



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 05:14 PM UTC

PDB ID : 7VD5 / pdb_00007vd5
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:

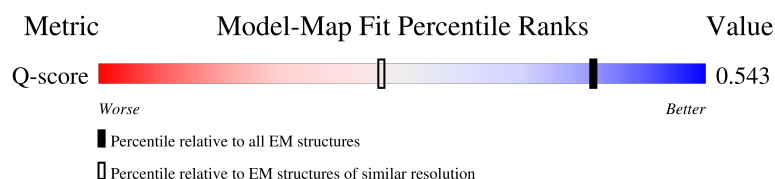
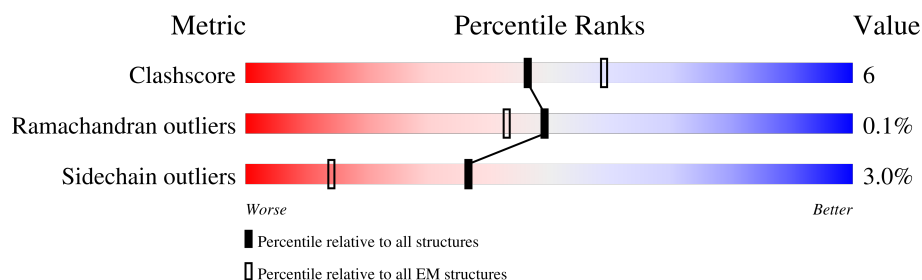
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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.



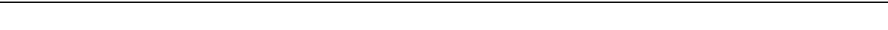
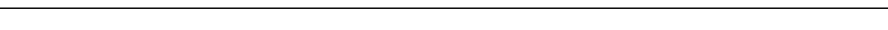
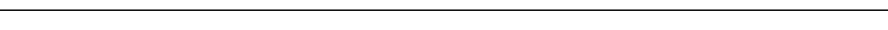
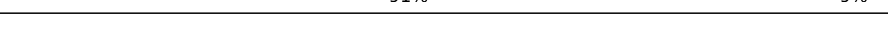
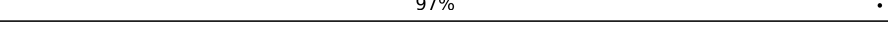
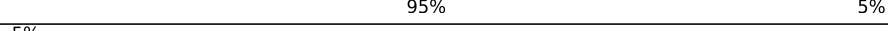
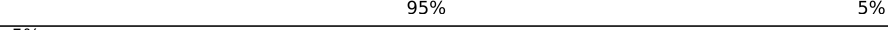
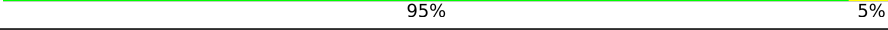
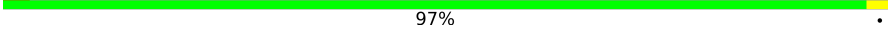
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	
1	a	334	
2	B	484	
2	b	484	

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Mol	Chain	Length	Quality of chain
3	C	451	 88% 11%
3	c	451	 89% 11%
4	D	341	 87% 13%
4	d	341	 87% 13%
5	E	75	 91% 9%
5	e	75	 91% 9%
6	F	28	 89% 11%
6	f	28	 86% 14%
7	H	66	 91% 9%
7	h	66	 88% 12%
8	I	35	 91% 9%
8	i	35	 94% 6%
9	J	34	 94% 6%
9	j	34	 91% 9%
10	K	37	 81% 19%
10	k	37	 89% 11%
11	L	38	 97% 5%
11	l	38	 95% 5%
12	M	42	 95% 5%
12	m	42	 95% 5%
13	O	245	 82% 16%
13	o	245	 80% 18%
14	T	30	 97% 5%
14	t	30	 87% 13%
15	U	93	 81% 19%

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Mol	Chain	Length	Quality of chain
15	u	93	82%18%
16	V	136	87%12%..
16	v	136	87%12%..
17	Y	34	88%12%
17	y	34	91%9%
18	X	37	5%92%8%
18	x	37	5%86%14%
19	Z	59	92%8%
19	z	59	97%.
20	Q	151	89%11%
20	q	151	87%13%
21	W	52	96%.
21	w	52	94%6%
22	0	31	97%.
22	5	31	97%.
23	1	30	100%
23	6	30	100%
24	11	176	86%13%.
24	31	176	84%16%
25	12	169	82%17%.
25	32	169	82%18%
26	13	169	6%83%17%.
26	33	169	5%81%18%.
27	14	172	80%19%.
27	34	172	77%22%.

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Mol	Chain	Length	Quality of chain
28	15	170	75% 77% 20% ..
28	35	170	75% 79% 19% ..
29	16	179	12% 79% 20% .
29	36	179	12% 80% 18% .
30	17	176	21% 81% 18% ..
30	37	176	21% 86% 14% .
31	18	168	78% 76% 21% .
31	38	168	80% 75% 21% .
32	19	227	8% 81% 19%
32	39	227	8% 81% 17% .
33	20	155	41% 77% 19% ..
33	40	155	47% 76% 21% ..
34	21	162	94% 73% 20% . .
34	41	162	94% 73% 21% . .

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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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		

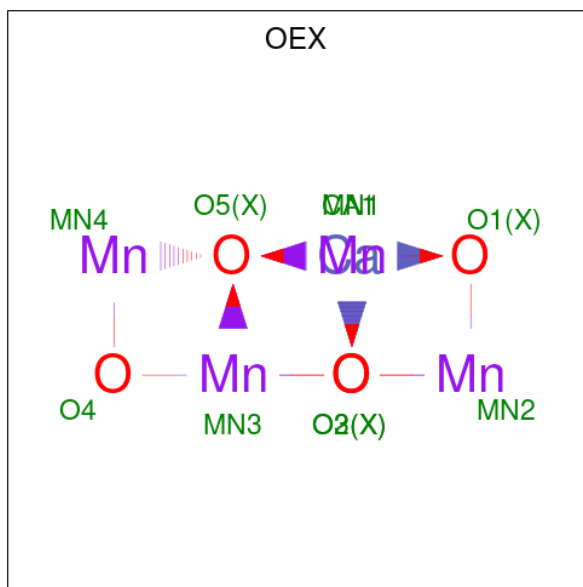
- Molecule 33 is a protein called Fcpb6, Fucoxanthin chlorophyll a/c-binding protein.

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 (CCD ID: OEX) (formula: CaMn_4O_5).

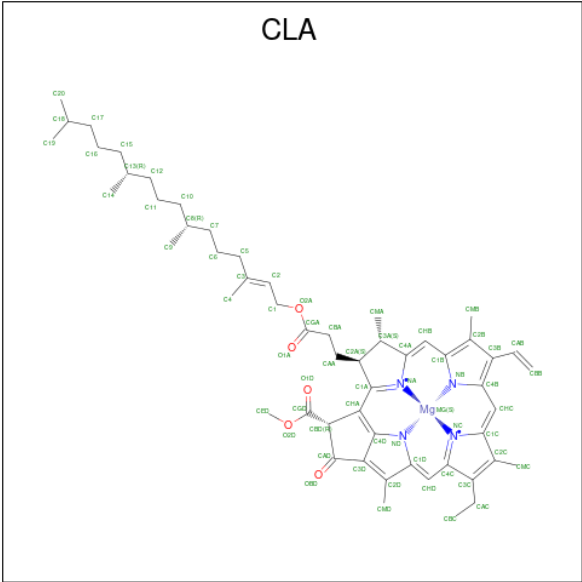


Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
35	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 36 is FE (II) ION (CCD ID: 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 (CCD ID: 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	
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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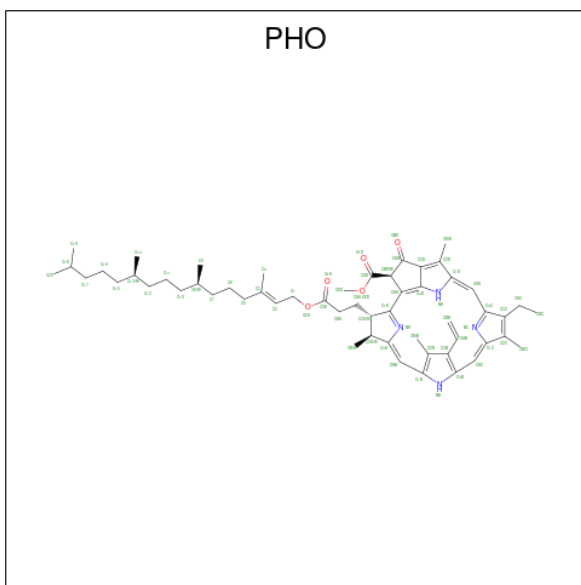
Mol	Chain	Residues	Atoms					AltConf
37	36	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	36	1	Total 57	C 47	Mg 1	N 4	O 5	0
37	36	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	36	1	Total 61	C 51	Mg 1	N 4	O 5	0
37	36	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	37	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	37	1	Total 56	C 46	Mg 1	N 4	O 5	0
37	37	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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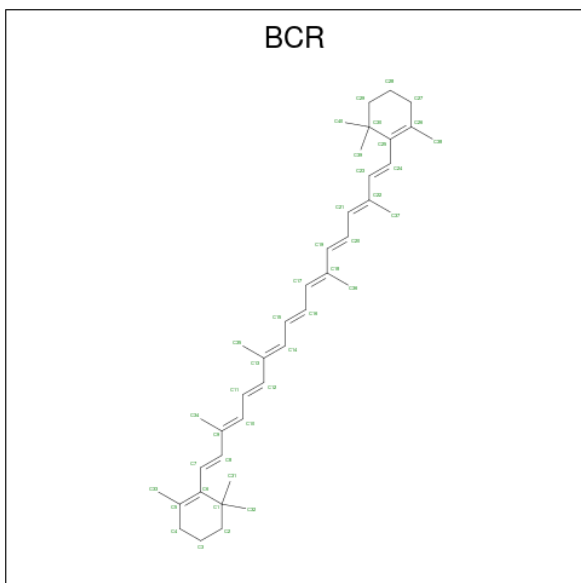
Mol	Chain	Residues	Atoms					AltConf
37	39	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
37	39	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
37	40	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
37	40	1	Total	C	Mg	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 (CCD ID: 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 (CCD ID: BCR) (formula: $C_{40}H_{56}$).



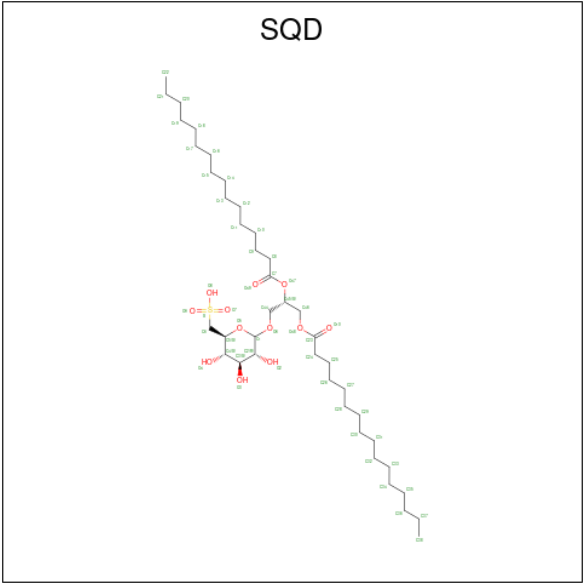
Mol	Chain	Residues	Atoms	AltConf
39	A	1	Total C 40 40	0
39	A	1	Total C 40 40	0
39	B	1	Total C 40 40	0
39	B	1	Total C 40 40	0
39	B	1	Total C 40 40	0
39	C	1	Total C 40 40	0
39	C	1	Total C 40 40	0
39	C	1	Total C 40 40	0
39	D	1	Total C 40 40	0
39	H	1	Total C 40 40	0
39	K	1	Total C 40 40	0
39	0	1	Total C 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 (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



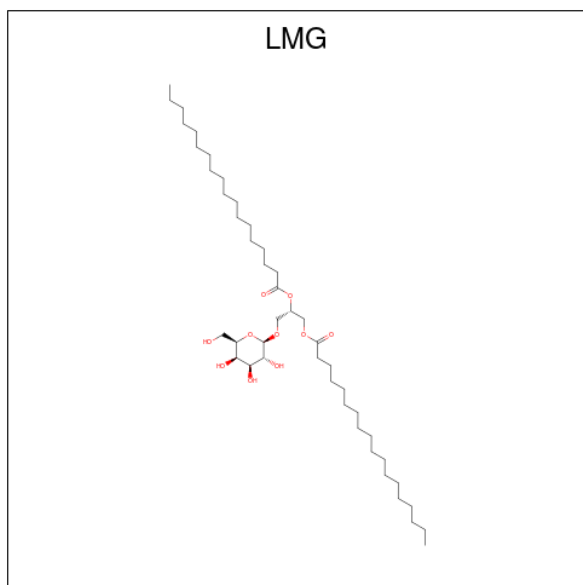
Mol	Chain	Residues	Atoms				AltConf
40	A	1	Total	C	O	S	0
			54	41	12	1	
40	B	1	Total	C	O	S	0
			54	41	12	1	
40	B	1	Total	C	O	S	0
			37	24	12	1	
40	L	1	Total	C	O	S	0
			54	41	12	1	
40	a	1	Total	C	O	S	0
			54	41	12	1	
40	b	1	Total	C	O	S	0
			37	24	12	1	
40	16	1	Total	C	O	S	0
			54	41	12	1	
40	17	1	Total	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 (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



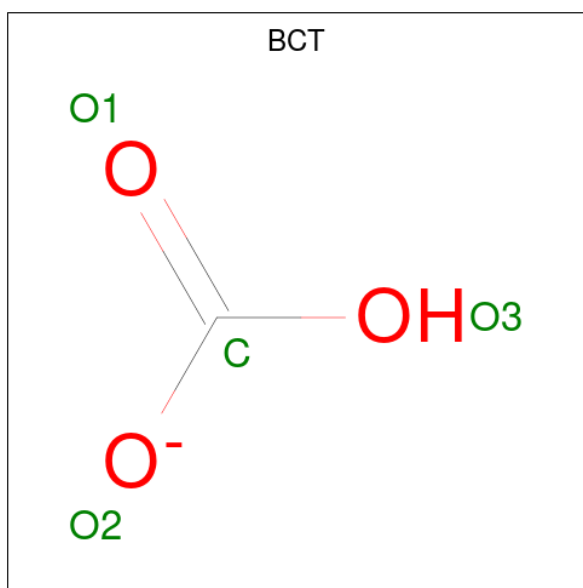
Mol	Chain	Residues	Atoms				AltConf
41	A	1	Total	C	O		0
			51	41	10		
41	B	1	Total	C	O		0
			51	41	10		
41	B	1	Total	C	O		0
			51	41	10		
41	C	1	Total	C	O		0
			51	41	10		
41	D	1	Total	C	O		0
			51	41	10		
41	L	1	Total	C	O		0
			40	30	10		
41	a	1	Total	C	O		0
			51	41	10		
41	b	1	Total	C	O		0
			51	41	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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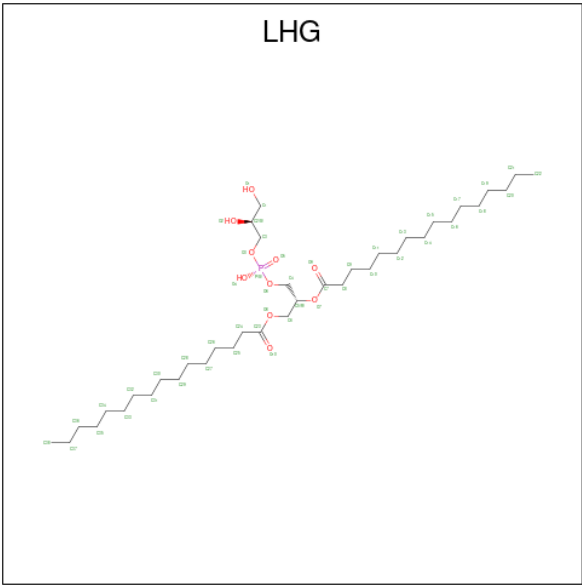
Mol	Chain	Residues	Atoms			AltConf
41	d	1	Total	C	O	0
			51	41	10	
41	l	1	Total	C	O	0
			40	30	10	
41	11	1	Total	C	O	0
			42	32	10	
41	11	1	Total	C	O	0
			32	22	10	
41	12	1	Total	C	O	0
			39	29	10	
41	16	1	Total	C	O	0
			36	26	10	
41	17	1	Total	C	O	0
			37	27	10	
41	31	1	Total	C	O	0
			42	32	10	
41	31	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 (CCD ID: 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 (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



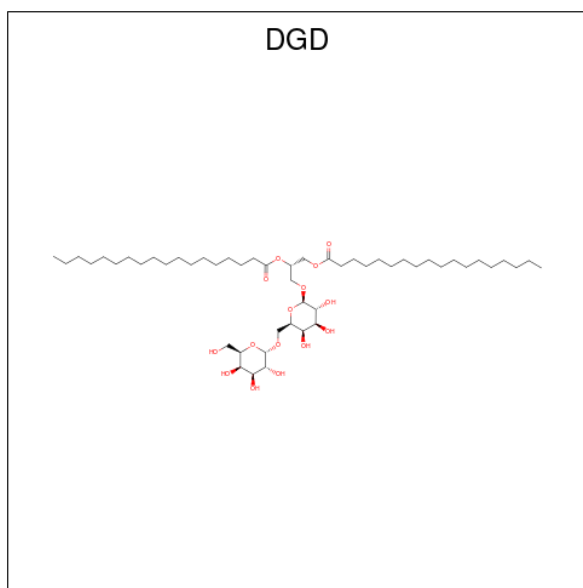
Mol	Chain	Residues	Atoms				AltConf
43	B	1	Total	C	O	P	0
			49	38	10	1	
43	D	1	Total	C	O	P	0
			49	38	10	1	
43	D	1	Total	C	O	P	0
			49	38	10	1	
43	D	1	Total	C	O	P	0
			46	35	10	1	
43	a	1	Total	C	O	P	0
			46	35	10	1	
43	b	1	Total	C	O	P	0
			49	38	10	1	
43	d	1	Total	C	O	P	0
			49	38	10	1	
43	d	1	Total	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) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



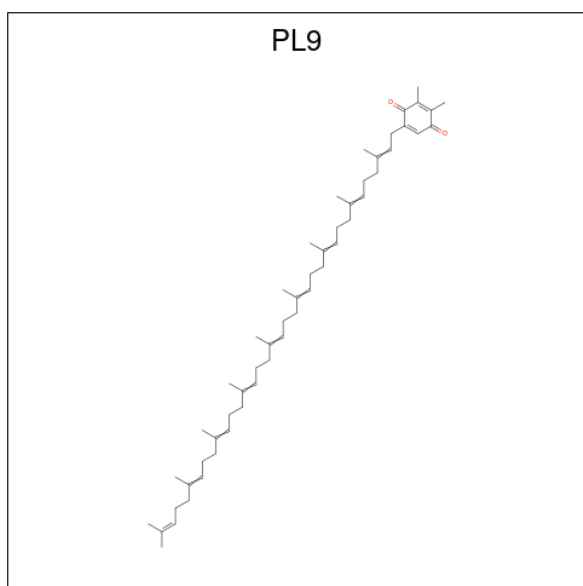
Mol	Chain	Residues	Atoms			AltConf
44	C	1	Total	C	O	0
			62	47	15	
44	C	1	Total	C	O	0
			62	47	15	
44	H	1	Total	C	O	0
			62	47	15	
44	J	1	Total	C	O	0
			62	47	15	

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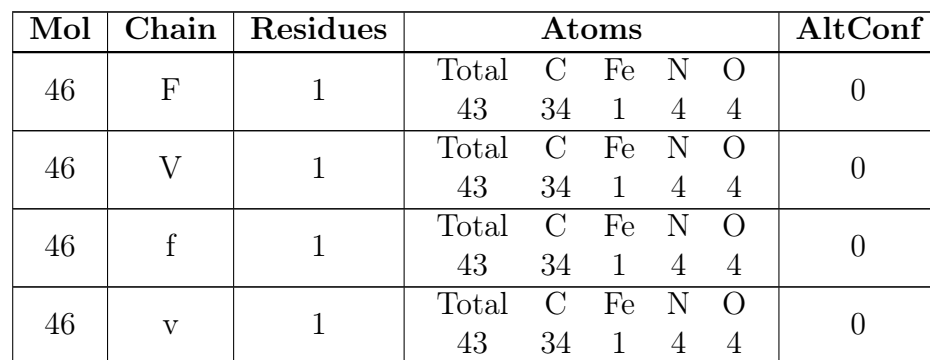
Mol	Chain	Residues	Atoms			AltConf
44	c	1	Total	C	O	0
			62	47	15	
44	c	1	Total	C	O	0
			62	47	15	
44	h	1	Total	C	O	0
			62	47	15	
44	j	1	Total	C	O	0
			62	47	15	

- 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 (CCD ID: 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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



- # KC1

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

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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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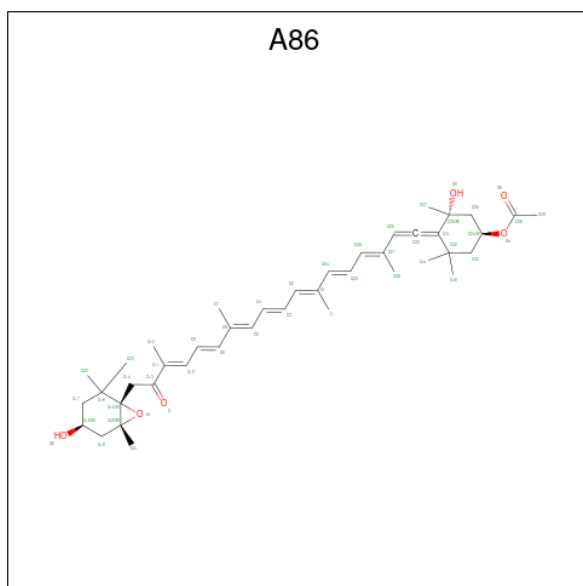
Mol	Chain	Residues	Atoms					AltConf
47	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	33	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	34	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	35	1	Total 45	C 35	Mg 1	N 4	O 5	0
47	35	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 (CCD ID: 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	
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	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	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	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	14	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	

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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	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	
48	19	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	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	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	
48	32	1	Total	C	O	0
			48	42	6	
48	33	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	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	
48	37	1	Total	C	O	0
			48	42	6	

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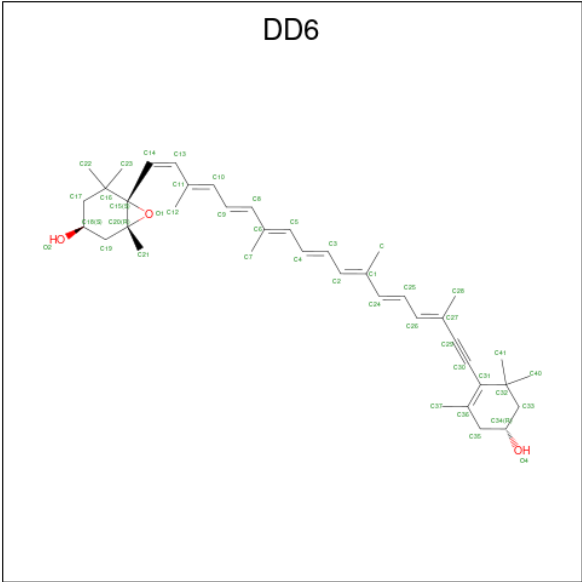
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Mol	Chain	Residues	Atoms			AltConf
48	37	1	Total	C	O	0
			48	42	6	
48	37	1	Total	C	O	0
			48	42	6	
48	37	1	Total	C	O	0
			48	42	6	
48	37	1	Total	C	O	0
			48	42	6	
48	37	1	Total	C	O	0
			48	42	6	
48	37	1	Total	C	O	0
			48	42	6	
48	38	1	Total	C	O	0
			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 (CCD ID: UNL) (formula:).

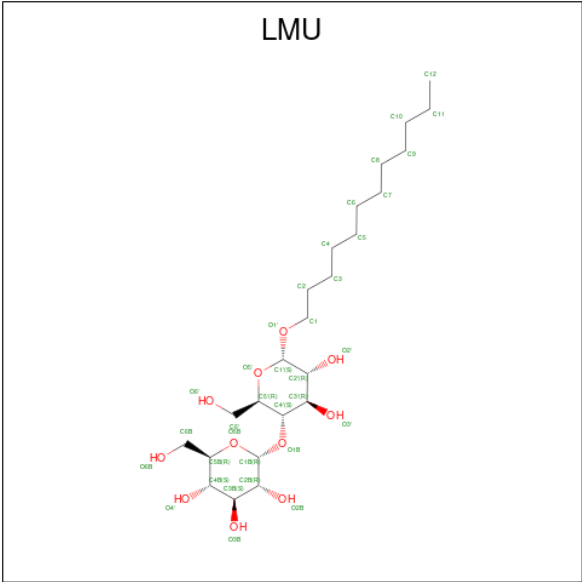
Mol	Chain	Residues	Atoms			AltConf
49	11	1	Total	C	O	0
			19	17	2	
49	12	2	Total	C	O	0
			34	32	2	
49	13	3	Total	C	O	0
			49	47	2	
49	14	1	Total	C		0
			16	16		
49	15	2	Total	C		0
			28	28		
49	16	2	Total	C		0
			24	24		
49	17	3	Total	C	O	0
			54	48	6	
49	18	4	Total	C		0
			58	58		
49	19	1	Total	C		0
			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 (CCD ID: 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 (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 52 is water.

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

Continued on next page...

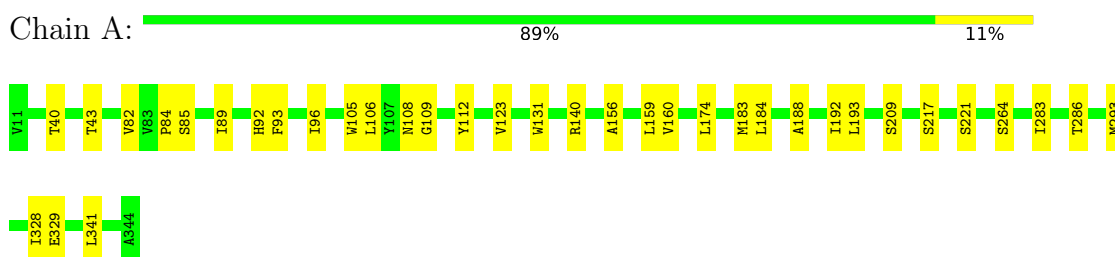
Continued from previous page...

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

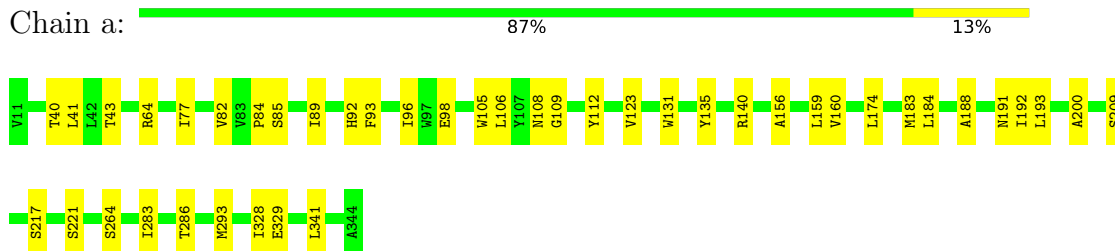
3 Residue-property plots [i](#)

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.

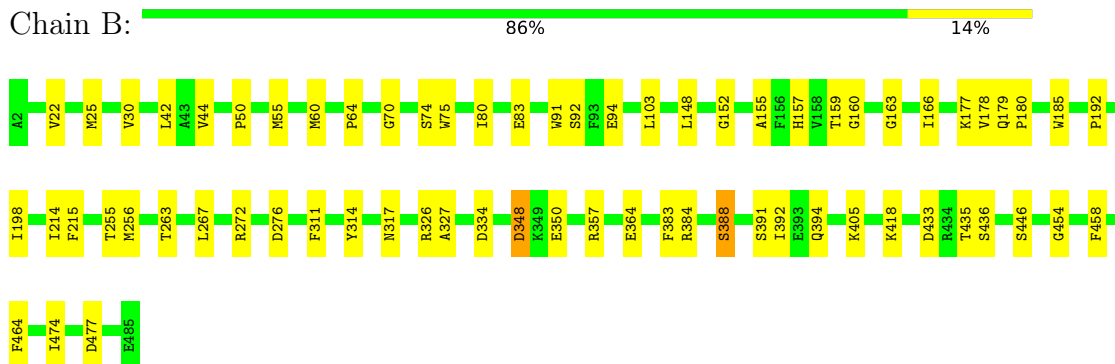
- Molecule 1: Photosystem II protein D1



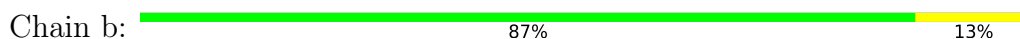
- Molecule 1: Photosystem II protein D1

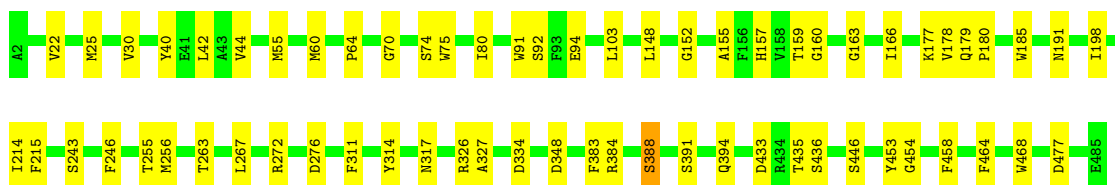


- Molecule 2: Photosystem II CP47 reaction center protein



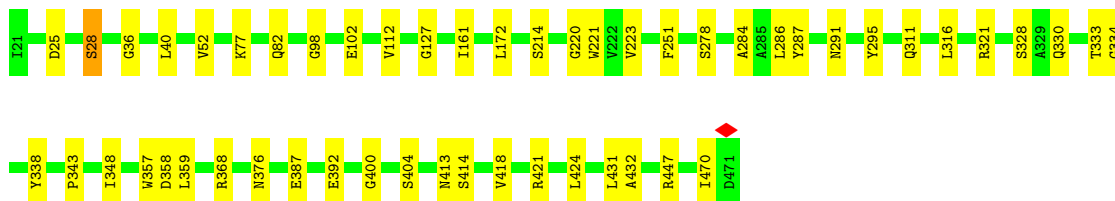
- Molecule 2: Photosystem II CP47 reaction center protein





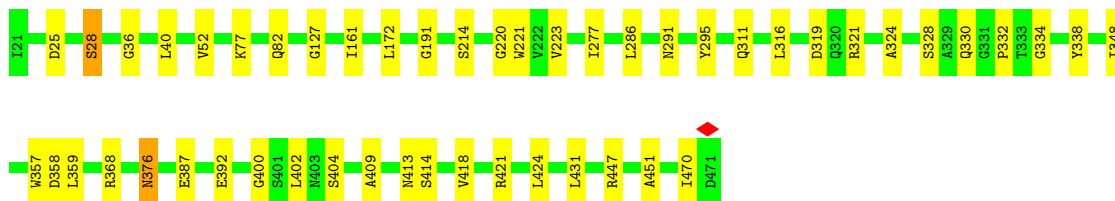
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 88% 11%



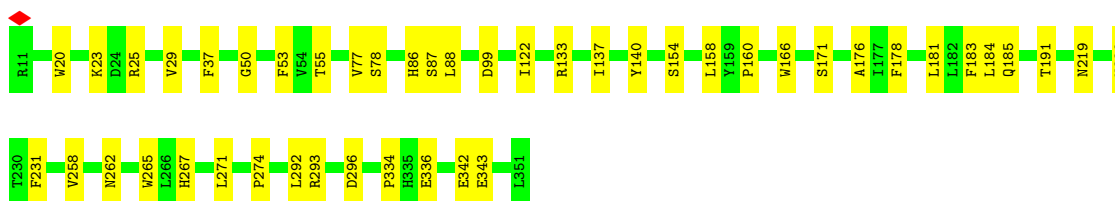
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 11%



• Molecule 4: Photosystem II D2 protein

Chain D: 87% 13%



• Molecule 4: Photosystem II D2 protein

Chain d: 87% 13%



• Molecule 5: Cytochrome b559 subunit alpha

Chain E:  91% 9%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e:  91% 9%



- Molecule 6: Cytochrome b559 subunit beta

Chain F:  89% 11%



- Molecule 6: Cytochrome b559 subunit beta

Chain f:  86% 14%



- Molecule 7: Photosystem II reaction center protein H

Chain H:  91% 9%



- Molecule 7: Photosystem II reaction center protein H

Chain h:  88% 12%

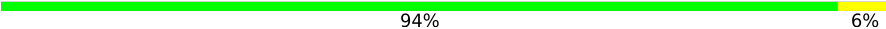


- Molecule 8: Photosystem II reaction center protein I

Chain I:  91% 9%



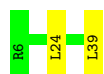
- Molecule 8: Photosystem II reaction center protein I

Chain i:  94% 6%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  94% 6%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  91% 9%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  81% 19%

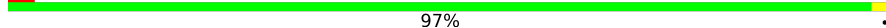


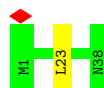
- Molecule 10: Photosystem II reaction center protein K

Chain k:  89% 11%

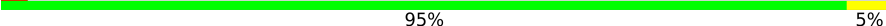


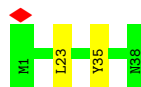
- Molecule 11: Photosystem II reaction center protein L

Chain L:  97% .



- Molecule 11: Photosystem II reaction center protein L

Chain l:  95% 5%



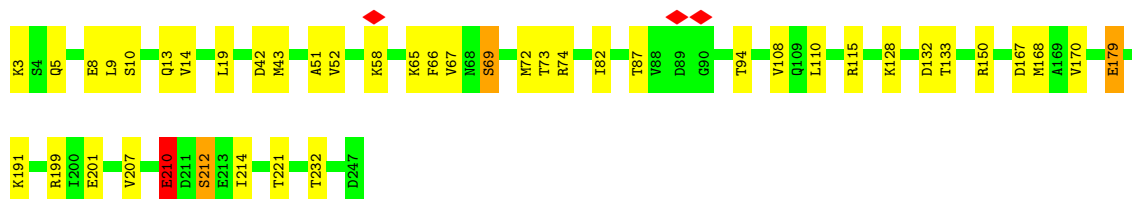
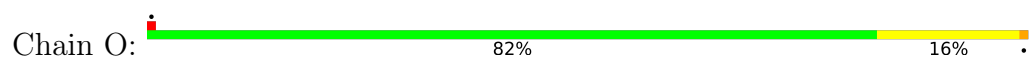
- Molecule 12: Photosystem II subunit



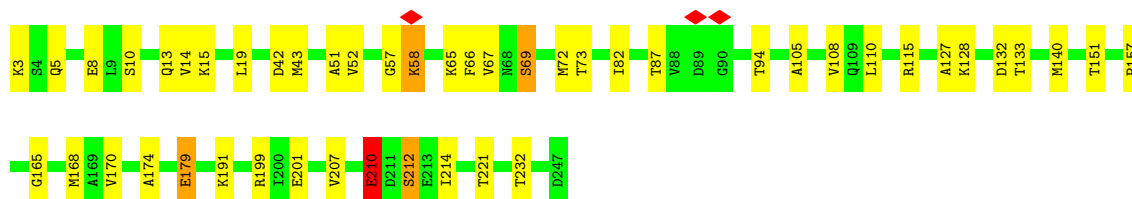
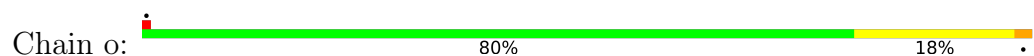
- Molecule 12: Photosystem II subunit



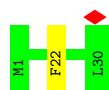
- Molecule 13: Extrinsic protein in photosystem II



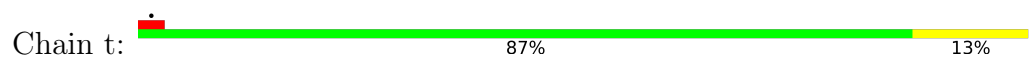
- Molecule 13: Extrinsic protein in photosystem II



- Molecule 14: Photosystem II reaction center protein T

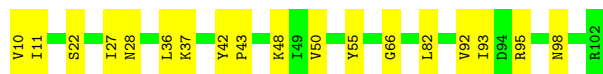


- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Extrinsic protein in photosystem II

Chain U:  81% 19%



- Molecule 15: Extrinsic protein in photosystem II

Chain u:  82% 18%



- Molecule 16: Cytochrome c-550

Chain V:  87% 12% ..



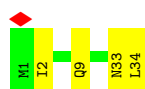
- Molecule 16: Cytochrome c-550

Chain v:  87% 12% ..



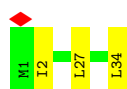
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  88% 12%



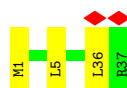
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  91% 9%

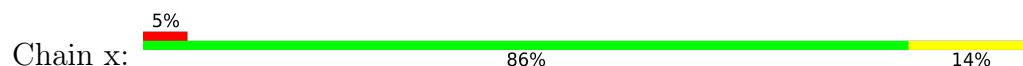


- Molecule 18: Photosystem II reaction center X protein

Chain X:  5% 92% 8%



- Molecule 18: Photosystem II reaction center X protein



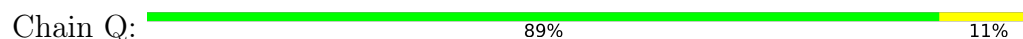
- Molecule 19: Photosystem II reaction center protein Z



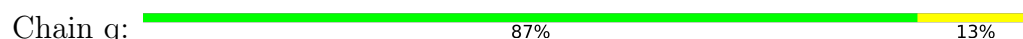
- Molecule 19: Photosystem II reaction center protein Z



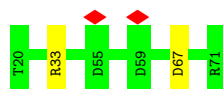
- Molecule 20: Extrinsic protein in photosystem II



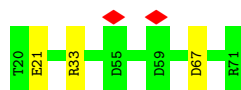
- Molecule 20: Extrinsic protein in photosystem II



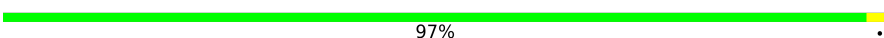
- Molecule 21: Photosystem II reaction center protein W

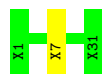


- Molecule 21: Photosystem II reaction center protein W

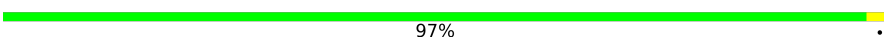


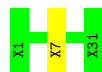
- Molecule 22: Unknown protein 0

Chain 0:  97%

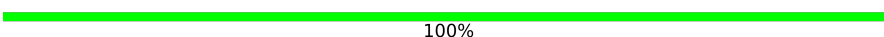


- Molecule 22: Unknown protein 0

Chain 5:  97%

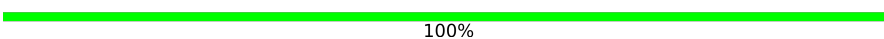


- Molecule 23: Unknown protein 1

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:  86% 13%



- Molecule 24: Chlorophyll a/b-binding protein

Chain 31:  84% 16%



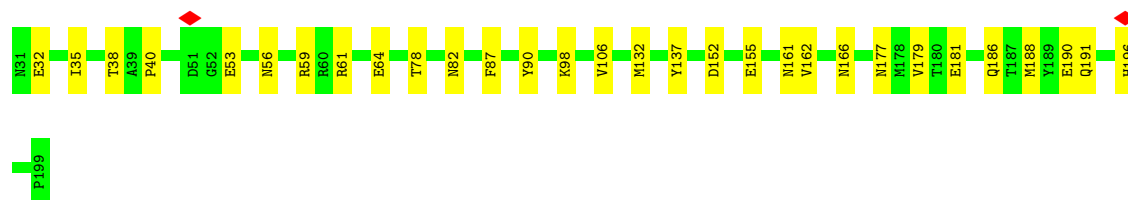
- Molecule 25: Fcpb2, Fucoxanthin chlorophyll a/c-binding protein

Chain 12:  82% 17%



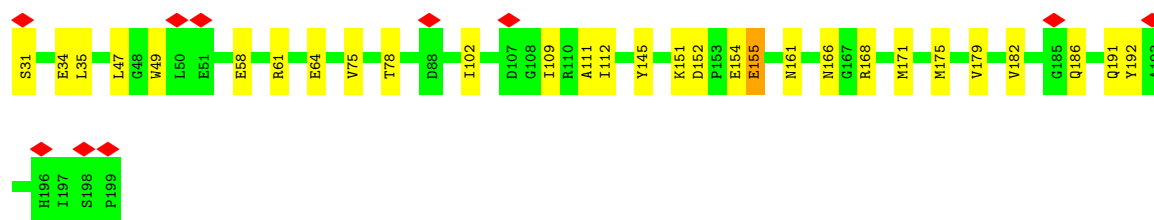
- Molecule 25: Fcpb2, Fucoxanthin chlorophyll a/c-binding protein

Chain 32:  82% 18%



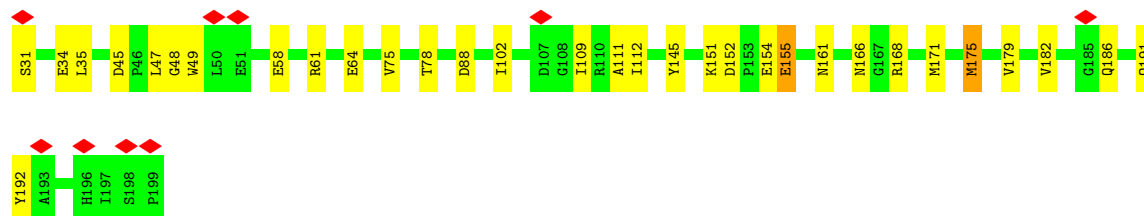
- Molecule 26: Chlorophyll a/b-binding protein

Chain 13:  6% 83% 17%



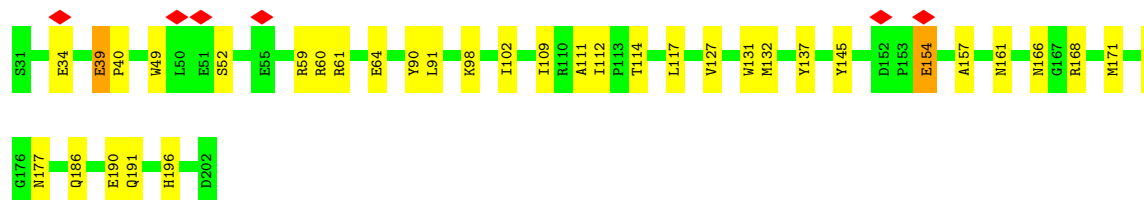
- Molecule 26: Chlorophyll a/b-binding protein

Chain 33:  5% 81% 18%



- Molecule 27: Chlorophyll a/b-binding protein

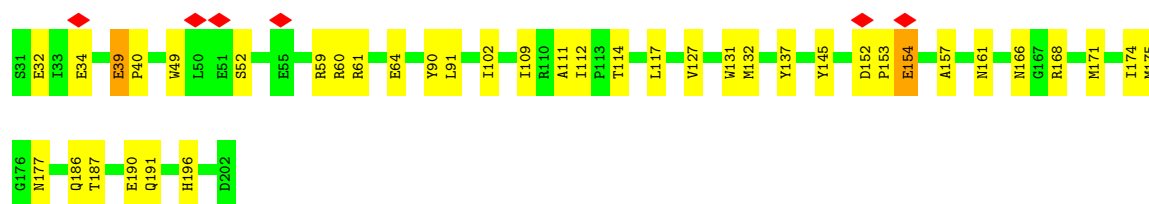
Chain 14:  80% 19%



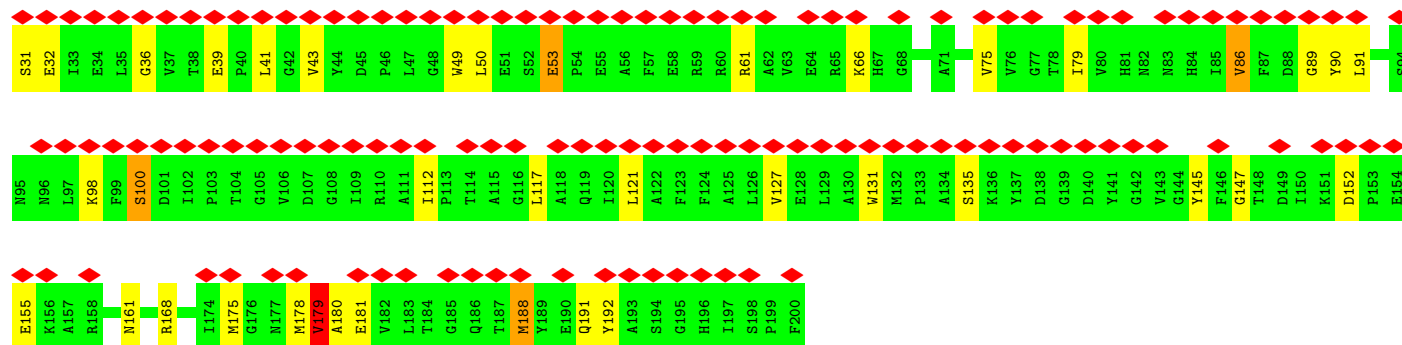
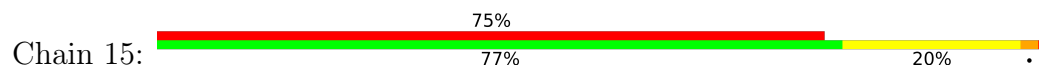
- Molecule 27: Chlorophyll a/b-binding protein

Chain 34:  77% 22%

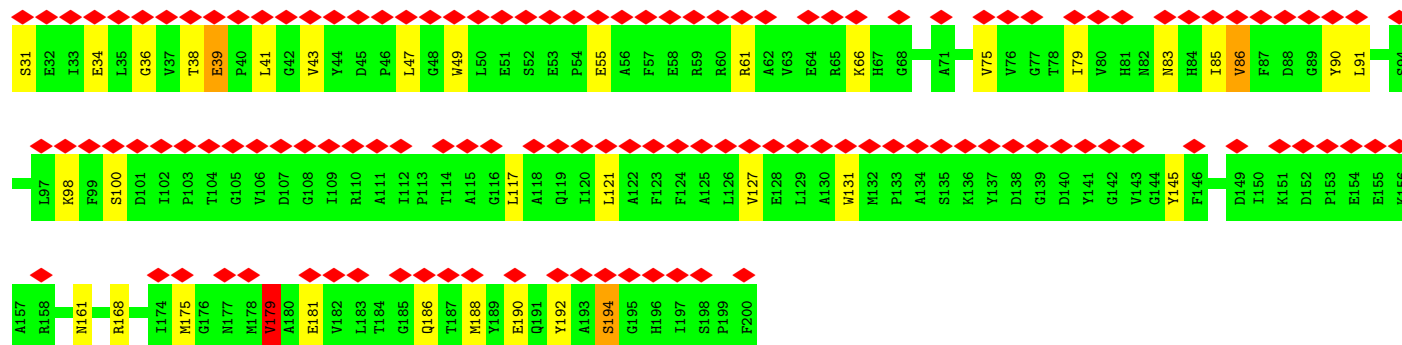
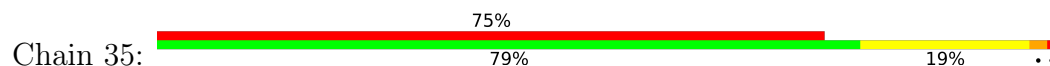




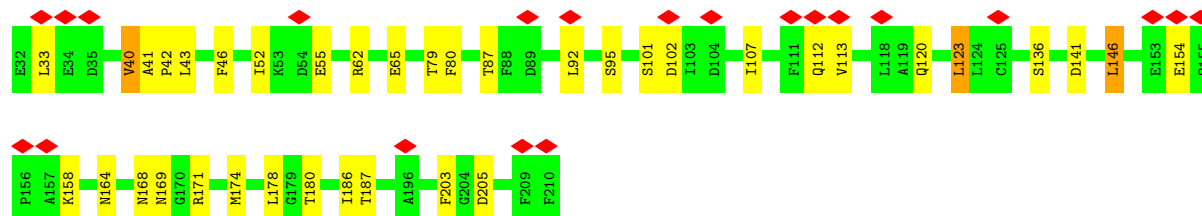
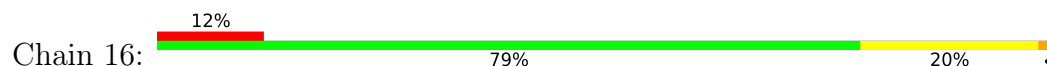
• Molecule 28: Chlorophyll a/b-binding protein



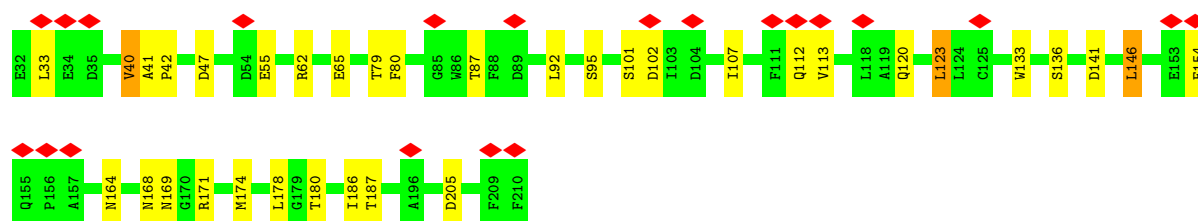
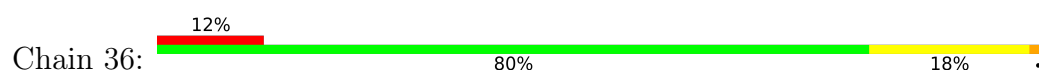
• Molecule 28: Chlorophyll a/b-binding protein



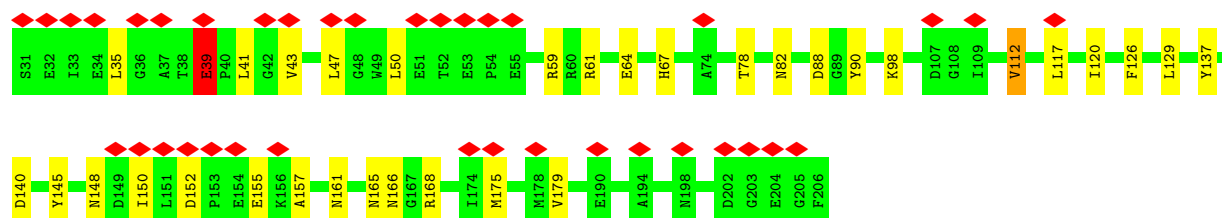
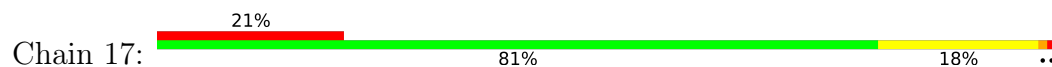
• Molecule 29: Fcpb3, Fucoxanthin chlorophyll a/c-binding protein



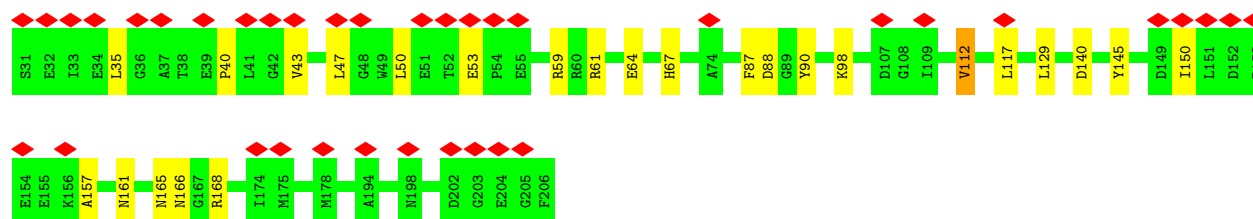
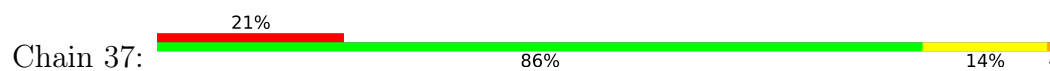
• Molecule 29: Fcpb3, Fucoxanthin chlorophyll a/c-binding protein



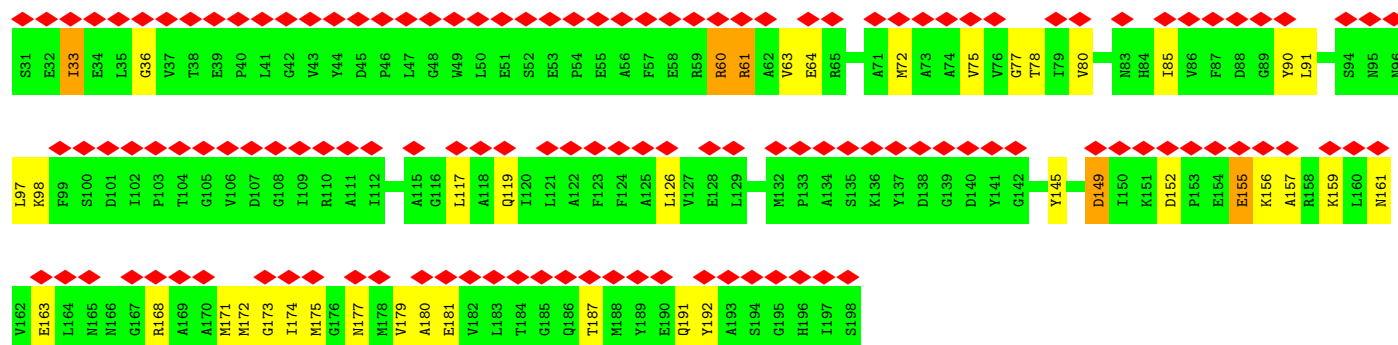
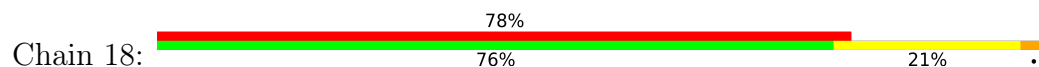
- Molecule 30: Fcpb4, Fucoxanthin chlorophyll a/c-binding protein



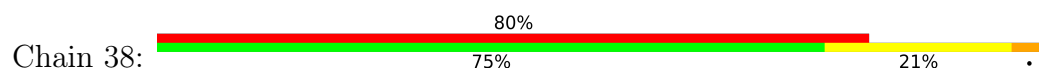
- Molecule 30: Fcpb4, Fucoxanthin chlorophyll a/c-binding protein

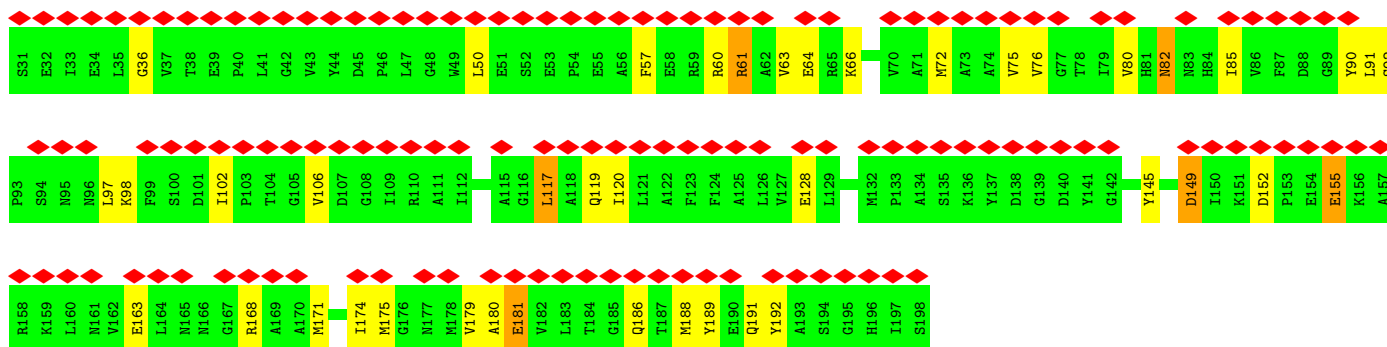


- Molecule 31: Chlorophyll a/b-binding protein

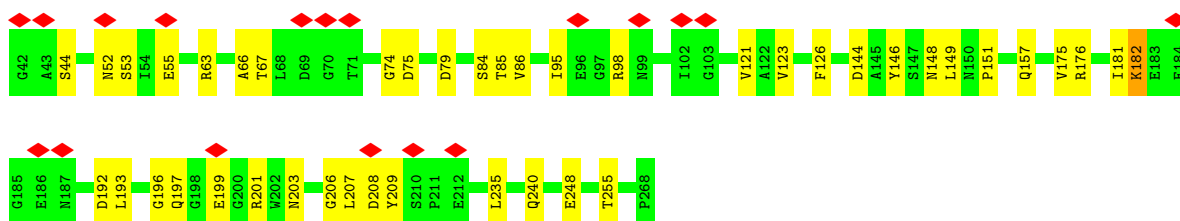
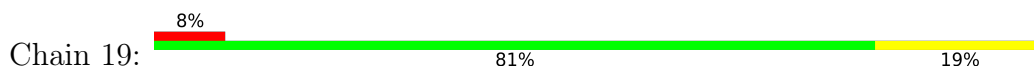


- Molecule 31: Chlorophyll a/b-binding protein

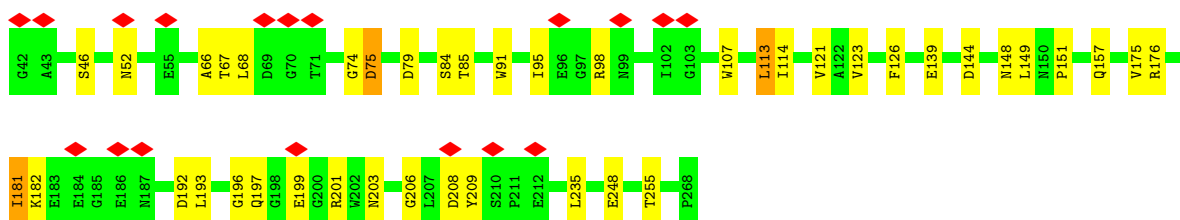
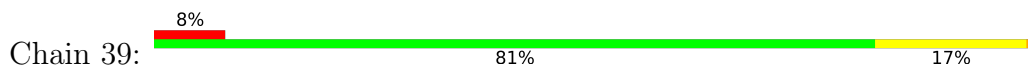




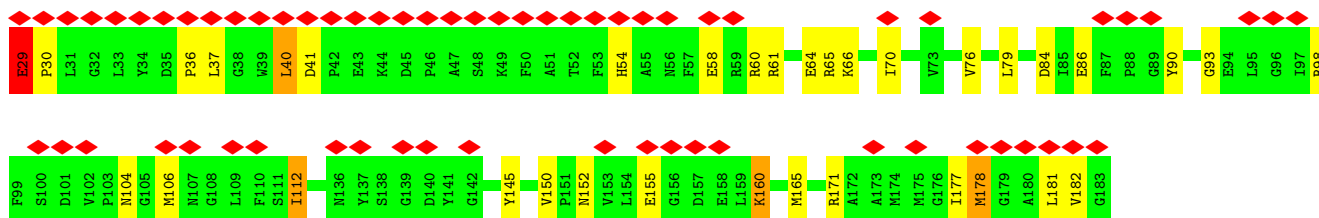
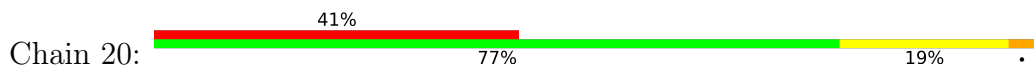
- Molecule 32: Fcpb5, Fucoxanthin chlorophyll a/c-binding protein



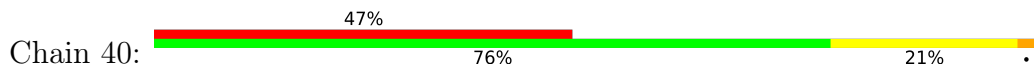
- Molecule 32: Fcpb5, Fucoxanthin chlorophyll a/c-binding protein

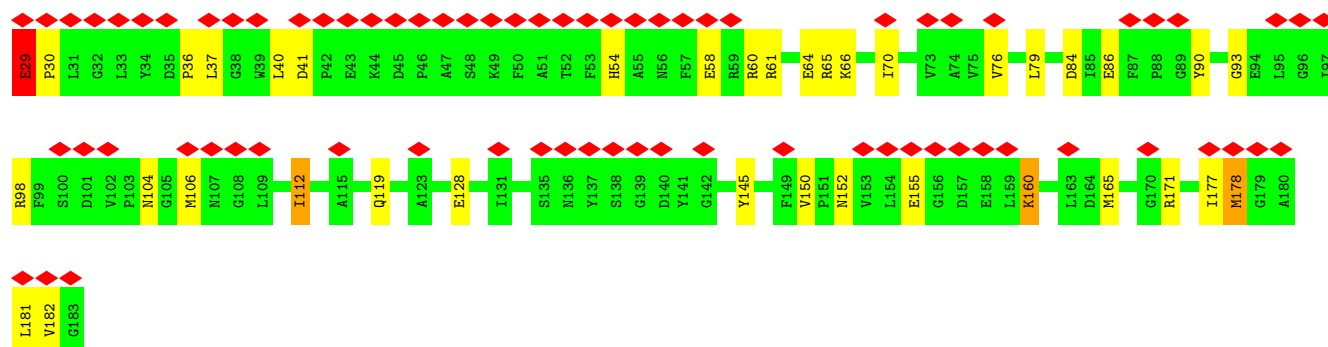


- Molecule 33: Fcpb6, Fucoxanthin chlorophyll a/c-binding protein

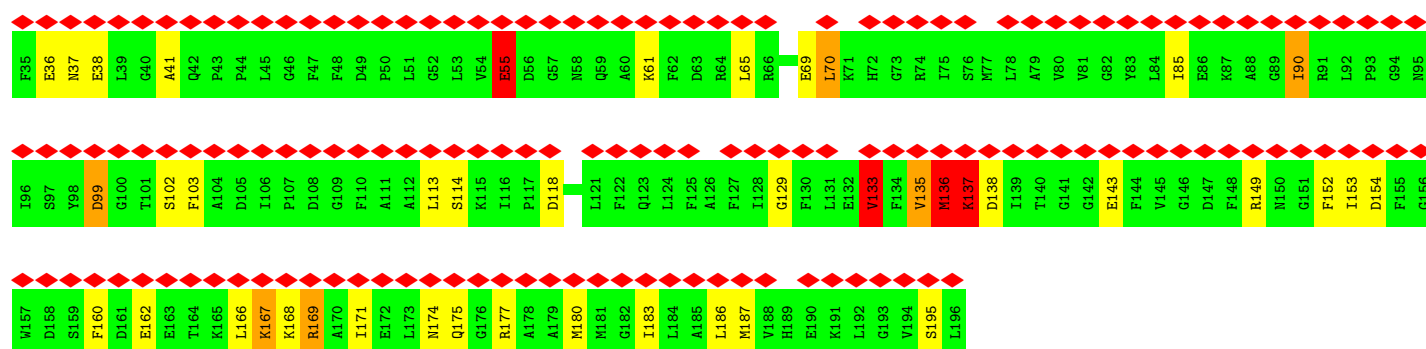
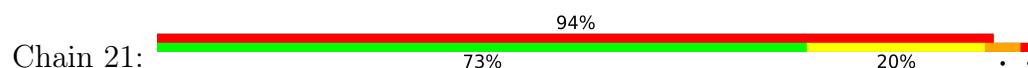


- Molecule 33: Fcpb6, Fucoxanthin chlorophyll a/c-binding protein

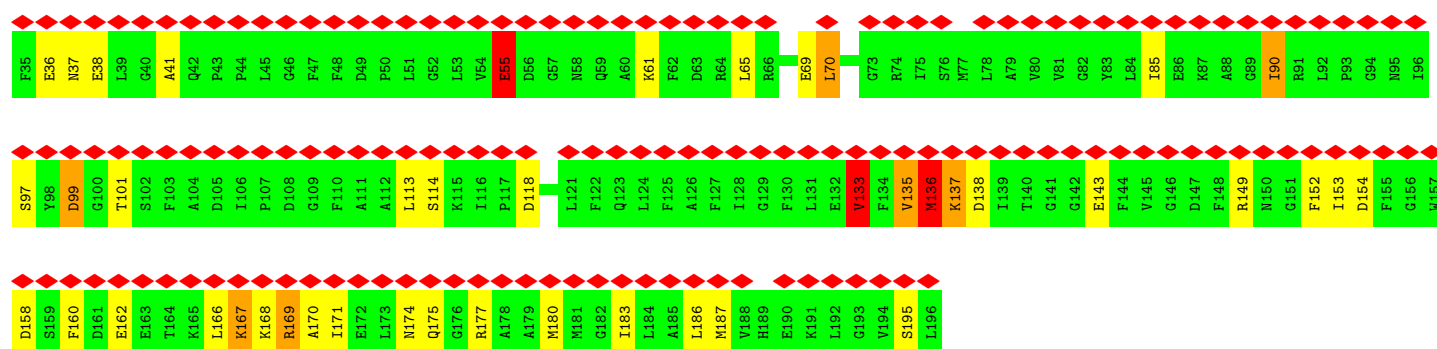




• Molecule 34: Fcpb7, Fucoxanthin chlorophyll a/c-binding protein



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



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: UNL, KC1, BCT, PL9, A86, LMU, OEX, DGD, SQD, DD6, HEM, BCR, FE2, PHO, CLA, LMG, LHG

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	0.39	0/2702	0.49	0/3682
1	a	0.39	0/2702	0.49	0/3682
2	B	0.39	0/3942	0.47	0/5362
2	b	0.39	0/3942	0.47	0/5362
3	C	0.40	0/3620	0.50	0/4933
3	c	0.40	0/3620	0.50	0/4933
4	D	0.40	0/2789	0.48	0/3803
4	d	0.40	0/2789	0.48	0/3803
5	E	0.30	0/634	0.46	0/864
5	e	0.30	0/634	0.46	0/864
6	F	0.36	0/235	0.53	0/316
6	f	0.36	0/235	0.53	0/316
7	H	0.36	0/523	0.54	0/714
7	h	0.36	0/523	0.54	0/714
8	I	0.38	0/294	0.64	0/397
8	i	0.38	0/294	0.64	0/397
9	J	0.26	0/260	0.40	0/351
9	j	0.26	0/260	0.40	0/351
10	K	0.38	0/313	0.62	0/429
10	k	0.38	0/313	0.62	0/429
11	L	0.39	0/319	0.45	0/433
11	l	0.39	0/319	0.45	0/433
12	M	0.36	0/321	0.56	0/433
12	m	0.36	0/321	0.55	0/433
13	O	0.32	0/1875	0.56	2/2528 (0.1%)
13	o	0.32	0/1875	0.56	2/2528 (0.1%)
14	T	0.31	0/256	0.41	0/346
14	t	0.31	0/256	0.41	0/346
15	U	0.29	0/728	0.51	0/989
15	u	0.29	0/728	0.51	0/989
16	V	0.33	0/1056	0.56	2/1435 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.33	0/1056	0.56	2/1435 (0.1%)
17	Y	0.26	0/252	0.61	1/341 (0.3%)
17	y	0.26	0/252	0.61	1/341 (0.3%)
18	X	0.24	0/263	0.40	0/355
18	x	0.24	0/263	0.41	0/355
19	Z	0.41	1/456 (0.2%)	0.54	0/624
19	z	0.41	1/456 (0.2%)	0.54	0/624
20	Q	0.28	0/1203	0.55	0/1623
20	q	0.28	0/1203	0.55	0/1623
21	W	0.35	0/434	0.53	0/590
21	w	0.35	0/434	0.53	0/590
24	11	0.42	0/1373	0.59	1/1861 (0.1%)
24	31	0.41	0/1373	0.53	0/1861
25	12	0.39	0/1334	0.55	0/1810
25	32	0.37	0/1334	0.53	0/1810
26	13	0.41	0/1325	0.68	2/1797 (0.1%)
26	33	0.44	0/1325	0.71	2/1797 (0.1%)
27	14	0.41	1/1349 (0.1%)	0.80	3/1829 (0.2%)
27	34	0.42	1/1349 (0.1%)	0.84	6/1829 (0.3%)
28	15	0.35	0/1337	0.92	4/1813 (0.2%)
28	35	0.39	0/1337	0.90	1/1813 (0.1%)
29	16	0.30	0/1425	0.70	3/1930 (0.2%)
29	36	0.30	0/1425	0.70	3/1930 (0.2%)
30	17	0.36	0/1386	0.77	2/1879 (0.1%)
30	37	0.39	0/1386	0.75	2/1879 (0.1%)
31	18	0.49	0/1317	1.09	10/1785 (0.6%)
31	38	0.54	2/1317 (0.2%)	1.10	7/1785 (0.4%)
32	19	0.36	0/1796	0.70	6/2445 (0.2%)
32	39	0.38	0/1796	0.74	6/2445 (0.2%)
33	20	0.39	0/1224	0.89	4/1656 (0.2%)
33	40	0.39	0/1224	0.89	4/1656 (0.2%)
34	21	0.48	0/1290	1.28	20/1735 (1.2%)
34	41	0.48	0/1290	1.28	20/1735 (1.2%)
All	All	0.38	6/75262 (0.0%)	0.66	116/102176 (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 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	20	VAL	CA-CB	-5.48	1.51	1.54
19	z	20	VAL	CA-CB	-5.45	1.51	1.54
31	38	82	ASN	CG-OD1	-5.41	1.13	1.23
31	38	60	ARG	CZ-NH1	-5.29	1.25	1.32
27	34	154	GLU	CB-CG	-5.24	1.36	1.52

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	21	70	LEU	CA-CB-CG	13.98	165.22	116.30
34	41	70	LEU	CA-CB-CG	13.96	165.18	116.30
34	21	136	MET	CB-CG-SD	13.02	151.75	112.70
34	41	136	MET	CB-CG-SD	13.02	151.75	112.70
27	34	154	GLU	CA-CB-CG	11.95	137.99	114.10

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2619	0	2520	28	0
1	a	2619	0	2520	35	0
2	B	3812	0	3690	50	0
2	b	3812	0	3690	48	0
3	C	3504	0	3410	35	0
3	c	3504	0	3410	36	0
4	D	2697	0	2596	35	0
4	d	2697	0	2596	34	0
5	E	616	0	602	6	0
5	e	616	0	602	6	0
6	F	228	0	234	4	0
6	f	228	0	234	5	0
7	H	513	0	541	7	0
7	h	513	0	541	8	0
8	I	287	0	306	5	0
8	i	287	0	306	2	0
9	J	254	0	266	2	0
9	j	254	0	266	3	0
10	K	302	0	316	5	0
10	k	302	0	316	2	0
11	L	310	0	313	1	0
11	l	310	0	313	2	0
12	M	316	0	319	2	0
12	m	316	0	319	2	0
13	O	1845	0	1841	26	0
13	o	1845	0	1841	30	0
14	T	250	0	268	1	0
14	t	250	0	268	3	0
15	U	713	0	715	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	u	713	0	715	11	0
16	V	1037	0	1031	15	0
16	v	1037	0	1031	15	0
17	Y	250	0	287	3	0
17	y	250	0	287	2	0
18	X	263	0	301	1	0
18	x	263	0	301	4	0
19	Z	447	0	490	4	0
19	z	447	0	490	1	0
20	Q	1180	0	1165	11	0
20	q	1180	0	1165	11	0
21	W	422	0	377	2	0
21	w	422	0	377	3	0
22	0	155	0	33	0	0
22	5	155	0	33	0	0
23	1	150	0	34	0	0
23	6	150	0	34	0	0
24	11	1343	0	1306	22	0
24	31	1343	0	1306	28	0
25	12	1302	0	1257	20	0
25	32	1302	0	1257	20	0
26	13	1296	0	1267	16	0
26	33	1296	0	1267	18	0
27	14	1319	0	1283	22	0
27	34	1319	0	1283	24	0
28	15	1307	0	1274	20	0
28	35	1307	0	1274	17	0
29	16	1386	0	1314	24	0
29	36	1386	0	1314	21	0
30	17	1353	0	1291	24	0
30	37	1353	0	1291	16	0
31	18	1289	0	1260	26	0
31	38	1289	0	1260	25	0
32	19	1746	0	1684	26	0
32	39	1746	0	1684	23	0
33	20	1193	0	1170	15	0
33	40	1193	0	1170	16	0
34	21	1262	0	1247	20	0
34	41	1262	0	1247	19	0
35	A	10	0	0	0	0
35	a	10	0	0	0	0
36	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	a	1	0	0	0	0
37	11	343	0	333	11	0
37	12	407	0	398	11	0
37	13	329	0	306	7	0
37	14	394	0	378	8	0
37	15	329	0	304	9	0
37	16	293	0	291	8	0
37	17	238	0	238	8	0
37	18	459	0	448	17	0
37	19	531	0	538	17	0
37	20	254	0	209	2	0
37	21	380	0	342	9	0
37	31	343	0	333	7	0
37	32	472	0	470	16	0
37	33	329	0	306	6	0
37	34	394	0	378	8	0
37	35	329	0	304	12	0
37	36	293	0	291	11	0
37	37	238	0	238	4	0
37	38	459	0	448	10	0
37	39	531	0	538	17	0
37	40	254	0	209	3	0
37	41	380	0	342	6	0
37	A	130	0	144	10	0
37	B	1102	0	1213	32	0
37	C	845	0	936	26	0
37	D	260	0	288	8	0
37	W	130	0	143	5	0
37	Z	110	0	103	5	0
37	a	195	0	216	14	0
37	b	1102	0	1213	38	0
37	c	845	0	936	30	0
37	d	195	0	216	5	0
37	w	65	0	71	1	0
37	z	110	0	104	3	0
38	A	64	0	74	2	0
38	D	64	0	74	1	0
38	a	128	0	148	3	0
39	0	40	0	56	5	0
39	5	40	0	56	3	0
39	A	80	0	112	6	0
39	B	120	0	167	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	C	120	0	168	5	0
39	D	40	0	56	4	0
39	H	40	0	56	2	0
39	K	40	0	56	4	0
39	a	80	0	112	5	0
39	b	120	0	167	8	0
39	c	120	0	168	4	0
39	d	40	0	56	3	0
39	h	40	0	56	1	0
39	y	40	0	56	4	0
40	16	54	0	77	1	0
40	17	49	0	65	3	0
40	36	49	0	65	3	0
40	40	54	0	77	2	0
40	A	54	0	77	1	0
40	B	91	0	114	5	0
40	L	54	0	77	3	0
40	a	54	0	77	0	0
40	b	37	0	37	1	0
41	11	74	0	88	0	0
41	12	39	0	48	0	0
41	16	36	0	42	1	0
41	17	37	0	44	0	0
41	31	74	0	88	0	0
41	32	39	0	48	0	0
41	36	36	0	42	0	0
41	37	37	0	44	0	0
41	A	51	0	72	4	0
41	B	102	0	144	7	0
41	C	51	0	72	1	0
41	D	51	0	72	2	0
41	L	40	0	50	2	0
41	a	51	0	72	4	0
41	b	102	0	144	8	0
41	c	51	0	72	3	0
41	d	51	0	72	2	0
41	l	40	0	50	1	0
42	A	4	0	0	1	0
42	a	4	0	0	1	0
43	17	44	0	61	1	0
43	19	49	0	74	10	0
43	21	80	0	102	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	37	89	0	124	4	0
43	39	49	0	74	8	0
43	41	35	0	39	0	0
43	B	49	0	74	0	0
43	D	144	0	213	6	0
43	a	46	0	65	3	0
43	b	49	0	74	0	0
43	d	98	0	148	3	0
44	C	124	0	164	4	0
44	H	62	0	82	2	0
44	J	62	0	81	1	0
44	c	124	0	164	4	0
44	h	62	0	82	3	0
44	j	62	0	81	2	0
45	D	110	0	157	5	0
45	d	110	0	157	5	0
46	F	43	0	30	2	0
46	V	43	0	30	2	0
46	f	43	0	30	2	0
46	v	43	0	30	2	0
47	11	180	0	0	4	0
47	12	135	0	0	0	0
47	13	180	0	0	0	0
47	14	135	0	0	0	0
47	15	180	0	0	0	0
47	16	180	0	0	1	0
47	17	180	0	0	2	0
47	18	135	0	0	1	0
47	19	45	0	0	0	0
47	20	135	0	0	2	0
47	21	90	0	0	0	0
47	31	180	0	0	1	0
47	32	135	0	0	0	0
47	33	180	0	0	1	0
47	34	135	0	0	0	0
47	35	180	0	0	0	0
47	36	180	0	0	1	0
47	37	180	0	0	2	0
47	38	135	0	0	2	0
47	39	45	0	0	0	0
47	40	135	0	0	2	0
47	41	90	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	11	288	0	0	11	0
48	12	336	0	0	0	0
48	13	240	0	0	1	0
48	14	288	0	0	3	0
48	15	336	0	0	1	0
48	16	192	0	0	0	0
48	17	336	0	0	0	0
48	18	192	0	0	1	0
48	19	96	0	0	0	0
48	20	96	0	0	0	0
48	21	192	0	0	0	0
48	31	288	0	0	14	0
48	32	336	0	0	0	0
48	33	240	0	0	1	0
48	34	288	0	0	3	0
48	35	336	0	0	1	0
48	36	144	0	0	0	0
48	37	336	0	0	0	0
48	38	192	0	0	1	0
48	39	96	0	0	1	0
48	40	144	0	0	0	0
48	41	192	0	0	0	0
49	11	19	0	0	0	0
49	12	34	0	0	0	0
49	13	49	0	0	0	0
49	14	16	0	0	0	0
49	15	28	0	0	0	0
49	16	24	0	0	0	0
49	17	54	0	0	0	0
49	18	58	0	0	0	0
49	19	12	0	0	0	0
49	31	19	0	0	0	0
49	32	34	0	0	0	0
49	33	49	0	0	0	0
49	34	16	0	0	0	0
49	35	28	0	0	0	0
49	36	24	0	0	0	0
49	37	54	0	0	0	0
49	38	58	0	0	0	0
49	39	12	0	0	0	0
50	16	43	0	0	0	0
50	19	43	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	20	86	0	0	1	0
50	21	86	0	0	0	0
50	36	43	0	0	0	0
50	39	43	0	0	2	0
50	40	86	0	0	1	0
50	41	86	0	0	0	0
51	19	35	0	46	0	0
51	39	35	0	46	0	0
52	11	3	0	0	0	0
52	12	2	0	0	0	0
52	13	1	0	0	0	0
52	14	1	0	0	0	0
52	15	1	0	0	0	0
52	16	1	0	0	0	0
52	17	2	0	0	0	0
52	18	1	0	0	0	0
52	19	1	0	0	0	0
52	31	3	0	0	0	0
52	32	2	0	0	0	0
52	33	1	0	0	0	0
52	34	1	0	0	0	0
52	35	1	0	0	0	0
52	36	1	0	0	0	0
52	37	2	0	0	0	0
52	38	1	0	0	0	0
52	39	1	0	0	0	0
52	B	5	0	0	0	0
52	C	3	0	0	0	0
52	D	4	0	0	0	0
52	Z	1	0	0	0	0
52	a	2	0	0	0	0
52	b	5	0	0	0	0
52	c	3	0	0	0	0
52	d	2	0	0	0	0
52	z	1	0	0	0	0
All	All	100884	0	91037	1161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1161 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:31:202:ASP:HB3	48:31:313:A86:C29	1.68	1.22
37:39:310:CLA:HBB2	43:39:314:LHG:H212	1.54	0.87
37:19:310:CLA:HBB2	43:19:314:LHG:H212	1.54	0.87
24:31:202:ASP:CB	48:31:313:A86:C29	2.57	0.81
24:11:204:GLN:HG3	48:11:313:A86:C25	2.12	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (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
8	i	33/35 (94%)	31 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
26	13	167/169 (99%)	160 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	33	167/169 (99%)	160 (96%)	7 (4%)	0	100	100
27	14	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	10	20
27	34	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	10	20
28	15	168/170 (99%)	147 (88%)	20 (12%)	1 (1%)	21	38
28	35	168/170 (99%)	147 (88%)	20 (12%)	1 (1%)	21	38
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%)	49	68

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%)	84	93
1	a	272/272 (100%)	271 (100%)	1 (0%)	84	93
2	B	385/385 (100%)	379 (98%)	6 (2%)	55	79
2	b	385/385 (100%)	379 (98%)	6 (2%)	55	79
3	C	356/356 (100%)	351 (99%)	5 (1%)	59	81
3	c	356/356 (100%)	351 (99%)	5 (1%)	59	81
4	D	273/273 (100%)	272 (100%)	1 (0%)	84	93
4	d	273/273 (100%)	272 (100%)	1 (0%)	84	93
5	E	69/69 (100%)	68 (99%)	1 (1%)	59	81
5	e	69/69 (100%)	68 (99%)	1 (1%)	59	81
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%)	16	34
10	k	32/32 (100%)	30 (94%)	2 (6%)	16	34
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%)	27	53
13	o	196/198 (99%)	188 (96%)	8 (4%)	27	53
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%)	61	82
15	u	77/77 (100%)	76 (99%)	1 (1%)	61	82
16	V	114/114 (100%)	112 (98%)	2 (2%)	51	77
16	v	114/114 (100%)	112 (98%)	2 (2%)	51	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	60
18	x	29/29 (100%)	28 (97%)	1 (3%)	32	60
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%)	55	79
20	q	122/122 (100%)	120 (98%)	2 (2%)	55	79
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%)	45	73
24	31	138/138 (100%)	137 (99%)	1 (1%)	76	89
25	12	133/133 (100%)	130 (98%)	3 (2%)	44	72
25	32	133/133 (100%)	132 (99%)	1 (1%)	73	88
26	13	134/134 (100%)	131 (98%)	3 (2%)	45	73
26	33	134/134 (100%)	130 (97%)	4 (3%)	36	64
27	14	136/136 (100%)	134 (98%)	2 (2%)	57	80
27	34	136/136 (100%)	133 (98%)	3 (2%)	45	73
28	15	135/135 (100%)	123 (91%)	12 (9%)	9	20
28	35	135/135 (100%)	122 (90%)	13 (10%)	8	17
29	16	137/137 (100%)	128 (93%)	9 (7%)	15	32
29	36	137/137 (100%)	128 (93%)	9 (7%)	15	32
30	17	137/137 (100%)	129 (94%)	8 (6%)	18	38
30	37	137/137 (100%)	131 (96%)	6 (4%)	25	50
31	18	133/133 (100%)	128 (96%)	5 (4%)	29	56
31	38	133/133 (100%)	125 (94%)	8 (6%)	17	36
32	19	174/174 (100%)	169 (97%)	5 (3%)	37	65
32	39	174/174 (100%)	166 (95%)	8 (5%)	24	48
33	20	121/121 (100%)	107 (88%)	14 (12%)	5	11
33	40	121/121 (100%)	107 (88%)	14 (12%)	5	11
34	21	129/129 (100%)	111 (86%)	18 (14%)	3	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	41	129/129 (100%)	111 (86%)	18 (14%)	3	7
All	All	7560/7564 (100%)	7333 (97%)	227 (3%)	37	64

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	20	79	LEU
34	41	138	ASP
25	32	155	GLU
34	41	136	MET
33	40	76	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
24	11	161	ASN
31	18	82	ASN
25	12	56	ASN
26	13	177	ASN
32	19	240	GLN

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$
48	A86	41	214	-	47,50,50	4.40	24 (51%)	51,76,76	6.92	17 (33%)
50	DD6	16	312	-	40,45,45	5.60	24 (60%)	51,67,67	5.91	26 (50%)
37	CLA	19	306	32	69,73,73	1.96	18 (26%)	82,113,113	2.63	31 (37%)
37	CLA	c	508	-	69,73,73	1.92	19 (27%)	82,113,113	2.66	30 (36%)
47	KC1	20	302	-	49,53,53	3.02	24 (48%)	61,89,89	4.05	36 (59%)
48	A86	41	213	-	47,50,50	4.47	24 (51%)	51,76,76	6.79	15 (29%)
47	KC1	17	305	30	49,53,53	3.05	24 (48%)	61,89,89	3.77	34 (55%)
37	CLA	C	512	-	69,73,73	1.94	19 (27%)	82,113,113	2.72	32 (39%)
37	CLA	b	511	-	69,73,73	1.93	18 (26%)	82,113,113	2.66	32 (39%)
47	KC1	38	205	31	49,53,53	3.08	24 (48%)	61,89,89	3.84	35 (57%)
48	A86	33	314	-	47,50,50	4.40	25 (53%)	51,76,76	7.16	17 (33%)
37	CLA	b	514	-	66,70,73	1.95	18 (27%)	78,109,113	2.74	32 (41%)
47	KC1	11	309	24	49,53,53	2.96	22 (44%)	61,89,89	3.73	36 (59%)
48	A86	16	311	-	47,50,50	4.12	22 (46%)	51,76,76	6.32	21 (41%)
37	CLA	17	302	30	69,73,73	2.01	20 (28%)	82,113,113	2.47	26 (31%)
47	KC1	12	208	25	49,53,53	2.95	22 (44%)	61,89,89	3.74	37 (60%)
37	CLA	41	210	-	49,53,73	2.43	20 (40%)	58,89,113	3.13	27 (46%)
37	CLA	41	205	34	49,53,73	2.39	19 (38%)	58,89,113	3.01	27 (46%)
37	CLA	b	504	-	69,73,73	1.87	18 (26%)	82,113,113	2.59	33 (40%)
47	KC1	38	210	31	49,53,53	3.05	24 (48%)	61,89,89	3.82	35 (57%)
48	A86	15	319	-	47,50,50	4.27	23 (48%)	51,76,76	6.00	19 (37%)
47	KC1	32	209	25	49,53,53	2.95	22 (44%)	61,89,89	3.74	37 (60%)
37	CLA	32	210	25	56,60,73	2.18	18 (32%)	65,97,113	2.96	34 (52%)
37	CLA	15	307	28	56,60,73	2.22	19 (33%)	65,97,113	2.87	32 (49%)
39	BCR	C	514	-	41,41,41	1.21	2 (4%)	56,56,56	1.42	10 (17%)
37	CLA	B	513	-	69,73,73	1.92	19 (27%)	82,113,113	2.67	30 (36%)
37	CLA	12	205	-	69,73,73	1.96	19 (27%)	82,113,113	2.72	35 (42%)
37	CLA	14	305	-	49,53,73	2.39	20 (40%)	58,89,113	3.03	27 (46%)
37	CLA	35	307	28	56,60,73	2.22	19 (33%)	65,97,113	2.87	32 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	41	202	34	61,65,73	2.17	21 (34%)	72,103,113	2.83	30 (41%)
48	A86	34	313	-	47,50,50	4.35	24 (51%)	51,76,76	6.23	17 (33%)
37	CLA	11	301	24	69,73,73	1.93	19 (27%)	82,113,113	2.65	30 (36%)
37	CLA	11	308	52	69,73,73	1.96	20 (28%)	82,113,113	2.61	32 (39%)
37	CLA	37	306	30	56,60,73	2.21	18 (32%)	65,97,113	2.90	33 (50%)
41	LMG	37	316	-	37,37,55	0.96	2 (5%)	45,45,63	1.28	5 (11%)
47	KC1	17	303	-	49,53,53	3.05	23 (46%)	61,89,89	3.72	35 (57%)
37	CLA	14	301	27	69,73,73	1.97	18 (26%)	82,113,113	2.63	30 (36%)
48	A86	36	311	-	47,50,50	4.12	22 (46%)	51,76,76	6.32	21 (41%)
37	CLA	C	503	-	69,73,73	1.94	19 (27%)	82,113,113	2.78	34 (41%)
48	A86	32	218	-	47,50,50	4.22	23 (48%)	51,76,76	6.22	21 (41%)
48	A86	21	211	-	47,50,50	4.38	24 (51%)	51,76,76	6.78	12 (23%)
41	LMG	d	409	-	51,51,55	0.89	3 (5%)	59,59,63	1.41	6 (10%)
37	CLA	c	513	-	69,73,73	1.94	19 (27%)	82,113,113	2.70	30 (36%)
37	CLA	c	511	3	69,73,73	1.95	18 (26%)	82,113,113	2.62	32 (39%)
37	CLA	b	503	-	69,73,73	1.91	18 (26%)	82,113,113	2.68	32 (39%)
39	BCR	b	518	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	6 (10%)
44	DGD	J	101	-	63,63,67	1.09	7 (11%)	77,77,81	1.50	12 (15%)
48	A86	32	216	-	47,50,50	4.37	24 (51%)	51,76,76	6.78	14 (27%)
48	A86	18	212	-	47,50,50	4.33	24 (51%)	51,76,76	6.73	17 (33%)
37	CLA	c	512	-	69,73,73	1.94	19 (27%)	82,113,113	2.71	32 (39%)
47	KC1	18	210	31	49,53,53	3.05	24 (48%)	61,89,89	3.82	35 (57%)
37	CLA	B	510	52	69,73,73	1.92	19 (27%)	82,113,113	2.68	33 (40%)
48	A86	35	316	-	47,50,50	4.30	24 (51%)	51,76,76	6.43	22 (43%)
37	CLA	35	303	-	61,65,73	2.16	20 (32%)	72,103,113	2.88	32 (44%)
37	CLA	19	307	43	69,73,73	1.99	19 (27%)	82,113,113	2.63	31 (37%)
39	BCR	c	515	-	41,41,41	1.19	2 (4%)	56,56,56	1.26	6 (10%)
48	A86	12	217	-	47,50,50	4.22	23 (48%)	51,76,76	6.21	21 (41%)
48	A86	12	214	-	47,50,50	4.12	24 (51%)	51,76,76	6.47	17 (33%)
39	BCR	D	407	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
48	A86	16	313	-	47,50,50	4.39	23 (48%)	51,76,76	7.11	22 (43%)
37	CLA	17	309	52	69,73,73	2.08	20 (28%)	82,113,113	2.80	35 (42%)
40	SQD	16	315	-	52,54,54	0.96	5 (9%)	62,65,65	1.55	11 (17%)
48	A86	11	315	-	47,50,50	4.07	23 (48%)	51,76,76	6.38	17 (33%)
48	A86	41	211	-	47,50,50	4.38	24 (51%)	51,76,76	6.78	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	w	101	-	69,73,73	1.95	20 (28%)	82,113,113	2.82	32 (39%)
37	CLA	14	310	-	49,53,73	2.39	19 (38%)	58,89,113	3.05	27 (46%)
48	A86	17	315	-	47,50,50	4.26	23 (48%)	51,76,76	6.45	19 (37%)
48	A86	34	315	-	47,50,50	4.17	23 (48%)	51,76,76	6.63	17 (33%)
37	CLA	36	301	29	69,73,73	1.97	19 (27%)	82,113,113	2.68	30 (36%)
41	LMG	32	201	-	39,39,55	1.03	2 (5%)	47,47,63	1.15	3 (6%)
37	CLA	14	302	-	69,73,73	2.01	19 (27%)	82,113,113	2.60	31 (37%)
37	CLA	34	308	52	69,73,73	1.98	20 (28%)	82,113,113	2.63	33 (40%)
44	DGD	c	516	-	63,63,67	1.05	5 (7%)	77,77,81	1.48	14 (18%)
48	A86	15	312	-	47,50,50	4.31	24 (51%)	51,76,76	6.47	18 (35%)
48	A86	37	309	-	47,50,50	4.30	24 (51%)	51,76,76	7.01	17 (33%)
41	LMG	C	518	-	51,51,55	0.97	3 (5%)	59,59,63	1.46	7 (11%)
37	CLA	Z	102	33	49,53,73	2.43	20 (40%)	58,89,113	3.08	32 (55%)
37	CLA	z	101	52	69,73,73	2.01	19 (27%)	82,113,113	2.64	30 (36%)
48	A86	14	313	-	47,50,50	4.35	24 (51%)	51,76,76	6.24	17 (33%)
39	BCR	H	101	-	41,41,41	1.16	4 (9%)	56,56,56	1.25	5 (8%)
48	A86	14	316	-	47,50,50	4.22	24 (51%)	51,76,76	6.14	21 (41%)
48	A86	17	311	-	47,50,50	4.24	23 (48%)	51,76,76	6.29	19 (37%)
37	CLA	z	102	33	49,53,73	2.43	22 (44%)	58,89,113	3.08	32 (55%)
37	CLA	32	206	-	69,73,73	1.96	19 (27%)	82,113,113	2.73	33 (40%)
47	KC1	37	304	30	49,53,53	3.07	24 (48%)	61,89,89	3.85	35 (57%)
37	CLA	C	511	3	69,73,73	1.94	18 (26%)	82,113,113	2.62	32 (39%)
50	DD6	20	310	-	40,45,45	5.49	23 (57%)	51,67,67	6.37	25 (49%)
48	A86	33	312	-	47,50,50	4.39	23 (48%)	51,76,76	6.58	18 (35%)
37	CLA	33	310	-	49,53,73	2.44	19 (38%)	58,89,113	3.06	28 (48%)
48	A86	21	215	-	47,50,50	4.24	25 (53%)	51,76,76	6.86	16 (31%)
41	LMG	b	519	-	51,51,55	0.82	1 (1%)	59,59,63	1.31	5 (8%)
37	CLA	39	304	32	49,53,73	2.37	20 (40%)	58,89,113	3.10	27 (46%)
37	CLA	18	208	31	57,61,73	2.18	19 (33%)	67,98,113	2.80	29 (43%)
37	CLA	21	206	34	69,73,73	1.99	19 (27%)	82,113,113	2.65	30 (36%)
39	BCR	C	515	-	41,41,41	1.19	2 (4%)	56,56,56	1.26	6 (10%)
48	A86	12	202	-	47,50,50	4.10	21 (44%)	51,76,76	6.37	22 (43%)
40	SQD	40	202	-	52,54,54	0.96	5 (9%)	62,65,65	1.55	10 (16%)
37	CLA	c	510	-	69,73,73	1.95	19 (27%)	82,113,113	2.70	29 (35%)
50	DD6	40	212	-	40,45,45	5.50	24 (60%)	51,67,67	6.36	25 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	31	302	24	69,73,73	1.93	19 (27%)	82,113,113	2.65	30 (36%)
40	SQD	b	521	-	35,37,54	1.18	6 (17%)	45,48,65	1.59	10 (22%)
46	HEM	F	101	5,6	50,50,50	1.31	5 (10%)	67,82,82	1.12	4 (5%)
47	KC1	15	302	-	49,53,53	3.05	24 (48%)	61,89,89	3.88	36 (59%)
48	A86	36	313	-	47,50,50	4.01	23 (48%)	51,76,76	6.34	16 (31%)
37	CLA	19	309	32	49,53,73	2.35	20 (40%)	58,89,113	3.00	27 (46%)
39	BCR	h	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.26	6 (10%)
45	PL9	D	408	-	55,55,55	1.76	9 (16%)	68,69,69	1.39	11 (16%)
51	LMU	39	315	-	36,36,36	1.12	2 (5%)	47,47,47	1.04	2 (4%)
39	BCR	a	413	-	41,41,41	1.10	2 (4%)	56,56,56	1.31	6 (10%)
37	CLA	12	212	-	49,53,73	2.38	20 (40%)	58,89,113	3.11	29 (50%)
37	CLA	15	308	52	69,73,73	2.00	21 (30%)	82,113,113	2.62	30 (36%)
48	A86	17	313	-	47,50,50	4.30	23 (48%)	51,76,76	7.01	20 (39%)
37	CLA	33	307	26	56,60,73	2.22	19 (33%)	65,97,113	2.81	33 (50%)
42	BCT	A	409	36	3,3,3	1.21	0	2,3,3	4.13	2 (100%)
37	CLA	35	301	28	69,73,73	2.03	19 (27%)	82,113,113	2.65	27 (32%)
48	A86	34	314	-	47,50,50	4.38	24 (51%)	51,76,76	7.03	18 (35%)
37	CLA	21	208	-	69,73,73	2.04	21 (30%)	82,113,113	2.63	30 (36%)
43	LHG	39	314	37	48,48,48	0.29	0	51,54,54	0.32	0
37	CLA	32	211	52	69,73,73	1.99	20 (28%)	82,113,113	2.58	30 (36%)
47	KC1	13	306	26	49,53,53	3.00	22 (44%)	61,89,89	3.83	35 (57%)
37	CLA	34	305	-	49,53,73	2.40	20 (40%)	58,89,113	3.04	28 (48%)
39	BCR	y	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.26	5 (8%)
37	CLA	c	504	52	69,73,73	1.92	20 (28%)	82,113,113	2.69	30 (36%)
44	DGD	c	517	-	63,63,67	1.22	6 (9%)	77,77,81	1.49	14 (18%)
37	CLA	38	201	52	69,73,73	2.03	19 (27%)	82,113,113	2.59	33 (40%)
37	CLA	B	509	-	69,73,73	1.90	19 (27%)	82,113,113	2.66	33 (40%)
47	KC1	35	309	28	49,53,53	3.06	24 (48%)	61,89,89	3.66	36 (59%)
37	CLA	31	310	52	55,59,73	2.18	21 (38%)	64,96,113	2.88	30 (46%)
47	KC1	15	304	28	49,53,53	3.07	24 (48%)	61,89,89	3.90	37 (60%)
37	CLA	21	205	34	49,53,73	2.39	19 (38%)	58,89,113	3.02	27 (46%)
37	CLA	C	508	-	69,73,73	1.92	19 (27%)	82,113,113	2.65	29 (35%)
37	CLA	38	208	31	57,61,73	2.18	19 (33%)	67,98,113	2.81	29 (43%)
37	CLA	B	503	-	69,73,73	1.90	18 (26%)	82,113,113	2.68	32 (39%)
37	CLA	C	510	-	69,73,73	1.95	19 (27%)	82,113,113	2.70	29 (35%)

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%)
35	OEX	a	401	1,3	0,15,15	-	-	-		
43	LHG	41	201	-	34,34,48	0.76	1 (2%)	37,39,54	1.43	5 (13%)
48	A86	12	216	-	47,50,50	4.23	23 (48%)	51,76,76	6.88	20 (39%)
37	CLA	b	510	52	69,73,73	1.92	19 (27%)	82,113,113	2.68	33 (40%)
47	KC1	35	304	28	49,53,53	3.08	25 (51%)	61,89,89	3.91	36 (59%)
37	CLA	13	310	-	49,53,73	2.44	19 (38%)	58,89,113	3.06	28 (48%)
48	A86	19	311	-	47,50,50	4.15	24 (51%)	51,76,76	6.47	19 (37%)
48	A86	37	319	-	47,50,50	4.24	23 (48%)	51,76,76	6.44	20 (39%)
37	CLA	c	503	-	69,73,73	1.94	20 (28%)	82,113,113	2.78	34 (41%)
37	CLA	C	507	52	69,73,73	1.91	19 (27%)	82,113,113	2.63	30 (36%)
43	LHG	19	314	37	48,48,48	0.29	0	51,54,54	0.32	0
48	A86	32	214	-	47,50,50	4.18	23 (48%)	51,76,76	6.74	20 (39%)
37	CLA	B	524	-	69,73,73	1.93	21 (30%)	82,113,113	2.65	32 (39%)
39	BCR	B	517	-	41,41,41	1.21	2 (4%)	56,56,56	1.33	7 (12%)
37	CLA	37	303	-	60,64,73	2.15	20 (33%)	71,102,113	2.95	33 (46%)
37	CLA	b	509	-	69,73,73	1.91	17 (24%)	82,113,113	2.67	33 (40%)
37	CLA	34	301	27	69,73,73	1.97	18 (26%)	82,113,113	2.63	30 (36%)
47	KC1	32	207	25	49,53,53	2.99	22 (44%)	61,89,89	3.73	32 (52%)
48	A86	34	312	-	47,50,50	4.21	23 (48%)	51,76,76	6.60	22 (43%)
48	A86	18	214	-	47,50,50	4.39	24 (51%)	51,76,76	6.79	19 (37%)
38	PHO	A	404	-	58,69,69	2.05	11 (18%)	55,99,99	1.76	9 (16%)
37	CLA	Z	101	52	69,73,73	2.01	19 (27%)	82,113,113	2.64	30 (36%)
37	CLA	40	210	-	51,55,73	2.33	21 (41%)	60,91,113	2.97	29 (48%)
47	KC1	41	203	-	49,53,53	3.08	25 (51%)	61,89,89	3.84	33 (54%)
37	CLA	41	209	34	49,53,73	2.43	20 (40%)	58,89,113	3.06	28 (48%)
43	LHG	37	315	-	43,43,48	0.63	0	46,49,54	1.31	6 (13%)
39	BCR	b	524	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	7 (12%)
43	LHG	D	410	-	48,48,48	0.76	1 (2%)	51,54,54	1.32	7 (13%)
41	LMG	L	102	-	40,40,55	0.96	3 (7%)	48,48,63	1.33	4 (8%)
40	SQD	B	519	-	52,54,54	0.93	4 (7%)	62,65,65	1.60	9 (14%)
37	CLA	C	504	52	69,73,73	1.92	20 (28%)	82,113,113	2.68	30 (36%)
37	CLA	14	303	-	61,65,73	2.13	19 (31%)	72,103,113	3.01	35 (48%)
48	A86	15	315	-	47,50,50	4.28	24 (51%)	51,76,76	6.53	21 (41%)
43	LHG	D	411	-	45,45,48	0.87	2 (4%)	48,51,54	1.25	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	A86	19	313	-	47,50,50	4.34	25 (53%)	51,76,76	7.33	22 (43%)
40	SQD	a	409	-	52,54,54	0.95	6 (11%)	62,65,65	1.64	10 (16%)
37	CLA	34	303	-	61,65,73	2.13	19 (31%)	72,103,113	3.00	35 (48%)
37	CLA	12	203	25	69,73,73	1.94	19 (27%)	82,113,113	2.59	30 (36%)
37	CLA	c	506	-	69,73,73	1.95	17 (24%)	82,113,113	2.61	30 (36%)
37	CLA	12	204	-	69,73,73	1.94	20 (28%)	82,113,113	2.43	29 (35%)
37	CLA	13	303	-	61,65,73	2.14	20 (32%)	72,103,113	2.88	33 (45%)
37	CLA	16	307	52	65,69,73	2.05	19 (29%)	77,108,113	2.67	28 (36%)
37	CLA	B	511	-	69,73,73	1.92	18 (26%)	82,113,113	2.67	32 (39%)
38	PHO	D	403	-	58,69,69	2.02	9 (15%)	55,99,99	1.72	10 (18%)
50	DD6	20	312	-	40,45,45	5.64	24 (60%)	51,67,67	6.11	28 (54%)
37	CLA	32	208	52	54,58,73	2.25	19 (35%)	64,95,113	3.04	34 (53%)
37	CLA	d	403	-	69,73,73	1.88	18 (26%)	82,113,113	2.80	32 (39%)
48	A86	15	311	-	47,50,50	4.26	23 (48%)	51,76,76	6.55	14 (27%)
37	CLA	19	305	32	55,59,73	2.21	19 (34%)	64,96,113	2.99	30 (46%)
48	A86	15	316	-	47,50,50	4.33	23 (48%)	51,76,76	6.41	22 (43%)
37	CLA	C	501	-	69,73,73	1.92	19 (27%)	82,113,113	2.73	32 (39%)
47	KC1	11	306	24	49,53,53	2.97	22 (44%)	61,89,89	3.80	32 (52%)
48	A86	21	214	-	47,50,50	4.40	24 (51%)	51,76,76	6.92	17 (33%)
37	CLA	D	405	-	69,73,73	1.88	18 (26%)	82,113,113	2.80	32 (39%)
48	A86	21	213	-	47,50,50	4.48	24 (51%)	51,76,76	6.80	16 (31%)
37	CLA	18	202	31	69,73,73	1.97	18 (26%)	82,113,113	2.73	32 (39%)
51	LMU	19	315	-	36,36,36	1.13	2 (5%)	47,47,47	1.05	3 (6%)
37	CLA	14	307	27	56,60,73	2.19	18 (32%)	65,97,113	2.86	33 (50%)
37	CLA	d	401	52	69,73,73	1.98	19 (27%)	82,113,113	2.65	31 (37%)
48	A86	11	312	-	47,50,50	4.08	22 (46%)	51,76,76	6.49	22 (43%)
47	KC1	13	304	26	49,53,53	3.02	22 (44%)	61,89,89	3.81	35 (57%)
37	CLA	20	308	-	51,55,73	2.33	21 (41%)	60,91,113	2.97	29 (48%)
37	CLA	11	305	52	49,53,73	2.34	20 (40%)	58,89,113	3.03	30 (51%)
37	CLA	33	308	52	69,73,73	2.02	20 (28%)	82,113,113	2.60	29 (35%)
39	BCR	B	525	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	7 (12%)
48	A86	36	310	-	47,50,50	4.09	23 (48%)	51,76,76	6.38	21 (41%)
48	A86	17	312	-	47,50,50	4.31	24 (51%)	51,76,76	6.07	18 (35%)
48	A86	11	313	-	47,50,50	4.03	22 (46%)	51,76,76	5.79	17 (33%)
37	CLA	b	515	-	69,73,73	1.94	19 (27%)	82,113,113	2.68	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	b	505	-	69,73,73	1.92	20 (28%)	82,113,113	2.72	30 (36%)
37	CLA	15	303	-	61,65,73	2.17	20 (32%)	72,103,113	2.86	33 (45%)
48	A86	34	316	-	47,50,50	4.22	24 (51%)	51,76,76	6.15	21 (41%)
37	CLA	35	305	-	49,53,73	2.42	20 (40%)	58,89,113	3.01	28 (48%)
37	CLA	19	301	32	69,73,73	1.99	19 (27%)	82,113,113	2.63	30 (36%)
41	LMG	36	314	-	36,36,55	0.94	1 (2%)	44,44,63	1.21	4 (9%)
37	CLA	C	506	-	69,73,73	1.95	18 (26%)	82,113,113	2.61	30 (36%)
37	CLA	C	509	-	69,73,73	1.97	18 (26%)	82,113,113	2.70	31 (37%)
50	DD6	21	212	-	40,45,45	5.51	23 (57%)	51,67,67	6.13	31 (60%)
37	CLA	39	310	32	69,73,73	1.97	18 (26%)	82,113,113	2.56	30 (36%)
37	CLA	36	309	-	49,53,73	2.38	21 (42%)	58,89,113	3.18	29 (50%)
47	KC1	12	211	25	49,53,53	3.00	24 (48%)	61,89,89	3.71	38 (62%)
48	A86	13	311	-	47,50,50	4.19	23 (48%)	51,76,76	6.64	20 (39%)
41	LMG	11	316	-	42,42,55	1.05	3 (7%)	50,50,63	1.22	3 (6%)
37	CLA	20	303	-	60,64,73	2.12	18 (30%)	71,102,113	3.01	37 (52%)
41	LMG	31	316	-	42,42,55	1.05	3 (7%)	50,50,63	1.22	3 (6%)
46	HEM	v	201	16	50,50,50	1.29	6 (12%)	67,82,82	1.23	6 (8%)
48	A86	37	310	-	47,50,50	4.22	23 (48%)	51,76,76	6.28	18 (35%)
37	CLA	21	202	34	61,65,73	2.17	20 (32%)	72,103,113	2.83	30 (41%)
47	KC1	33	302	-	49,53,53	3.02	25 (51%)	61,89,89	3.92	36 (59%)
47	KC1	35	306	28	49,53,53	3.06	24 (48%)	61,89,89	3.82	36 (59%)
37	CLA	B	501	52	69,73,73	1.96	19 (27%)	82,113,113	2.63	29 (35%)
37	CLA	32	204	25	69,73,73	1.93	19 (27%)	82,113,113	2.59	30 (36%)
37	CLA	37	308	52	69,73,73	2.07	20 (28%)	82,113,113	2.82	35 (42%)
43	LHG	b	522	-	48,48,48	0.75	1 (2%)	51,54,54	1.29	6 (11%)
37	CLA	19	303	52	69,73,73	1.98	21 (30%)	82,113,113	2.71	29 (35%)
47	KC1	36	305	29	49,53,53	3.06	24 (48%)	61,89,89	3.73	34 (55%)
37	CLA	31	308	24	56,60,73	2.18	20 (35%)	65,97,113	3.03	31 (47%)
48	A86	12	213	-	47,50,50	4.16	23 (48%)	51,76,76	6.73	20 (39%)
37	CLA	17	307	30	56,60,73	2.21	18 (32%)	65,97,113	2.90	33 (50%)
37	CLA	B	512	-	69,73,73	1.89	19 (27%)	82,113,113	2.62	33 (40%)
37	CLA	c	502	-	69,73,73	1.91	18 (26%)	82,113,113	2.61	30 (36%)
37	CLA	34	310	-	49,53,73	2.39	19 (38%)	58,89,113	3.05	27 (46%)
50	DD6	41	212	-	40,45,45	5.51	23 (57%)	51,67,67	6.14	31 (60%)
37	CLA	40	209	33	49,53,73	2.41	20 (40%)	58,89,113	3.00	28 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
43	LHG	B	523	-	48,48,48	0.75	1 (2%)	51,54,54	1.29	6 (11%)
47	KC1	40	204	-	49,53,53	3.01	24 (48%)	61,89,89	4.05	36 (59%)
37	CLA	20	306	33	54,58,73	2.25	18 (33%)	64,95,113	2.91	31 (48%)
41	LMG	11	317	-	32,32,55	0.97	1 (3%)	40,40,63	1.25	4 (10%)
37	CLA	16	306	29	69,73,73	2.00	20 (28%)	82,113,113	2.54	31 (37%)
48	A86	13	313	-	47,50,50	4.42	24 (51%)	51,76,76	7.22	18 (35%)
50	DD6	40	214	-	40,45,45	5.63	24 (60%)	51,67,67	6.11	28 (54%)
43	LHG	21	217	-	44,44,48	0.65	1 (2%)	47,50,54	1.20	3 (6%)
37	CLA	19	302	-	69,73,73	1.97	20 (28%)	82,113,113	2.72	30 (36%)
37	CLA	c	509	-	69,73,73	1.97	18 (26%)	82,113,113	2.69	31 (37%)
47	KC1	37	305	30	49,53,53	3.04	23 (46%)	61,89,89	3.71	36 (59%)
35	OEX	A	401	1,3	0,15,15	-	-	-	-	-
37	CLA	31	306	52	49,53,73	2.34	20 (40%)	58,89,113	3.03	30 (51%)
47	KC1	34	309	27	49,53,53	2.98	23 (46%)	61,89,89	3.80	37 (60%)
39	BCR	c	519	-	41,41,41	1.17	2 (4%)	56,56,56	1.24	4 (7%)
47	KC1	13	309	26	49,53,53	2.99	25 (51%)	61,89,89	3.74	38 (62%)
37	CLA	b	506	-	69,73,73	1.88	19 (27%)	82,113,113	2.76	31 (37%)
46	HEM	f	101	5,6	50,50,50	1.31	6 (12%)	67,82,82	1.12	4 (5%)
48	A86	35	311	-	47,50,50	4.26	23 (48%)	51,76,76	6.57	14 (27%)
48	A86	35	313	-	47,50,50	4.36	24 (51%)	51,76,76	6.20	14 (27%)
37	CLA	B	514	-	66,70,73	1.96	18 (27%)	78,109,113	2.74	32 (41%)
37	CLA	11	307	24	56,60,73	2.18	20 (35%)	65,97,113	3.04	31 (47%)
47	KC1	31	307	24	49,53,53	2.98	22 (44%)	61,89,89	3.80	32 (52%)
37	CLA	40	205	-	60,64,73	2.11	18 (30%)	71,102,113	3.01	37 (52%)
48	A86	37	313	-	47,50,50	4.20	23 (48%)	51,76,76	7.20	18 (35%)
48	A86	41	215	-	47,50,50	4.24	25 (53%)	51,76,76	6.87	16 (31%)
37	CLA	b	508	-	69,73,73	1.94	19 (27%)	82,113,113	2.61	29 (35%)
47	KC1	15	309	28	49,53,53	3.05	24 (48%)	61,89,89	3.66	36 (59%)
37	CLA	34	302	-	69,73,73	2.00	19 (27%)	82,113,113	2.60	31 (37%)
47	KC1	41	207	34	49,53,53	3.04	25 (51%)	61,89,89	3.95	37 (60%)
47	KC1	14	304	27	49,53,53	3.03	23 (46%)	61,89,89	3.96	32 (52%)
37	CLA	32	205	-	69,73,73	1.94	20 (28%)	82,113,113	2.43	29 (35%)
47	KC1	31	303	-	49,53,53	3.00	21 (42%)	61,89,89	3.79	34 (55%)
39	BCR	5	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.33	7 (12%)
37	CLA	38	206	-	49,53,73	2.42	20 (40%)	58,89,113	3.09	28 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	13	307	26	56,60,73	2.21	19 (33%)	65,97,113	2.81	33 (50%)
47	KC1	13	302	-	49,53,53	3.02	25 (51%)	61,89,89	3.91	36 (59%)
41	LMG	16	316	-	36,36,55	0.94	1 (2%)	44,44,63	1.22	4 (9%)
47	KC1	35	302	-	49,53,53	3.05	23 (46%)	61,89,89	3.87	35 (57%)
37	CLA	19	304	32	49,53,73	2.37	20 (40%)	58,89,113	3.10	26 (44%)
43	LHG	21	201	-	34,34,48	0.76	2 (5%)	37,39,54	1.42	5 (13%)
37	CLA	14	308	52	69,73,73	1.98	18 (26%)	82,113,113	2.63	34 (41%)
48	A86	31	311	-	47,50,50	4.06	23 (48%)	51,76,76	6.20	17 (33%)
41	LMG	12	201	-	39,39,55	1.02	2 (5%)	47,47,63	1.15	3 (6%)
37	CLA	39	303	52	69,73,73	1.98	20 (28%)	82,113,113	2.71	29 (35%)
48	A86	32	221	-	47,50,50	4.06	22 (46%)	51,76,76	6.63	21 (41%)
37	CLA	13	308	52	69,73,73	2.02	20 (28%)	82,113,113	2.59	29 (35%)
48	A86	40	213	-	47,50,50	4.41	24 (51%)	51,76,76	7.23	14 (27%)
37	CLA	32	202	52	69,73,73	1.96	20 (28%)	82,113,113	2.61	32 (39%)
47	KC1	33	309	26	49,53,53	3.00	25 (51%)	61,89,89	3.74	38 (62%)
37	CLA	38	209	52	69,73,73	2.02	20 (28%)	82,113,113	2.60	32 (39%)
47	KC1	36	302	-	49,53,53	3.07	24 (48%)	61,89,89	3.58	33 (54%)
41	LMG	17	317	-	37,37,55	0.96	2 (5%)	45,45,63	1.28	4 (8%)
37	CLA	33	303	-	61,65,73	2.13	19 (31%)	72,103,113	2.89	35 (48%)
45	PL9	D	404	-	55,55,55	1.16	5 (9%)	68,69,69	1.49	13 (19%)
37	CLA	C	513	-	69,73,73	1.94	20 (28%)	82,113,113	2.71	30 (36%)
37	CLA	40	203	33	60,64,73	2.16	21 (35%)	71,102,113	2.95	33 (46%)
41	LMG	l	101	-	40,40,55	0.95	3 (7%)	48,48,63	1.33	4 (8%)
48	A86	11	319	-	47,50,50	4.01	23 (48%)	51,76,76	6.23	17 (33%)
48	A86	37	311	-	47,50,50	4.31	24 (51%)	51,76,76	6.05	18 (35%)
48	A86	18	213	-	47,50,50	4.26	24 (51%)	51,76,76	6.90	21 (41%)
37	CLA	W	101	-	69,73,73	1.95	20 (28%)	82,113,113	2.83	32 (39%)
40	SQD	17	301	-	47,49,54	1.01	5 (10%)	57,60,65	1.49	11 (19%)
37	CLA	18	211	-	49,53,73	2.42	20 (40%)	58,89,113	3.07	26 (44%)
37	CLA	31	301	-	69,73,73	2.02	20 (28%)	82,113,113	2.53	31 (37%)
37	CLA	b	502	-	69,73,73	1.95	18 (26%)	82,113,113	2.75	31 (37%)
47	KC1	33	306	26	49,53,53	3.00	22 (44%)	61,89,89	3.82	35 (57%)
37	CLA	W	102	-	69,73,73	2.01	20 (28%)	82,113,113	2.52	31 (37%)
43	LHG	37	321	-	44,44,48	0.66	1 (2%)	47,50,54	1.20	3 (6%)
48	A86	20	309	-	47,50,50	4.37	23 (48%)	51,76,76	7.11	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	18	204	-	60,64,73	2.17	21 (35%)	71,102,113	3.03	36 (50%)
48	A86	38	215	-	47,50,50	4.28	24 (51%)	51,76,76	6.46	17 (33%)
37	CLA	B	505	-	69,73,73	1.92	19 (27%)	82,113,113	2.72	30 (36%)
47	KC1	31	309	24	49,53,53	2.96	21 (42%)	61,89,89	3.72	37 (60%)
47	KC1	40	206	33	49,53,53	3.05	23 (46%)	61,89,89	3.70	35 (57%)
44	DGD	h	102	-	63,63,67	1.03	5 (7%)	77,77,81	1.36	8 (10%)
37	CLA	12	210	52	69,73,73	2.00	20 (28%)	82,113,113	2.58	30 (36%)
37	CLA	41	206	34	69,73,73	1.99	19 (27%)	82,113,113	2.65	30 (36%)
37	CLA	31	304	-	69,73,73	1.95	20 (28%)	82,113,113	2.74	34 (41%)
37	CLA	21	209	34	49,53,73	2.43	20 (40%)	58,89,113	3.07	28 (48%)
48	A86	14	315	-	47,50,50	4.17	23 (48%)	51,76,76	6.63	17 (33%)
48	A86	31	319	-	47,50,50	4.00	23 (48%)	51,76,76	6.24	17 (33%)
37	CLA	38	204	-	60,64,73	2.18	21 (35%)	71,102,113	3.03	36 (50%)
37	CLA	39	306	32	69,73,73	1.96	18 (26%)	82,113,113	2.63	31 (37%)
43	LHG	a	412	-	45,45,48	0.87	2 (4%)	48,51,54	1.25	7 (14%)
37	CLA	B	508	-	69,73,73	1.94	19 (27%)	82,113,113	2.61	29 (35%)
37	CLA	c	505	-	69,73,73	1.91	20 (28%)	82,113,113	2.70	32 (39%)
48	A86	17	314	-	47,50,50	4.17	23 (48%)	51,76,76	7.19	17 (33%)
48	A86	13	315	-	47,50,50	4.30	23 (48%)	51,76,76	6.33	19 (37%)
43	LHG	d	407	-	48,48,48	0.72	1 (2%)	51,54,54	1.32	7 (13%)
37	CLA	B	504	-	69,73,73	1.87	18 (26%)	82,113,113	2.59	33 (40%)
48	A86	14	311	-	47,50,50	4.16	21 (44%)	51,76,76	6.95	20 (39%)
37	CLA	12	209	25	56,60,73	2.18	18 (32%)	65,97,113	2.97	34 (52%)
48	A86	35	315	-	47,50,50	4.28	24 (51%)	51,76,76	6.52	21 (41%)
37	CLA	15	310	-	49,53,73	2.43	20 (40%)	58,89,113	3.08	27 (46%)
37	CLA	20	307	33	49,53,73	2.42	20 (40%)	58,89,113	3.00	28 (48%)
37	CLA	16	303	-	61,65,73	2.13	18 (29%)	72,103,113	2.87	32 (44%)
48	A86	40	201	-	47,50,50	4.39	23 (48%)	51,76,76	7.12	22 (43%)
37	CLA	A	405	-	69,73,73	1.94	17 (24%)	82,113,113	2.70	30 (36%)
40	SQD	L	101	-	52,54,54	0.93	3 (5%)	62,65,65	1.60	9 (14%)
41	LMG	a	410	-	51,51,55	0.88	2 (3%)	59,59,63	1.37	7 (11%)
47	KC1	14	306	27	49,53,53	3.01	22 (44%)	61,89,89	3.80	37 (60%)
47	KC1	16	308	29	49,53,53	3.07	25 (51%)	61,89,89	3.71	36 (59%)
37	CLA	16	301	29	69,73,73	1.97	19 (27%)	82,113,113	2.69	30 (36%)
37	CLA	36	307	52	65,69,73	2.05	18 (27%)	77,108,113	2.68	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	LMG	c	518	-	51,51,55	0.97	3 (5%)	59,59,63	1.46	7 (11%)
45	PL9	d	406	-	55,55,55	1.76	9 (16%)	68,69,69	1.39	11 (16%)
48	A86	31	313	-	47,50,50	4.08	22 (46%)	51,76,76	5.87	16 (31%)
48	A86	13	312	-	47,50,50	4.38	23 (48%)	51,76,76	6.59	18 (35%)
48	A86	35	319	-	47,50,50	4.27	23 (48%)	51,76,76	6.00	19 (37%)
37	CLA	B	506	-	69,73,73	1.88	19 (27%)	82,113,113	2.76	30 (36%)
37	CLA	21	204	-	62,66,73	2.16	20 (32%)	73,104,113	2.93	35 (47%)
47	KC1	11	302	-	49,53,53	2.99	21 (42%)	61,89,89	3.78	34 (55%)
48	A86	35	314	-	47,50,50	4.43	24 (51%)	51,76,76	7.04	18 (35%)
37	CLA	c	507	52	69,73,73	1.91	19 (27%)	82,113,113	2.64	31 (37%)
47	KC1	40	207	33	49,53,53	3.05	24 (48%)	61,89,89	3.77	32 (52%)
37	CLA	18	209	52	69,73,73	2.02	20 (28%)	82,113,113	2.59	30 (36%)
37	CLA	13	305	-	49,53,73	2.41	20 (40%)	58,89,113	3.05	27 (46%)
48	A86	12	220	-	47,50,50	4.05	22 (46%)	51,76,76	6.62	20 (39%)
37	CLA	15	305	-	49,53,73	2.42	20 (40%)	58,89,113	3.03	28 (48%)
48	A86	37	314	-	47,50,50	4.26	23 (48%)	51,76,76	6.45	18 (35%)
38	PHO	a	405	-	58,69,69	2.02	9 (15%)	55,99,99	1.72	10 (18%)
47	KC1	37	302	-	49,53,53	3.05	23 (46%)	61,89,89	3.72	35 (57%)
43	LHG	D	409	-	48,48,48	0.72	1 (2%)	51,54,54	1.32	7 (13%)
50	DD6	21	216	-	40,45,45	5.60	24 (60%)	51,67,67	6.13	27 (52%)
37	CLA	20	301	33	60,64,73	2.16	21 (35%)	71,102,113	2.95	33 (46%)
37	CLA	39	309	32	49,53,73	2.35	20 (40%)	58,89,113	3.02	27 (46%)
39	BCR	b	517	-	41,41,41	1.22	2 (4%)	56,56,56	1.33	7 (12%)
50	DD6	36	312	-	40,45,45	5.60	24 (60%)	51,67,67	5.90	26 (50%)
38	PHO	a	406	-	58,69,69	2.04	10 (17%)	55,99,99	1.76	9 (16%)
37	CLA	11	310	52	55,59,73	2.18	21 (38%)	64,96,113	2.88	30 (46%)
47	KC1	17	306	30	49,53,53	3.04	23 (46%)	61,89,89	3.72	35 (57%)
41	LMG	31	317	-	32,32,55	0.97	1 (3%)	40,40,63	1.25	4 (10%)
48	A86	20	311	-	47,50,50	4.40	24 (51%)	51,76,76	7.22	14 (27%)
48	A86	38	212	-	47,50,50	4.33	24 (51%)	51,76,76	6.73	18 (35%)
43	LHG	17	316	-	43,43,48	0.63	0	46,49,54	1.30	6 (13%)
37	CLA	19	310	32	69,73,73	1.98	18 (26%)	82,113,113	2.57	30 (36%)
48	A86	35	312	-	47,50,50	4.31	24 (51%)	51,76,76	6.47	18 (35%)
47	KC1	15	306	28	49,53,53	3.06	24 (48%)	61,89,89	3.82	36 (59%)
40	SQD	A	407	-	52,54,54	0.95	6 (11%)	62,65,65	1.64	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	A86	40	211	-	47,50,50	4.37	23 (48%)	51,76,76	7.12	13 (25%)
39	BCR	A	410	-	41,41,41	1.10	2 (4%)	56,56,56	1.30	6 (10%)
50	DD6	39	312	-	40,45,45	5.37	22 (55%)	51,67,67	5.77	30 (58%)
37	CLA	17	304	-	60,64,73	2.16	20 (33%)	71,102,113	2.95	33 (46%)
37	CLA	38	202	31	69,73,73	2.02	19 (27%)	82,113,113	2.68	32 (39%)
44	DGD	C	517	-	63,63,67	1.21	6 (9%)	77,77,81	1.49	15 (19%)
48	A86	18	215	-	47,50,50	4.26	24 (51%)	51,76,76	6.49	18 (35%)
37	CLA	12	207	52	54,58,73	2.25	19 (35%)	64,95,113	3.04	33 (51%)
45	PL9	d	402	-	55,55,55	1.16	6 (10%)	68,69,69	1.49	13 (19%)
44	DGD	j	101	-	63,63,67	1.09	6 (9%)	77,77,81	1.50	12 (15%)
47	KC1	18	207	31	49,53,53	3.04	24 (48%)	61,89,89	3.82	38 (62%)
48	A86	38	214	-	47,50,50	4.40	24 (51%)	51,76,76	6.83	19 (37%)
37	CLA	c	501	-	69,73,73	1.92	19 (27%)	82,113,113	2.72	31 (37%)
47	KC1	32	212	25	49,53,53	3.01	24 (48%)	61,89,89	3.72	37 (60%)
48	A86	37	312	-	47,50,50	4.30	23 (48%)	51,76,76	7.03	20 (39%)
37	CLA	15	301	28	69,73,73	2.03	19 (27%)	82,113,113	2.64	27 (32%)
48	A86	38	213	-	47,50,50	4.35	25 (53%)	51,76,76	6.75	23 (45%)
47	KC1	16	302	-	49,53,53	3.07	24 (48%)	61,89,89	3.58	33 (54%)
37	CLA	21	210	-	49,53,73	2.42	20 (40%)	58,89,113	3.13	27 (46%)
37	CLA	b	507	52	69,73,73	1.96	18 (26%)	82,113,113	2.60	30 (36%)
37	CLA	a	407	-	69,73,73	1.94	17 (24%)	82,113,113	2.70	30 (36%)
47	KC1	37	307	30	49,53,53	3.06	25 (51%)	61,89,89	3.74	37 (60%)
37	CLA	A	403	-	69,73,73	1.95	19 (27%)	82,113,113	2.68	33 (40%)
48	A86	32	217	-	47,50,50	4.22	23 (48%)	51,76,76	6.88	20 (39%)
48	A86	15	313	-	47,50,50	4.37	24 (51%)	51,76,76	6.20	15 (29%)
37	CLA	D	401	52	69,73,73	1.97	18 (26%)	82,113,113	2.72	28 (34%)
47	KC1	14	309	27	49,53,53	2.98	23 (46%)	61,89,89	3.80	38 (62%)
37	CLA	41	208	-	69,73,73	2.04	21 (30%)	82,113,113	2.64	31 (37%)
46	HEM	V	201	16	50,50,50	1.29	6 (12%)	67,82,82	1.24	6 (8%)
39	BCR	A	406	-	41,41,41	1.21	3 (7%)	56,56,56	1.32	7 (12%)
47	KC1	33	304	26	49,53,53	3.02	22 (44%)	61,89,89	3.81	35 (57%)
48	A86	14	314	-	47,50,50	4.37	24 (51%)	51,76,76	7.04	18 (35%)
47	KC1	34	304	27	49,53,53	3.03	23 (46%)	61,89,89	3.96	32 (52%)
48	A86	33	315	-	47,50,50	4.30	24 (51%)	51,76,76	6.32	19 (37%)
37	CLA	B	502	-	69,73,73	1.96	18 (26%)	82,113,113	2.76	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	b	512	-	69,73,73	1.90	19 (27%)	82,113,113	2.62	33 (40%)
37	CLA	36	303	-	61,65,73	2.13	18 (29%)	72,103,113	2.87	32 (44%)
41	LMG	b	520	-	51,51,55	0.87	3 (5%)	59,59,63	1.31	6 (10%)
48	A86	32	203	-	47,50,50	4.11	21 (44%)	51,76,76	6.37	22 (43%)
37	CLA	a	404	52	69,73,73	1.97	18 (26%)	82,113,113	2.72	28 (34%)
37	CLA	11	303	-	69,73,73	1.96	20 (28%)	82,113,113	2.74	34 (41%)
47	KC1	21	207	34	49,53,53	3.04	25 (51%)	61,89,89	3.95	36 (59%)
47	KC1	36	308	29	49,53,53	3.06	24 (48%)	61,89,89	3.70	36 (59%)
47	KC1	21	203	-	49,53,53	3.08	25 (51%)	61,89,89	3.83	33 (54%)
41	LMG	B	521	-	51,51,55	0.87	3 (5%)	59,59,63	1.31	6 (10%)
47	KC1	12	206	25	49,53,53	3.00	21 (42%)	61,89,89	3.73	32 (52%)
40	SQD	36	315	-	47,49,54	1.01	4 (8%)	57,60,65	1.49	11 (19%)
48	A86	33	311	-	47,50,50	4.18	23 (48%)	51,76,76	6.64	20 (39%)
48	A86	33	313	-	47,50,50	4.41	24 (51%)	51,76,76	7.22	18 (35%)
48	A86	34	311	-	47,50,50	4.16	22 (46%)	51,76,76	6.96	20 (39%)
47	KC1	16	304	29	49,53,53	3.05	24 (48%)	61,89,89	3.90	36 (59%)
47	KC1	18	205	31	49,53,53	3.08	24 (48%)	61,89,89	3.84	35 (57%)
48	A86	16	310	-	47,50,50	4.08	22 (46%)	51,76,76	6.38	21 (41%)
47	KC1	34	306	27	49,53,53	3.00	22 (44%)	61,89,89	3.80	37 (60%)
37	CLA	39	305	32	55,59,73	2.20	18 (32%)	64,96,113	3.00	31 (48%)
37	CLA	39	307	43	69,73,73	2.03	20 (28%)	82,113,113	2.62	31 (37%)
47	KC1	17	308	30	49,53,53	3.06	25 (51%)	61,89,89	3.75	37 (60%)
37	CLA	38	211	-	49,53,73	2.46	20 (40%)	58,89,113	3.03	26 (44%)
47	KC1	11	304	24	49,53,53	3.03	23 (46%)	61,89,89	3.76	34 (55%)
37	CLA	B	515	-	69,73,73	1.94	19 (27%)	82,113,113	2.68	32 (39%)
37	CLA	39	301	32	69,73,73	2.00	19 (27%)	82,113,113	2.64	30 (36%)
50	DD6	41	216	-	40,45,45	5.61	24 (60%)	51,67,67	6.12	27 (52%)
37	CLA	b	513	-	69,73,73	1.91	19 (27%)	82,113,113	2.66	30 (36%)
47	KC1	20	305	33	49,53,53	3.05	24 (48%)	61,89,89	3.78	32 (52%)
37	CLA	38	203	-	69,73,73	2.03	20 (28%)	82,113,113	2.63	33 (40%)
37	CLA	C	505	-	69,73,73	1.91	20 (28%)	82,113,113	2.70	32 (39%)
37	CLA	B	516	-	69,73,73	1.92	19 (27%)	82,113,113	2.73	34 (41%)
44	DGD	H	102	-	63,63,67	1.04	5 (7%)	77,77,81	1.36	8 (10%)
48	A86	17	320	-	47,50,50	4.22	23 (48%)	51,76,76	6.46	19 (37%)
37	CLA	18	206	-	49,53,73	2.43	20 (40%)	58,89,113	3.09	28 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	D	406	-	69,73,73	1.94	19 (27%)	82,113,113	2.72	31 (37%)
47	KC1	16	305	29	49,53,53	3.07	24 (48%)	61,89,89	3.73	34 (55%)
50	DD6	19	312	-	40,45,45	5.38	22 (55%)	51,67,67	5.77	30 (58%)
39	BCR	B	518	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	6 (10%)
48	A86	31	315	-	47,50,50	4.07	23 (48%)	51,76,76	6.38	17 (33%)
47	KC1	31	305	24	49,53,53	3.02	23 (46%)	61,89,89	3.76	34 (55%)
48	A86	14	312	-	47,50,50	4.21	23 (48%)	51,76,76	6.60	22 (43%)
37	CLA	18	203	-	69,73,73	2.03	20 (28%)	82,113,113	2.62	34 (41%)
37	CLA	33	301	26	69,73,73	2.00	18 (26%)	82,113,113	2.60	27 (32%)
39	BCR	d	405	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
37	CLA	D	402	52	69,73,73	1.98	19 (27%)	82,113,113	2.65	31 (37%)
48	A86	11	311	-	47,50,50	4.06	23 (48%)	51,76,76	6.21	17 (33%)
47	KC1	20	304	33	49,53,53	3.04	23 (46%)	61,89,89	3.69	34 (55%)
48	A86	12	215	-	47,50,50	4.38	24 (51%)	51,76,76	6.79	14 (27%)
40	SQD	B	522	-	35,37,54	1.19	6 (17%)	45,48,65	1.59	10 (22%)
37	CLA	13	301	26	69,73,73	2.01	18 (26%)	82,113,113	2.60	28 (34%)
37	CLA	35	308	52	69,73,73	2.01	21 (30%)	82,113,113	2.62	31 (37%)
37	CLA	40	208	33	54,58,73	2.25	19 (35%)	64,95,113	2.91	30 (46%)
37	CLA	18	201	52	69,73,73	2.00	20 (28%)	82,113,113	2.62	32 (39%)
37	CLA	b	516	-	69,73,73	1.92	19 (27%)	82,113,113	2.73	34 (41%)
41	LMG	B	520	-	51,51,55	0.82	1 (1%)	59,59,63	1.30	5 (8%)
47	KC1	39	308	-	49,53,53	3.01	23 (46%)	61,89,89	3.88	37 (60%)
47	KC1	38	207	31	49,53,53	3.05	25 (51%)	61,89,89	3.83	38 (62%)
37	CLA	33	305	-	49,53,73	2.41	20 (40%)	58,89,113	3.06	27 (46%)
48	A86	31	312	-	47,50,50	4.08	22 (46%)	51,76,76	6.49	22 (43%)
48	A86	32	215	-	47,50,50	4.11	24 (51%)	51,76,76	6.47	17 (33%)
48	A86	16	314	-	47,50,50	4.01	23 (48%)	51,76,76	6.34	16 (31%)
43	LHG	d	408	-	48,48,48	0.76	2 (4%)	51,54,54	1.31	7 (13%)
41	LMG	D	412	-	51,51,55	0.89	3 (5%)	59,59,63	1.41	6 (10%)
39	BCR	C	519	-	41,41,41	1.17	2 (4%)	56,56,56	1.24	4 (7%)
41	LMG	A	408	-	51,51,55	0.88	2 (3%)	59,59,63	1.37	7 (11%)
48	A86	31	314	-	47,50,50	4.17	23 (48%)	51,76,76	7.00	22 (43%)
48	A86	39	311	-	47,50,50	4.15	23 (48%)	51,76,76	6.47	19 (37%)
48	A86	39	313	-	47,50,50	4.40	26 (55%)	51,76,76	7.35	21 (41%)
48	A86	11	314	-	47,50,50	4.18	23 (48%)	51,76,76	7.00	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CLA	41	204	-	62,66,73	2.16	20 (32%)	73,104,113	2.93	35 (47%)
37	CLA	b	523	-	69,73,73	1.92	21 (30%)	82,113,113	2.65	32 (39%)
39	BCR	c	514	-	41,41,41	1.21	2 (4%)	56,56,56	1.43	10 (17%)
37	CLA	37	301	30	69,73,73	2.03	20 (28%)	82,113,113	2.59	27 (32%)
37	CLA	34	307	27	56,60,73	2.19	18 (32%)	65,97,113	2.86	33 (50%)
47	KC1	36	304	29	49,53,53	3.05	24 (48%)	61,89,89	3.90	36 (59%)
37	CLA	b	501	52	69,73,73	1.96	19 (27%)	82,113,113	2.63	29 (35%)
37	CLA	B	507	52	69,73,73	1.96	19 (27%)	82,113,113	2.61	30 (36%)
48	A86	13	314	-	47,50,50	4.41	24 (51%)	51,76,76	7.15	17 (33%)
37	CLA	a	403	-	69,73,73	1.95	20 (28%)	82,113,113	2.68	33 (40%)
47	KC1	19	308	-	49,53,53	3.01	23 (46%)	61,89,89	3.88	38 (62%)
48	A86	15	314	-	47,50,50	4.45	24 (51%)	51,76,76	6.97	18 (35%)
42	BCT	a	411	36	3,3,3	1.21	0	2,3,3	4.13	2 (100%)
37	CLA	d	404	-	69,73,73	1.94	18 (26%)	82,113,113	2.72	32 (39%)
48	A86	17	310	-	47,50,50	4.30	23 (48%)	51,76,76	7.02	17 (33%)
37	CLA	16	309	-	49,53,73	2.38	20 (40%)	58,89,113	3.18	29 (50%)
37	CLA	32	213	-	49,53,73	2.38	19 (38%)	58,89,113	3.11	28 (48%)
39	BCR	K	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.27	7 (12%)
37	CLA	39	302	-	69,73,73	1.97	21 (30%)	82,113,113	2.73	30 (36%)
37	CLA	C	502	-	69,73,73	1.91	18 (26%)	82,113,113	2.60	30 (36%)
39	BCR	a	408	-	41,41,41	1.20	3 (7%)	56,56,56	1.32	7 (12%)
37	CLA	36	306	29	69,73,73	2.00	20 (28%)	82,113,113	2.55	31 (37%)
37	CLA	35	310	-	49,53,73	2.43	20 (40%)	58,89,113	3.09	27 (46%)
39	BCR	0	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.34	7 (12%)

