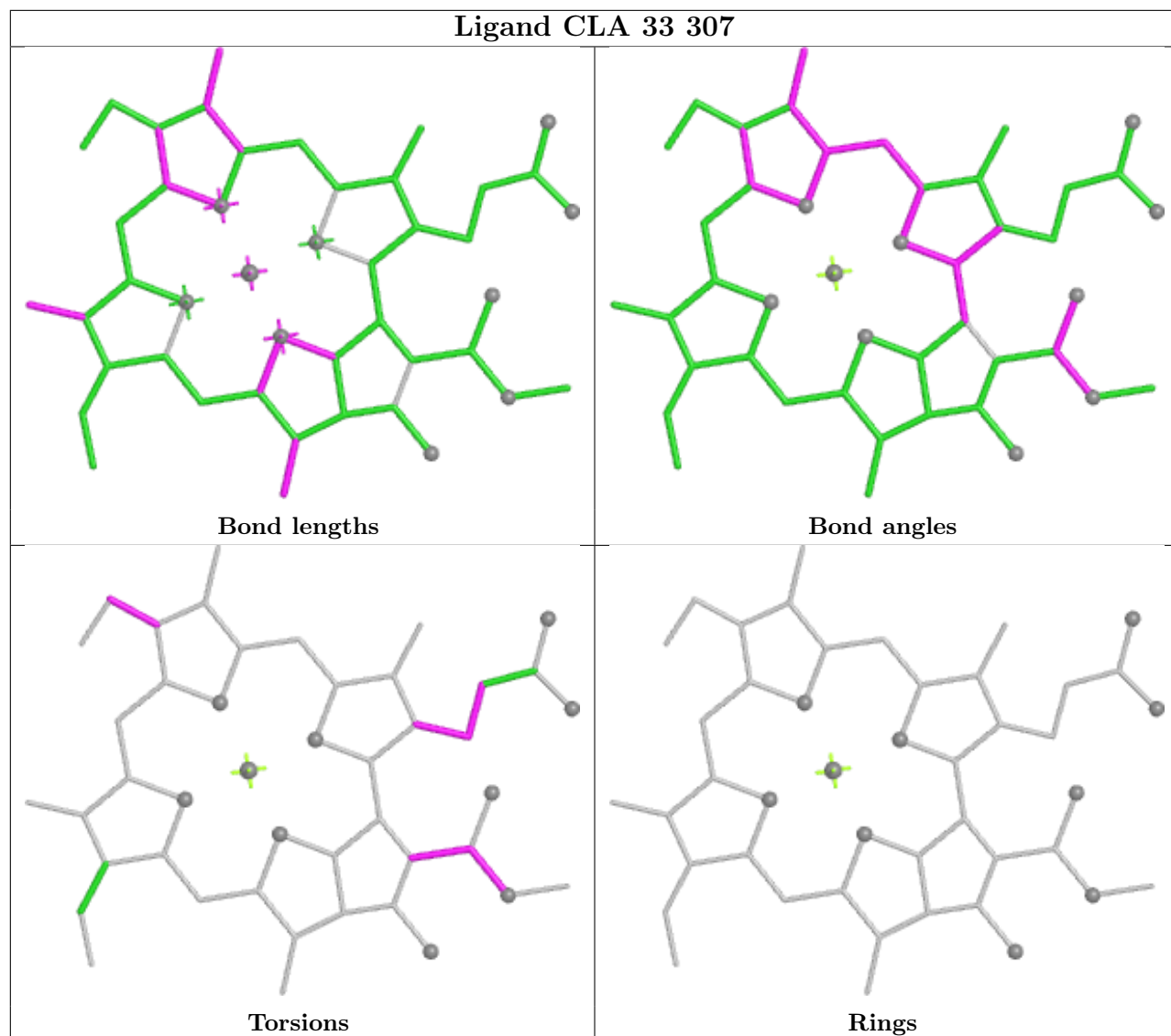


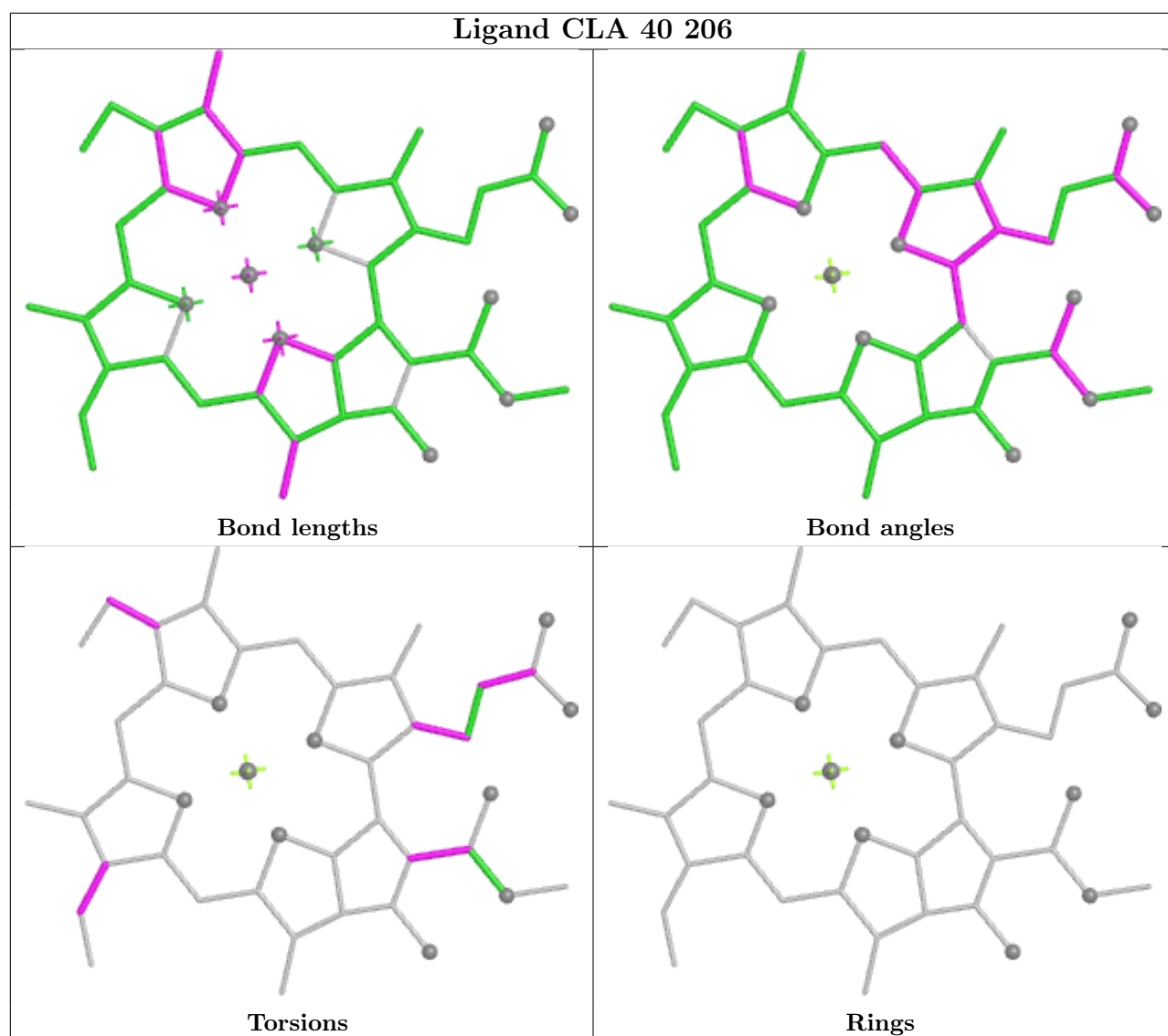


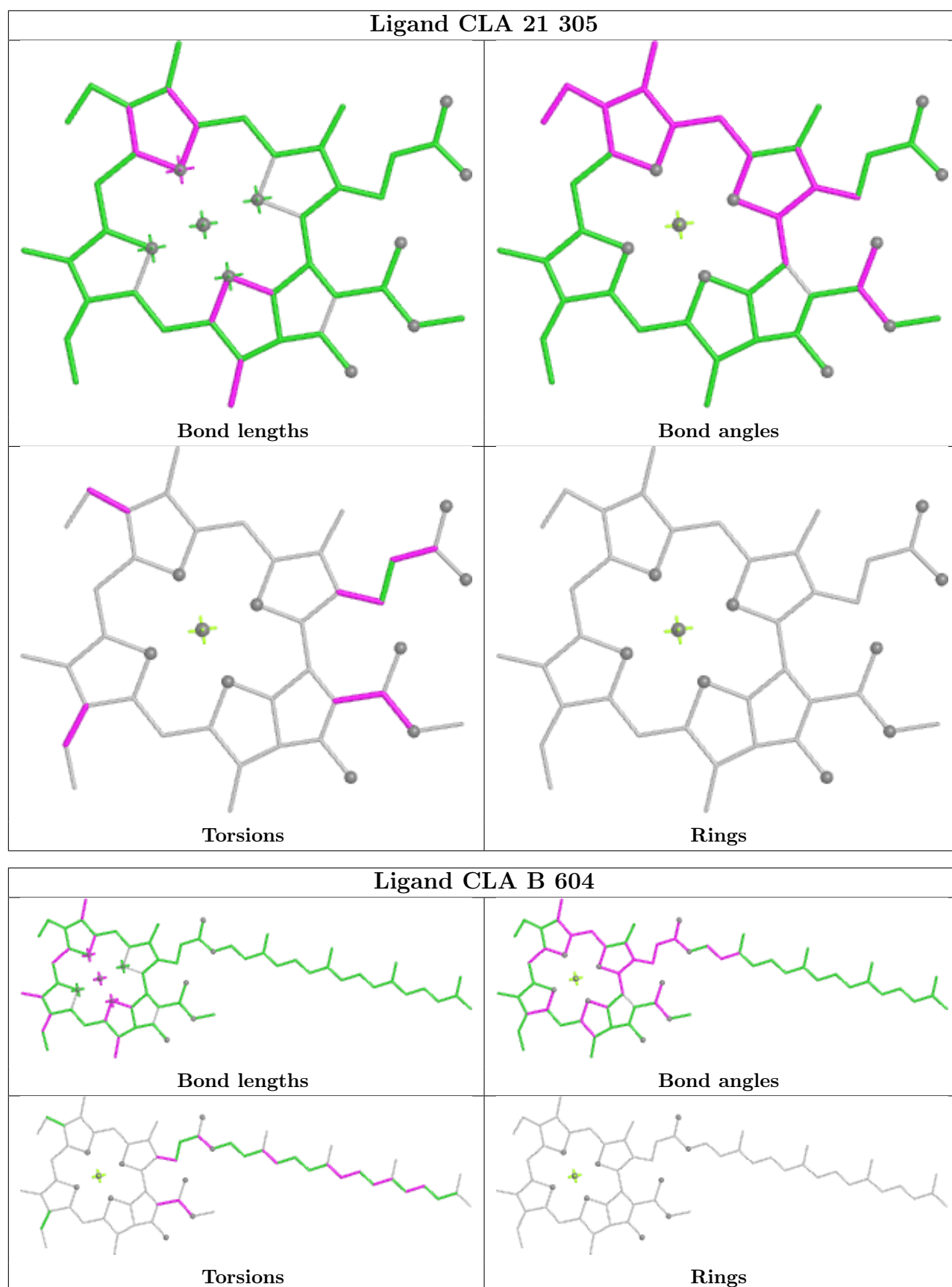


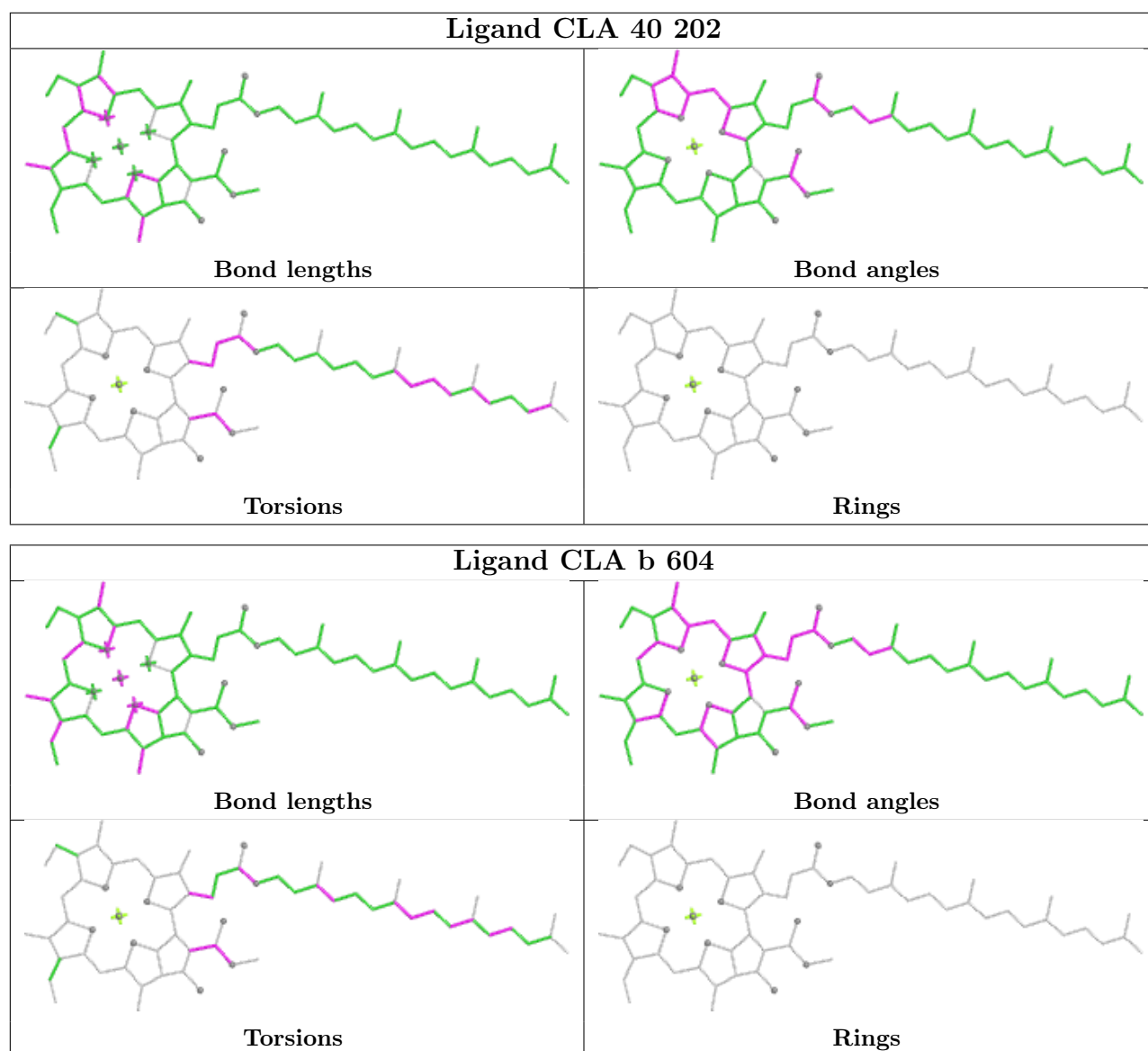


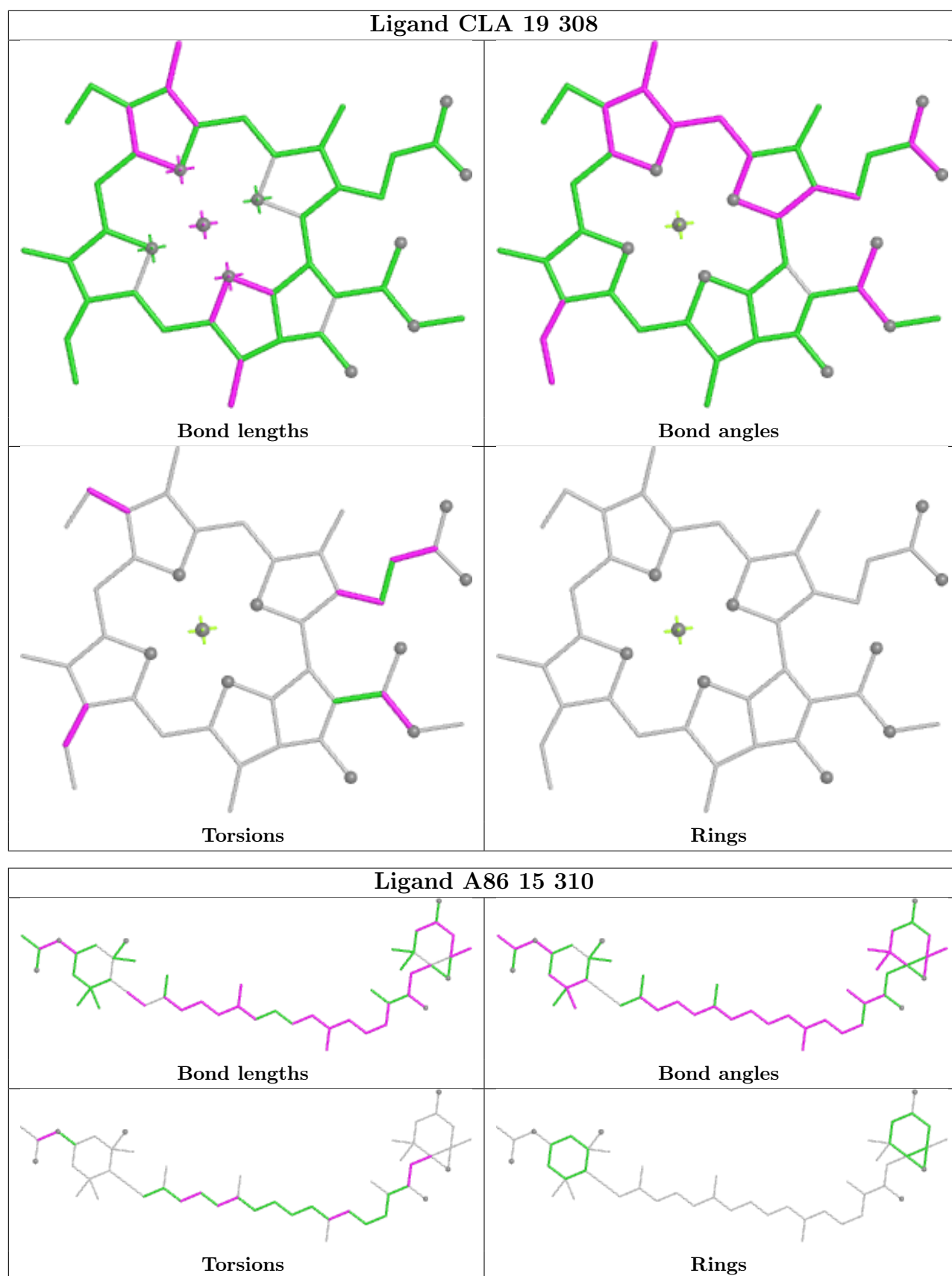


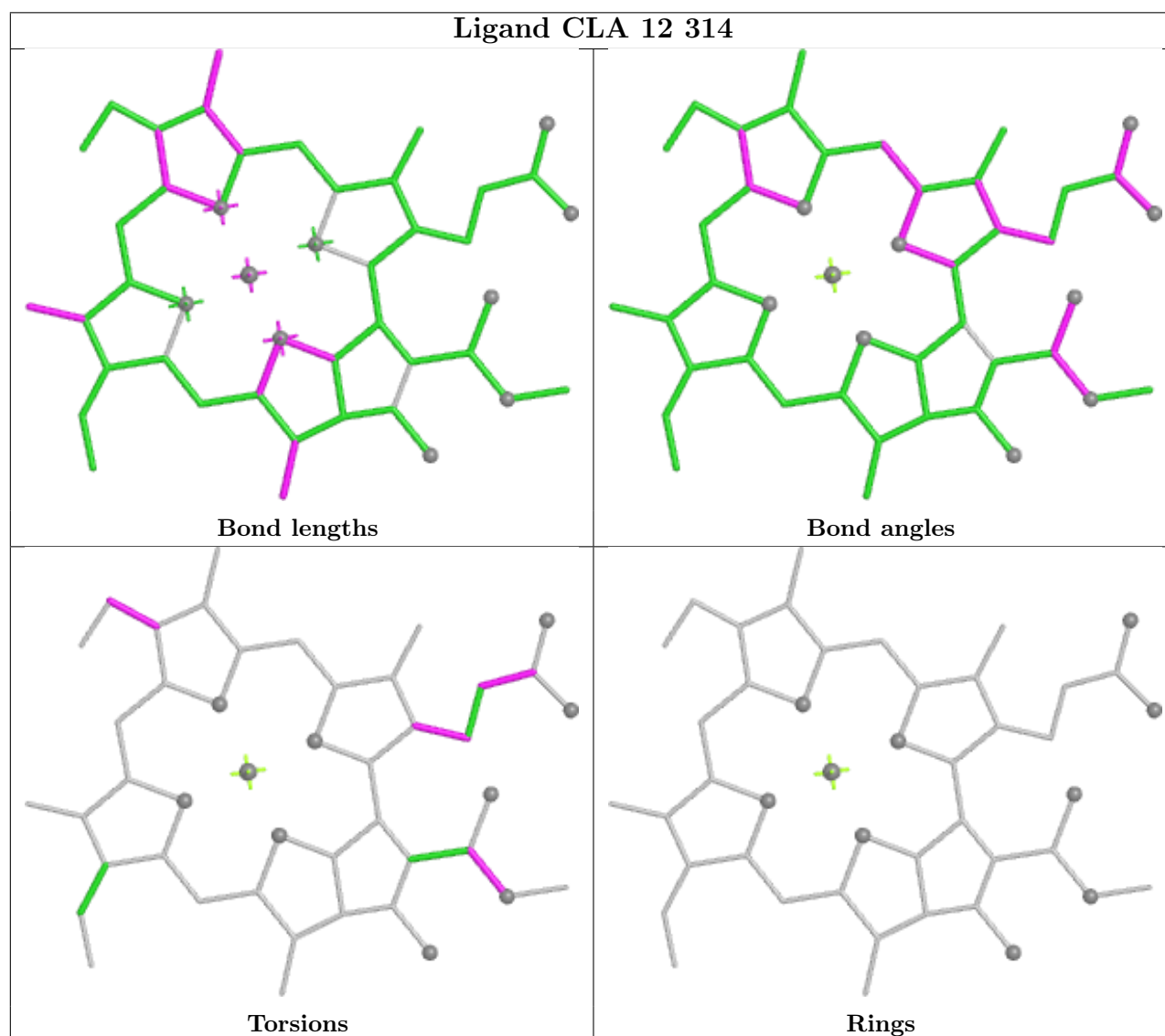
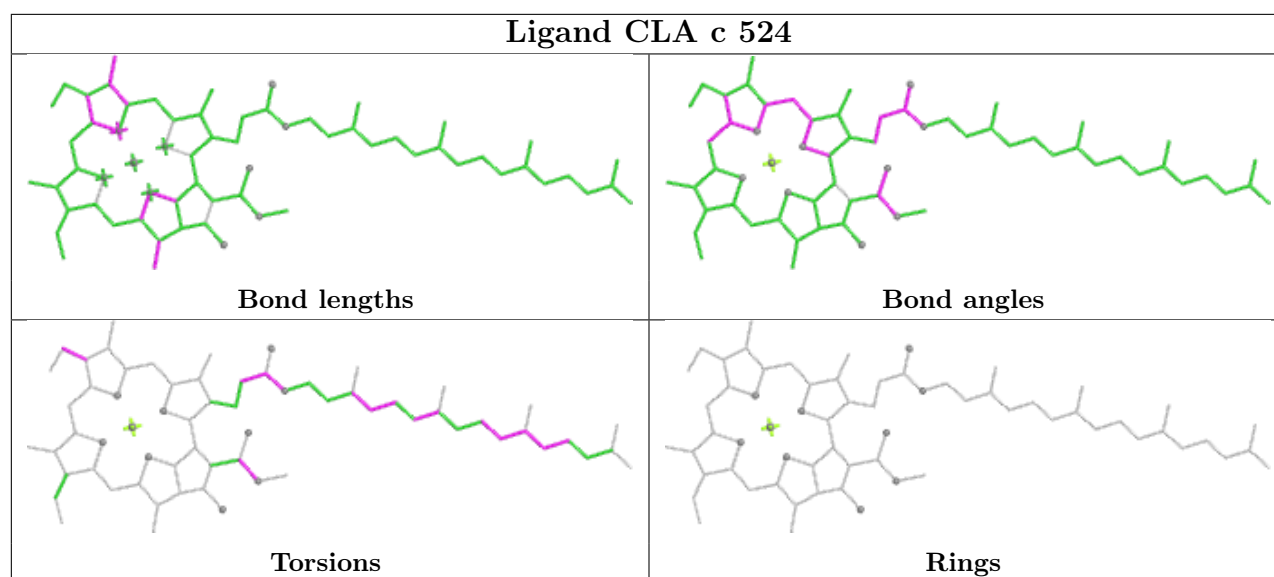


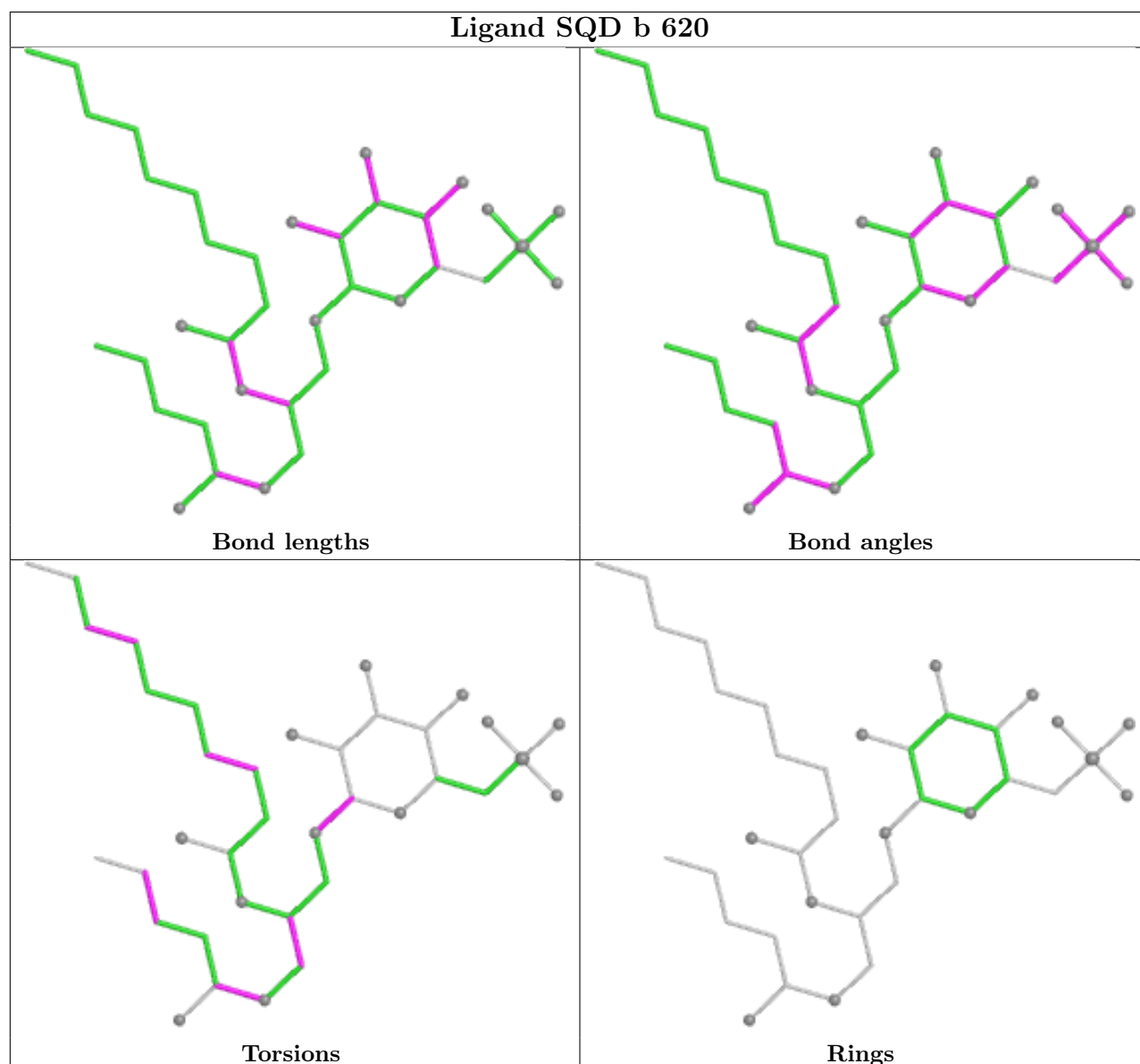
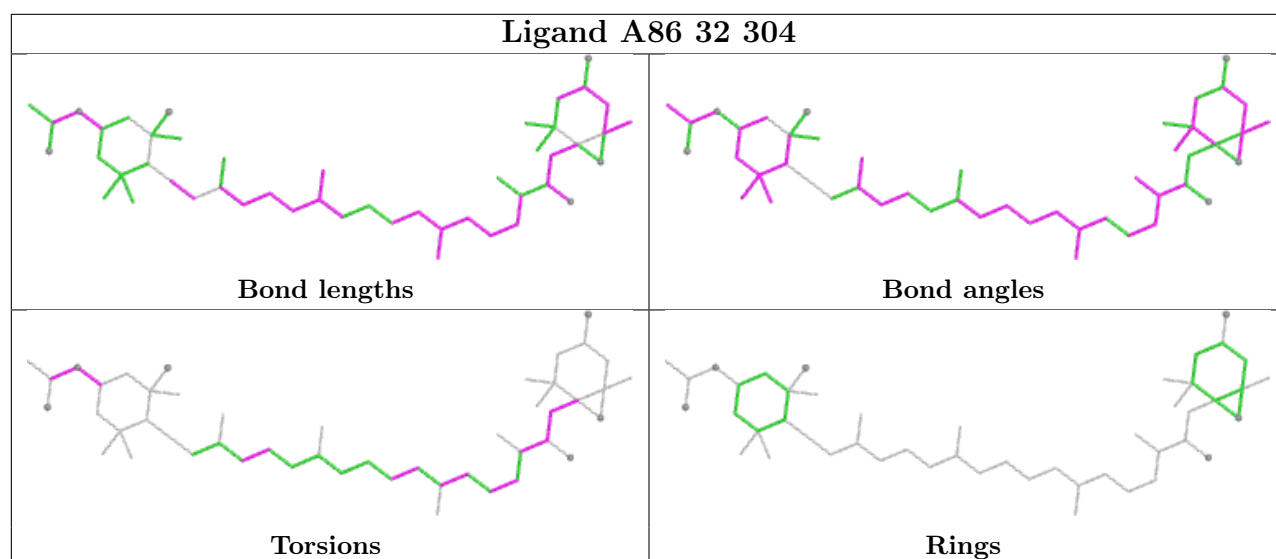


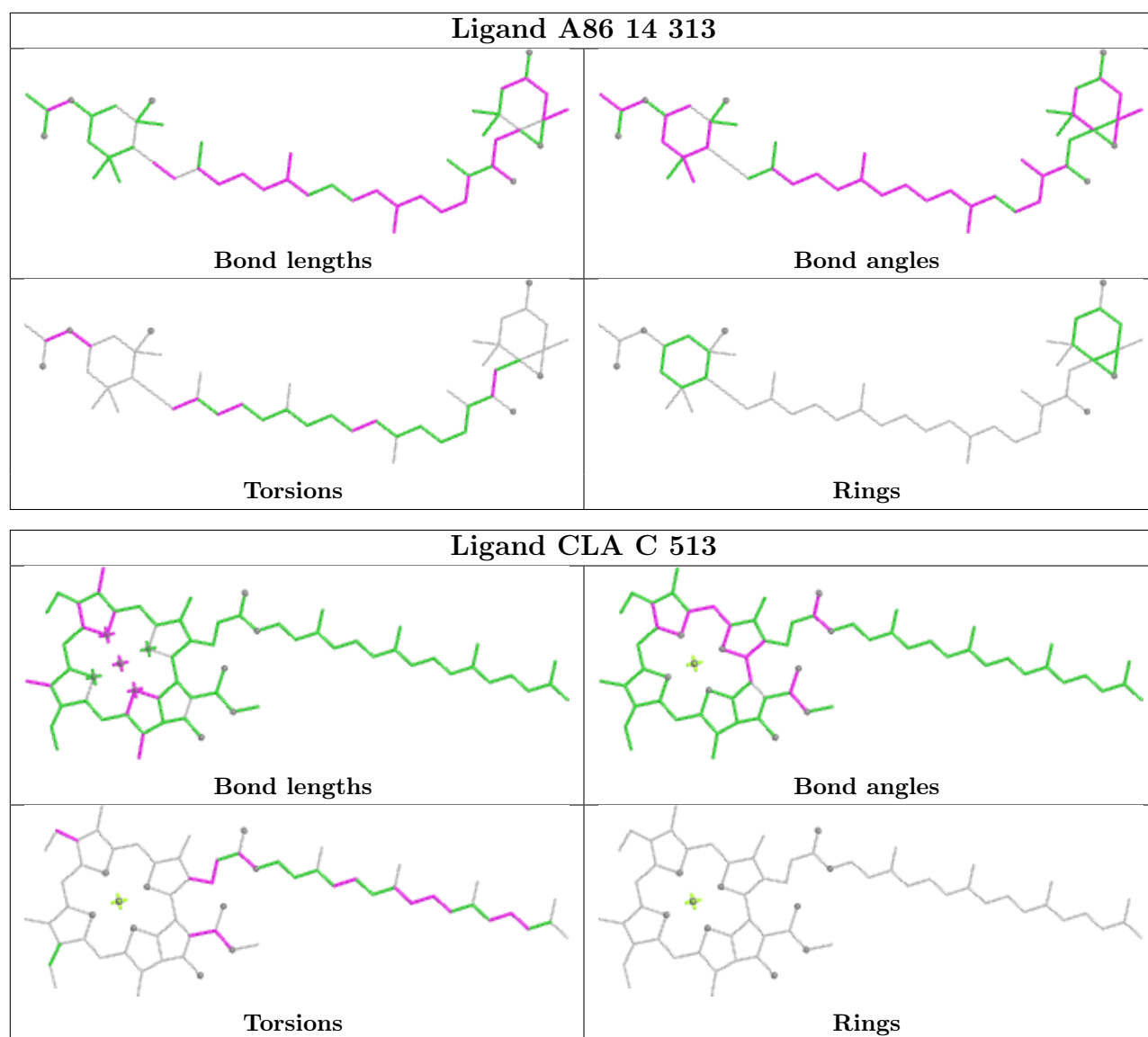


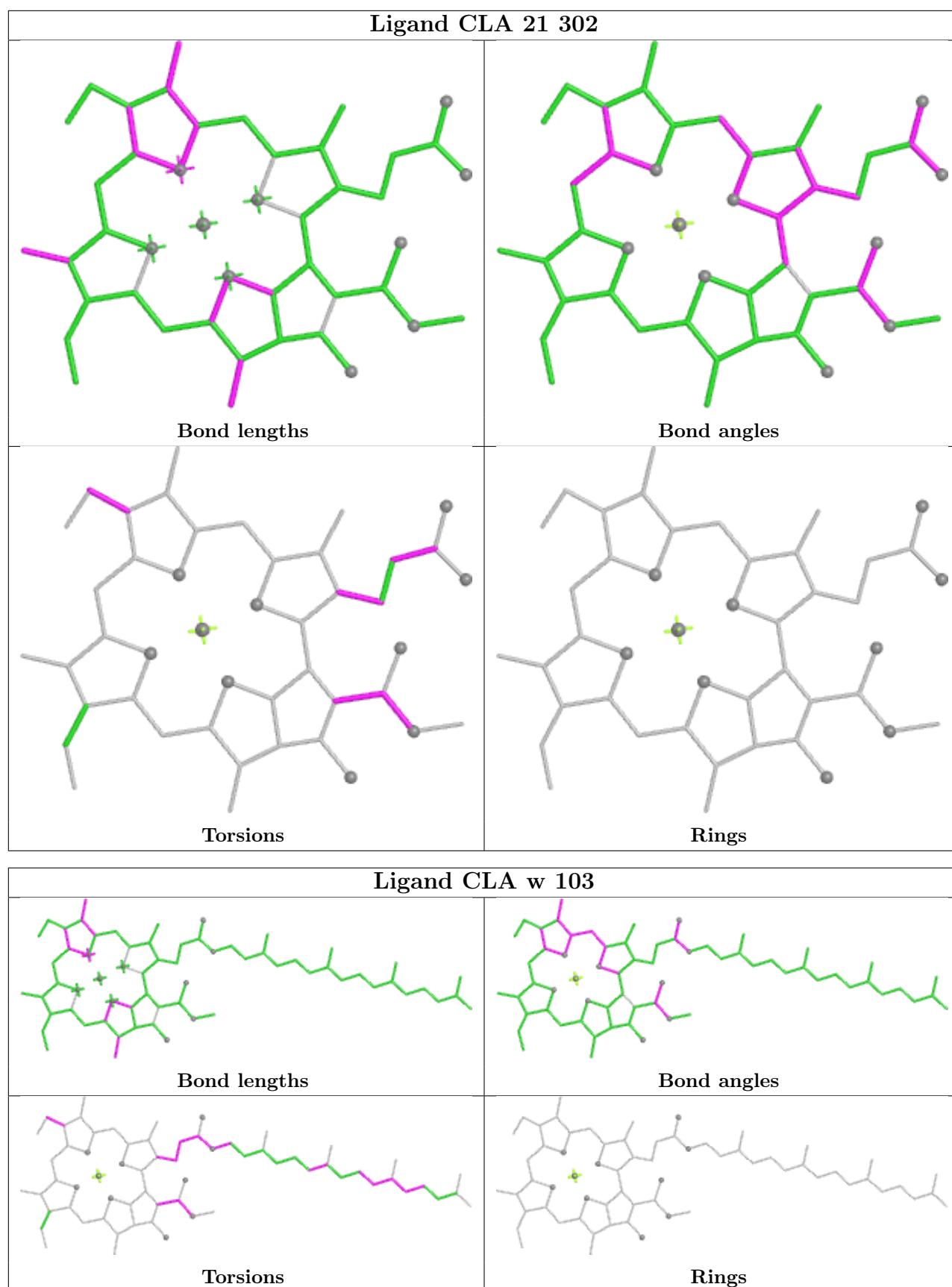


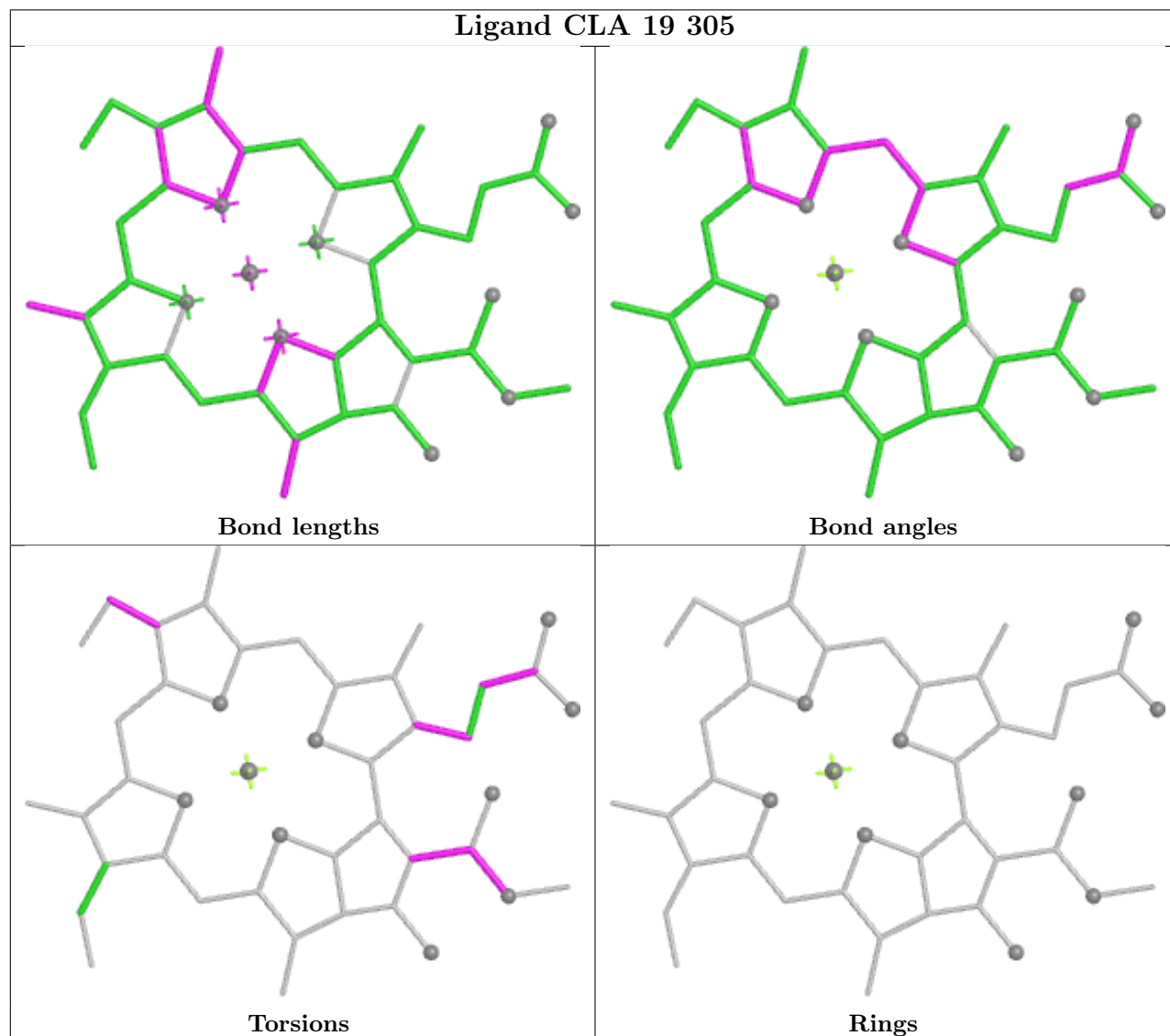
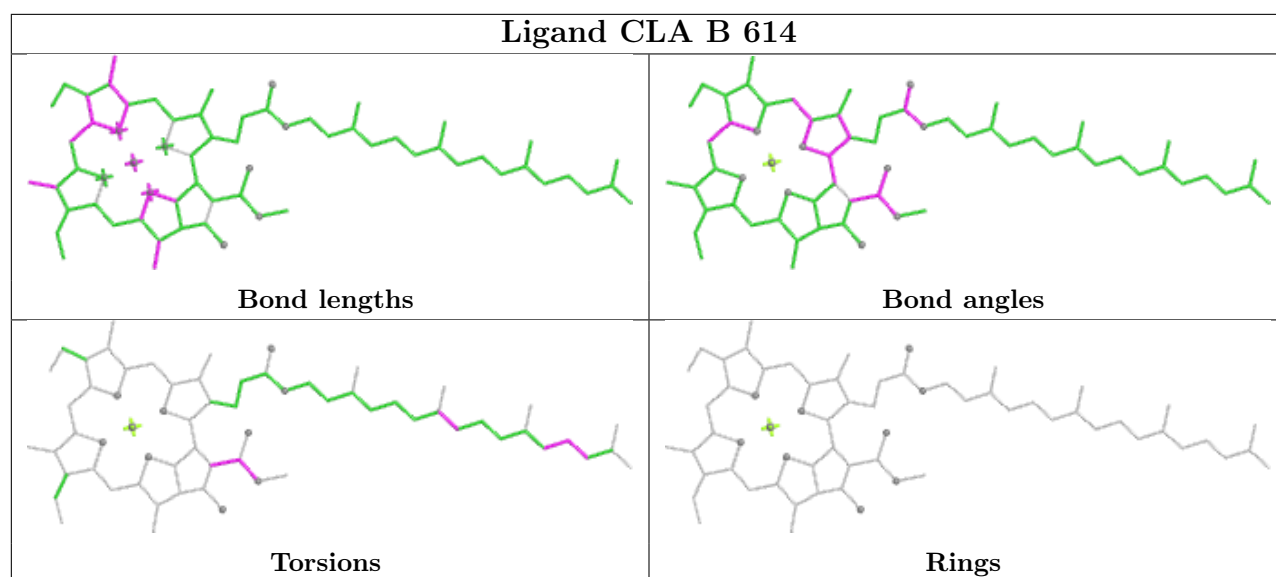


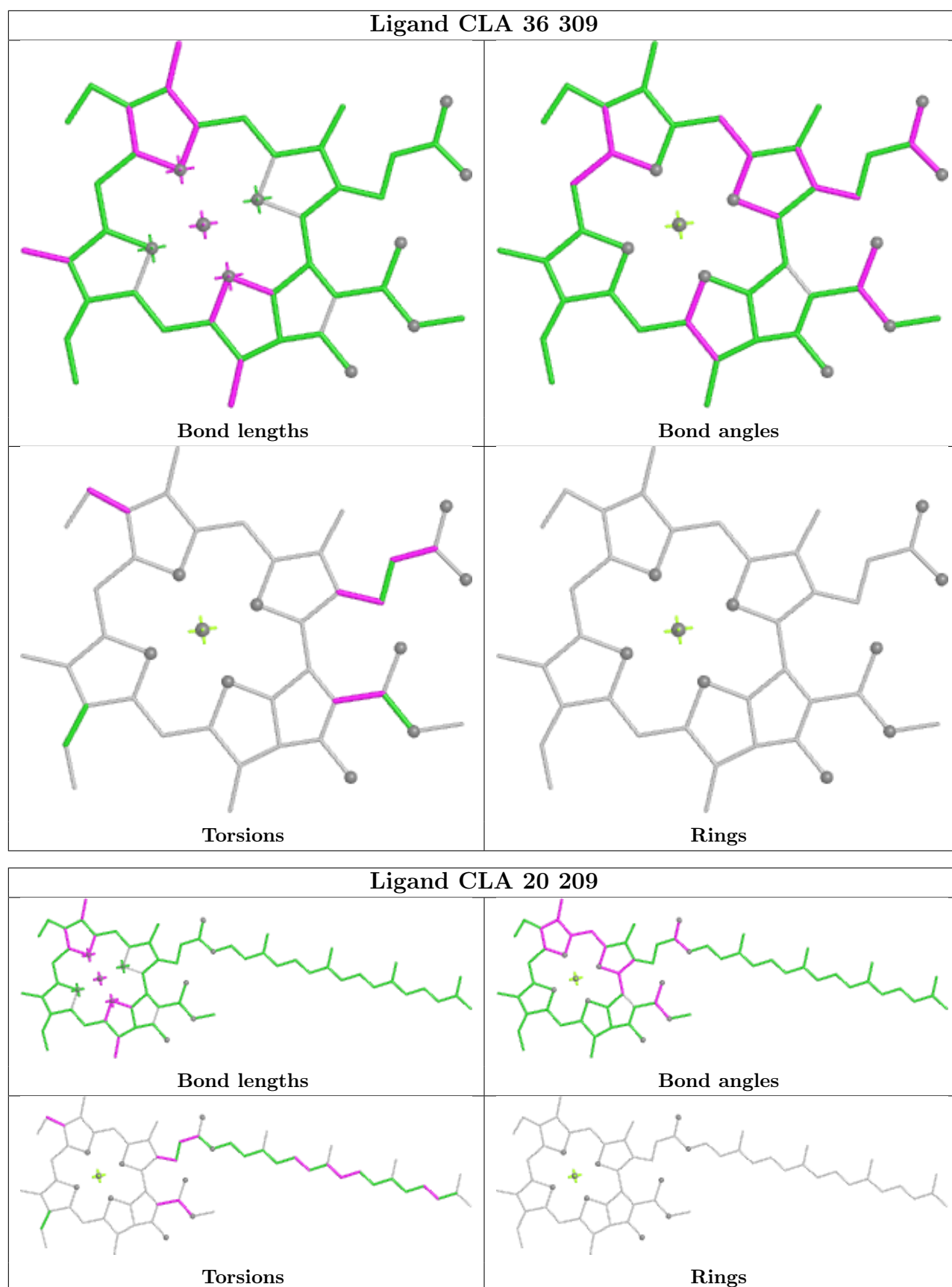


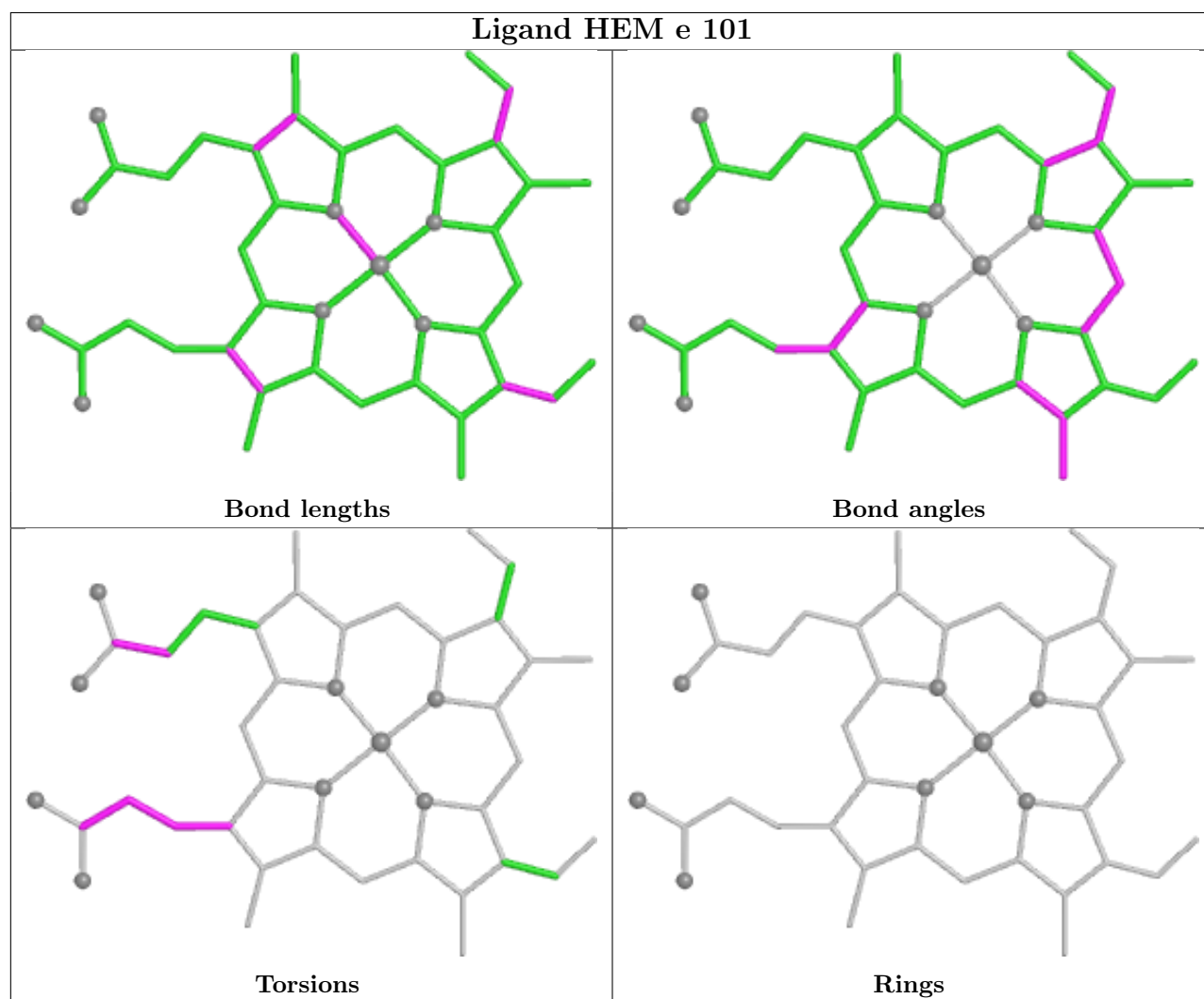
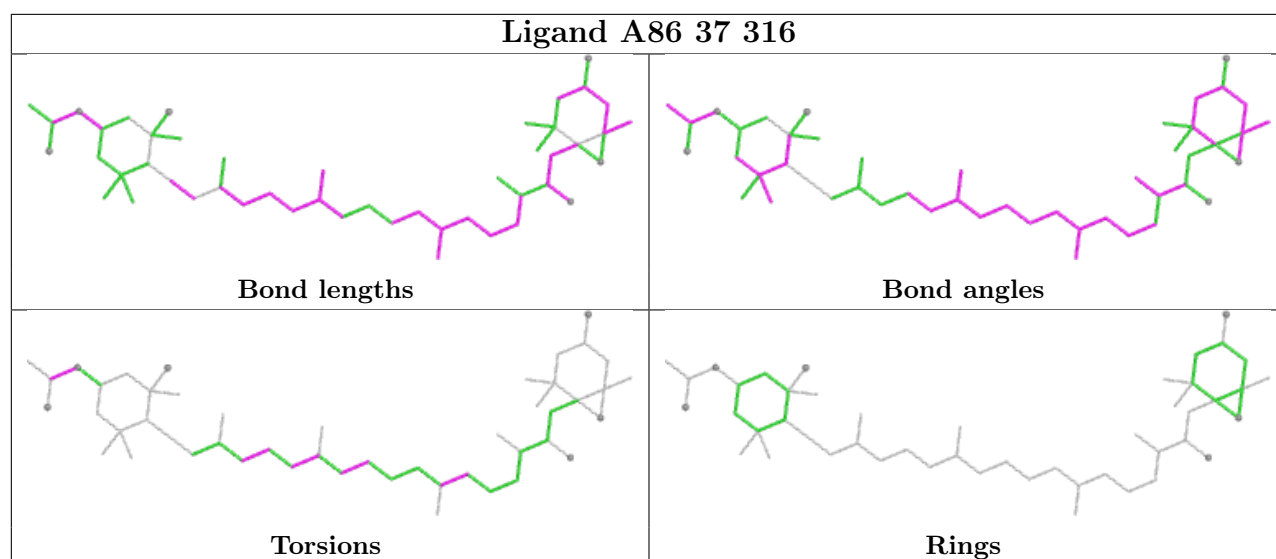


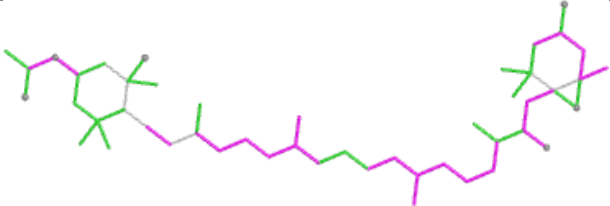
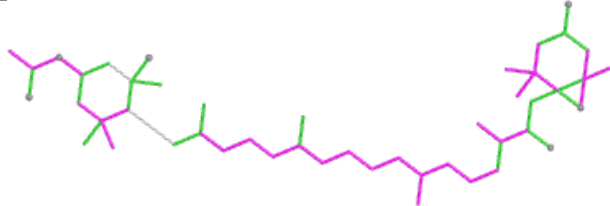
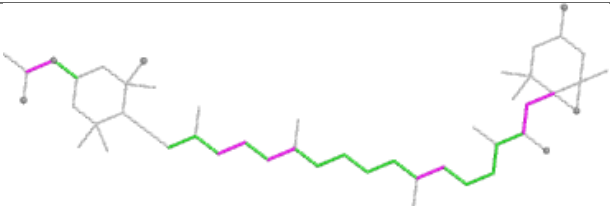
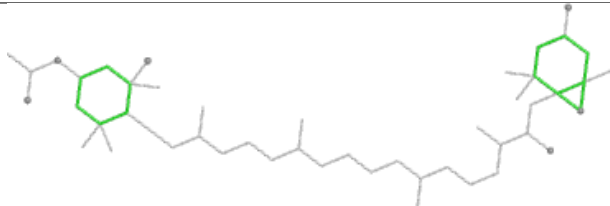
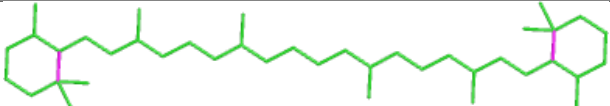
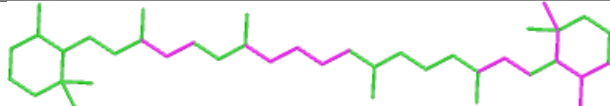
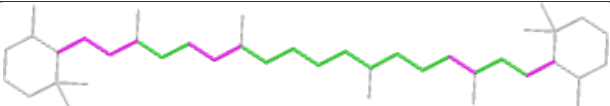
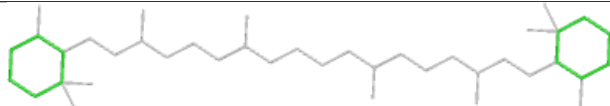
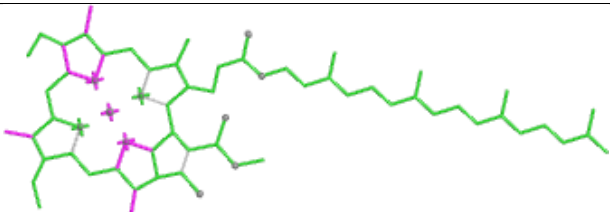
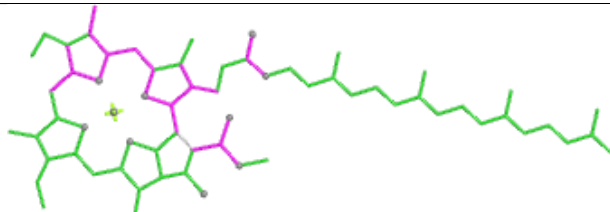
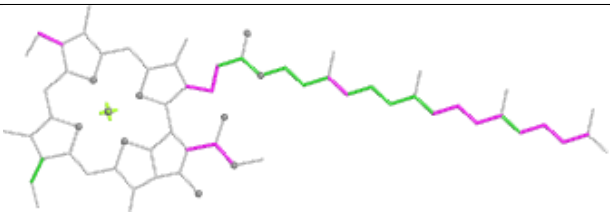
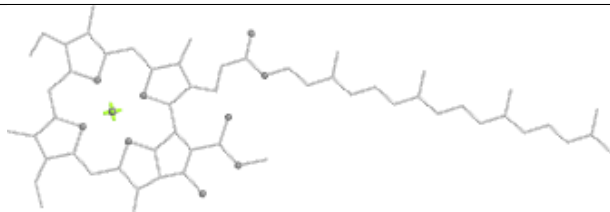


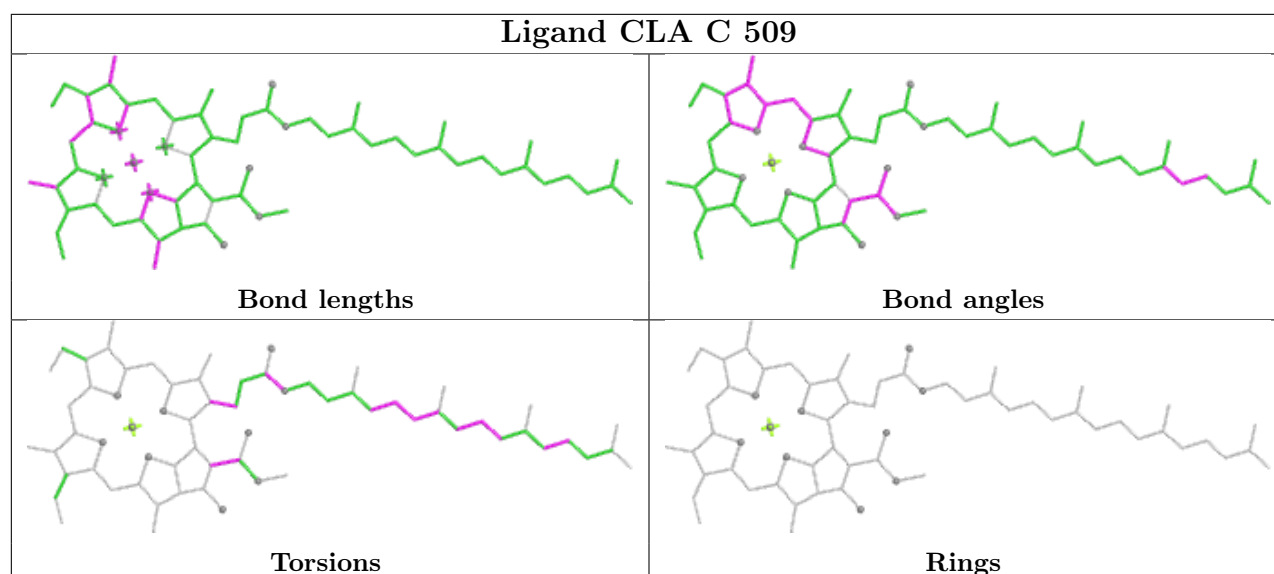
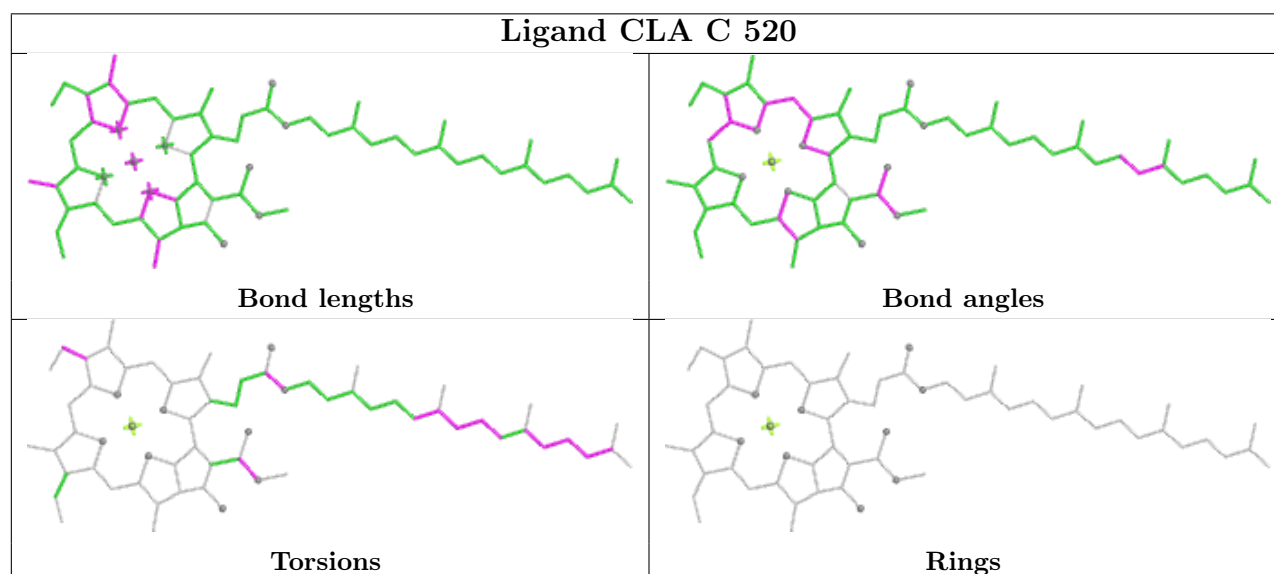
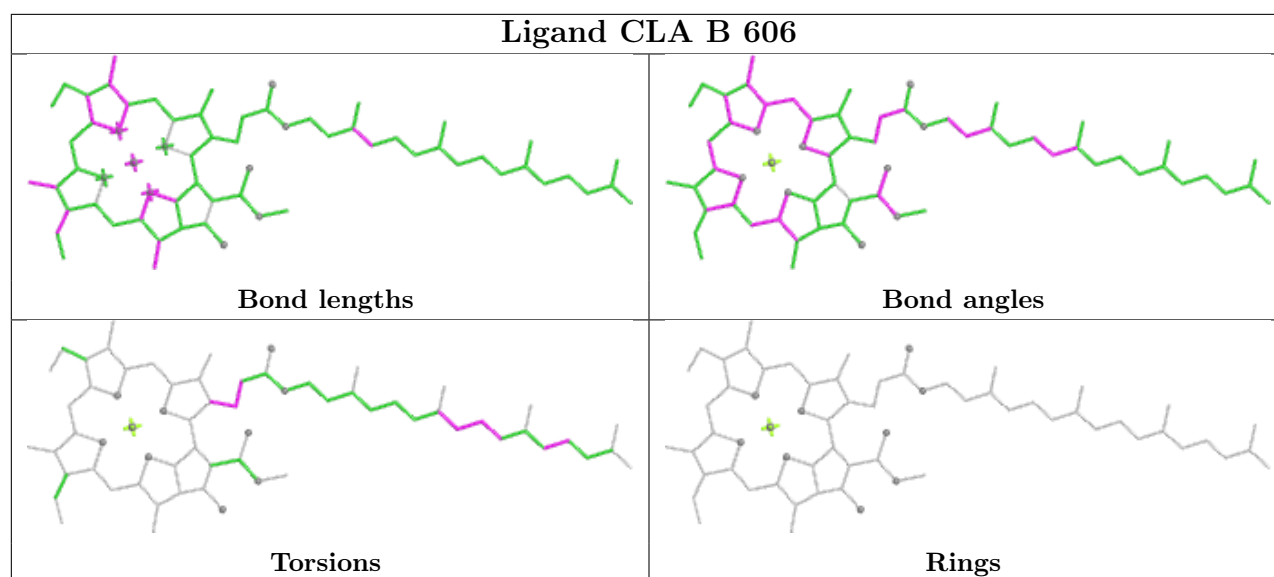


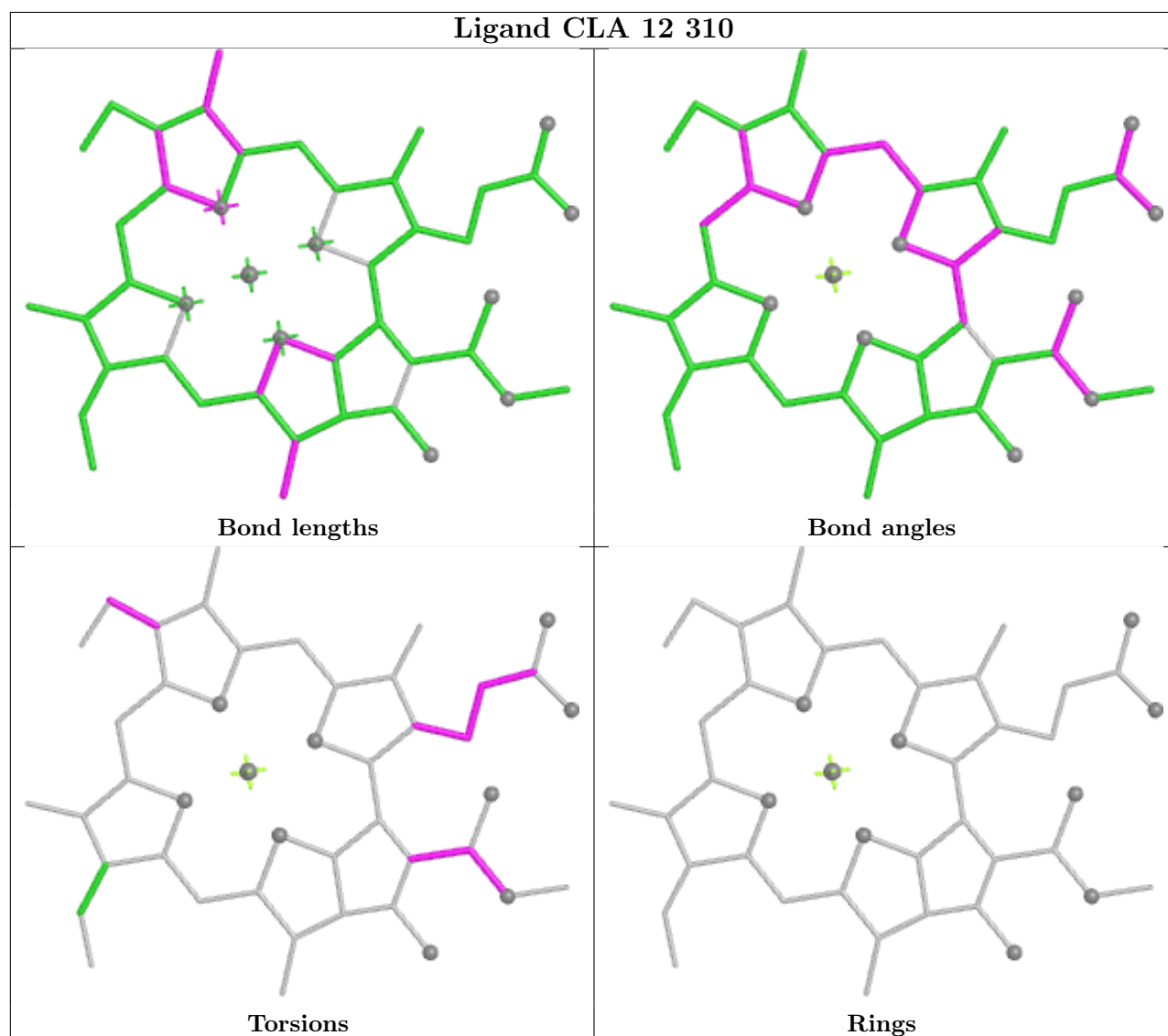
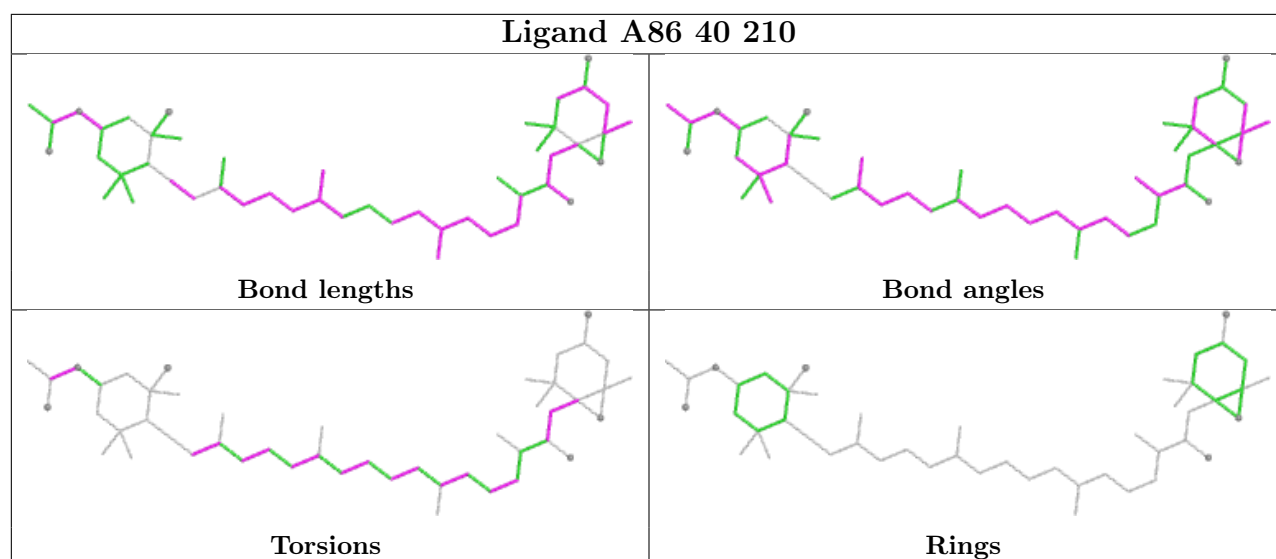


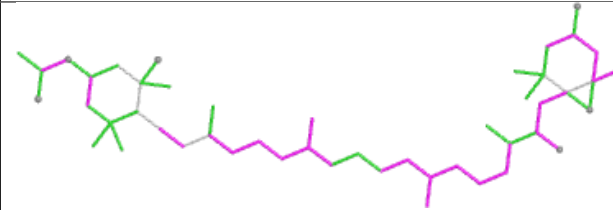
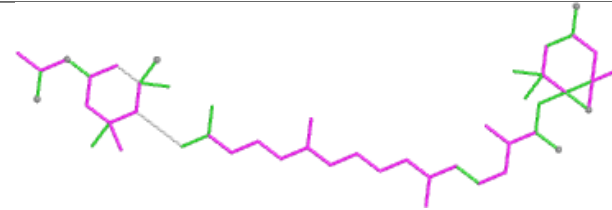
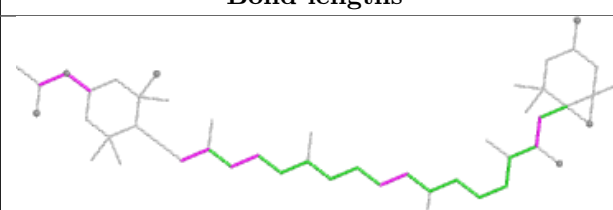
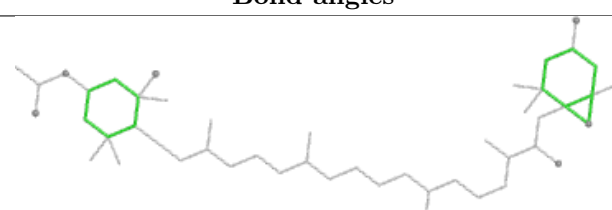


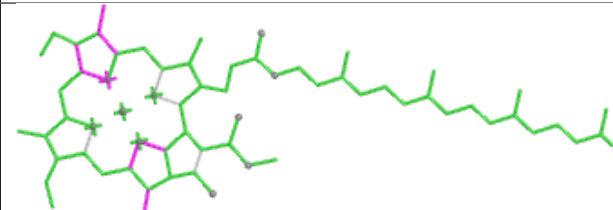
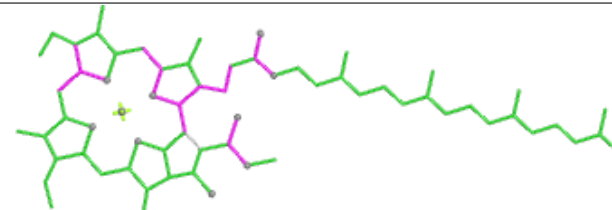
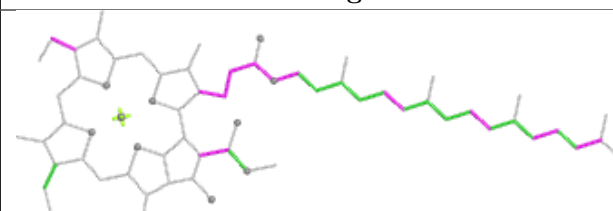
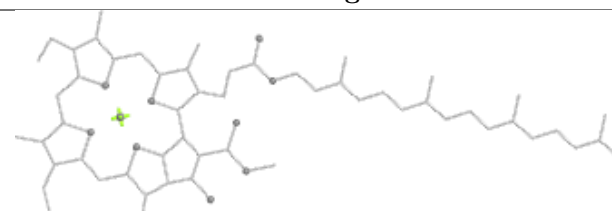


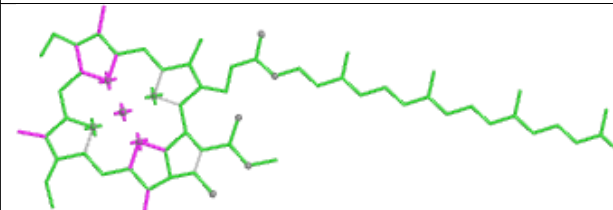
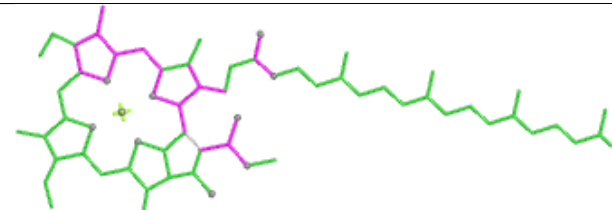
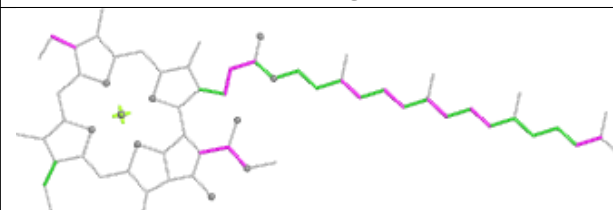
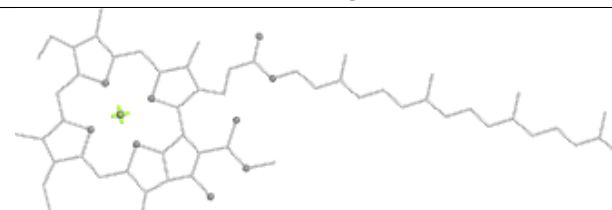
Ligand A86 34 311	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA c 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

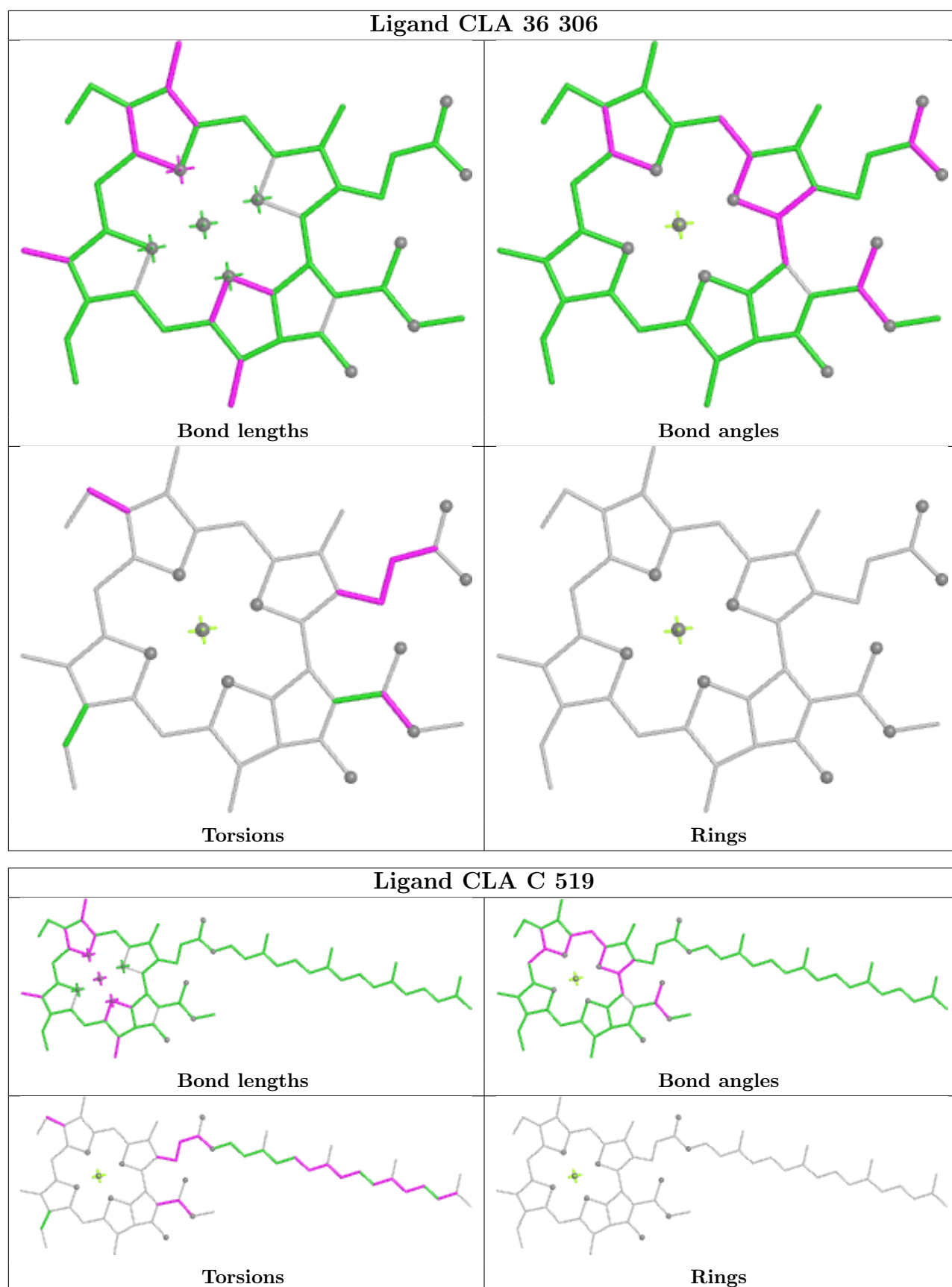


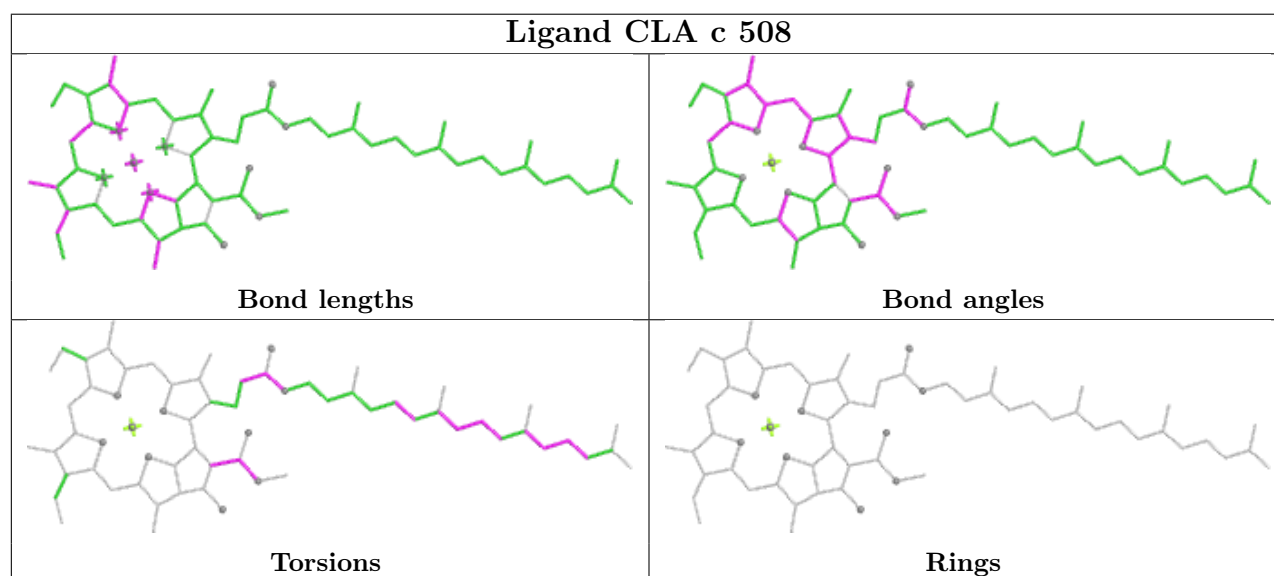
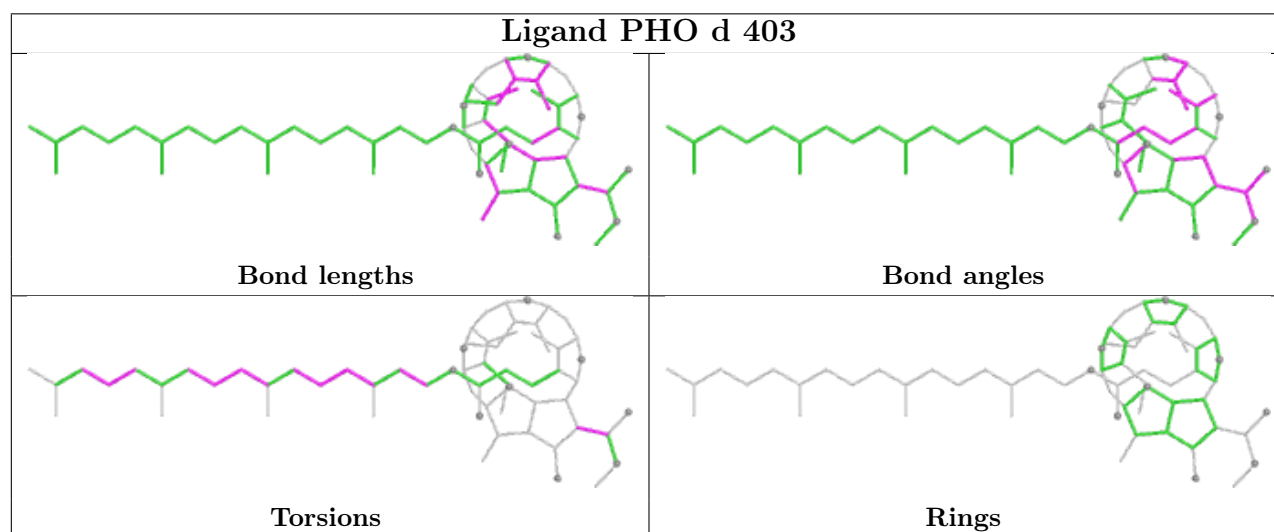
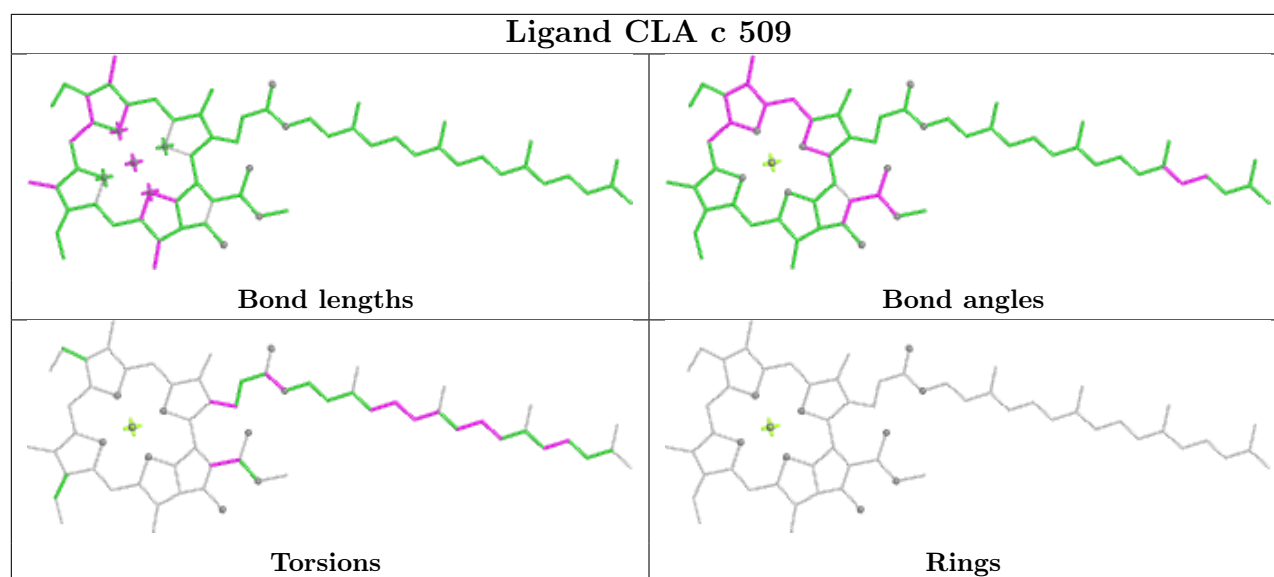


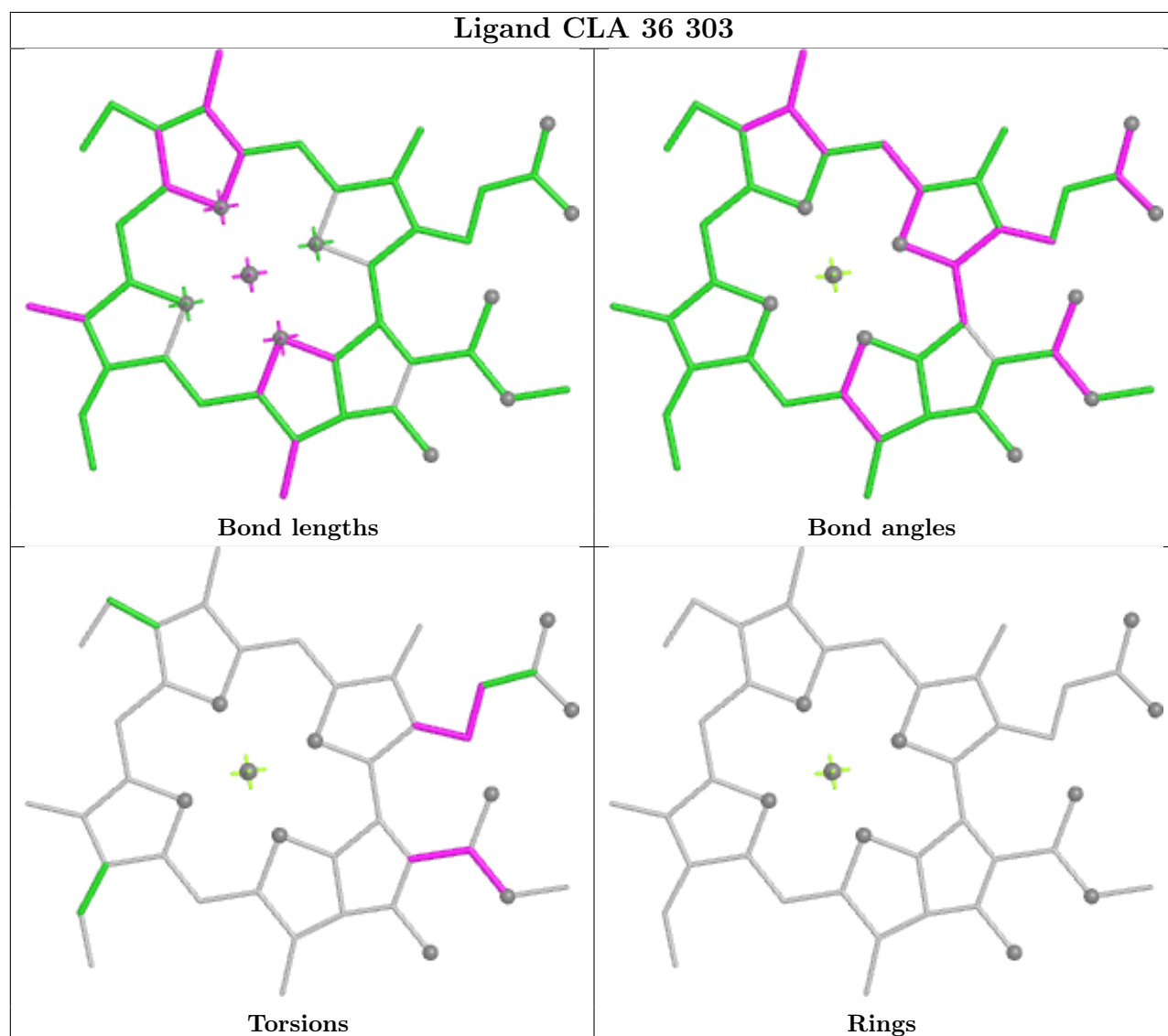
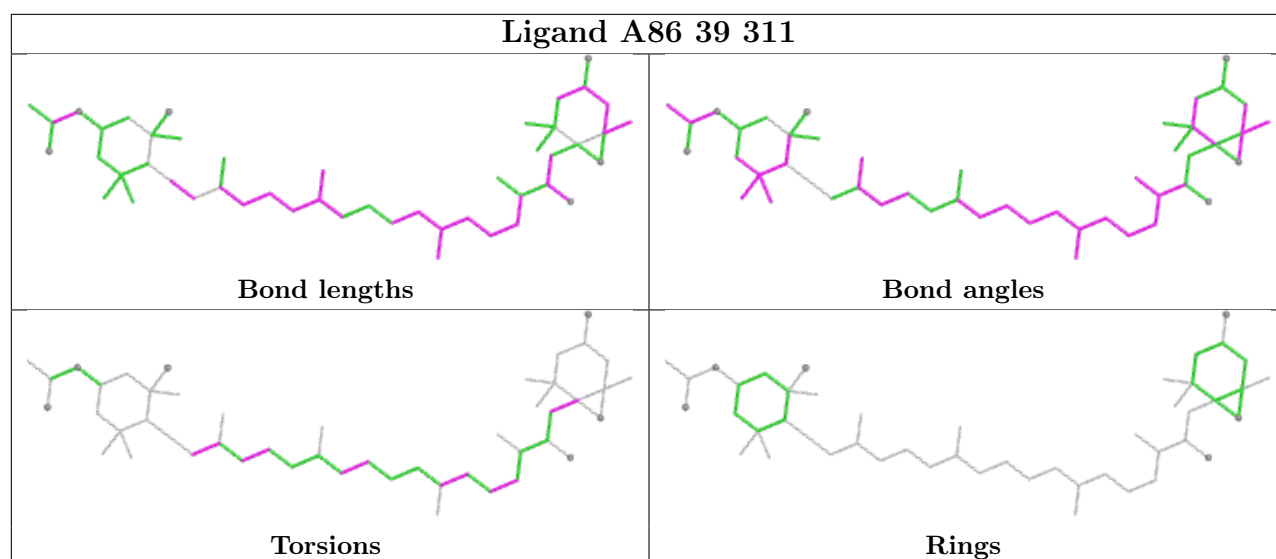
Ligand A86 31 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

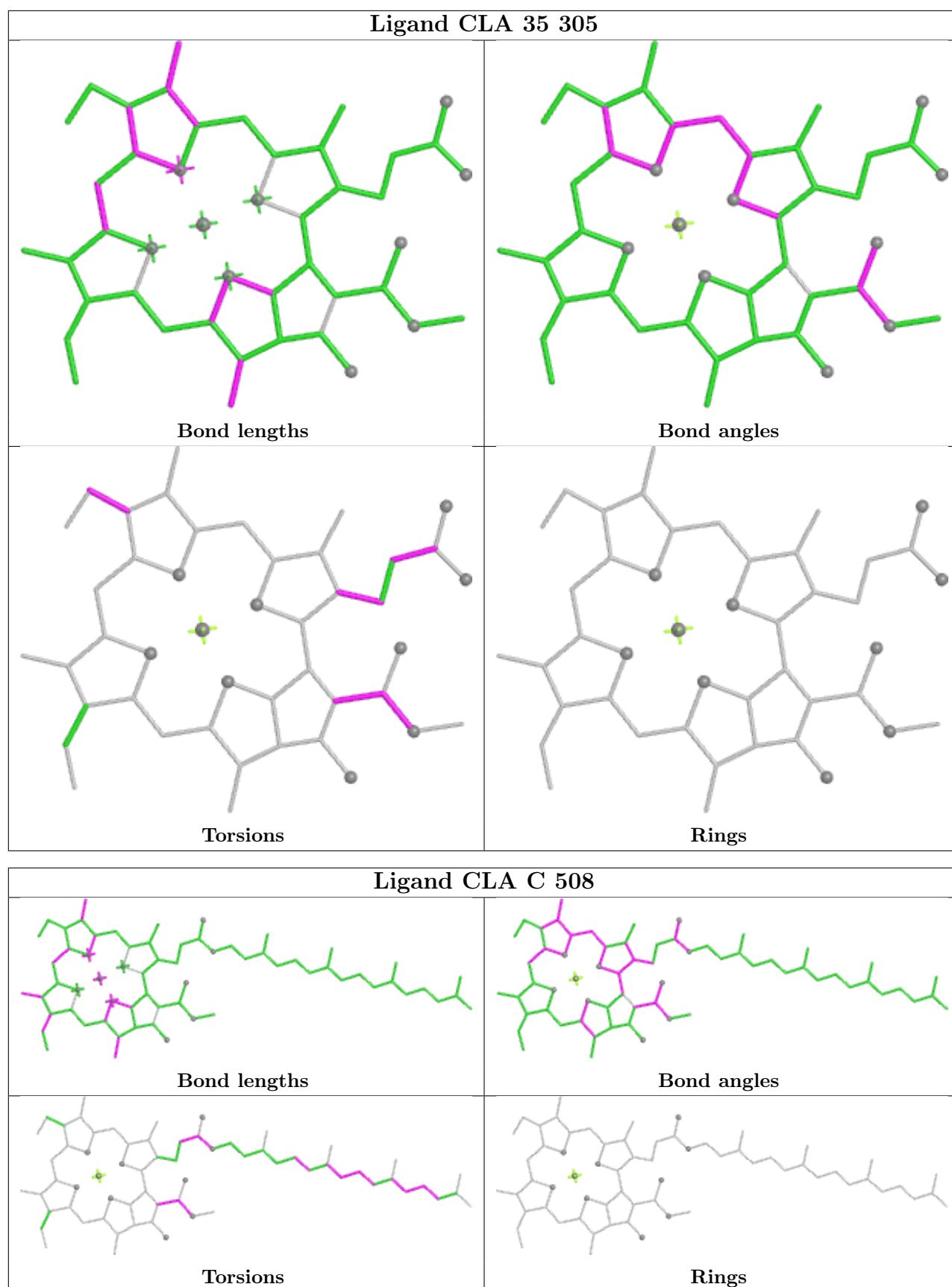
Ligand CLA 41 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

