



wwPDB EM Validation Summary Report ⓘ

Dec 29, 2024 – 07:50 PM EST

PDB ID : 7VD5
EMDB ID : EMD-31905
Title : Structure of C2S2M2-type PSII-FCPII supercomplex from diatom
Authors : Nagao, R.; Kato, K.; Akita, F.; Miyazaki, N.; Shen, J.R.
Deposited on : 2021-09-06
Resolution : 2.50 Å(reported)
Based on initial model : 6J40

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

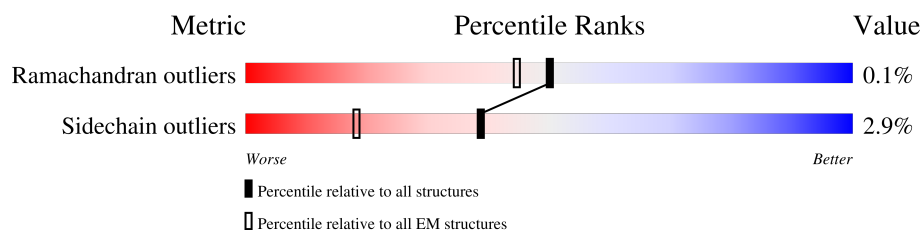
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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


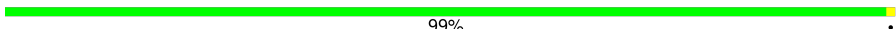
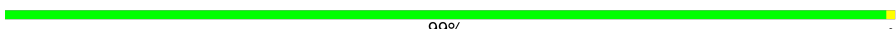
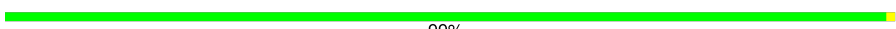





The reported resolution of this entry is 2.50 Å.

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



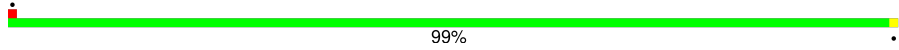


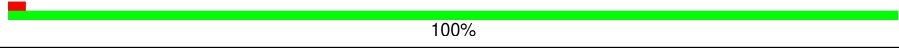



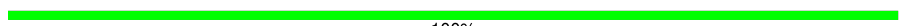
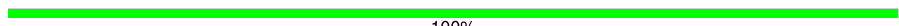
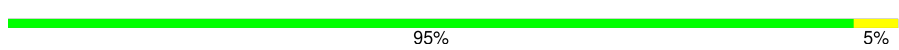
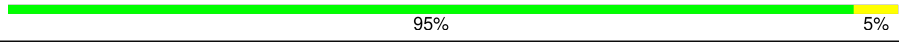
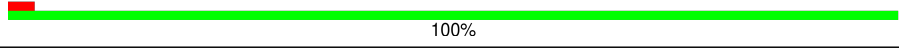


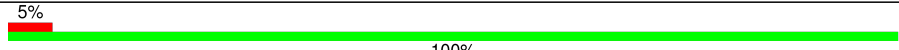
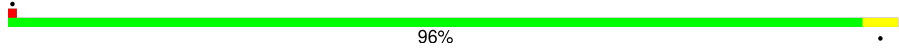
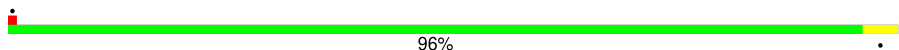


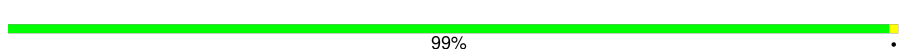
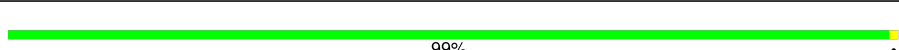

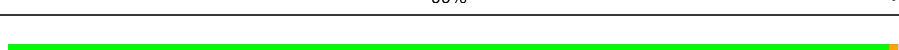
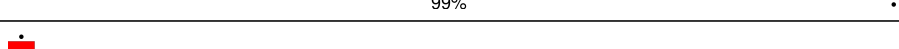
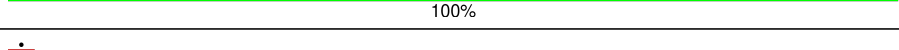
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	334	 99% .
1	a	334	 99% .
2	B	484	 99% .
2	b	484	 99% .
3	C	451	 99% .
3	c	451	 99% .
4	D	341	 100%
4	d	341	 100%
5	E	75	 99% .

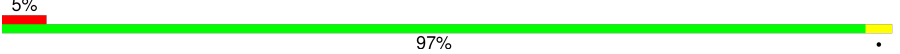
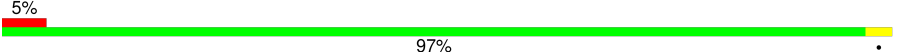
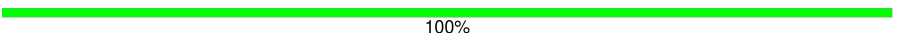
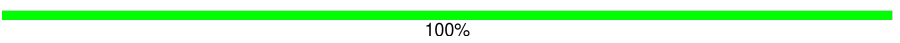
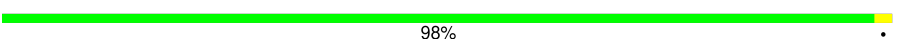
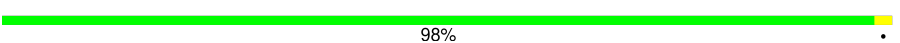


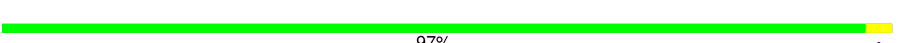
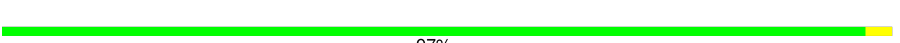

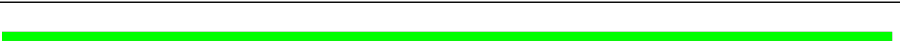

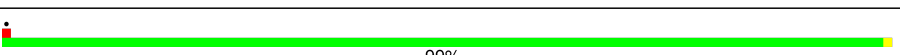
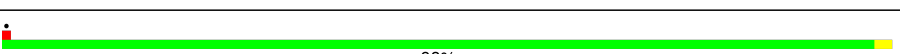
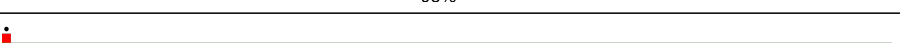
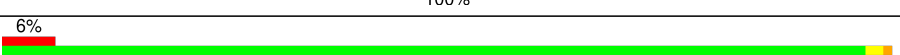
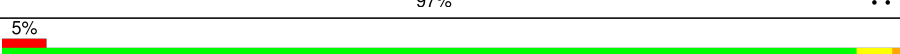
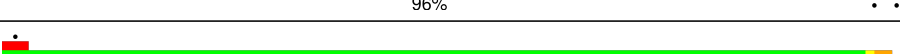
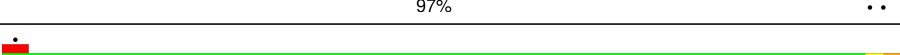



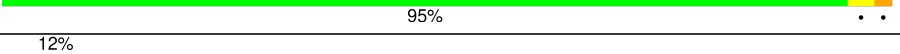
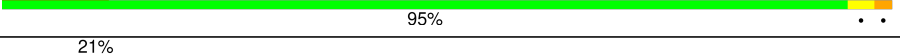
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Mol	Chain	Length	Quality of chain
5	e	75	 99%
6	F	28	 100%
6	f	28	 100%
7	H	66	 100%
7	h	66	 100%
8	I	35	 100%
8	i	35	 100%
9	J	34	 100%
9	j	34	 100%
10	K	37	 95% 5%
10	k	37	 95% 5%
11	L	38	 100%
11	l	38	 100%
12	M	42	 100% 5%
12	m	42	 100% 5%
13	O	245	 96% .
13	o	245	 96% .
14	T	30	 100%
14	t	30	 100%
15	U	93	 99% .
15	u	93	 99% .
16	V	136	 99% .
16	v	136	 99% .
17	Y	34	 100%
17	y	34	 100%

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Mol	Chain	Length	Quality of chain
18	X	37	
18	x	37	
19	Z	59	
19	z	59	
20	Q	151	
20	q	151	
21	W	52	
21	w	52	
22	0	31	
22	5	31	
23	1	30	
23	6	30	
24	11	176	
24	31	176	
25	12	169	
25	32	169	
26	13	169	
26	33	169	
27	14	172	
27	34	172	
28	15	170	
28	35	170	
29	16	179	
29	36	179	
30	17	176	

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Mol	Chain	Length	Quality of chain
30	37	176	
31	18	168	
31	38	168	
32	19	227	
32	39	227	
33	20	155	
33	40	155	
34	21	162	
34	41	162	

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
37	CLA	11	303	X	-	-	-
37	CLA	11	305	X	-	-	-
37	CLA	11	308	X	-	-	-
37	CLA	11	310	X	-	-	-
37	CLA	12	203	X	-	-	-
37	CLA	12	204	X	-	-	-
37	CLA	12	205	X	-	-	-
37	CLA	12	207	X	-	-	-
37	CLA	12	209	X	-	-	-
37	CLA	12	212	X	-	-	-
37	CLA	13	303	X	-	-	-
37	CLA	13	305	X	-	-	-
37	CLA	13	307	X	-	-	-
37	CLA	14	302	X	-	-	-
37	CLA	14	305	X	-	-	-
37	CLA	14	307	X	-	-	-
37	CLA	14	308	X	-	-	-
37	CLA	14	310	X	-	-	-
37	CLA	15	305	X	-	-	-
37	CLA	15	307	X	-	-	-
37	CLA	15	308	X	-	-	-
37	CLA	15	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CLA	16	303	X	-	-	-
37	CLA	16	306	X	-	-	-
37	CLA	16	307	X	-	-	-
37	CLA	16	309	X	-	-	-
37	CLA	17	304	X	-	-	-
37	CLA	17	307	X	-	-	-
37	CLA	17	309	X	-	-	-
37	CLA	18	201	X	-	-	-
37	CLA	18	203	X	-	-	-
37	CLA	18	204	X	-	-	-
37	CLA	18	206	X	-	-	-
37	CLA	18	208	X	-	-	-
37	CLA	18	209	X	-	-	-
37	CLA	19	301	X	-	-	-
37	CLA	19	302	X	-	-	-
37	CLA	19	303	X	-	-	-
37	CLA	19	304	X	-	-	-
37	CLA	19	305	X	-	-	-
37	CLA	19	306	X	-	-	-
37	CLA	19	307	X	-	-	-
37	CLA	19	309	X	-	-	-
37	CLA	19	310	X	-	-	-
37	CLA	20	303	X	-	-	-
37	CLA	20	306	X	-	-	-
37	CLA	20	307	X	-	-	-
37	CLA	20	308	X	-	-	-
37	CLA	21	202	X	-	-	-
37	CLA	21	205	X	-	-	-
37	CLA	21	206	X	-	-	-
37	CLA	21	208	X	-	-	-
37	CLA	21	209	X	-	-	-
37	CLA	31	301	X	-	-	-
37	CLA	31	304	X	-	-	-
37	CLA	31	306	X	-	-	-
37	CLA	31	310	X	-	-	-
37	CLA	32	202	X	-	-	-
37	CLA	32	204	X	-	-	-
37	CLA	32	205	X	-	-	-
37	CLA	32	206	X	-	-	-
37	CLA	32	208	X	-	-	-
37	CLA	32	210	X	-	-	-
37	CLA	32	213	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CLA	33	303	X	-	-	-
37	CLA	33	305	X	-	-	-
37	CLA	33	307	X	-	-	-
37	CLA	34	302	X	-	-	-
37	CLA	34	305	X	-	-	-
37	CLA	34	307	X	-	-	-
37	CLA	34	308	X	-	-	-
37	CLA	34	310	X	-	-	-
37	CLA	35	305	X	-	-	-
37	CLA	35	307	X	-	-	-
37	CLA	35	310	X	-	-	-
37	CLA	36	303	X	-	-	-
37	CLA	36	306	X	-	-	-
37	CLA	36	307	X	-	-	-
37	CLA	36	309	X	-	-	-
37	CLA	37	303	X	-	-	-
37	CLA	37	306	X	-	-	-
37	CLA	37	308	X	-	-	-
37	CLA	38	201	X	-	-	-
37	CLA	38	203	X	-	-	-
37	CLA	38	204	X	-	-	-
37	CLA	38	208	X	-	-	-
37	CLA	38	209	X	-	-	-
37	CLA	39	301	X	-	-	-
37	CLA	39	302	X	-	-	-
37	CLA	39	303	X	-	-	-
37	CLA	39	304	X	-	-	-
37	CLA	39	305	X	-	-	-
37	CLA	39	307	X	-	-	-
37	CLA	39	309	X	-	-	-
37	CLA	39	310	X	-	-	-
37	CLA	40	205	X	-	-	-
37	CLA	40	208	X	-	-	-
37	CLA	40	209	X	-	-	-
37	CLA	40	210	X	-	-	-
37	CLA	41	202	X	-	-	-
37	CLA	41	205	X	-	-	-
37	CLA	41	206	X	-	-	-
37	CLA	41	208	X	-	-	-
37	CLA	41	209	X	-	-	-
37	CLA	A	403	X	-	-	-
37	CLA	B	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CLA	B	502	X	-	-	-
37	CLA	B	503	X	-	-	-
37	CLA	B	504	X	-	-	-
37	CLA	B	505	X	-	-	-
37	CLA	B	506	X	-	-	-
37	CLA	B	507	X	-	-	-
37	CLA	B	509	X	-	-	-
37	CLA	B	510	X	-	-	-
37	CLA	B	511	X	-	-	-
37	CLA	B	512	X	-	-	-
37	CLA	B	513	X	-	-	-
37	CLA	B	514	X	-	-	-
37	CLA	B	515	X	-	-	-
37	CLA	B	516	X	-	-	-
37	CLA	B	524	X	-	-	-
37	CLA	C	501	X	-	-	-
37	CLA	C	502	X	-	-	-
37	CLA	C	503	X	-	-	-
37	CLA	C	504	X	-	-	-
37	CLA	C	505	X	-	-	-
37	CLA	C	506	X	-	-	-
37	CLA	C	507	X	-	-	-
37	CLA	C	508	X	-	-	-
37	CLA	C	509	X	-	-	-
37	CLA	C	510	X	-	-	-
37	CLA	C	511	X	-	-	-
37	CLA	C	512	X	-	-	-
37	CLA	C	513	X	-	-	-
37	CLA	D	401	X	-	-	-
37	CLA	D	405	X	-	-	-
37	CLA	D	406	X	-	-	-
37	CLA	W	101	X	-	-	-
37	CLA	W	102	X	-	-	-
37	CLA	Z	101	X	-	-	-
37	CLA	Z	102	X	-	-	-
37	CLA	a	403	X	-	-	-
37	CLA	a	404	X	-	-	-
37	CLA	b	501	X	-	-	-
37	CLA	b	502	X	-	-	-
37	CLA	b	503	X	-	-	-
37	CLA	b	504	X	-	-	-
37	CLA	b	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CLA	b	506	X	-	-	-
37	CLA	b	507	X	-	-	-
37	CLA	b	509	X	-	-	-
37	CLA	b	510	X	-	-	-
37	CLA	b	511	X	-	-	-
37	CLA	b	512	X	-	-	-
37	CLA	b	513	X	-	-	-
37	CLA	b	514	X	-	-	-
37	CLA	b	515	X	-	-	-
37	CLA	b	516	X	-	-	-
37	CLA	b	523	X	-	-	-
37	CLA	c	501	X	-	-	-
37	CLA	c	502	X	-	-	-
37	CLA	c	503	X	-	-	-
37	CLA	c	504	X	-	-	-
37	CLA	c	505	X	-	-	-
37	CLA	c	506	X	-	-	-
37	CLA	c	507	X	-	-	-
37	CLA	c	508	X	-	-	-
37	CLA	c	509	X	-	-	-
37	CLA	c	510	X	-	-	-
37	CLA	c	511	X	-	-	-
37	CLA	c	512	X	-	-	-
37	CLA	c	513	X	-	-	-
37	CLA	d	403	X	-	-	-
37	CLA	d	404	X	-	-	-
37	CLA	w	101	X	-	-	-
37	CLA	z	101	X	-	-	-
37	CLA	z	102	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 100884 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 protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2619	1712	429	463	15		
1	a	334	Total	C	N	O	S	0	0
			2619	1712	429	463	15		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

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 CP43 reaction center protein.

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 D2 protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 12 is a protein called Photosystem II subunit.

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	151	Total	C	N	O	S	0	0
			1180	749	196	234	1		
20	q	151	Total	C	N	O	S	0	0
			1180	749	196	234	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 Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	11	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		
24	31	176	Total	C	N	O	S	0	0
			1343	852	228	256	7		

- Molecule 25 is a protein called Fcpb2, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	12	169	Total	C	N	O	S	0	0
			1302	828	222	244	8		
25	32	169	Total	C	N	O	S	0	0
			1302	828	222	244	8		

- Molecule 26 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	13	169	Total	C	N	O	S	0	0
			1296	823	220	246	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	33	169	Total	C	N	O	S	0	0
			1296	823	220	246	7		

- Molecule 27 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	14	172	Total	C	N	O	S	0	0
			1319	838	223	251	7		
27	34	172	Total	C	N	O	S	0	0
			1319	838	223	251	7		

- Molecule 28 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	15	170	Total	C	N	O	S	0	0
			1307	832	221	247	7		
28	35	170	Total	C	N	O	S	0	0
			1307	832	221	247	7		

- Molecule 29 is a protein called Fcpb3, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	16	179	Total	C	N	O	S	0	0
			1386	891	233	256	6		
29	36	179	Total	C	N	O	S	0	0
			1386	891	233	256	6		

- Molecule 30 is a protein called Fcpb4, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	17	176	Total	C	N	O	S	0	0
			1353	862	227	258	6		
30	37	176	Total	C	N	O	S	0	0
			1353	862	227	258	6		

- Molecule 31 is a protein called Chlorophyll a/b-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	18	168	Total	C	N	O	S	0	0
			1289	818	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	38	168	Total	C	N	O	S	0	0
			1289	818	219	245	7		

- Molecule 32 is a protein called Fcpb5, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	19	227	Total	C	N	O	S	0	0
			1746	1128	291	322	5		
32	39	227	Total	C	N	O	S	0	0
			1746	1128	291	322	5		

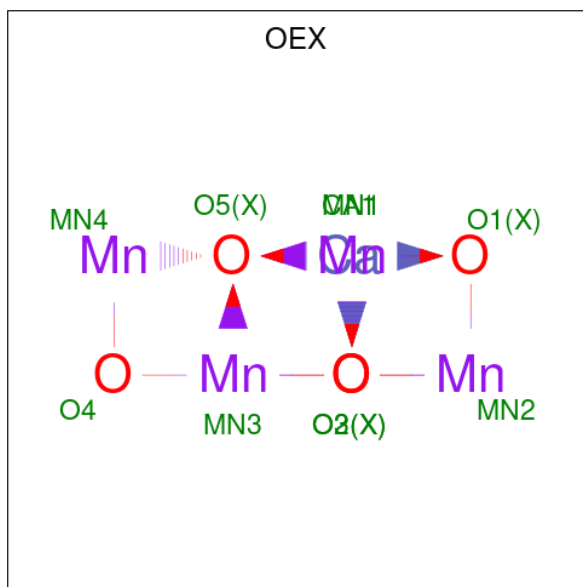
- Molecule 33 is a protein called Fcpb6, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	20	155	Total	C	N	O	S	0	0
			1193	769	201	215	8		
33	40	155	Total	C	N	O	S	0	0
			1193	769	201	215	8		

- Molecule 34 is a protein called Fcpb7, Fucoxanthin chlorophyll a/c-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	21	162	Total	C	N	O	S	0	0
			1262	822	206	229	5		
34	41	162	Total	C	N	O	S	0	0
			1262	822	206	229	5		

- Molecule 35 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).

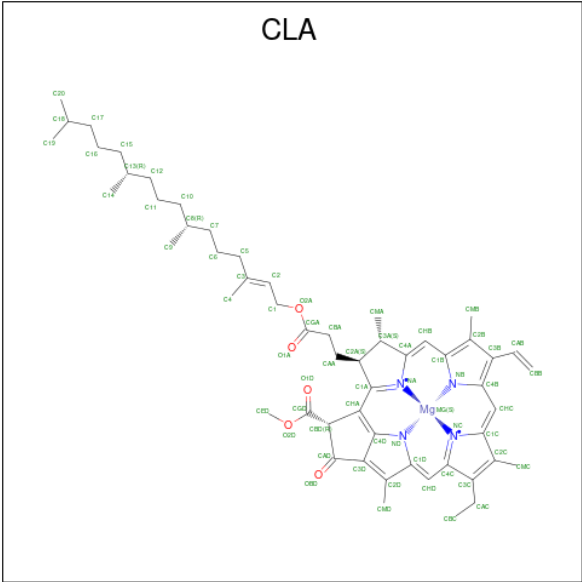


Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
35	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 36 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 37 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					AltConf
37	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
37	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
37	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
37	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	z	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
37	z	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	w	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	11	1	Total 52	C 42	Mg 1	N 4	O 5	0
37	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	11	1	Total 51	C 41	Mg 1	N 4	O 5	0
37	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	12	1	Total 50	C 40	Mg 1	N 4	O 5	0
37	12	1	Total 52	C 42	Mg 1	N 4	O 5	0
37	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	13	1	Total 57	C 47	Mg 1	N 4	O 5	0
37	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	13	1	Total 52	C 42	Mg 1	N 4	O 5	0
37	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	13	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
37	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	14	1	Total 57	C 47	Mg 1	N 4	O 5	0
37	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	14	1	Total 52	C 42	Mg 1	N 4	O 5	0
37	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	15	1	Total 57	C 47	Mg 1	N 4	O 5	0
37	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	15	1	Total 52	C 42	Mg 1	N 4	O 5	0
37	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	16	1	Total 57	C 47	Mg 1	N 4	O 5	0
37	16	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	16	1	Total 61	C 51	Mg 1	N 4	O 5	0
37	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	17	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	17	1	Total 56	C 46	Mg 1	N 4	O 5	0
37	17	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
37	17	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	18	1	Total 56	C 46	Mg 1	N 4	O 5	0
37	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	18	1	Total 53	C 43	Mg 1	N 4	O 5	0
37	18	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	19	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	19	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	19	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	19	1	Total 51	C 41	Mg 1	N 4	O 5	0
37	19	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	19	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	19	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	20	1	Total 56	C 46	Mg 1	N 4	O 5	0
37	20	1	Total 56	C 46	Mg 1	N 4	O 5	0
37	20	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
37	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	20	1	Total 47	C 37	Mg 1	N 4	O 5	0
37	21	1	Total 57	C 47	Mg 1	N 4	O 5	0
37	21	1	Total 58	C 48	Mg 1	N 4	O 5	0
37	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	21	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	21	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	31	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	31	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	31	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	31	1	Total 52	C 42	Mg 1	N 4	O 5	0
37	31	1	Total 51	C 41	Mg 1	N 4	O 5	0
37	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	32	1	Total 50	C 40	Mg 1	N 4	O 5	0
37	32	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
37	32	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	33	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	33	1	Total 57	C 47	Mg 1	N 4	O 5	0
37	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	33	1	Total 52	C 42	Mg 1	N 4	O 5	0
37	33	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	34	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	34	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	34	1	Total 57	C 47	Mg 1	N 4	O 5	0
37	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	34	1	Total 52	C 42	Mg 1	N 4	O 5	0
37	34	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	35	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	35	1	Total 57	C 47	Mg 1	N 4	O 5	0
37	35	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	35	1	Total 52	C 42	Mg 1	N 4	O 5	0
37	35	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	35	1	Total 45	C 35	Mg 1	N 4	O 5	0

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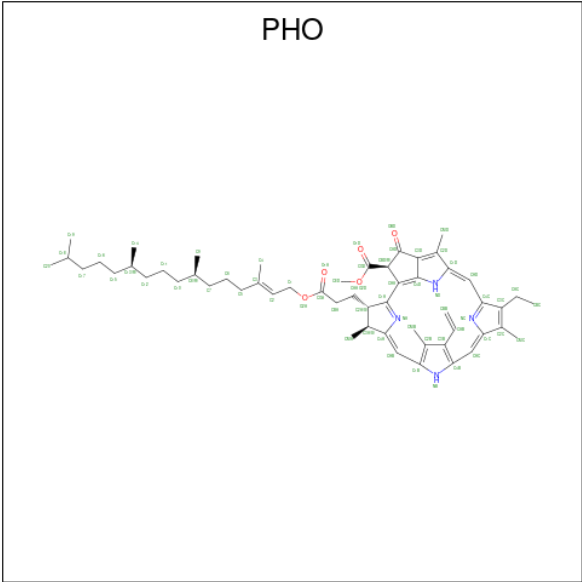
Mol	Chain	Residues	Atoms					AltConf
37	36	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	36	1	Total 57	C 47	Mg 1	N 4	O 5	0
37	36	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	36	1	Total 61	C 51	Mg 1	N 4	O 5	0
37	36	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	37	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	37	1	Total 56	C 46	Mg 1	N 4	O 5	0
37	37	1	Total 52	C 42	Mg 1	N 4	O 5	0
37	37	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	38	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	38	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	38	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	38	1	Total 56	C 46	Mg 1	N 4	O 5	0
37	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	38	1	Total 53	C 43	Mg 1	N 4	O 5	0
37	38	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	39	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	39	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	39	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	39	1	Total 45	C 35	Mg 1	N 4	O 5	0

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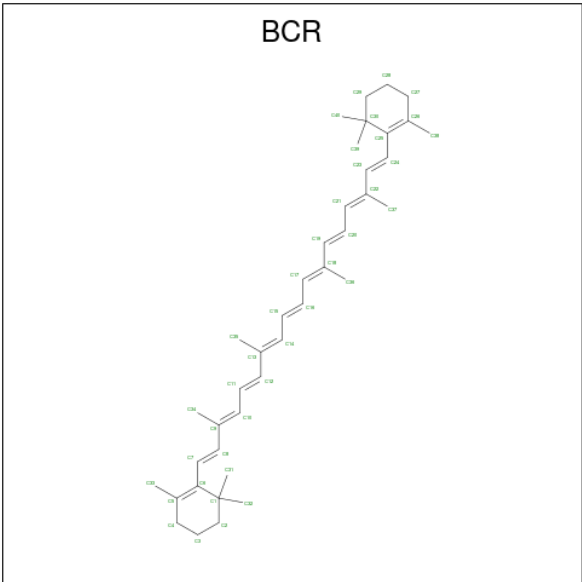
Mol	Chain	Residues	Atoms					AltConf
37	39	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	40	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
37	40	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
37	40	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
37	40	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	40	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 38 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 39 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



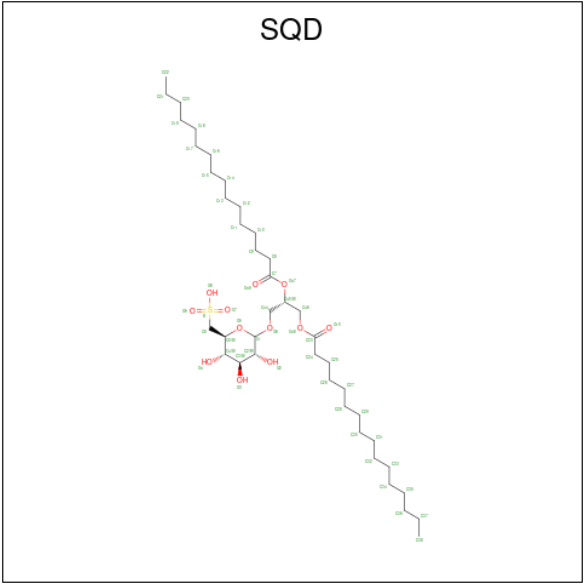
Mol	Chain	Residues	Atoms	AltConf
39	A	1	Total C 40 40	0
39	A	1	Total C 40 40	0
39	B	1	Total C 40 40	0
39	B	1	Total C 40 40	0
39	B	1	Total C 40 40	0
39	C	1	Total C 40 40	0
39	C	1	Total C 40 40	0
39	C	1	Total C 40 40	0
39	D	1	Total C 40 40	0
39	H	1	Total C 40 40	0
39	K	1	Total C 40 40	0
39	0	1	Total C 40 40	0
39	a	1	Total C 40 40	0
39	a	1	Total C 40 40	0
39	b	1	Total C 40 40	0
39	b	1	Total C 40 40	0
39	b	1	Total C 40 40	0
39	c	1	Total C 40 40	0
39	c	1	Total C 40 40	0
39	c	1	Total C 40 40	0
39	d	1	Total C 40 40	0
39	h	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
39	y	1	Total	C	0
			40	40	
39	5	1	Total	C	0
			40	40	

- Molecule 40 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



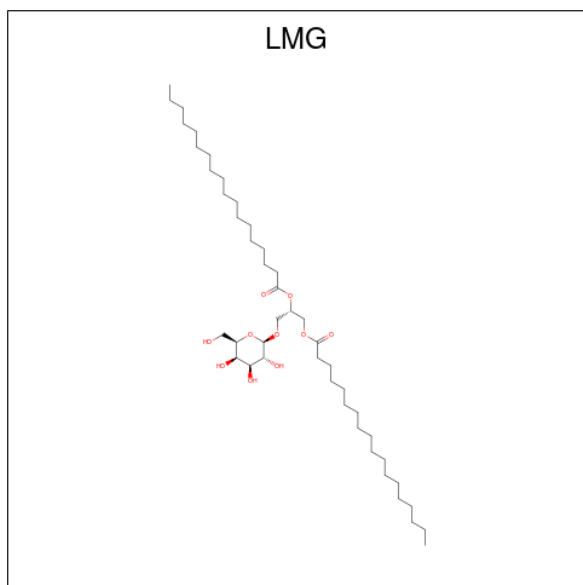
Mol	Chain	Residues	Atoms				AltConf
40	A	1	Total	C	O	S	0
			54	41	12	1	
40	B	1	Total	C	O	S	0
			54	41	12	1	
40	B	1	Total	C	O	S	0
			37	24	12	1	
40	L	1	Total	C	O	S	0
			54	41	12	1	
40	a	1	Total	C	O	S	0
			54	41	12	1	
40	b	1	Total	C	O	S	0
			37	24	12	1	
40	16	1	Total	C	O	S	0
			54	41	12	1	
40	17	1	Total	C	O	S	0
			49	36	12	1	
40	36	1	Total	C	O	S	0
			49	36	12	1	

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Mol	Chain	Residues	Atoms				AltConf
40	40	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 41 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



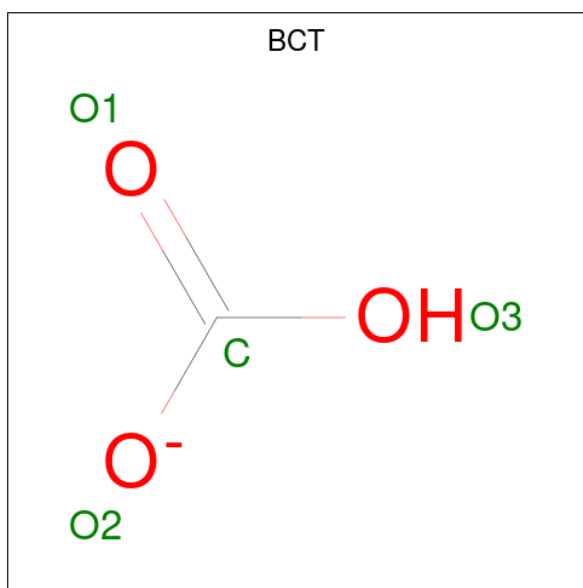
Mol	Chain	Residues	Atoms			AltConf
41	A	1	Total	C	O	0
			51	41	10	
41	B	1	Total	C	O	0
			51	41	10	
41	B	1	Total	C	O	0
			51	41	10	
41	C	1	Total	C	O	0
			51	41	10	
41	D	1	Total	C	O	0
			51	41	10	
41	L	1	Total	C	O	0
			40	30	10	
41	a	1	Total	C	O	0
			51	41	10	
41	b	1	Total	C	O	0
			51	41	10	
41	b	1	Total	C	O	0
			51	41	10	
41	c	1	Total	C	O	0
			51	41	10	

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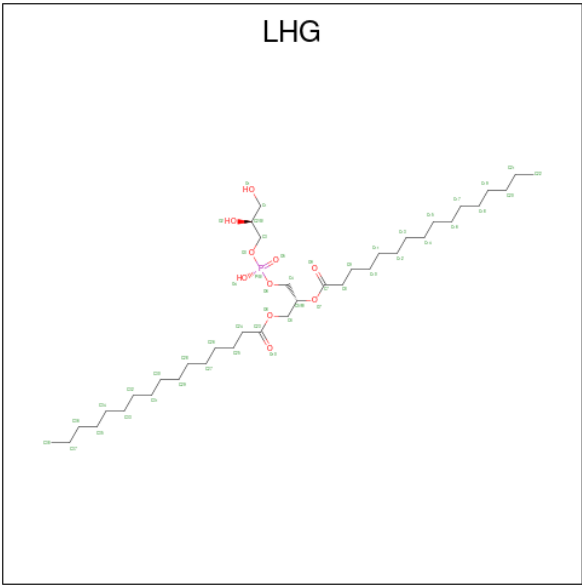
Mol	Chain	Residues	Atoms			AltConf
41	d	1	Total	C	O	0
			51	41	10	
41	l	1	Total	C	O	0
			40	30	10	
41	11	1	Total	C	O	0
			42	32	10	
41	11	1	Total	C	O	0
			32	22	10	
41	12	1	Total	C	O	0
			39	29	10	
41	16	1	Total	C	O	0
			36	26	10	
41	17	1	Total	C	O	0
			37	27	10	
41	31	1	Total	C	O	0
			42	32	10	
41	31	1	Total	C	O	0
			32	22	10	
41	32	1	Total	C	O	0
			39	29	10	
41	36	1	Total	C	O	0
			36	26	10	
41	37	1	Total	C	O	0
			37	27	10	

- Molecule 42 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3^-).



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

- Molecule 43 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



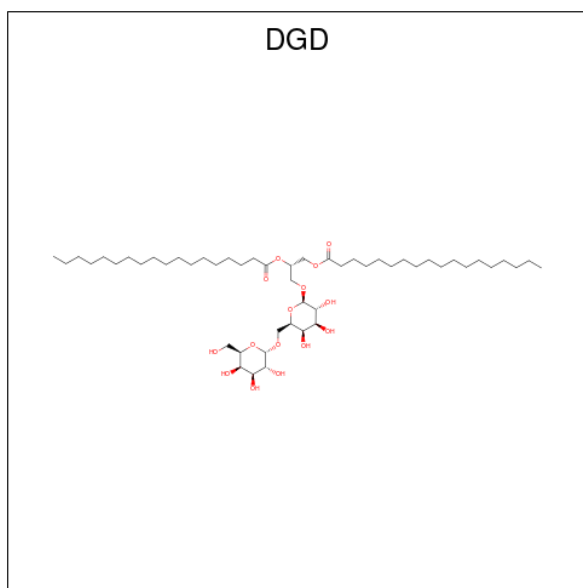
Mol	Chain	Residues	Atoms				AltConf
43	B	1	Total	C	O	P	0
			49	38	10	1	
43	D	1	Total	C	O	P	0
			49	38	10	1	
43	D	1	Total	C	O	P	0
			49	38	10	1	
43	D	1	Total	C	O	P	0
			46	35	10	1	
43	a	1	Total	C	O	P	0
			46	35	10	1	
43	b	1	Total	C	O	P	0
			49	38	10	1	
43	d	1	Total	C	O	P	0
			49	38	10	1	
43	d	1	Total	C	O	P	0
			49	38	10	1	
43	17	1	Total	C	O	P	0
			44	33	10	1	

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Mol	Chain	Residues	Atoms				AltConf
43	19	1	Total	C	O	P	0
			49	38	10	1	
43	21	1	Total	C	O	P	0
			35	25	9	1	
43	21	1	Total	C	O	P	0
			45	34	10	1	
43	37	1	Total	C	O	P	0
			44	33	10	1	
43	37	1	Total	C	O	P	0
			45	34	10	1	
43	39	1	Total	C	O	P	0
			49	38	10	1	
43	41	1	Total	C	O	P	0
			35	25	9	1	

- Molecule 44 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



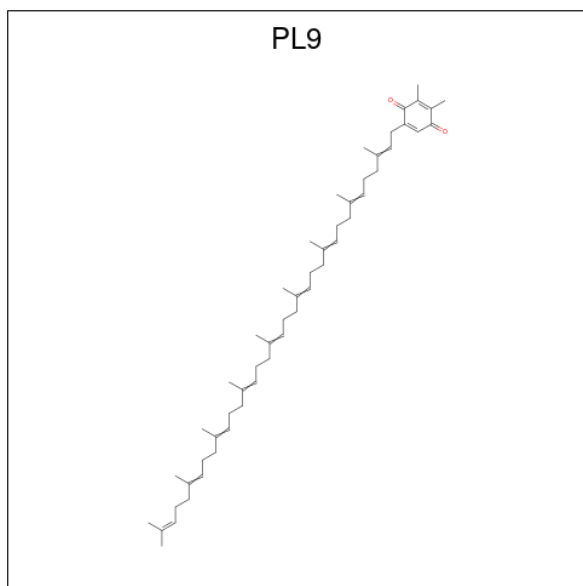
Mol	Chain	Residues	Atoms			AltConf
44	C	1	Total	C	O	0
			62	47	15	
44	C	1	Total	C	O	0
			62	47	15	
44	H	1	Total	C	O	0
			62	47	15	
44	J	1	Total	C	O	0
			62	47	15	

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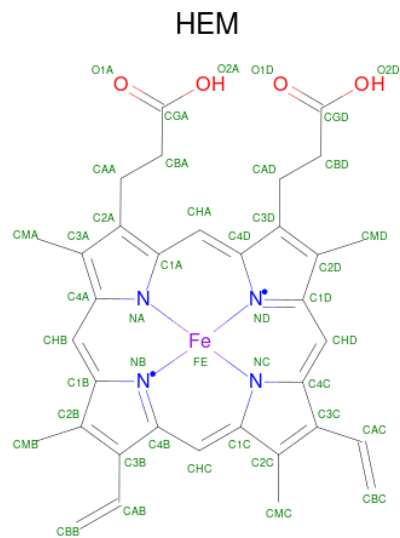
Mol	Chain	Residues	Atoms			AltConf
44	c	1	Total	C	O	0
			62	47	15	
44	c	1	Total	C	O	0
			62	47	15	
44	h	1	Total	C	O	0
			62	47	15	
44	j	1	Total	C	O	0
			62	47	15	

- Molecule 45 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



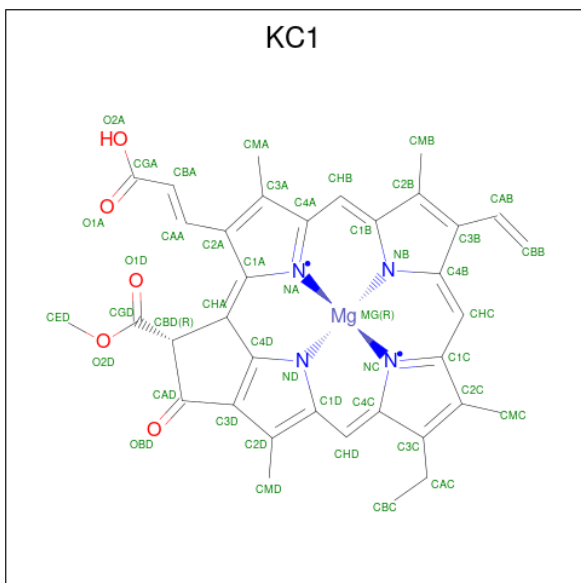
Mol	Chain	Residues	Atoms			AltConf
45	D	1	Total	C	O	0
			55	53	2	
45	D	1	Total	C	O	0
			55	53	2	
45	d	1	Total	C	O	0
			55	53	2	
45	d	1	Total	C	O	0
			55	53	2	

- Molecule 46 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 47 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
47	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
47	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	18	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	19	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	20	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	21	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	31	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	32	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	33	1	Total 45	C 35	Mg 1	N 4	O 5	0

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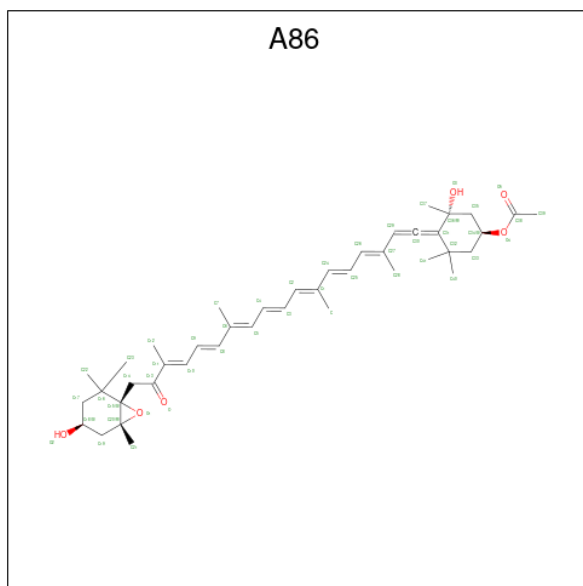
Mol	Chain	Residues	Atoms					AltConf
47	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	35	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	35	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	35	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	35	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	36	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	36	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	36	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	36	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	37	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	37	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	37	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	37	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	38	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	38	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
47	39	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	40	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	40	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	40	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
47	41	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 48 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (three-letter code: A86) (formula: C₄₂H₅₈O₆).



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

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Mol	Chain	Residues	Atoms			AltConf
48	11	1	Total	C	O	0
			48	42	6	
48	11	1	Total	C	O	0
			48	42	6	
48	12	1	Total	C	O	0
			48	42	6	
48	12	1	Total	C	O	0
			48	42	6	
48	12	1	Total	C	O	0
			48	42	6	
48	12	1	Total	C	O	0
			48	42	6	
48	12	1	Total	C	O	0
			48	42	6	
48	12	1	Total	C	O	0
			48	42	6	
48	13	1	Total	C	O	0
			48	42	6	
48	13	1	Total	C	O	0
			48	42	6	
48	13	1	Total	C	O	0
			48	42	6	
48	13	1	Total	C	O	0
			48	42	6	
48	14	1	Total	C	O	0
			48	42	6	
48	14	1	Total	C	O	0
			48	42	6	
48	14	1	Total	C	O	0
			48	42	6	
48	14	1	Total	C	O	0
			48	42	6	
48	14	1	Total	C	O	0
			48	42	6	
48	15	1	Total	C	O	0
			48	42	6	

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

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Mol	Chain	Residues	Atoms			AltConf
48	19	1	Total	C	O	0
			48	42	6	
48	19	1	Total	C	O	0
			48	42	6	
48	20	1	Total	C	O	0
			48	42	6	
48	20	1	Total	C	O	0
			48	42	6	
48	21	1	Total	C	O	0
			48	42	6	
48	21	1	Total	C	O	0
			48	42	6	
48	21	1	Total	C	O	0
			48	42	6	
48	21	1	Total	C	O	0
			48	42	6	
48	31	1	Total	C	O	0
			48	42	6	
48	31	1	Total	C	O	0
			48	42	6	
48	31	1	Total	C	O	0
			48	42	6	
48	31	1	Total	C	O	0
			48	42	6	
48	31	1	Total	C	O	0
			48	42	6	
48	31	1	Total	C	O	0
			48	42	6	
48	32	1	Total	C	O	0
			48	42	6	
48	32	1	Total	C	O	0
			48	42	6	
48	32	1	Total	C	O	0
			48	42	6	
48	32	1	Total	C	O	0
			48	42	6	
48	32	1	Total	C	O	0
			48	42	6	
48	32	1	Total	C	O	0
			48	42	6	

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

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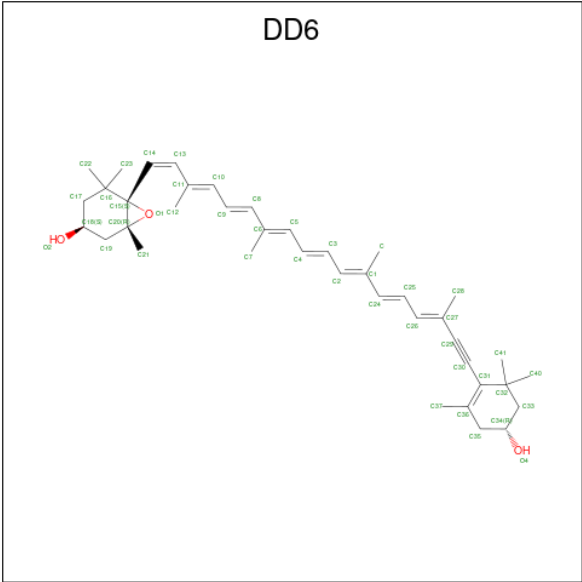
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Mol	Chain	Residues	Atoms			AltConf
48	37	1	Total	C	O	0
			48	42	6	
48	37	1	Total	C	O	0
			48	42	6	
48	37	1	Total	C	O	0
			48	42	6	
48	37	1	Total	C	O	0
			48	42	6	
48	37	1	Total	C	O	0
			48	42	6	
48	37	1	Total	C	O	0
			48	42	6	
48	38	1	Total	C	O	0
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

- Molecule 49 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			AltConf
49	11	1	Total	C	O	0
			19	17	2	
49	12	2	Total	C	O	0
			34	32	2	
49	13	3	Total	C	O	0
			49	47	2	
49	14	1	Total	C		0
			16	16		
49	15	2	Total	C		0
			28	28		
49	16	2	Total	C		0
			24	24		
49	17	3	Total	C	O	0
			54	48	6	
49	18	4	Total	C		0
			58	58		
49	19	1	Total	C		0
			12	12		
49	31	1	Total	C	O	0
			19	17	2	
49	32	2	Total	C	O	0
			34	32	2	
49	33	3	Total	C	O	0
			49	47	2	
49	34	1	Total	C		0
			16	16		
49	35	2	Total	C		0
			28	28		
49	36	2	Total	C		0
			24	24		
49	37	3	Total	C	O	0
			54	48	6	
49	38	4	Total	C		0
			58	58		
49	39	1	Total	C		0
			12	12		

- Molecule 50 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (three-letter code: DD6) (formula: C₄₀H₅₄O₃).



Mol	Chain	Residues	Atoms			AltConf
50	16	1	Total	C	O	0
			43	40	3	
50	19	1	Total	C	O	0
			43	40	3	
50	20	1	Total	C	O	0
			43	40	3	
50	20	1	Total	C	O	0
			43	40	3	
50	21	1	Total	C	O	0
			43	40	3	
50	21	1	Total	C	O	0
			43	40	3	
50	36	1	Total	C	O	0
			43	40	3	
50	39	1	Total	C	O	0
			43	40	3	
50	40	1	Total	C	O	0
			43	40	3	
50	40	1	Total	C	O	0
			43	40	3	
50	41	1	Total	C	O	0
			43	40	3	
50	41	1	Total	C	O	0
			43	40	3	

- Molecule 51 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
51	19	1	Total 35	C 24	O 11	0
51	39	1	Total 35	C 24	O 11	0

- Molecule 52 is water.

Mol	Chain	Residues	Atoms		AltConf
52	B	5	Total 5	O 5	0
52	C	3	Total 3	O 3	0
52	D	4	Total 4	O 4	0
52	Z	1	Total 1	O 1	0
52	a	2	Total 2	O 2	0
52	b	5	Total 5	O 5	0
52	c	3	Total 3	O 3	0
52	d	2	Total 2	O 2	0
52	z	1	Total 1	O 1	0
52	11	3	Total 3	O 3	0

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Mol	Chain	Residues	Atoms		AltConf
52	12	2	Total 2	O 2	0
52	13	1	Total 1	O 1	0
52	14	1	Total 1	O 1	0
52	15	1	Total 1	O 1	0
52	16	1	Total 1	O 1	0
52	17	2	Total 2	O 2	0
52	18	1	Total 1	O 1	0
52	19	1	Total 1	O 1	0
52	31	3	Total 3	O 3	0
52	32	2	Total 2	O 2	0
52	33	1	Total 1	O 1	0
52	34	1	Total 1	O 1	0
52	35	1	Total 1	O 1	0
52	36	1	Total 1	O 1	0
52	37	2	Total 2	O 2	0
52	38	1	Total 1	O 1	0
52	39	1	Total 1	O 1	0

3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1

Chain A:  99%



- Molecule 1: Photosystem II protein D1

Chain a:  99%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  99%



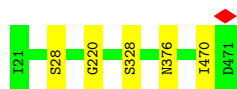
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  99%



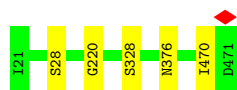
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  99%



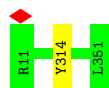
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  99%



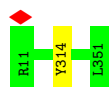
- Molecule 4: Photosystem II D2 protein

Chain D:  100%



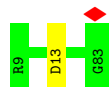
- Molecule 4: Photosystem II D2 protein

Chain d:  100%



- Molecule 5: Cytochrome b559 subunit alpha

Chain E:  99%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  99%



- Molecule 6: Cytochrome b559 subunit beta

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Cytochrome b559 subunit beta

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 7: Photosystem II reaction center protein H

Chain H:  100%



- Molecule 7: Photosystem II reaction center protein H

Chain h:  100%



- Molecule 8: Photosystem II reaction center protein I

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem II reaction center protein I

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein J

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein J

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 10: Photosystem II reaction center protein K

Chain K:  95% 5%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  95% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  100%



- Molecule 11: Photosystem II reaction center protein L

Chain l:  100%



- Molecule 12: Photosystem II subunit

Chain M:  5% 100%



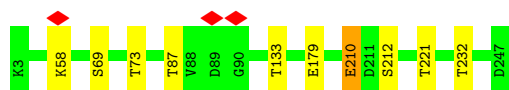
- Molecule 12: Photosystem II subunit

Chain m:  5% 100%



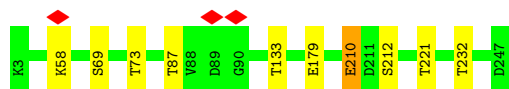
- Molecule 13: Extrinsic protein in photosystem II

Chain O:  96%



- Molecule 13: Extrinsic protein in photosystem II

Chain o:  96%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  100%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  100%



- Molecule 15: Extrinsic protein in photosystem II

Chain U:  99%



- Molecule 15: Extrinsic protein in photosystem II

Chain u:  99%



- Molecule 16: Cytochrome c-550

Chain V:  99%



- Molecule 16: Cytochrome c-550

Chain v:  99%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  100%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  100%



- Molecule 18: Photosystem II reaction center X protein

Chain X:  5% 97%



- Molecule 18: Photosystem II reaction center X protein

Chain x:  5% 97%



- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  100%

There are no outlier residues recorded for this chain.

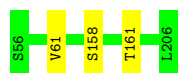
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  100%

There are no outlier residues recorded for this chain.

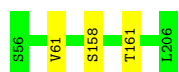
- Molecule 20: Extrinsic protein in photosystem II

Chain Q:  98%



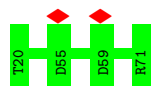
- Molecule 20: Extrinsic protein in photosystem II

Chain q:  98%



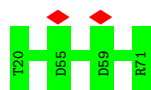
- Molecule 21: Photosystem II reaction center protein W

Chain W:  100%



- Molecule 21: Photosystem II reaction center protein W

Chain w:  100%



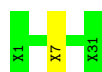
- Molecule 22: Unknown protein 0

Chain 0:  97%



- Molecule 22: Unknown protein 0

Chain 5:  97%



- Molecule 23: Unknown protein 1

Chain 1:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: Unknown protein 1

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: Chlorophyll a/b-binding protein

Chain 11:  98%



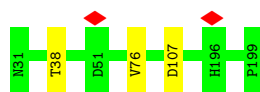
- Molecule 24: Chlorophyll a/b-binding protein

Chain 31:  99%

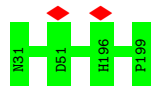


- Molecule 25: Fcpb2, Fucoxanthin chlorophyll a/c-binding protein

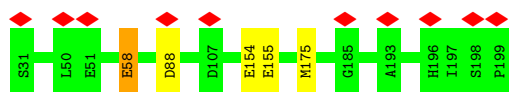
Chain 12:  98%



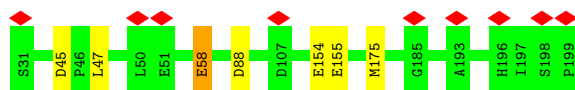
- Molecule 25: Fcpb2, Fucoxanthin chlorophyll a/c-binding protein



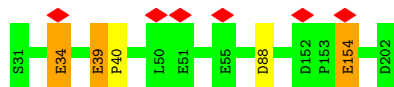
- Molecule 26: Chlorophyll a/b-binding protein



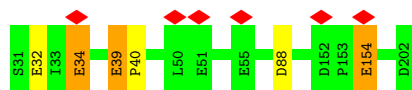
- Molecule 26: Chlorophyll a/b-binding protein



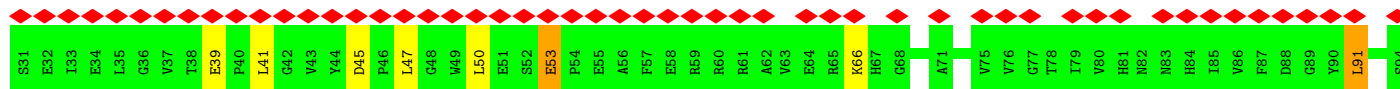
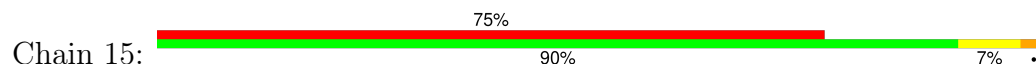
- Molecule 27: Chlorophyll a/b-binding protein

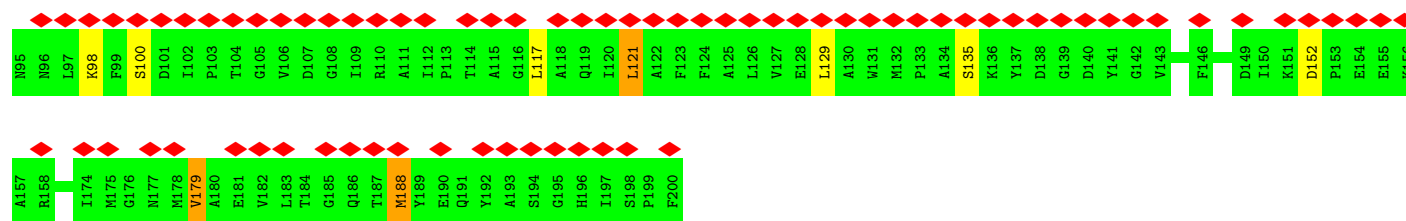


- Molecule 27: Chlorophyll a/b-binding protein

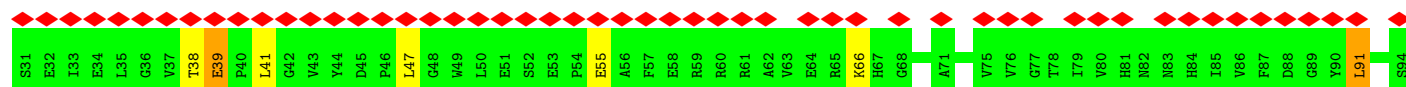
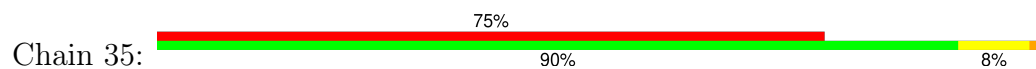


- Molecule 28: Chlorophyll a/b-binding protein





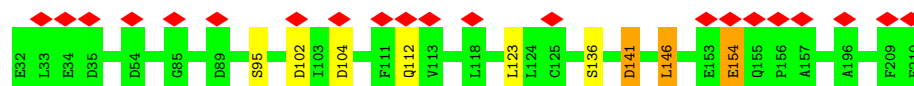
- Molecule 28: Chlorophyll a/b-binding protein



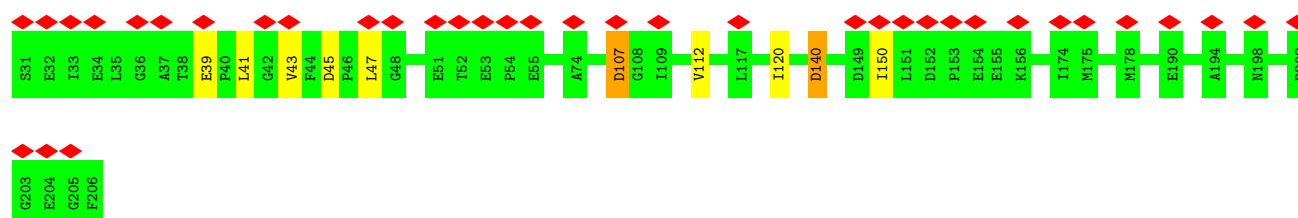
- Molecule 29: Fcpb3, Fucoxanthin chlorophyll a/c-binding protein



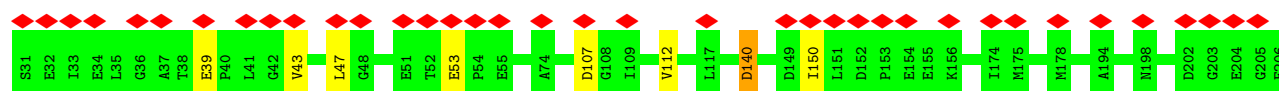
- Molecule 29: Fcpb3, Fucoxanthin chlorophyll a/c-binding protein



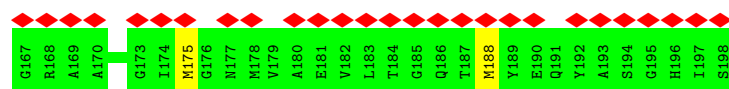
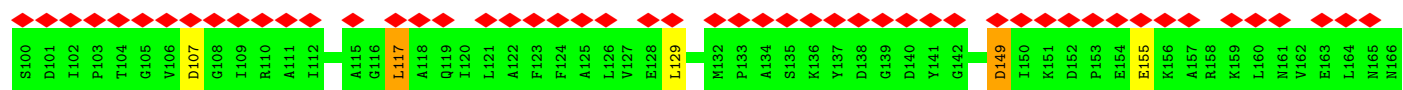
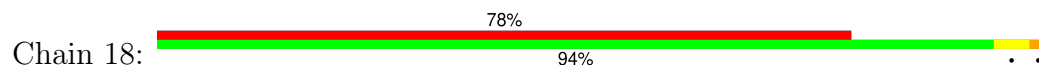
- Molecule 30: Fcpb4, Fucoxanthin chlorophyll a/c-binding protein



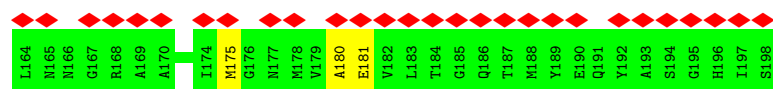
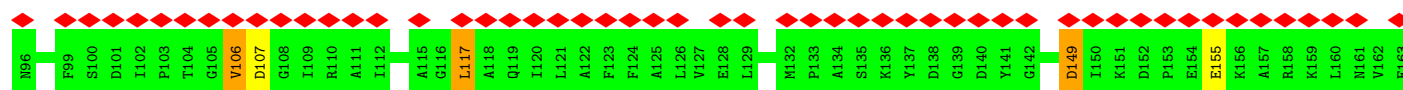
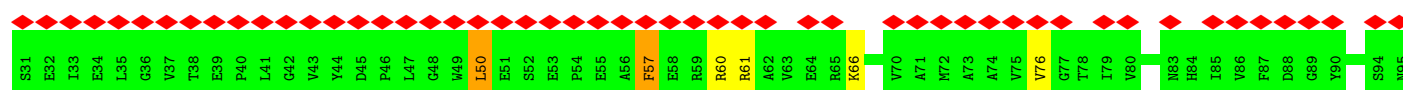
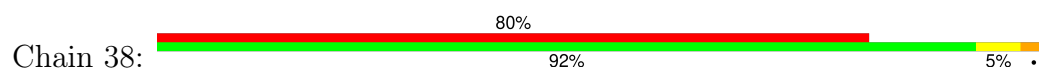
- Molecule 30: Fcpb4, Fucoxanthin chlorophyll a/c-binding protein



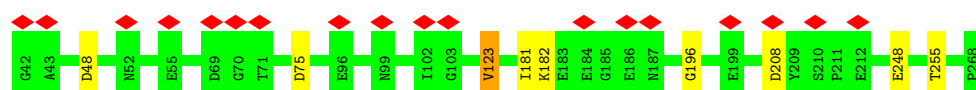
• Molecule 31: Chlorophyll a/b-binding protein



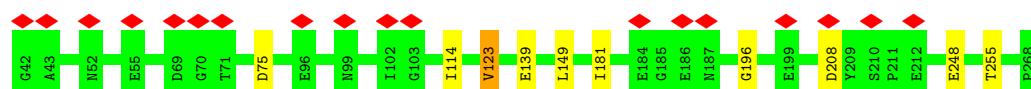
• Molecule 31: Chlorophyll a/b-binding protein



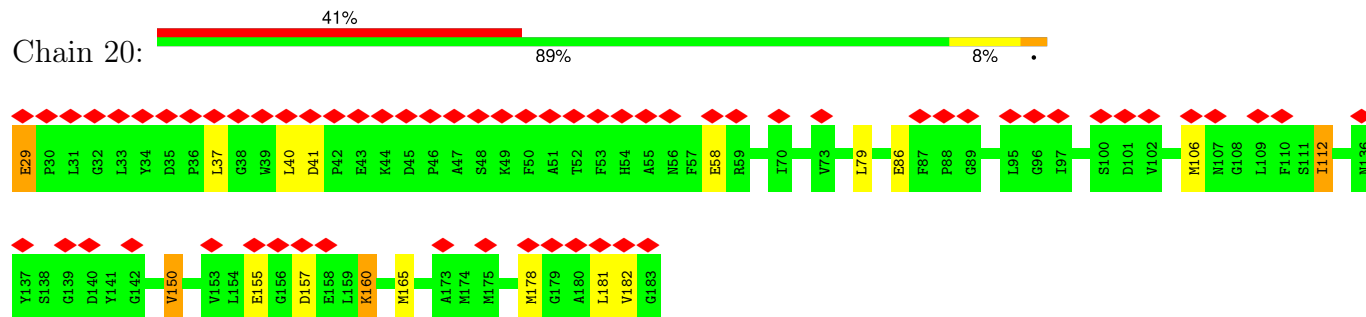
• Molecule 32: Fcpb5, Fucoxanthin chlorophyll a/c-binding protein



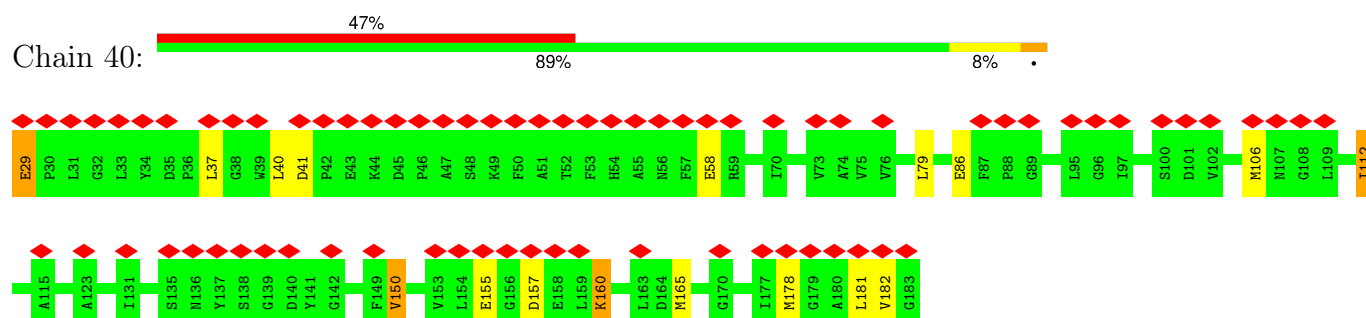
• Molecule 32: Fcpb5, Fucoxanthin chlorophyll a/c-binding protein



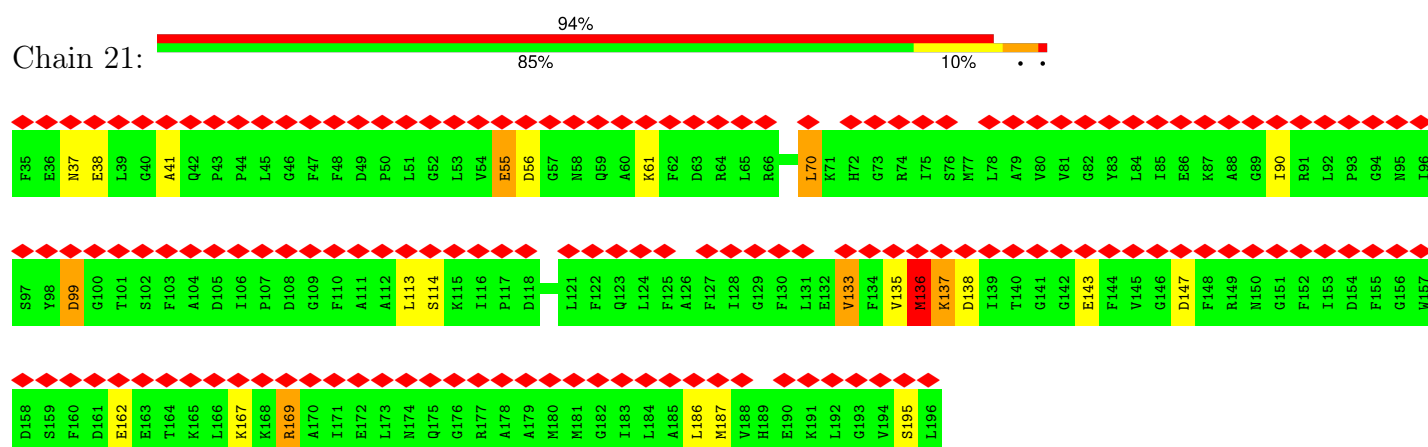
- Molecule 33: Fcpb6, Fucoxanthin chlorophyll a/c-binding protein



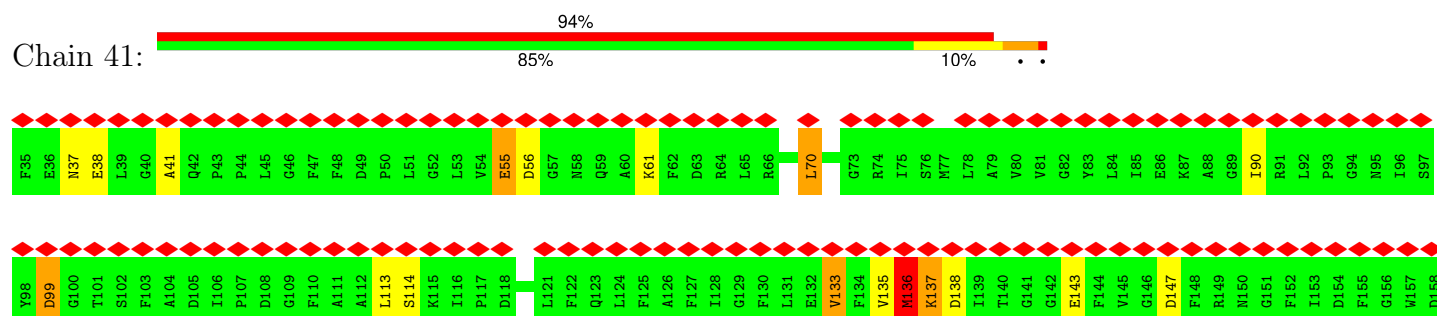
- Molecule 33: Fcpb6, Fucoxanthin chlorophyll a/c-binding protein



- Molecule 34: Fcpb7, Fucoxanthin chlorophyll a/c-binding protein



- Molecule 34: Fcpb7, Fucoxanthin chlorophyll a/c-binding protein



S159	F160	D161	E162	E163	T164	K165	L166	K167	K168	R169	A170	I171	E172	L173	N174	Q175	G176	R177	A178	A179	M180	M181	G182	I183	L184	A185	L186	M187	V188	H189	E190	K191	L192	G193	V194	S195	L196
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	210825	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	0.369	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	569.856, 569.856, 569.856	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OEX, BCT, LHG, PHO, BCR, UNL, LMG, SQD, DD6, FE2, LMU, DGD, CLA, A86, HEM, KC1, PL9

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	0.44	0/2702	0.52	1/3682 (0.0%)
1	a	0.44	0/2702	0.52	1/3682 (0.0%)
2	B	0.46	0/3942	0.52	0/5362
2	b	0.46	0/3942	0.52	0/5362
3	C	0.48	0/3620	0.52	0/4933
3	c	0.48	0/3620	0.52	0/4933
4	D	0.48	1/2789 (0.0%)	0.53	0/3803
4	d	0.48	1/2789 (0.0%)	0.53	0/3803
5	E	0.38	0/634	0.48	0/864
5	e	0.38	0/634	0.48	0/864
6	F	0.38	0/235	0.56	0/316
6	f	0.38	0/235	0.56	0/316
7	H	0.39	0/523	0.56	0/714
7	h	0.39	0/523	0.56	0/714
8	I	0.42	0/294	0.58	0/397
8	i	0.42	0/294	0.58	0/397
9	J	0.36	0/260	0.47	0/351
9	j	0.36	0/260	0.46	0/351
10	K	0.45	0/313	0.61	0/429
10	k	0.45	0/313	0.61	0/429
11	L	0.50	0/319	0.49	0/433
11	l	0.50	0/319	0.49	0/433
12	M	0.37	0/321	0.56	0/433
12	m	0.37	0/321	0.56	0/433
13	O	0.40	0/1875	0.58	1/2528 (0.0%)
13	o	0.40	0/1875	0.58	1/2528 (0.0%)
14	T	0.41	0/256	0.44	0/346
14	t	0.41	0/256	0.45	0/346
15	U	0.37	0/728	0.54	0/989
15	u	0.37	0/728	0.54	0/989
16	V	0.41	0/1056	0.56	1/1435 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.41	0/1056	0.56	1/1435 (0.1%)
17	Y	0.28	0/252	0.55	0/341
17	y	0.28	0/252	0.55	0/341
18	X	0.29	0/263	0.45	0/355
18	x	0.29	0/263	0.45	0/355
19	Z	0.36	0/456	0.56	0/624
19	z	0.36	0/456	0.56	0/624
20	Q	0.36	0/1203	0.55	0/1623
20	q	0.36	0/1203	0.55	0/1623
21	W	0.40	0/434	0.57	0/590
21	w	0.40	0/434	0.57	0/590
24	11	0.53	2/1373 (0.1%)	0.61	3/1861 (0.2%)
24	31	0.46	0/1373	0.57	1/1861 (0.1%)
25	12	0.44	0/1334	0.61	2/1810 (0.1%)
25	32	0.43	0/1334	0.56	0/1810
26	13	0.48	1/1325 (0.1%)	0.75	4/1797 (0.2%)
26	33	0.49	1/1325 (0.1%)	0.75	4/1797 (0.2%)
27	14	0.50	2/1349 (0.1%)	0.73	3/1829 (0.2%)
27	34	0.51	2/1349 (0.1%)	0.76	5/1829 (0.3%)
28	15	0.40	0/1337	0.90	9/1813 (0.5%)
28	35	0.43	0/1337	0.86	6/1813 (0.3%)
29	16	0.40	1/1425 (0.1%)	0.69	2/1930 (0.1%)
29	36	0.40	1/1425 (0.1%)	0.69	2/1930 (0.1%)
30	17	0.42	0/1386	0.77	4/1879 (0.2%)
30	37	0.48	2/1386 (0.1%)	0.76	4/1879 (0.2%)
31	18	0.53	0/1317	1.07	12/1785 (0.7%)
31	38	0.60	3/1317 (0.2%)	1.07	12/1785 (0.7%)
32	19	0.44	0/1796	0.66	4/2445 (0.2%)
32	39	0.46	1/1796 (0.1%)	0.66	2/2445 (0.1%)
33	20	0.45	1/1224 (0.1%)	0.85	7/1656 (0.4%)
33	40	0.45	1/1224 (0.1%)	0.85	7/1656 (0.4%)
34	21	0.53	0/1290	1.33	17/1735 (1.0%)
34	41	0.53	0/1290	1.33	17/1735 (1.0%)
All	All	0.45	20/75262 (0.0%)	0.67	133/102176 (0.1%)

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
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	c	0	1
13	O	0	2
13	o	0	2
20	Q	0	1
20	q	0	1
22	0	0	1
22	5	0	1
27	14	0	1
27	34	0	1
28	35	0	2
29	16	0	1
29	36	0	1
32	19	0	1
32	39	0	1
33	20	0	3
33	40	0	3
34	21	0	3
34	41	0	3
All	All	0	30

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	34	154	GLU	CB-CG	-8.12	1.36	1.52
27	14	154	GLU	CB-CG	-8.09	1.36	1.52
31	38	106	VAL	CB-CG1	-7.57	1.36	1.52
24	11	58	GLU	CD-OE1	-7.35	1.17	1.25
32	39	248	GLU	CG-CD	-7.11	1.41	1.51

The worst 5 of 133 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	21	70	LEU	CA-CB-CG	21.70	165.22	115.30
34	41	70	LEU	CA-CB-CG	21.69	165.18	115.30
34	21	136	MET	CB-CG-SD	13.12	151.75	112.40
34	41	136	MET	CB-CG-SD	13.12	151.75	112.40
34	41	136	MET	CA-CB-CG	-12.95	91.28	113.30

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	0	7	UNK	Peptide
3	C	220	GLY	Peptide
13	O	58	LYS	Peptide
13	O	73	THR	Peptide
20	Q	61	VAL	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	324 (98%)	8 (2%)	0	100	100
1	a	332/334 (99%)	324 (98%)	8 (2%)	0	100	100
2	B	482/484 (100%)	467 (97%)	15 (3%)	0	100	100
2	b	482/484 (100%)	467 (97%)	15 (3%)	0	100	100
3	C	449/451 (100%)	431 (96%)	18 (4%)	0	100	100
3	c	449/451 (100%)	431 (96%)	18 (4%)	0	100	100
4	D	339/341 (99%)	327 (96%)	12 (4%)	0	100	100
4	d	339/341 (99%)	327 (96%)	12 (4%)	0	100	100
5	E	73/75 (97%)	73 (100%)	0	0	100	100
5	e	73/75 (97%)	73 (100%)	0	0	100	100
6	F	26/28 (93%)	26 (100%)	0	0	100	100
6	f	26/28 (93%)	26 (100%)	0	0	100	100
7	H	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
7	h	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
8	I	33/35 (94%)	31 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	i	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
9	J	32/34 (94%)	32 (100%)	0	0	100	100
9	j	32/34 (94%)	32 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	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	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
12	m	40/42 (95%)	37 (92%)	3 (8%)	0	100	100
13	O	243/245 (99%)	232 (96%)	11 (4%)	0	100	100
13	o	243/245 (99%)	231 (95%)	12 (5%)	0	100	100
14	T	28/30 (93%)	28 (100%)	0	0	100	100
14	t	28/30 (93%)	28 (100%)	0	0	100	100
15	U	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
15	u	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
16	V	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
16	v	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
17	Y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
17	y	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
18	X	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
18	x	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
19	Z	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
19	z	57/59 (97%)	55 (96%)	2 (4%)	0	100	100
20	Q	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
20	q	149/151 (99%)	140 (94%)	9 (6%)	0	100	100
21	W	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
21	w	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
24	11	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
24	31	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
25	12	167/169 (99%)	160 (96%)	7 (4%)	0	100	100
25	32	167/169 (99%)	159 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	13	167/169 (99%)	160 (96%)	7 (4%)	0	100	100
26	33	167/169 (99%)	160 (96%)	7 (4%)	0	100	100
27	14	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	11	21
27	34	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	11	21
28	15	168/170 (99%)	147 (88%)	20 (12%)	1 (1%)	22	39
28	35	168/170 (99%)	147 (88%)	20 (12%)	1 (1%)	22	39
29	16	177/179 (99%)	171 (97%)	6 (3%)	0	100	100
29	36	177/179 (99%)	171 (97%)	6 (3%)	0	100	100
30	17	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
30	37	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
31	18	166/168 (99%)	156 (94%)	10 (6%)	0	100	100
31	38	166/168 (99%)	156 (94%)	10 (6%)	0	100	100
32	19	225/227 (99%)	211 (94%)	14 (6%)	0	100	100
32	39	225/227 (99%)	214 (95%)	11 (5%)	0	100	100
33	20	153/155 (99%)	133 (87%)	20 (13%)	0	100	100
33	40	153/155 (99%)	133 (87%)	20 (13%)	0	100	100
34	21	160/162 (99%)	142 (89%)	18 (11%)	0	100	100
34	41	160/162 (99%)	142 (89%)	18 (11%)	0	100	100
All	All	9322/9450 (99%)	8876 (95%)	440 (5%)	6 (0%)	50	69

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	14	39	GLU
27	34	39	GLU
27	14	40	PRO
28	15	39	GLU
27	34	40	PRO

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	272/272 (100%)	271 (100%)	1 (0%)	89	96
1	a	272/272 (100%)	271 (100%)	1 (0%)	89	96
2	B	385/385 (100%)	379 (98%)	6 (2%)	58	80
2	b	385/385 (100%)	379 (98%)	6 (2%)	58	80
3	C	356/356 (100%)	352 (99%)	4 (1%)	70	87
3	c	356/356 (100%)	352 (99%)	4 (1%)	70	87
4	D	273/273 (100%)	273 (100%)	0	100	100
4	d	273/273 (100%)	273 (100%)	0	100	100
5	E	69/69 (100%)	68 (99%)	1 (1%)	62	83
5	e	69/69 (100%)	68 (99%)	1 (1%)	62	83
6	F	22/22 (100%)	22 (100%)	0	100	100
6	f	22/22 (100%)	22 (100%)	0	100	100
7	H	55/55 (100%)	55 (100%)	0	100	100
7	h	55/55 (100%)	55 (100%)	0	100	100
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	34 (100%)	0	100	100
9	J	27/27 (100%)	27 (100%)	0	100	100
9	j	27/27 (100%)	27 (100%)	0	100	100
10	K	32/32 (100%)	30 (94%)	2 (6%)	15	30
10	k	32/32 (100%)	30 (94%)	2 (6%)	15	30
11	L	34/34 (100%)	34 (100%)	0	100	100
11	l	34/34 (100%)	34 (100%)	0	100	100
12	M	31/31 (100%)	31 (100%)	0	100	100
12	m	31/31 (100%)	31 (100%)	0	100	100
13	O	196/198 (99%)	188 (96%)	8 (4%)	26	50
13	o	196/198 (99%)	188 (96%)	8 (4%)	26	50
14	T	27/27 (100%)	27 (100%)	0	100	100
14	t	27/27 (100%)	27 (100%)	0	100	100
15	U	77/77 (100%)	76 (99%)	1 (1%)	65	85
15	u	77/77 (100%)	76 (99%)	1 (1%)	65	85
16	V	114/114 (100%)	113 (99%)	1 (1%)	75	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	114/114 (100%)	113 (99%)	1 (1%)	75	90
17	Y	27/27 (100%)	27 (100%)	0	100	100
17	y	27/27 (100%)	27 (100%)	0	100	100
18	X	29/29 (100%)	28 (97%)	1 (3%)	32	58
18	x	29/29 (100%)	28 (97%)	1 (3%)	32	58
19	Z	48/48 (100%)	48 (100%)	0	100	100
19	z	48/48 (100%)	48 (100%)	0	100	100
20	Q	122/122 (100%)	120 (98%)	2 (2%)	58	80
20	q	122/122 (100%)	120 (98%)	2 (2%)	58	80
21	W	43/43 (100%)	43 (100%)	0	100	100
21	w	43/43 (100%)	43 (100%)	0	100	100
24	11	138/138 (100%)	135 (98%)	3 (2%)	47	73
24	31	138/138 (100%)	137 (99%)	1 (1%)	81	93
25	12	133/133 (100%)	132 (99%)	1 (1%)	79	91
25	32	133/133 (100%)	133 (100%)	0	100	100
26	13	134/134 (100%)	131 (98%)	3 (2%)	47	73
26	33	134/134 (100%)	130 (97%)	4 (3%)	36	63
27	14	136/136 (100%)	134 (98%)	2 (2%)	60	82
27	34	136/136 (100%)	133 (98%)	3 (2%)	47	73
28	15	135/135 (100%)	122 (90%)	13 (10%)	7	14
28	35	135/135 (100%)	122 (90%)	13 (10%)	7	14
29	16	137/137 (100%)	129 (94%)	8 (6%)	17	34
29	36	137/137 (100%)	129 (94%)	8 (6%)	17	34
30	17	137/137 (100%)	128 (93%)	9 (7%)	14	28
30	37	137/137 (100%)	131 (96%)	6 (4%)	24	47
31	18	133/133 (100%)	126 (95%)	7 (5%)	19	38
31	38	133/133 (100%)	123 (92%)	10 (8%)	11	23
32	19	174/174 (100%)	168 (97%)	6 (3%)	32	58
32	39	174/174 (100%)	166 (95%)	8 (5%)	23	45
33	20	121/121 (100%)	110 (91%)	11 (9%)	7	16
33	40	121/121 (100%)	110 (91%)	11 (9%)	7	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	21	129/129 (100%)	111 (86%)	18 (14%)	3	5
34	41	129/129 (100%)	111 (86%)	18 (14%)	3	5
All	All	7560/7564 (100%)	7343 (97%)	217 (3%)	39	64

5 of 217 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	20	165	MET
28	35	41	LEU
34	41	37	ASN
34	21	61	LYS
34	21	162	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	416	ASN
31	38	83	ASN
15	u	28	ASN
30	37	83	ASN
24	31	161	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 548 ligands modelled in this entry, 2 are monoatomic and 38 are unknown - leaving 508 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	$\# Z > 2$
44	DGD	c	516	-	63,63,67	1.05	5 (7%)	77,77,81	1.48	14 (18%)
46	HEM	V	201	16	42,50,50	1.58	4 (9%)	46,82,82	1.36	5 (10%)
48	A86	17	312	-	47,50,50	4.31	24 (51%)	51,76,76	6.07	18 (35%)
37	CLA	41	202	34	55,65,73	2.22	16 (29%)	64,103,113	2.80	26 (40%)
48	A86	13	311	-	47,50,50	4.19	23 (48%)	51,76,76	6.64	20 (39%)
48	A86	20	309	-	47,50,50	4.37	23 (48%)	51,76,76	7.11	13 (25%)
37	CLA	34	301	27	63,73,73	2.00	15 (23%)	74,113,113	2.61	26 (35%)
47	KC1	17	303	-	48,53,53	3.16	24 (50%)	54,89,89	3.57	29 (53%)
51	LMU	39	315	-	36,36,36	1.12	2 (5%)	47,47,47	1.04	2 (4%)
37	CLA	32	202	52	63,73,73	1.95	16 (25%)	74,113,113	2.56	28 (37%)
37	CLA	38	203	-	63,73,73	2.08	16 (25%)	74,113,113	2.60	30 (40%)
48	A86	12	220	-	47,50,50	4.05	22 (46%)	51,76,76	6.62	20 (39%)
37	CLA	W	101	-	63,73,73	1.95	15 (23%)	74,113,113	2.81	29 (39%)
47	KC1	36	308	29	48,53,53	3.15	23 (47%)	54,89,89	3.51	30 (55%)
47	KC1	21	203	-	48,53,53	3.18	25 (52%)	54,89,89	3.71	27 (50%)
47	KC1	32	212	25	48,53,53	3.10	23 (47%)	54,89,89	3.54	31 (57%)
40	SQD	40	202	-	52,54,54	0.96	5 (9%)	62,65,65	1.55	10 (16%)
39	BCR	d	405	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
37	CLA	38	201	52	63,73,73	2.05	15 (23%)	74,113,113	2.56	29 (39%)
40	SQD	16	315	-	52,54,54	0.96	5 (9%)	62,65,65	1.55	11 (17%)
37	CLA	19	305	32	49,59,73	2.26	16 (32%)	56,96,113	3.01	26 (46%)
37	CLA	31	306	52	43,53,73	2.40	15 (34%)	50,89,113	3.06	26 (52%)
48	A86	35	312	-	47,50,50	4.31	24 (51%)	51,76,76	6.47	18 (35%)
47	KC1	34	309	27	48,53,53	3.07	22 (45%)	54,89,89	3.62	31 (57%)
48	A86	34	316	-	47,50,50	4.22	24 (51%)	51,76,76	6.15	21 (41%)
41	LMG	31	316	-	42,42,55	1.05	3 (7%)	50,50,63	1.22	3 (6%)
37	CLA	A	405	-	63,73,73	1.94	14 (22%)	74,113,113	2.68	27 (36%)
37	CLA	20	306	33	48,58,73	2.31	14 (29%)	56,95,113	2.93	27 (48%)
41	LMG	B	521	-	51,51,55	0.87	3 (5%)	59,59,63	1.31	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	HEM	F	101	5,6	42,50,50	1.44	5 (11%)	46,82,82	1.35	5 (10%)
48	A86	17	320	-	47,50,50	4.22	23 (48%)	51,76,76	6.46	19 (37%)
48	A86	32	203	-	47,50,50	4.11	21 (44%)	51,76,76	6.37	22 (43%)
39	BCR	B	525	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	7 (12%)
47	KC1	35	309	28	48,53,53	3.17	24 (50%)	54,89,89	3.49	30 (55%)
47	KC1	13	304	26	48,53,53	3.11	20 (41%)	54,89,89	3.62	29 (53%)
47	KC1	15	302	-	48,53,53	3.15	25 (52%)	54,89,89	3.73	30 (55%)
48	A86	31	312	-	47,50,50	4.08	22 (46%)	51,76,76	6.49	22 (43%)
50	DD6	19	312	-	40,45,45	5.38	22 (55%)	51,67,67	5.77	30 (58%)
47	KC1	41	207	34	48,53,53	3.16	26 (54%)	54,89,89	3.81	32 (59%)
48	A86	15	316	-	47,50,50	4.33	23 (48%)	51,76,76	6.41	22 (43%)
43	LHG	b	522	-	48,48,48	0.75	1 (2%)	51,54,54	1.29	6 (11%)
42	BCT	A	409	36	3,3,3	1.21	0	2,3,3	4.13	2 (100%)
47	KC1	14	306	27	48,53,53	3.11	22 (45%)	54,89,89	3.61	31 (57%)
37	CLA	39	304	32	43,53,73	2.46	16 (37%)	50,89,113	3.14	24 (48%)
37	CLA	A	403	-	63,73,73	1.97	14 (22%)	74,113,113	2.66	30 (40%)
37	CLA	39	302	-	63,73,73	2.01	17 (26%)	74,113,113	2.74	27 (36%)
48	A86	41	215	-	47,50,50	4.24	25 (53%)	51,76,76	6.87	16 (31%)
47	KC1	31	303	-	48,53,53	3.11	21 (43%)	54,89,89	3.61	28 (51%)
37	CLA	12	205	-	63,73,73	1.98	14 (22%)	74,113,113	2.72	32 (43%)
48	A86	18	214	-	47,50,50	4.39	24 (51%)	51,76,76	6.79	19 (37%)
37	CLA	b	513	-	63,73,73	1.93	15 (23%)	74,113,113	2.64	28 (37%)
47	KC1	38	207	31	48,53,53	3.17	25 (52%)	54,89,89	3.69	32 (59%)
39	BCR	A	410	-	41,41,41	1.10	2 (4%)	56,56,56	1.30	6 (10%)
37	CLA	40	210	-	45,55,73	2.43	17 (37%)	52,91,113	2.99	26 (50%)
37	CLA	35	310	-	43,53,73	2.55	16 (37%)	50,89,113	3.13	24 (48%)
39	BCR	C	519	-	41,41,41	1.17	2 (4%)	56,56,56	1.24	4 (7%)
50	DD6	20	312	-	40,45,45	5.64	24 (60%)	51,67,67	6.11	28 (54%)
47	KC1	34	304	27	48,53,53	3.13	21 (43%)	54,89,89	3.79	26 (48%)
47	KC1	12	211	25	48,53,53	3.09	23 (47%)	54,89,89	3.54	32 (59%)
48	A86	15	314	-	47,50,50	4.45	24 (51%)	51,76,76	6.97	18 (35%)
48	A86	18	215	-	47,50,50	4.26	24 (51%)	51,76,76	6.49	18 (35%)
37	CLA	35	305	-	43,53,73	2.53	16 (37%)	50,89,113	3.02	25 (50%)
47	KC1	38	210	31	48,53,53	3.16	24 (50%)	54,89,89	3.65	29 (53%)
48	A86	36	310	-	47,50,50	4.09	23 (48%)	51,76,76	6.38	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	BCR	5	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.33	7 (12%)
37	CLA	b	509	-	63,73,73	1.89	13 (20%)	74,113,113	2.66	29 (39%)
48	A86	12	213	-	47,50,50	4.16	23 (48%)	51,76,76	6.73	20 (39%)
39	BCR	c	519	-	41,41,41	1.17	2 (4%)	56,56,56	1.24	4 (7%)
37	CLA	33	307	26	50,60,73	2.26	14 (28%)	57,97,113	2.79	30 (52%)
37	CLA	18	204	-	54,64,73	2.24	16 (29%)	63,102,113	3.04	32 (50%)
45	PL9	D	408	-	55,55,55	1.76	9 (16%)	68,69,69	1.39	11 (16%)
41	LMG	B	520	-	51,51,55	0.82	1 (1%)	59,59,63	1.30	5 (8%)
48	A86	33	315	-	47,50,50	4.30	24 (51%)	51,76,76	6.32	19 (37%)
48	A86	21	214	-	47,50,50	4.40	24 (51%)	51,76,76	6.92	17 (33%)
37	CLA	38	208	31	51,61,73	2.26	15 (29%)	59,98,113	2.82	27 (45%)
37	CLA	b	516	-	63,73,73	1.90	14 (22%)	74,113,113	2.71	29 (39%)
41	LMG	L	102	-	40,40,55	0.96	3 (7%)	48,48,63	1.33	4 (8%)
47	KC1	33	306	26	48,53,53	3.11	22 (45%)	54,89,89	3.60	29 (53%)
37	CLA	21	208	-	63,73,73	2.10	17 (26%)	74,113,113	2.61	27 (36%)
46	HEM	f	101	5,6	42,50,50	1.44	5 (11%)	46,82,82	1.36	5 (10%)
37	CLA	31	310	52	49,59,73	2.22	16 (32%)	56,96,113	2.90	27 (48%)
48	A86	13	313	-	47,50,50	4.42	24 (51%)	51,76,76	7.22	18 (35%)
47	KC1	40	204	-	48,53,53	3.11	23 (47%)	54,89,89	3.90	30 (55%)
37	CLA	34	303	-	55,65,73	2.18	14 (25%)	64,103,113	3.00	32 (50%)
41	LMG	l	101	-	40,40,55	0.95	3 (7%)	48,48,63	1.33	4 (8%)
37	CLA	a	404	52	63,73,73	1.99	13 (20%)	74,113,113	2.71	26 (35%)
37	CLA	C	502	-	63,73,73	1.88	14 (22%)	74,113,113	2.57	27 (36%)
47	KC1	18	210	31	48,53,53	3.16	25 (52%)	54,89,89	3.66	29 (53%)
37	CLA	D	401	52	63,73,73	1.99	13 (20%)	74,113,113	2.70	26 (35%)
46	HEM	v	201	16	42,50,50	1.58	4 (9%)	46,82,82	1.35	5 (10%)
48	A86	18	213	-	47,50,50	4.26	24 (51%)	51,76,76	6.90	21 (41%)
37	CLA	19	302	-	63,73,73	2.01	16 (25%)	74,113,113	2.72	27 (36%)
37	CLA	19	301	32	63,73,73	2.01	15 (23%)	74,113,113	2.60	27 (36%)
37	CLA	b	515	-	63,73,73	1.94	15 (23%)	74,113,113	2.62	29 (39%)
40	SQD	L	101	-	52,54,54	0.93	3 (5%)	62,65,65	1.60	9 (14%)
37	CLA	12	209	25	50,60,73	2.20	14 (28%)	57,97,113	2.97	30 (52%)
37	CLA	C	511	3	63,73,73	1.96	15 (23%)	74,113,113	2.60	29 (39%)
37	CLA	19	309	32	43,53,73	2.43	15 (34%)	50,89,113	3.03	24 (48%)
37	CLA	21	205	34	43,53,73	2.51	15 (34%)	50,89,113	3.02	24 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	KC1	13	309	26	48,53,53	3.11	25 (52%)	54,89,89	3.59	32 (59%)
48	A86	16	313	-	47,50,50	4.39	23 (48%)	51,76,76	7.11	22 (43%)
48	A86	32	214	-	47,50,50	4.18	23 (48%)	51,76,76	6.74	20 (39%)
48	A86	32	216	-	47,50,50	4.37	24 (51%)	51,76,76	6.78	14 (27%)
40	SQD	17	301	-	47,49,54	1.01	5 (10%)	57,60,65	1.49	11 (19%)
39	BCR	b	517	-	41,41,41	1.22	2 (4%)	56,56,56	1.33	7 (12%)
48	A86	35	314	-	47,50,50	4.43	24 (51%)	51,76,76	7.04	18 (35%)
37	CLA	z	101	52	63,73,73	2.07	15 (23%)	74,113,113	2.65	28 (37%)
44	DGD	j	101	-	63,63,67	1.09	6 (9%)	77,77,81	1.50	12 (15%)
37	CLA	16	309	-	43,53,73	2.48	15 (34%)	50,89,113	3.24	25 (50%)
41	LMG	C	518	-	51,51,55	0.97	3 (5%)	59,59,63	1.46	7 (11%)
37	CLA	13	307	26	50,60,73	2.26	14 (28%)	57,97,113	2.79	30 (52%)
37	CLA	Z	101	52	63,73,73	2.08	15 (23%)	74,113,113	2.65	28 (37%)
37	CLA	c	501	-	63,73,73	1.92	16 (25%)	74,113,113	2.71	27 (36%)
37	CLA	12	212	-	43,53,73	2.47	15 (34%)	50,89,113	3.13	25 (50%)
41	LMG	c	518	-	51,51,55	0.97	3 (5%)	59,59,63	1.46	7 (11%)
39	BCR	b	518	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	6 (10%)
37	CLA	c	511	3	63,73,73	1.97	15 (23%)	74,113,113	2.60	29 (39%)
48	A86	35	313	-	47,50,50	4.36	24 (51%)	51,76,76	6.20	14 (27%)
47	KC1	38	205	31	48,53,53	3.16	25 (52%)	54,89,89	3.63	29 (53%)
48	A86	32	215	-	47,50,50	4.11	24 (51%)	51,76,76	6.47	17 (33%)
47	KC1	20	302	-	48,53,53	3.11	23 (47%)	54,89,89	3.90	30 (55%)
37	CLA	B	510	52	63,73,73	1.92	15 (23%)	74,113,113	2.67	29 (39%)
50	DD6	16	312	-	40,45,45	5.60	24 (60%)	51,67,67	5.91	26 (50%)
37	CLA	C	510	-	63,73,73	1.96	15 (23%)	74,113,113	2.69	27 (36%)
37	CLA	20	301	33	54,64,73	2.23	17 (31%)	63,102,113	2.95	29 (46%)
37	CLA	39	305	32	49,59,73	2.26	15 (30%)	56,96,113	3.02	27 (48%)
41	LMG	b	520	-	51,51,55	0.87	3 (5%)	59,59,63	1.31	6 (10%)
47	KC1	15	306	28	48,53,53	3.16	25 (52%)	54,89,89	3.63	30 (55%)
48	A86	31	311	-	47,50,50	4.06	23 (48%)	51,76,76	6.20	17 (33%)
48	A86	39	313	-	47,50,50	4.40	26 (55%)	51,76,76	7.35	21 (41%)
48	A86	37	310	-	47,50,50	4.22	23 (48%)	51,76,76	6.28	18 (35%)
39	BCR	K	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.27	7 (12%)
50	DD6	39	312	-	40,45,45	5.37	22 (55%)	51,67,67	5.77	30 (58%)
43	LHG	d	407	-	48,48,48	0.72	1 (2%)	51,54,54	1.32	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	11	305	52	43,53,73	2.40	15 (34%)	50,89,113	3.05	26 (52%)
48	A86	37	314	-	47,50,50	4.26	23 (48%)	51,76,76	6.45	18 (35%)
37	CLA	34	310	-	43,53,73	2.49	15 (34%)	50,89,113	3.09	24 (48%)
37	CLA	c	513	-	63,73,73	1.96	15 (23%)	74,113,113	2.66	26 (35%)
37	CLA	34	308	52	63,73,73	2.02	16 (25%)	74,113,113	2.61	30 (40%)
37	CLA	16	307	52	59,69,73	2.10	15 (25%)	69,108,113	2.67	25 (36%)
37	CLA	C	509	-	63,73,73	1.99	14 (22%)	74,113,113	2.71	29 (39%)
37	CLA	37	303	-	54,64,73	2.21	14 (25%)	63,102,113	2.96	30 (47%)
48	A86	12	214	-	47,50,50	4.12	24 (51%)	51,76,76	6.47	17 (33%)
47	KC1	37	304	30	48,53,53	3.13	24 (50%)	54,89,89	3.67	30 (55%)
39	BCR	D	407	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
40	SQD	a	409	-	52,54,54	0.95	6 (11%)	62,65,65	1.64	10 (16%)
41	LMG	17	317	-	37,37,55	0.96	2 (5%)	45,45,63	1.28	4 (8%)
39	BCR	h	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.26	6 (10%)
41	LMG	31	317	-	32,32,55	0.97	1 (3%)	40,40,63	1.25	4 (10%)
44	DGD	c	517	-	63,63,67	1.22	6 (9%)	77,77,81	1.49	14 (18%)
48	A86	37	311	-	47,50,50	4.31	24 (51%)	51,76,76	6.05	18 (35%)
47	KC1	19	308	-	48,53,53	3.12	21 (43%)	54,89,89	3.71	32 (59%)
47	KC1	33	302	-	48,53,53	3.11	25 (52%)	54,89,89	3.79	30 (55%)
37	CLA	33	305	-	43,53,73	2.52	16 (37%)	50,89,113	3.08	24 (48%)
43	LHG	21	201	-	34,34,48	0.76	2 (5%)	37,39,54	1.42	5 (13%)
37	CLA	41	204	-	56,66,73	2.22	15 (26%)	65,104,113	2.93	32 (49%)
47	KC1	36	304	29	48,53,53	3.15	25 (52%)	54,89,89	3.73	30 (55%)
37	CLA	c	509	-	63,73,73	1.98	14 (22%)	74,113,113	2.71	29 (39%)
39	BCR	b	524	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	7 (12%)
43	LHG	d	408	-	48,48,48	0.76	2 (4%)	51,54,54	1.31	7 (13%)
48	A86	34	314	-	47,50,50	4.38	24 (51%)	51,76,76	7.03	18 (35%)
37	CLA	C	505	-	63,73,73	1.90	15 (23%)	74,113,113	2.68	27 (36%)
48	A86	38	215	-	47,50,50	4.28	24 (51%)	51,76,76	6.46	17 (33%)
37	CLA	38	204	-	54,64,73	2.25	16 (29%)	63,102,113	3.05	32 (50%)
37	CLA	21	206	34	63,73,73	2.03	15 (23%)	74,113,113	2.63	27 (36%)
43	LHG	a	412	-	45,45,48	0.87	2 (4%)	48,51,54	1.25	7 (14%)
37	CLA	18	202	31	63,73,73	2.01	14 (22%)	74,113,113	2.72	28 (37%)
47	KC1	16	305	29	48,53,53	3.18	24 (50%)	54,89,89	3.57	28 (51%)
44	DGD	C	516	-	63,63,67	1.05	5 (7%)	77,77,81	1.48	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	KC1	18	207	31	48,53,53	3.16	25 (52%)	54,89,89	3.67	32 (59%)
48	A86	34	311	-	47,50,50	4.16	22 (46%)	51,76,76	6.96	20 (39%)
37	CLA	B	504	-	63,73,73	1.84	15 (23%)	74,113,113	2.58	30 (40%)
41	LMG	a	410	-	51,51,55	0.88	2 (3%)	59,59,63	1.37	7 (11%)
50	DD6	20	310	-	40,45,45	5.49	23 (57%)	51,67,67	6.37	25 (49%)
37	CLA	19	303	52	63,73,73	2.02	17 (26%)	74,113,113	2.71	26 (35%)
48	A86	16	310	-	47,50,50	4.08	22 (46%)	51,76,76	6.38	21 (41%)
37	CLA	33	310	-	43,53,73	2.56	15 (34%)	50,89,113	3.08	24 (48%)
37	CLA	19	306	32	63,73,73	1.96	14 (22%)	74,113,113	2.60	26 (35%)
37	CLA	d	404	-	63,73,73	1.95	14 (22%)	74,113,113	2.69	28 (37%)
39	BCR	a	413	-	41,41,41	1.10	2 (4%)	56,56,56	1.31	6 (10%)
37	CLA	34	302	-	63,73,73	2.01	15 (23%)	74,113,113	2.54	27 (36%)
47	KC1	32	207	25	48,53,53	3.10	21 (43%)	54,89,89	3.50	26 (48%)
37	CLA	39	301	32	63,73,73	2.02	15 (23%)	74,113,113	2.61	27 (36%)
37	CLA	16	303	-	55,65,73	2.18	14 (25%)	64,103,113	2.86	29 (45%)
40	SQD	B	519	-	52,54,54	0.93	4 (7%)	62,65,65	1.60	9 (14%)
47	KC1	41	203	-	48,53,53	3.18	25 (52%)	54,89,89	3.71	27 (50%)
48	A86	13	314	-	47,50,50	4.41	24 (51%)	51,76,76	7.15	17 (33%)
48	A86	18	212	-	47,50,50	4.33	24 (51%)	51,76,76	6.73	17 (33%)
37	CLA	41	210	-	43,53,73	2.53	16 (37%)	50,89,113	3.15	24 (48%)
48	A86	14	313	-	47,50,50	4.35	24 (51%)	51,76,76	6.24	17 (33%)
48	A86	15	313	-	47,50,50	4.37	24 (51%)	51,76,76	6.20	15 (29%)
43	LHG	B	523	-	48,48,48	0.75	1 (2%)	51,54,54	1.29	6 (11%)
37	CLA	z	102	33	43,53,73	2.55	16 (37%)	50,89,113	3.11	28 (56%)
37	CLA	11	308	52	63,73,73	1.95	16 (25%)	74,113,113	2.57	28 (37%)
37	CLA	19	307	43	63,73,73	1.99	15 (23%)	74,113,113	2.58	28 (37%)
37	CLA	32	204	25	63,73,73	1.95	14 (22%)	74,113,113	2.55	27 (36%)
37	CLA	21	202	34	55,65,73	2.22	16 (29%)	64,103,113	2.81	26 (40%)
48	A86	11	314	-	47,50,50	4.18	23 (48%)	51,76,76	7.00	22 (43%)
37	CLA	15	308	52	63,73,73	2.05	17 (26%)	74,113,113	2.62	27 (36%)
37	CLA	21	204	-	56,66,73	2.22	15 (26%)	65,104,113	2.94	32 (49%)
37	CLA	33	308	52	63,73,73	2.06	16 (25%)	74,113,113	2.59	26 (35%)
47	KC1	16	304	29	48,53,53	3.15	24 (50%)	54,89,89	3.73	30 (55%)
39	BCR	B	517	-	41,41,41	1.21	2 (4%)	56,56,56	1.33	7 (12%)
37	CLA	13	303	-	55,65,73	2.17	15 (27%)	64,103,113	2.85	31 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	18	201	52	63,73,73	2.03	17 (26%)	74,113,113	2.60	28 (37%)
37	CLA	C	506	-	63,73,73	1.93	16 (25%)	74,113,113	2.63	28 (37%)
41	LMG	d	409	-	51,51,55	0.89	3 (5%)	59,59,63	1.41	6 (10%)
48	A86	33	312	-	47,50,50	4.39	23 (48%)	51,76,76	6.58	18 (35%)
47	KC1	14	304	27	48,53,53	3.13	21 (43%)	54,89,89	3.79	26 (48%)
37	CLA	13	310	-	43,53,73	2.55	15 (34%)	50,89,113	3.08	24 (48%)
37	CLA	15	310	-	43,53,73	2.55	16 (37%)	50,89,113	3.11	24 (48%)
48	A86	37	309	-	47,50,50	4.30	24 (51%)	51,76,76	7.01	17 (33%)
41	LMG	32	201	-	39,39,55	1.03	2 (5%)	47,47,63	1.15	3 (6%)
35	OEX	a	401	1,3	0,15,15	-	-	-	-	-
40	SQD	b	521	-	35,37,54	1.18	6 (17%)	45,48,65	1.59	10 (22%)
41	LMG	D	412	-	51,51,55	0.89	3 (5%)	59,59,63	1.41	6 (10%)
37	CLA	17	304	-	54,64,73	2.21	15 (27%)	63,102,113	2.95	30 (47%)
48	A86	11	315	-	47,50,50	4.07	23 (48%)	51,76,76	6.38	17 (33%)
40	SQD	B	522	-	35,37,54	1.19	6 (17%)	45,48,65	1.59	10 (22%)
47	KC1	37	305	30	48,53,53	3.15	24 (50%)	54,89,89	3.59	30 (55%)
48	A86	13	315	-	47,50,50	4.30	23 (48%)	51,76,76	6.33	19 (37%)
47	KC1	12	208	25	48,53,53	3.05	22 (45%)	54,89,89	3.56	31 (57%)
48	A86	11	313	-	47,50,50	4.03	22 (46%)	51,76,76	5.79	17 (33%)
48	A86	16	314	-	47,50,50	4.01	23 (48%)	51,76,76	6.34	16 (31%)
44	DGD	J	101	-	63,63,67	1.09	7 (11%)	77,77,81	1.50	12 (15%)
48	A86	35	319	-	47,50,50	4.27	23 (48%)	51,76,76	6.00	19 (37%)
44	DGD	H	102	-	63,63,67	1.04	5 (7%)	77,77,81	1.36	8 (10%)
48	A86	15	315	-	47,50,50	4.28	24 (51%)	51,76,76	6.53	21 (41%)
38	PHO	a	406	-	50,69,69	1.03	6 (12%)	48,99,99	1.28	6 (12%)
37	CLA	Z	102	33	43,53,73	2.55	14 (32%)	50,89,113	3.11	28 (56%)
47	KC1	32	209	25	48,53,53	3.06	22 (45%)	54,89,89	3.56	31 (57%)
48	A86	37	313	-	47,50,50	4.20	23 (48%)	51,76,76	7.20	18 (35%)
37	CLA	15	301	28	63,73,73	2.07	15 (23%)	74,113,113	2.63	24 (32%)
50	DD6	41	212	-	40,45,45	5.51	23 (57%)	51,67,67	6.14	31 (60%)
44	DGD	h	102	-	63,63,67	1.03	5 (7%)	77,77,81	1.36	8 (10%)
37	CLA	b	514	-	60,70,73	1.96	14 (23%)	70,109,113	2.74	28 (40%)
37	CLA	38	211	-	43,53,73	2.58	16 (37%)	50,89,113	3.04	23 (46%)
47	KC1	35	304	28	48,53,53	3.17	25 (52%)	54,89,89	3.76	30 (55%)
35	OEX	A	401	1,3	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	A86	15	312	-	47,50,50	4.31	24 (51%)	51,76,76	6.47	18 (35%)
48	A86	40	201	-	47,50,50	4.39	23 (48%)	51,76,76	7.12	22 (43%)
43	LHG	37	321	-	44,44,48	0.66	1 (2%)	47,50,54	1.20	3 (6%)
48	A86	39	311	-	47,50,50	4.15	23 (48%)	51,76,76	6.47	19 (37%)
47	KC1	40	207	33	48,53,53	3.16	25 (52%)	54,89,89	3.66	26 (48%)
37	CLA	31	304	-	63,73,73	1.97	15 (23%)	74,113,113	2.72	32 (43%)
37	CLA	B	514	-	60,70,73	1.96	15 (25%)	70,109,113	2.74	28 (40%)
37	CLA	40	203	33	54,64,73	2.23	17 (31%)	63,102,113	2.96	29 (46%)
37	CLA	17	302	30	63,73,73	2.04	15 (23%)	74,113,113	2.42	23 (31%)
37	CLA	b	506	-	63,73,73	1.88	15 (23%)	74,113,113	2.76	28 (37%)
48	A86	34	313	-	47,50,50	4.35	24 (51%)	51,76,76	6.23	17 (33%)
47	KC1	36	302	-	48,53,53	3.18	25 (52%)	54,89,89	3.41	27 (50%)
37	CLA	b	510	52	63,73,73	1.92	15 (23%)	74,113,113	2.67	29 (39%)
37	CLA	15	307	28	50,60,73	2.28	14 (28%)	57,97,113	2.86	28 (49%)
48	A86	17	311	-	47,50,50	4.24	23 (48%)	51,76,76	6.29	19 (37%)
39	BCR	y	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.26	5 (8%)
37	CLA	38	206	-	43,53,73	2.54	16 (37%)	50,89,113	3.13	25 (50%)
37	CLA	41	208	-	63,73,73	2.10	17 (26%)	74,113,113	2.62	28 (37%)
37	CLA	18	211	-	43,53,73	2.55	16 (37%)	50,89,113	3.08	23 (46%)
43	LHG	D	409	-	48,48,48	0.72	1 (2%)	51,54,54	1.32	7 (13%)
37	CLA	35	303	-	55,65,73	2.24	16 (29%)	64,103,113	2.90	30 (46%)
48	A86	14	312	-	47,50,50	4.21	23 (48%)	51,76,76	6.60	22 (43%)
37	CLA	C	507	52	63,73,73	1.93	14 (22%)	74,113,113	2.61	28 (37%)
37	CLA	C	501	-	63,73,73	1.93	16 (25%)	74,113,113	2.71	28 (37%)
37	CLA	B	502	-	63,73,73	1.97	14 (22%)	74,113,113	2.74	28 (37%)
48	A86	38	213	-	47,50,50	4.35	25 (53%)	51,76,76	6.75	23 (45%)
47	KC1	11	309	24	48,53,53	3.05	22 (45%)	54,89,89	3.56	30 (55%)
48	A86	11	312	-	47,50,50	4.08	22 (46%)	51,76,76	6.49	22 (43%)
37	CLA	32	211	52	63,73,73	2.01	16 (25%)	74,113,113	2.55	27 (36%)
37	CLA	12	203	25	63,73,73	1.95	15 (23%)	74,113,113	2.55	27 (36%)
47	KC1	14	309	27	48,53,53	3.07	22 (45%)	54,89,89	3.63	32 (59%)
47	KC1	15	309	28	48,53,53	3.17	24 (50%)	54,89,89	3.49	30 (55%)
50	DD6	40	212	-	40,45,45	5.50	24 (60%)	51,67,67	6.36	25 (49%)
37	CLA	B	511	-	63,73,73	1.94	14 (22%)	74,113,113	2.67	29 (39%)
48	A86	17	313	-	47,50,50	4.30	23 (48%)	51,76,76	7.01	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	14	307	27	50,60,73	2.22	14 (28%)	57,97,113	2.84	29 (50%)
48	A86	38	212	-	47,50,50	4.33	24 (51%)	51,76,76	6.73	18 (35%)
48	A86	11	311	-	47,50,50	4.06	23 (48%)	51,76,76	6.21	17 (33%)
37	CLA	31	302	24	63,73,73	1.94	15 (23%)	74,113,113	2.62	27 (36%)
37	CLA	19	310	32	63,73,73	2.00	15 (23%)	74,113,113	2.54	27 (36%)
47	KC1	11	306	24	48,53,53	3.08	23 (47%)	54,89,89	3.60	26 (48%)
37	CLA	B	506	-	63,73,73	1.88	15 (23%)	74,113,113	2.76	27 (36%)
37	CLA	15	303	-	55,65,73	2.24	16 (29%)	64,103,113	2.88	30 (46%)
47	KC1	13	306	26	48,53,53	3.11	22 (45%)	54,89,89	3.60	29 (53%)
41	LMG	16	316	-	36,36,55	0.94	1 (2%)	44,44,63	1.22	4 (9%)
37	CLA	B	513	-	63,73,73	1.94	15 (23%)	74,113,113	2.65	28 (37%)
48	A86	41	213	-	47,50,50	4.47	24 (51%)	51,76,76	6.79	15 (29%)
48	A86	12	215	-	47,50,50	4.38	24 (51%)	51,76,76	6.79	14 (27%)
39	BCR	A	406	-	41,41,41	1.21	3 (7%)	56,56,56	1.32	7 (12%)
37	CLA	C	504	52	63,73,73	1.93	15 (23%)	74,113,113	2.64	27 (36%)
41	LMG	A	408	-	51,51,55	0.88	2 (3%)	59,59,63	1.37	7 (11%)
37	CLA	32	208	52	48,58,73	2.31	15 (31%)	56,95,113	3.06	31 (55%)
37	CLA	B	503	-	63,73,73	1.88	14 (22%)	74,113,113	2.68	28 (37%)
48	A86	37	319	-	47,50,50	4.24	23 (48%)	51,76,76	6.44	20 (39%)
37	CLA	33	303	-	55,65,73	2.18	14 (25%)	64,103,113	2.88	32 (50%)
37	CLA	12	207	52	48,58,73	2.31	15 (31%)	56,95,113	3.06	30 (53%)
48	A86	17	314	-	47,50,50	4.17	23 (48%)	51,76,76	7.19	17 (33%)
48	A86	35	311	-	47,50,50	4.26	23 (48%)	51,76,76	6.57	14 (27%)
37	CLA	35	308	52	63,73,73	2.06	17 (26%)	74,113,113	2.62	28 (37%)
37	CLA	41	205	34	43,53,73	2.51	15 (34%)	50,89,113	3.02	24 (48%)
47	KC1	18	205	31	48,53,53	3.17	25 (52%)	54,89,89	3.62	29 (53%)
38	PHO	A	404	-	50,69,69	1.03	6 (12%)	48,99,99	1.28	6 (12%)
48	A86	14	316	-	47,50,50	4.22	24 (51%)	51,76,76	6.14	21 (41%)
48	A86	31	314	-	47,50,50	4.17	23 (48%)	51,76,76	7.00	22 (43%)
37	CLA	36	309	-	43,53,73	2.47	16 (37%)	50,89,113	3.23	25 (50%)
48	A86	35	316	-	47,50,50	4.30	24 (51%)	51,76,76	6.43	22 (43%)
37	CLA	39	306	32	63,73,73	1.96	14 (22%)	74,113,113	2.60	26 (35%)
48	A86	35	315	-	47,50,50	4.28	24 (51%)	51,76,76	6.52	21 (41%)
37	CLA	20	307	33	43,53,73	2.54	16 (37%)	50,89,113	3.05	25 (50%)
45	PL9	d	402	-	55,55,55	1.16	6 (10%)	68,69,69	1.49	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	14	305	-	43,53,73	2.50	16 (37%)	50,89,113	3.07	24 (48%)
47	KC1	35	306	28	48,53,53	3.16	25 (52%)	54,89,89	3.63	30 (55%)
37	CLA	40	208	33	48,58,73	2.31	14 (29%)	56,95,113	2.92	26 (46%)
50	DD6	21	212	-	40,45,45	5.51	23 (57%)	51,67,67	6.13	31 (60%)
37	CLA	d	401	52	63,73,73	1.98	15 (23%)	74,113,113	2.63	27 (36%)
48	A86	41	211	-	47,50,50	4.38	24 (51%)	51,76,76	6.78	12 (23%)
37	CLA	B	512	-	63,73,73	1.90	16 (25%)	74,113,113	2.61	30 (40%)
47	KC1	33	309	26	48,53,53	3.11	25 (52%)	54,89,89	3.59	32 (59%)
47	KC1	15	304	28	48,53,53	3.16	25 (52%)	54,89,89	3.76	31 (57%)
37	CLA	B	516	-	63,73,73	1.90	14 (22%)	74,113,113	2.71	29 (39%)
37	CLA	14	302	-	63,73,73	2.02	15 (23%)	74,113,113	2.54	27 (36%)
48	A86	32	221	-	47,50,50	4.06	22 (46%)	51,76,76	6.63	21 (41%)
48	A86	11	319	-	47,50,50	4.01	23 (48%)	51,76,76	6.23	17 (33%)
37	CLA	W	102	-	63,73,73	2.08	16 (25%)	74,113,113	2.50	28 (37%)
37	CLA	B	507	52	63,73,73	1.96	15 (23%)	74,113,113	2.60	28 (37%)
37	CLA	39	303	52	63,73,73	2.02	16 (25%)	74,113,113	2.70	26 (35%)
48	A86	19	311	-	47,50,50	4.15	24 (51%)	51,76,76	6.47	19 (37%)
37	CLA	32	213	-	43,53,73	2.47	14 (32%)	50,89,113	3.13	24 (48%)
37	CLA	36	307	52	59,69,73	2.10	14 (23%)	69,108,113	2.68	25 (36%)
40	SQD	A	407	-	52,54,54	0.95	6 (11%)	62,65,65	1.64	10 (16%)
45	PL9	D	404	-	55,55,55	1.16	5 (9%)	68,69,69	1.49	13 (19%)
37	CLA	20	308	-	45,55,73	2.43	17 (37%)	52,91,113	3.00	26 (50%)
37	CLA	32	210	25	50,60,73	2.20	14 (28%)	57,97,113	2.96	30 (52%)
48	A86	12	216	-	47,50,50	4.23	23 (48%)	51,76,76	6.88	20 (39%)
37	CLA	38	202	31	63,73,73	2.05	14 (22%)	74,113,113	2.65	28 (37%)
48	A86	31	315	-	47,50,50	4.07	23 (48%)	51,76,76	6.38	17 (33%)
37	CLA	32	205	-	63,73,73	1.92	16 (25%)	74,113,113	2.40	25 (33%)
37	CLA	33	301	26	63,73,73	2.02	14 (22%)	74,113,113	2.55	24 (32%)
48	A86	32	218	-	47,50,50	4.22	23 (48%)	51,76,76	6.22	21 (41%)
37	CLA	13	308	52	63,73,73	2.05	16 (25%)	74,113,113	2.59	26 (35%)
47	KC1	31	305	24	48,53,53	3.12	22 (45%)	54,89,89	3.62	29 (53%)
37	CLA	41	206	34	63,73,73	2.03	15 (23%)	74,113,113	2.62	27 (36%)
47	KC1	31	307	24	48,53,53	3.09	23 (47%)	54,89,89	3.60	26 (48%)
50	DD6	40	214	-	40,45,45	5.63	24 (60%)	51,67,67	6.11	28 (54%)
37	CLA	35	307	28	50,60,73	2.28	14 (28%)	57,97,113	2.86	28 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	40	205	-	54,64,73	2.17	15 (27%)	63,102,113	3.05	34 (53%)
48	A86	14	311	-	47,50,50	4.16	21 (44%)	51,76,76	6.95	20 (39%)
37	CLA	32	206	-	63,73,73	1.97	14 (22%)	74,113,113	2.72	31 (41%)
48	A86	14	314	-	47,50,50	4.37	24 (51%)	51,76,76	7.04	18 (35%)
37	CLA	c	508	-	63,73,73	1.93	14 (22%)	74,113,113	2.67	26 (35%)
48	A86	34	315	-	47,50,50	4.17	23 (48%)	51,76,76	6.63	17 (33%)
43	LHG	37	315	-	43,43,48	0.63	0	46,49,54	1.31	6 (13%)
38	PHO	a	405	-	50,69,69	1.03	5 (10%)	48,99,99	1.30	7 (14%)
37	CLA	11	301	24	63,73,73	1.94	15 (23%)	74,113,113	2.62	27 (36%)
48	A86	21	211	-	47,50,50	4.38	24 (51%)	51,76,76	6.78	12 (23%)
47	KC1	21	207	34	48,53,53	3.15	26 (54%)	54,89,89	3.81	31 (57%)
37	CLA	38	209	52	63,73,73	2.06	16 (25%)	74,113,113	2.58	28 (37%)
37	CLA	21	209	34	43,53,73	2.55	16 (37%)	50,89,113	3.09	25 (50%)
43	LHG	21	217	-	44,44,48	0.65	1 (2%)	47,50,54	1.20	3 (6%)
37	CLA	C	513	-	63,73,73	1.97	16 (25%)	74,113,113	2.67	26 (35%)
37	CLA	C	503	-	63,73,73	1.94	14 (22%)	74,113,113	2.72	30 (40%)
48	A86	37	312	-	47,50,50	4.30	23 (48%)	51,76,76	7.03	20 (39%)
37	CLA	20	303	-	54,64,73	2.17	15 (27%)	63,102,113	3.05	34 (53%)
37	CLA	18	206	-	43,53,73	2.52	16 (37%)	50,89,113	3.10	25 (50%)
37	CLA	14	303	-	55,65,73	2.18	14 (25%)	64,103,113	3.01	32 (50%)
37	CLA	39	310	32	63,73,73	2.00	14 (22%)	74,113,113	2.53	27 (36%)
38	PHO	D	403	-	50,69,69	1.03	5 (10%)	48,99,99	1.30	7 (14%)
47	KC1	17	305	30	48,53,53	3.13	25 (52%)	54,89,89	3.55	28 (51%)
47	KC1	20	305	33	48,53,53	3.16	25 (52%)	54,89,89	3.67	26 (48%)
47	KC1	13	302	-	48,53,53	3.11	25 (52%)	54,89,89	3.78	30 (55%)
37	CLA	13	305	-	43,53,73	2.52	16 (37%)	50,89,113	3.07	24 (48%)
48	A86	12	202	-	47,50,50	4.10	21 (44%)	51,76,76	6.37	22 (43%)
39	BCR	C	515	-	41,41,41	1.19	2 (4%)	56,56,56	1.26	6 (10%)
37	CLA	31	308	24	50,60,73	2.20	16 (32%)	57,97,113	3.02	27 (47%)
48	A86	36	313	-	47,50,50	4.01	23 (48%)	51,76,76	6.34	16 (31%)
41	LMG	36	314	-	36,36,55	0.94	1 (2%)	44,44,63	1.21	4 (9%)
37	CLA	c	503	-	63,73,73	1.94	14 (22%)	74,113,113	2.72	30 (40%)
37	CLA	41	209	34	43,53,73	2.55	16 (37%)	50,89,113	3.09	25 (50%)
48	A86	14	315	-	47,50,50	4.17	23 (48%)	51,76,76	6.63	17 (33%)
48	A86	33	311	-	47,50,50	4.18	23 (48%)	51,76,76	6.64	20 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	17	309	52	63,73,73	2.13	15 (23%)	74,113,113	2.80	31 (41%)
37	CLA	b	523	-	63,73,73	1.92	18 (28%)	74,113,113	2.66	29 (39%)
48	A86	36	311	-	47,50,50	4.12	22 (46%)	51,76,76	6.32	21 (41%)
48	A86	38	214	-	47,50,50	4.40	24 (51%)	51,76,76	6.83	19 (37%)
48	A86	15	311	-	47,50,50	4.26	23 (48%)	51,76,76	6.55	14 (27%)
37	CLA	c	507	52	63,73,73	1.93	14 (22%)	74,113,113	2.61	28 (37%)
48	A86	33	314	-	47,50,50	4.40	25 (53%)	51,76,76	7.16	17 (33%)
37	CLA	c	506	-	63,73,73	1.93	15 (23%)	74,113,113	2.63	28 (37%)
48	A86	34	312	-	47,50,50	4.21	23 (48%)	51,76,76	6.60	22 (43%)
51	LMU	19	315	-	36,36,36	1.13	2 (5%)	47,47,47	1.05	3 (6%)
47	KC1	12	206	25	48,53,53	3.10	20 (41%)	54,89,89	3.50	26 (48%)
39	BCR	C	514	-	41,41,41	1.21	2 (4%)	56,56,56	1.42	10 (17%)
39	BCR	0	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.34	7 (12%)
48	A86	33	313	-	47,50,50	4.41	24 (51%)	51,76,76	7.22	18 (35%)
37	CLA	11	310	52	49,59,73	2.22	16 (32%)	56,96,113	2.90	27 (48%)
45	PL9	d	406	-	55,55,55	1.76	9 (16%)	68,69,69	1.39	11 (16%)
42	BCT	a	411	36	3,3,3	1.21	0	2,3,3	4.13	2 (100%)
37	CLA	c	512	-	63,73,73	1.94	15 (23%)	74,113,113	2.65	28 (37%)
37	CLA	B	509	-	63,73,73	1.88	13 (20%)	74,113,113	2.65	29 (39%)
37	CLA	14	301	27	63,73,73	1.99	15 (23%)	74,113,113	2.60	26 (35%)
37	CLA	18	203	-	63,73,73	2.07	15 (23%)	74,113,113	2.59	30 (40%)
48	A86	17	310	-	47,50,50	4.30	23 (48%)	51,76,76	7.02	17 (33%)
47	KC1	37	307	30	48,53,53	3.16	25 (52%)	54,89,89	3.55	31 (57%)
37	CLA	C	508	-	63,73,73	1.92	14 (22%)	74,113,113	2.65	25 (33%)
37	CLA	18	209	52	63,73,73	2.06	16 (25%)	74,113,113	2.56	26 (35%)
39	BCR	c	514	-	41,41,41	1.21	2 (4%)	56,56,56	1.43	10 (17%)
47	KC1	20	304	33	48,53,53	3.13	24 (50%)	54,89,89	3.49	28 (51%)
47	KC1	11	302	-	48,53,53	3.11	21 (43%)	54,89,89	3.61	28 (51%)
37	CLA	b	503	-	63,73,73	1.88	14 (22%)	74,113,113	2.68	28 (37%)
37	CLA	14	310	-	43,53,73	2.48	15 (34%)	50,89,113	3.08	24 (48%)
48	A86	40	213	-	47,50,50	4.41	24 (51%)	51,76,76	7.23	14 (27%)
41	LMG	12	201	-	39,39,55	1.02	2 (5%)	47,47,63	1.15	3 (6%)
43	LHG	19	314	37	48,48,48	0.29	0	51,54,54	0.32	0
37	CLA	36	301	29	63,73,73	1.99	16 (25%)	74,113,113	2.67	27 (36%)
48	A86	41	214	-	47,50,50	4.40	24 (51%)	51,76,76	6.92	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	SQD	36	315	-	47,49,54	1.01	4 (8%)	57,60,65	1.49	11 (19%)
37	CLA	37	306	30	50,60,73	2.28	14 (28%)	57,97,113	2.90	29 (50%)
43	LHG	D	410	-	48,48,48	0.76	1 (2%)	51,54,54	1.32	7 (13%)
48	A86	31	319	-	47,50,50	4.00	23 (48%)	51,76,76	6.24	17 (33%)
37	CLA	b	504	-	63,73,73	1.84	15 (23%)	74,113,113	2.59	30 (40%)
37	CLA	18	208	31	51,61,73	2.27	15 (29%)	59,98,113	2.81	27 (45%)
41	LMG	37	316	-	37,37,55	0.96	2 (5%)	45,45,63	1.28	5 (11%)
47	KC1	33	304	26	48,53,53	3.11	20 (41%)	54,89,89	3.63	29 (53%)
39	BCR	H	101	-	41,41,41	1.16	4 (9%)	56,56,56	1.25	5 (8%)
41	LMG	11	316	-	42,42,55	1.05	3 (7%)	50,50,63	1.22	3 (6%)
37	CLA	40	209	33	43,53,73	2.54	16 (37%)	50,89,113	3.04	25 (50%)
37	CLA	12	210	52	63,73,73	2.02	16 (25%)	74,113,113	2.55	27 (36%)
47	KC1	17	308	30	48,53,53	3.16	25 (52%)	54,89,89	3.56	31 (57%)
43	LHG	39	314	37	48,48,48	0.29	0	51,54,54	0.32	0
47	KC1	16	308	29	48,53,53	3.16	24 (50%)	54,89,89	3.52	30 (55%)
47	KC1	16	302	-	48,53,53	3.18	25 (52%)	54,89,89	3.41	27 (50%)
48	A86	13	312	-	47,50,50	4.38	23 (48%)	51,76,76	6.59	18 (35%)
37	CLA	B	501	52	63,73,73	1.96	15 (23%)	74,113,113	2.58	26 (35%)
37	CLA	w	101	-	63,73,73	1.95	15 (23%)	74,113,113	2.80	29 (39%)
37	CLA	13	301	26	63,73,73	2.03	14 (22%)	74,113,113	2.55	25 (33%)
37	CLA	21	210	-	43,53,73	2.52	16 (37%)	50,89,113	3.15	24 (48%)
37	CLA	B	524	-	63,73,73	1.93	18 (28%)	74,113,113	2.66	29 (39%)
47	KC1	34	306	27	48,53,53	3.11	23 (47%)	54,89,89	3.61	31 (57%)
48	A86	20	311	-	47,50,50	4.40	24 (51%)	51,76,76	7.22	14 (27%)
50	DD6	21	216	-	40,45,45	5.60	24 (60%)	51,67,67	6.13	27 (52%)
39	BCR	B	518	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	6 (10%)
37	CLA	b	507	52	63,73,73	1.96	14 (22%)	74,113,113	2.59	28 (37%)
37	CLA	b	508	-	63,73,73	1.93	15 (23%)	74,113,113	2.59	26 (35%)
37	CLA	15	305	-	43,53,73	2.54	16 (37%)	50,89,113	3.05	25 (50%)
37	CLA	34	305	-	43,53,73	2.51	16 (37%)	50,89,113	3.07	25 (50%)
37	CLA	a	403	-	63,73,73	1.97	15 (23%)	74,113,113	2.66	30 (40%)
37	CLA	12	204	-	63,73,73	1.93	16 (25%)	74,113,113	2.40	25 (33%)
48	A86	12	217	-	47,50,50	4.22	23 (48%)	51,76,76	6.21	21 (41%)
37	CLA	39	309	32	43,53,73	2.43	15 (34%)	50,89,113	3.05	24 (48%)
47	KC1	40	206	33	48,53,53	3.14	24 (50%)	54,89,89	3.50	29 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	C	512	-	63,73,73	1.95	15 (23%)	74,113,113	2.66	28 (37%)
37	CLA	D	406	-	63,73,73	1.95	14 (22%)	74,113,113	2.69	27 (36%)
37	CLA	16	301	29	63,73,73	1.99	16 (25%)	74,113,113	2.67	27 (36%)
37	CLA	19	304	32	43,53,73	2.46	16 (37%)	50,89,113	3.14	23 (46%)
37	CLA	c	502	-	63,73,73	1.88	14 (22%)	74,113,113	2.57	27 (36%)
37	CLA	a	407	-	63,73,73	1.94	14 (22%)	74,113,113	2.68	27 (36%)
37	CLA	d	403	-	63,73,73	1.89	16 (25%)	74,113,113	2.80	29 (39%)
43	LHG	17	316	-	43,43,48	0.63	0	46,49,54	1.30	6 (13%)
37	CLA	16	306	29	63,73,73	2.02	15 (23%)	74,113,113	2.57	29 (39%)
47	KC1	35	302	-	48,53,53	3.16	24 (50%)	54,89,89	3.70	29 (53%)
48	A86	21	215	-	47,50,50	4.24	25 (53%)	51,76,76	6.86	16 (31%)
48	A86	17	315	-	47,50,50	4.26	23 (48%)	51,76,76	6.45	19 (37%)
48	A86	15	319	-	47,50,50	4.27	23 (48%)	51,76,76	6.00	19 (37%)
44	DGD	C	517	-	63,63,67	1.21	6 (9%)	77,77,81	1.49	15 (19%)
37	CLA	11	303	-	63,73,73	1.97	15 (23%)	74,113,113	2.73	32 (43%)
43	LHG	41	201	-	34,34,48	0.76	1 (2%)	37,39,54	1.43	5 (13%)
47	KC1	36	305	29	48,53,53	3.17	24 (50%)	54,89,89	3.56	28 (51%)
41	LMG	b	519	-	51,51,55	0.82	1 (1%)	59,59,63	1.31	5 (8%)
48	A86	31	313	-	47,50,50	4.08	22 (46%)	51,76,76	5.87	16 (31%)
39	BCR	a	408	-	41,41,41	1.20	3 (7%)	56,56,56	1.32	7 (12%)
37	CLA	31	301	-	63,73,73	2.08	16 (25%)	74,113,113	2.51	29 (39%)
47	KC1	11	304	24	48,53,53	3.12	22 (45%)	54,89,89	3.62	29 (53%)
37	CLA	b	502	-	63,73,73	1.97	14 (22%)	74,113,113	2.74	28 (37%)
37	CLA	11	307	24	50,60,73	2.20	16 (32%)	57,97,113	3.04	27 (47%)
37	CLA	37	308	52	63,73,73	2.12	15 (23%)	74,113,113	2.81	31 (41%)
47	KC1	37	302	-	48,53,53	3.16	23 (47%)	54,89,89	3.57	29 (53%)
50	DD6	41	216	-	40,45,45	5.61	24 (60%)	51,67,67	6.12	27 (52%)
37	CLA	b	501	52	63,73,73	1.97	15 (23%)	74,113,113	2.58	26 (35%)
37	CLA	c	505	-	63,73,73	1.90	15 (23%)	74,113,113	2.68	27 (36%)
37	CLA	39	307	43	63,73,73	2.04	16 (25%)	74,113,113	2.58	27 (36%)
41	LMG	11	317	-	32,32,55	0.97	1 (3%)	40,40,63	1.25	4 (10%)
39	BCR	c	515	-	41,41,41	1.19	2 (4%)	56,56,56	1.26	6 (10%)
37	CLA	35	301	28	63,73,73	2.08	15 (23%)	74,113,113	2.63	24 (32%)
37	CLA	36	303	-	55,65,73	2.19	15 (27%)	64,103,113	2.86	29 (45%)
47	KC1	31	309	24	48,53,53	3.06	21 (43%)	54,89,89	3.55	31 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	A86	21	213	-	47,50,50	4.48	24 (51%)	51,76,76	6.80	16 (31%)
37	CLA	c	504	52	63,73,73	1.92	15 (23%)	74,113,113	2.64	27 (36%)
37	CLA	17	307	30	50,60,73	2.28	14 (28%)	57,97,113	2.90	29 (50%)
37	CLA	36	306	29	63,73,73	2.02	15 (23%)	74,113,113	2.57	28 (37%)
37	CLA	D	402	52	63,73,73	1.99	15 (23%)	74,113,113	2.63	27 (36%)
48	A86	32	217	-	47,50,50	4.22	23 (48%)	51,76,76	6.88	20 (39%)
37	CLA	b	512	-	63,73,73	1.90	17 (26%)	74,113,113	2.61	30 (40%)
37	CLA	14	308	52	63,73,73	2.02	14 (22%)	74,113,113	2.62	31 (41%)
37	CLA	B	505	-	63,73,73	1.91	15 (23%)	74,113,113	2.70	25 (33%)
48	A86	16	311	-	47,50,50	4.12	22 (46%)	51,76,76	6.32	21 (41%)
37	CLA	b	511	-	63,73,73	1.94	14 (22%)	74,113,113	2.66	29 (39%)
37	CLA	c	510	-	63,73,73	1.96	15 (23%)	74,113,113	2.69	27 (36%)
47	KC1	17	306	30	48,53,53	3.15	24 (50%)	54,89,89	3.60	29 (53%)
37	CLA	B	508	-	63,73,73	1.93	15 (23%)	74,113,113	2.59	26 (35%)
37	CLA	37	301	30	63,73,73	2.07	15 (23%)	74,113,113	2.56	24 (32%)
47	KC1	39	308	-	48,53,53	3.12	21 (43%)	54,89,89	3.71	31 (57%)
37	CLA	B	515	-	63,73,73	1.94	15 (23%)	74,113,113	2.62	29 (39%)
37	CLA	b	505	-	63,73,73	1.91	15 (23%)	74,113,113	2.70	25 (33%)
48	A86	19	313	-	47,50,50	4.34	25 (53%)	51,76,76	7.33	22 (43%)
37	CLA	D	405	-	63,73,73	1.89	16 (25%)	74,113,113	2.80	29 (39%)
37	CLA	34	307	27	50,60,73	2.22	14 (28%)	57,97,113	2.84	29 (50%)
48	A86	40	211	-	47,50,50	4.37	23 (48%)	51,76,76	7.12	13 (25%)
50	DD6	36	312	-	40,45,45	5.60	24 (60%)	51,67,67	5.90	26 (50%)
43	LHG	D	411	-	45,45,48	0.87	2 (4%)	48,51,54	1.25	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	DGD	c	516	-	-	17/51/91/95	0/2/2/2
46	HEM	V	201	16	-	4/12/54/54	-
48	A86	17	312	-	-	8/34/90/90	0/3/3/3
37	CLA	41	202	34	1/1/13/20	7/28/106/115	-
48	A86	13	311	-	-	5/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	20	309	-	-	5/34/90/90	0/3/3/3
37	CLA	34	301	27	-	12/37/115/115	-
47	KC1	17	303	-	-	6/15/71/71	-
51	LMU	39	315	-	-	6/21/61/61	0/2/2/2
37	CLA	32	202	52	1/1/15/20	13/37/115/115	-
37	CLA	38	203	-	1/1/15/20	6/37/115/115	-
48	A86	12	220	-	-	9/34/90/90	0/3/3/3
37	CLA	W	101	-	1/1/15/20	15/37/115/115	-
47	KC1	36	308	29	-	4/15/71/71	-
47	KC1	21	203	-	-	4/15/71/71	-
47	KC1	32	212	25	-	6/15/71/71	-
40	SQD	40	202	-	-	24/49/69/69	0/1/1/1
39	BCR	d	405	-	-	12/29/63/63	0/2/2/2
37	CLA	38	201	52	1/1/15/20	7/37/115/115	-
40	SQD	16	315	-	-	24/49/69/69	0/1/1/1
37	CLA	19	305	32	1/1/12/20	5/21/99/115	-
37	CLA	31	306	52	1/1/11/20	1/13/91/115	-
48	A86	35	312	-	-	8/34/90/90	0/3/3/3
47	KC1	34	309	27	-	6/15/71/71	-
48	A86	34	316	-	-	13/34/90/90	0/3/3/3
41	LMG	31	316	-	-	19/37/57/70	0/1/1/1
37	CLA	A	405	-	-	6/37/115/115	-
37	CLA	20	306	33	1/1/12/20	3/19/97/115	-
41	LMG	B	521	-	-	24/46/66/70	0/1/1/1
46	HEM	F	101	5,6	-	8/12/54/54	-
48	A86	17	320	-	-	8/34/90/90	0/3/3/3
48	A86	32	203	-	-	14/34/90/90	0/3/3/3
39	BCR	B	525	-	-	18/29/63/63	0/2/2/2
47	KC1	35	309	28	-	8/15/71/71	-
47	KC1	13	304	26	-	7/15/71/71	-
47	KC1	15	302	-	-	6/15/71/71	-
48	A86	31	312	-	-	6/34/90/90	0/3/3/3
50	DD6	19	312	-	-	12/26/80/80	0/3/3/3
47	KC1	41	207	34	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	15	316	-	-	14/34/90/90	0/3/3/3
43	LHG	b	522	-	-	18/53/53/53	-
47	KC1	14	306	27	-	6/15/71/71	-
37	CLA	39	304	32	1/1/11/20	4/13/91/115	-
37	CLA	A	403	-	1/1/15/20	4/37/115/115	-
37	CLA	39	302	-	1/1/15/20	9/37/115/115	-
48	A86	41	215	-	-	6/34/90/90	0/3/3/3
47	KC1	31	303	-	-	2/15/71/71	-
37	CLA	12	205	-	1/1/15/20	9/37/115/115	-
48	A86	18	214	-	-	12/34/90/90	0/3/3/3
37	CLA	b	513	-	1/1/15/20	8/37/115/115	-
47	KC1	38	207	31	-	5/15/71/71	-
39	BCR	A	410	-	-	7/29/63/63	0/2/2/2
37	CLA	40	210	-	1/1/11/20	2/16/94/115	-
37	CLA	35	310	-	1/1/11/20	2/13/91/115	-
39	BCR	C	519	-	-	6/29/63/63	0/2/2/2
50	DD6	20	312	-	-	12/26/80/80	0/3/3/3
47	KC1	34	304	27	-	6/15/71/71	-
47	KC1	12	211	25	-	6/15/71/71	-
48	A86	15	314	-	-	14/34/90/90	0/3/3/3
48	A86	18	215	-	-	13/34/90/90	0/3/3/3
37	CLA	35	305	-	1/1/11/20	3/13/91/115	-
47	KC1	38	210	31	-	8/15/71/71	-
48	A86	36	310	-	-	5/34/90/90	0/3/3/3
39	BCR	5	101	-	-	8/29/63/63	0/2/2/2
37	CLA	b	509	-	1/1/15/20	9/37/115/115	-
48	A86	12	213	-	-	5/34/90/90	0/3/3/3
39	BCR	c	519	-	-	6/29/63/63	0/2/2/2
37	CLA	33	307	26	1/1/12/20	10/22/100/115	-
37	CLA	18	204	-	1/1/13/20	8/27/105/115	-
45	PL9	D	408	-	-	9/53/73/73	0/1/1/1
41	LMG	B	520	-	-	15/46/66/70	0/1/1/1
48	A86	33	315	-	-	11/34/90/90	0/3/3/3
48	A86	21	214	-	-	5/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	38	208	31	1/1/12/20	11/23/101/115	-
37	CLA	b	516	-	1/1/15/20	13/37/115/115	-
41	LMG	L	102	-	-	15/35/55/70	0/1/1/1
47	KC1	33	306	26	-	6/15/71/71	-
37	CLA	21	208	-	1/1/15/20	11/37/115/115	-
46	HEM	f	101	5,6	-	8/12/54/54	-
37	CLA	31	310	52	1/1/12/20	6/21/99/115	-
48	A86	13	313	-	-	18/34/90/90	0/3/3/3
47	KC1	40	204	-	-	7/15/71/71	-
37	CLA	34	303	-	-	4/28/106/115	-
41	LMG	l	101	-	-	15/35/55/70	0/1/1/1
37	CLA	a	404	52	1/1/15/20	6/37/115/115	-
37	CLA	C	502	-	1/1/15/20	7/37/115/115	-
47	KC1	18	210	31	-	8/15/71/71	-
37	CLA	D	401	52	1/1/15/20	6/37/115/115	-
46	HEM	v	201	16	-	4/12/54/54	-
48	A86	18	213	-	-	9/34/90/90	0/3/3/3
37	CLA	19	302	-	1/1/15/20	9/37/115/115	-
37	CLA	19	301	32	1/1/15/20	8/37/115/115	-
37	CLA	b	515	-	1/1/15/20	3/37/115/115	-
40	SQD	L	101	-	-	26/49/69/69	0/1/1/1
37	CLA	12	209	25	1/1/12/20	11/22/100/115	-
37	CLA	C	511	3	1/1/15/20	6/37/115/115	-
37	CLA	19	309	32	1/1/11/20	3/13/91/115	-
37	CLA	21	205	34	1/1/11/20	7/13/91/115	-
47	KC1	13	309	26	-	4/15/71/71	-
48	A86	16	313	-	-	13/34/90/90	0/3/3/3
48	A86	32	214	-	-	5/34/90/90	0/3/3/3
48	A86	32	216	-	-	13/34/90/90	0/3/3/3
40	SQD	17	301	-	-	24/44/64/69	0/1/1/1
39	BCR	b	517	-	-	6/29/63/63	0/2/2/2
48	A86	35	314	-	-	14/34/90/90	0/3/3/3
37	CLA	z	101	52	1/1/15/20	18/37/115/115	-
44	DGD	j	101	-	-	16/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	16	309	-	1/1/11/20	6/13/91/115	-
41	LMG	C	518	-	-	25/46/66/70	0/1/1/1
37	CLA	13	307	26	1/1/12/20	10/22/100/115	-
37	CLA	Z	101	52	1/1/15/20	18/37/115/115	-
37	CLA	c	501	-	1/1/15/20	10/37/115/115	-
37	CLA	12	212	-	1/1/11/20	7/13/91/115	-
41	LMG	c	518	-	-	25/46/66/70	0/1/1/1
39	BCR	b	518	-	-	6/29/63/63	0/2/2/2
37	CLA	c	511	3	1/1/15/20	6/37/115/115	-
48	A86	35	313	-	-	9/34/90/90	0/3/3/3
47	KC1	38	205	31	-	6/15/71/71	-
48	A86	32	215	-	-	3/34/90/90	0/3/3/3
47	KC1	20	302	-	-	7/15/71/71	-
37	CLA	B	510	52	1/1/15/20	7/37/115/115	-
50	DD6	16	312	-	-	12/26/80/80	0/3/3/3
37	CLA	C	510	-	1/1/15/20	12/37/115/115	-
37	CLA	39	305	32	1/1/12/20	5/21/99/115	-
37	CLA	20	301	33	-	11/27/105/115	-
41	LMG	b	520	-	-	24/46/66/70	0/1/1/1
47	KC1	15	306	28	-	6/15/71/71	-
48	A86	31	311	-	-	6/34/90/90	0/3/3/3
48	A86	39	313	-	-	7/34/90/90	0/3/3/3
48	A86	37	310	-	-	8/34/90/90	0/3/3/3
39	BCR	K	101	-	-	15/29/63/63	0/2/2/2
50	DD6	39	312	-	-	12/26/80/80	0/3/3/3
43	LHG	d	407	-	-	27/53/53/53	-
37	CLA	11	305	52	1/1/11/20	1/13/91/115	-
48	A86	37	314	-	-	12/34/90/90	0/3/3/3
37	CLA	34	310	-	1/1/11/20	2/13/91/115	-
37	CLA	c	513	-	1/1/15/20	7/37/115/115	-
37	CLA	34	308	52	1/1/15/20	10/37/115/115	-
37	CLA	16	307	52	1/1/14/20	12/33/111/115	-
37	CLA	C	509	-	1/1/15/20	7/37/115/115	-
37	CLA	37	303	-	1/1/13/20	6/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	12	214	-	-	3/34/90/90	0/3/3/3
47	KC1	37	304	30	-	6/15/71/71	-
39	BCR	D	407	-	-	12/29/63/63	0/2/2/2
40	SQD	a	409	-	-	17/49/69/69	0/1/1/1
41	LMG	17	317	-	-	15/32/52/70	0/1/1/1
39	BCR	h	101	-	-	6/29/63/63	0/2/2/2
41	LMG	31	317	-	-	13/27/47/70	0/1/1/1
44	DGD	c	517	-	-	19/51/91/95	0/2/2/2
48	A86	37	311	-	-	7/34/90/90	0/3/3/3
47	KC1	19	308	-	-	4/15/71/71	-
47	KC1	33	302	-	-	5/15/71/71	-
37	CLA	33	305	-	1/1/11/20	2/13/91/115	-
43	LHG	21	201	-	-	19/38/38/53	-
37	CLA	41	204	-	-	10/29/107/115	-
47	KC1	36	304	29	-	6/15/71/71	-
37	CLA	c	509	-	1/1/15/20	7/37/115/115	-
39	BCR	b	524	-	-	17/29/63/63	0/2/2/2
43	LHG	d	408	-	-	26/53/53/53	-
48	A86	34	314	-	-	13/34/90/90	0/3/3/3
37	CLA	C	505	-	1/1/15/20	10/37/115/115	-
48	A86	38	215	-	-	13/34/90/90	0/3/3/3
37	CLA	38	204	-	1/1/13/20	6/27/105/115	-
37	CLA	21	206	34	1/1/15/20	13/37/115/115	-
43	LHG	a	412	-	-	26/50/50/53	-
37	CLA	18	202	31	-	13/37/115/115	-
47	KC1	16	305	29	-	6/15/71/71	-
44	DGD	C	516	-	-	17/51/91/95	0/2/2/2
47	KC1	18	207	31	-	6/15/71/71	-
48	A86	34	311	-	-	7/34/90/90	0/3/3/3
37	CLA	B	504	-	1/1/15/20	3/37/115/115	-
41	LMG	a	410	-	-	32/46/66/70	0/1/1/1
50	DD6	20	310	-	-	14/26/80/80	0/3/3/3
37	CLA	19	303	52	1/1/15/20	12/37/115/115	-
48	A86	16	310	-	-	5/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	33	310	-	-	0/13/91/115	-
37	CLA	19	306	32	1/1/15/20	6/37/115/115	-
37	CLA	d	404	-	1/1/15/20	17/37/115/115	-
39	BCR	a	413	-	-	7/29/63/63	0/2/2/2
37	CLA	34	302	-	1/1/15/20	16/37/115/115	-
47	KC1	32	207	25	-	6/15/71/71	-
37	CLA	39	301	32	1/1/15/20	8/37/115/115	-
37	CLA	16	303	-	1/1/13/20	8/28/106/115	-
40	SQD	B	519	-	-	26/49/69/69	0/1/1/1
47	KC1	41	203	-	-	4/15/71/71	-
48	A86	13	314	-	-	9/34/90/90	0/3/3/3
48	A86	18	212	-	-	8/34/90/90	0/3/3/3
37	CLA	41	210	-	-	4/13/91/115	-
48	A86	14	313	-	-	12/34/90/90	0/3/3/3
48	A86	15	313	-	-	9/34/90/90	0/3/3/3
43	LHG	B	523	-	-	18/53/53/53	-
37	CLA	z	102	33	1/1/11/20	5/13/91/115	-
37	CLA	11	308	52	1/1/15/20	13/37/115/115	-
37	CLA	19	307	43	1/1/15/20	8/37/115/115	-
37	CLA	32	204	25	1/1/15/20	12/37/115/115	-
37	CLA	21	202	34	1/1/13/20	7/28/106/115	-
48	A86	11	314	-	-	9/34/90/90	0/3/3/3
37	CLA	15	308	52	1/1/15/20	8/37/115/115	-
37	CLA	21	204	-	-	10/29/107/115	-
37	CLA	33	308	52	-	8/37/115/115	-
47	KC1	16	304	29	-	6/15/71/71	-
39	BCR	B	517	-	-	6/29/63/63	0/2/2/2
37	CLA	13	303	-	1/1/13/20	9/28/106/115	-
37	CLA	18	201	52	1/1/15/20	7/37/115/115	-
37	CLA	C	506	-	1/1/15/20	13/37/115/115	-
41	LMG	d	409	-	-	13/46/66/70	0/1/1/1
48	A86	33	312	-	-	8/34/90/90	0/3/3/3
47	KC1	14	304	27	-	6/15/71/71	-
37	CLA	13	310	-	-	0/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	15	310	-	1/1/11/20	2/13/91/115	-
48	A86	37	309	-	-	8/34/90/90	0/3/3/3
41	LMG	32	201	-	-	14/34/54/70	0/1/1/1
40	SQD	b	521	-	-	11/32/52/69	0/1/1/1
41	LMG	D	412	-	-	13/46/66/70	0/1/1/1
37	CLA	17	304	-	1/1/13/20	6/27/105/115	-
48	A86	11	315	-	-	6/34/90/90	0/3/3/3
40	SQD	B	522	-	-	11/32/52/69	0/1/1/1
47	KC1	37	305	30	-	9/15/71/71	-
48	A86	13	315	-	-	11/34/90/90	0/3/3/3
47	KC1	12	208	25	-	4/15/71/71	-
48	A86	11	313	-	-	6/34/90/90	1/3/3/3
48	A86	16	314	-	-	8/34/90/90	0/3/3/3
44	DGD	J	101	-	-	16/51/91/95	0/2/2/2
48	A86	35	319	-	-	8/34/90/90	0/3/3/3
44	DGD	H	102	-	-	16/51/91/95	0/2/2/2
48	A86	15	315	-	-	8/34/90/90	0/3/3/3
38	PHO	a	406	-	-	6/37/103/103	0/5/6/6
37	CLA	Z	102	33	1/1/11/20	5/13/91/115	-
47	KC1	32	209	25	-	4/15/71/71	-
48	A86	37	313	-	-	9/34/90/90	0/3/3/3
37	CLA	15	301	28	-	8/37/115/115	-
50	DD6	41	212	-	-	12/26/80/80	0/3/3/3
44	DGD	h	102	-	-	16/51/91/95	0/2/2/2
37	CLA	b	514	-	1/1/14/20	11/34/112/115	-
37	CLA	38	211	-	-	2/13/91/115	-
47	KC1	35	304	28	-	6/15/71/71	-
48	A86	40	201	-	-	13/34/90/90	0/3/3/3
48	A86	15	312	-	-	8/34/90/90	0/3/3/3
43	LHG	37	321	-	-	27/49/49/53	-
48	A86	39	311	-	-	6/34/90/90	0/3/3/3
47	KC1	40	207	33	-	12/15/71/71	-
37	CLA	31	304	-	1/1/15/20	8/37/115/115	-
37	CLA	B	514	-	1/1/14/20	11/34/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	40	203	33	-	11/27/105/115	-
37	CLA	17	302	30	-	10/37/115/115	-
37	CLA	b	506	-	1/1/15/20	7/37/115/115	-
48	A86	34	313	-	-	12/34/90/90	0/3/3/3
47	KC1	36	302	-	-	2/15/71/71	-
37	CLA	b	510	52	1/1/15/20	7/37/115/115	-
37	CLA	15	307	28	1/1/12/20	10/22/100/115	-
48	A86	17	311	-	-	8/34/90/90	0/3/3/3
39	BCR	y	101	-	-	15/29/63/63	0/2/2/2
37	CLA	38	206	-	-	4/13/91/115	-
37	CLA	41	208	-	1/1/15/20	11/37/115/115	-
37	CLA	18	211	-	-	2/13/91/115	-
43	LHG	D	409	-	-	27/53/53/53	-
37	CLA	35	303	-	-	8/28/106/115	-
48	A86	14	312	-	-	4/34/90/90	0/3/3/3
37	CLA	C	507	52	1/1/15/20	8/37/115/115	-
37	CLA	C	501	-	1/1/15/20	10/37/115/115	-
37	CLA	B	502	-	1/1/15/20	9/37/115/115	-
48	A86	38	213	-	-	9/34/90/90	0/3/3/3
47	KC1	11	309	24	-	8/15/71/71	-
48	A86	11	312	-	-	6/34/90/90	0/3/3/3
37	CLA	32	211	52	-	8/37/115/115	-
37	CLA	12	203	25	1/1/15/20	12/37/115/115	-
47	KC1	14	309	27	-	6/15/71/71	-
47	KC1	15	309	28	-	8/15/71/71	-
50	DD6	40	212	-	-	14/26/80/80	0/3/3/3
37	CLA	B	511	-	1/1/15/20	11/37/115/115	-
48	A86	17	313	-	-	8/34/90/90	0/3/3/3
37	CLA	14	307	27	1/1/12/20	13/22/100/115	-
48	A86	38	212	-	-	8/34/90/90	0/3/3/3
48	A86	11	311	-	-	6/34/90/90	0/3/3/3
37	CLA	31	302	24	-	10/37/115/115	-
37	CLA	19	310	32	1/1/15/20	7/37/115/115	-
47	KC1	11	306	24	-	8/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	B	506	-	1/1/15/20	7/37/115/115	-
37	CLA	15	303	-	-	7/28/106/115	-
47	KC1	13	306	26	-	6/15/71/71	-
41	LMG	16	316	-	-	14/31/51/70	0/1/1/1
37	CLA	B	513	-	1/1/15/20	8/37/115/115	-
48	A86	41	213	-	-	8/34/90/90	0/3/3/3
48	A86	12	215	-	-	13/34/90/90	0/3/3/3
39	BCR	A	406	-	-	8/29/63/63	0/2/2/2
37	CLA	C	504	52	1/1/15/20	7/37/115/115	-
41	LMG	A	408	-	-	32/46/66/70	0/1/1/1
37	CLA	32	208	52	1/1/12/20	0/19/97/115	-
37	CLA	B	503	-	1/1/15/20	9/37/115/115	-
48	A86	37	319	-	-	8/34/90/90	0/3/3/3
37	CLA	33	303	-	1/1/13/20	10/28/106/115	-
37	CLA	12	207	52	1/1/12/20	0/19/97/115	-
48	A86	17	314	-	-	8/34/90/90	0/3/3/3
48	A86	35	311	-	-	6/34/90/90	0/3/3/3
37	CLA	35	308	52	-	8/37/115/115	-
37	CLA	41	205	34	1/1/11/20	7/13/91/115	-
47	KC1	18	205	31	-	6/15/71/71	-
38	PHO	A	404	-	-	6/37/103/103	0/5/6/6
48	A86	14	316	-	-	13/34/90/90	0/3/3/3
48	A86	31	314	-	-	9/34/90/90	0/3/3/3
37	CLA	36	309	-	1/1/11/20	6/13/91/115	-
48	A86	35	316	-	-	14/34/90/90	0/3/3/3
37	CLA	39	306	32	-	6/37/115/115	-
48	A86	35	315	-	-	8/34/90/90	0/3/3/3
37	CLA	20	307	33	1/1/11/20	6/13/91/115	-
45	PL9	d	402	-	-	17/53/73/73	0/1/1/1
37	CLA	14	305	-	1/1/11/20	2/13/91/115	-
47	KC1	35	306	28	-	6/15/71/71	-
37	CLA	40	208	33	1/1/12/20	3/19/97/115	-
50	DD6	21	212	-	-	12/26/80/80	0/3/3/3
37	CLA	d	401	52	-	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	41	211	-	-	9/34/90/90	0/3/3/3
37	CLA	B	512	-	1/1/15/20	8/37/115/115	-
47	KC1	33	309	26	-	4/15/71/71	-
47	KC1	15	304	28	-	6/15/71/71	-
37	CLA	B	516	-	1/1/15/20	13/37/115/115	-
37	CLA	14	302	-	1/1/15/20	16/37/115/115	-
48	A86	32	221	-	-	9/34/90/90	0/3/3/3
48	A86	11	319	-	-	7/34/90/90	0/3/3/3
37	CLA	W	102	-	1/1/15/20	19/37/115/115	-
37	CLA	B	507	52	1/1/15/20	9/37/115/115	-
37	CLA	39	303	52	1/1/15/20	12/37/115/115	-
48	A86	19	311	-	-	6/34/90/90	0/3/3/3
37	CLA	32	213	-	1/1/11/20	7/13/91/115	-
37	CLA	36	307	52	1/1/14/20	12/33/111/115	-
40	SQD	A	407	-	-	17/49/69/69	0/1/1/1
45	PL9	D	404	-	-	17/53/73/73	0/1/1/1
37	CLA	20	308	-	1/1/11/20	2/16/94/115	-
37	CLA	32	210	25	1/1/12/20	11/22/100/115	-
48	A86	12	216	-	-	9/34/90/90	0/3/3/3
37	CLA	38	202	31	-	13/37/115/115	-
48	A86	31	315	-	-	6/34/90/90	0/3/3/3
37	CLA	32	205	-	1/1/15/20	9/37/115/115	-
37	CLA	33	301	26	-	12/37/115/115	-
48	A86	32	218	-	-	13/34/90/90	0/3/3/3
37	CLA	13	308	52	-	8/37/115/115	-
47	KC1	31	305	24	-	4/15/71/71	-
37	CLA	41	206	34	1/1/15/20	13/37/115/115	-
47	KC1	31	307	24	-	8/15/71/71	-
50	DD6	40	214	-	-	12/26/80/80	0/3/3/3
37	CLA	35	307	28	1/1/12/20	10/22/100/115	-
37	CLA	40	205	-	1/1/13/20	8/27/105/115	-
48	A86	14	311	-	-	7/34/90/90	0/3/3/3
37	CLA	32	206	-	1/1/15/20	9/37/115/115	-
48	A86	14	314	-	-	13/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	c	508	-	1/1/15/20	8/37/115/115	-
48	A86	34	315	-	-	6/34/90/90	0/3/3/3
43	LHG	37	315	-	-	26/48/48/53	-
38	PHO	a	405	-	-	9/37/103/103	0/5/6/6
37	CLA	11	301	24	-	10/37/115/115	-
48	A86	21	211	-	-	9/34/90/90	0/3/3/3
47	KC1	21	207	34	-	7/15/71/71	-
37	CLA	38	209	52	1/1/15/20	7/37/115/115	-
37	CLA	21	209	34	1/1/11/20	6/13/91/115	-
43	LHG	21	217	-	-	27/49/49/53	-
37	CLA	C	513	-	1/1/15/20	7/37/115/115	-
37	CLA	C	503	-	1/1/15/20	19/37/115/115	-
48	A86	37	312	-	-	7/34/90/90	0/3/3/3
37	CLA	20	303	-	1/1/13/20	8/27/105/115	-
37	CLA	18	206	-	1/1/11/20	3/13/91/115	-
37	CLA	14	303	-	-	4/28/106/115	-
37	CLA	39	310	32	1/1/15/20	7/37/115/115	-
38	PHO	D	403	-	-	9/37/103/103	0/5/6/6
47	KC1	17	305	30	-	6/15/71/71	-
47	KC1	20	305	33	-	12/15/71/71	-
47	KC1	13	302	-	-	5/15/71/71	-
37	CLA	13	305	-	1/1/11/20	2/13/91/115	-
48	A86	12	202	-	-	14/34/90/90	0/3/3/3
39	BCR	C	515	-	-	7/29/63/63	0/2/2/2
37	CLA	31	308	24	-	6/22/100/115	-
48	A86	36	313	-	-	8/34/90/90	0/3/3/3
41	LMG	36	314	-	-	14/31/51/70	0/1/1/1
37	CLA	c	503	-	1/1/15/20	19/37/115/115	-
37	CLA	41	209	34	1/1/11/20	6/13/91/115	-
48	A86	14	315	-	-	6/34/90/90	0/3/3/3
48	A86	33	311	-	-	5/34/90/90	0/3/3/3
37	CLA	17	309	52	1/1/15/20	11/37/115/115	-
37	CLA	b	523	-	1/1/15/20	11/37/115/115	-
48	A86	36	311	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	38	214	-	-	12/34/90/90	0/3/3/3
48	A86	15	311	-	-	6/34/90/90	0/3/3/3
37	CLA	c	507	52	1/1/15/20	8/37/115/115	-
48	A86	33	314	-	-	9/34/90/90	0/3/3/3
37	CLA	c	506	-	1/1/15/20	13/37/115/115	-
48	A86	34	312	-	-	4/34/90/90	0/3/3/3
51	LMU	19	315	-	-	6/21/61/61	0/2/2/2
47	KC1	12	206	25	-	6/15/71/71	-
39	BCR	C	514	-	-	6/29/63/63	0/2/2/2
39	BCR	0	101	-	-	8/29/63/63	0/2/2/2
48	A86	33	313	-	-	18/34/90/90	0/3/3/3
37	CLA	11	310	52	1/1/12/20	6/21/99/115	-
45	PL9	d	406	-	-	9/53/73/73	0/1/1/1
37	CLA	c	512	-	1/1/15/20	6/37/115/115	-
37	CLA	B	509	-	1/1/15/20	9/37/115/115	-
37	CLA	18	203	-	1/1/15/20	6/37/115/115	-
37	CLA	14	301	27	-	12/37/115/115	-
48	A86	17	310	-	-	8/34/90/90	0/3/3/3
47	KC1	37	307	30	-	4/15/71/71	-
37	CLA	C	508	-	1/1/15/20	8/37/115/115	-
37	CLA	18	209	52	1/1/15/20	8/37/115/115	-
39	BCR	c	514	-	-	6/29/63/63	0/2/2/2
47	KC1	20	304	33	-	6/15/71/71	-
47	KC1	11	302	-	-	2/15/71/71	-
37	CLA	b	503	-	1/1/15/20	9/37/115/115	-
37	CLA	14	310	-	1/1/11/20	2/13/91/115	-
48	A86	40	213	-	-	16/34/90/90	0/3/3/3
41	LMG	12	201	-	-	14/34/54/70	0/1/1/1
43	LHG	19	314	37	-	28/53/53/53	-
37	CLA	36	301	29	-	9/37/115/115	-
48	A86	41	214	-	-	5/34/90/90	0/3/3/3
40	SQD	36	315	-	-	24/44/64/69	0/1/1/1
37	CLA	37	306	30	1/1/12/20	9/22/100/115	-
43	LHG	D	410	-	-	26/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	31	319	-	-	7/34/90/90	0/3/3/3
37	CLA	b	504	-	1/1/15/20	3/37/115/115	-
37	CLA	18	208	31	1/1/12/20	11/23/101/115	-
41	LMG	37	316	-	-	15/32/52/70	0/1/1/1
47	KC1	33	304	26	-	7/15/71/71	-
39	BCR	H	101	-	-	6/29/63/63	0/2/2/2
41	LMG	11	316	-	-	19/37/57/70	0/1/1/1
37	CLA	40	209	33	1/1/11/20	6/13/91/115	-
37	CLA	12	210	52	-	8/37/115/115	-
47	KC1	17	308	30	-	4/15/71/71	-
43	LHG	39	314	37	-	28/53/53/53	-
47	KC1	16	308	29	-	4/15/71/71	-
47	KC1	16	302	-	-	2/15/71/71	-
48	A86	13	312	-	-	8/34/90/90	0/3/3/3
37	CLA	B	501	52	1/1/15/20	16/37/115/115	-
37	CLA	w	101	-	1/1/15/20	15/37/115/115	-
37	CLA	13	301	26	-	12/37/115/115	-
37	CLA	21	210	-	-	4/13/91/115	-
37	CLA	B	524	-	1/1/15/20	11/37/115/115	-
47	KC1	34	306	27	-	6/15/71/71	-
48	A86	20	311	-	-	16/34/90/90	0/3/3/3
50	DD6	21	216	-	-	15/26/80/80	0/3/3/3
39	BCR	B	518	-	-	6/29/63/63	0/2/2/2
37	CLA	b	507	52	1/1/15/20	9/37/115/115	-
37	CLA	b	508	-	-	5/37/115/115	-
37	CLA	15	305	-	1/1/11/20	3/13/91/115	-
37	CLA	34	305	-	1/1/11/20	2/13/91/115	-
37	CLA	a	403	-	1/1/15/20	4/37/115/115	-
37	CLA	12	204	-	1/1/15/20	9/37/115/115	-
48	A86	12	217	-	-	13/34/90/90	0/3/3/3
37	CLA	39	309	32	1/1/11/20	3/13/91/115	-
47	KC1	40	206	33	-	6/15/71/71	-
37	CLA	C	512	-	1/1/15/20	6/37/115/115	-
37	CLA	D	406	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	16	301	29	-	9/37/115/115	-
37	CLA	19	304	32	1/1/11/20	4/13/91/115	-
37	CLA	c	502	-	1/1/15/20	7/37/115/115	-
37	CLA	a	407	-	-	6/37/115/115	-
37	CLA	d	403	-	1/1/15/20	6/37/115/115	-
43	LHG	17	316	-	-	26/48/48/53	-
37	CLA	16	306	29	1/1/15/20	11/37/115/115	-
47	KC1	35	302	-	-	6/15/71/71	-
48	A86	21	215	-	-	6/34/90/90	0/3/3/3
48	A86	17	315	-	-	12/34/90/90	0/3/3/3
48	A86	15	319	-	-	8/34/90/90	0/3/3/3
44	DGD	C	517	-	-	19/51/91/95	0/2/2/2
37	CLA	11	303	-	1/1/15/20	8/37/115/115	-
43	LHG	41	201	-	-	19/38/38/53	-
47	KC1	36	305	29	-	6/15/71/71	-
41	LMG	b	519	-	-	15/46/66/70	0/1/1/1
48	A86	31	313	-	-	6/34/90/90	1/3/3/3
39	BCR	a	408	-	-	8/29/63/63	0/2/2/2
37	CLA	31	301	-	1/1/15/20	19/37/115/115	-
47	KC1	11	304	24	-	4/15/71/71	-
37	CLA	b	502	-	1/1/15/20	9/37/115/115	-
37	CLA	37	308	52	1/1/15/20	11/37/115/115	-
37	CLA	11	307	24	-	6/22/100/115	-
47	KC1	37	302	-	-	6/15/71/71	-
50	DD6	41	216	-	-	15/26/80/80	0/3/3/3
37	CLA	b	501	52	1/1/15/20	15/37/115/115	-
37	CLA	c	505	-	1/1/15/20	10/37/115/115	-
37	CLA	39	307	43	1/1/15/20	8/37/115/115	-
41	LMG	11	317	-	-	13/27/47/70	0/1/1/1
39	BCR	c	515	-	-	7/29/63/63	0/2/2/2
37	CLA	35	301	28	-	8/37/115/115	-
37	CLA	36	303	-	1/1/13/20	8/28/106/115	-
47	KC1	31	309	24	-	8/15/71/71	-
48	A86	21	213	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	c	504	52	1/1/15/20	7/37/115/115	-
37	CLA	17	307	30	1/1/12/20	9/22/100/115	-
37	CLA	36	306	29	1/1/15/20	11/37/115/115	-
37	CLA	D	402	52	-	12/37/115/115	-
48	A86	32	217	-	-	9/34/90/90	0/3/3/3
37	CLA	b	512	-	1/1/15/20	8/37/115/115	-
37	CLA	14	308	52	1/1/15/20	10/37/115/115	-
37	CLA	B	505	-	1/1/15/20	6/37/115/115	-
48	A86	16	311	-	-	8/34/90/90	0/3/3/3
37	CLA	b	511	-	1/1/15/20	11/37/115/115	-
37	CLA	c	510	-	1/1/15/20	12/37/115/115	-
47	KC1	17	306	30	-	8/15/71/71	-
37	CLA	B	508	-	-	5/37/115/115	-
37	CLA	37	301	30	-	10/37/115/115	-
47	KC1	39	308	-	-	4/15/71/71	-
37	CLA	B	515	-	1/1/15/20	3/37/115/115	-
37	CLA	b	505	-	1/1/15/20	6/37/115/115	-
48	A86	19	313	-	-	8/34/90/90	0/3/3/3
37	CLA	D	405	-	1/1/15/20	6/37/115/115	-
37	CLA	34	307	27	1/1/12/20	13/22/100/115	-
48	A86	40	211	-	-	5/34/90/90	0/3/3/3
50	DD6	36	312	-	-	12/26/80/80	0/3/3/3
43	LHG	D	411	-	-	26/50/50/53	-

The worst 5 of 8062 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	40	213	A86	C14-C13	16.10	1.69	1.51
48	39	313	A86	C14-C13	16.10	1.69	1.51
48	20	311	A86	C14-C13	16.10	1.69	1.51
48	35	319	A86	C14-C13	15.94	1.69	1.51
48	15	319	A86	C14-C13	15.94	1.69	1.51

The worst 5 of 11064 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	17	314	A86	O1-C20-C19	46.24	156.82	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	37	313	A86	O1-C20-C19	46.19	156.78	113.49
48	39	313	A86	O1-C20-C19	46.06	156.66	113.49
48	40	213	A86	O1-C20-C19	45.80	156.42	113.49
48	20	311	A86	O1-C20-C19	45.78	156.40	113.49

5 of 177 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
37	A	403	CLA	ND
37	B	501	CLA	ND
37	B	502	CLA	ND
37	B	503	CLA	ND
37	B	504	CLA	ND

5 of 4780 torsion outliers are listed below:

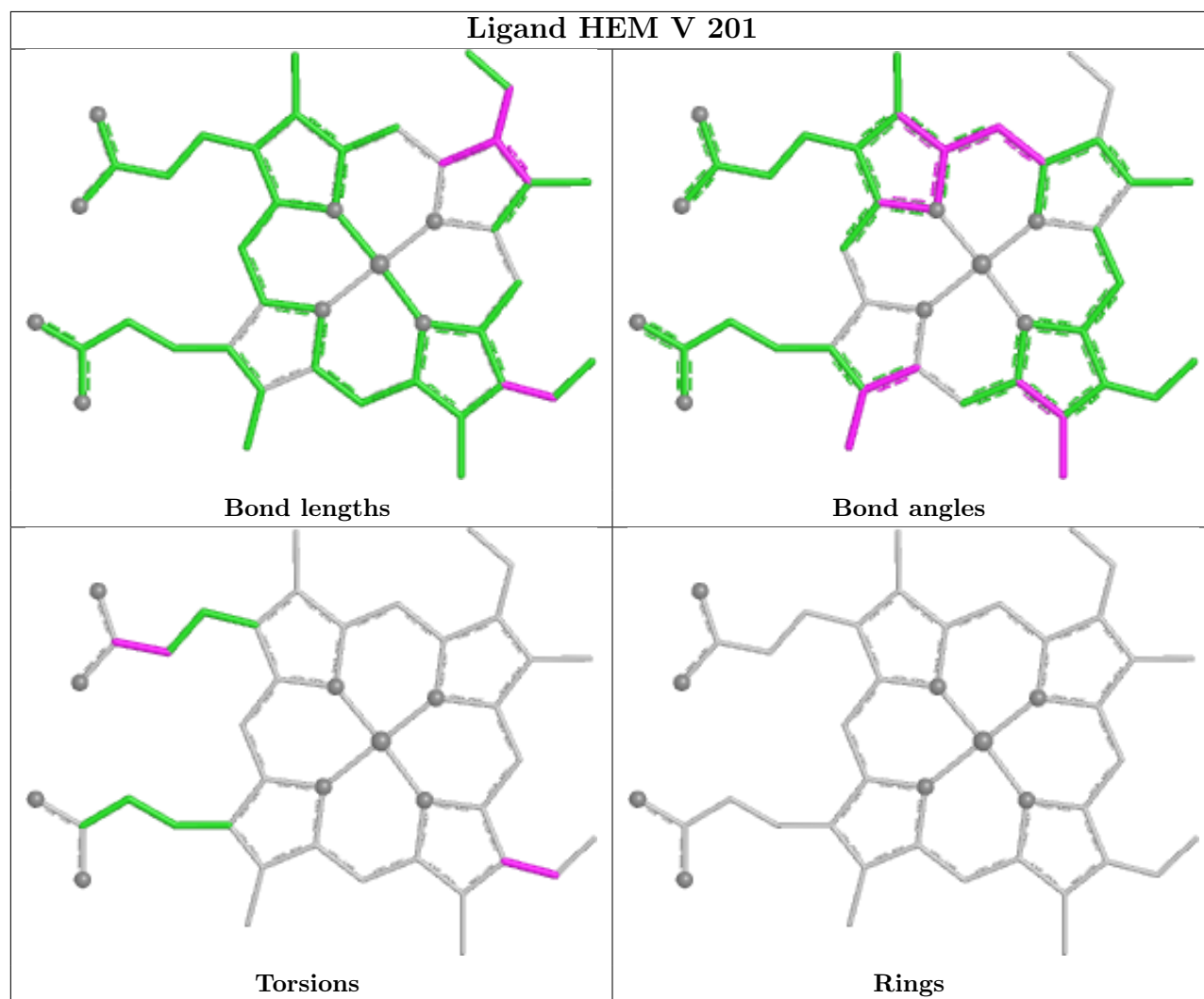
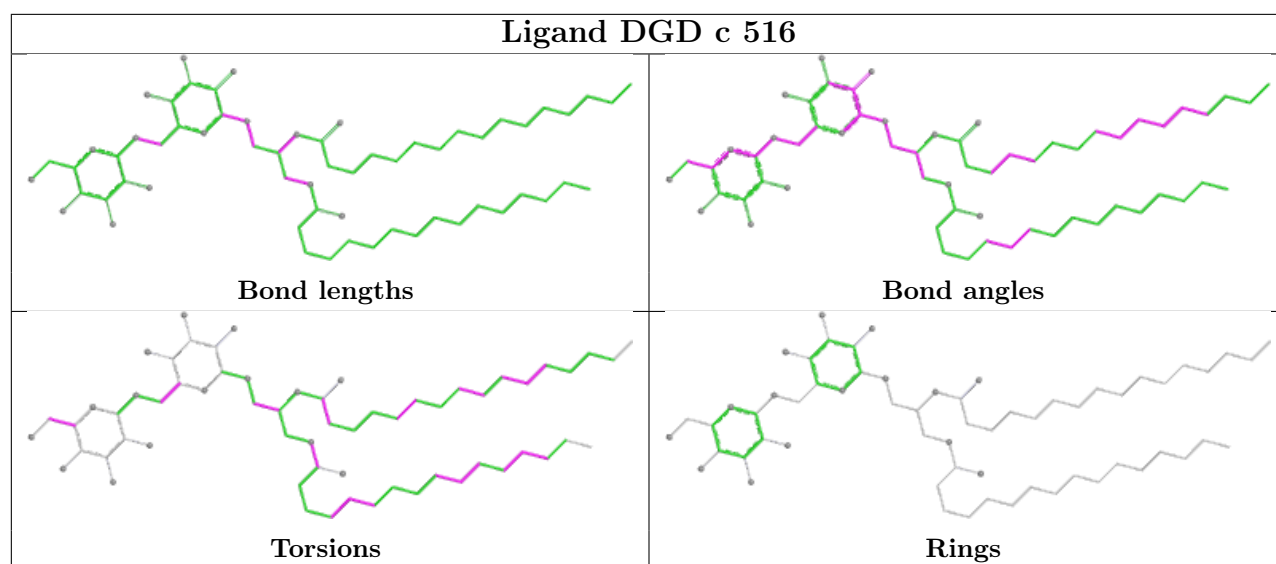
Mol	Chain	Res	Type	Atoms
37	B	514	CLA	CAD-CBD-CGD-O1D
37	B	514	CLA	CAD-CBD-CGD-O2D
37	B	516	CLA	CHA-CBD-CGD-O1D
37	B	516	CLA	CHA-CBD-CGD-O2D
37	C	501	CLA	C1A-C2A-CAA-CBA

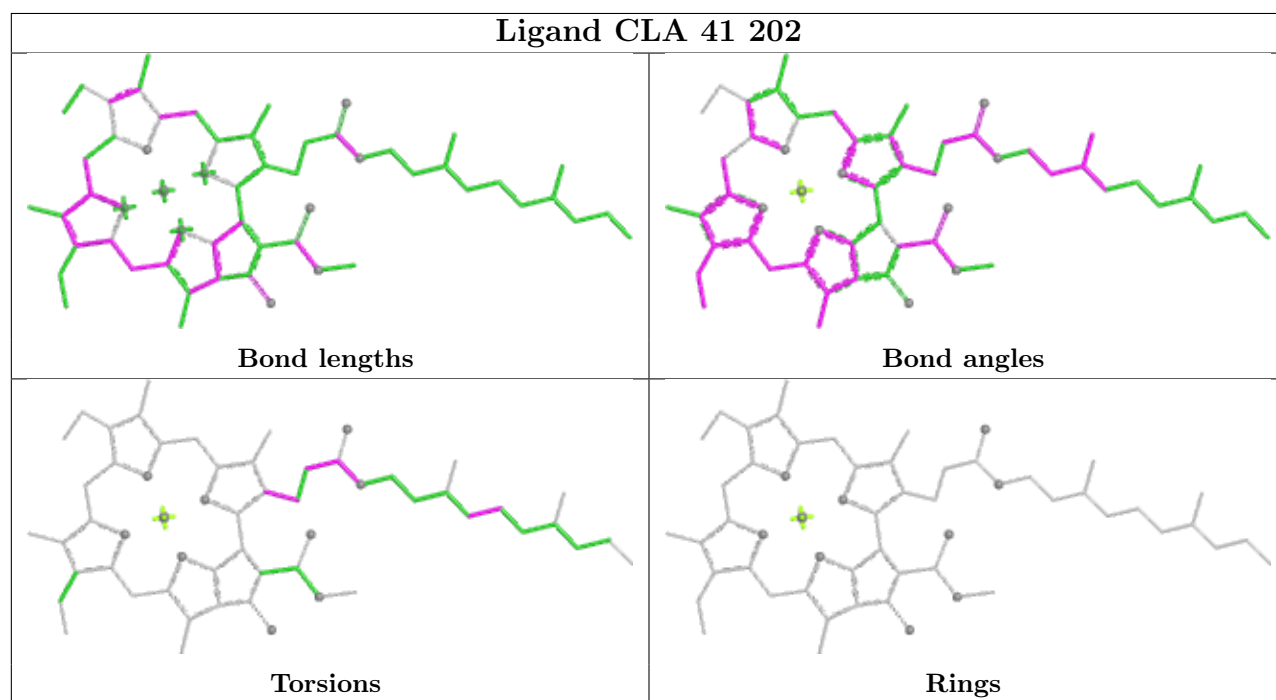
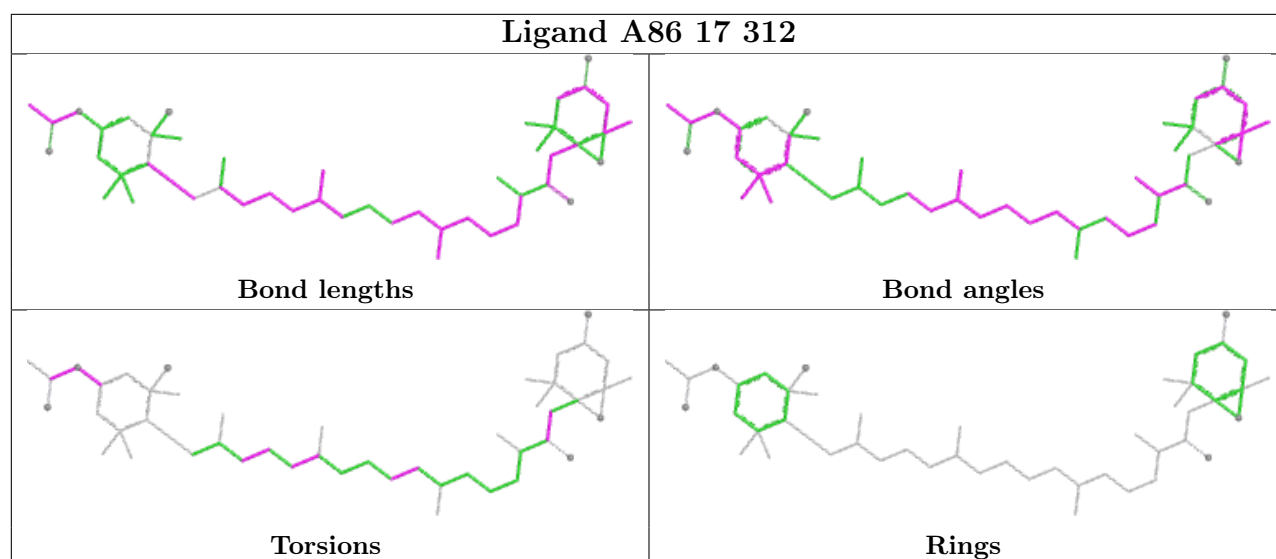
All (2) ring outliers are listed below:

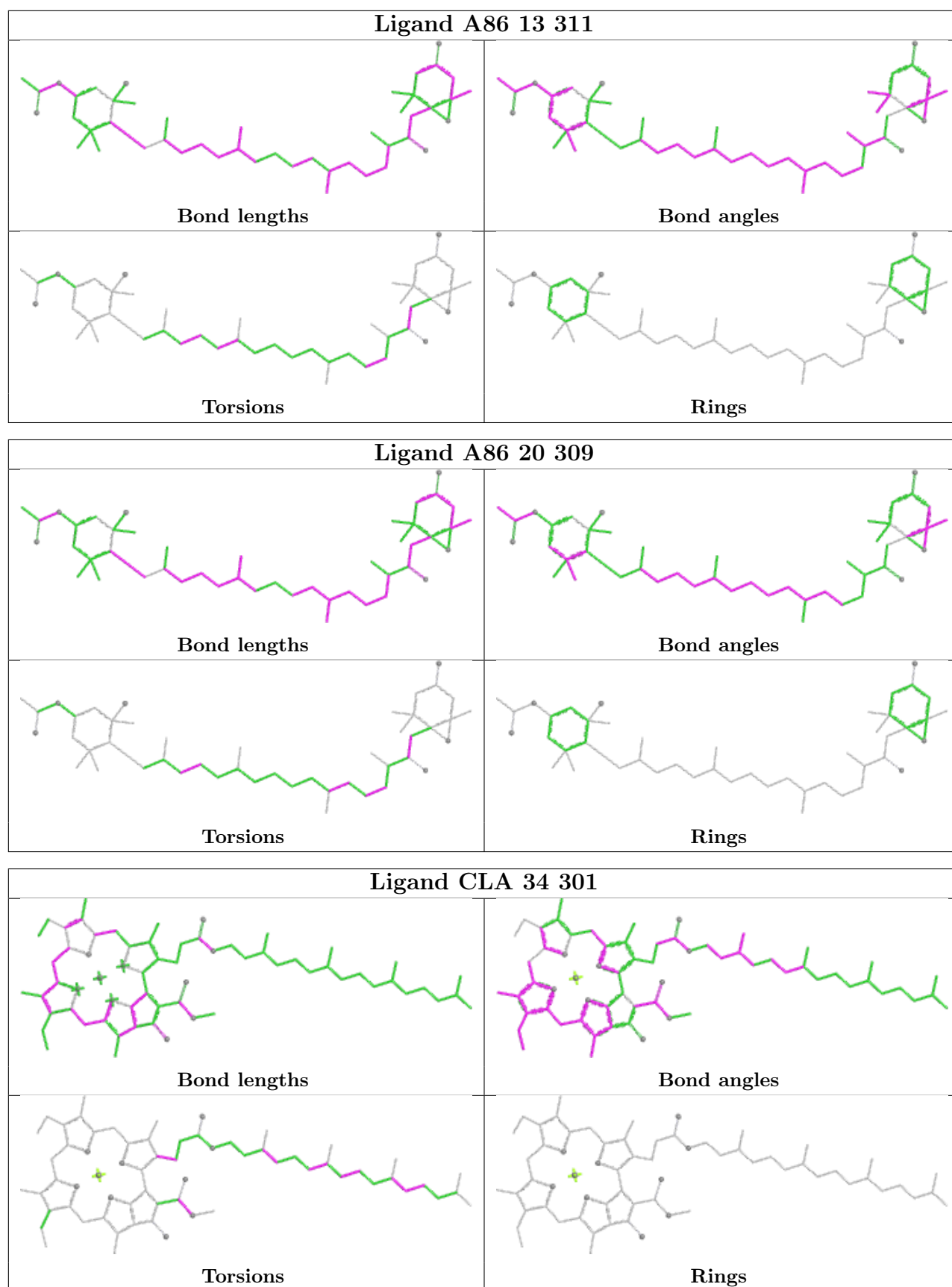
Mol	Chain	Res	Type	Atoms
48	31	313	A86	C31-C32-C33-C34-C35-C36
48	11	313	A86	C31-C32-C33-C34-C35-C36

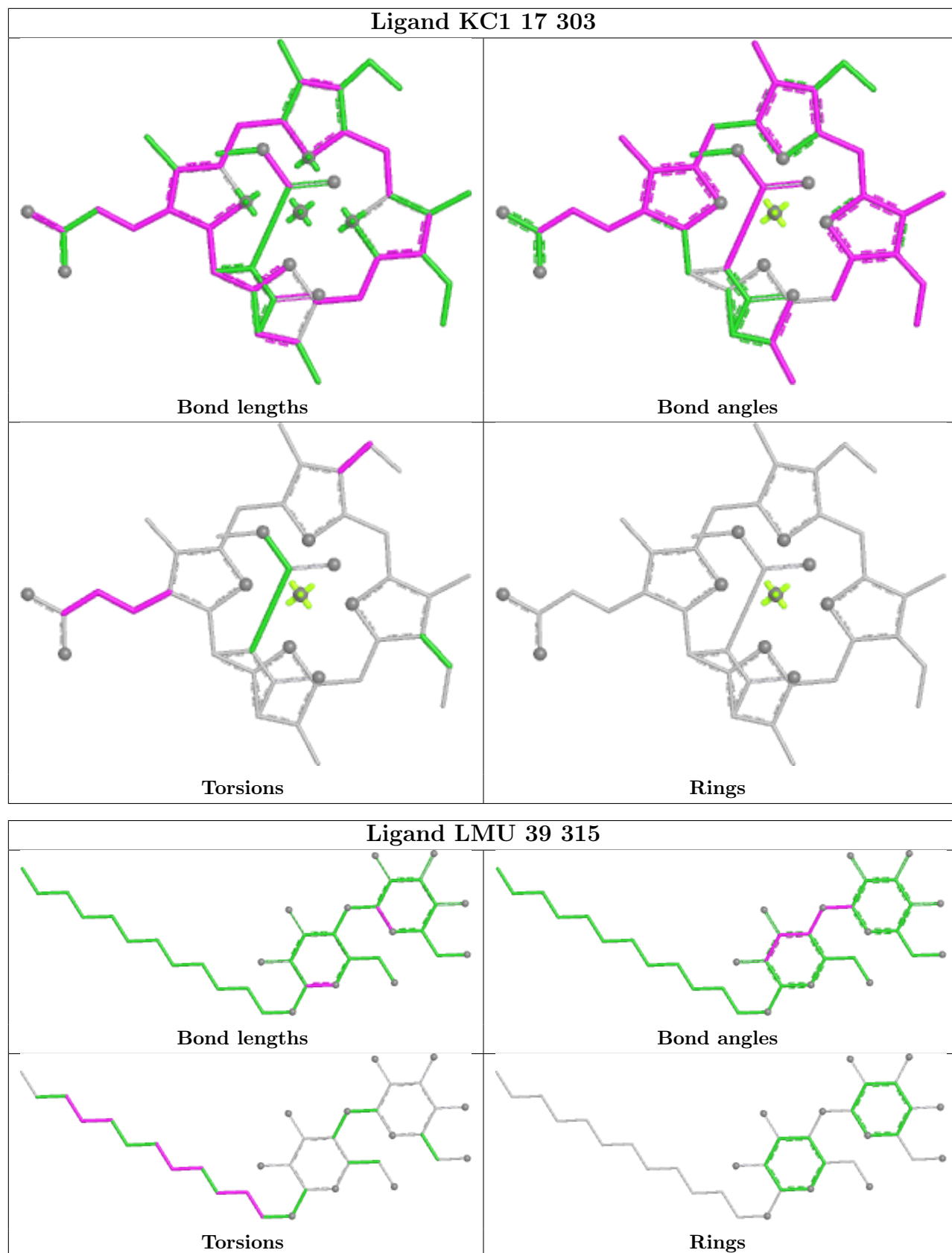
No monomer is involved in short contacts.