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
48	A86	41	214	-	-	5/34/90/90	0/3/3/3
50	DD6	16	312	-	-	12/26/80/80	0/3/3/3
37	CLA	19	306	32	1/1/15/20	7/39/115/115	-
37	CLA	c	508	-	1/1/15/20	8/39/115/115	-
47	KC1	20	302	-	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	41	213	-	-	8/34/90/90	0/3/3/3
47	KC1	17	305	30	-	6/15/71/71	-
37	CLA	C	512	-	1/1/15/20	6/39/115/115	-
37	CLA	b	511	-	1/1/15/20	11/39/115/115	-
47	KC1	38	205	31	-	6/15/71/71	-
48	A86	33	314	-	-	9/34/90/90	0/3/3/3
37	CLA	b	514	-	1/1/14/20	13/36/112/115	-
47	KC1	11	309	24	-	8/15/71/71	-
48	A86	16	311	-	-	8/34/90/90	0/3/3/3
37	CLA	17	302	30	-	12/39/115/115	-
47	KC1	12	208	25	-	4/15/71/71	-
37	CLA	41	210	-	-	6/15/91/115	-
37	CLA	41	205	34	1/1/11/20	9/15/91/115	-
37	CLA	b	504	-	1/1/15/20	5/39/115/115	-
47	KC1	38	210	31	-	8/15/71/71	-
48	A86	15	319	-	-	8/34/90/90	0/3/3/3
47	KC1	32	209	25	-	4/15/71/71	-
37	CLA	32	210	25	1/1/12/20	13/24/100/115	-
37	CLA	15	307	28	1/1/12/20	12/24/100/115	-
39	BCR	C	514	-	-	6/29/63/63	0/2/2/2
37	CLA	B	513	-	1/1/15/20	8/39/115/115	-
37	CLA	12	205	-	1/1/15/20	11/39/115/115	-
37	CLA	14	305	-	1/1/11/20	4/15/91/115	-
37	CLA	35	307	28	1/1/12/20	12/24/100/115	-
37	CLA	41	202	34	1/1/13/20	9/30/106/115	-
48	A86	34	313	-	-	12/34/90/90	0/3/3/3
37	CLA	11	301	24	-	12/39/115/115	-
37	CLA	11	308	52	1/1/15/20	13/39/115/115	-
37	CLA	37	306	30	1/1/12/20	11/24/100/115	-
41	LMG	37	316	-	-	15/32/52/70	0/1/1/1
47	KC1	17	303	-	-	6/15/71/71	-
37	CLA	14	301	27	-	14/39/115/115	-
48	A86	36	311	-	-	8/34/90/90	0/3/3/3
37	CLA	C	503	-	1/1/15/20	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	32	218	-	-	13/34/90/90	0/3/3/3
48	A86	21	211	-	-	9/34/90/90	0/3/3/3
41	LMG	d	409	-	-	13/46/66/70	0/1/1/1
37	CLA	c	513	-	1/1/15/20	9/39/115/115	-
37	CLA	c	511	3	1/1/15/20	8/39/115/115	-
37	CLA	b	503	-	1/1/15/20	11/39/115/115	-
39	BCR	b	518	-	-	6/29/63/63	0/2/2/2
44	DGD	J	101	-	-	16/51/91/95	0/2/2/2
48	A86	32	216	-	-	13/34/90/90	0/3/3/3
48	A86	18	212	-	-	8/34/90/90	0/3/3/3
37	CLA	c	512	-	1/1/15/20	6/39/115/115	-
47	KC1	18	210	31	-	8/15/71/71	-
37	CLA	B	510	52	1/1/15/20	7/39/115/115	-
48	A86	35	316	-	-	14/34/90/90	0/3/3/3
37	CLA	35	303	-	-	8/30/106/115	-
37	CLA	19	307	43	1/1/15/20	8/39/115/115	-
39	BCR	c	515	-	-	7/29/63/63	0/2/2/2
48	A86	12	217	-	-	13/34/90/90	0/3/3/3
48	A86	12	214	-	-	3/34/90/90	0/3/3/3
39	BCR	D	407	-	-	12/29/63/63	0/2/2/2
48	A86	16	313	-	-	13/34/90/90	0/3/3/3
37	CLA	17	309	52	1/1/15/20	11/39/115/115	-
40	SQD	16	315	-	-	24/49/69/69	0/1/1/1
48	A86	11	315	-	-	6/34/90/90	0/3/3/3
48	A86	41	211	-	-	9/34/90/90	0/3/3/3
37	CLA	w	101	-	1/1/15/20	17/39/115/115	-
37	CLA	14	310	-	1/1/11/20	4/15/91/115	-
48	A86	17	315	-	-	12/34/90/90	0/3/3/3
48	A86	34	315	-	-	6/34/90/90	0/3/3/3
37	CLA	36	301	29	-	11/39/115/115	-
41	LMG	32	201	-	-	14/34/54/70	0/1/1/1
37	CLA	14	302	-	1/1/15/20	18/39/115/115	-
37	CLA	34	308	52	1/1/15/20	11/39/115/115	-
44	DGD	c	516	-	-	17/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	15	312	-	-	8/34/90/90	0/3/3/3
48	A86	37	309	-	-	8/34/90/90	0/3/3/3
41	LMG	C	518	-	-	25/46/66/70	0/1/1/1
37	CLA	Z	102	33	1/1/11/20	7/15/91/115	-
37	CLA	z	101	52	1/1/15/20	20/39/115/115	-
48	A86	14	313	-	-	12/34/90/90	0/3/3/3
39	BCR	H	101	-	-	6/29/63/63	0/2/2/2
48	A86	14	316	-	-	13/34/90/90	0/3/3/3
48	A86	17	311	-	-	8/34/90/90	0/3/3/3
37	CLA	z	102	33	1/1/11/20	7/15/91/115	-
37	CLA	32	206	-	1/1/15/20	11/39/115/115	-
47	KC1	37	304	30	-	6/15/71/71	-
37	CLA	C	511	3	1/1/15/20	8/39/115/115	-
50	DD6	20	310	-	-	14/26/80/80	0/3/3/3
48	A86	33	312	-	-	8/34/90/90	0/3/3/3
37	CLA	33	310	-	-	2/15/91/115	-
48	A86	21	215	-	-	6/34/90/90	0/3/3/3
41	LMG	b	519	-	-	15/46/66/70	0/1/1/1
37	CLA	39	304	32	1/1/11/20	6/15/91/115	-
37	CLA	18	208	31	1/1/12/20	13/25/101/115	-
37	CLA	21	206	34	1/1/15/20	15/39/115/115	-
39	BCR	C	515	-	-	7/29/63/63	0/2/2/2
48	A86	12	202	-	-	14/34/90/90	0/3/3/3
40	SQD	40	202	-	-	24/49/69/69	0/1/1/1
37	CLA	c	510	-	1/1/15/20	12/39/115/115	-
50	DD6	40	212	-	-	14/26/80/80	0/3/3/3
37	CLA	31	302	24	-	12/39/115/115	-
40	SQD	b	521	-	-	11/32/52/69	0/1/1/1
46	HEM	F	101	5,6	-	8/14/54/54	-
47	KC1	15	302	-	-	6/15/71/71	-
48	A86	36	313	-	-	8/34/90/90	0/3/3/3
37	CLA	19	309	32	1/1/11/20	5/15/91/115	-
39	BCR	h	101	-	-	6/29/63/63	0/2/2/2
45	PL9	D	408	-	-	9/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	LMU	39	315	-	-	6/21/61/61	0/2/2/2
39	BCR	a	413	-	-	7/29/63/63	0/2/2/2
37	CLA	12	212	-	1/1/11/20	7/15/91/115	-
37	CLA	15	308	52	1/1/15/20	10/39/115/115	-
48	A86	17	313	-	-	8/34/90/90	0/3/3/3
37	CLA	33	307	26	1/1/12/20	12/24/100/115	-
37	CLA	35	301	28	-	10/39/115/115	-
48	A86	34	314	-	-	13/34/90/90	0/3/3/3
37	CLA	21	208	-	1/1/15/20	13/39/115/115	-
43	LHG	39	314	37	-	28/53/53/53	-
37	CLA	32	211	52	-	9/39/115/115	-
47	KC1	13	306	26	-	6/15/71/71	-
37	CLA	34	305	-	1/1/11/20	4/15/91/115	-
39	BCR	y	101	-	-	15/29/63/63	0/2/2/2
37	CLA	c	504	52	1/1/15/20	9/39/115/115	-
44	DGD	c	517	-	-	19/51/91/95	0/2/2/2
37	CLA	38	201	52	1/1/15/20	8/39/115/115	-
37	CLA	B	509	-	1/1/15/20	11/39/115/115	-
47	KC1	35	309	28	-	8/15/71/71	-
37	CLA	31	310	52	1/1/12/20	6/23/99/115	-
47	KC1	15	304	28	-	6/15/71/71	-
37	CLA	21	205	34	1/1/11/20	9/15/91/115	-
37	CLA	C	508	-	1/1/15/20	8/39/115/115	-
37	CLA	38	208	31	1/1/12/20	13/25/101/115	-
37	CLA	B	503	-	1/1/15/20	11/39/115/115	-
37	CLA	C	510	-	1/1/15/20	12/39/115/115	-
44	DGD	C	516	-	-	17/51/91/95	0/2/2/2
48	A86	12	216	-	-	9/34/90/90	0/3/3/3
43	LHG	41	201	-	-	19/38/38/53	-
37	CLA	b	510	52	1/1/15/20	7/39/115/115	-
47	KC1	35	304	28	-	6/15/71/71	-
37	CLA	13	310	-	-	2/15/91/115	-
48	A86	19	311	-	-	6/34/90/90	0/3/3/3
48	A86	37	319	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	c	503	-	1/1/15/20	21/39/115/115	-
37	CLA	C	507	52	1/1/15/20	8/39/115/115	-
43	LHG	19	314	37	-	28/53/53/53	-
48	A86	32	214	-	-	5/34/90/90	0/3/3/3
37	CLA	B	524	-	1/1/15/20	13/39/115/115	-
39	BCR	B	517	-	-	6/29/63/63	0/2/2/2
37	CLA	37	303	-	1/1/13/20	8/29/105/115	-
37	CLA	b	509	-	1/1/15/20	11/39/115/115	-
37	CLA	34	301	27	-	14/39/115/115	-
47	KC1	32	207	25	-	6/15/71/71	-
48	A86	34	312	-	-	4/34/90/90	0/3/3/3
48	A86	18	214	-	-	12/34/90/90	0/3/3/3
38	PHO	A	404	-	-	6/37/103/103	0/5/6/6
37	CLA	Z	101	52	1/1/15/20	20/39/115/115	-
37	CLA	40	210	-	1/1/11/20	4/18/94/115	-
47	KC1	41	203	-	-	4/15/71/71	-
37	CLA	41	209	34	1/1/11/20	6/15/91/115	-
43	LHG	37	315	-	-	26/48/48/53	-
39	BCR	b	524	-	-	17/29/63/63	0/2/2/2
43	LHG	D	410	-	-	26/53/53/53	-
41	LMG	L	102	-	-	15/35/55/70	0/1/1/1
40	SQD	B	519	-	-	26/49/69/69	0/1/1/1
37	CLA	C	504	52	1/1/15/20	9/39/115/115	-
37	CLA	14	303	-	-	6/30/106/115	-
48	A86	15	315	-	-	8/34/90/90	0/3/3/3
43	LHG	D	411	-	-	26/50/50/53	-
48	A86	19	313	-	-	8/34/90/90	0/3/3/3
40	SQD	a	409	-	-	17/49/69/69	0/1/1/1
37	CLA	34	303	-	-	6/30/106/115	-
37	CLA	12	203	25	1/1/15/20	14/39/115/115	-
37	CLA	c	506	-	1/1/15/20	13/39/115/115	-
37	CLA	12	204	-	1/1/15/20	9/39/115/115	-
37	CLA	13	303	-	1/1/13/20	11/30/106/115	-
37	CLA	16	307	52	1/1/14/20	13/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	B	511	-	1/1/15/20	11/39/115/115	-
38	PHO	D	403	-	-	9/37/103/103	0/5/6/6
50	DD6	20	312	-	-	12/26/80/80	0/3/3/3
37	CLA	32	208	52	1/1/12/20	2/21/97/115	-
37	CLA	d	403	-	1/1/15/20	8/39/115/115	-
48	A86	15	311	-	-	6/34/90/90	0/3/3/3
37	CLA	19	305	32	1/1/12/20	7/23/99/115	-
48	A86	15	316	-	-	14/34/90/90	0/3/3/3
37	CLA	C	501	-	1/1/15/20	12/39/115/115	-
47	KC1	11	306	24	-	8/15/71/71	-
48	A86	21	214	-	-	5/34/90/90	0/3/3/3
37	CLA	D	405	-	1/1/15/20	8/39/115/115	-
48	A86	21	213	-	-	8/34/90/90	0/3/3/3
37	CLA	18	202	31	-	14/39/115/115	-
51	LMU	19	315	-	-	6/21/61/61	0/2/2/2
37	CLA	14	307	27	1/1/12/20	15/24/100/115	-
37	CLA	d	401	52	-	14/39/115/115	-
48	A86	11	312	-	-	6/34/90/90	0/3/3/3
47	KC1	13	304	26	-	7/15/71/71	-
37	CLA	20	308	-	1/1/11/20	4/18/94/115	-
37	CLA	11	305	52	1/1/11/20	3/15/91/115	-
37	CLA	33	308	52	-	8/39/115/115	-
39	BCR	B	525	-	-	18/29/63/63	0/2/2/2
48	A86	36	310	-	-	5/34/90/90	0/3/3/3
48	A86	17	312	-	-	8/34/90/90	0/3/3/3
48	A86	11	313	-	-	6/34/90/90	1/3/3/3
37	CLA	b	515	-	1/1/15/20	5/39/115/115	-
37	CLA	b	505	-	1/1/15/20	6/39/115/115	-
37	CLA	15	303	-	-	7/30/106/115	-
48	A86	34	316	-	-	13/34/90/90	0/3/3/3
37	CLA	35	305	-	1/1/11/20	5/15/91/115	-
37	CLA	19	301	32	1/1/15/20	10/39/115/115	-
41	LMG	36	314	-	-	14/31/51/70	0/1/1/1
37	CLA	C	506	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	C	509	-	1/1/15/20	7/39/115/115	-
50	DD6	21	212	-	-	12/26/80/80	0/3/3/3
37	CLA	39	310	32	1/1/15/20	9/39/115/115	-
37	CLA	36	309	-	1/1/11/20	6/15/91/115	-
47	KC1	12	211	25	-	6/15/71/71	-
48	A86	13	311	-	-	5/34/90/90	0/3/3/3
41	LMG	11	316	-	-	19/37/57/70	0/1/1/1
37	CLA	20	303	-	1/1/13/20	10/29/105/115	-
41	LMG	31	316	-	-	19/37/57/70	0/1/1/1
46	HEM	v	201	16	-	6/14/54/54	-
48	A86	37	310	-	-	8/34/90/90	0/3/3/3
37	CLA	21	202	34	1/1/13/20	9/30/106/115	-
47	KC1	33	302	-	-	5/15/71/71	-
47	KC1	35	306	28	-	6/15/71/71	-
37	CLA	B	501	52	1/1/15/20	18/39/115/115	-
37	CLA	32	204	25	1/1/15/20	14/39/115/115	-
37	CLA	37	308	52	1/1/15/20	11/39/115/115	-
43	LHG	b	522	-	-	18/53/53/53	-
37	CLA	19	303	52	1/1/15/20	14/39/115/115	-
47	KC1	36	305	29	-	6/15/71/71	-
37	CLA	31	308	24	-	8/24/100/115	-
48	A86	12	213	-	-	5/34/90/90	0/3/3/3
37	CLA	17	307	30	1/1/12/20	11/24/100/115	-
37	CLA	B	512	-	1/1/15/20	8/39/115/115	-
37	CLA	c	502	-	1/1/15/20	9/39/115/115	-
37	CLA	34	310	-	1/1/11/20	4/15/91/115	-
50	DD6	41	212	-	-	12/26/80/80	0/3/3/3
37	CLA	40	209	33	1/1/11/20	8/15/91/115	-
43	LHG	B	523	-	-	18/53/53/53	-
47	KC1	40	204	-	-	7/15/71/71	-
37	CLA	20	306	33	1/1/12/20	5/21/97/115	-
41	LMG	11	317	-	-	13/27/47/70	0/1/1/1
37	CLA	16	306	29	1/1/15/20	13/39/115/115	-
48	A86	13	313	-	-	18/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	DD6	40	214	-	-	12/26/80/80	0/3/3/3
43	LHG	21	217	-	-	27/49/49/53	-
37	CLA	19	302	-	1/1/15/20	11/39/115/115	-
37	CLA	c	509	-	1/1/15/20	7/39/115/115	-
47	KC1	37	305	30	-	9/15/71/71	-
37	CLA	31	306	52	1/1/11/20	3/15/91/115	-
47	KC1	34	309	27	-	6/15/71/71	-
39	BCR	c	519	-	-	6/29/63/63	0/2/2/2
47	KC1	13	309	26	-	4/15/71/71	-
37	CLA	b	506	-	1/1/15/20	7/39/115/115	-
46	HEM	f	101	5,6	-	8/14/54/54	-
48	A86	35	311	-	-	6/34/90/90	0/3/3/3
48	A86	35	313	-	-	9/34/90/90	0/3/3/3
37	CLA	B	514	-	1/1/14/20	13/36/112/115	-
37	CLA	11	307	24	-	8/24/100/115	-
47	KC1	31	307	24	-	8/15/71/71	-
37	CLA	40	205	-	1/1/13/20	10/29/105/115	-
48	A86	37	313	-	-	9/34/90/90	0/3/3/3
48	A86	41	215	-	-	6/34/90/90	0/3/3/3
37	CLA	b	508	-	-	5/39/115/115	-
47	KC1	15	309	28	-	8/15/71/71	-
37	CLA	34	302	-	1/1/15/20	18/39/115/115	-
47	KC1	41	207	34	-	7/15/71/71	-
47	KC1	14	304	27	-	6/15/71/71	-
37	CLA	32	205	-	1/1/15/20	9/39/115/115	-
47	KC1	31	303	-	-	2/15/71/71	-
39	BCR	5	101	-	-	8/29/63/63	0/2/2/2
37	CLA	38	206	-	-	6/15/91/115	-
37	CLA	13	307	26	1/1/12/20	12/24/100/115	-
47	KC1	13	302	-	-	5/15/71/71	-
41	LMG	16	316	-	-	14/31/51/70	0/1/1/1
47	KC1	35	302	-	-	6/15/71/71	-
37	CLA	19	304	32	1/1/11/20	6/15/91/115	-
43	LHG	21	201	-	-	19/38/38/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	14	308	52	1/1/15/20	11/39/115/115	-
48	A86	31	311	-	-	6/34/90/90	0/3/3/3
41	LMG	12	201	-	-	14/34/54/70	0/1/1/1
37	CLA	39	303	52	1/1/15/20	14/39/115/115	-
48	A86	32	221	-	-	9/34/90/90	0/3/3/3
37	CLA	13	308	52	-	8/39/115/115	-
48	A86	40	213	-	-	16/34/90/90	0/3/3/3
37	CLA	32	202	52	1/1/15/20	13/39/115/115	-
47	KC1	33	309	26	-	4/15/71/71	-
37	CLA	38	209	52	1/1/15/20	9/39/115/115	-
47	KC1	36	302	-	-	2/15/71/71	-
41	LMG	17	317	-	-	15/32/52/70	0/1/1/1
37	CLA	33	303	-	1/1/13/20	12/30/106/115	-
45	PL9	D	404	-	-	17/53/73/73	0/1/1/1
37	CLA	C	513	-	1/1/15/20	9/39/115/115	-
37	CLA	40	203	33	-	13/29/105/115	-
41	LMG	l	101	-	-	15/35/55/70	0/1/1/1
48	A86	11	319	-	-	7/34/90/90	0/3/3/3
48	A86	37	311	-	-	7/34/90/90	0/3/3/3
48	A86	18	213	-	-	9/34/90/90	0/3/3/3
37	CLA	W	101	-	1/1/15/20	17/39/115/115	-
40	SQD	17	301	-	-	24/44/64/69	0/1/1/1
37	CLA	18	211	-	-	4/15/91/115	-
37	CLA	31	301	-	1/1/15/20	21/39/115/115	-
37	CLA	b	502	-	1/1/15/20	10/39/115/115	-
47	KC1	33	306	26	-	6/15/71/71	-
37	CLA	W	102	-	1/1/15/20	21/39/115/115	-
43	LHG	37	321	-	-	27/49/49/53	-
48	A86	20	309	-	-	5/34/90/90	0/3/3/3
37	CLA	18	204	-	1/1/13/20	10/29/105/115	-
48	A86	38	215	-	-	13/34/90/90	0/3/3/3
37	CLA	B	505	-	1/1/15/20	6/39/115/115	-
47	KC1	31	309	24	-	8/15/71/71	-
47	KC1	40	206	33	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	DGD	h	102	-	-	16/51/91/95	0/2/2/2
37	CLA	12	210	52	-	9/39/115/115	-
37	CLA	41	206	34	1/1/15/20	15/39/115/115	-
37	CLA	31	304	-	1/1/15/20	10/39/115/115	-
37	CLA	21	209	34	1/1/11/20	6/15/91/115	-
48	A86	14	315	-	-	6/34/90/90	0/3/3/3
48	A86	31	319	-	-	7/34/90/90	0/3/3/3
37	CLA	38	204	-	1/1/13/20	8/29/105/115	-
37	CLA	39	306	32	-	8/39/115/115	-
43	LHG	a	412	-	-	26/50/50/53	-
37	CLA	c	505	-	1/1/15/20	10/39/115/115	-
37	CLA	B	508	-	-	5/39/115/115	-
48	A86	17	314	-	-	8/34/90/90	0/3/3/3
48	A86	13	315	-	-	11/34/90/90	0/3/3/3
43	LHG	d	407	-	-	27/53/53/53	-
37	CLA	B	504	-	1/1/15/20	5/39/115/115	-
48	A86	14	311	-	-	7/34/90/90	0/3/3/3
37	CLA	12	209	25	1/1/12/20	13/24/100/115	-
48	A86	35	315	-	-	8/34/90/90	0/3/3/3
37	CLA	15	310	-	1/1/11/20	4/15/91/115	-
37	CLA	20	307	33	1/1/11/20	8/15/91/115	-
37	CLA	16	303	-	1/1/13/20	10/30/106/115	-
48	A86	40	201	-	-	13/34/90/90	0/3/3/3
37	CLA	A	405	-	-	8/39/115/115	-
40	SQD	L	101	-	-	26/49/69/69	0/1/1/1
41	LMG	a	410	-	-	32/46/66/70	0/1/1/1
47	KC1	14	306	27	-	6/15/71/71	-
47	KC1	16	308	29	-	4/15/71/71	-
37	CLA	16	301	29	-	11/39/115/115	-
37	CLA	36	307	52	1/1/14/20	13/35/111/115	-
41	LMG	c	518	-	-	25/46/66/70	0/1/1/1
45	PL9	d	406	-	-	9/53/73/73	0/1/1/1
48	A86	31	313	-	-	6/34/90/90	1/3/3/3
48	A86	13	312	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	A86	35	319	-	-	8/34/90/90	0/3/3/3
37	CLA	B	506	-	1/1/15/20	7/39/115/115	-
37	CLA	21	204	-	-	12/31/107/115	-
47	KC1	11	302	-	-	2/15/71/71	-
48	A86	35	314	-	-	14/34/90/90	0/3/3/3
37	CLA	c	507	52	1/1/15/20	8/39/115/115	-
47	KC1	40	207	33	-	12/15/71/71	-
37	CLA	18	209	52	1/1/15/20	10/39/115/115	-
37	CLA	13	305	-	1/1/11/20	4/15/91/115	-
48	A86	12	220	-	-	9/34/90/90	0/3/3/3
37	CLA	15	305	-	1/1/11/20	5/15/91/115	-
48	A86	37	314	-	-	12/34/90/90	0/3/3/3
38	PHO	a	405	-	-	9/37/103/103	0/5/6/6
47	KC1	37	302	-	-	6/15/71/71	-
43	LHG	D	409	-	-	27/53/53/53	-
50	DD6	21	216	-	-	15/26/80/80	0/3/3/3
37	CLA	20	301	33	-	13/29/105/115	-
37	CLA	39	309	32	1/1/11/20	5/15/91/115	-
39	BCR	b	517	-	-	6/29/63/63	0/2/2/2
50	DD6	36	312	-	-	12/26/80/80	0/3/3/3
38	PHO	a	406	-	-	6/37/103/103	0/5/6/6
37	CLA	11	310	52	1/1/12/20	6/23/99/115	-
47	KC1	17	306	30	-	8/15/71/71	-
41	LMG	31	317	-	-	13/27/47/70	0/1/1/1
48	A86	20	311	-	-	16/34/90/90	0/3/3/3
48	A86	38	212	-	-	8/34/90/90	0/3/3/3
43	LHG	17	316	-	-	26/48/48/53	-
37	CLA	19	310	32	1/1/15/20	9/39/115/115	-
48	A86	35	312	-	-	8/34/90/90	0/3/3/3
47	KC1	15	306	28	-	6/15/71/71	-
40	SQD	A	407	-	-	17/49/69/69	0/1/1/1
48	A86	40	211	-	-	5/34/90/90	0/3/3/3
39	BCR	A	410	-	-	7/29/63/63	0/2/2/2
50	DD6	39	312	-	-	12/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	17	304	-	1/1/13/20	8/29/105/115	-
37	CLA	38	202	31	-	14/39/115/115	-
44	DGD	C	517	-	-	19/51/91/95	0/2/2/2
48	A86	18	215	-	-	13/34/90/90	0/3/3/3
37	CLA	12	207	52	1/1/12/20	2/21/97/115	-
45	PL9	d	402	-	-	17/53/73/73	0/1/1/1
44	DGD	j	101	-	-	16/51/91/95	0/2/2/2
47	KC1	18	207	31	-	6/15/71/71	-
48	A86	38	214	-	-	12/34/90/90	0/3/3/3
37	CLA	c	501	-	1/1/15/20	12/39/115/115	-
47	KC1	32	212	25	-	6/15/71/71	-
48	A86	37	312	-	-	7/34/90/90	0/3/3/3
37	CLA	15	301	28	-	10/39/115/115	-
48	A86	38	213	-	-	9/34/90/90	0/3/3/3
47	KC1	16	302	-	-	2/15/71/71	-
37	CLA	21	210	-	-	6/15/91/115	-
37	CLA	b	507	52	1/1/15/20	9/39/115/115	-
37	CLA	a	407	-	-	8/39/115/115	-
47	KC1	37	307	30	-	4/15/71/71	-
37	CLA	A	403	-	1/1/15/20	4/39/115/115	-
48	A86	32	217	-	-	9/34/90/90	0/3/3/3
48	A86	15	313	-	-	9/34/90/90	0/3/3/3
37	CLA	D	401	52	1/1/15/20	6/39/115/115	-
47	KC1	14	309	27	-	6/15/71/71	-
37	CLA	41	208	-	1/1/15/20	13/39/115/115	-
46	HEM	V	201	16	-	6/14/54/54	-
39	BCR	A	406	-	-	8/29/63/63	0/2/2/2
47	KC1	33	304	26	-	7/15/71/71	-
48	A86	14	314	-	-	13/34/90/90	0/3/3/3
47	KC1	34	304	27	-	6/15/71/71	-
48	A86	33	315	-	-	11/34/90/90	0/3/3/3
37	CLA	B	502	-	1/1/15/20	10/39/115/115	-
37	CLA	b	512	-	1/1/15/20	8/39/115/115	-
37	CLA	36	303	-	1/1/13/20	10/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LMG	b	520	-	-	24/46/66/70	0/1/1/1
48	A86	32	203	-	-	14/34/90/90	0/3/3/3
37	CLA	a	404	52	1/1/15/20	6/39/115/115	-
37	CLA	11	303	-	1/1/15/20	10/39/115/115	-
47	KC1	21	207	34	-	7/15/71/71	-
47	KC1	36	308	29	-	4/15/71/71	-
47	KC1	21	203	-	-	4/15/71/71	-
41	LMG	B	521	-	-	24/46/66/70	0/1/1/1
47	KC1	12	206	25	-	6/15/71/71	-
40	SQD	36	315	-	-	24/44/64/69	0/1/1/1
48	A86	33	311	-	-	5/34/90/90	0/3/3/3
48	A86	33	313	-	-	18/34/90/90	0/3/3/3
48	A86	34	311	-	-	7/34/90/90	0/3/3/3
47	KC1	16	304	29	-	6/15/71/71	-
47	KC1	18	205	31	-	6/15/71/71	-
48	A86	16	310	-	-	5/34/90/90	0/3/3/3
47	KC1	34	306	27	-	6/15/71/71	-
37	CLA	39	305	32	1/1/12/20	7/23/99/115	-
37	CLA	39	307	43	1/1/15/20	8/39/115/115	-
47	KC1	17	308	30	-	4/15/71/71	-
37	CLA	38	211	-	-	4/15/91/115	-
47	KC1	11	304	24	-	4/15/71/71	-
37	CLA	B	515	-	1/1/15/20	5/39/115/115	-
37	CLA	39	301	32	1/1/15/20	10/39/115/115	-
50	DD6	41	216	-	-	15/26/80/80	0/3/3/3
37	CLA	b	513	-	1/1/15/20	8/39/115/115	-
47	KC1	20	305	33	-	12/15/71/71	-
37	CLA	38	203	-	1/1/15/20	8/39/115/115	-
37	CLA	C	505	-	1/1/15/20	10/39/115/115	-
37	CLA	B	516	-	1/1/15/20	13/39/115/115	-
44	DGD	H	102	-	-	16/51/91/95	0/2/2/2
48	A86	17	320	-	-	8/34/90/90	0/3/3/3
37	CLA	18	206	-	1/1/11/20	5/15/91/115	-
37	CLA	D	406	-	1/1/15/20	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	KC1	16	305	29	-	6/15/71/71	-
50	DD6	19	312	-	-	12/26/80/80	0/3/3/3
39	BCR	B	518	-	-	6/29/63/63	0/2/2/2
48	A86	31	315	-	-	6/34/90/90	0/3/3/3
47	KC1	31	305	24	-	4/15/71/71	-
48	A86	14	312	-	-	4/34/90/90	0/3/3/3
37	CLA	18	203	-	1/1/15/20	8/39/115/115	-
37	CLA	33	301	26	-	14/39/115/115	-
39	BCR	d	405	-	-	12/29/63/63	0/2/2/2
37	CLA	D	402	52	-	14/39/115/115	-
48	A86	11	311	-	-	6/34/90/90	0/3/3/3
47	KC1	20	304	33	-	6/15/71/71	-
48	A86	12	215	-	-	13/34/90/90	0/3/3/3
40	SQD	B	522	-	-	11/32/52/69	0/1/1/1
37	CLA	13	301	26	-	14/39/115/115	-
37	CLA	35	308	52	-	10/39/115/115	-
37	CLA	40	208	33	1/1/12/20	5/21/97/115	-
37	CLA	18	201	52	1/1/15/20	7/39/115/115	-
37	CLA	b	516	-	1/1/15/20	13/39/115/115	-
41	LMG	B	520	-	-	15/46/66/70	0/1/1/1
47	KC1	39	308	-	-	4/15/71/71	-
47	KC1	38	207	31	-	5/15/71/71	-
37	CLA	33	305	-	1/1/11/20	4/15/91/115	-
48	A86	31	312	-	-	6/34/90/90	0/3/3/3
48	A86	32	215	-	-	3/34/90/90	0/3/3/3
48	A86	16	314	-	-	8/34/90/90	0/3/3/3
43	LHG	d	408	-	-	26/53/53/53	-
41	LMG	D	412	-	-	13/46/66/70	0/1/1/1
39	BCR	C	519	-	-	6/29/63/63	0/2/2/2
41	LMG	A	408	-	-	32/46/66/70	0/1/1/1
48	A86	31	314	-	-	9/34/90/90	0/3/3/3
48	A86	39	311	-	-	6/34/90/90	0/3/3/3
48	A86	39	313	-	-	7/34/90/90	0/3/3/3
48	A86	11	314	-	-	9/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CLA	41	204	-	-	12/31/107/115	-
37	CLA	b	523	-	1/1/15/20	13/39/115/115	-
39	BCR	c	514	-	-	6/29/63/63	0/2/2/2
37	CLA	37	301	30	-	12/39/115/115	-
37	CLA	34	307	27	1/1/12/20	15/24/100/115	-
47	KC1	36	304	29	-	6/15/71/71	-
37	CLA	b	501	52	1/1/15/20	17/39/115/115	-
37	CLA	B	507	52	1/1/15/20	9/39/115/115	-
48	A86	13	314	-	-	9/34/90/90	0/3/3/3
37	CLA	a	403	-	1/1/15/20	4/39/115/115	-
47	KC1	19	308	-	-	4/15/71/71	-
48	A86	15	314	-	-	14/34/90/90	0/3/3/3
37	CLA	d	404	-	1/1/15/20	19/39/115/115	-
48	A86	17	310	-	-	8/34/90/90	0/3/3/3
37	CLA	16	309	-	1/1/11/20	6/15/91/115	-
37	CLA	32	213	-	1/1/11/20	7/15/91/115	-
39	BCR	K	101	-	-	15/29/63/63	0/2/2/2
37	CLA	39	302	-	1/1/15/20	11/39/115/115	-
37	CLA	C	502	-	1/1/15/20	9/39/115/115	-
39	BCR	a	408	-	-	8/29/63/63	0/2/2/2
37	CLA	36	306	29	1/1/15/20	13/39/115/115	-
37	CLA	35	310	-	1/1/11/20	4/15/91/115	-
39	BCR	0	101	-	-	8/29/63/63	0/2/2/2

The worst 5 of 8997 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 12213 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 5098 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	B	503	CLA	C2B-C3B-CAB-CBB
37	B	503	CLA	C4B-C3B-CAB-CBB
37	B	504	CLA	C2B-C3B-CAB-CBB
37	B	504	CLA	C4B-C3B-CAB-CBB
37	B	514	CLA	CAD-CBD-CGD-O1D

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

281 monomers are involved in 580 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	19	306	CLA	1	0
37	c	508	CLA	1	0
47	20	302	KC1	1	0
37	C	512	CLA	4	0
37	b	511	CLA	1	0
47	38	205	KC1	2	0
37	b	514	CLA	3	0
37	17	302	CLA	3	0
37	b	504	CLA	5	0
37	32	210	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	15	307	CLA	1	0
39	C	514	BCR	2	0
37	B	513	CLA	2	0
37	12	205	CLA	3	0
37	35	307	CLA	1	0
37	41	202	CLA	2	0
37	11	301	CLA	1	0
37	11	308	CLA	5	0
37	37	306	CLA	1	0
47	17	303	KC1	2	0
37	14	301	CLA	2	0
37	C	503	CLA	3	0
41	d	409	LMG	2	0
37	c	513	CLA	2	0
37	c	511	CLA	5	0
37	b	503	CLA	3	0
39	b	518	BCR	2	0
44	J	101	DGD	1	0
48	18	212	A86	1	0
37	c	512	CLA	3	0
37	19	307	CLA	2	0
39	c	515	BCR	2	0
39	D	407	BCR	4	0
37	17	309	CLA	4	0
40	16	315	SQD	1	0
37	w	101	CLA	1	0
48	34	315	A86	1	0
37	36	301	CLA	4	0
37	14	302	CLA	3	0
37	34	308	CLA	1	0
44	c	516	DGD	4	0
41	C	518	LMG	1	0
37	Z	102	CLA	2	0
37	z	101	CLA	2	0
39	H	101	BCR	2	0
37	z	102	CLA	1	0
37	32	206	CLA	3	0
37	C	511	CLA	4	0
37	33	310	CLA	1	0
41	b	519	LMG	4	0
37	18	208	CLA	4	0
37	21	206	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	C	515	BCR	2	0
40	40	202	SQD	2	0
37	c	510	CLA	4	0
37	31	302	CLA	1	0
40	b	521	SQD	1	0
46	F	101	HEM	2	0
39	h	101	BCR	1	0
45	D	408	PL9	1	0
37	12	212	CLA	1	0
37	15	308	CLA	2	0
37	33	307	CLA	1	0
42	A	409	BCT	1	0
37	35	301	CLA	4	0
48	34	314	A86	1	0
37	21	208	CLA	1	0
43	39	314	LHG	8	0
37	32	211	CLA	2	0
39	y	101	BCR	4	0
37	c	504	CLA	3	0
37	38	201	CLA	4	0
37	B	509	CLA	2	0
37	C	508	CLA	2	0
37	38	208	CLA	3	0
37	B	503	CLA	2	0
37	C	510	CLA	4	0
44	C	516	DGD	4	0
37	13	310	CLA	2	0
37	c	503	CLA	4	0
43	19	314	LHG	10	0
37	B	524	CLA	3	0
39	B	517	BCR	3	0
37	b	509	CLA	2	0
37	34	301	CLA	2	0
38	A	404	PHO	2	0
37	Z	101	CLA	3	0
37	41	209	CLA	1	0
43	37	315	LHG	1	0
39	b	524	BCR	2	0
43	D	410	LHG	2	0
41	L	102	LMG	2	0
40	B	519	SQD	3	0
37	C	504	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	14	303	CLA	1	0
43	D	411	LHG	3	0
37	34	303	CLA	1	0
37	12	203	CLA	2	0
37	c	506	CLA	2	0
37	12	204	CLA	2	0
37	16	307	CLA	3	0
37	B	511	CLA	1	0
38	D	403	PHO	1	0
50	20	312	DD6	1	0
37	d	403	CLA	4	0
48	15	311	A86	1	0
37	19	305	CLA	2	0
37	C	501	CLA	3	0
47	11	306	KC1	4	0
37	D	405	CLA	4	0
37	18	202	CLA	2	0
37	14	307	CLA	1	0
37	33	308	CLA	4	0
39	B	525	BCR	2	0
48	11	313	A86	9	0
37	b	515	CLA	1	0
37	b	505	CLA	3	0
37	15	303	CLA	1	0
37	19	301	CLA	1	0
37	C	506	CLA	2	0
37	C	509	CLA	1	0
37	39	310	CLA	5	0
37	36	309	CLA	1	0
48	13	311	A86	1	0
46	v	201	HEM	2	0
37	21	202	CLA	2	0
47	33	302	KC1	1	0
37	B	501	CLA	1	0
37	32	204	CLA	3	0
37	37	308	CLA	1	0
37	19	303	CLA	1	0
37	31	308	CLA	3	0
37	17	307	CLA	1	0
37	B	512	CLA	3	0
37	c	502	CLA	5	0
47	40	204	KC1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	20	306	CLA	1	0
50	40	214	DD6	1	0
43	21	217	LHG	3	0
37	19	302	CLA	3	0
37	c	509	CLA	1	0
37	b	506	CLA	3	0
46	f	101	HEM	2	0
48	35	311	A86	1	0
37	B	514	CLA	3	0
37	11	307	CLA	4	0
37	40	205	CLA	1	0
37	b	508	CLA	1	0
37	34	302	CLA	3	0
37	32	205	CLA	2	0
39	5	101	BCR	3	0
37	13	307	CLA	1	0
41	16	316	LMG	1	0
37	19	304	CLA	2	0
37	14	308	CLA	1	0
48	31	311	A86	2	0
37	39	303	CLA	1	0
37	13	308	CLA	4	0
37	32	202	CLA	4	0
45	D	404	PL9	4	0
37	C	513	CLA	2	0
37	40	203	CLA	1	0
41	l	101	LMG	1	0
48	11	319	A86	1	0
37	W	101	CLA	3	0
40	17	301	SQD	3	0
37	18	211	CLA	1	0
37	31	301	CLA	2	0
37	b	502	CLA	7	0
37	W	102	CLA	2	0
43	37	321	LHG	3	0
37	B	505	CLA	2	0
47	31	309	KC1	1	0
47	40	206	KC1	1	0
44	h	102	DGD	3	0
37	12	210	CLA	2	0
37	41	206	CLA	2	0
37	31	304	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	21	209	CLA	1	0
48	14	315	A86	1	0
48	31	319	A86	1	0
37	39	306	CLA	1	0
43	a	412	LHG	3	0
37	B	508	CLA	2	0
37	c	505	CLA	2	0
43	d	407	LHG	1	0
37	B	504	CLA	5	0
48	14	311	A86	1	0
37	A	405	CLA	6	0
40	L	101	SQD	3	0
41	a	410	LMG	4	0
37	16	301	CLA	4	0
37	36	307	CLA	4	0
41	c	518	LMG	3	0
45	d	406	PL9	3	0
48	31	313	A86	11	0
37	B	506	CLA	3	0
37	18	209	CLA	1	0
38	a	405	PHO	2	0
47	37	302	KC1	2	0
43	D	409	LHG	1	0
37	20	301	CLA	1	0
39	b	517	BCR	4	0
38	a	406	PHO	1	0
48	38	212	A86	1	0
43	17	316	LHG	1	0
37	19	310	CLA	5	0
40	A	407	SQD	1	0
39	A	410	BCR	2	0
50	39	312	DD6	2	0
37	12	207	CLA	1	0
45	d	402	PL9	2	0
44	j	101	DGD	2	0
37	c	501	CLA	4	0
37	15	301	CLA	5	0
37	b	507	CLA	2	0
37	a	407	CLA	6	0
37	A	403	CLA	4	0
37	D	401	CLA	2	0
37	41	208	CLA	1	0

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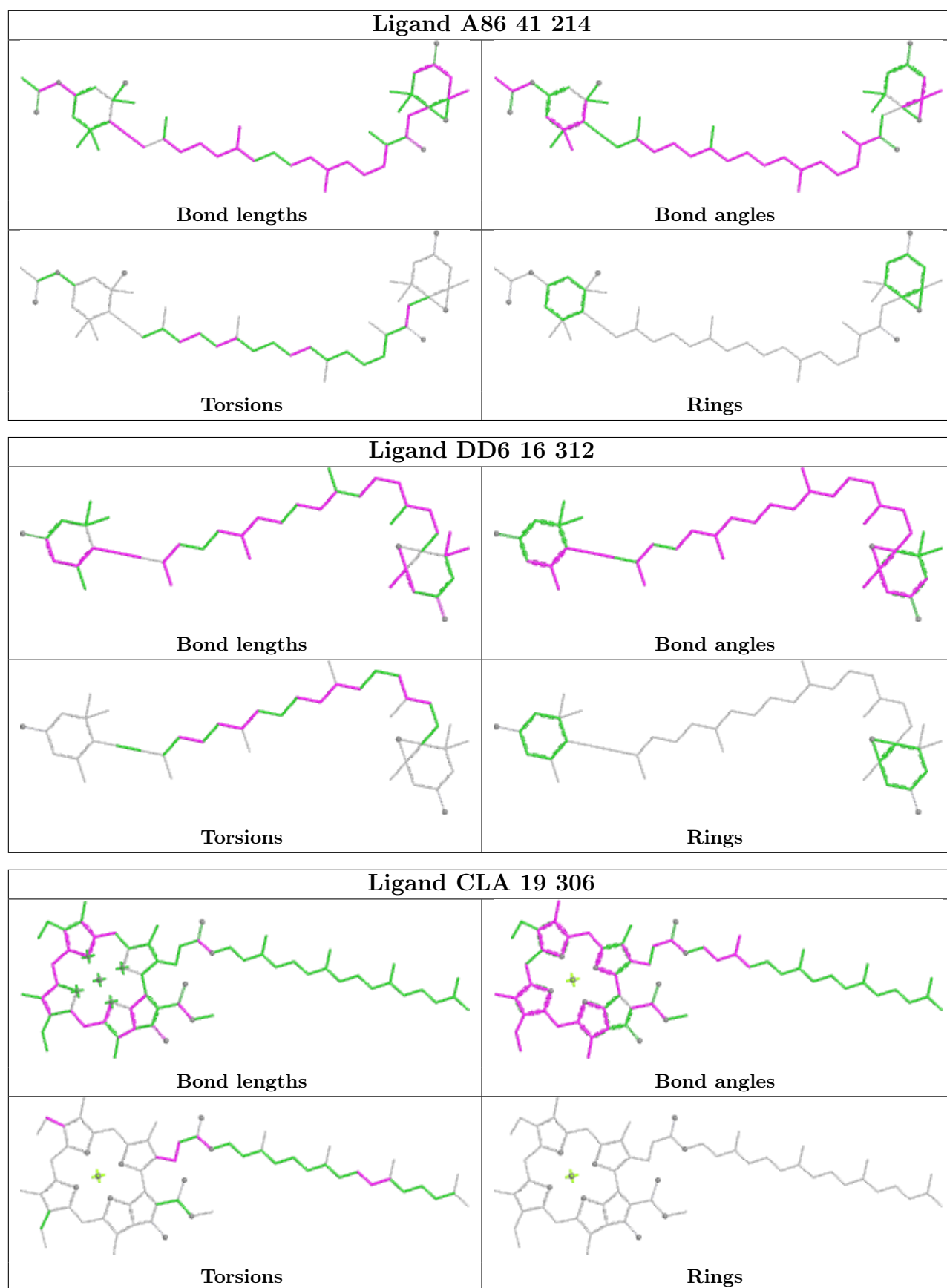
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	V	201	HEM	2	0
39	A	406	BCR	4	0
48	14	314	A86	1	0
37	B	502	CLA	4	0
37	b	512	CLA	3	0
41	b	520	LMG	4	0
37	a	404	CLA	2	0
37	11	303	CLA	1	0
41	B	521	LMG	4	0
40	36	315	SQD	3	0
48	33	311	A86	1	0
48	34	311	A86	1	0
47	16	304	KC1	1	0
47	18	205	KC1	1	0
37	39	305	CLA	2	0
37	39	307	CLA	3	0
37	38	211	CLA	1	0
37	B	515	CLA	1	0
37	39	301	CLA	2	0
37	b	513	CLA	2	0
37	38	203	CLA	2	0
37	C	505	CLA	1	0
37	B	516	CLA	2	0
44	H	102	DGD	2	0
37	D	406	CLA	2	0
50	19	312	DD6	2	0
39	B	518	BCR	2	0
37	18	203	CLA	3	0
39	d	405	BCR	3	0
48	11	311	A86	1	0
47	20	304	KC1	1	0
40	B	522	SQD	2	0
37	35	308	CLA	6	0
37	40	208	CLA	1	0
37	18	201	CLA	6	0
37	b	516	CLA	1	0
41	B	520	LMG	3	0
43	d	408	LHG	2	0
41	D	412	LMG	2	0
39	C	519	BCR	1	0
41	A	408	LMG	4	0
48	39	313	A86	1	0

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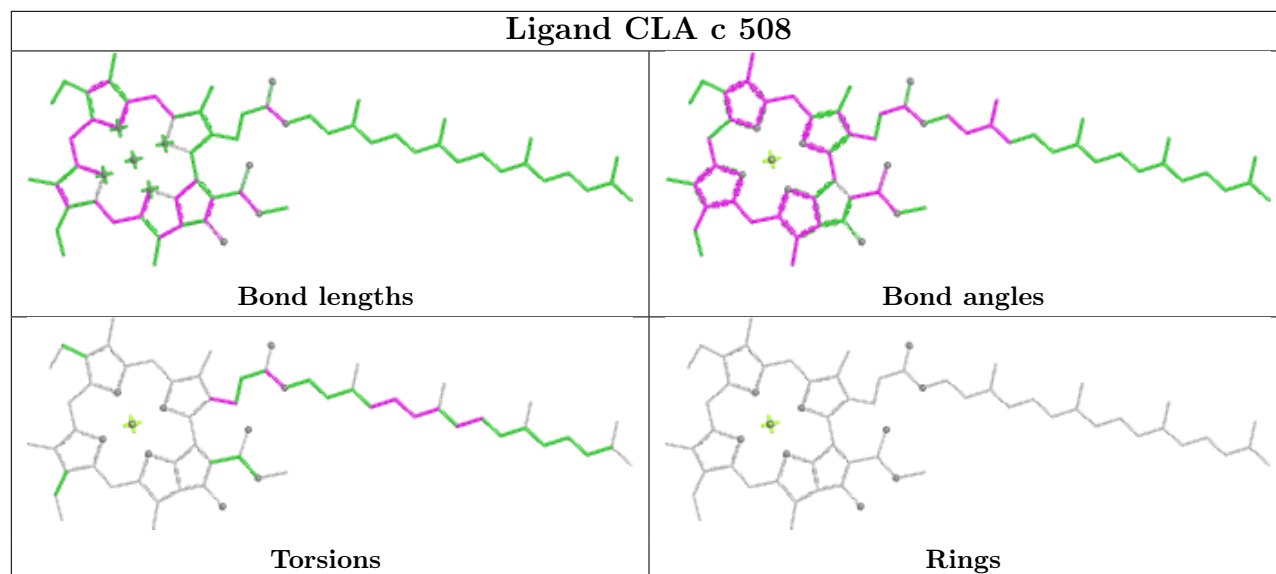
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	b	523	CLA	4	0
39	c	514	BCR	2	0
37	37	301	CLA	2	0
37	34	307	CLA	1	0
47	36	304	KC1	1	0
37	b	501	CLA	3	0
37	B	507	CLA	2	0
37	a	403	CLA	6	0
42	a	411	BCT	1	0
37	d	404	CLA	1	0
37	16	309	CLA	1	0
37	32	213	CLA	1	0
39	K	101	BCR	4	0
37	39	302	CLA	3	0
37	C	502	CLA	4	0
39	a	408	BCR	5	0
37	36	306	CLA	2	0
37	35	310	CLA	1	0
39	0	101	BCR	5	0

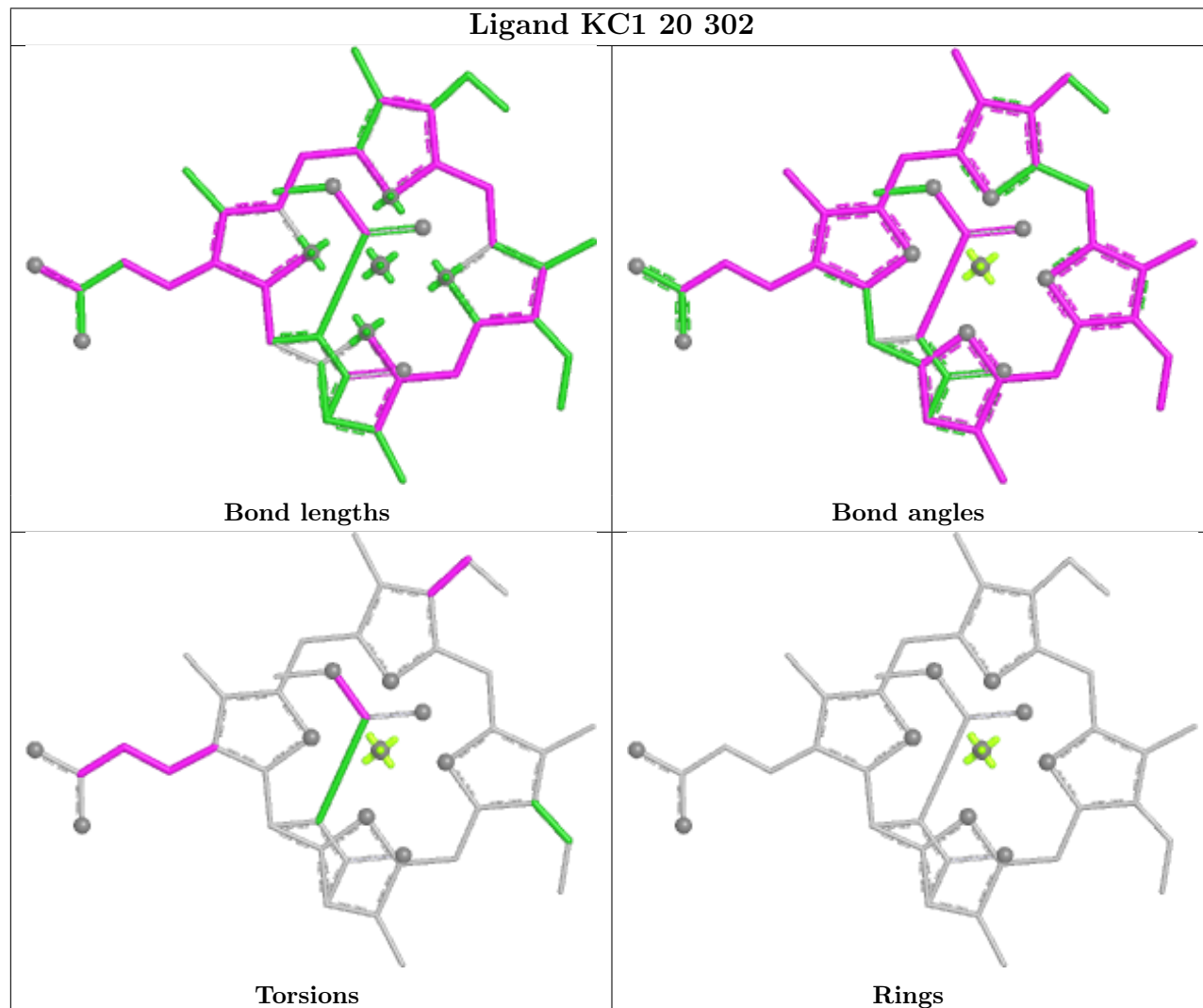
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

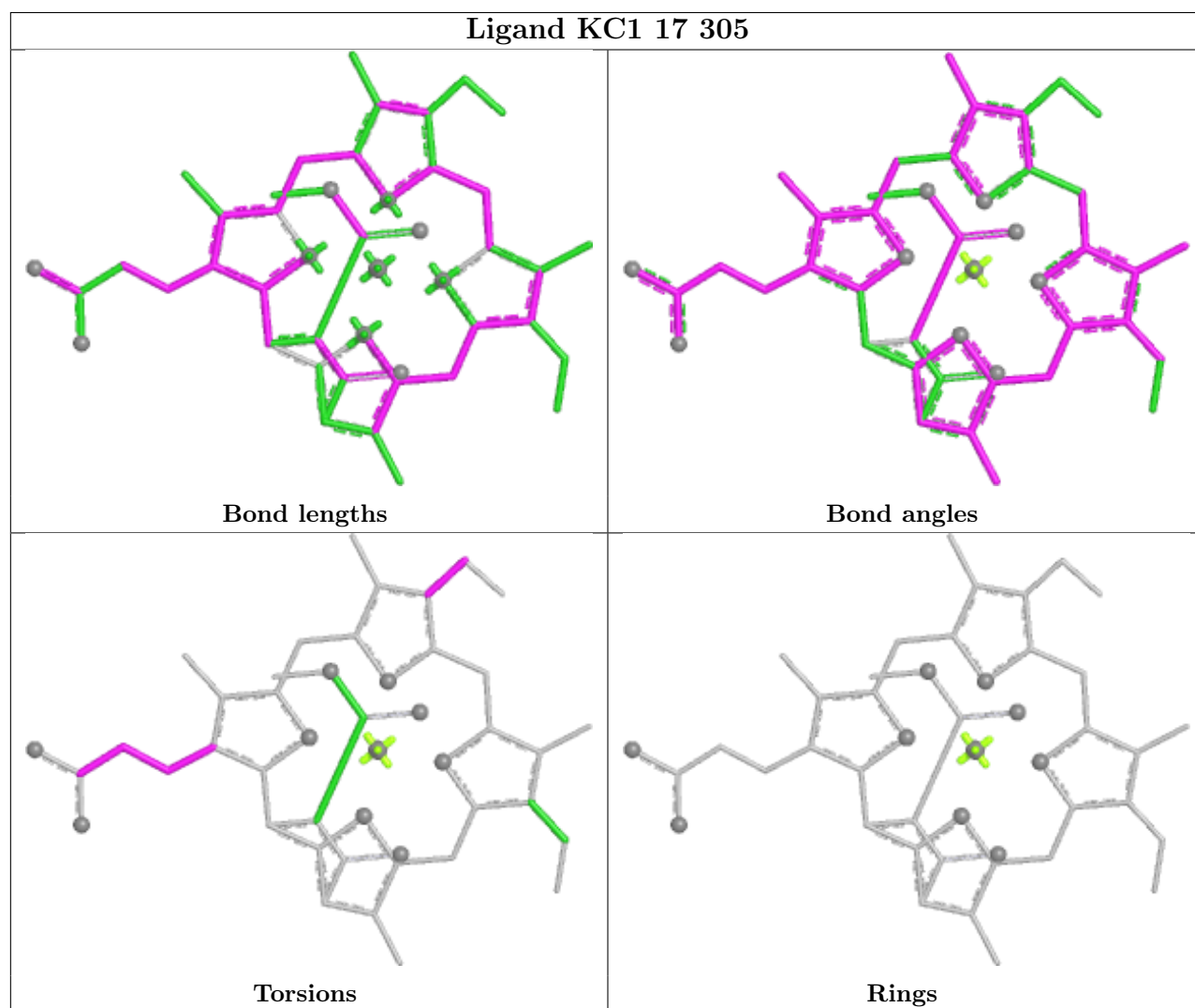
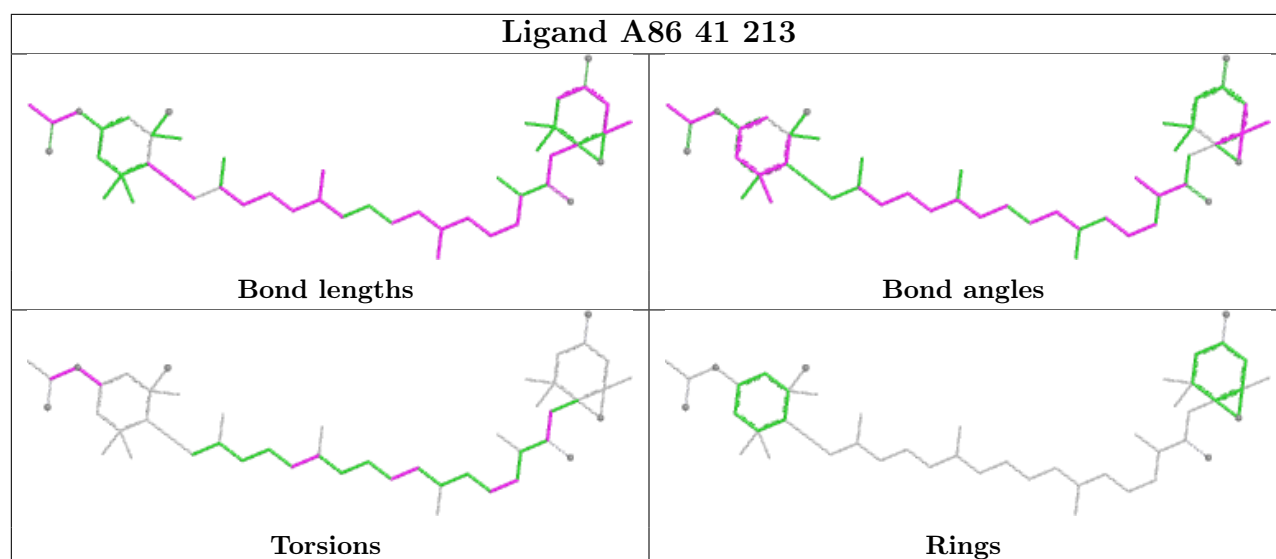


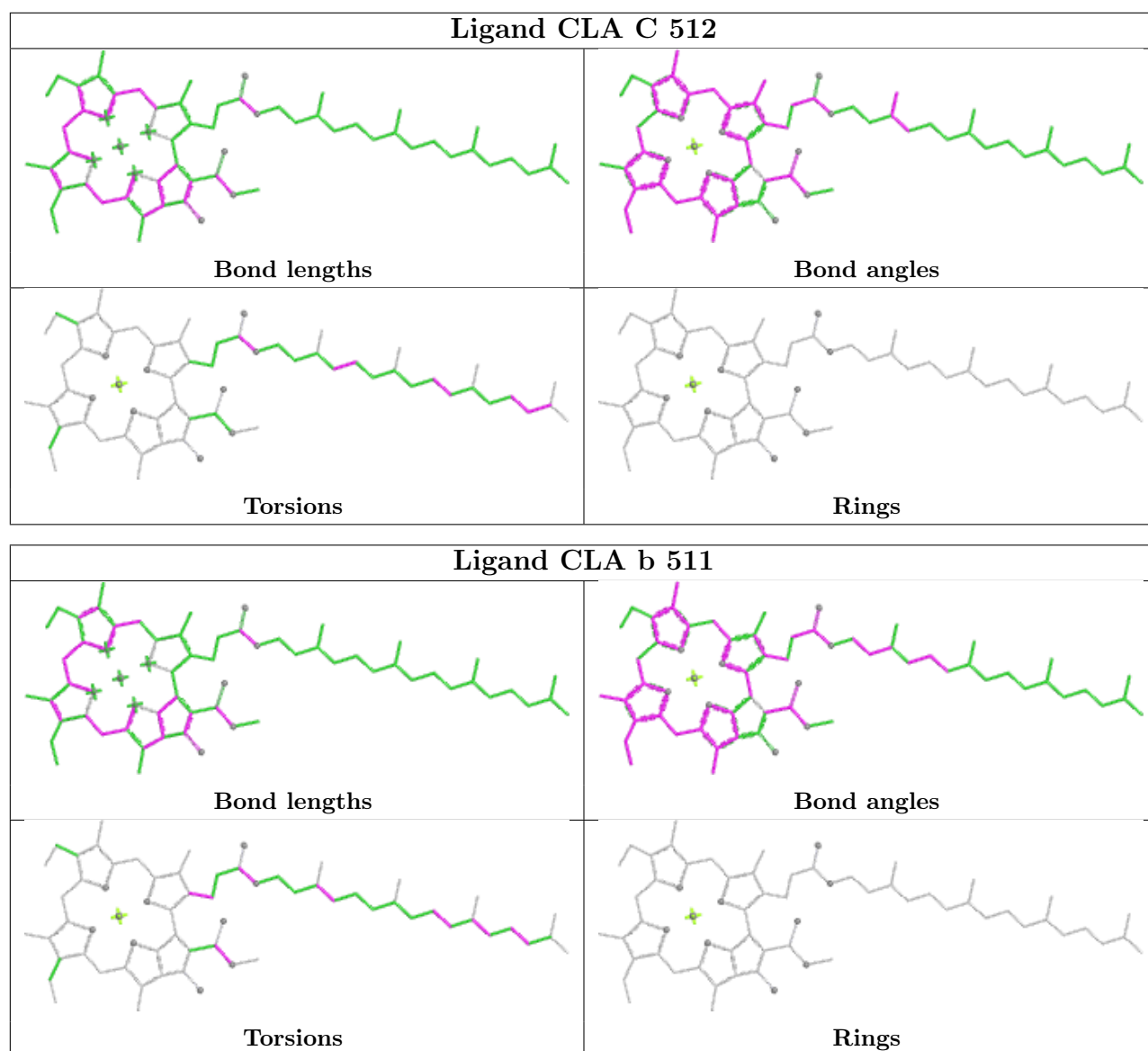
Ligand CLA c 508

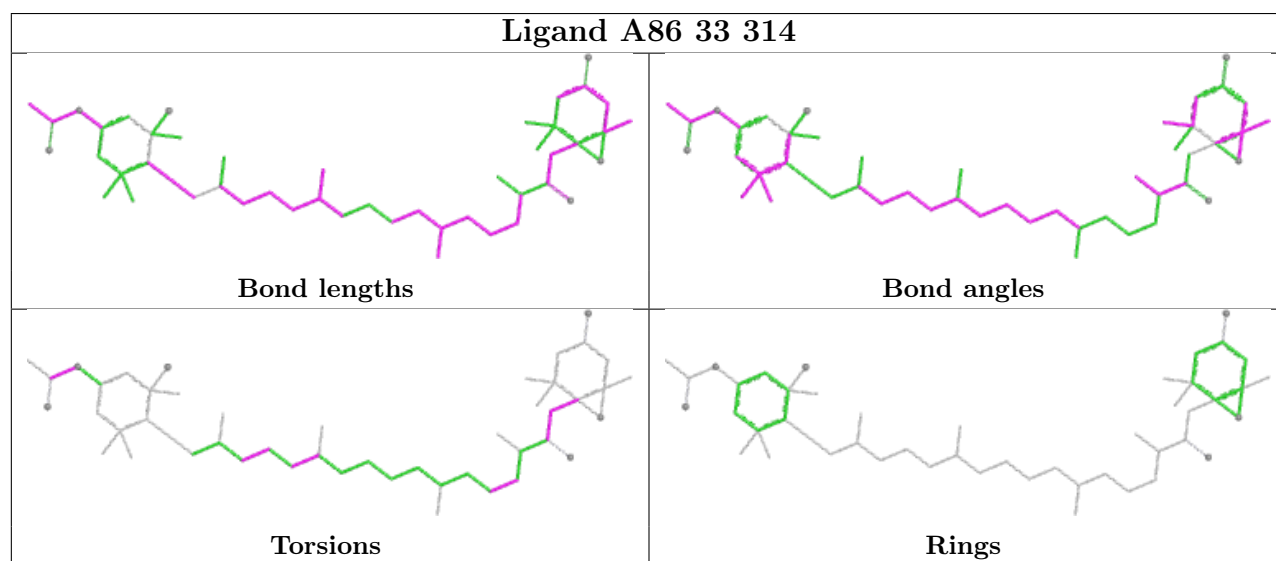
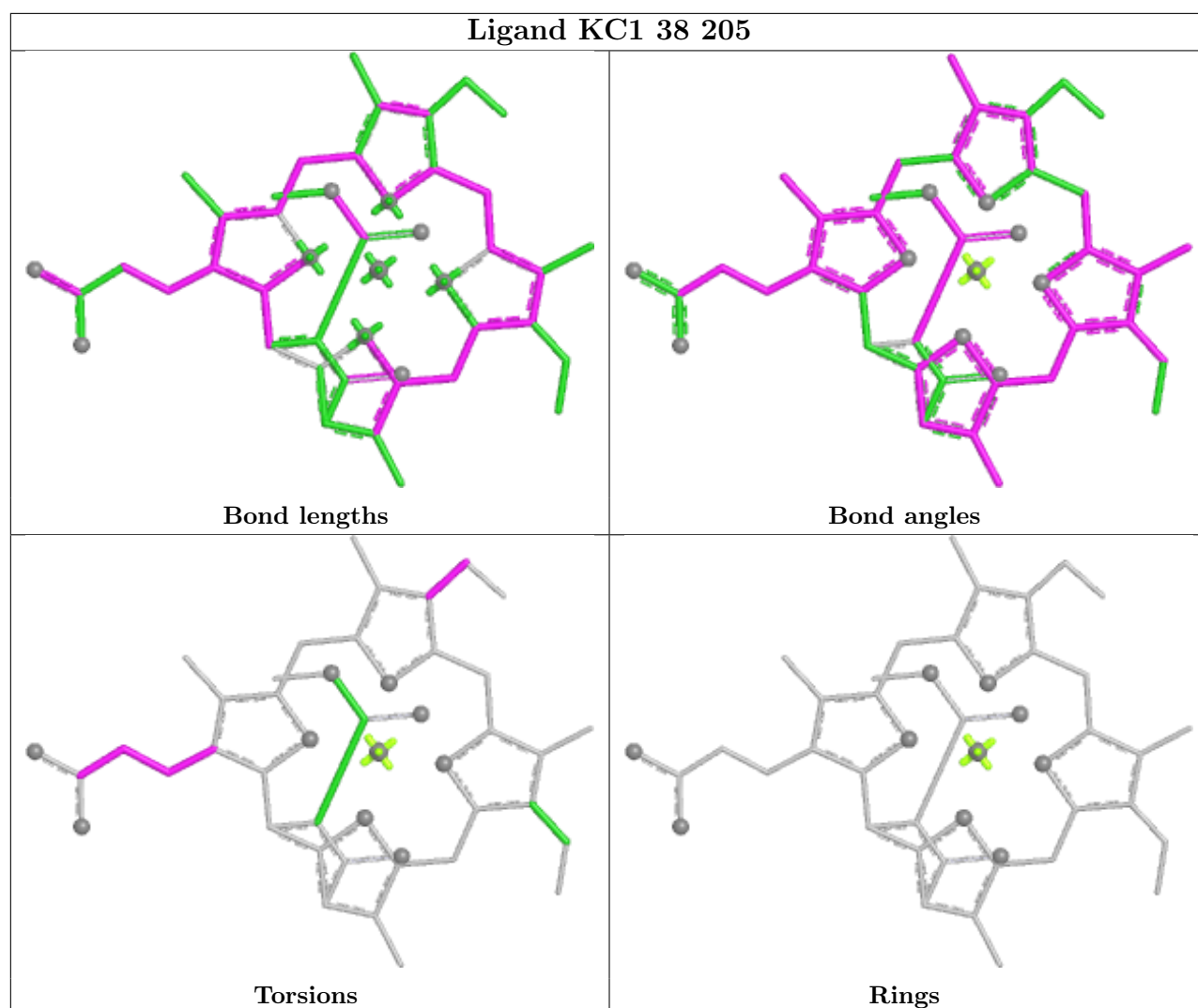


Ligand KC1 20 302

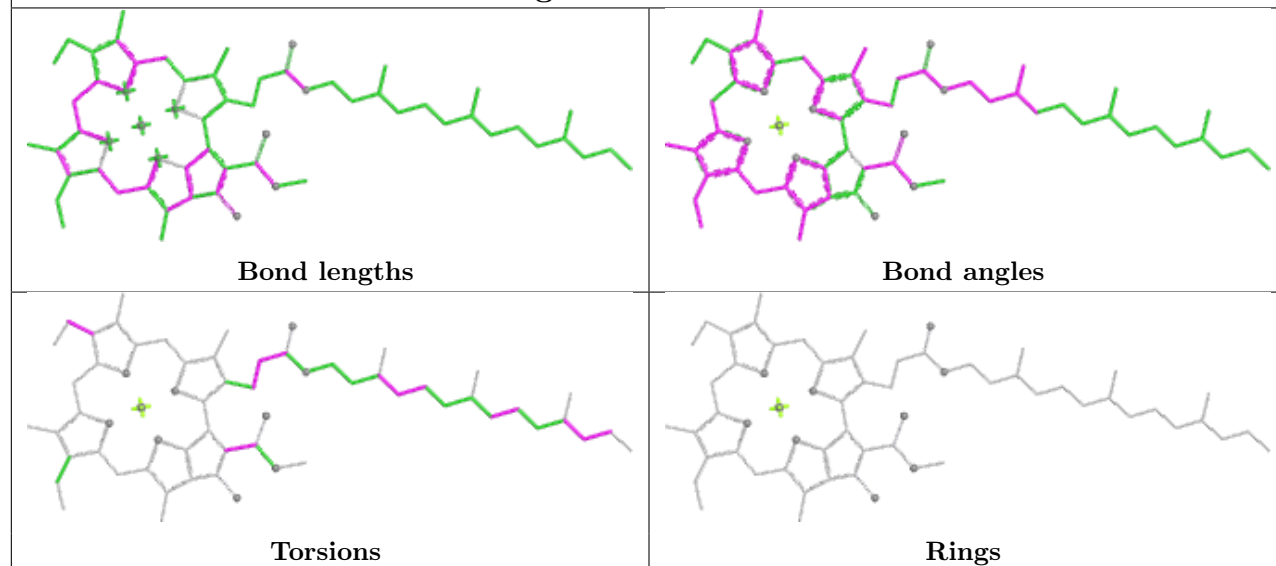




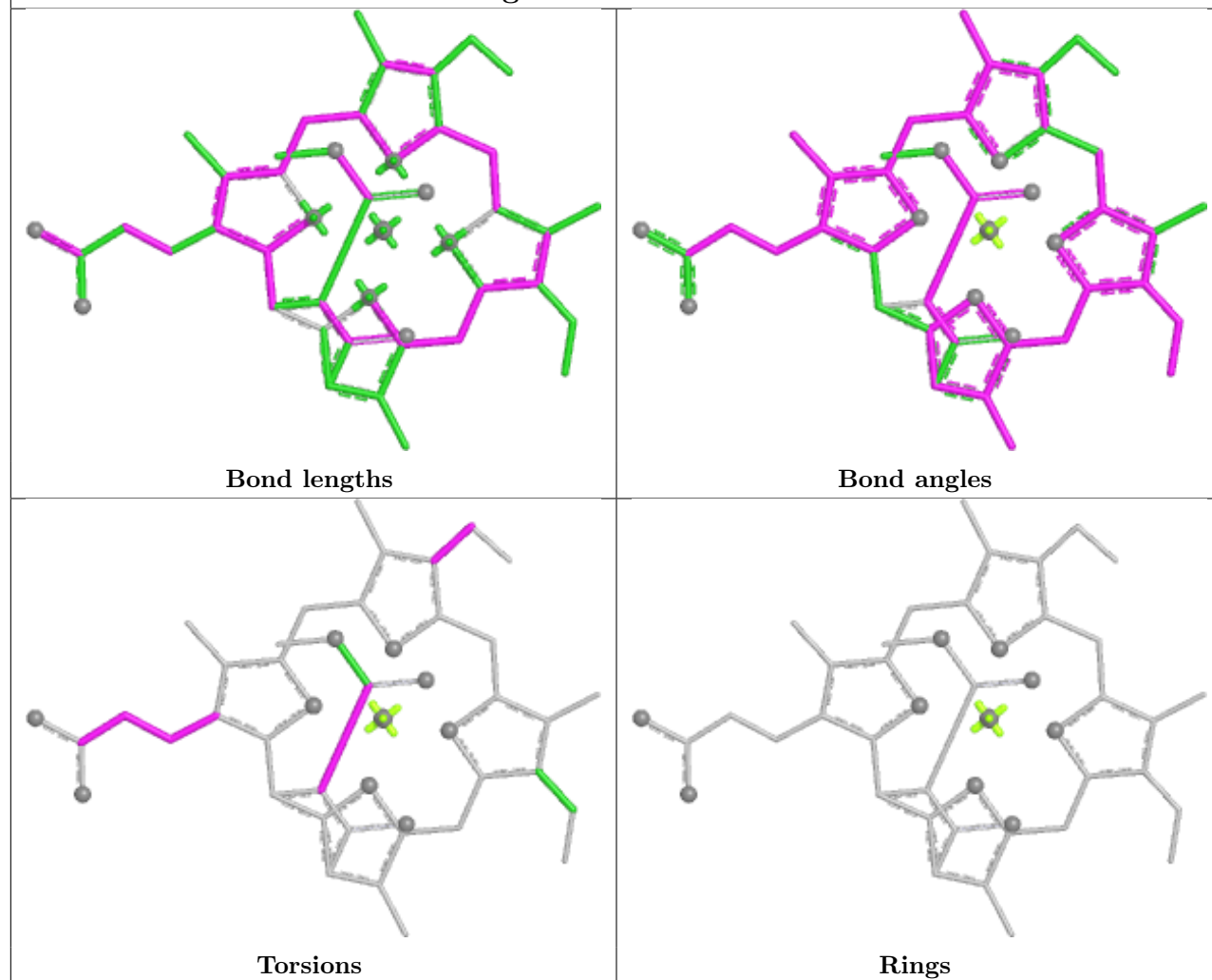


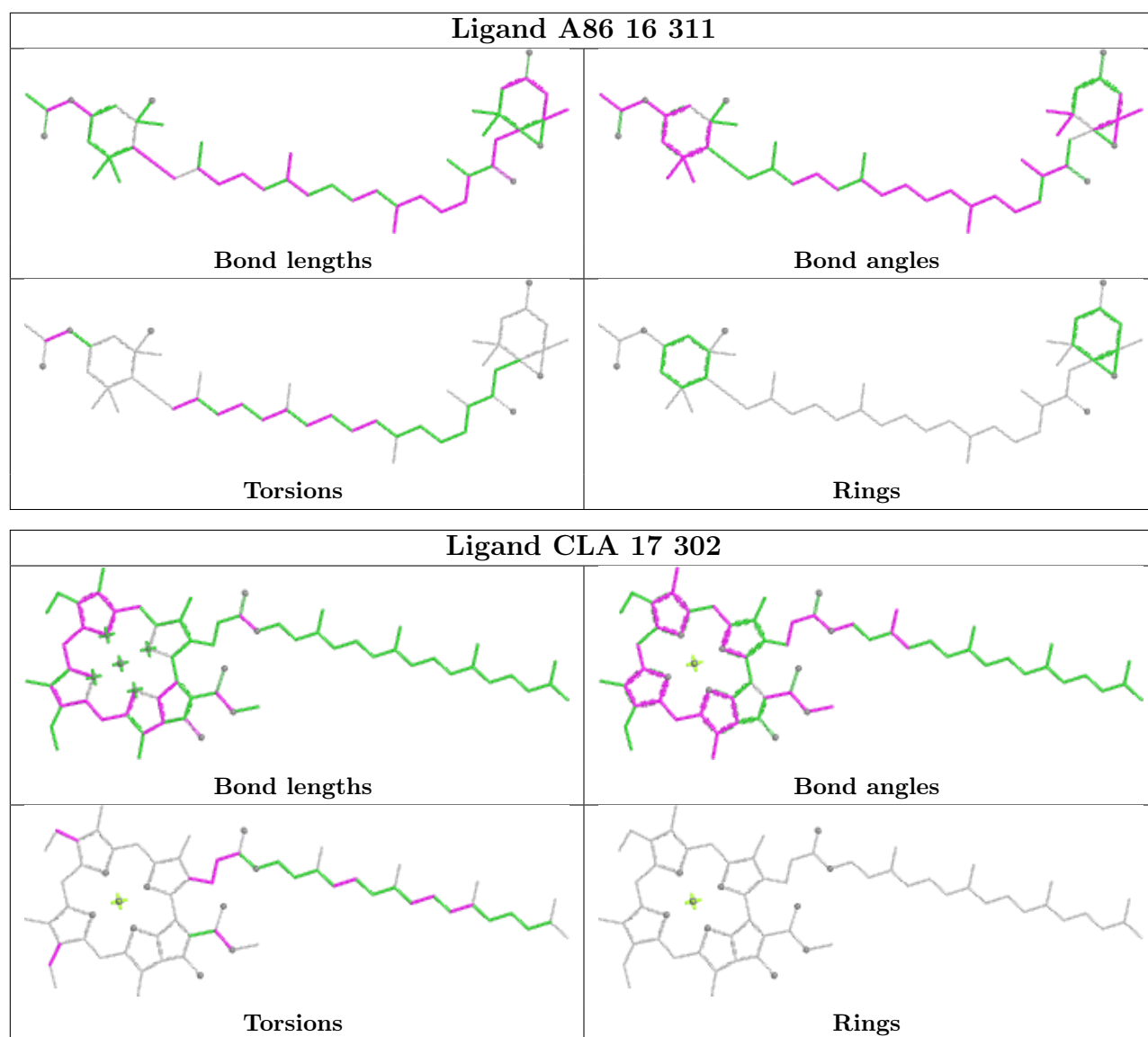


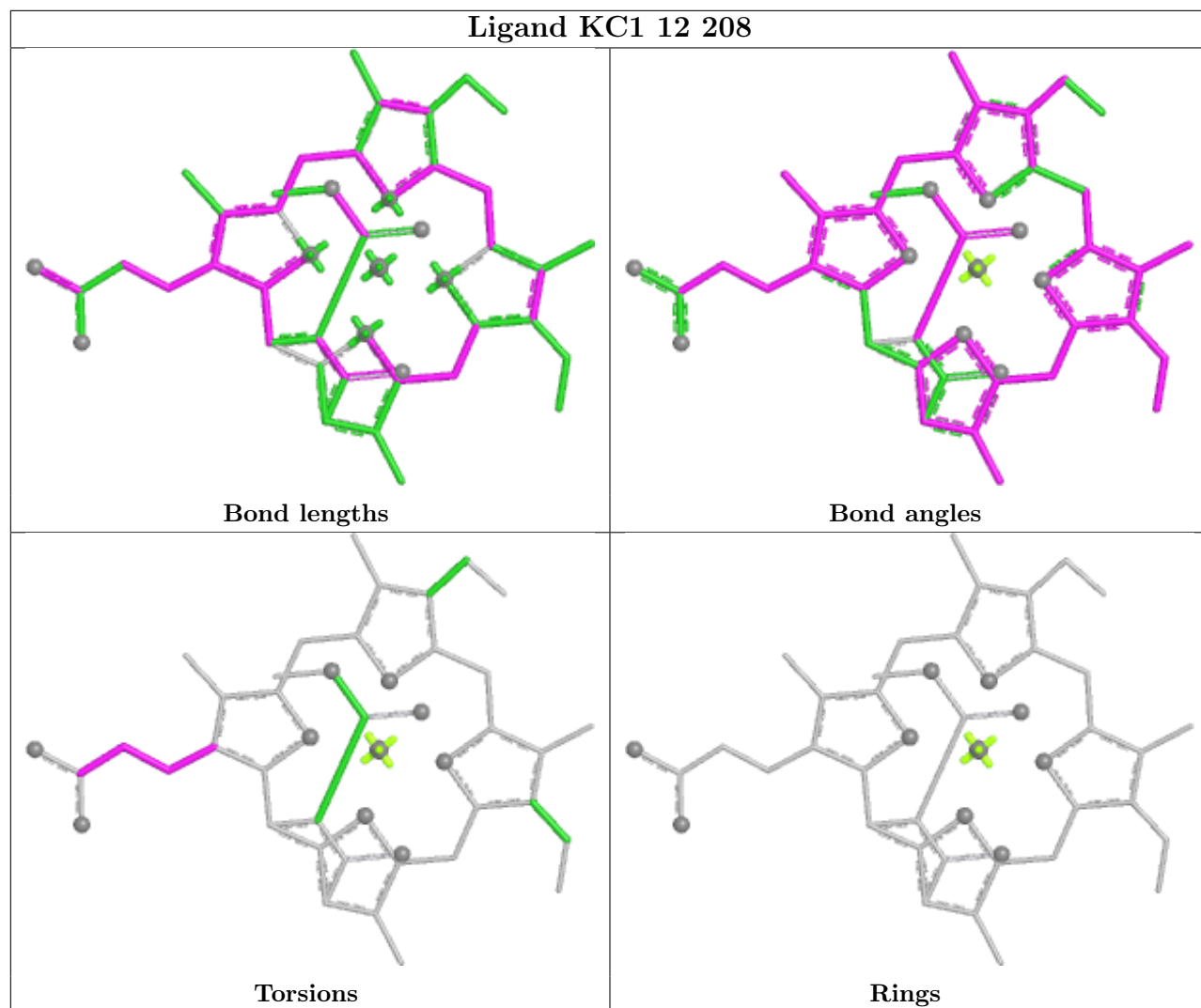
Ligand CLA b 514

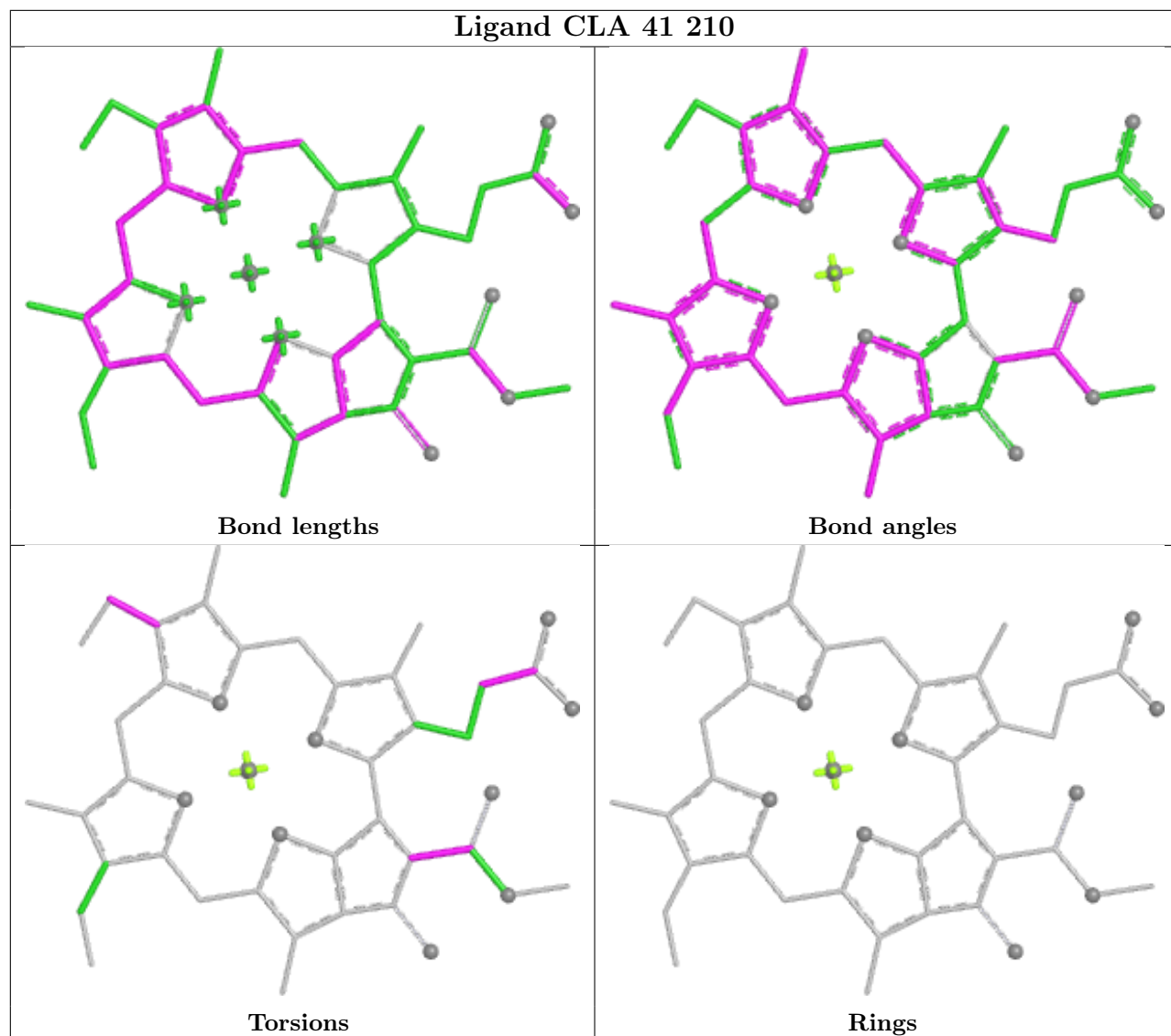


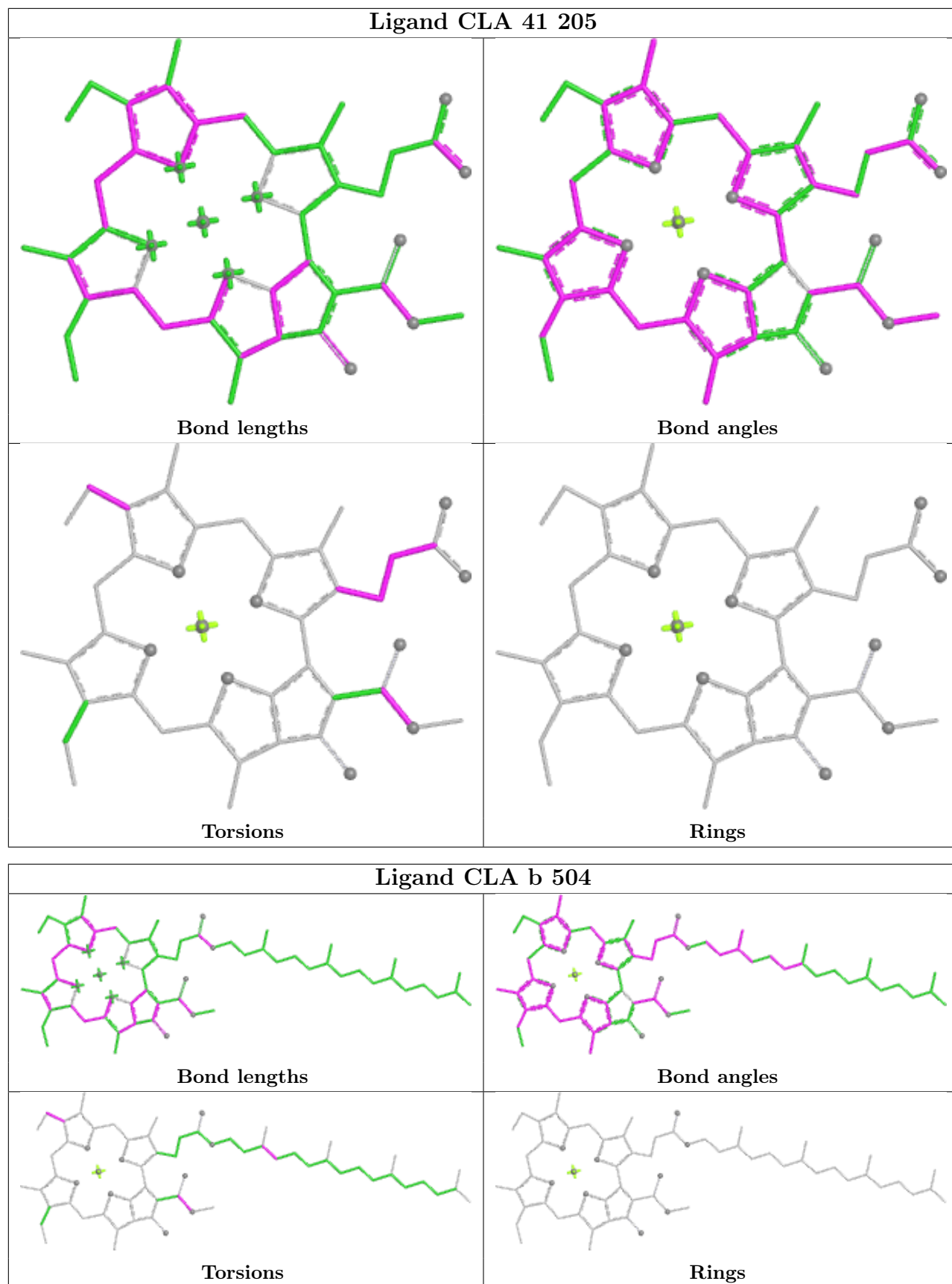
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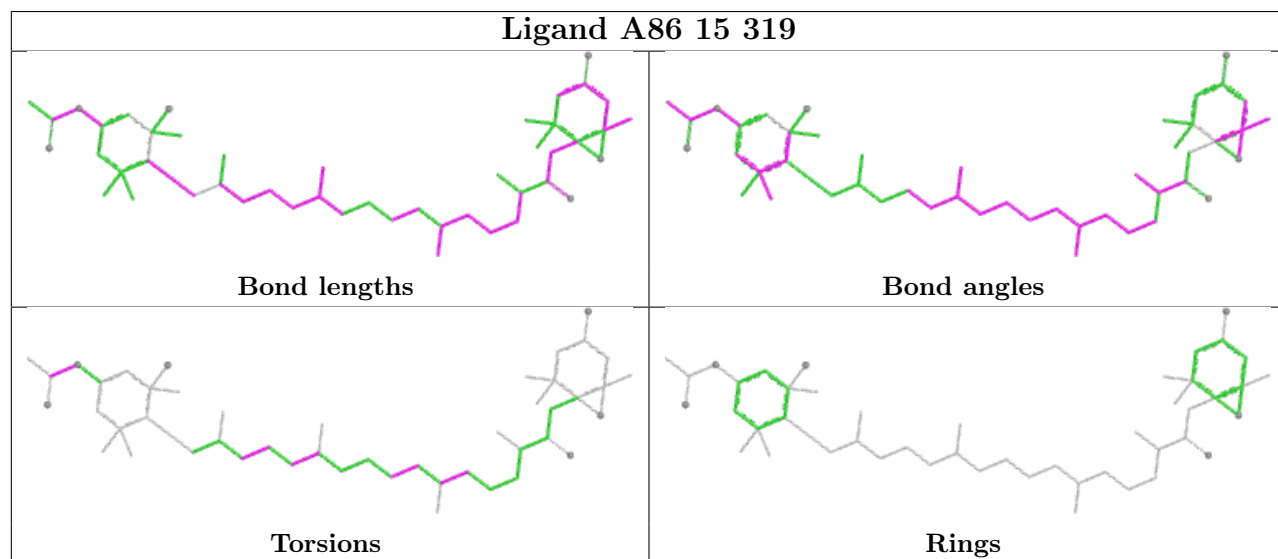
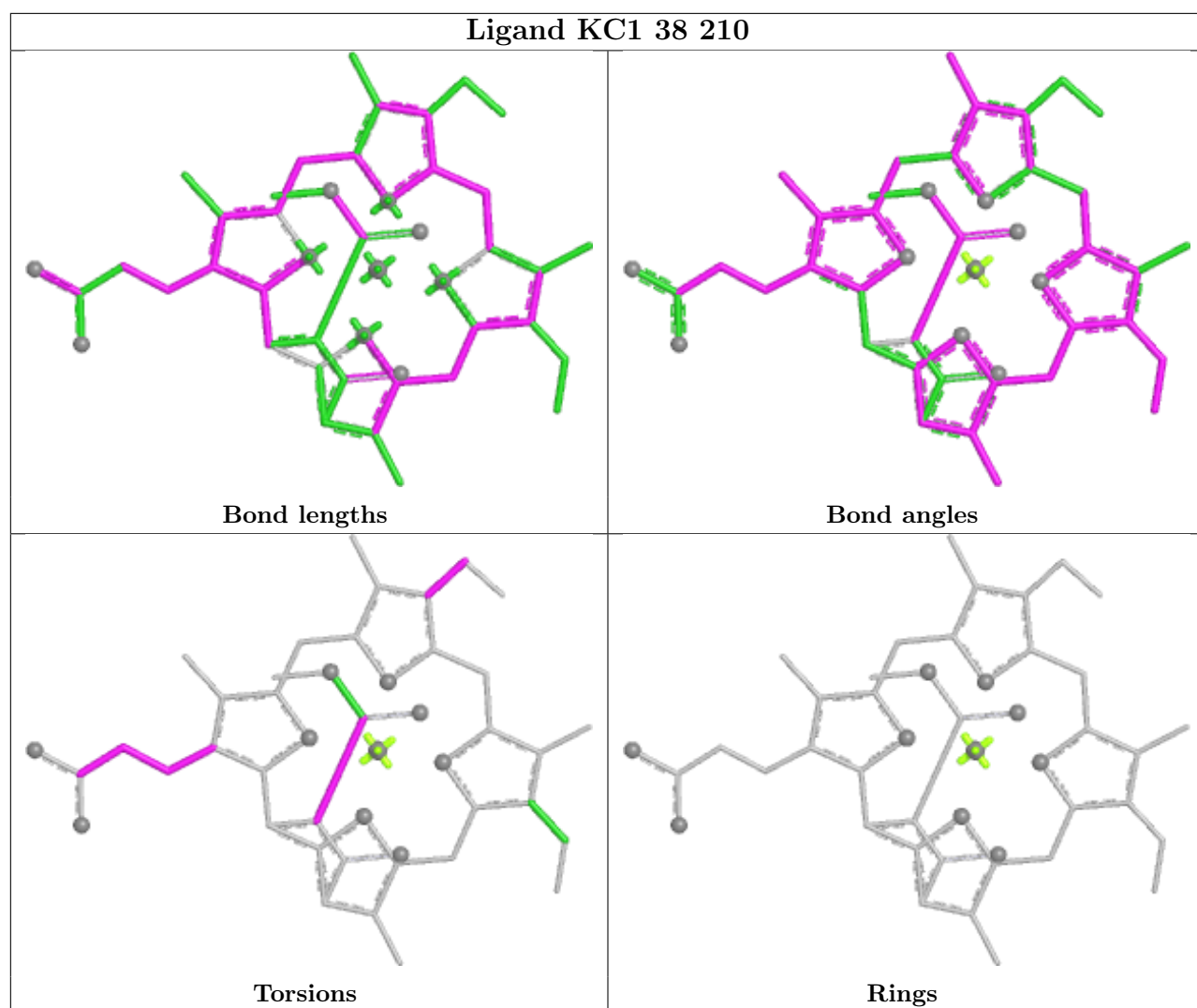


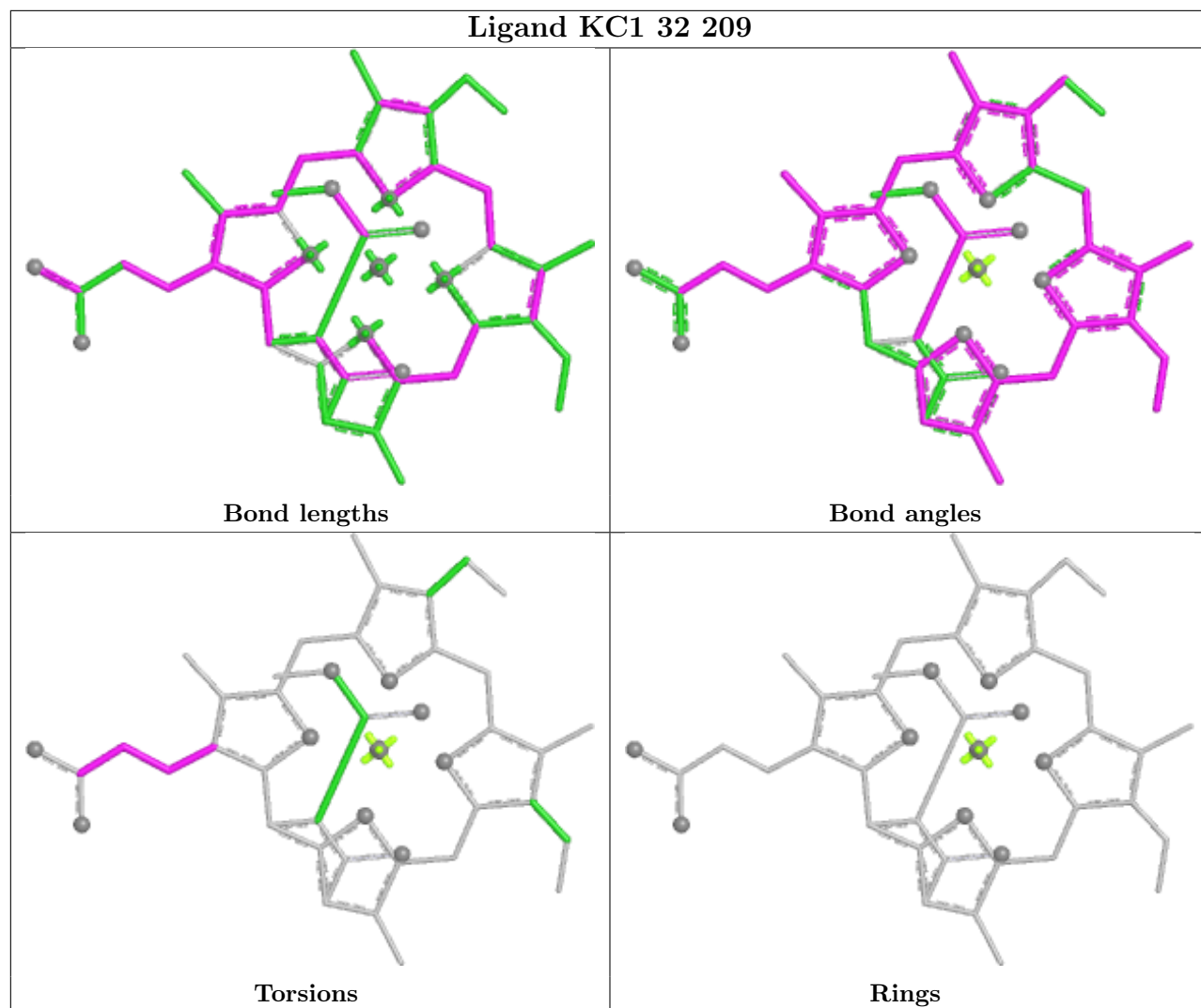


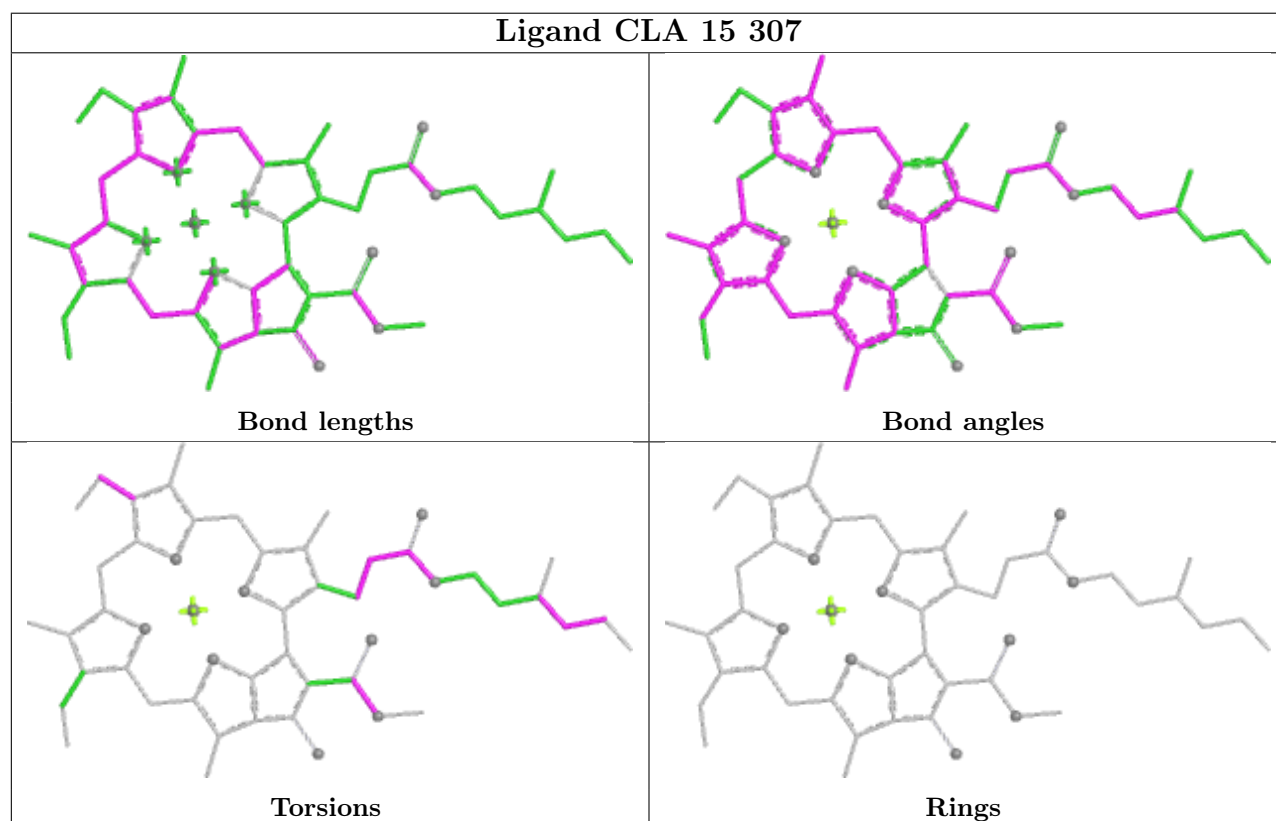
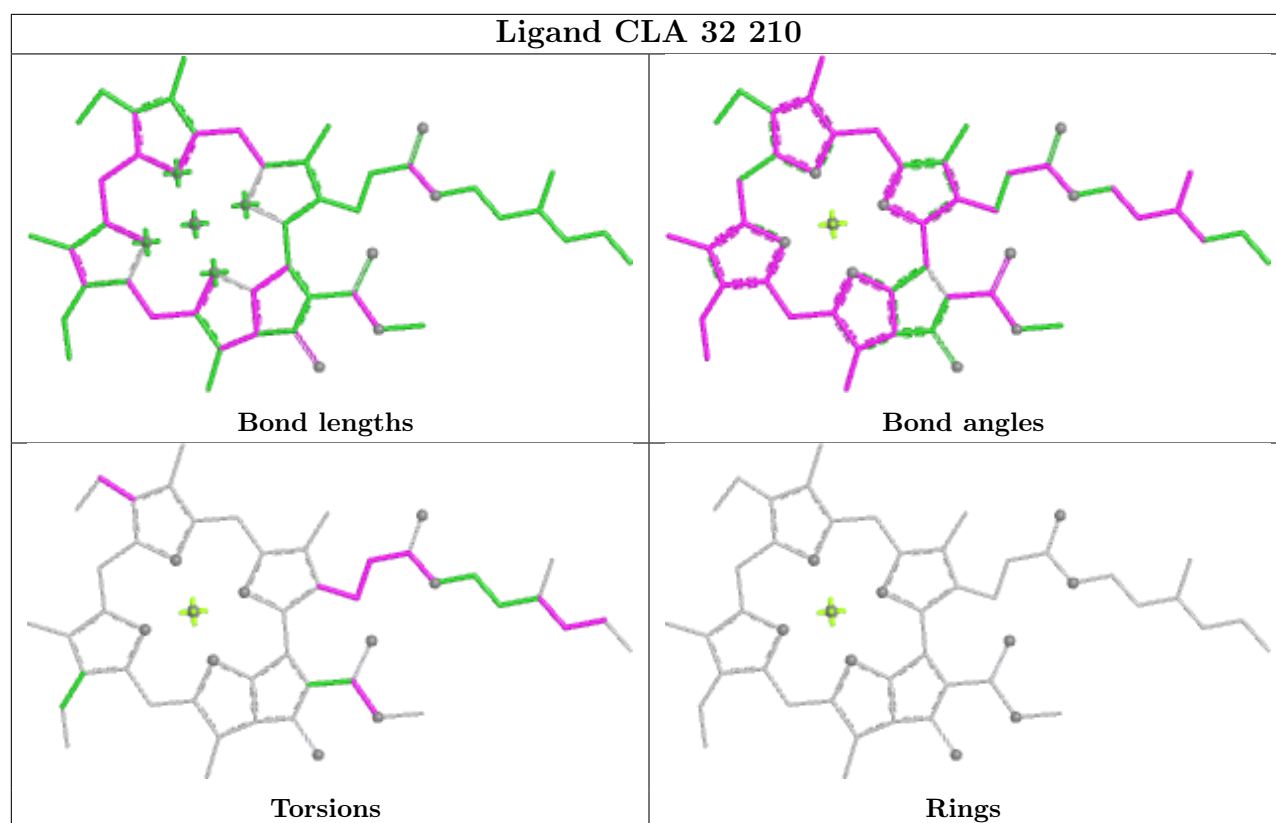