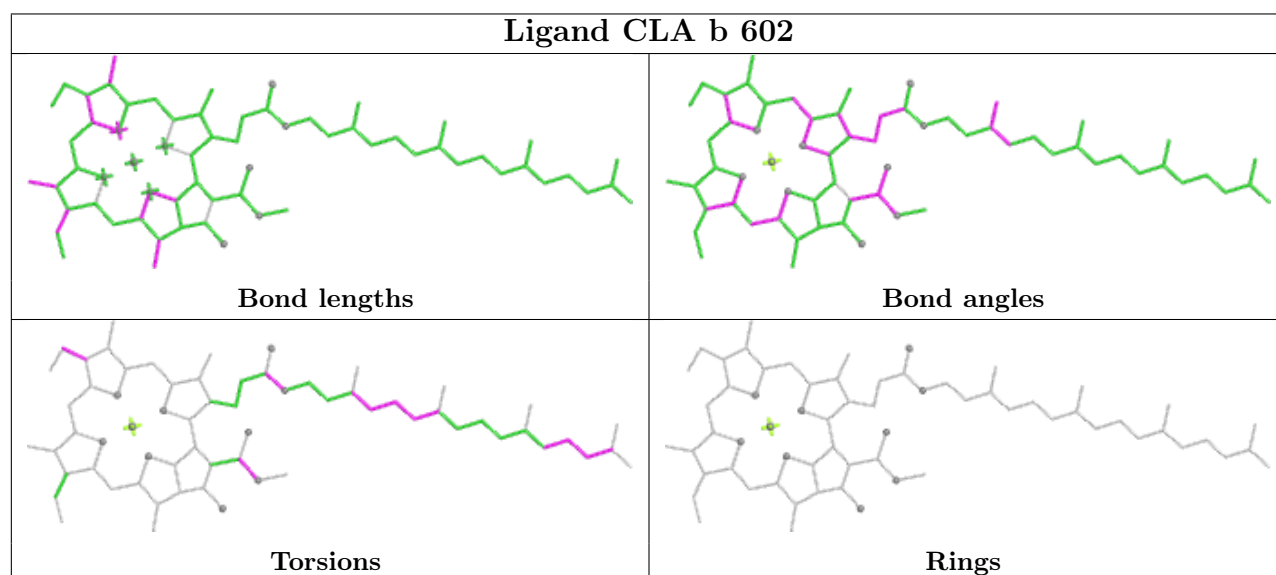
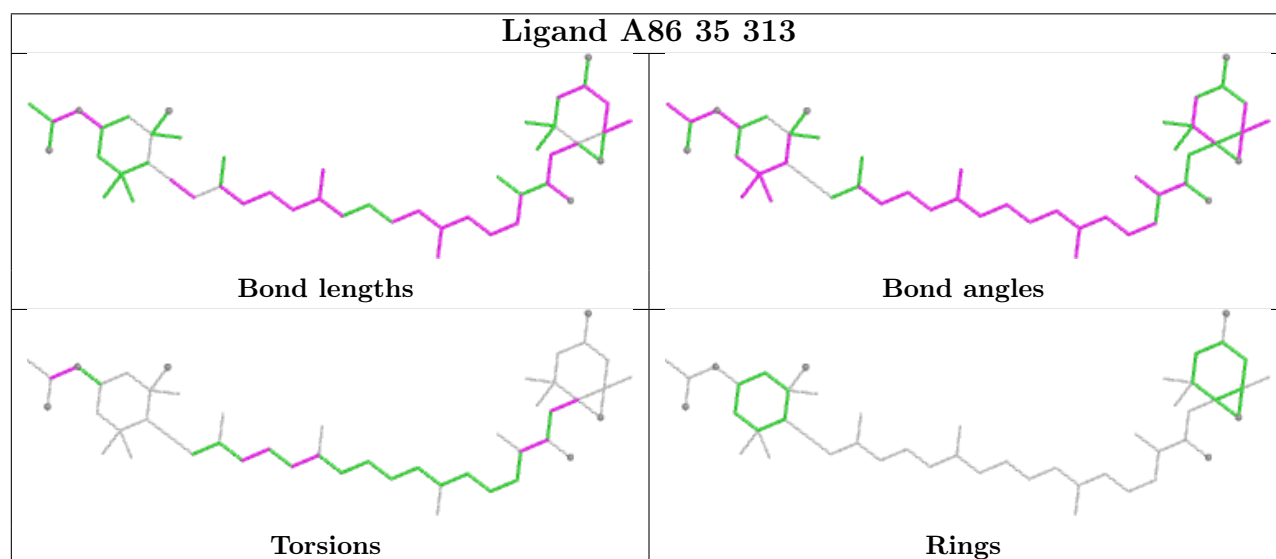
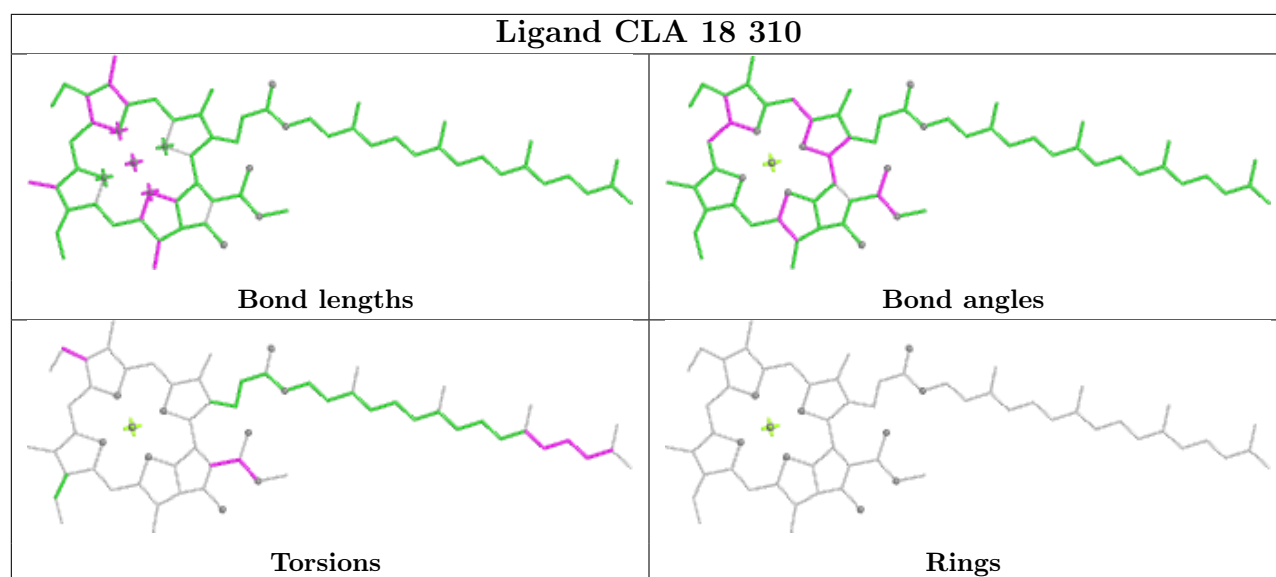
Ligand CLA C 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

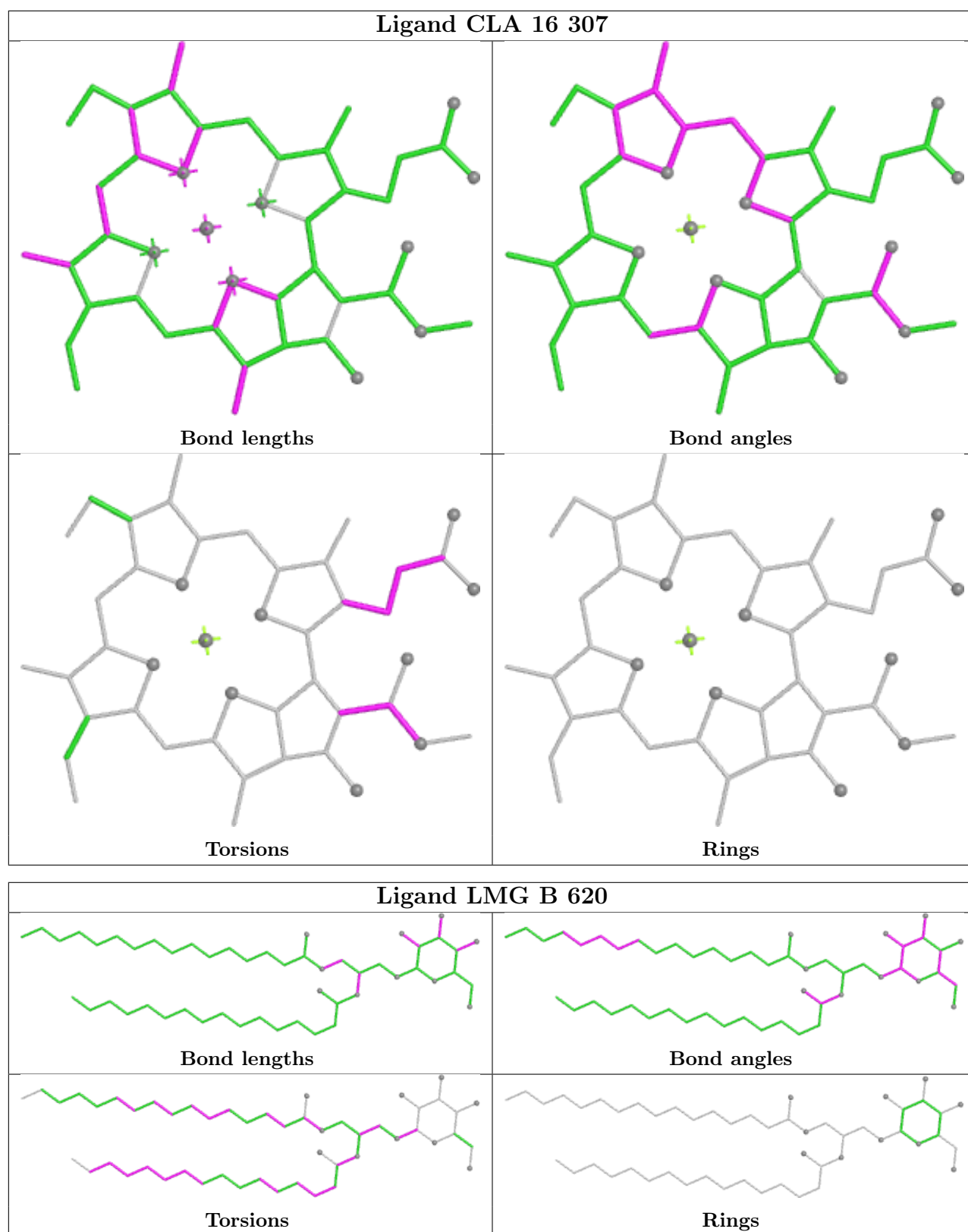


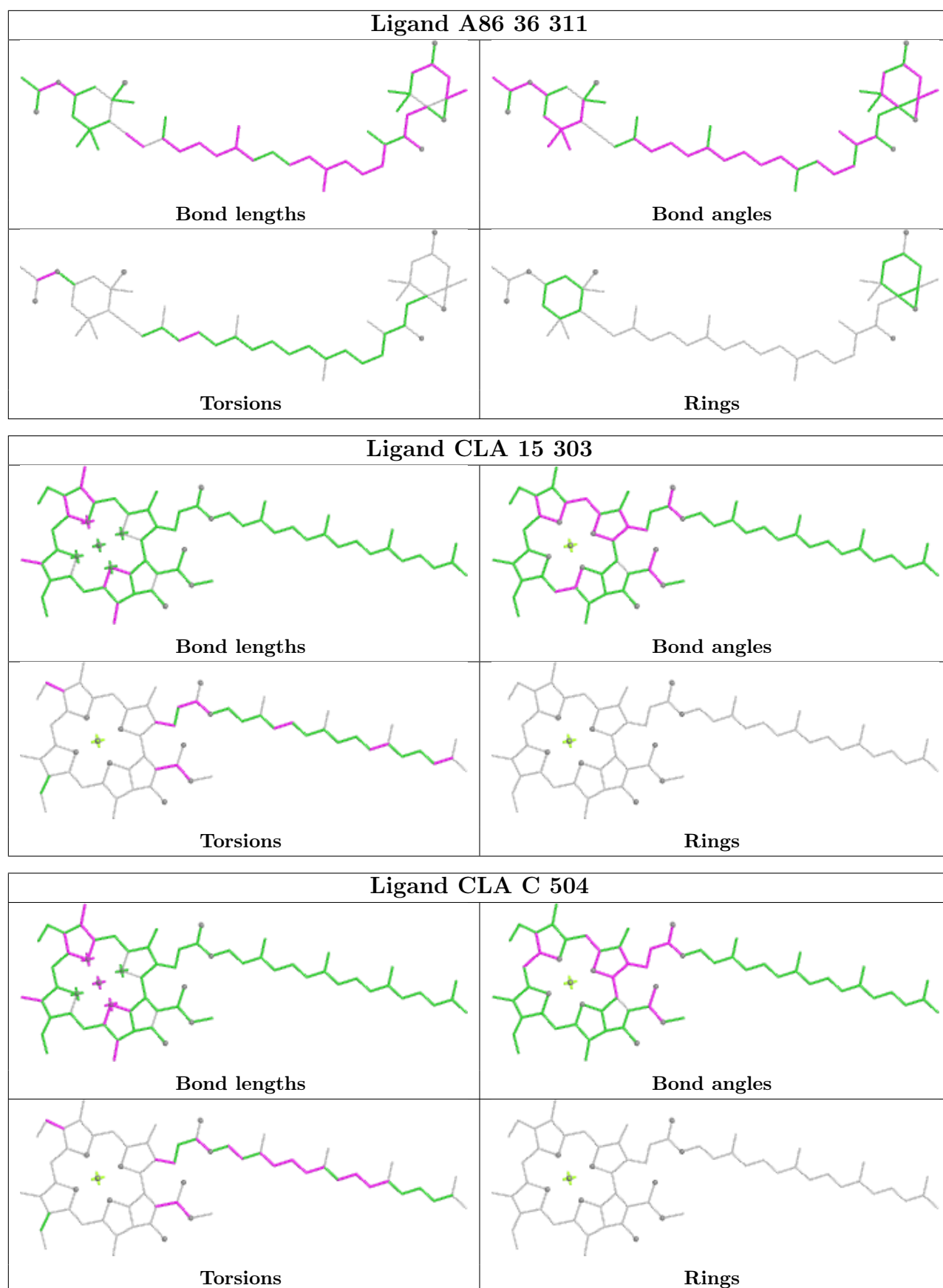


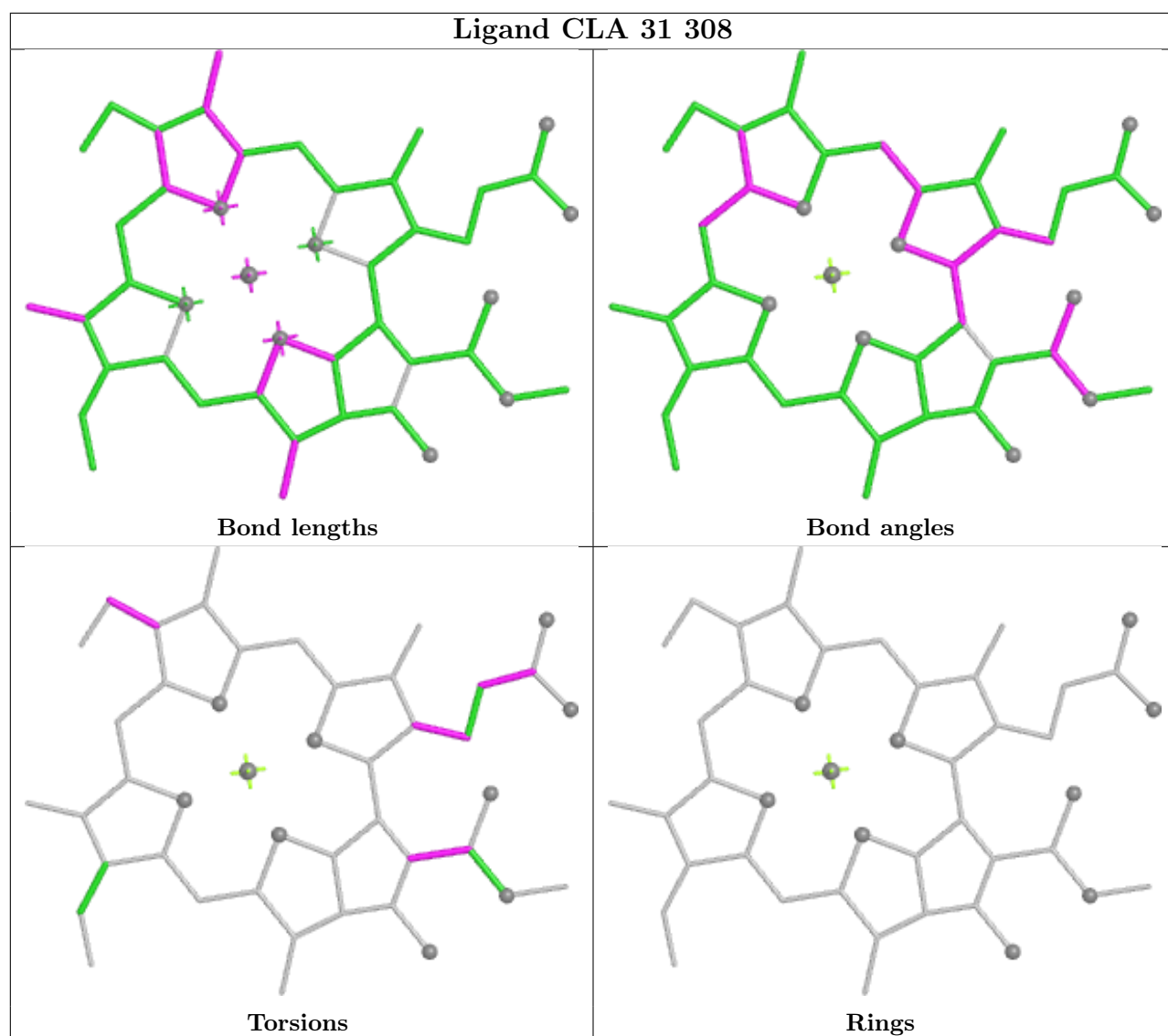


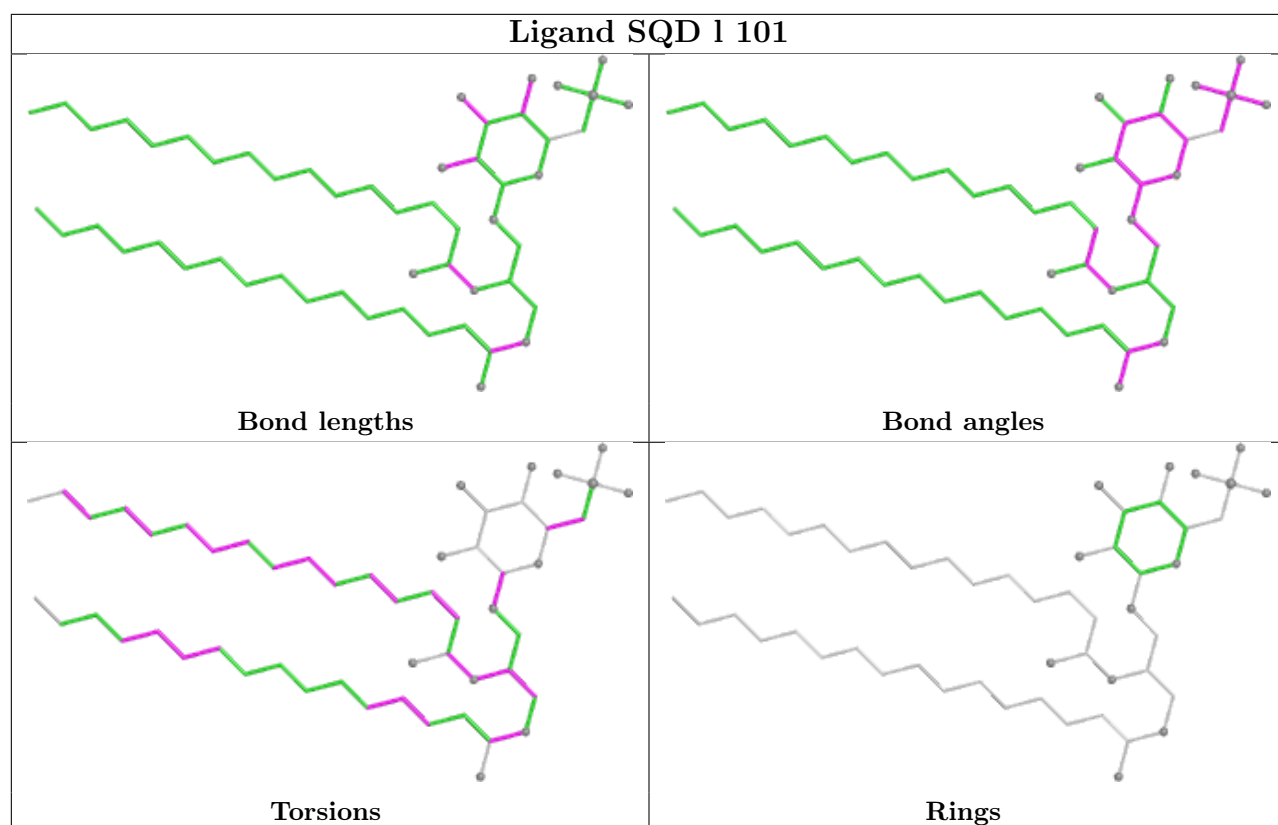


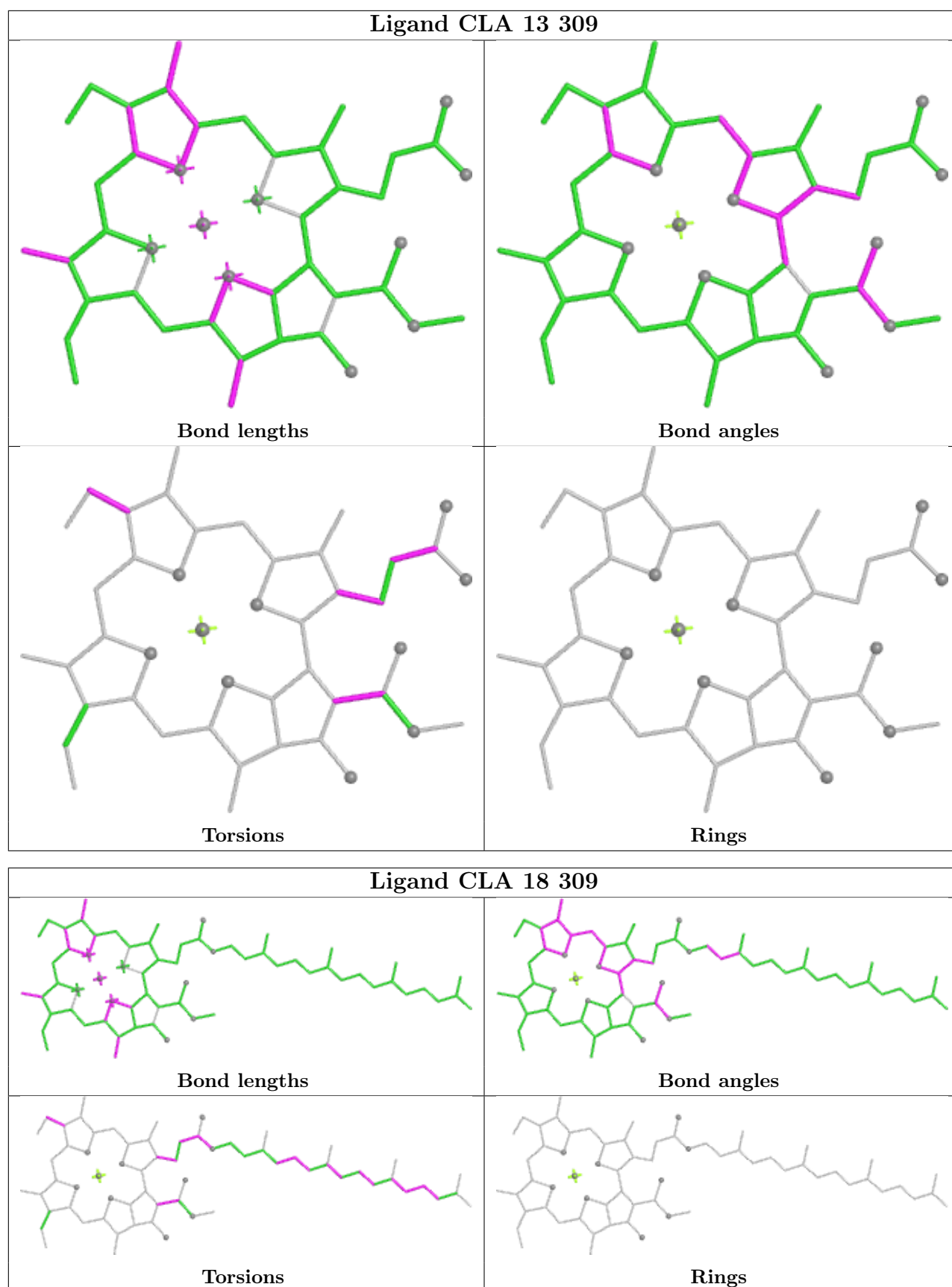


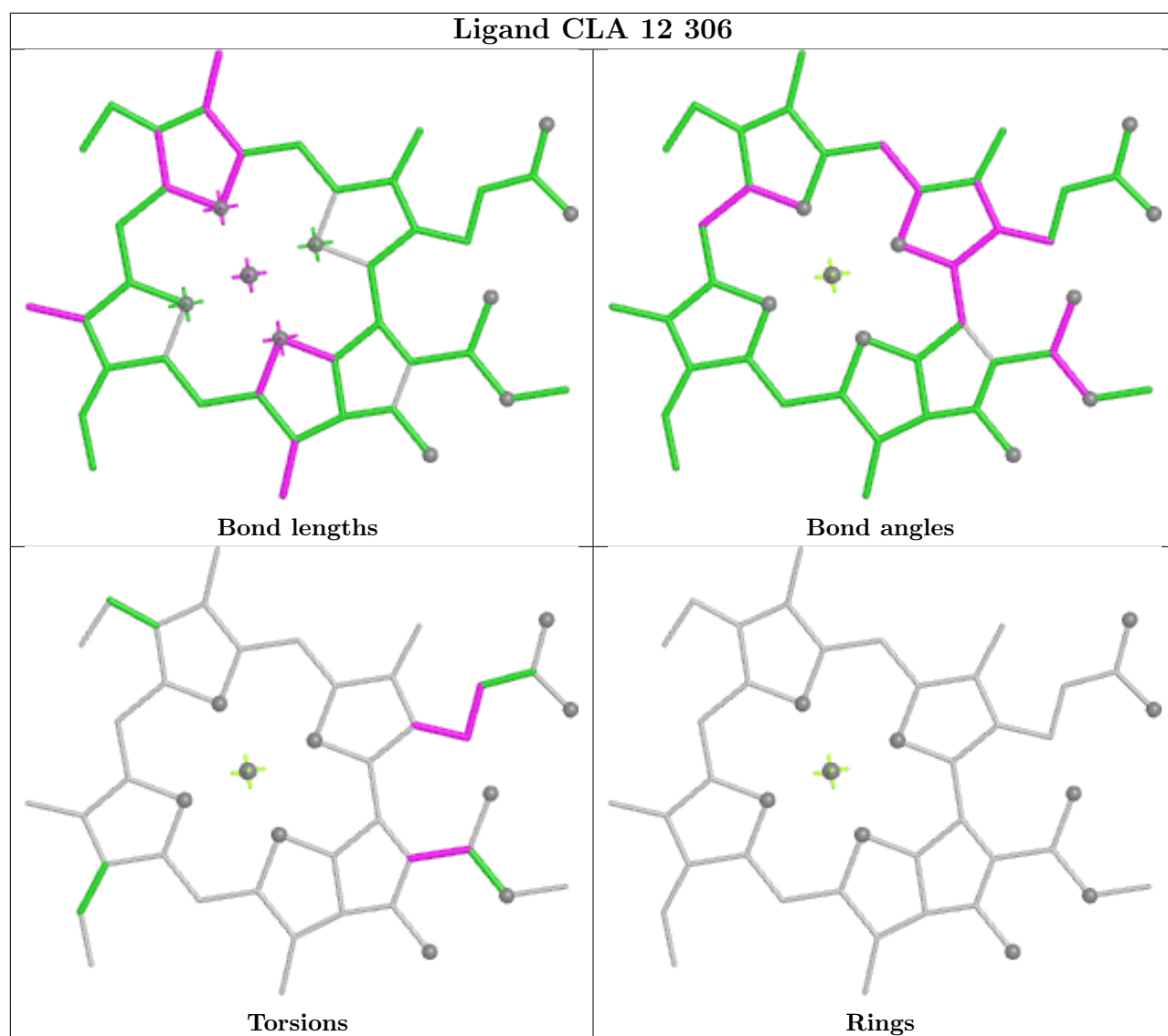


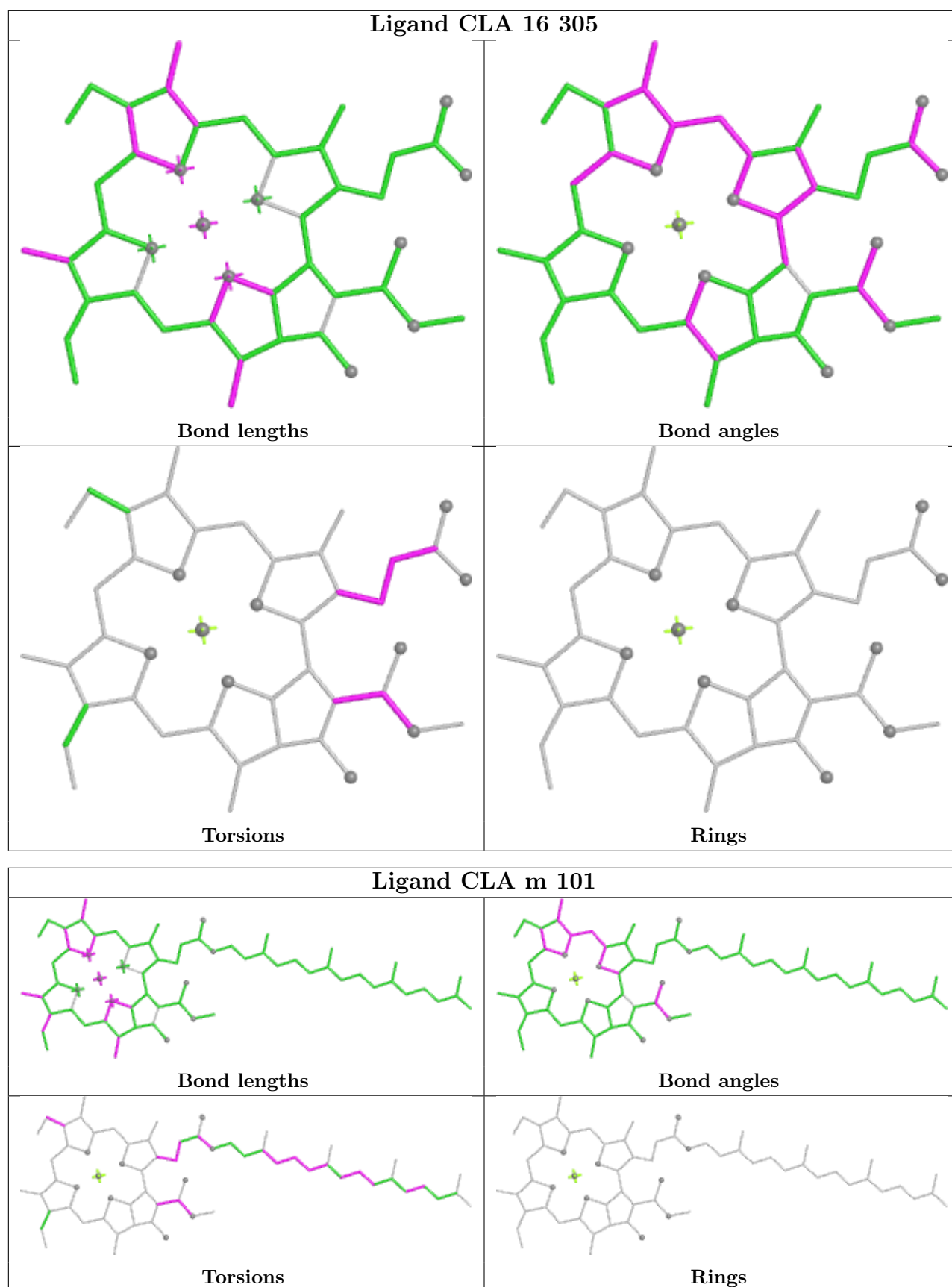


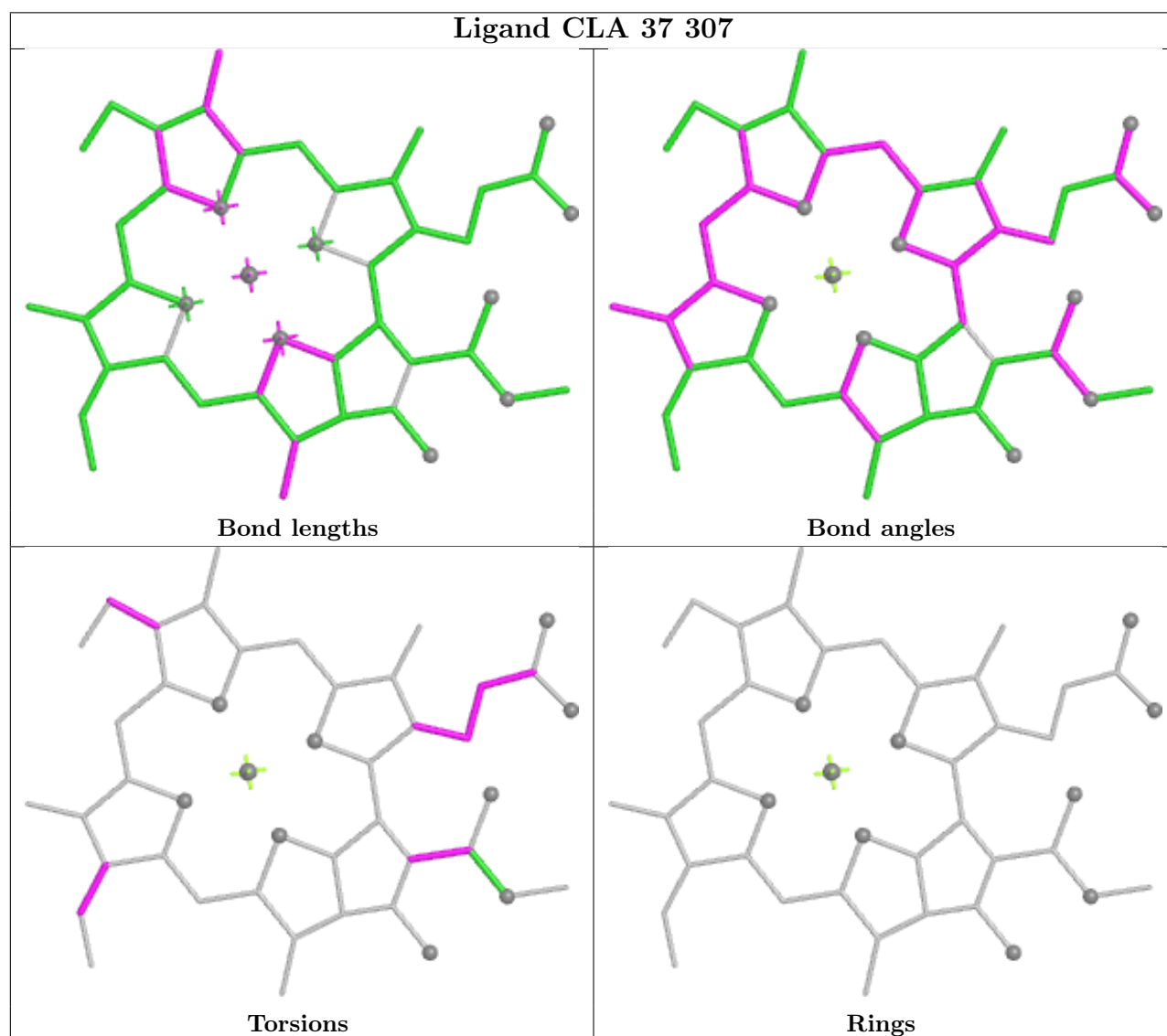
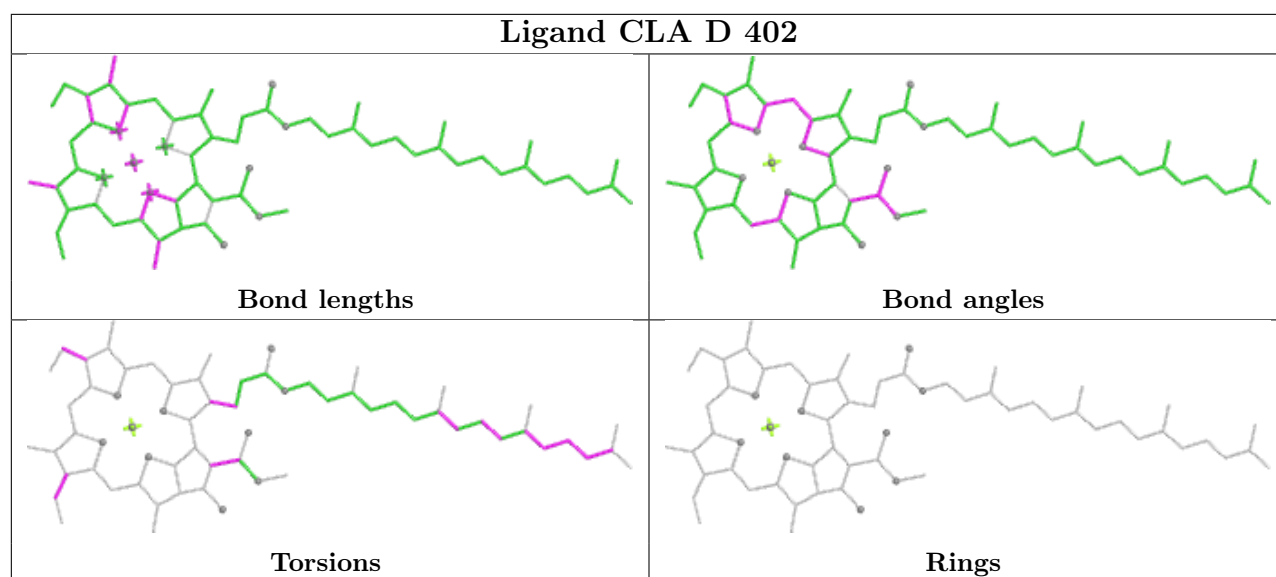


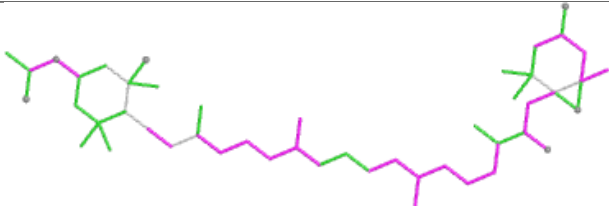
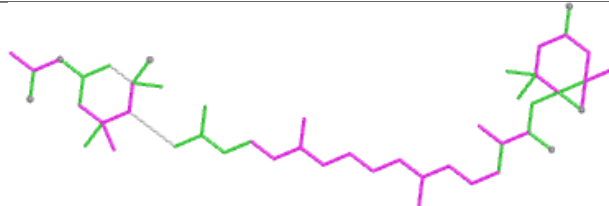
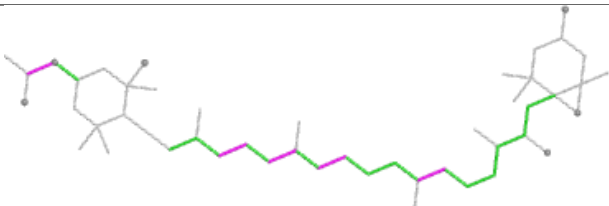
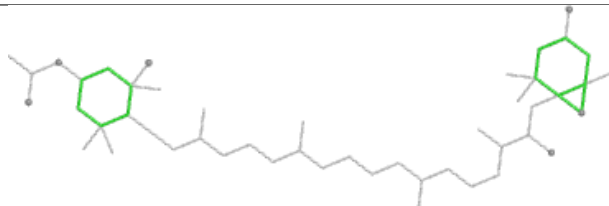


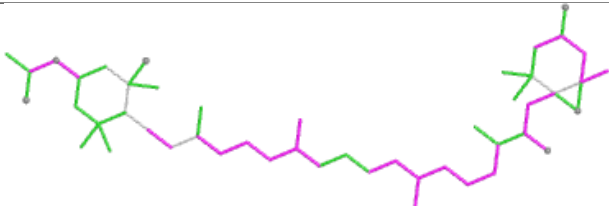
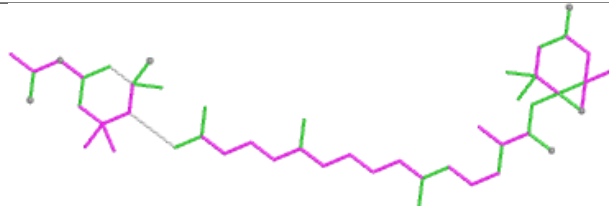
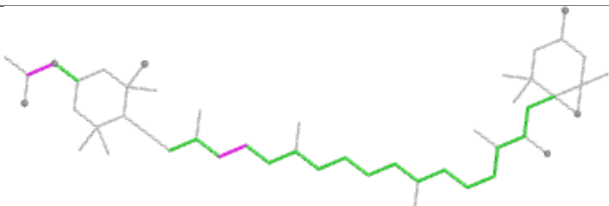
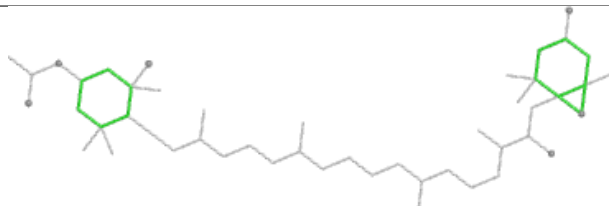


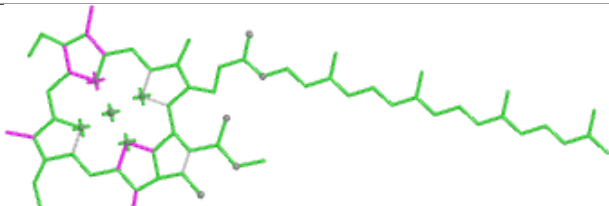
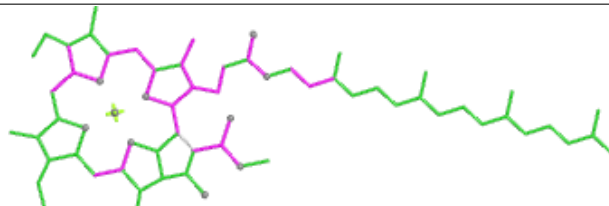
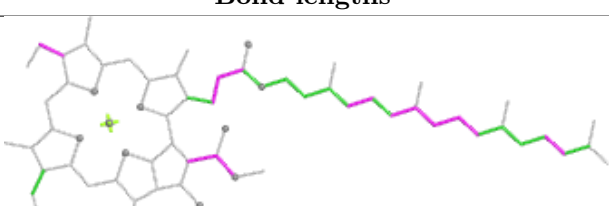
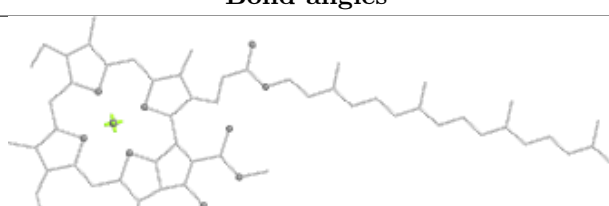


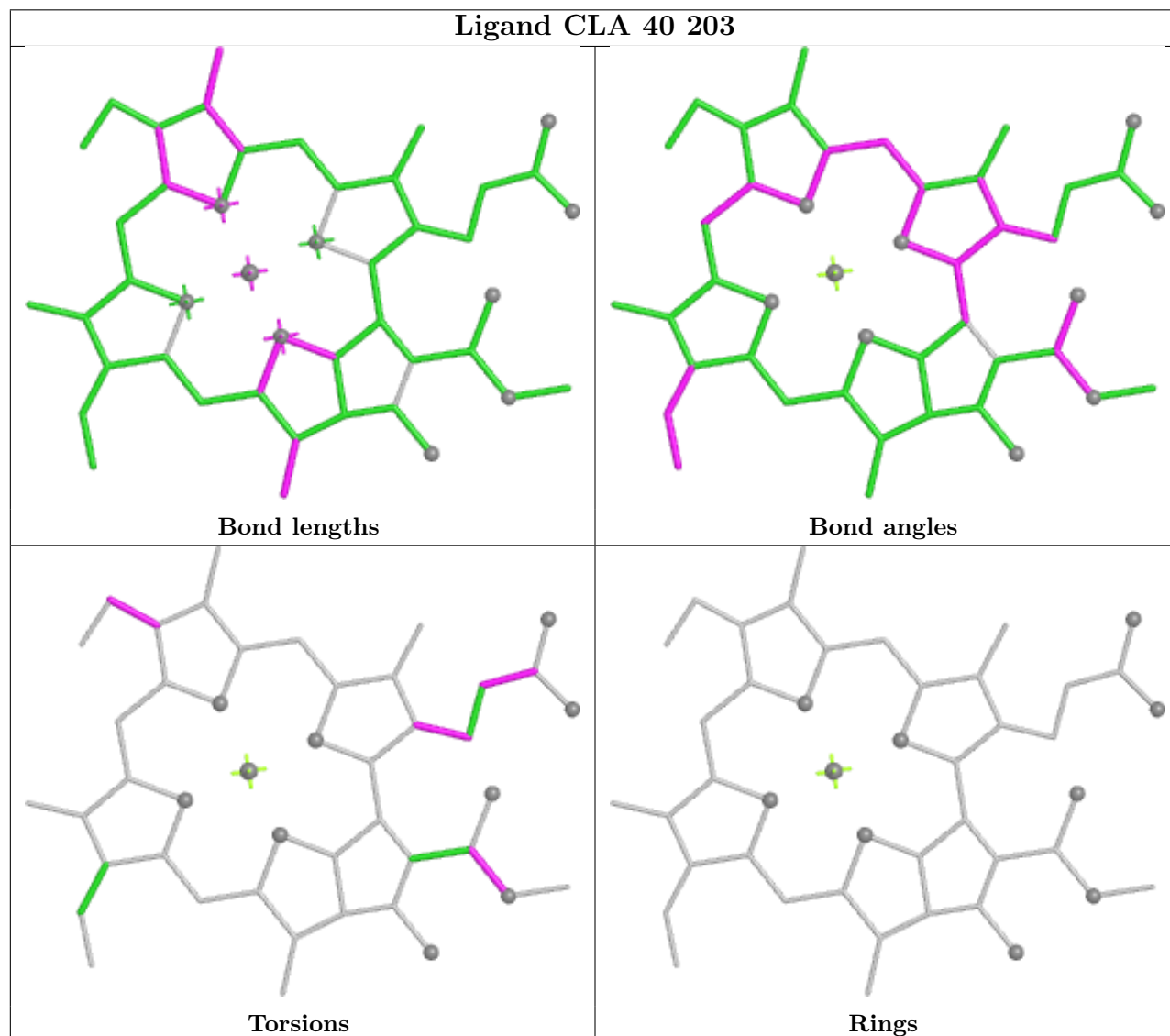
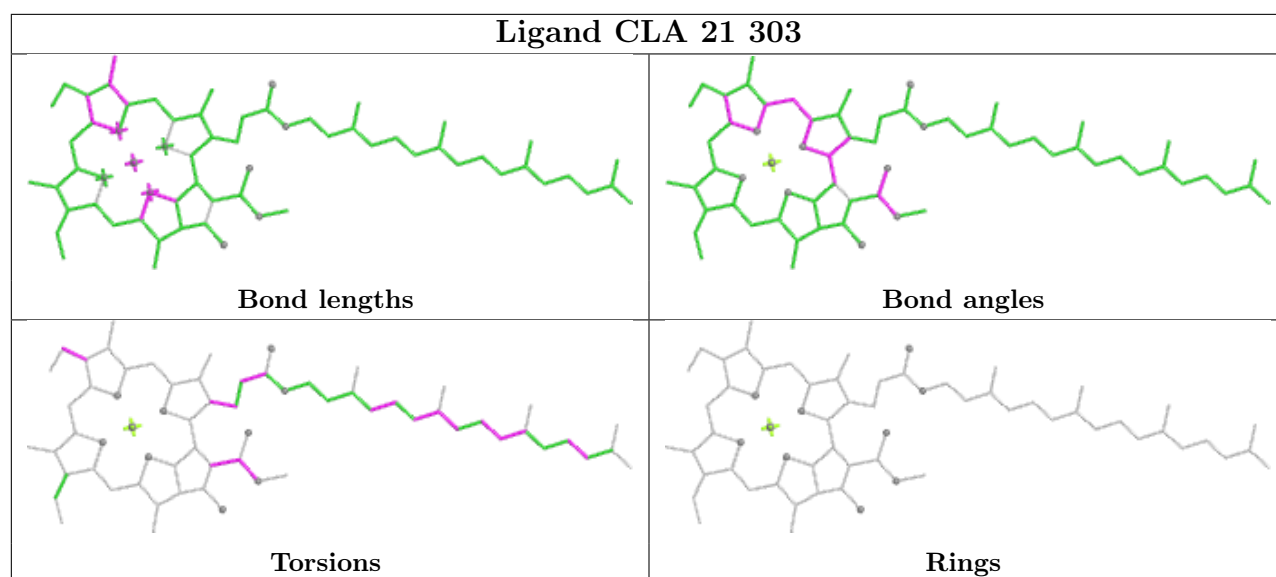


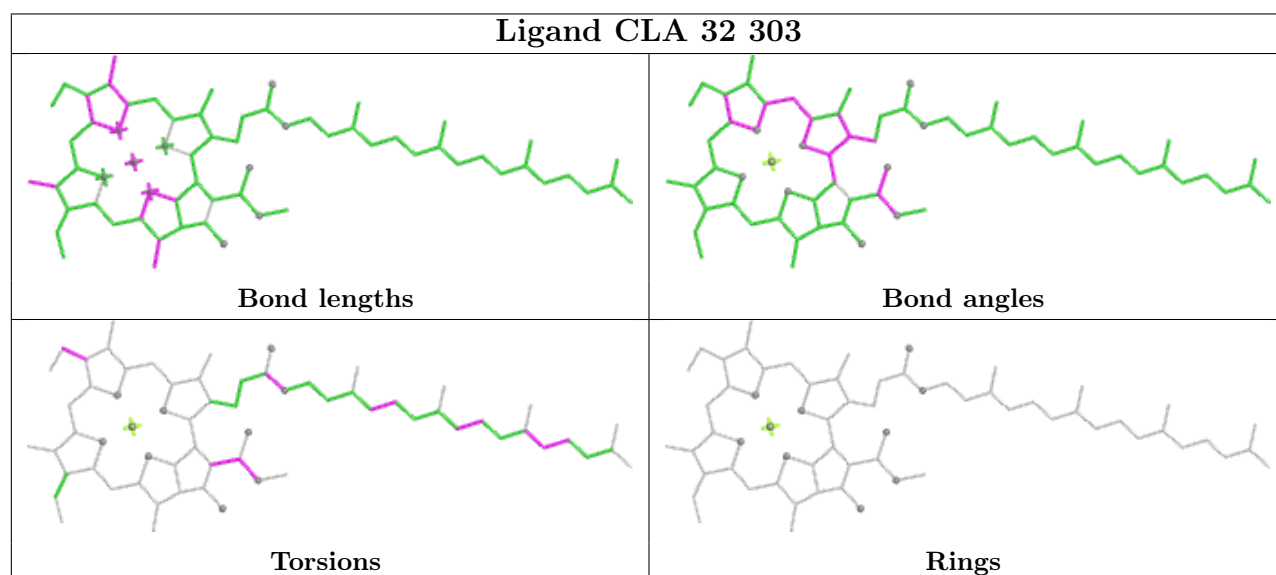
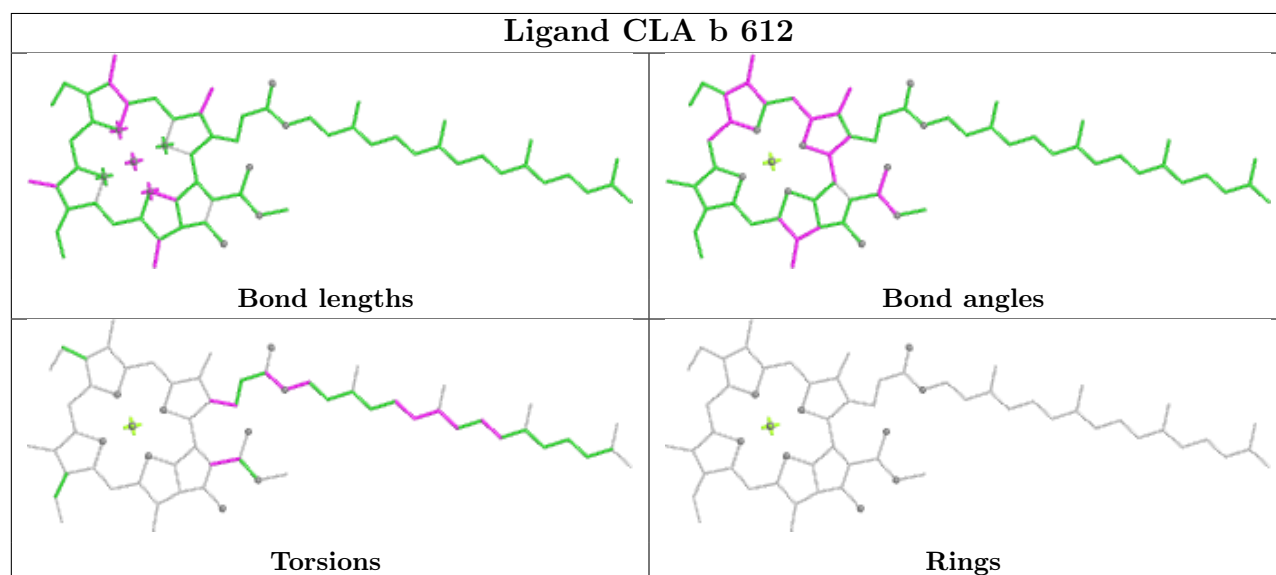
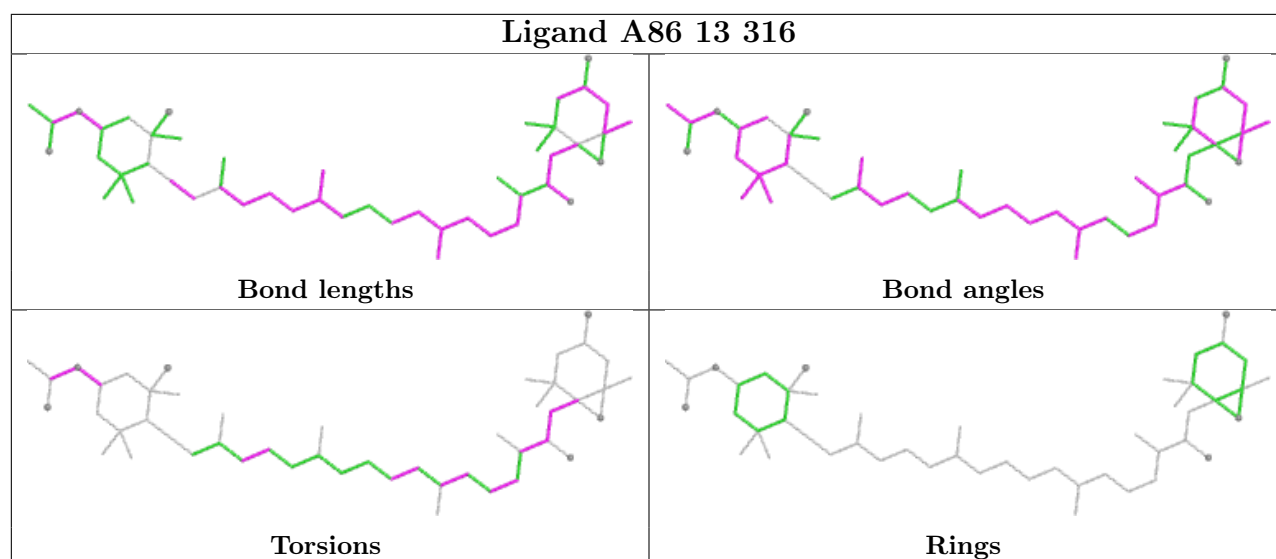


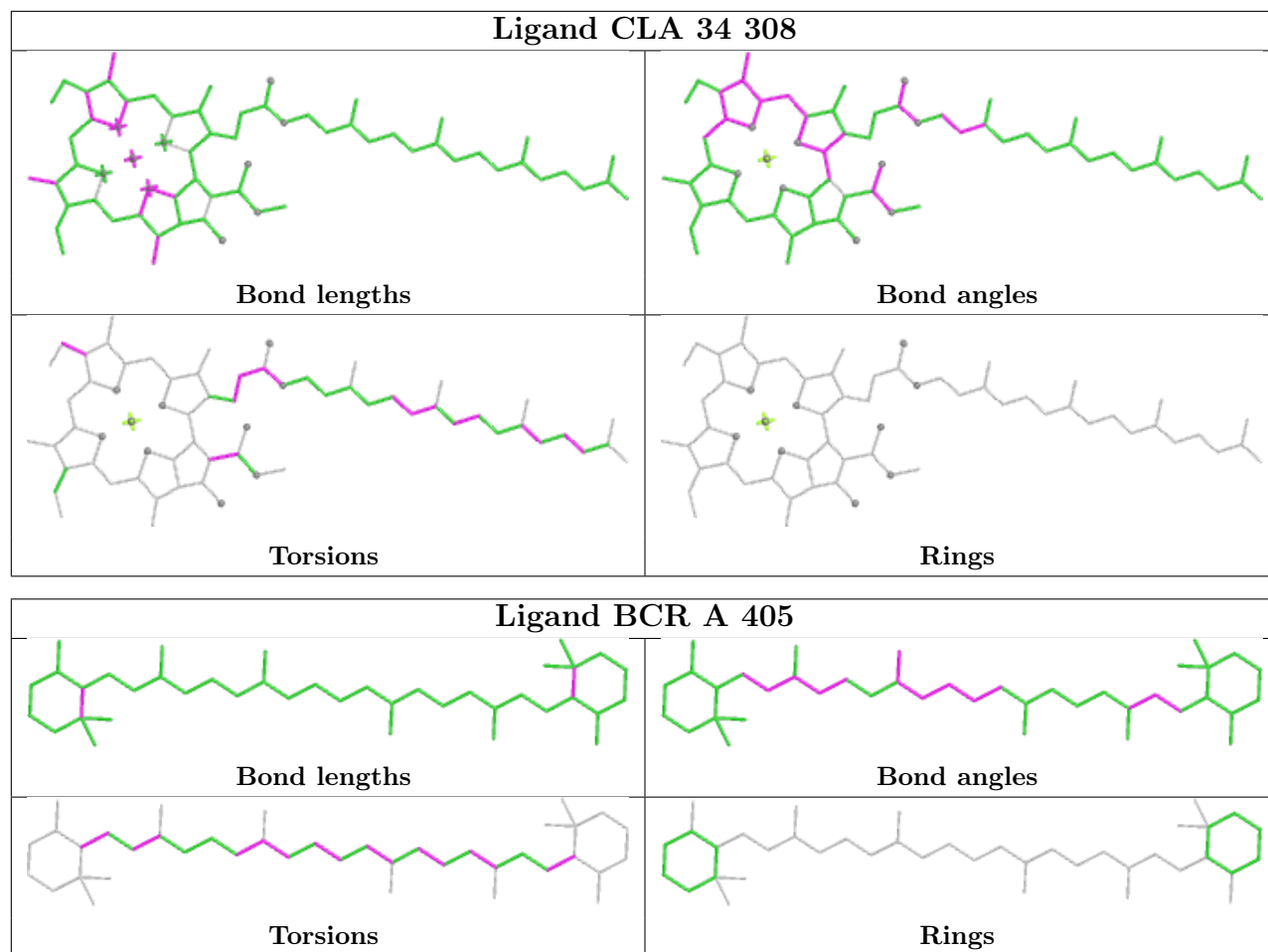
Ligand A86 32 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

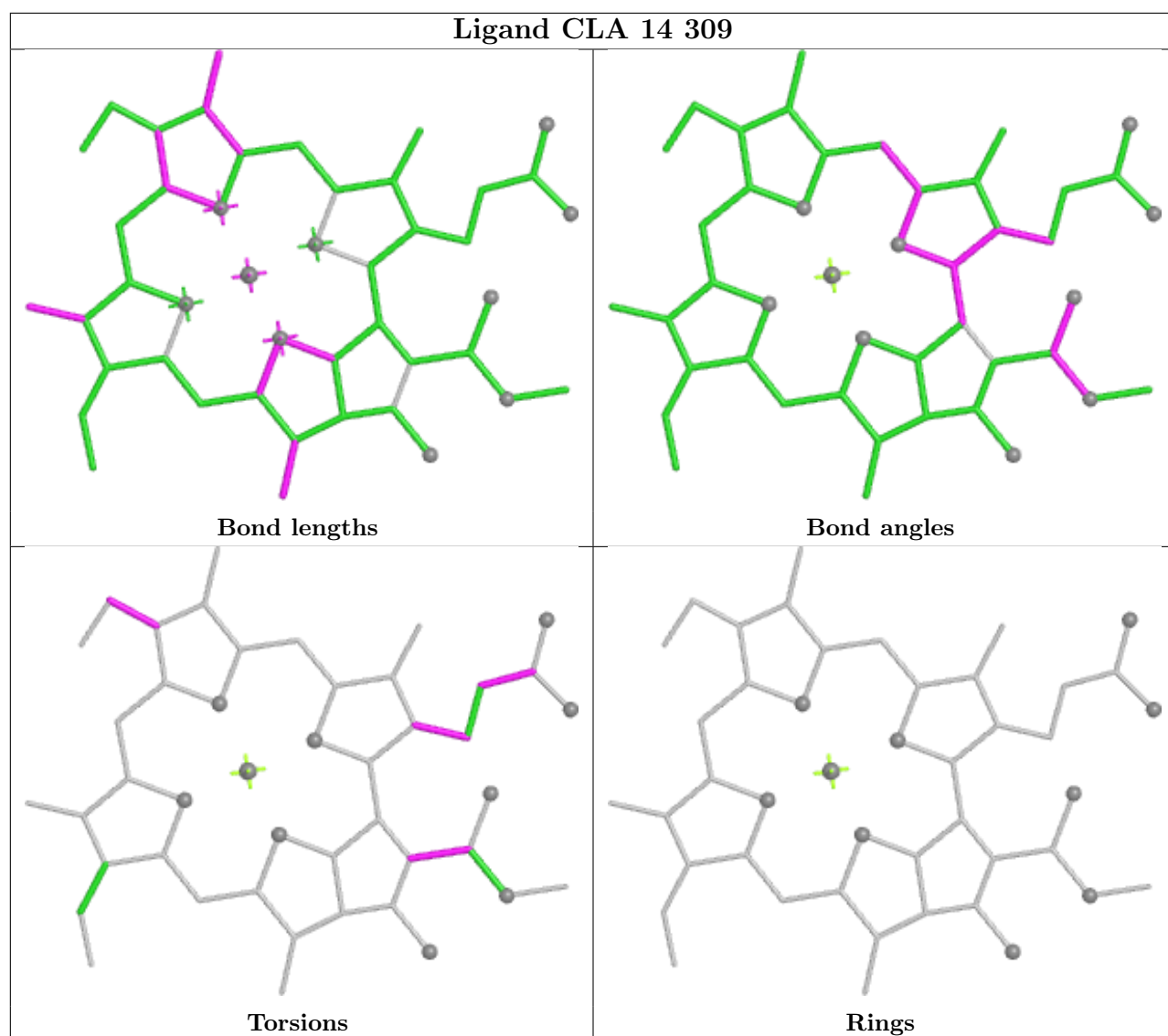
Ligand A86 15 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

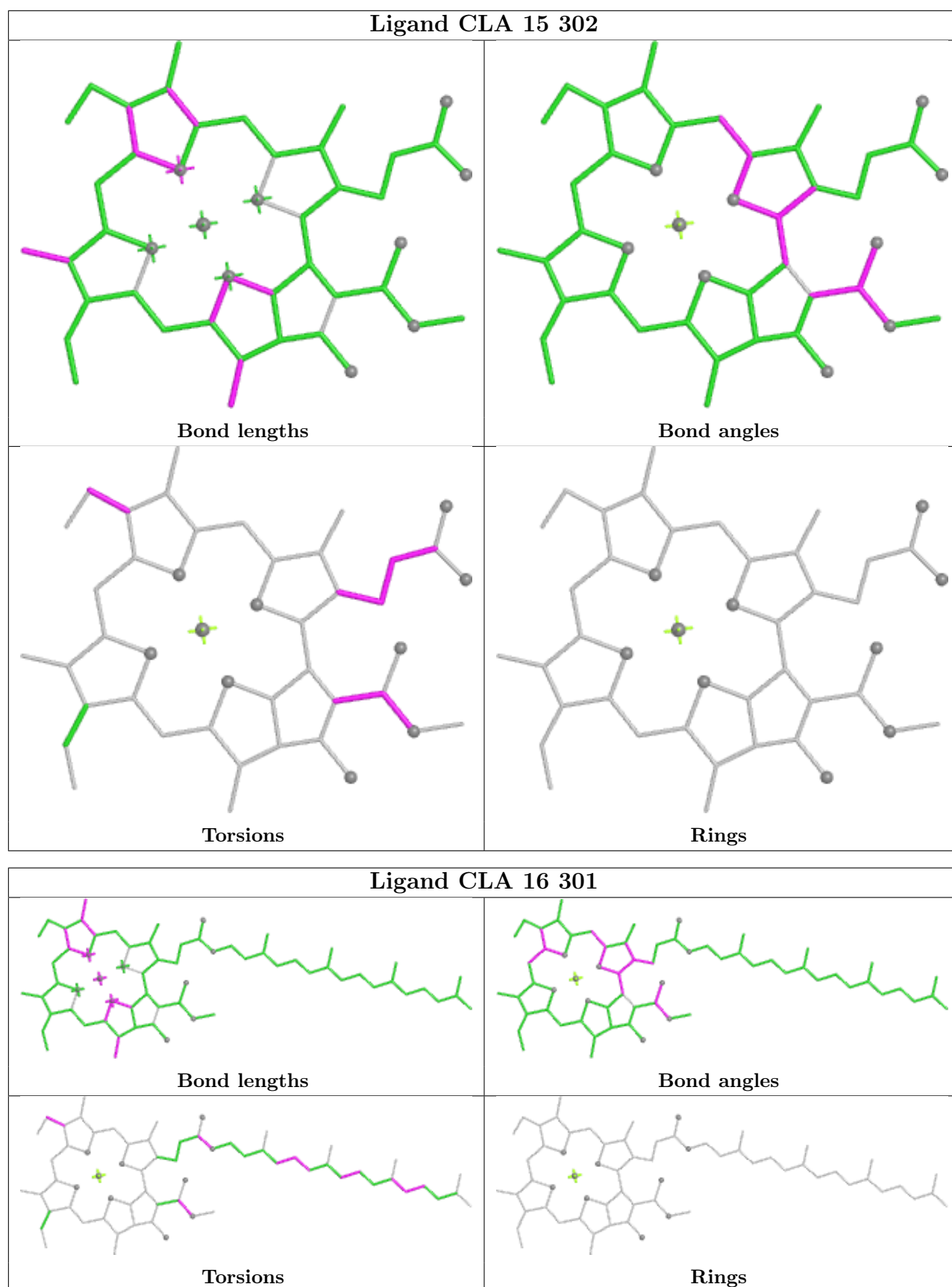
Ligand CLA 36 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

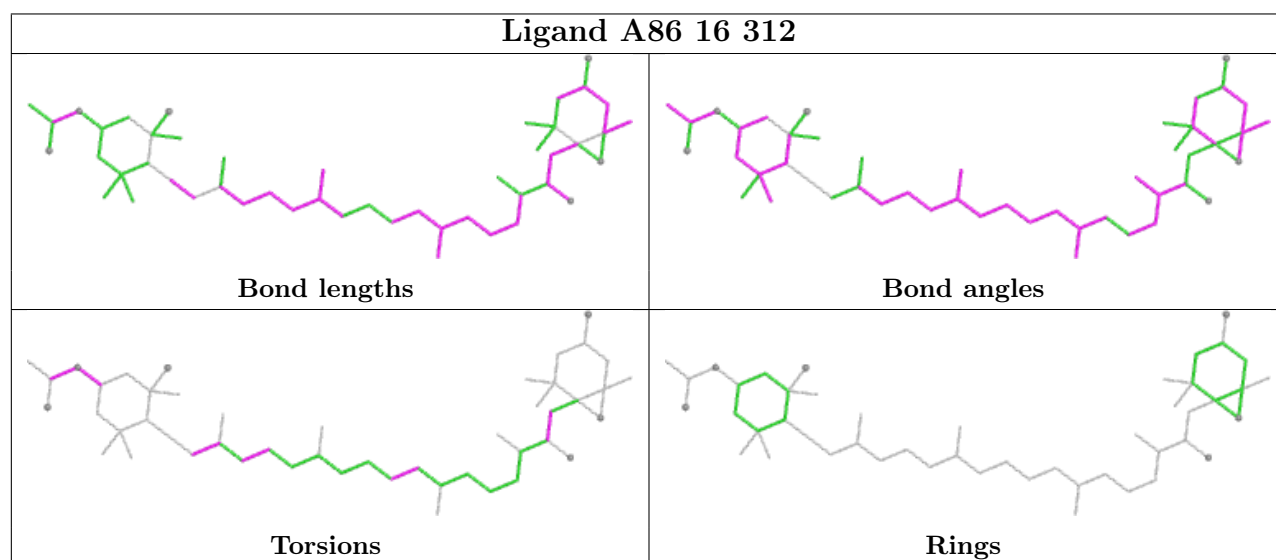
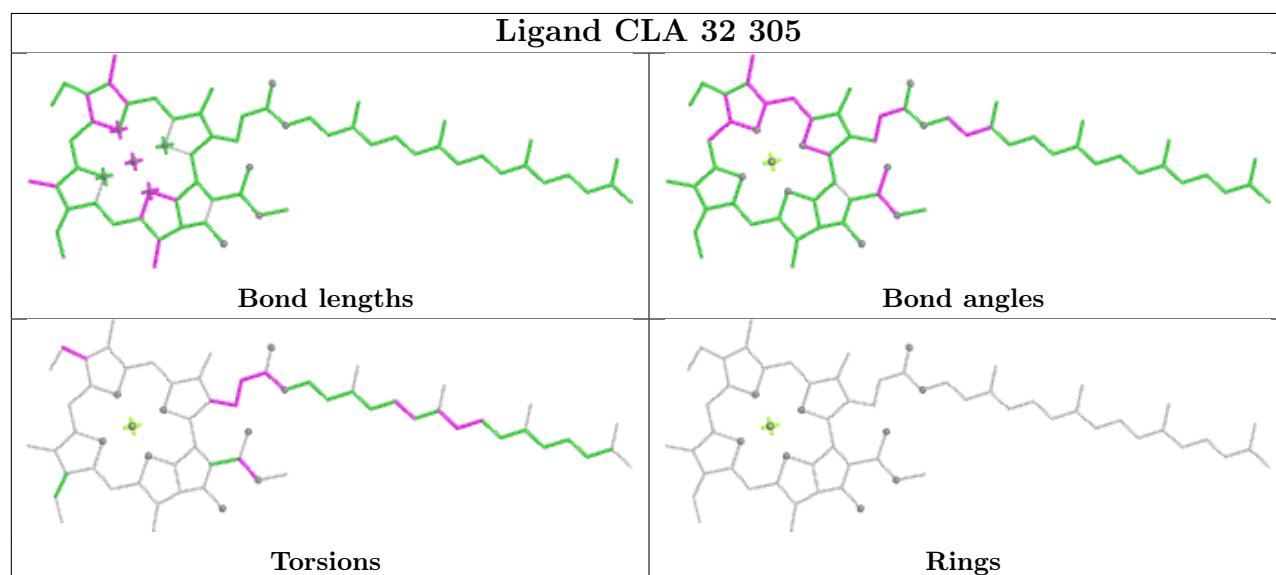
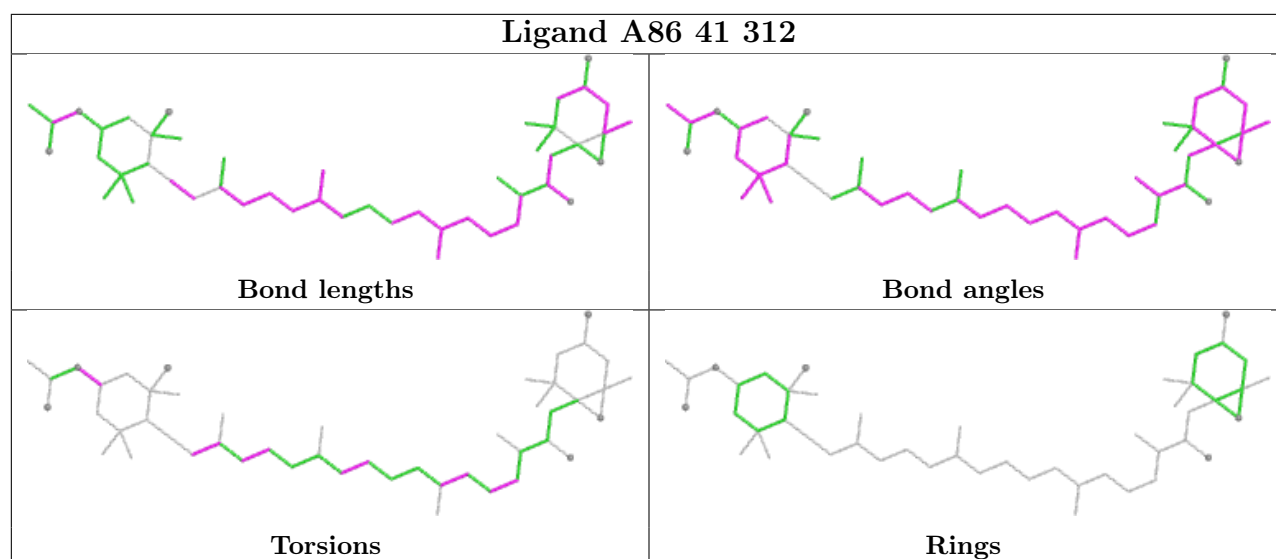


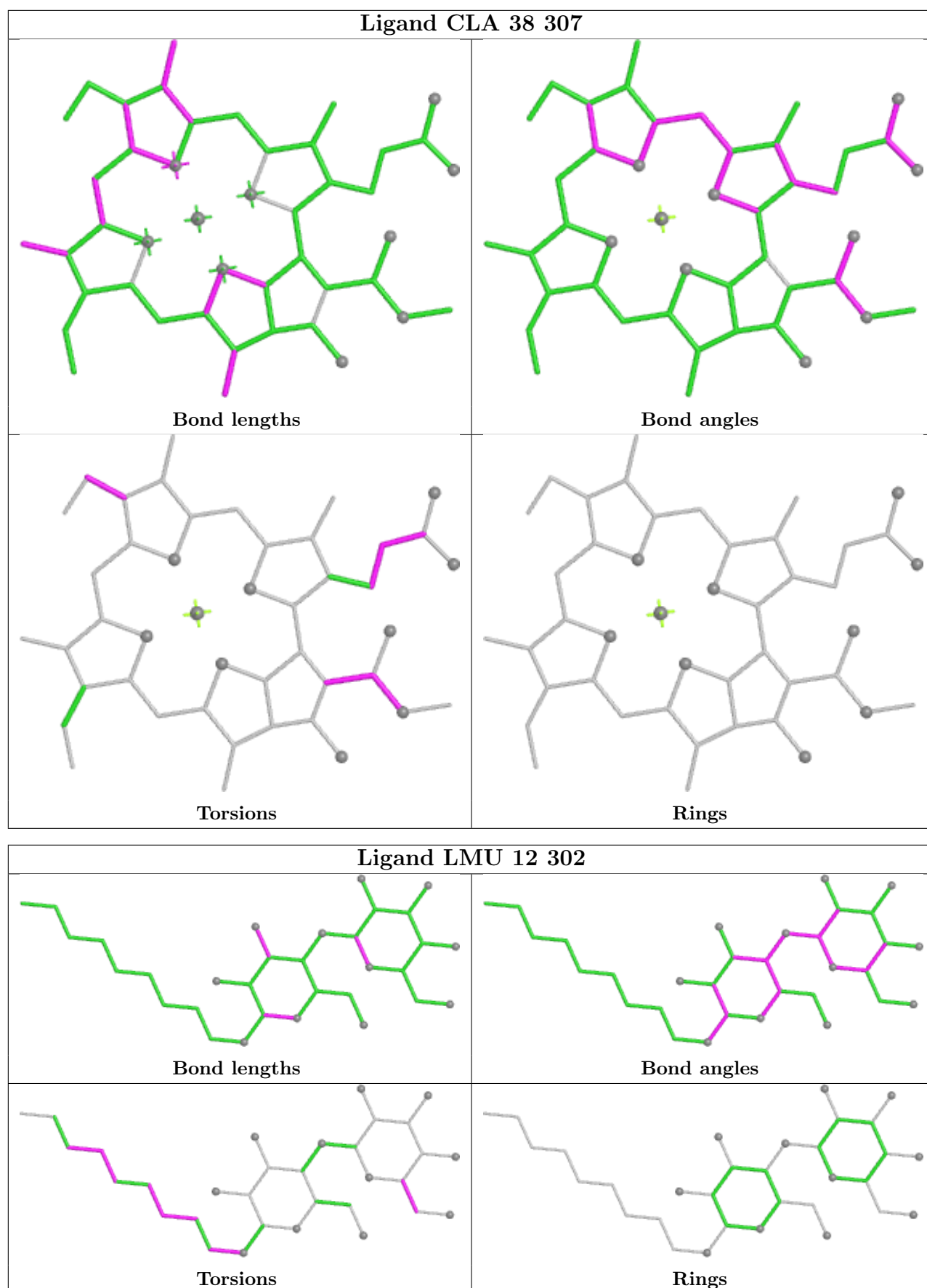


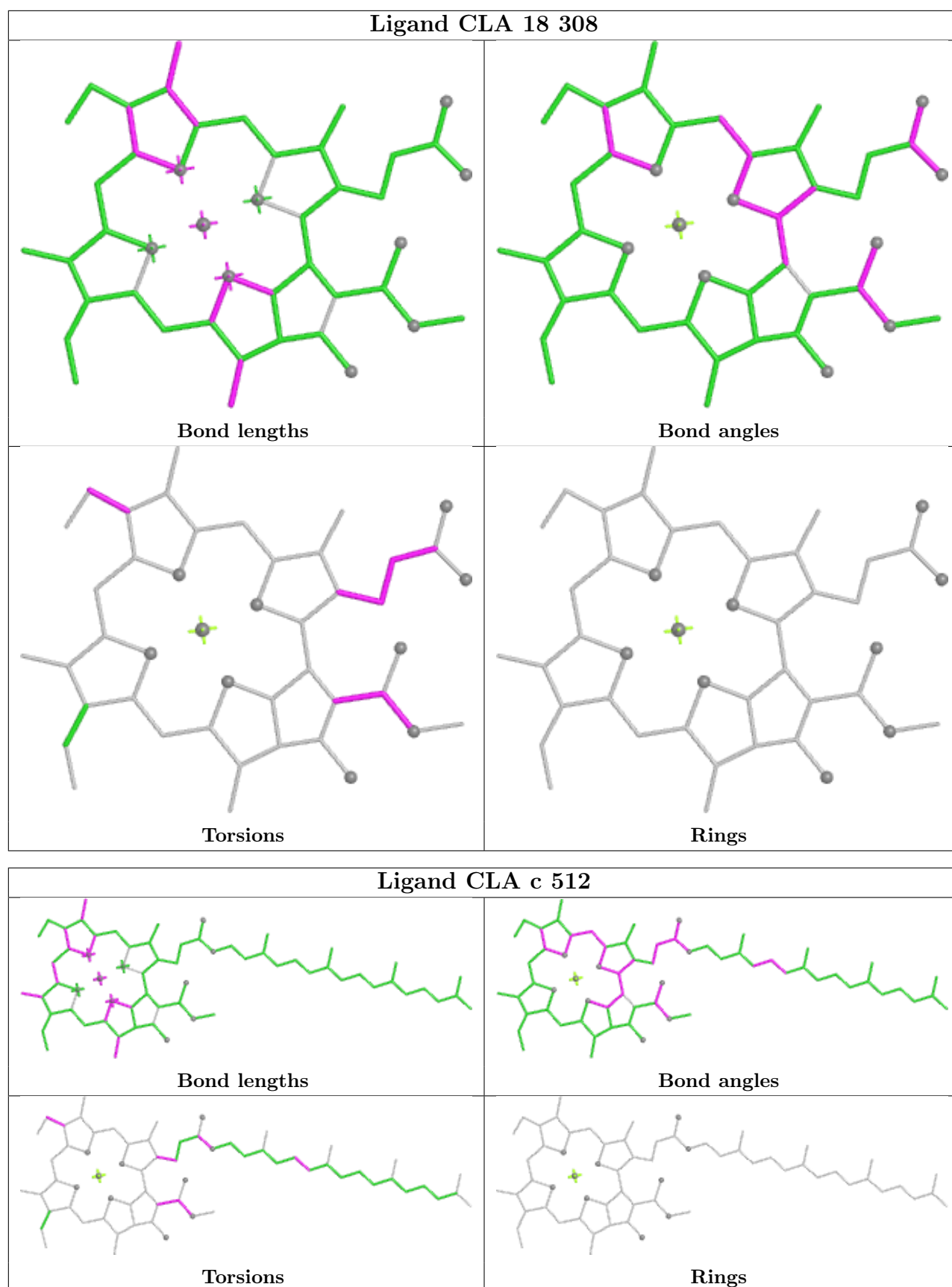


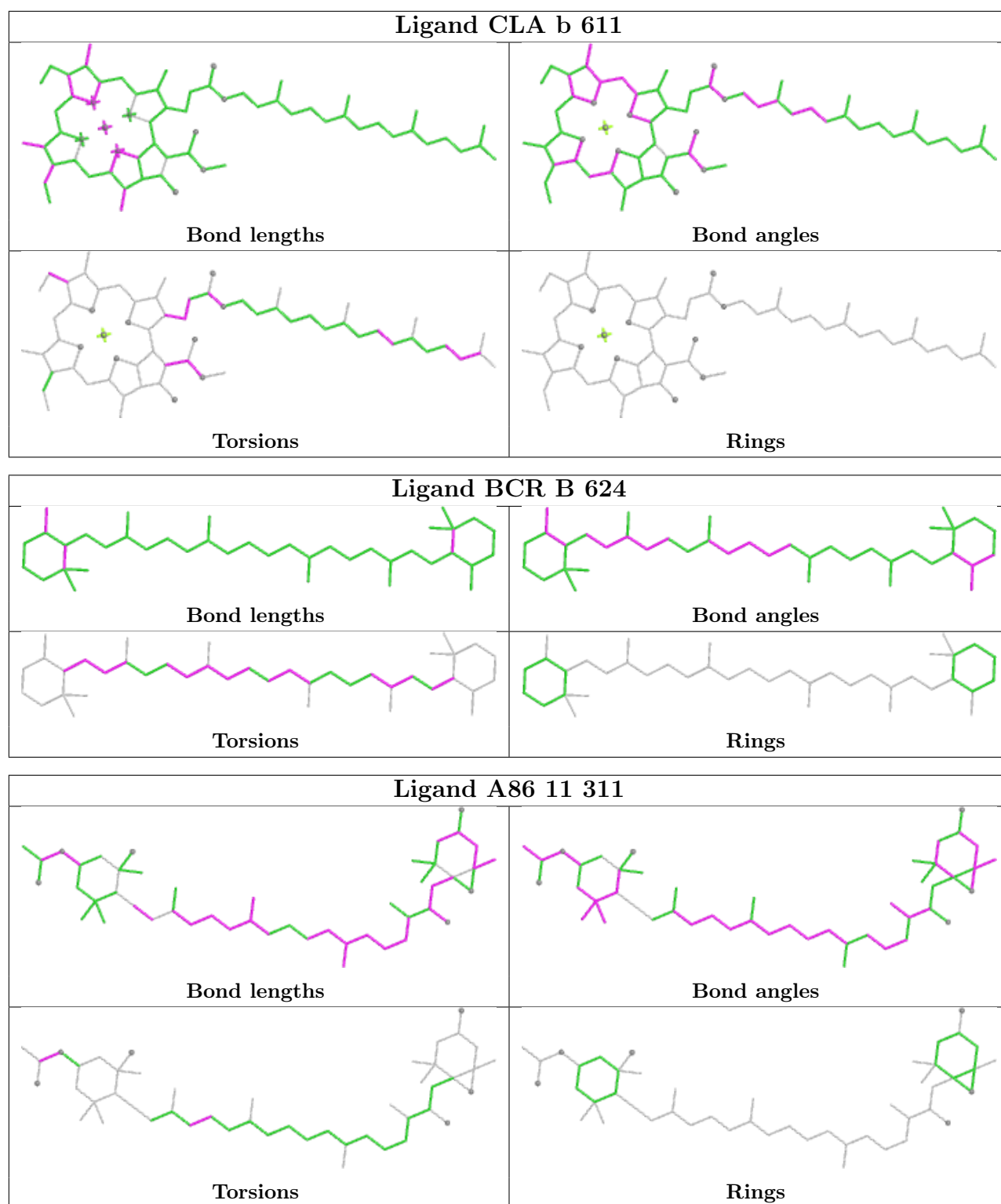


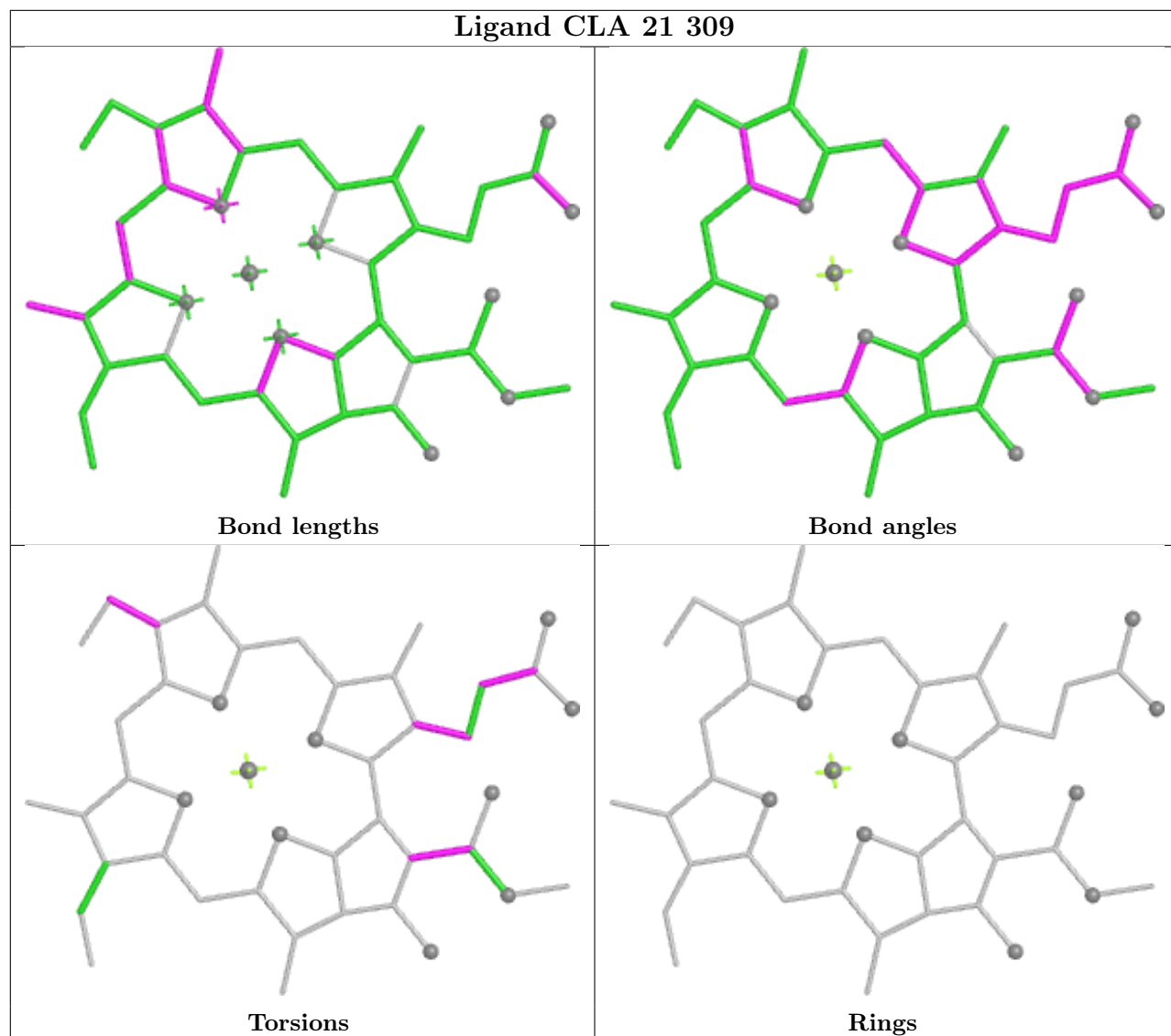


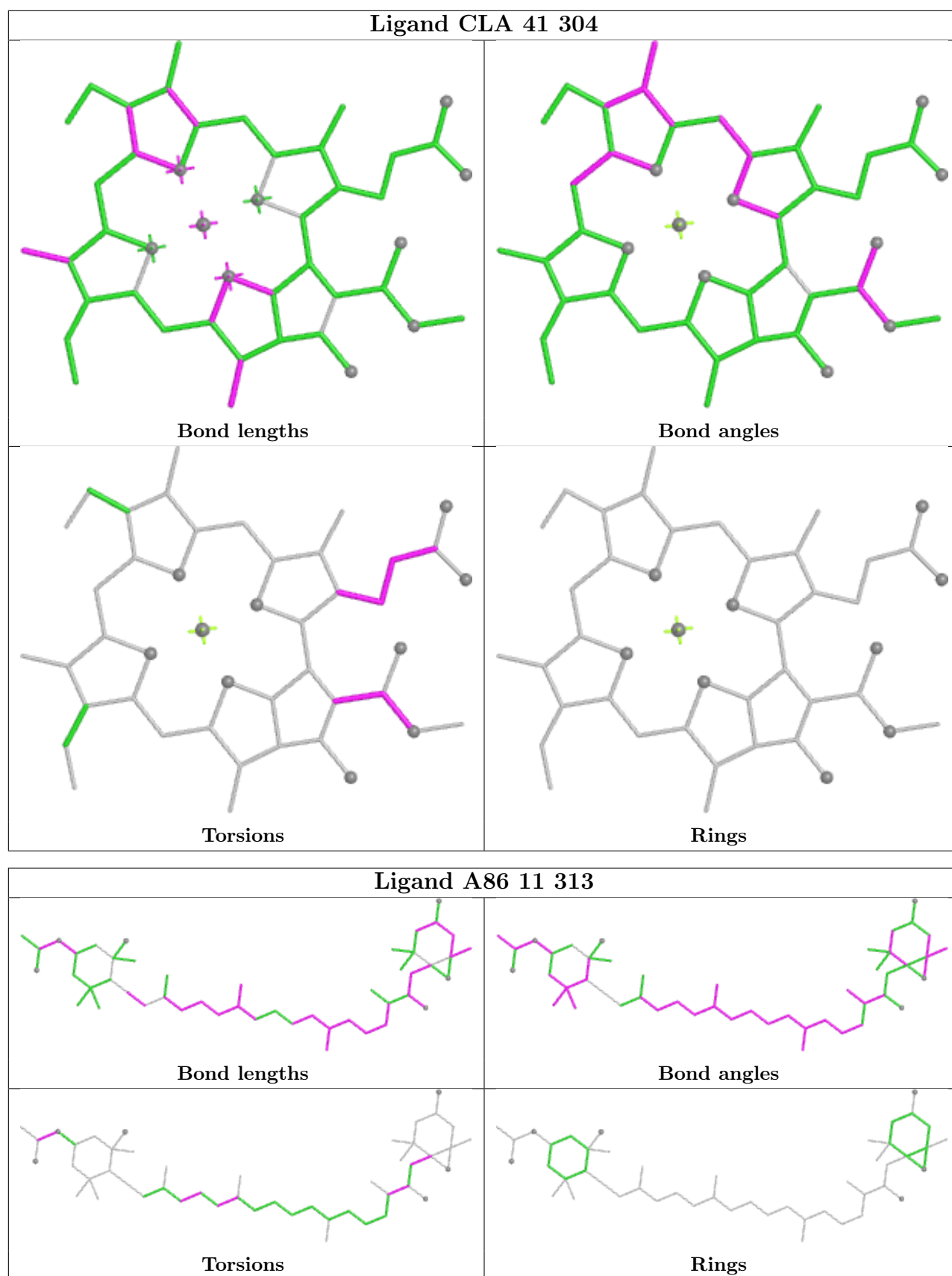


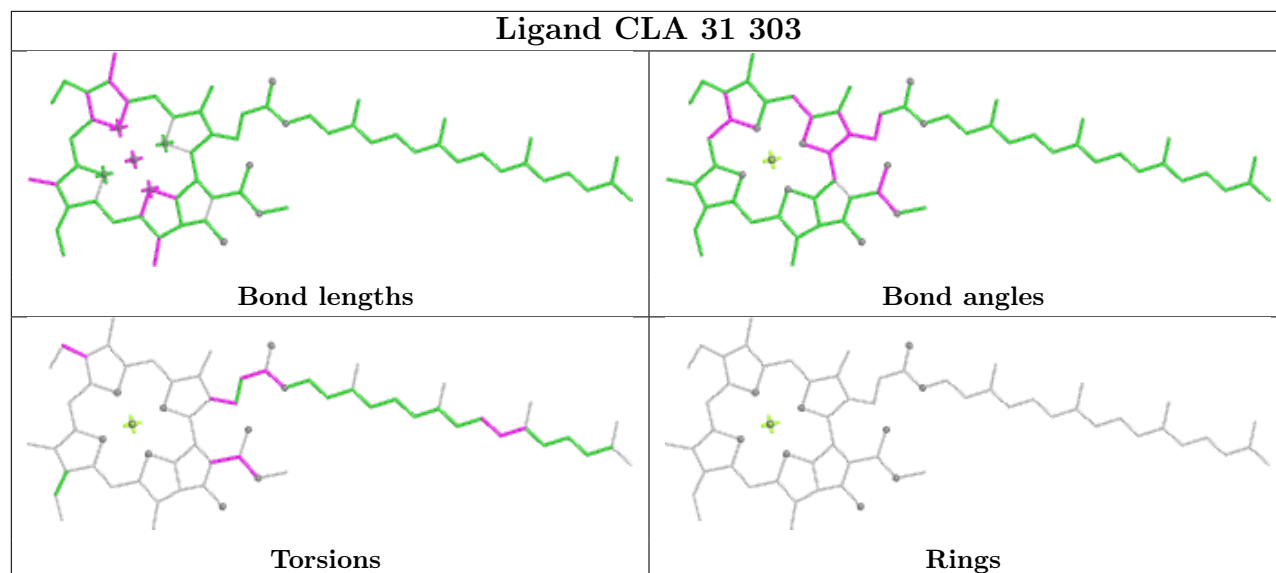
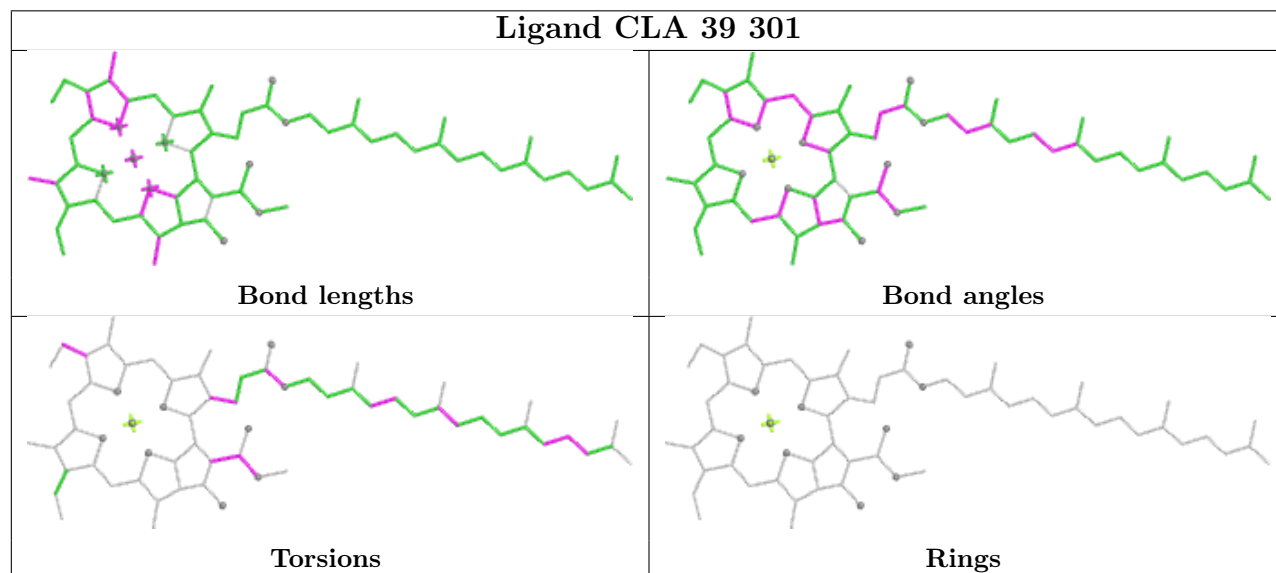
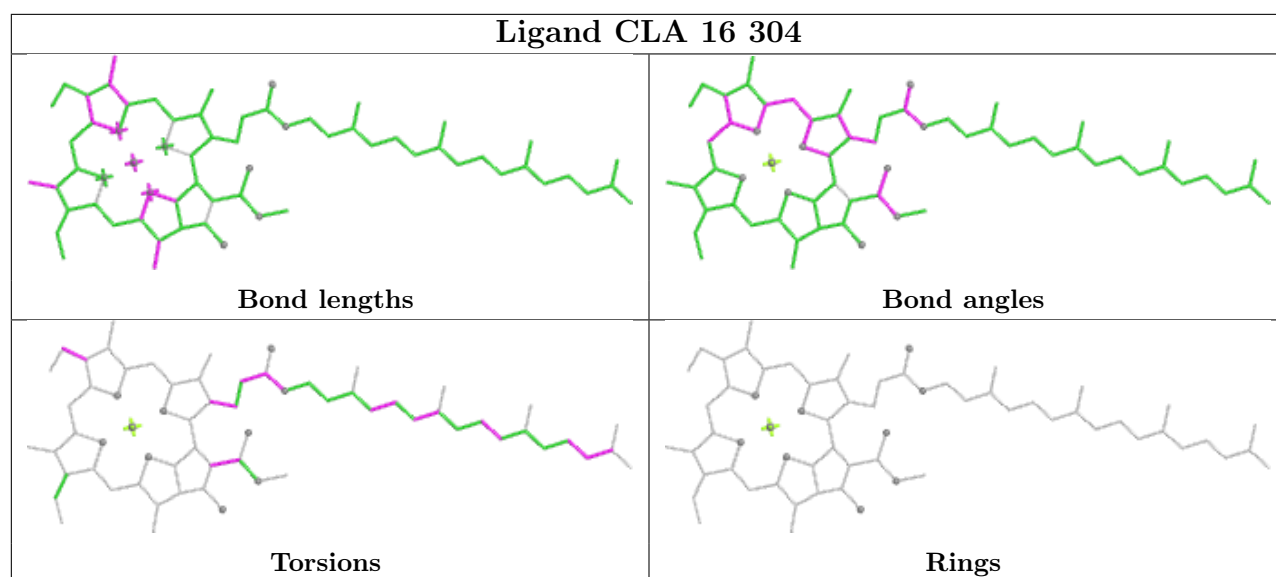