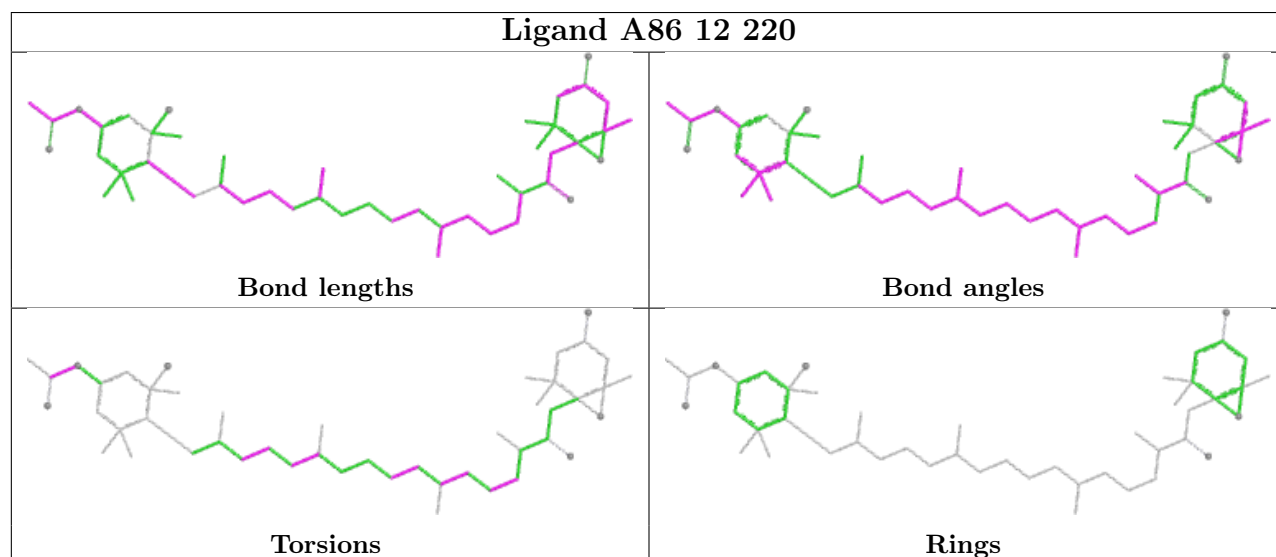
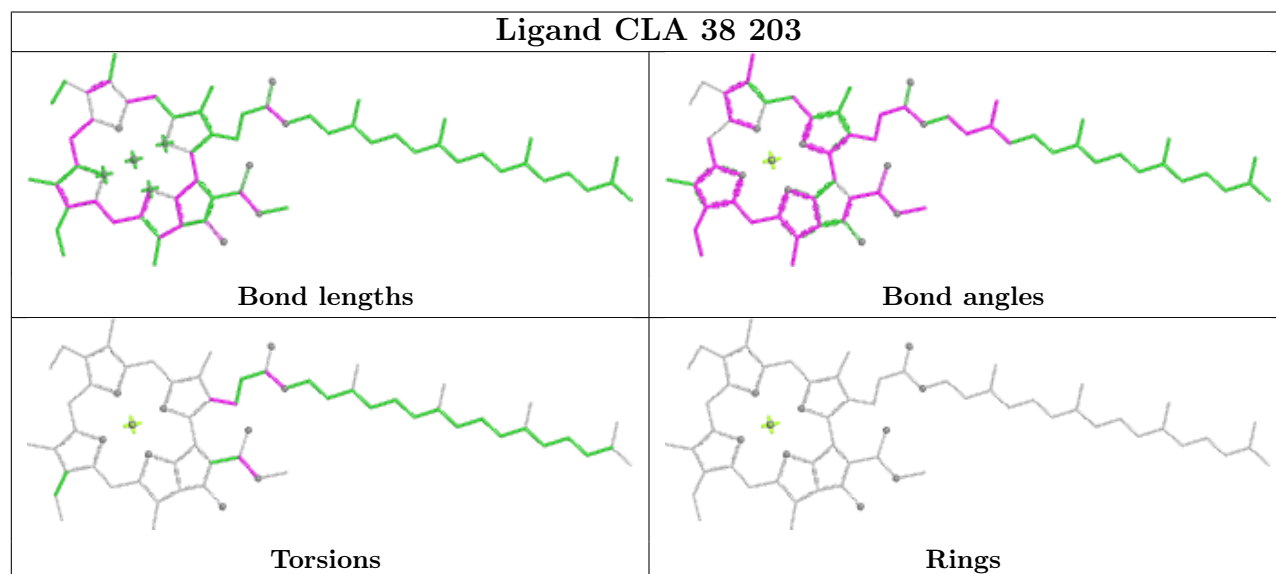
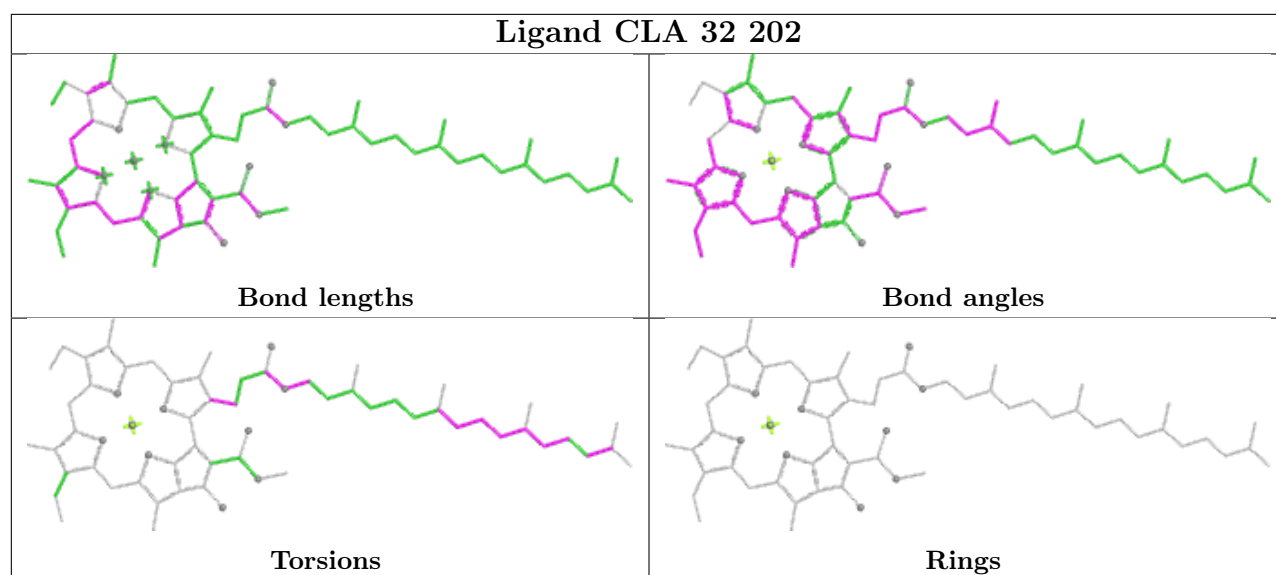
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

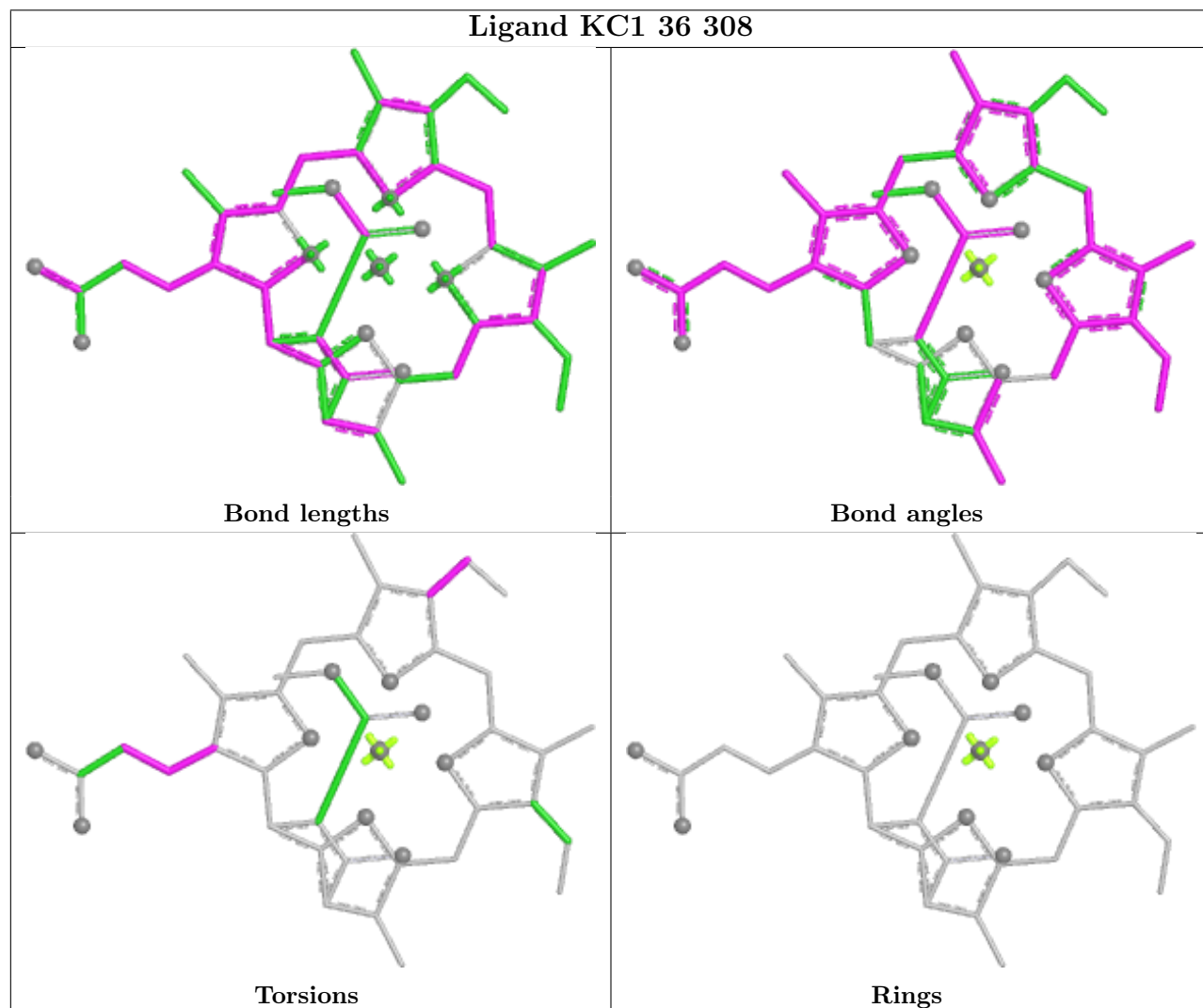
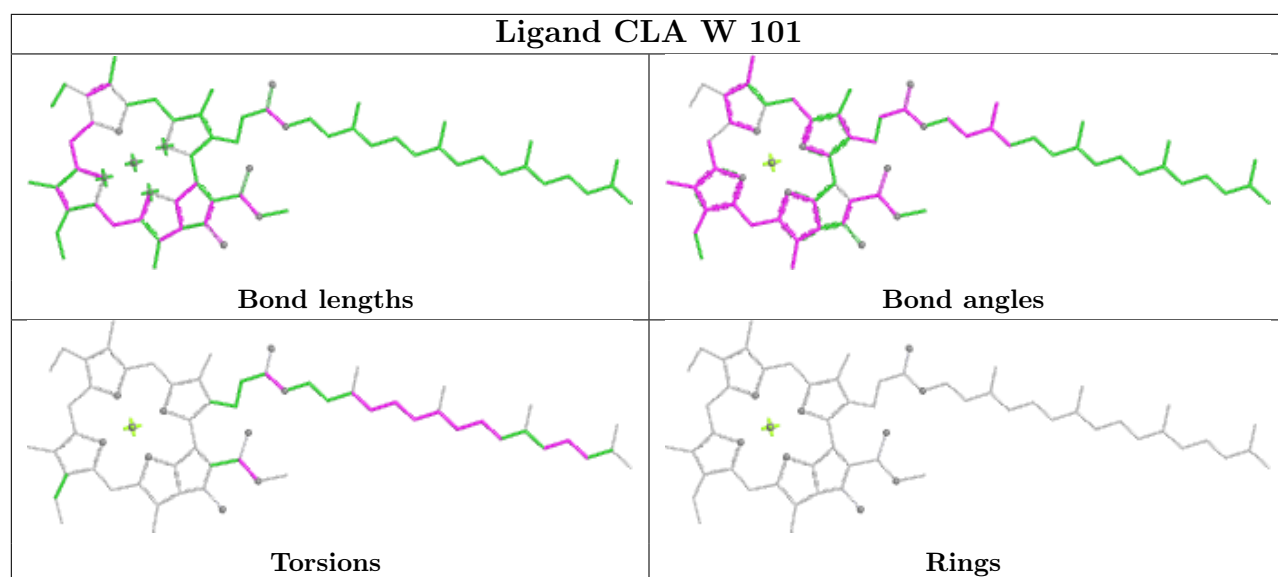


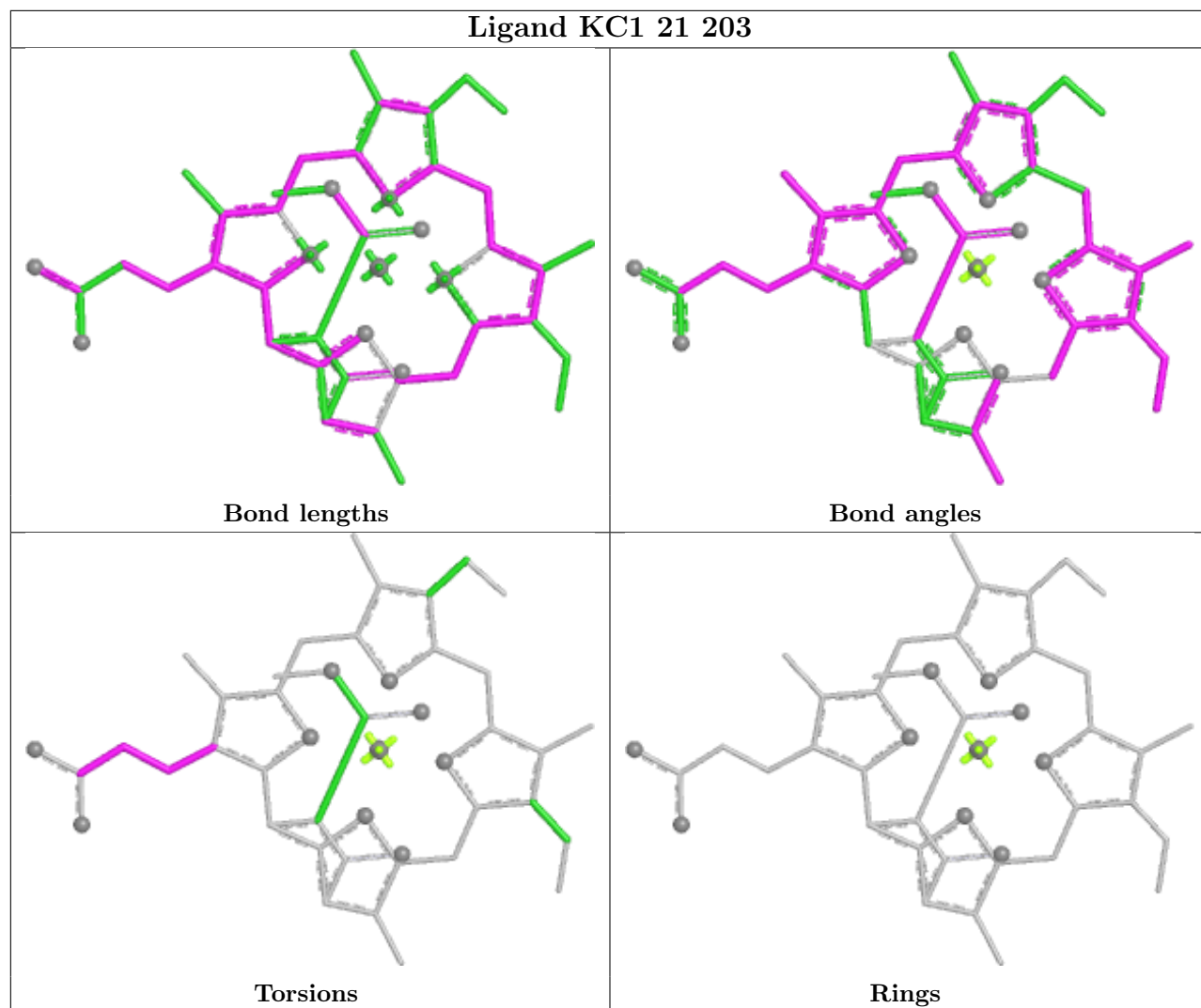


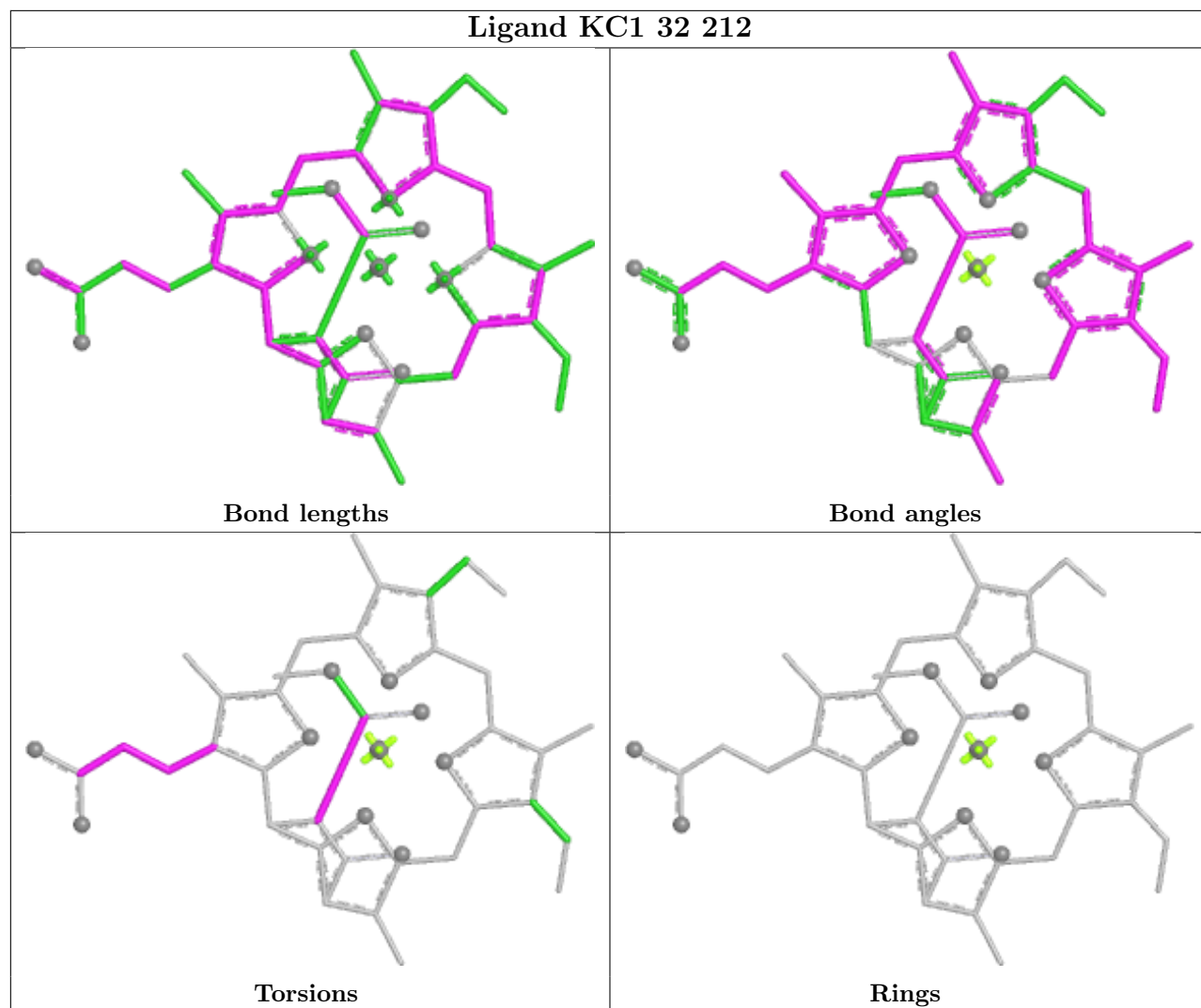


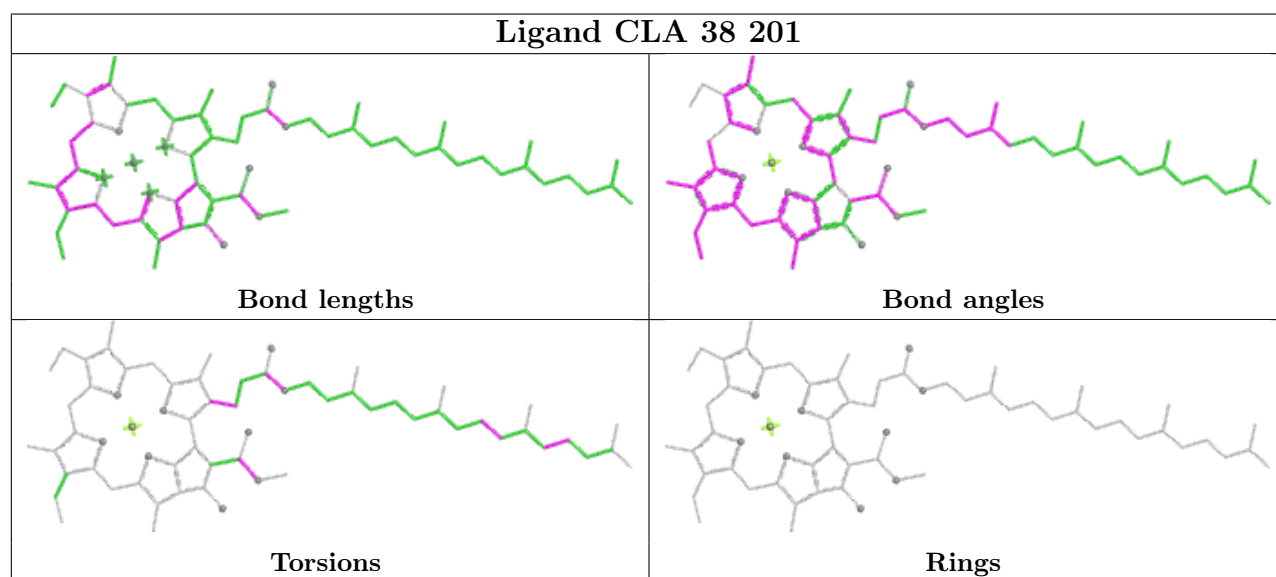
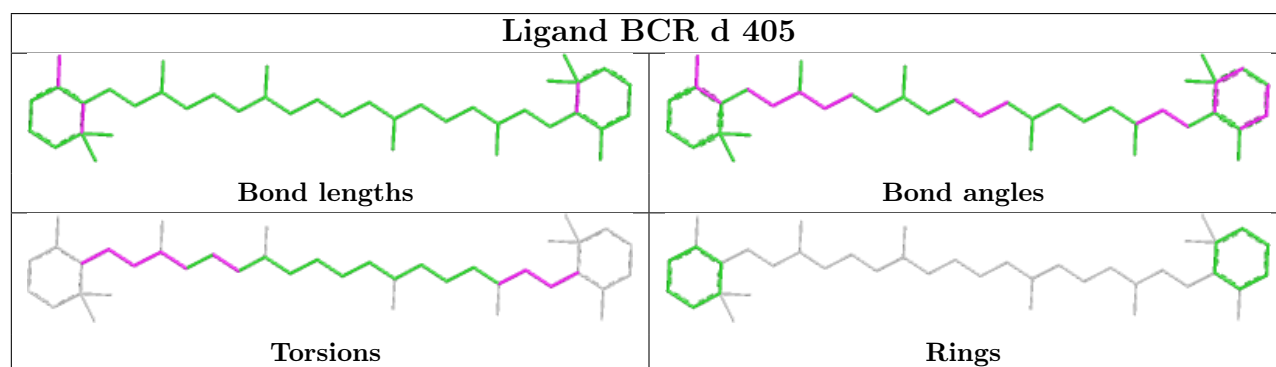
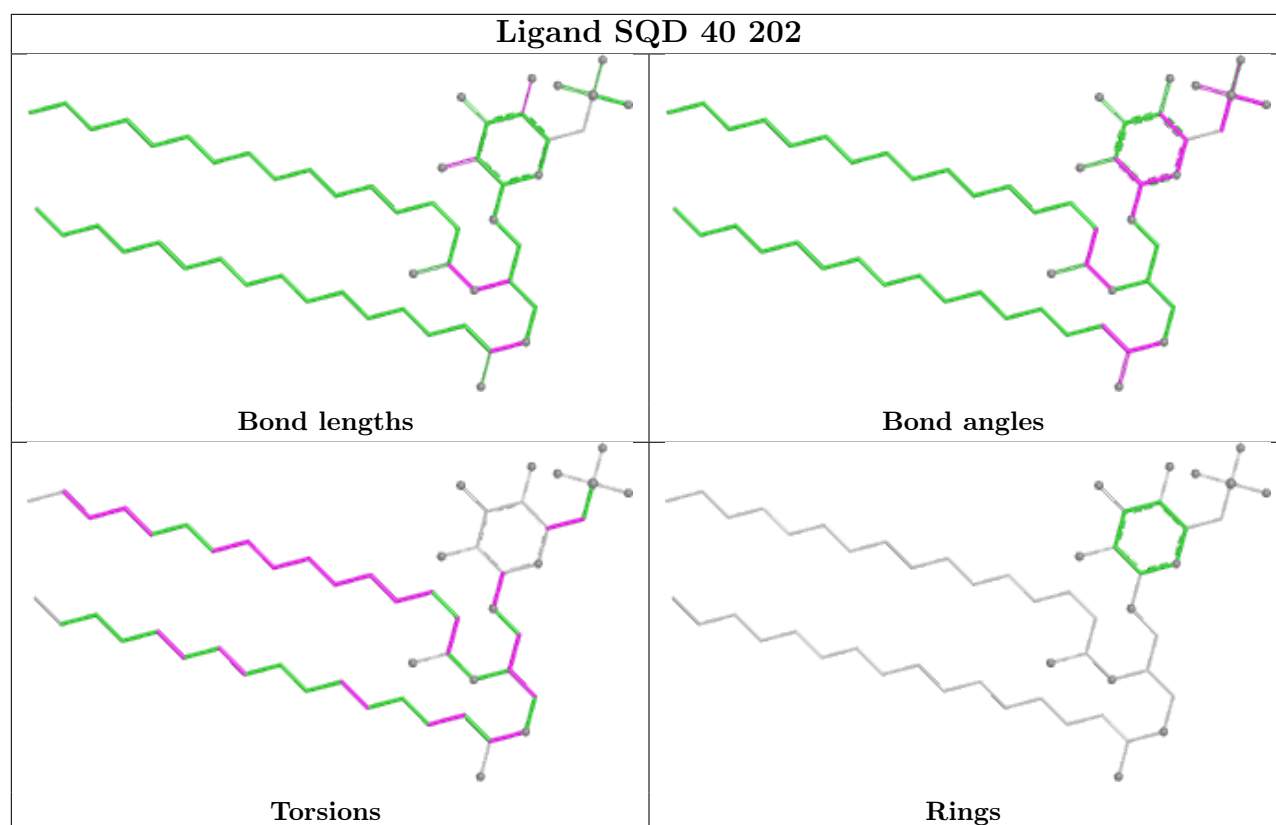


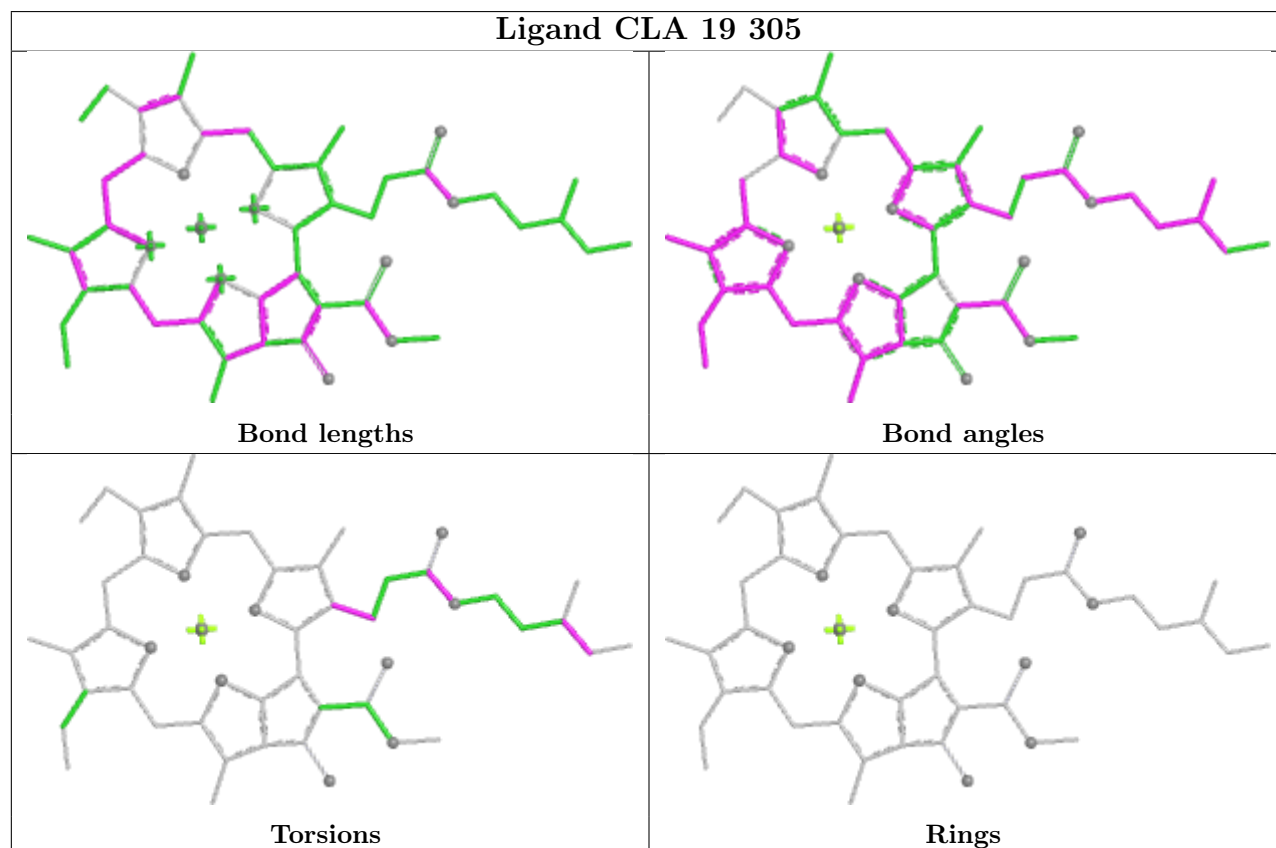
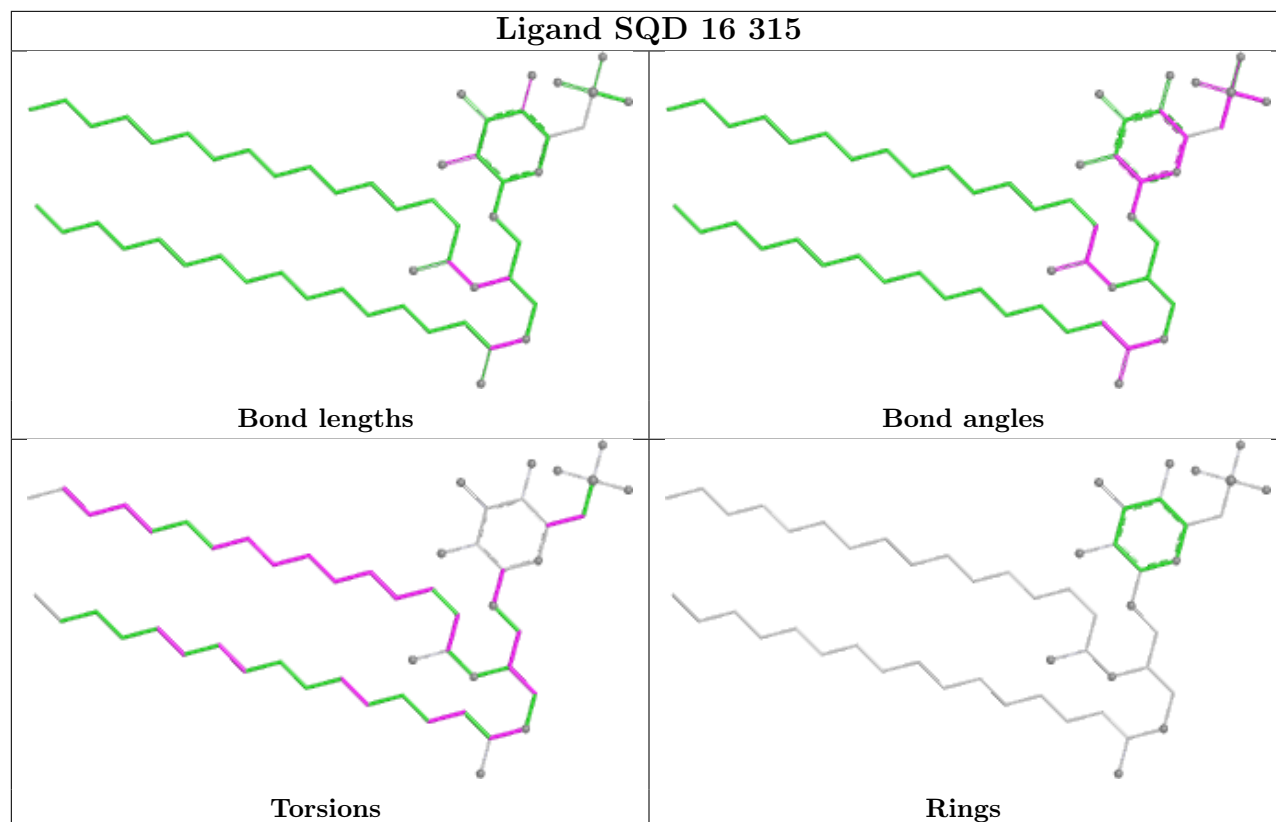


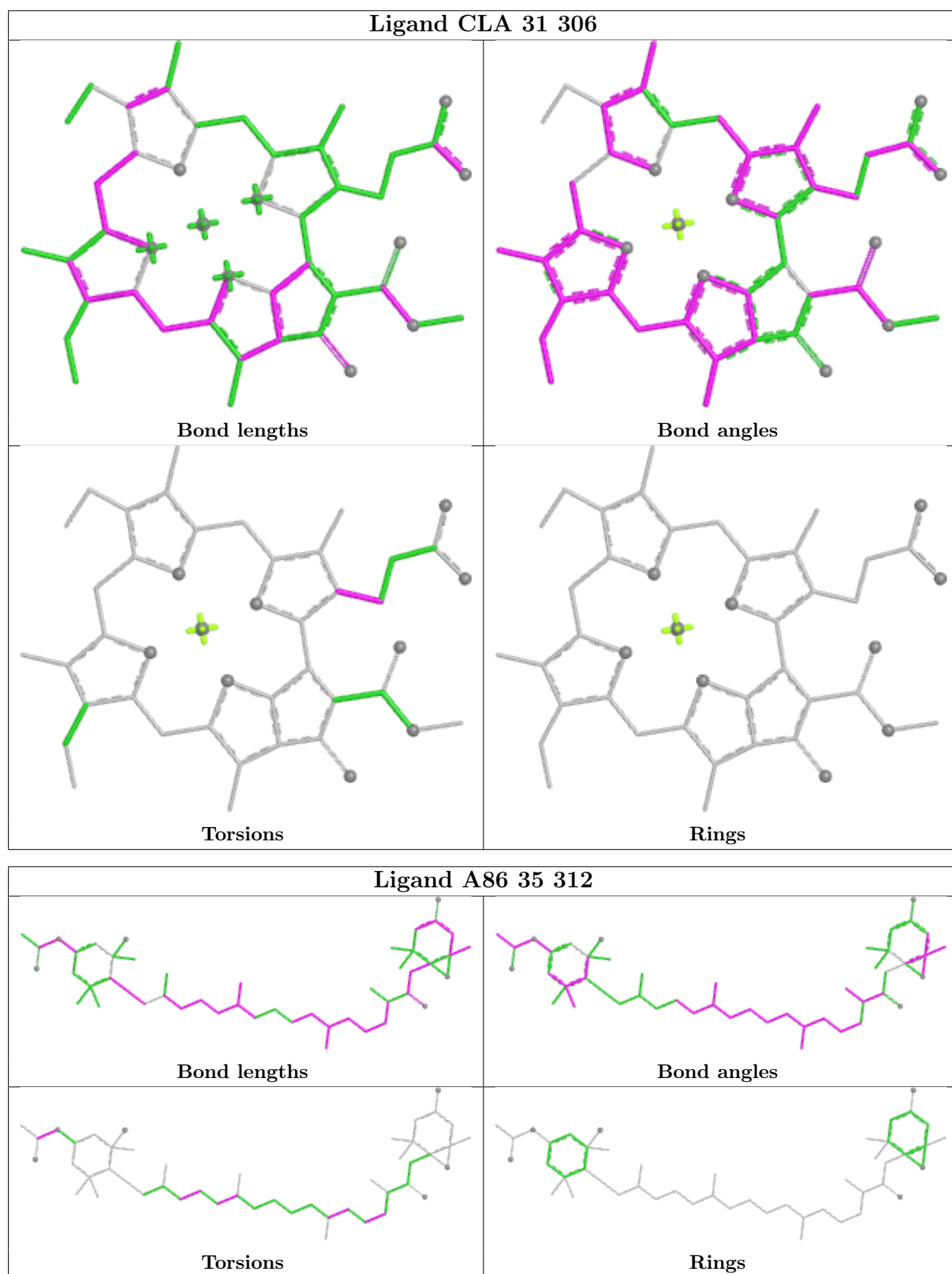


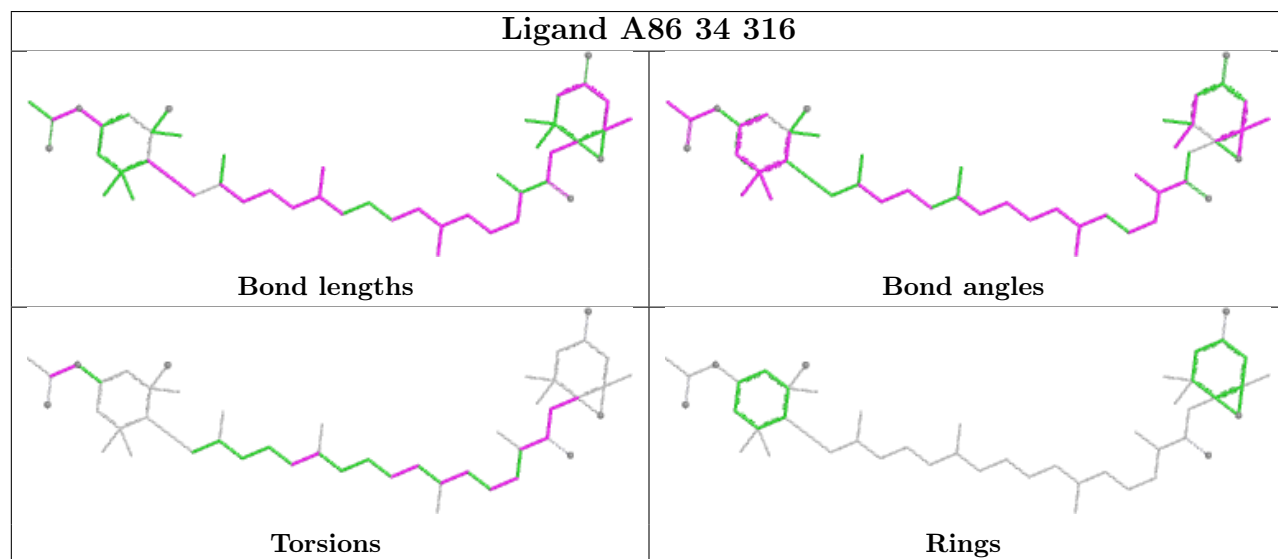
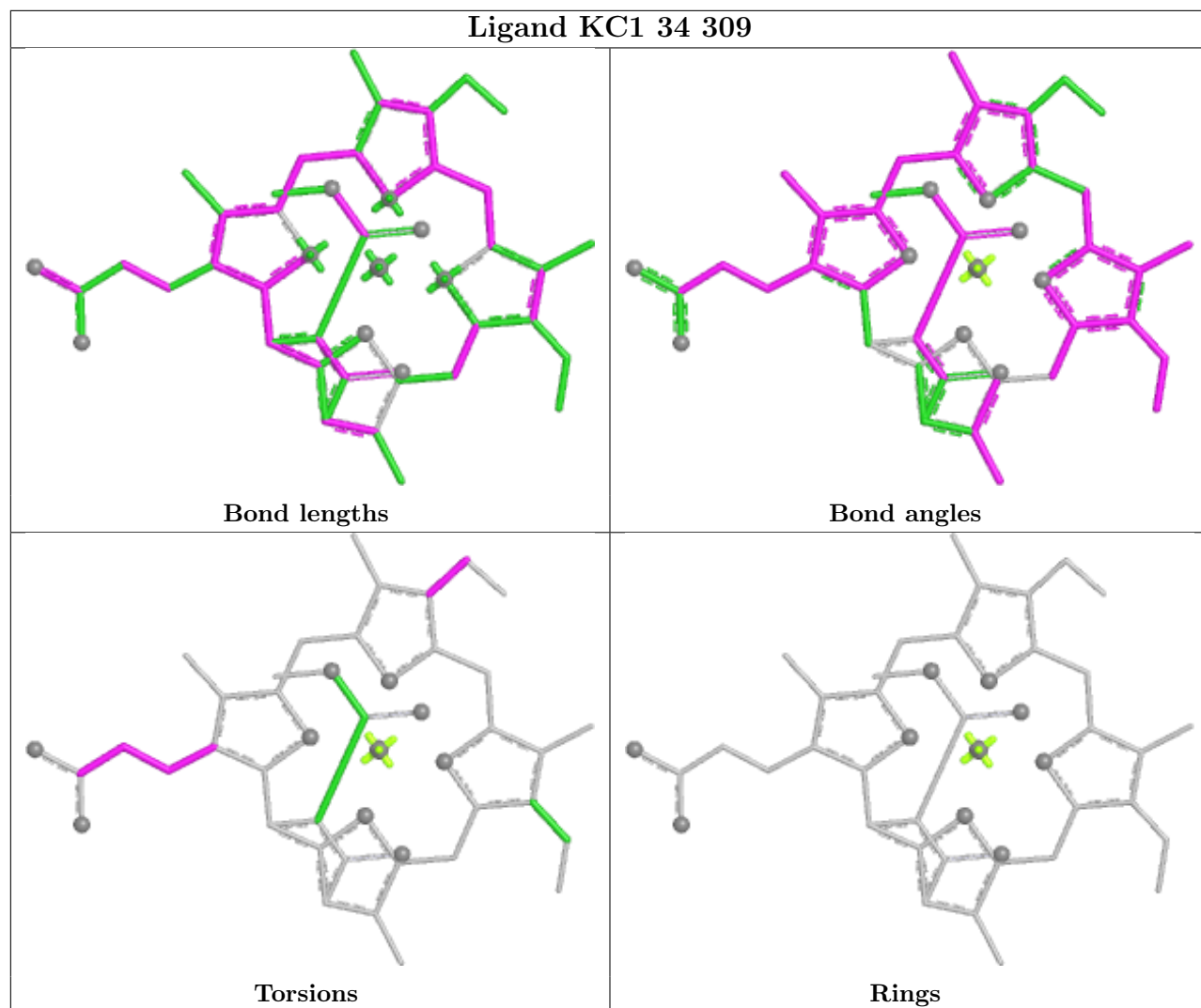


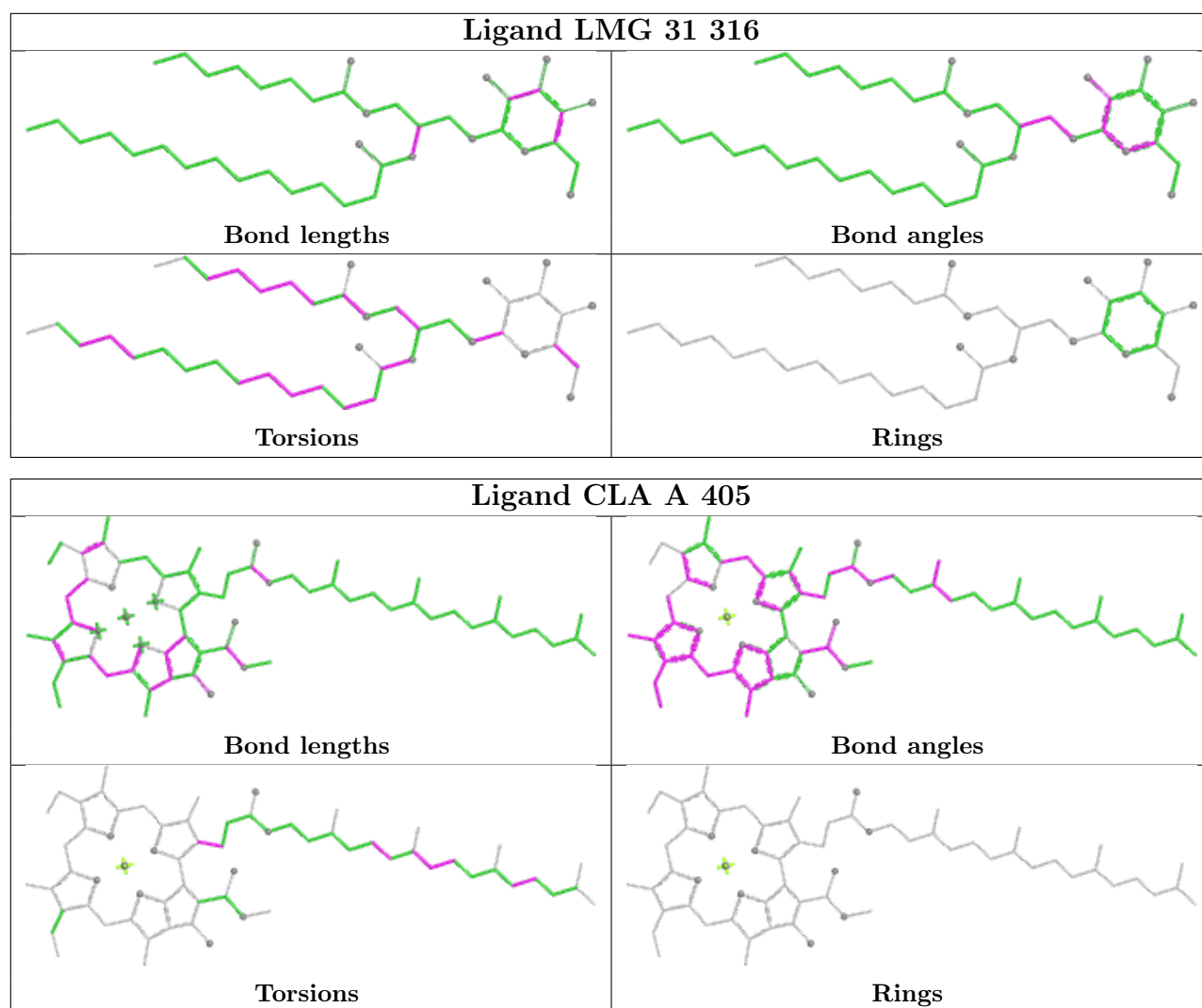


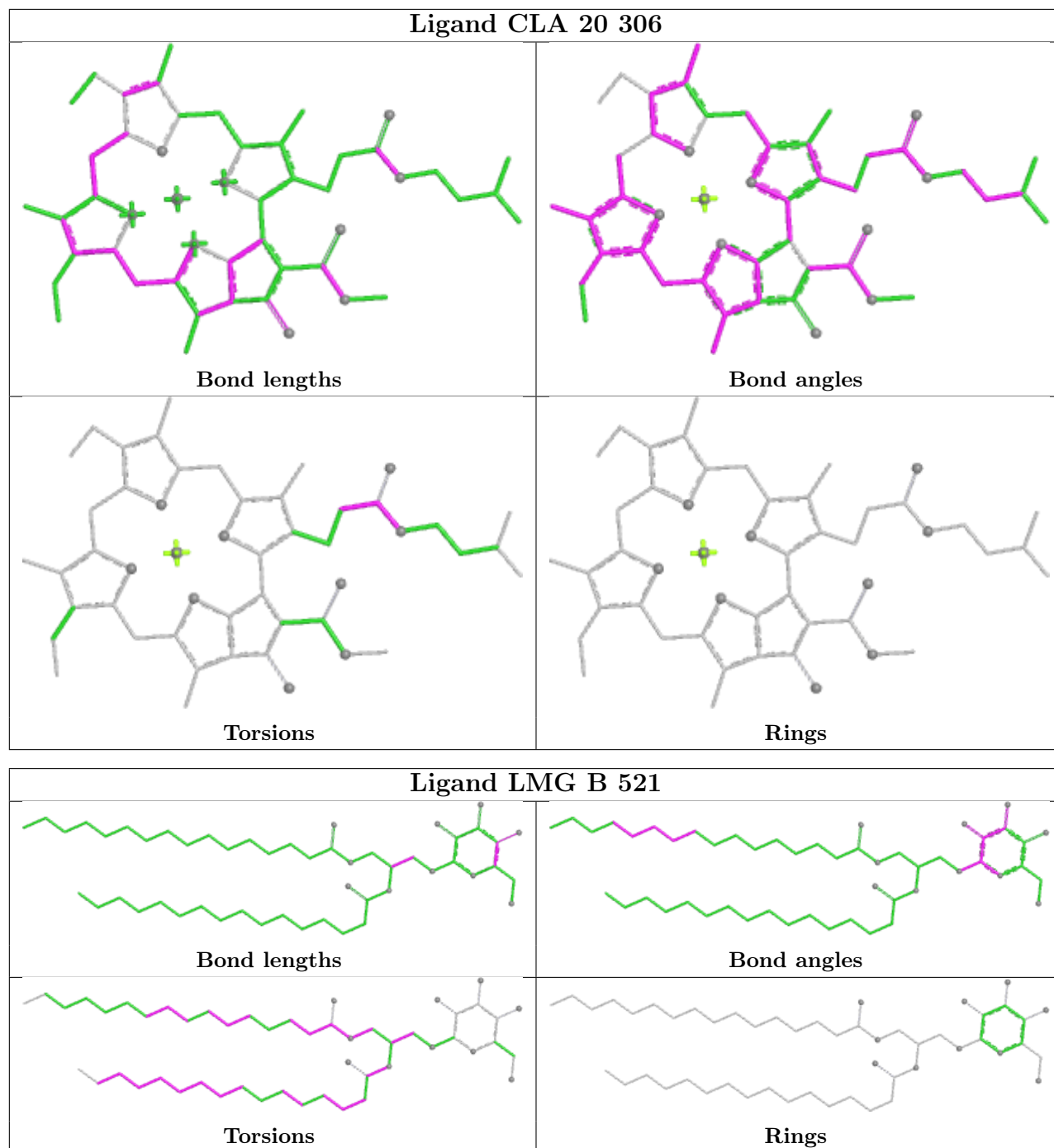


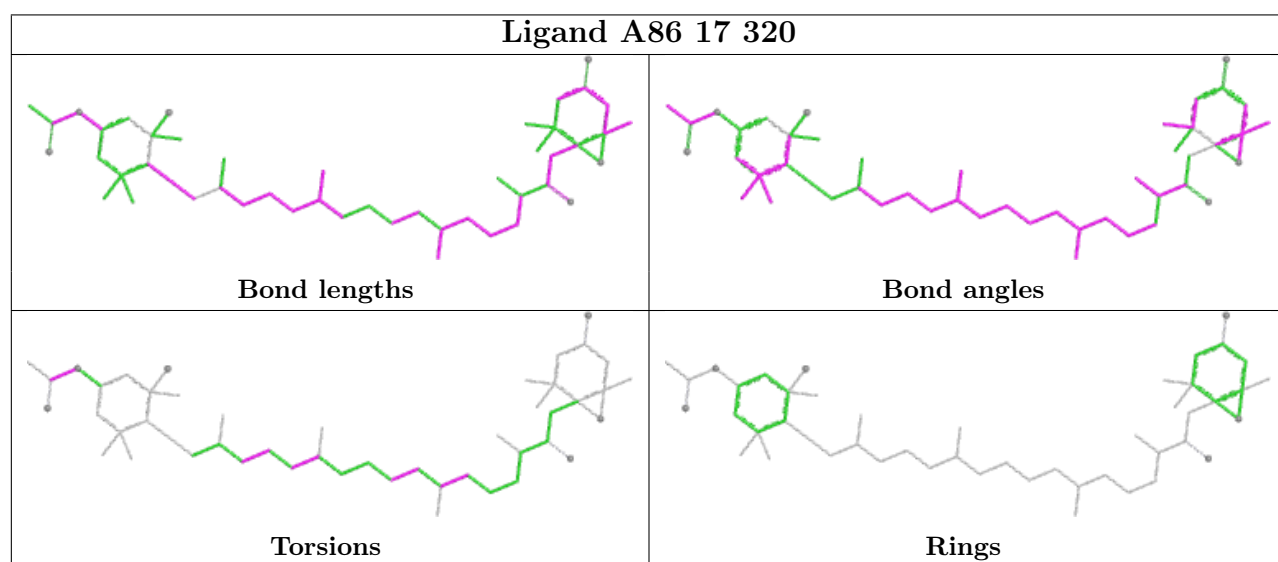
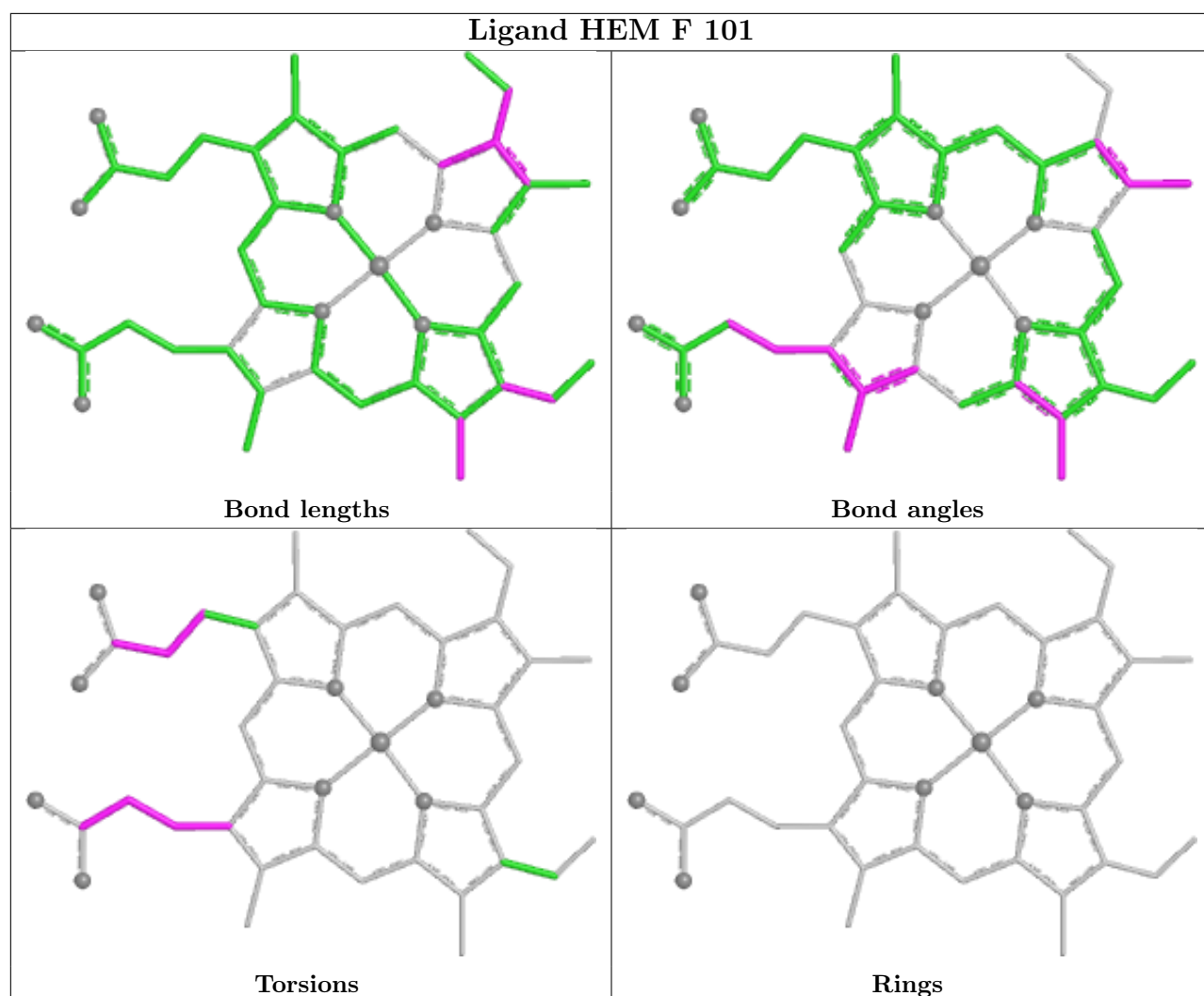


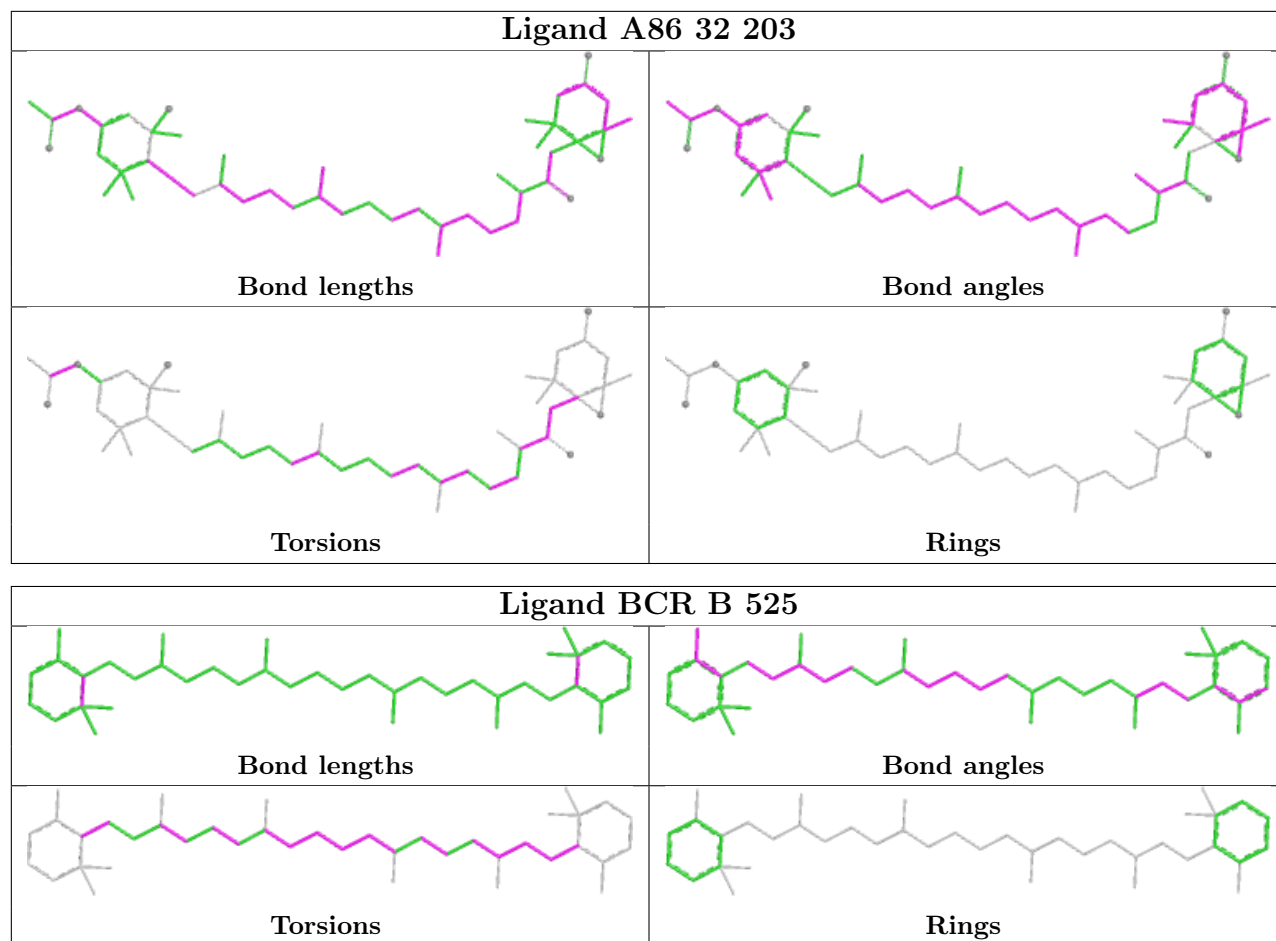


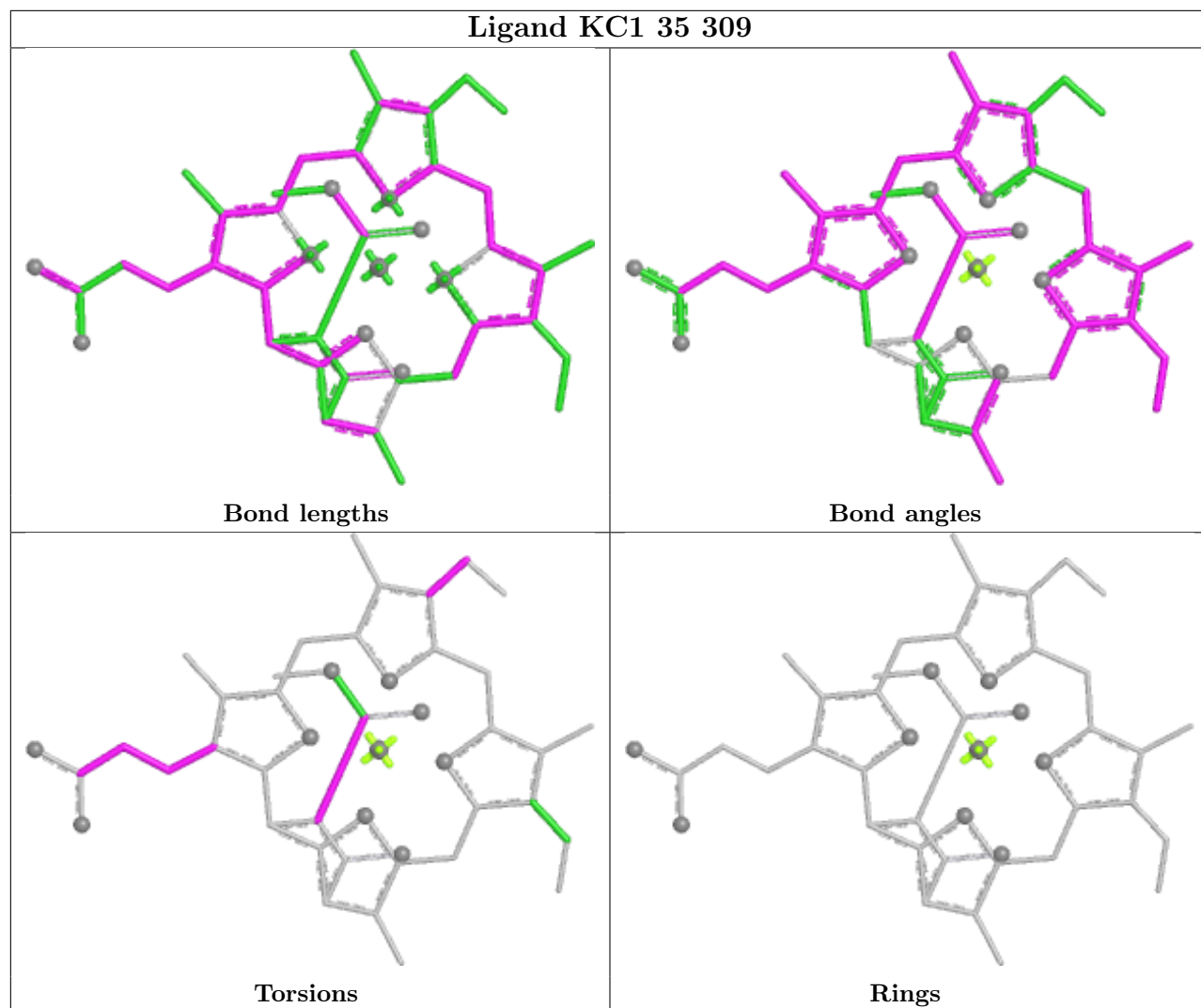


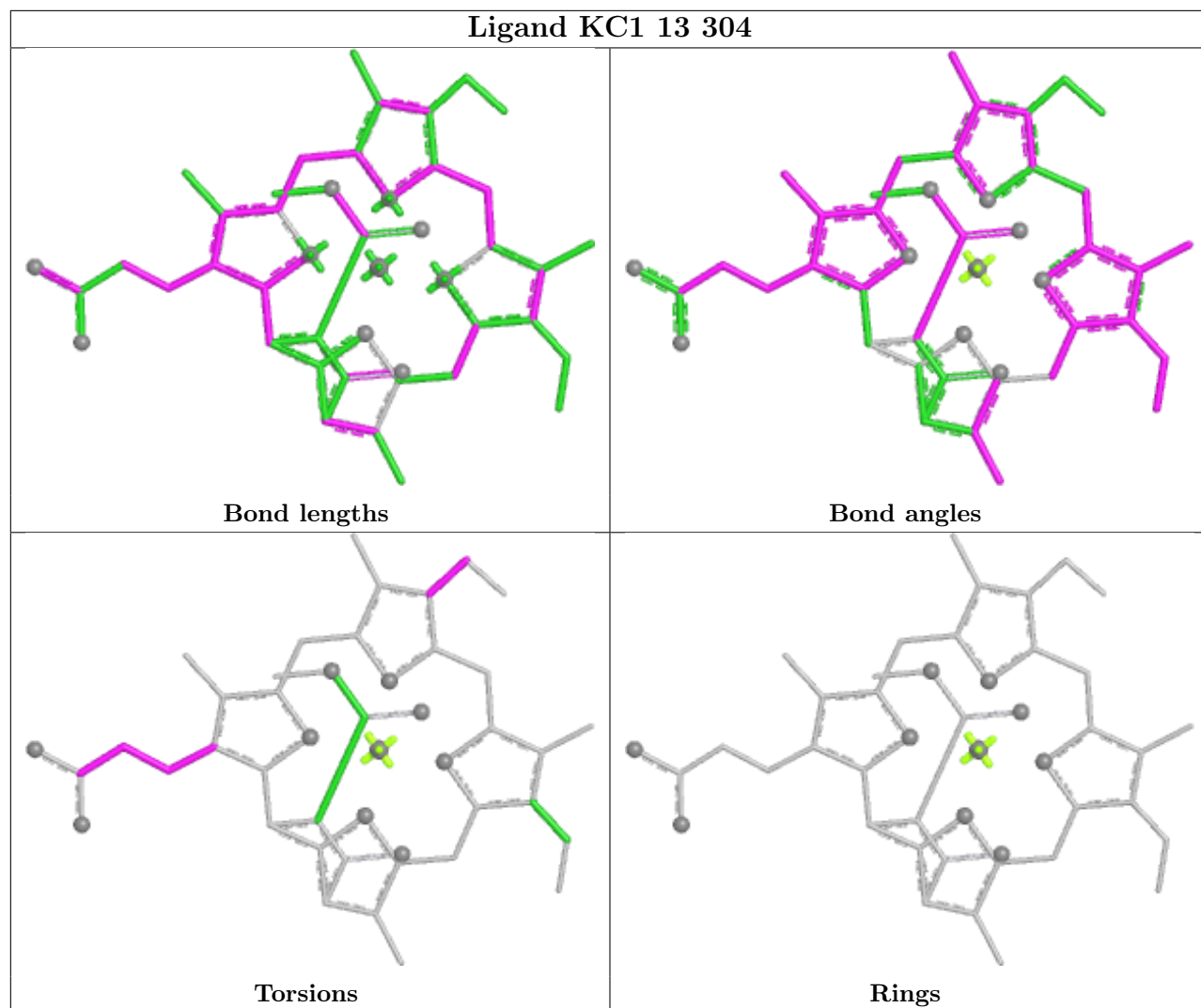


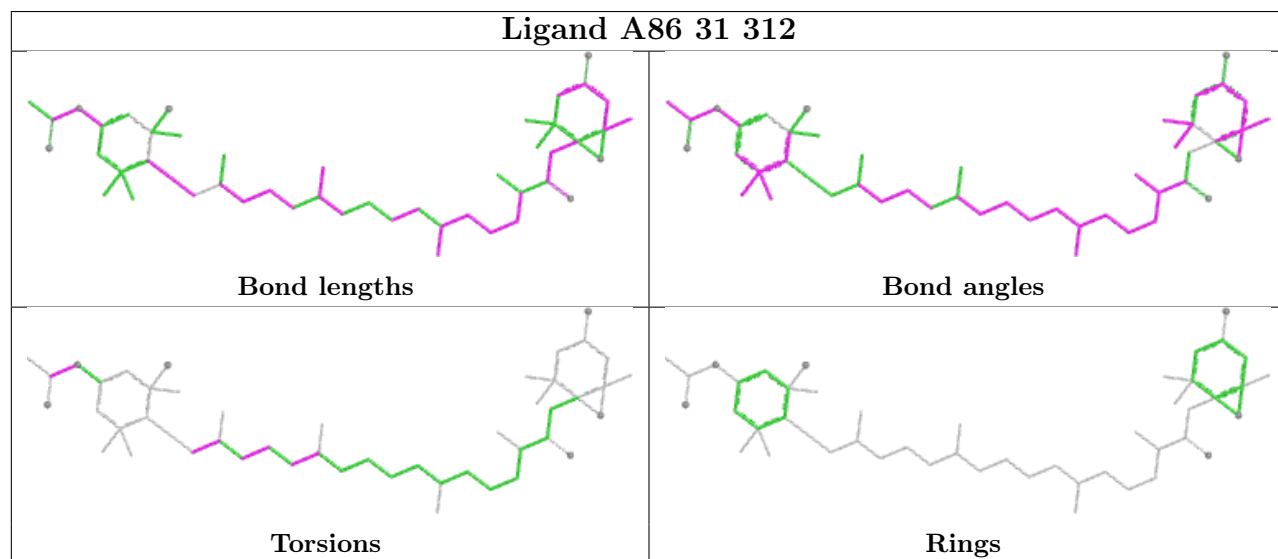
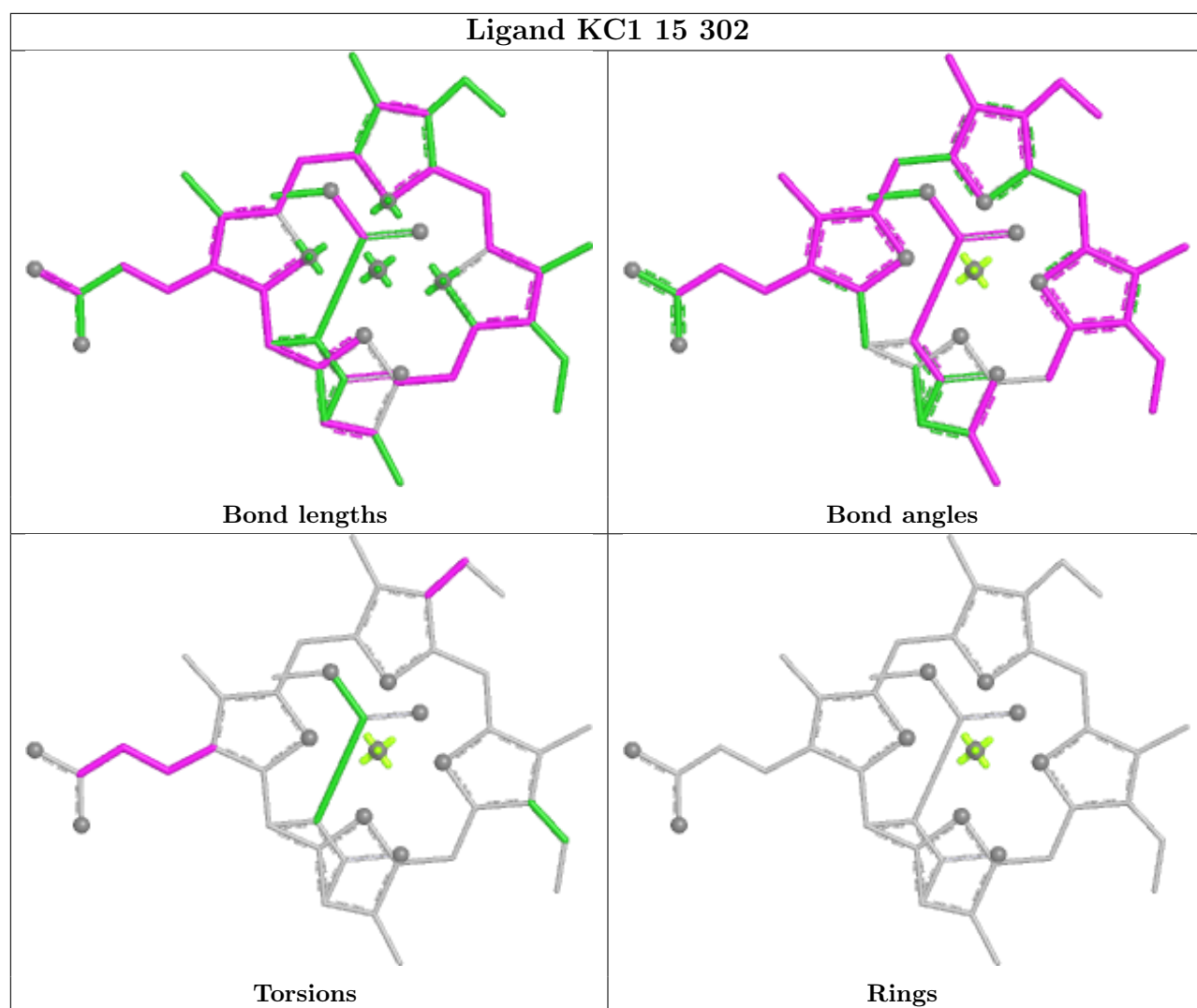


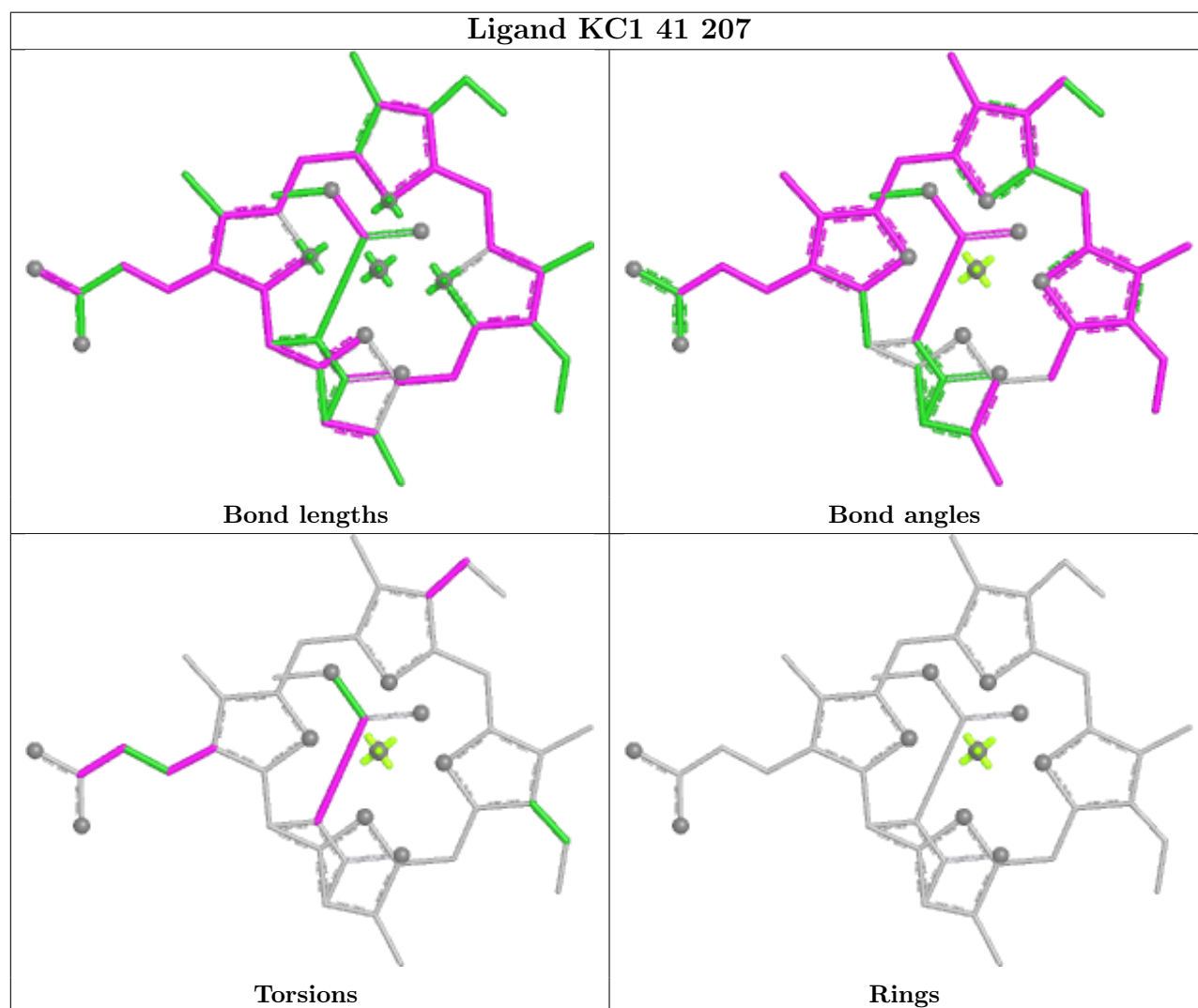
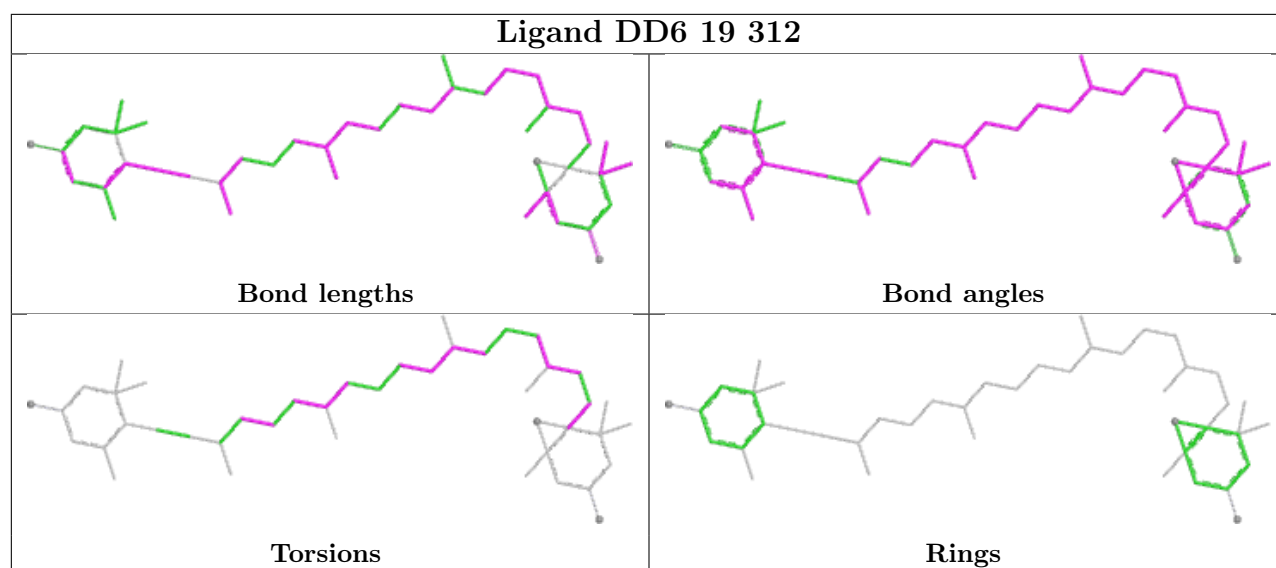


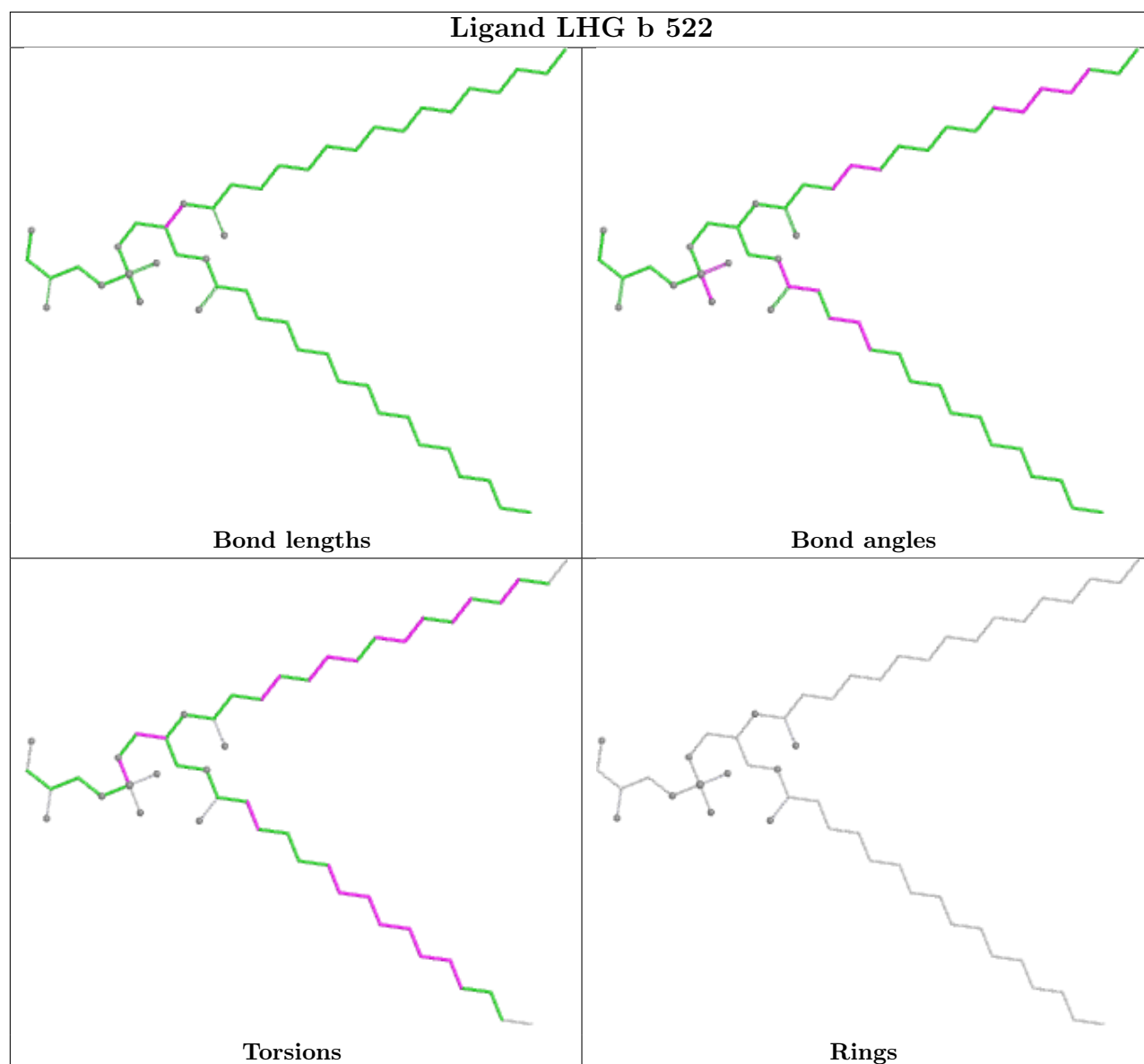
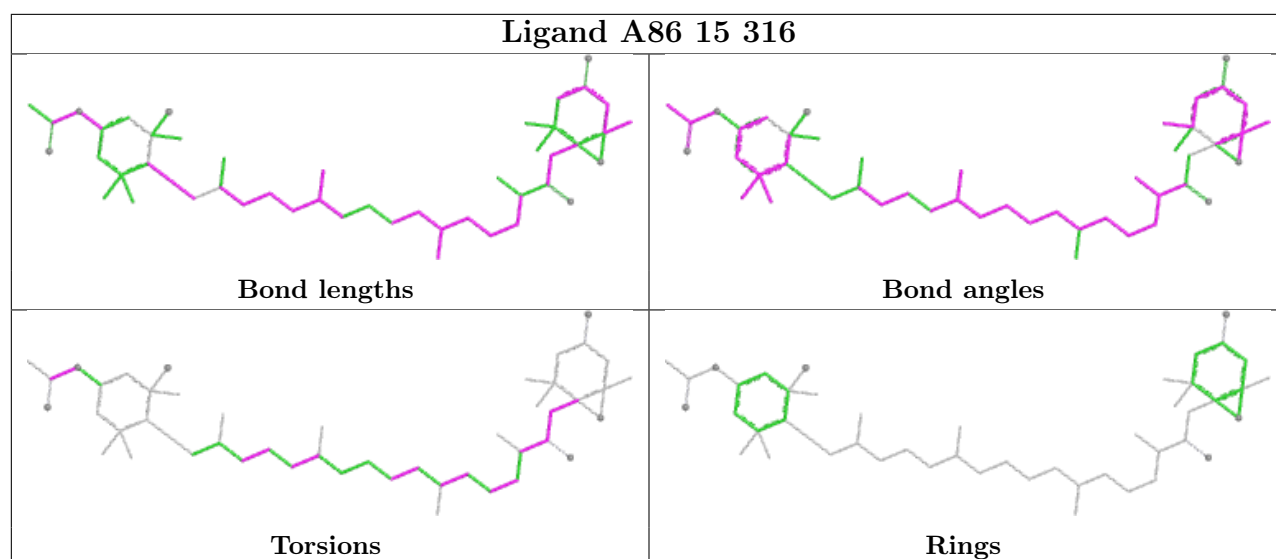


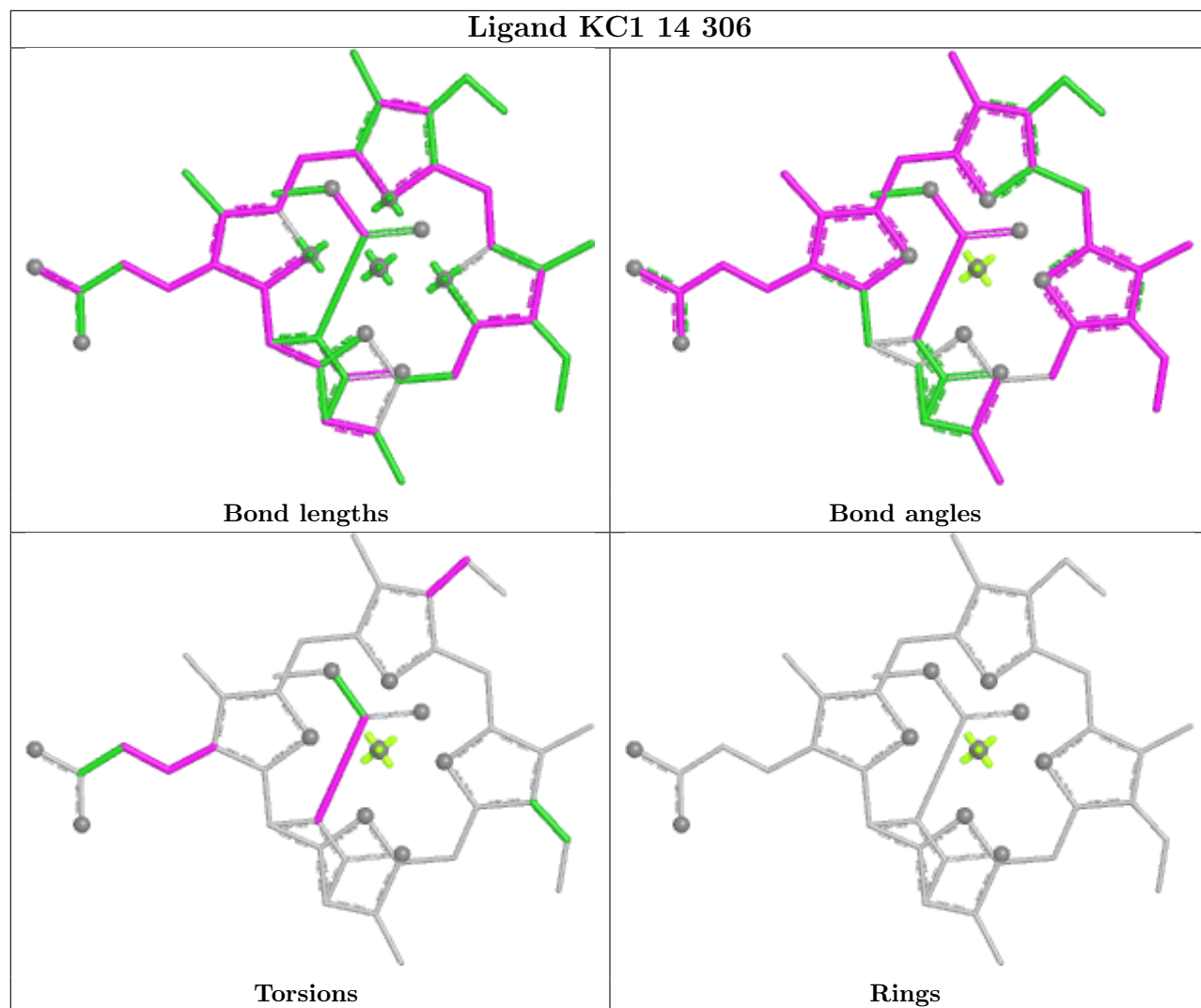


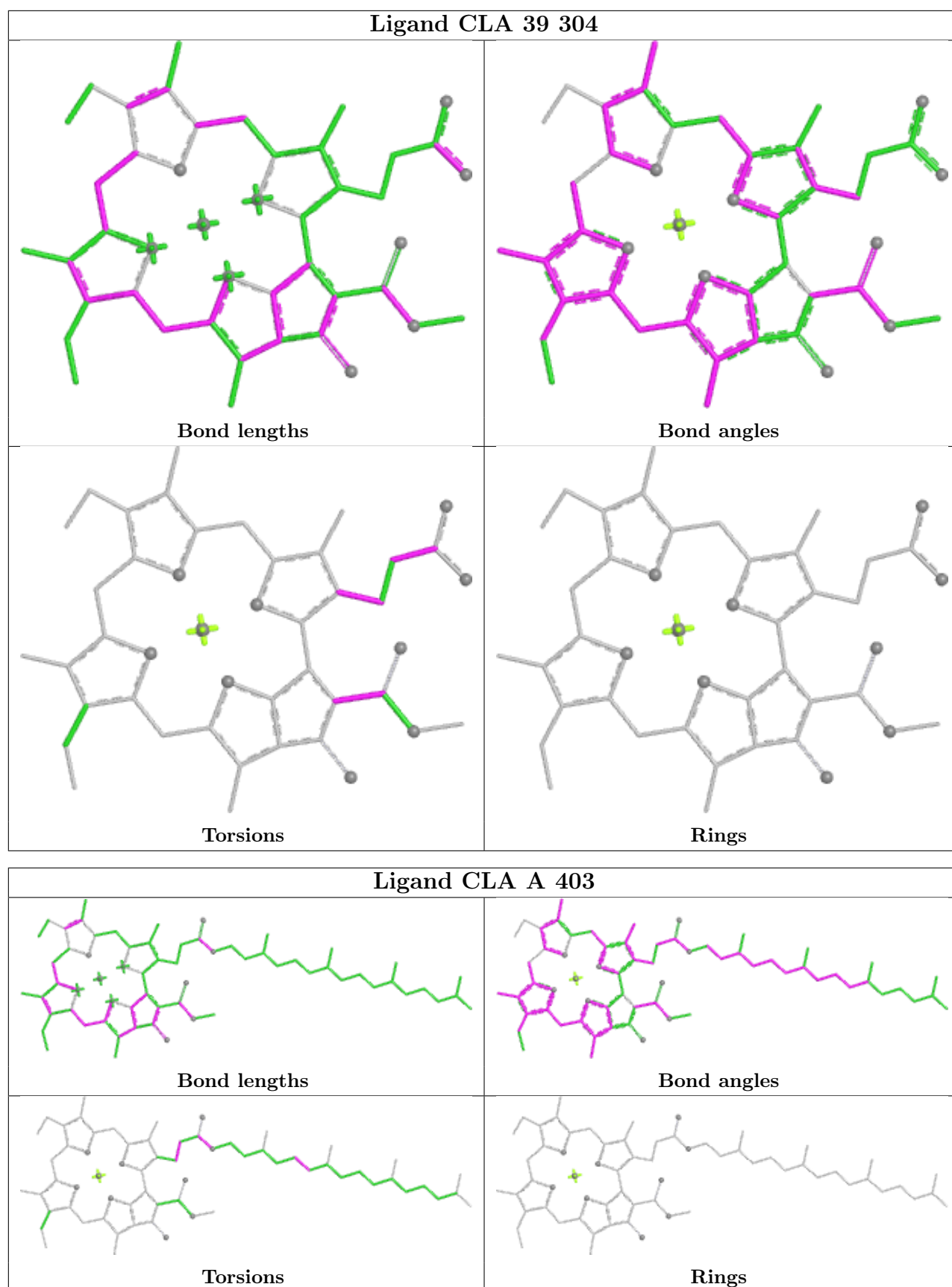


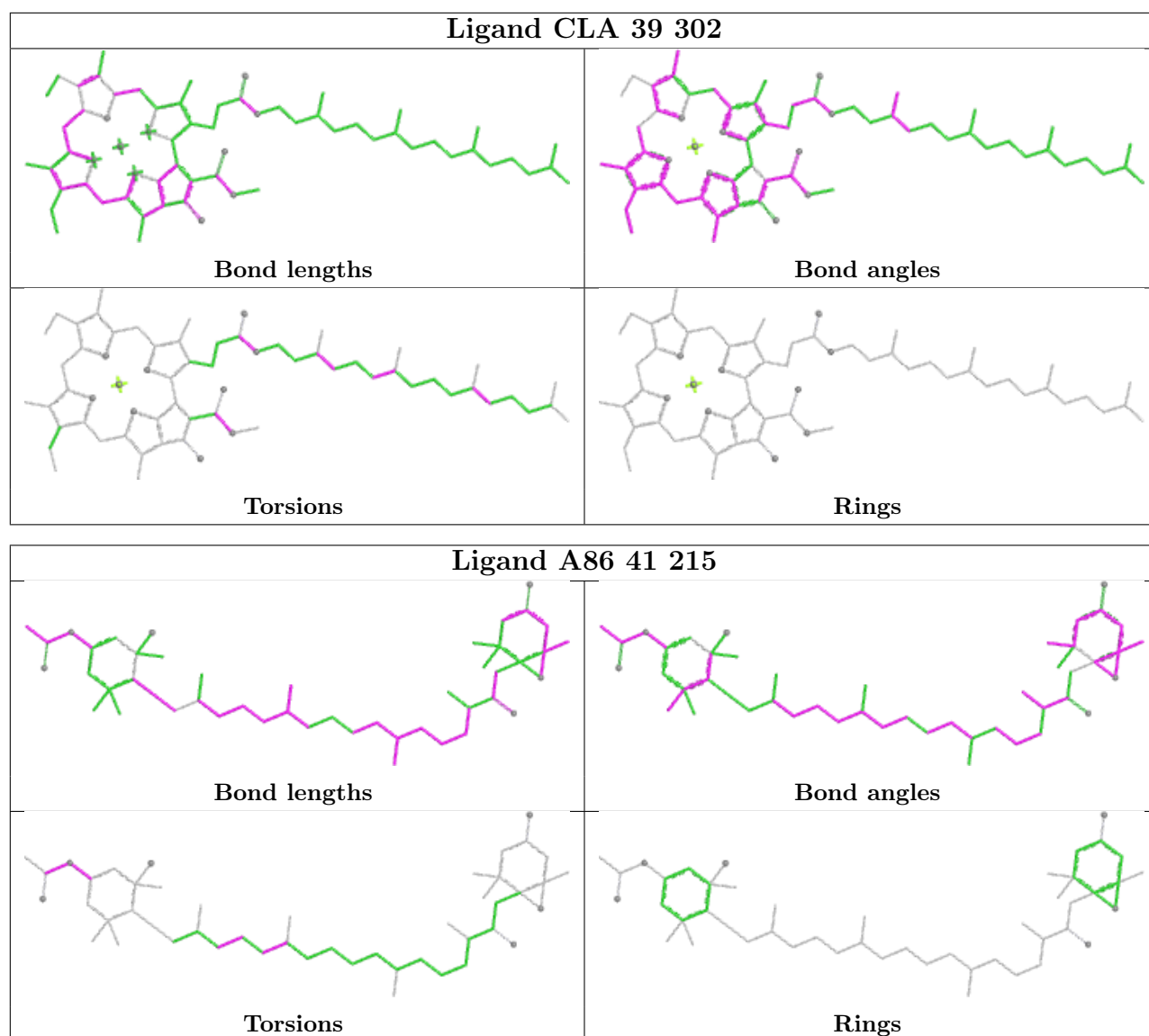


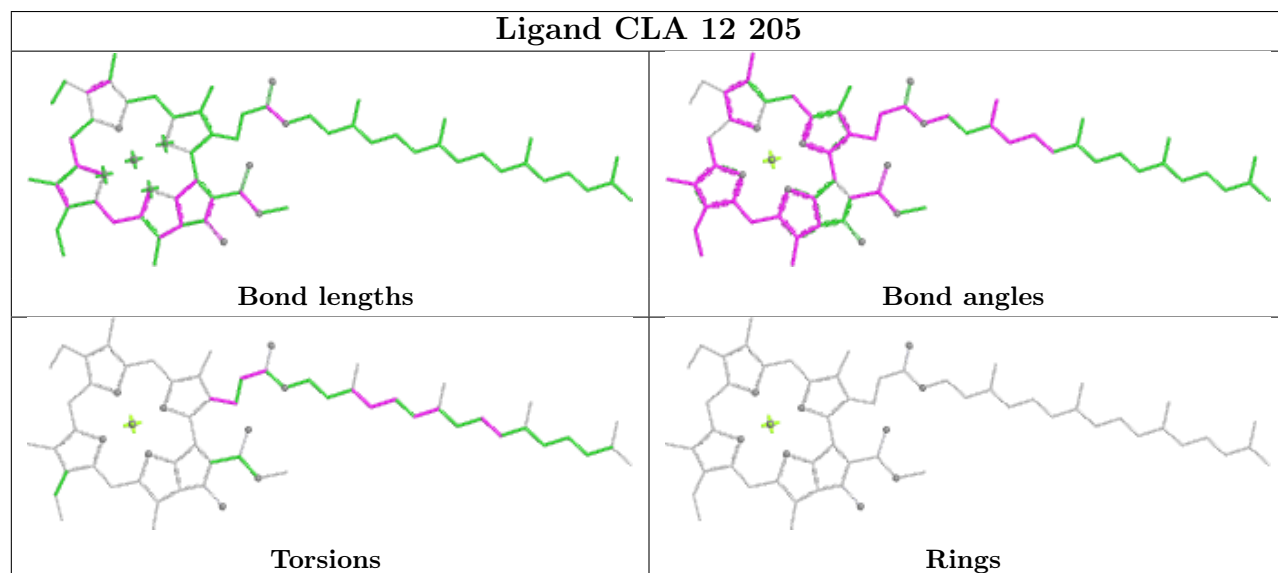
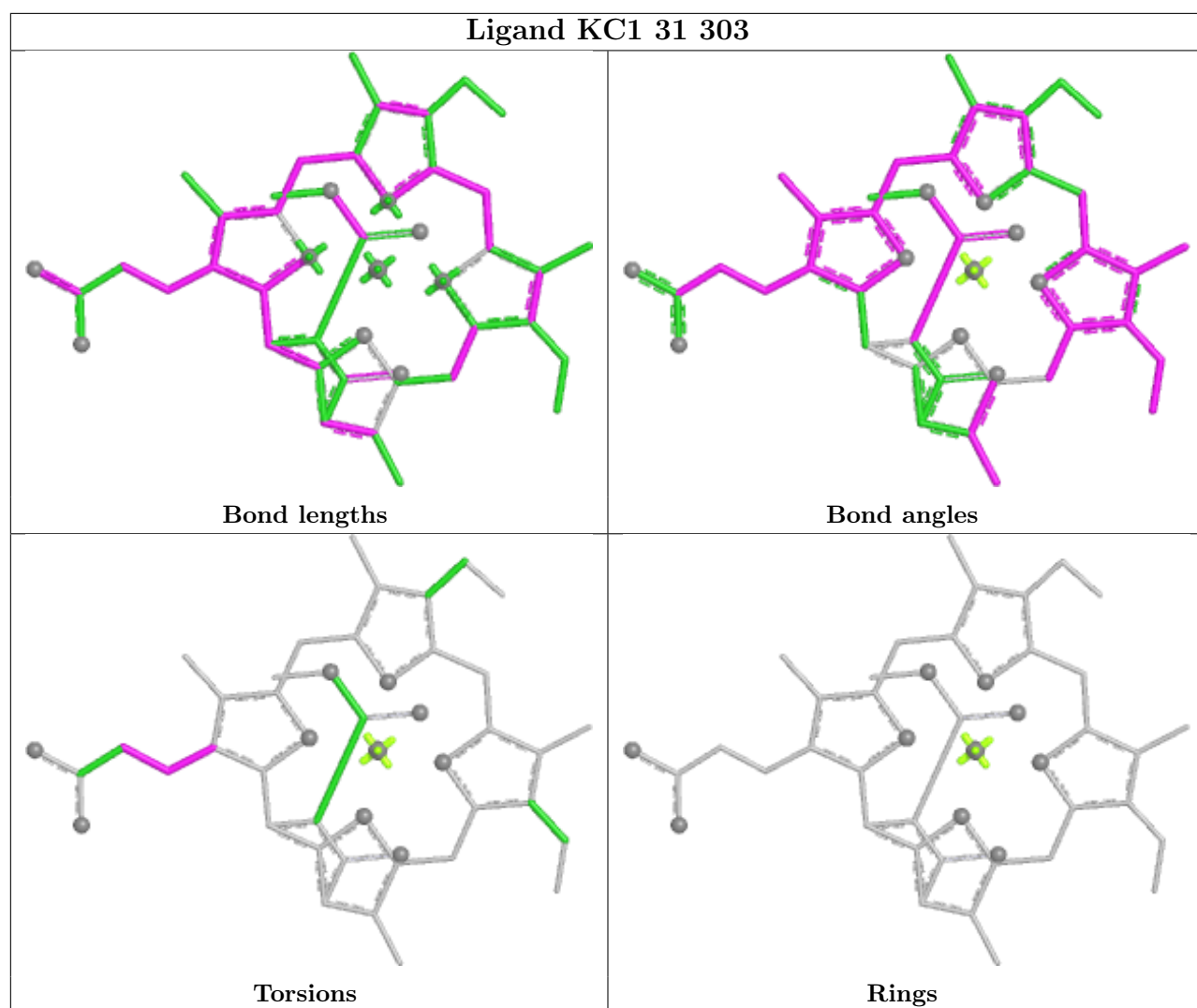


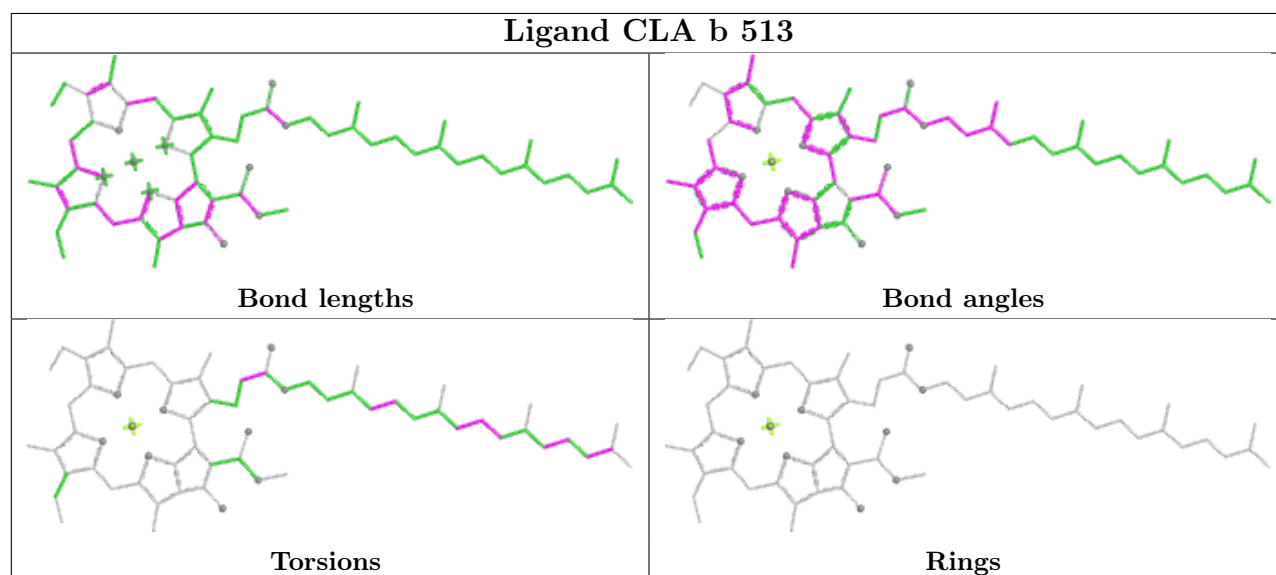
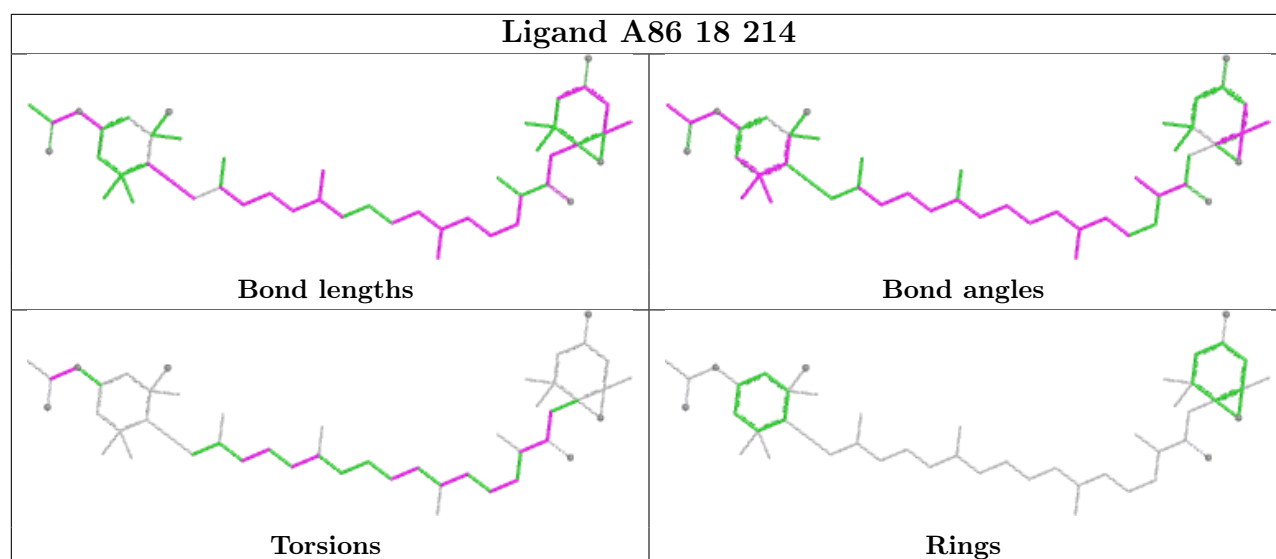


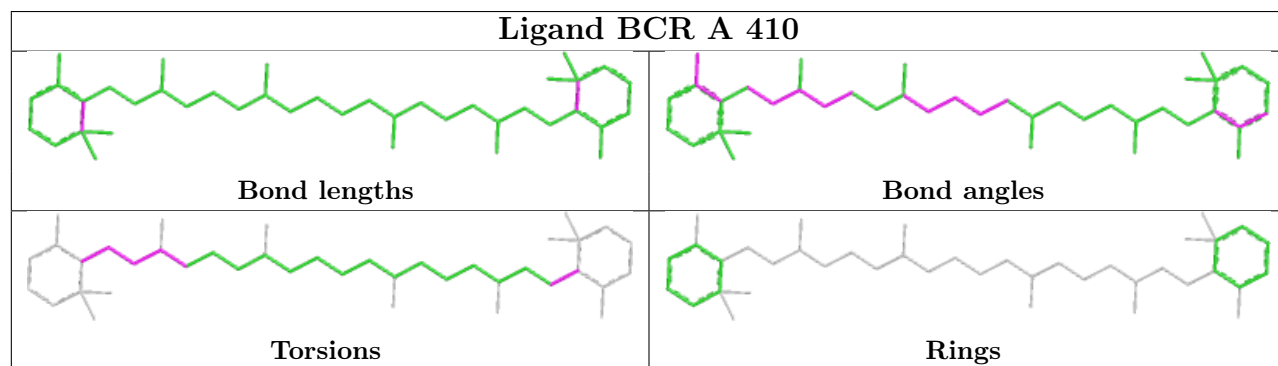
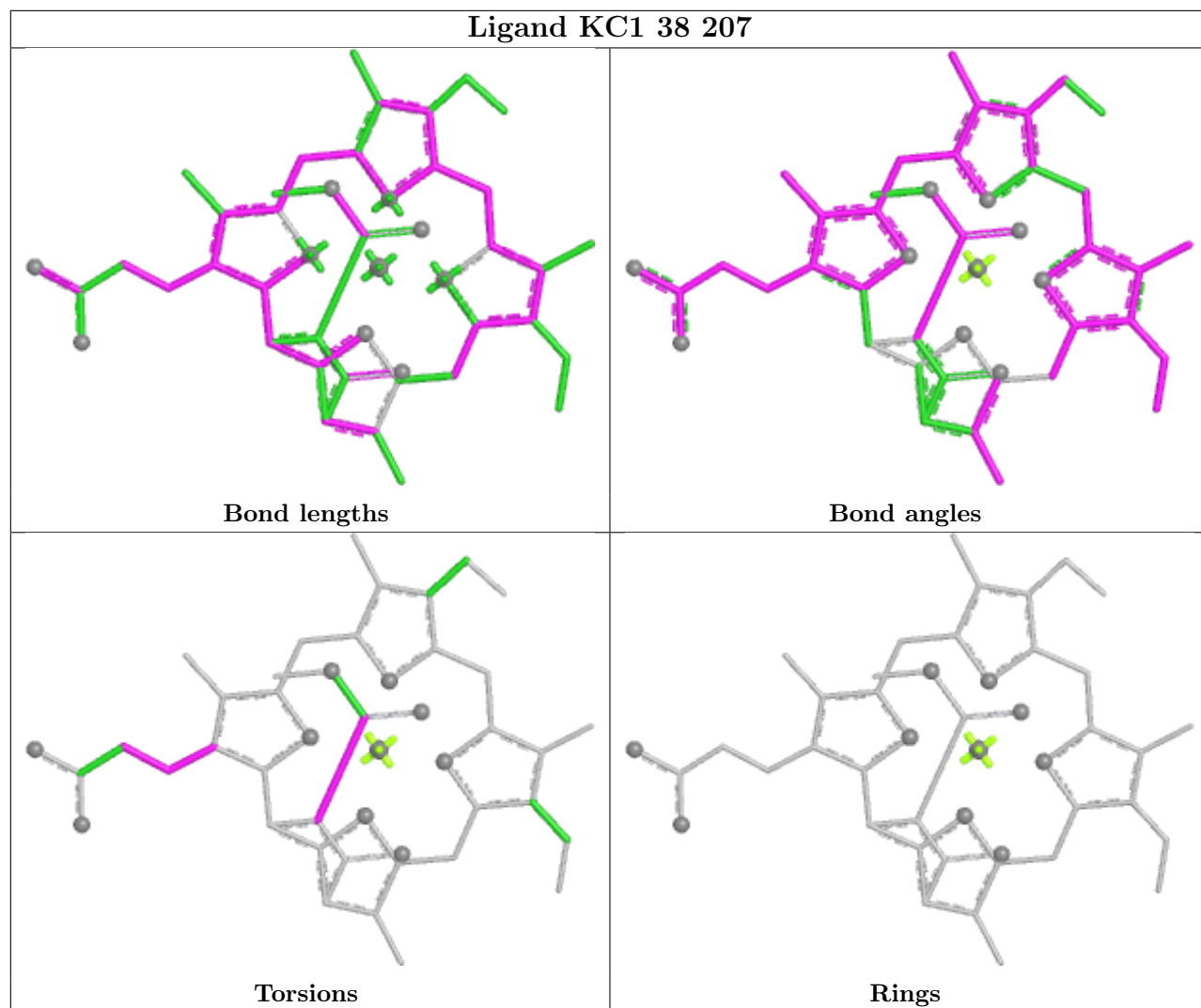


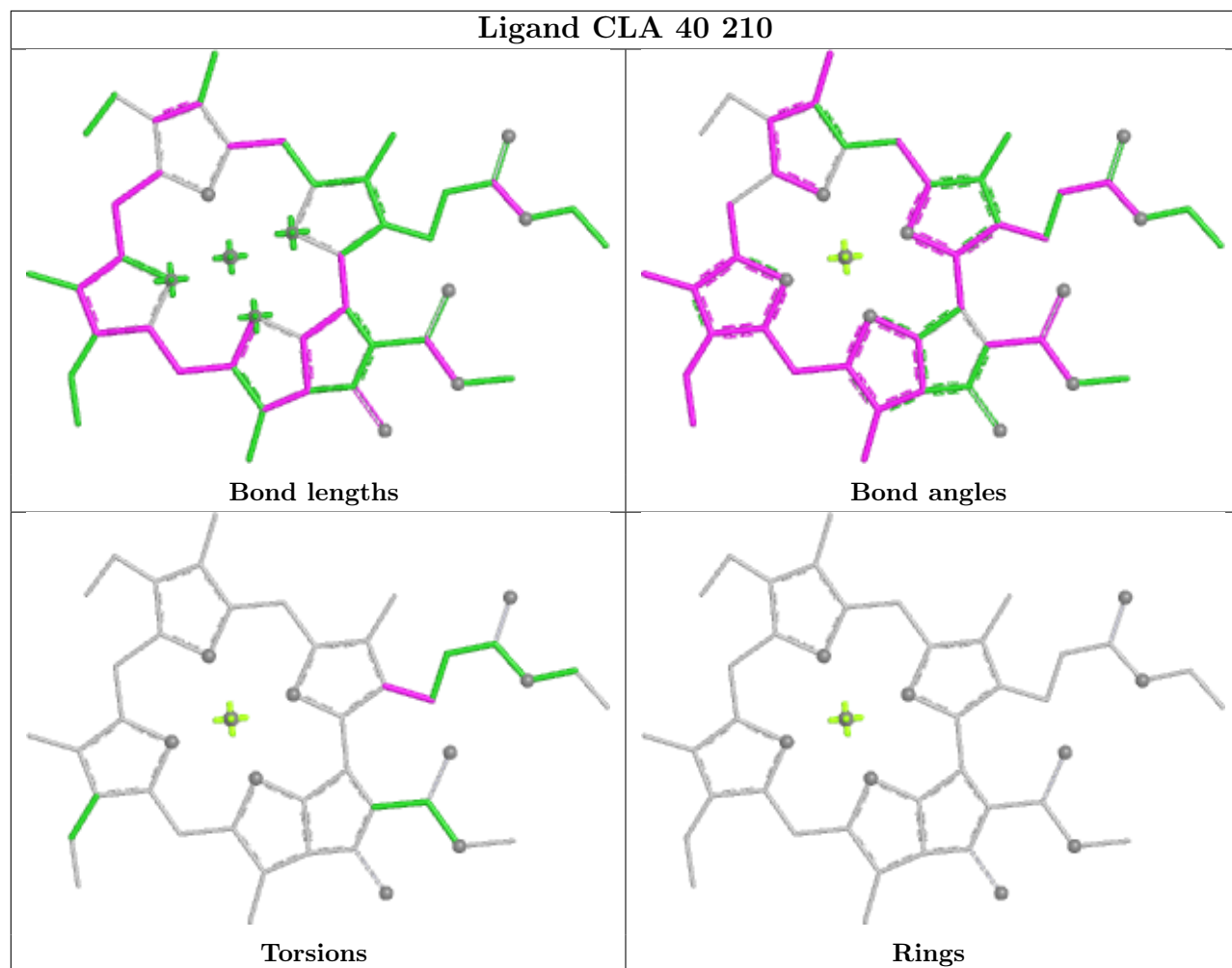


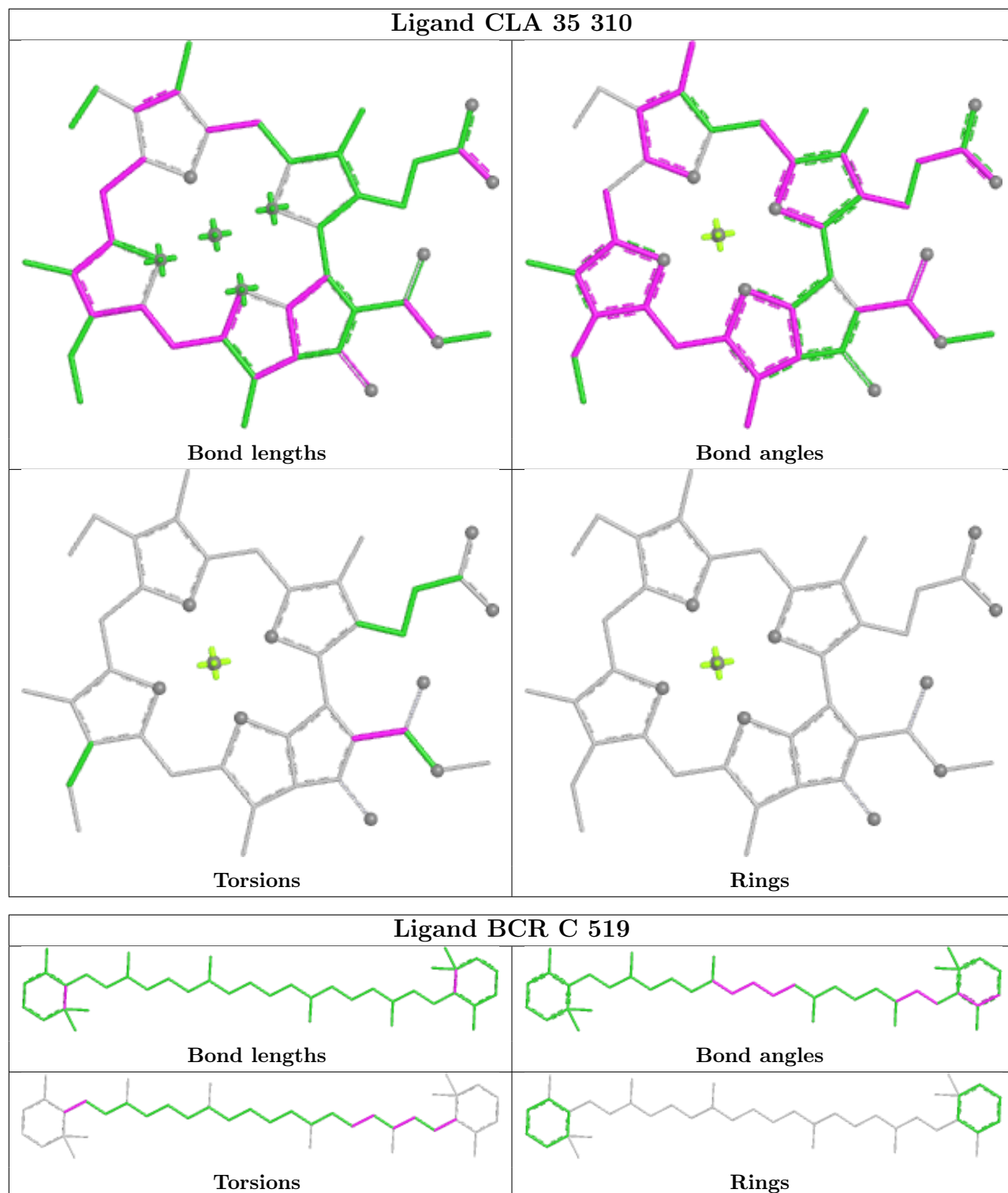


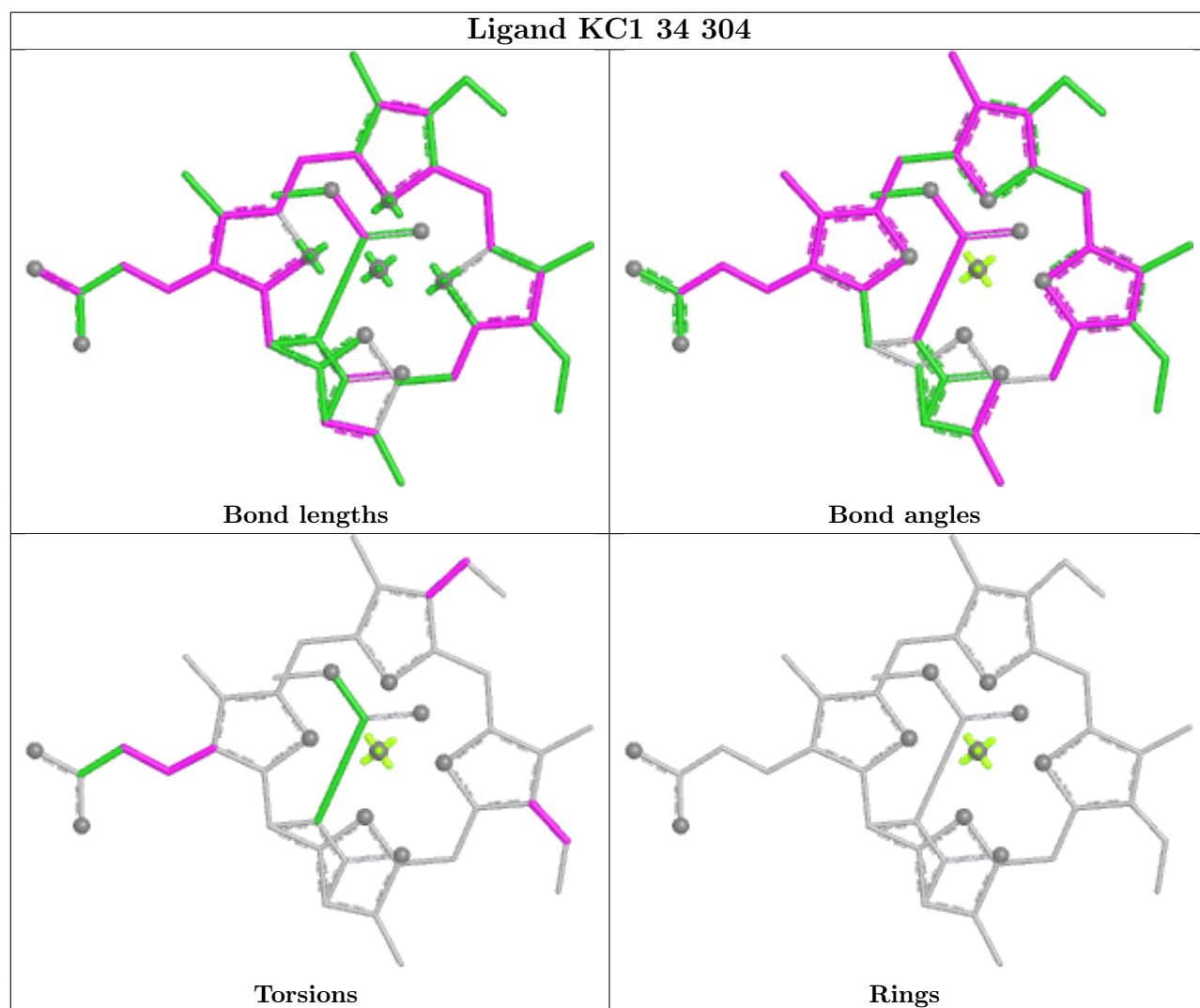
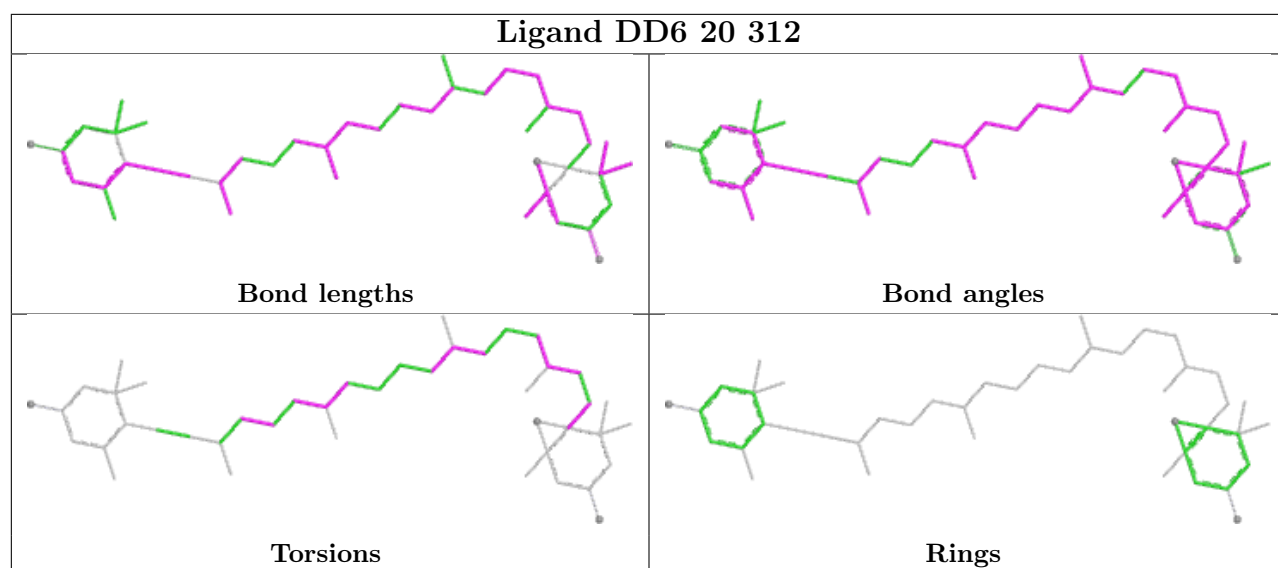


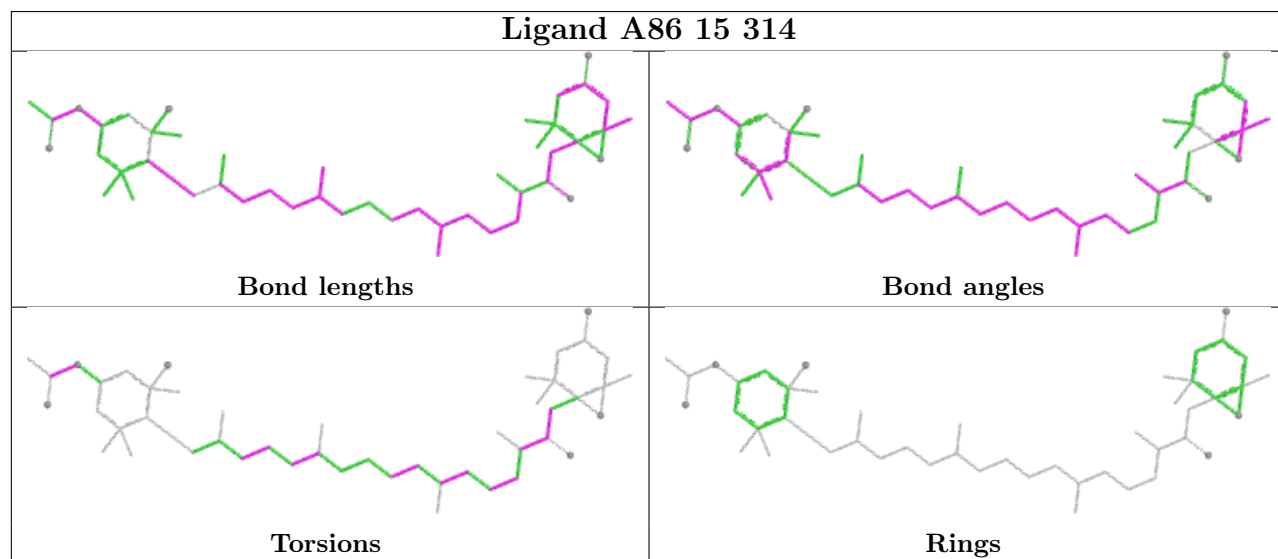
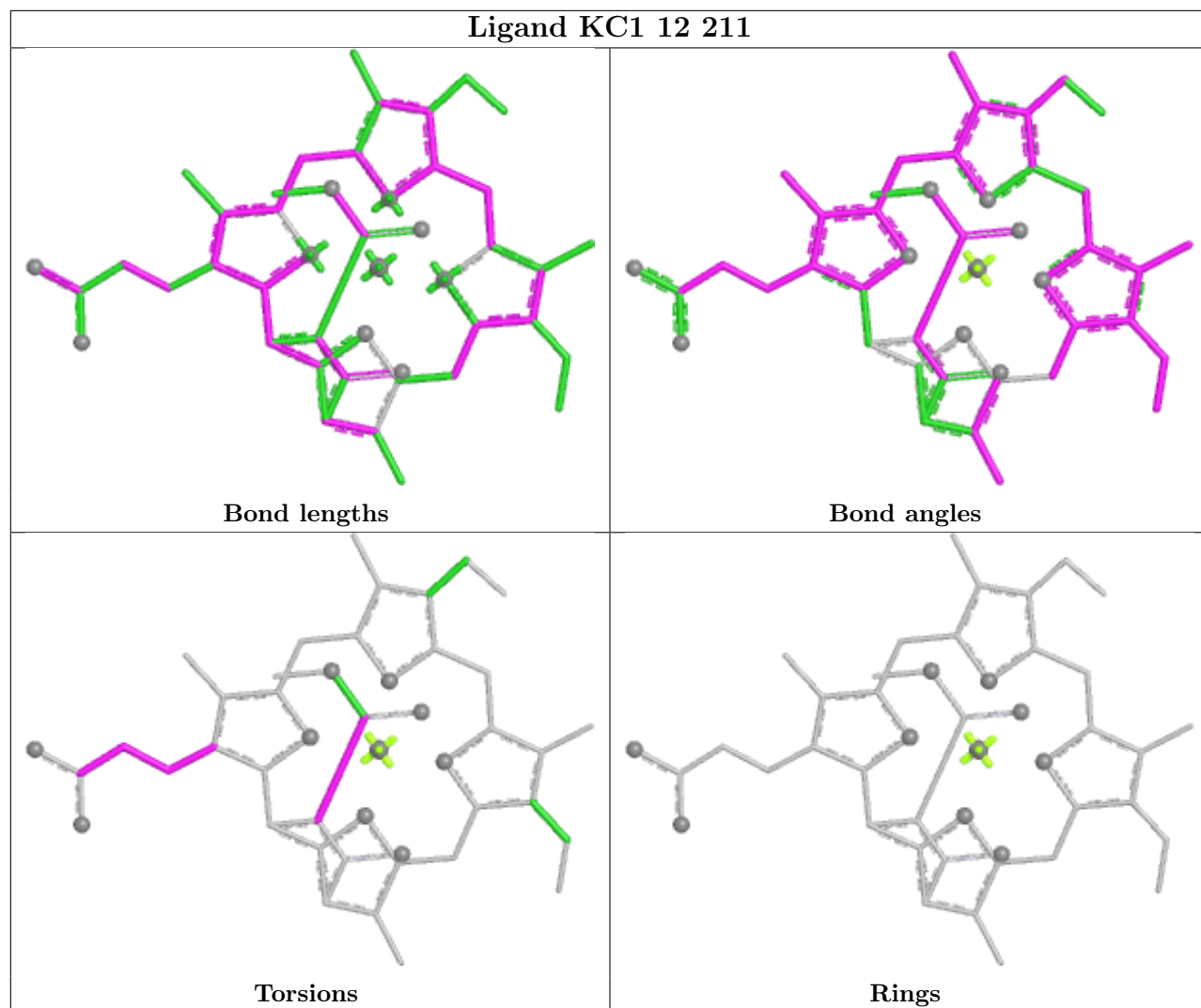


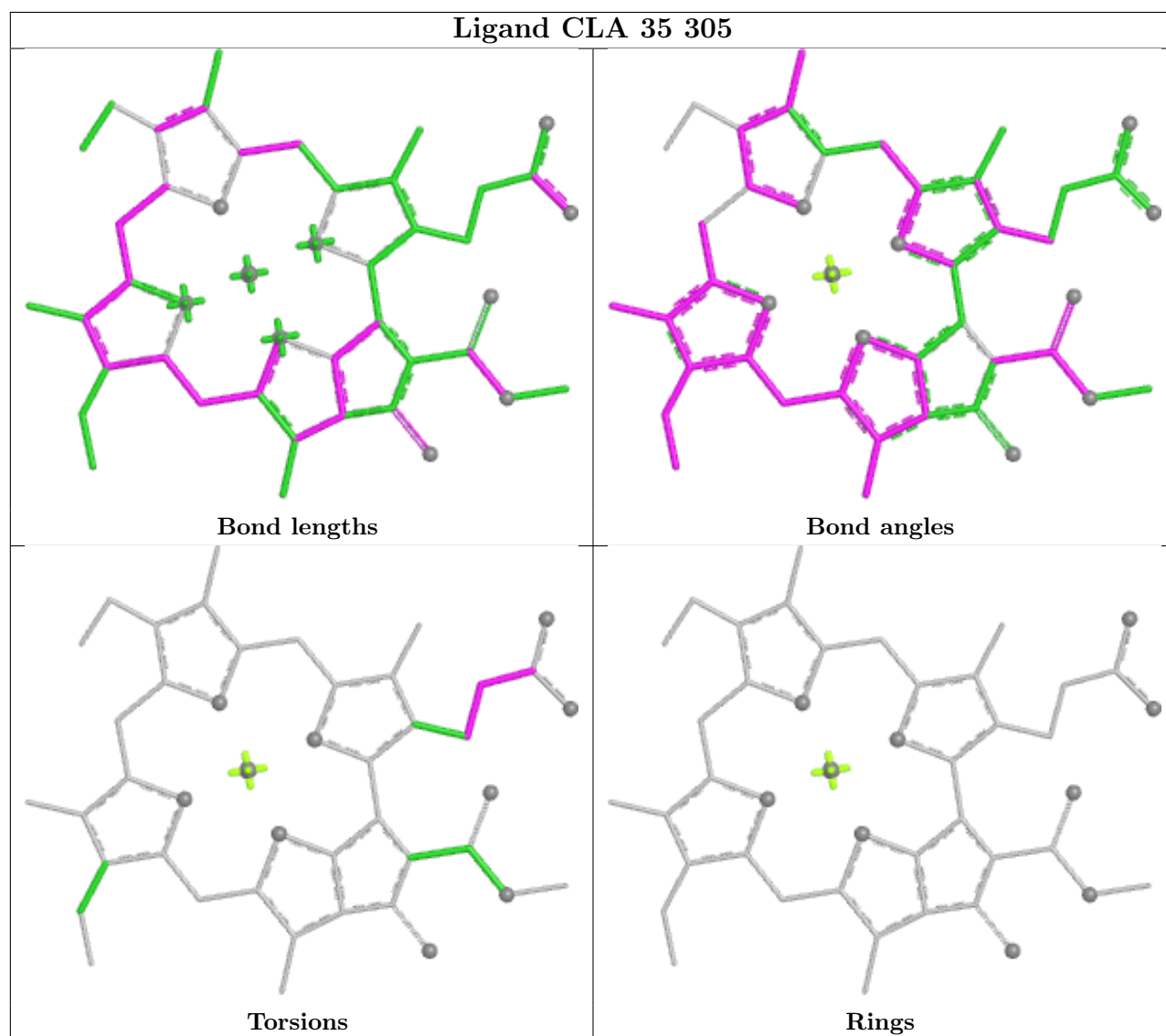
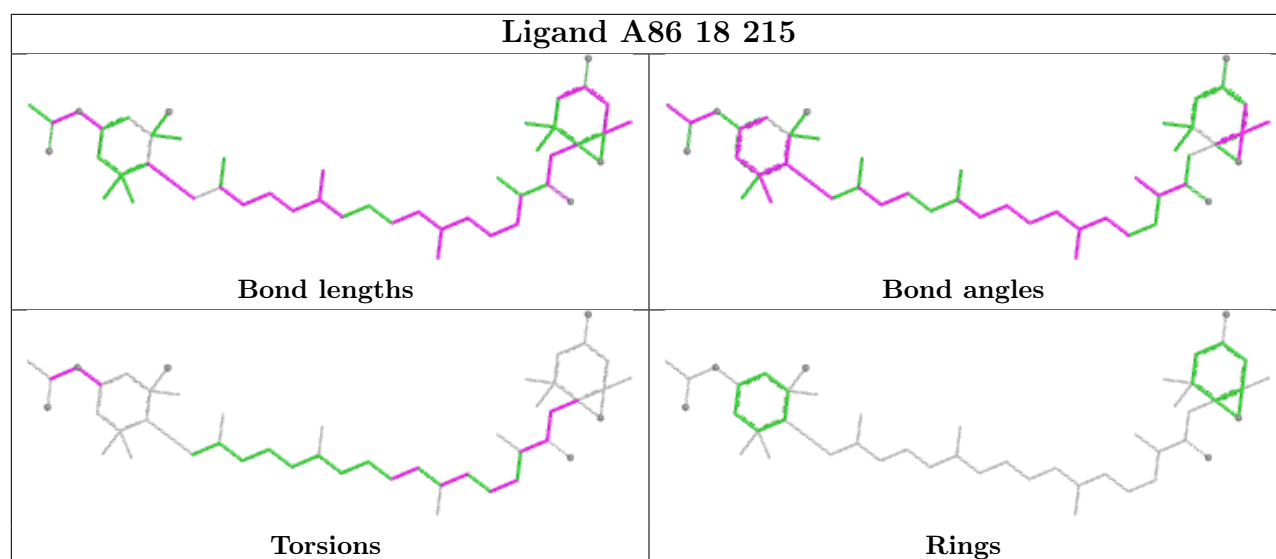


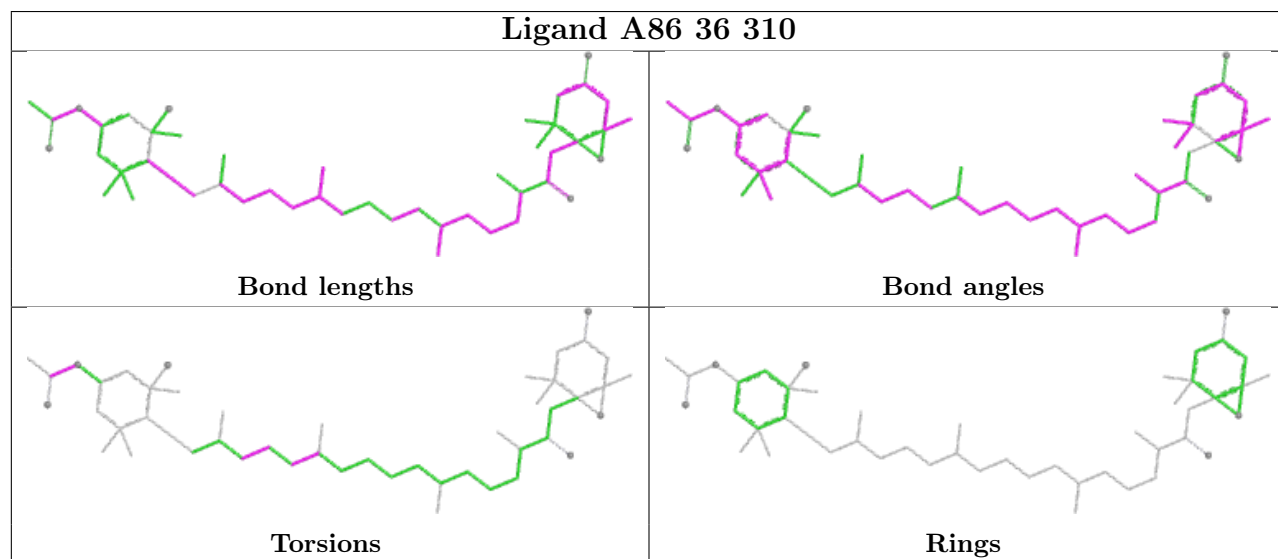
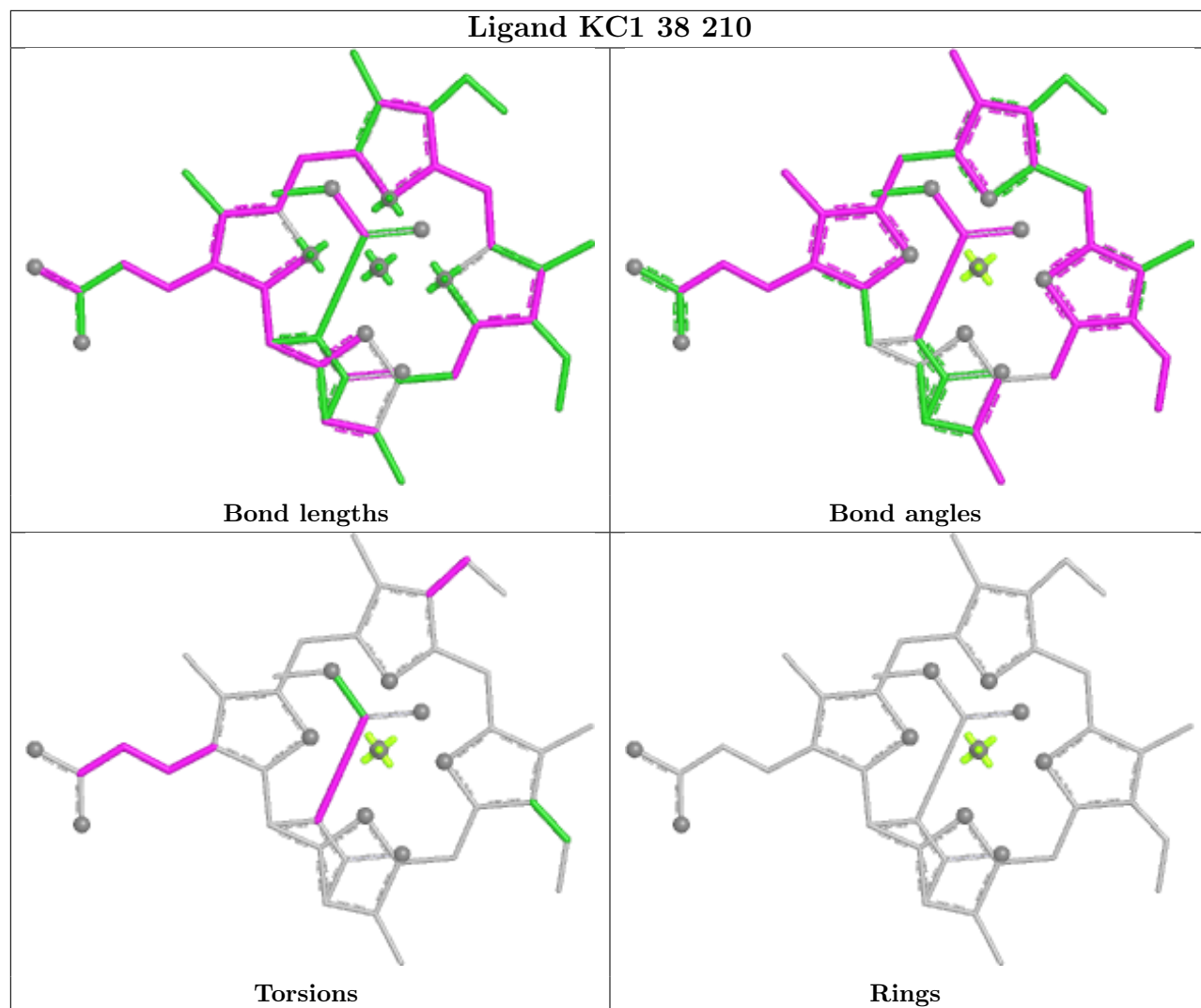


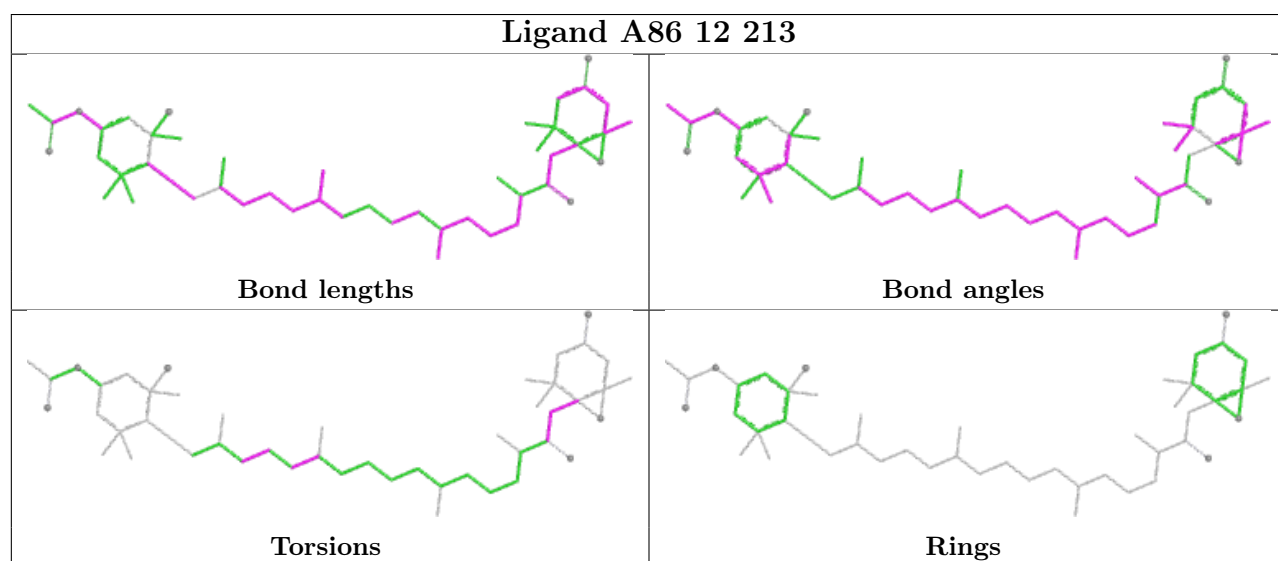
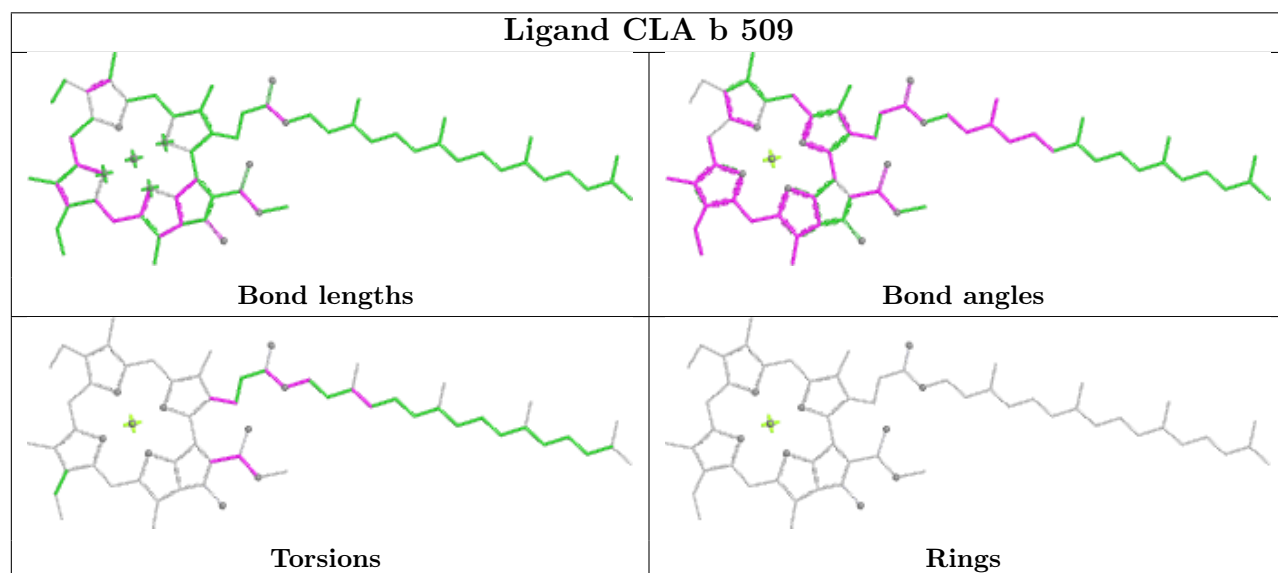
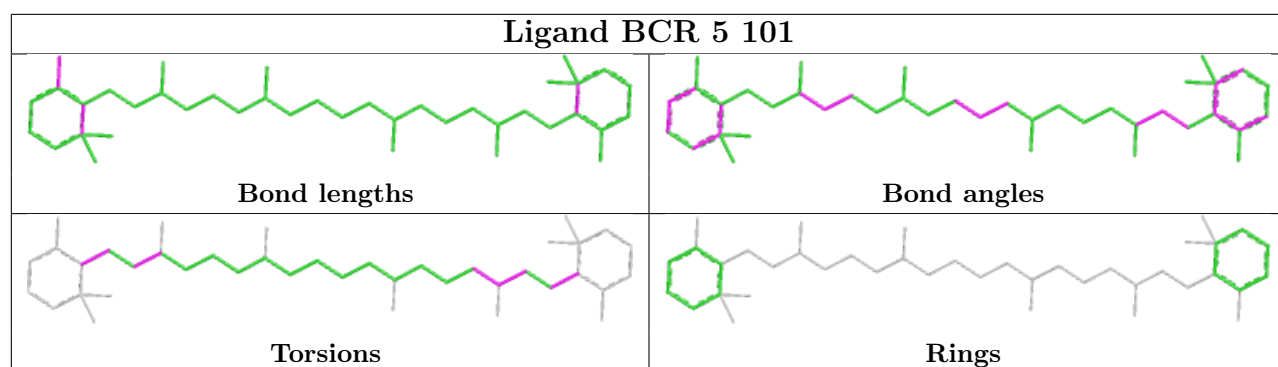


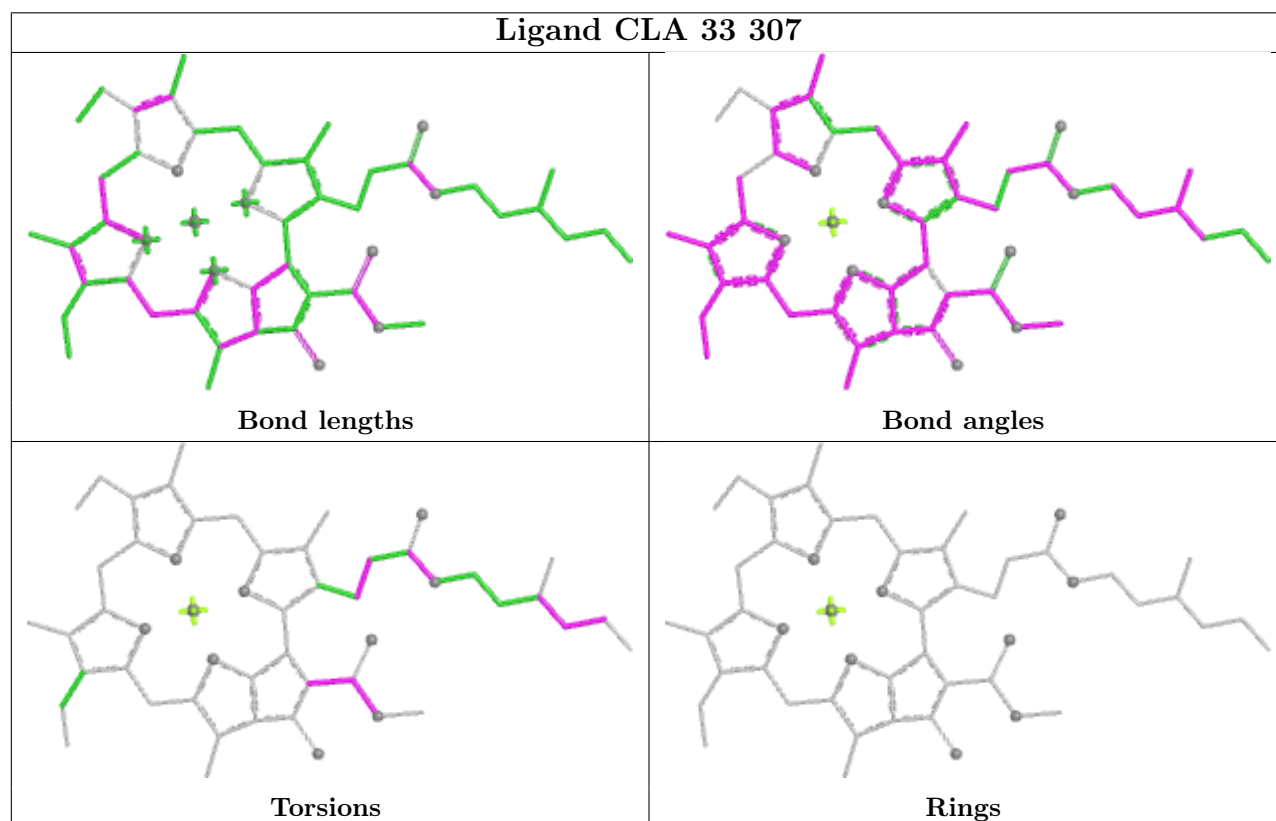
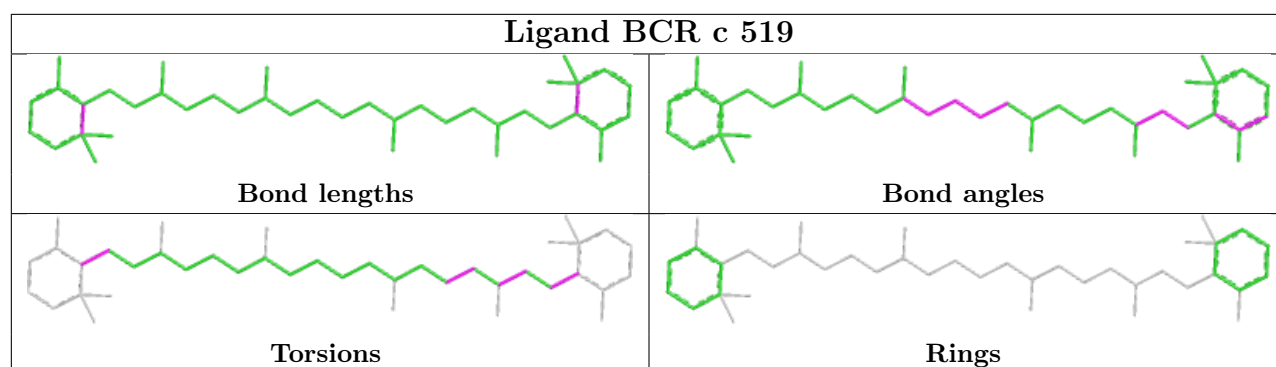


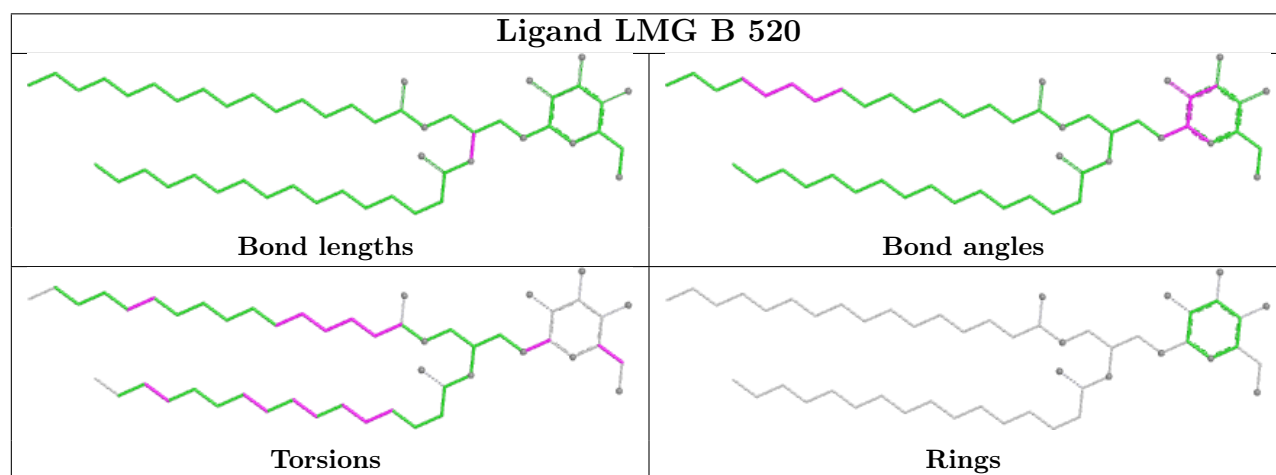
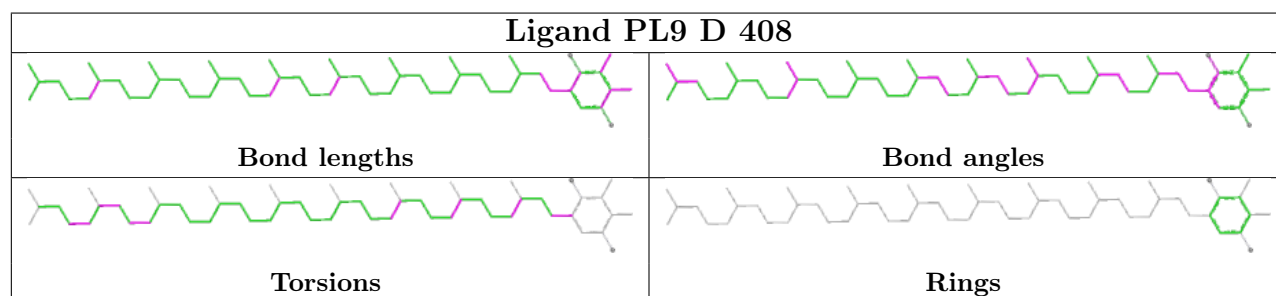
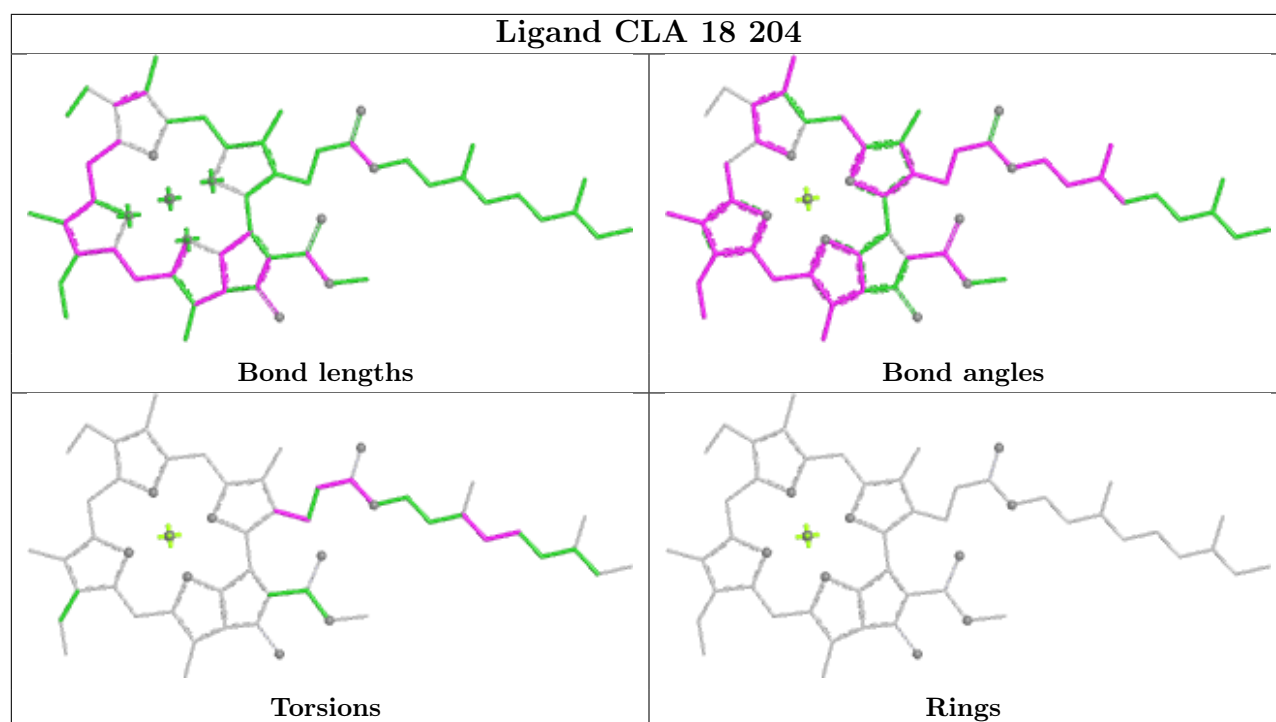