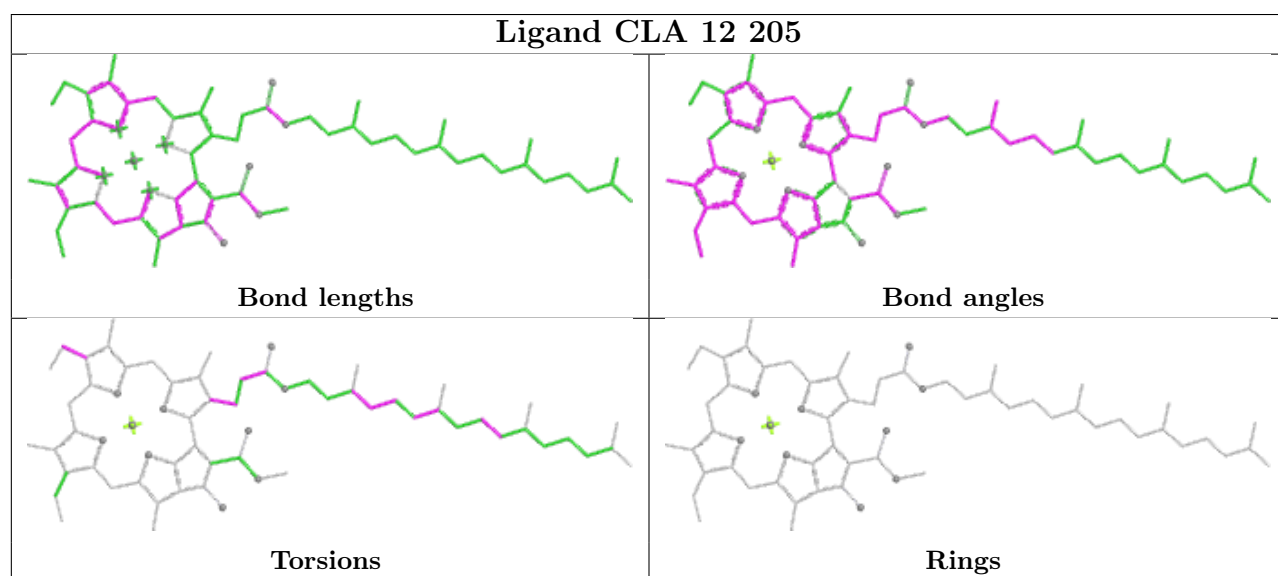
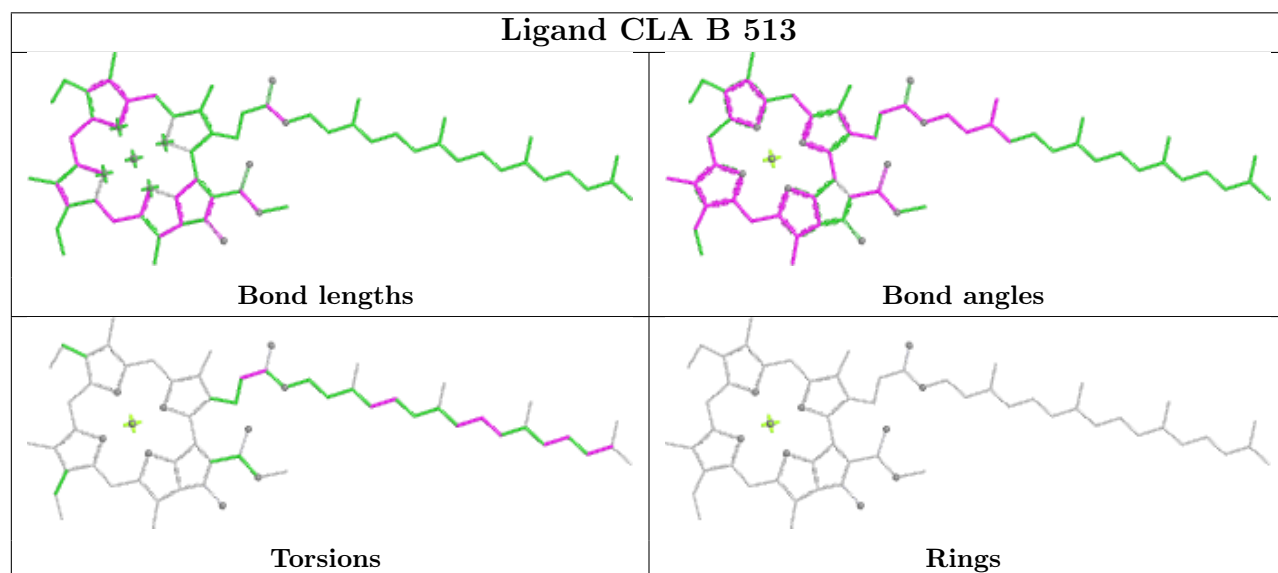
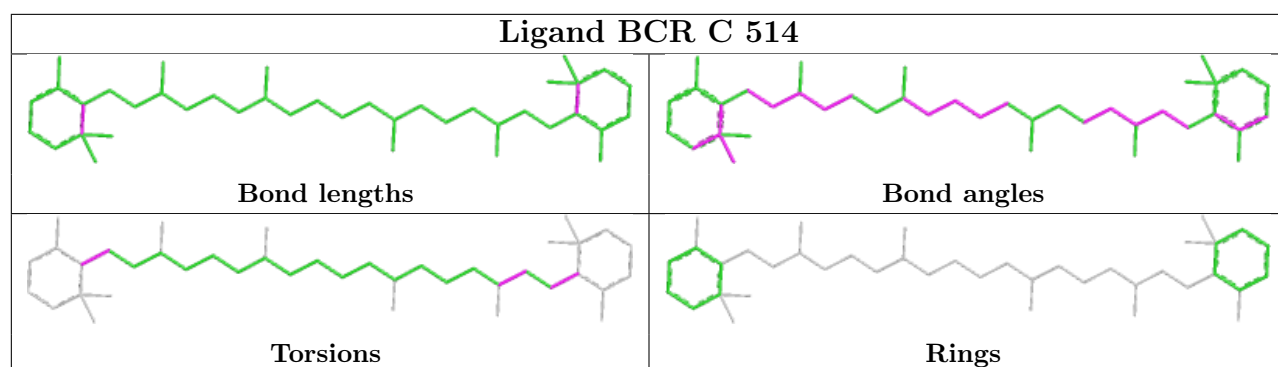


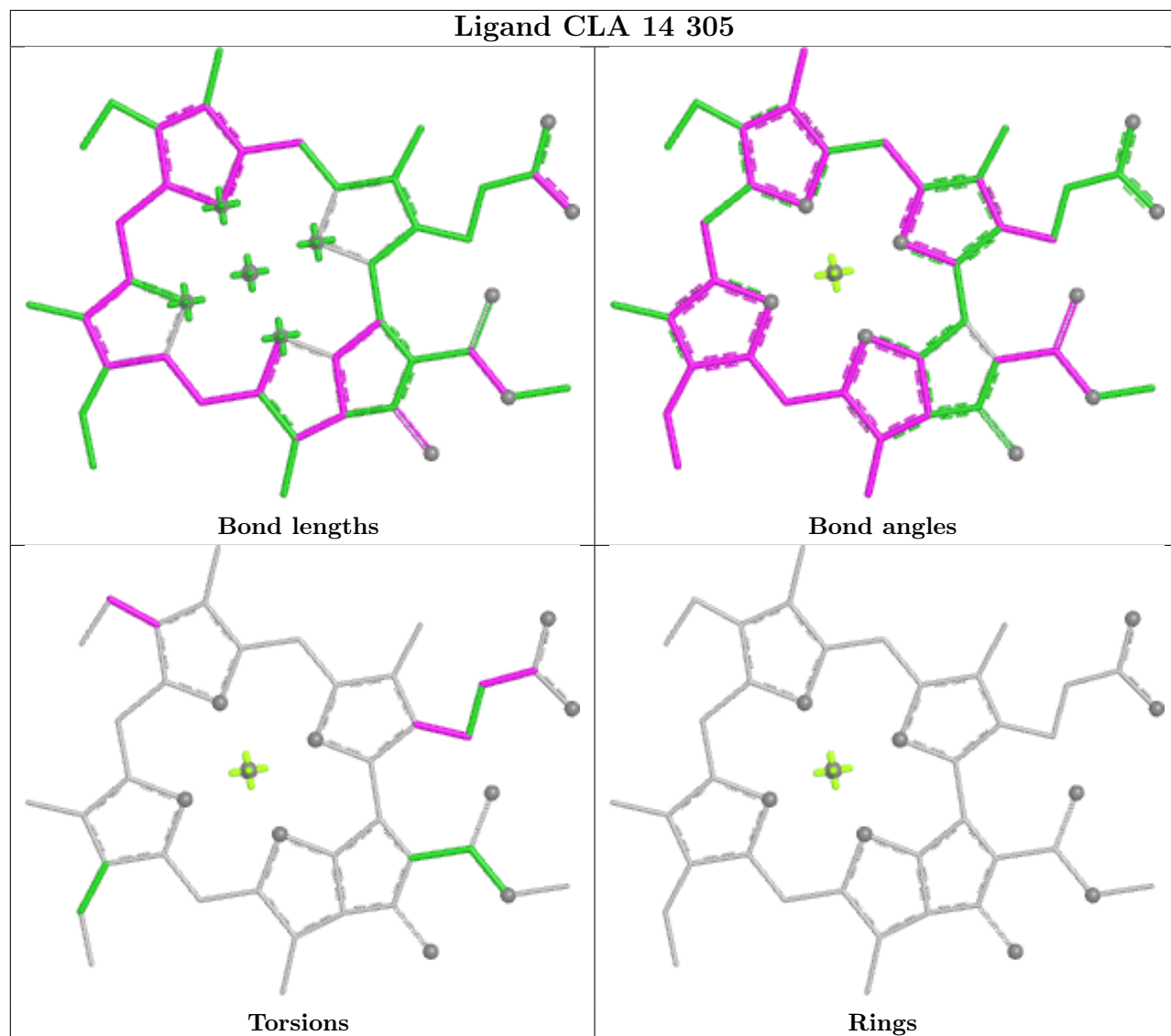


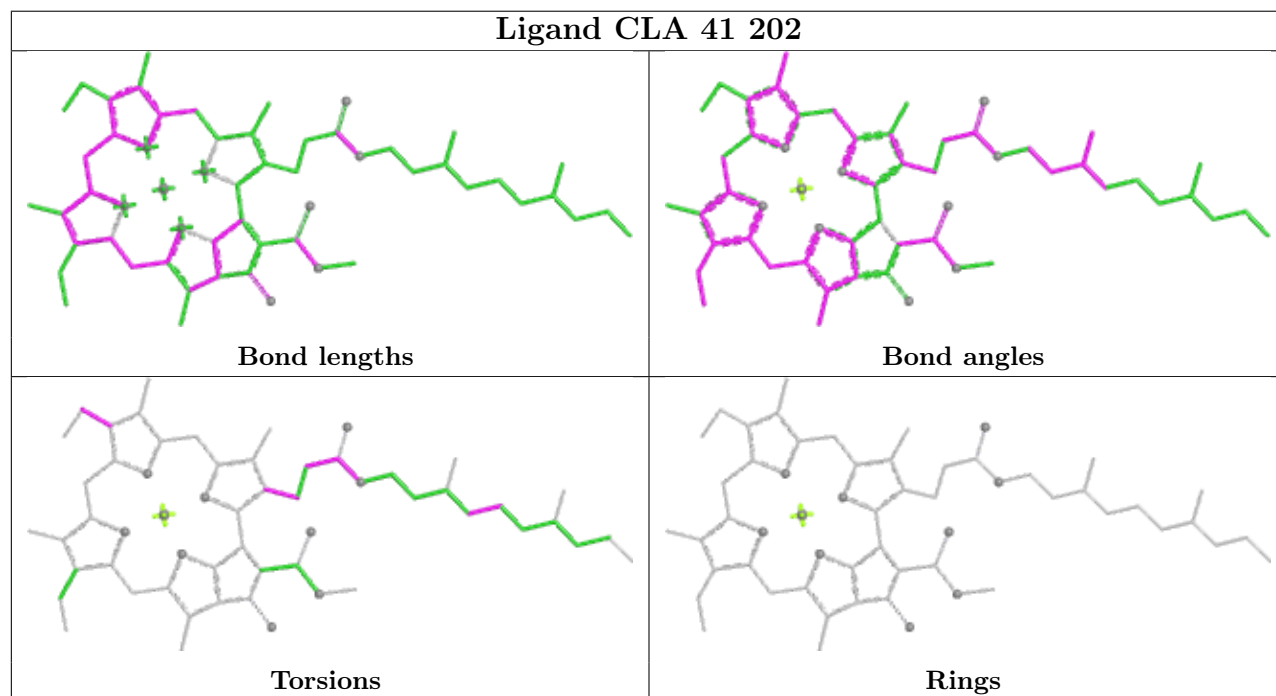
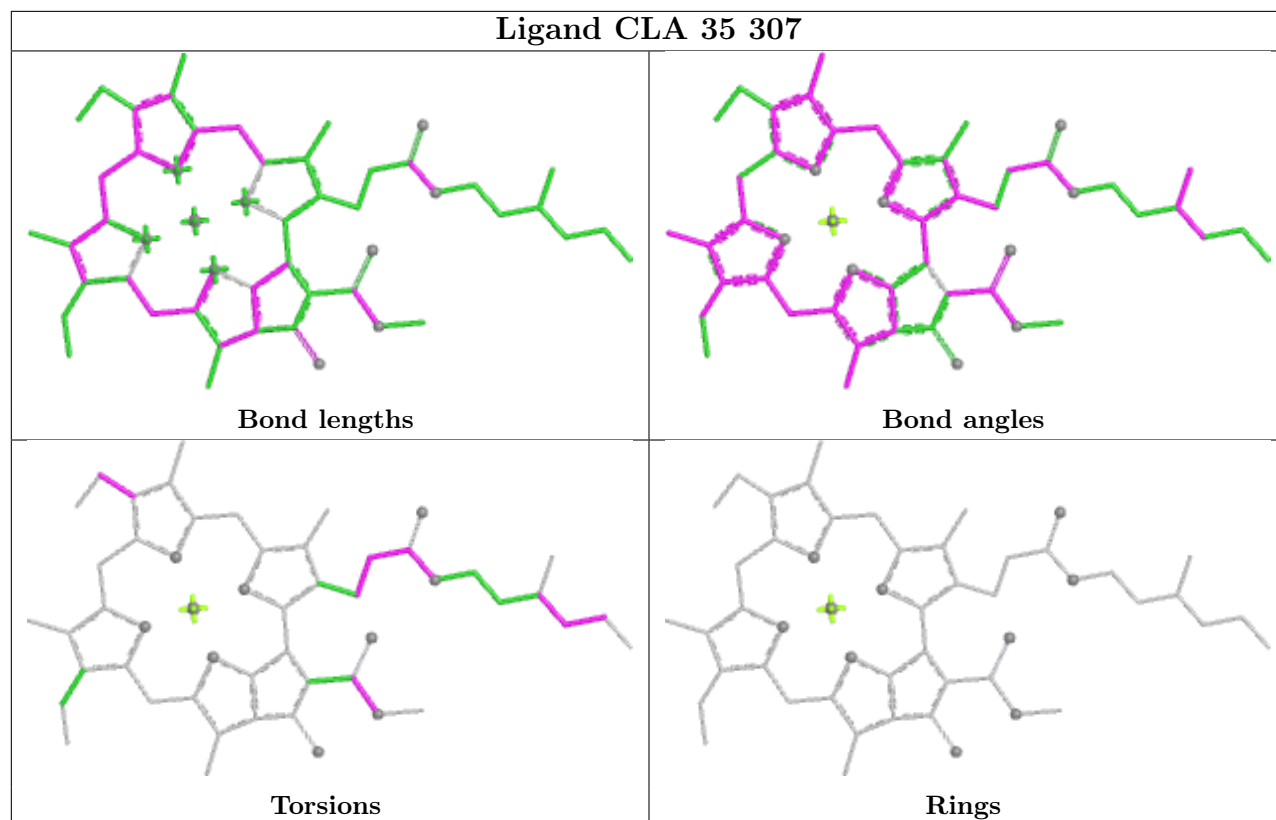


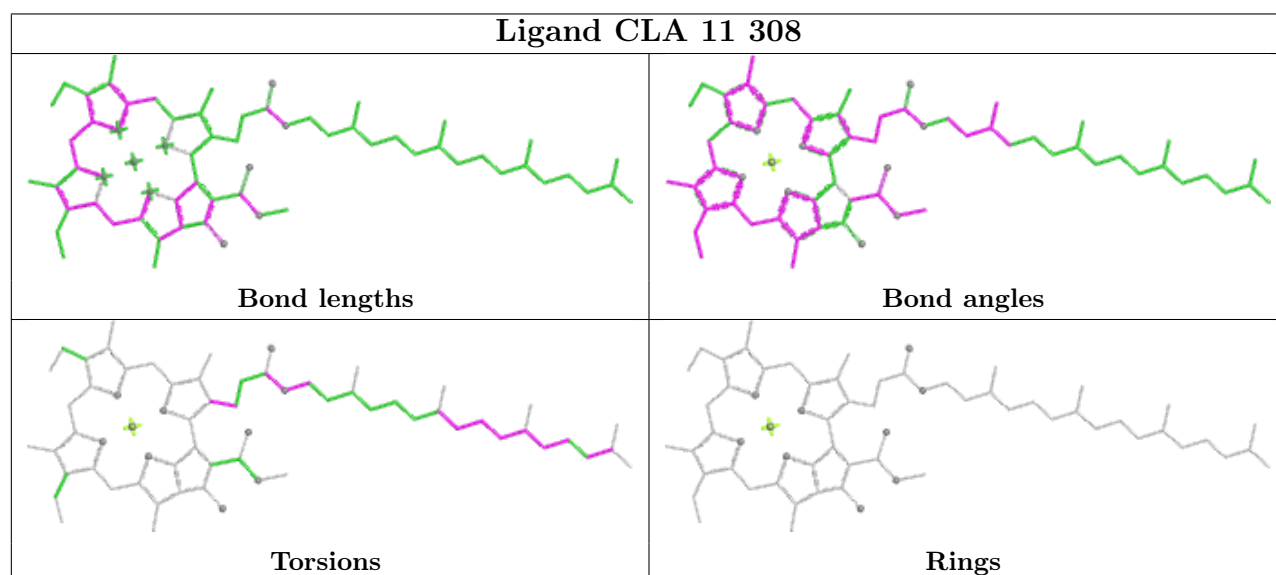
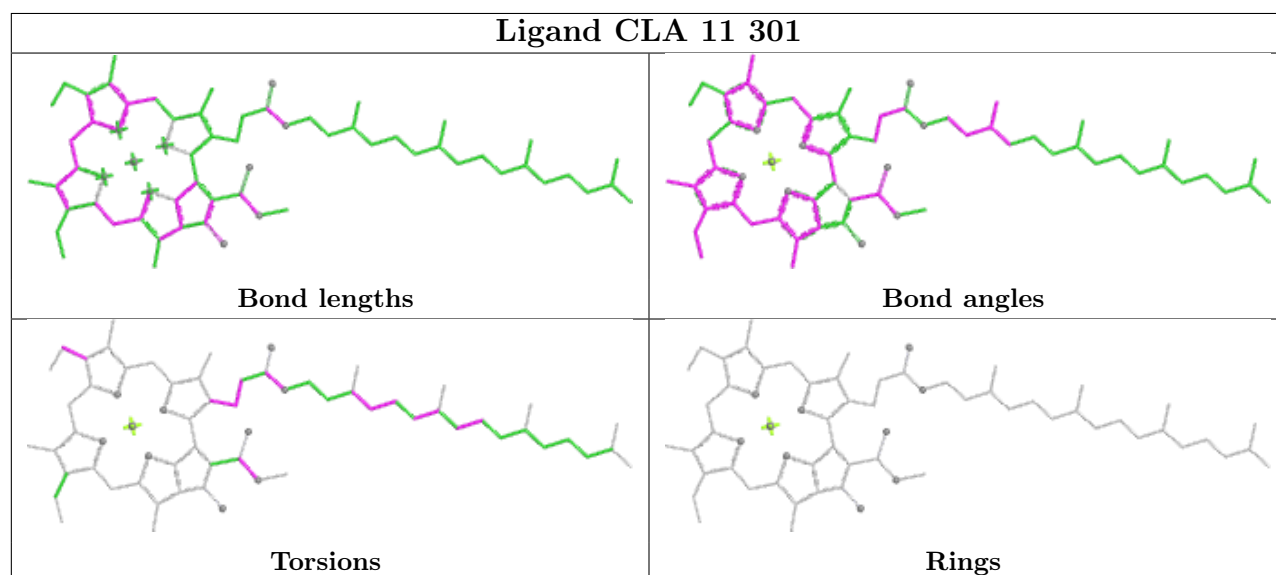
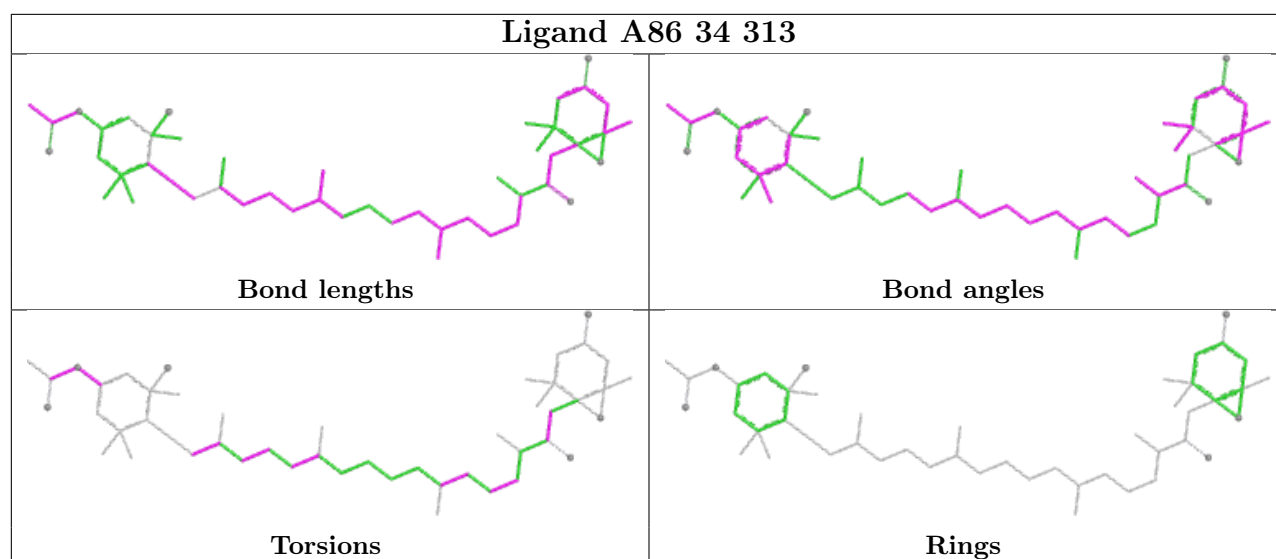


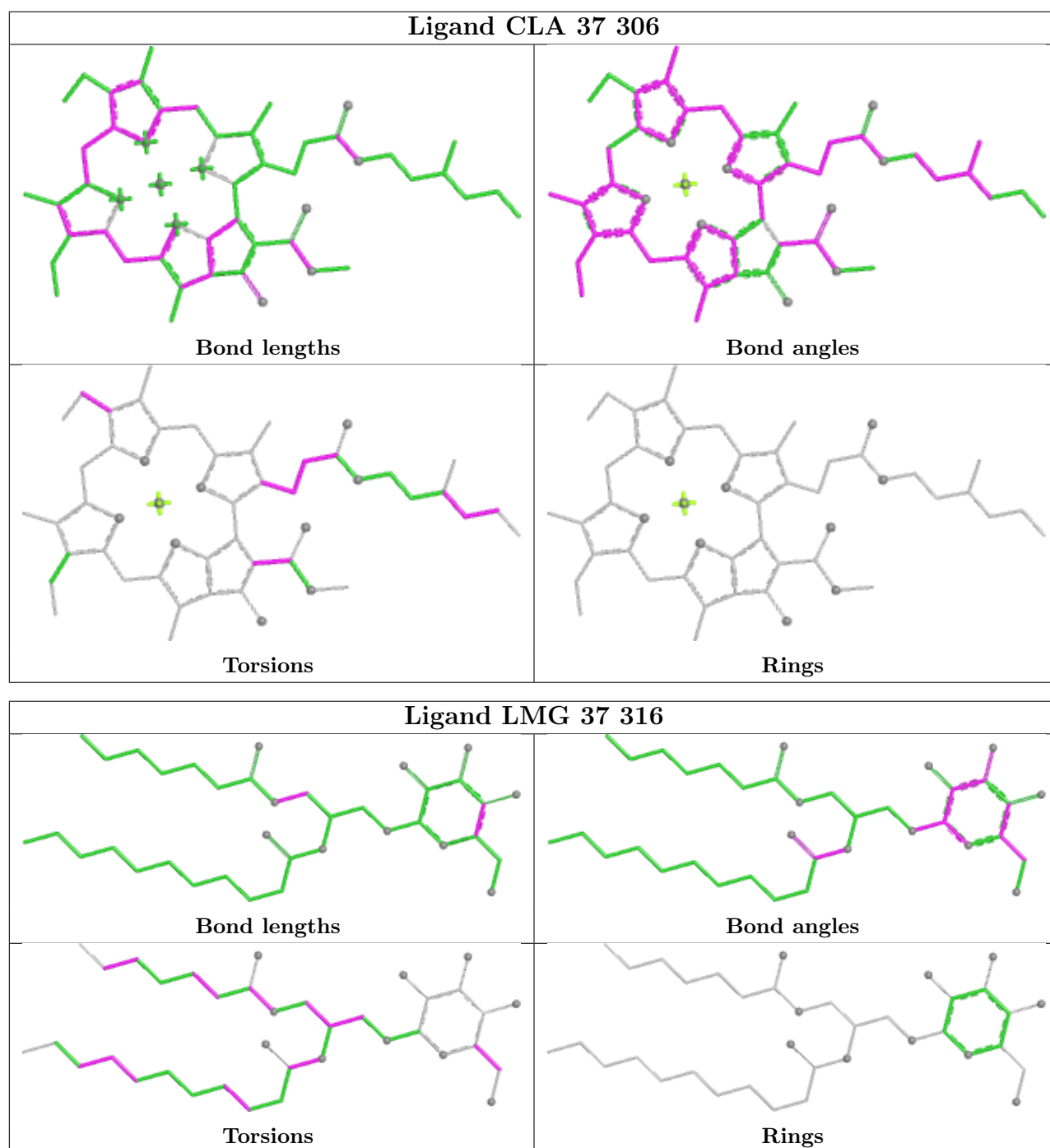


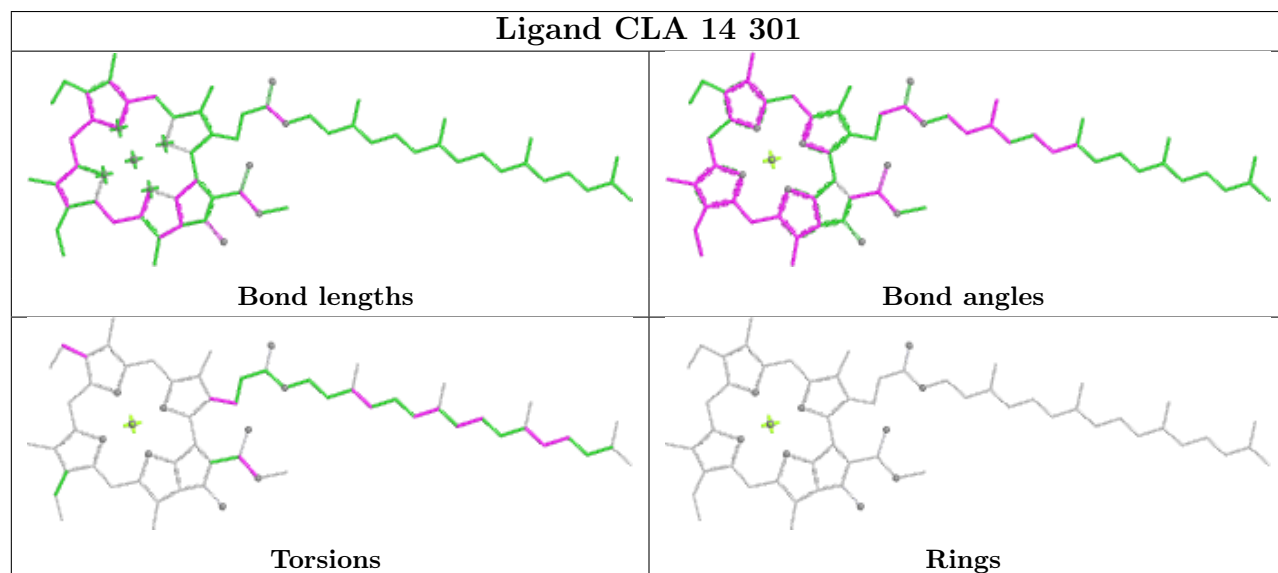
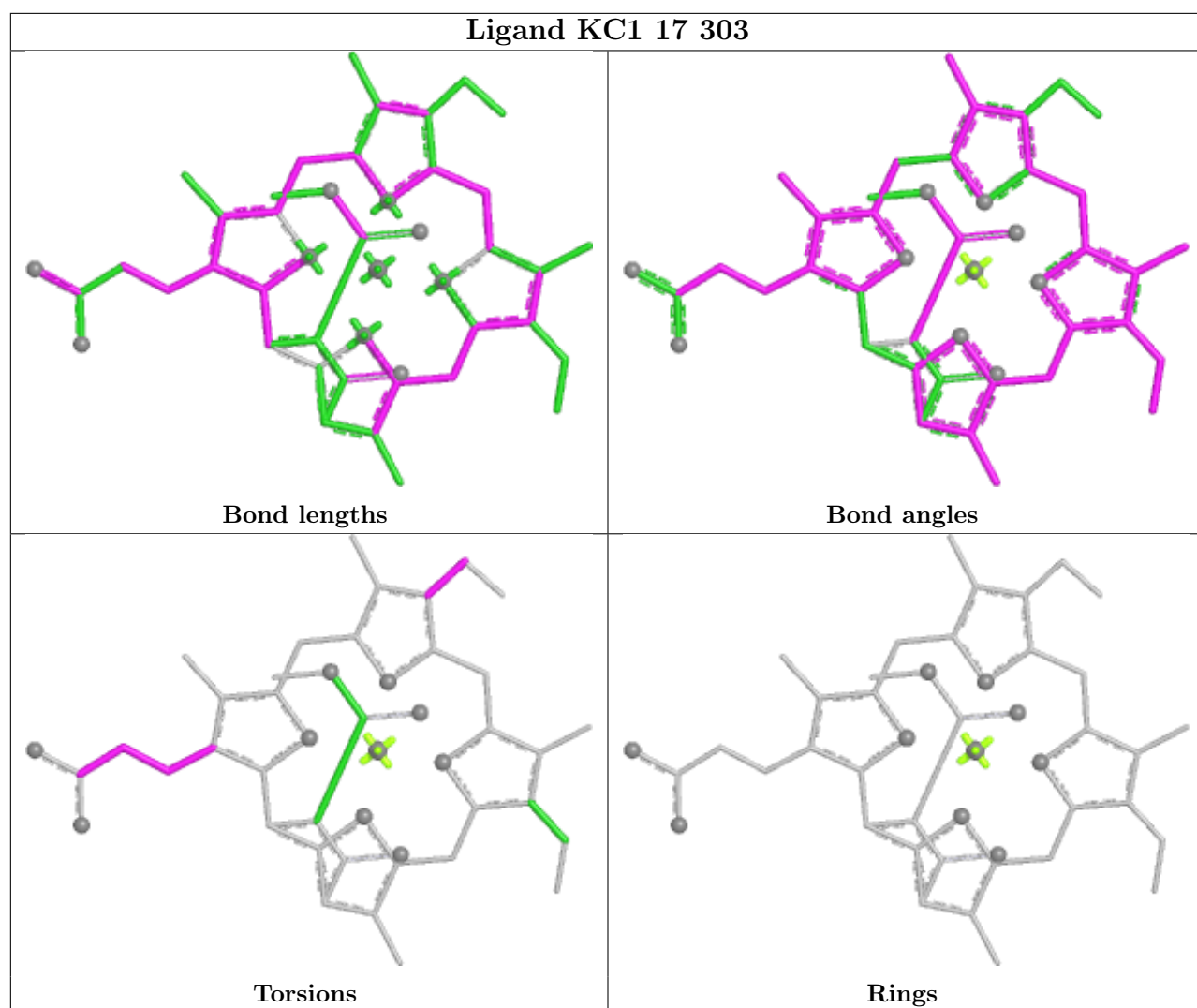


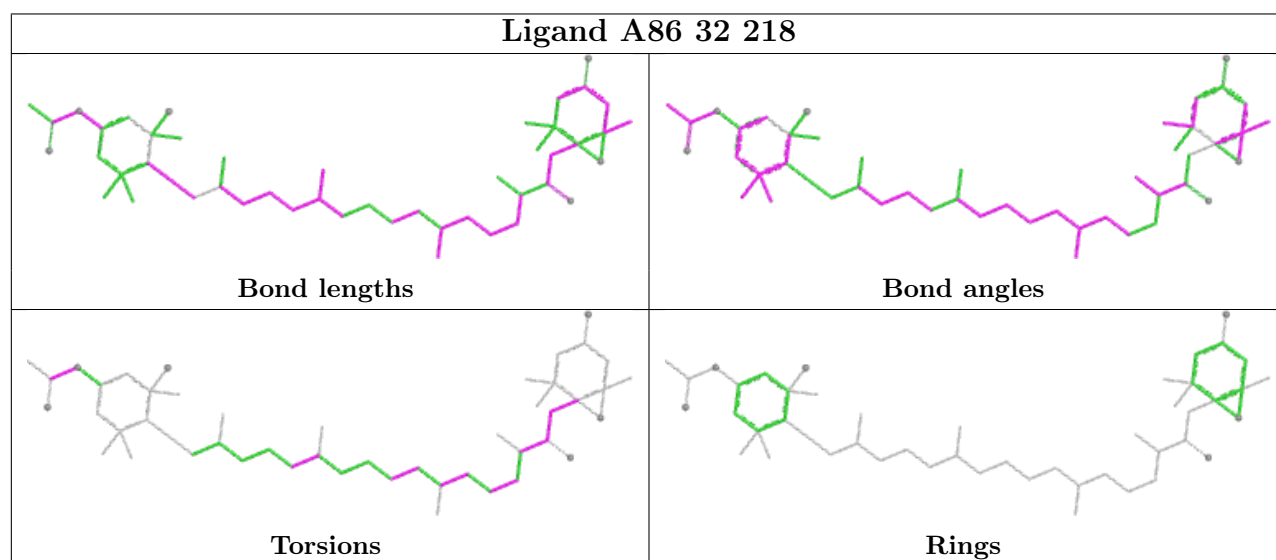
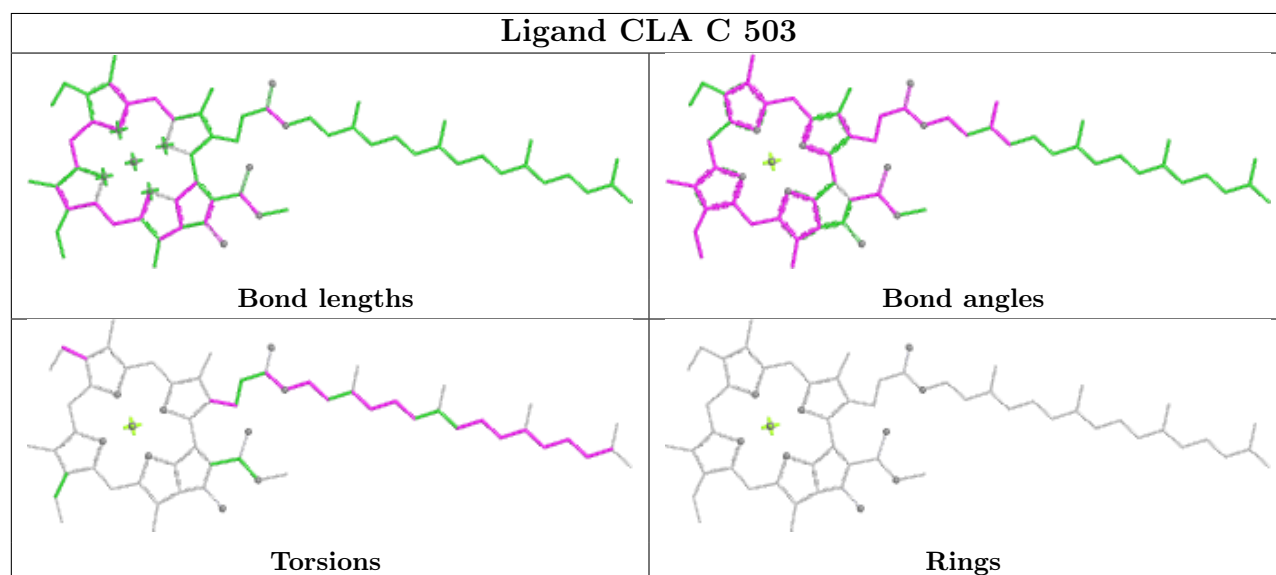
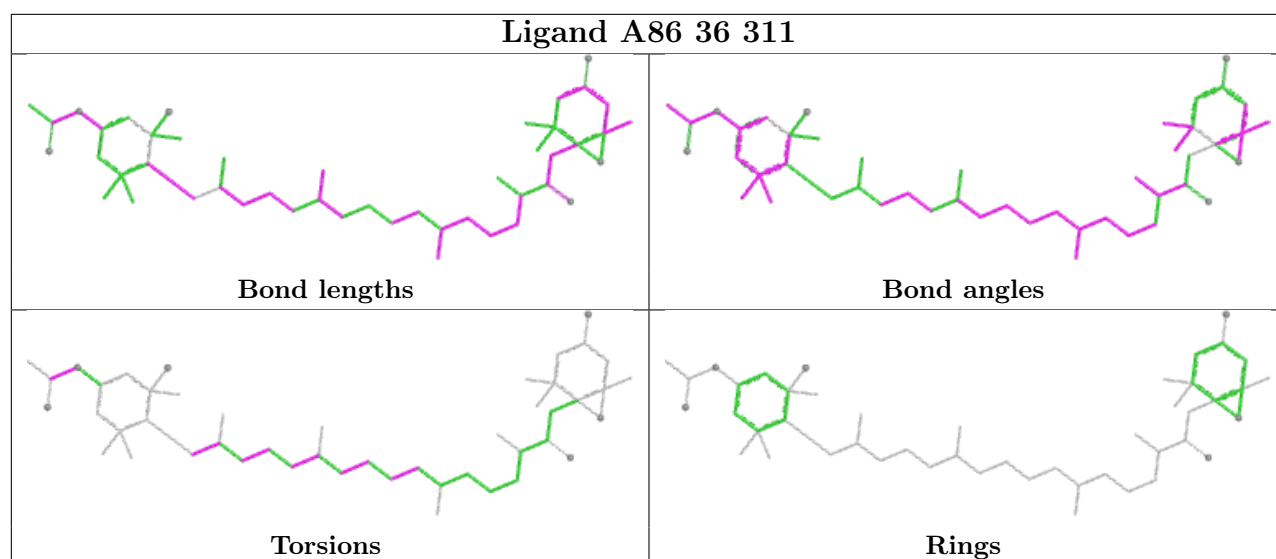


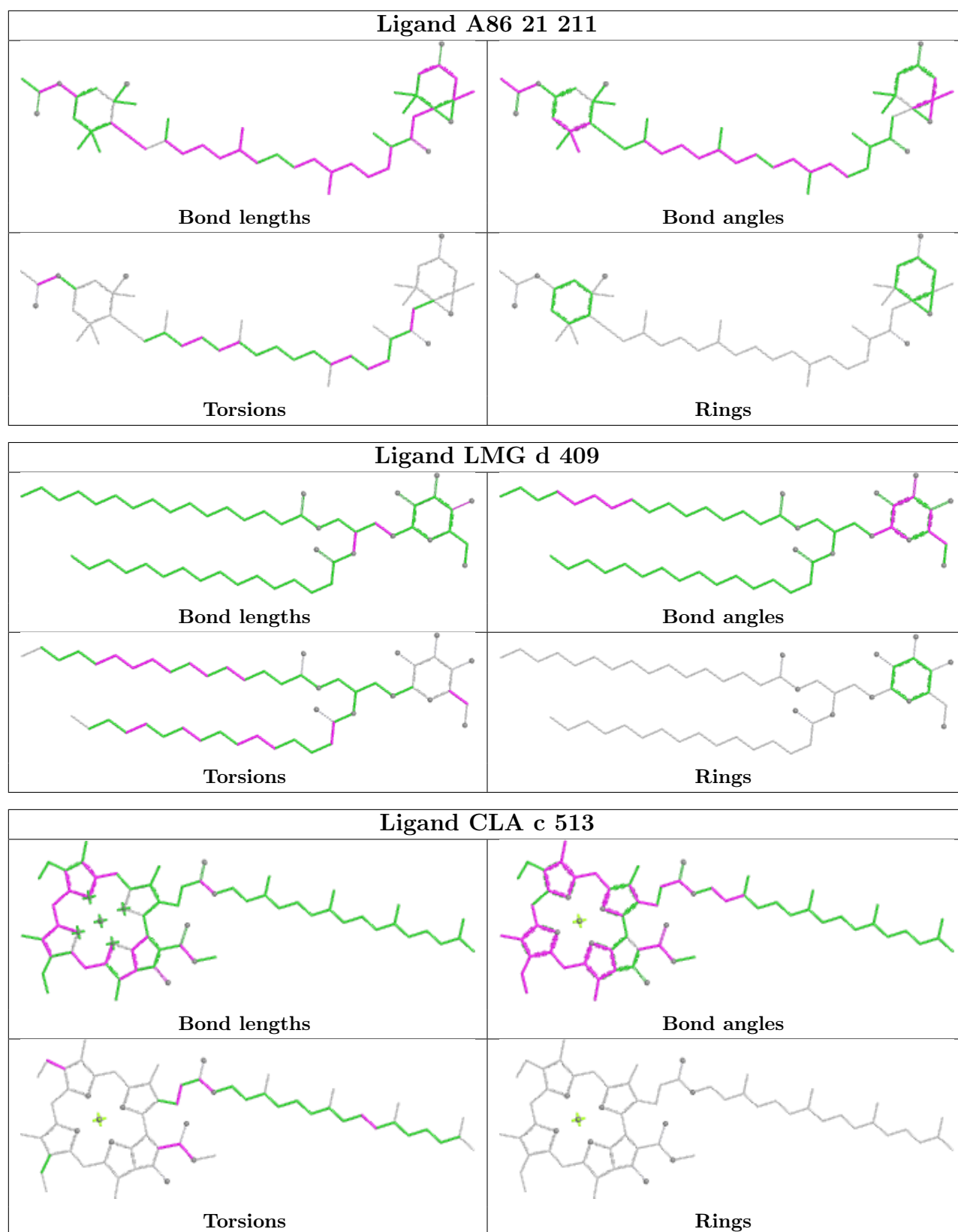


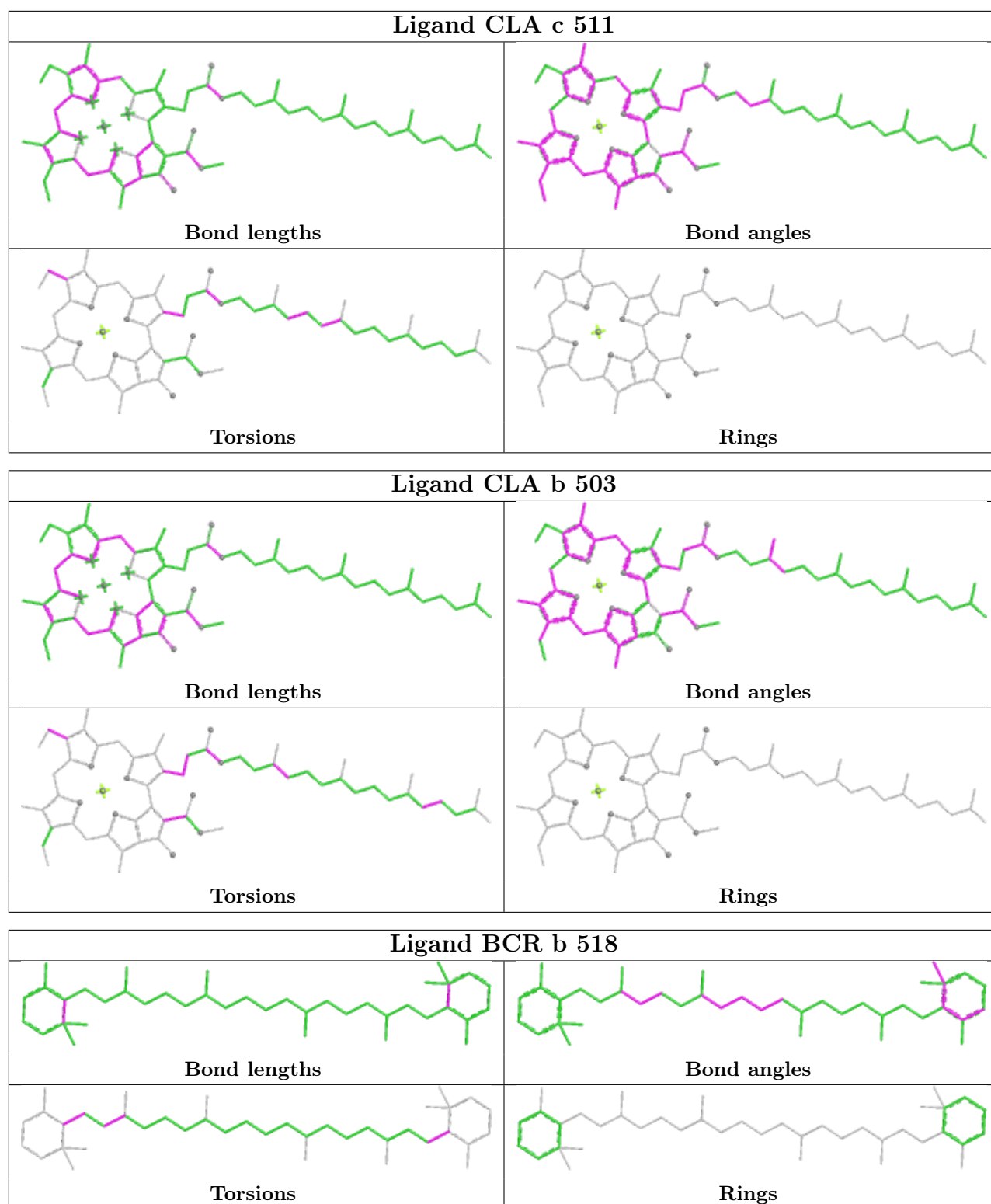


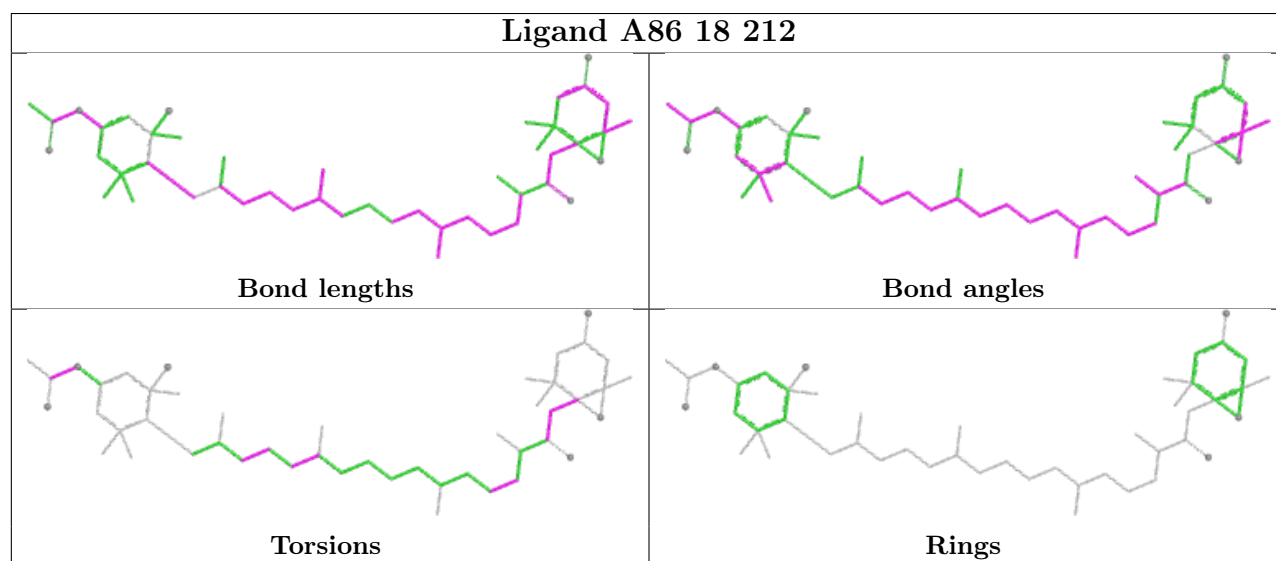
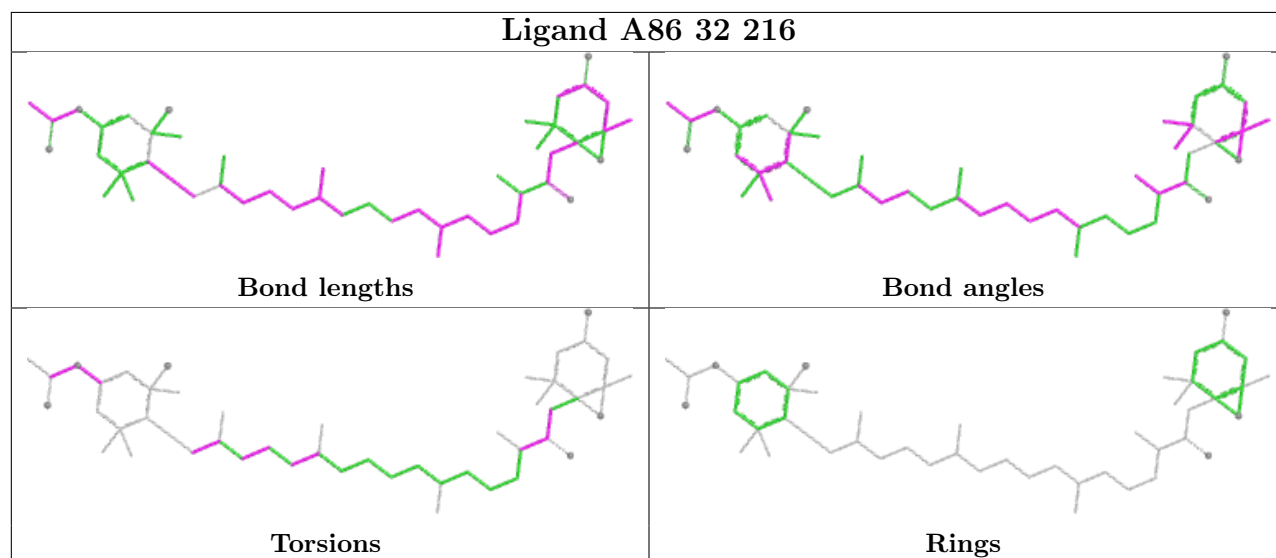
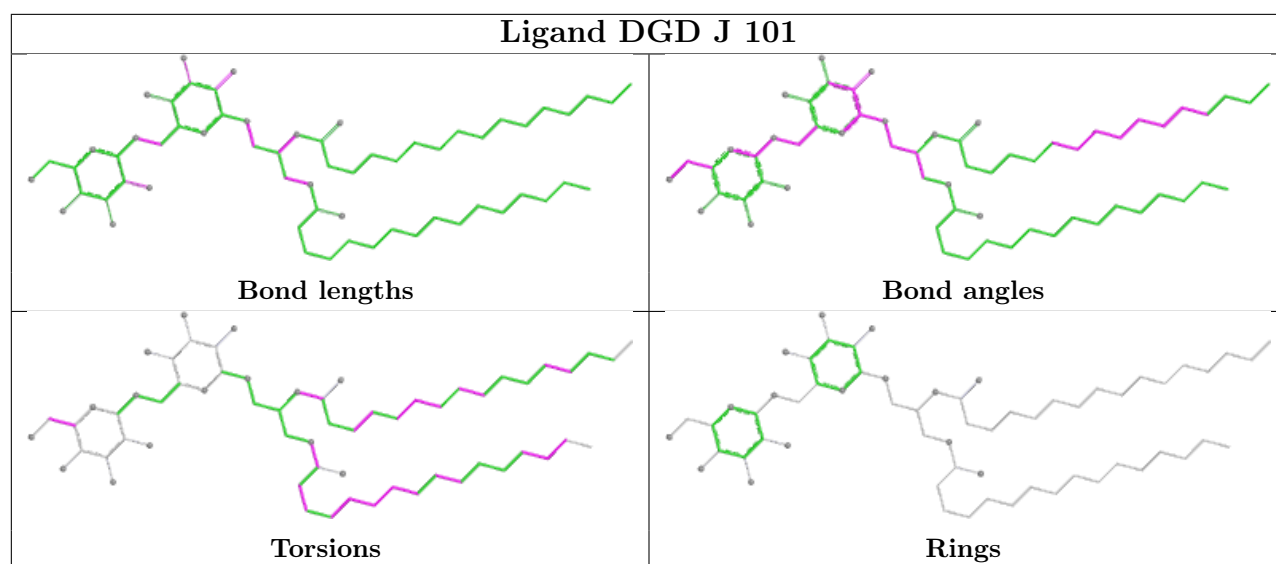


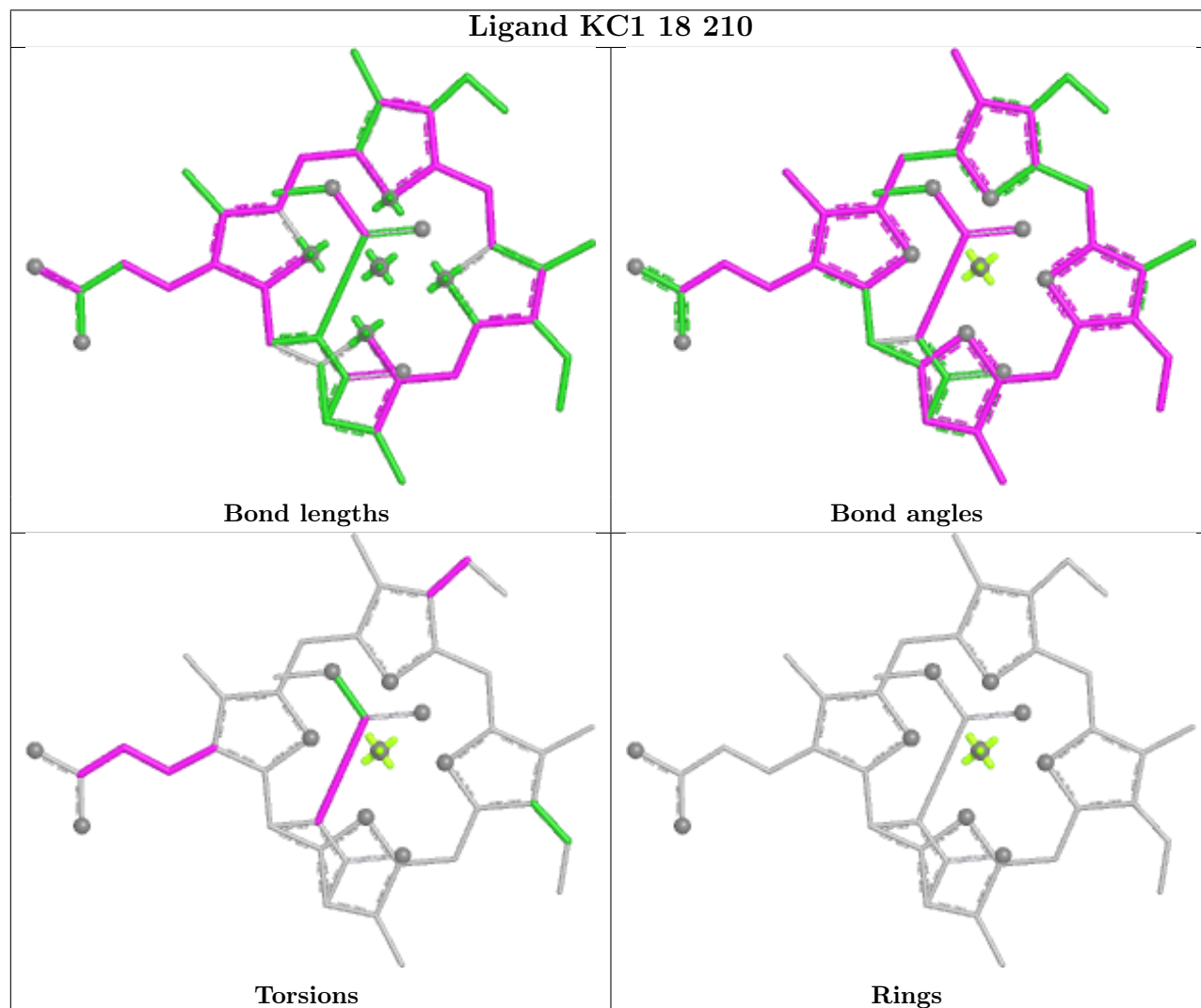
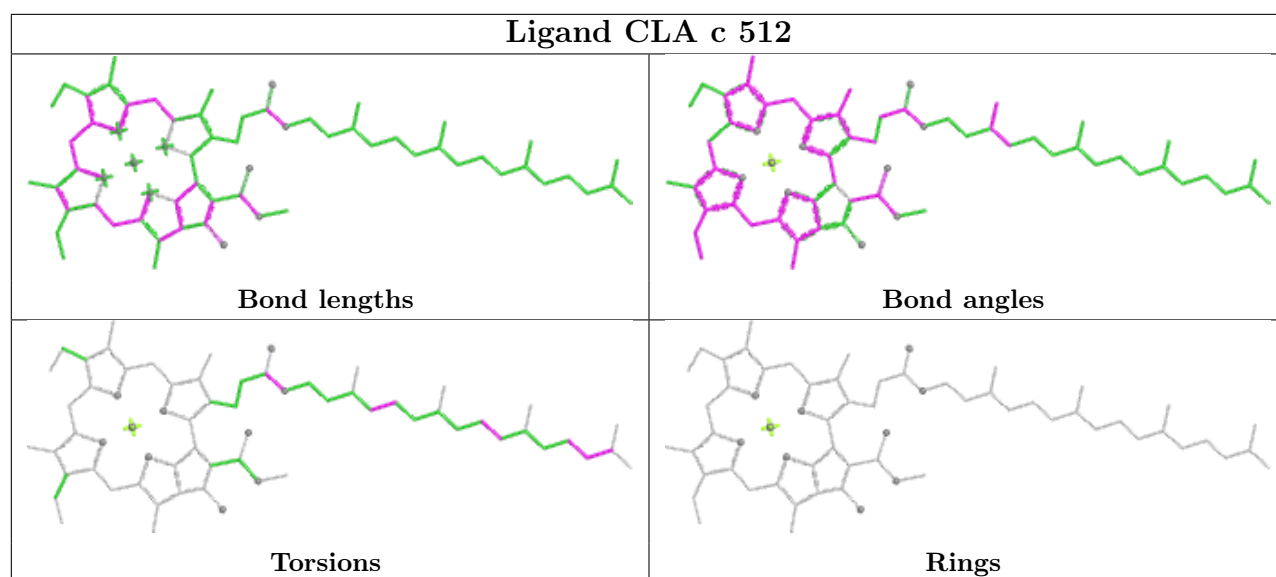


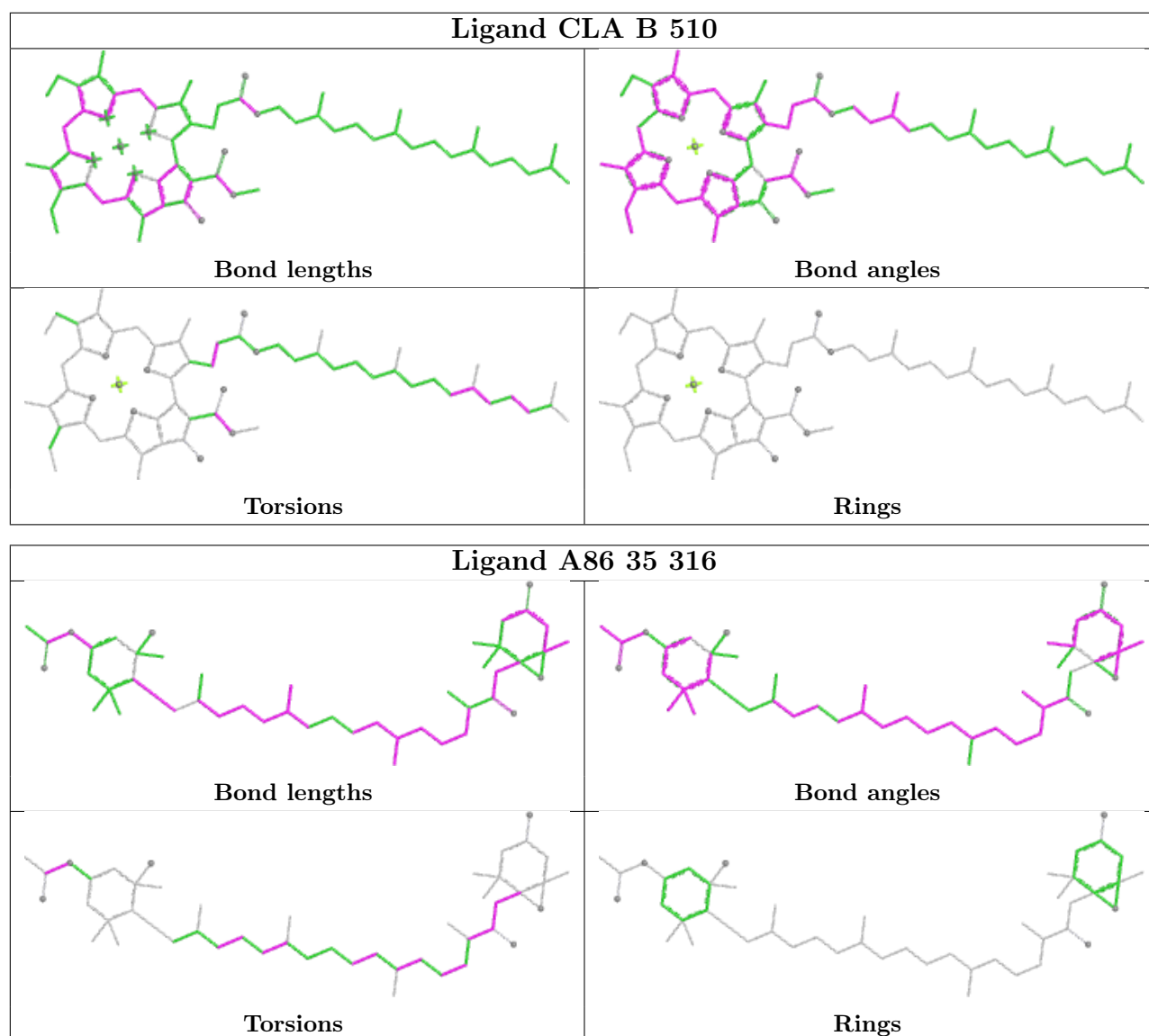


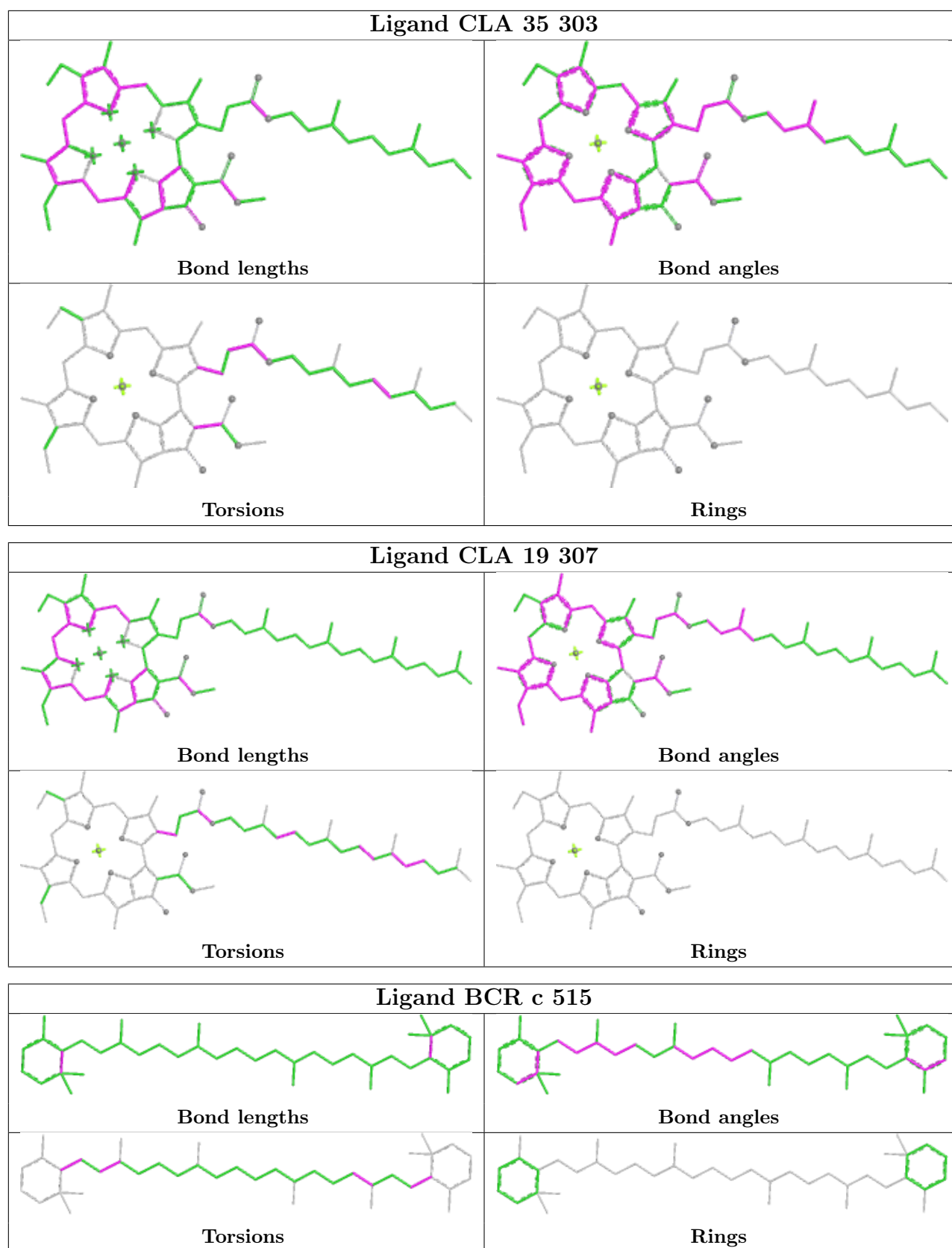


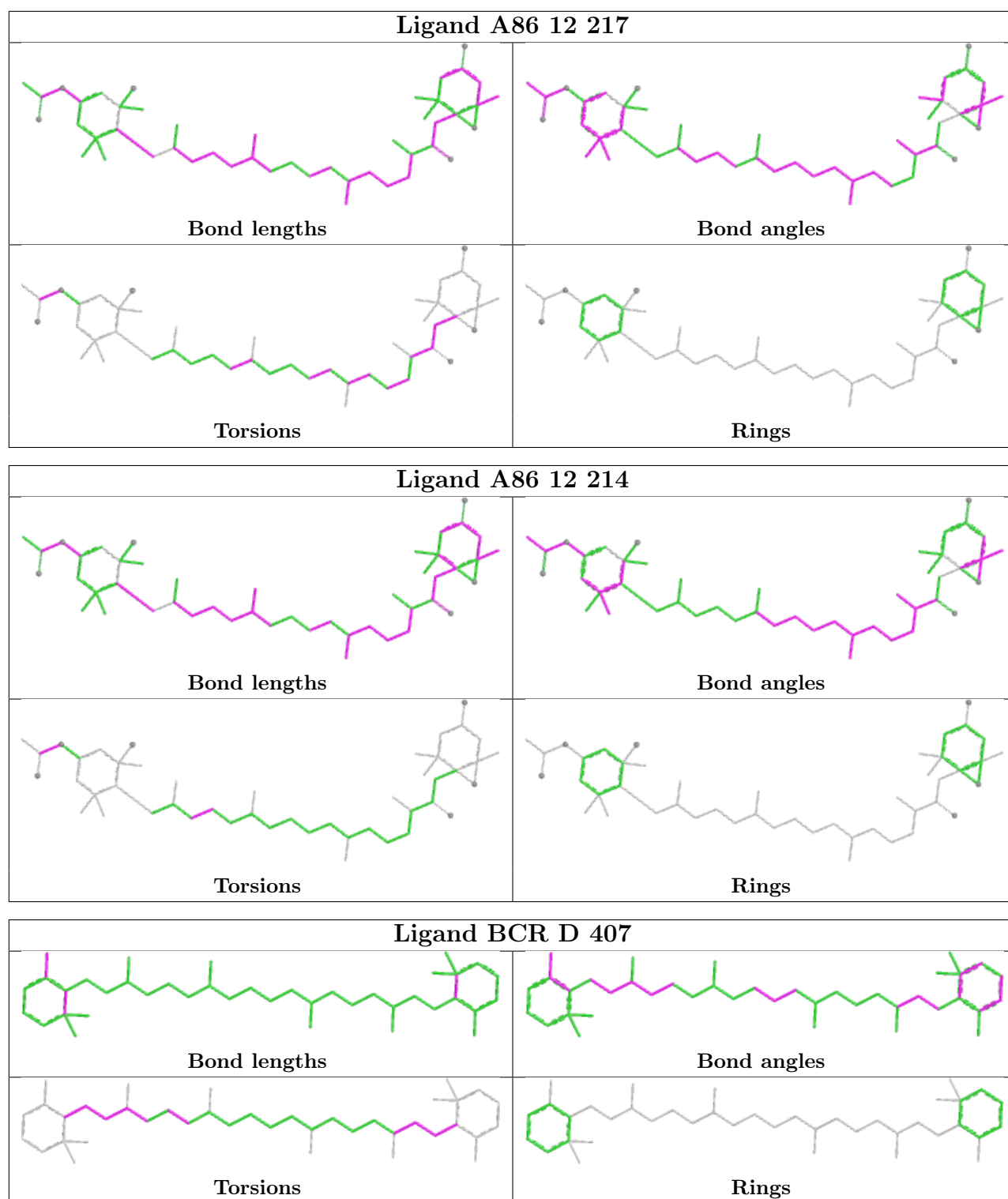


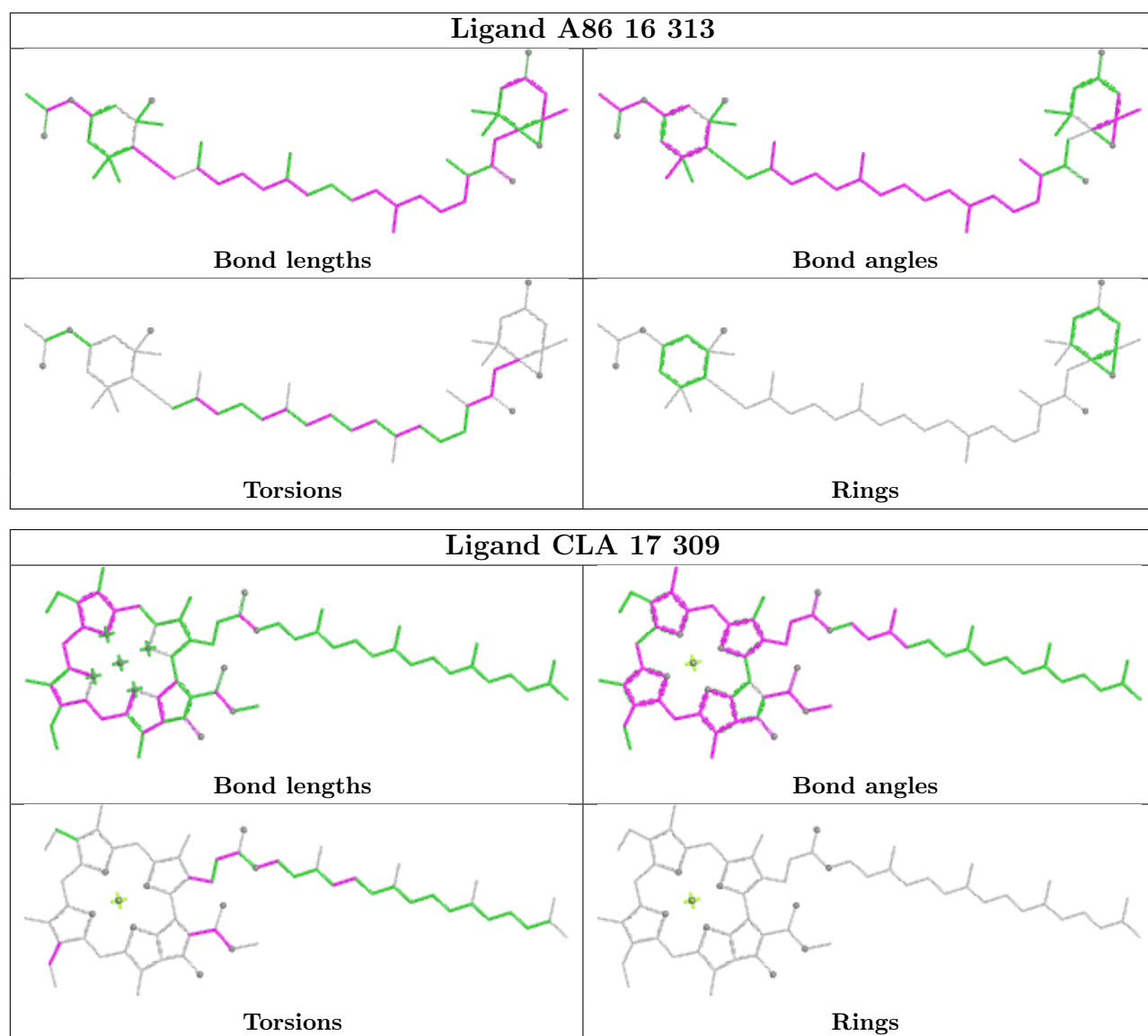


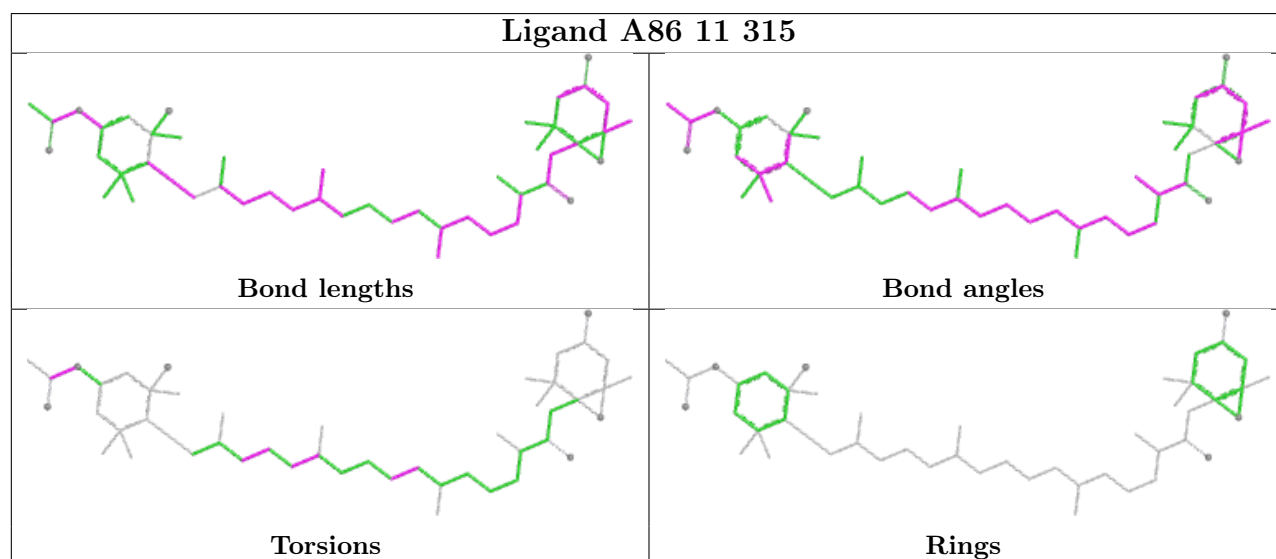
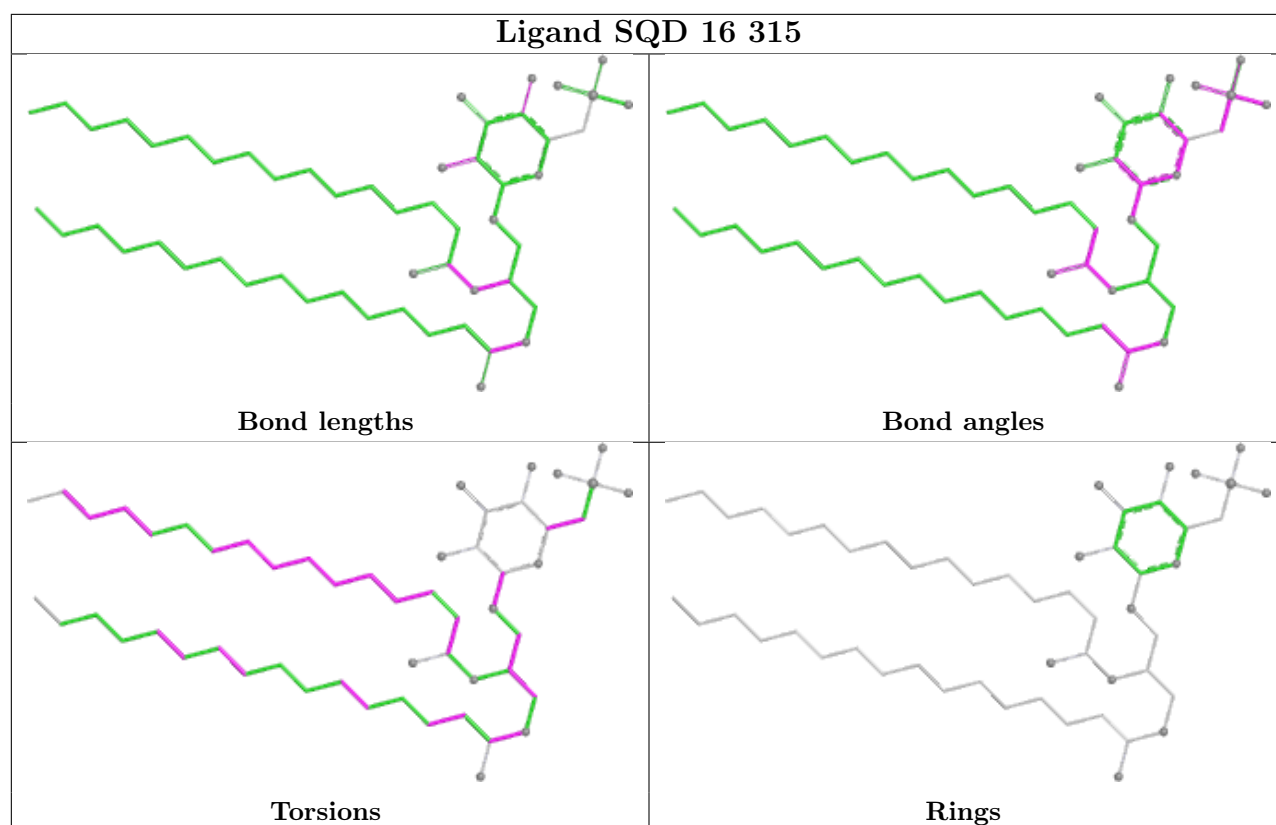


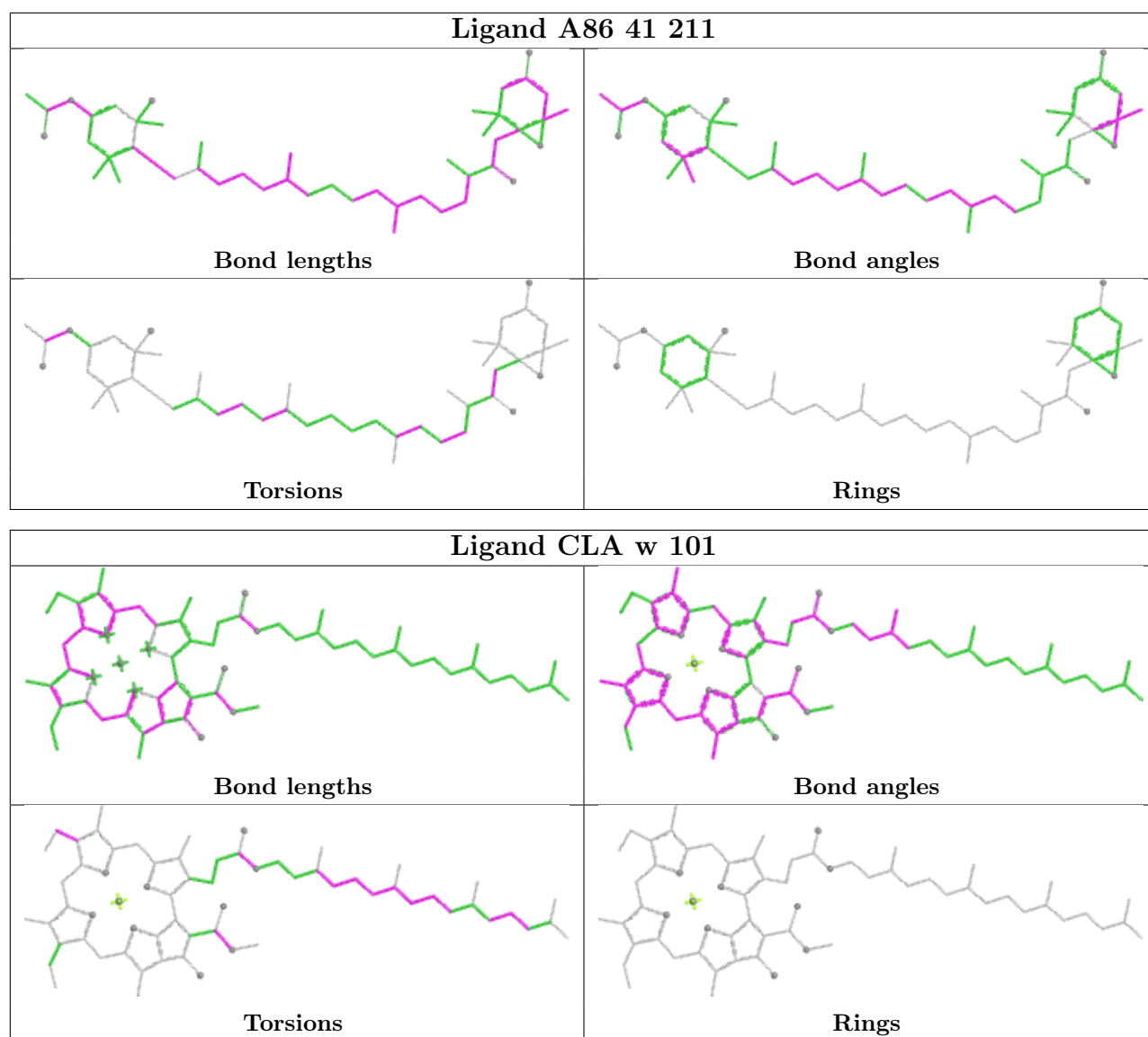


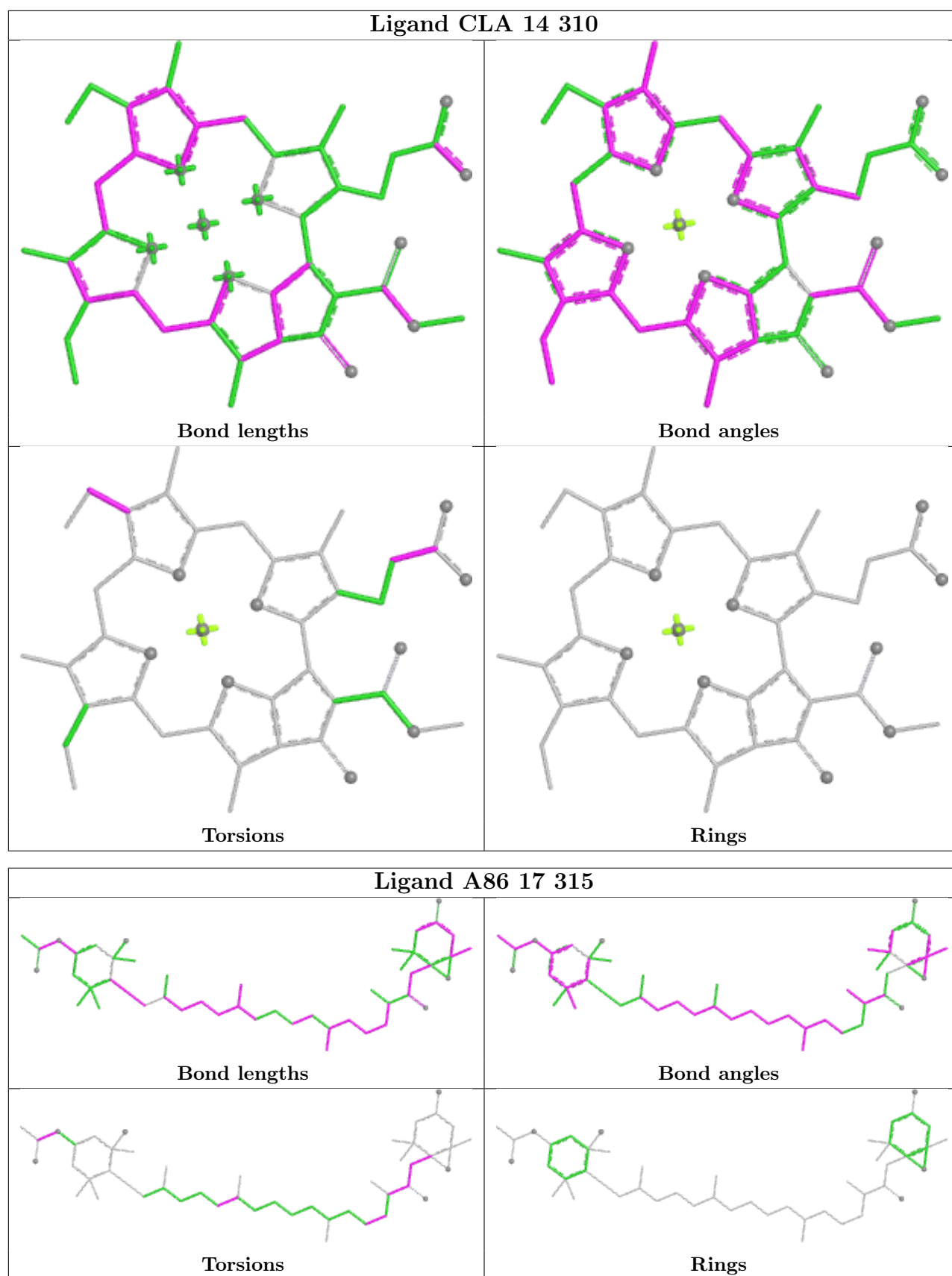


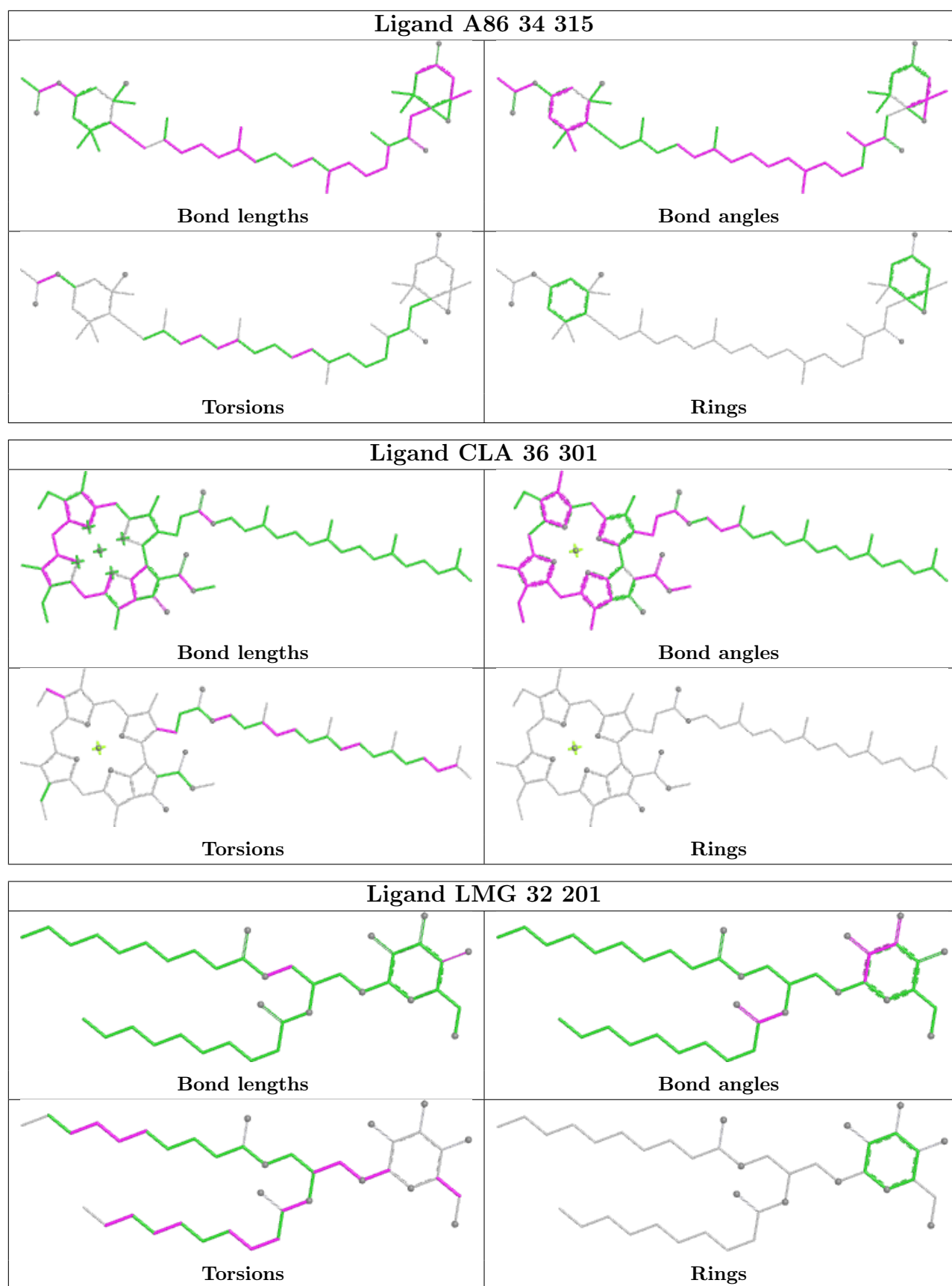


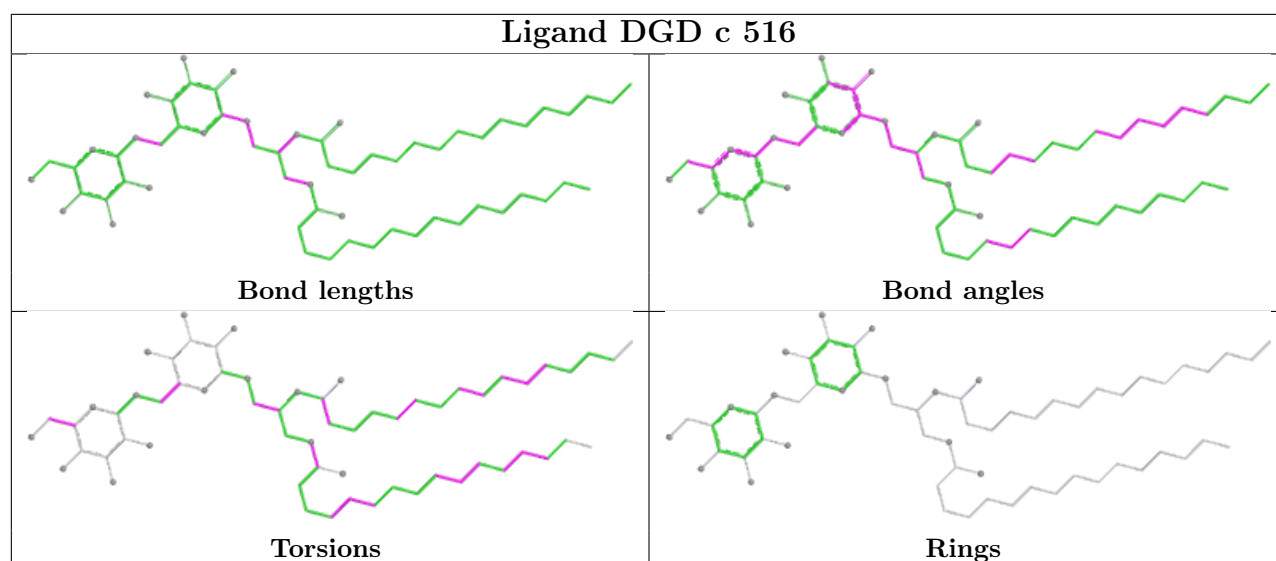
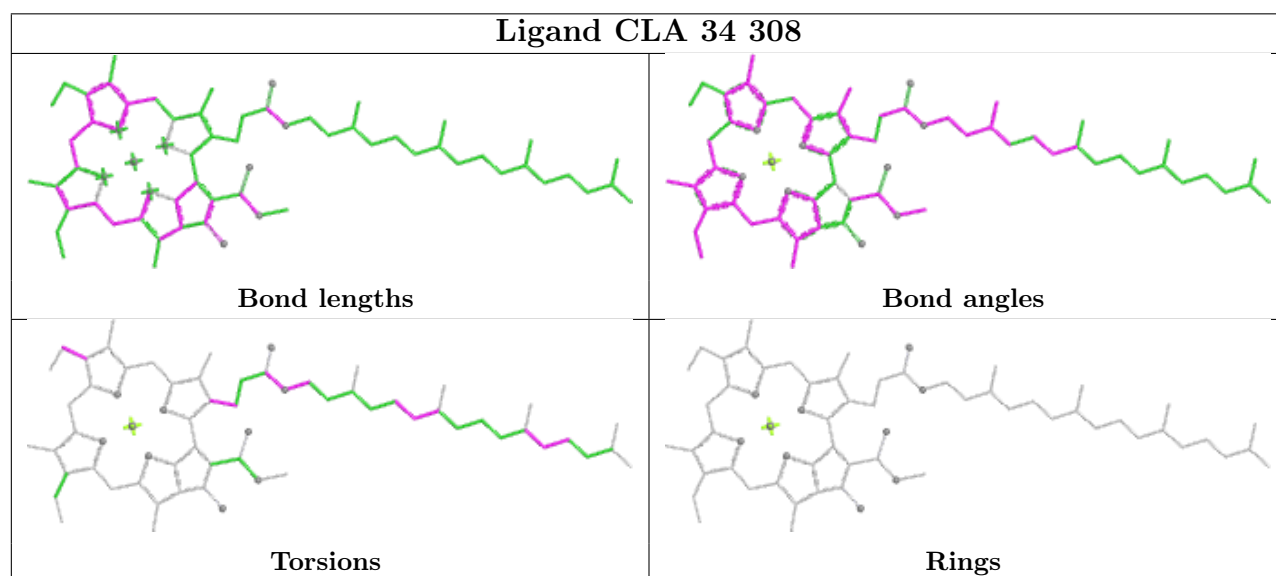
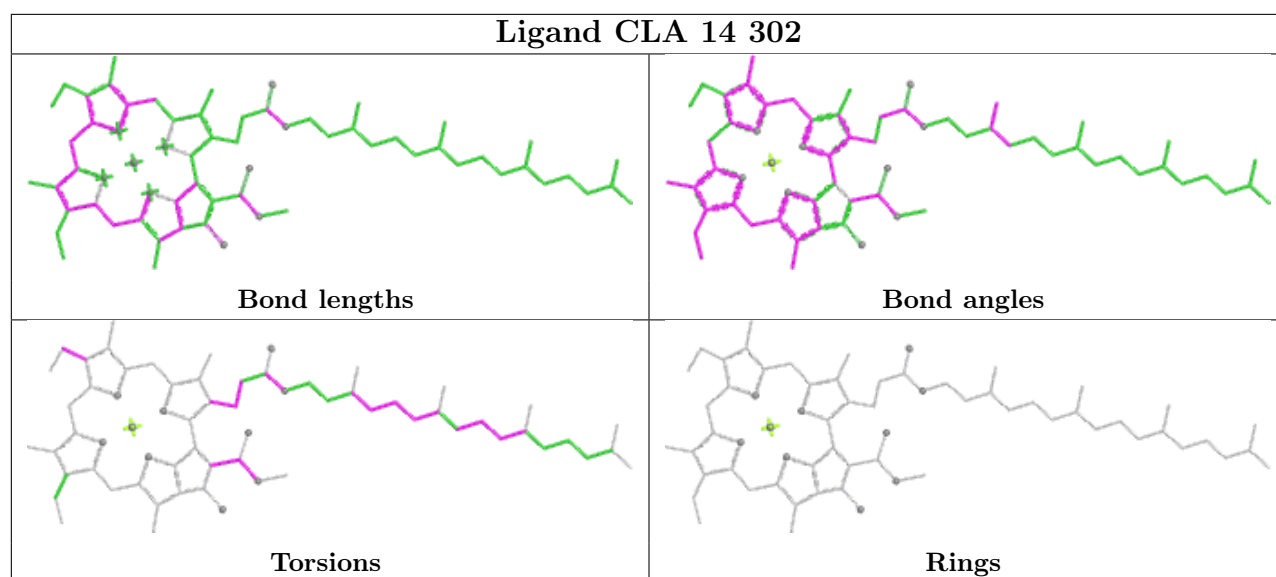


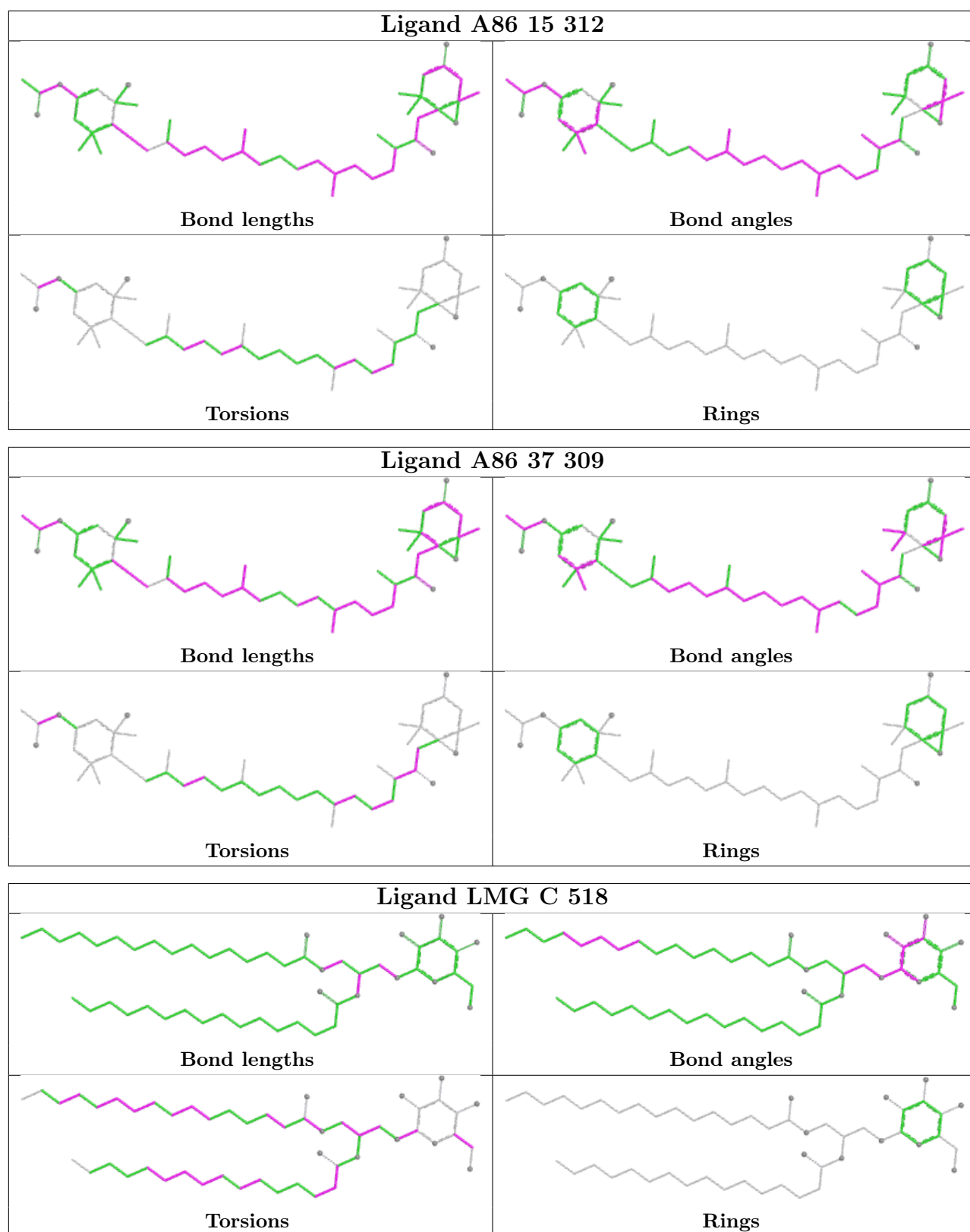




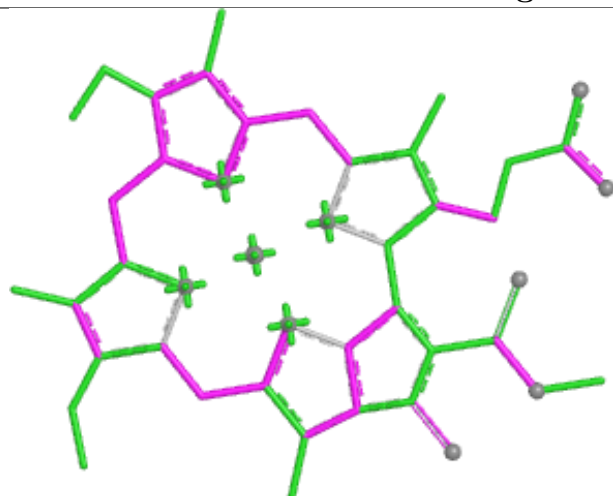




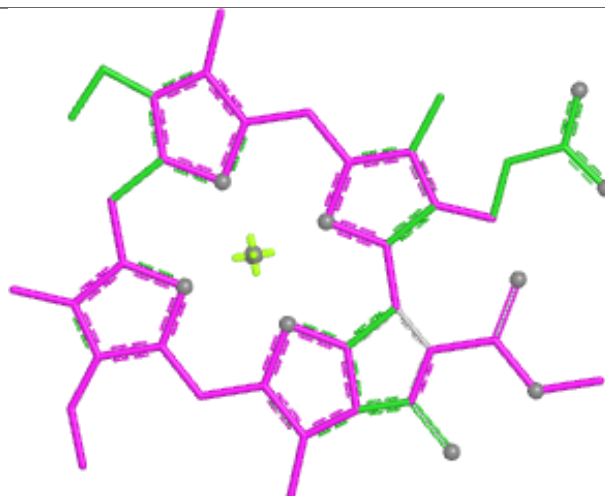




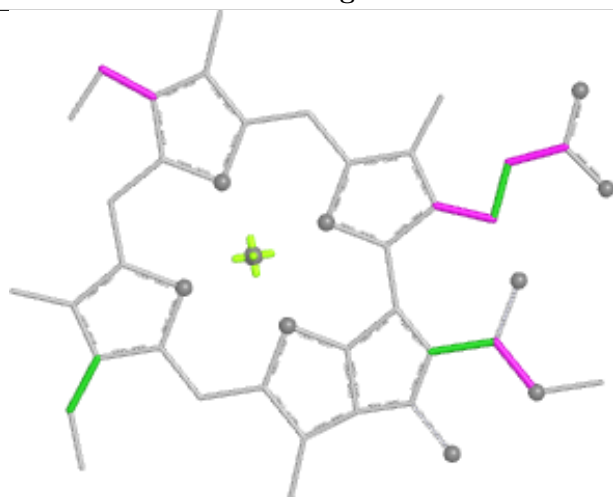
Ligand CLA Z 102



Bond lengths



Bond angles

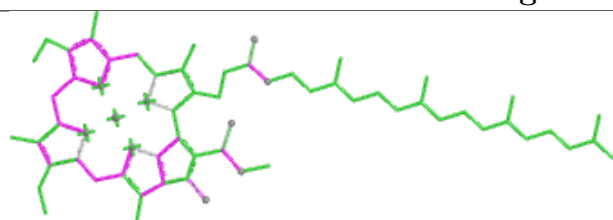


Torsions

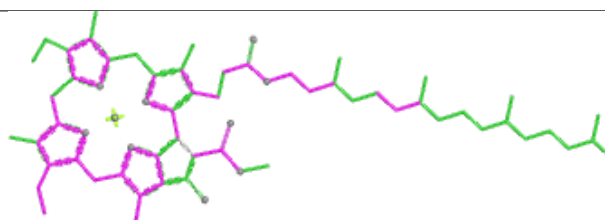


Rings

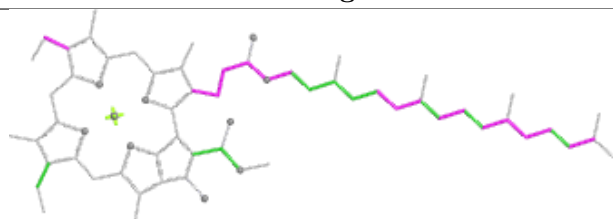
Ligand CLA z 101



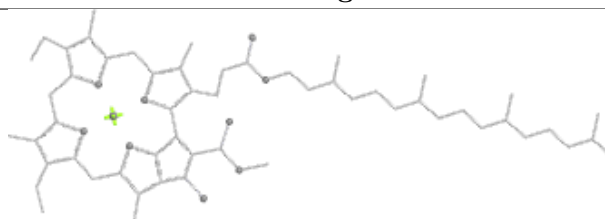
Bond lengths



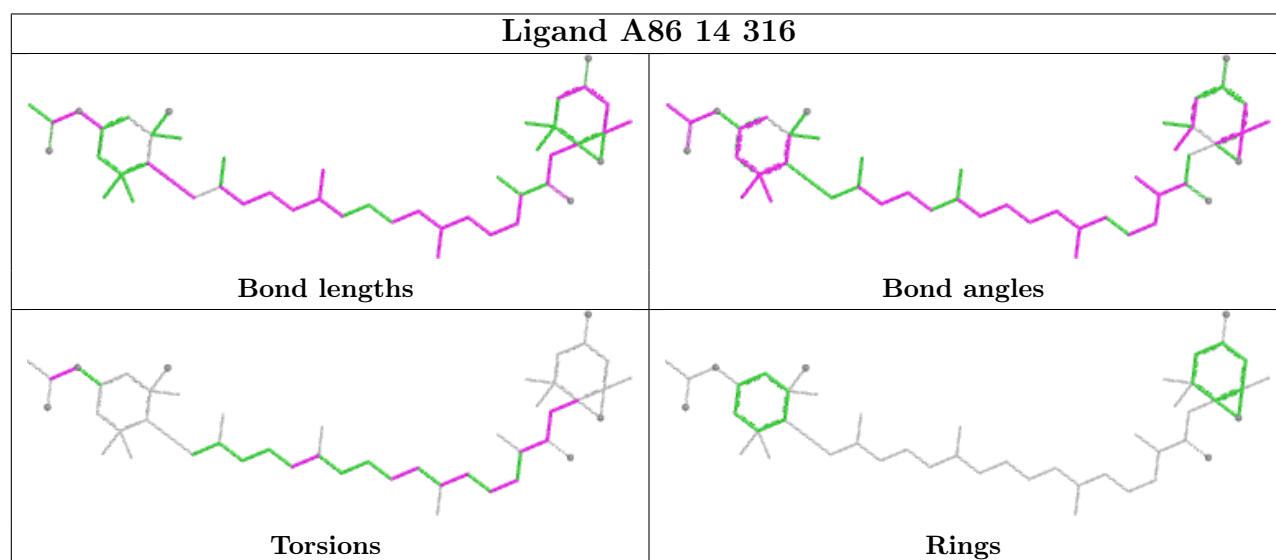
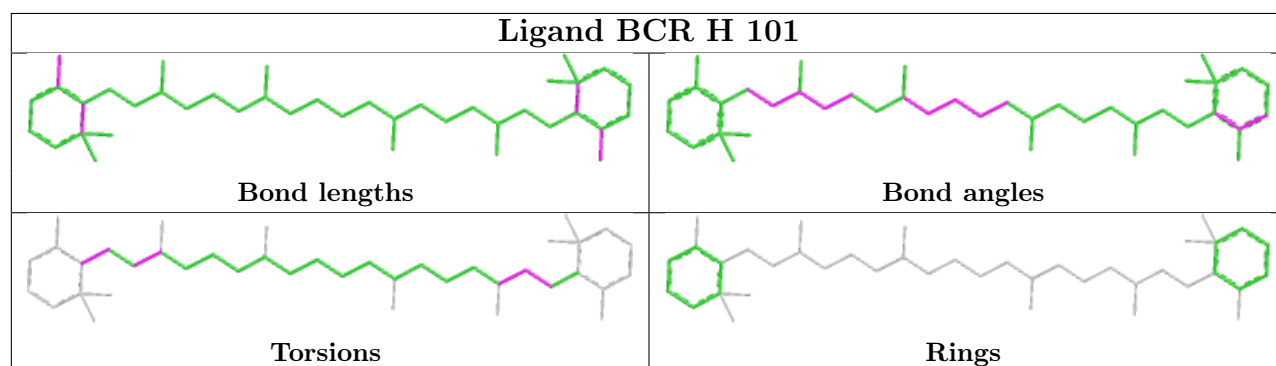
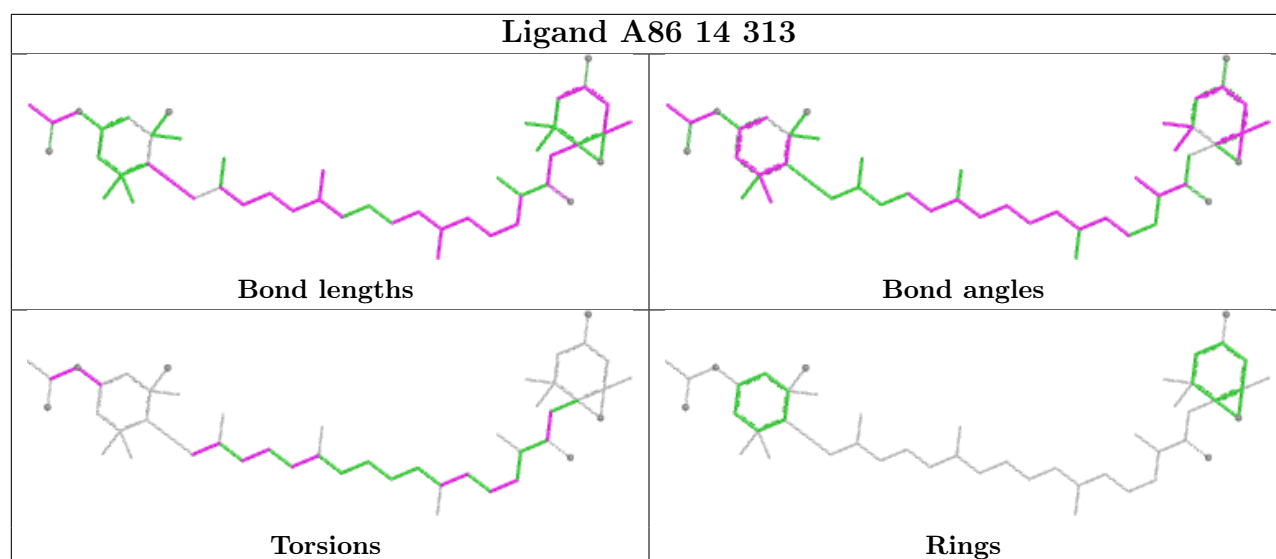
Bond angles

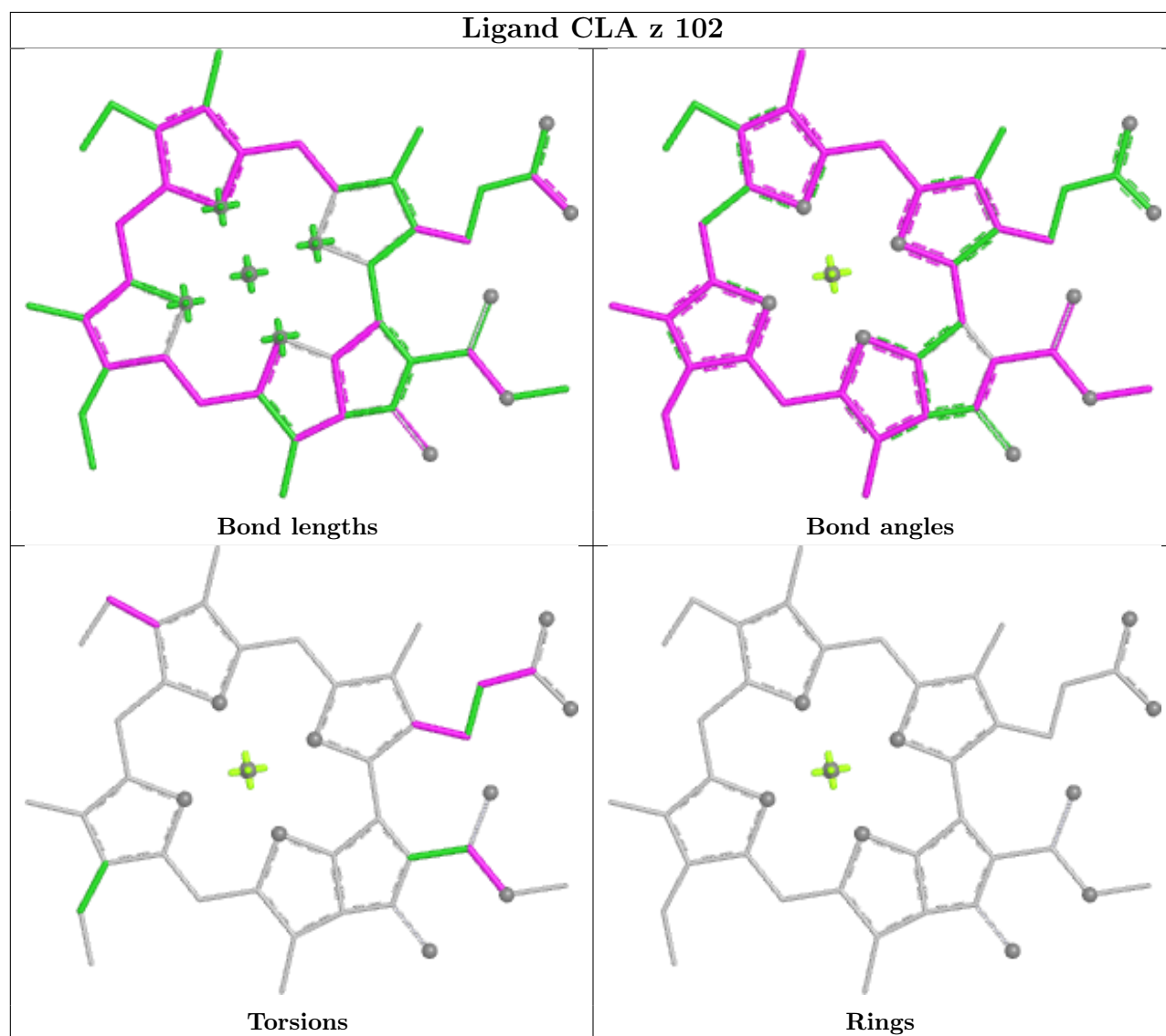
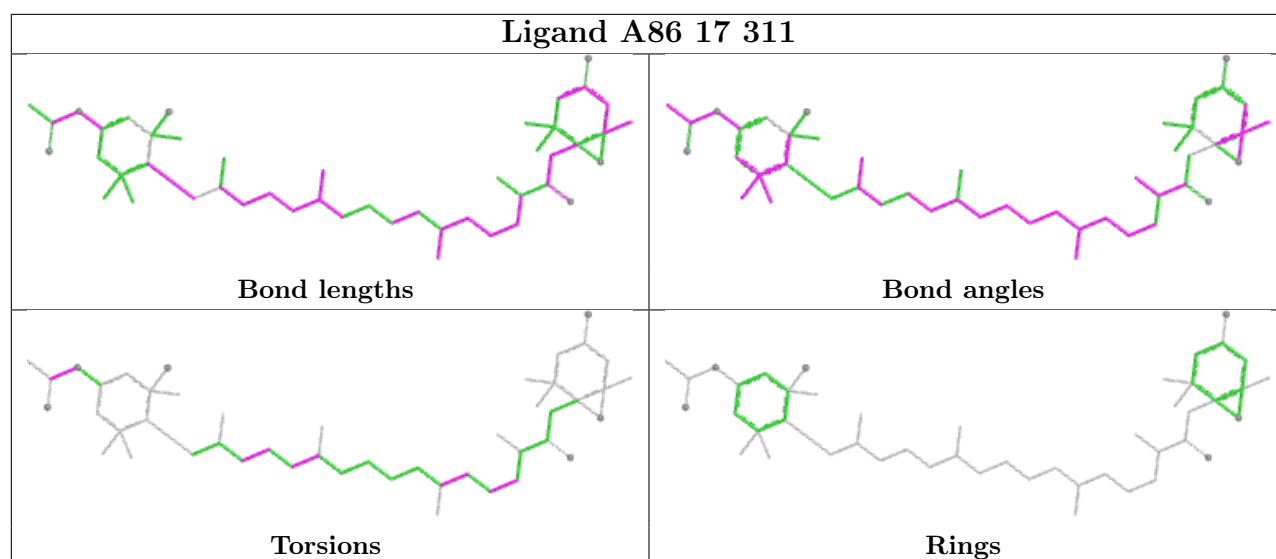


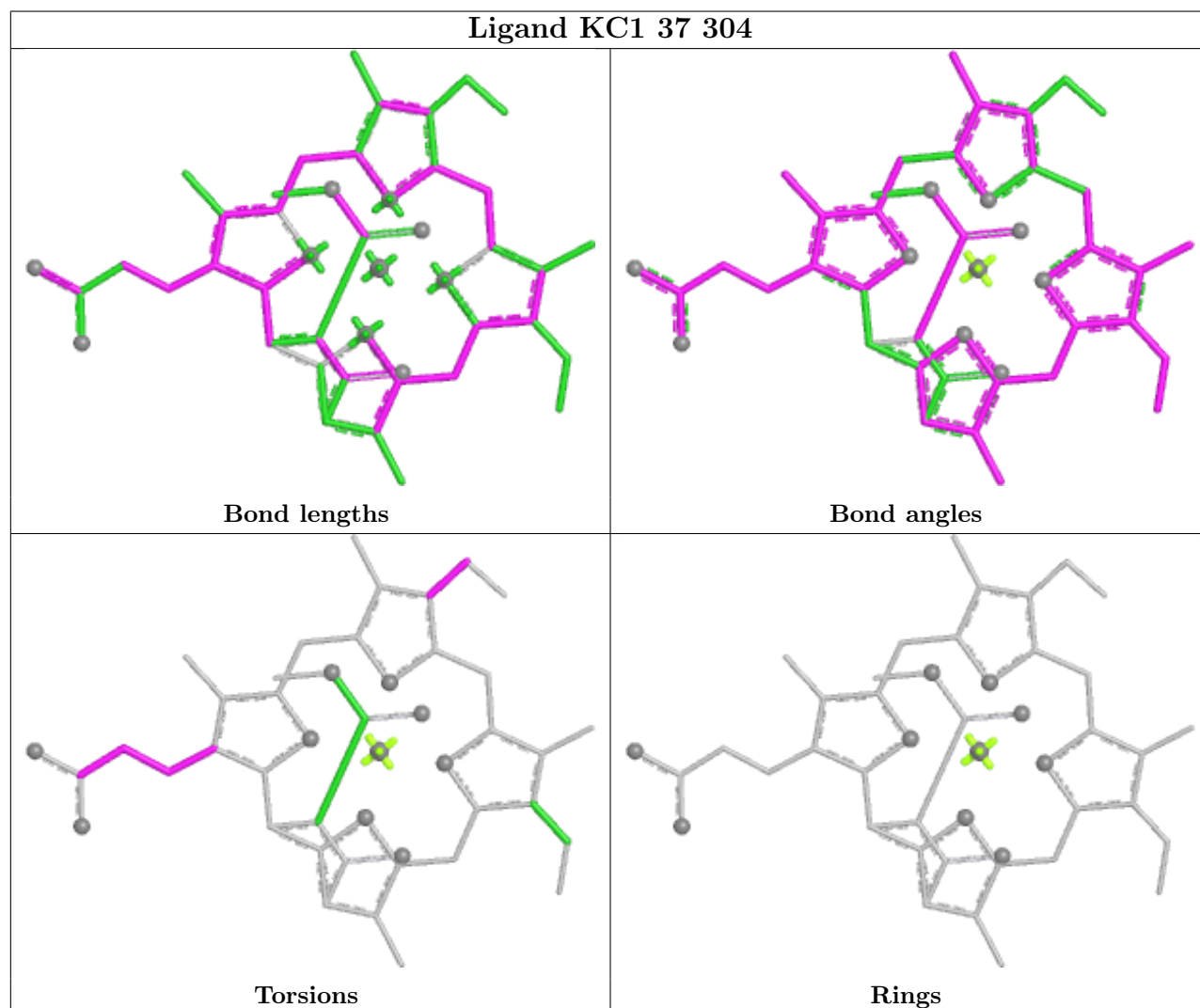
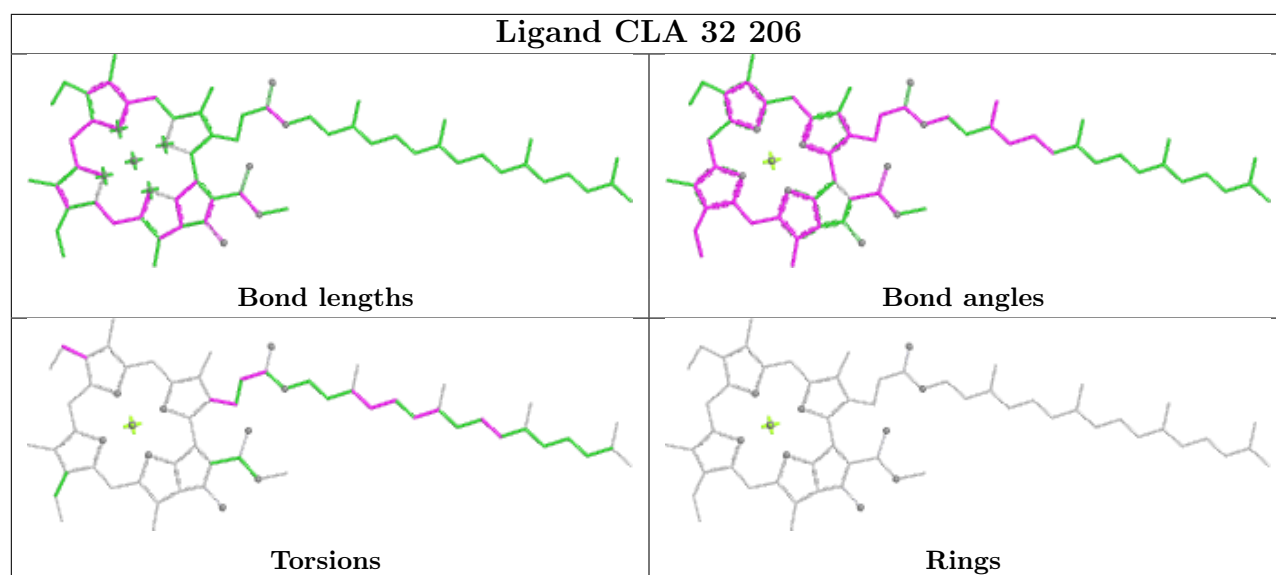
Torsions