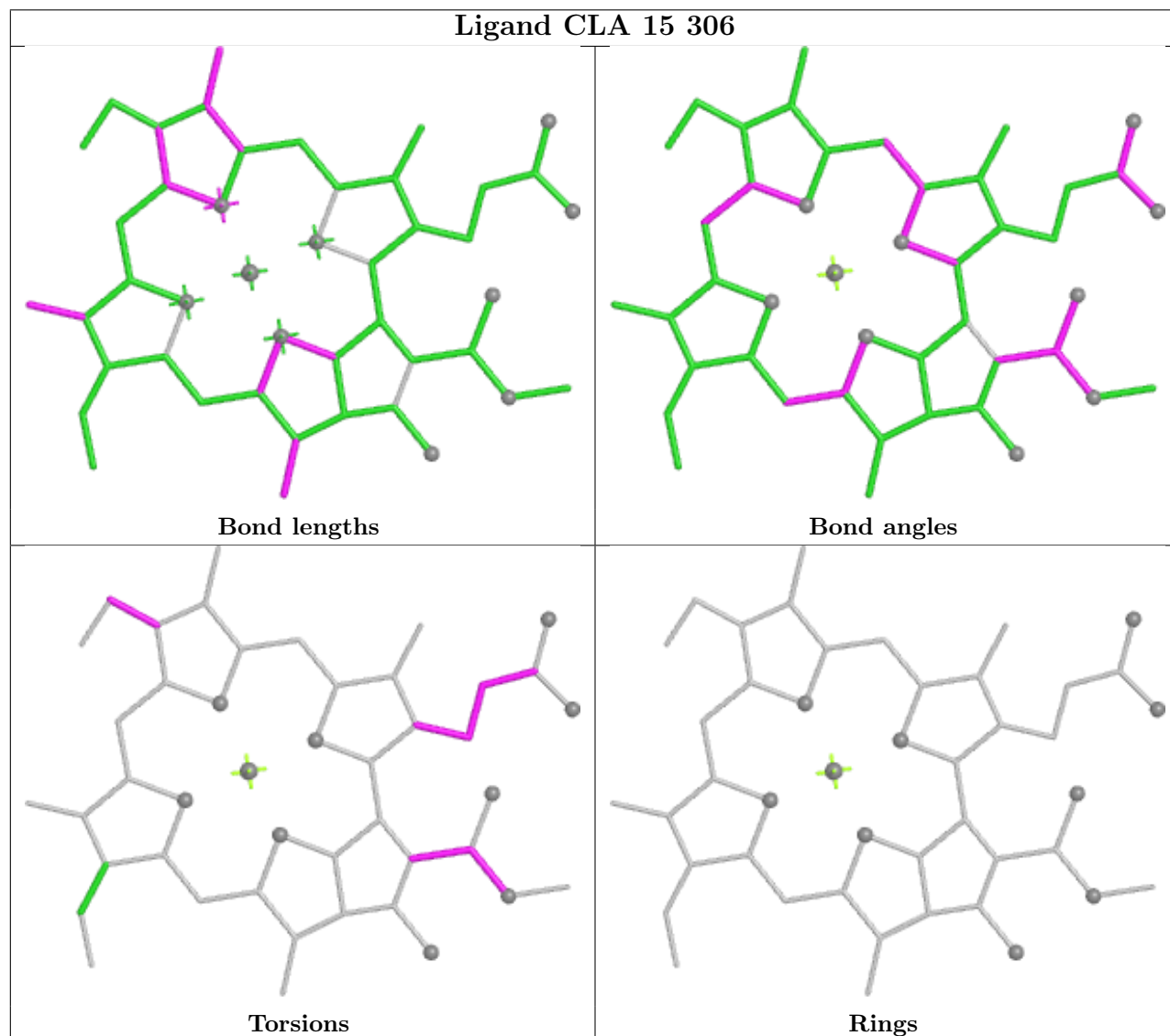
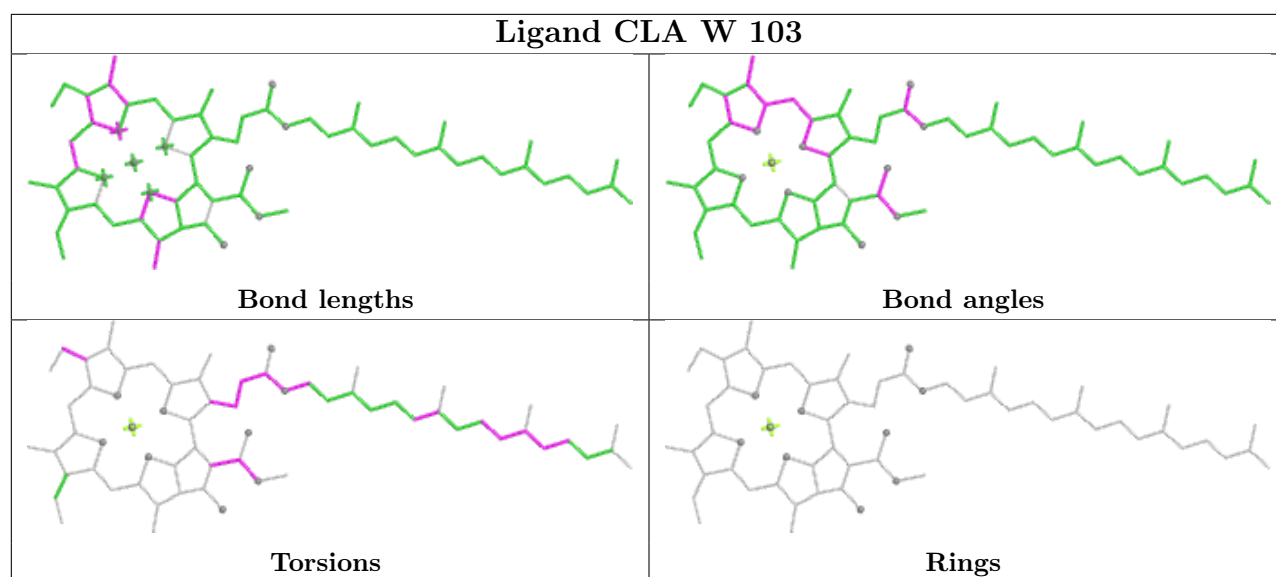


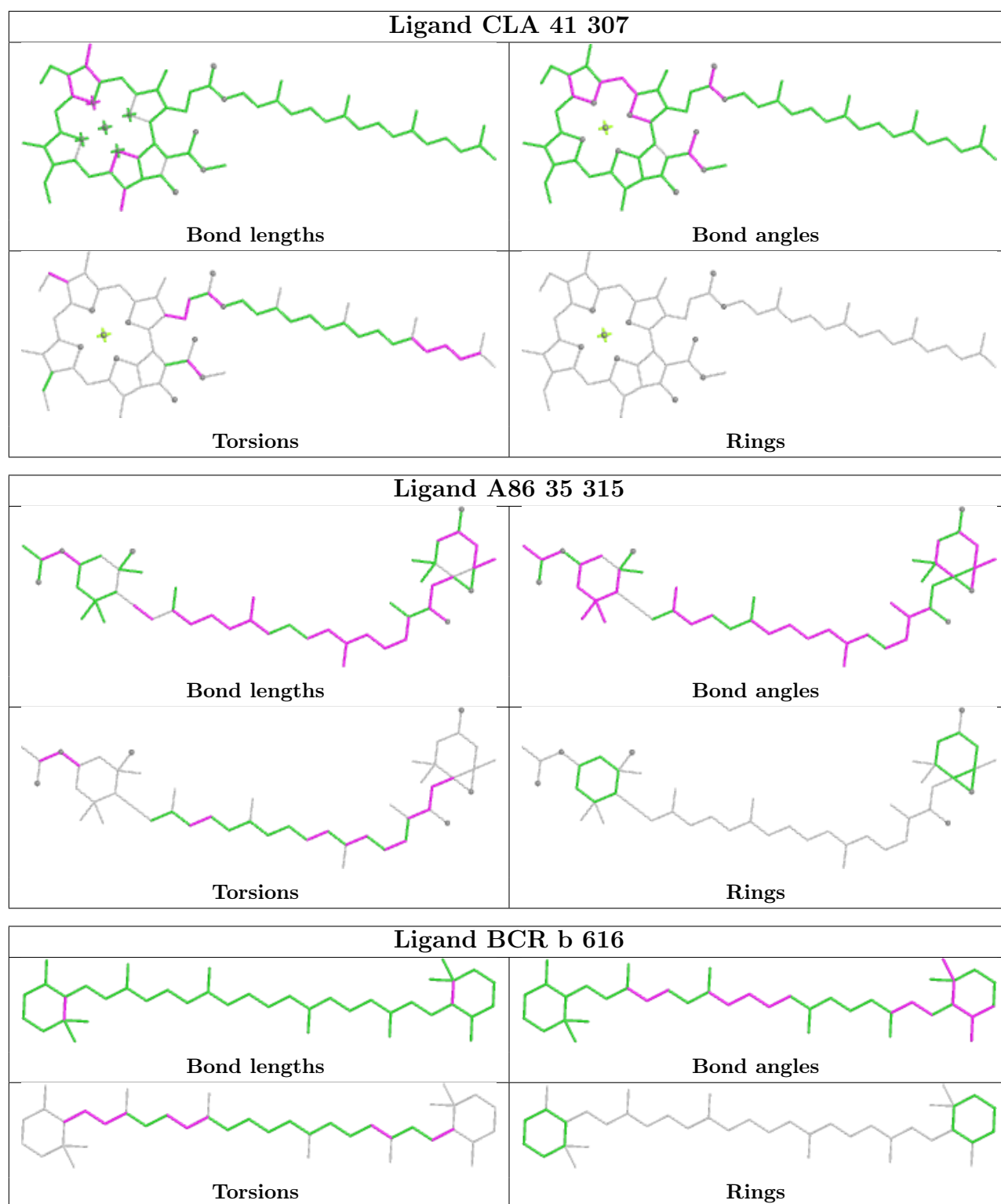


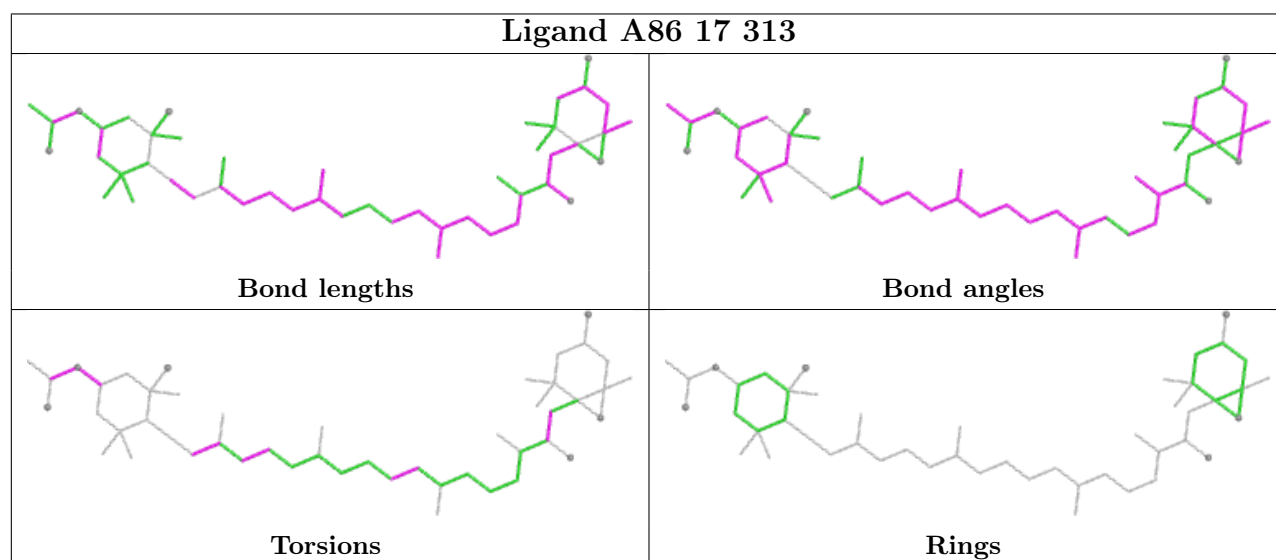
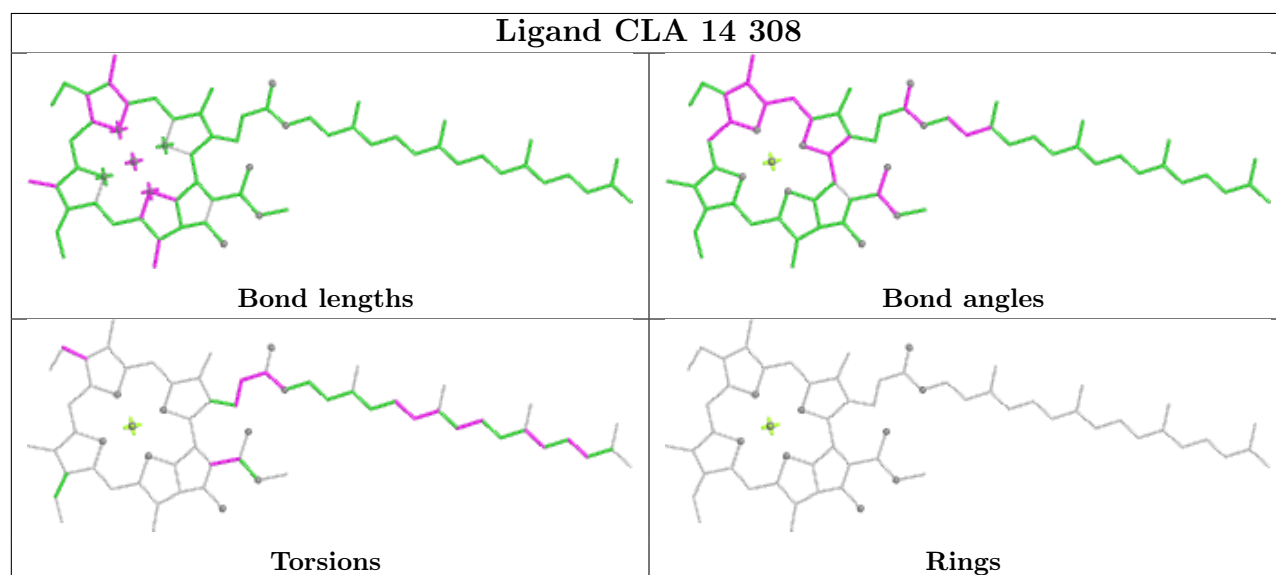
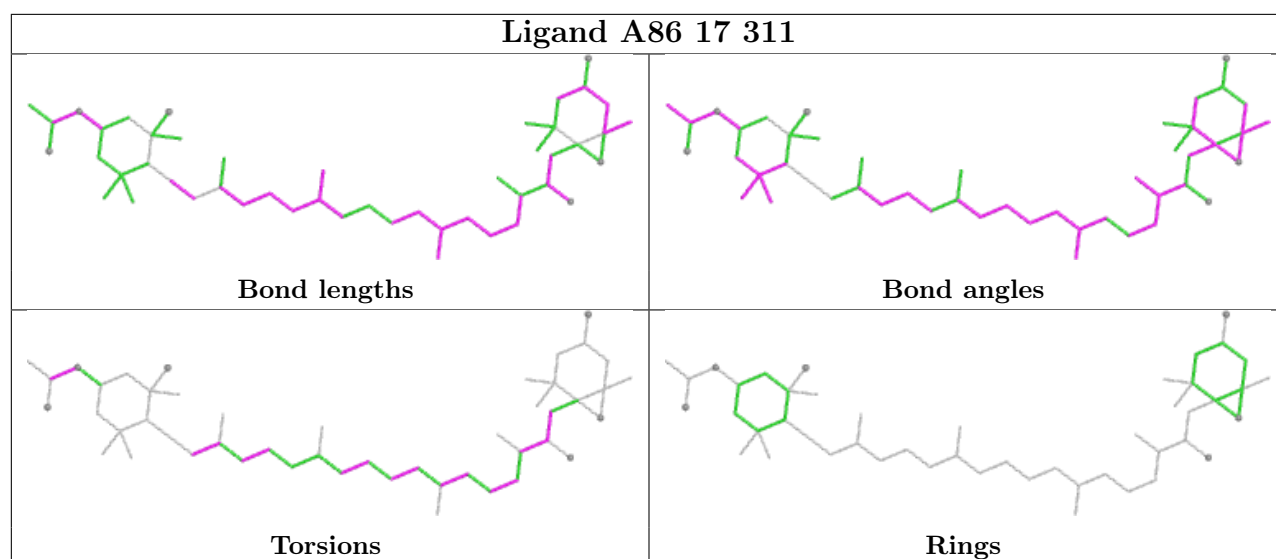


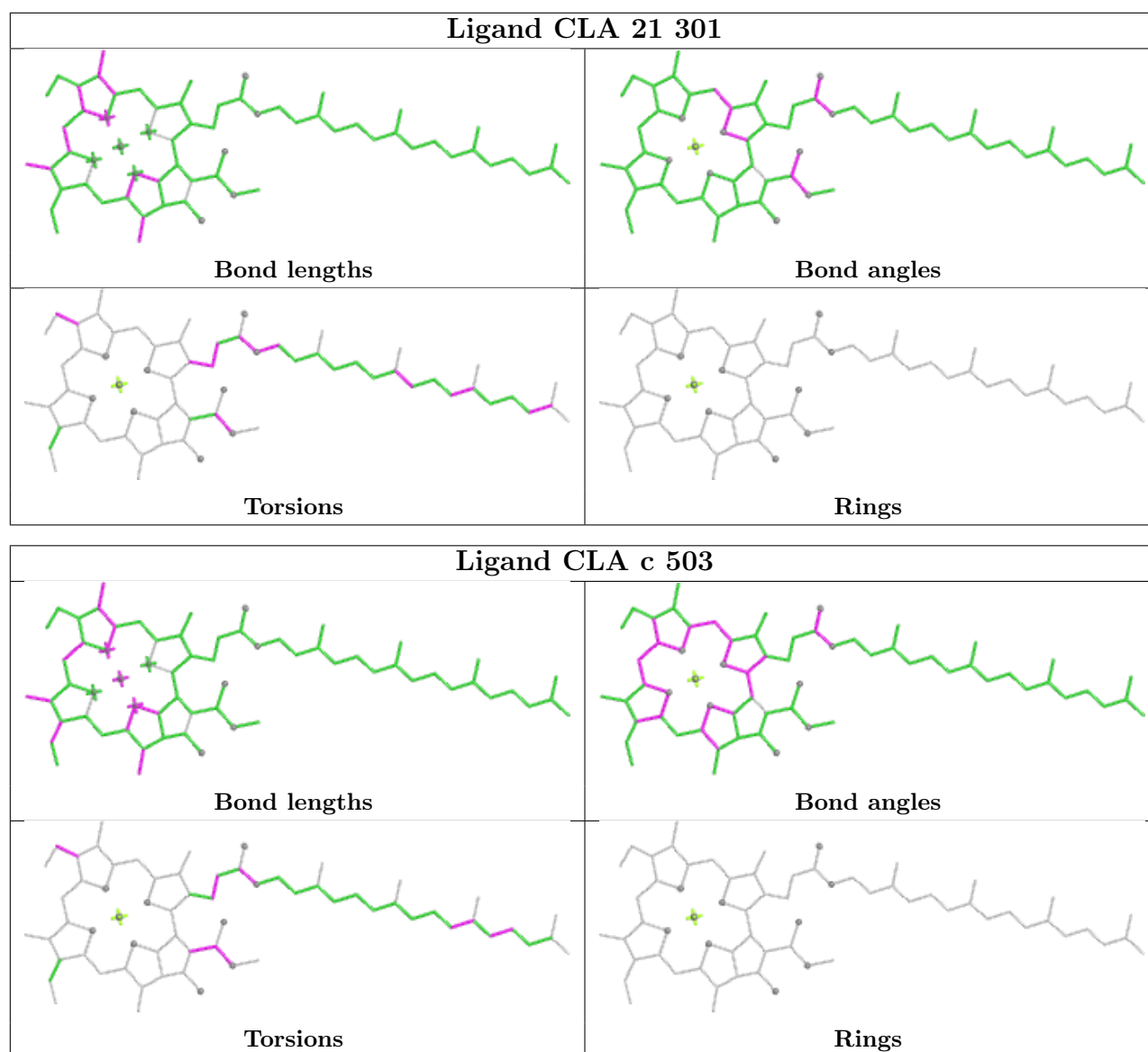


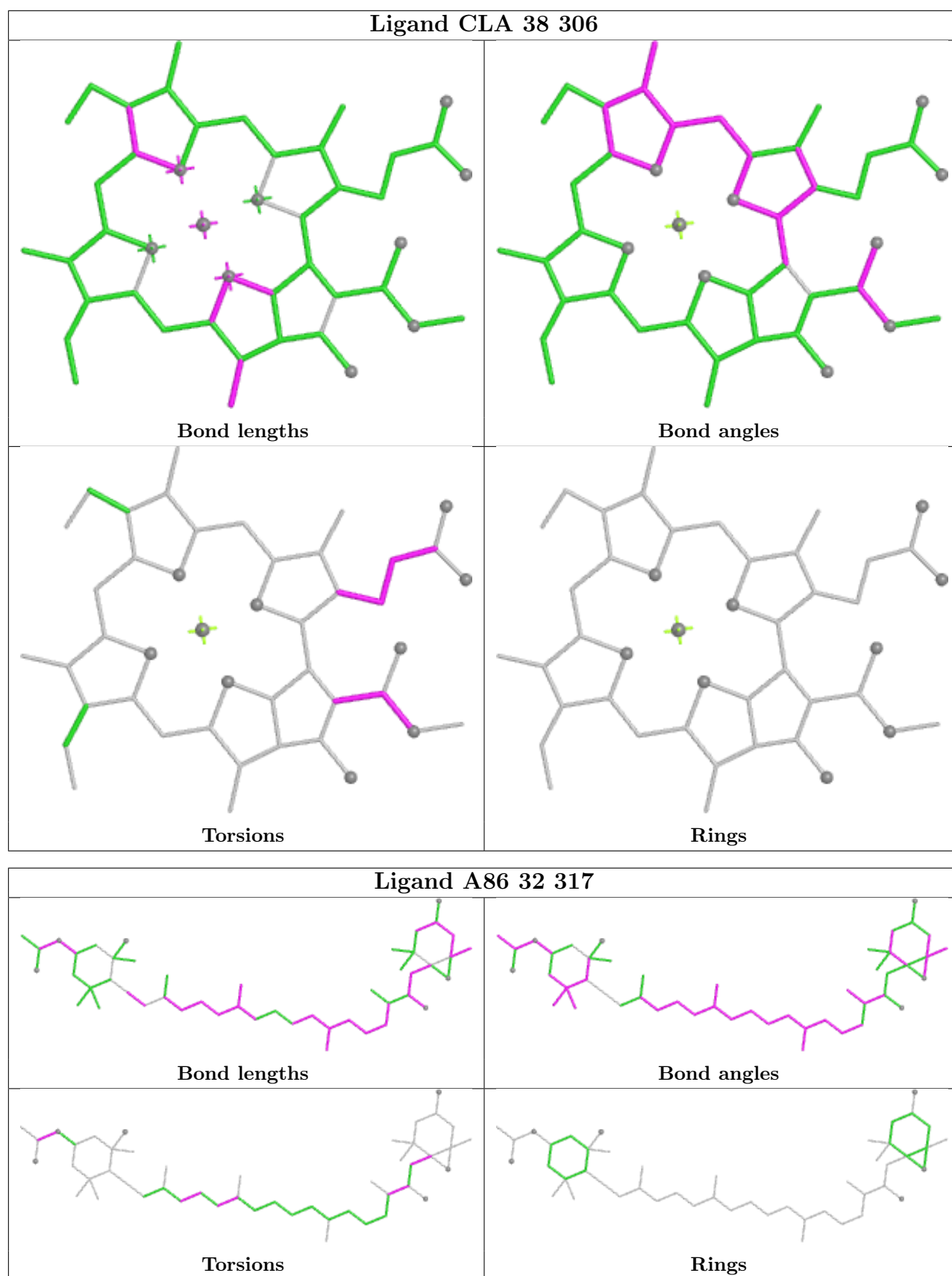


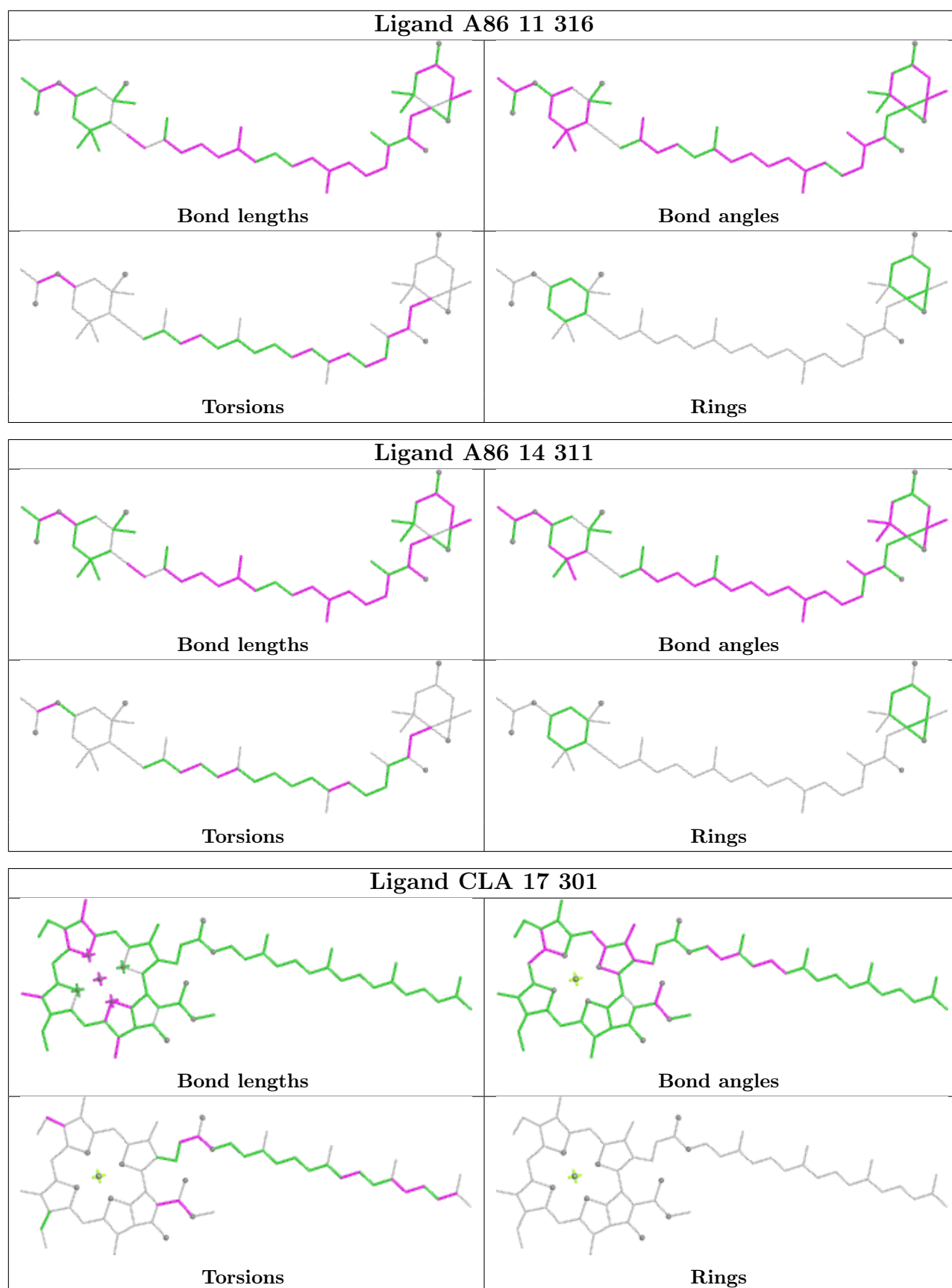


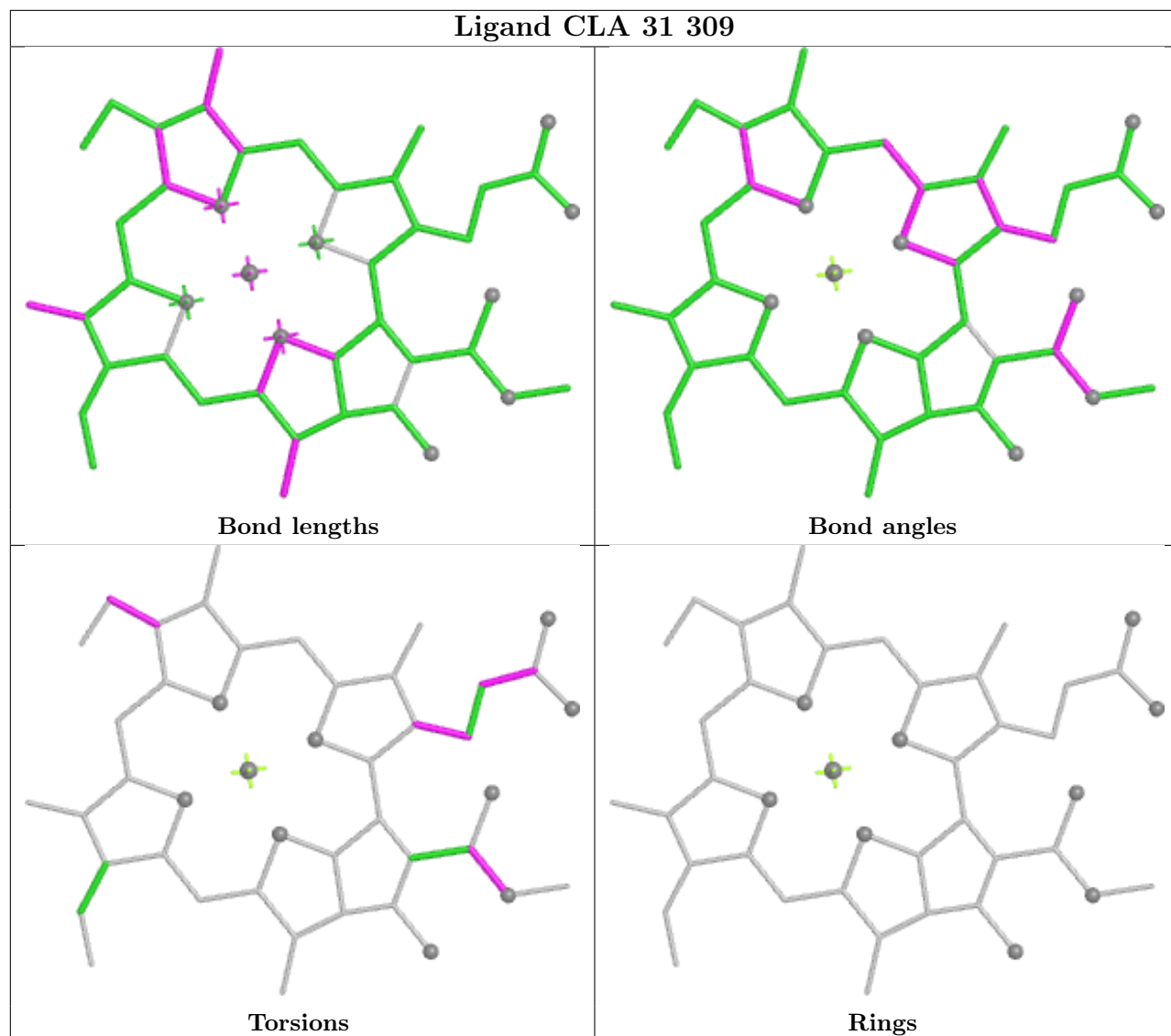


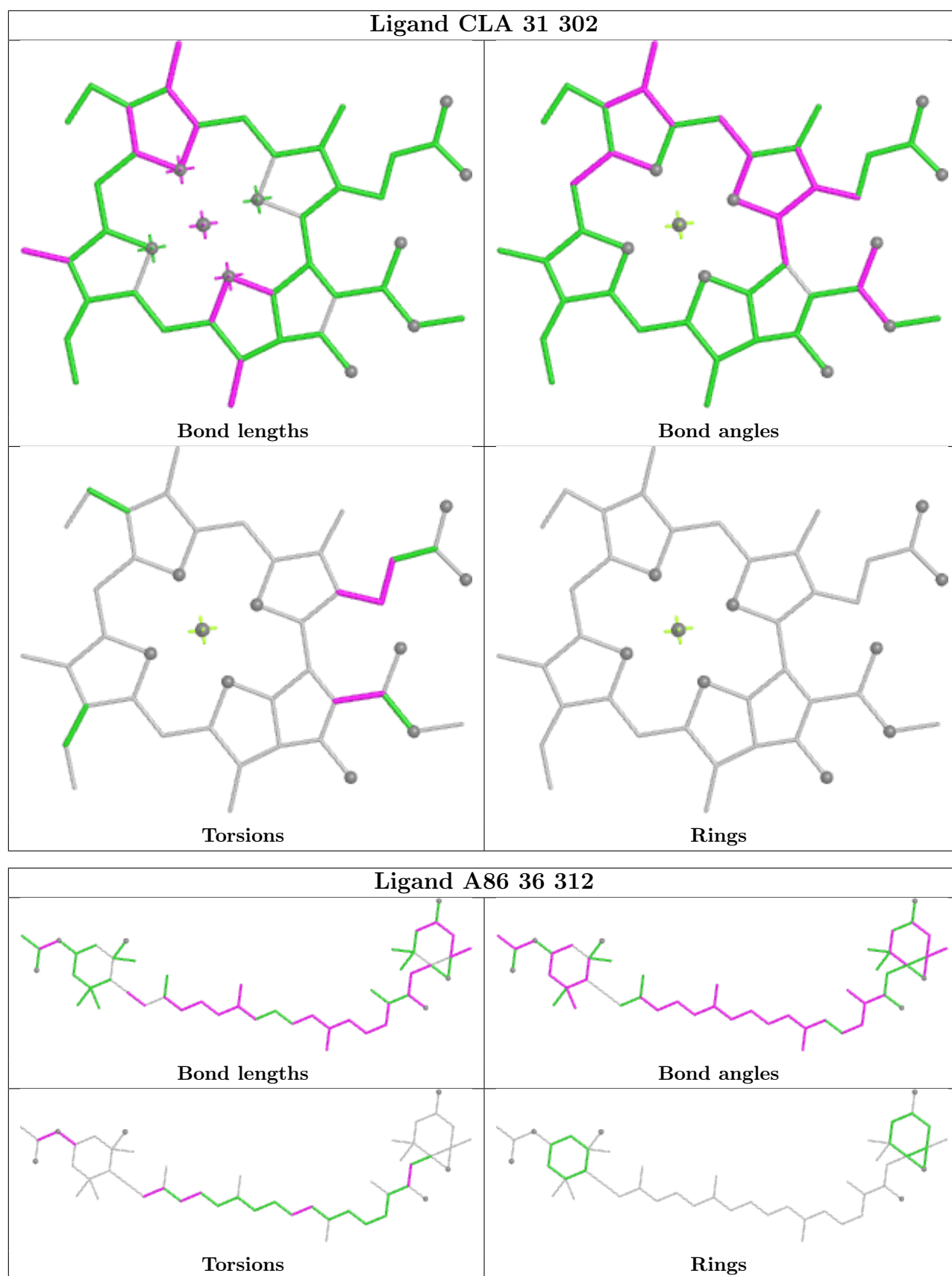


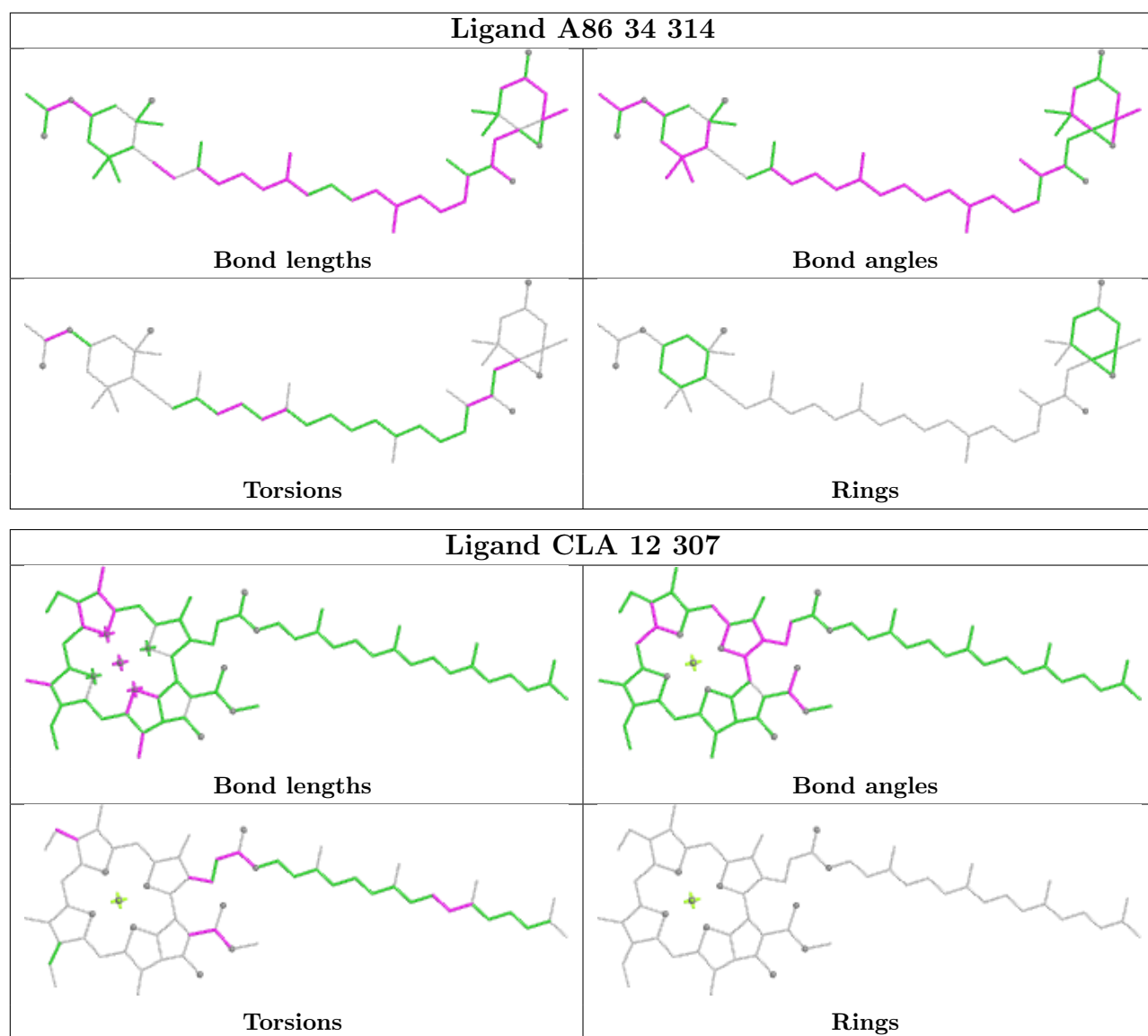


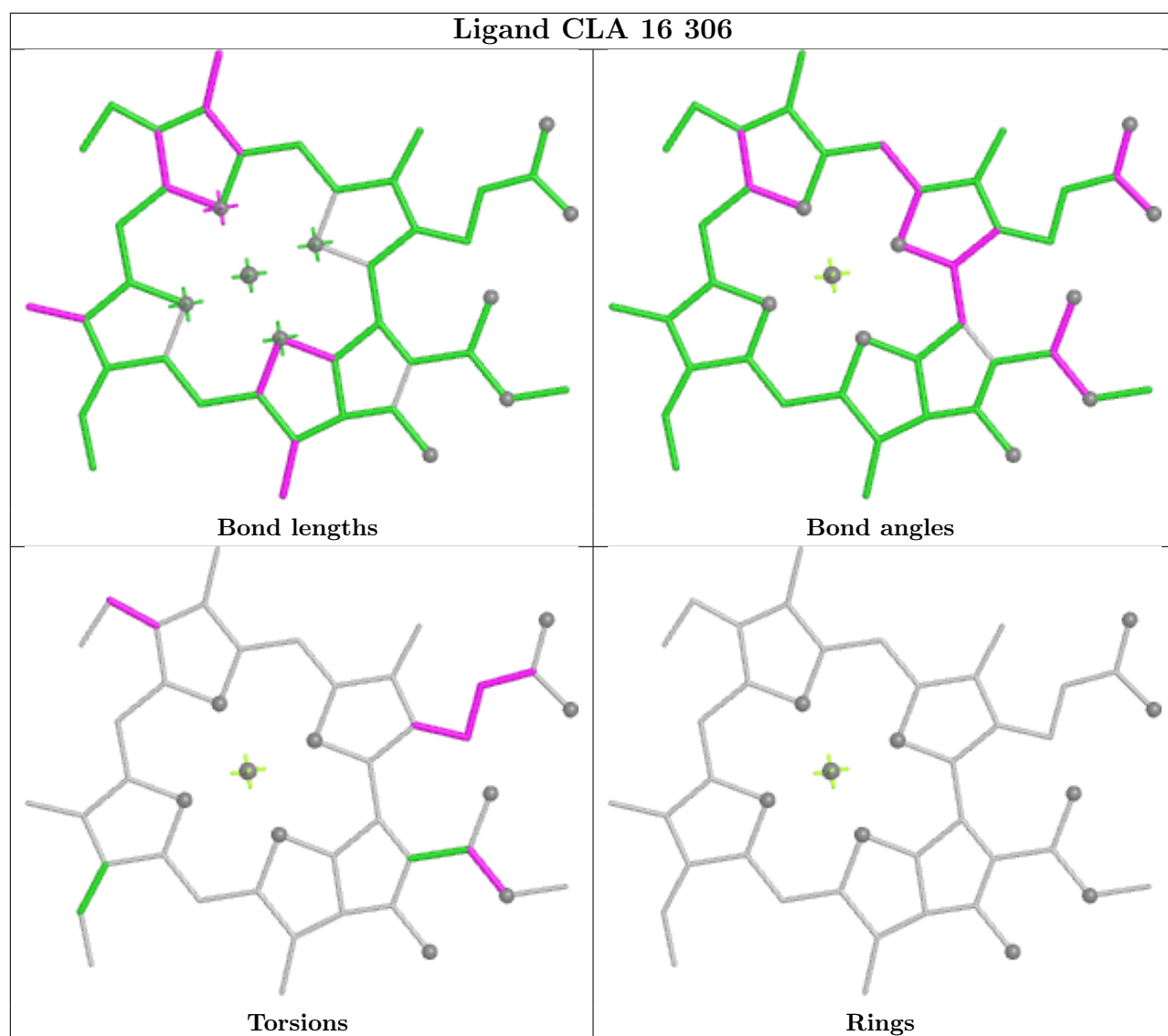


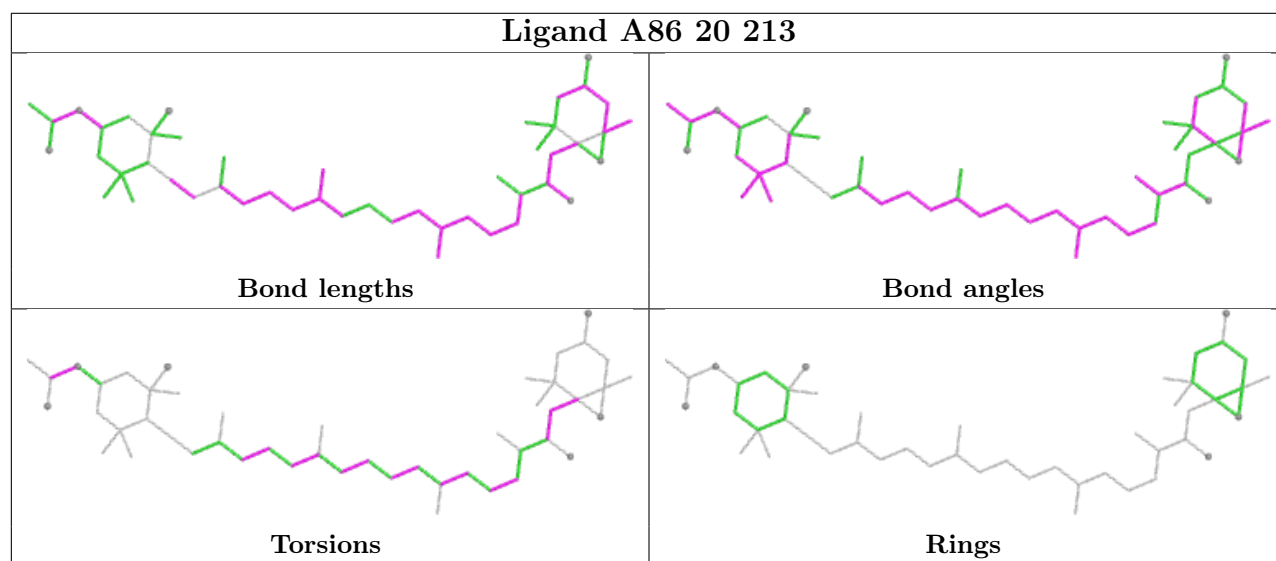
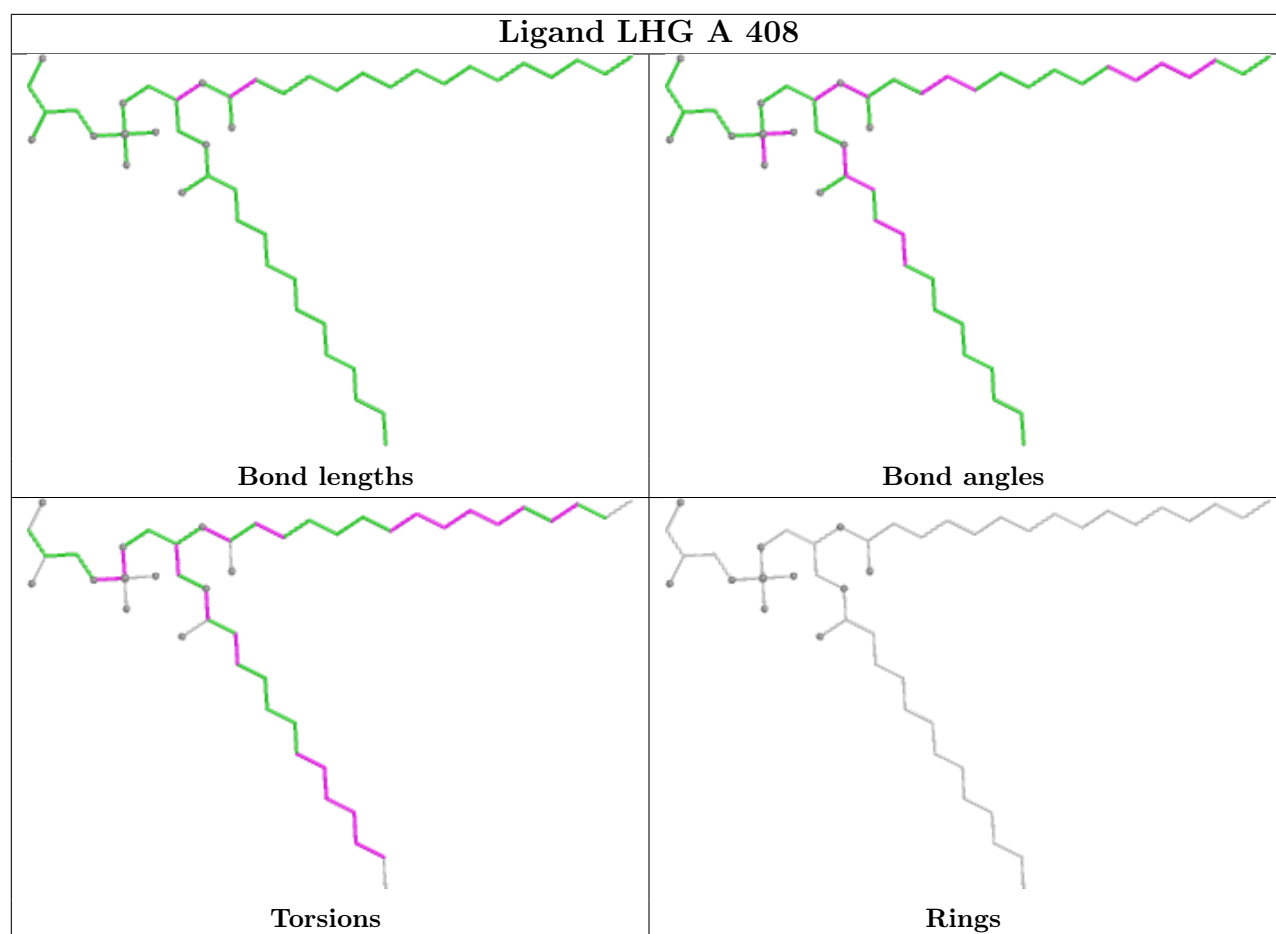


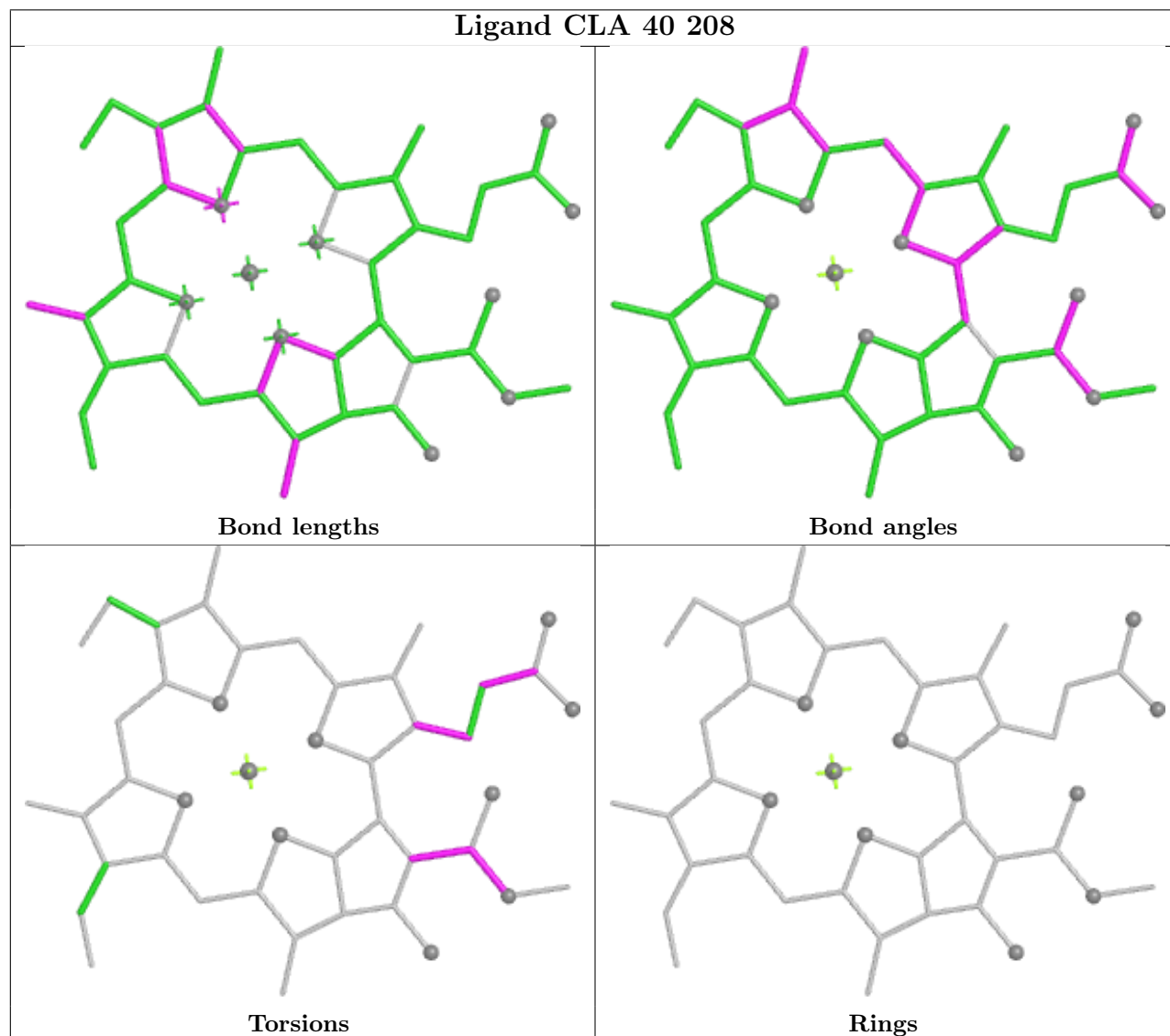
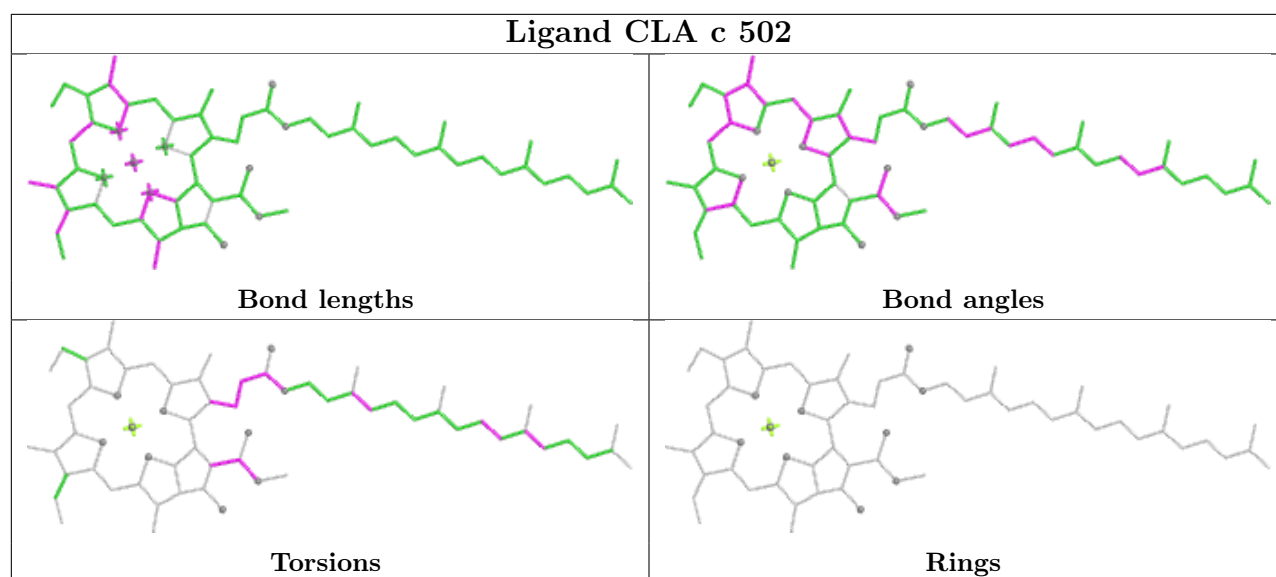


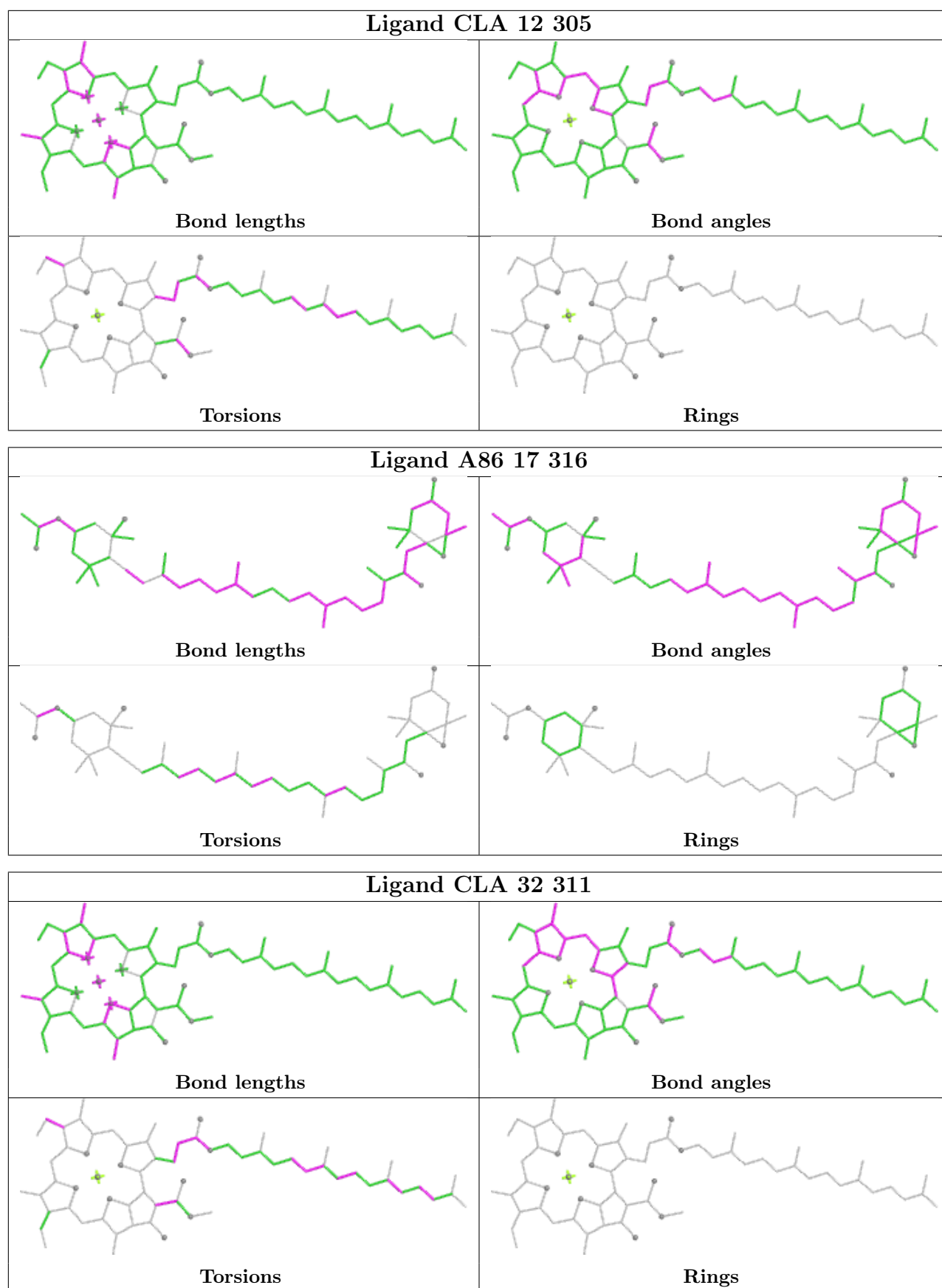


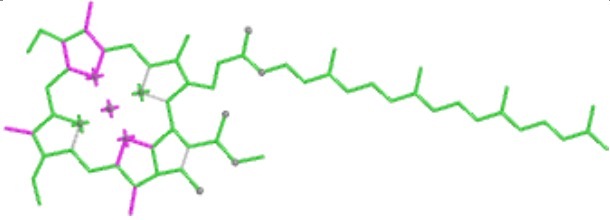
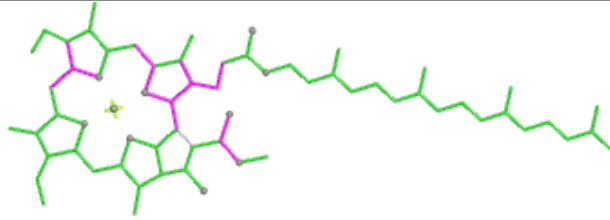
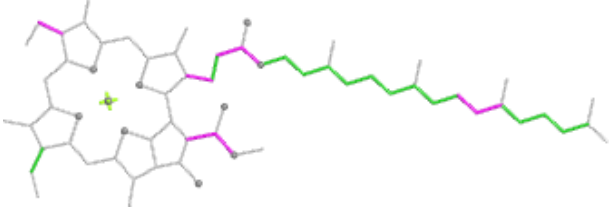
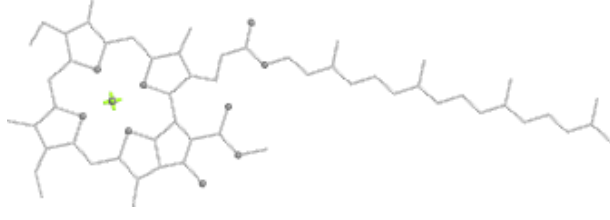


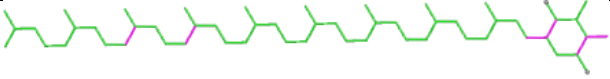
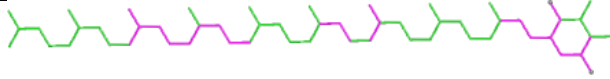
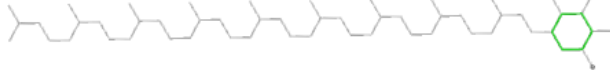


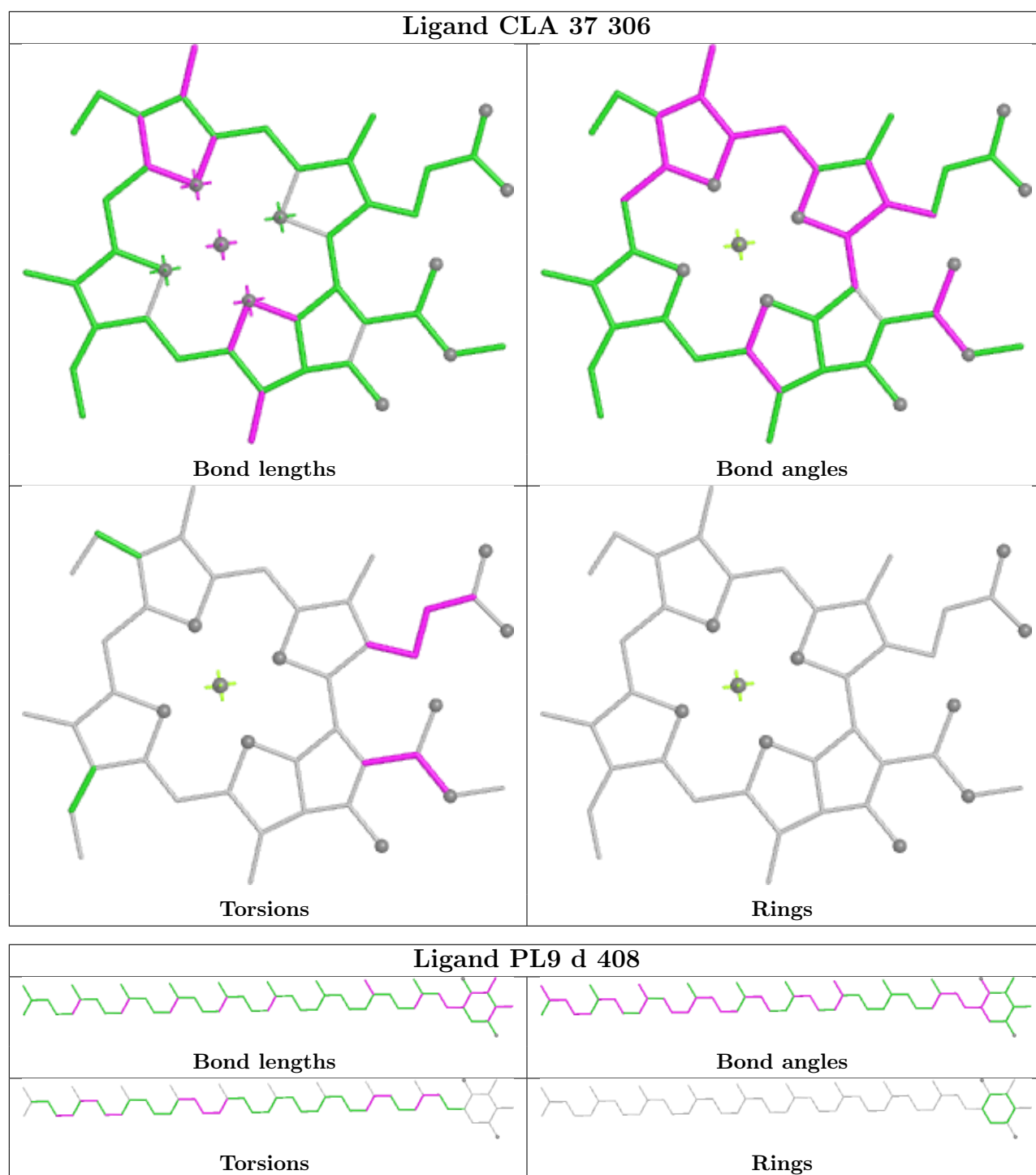


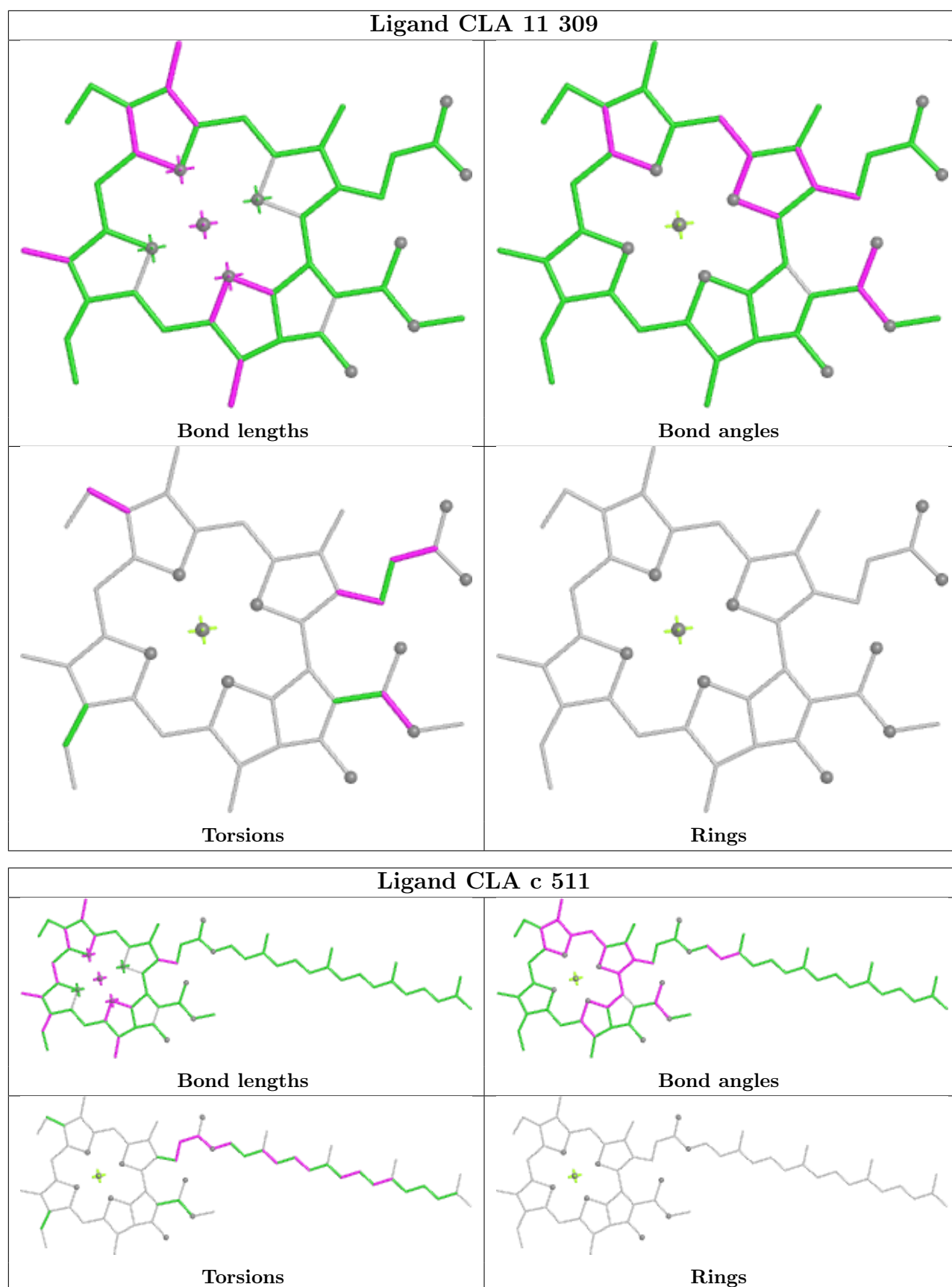


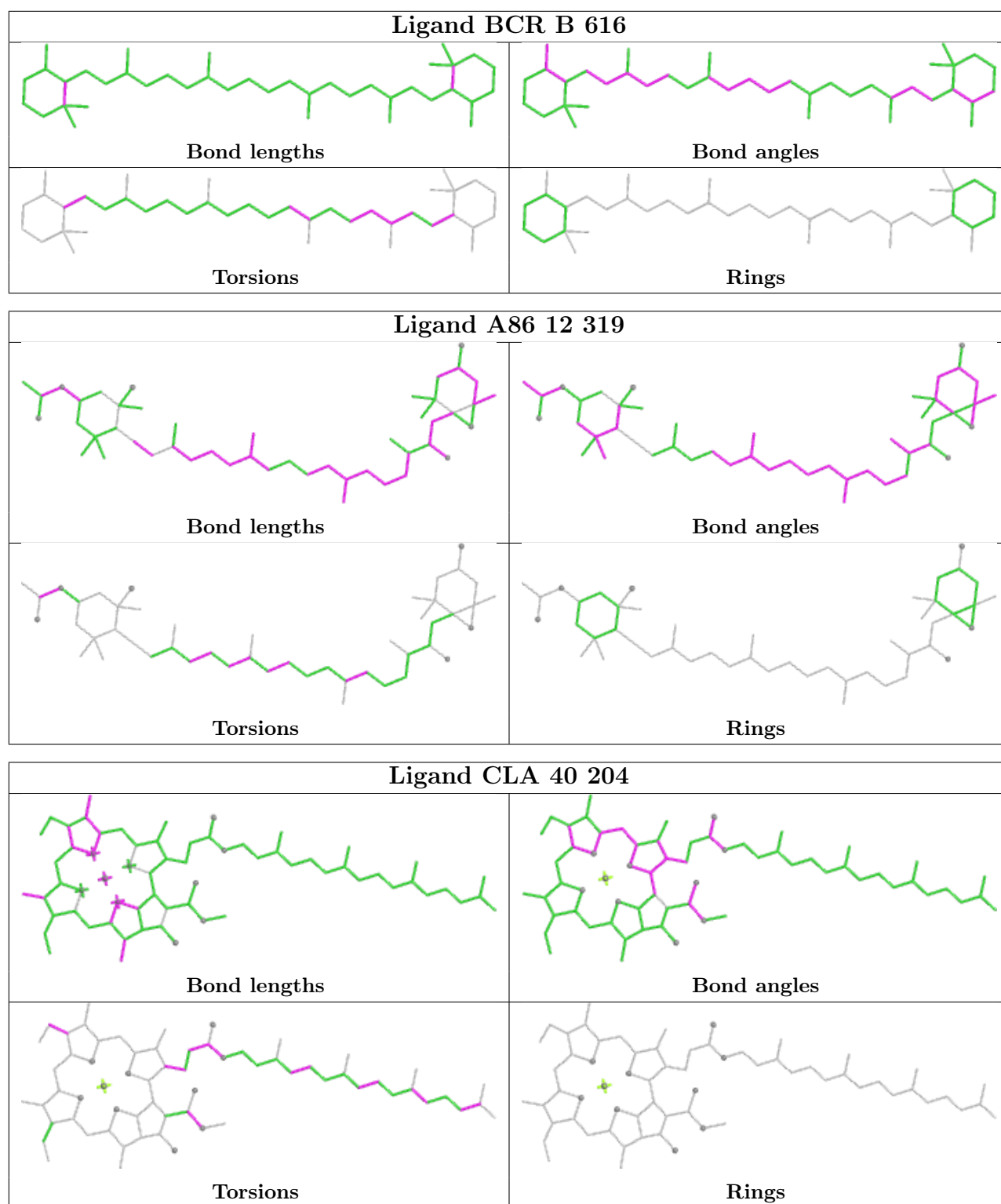


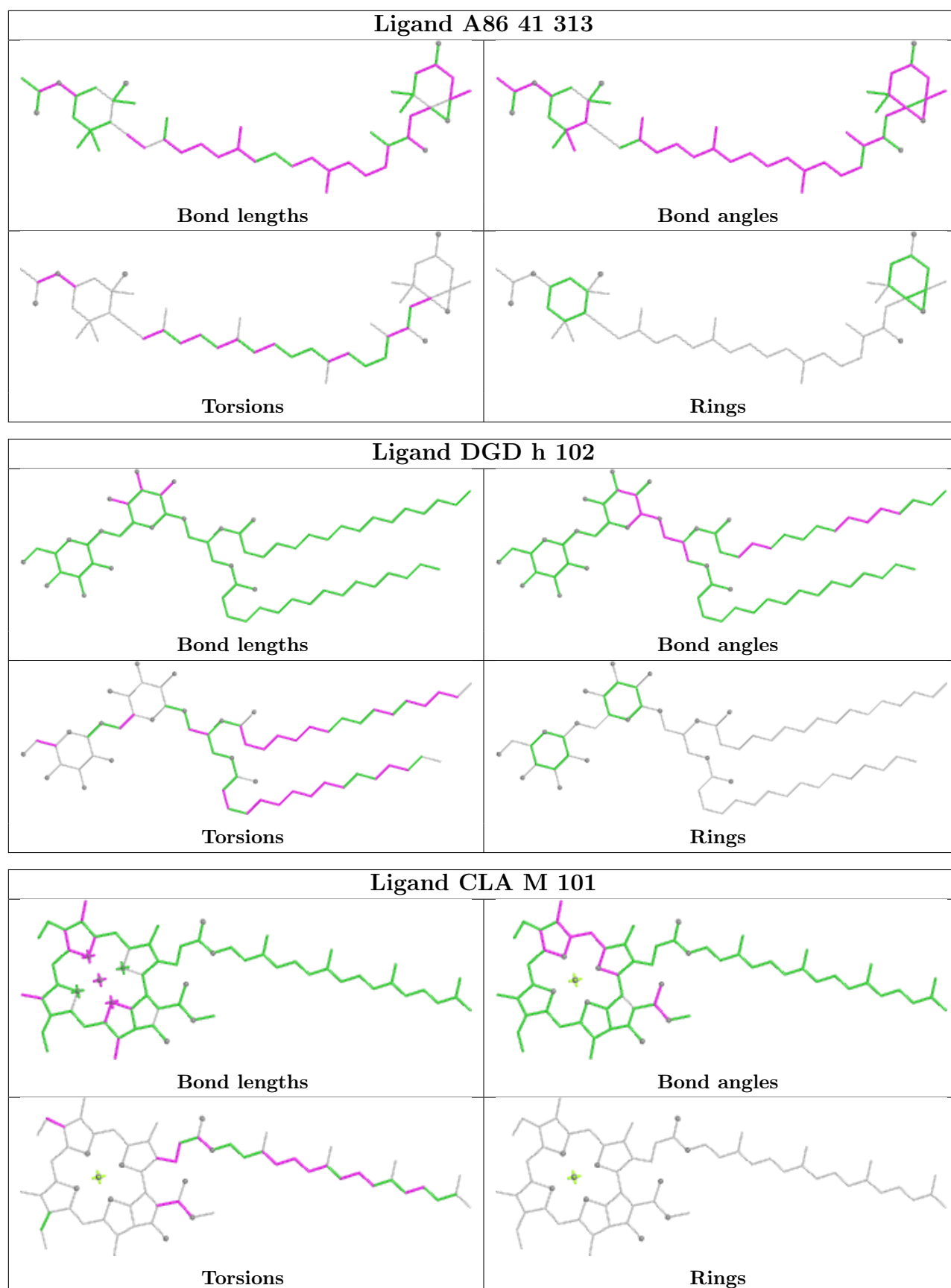
Ligand CLA 34 304			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

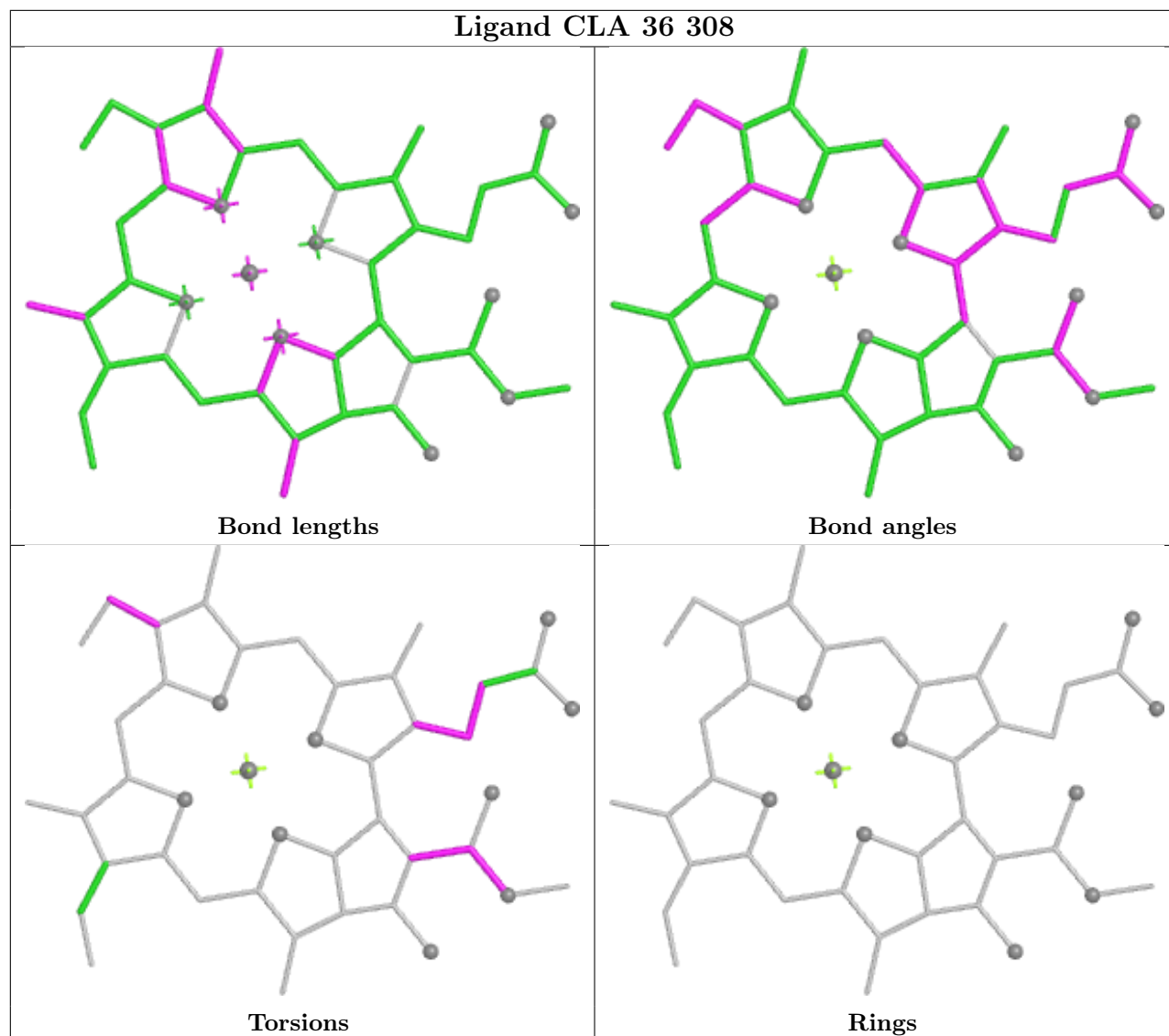
Ligand PL9 D 404			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

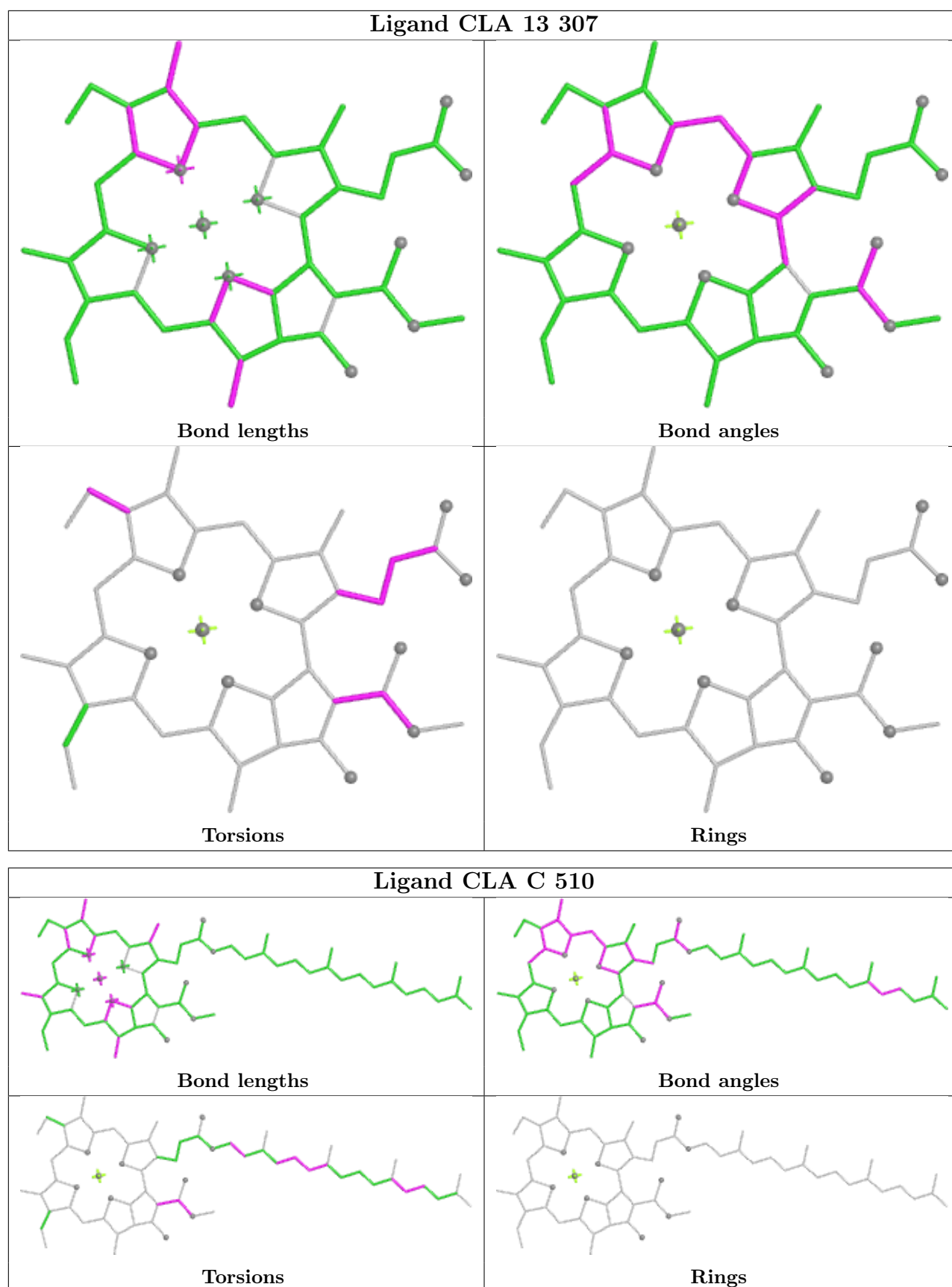


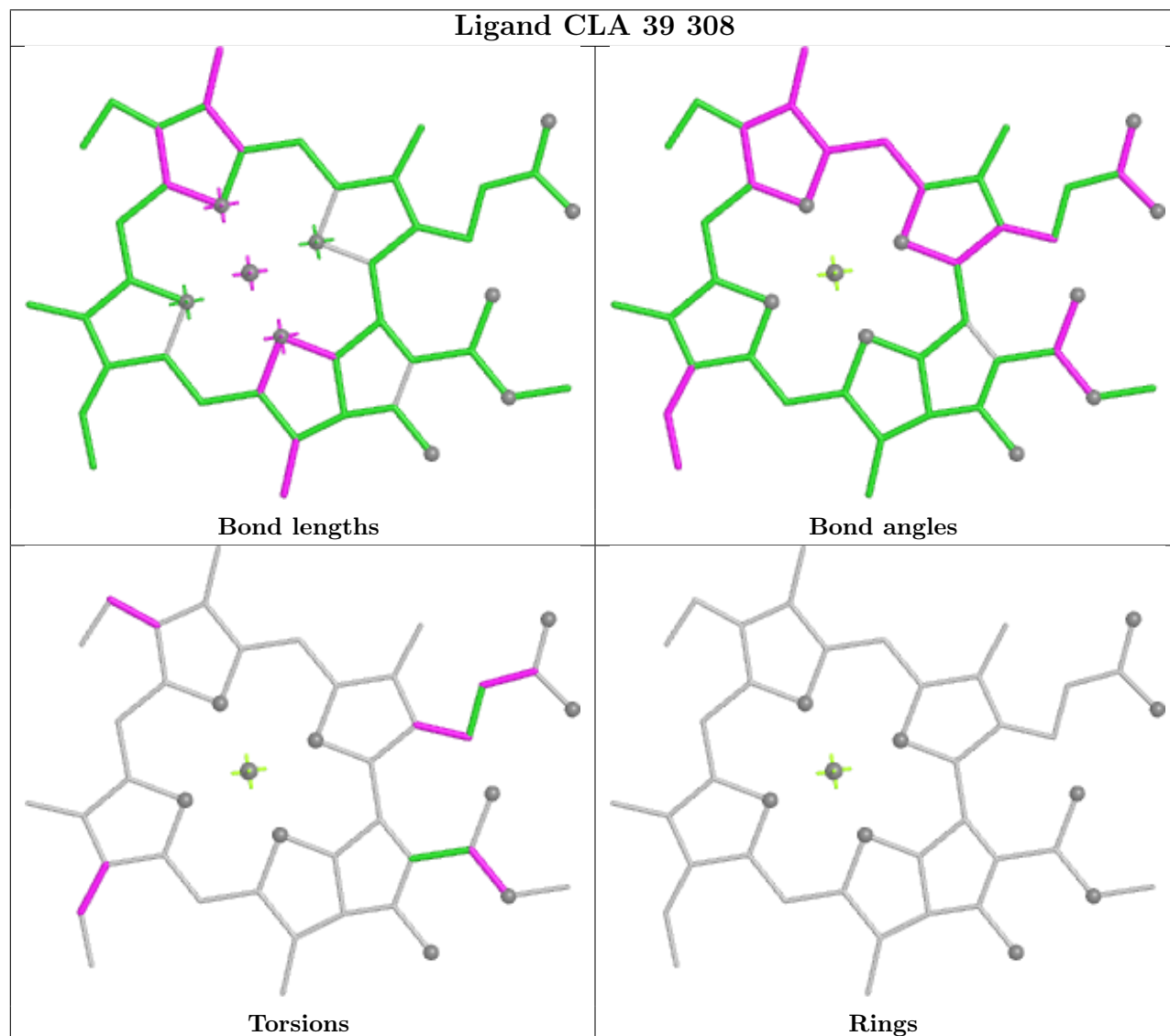
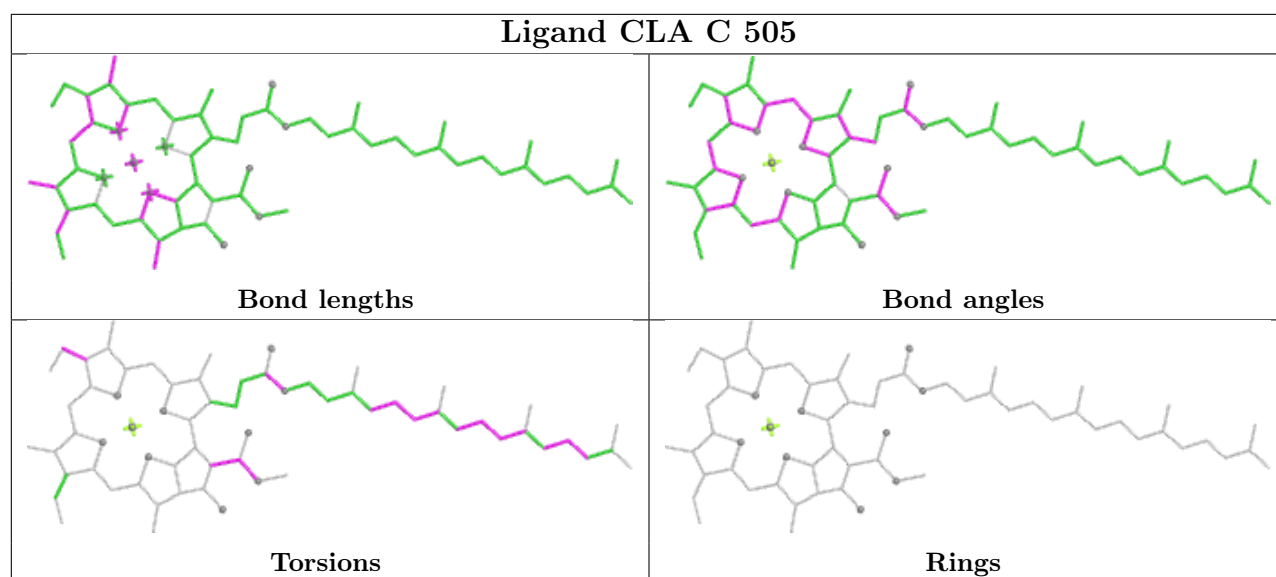


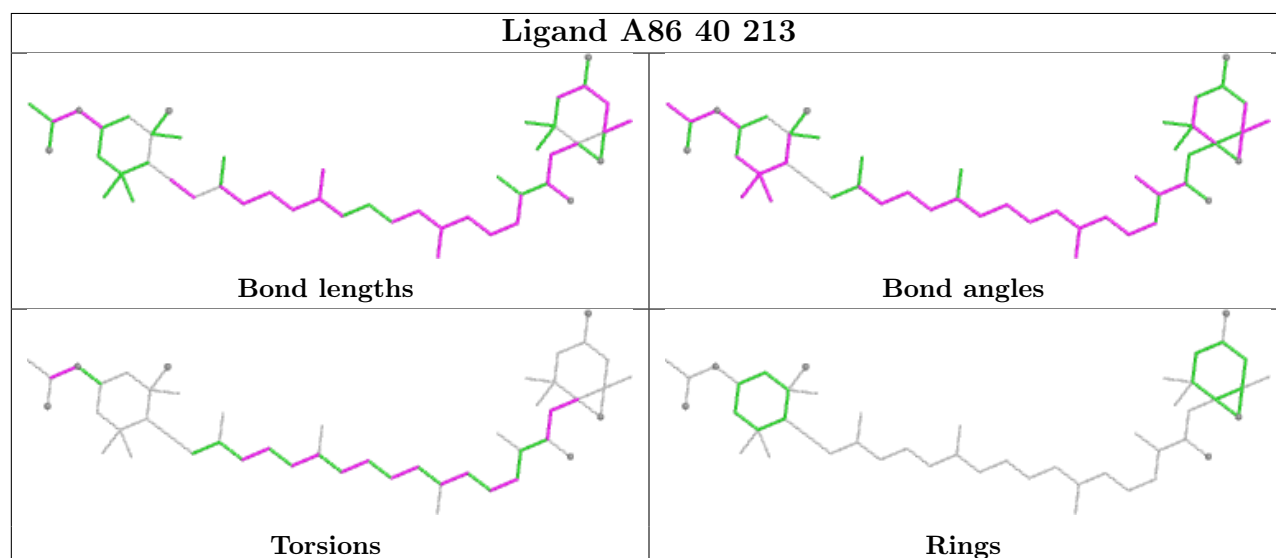
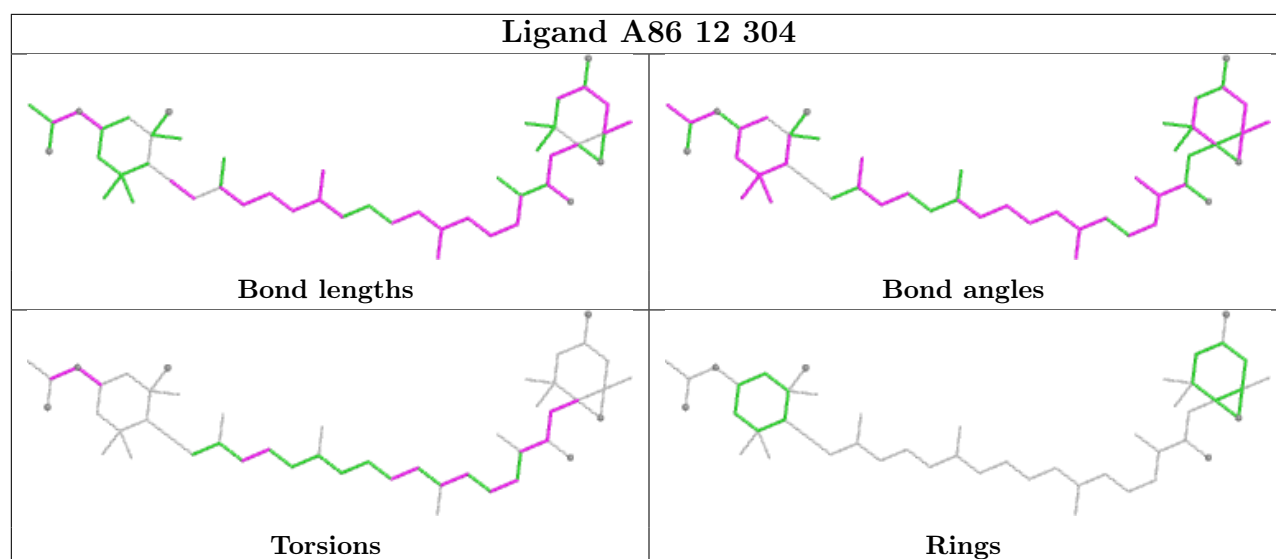