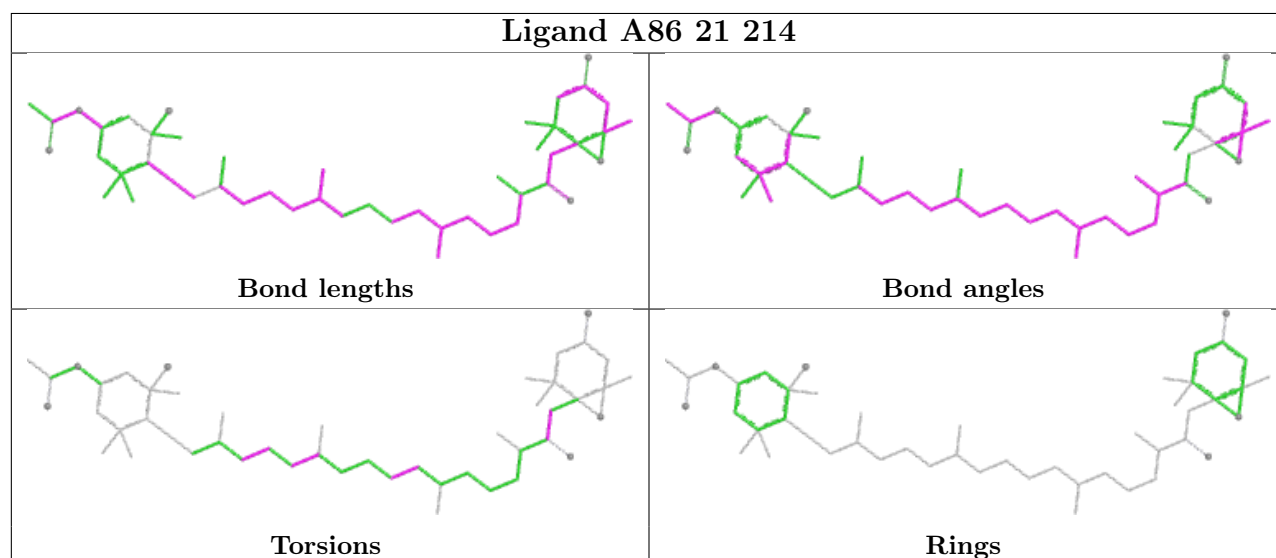
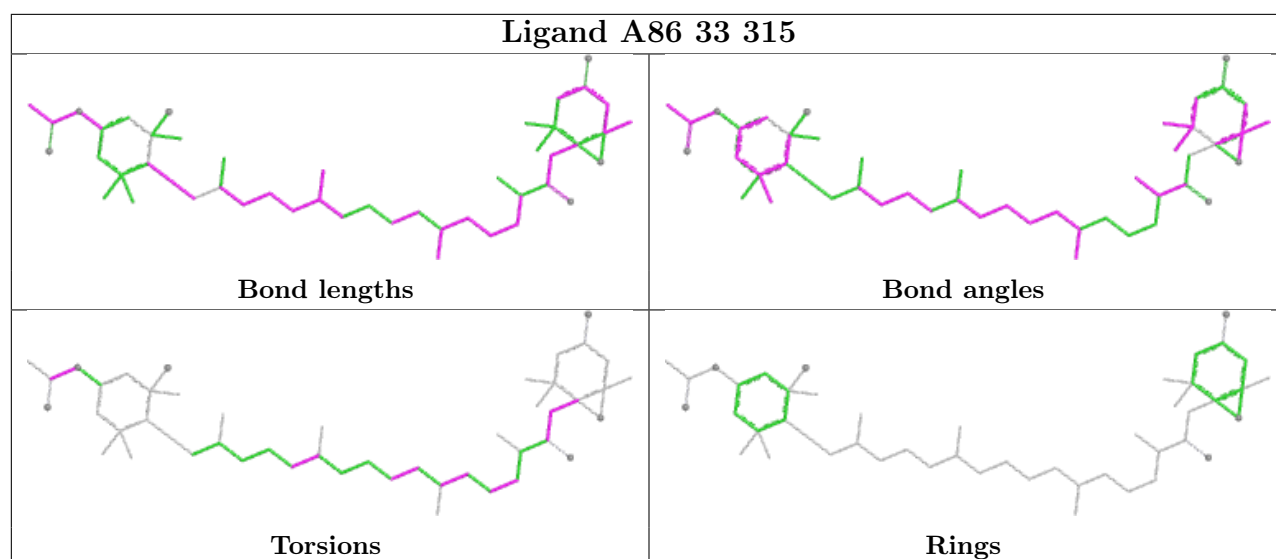


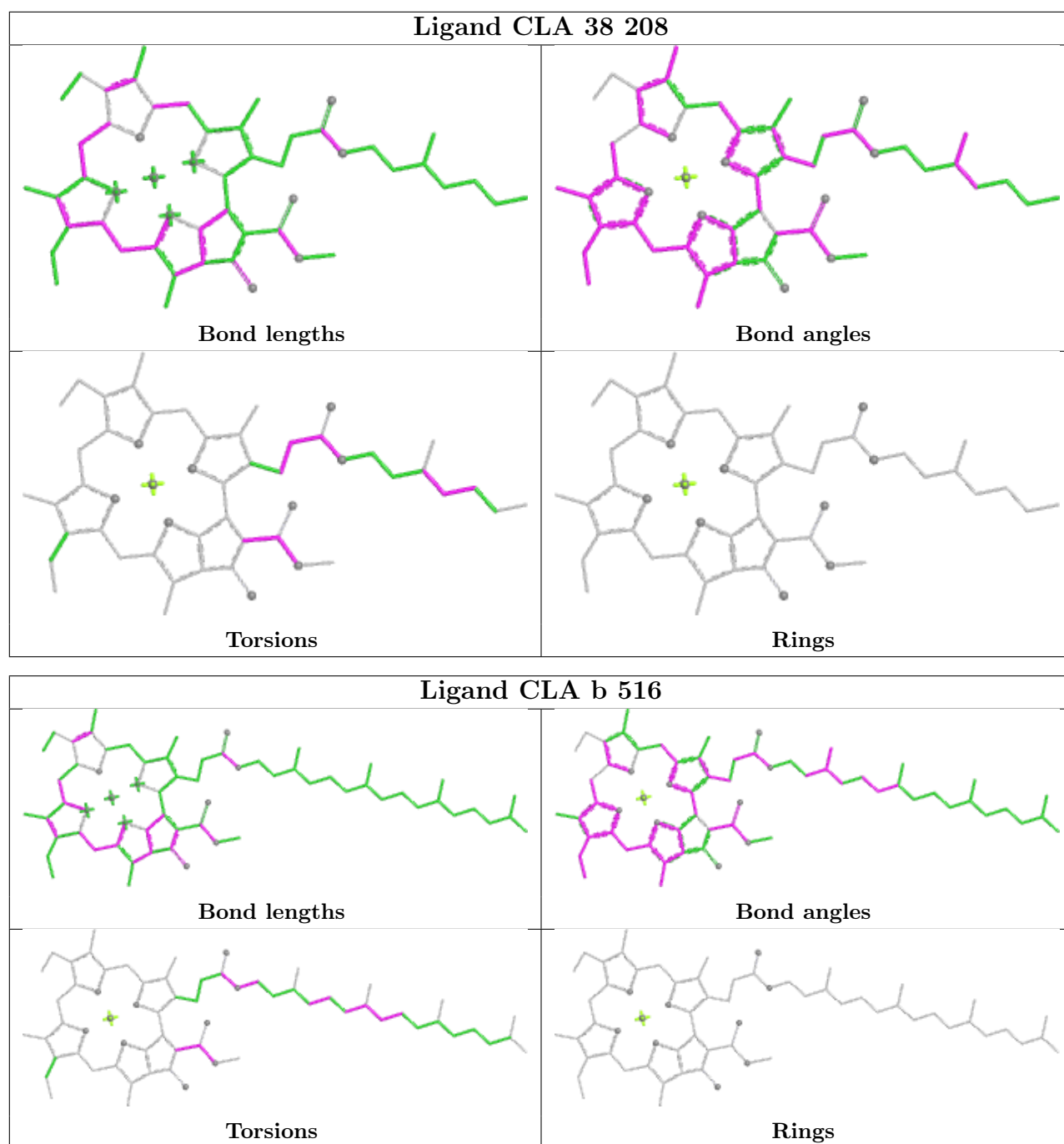


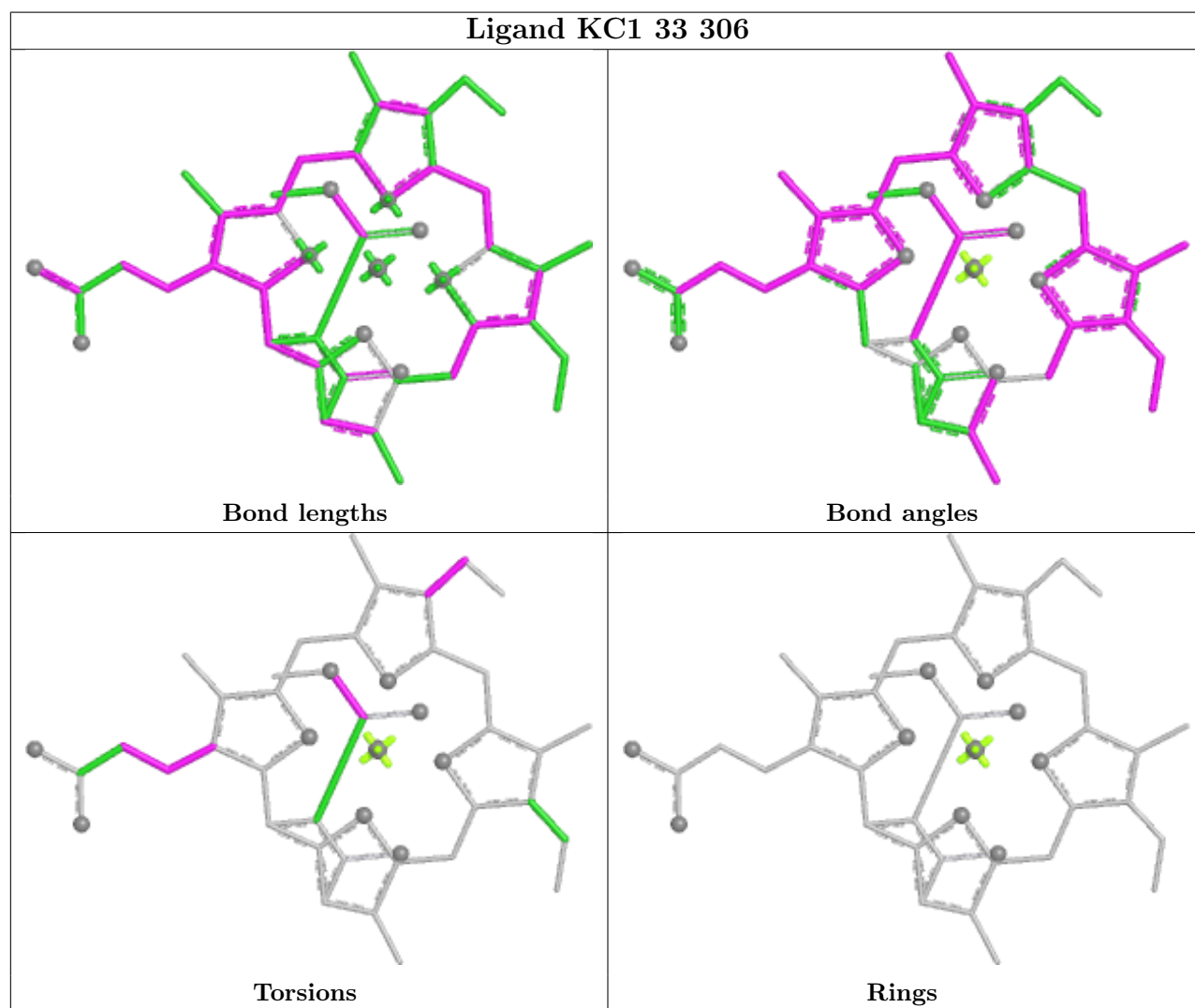
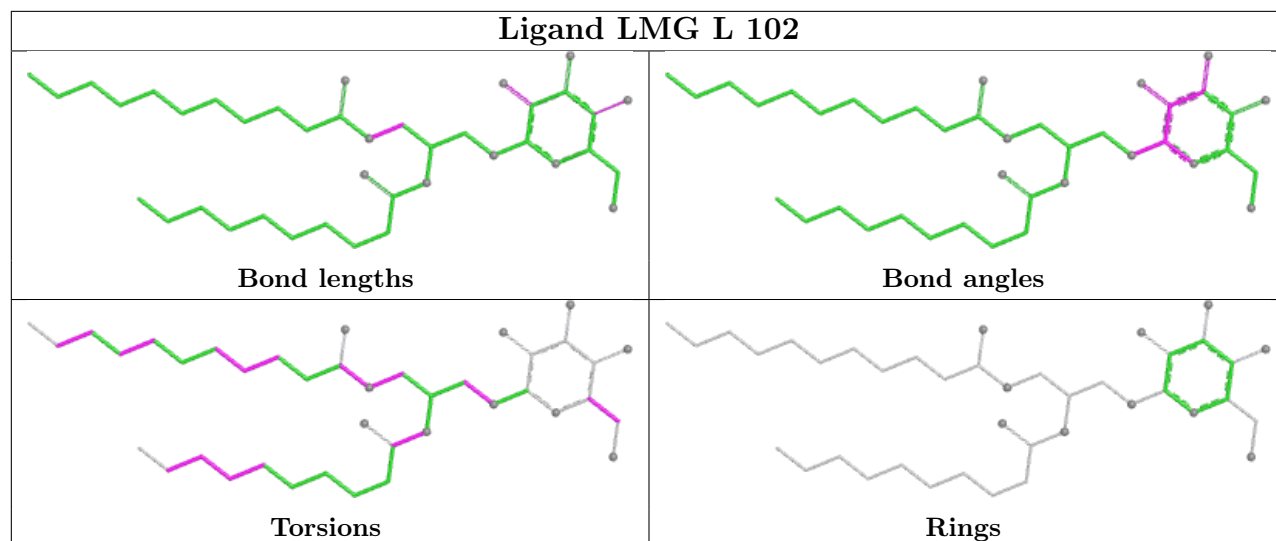


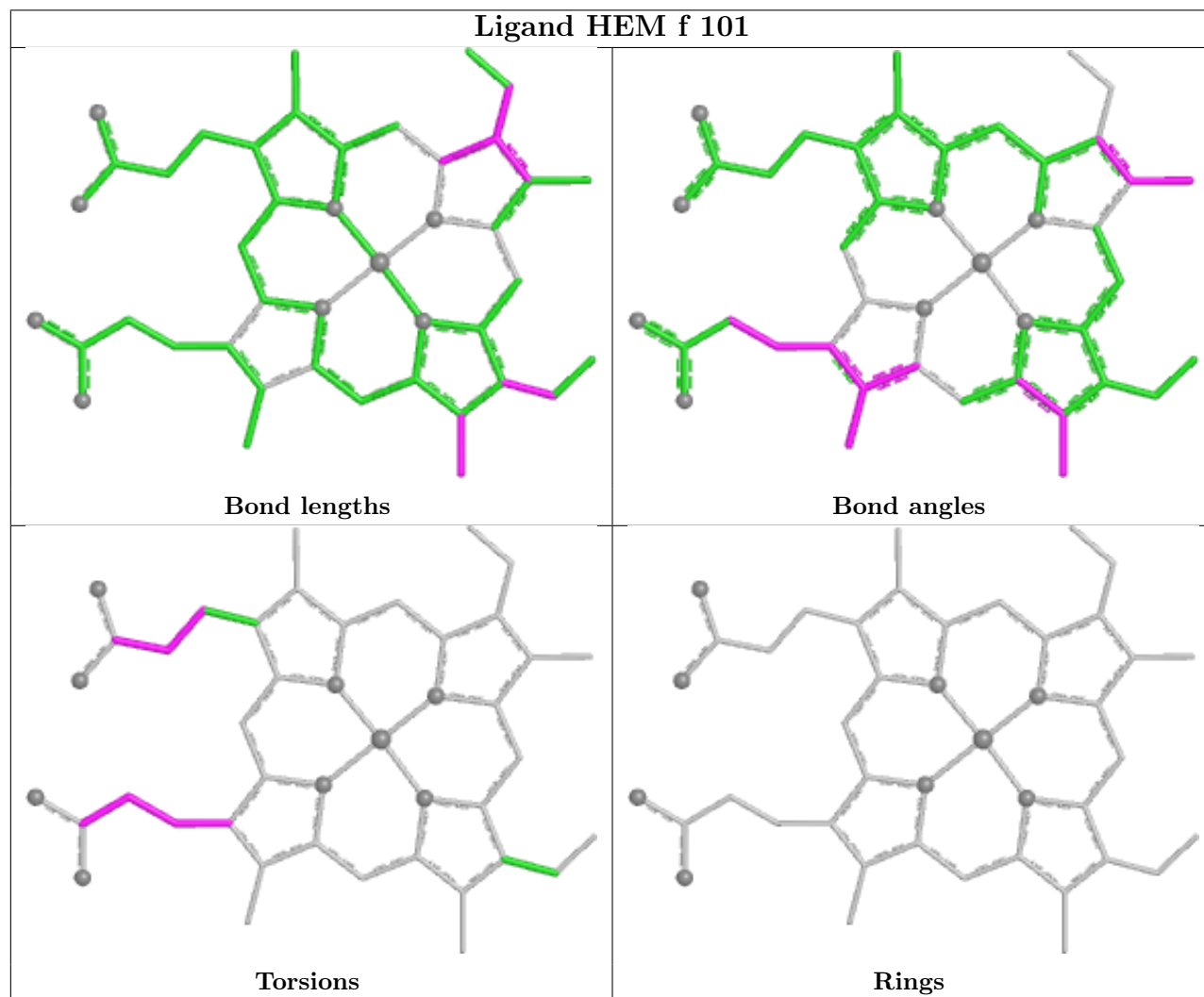
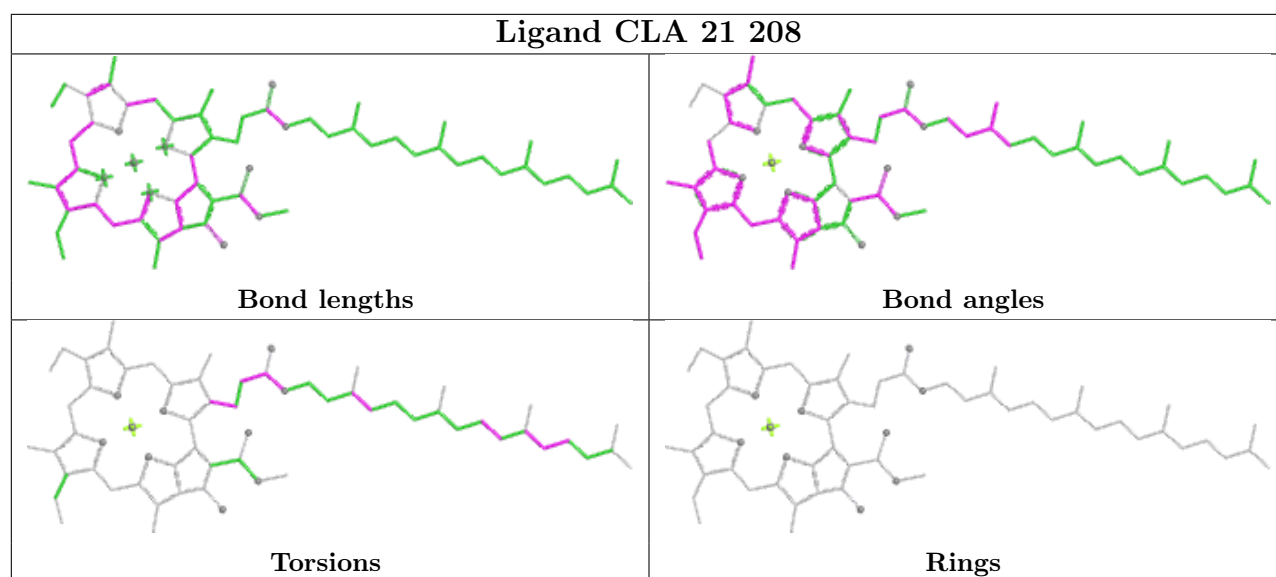


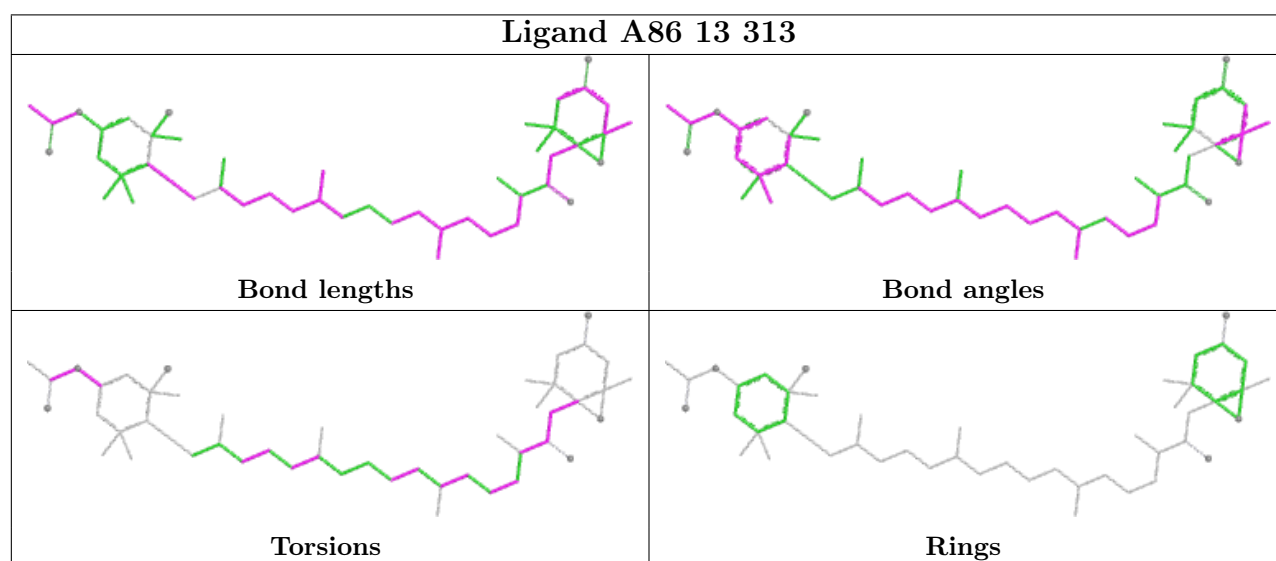
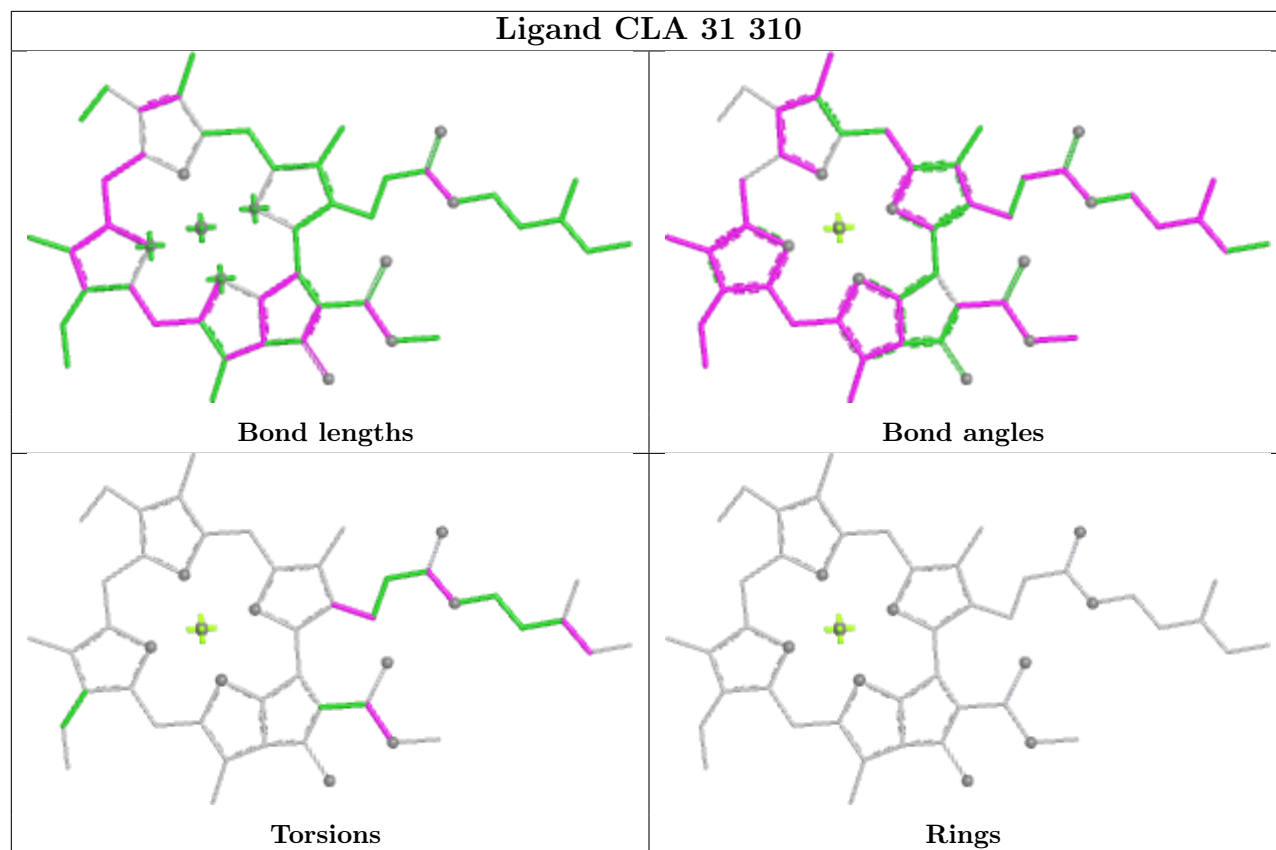


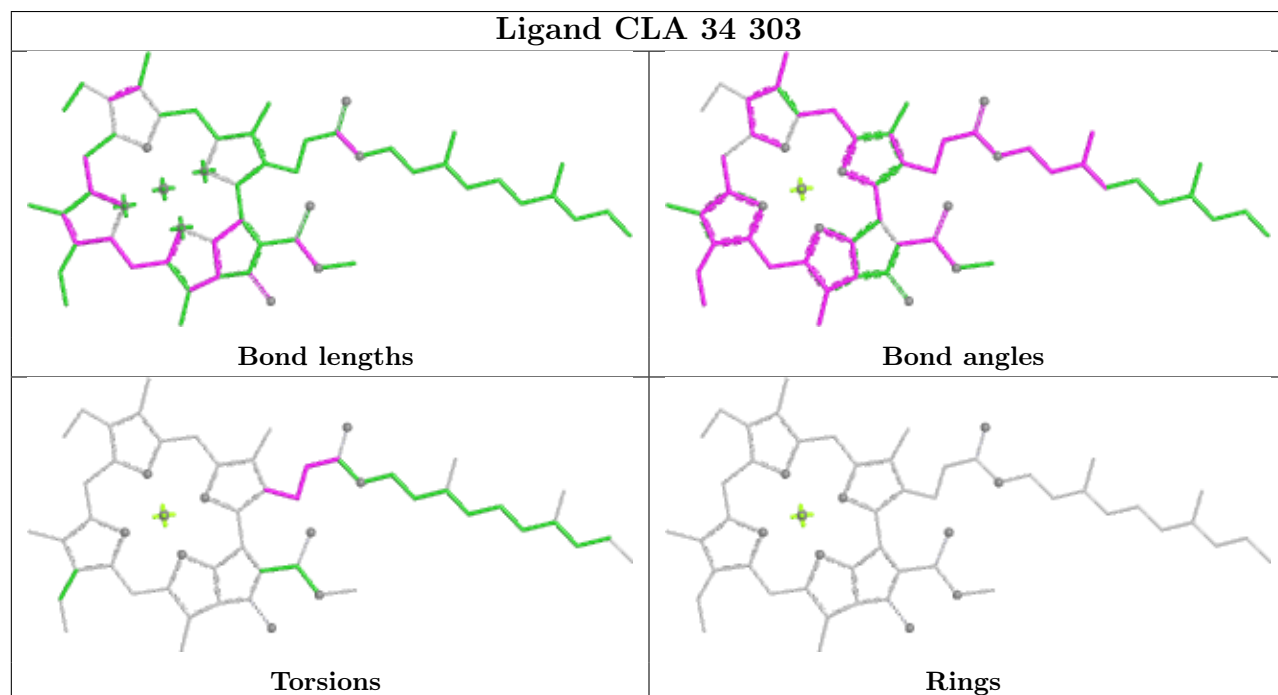
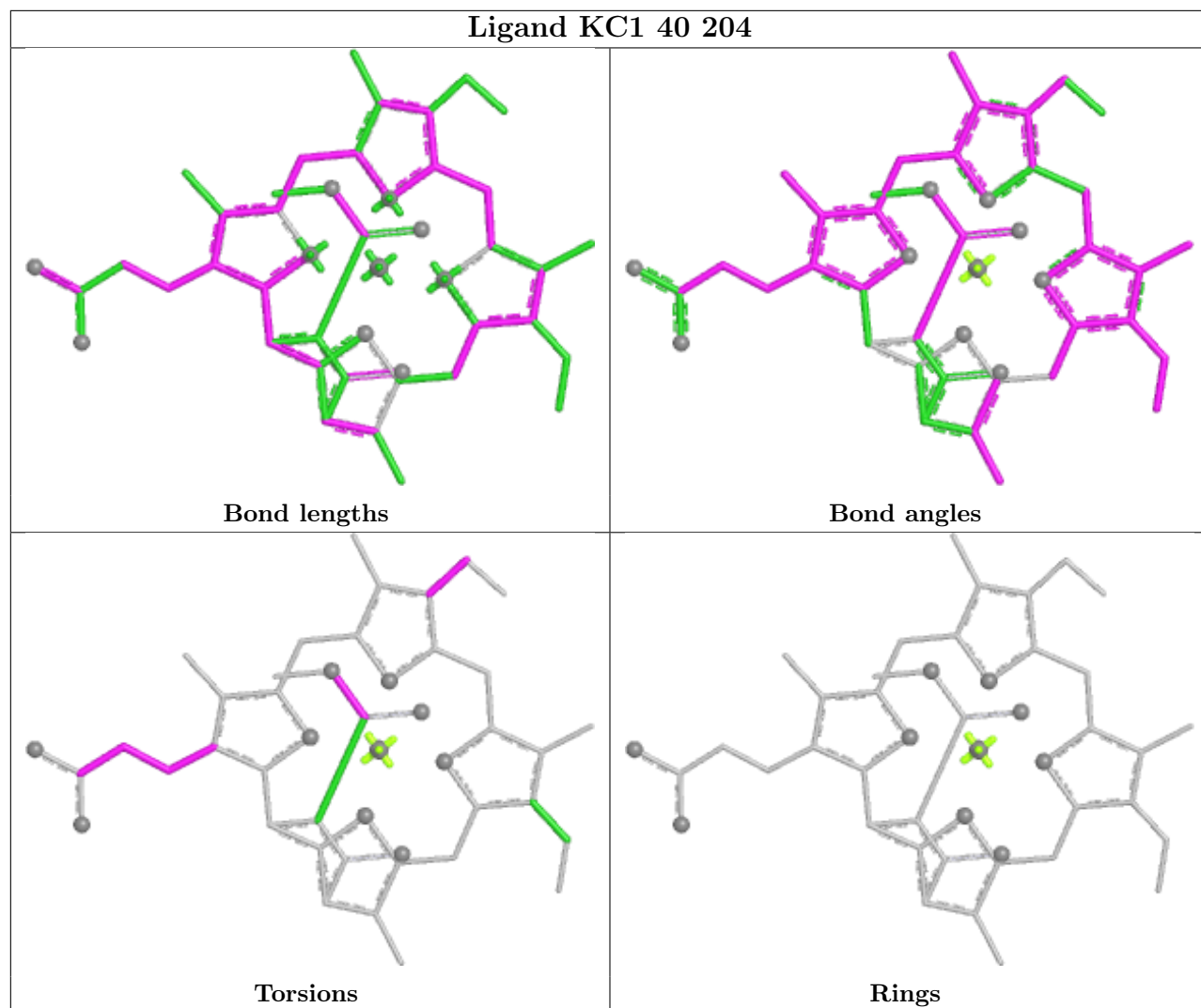


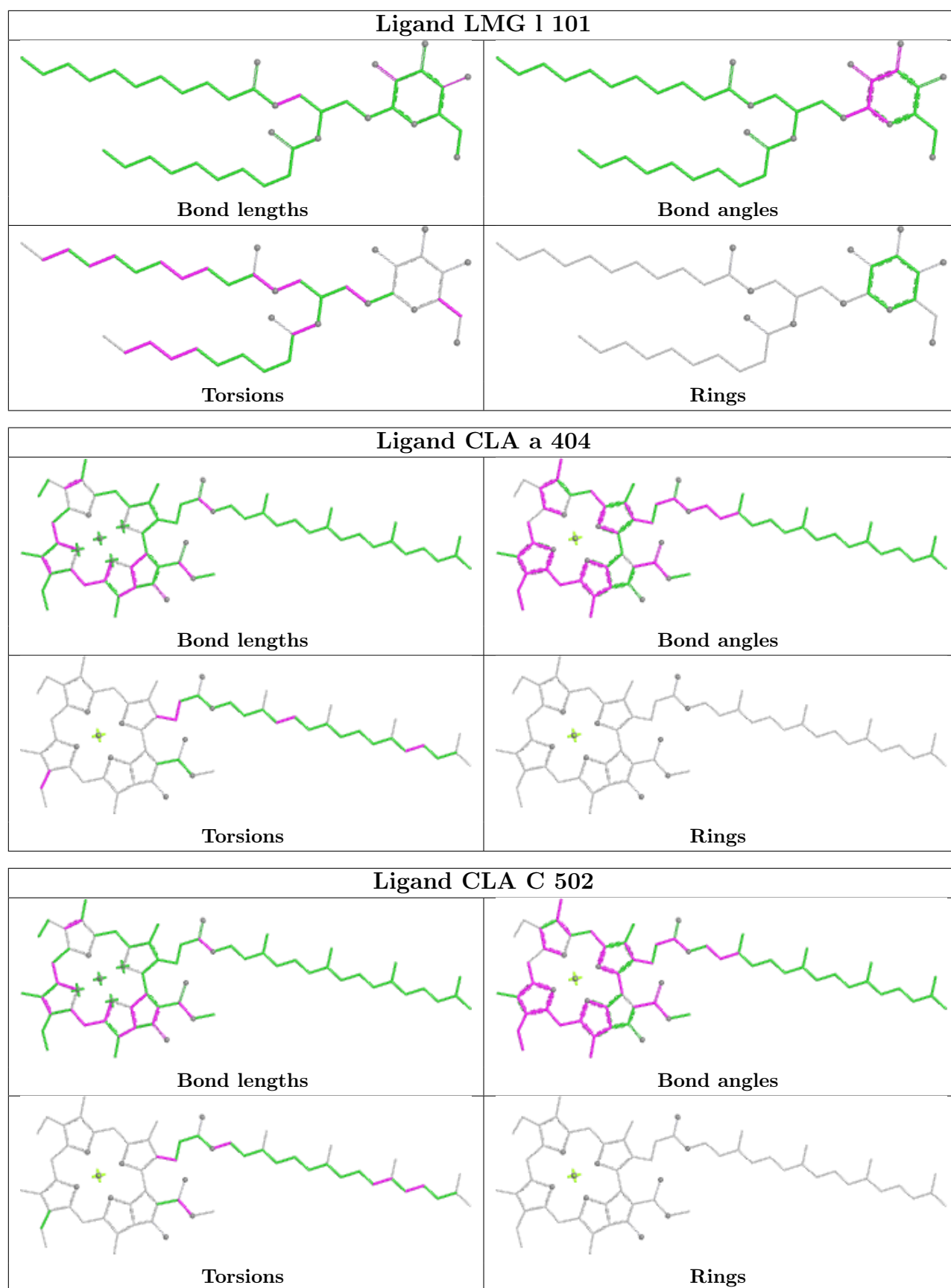


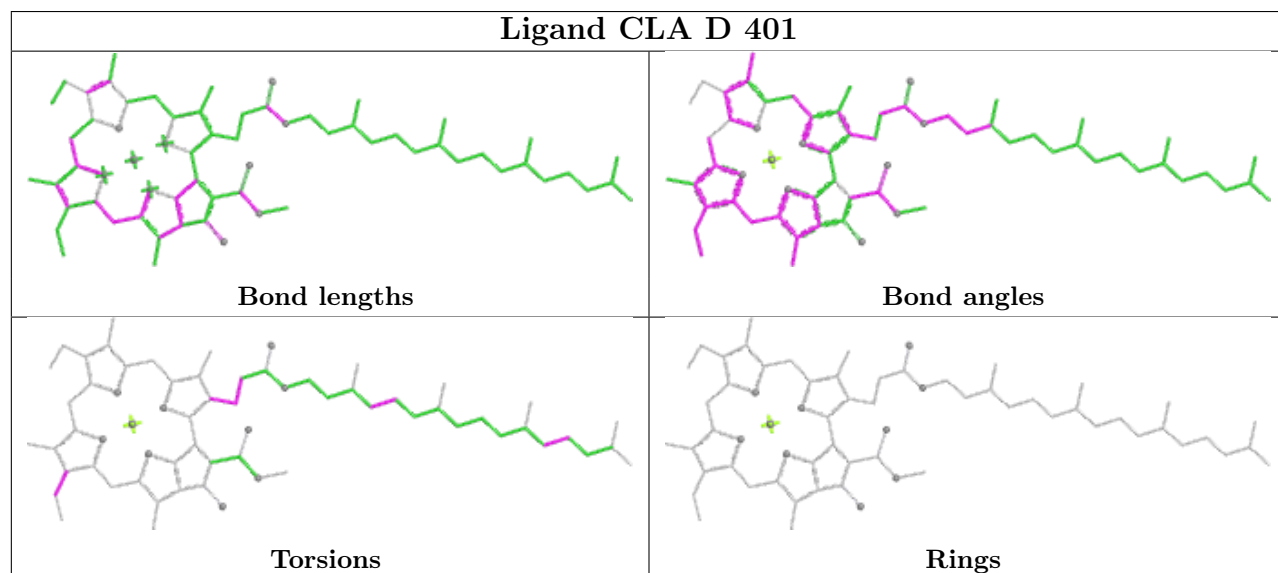
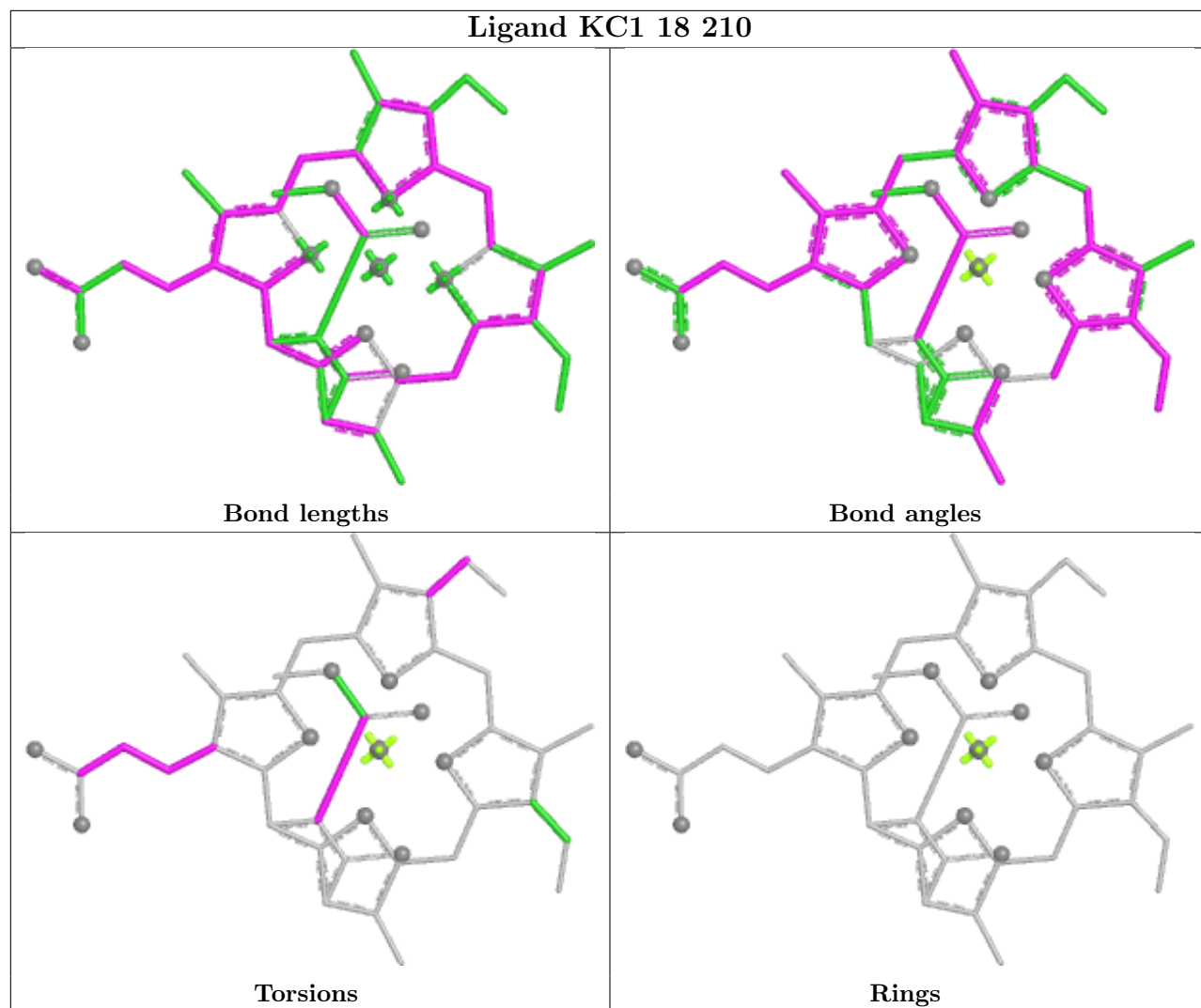


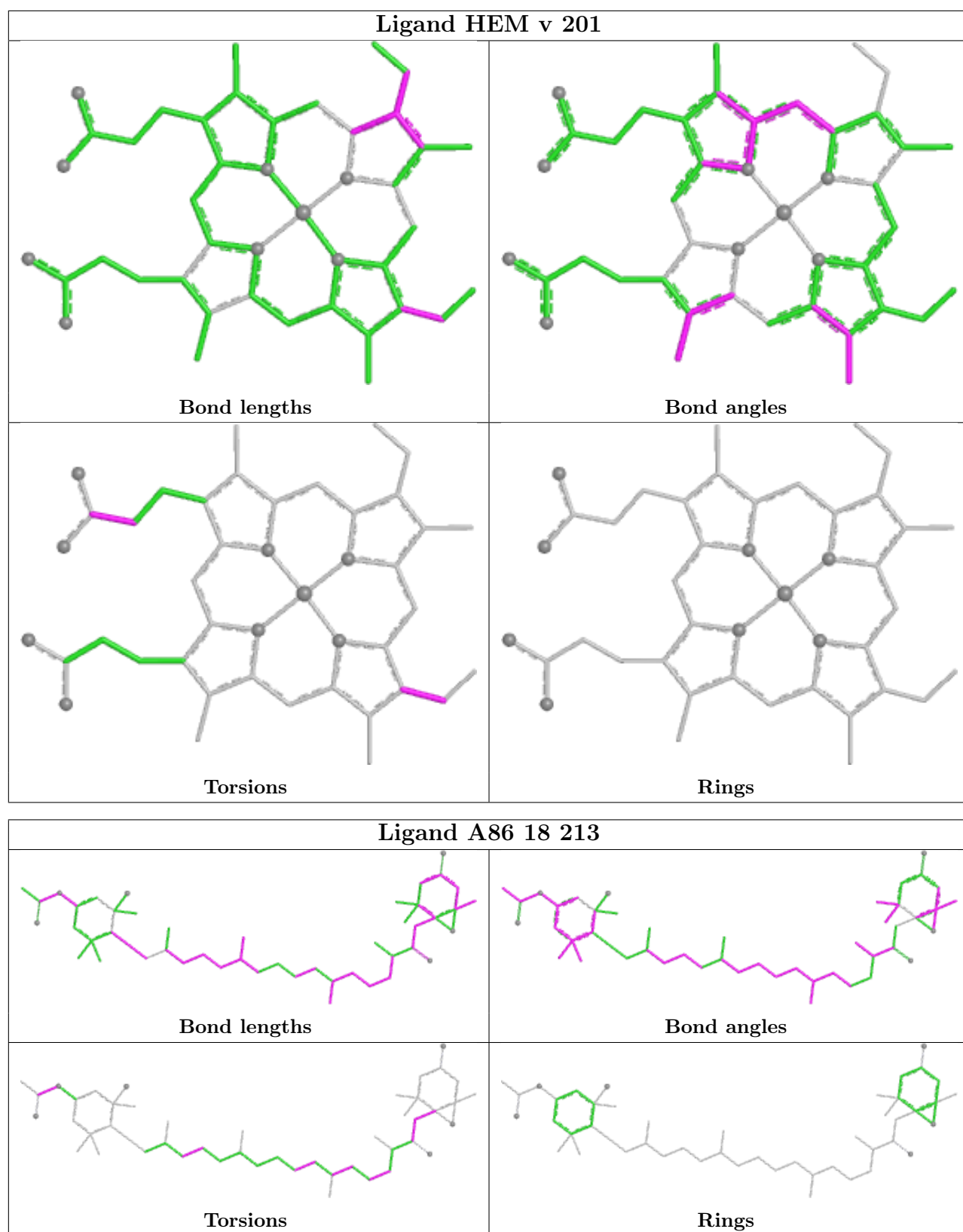


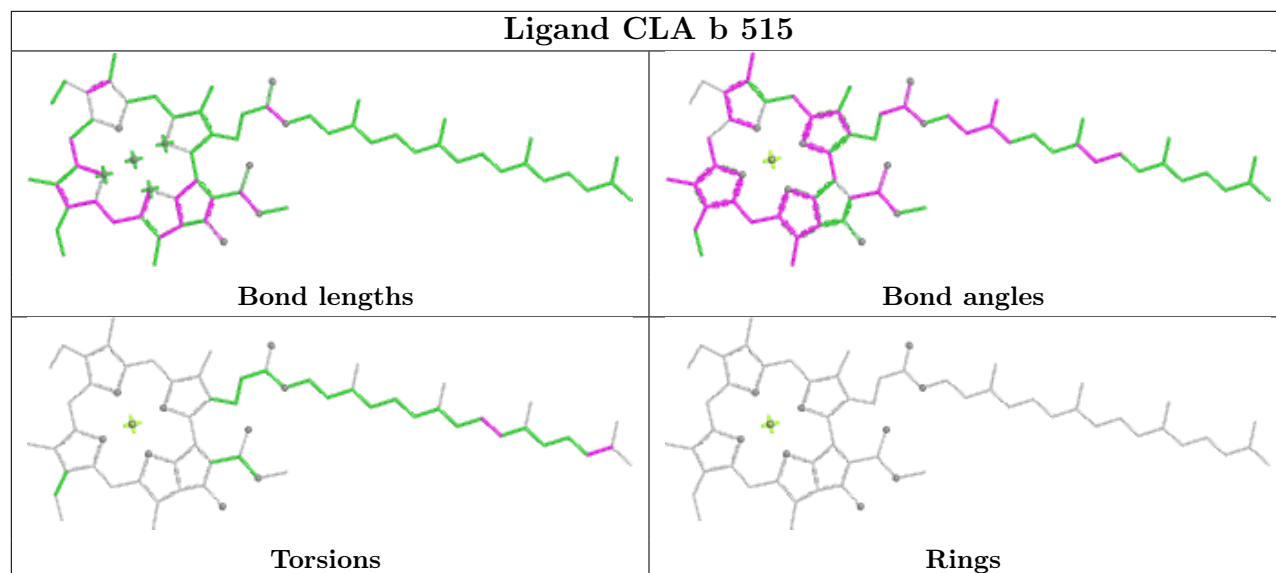
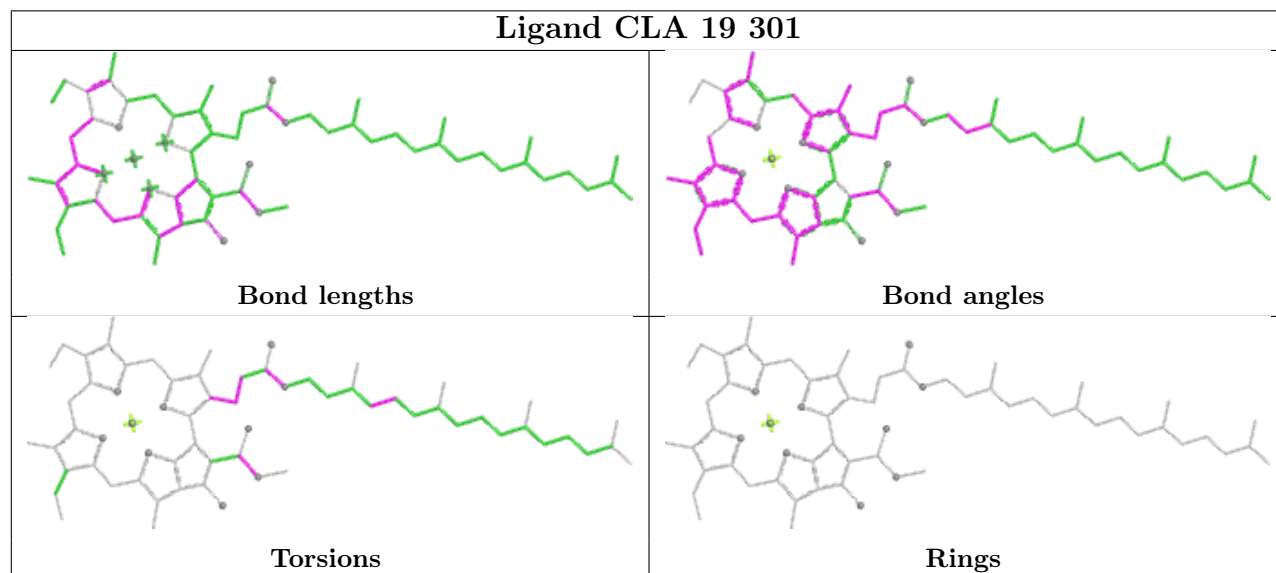
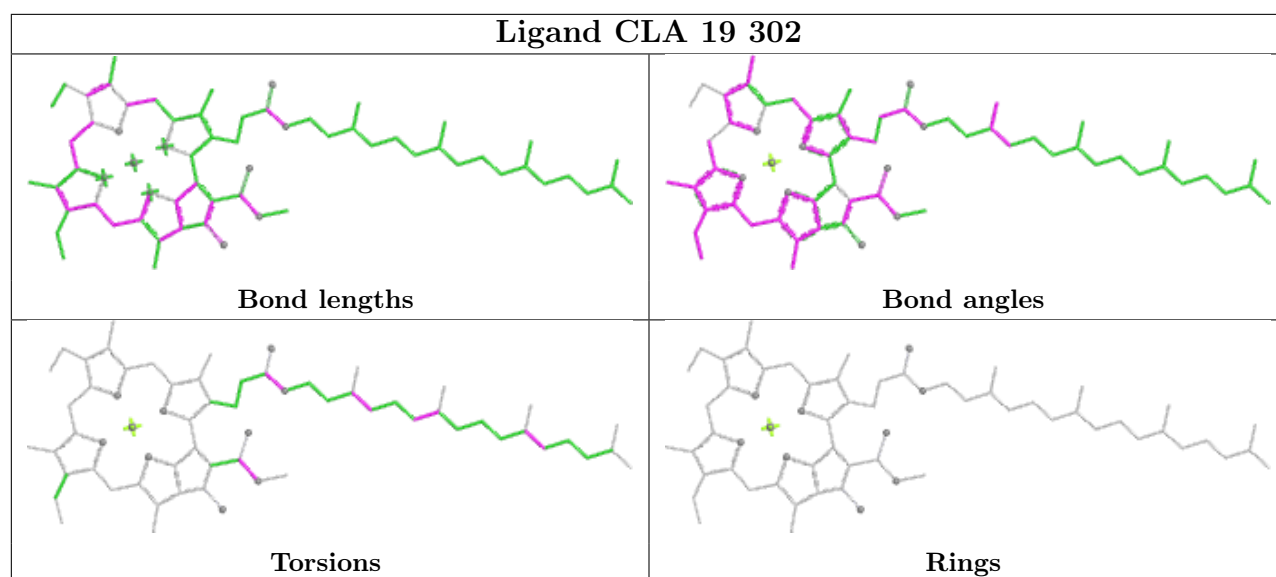


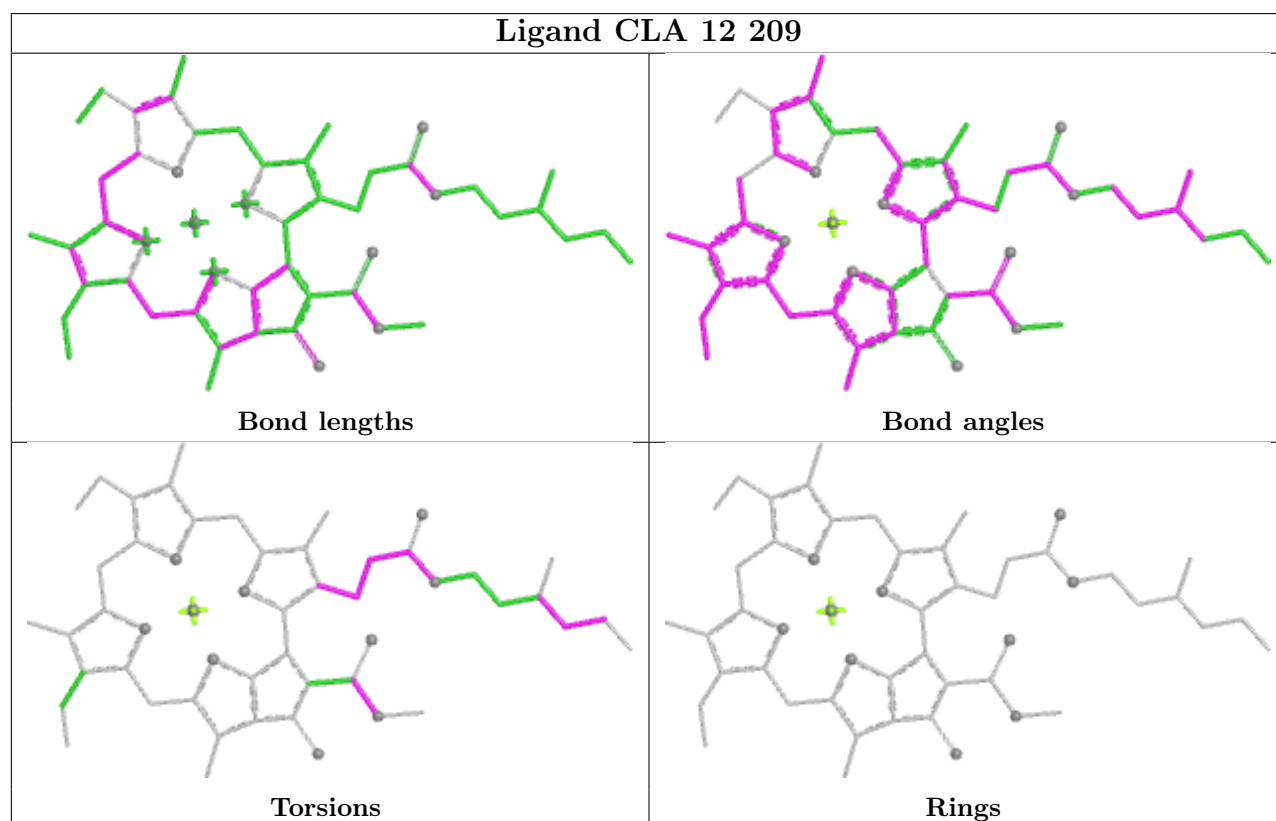
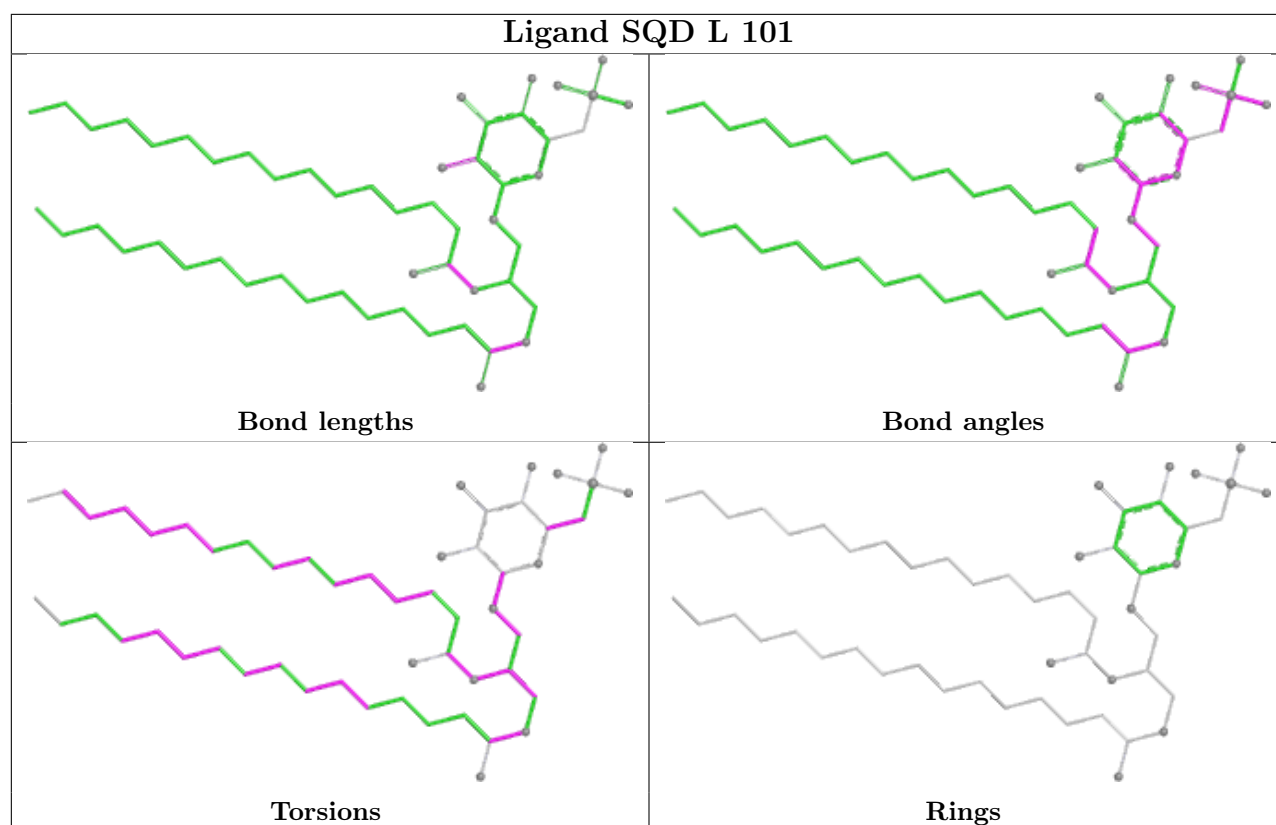


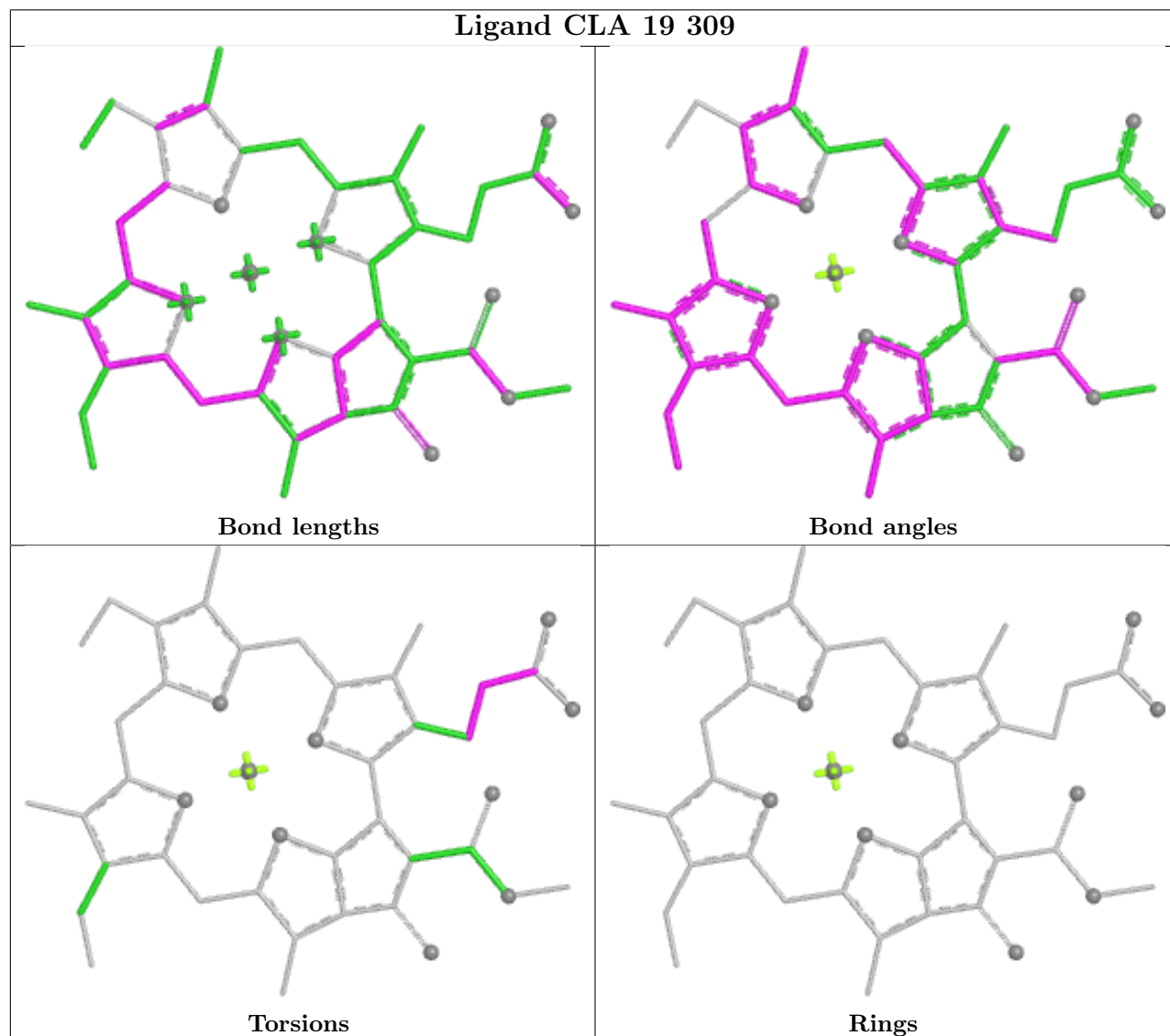
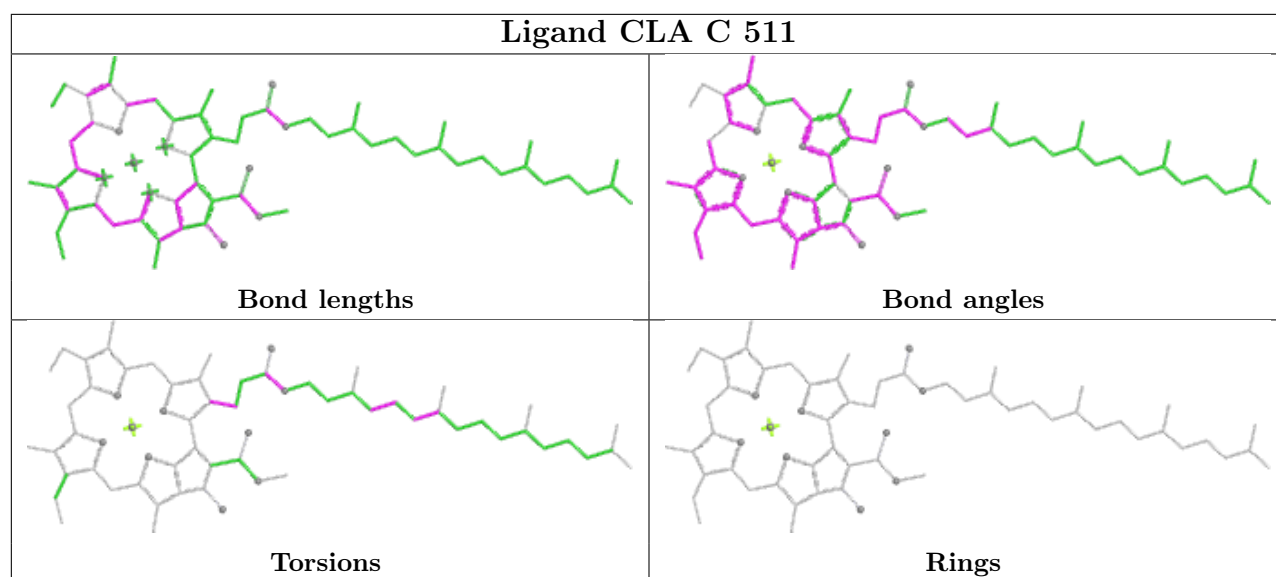


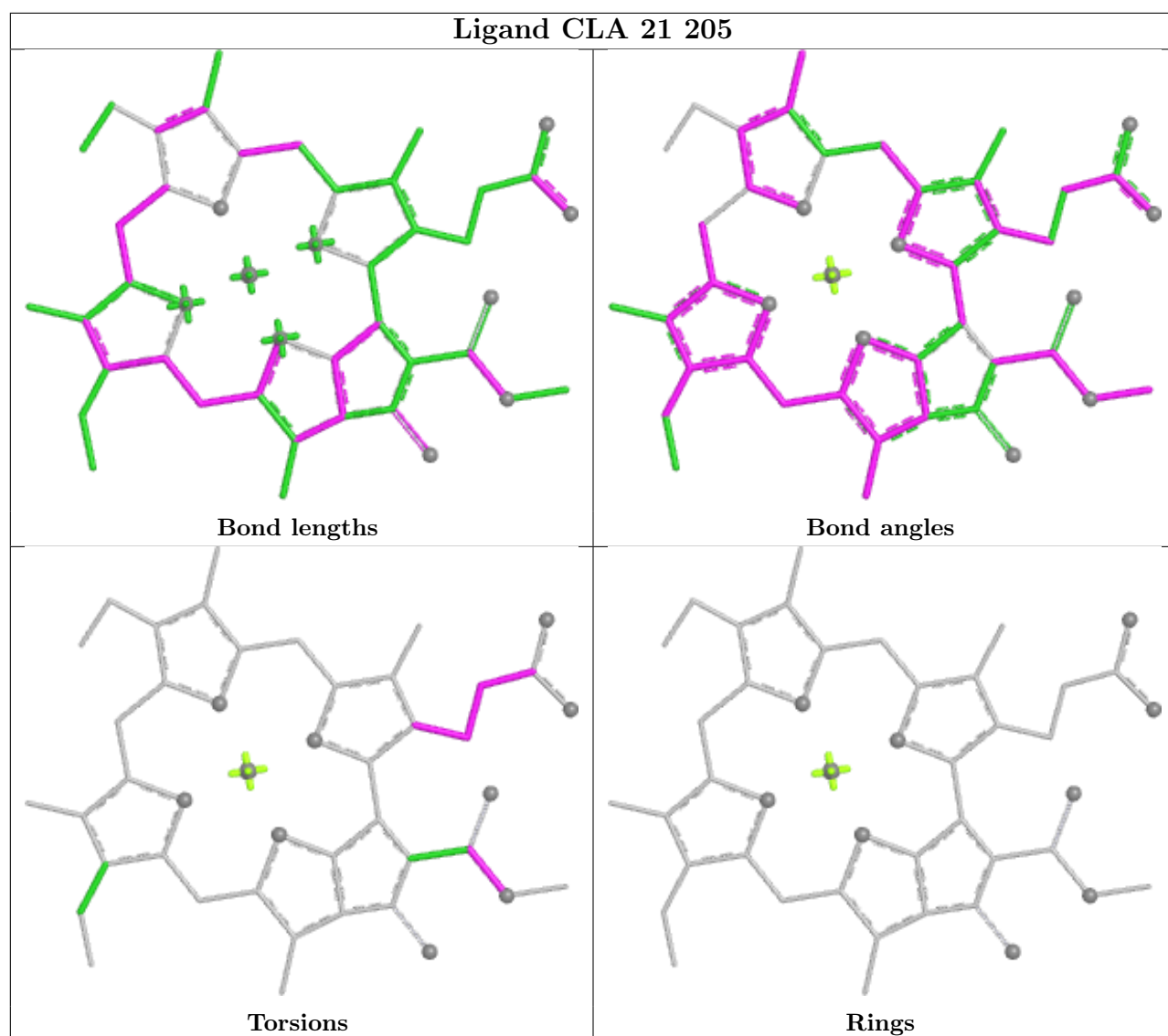


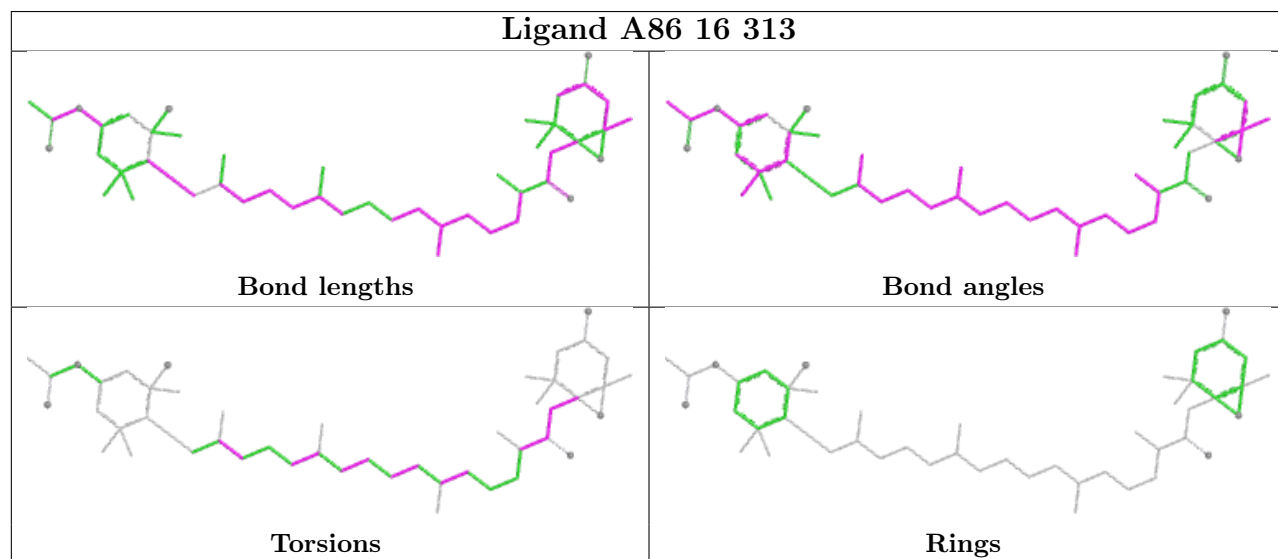
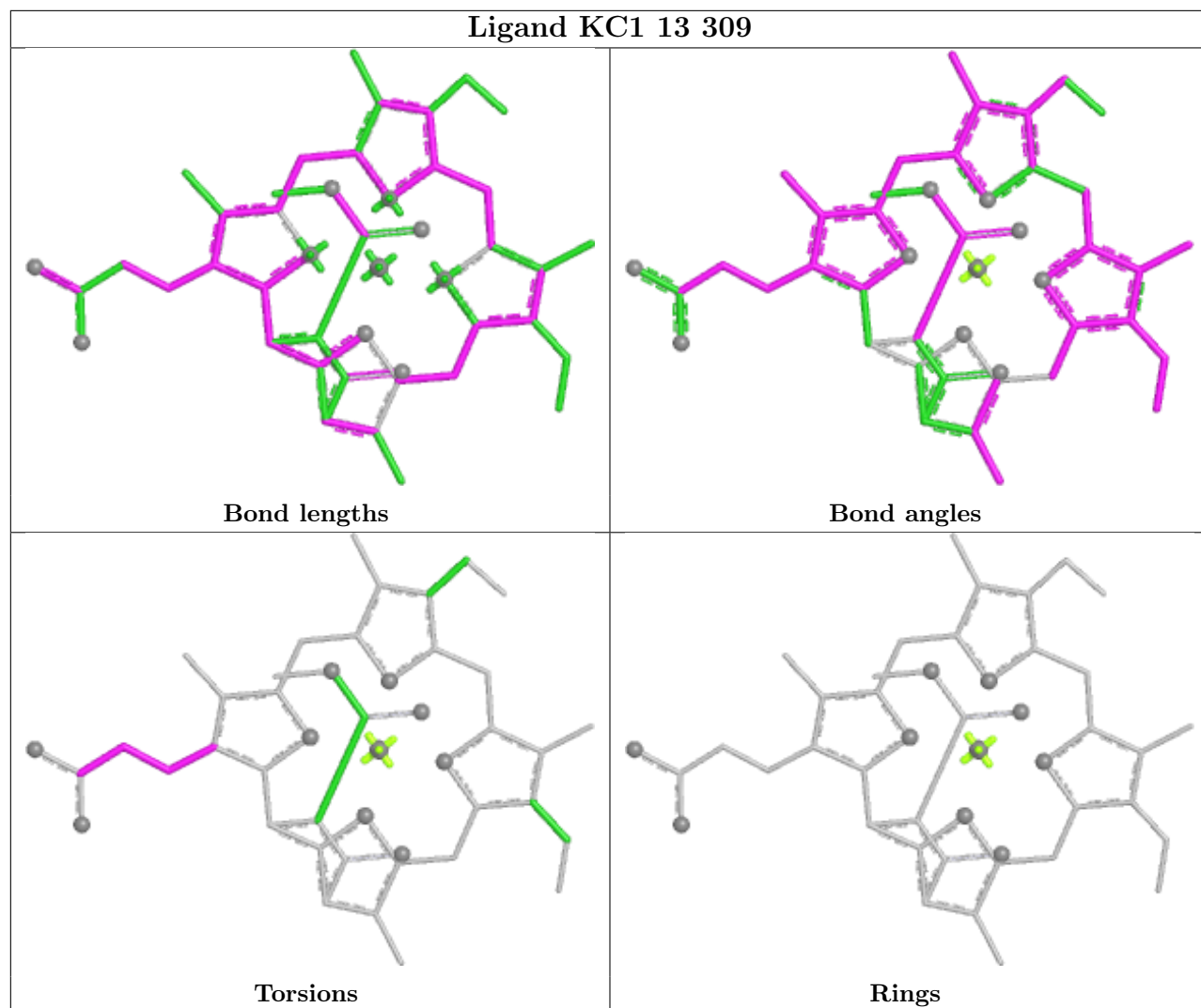


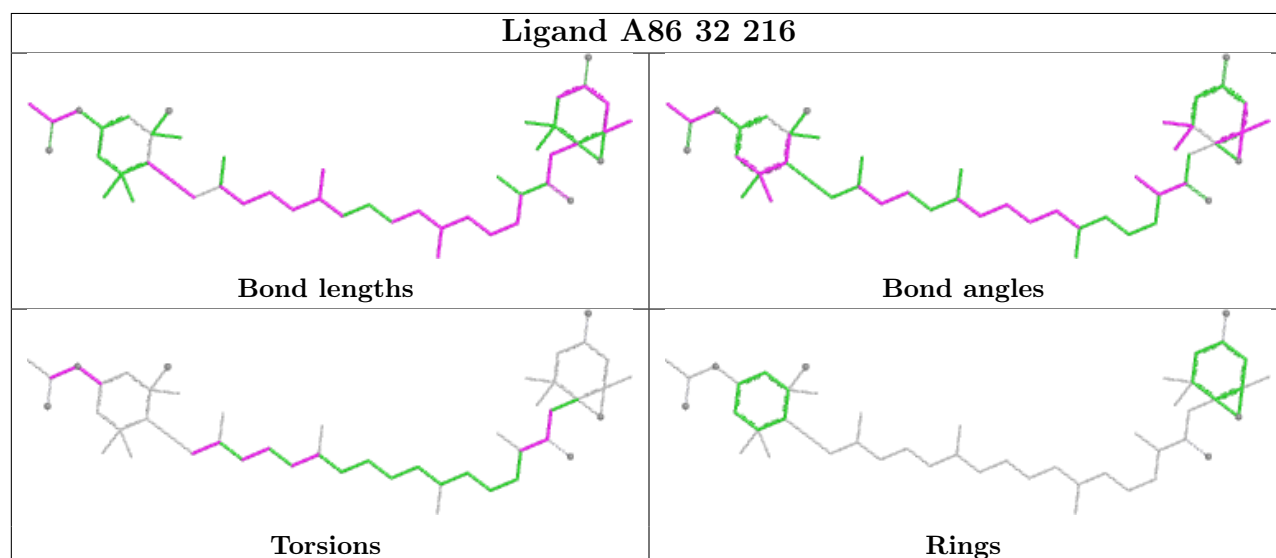
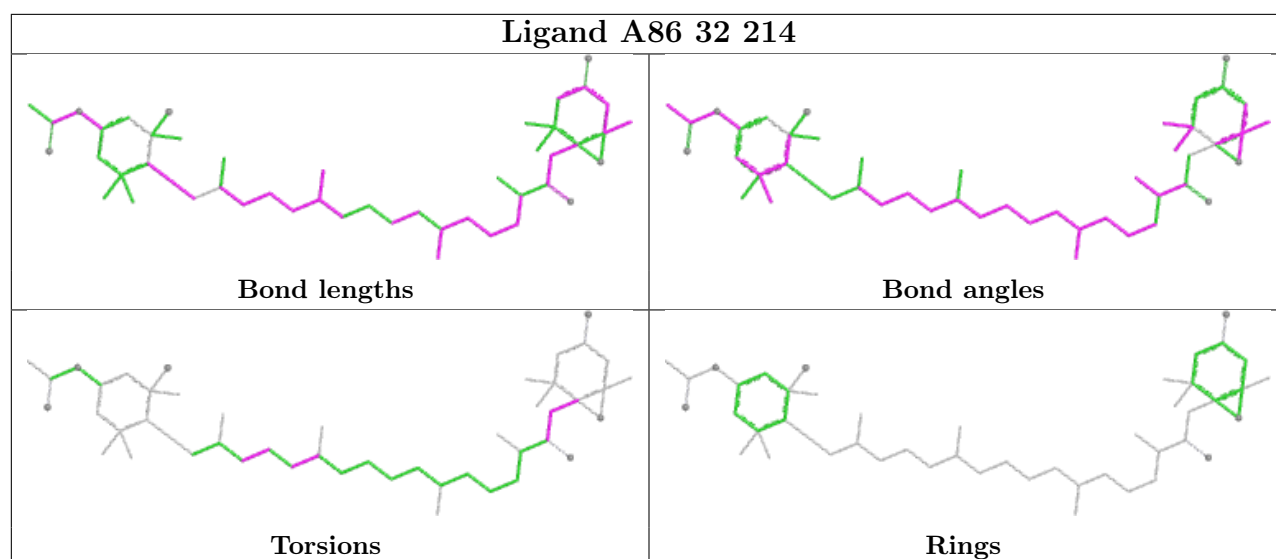


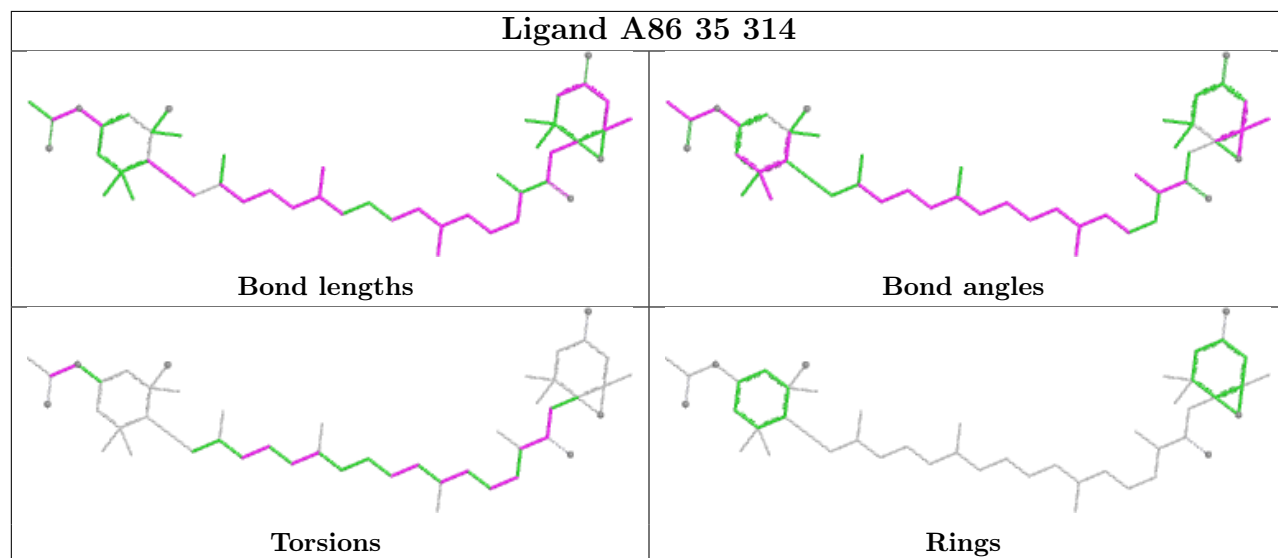
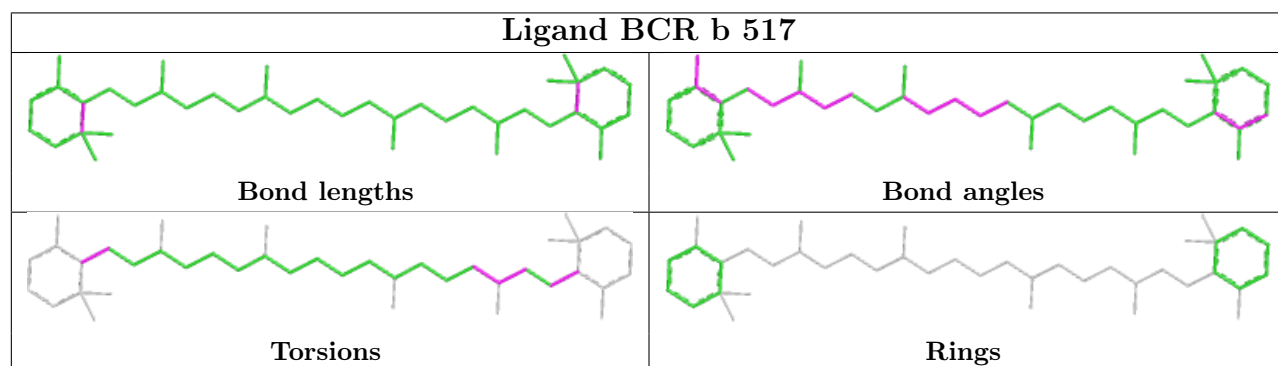
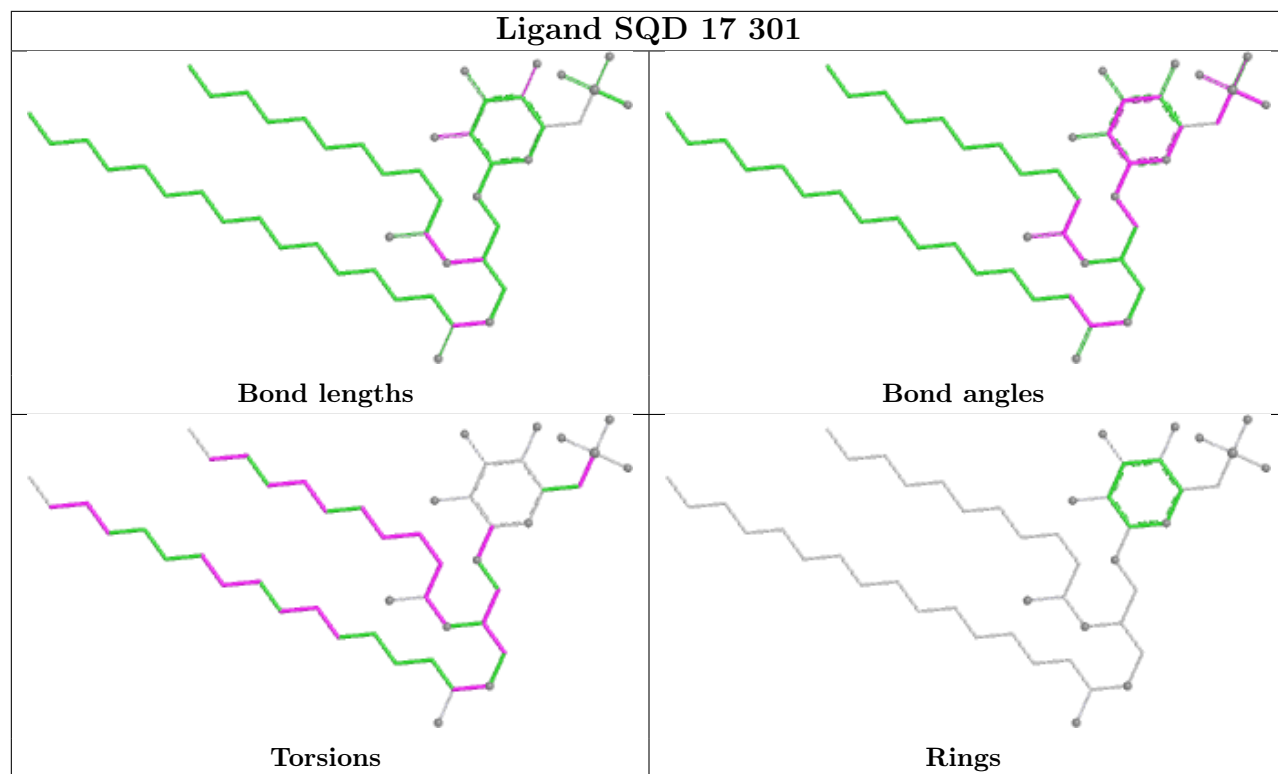


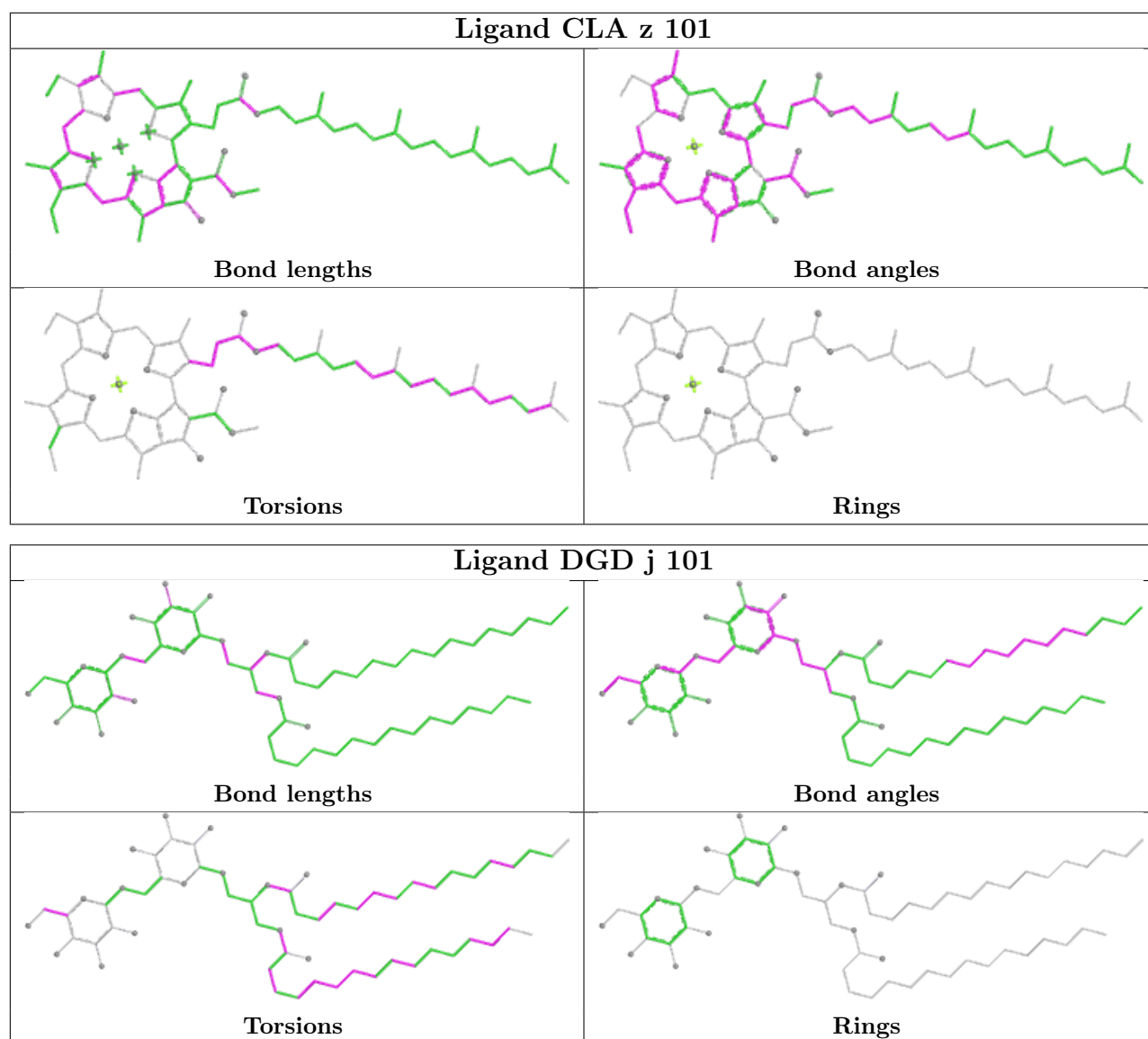


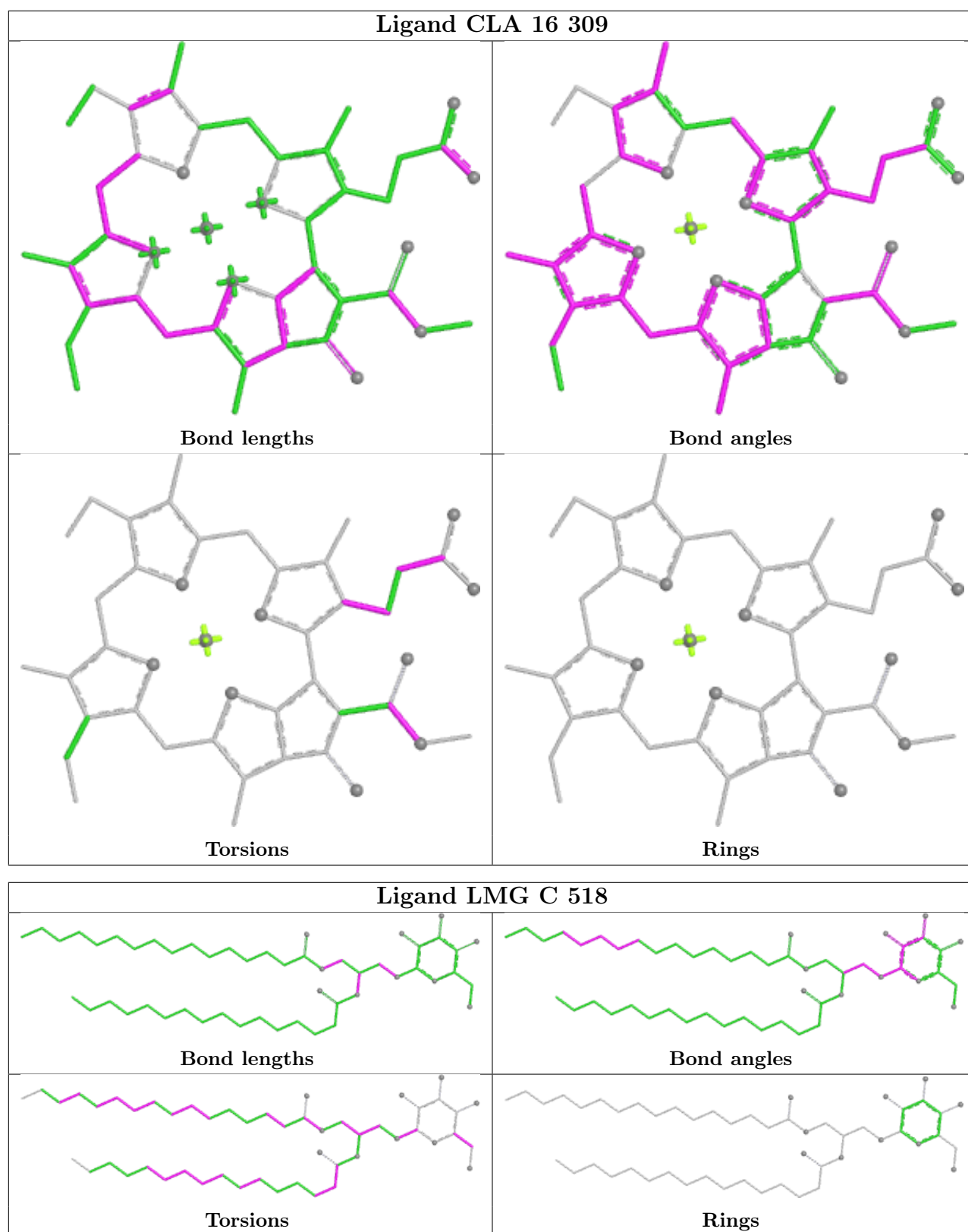


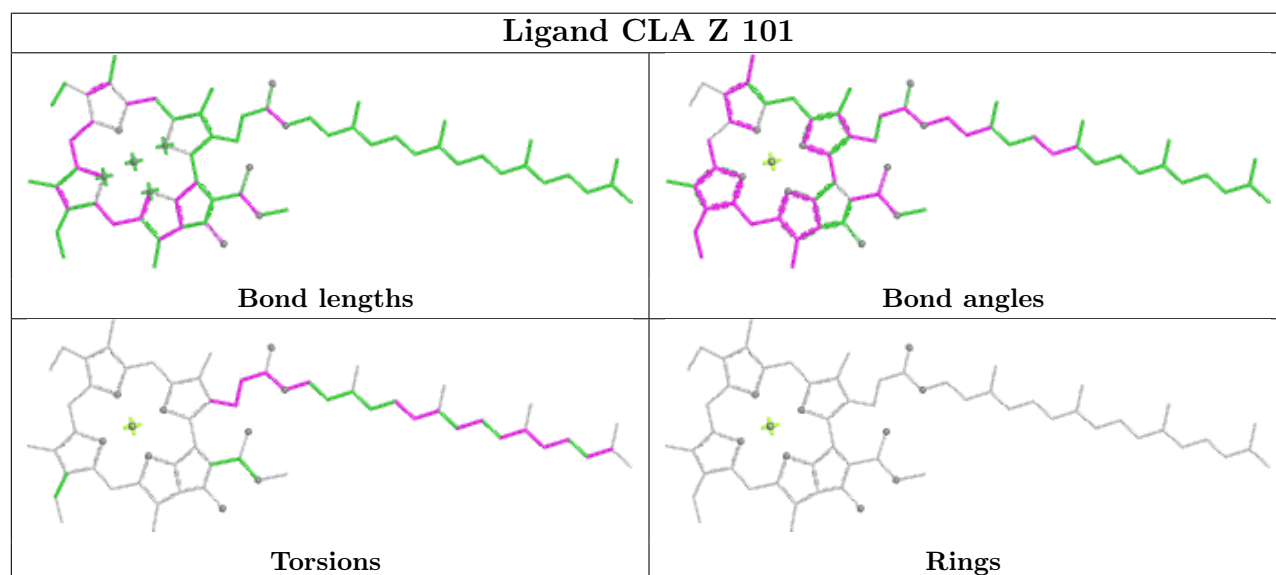
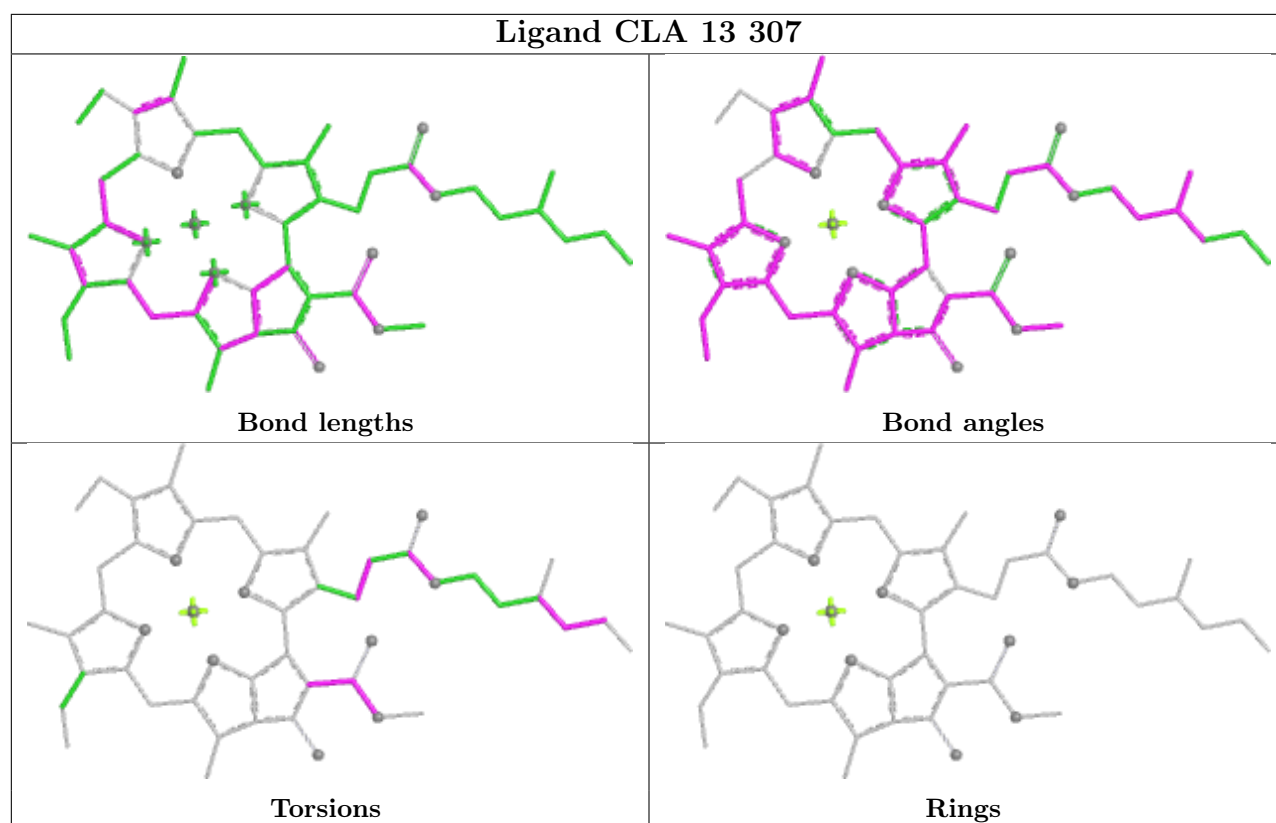


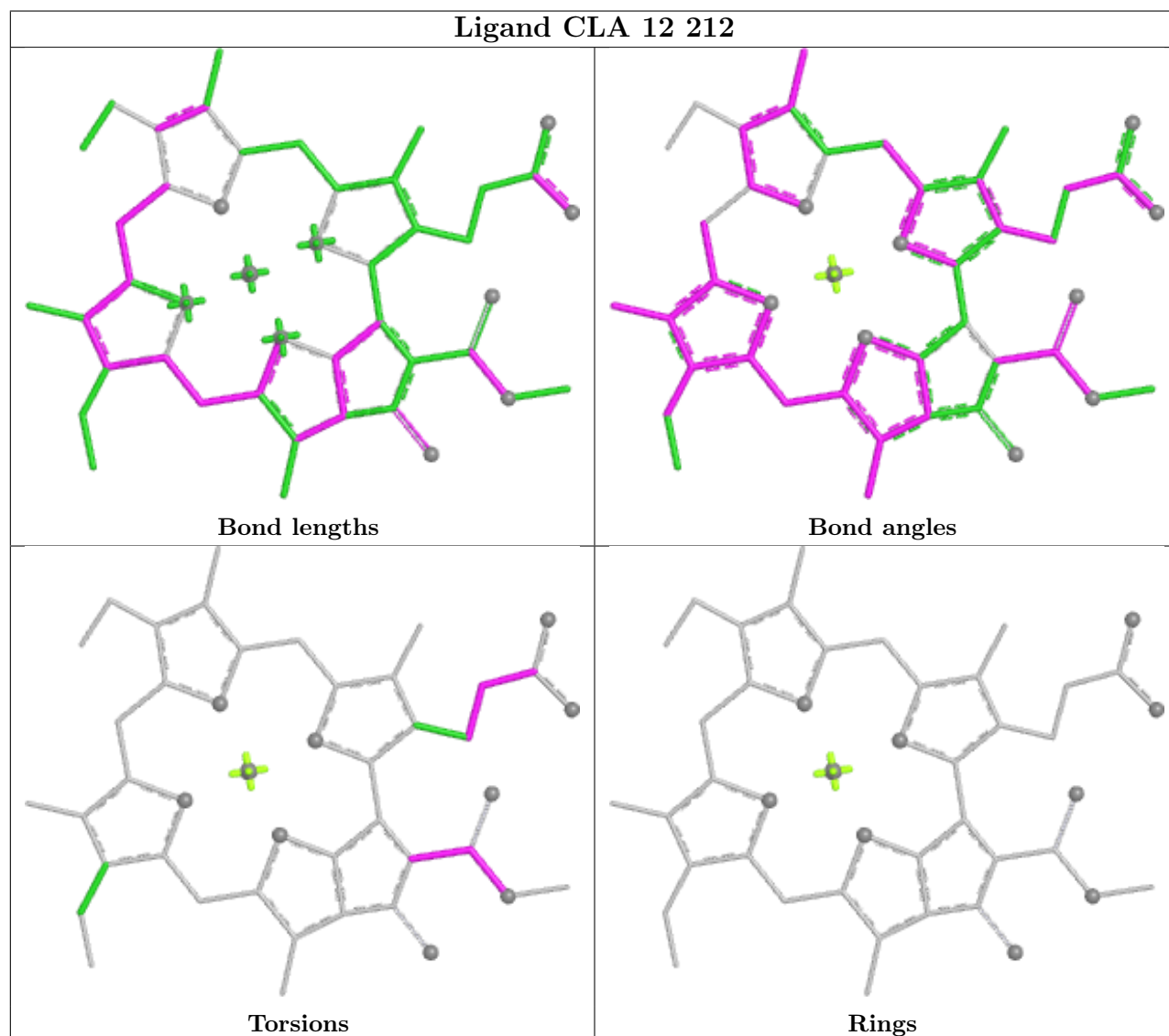
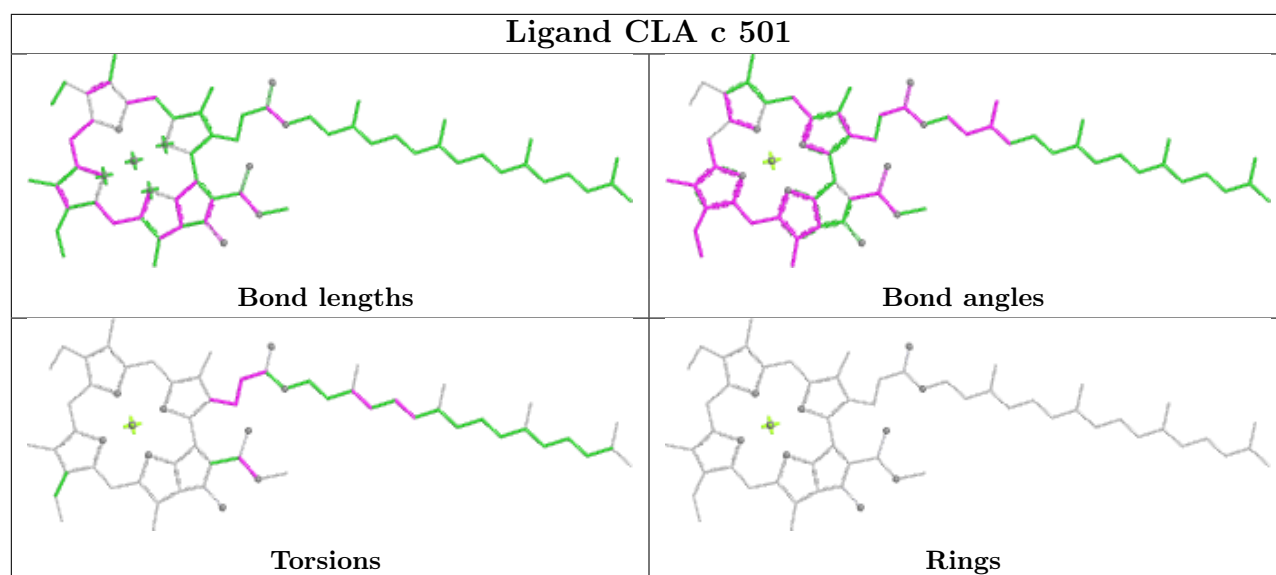


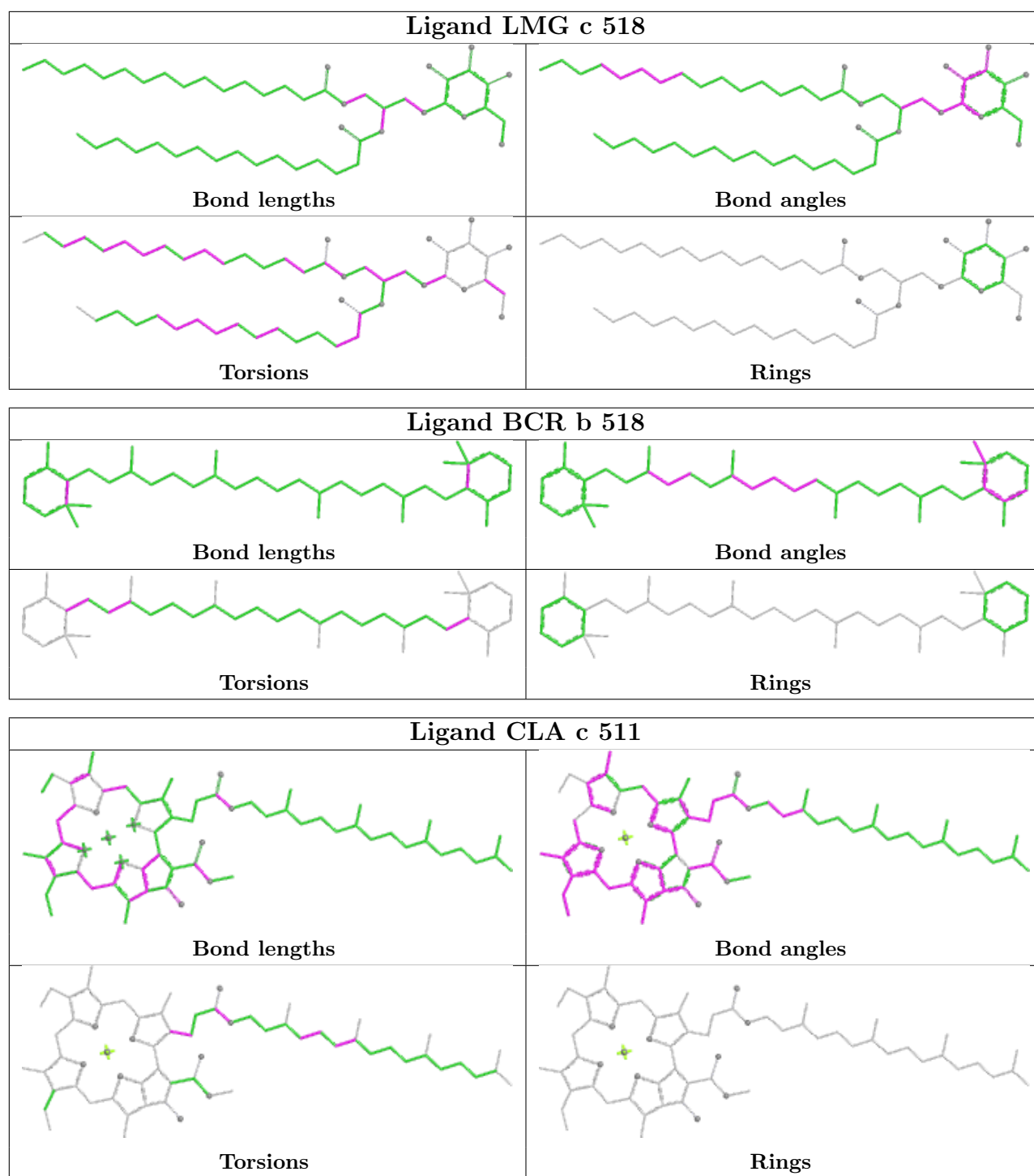


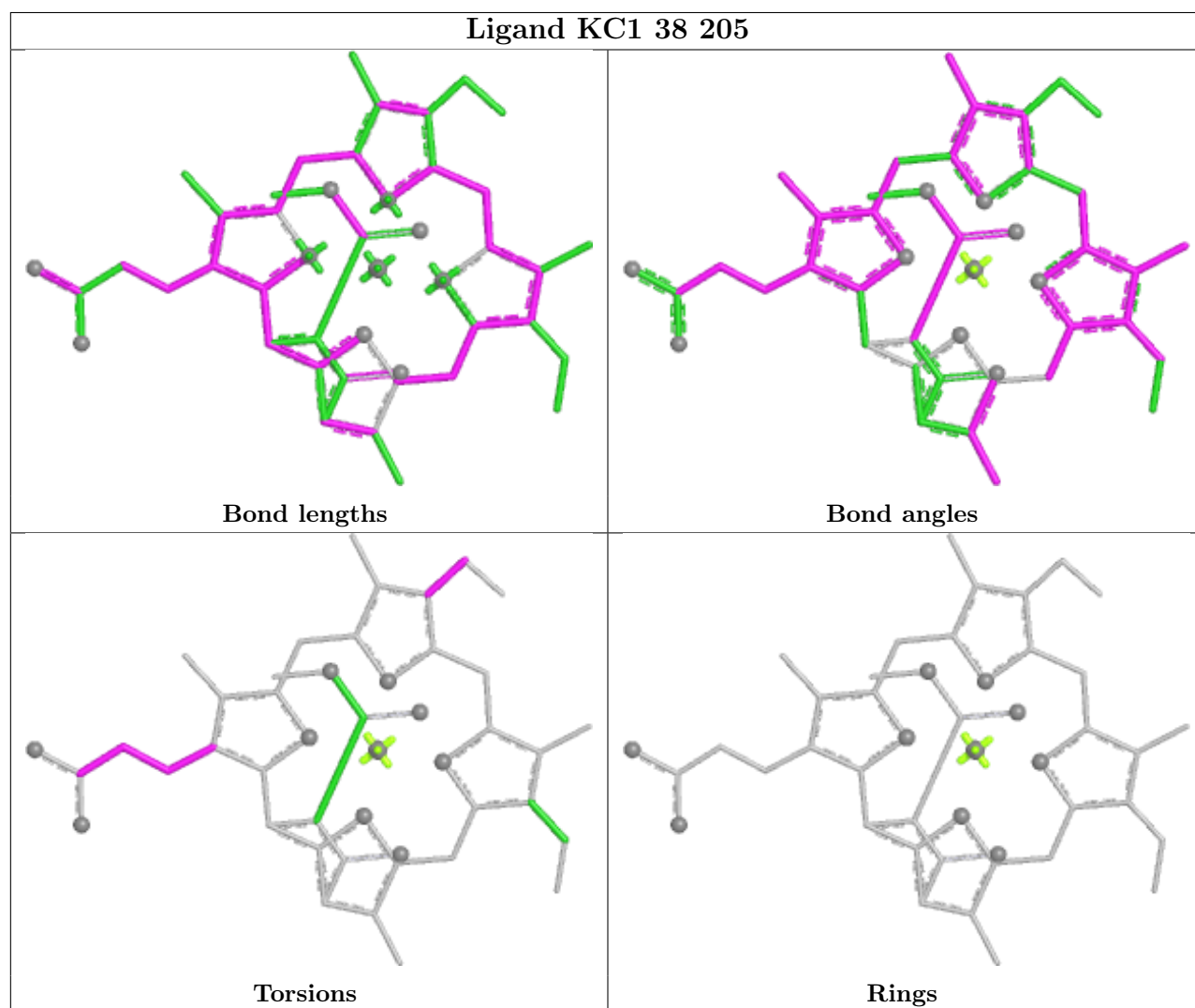
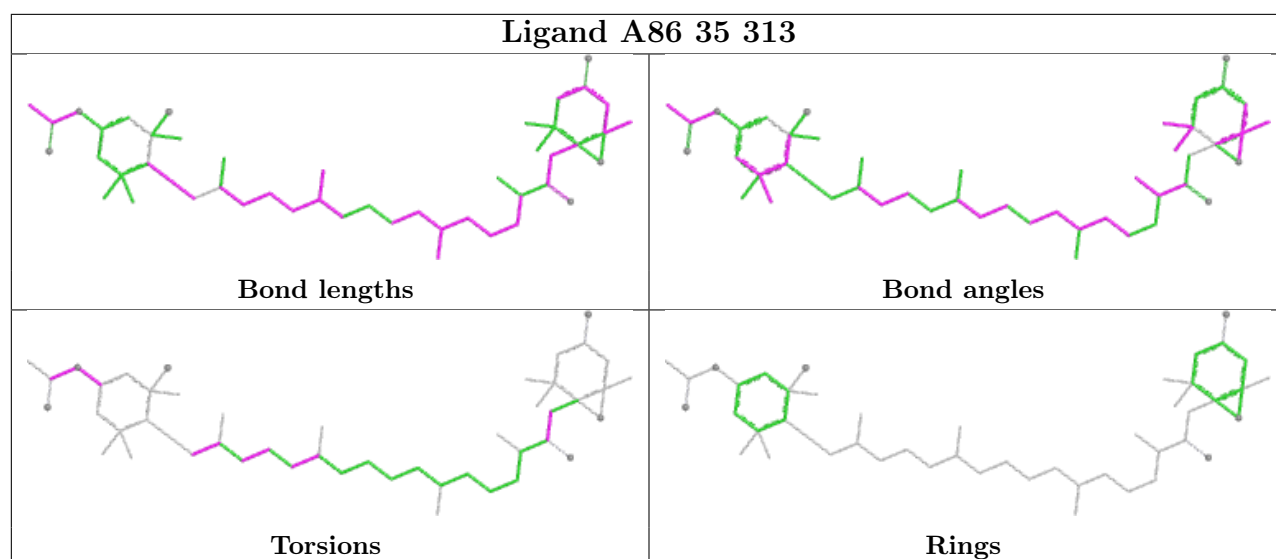


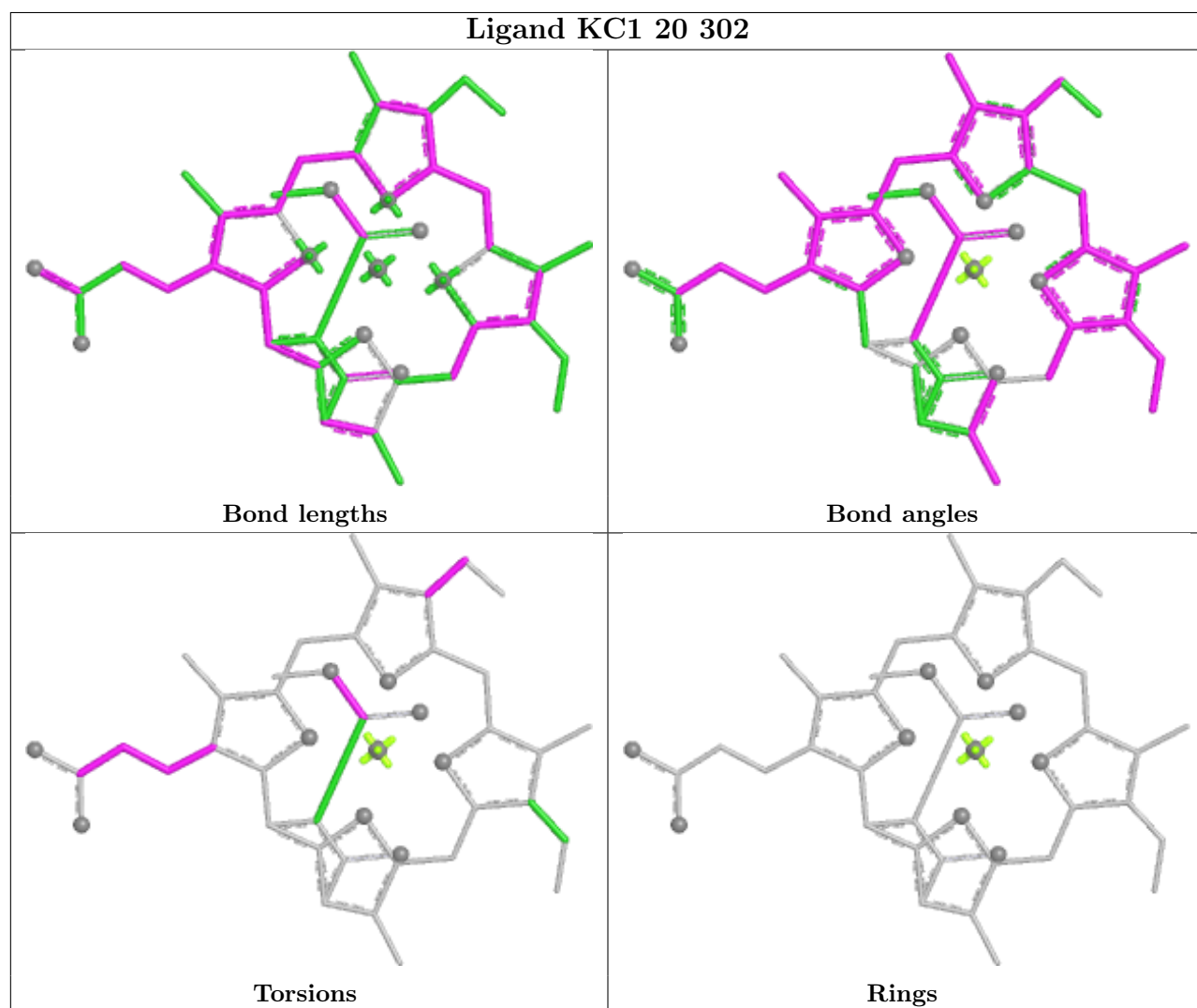
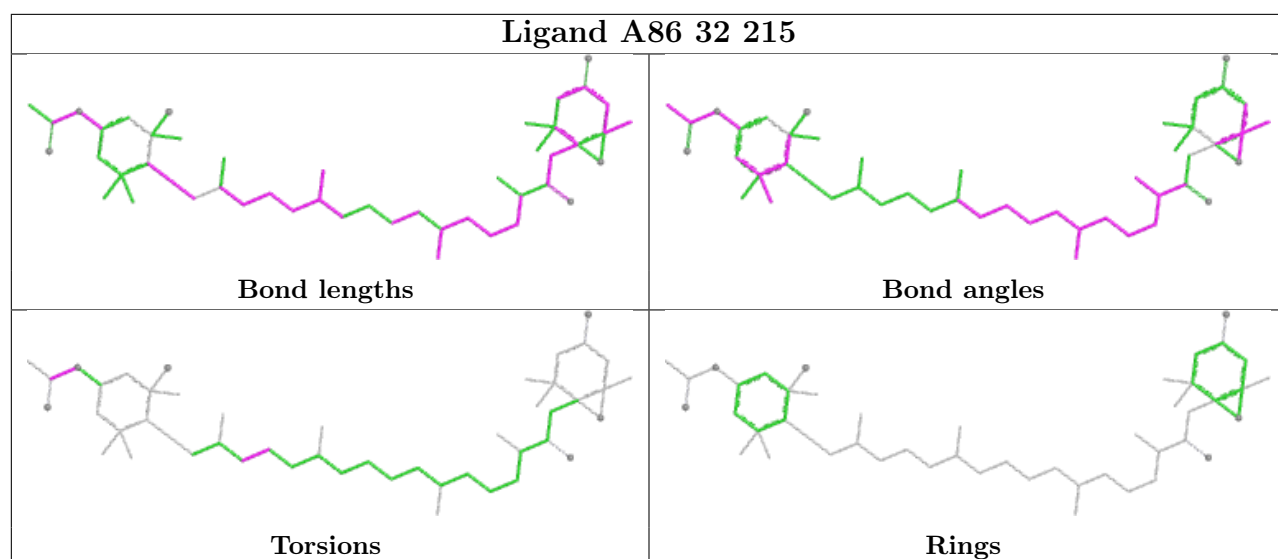


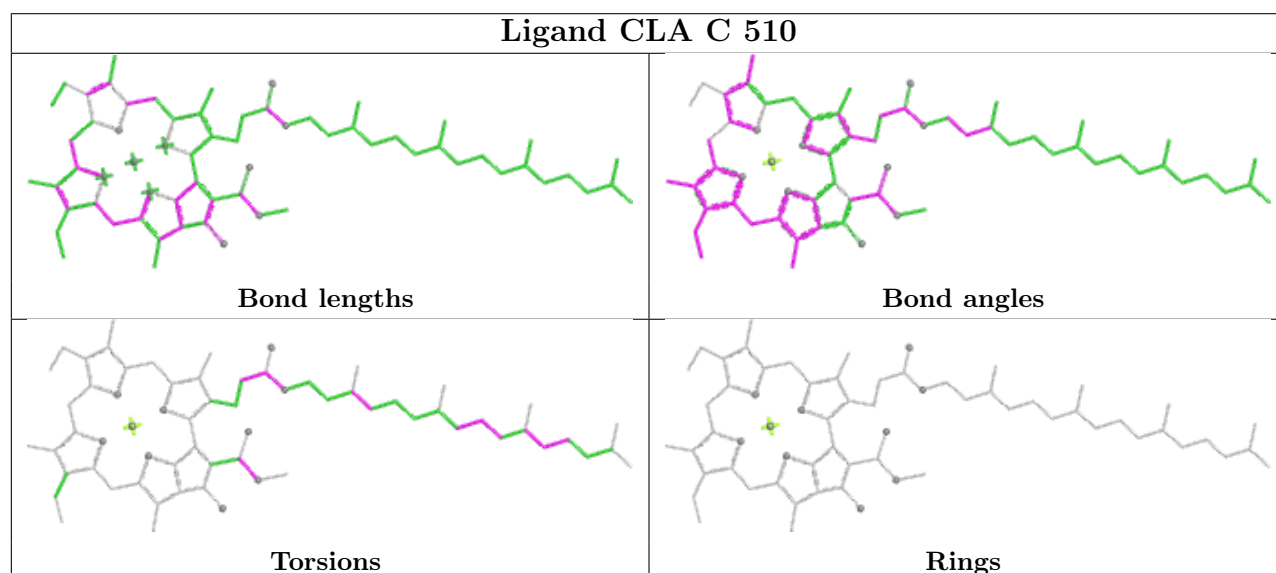
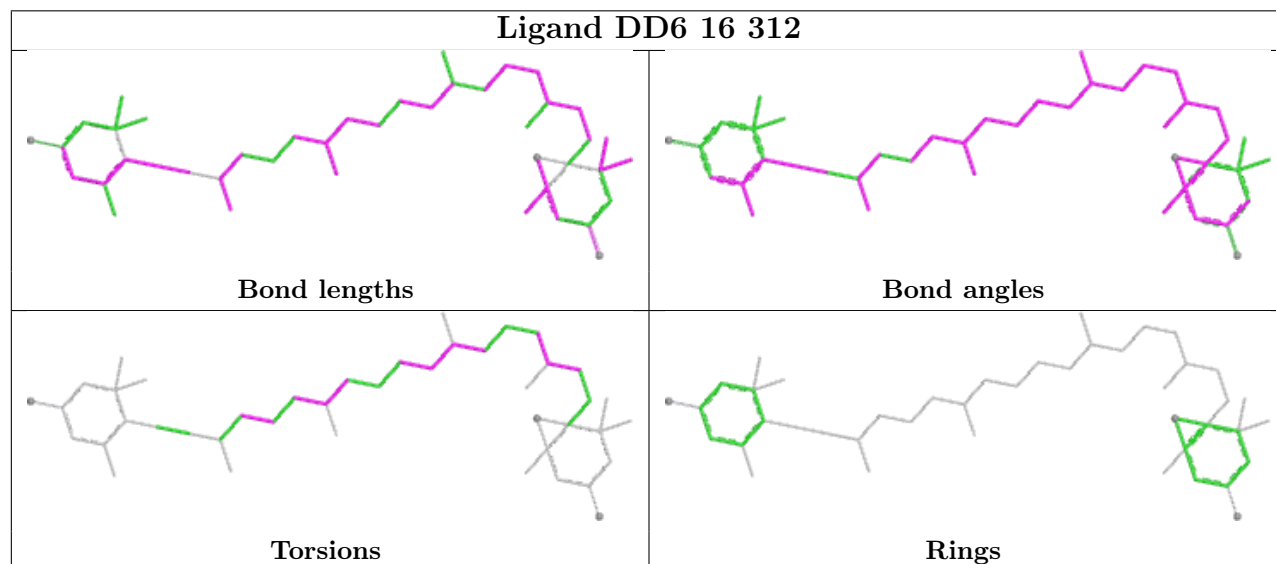
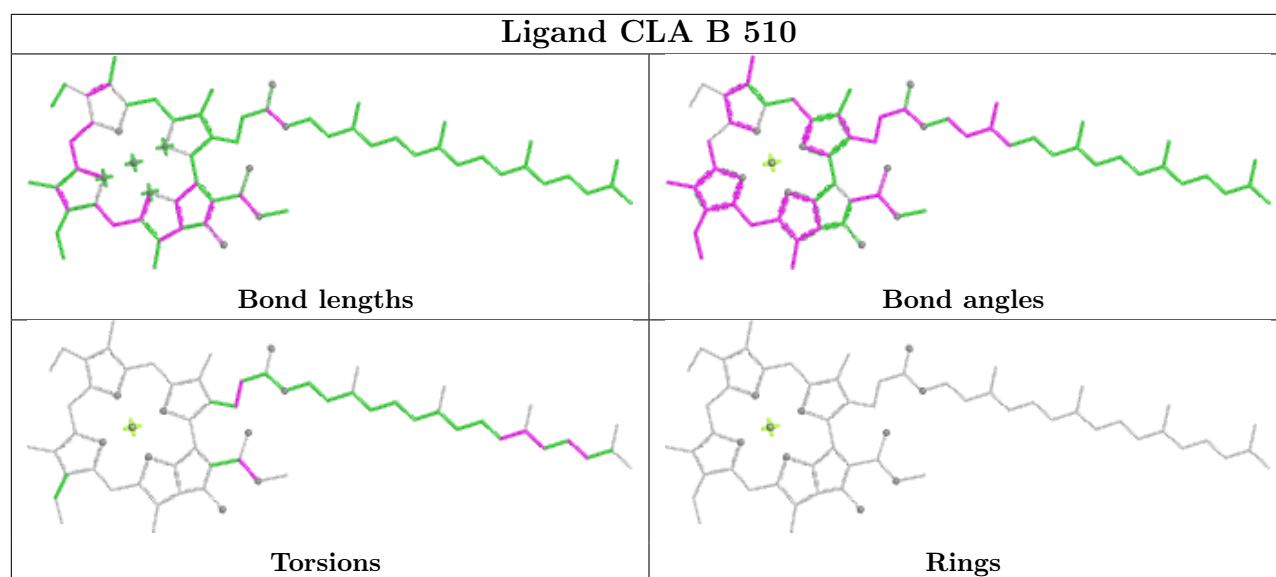


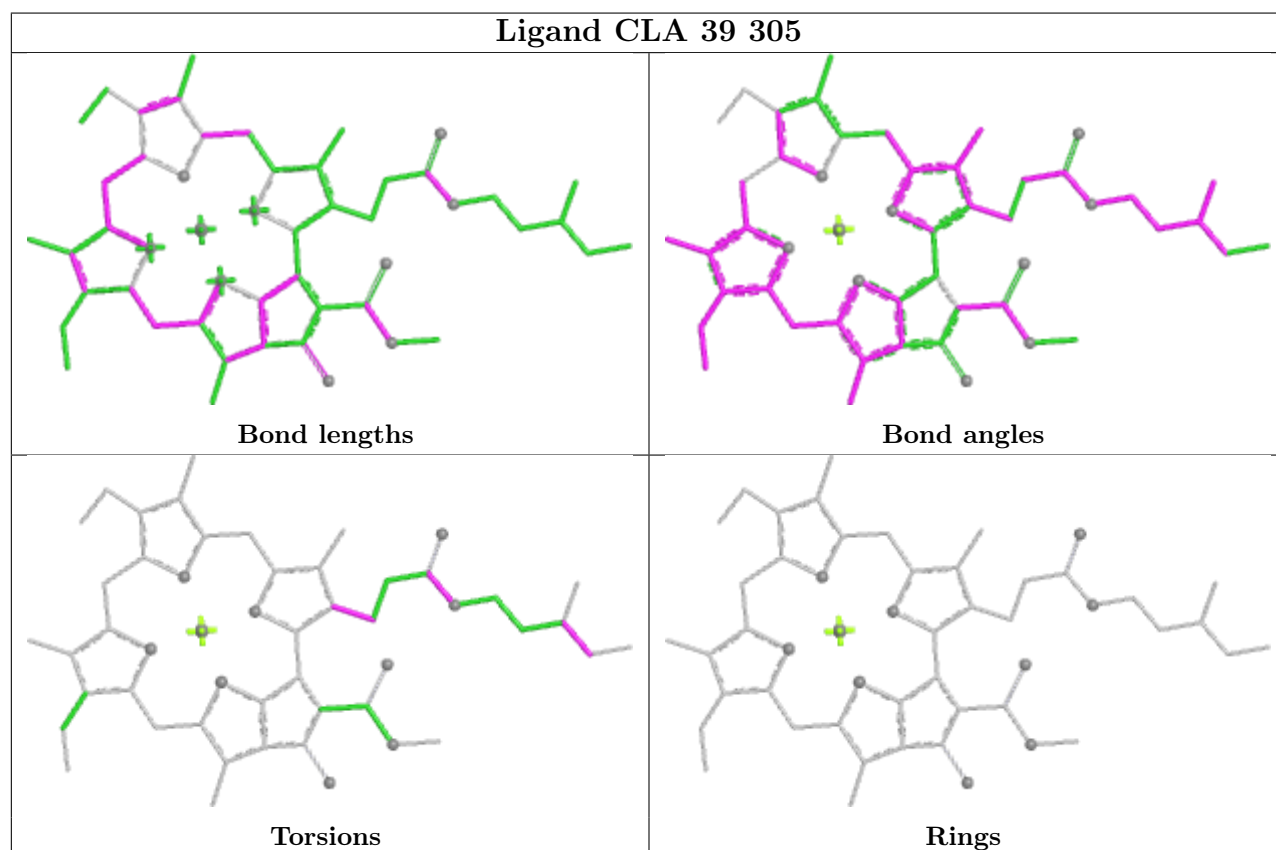
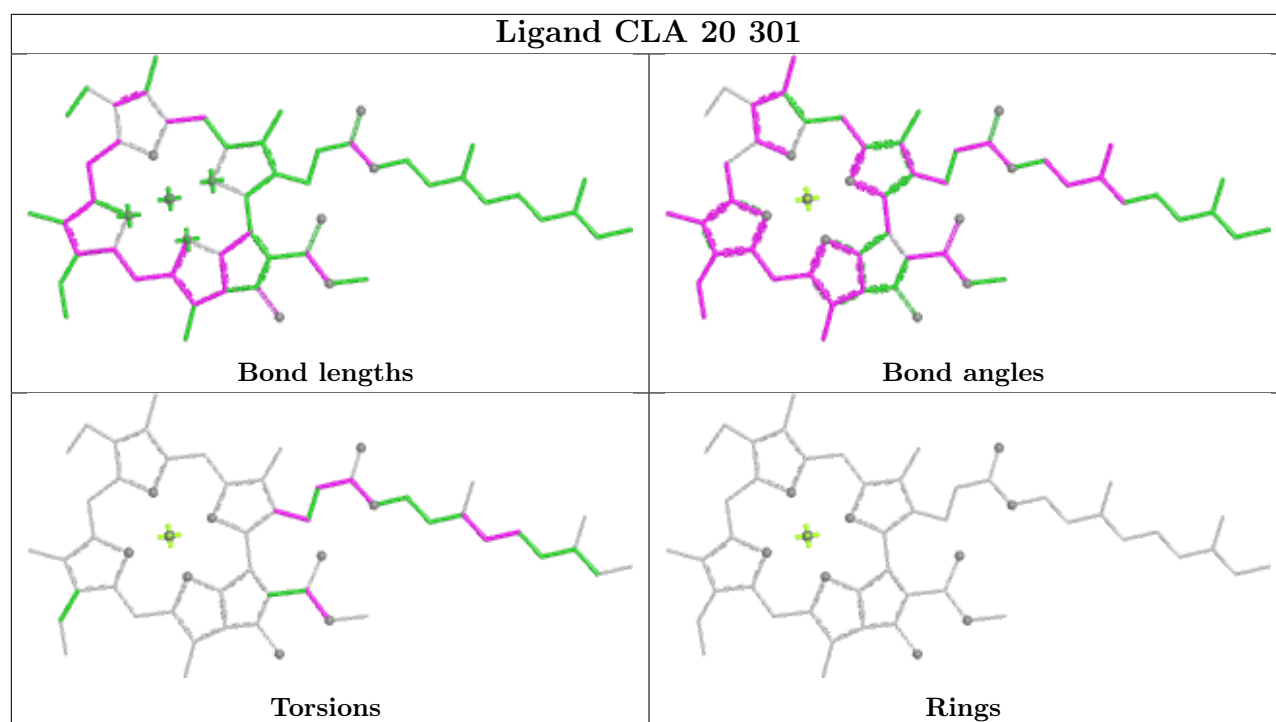


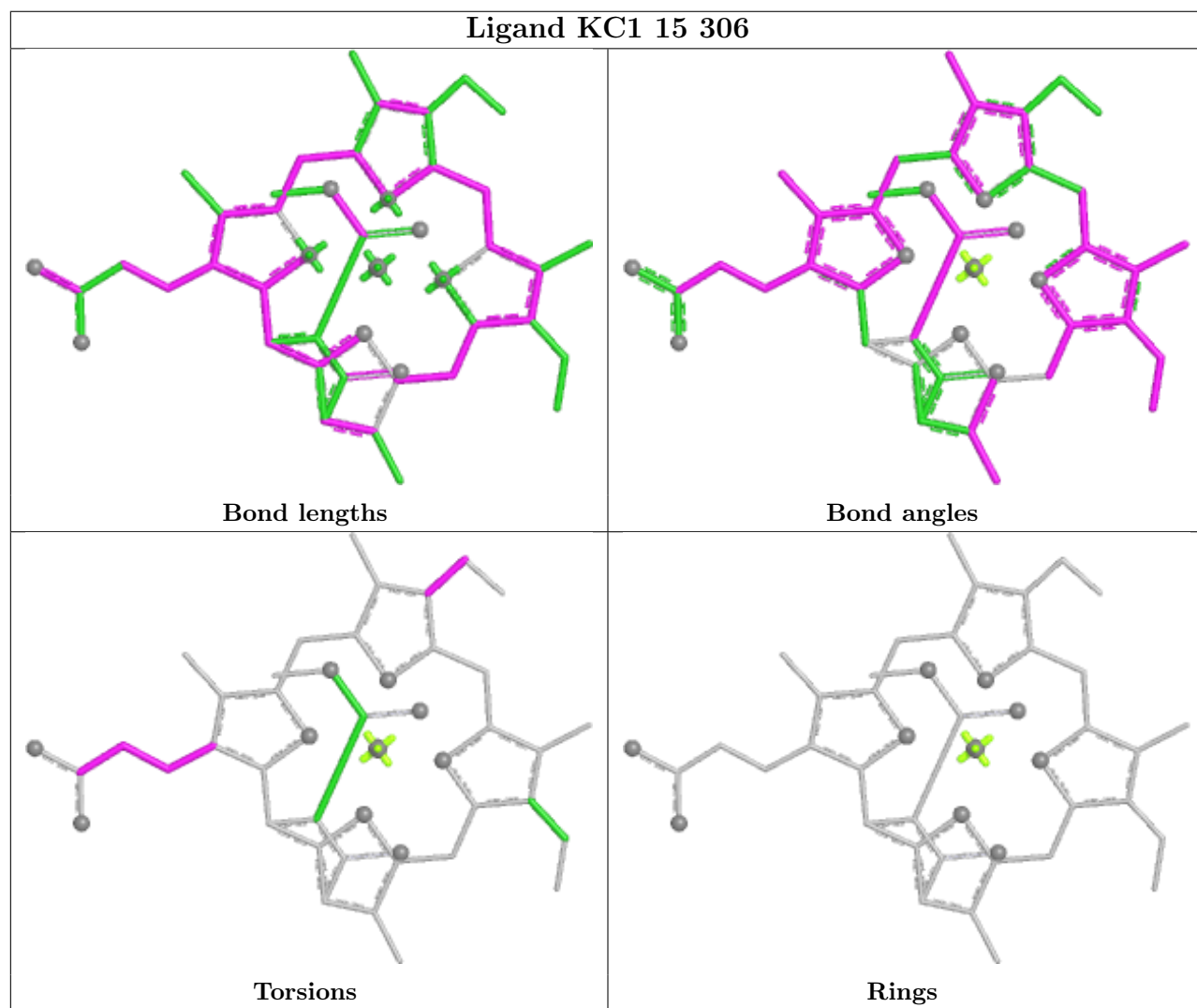
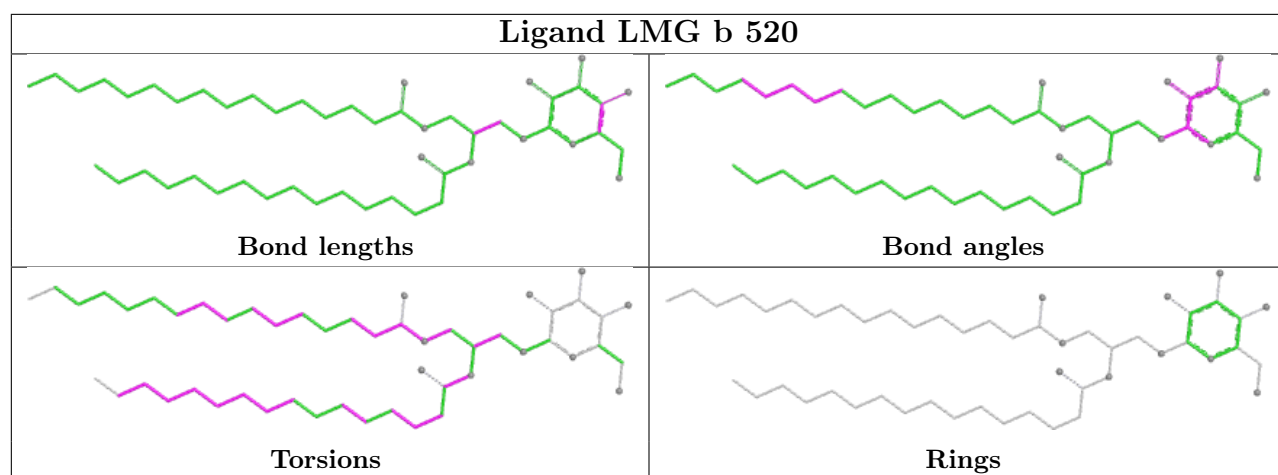


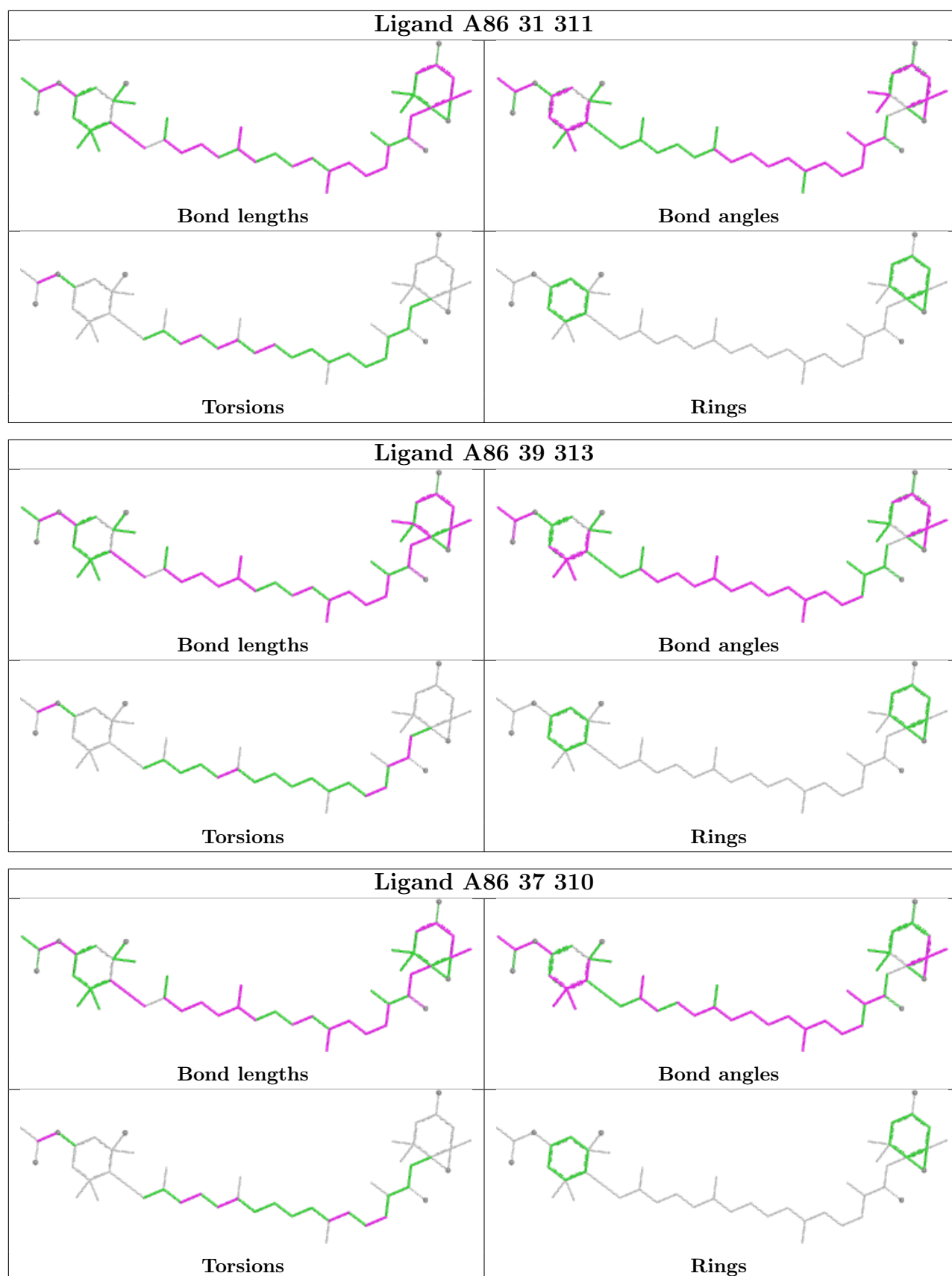


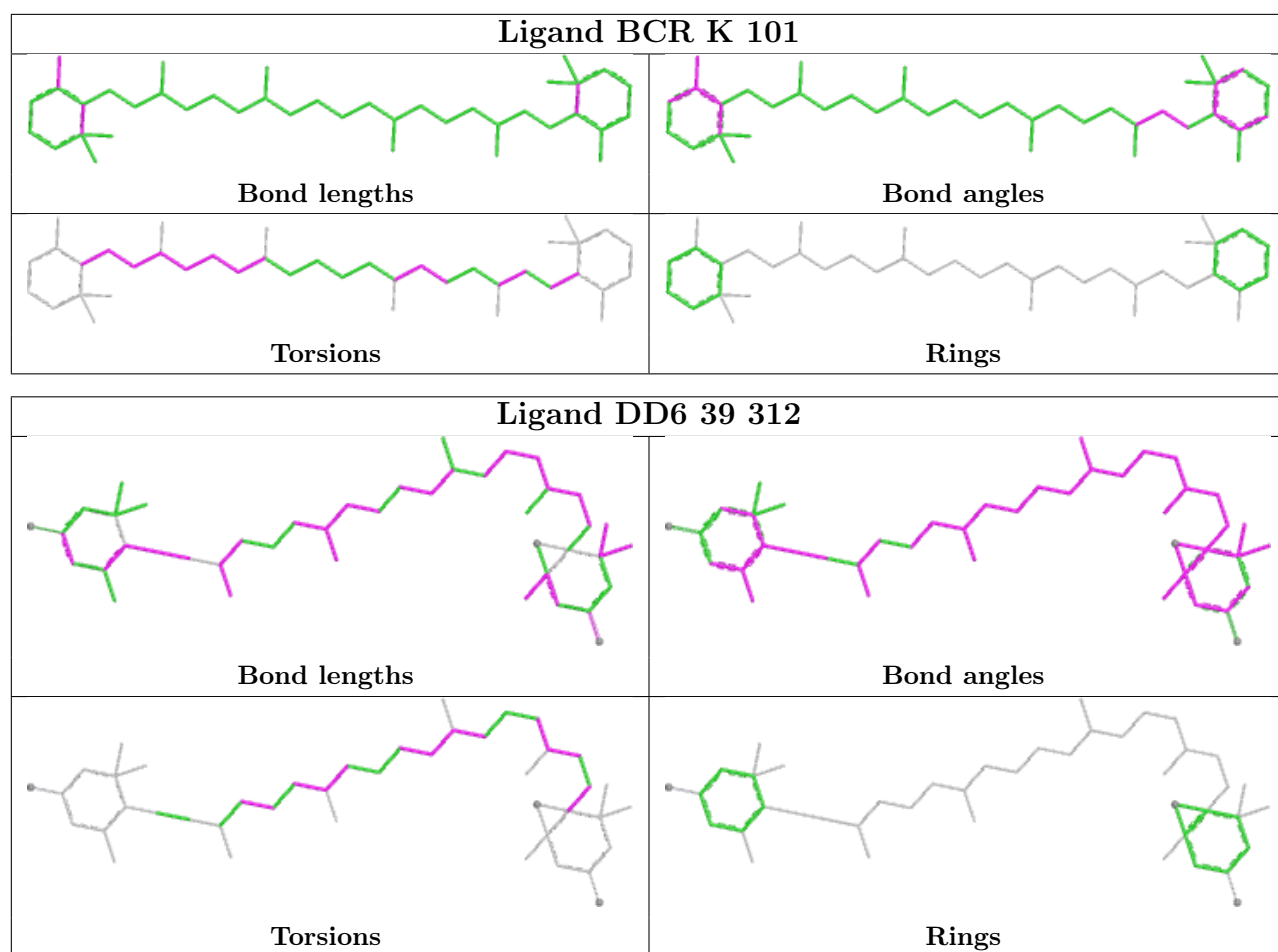


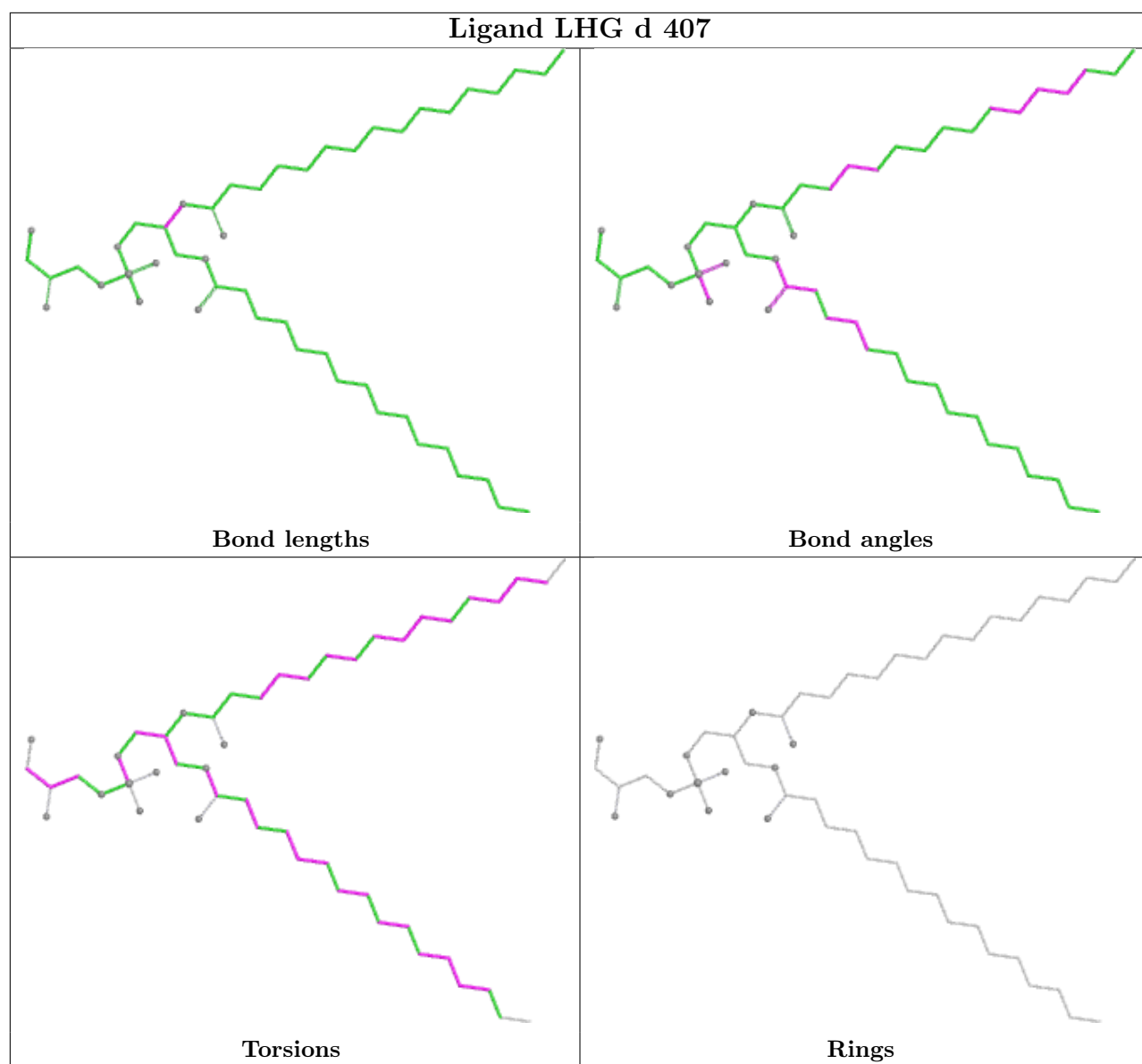


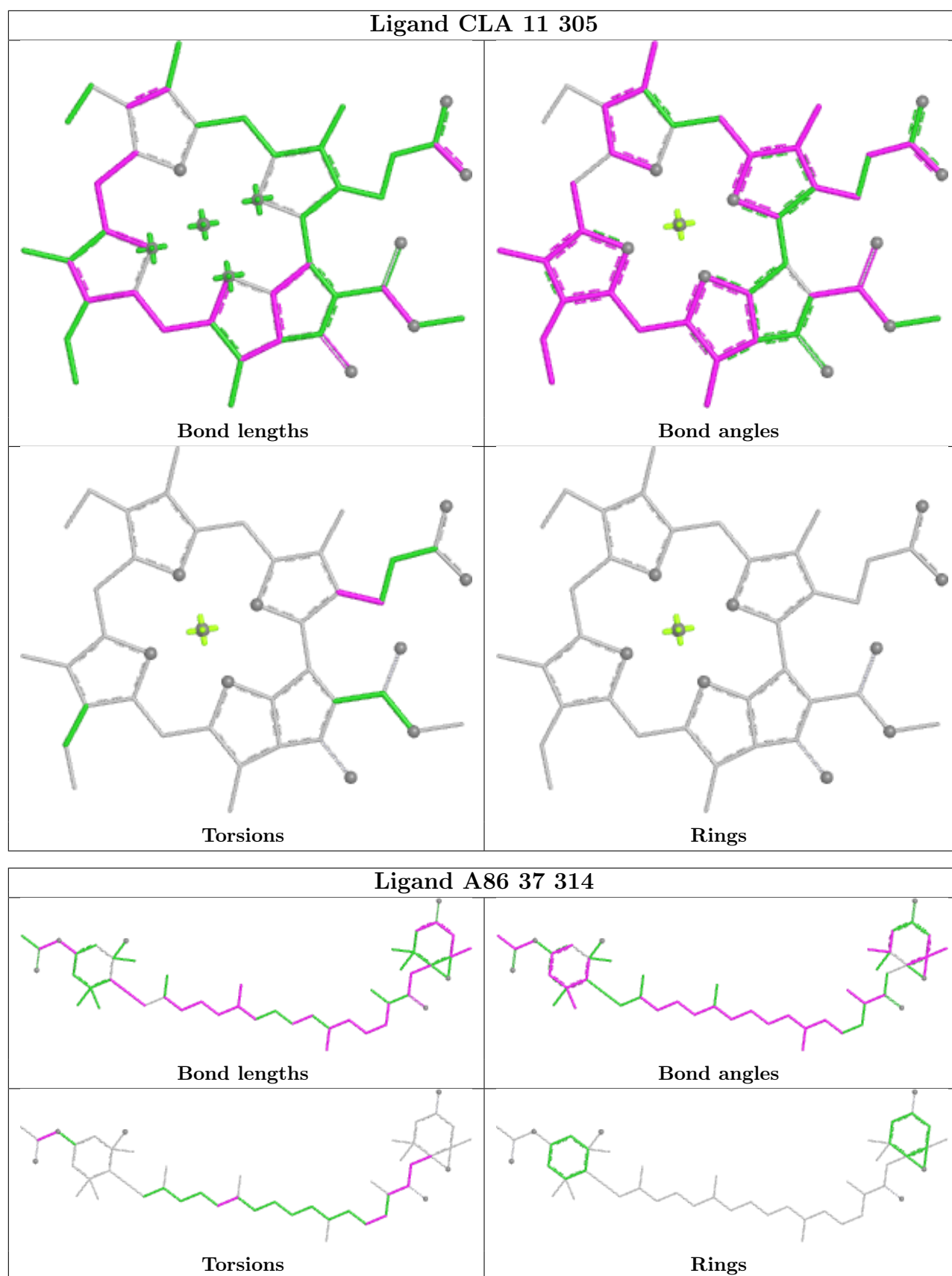


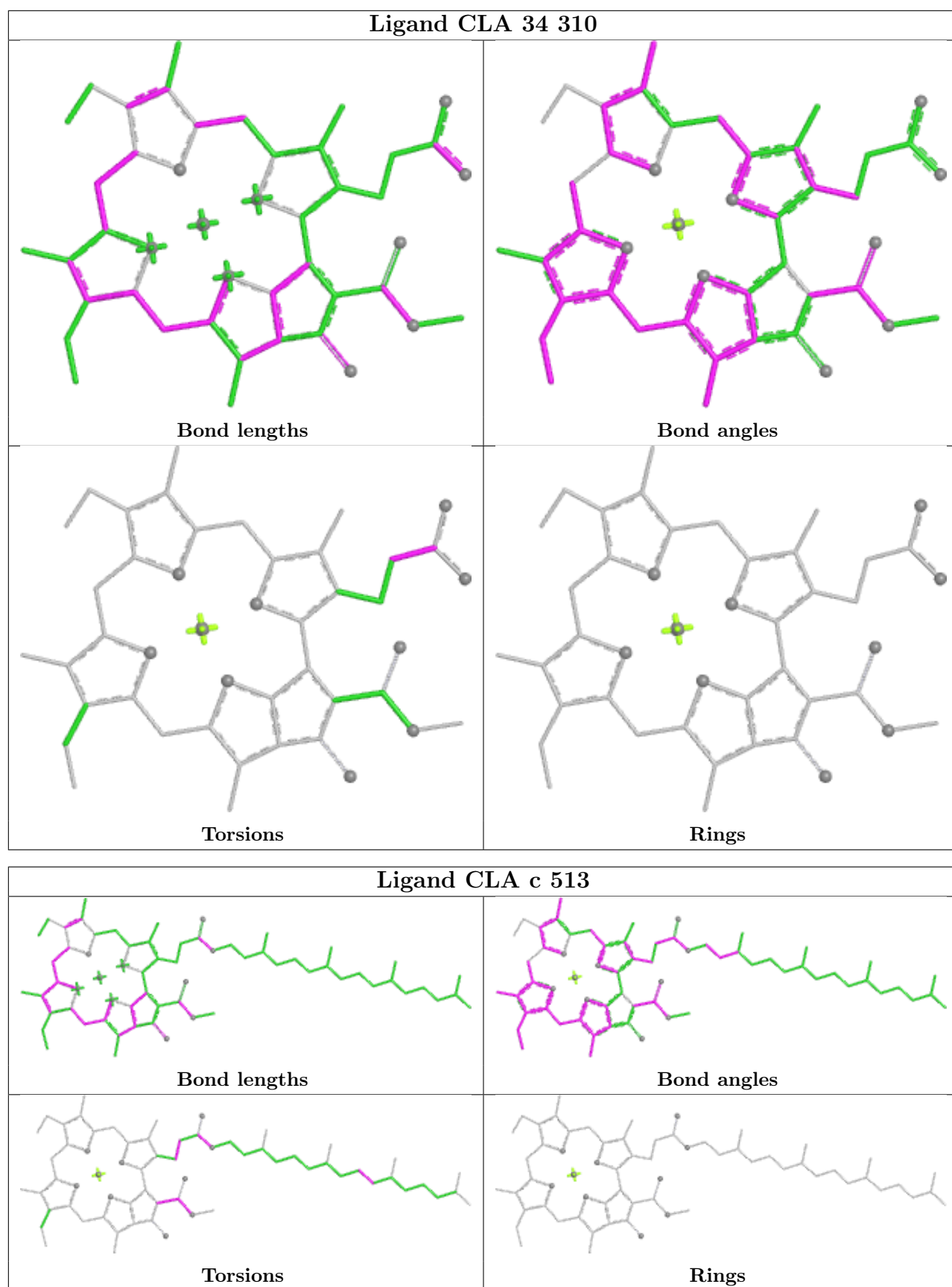


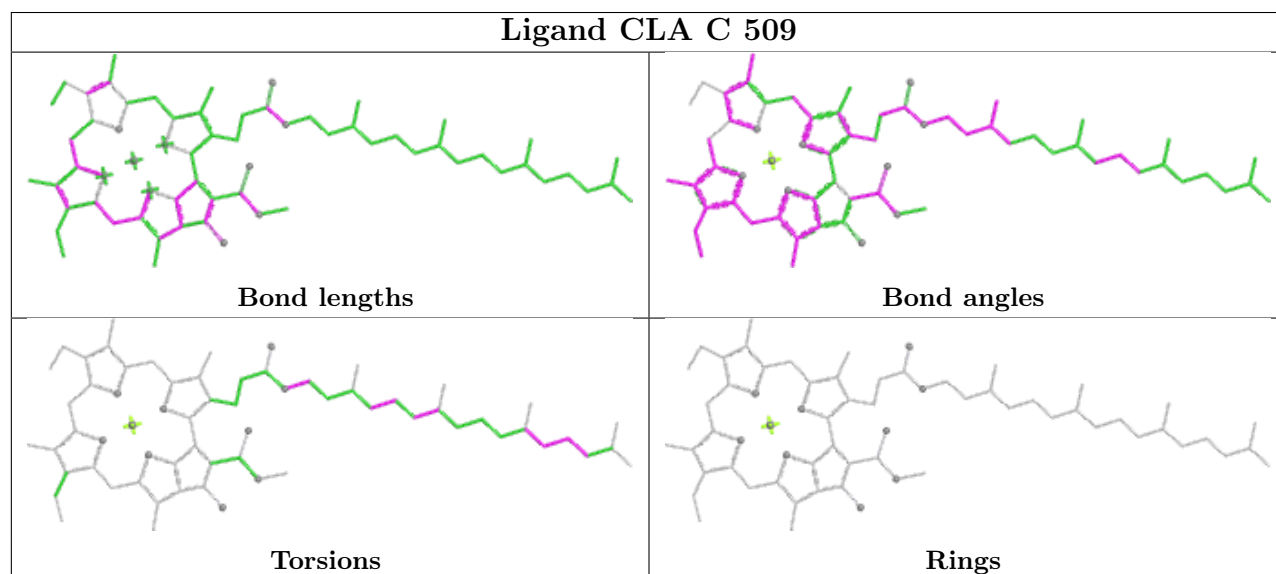
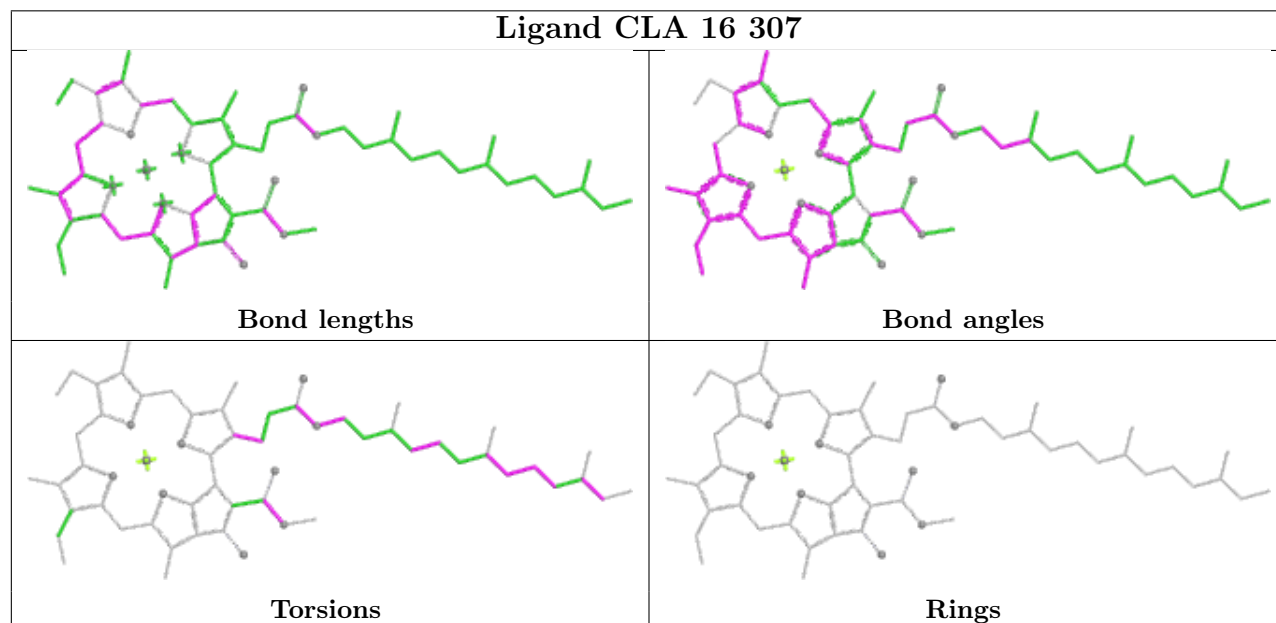
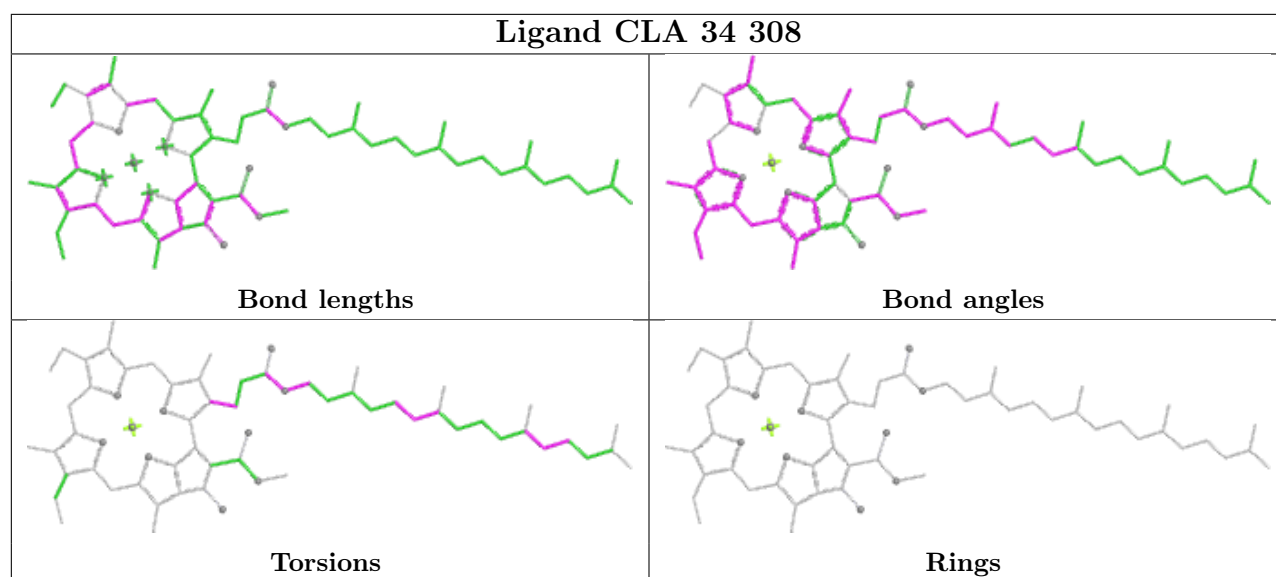


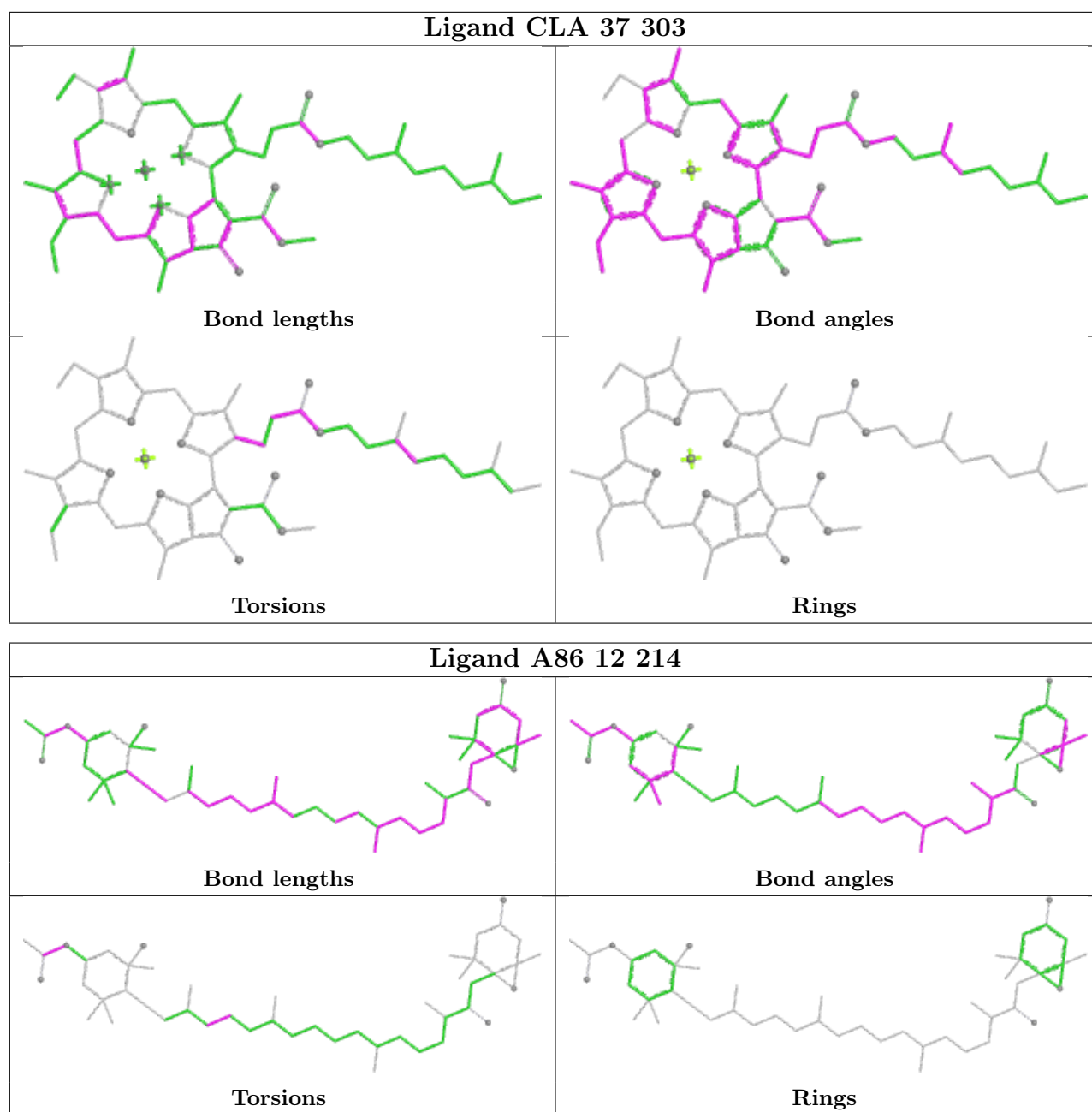


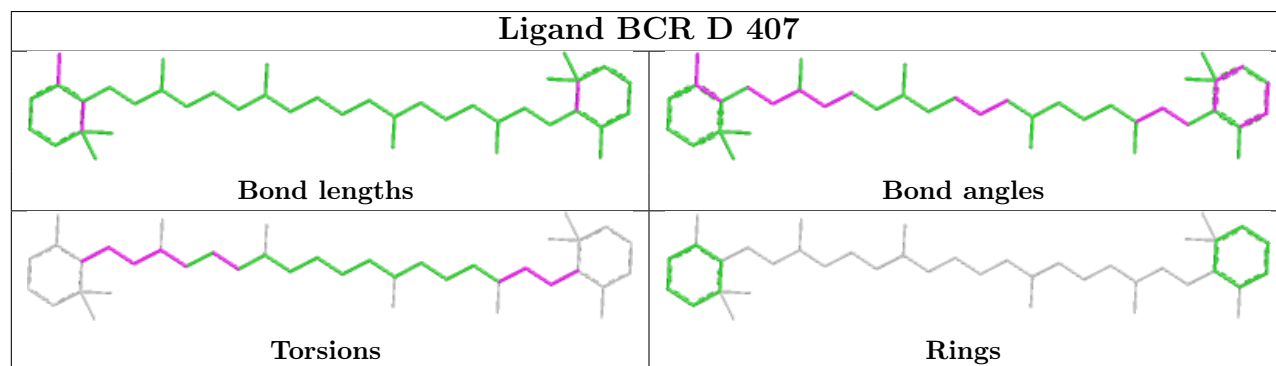
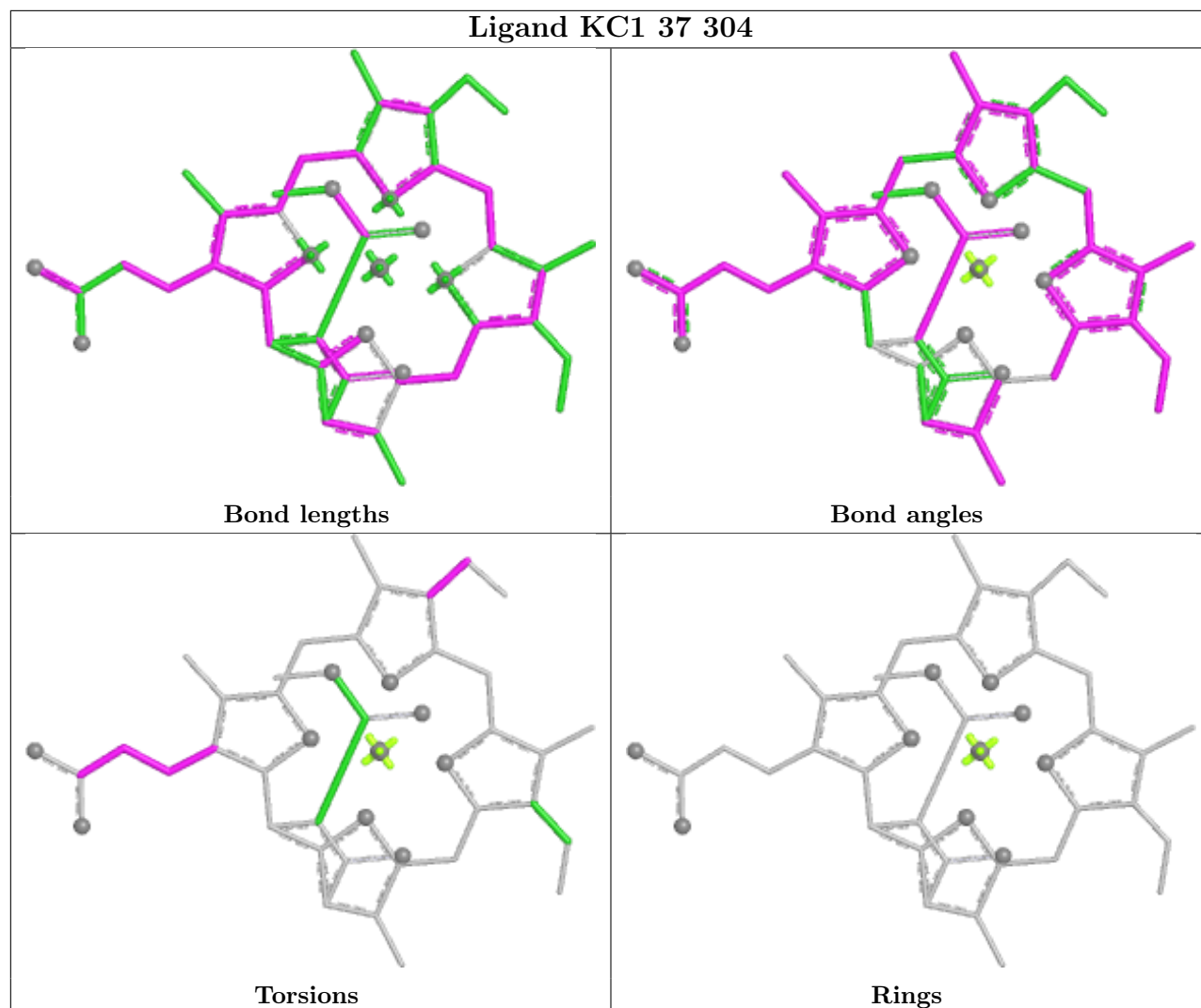