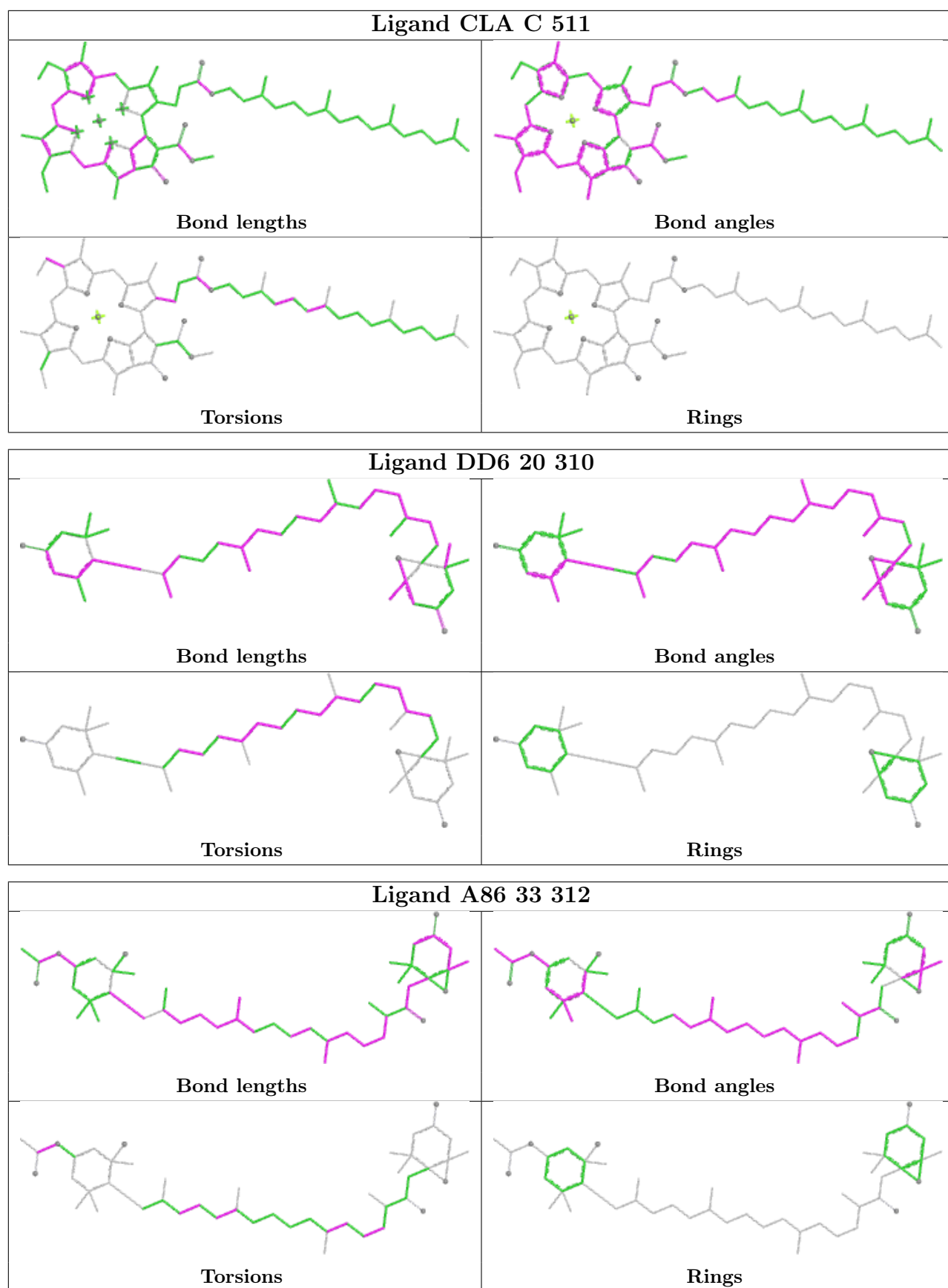


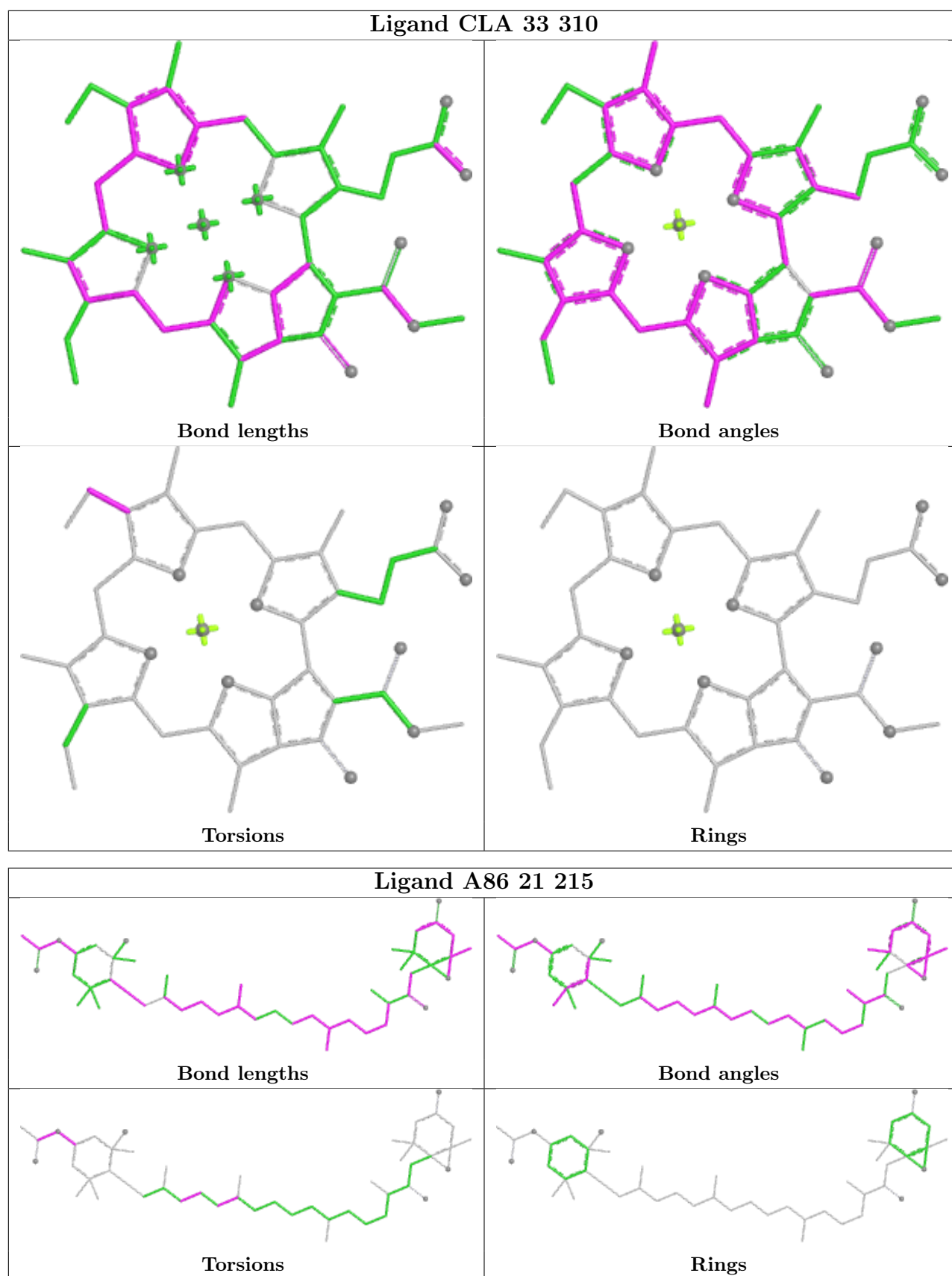
Rings

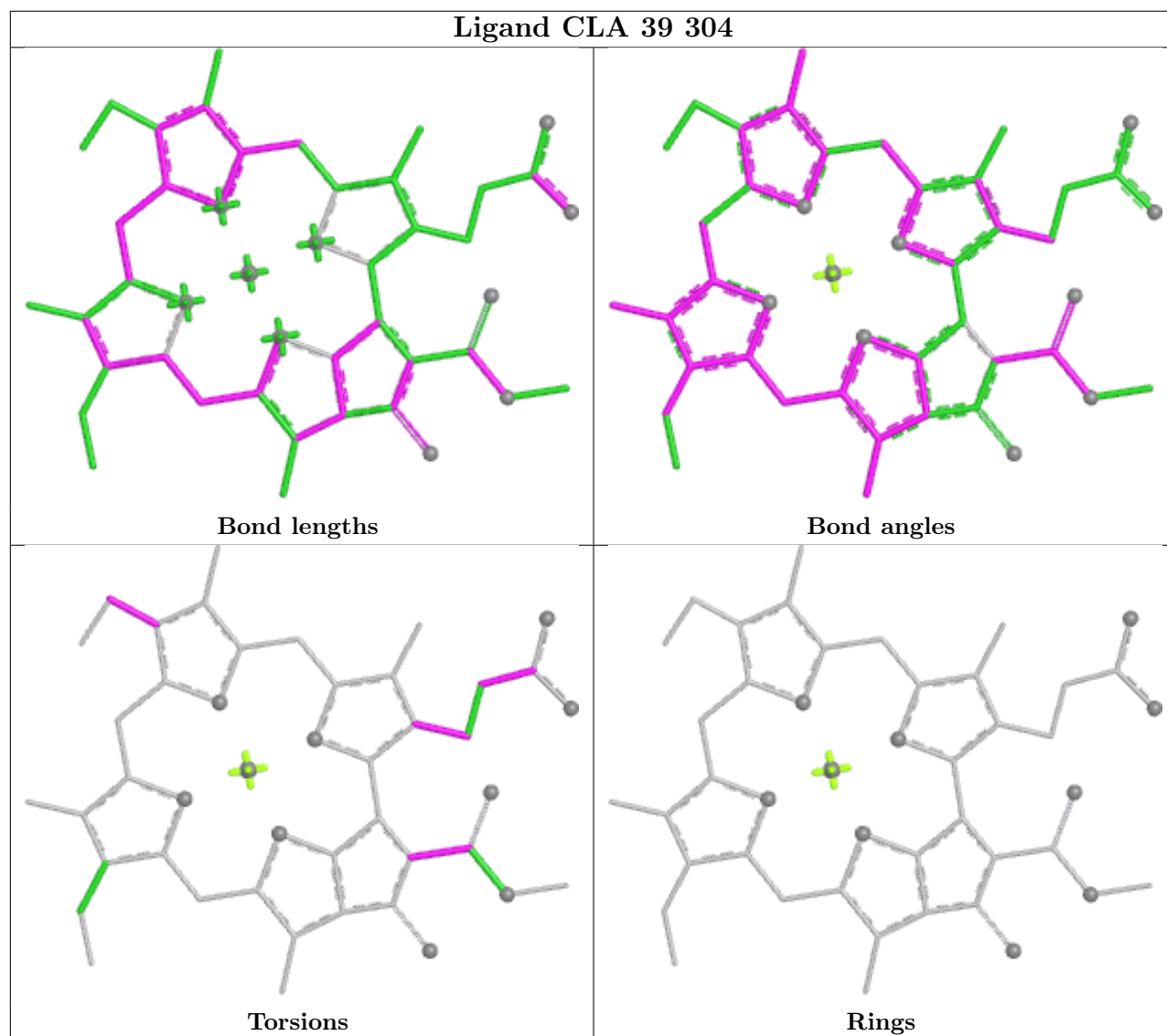
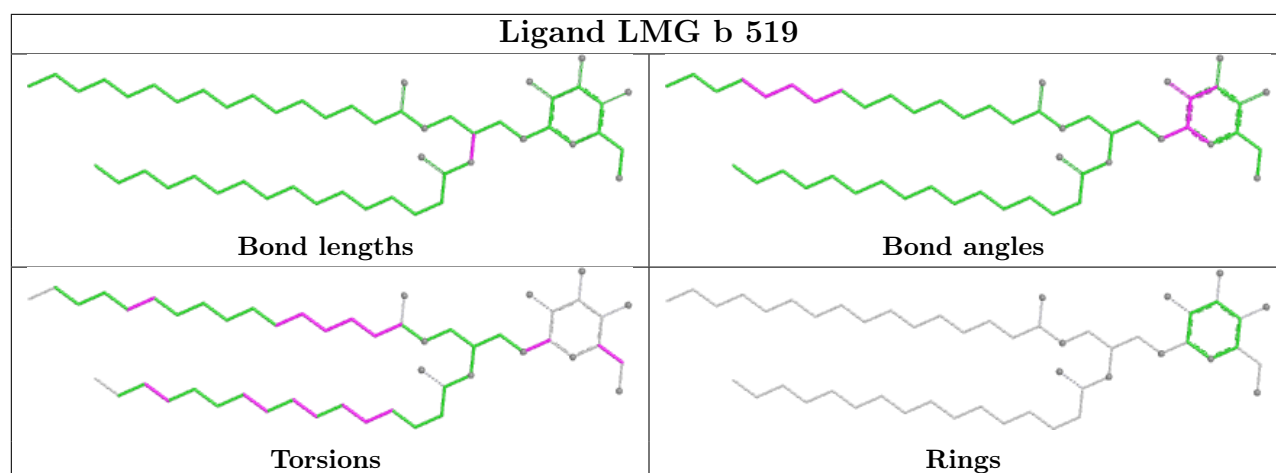


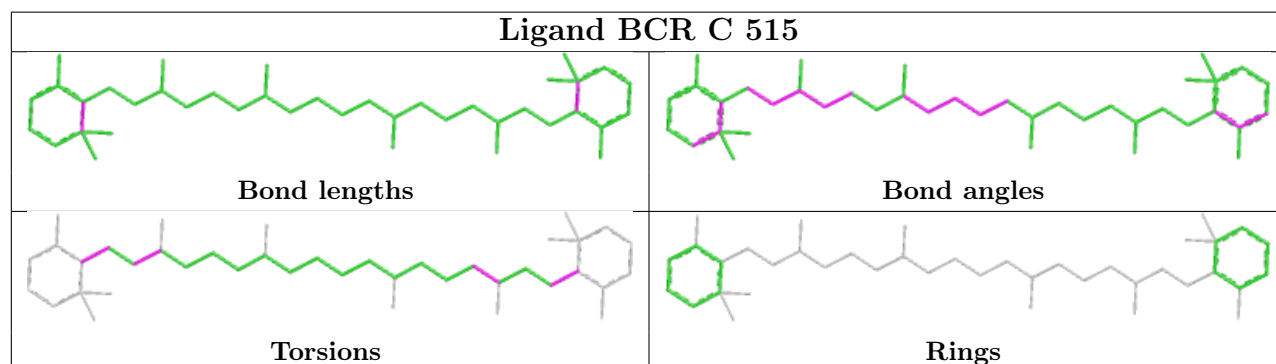
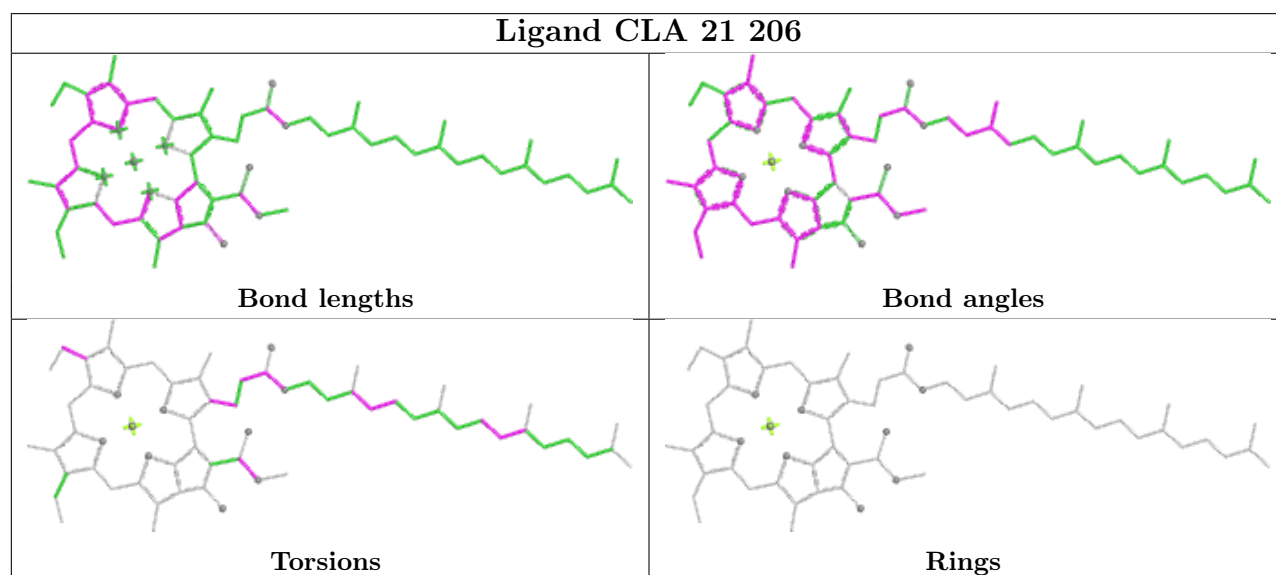
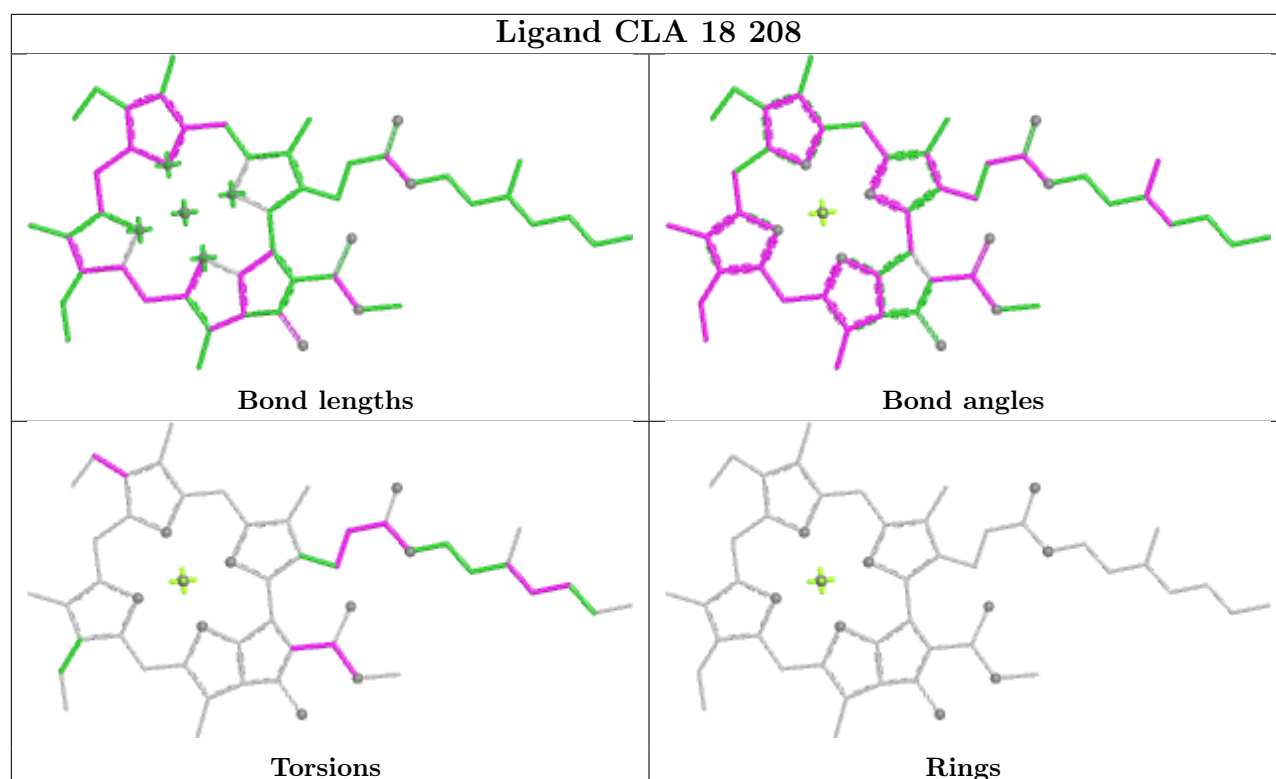


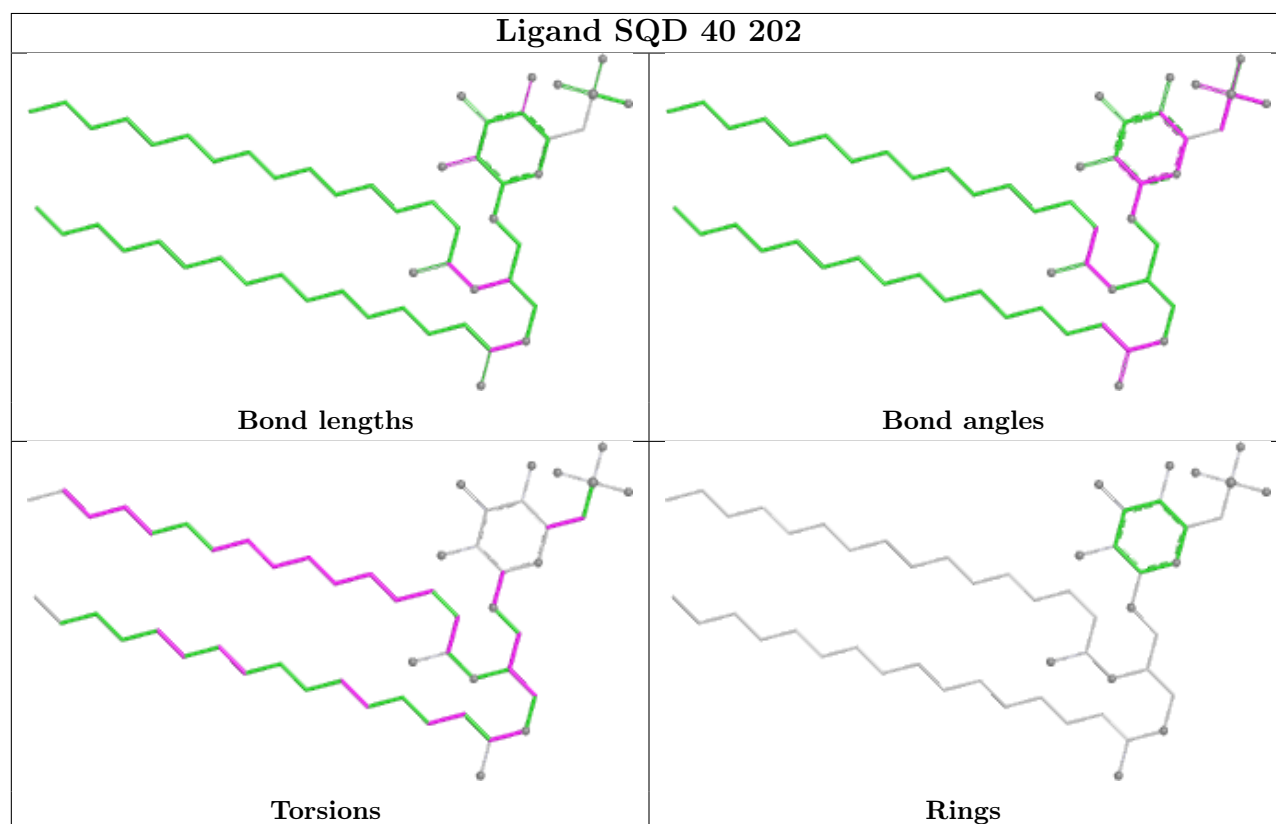
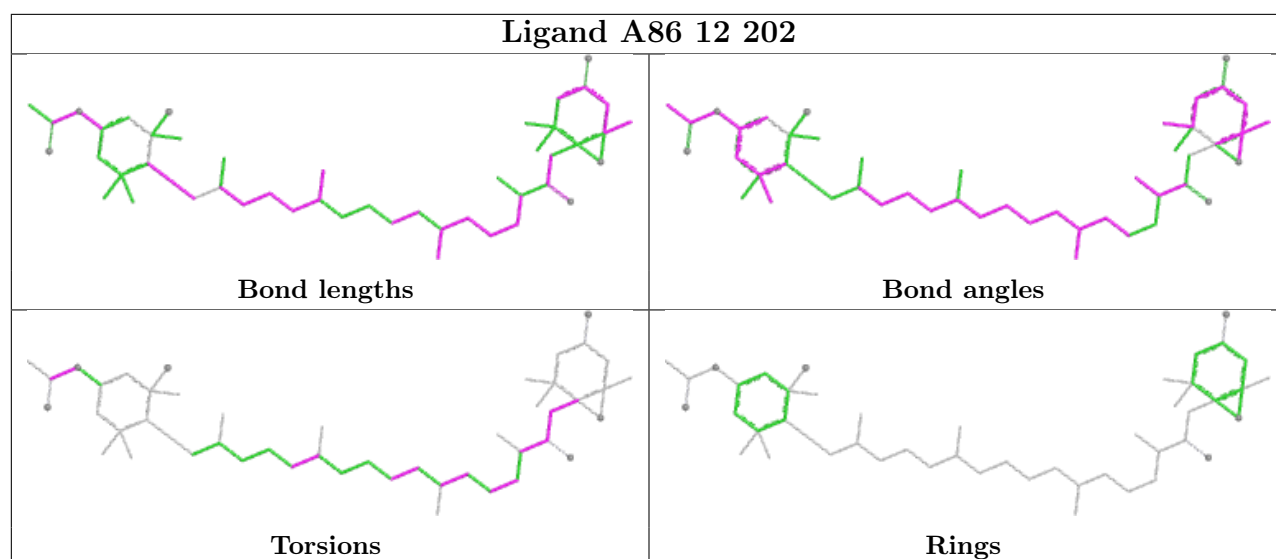


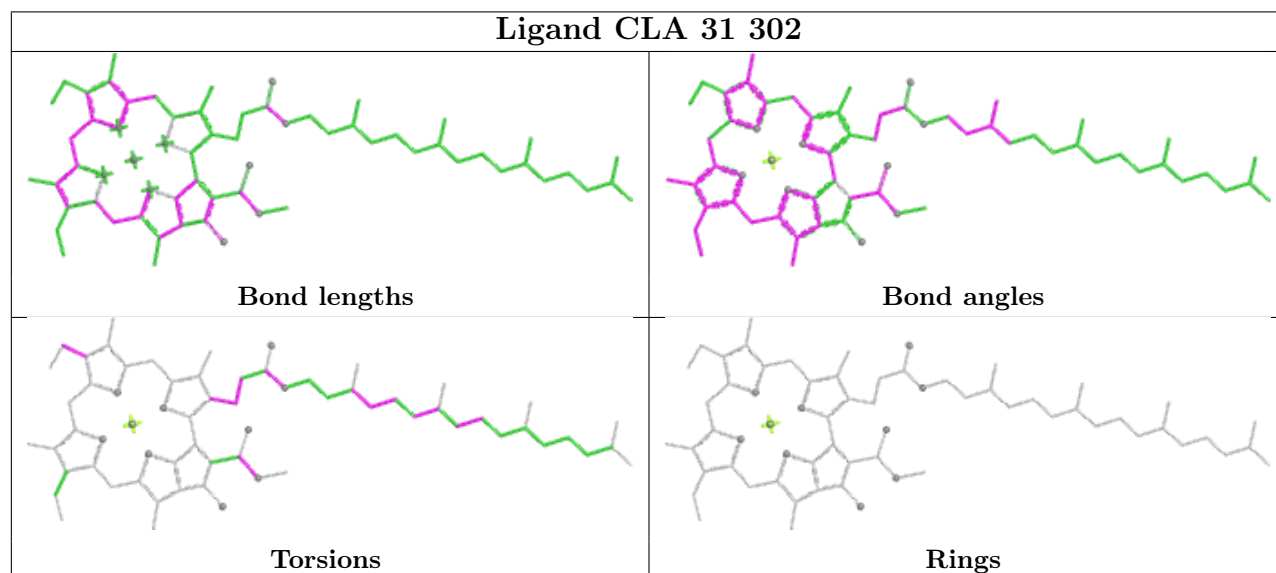
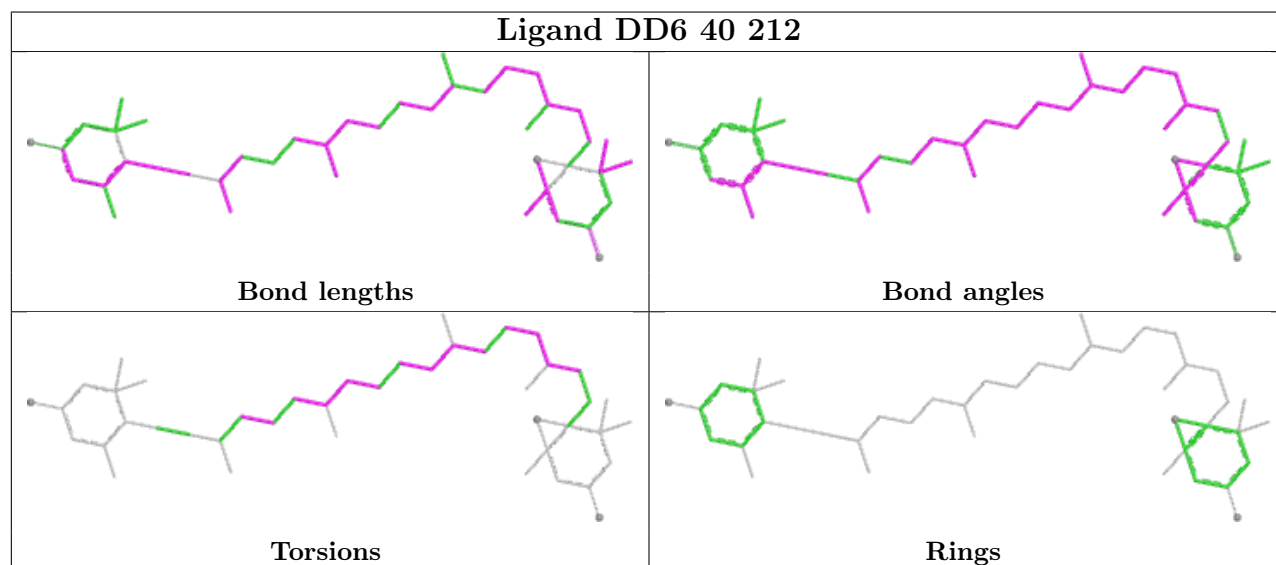
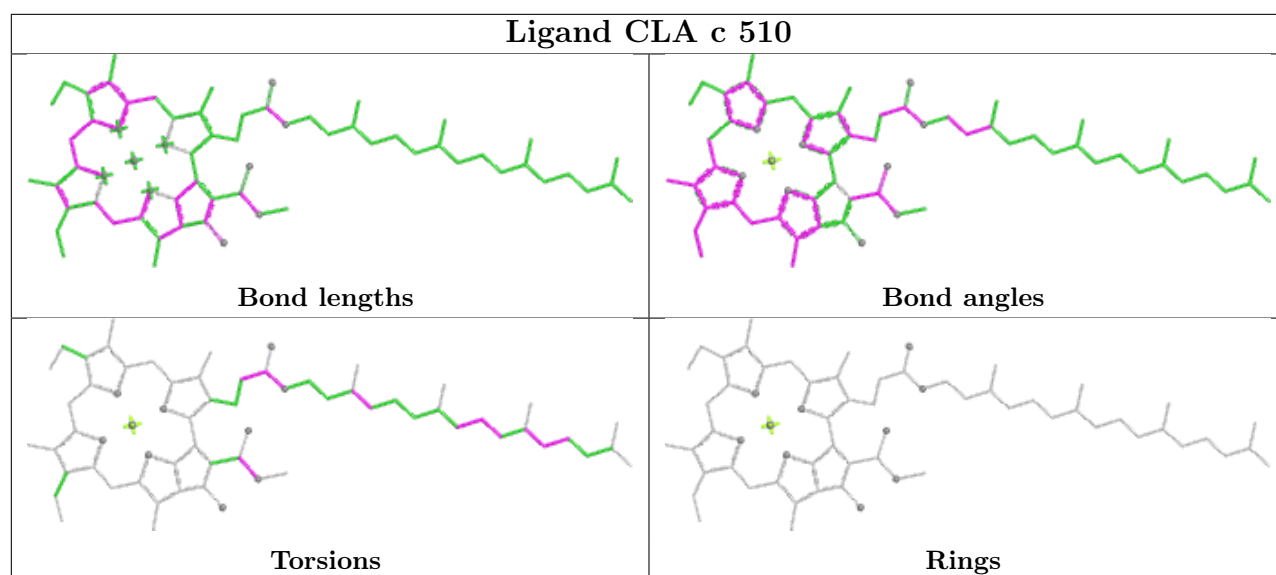


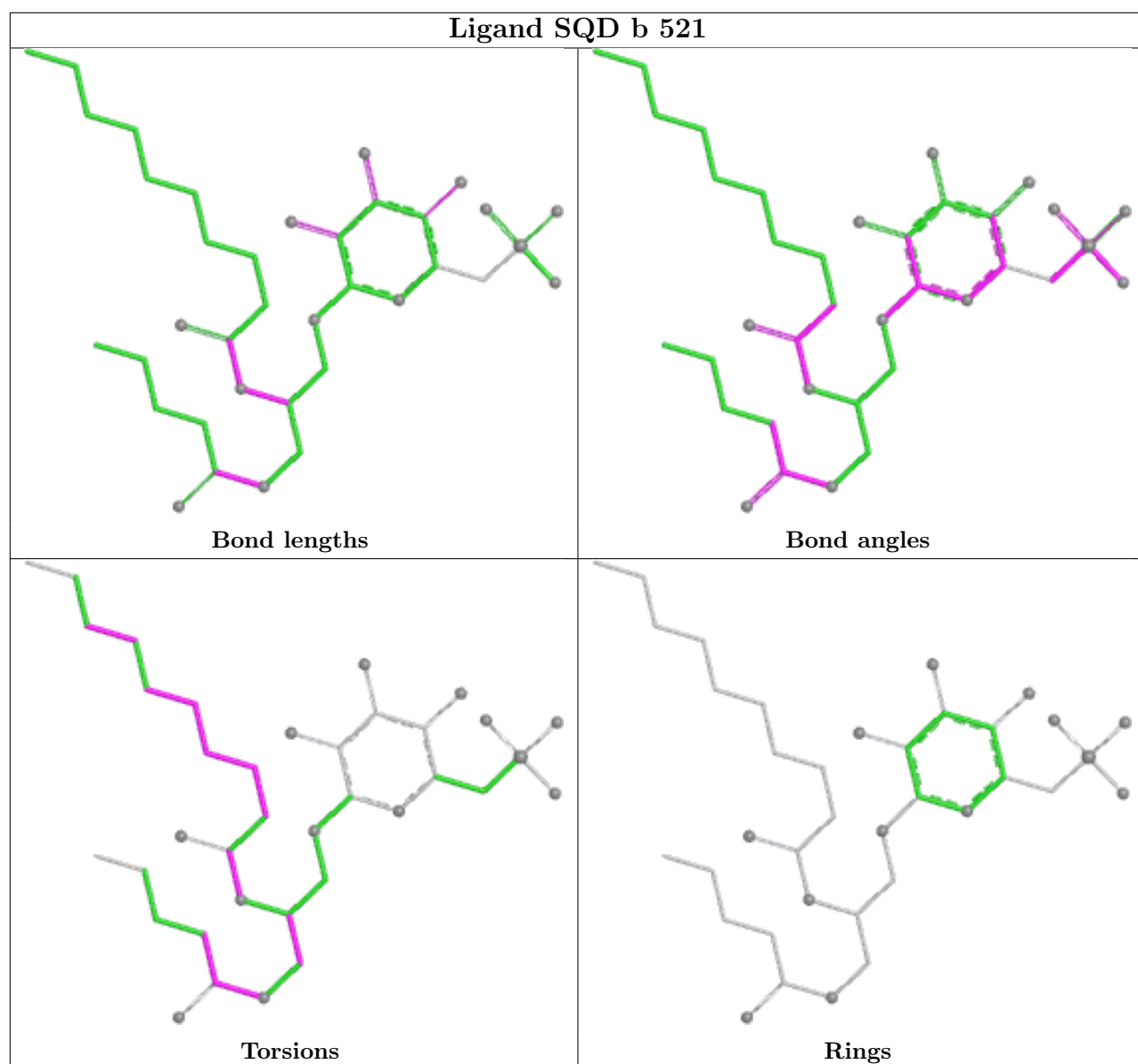


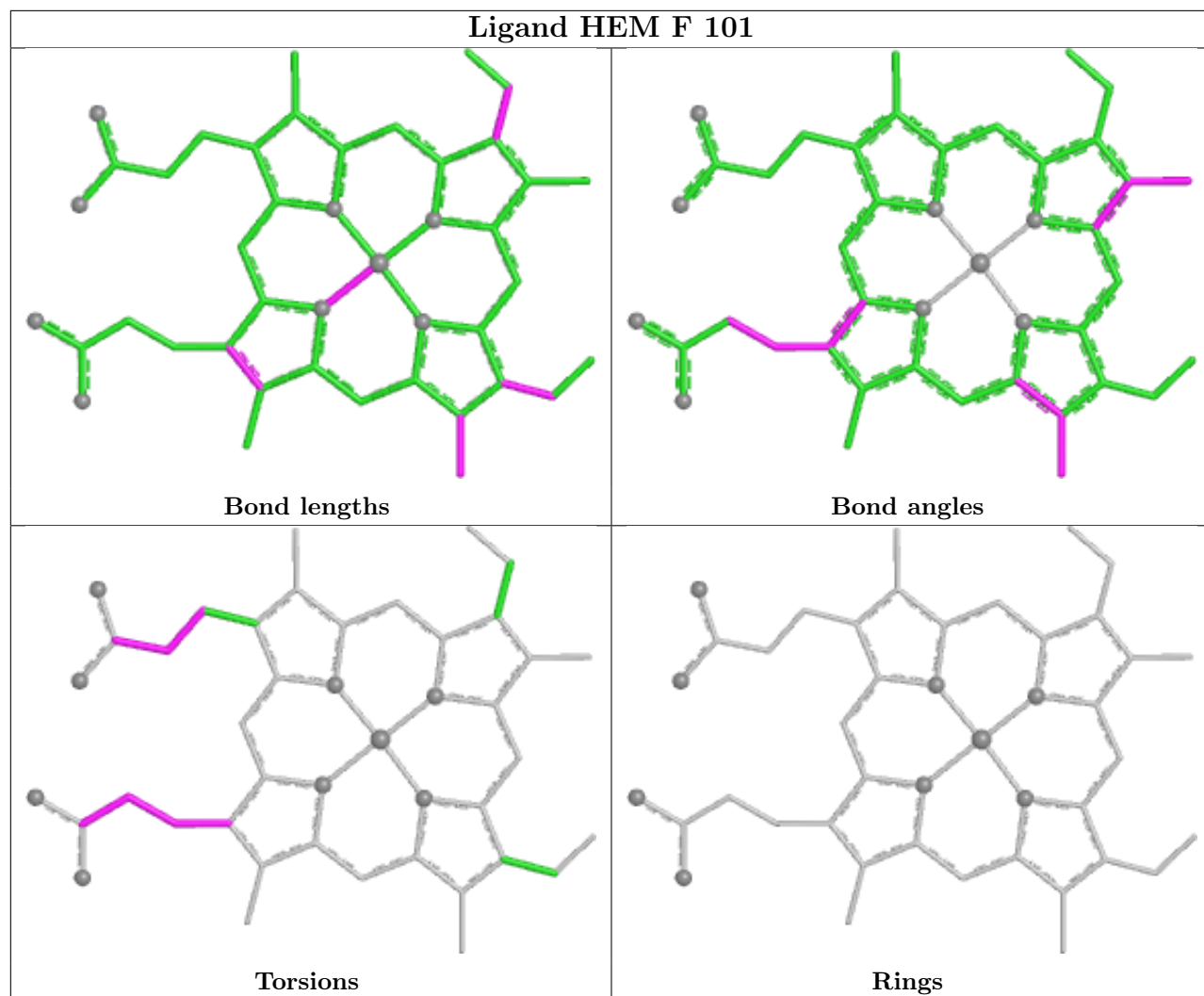


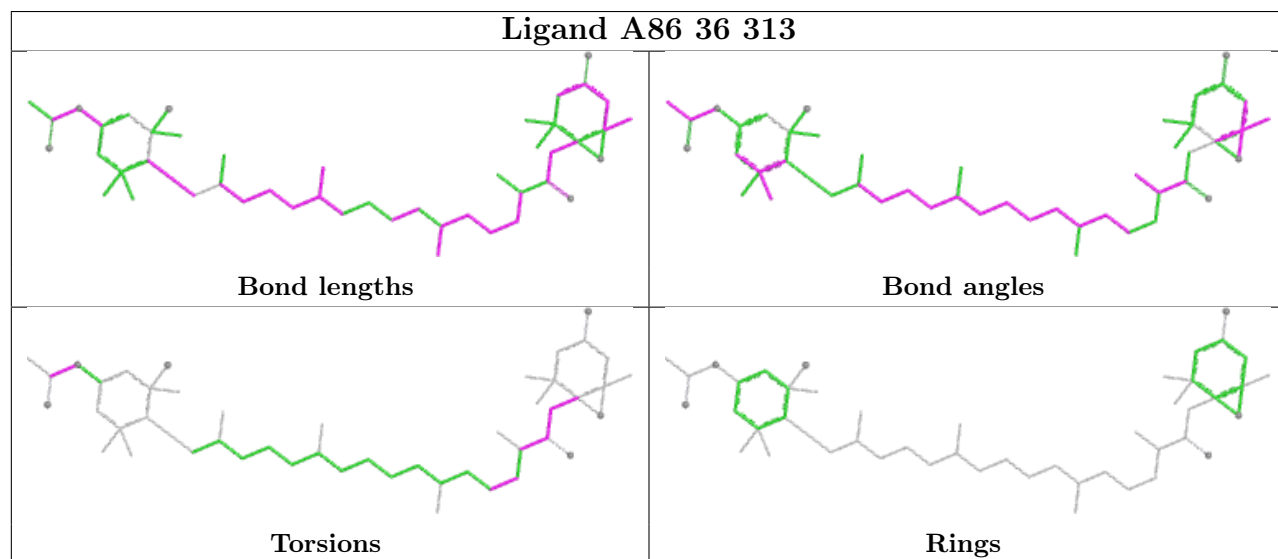
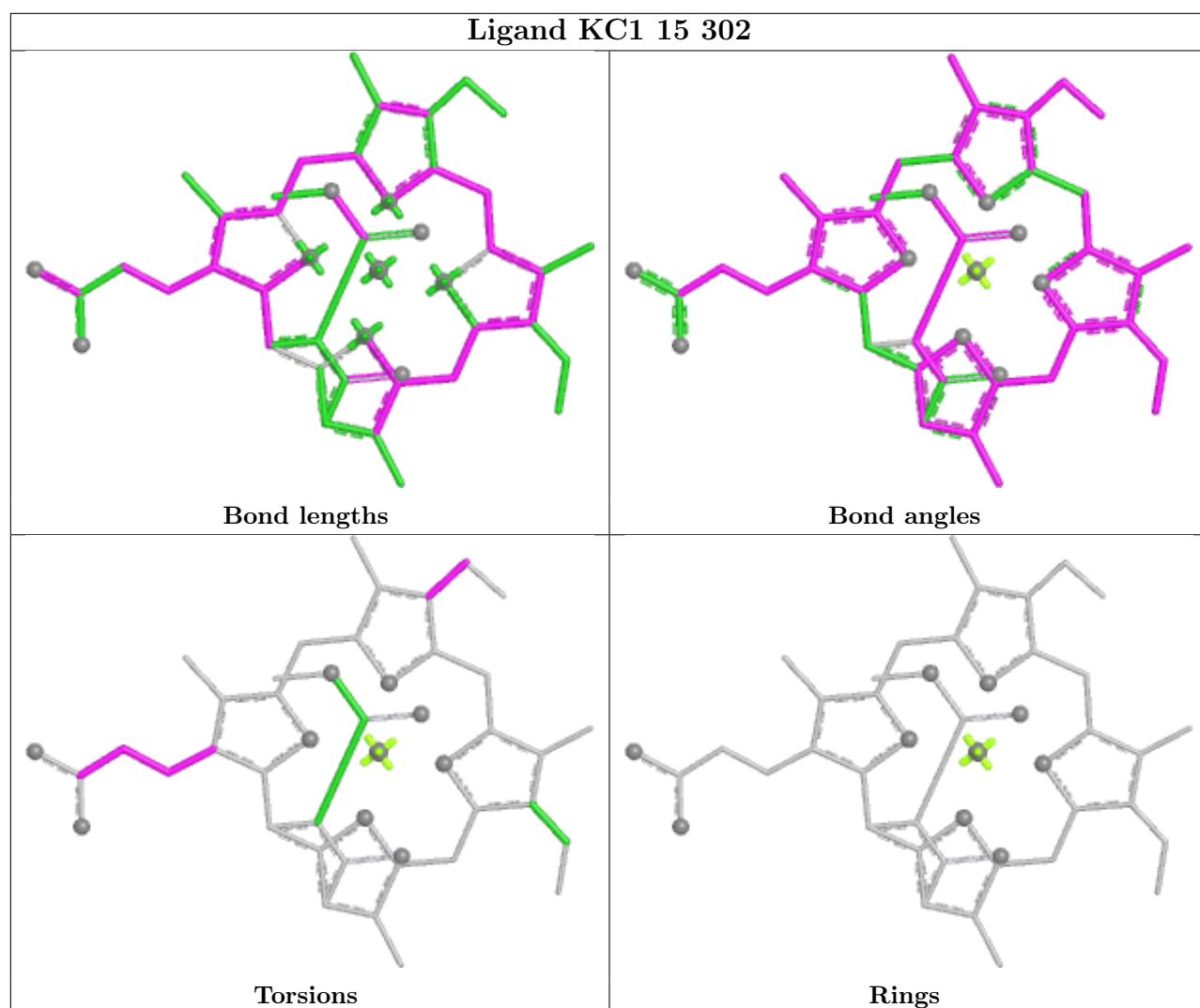


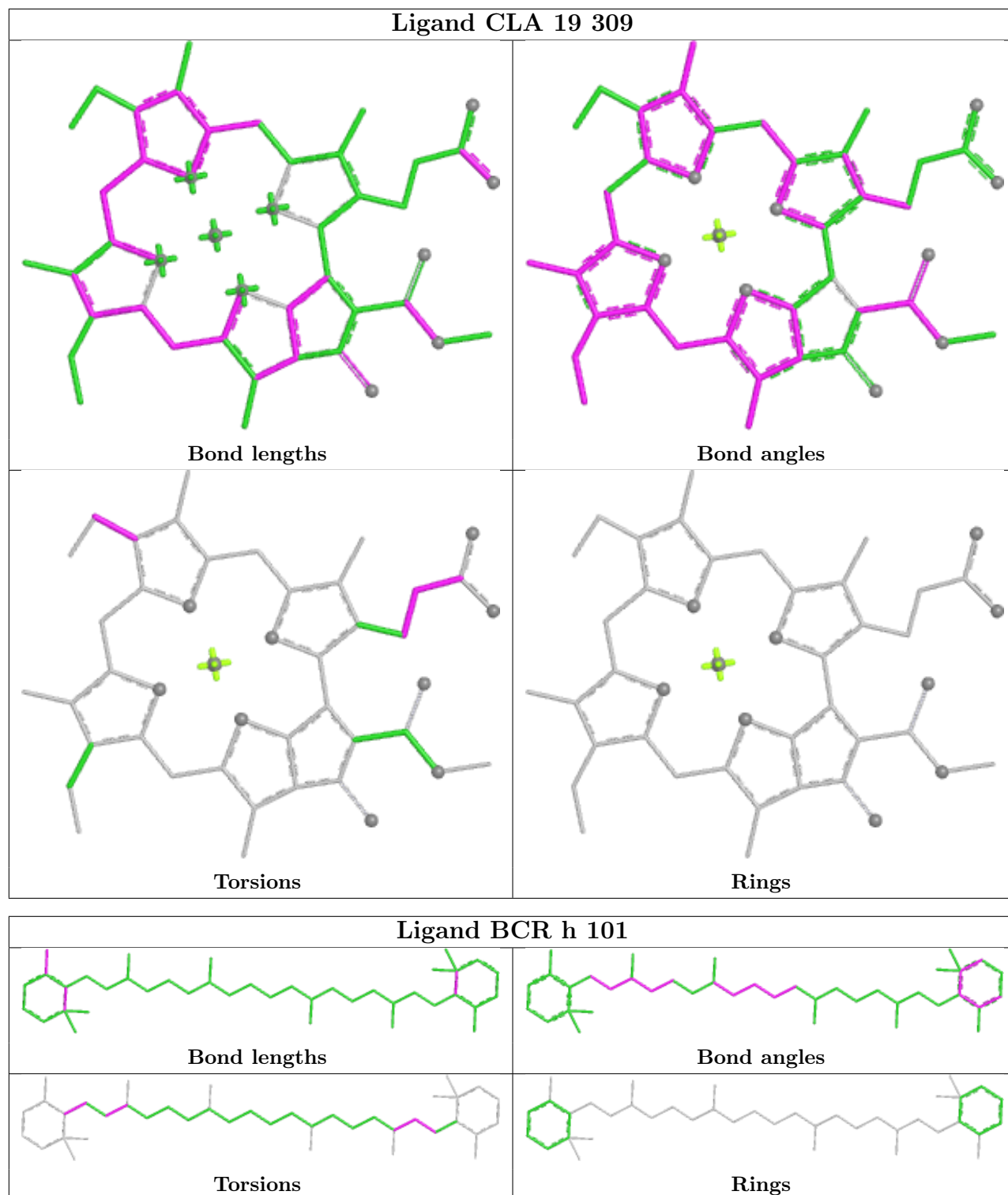


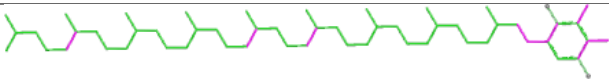
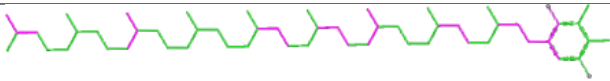
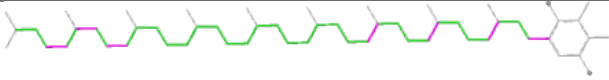
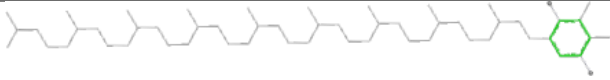


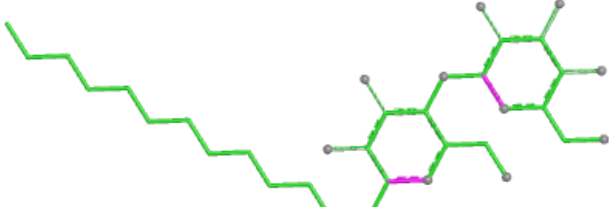
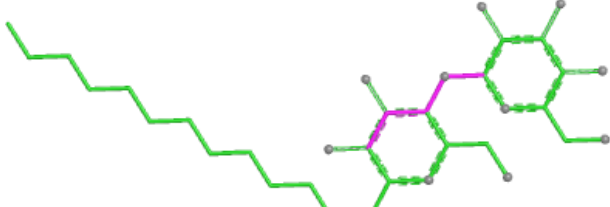
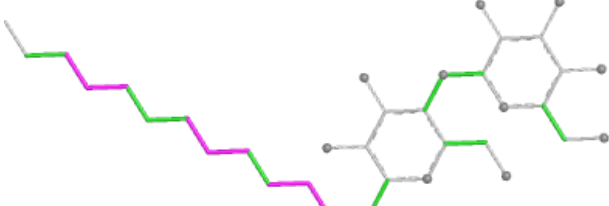
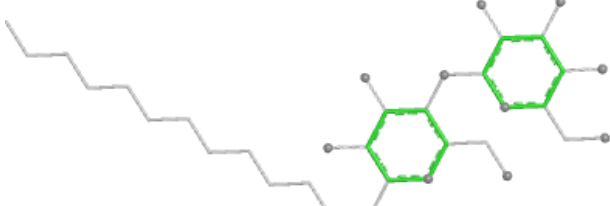


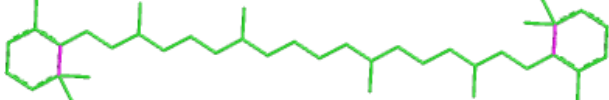
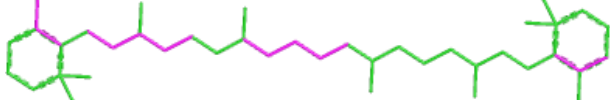
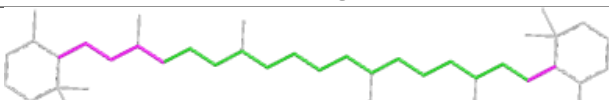
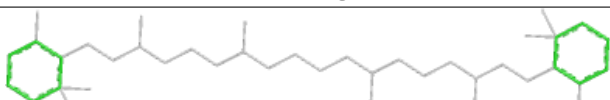


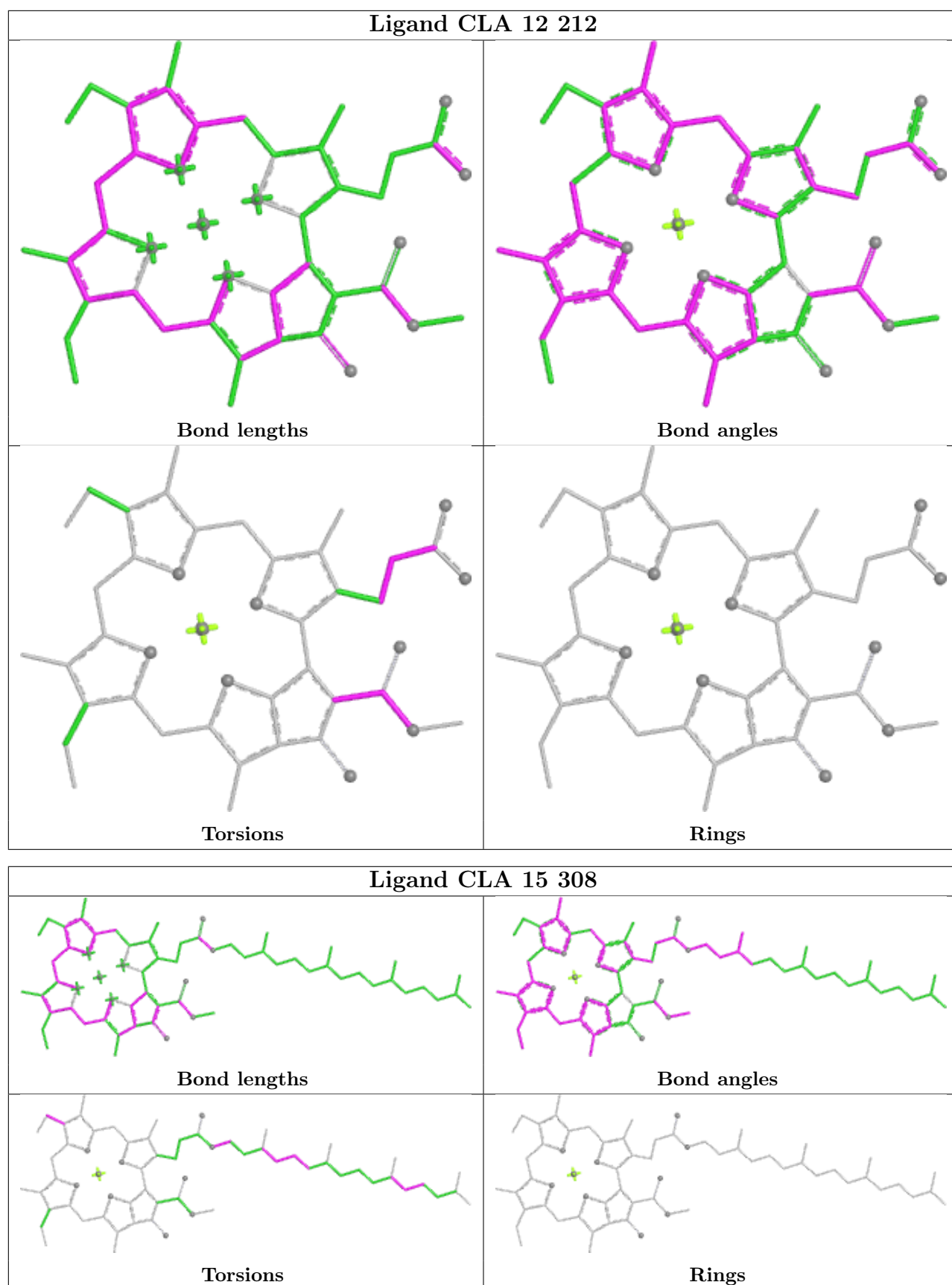


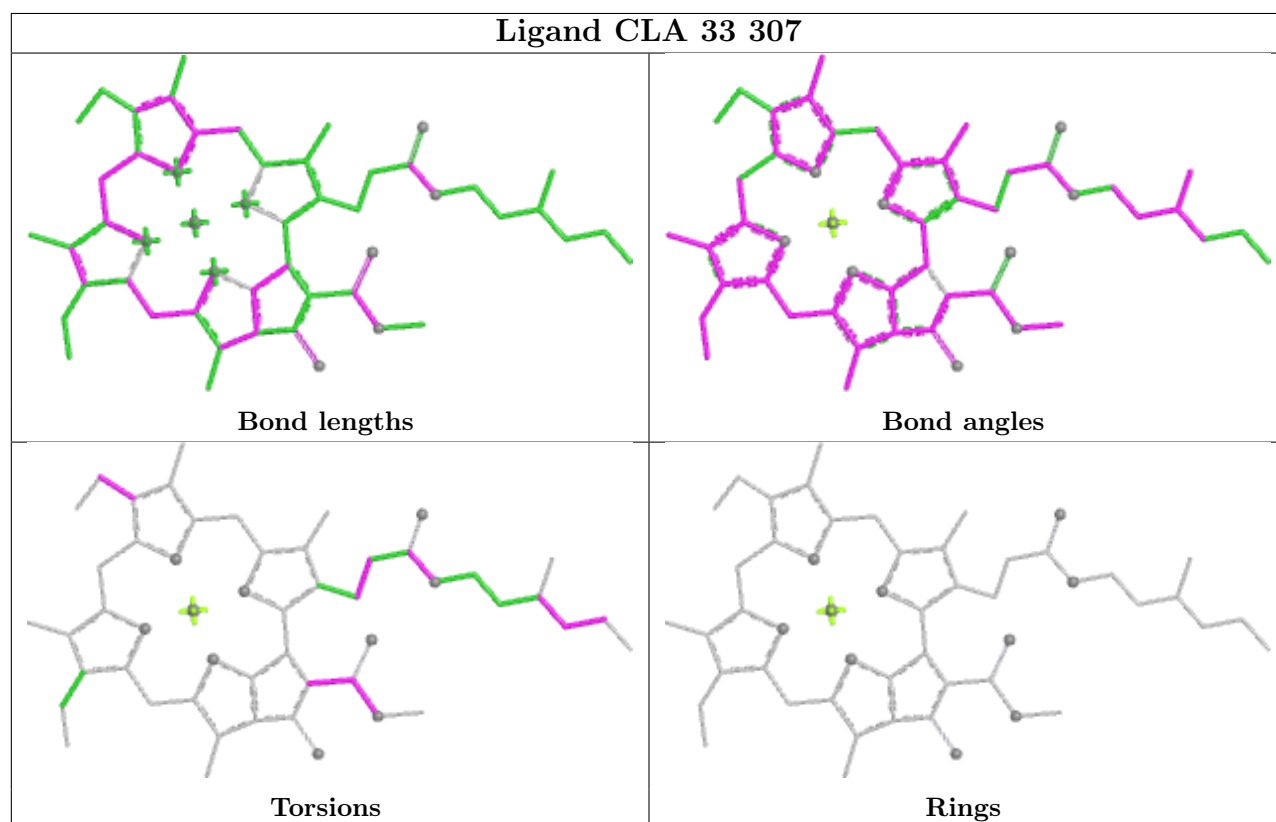
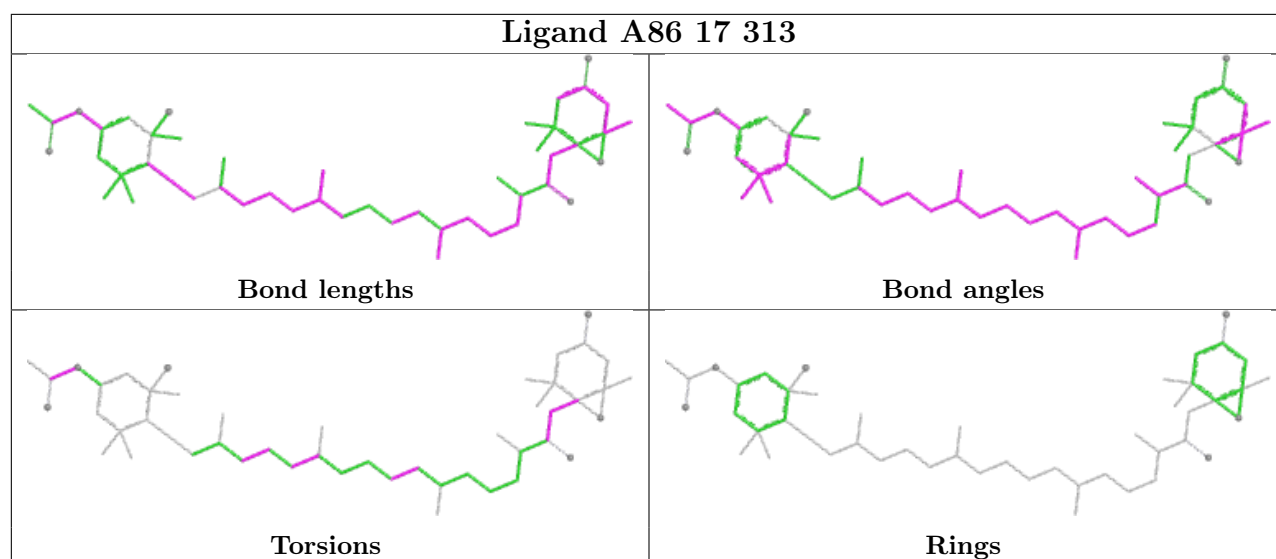


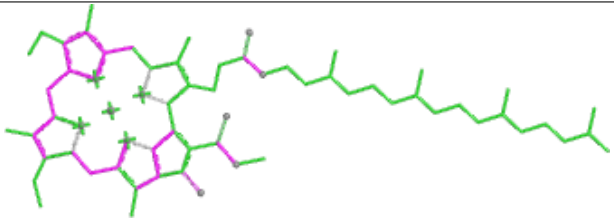
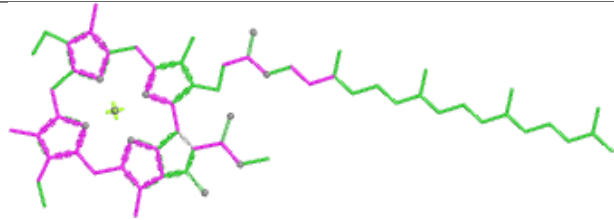
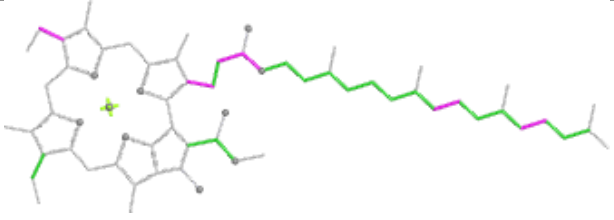
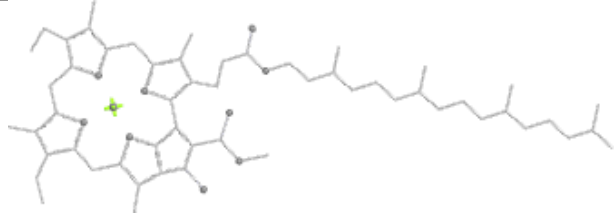
Ligand PL9 D 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

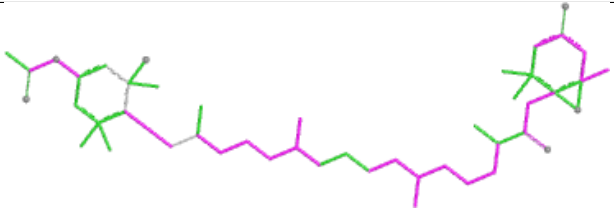
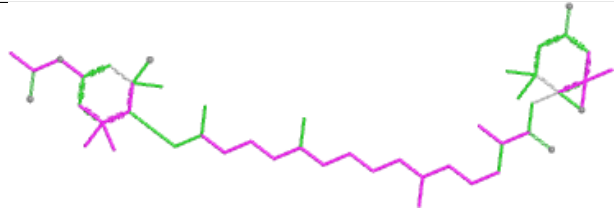
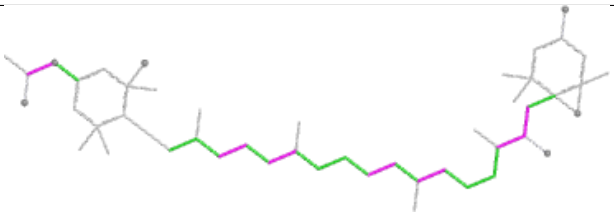
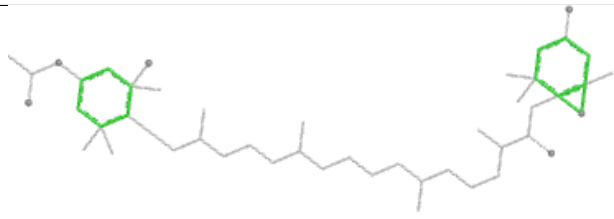
Ligand LMU 39 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

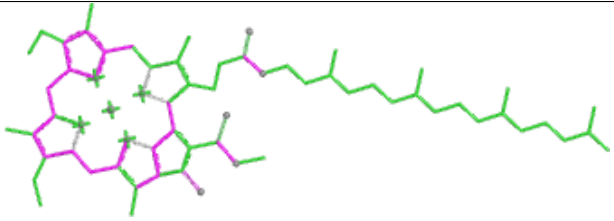
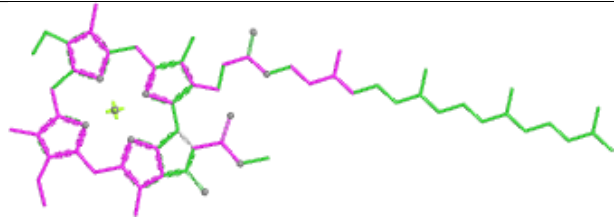
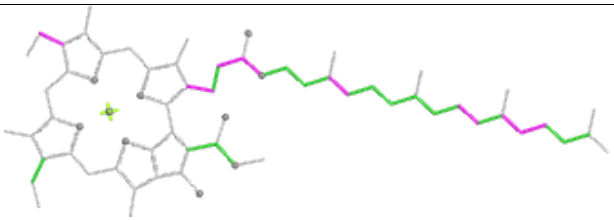
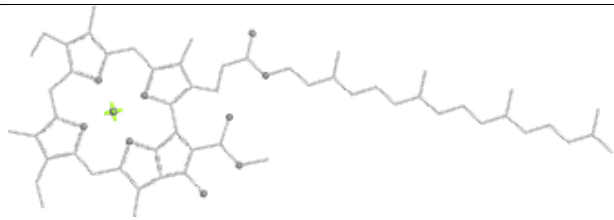
Ligand BCR a 413	
 Bond lengths	 Bond angles
 Torsions	 Rings

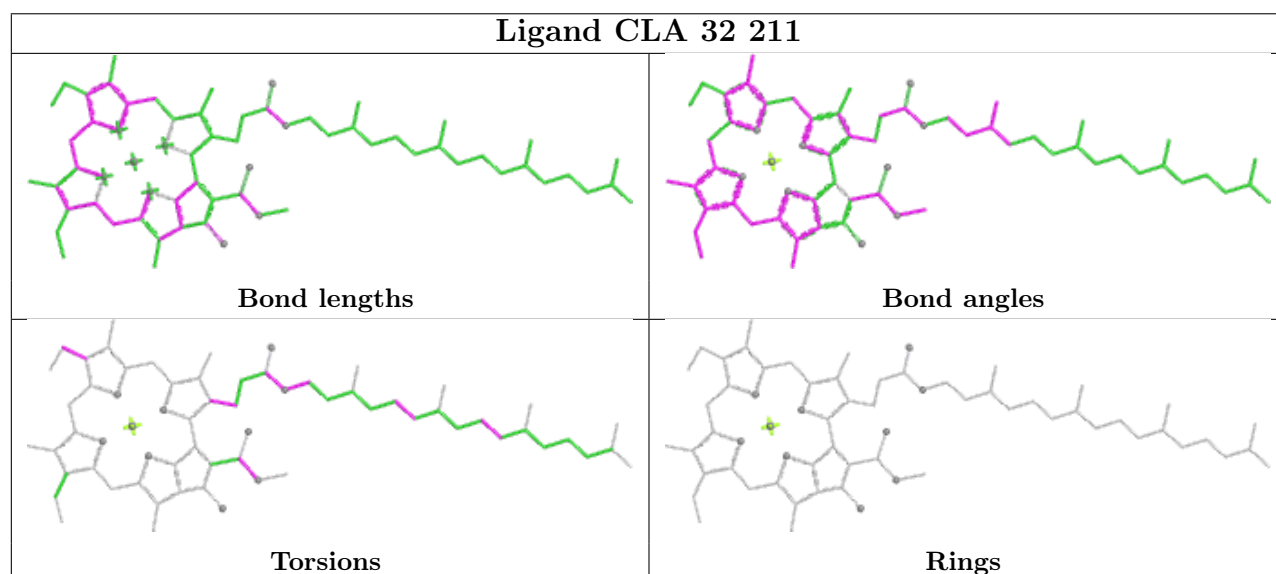
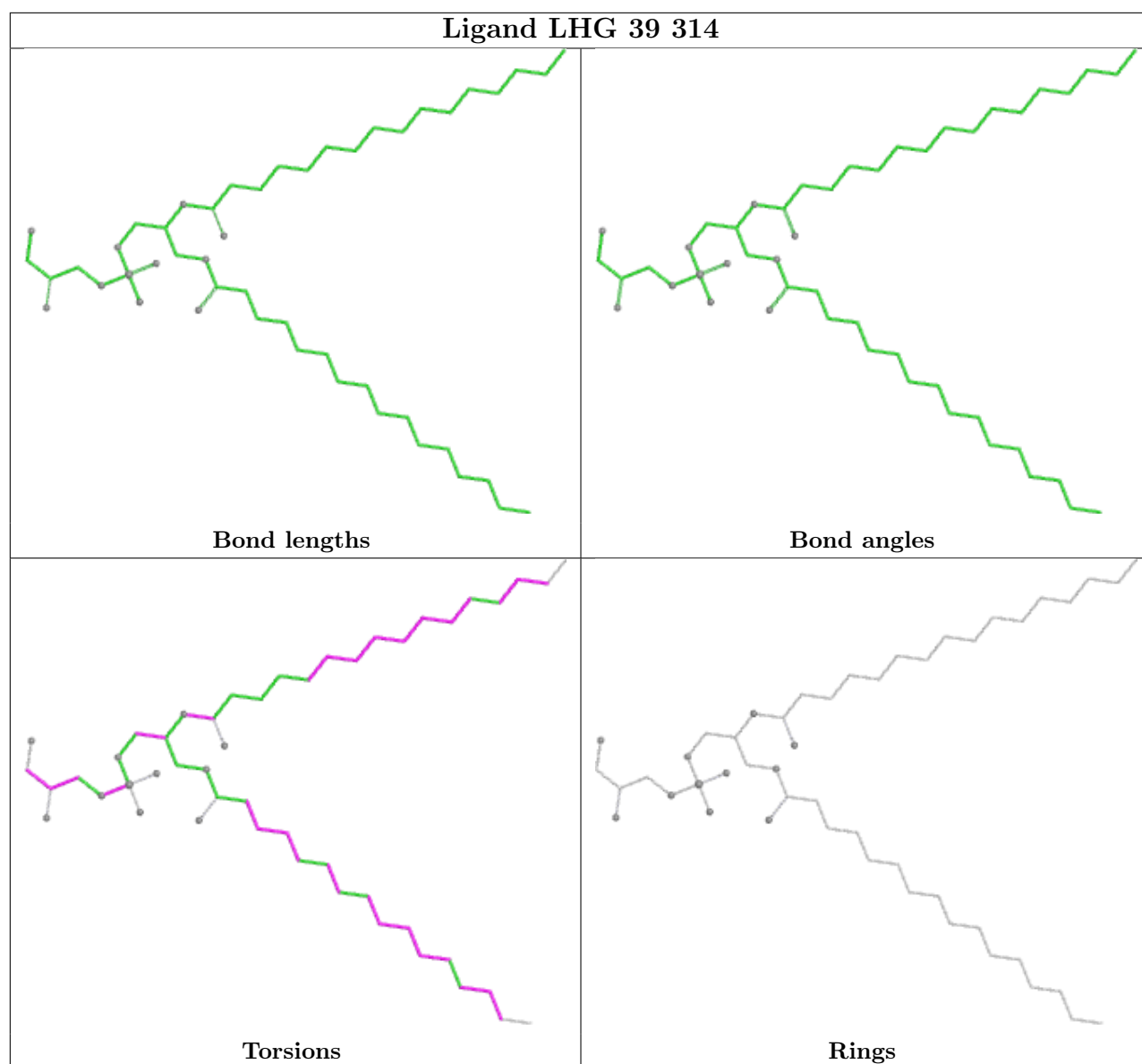


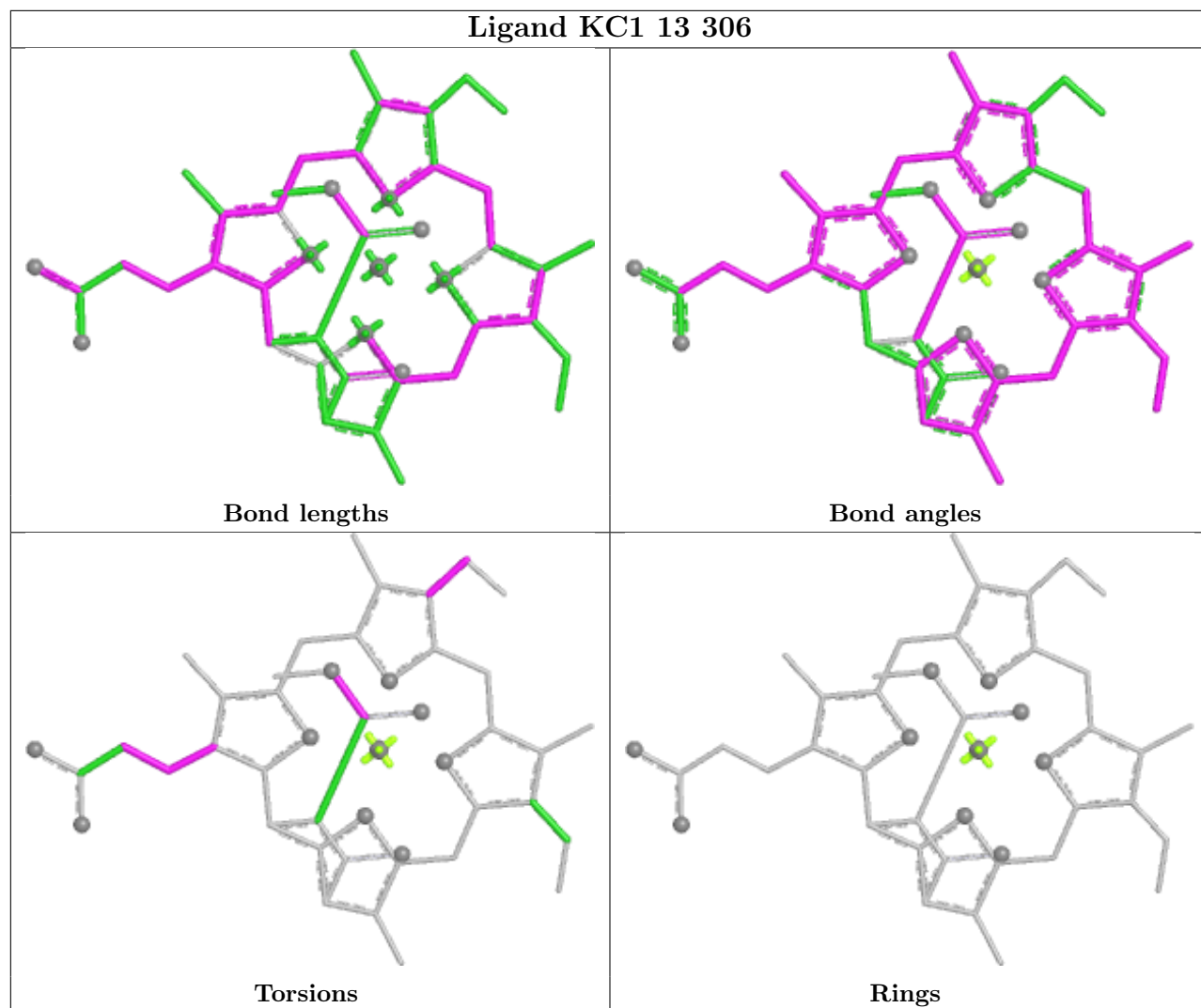


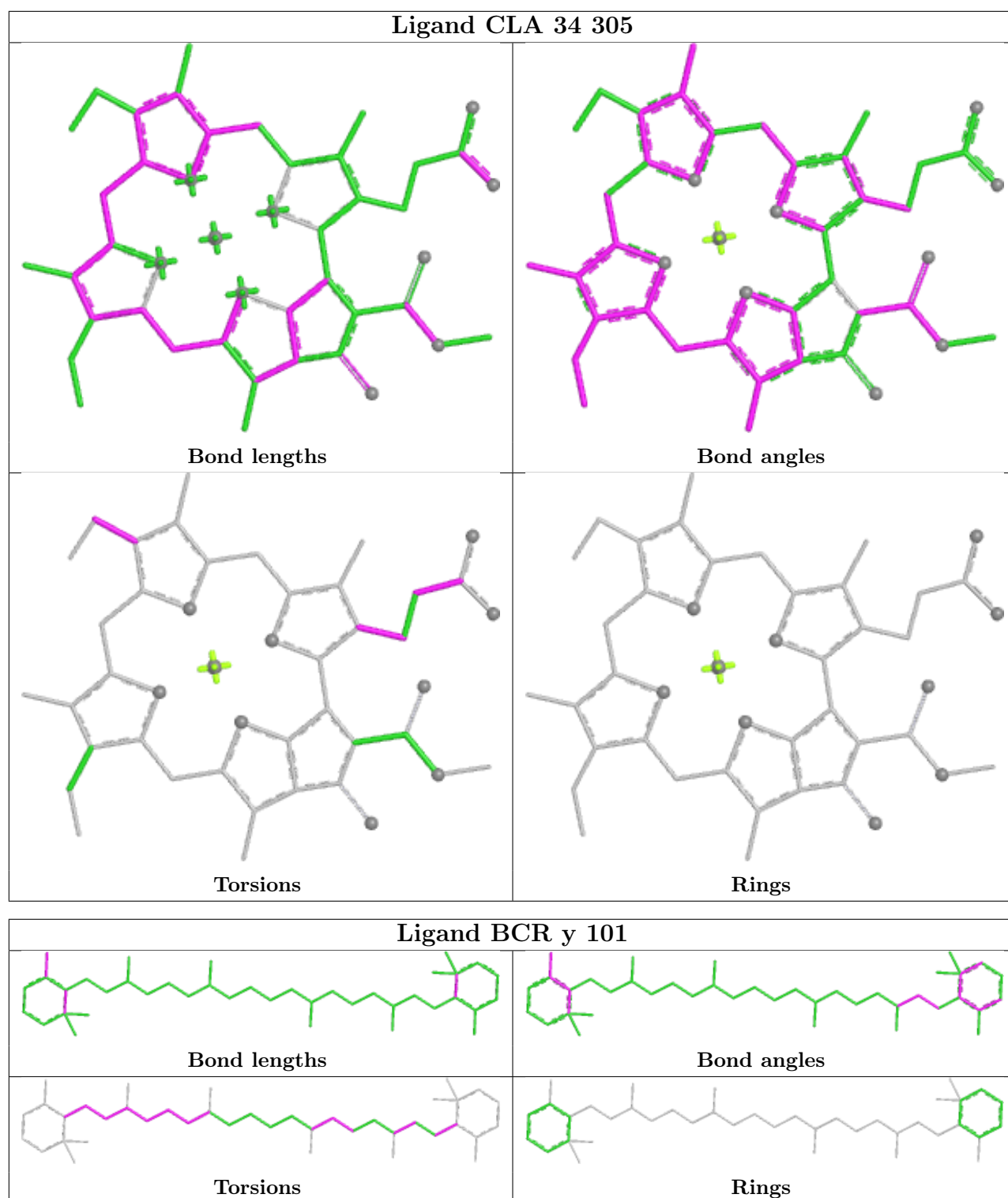
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Bond lengths	Bond angles
	
Torsions	Rings

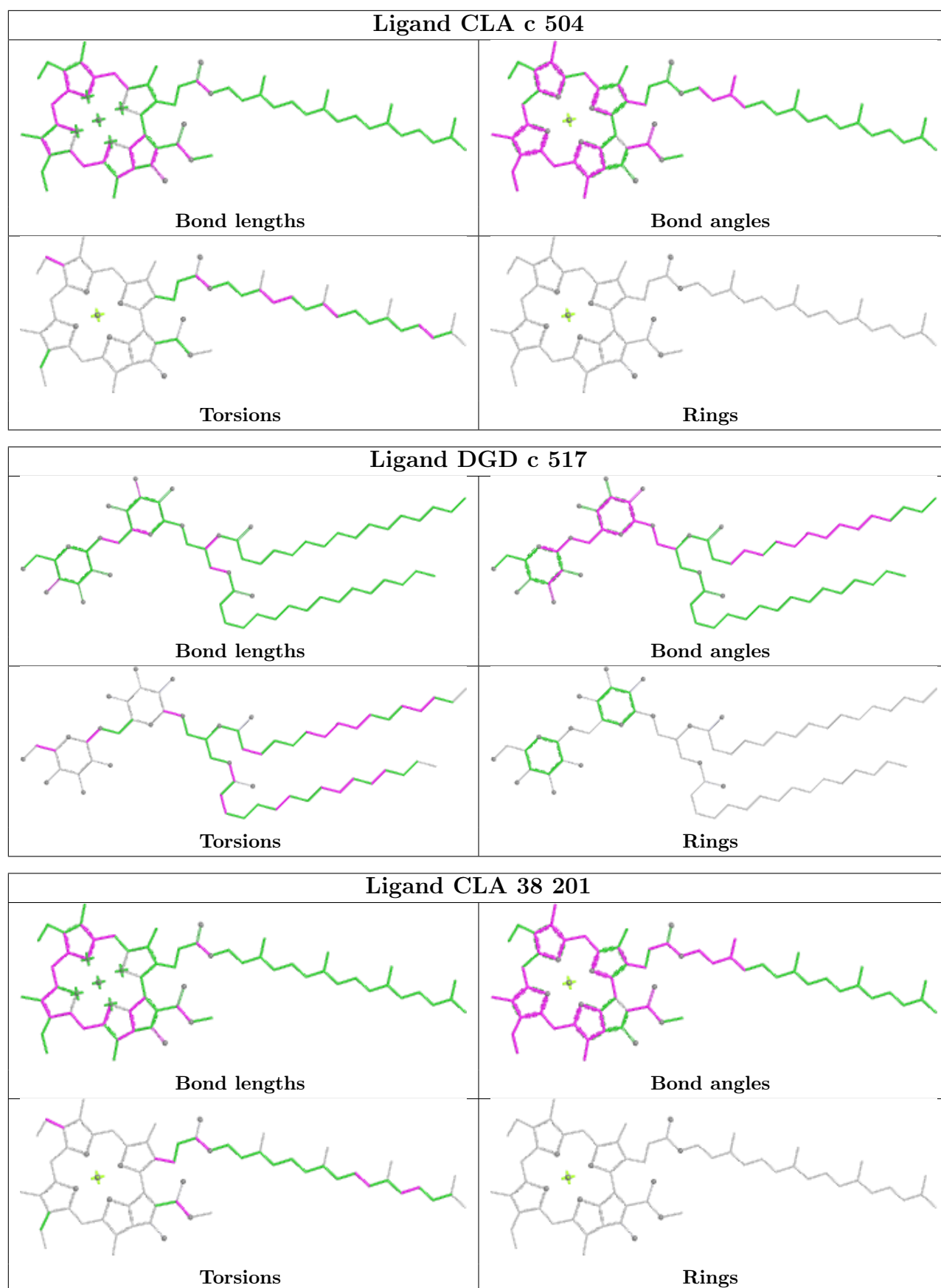
Ligand A86 34 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

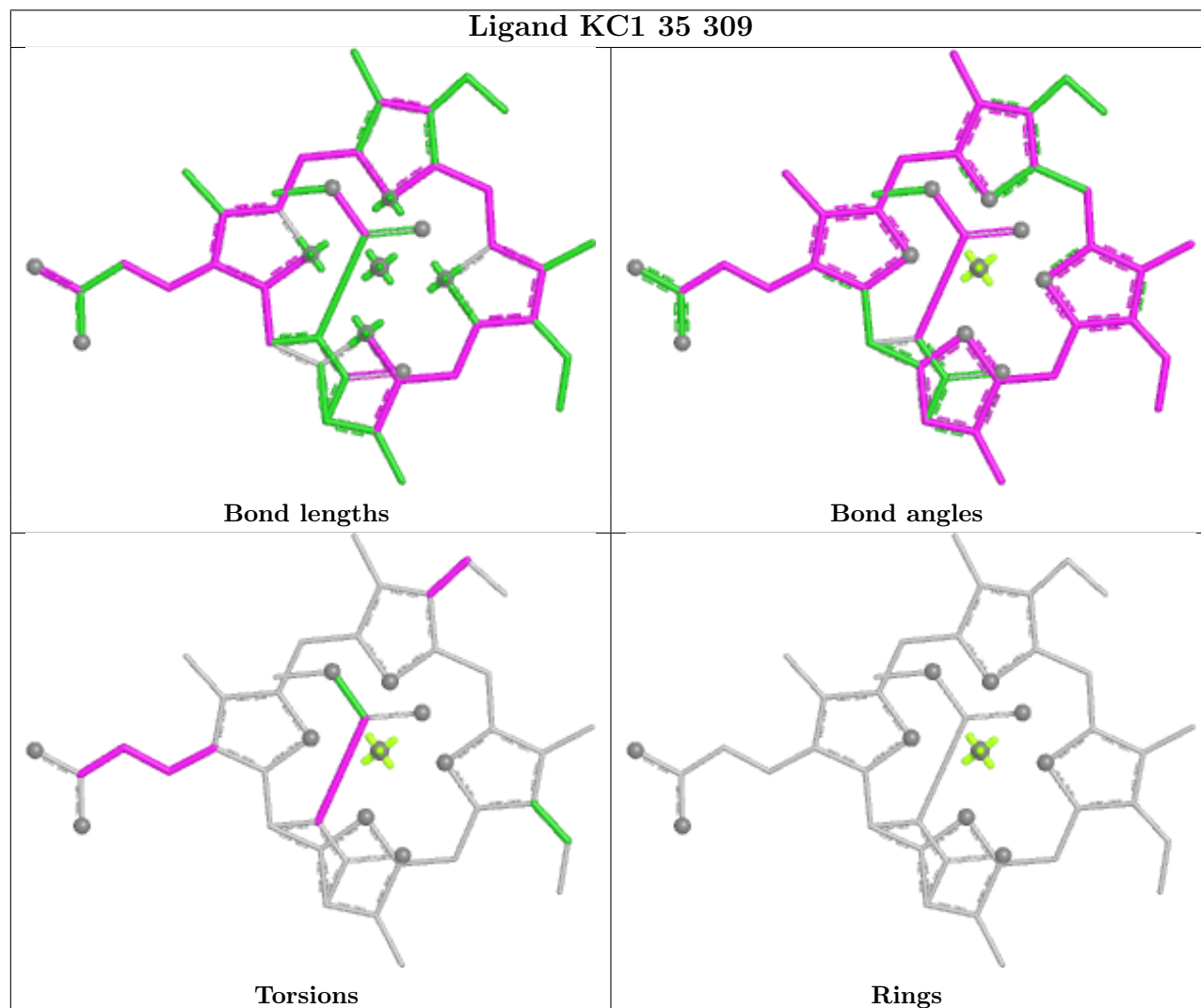
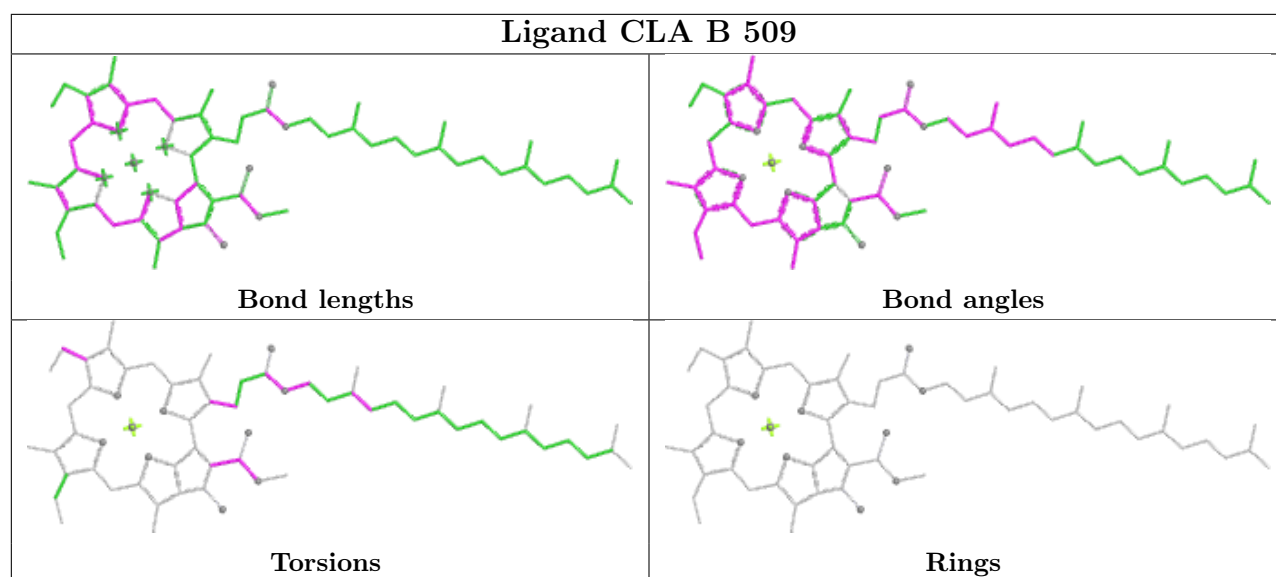
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Bond lengths	Bond angles
	
Torsions	Rings

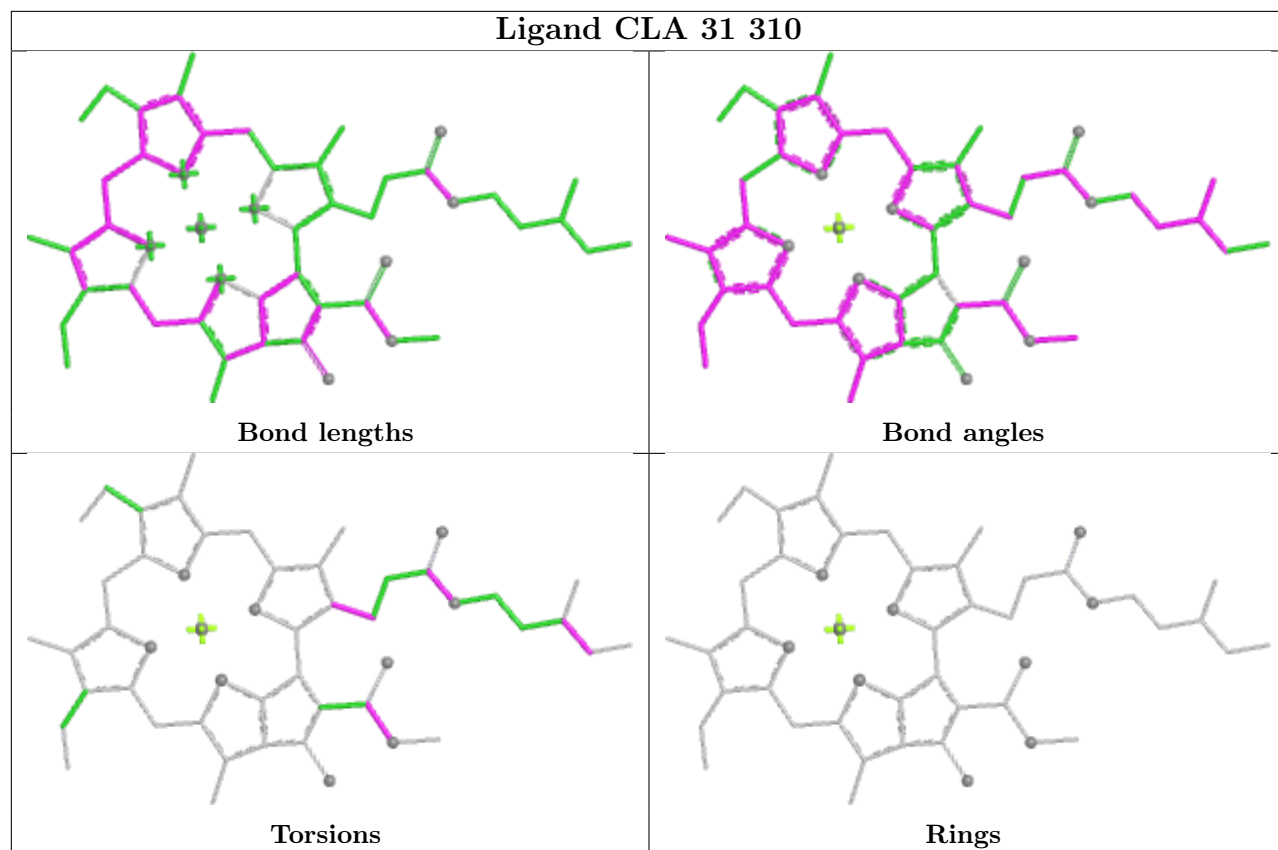


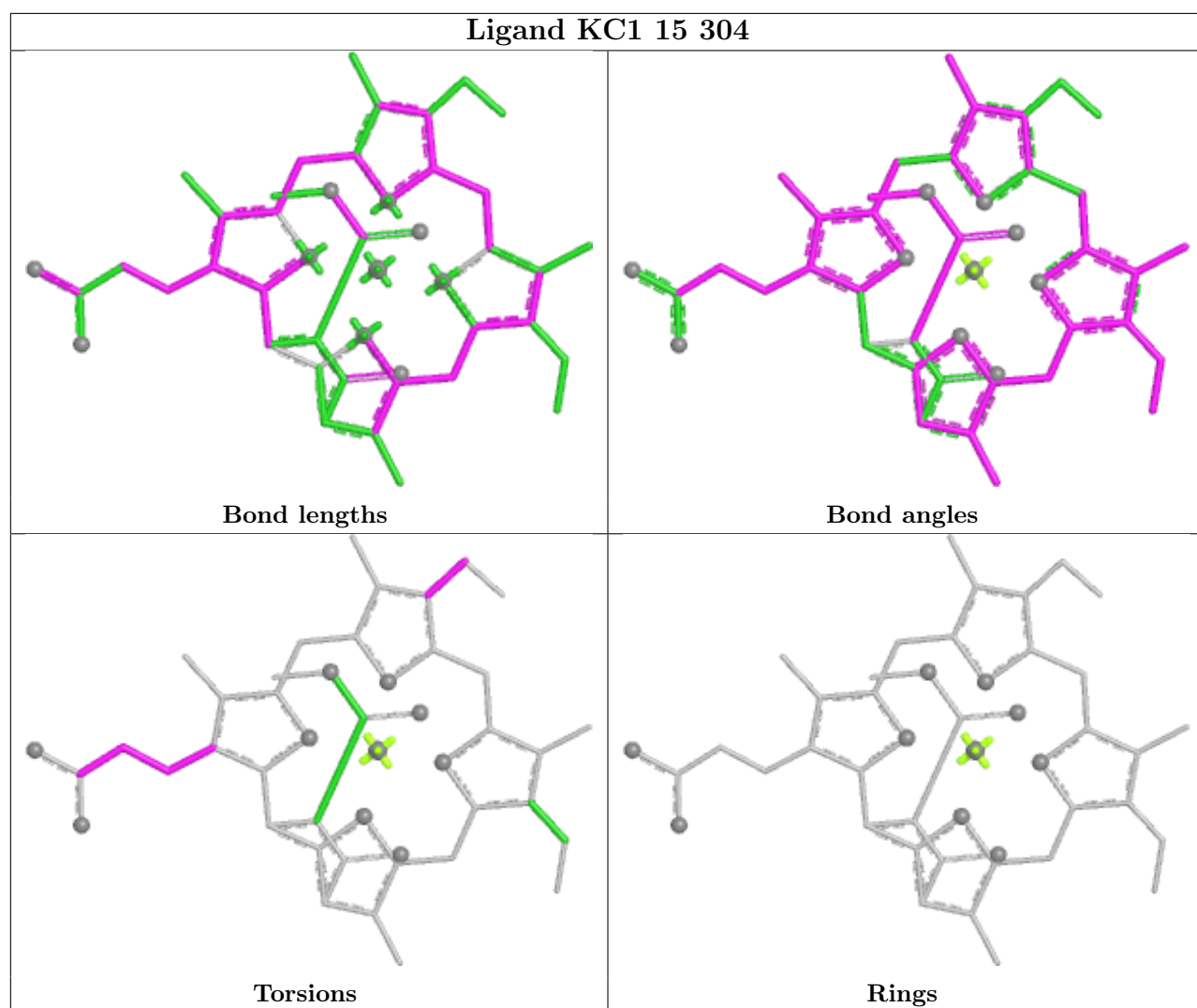


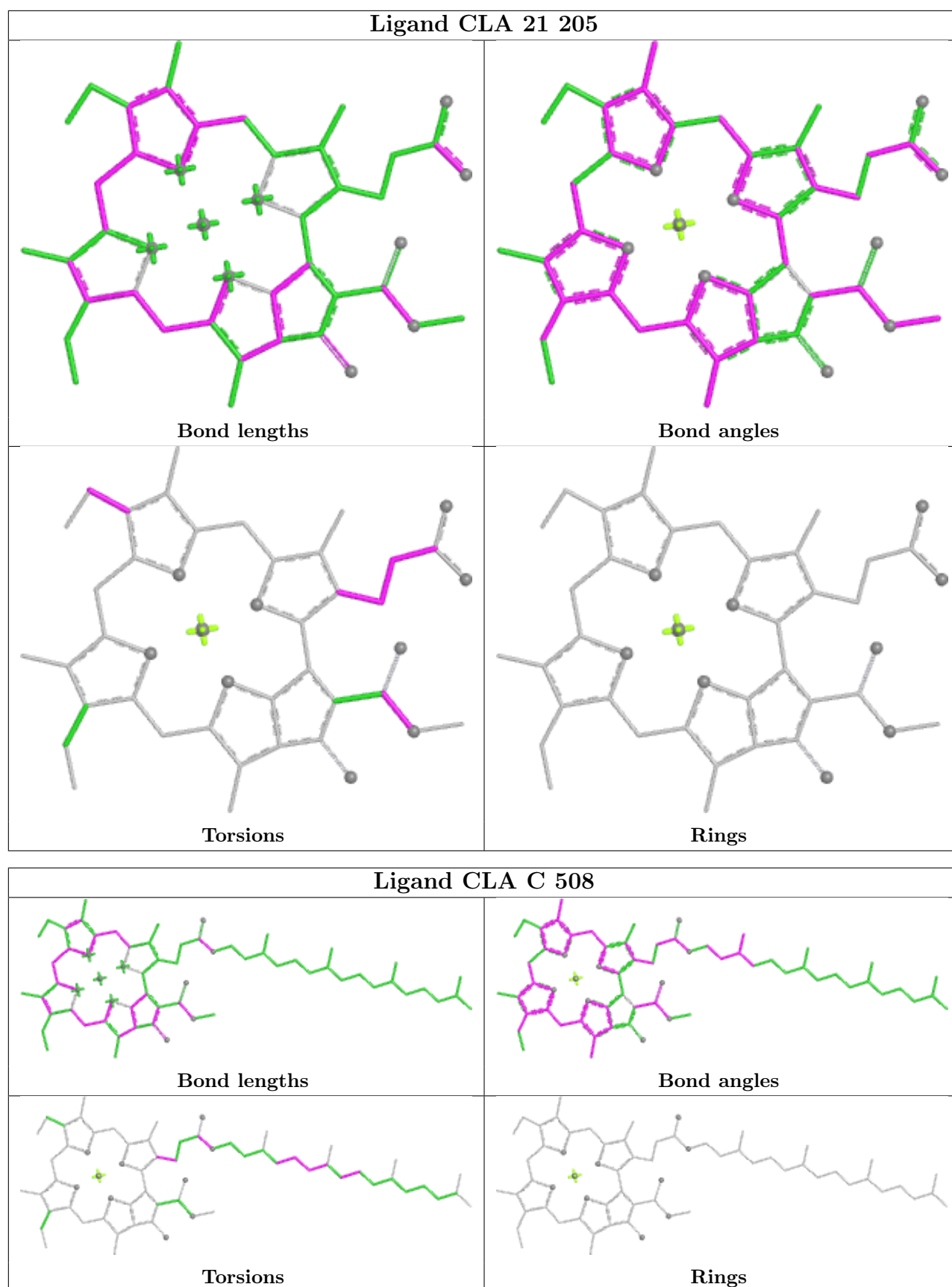


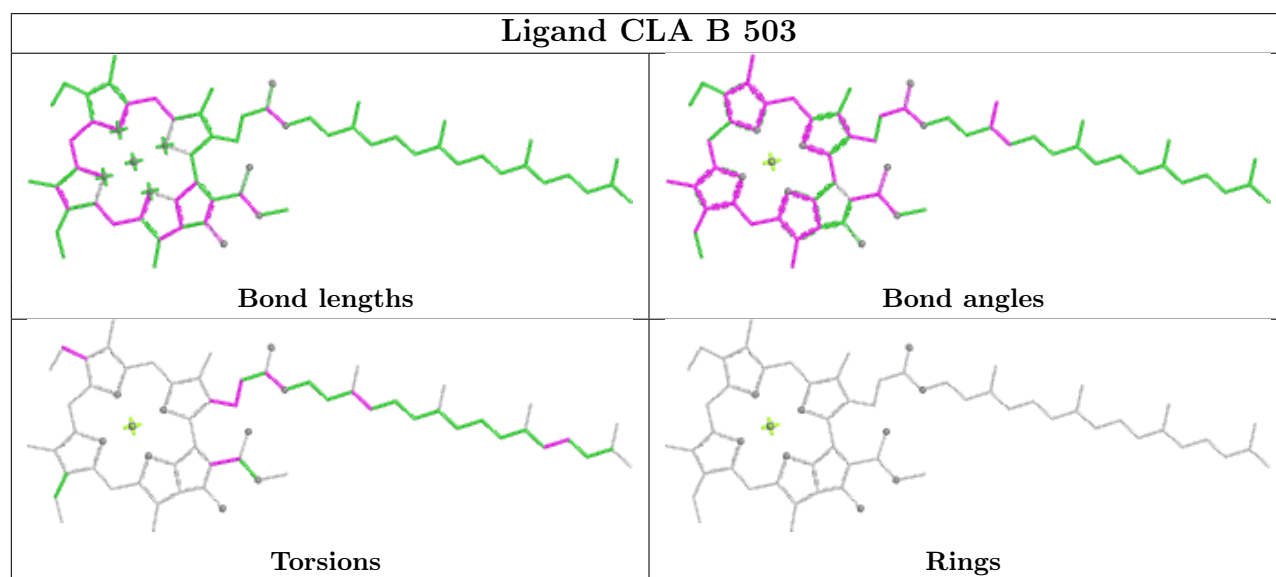
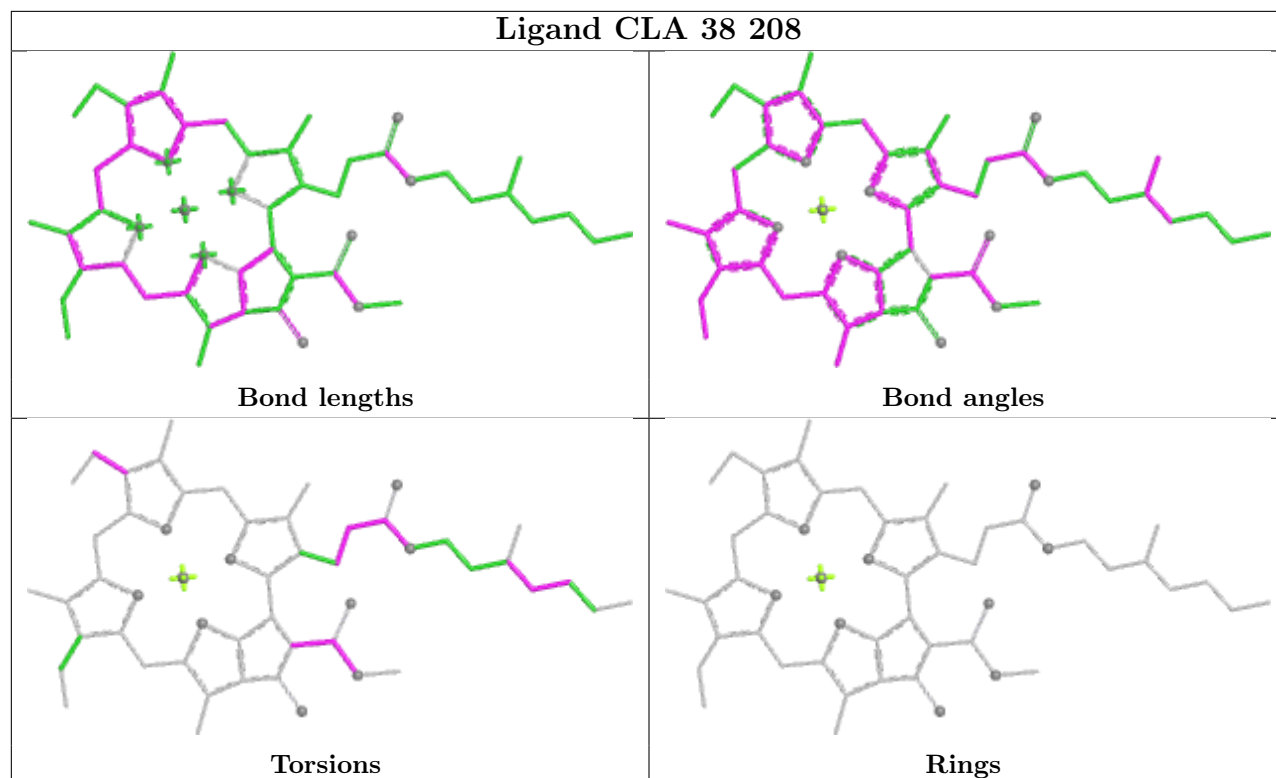


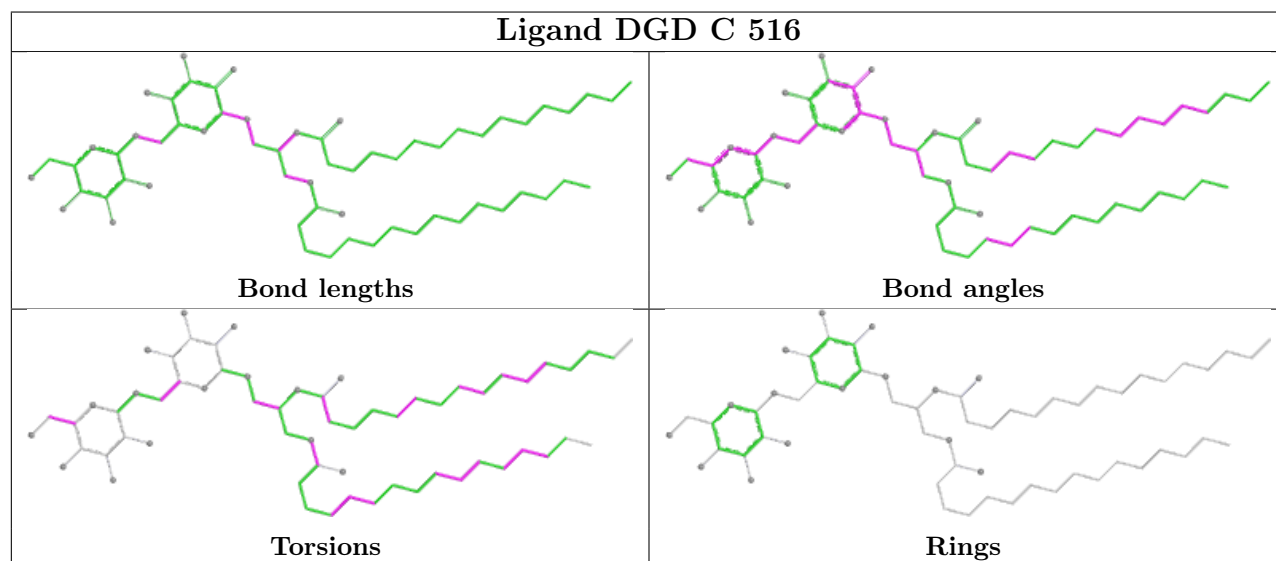
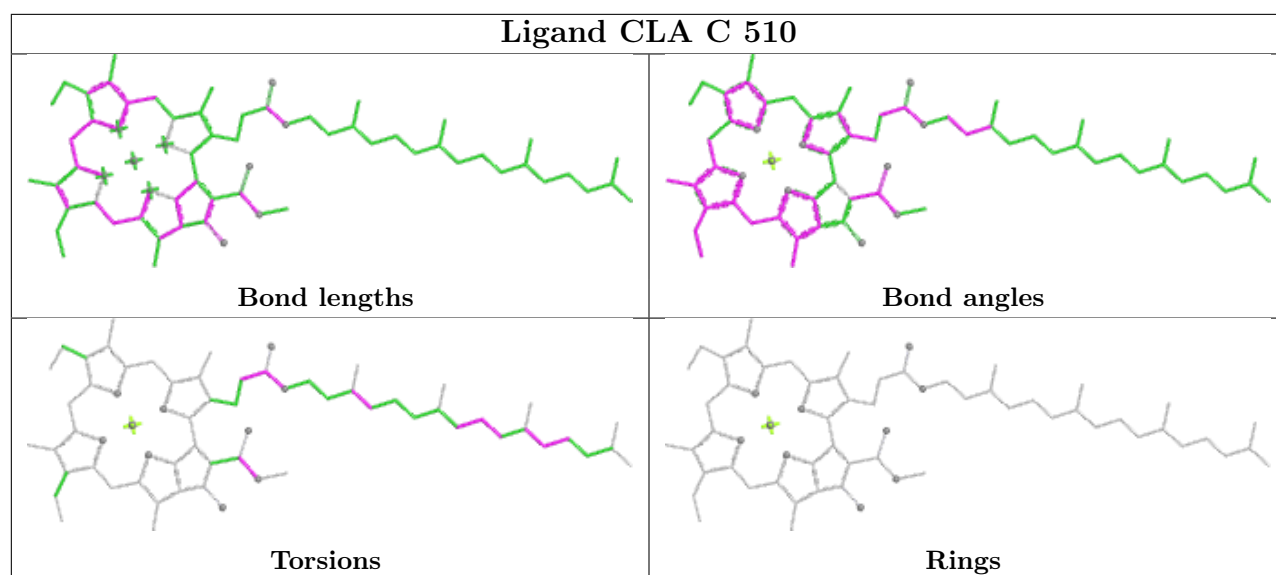


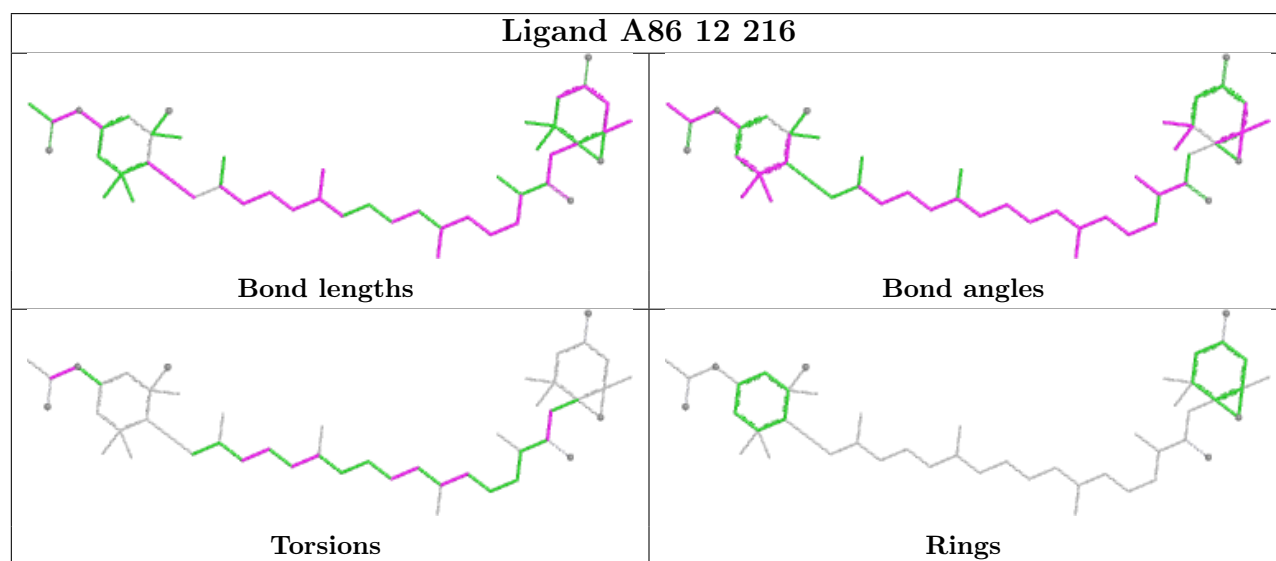
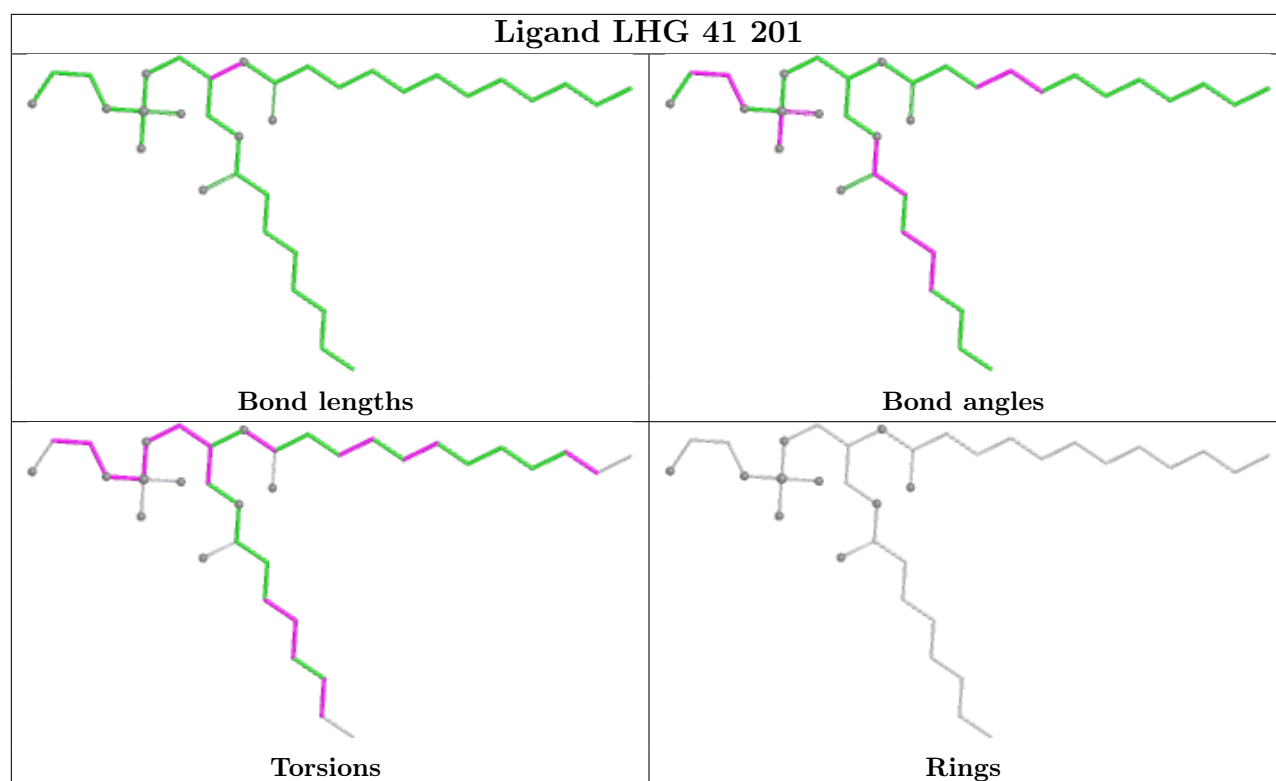


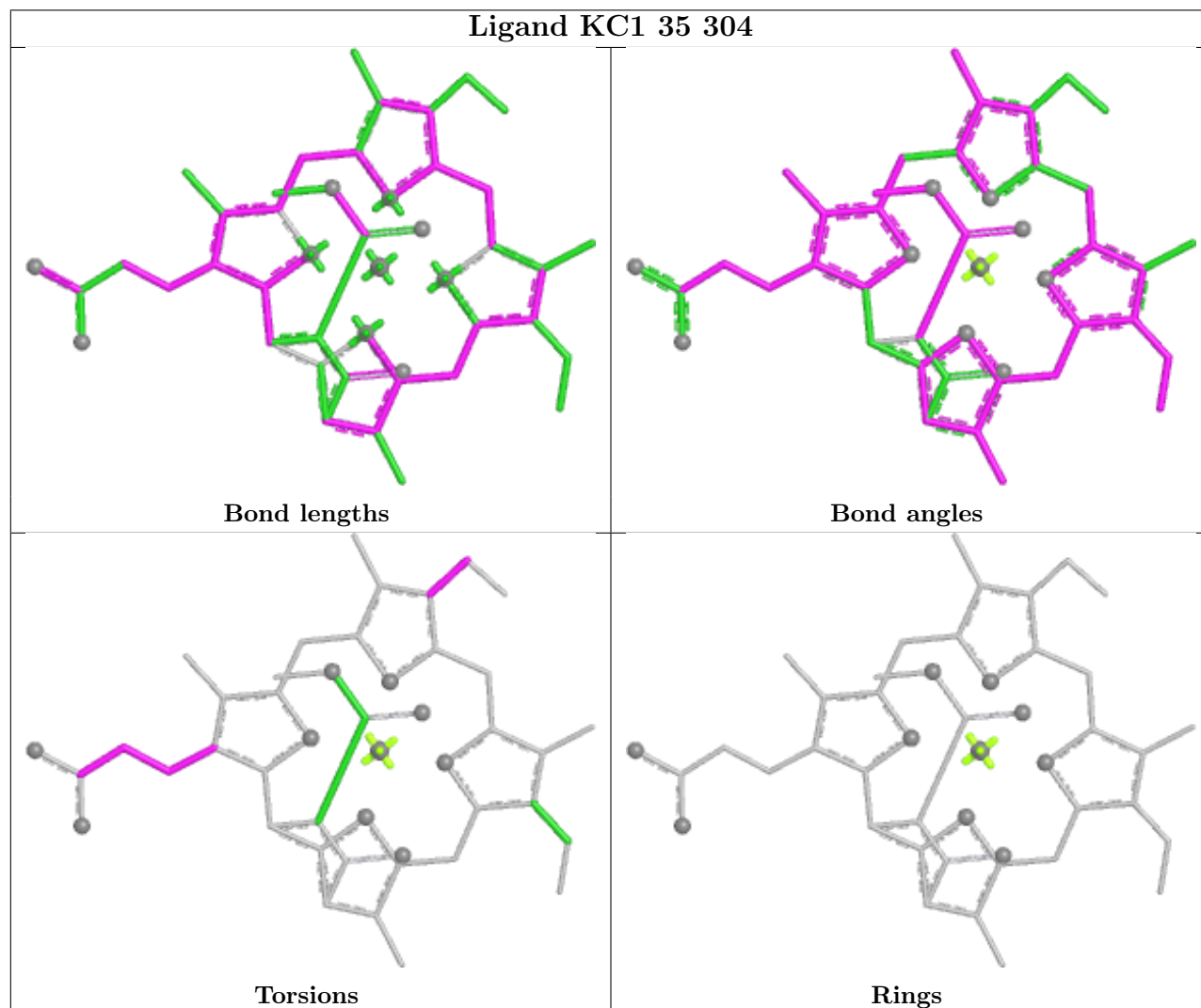
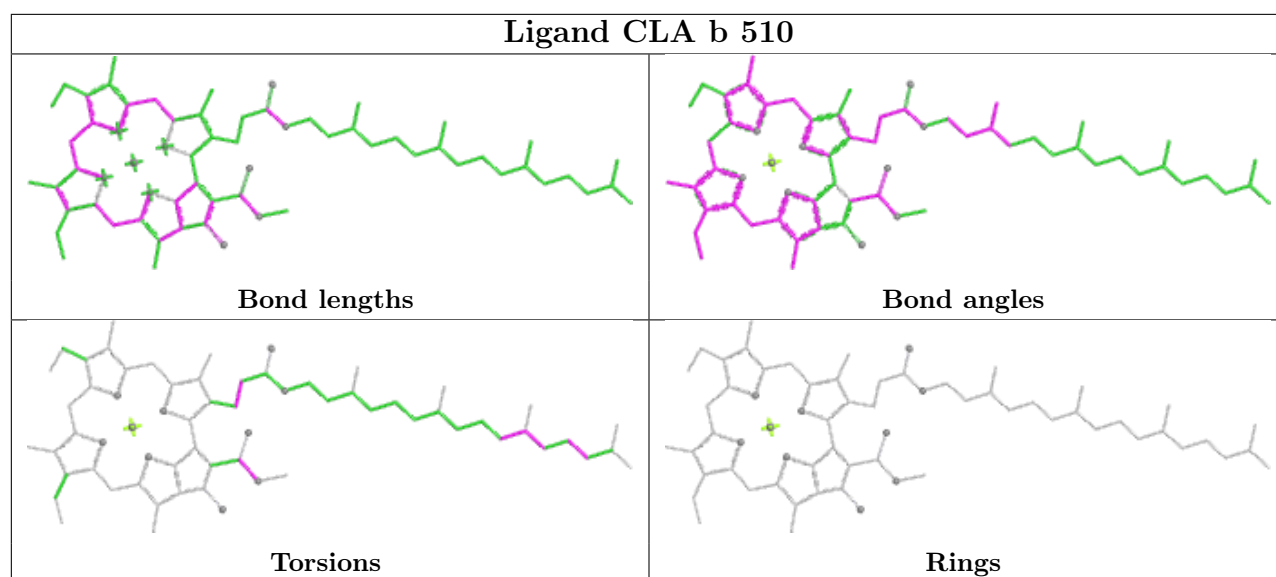