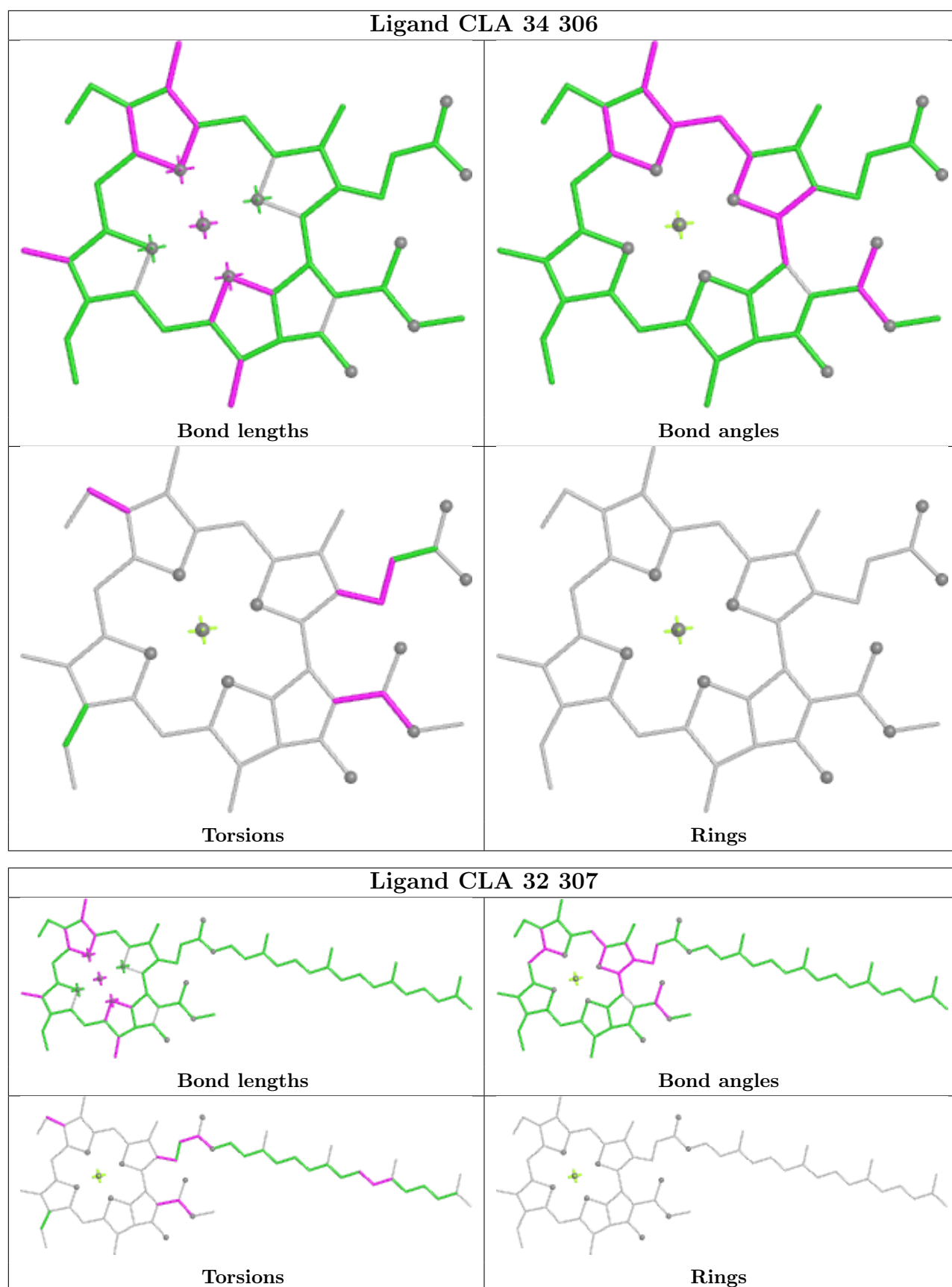


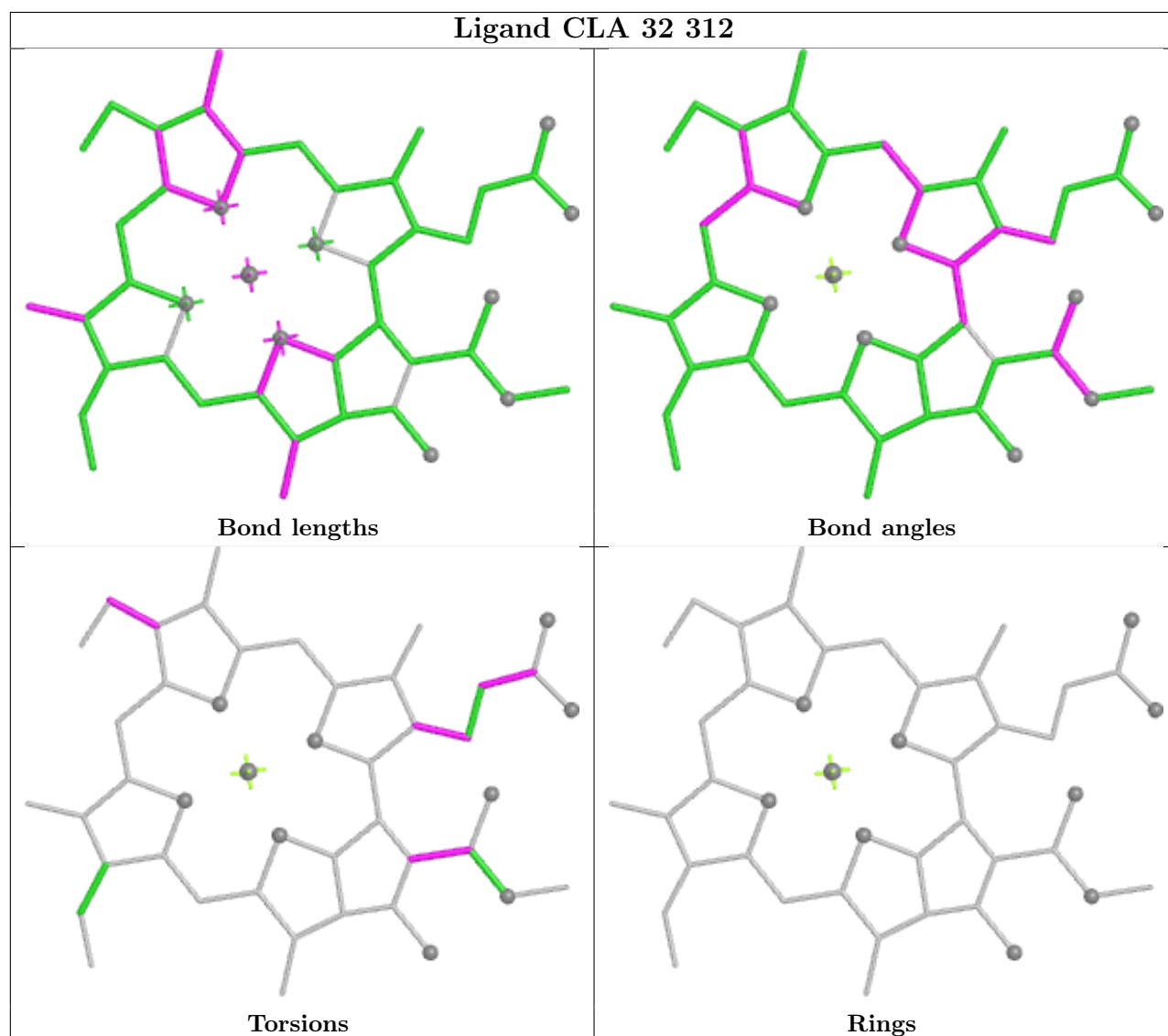
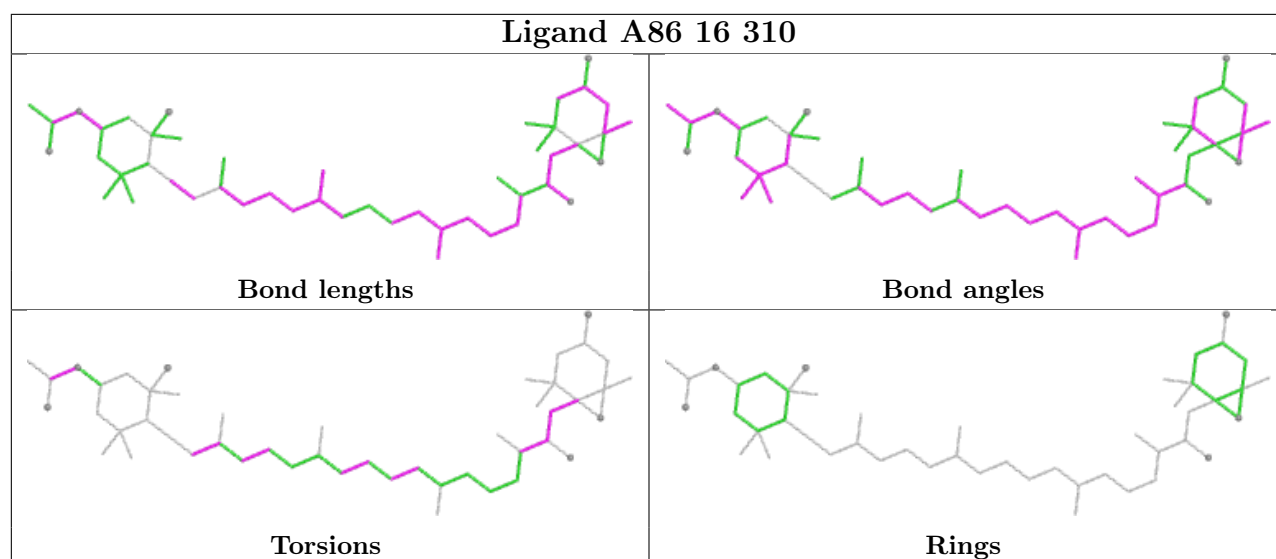


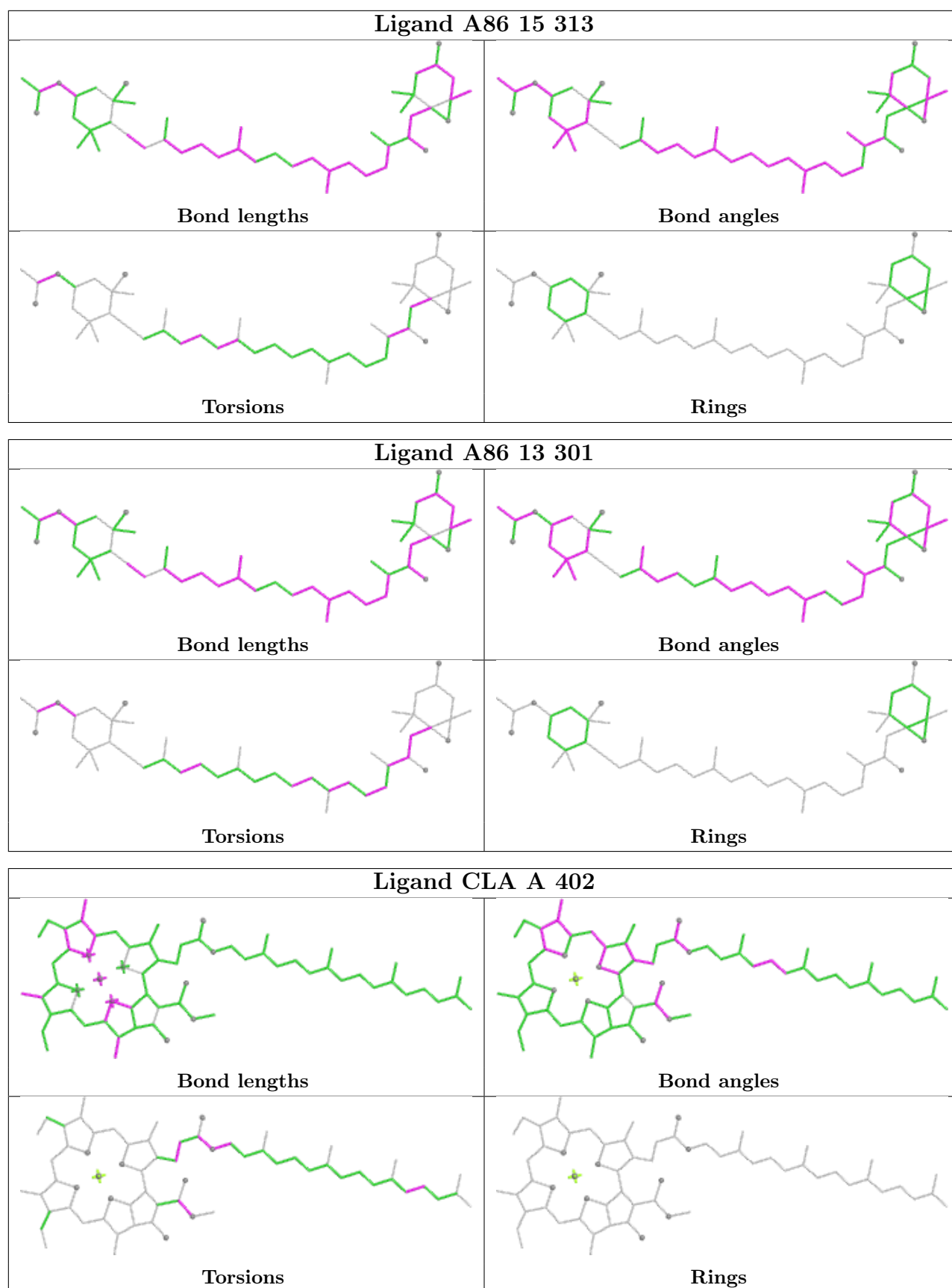


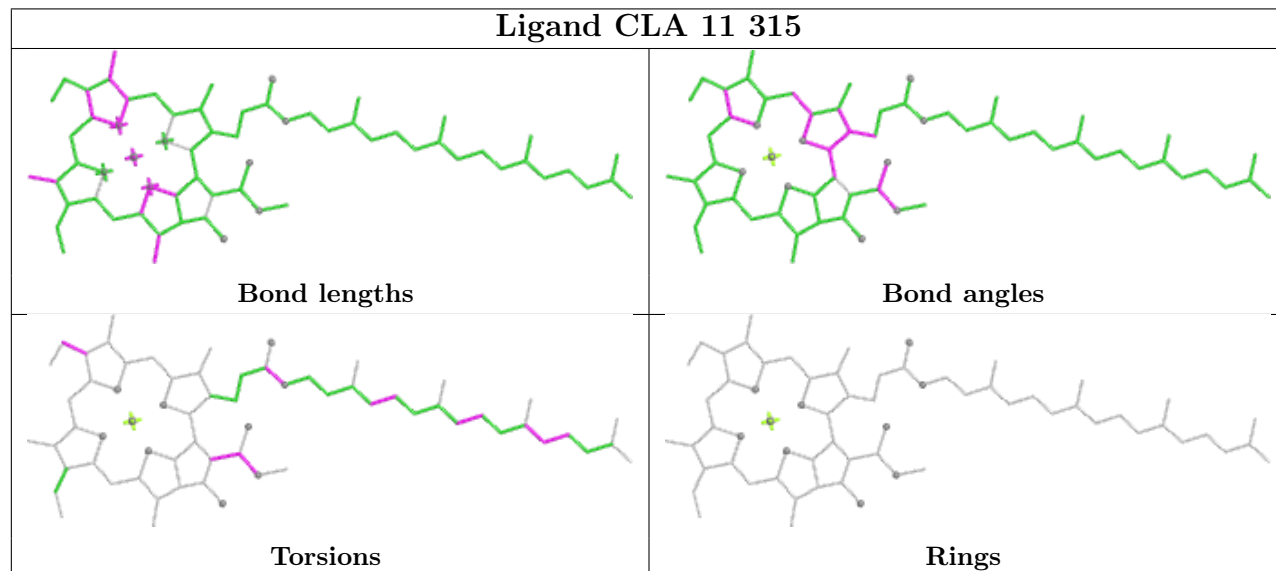
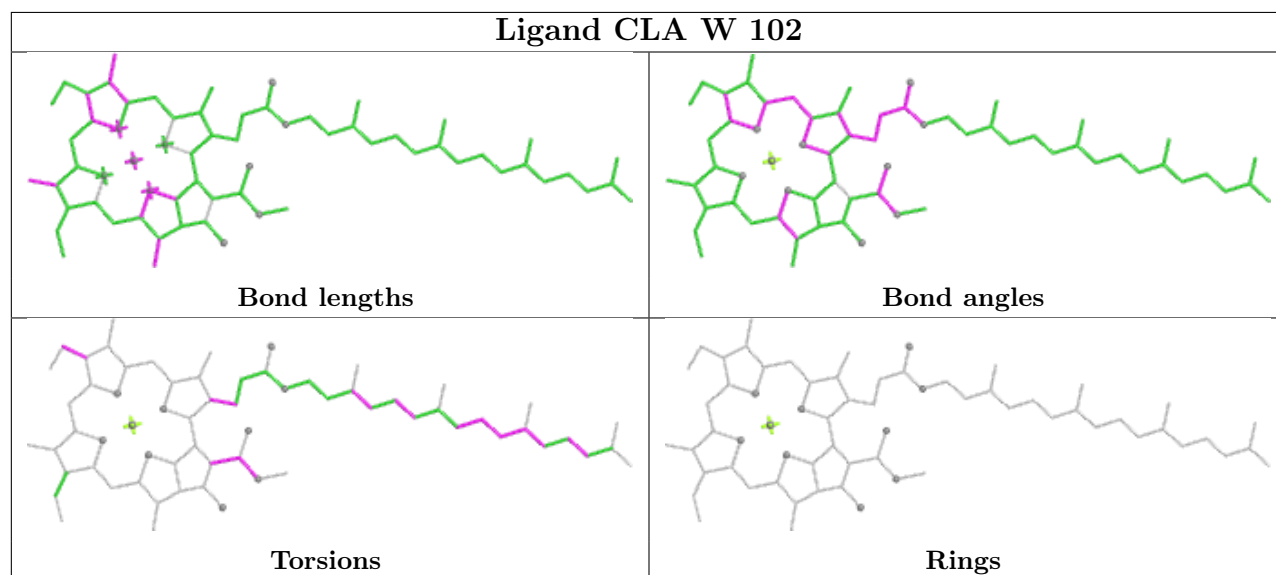
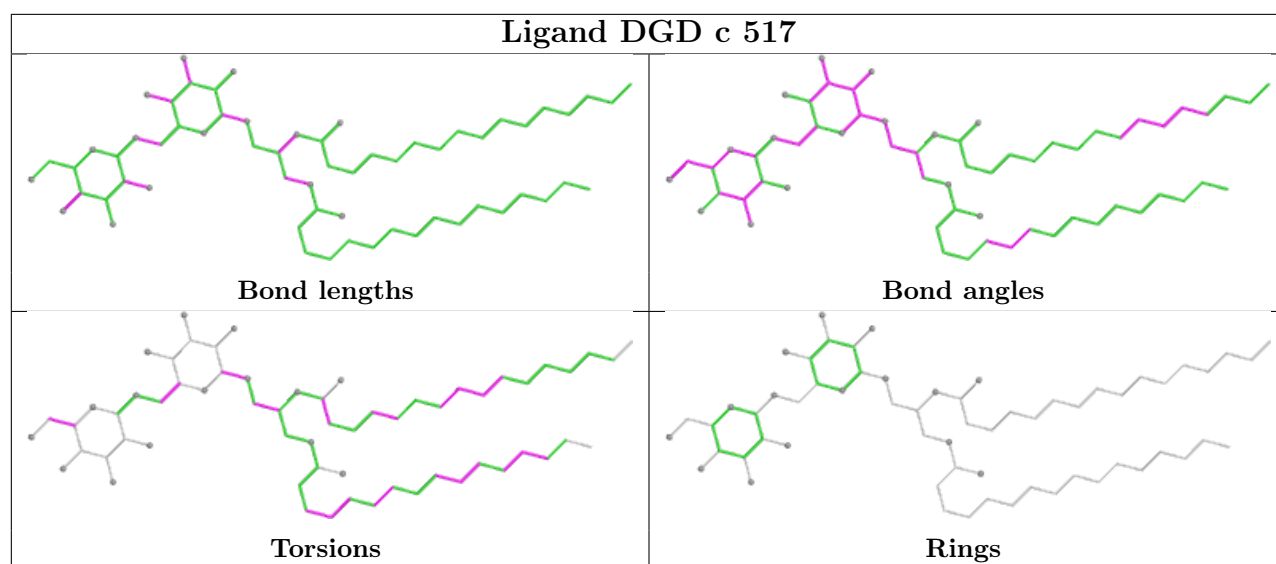


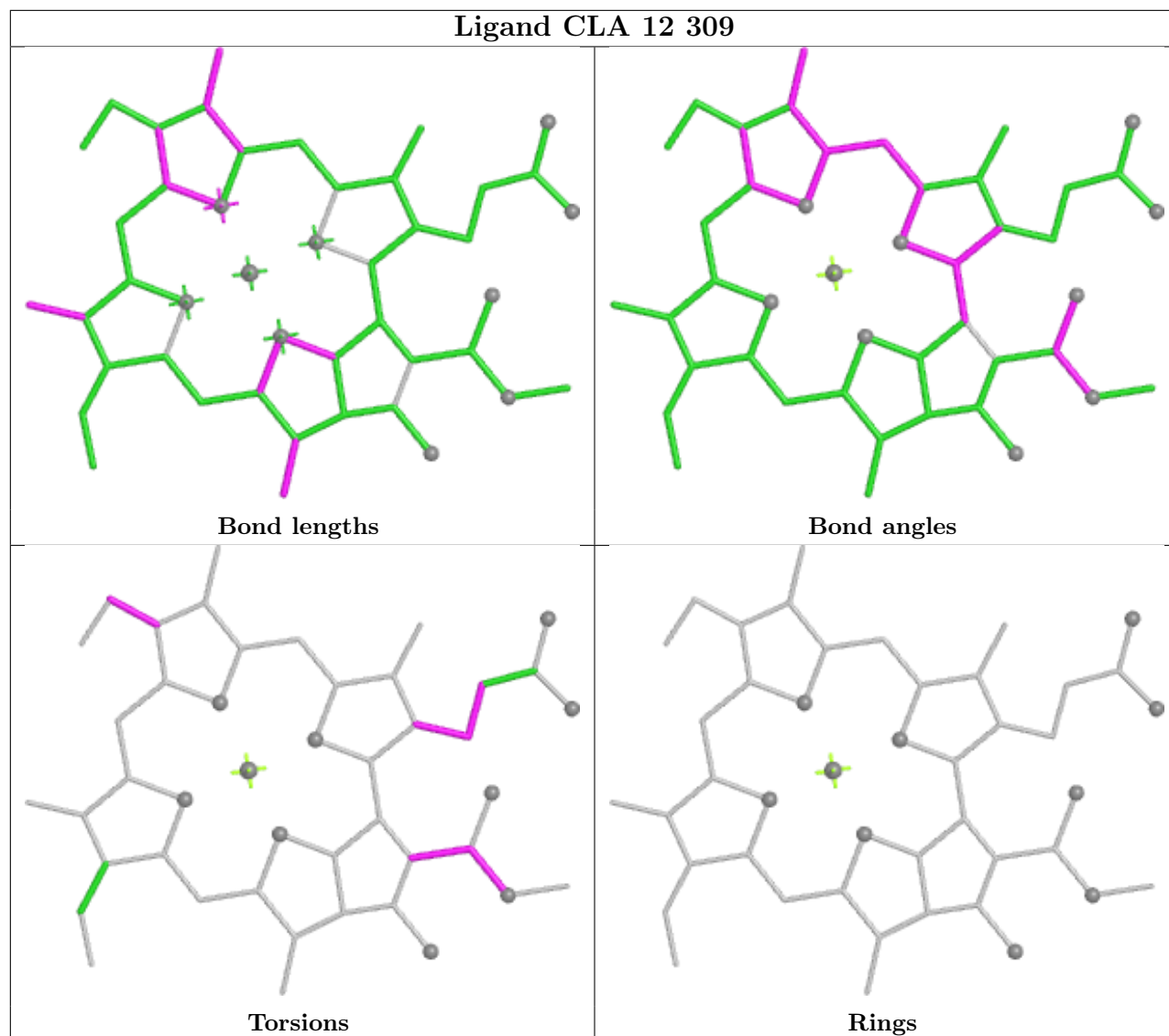


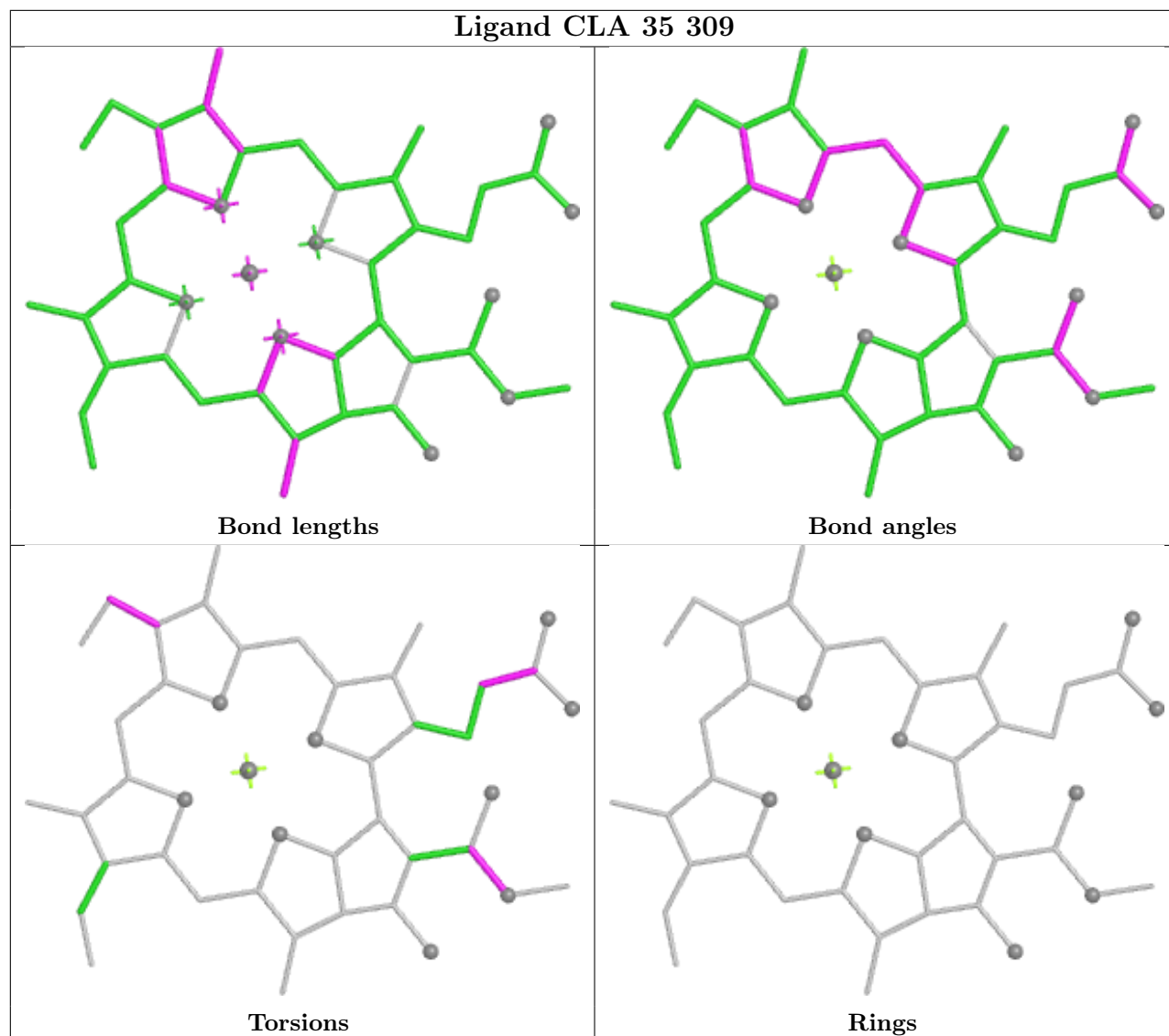


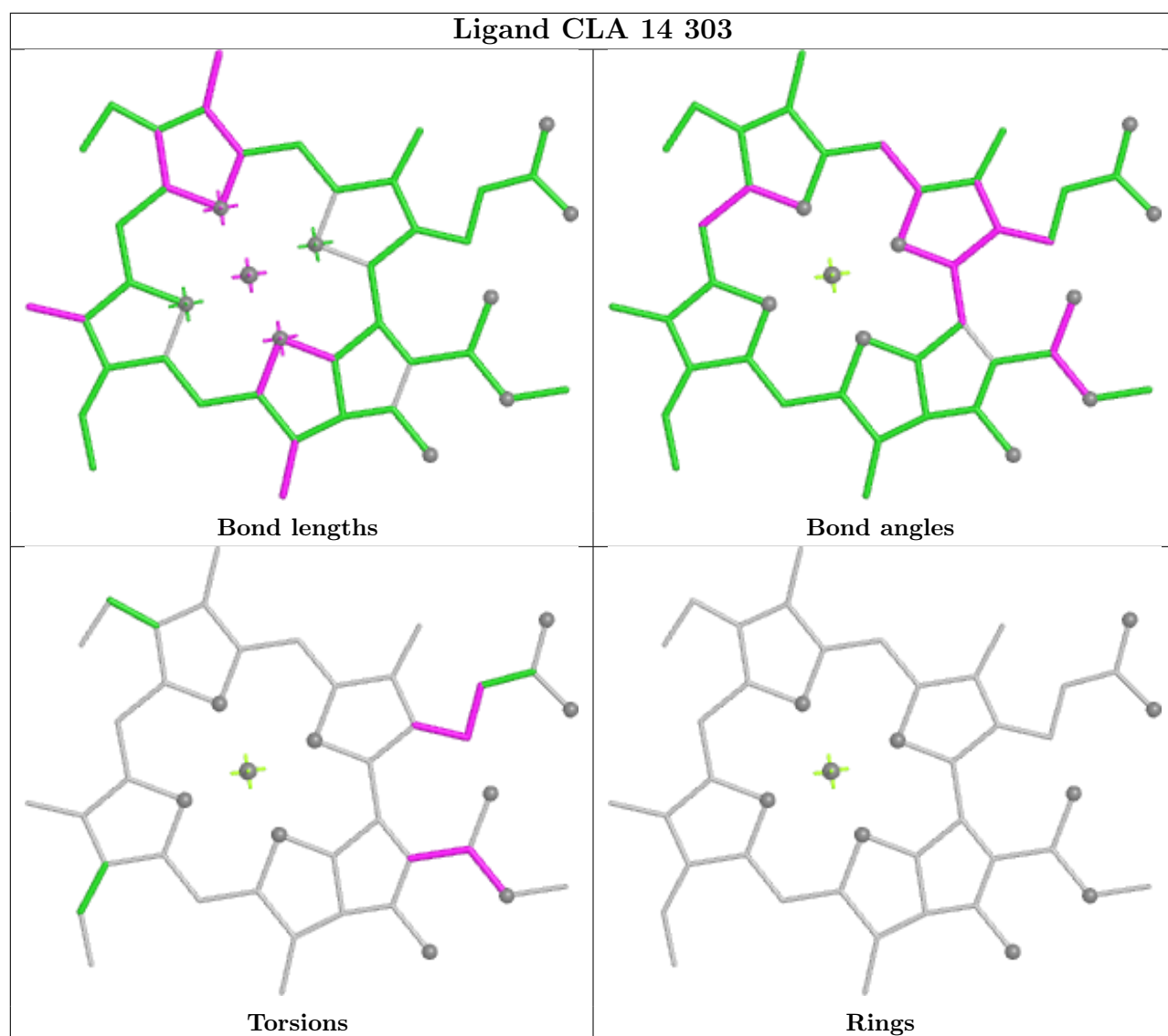


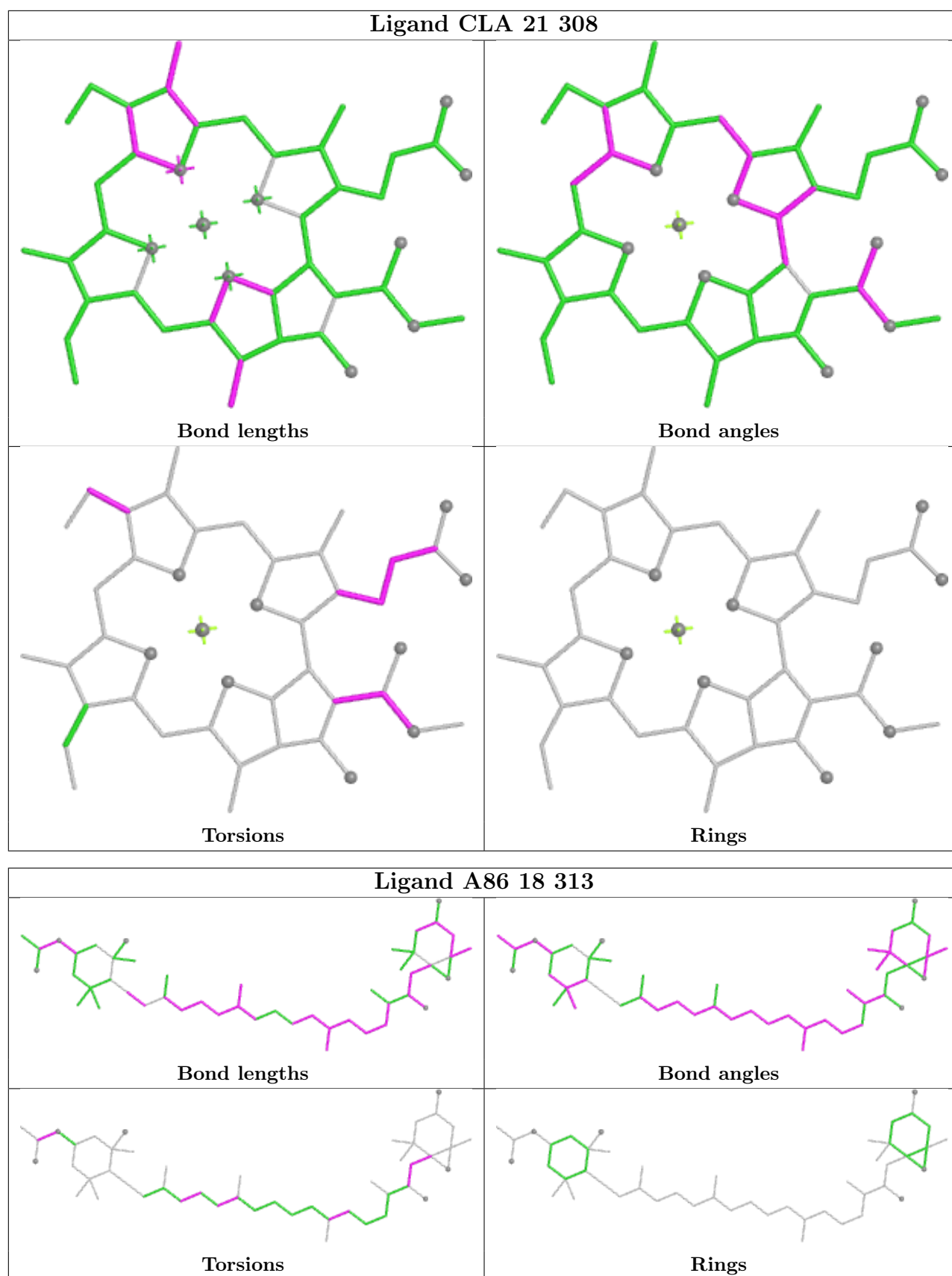


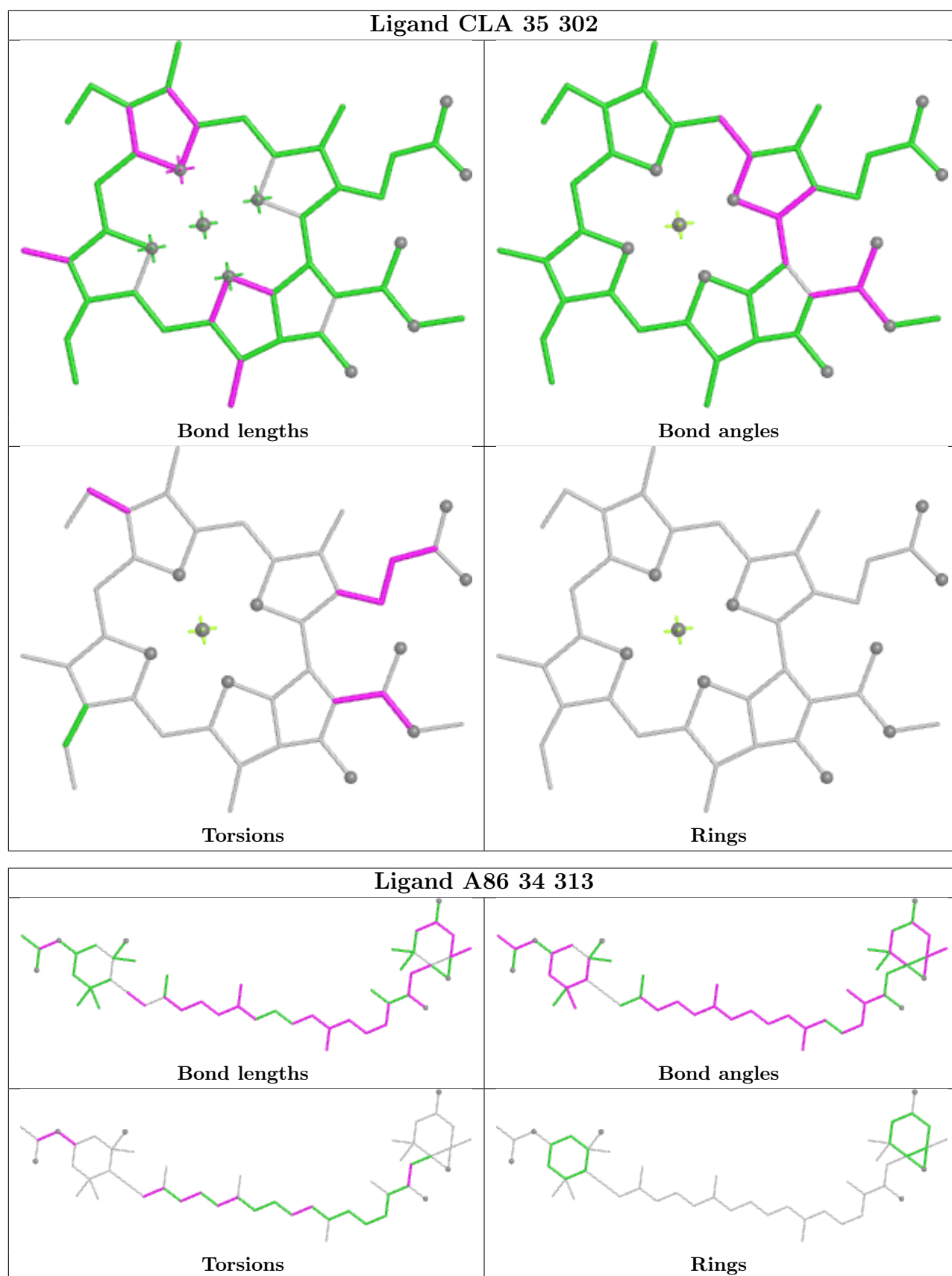


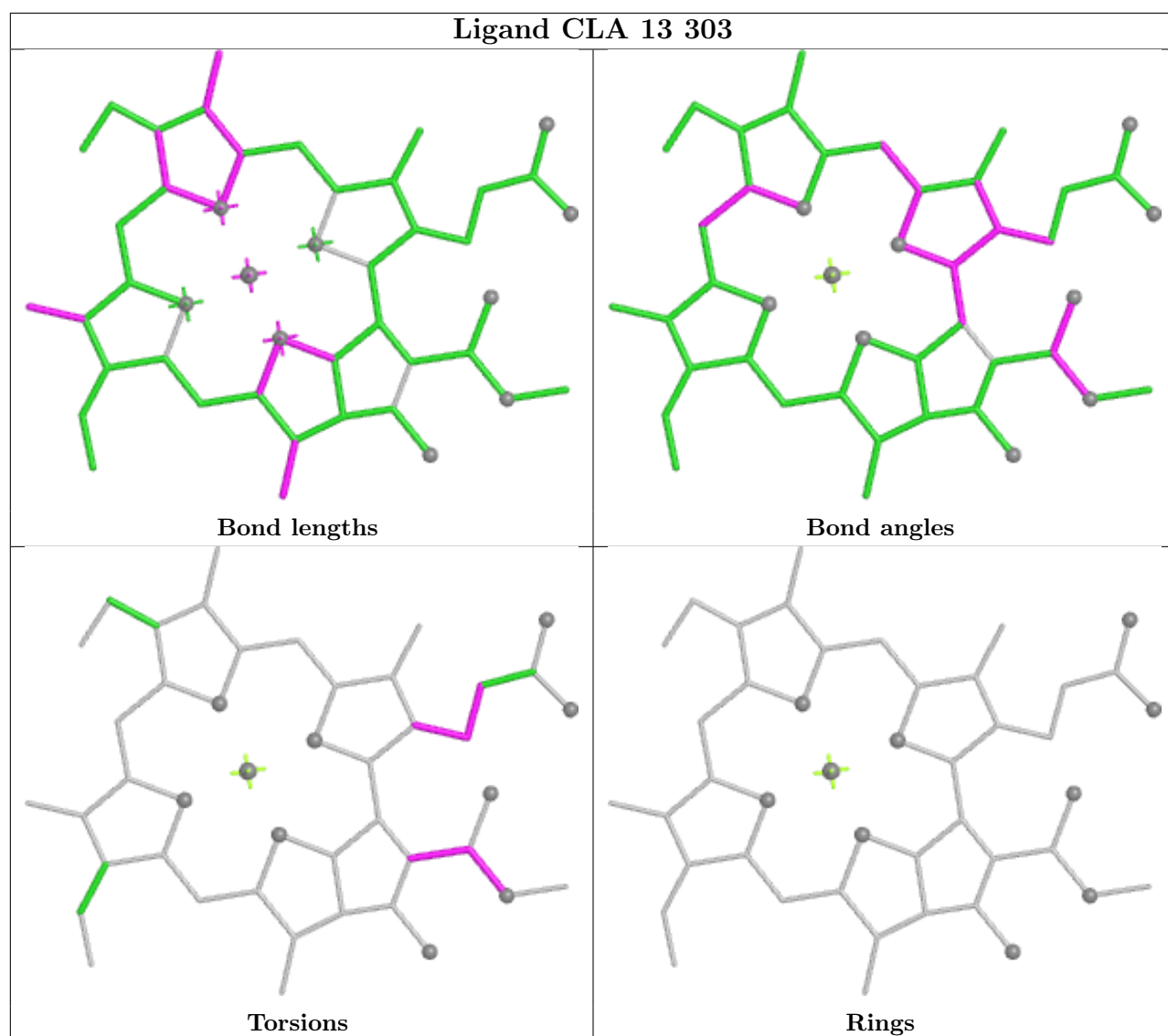


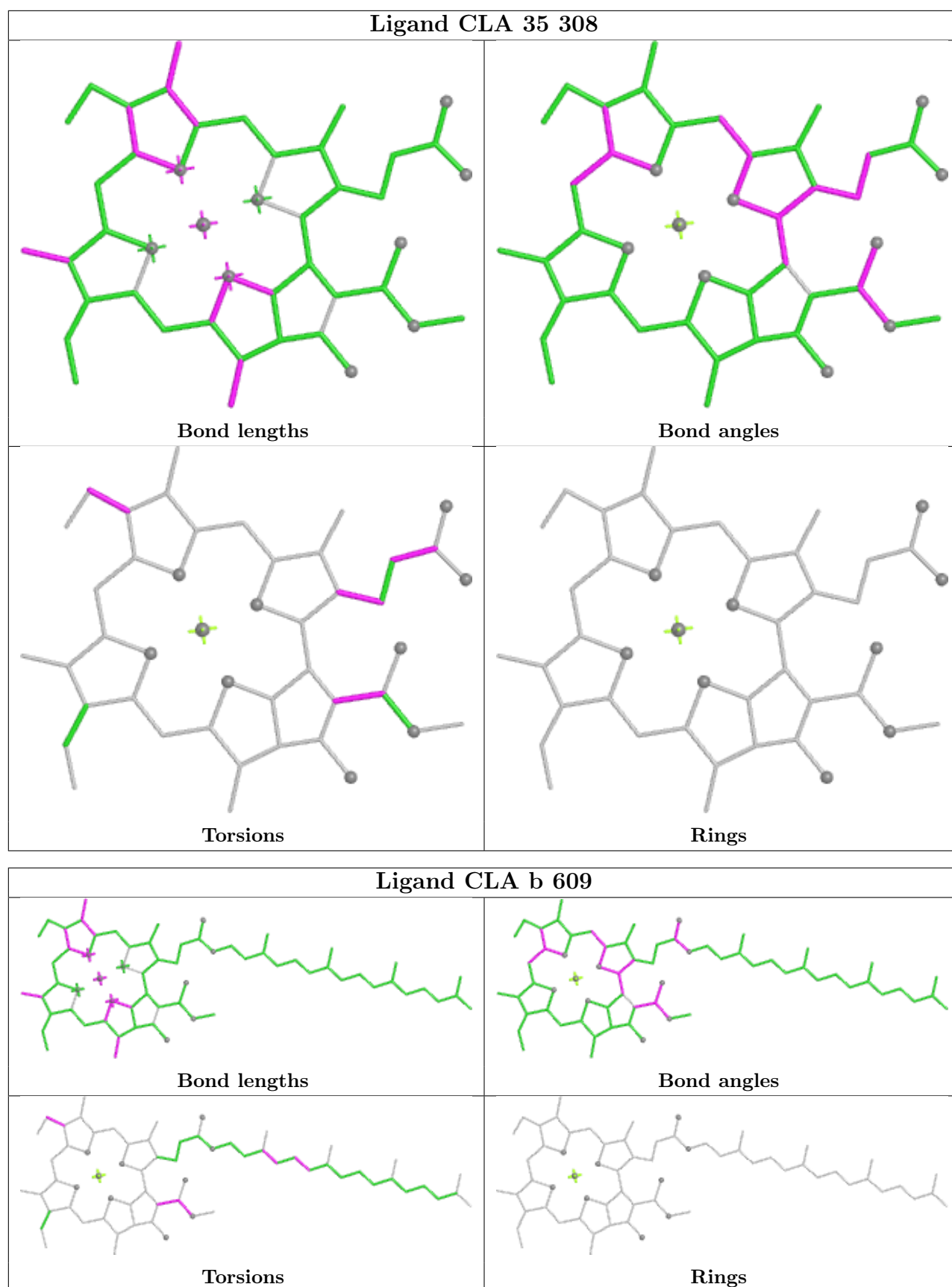


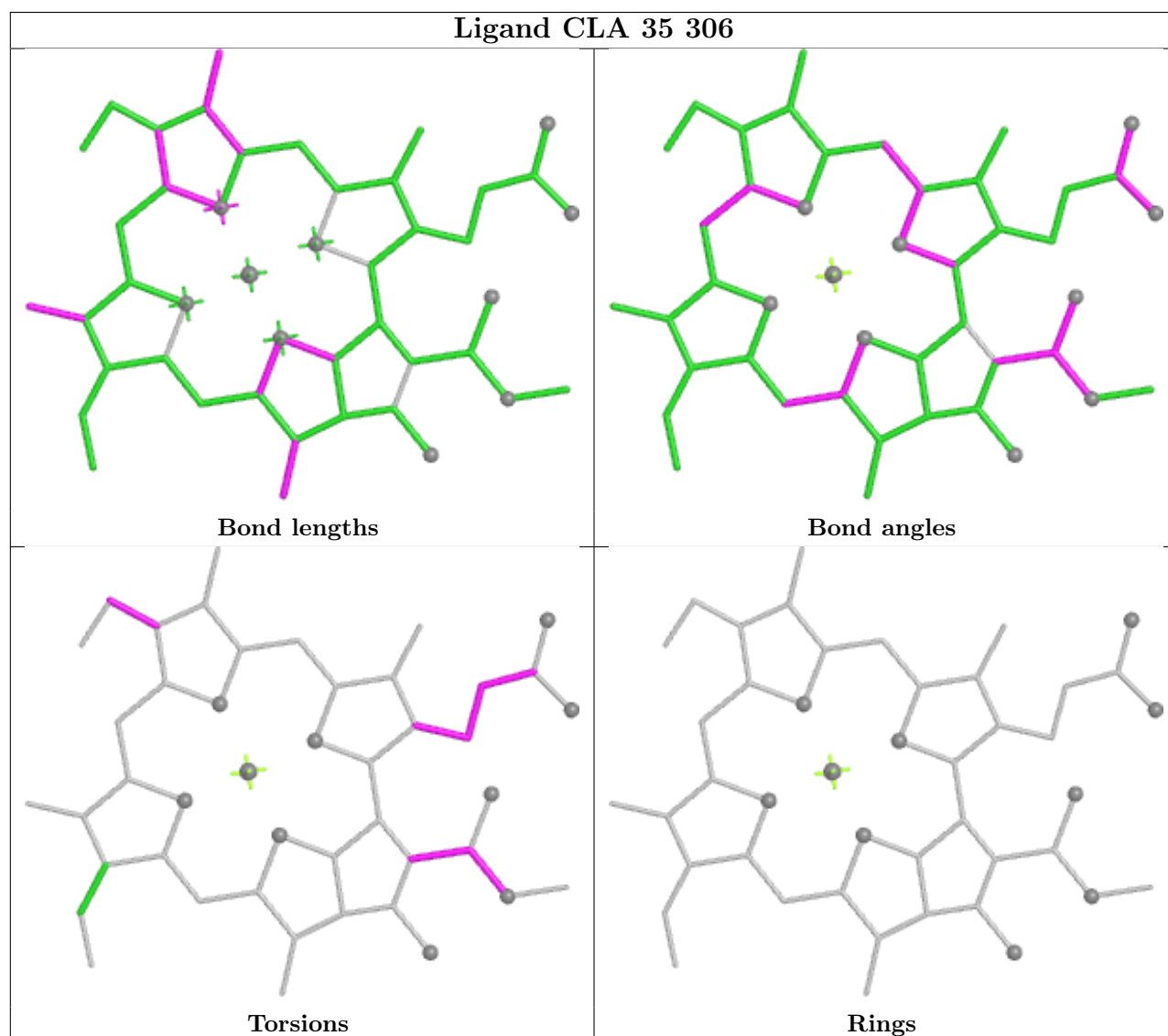
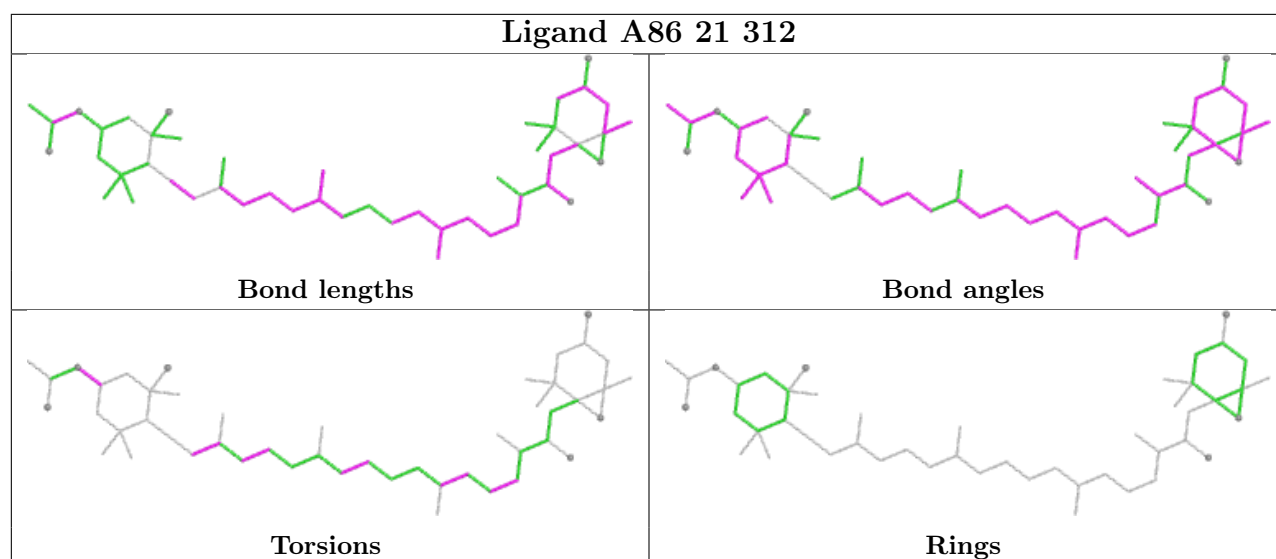


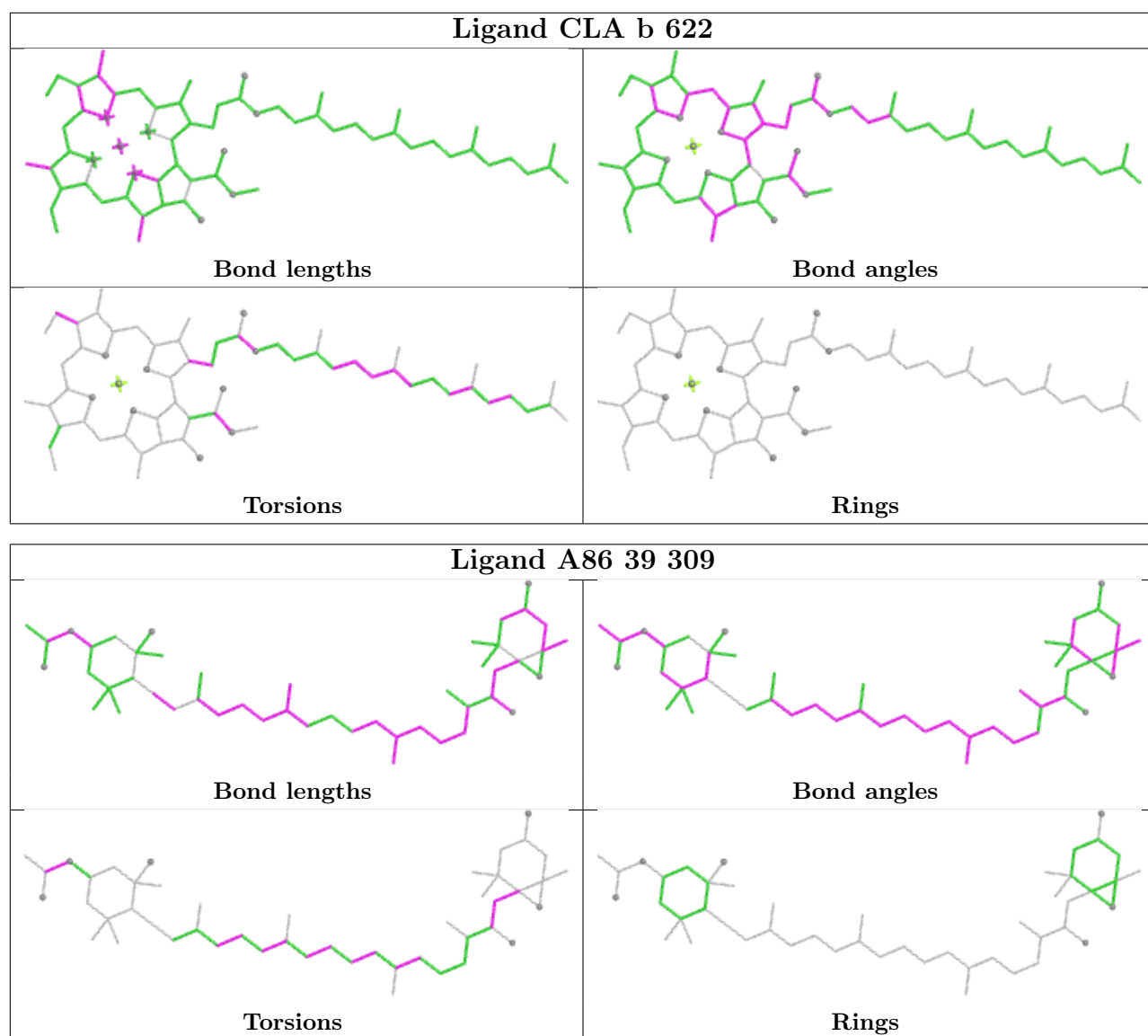


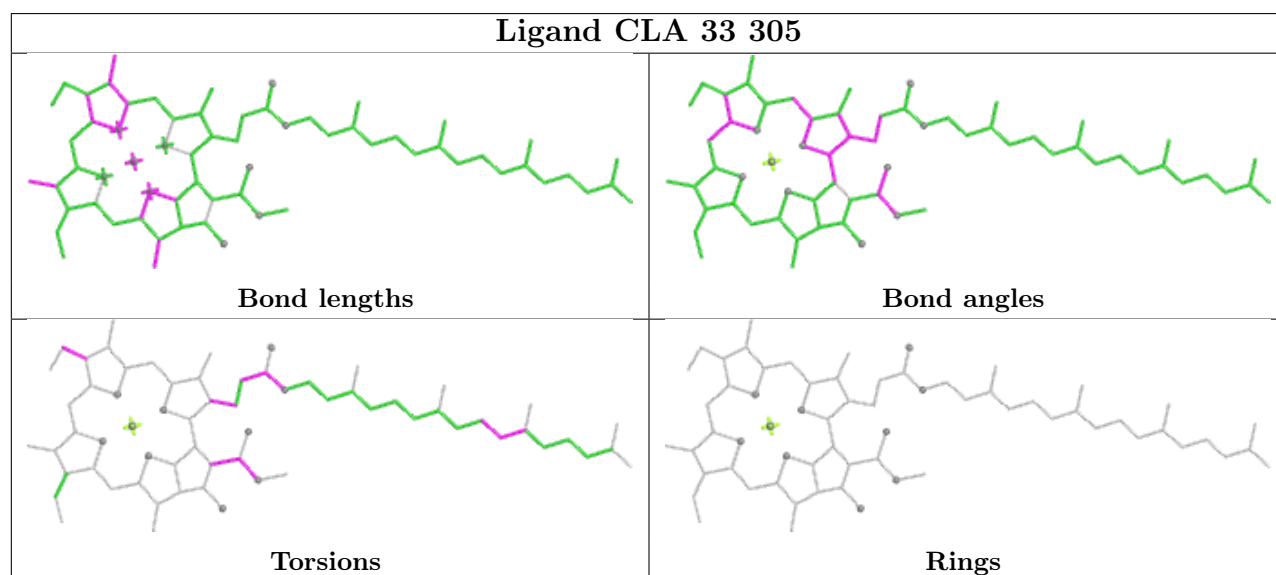
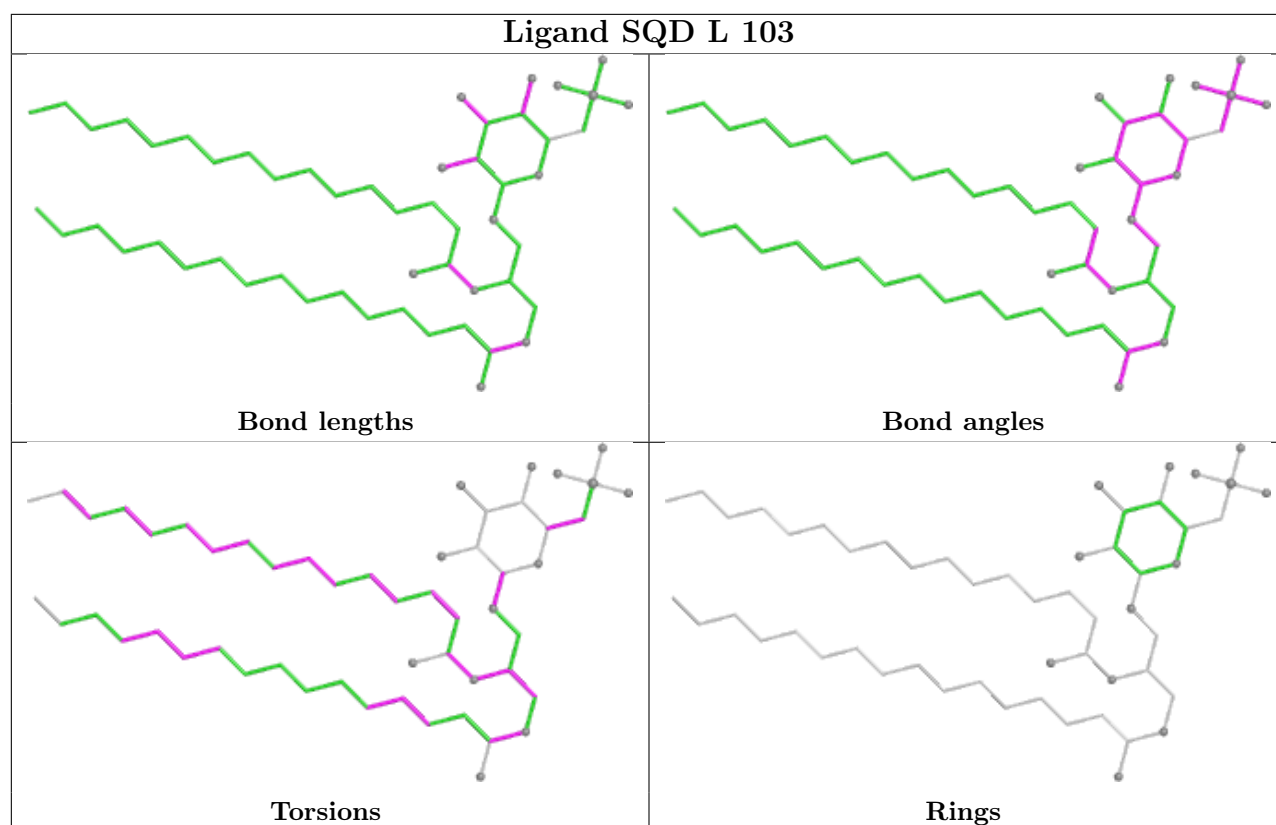


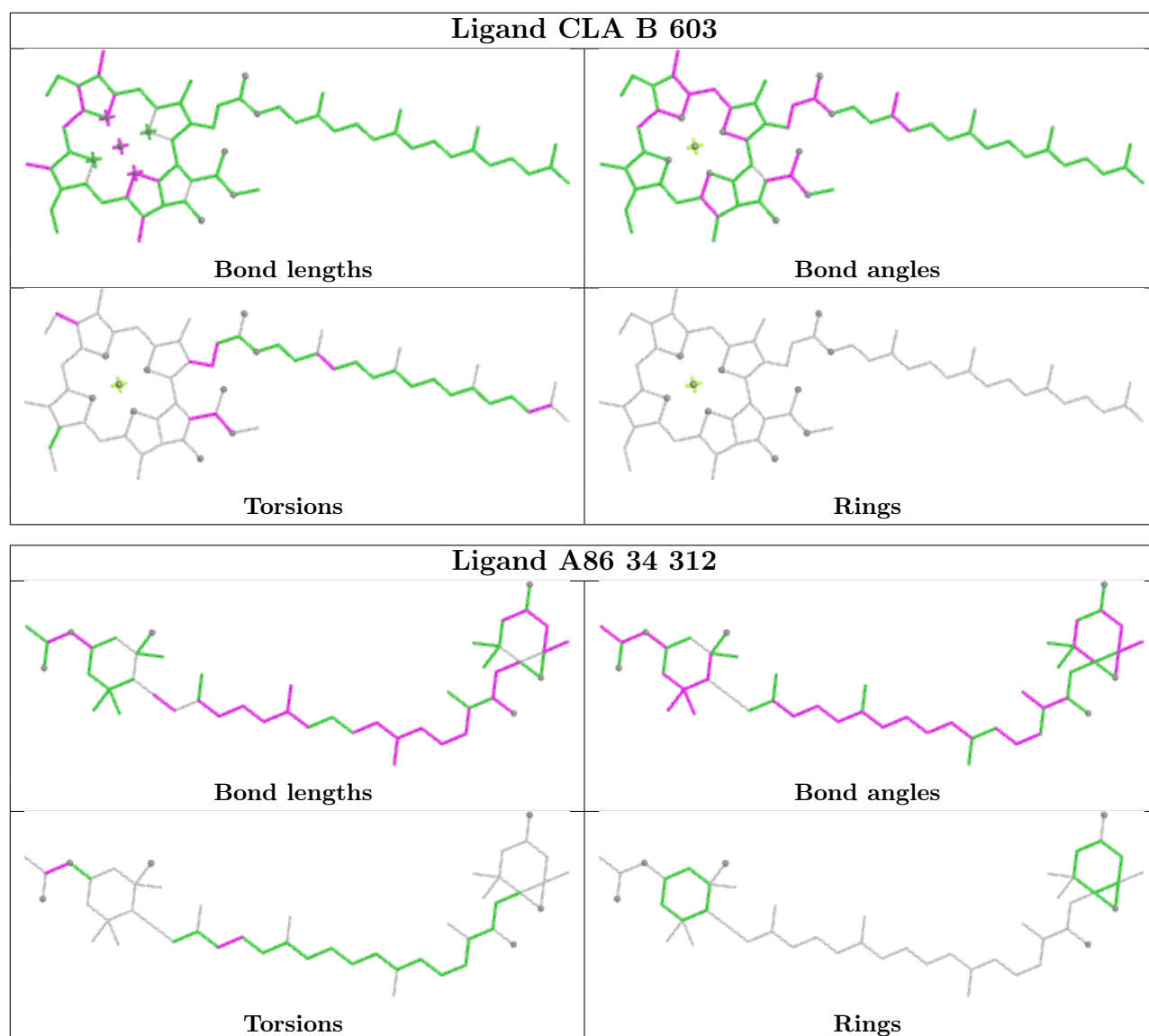


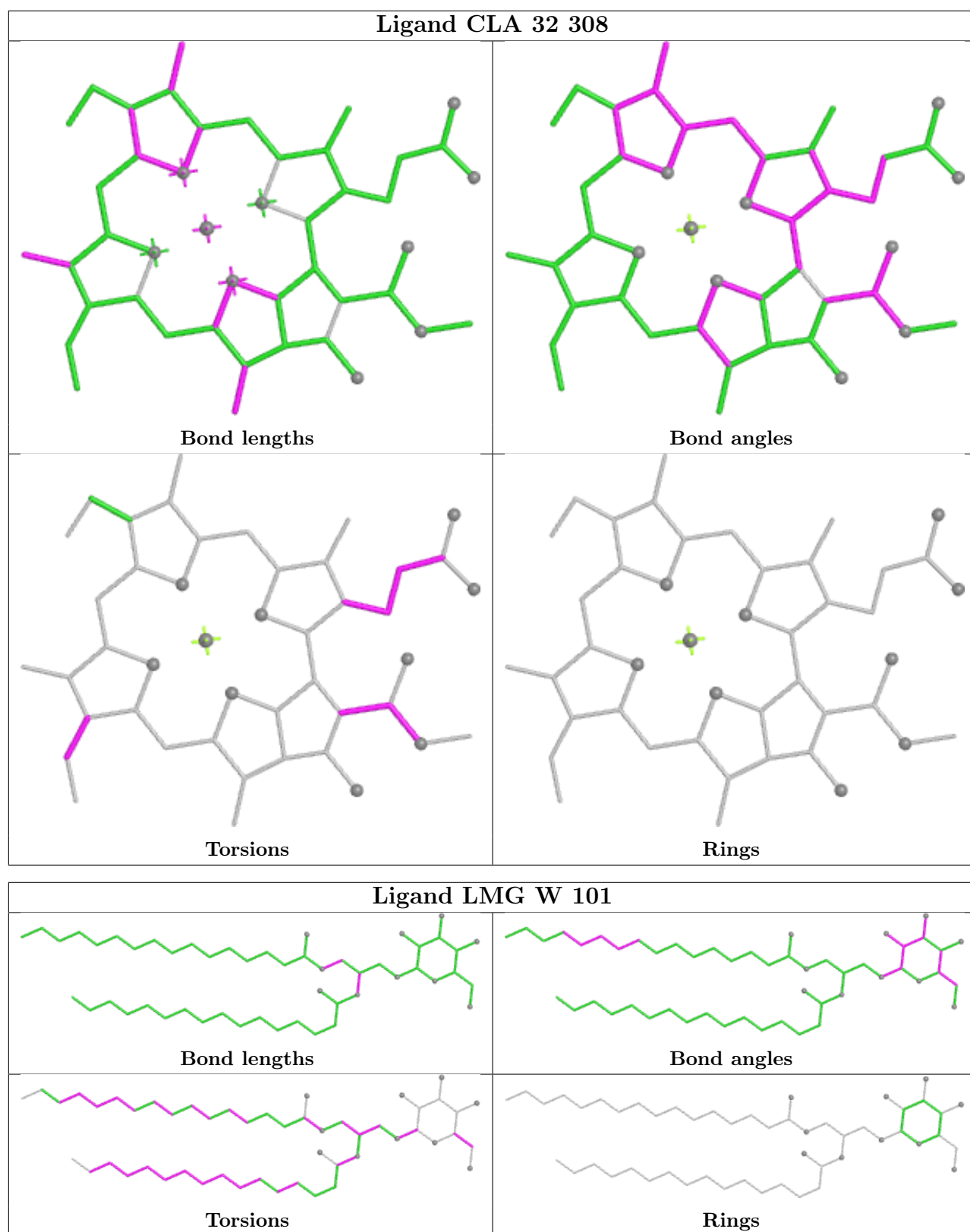


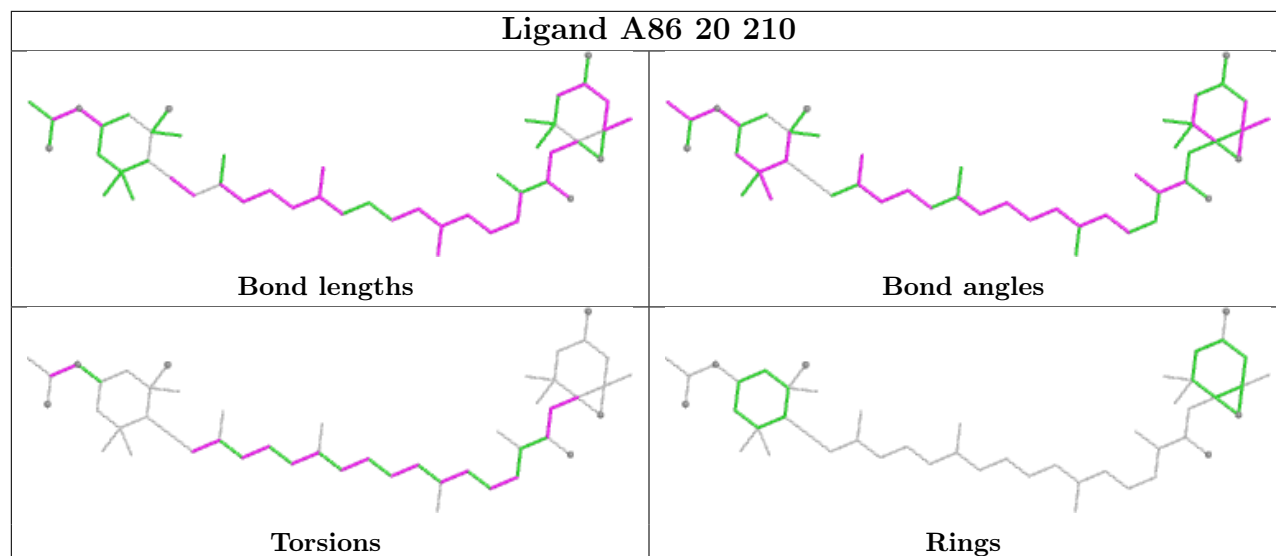
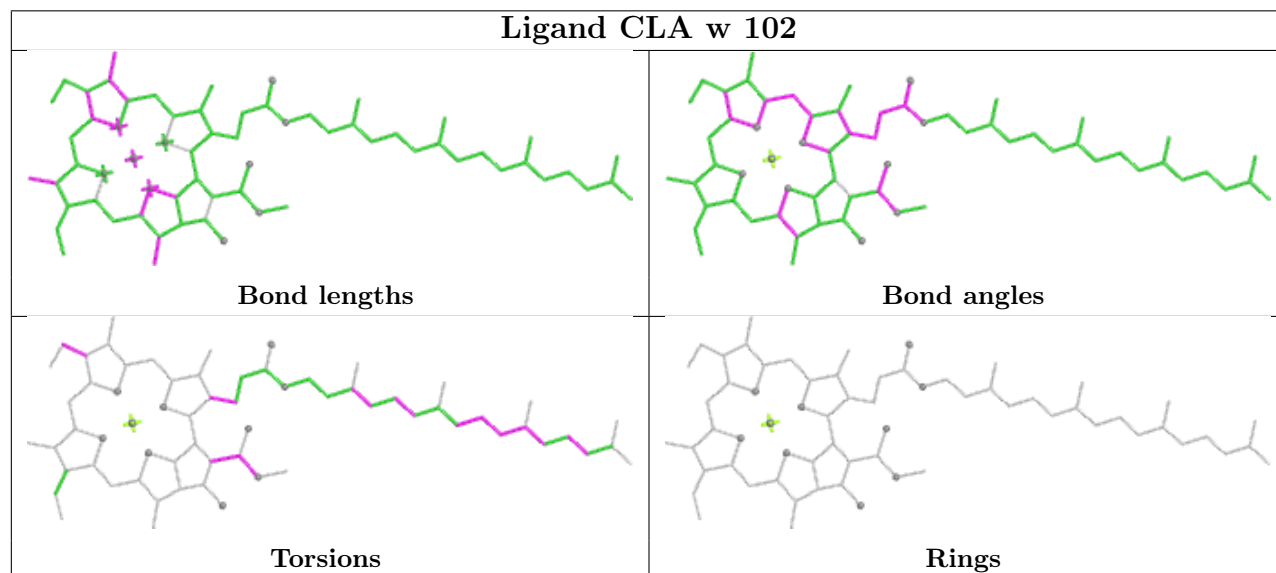
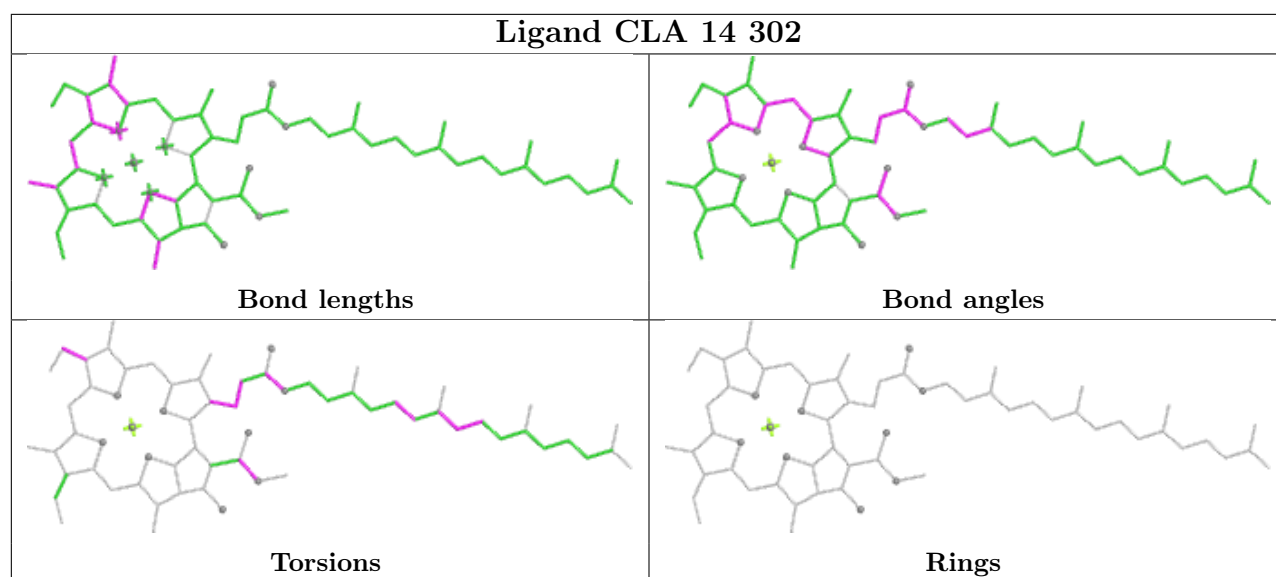


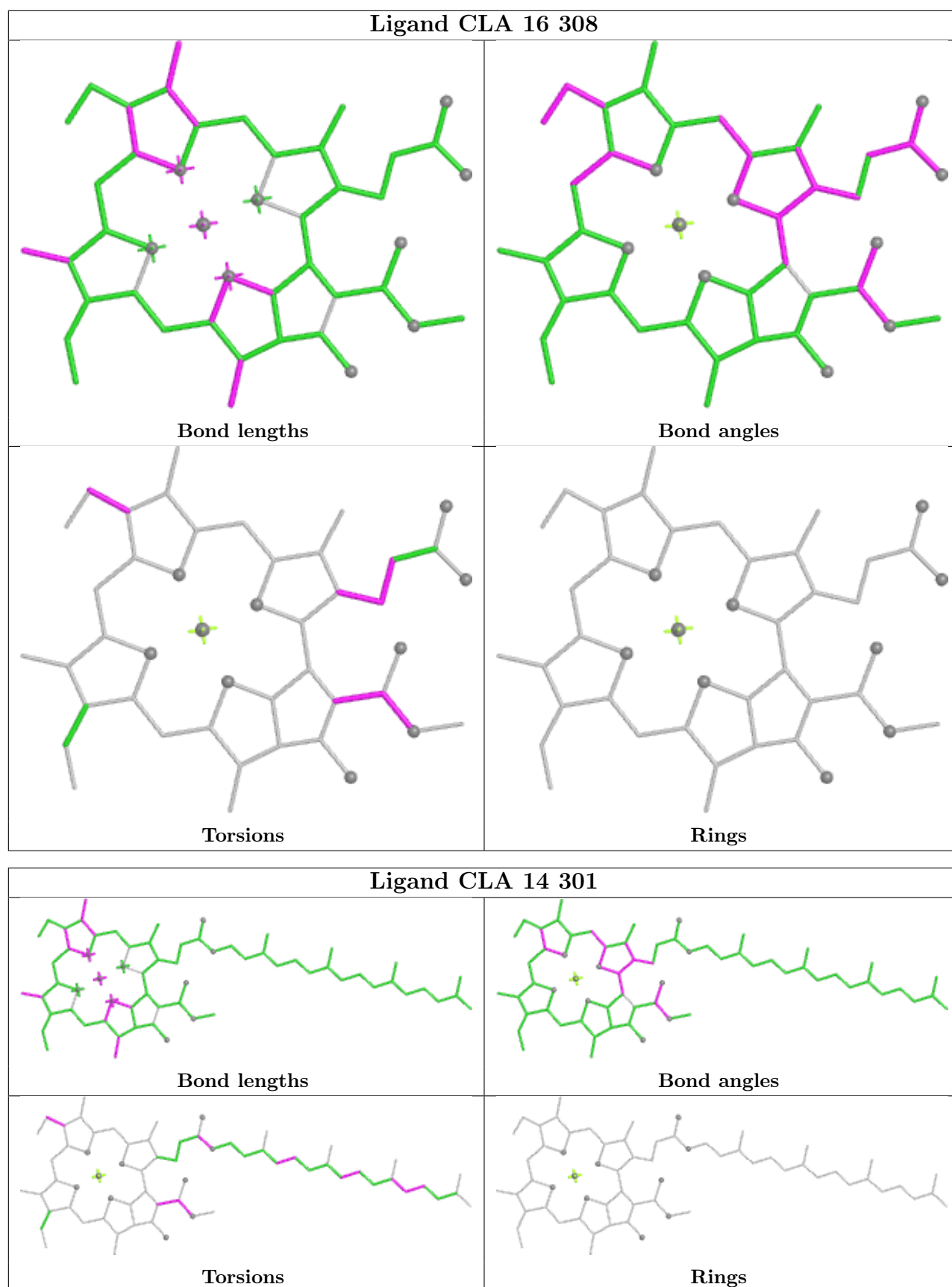


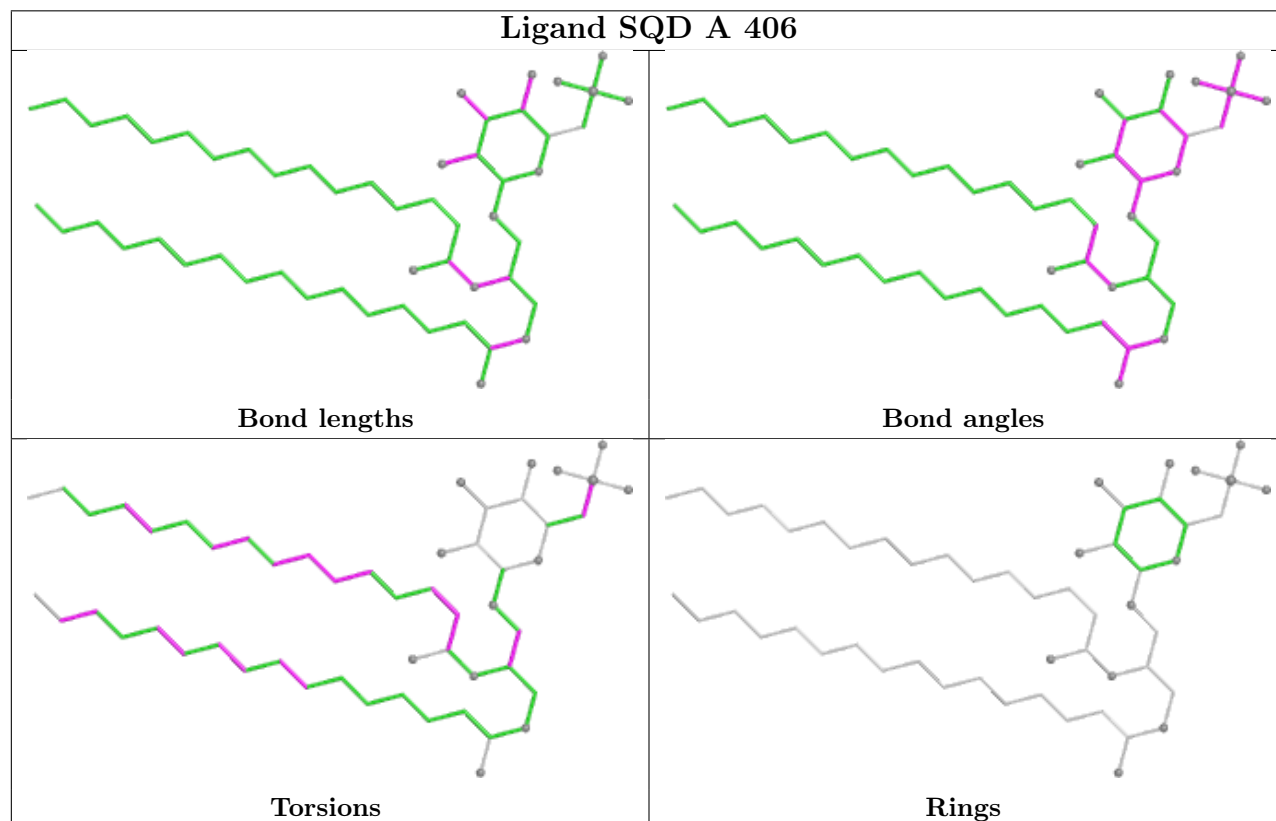
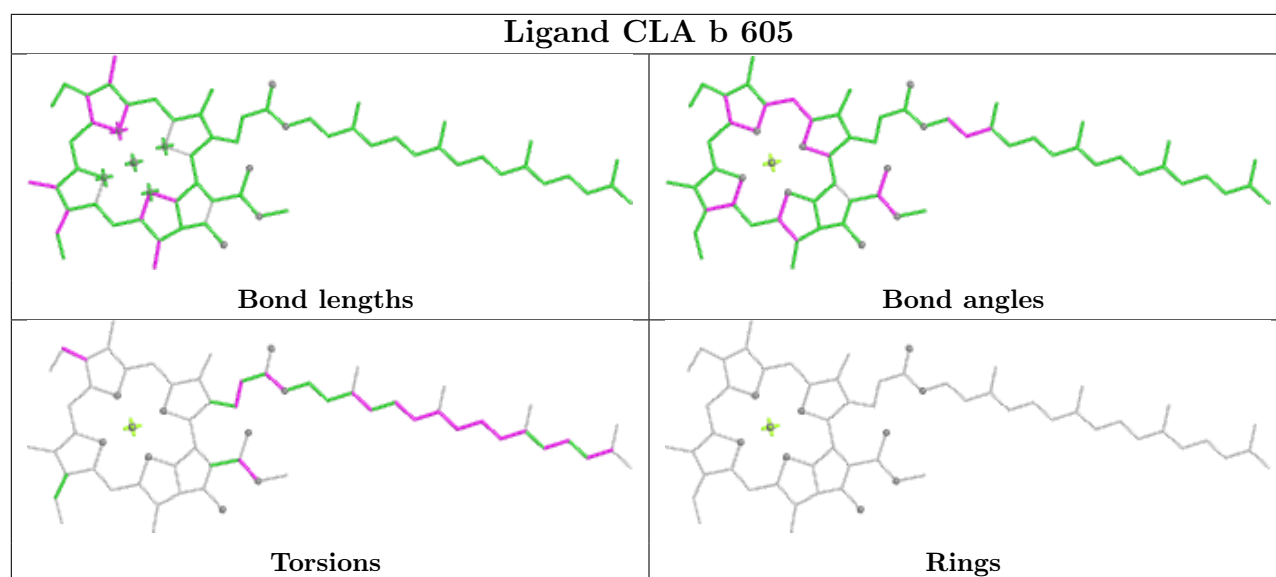


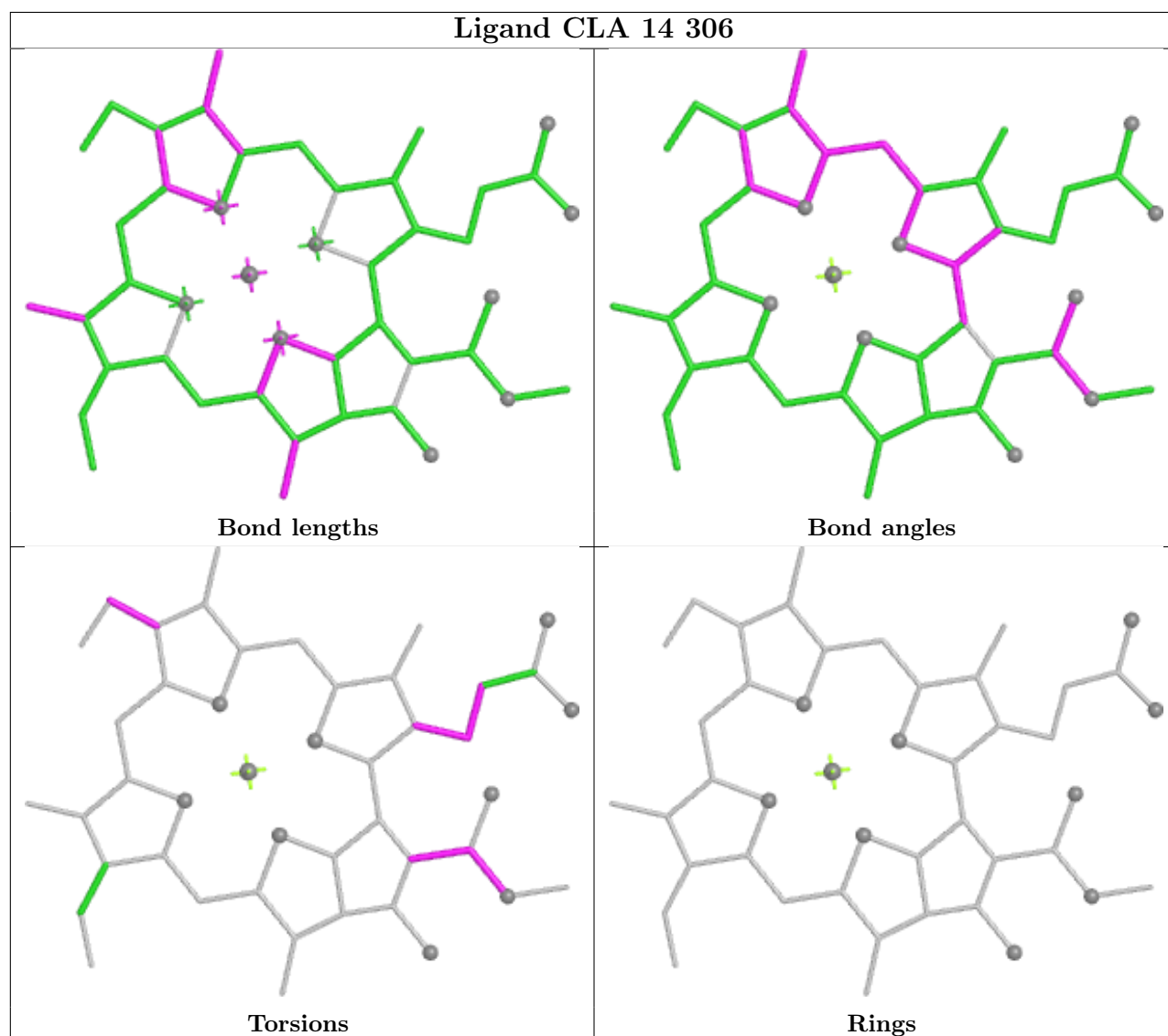
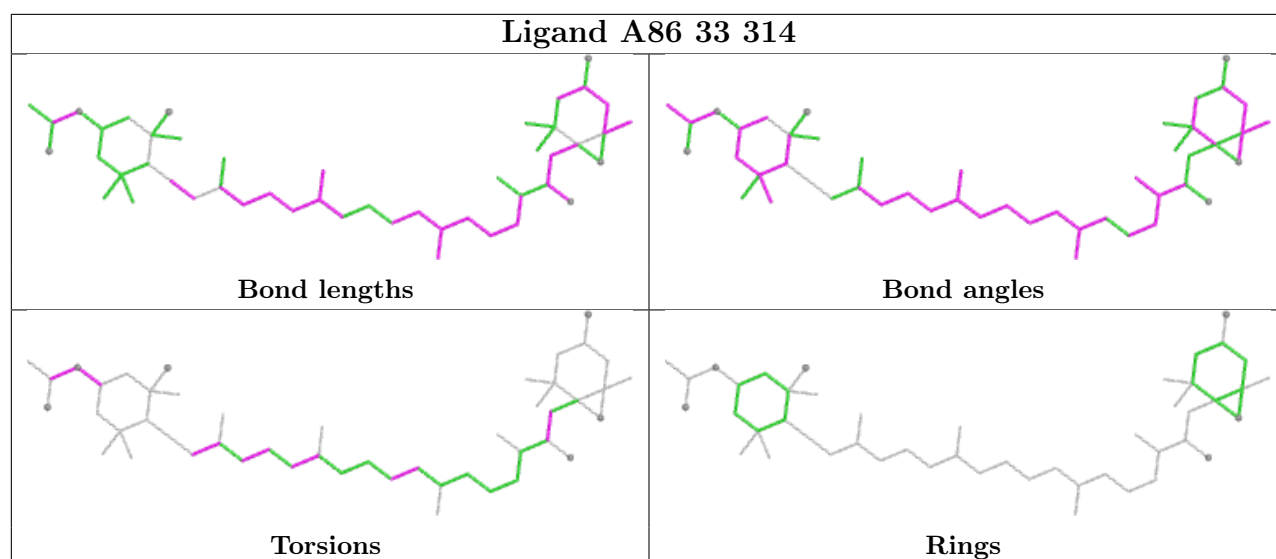


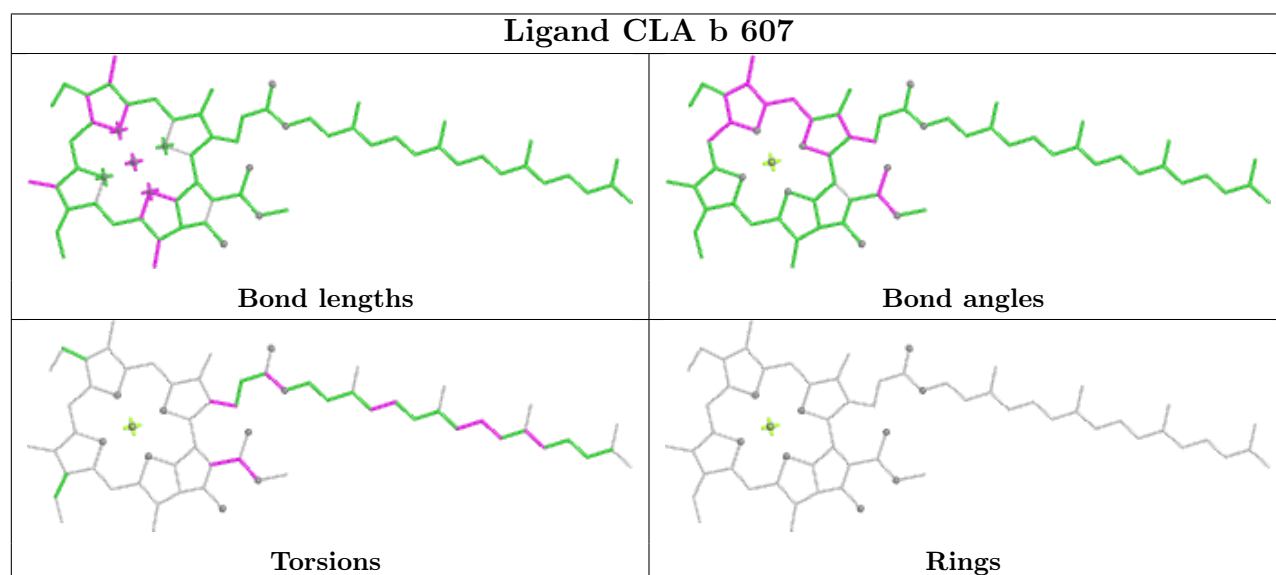
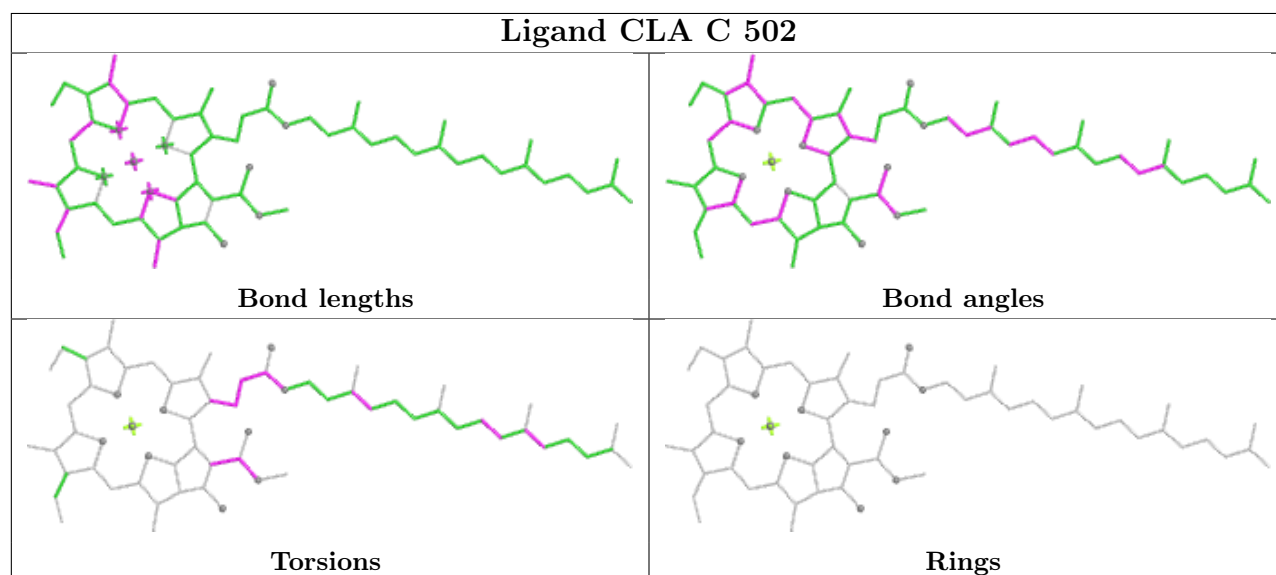
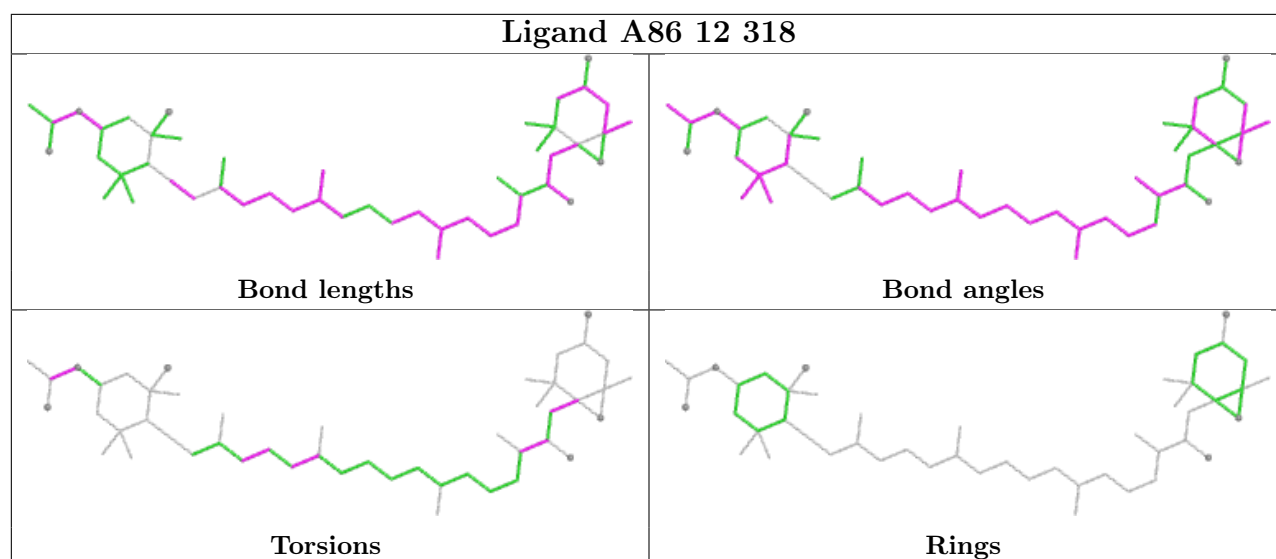


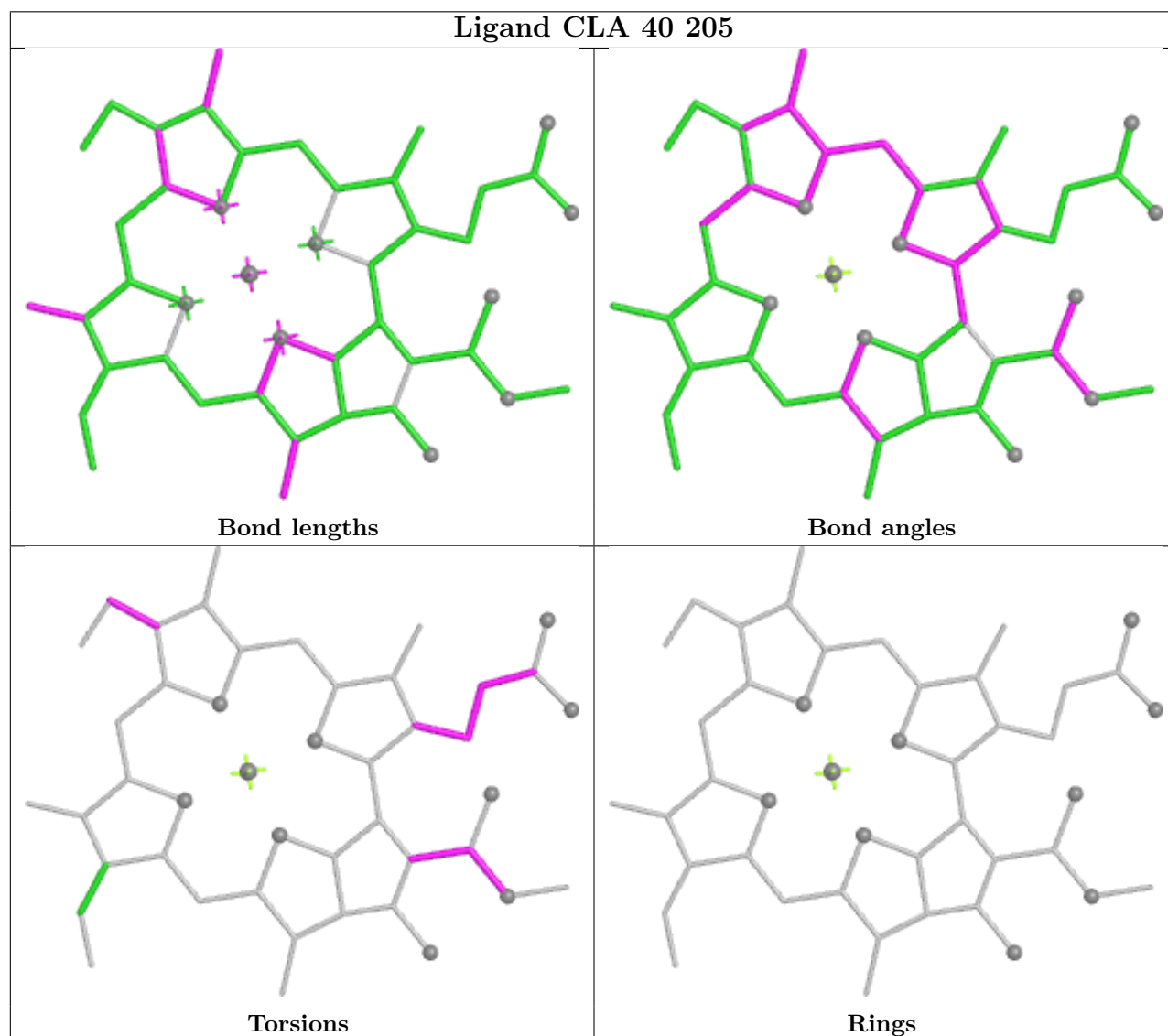
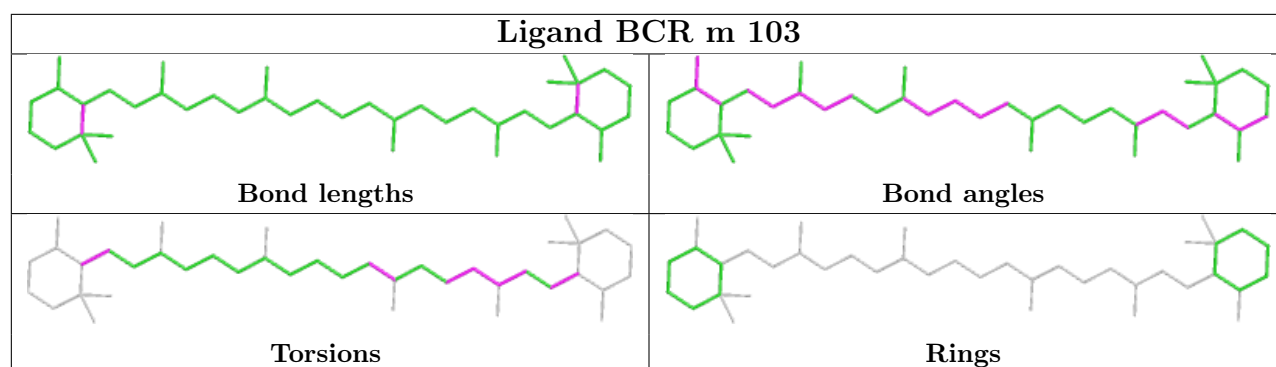