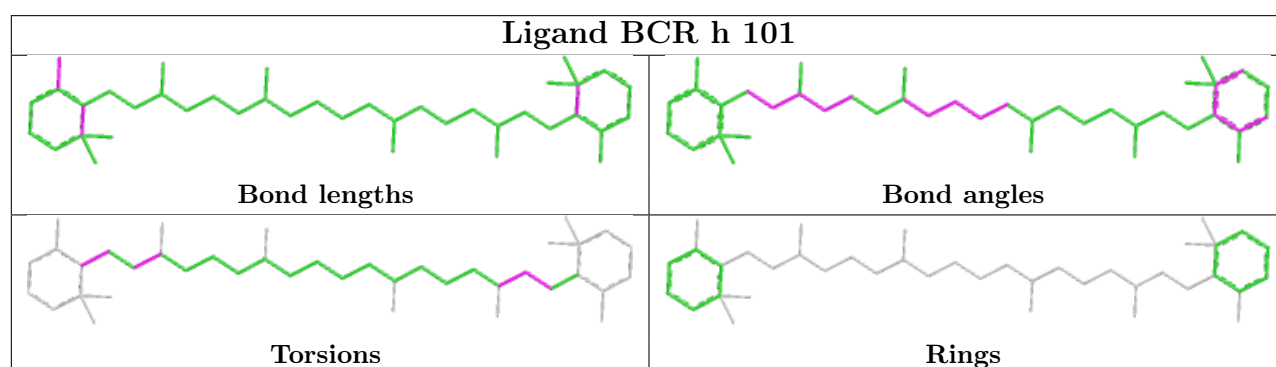
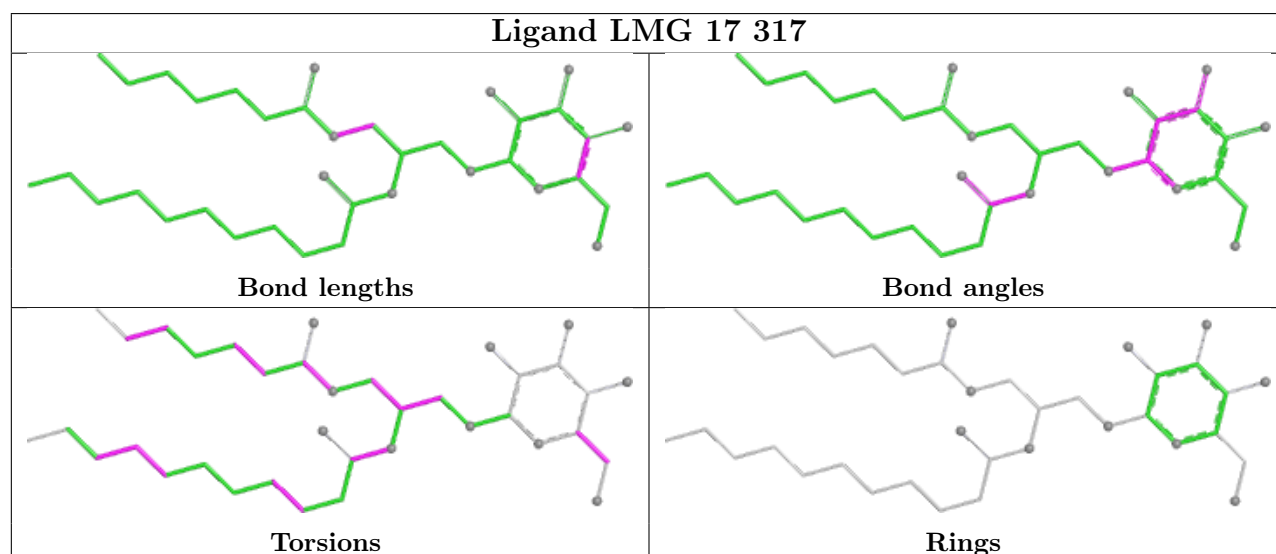
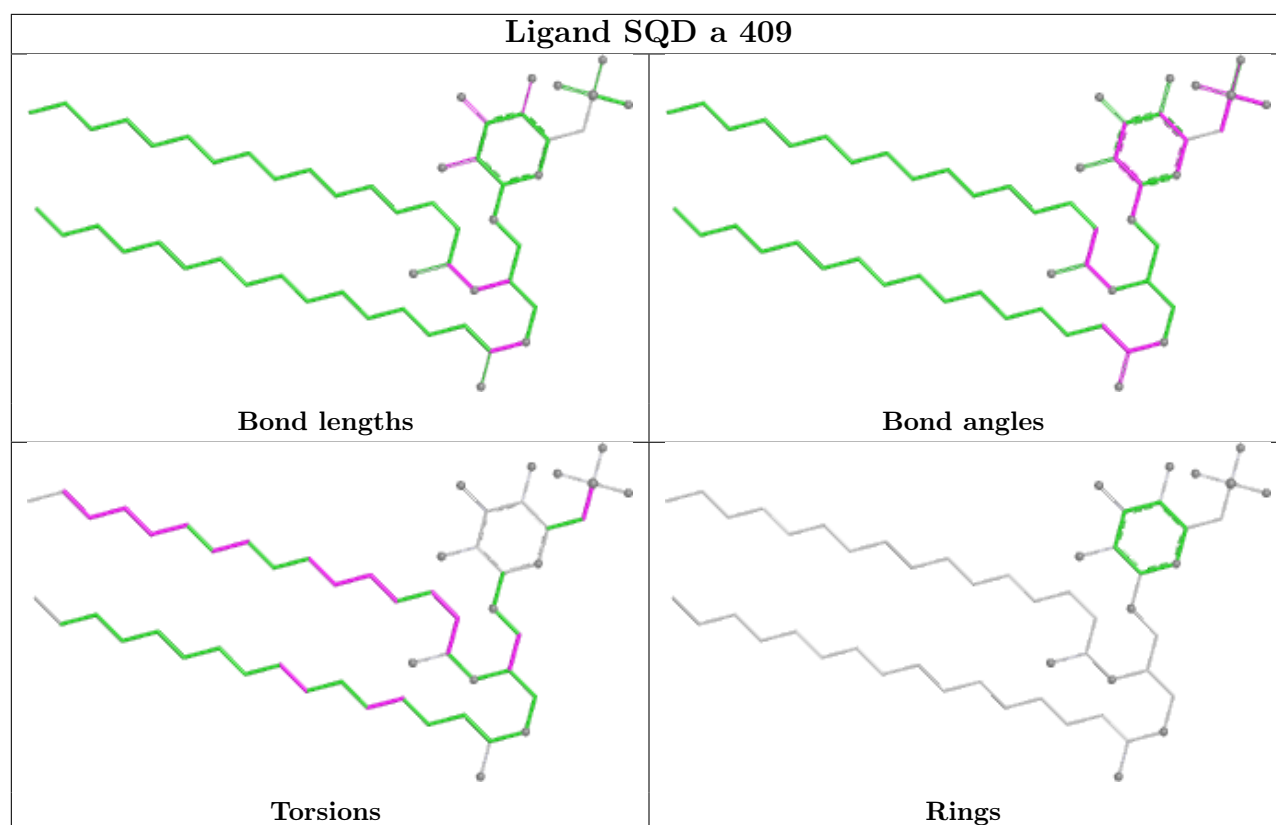


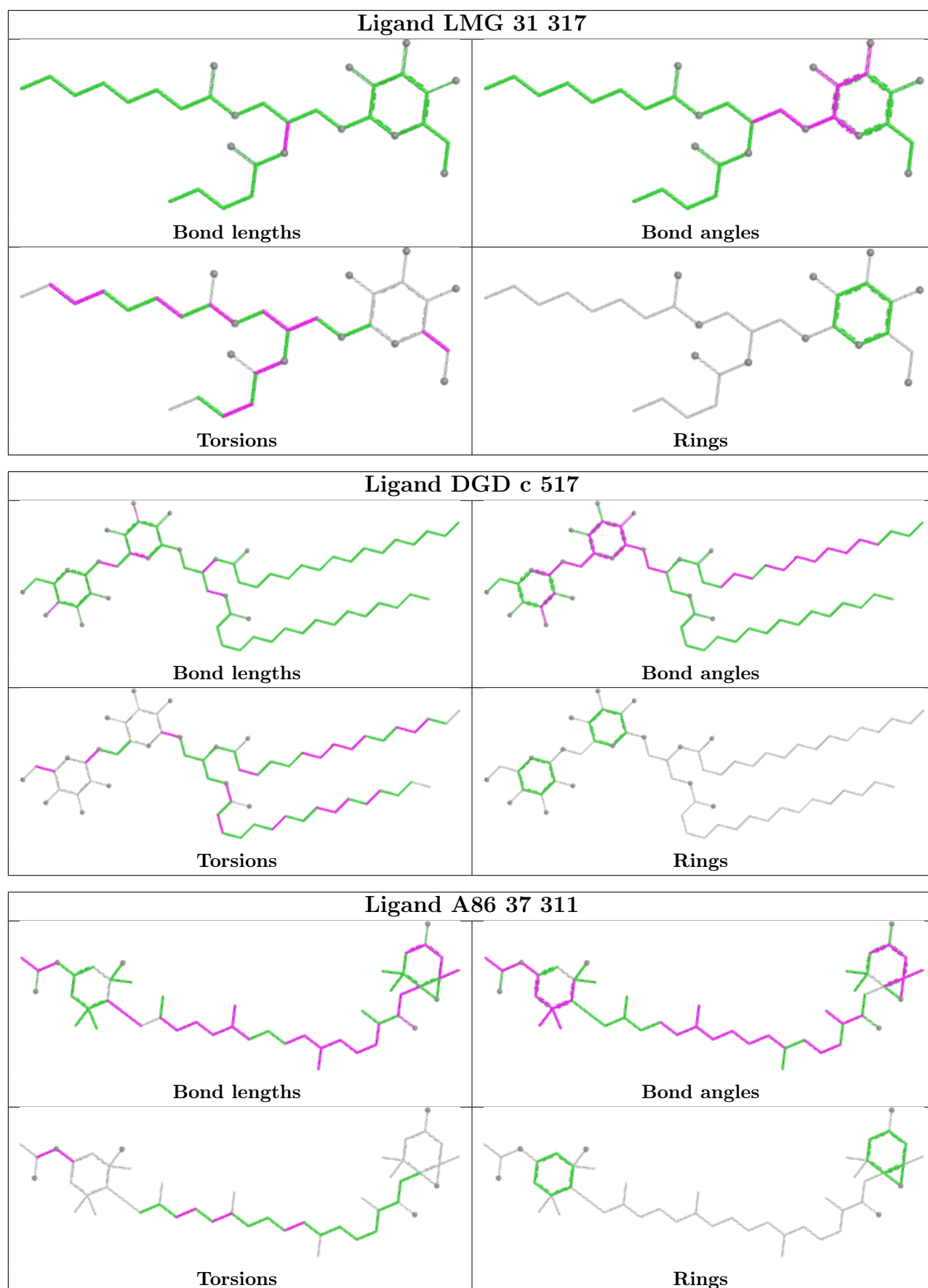


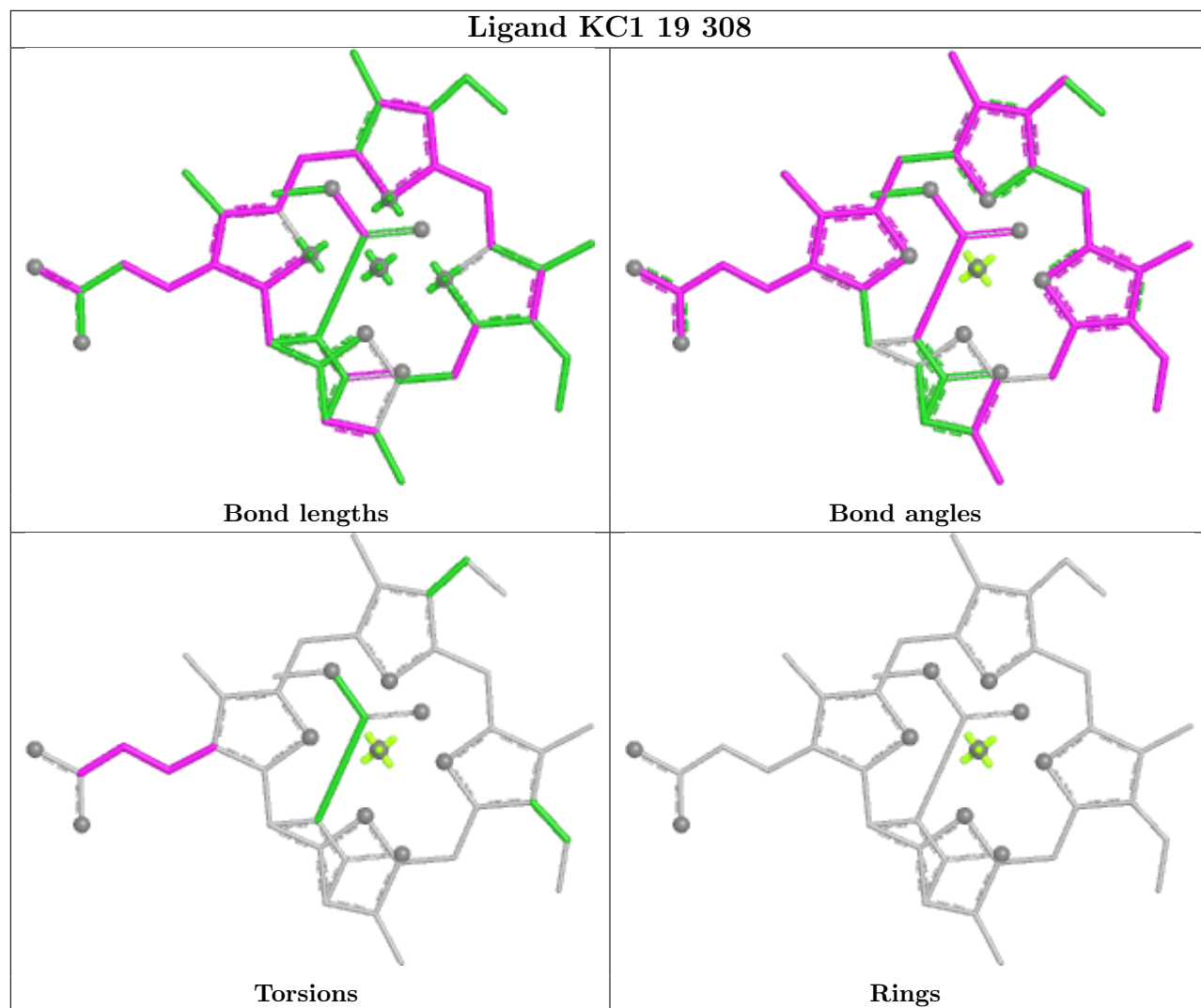


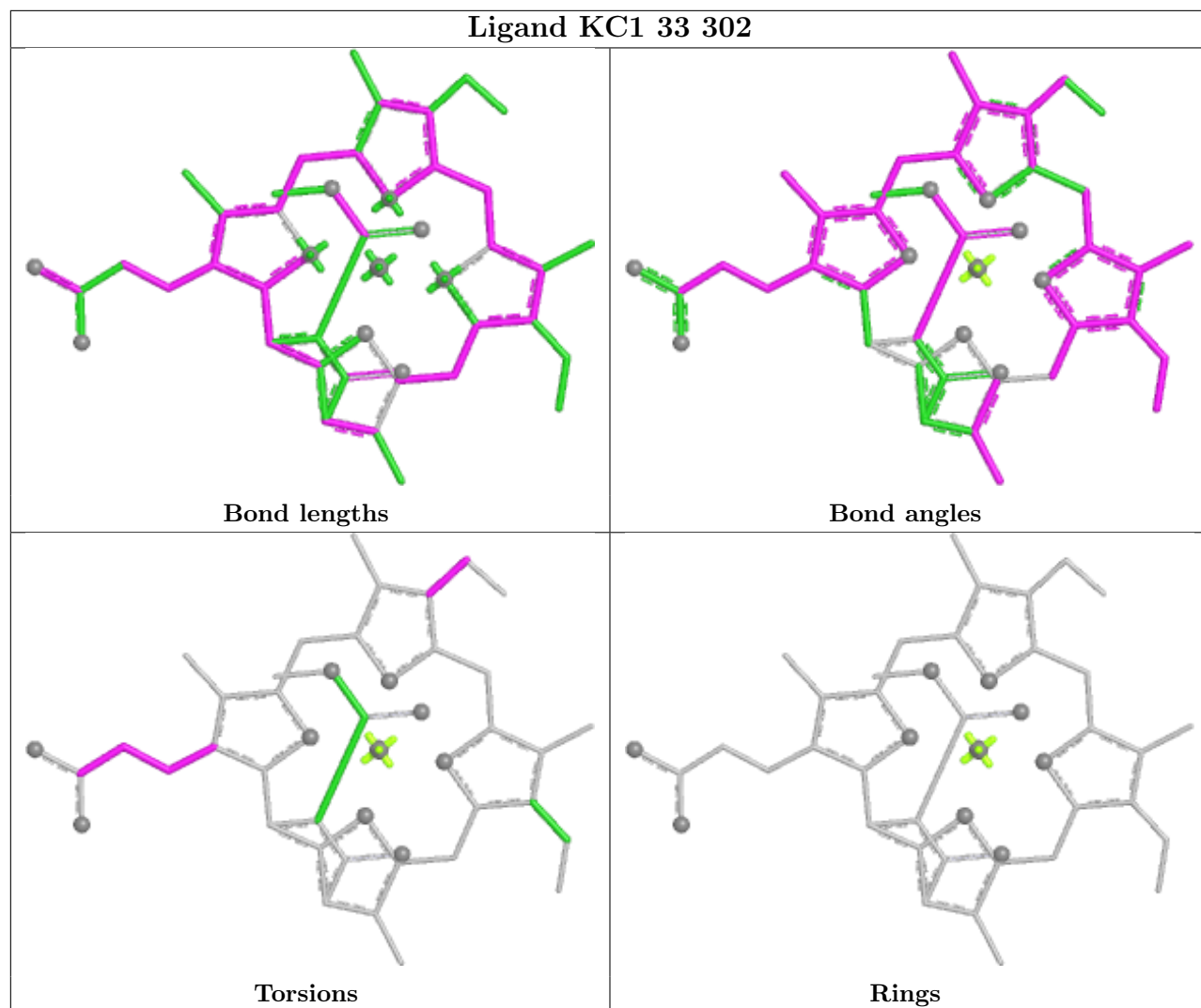


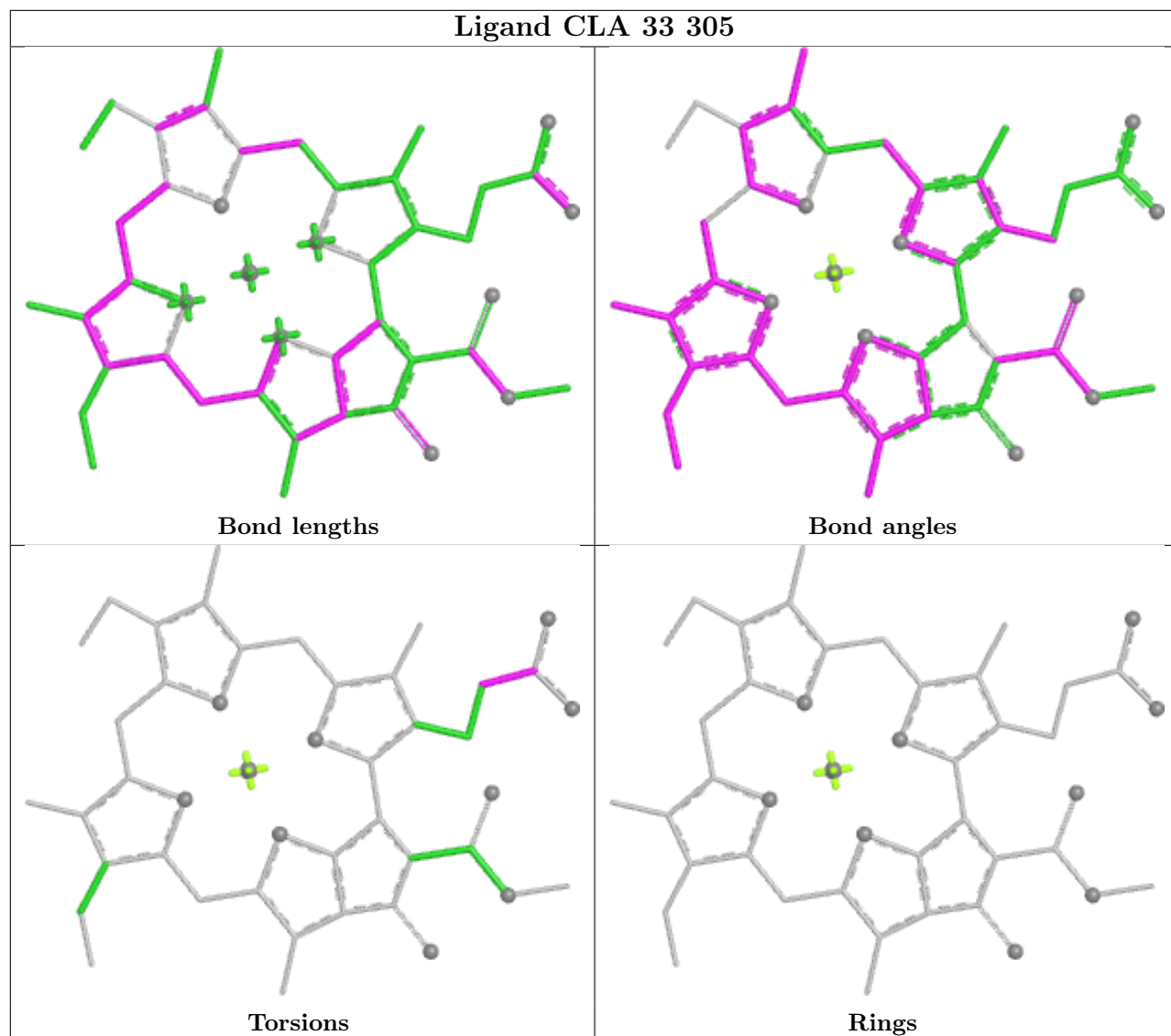


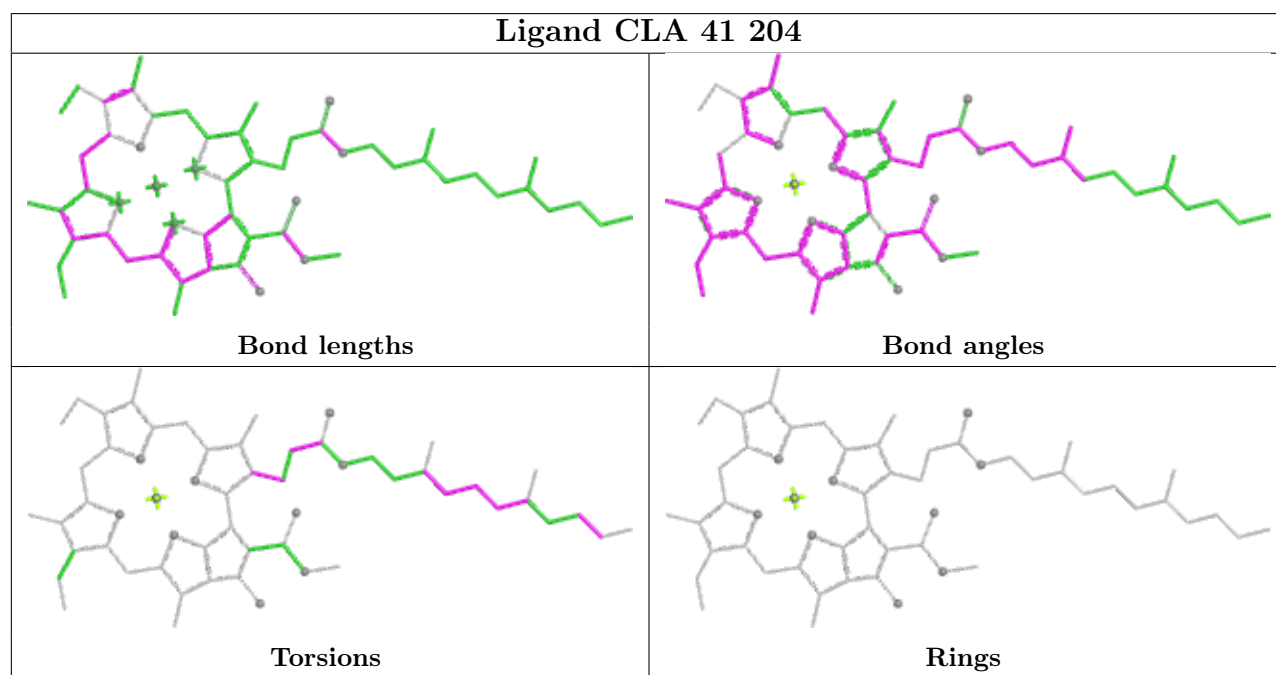
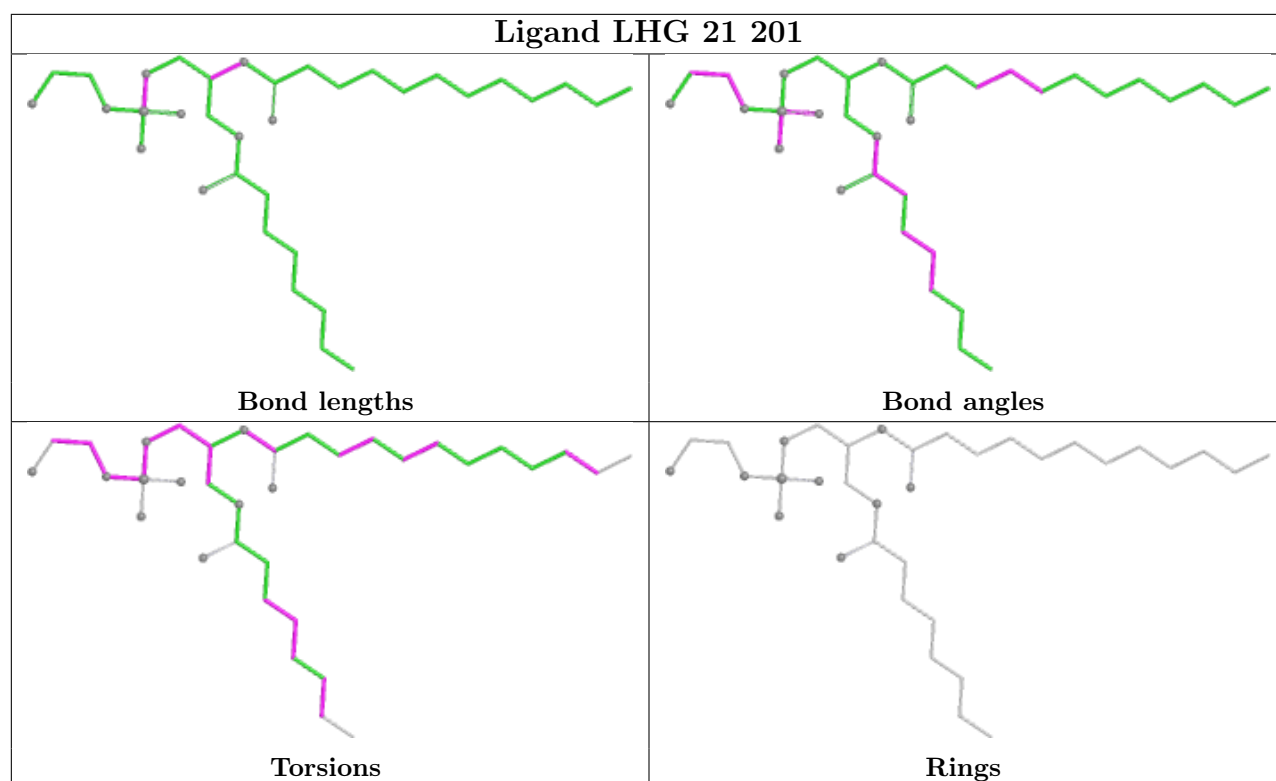


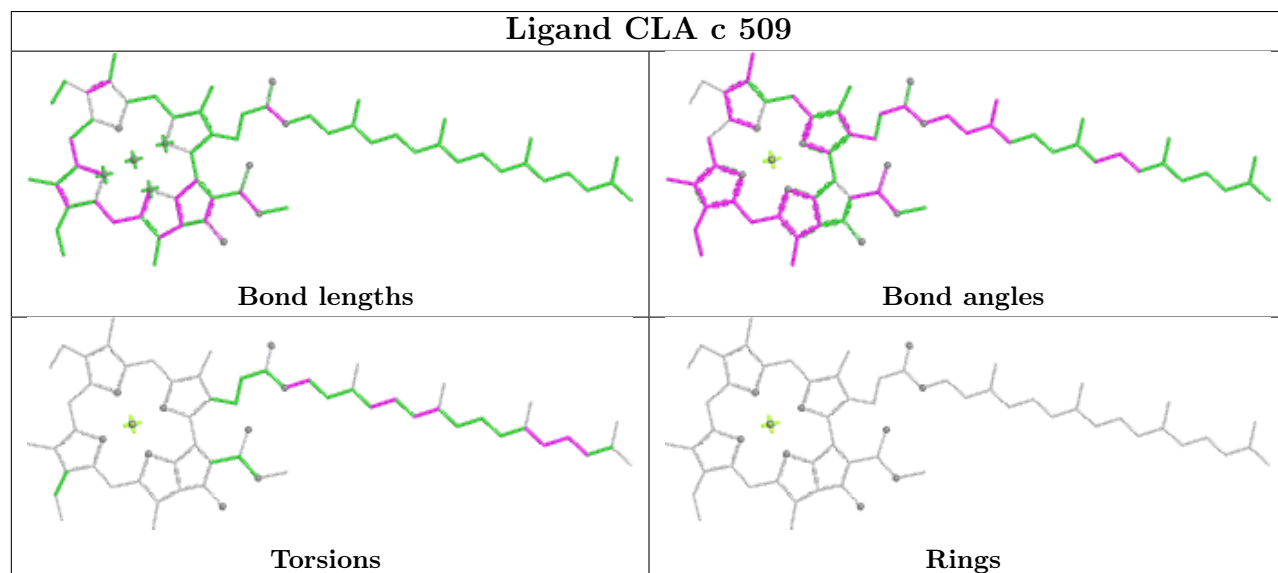
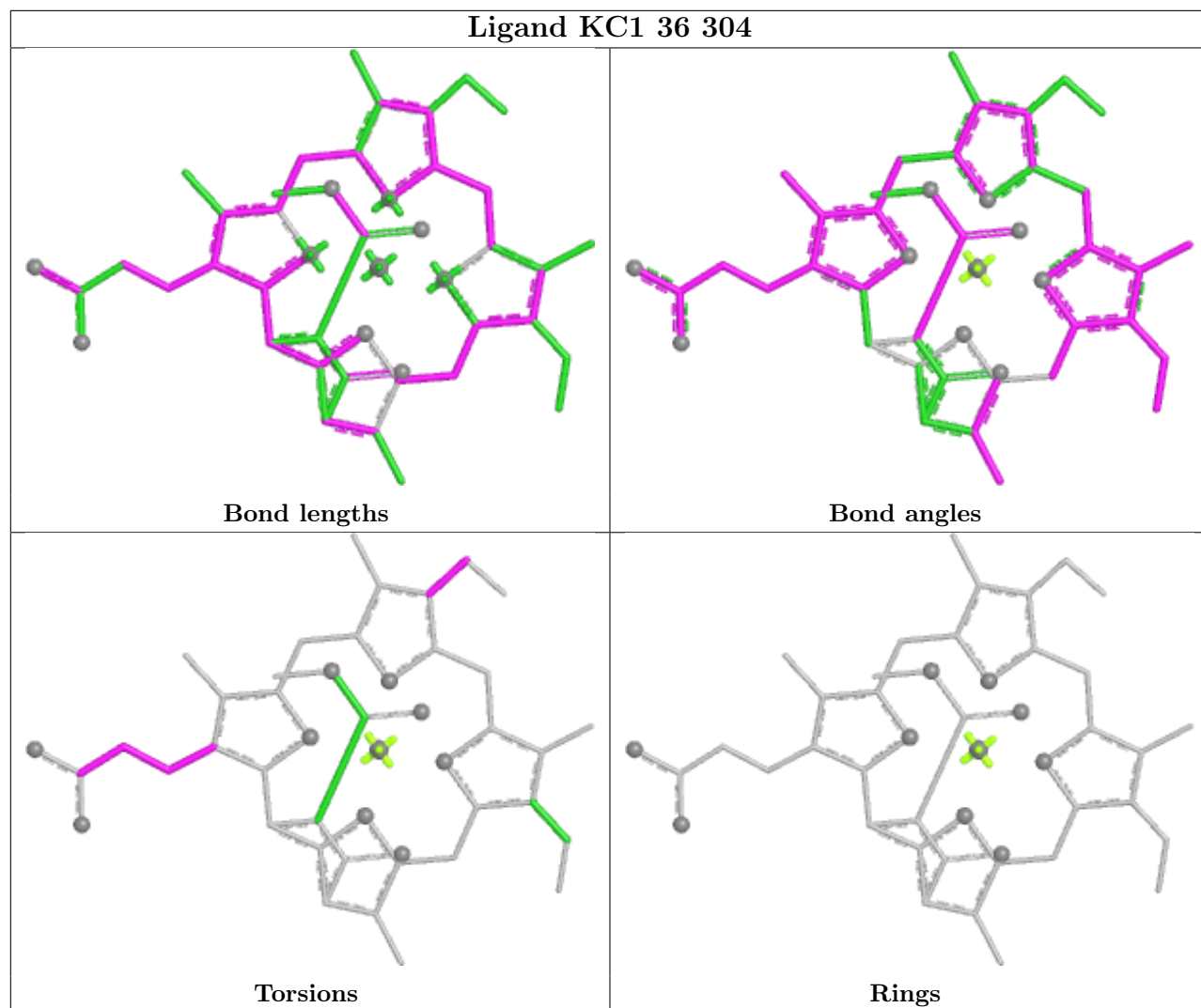


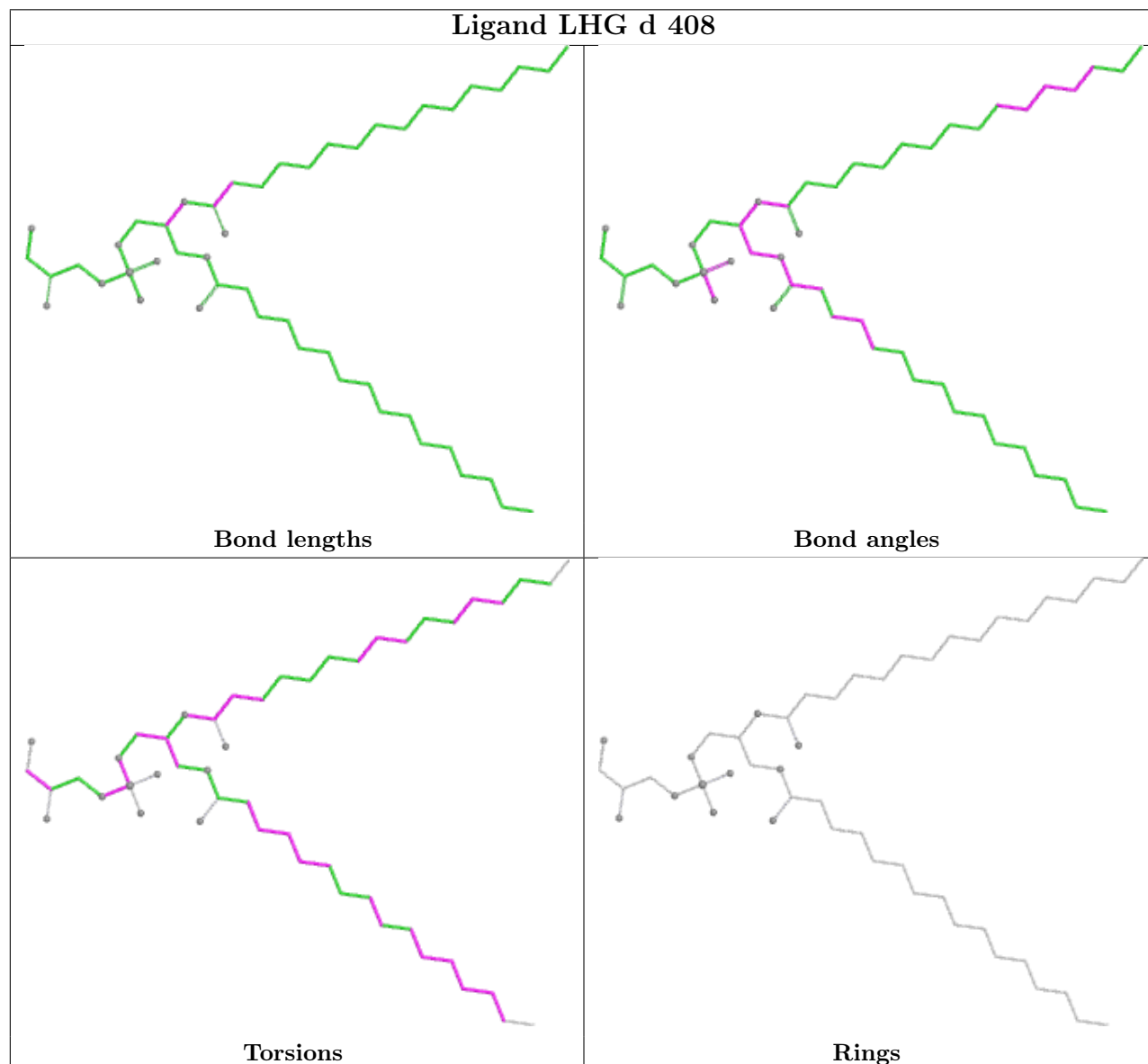
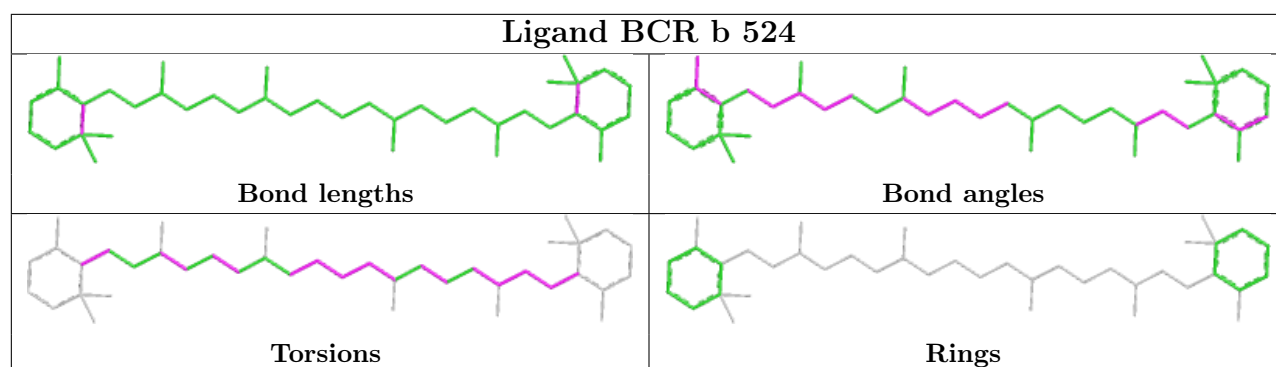


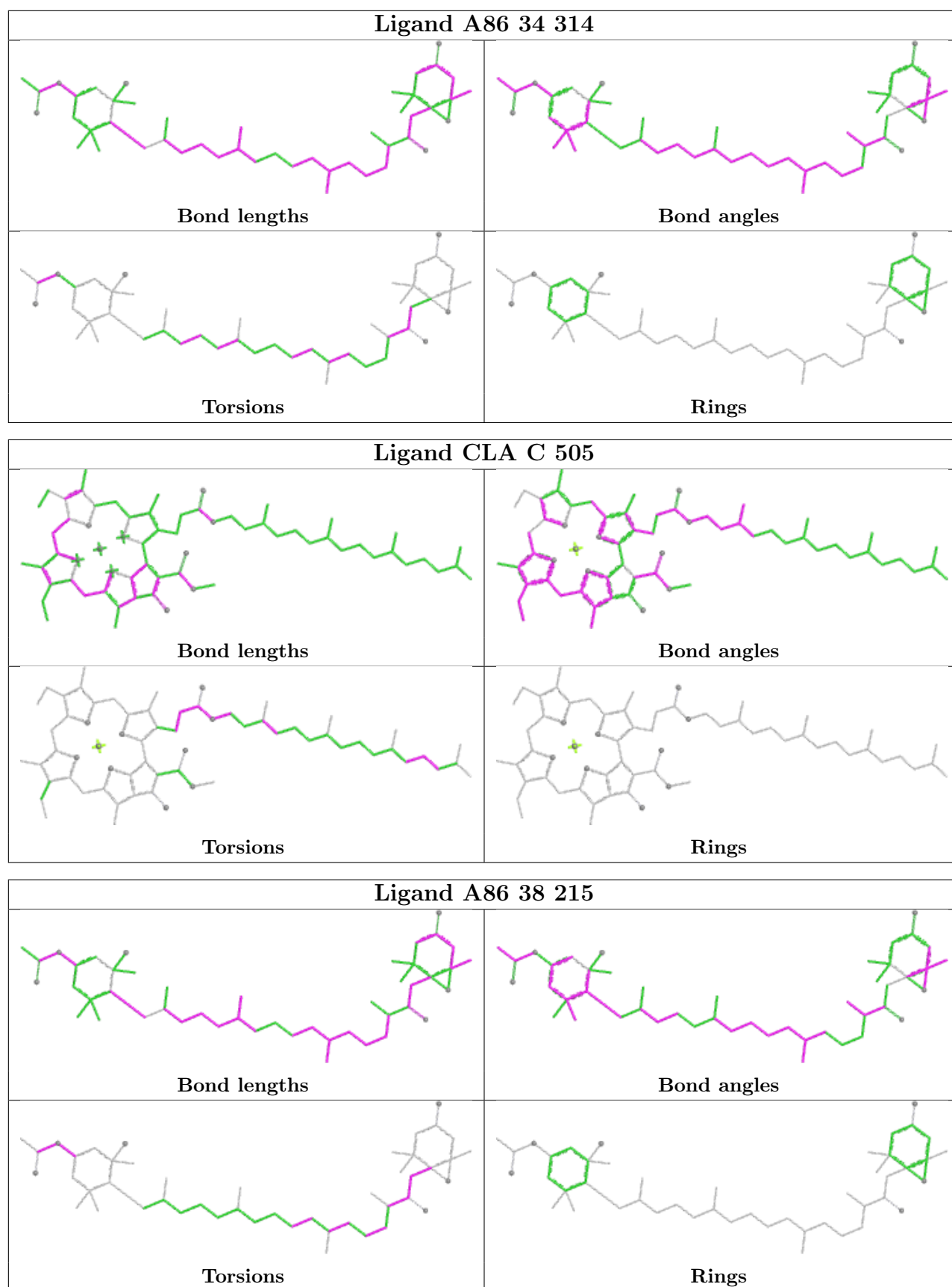


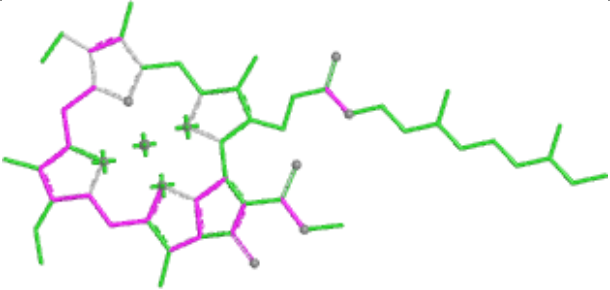
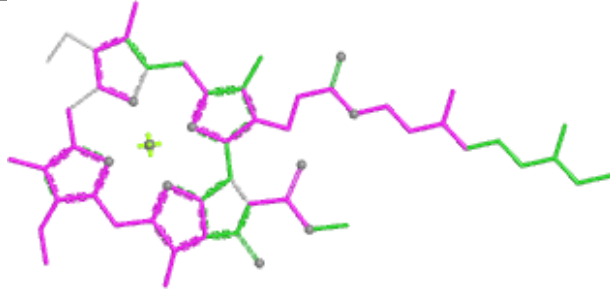
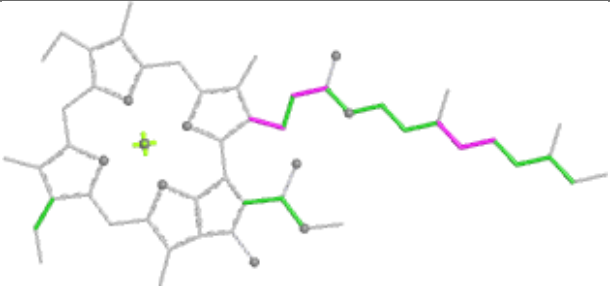
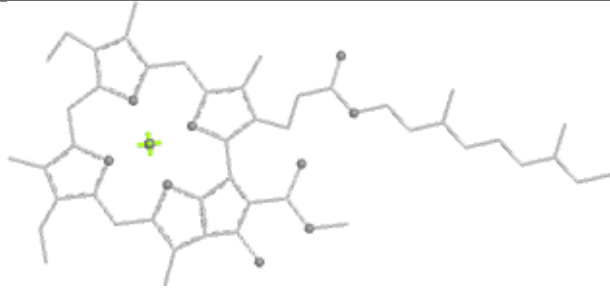
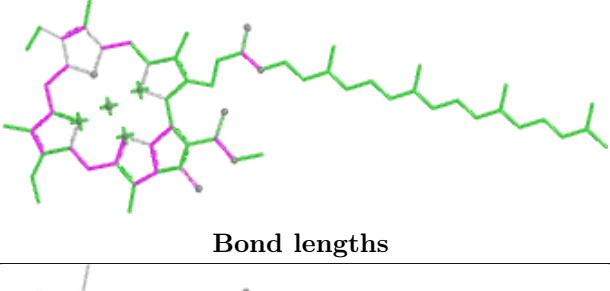
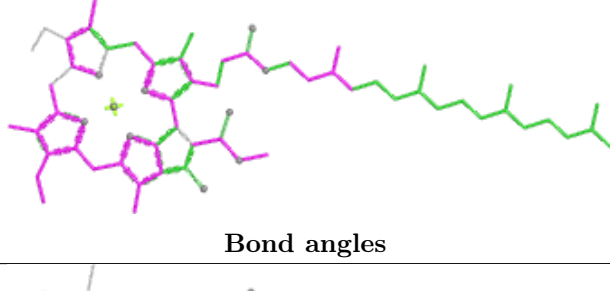
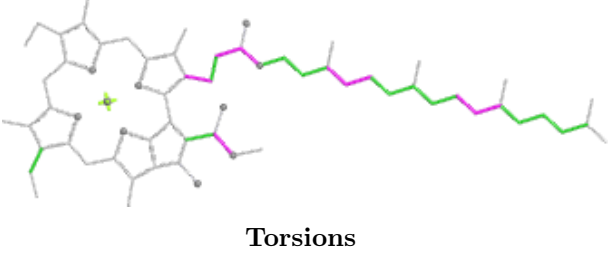
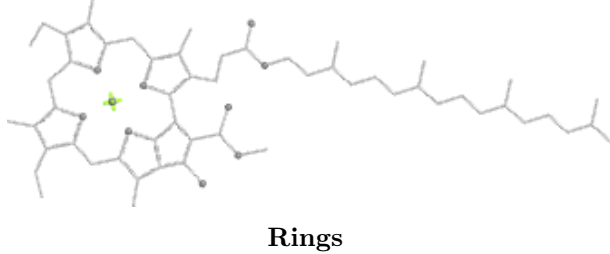


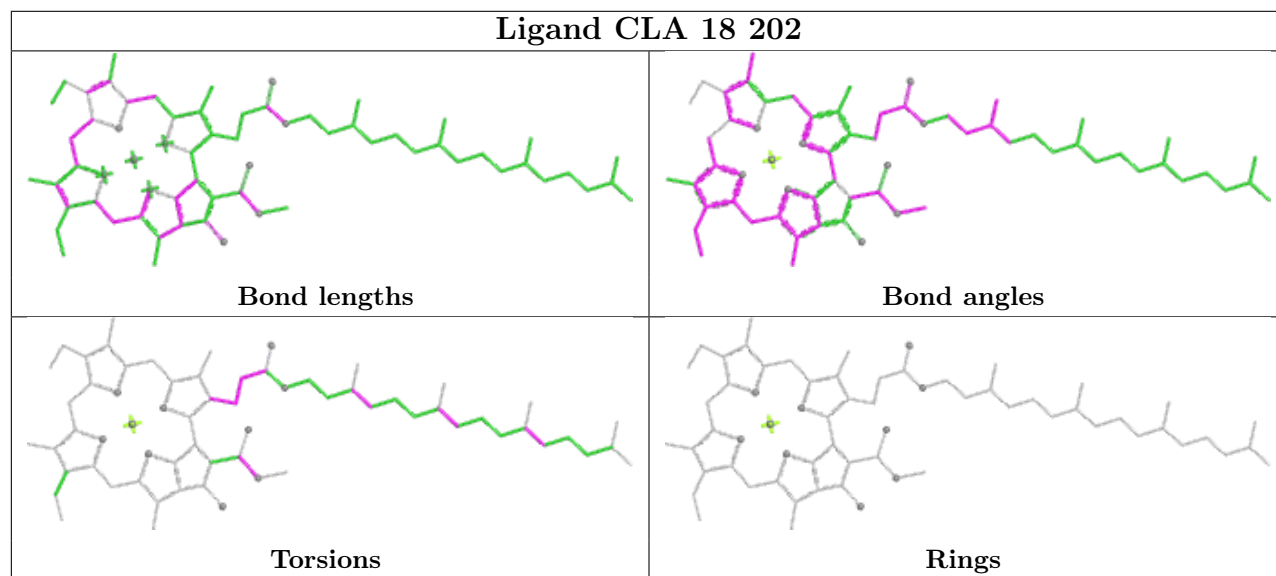
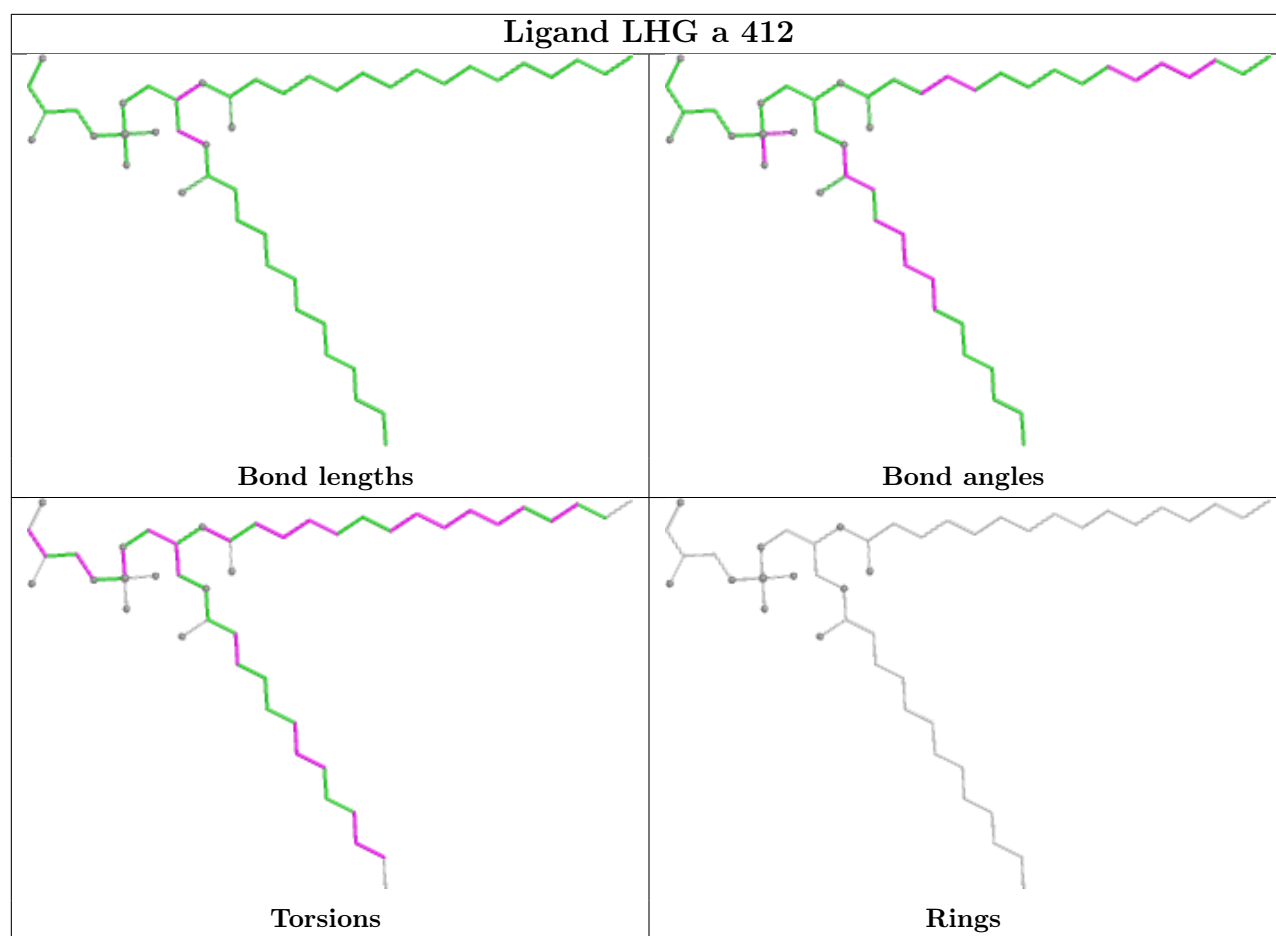


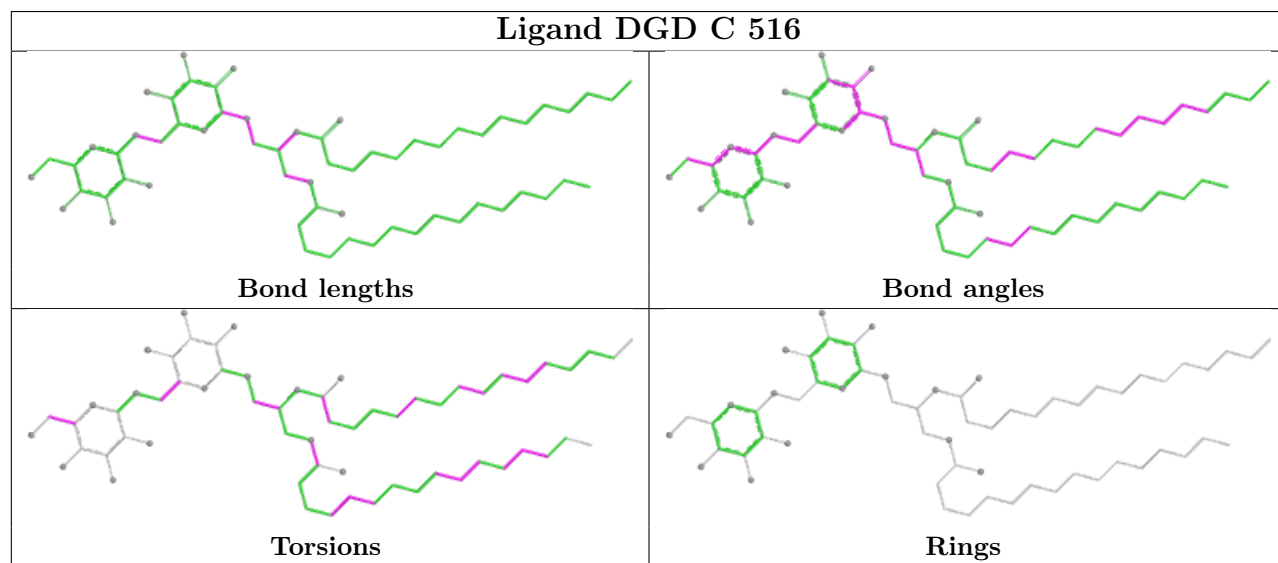
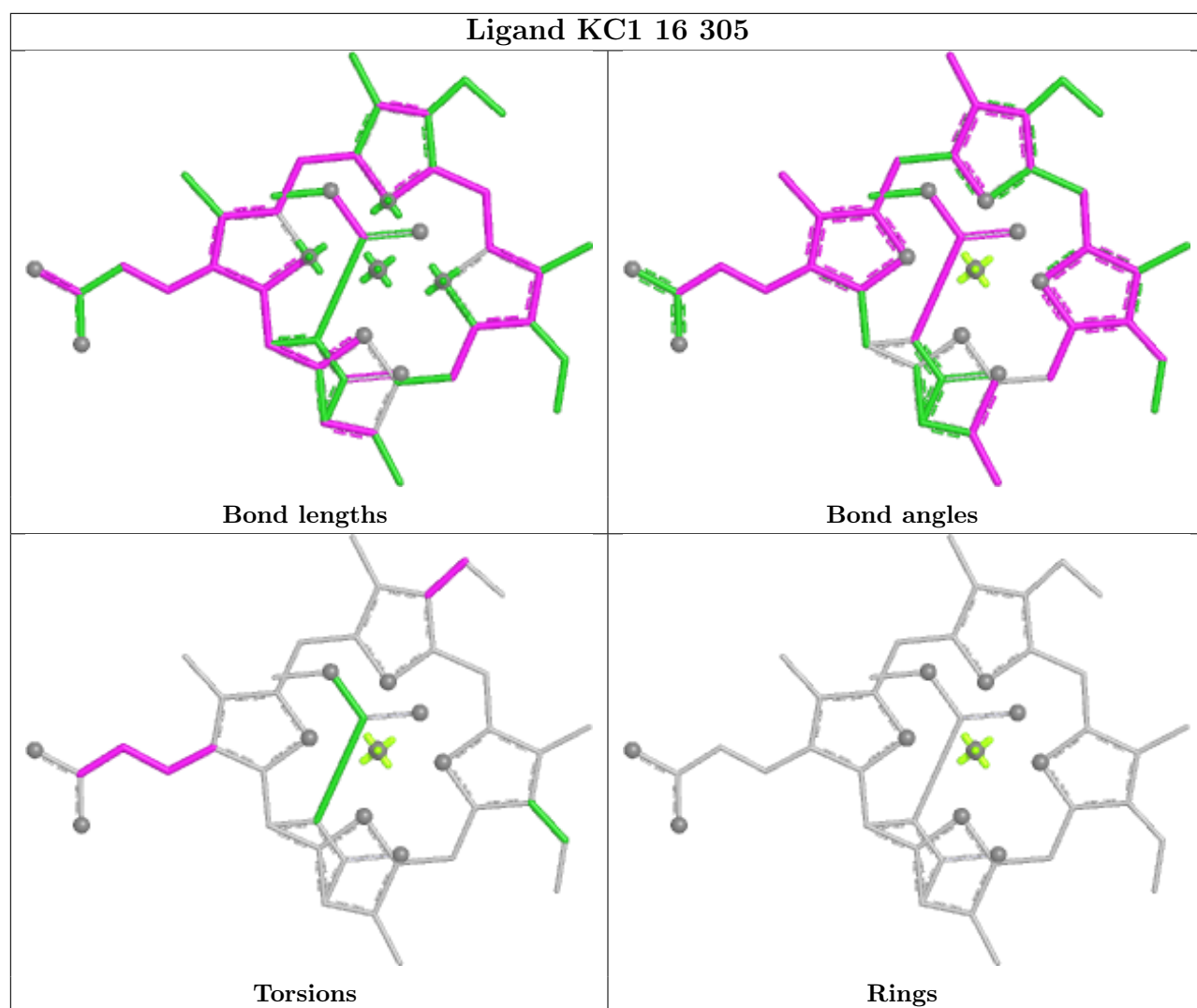


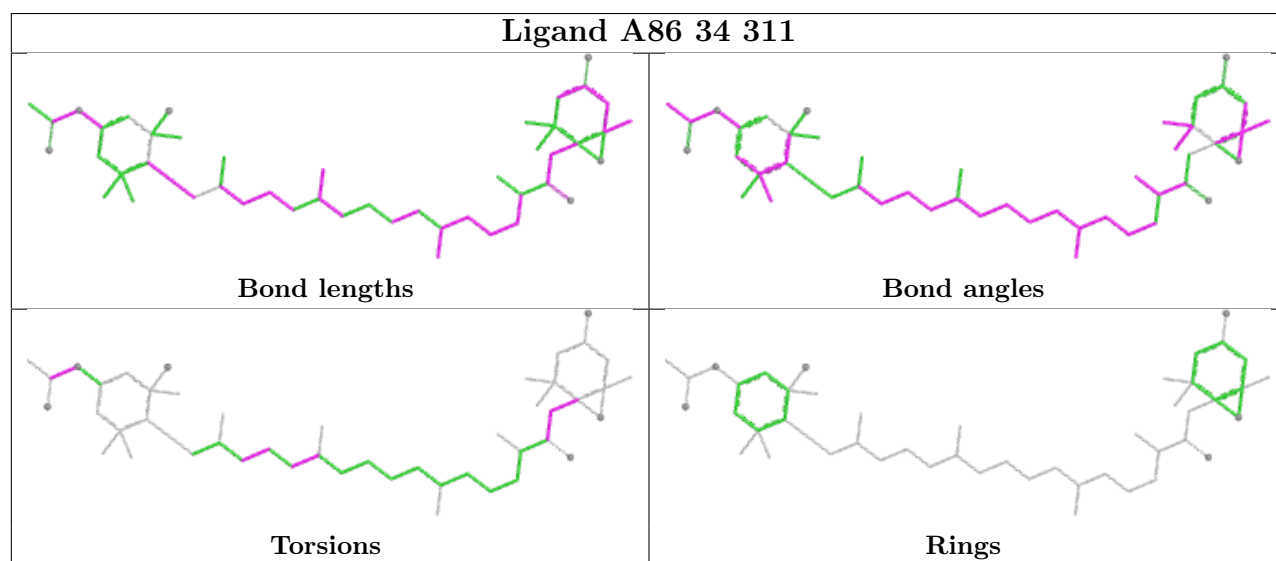
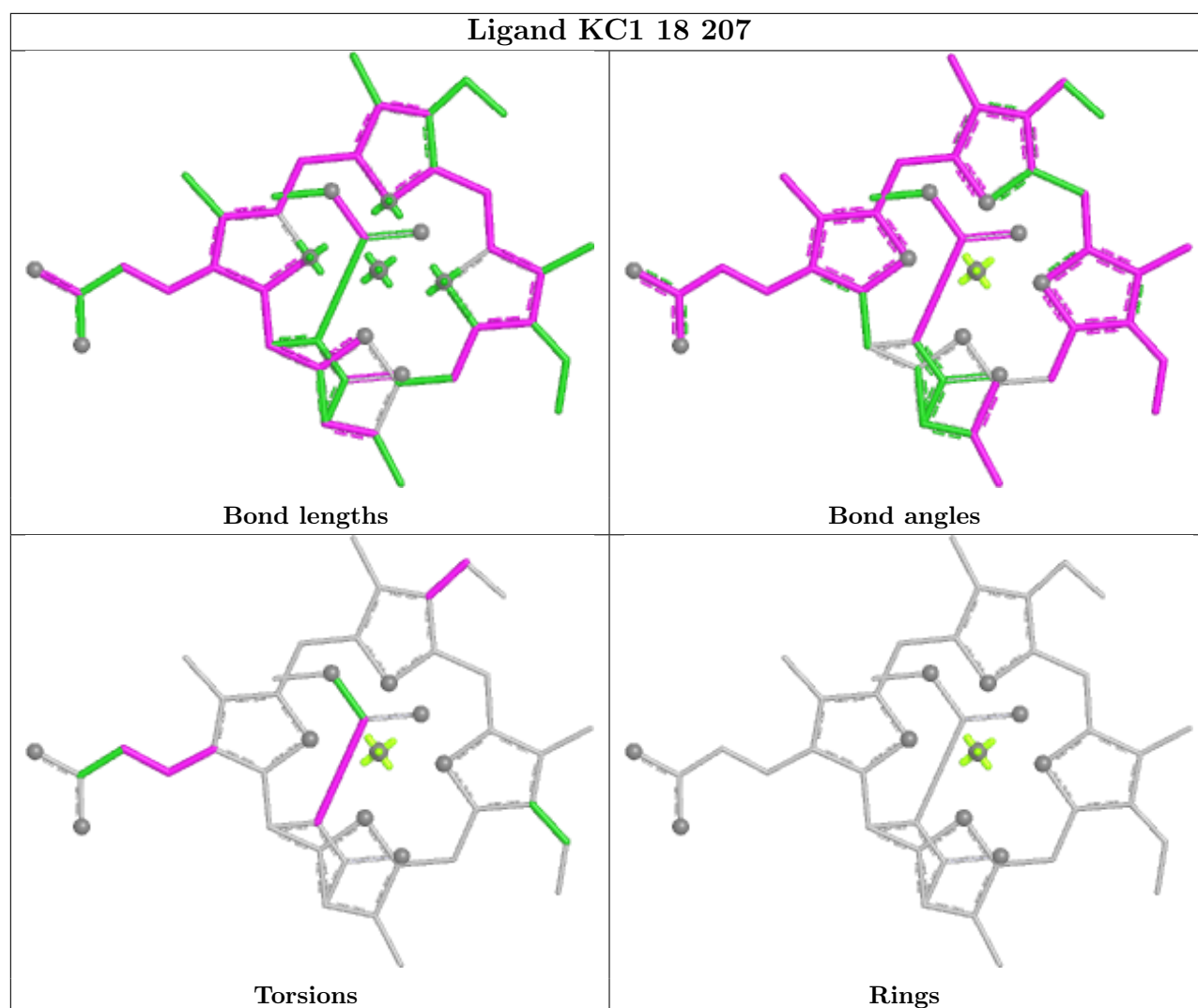


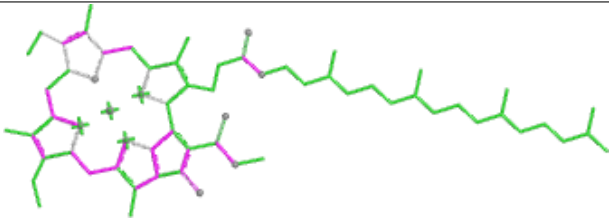
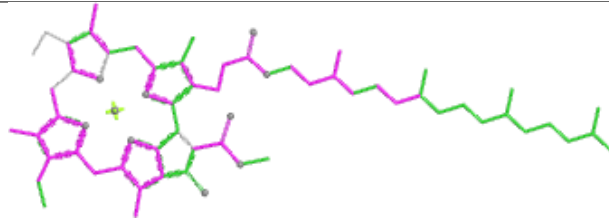
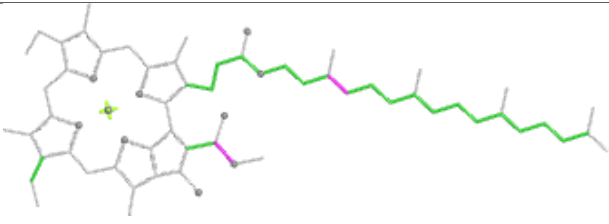
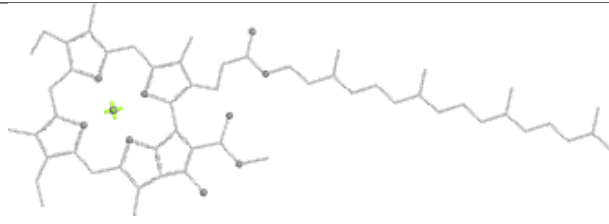


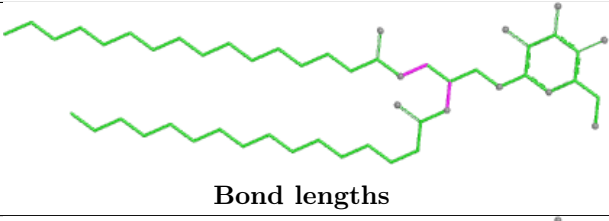
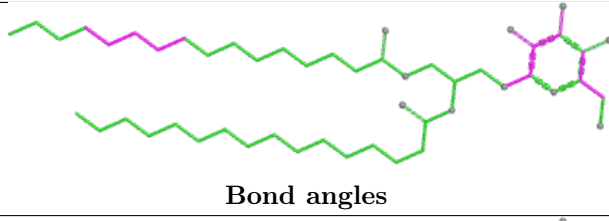
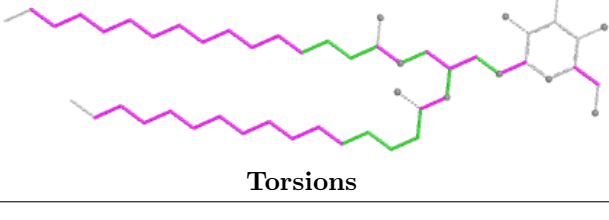
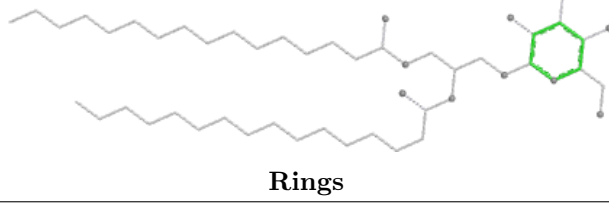
Ligand CLA 38 204	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA 21 206	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

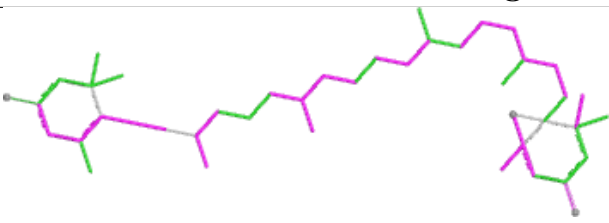
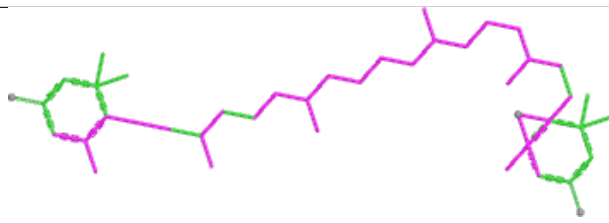
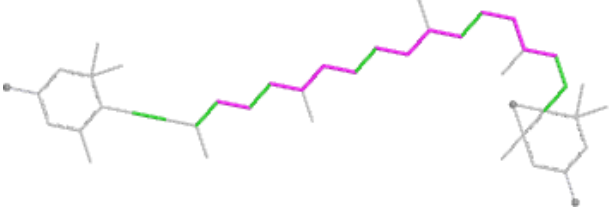
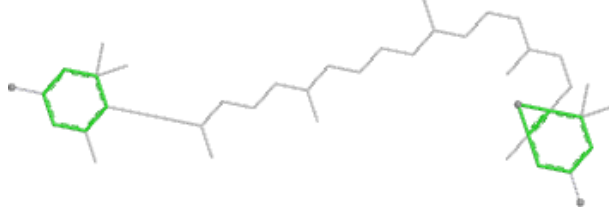


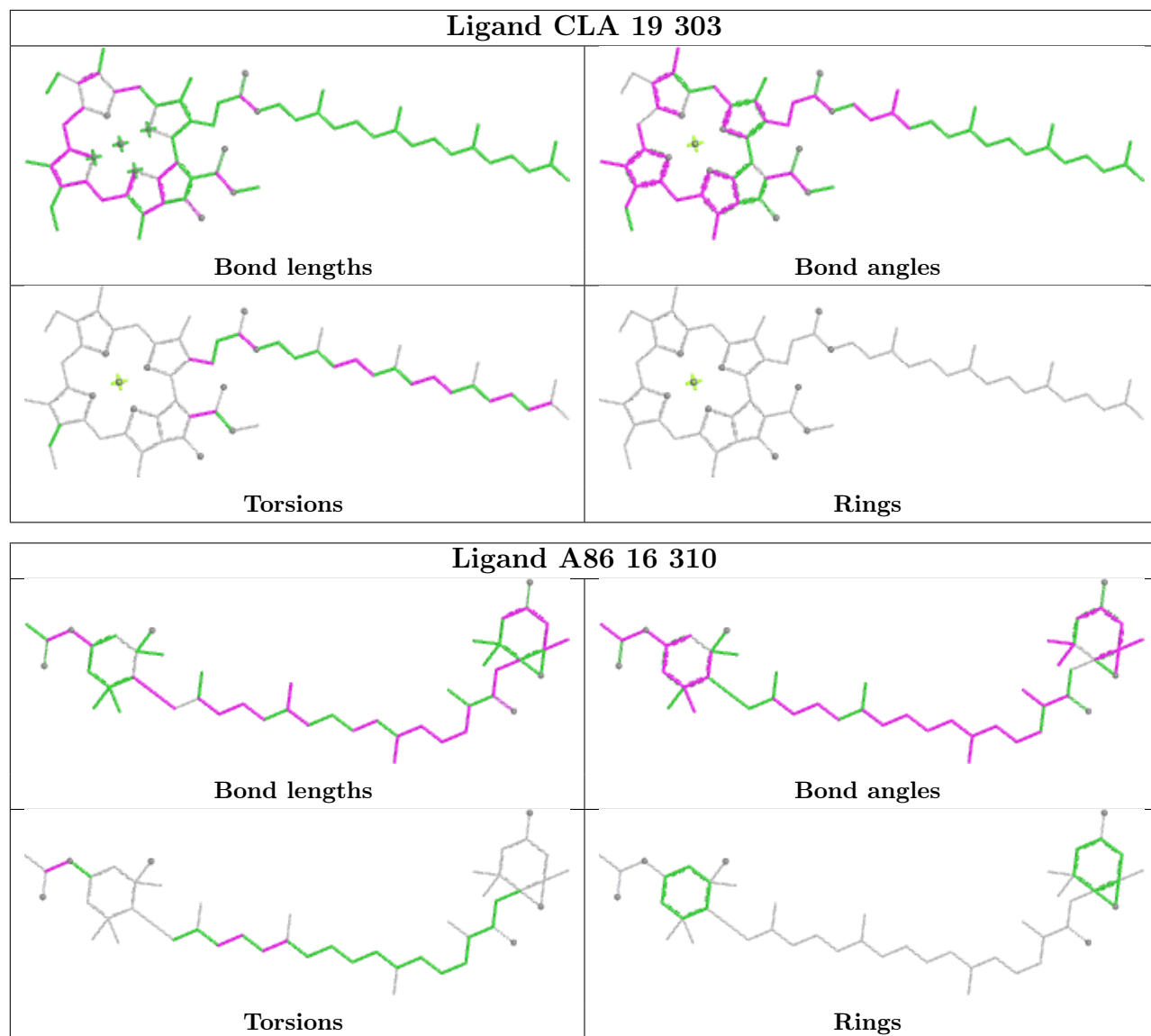


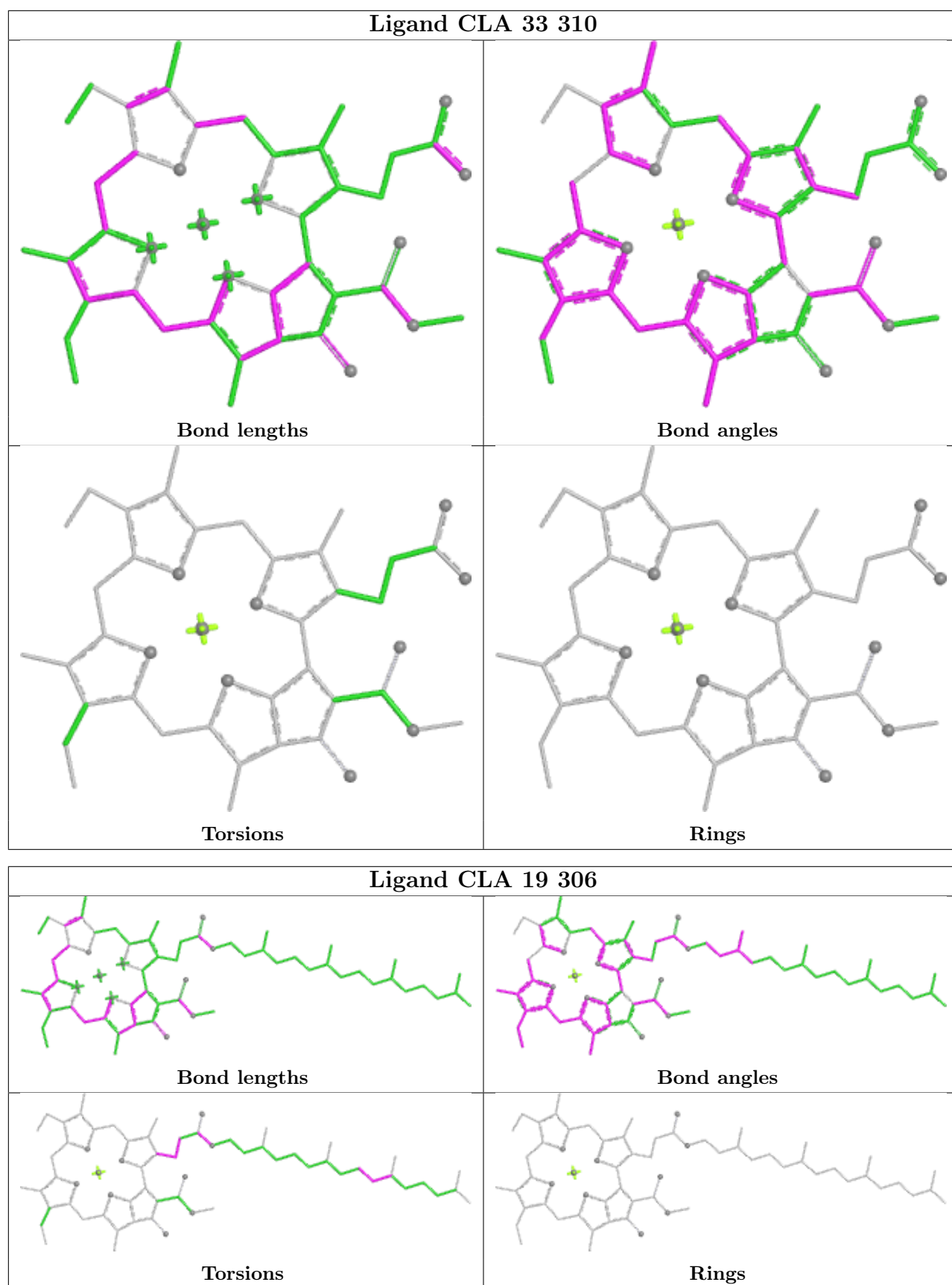


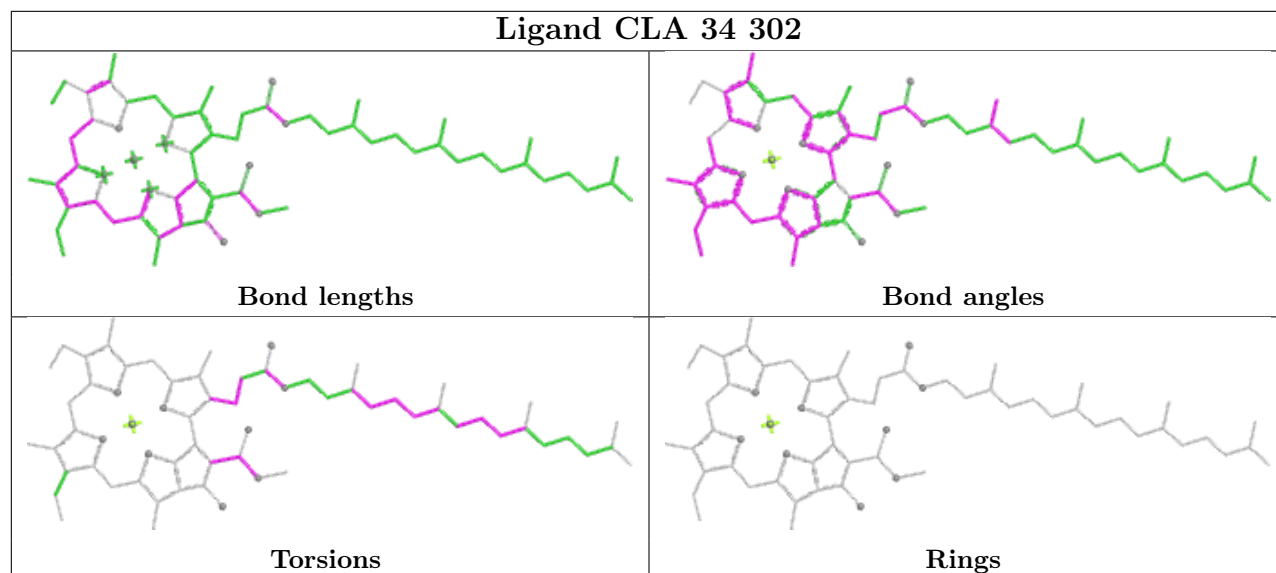
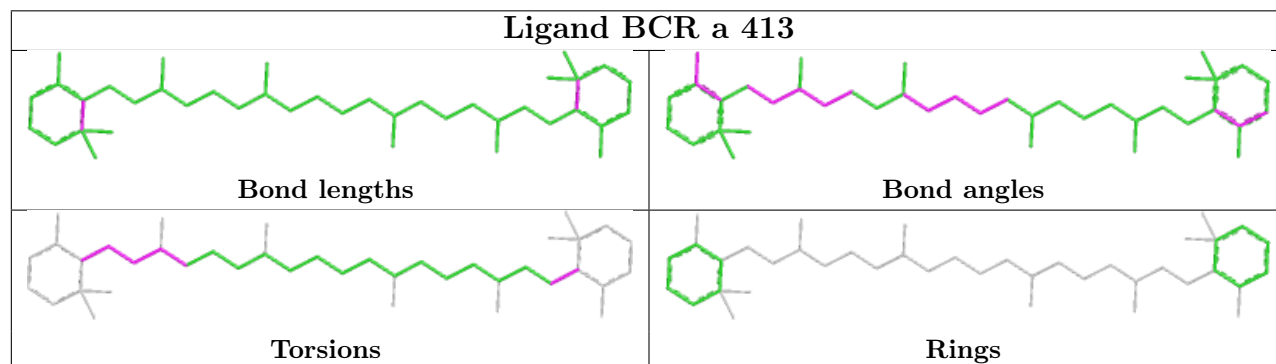
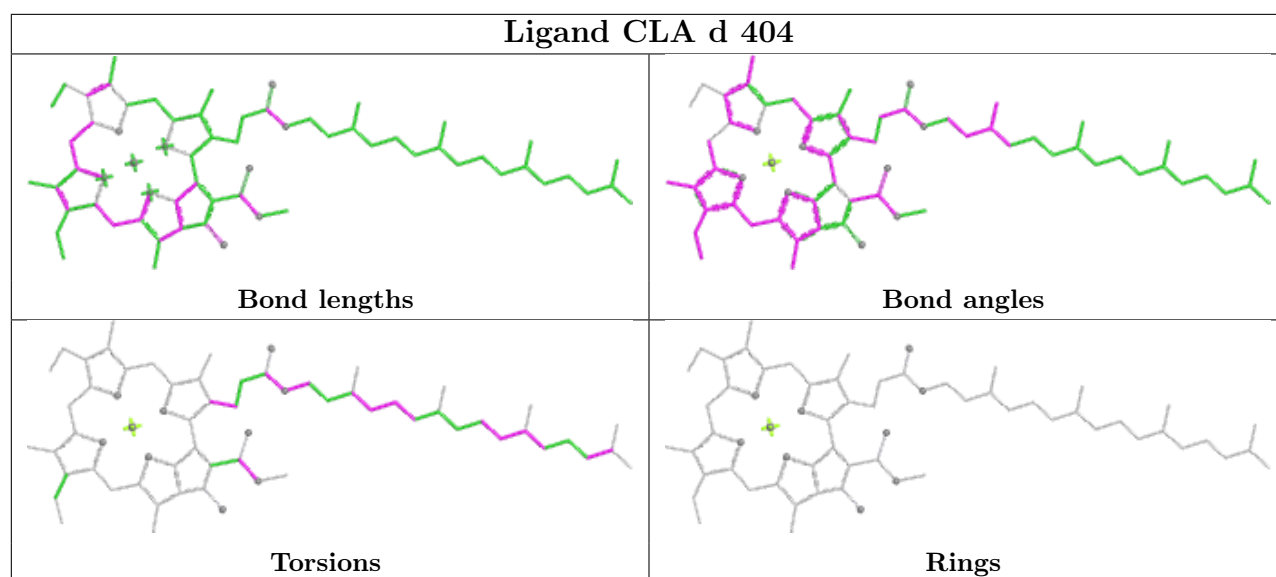
Ligand CLA B 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

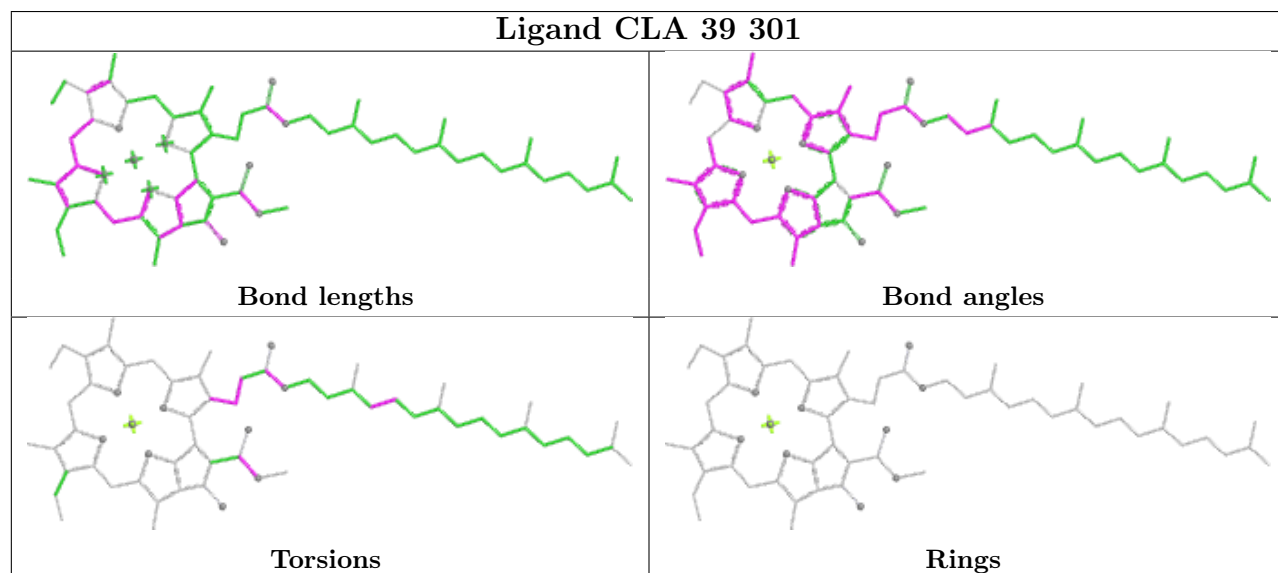
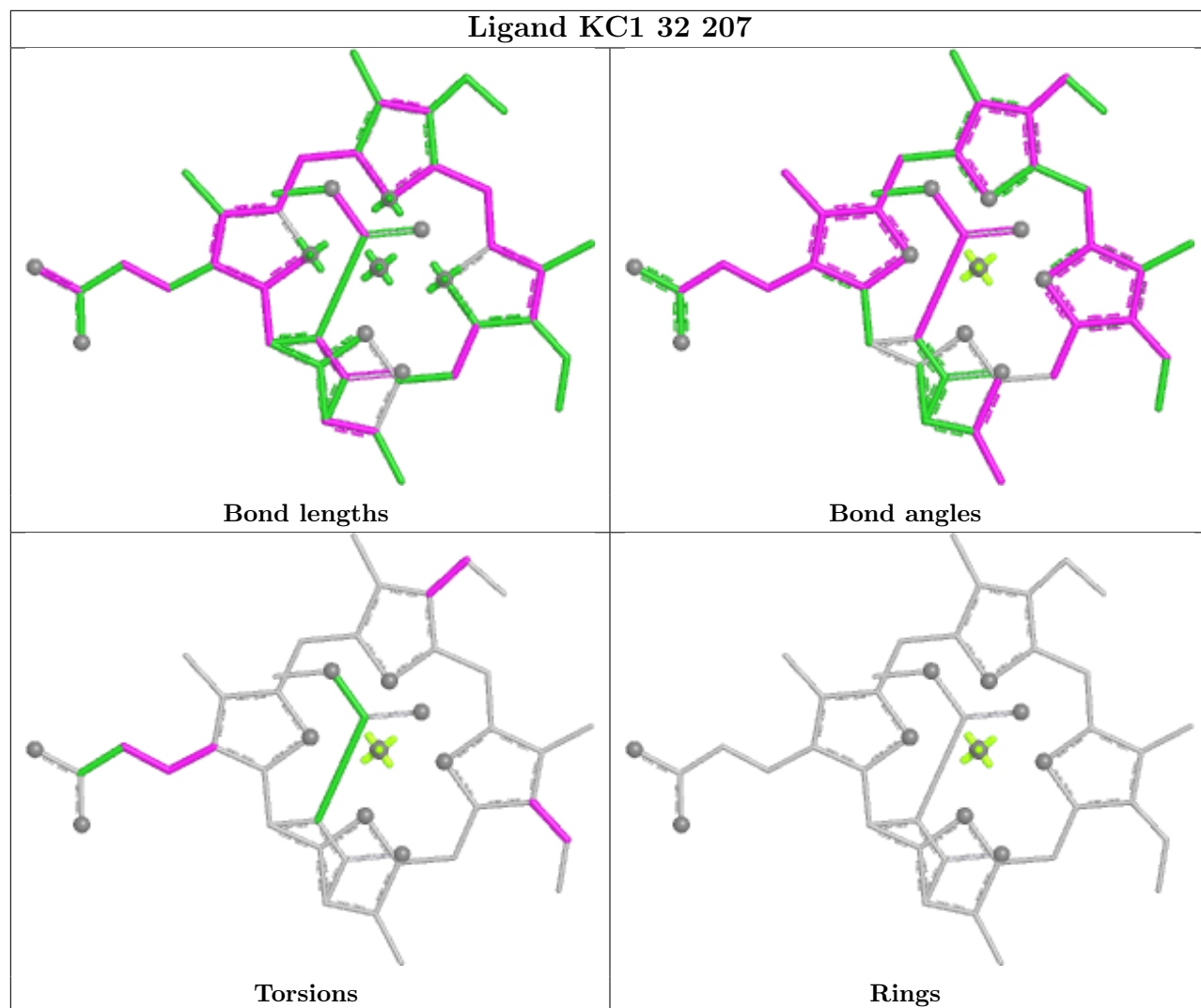
Ligand LMG a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

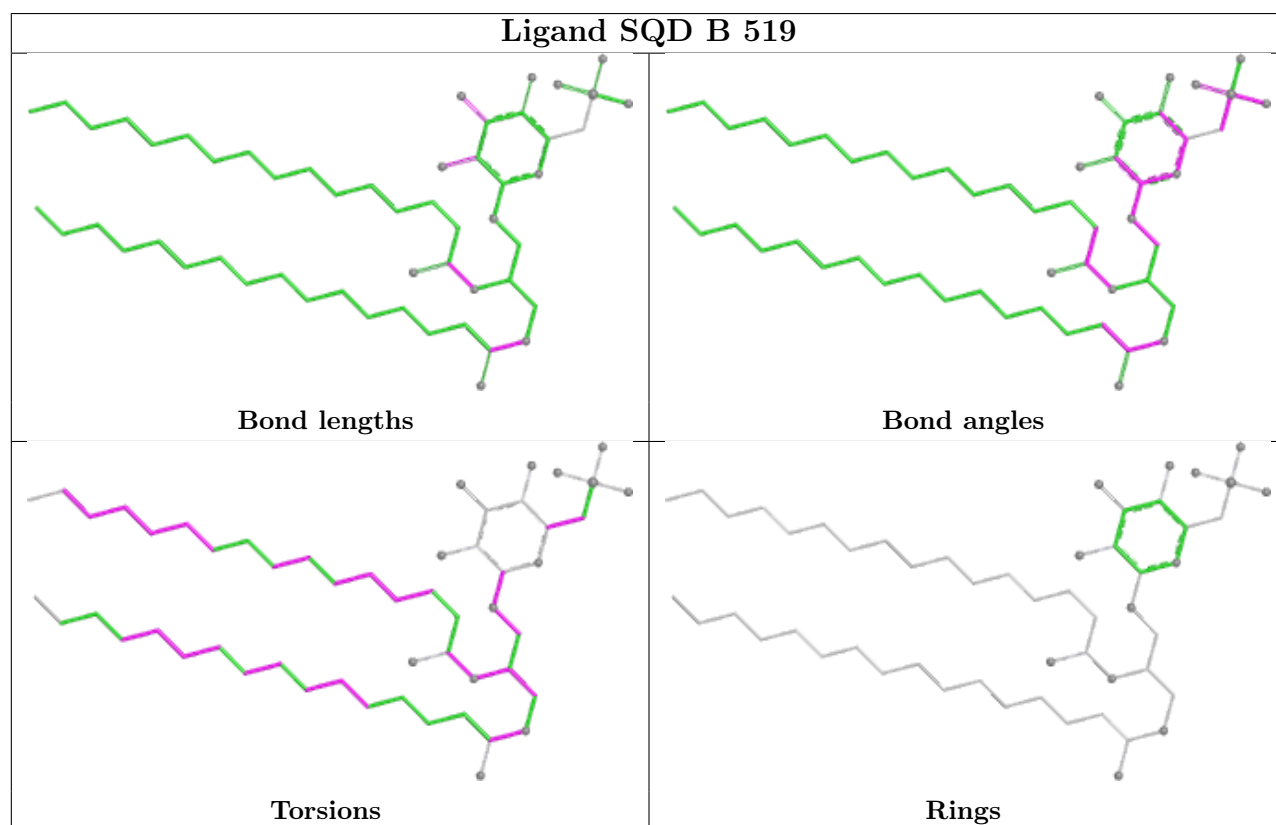
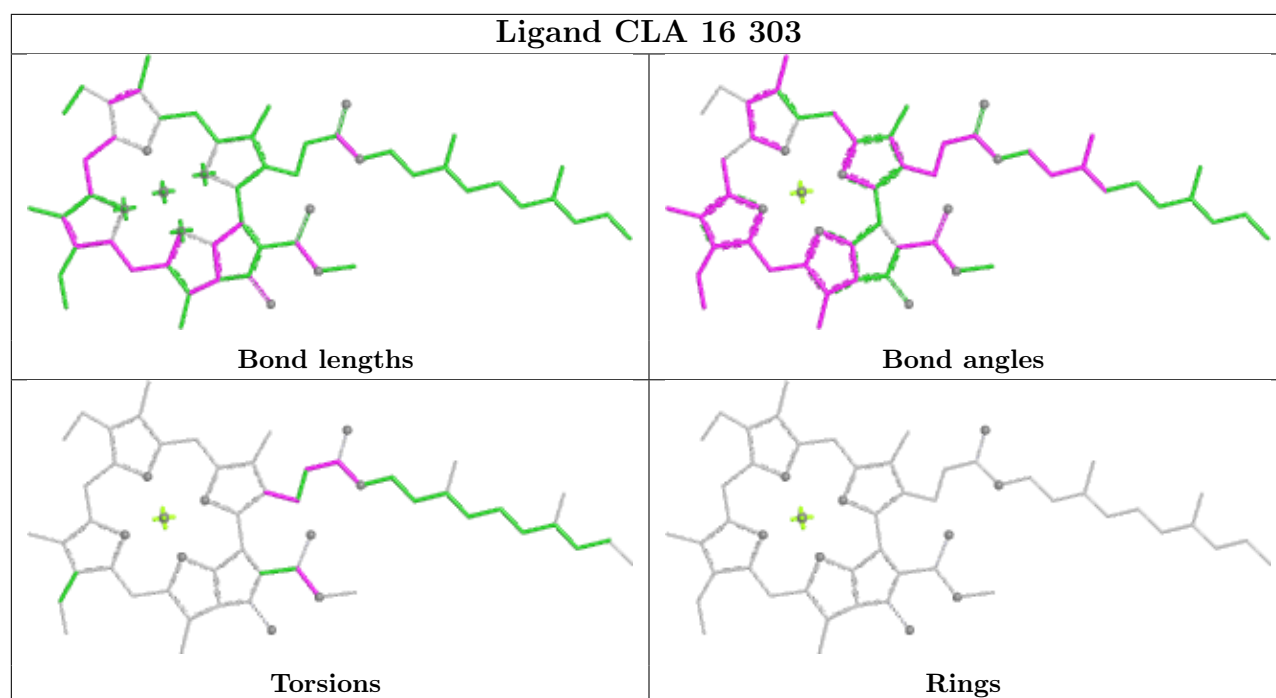
Ligand DD6 20 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

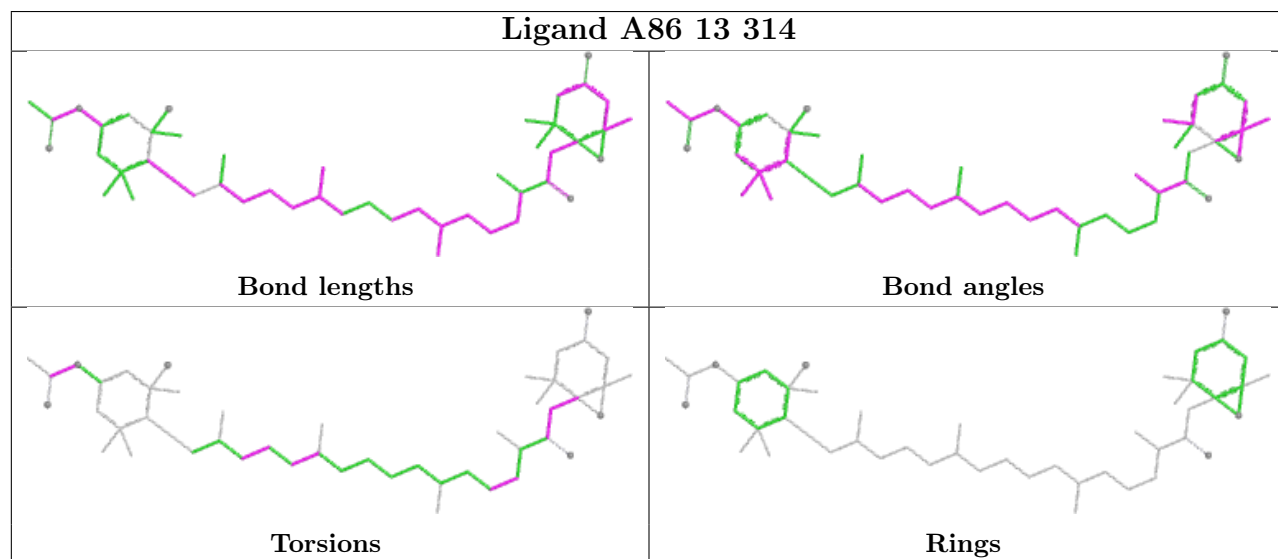
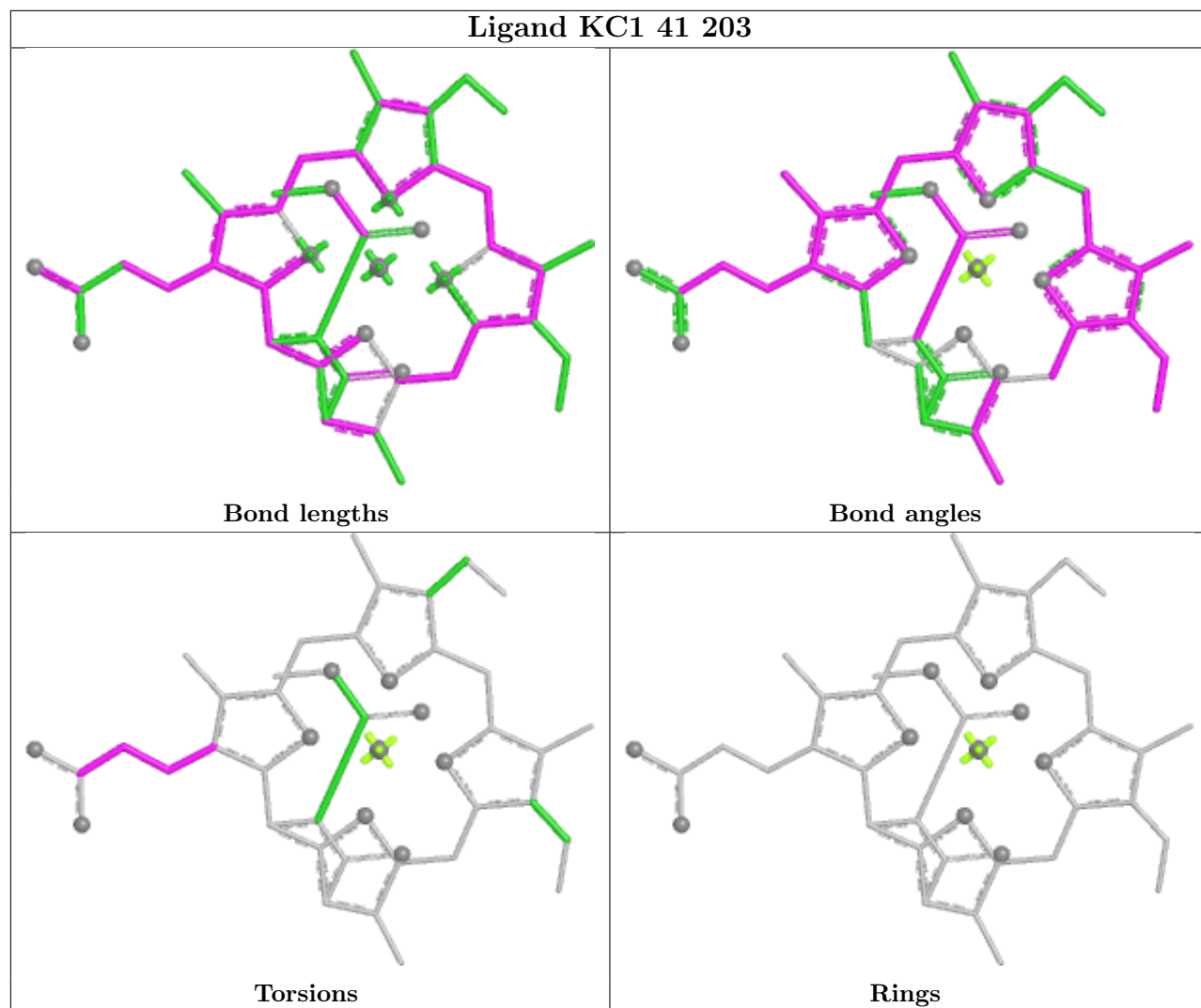


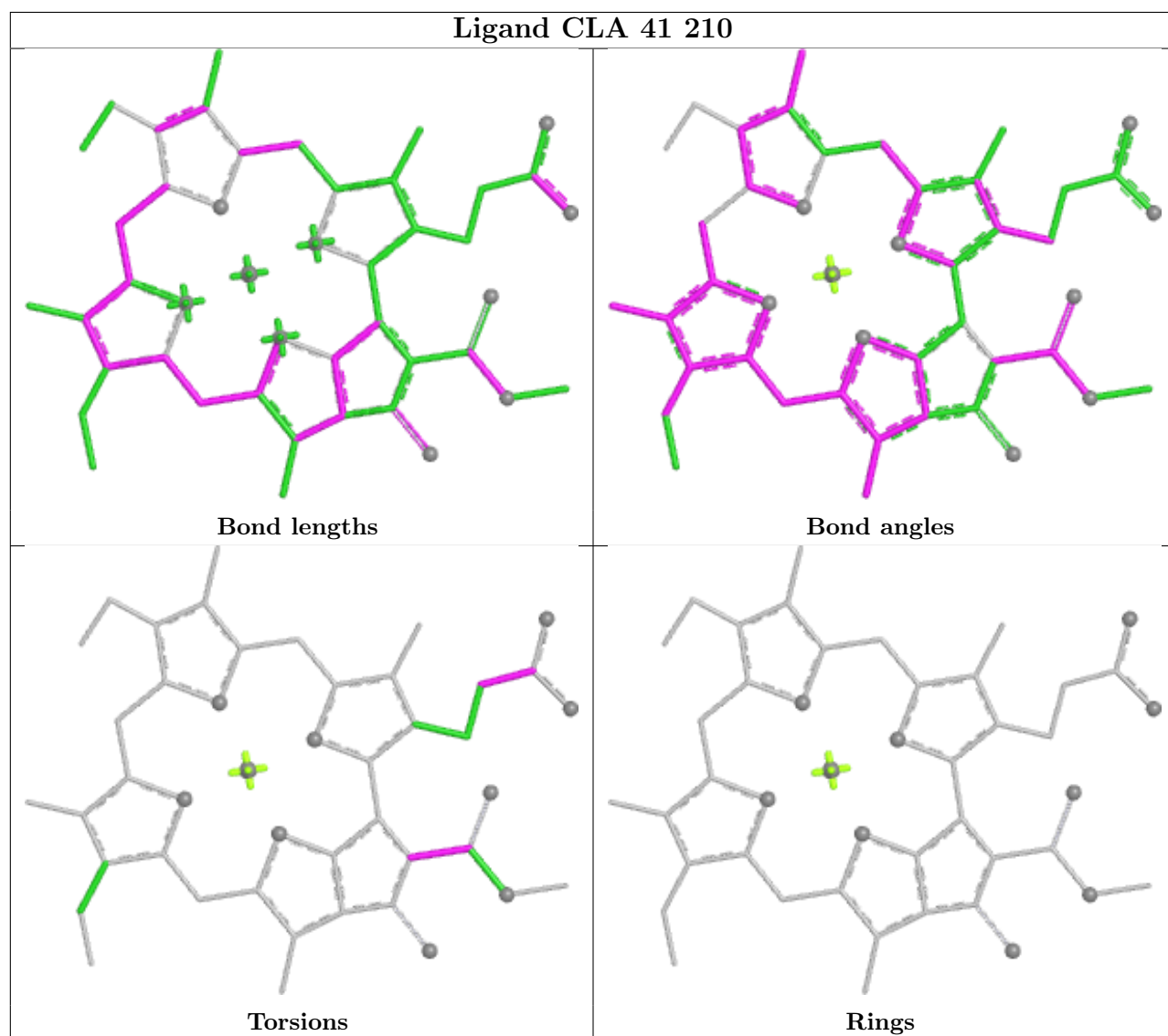
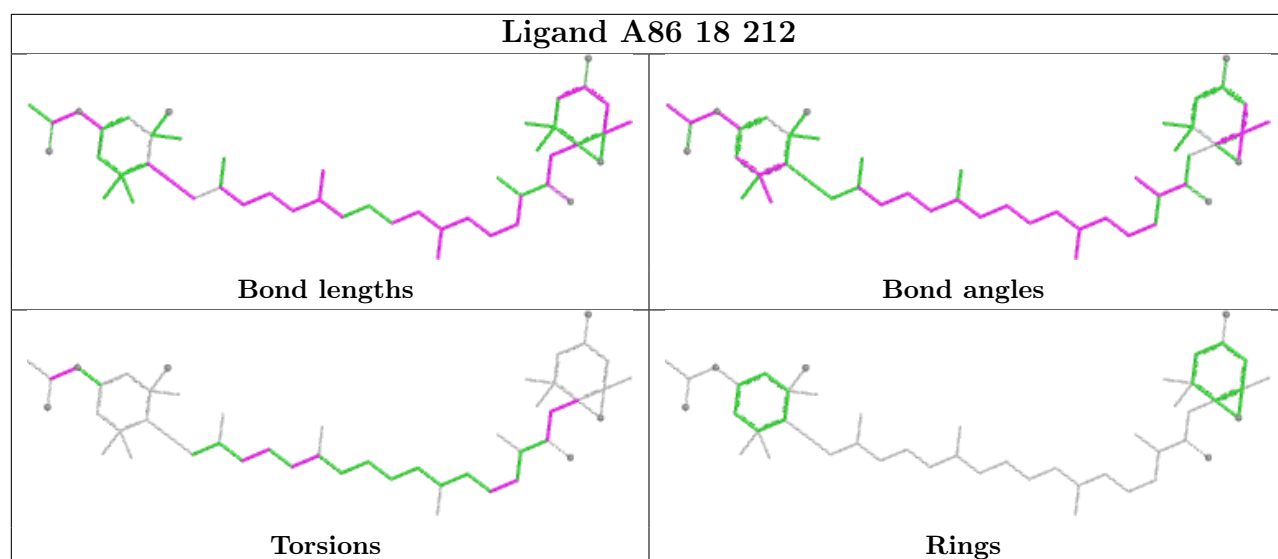


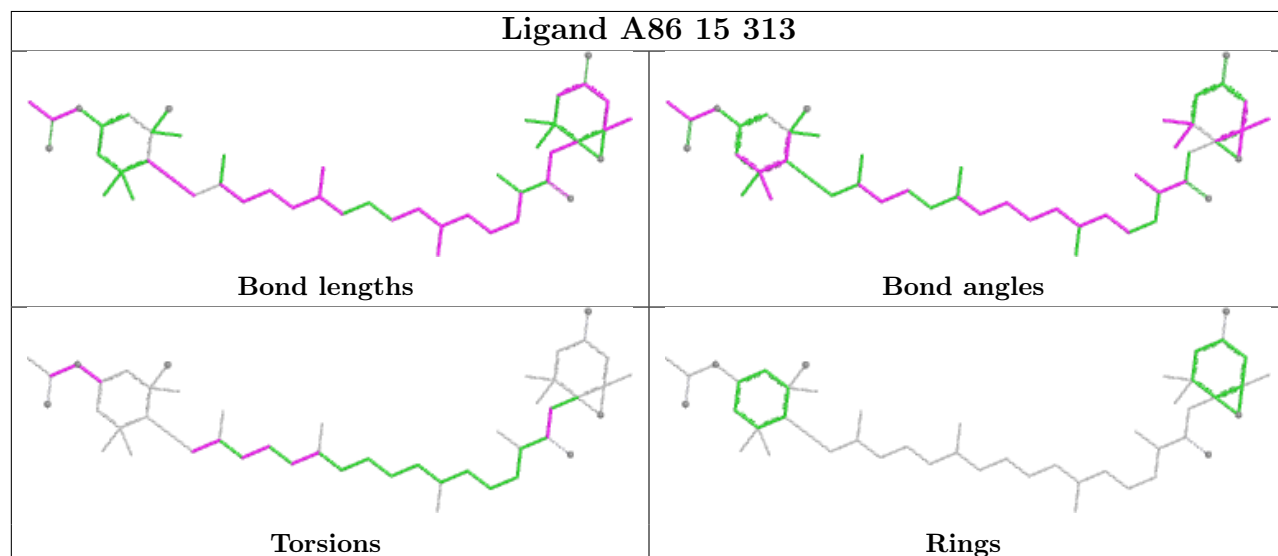
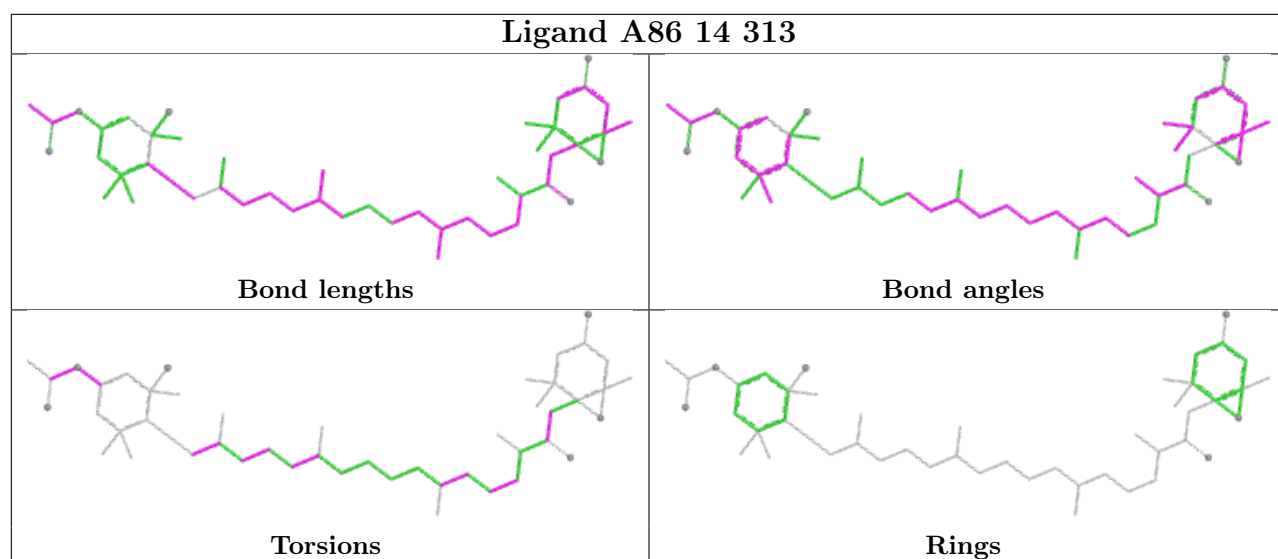


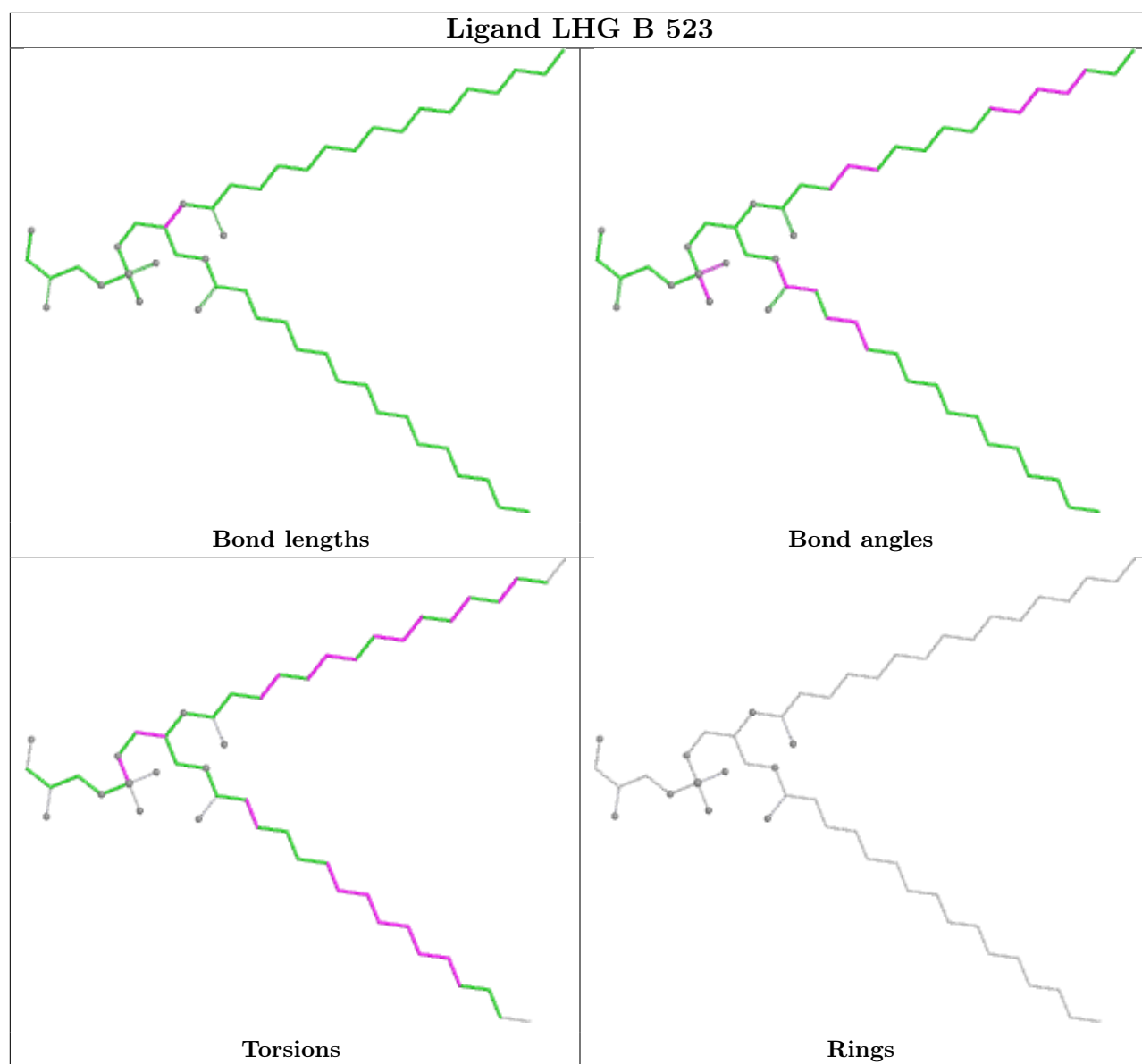




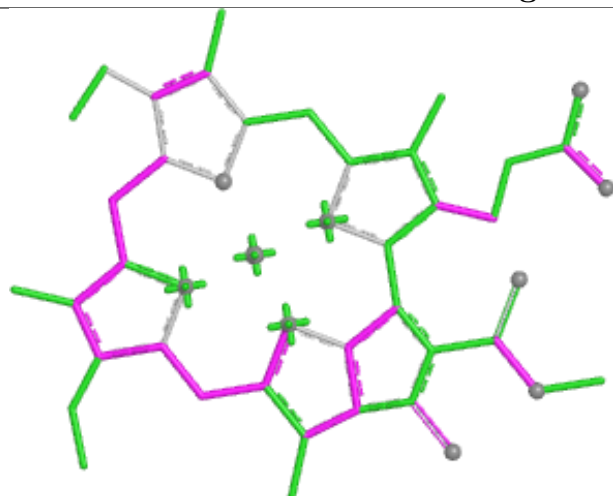




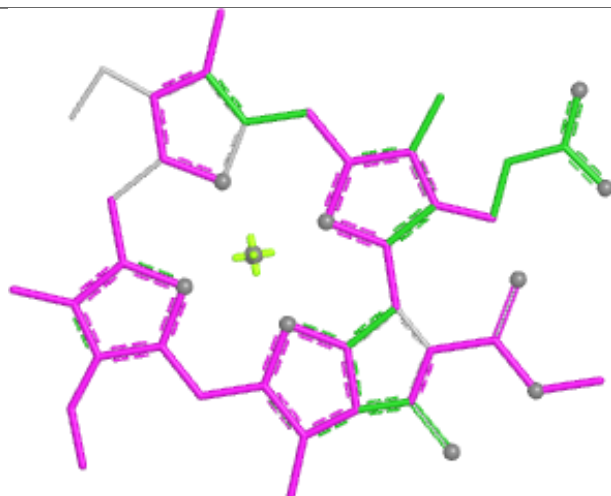




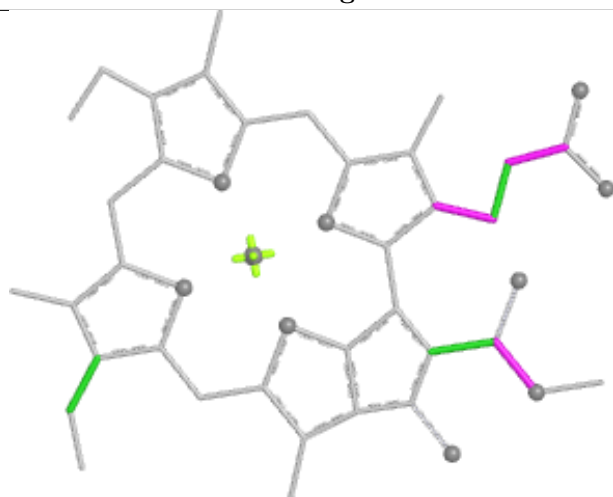
Ligand CLA z 102



Bond lengths



Bond angles

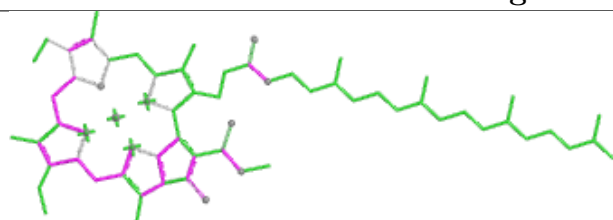


Torsions

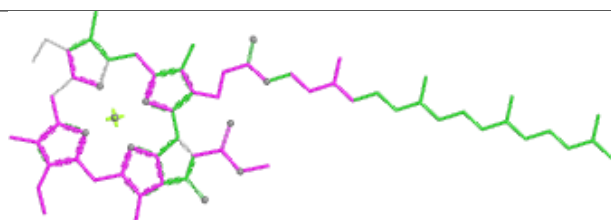


Rings

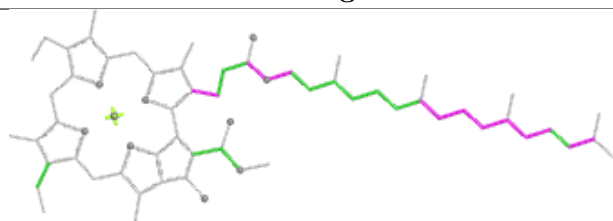
Ligand CLA 11 308



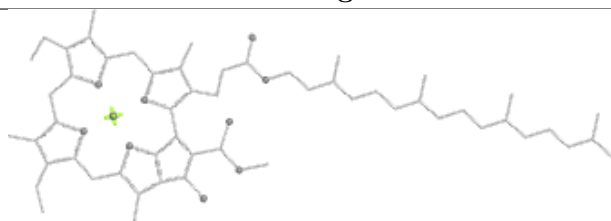
Bond lengths



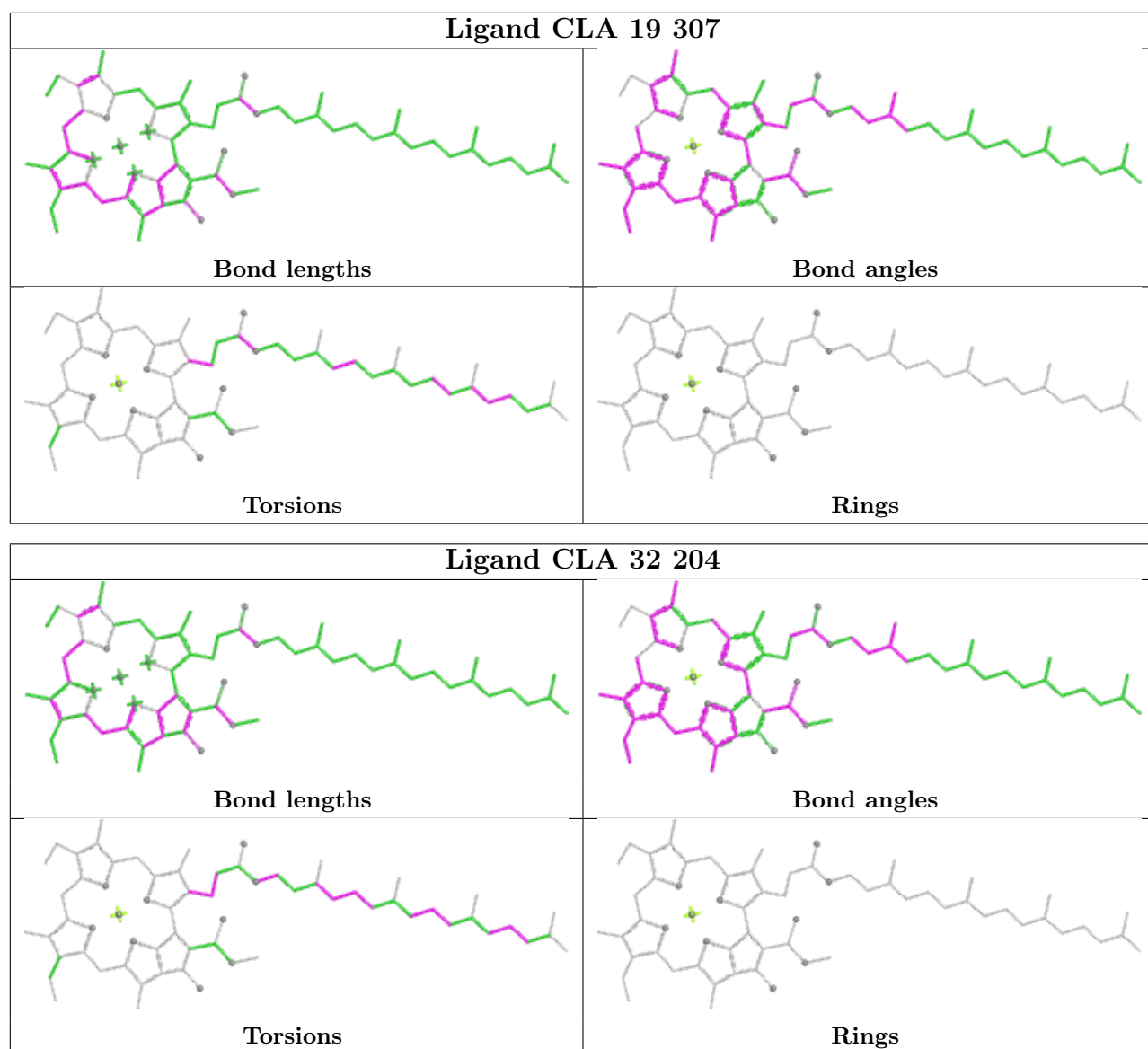
Bond angles

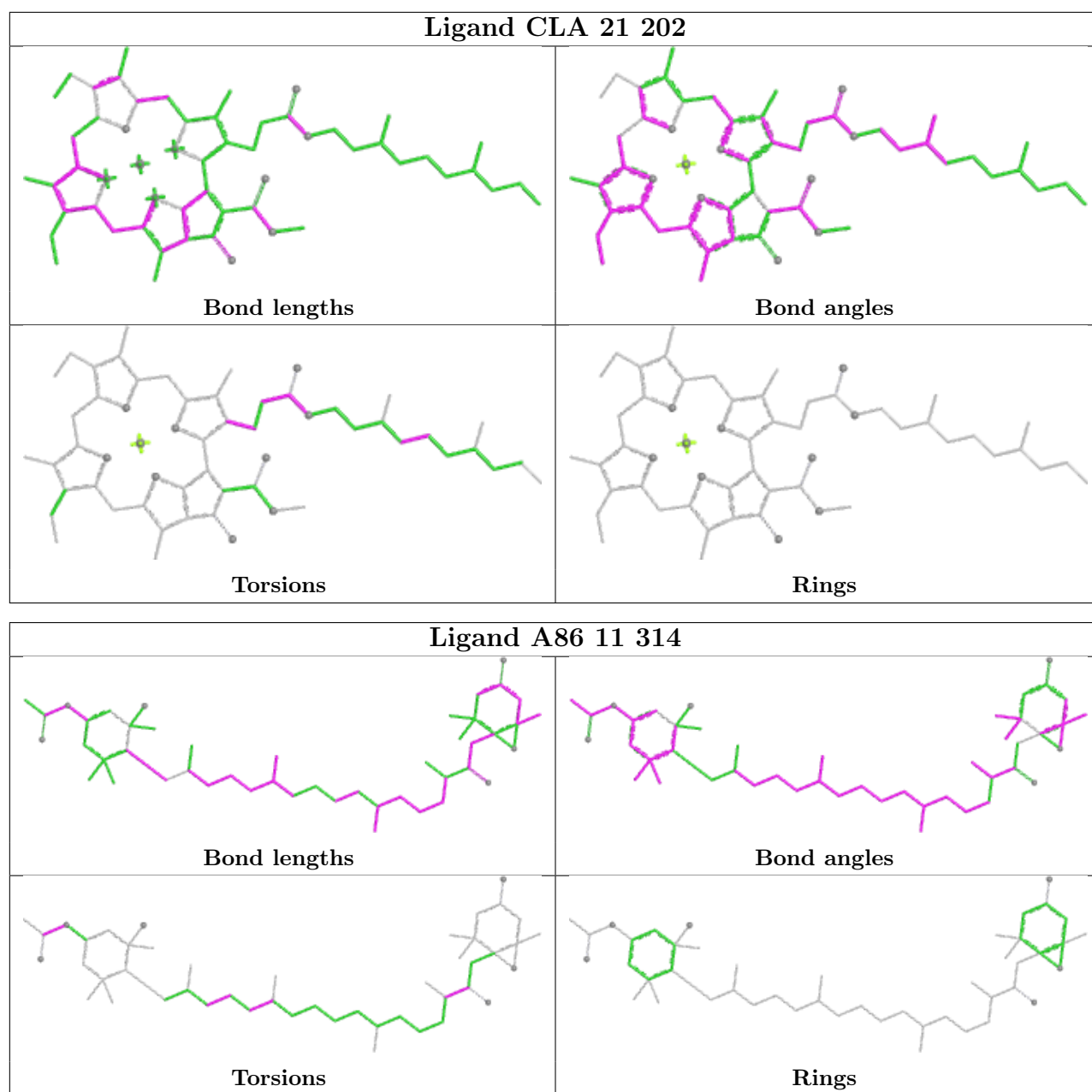


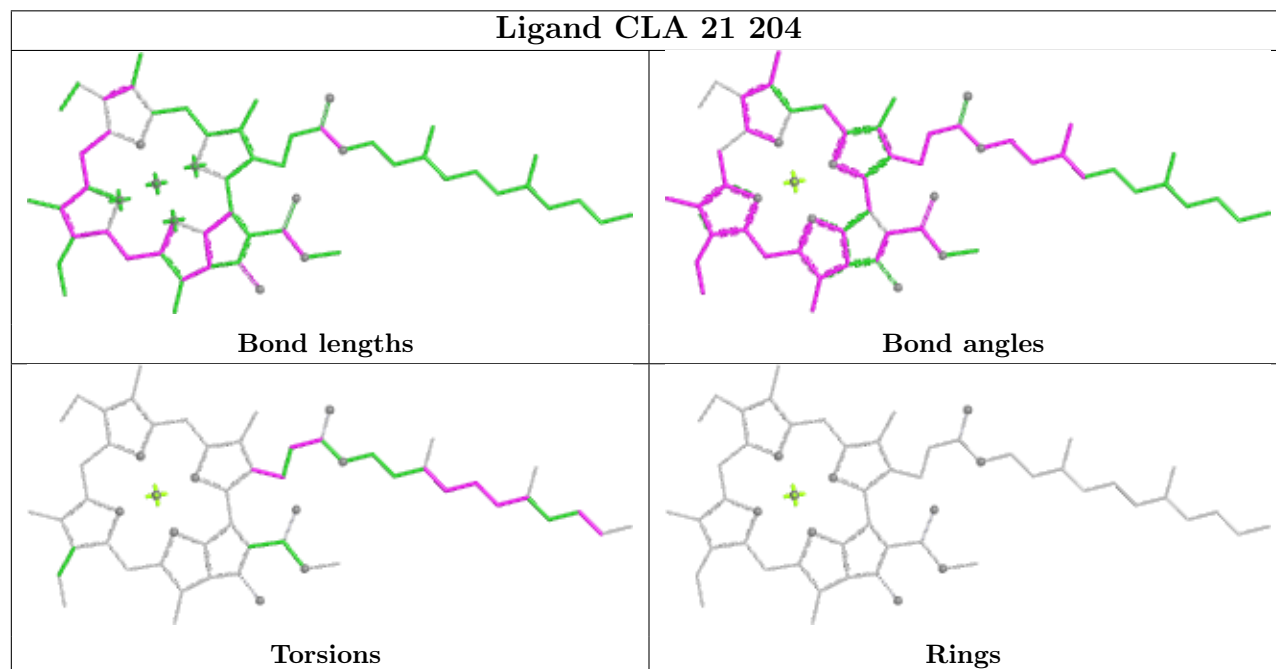
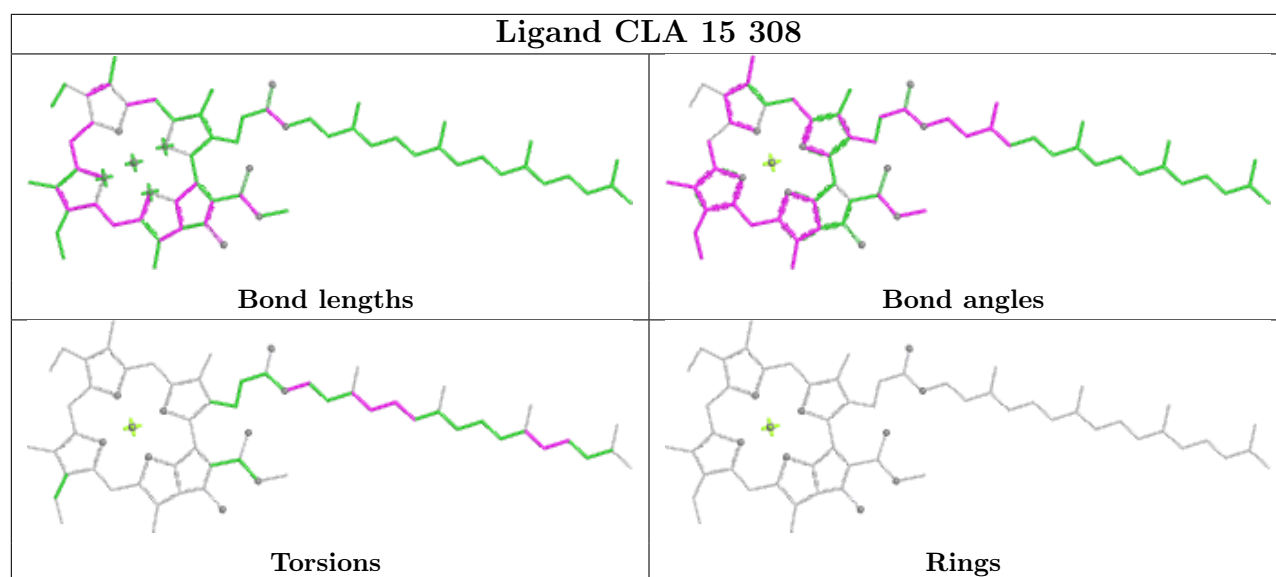
Torsions

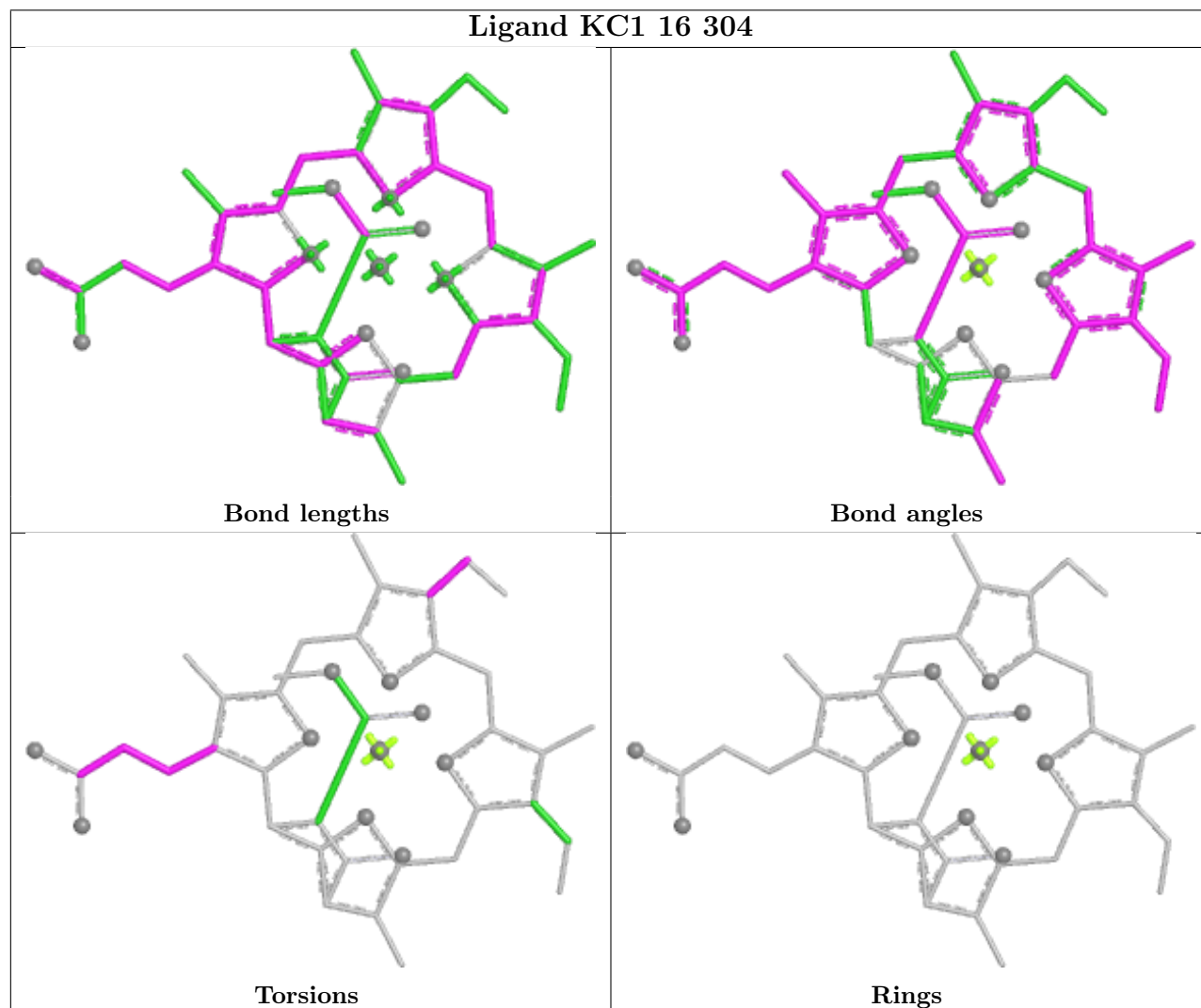
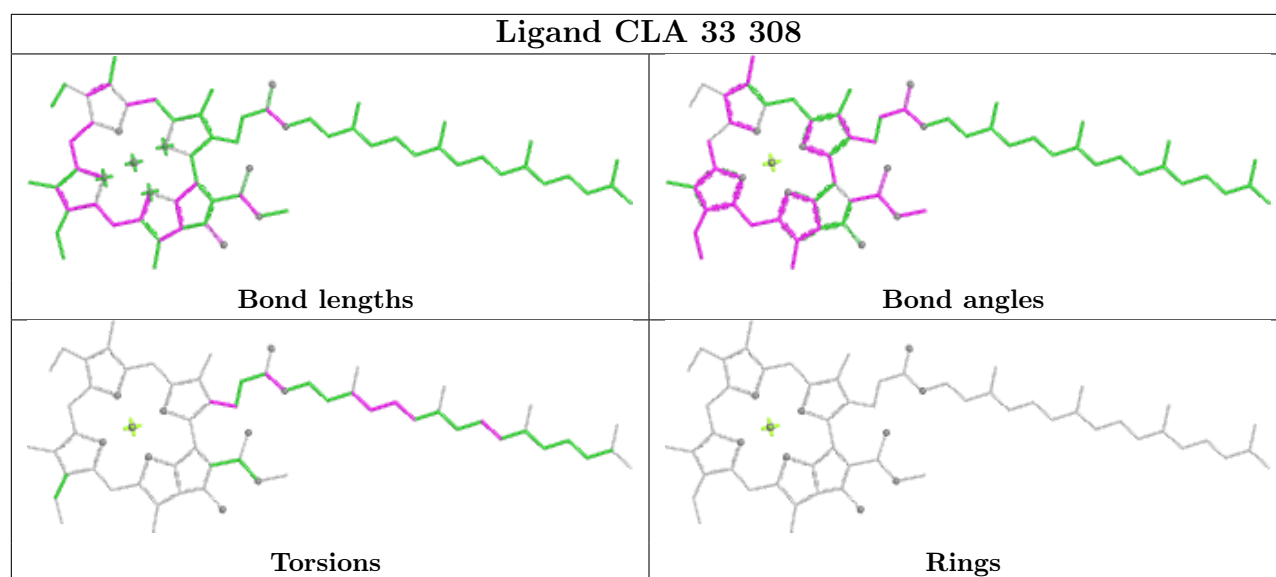


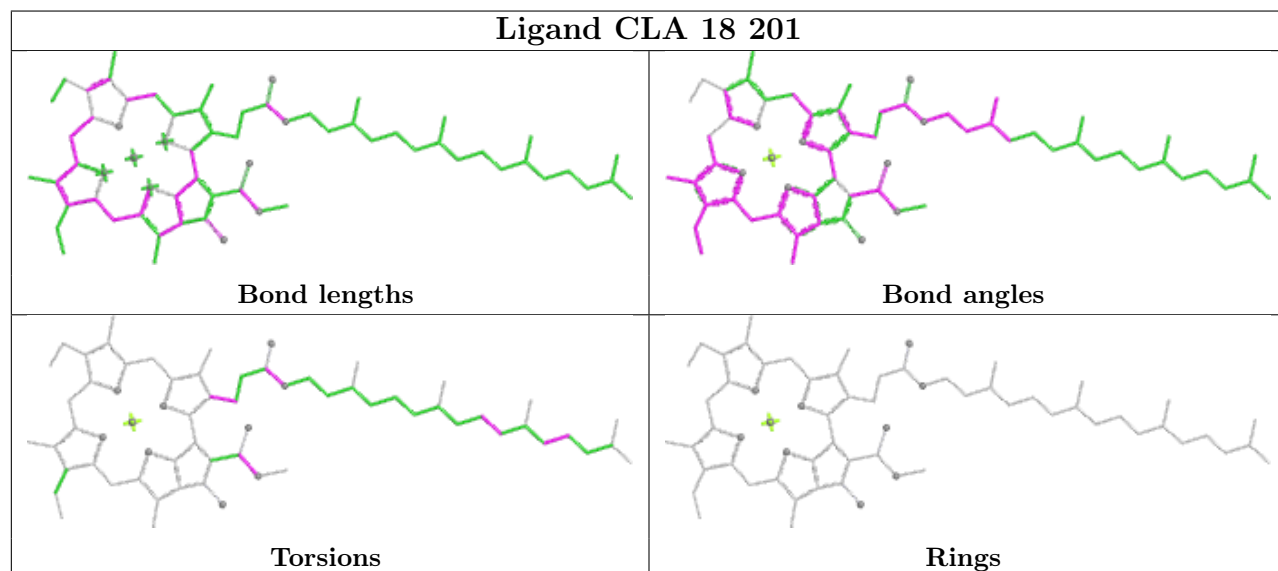
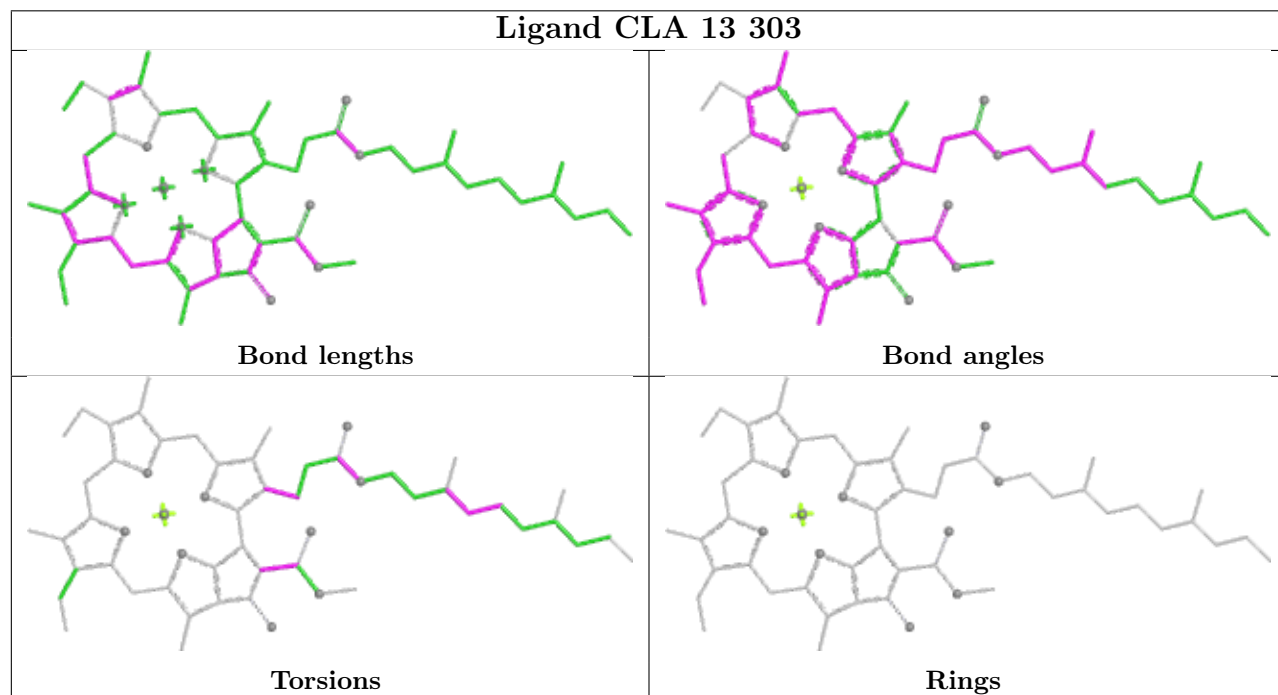
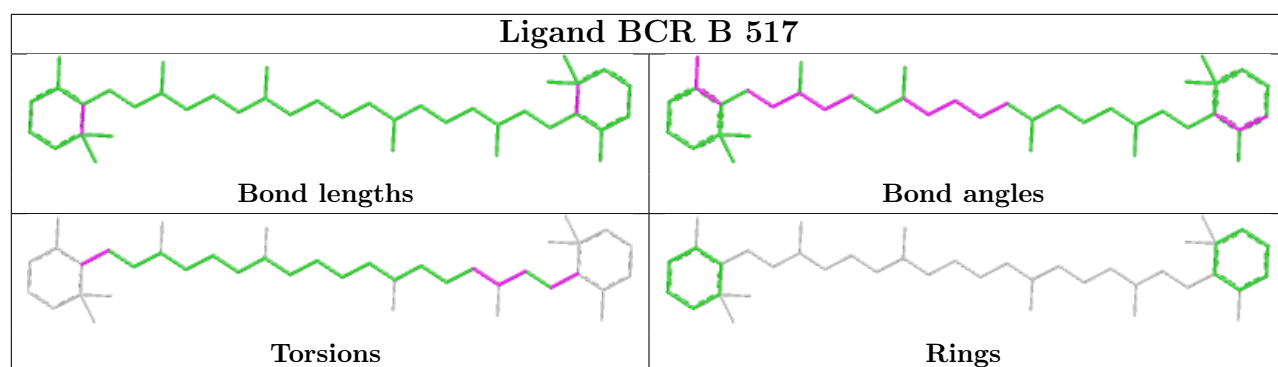
Rings

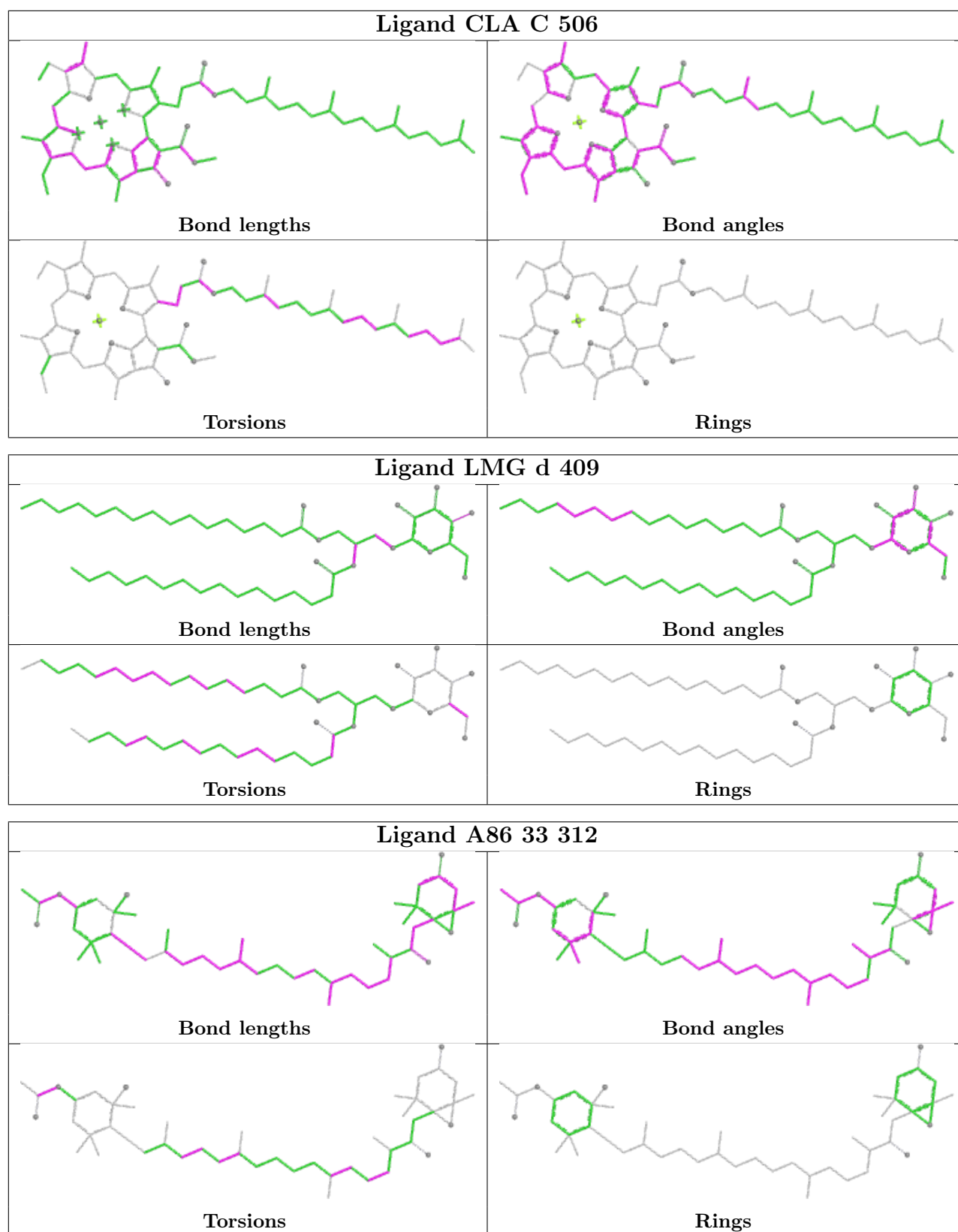


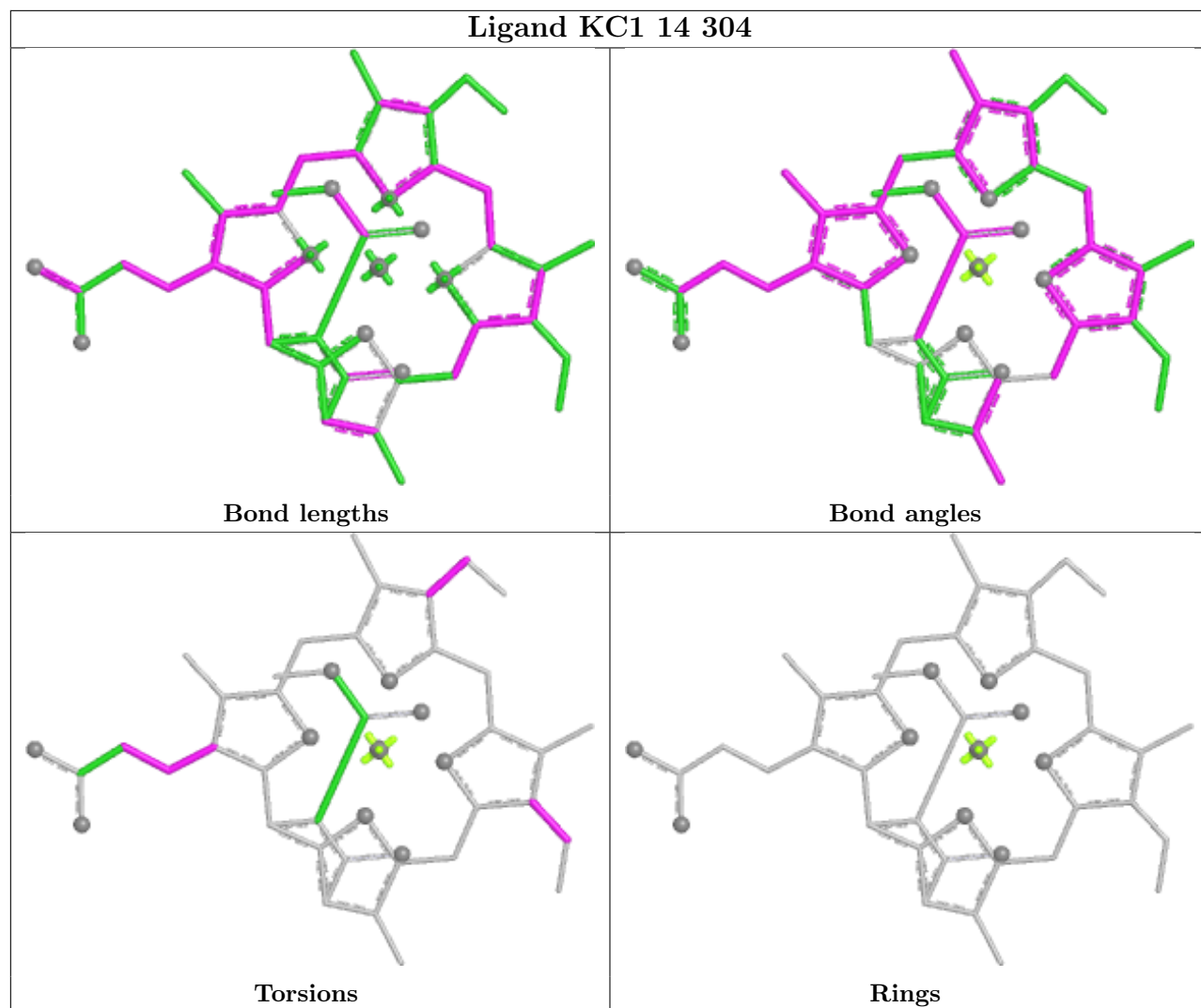


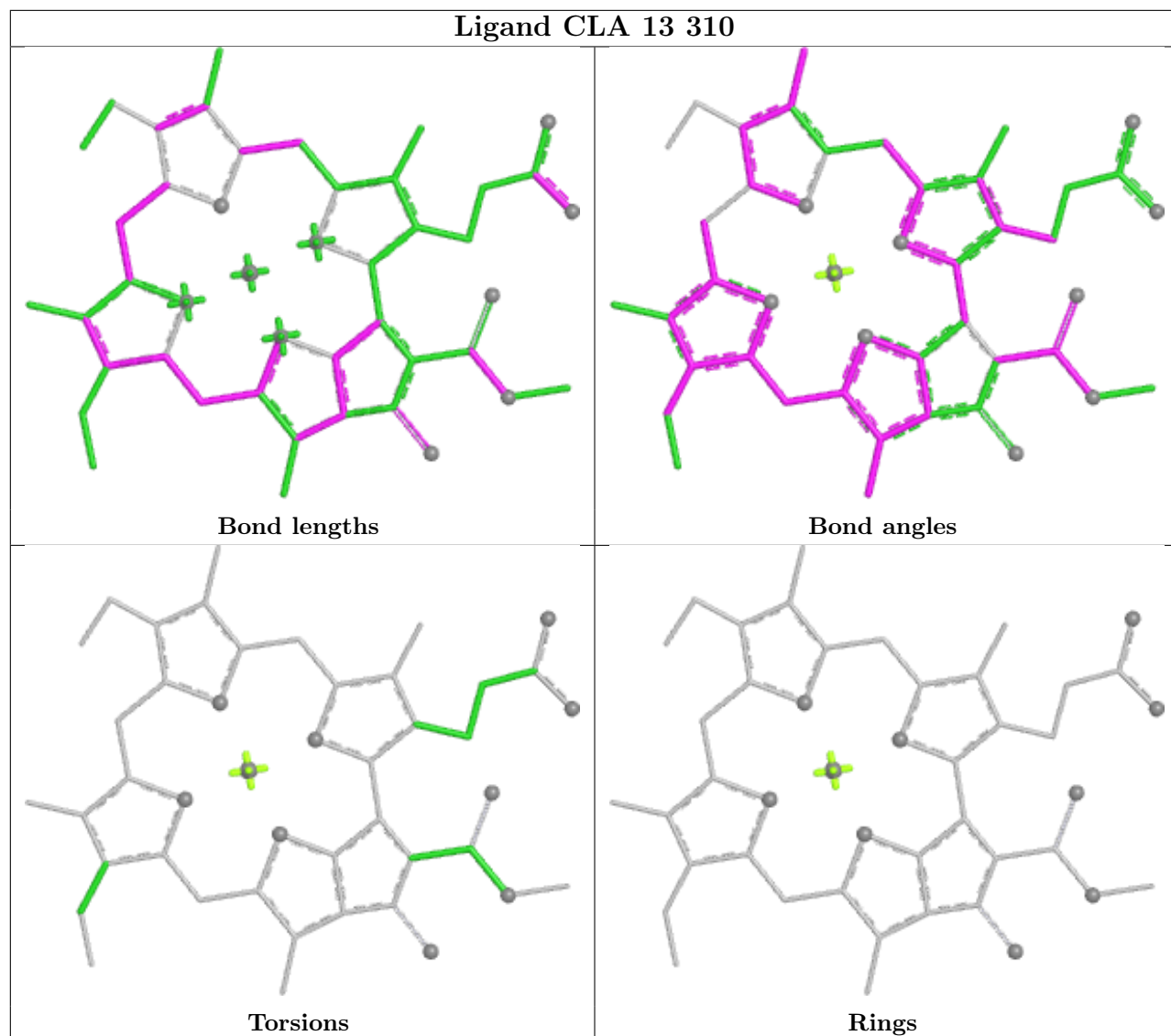


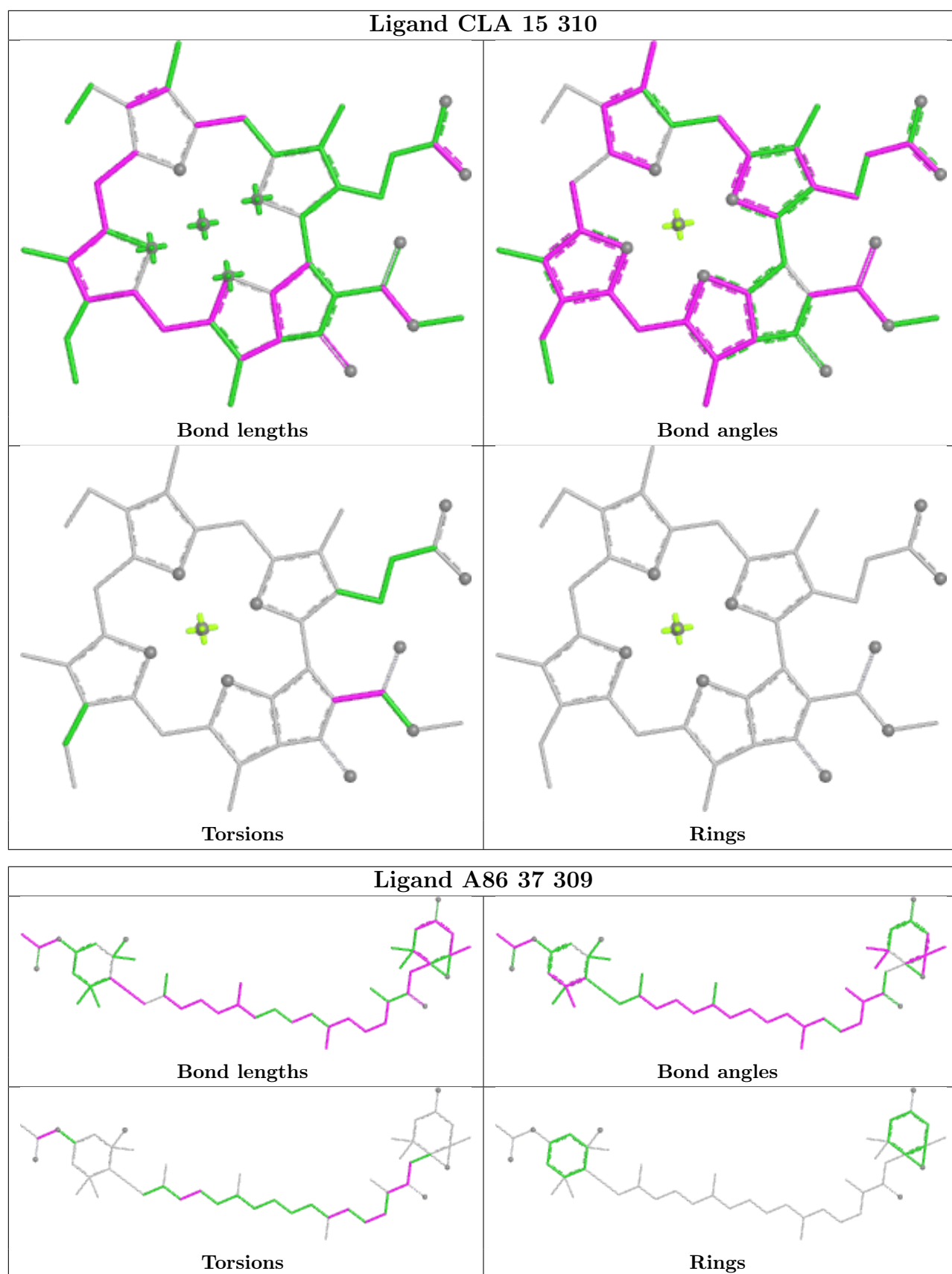


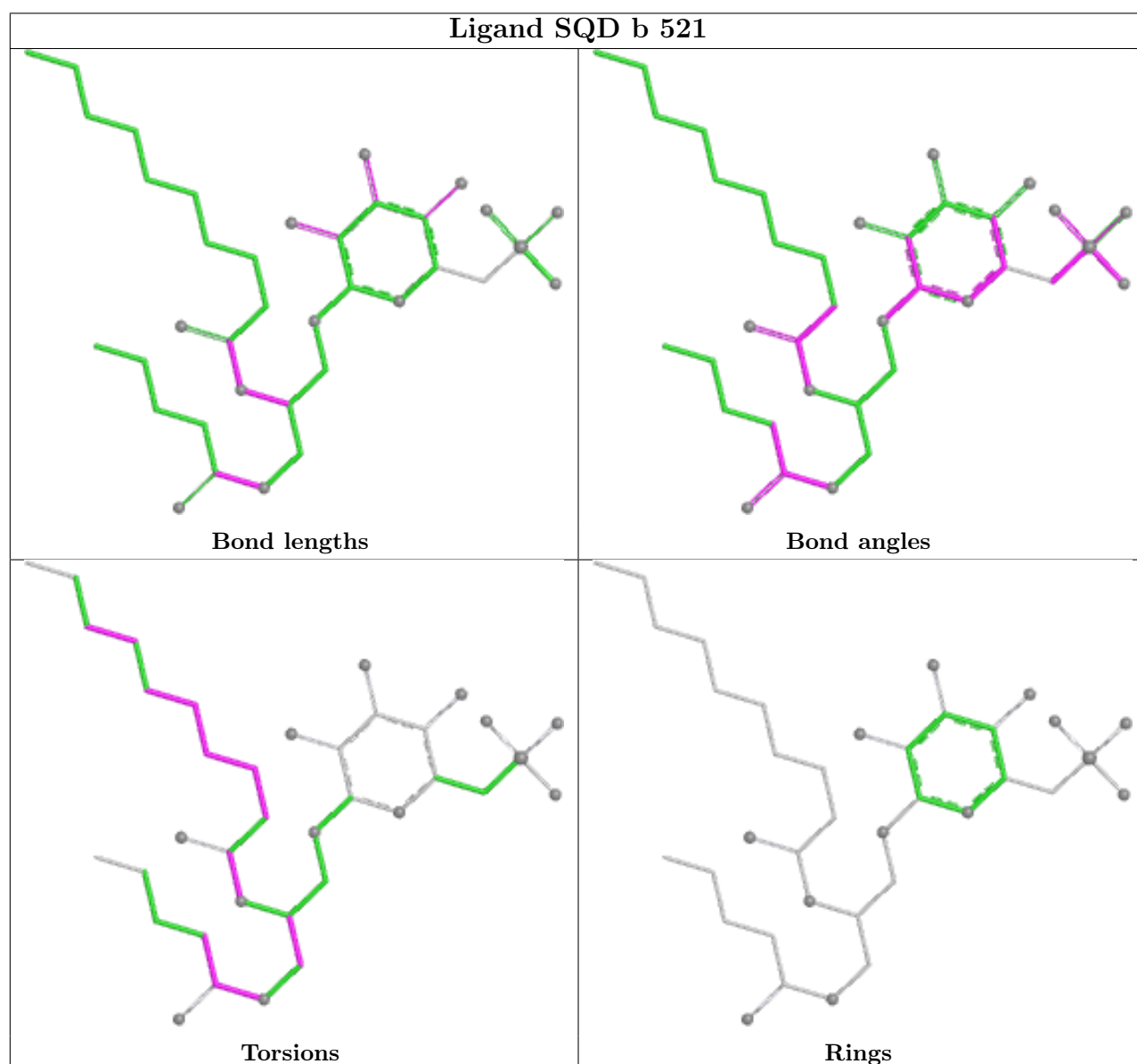
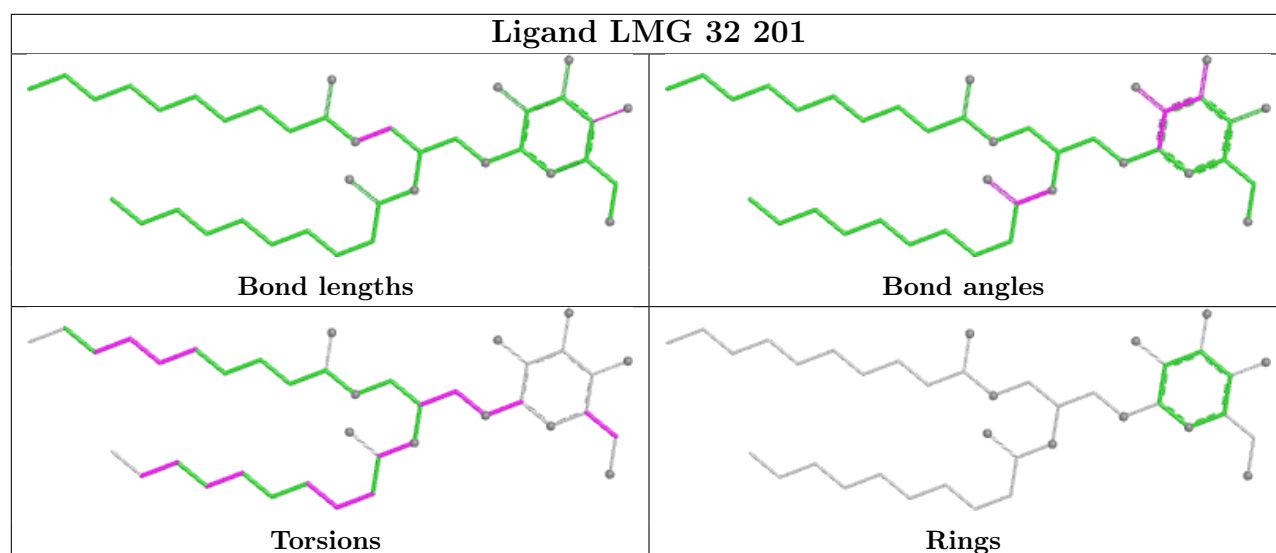