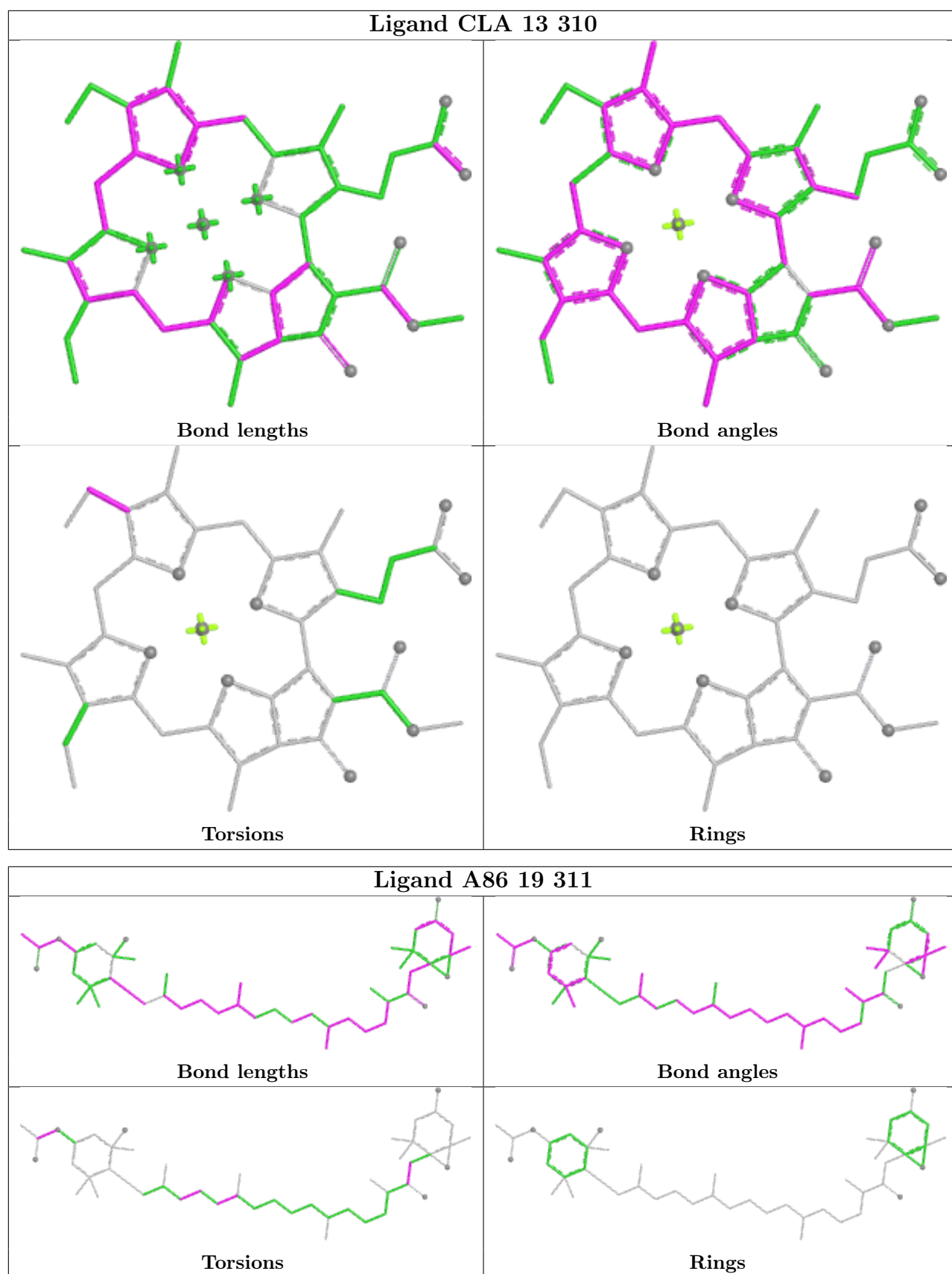


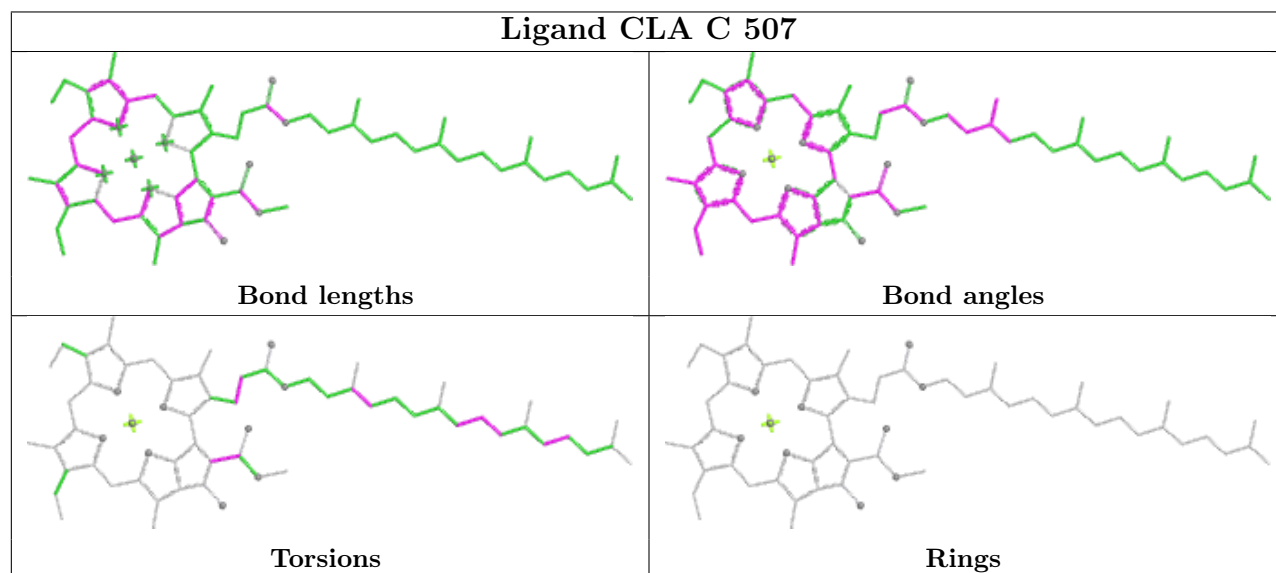
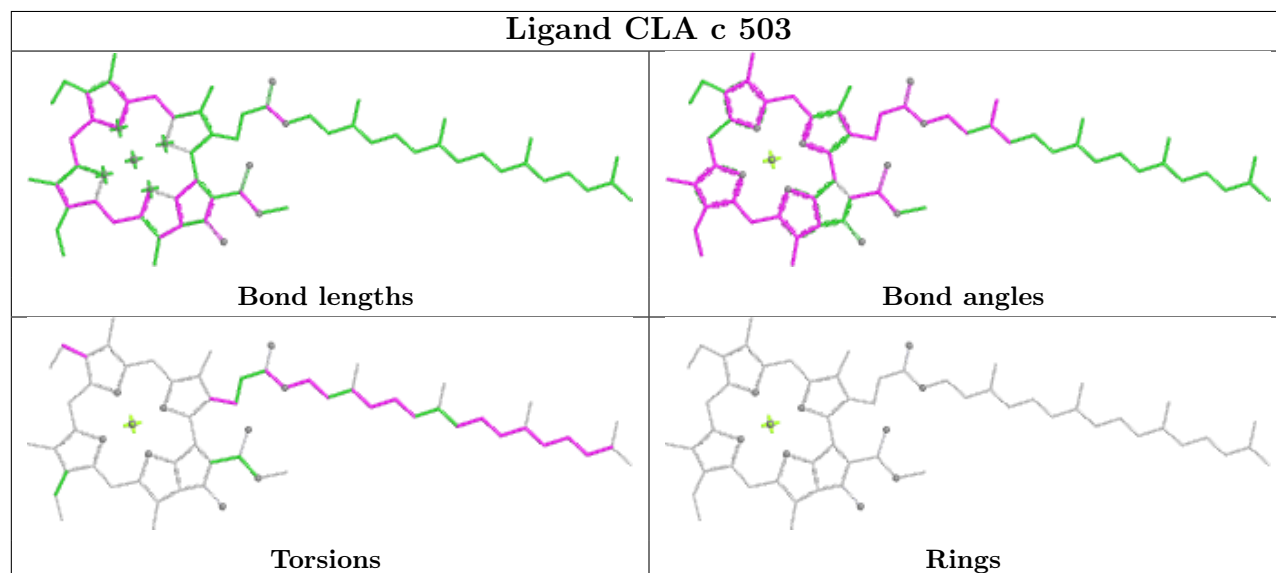
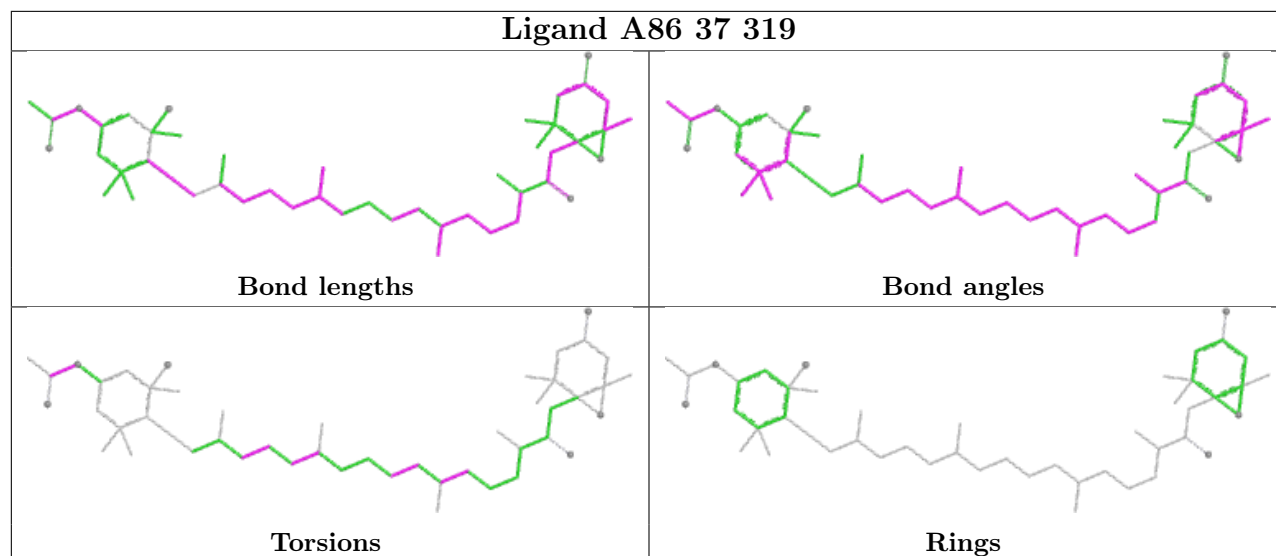


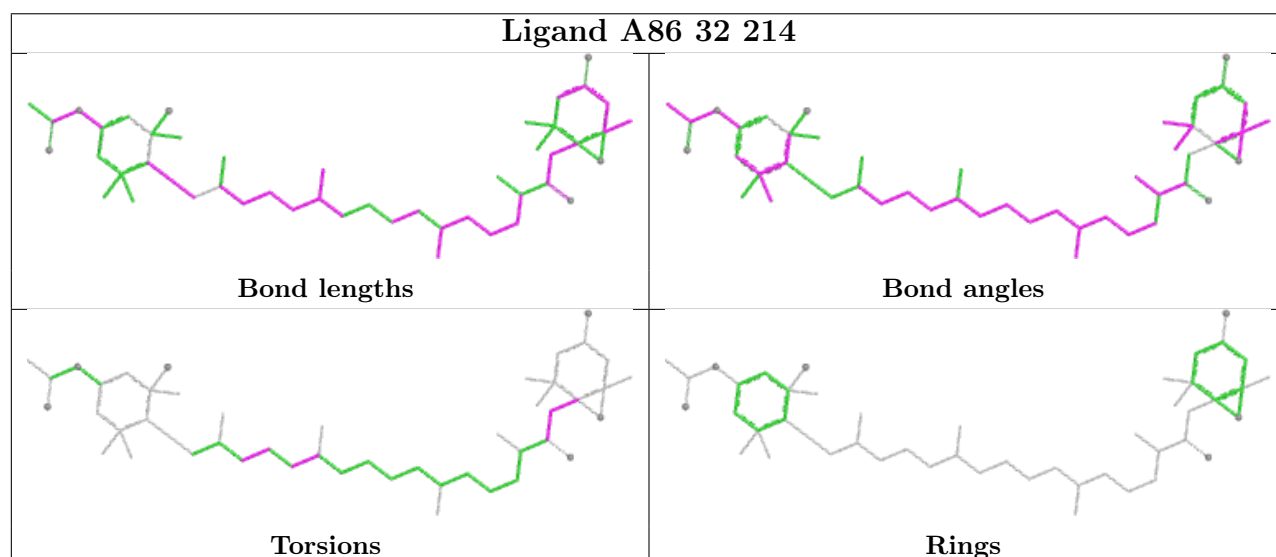
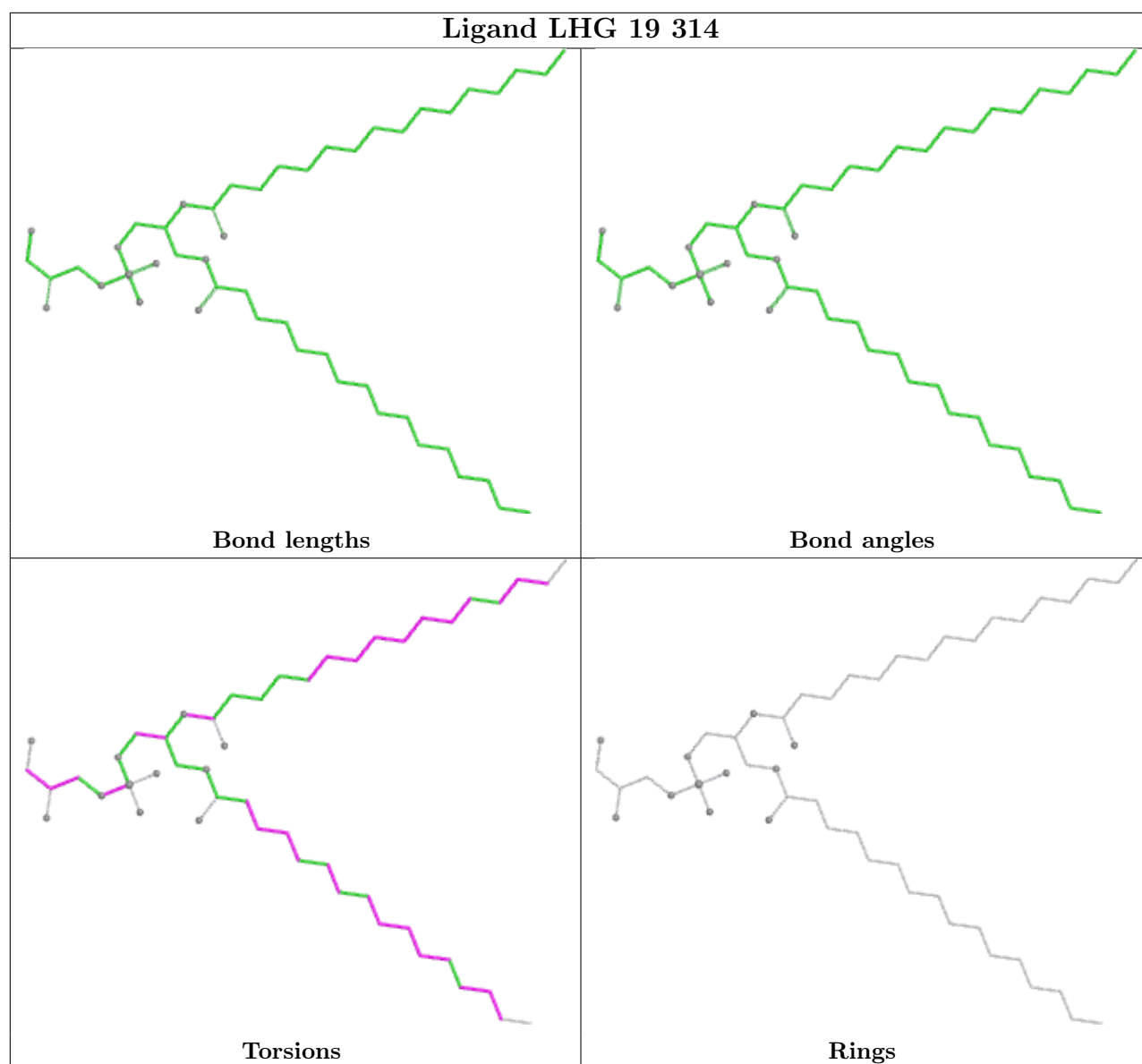


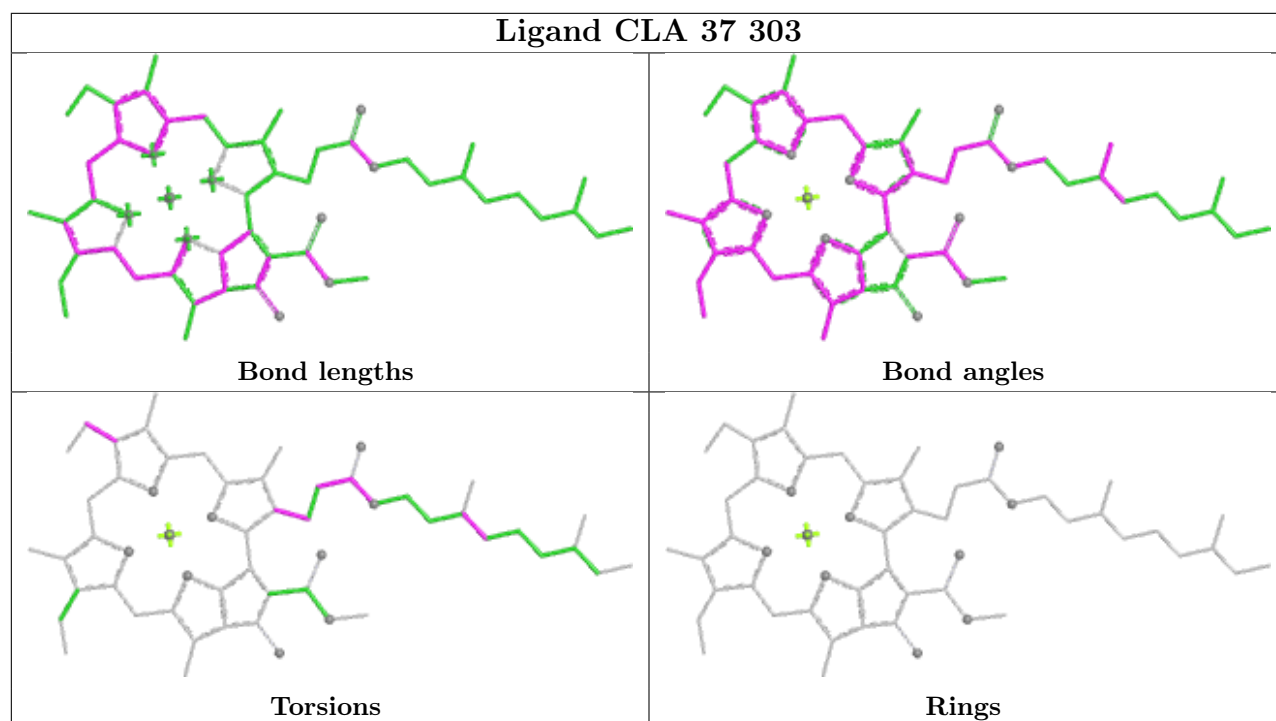
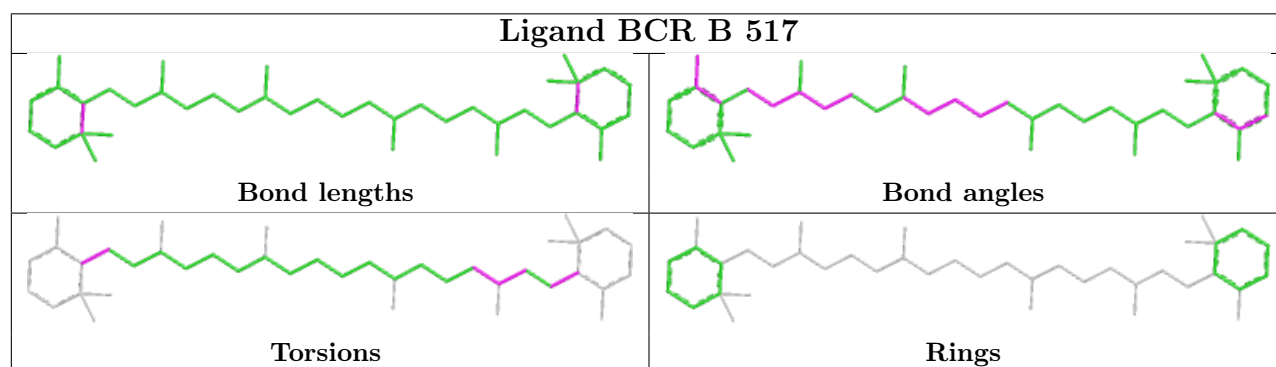
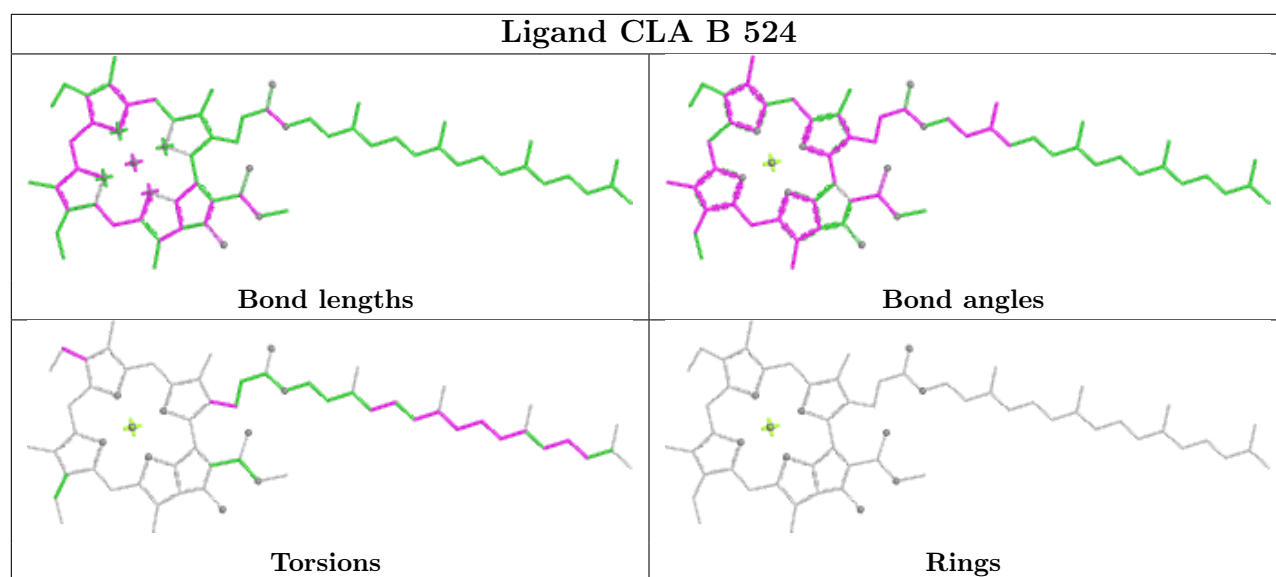


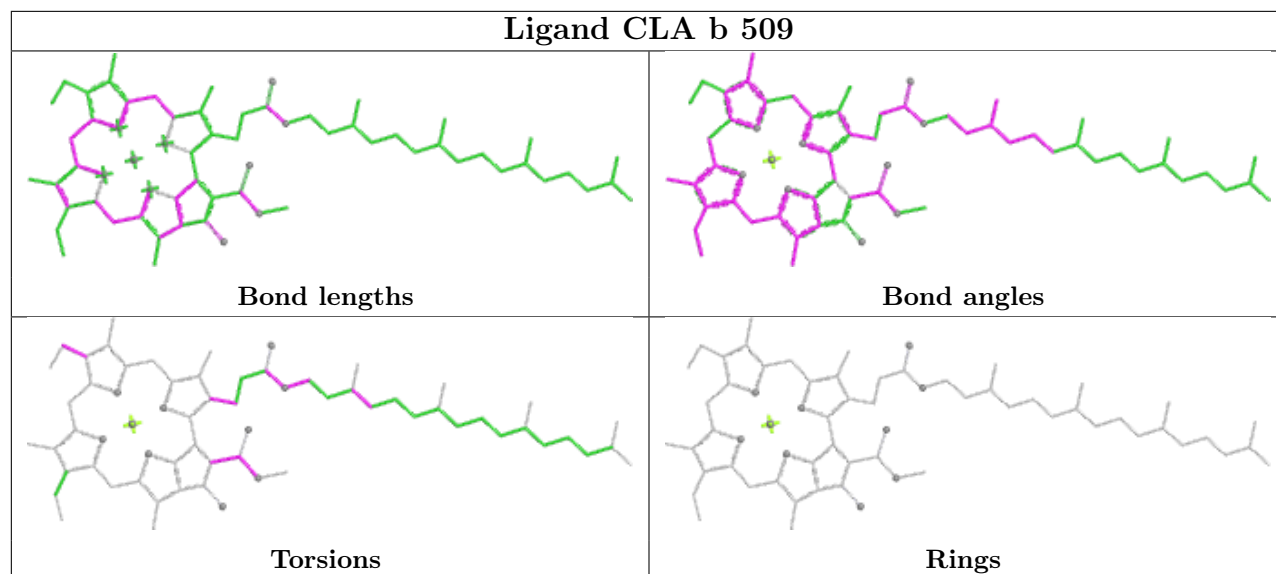
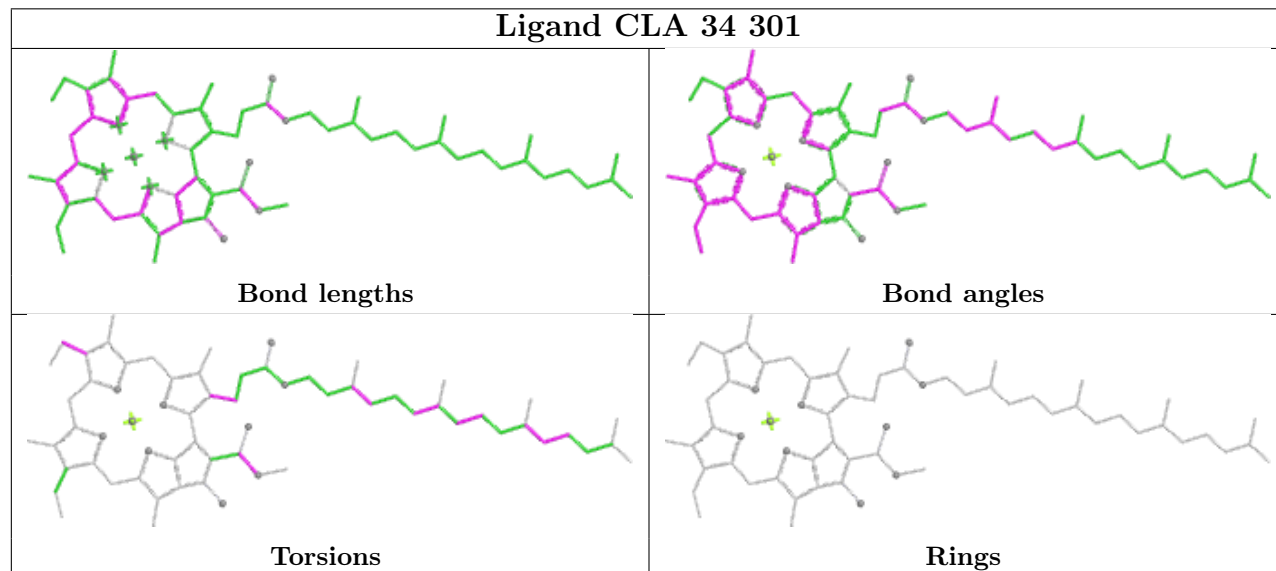


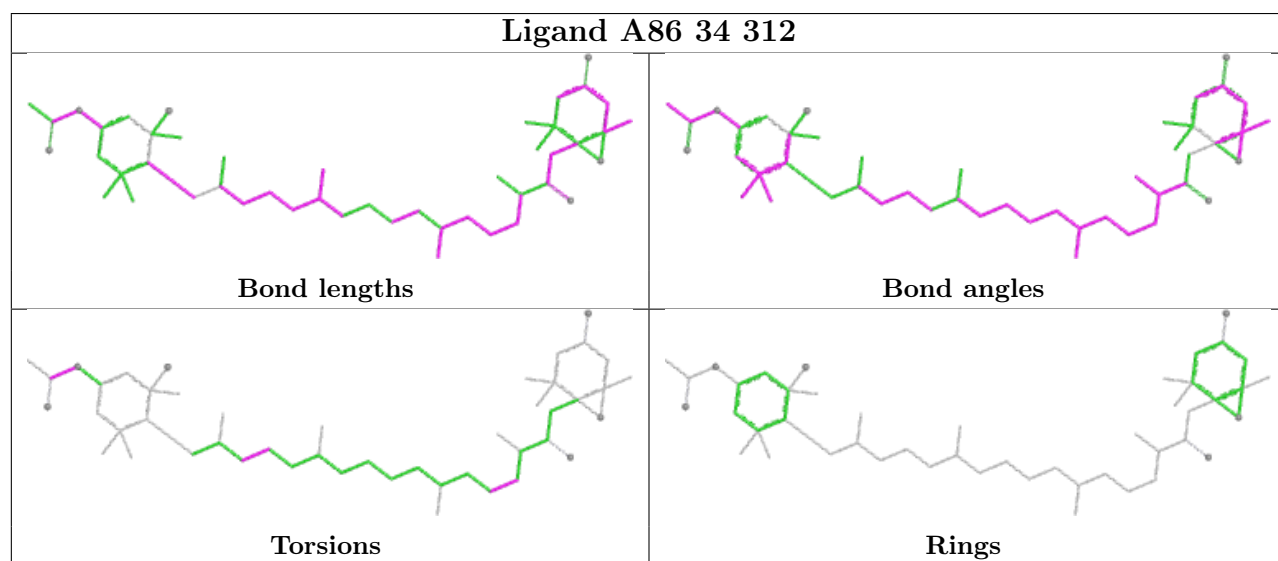
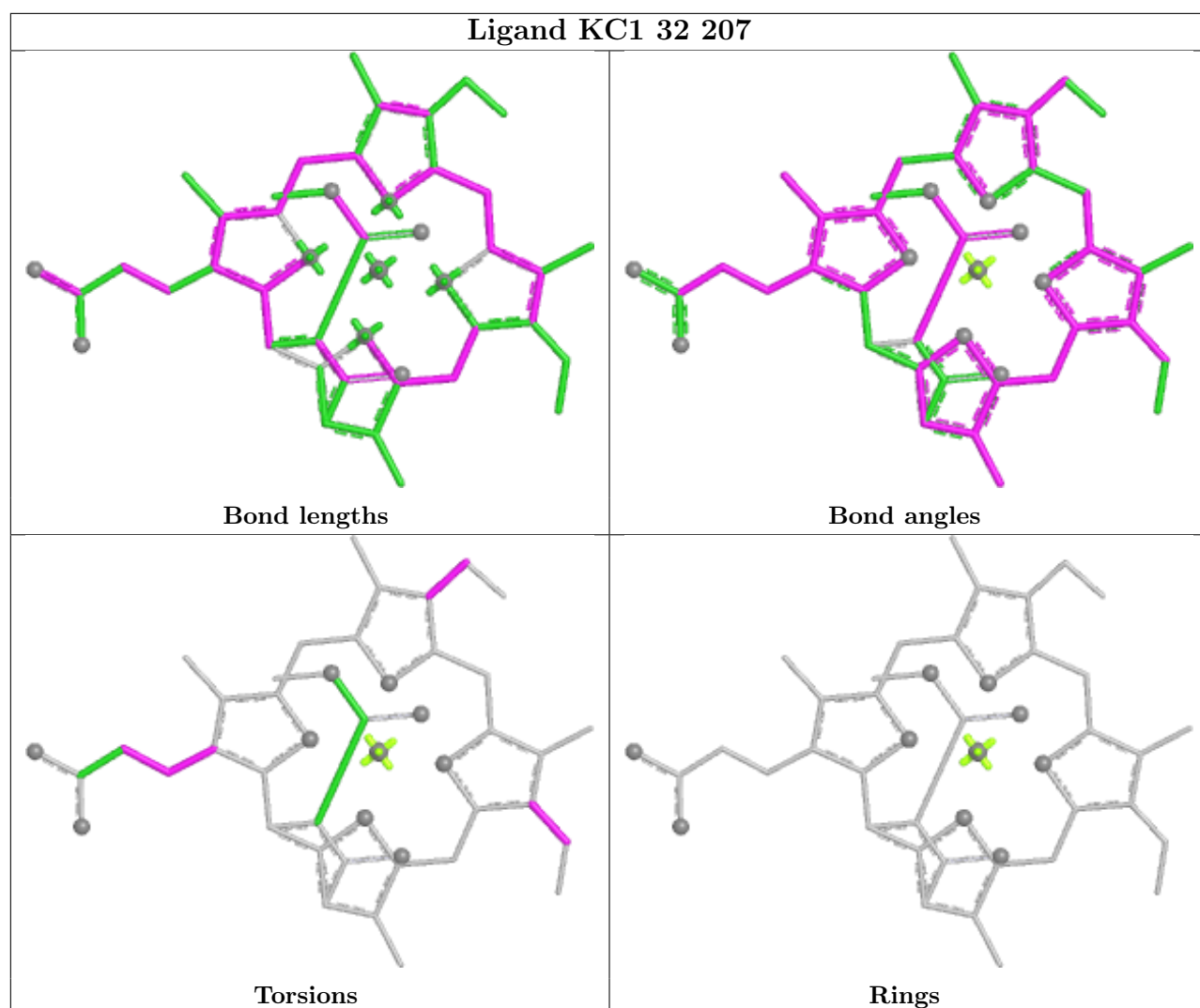


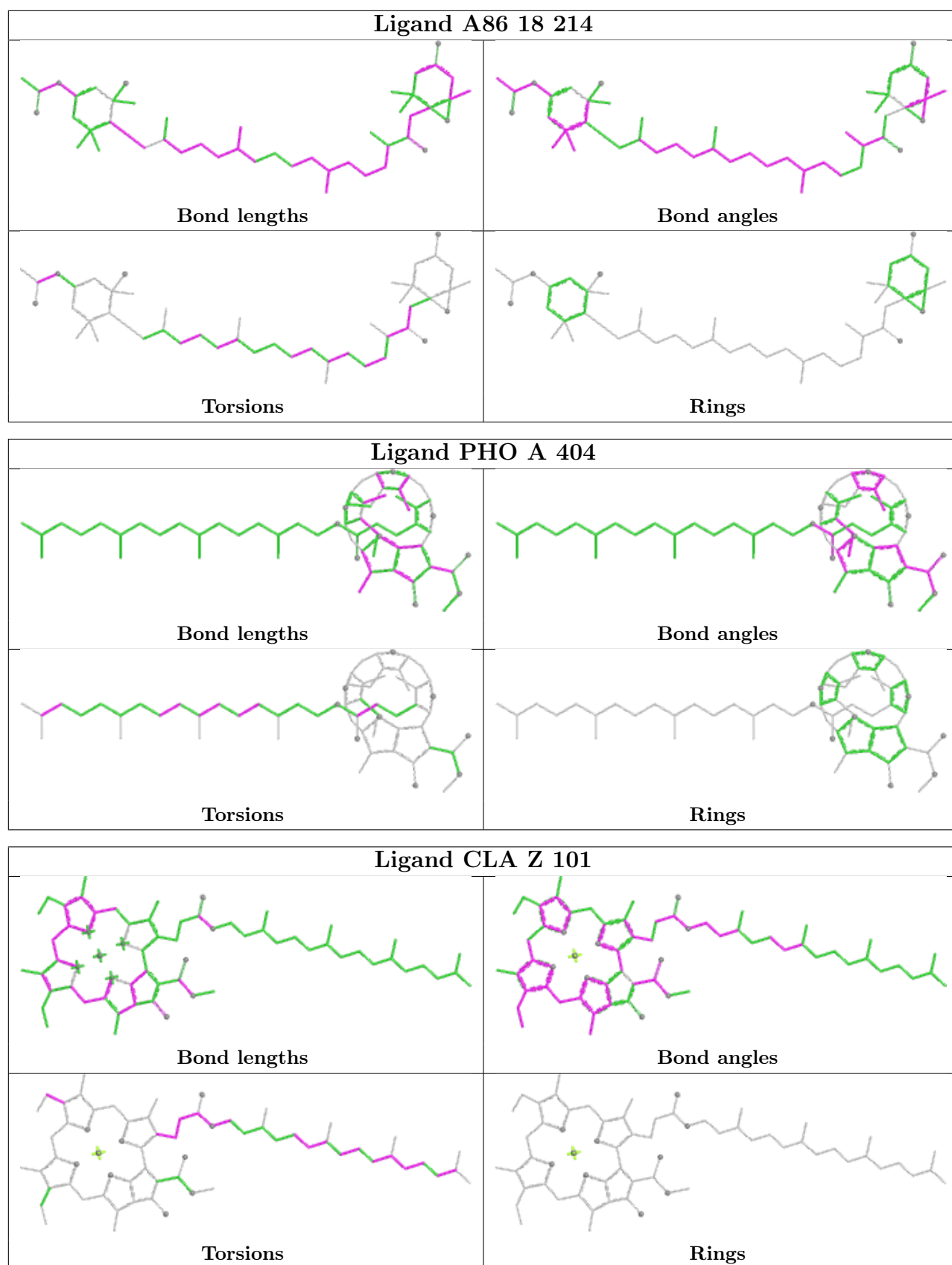


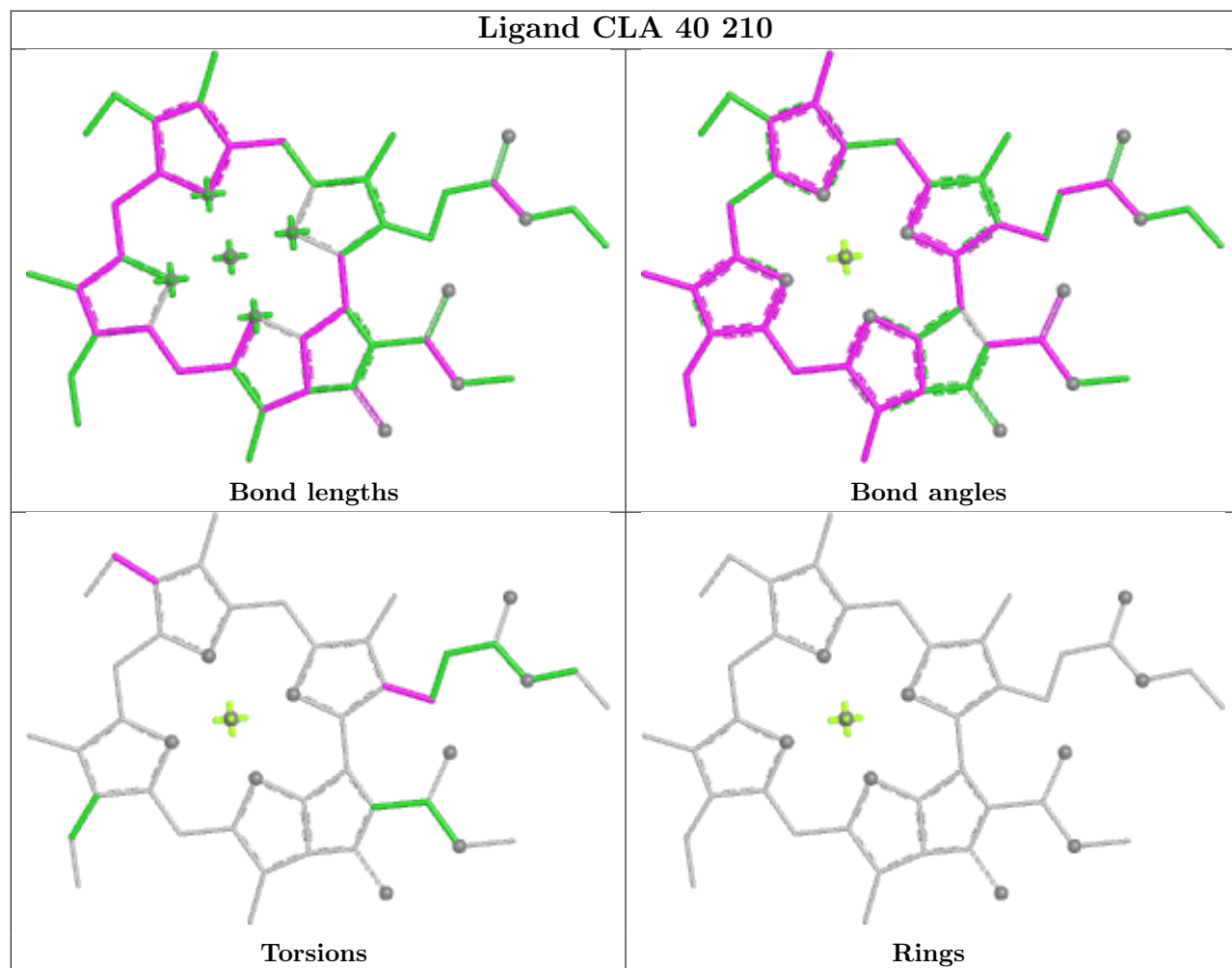


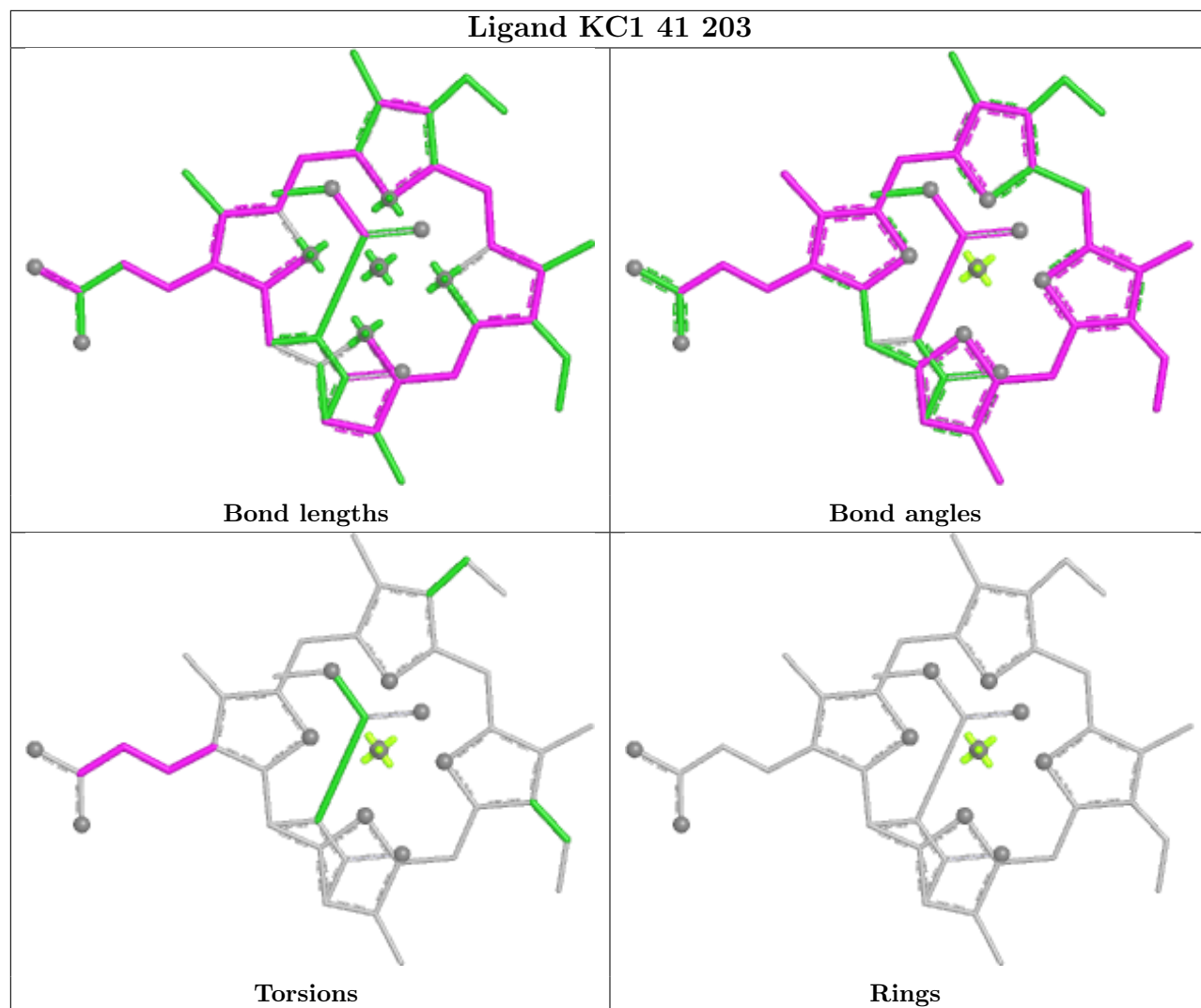


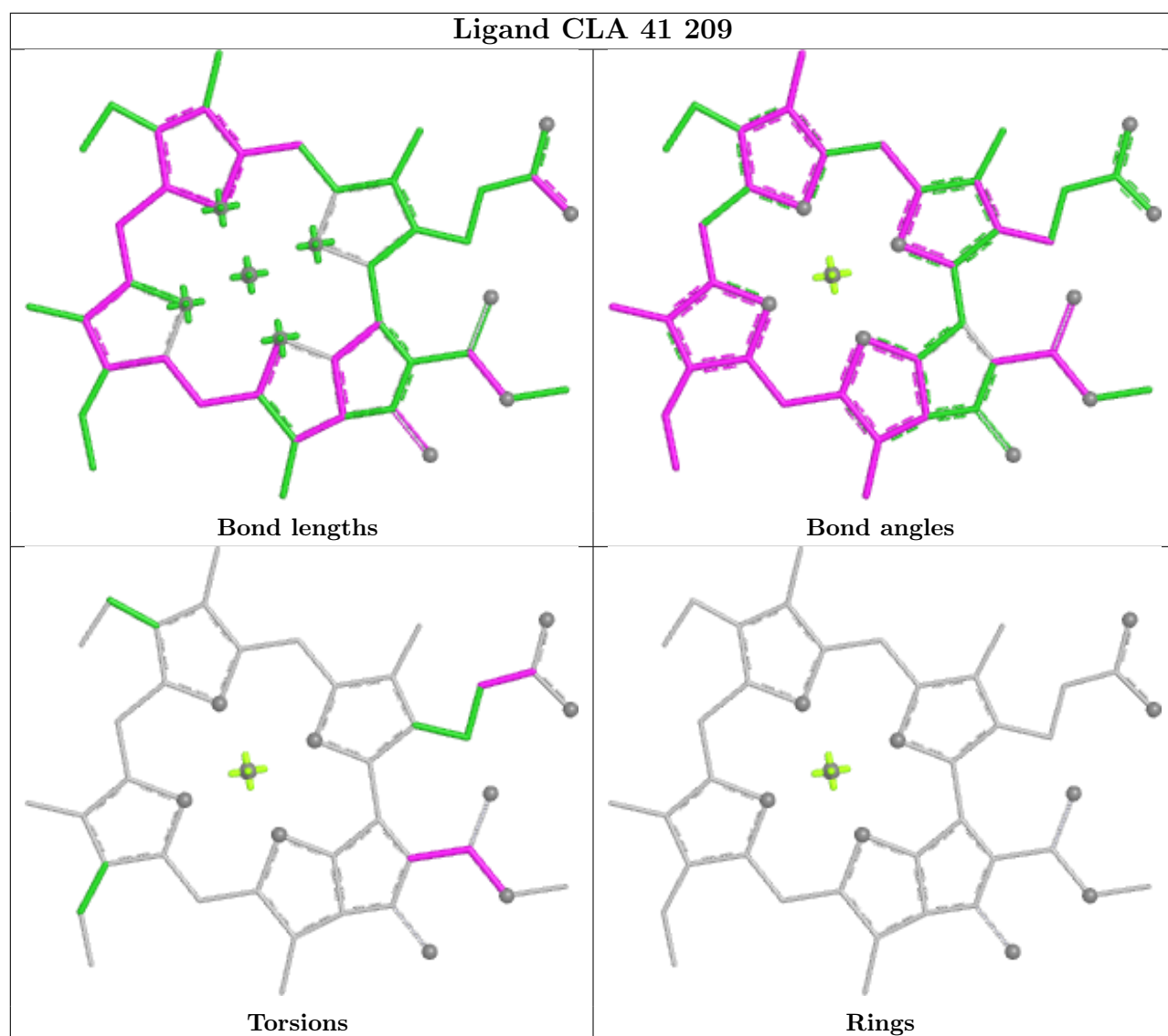
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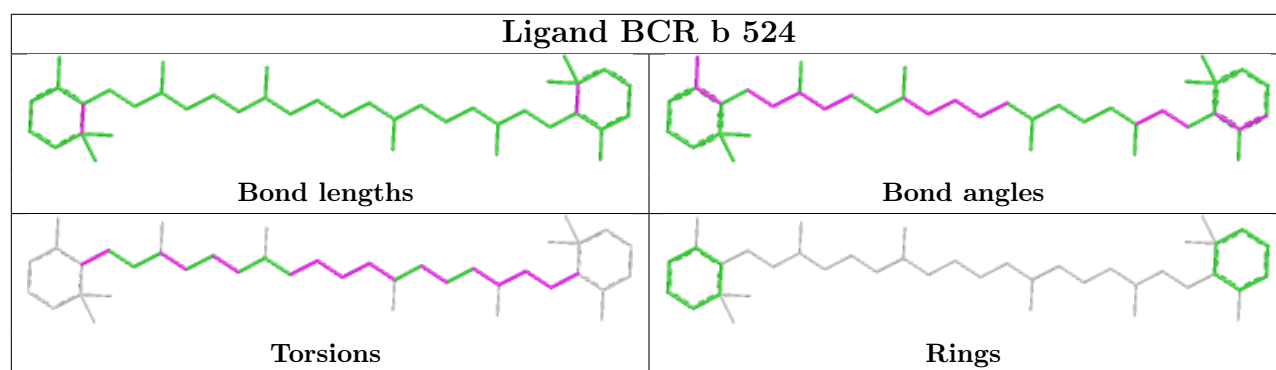
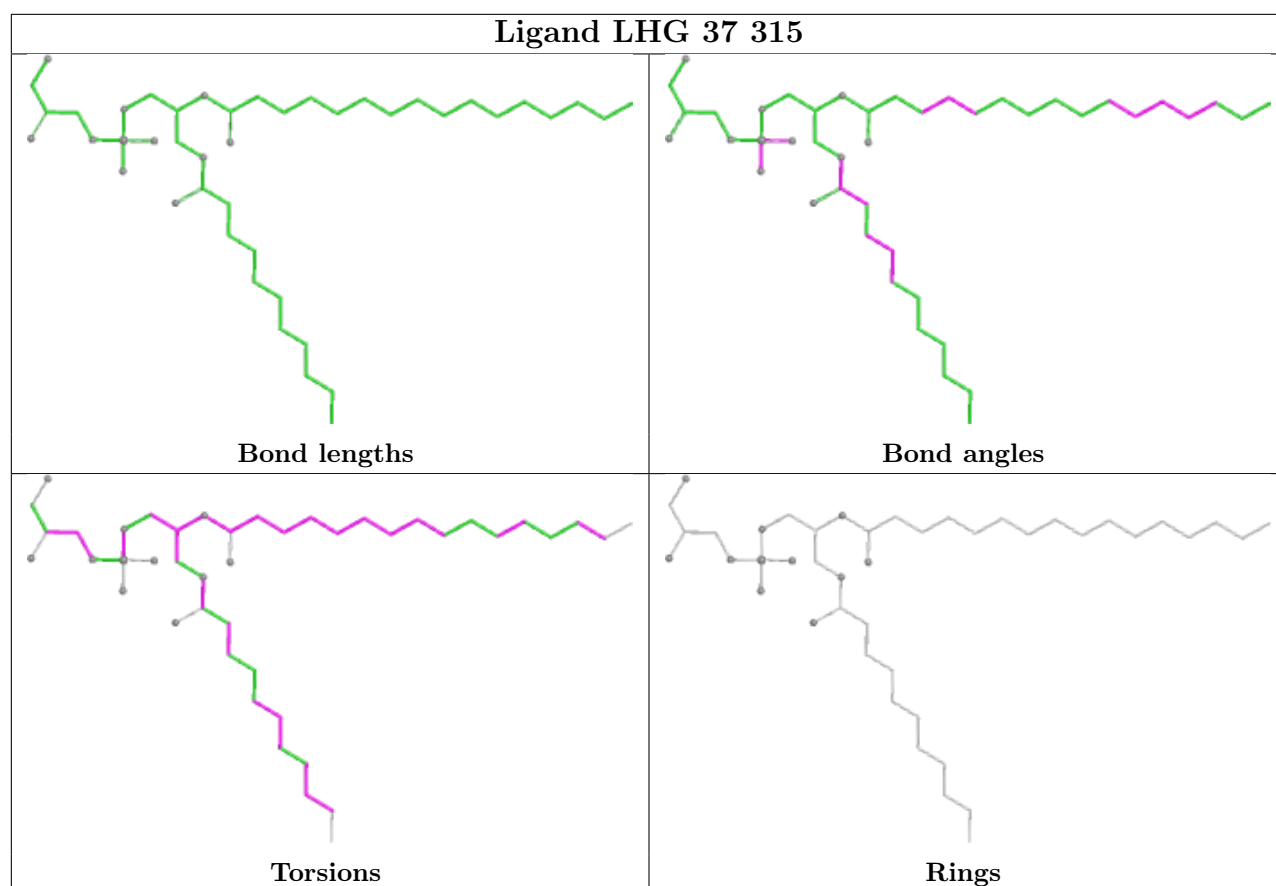


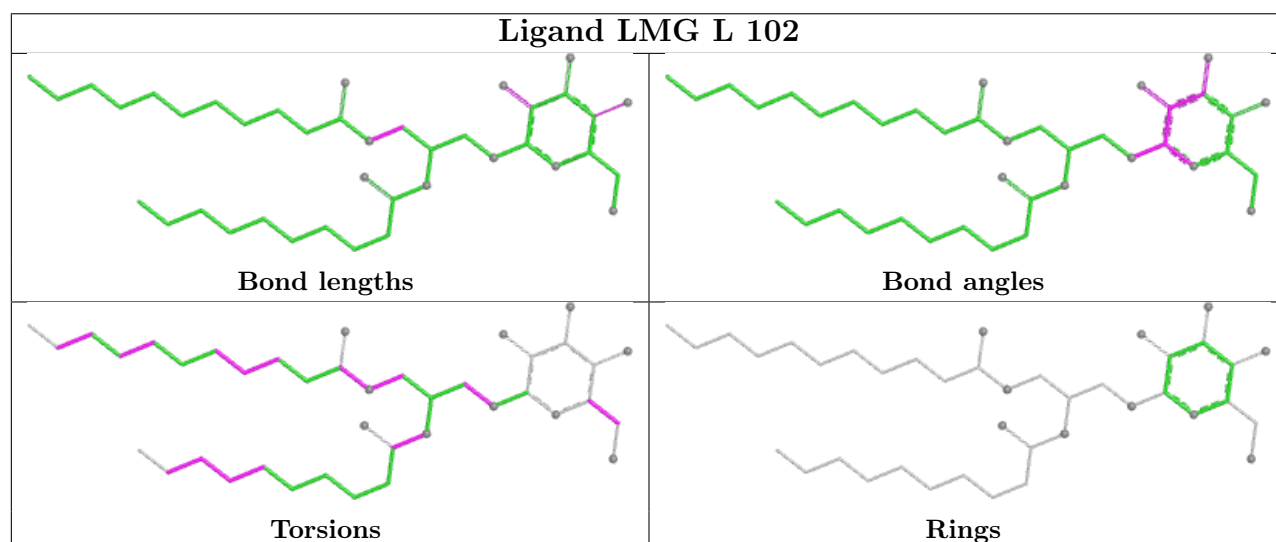
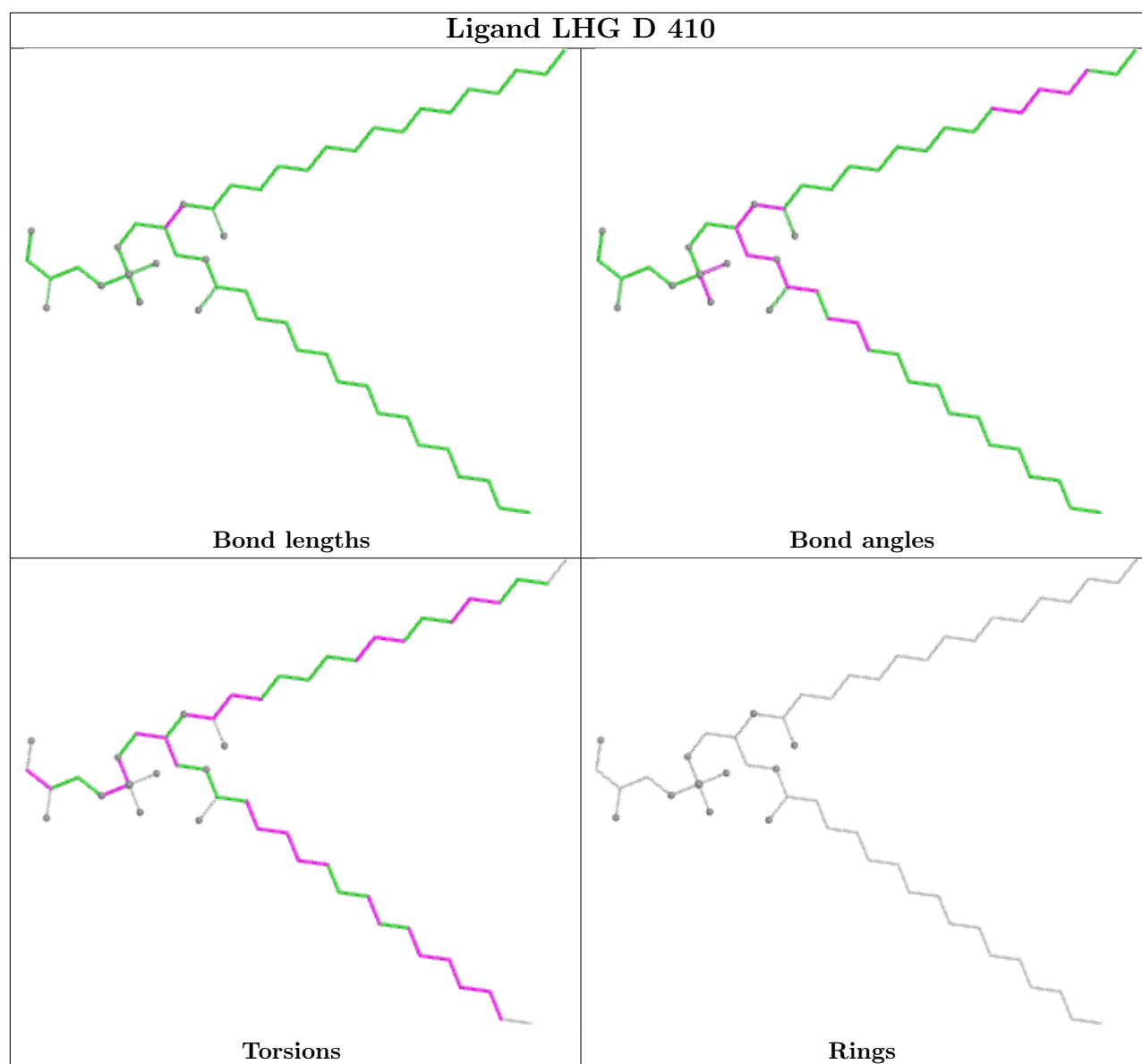


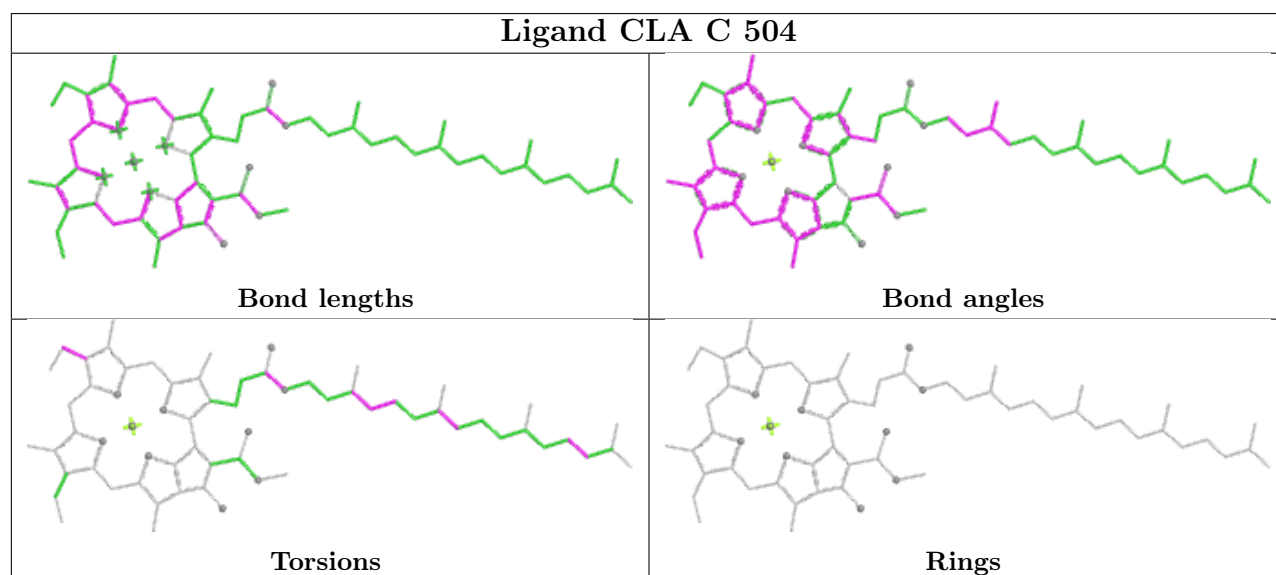
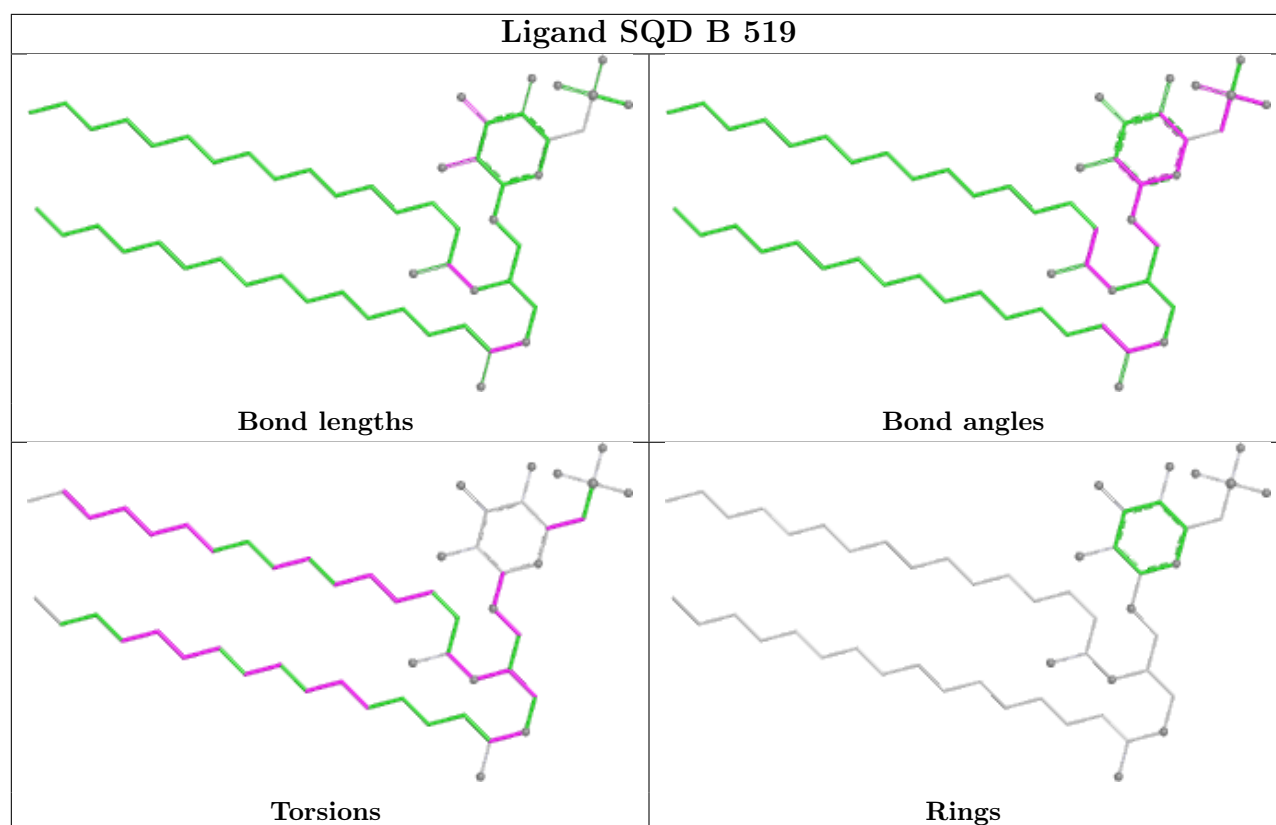


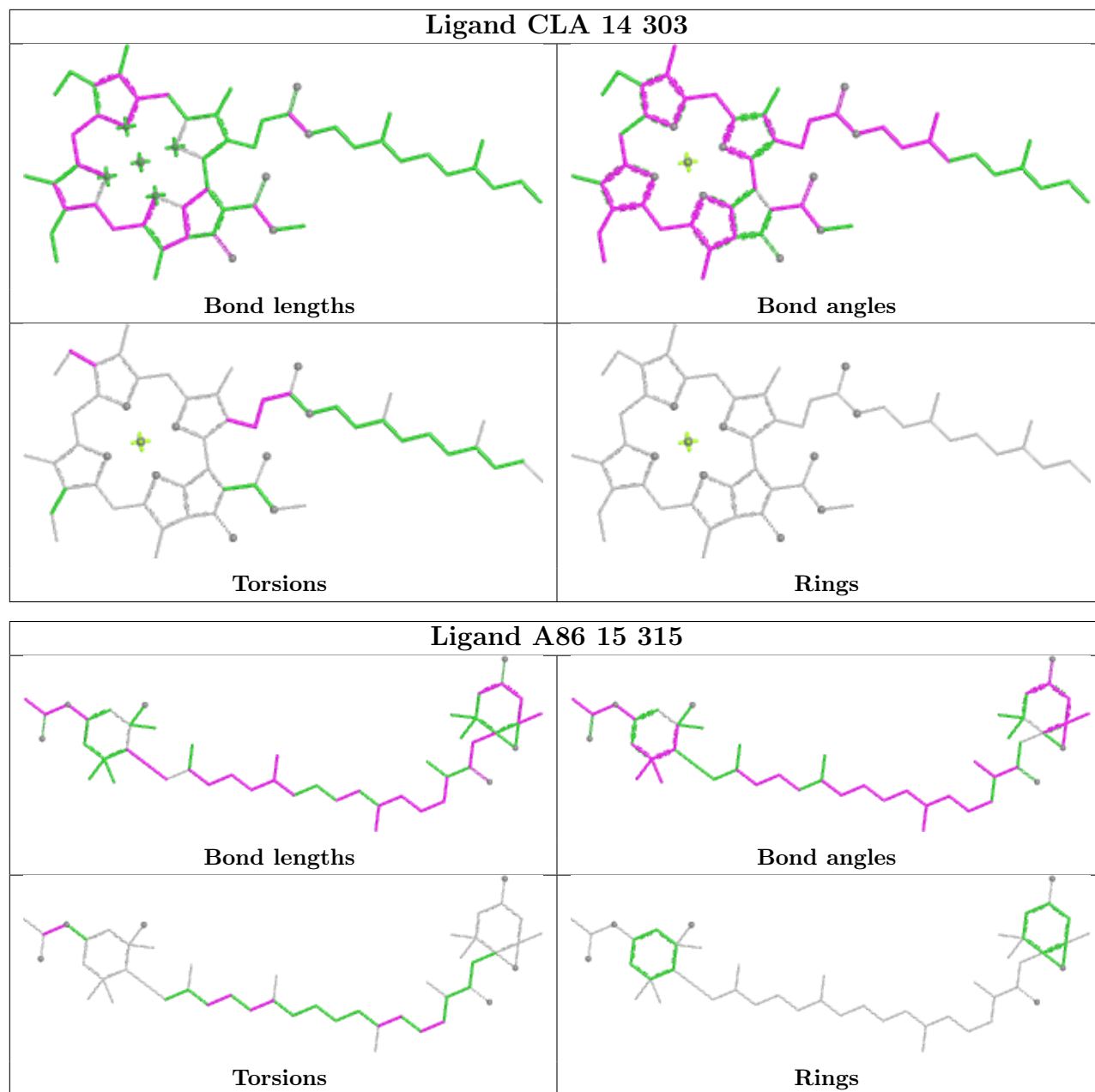


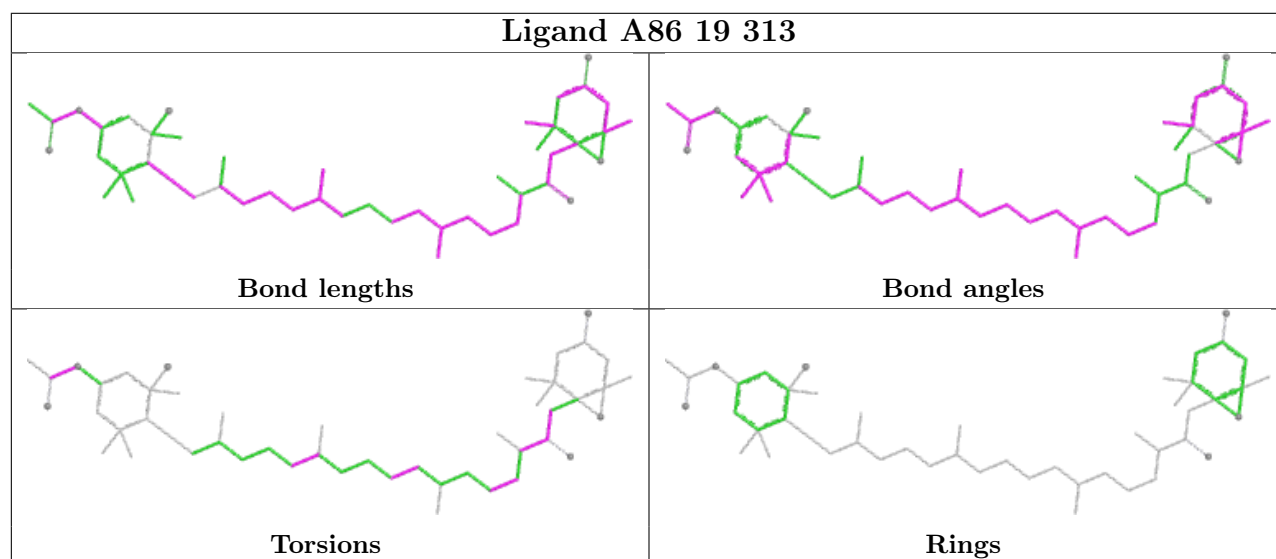
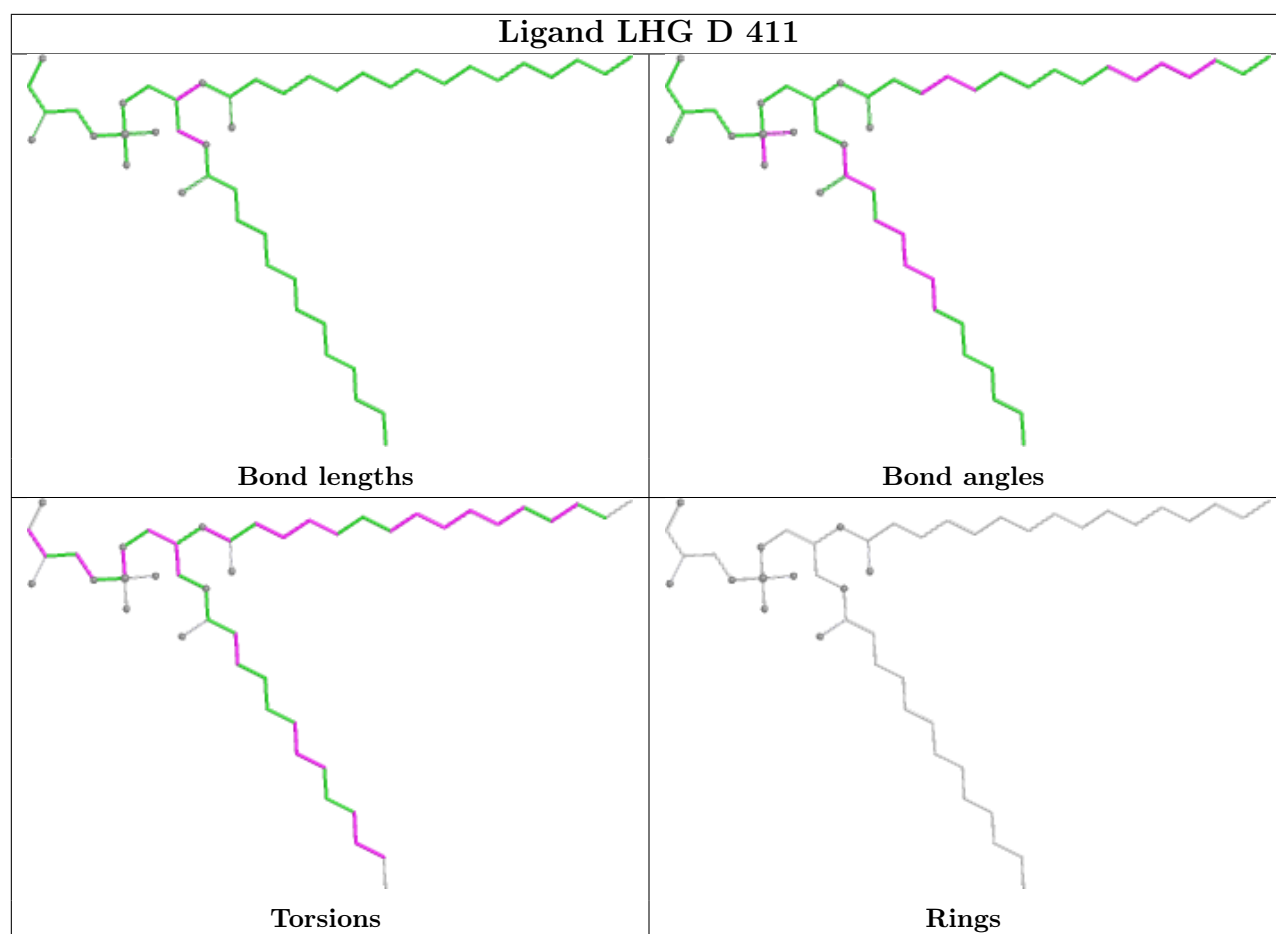


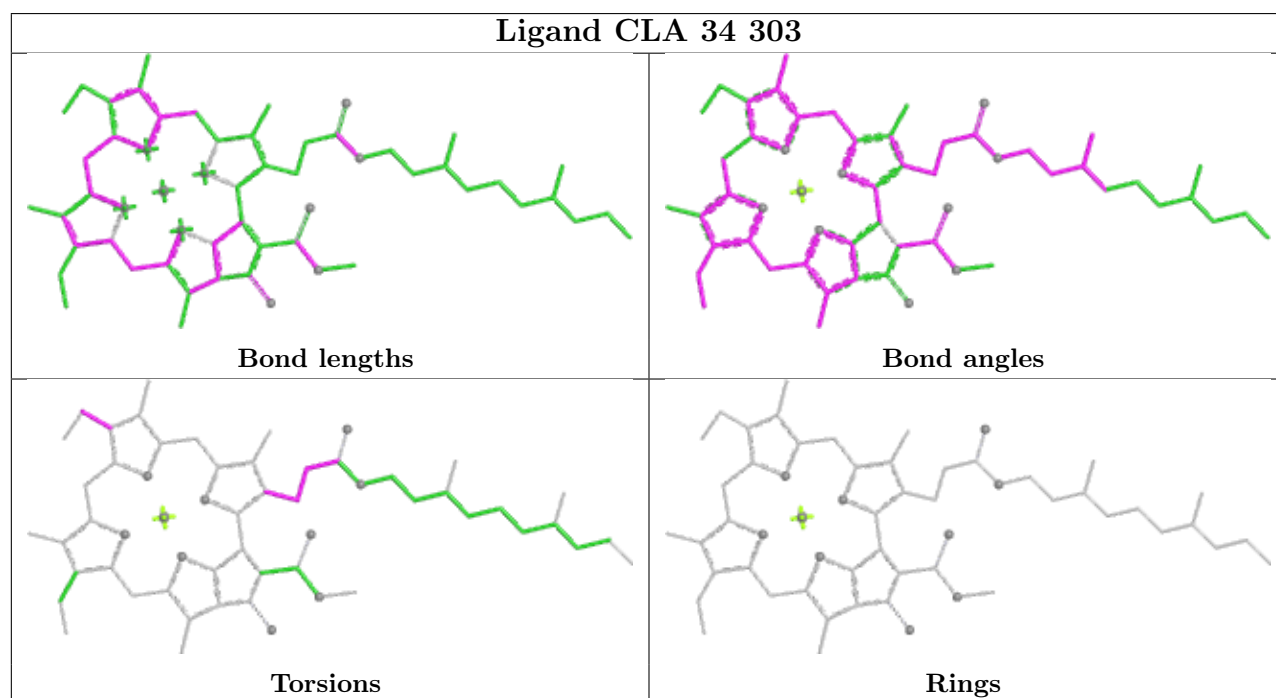
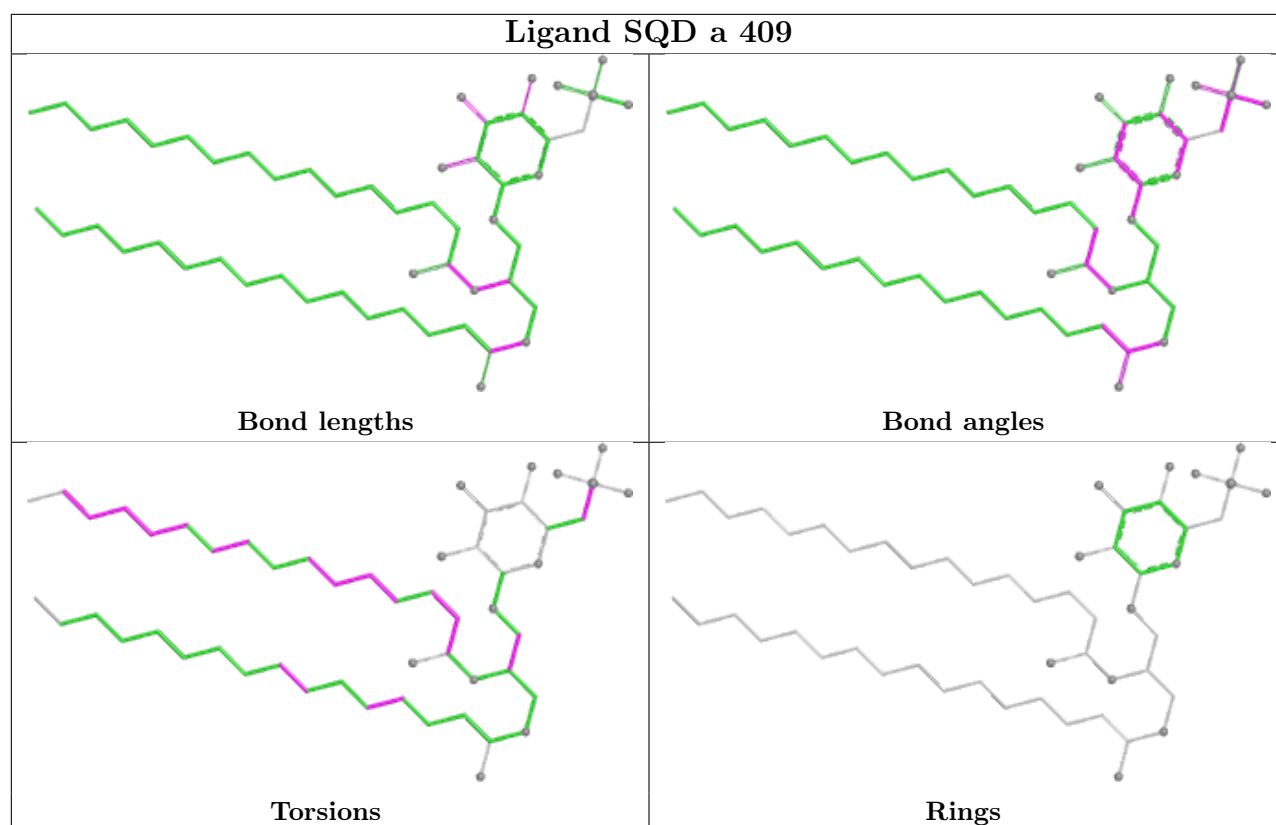


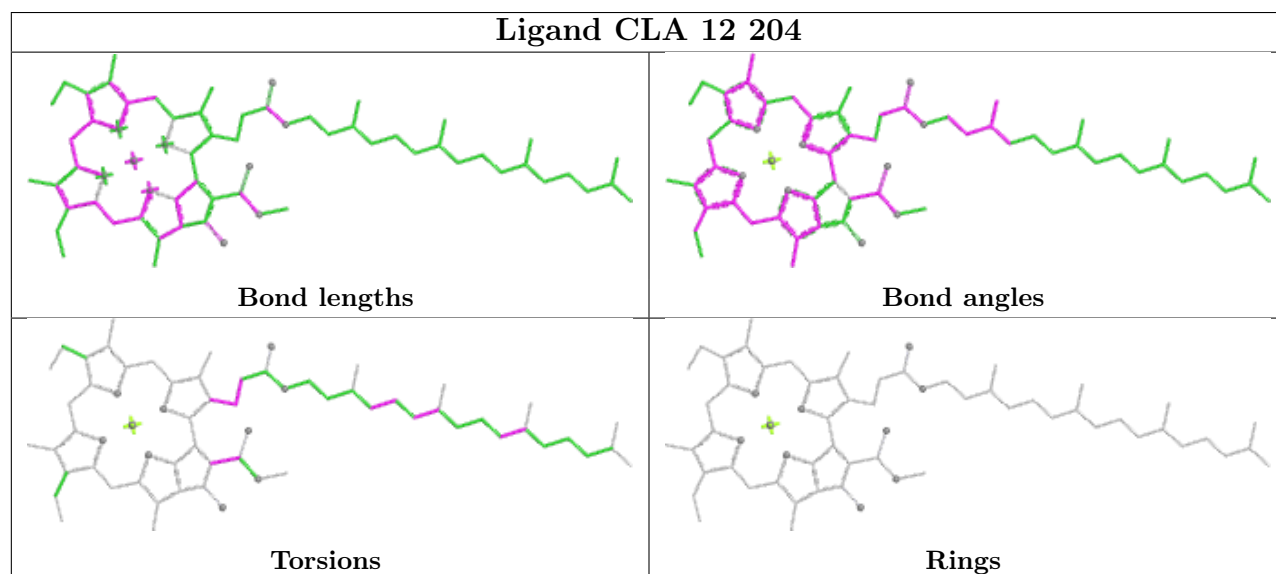
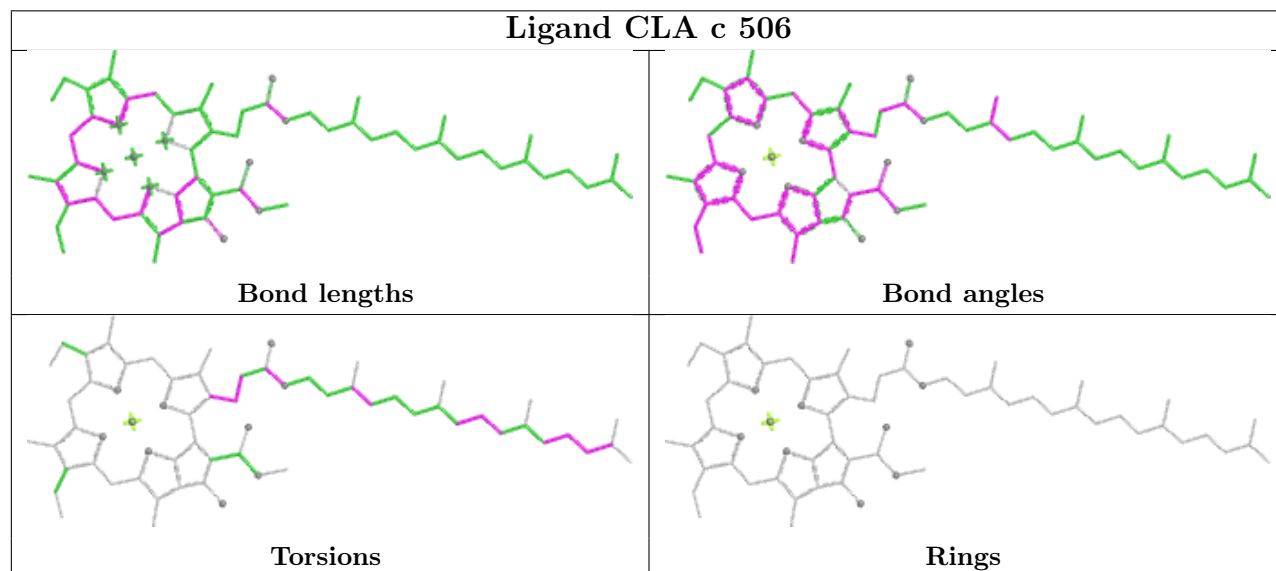
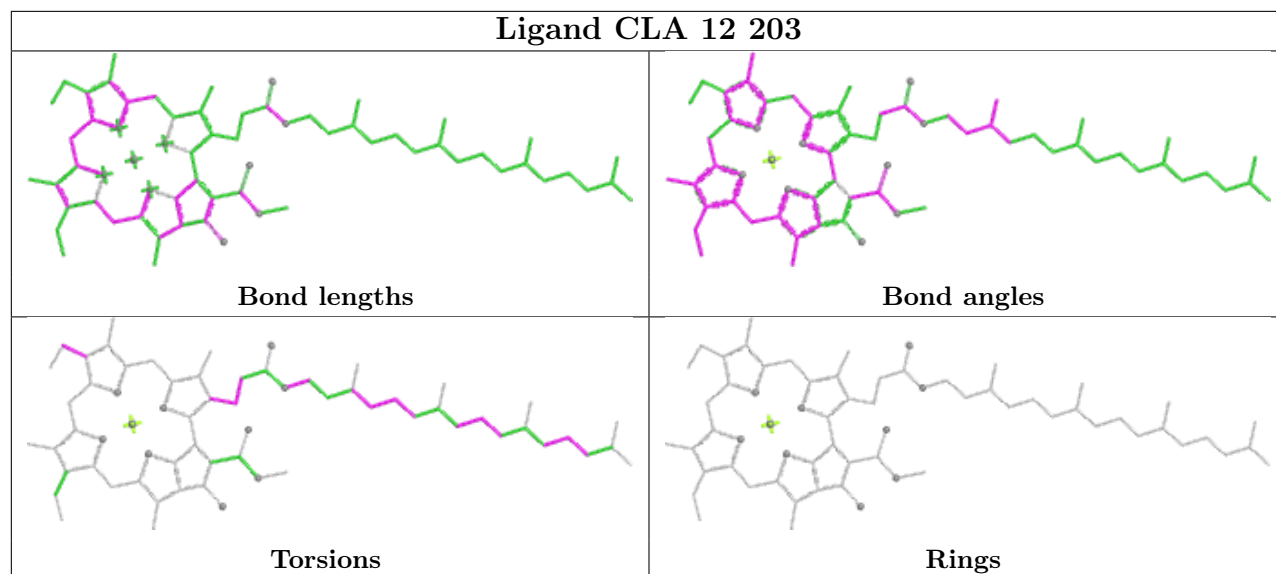


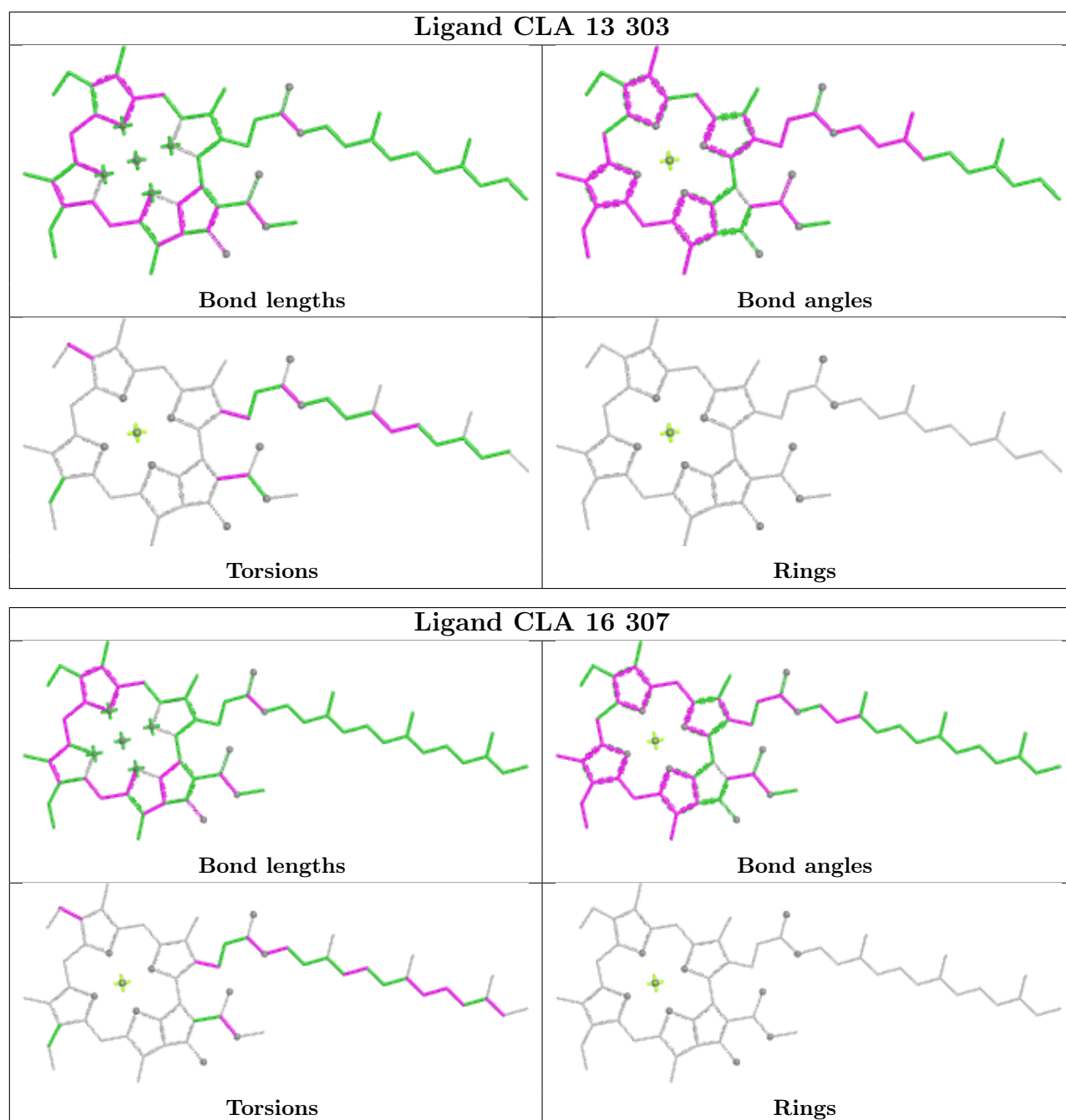


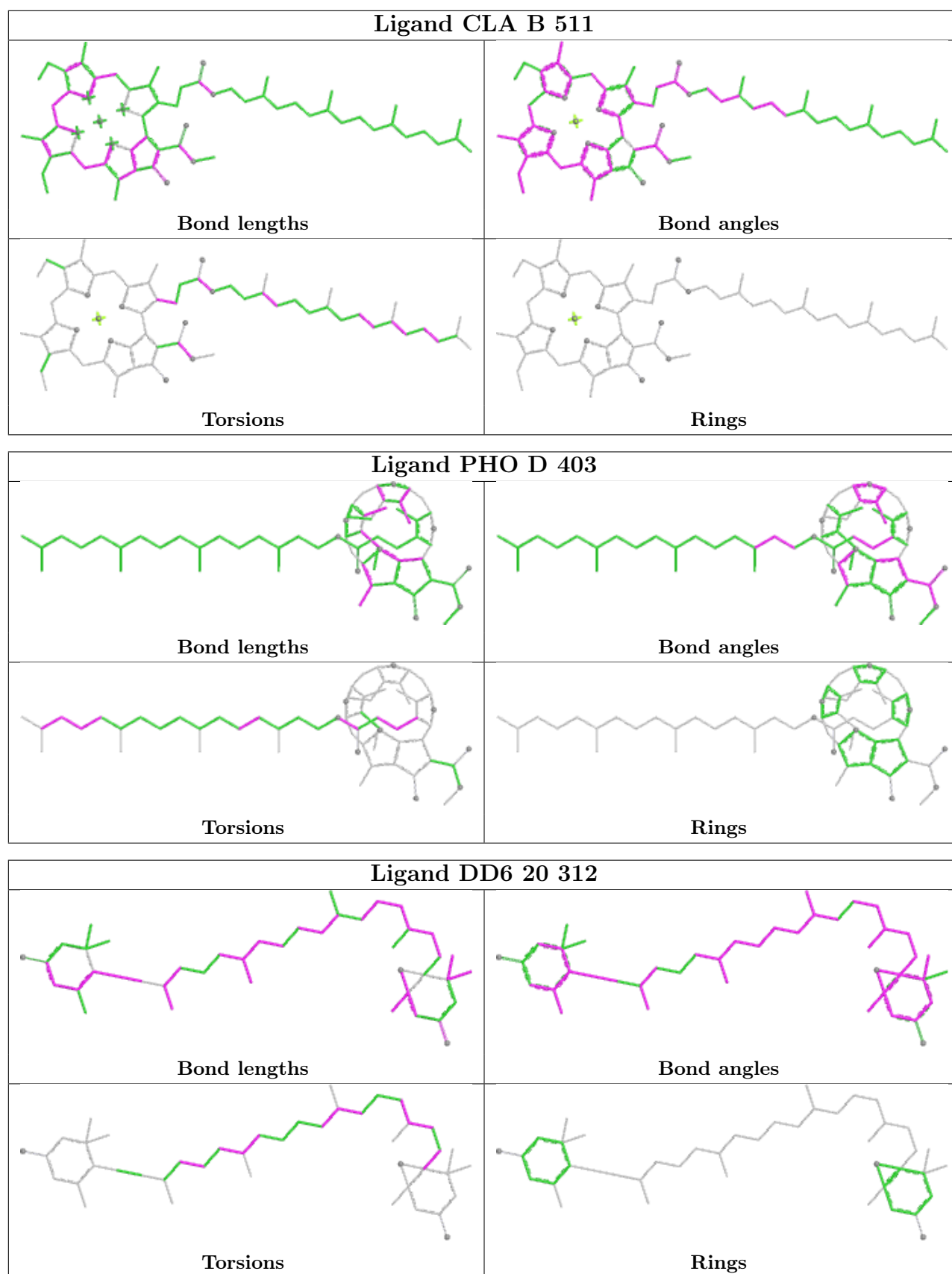


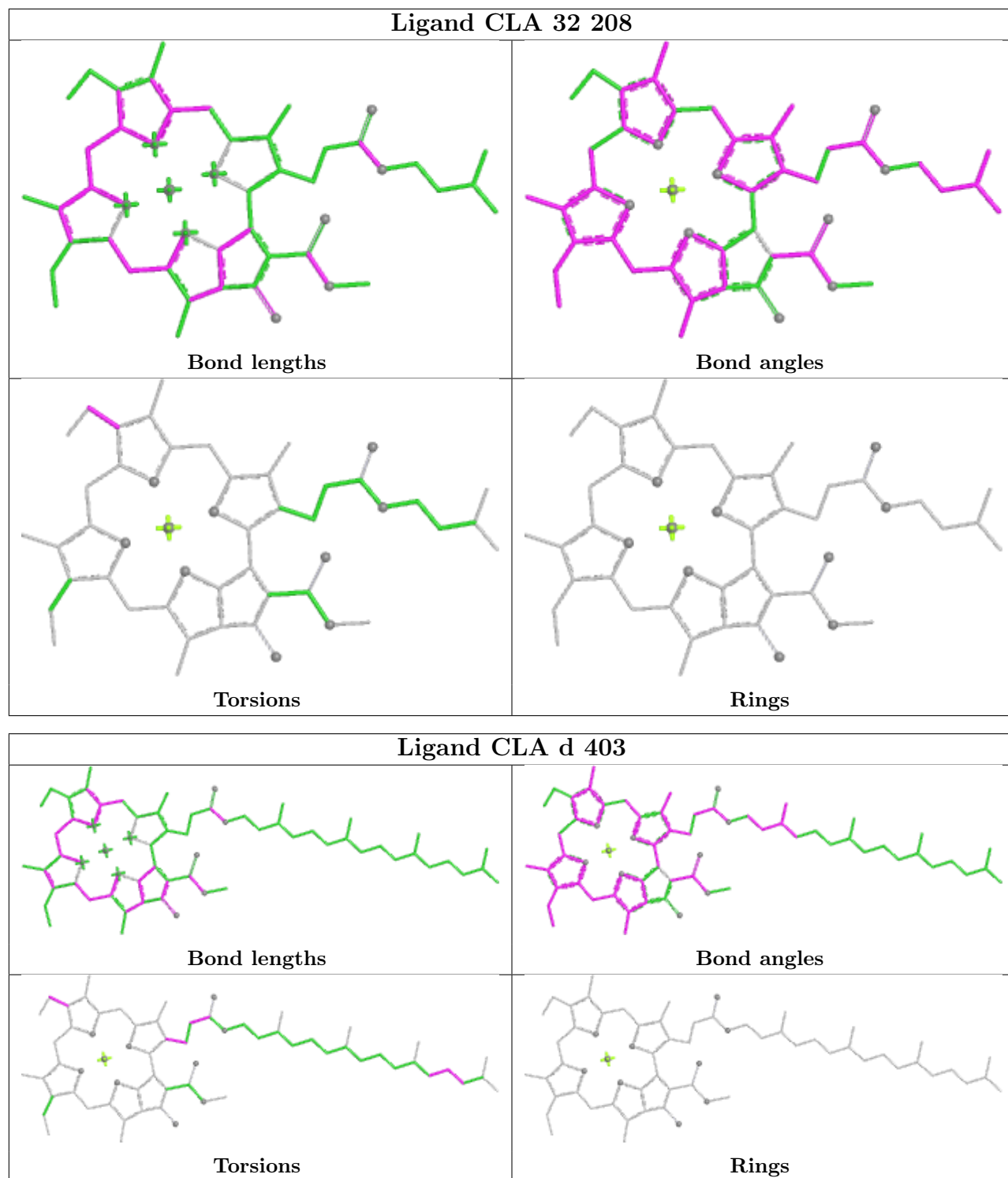


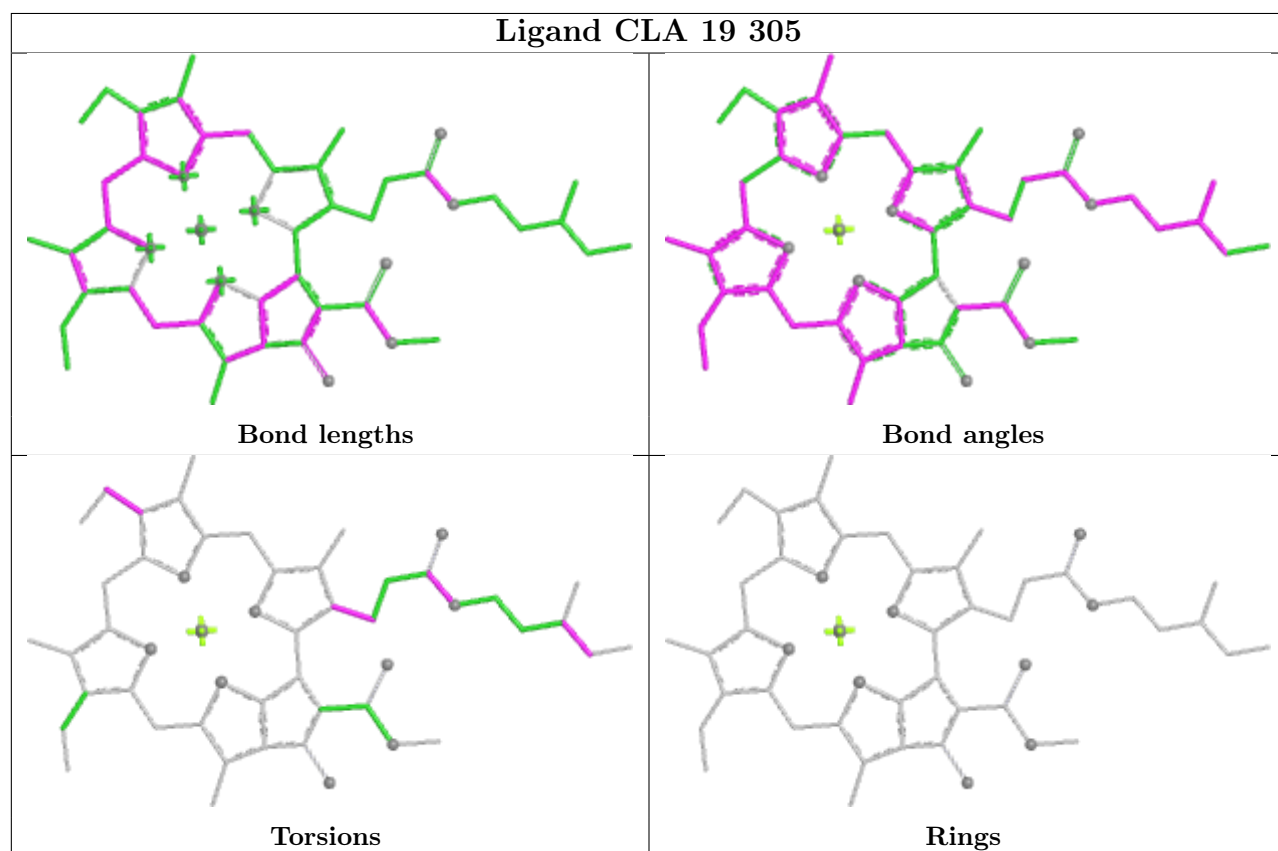
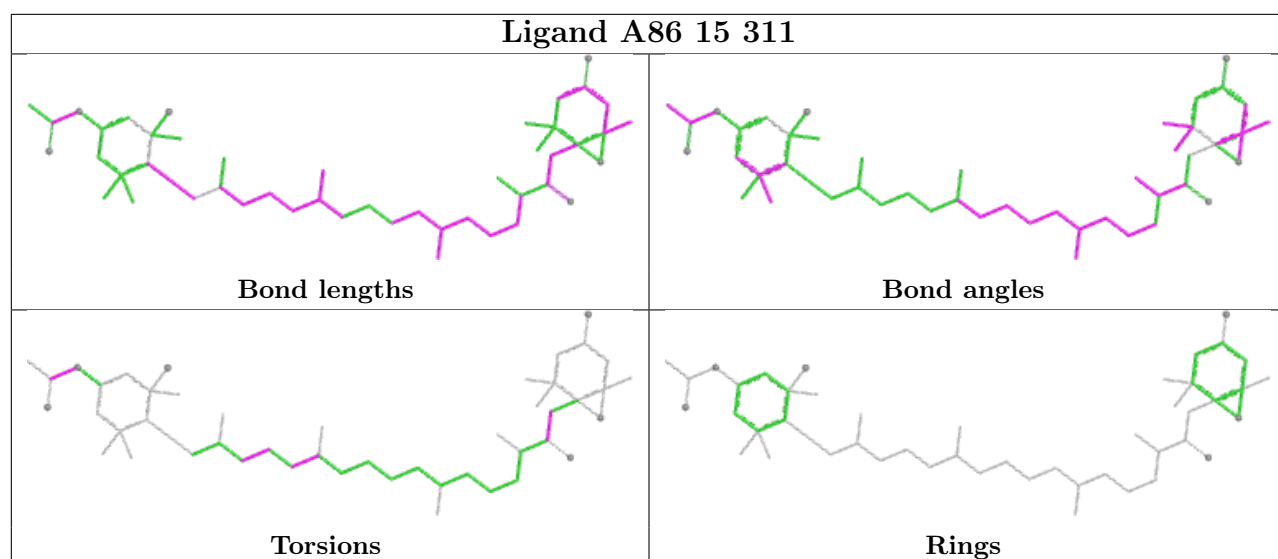


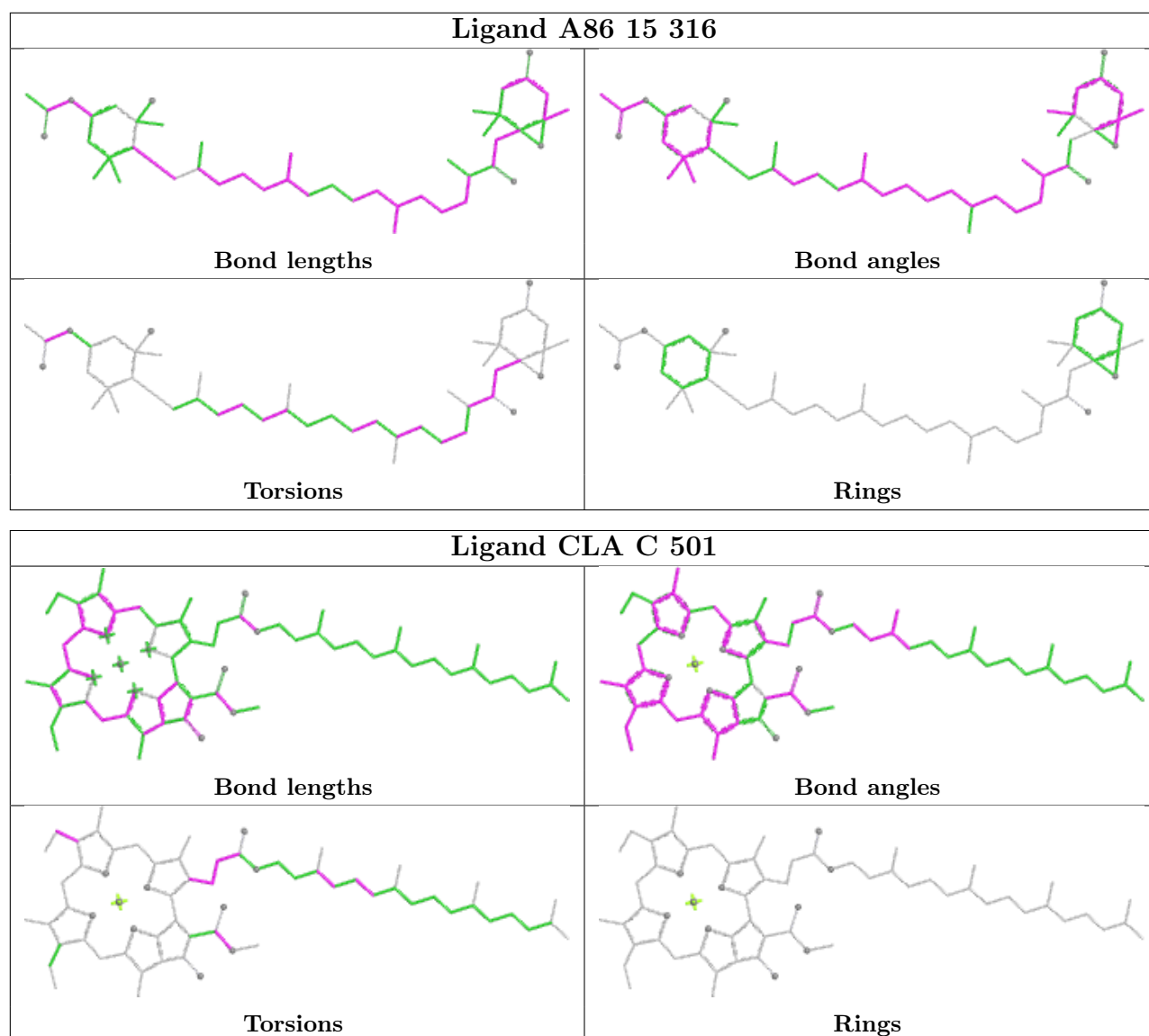


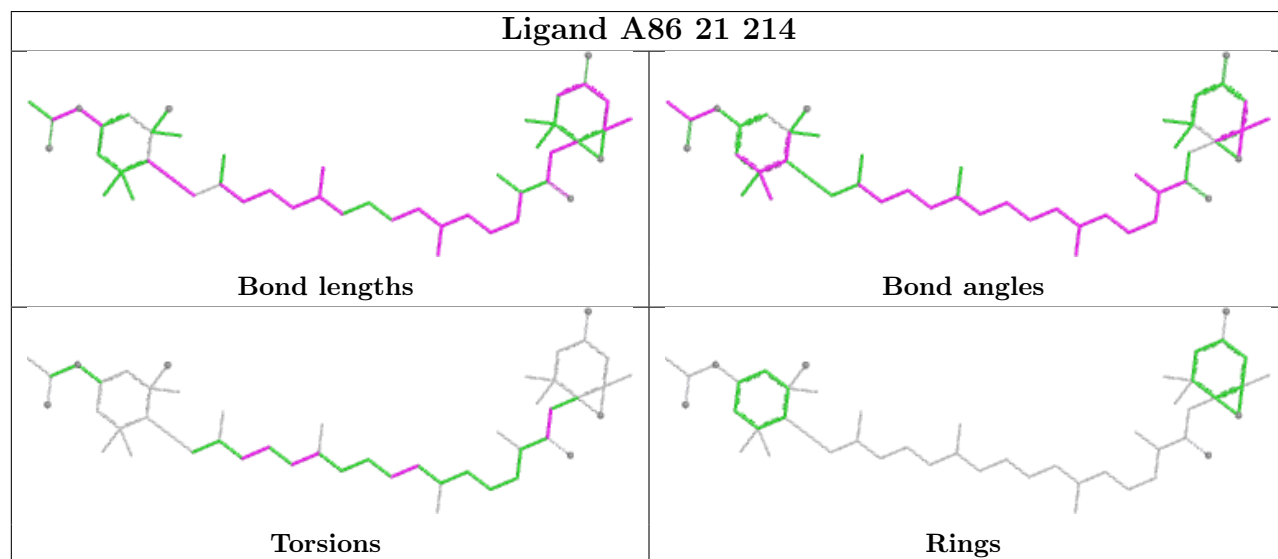
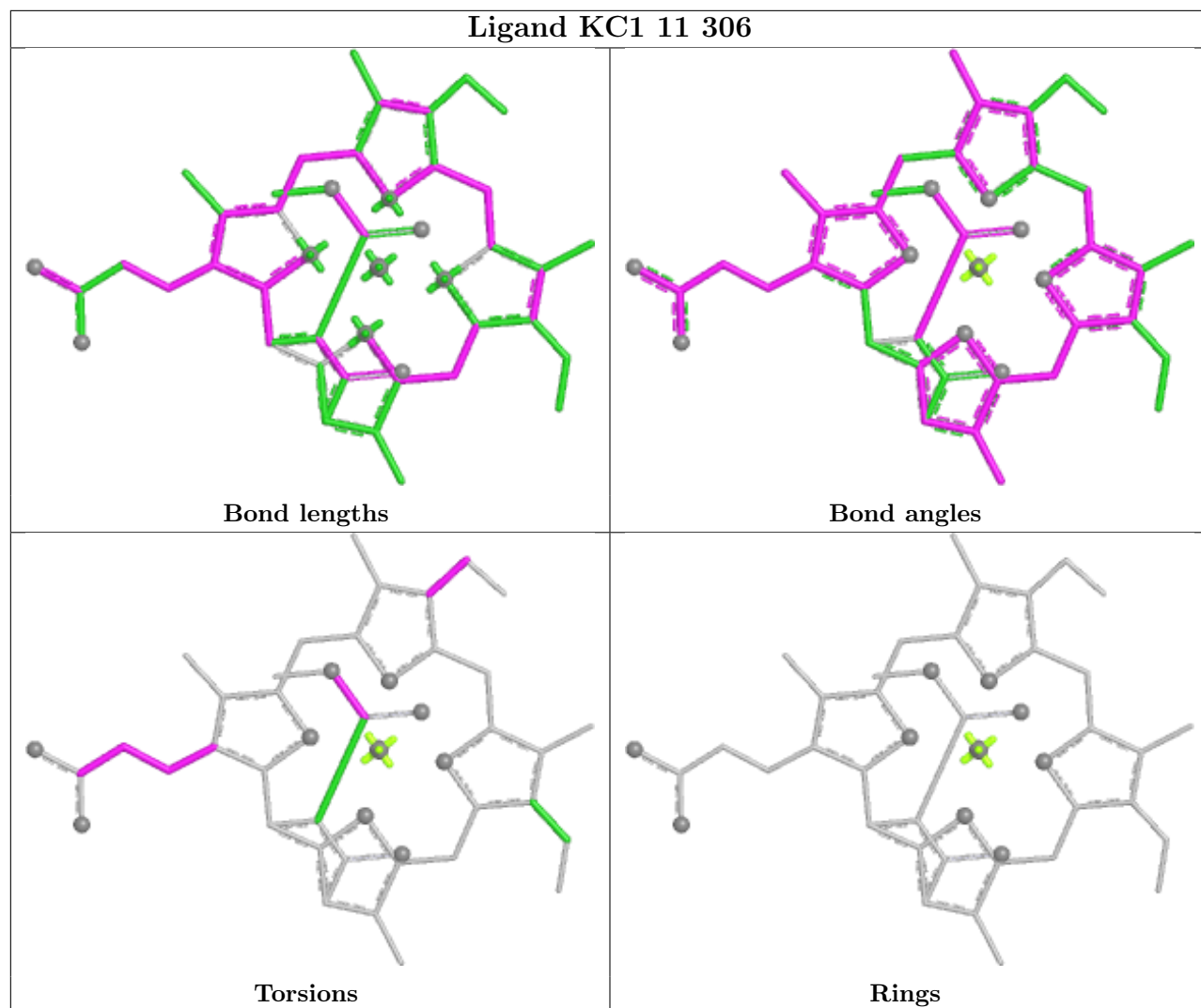


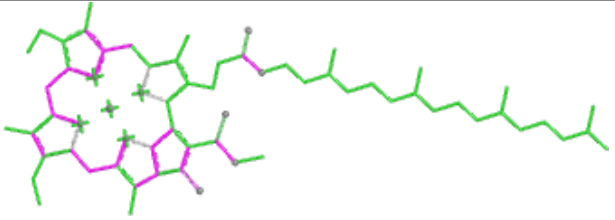
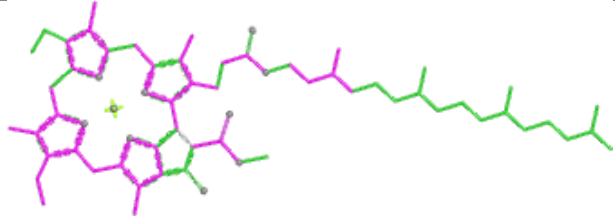
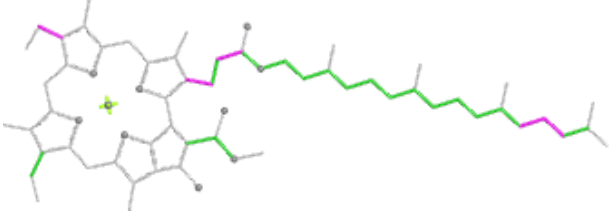
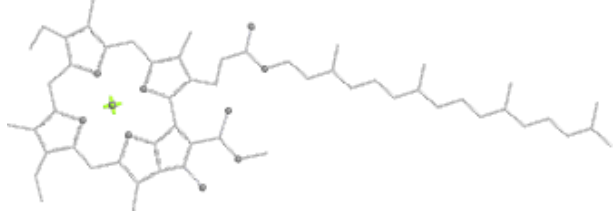
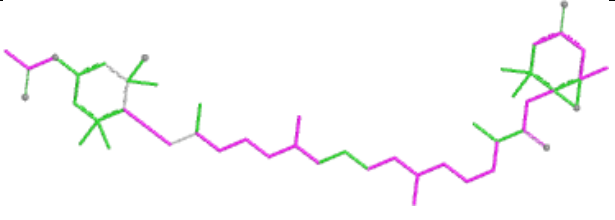
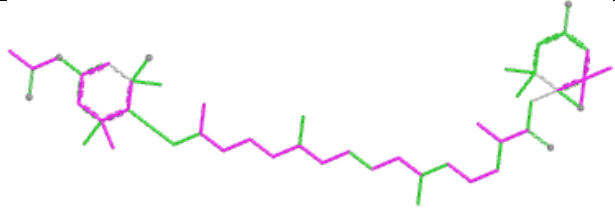
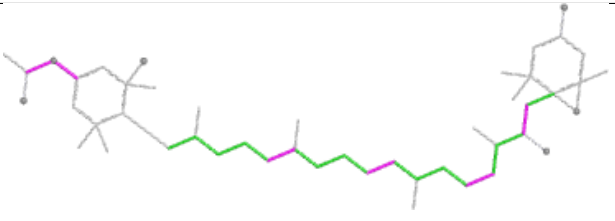
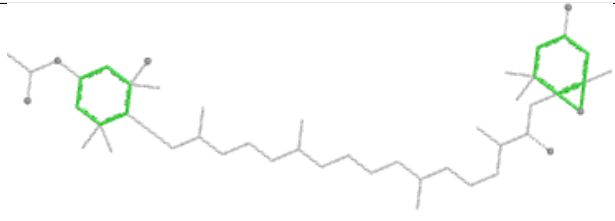
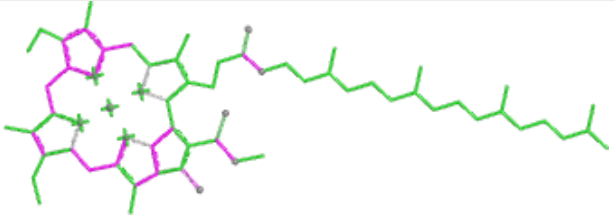
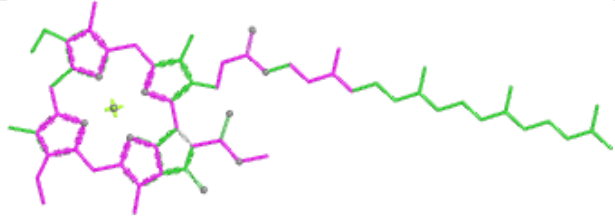
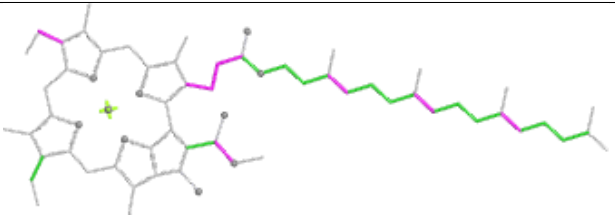
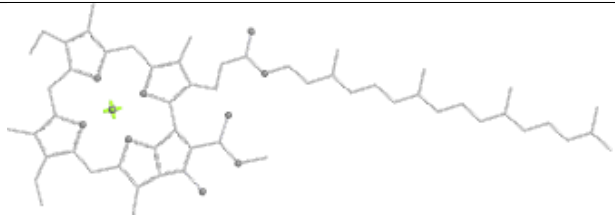