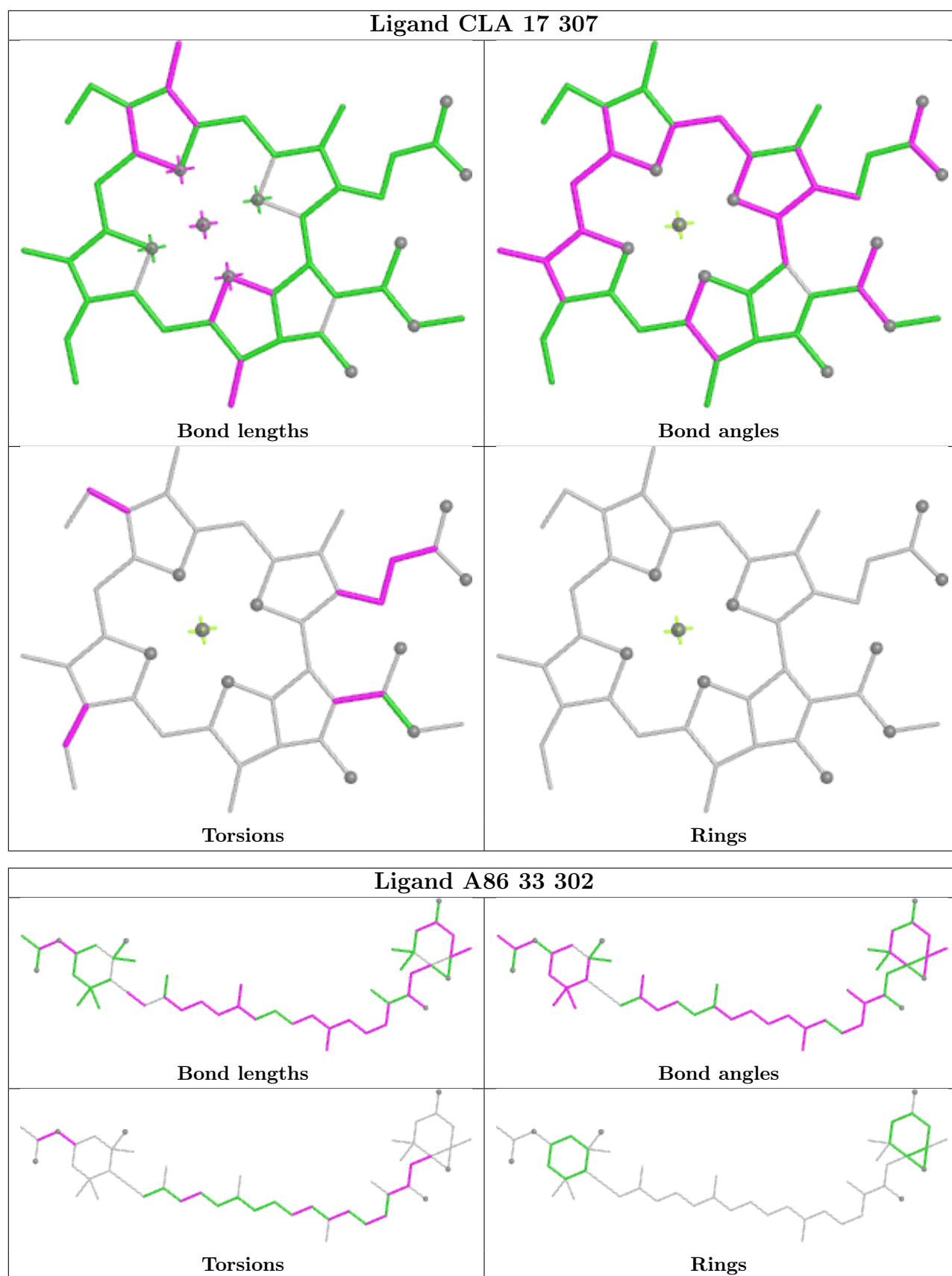


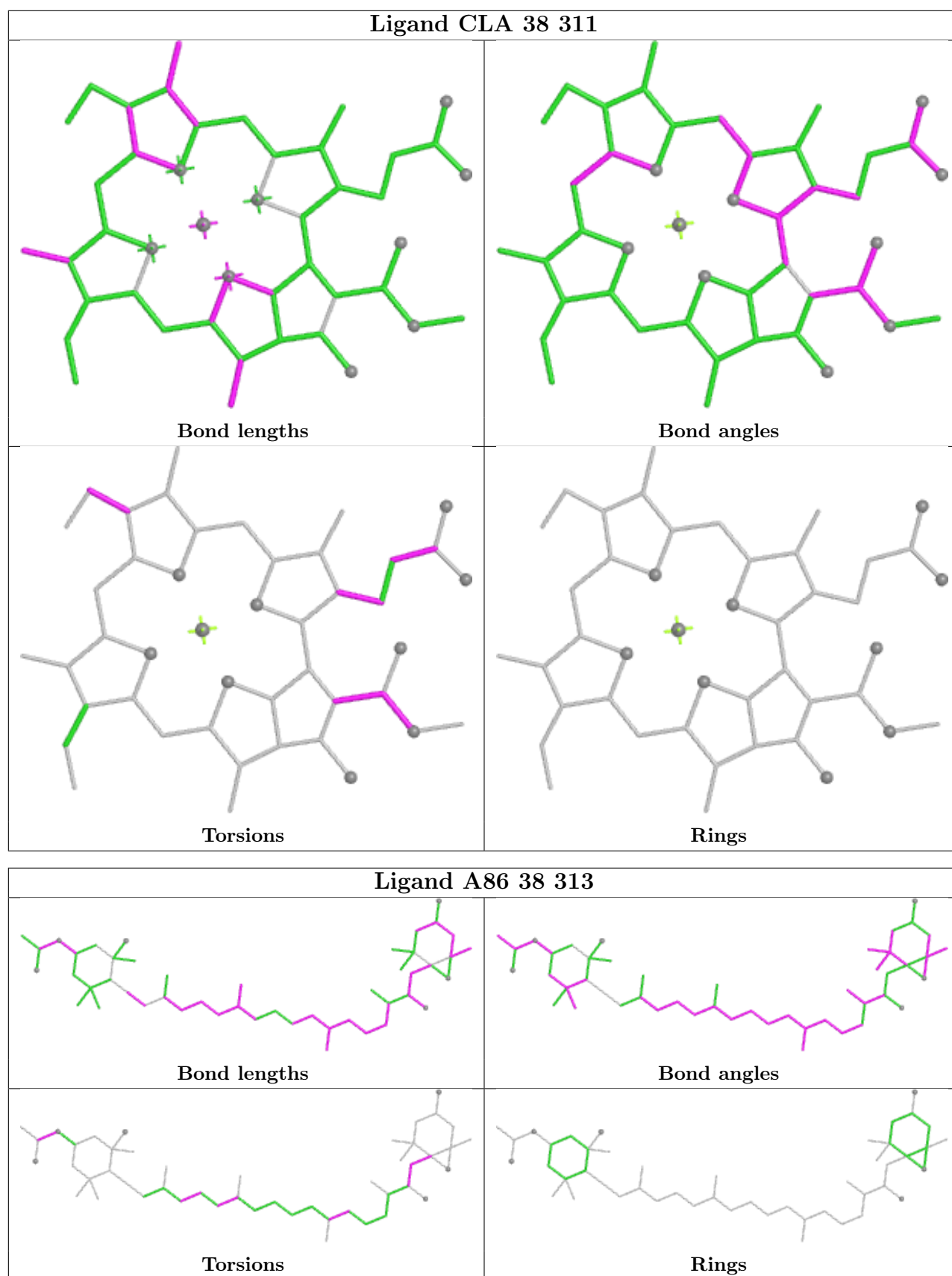


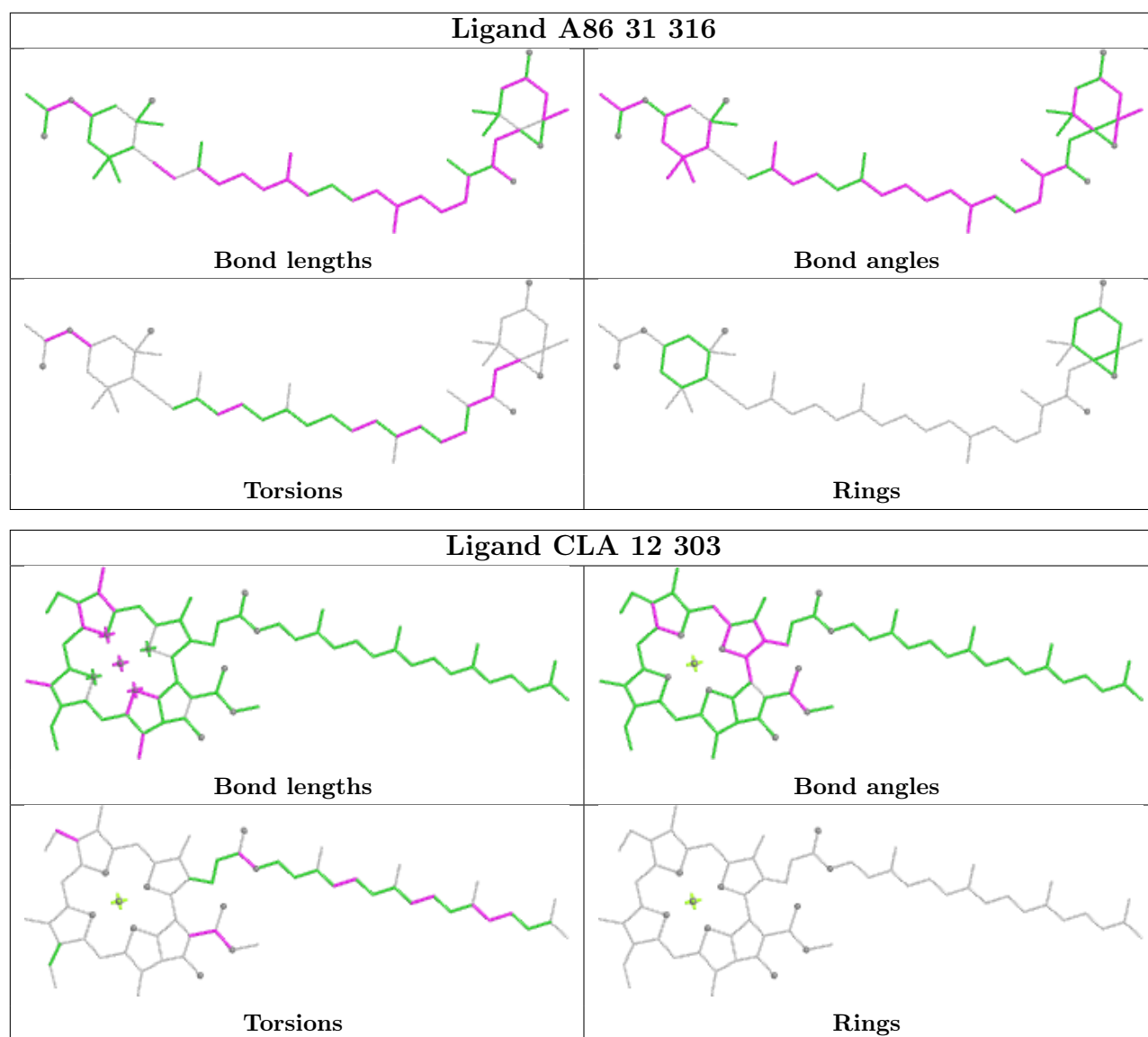


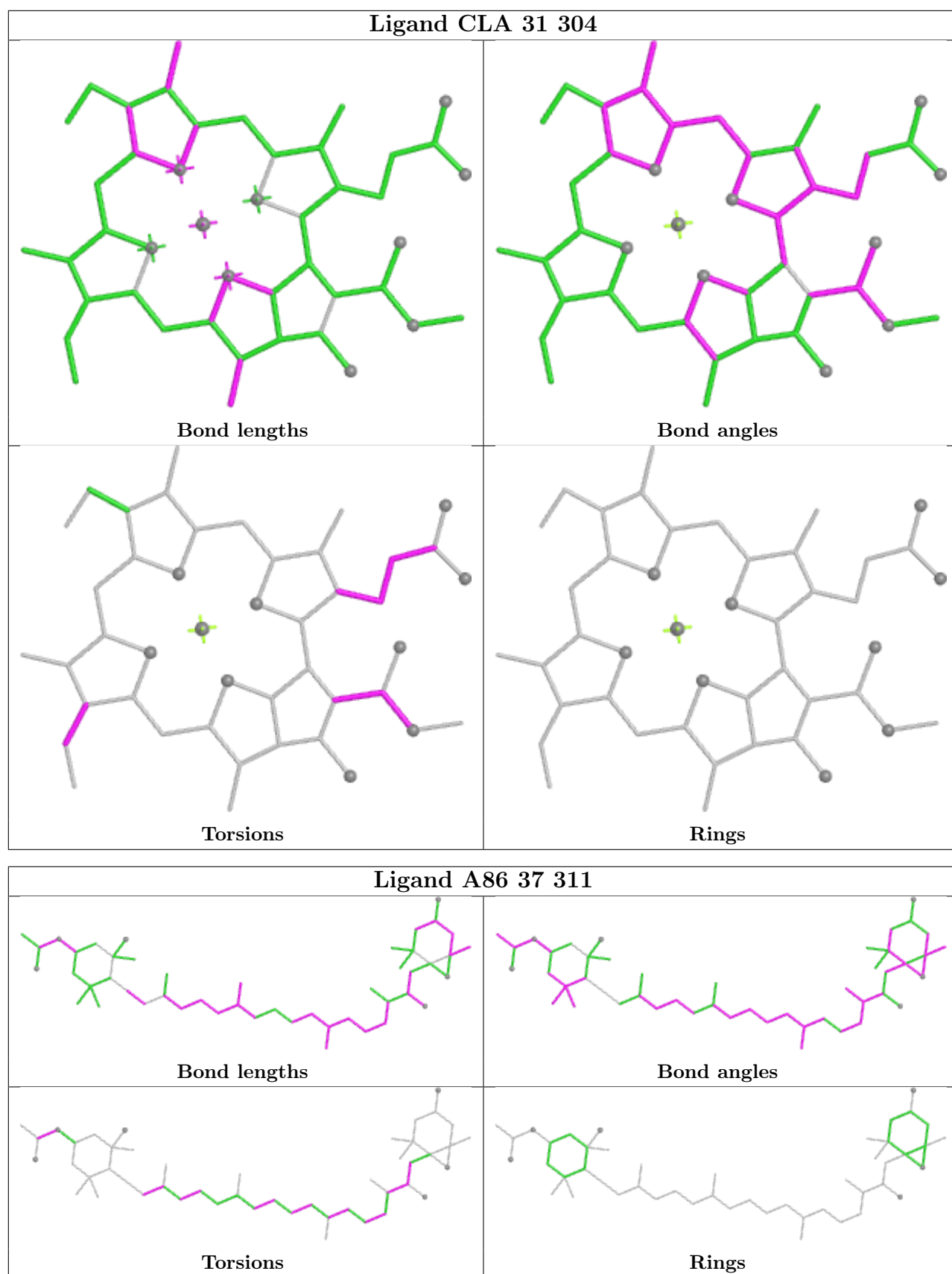


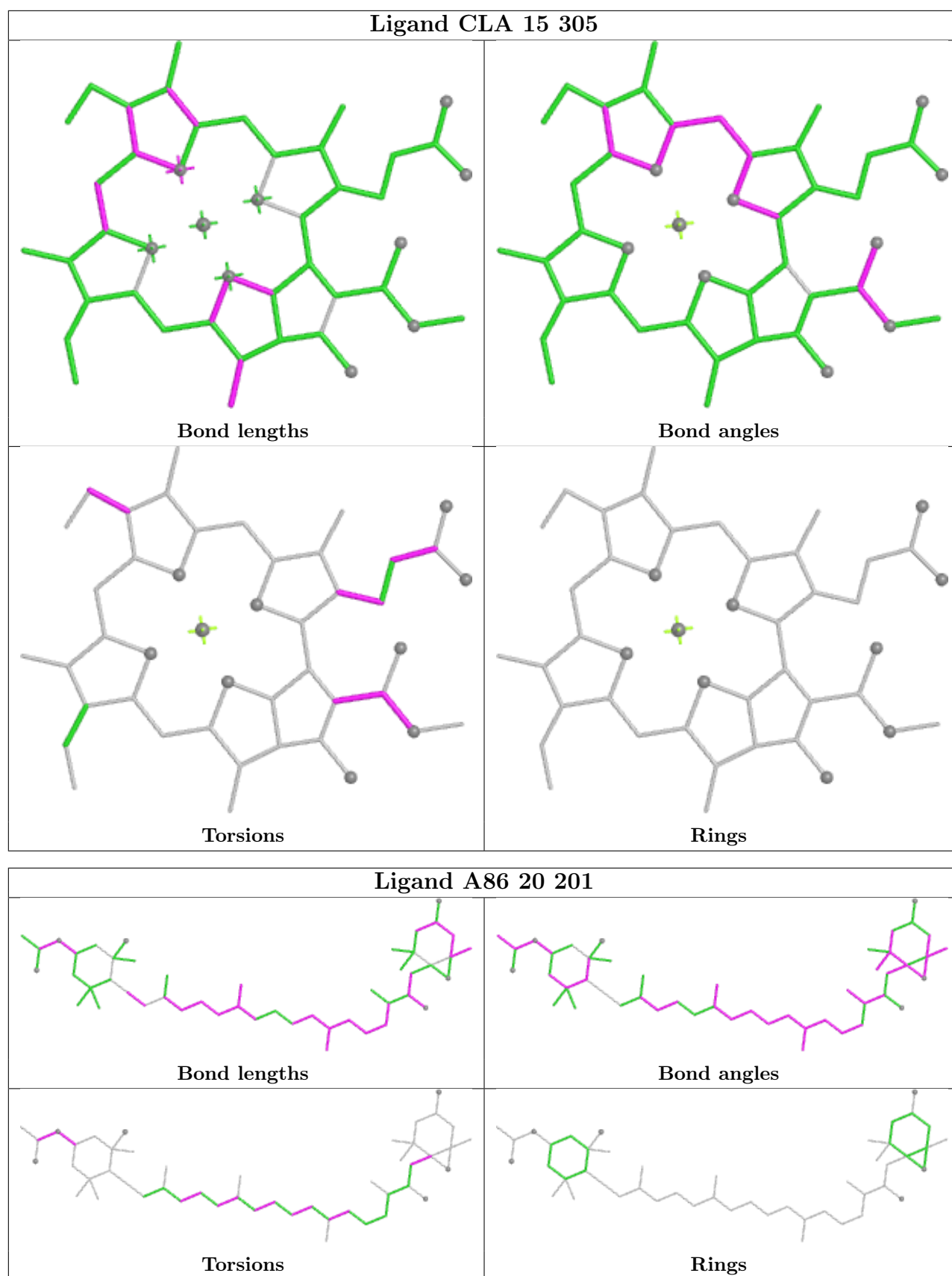


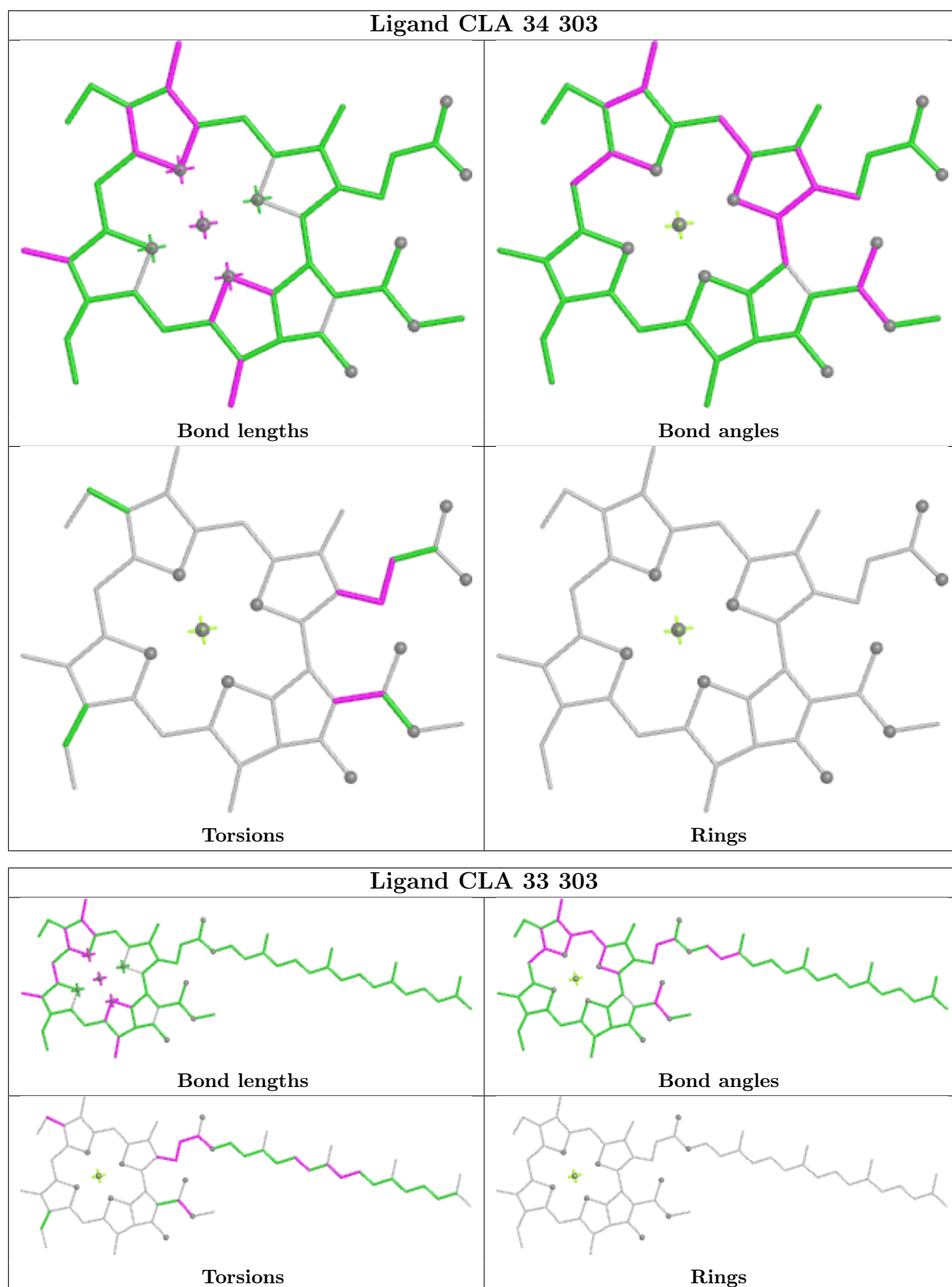


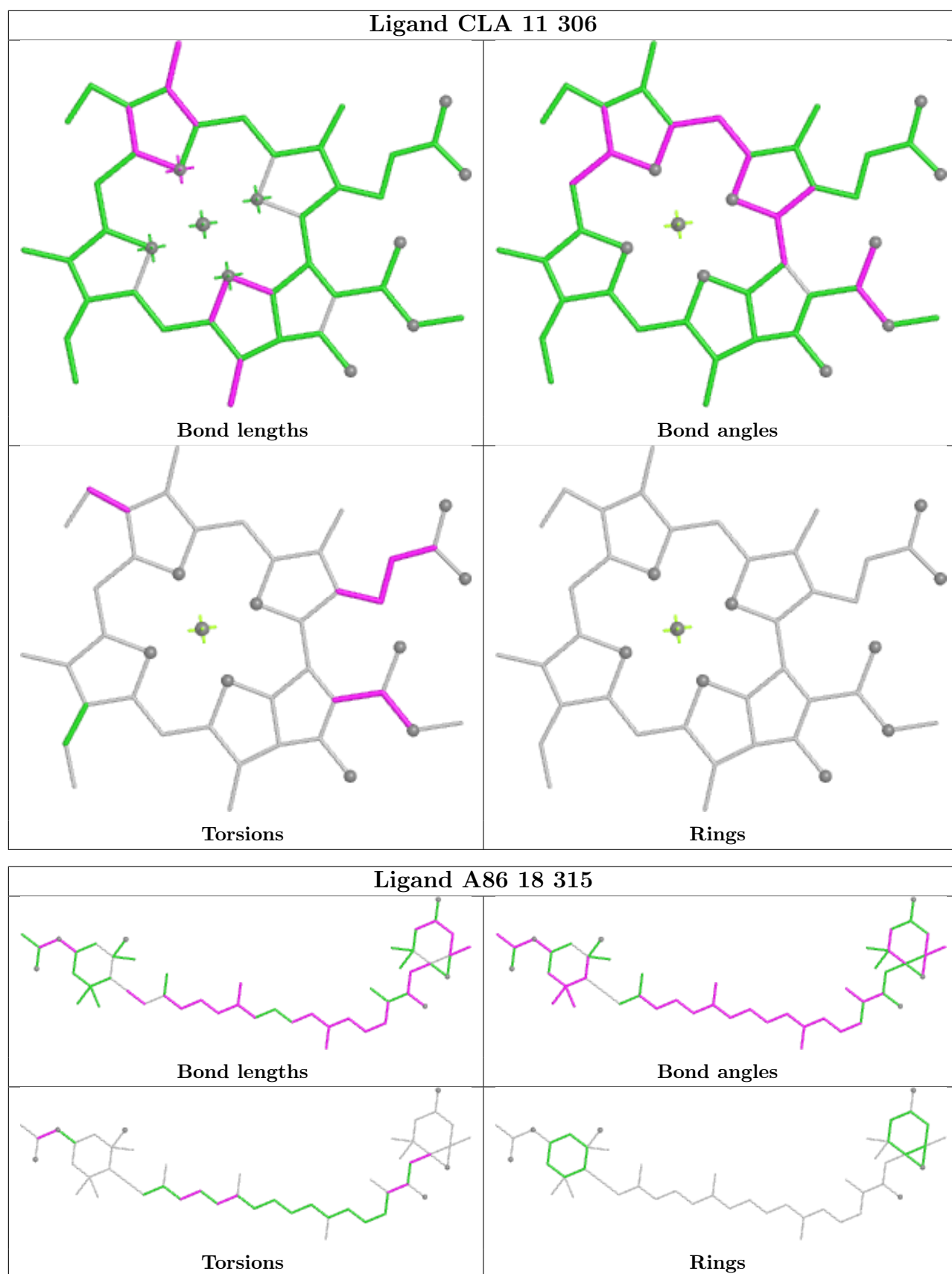


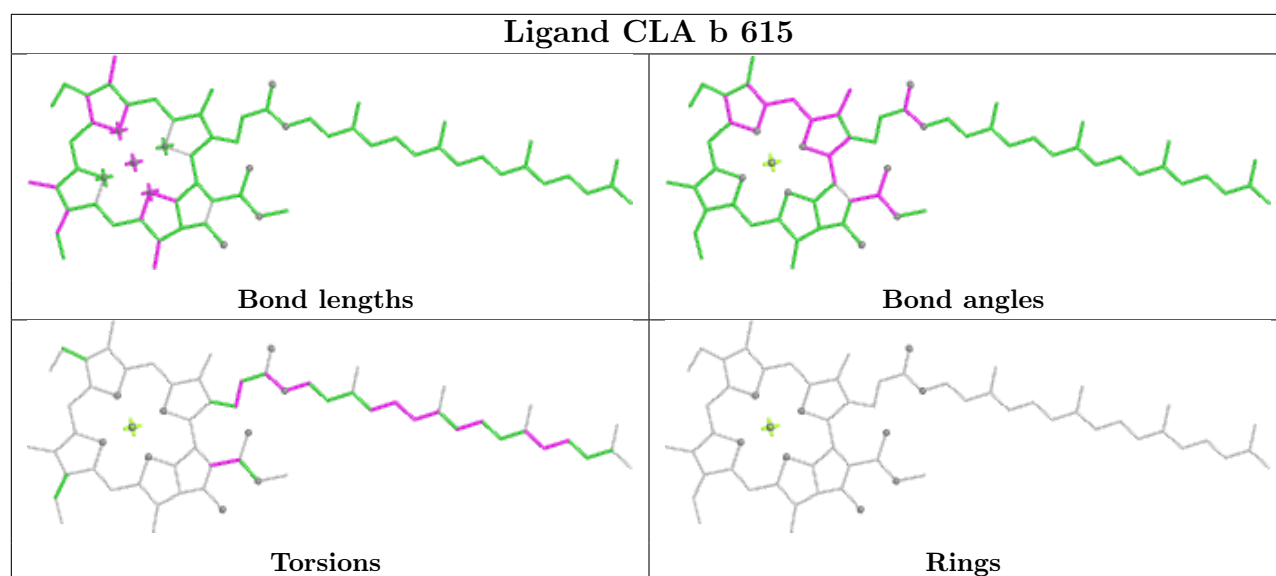
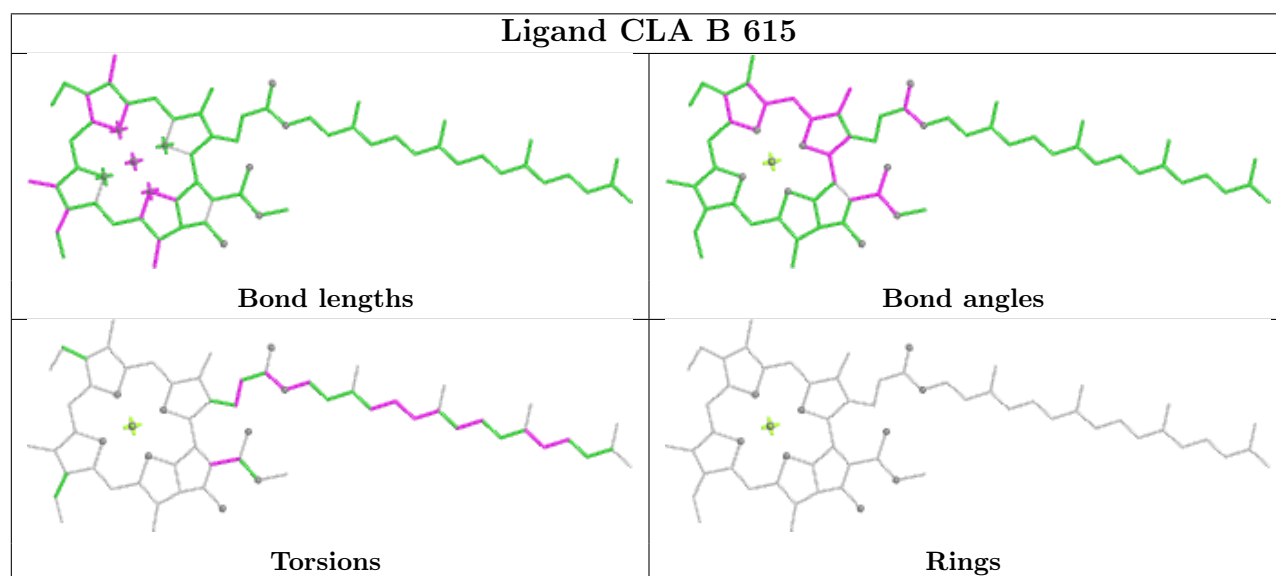
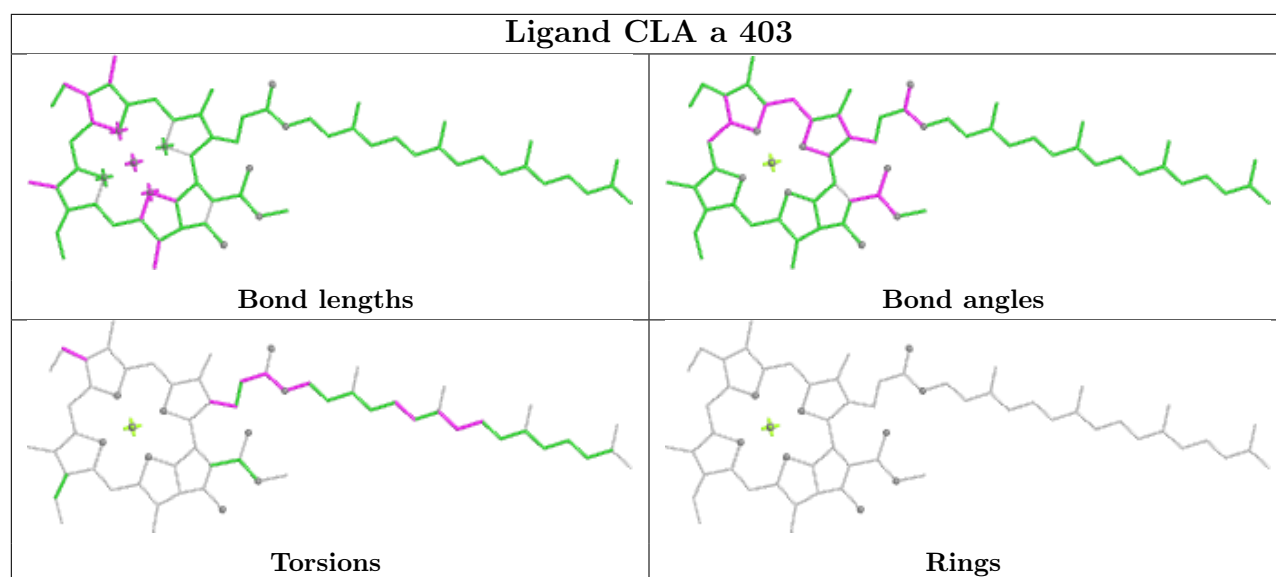


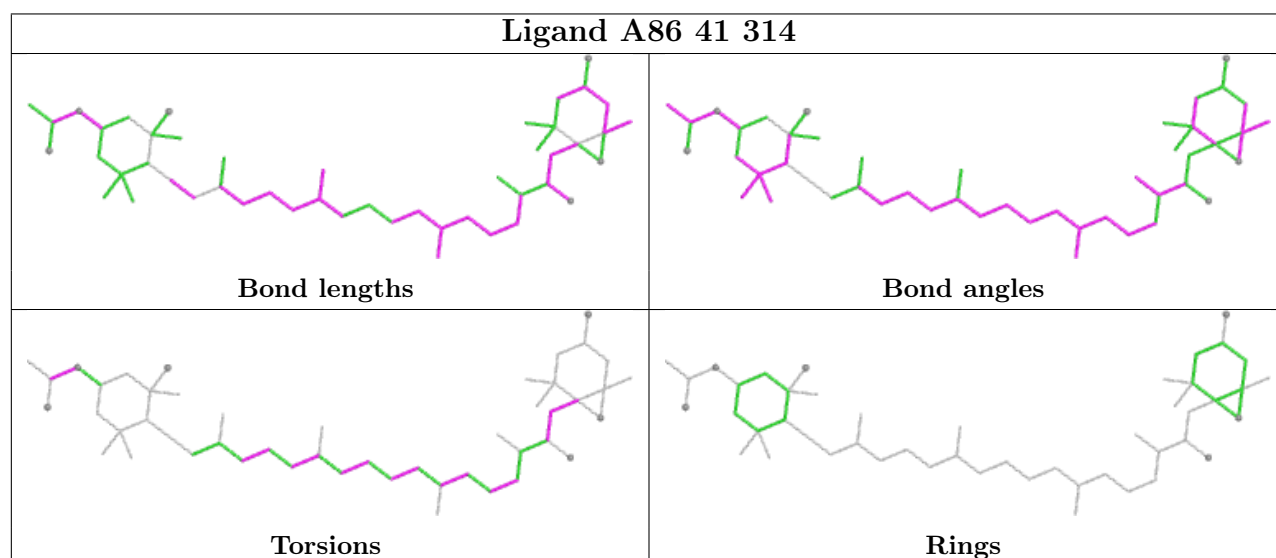
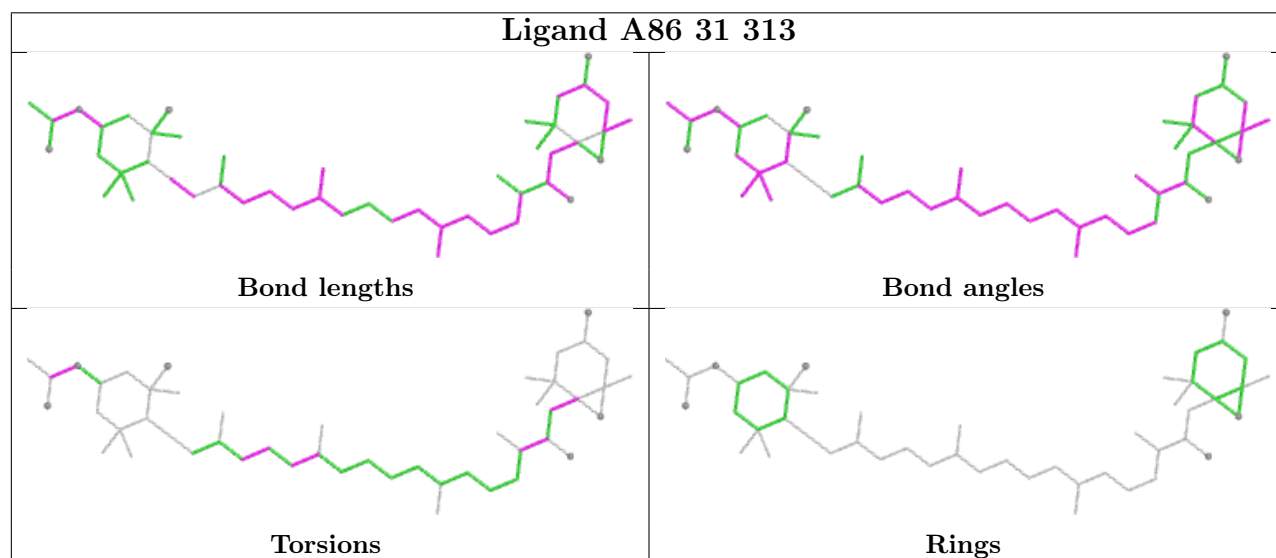
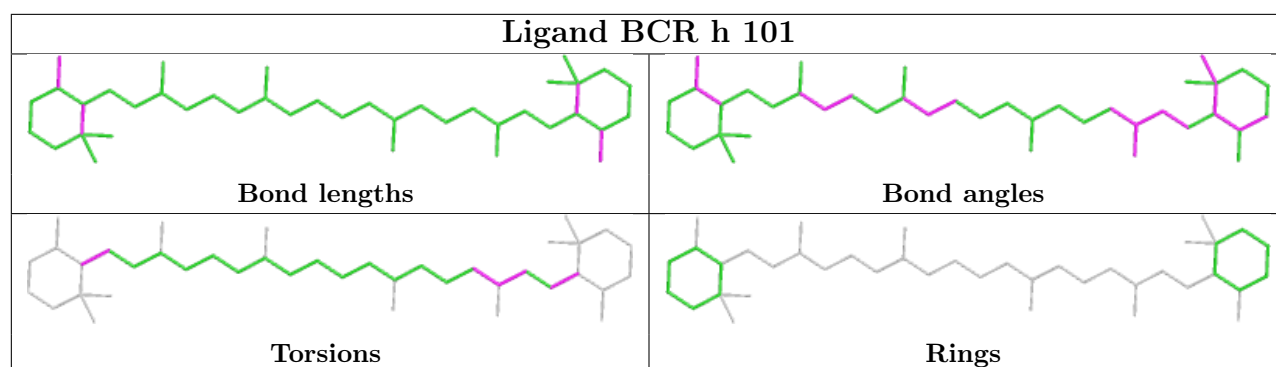


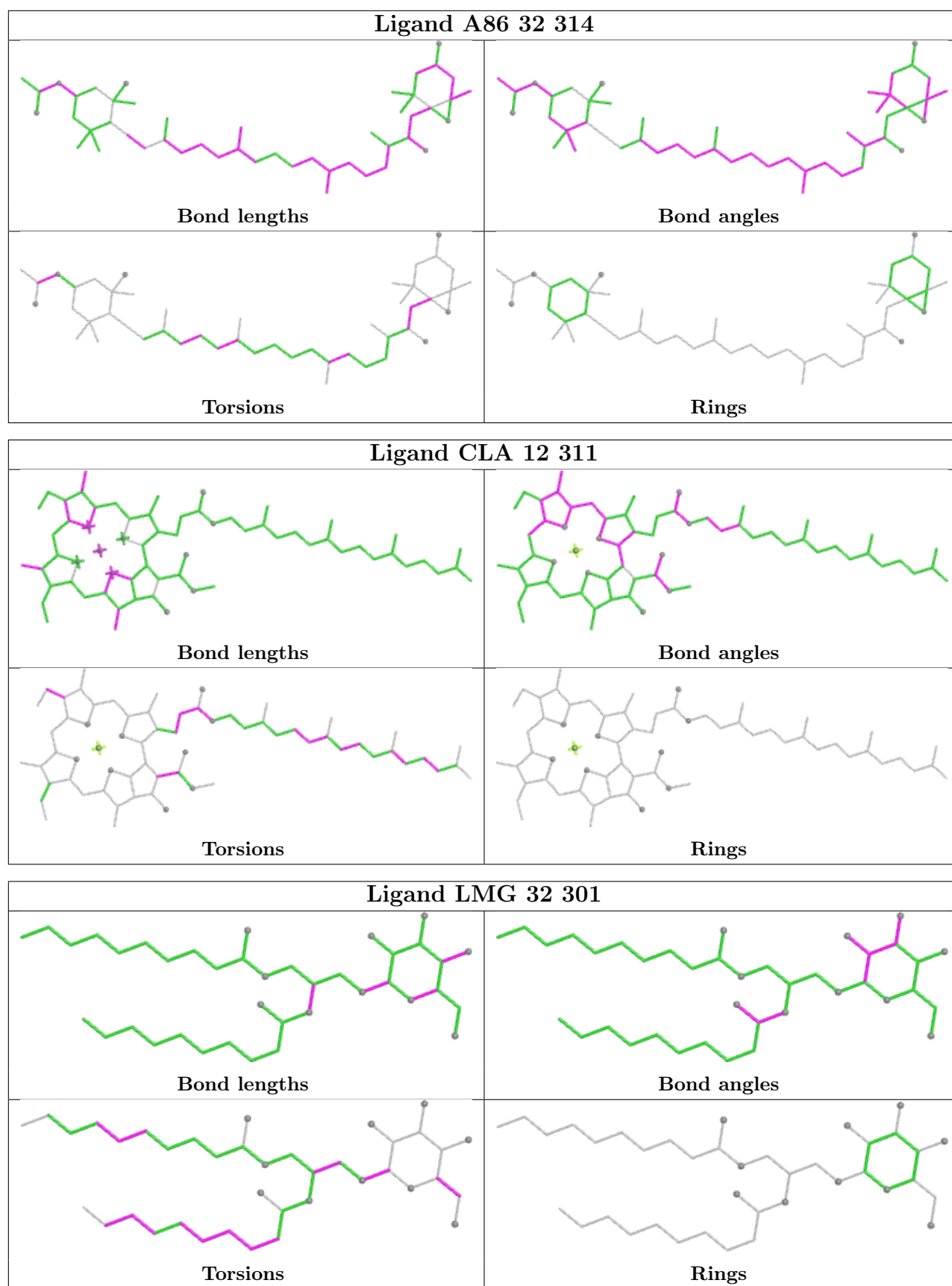


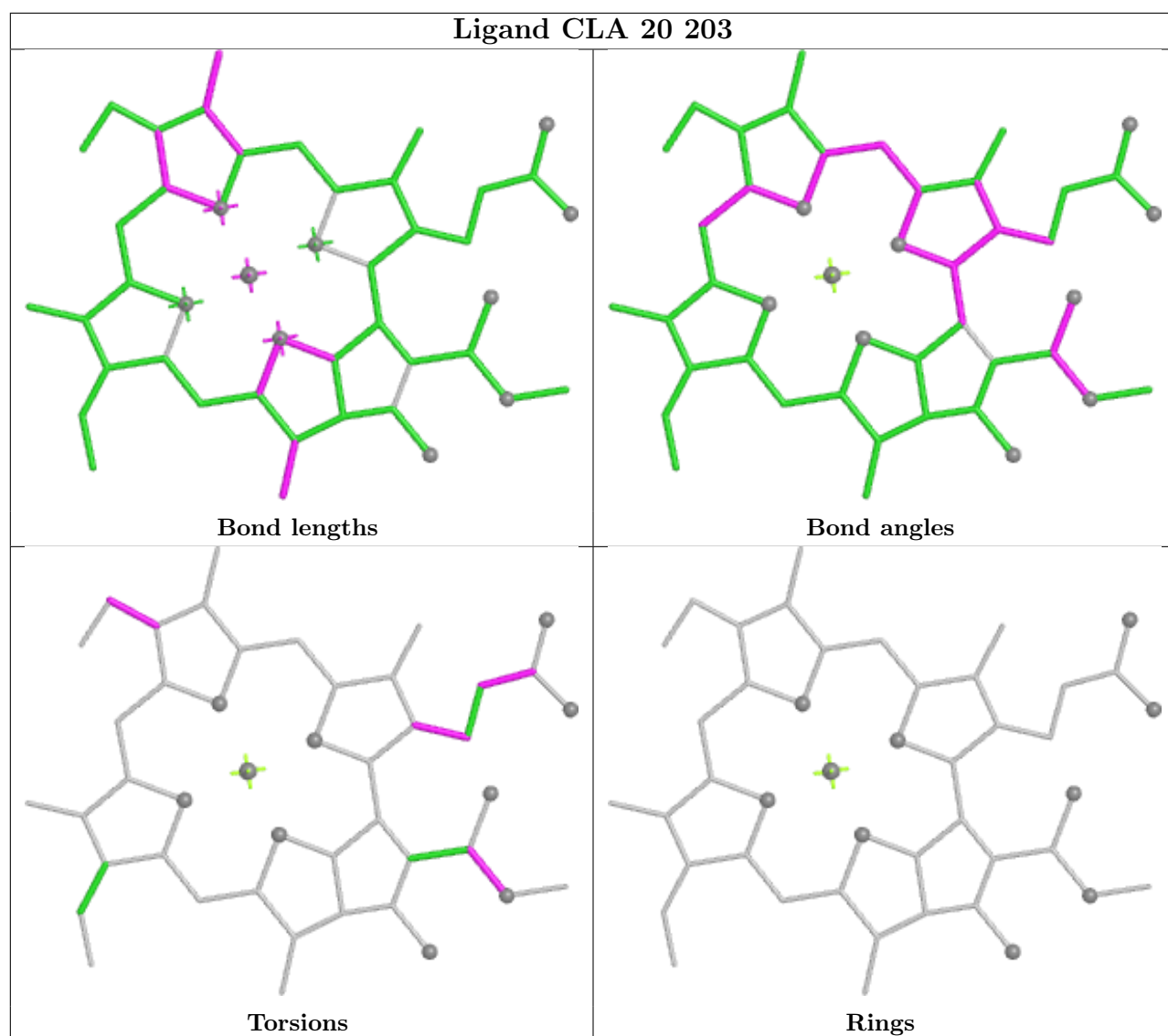


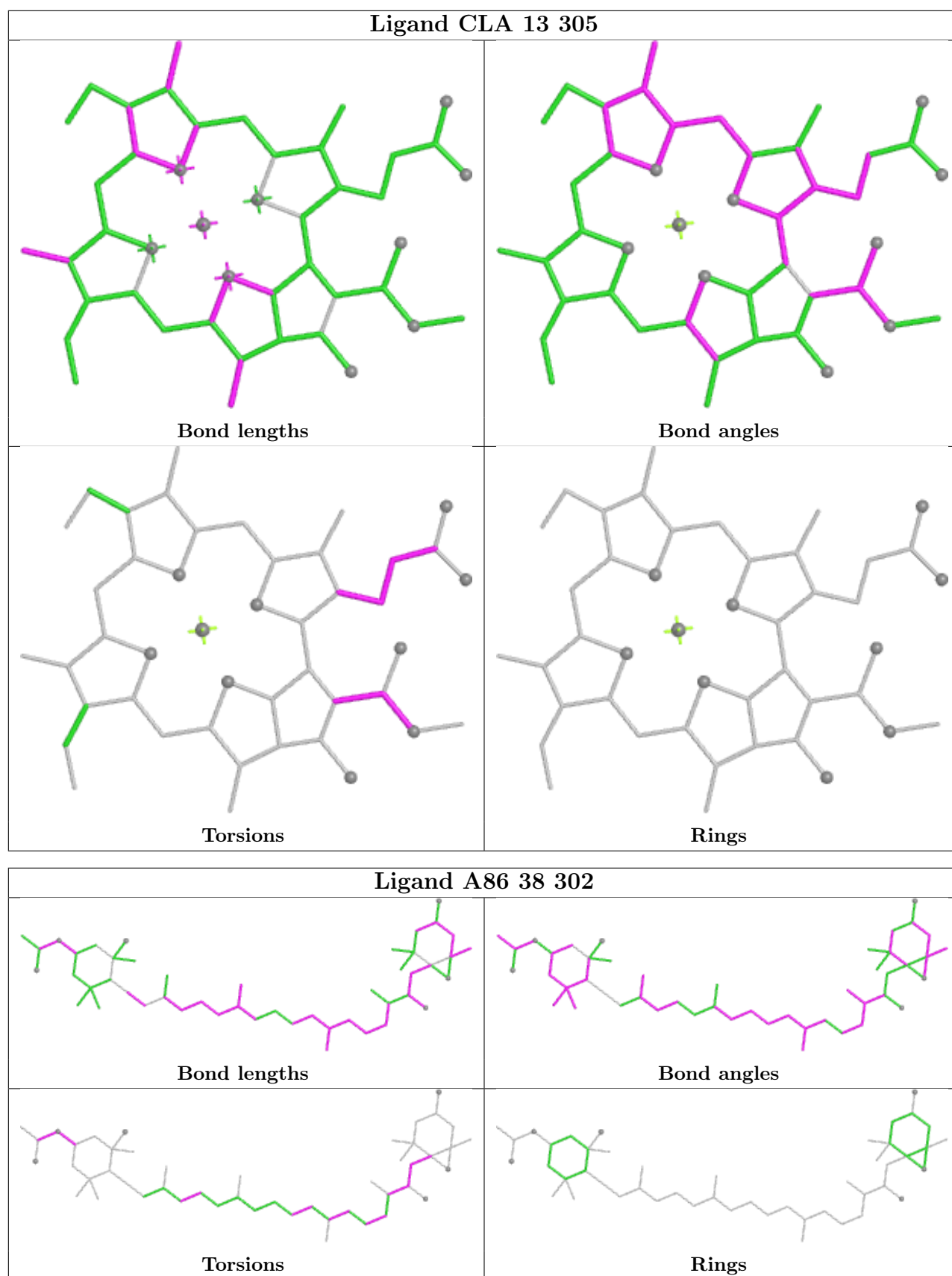


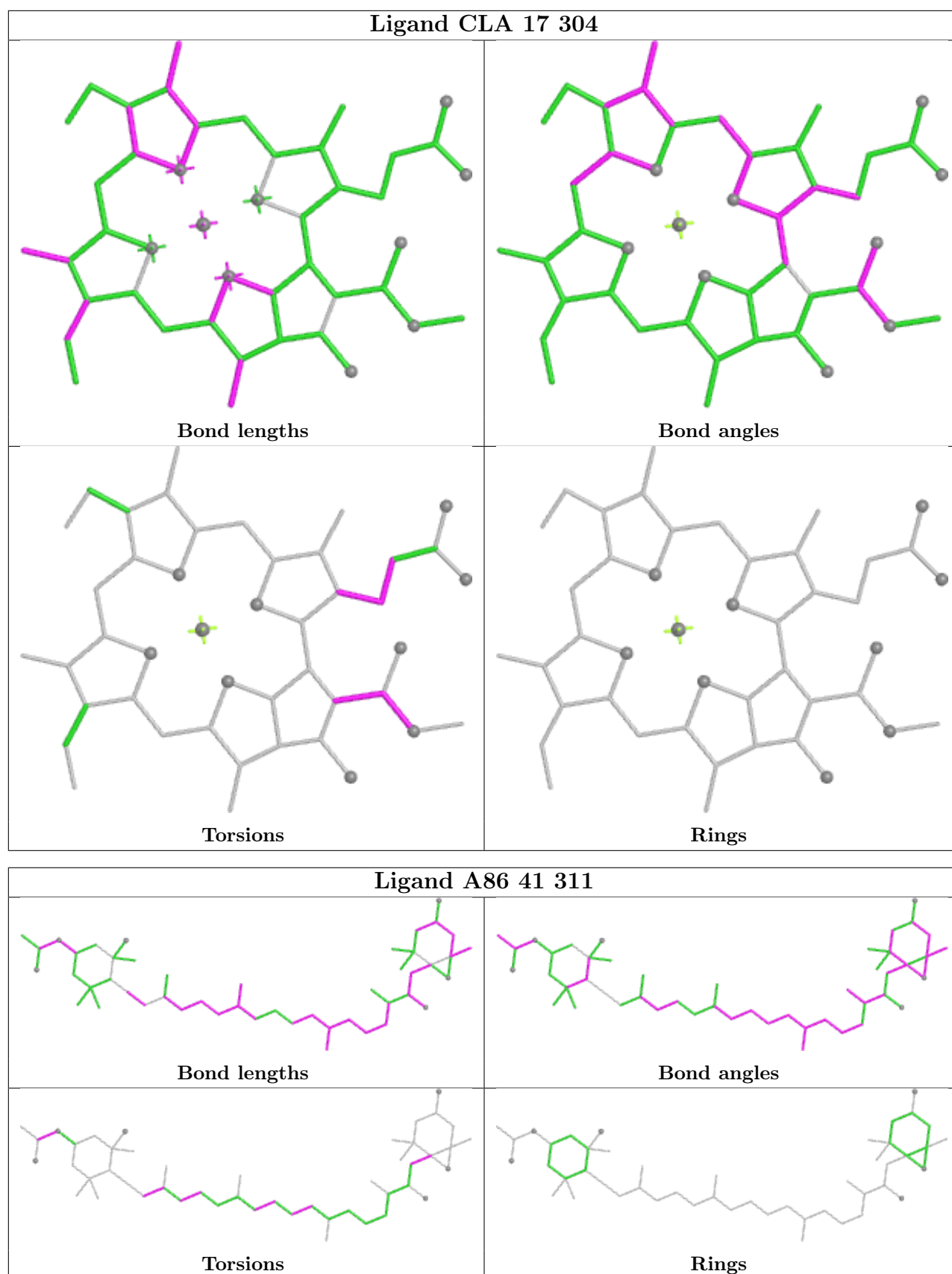


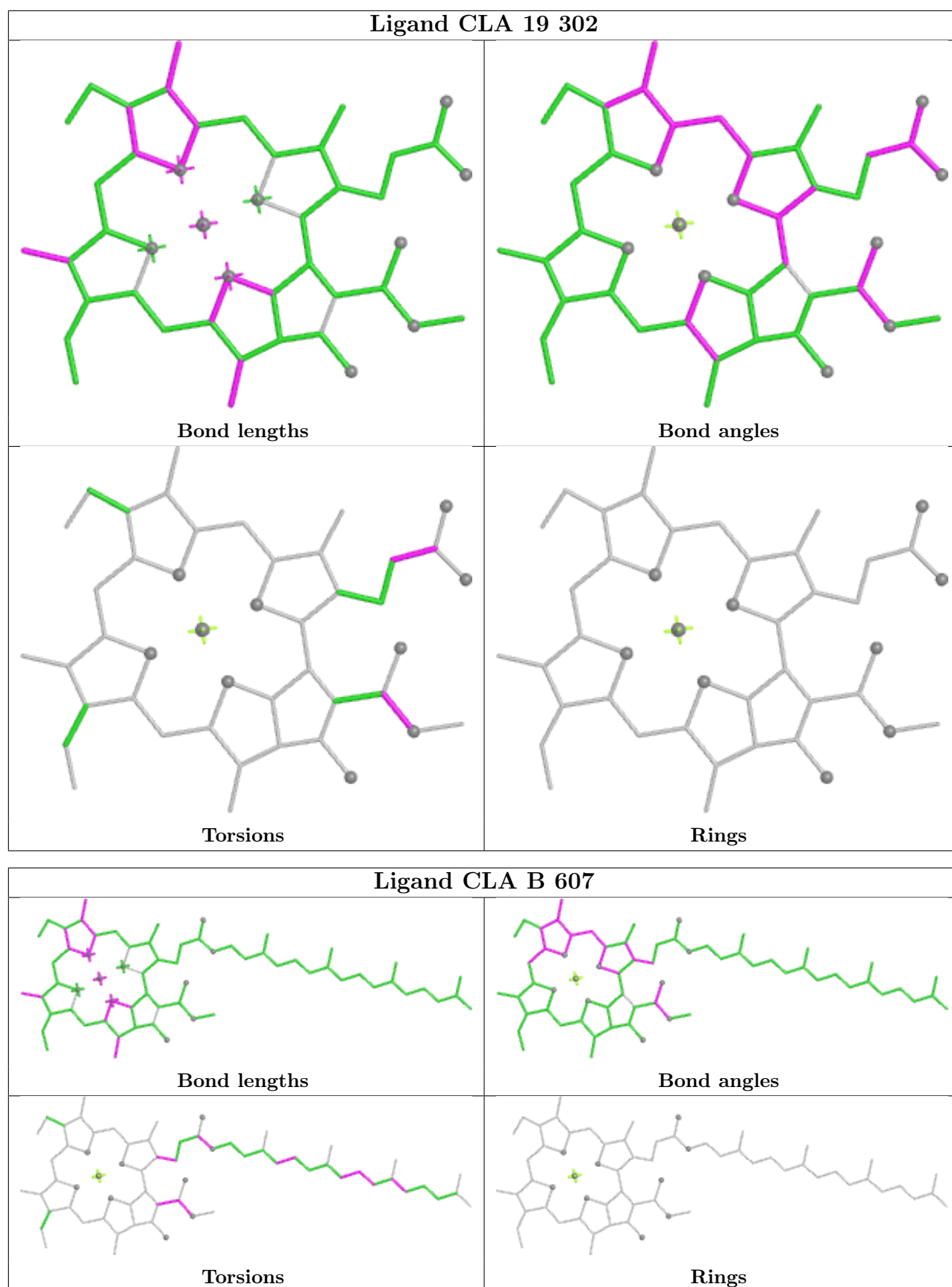


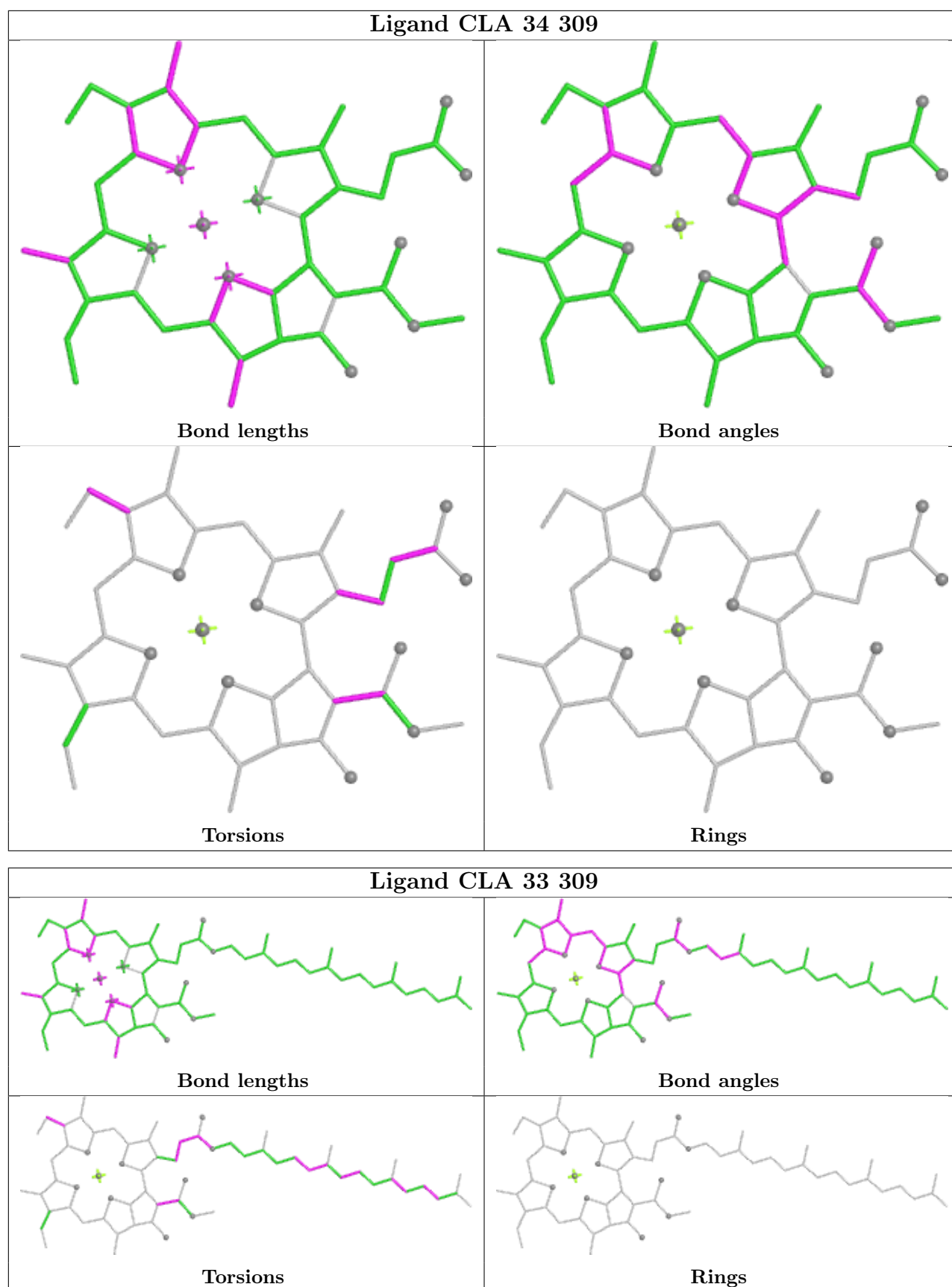


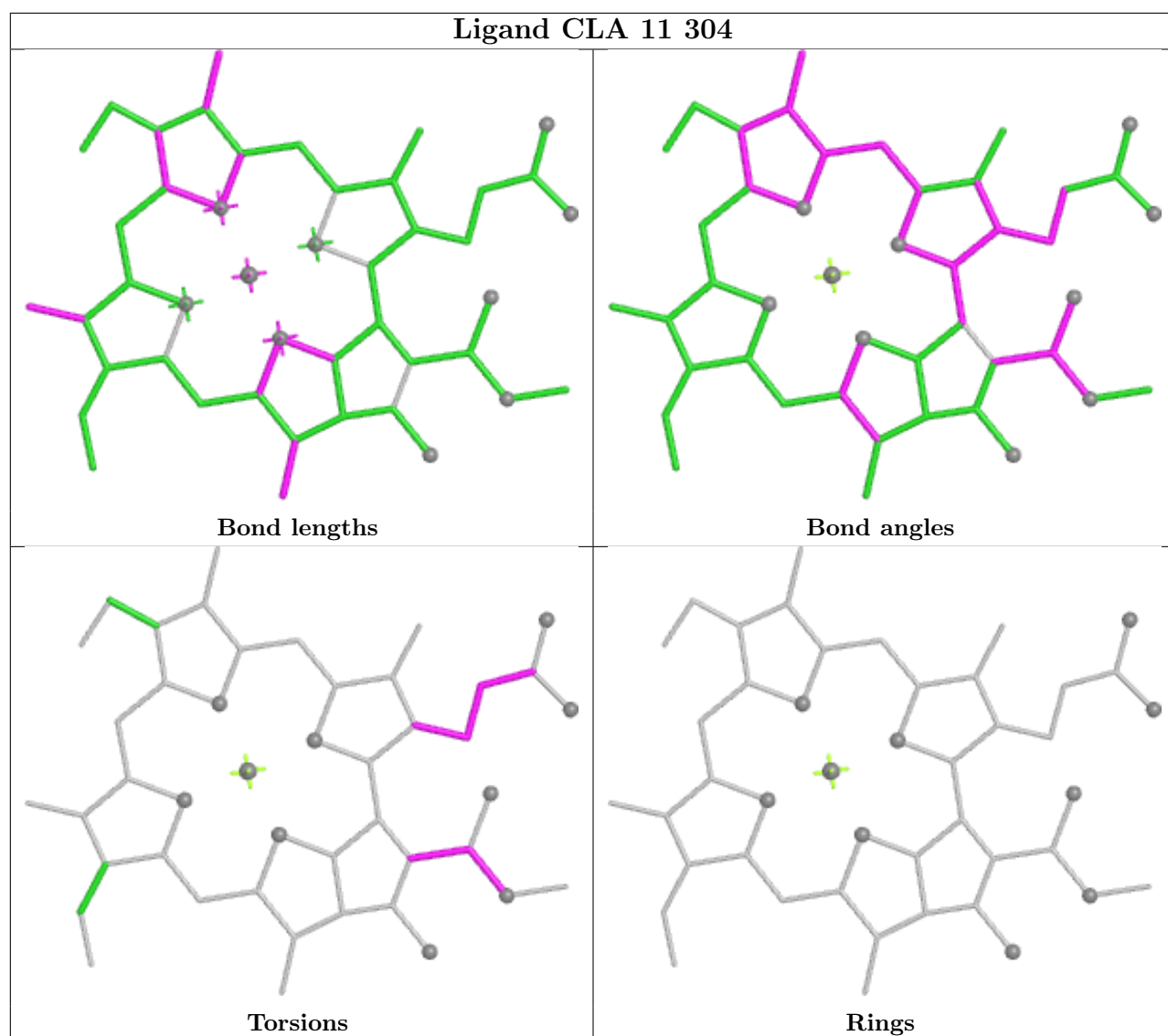


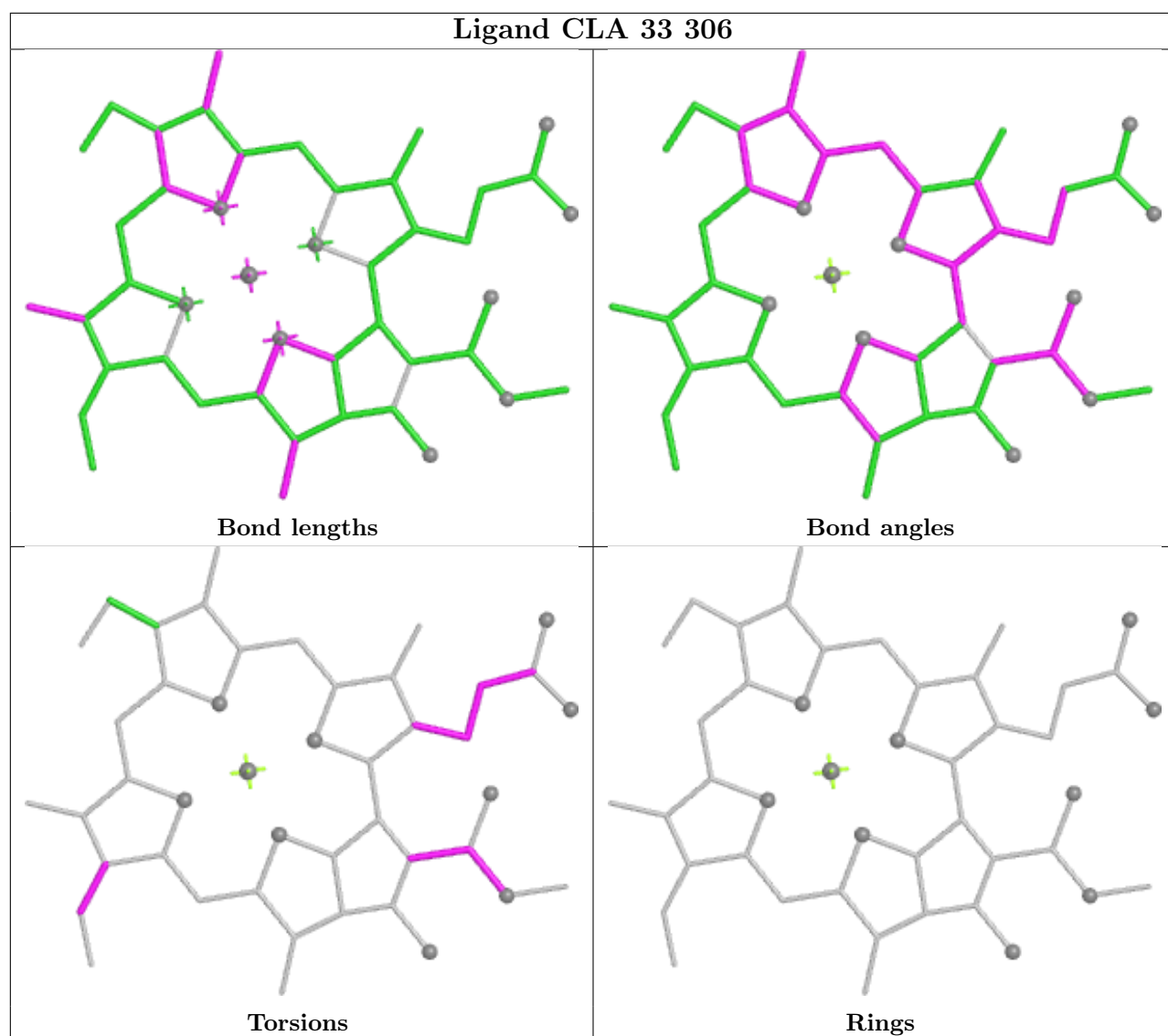


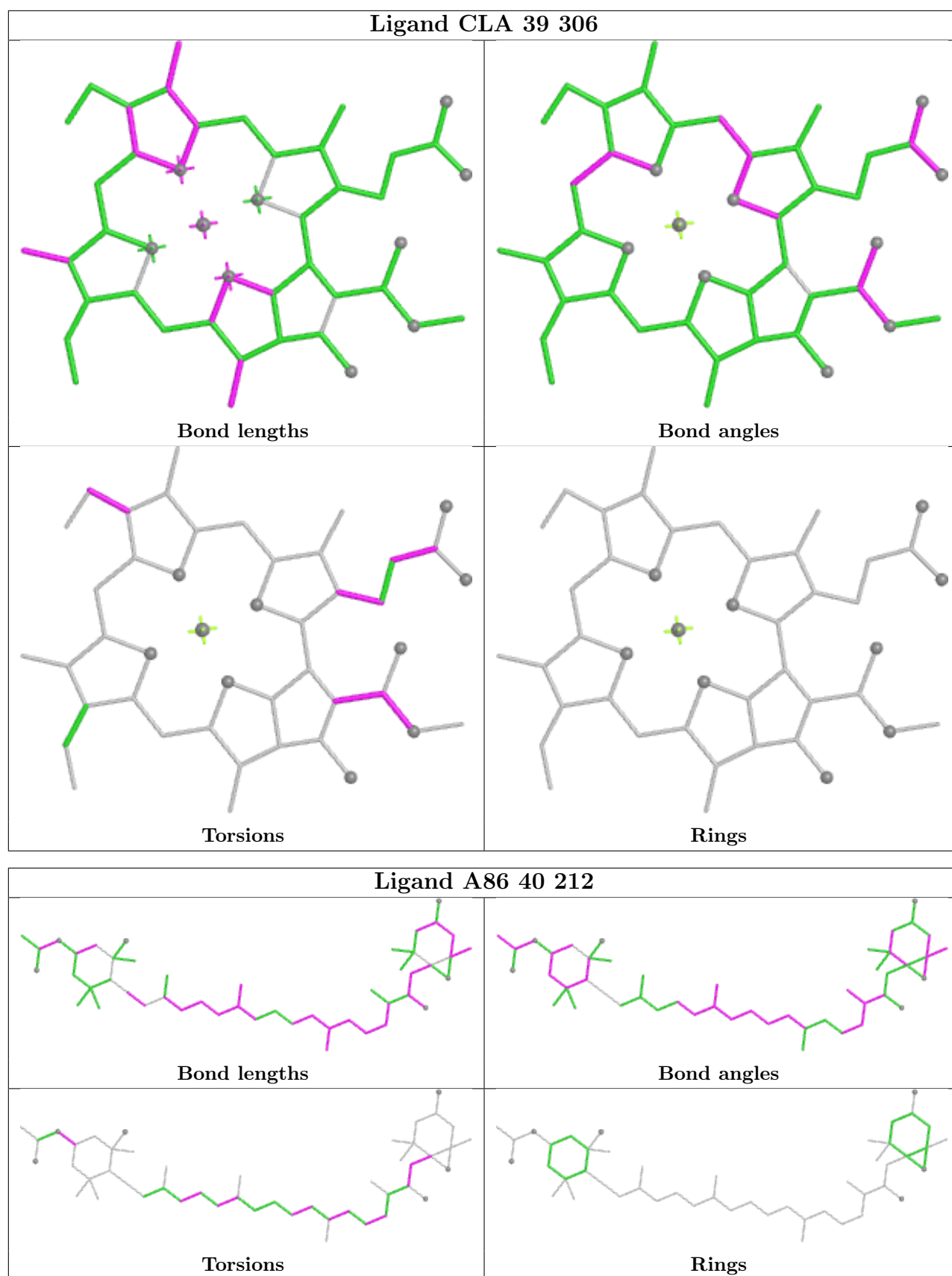


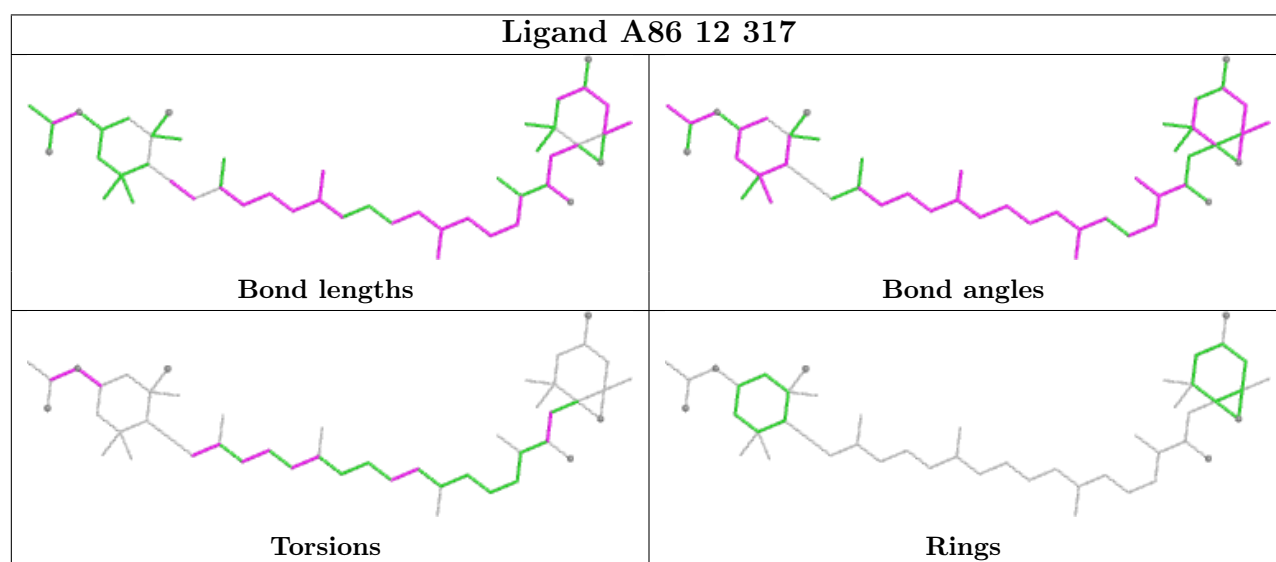
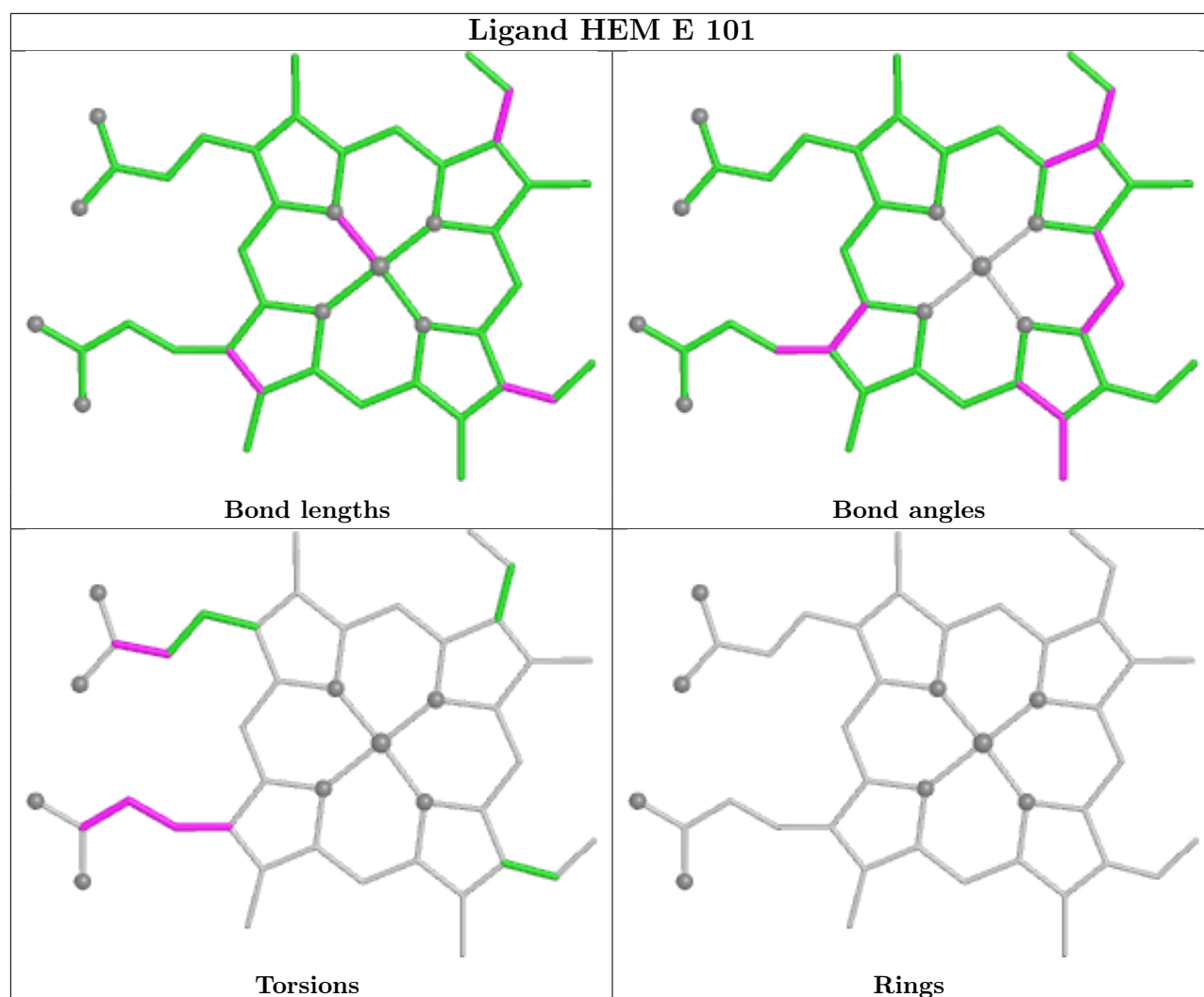


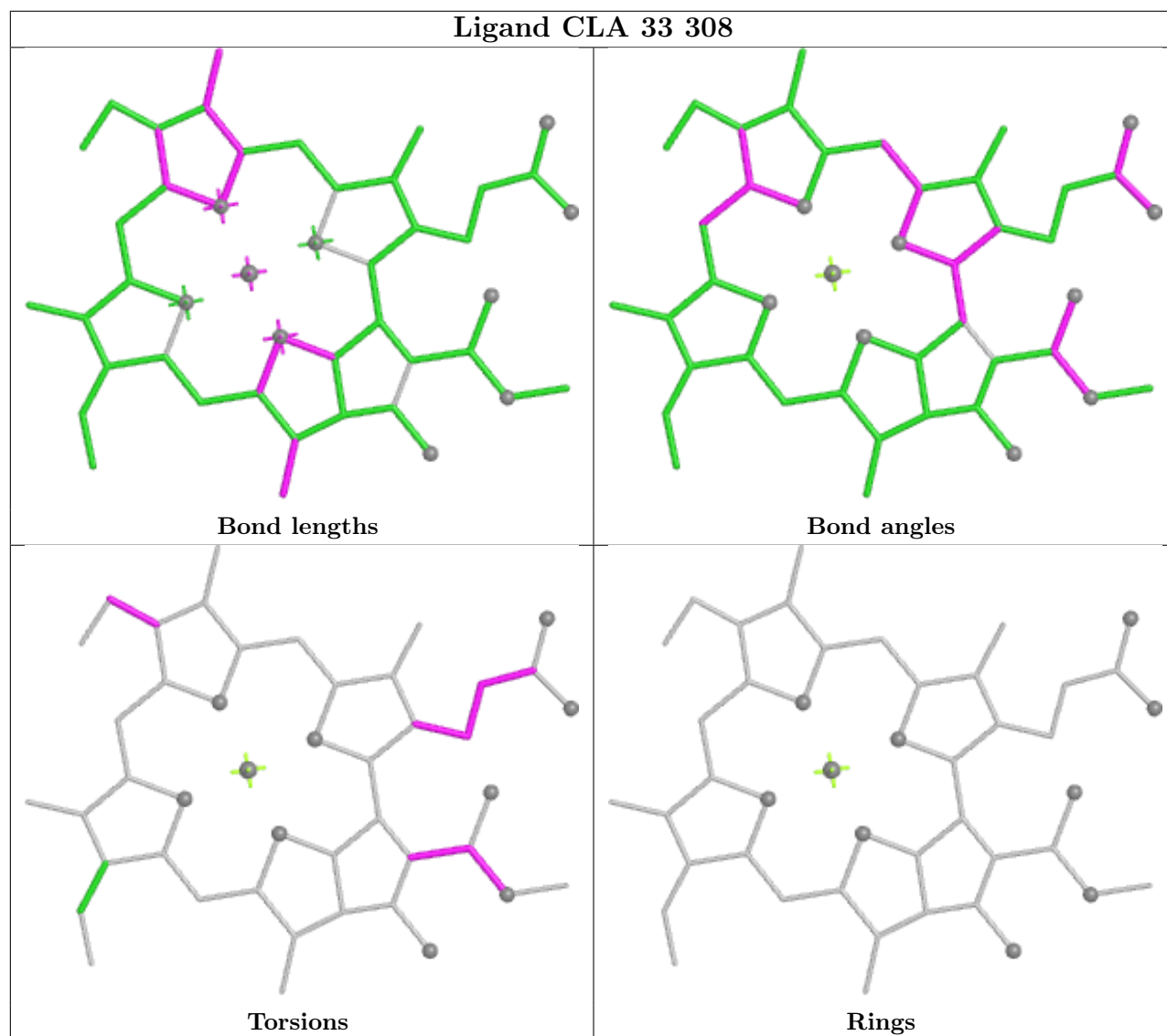
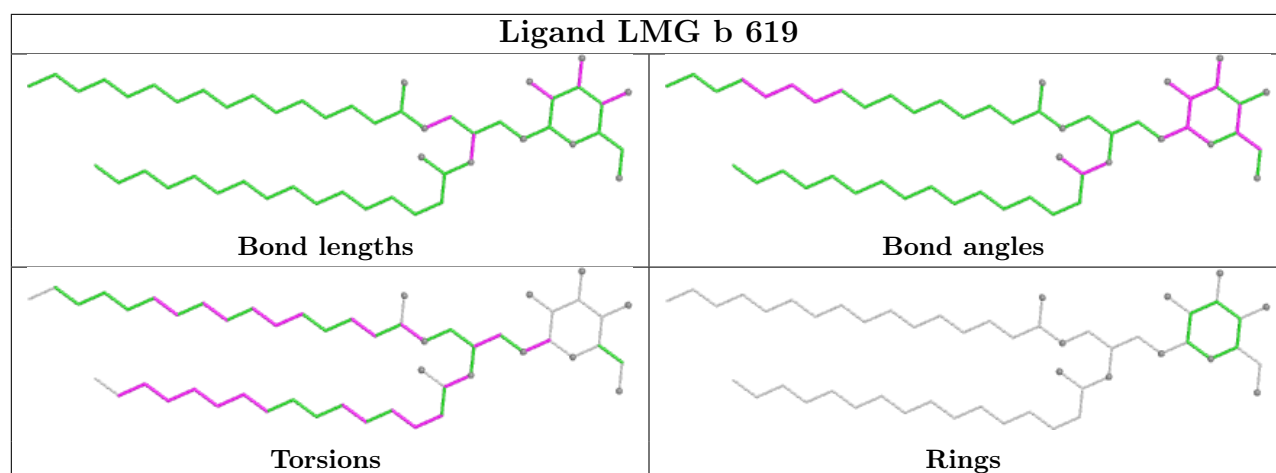


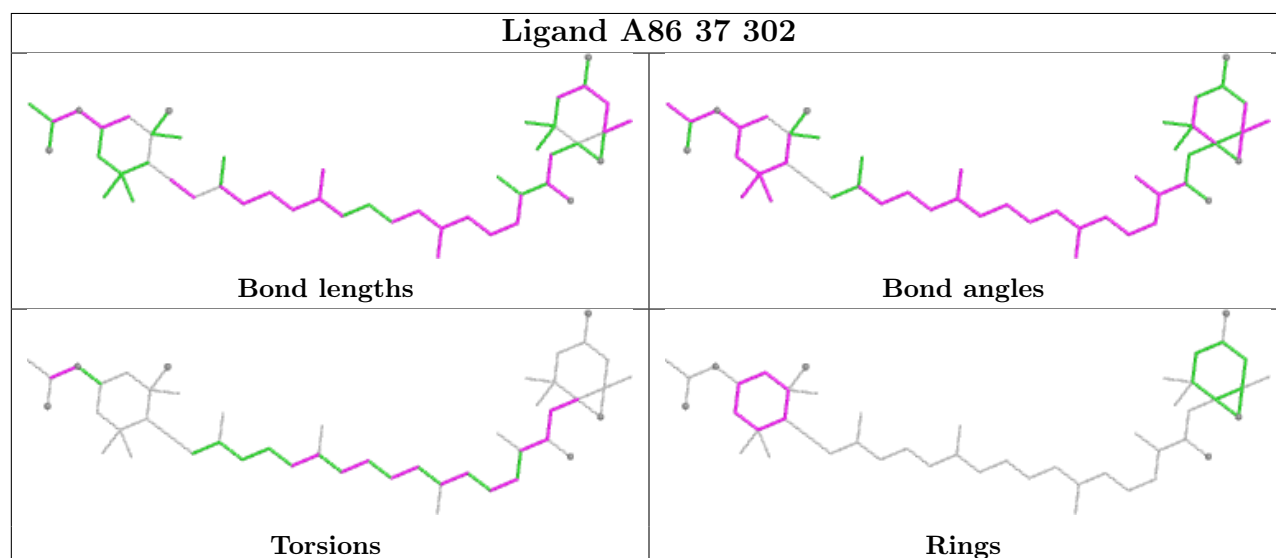
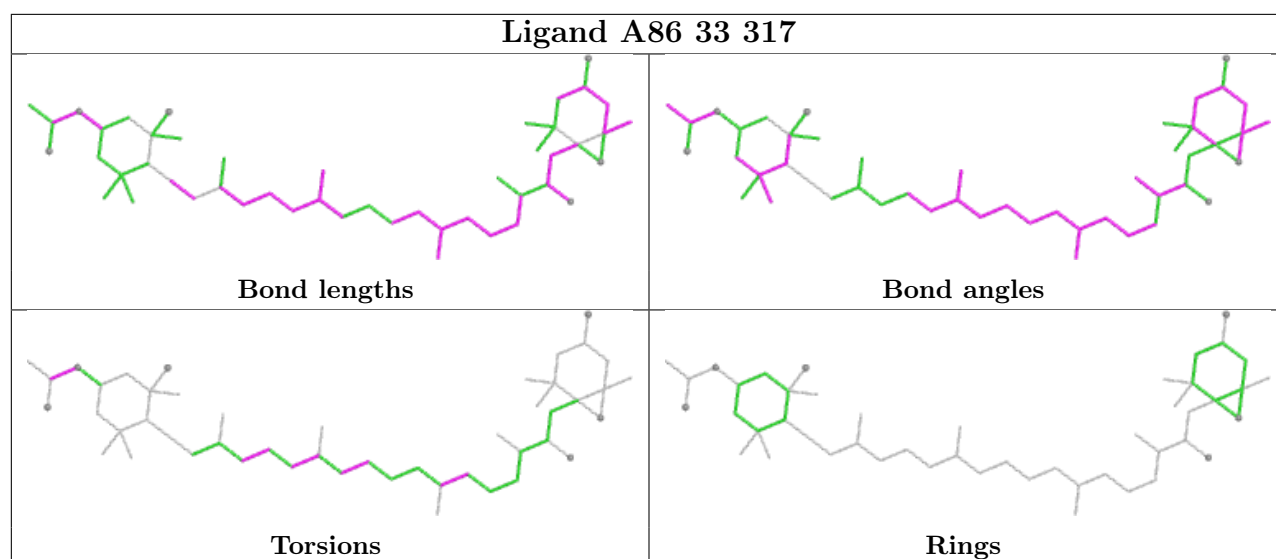


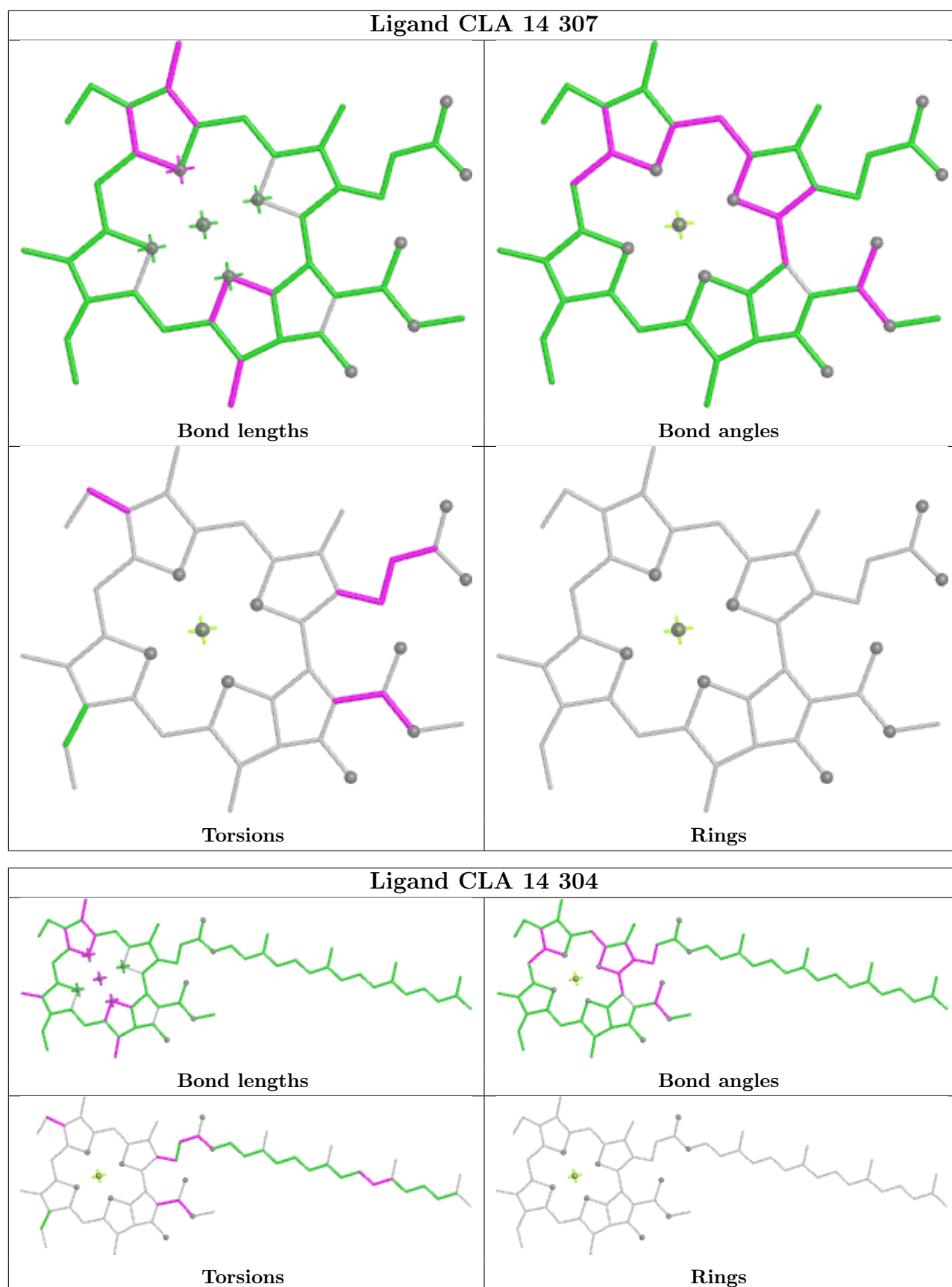


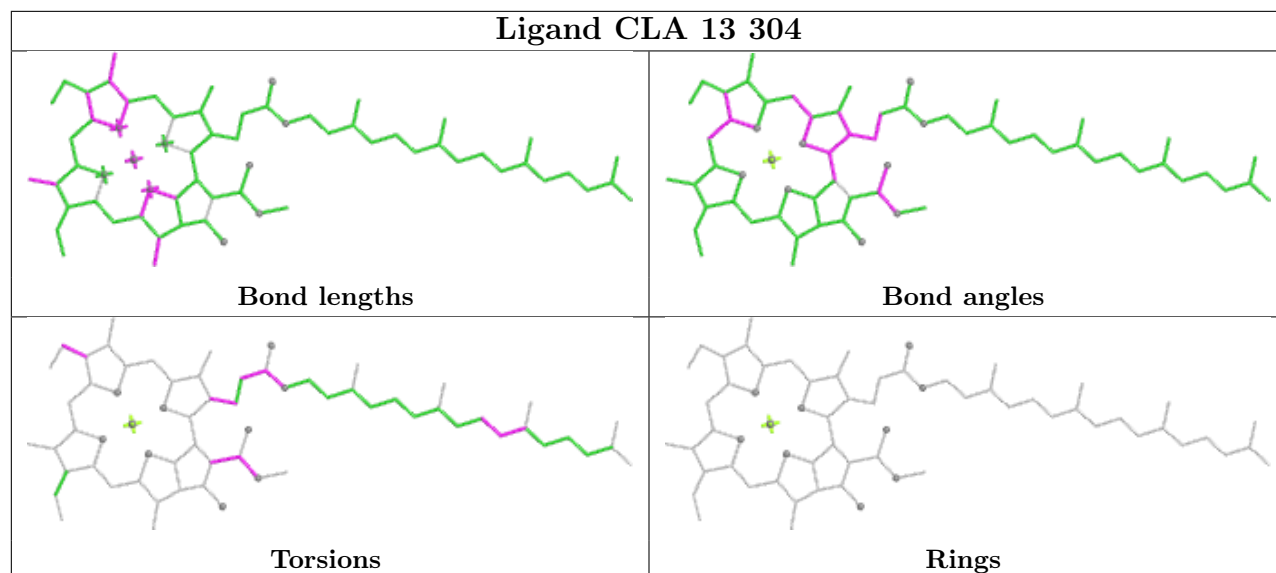
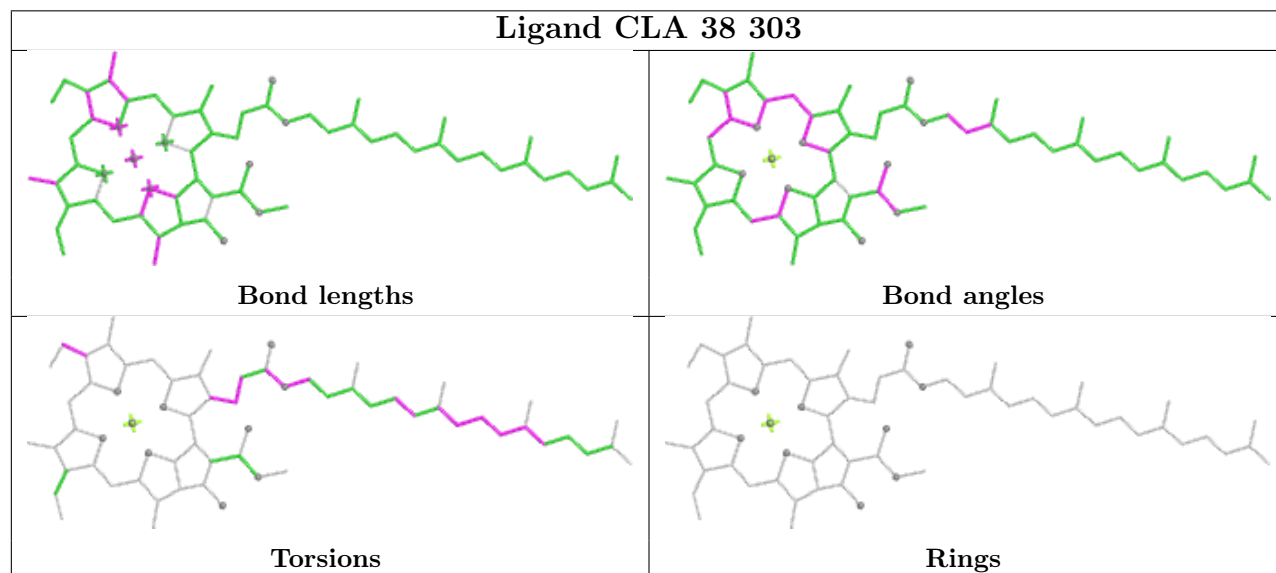
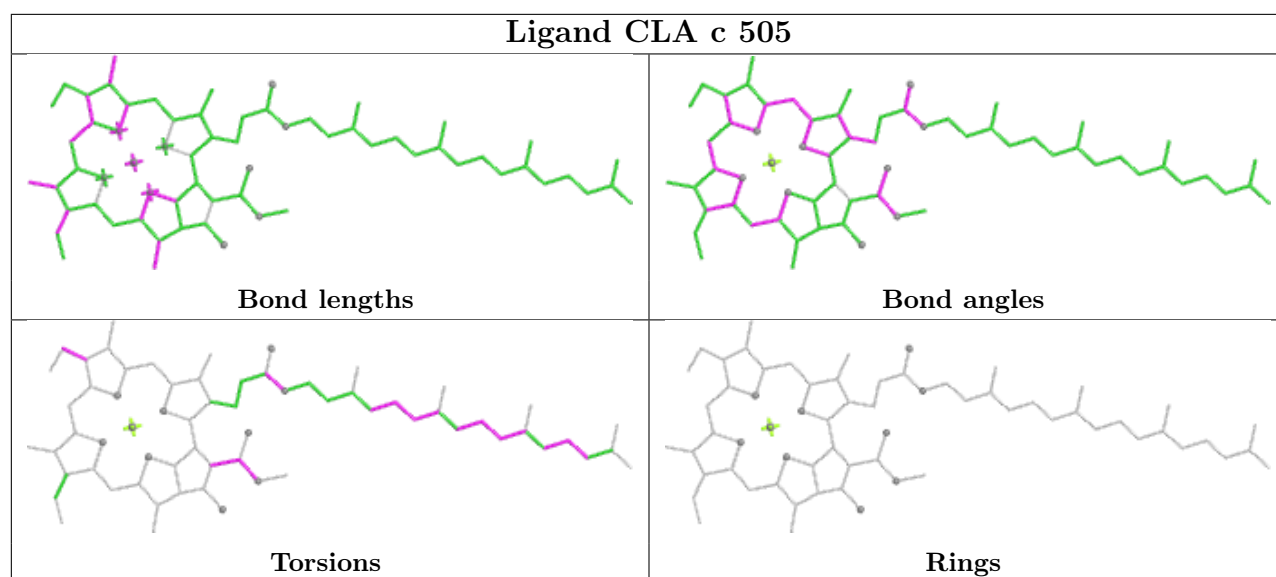