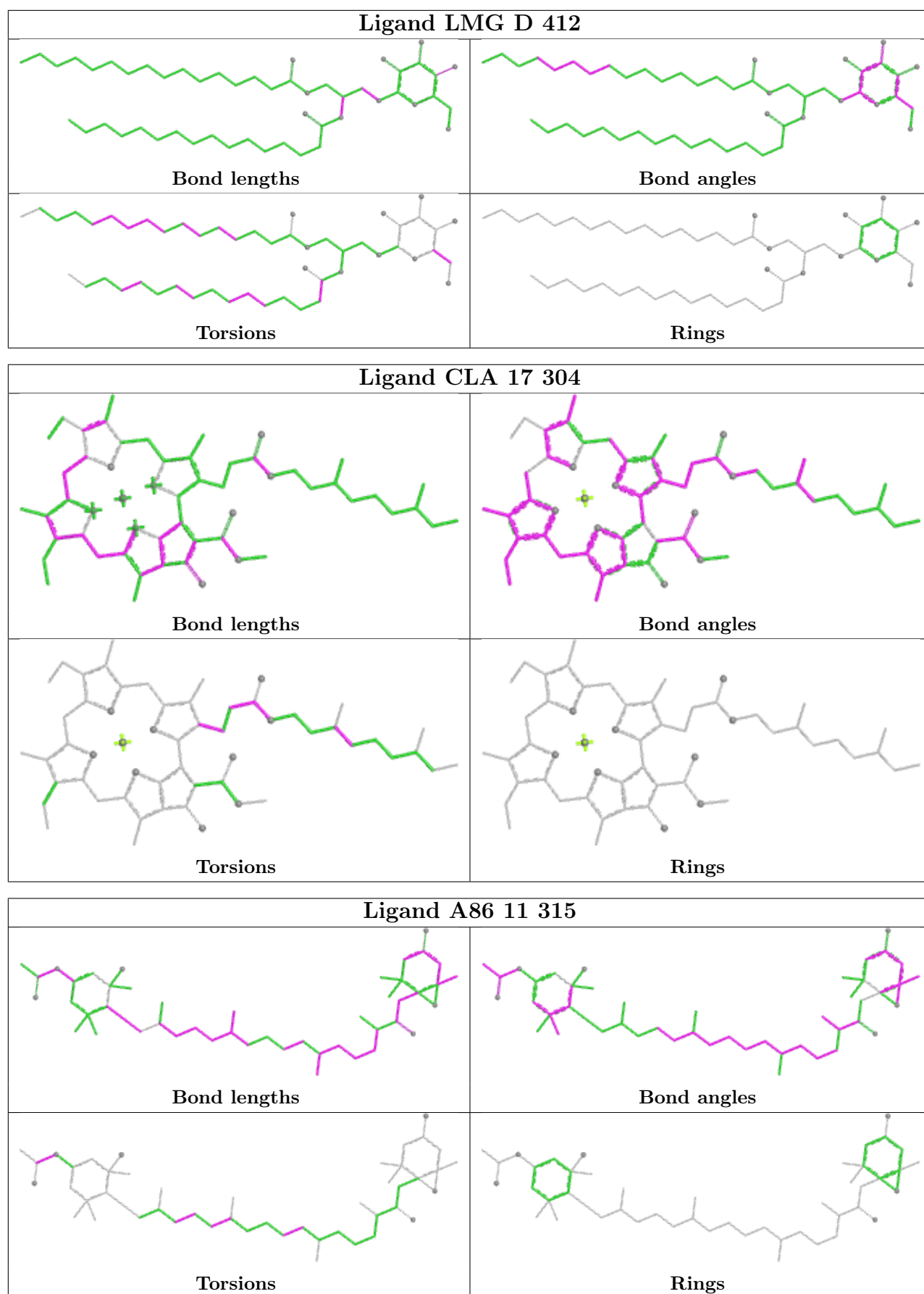


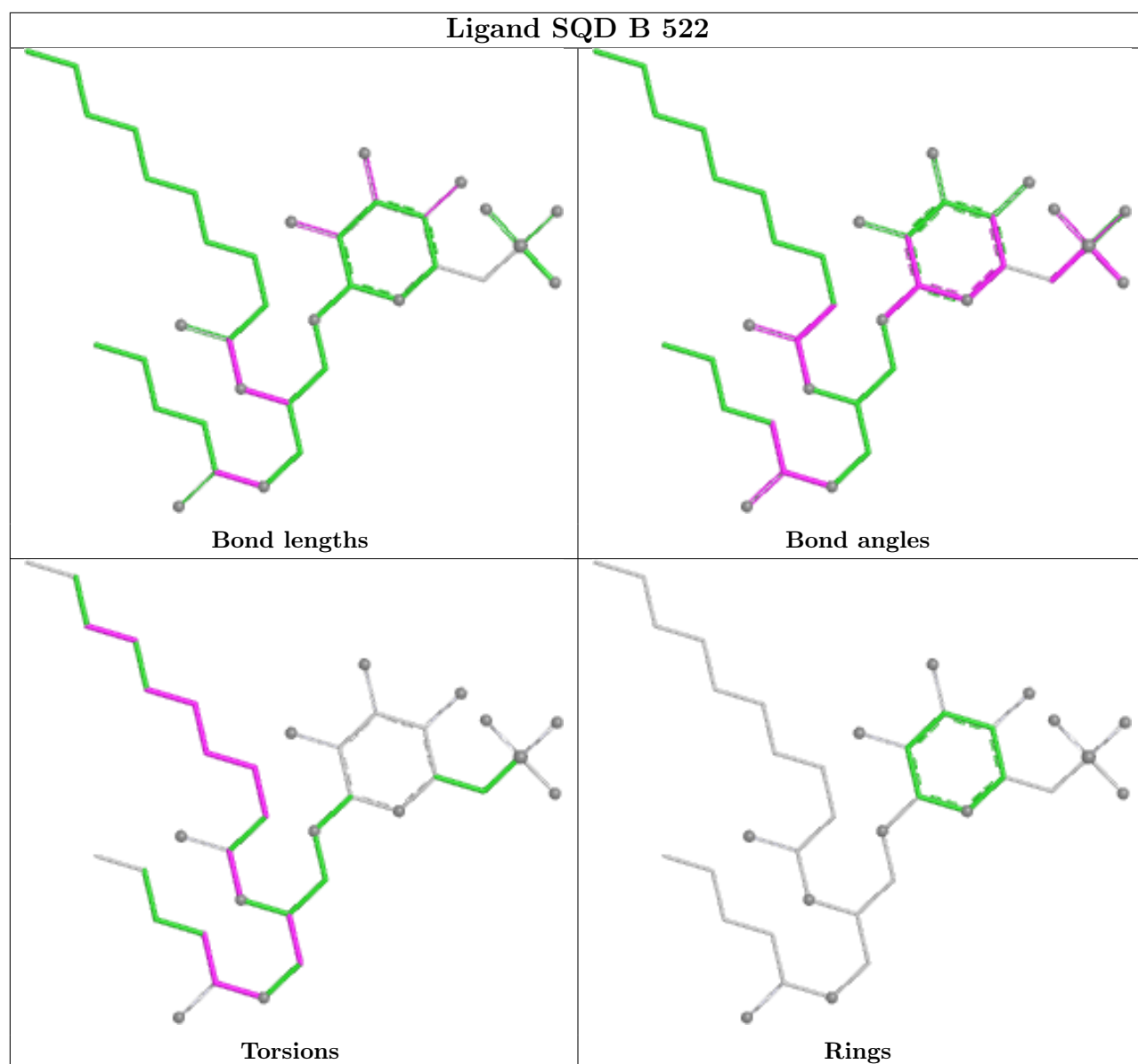


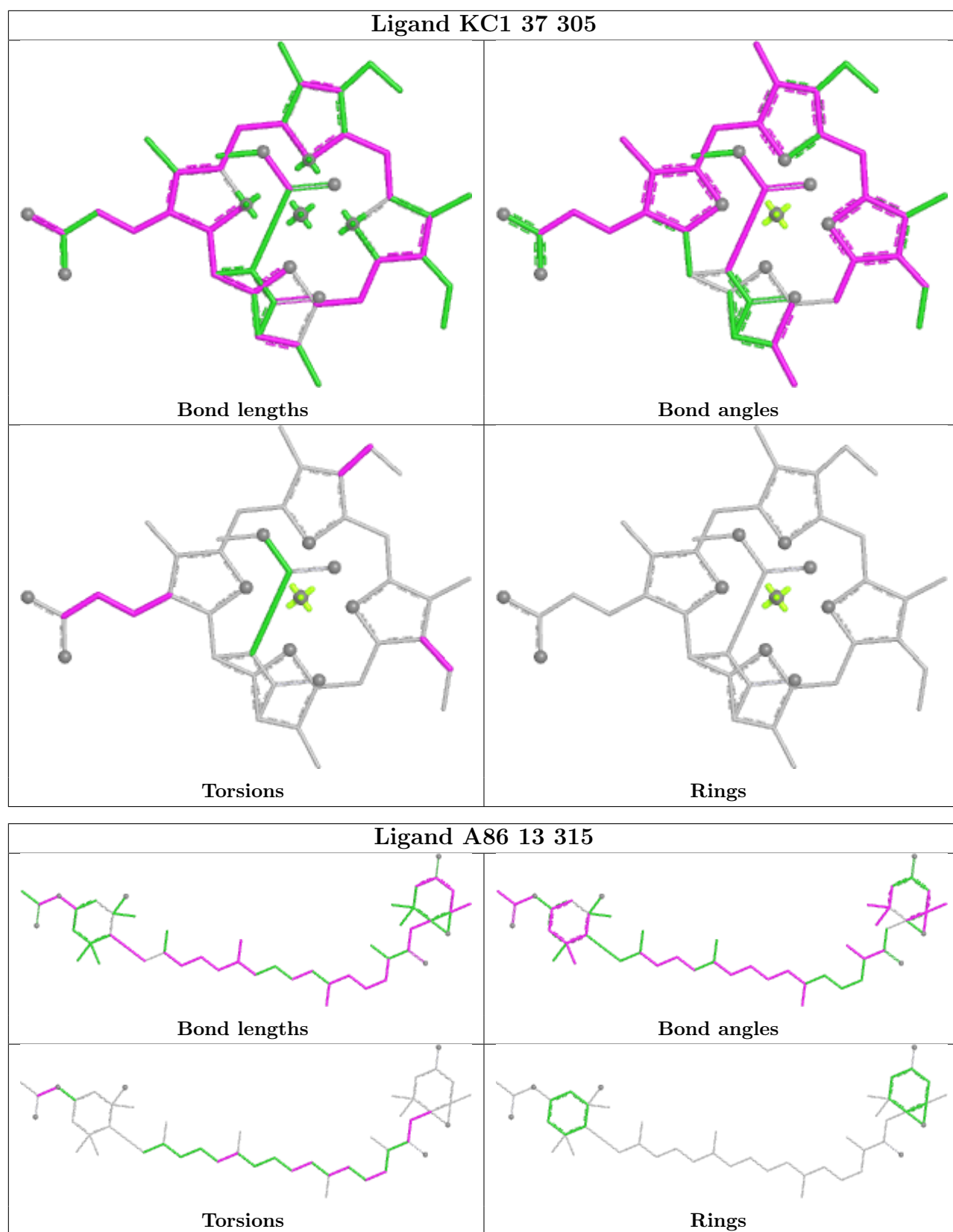


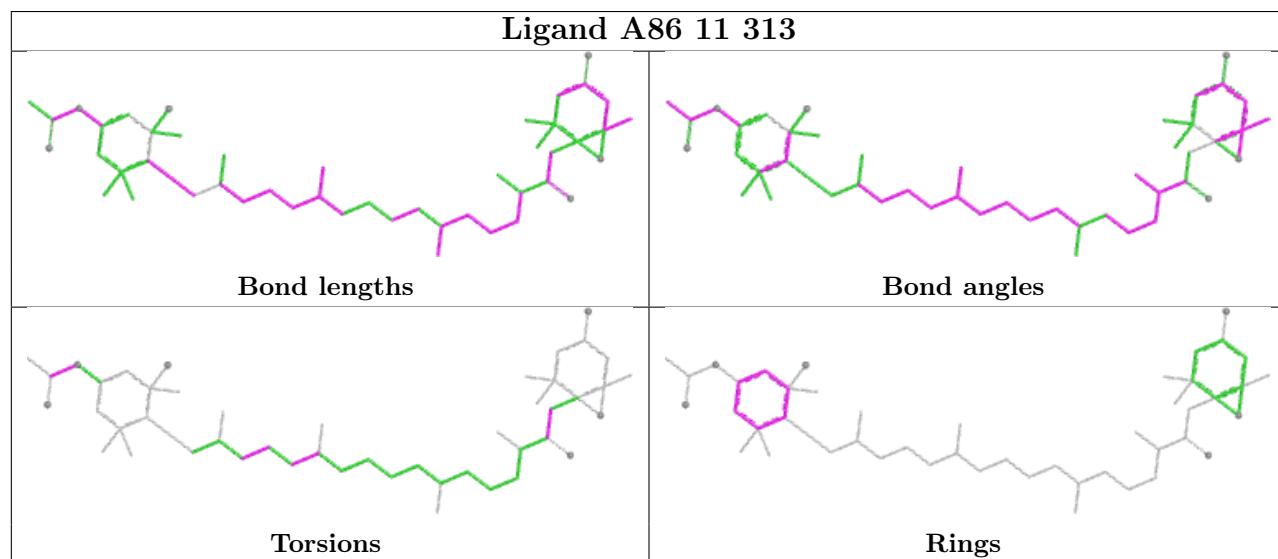
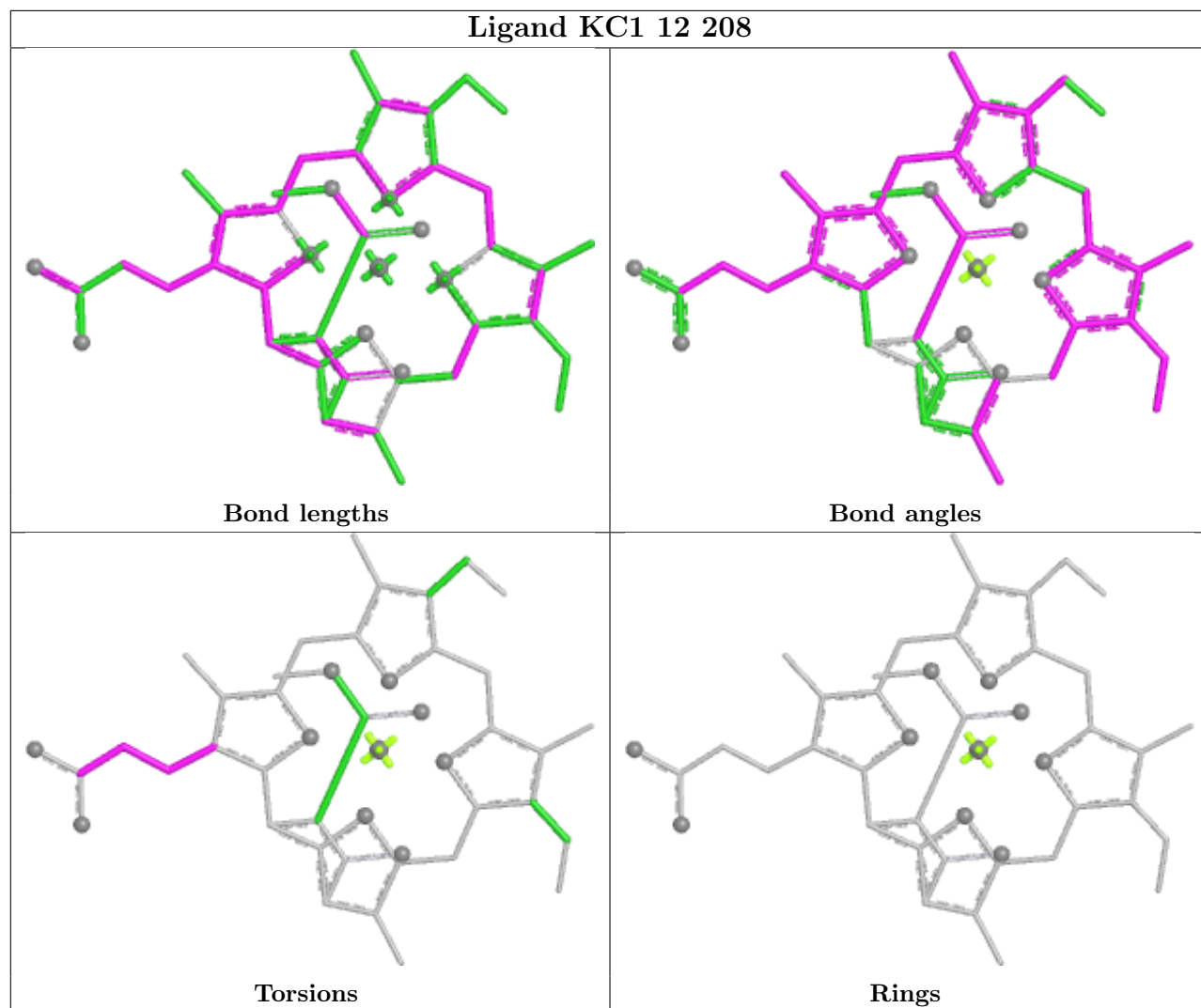


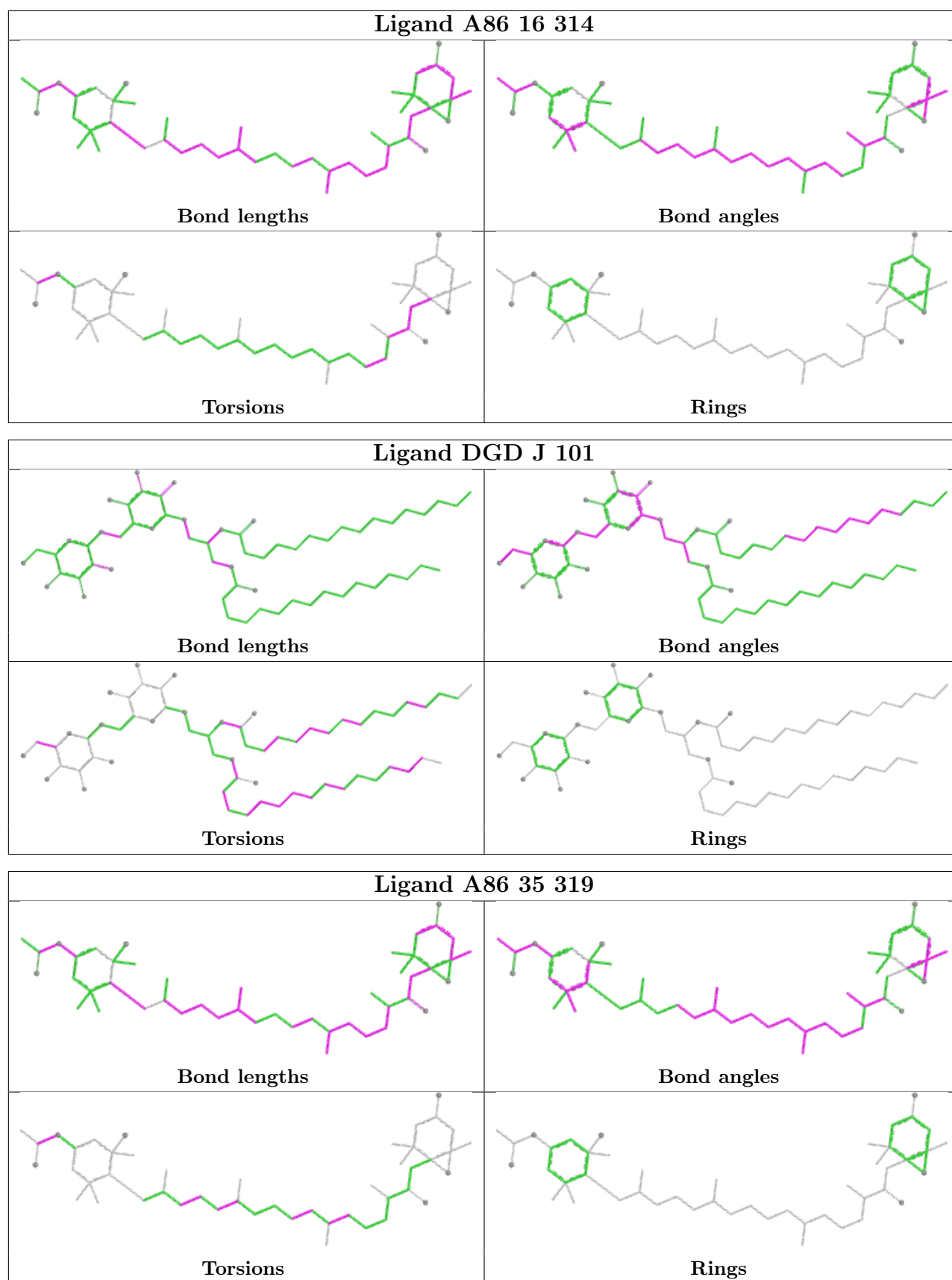


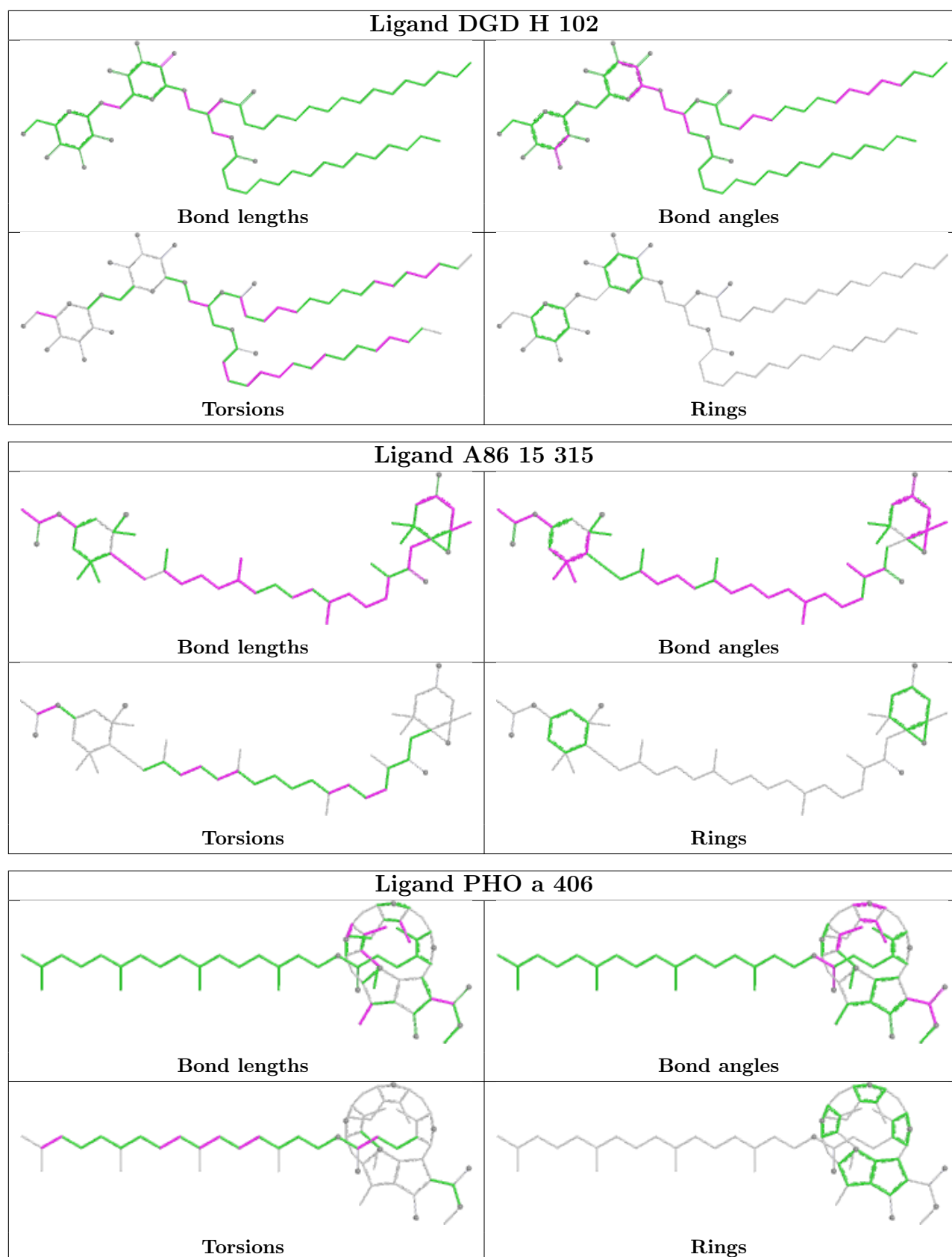




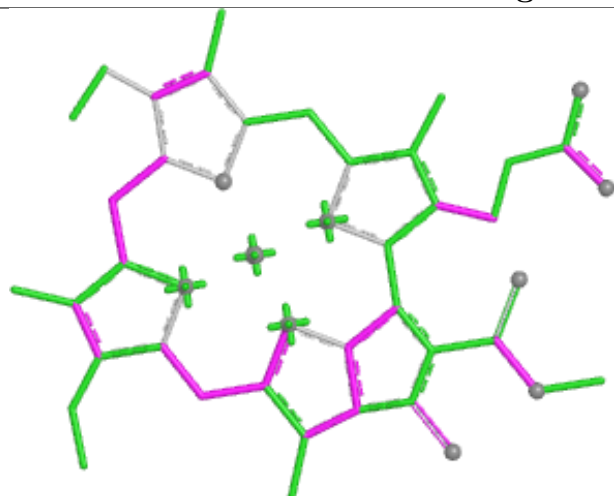




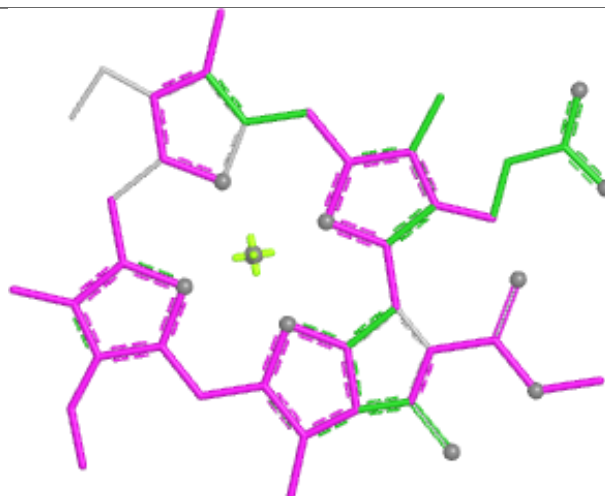




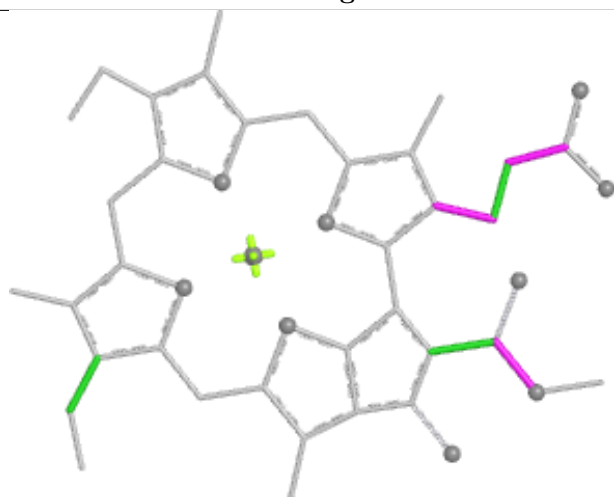
Ligand CLA Z 102



Bond lengths



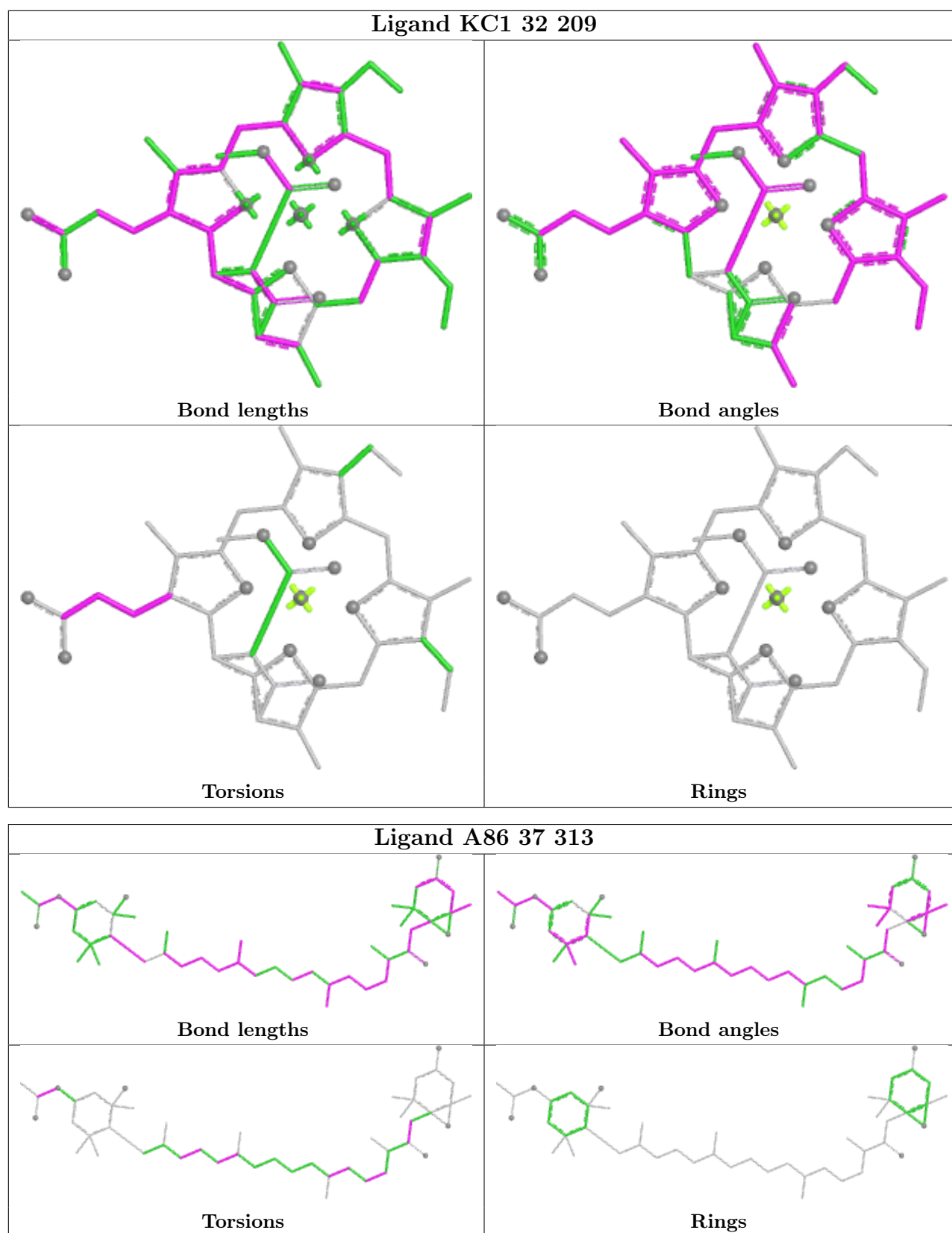
Bond angles

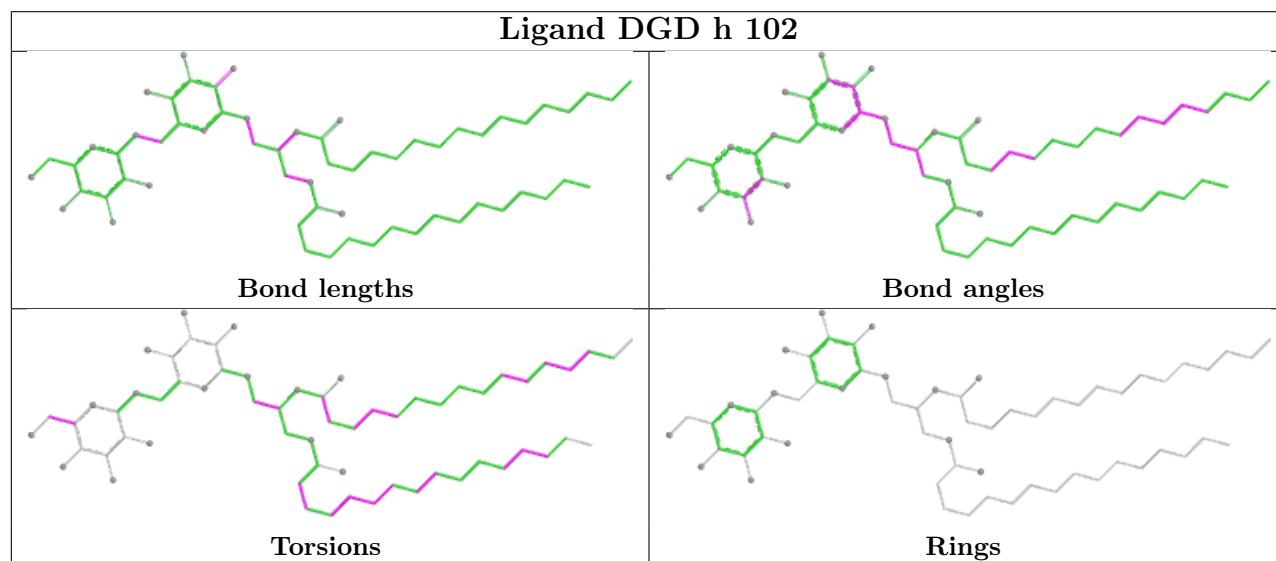
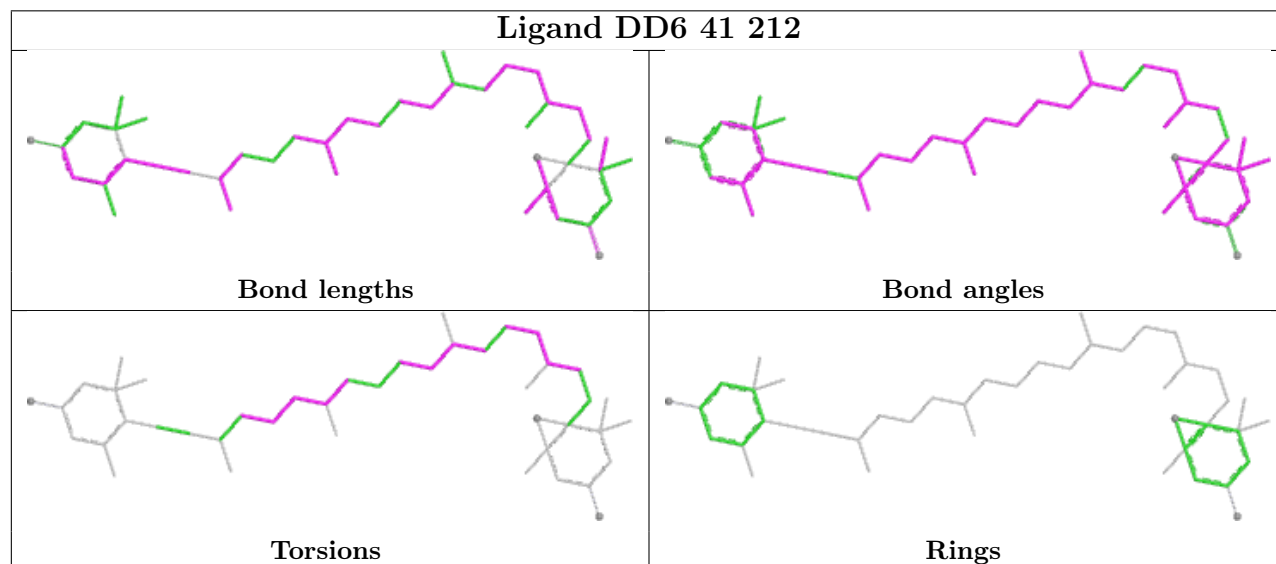
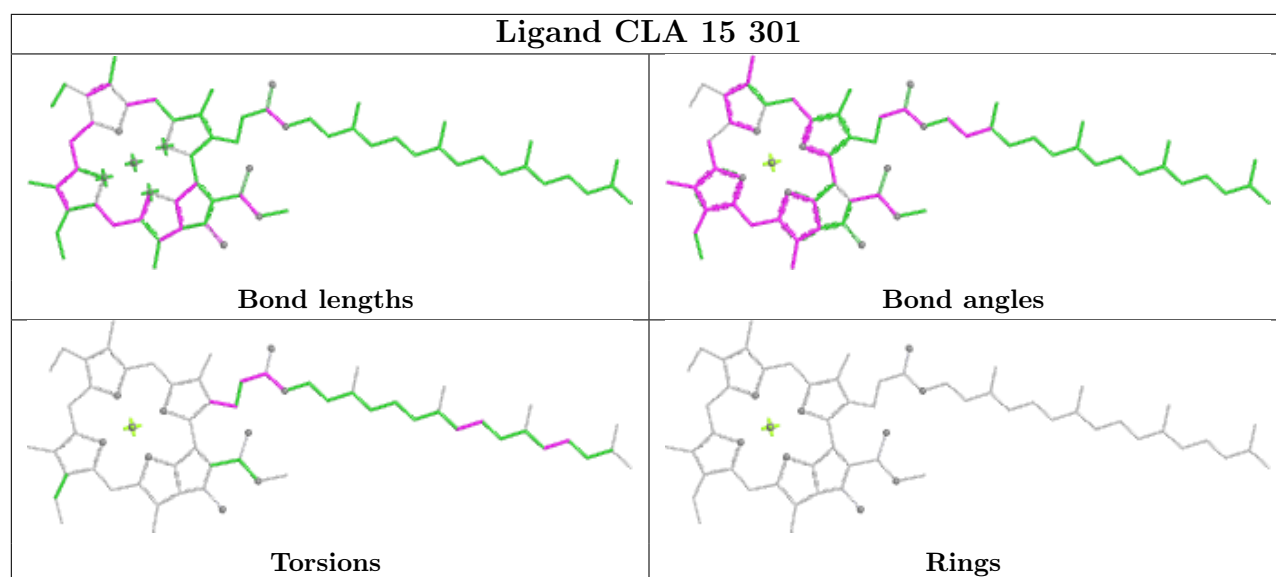


Torsions

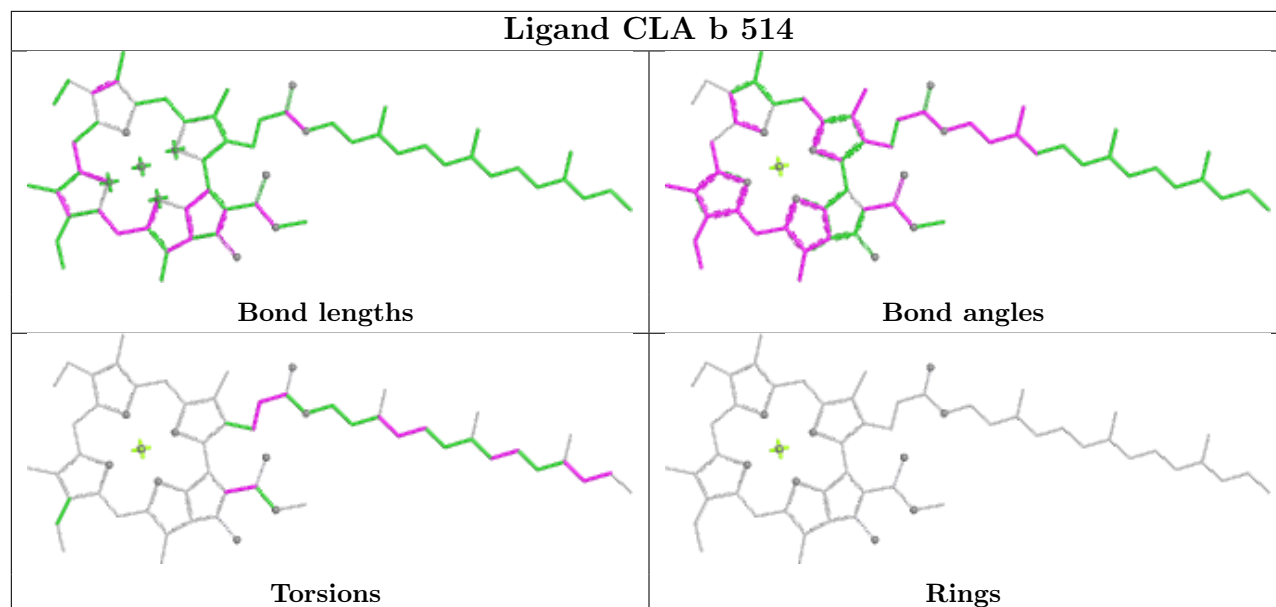


Rings

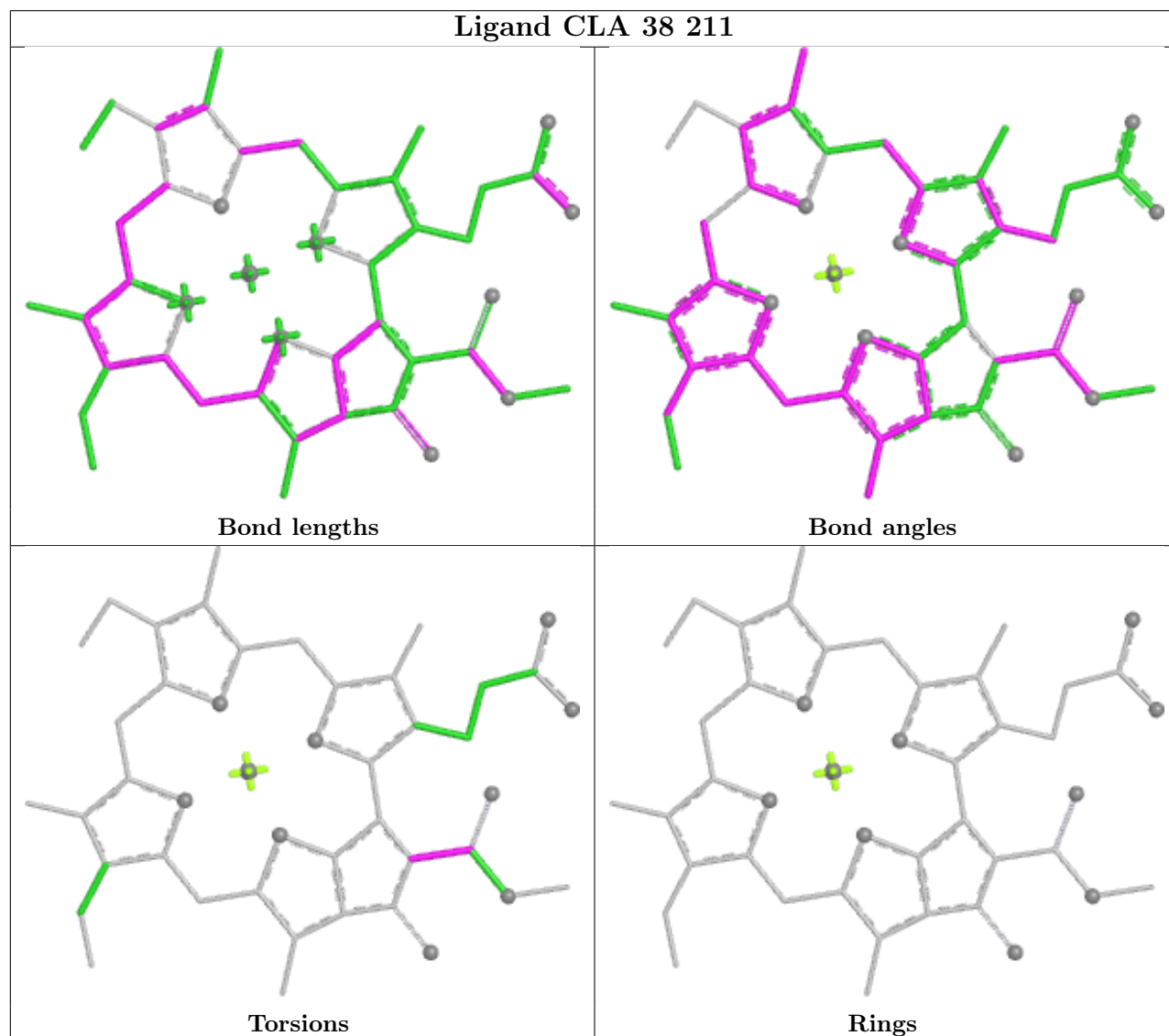


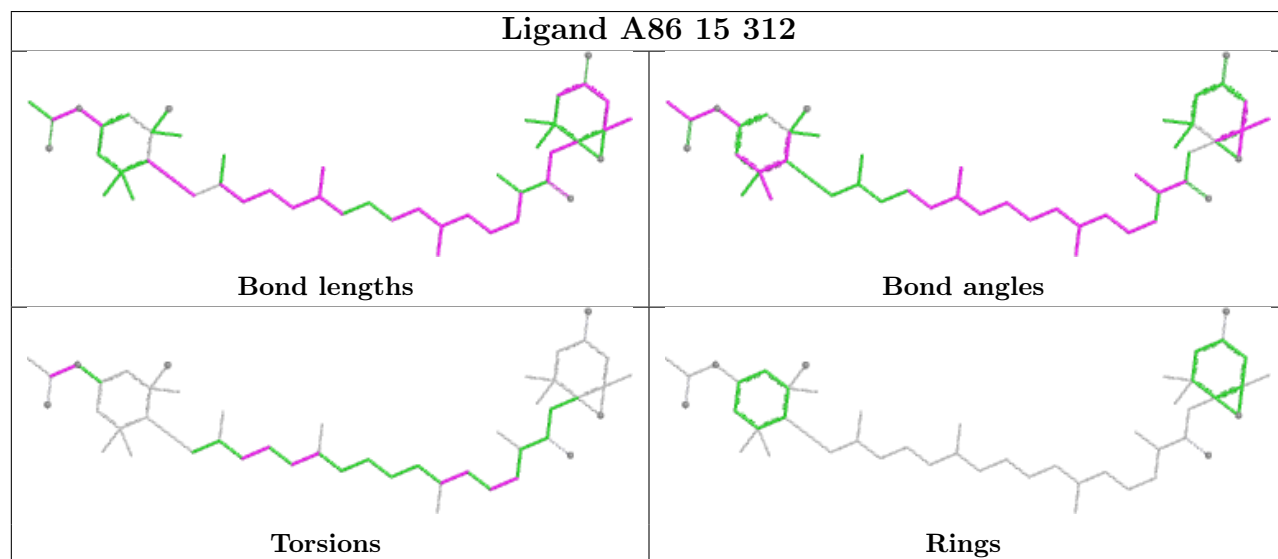
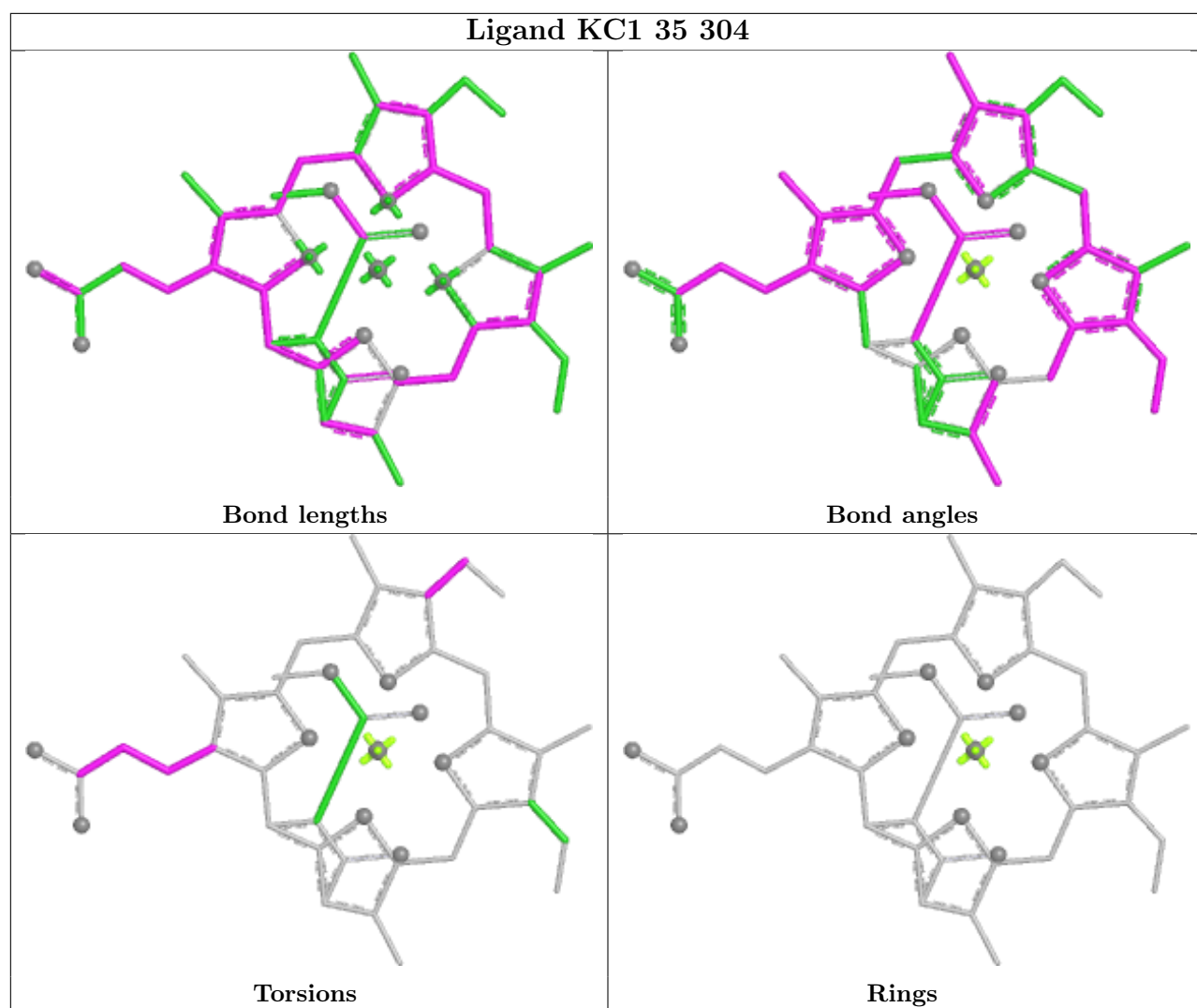


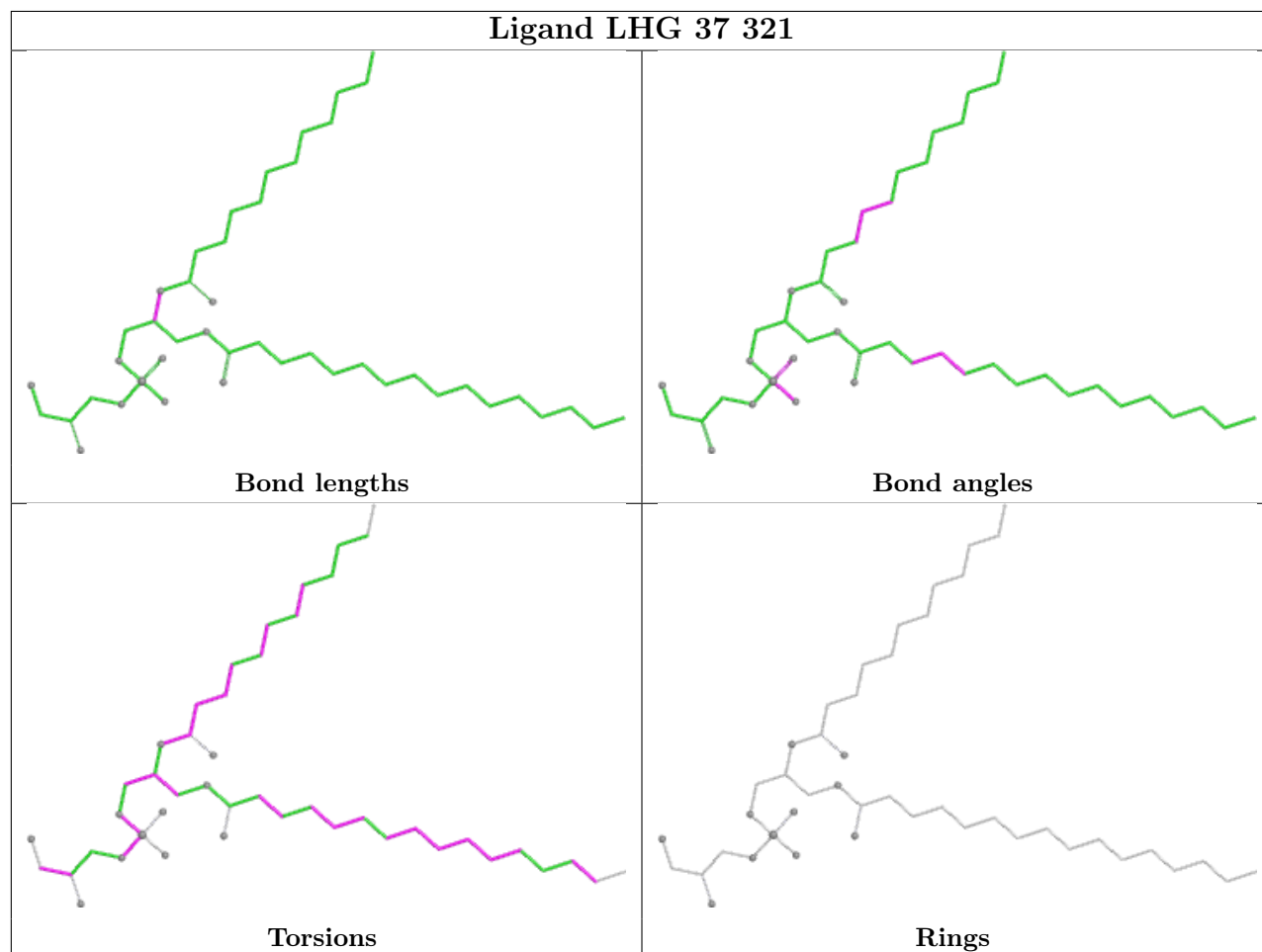
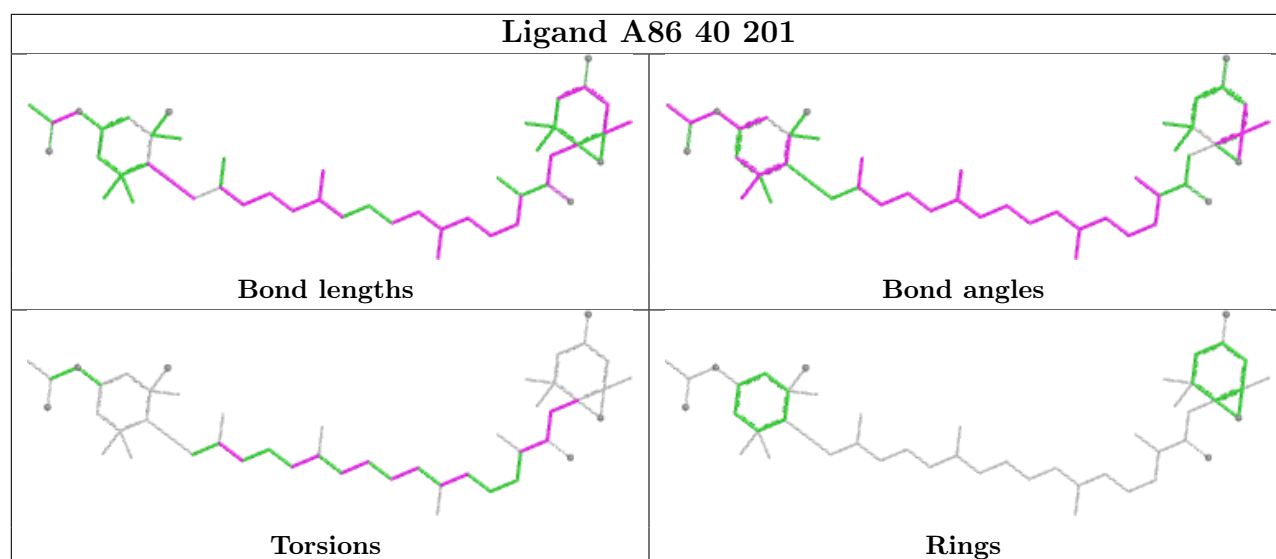
Ligand CLA b 514

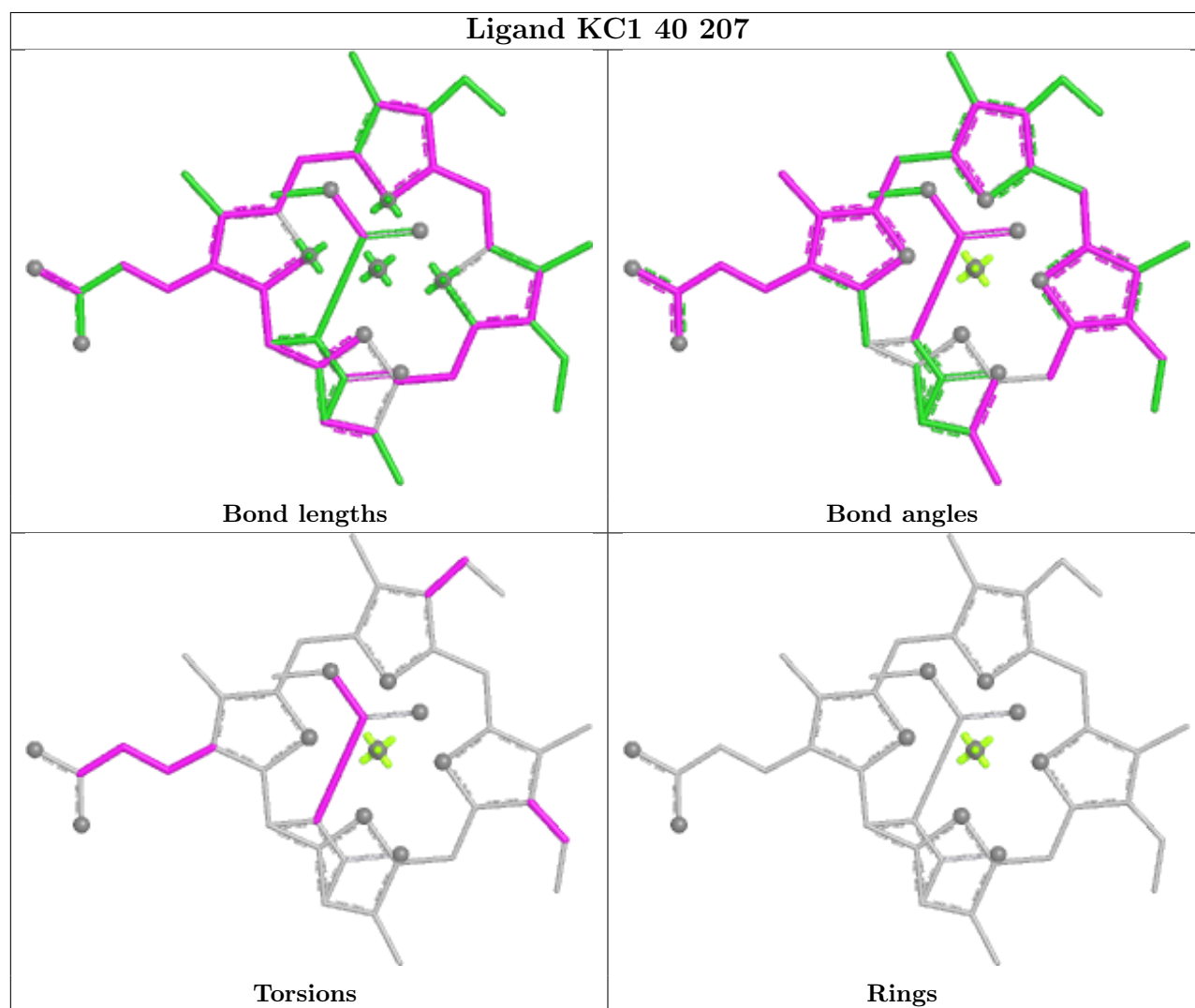
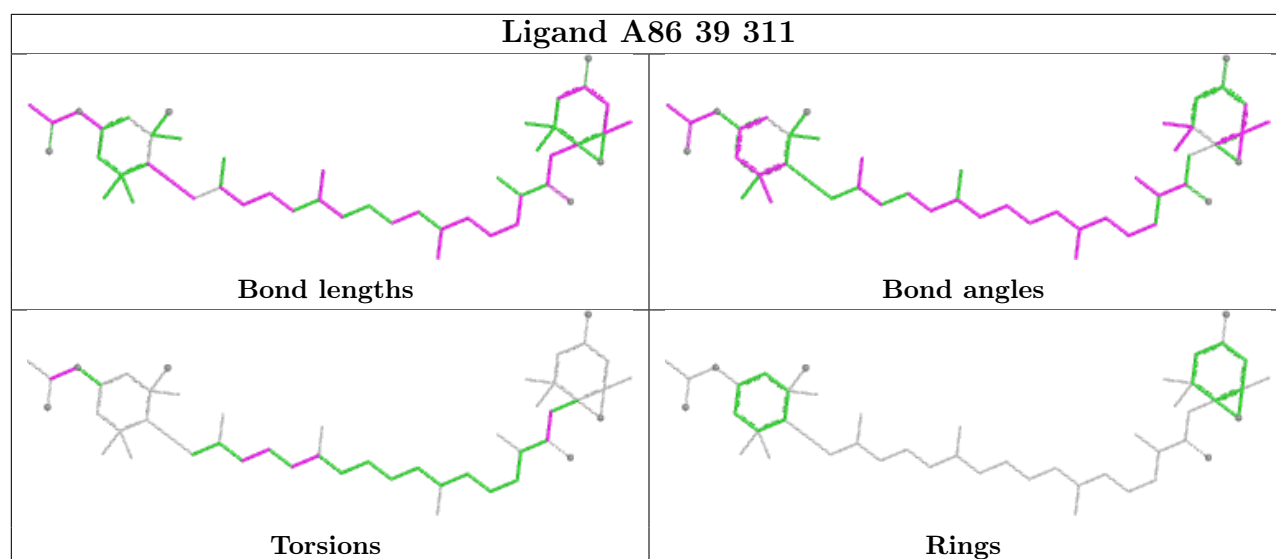


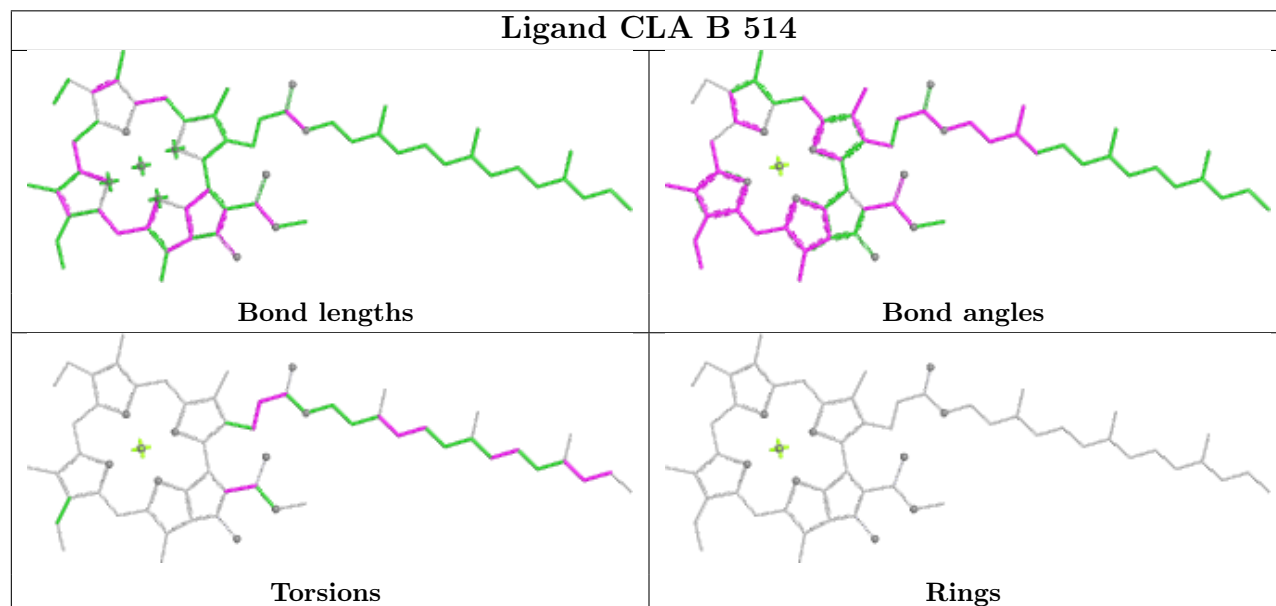
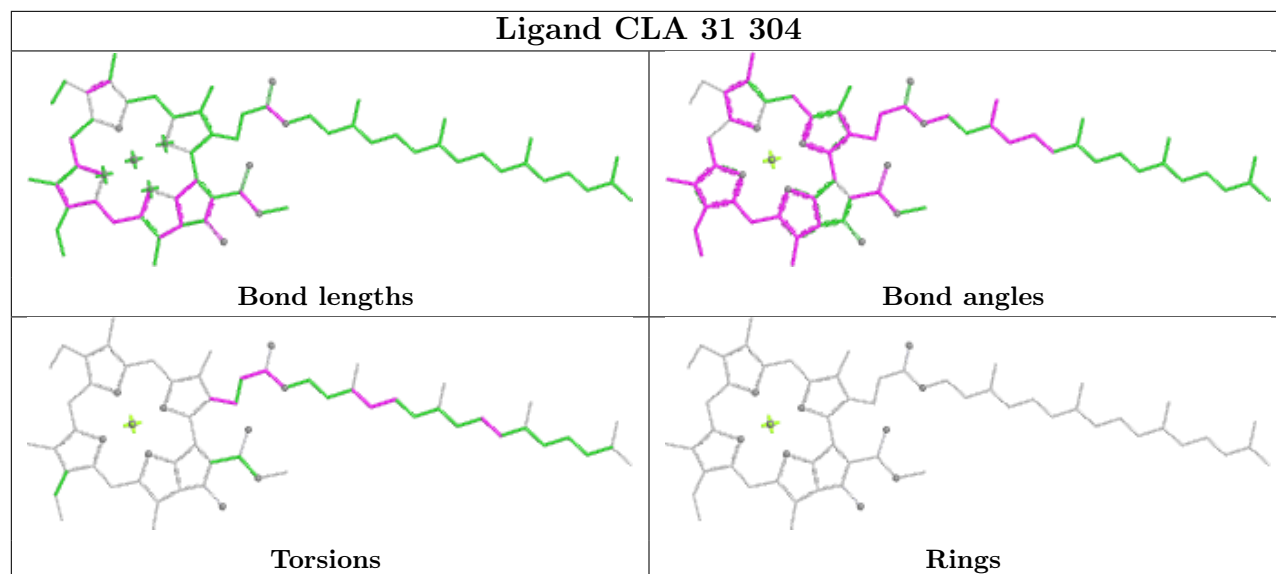
Ligand CLA 38 211

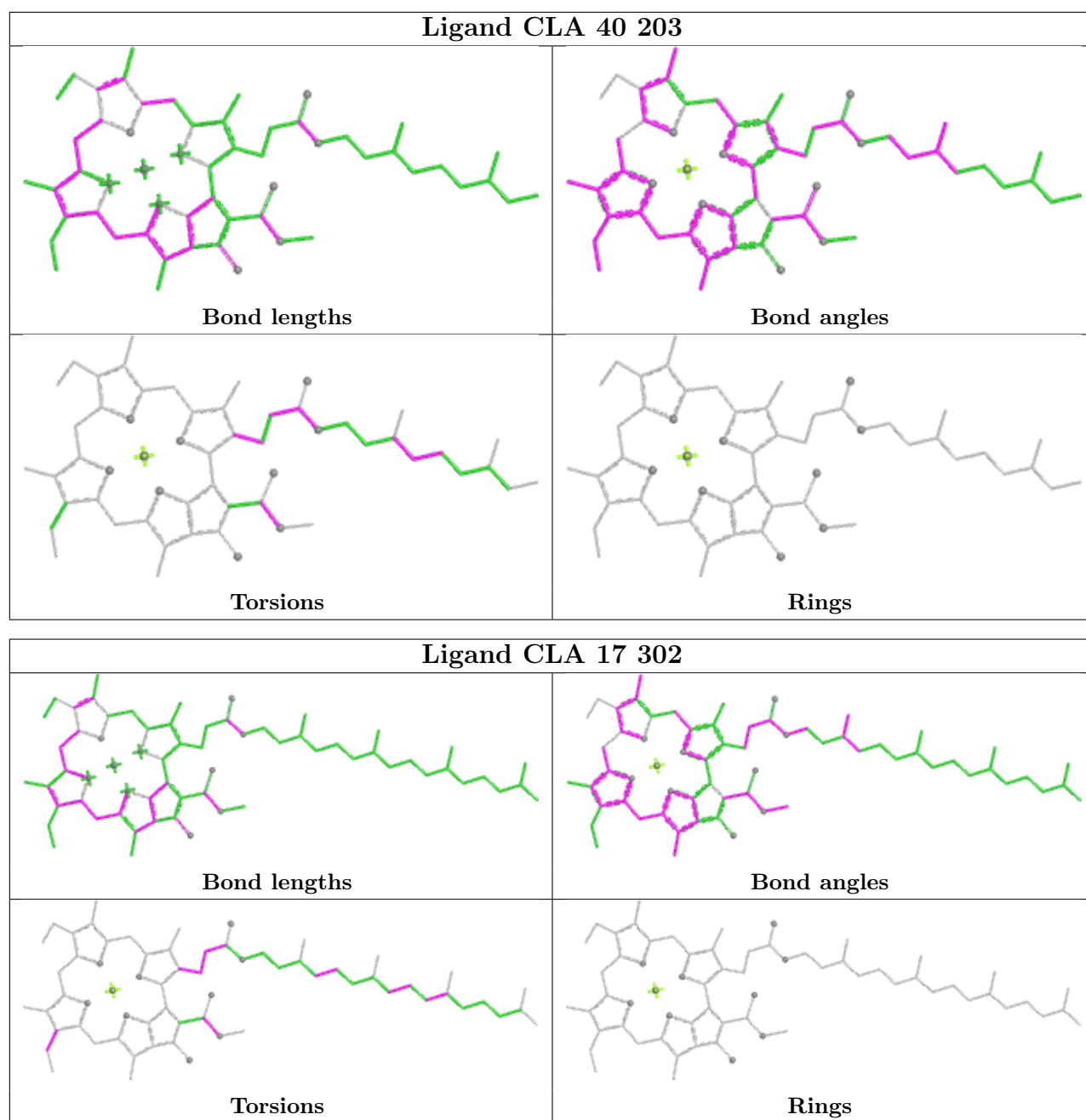


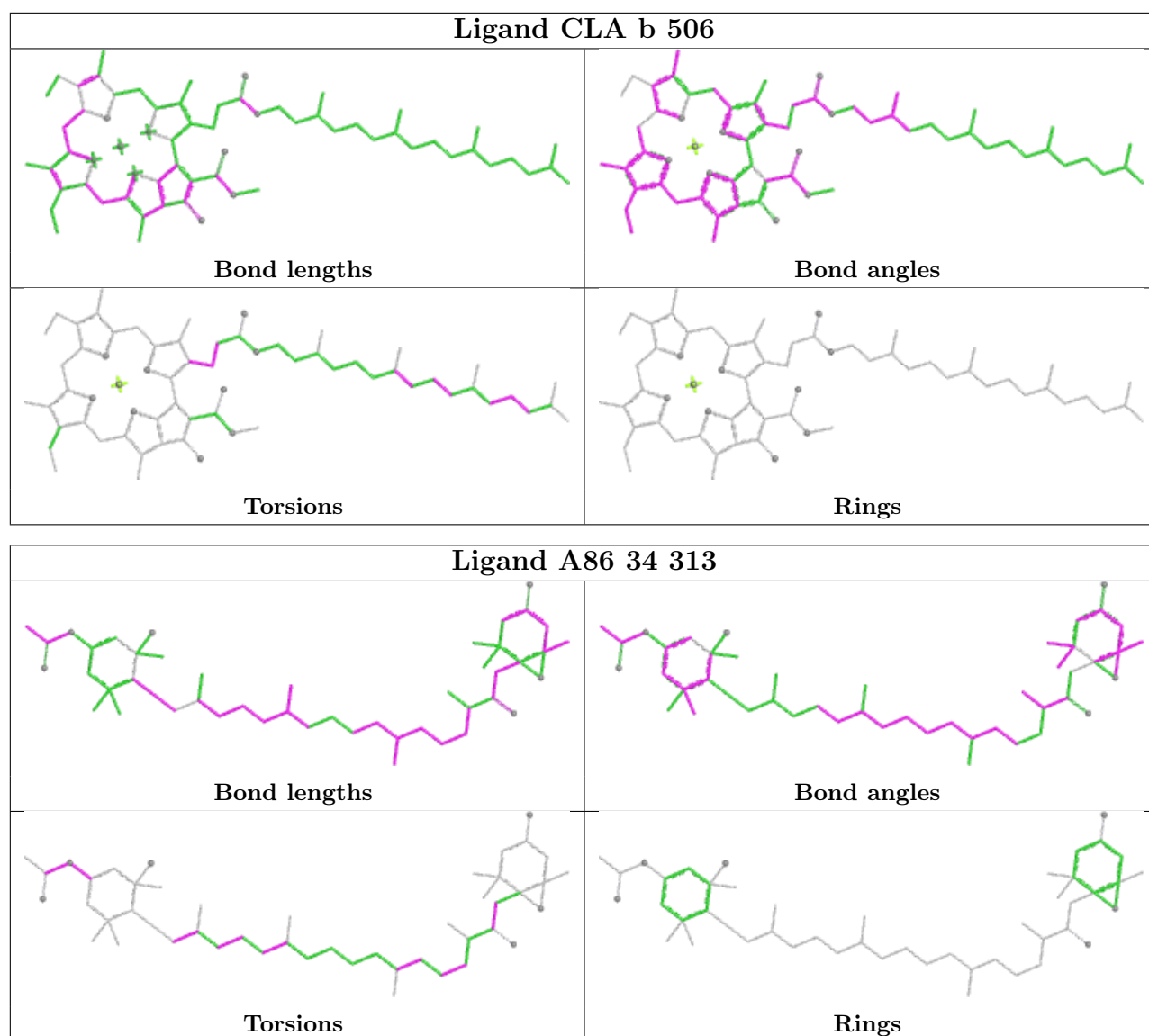


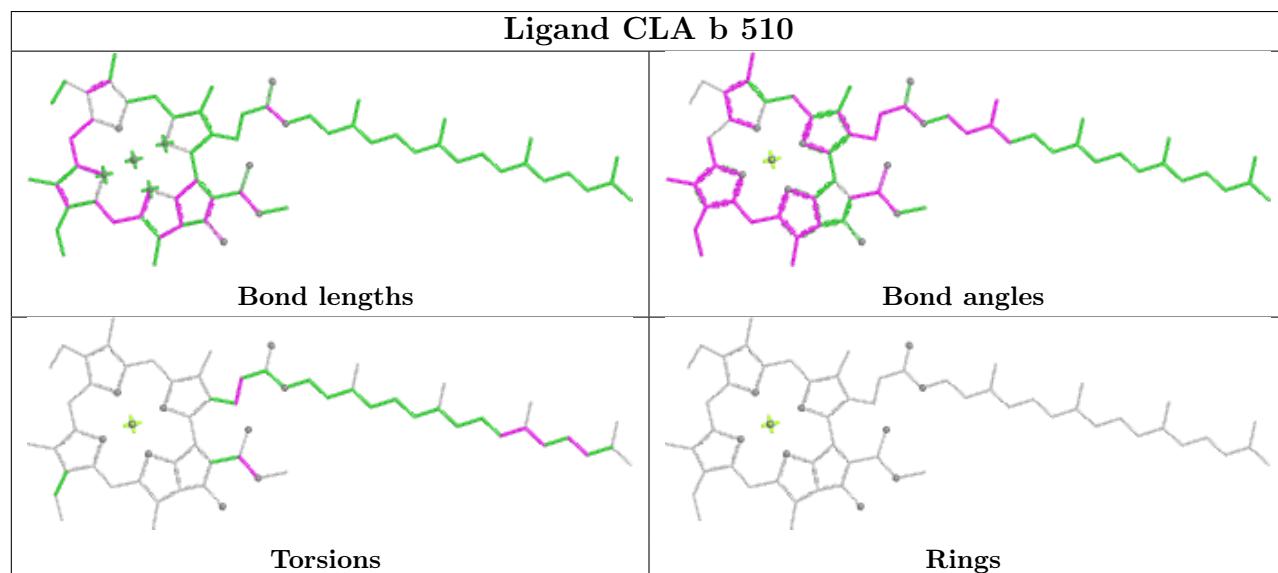
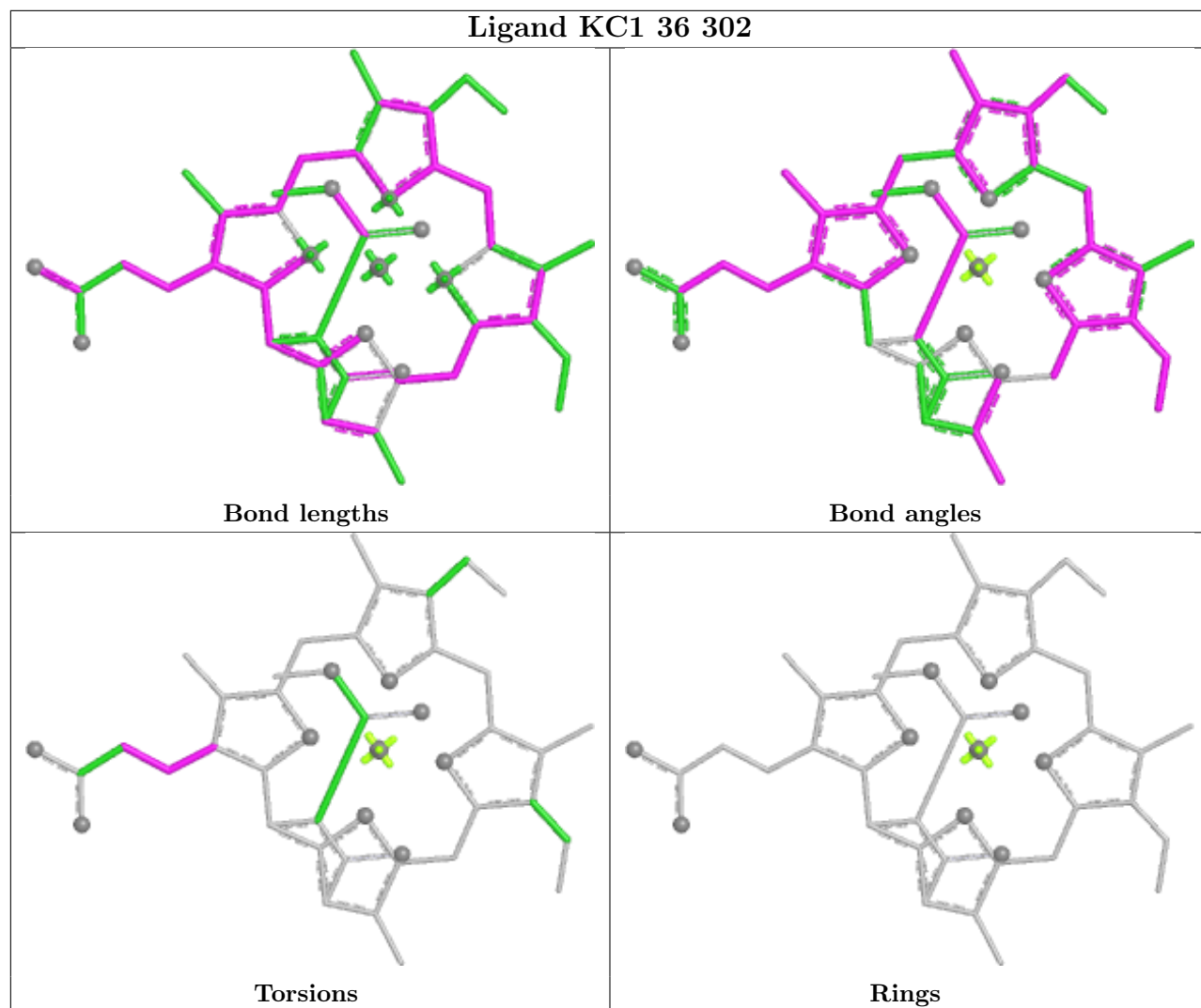


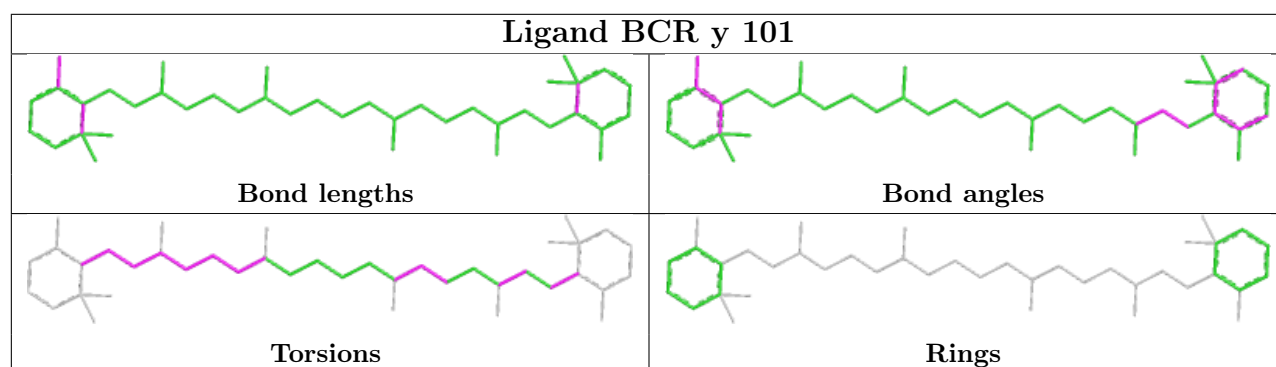
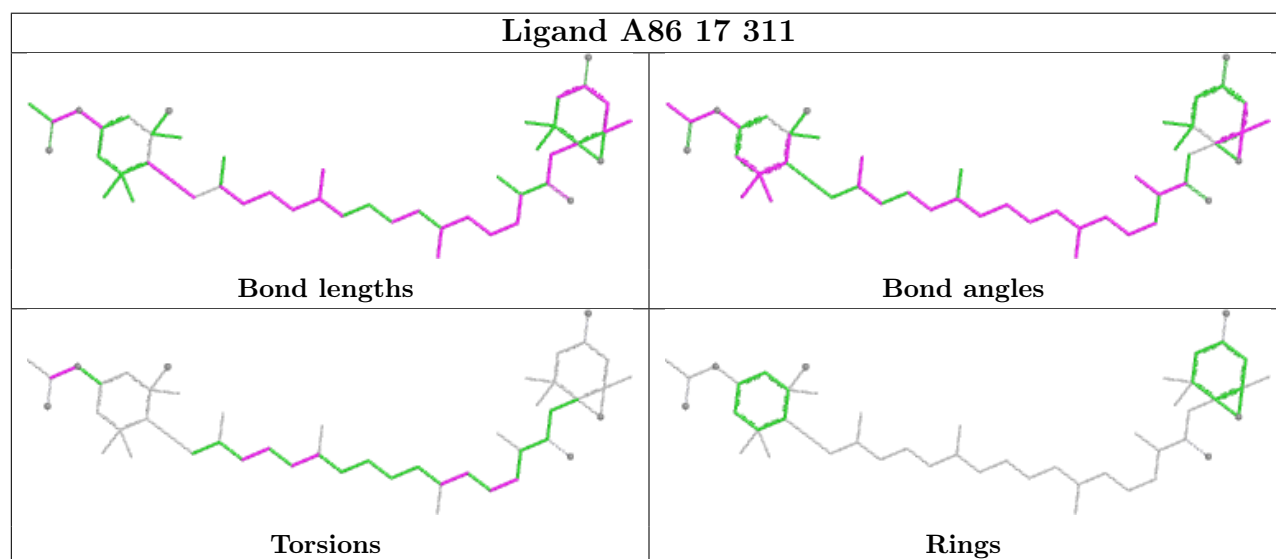
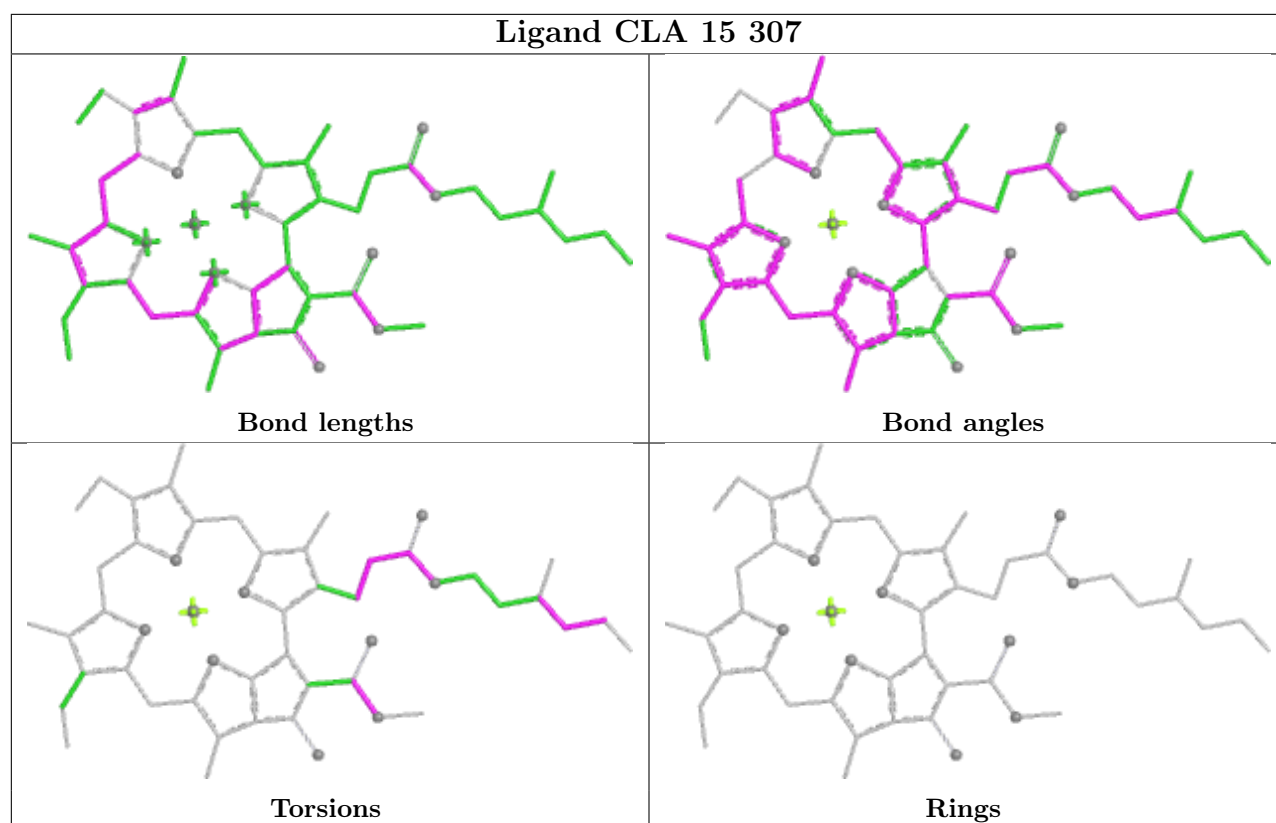


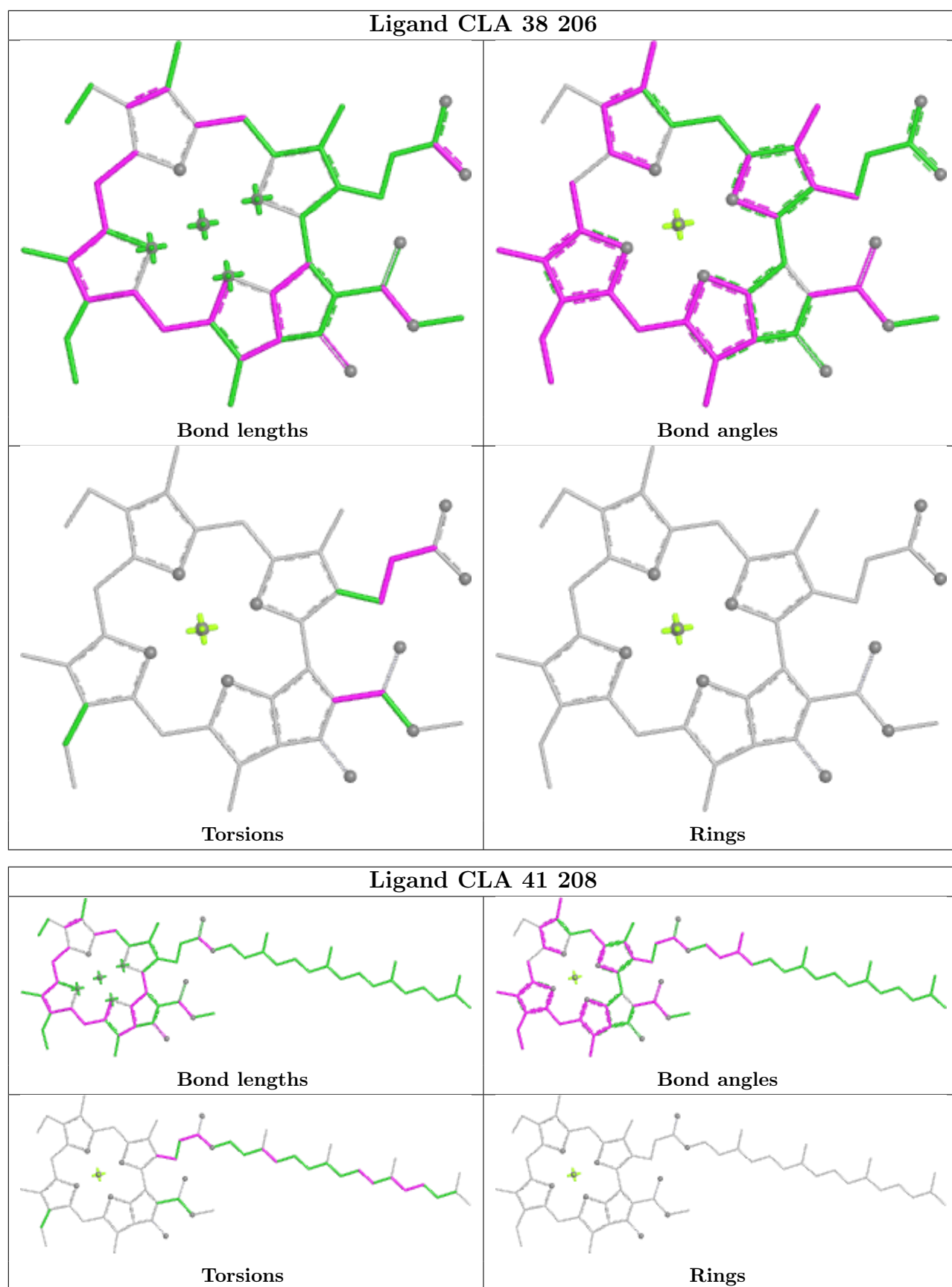


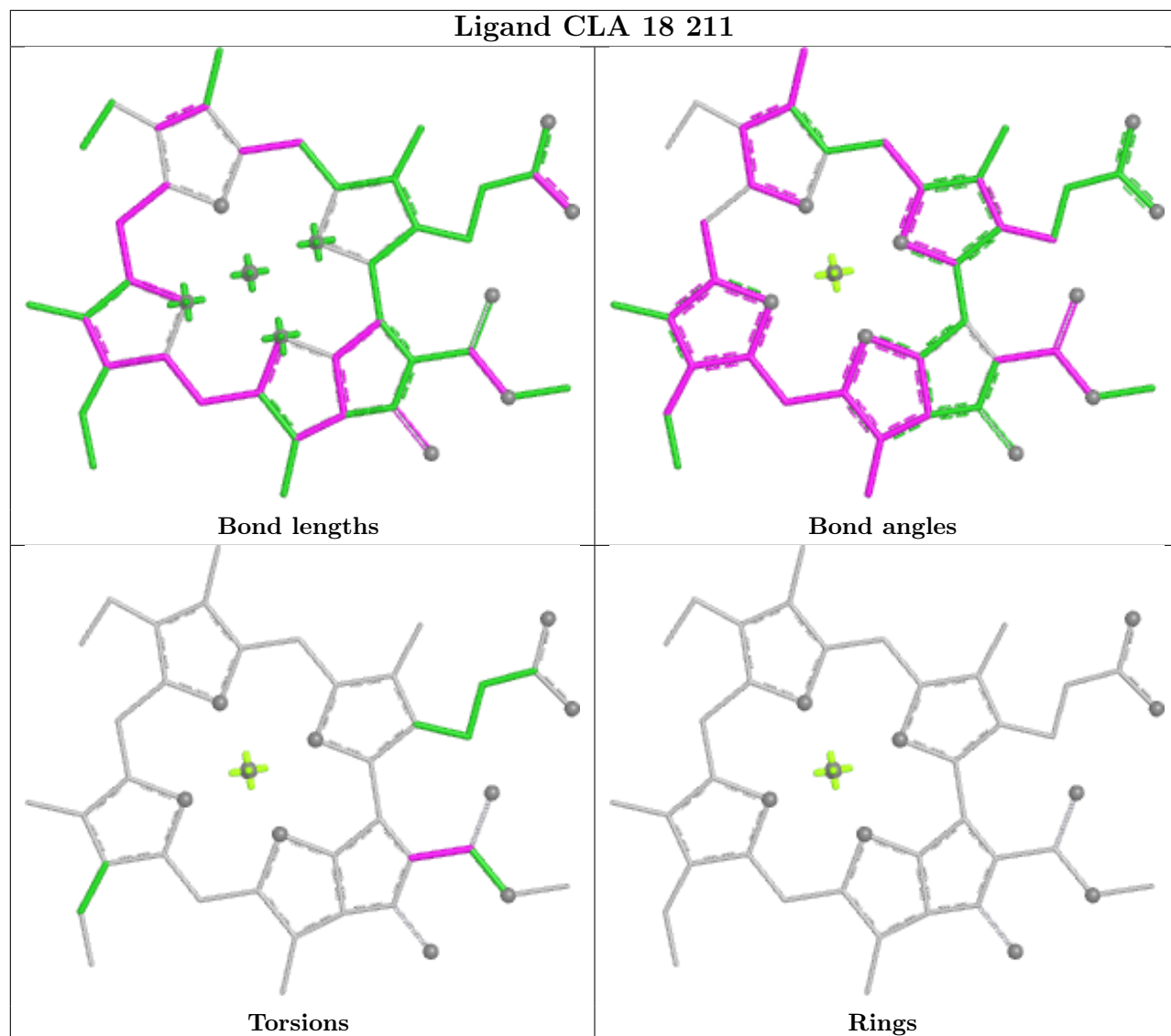


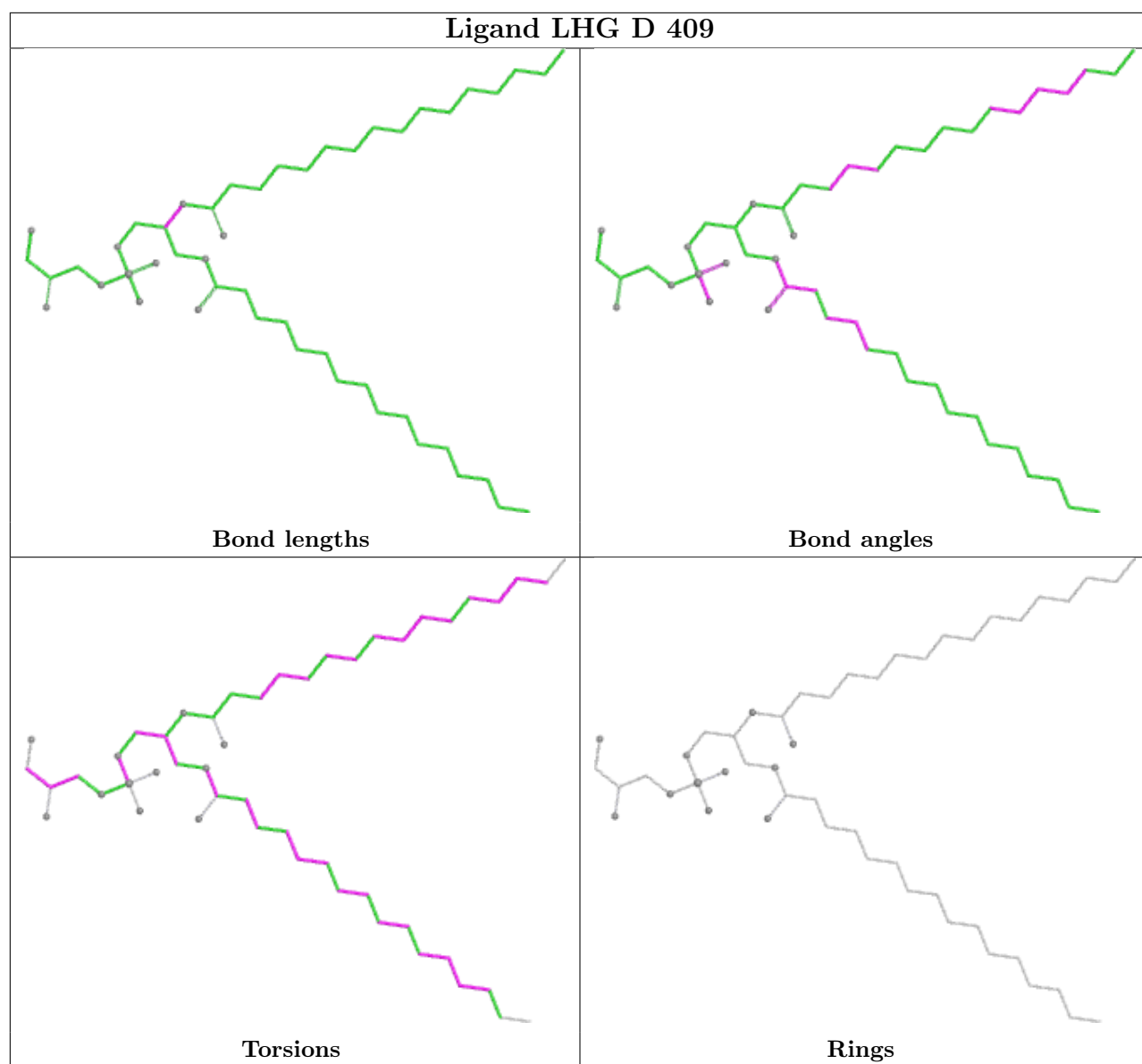


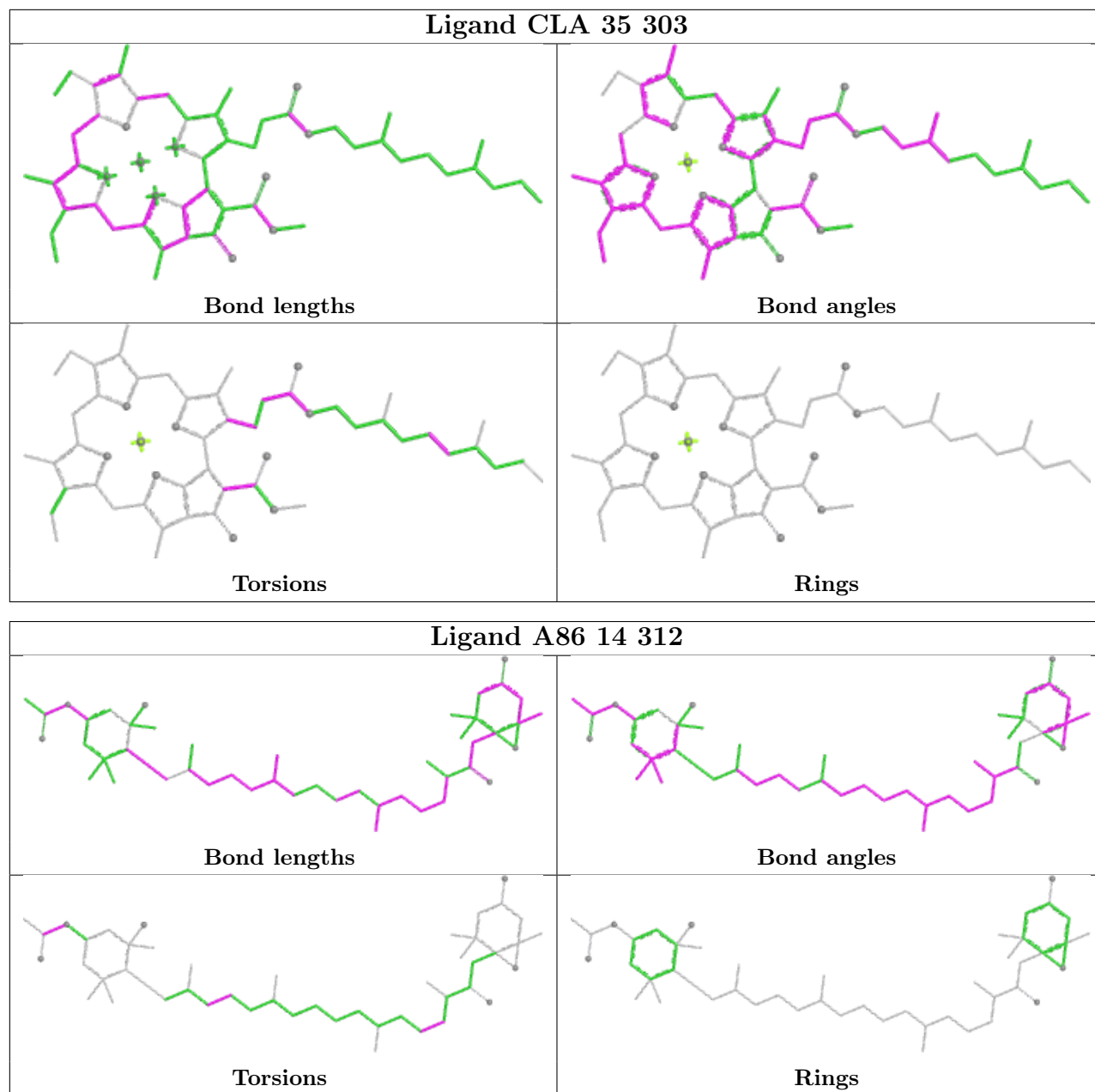


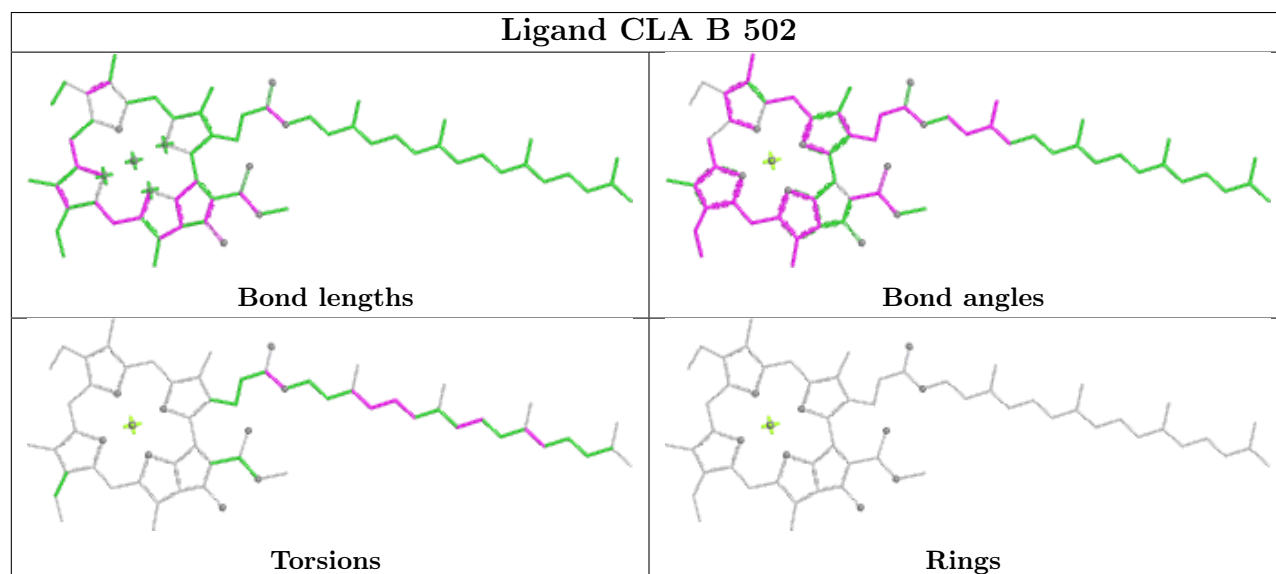
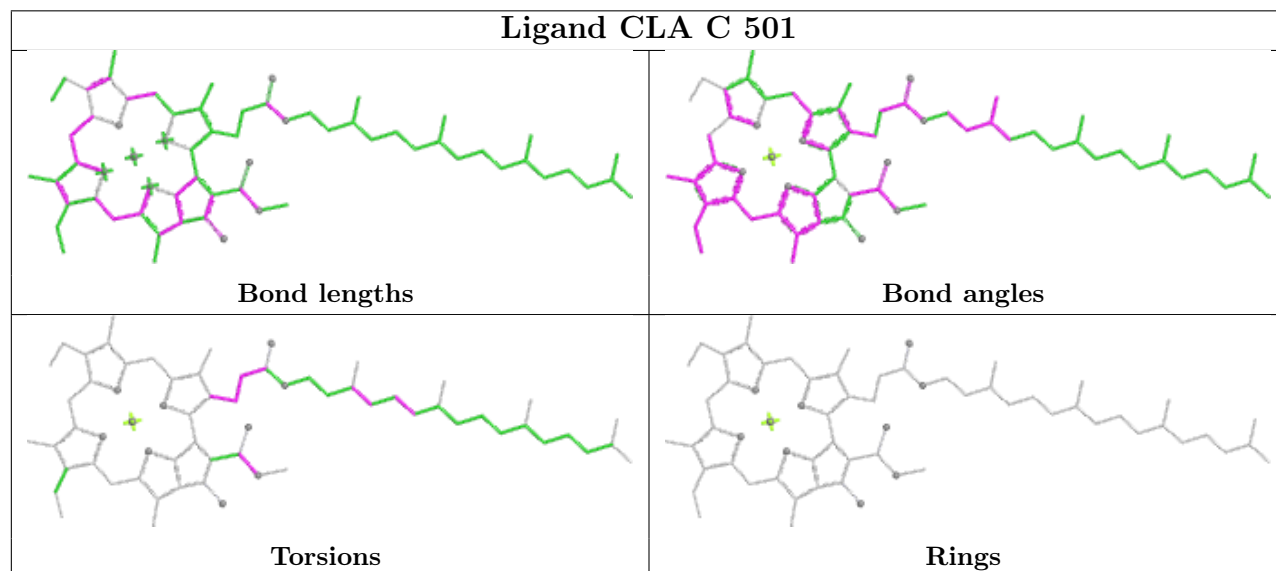
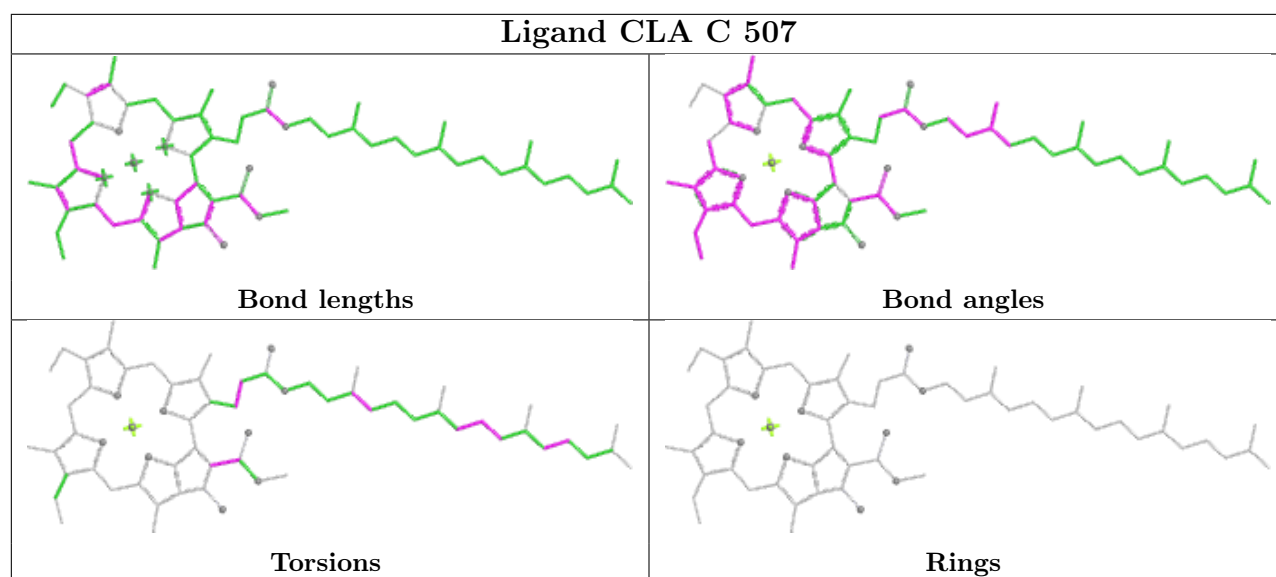


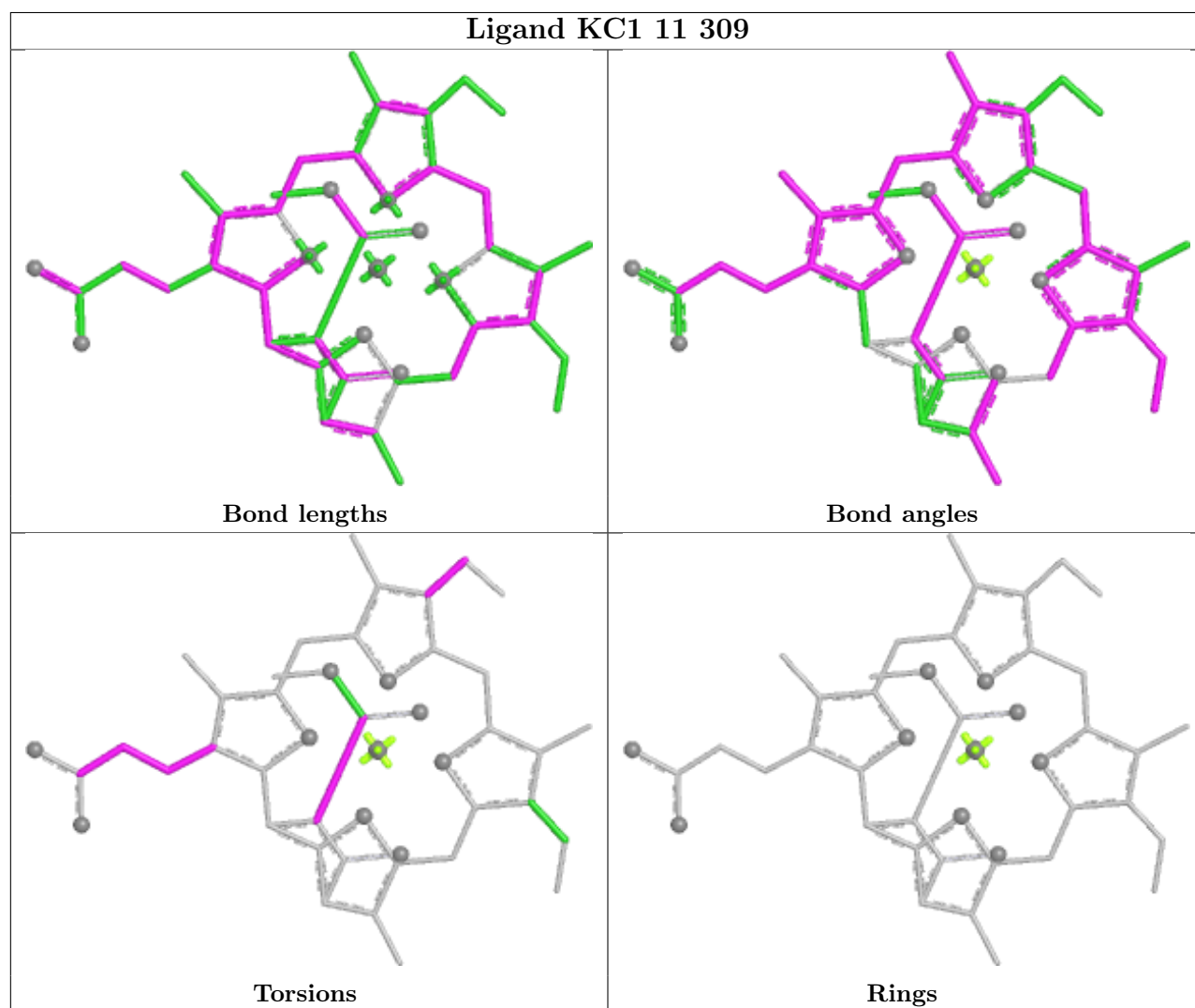
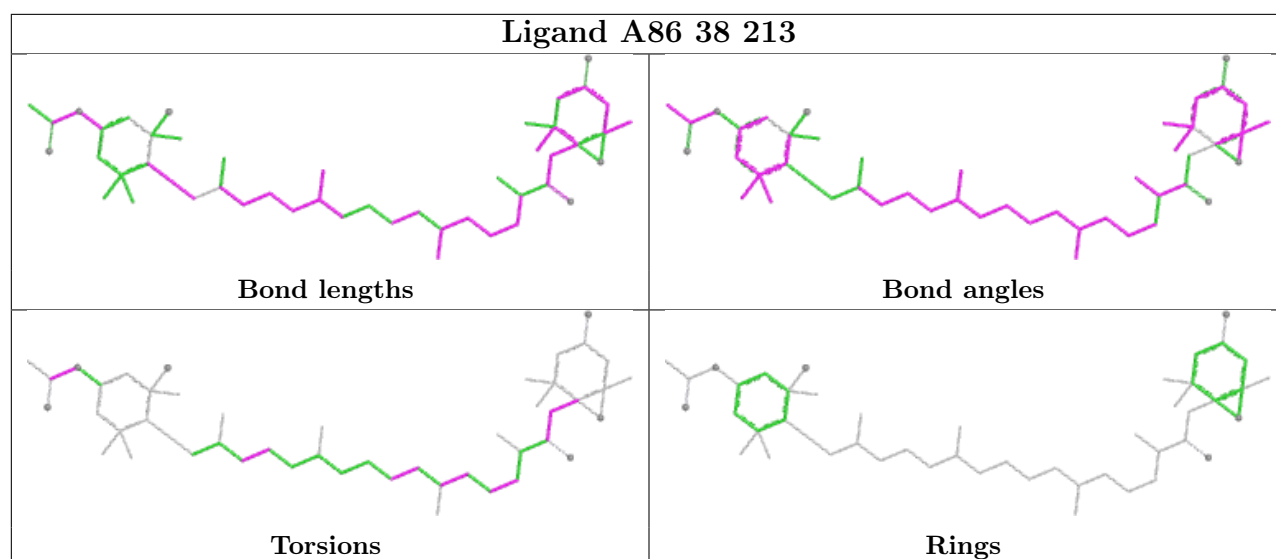


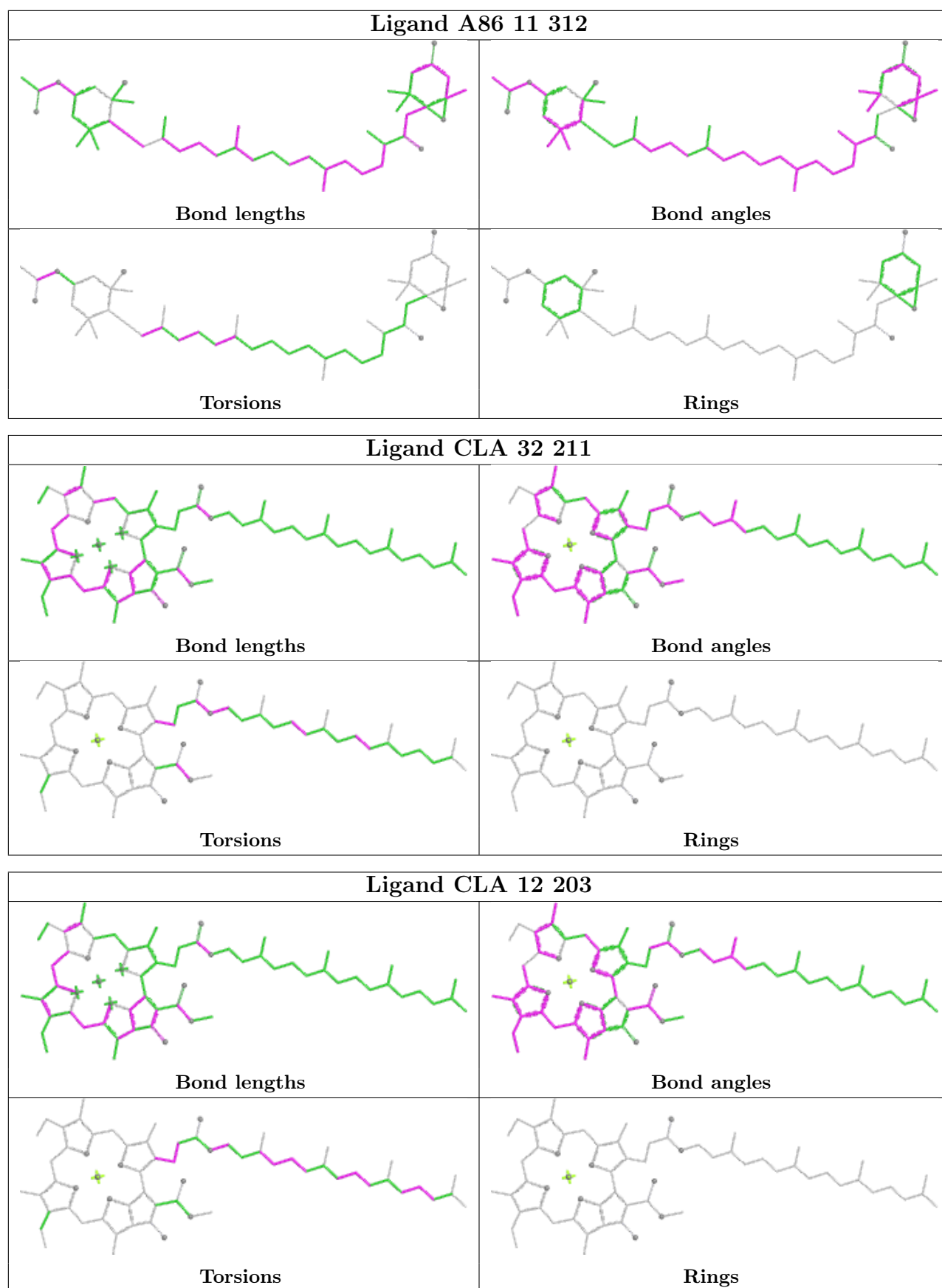


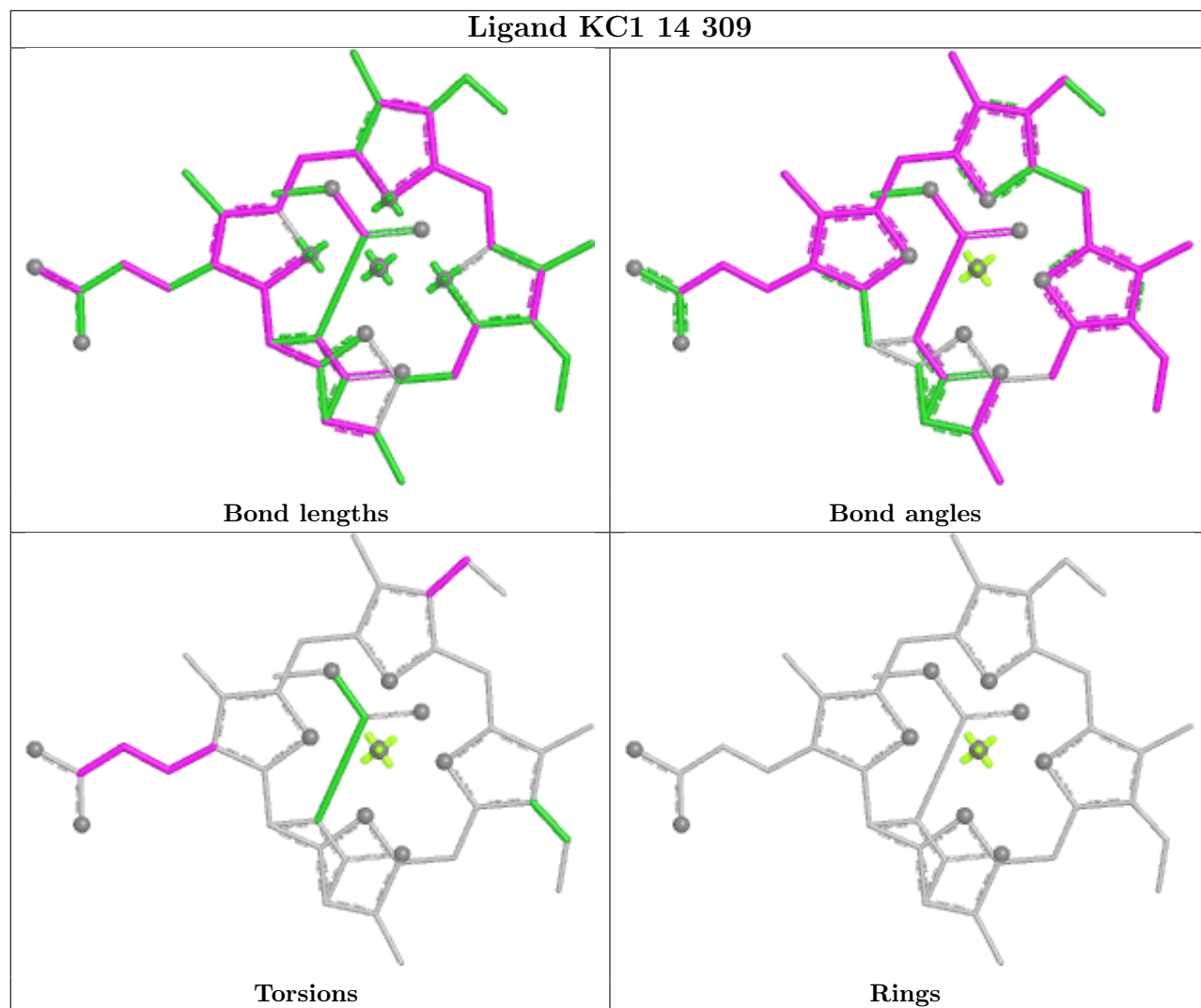


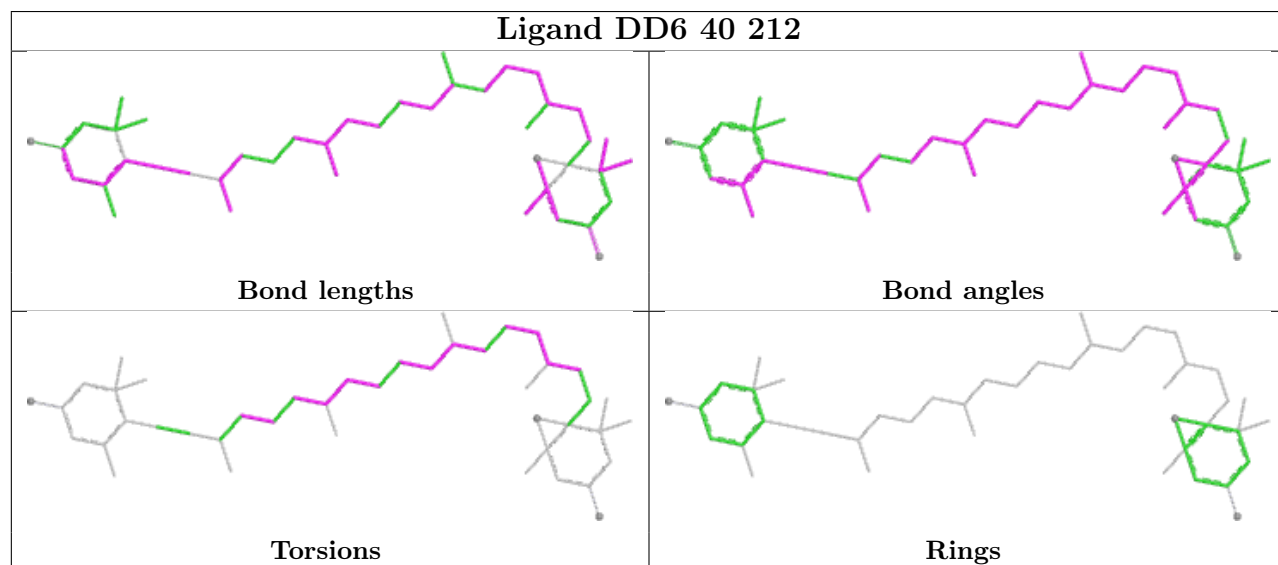
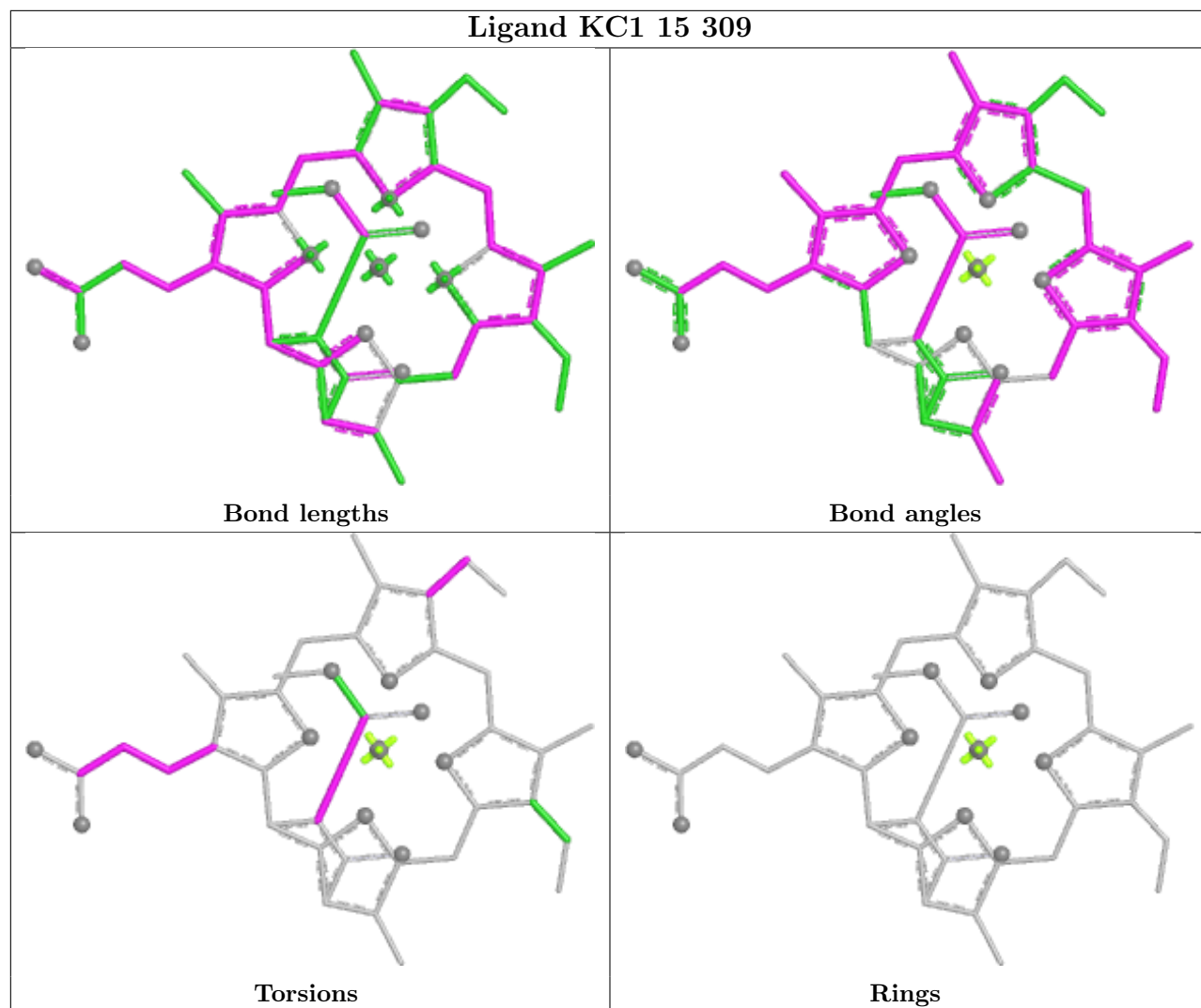


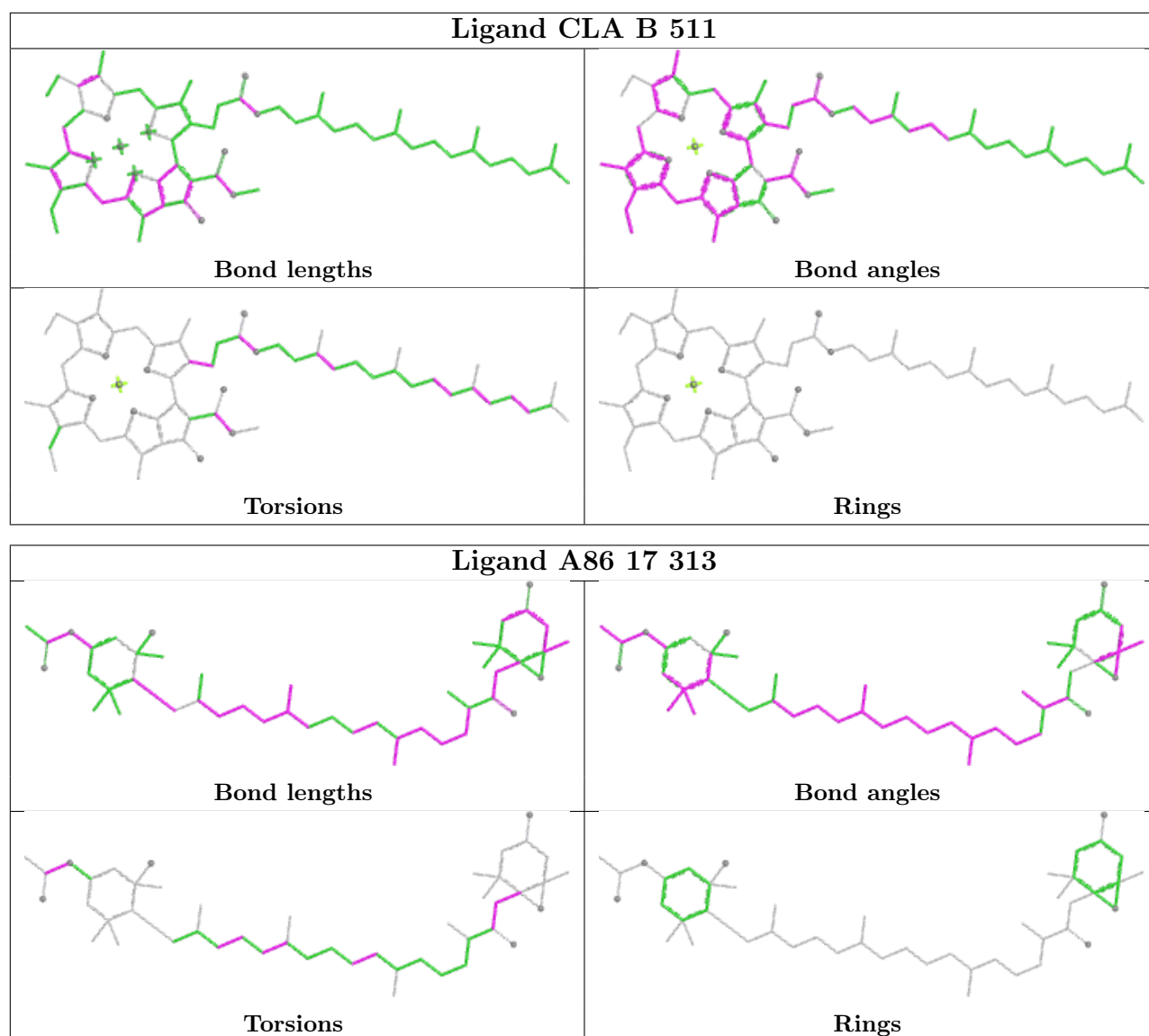


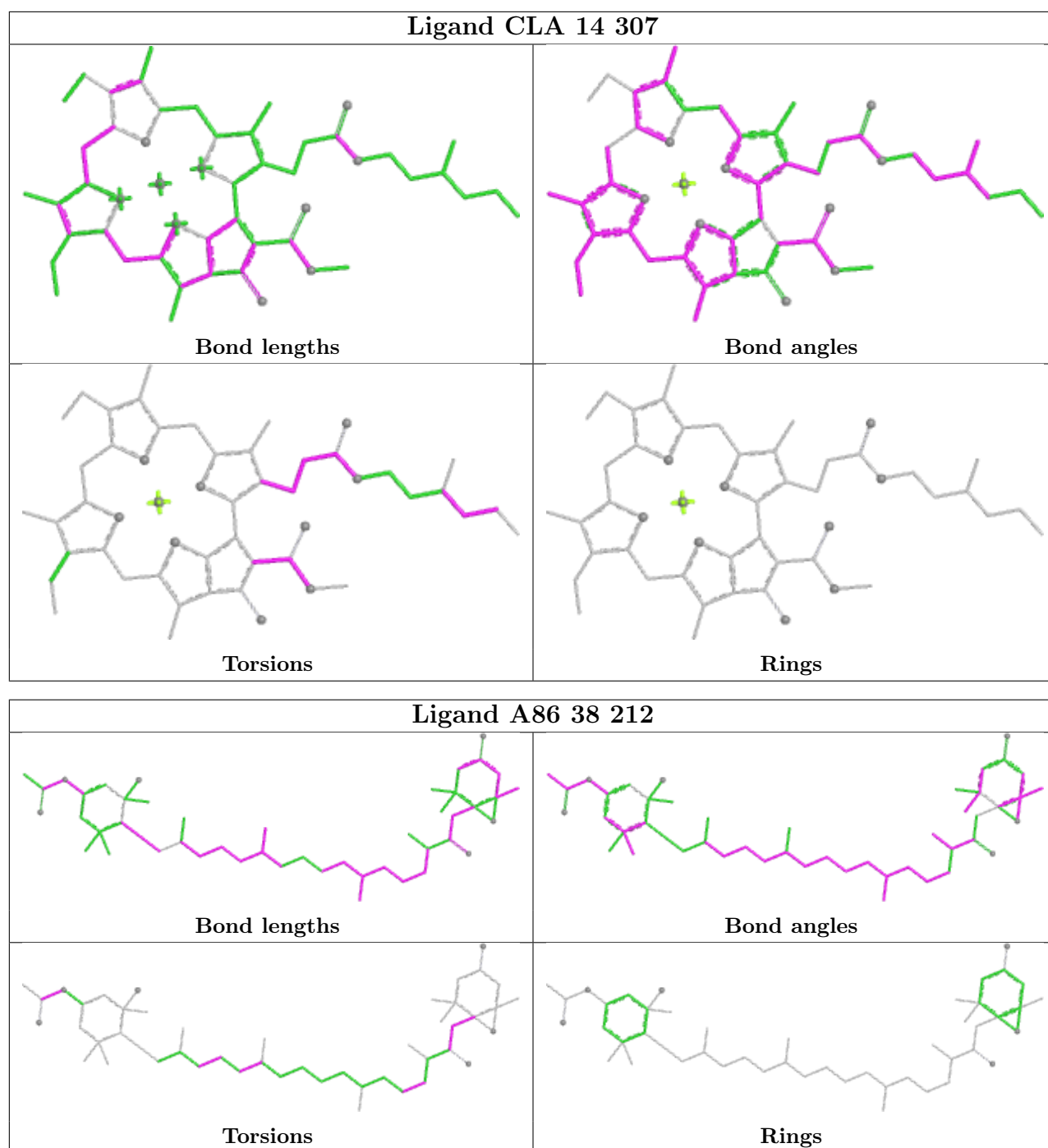


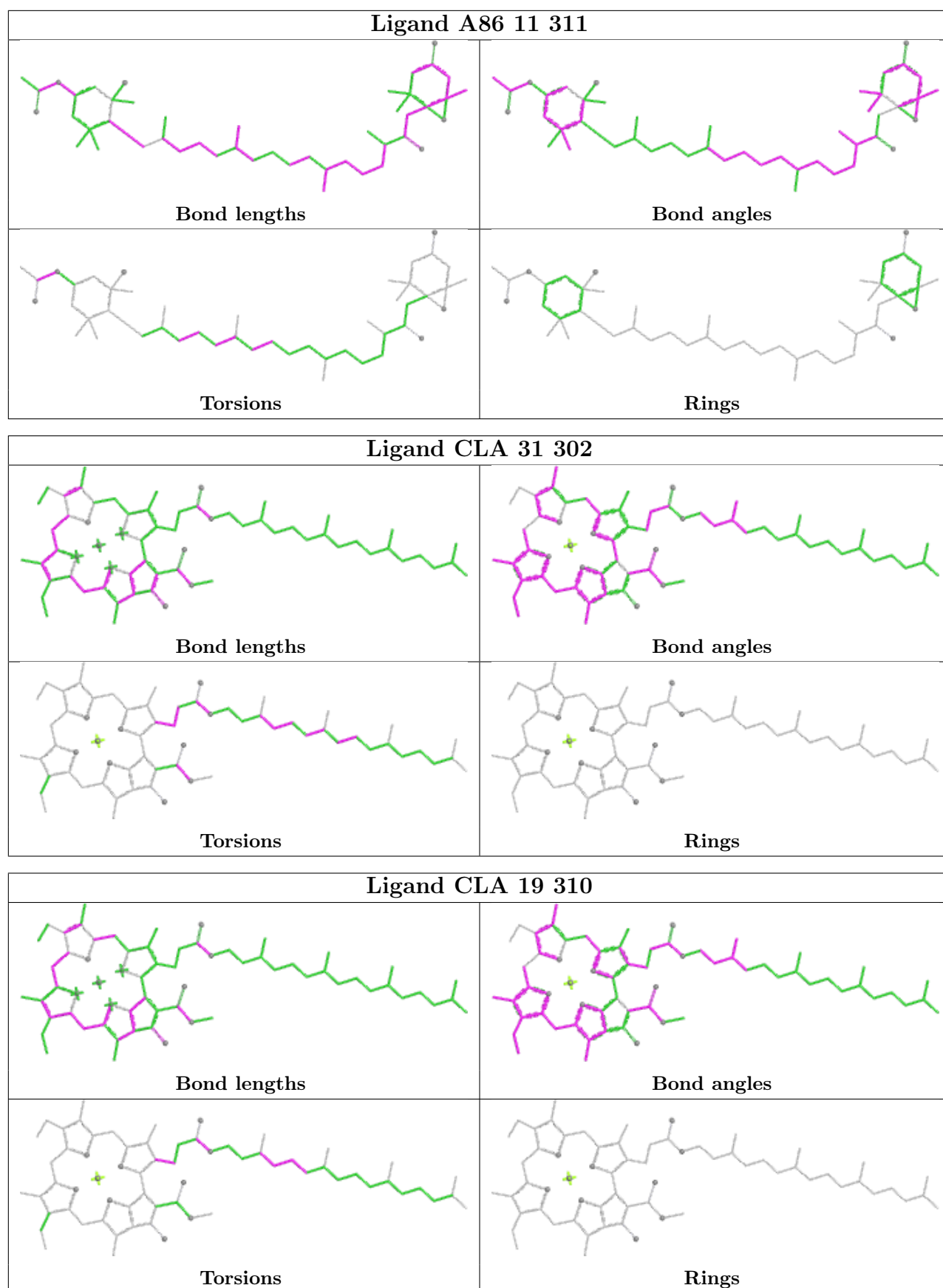


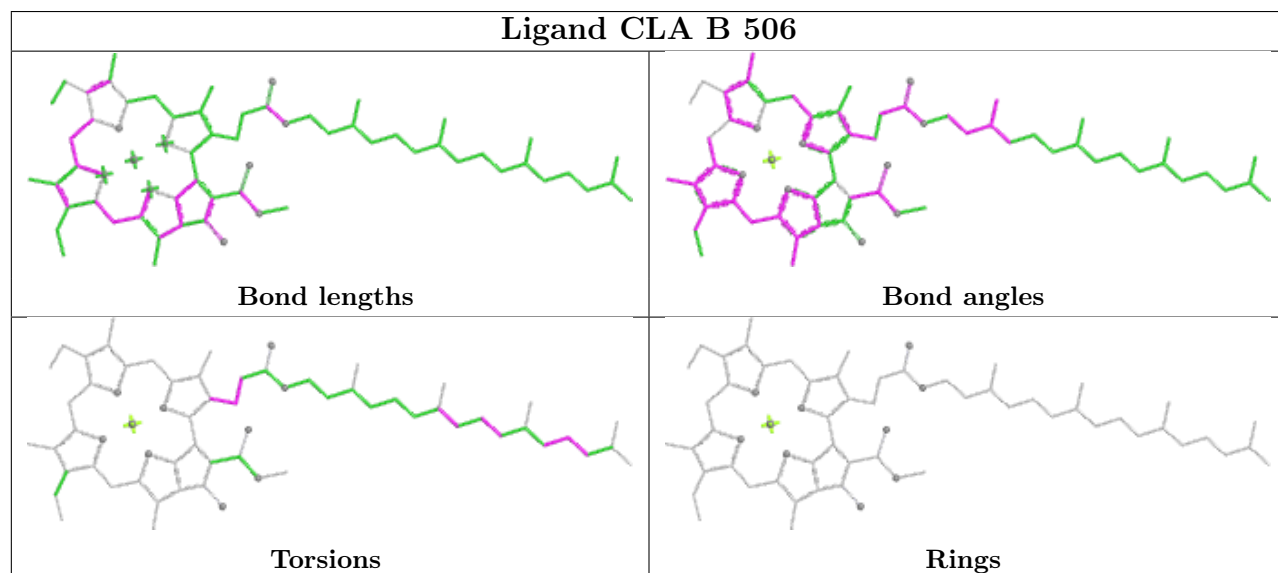
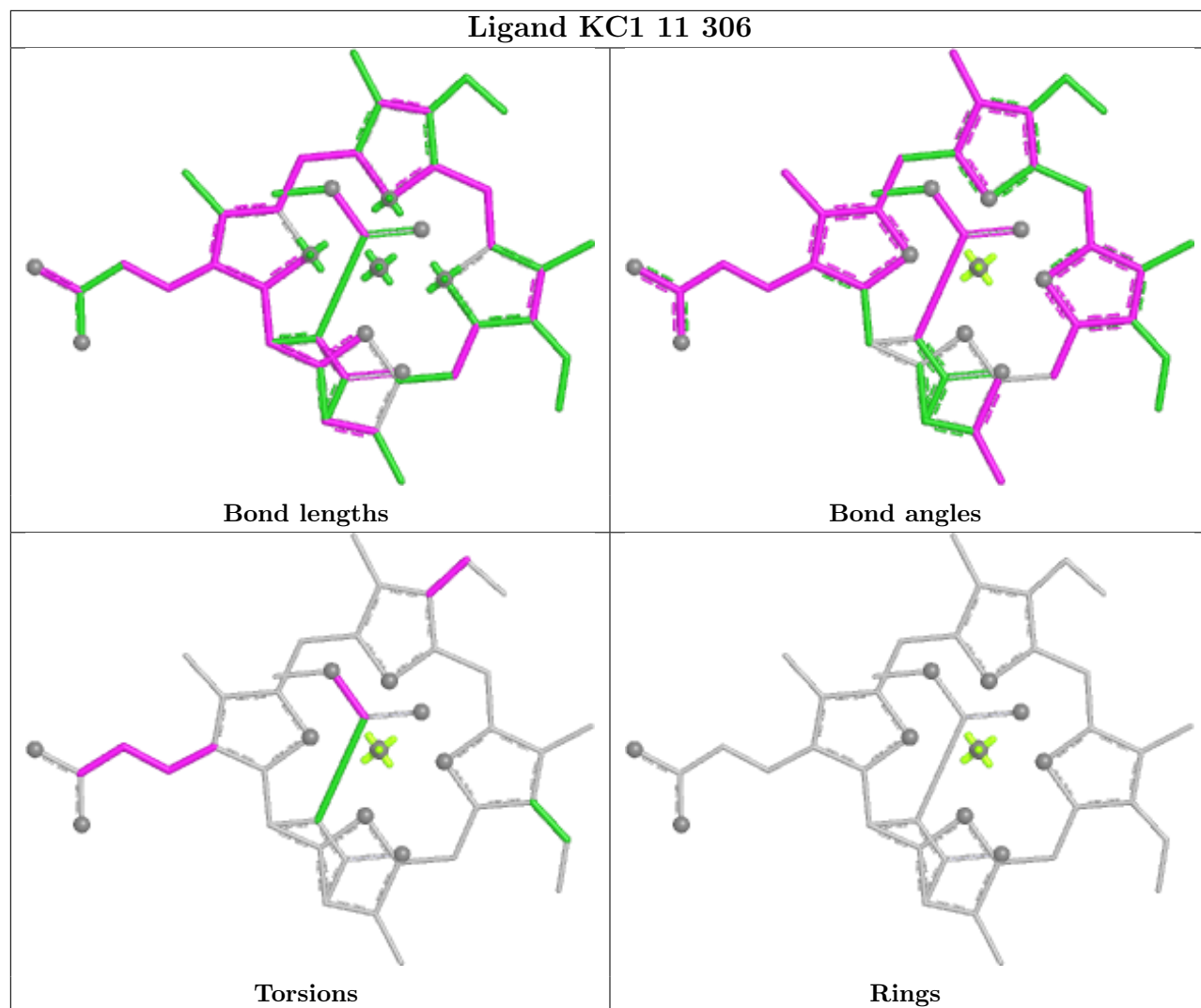


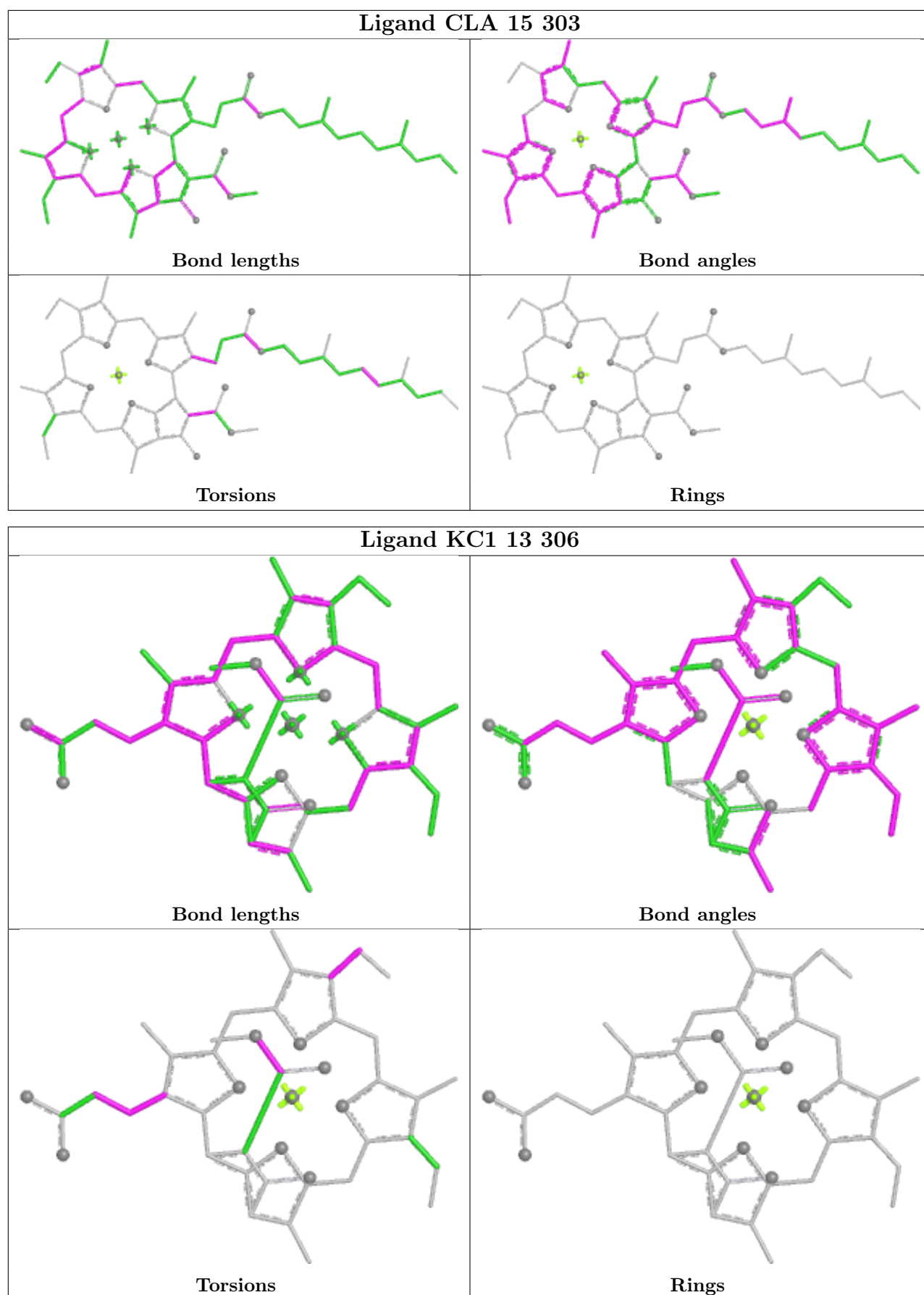


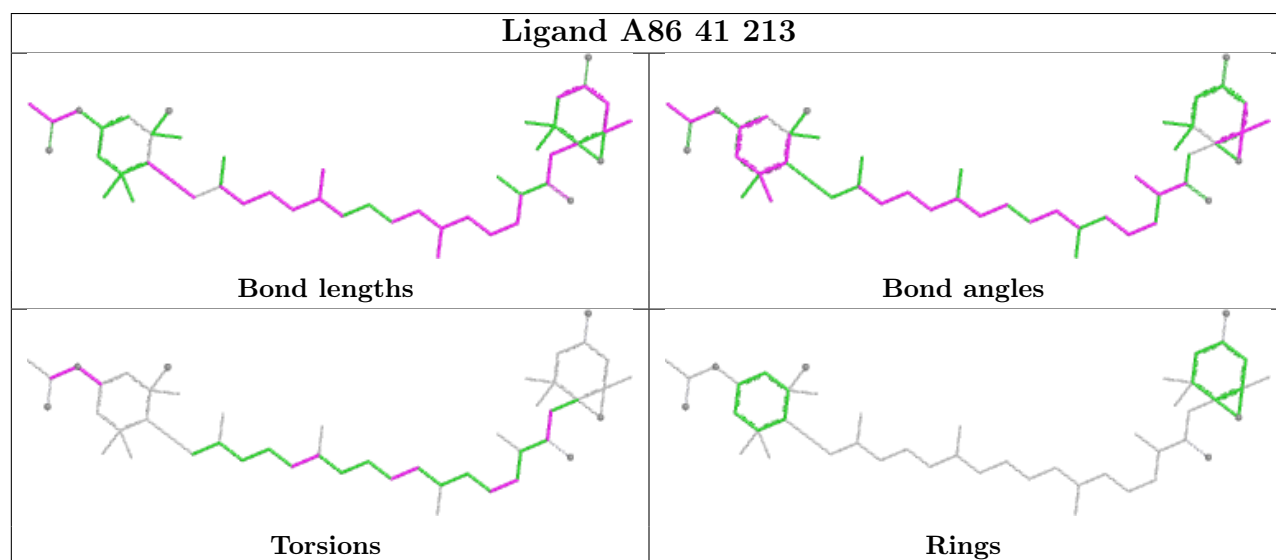
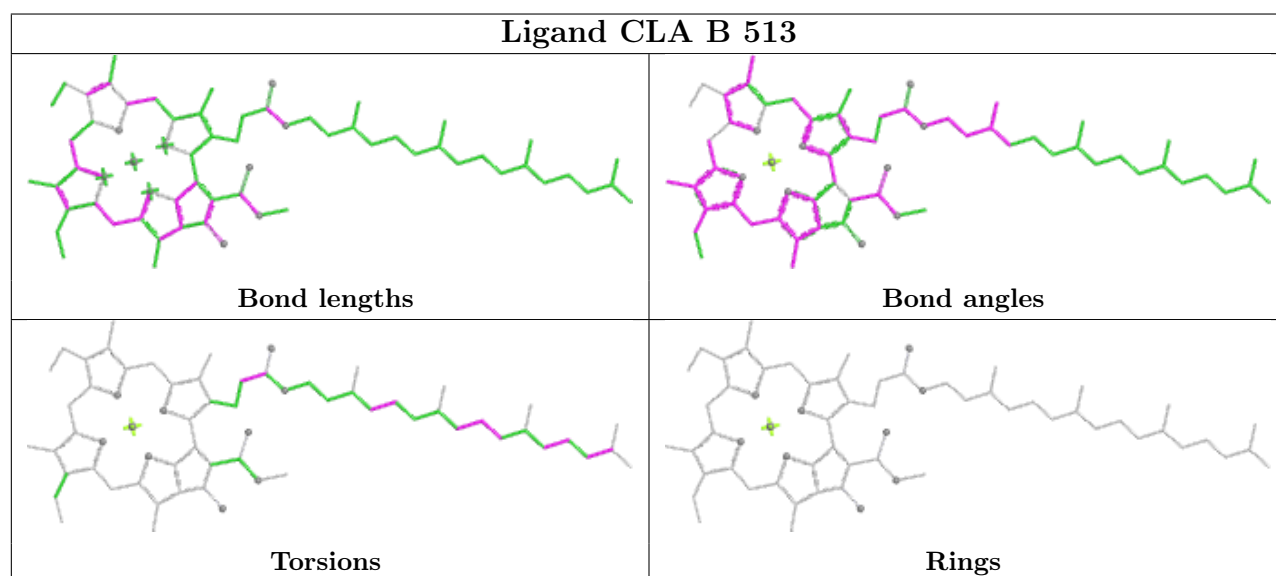
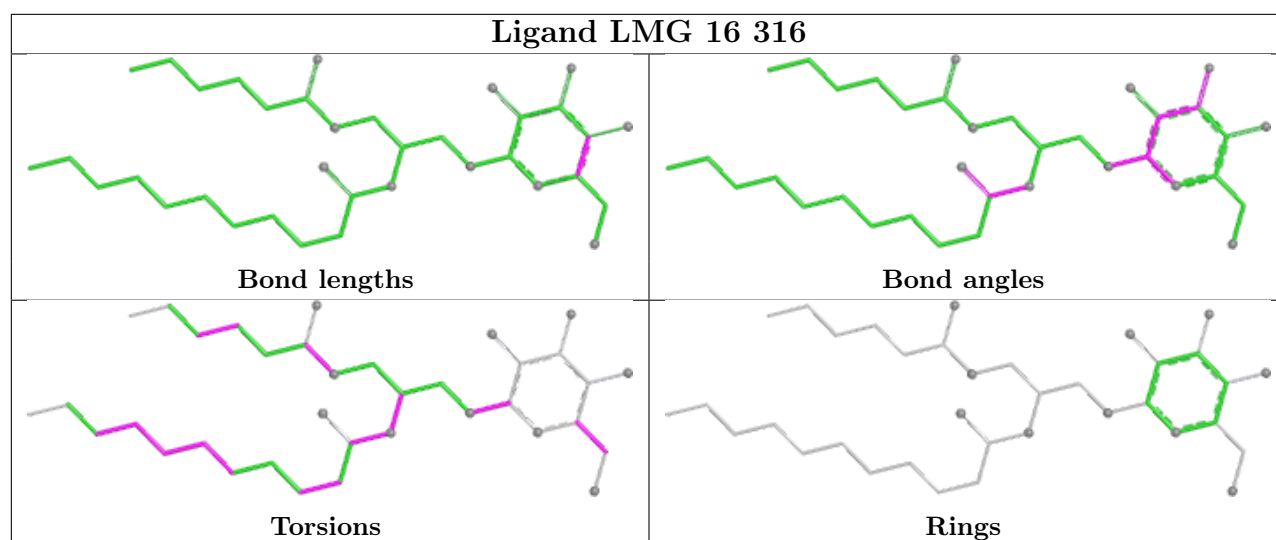


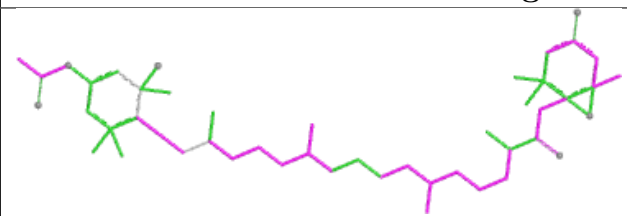
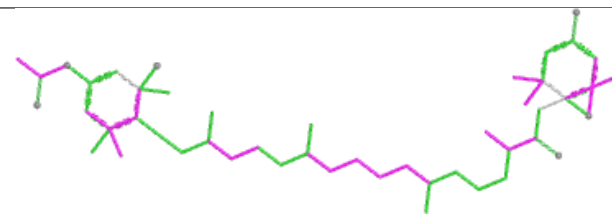
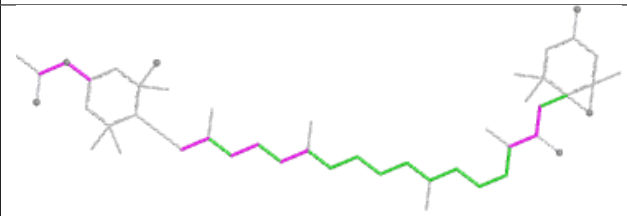
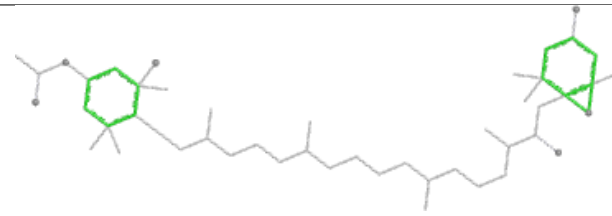



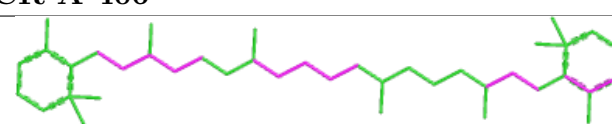
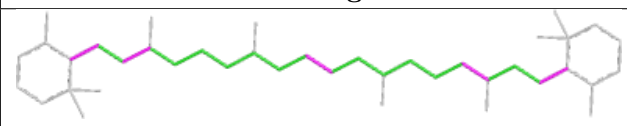
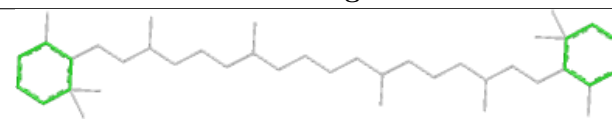


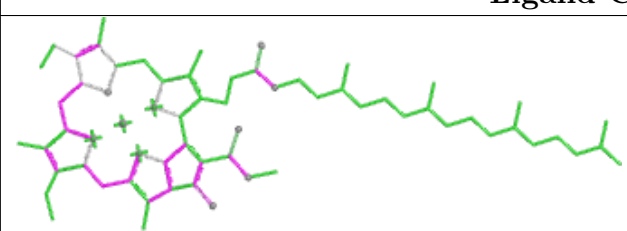
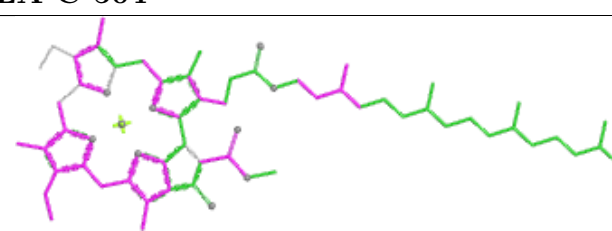
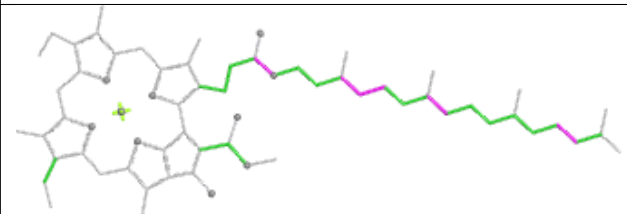
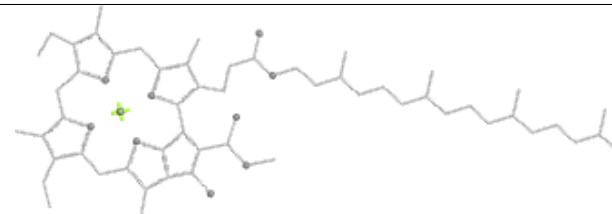


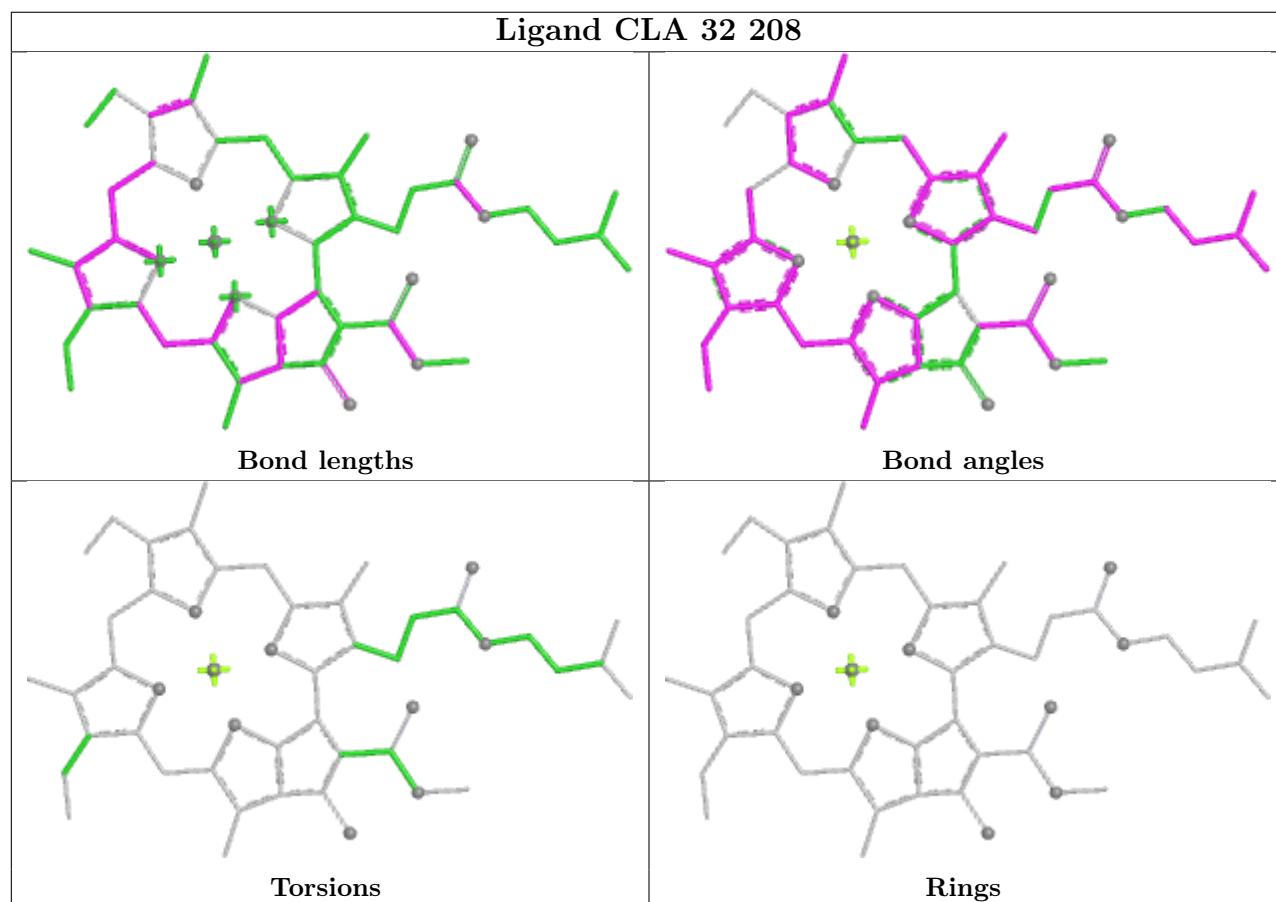
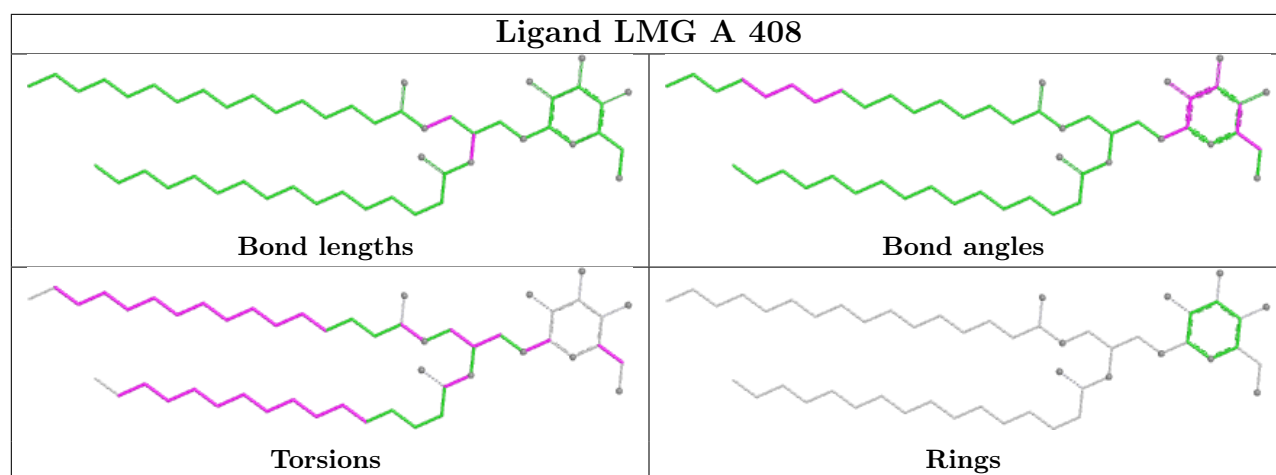


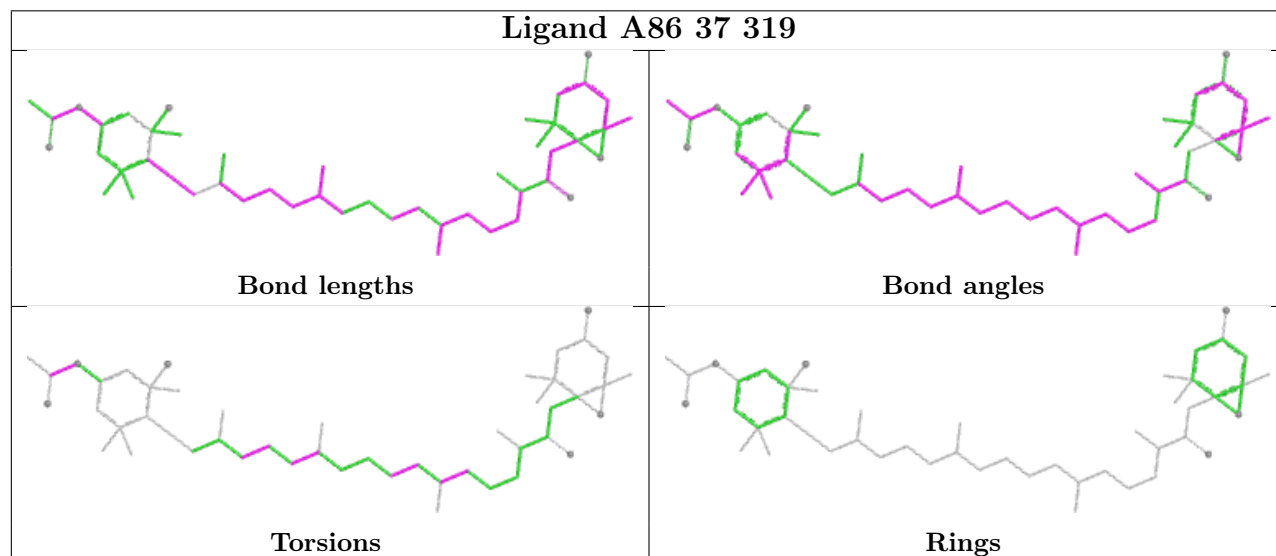
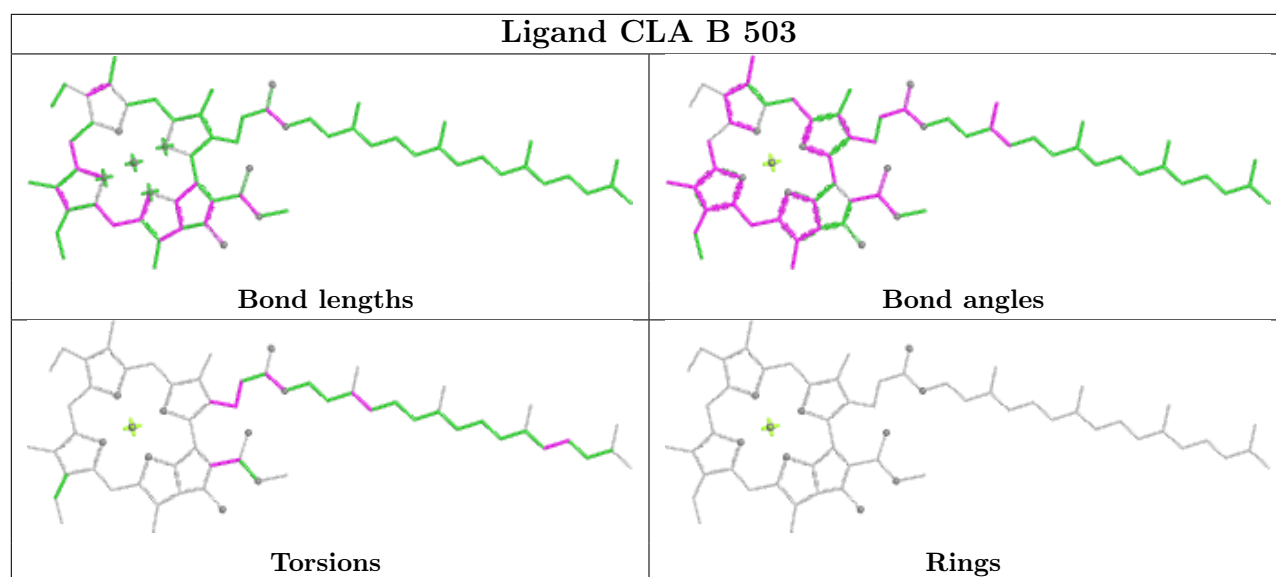


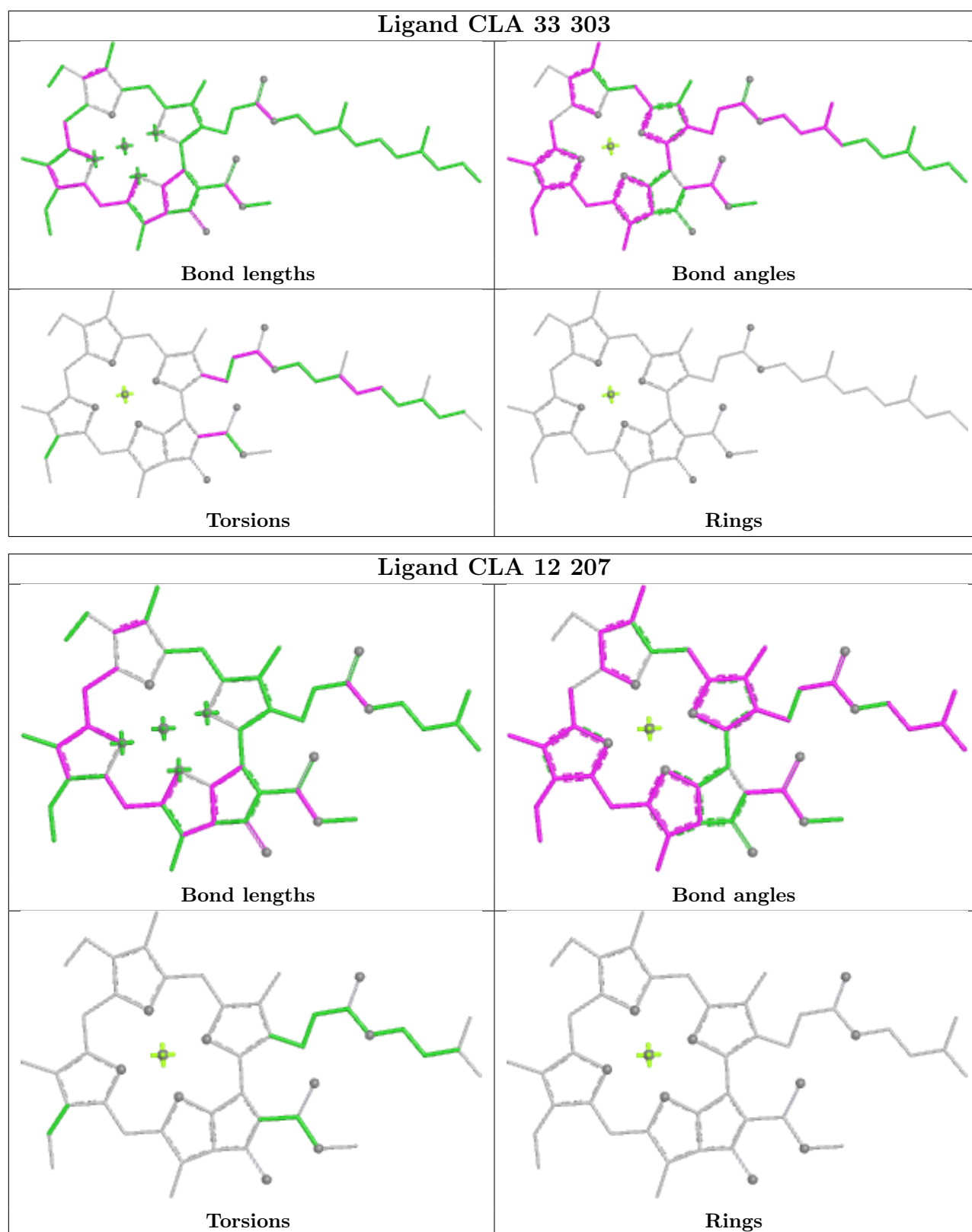
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Bond lengths	Bond angles
	
Torsions	Rings

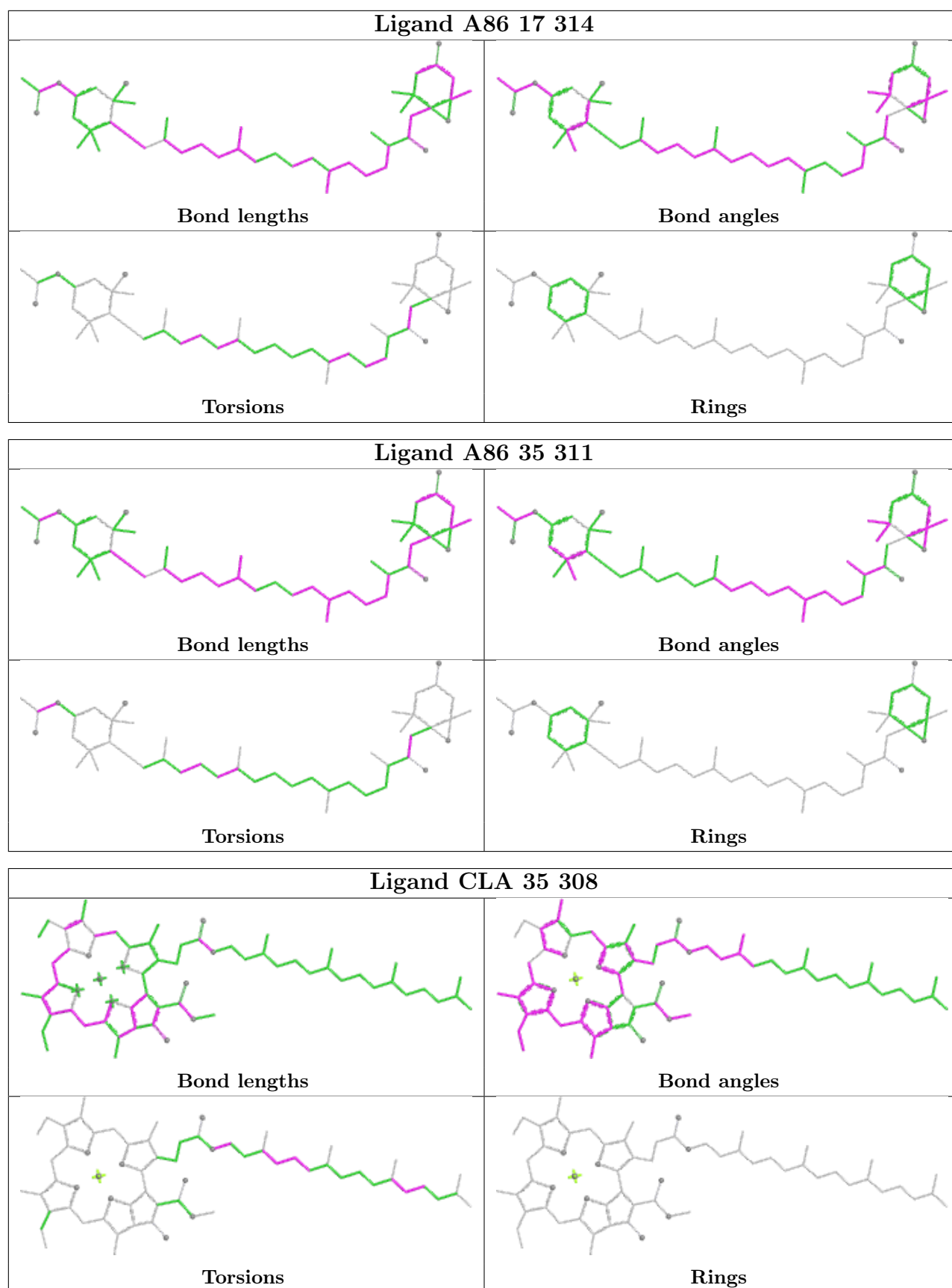
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Bond lengths	Bond angles
	