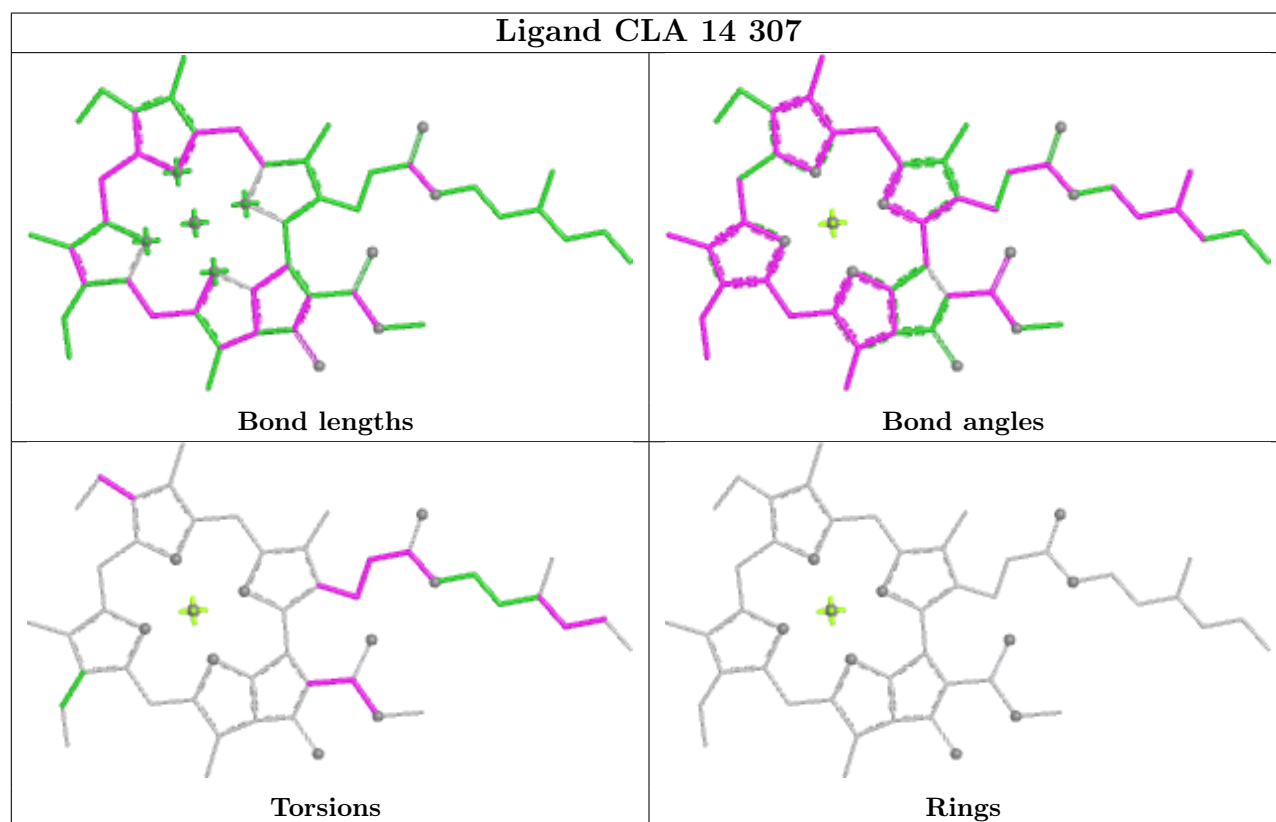
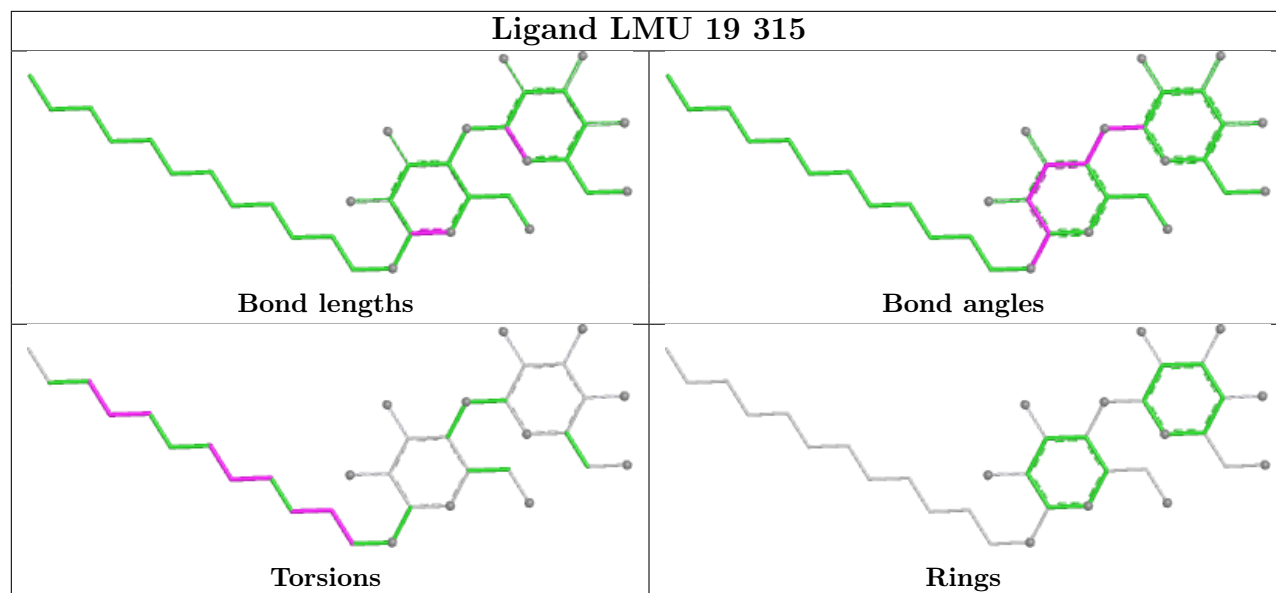


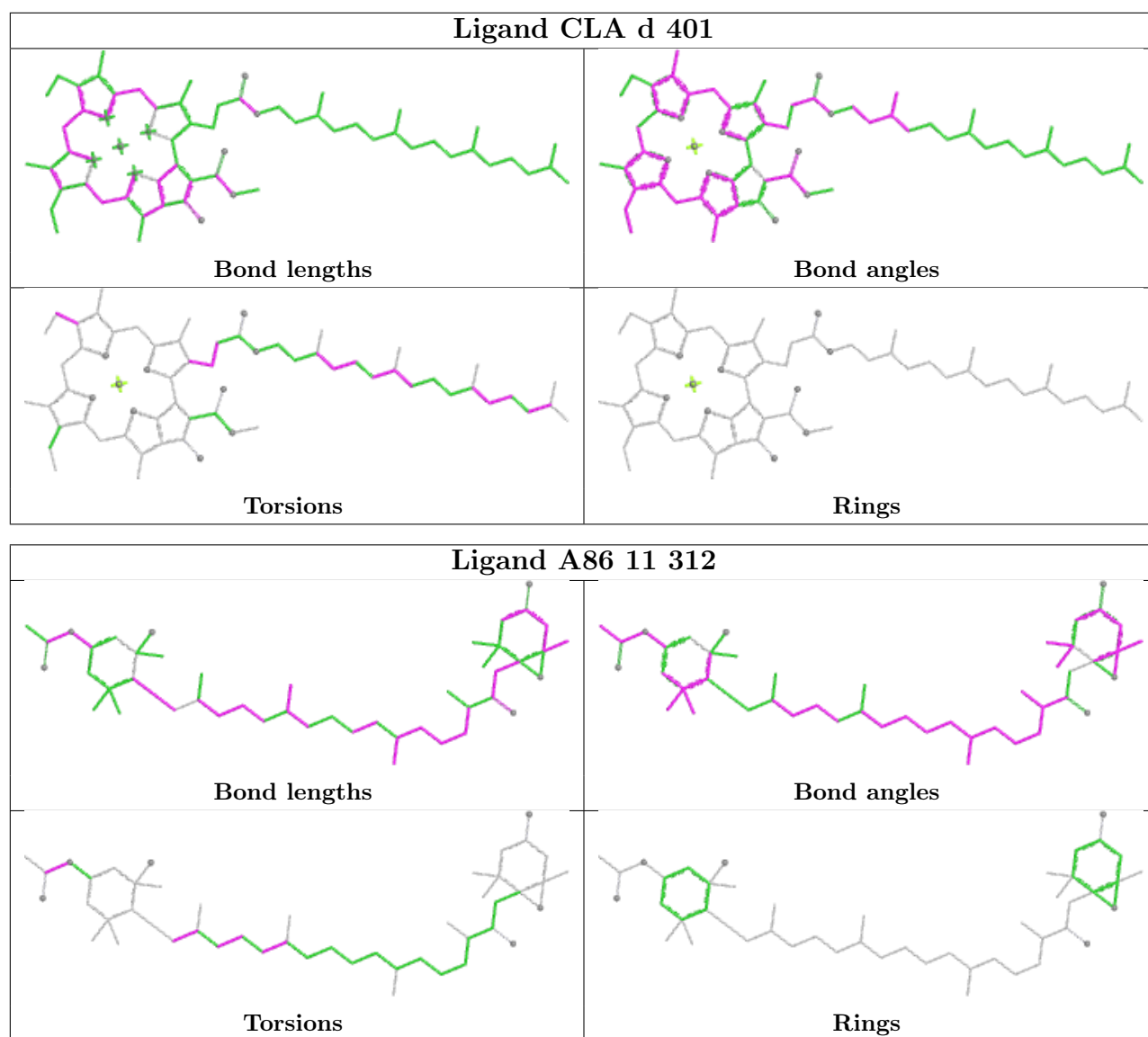


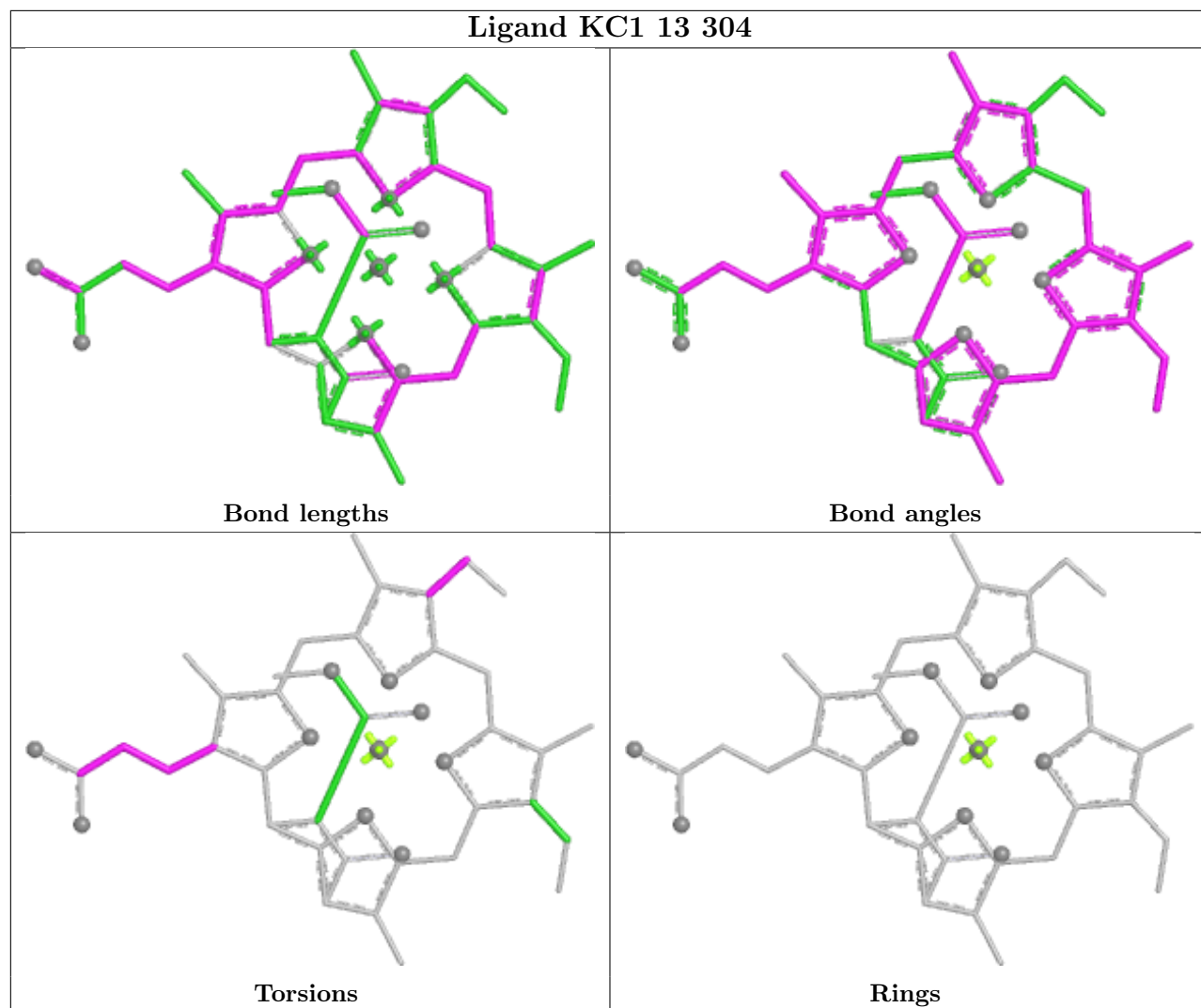


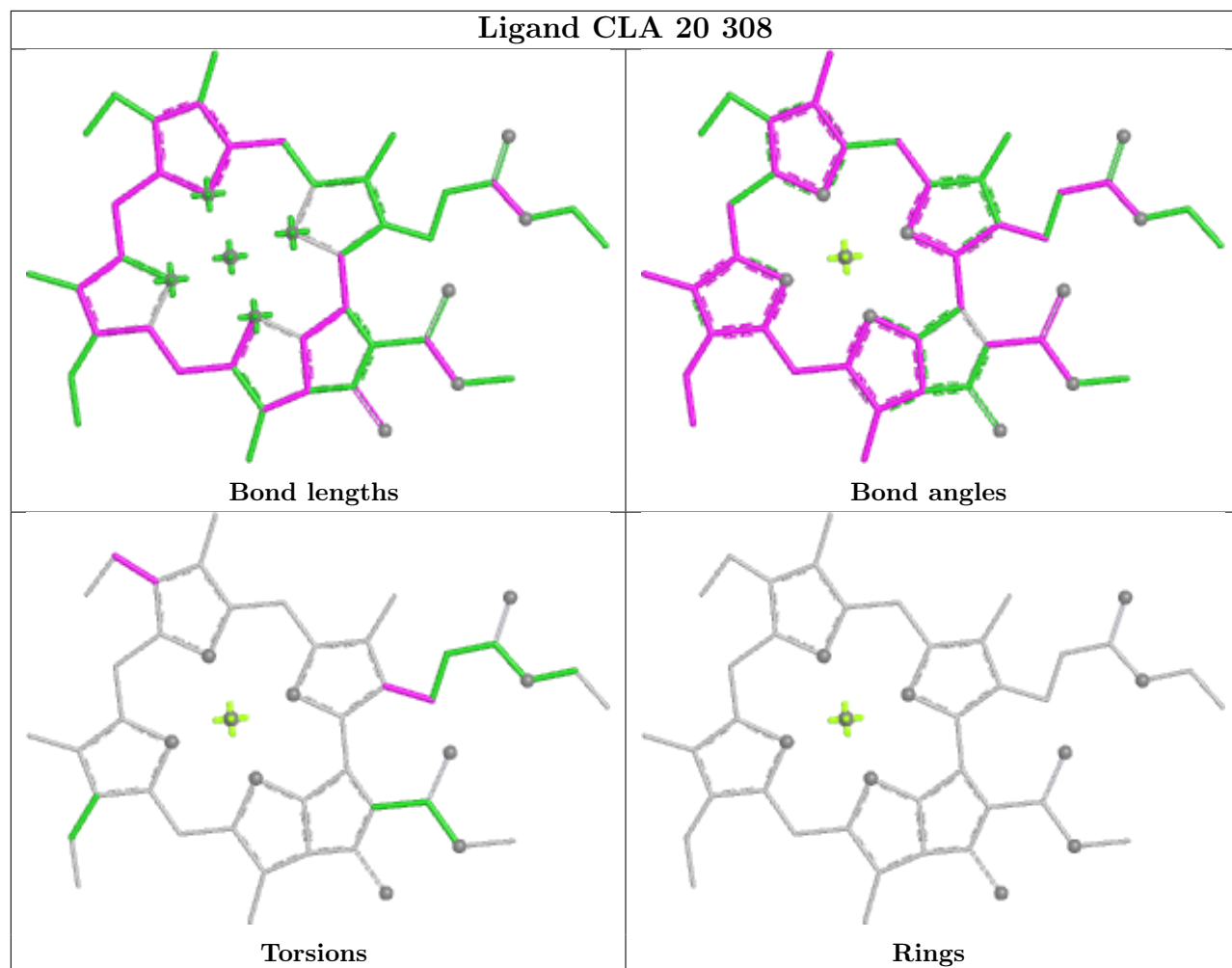


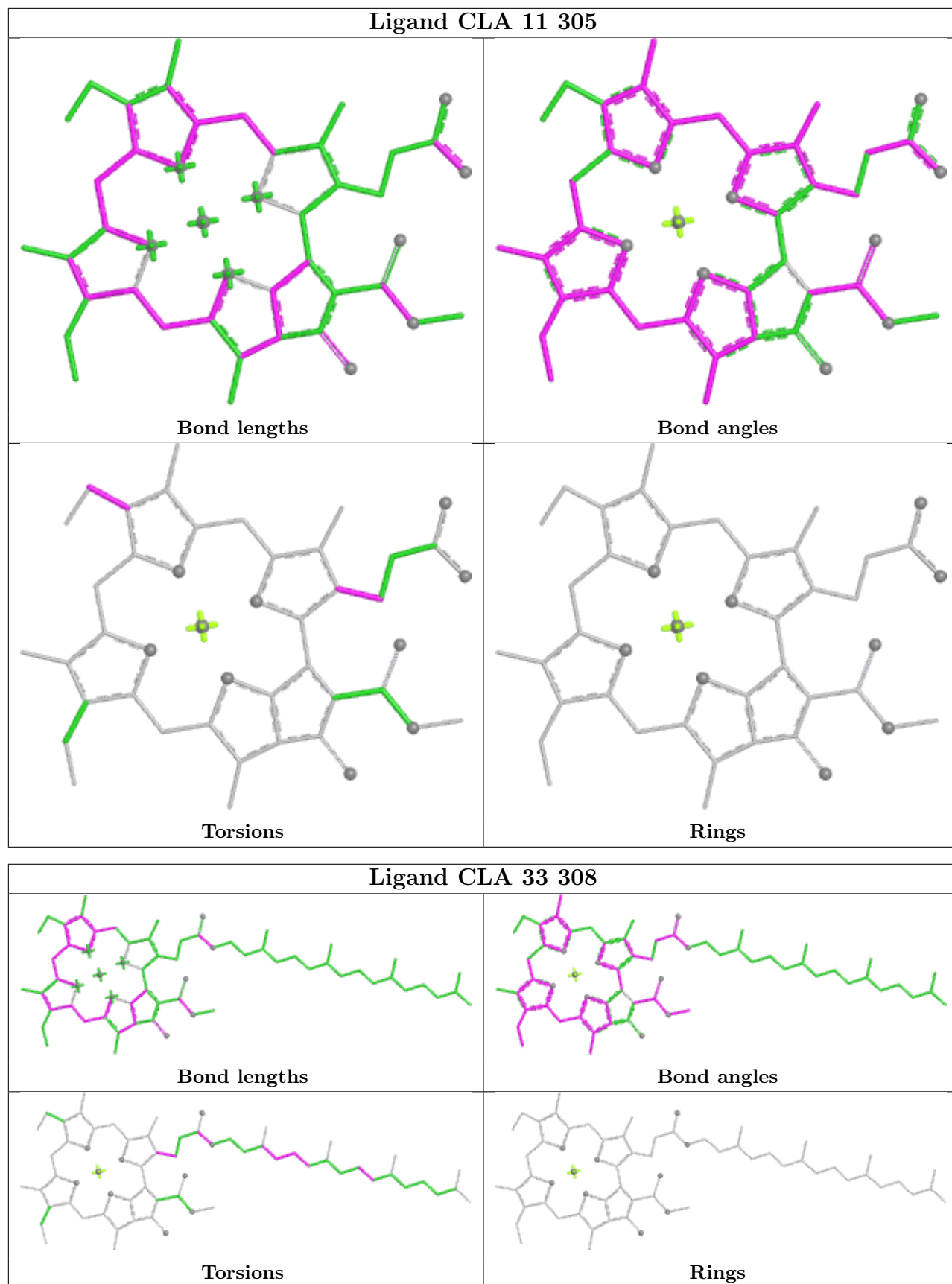
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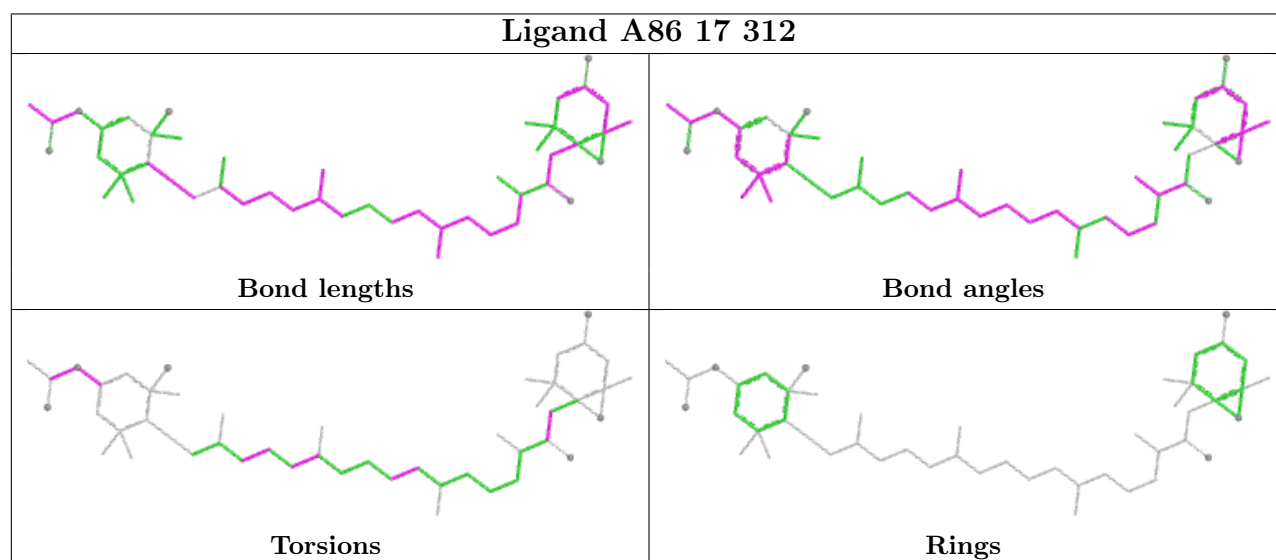
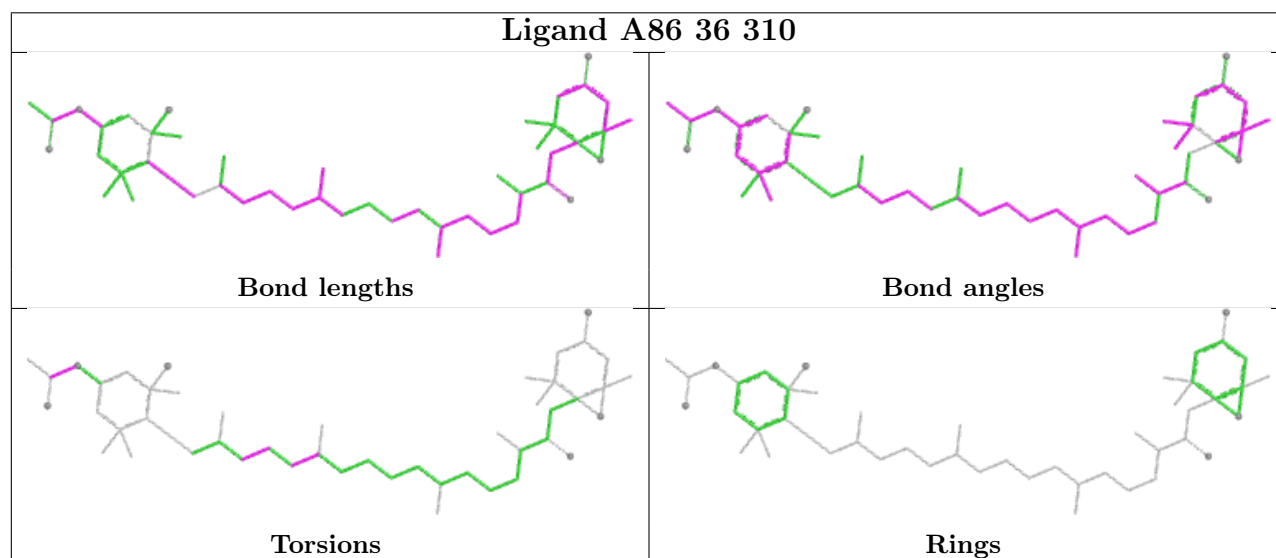
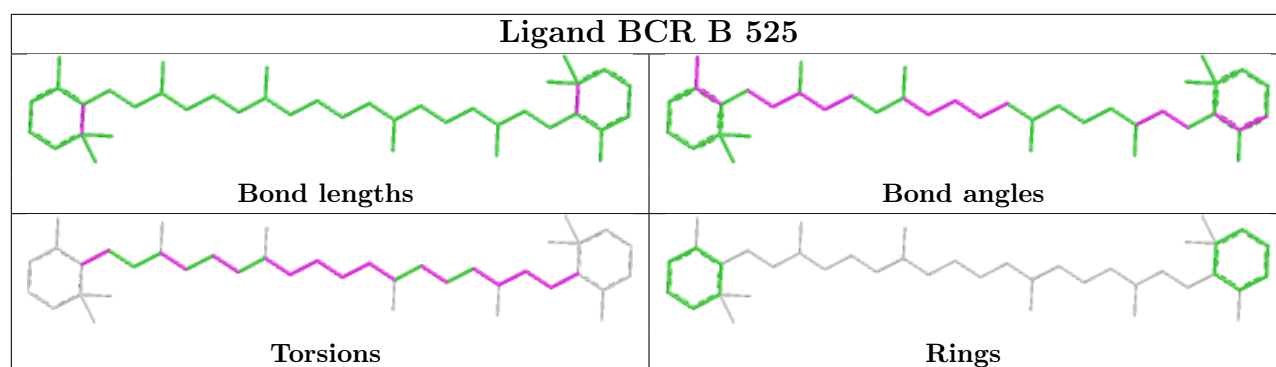


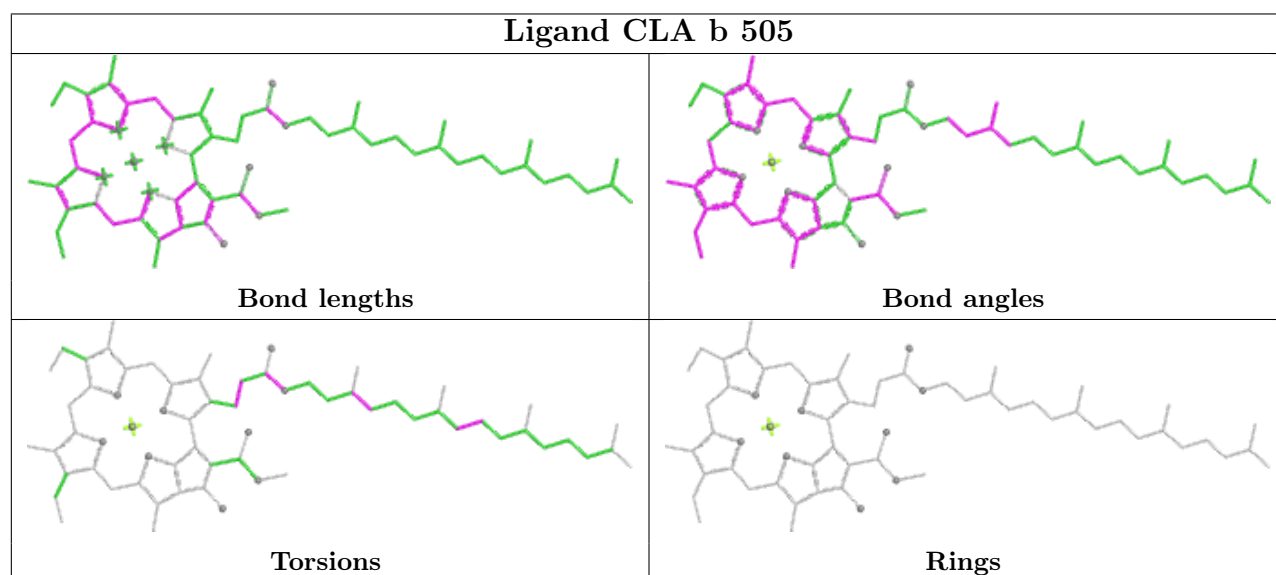
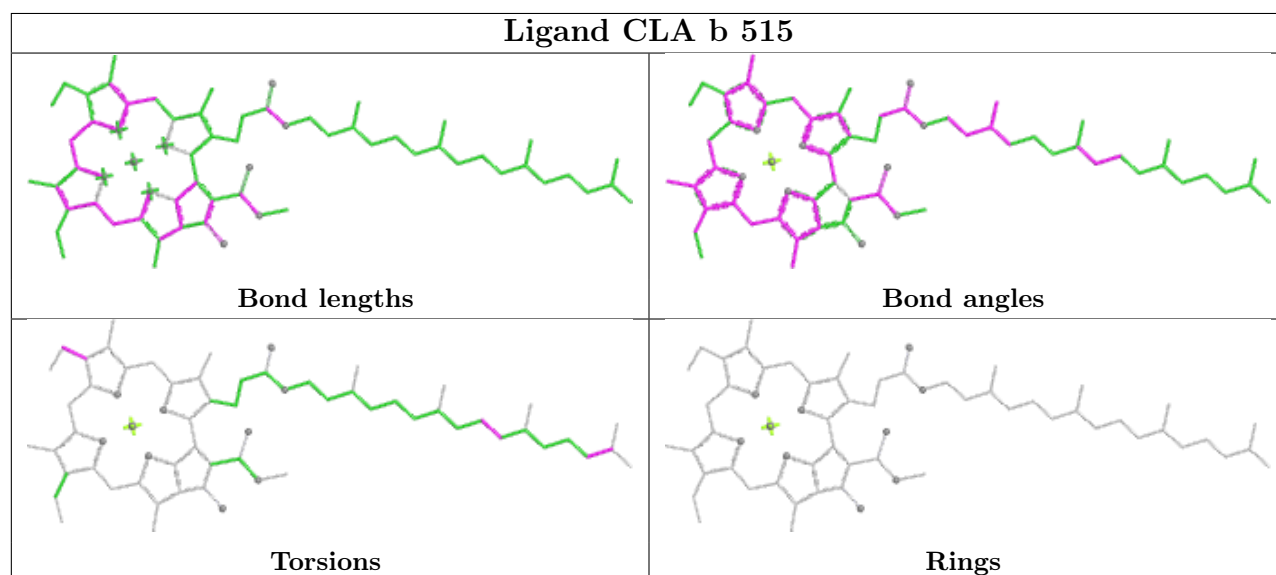
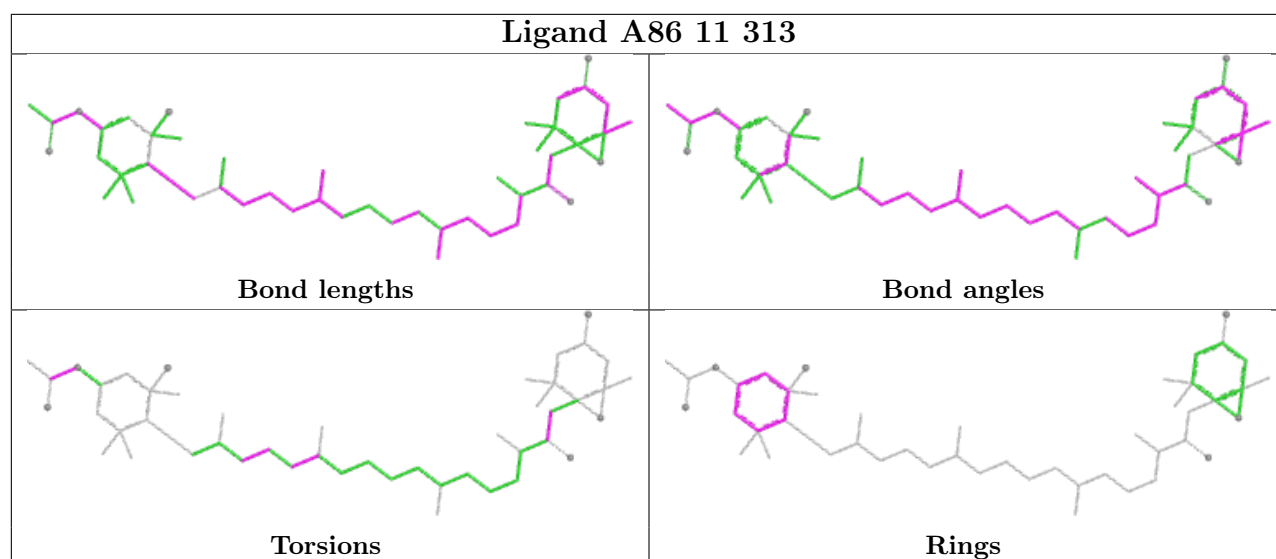


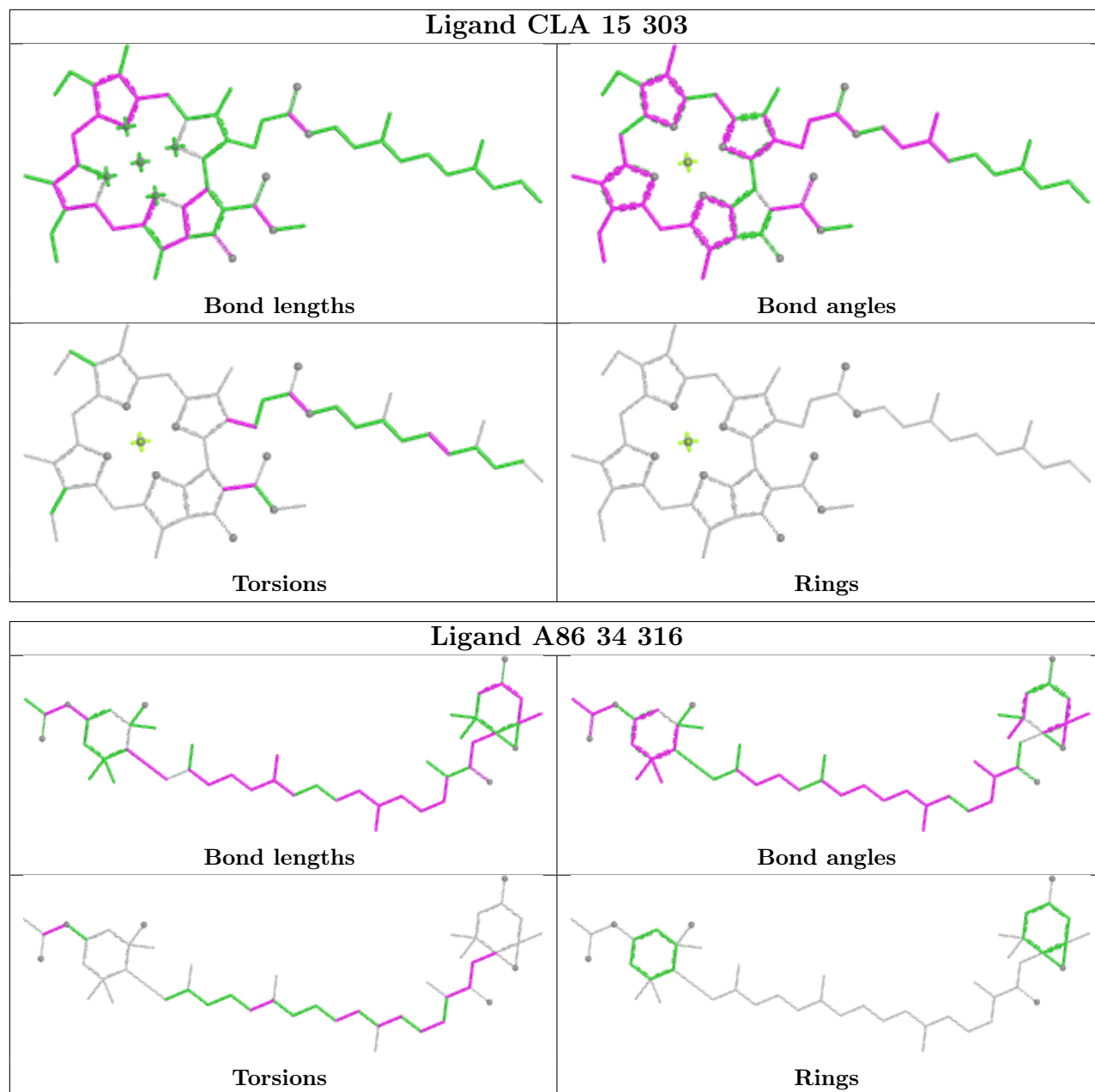


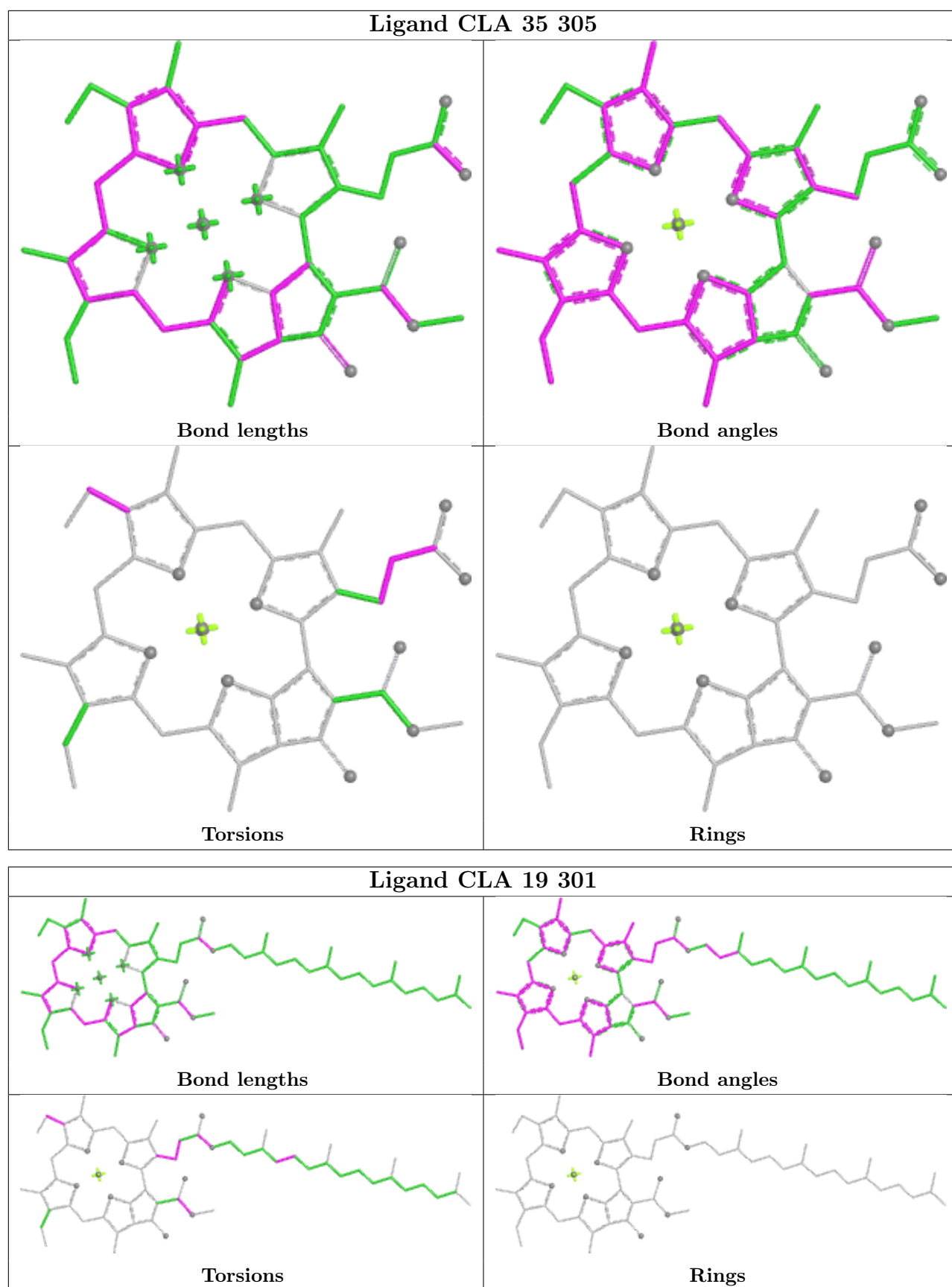


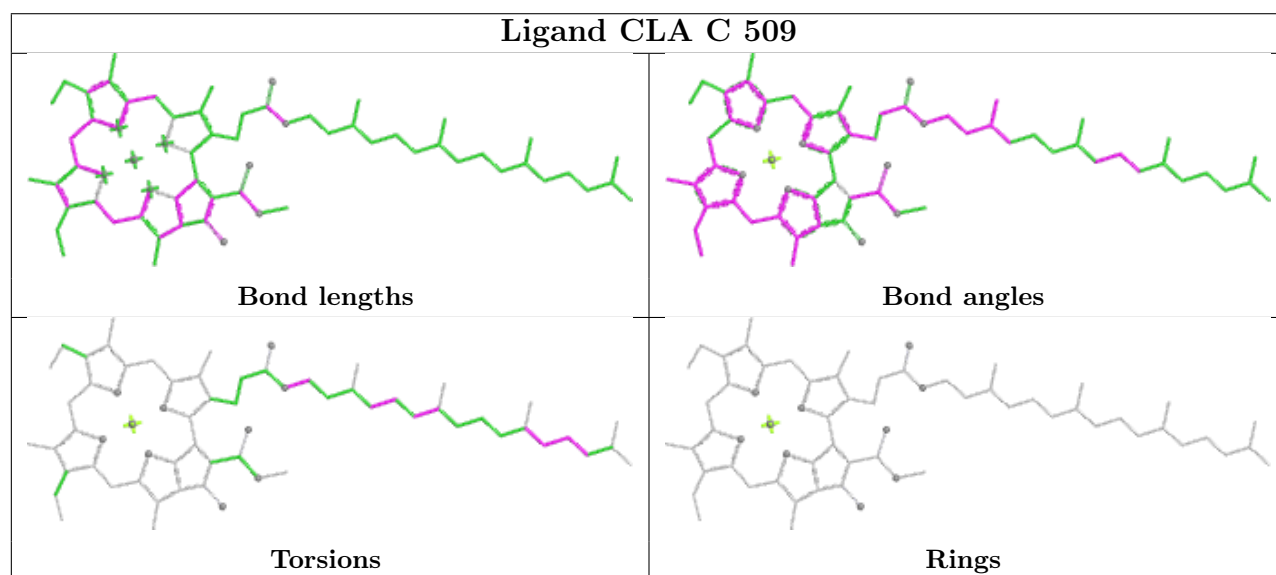
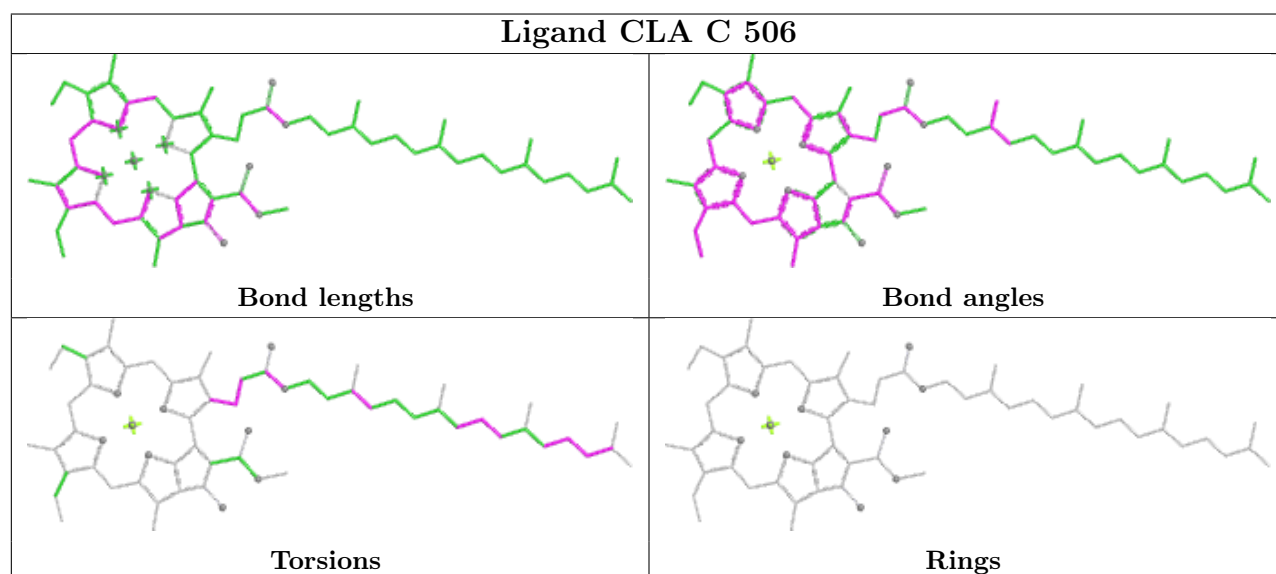
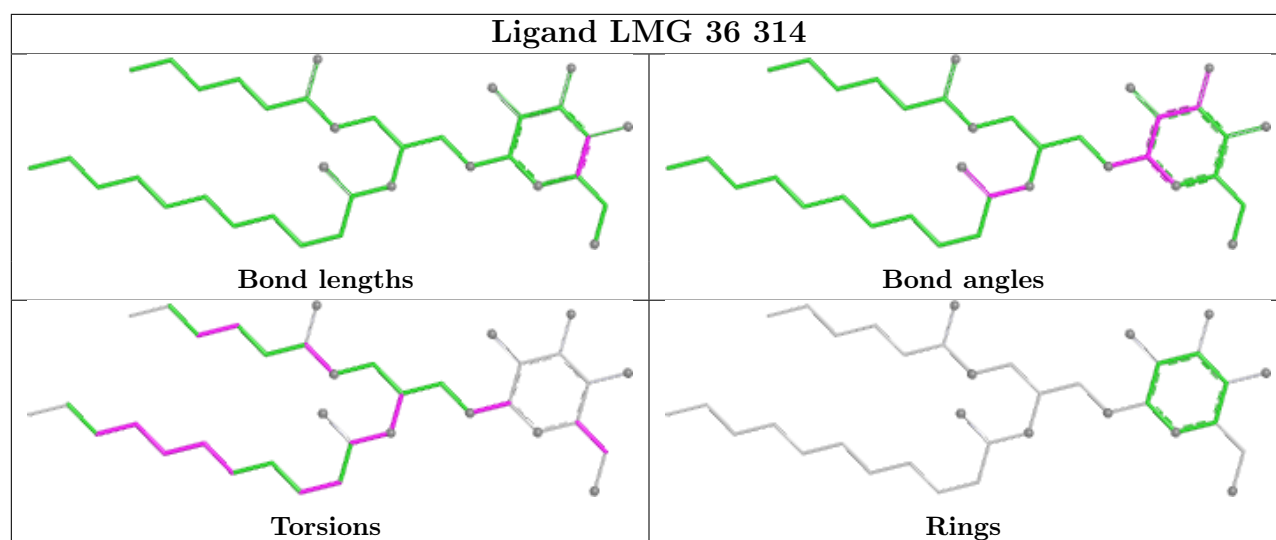


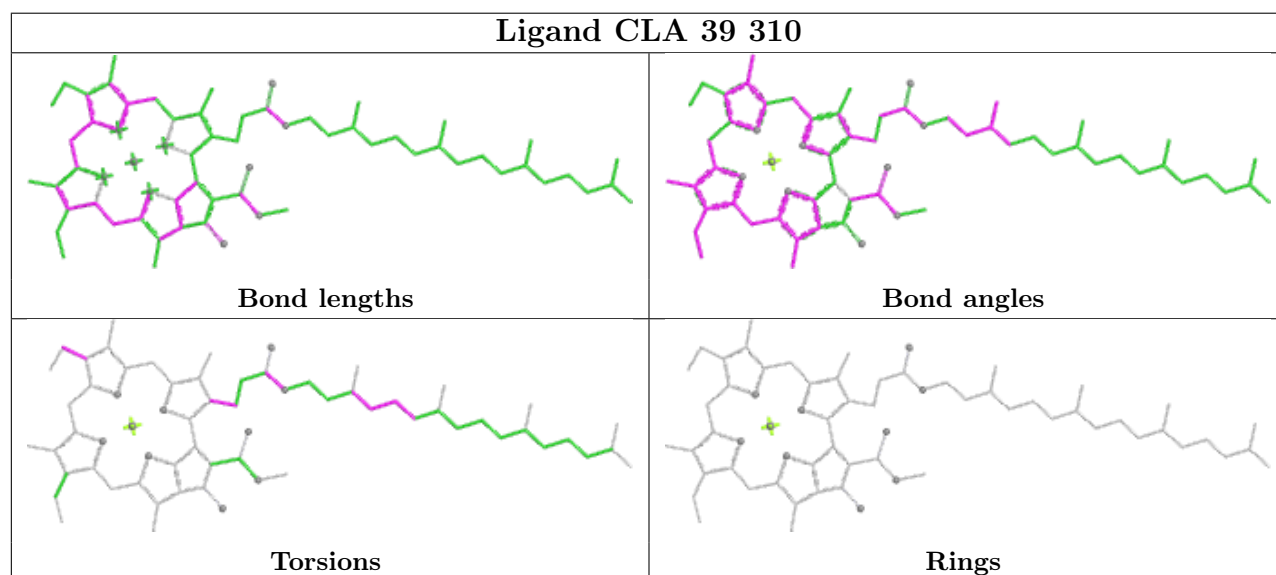
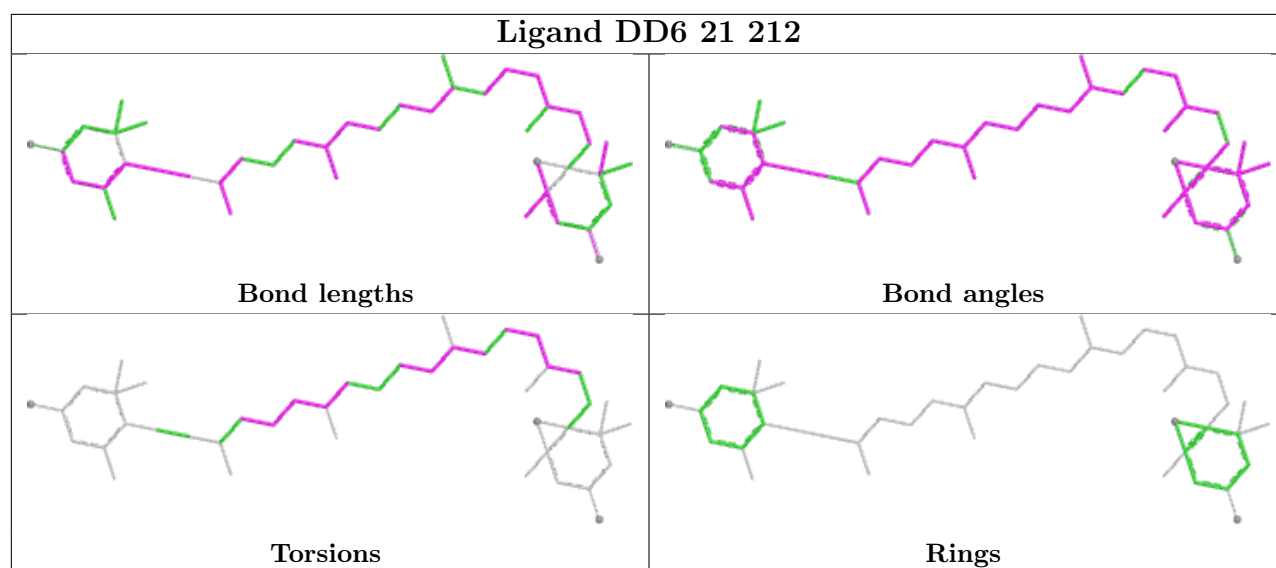


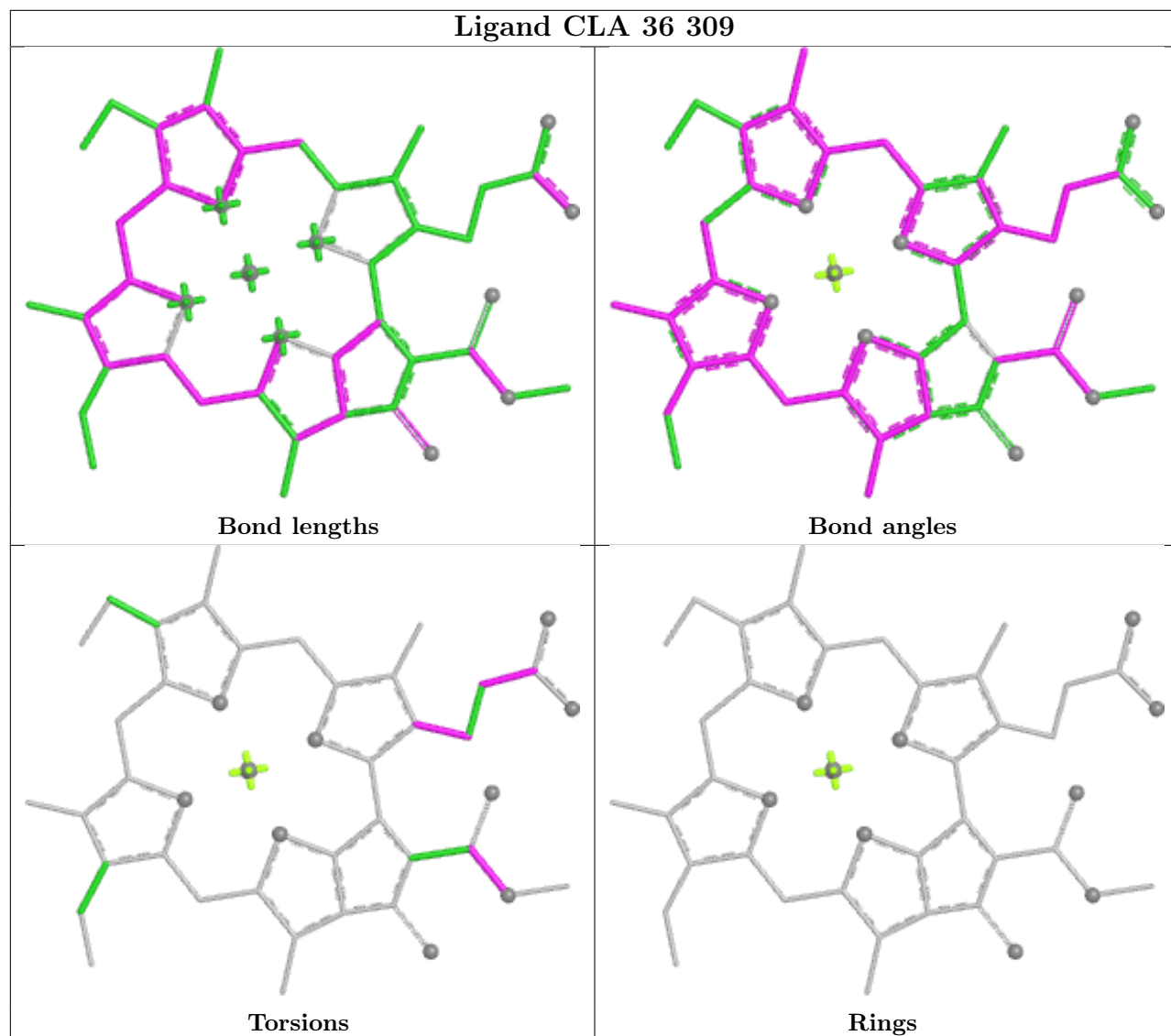


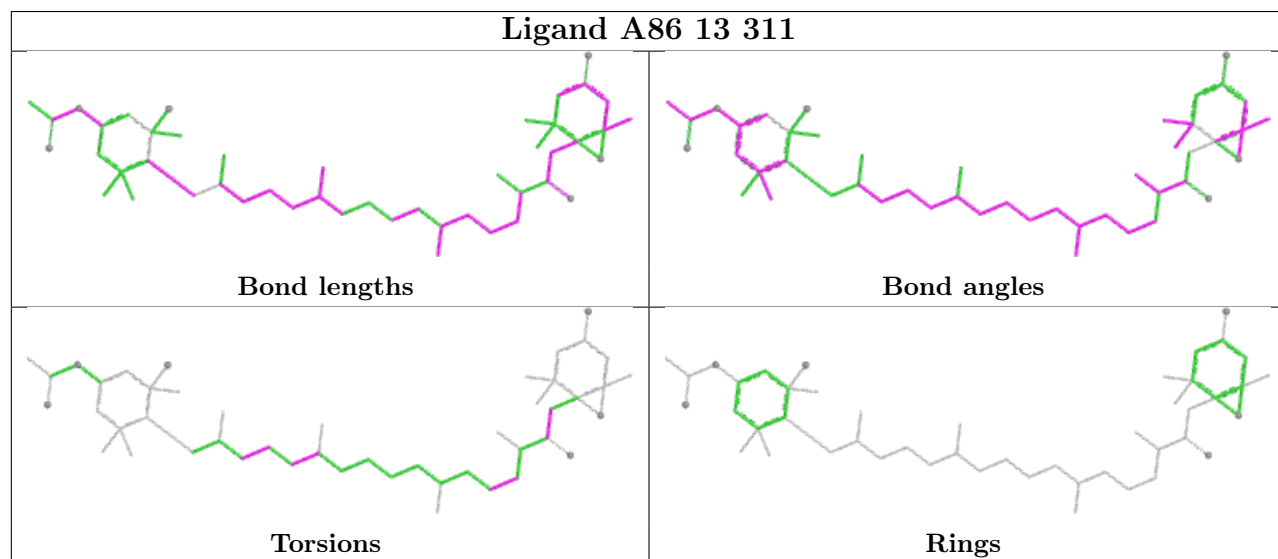
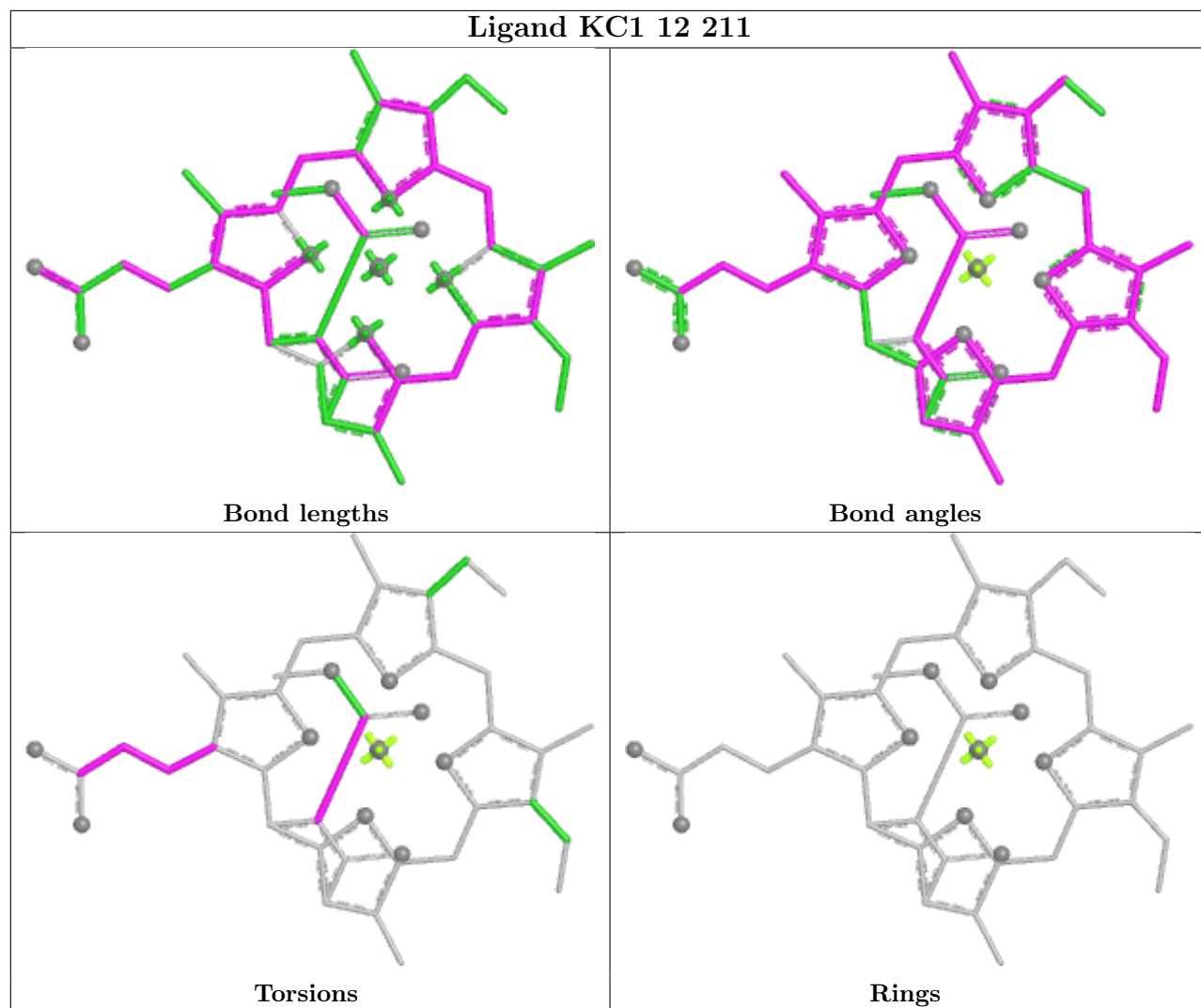


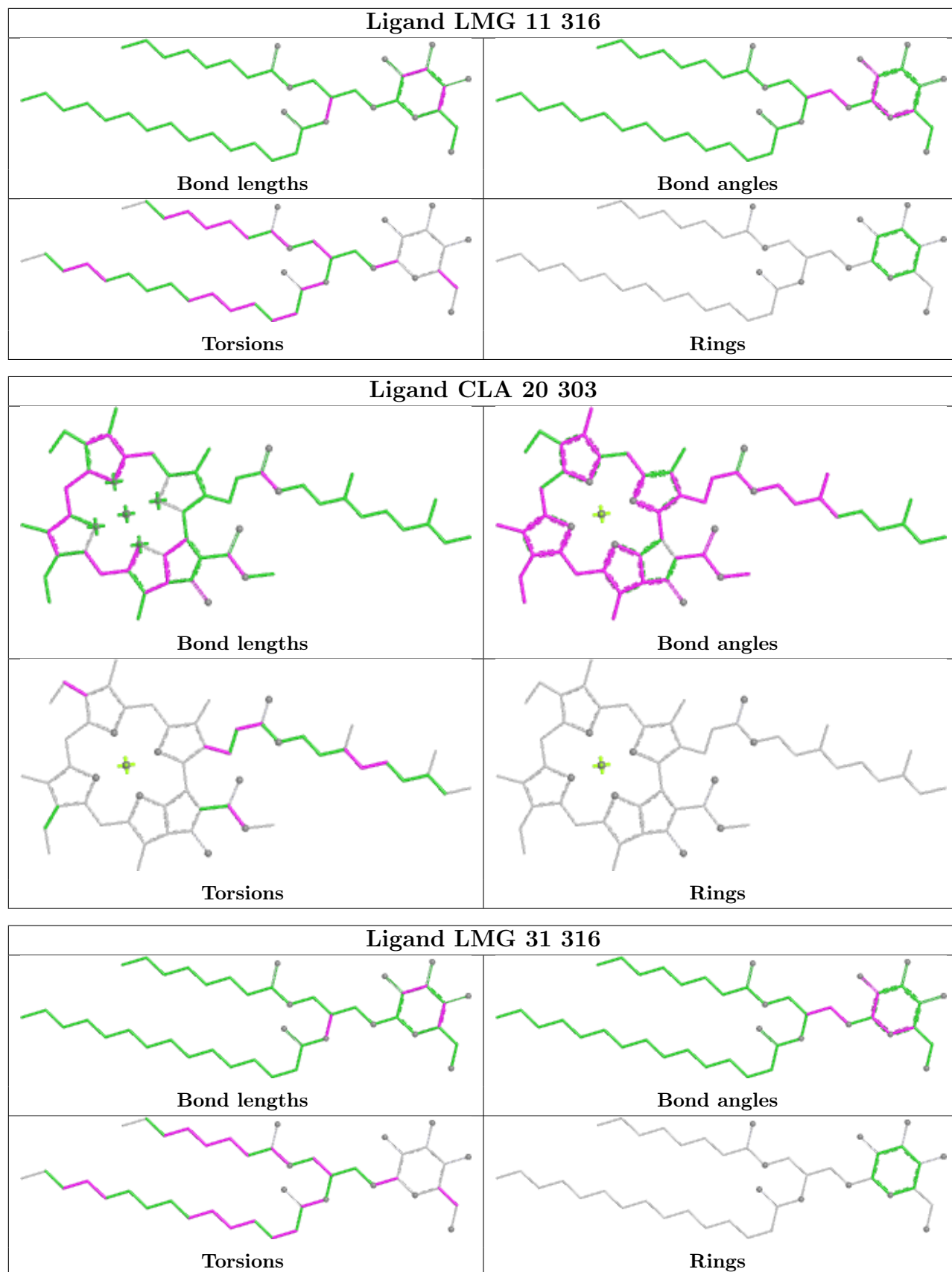


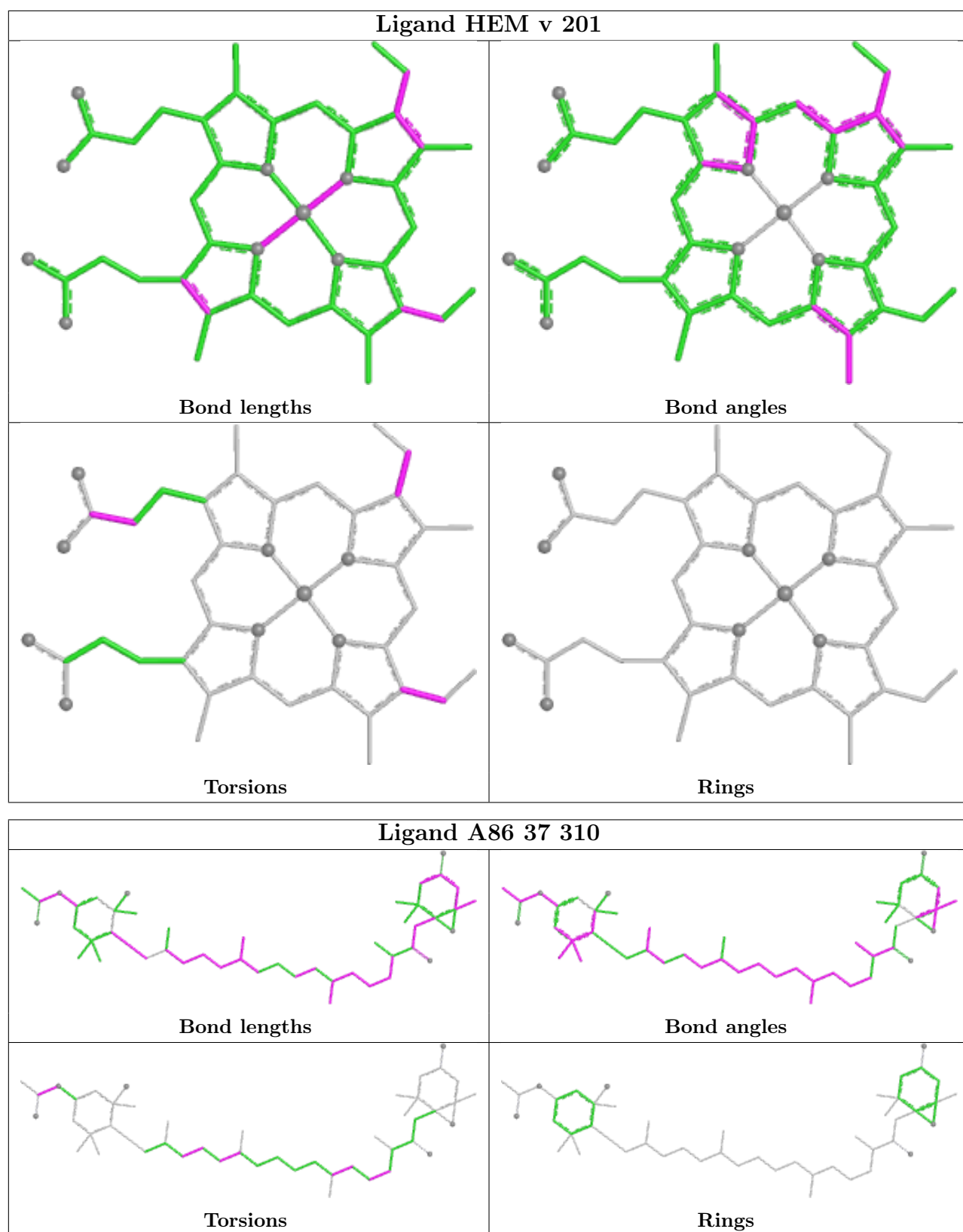


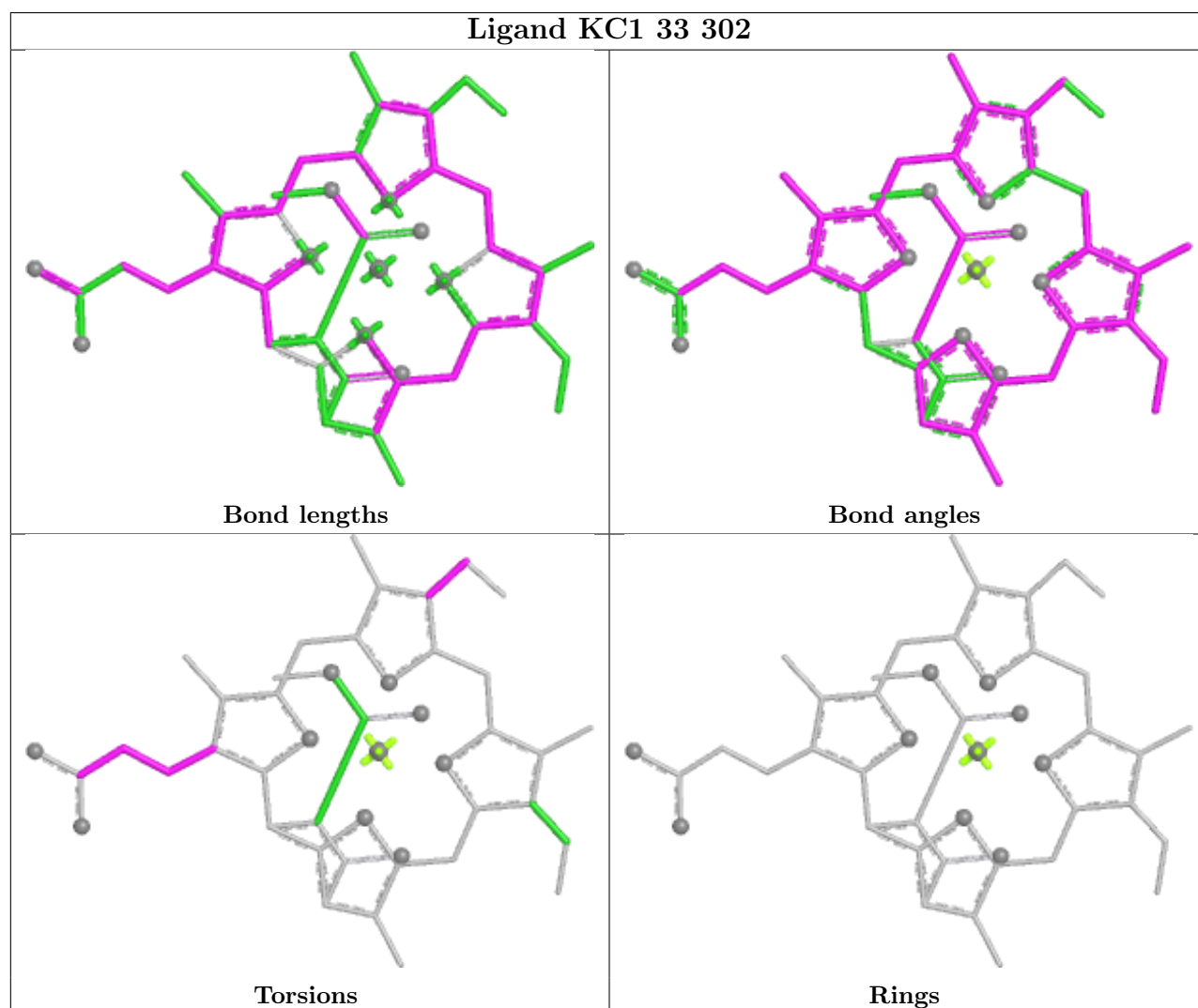
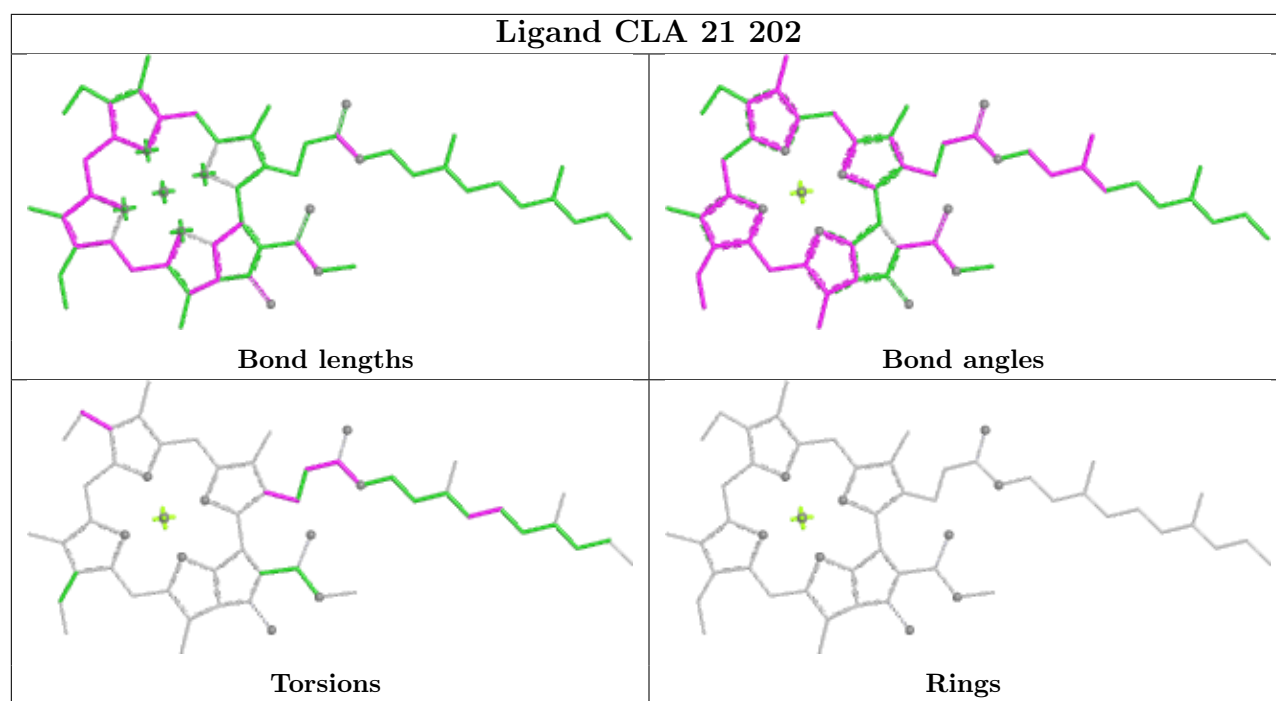


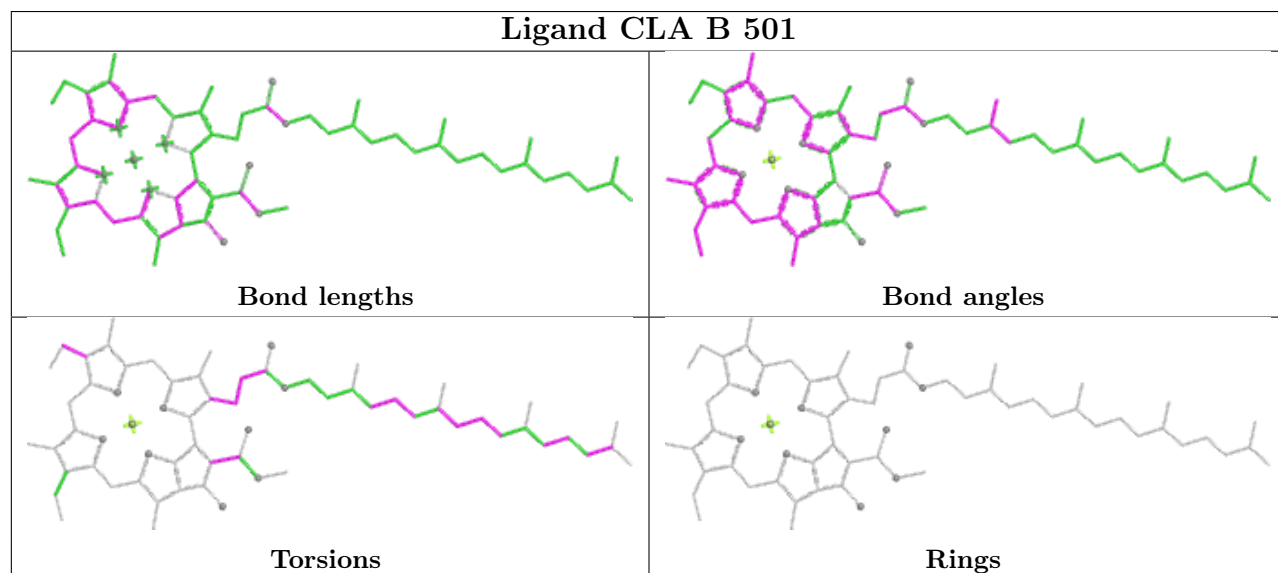
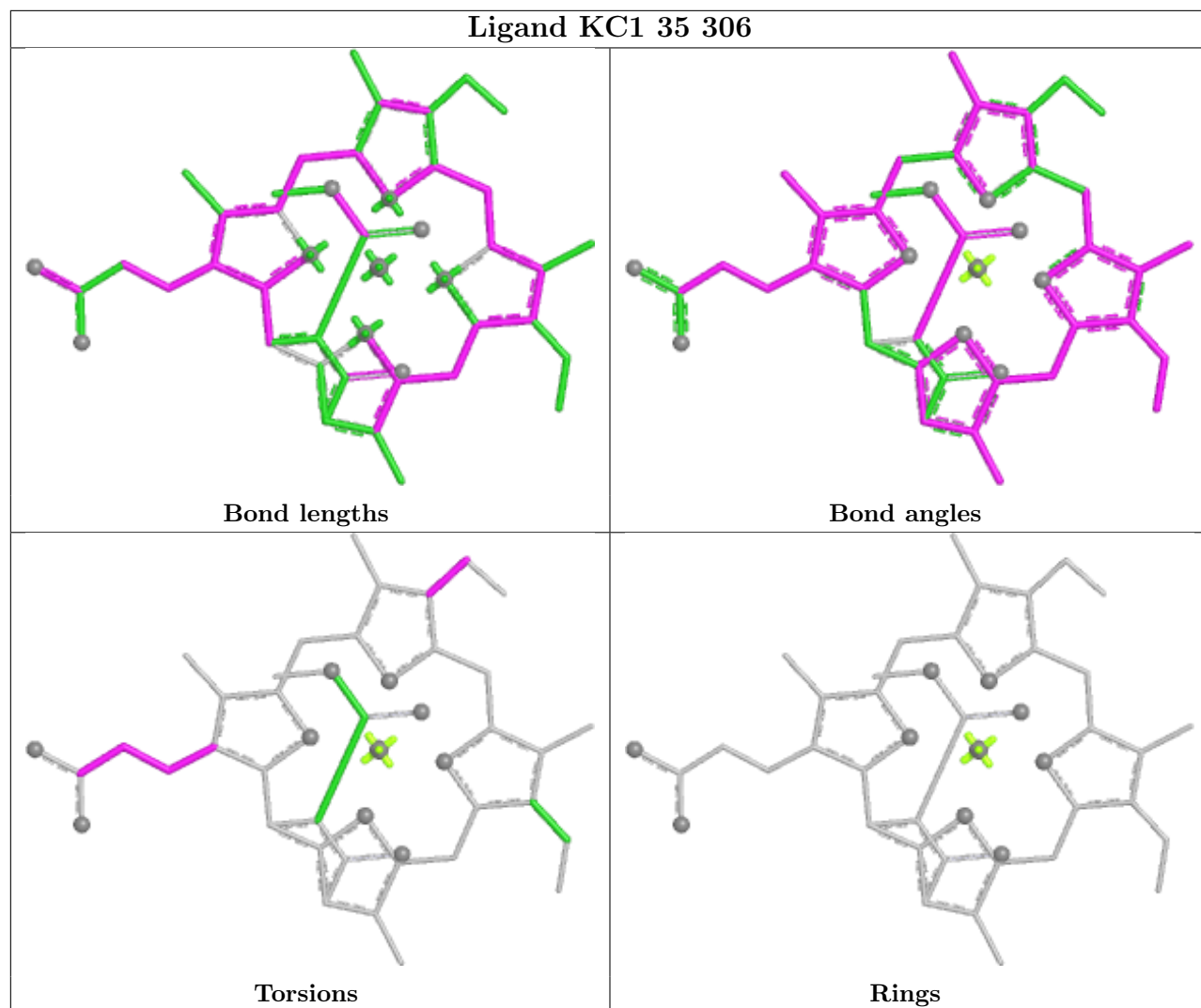


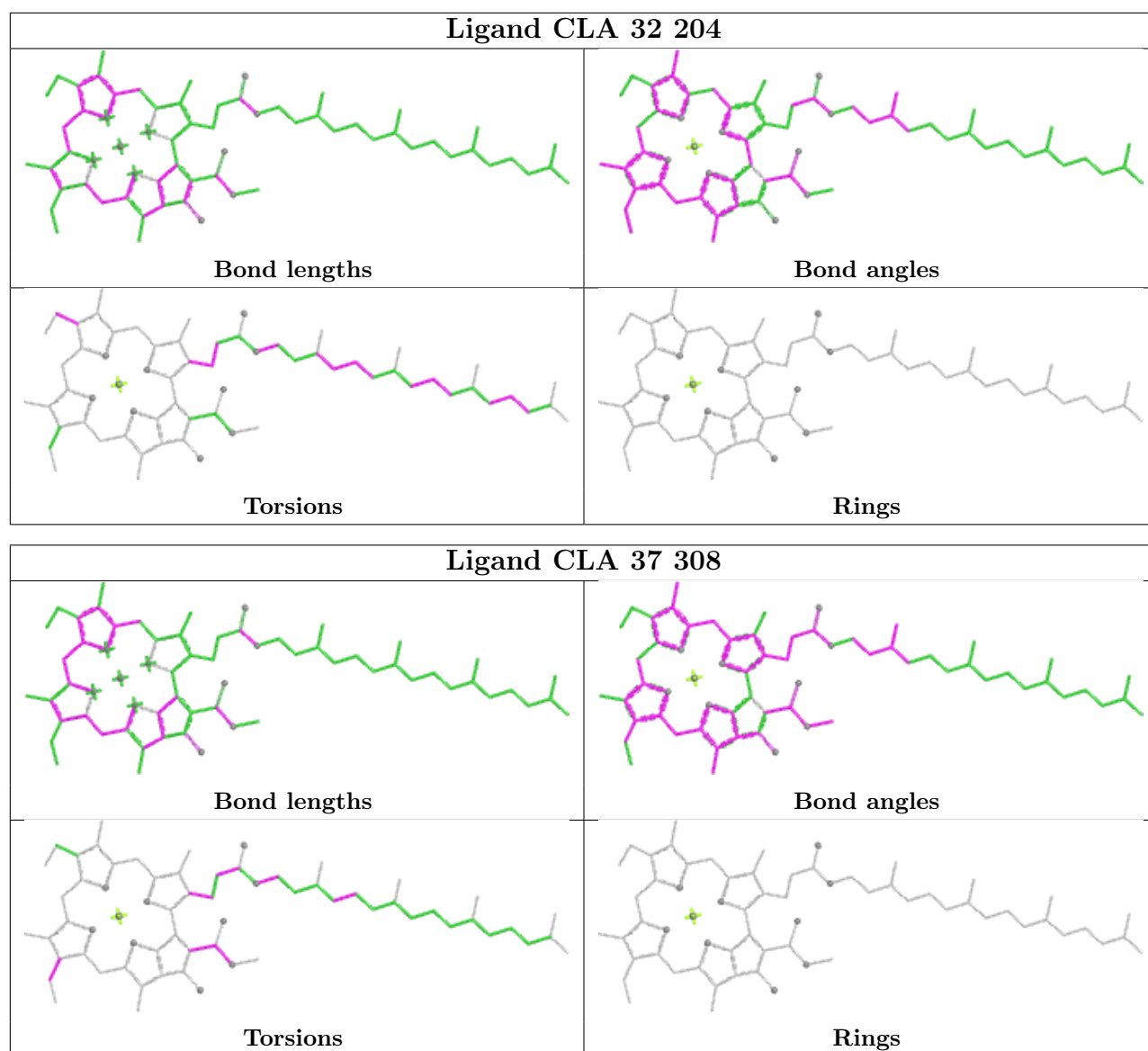


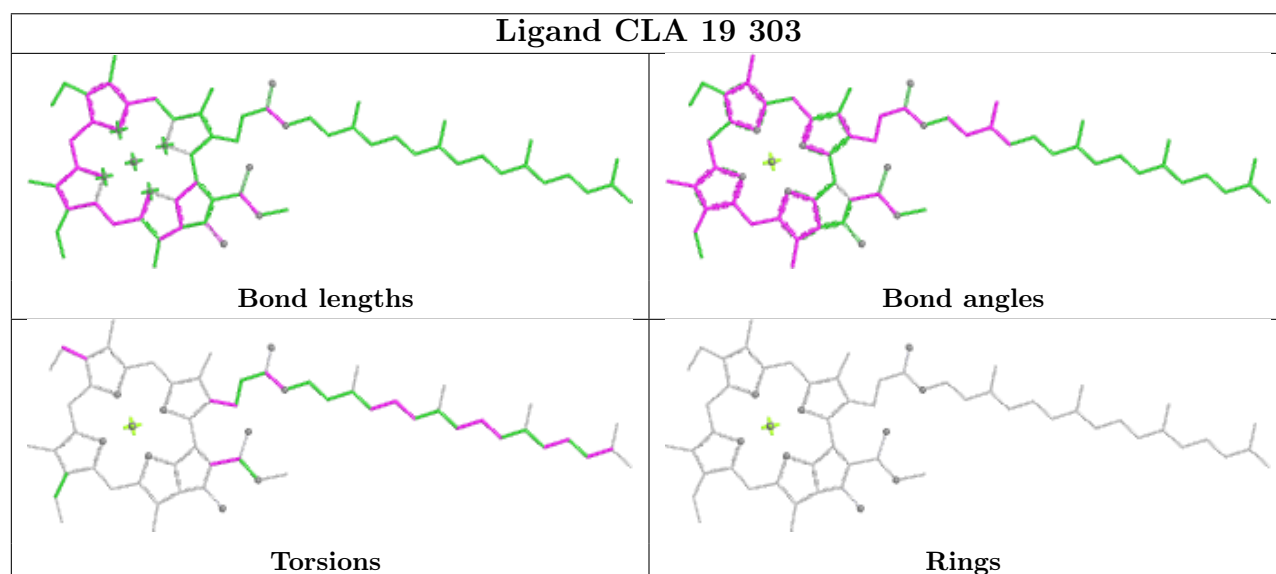
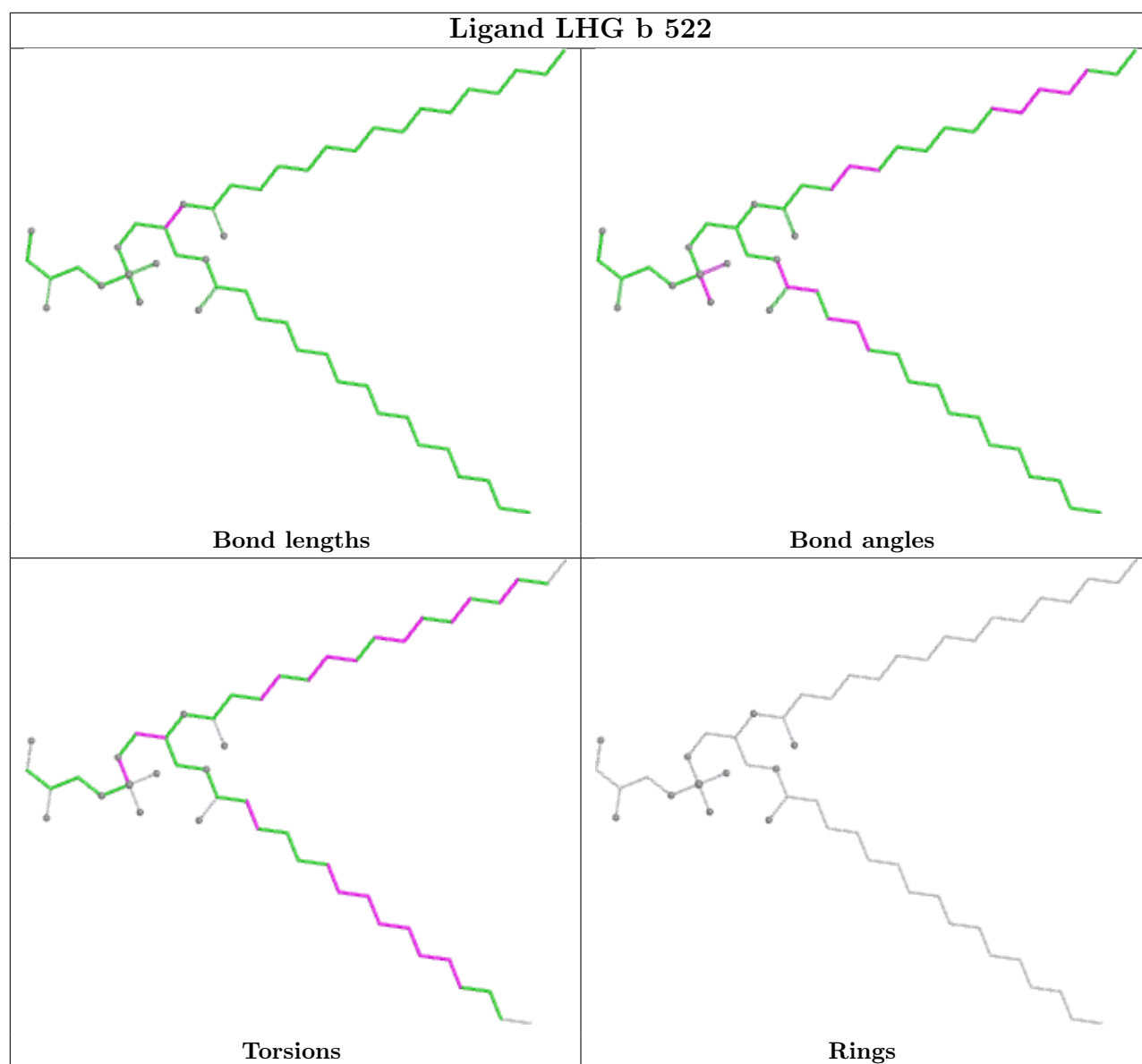


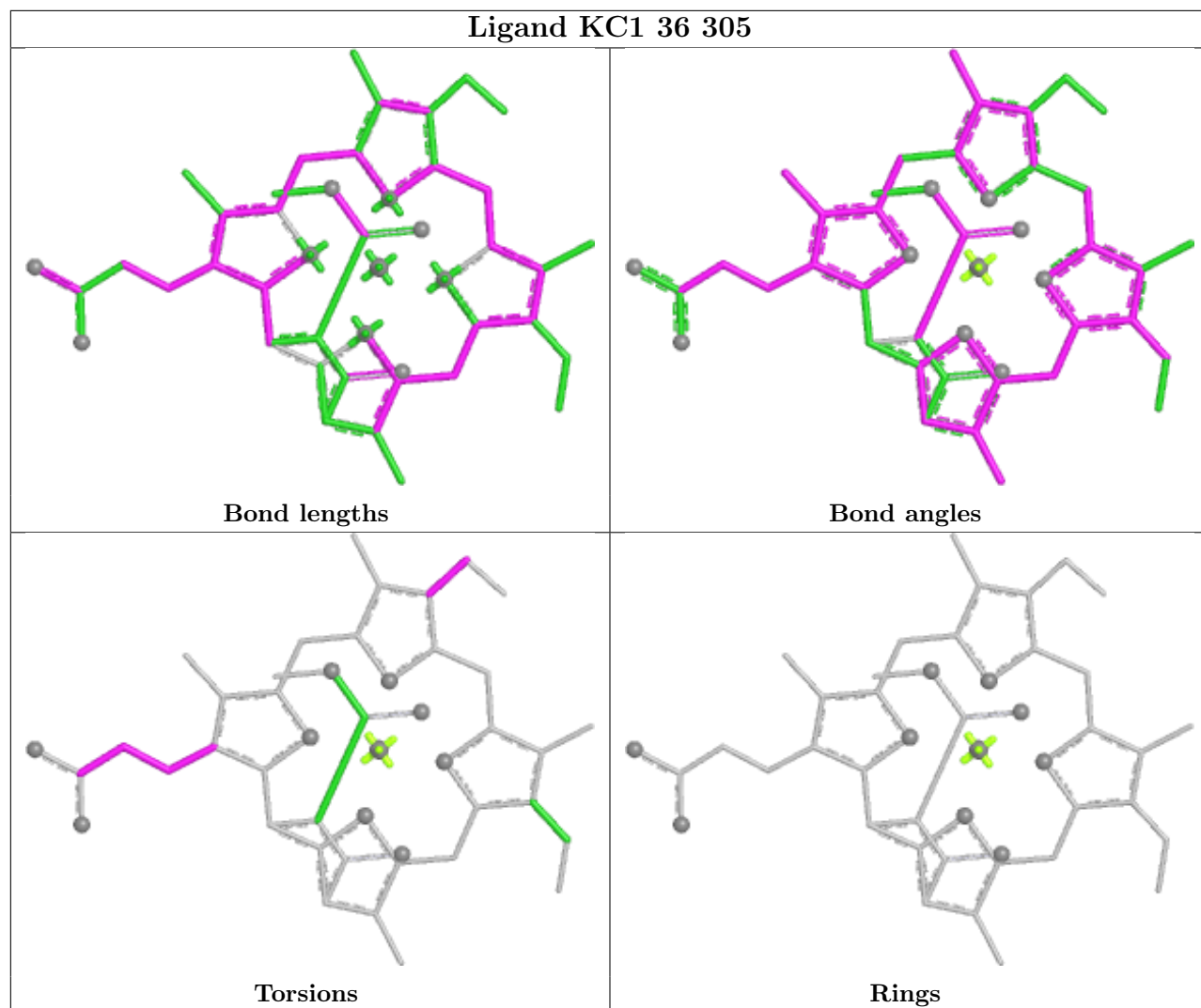


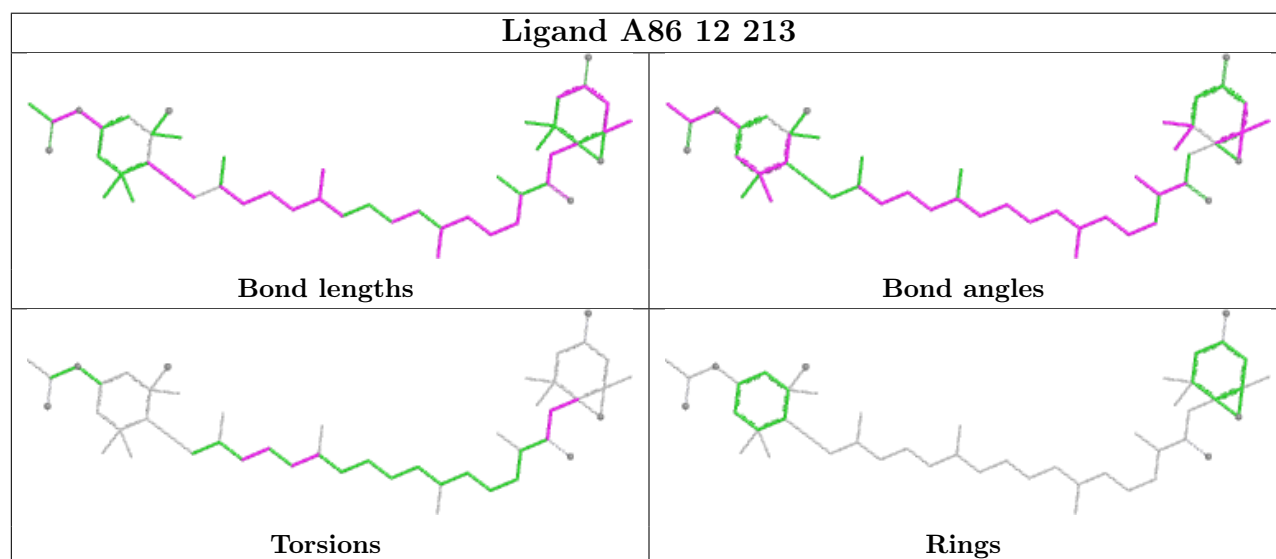
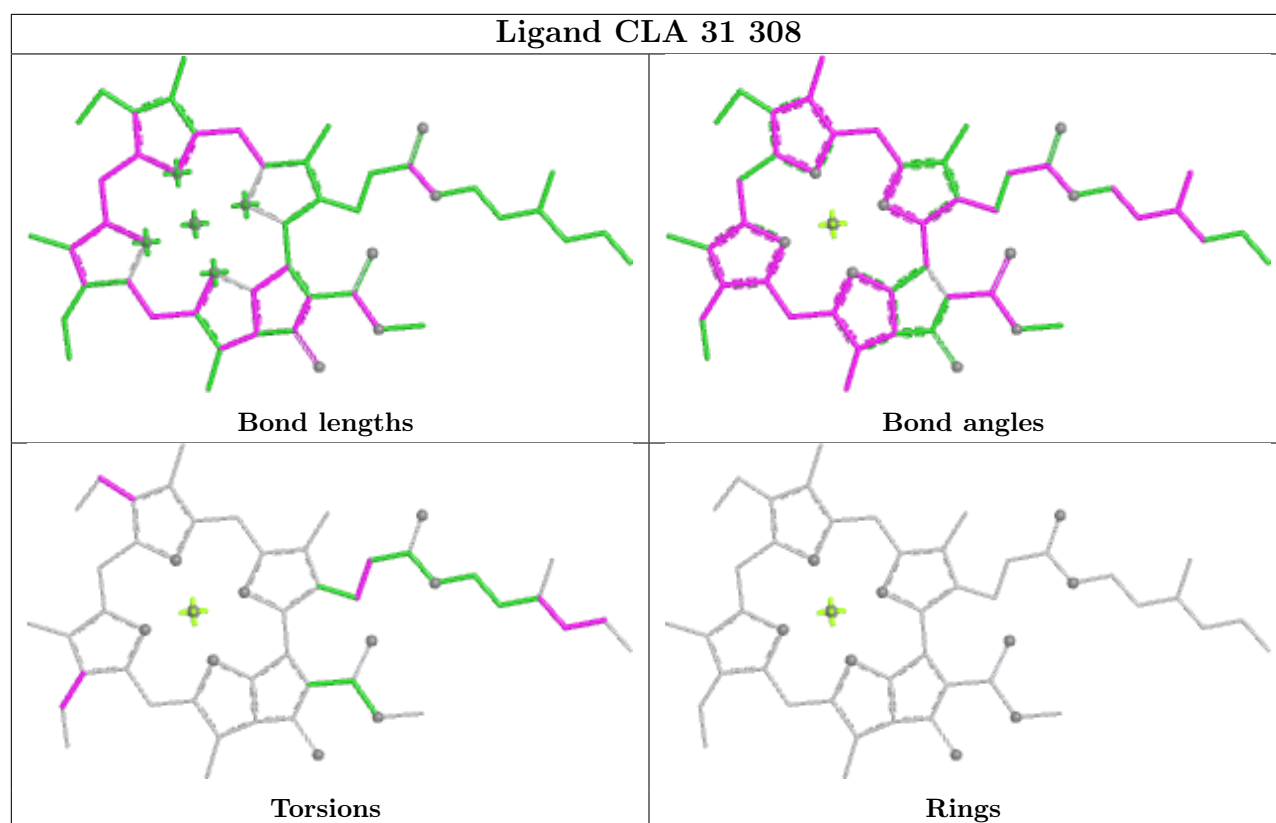


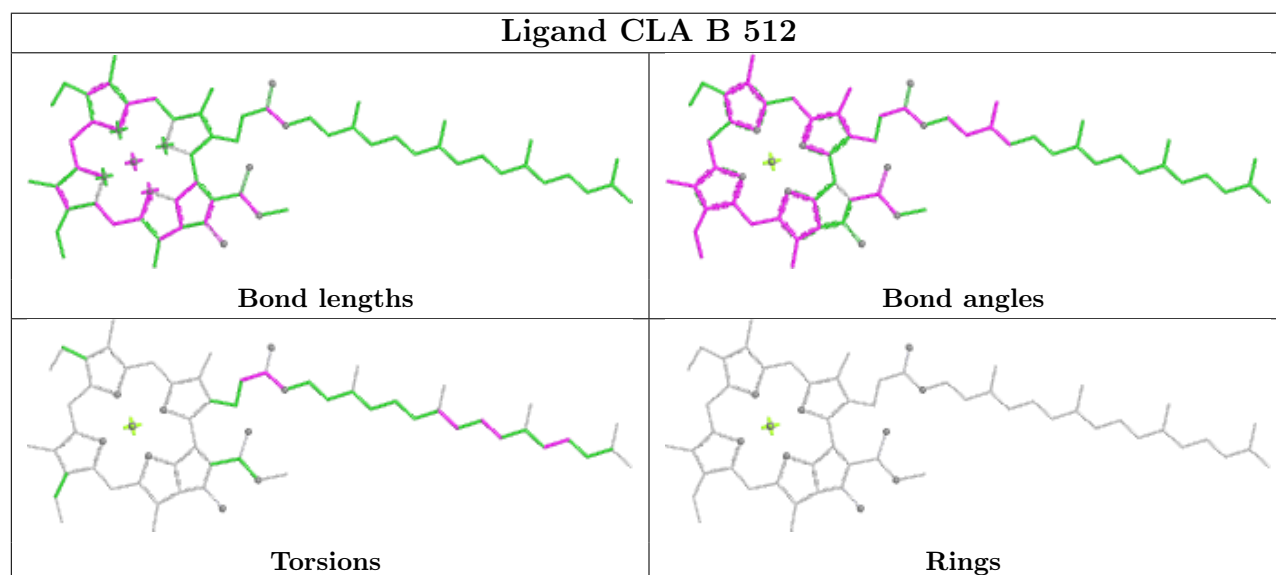
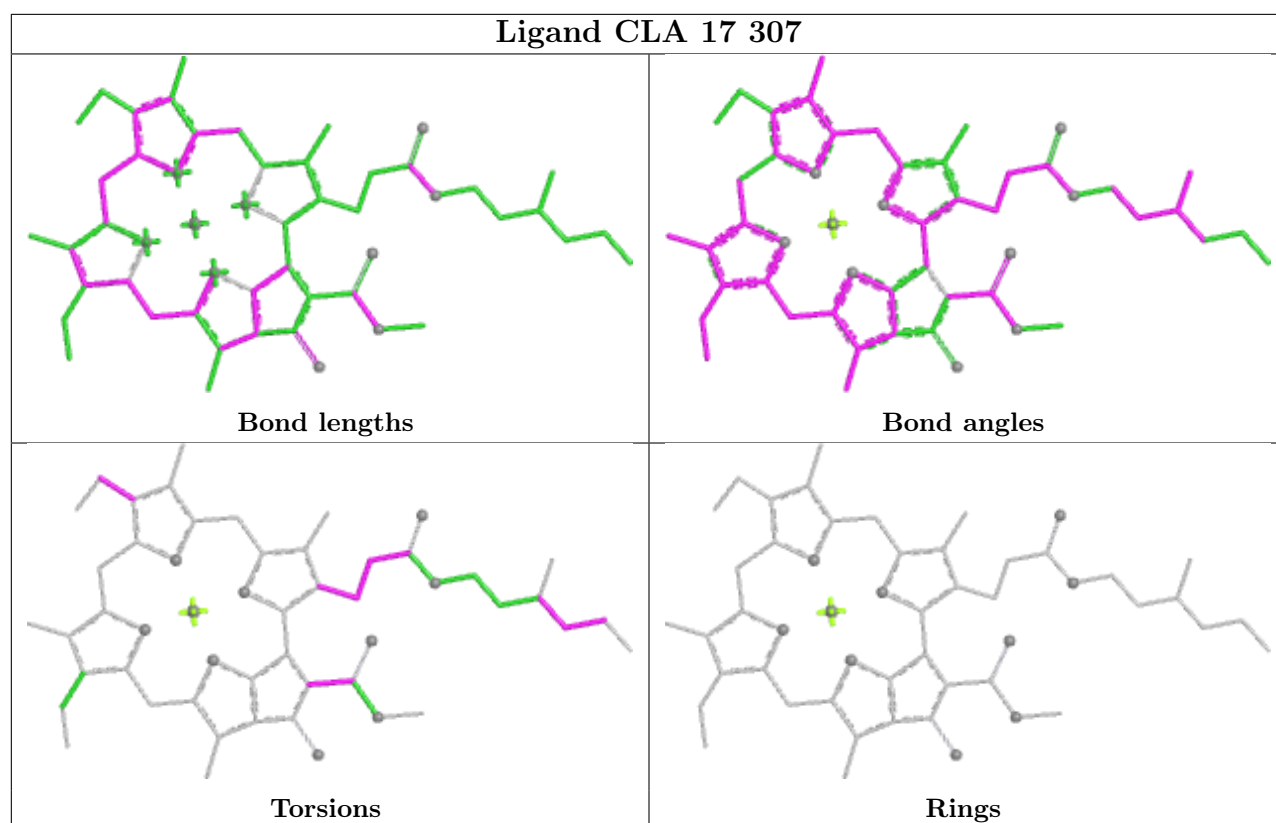


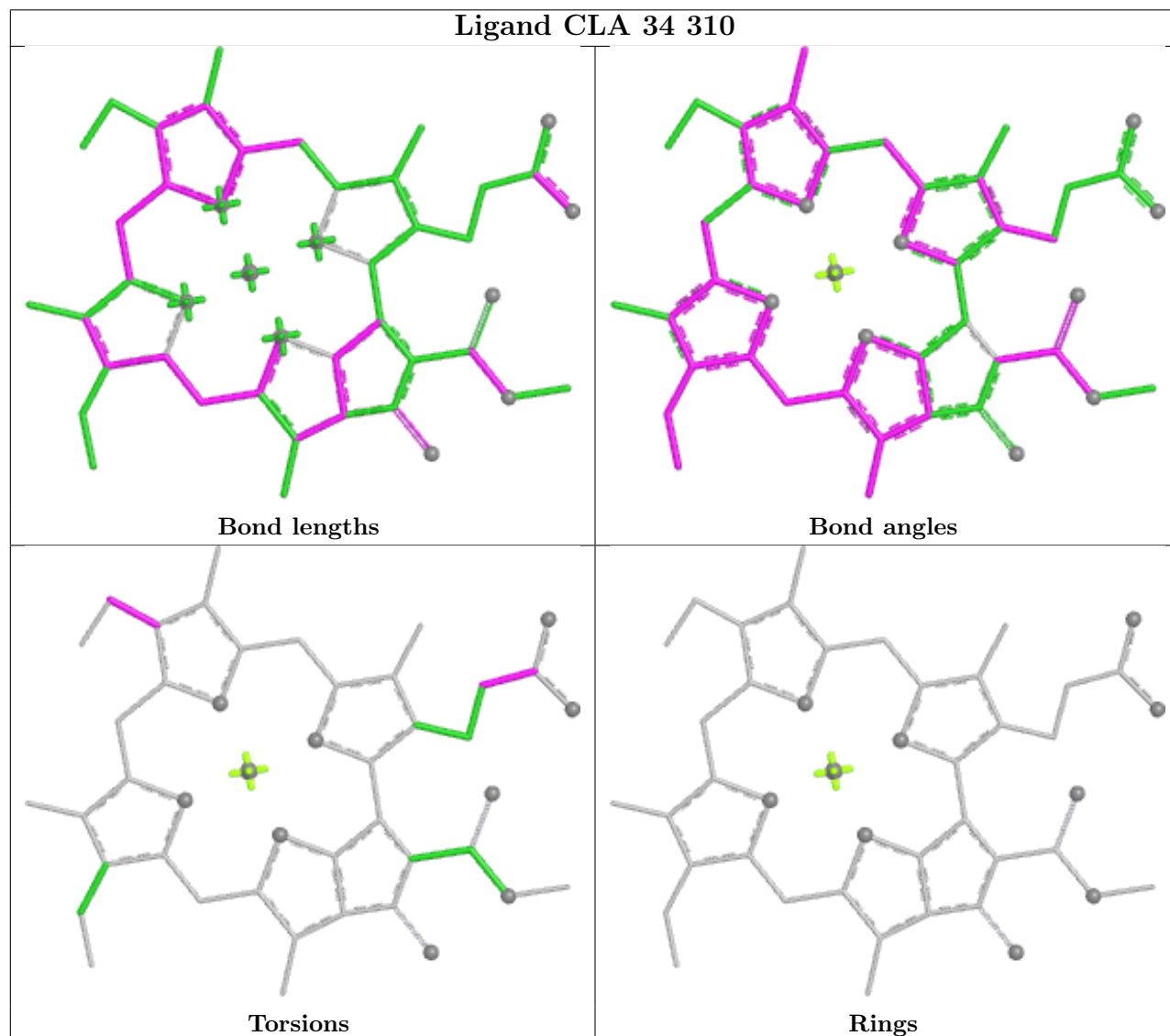
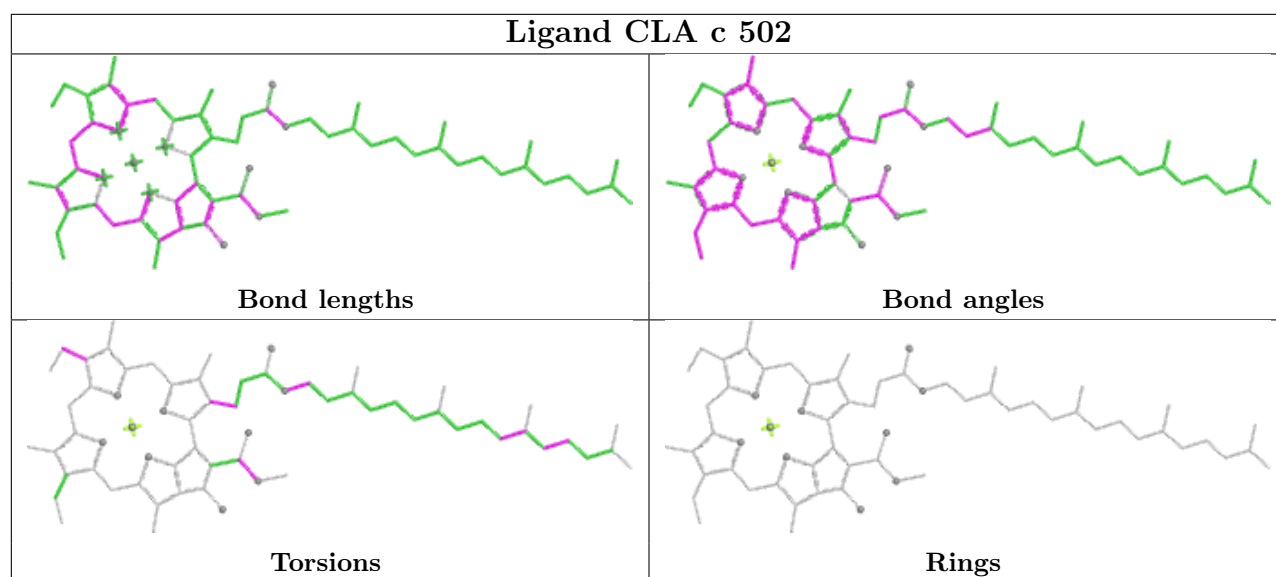


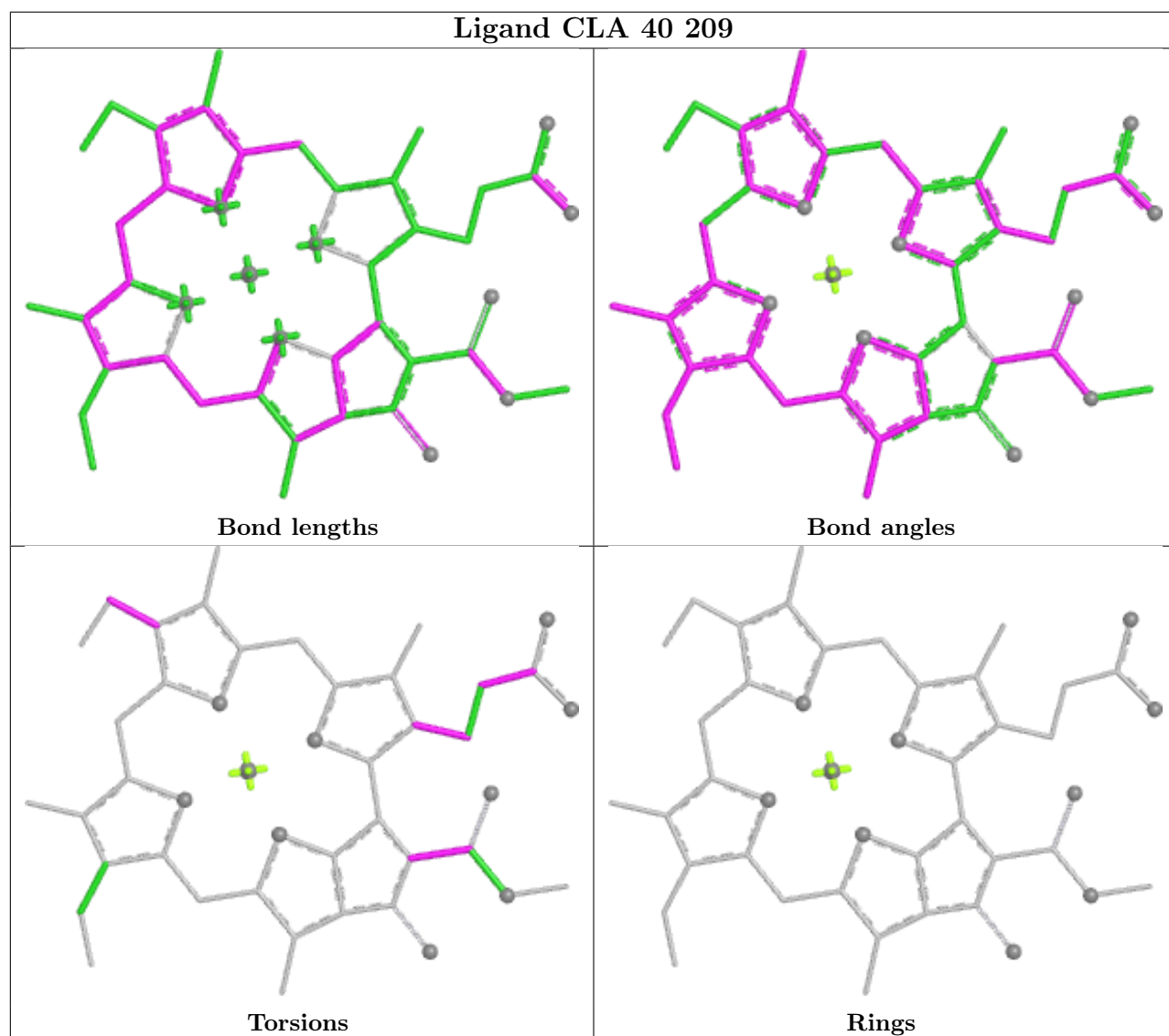
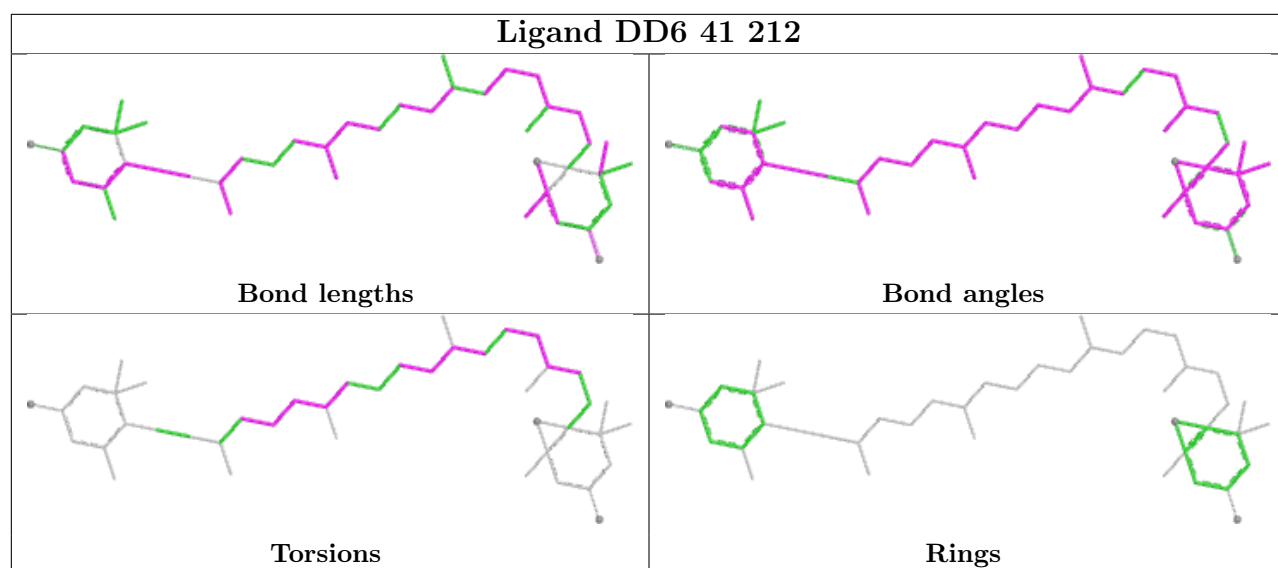