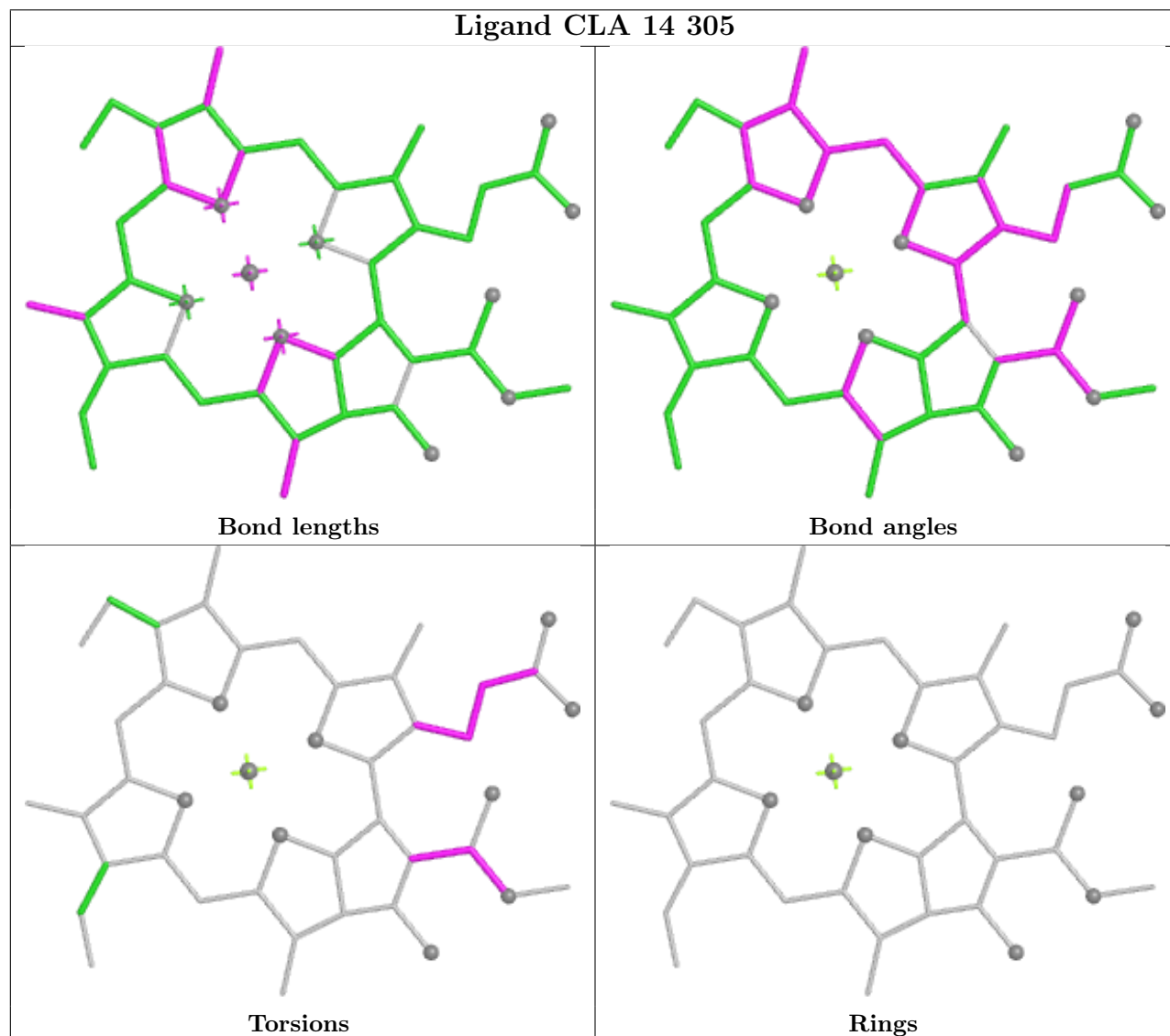
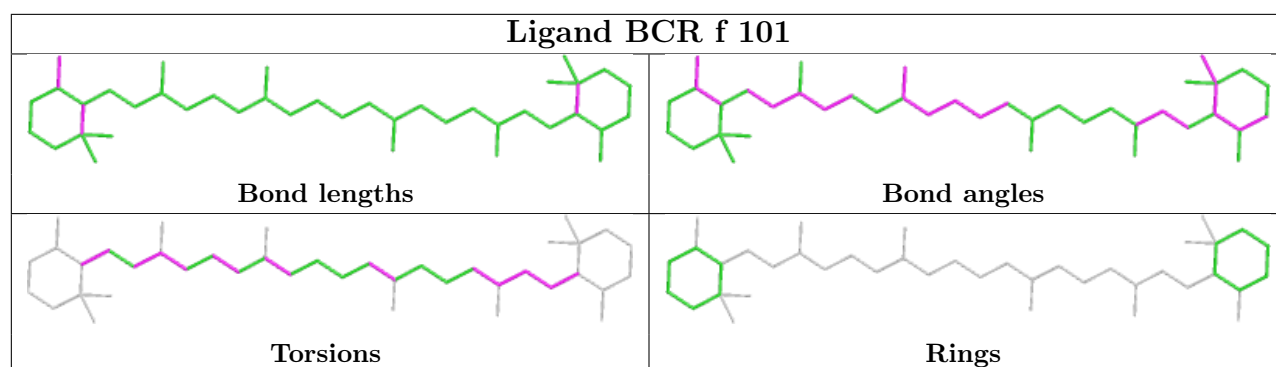


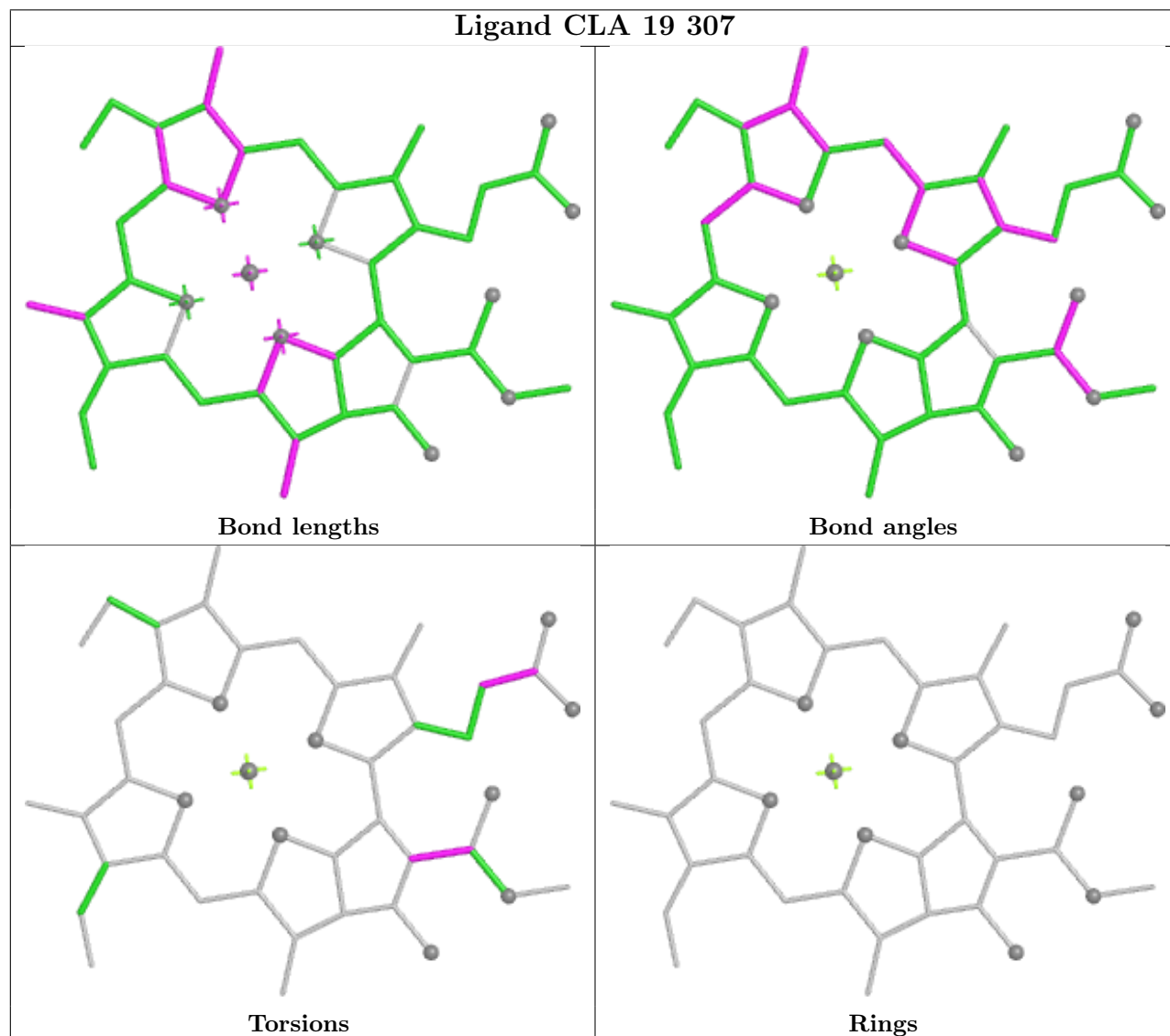
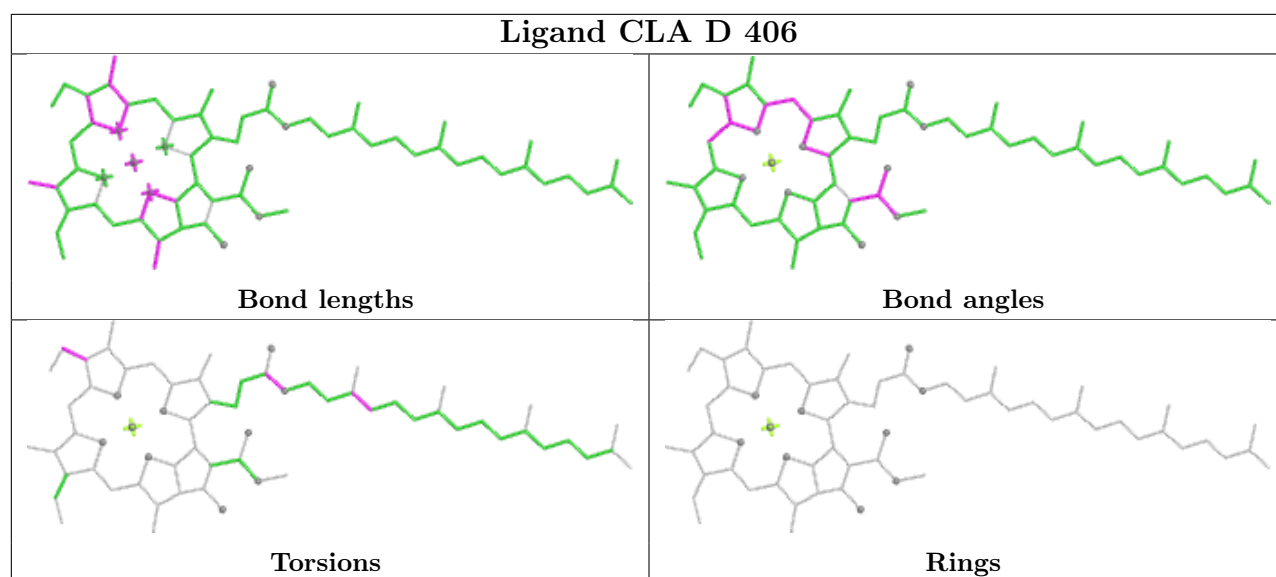


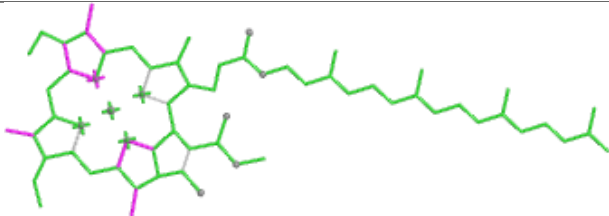
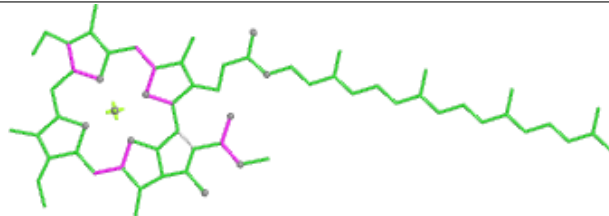
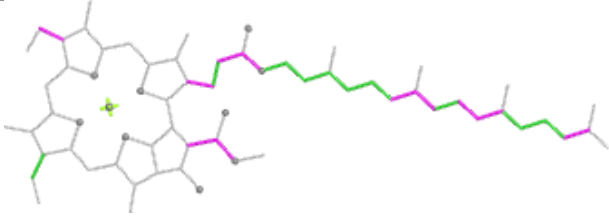
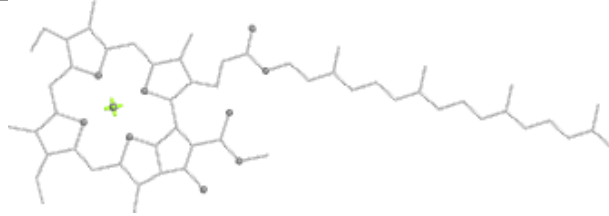


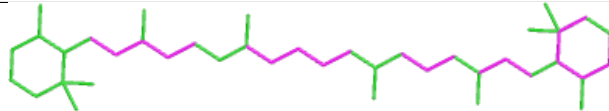
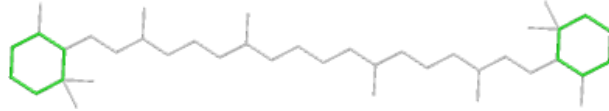


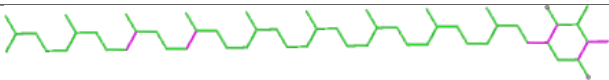
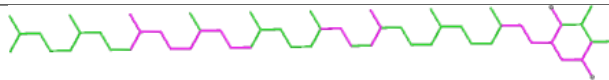
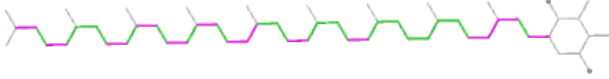
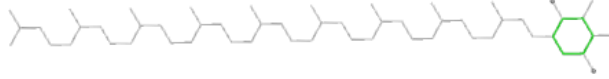


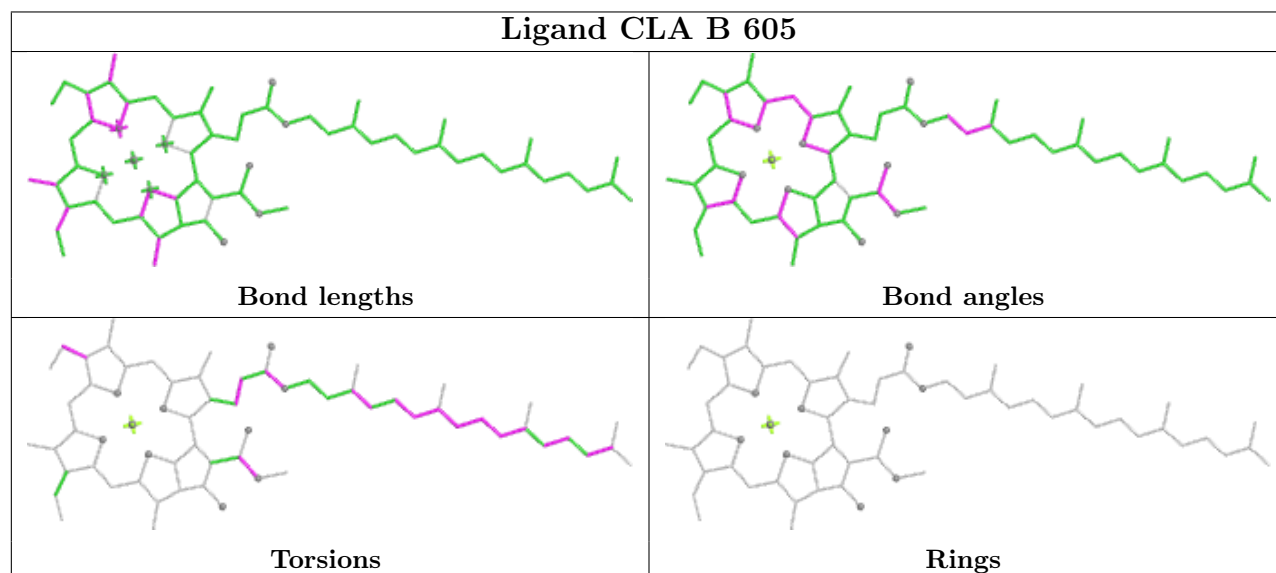
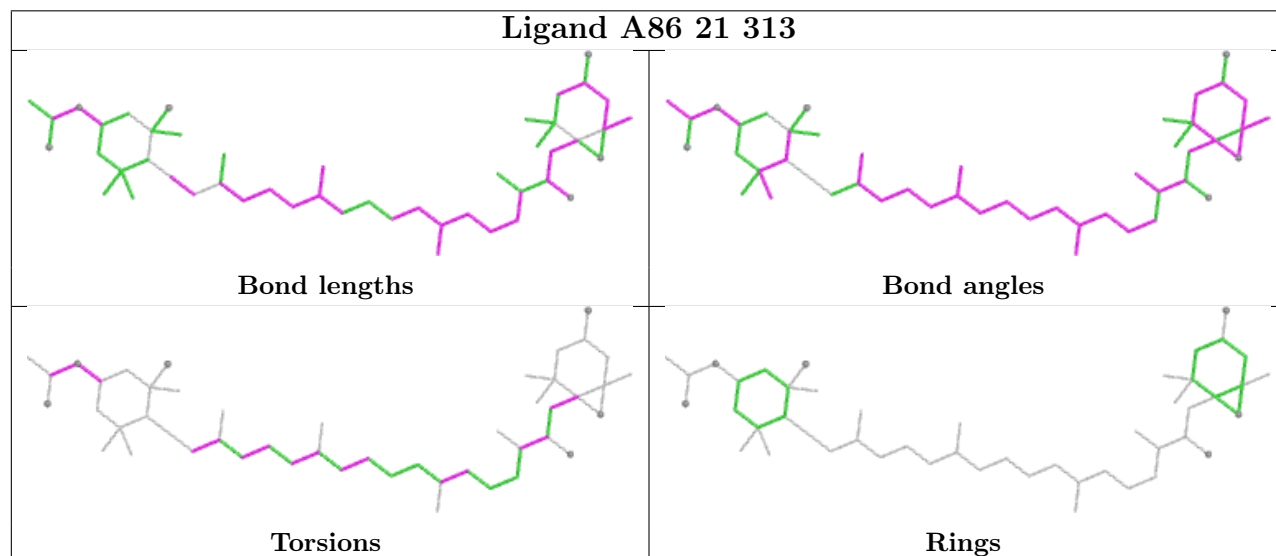
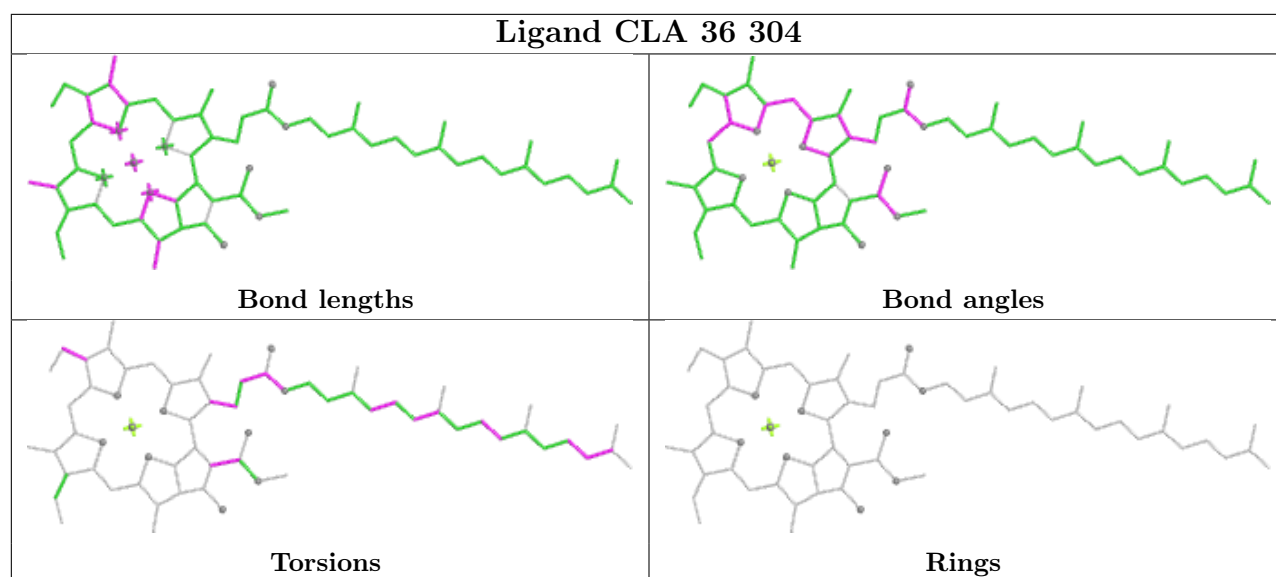


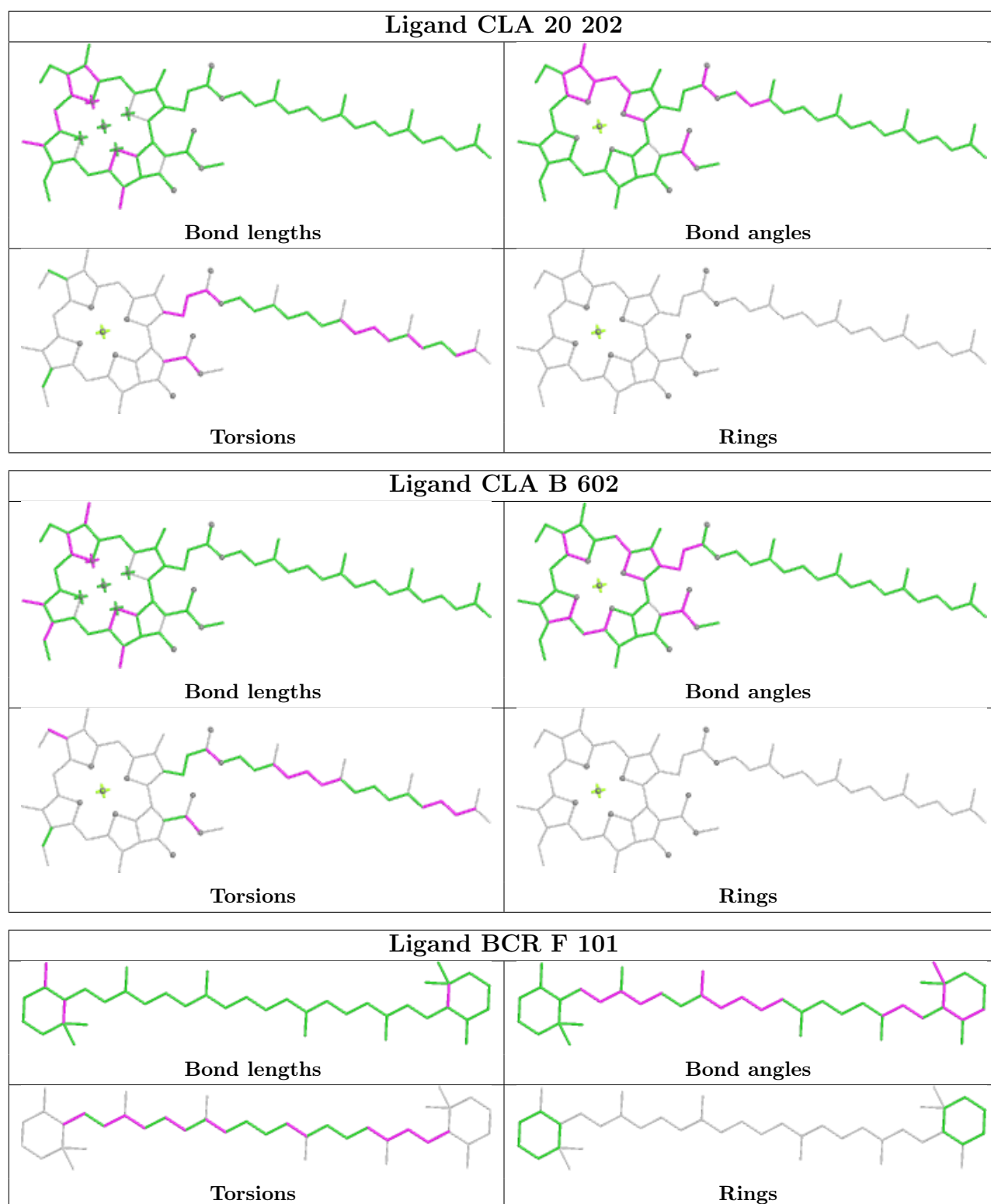


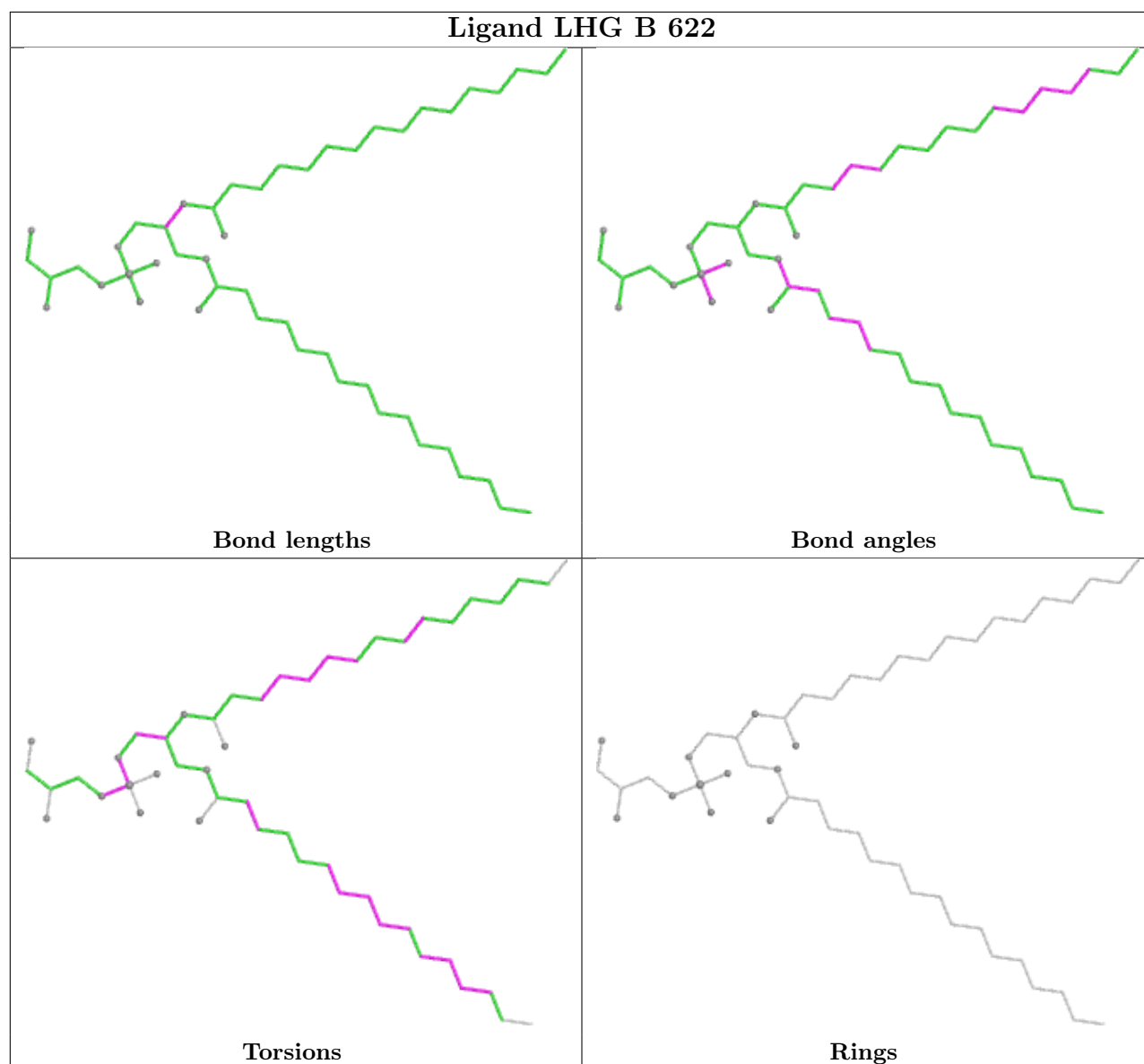
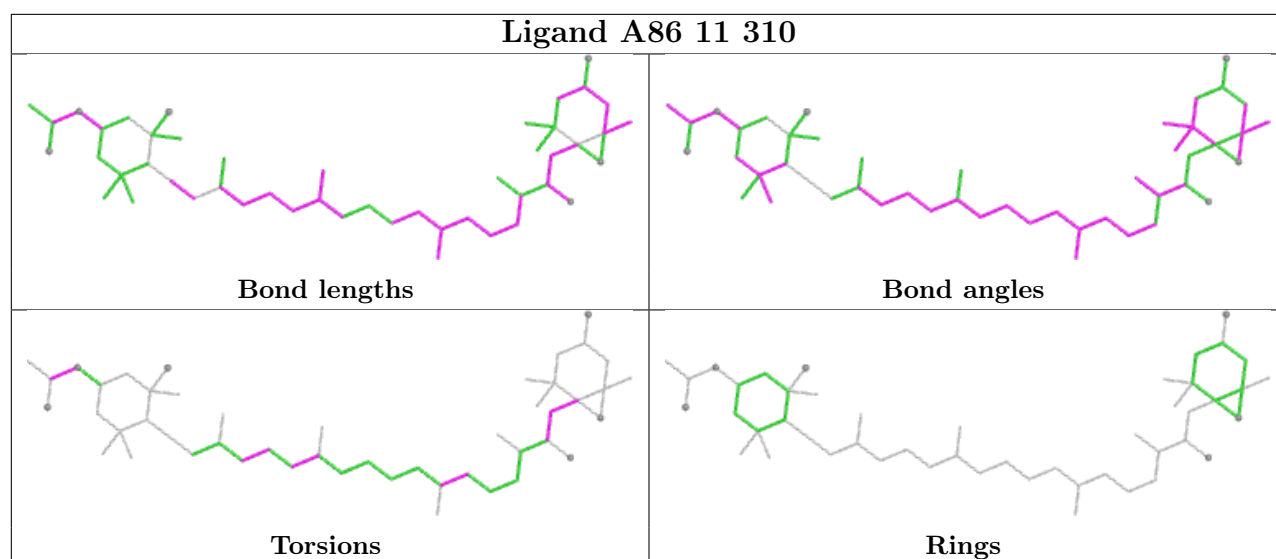
Ligand CLA 38 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

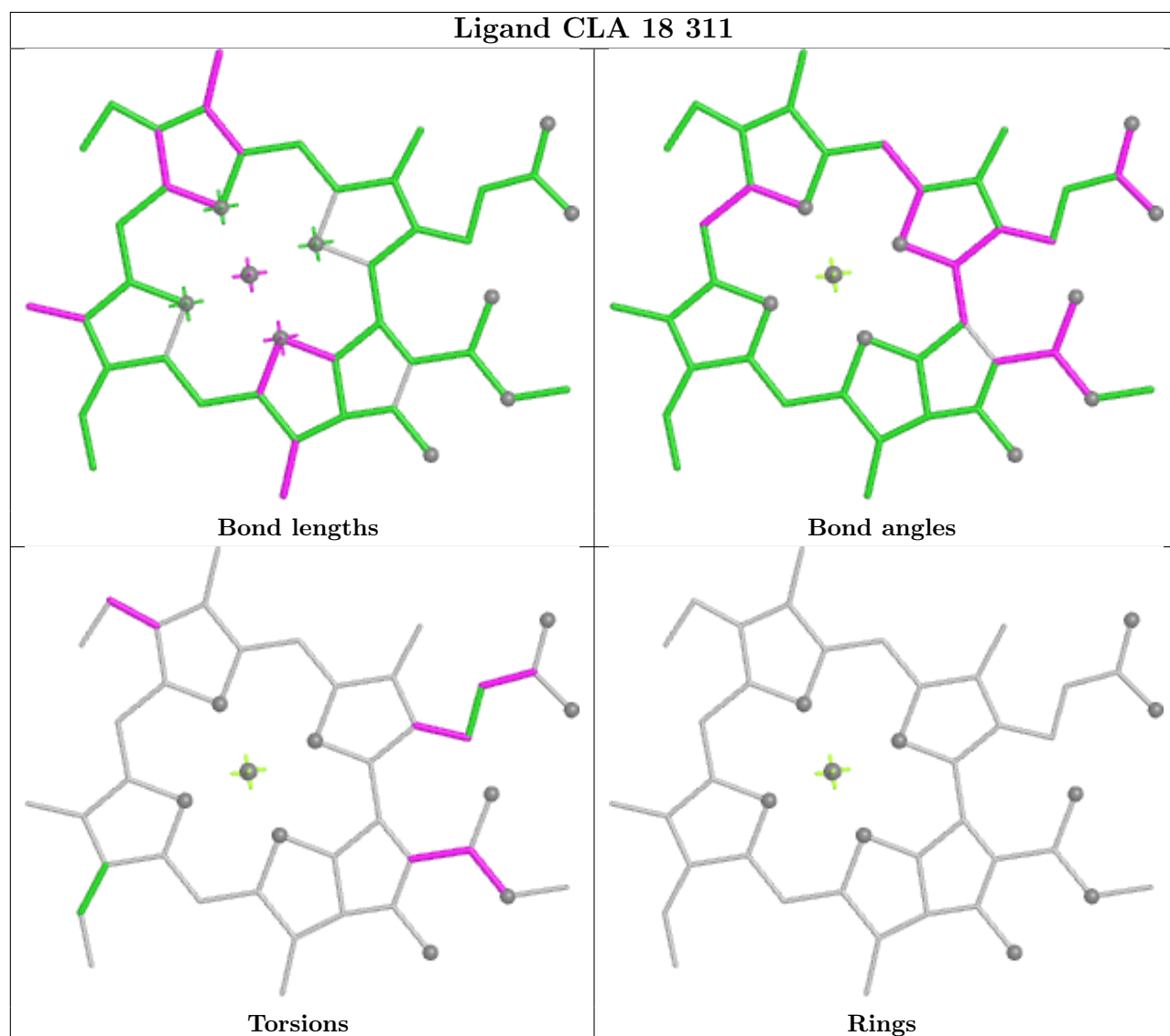
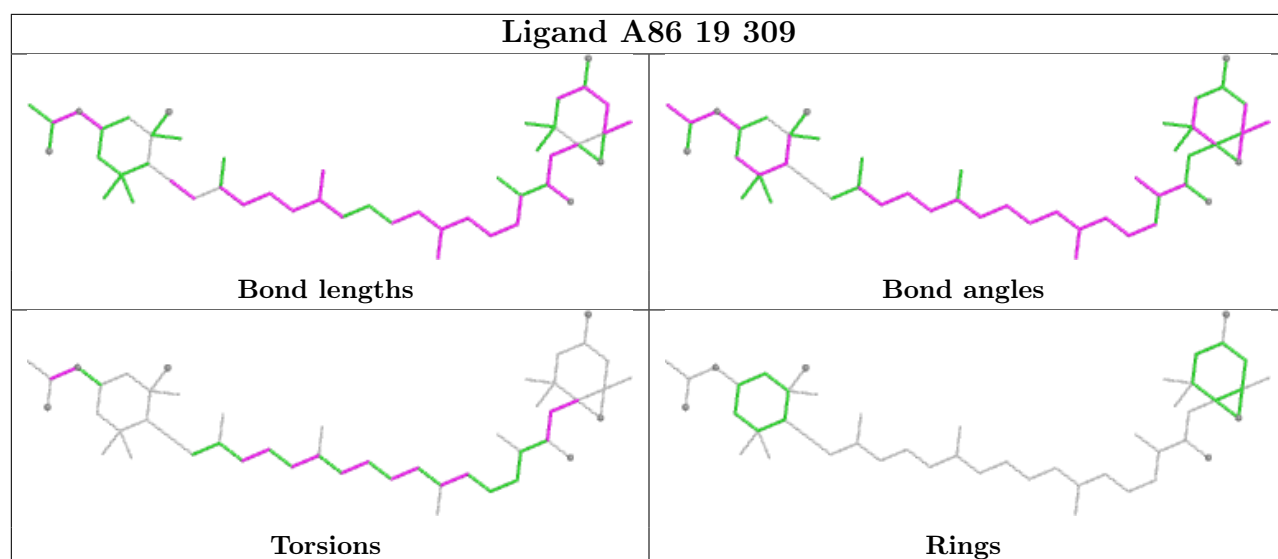
Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

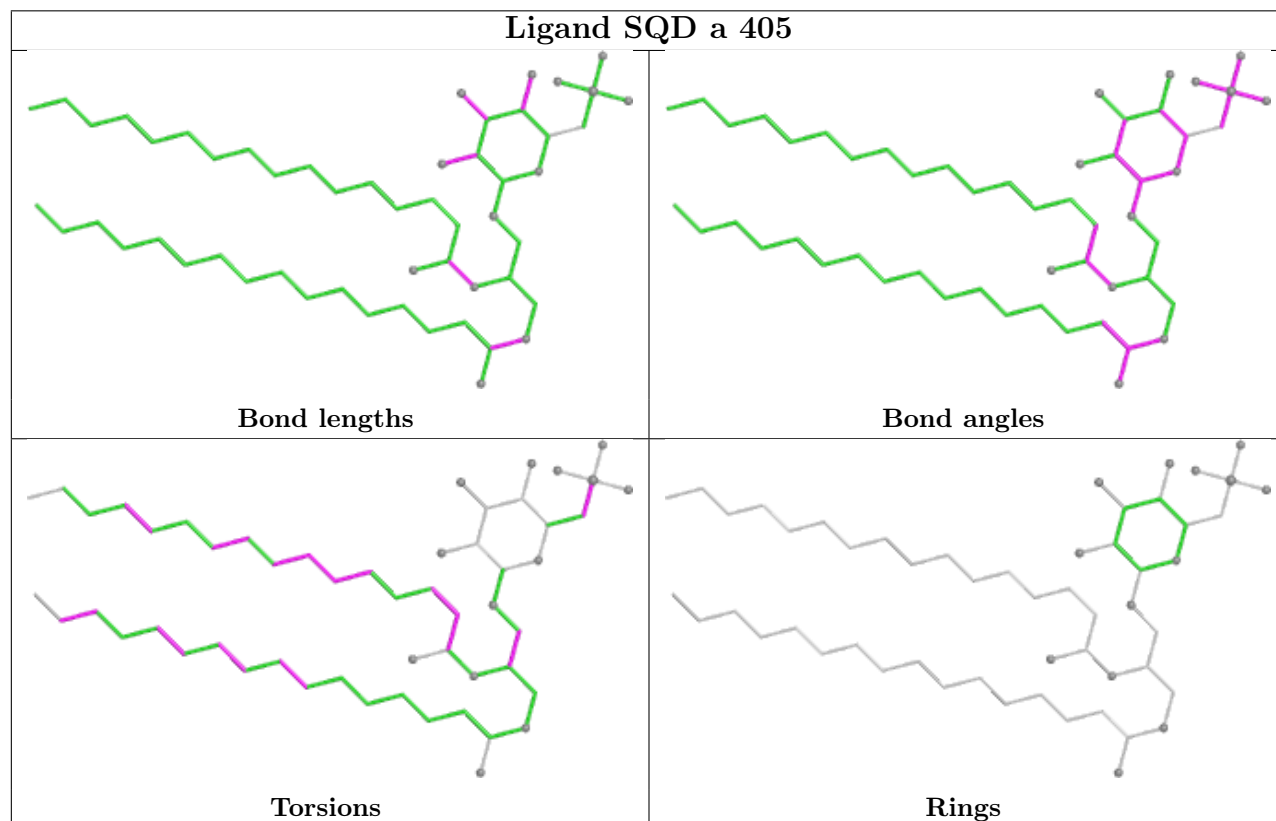
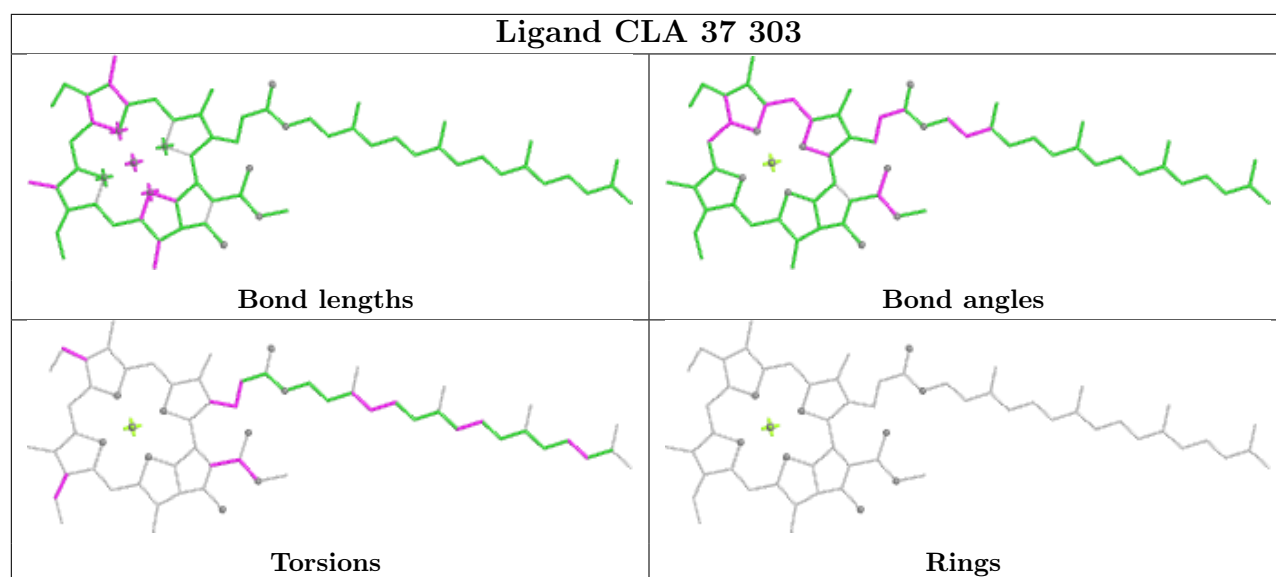
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

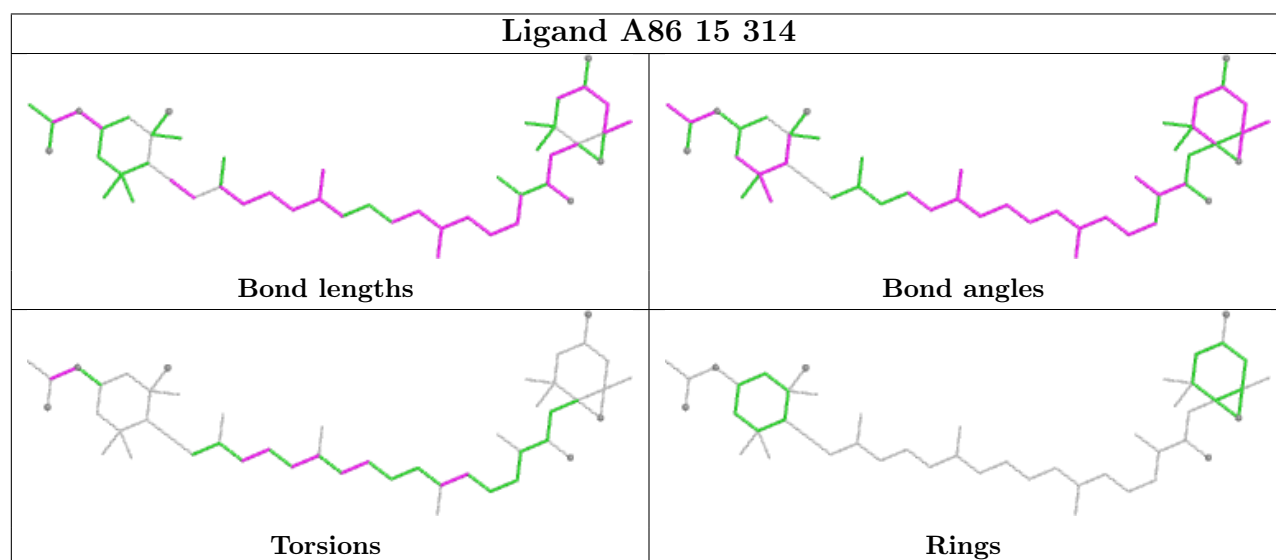
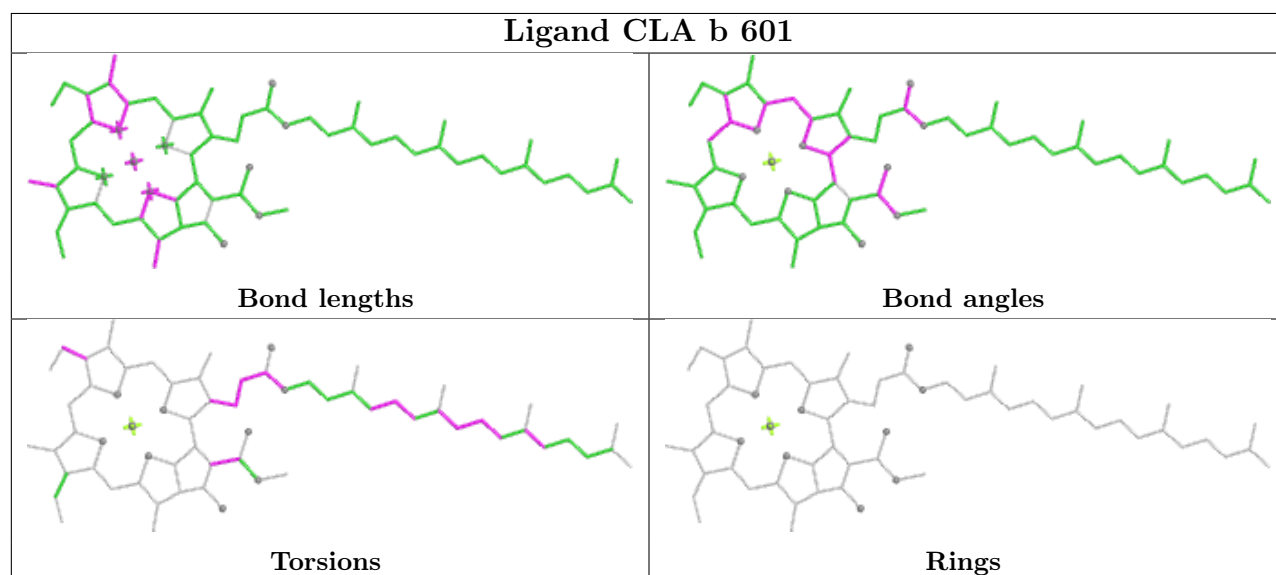
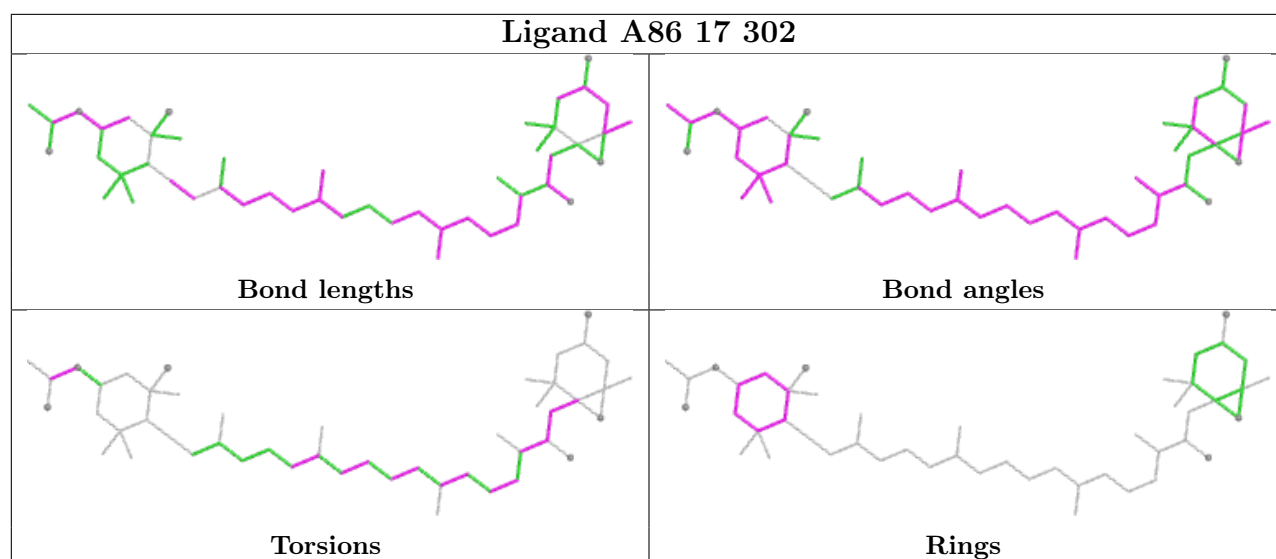


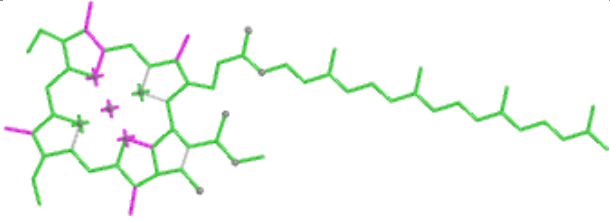
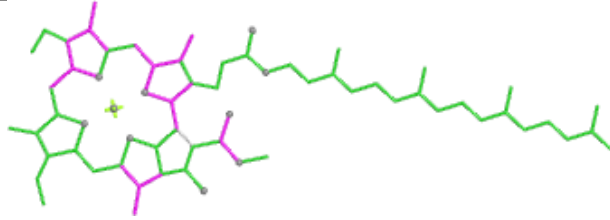
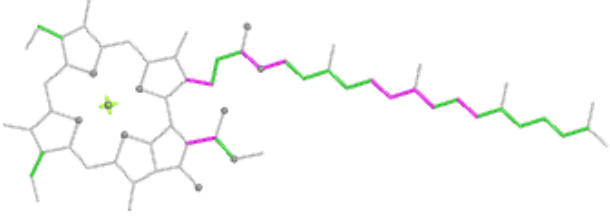
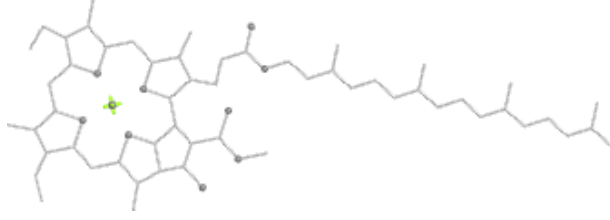
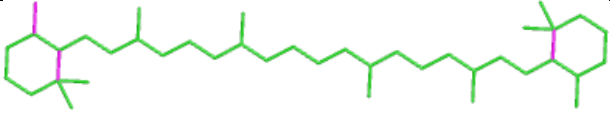
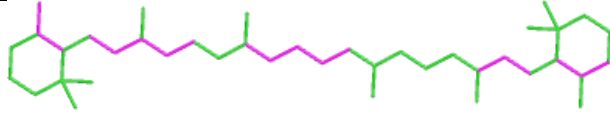
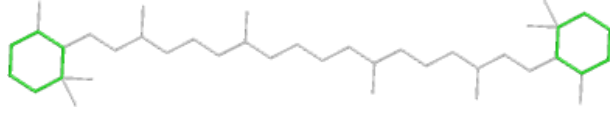
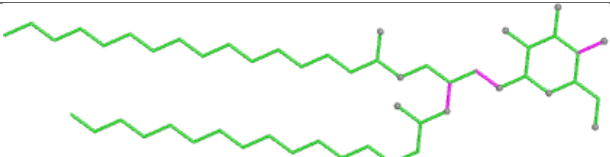
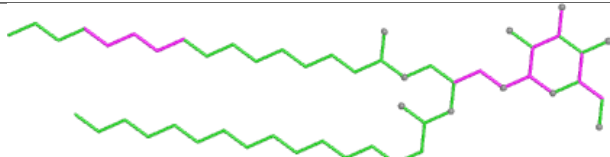
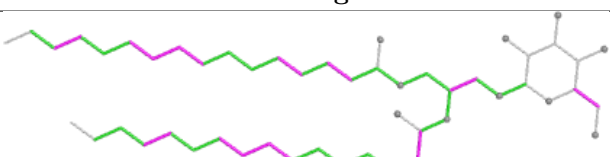
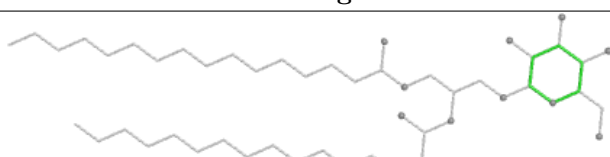


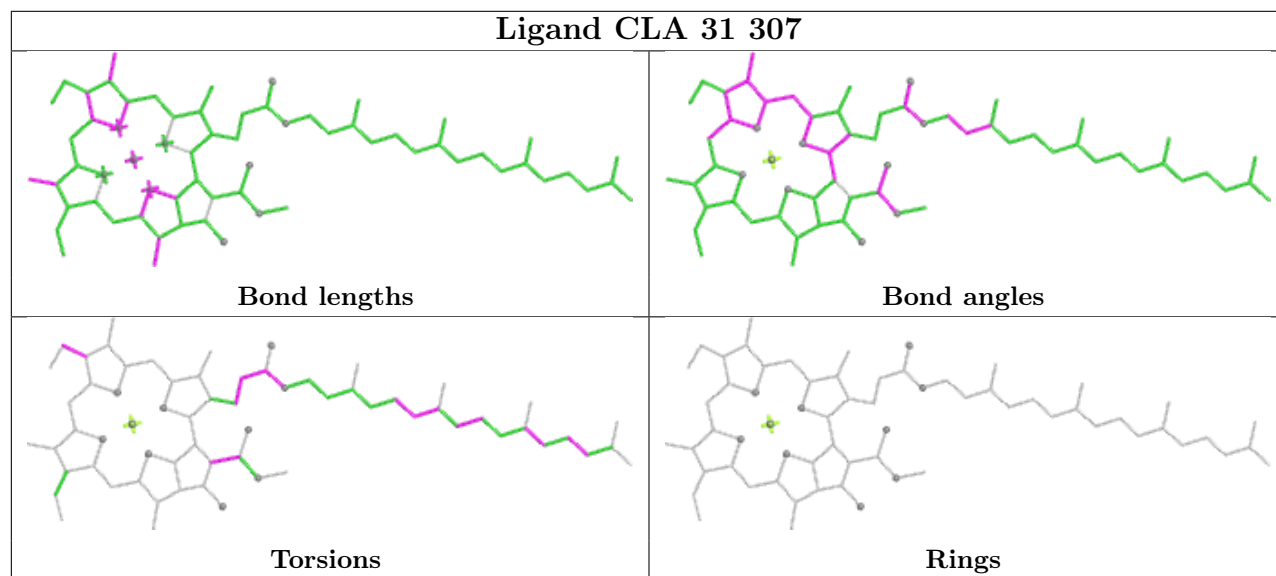
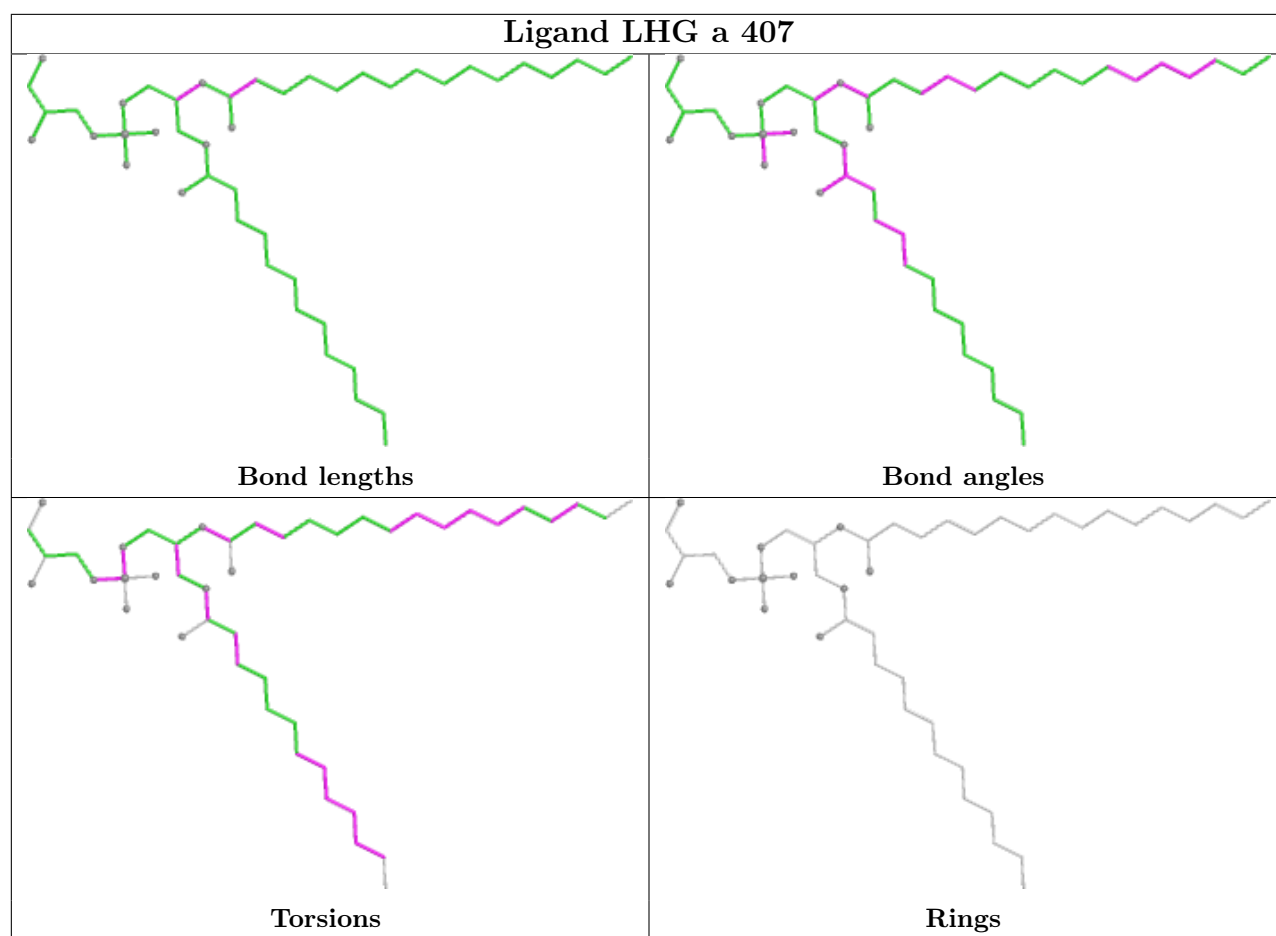


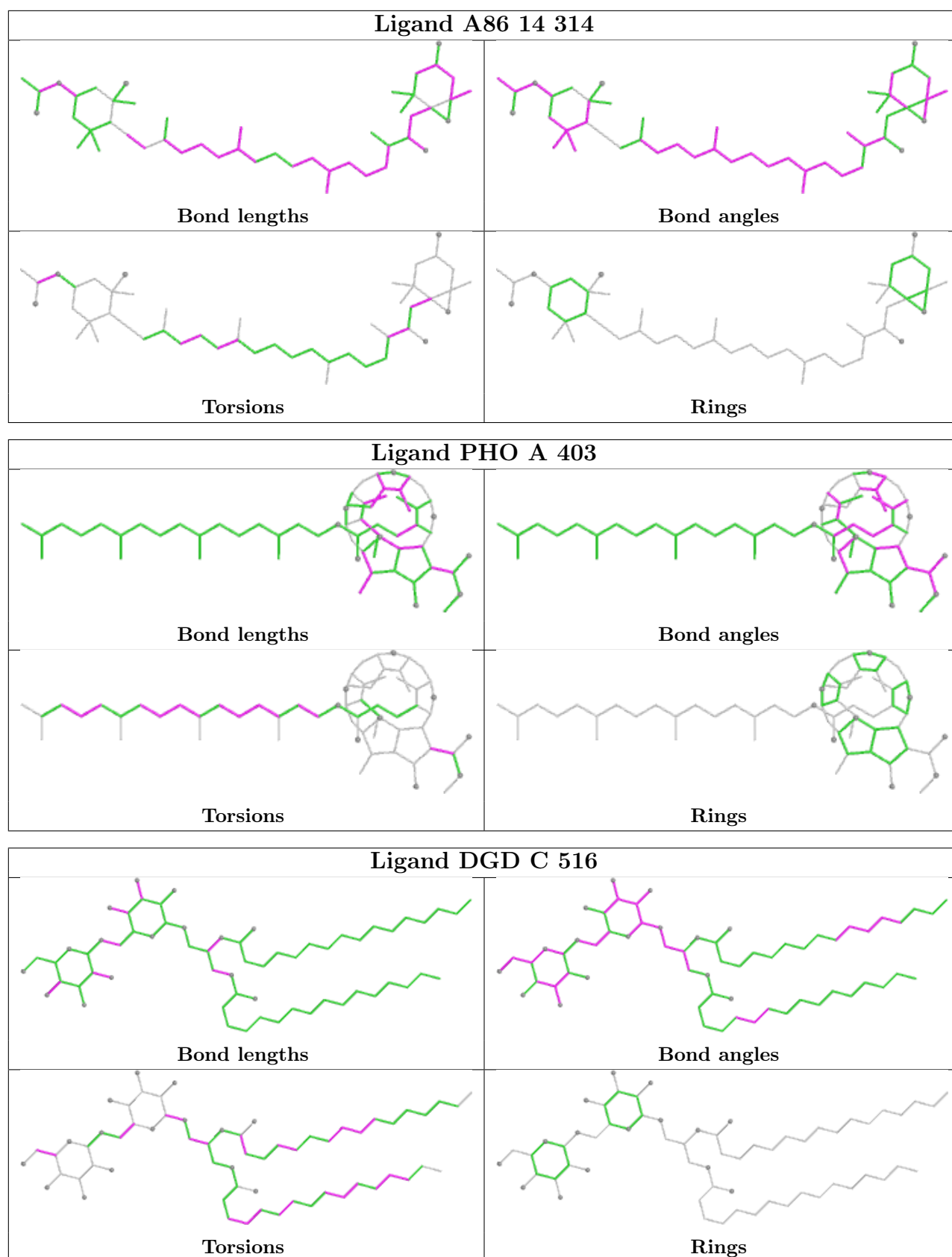


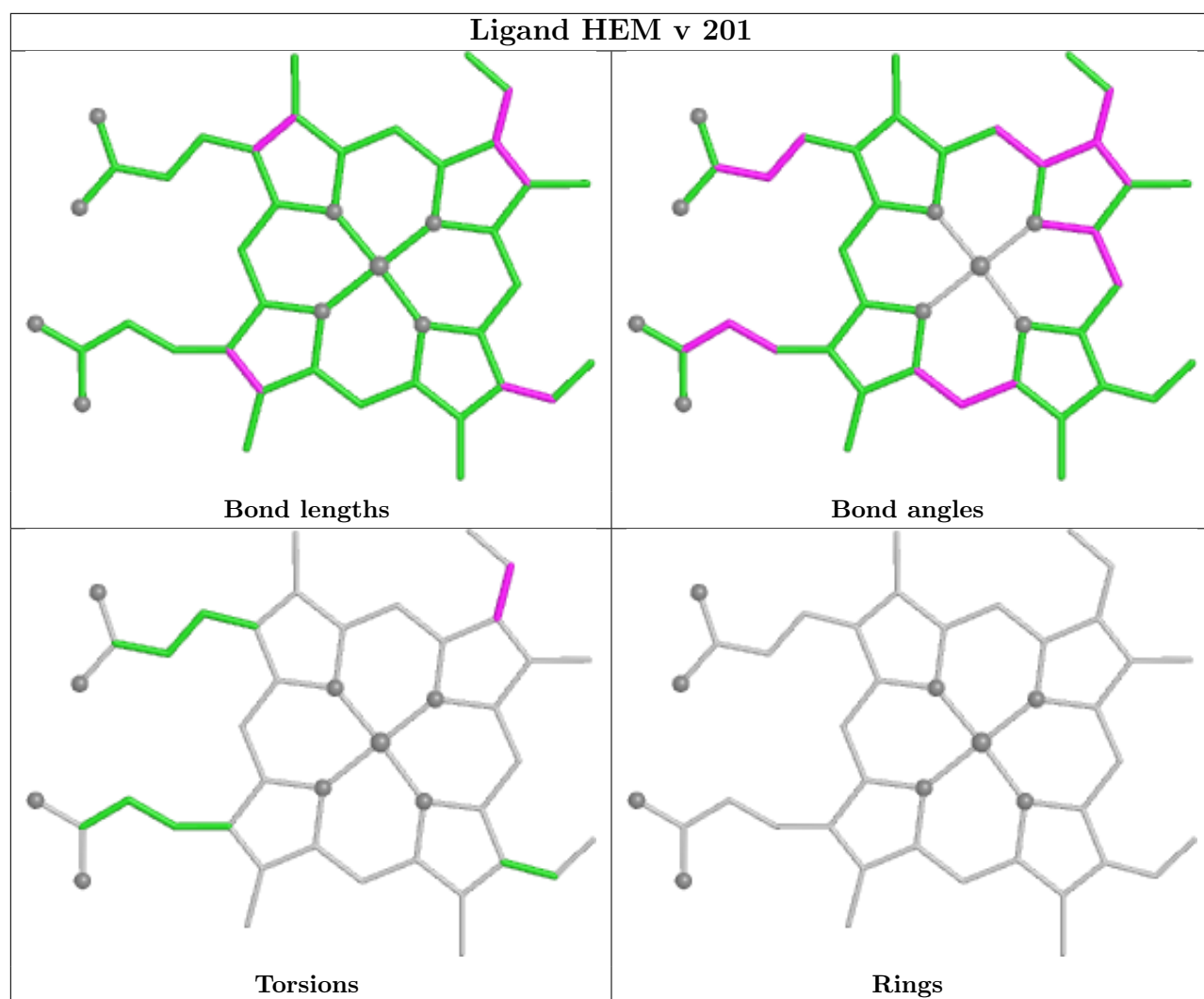


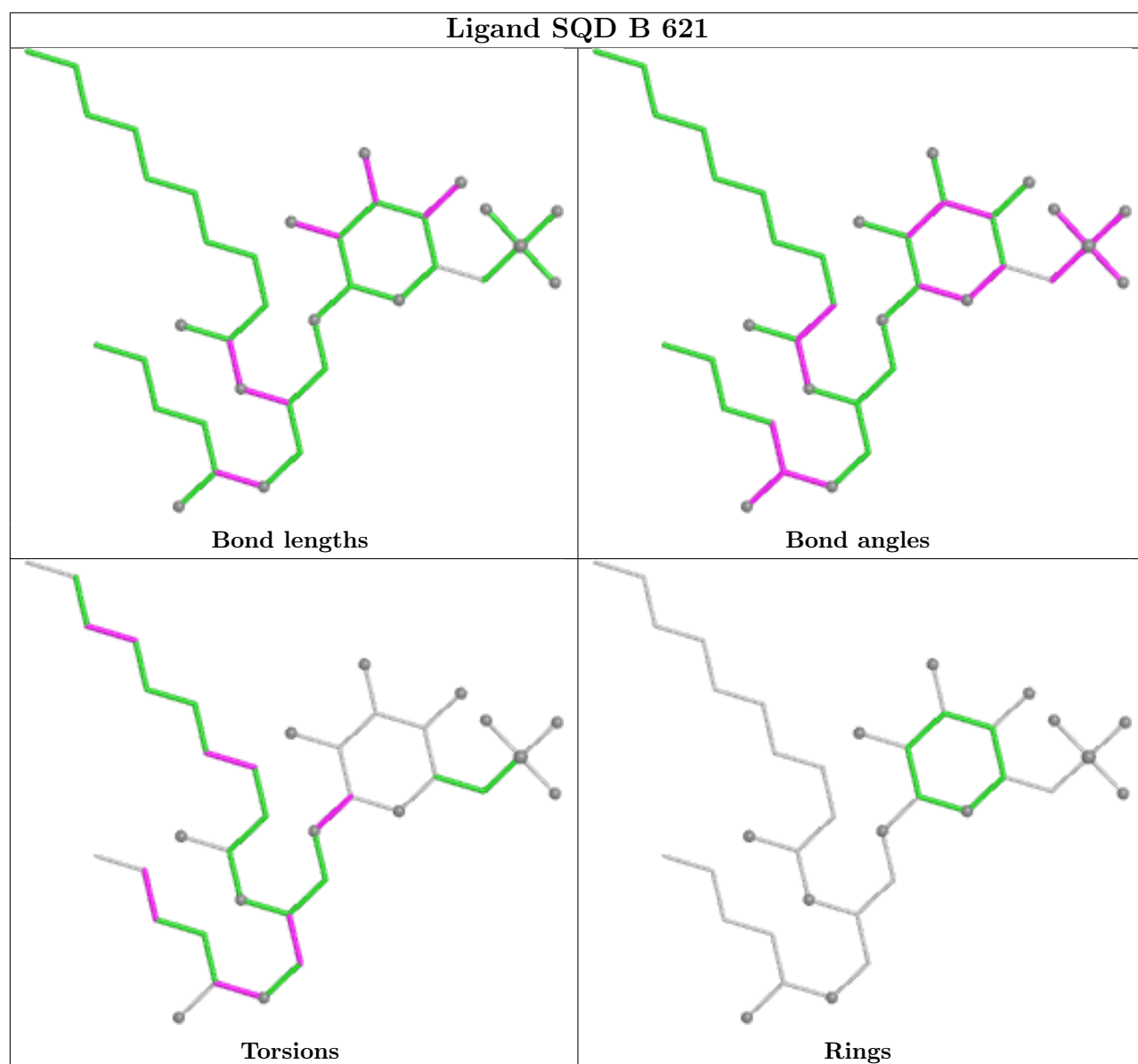


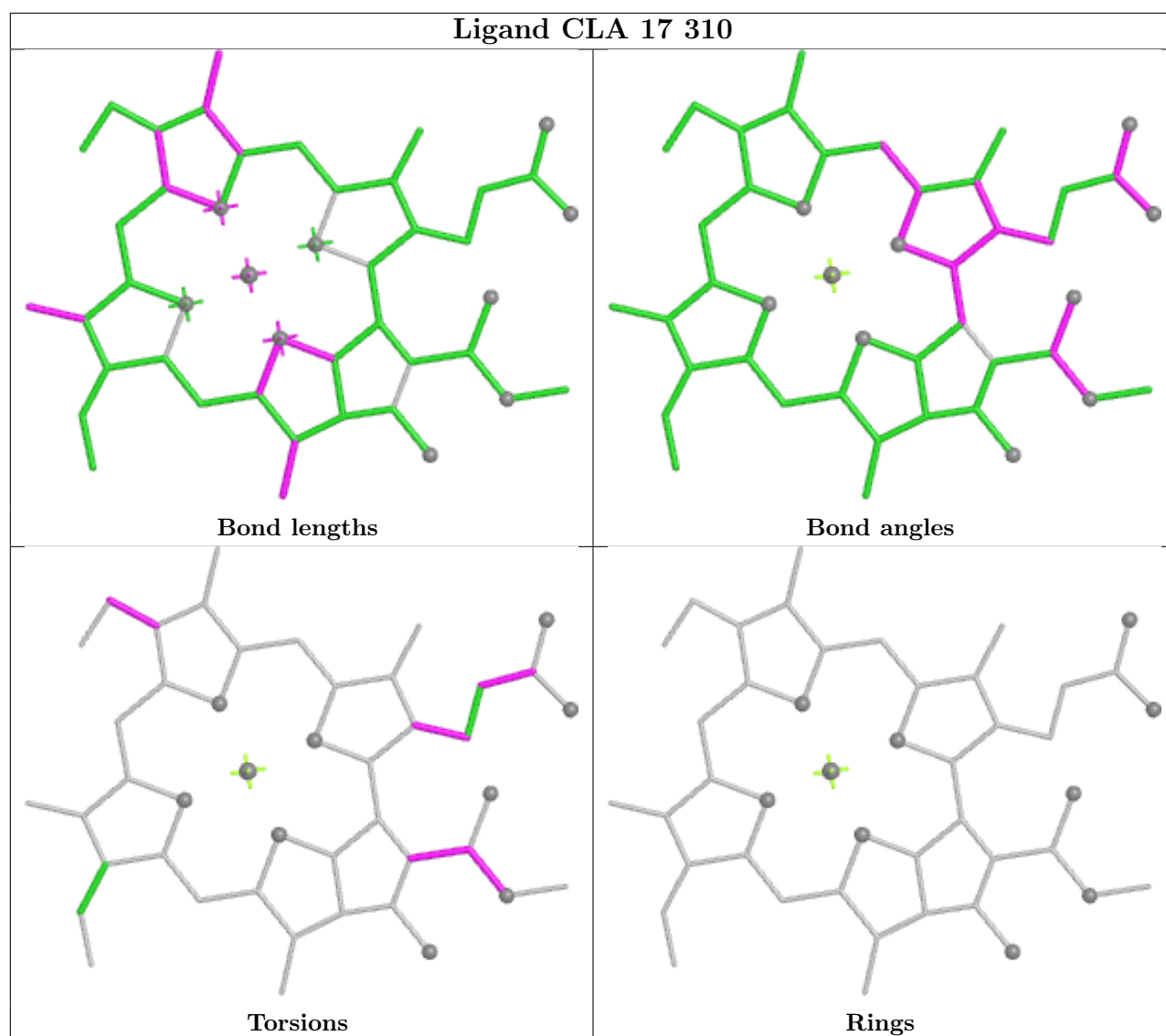
Ligand CLA B 612	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG d 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

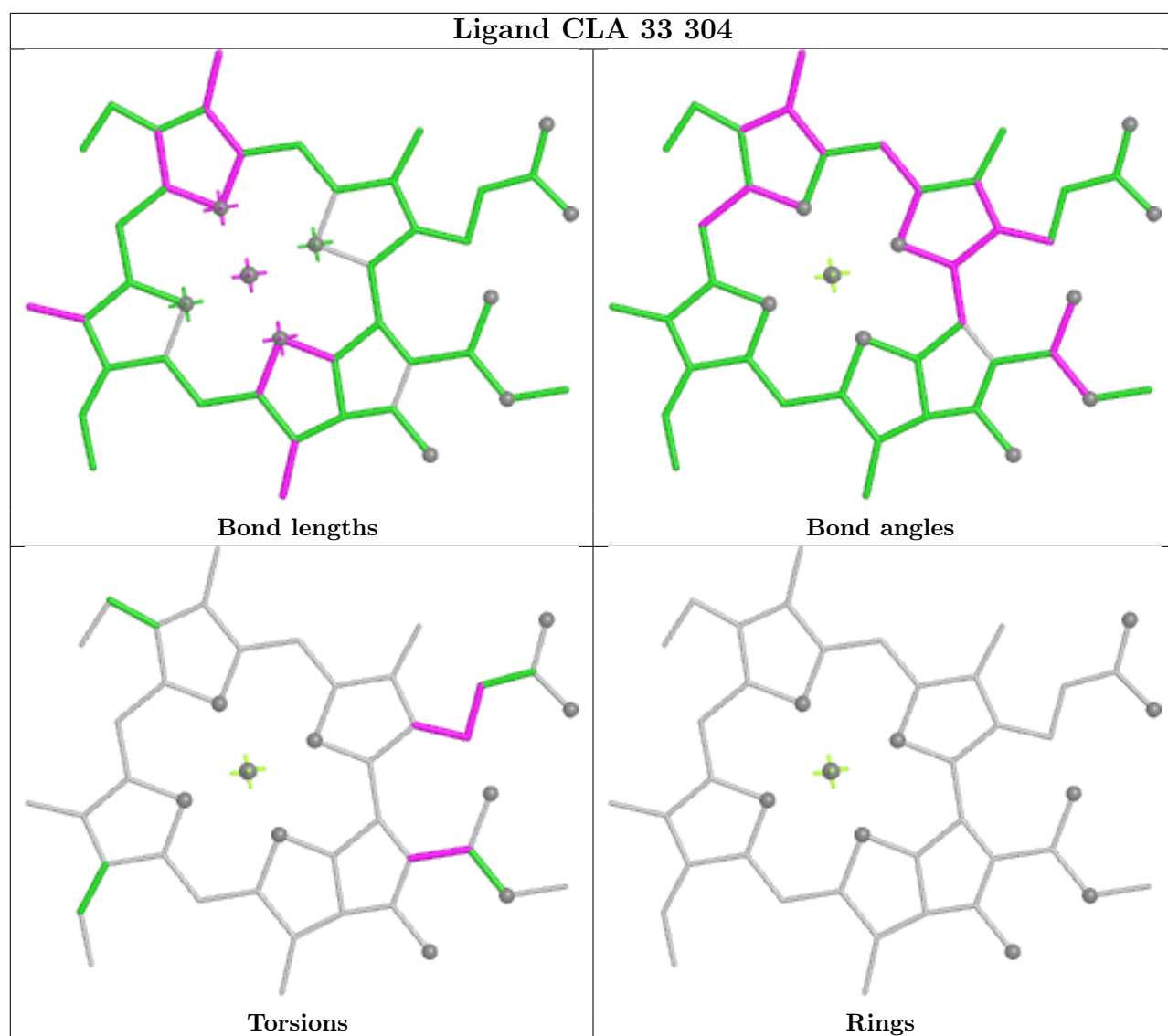


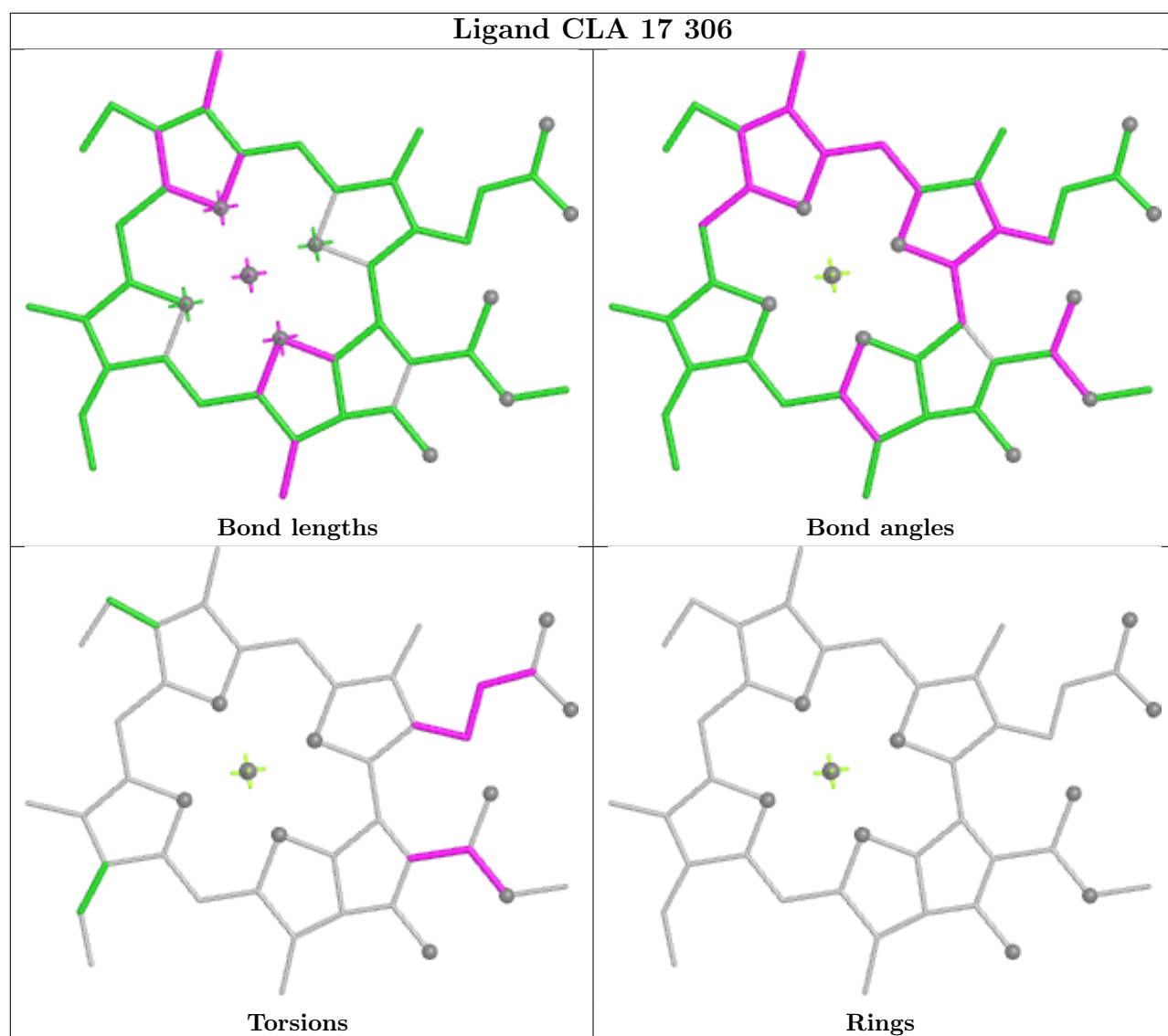


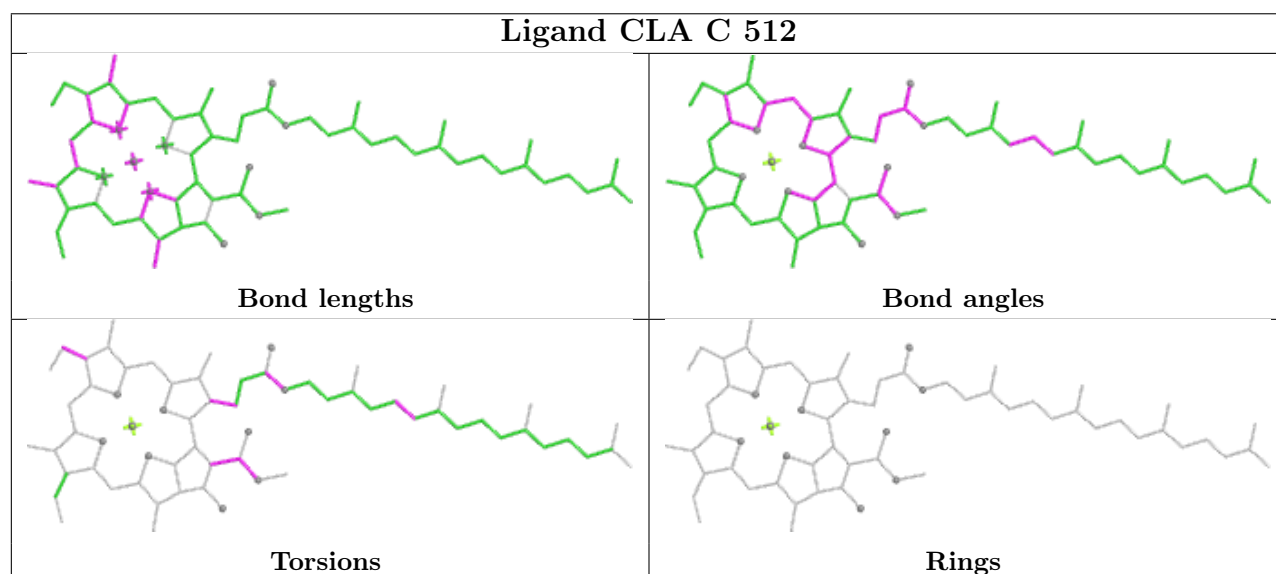
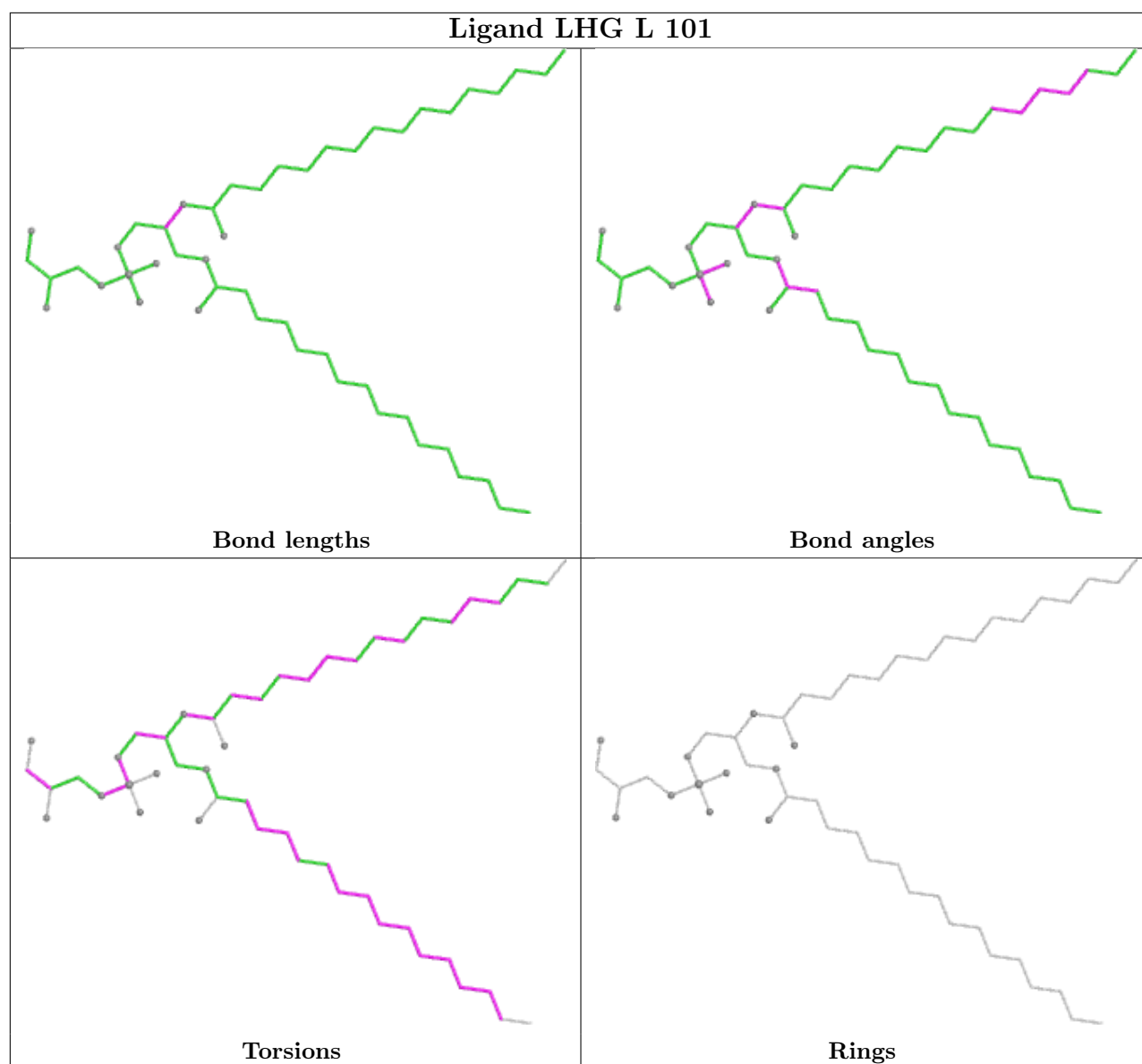


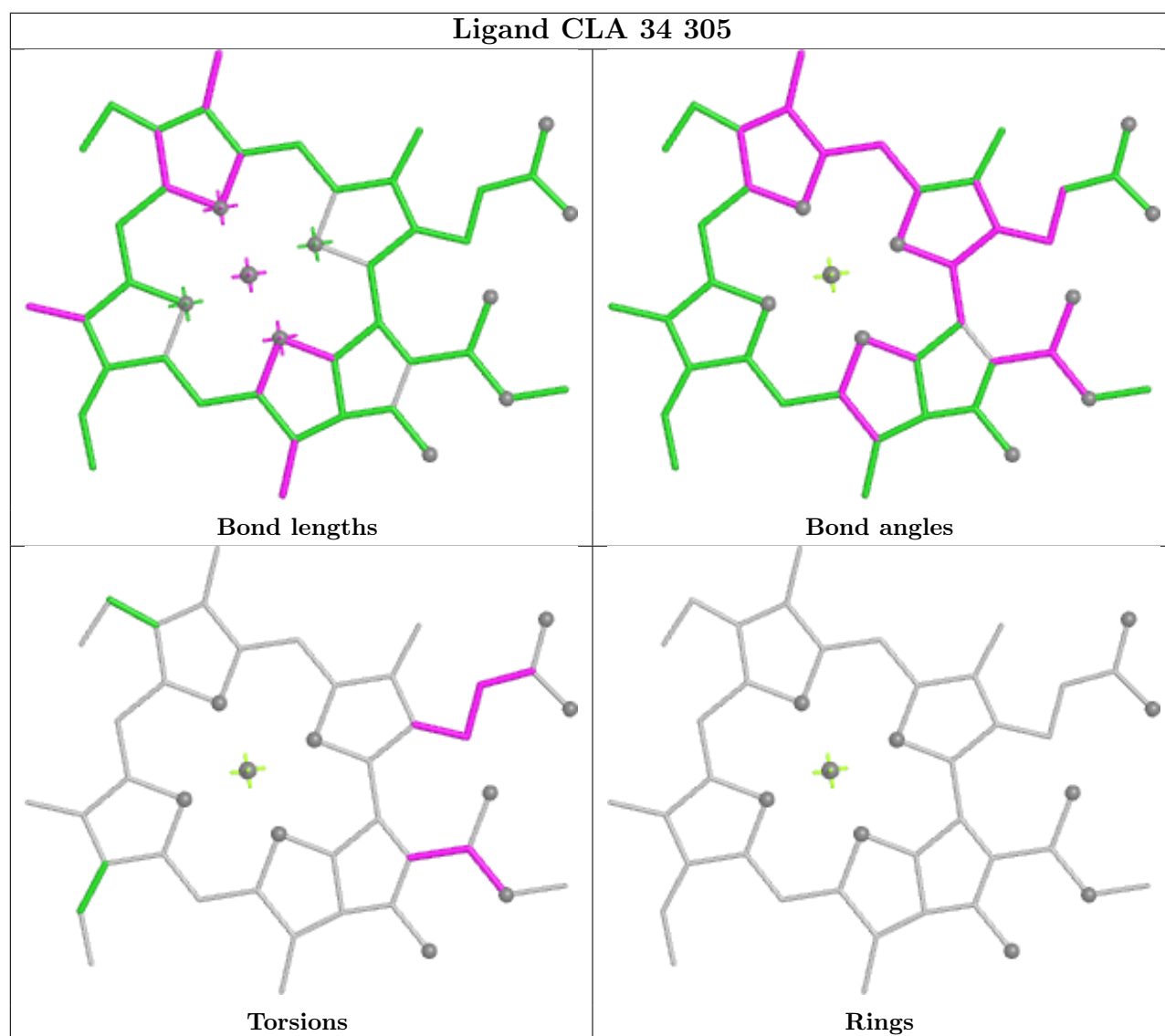
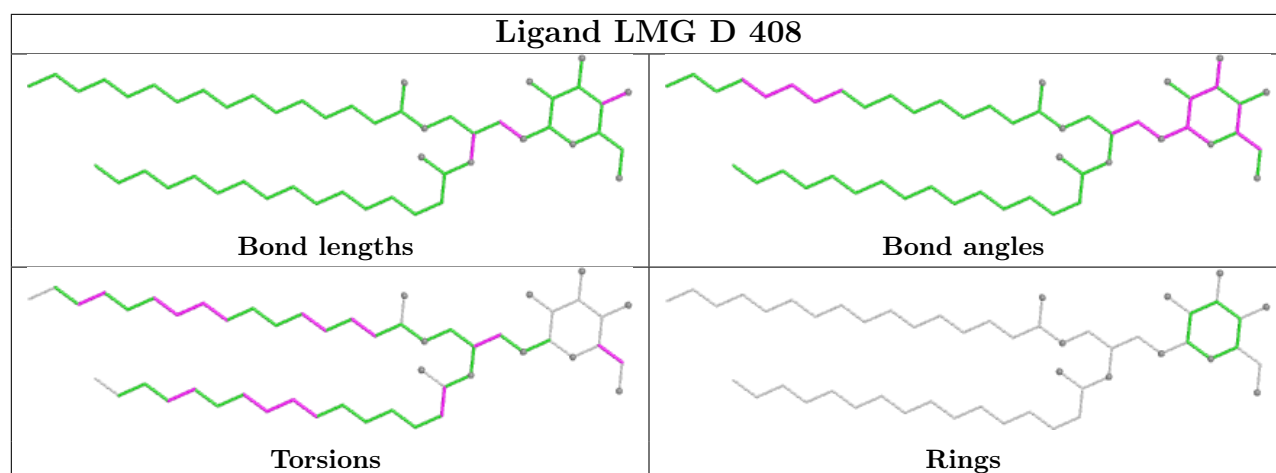