Torsions	Rings

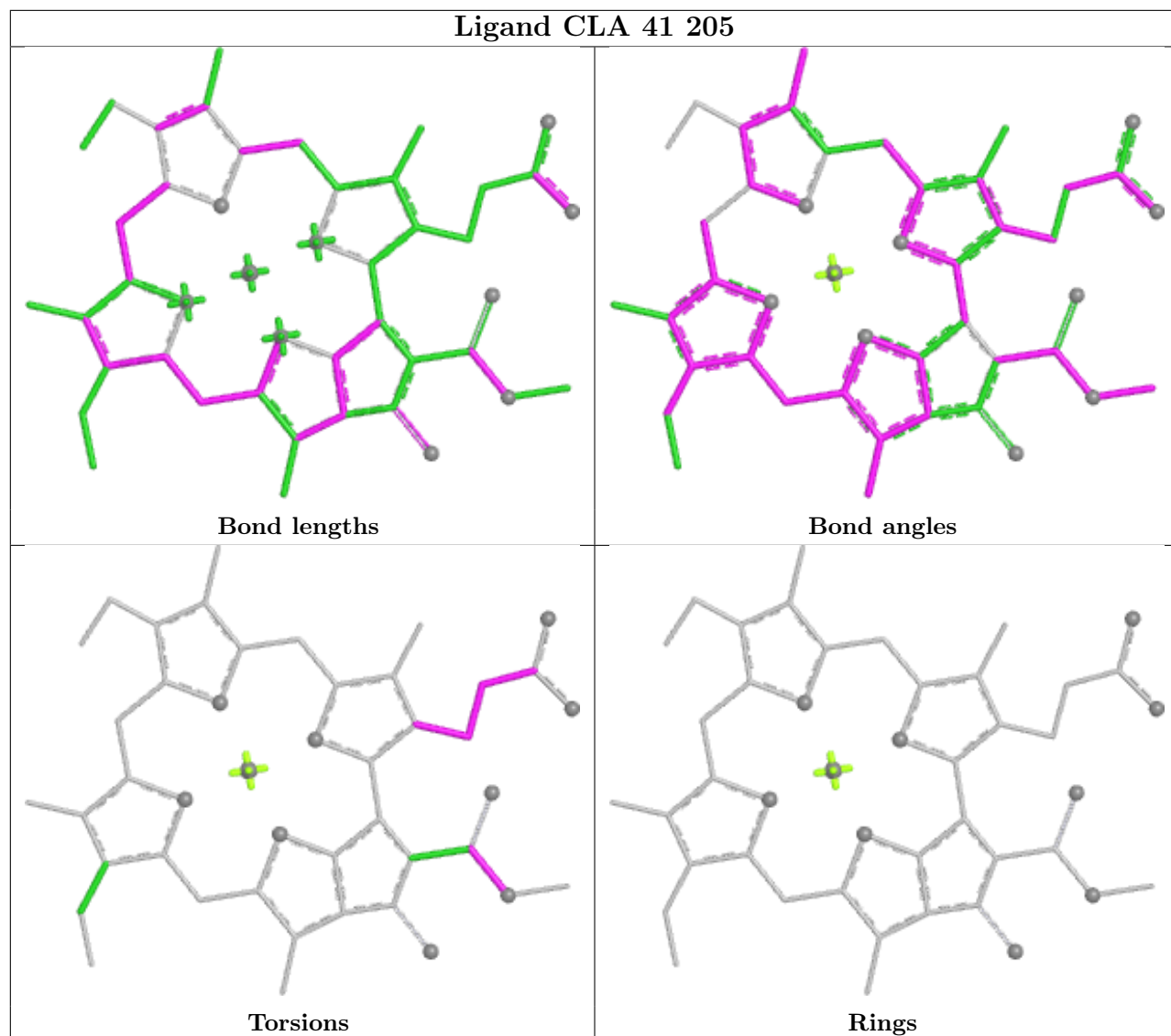
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Bond lengths	Bond angles
	
Torsions	Rings

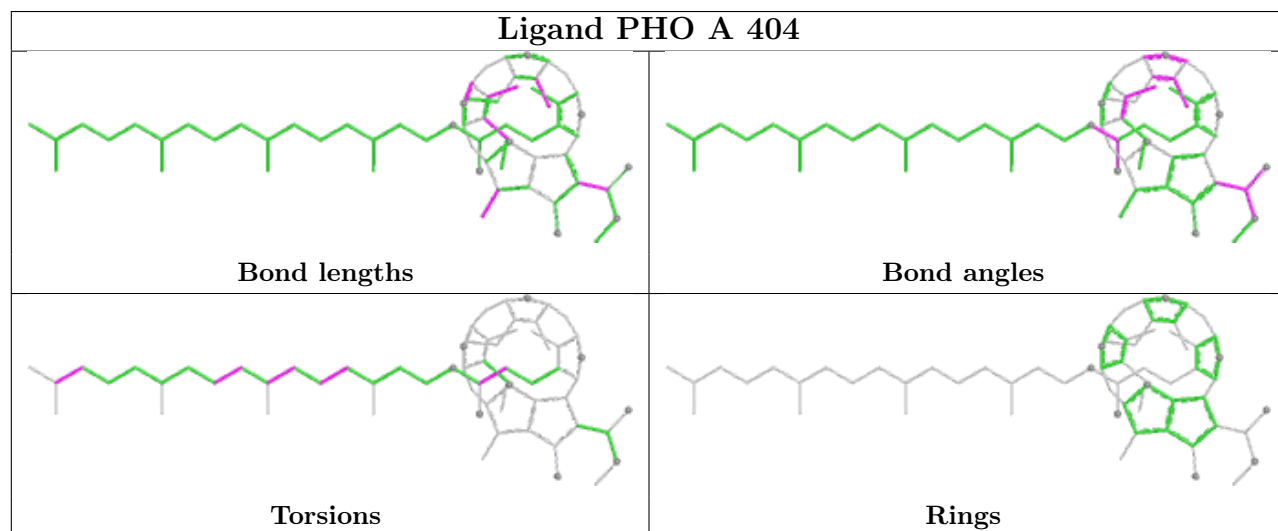
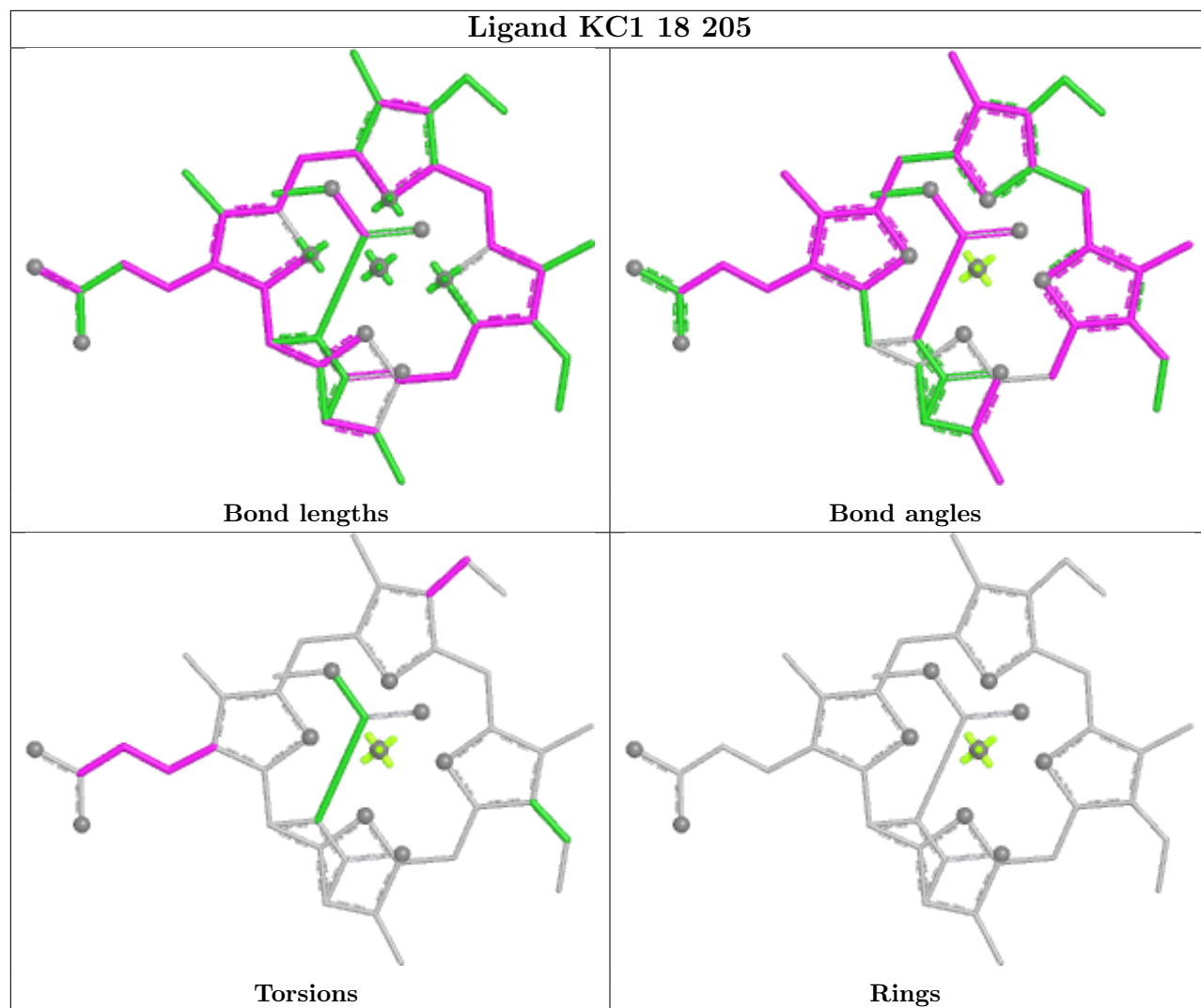


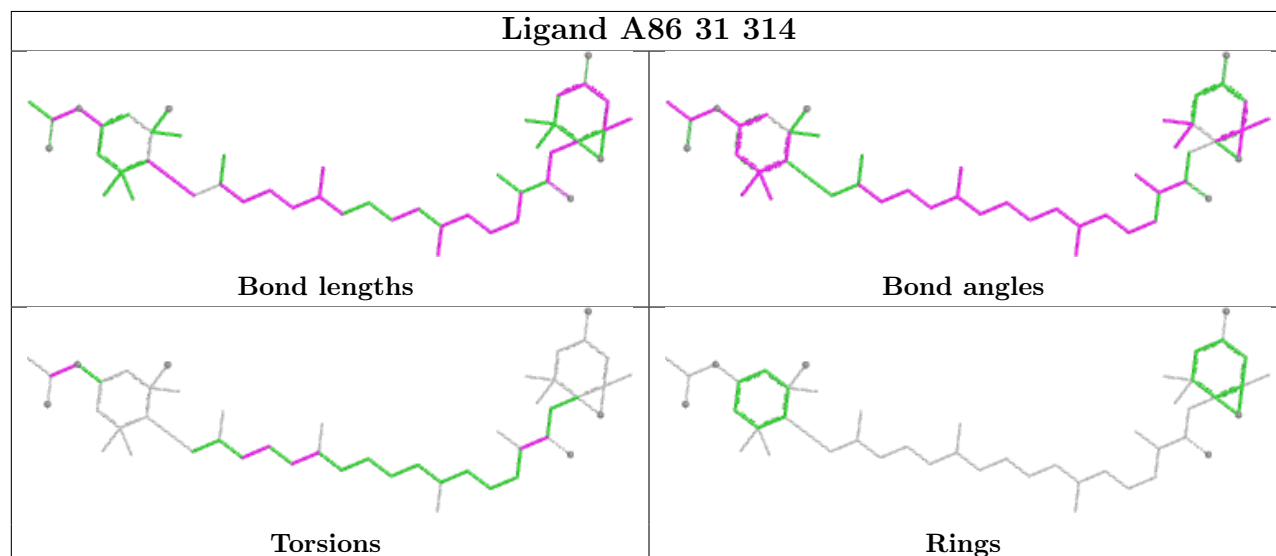
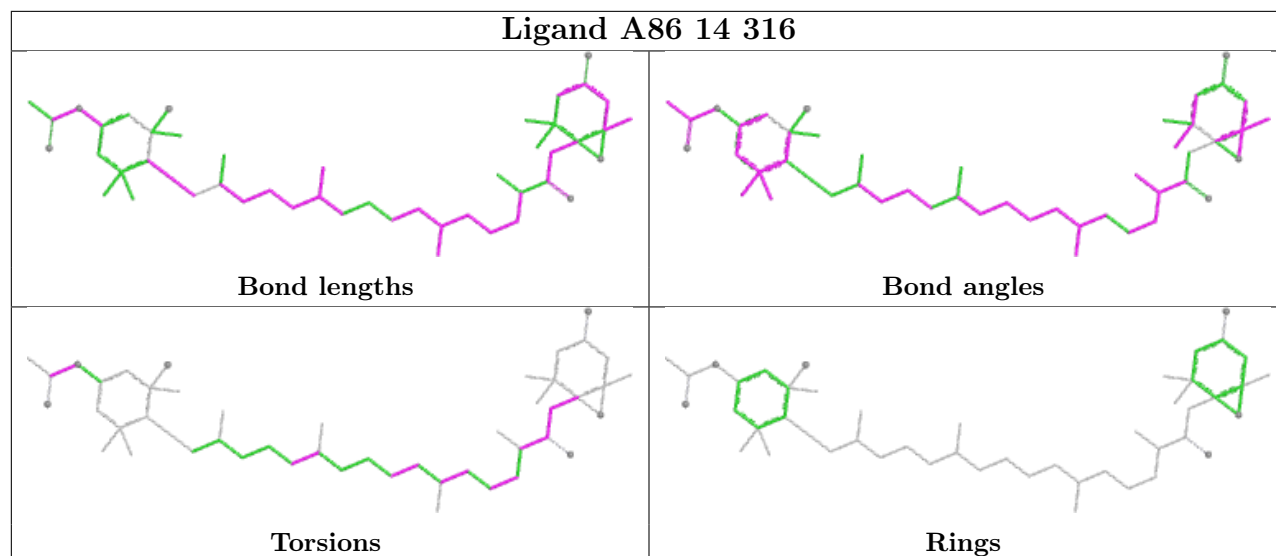


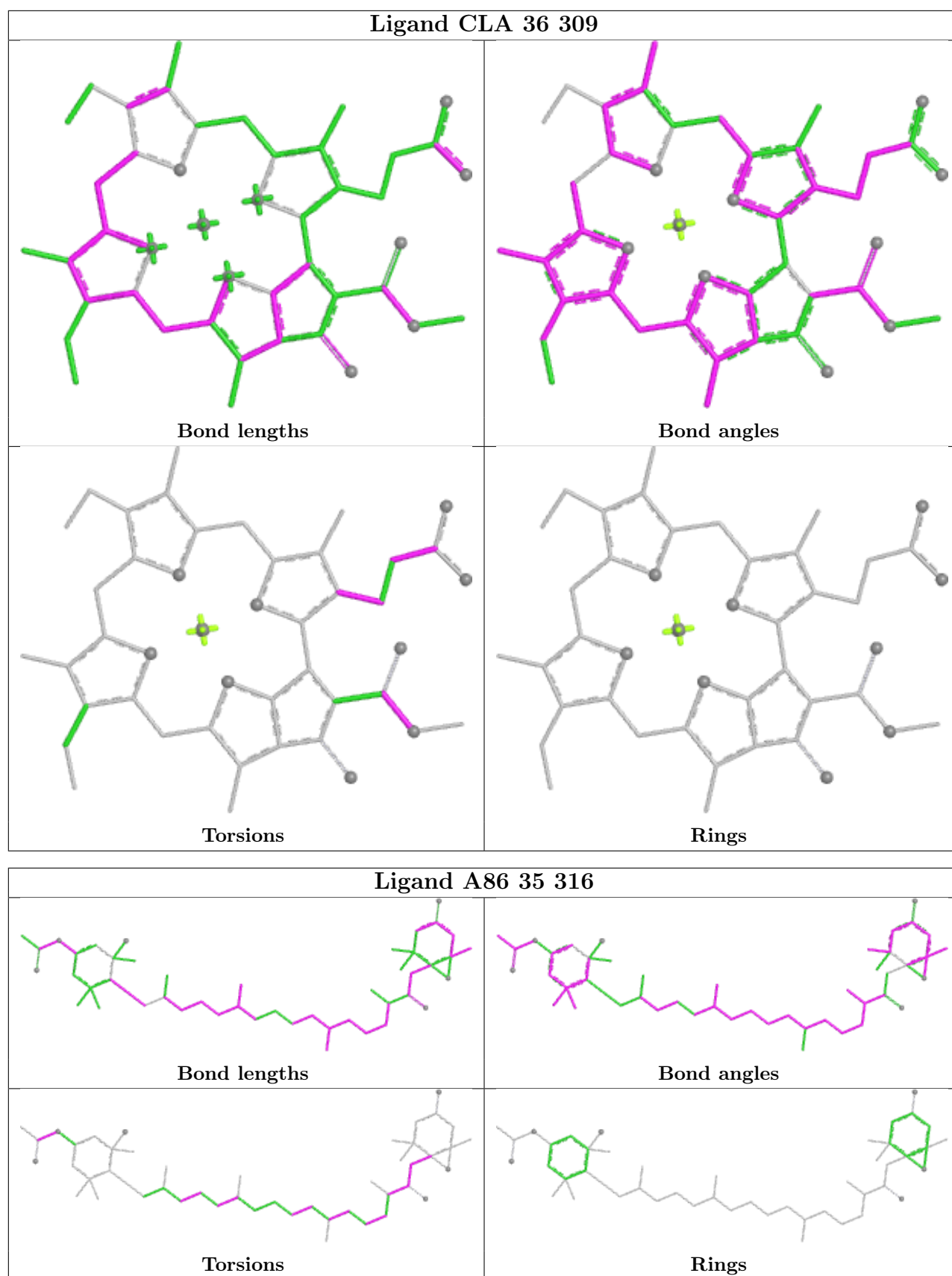


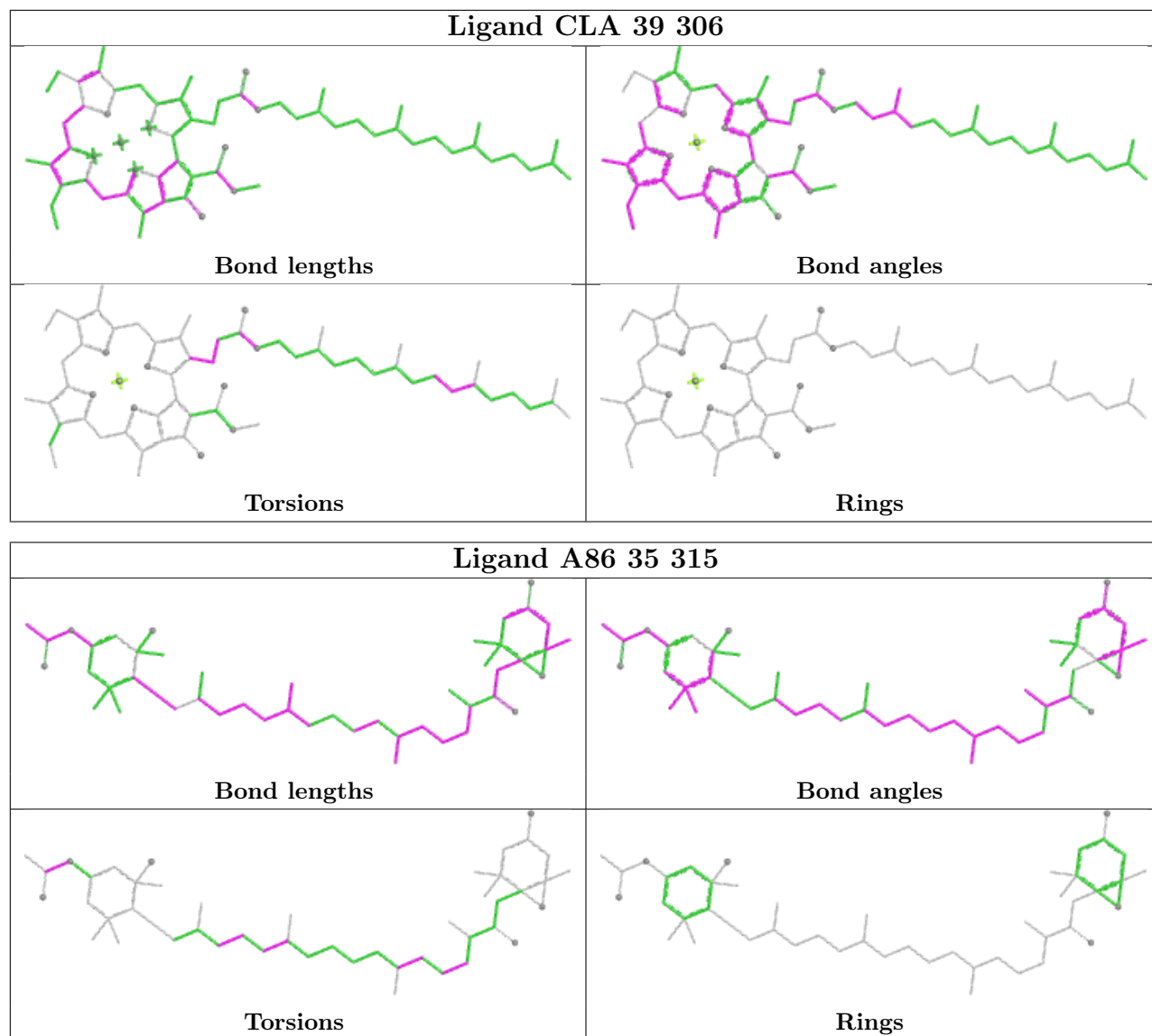


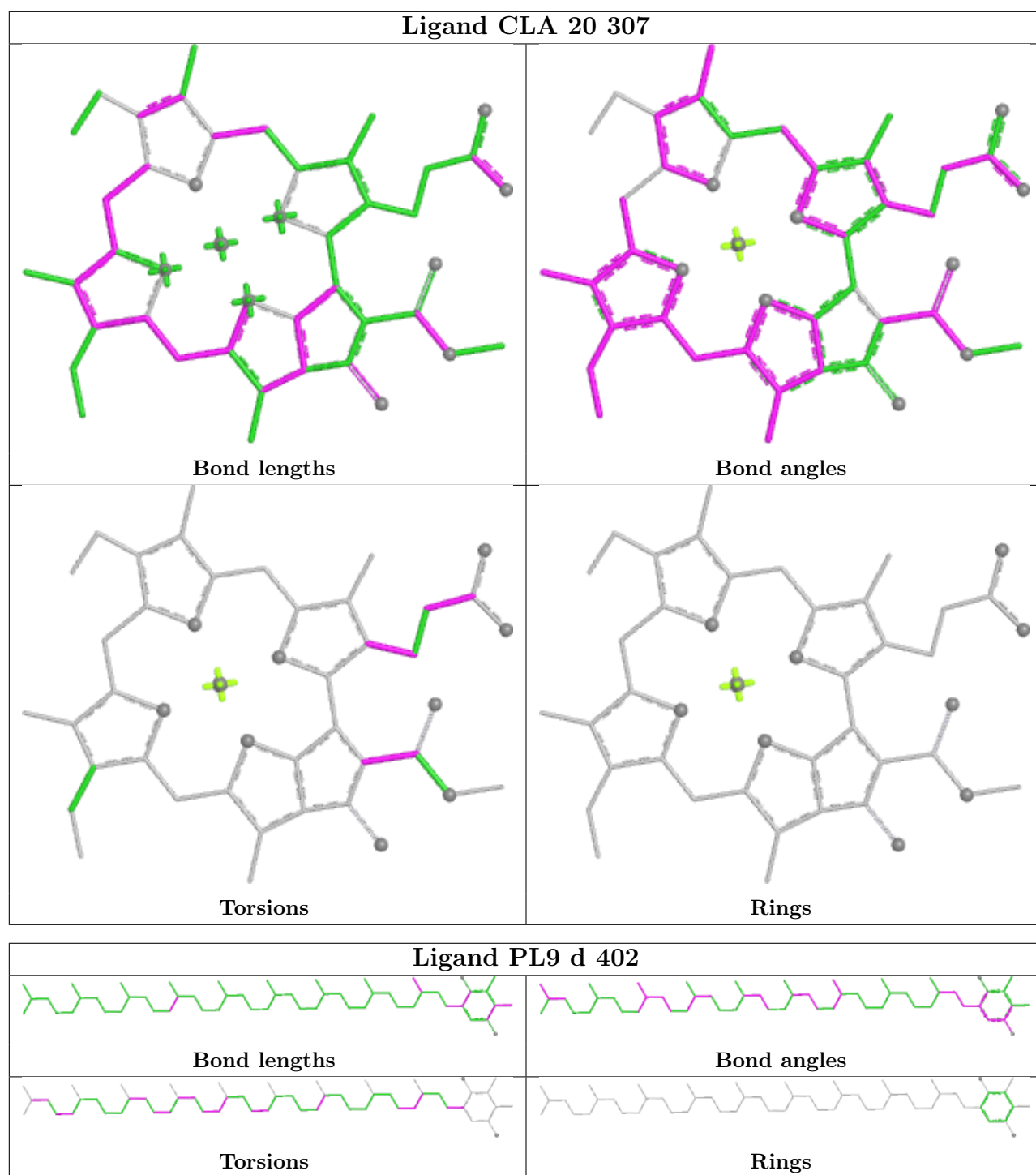


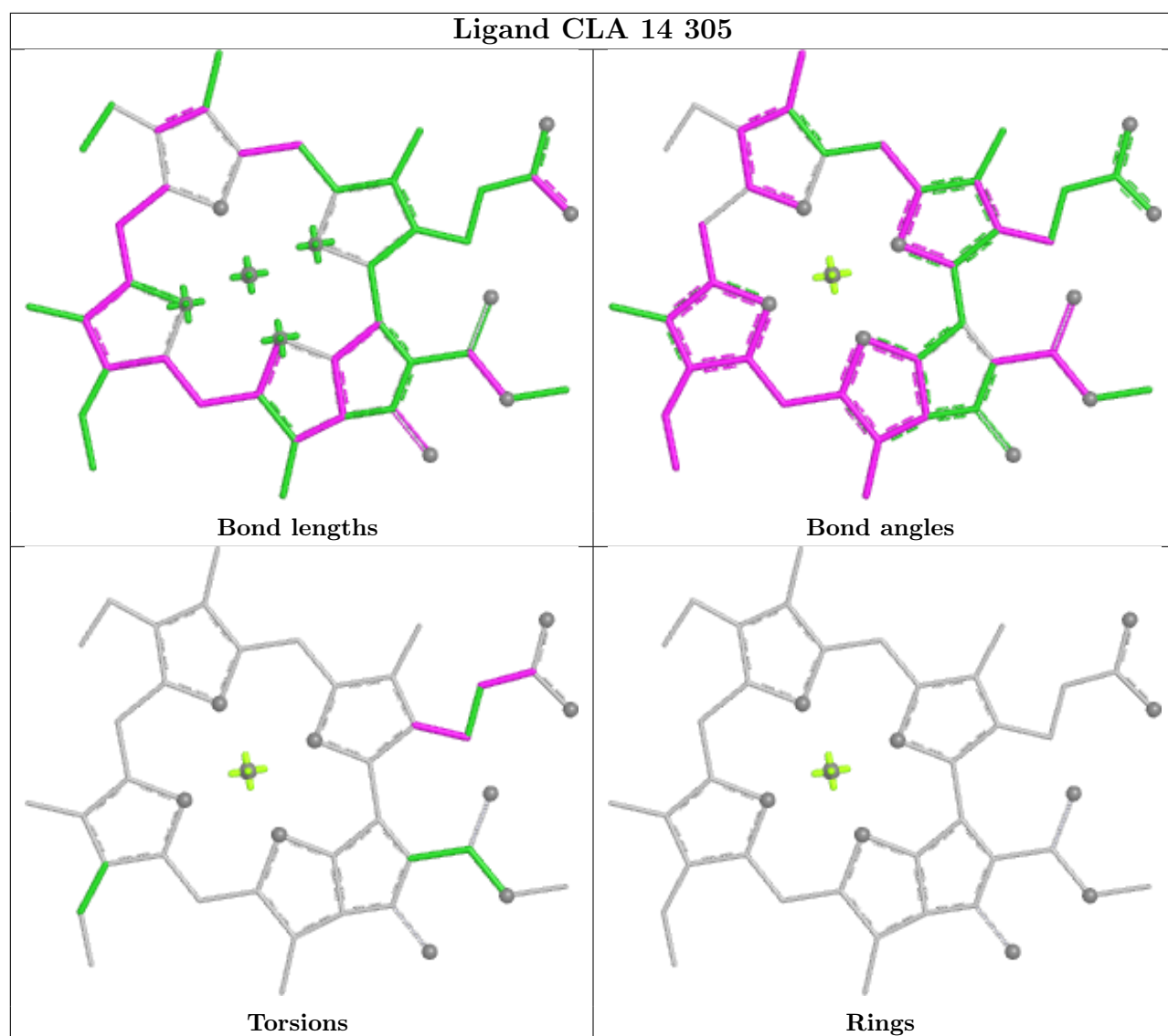


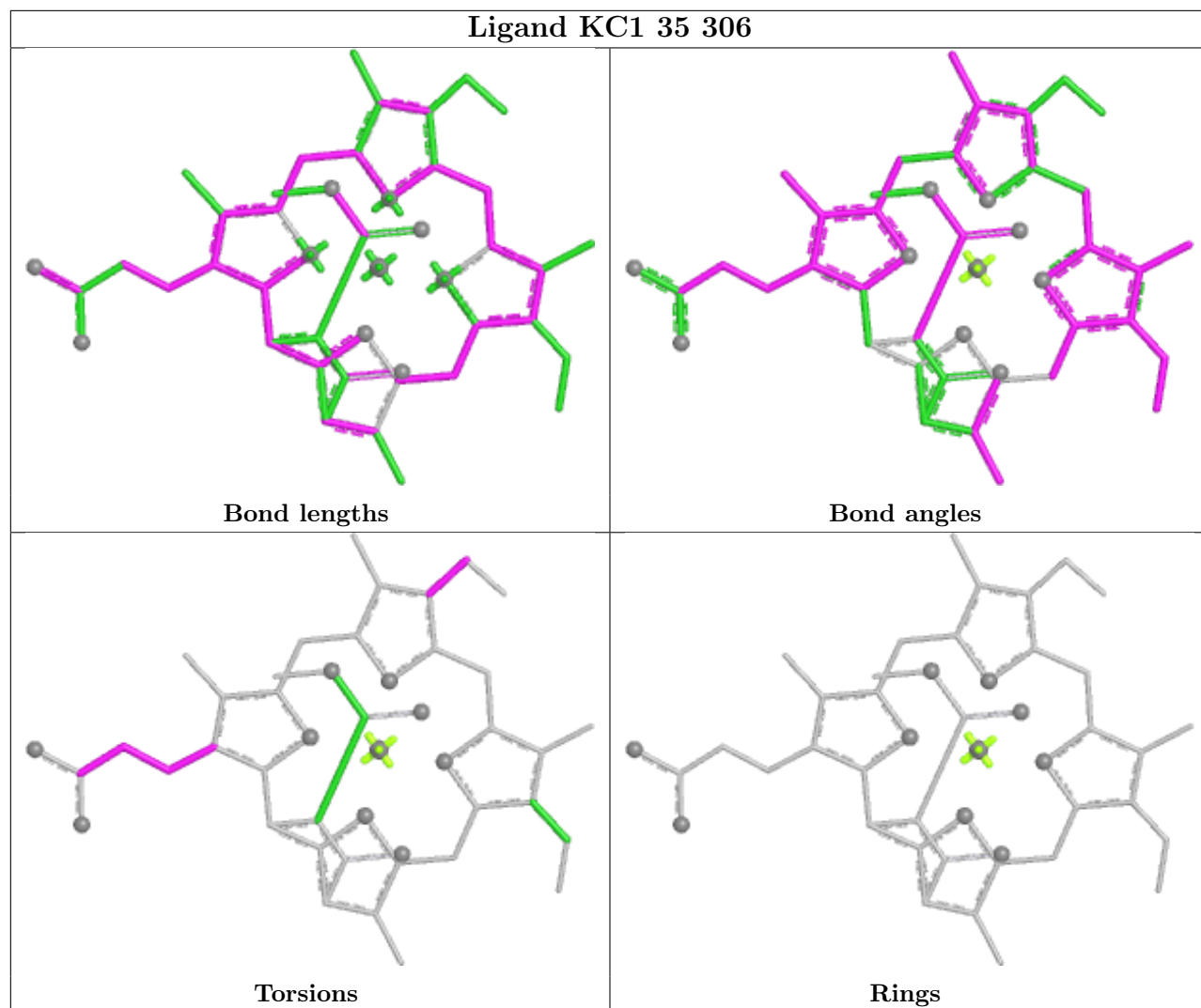


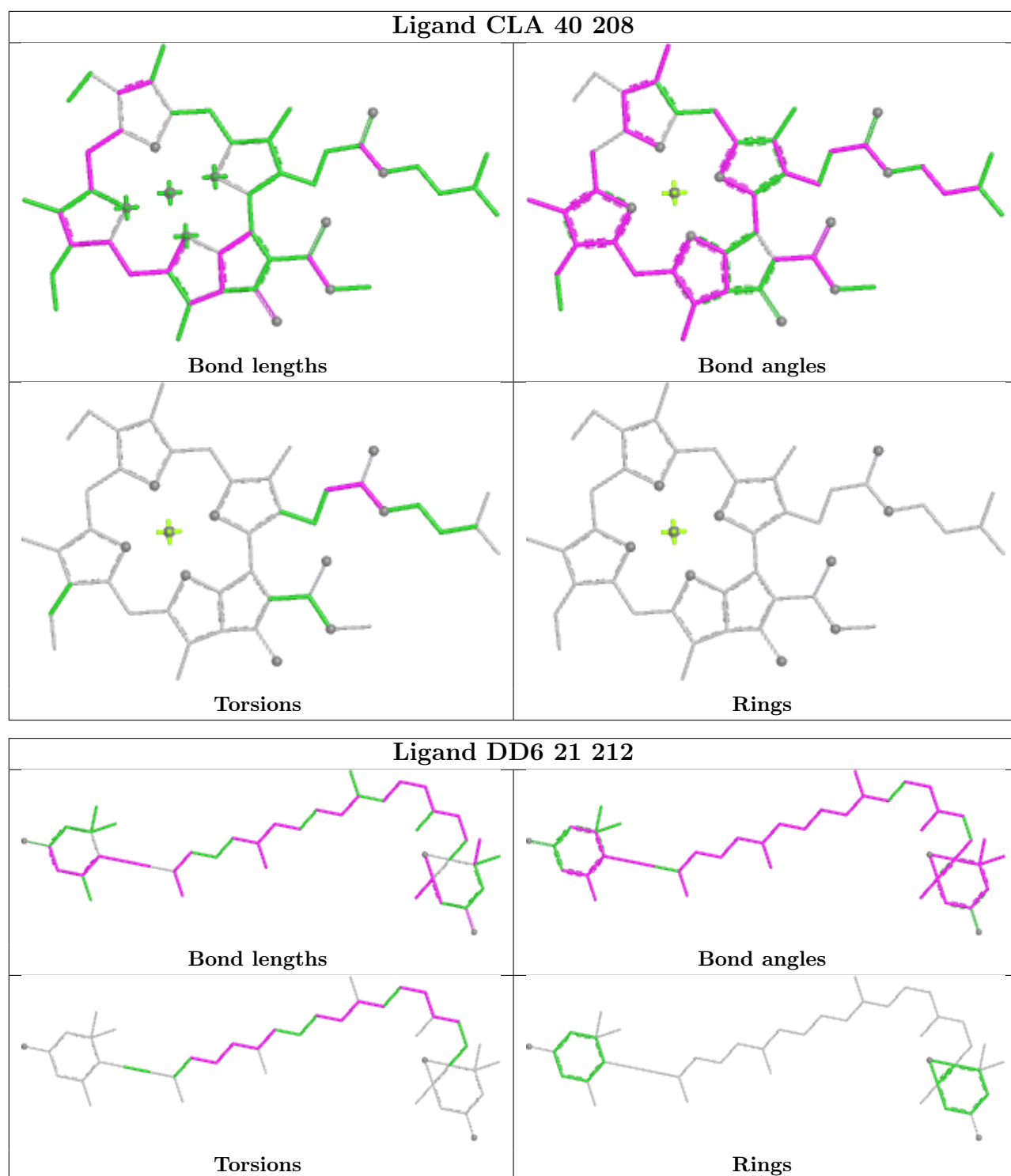


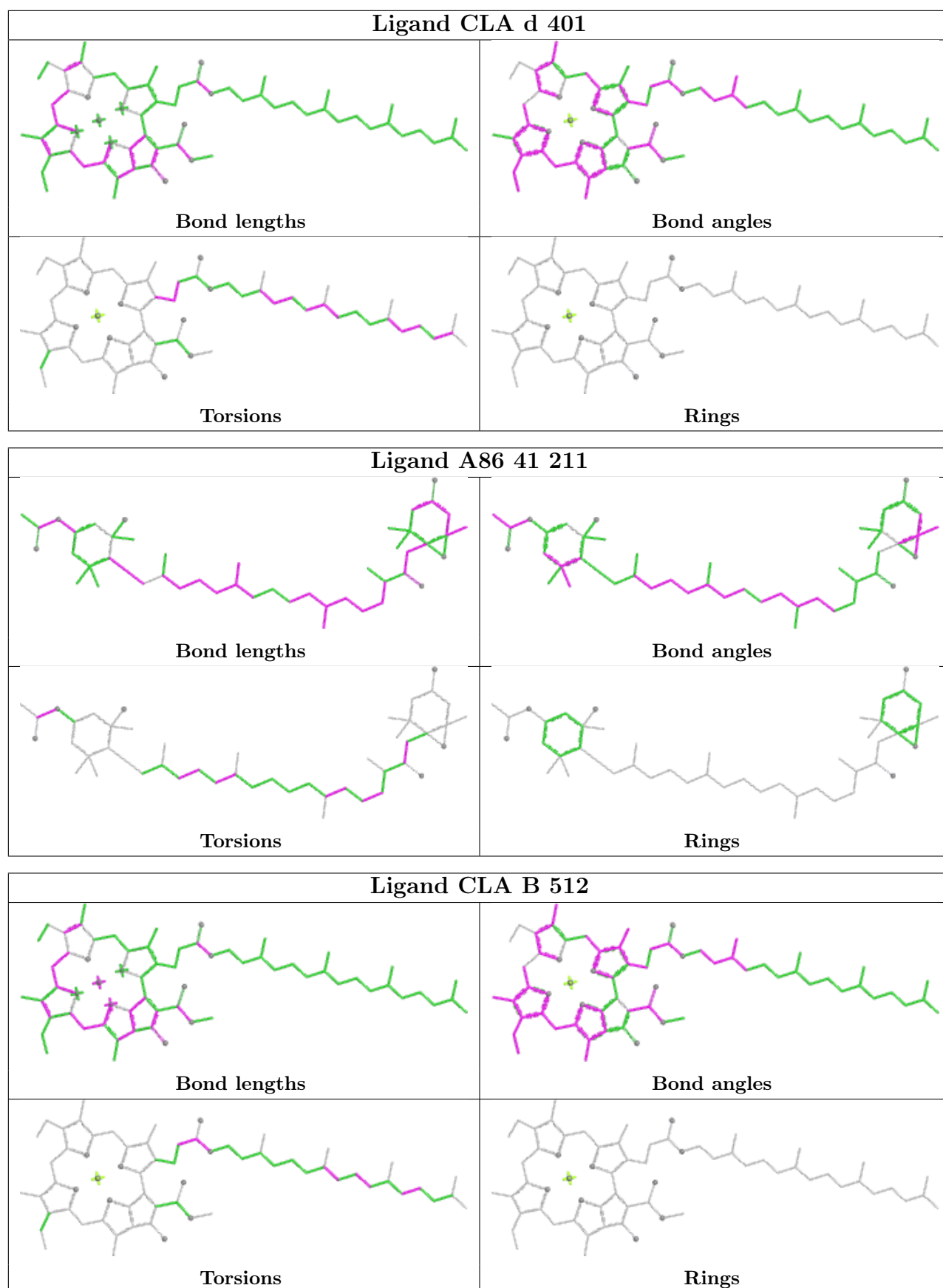


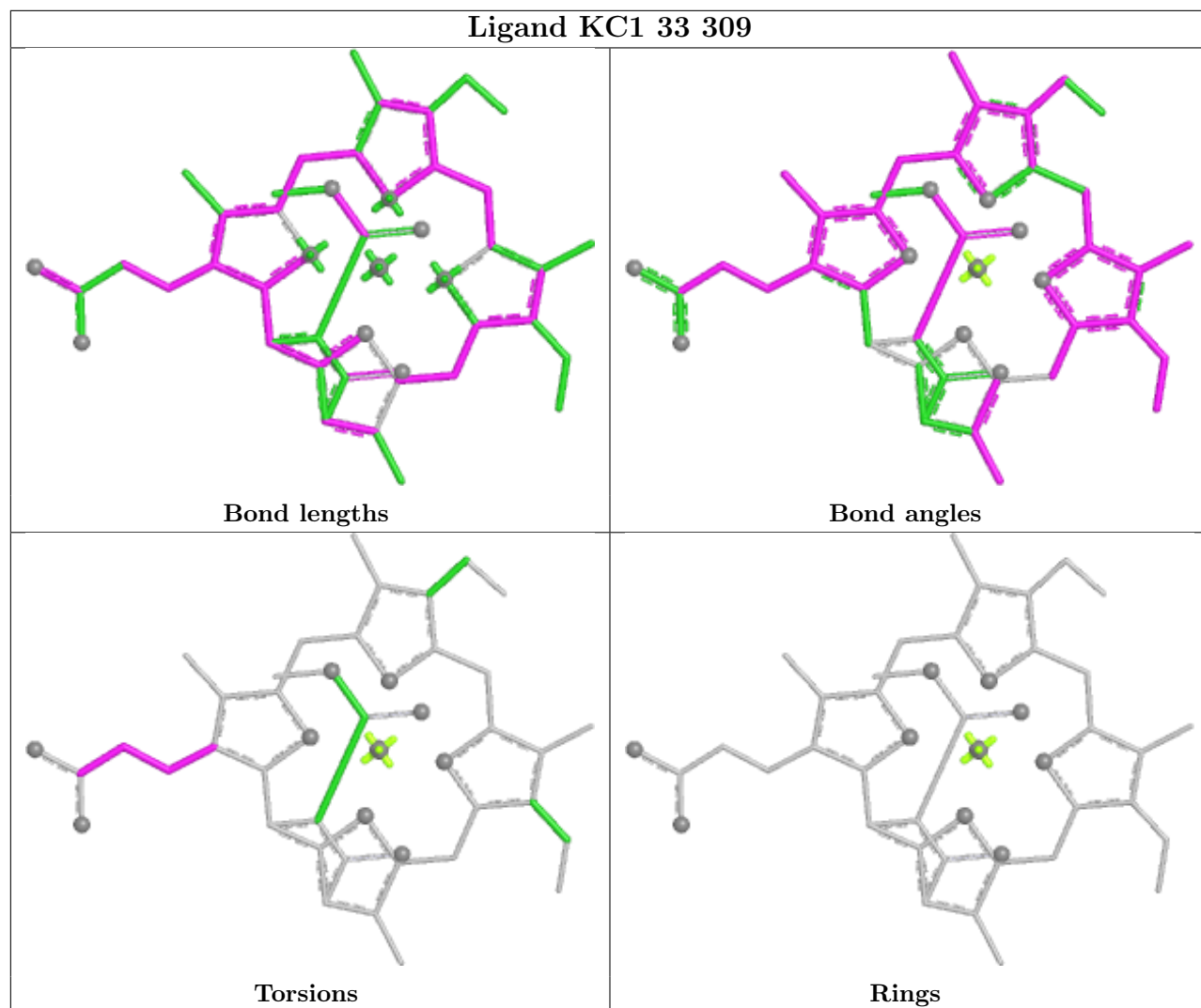


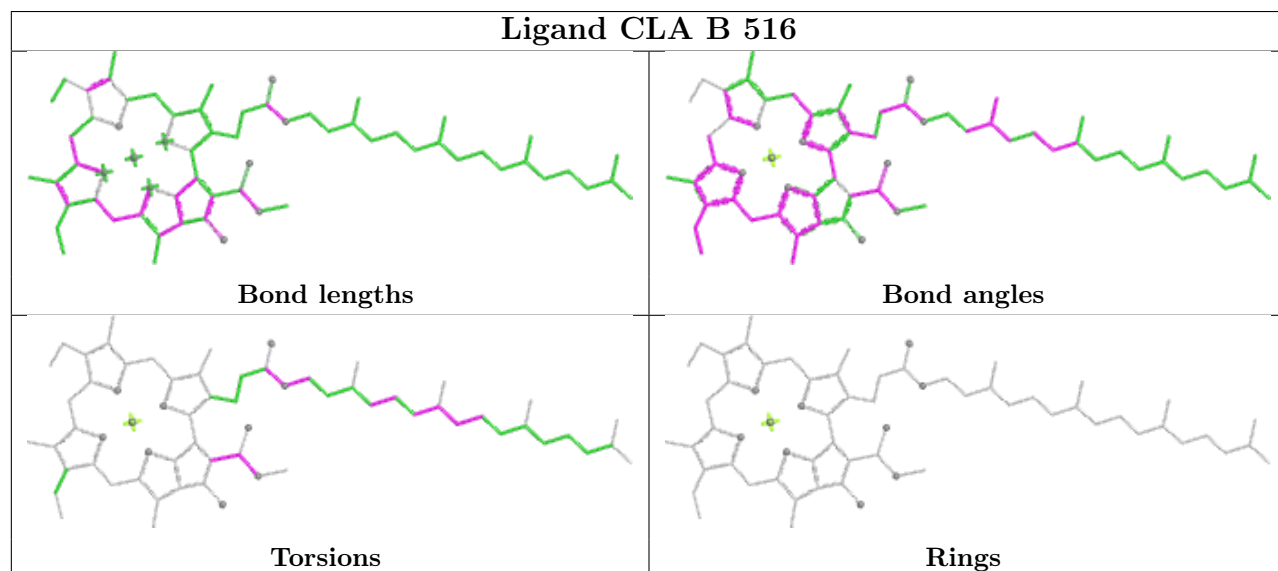
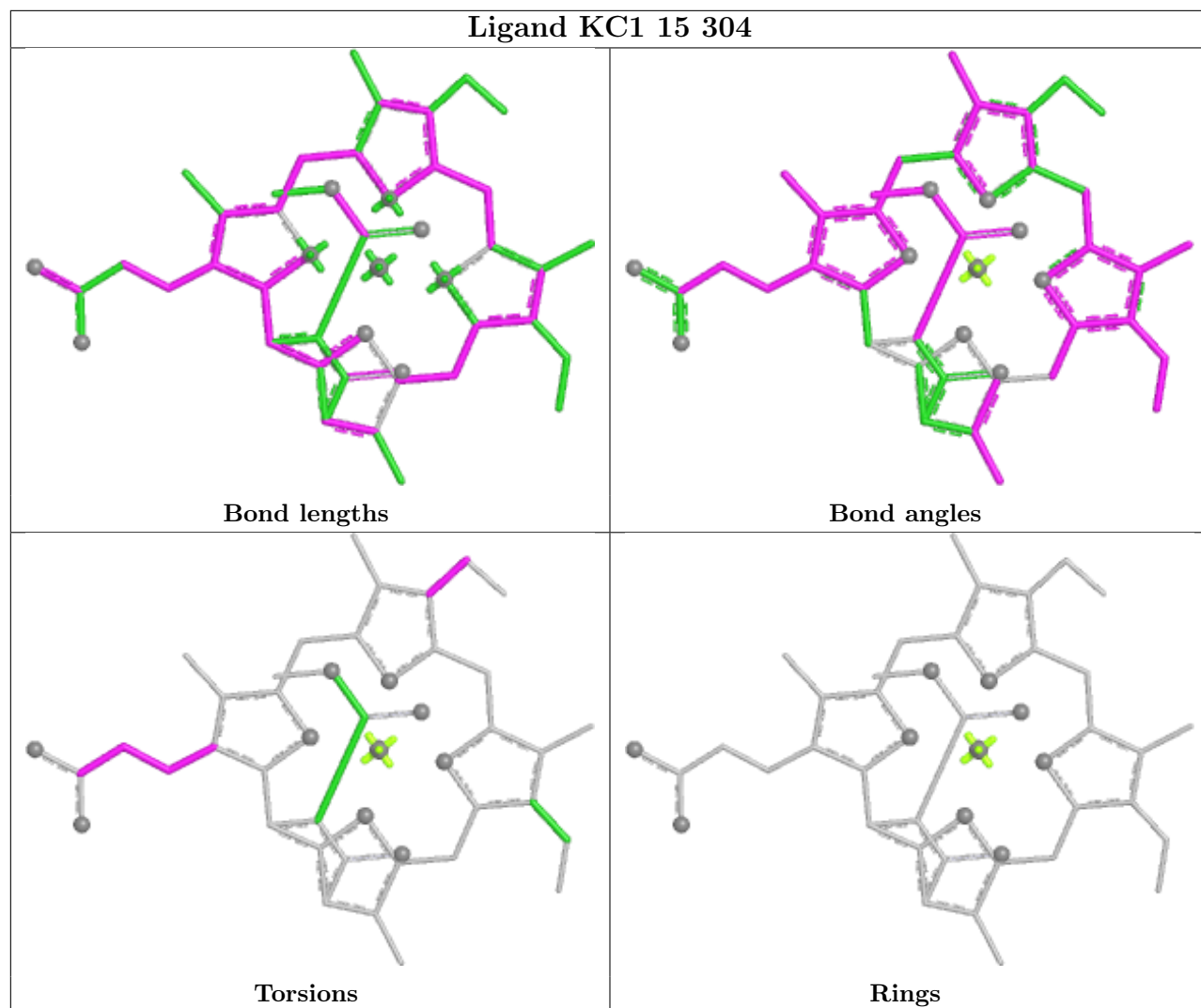


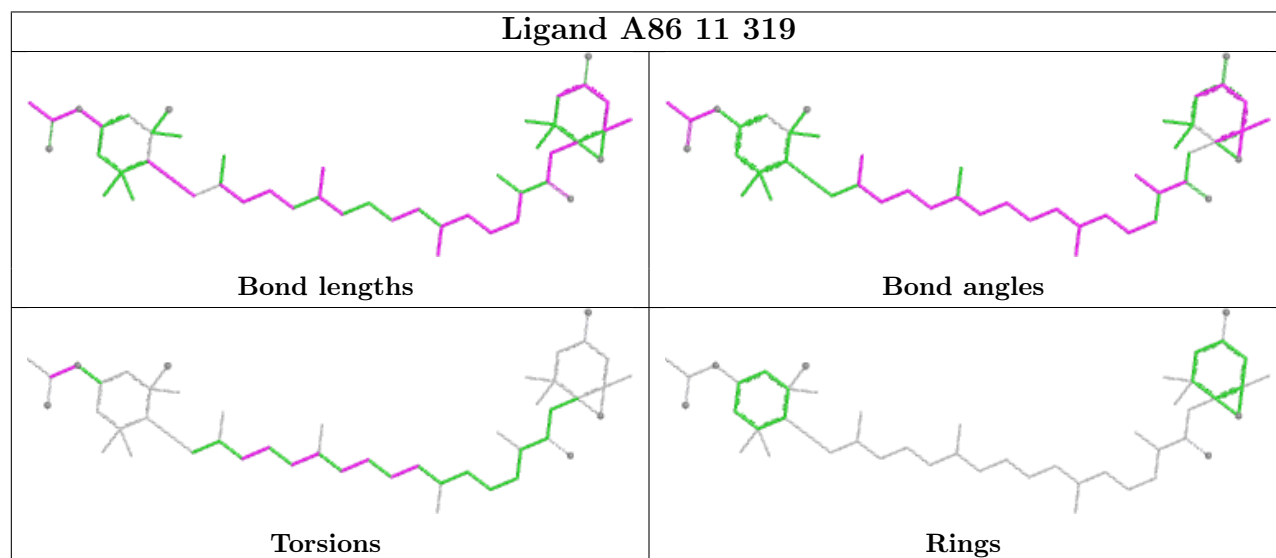
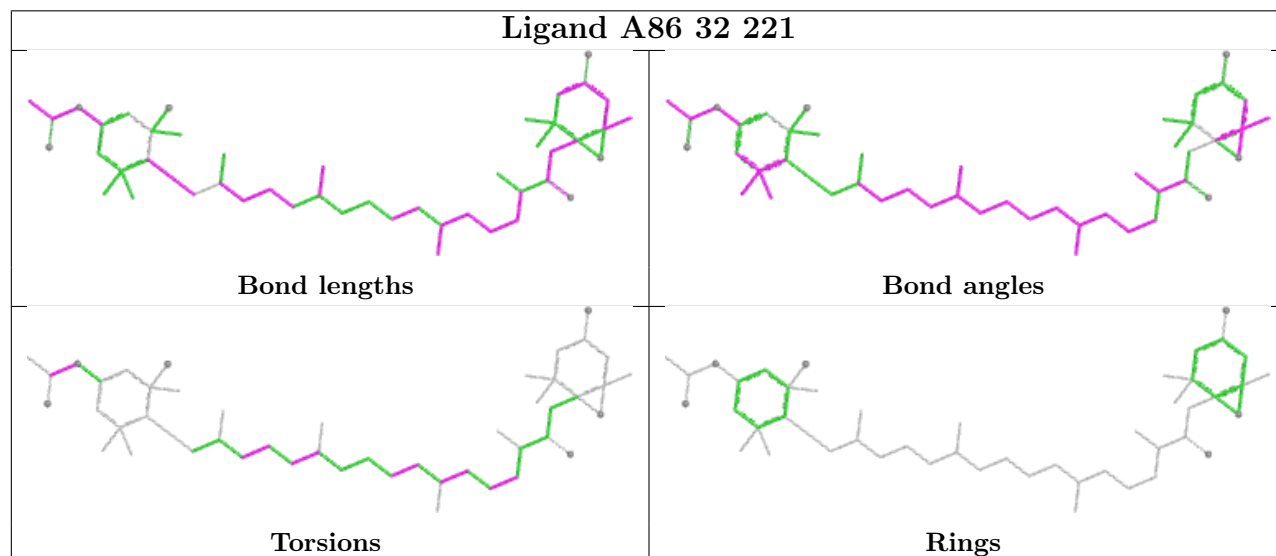
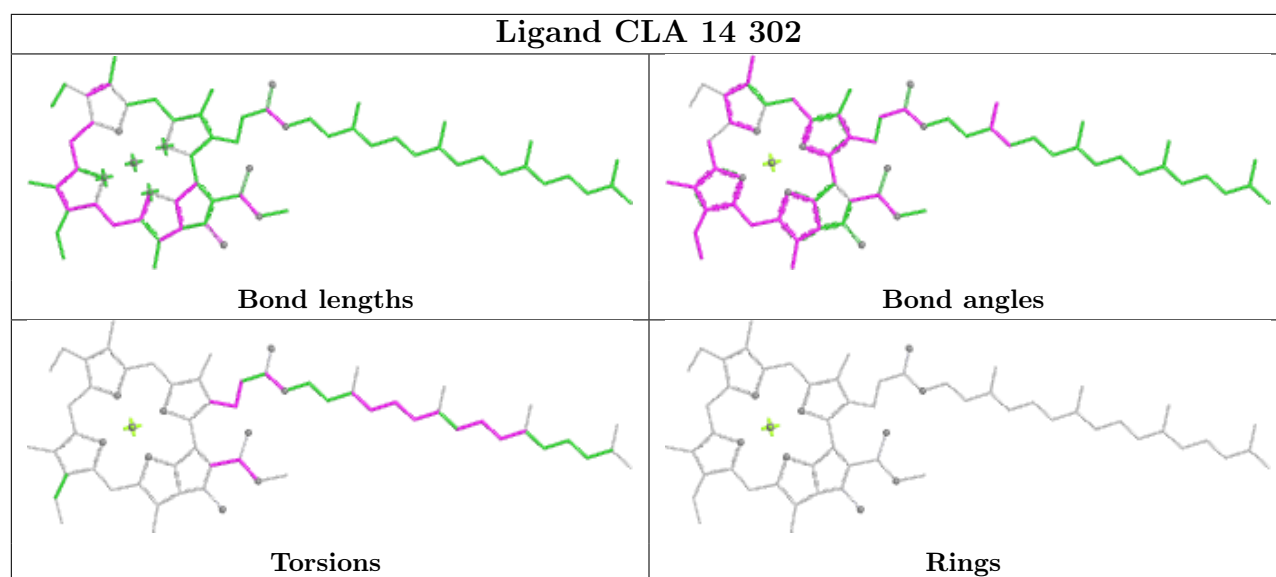


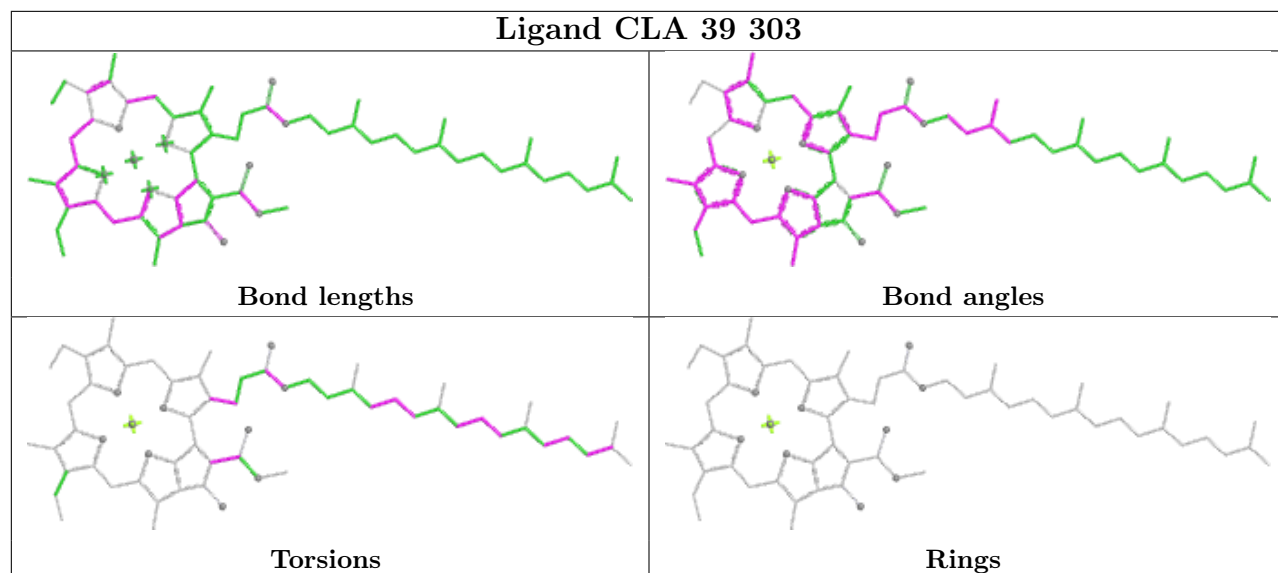
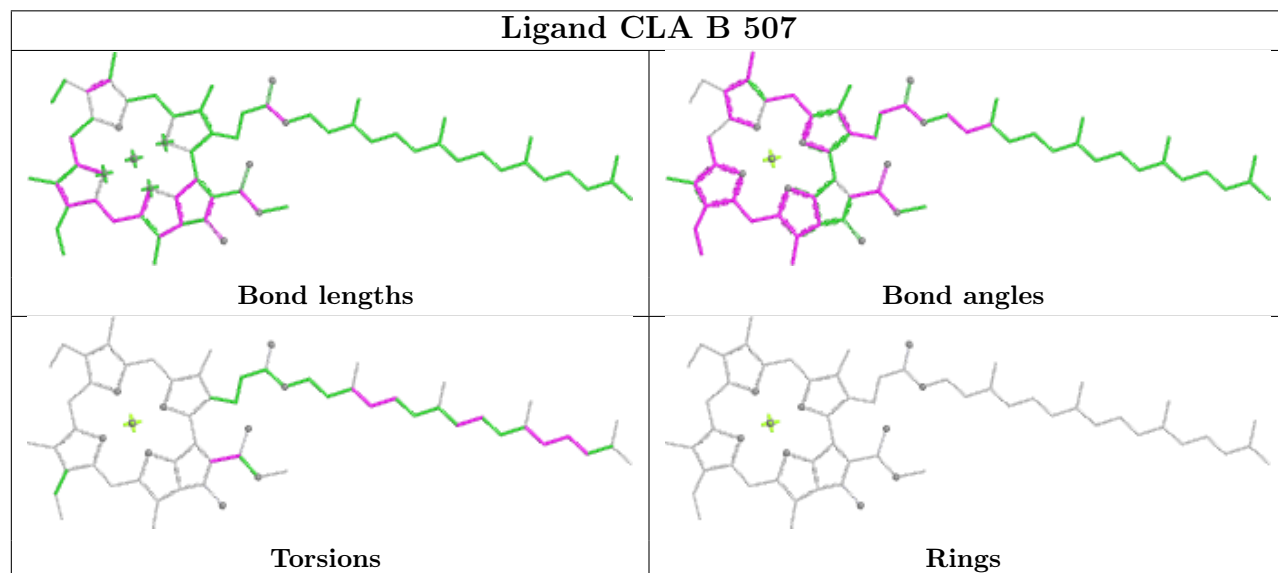
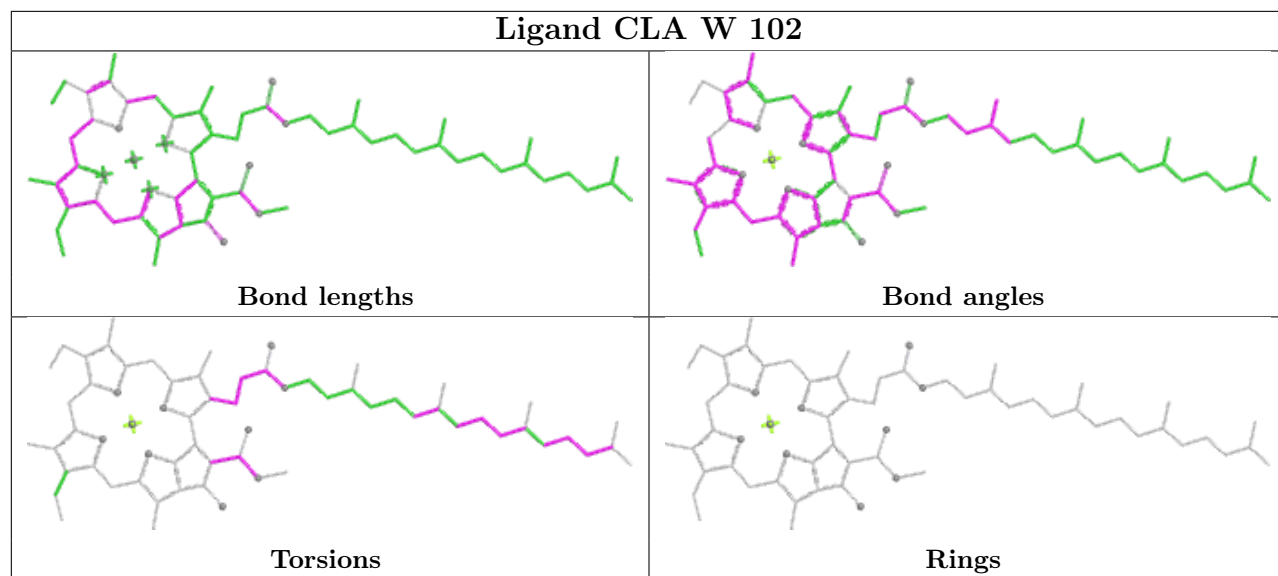


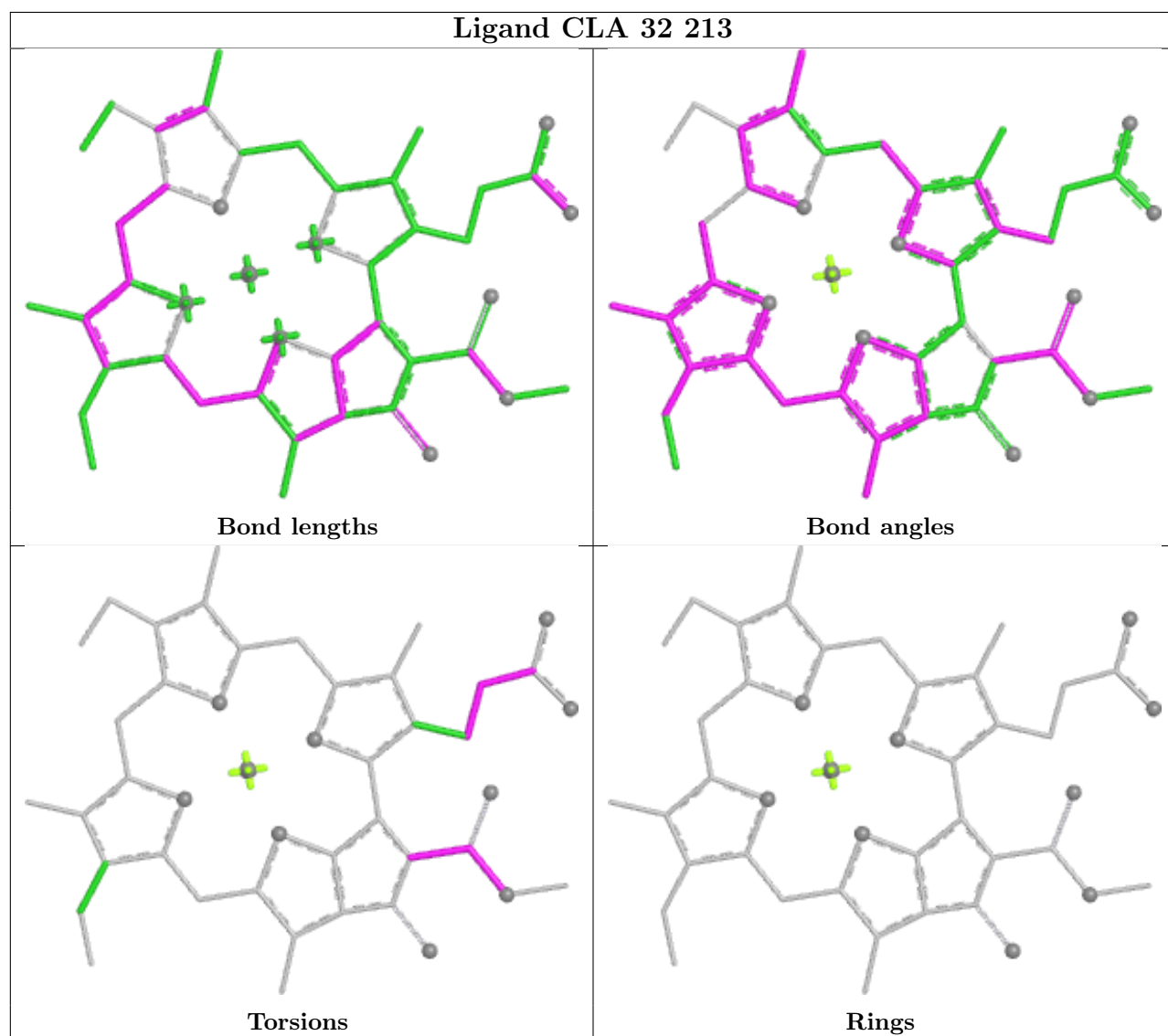
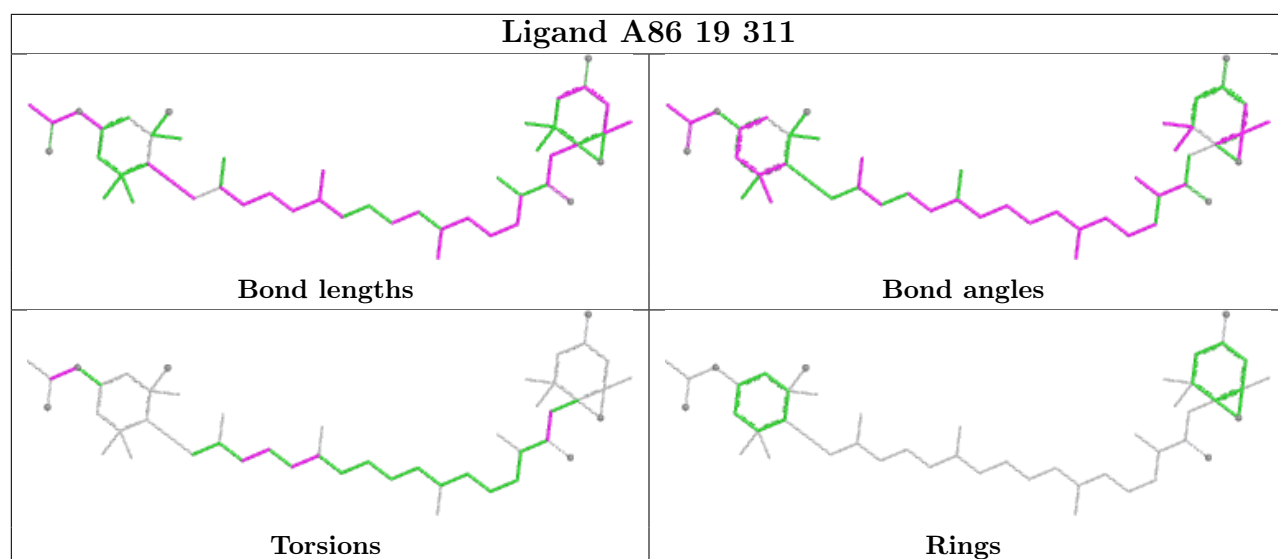


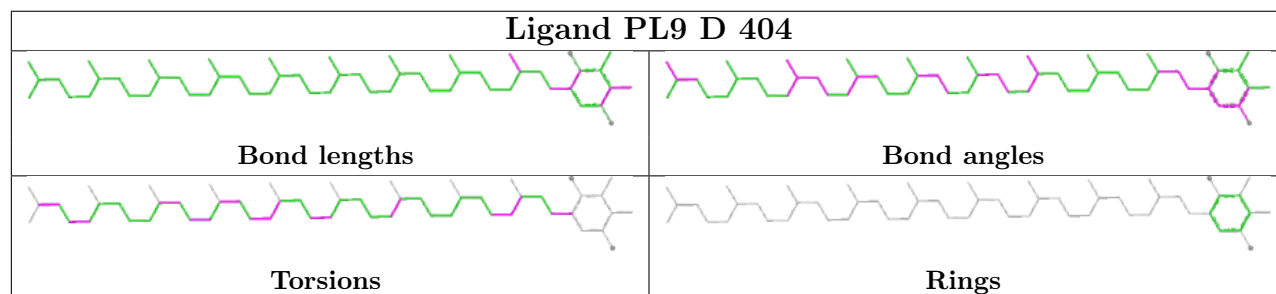
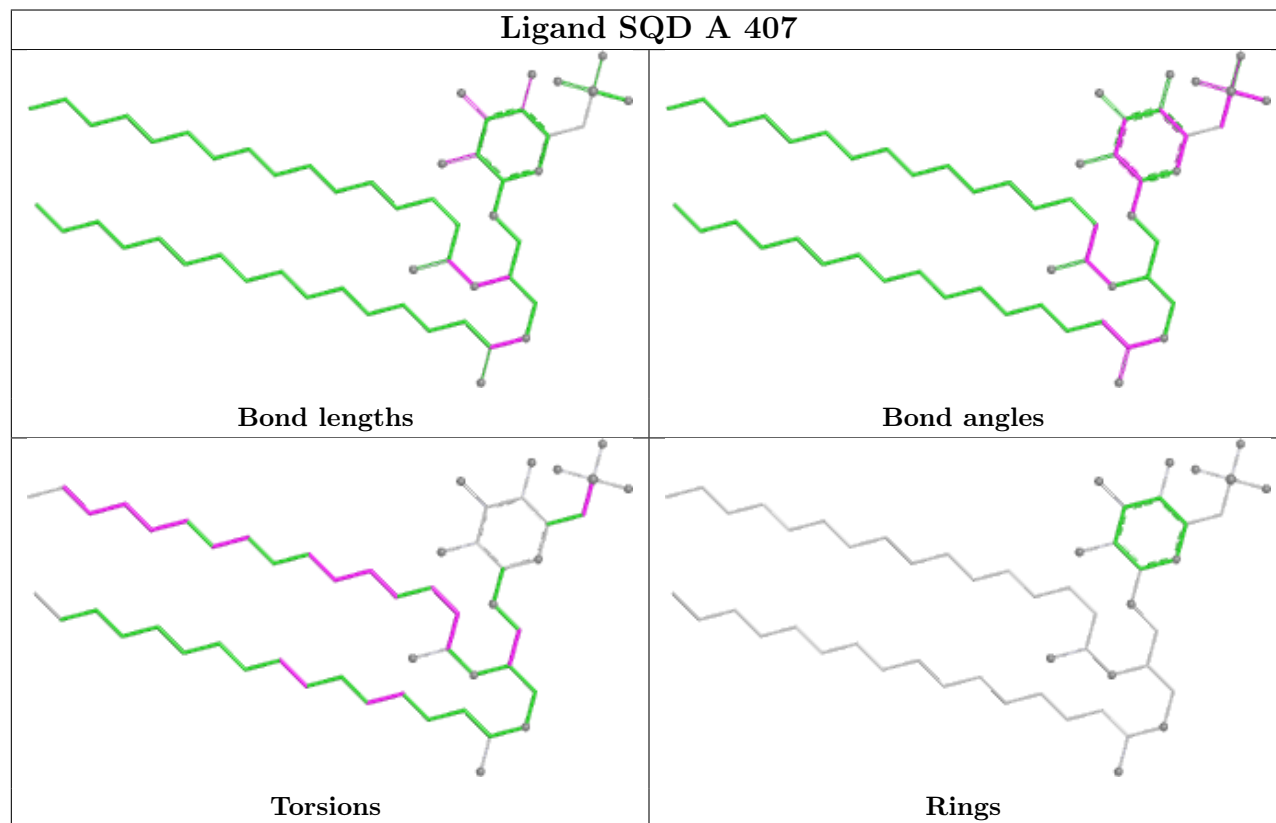
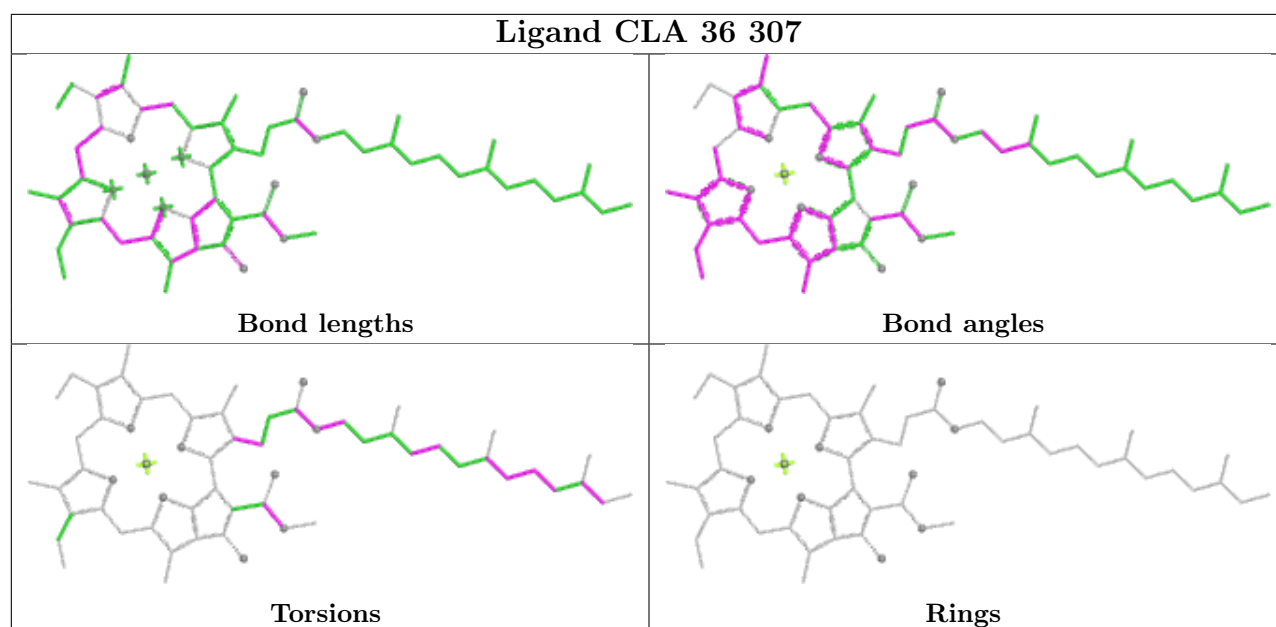


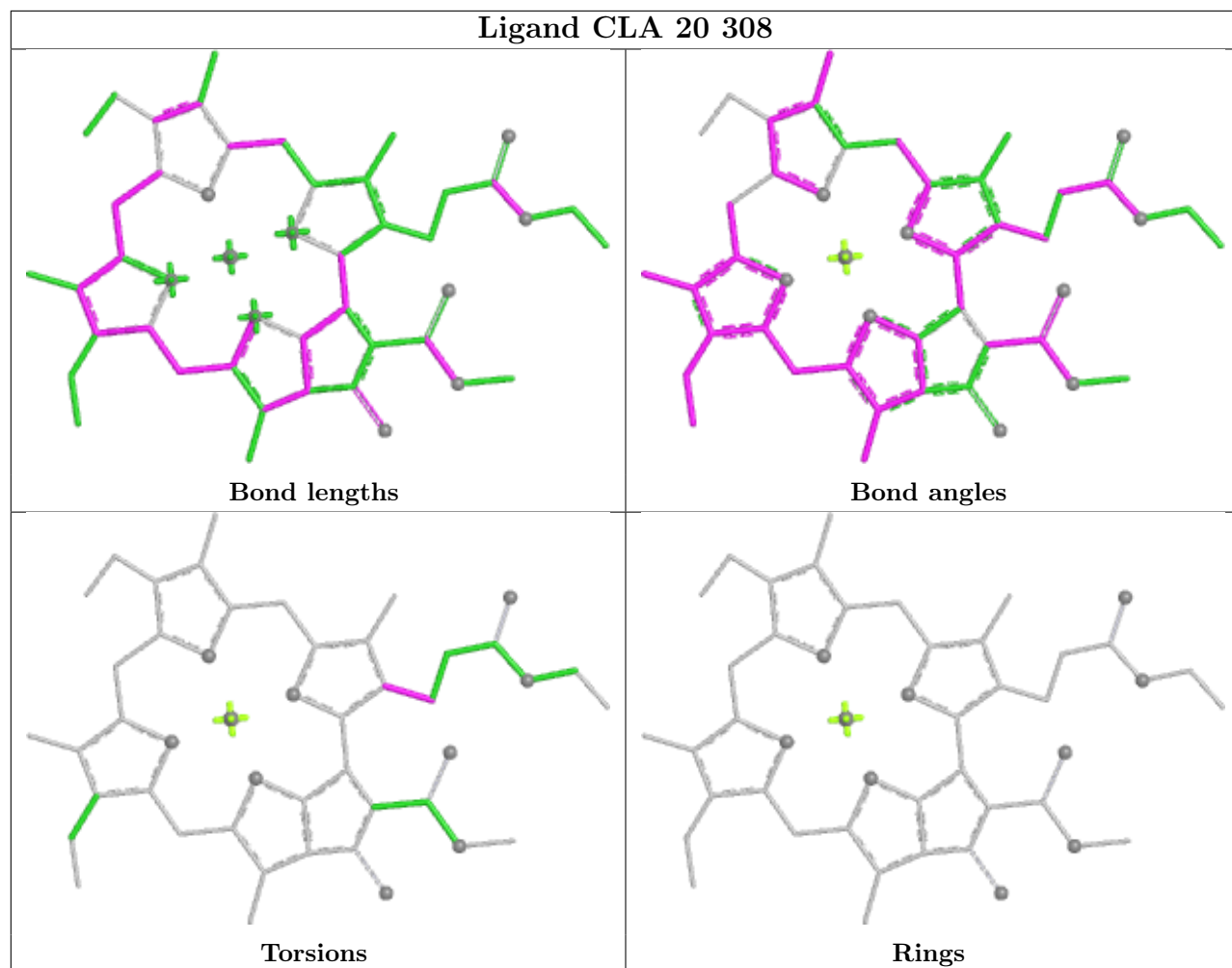


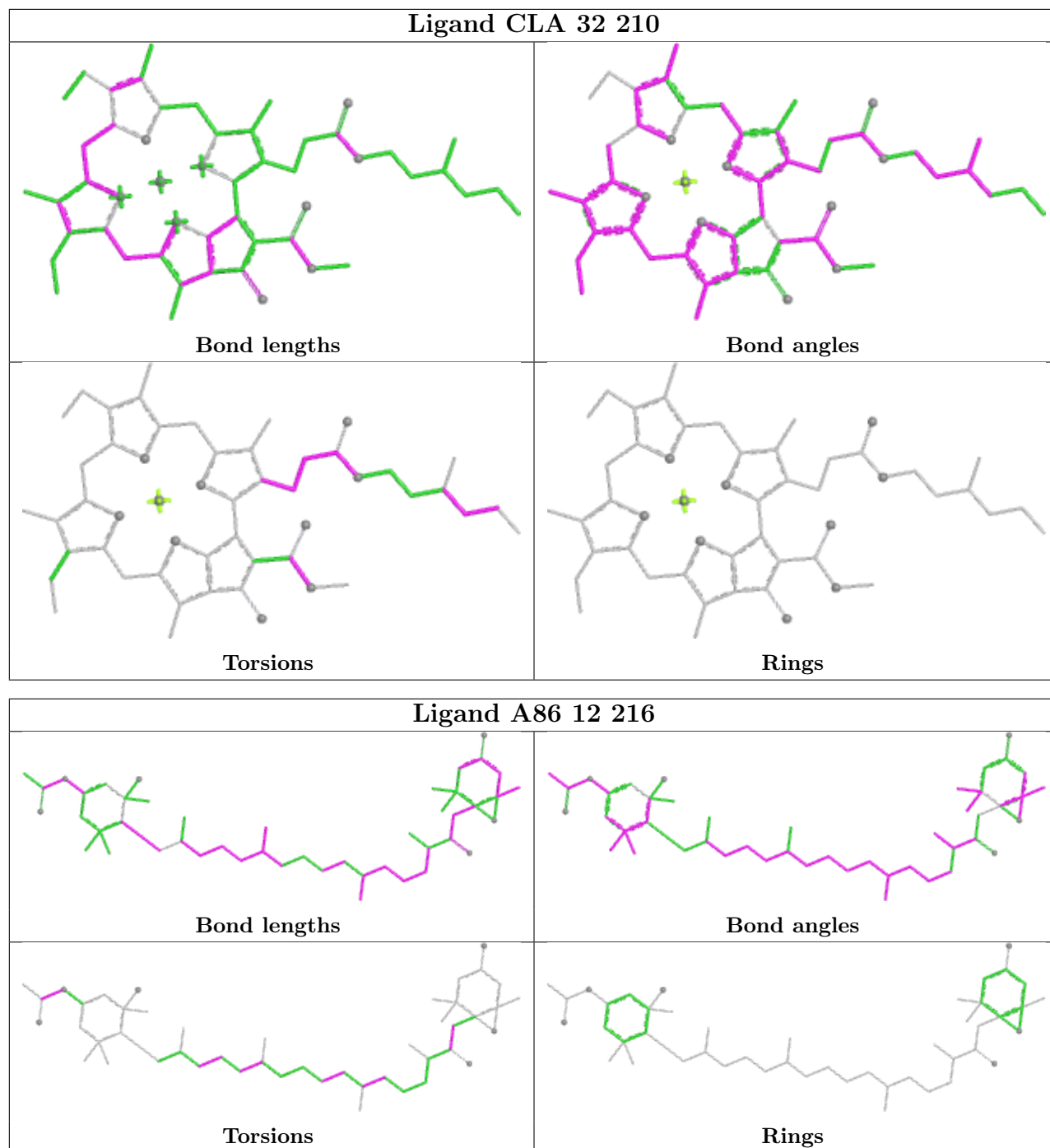


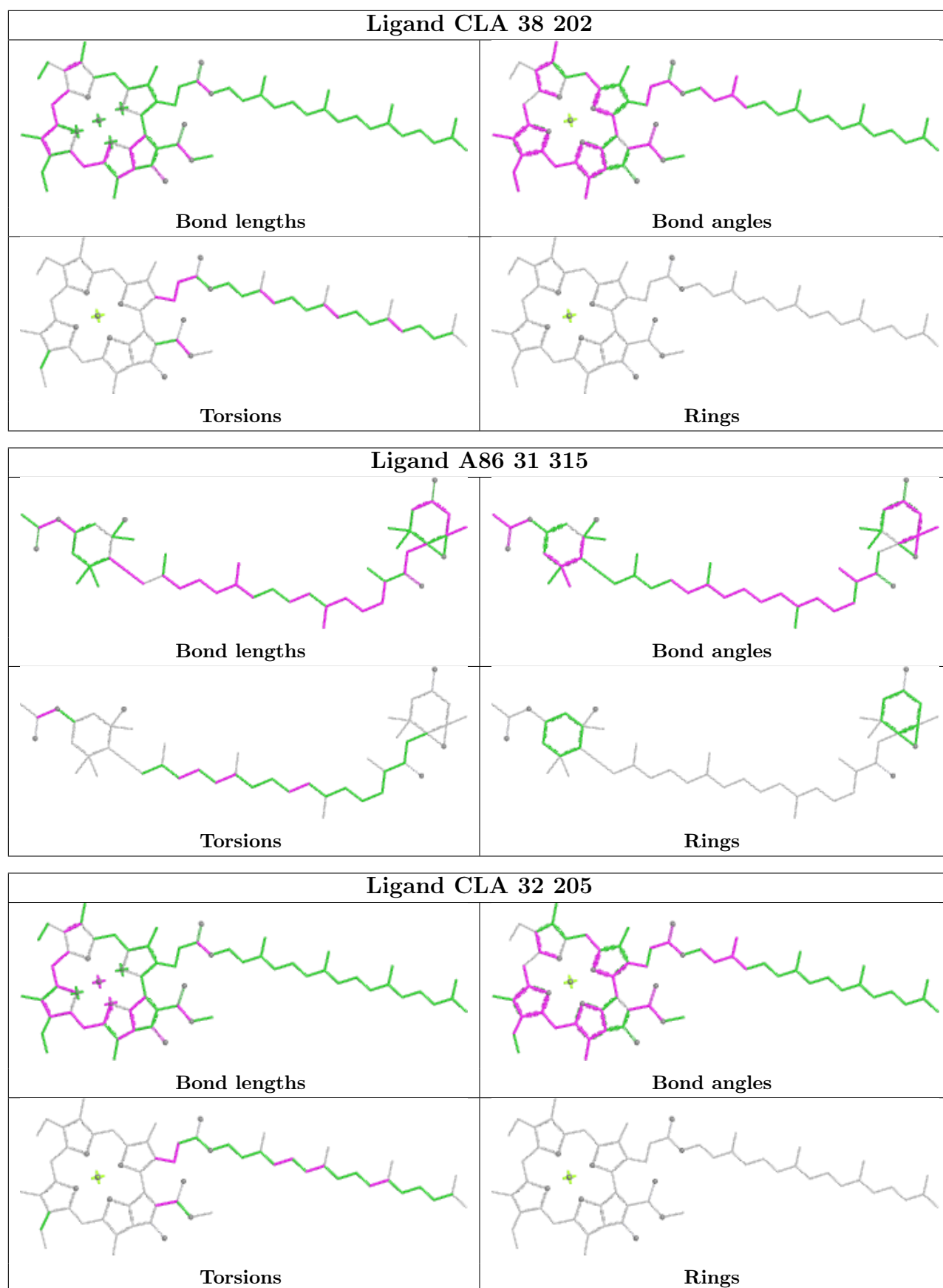


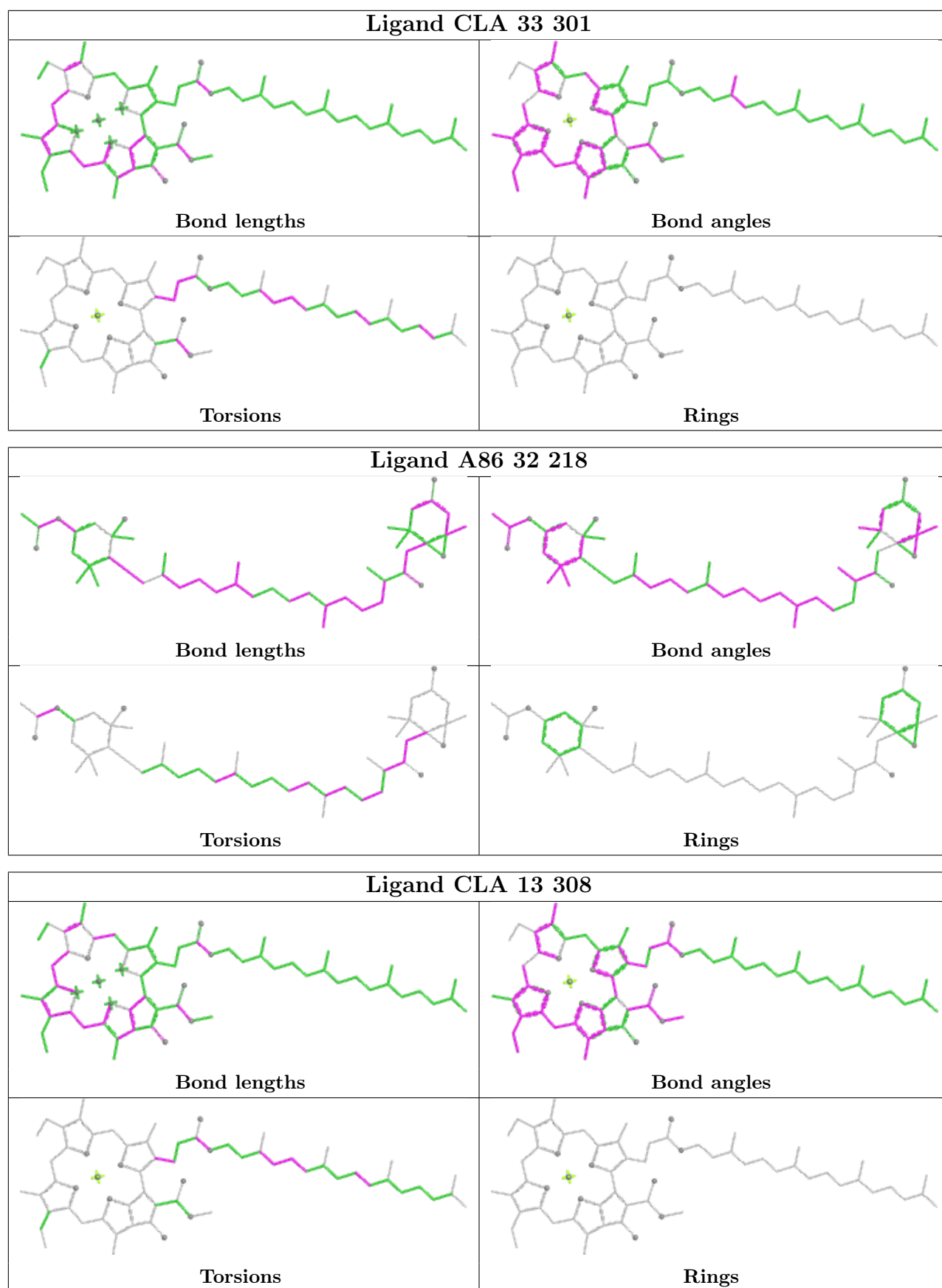


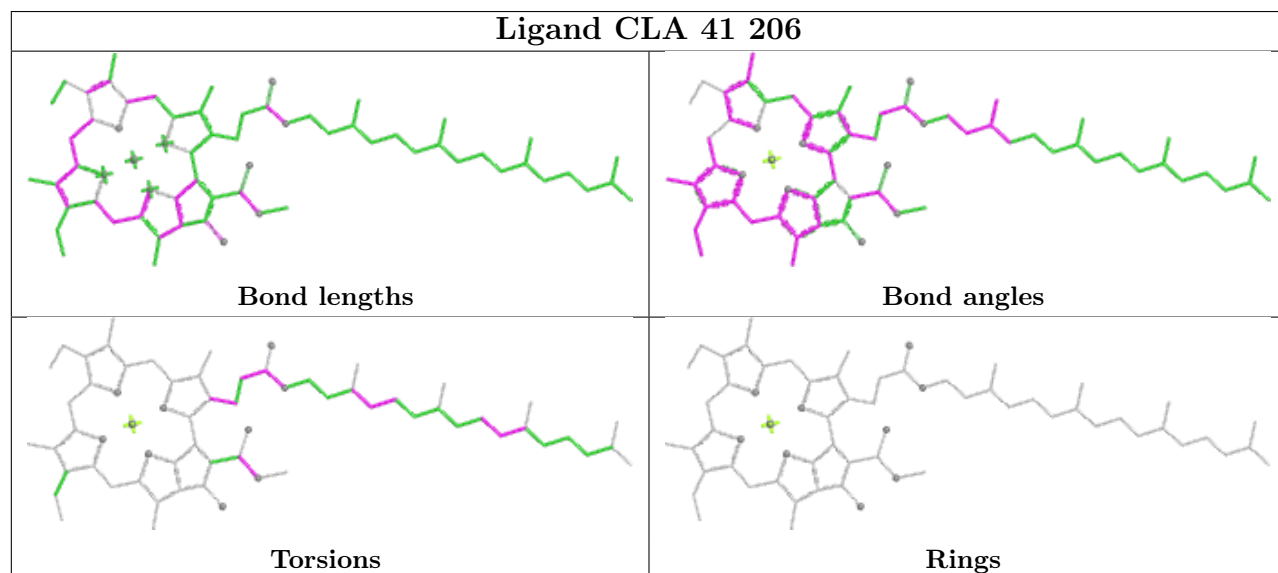
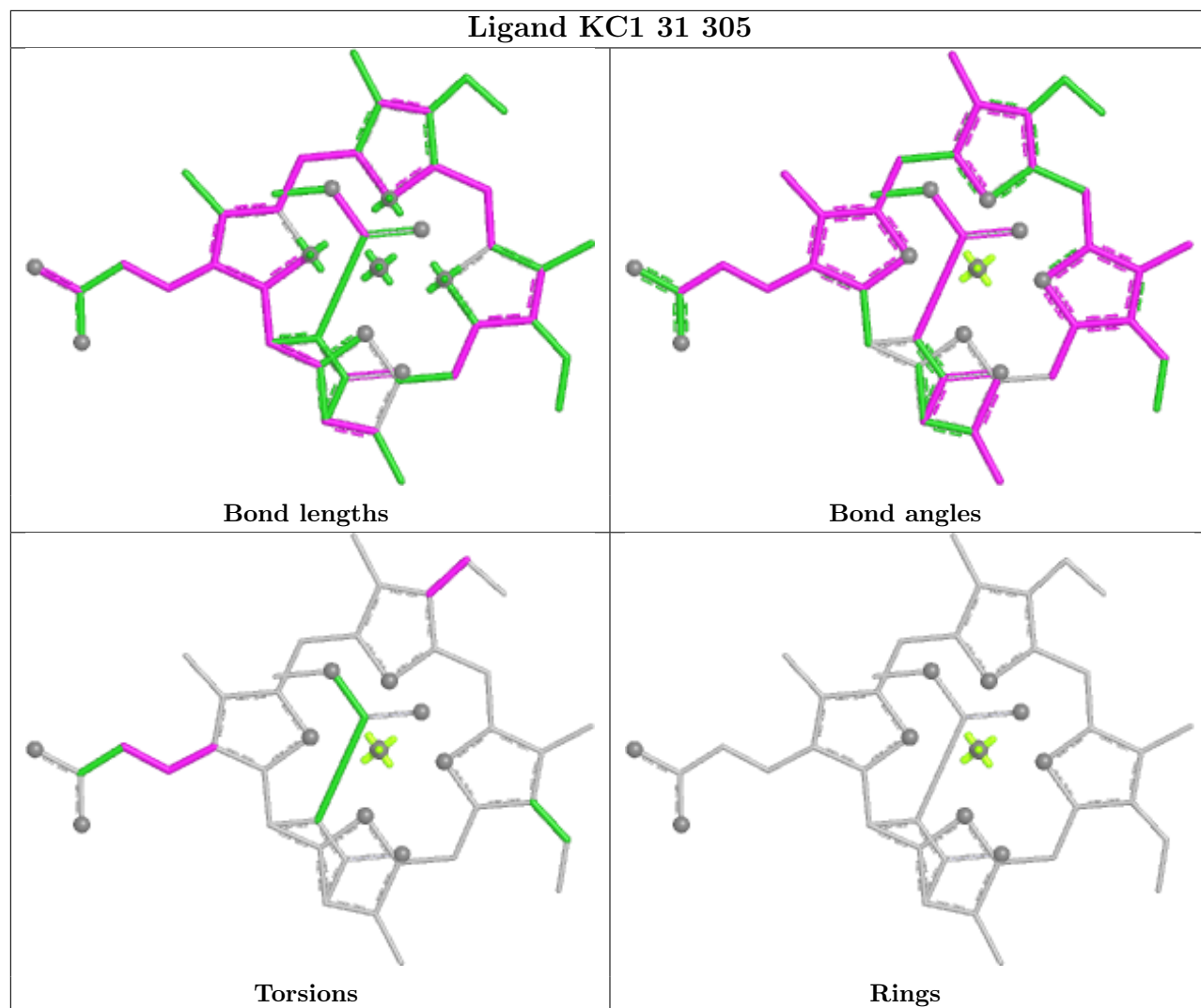


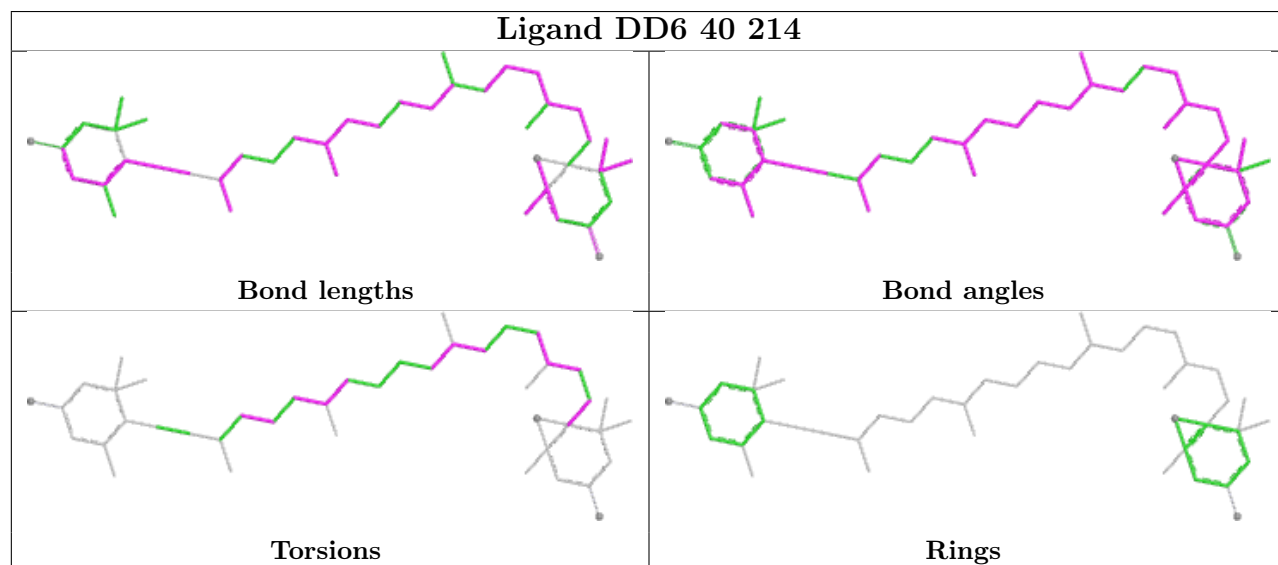
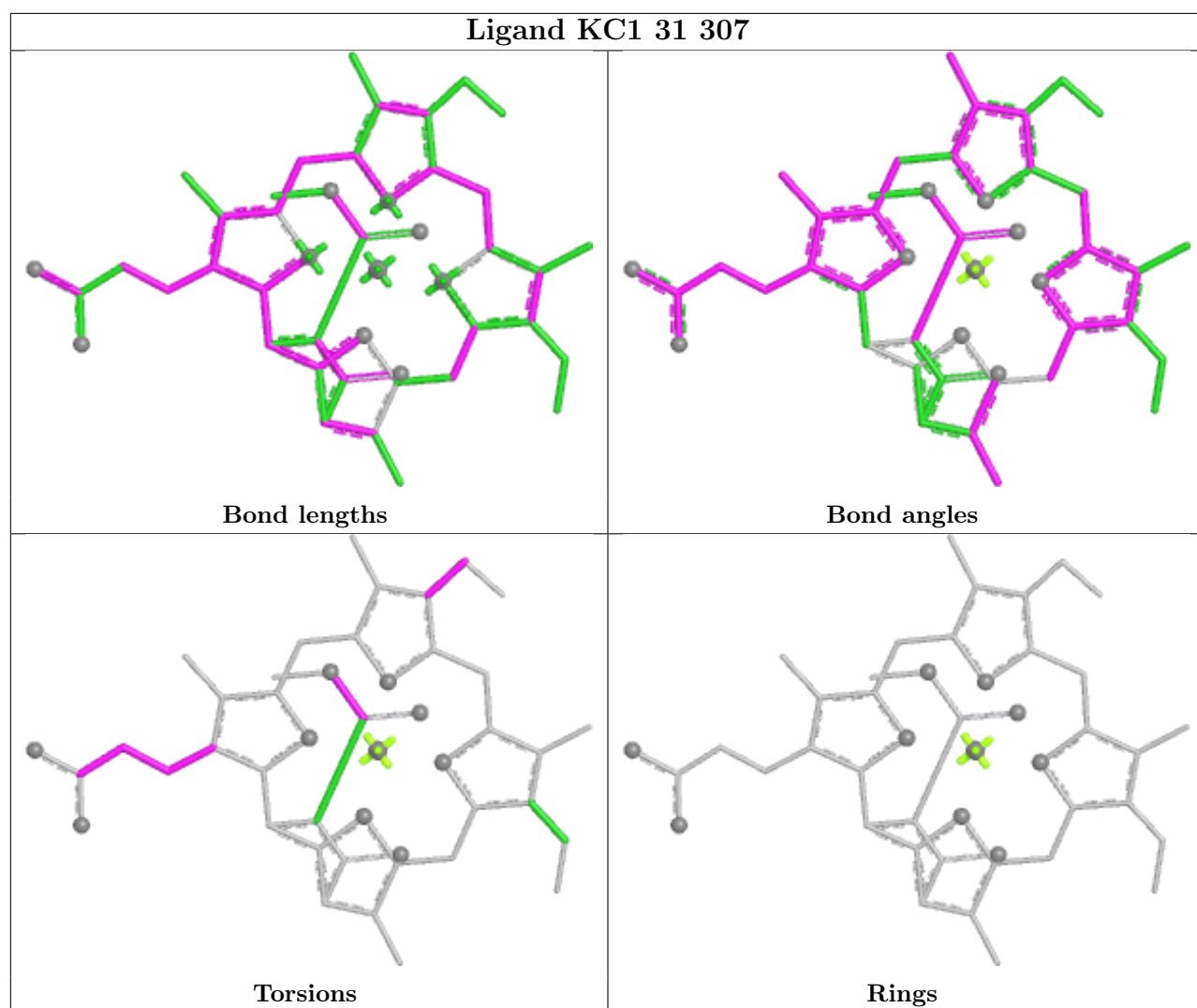


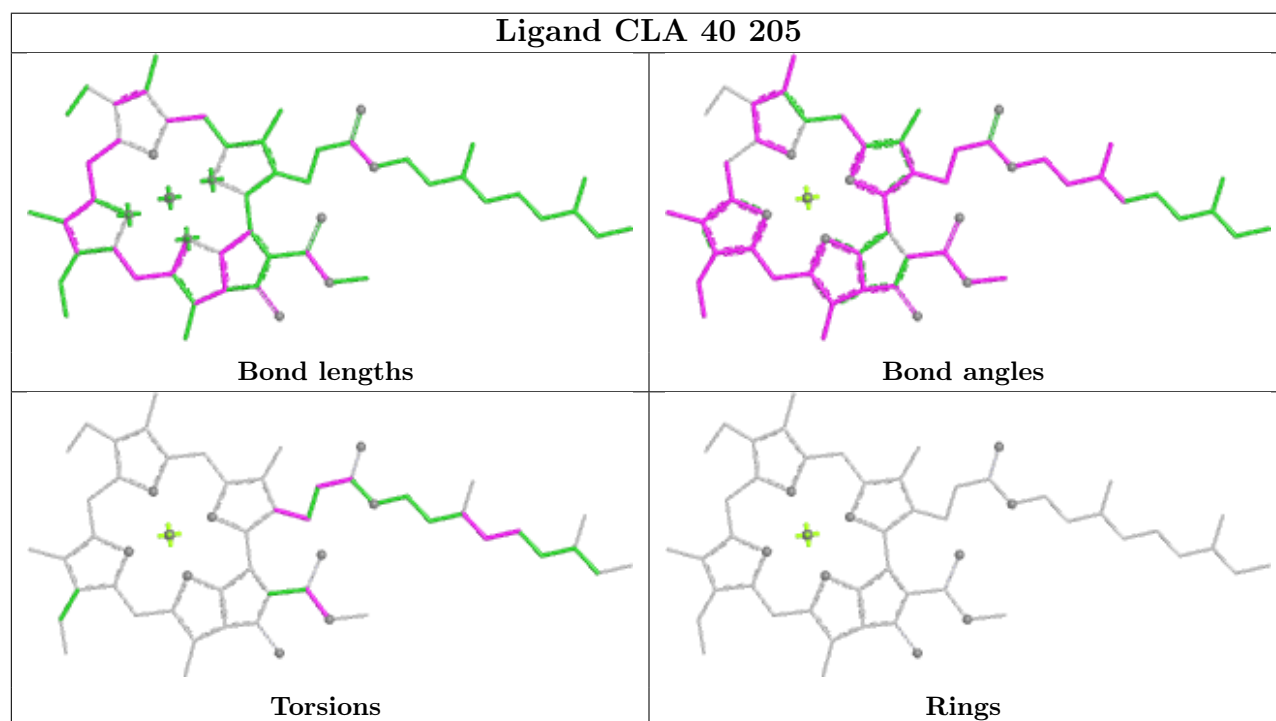
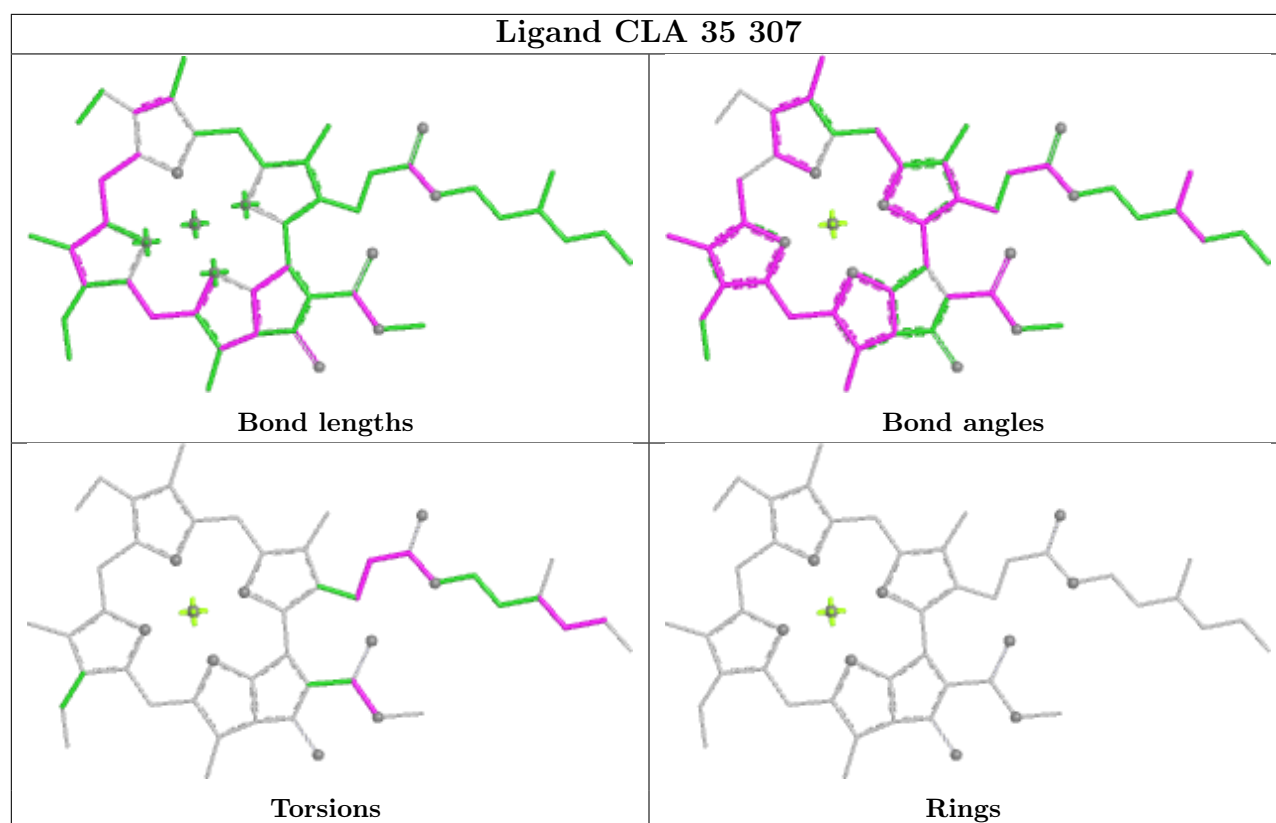


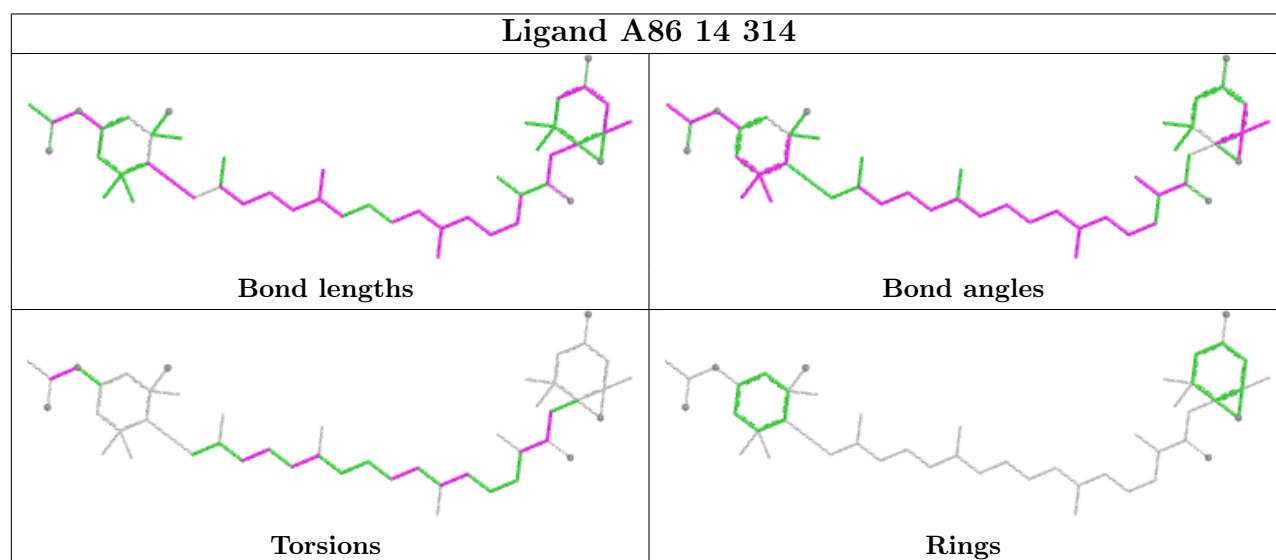
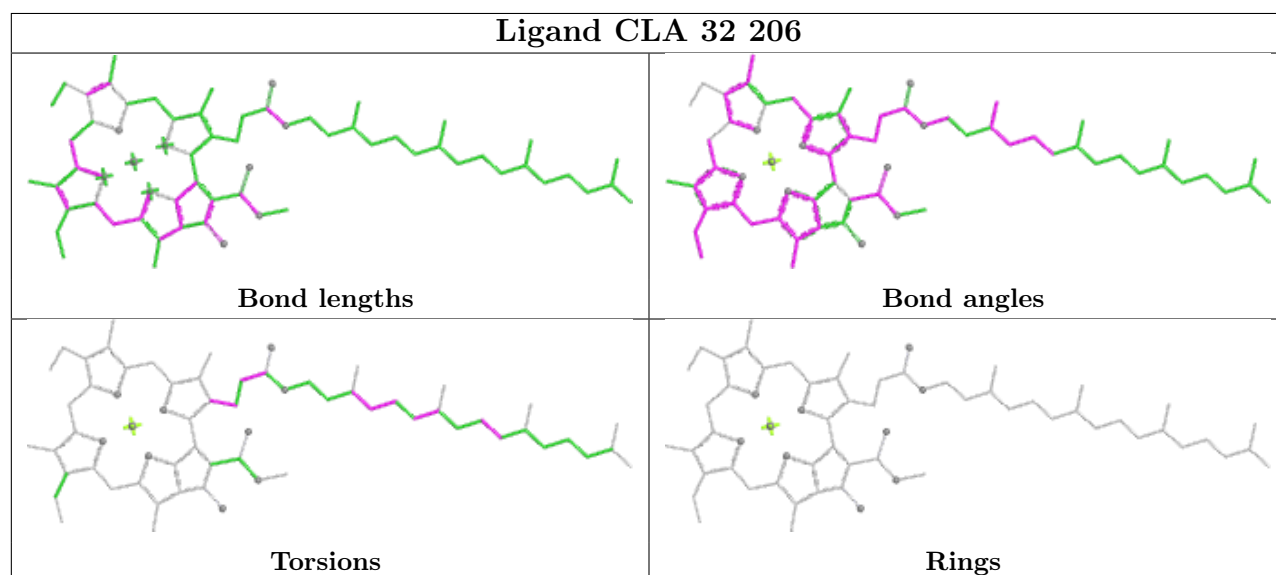
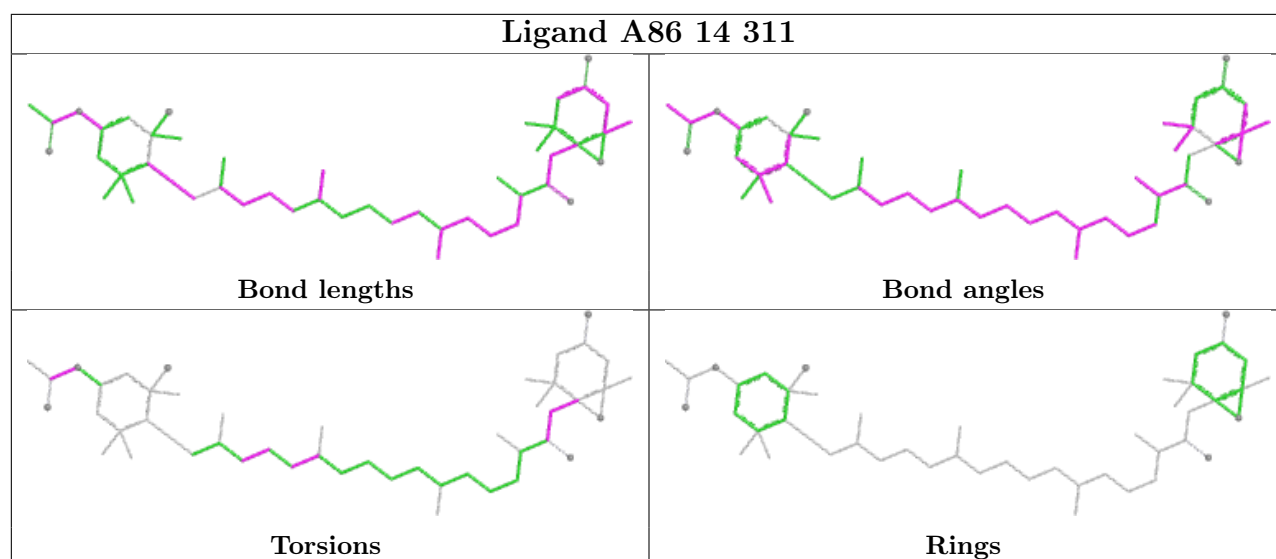


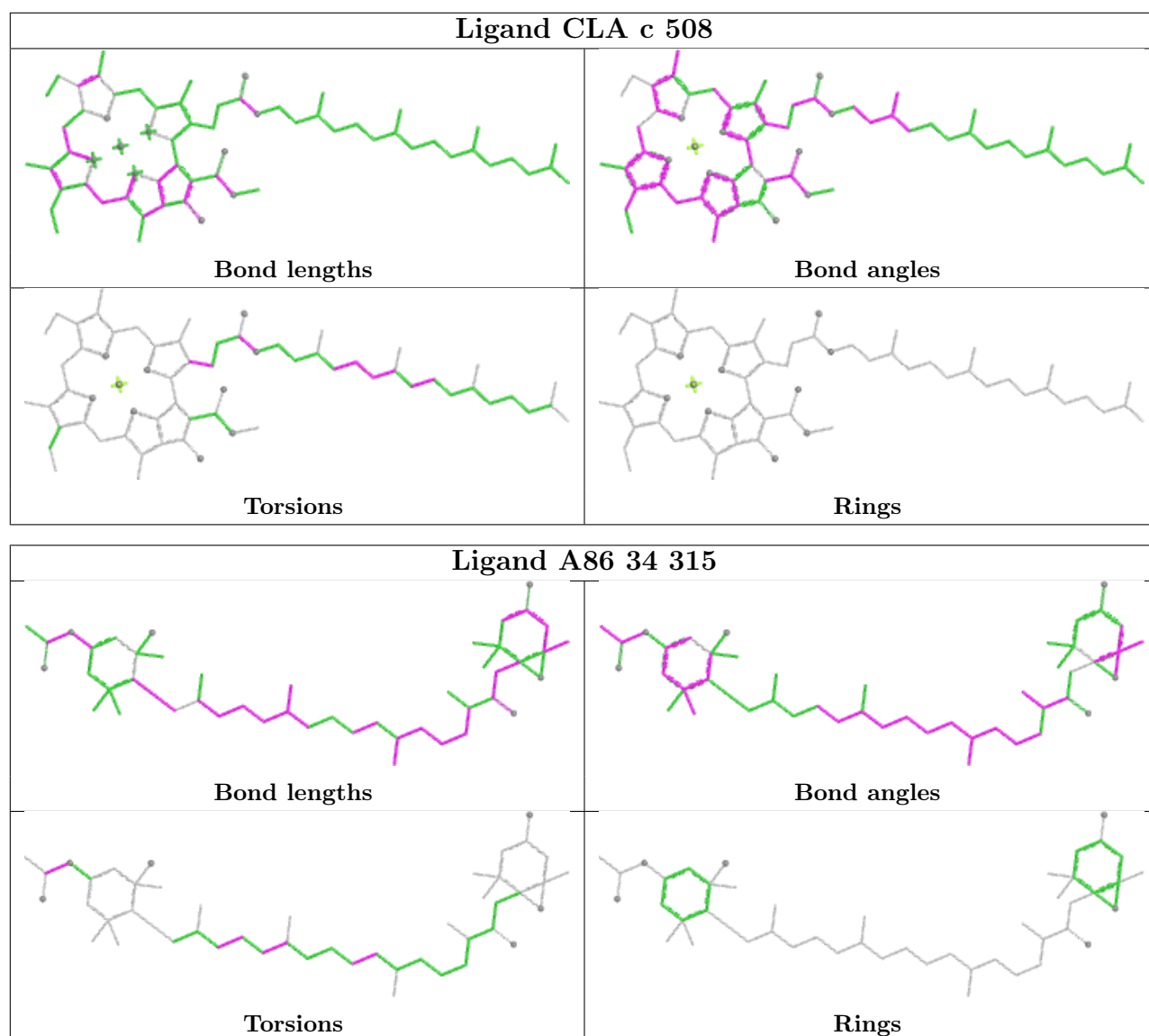


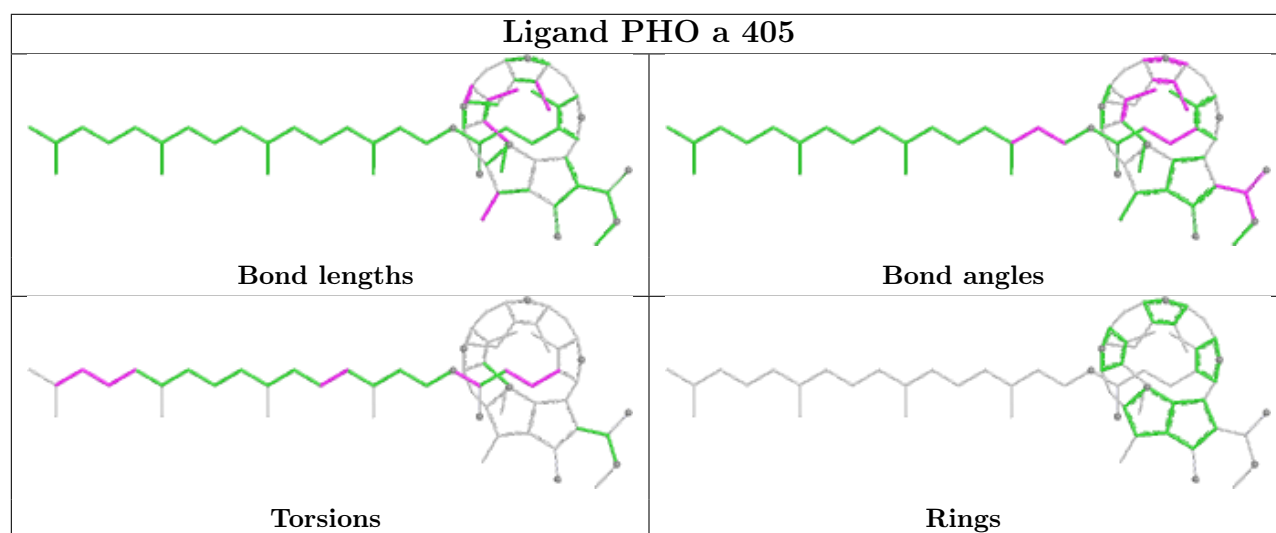
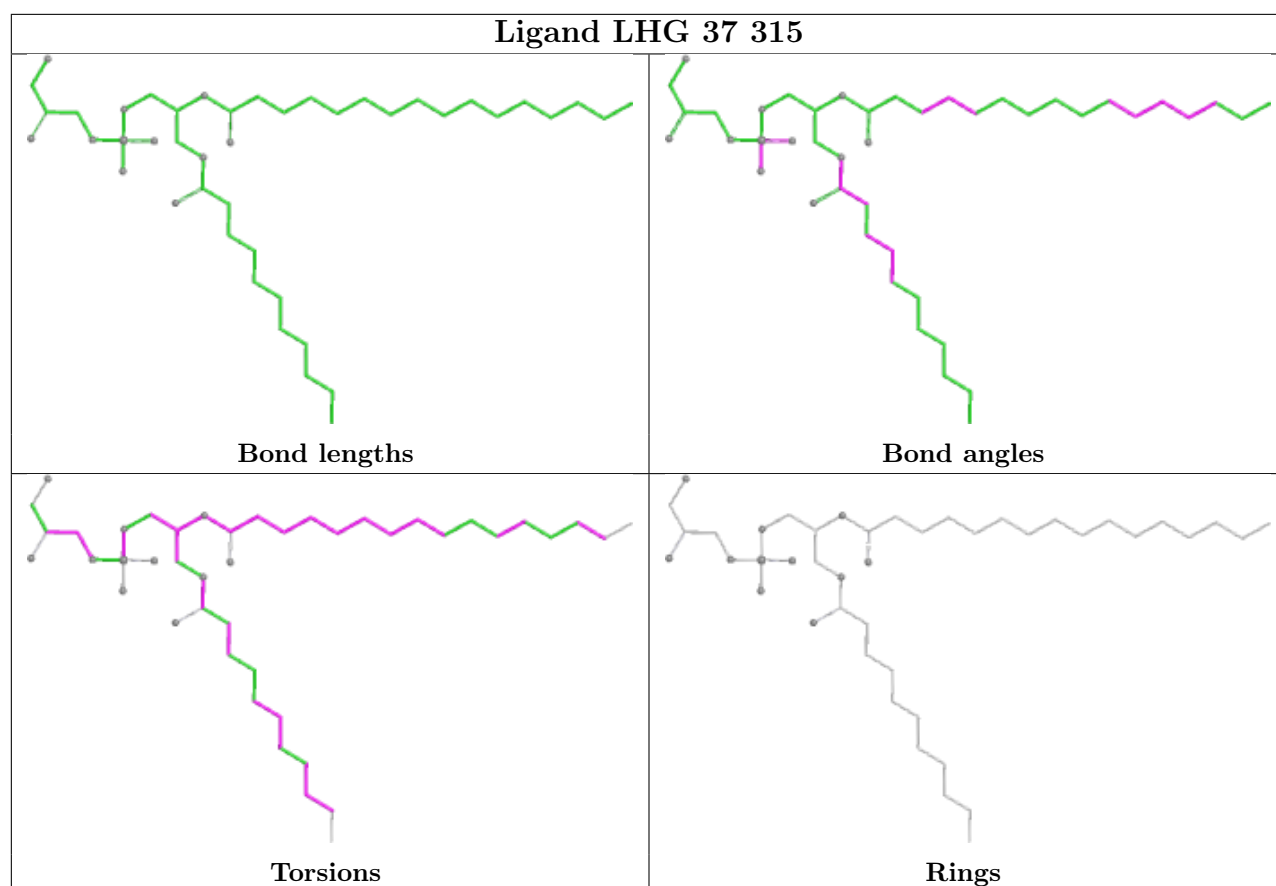


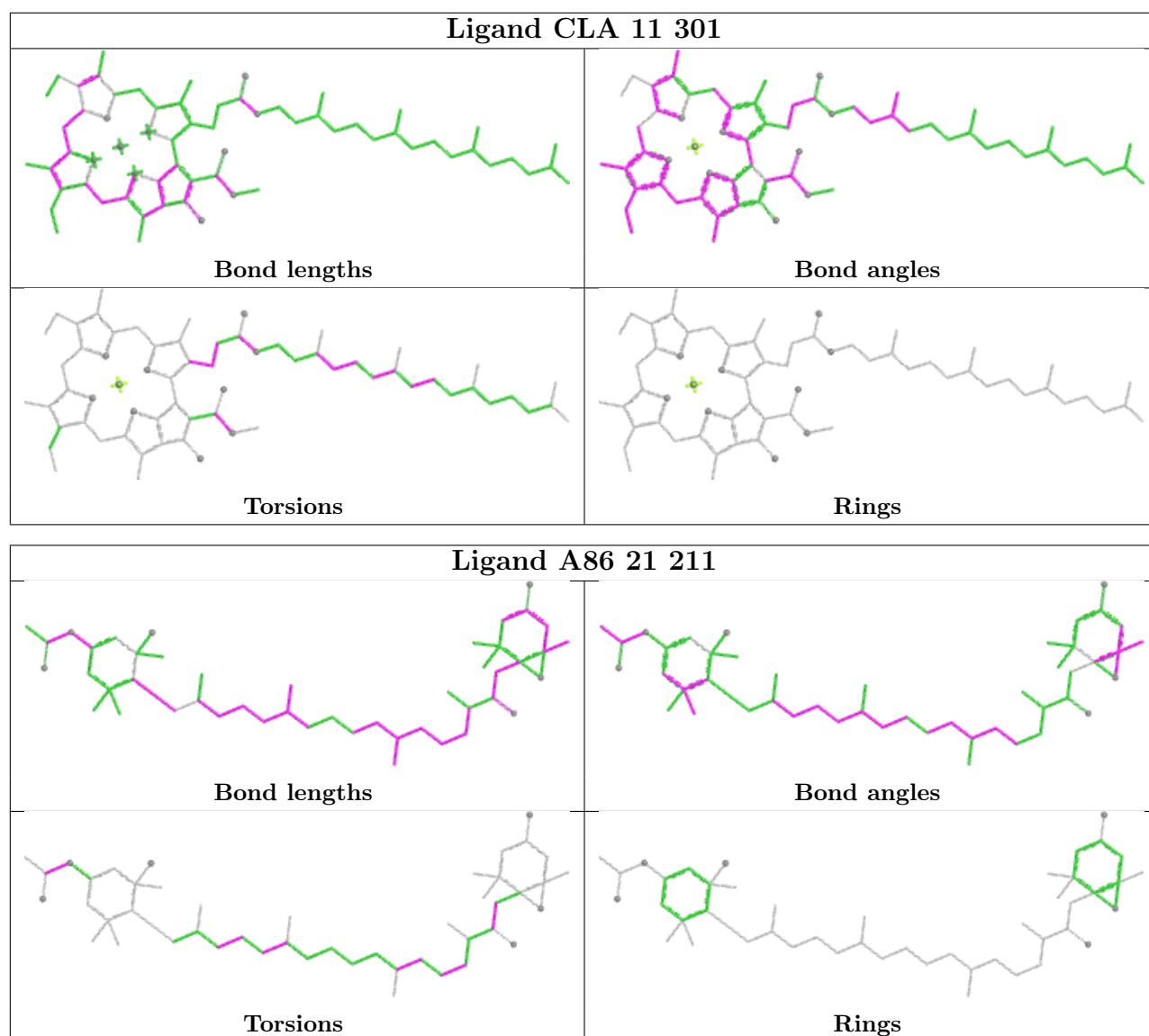


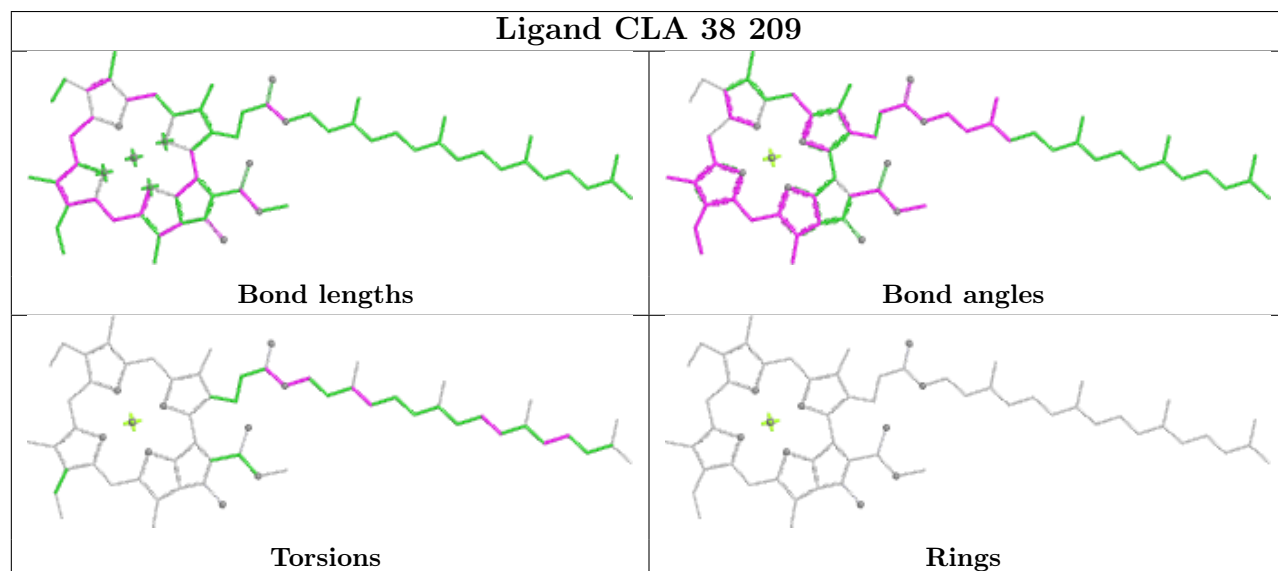
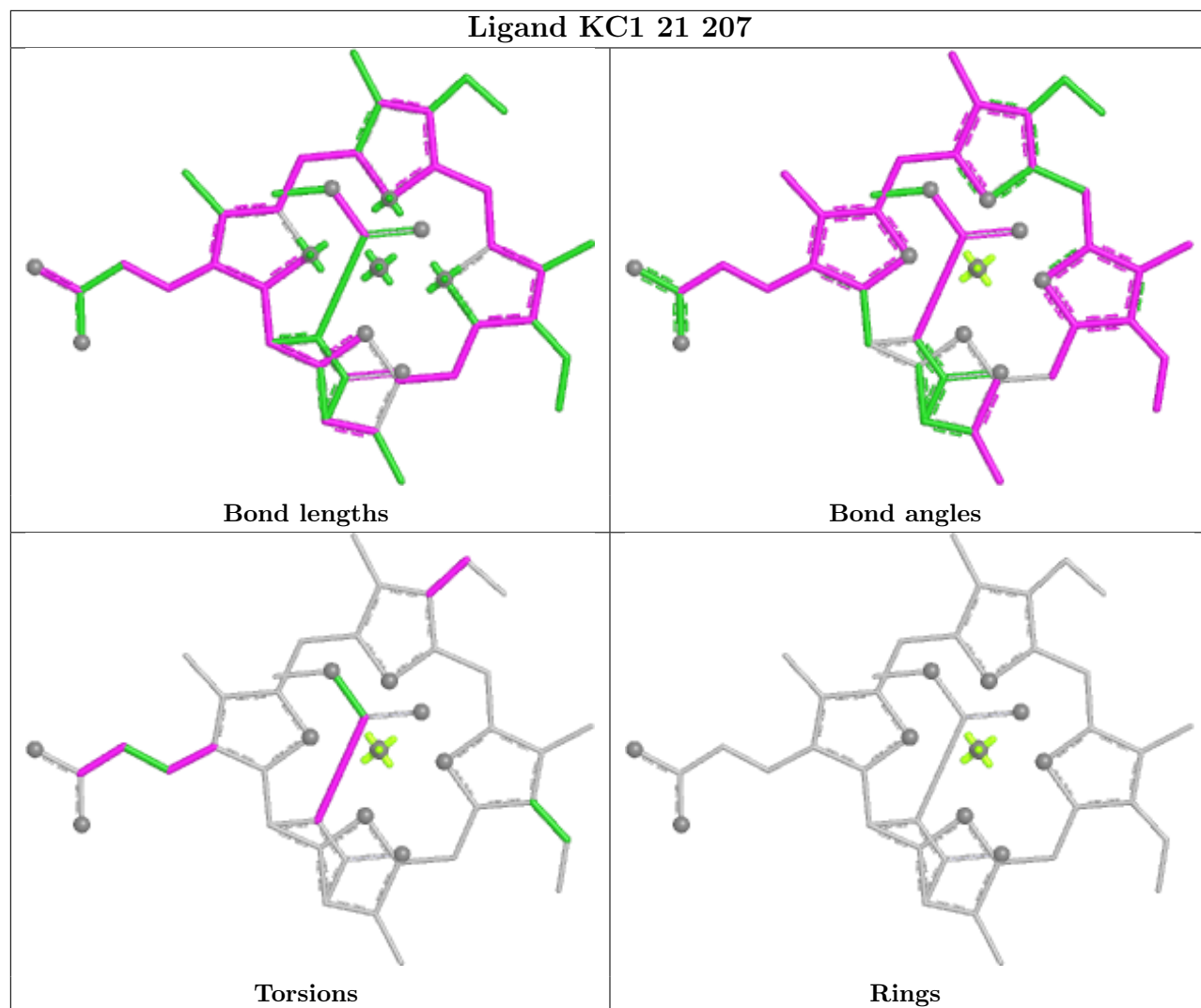


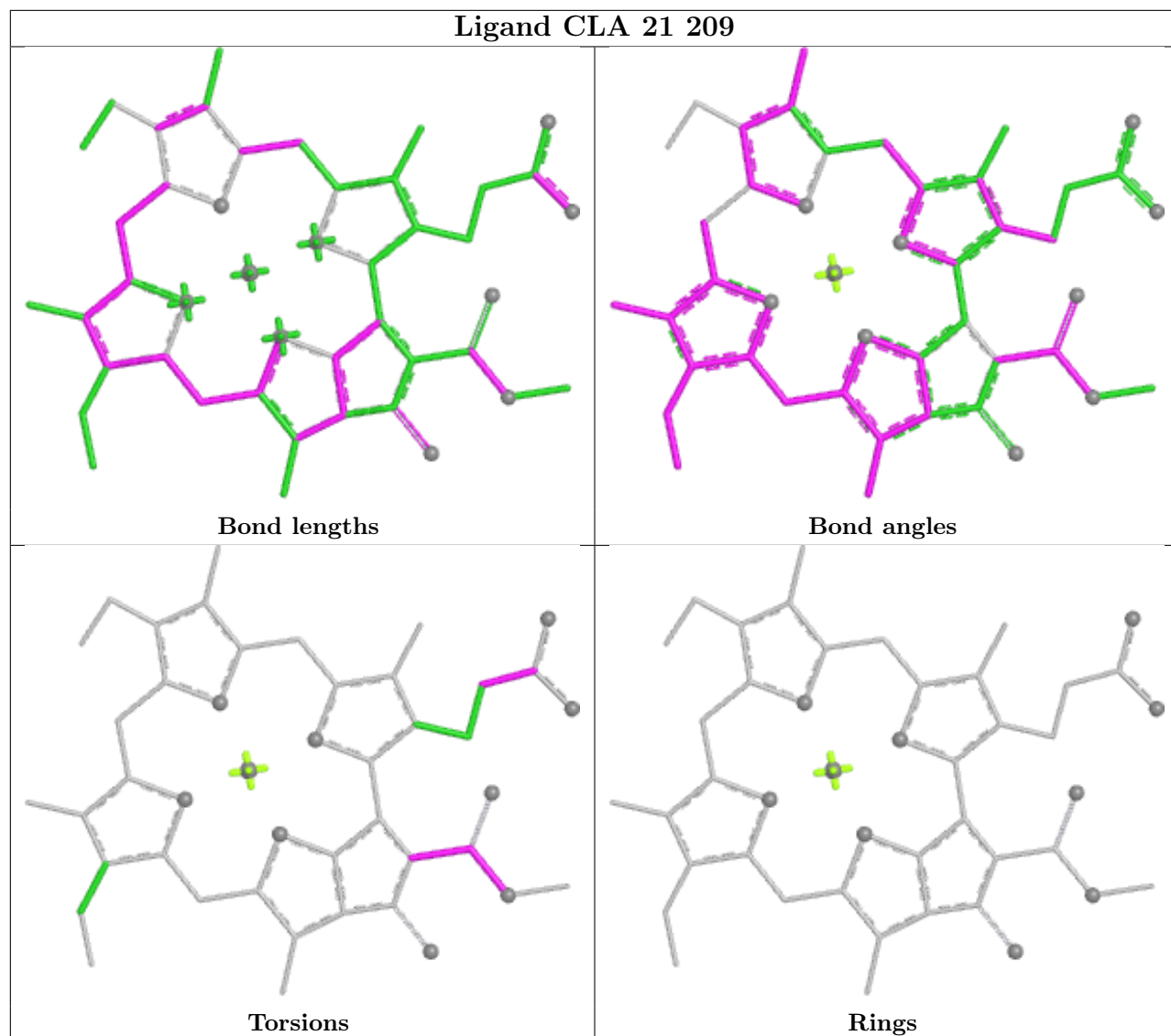


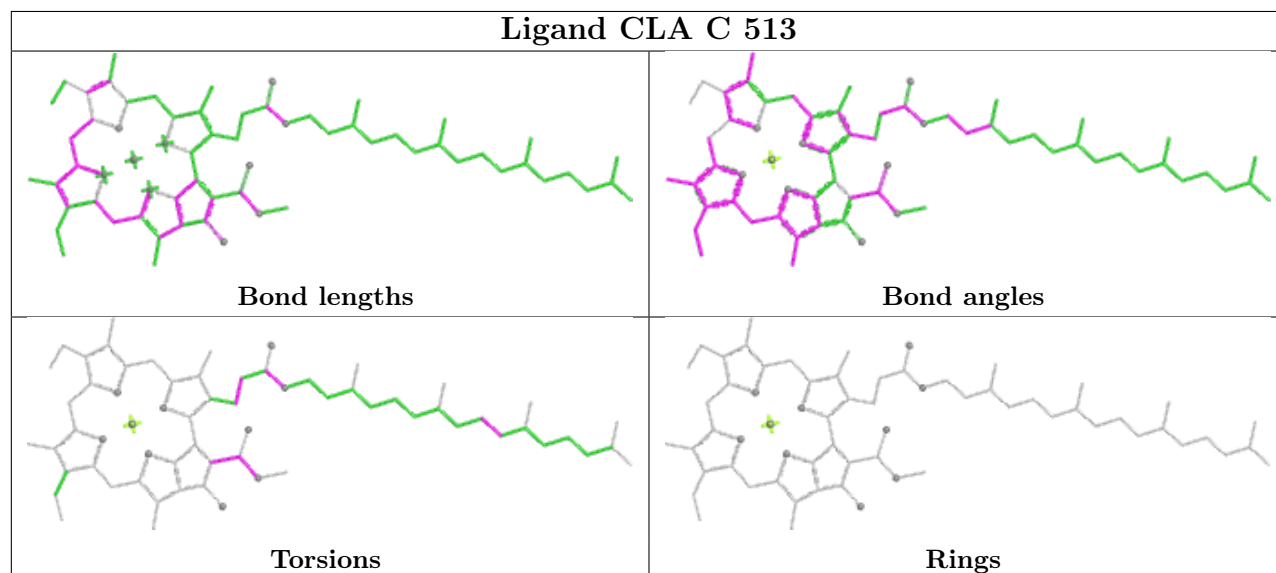
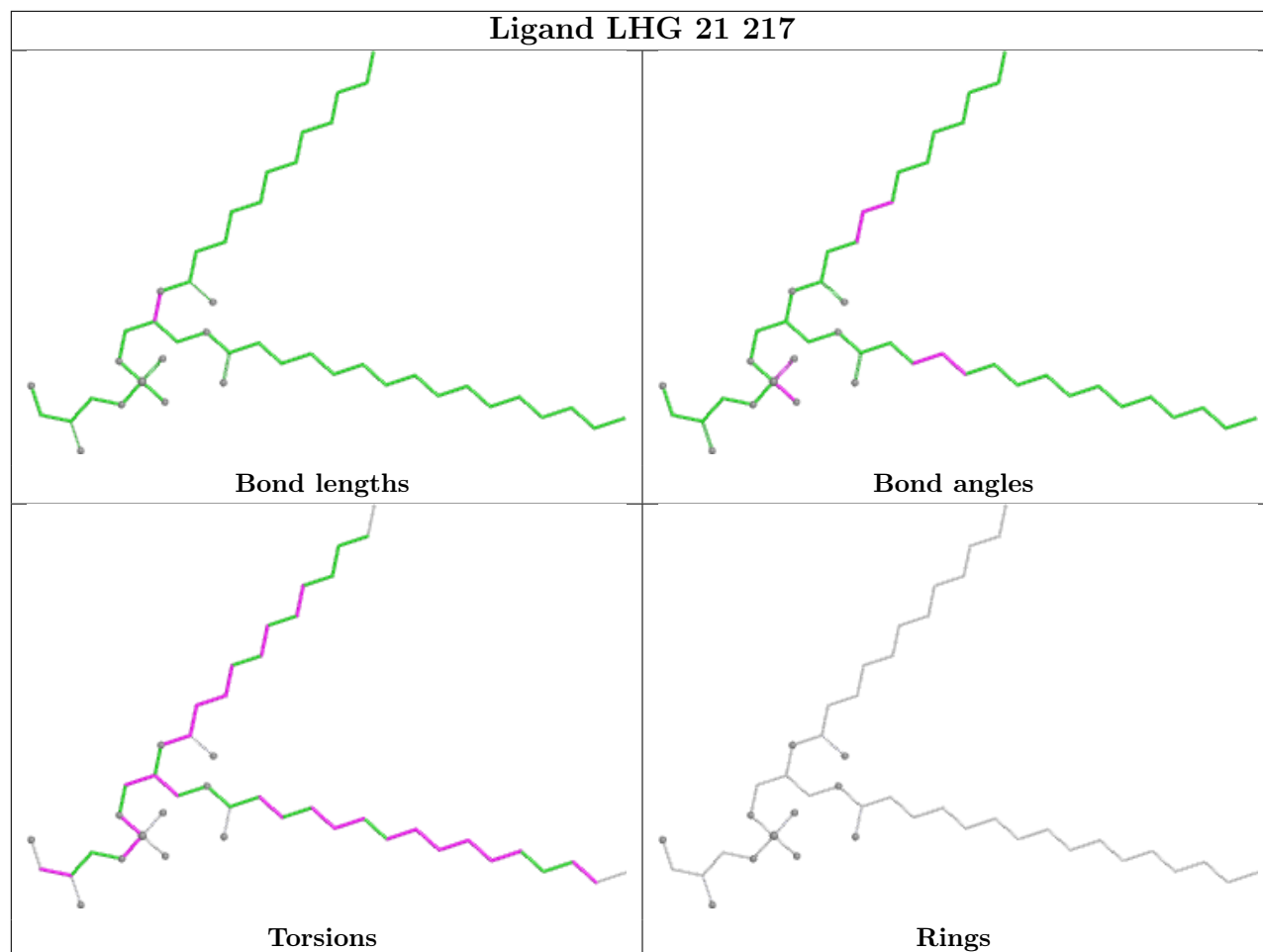


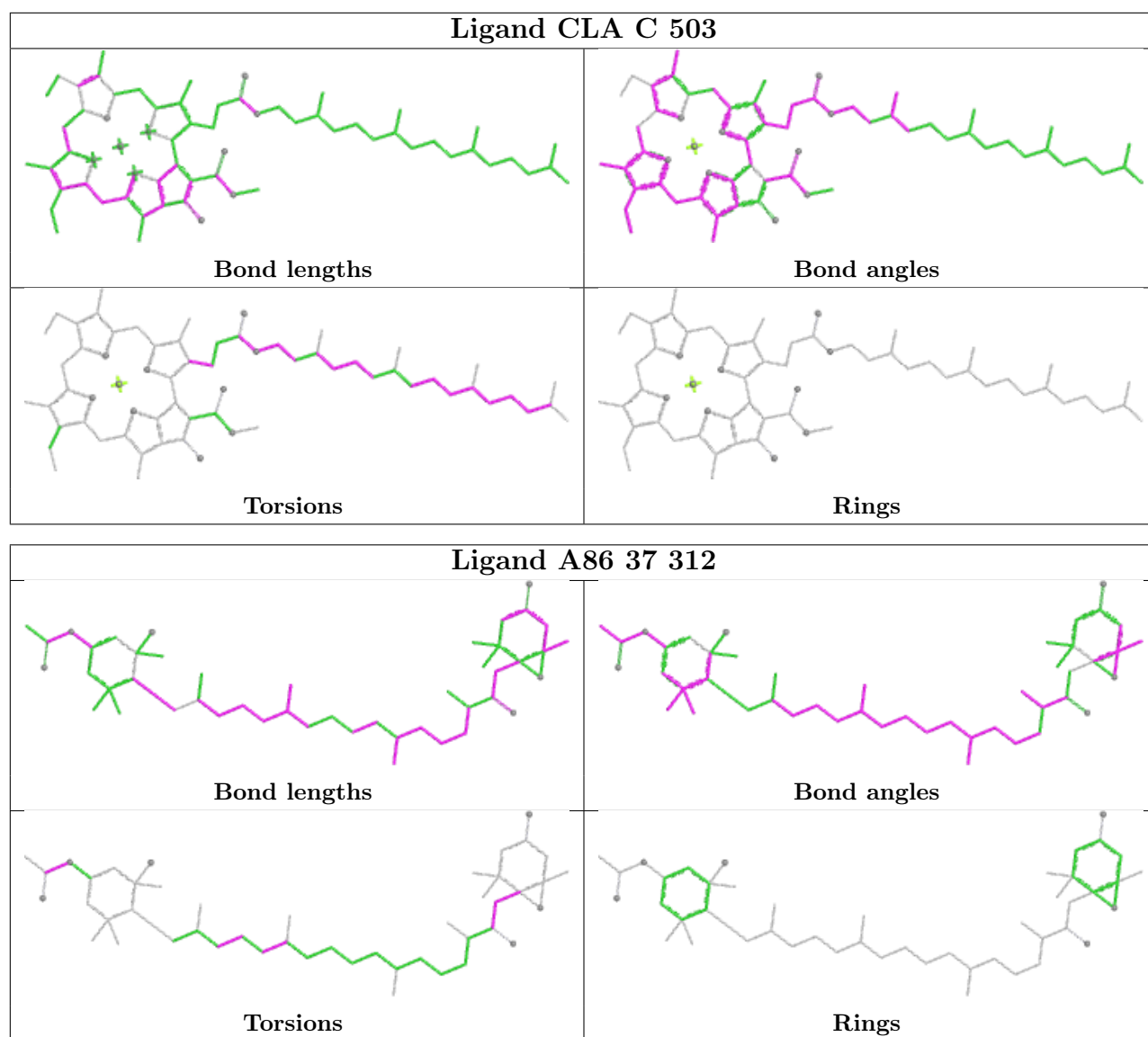


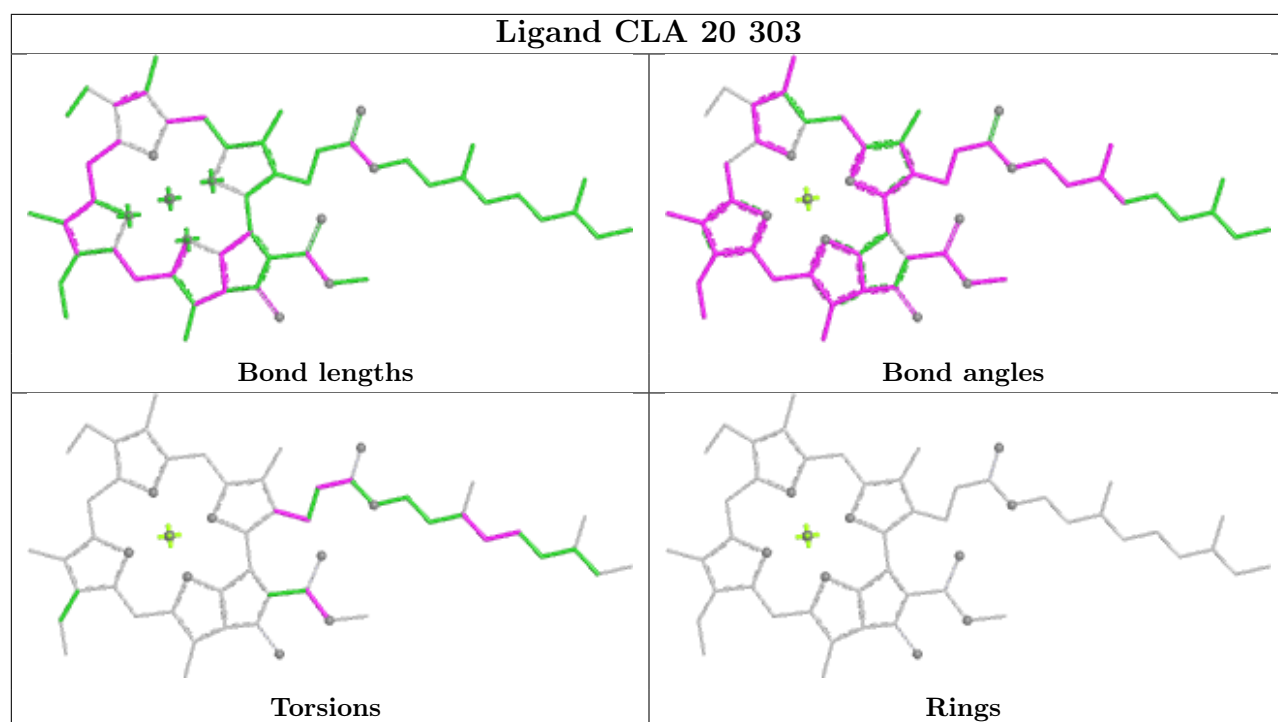


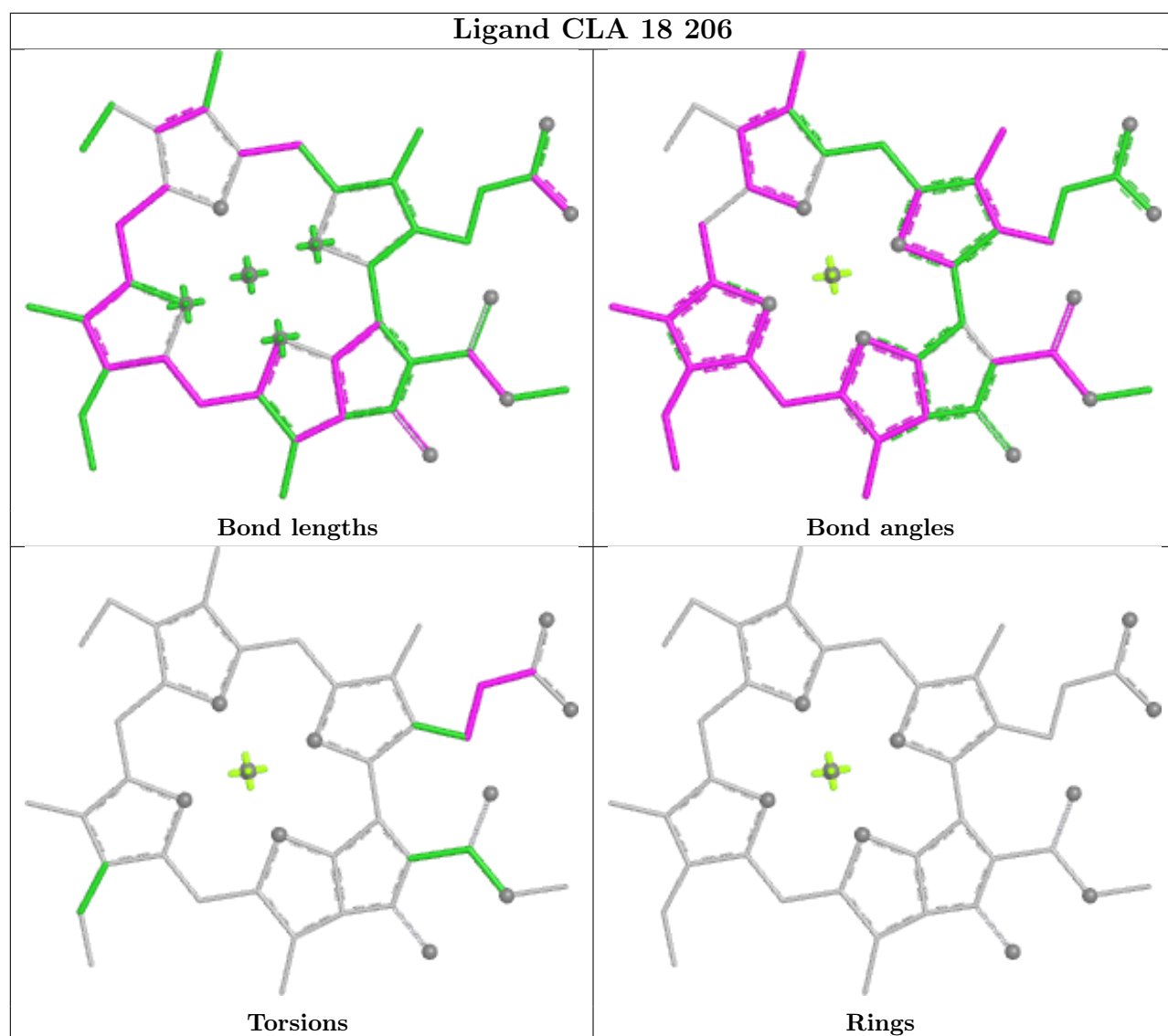


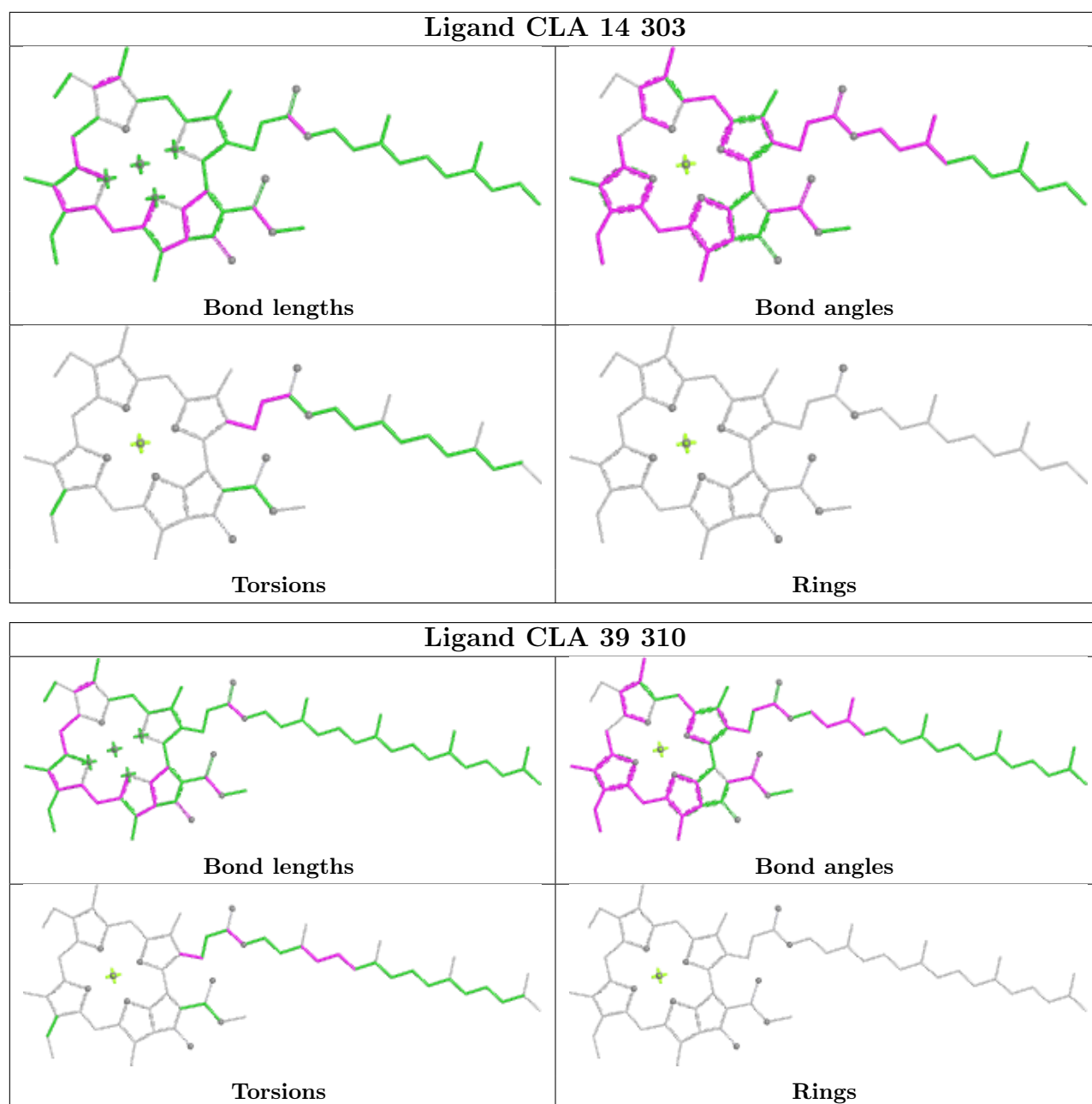


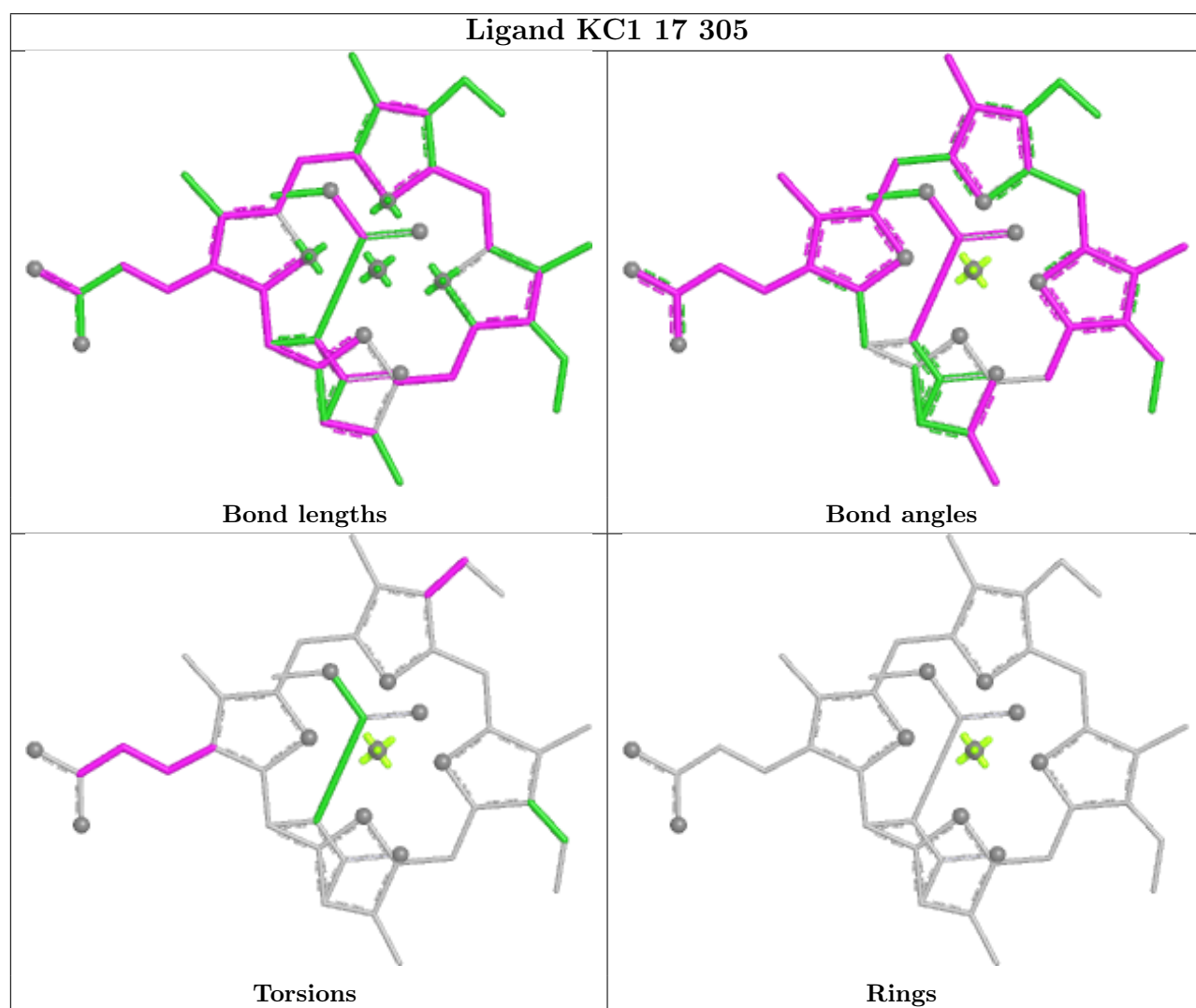
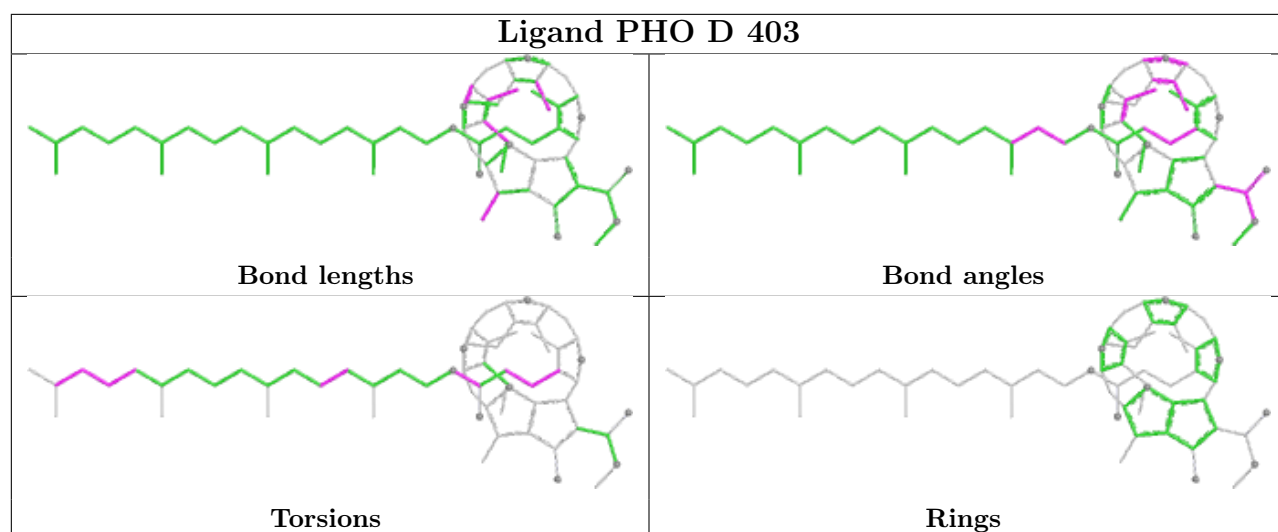


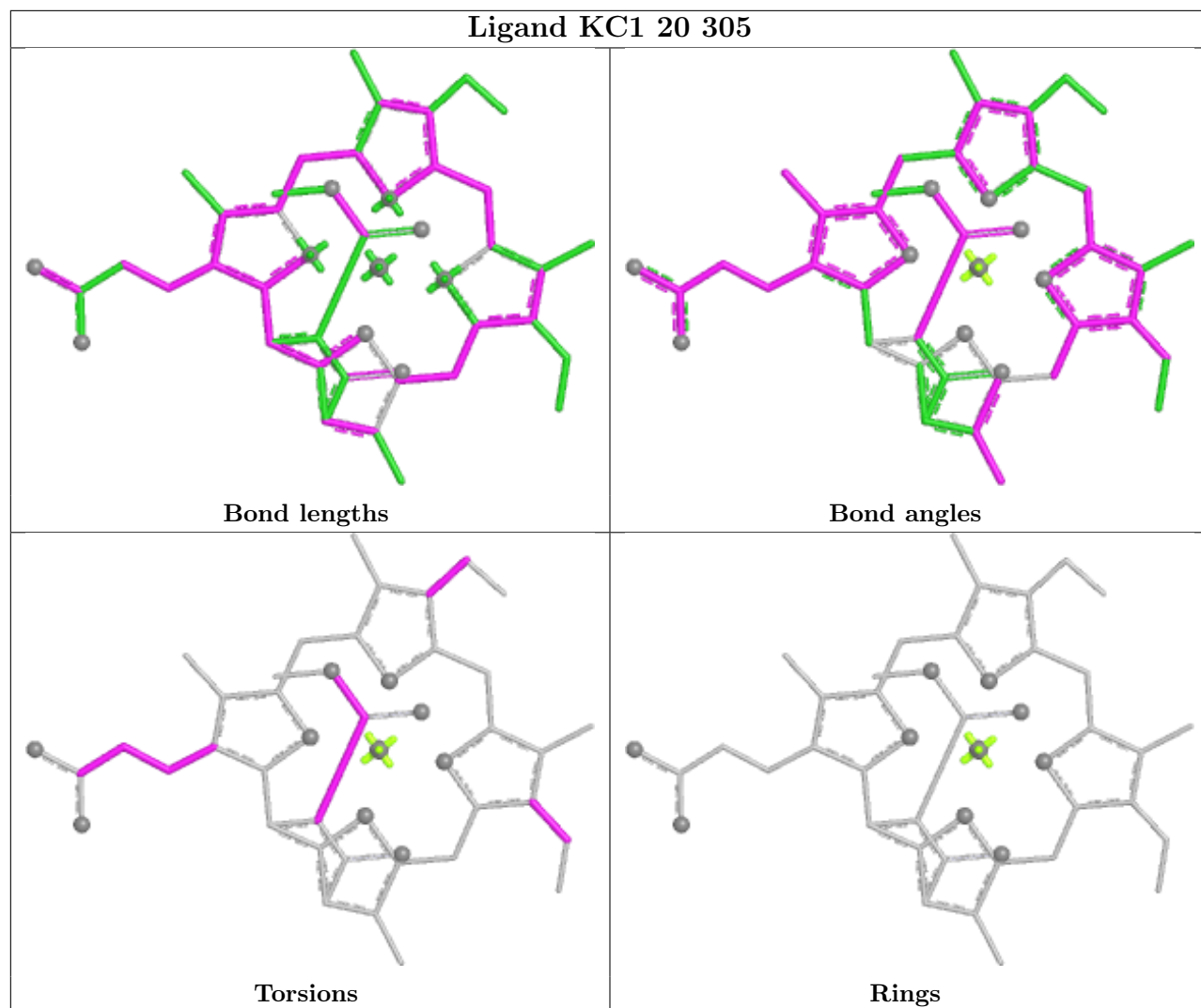


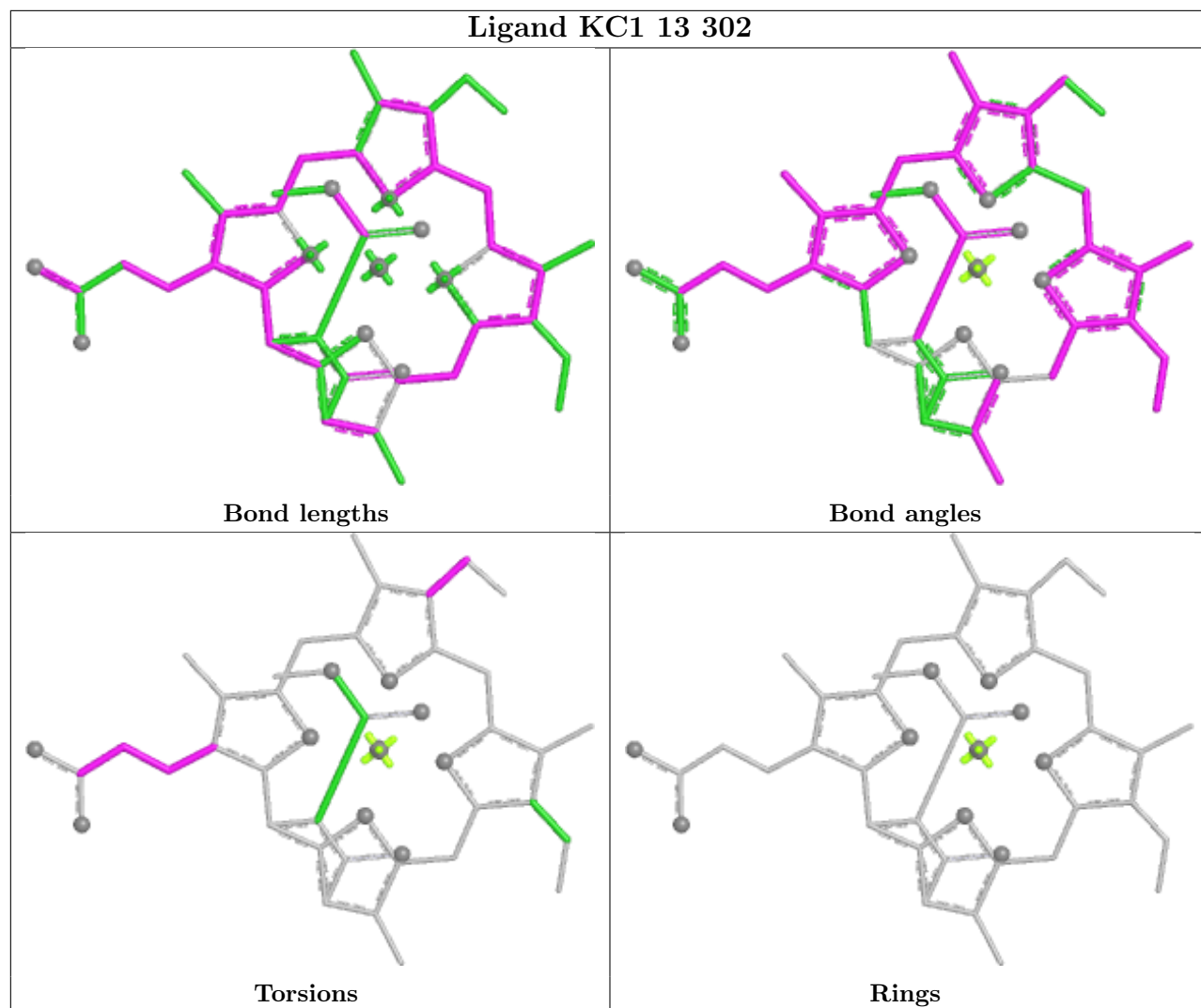


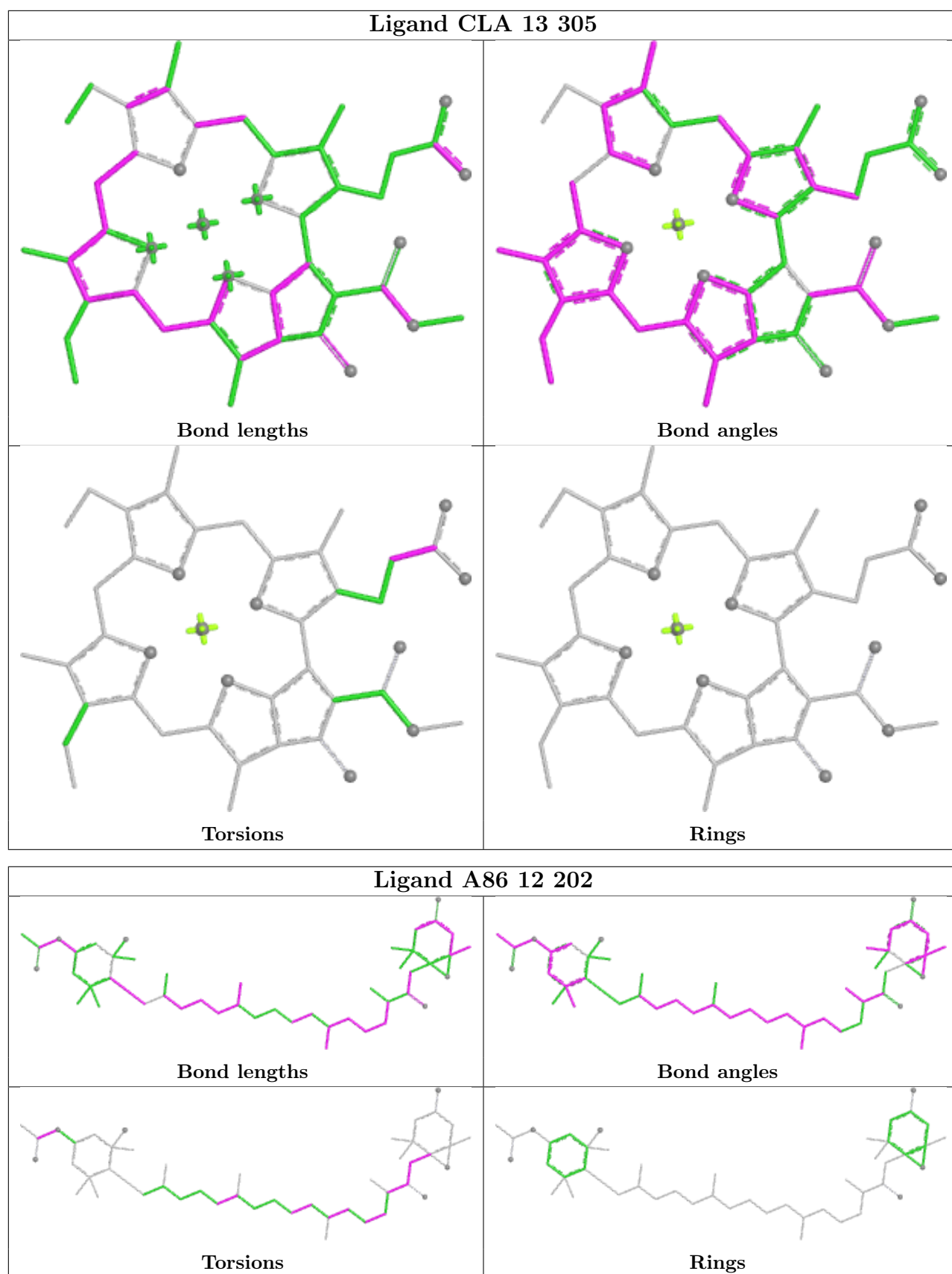


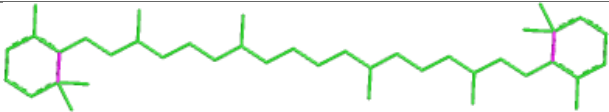
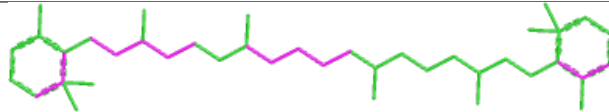
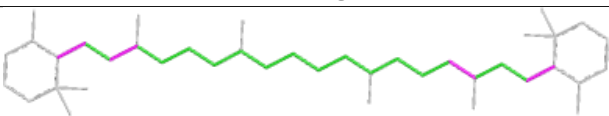
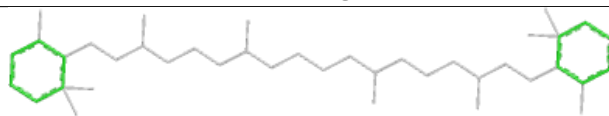