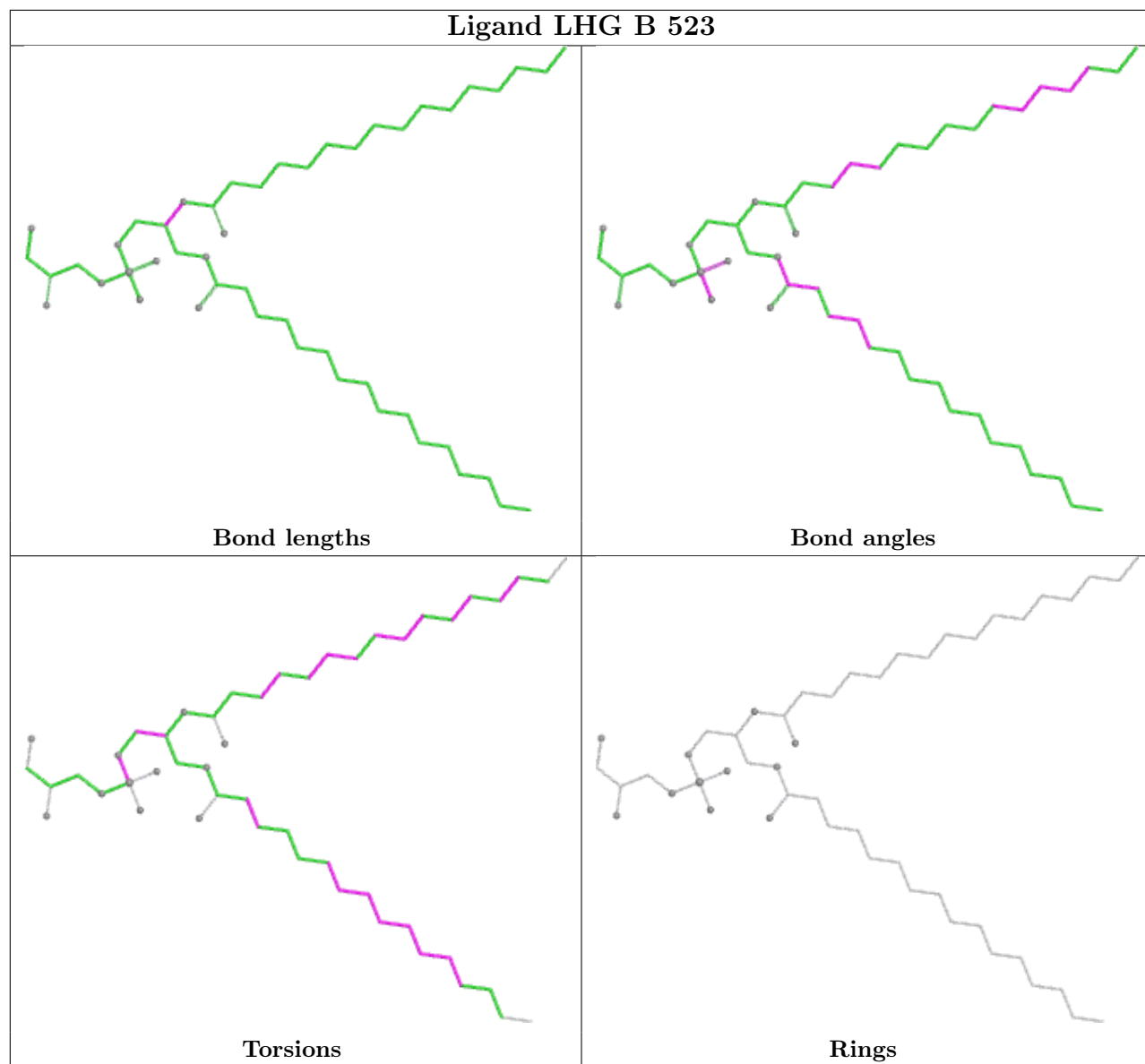


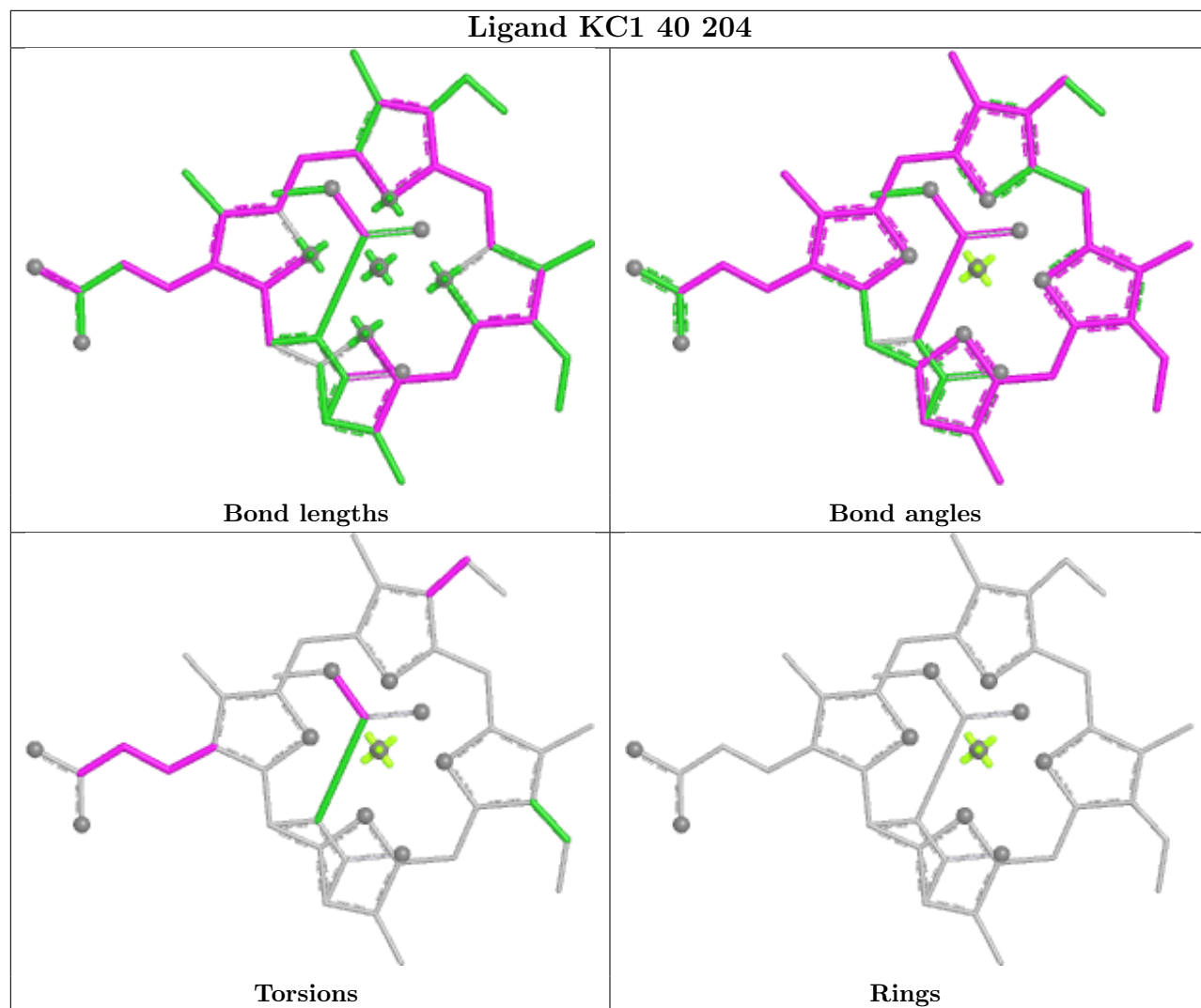


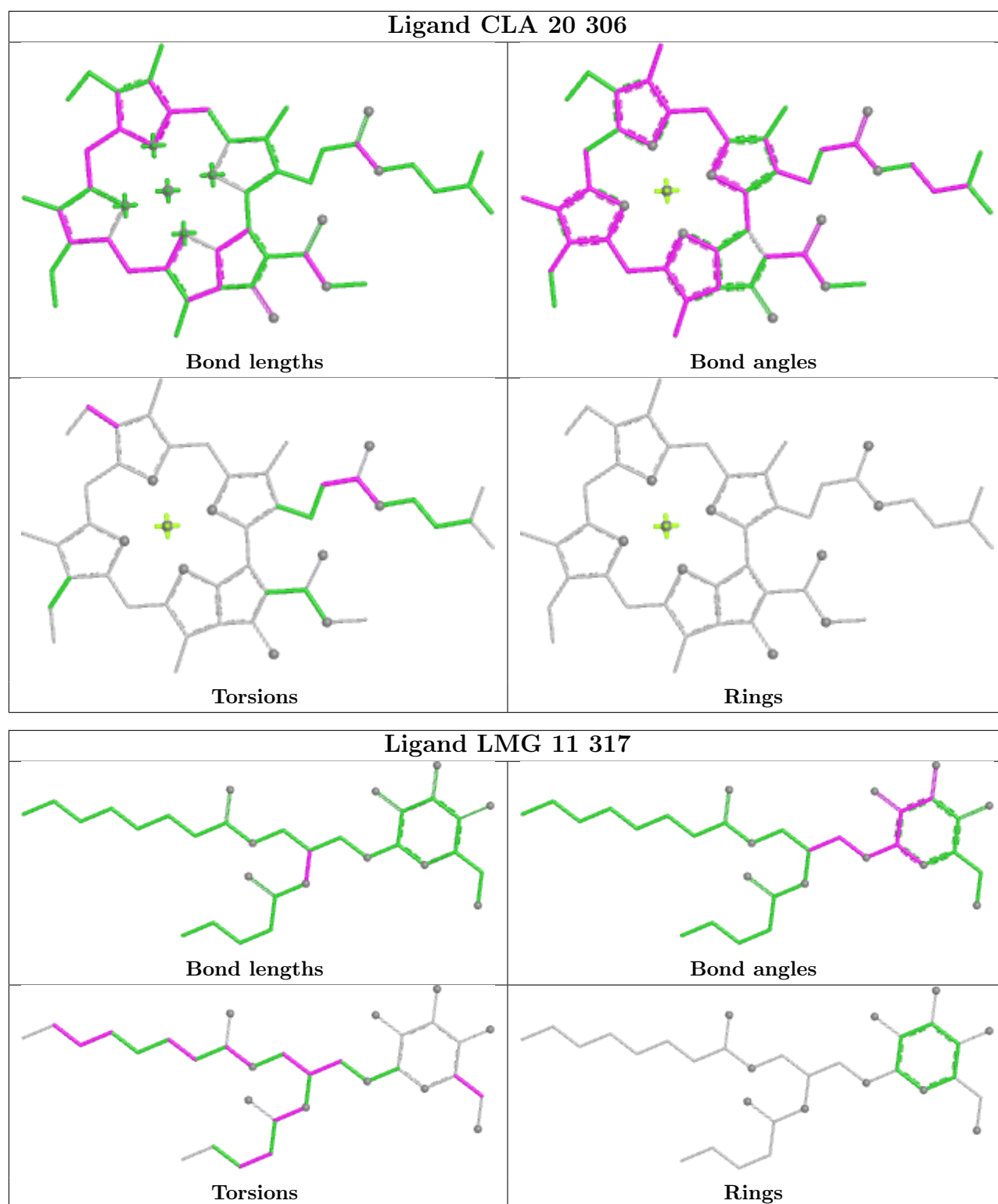


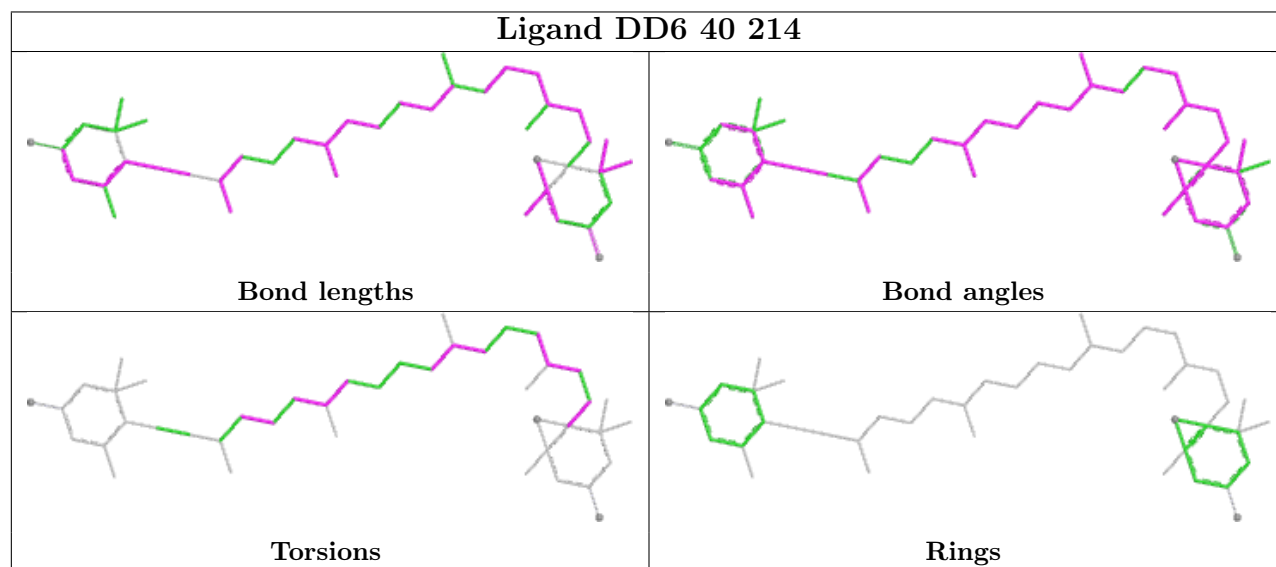
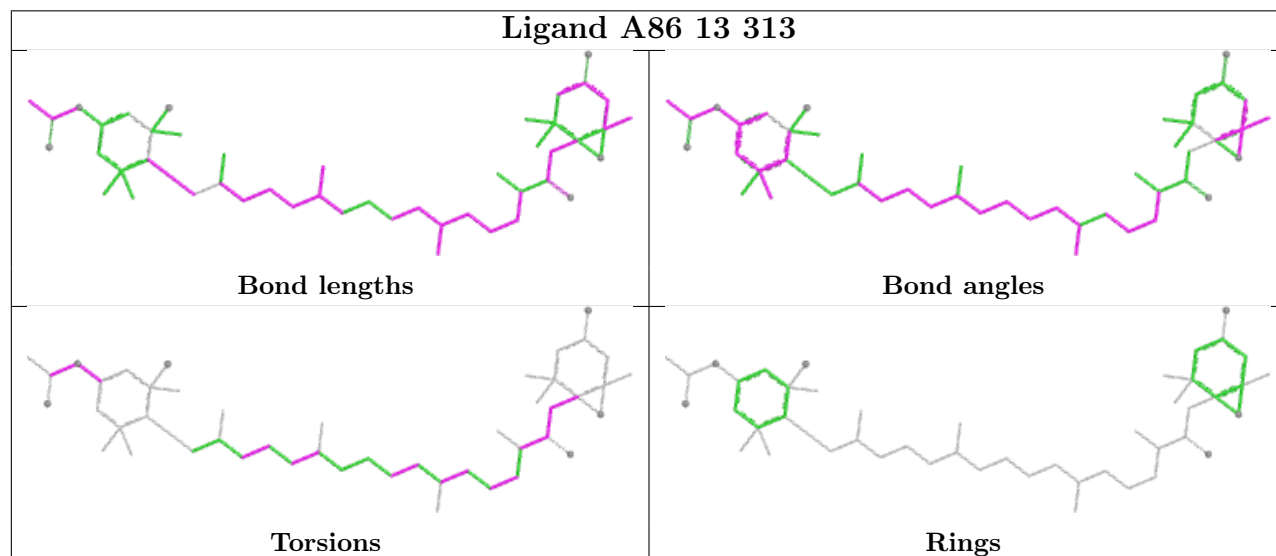
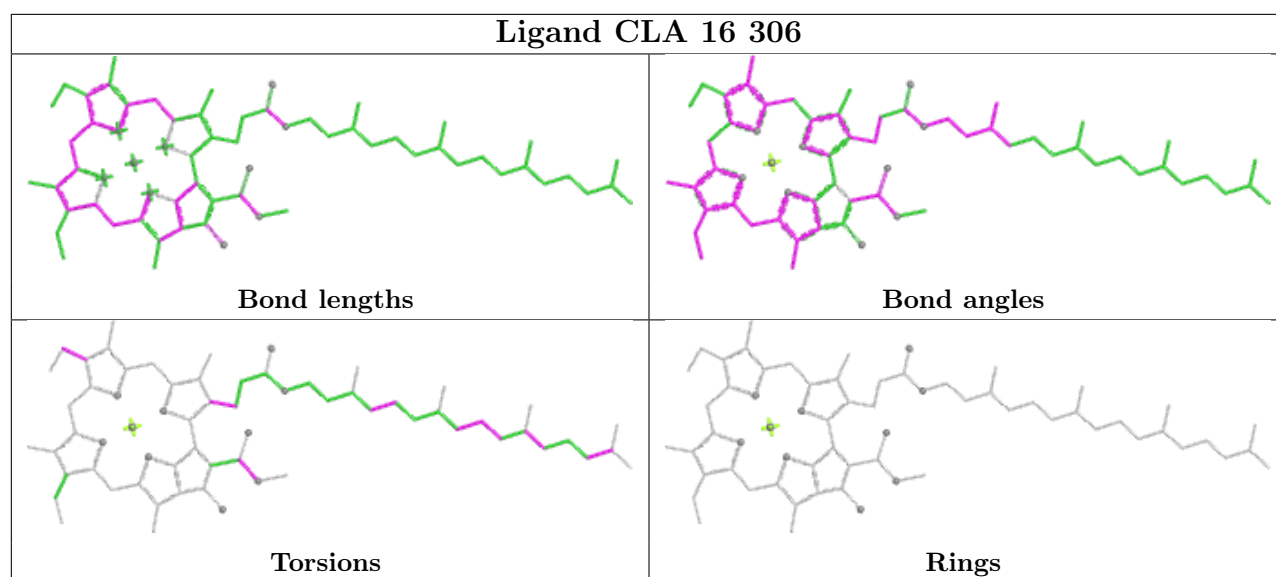


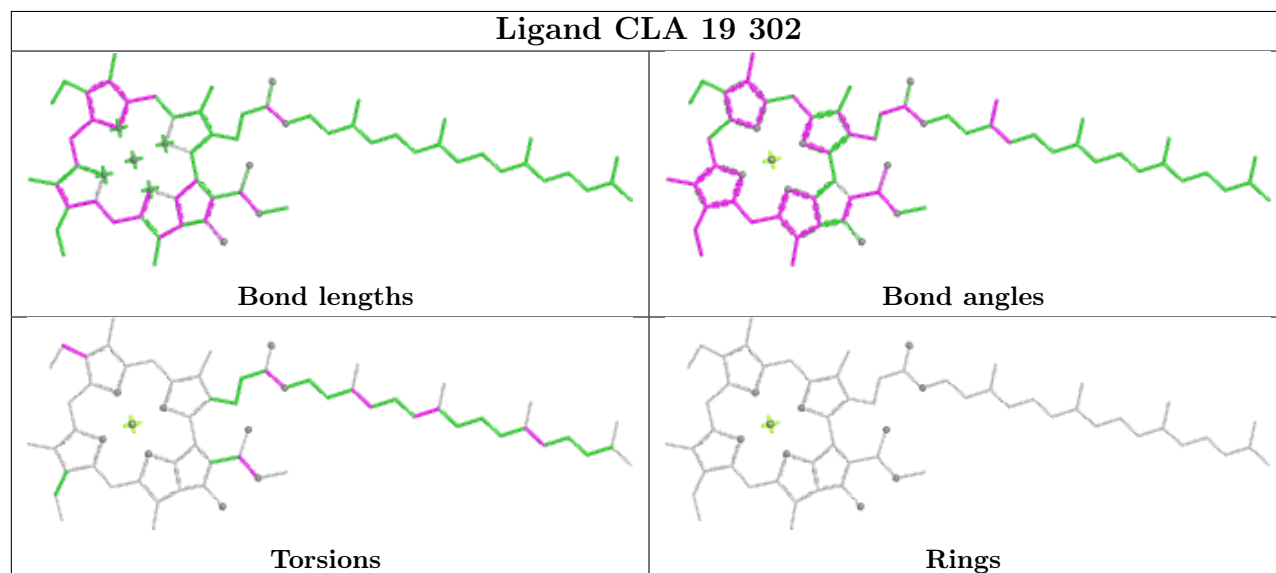
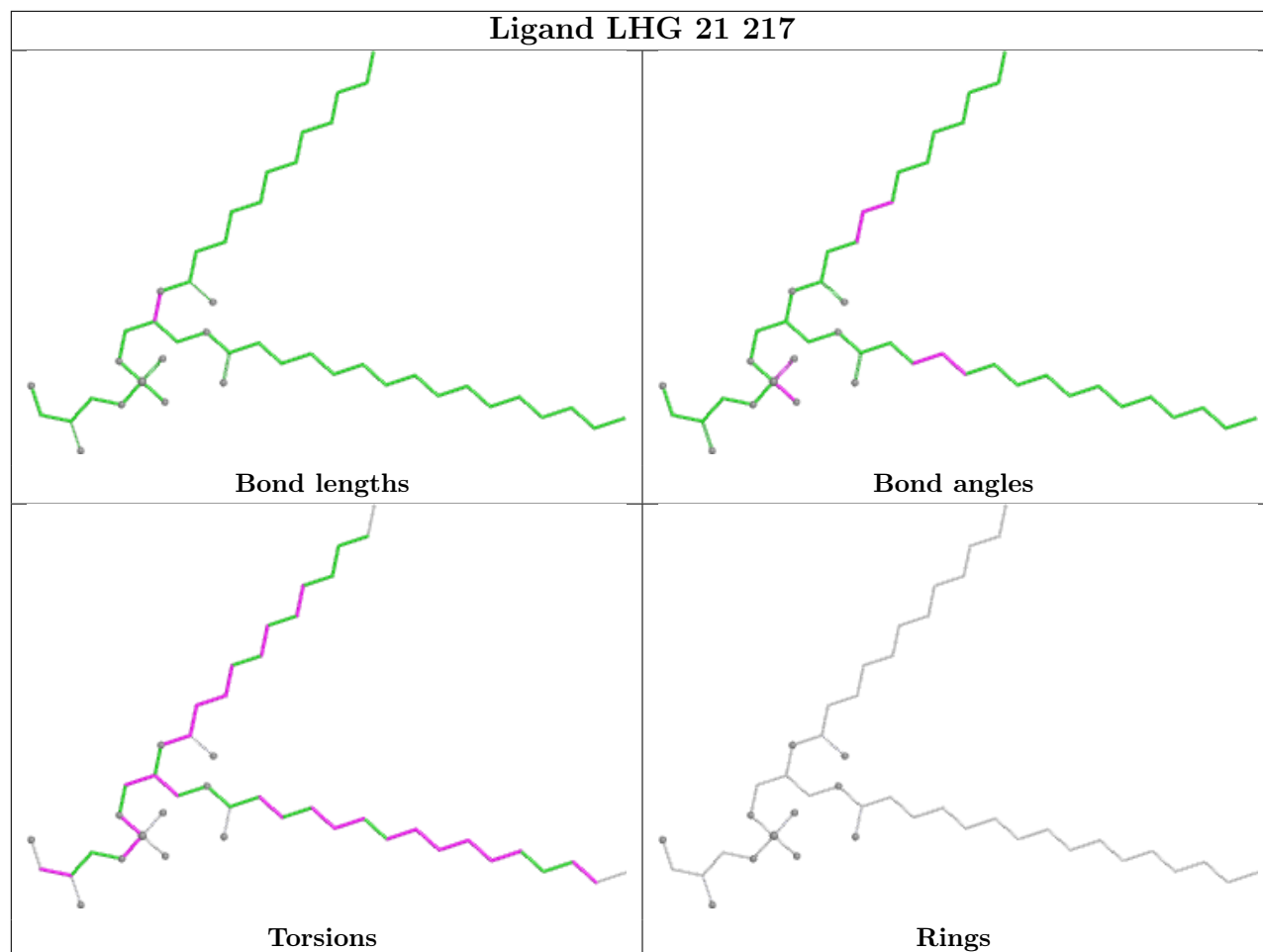


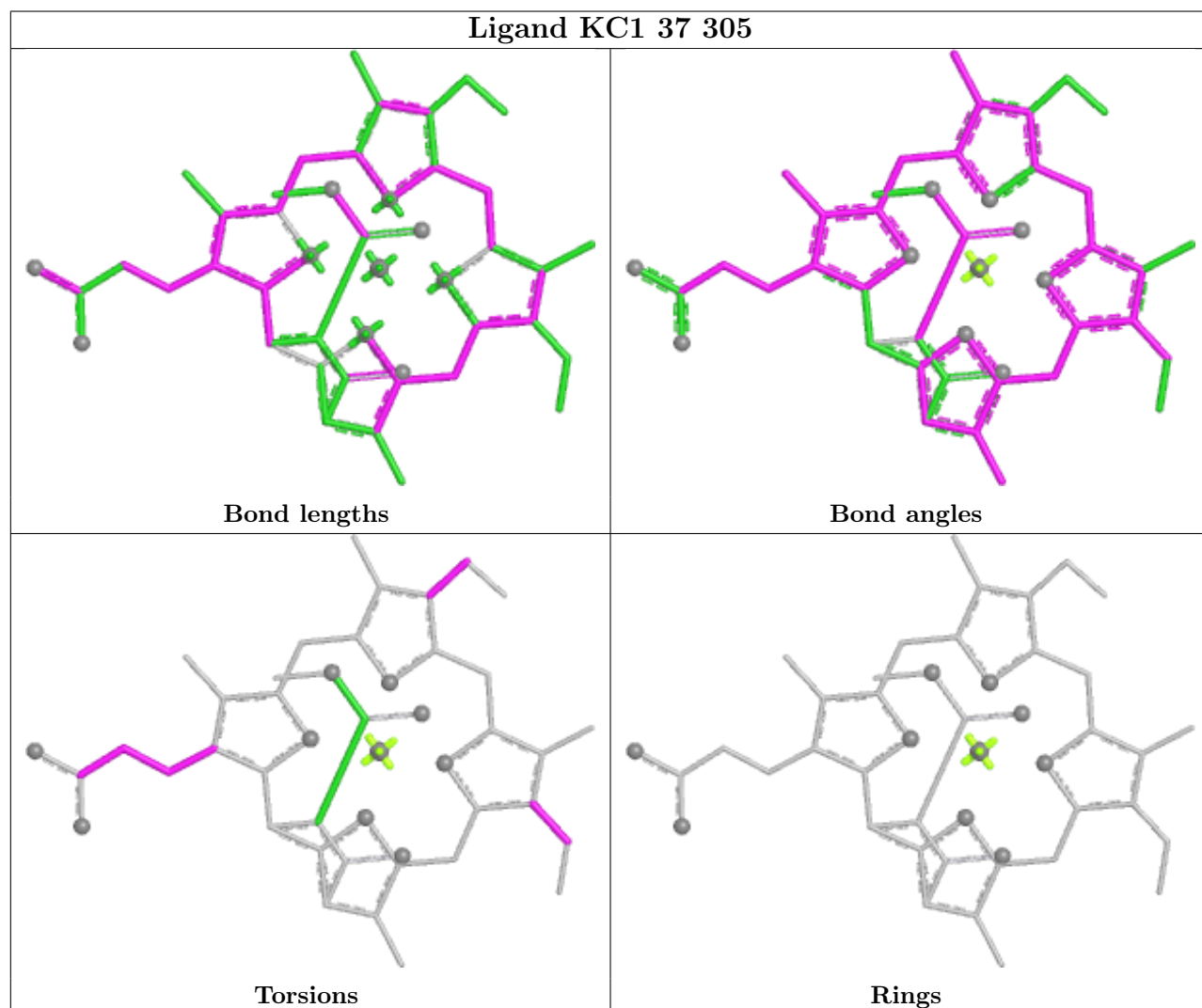
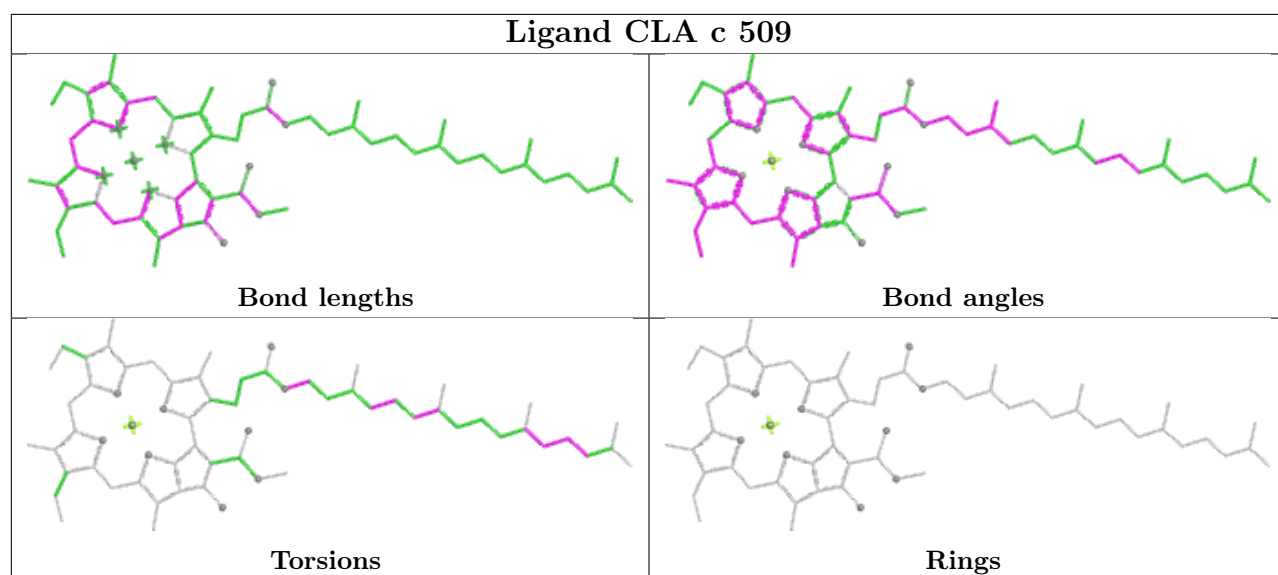


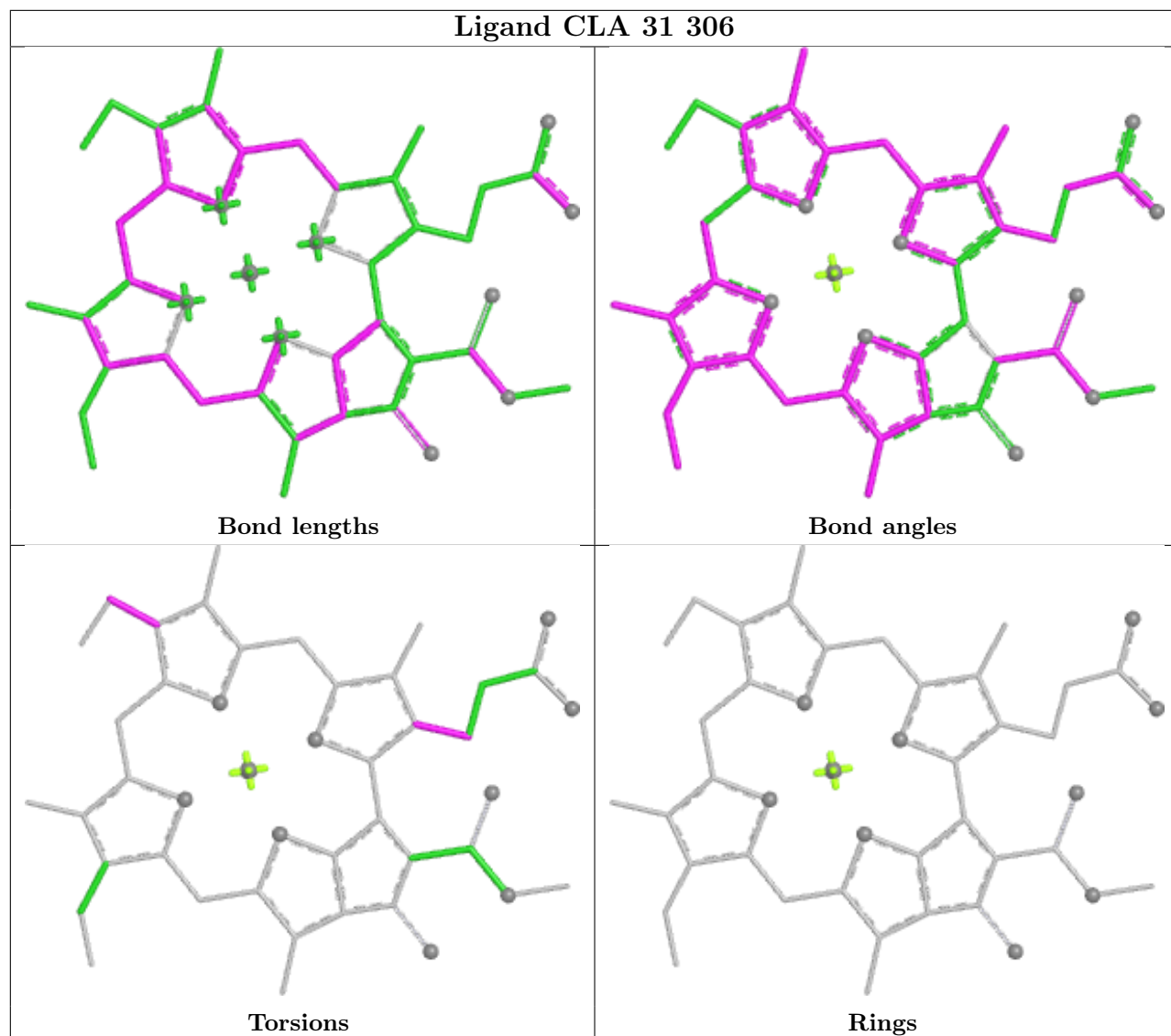


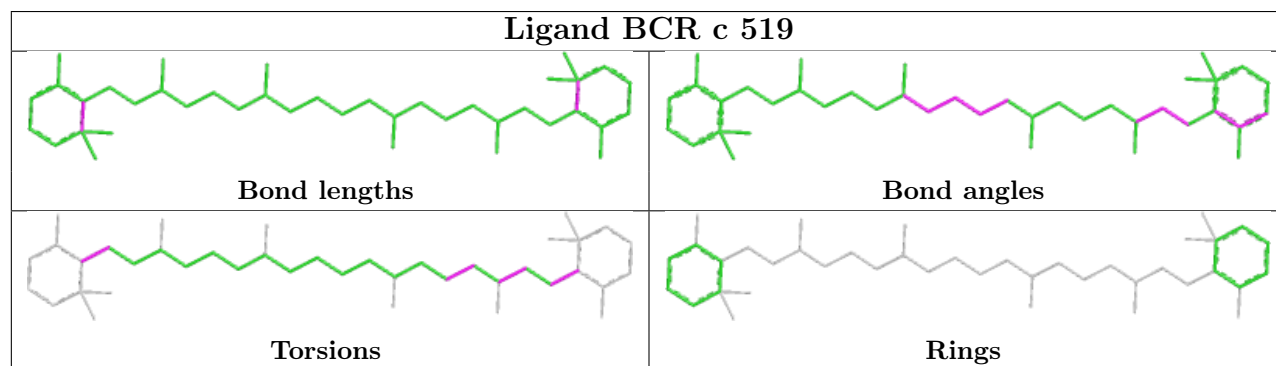
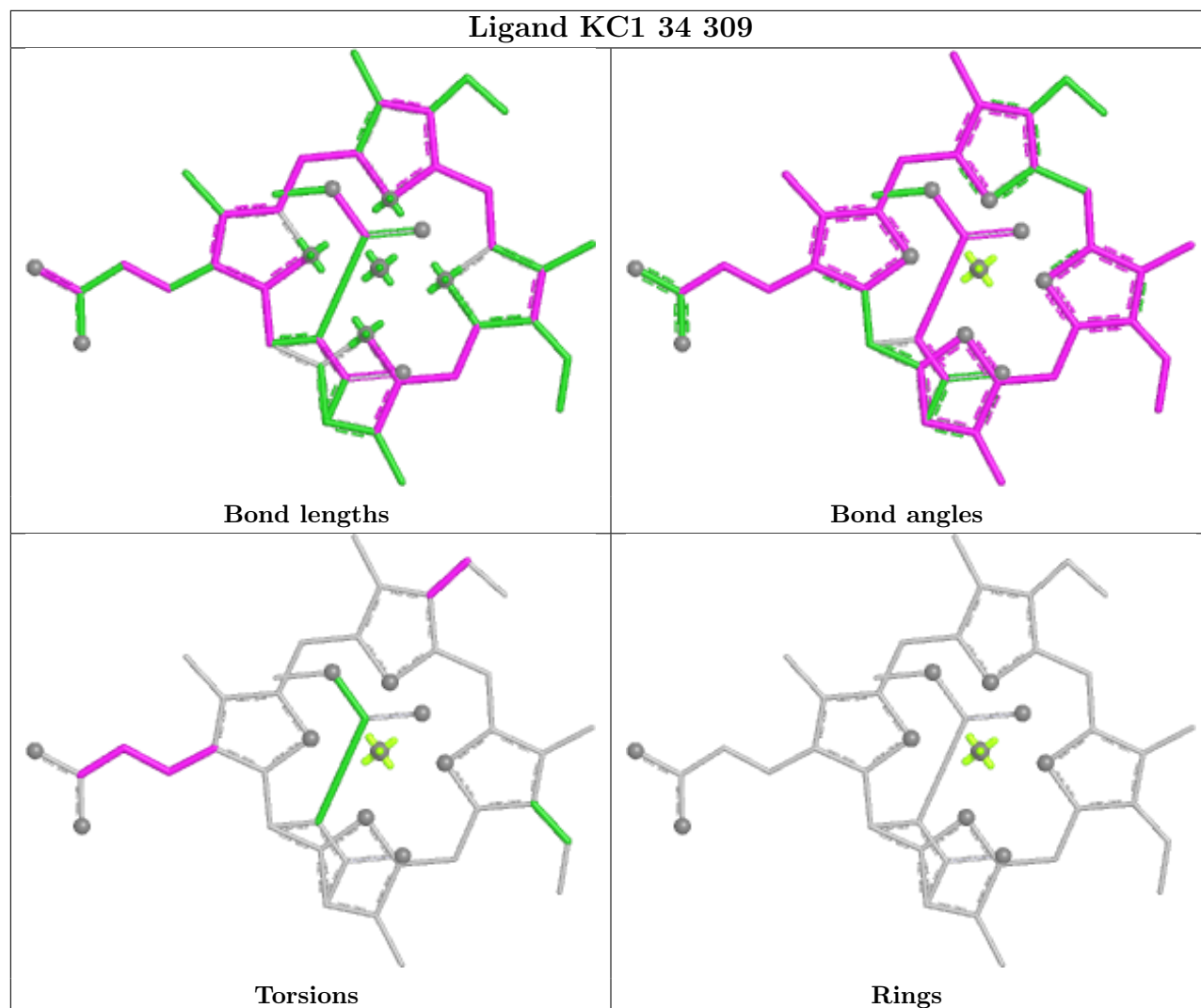


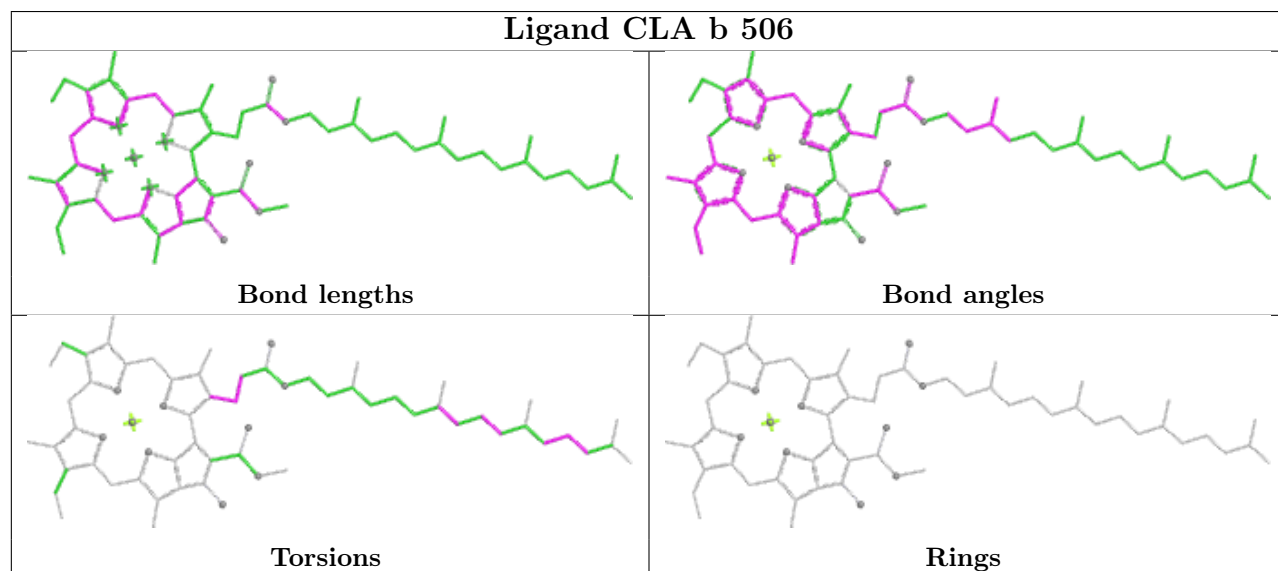
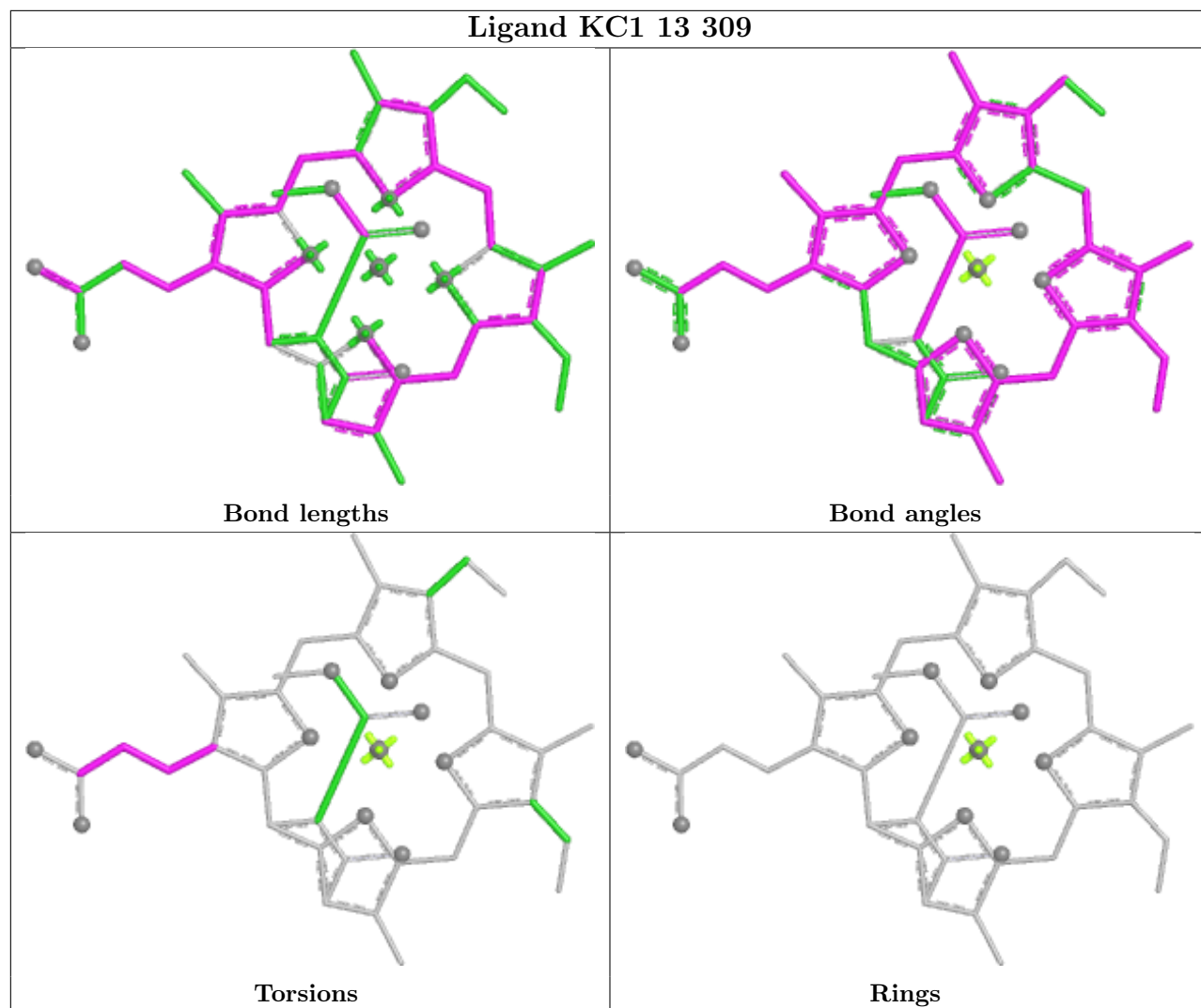




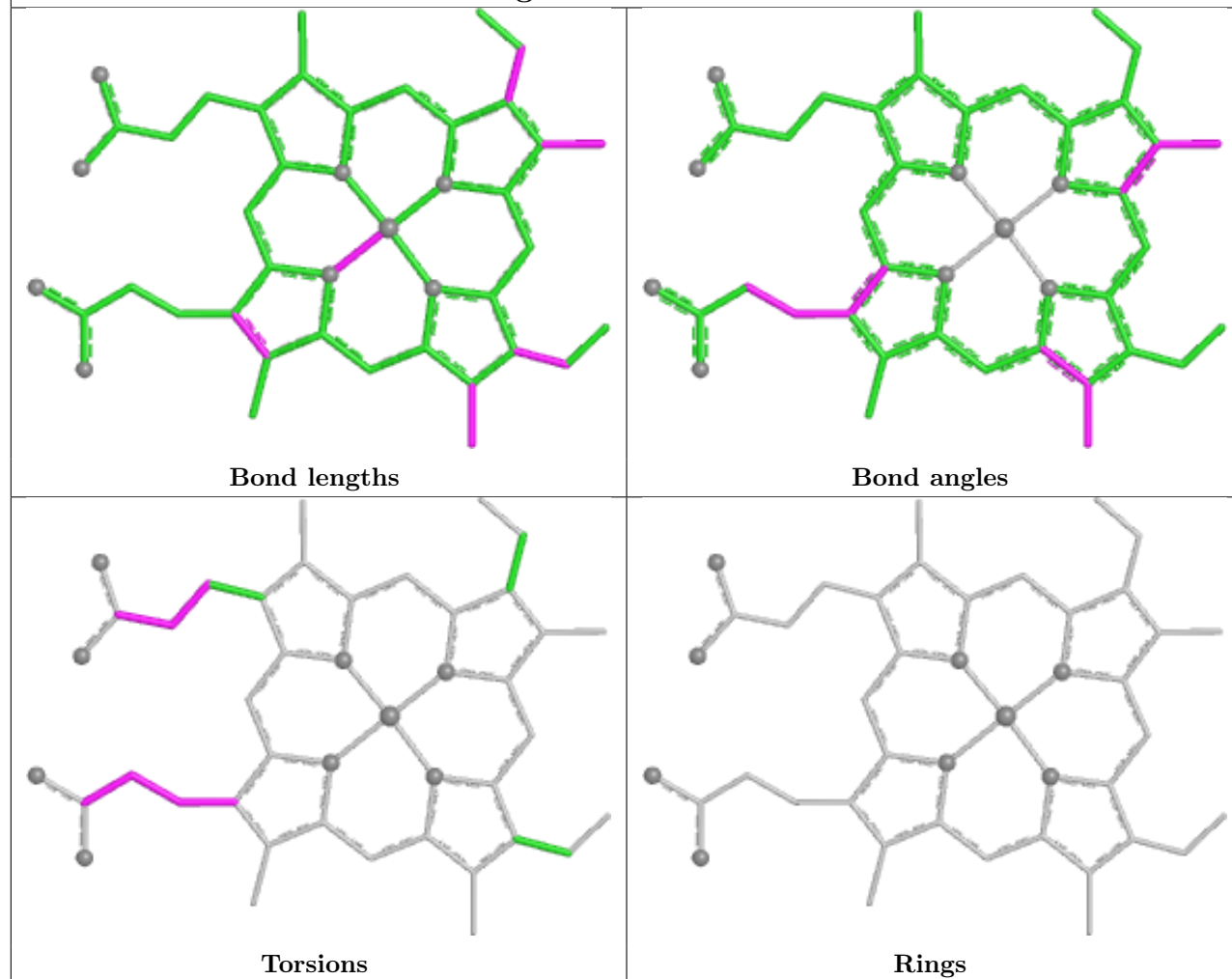




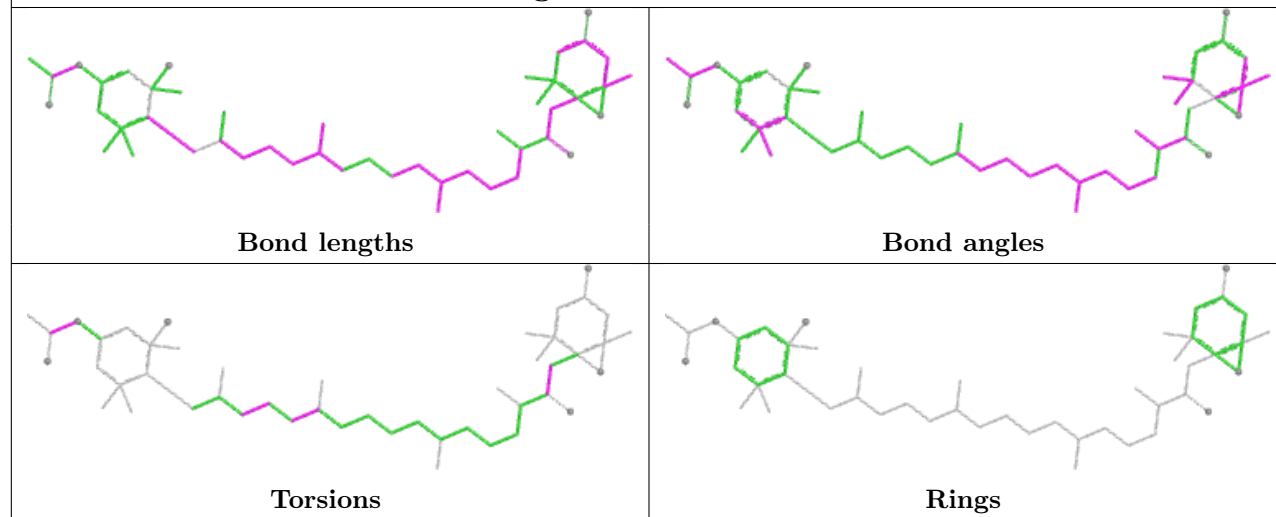


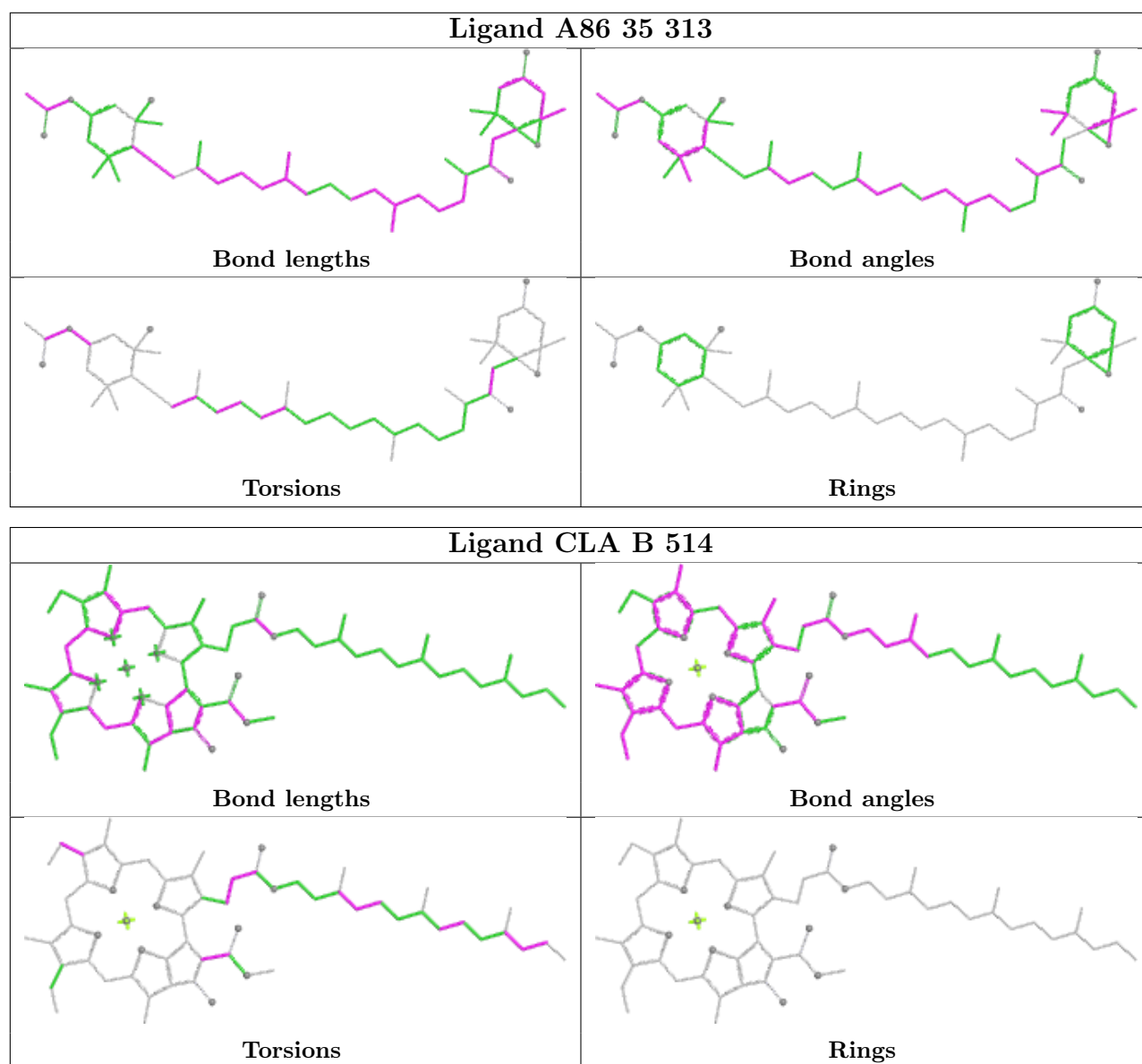


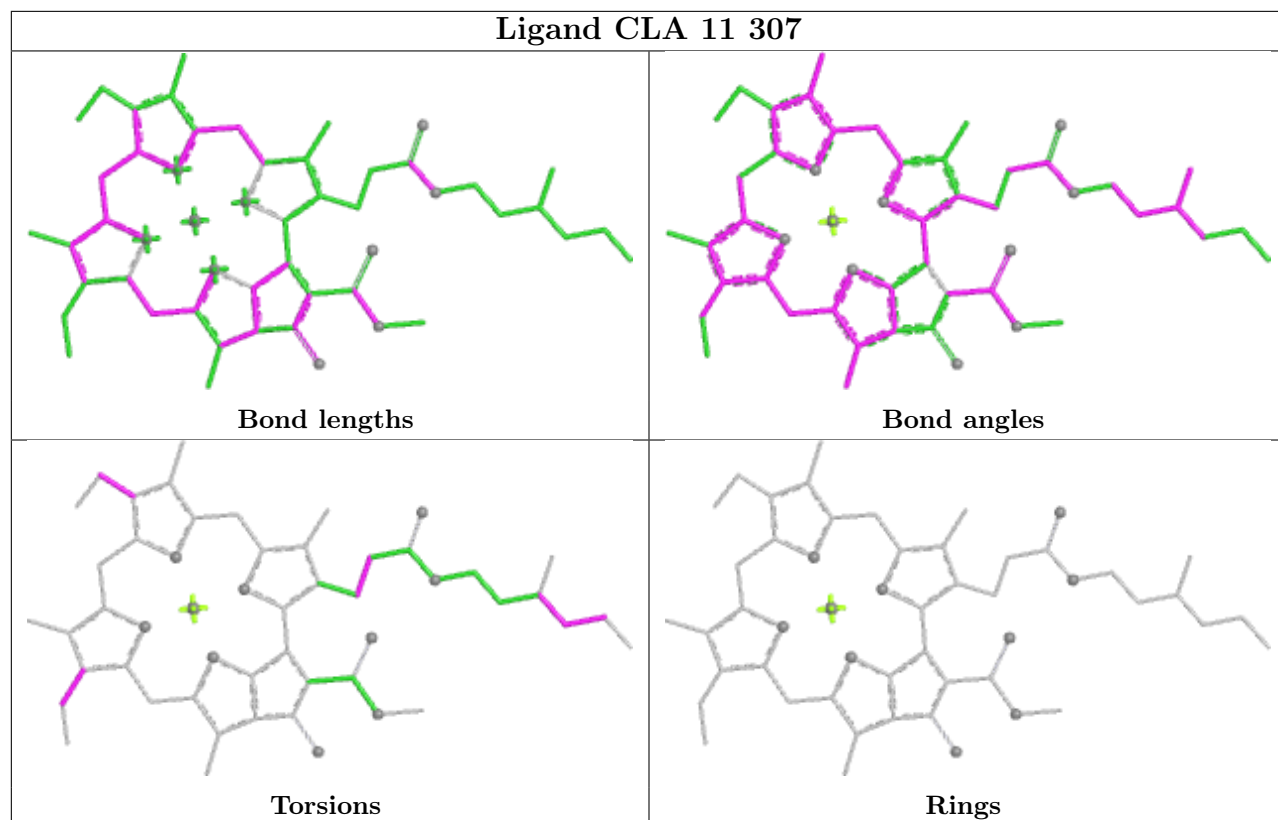
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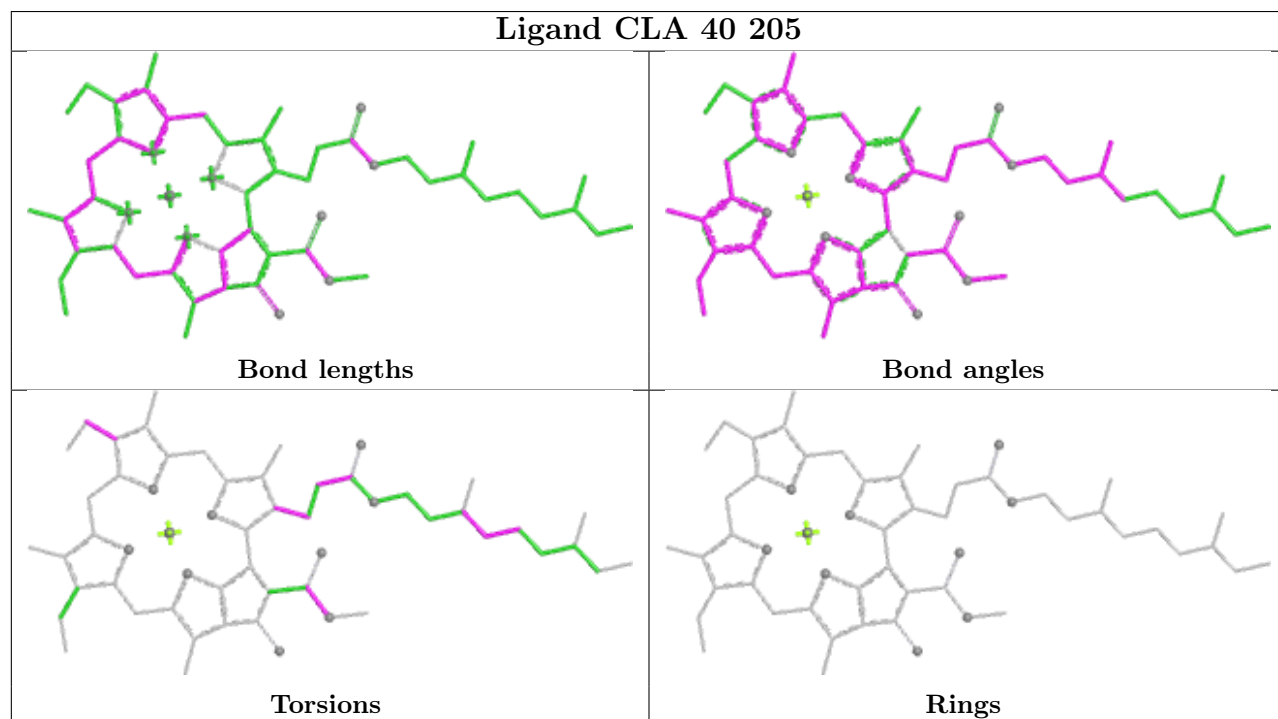
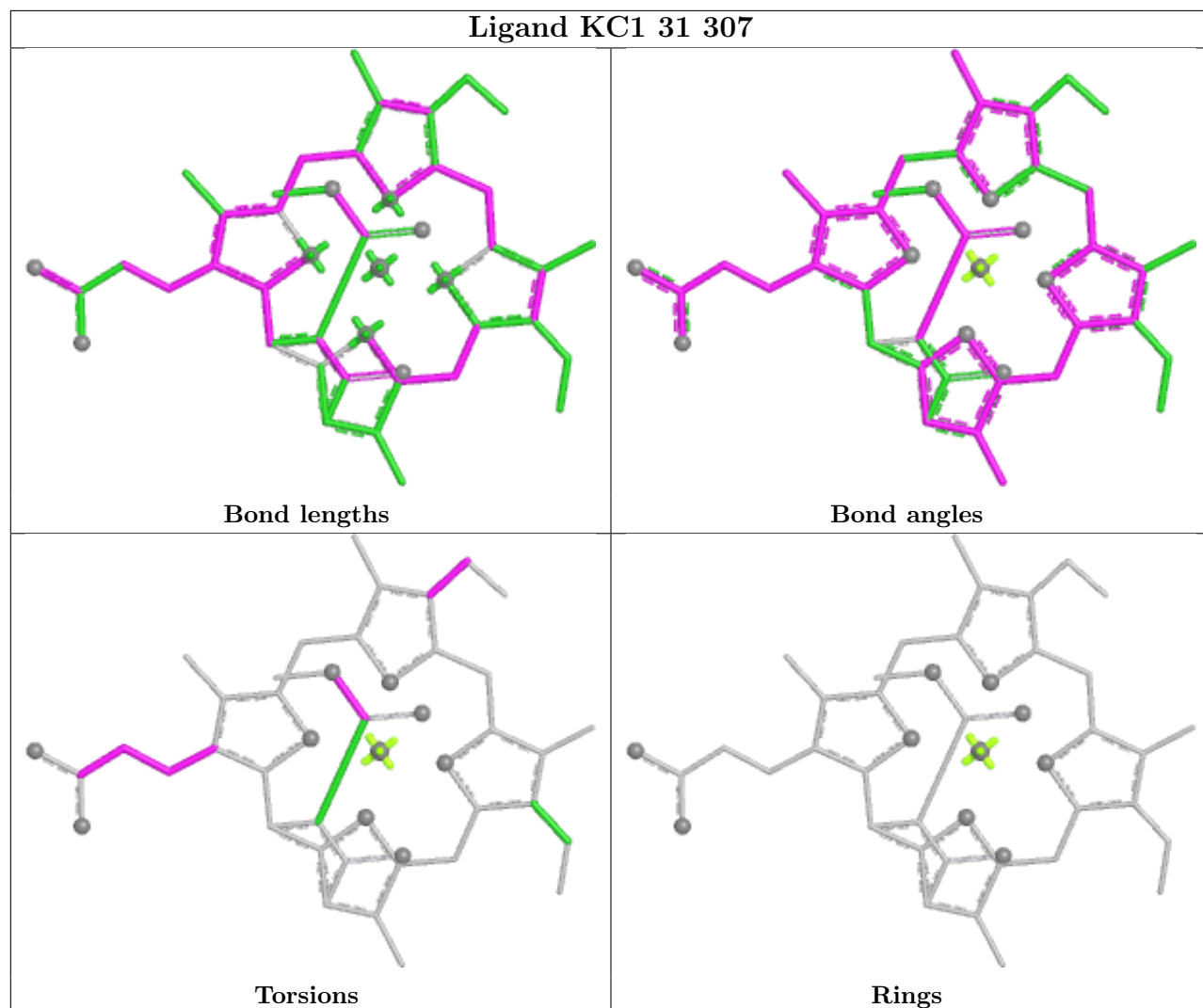


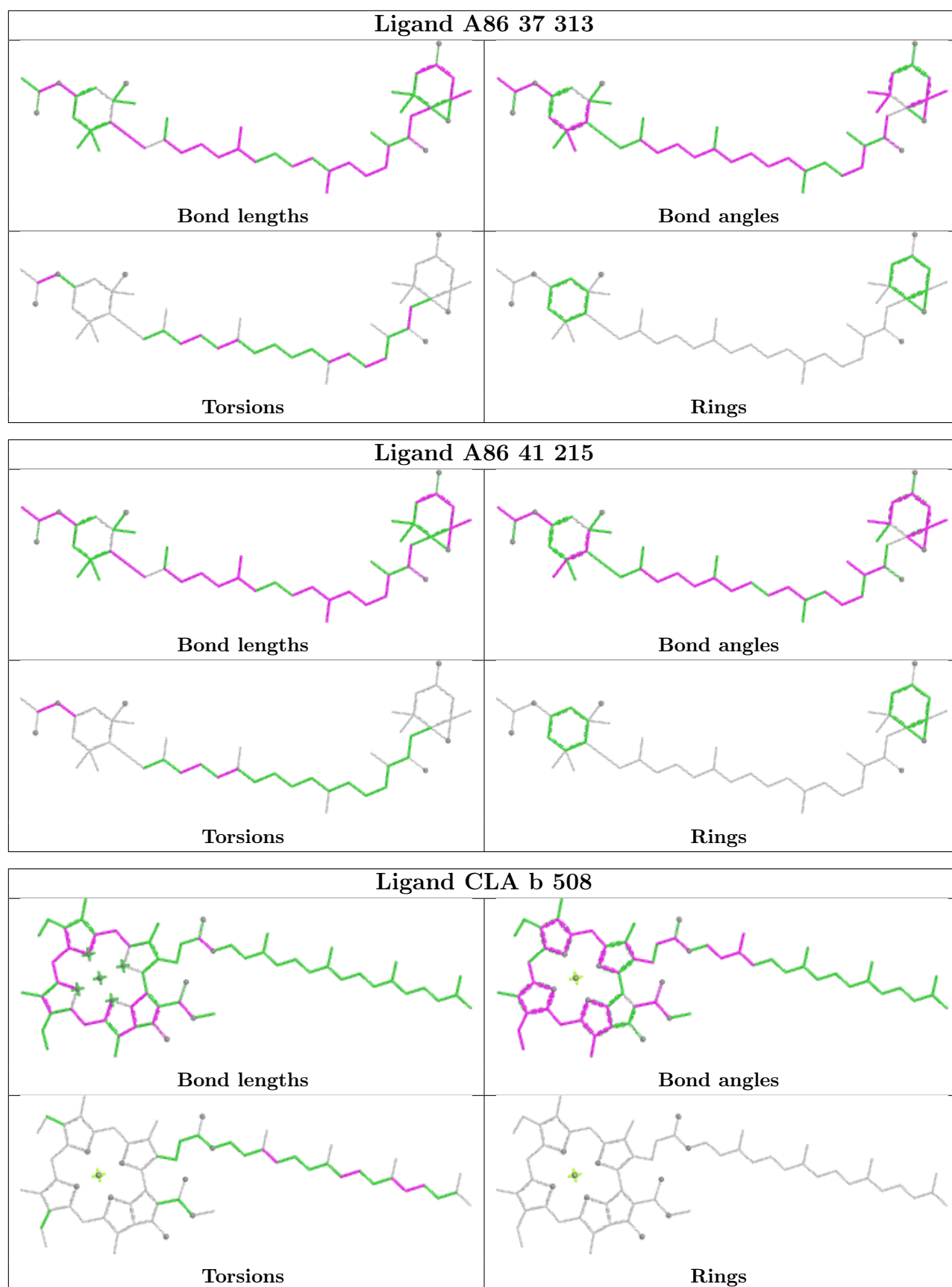
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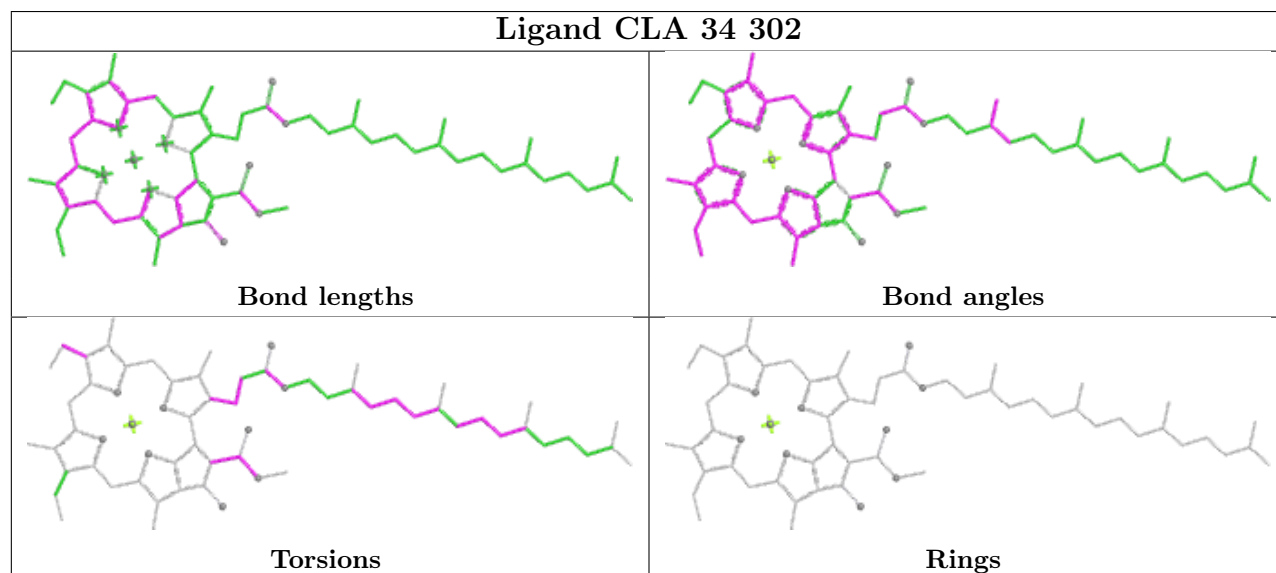
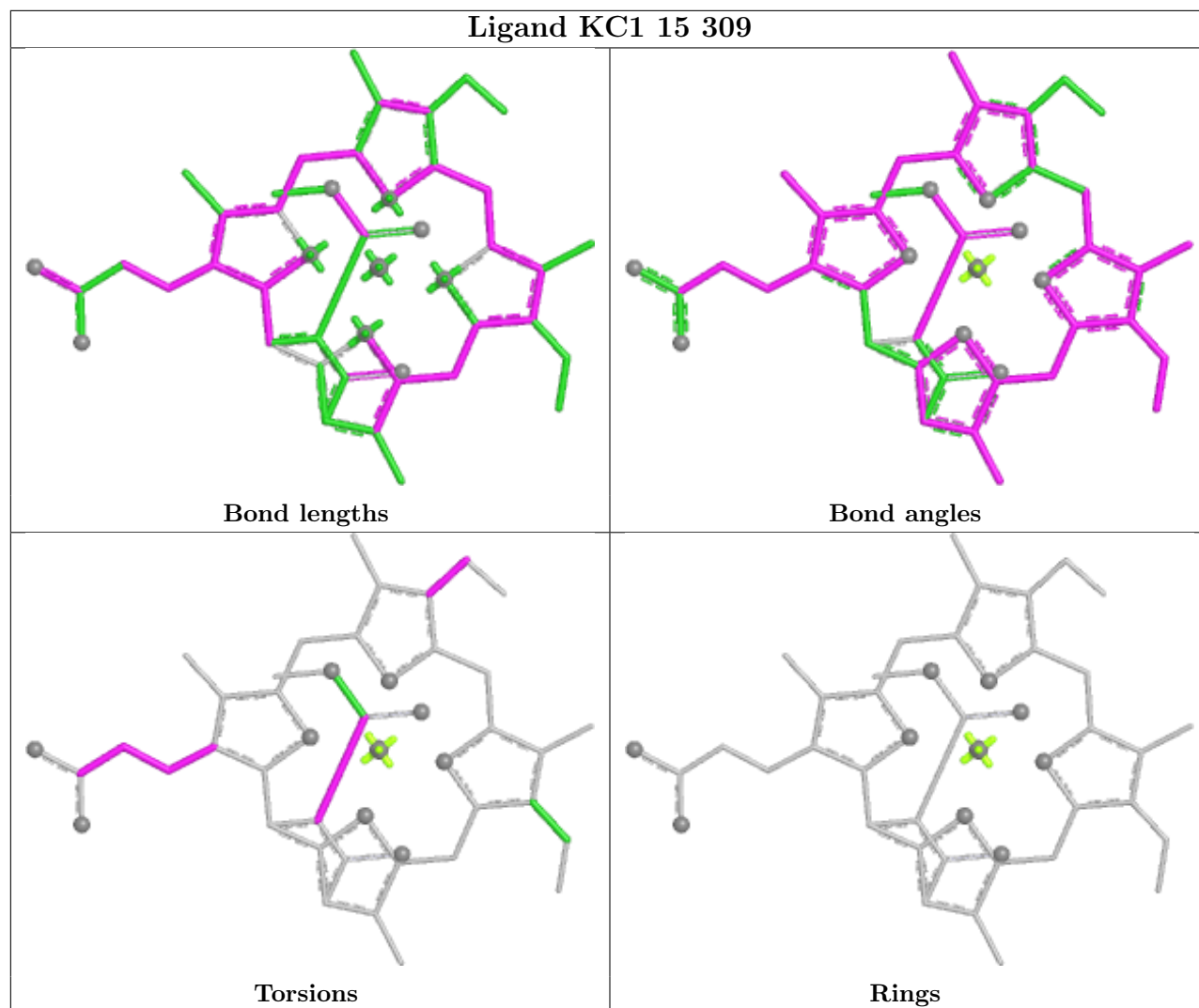


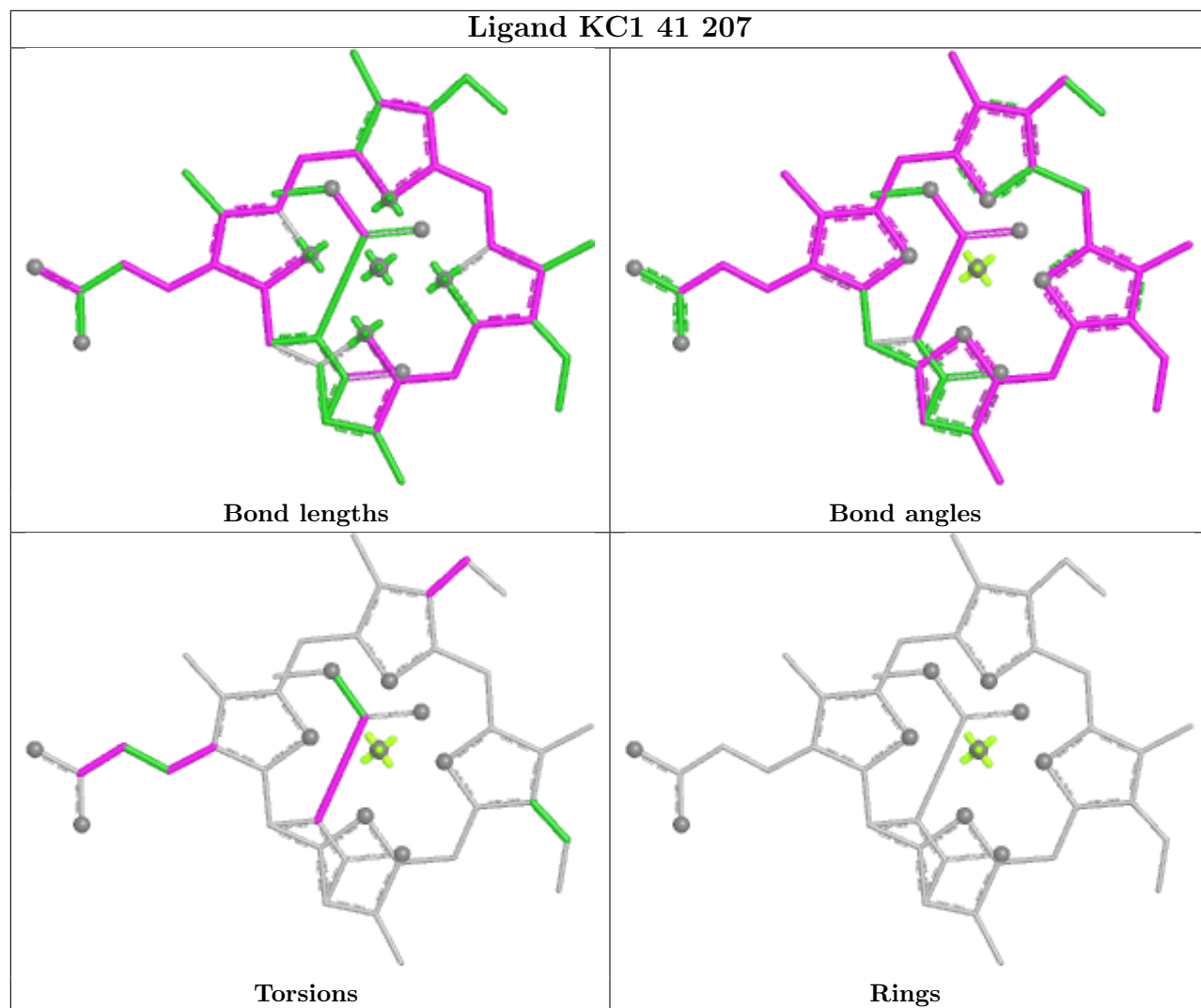


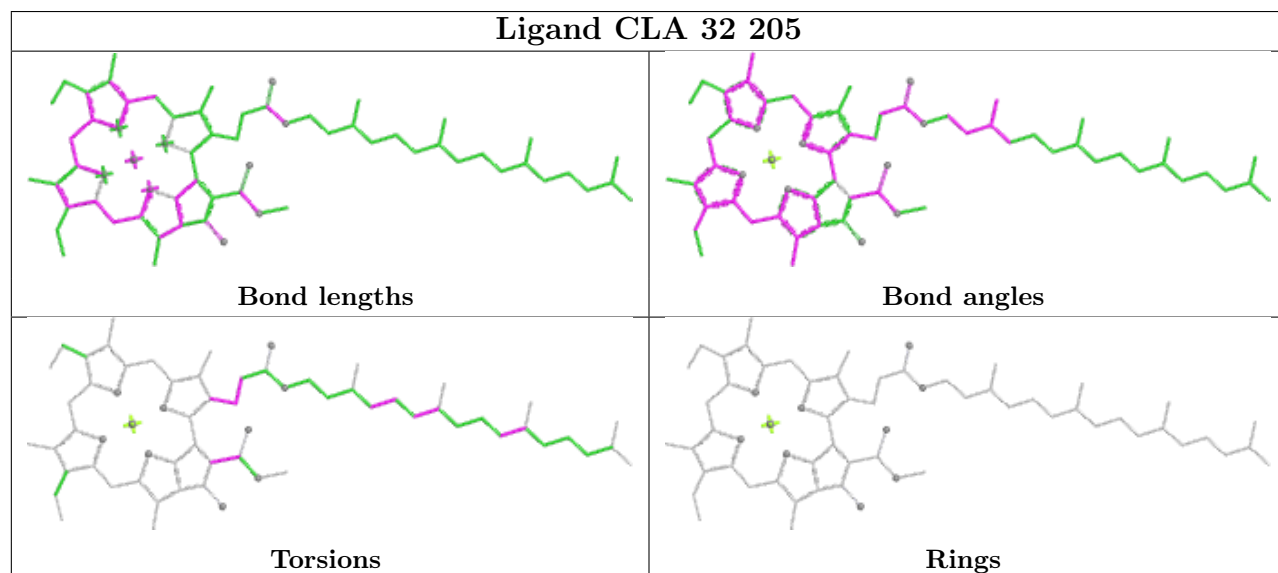
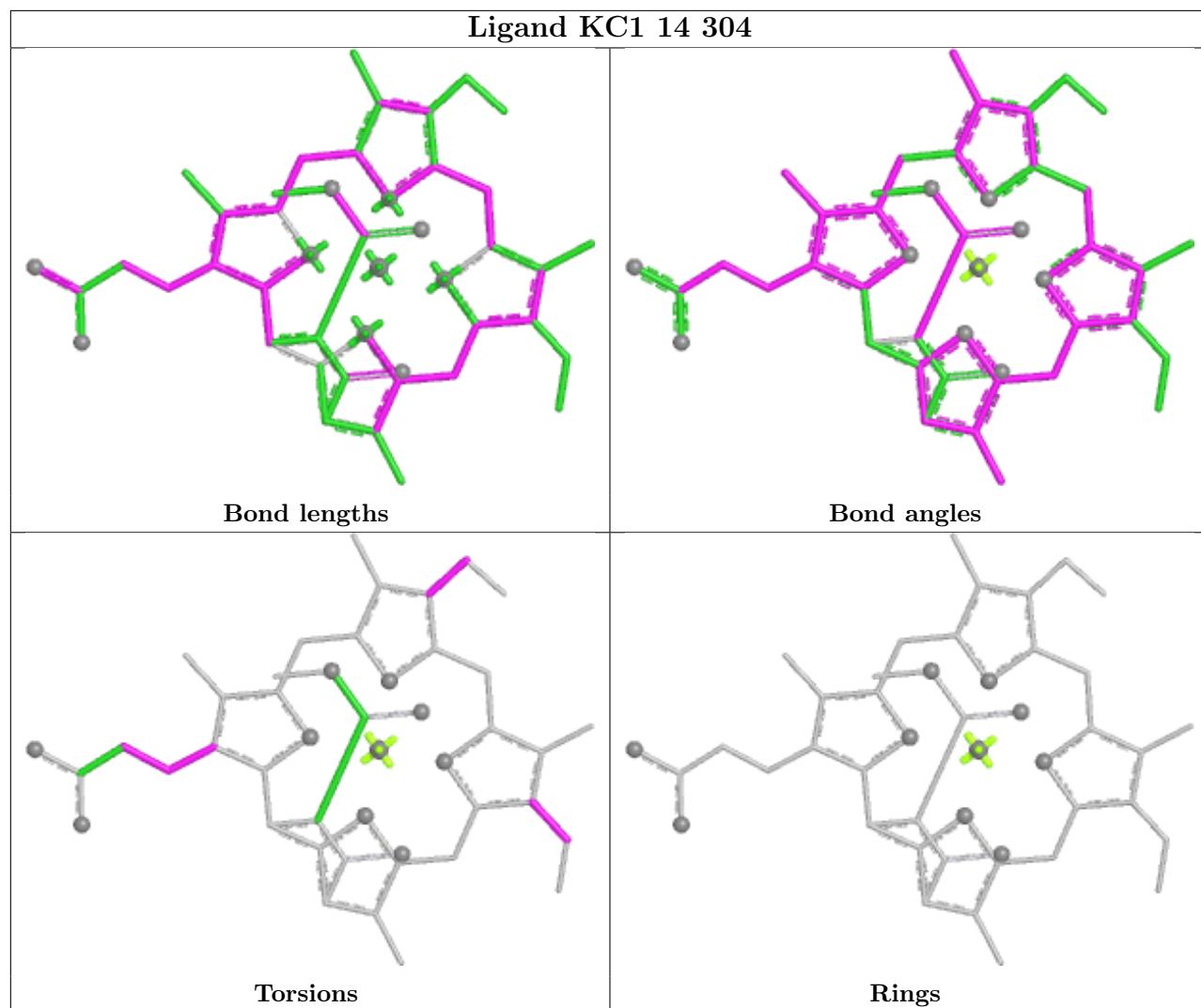


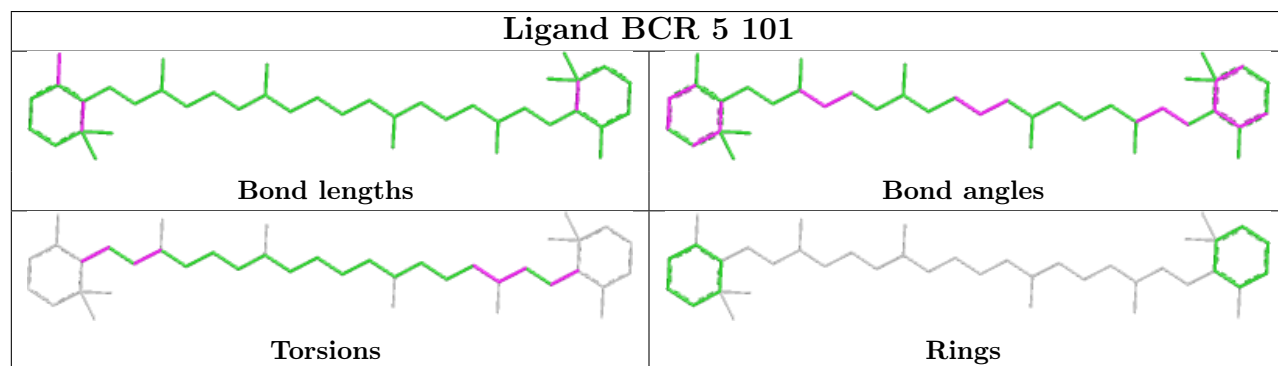
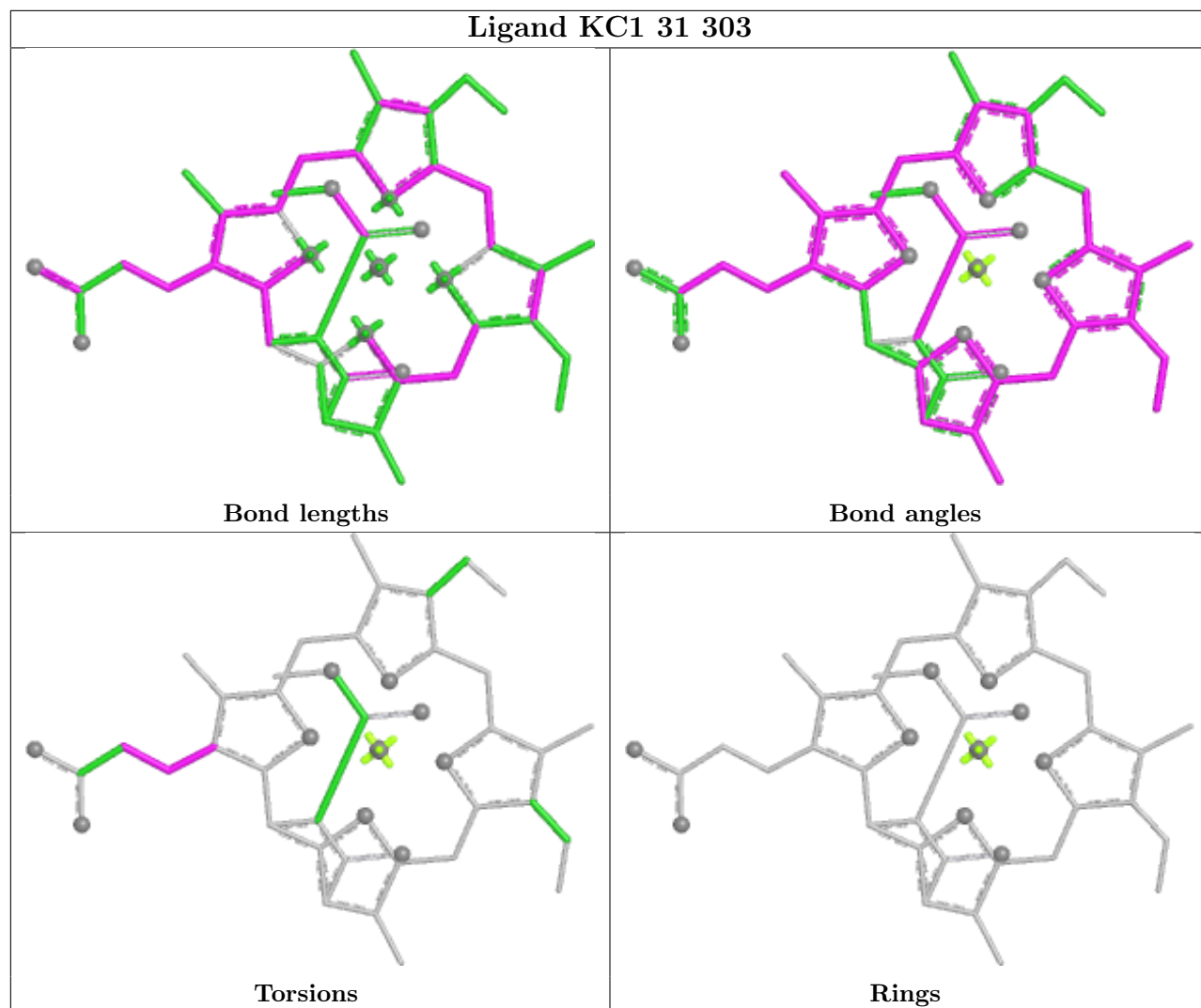


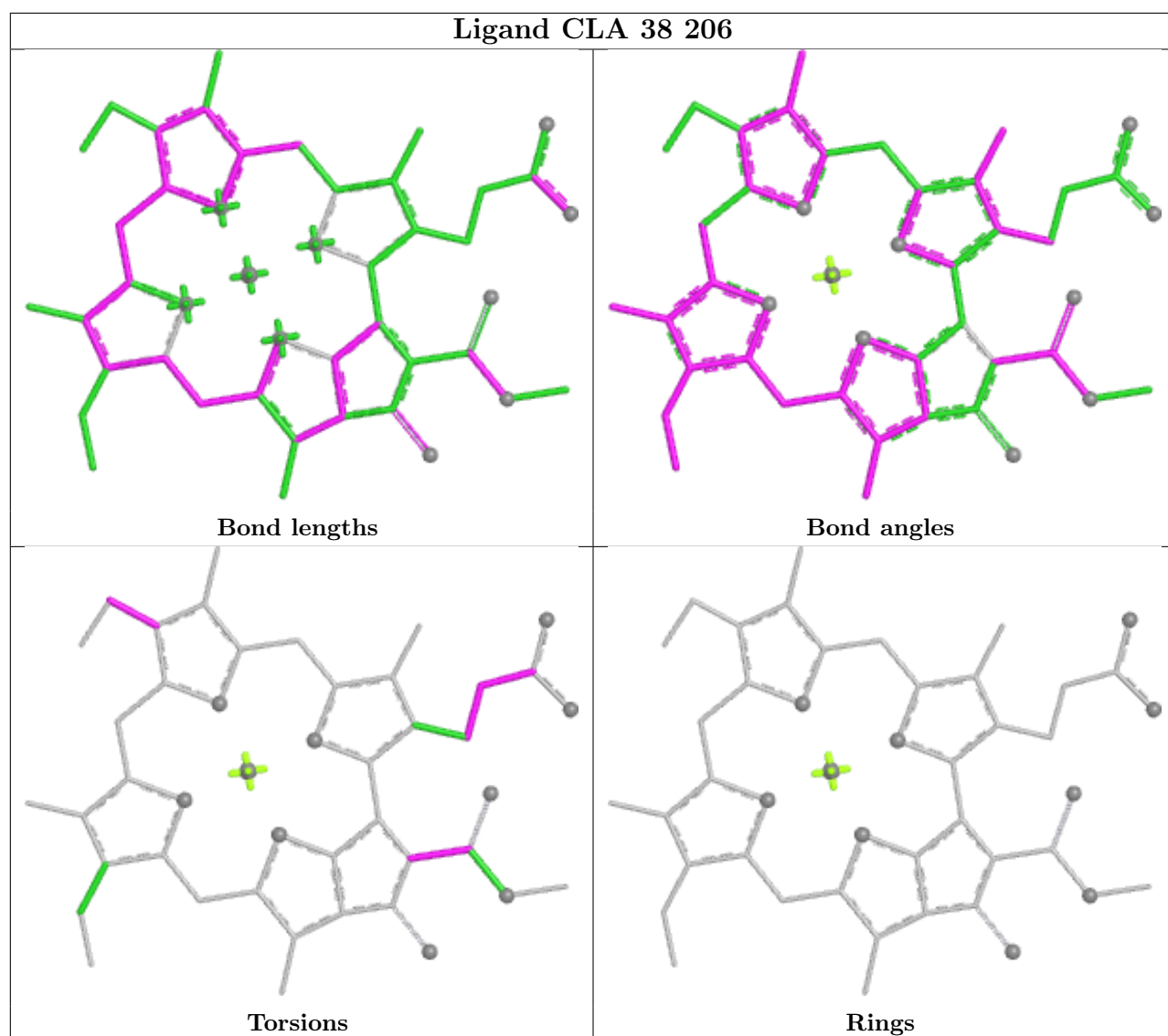


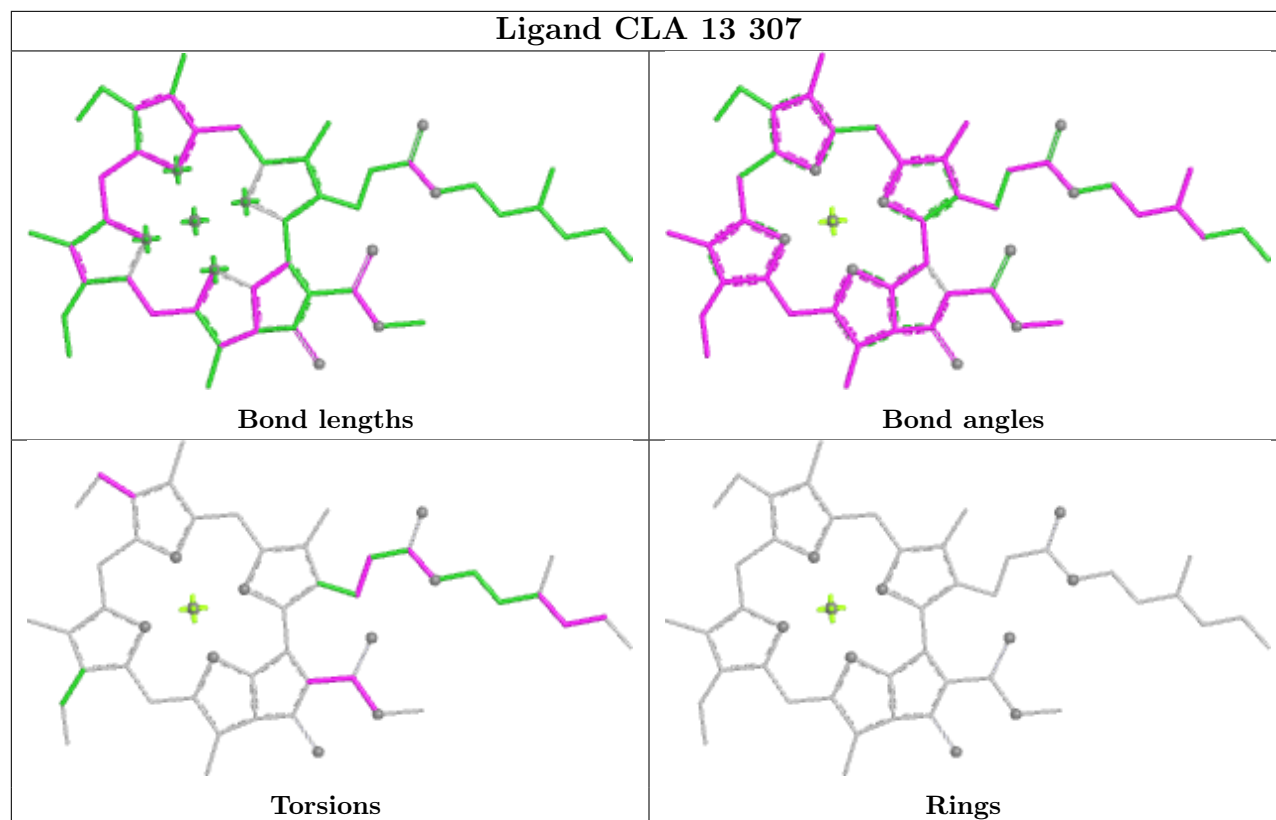


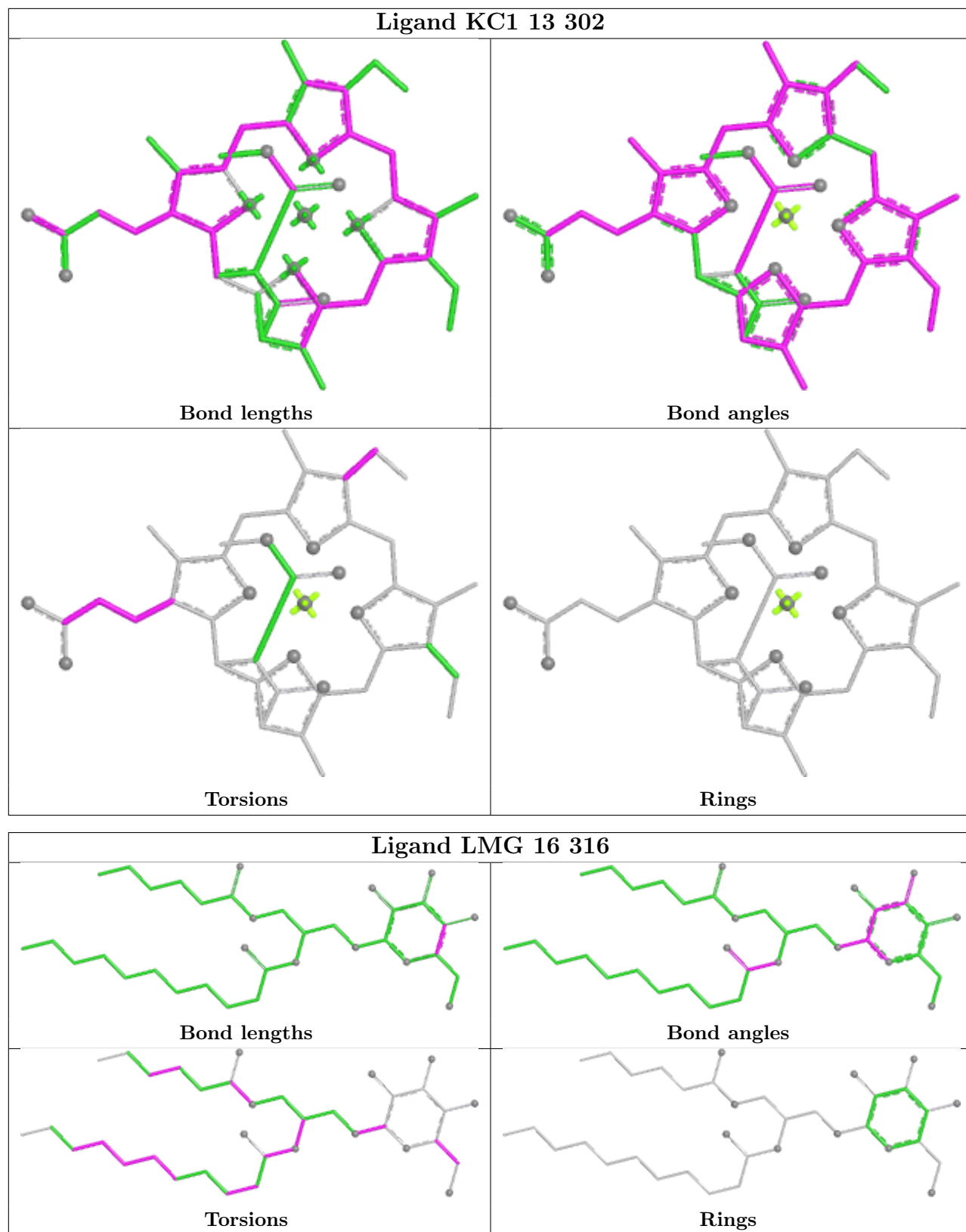


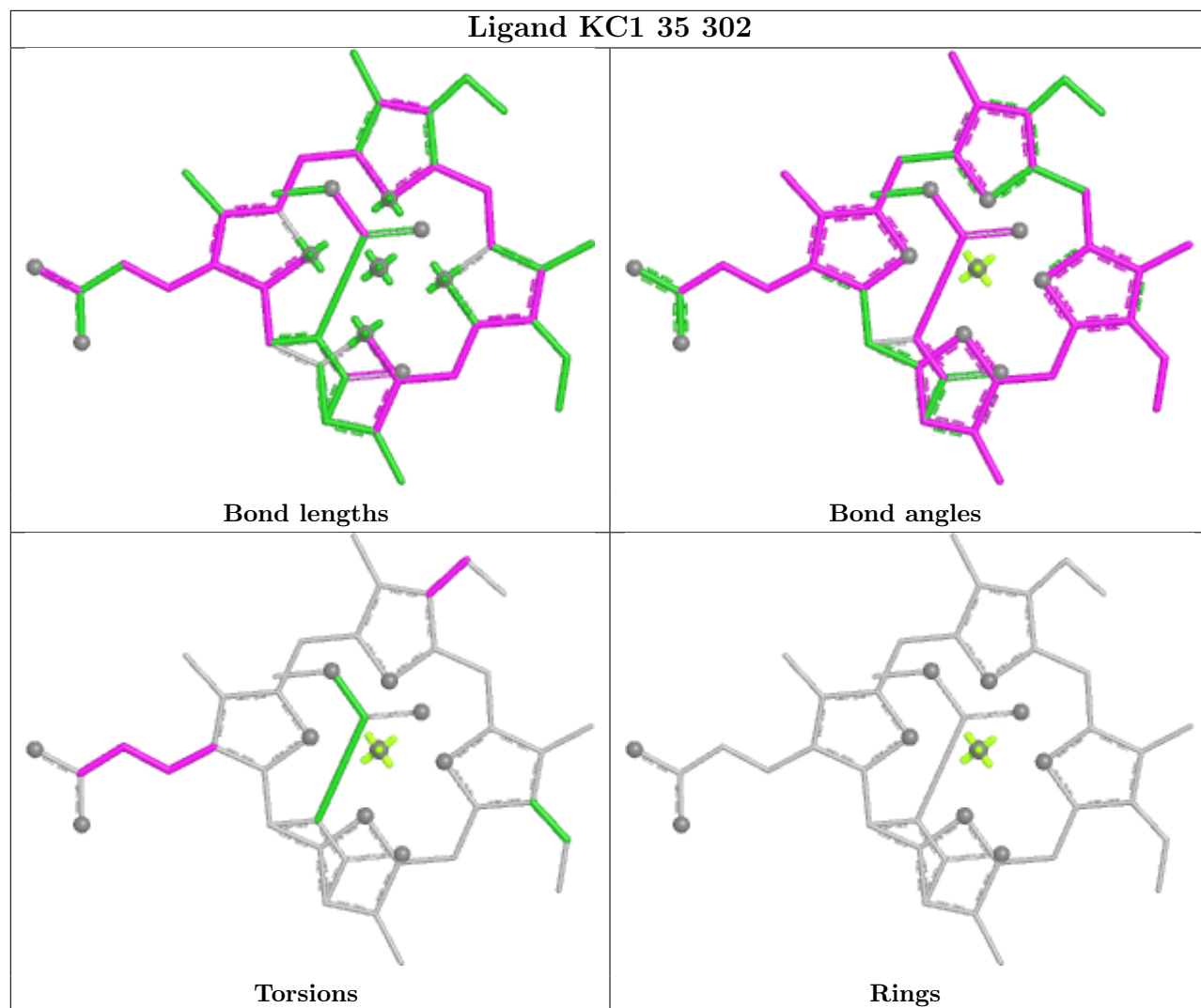


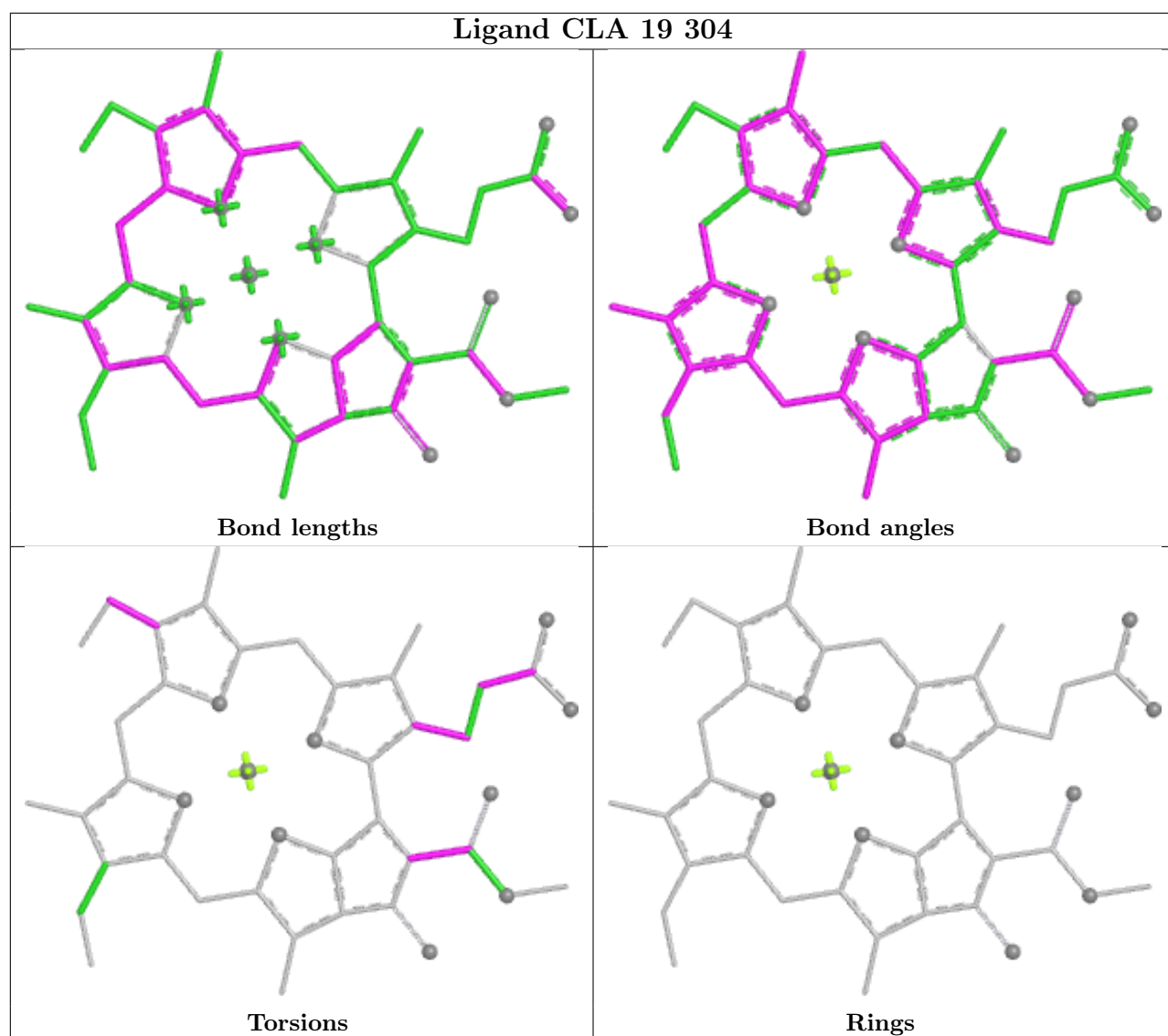


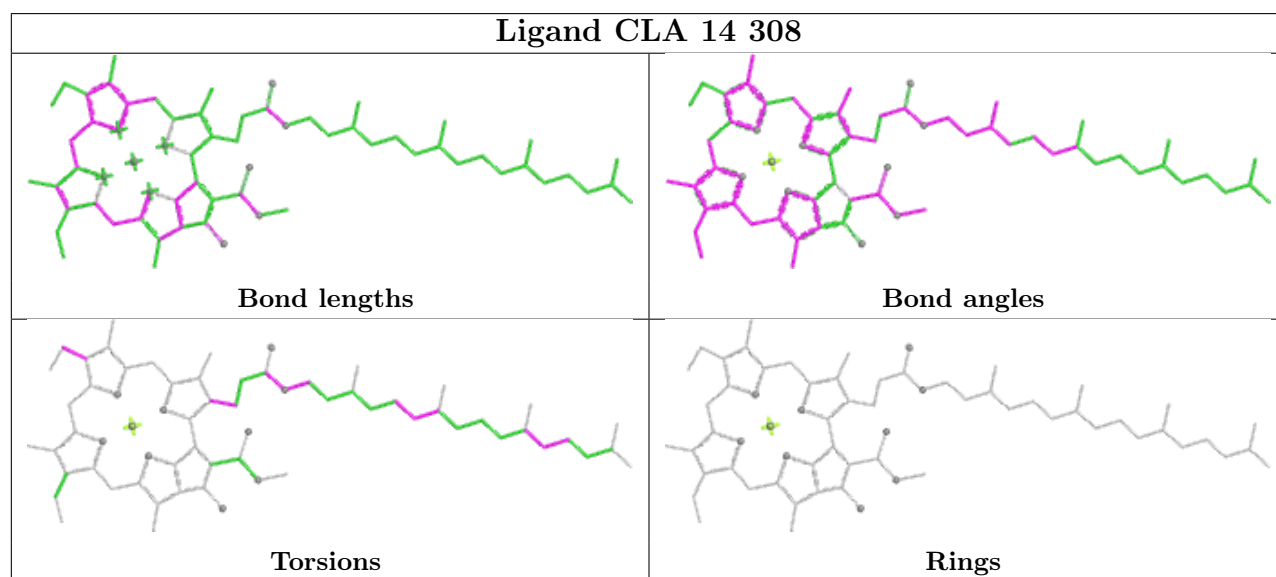
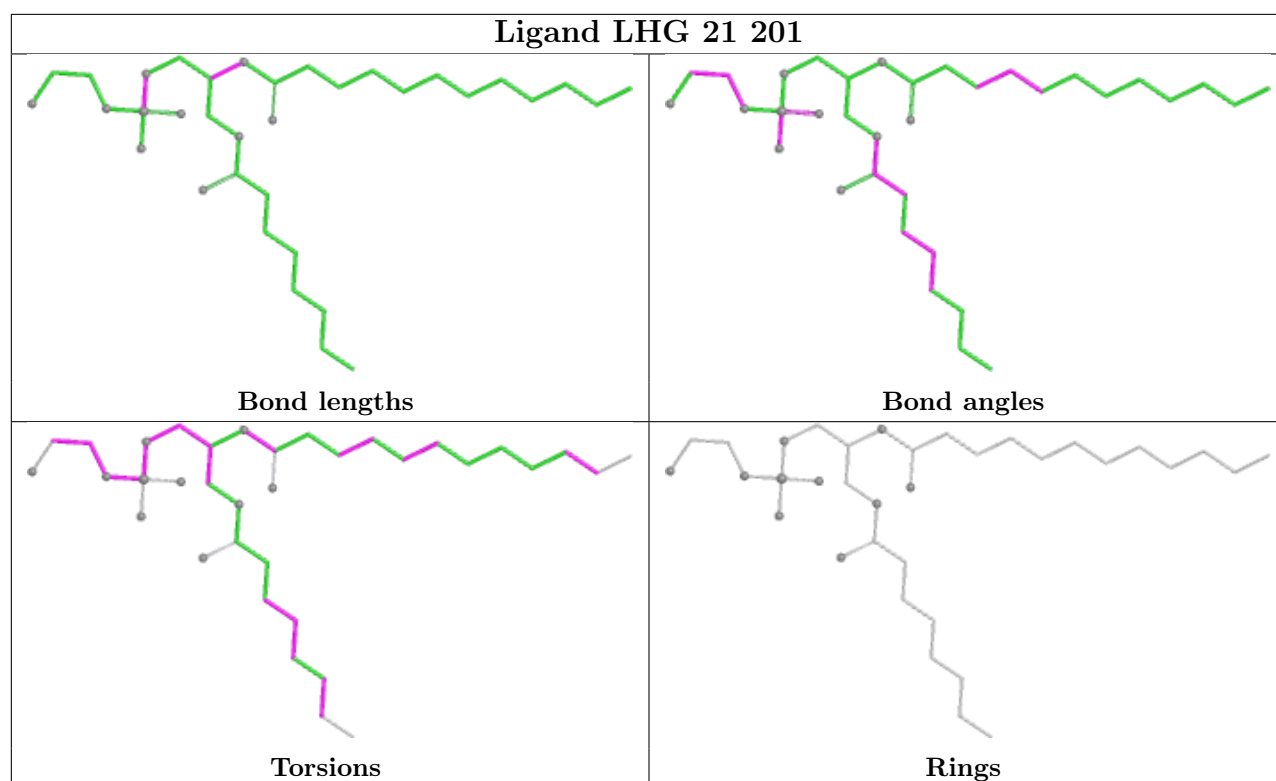


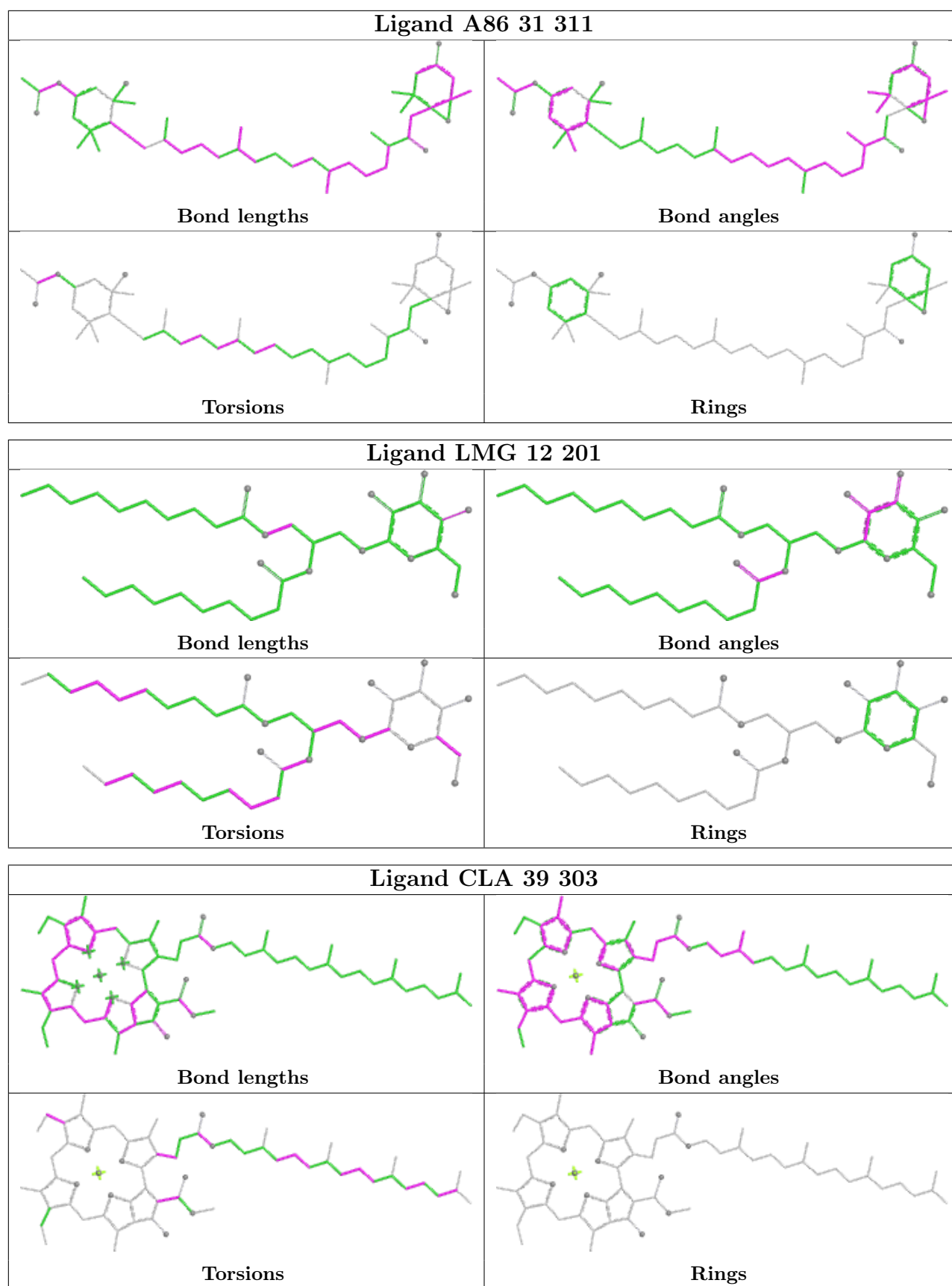


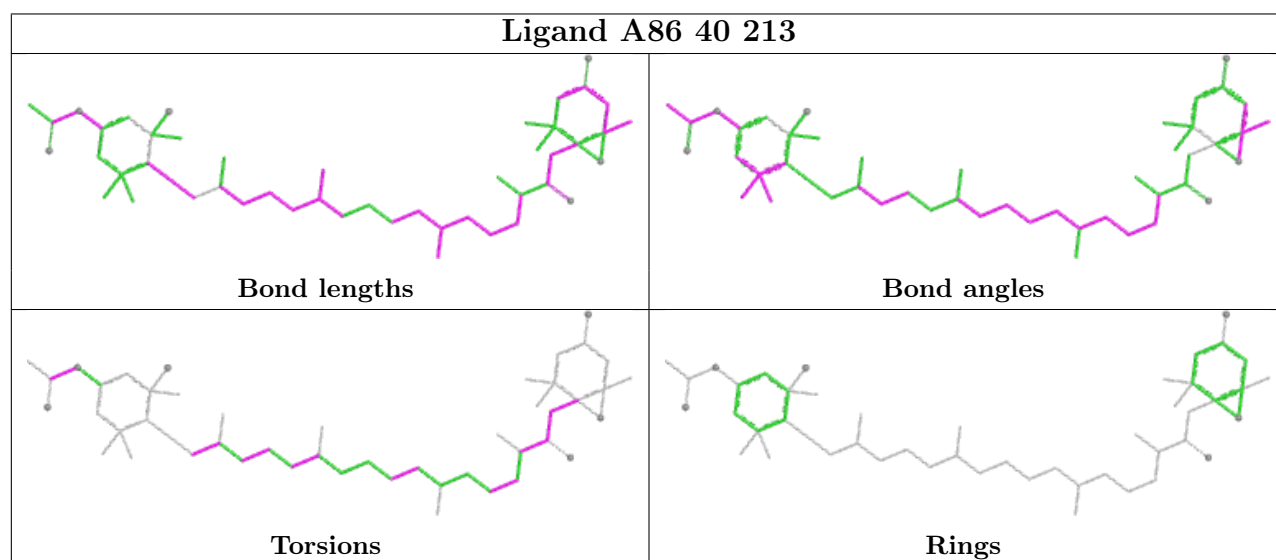
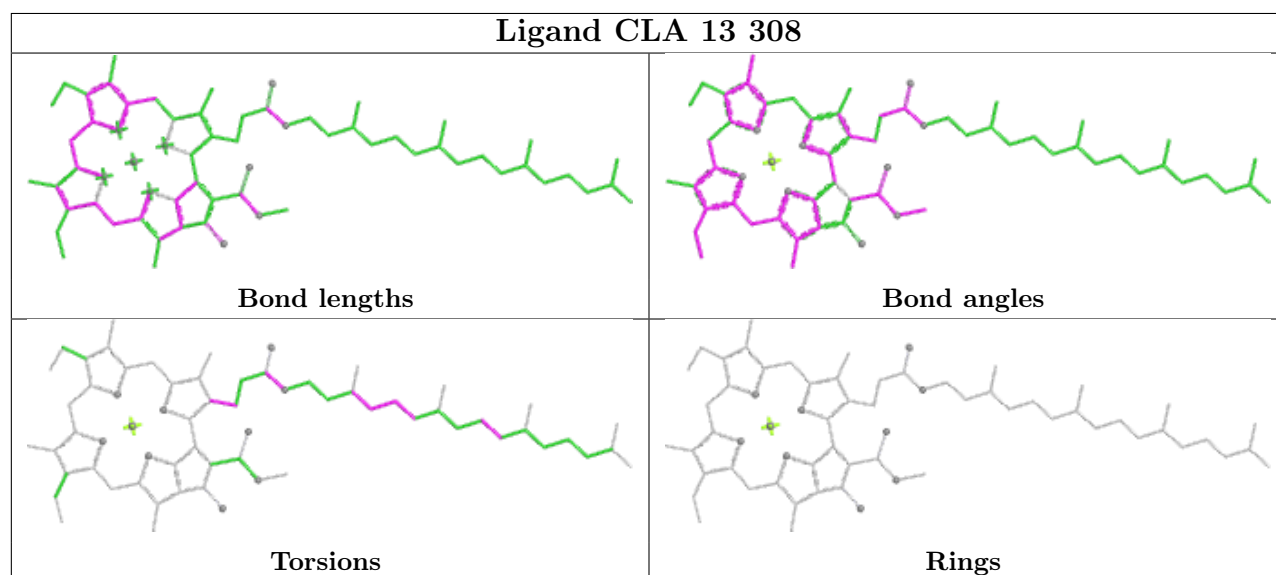
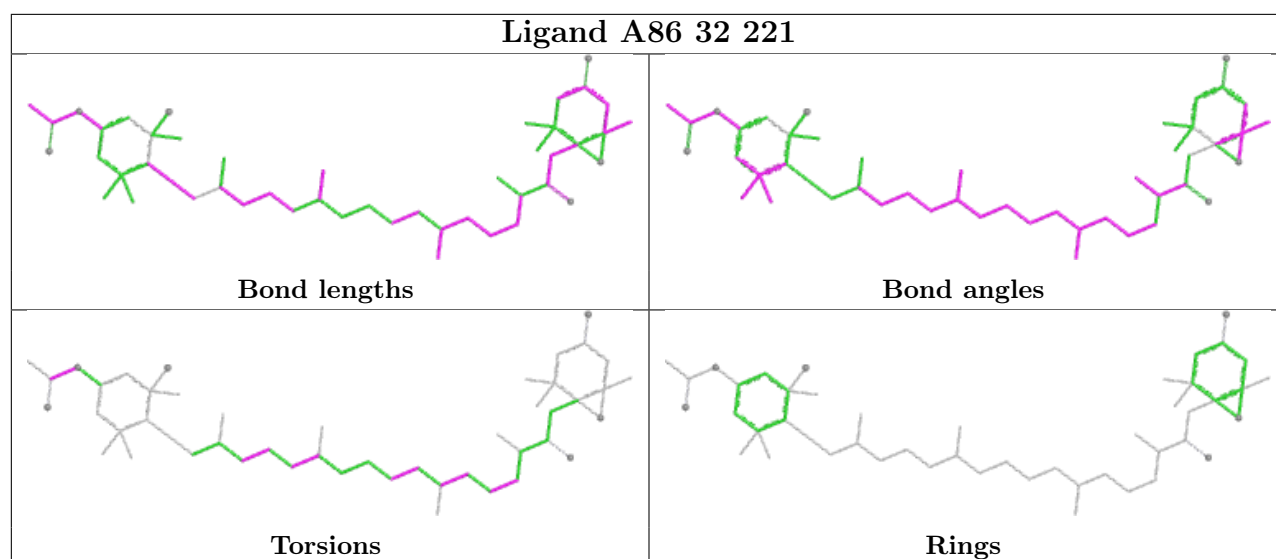


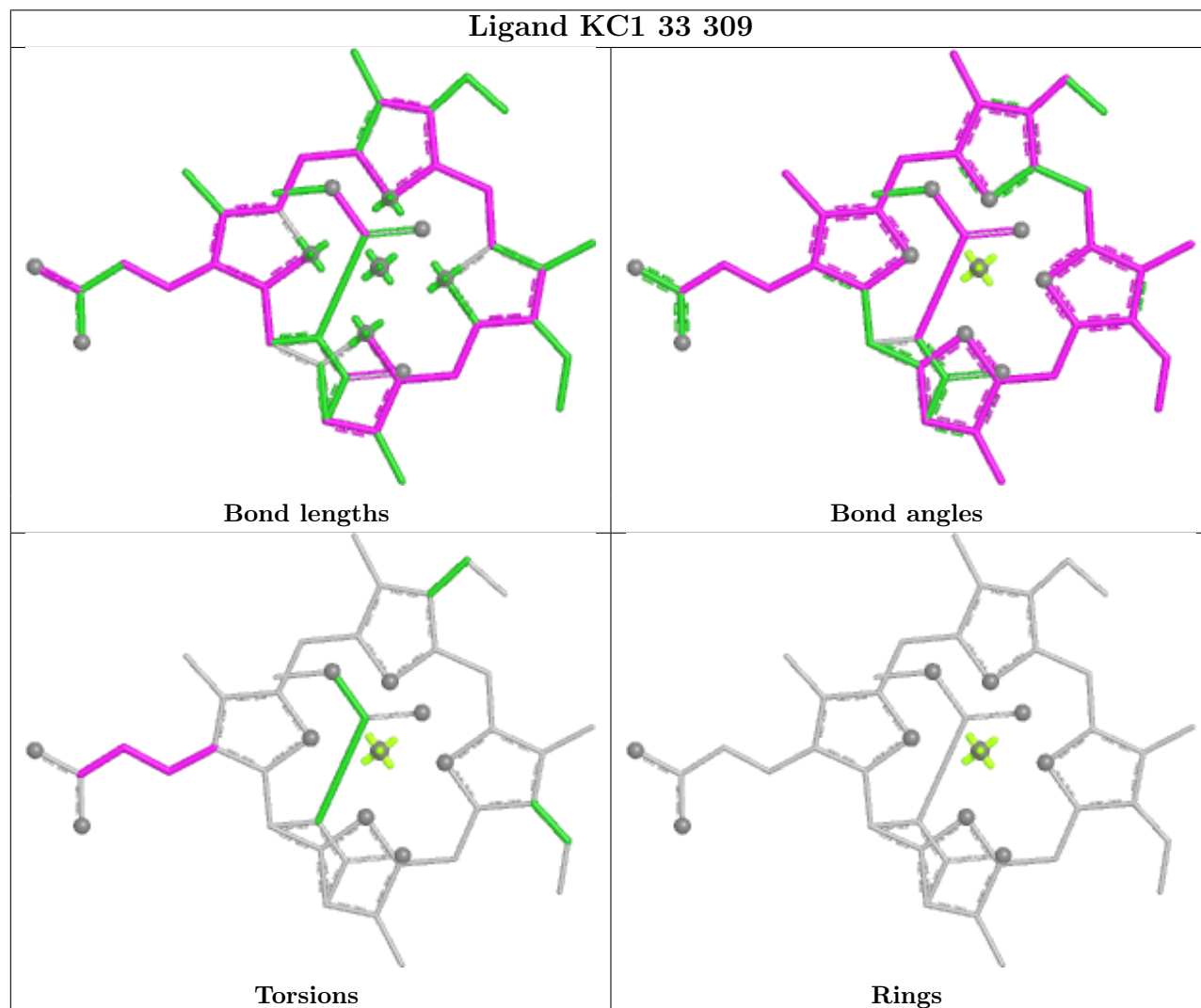
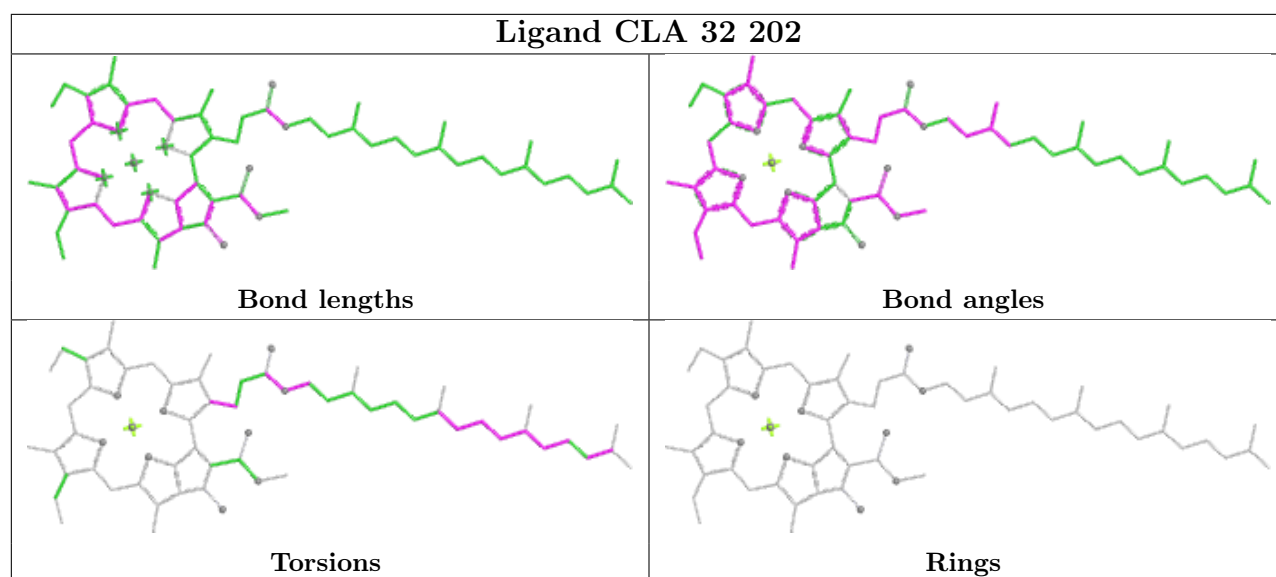