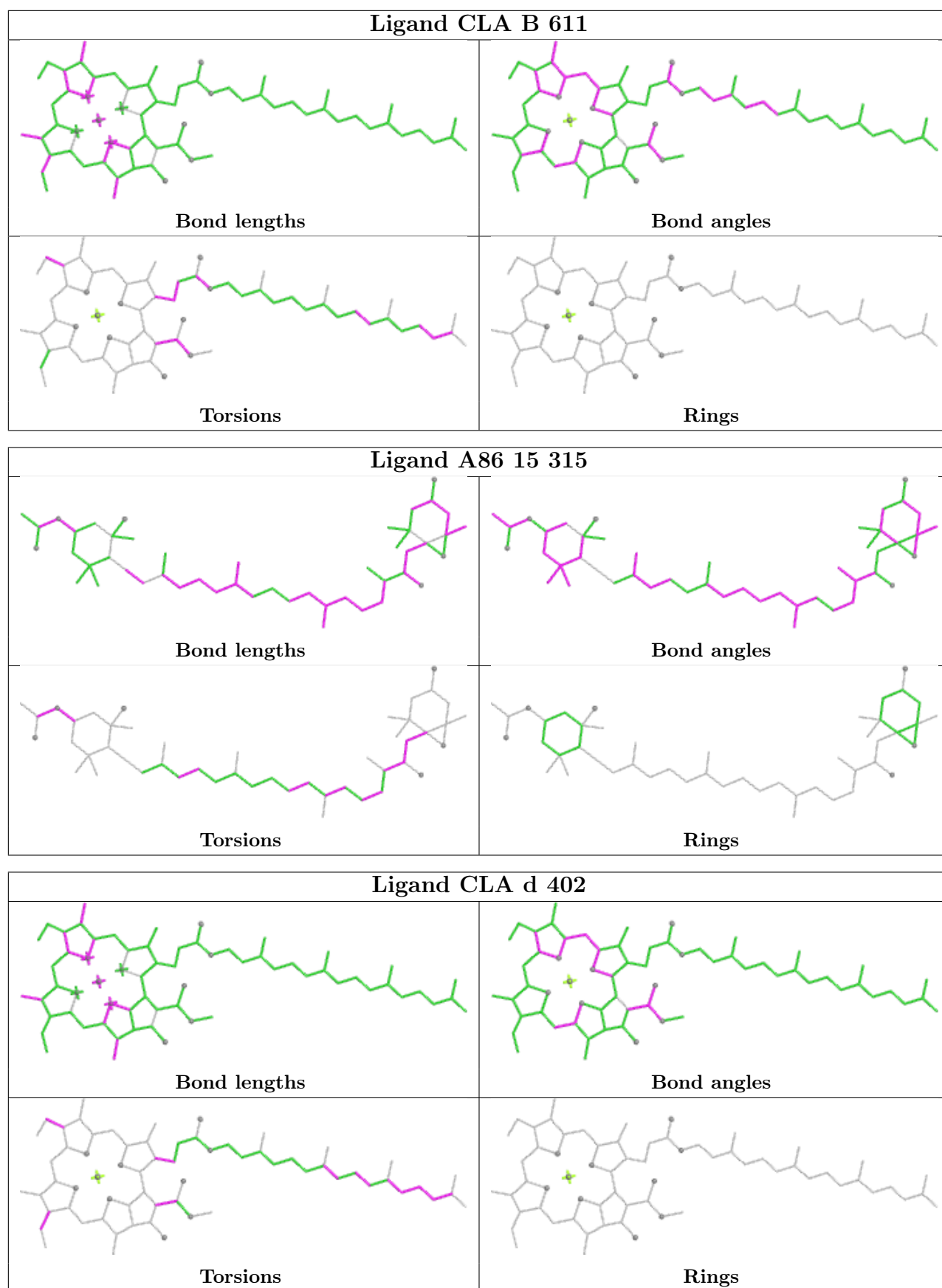


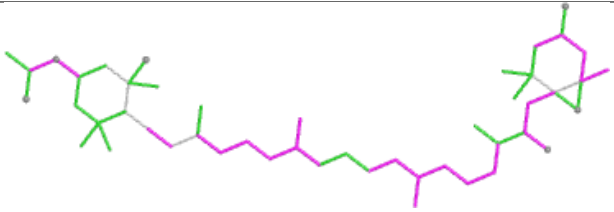
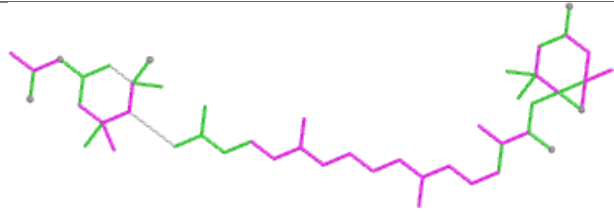
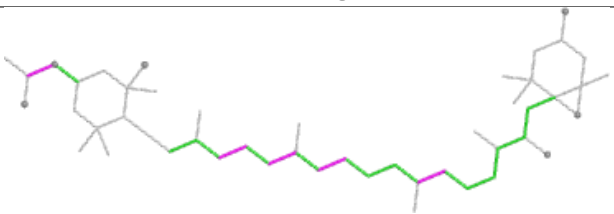
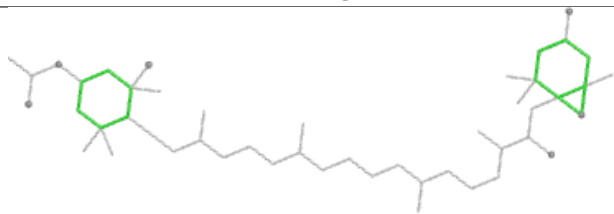


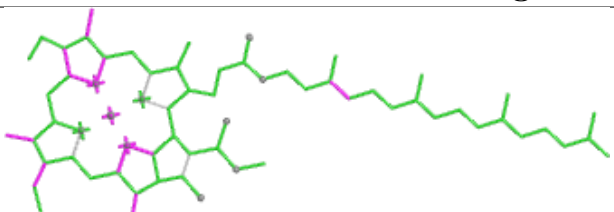
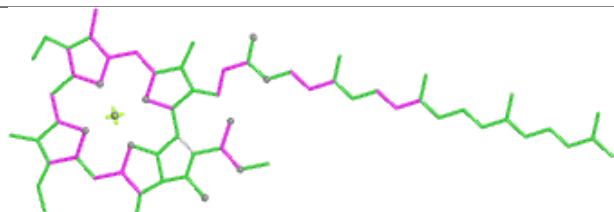
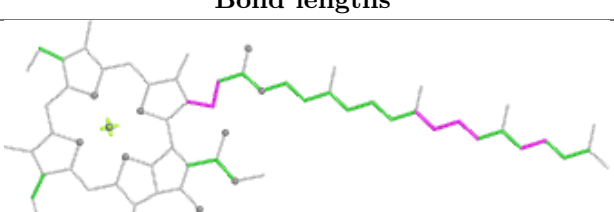
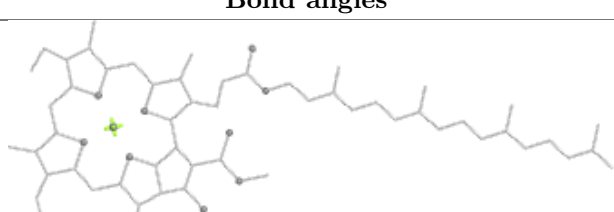


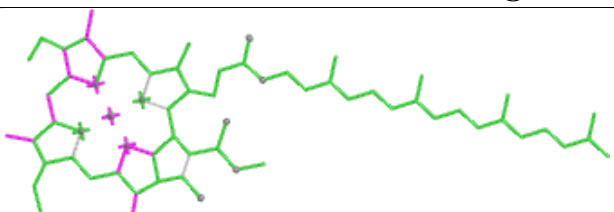
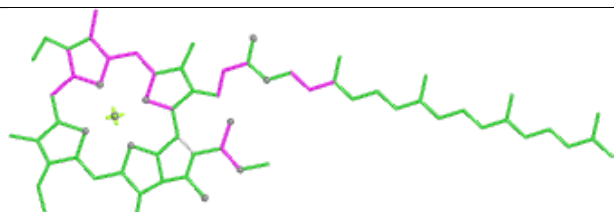
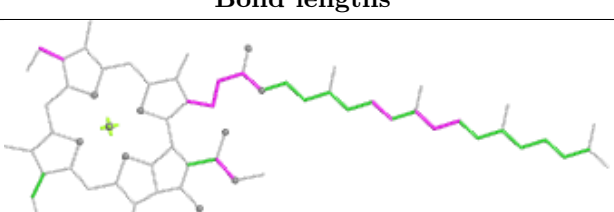
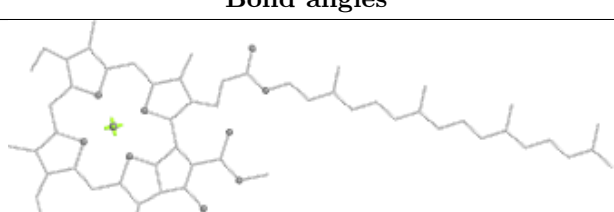


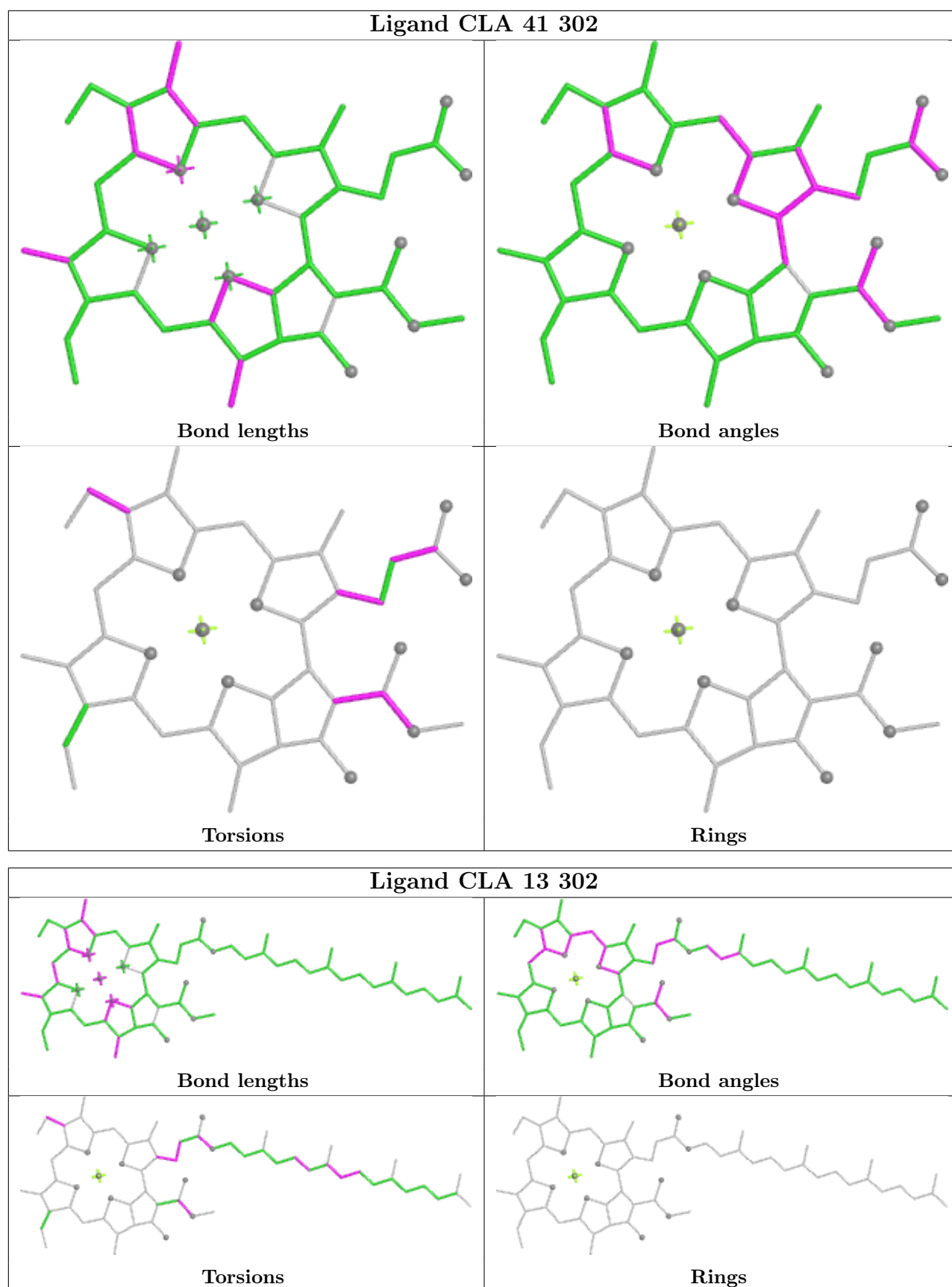


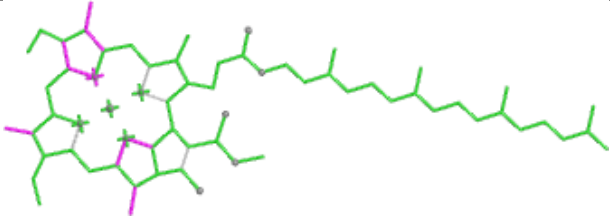
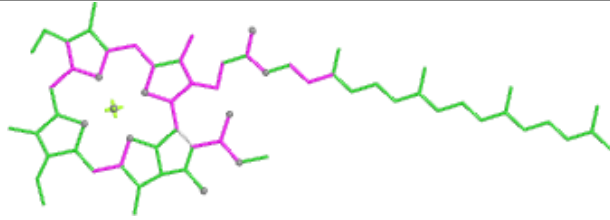
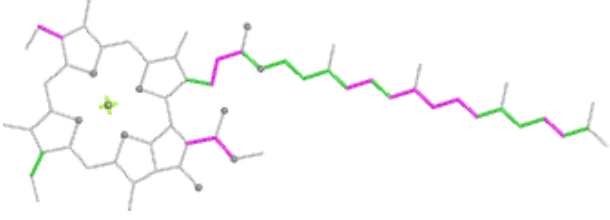
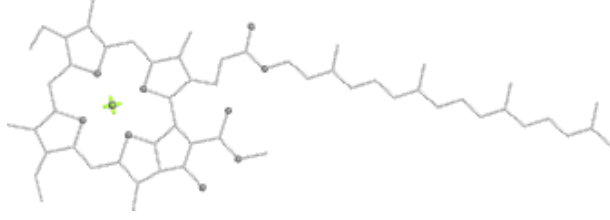


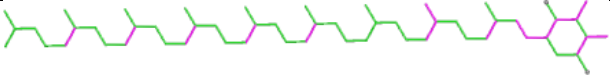
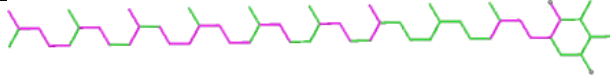
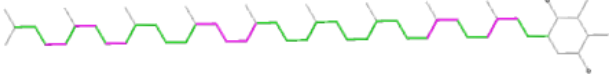
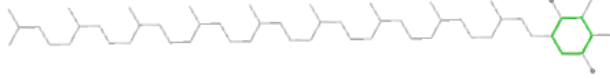
Ligand A86 36 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

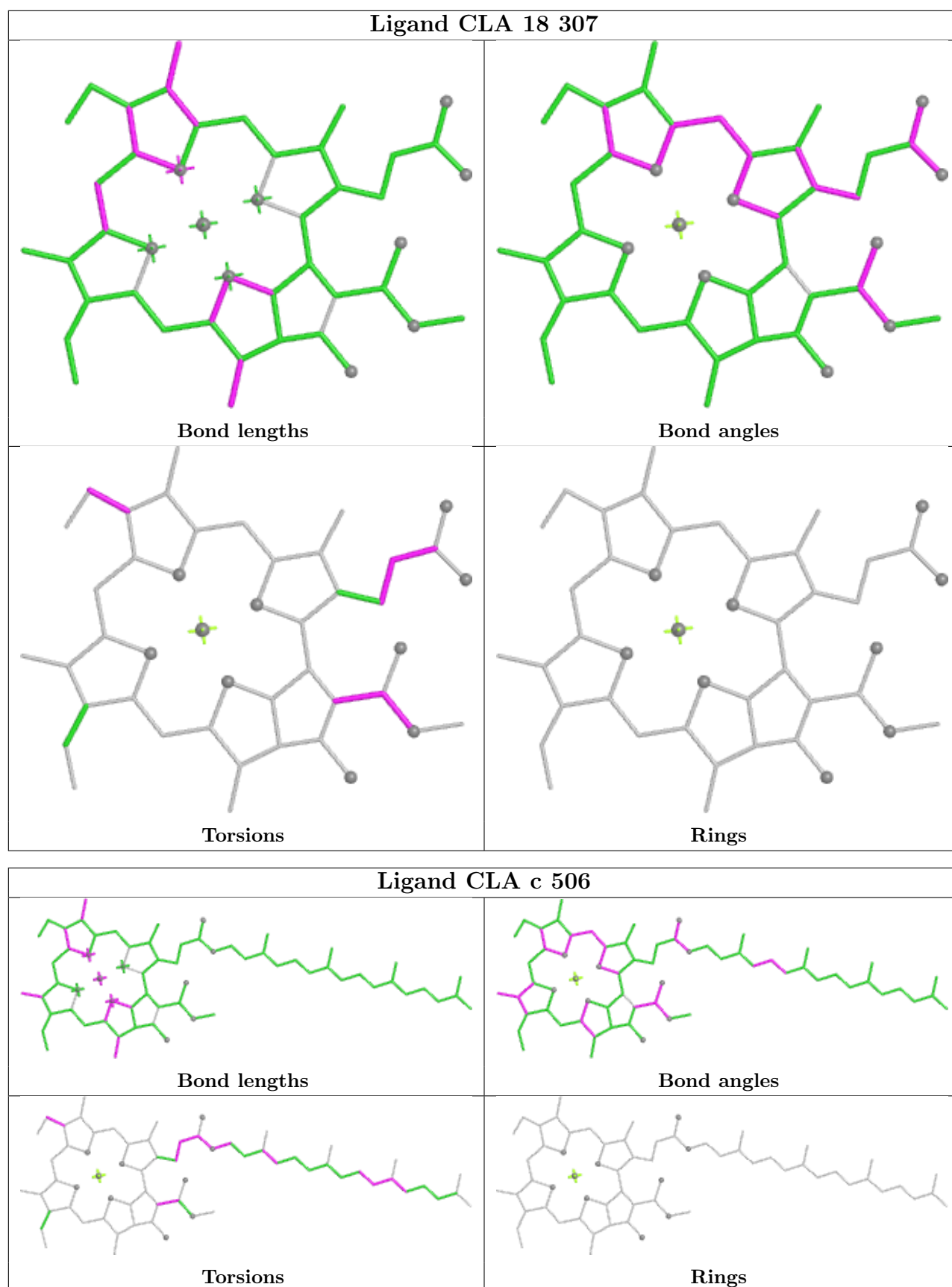
Ligand CLA b 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

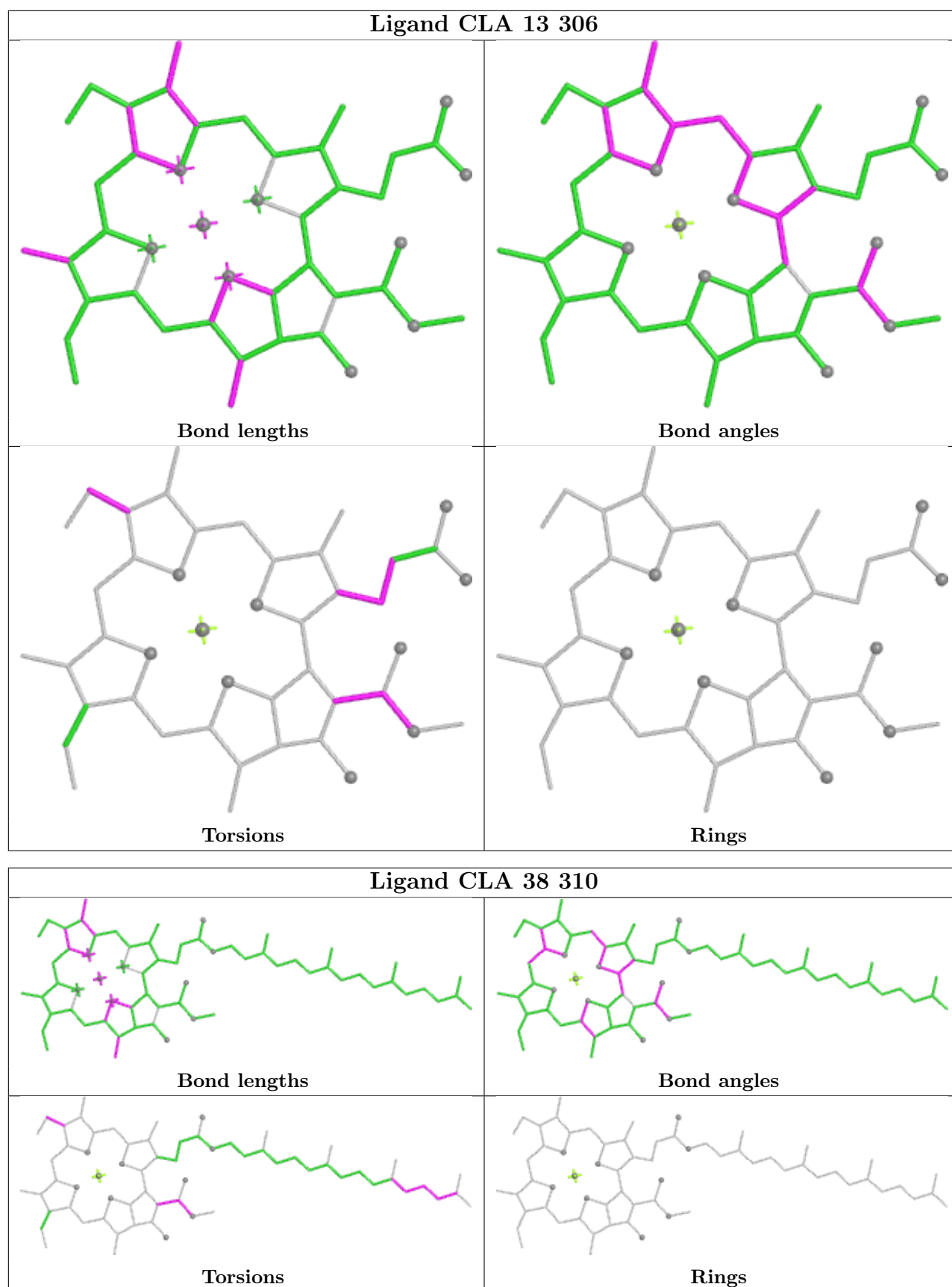
Ligand CLA 31 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

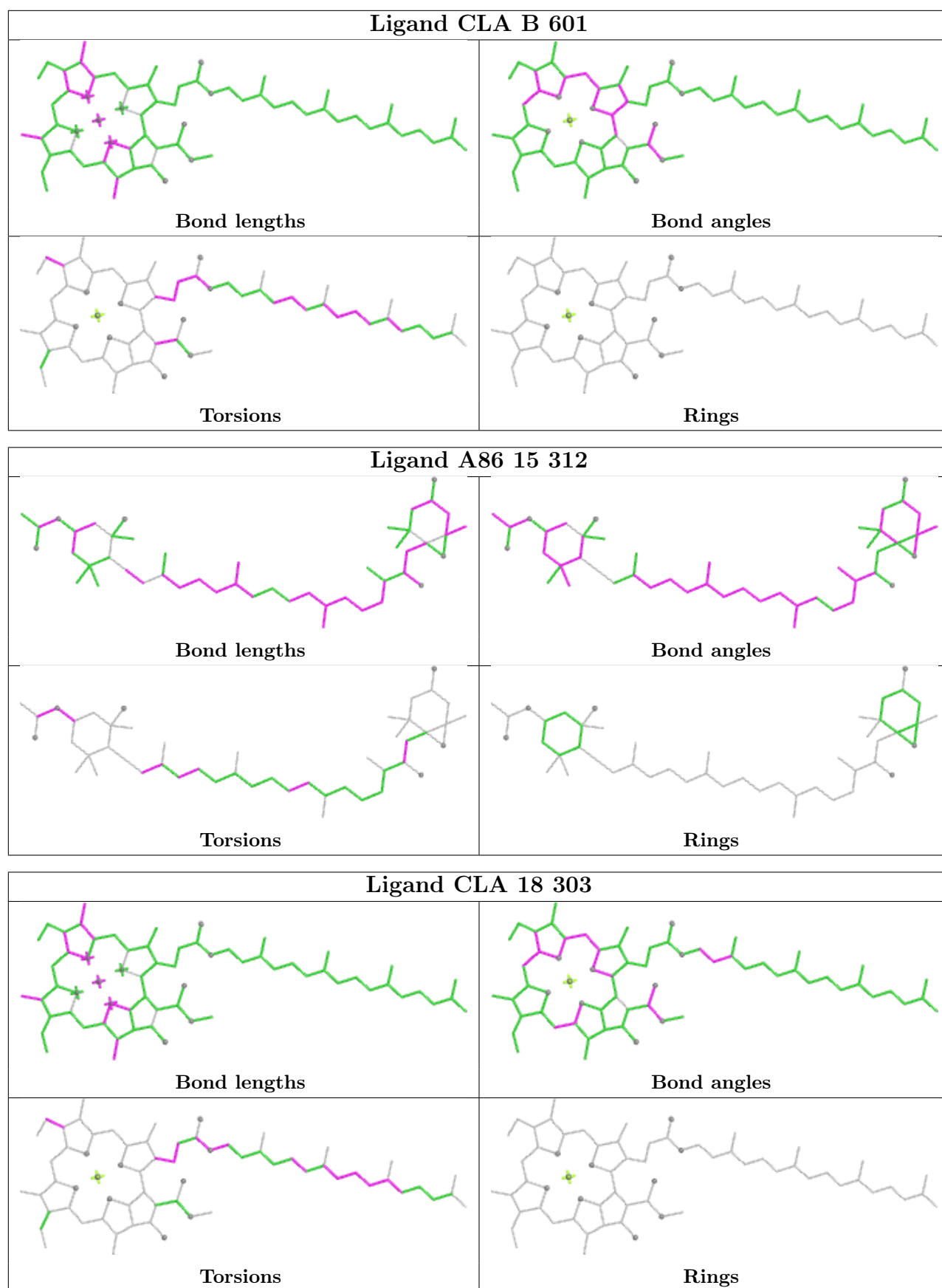


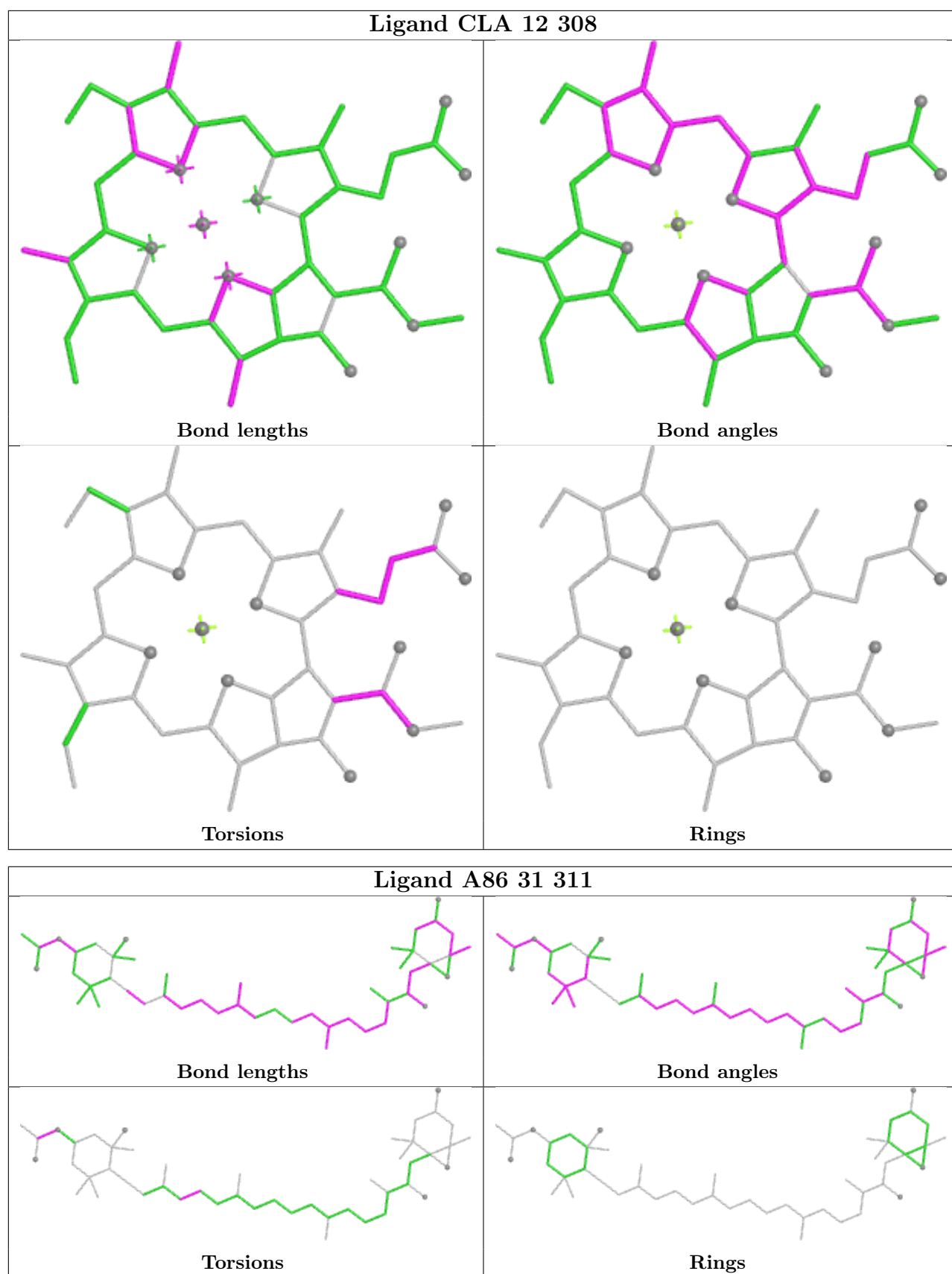
Ligand CLA 16 302			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

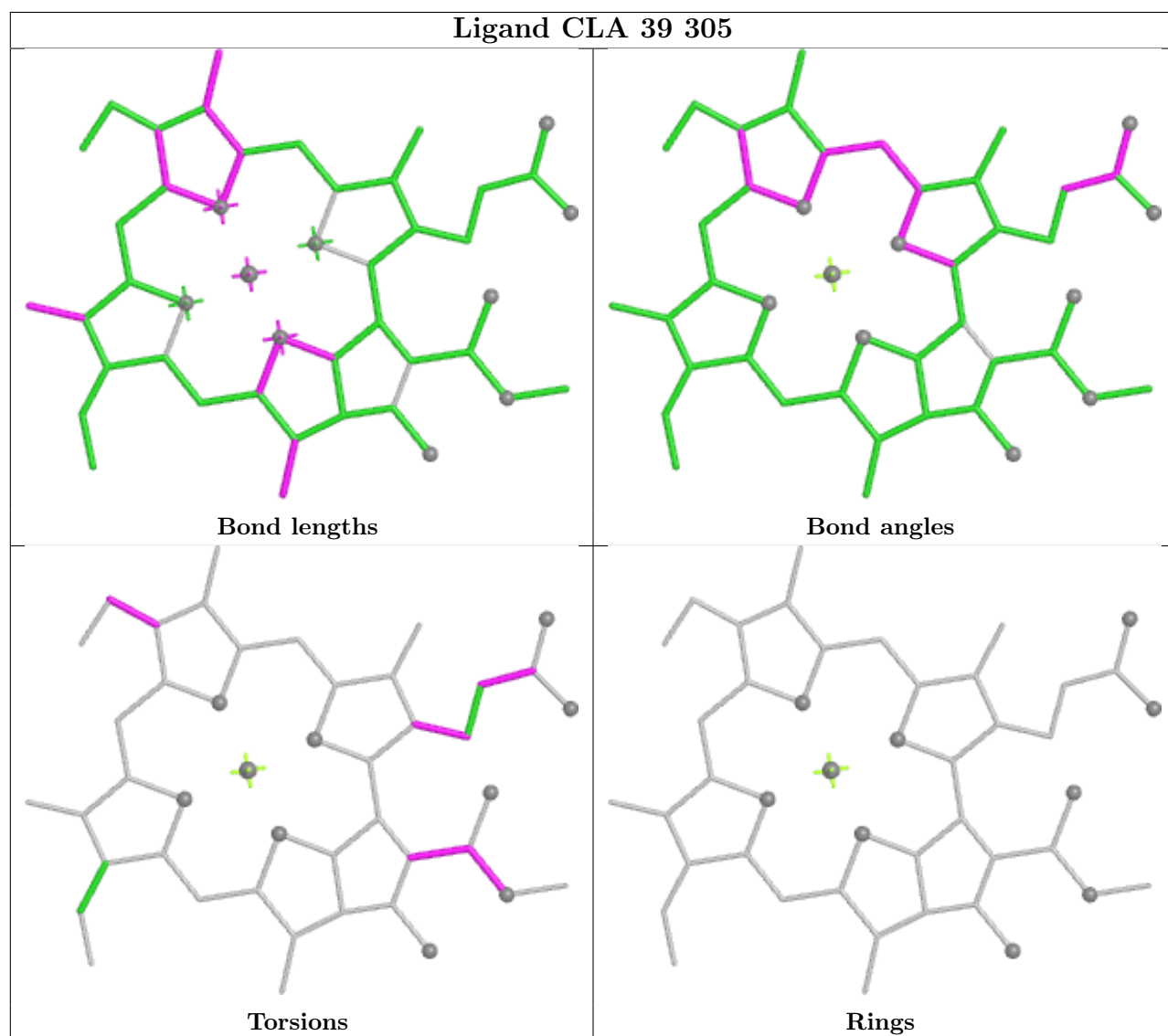
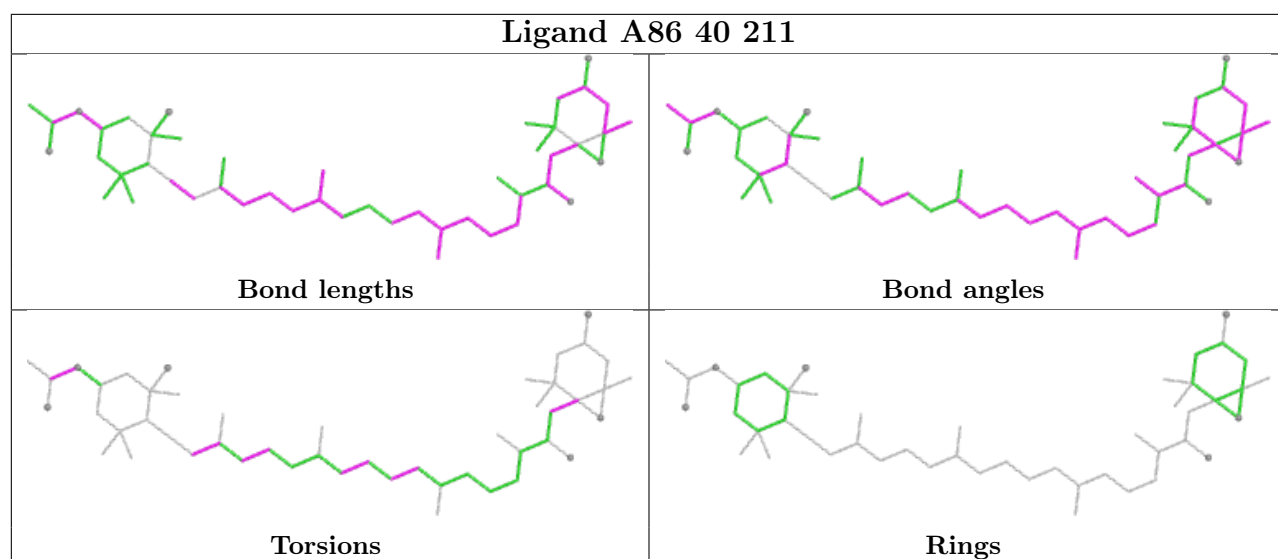
Ligand PL9 D 407			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

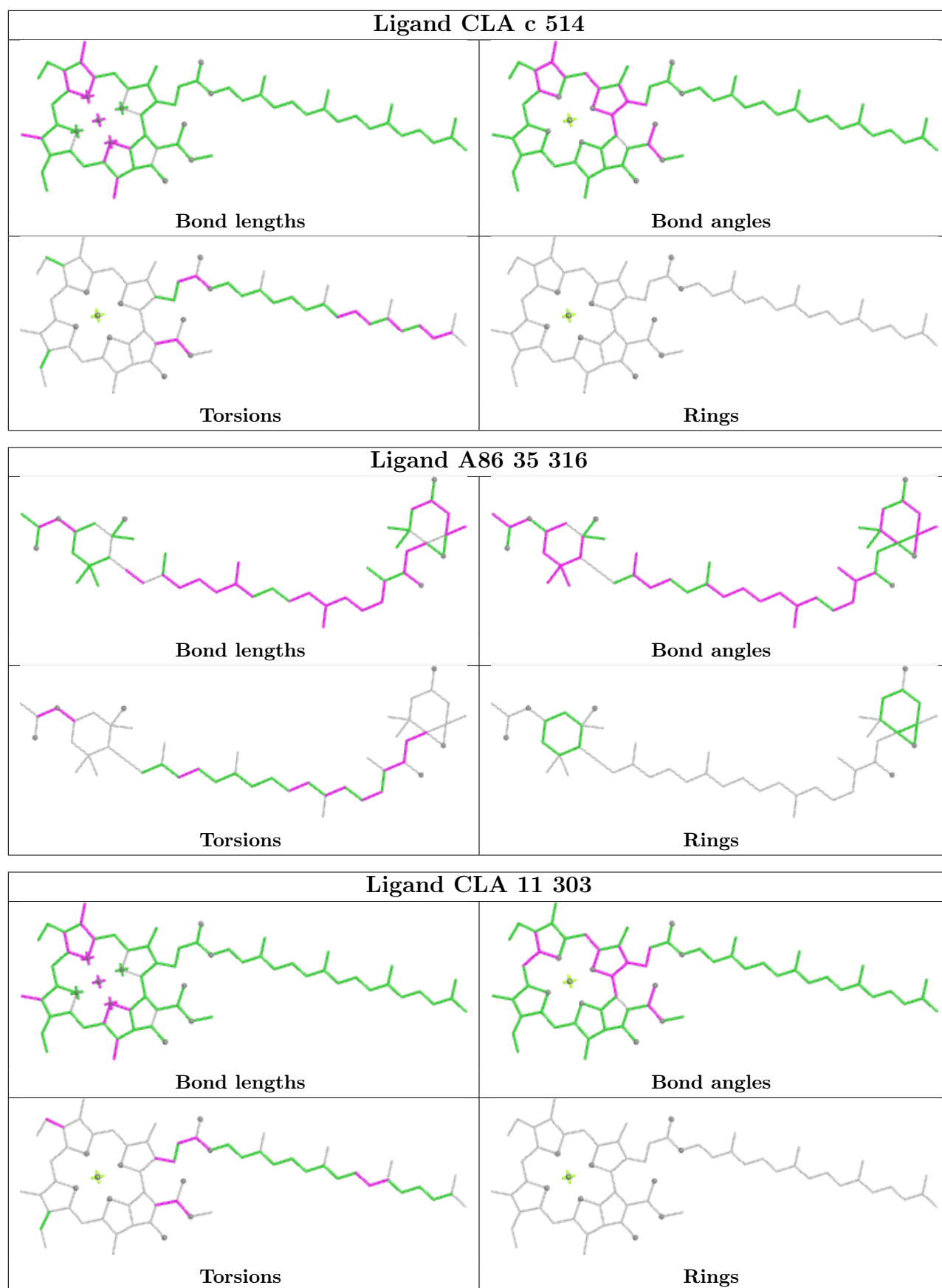


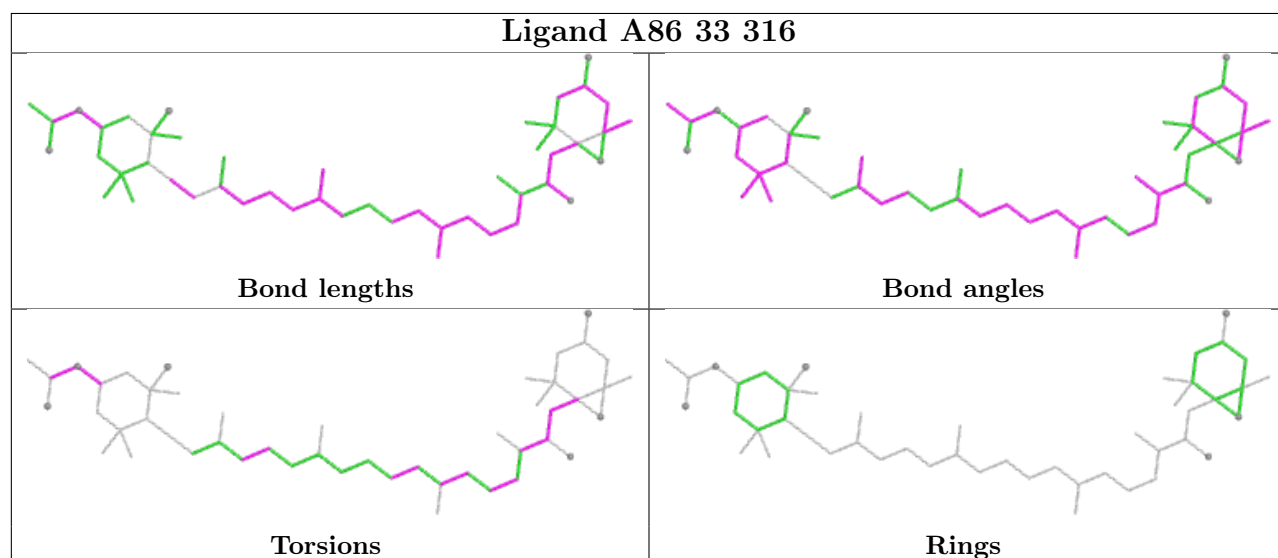
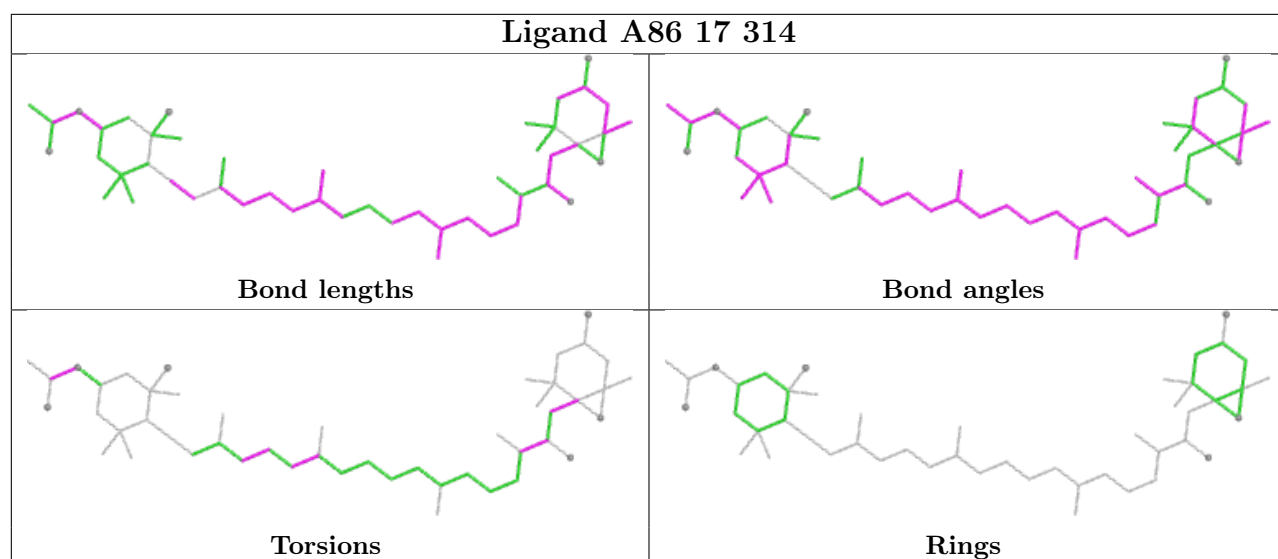


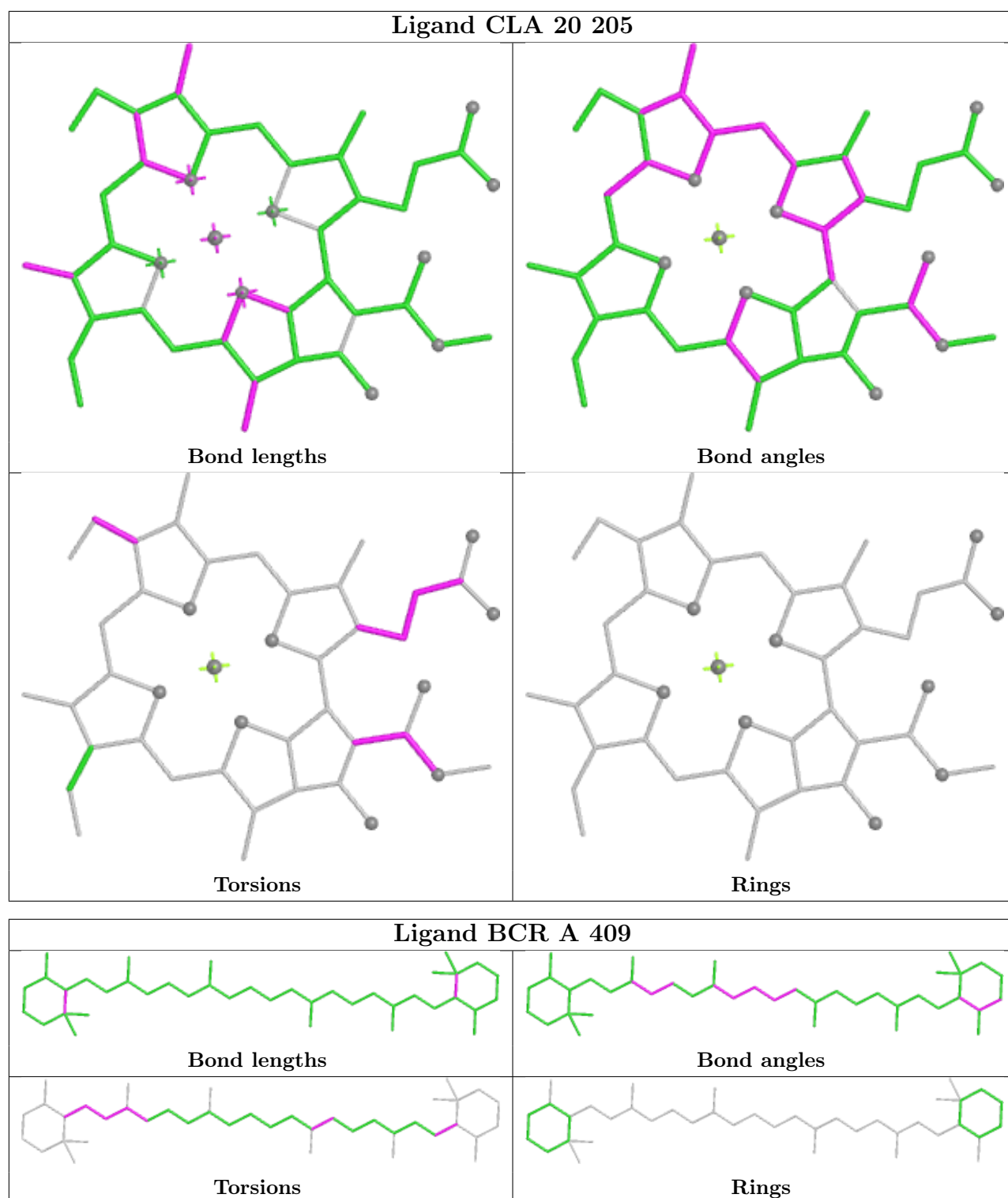


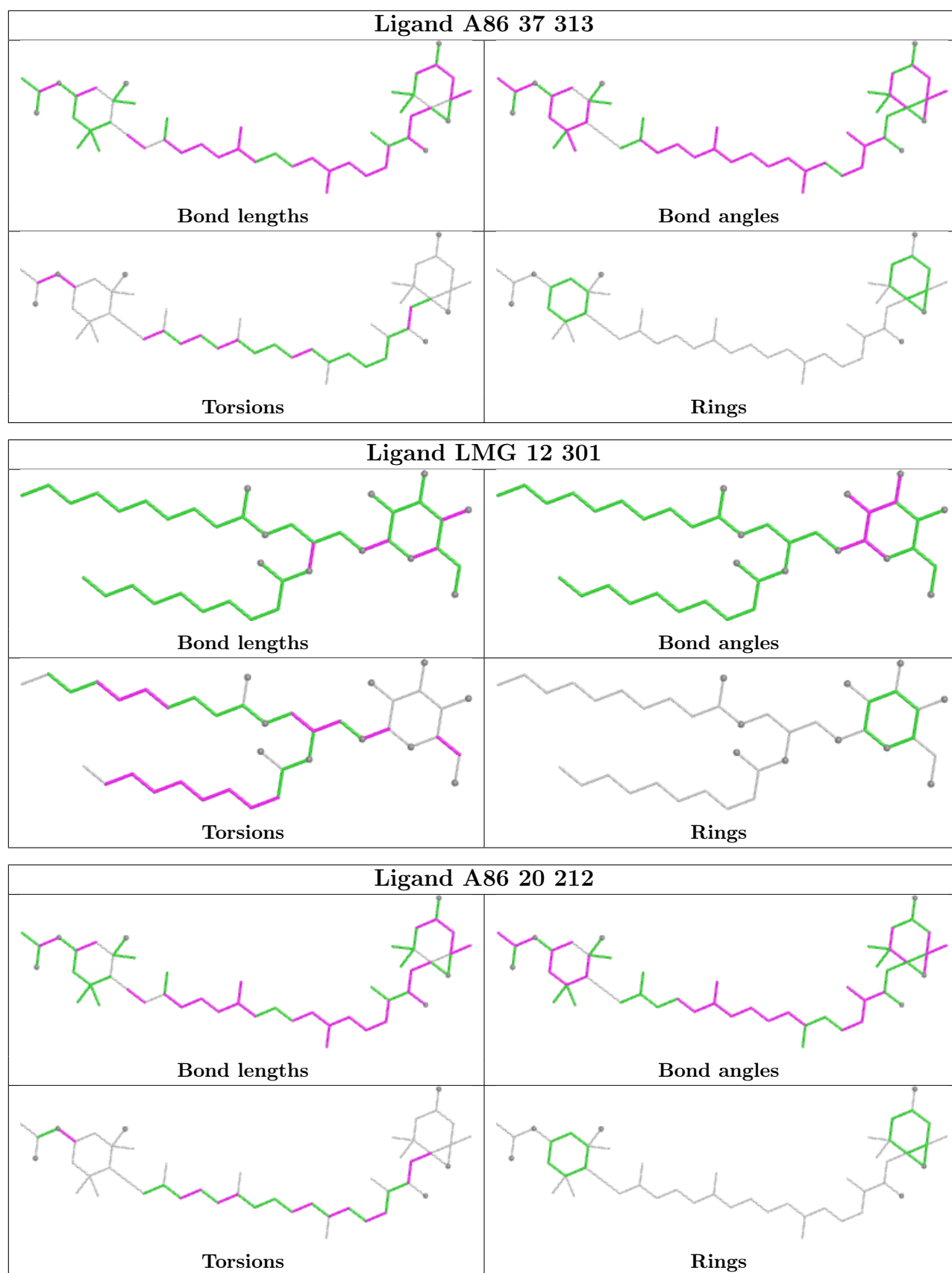


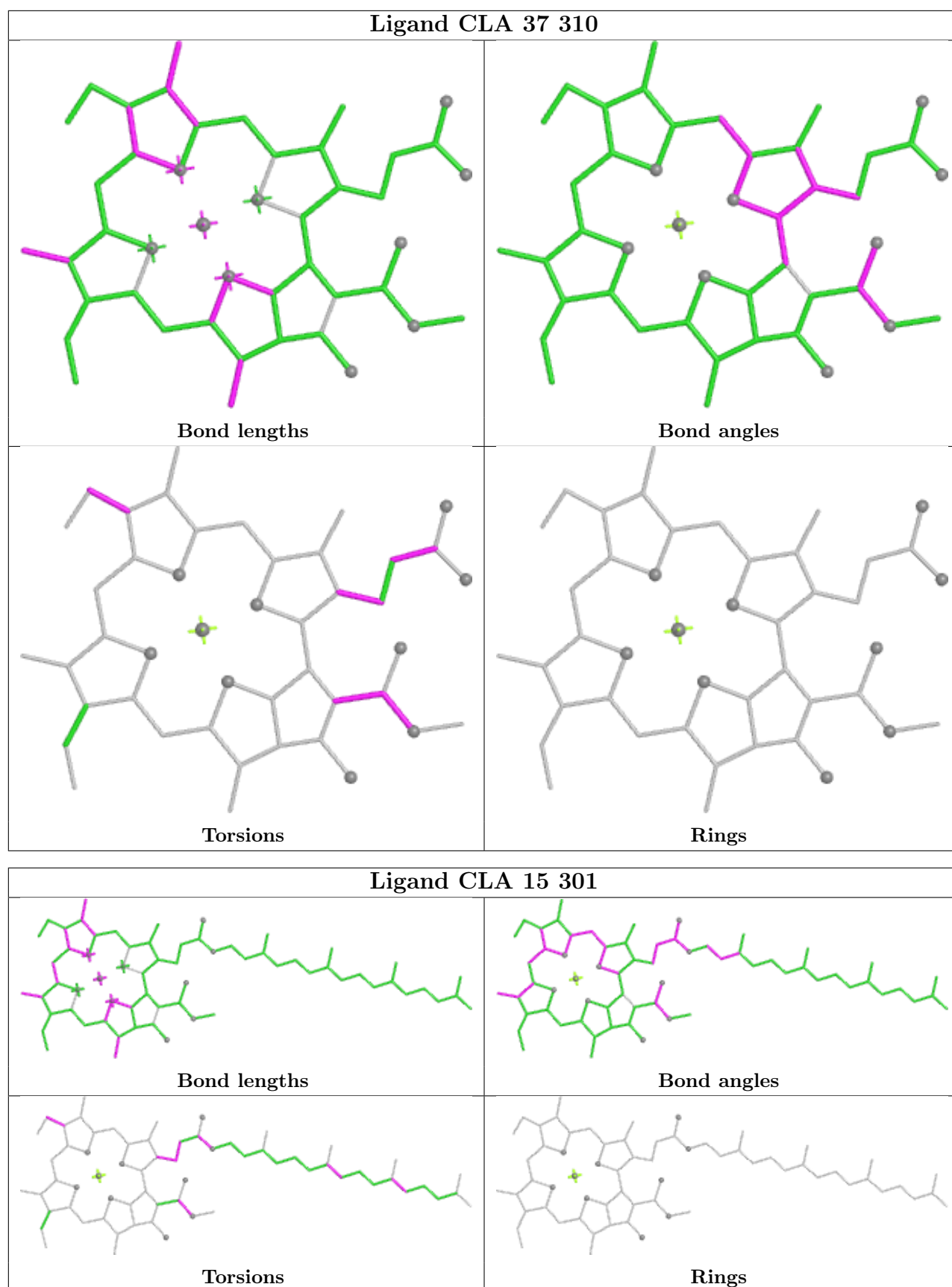


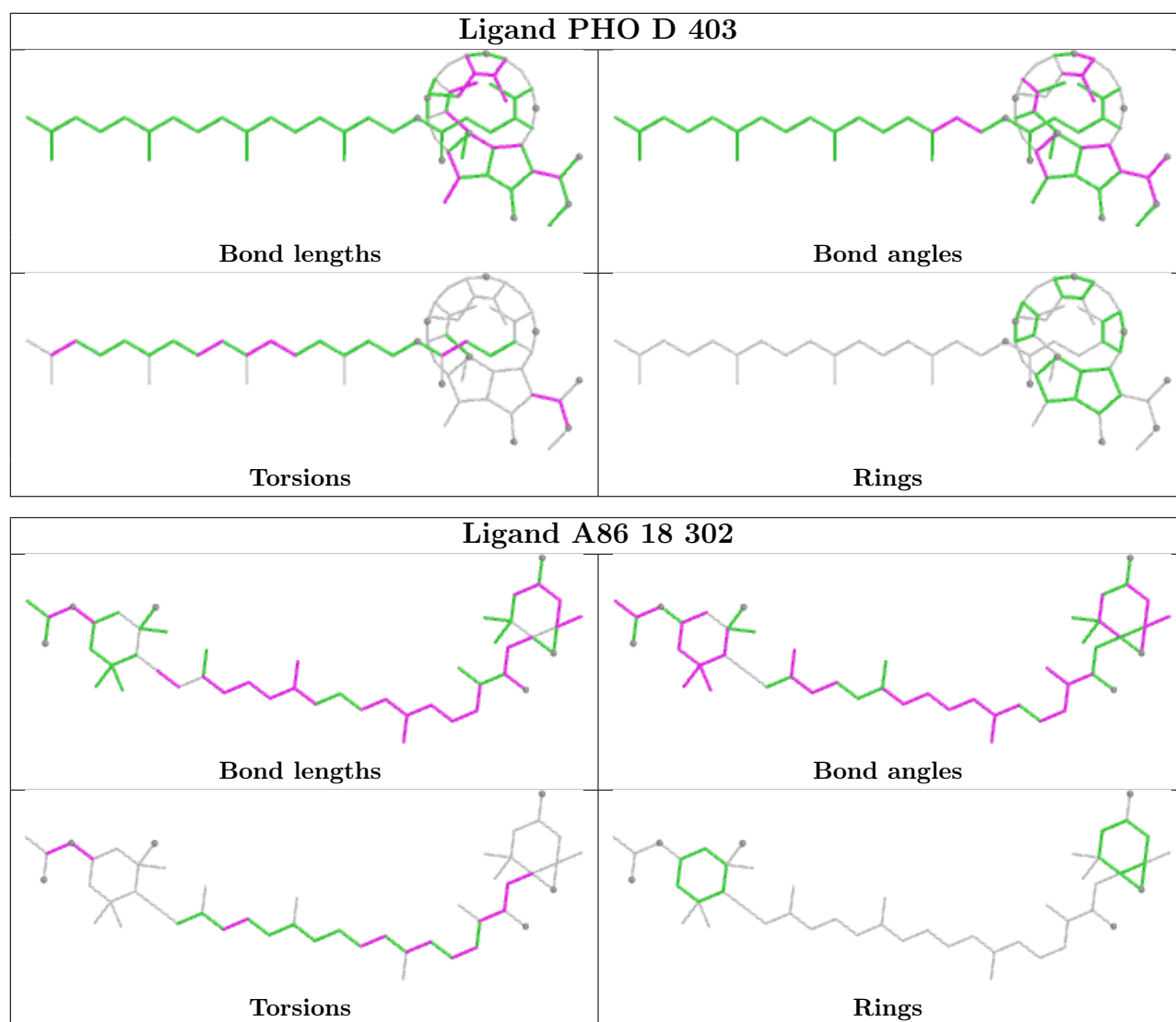


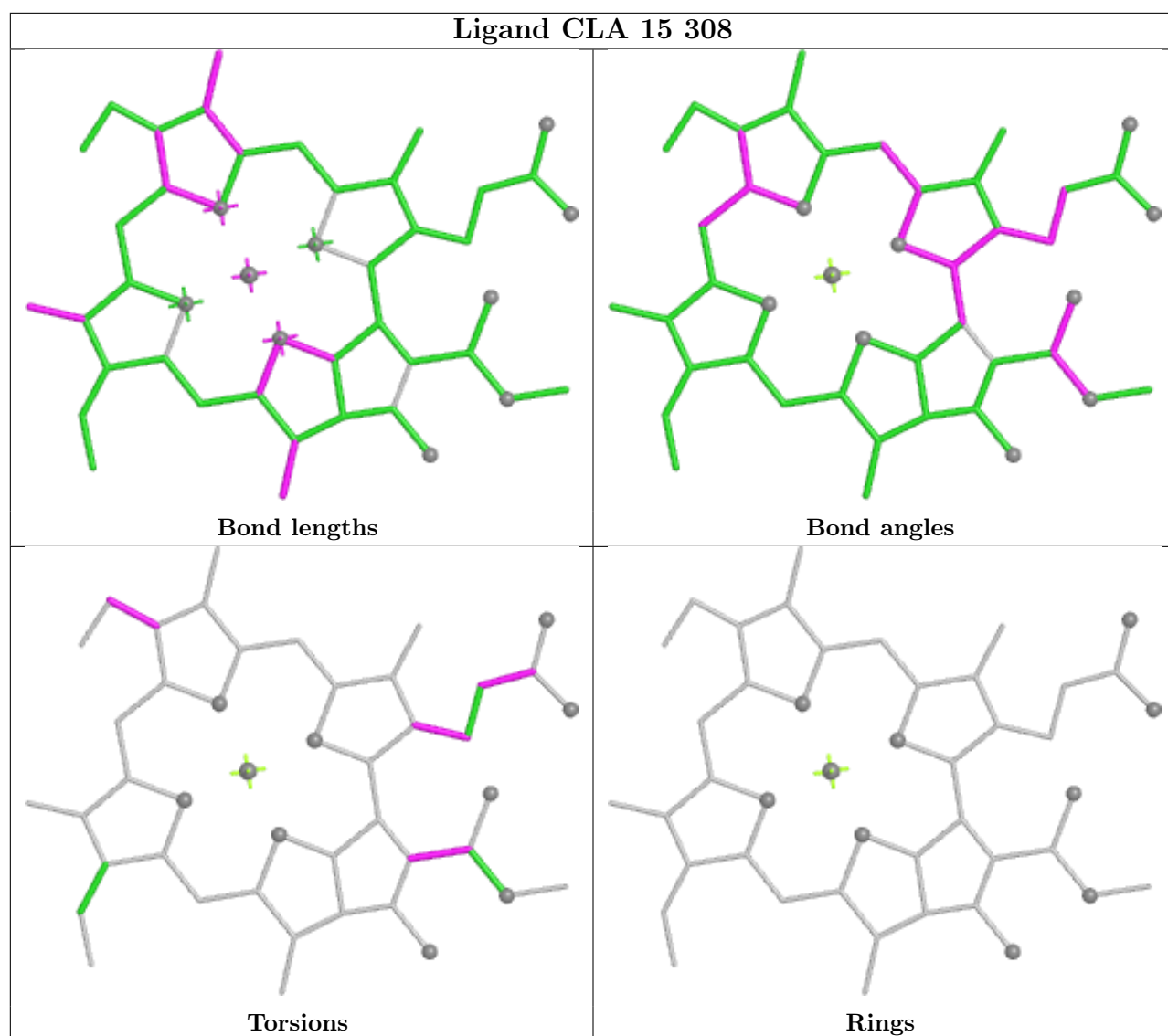


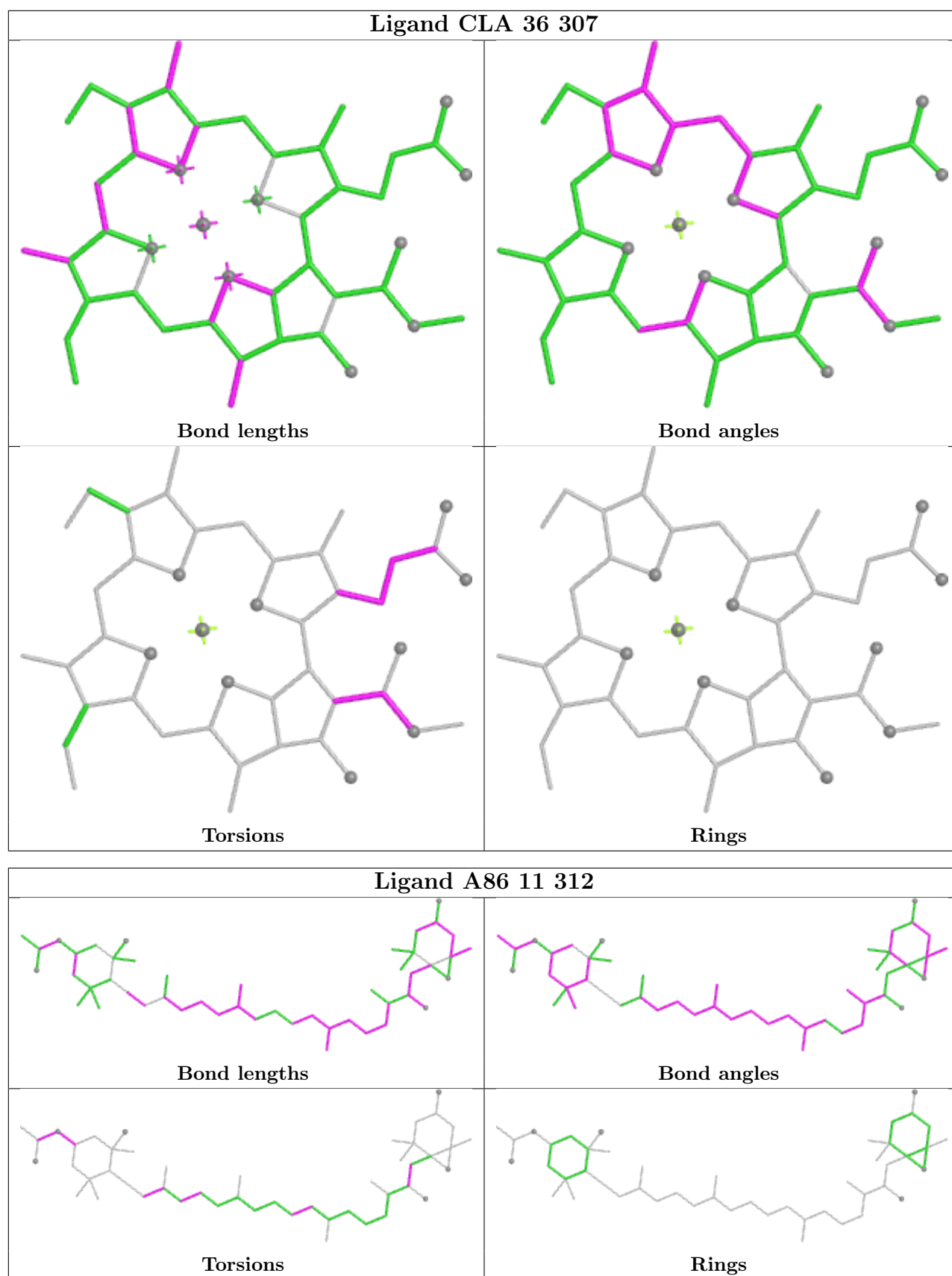


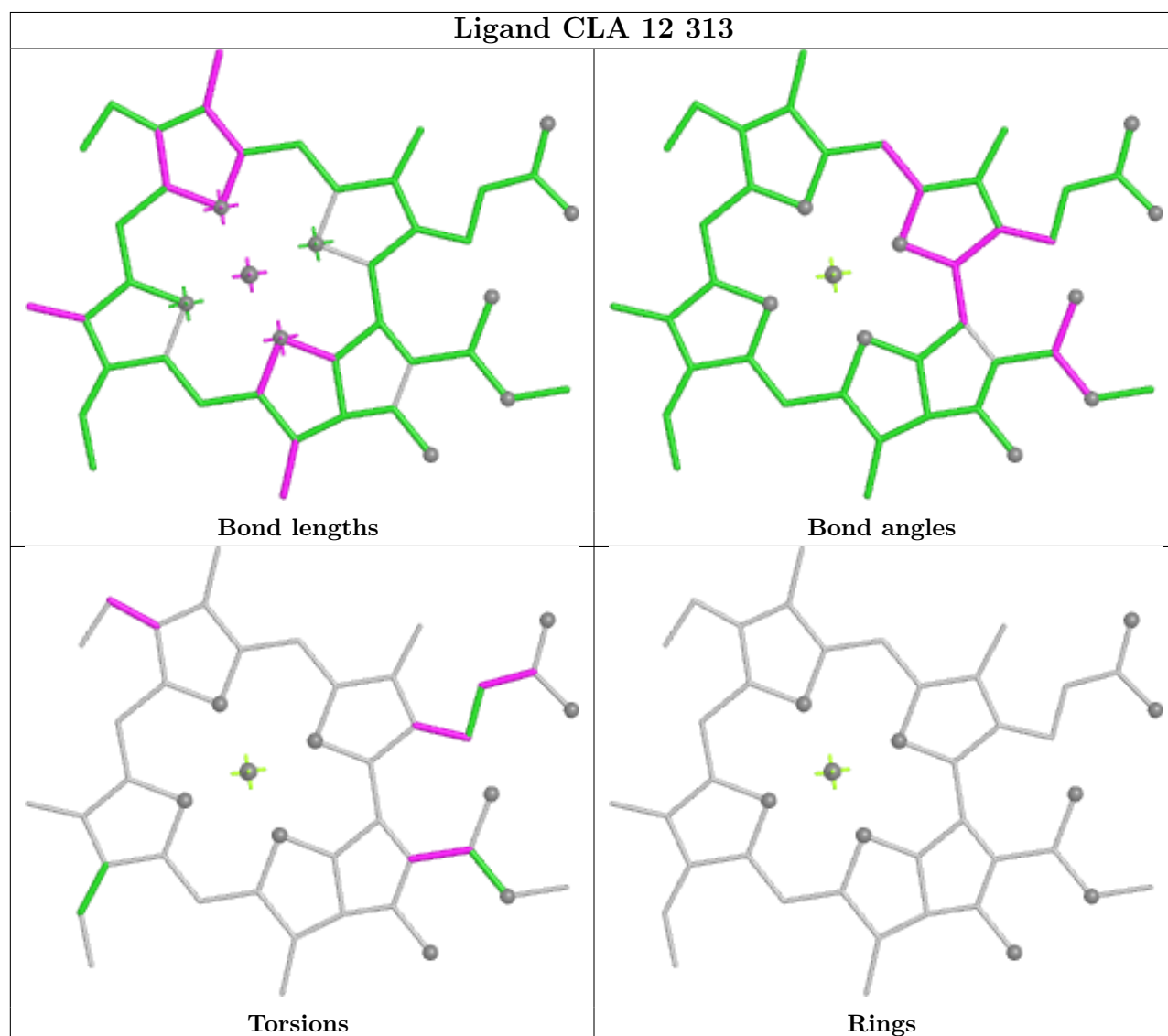
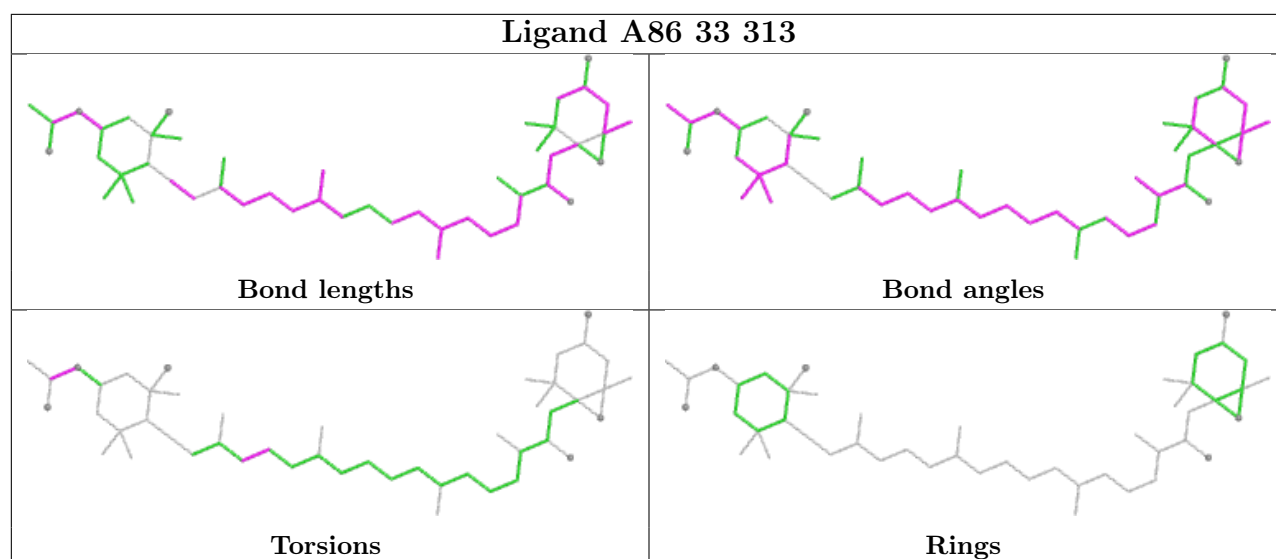


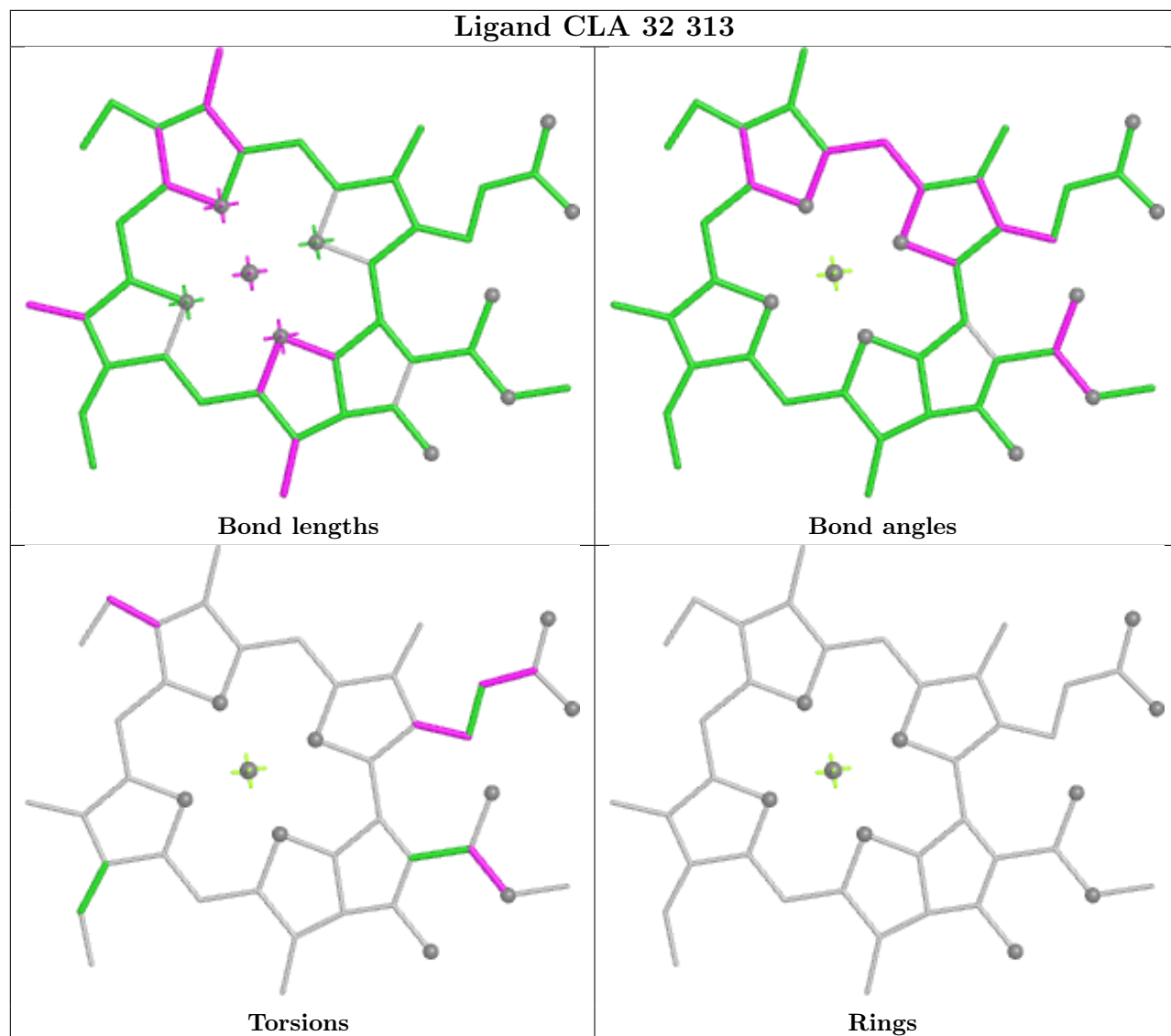


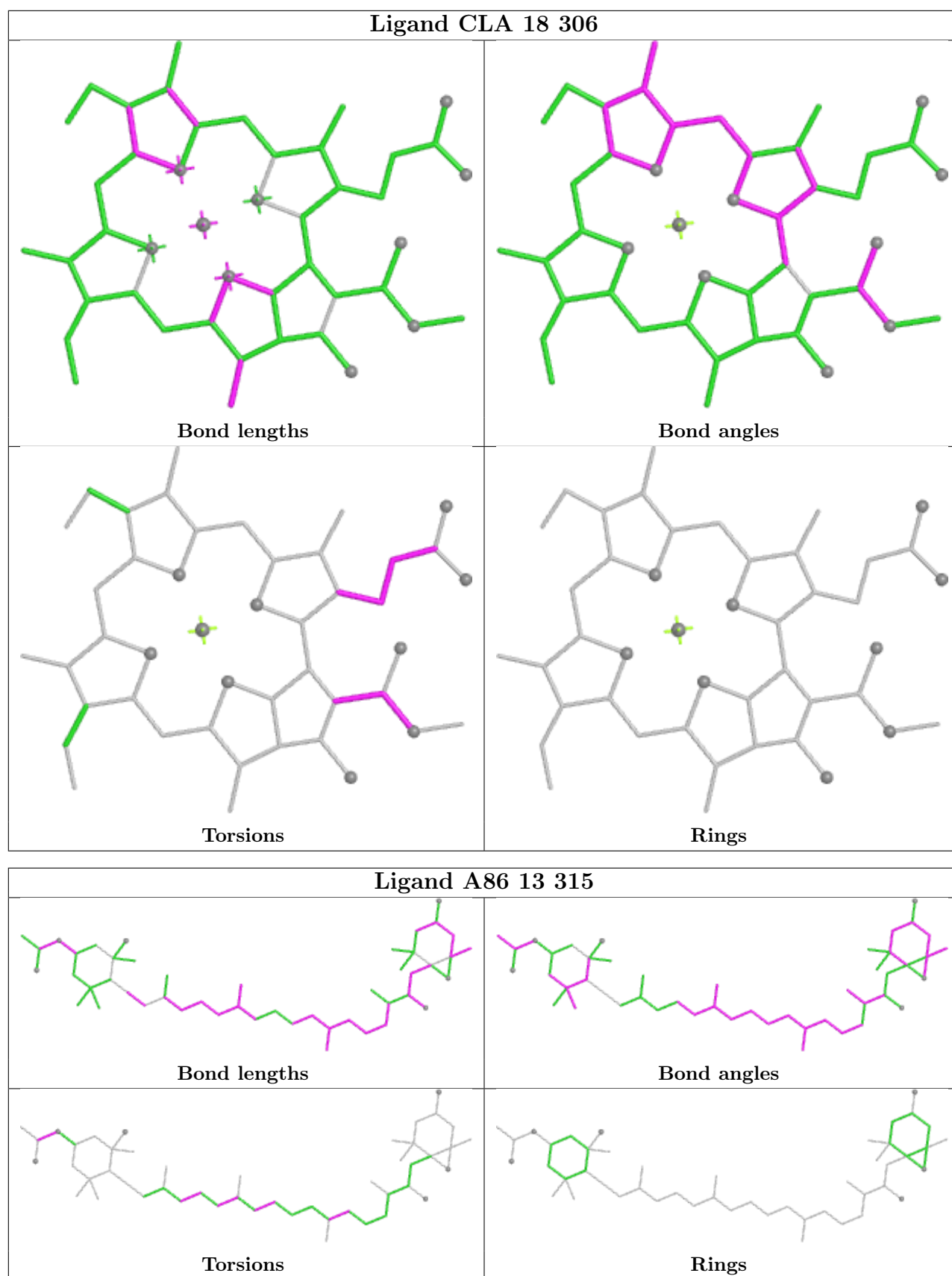


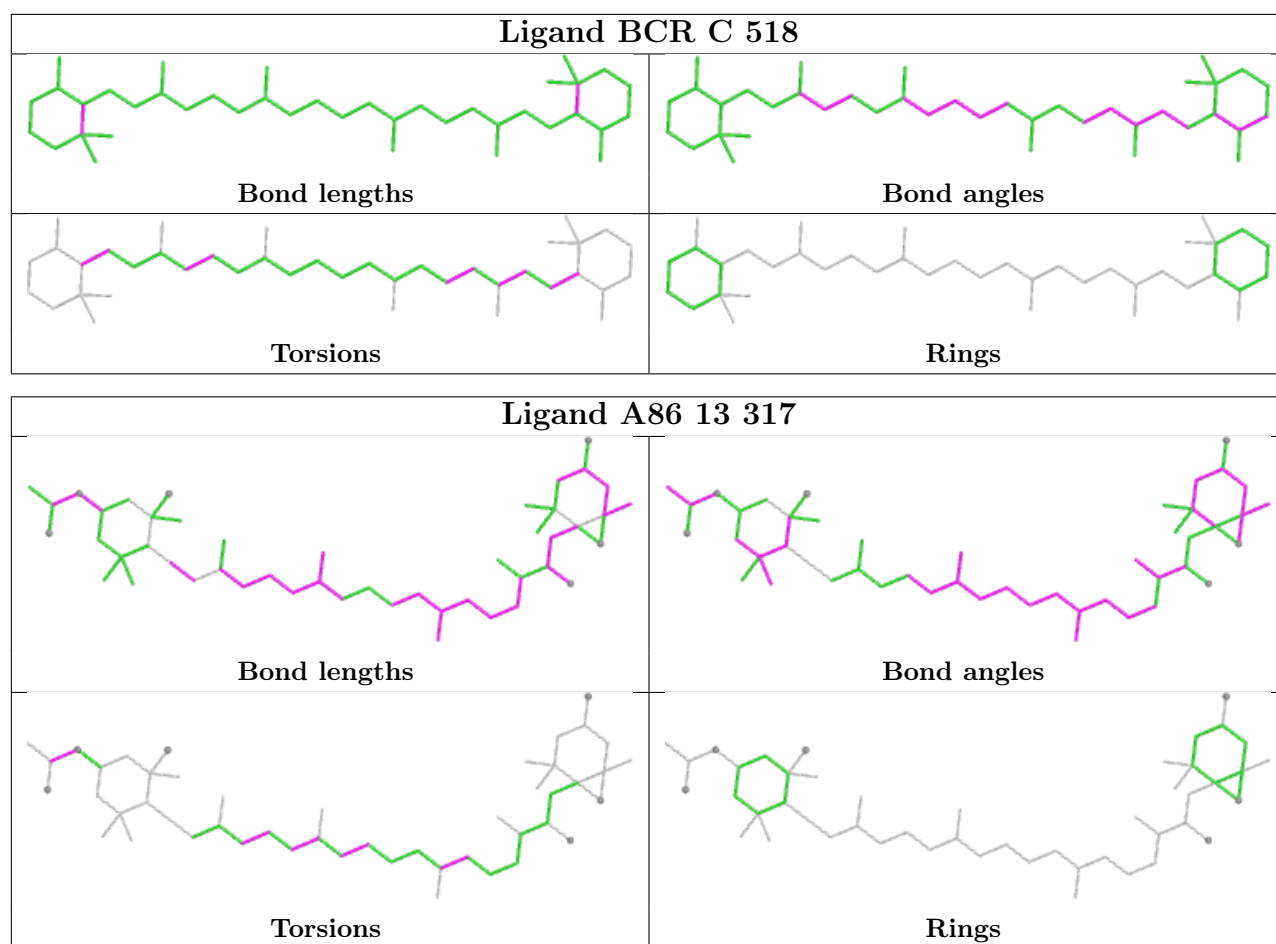


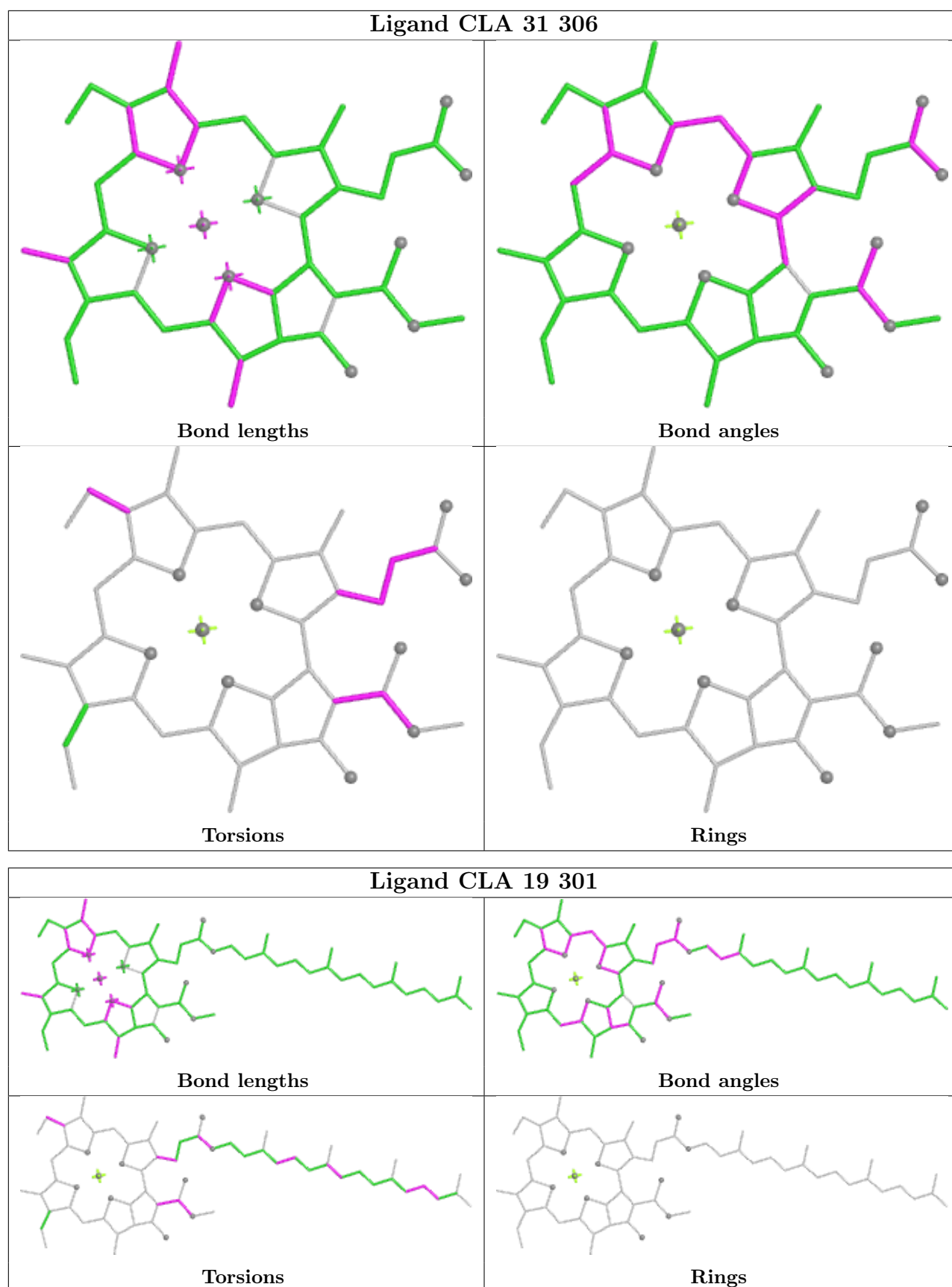


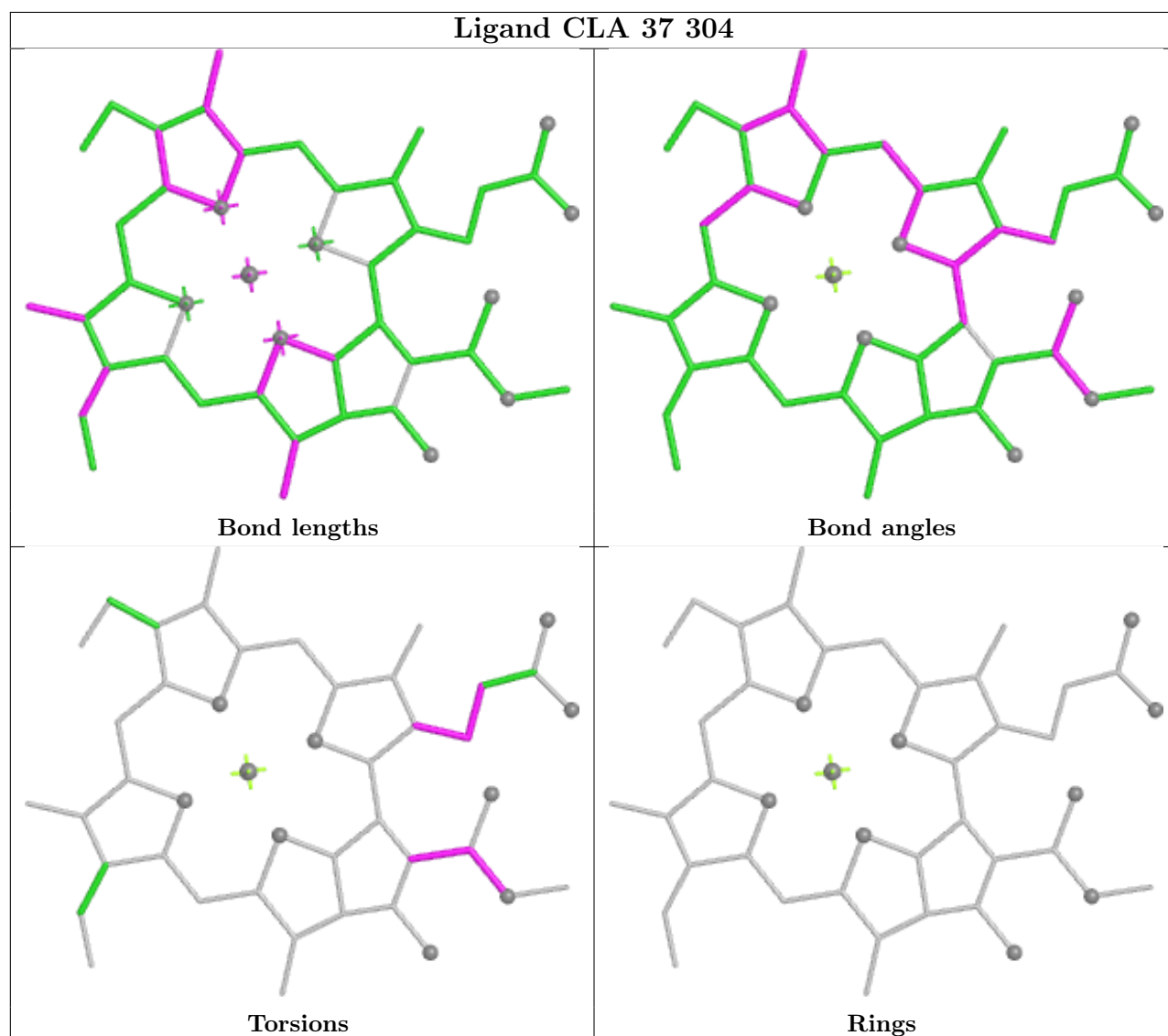
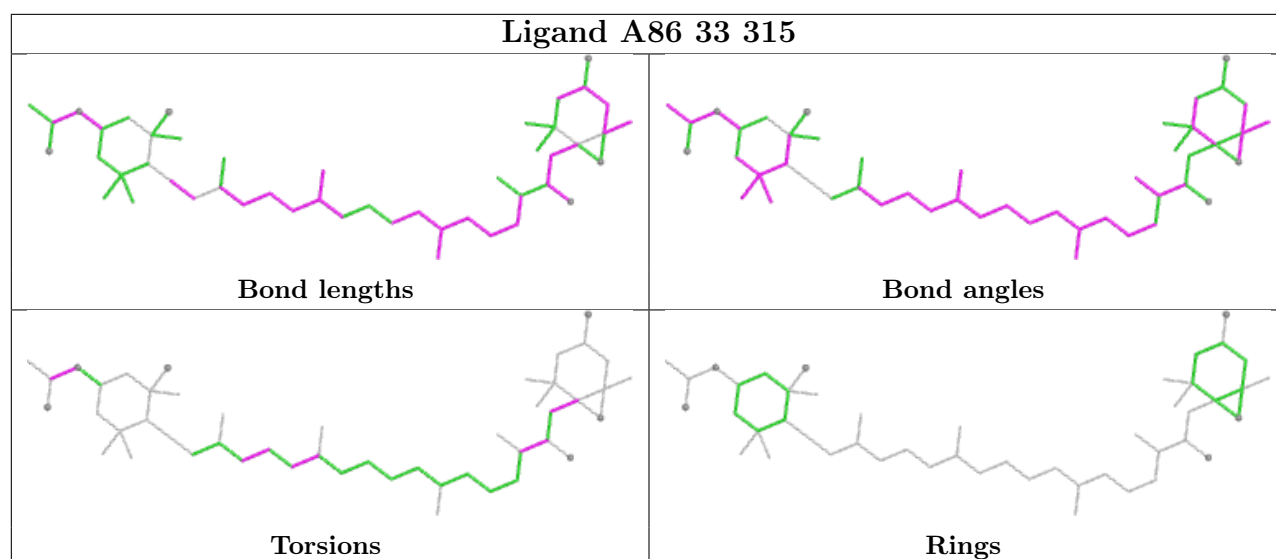


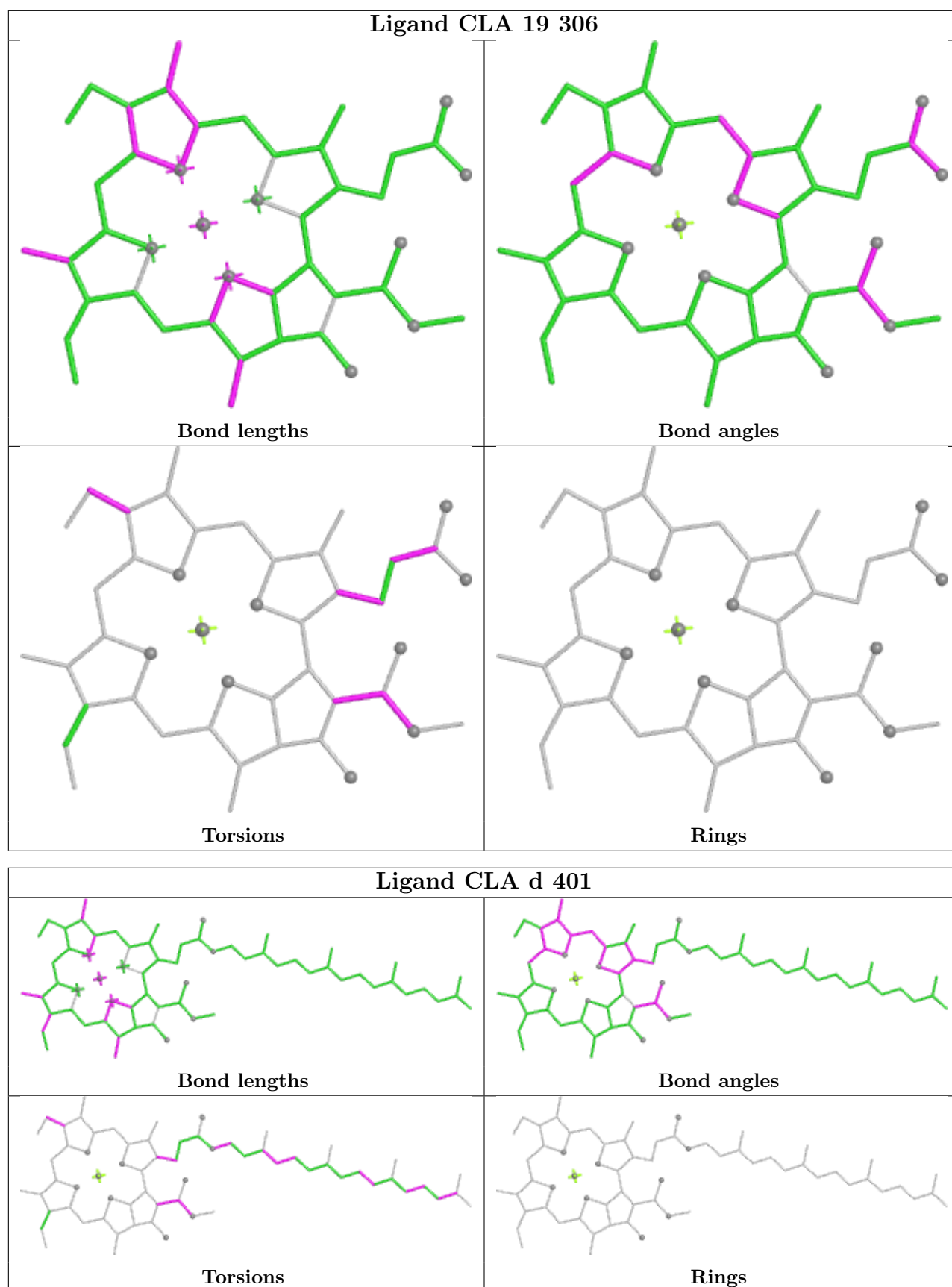


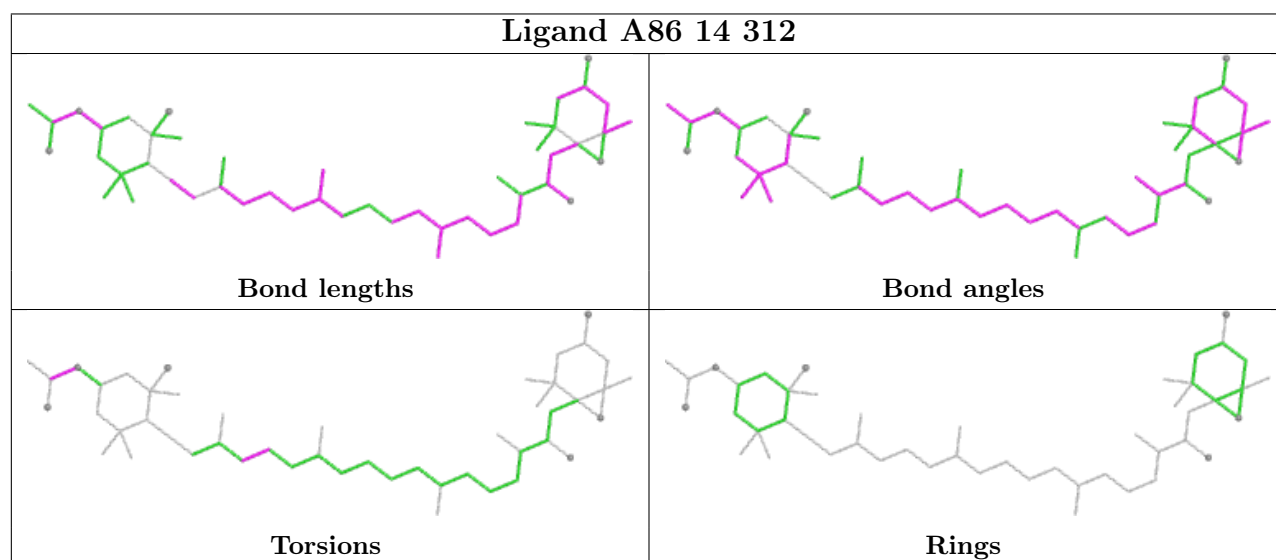
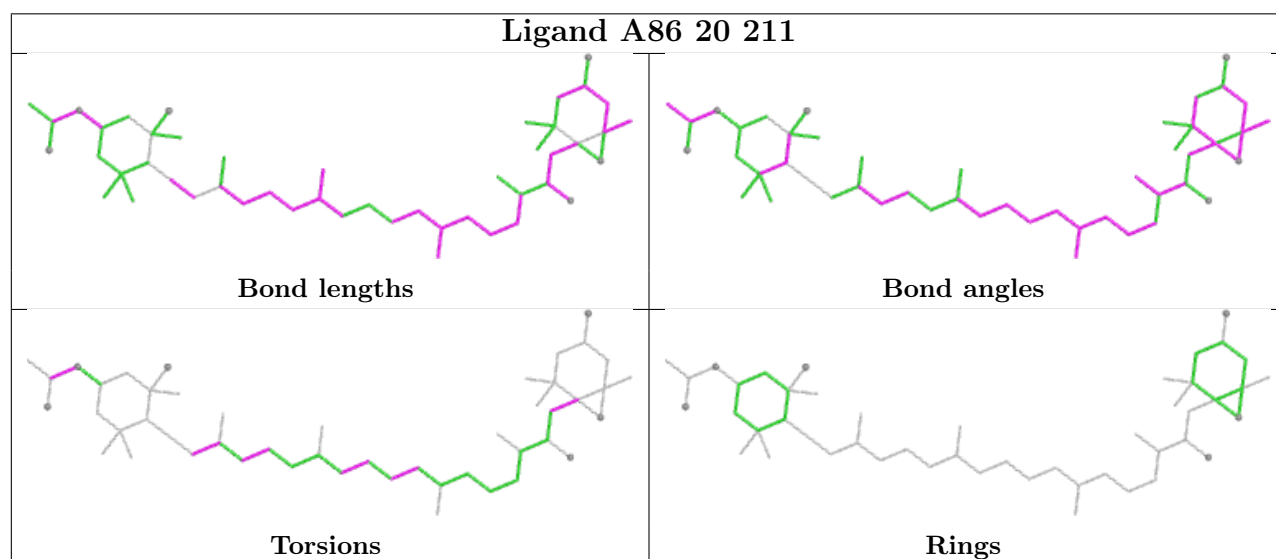
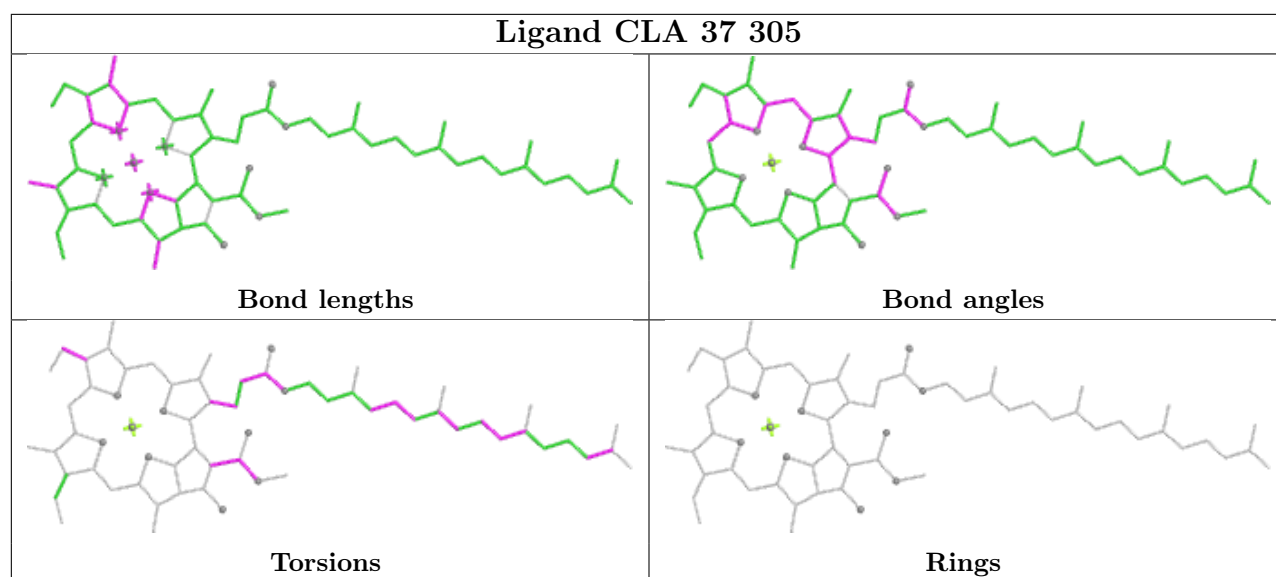