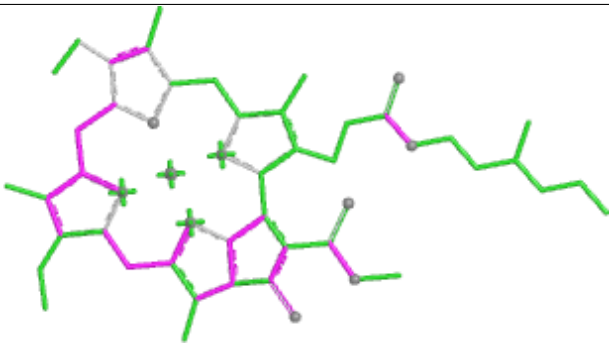
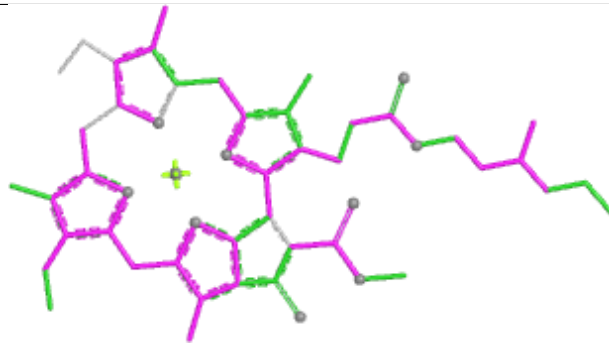
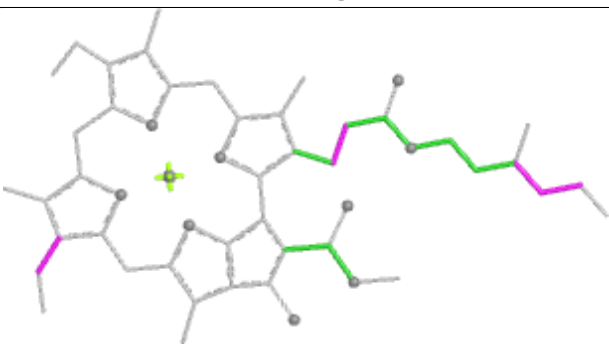
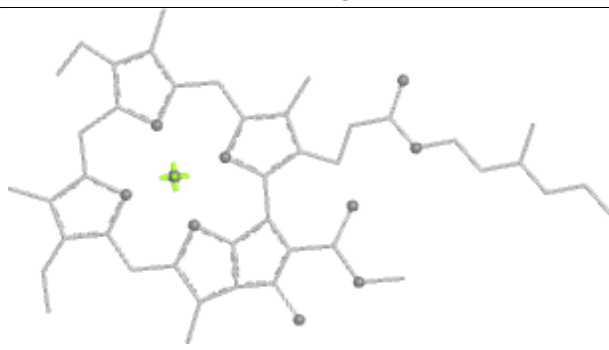


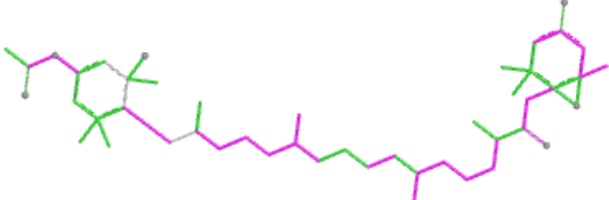
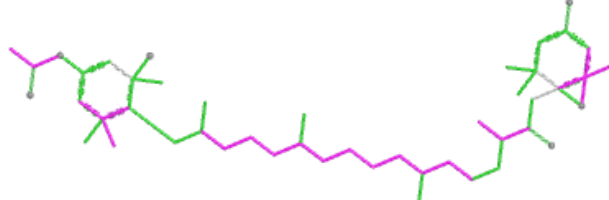
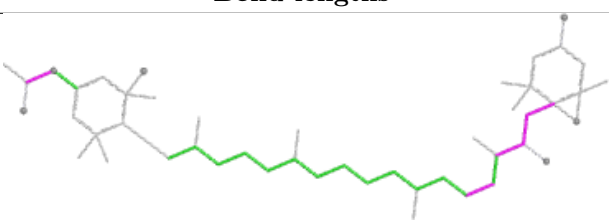
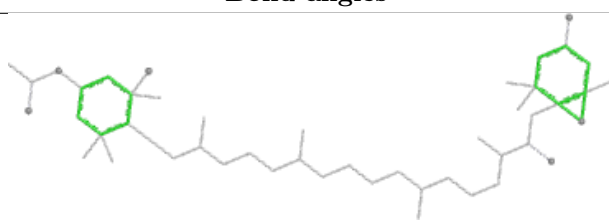


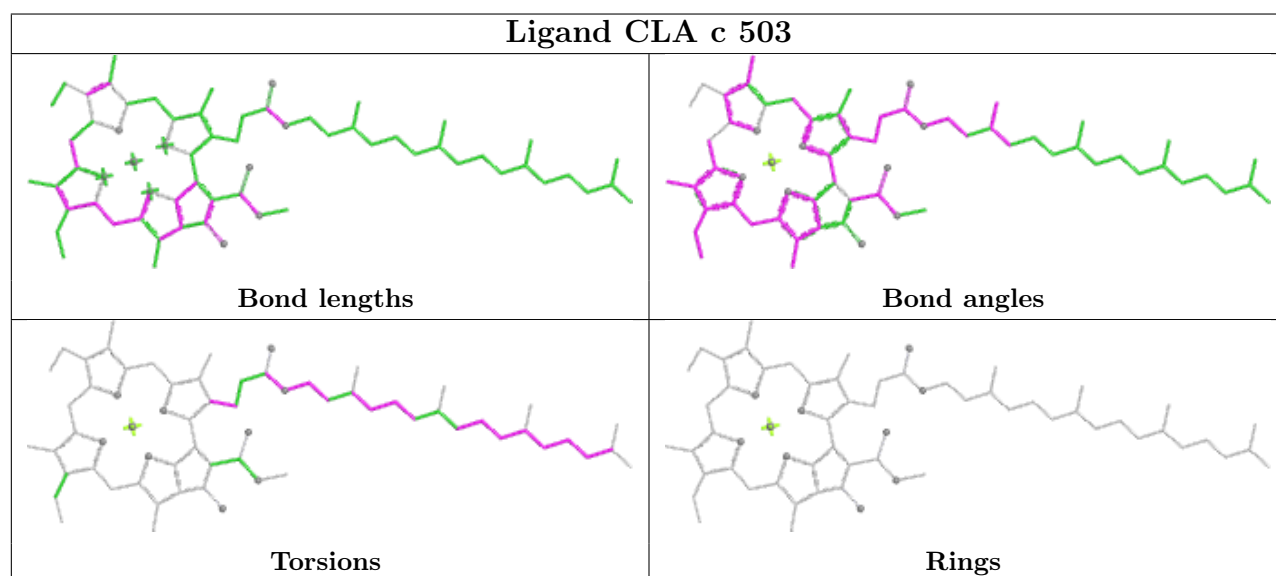
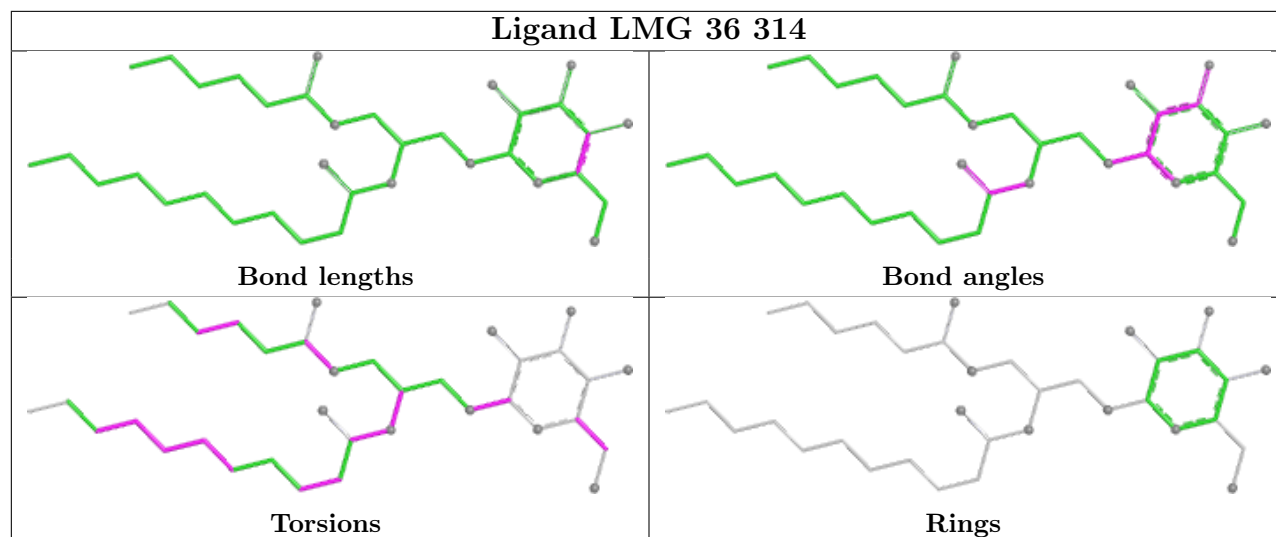


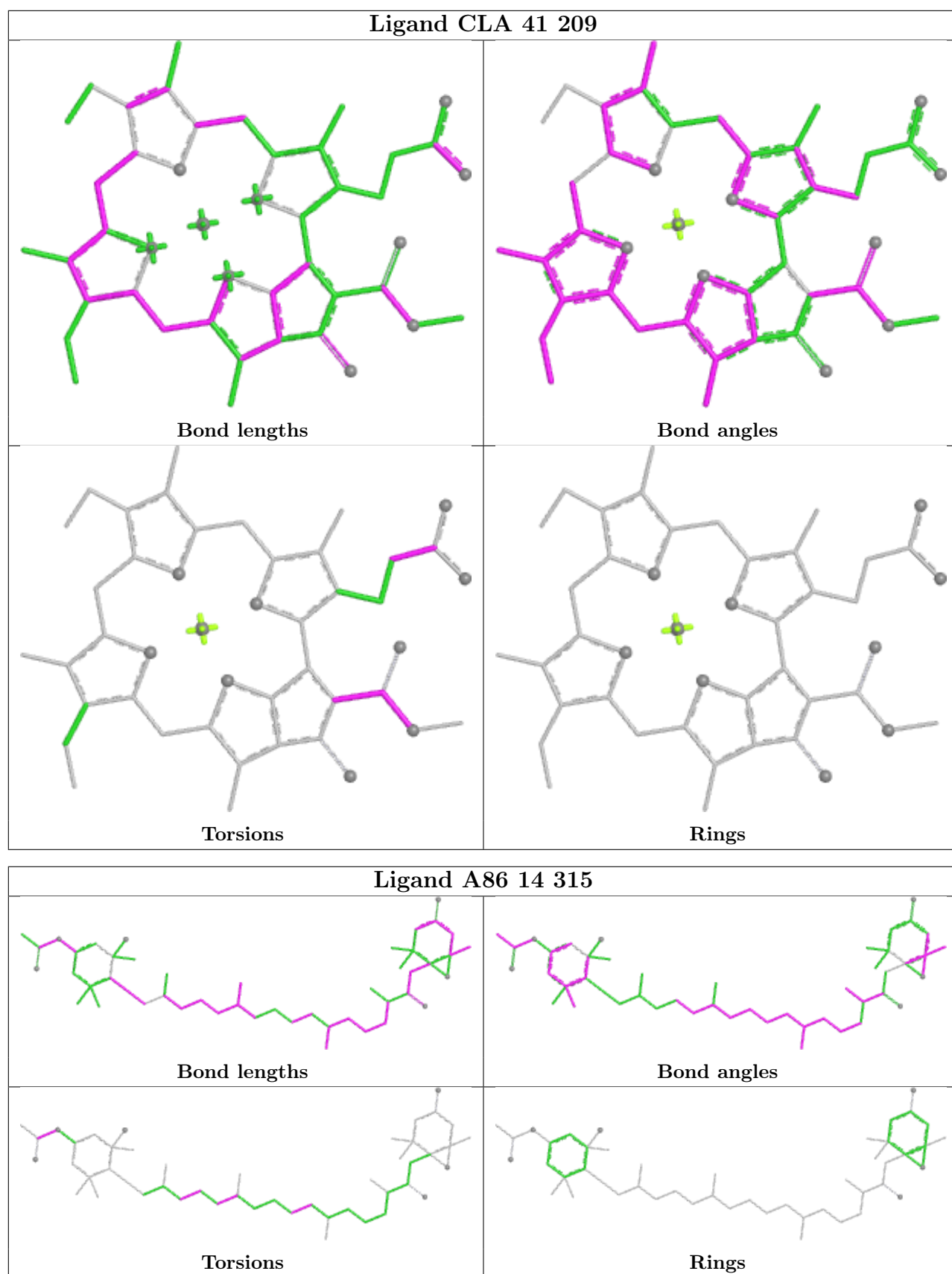


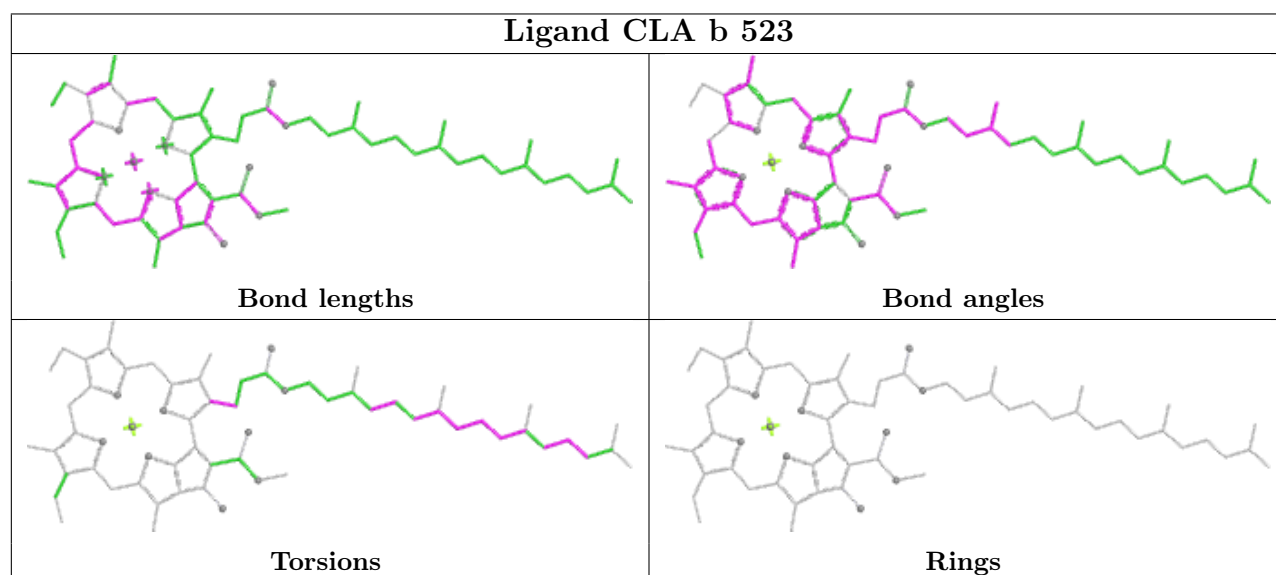
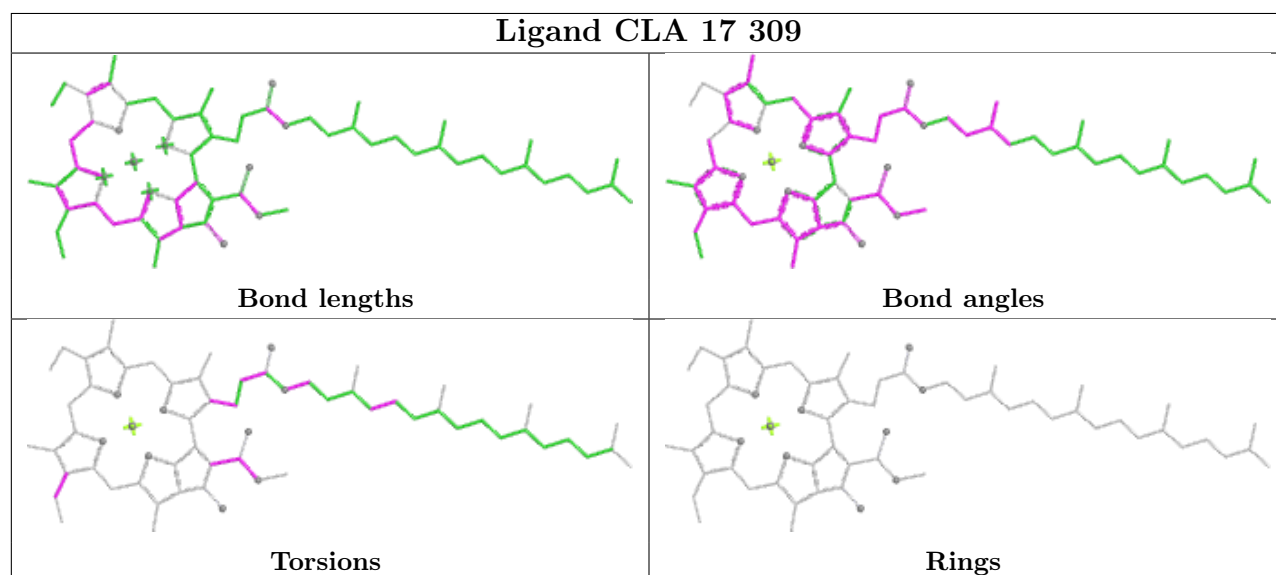
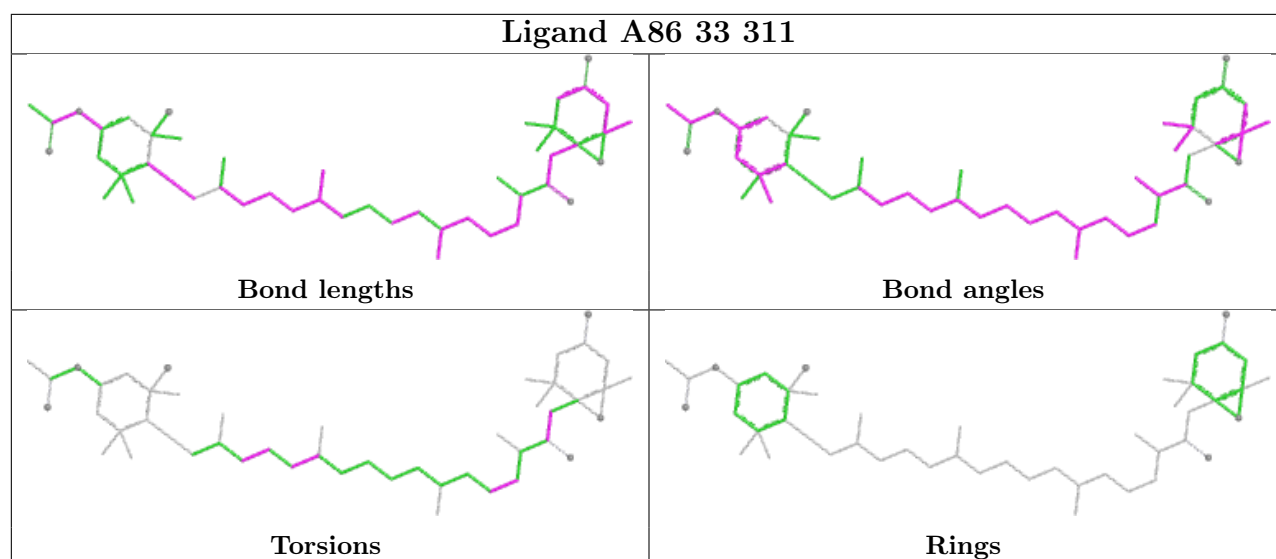
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Bond lengths	Bond angles
	
Torsions	Rings

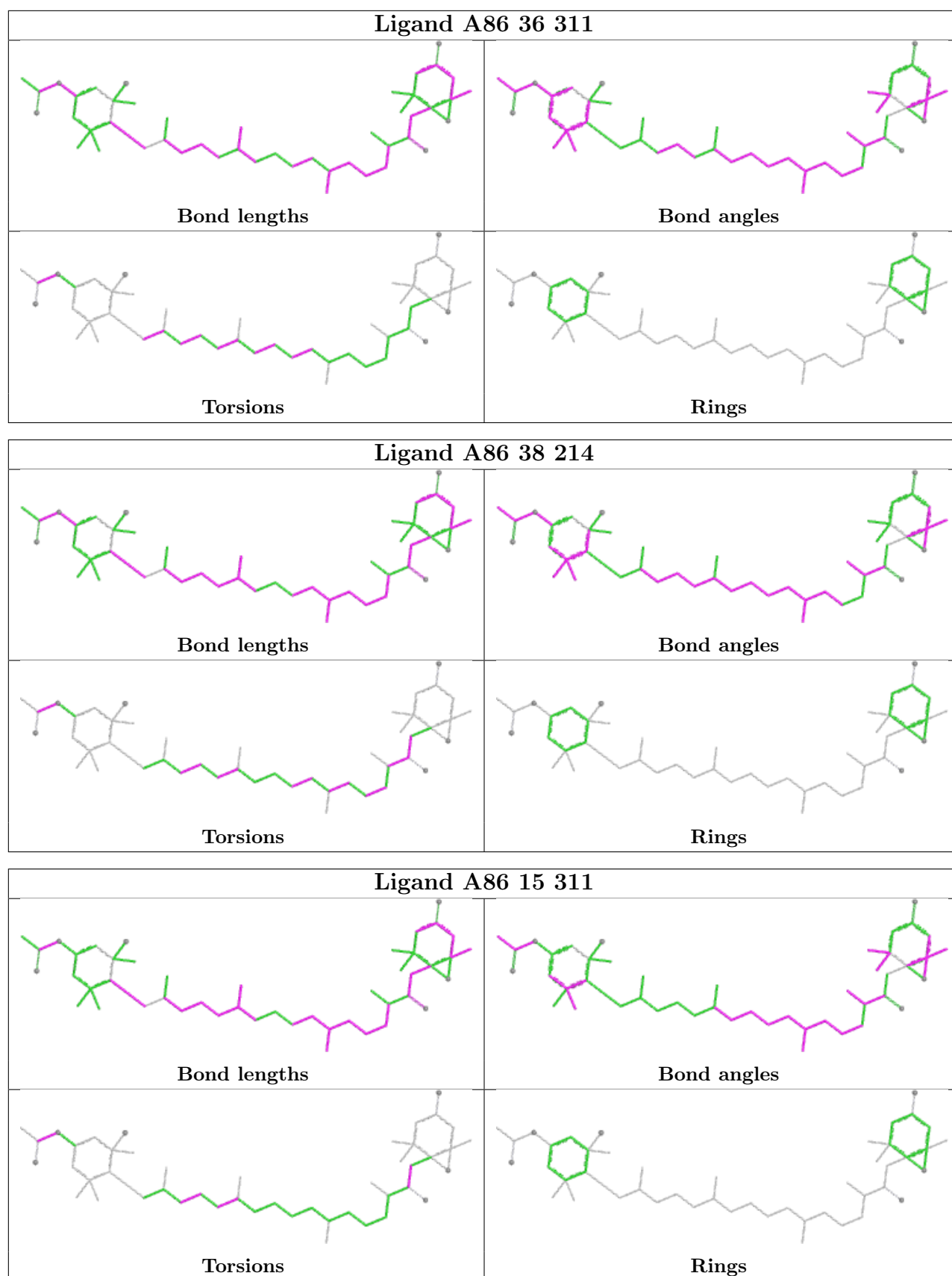
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Bond lengths	Bond angles
	
Torsions	Rings

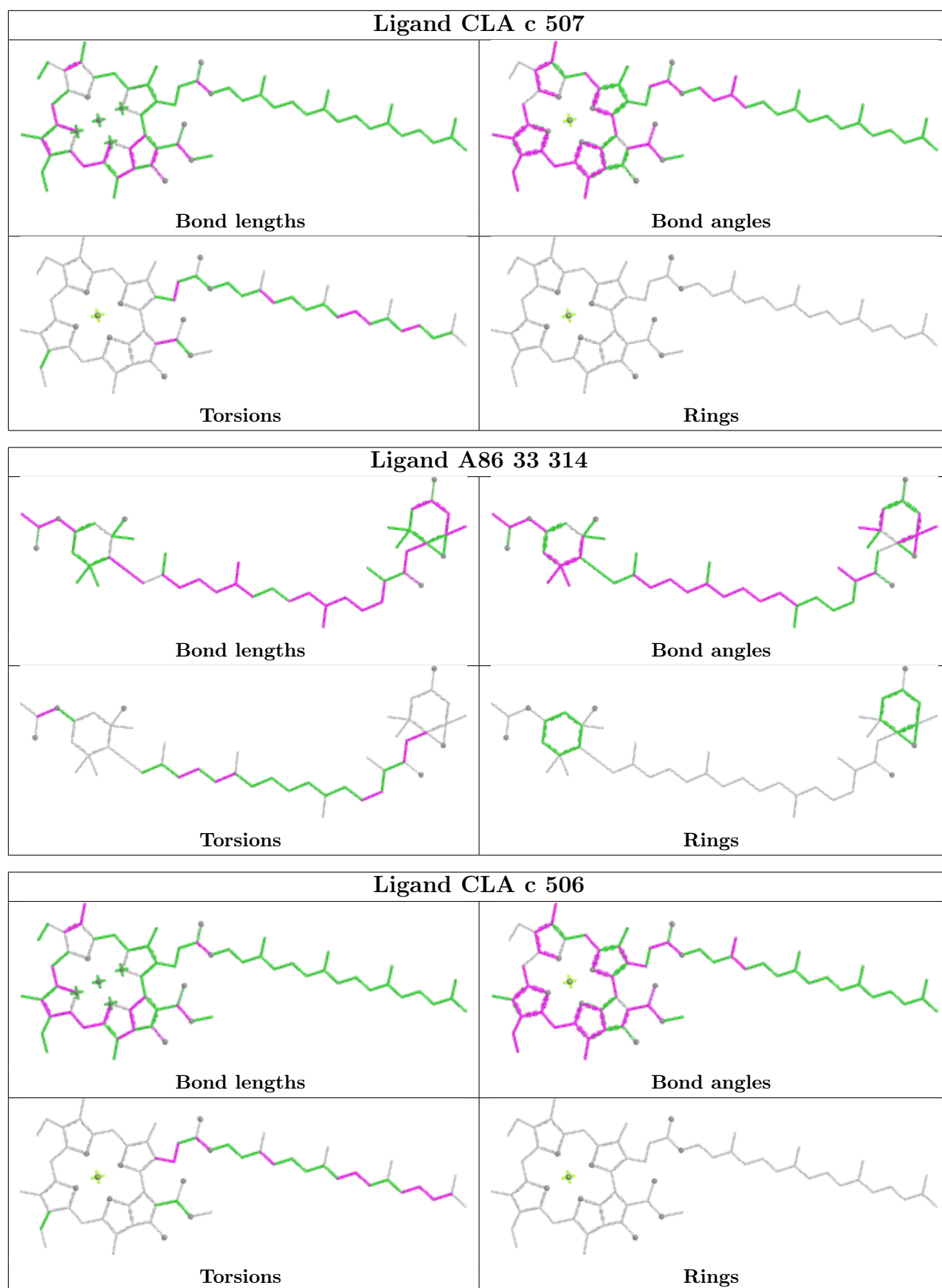
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Bond lengths	Bond angles
	
Torsions	Rings

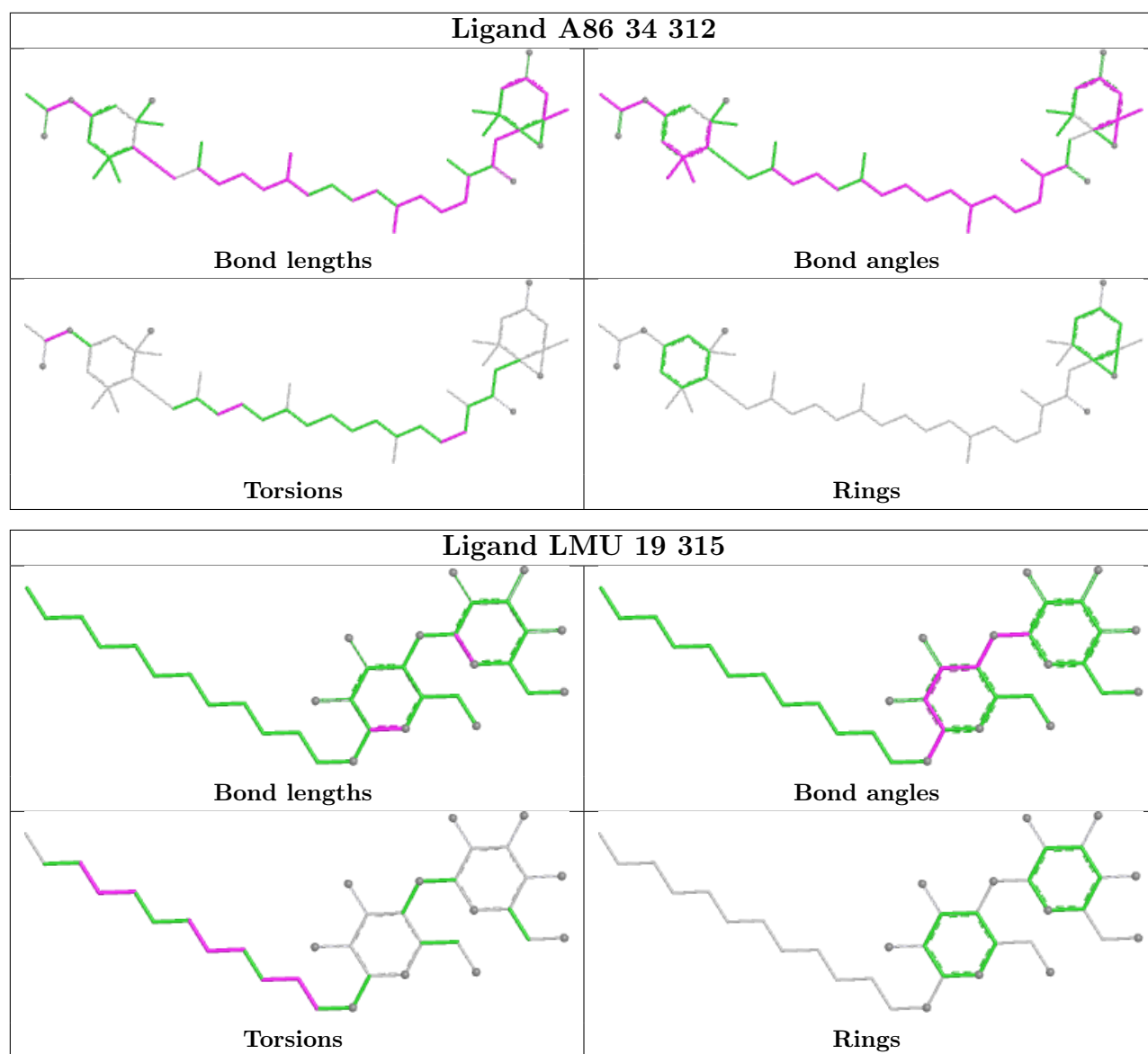


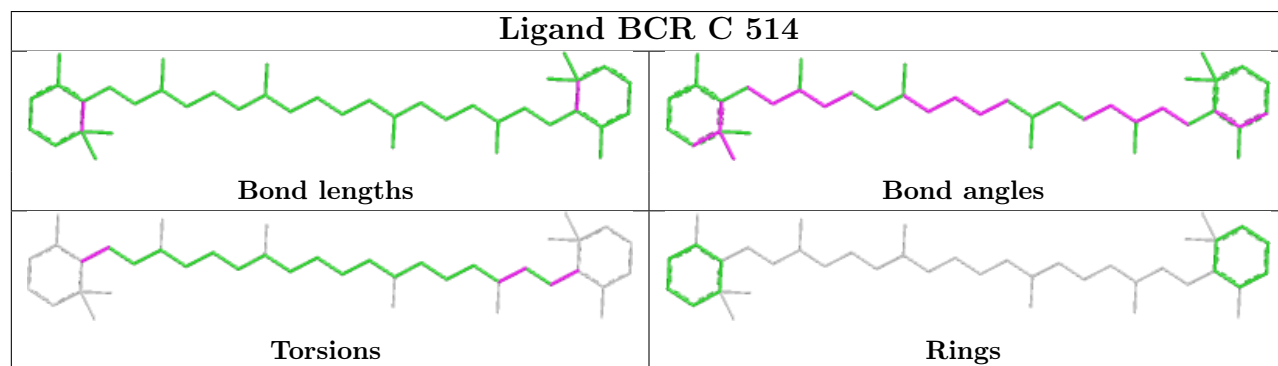
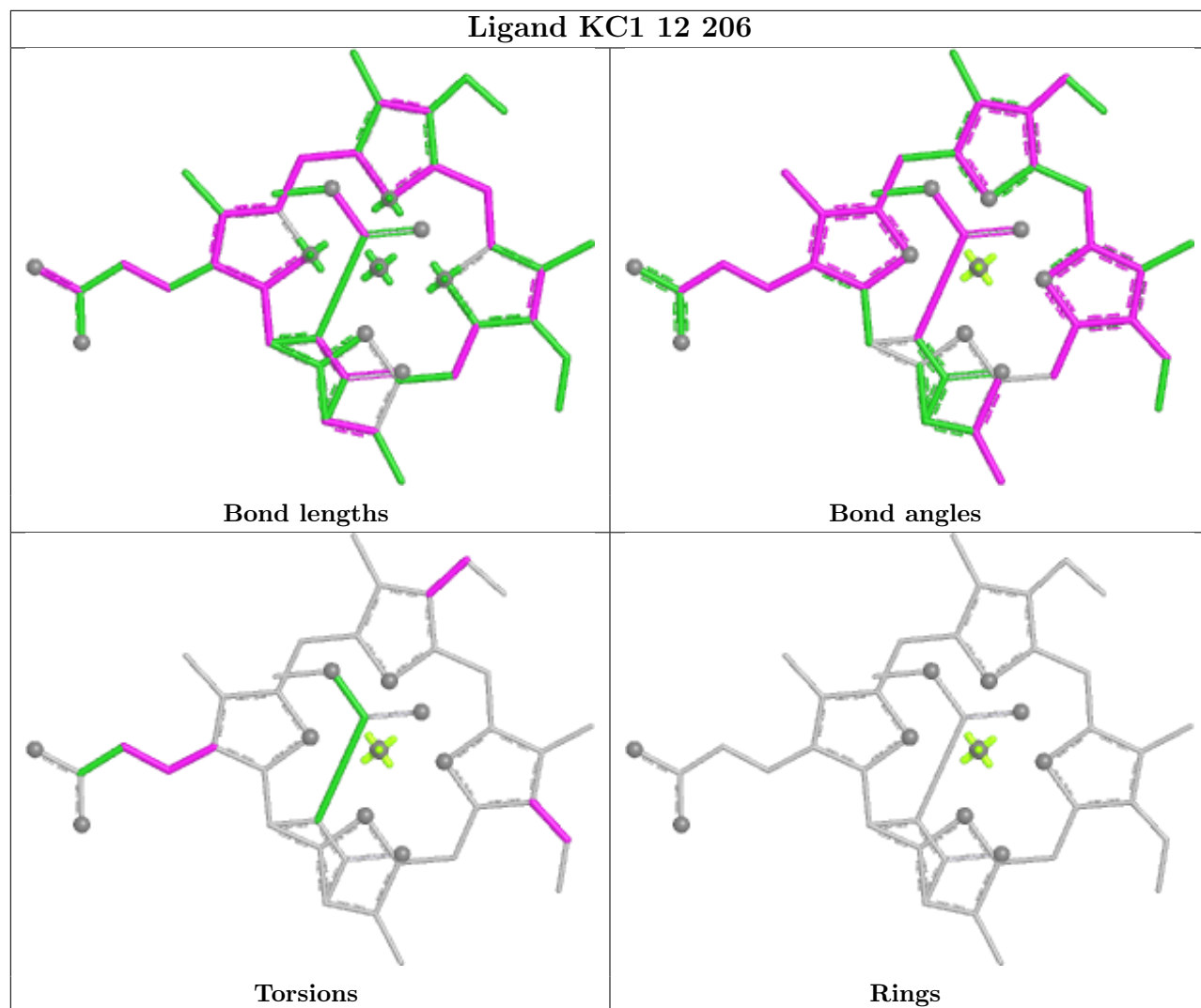


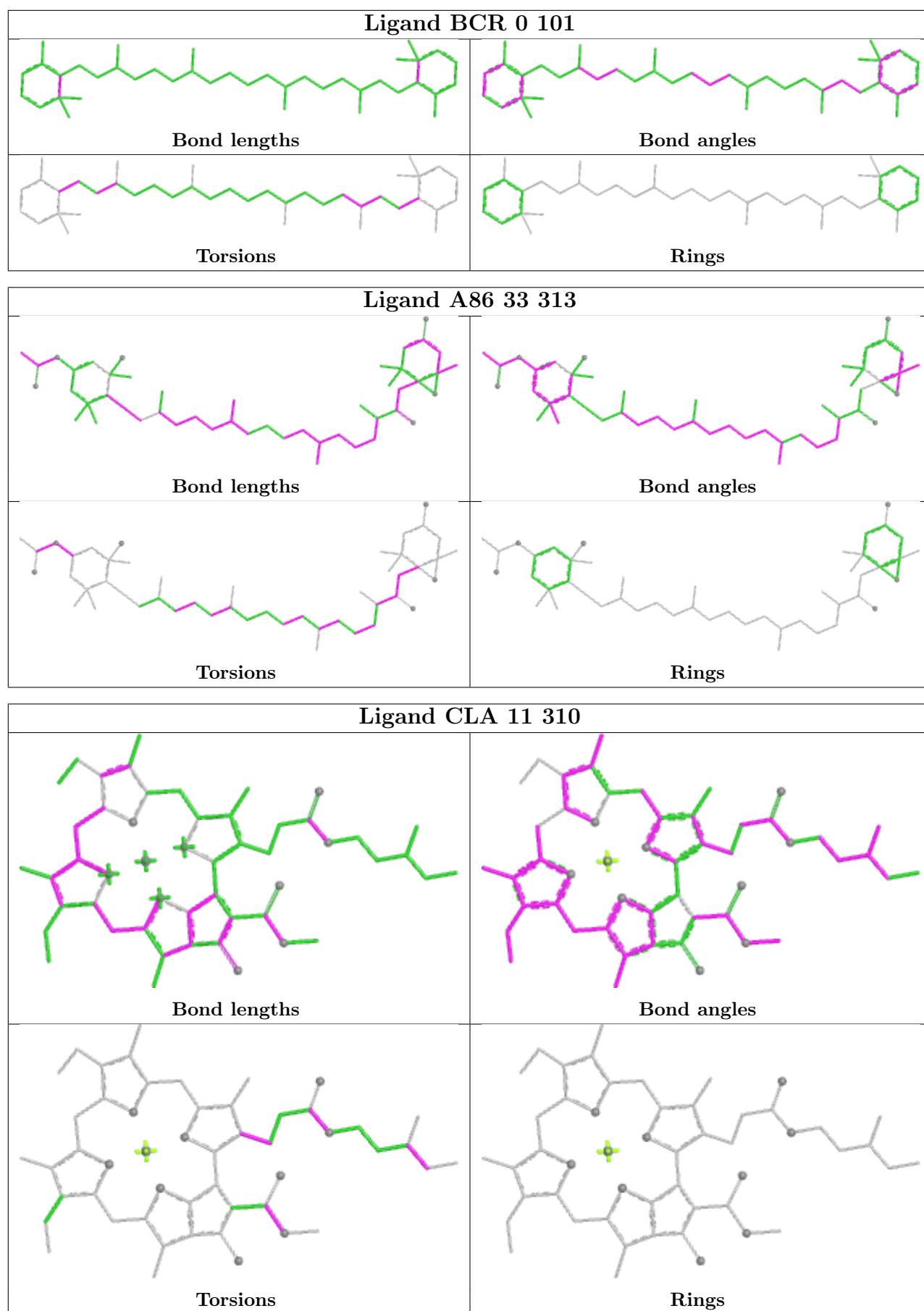


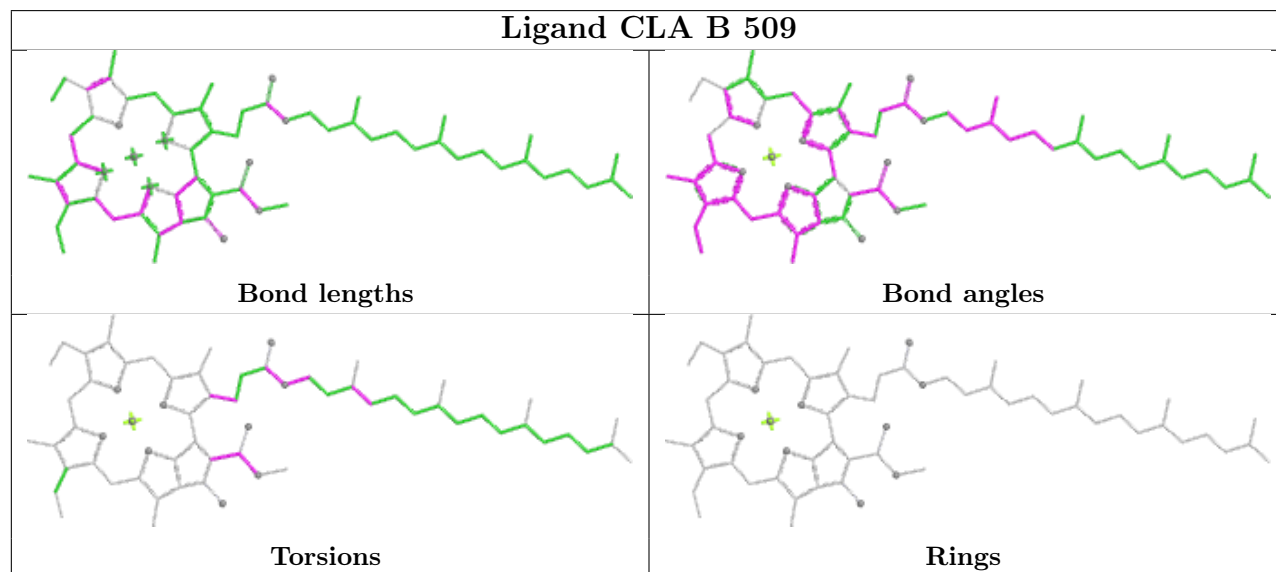
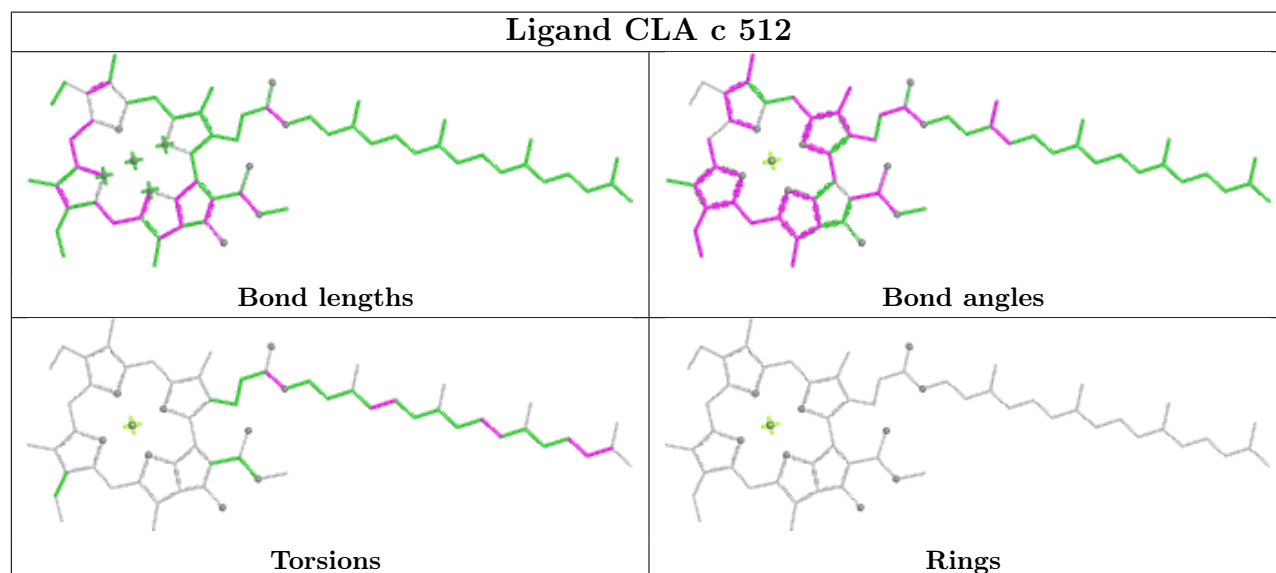
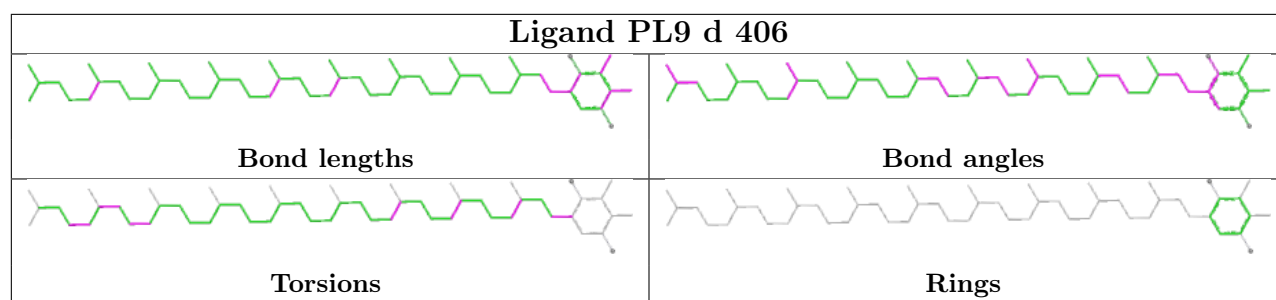


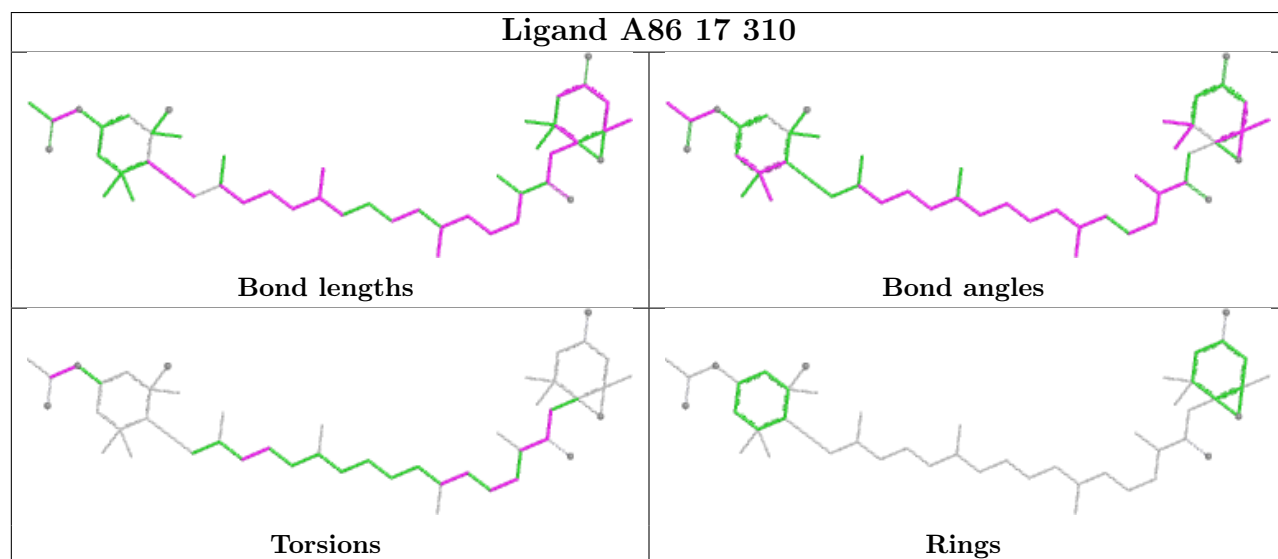
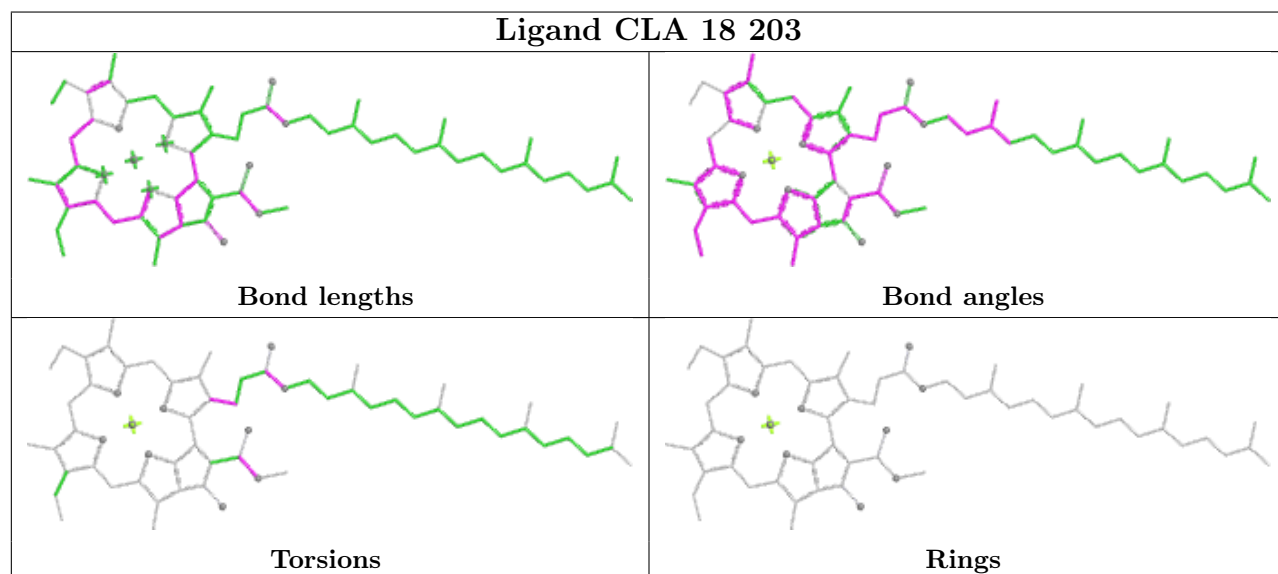
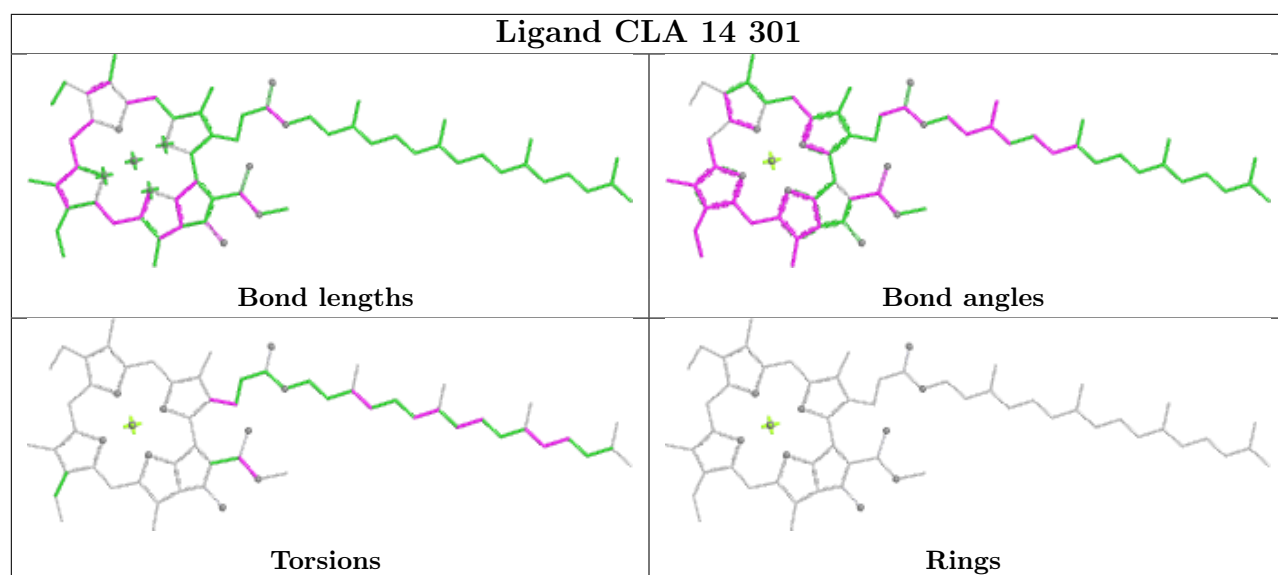


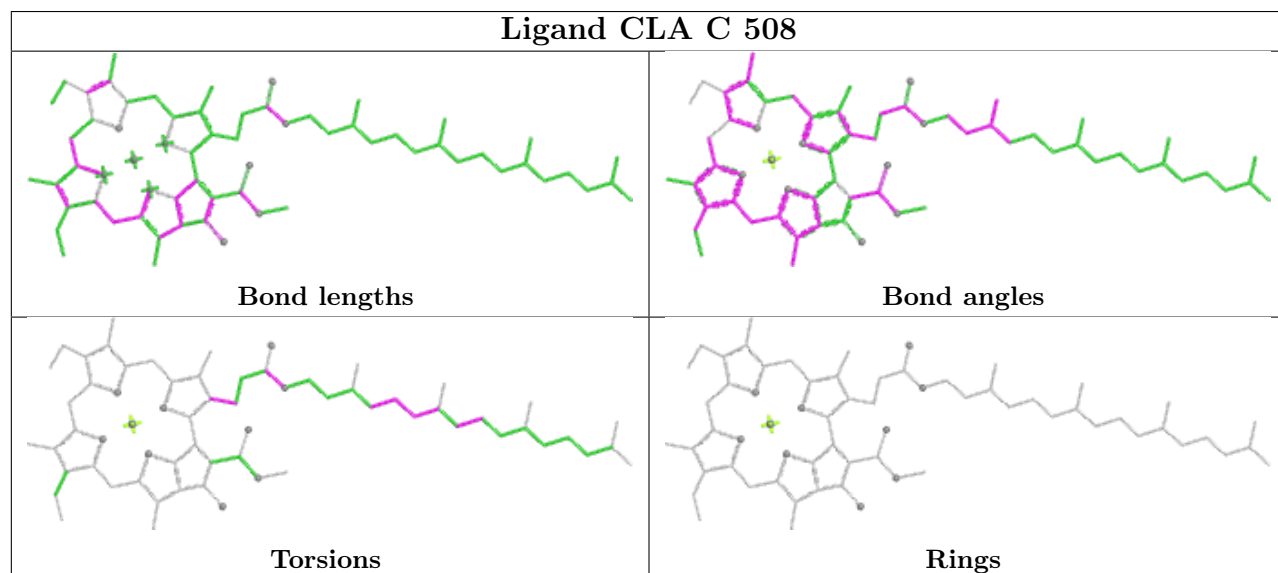
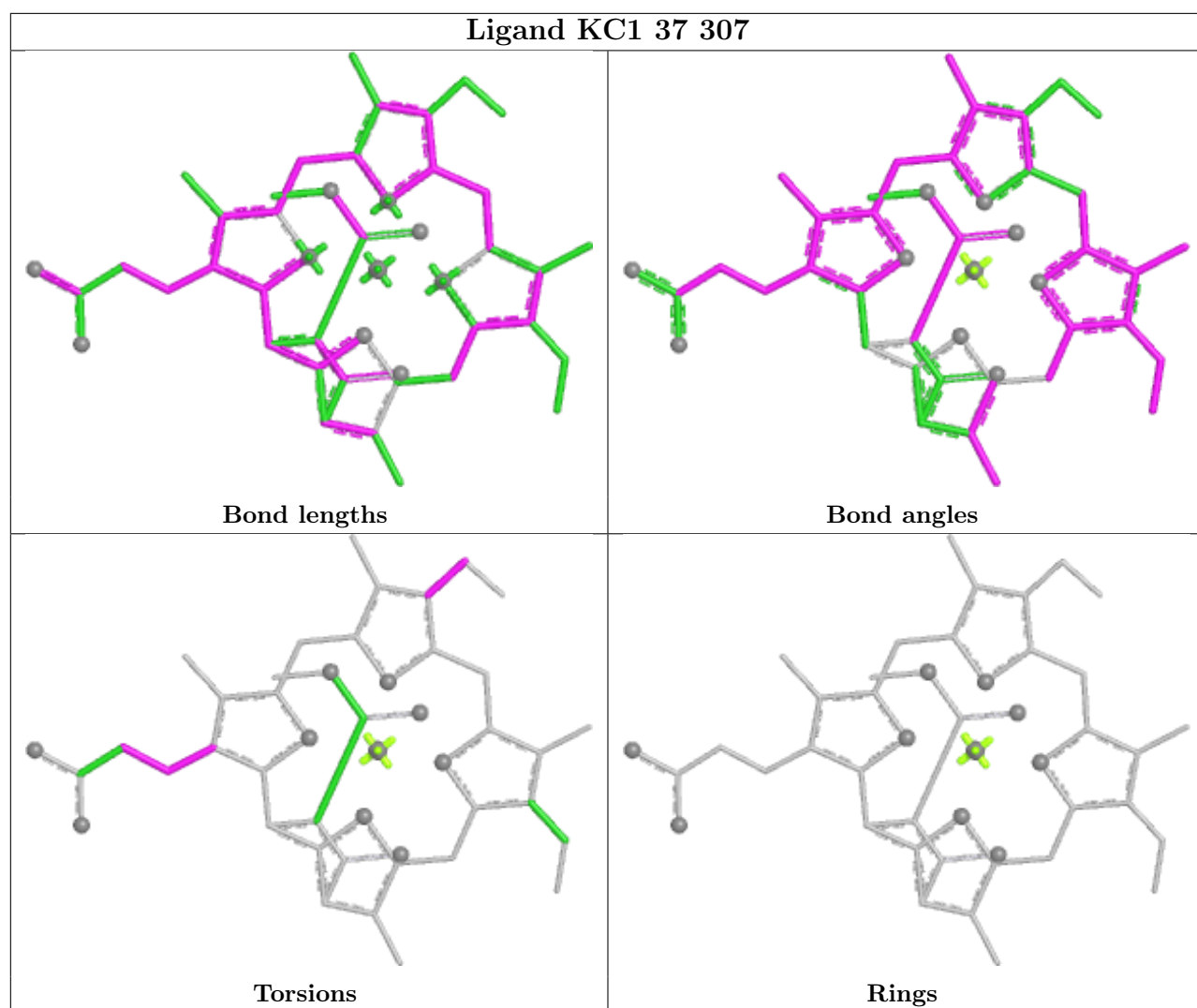


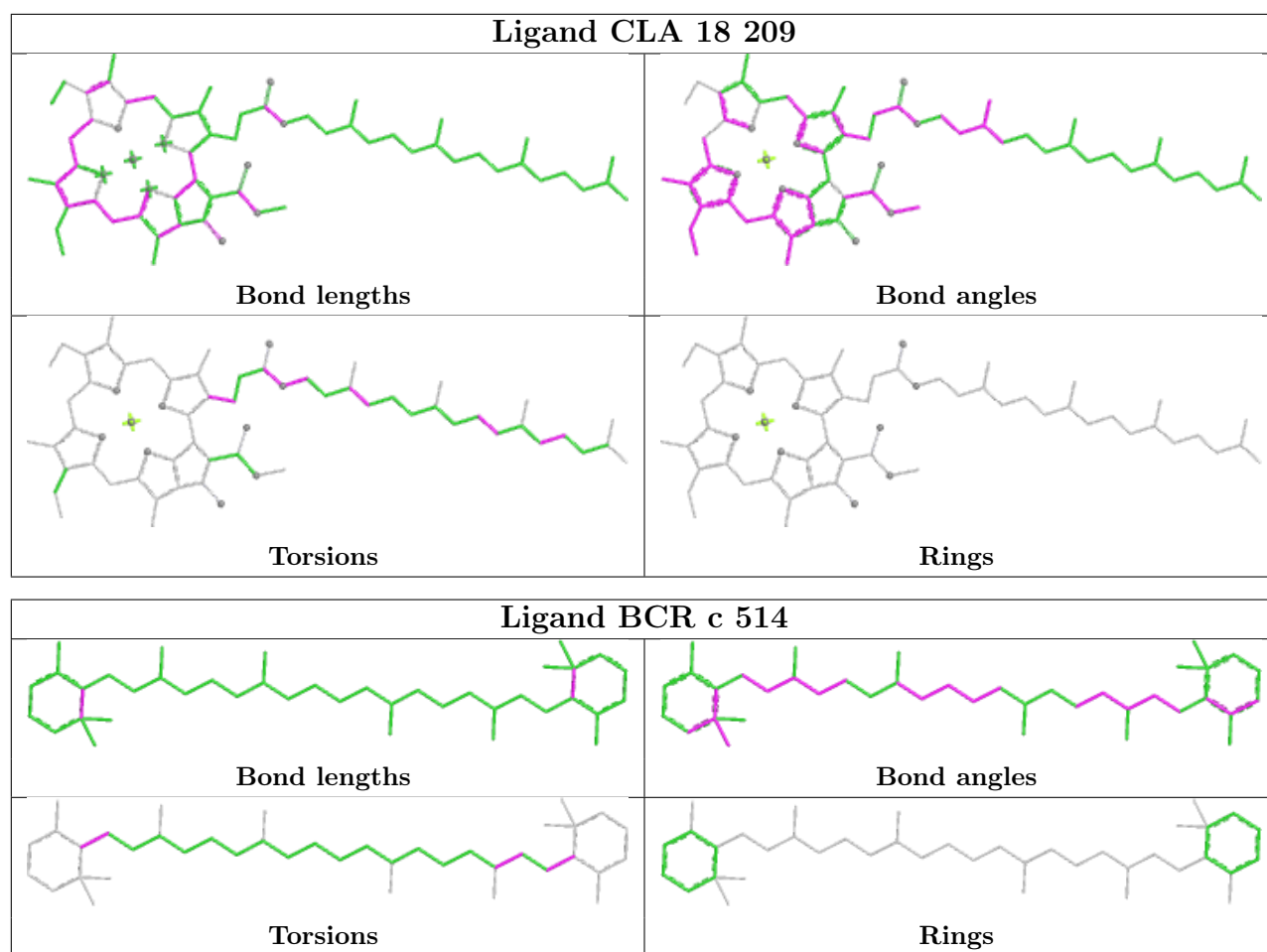


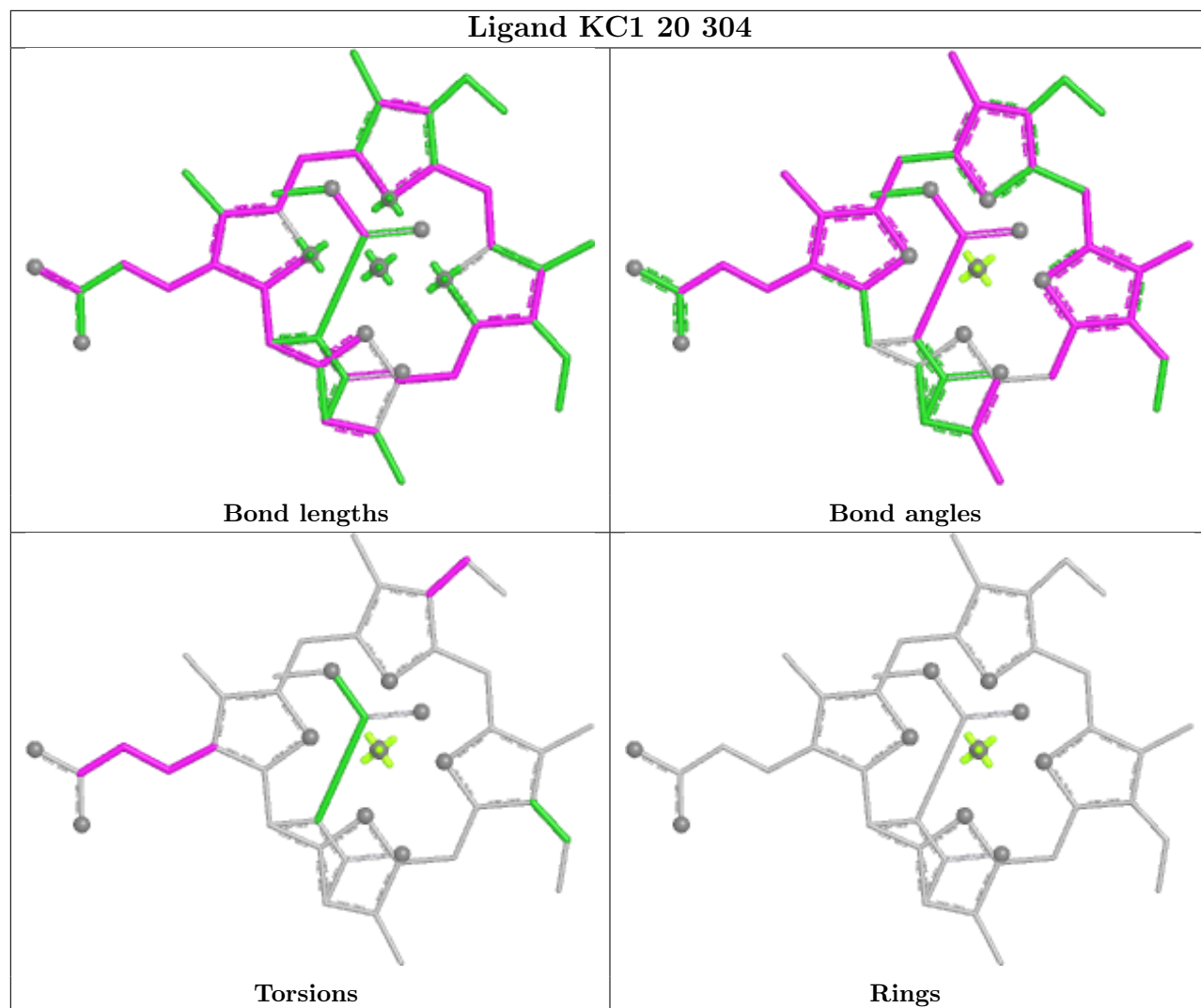


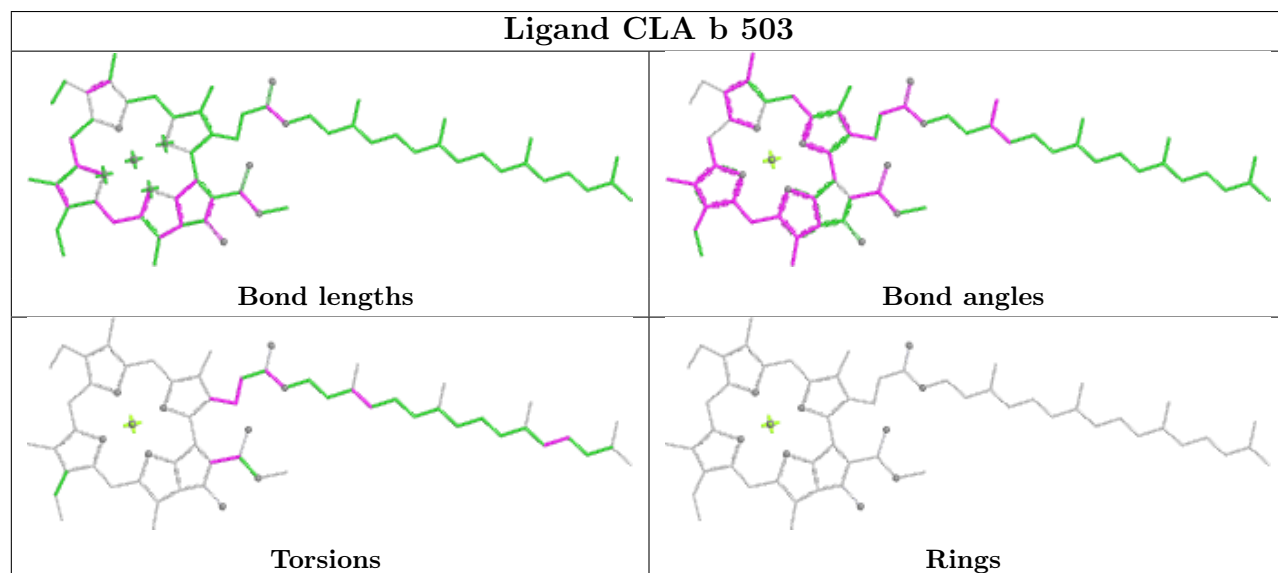
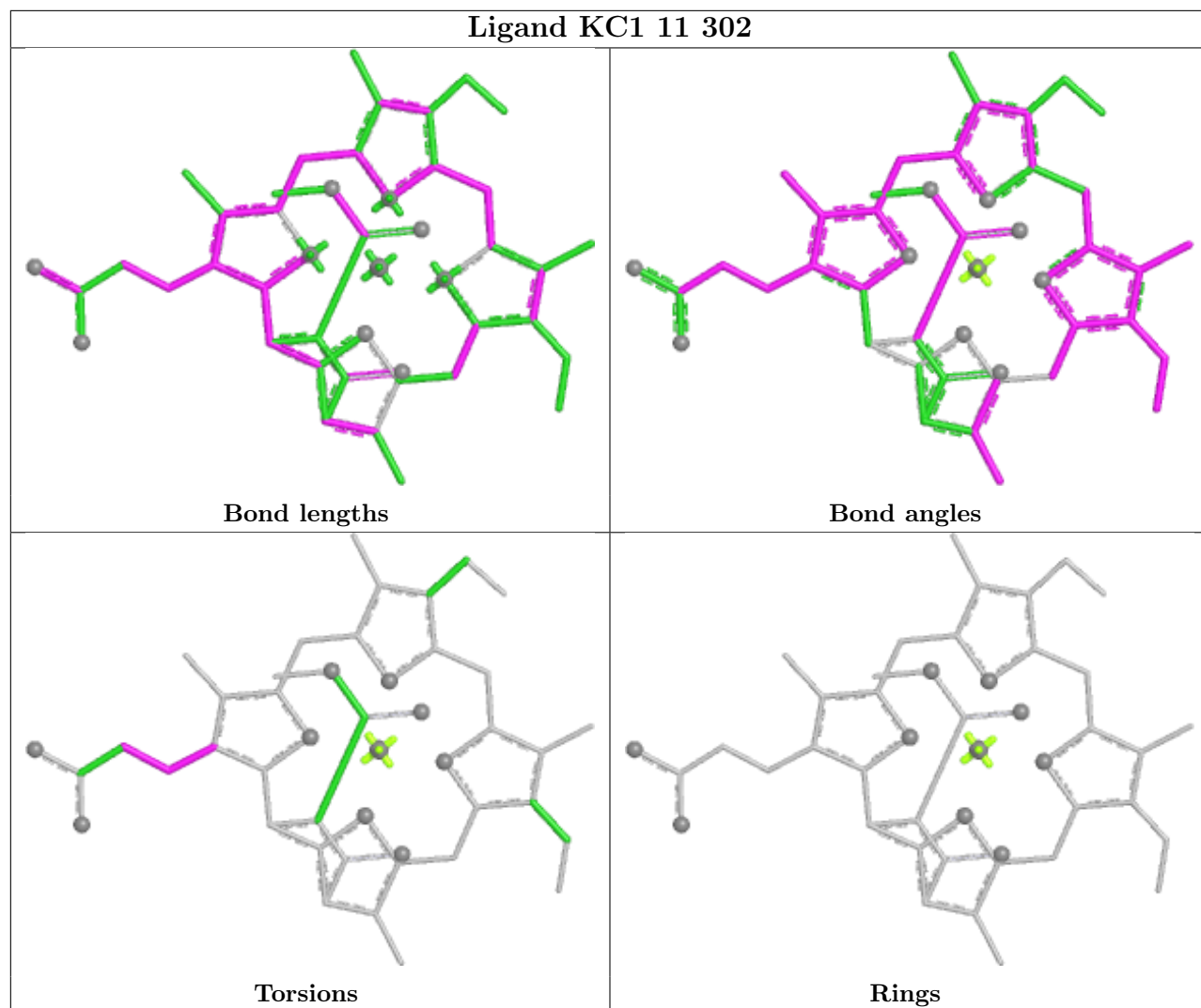


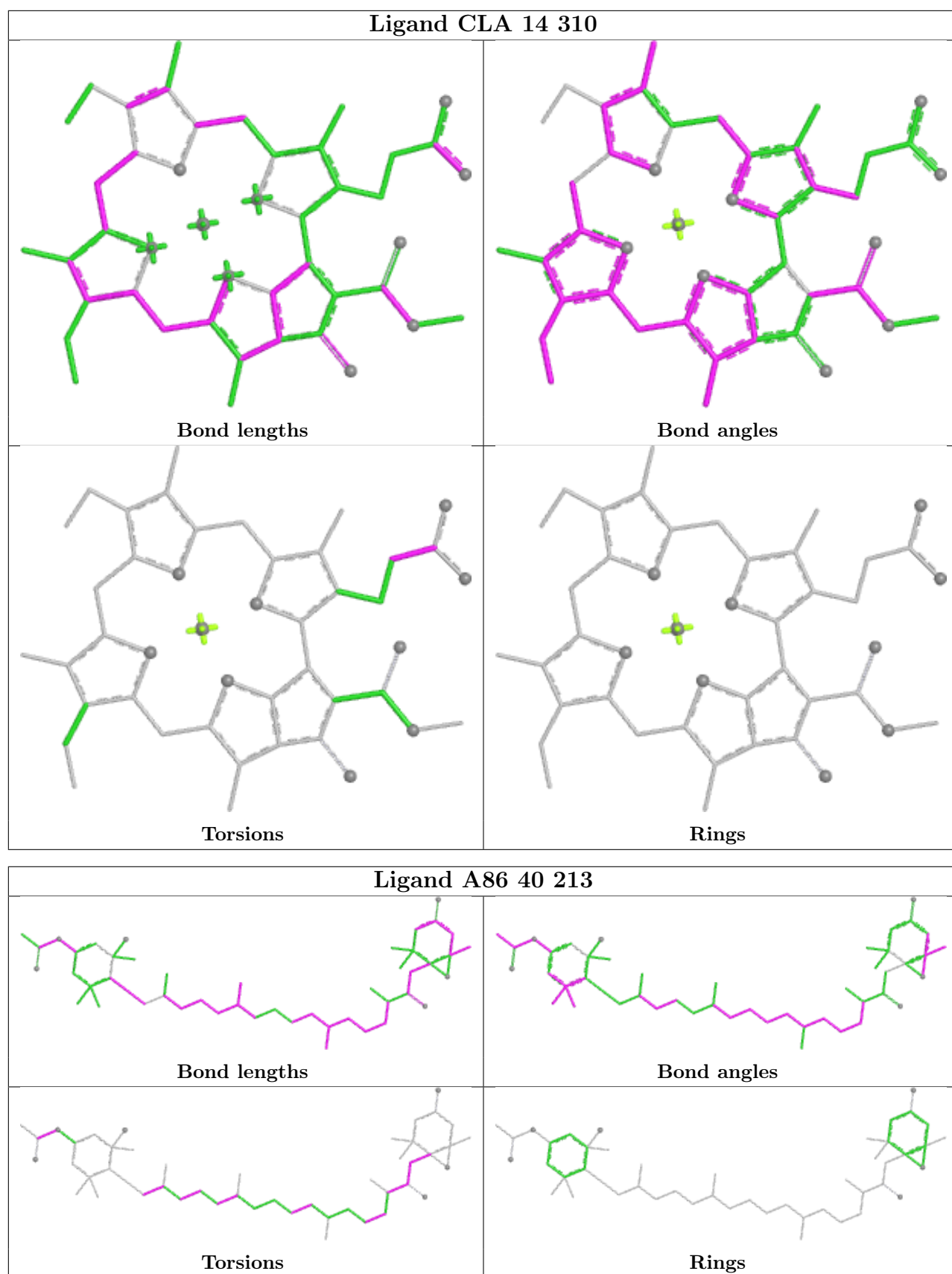


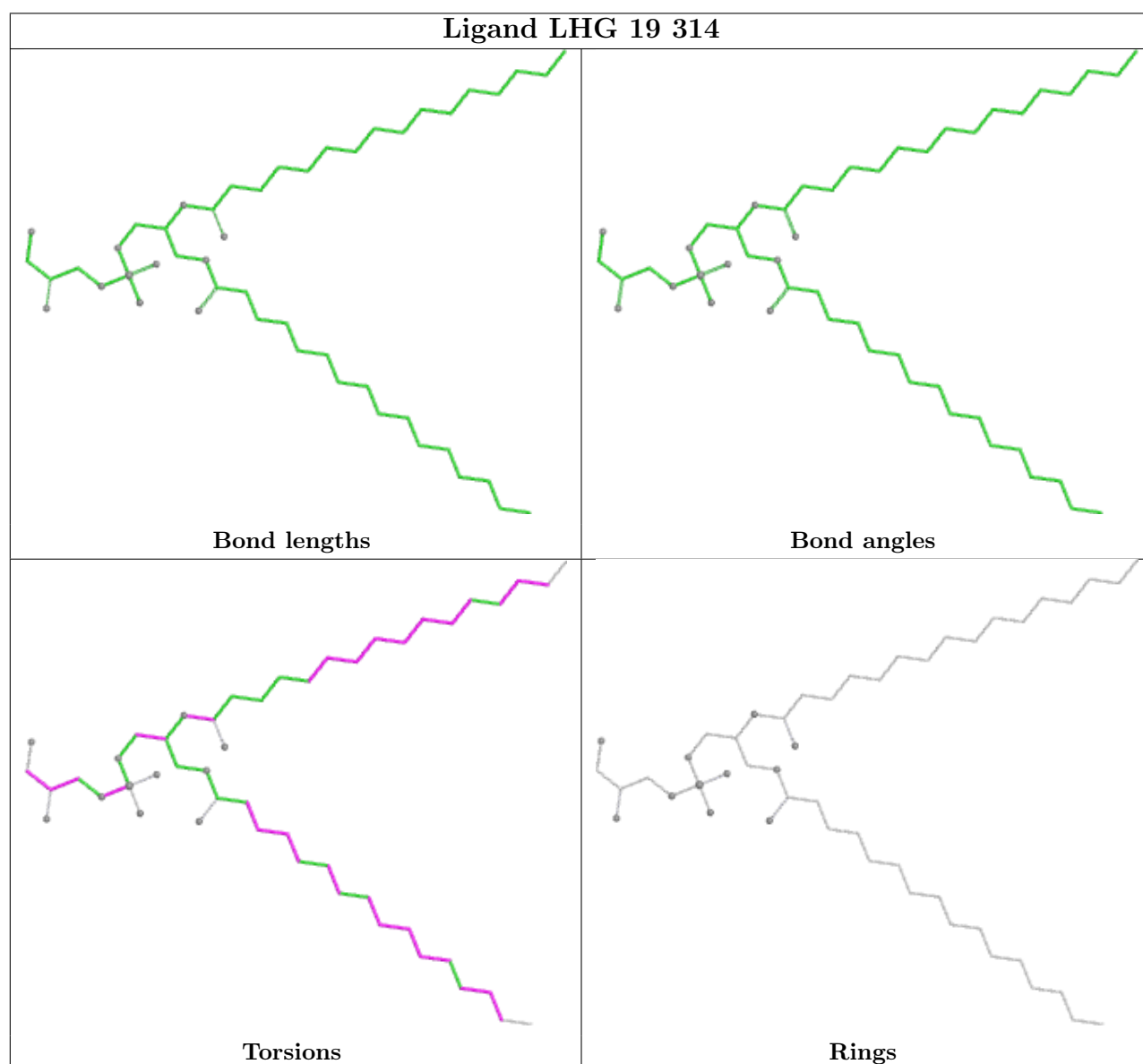
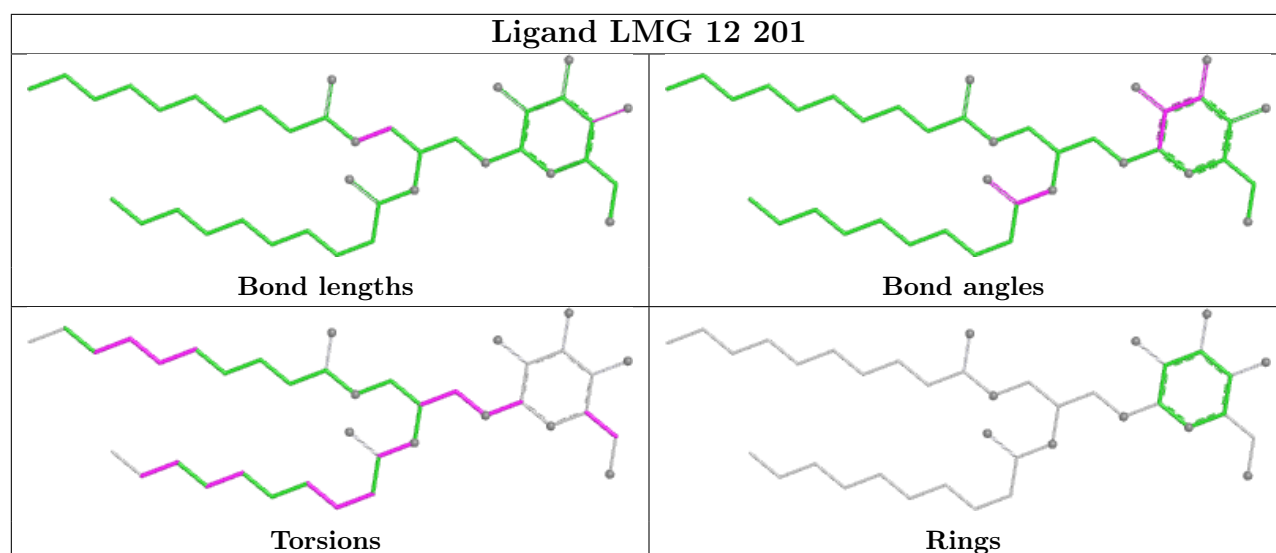


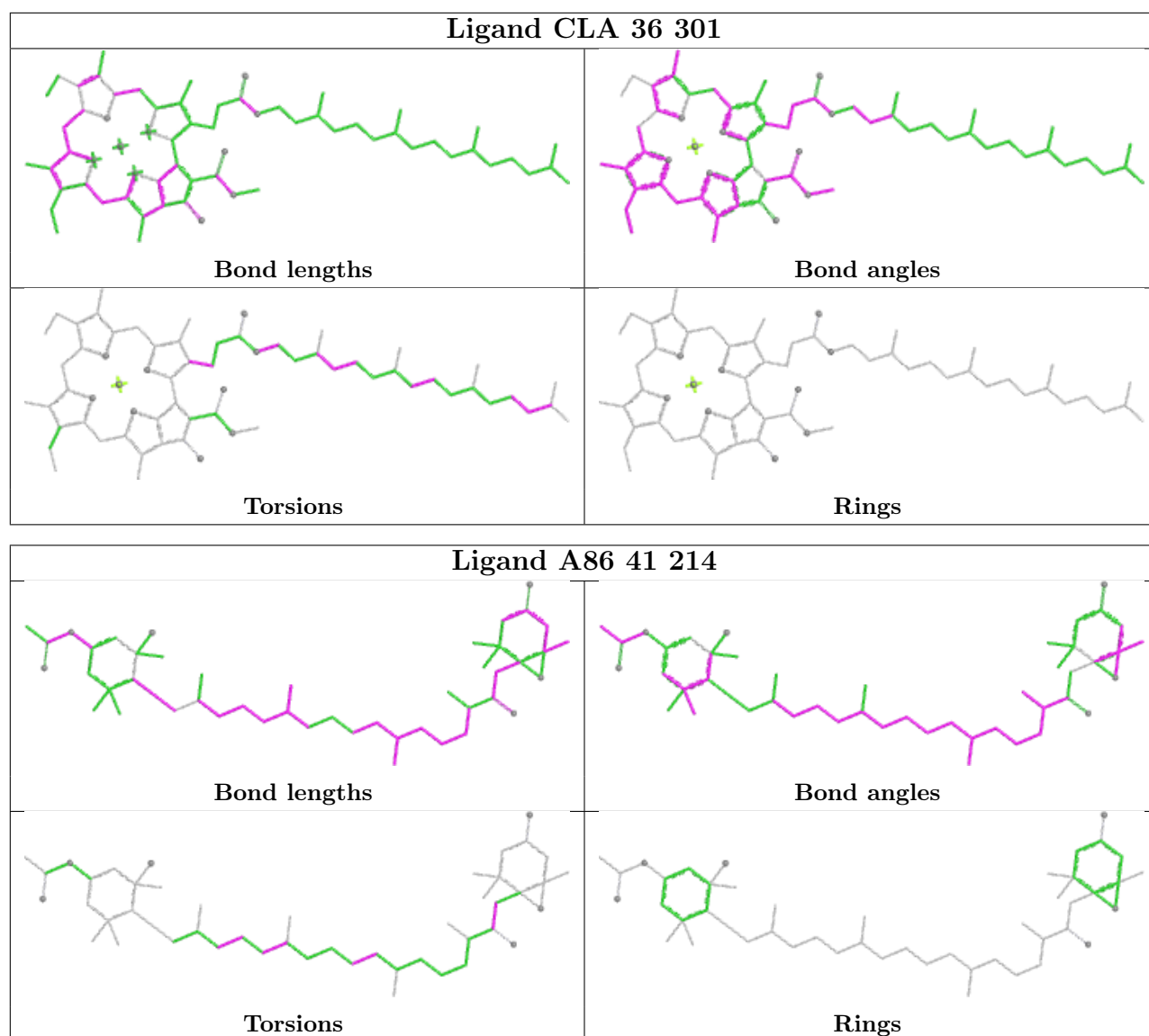


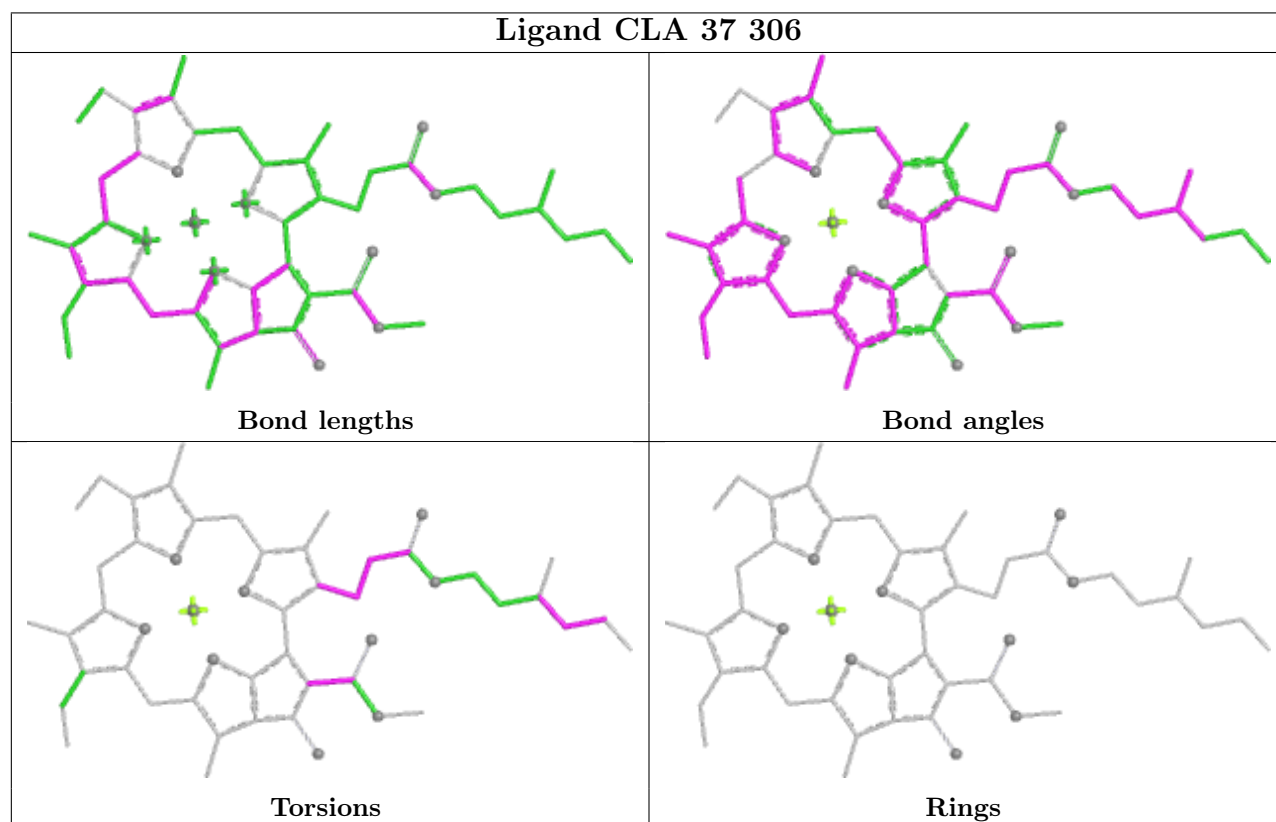
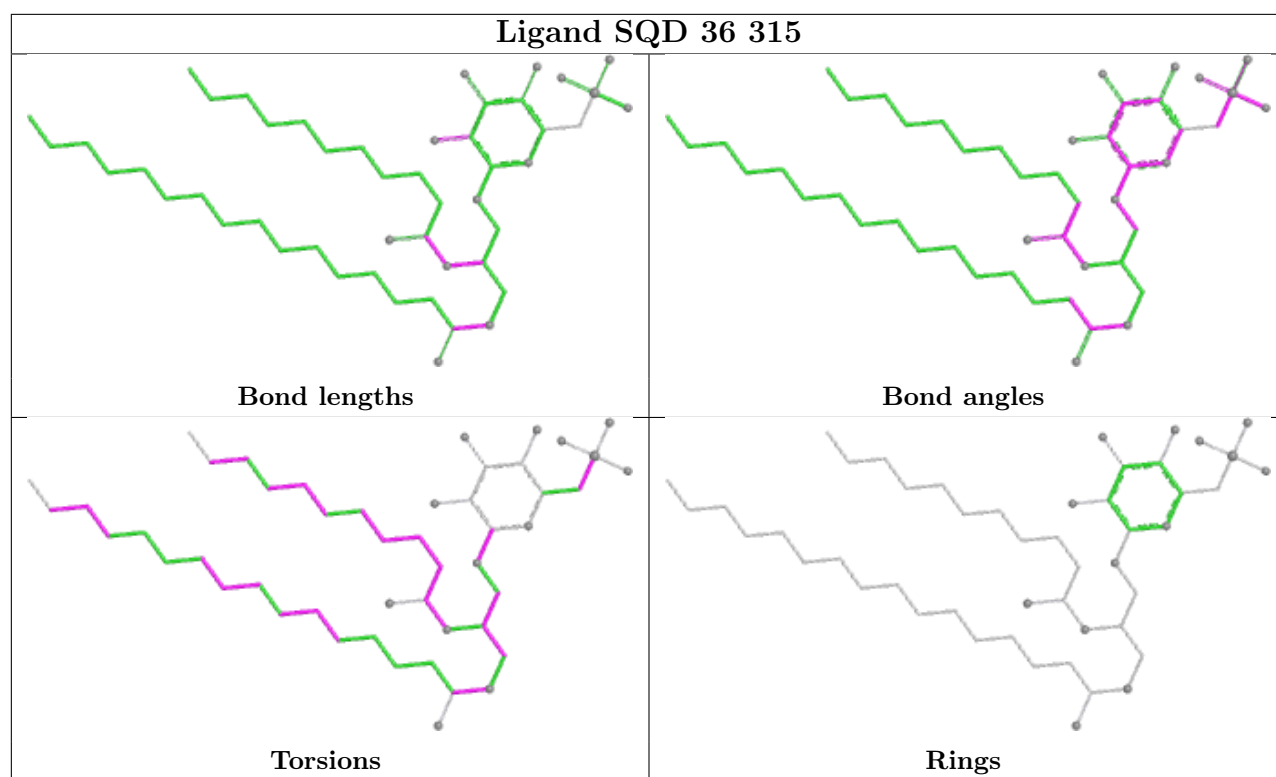


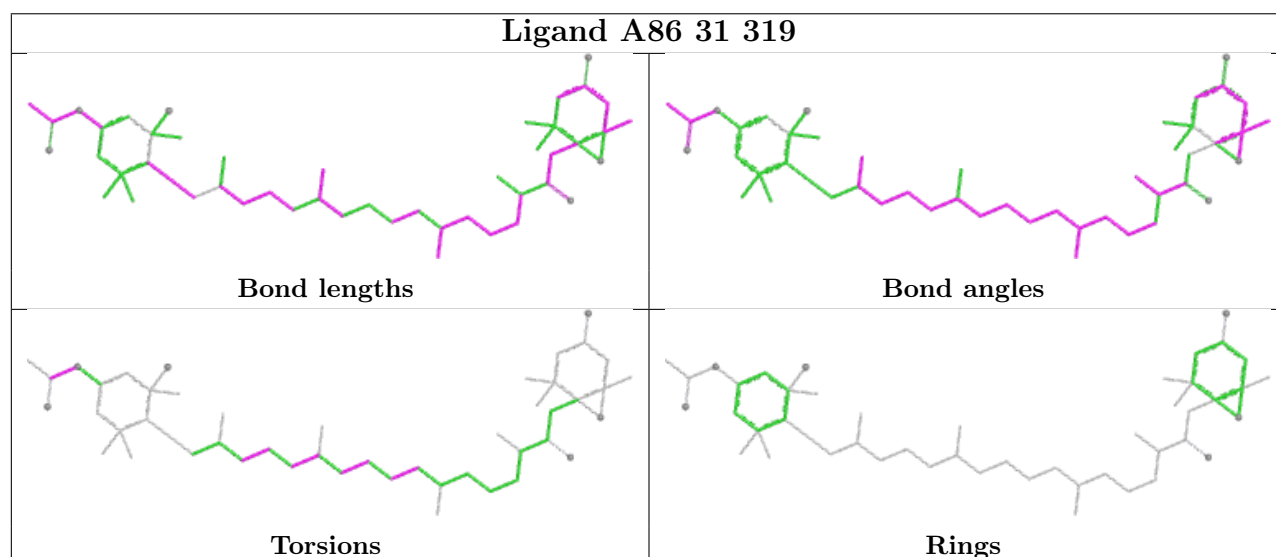
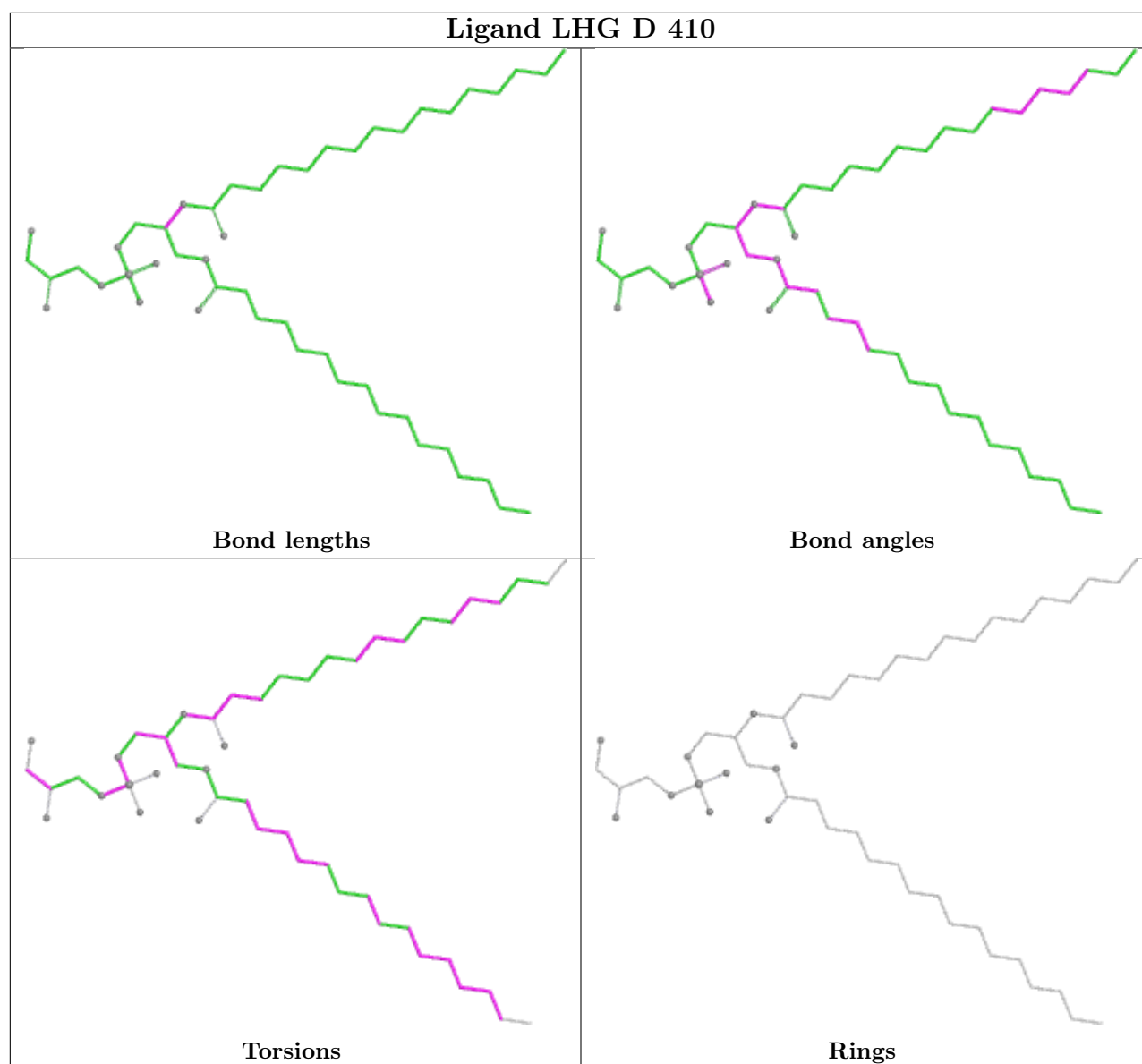


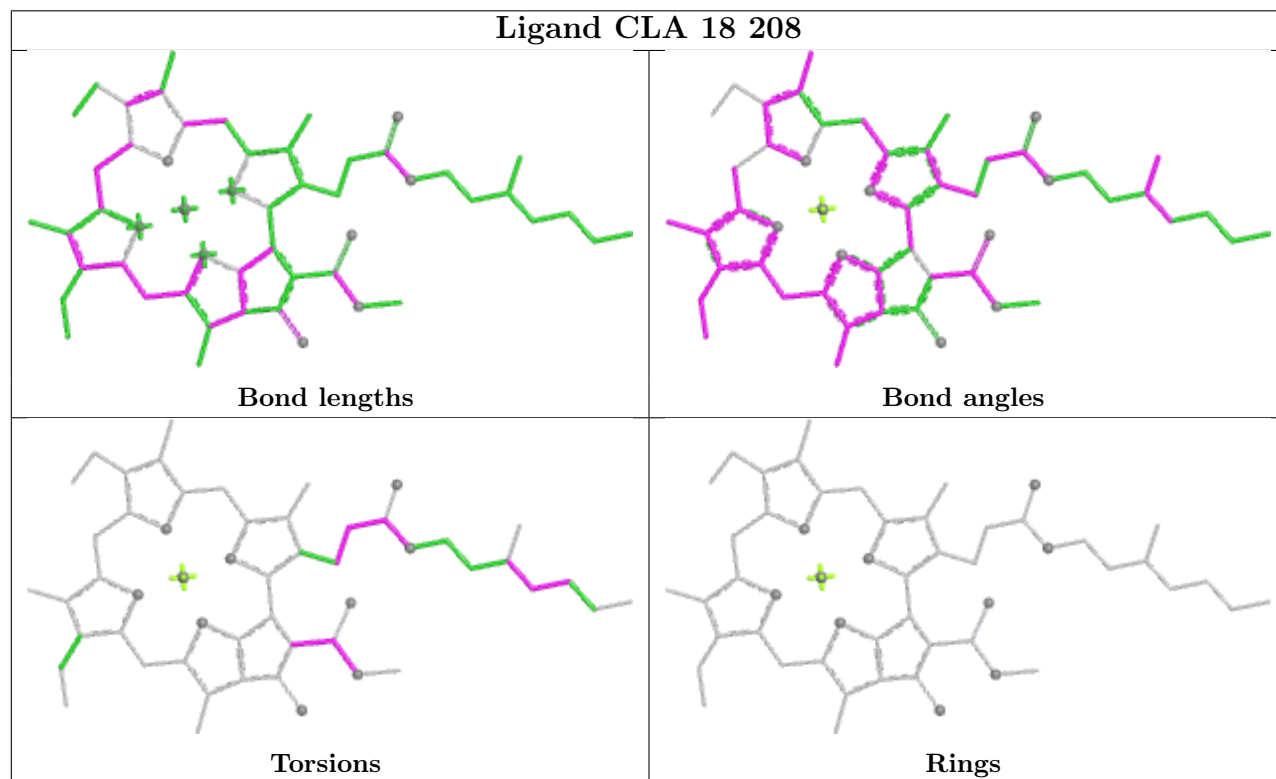
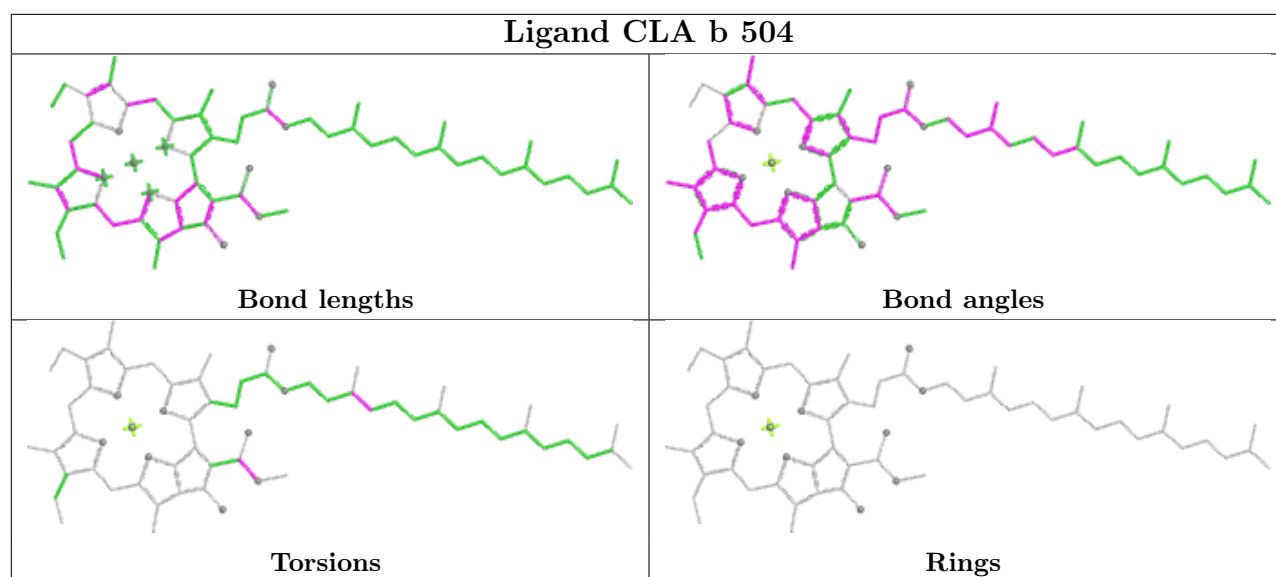


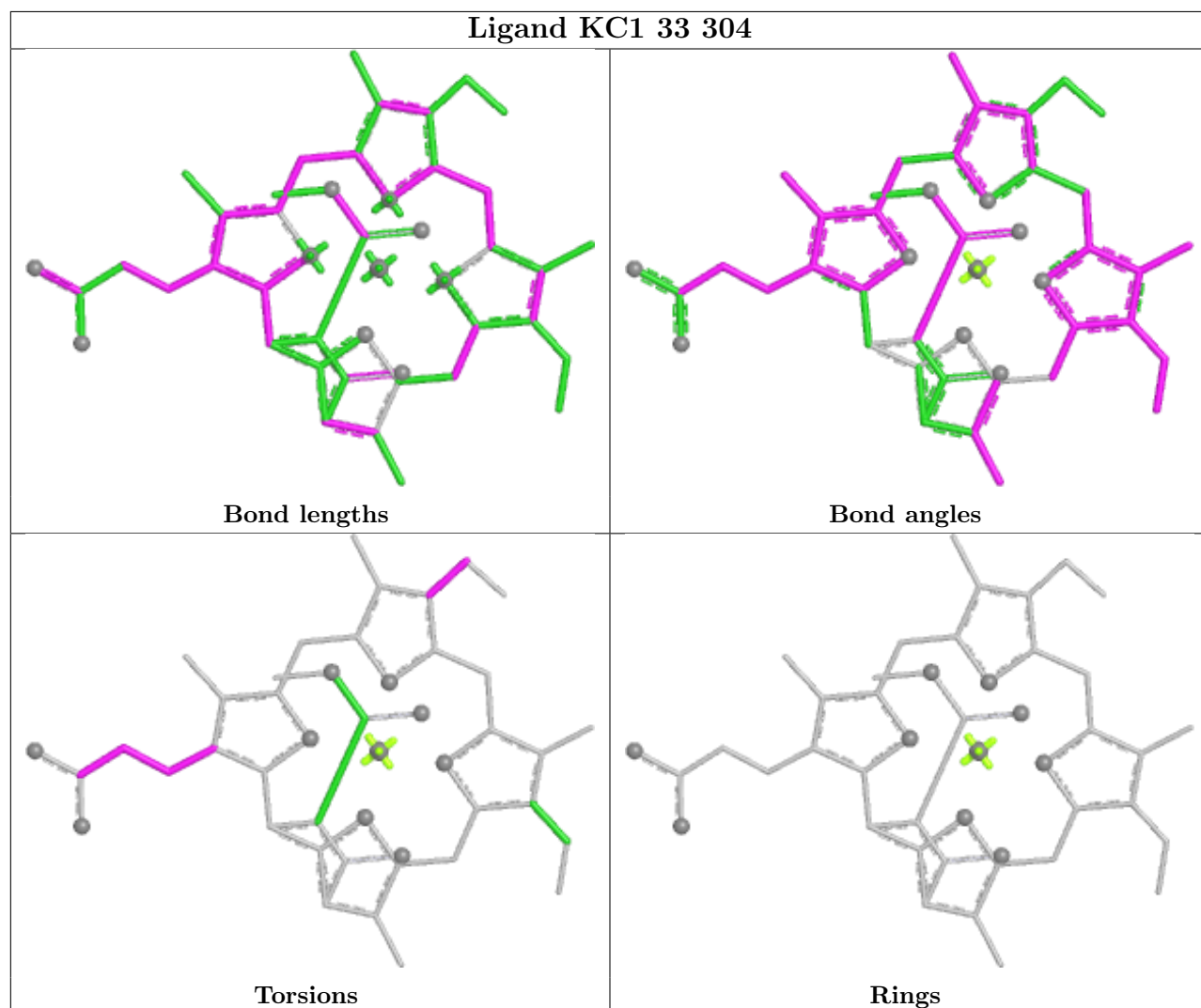
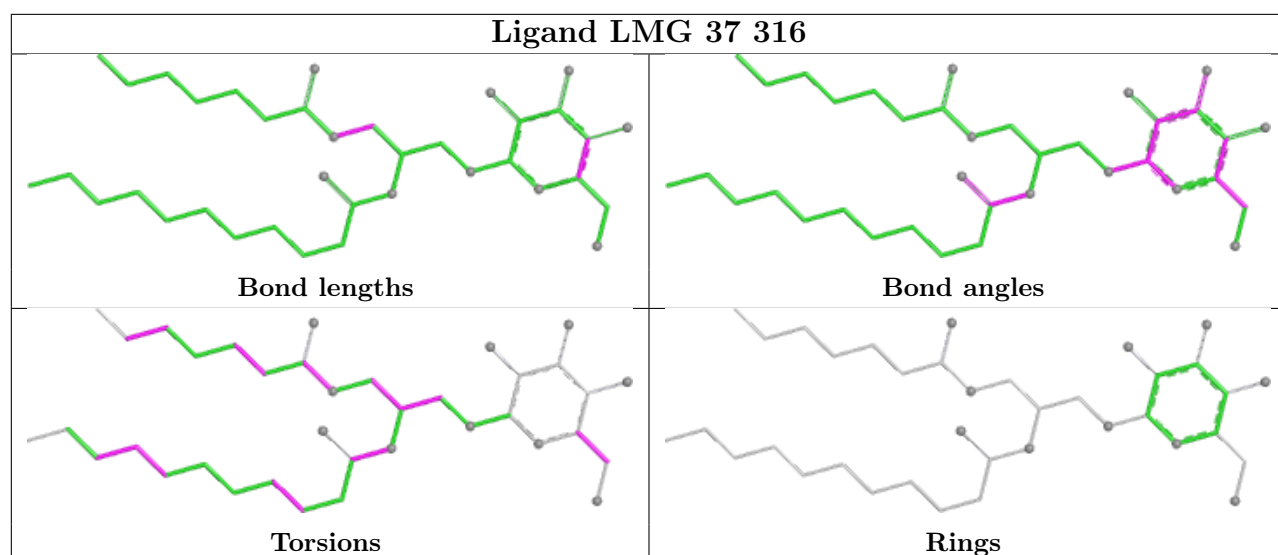


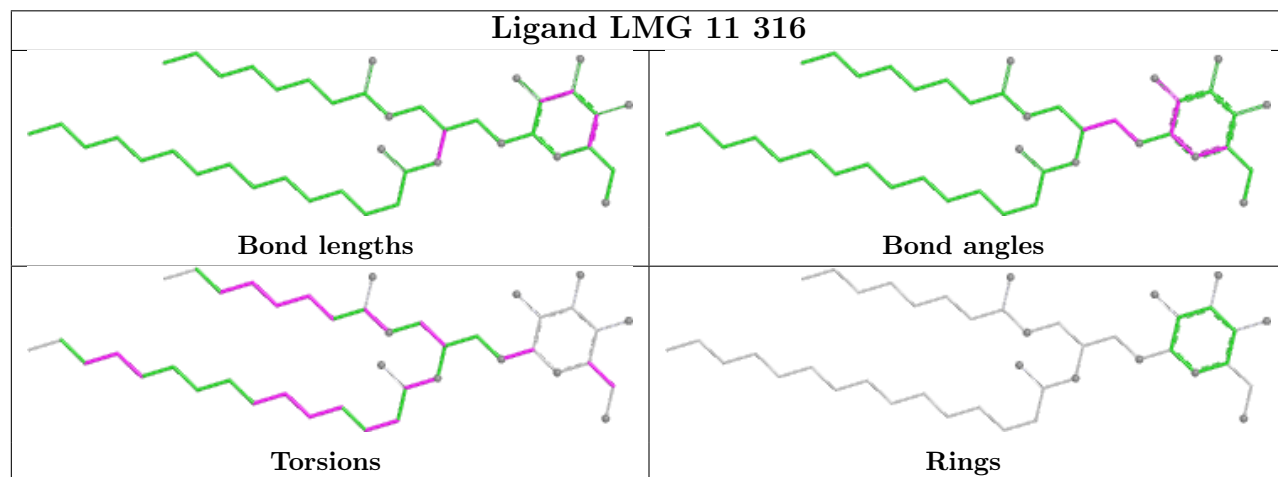
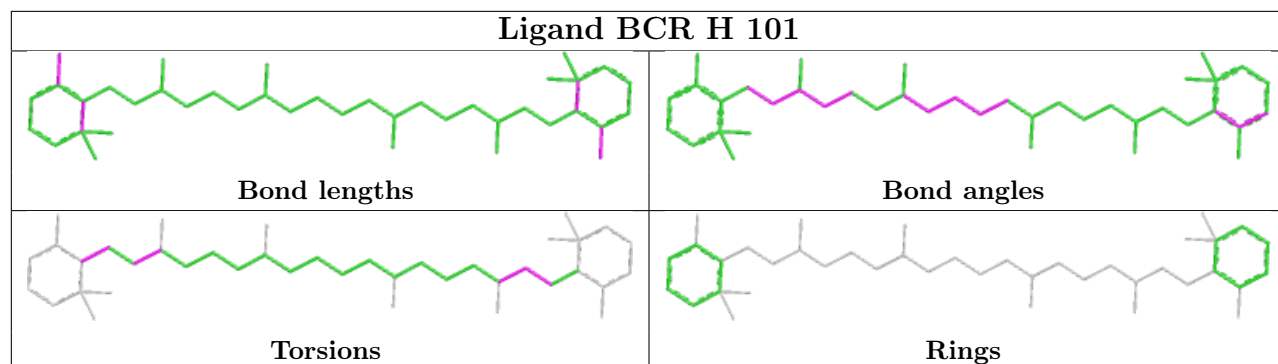


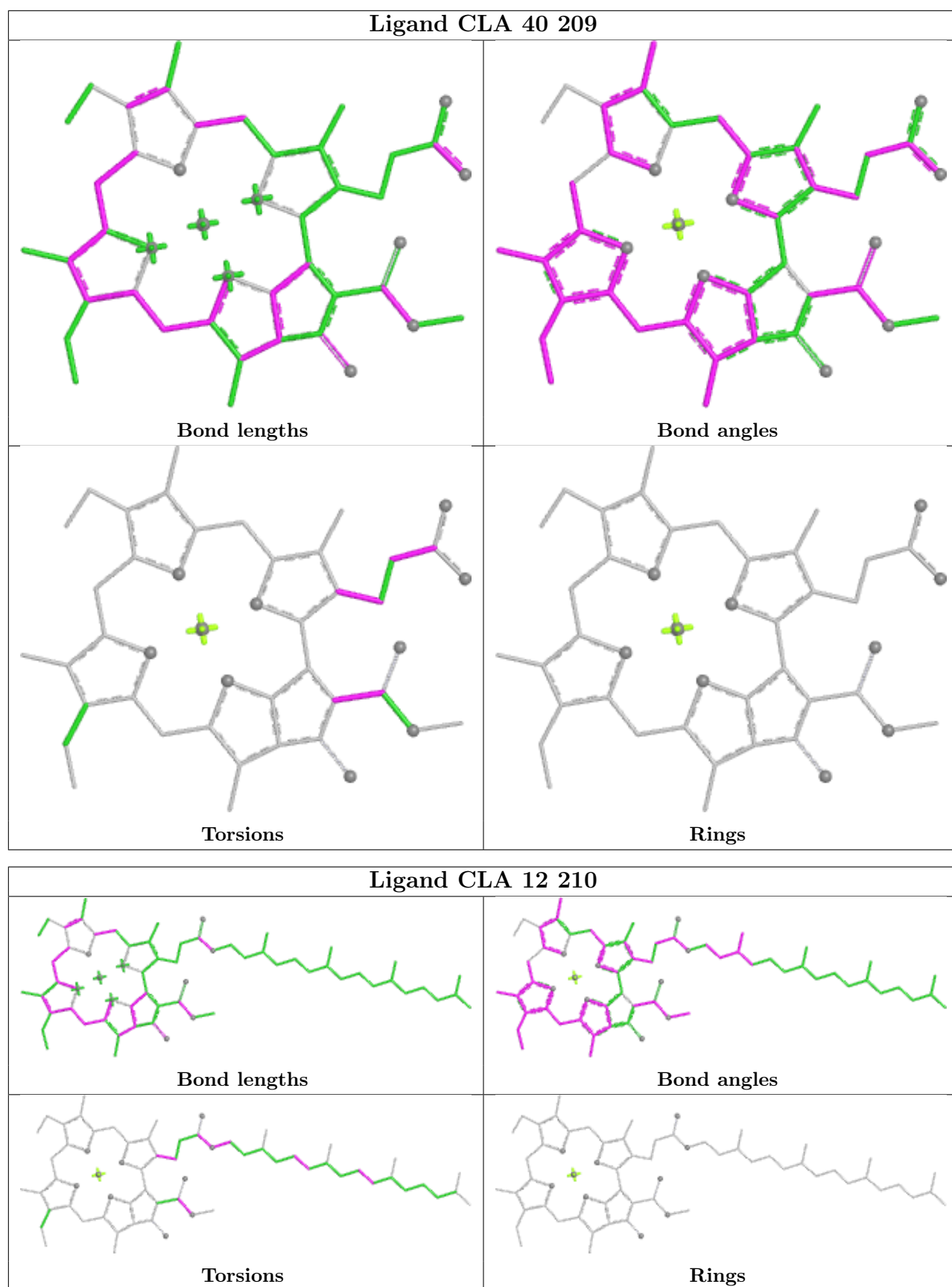


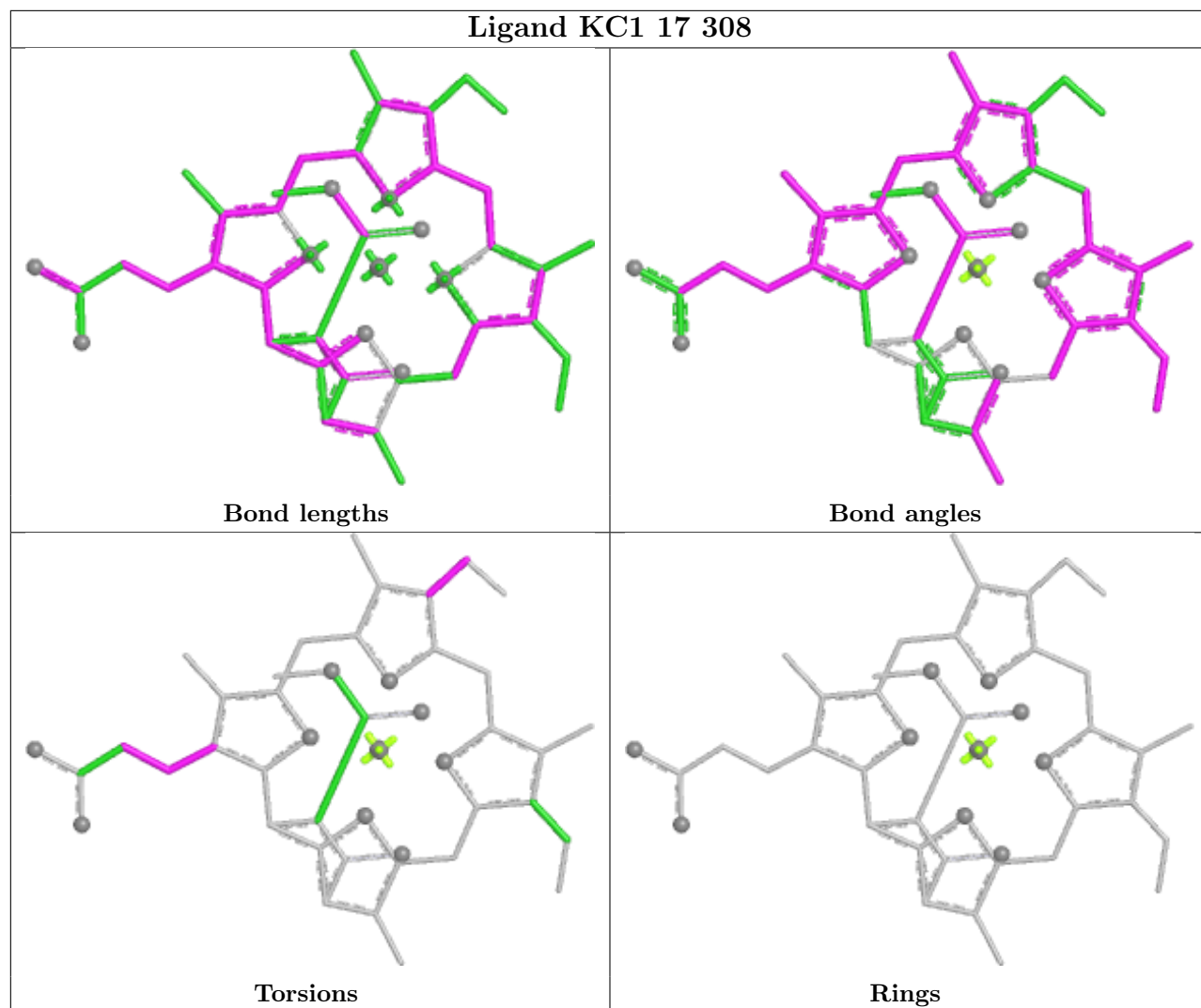


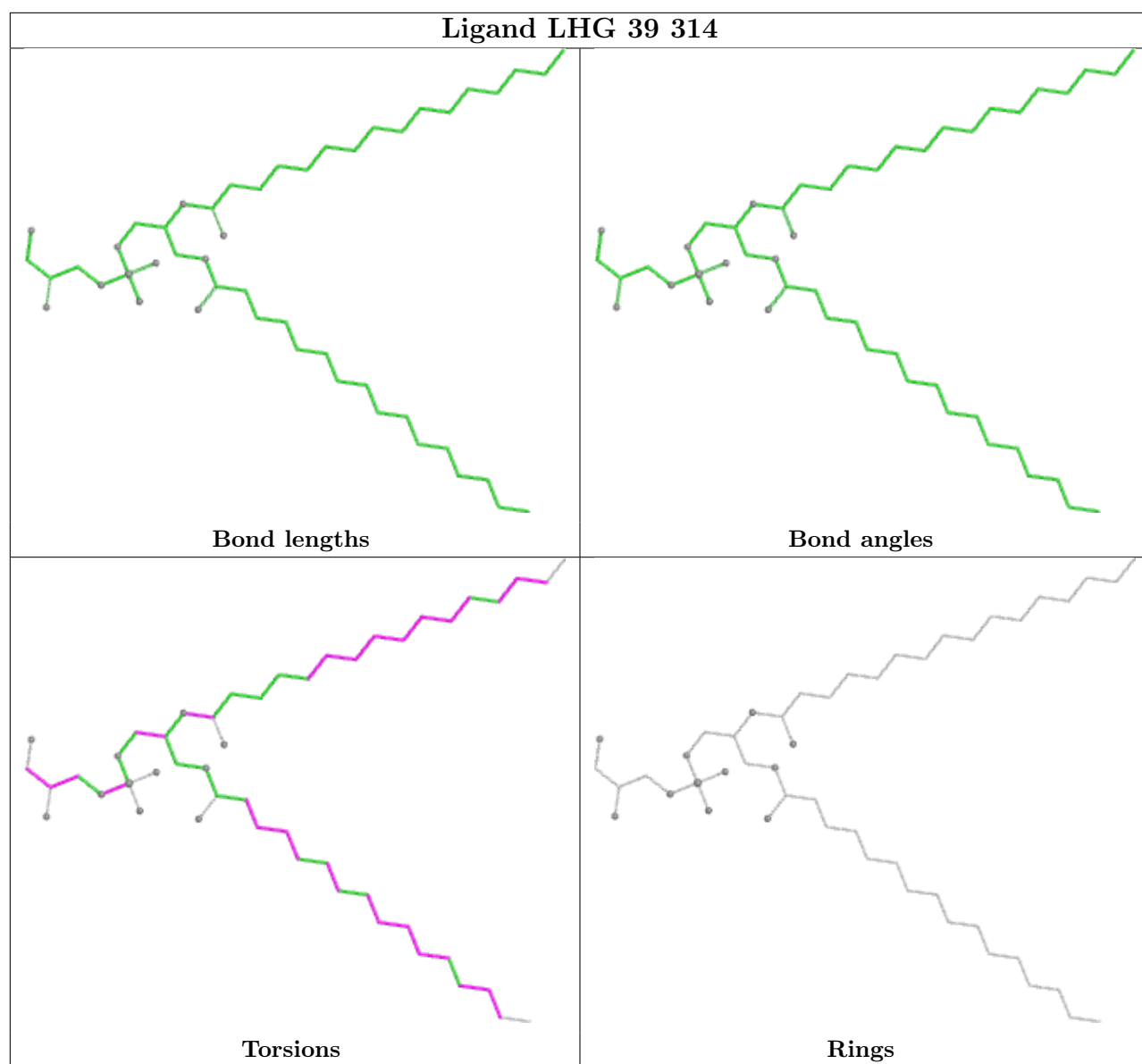


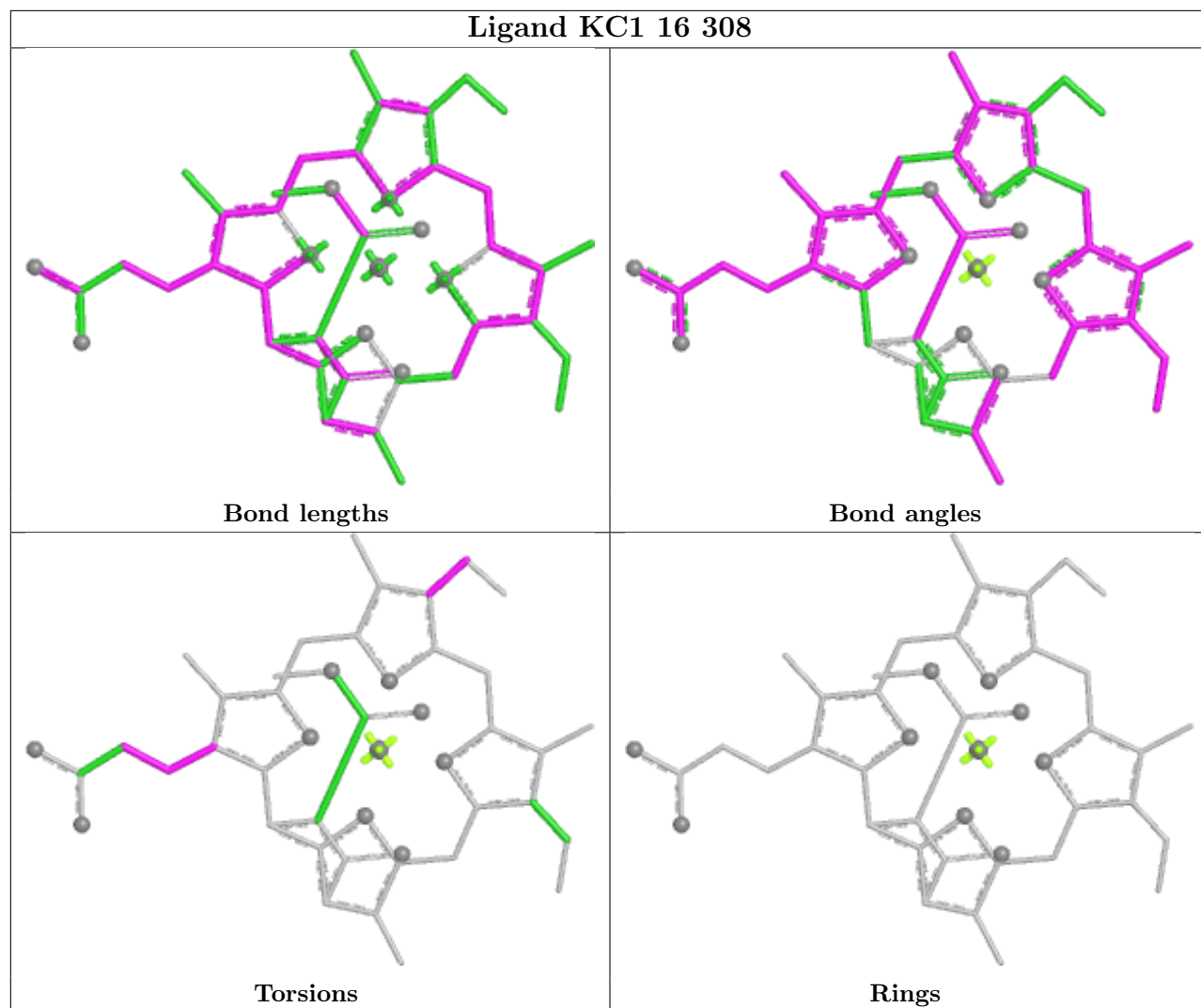


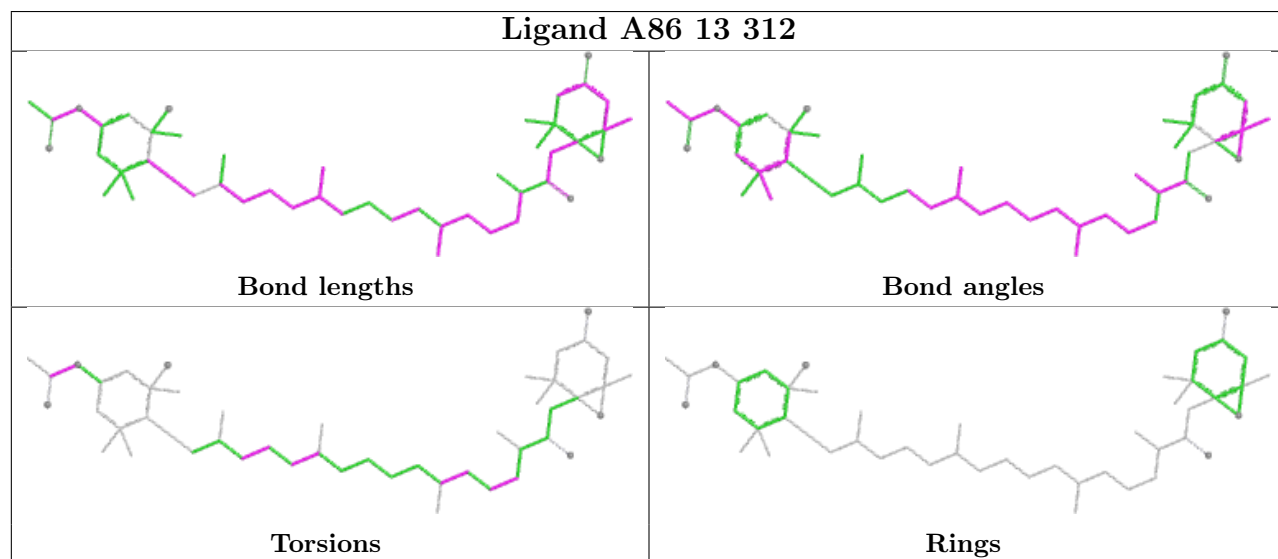
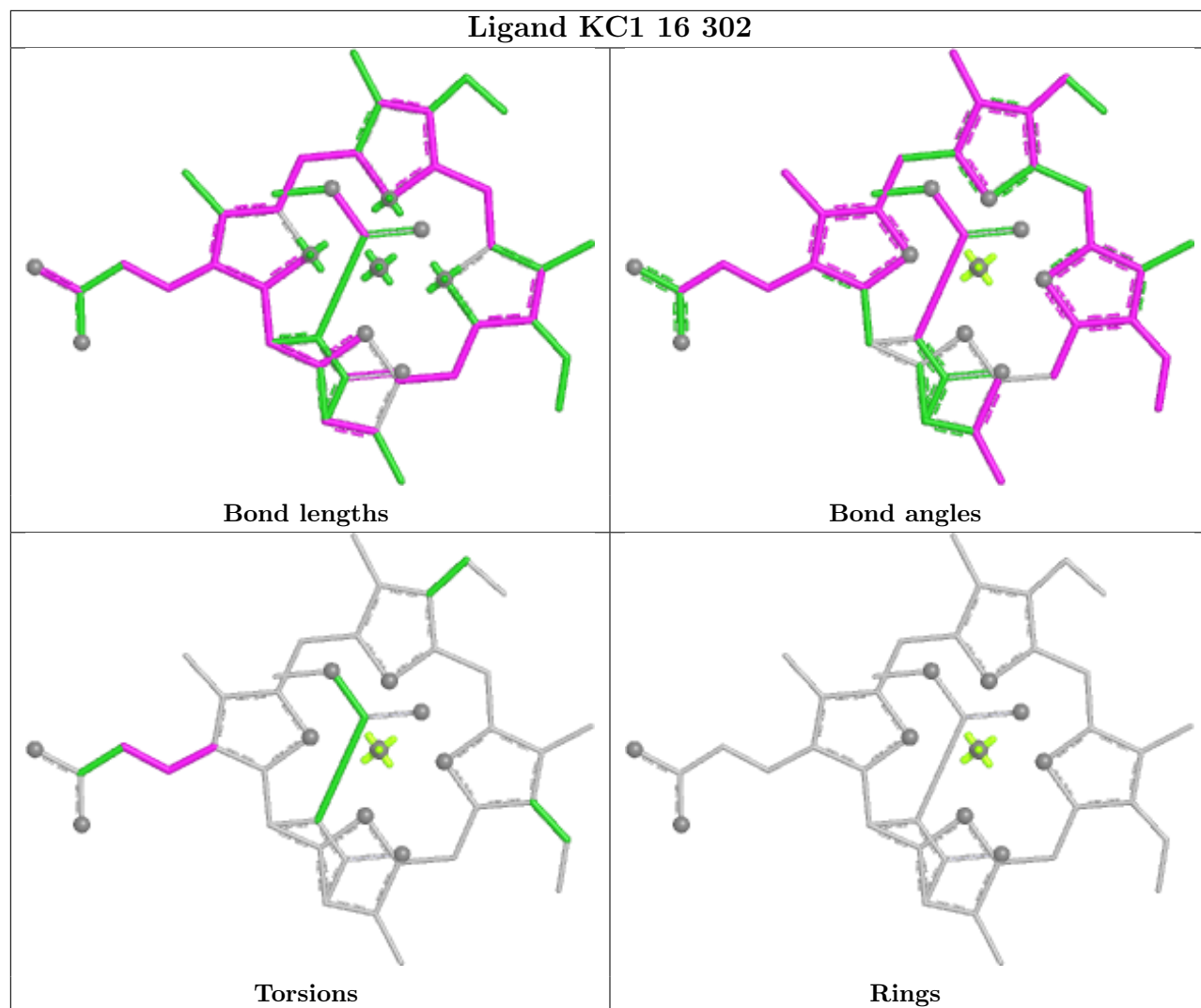


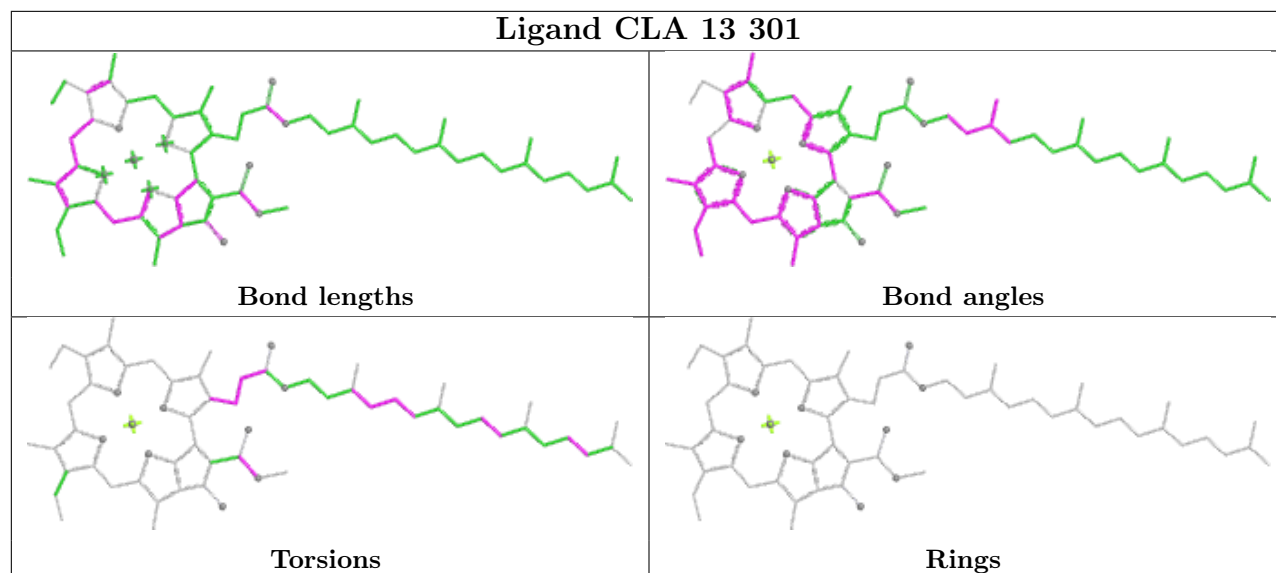
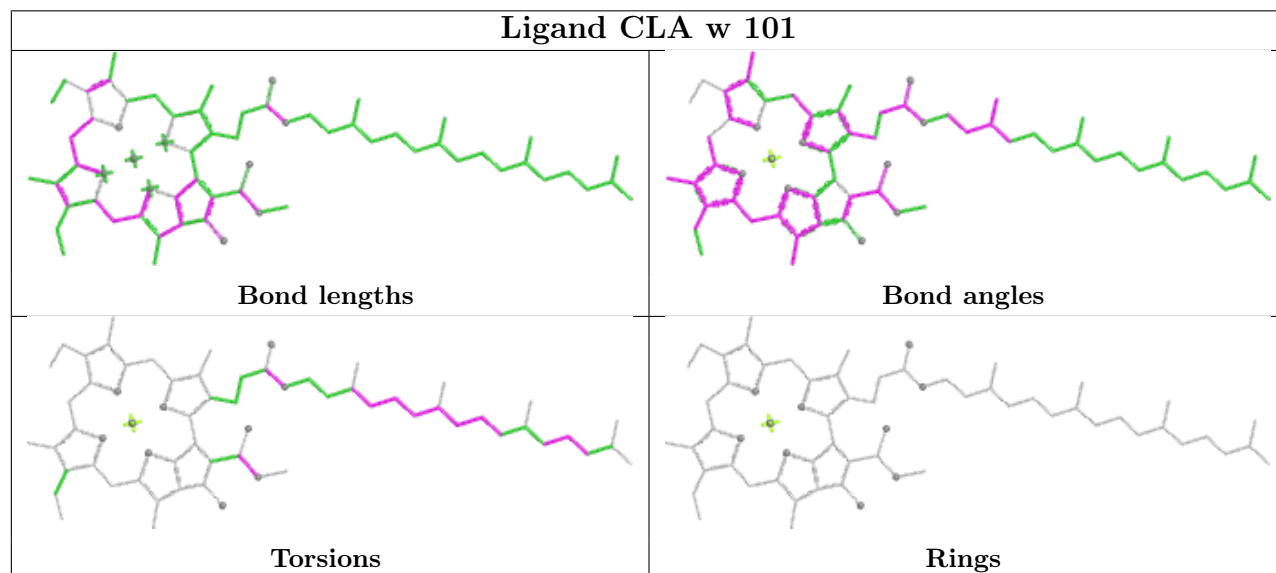
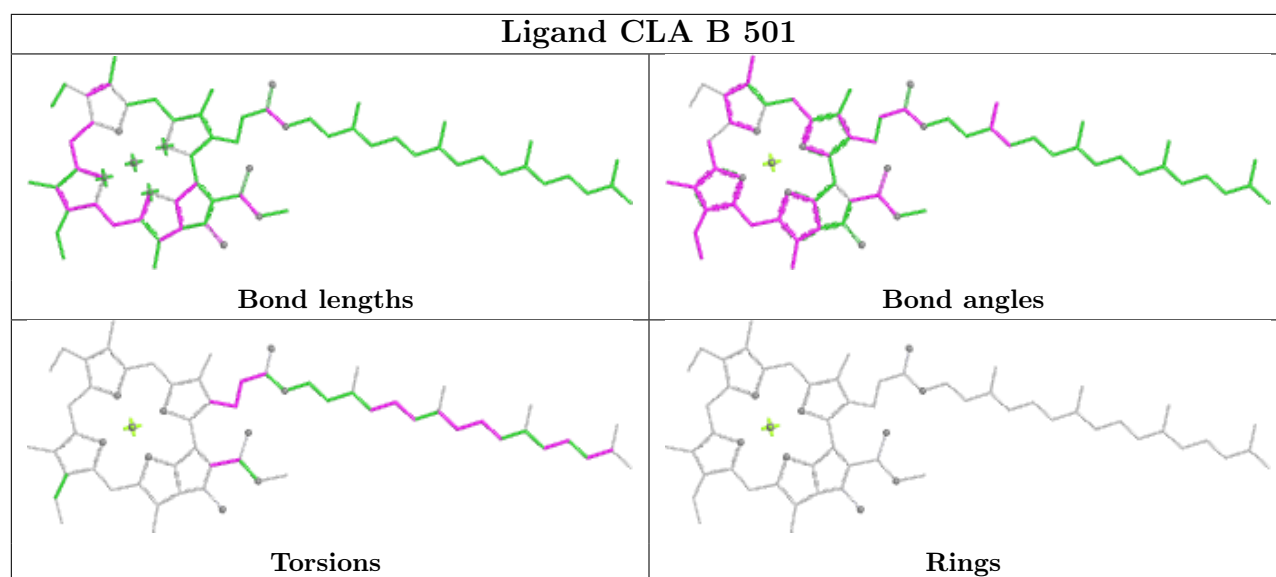


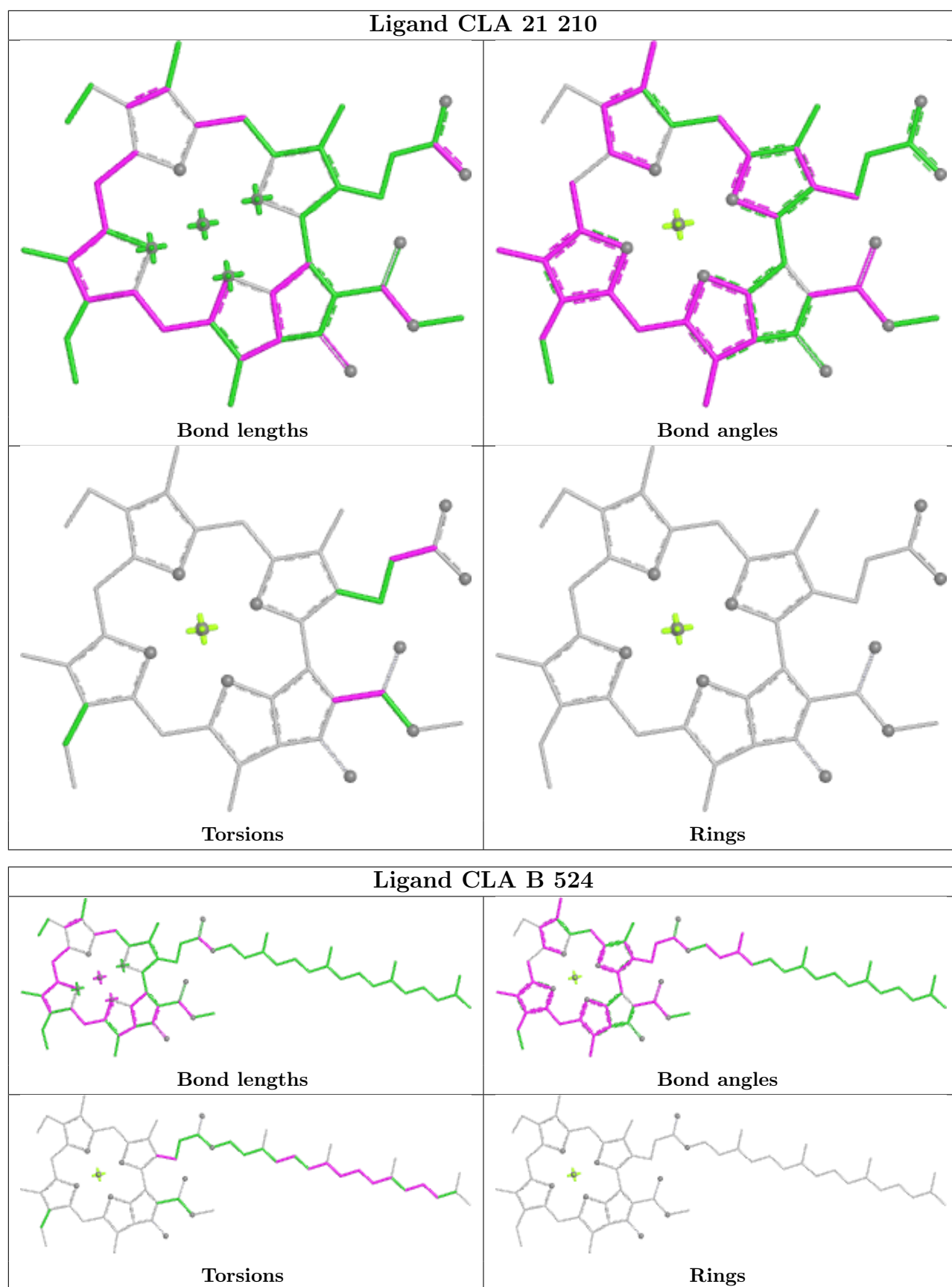


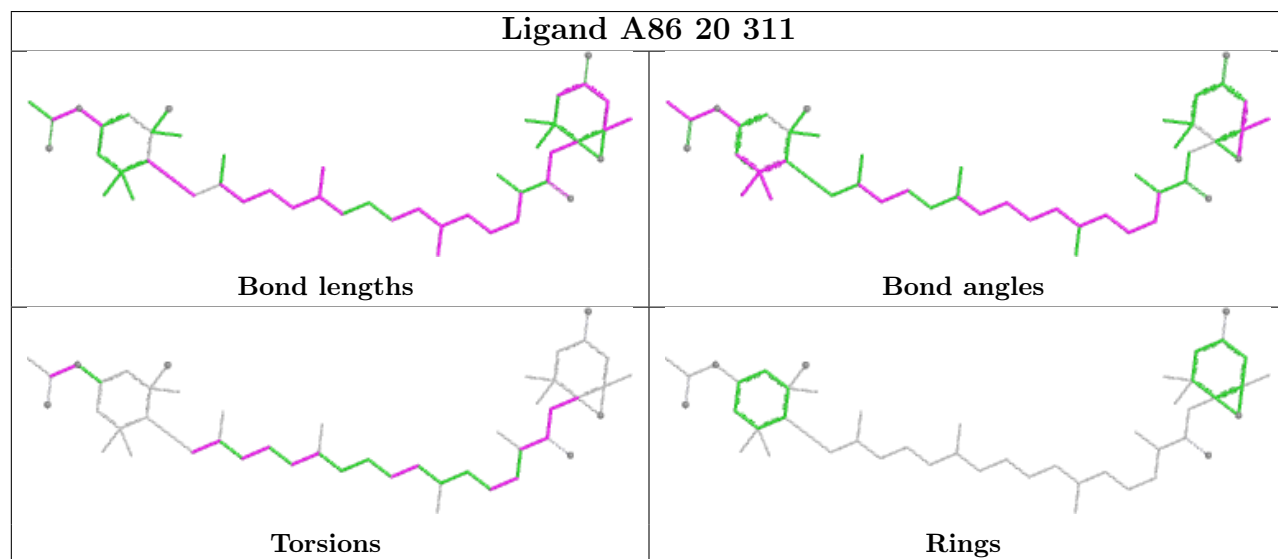
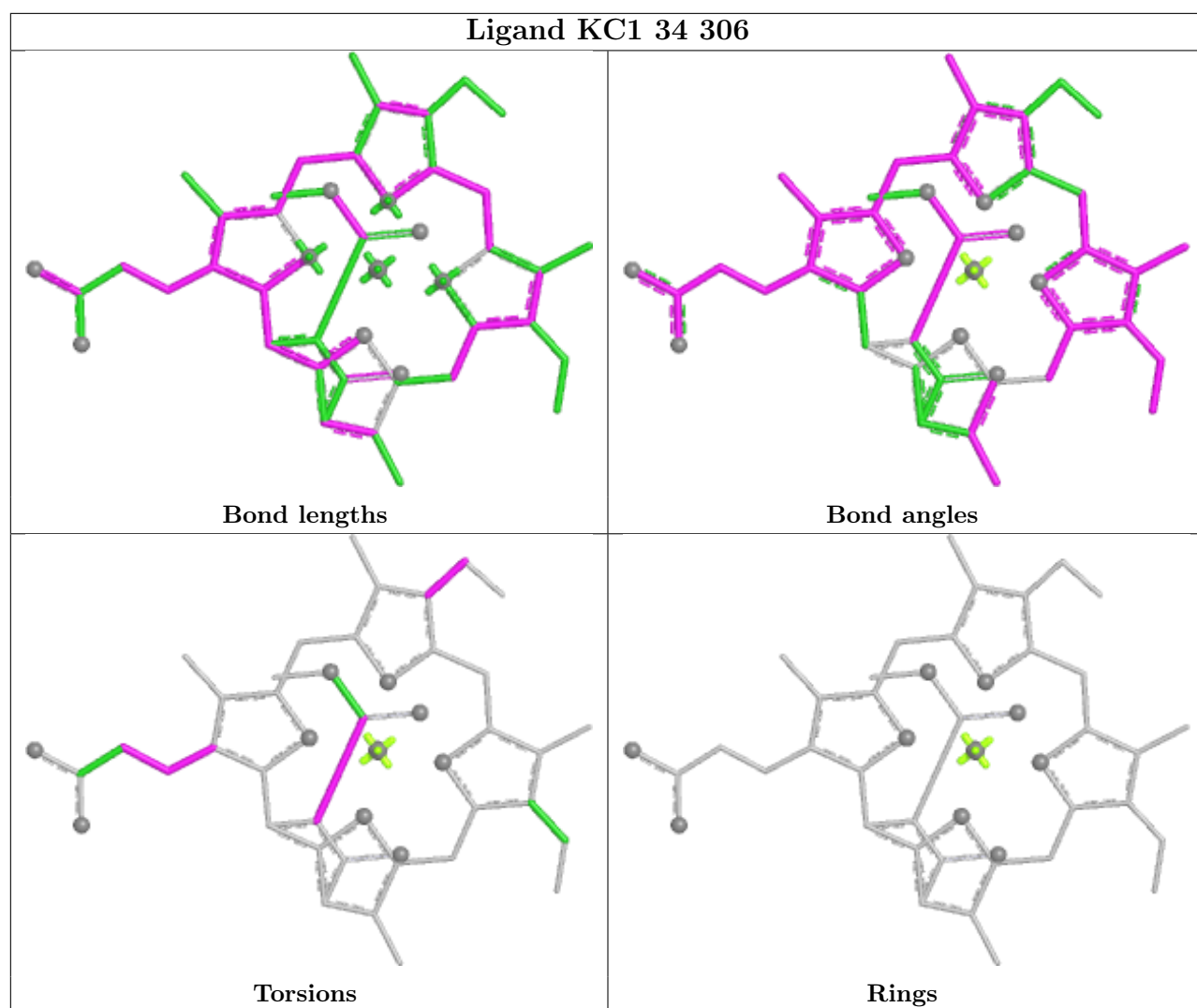


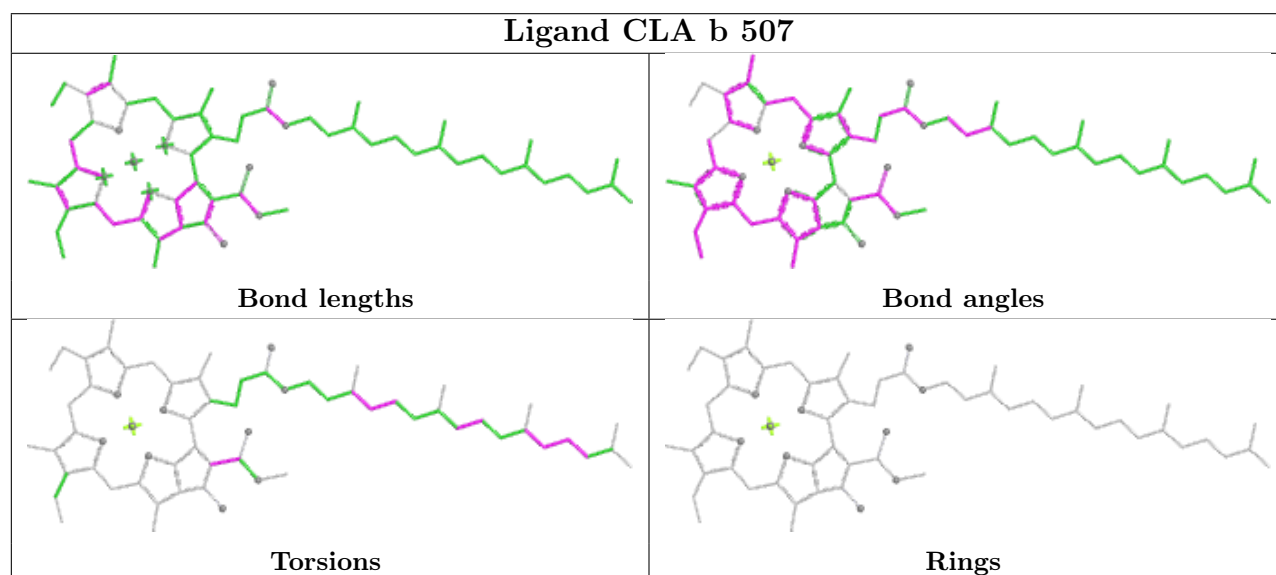
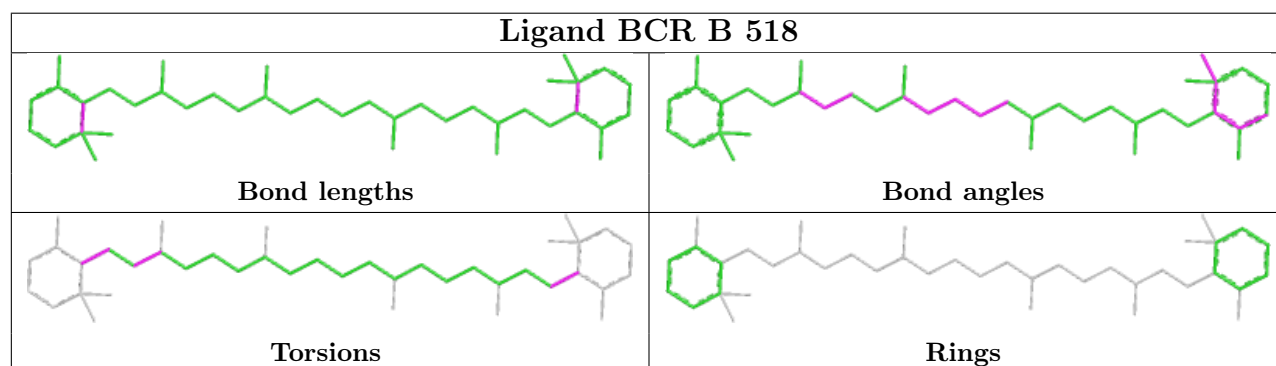
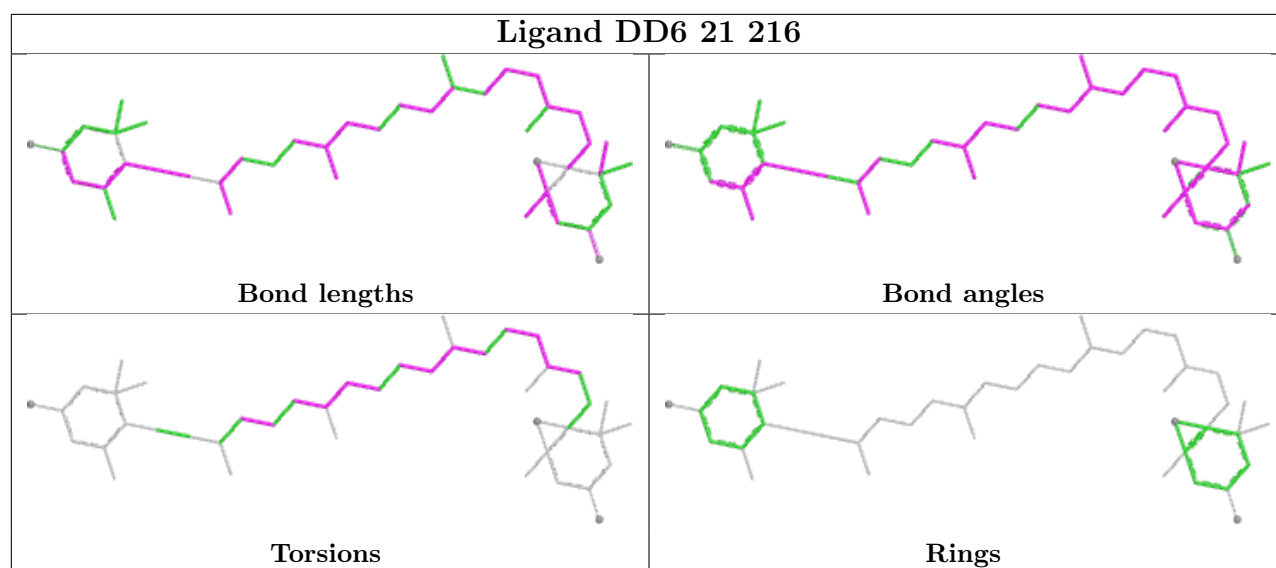


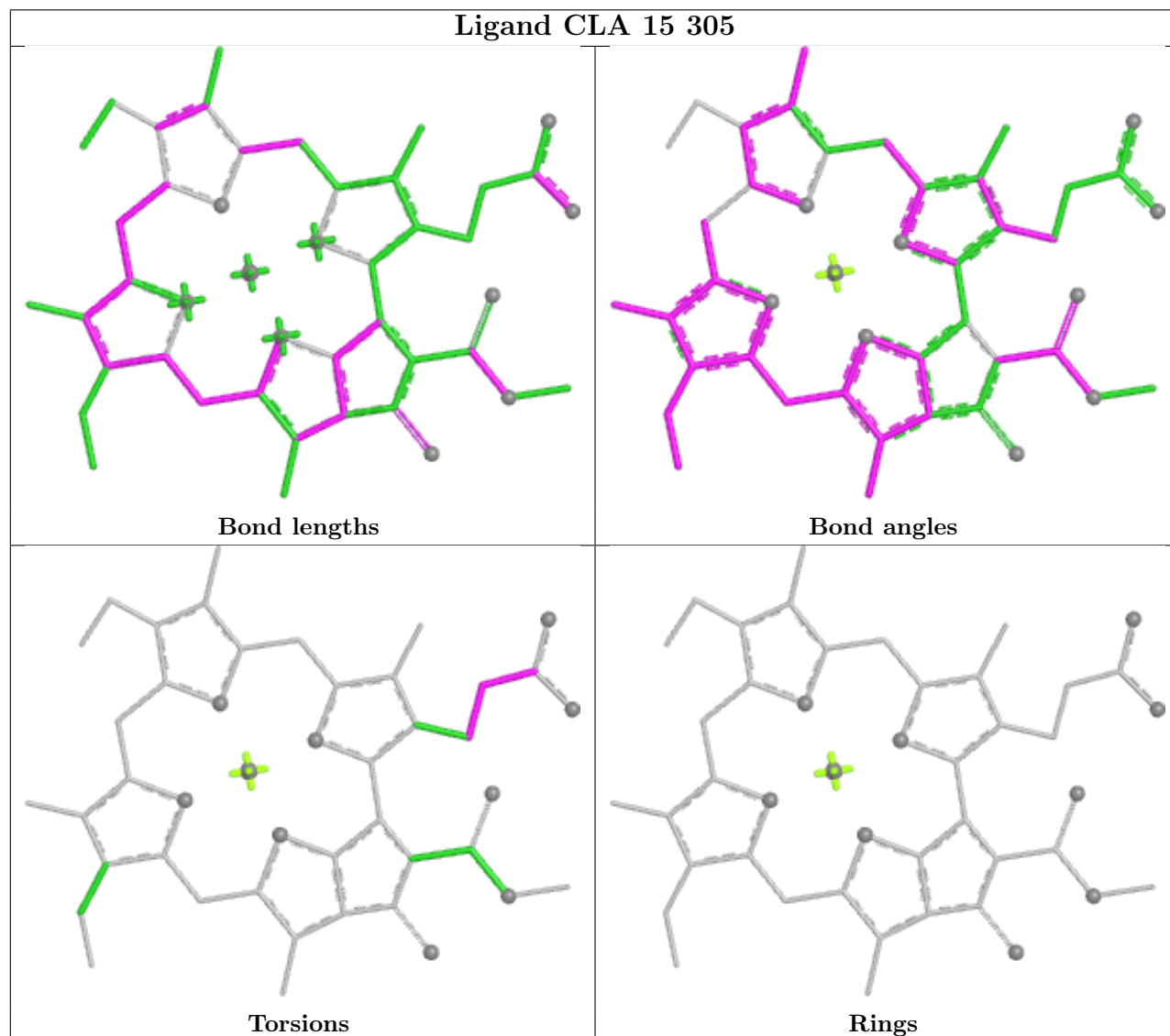
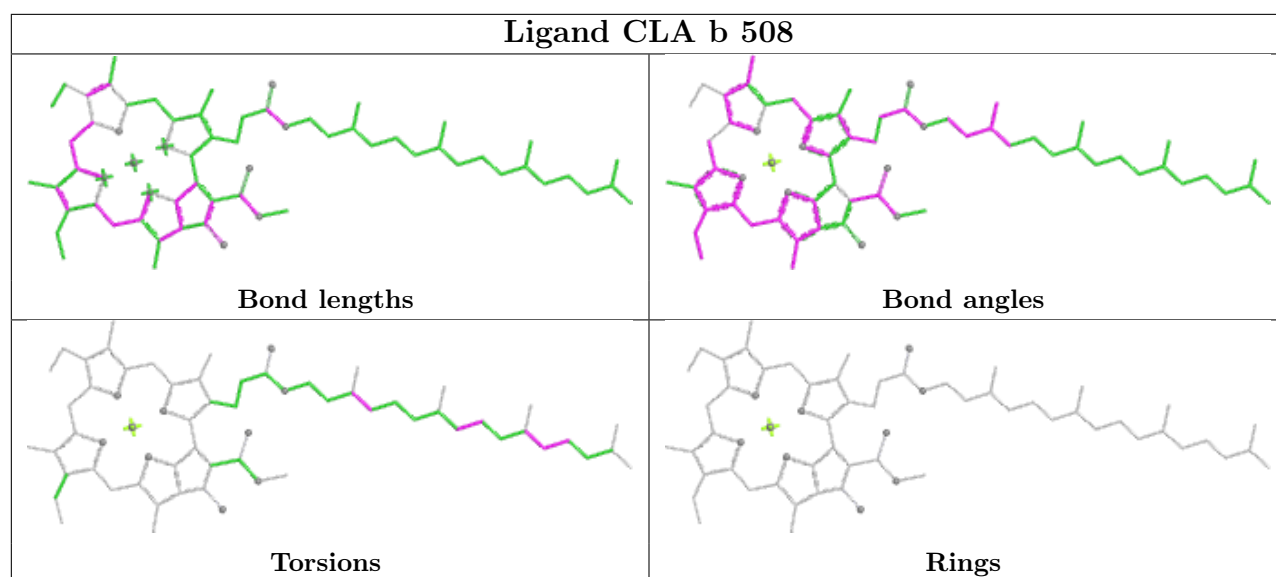


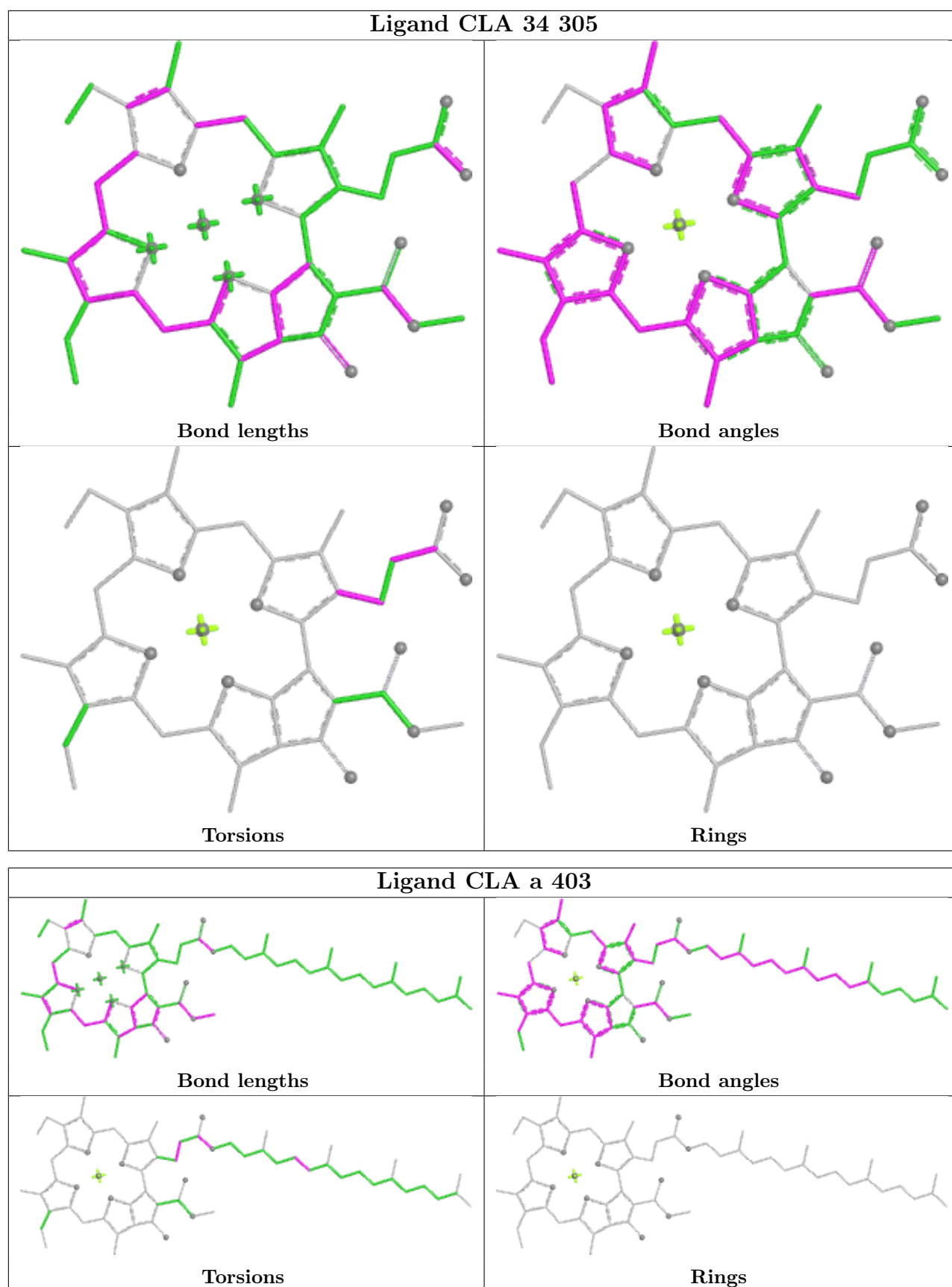


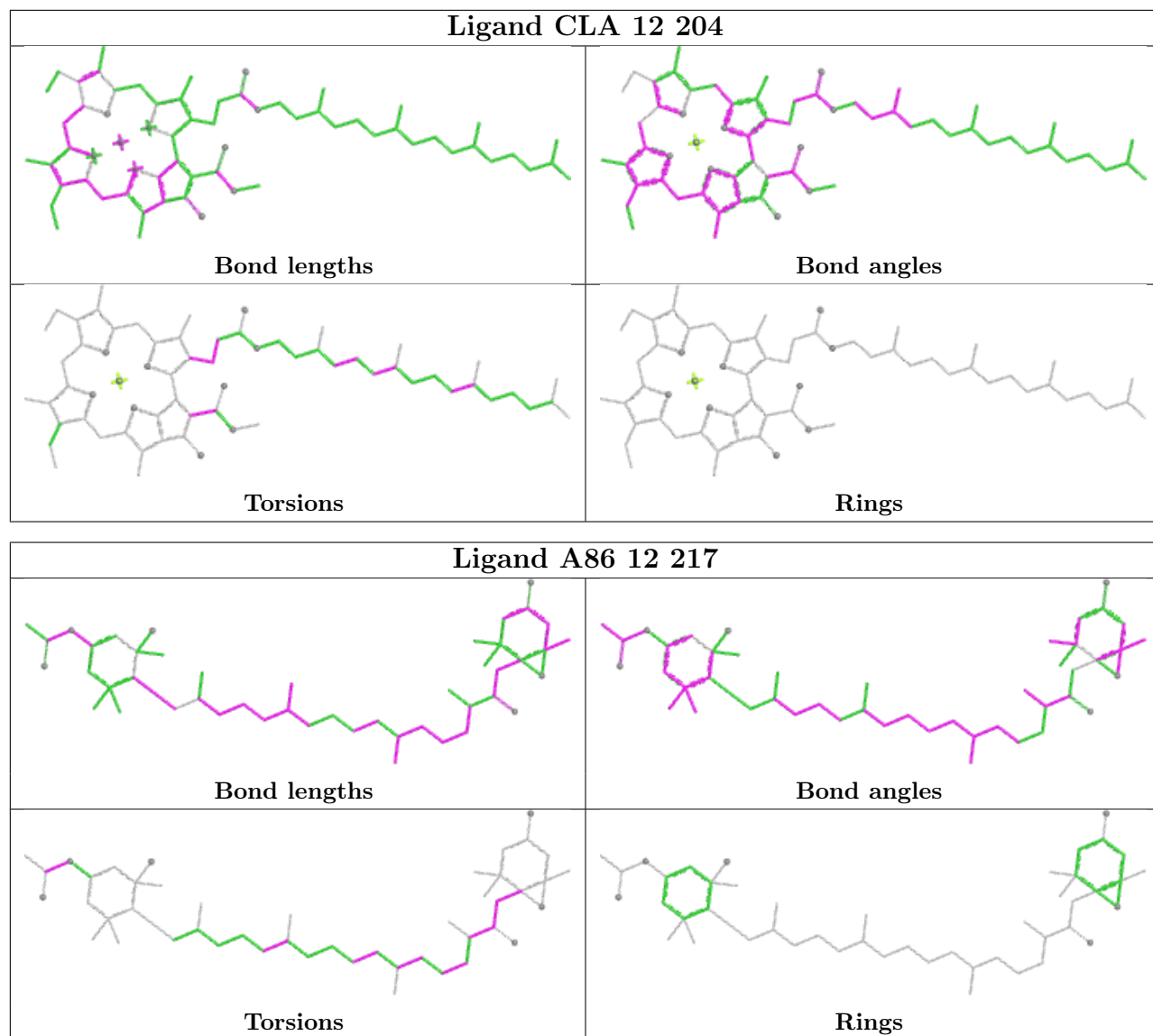


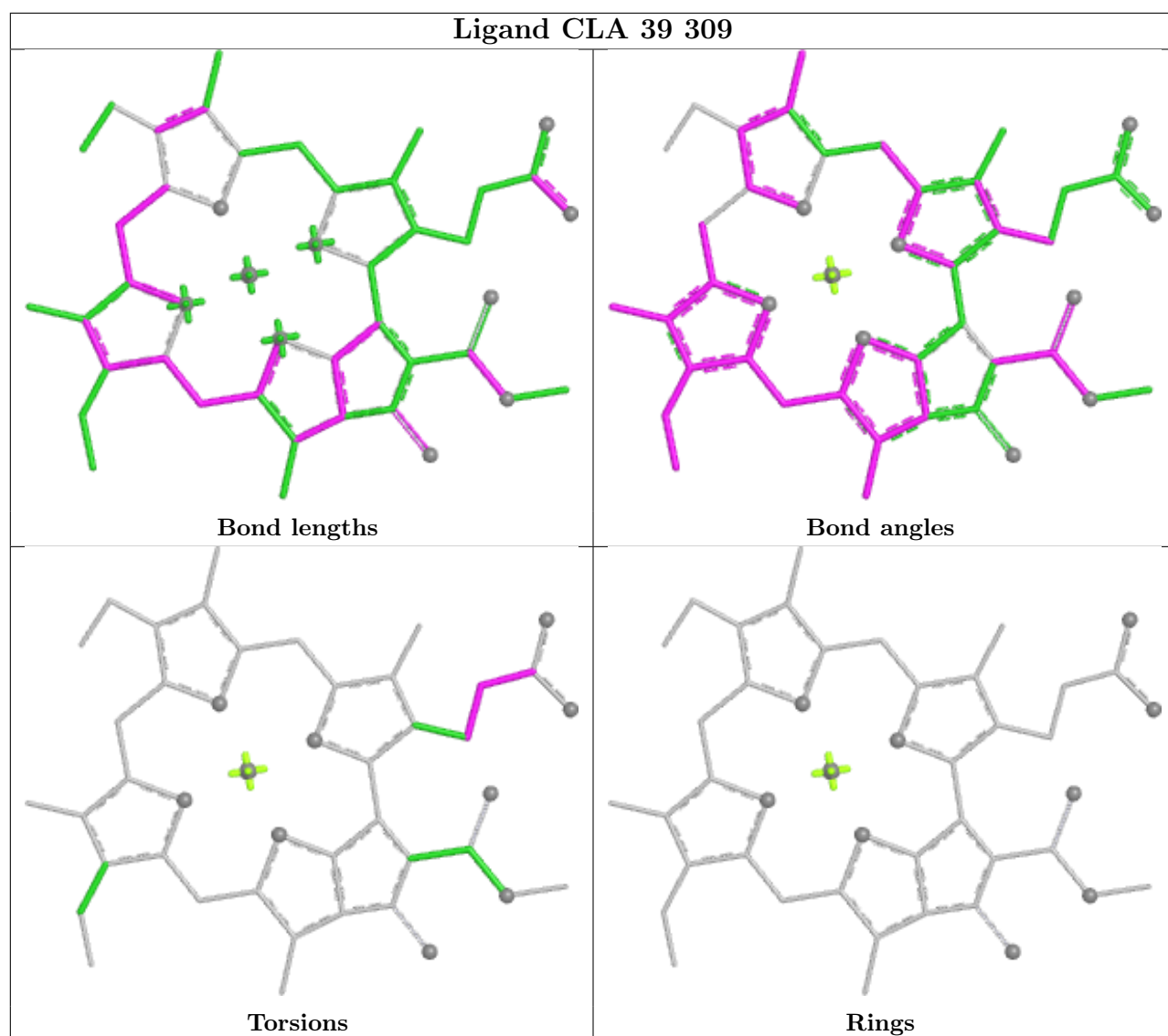


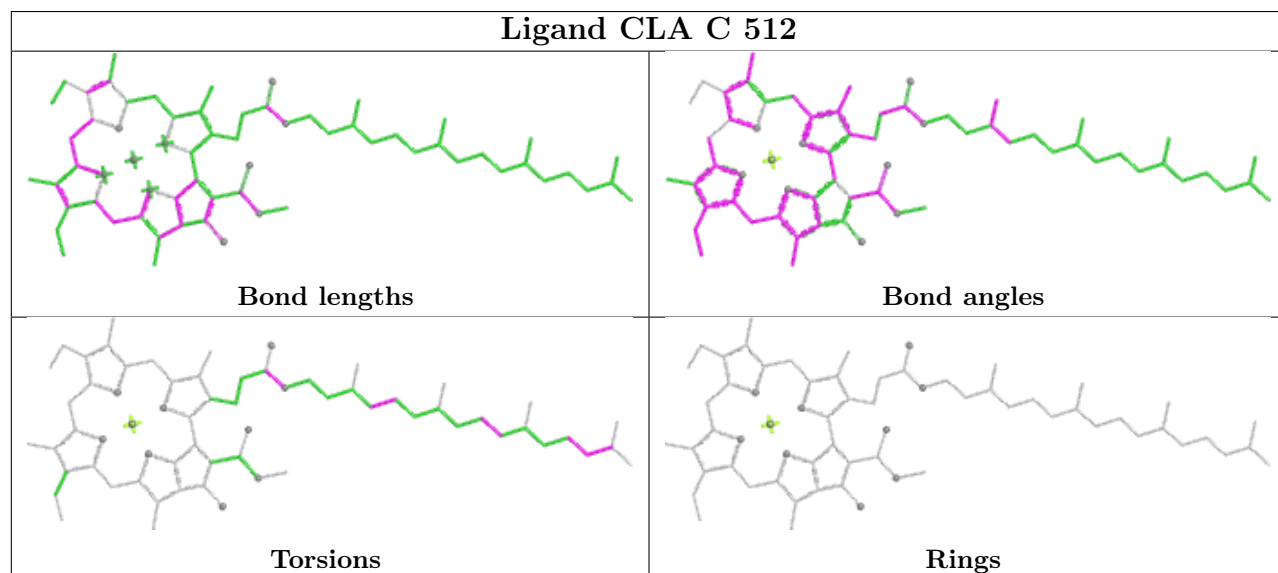
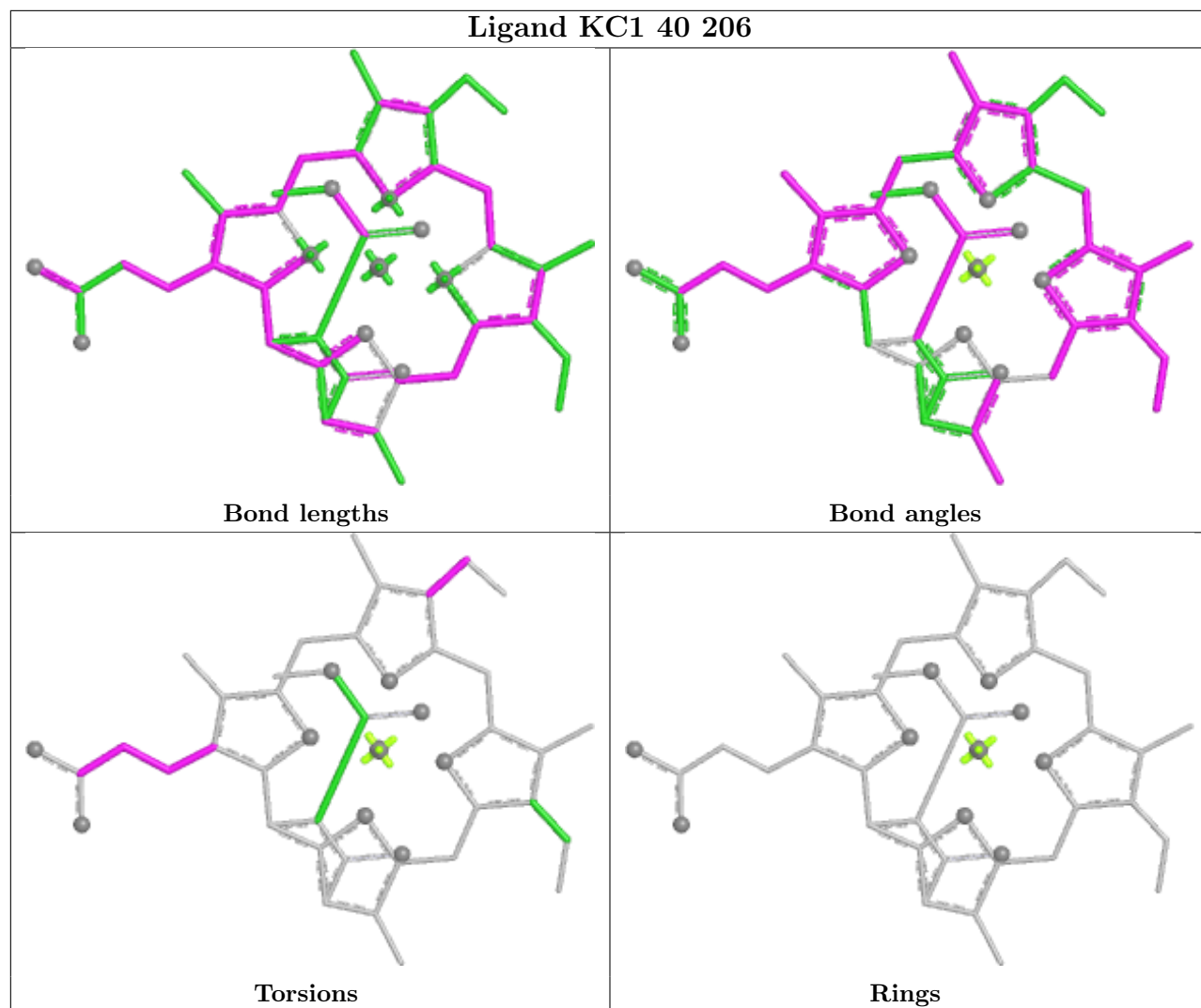