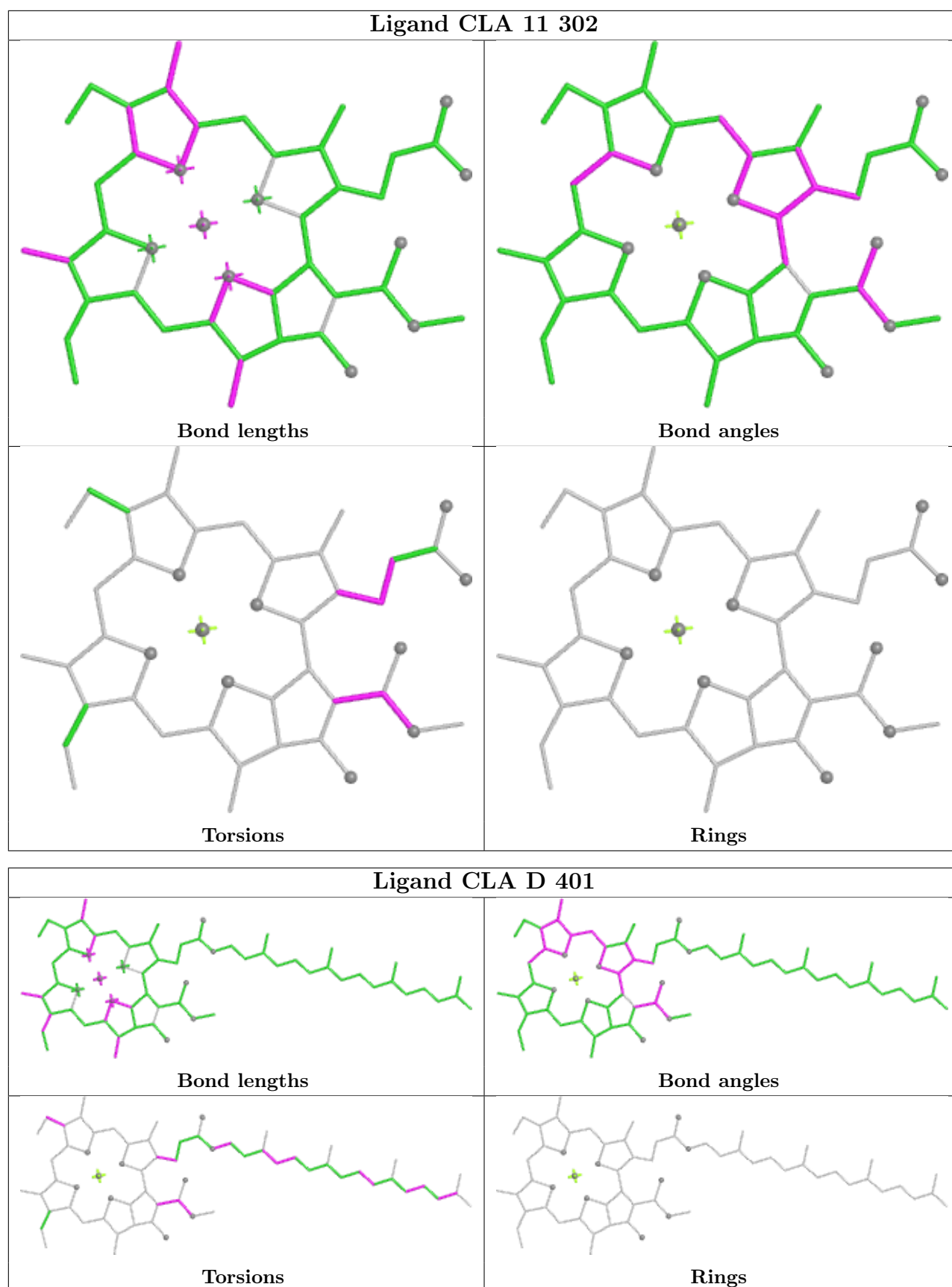


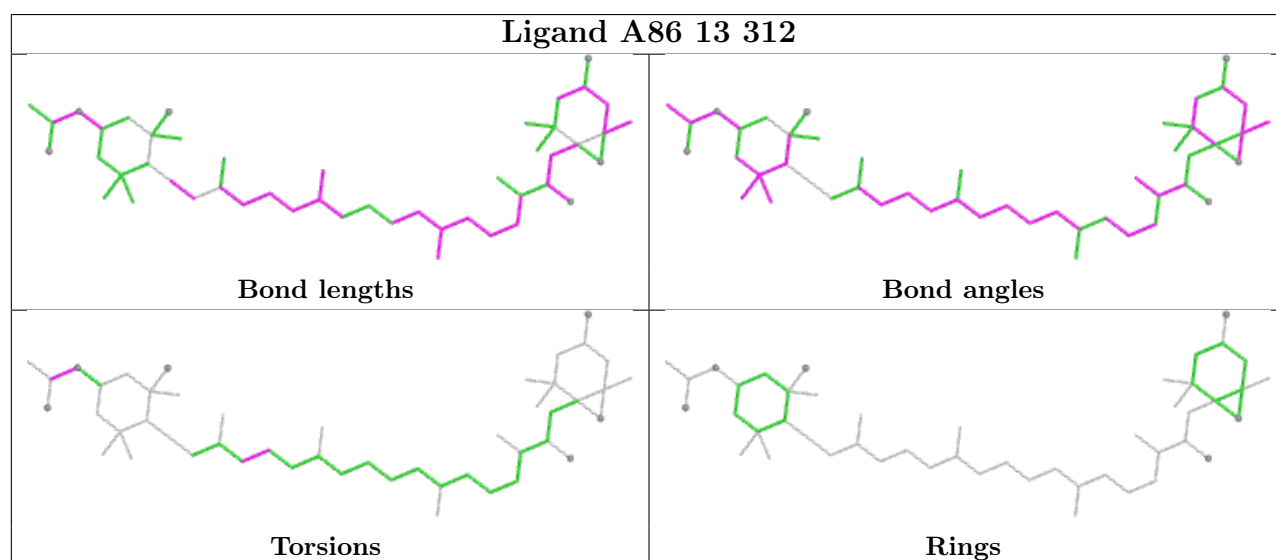
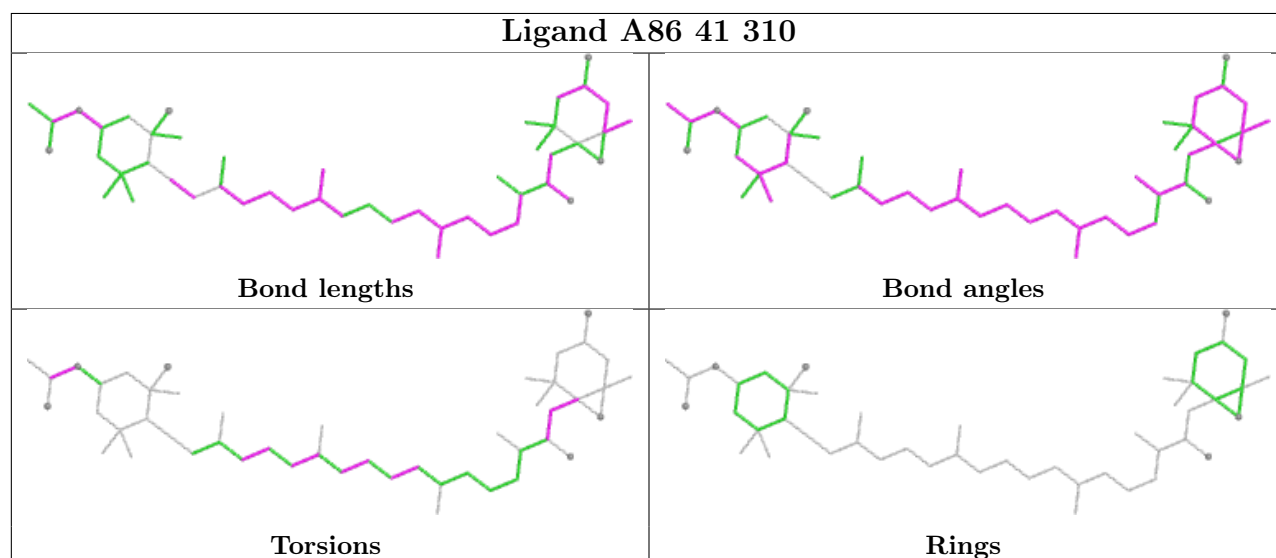
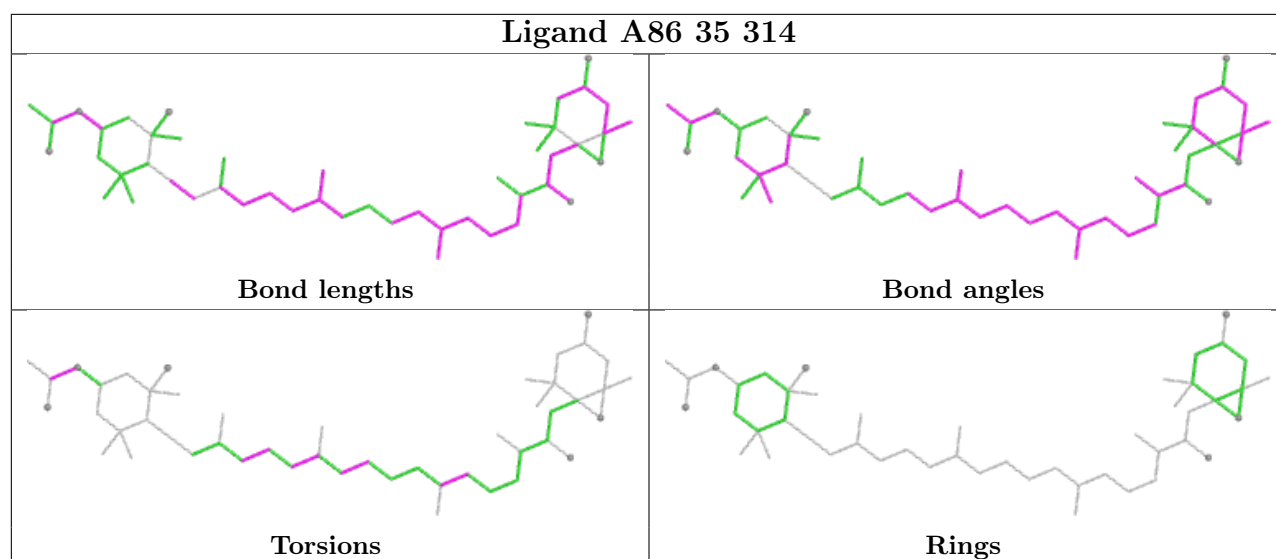


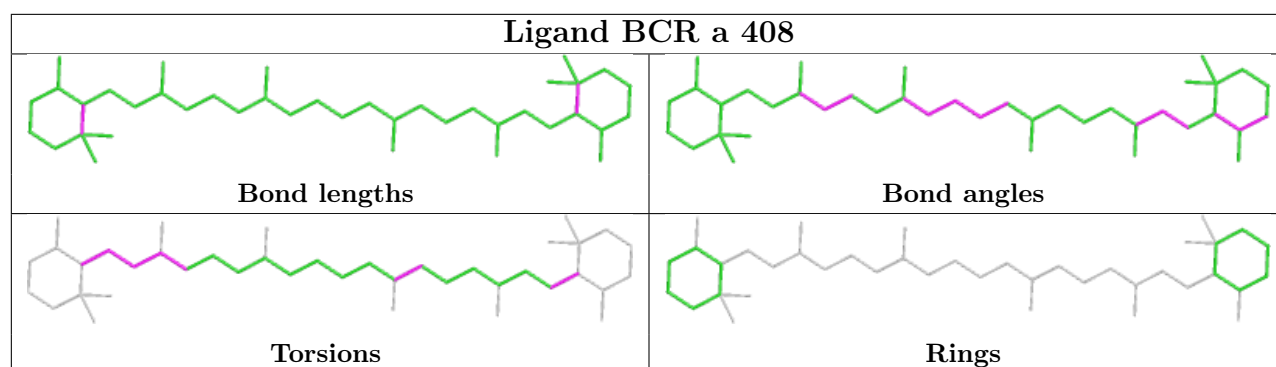
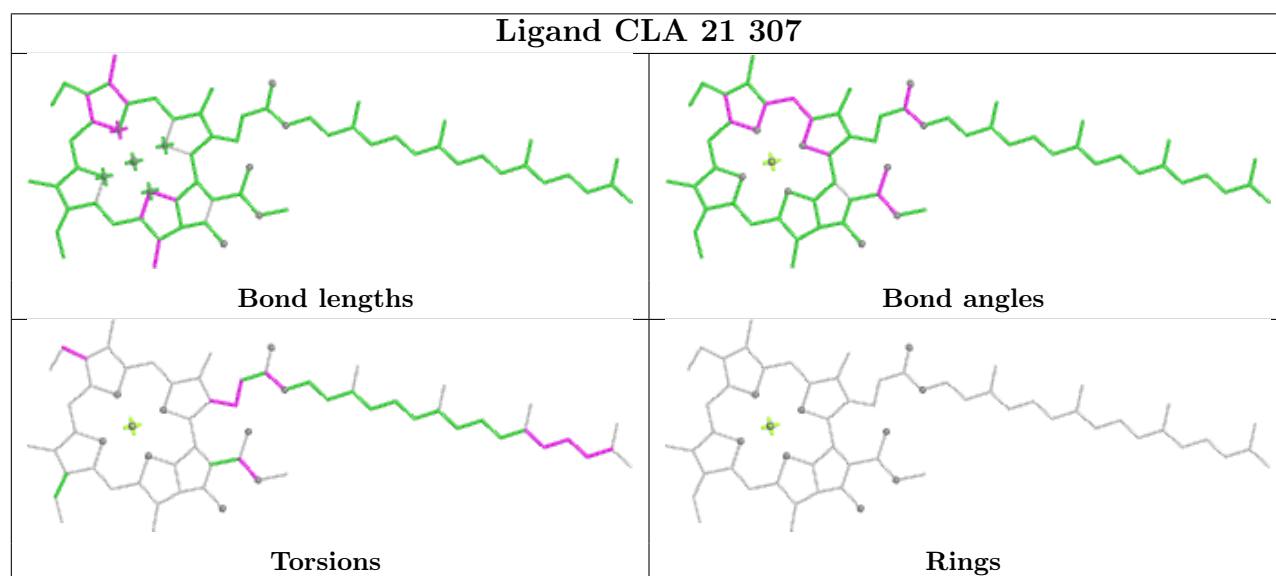
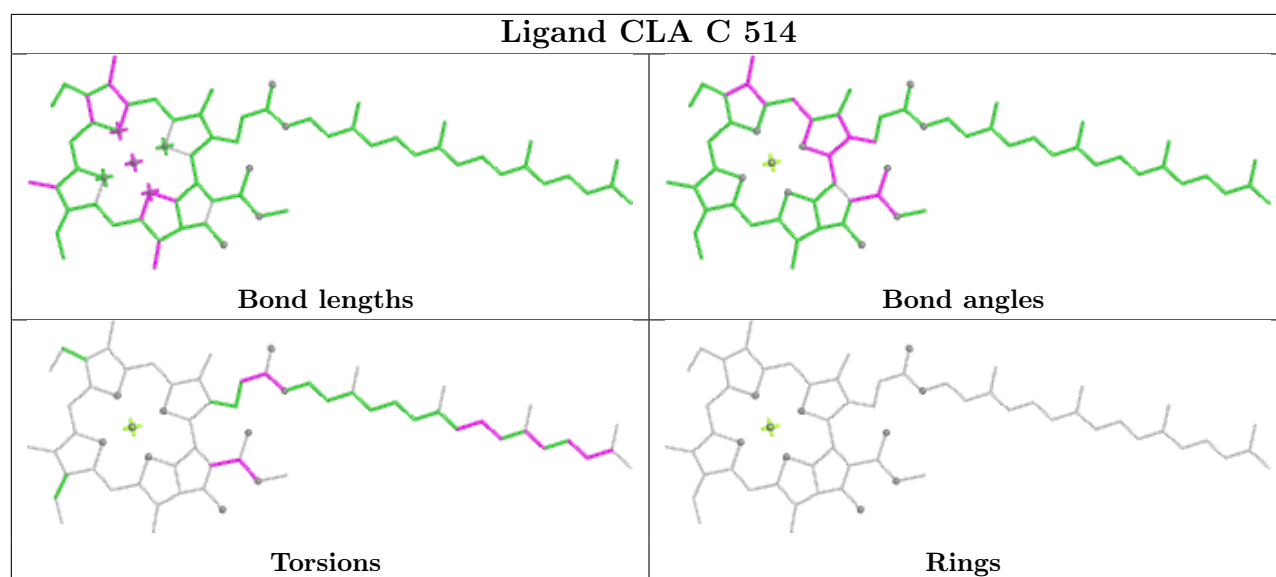


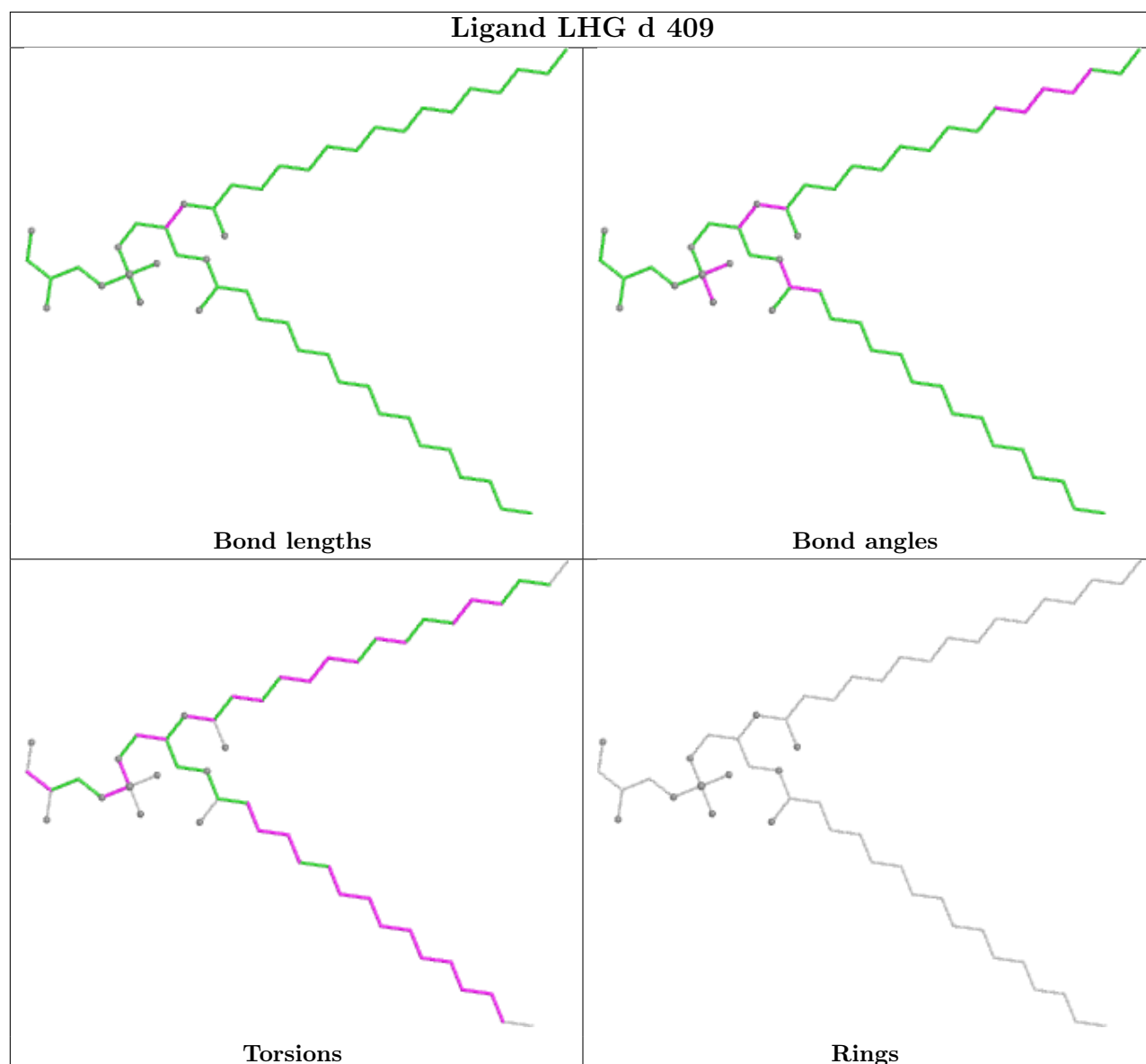
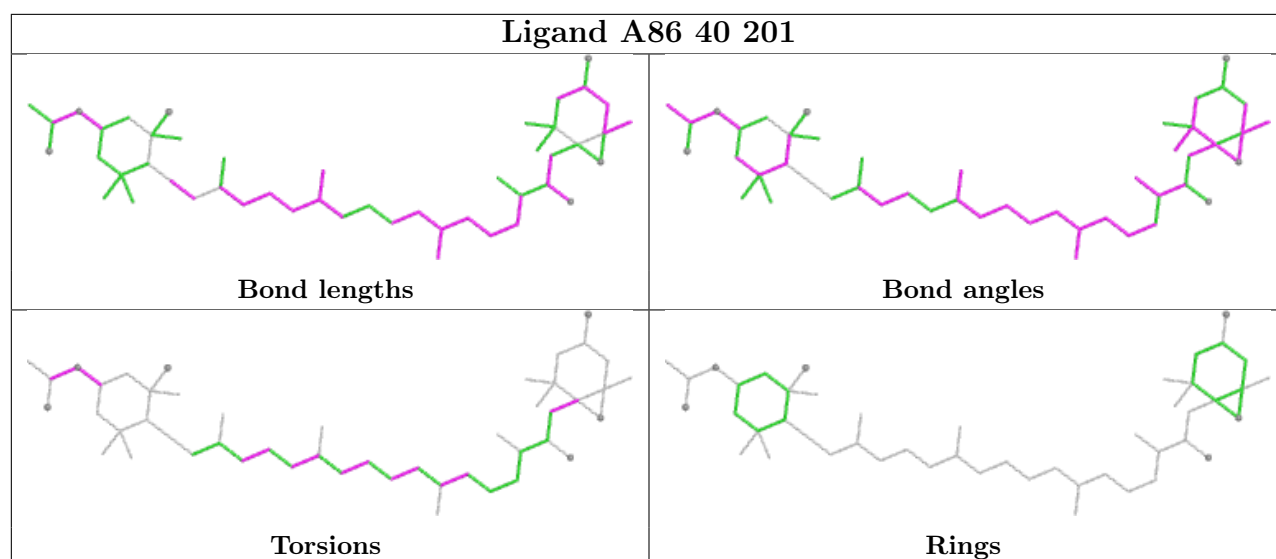


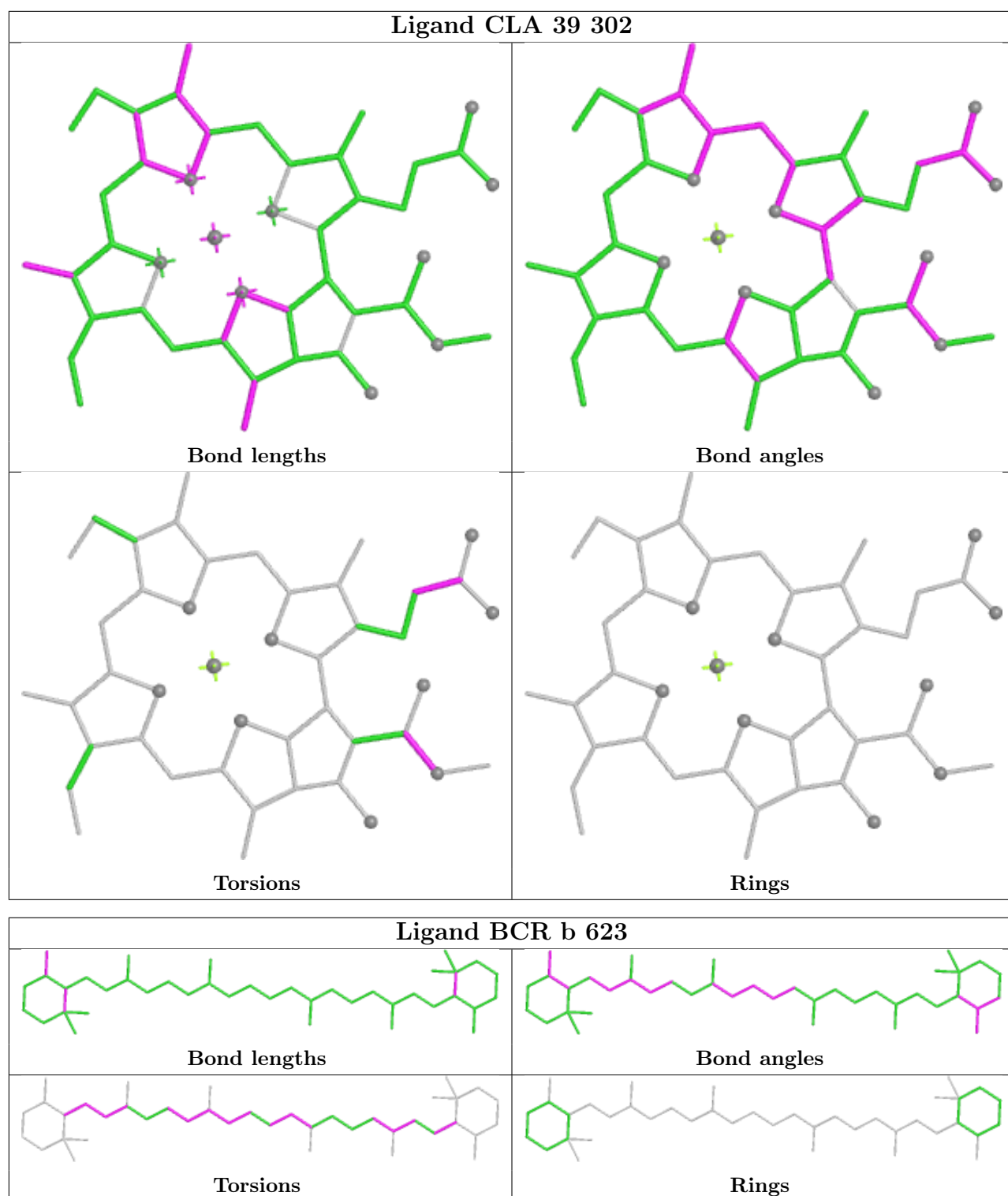


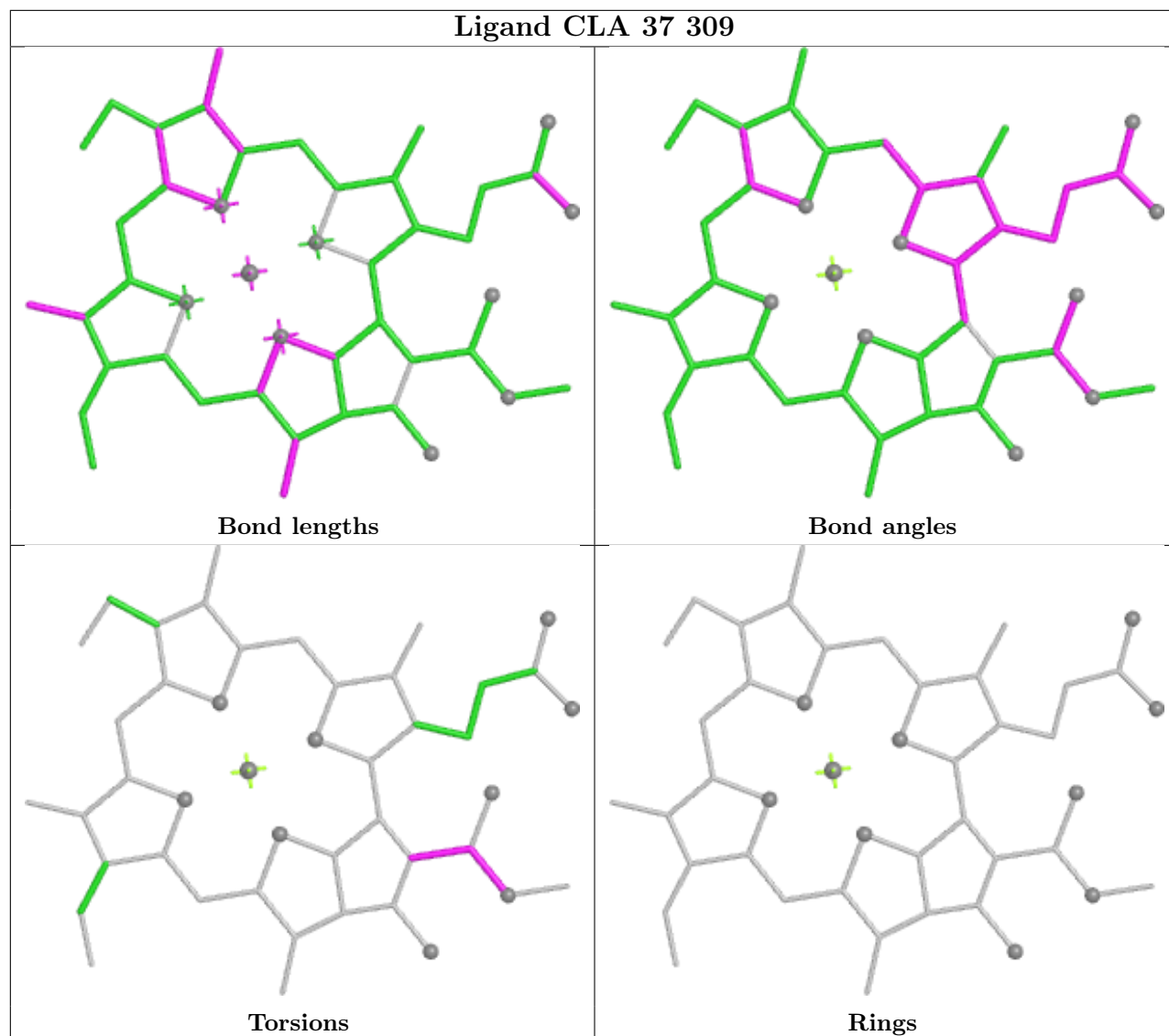


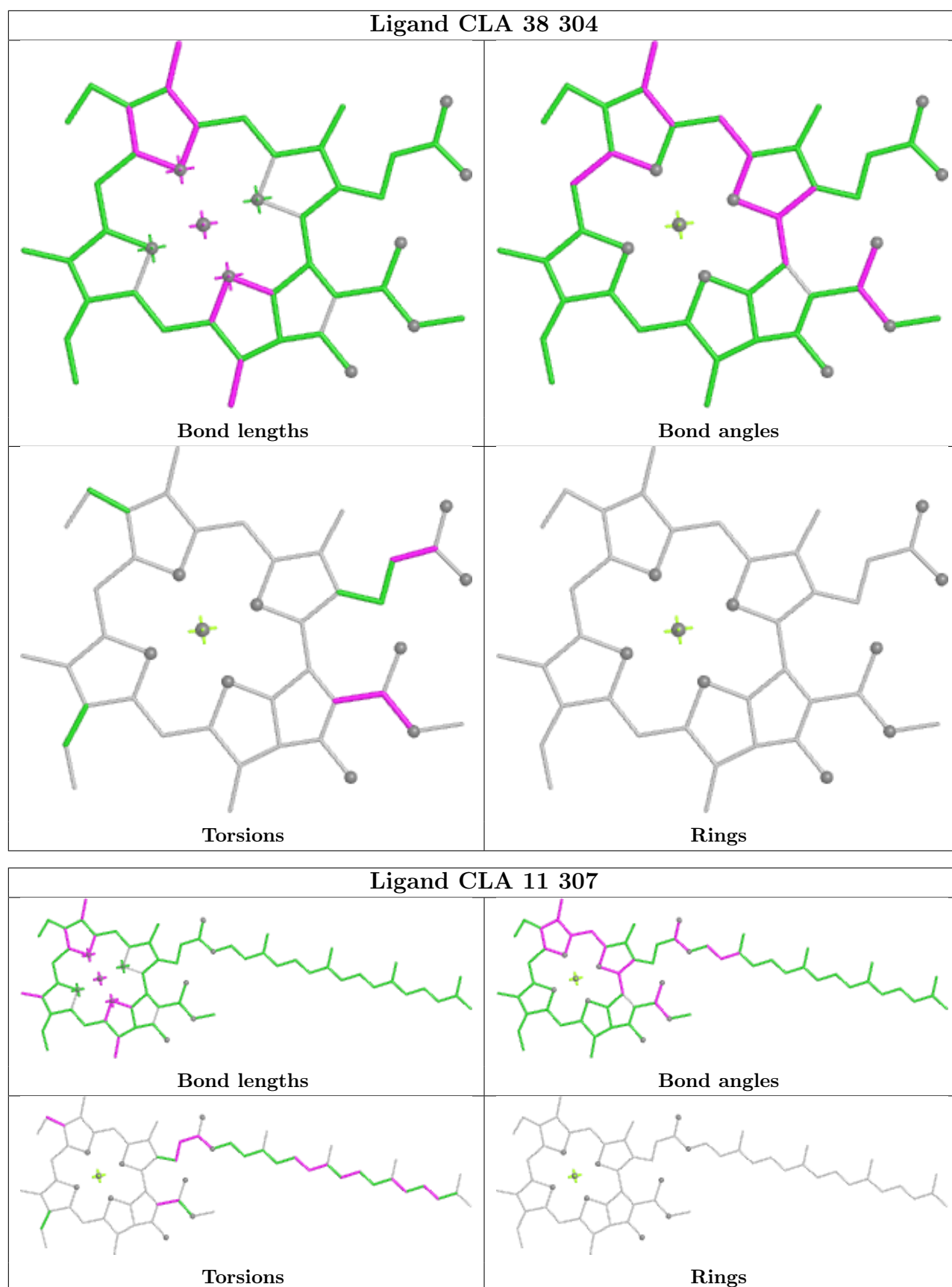


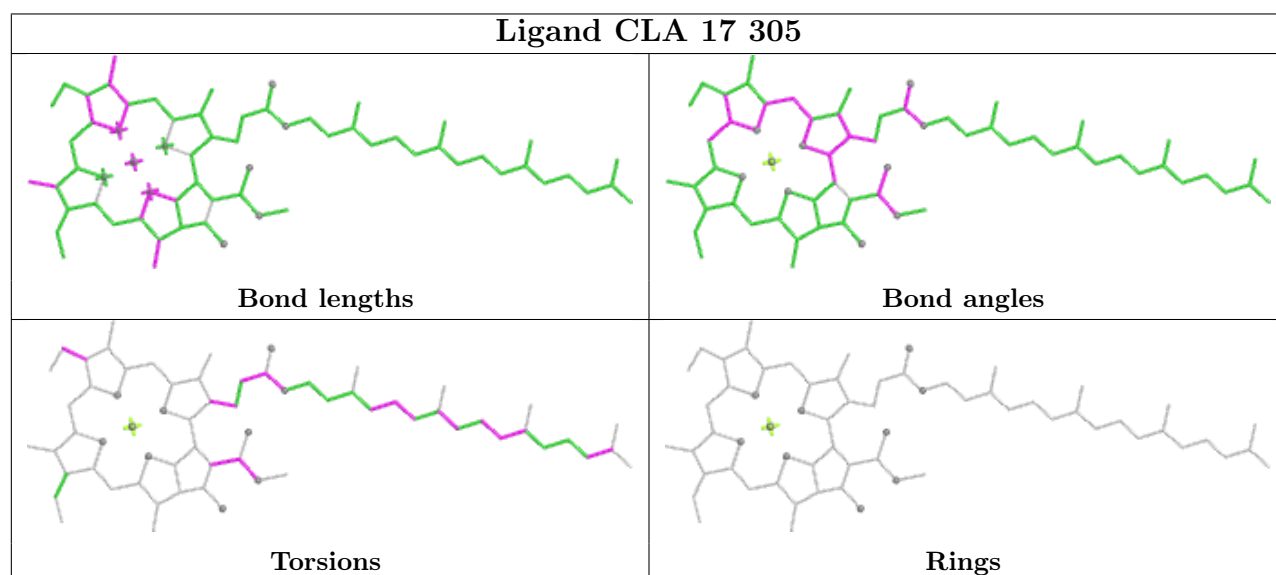
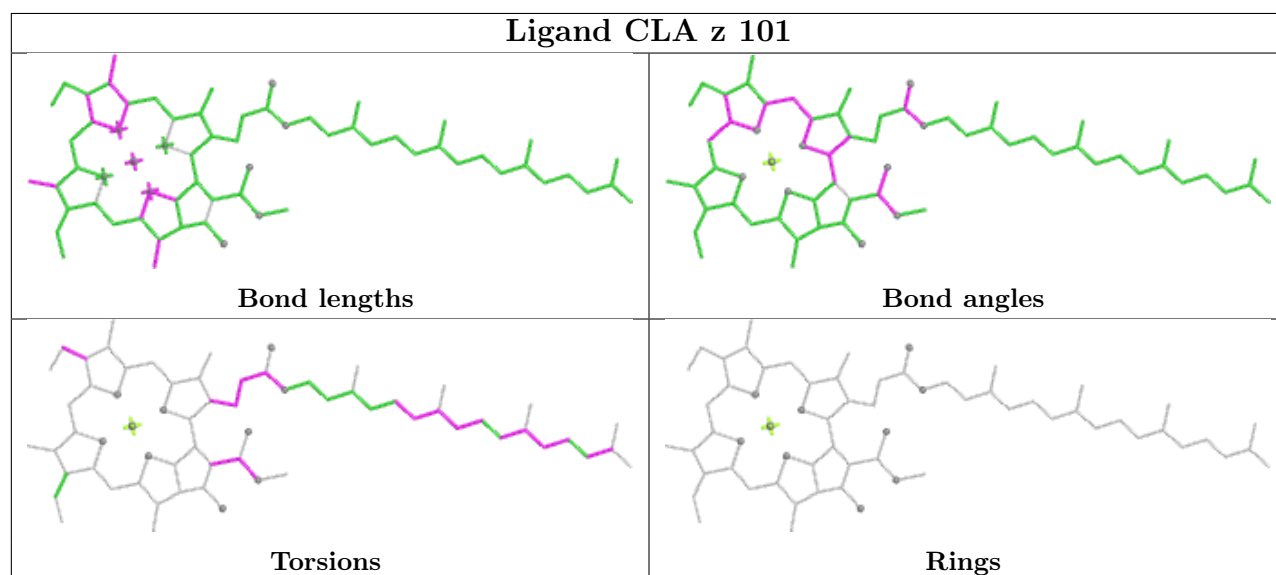
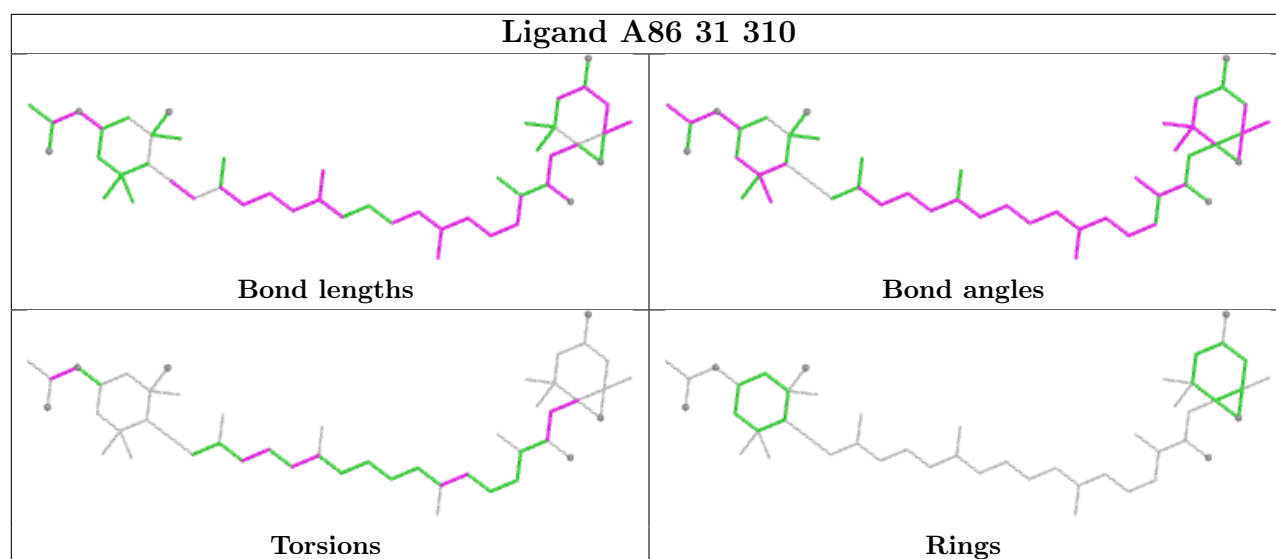


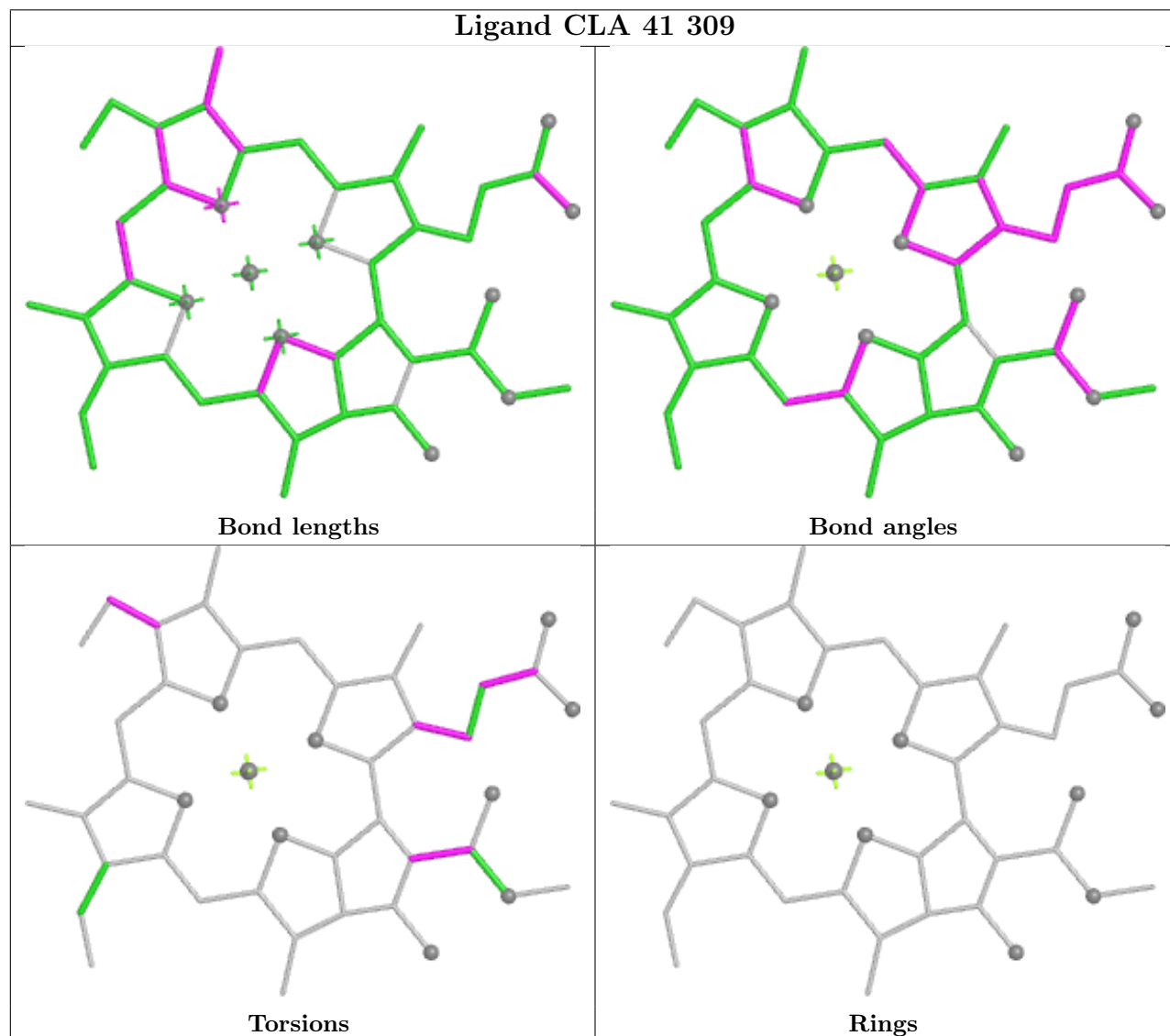
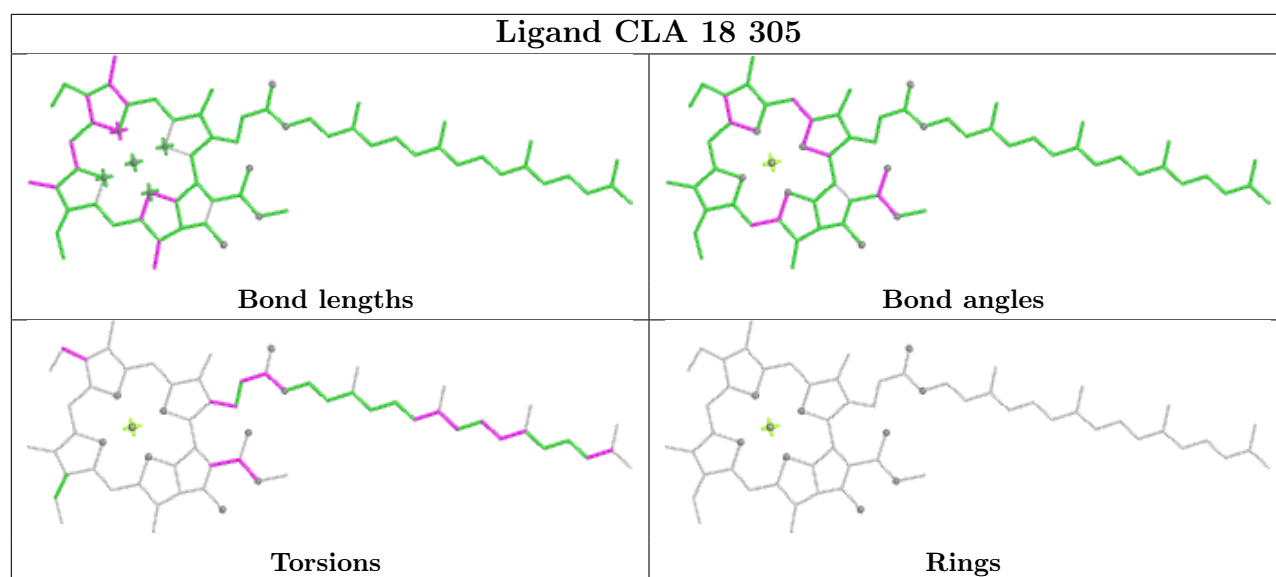


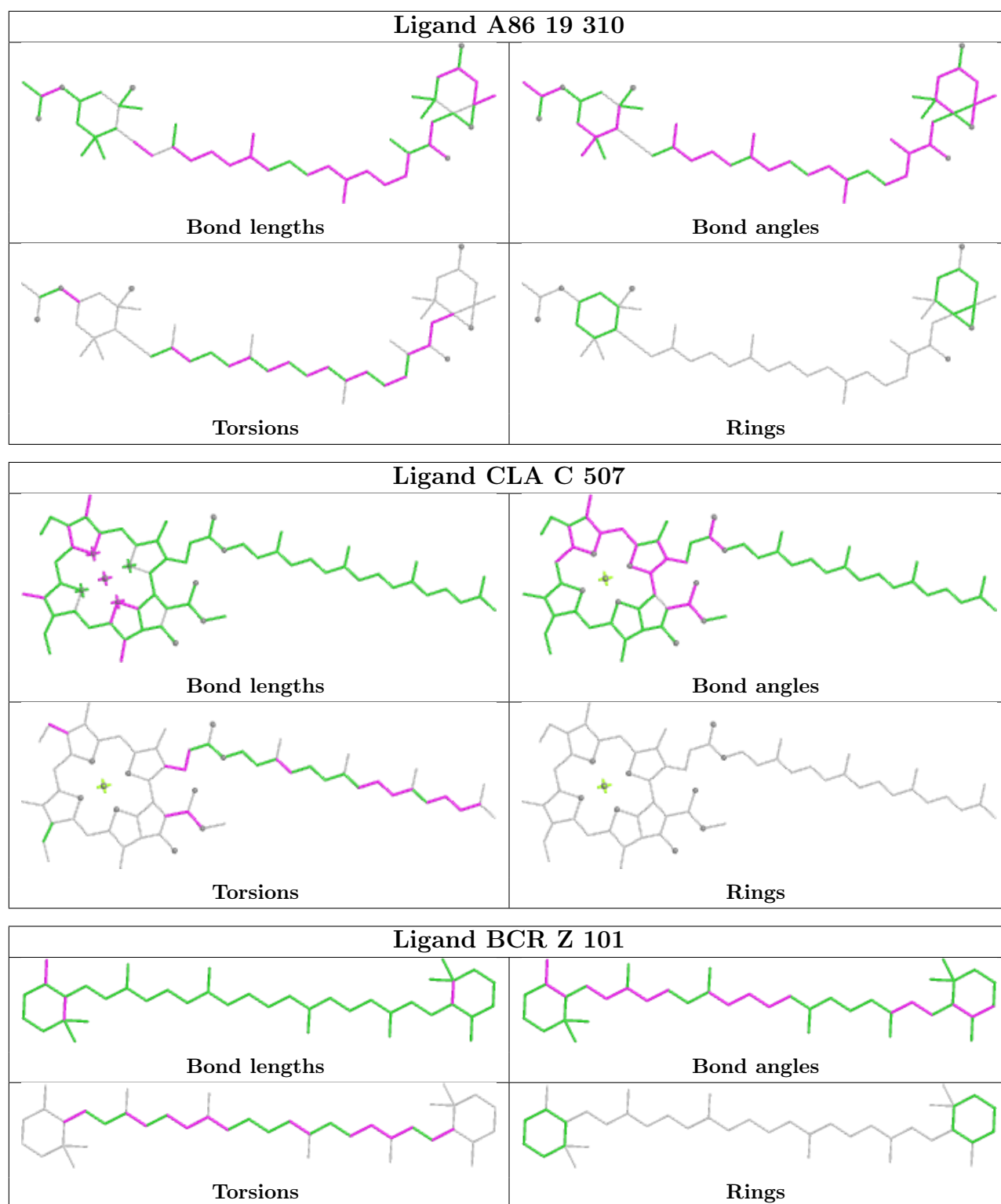


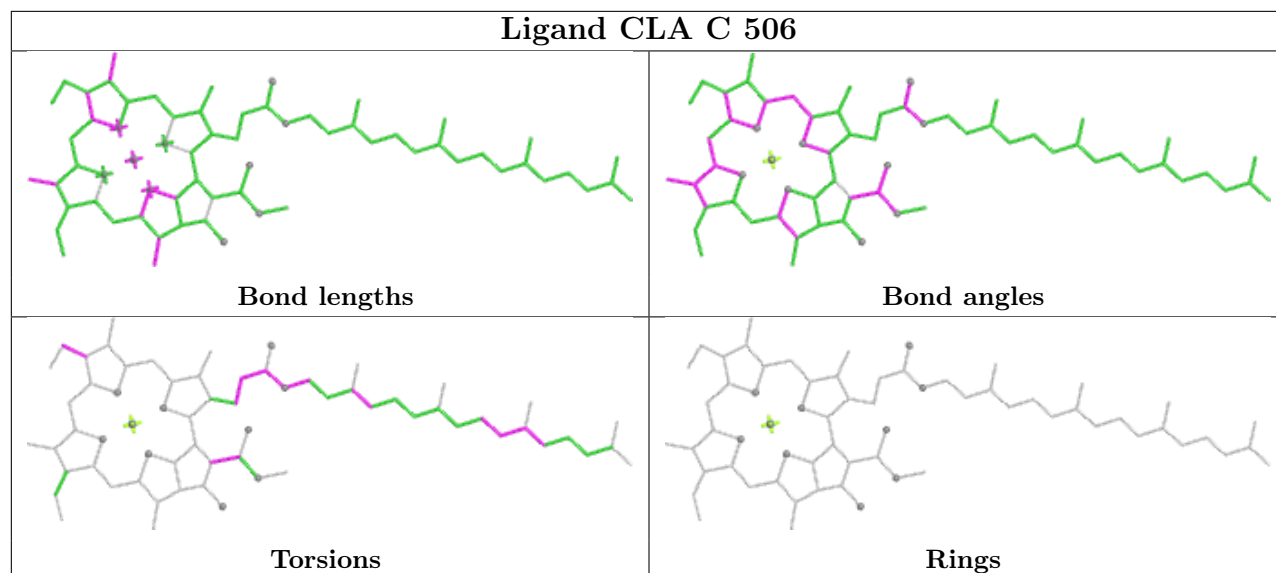
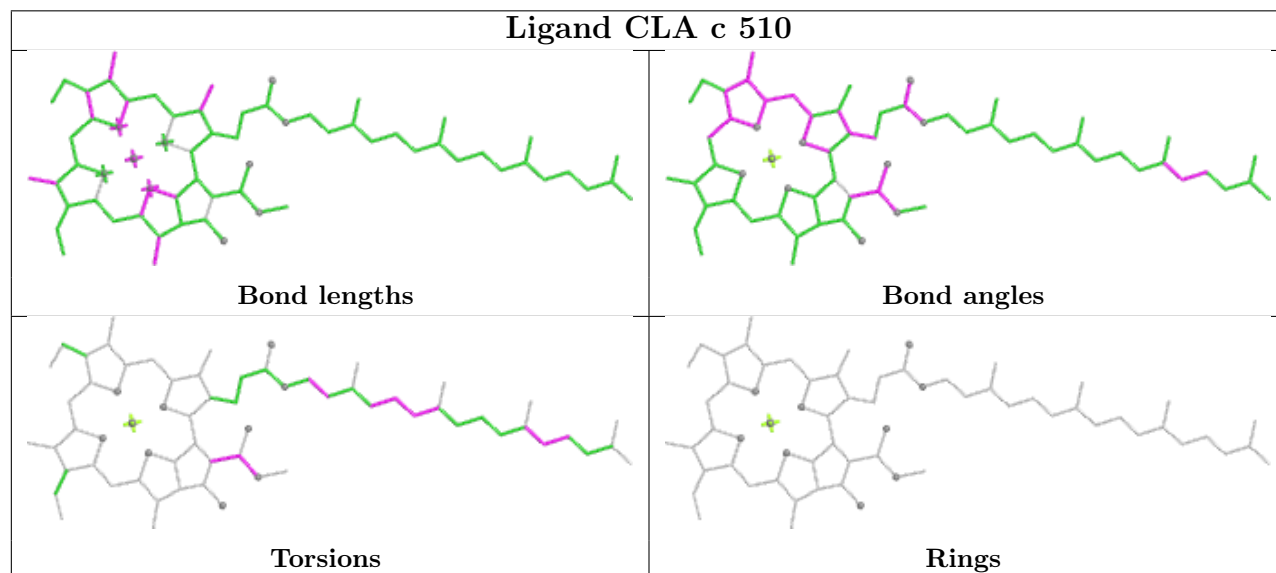
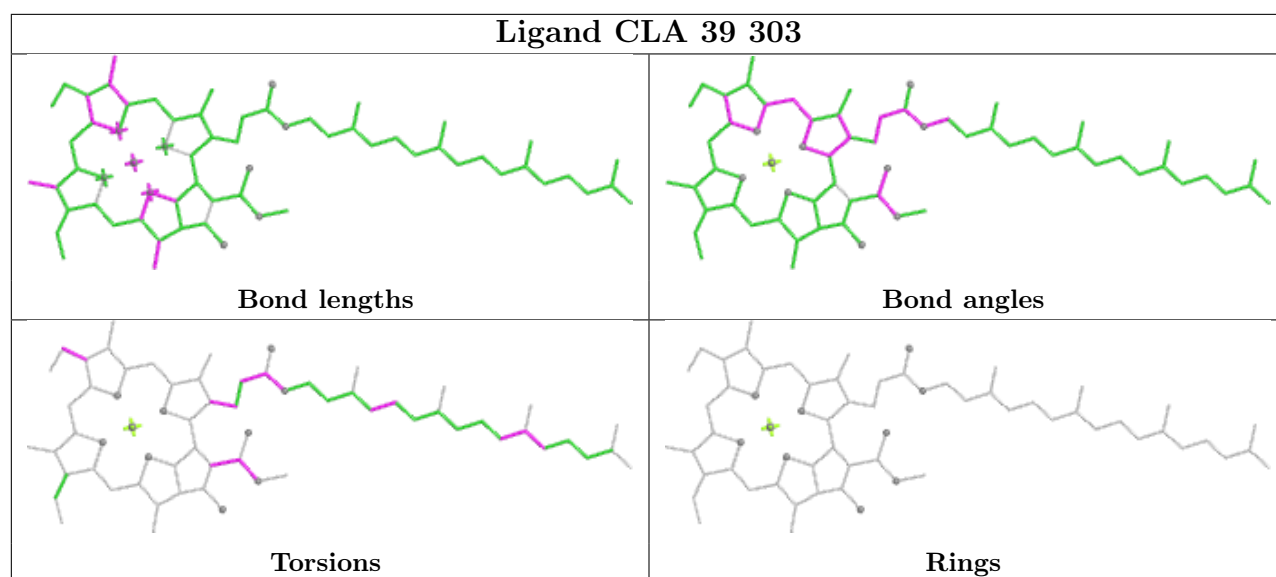


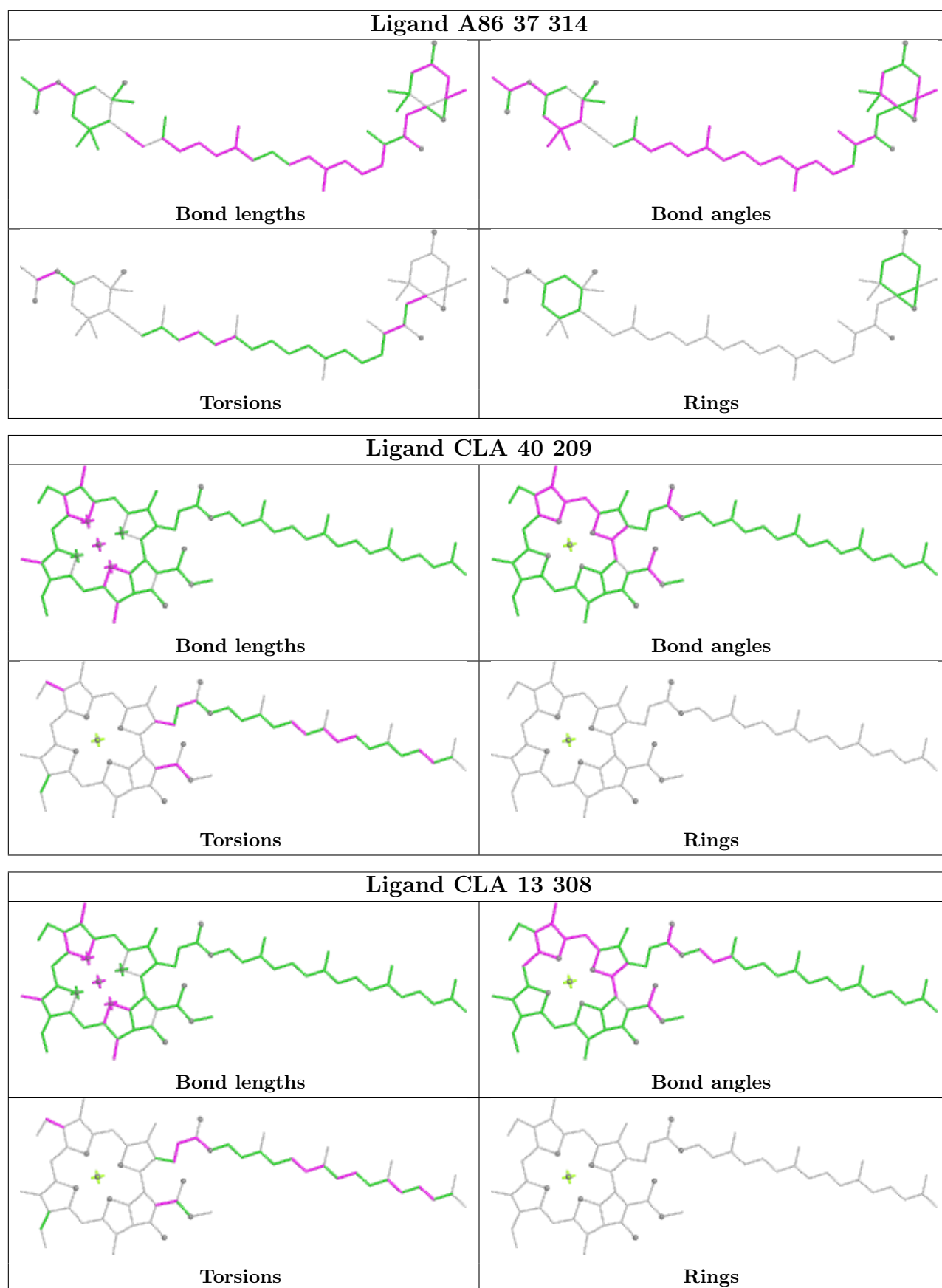












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

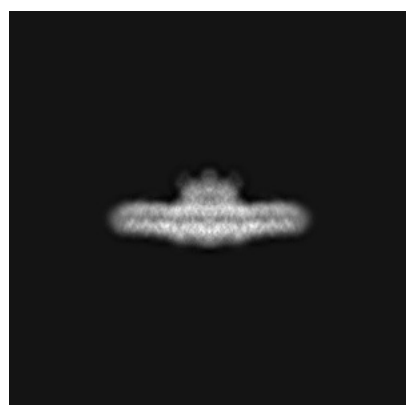
6 Map visualisation [i](#)

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

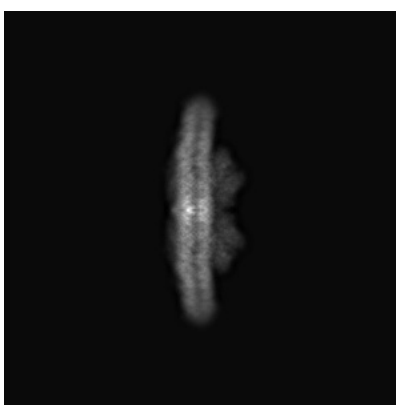
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

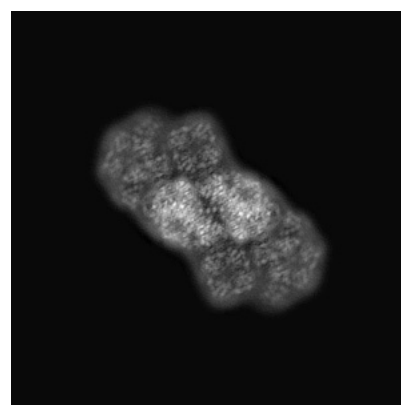
6.1.1 Primary map



X



Y



Z

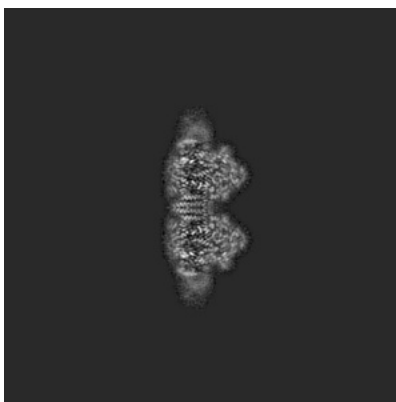
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

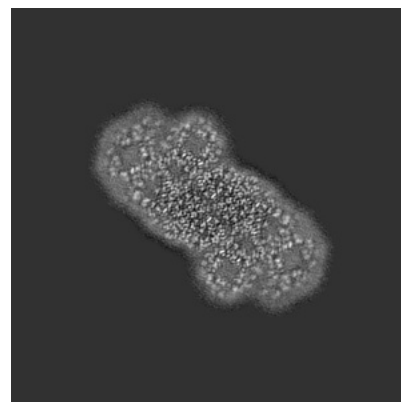
6.2.1 Primary map



X Index: 256



Y Index: 256

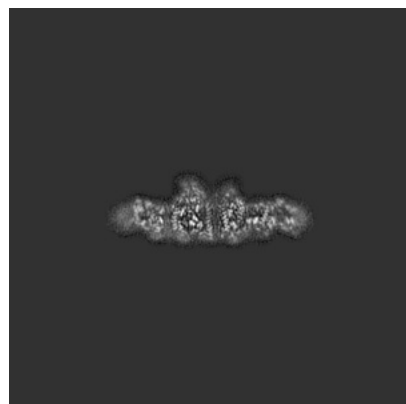


Z Index: 256

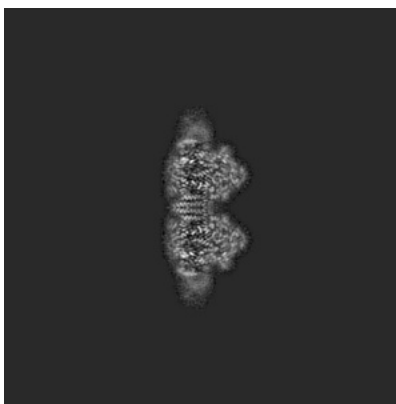
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

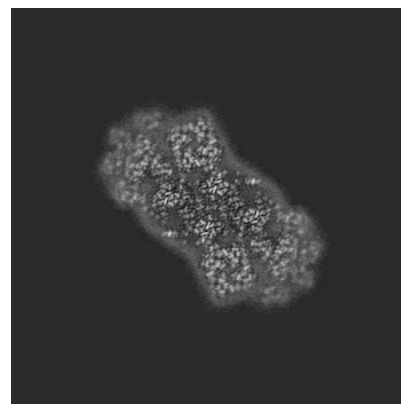
6.3.1 Primary map



X Index: 253



Y Index: 256

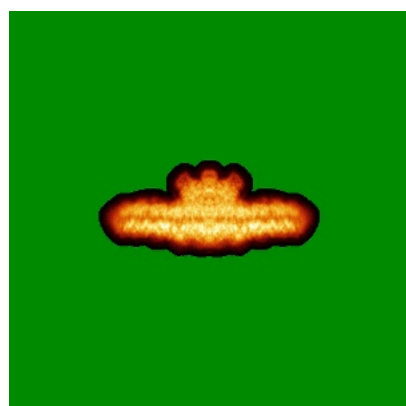


Z Index: 235

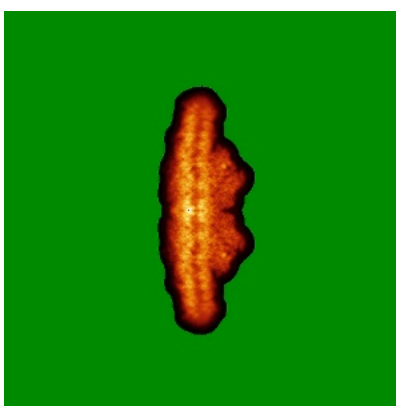
The images above show the largest variance slices of the map in three orthogonal directions.

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

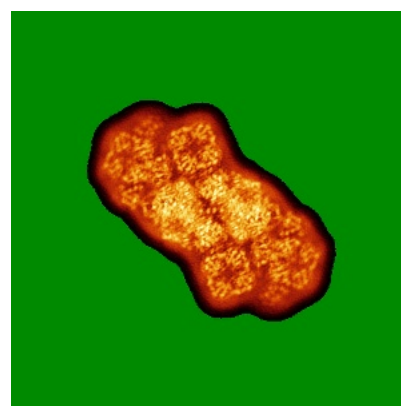
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

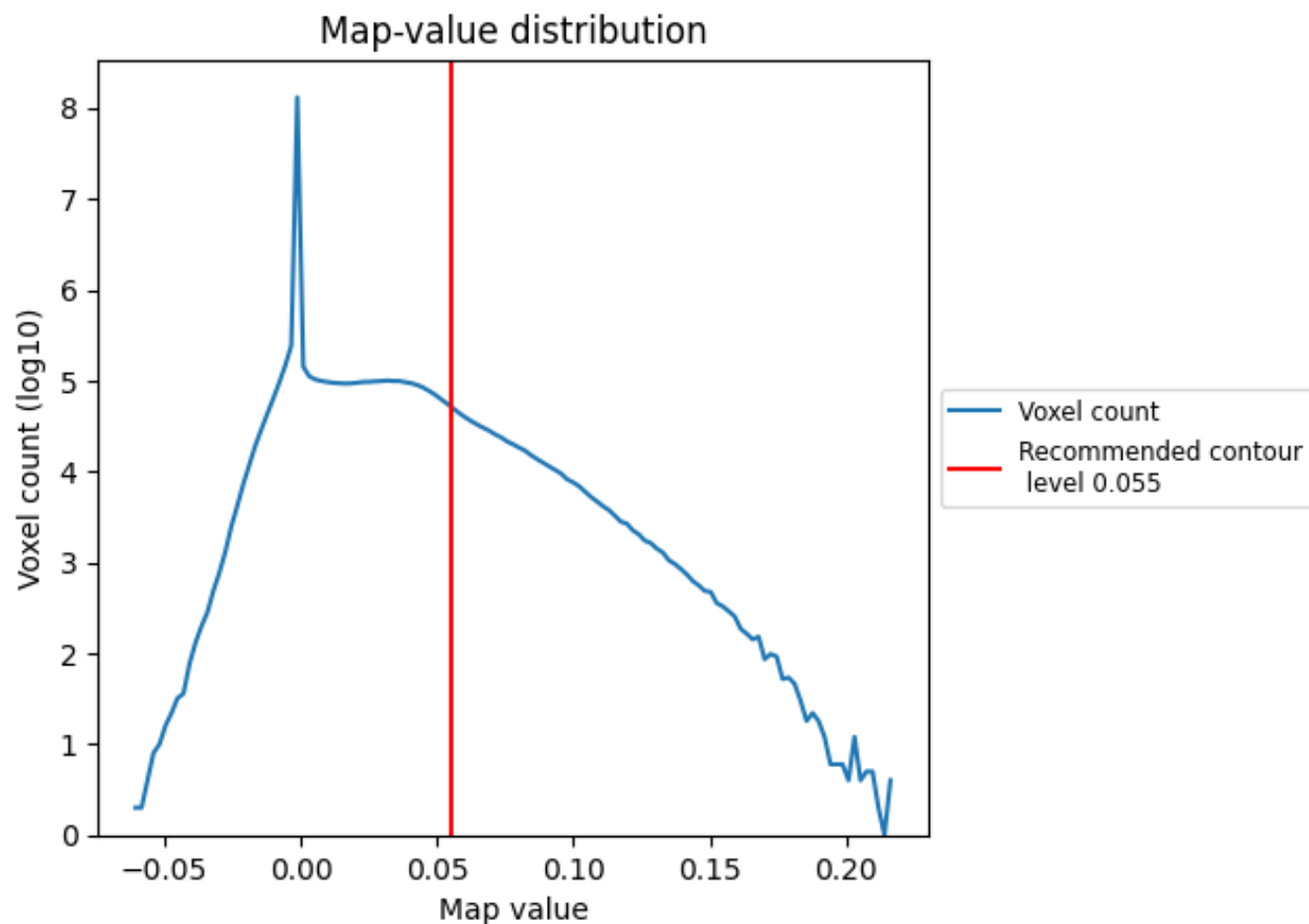
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

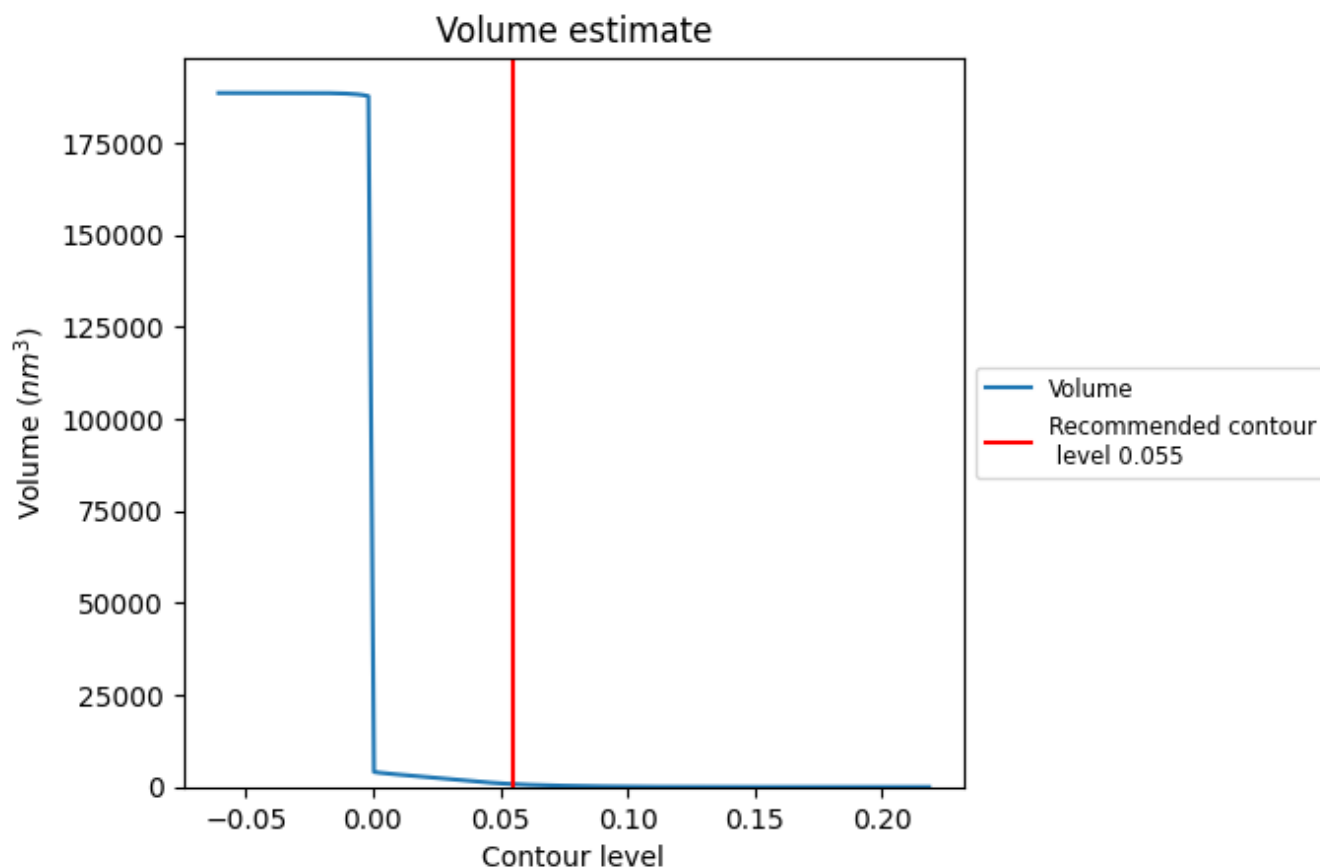
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

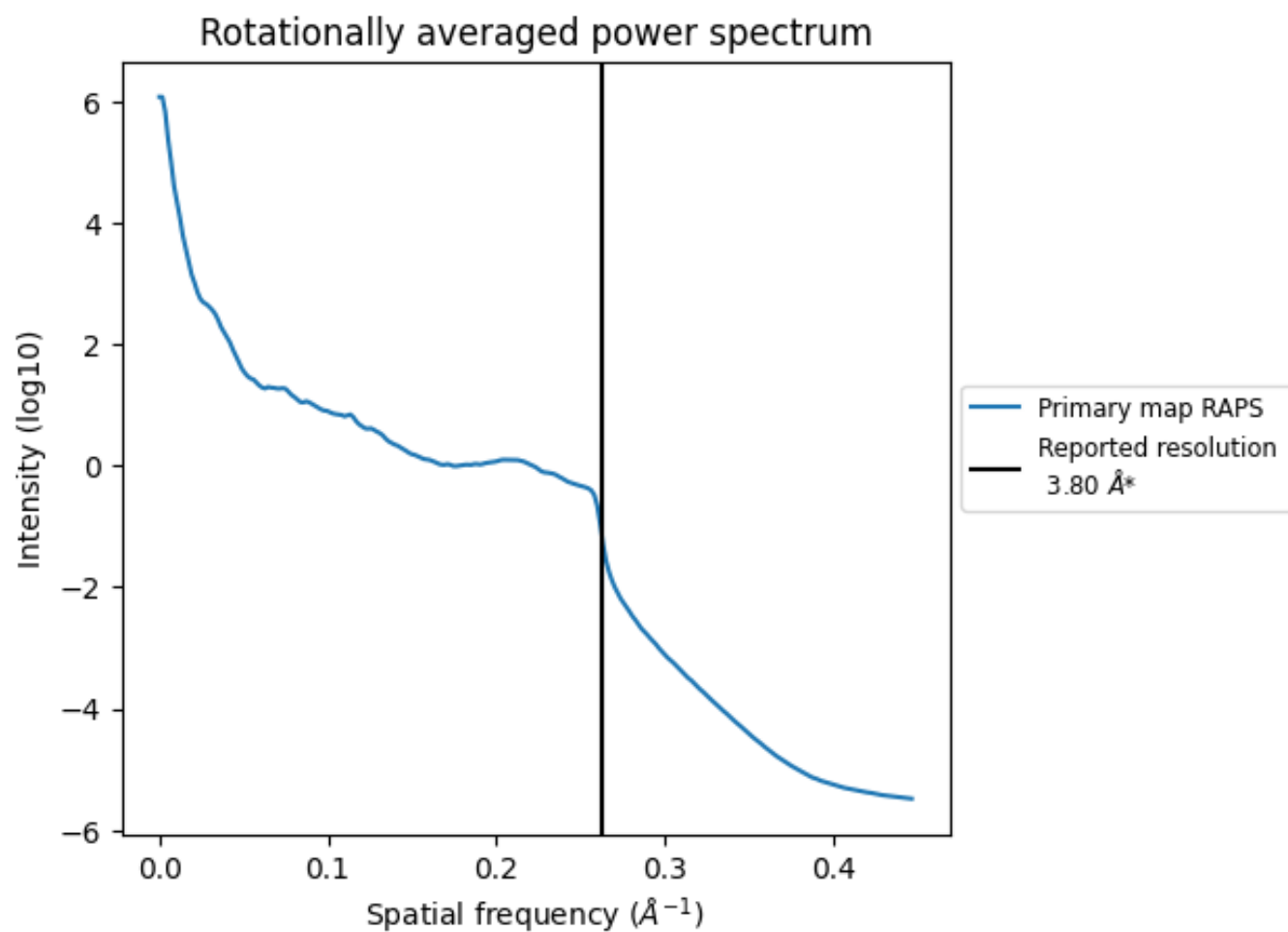
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 777 nm^3 ; this corresponds to an approximate mass of 701 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

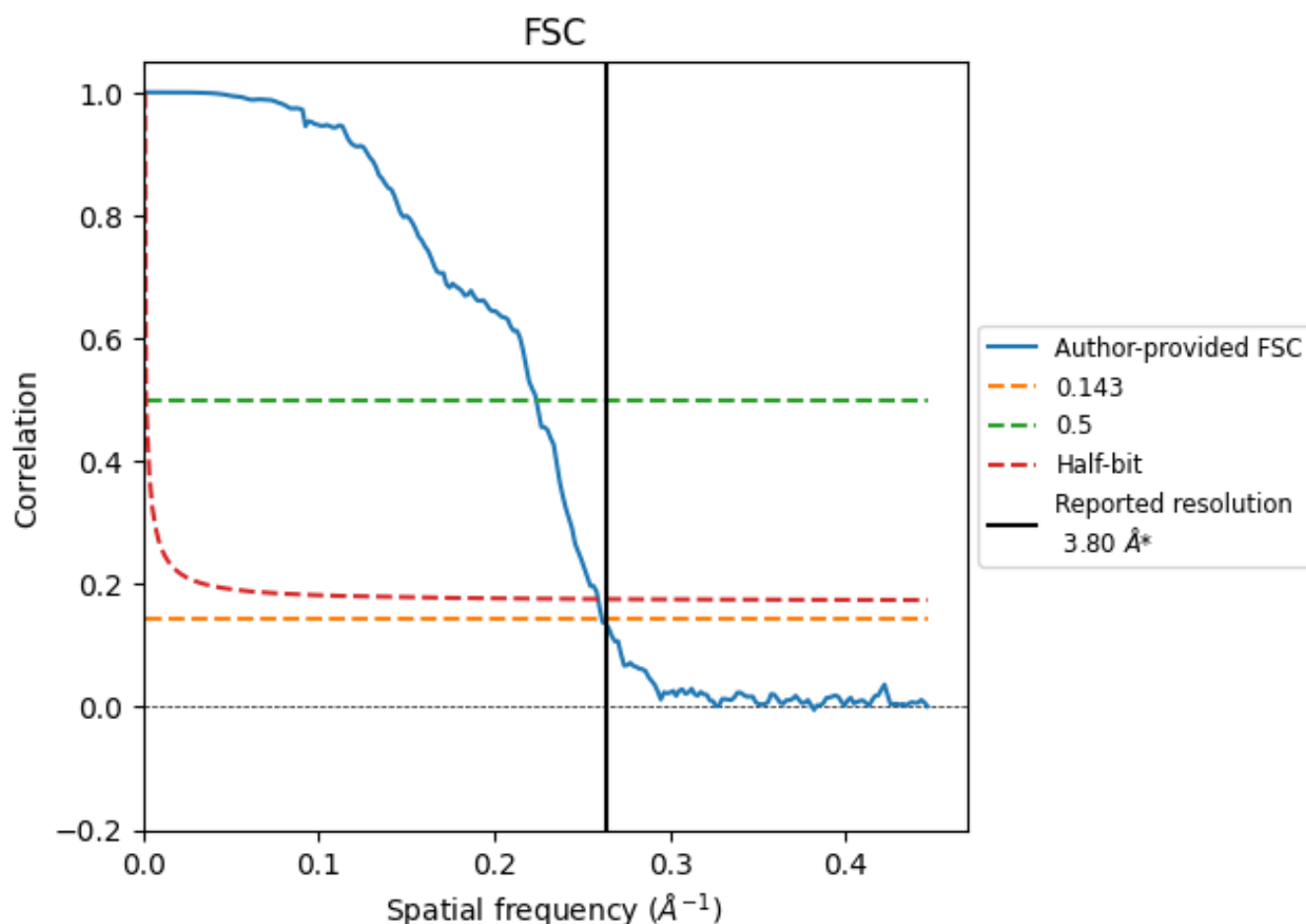


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

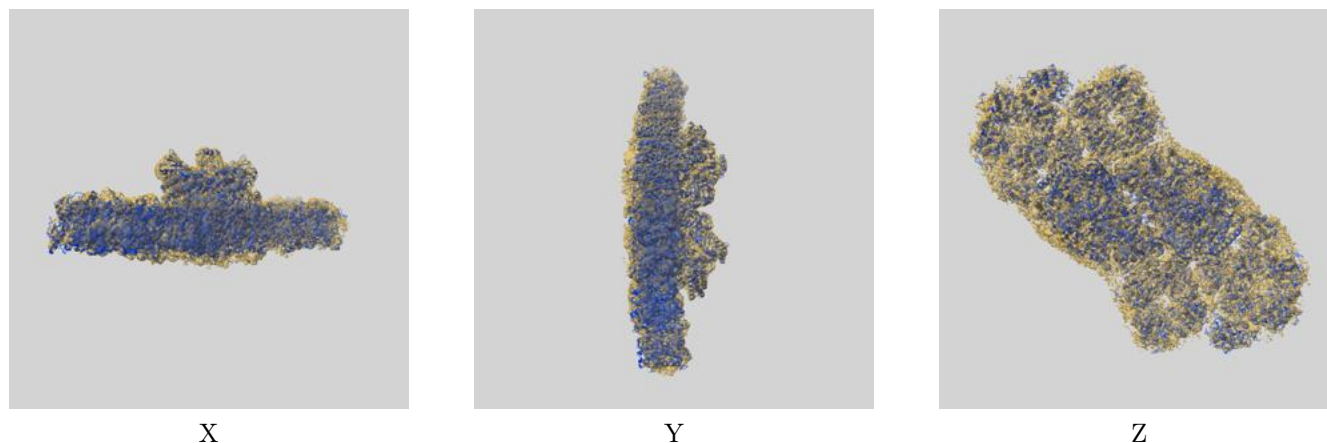
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	4.47	3.86
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

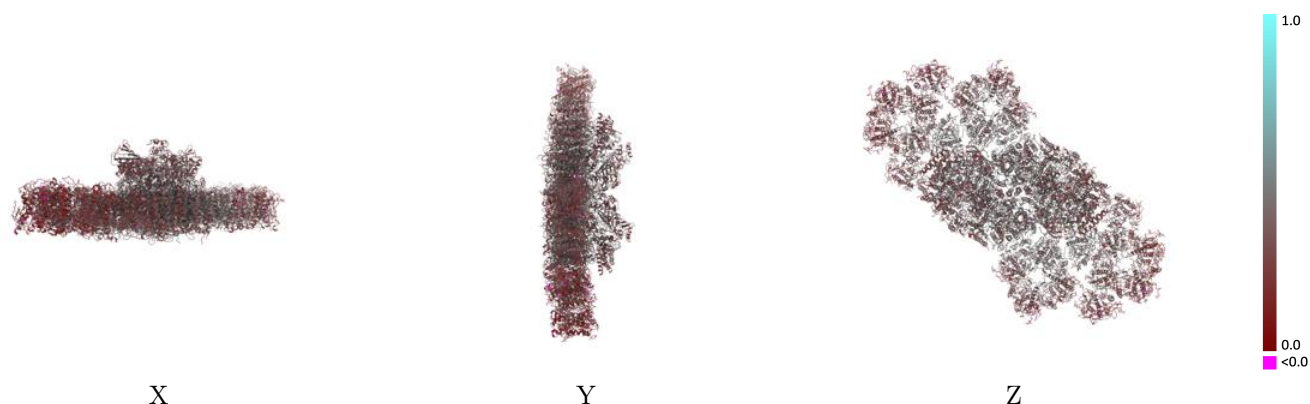
This section contains information regarding the fit between EMDB map EMD-9777 and PDB model 6J40. Per-residue inclusion information can be found in [section 3](#) on [page 42](#).

9.1 Map-model overlay [i](#)



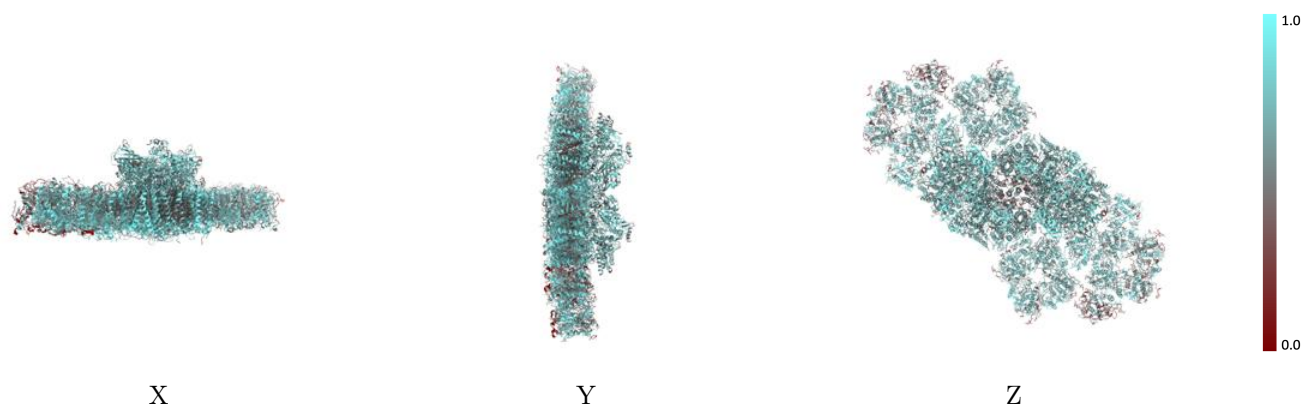
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



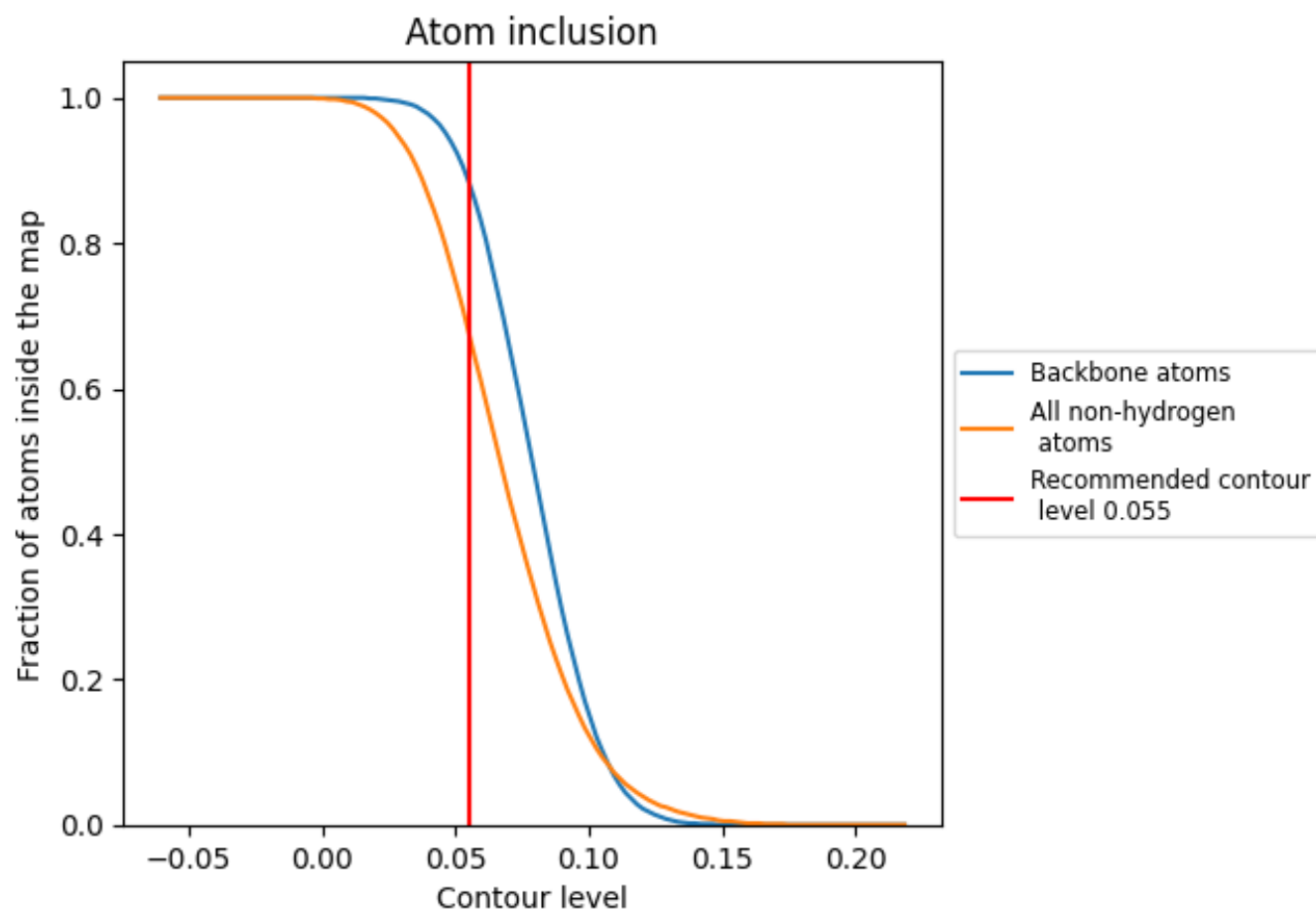
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6760	 0.3490
0	 0.7870	 0.4230
1	 0.8730	 0.4170
11	 0.7110	 0.3840
12	 0.6960	 0.3490
13	 0.6420	 0.2830
14	 0.6830	 0.3150
15	 0.5520	 0.2140
16	 0.7170	 0.3000
17	 0.6860	 0.3060
18	 0.5890	 0.2310
19	 0.8290	 0.4090
2	 0.9400	 0.3970
20	 0.7420	 0.2860
21	 0.4230	 0.2190
31	 0.7120	 0.3840
32	 0.7010	 0.3430
33	 0.6540	 0.2860
34	 0.6850	 0.3140
35	 0.5520	 0.2140
36	 0.7150	 0.3040
37	 0.6950	 0.3120
38	 0.5870	 0.2260
39	 0.8310	 0.4100
40	 0.7390	 0.2890
41	 0.4260	 0.2260
5	 0.8190	 0.4340
6	 0.8600	 0.4310
7	 0.8800	 0.3920
A	 0.6980	 0.4220
B	 0.7030	 0.4120
C	 0.7130	 0.3990
D	 0.6750	 0.4070
E	 0.7580	 0.3350
F	 0.6690	 0.3530



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
H	 0.7010	 0.3950
I	 0.6950	 0.3930
J	 0.6050	 0.3660
K	 0.7100	 0.3670
L	 0.5270	 0.4190
M	 0.5240	 0.3750
O	 0.6930	 0.3620
Q	 0.6240	 0.3190
T	 0.5630	 0.3730
U	 0.7080	 0.3380
V	 0.7640	 0.3530
W	 0.5370	 0.3630
X	 0.6250	 0.2750
Y	 0.5640	 0.3240
Z	 0.6750	 0.3140
a	 0.7020	 0.4220
b	 0.7100	 0.4180
c	 0.6990	 0.3950
d	 0.6630	 0.4120
e	 0.7700	 0.3360
f	 0.6690	 0.3530
h	 0.7040	 0.3980
i	 0.7090	 0.3880
j	 0.6140	 0.3590
k	 0.7060	 0.3710
l	 0.5420	 0.4100
m	 0.5040	 0.3780
o	 0.6940	 0.3620
q	 0.6400	 0.3130
t	 0.5550	 0.3790
u	 0.6970	 0.3390
v	 0.7590	 0.3510
w	 0.5440	 0.3590
x	 0.6290	 0.2800
y	 0.5940	 0.3020
z	 0.6930	 0.3120