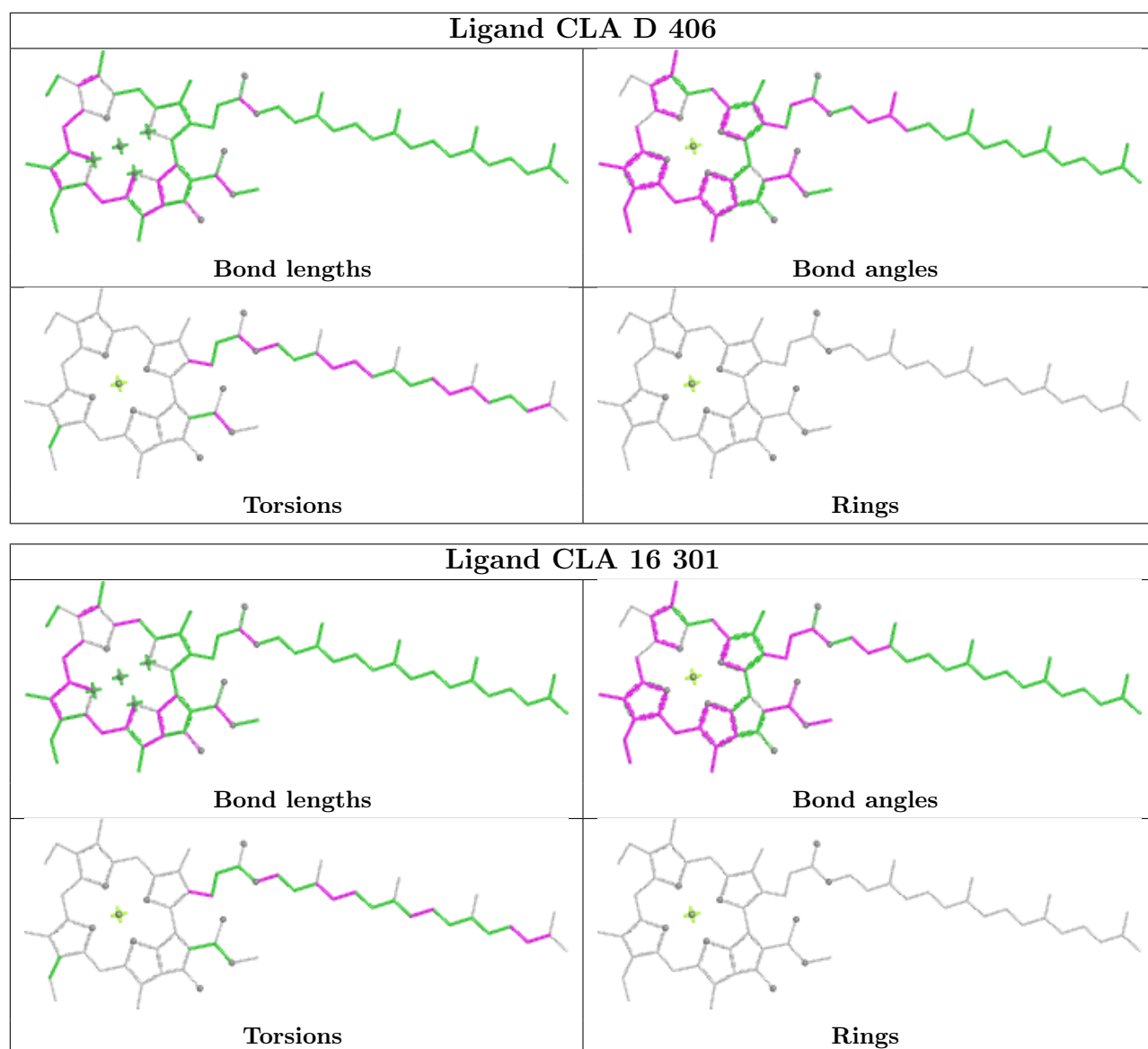


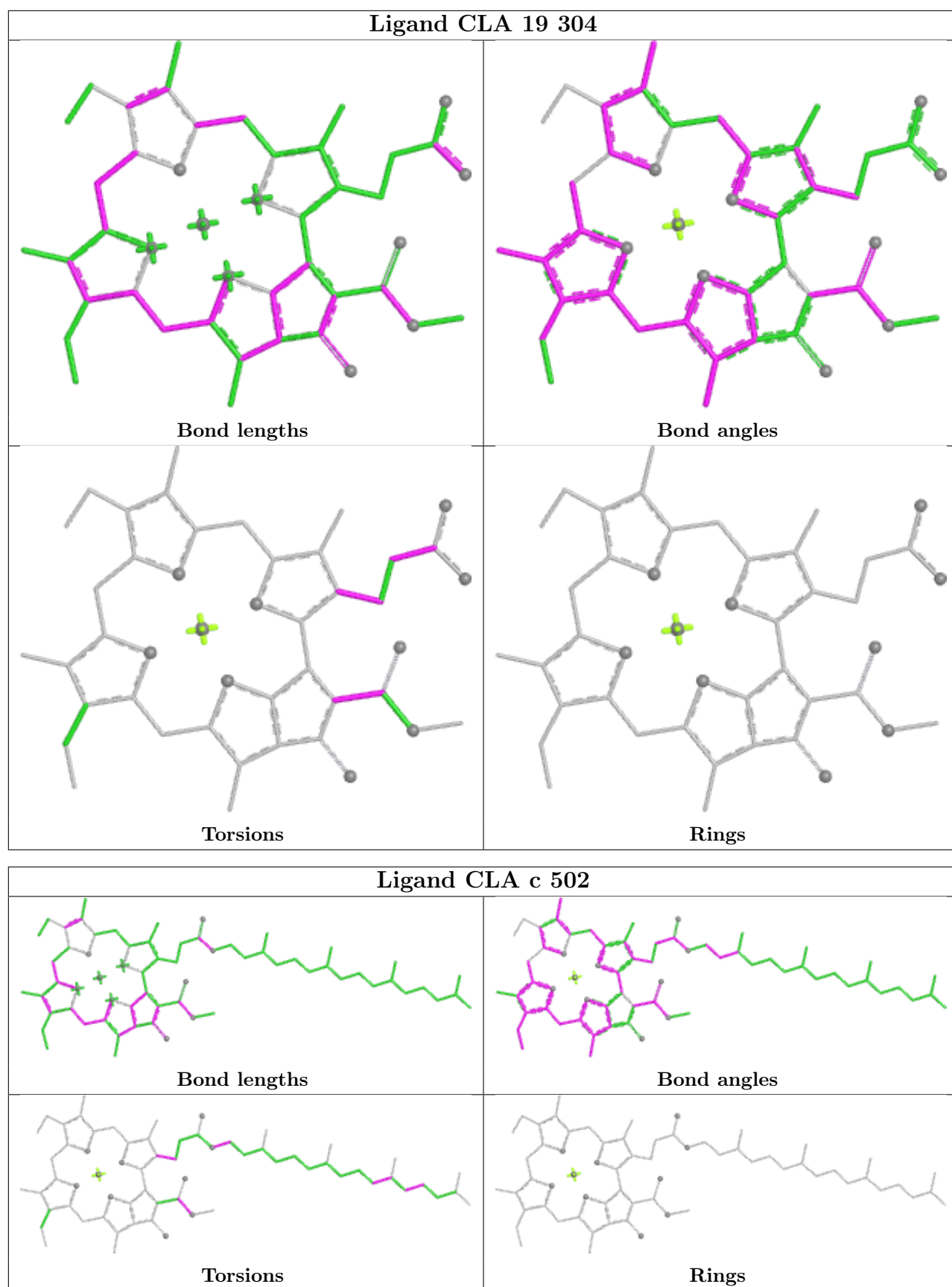


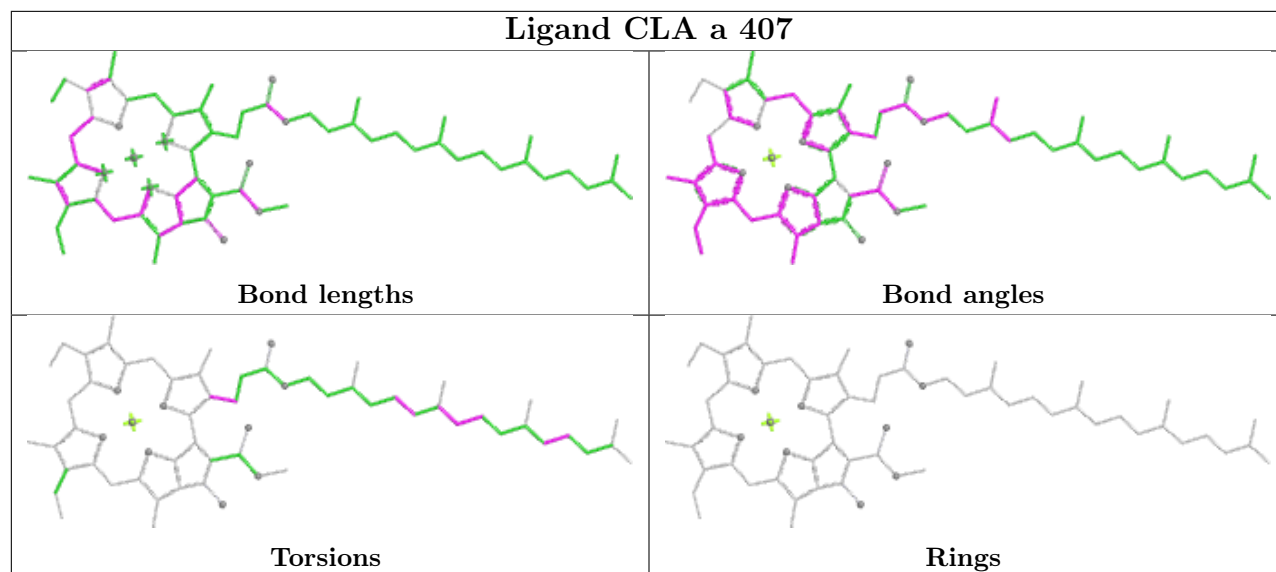
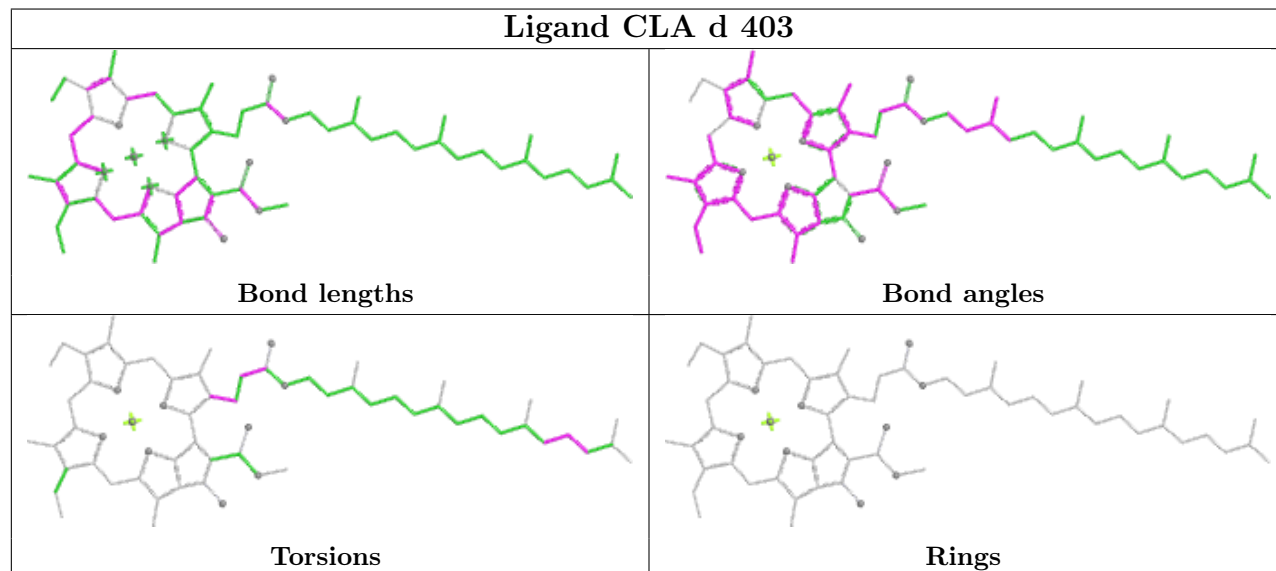


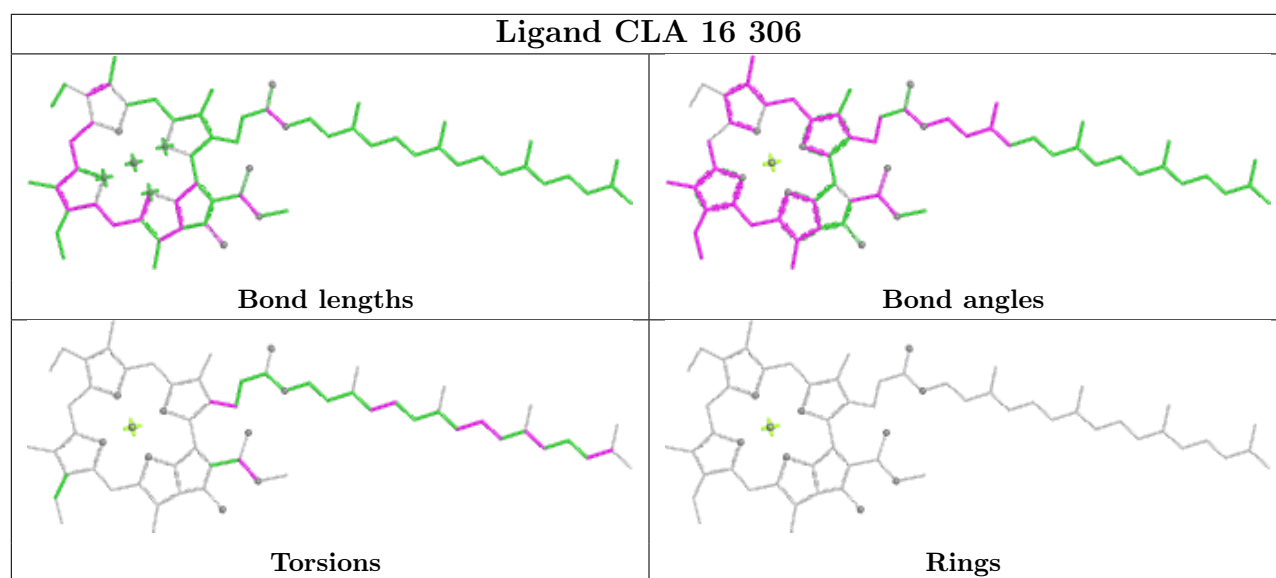
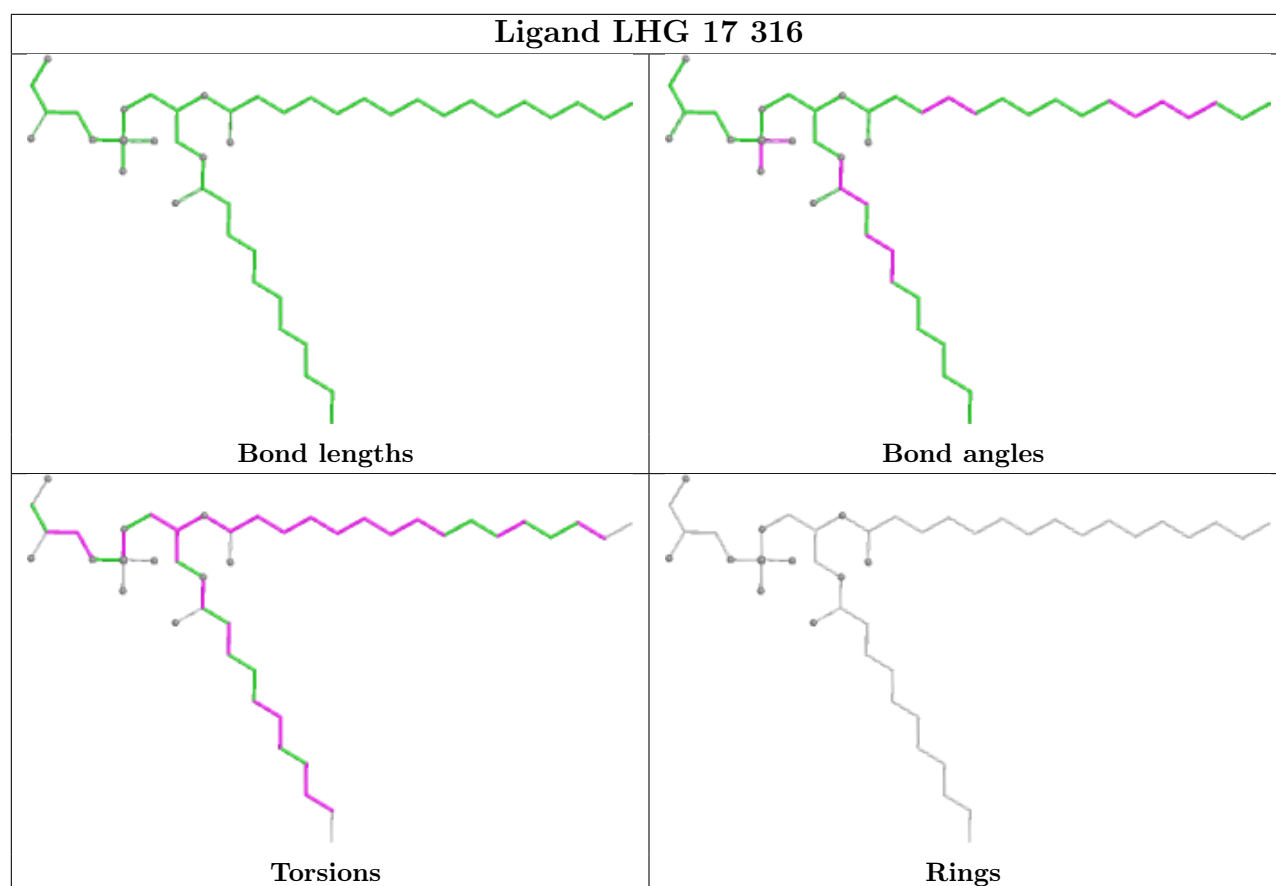


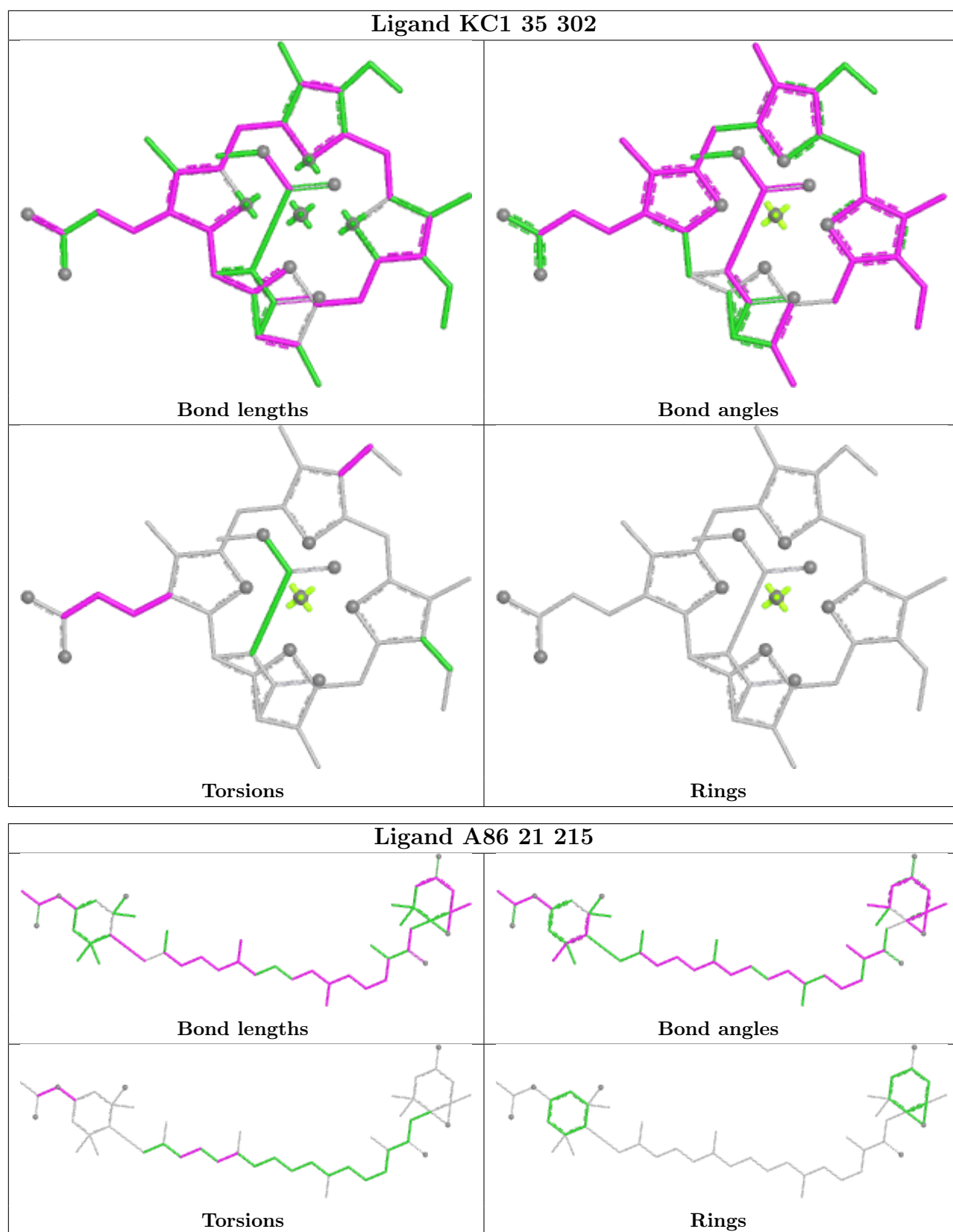


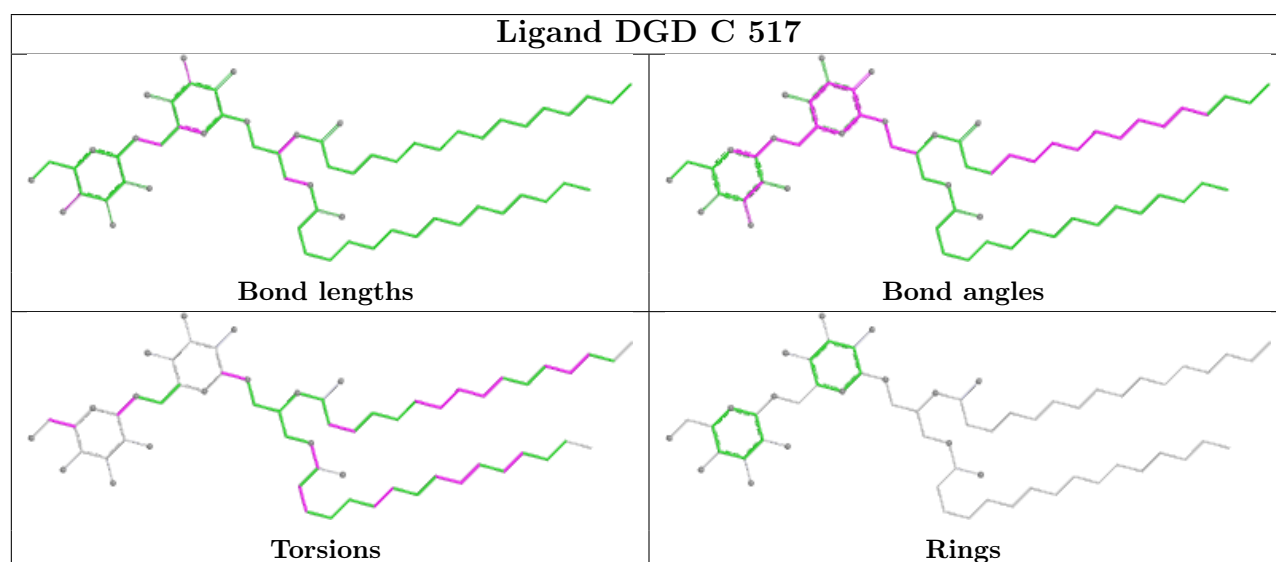
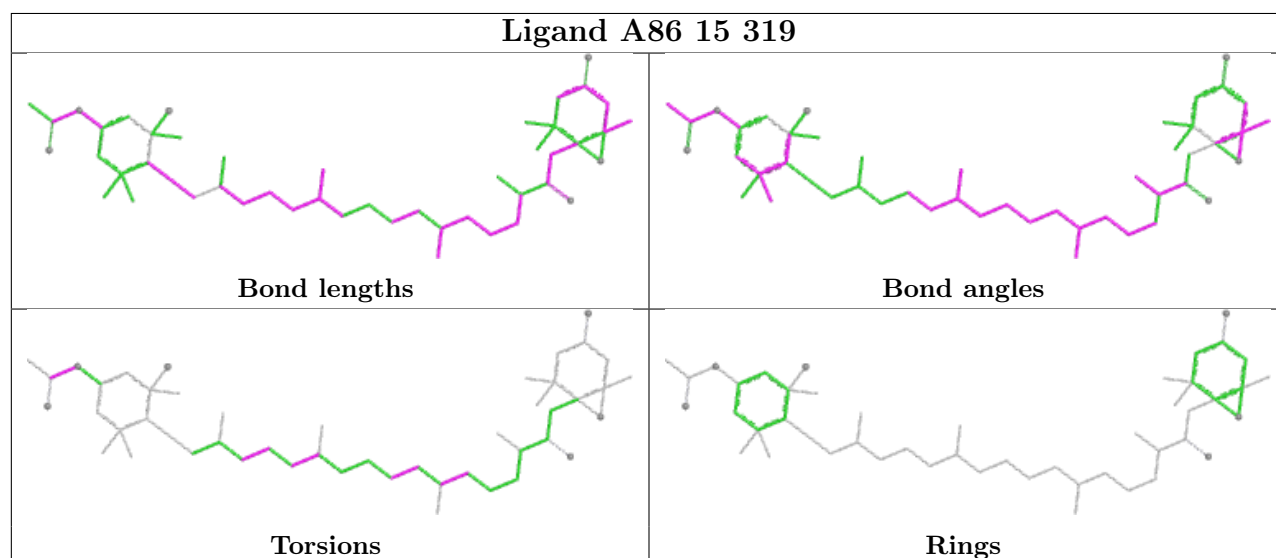
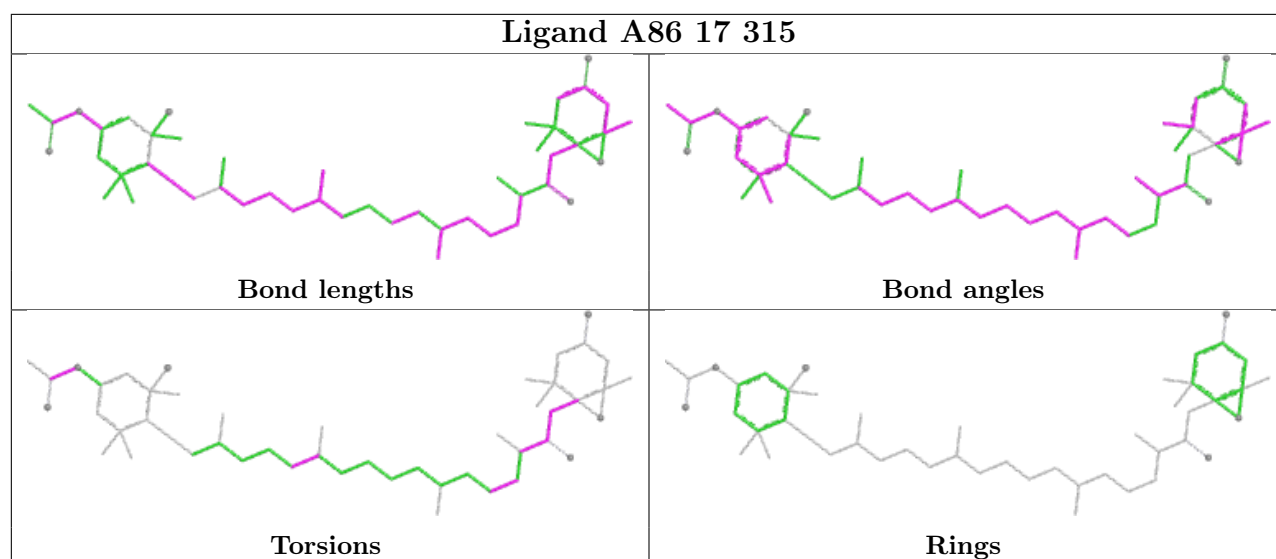


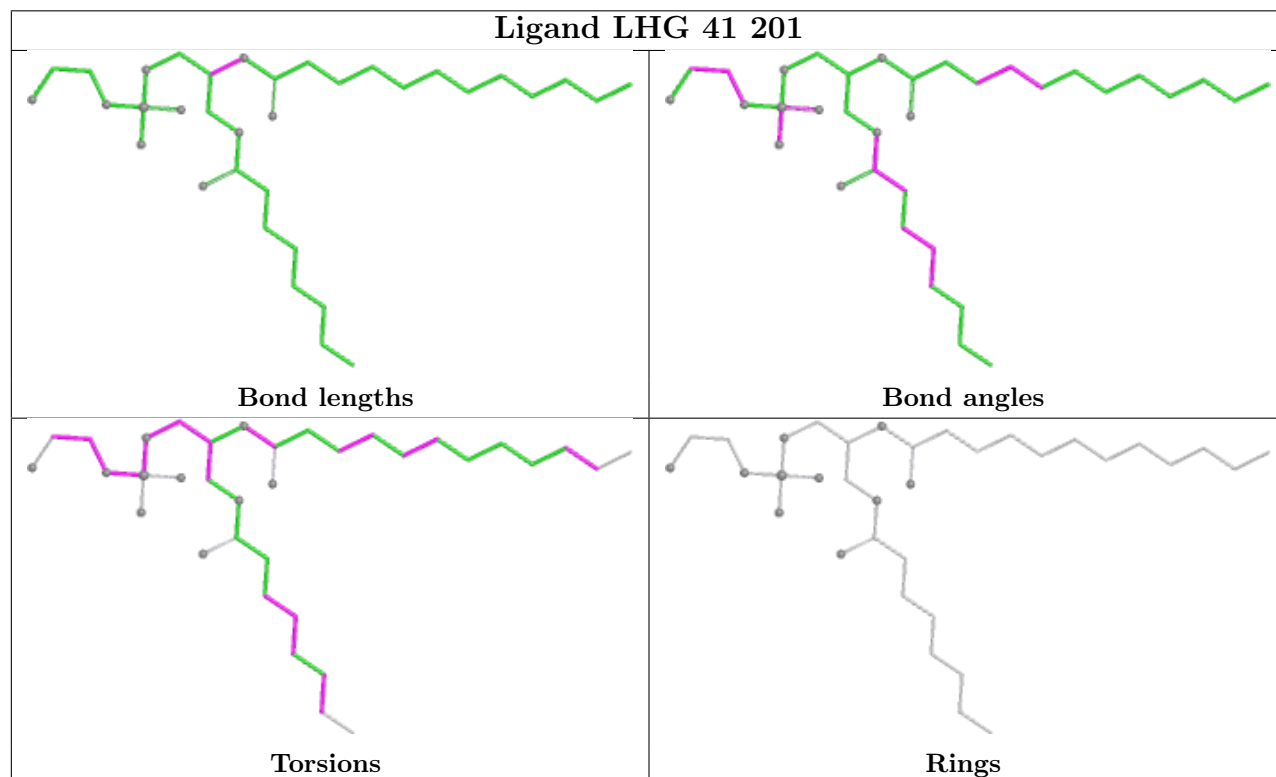
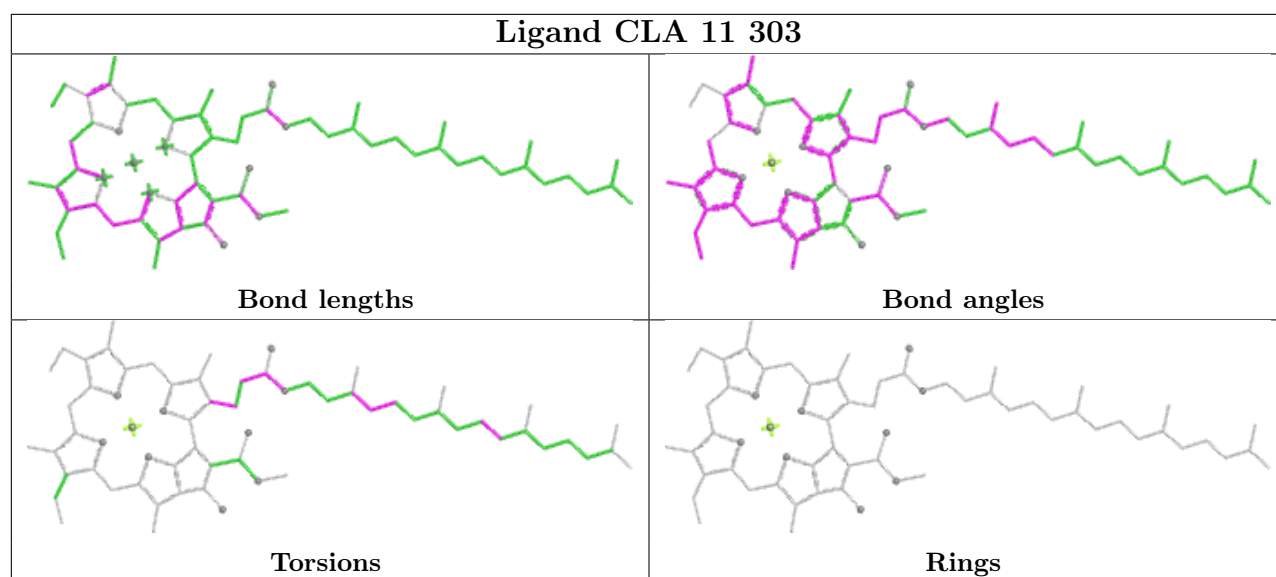


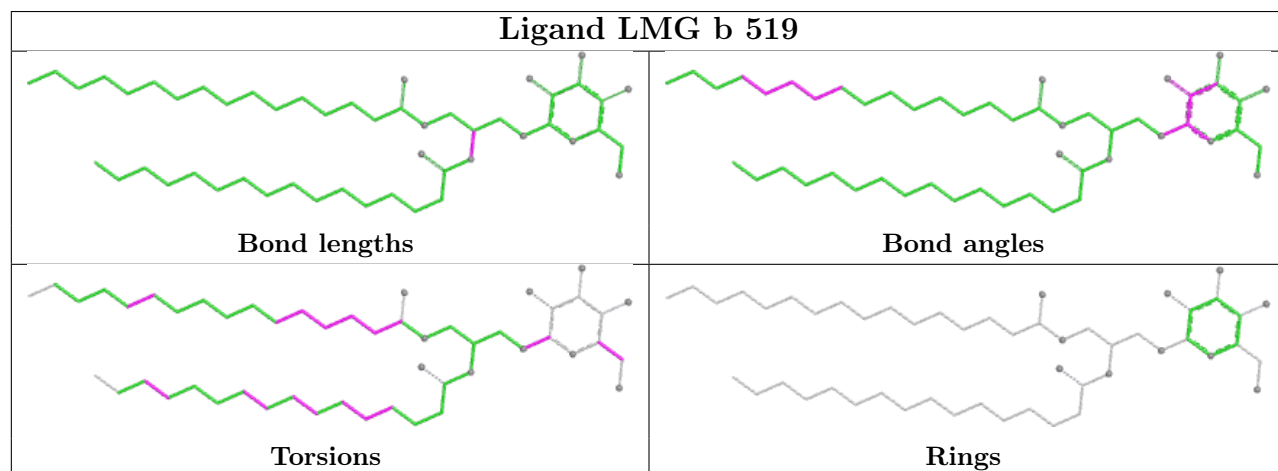
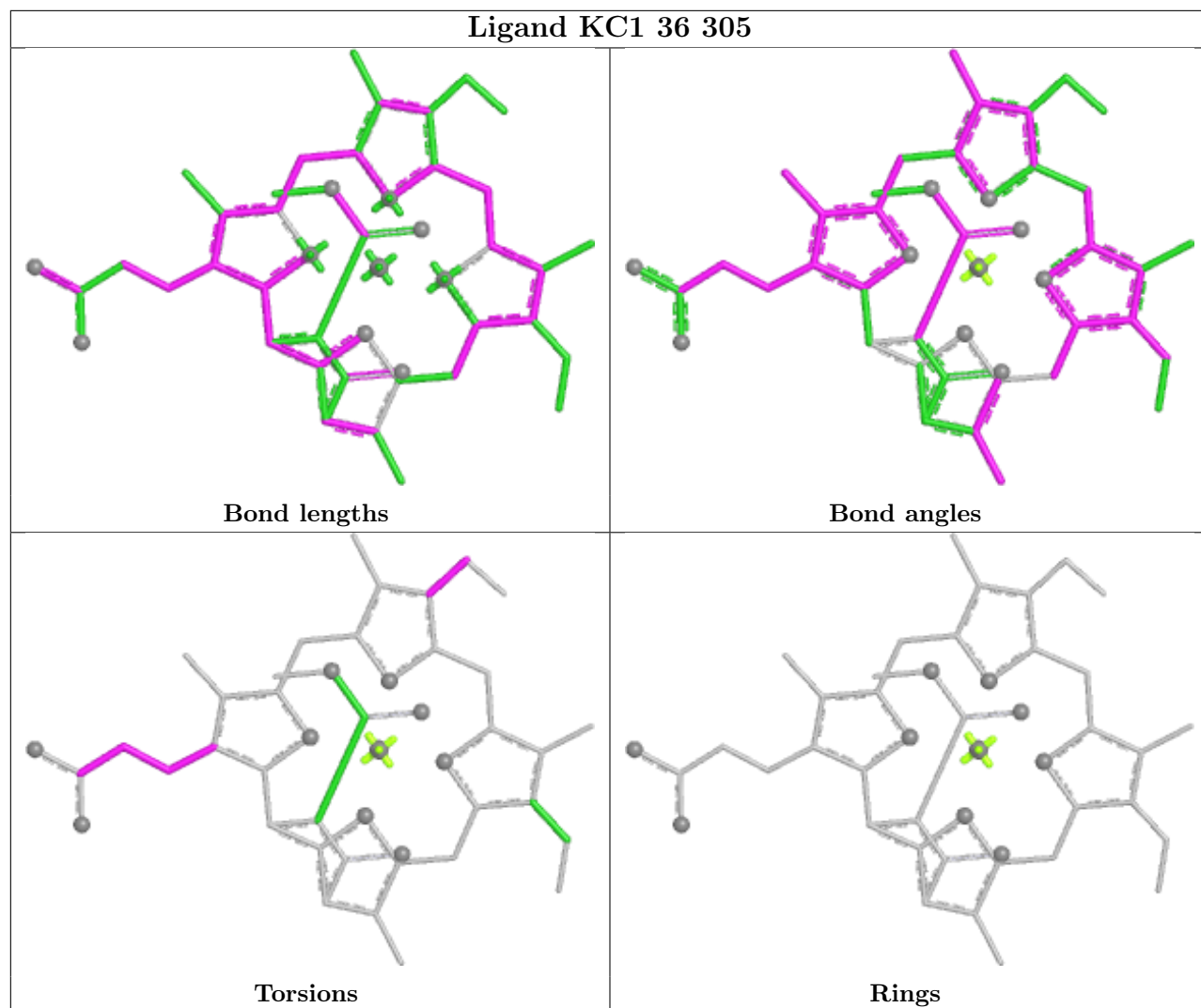
Ligand CLA a 407**Ligand CLA d 403**

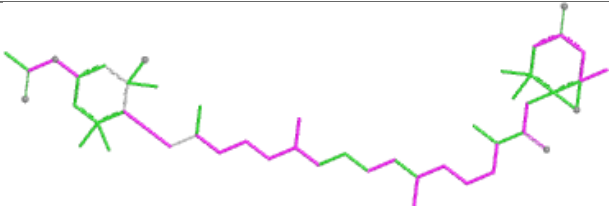
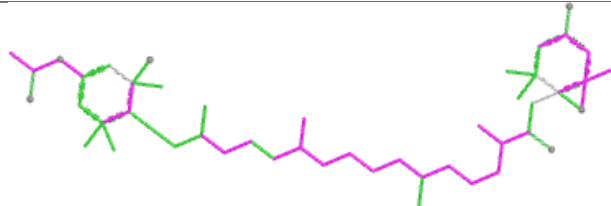
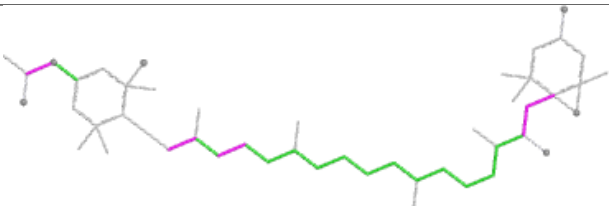
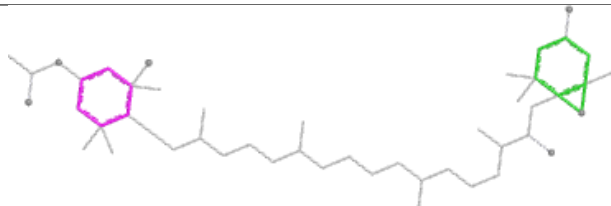


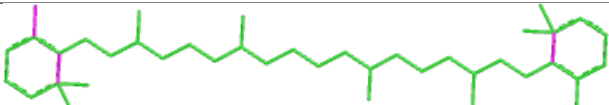
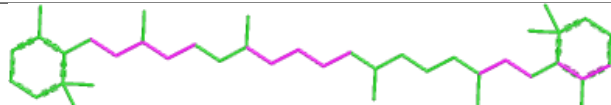
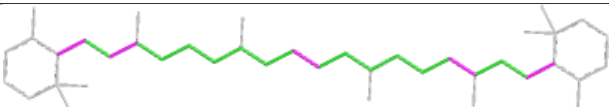
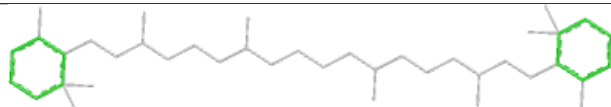


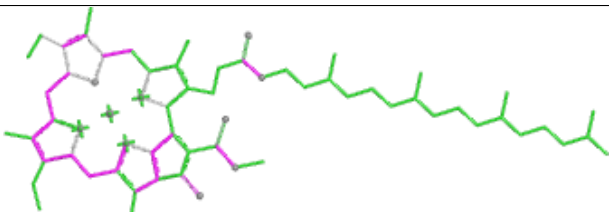
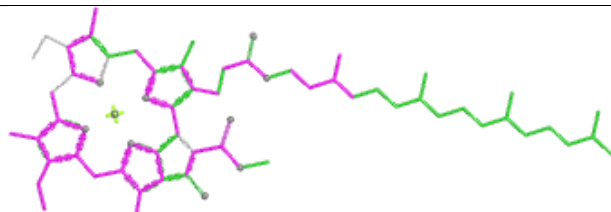
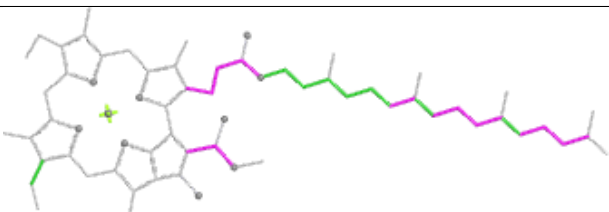
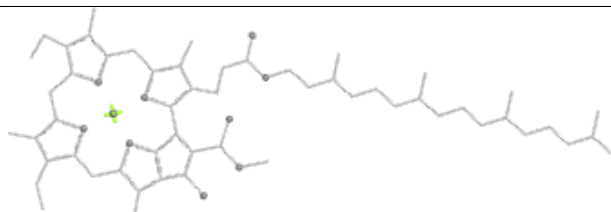


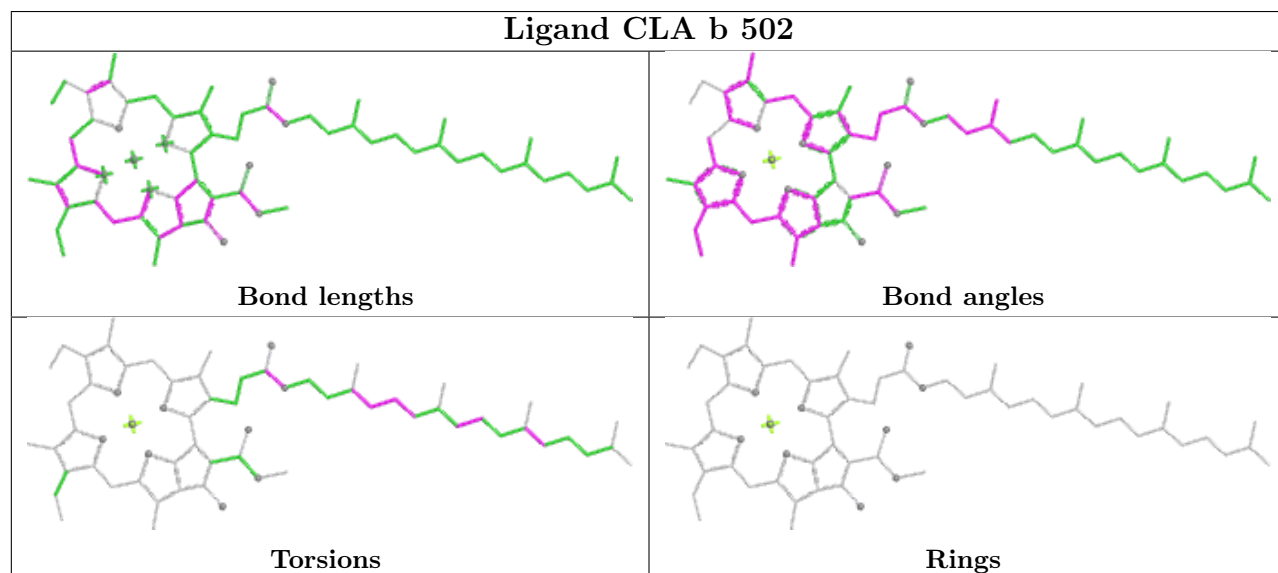
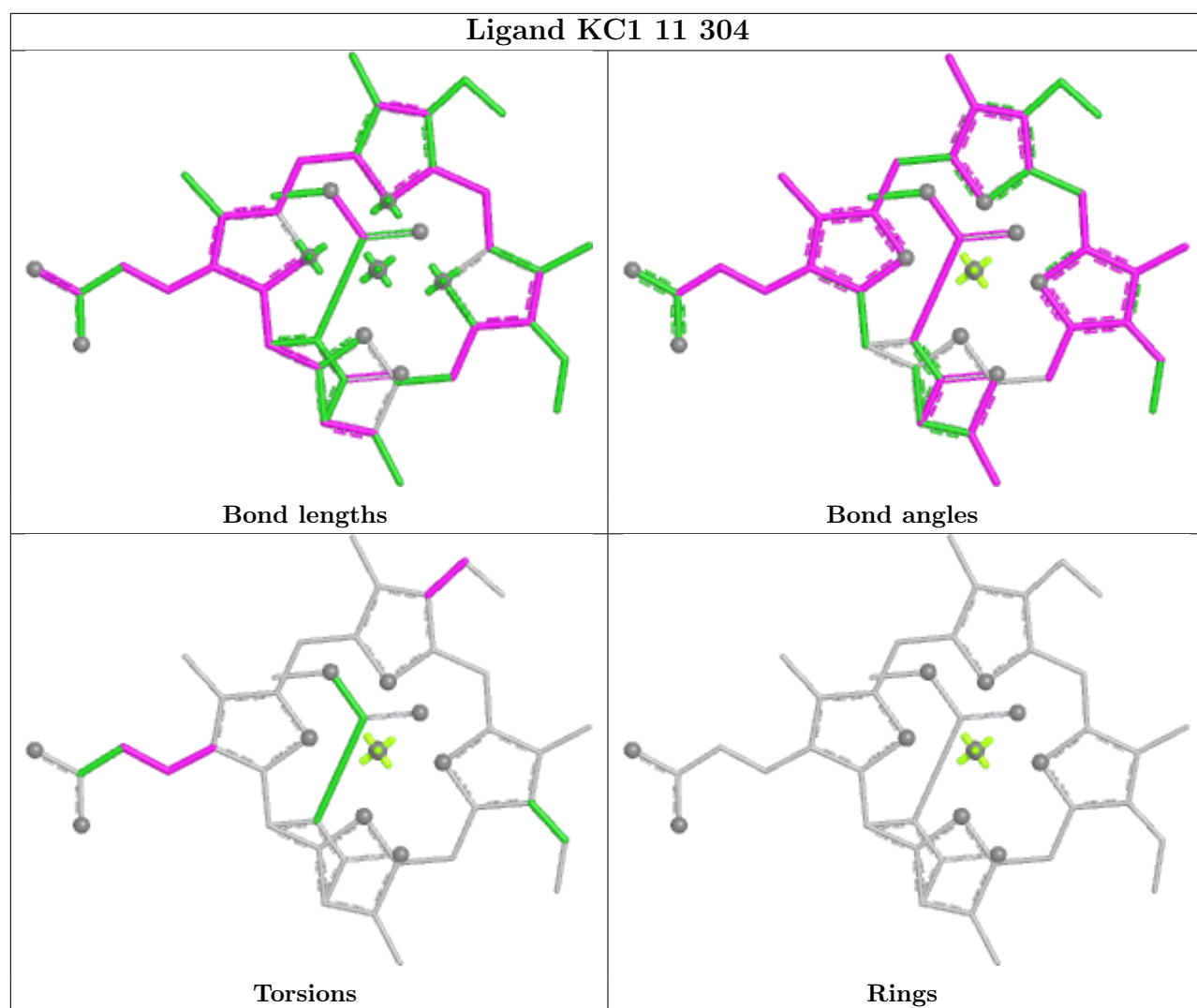


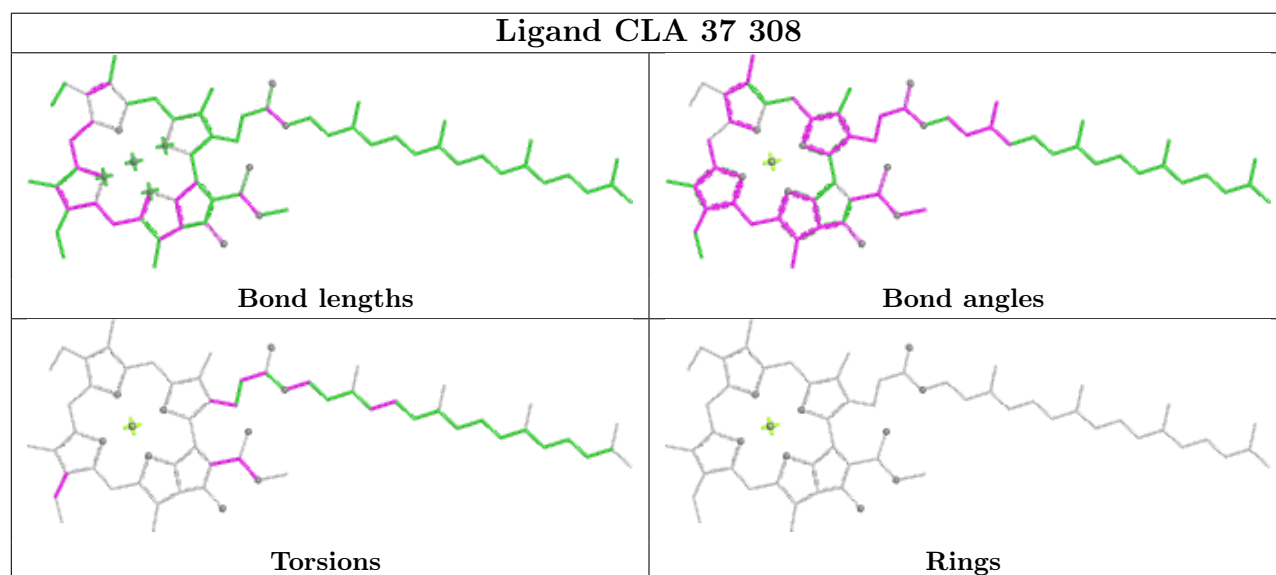
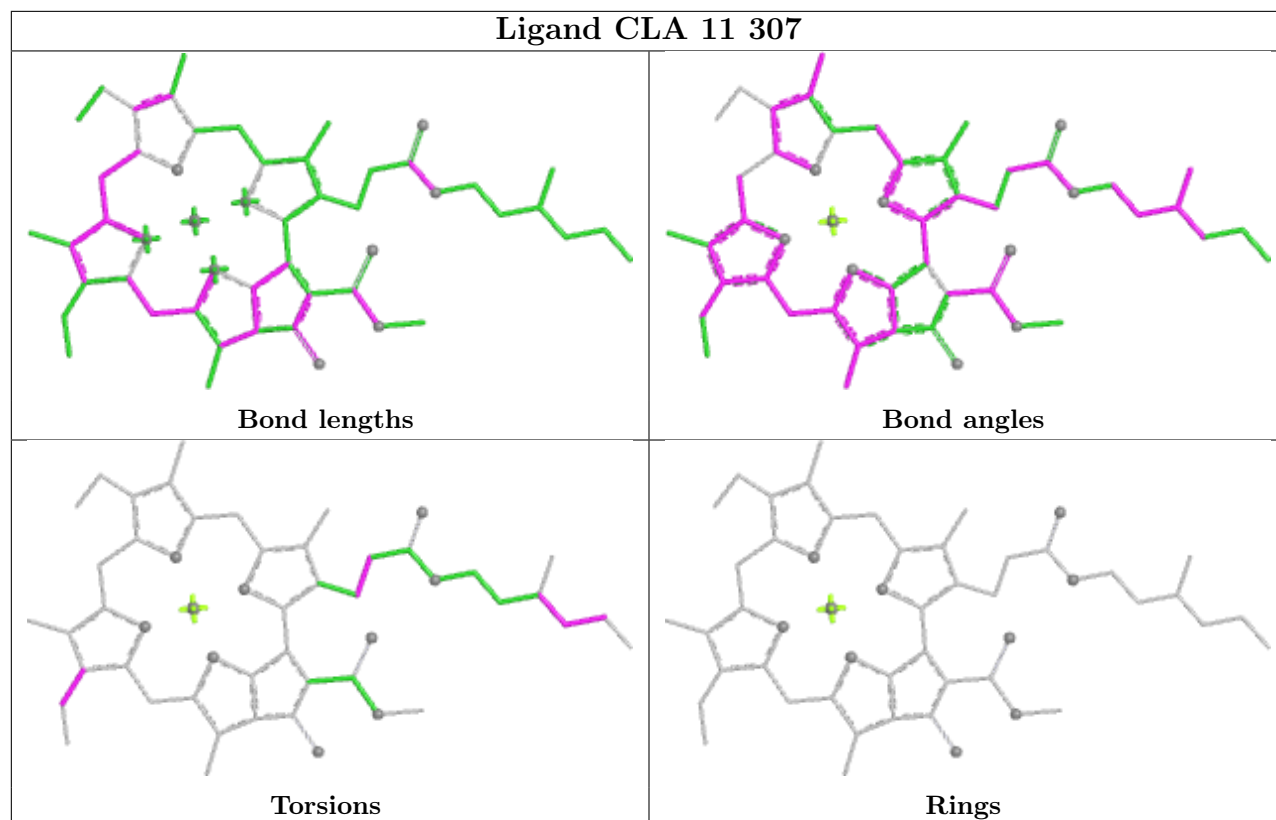


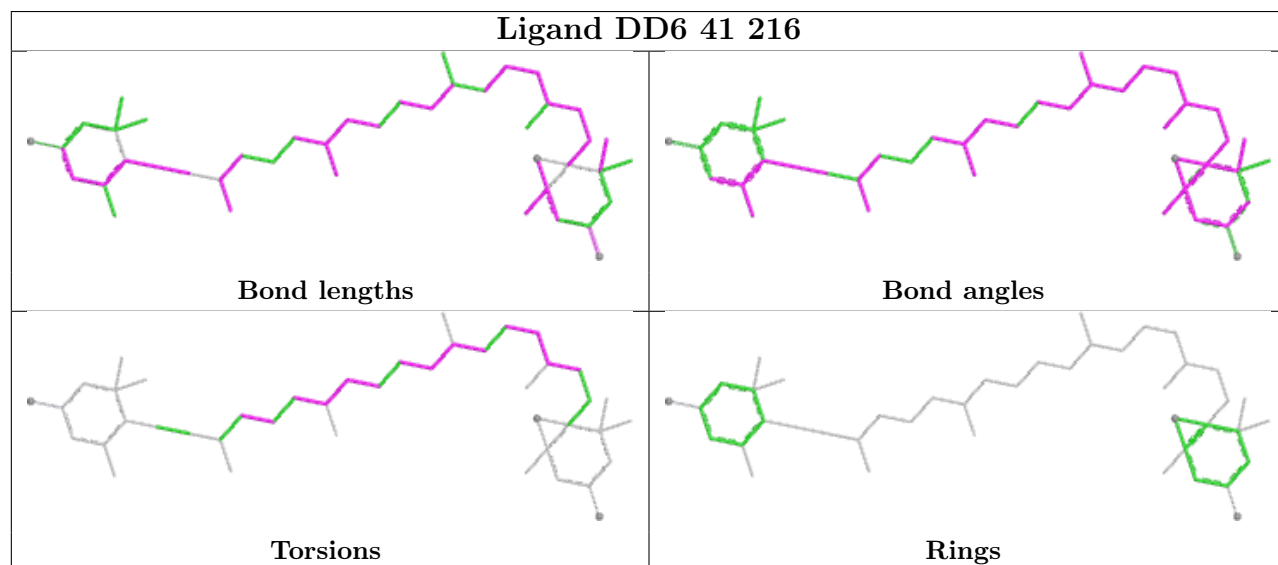
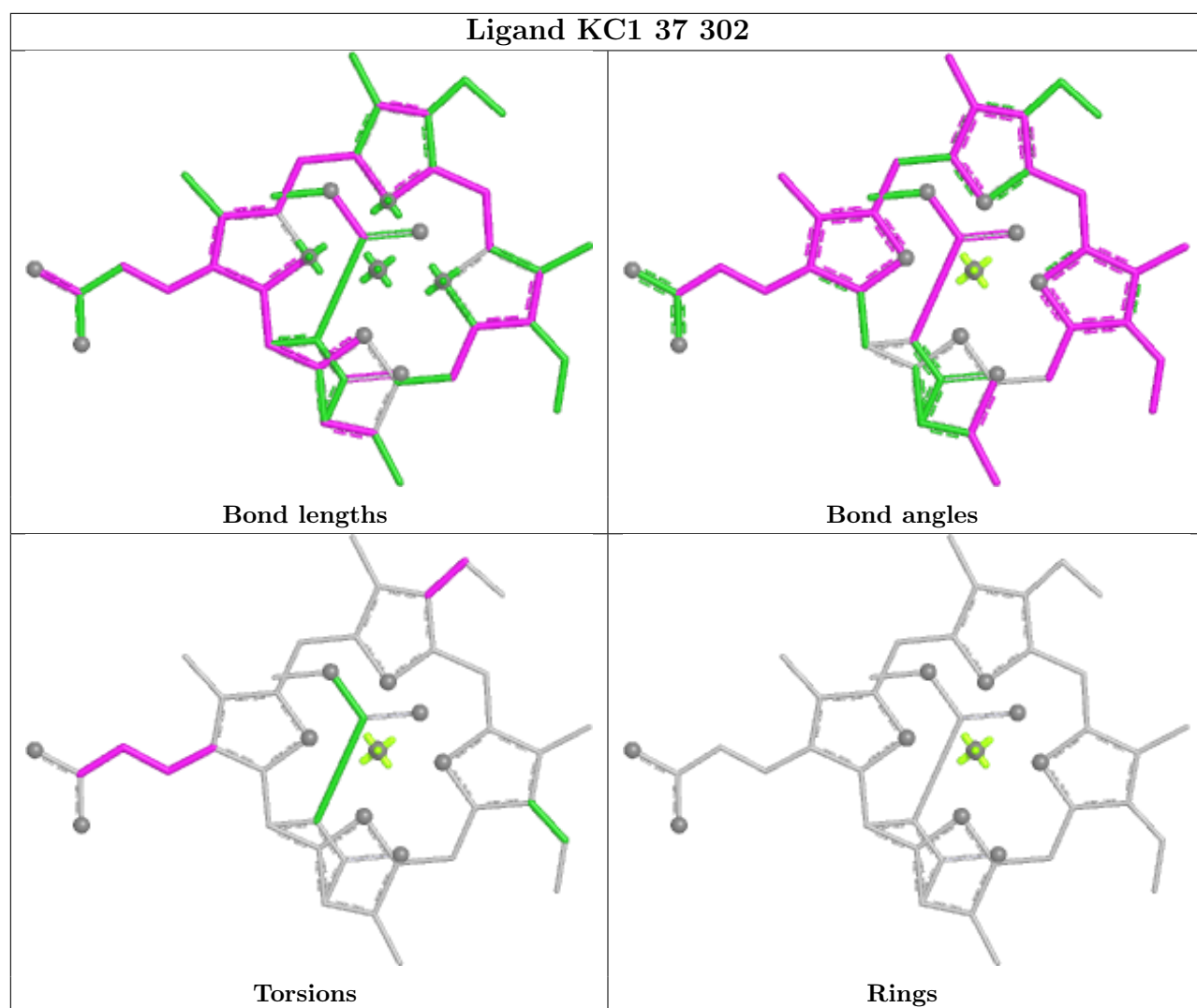
Ligand A86 31 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

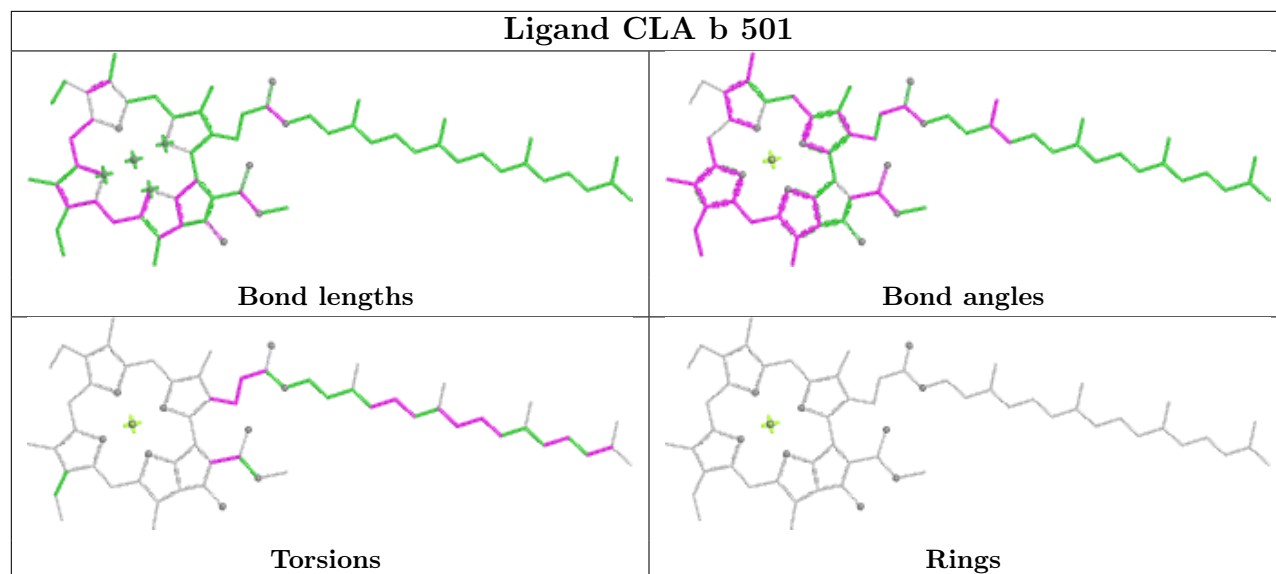
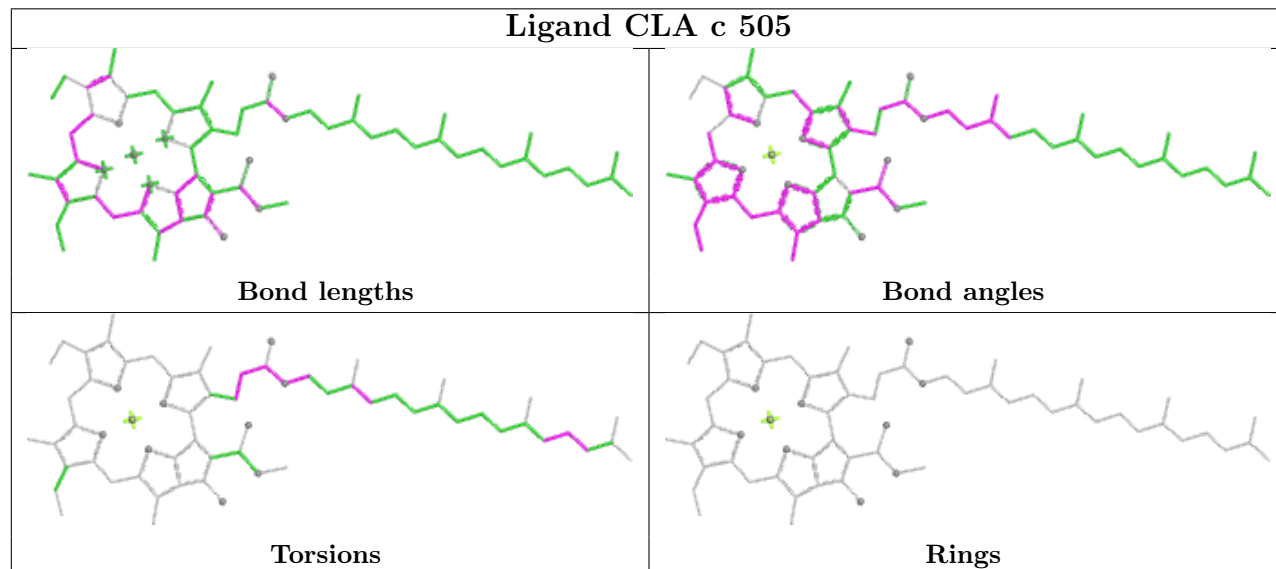
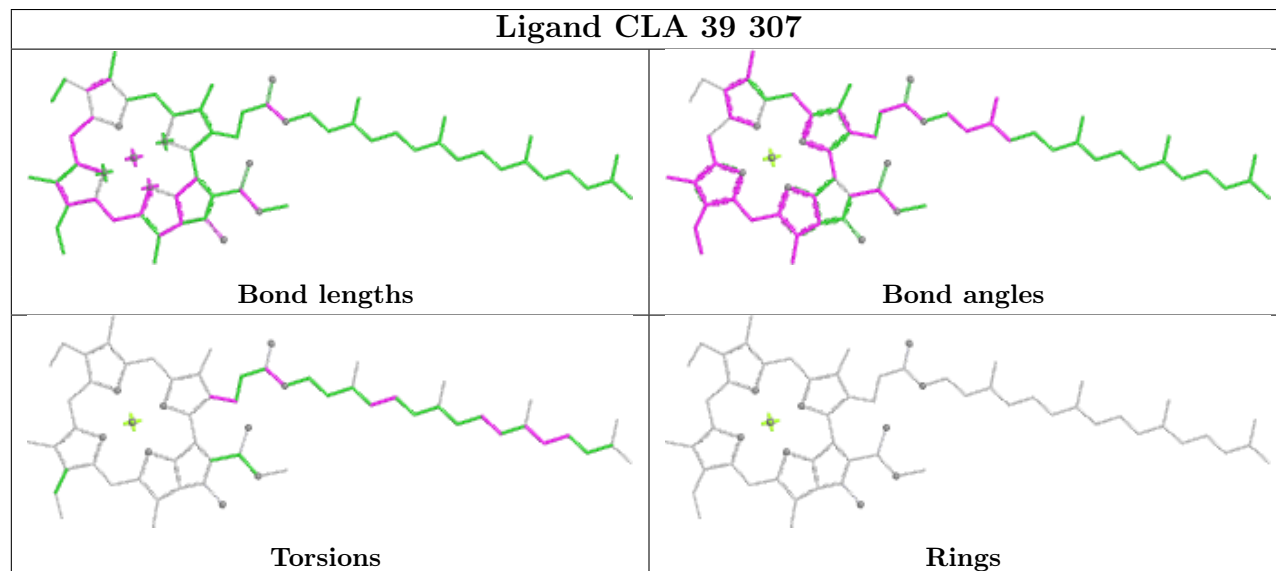
Ligand BCR a 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

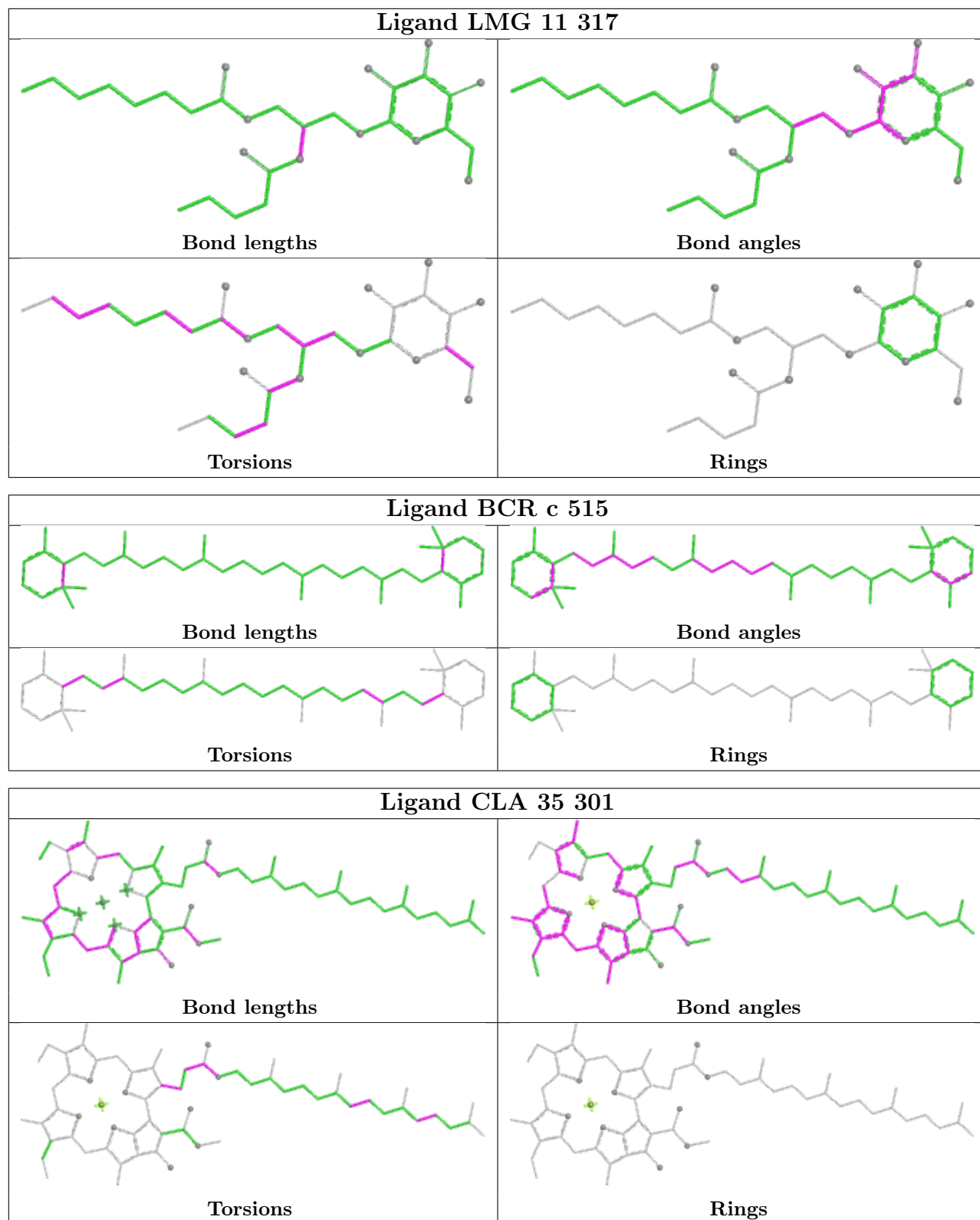
Ligand CLA 31 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

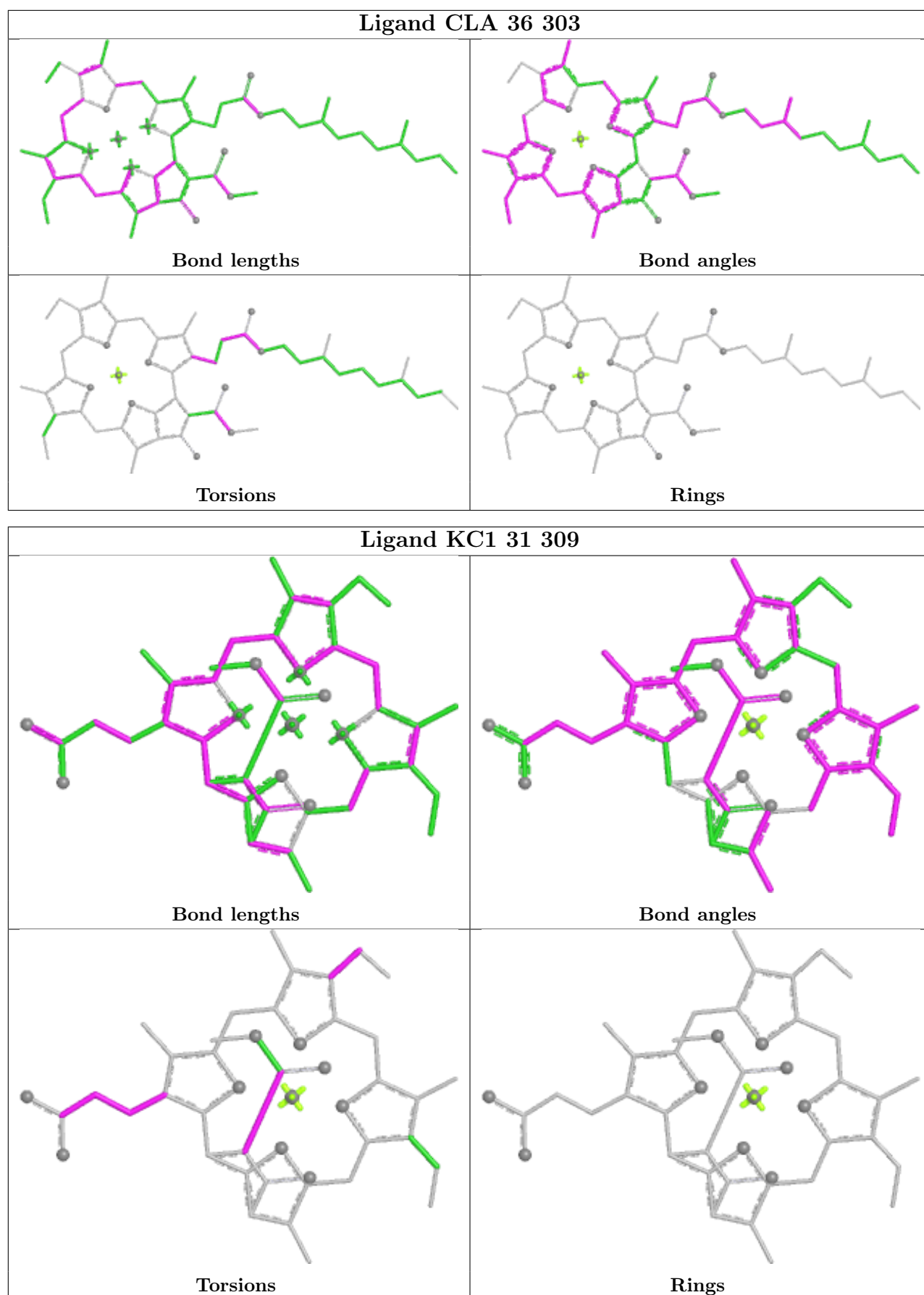


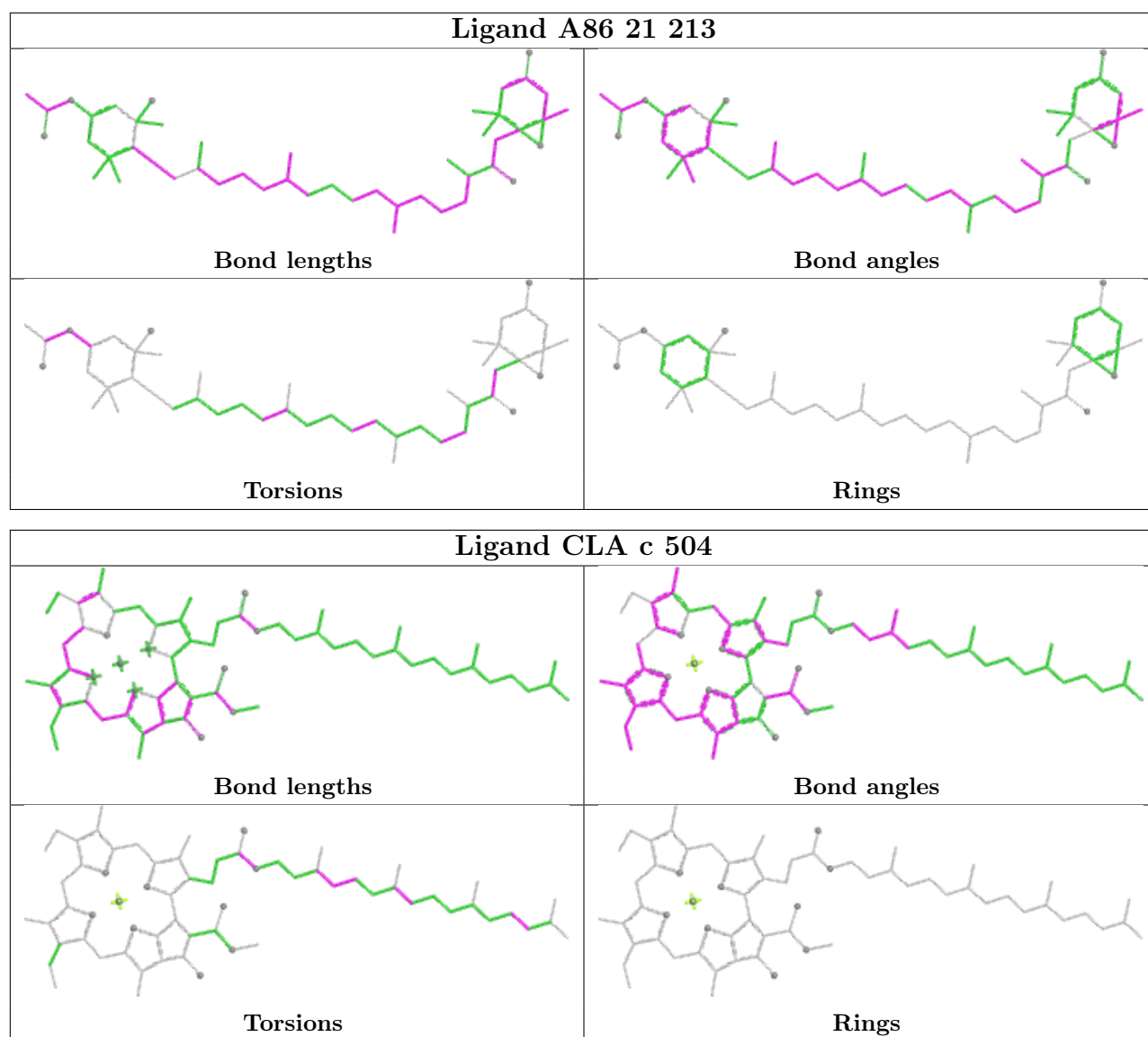


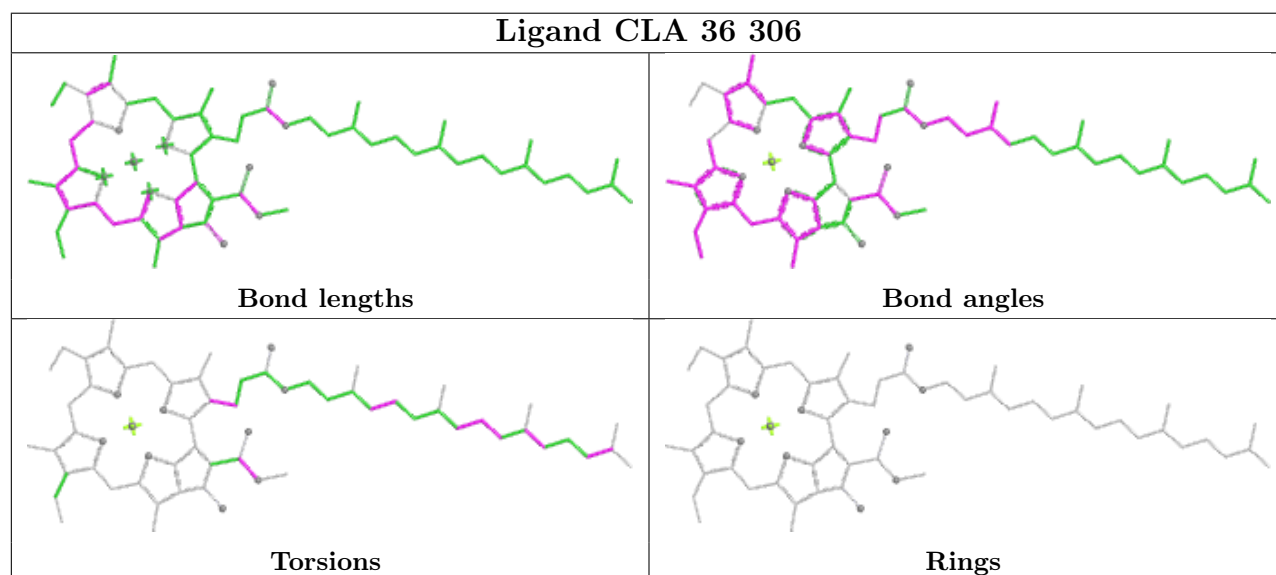
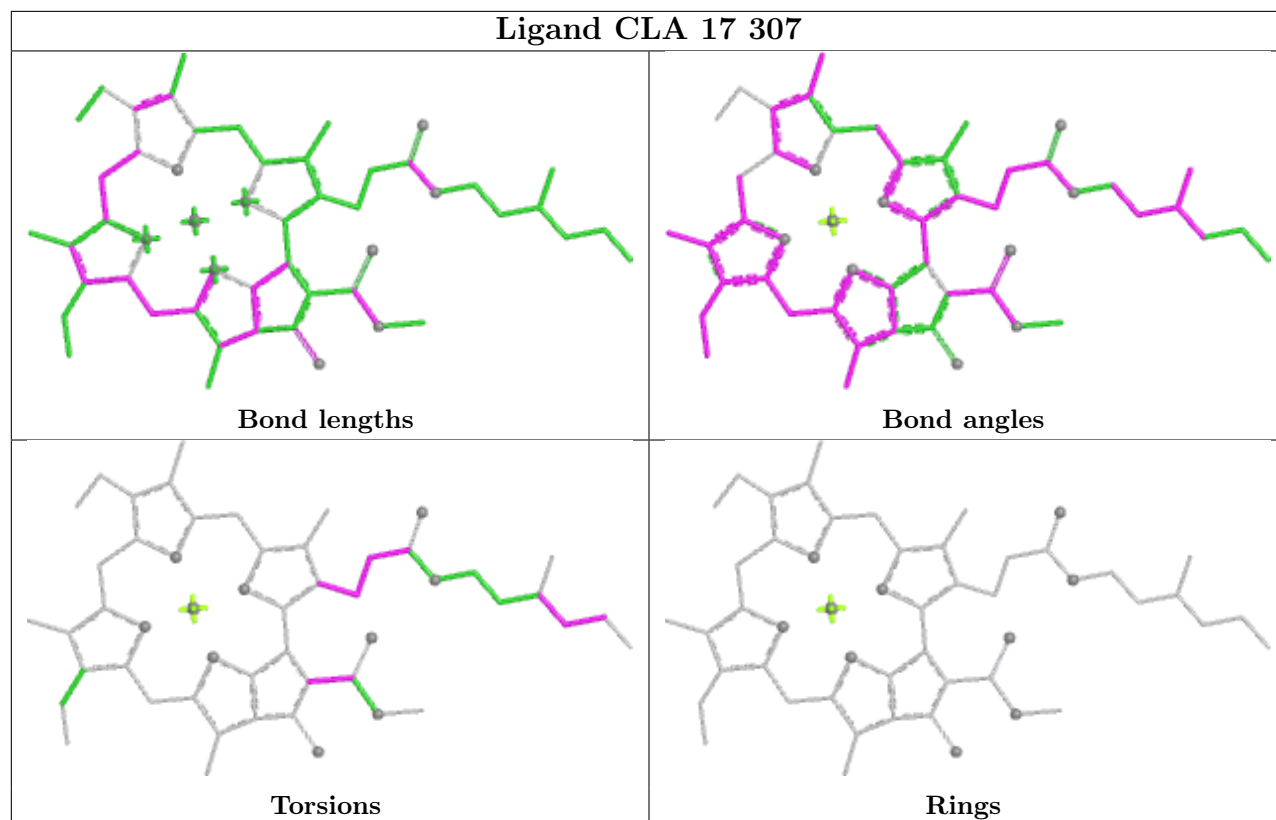


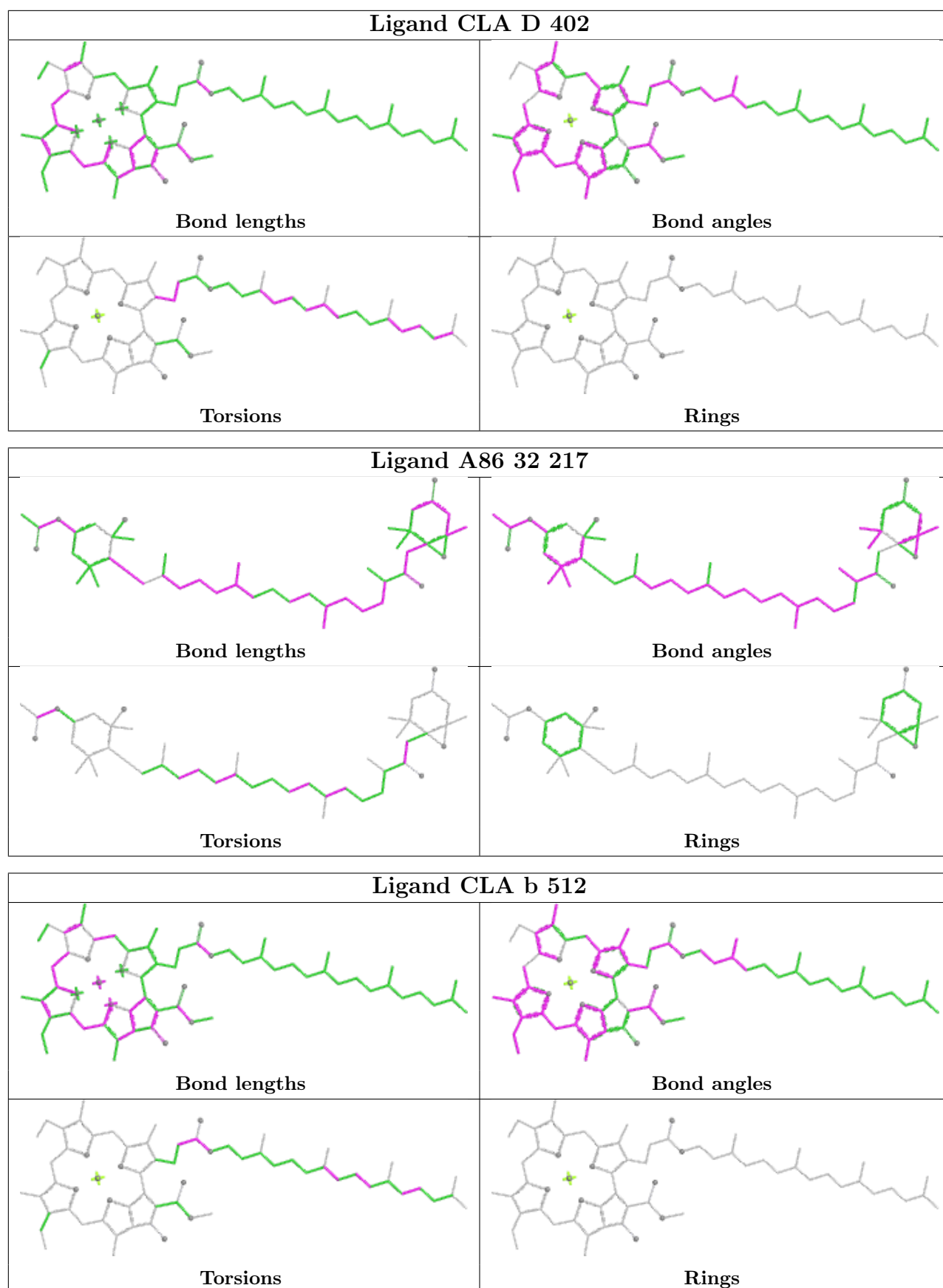
Ligand CLA b 501**Ligand CLA c 505****Ligand CLA 39 307**

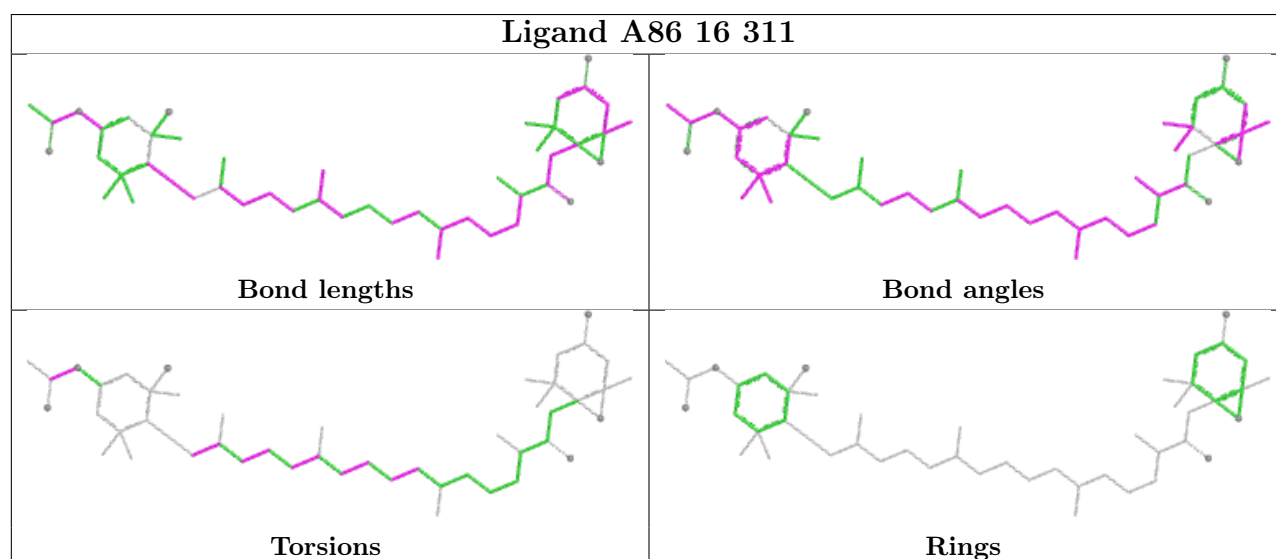
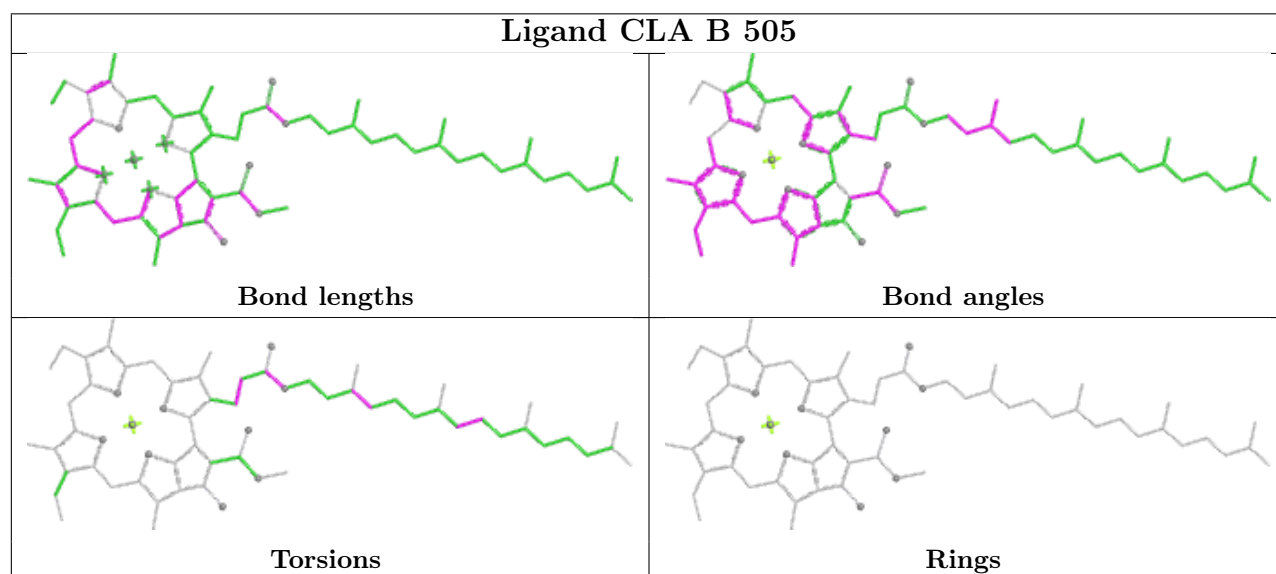
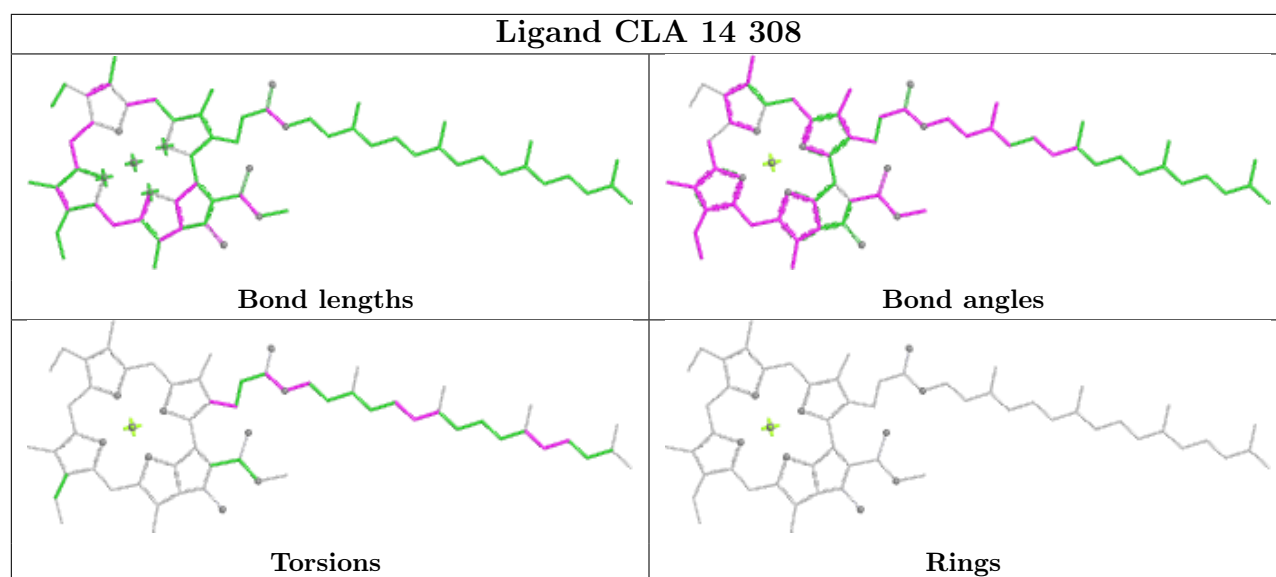


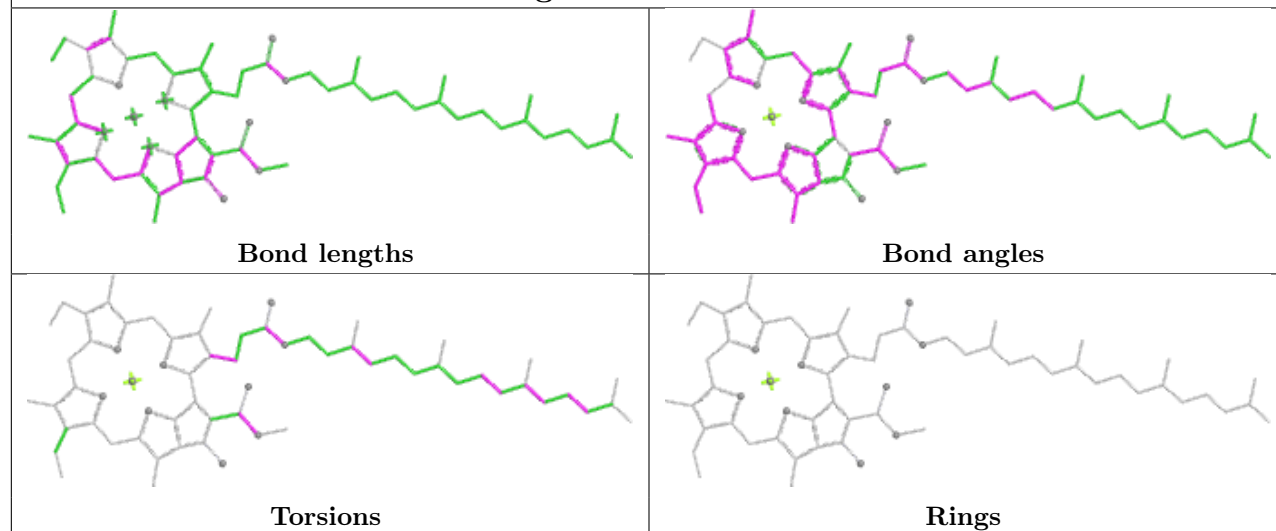
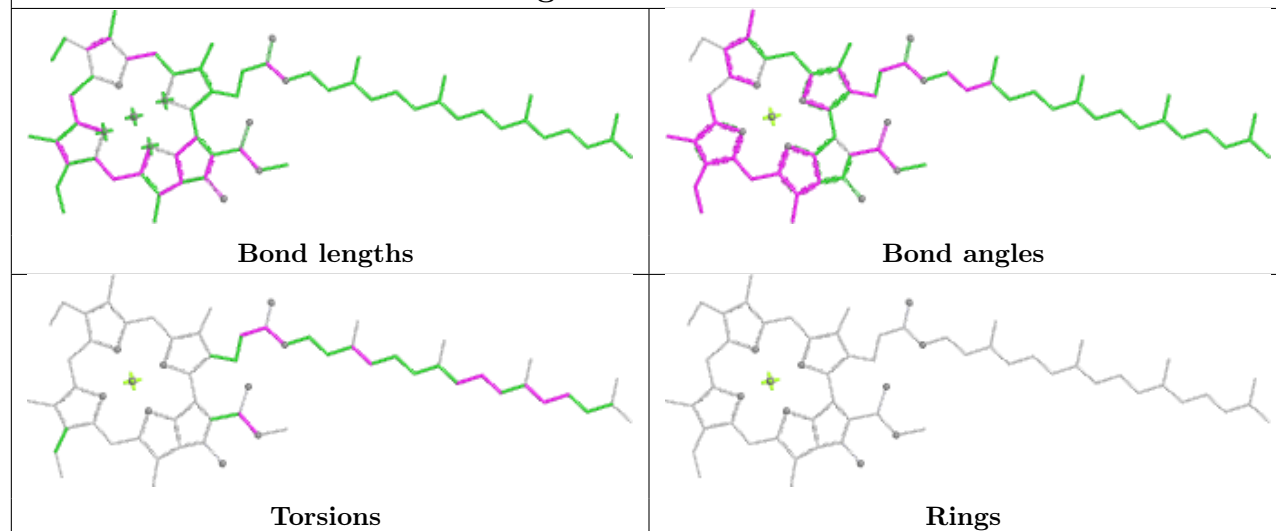


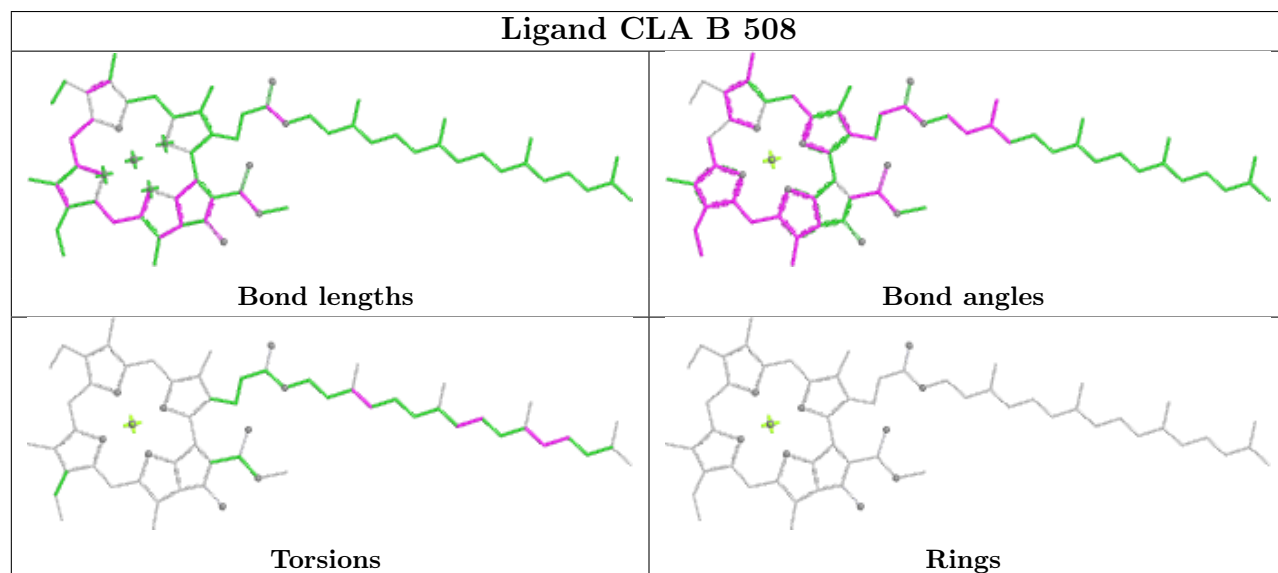
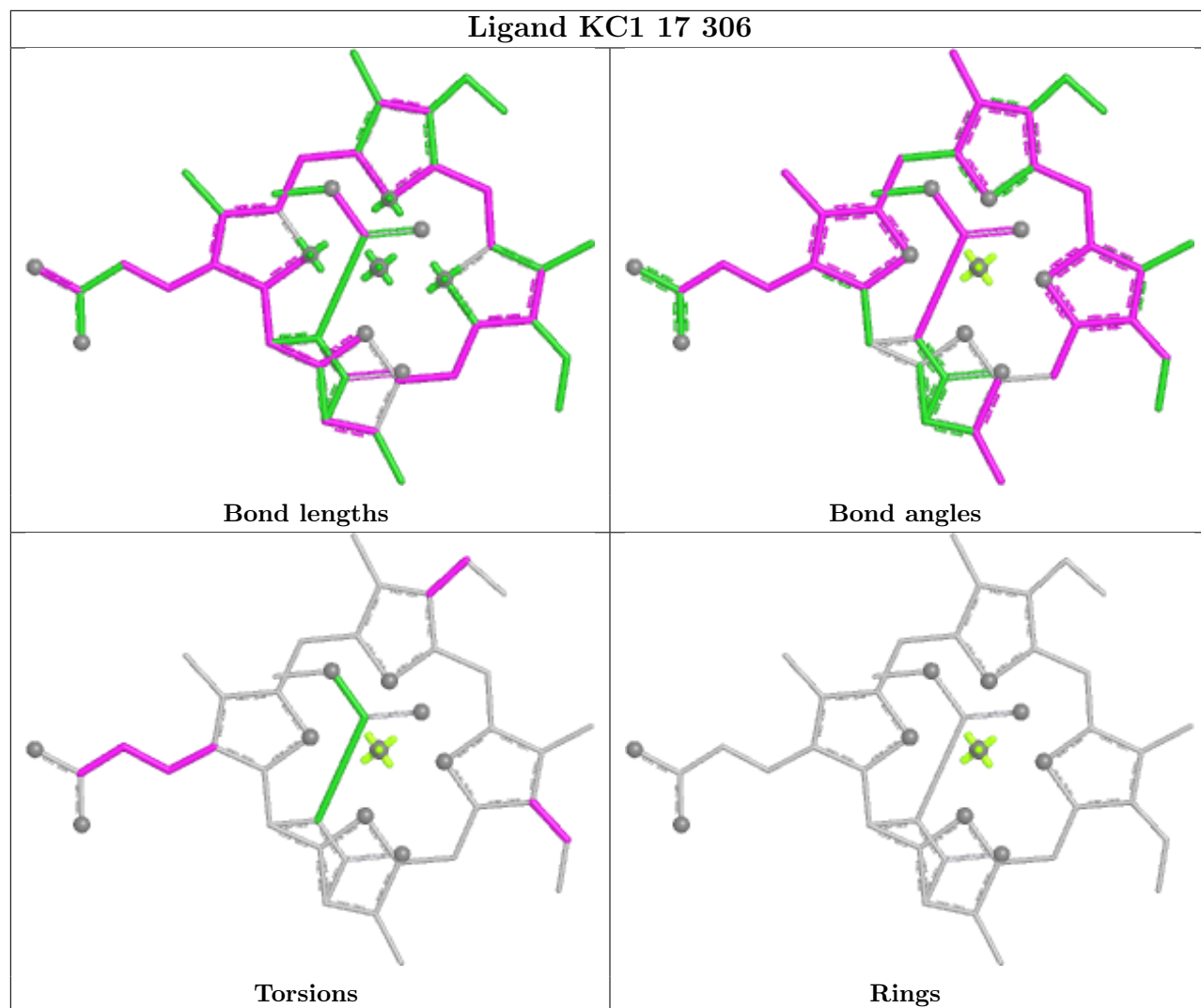


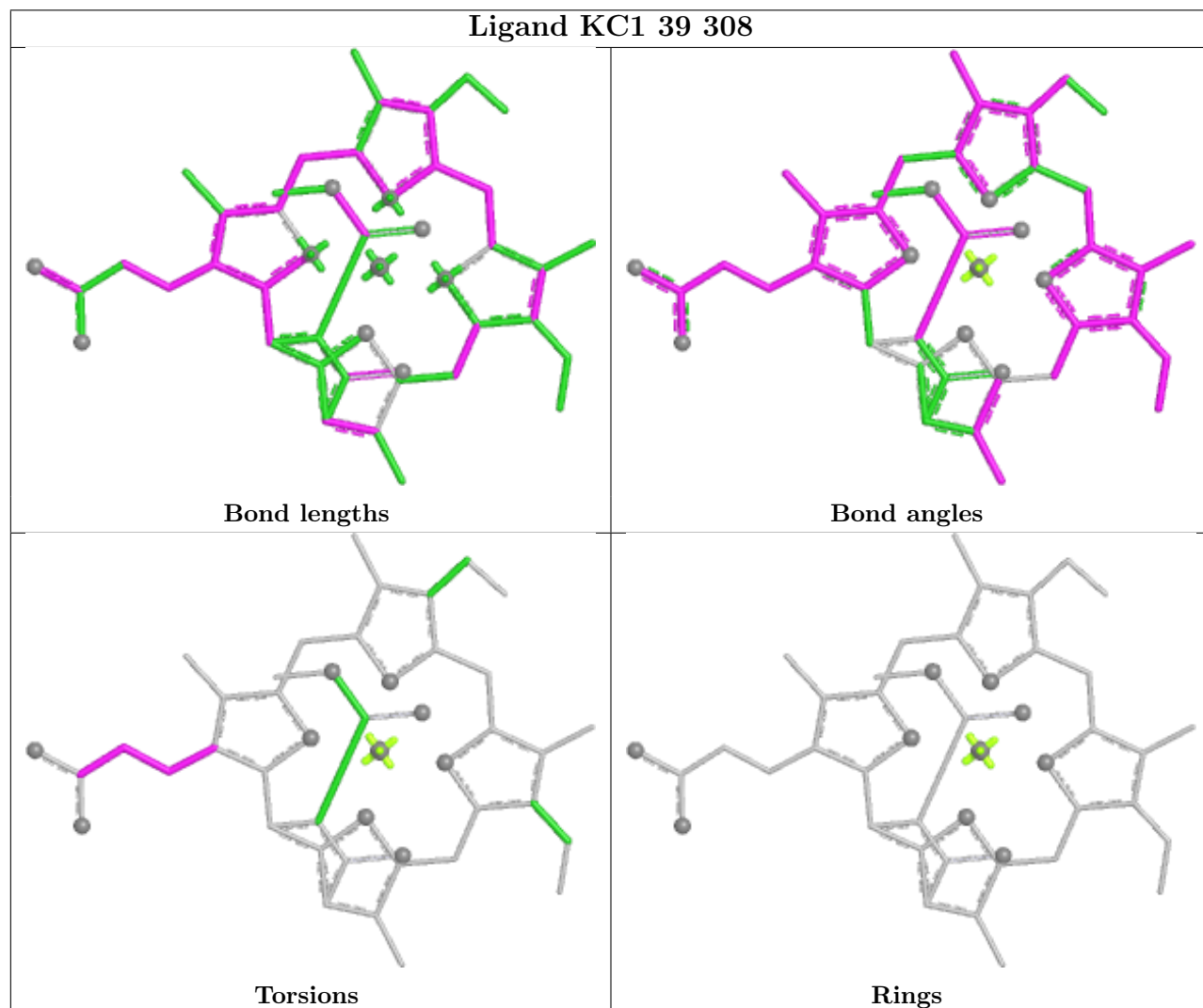
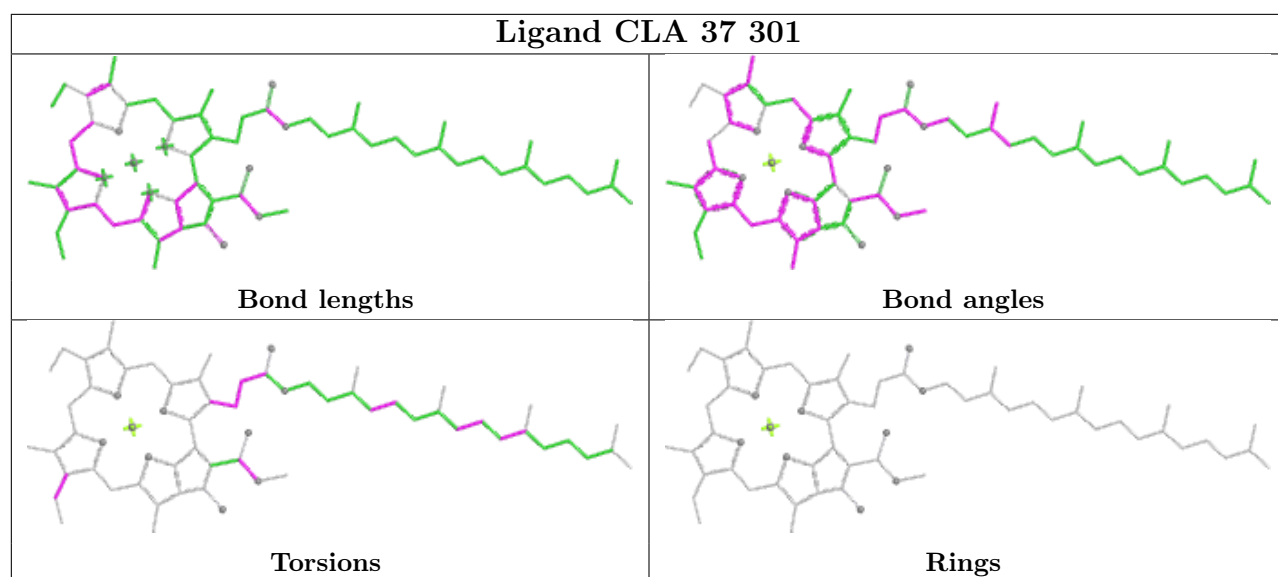


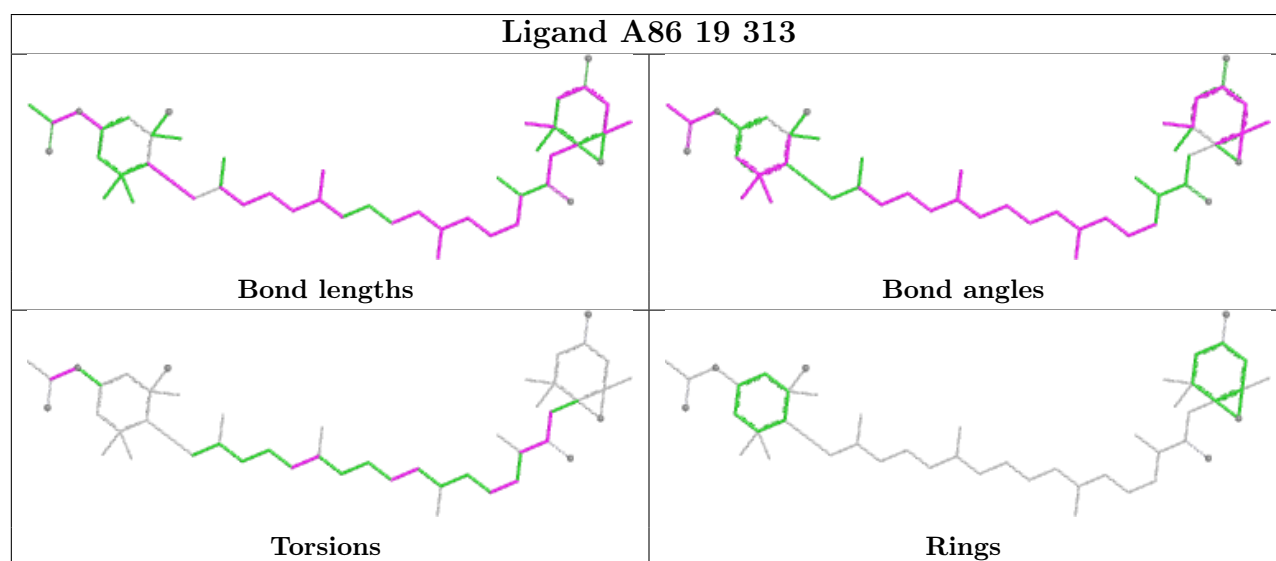
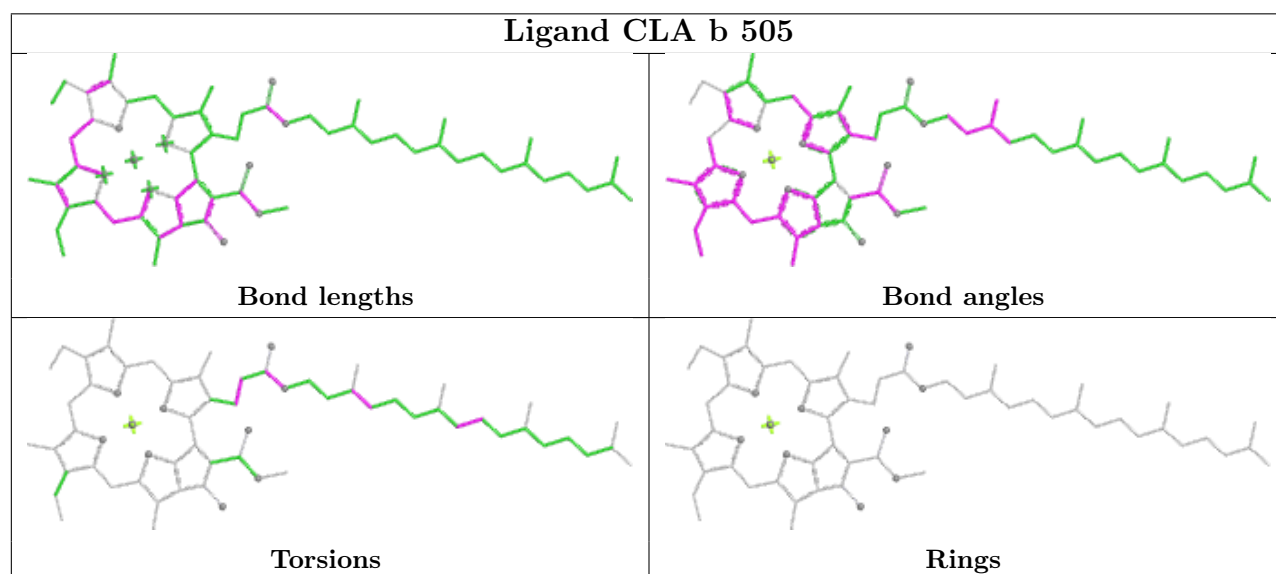
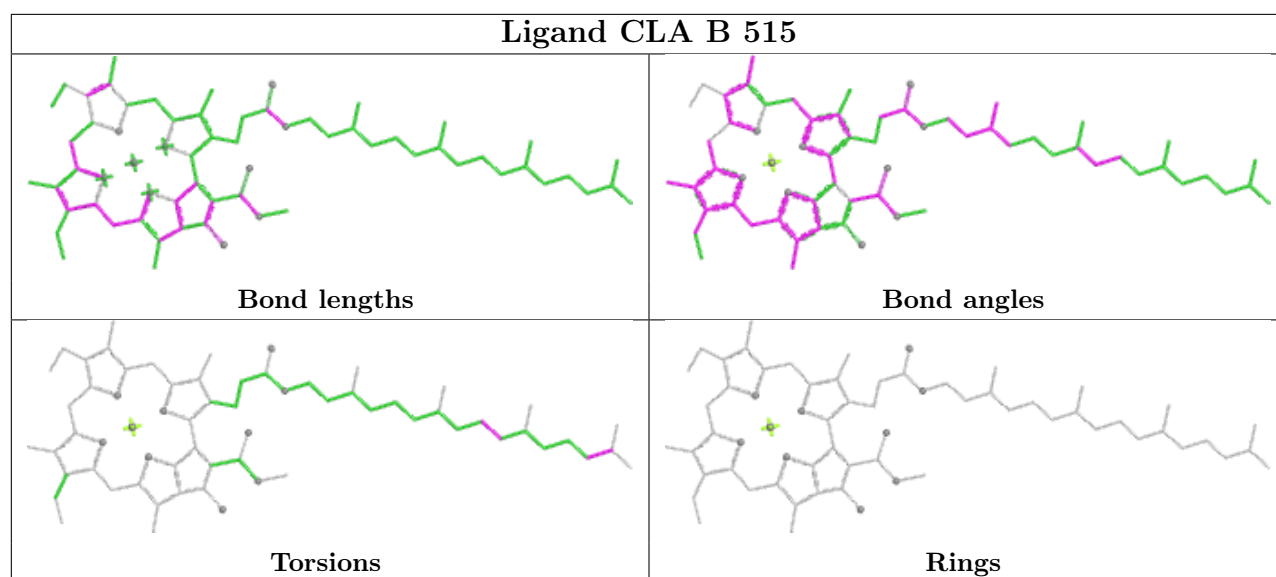


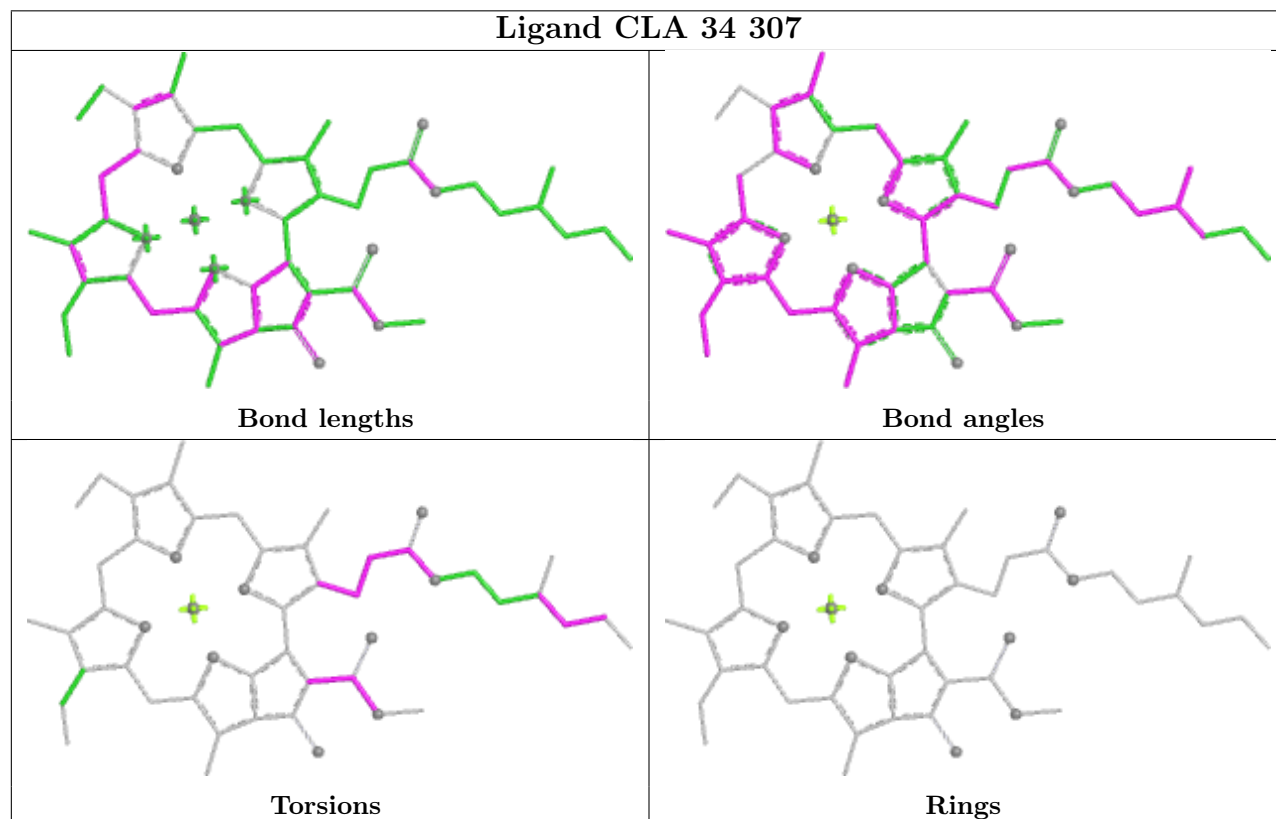
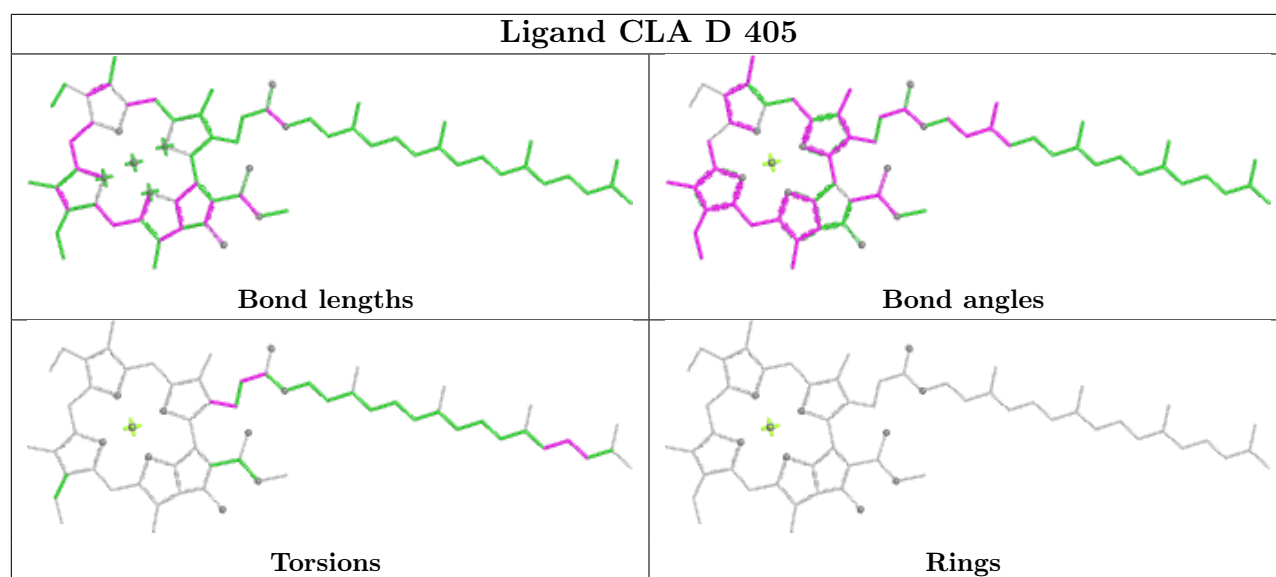


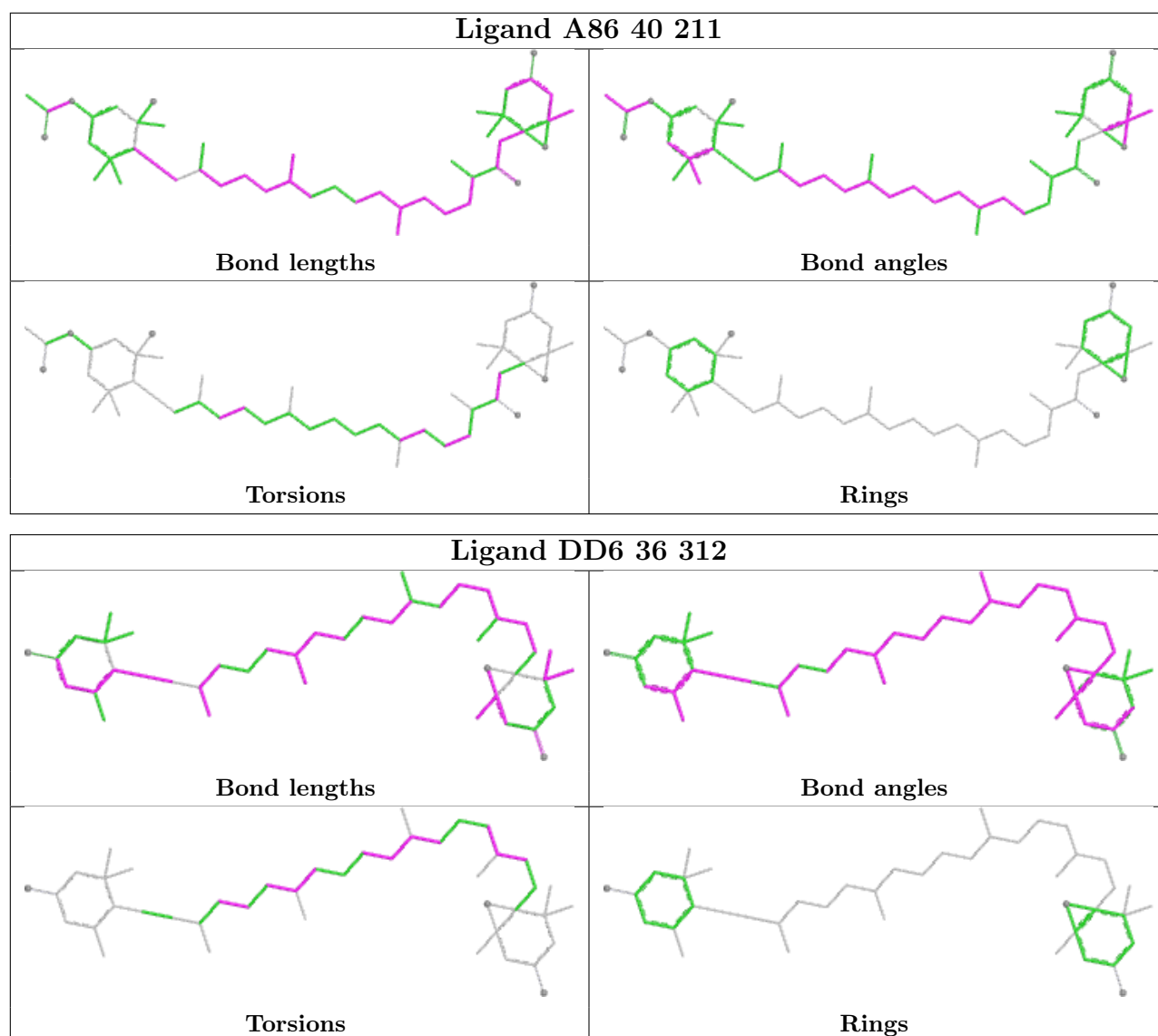
Ligand CLA b 511**Ligand CLA c 510**

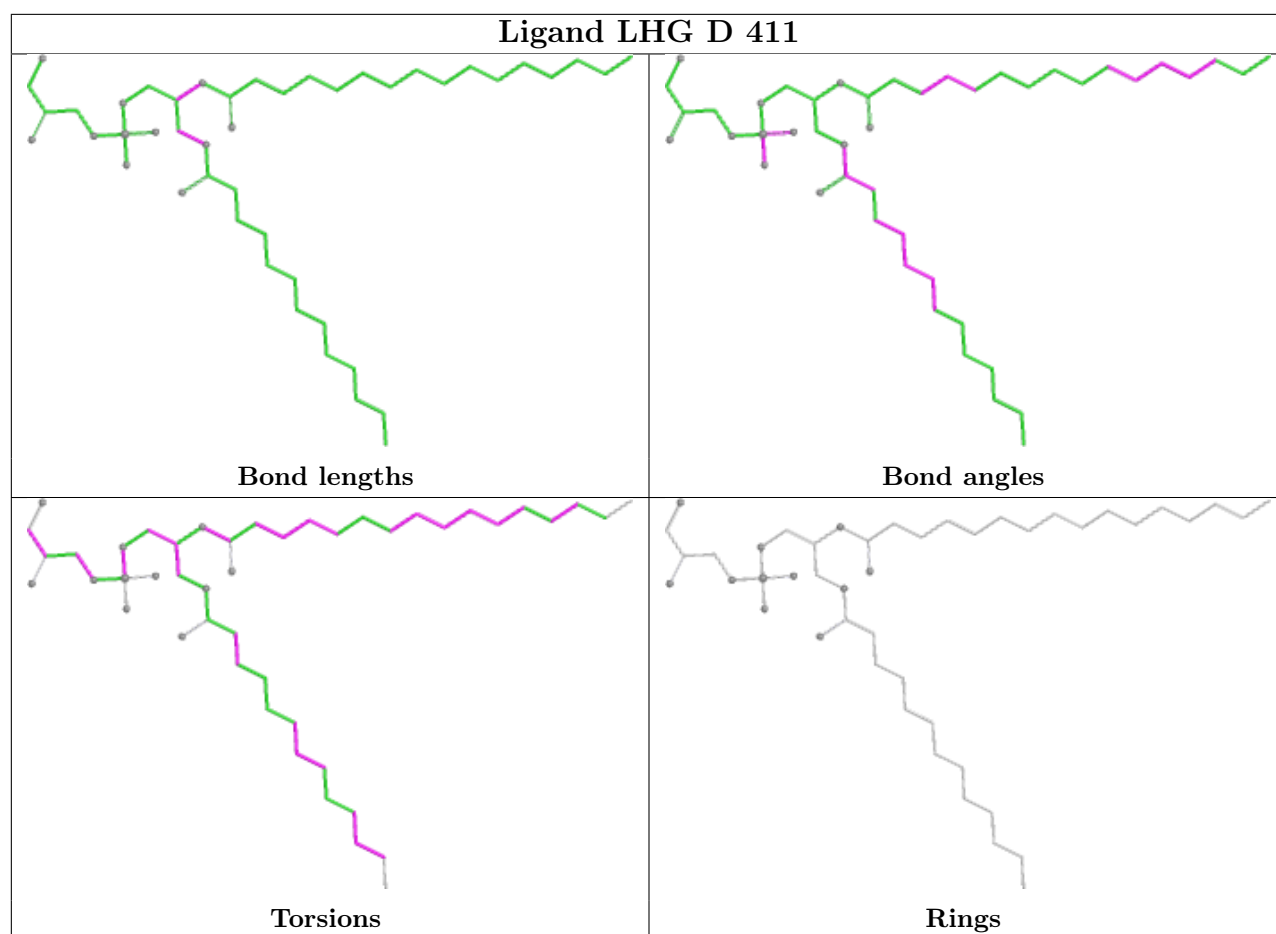












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

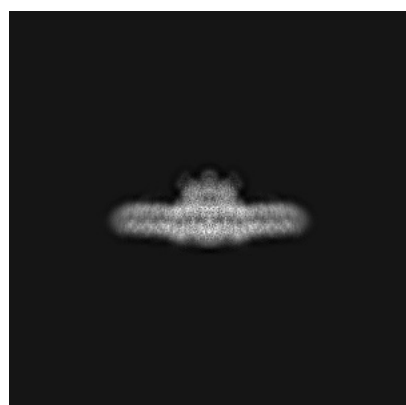
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31905. These allow visual inspection of the internal detail of the map and identification of artifacts.

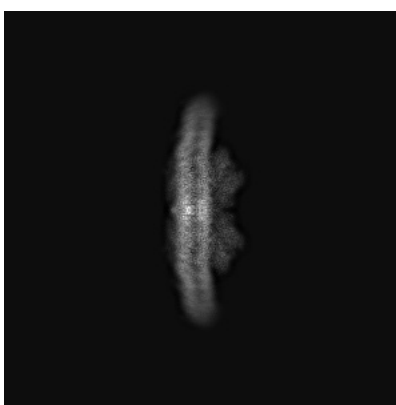
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

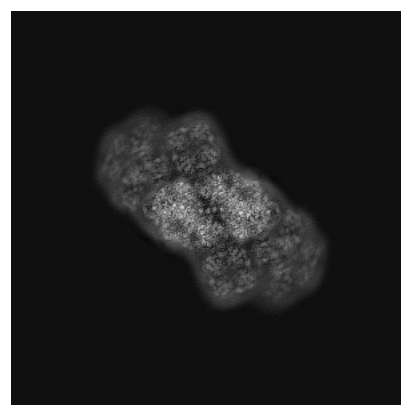
6.1.1 Primary map



X



Y

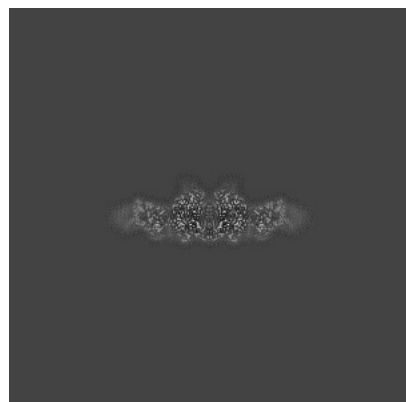


Z

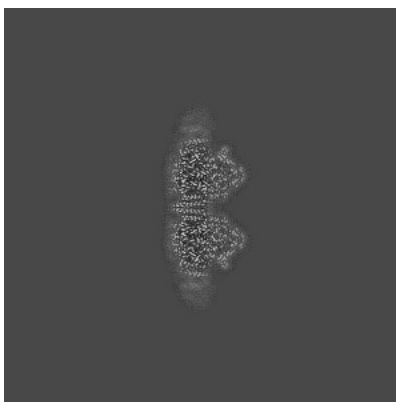
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

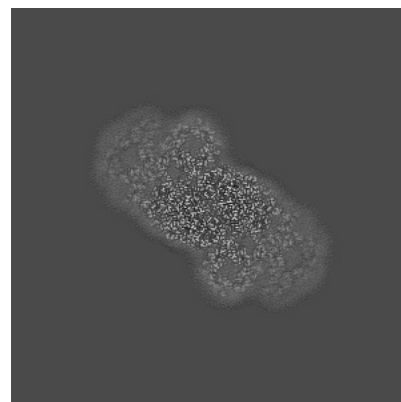
6.2.1 Primary map



X Index: 256



Y Index: 256

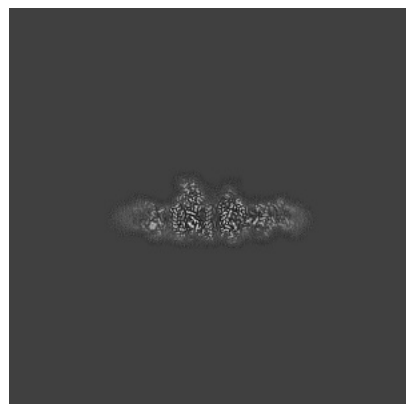


Z Index: 256

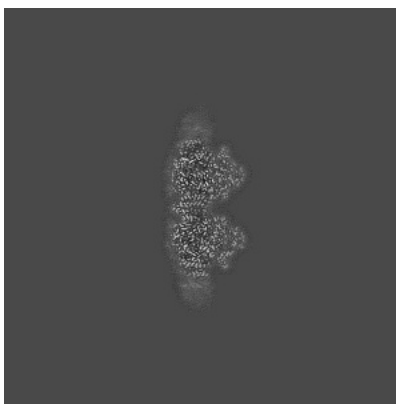
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

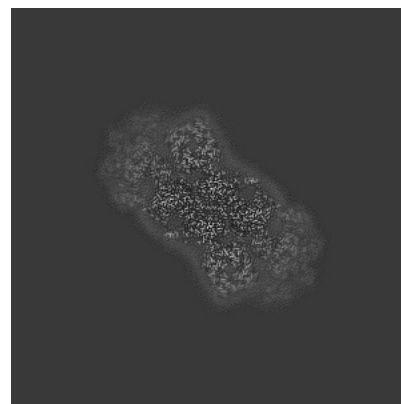
6.3.1 Primary map



X Index: 252



Y Index: 257

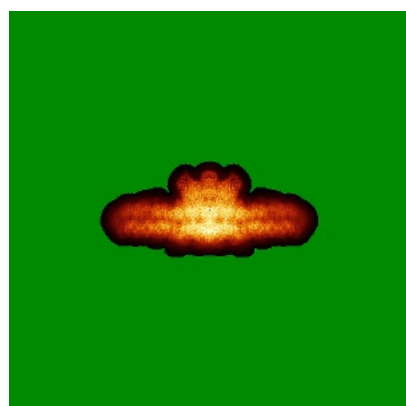


Z Index: 234

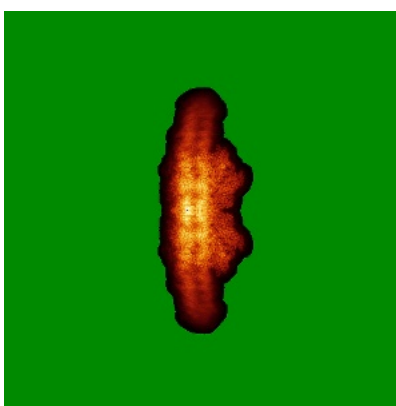
The images above show the largest variance slices of the map in three orthogonal directions.

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

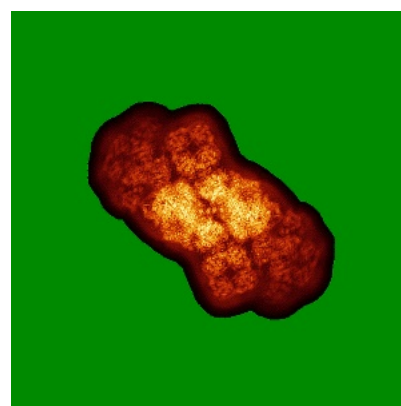
6.4.1 Primary map



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 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

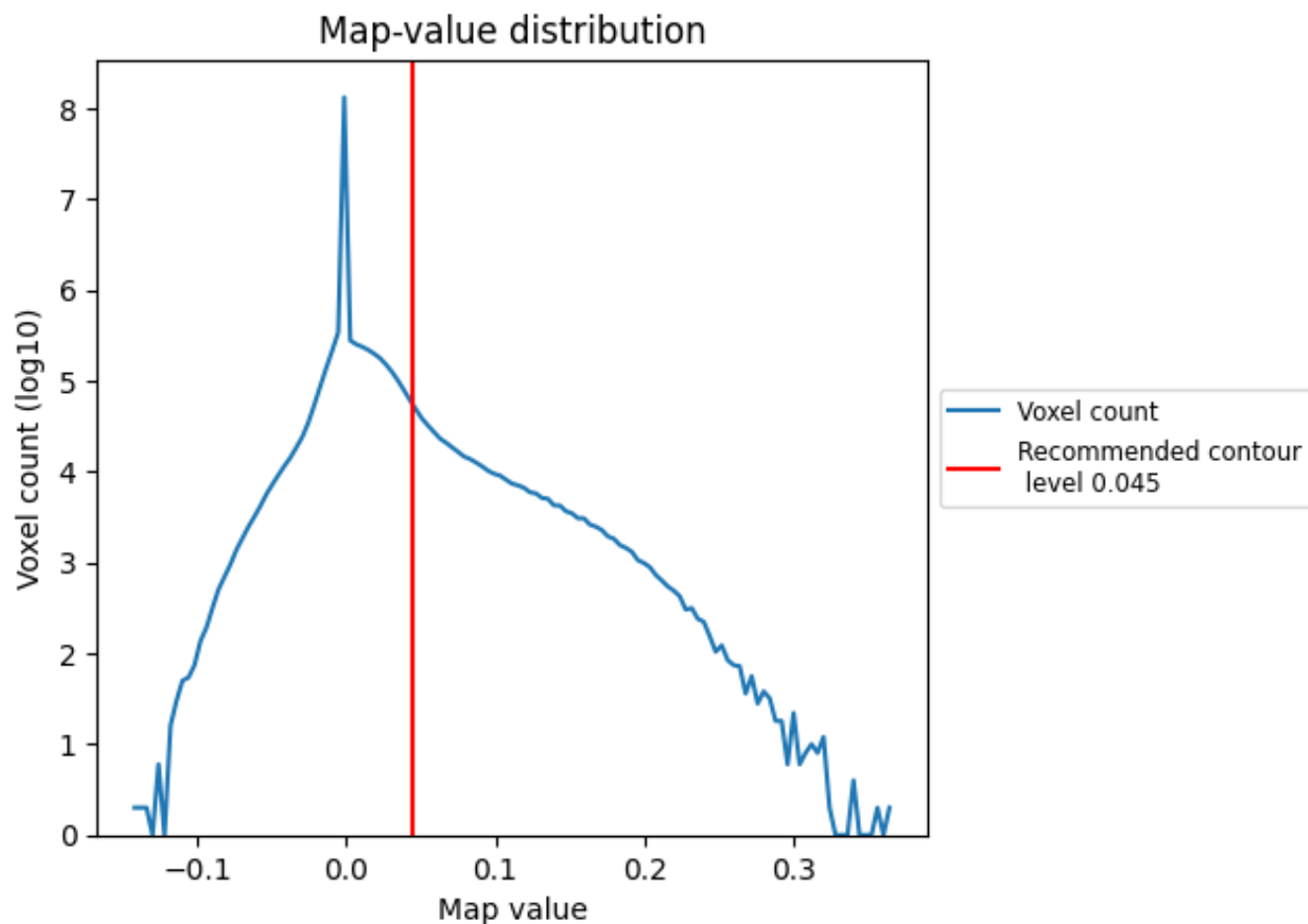
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

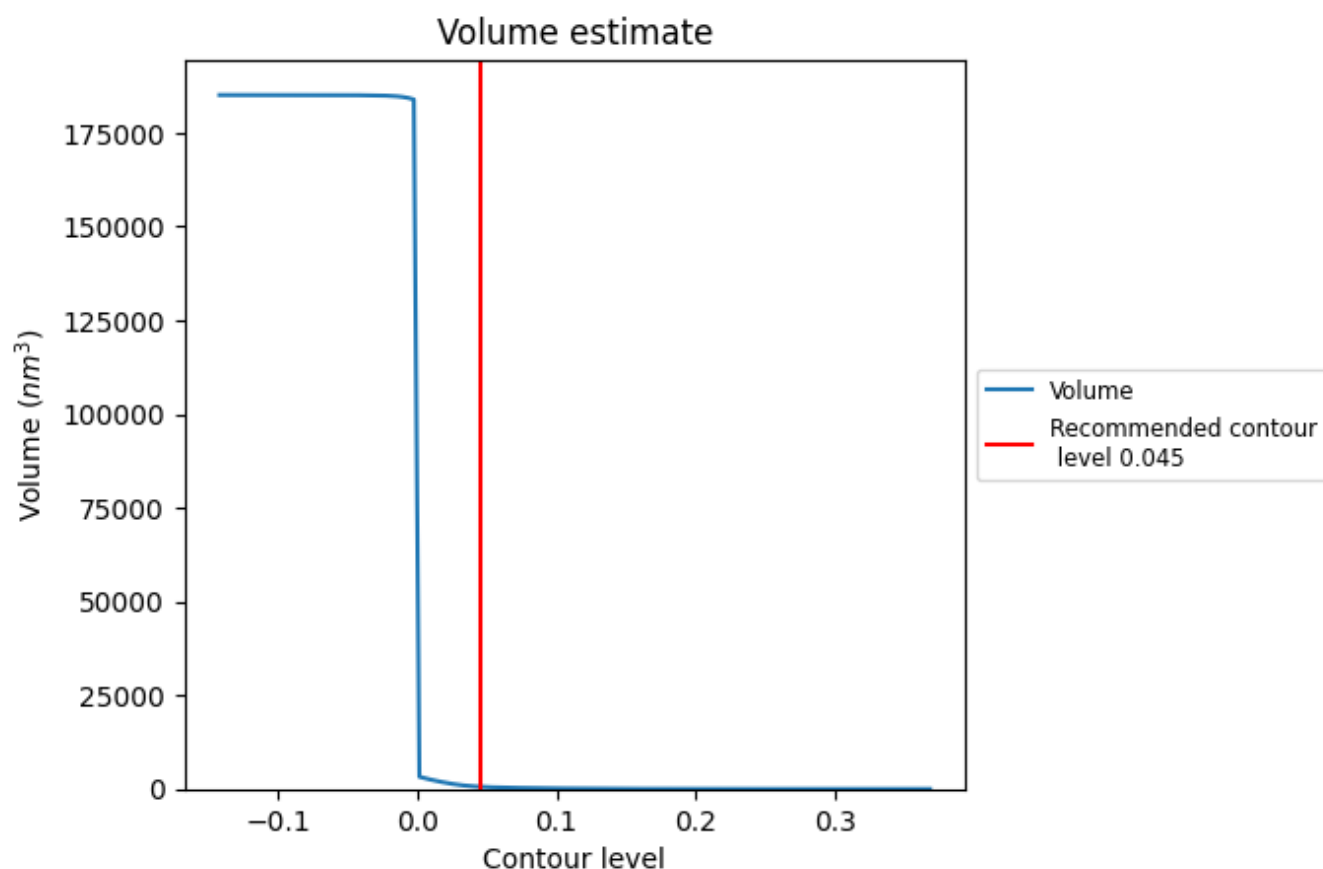
This section contains the results of statistical analysis of the map.

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.

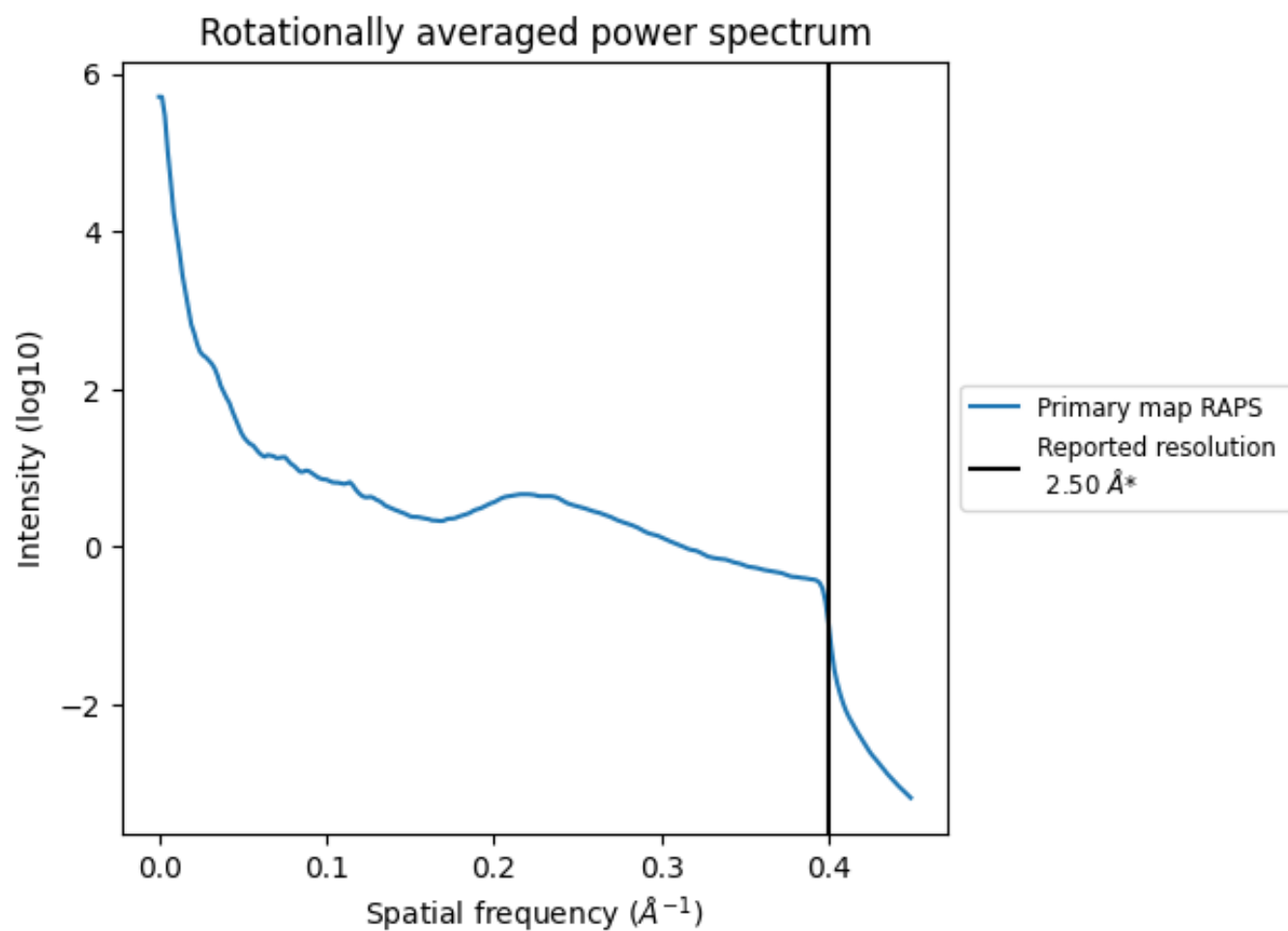
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 588 nm^3 ; this corresponds to an approximate mass of 532 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 ⓘ

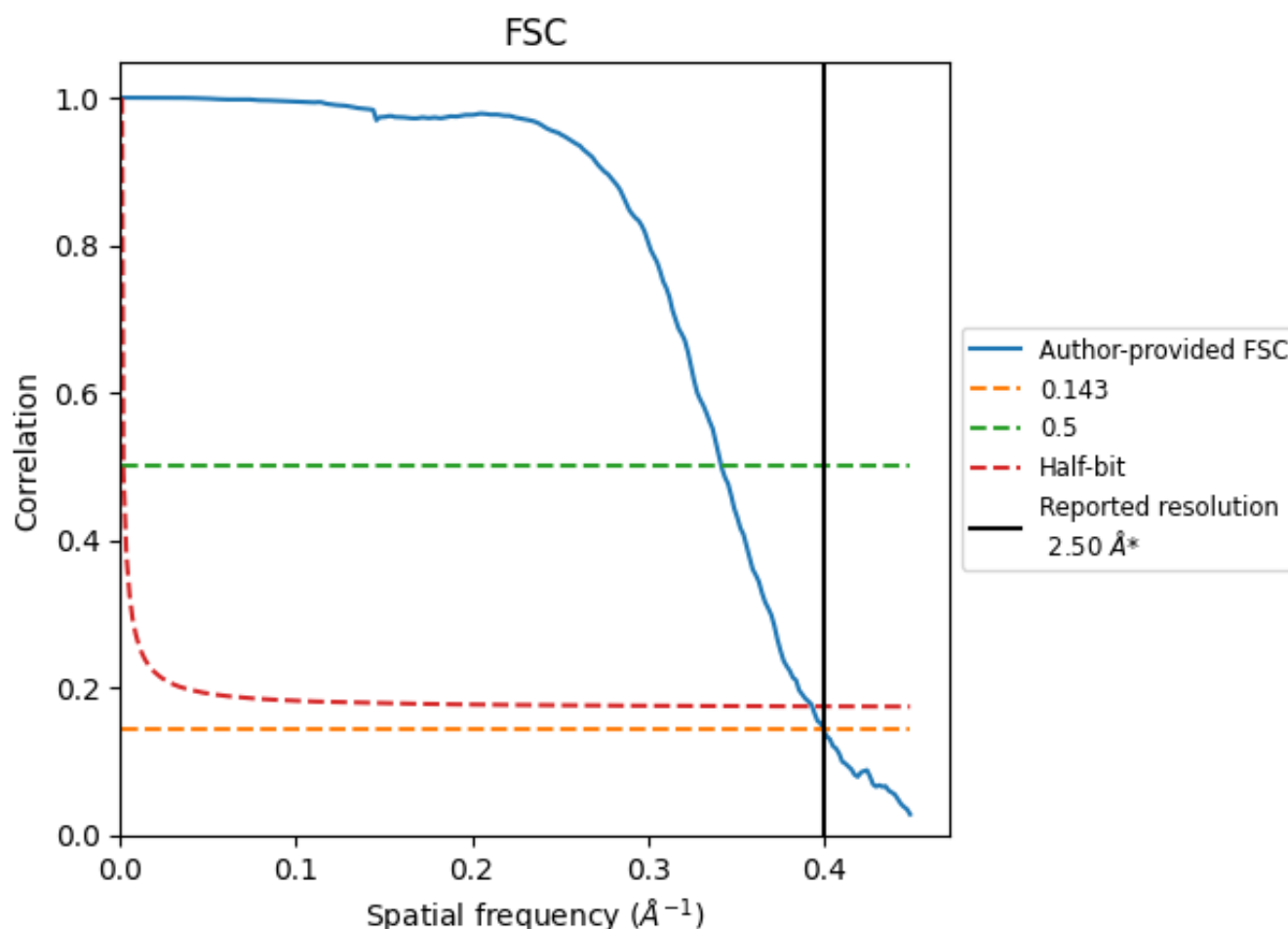


*Reported resolution corresponds to spatial frequency of 0.400 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 \AA^{-1}

8.2 Resolution estimates [i](#)

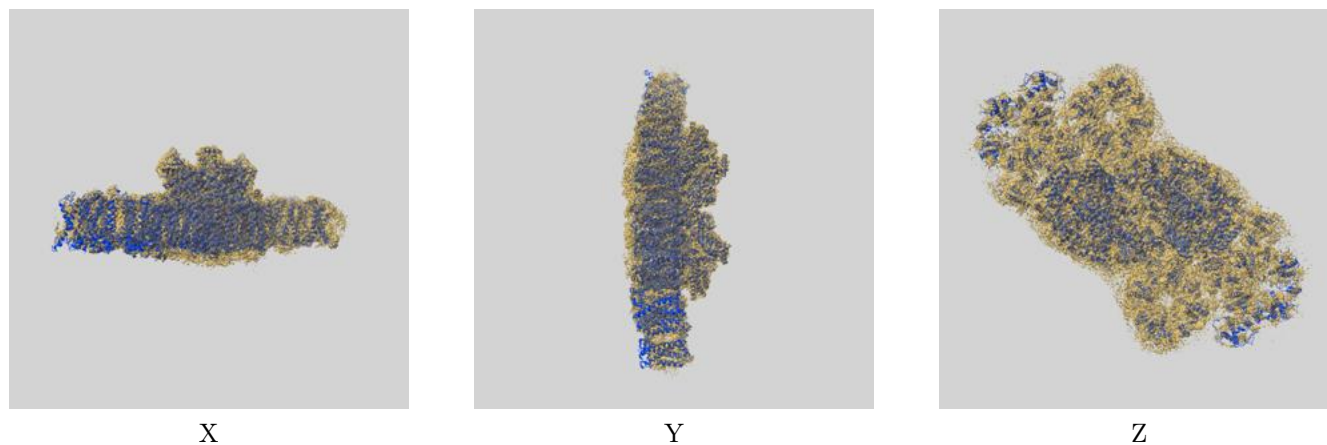
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.50	2.92	2.54
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

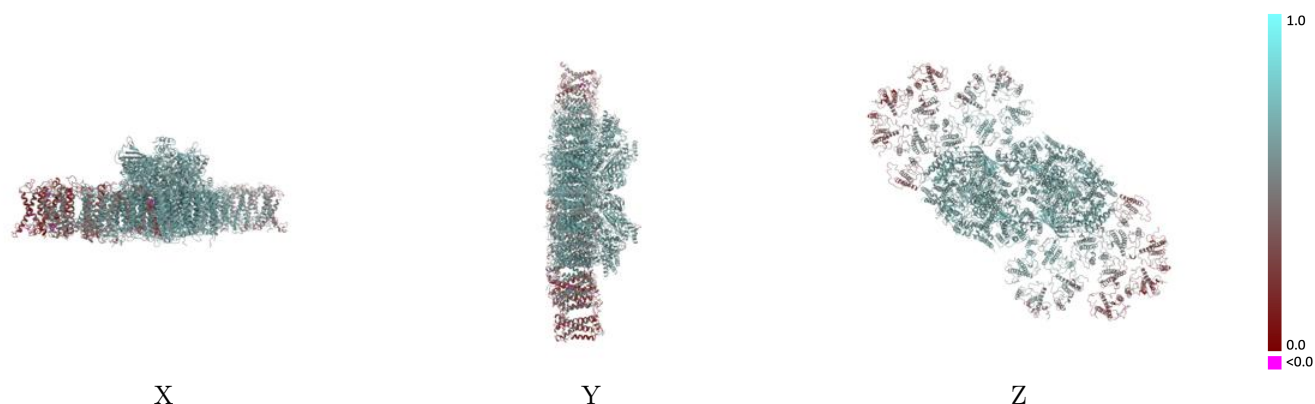
This section contains information regarding the fit between EMDB map EMD-31905 and PDB model 7VD5. Per-residue inclusion information can be found in section [3](#) on page [51](#).

9.1 Map-model overlay [i](#)



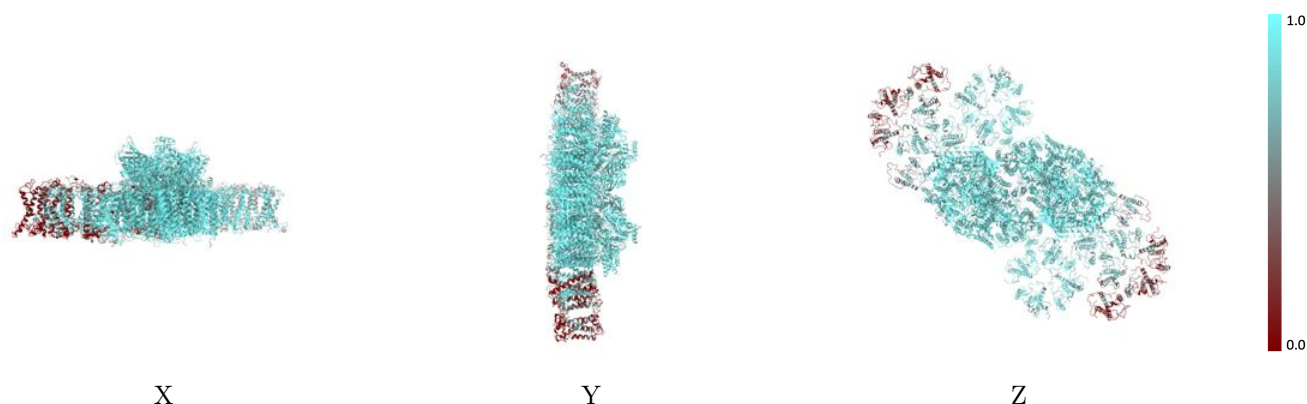
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



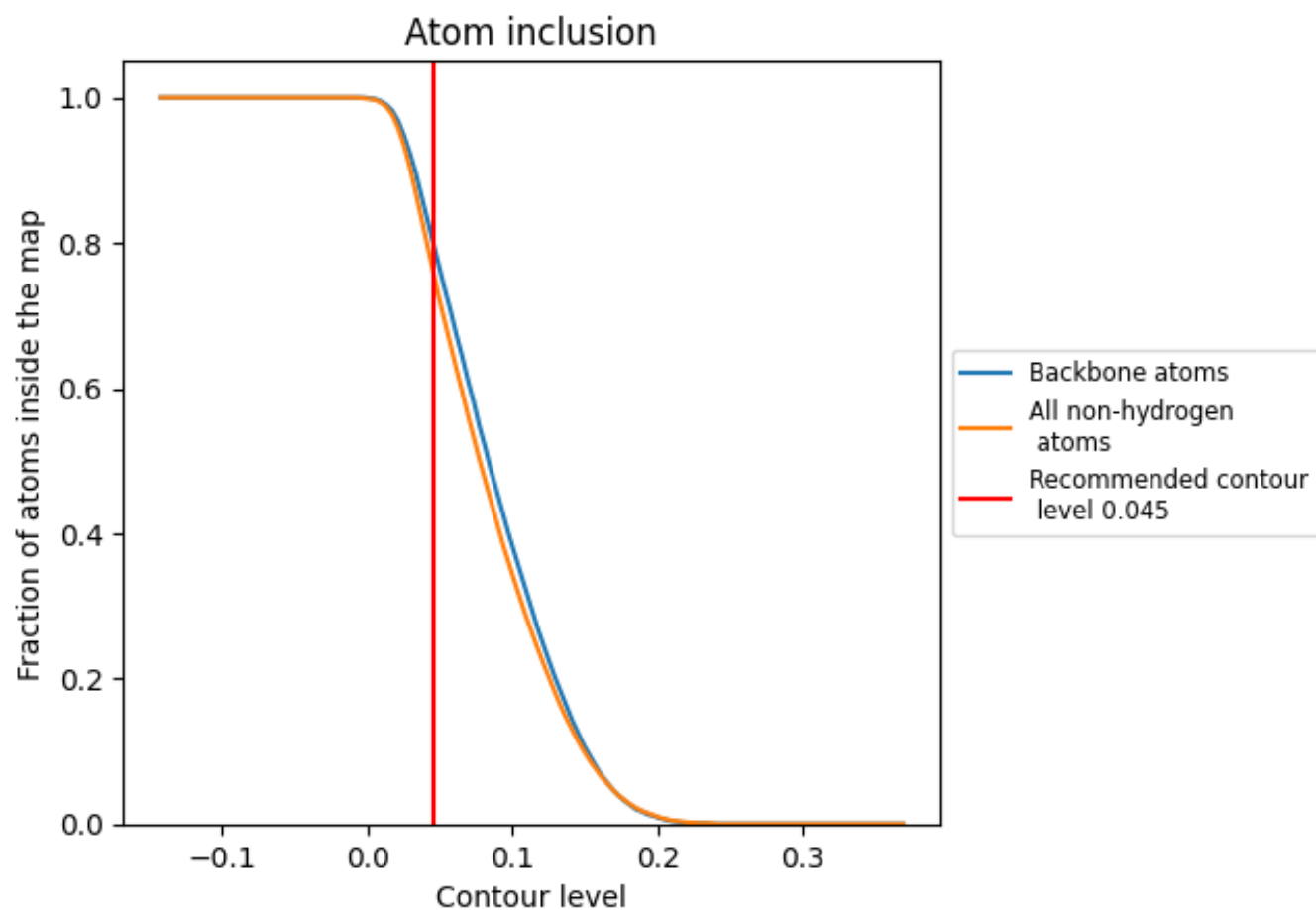
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 76% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7640	 0.5430
0	 0.9590	 0.6360
1	 0.9330	 0.6130
11	 0.8820	 0.6000
12	 0.8680	 0.5780
13	 0.7230	 0.4570
14	 0.7450	 0.4800
15	 0.2430	 0.2840
16	 0.6780	 0.4740
17	 0.5850	 0.4350
18	 0.2380	 0.2830
19	 0.7830	 0.5510
20	 0.5020	 0.3420
21	 0.1260	 0.2530
31	 0.8690	 0.5900
32	 0.8710	 0.5790
33	 0.7220	 0.4550
34	 0.7460	 0.4770
35	 0.2400	 0.2850
36	 0.6890	 0.4790
37	 0.5830	 0.4360
38	 0.2400	 0.2860
39	 0.7830	 0.5490
40	 0.4820	 0.3370
41	 0.1300	 0.2520
5	 0.9590	 0.6400
6	 0.9330	 0.6080
A	 0.9630	 0.6690
B	 0.9350	 0.6540
C	 0.9440	 0.6550
D	 0.9420	 0.6620
E	 0.9020	 0.6110
F	 0.9200	 0.5950
H	 0.9340	 0.6390
I	 0.9540	 0.6560



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Chain	Atom inclusion	Q-score
J	 0.8940	 0.6380
K	 0.9200	 0.6260
L	 0.8900	 0.6400
M	 0.8590	 0.6400
O	 0.8830	 0.6120
Q	 0.8670	 0.5980
T	 0.9100	 0.6520
U	 0.9070	 0.6120
V	 0.9320	 0.6200
W	 0.8070	 0.5830
X	 0.8380	 0.5580
Y	 0.8270	 0.5920
Z	 0.8640	 0.5670
a	 0.9630	 0.6680
b	 0.9370	 0.6550
c	 0.9430	 0.6530
d	 0.9390	 0.6610
e	 0.8920	 0.6110
f	 0.9200	 0.5950
h	 0.9390	 0.6350
i	 0.9540	 0.6570
j	 0.8870	 0.6360
k	 0.9360	 0.6190
l	 0.9480	 0.6530
m	 0.8630	 0.6410
o	 0.8870	 0.6120
q	 0.8730	 0.6000
t	 0.9100	 0.6570
u	 0.9070	 0.6140
v	 0.9300	 0.6220
w	 0.8520	 0.6140
x	 0.8220	 0.5620
y	 0.8410	 0.6050
z	 0.8720	 0.5650