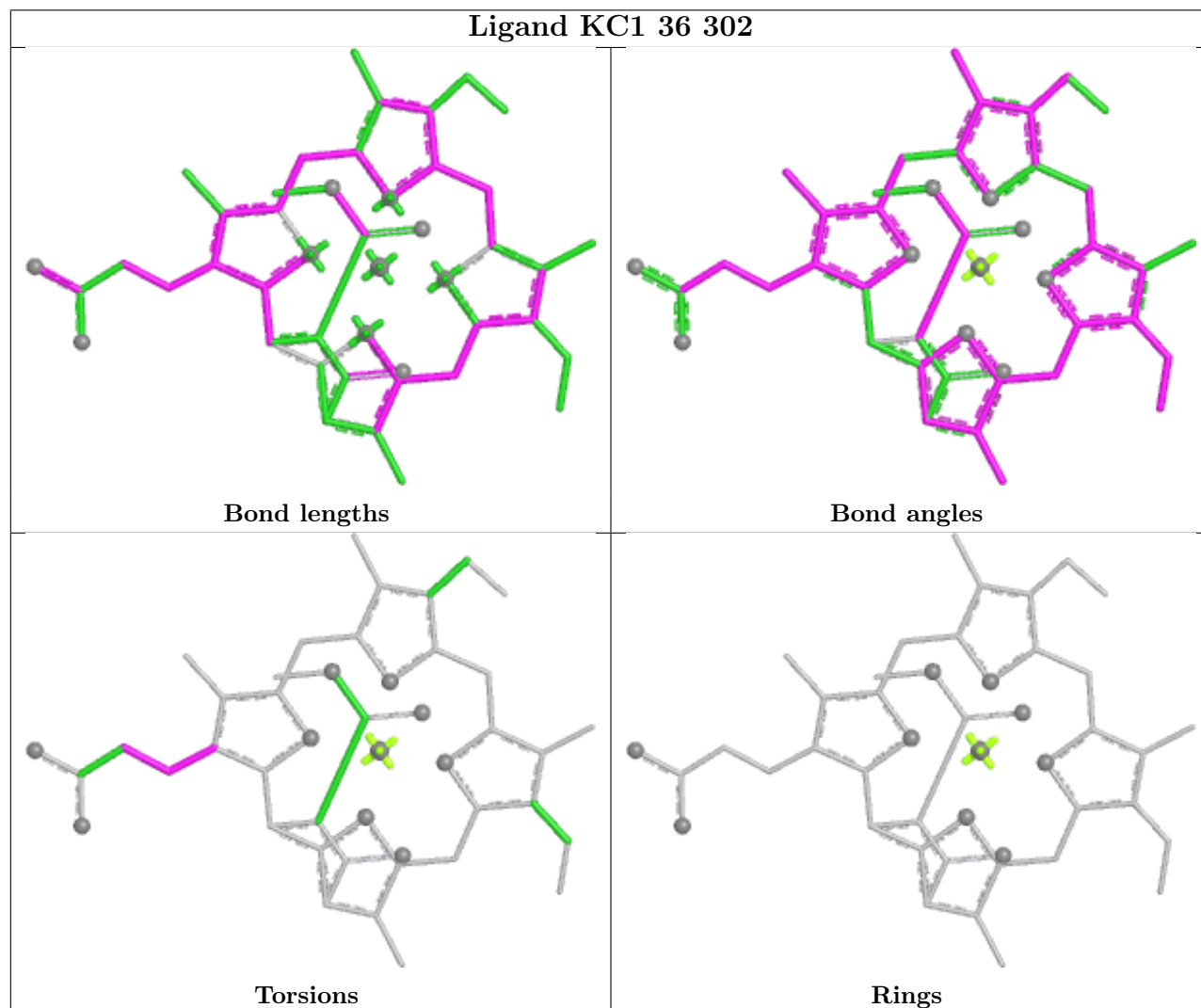
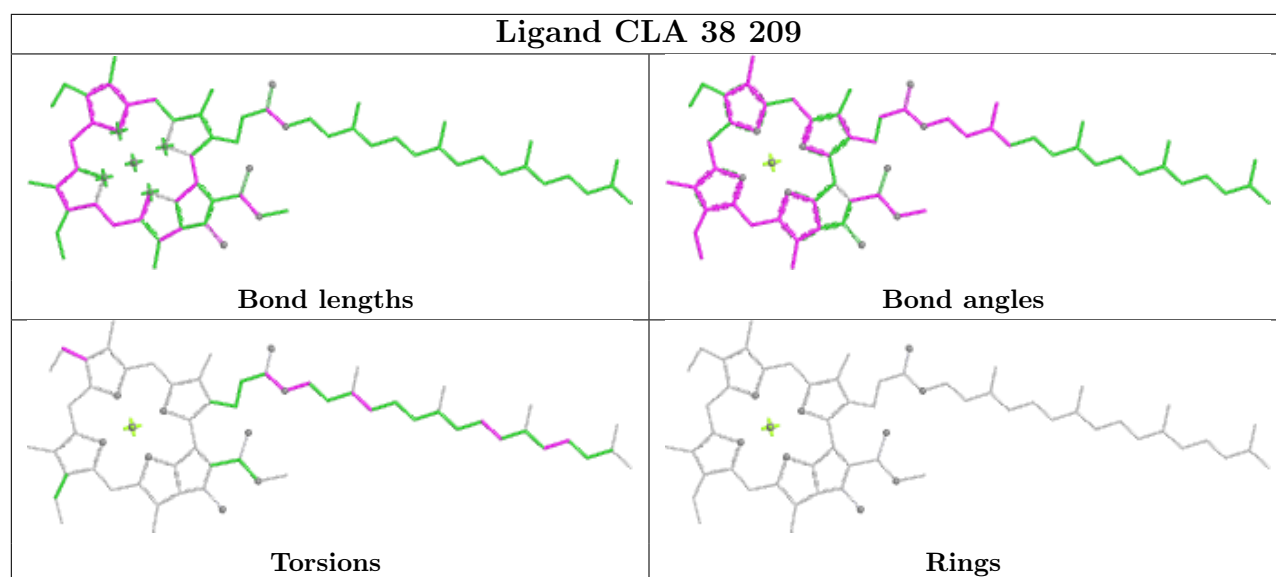


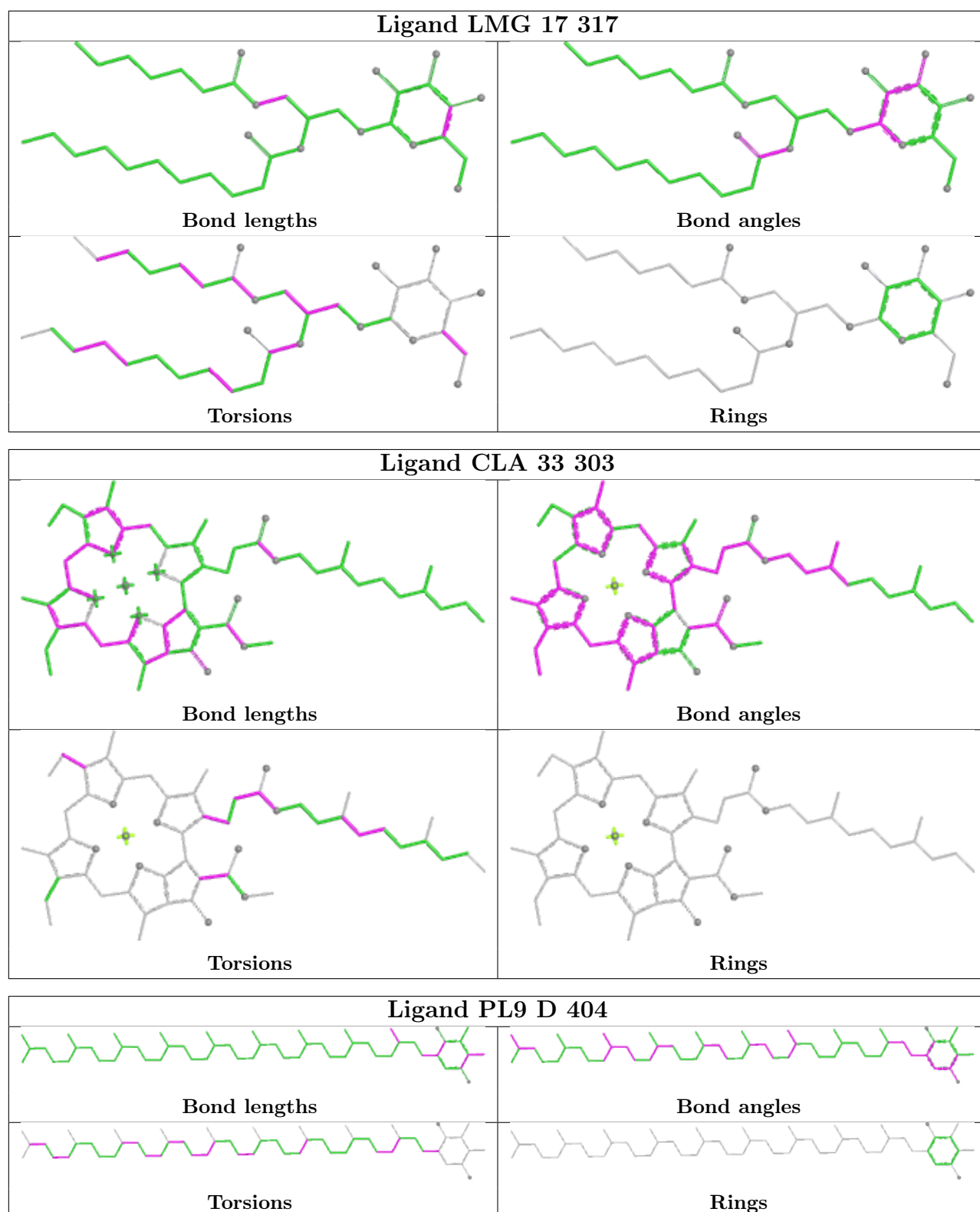


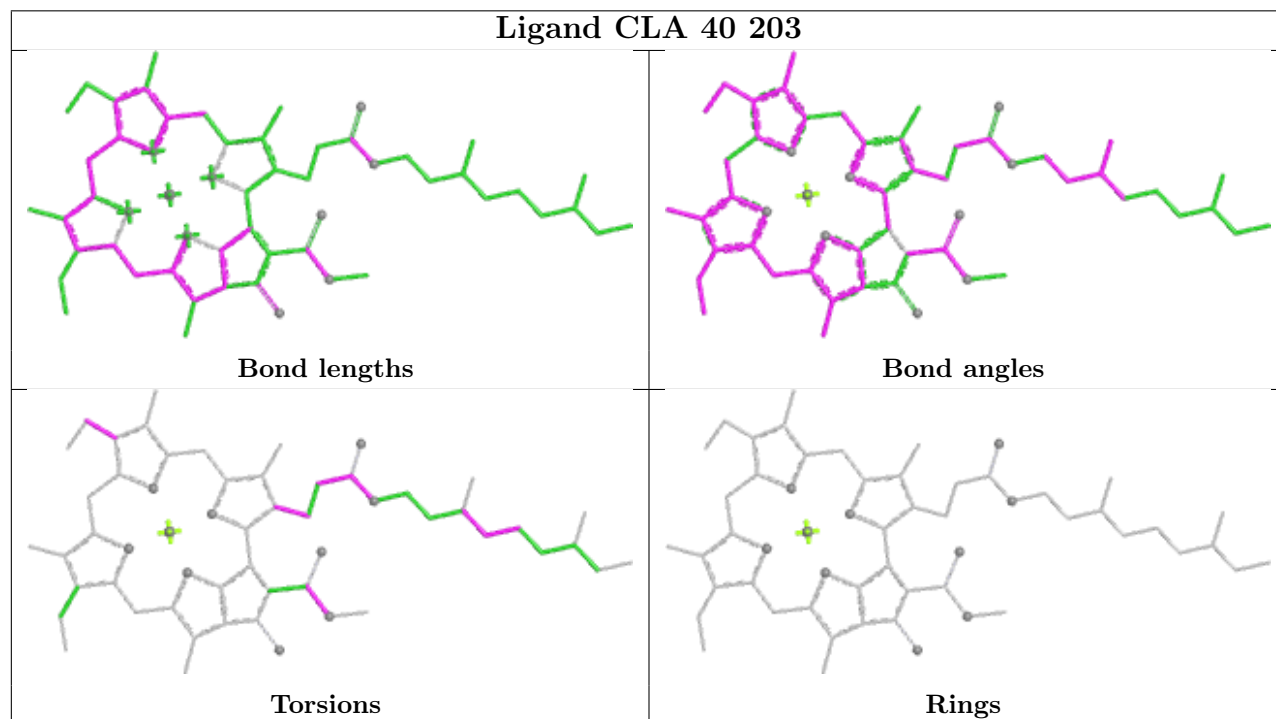
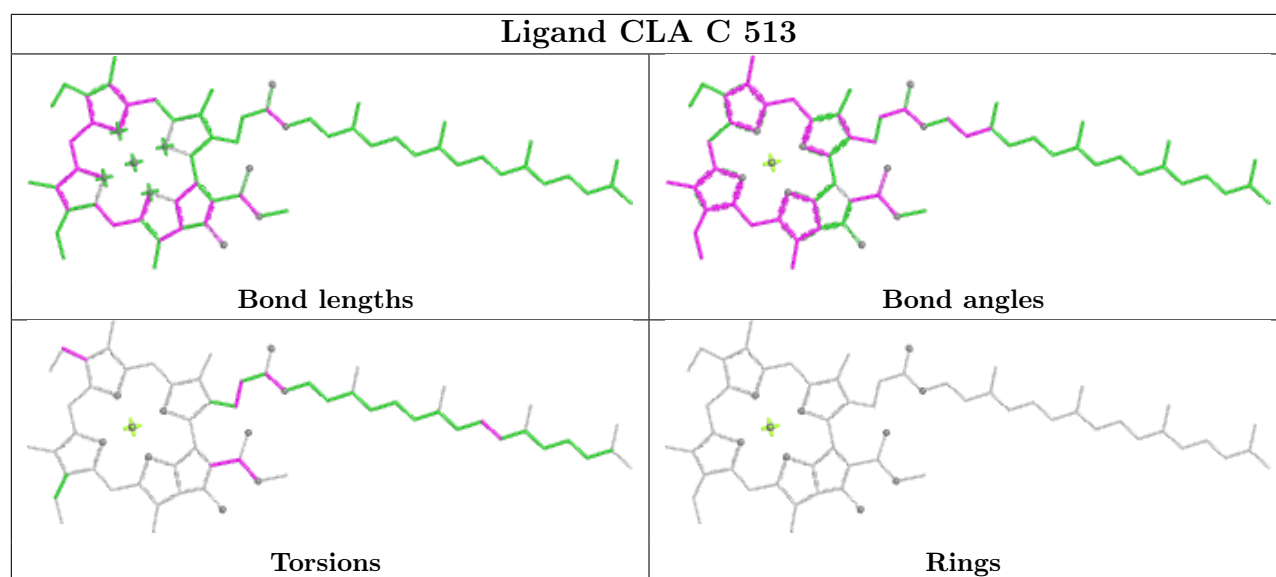


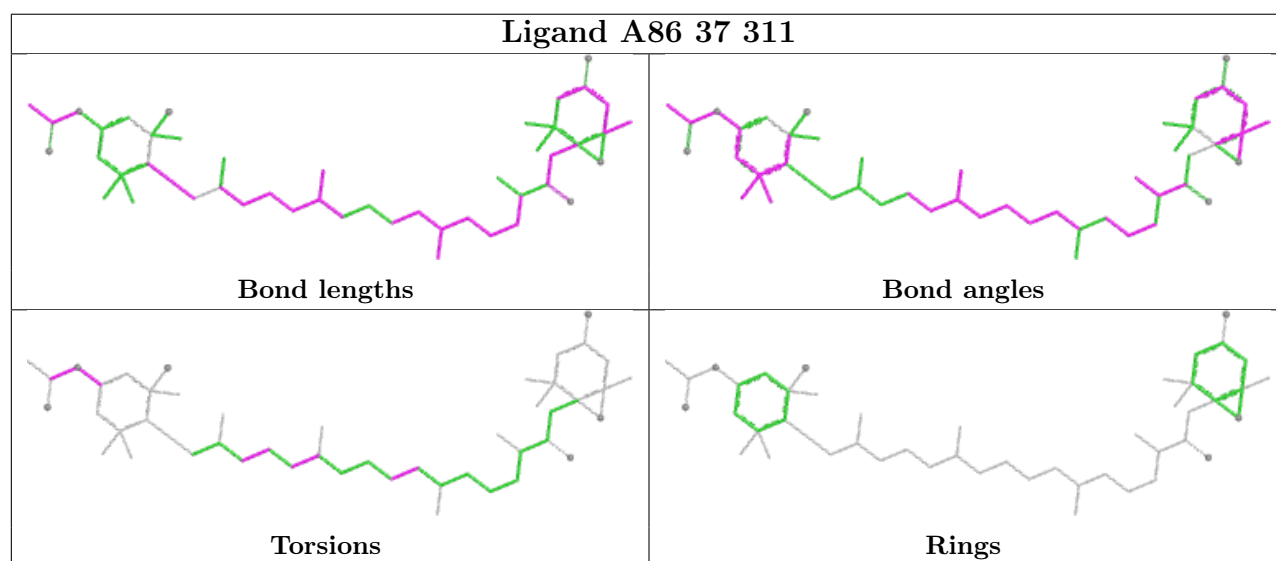
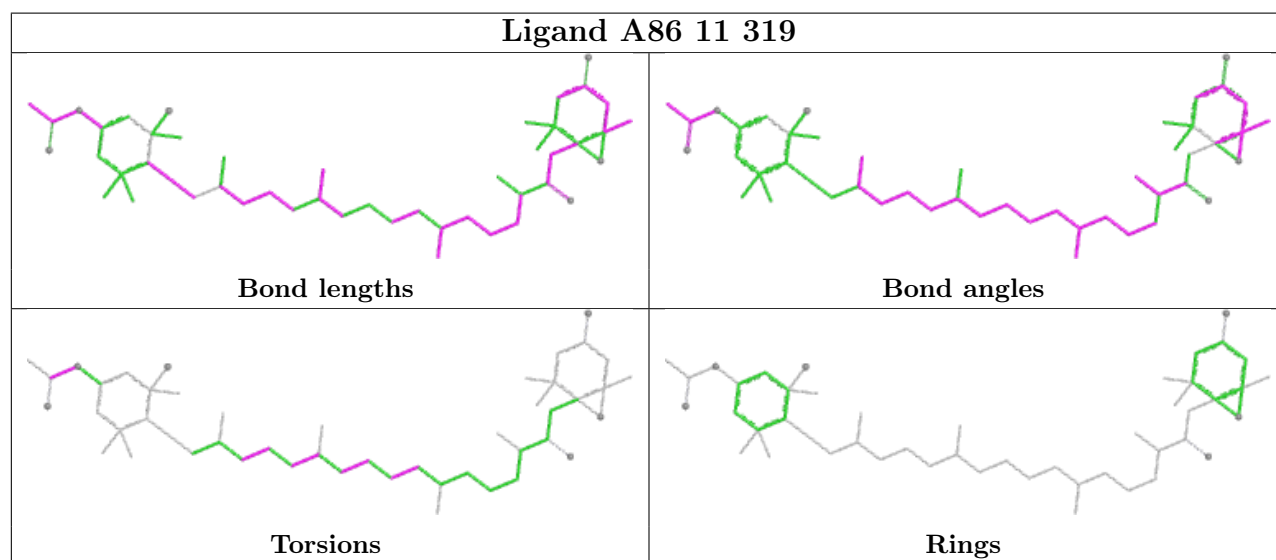
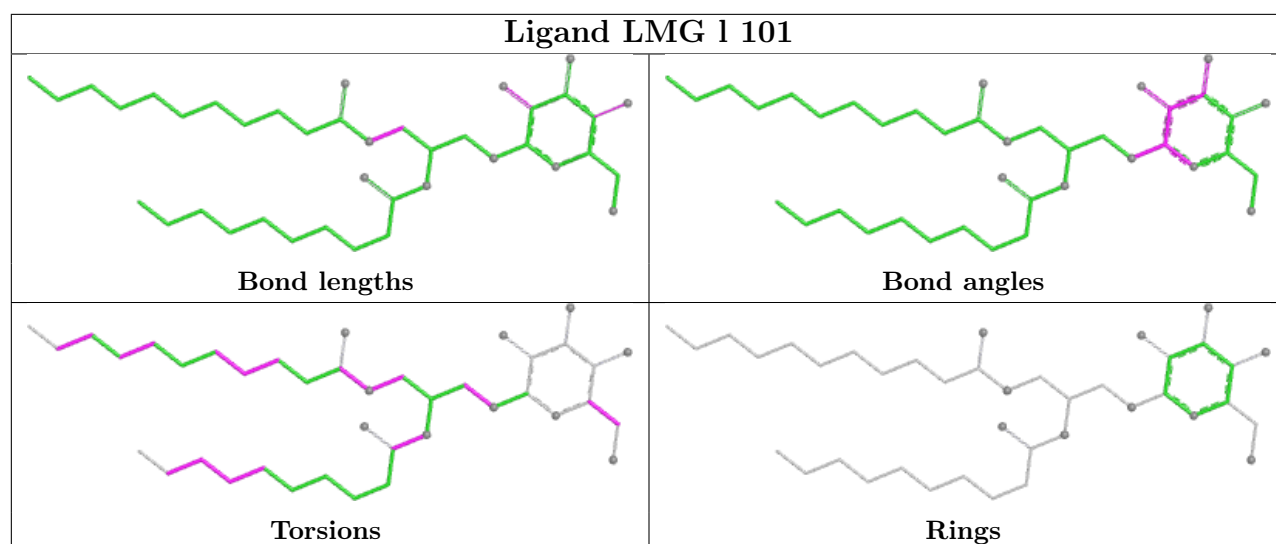


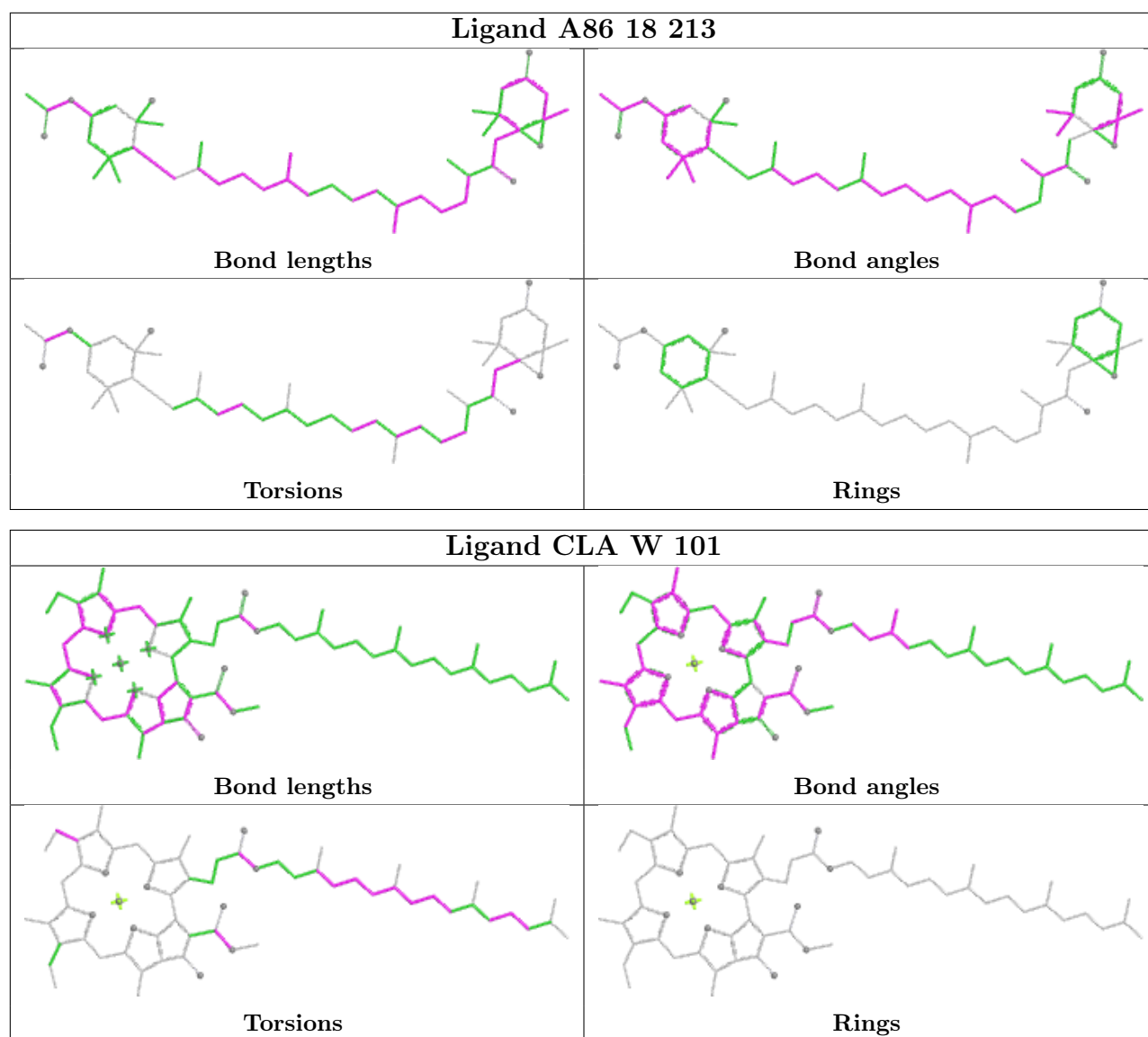


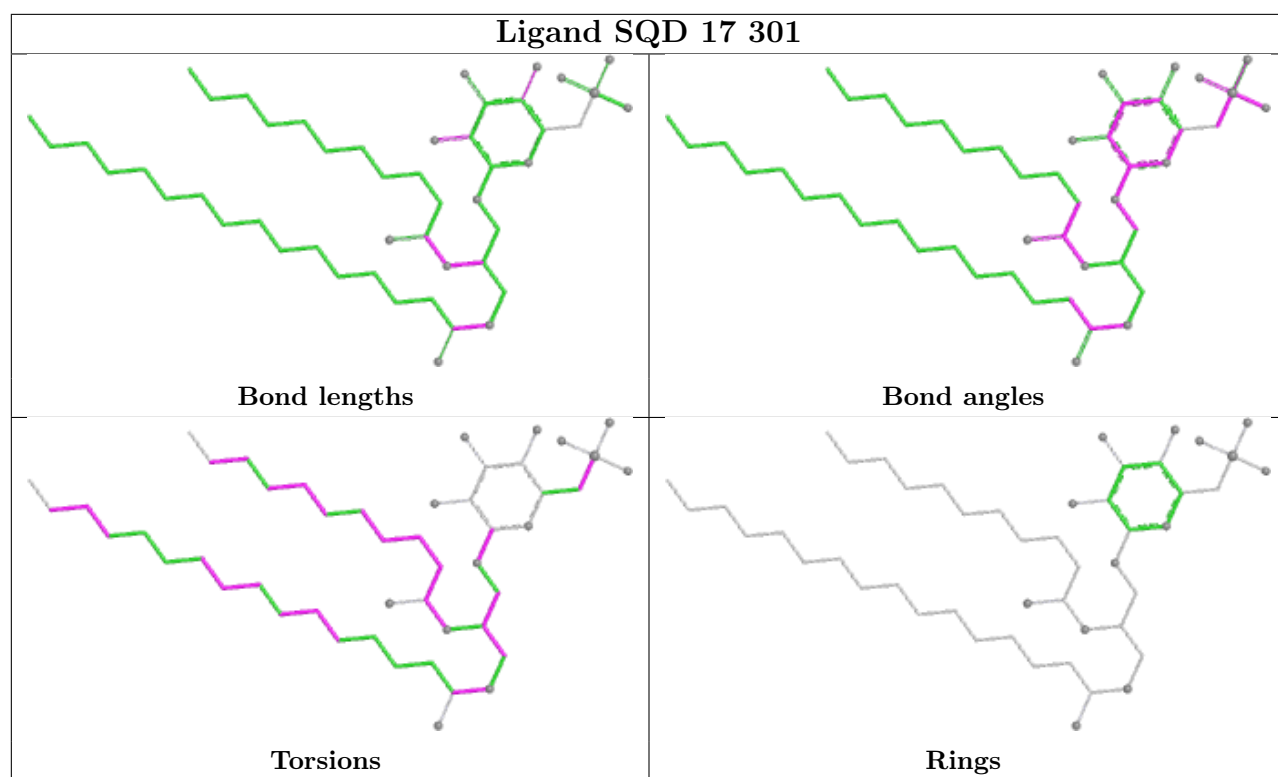


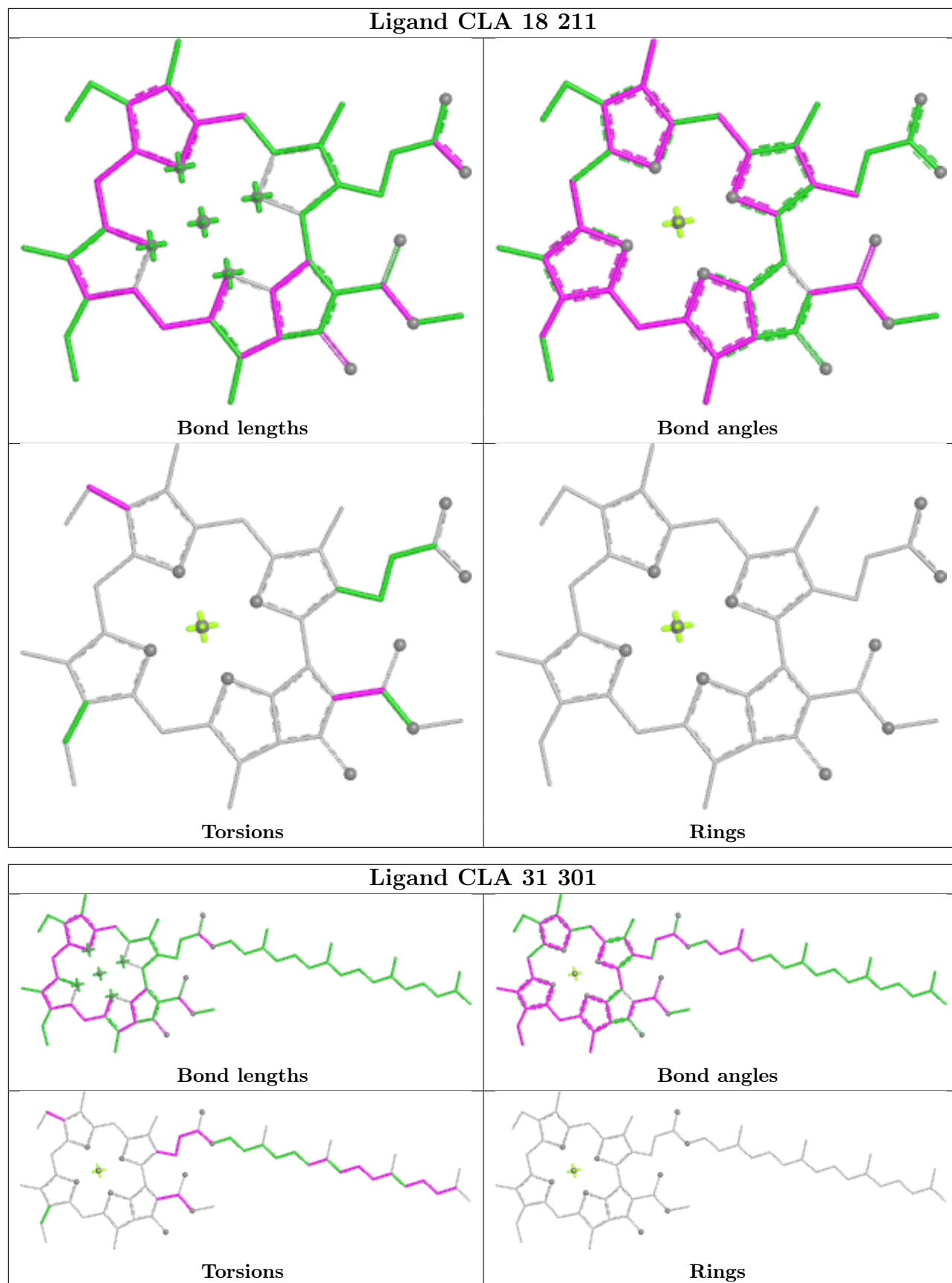




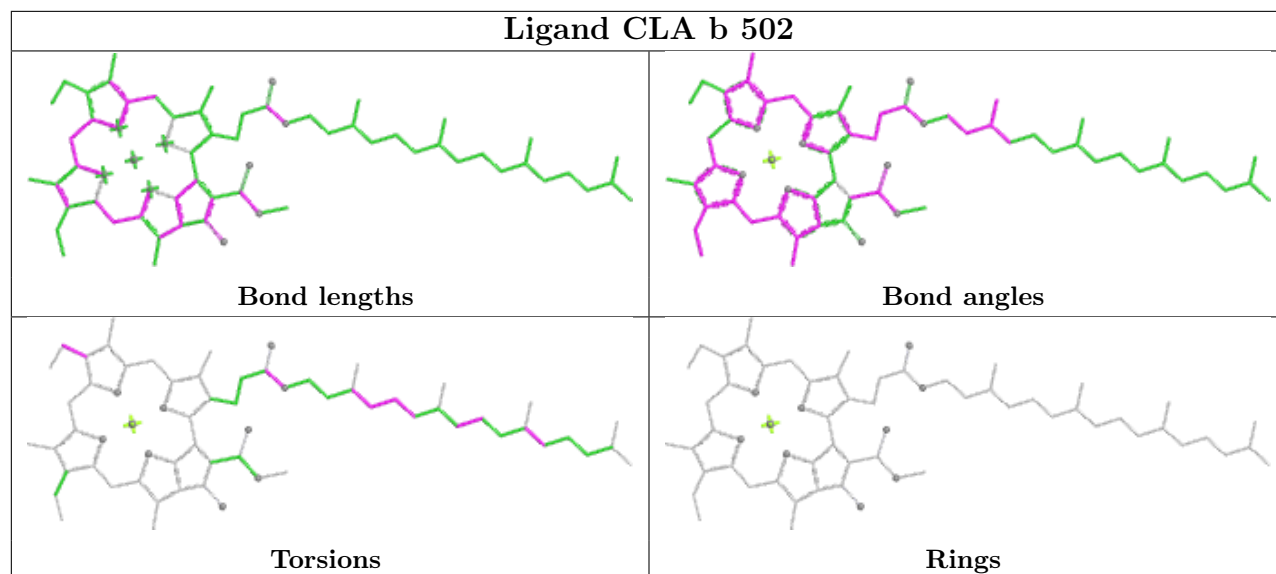




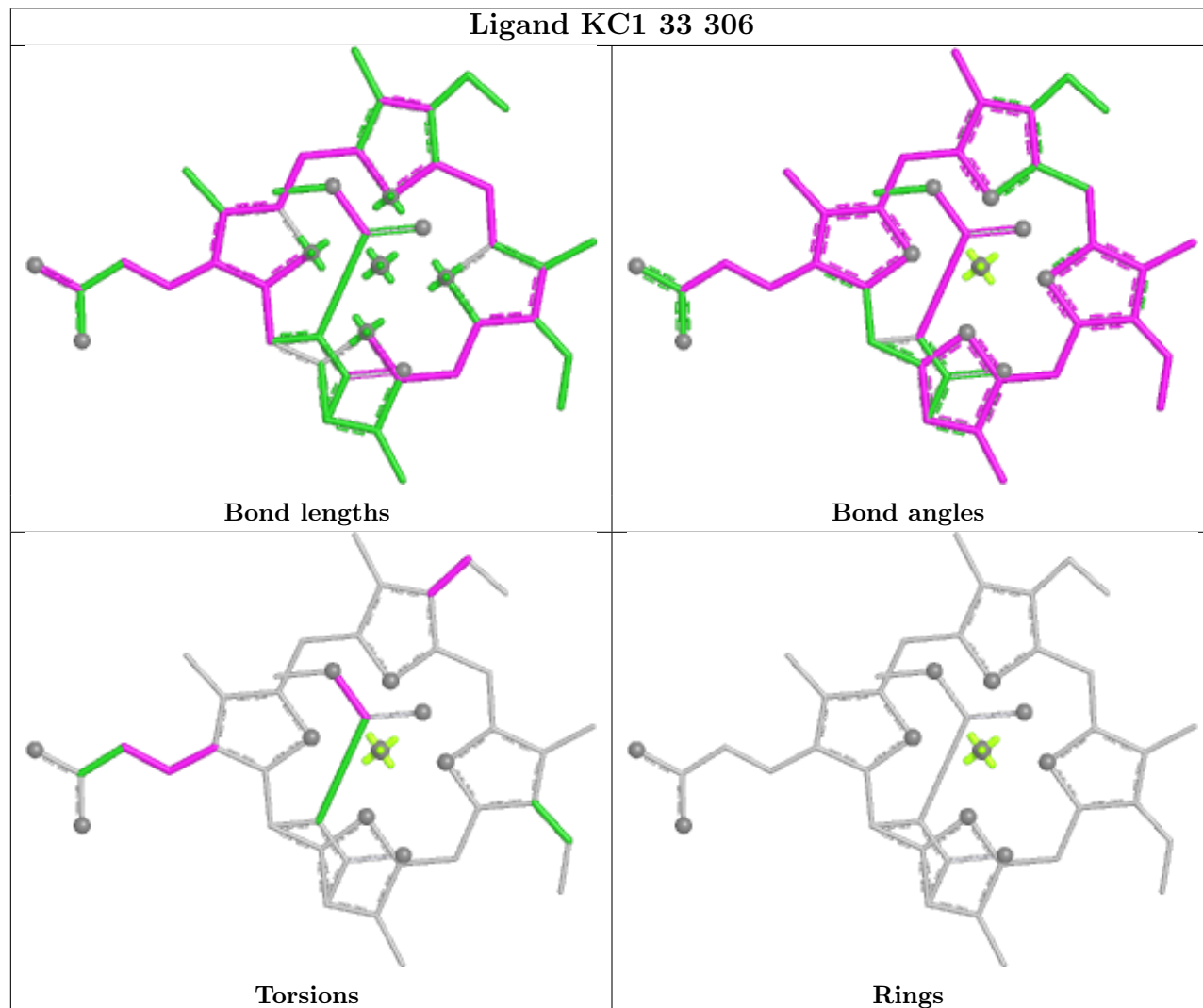


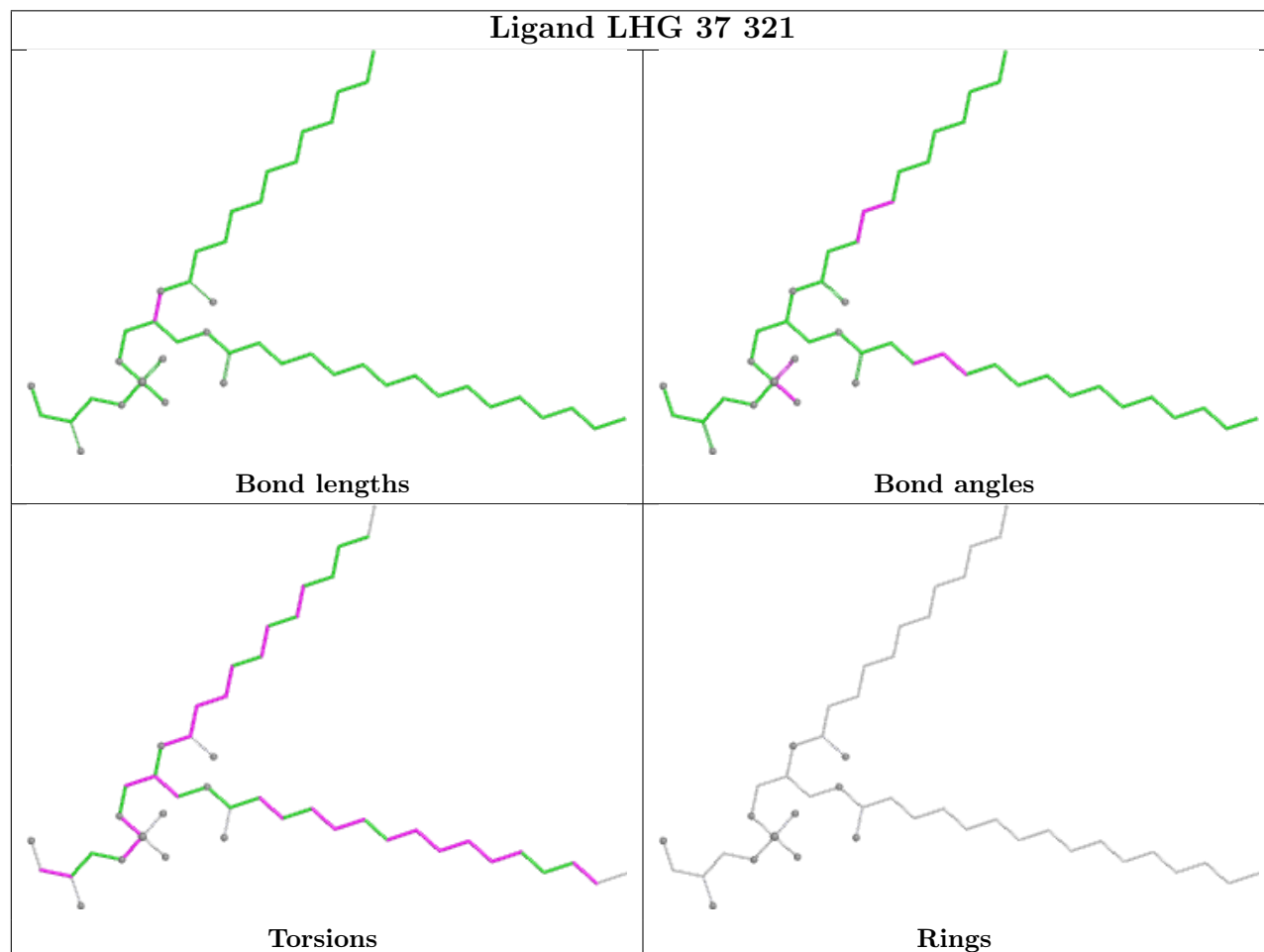
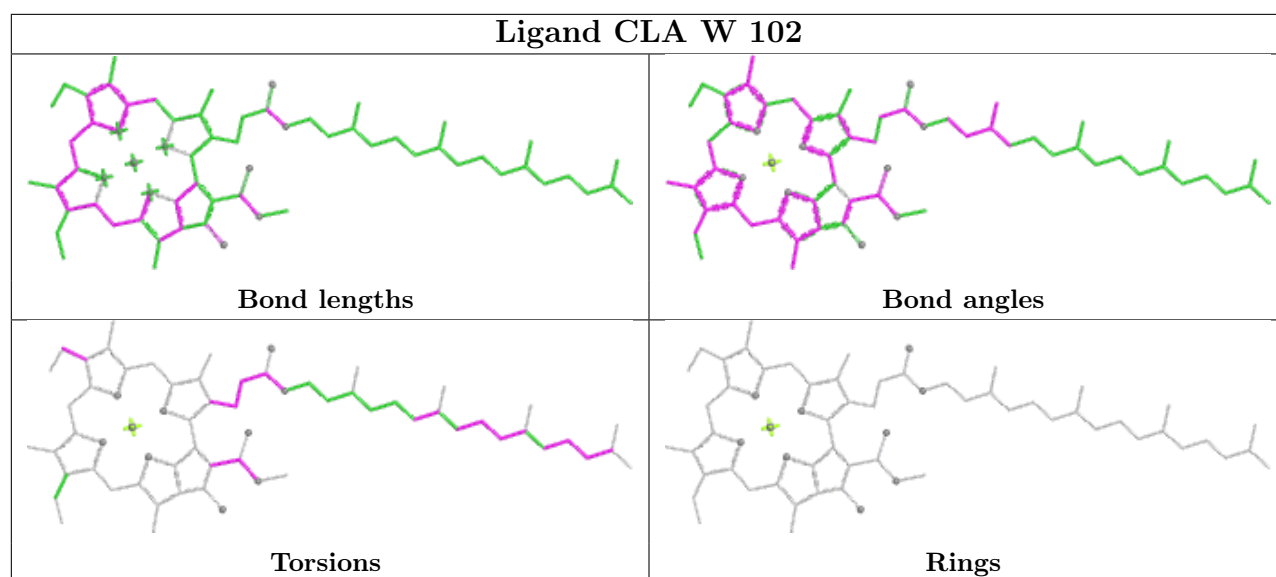


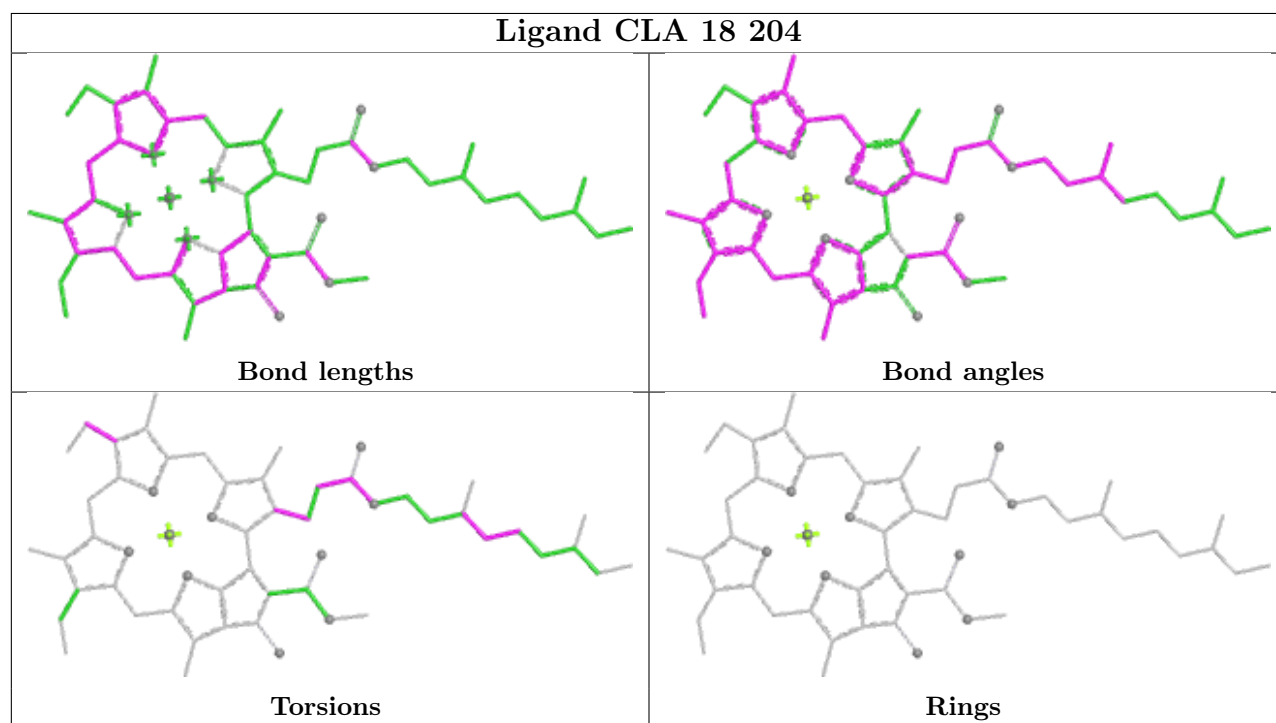
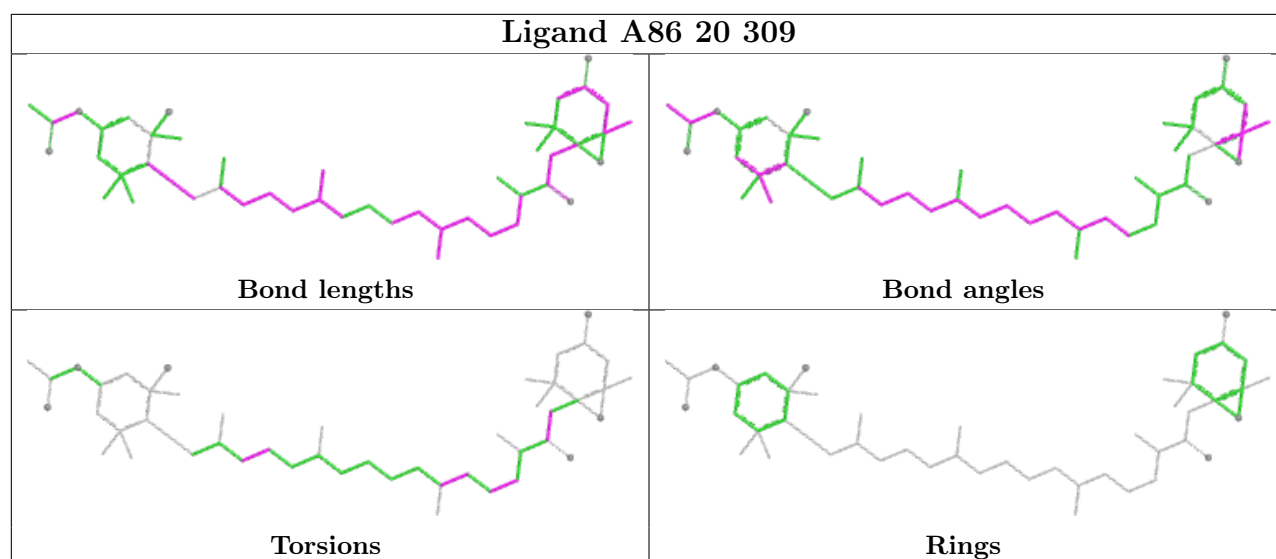
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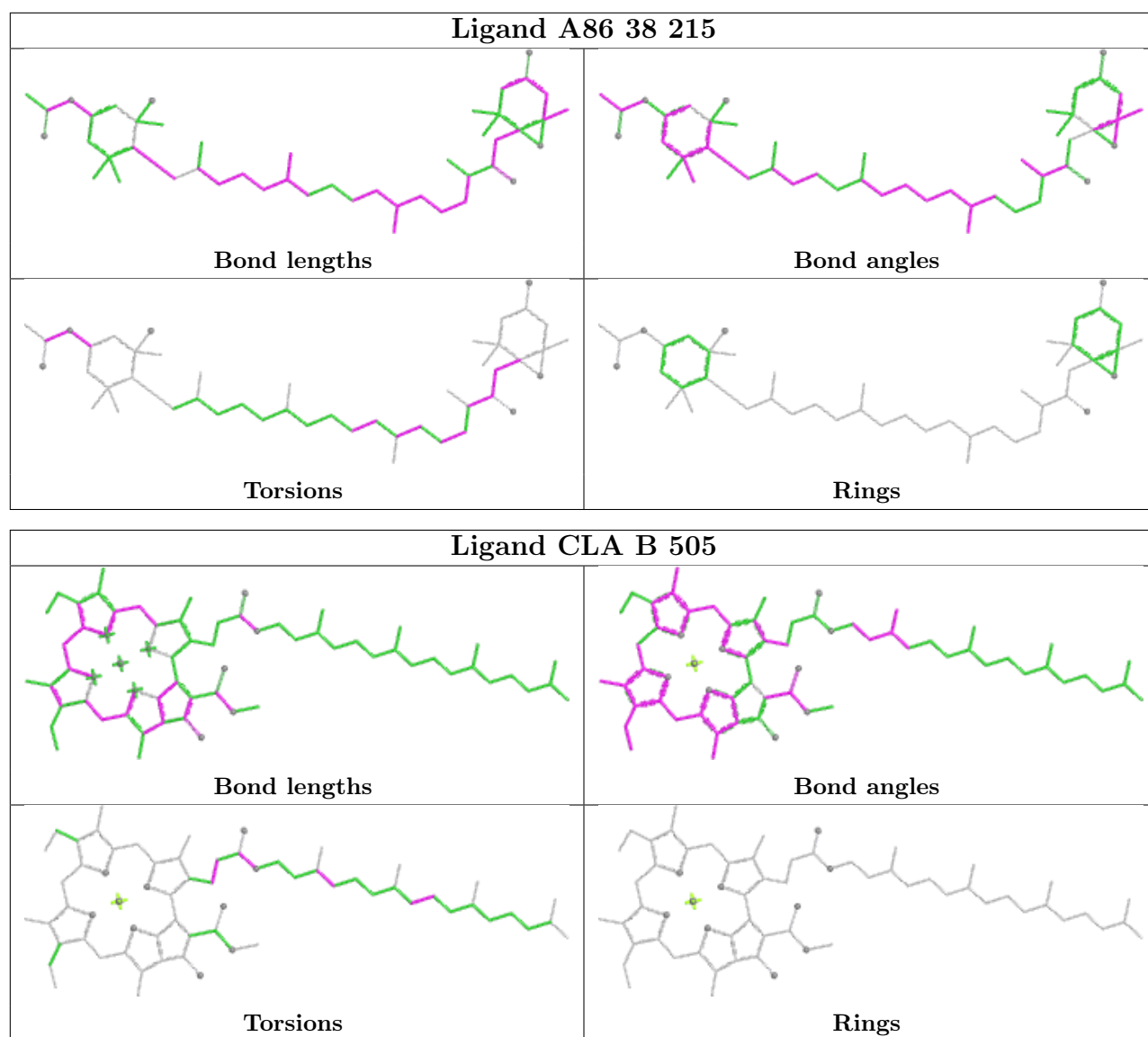


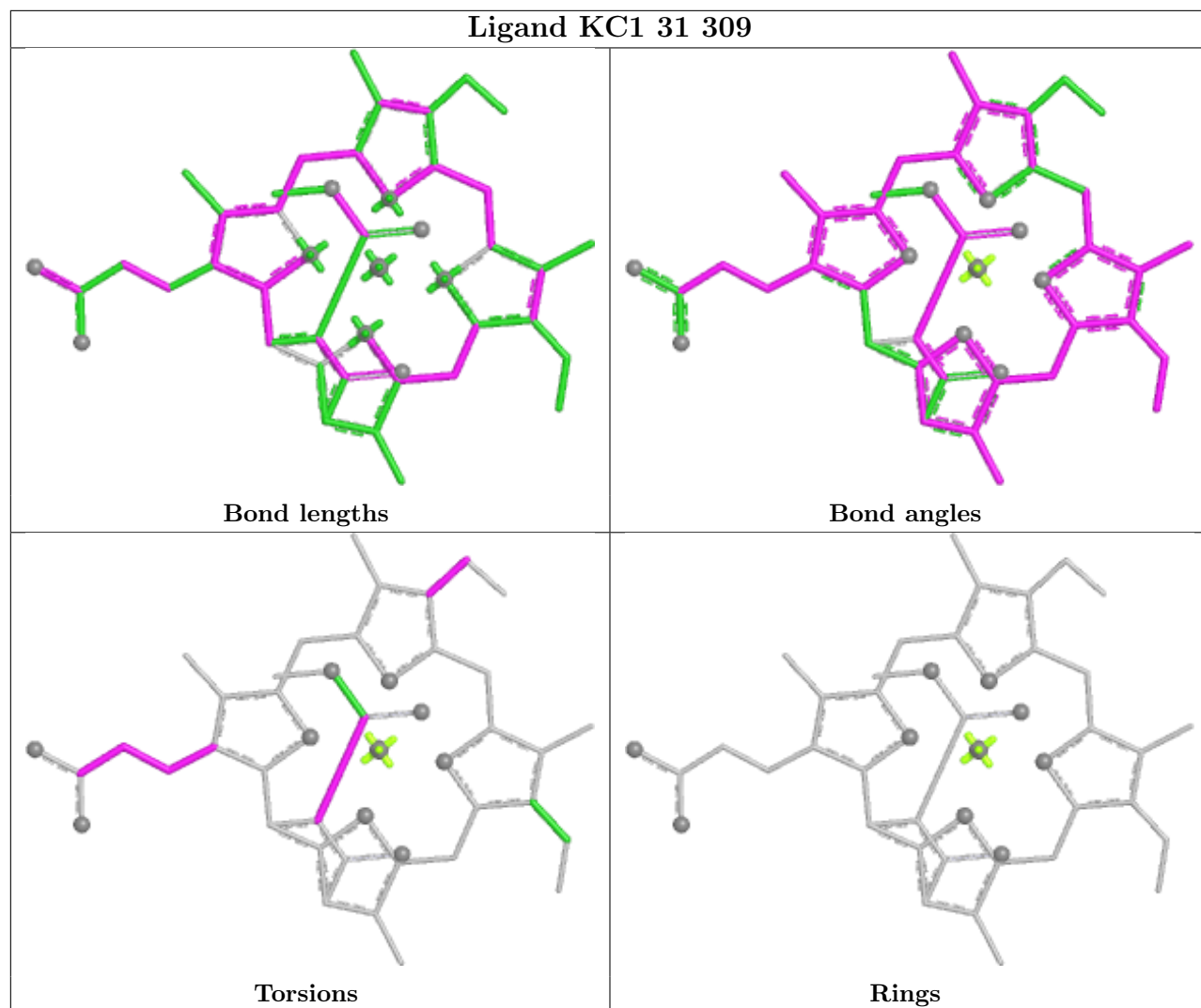
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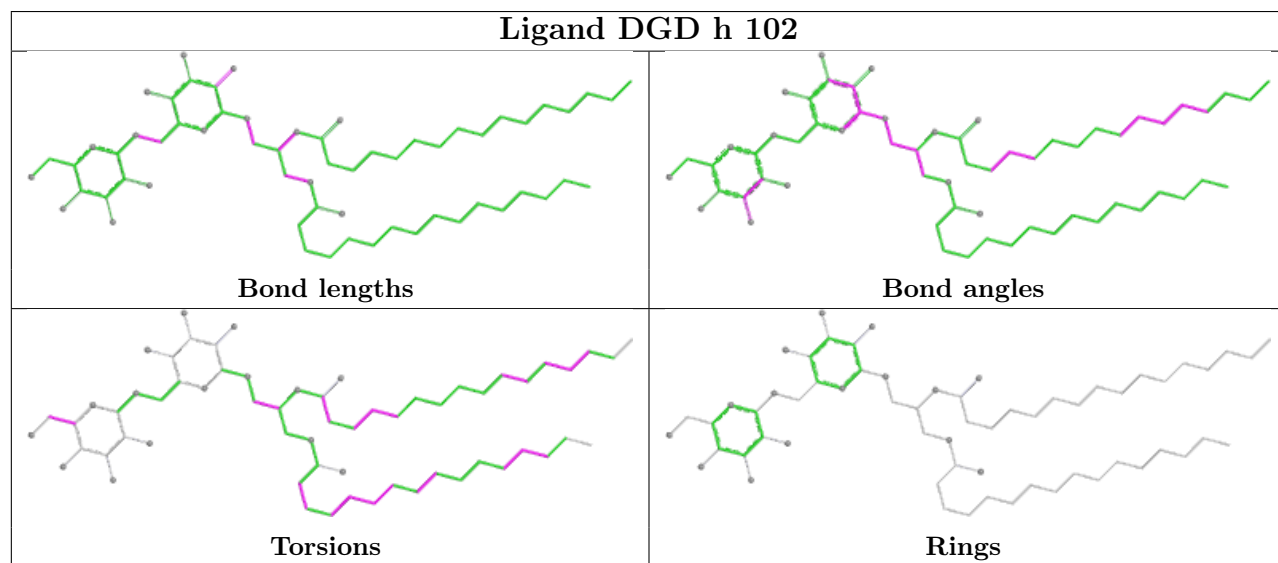
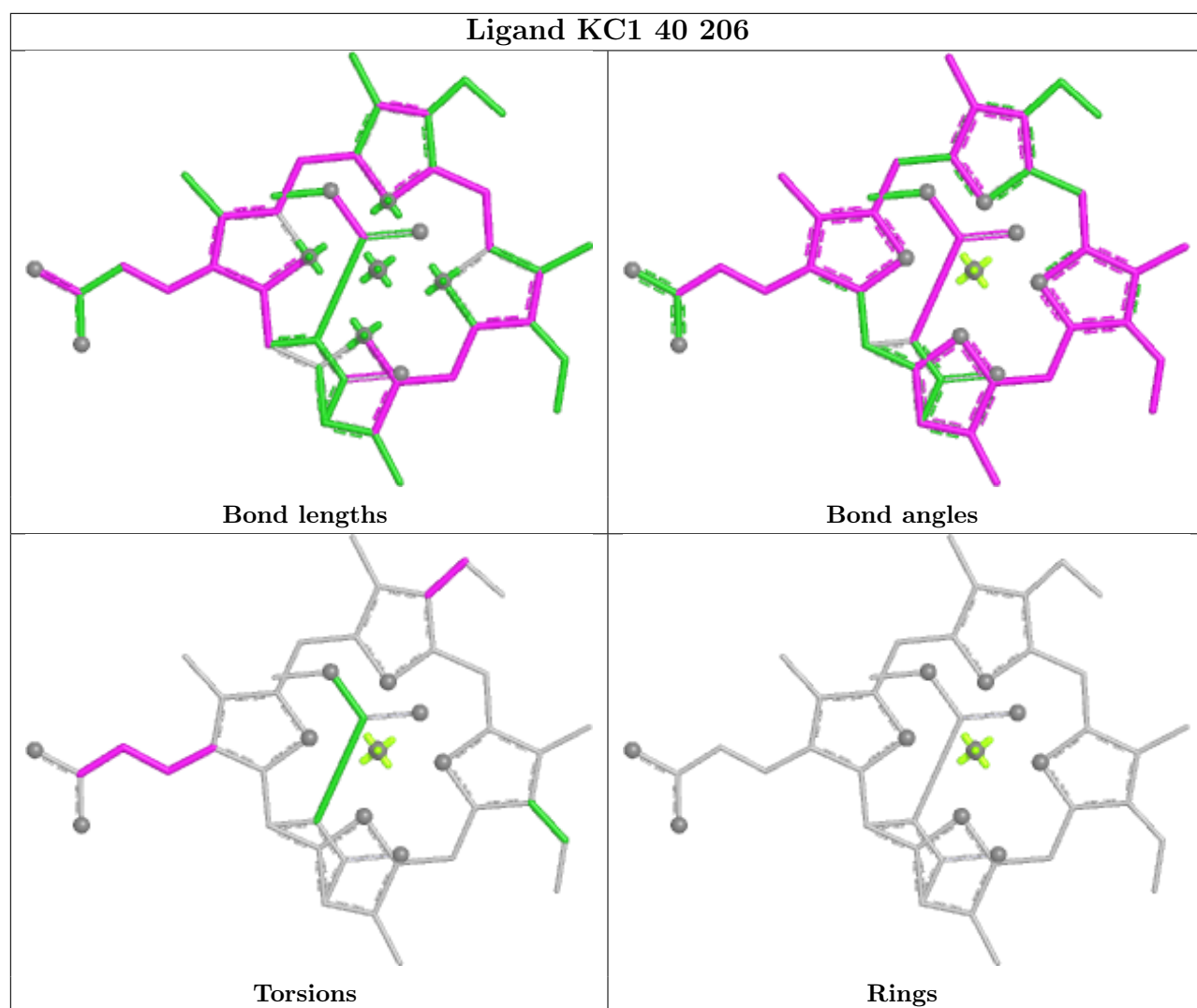


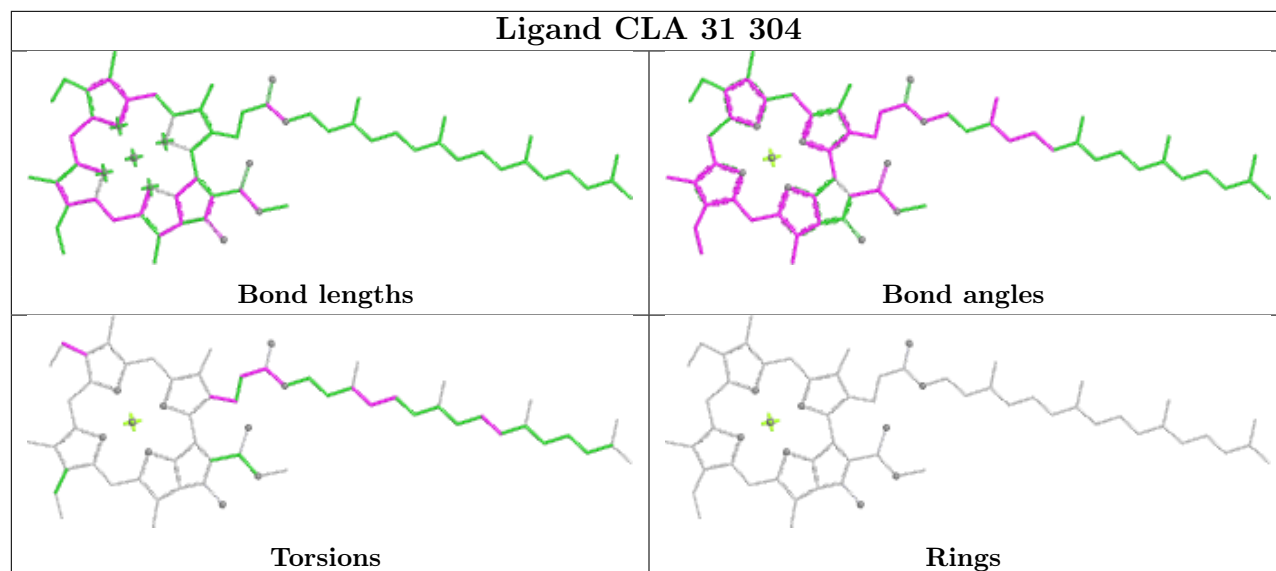
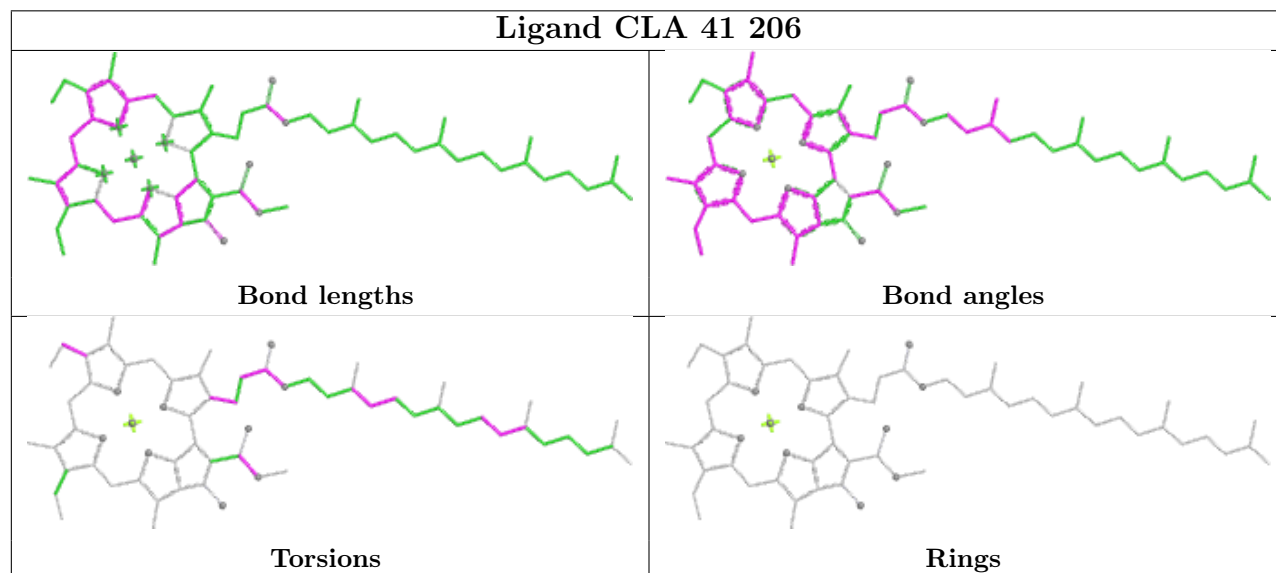
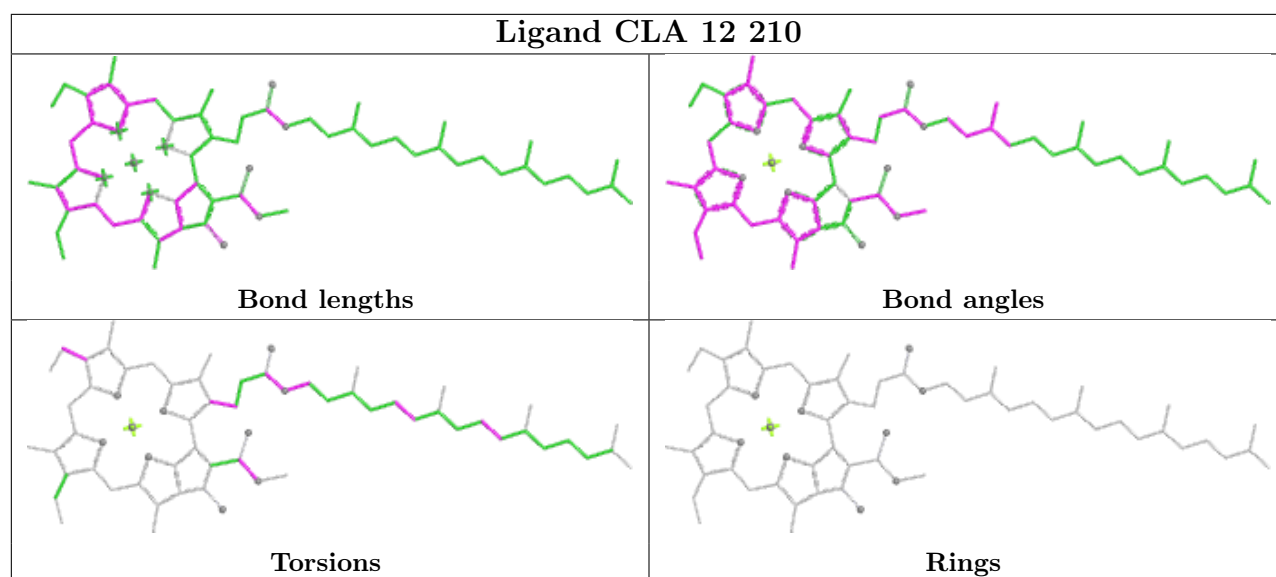


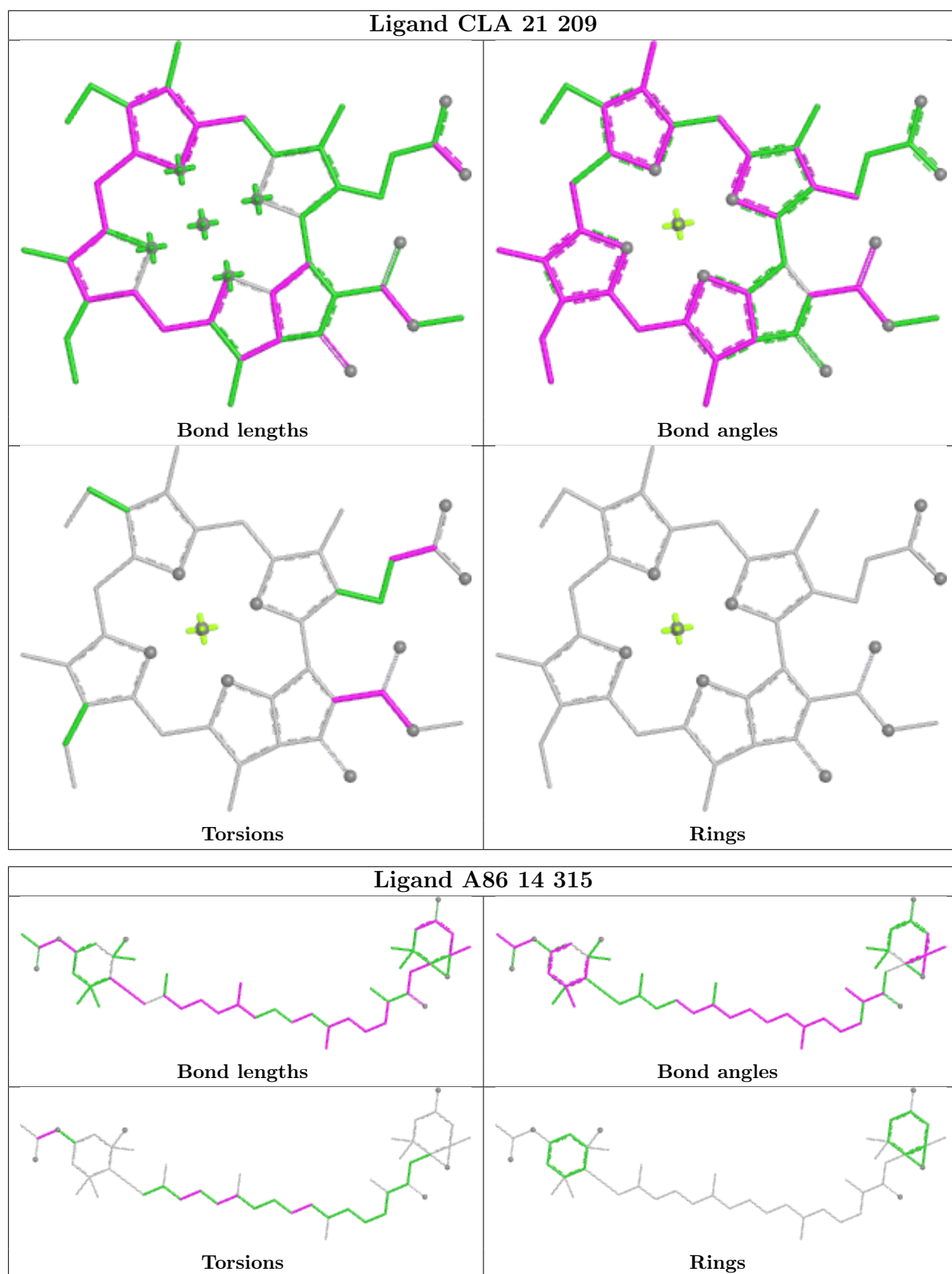


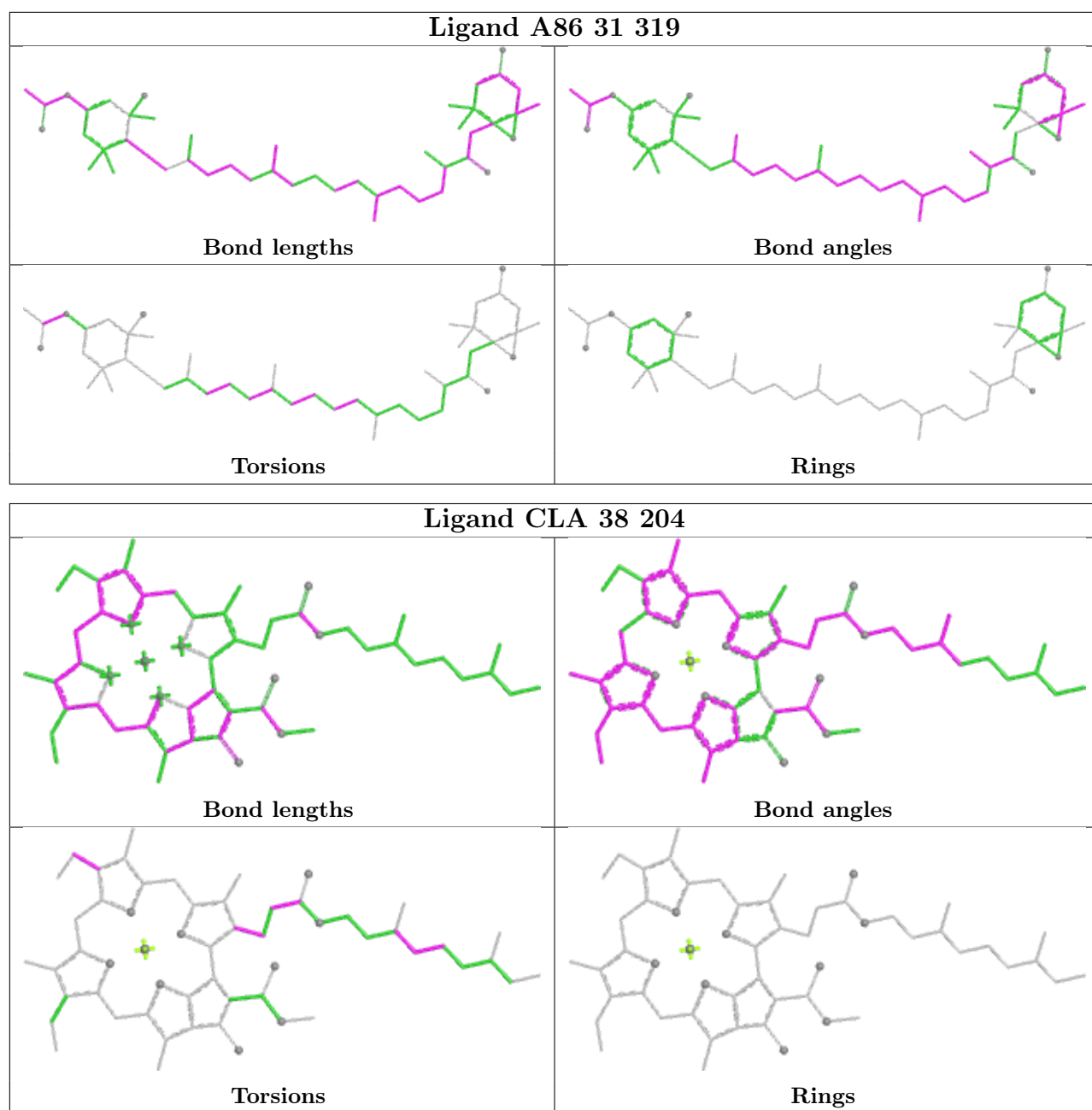


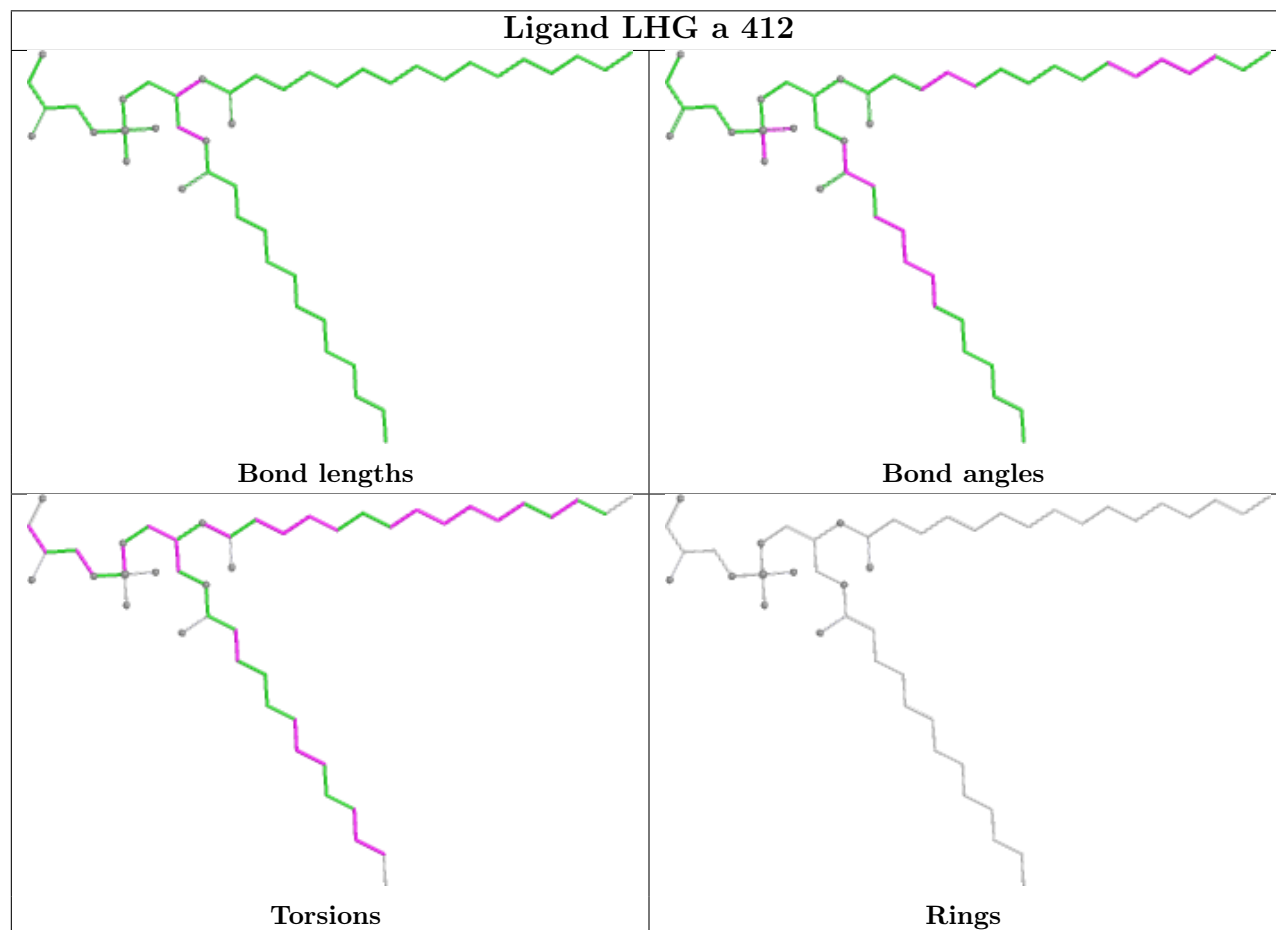
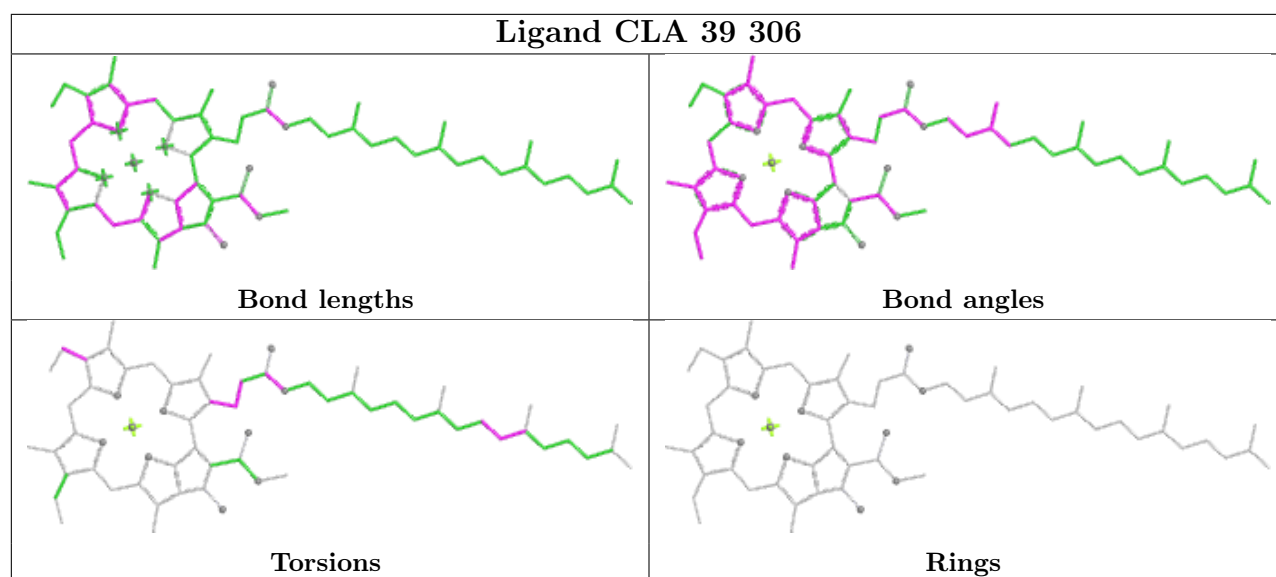


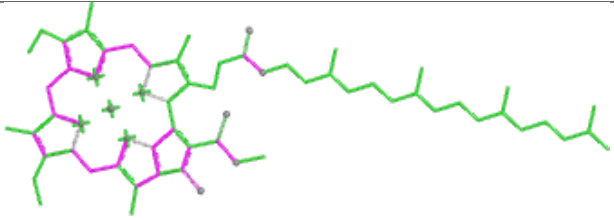
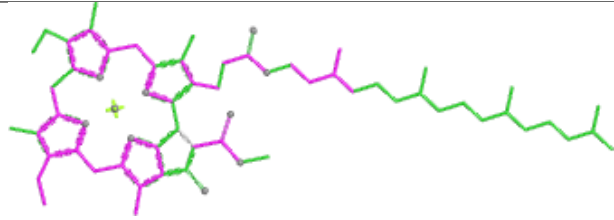
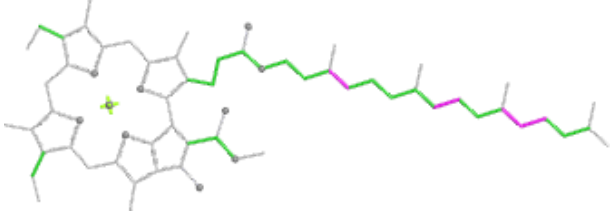
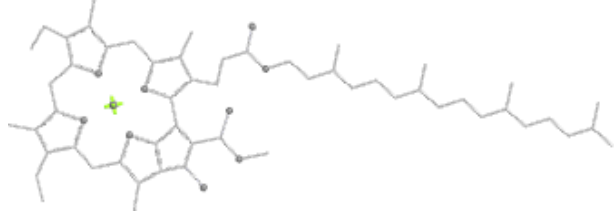


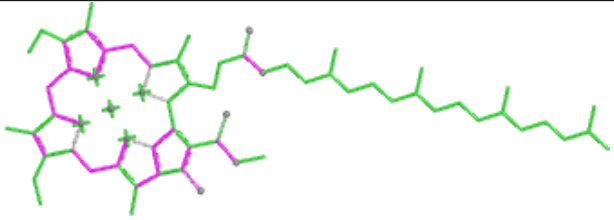
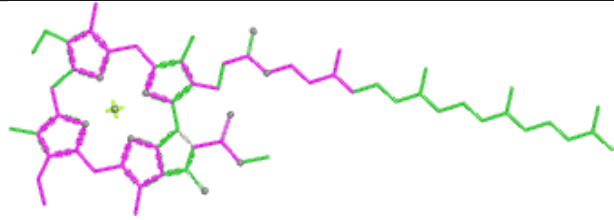
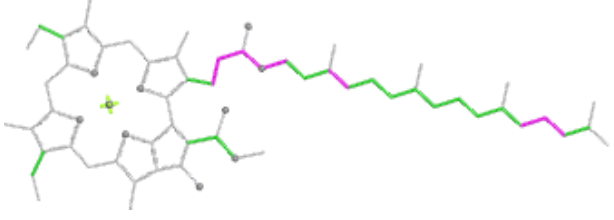
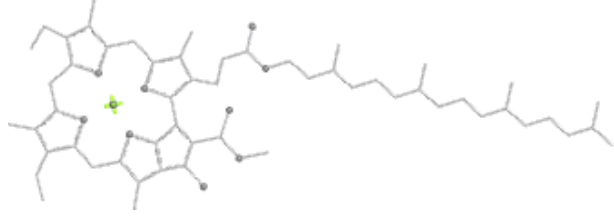


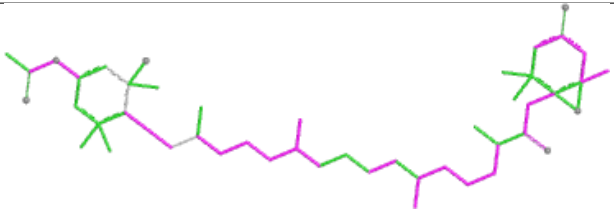
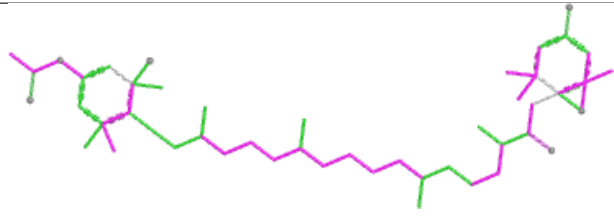
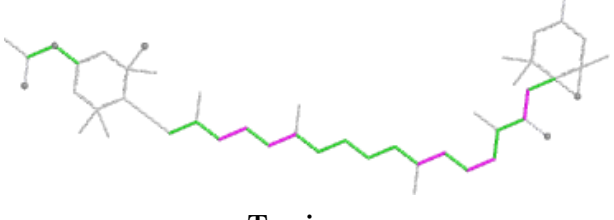
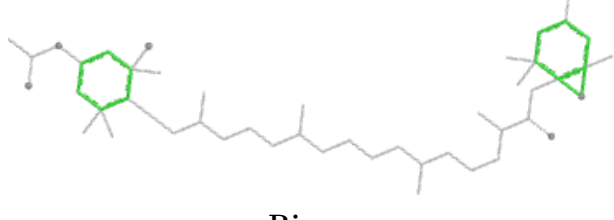


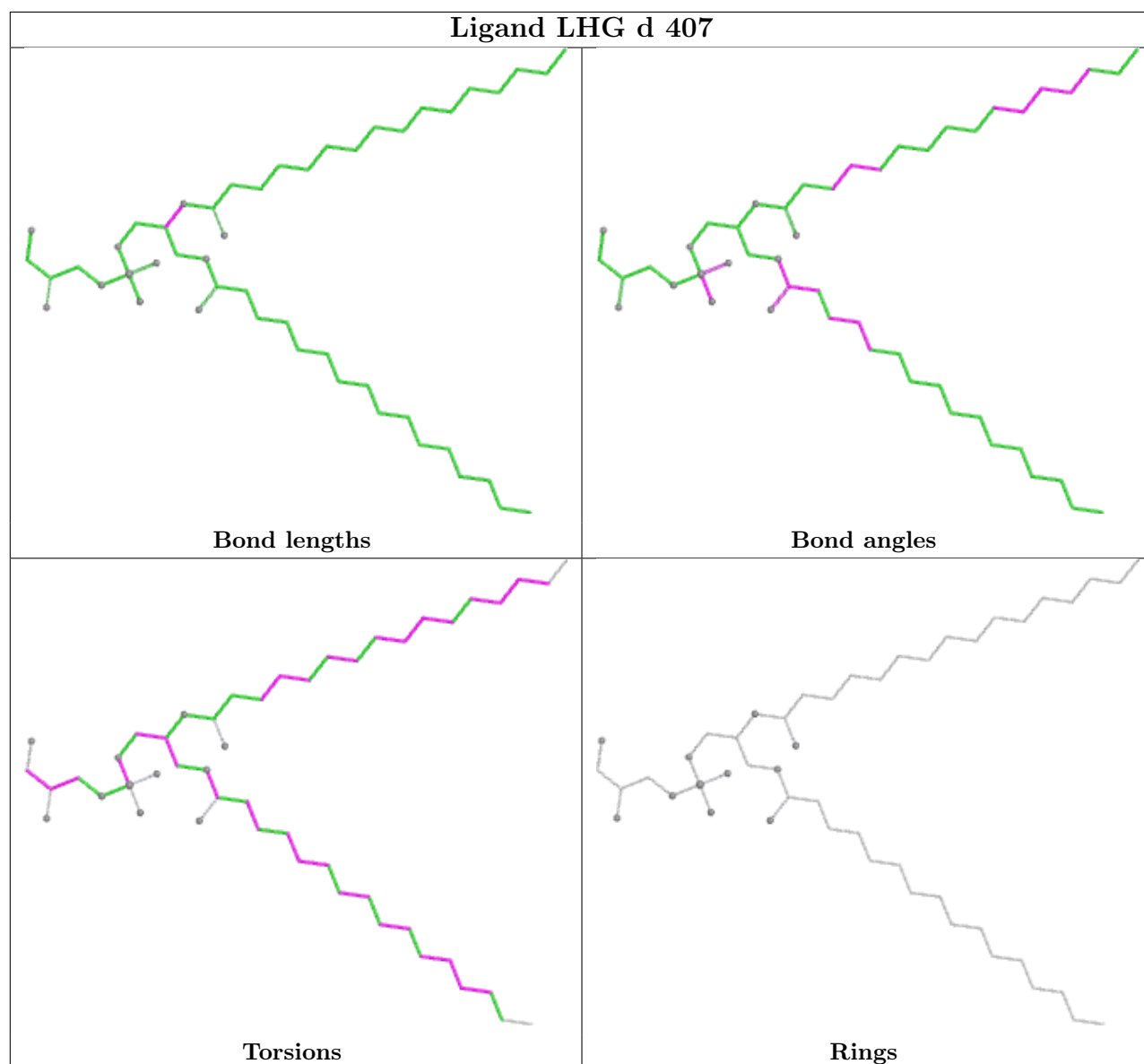
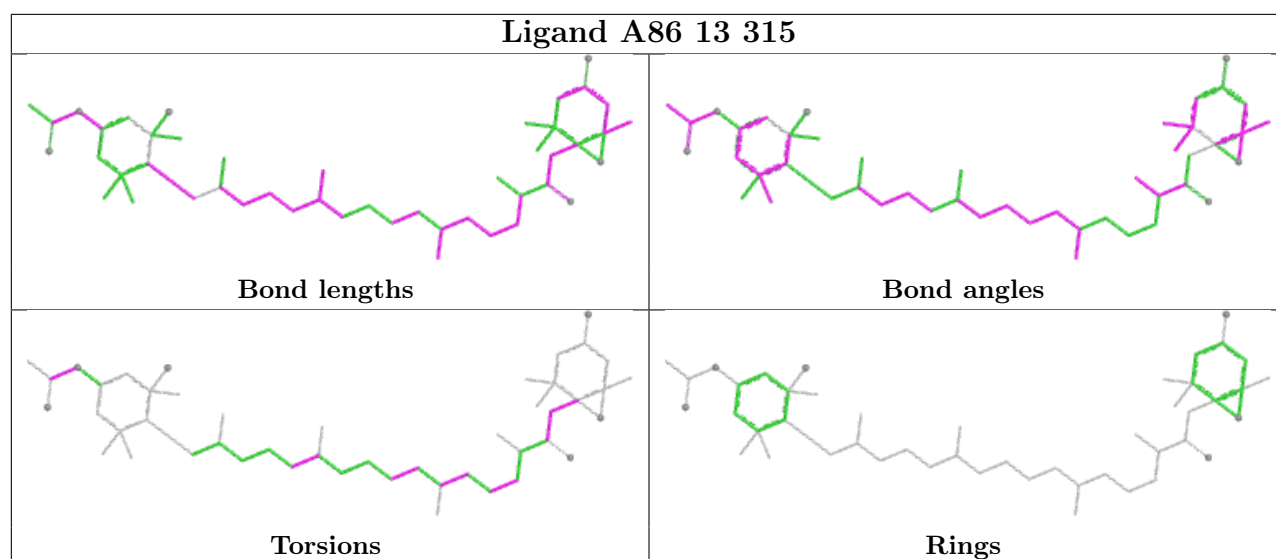


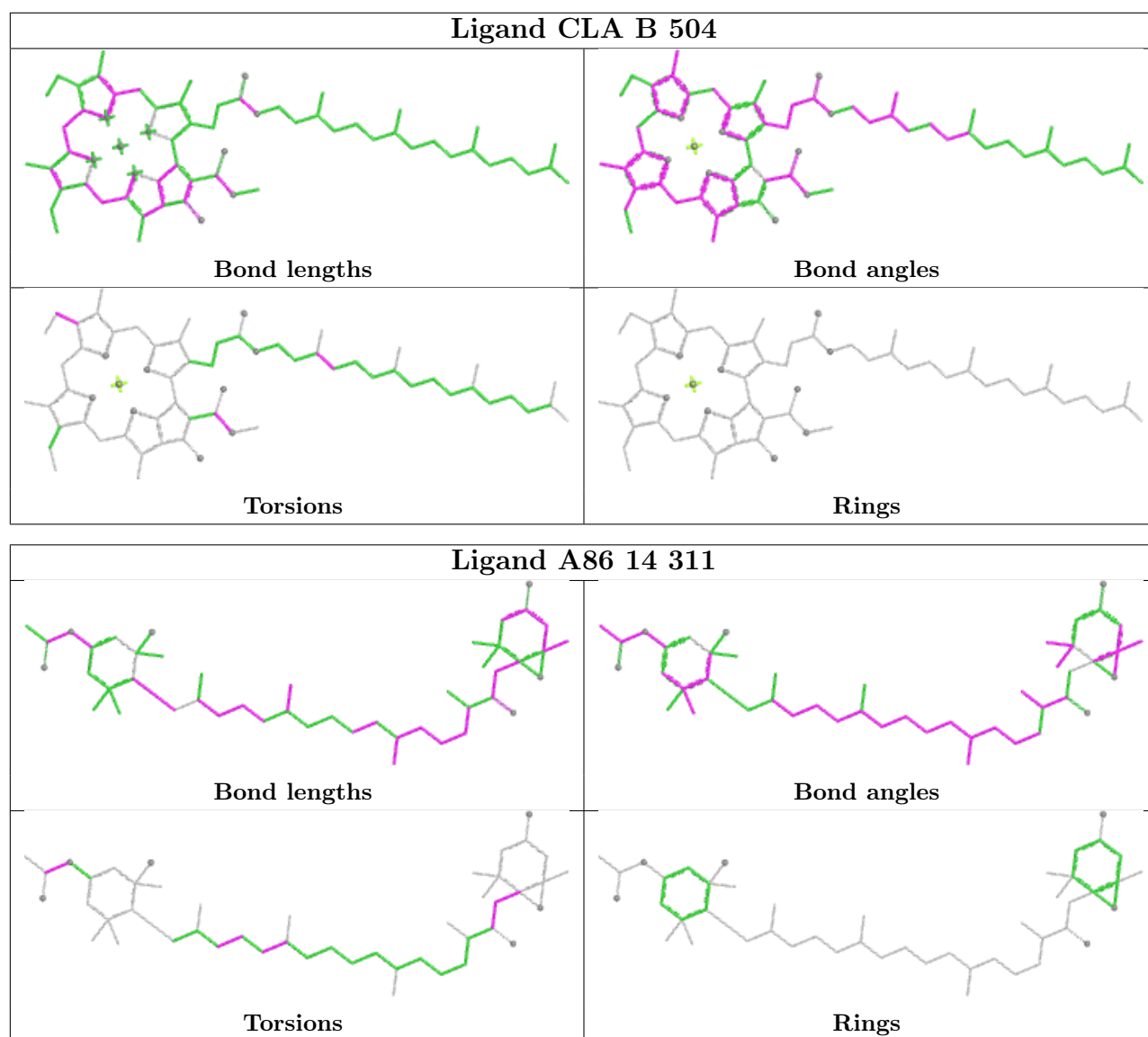


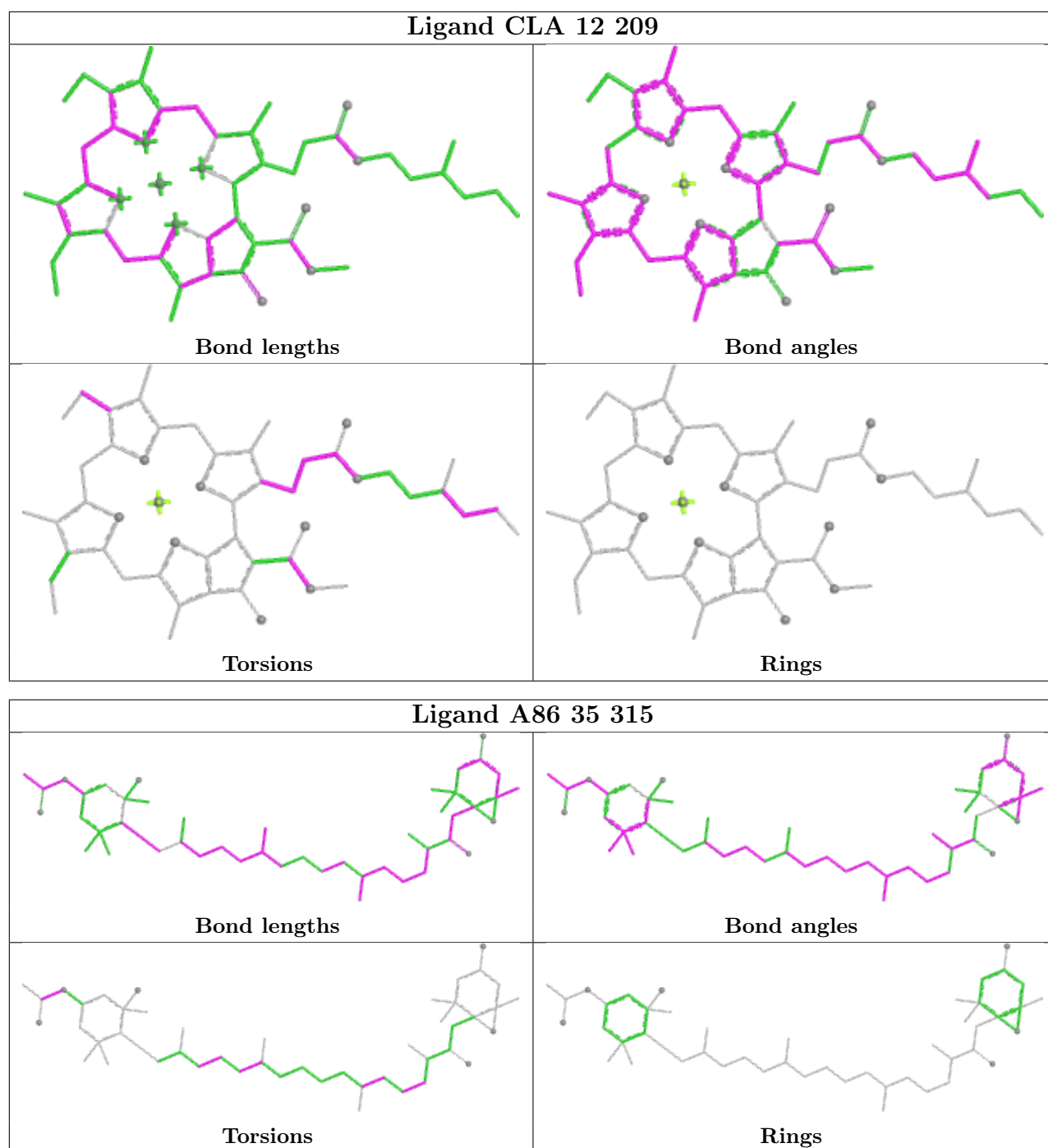
Ligand CLA B 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

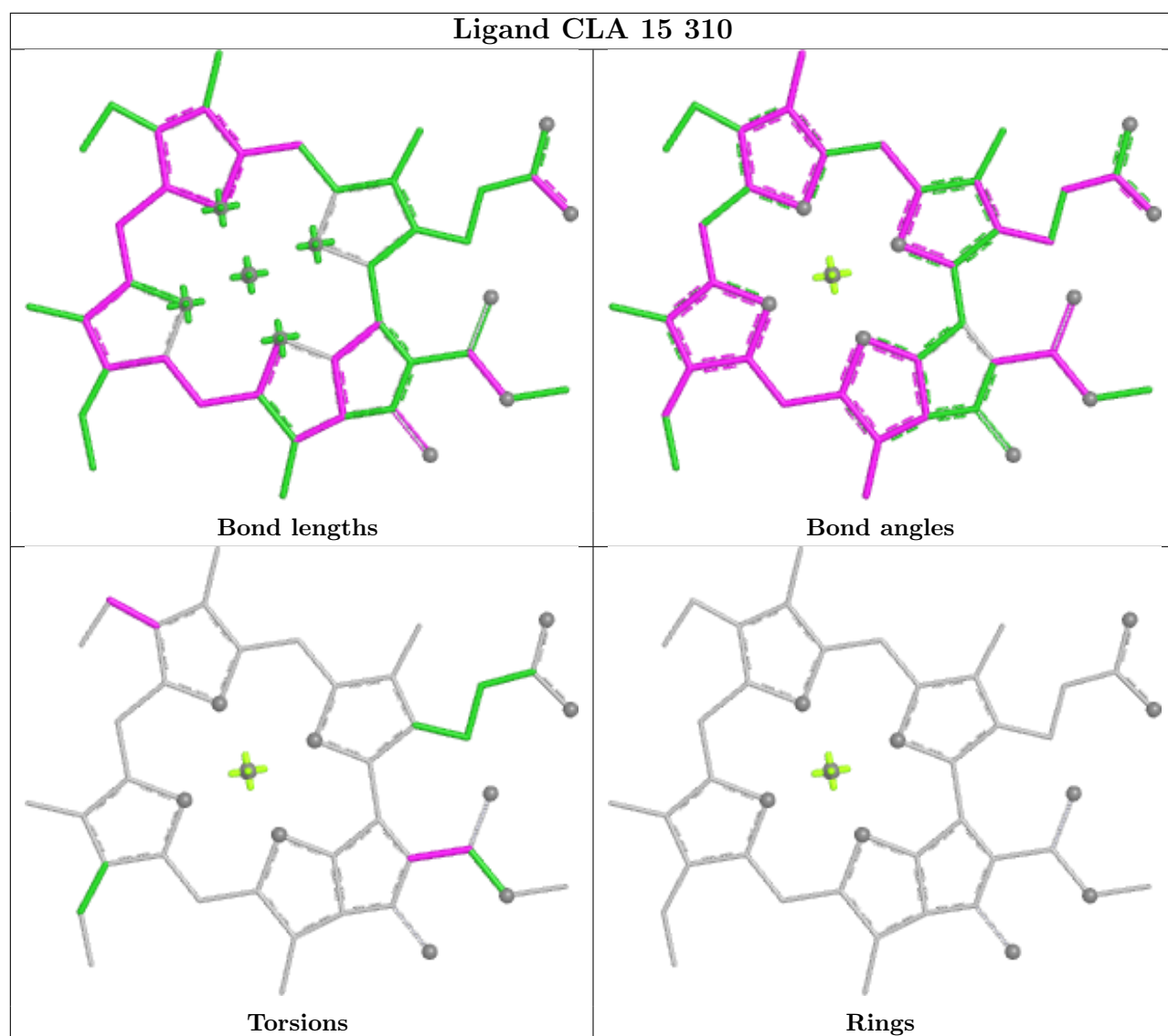
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Bond lengths	Bond angles
	
Torsions	Rings

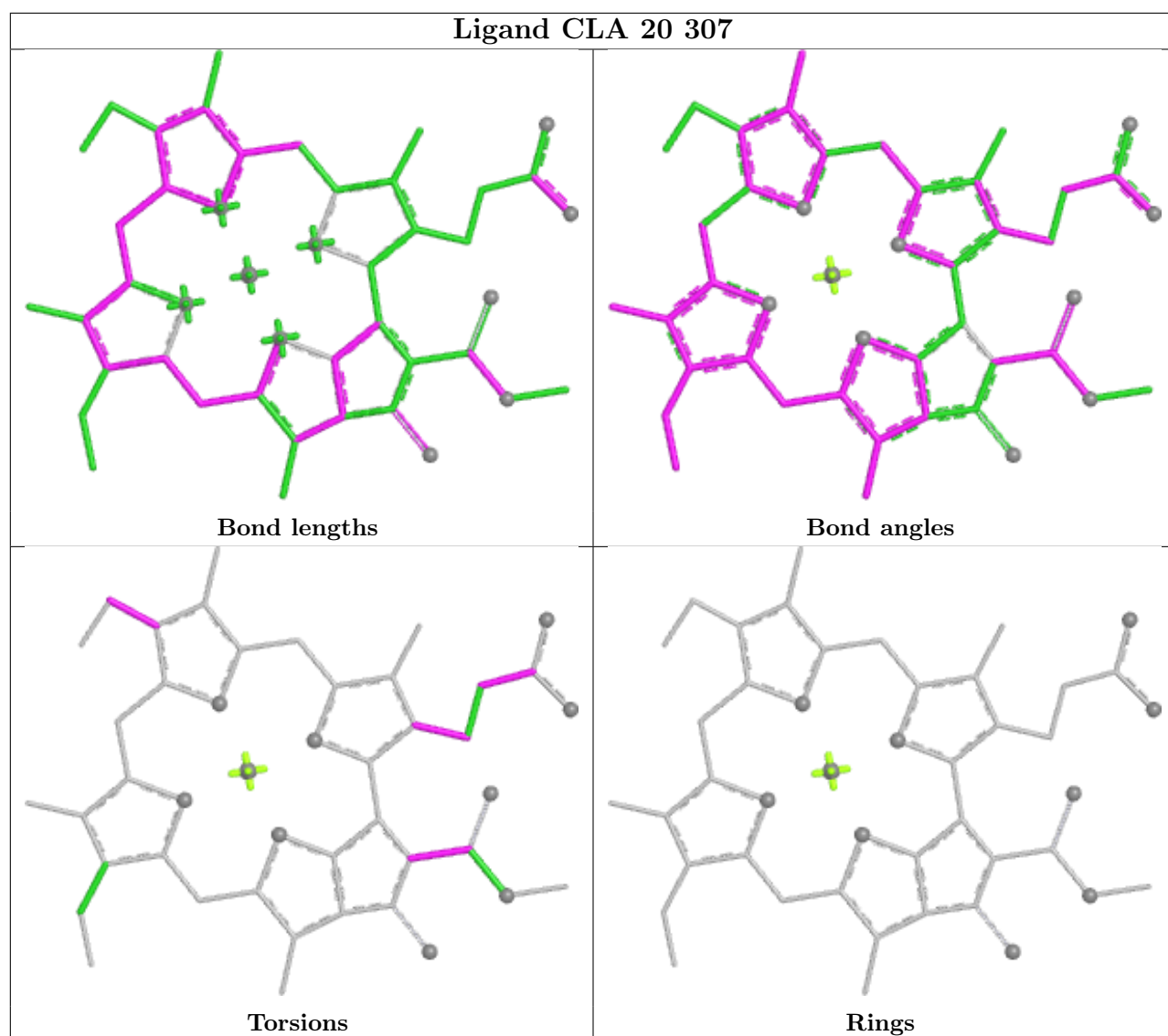
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Bond lengths	Bond angles
	
Torsions	Rings

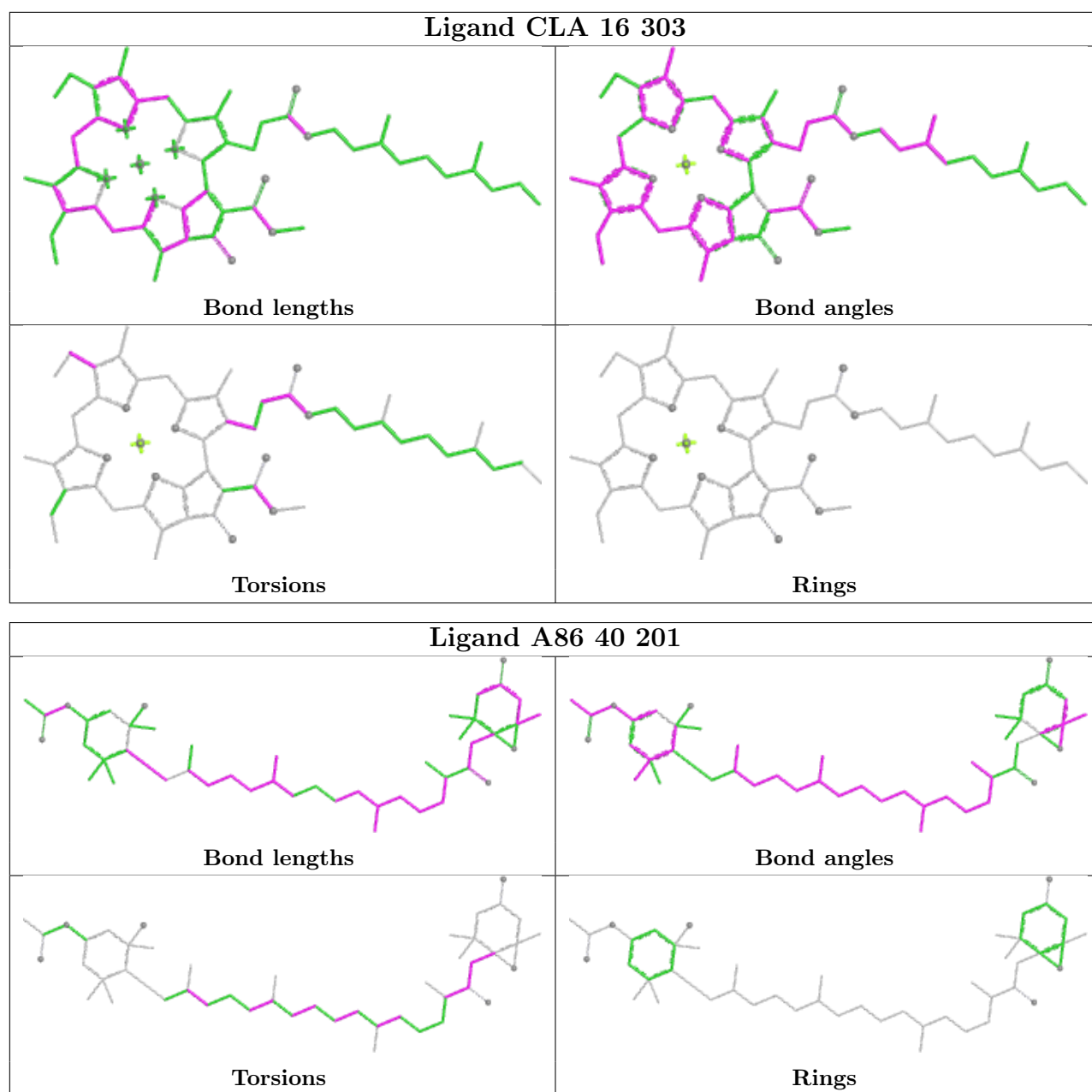


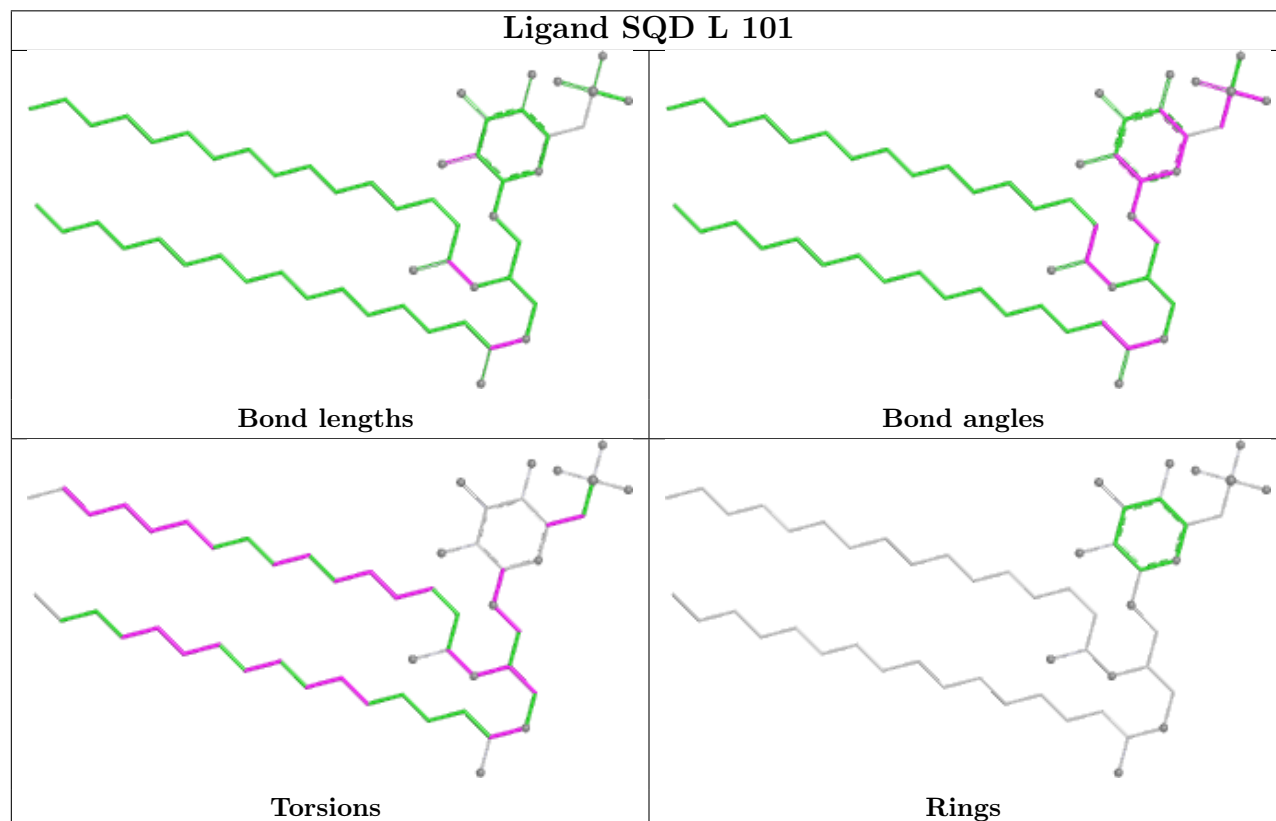
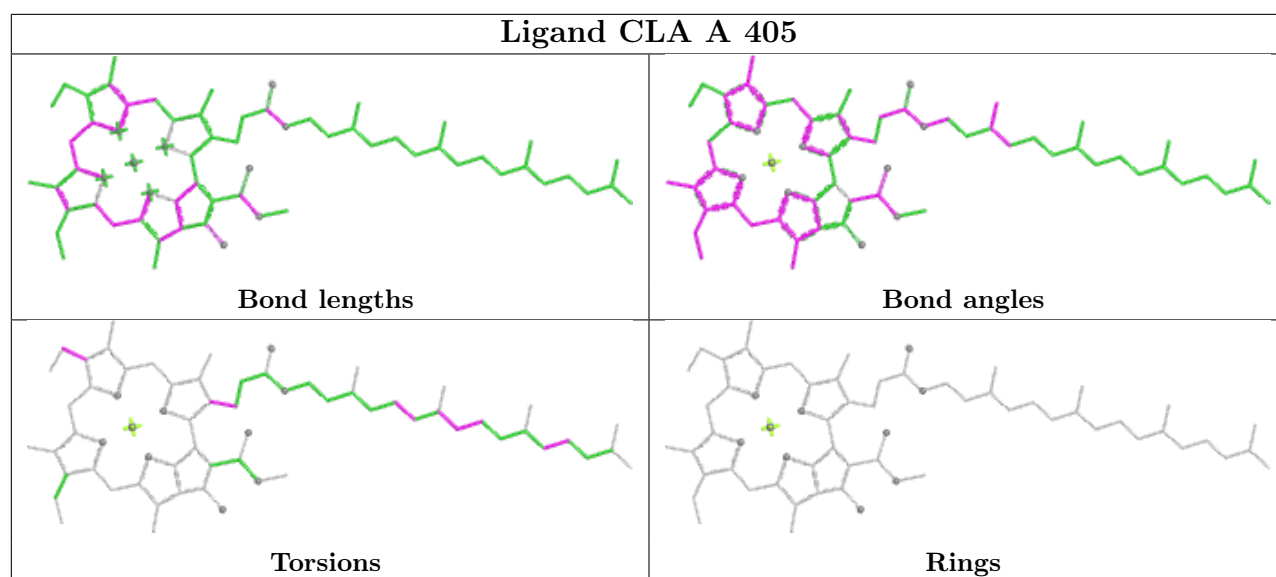


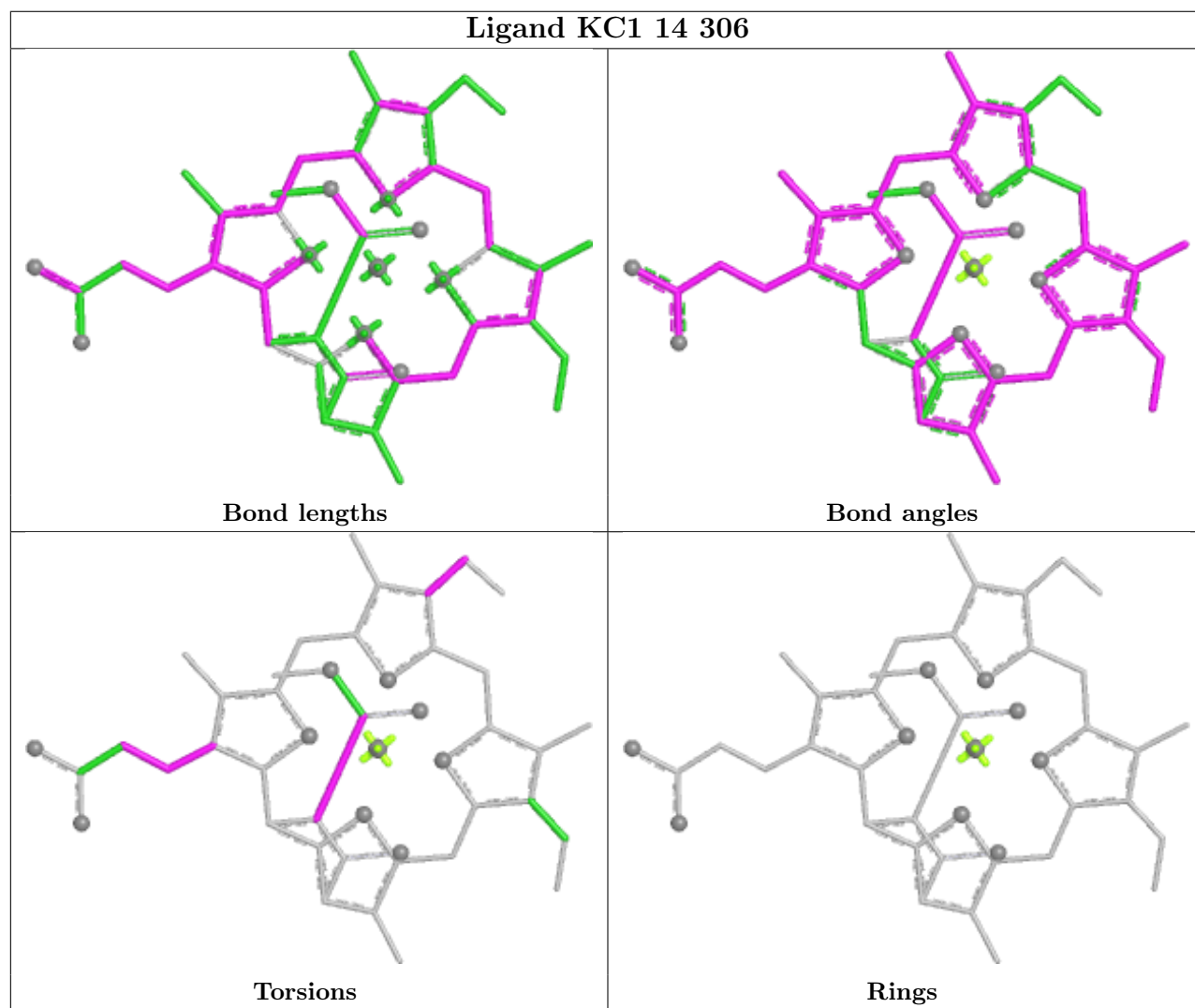
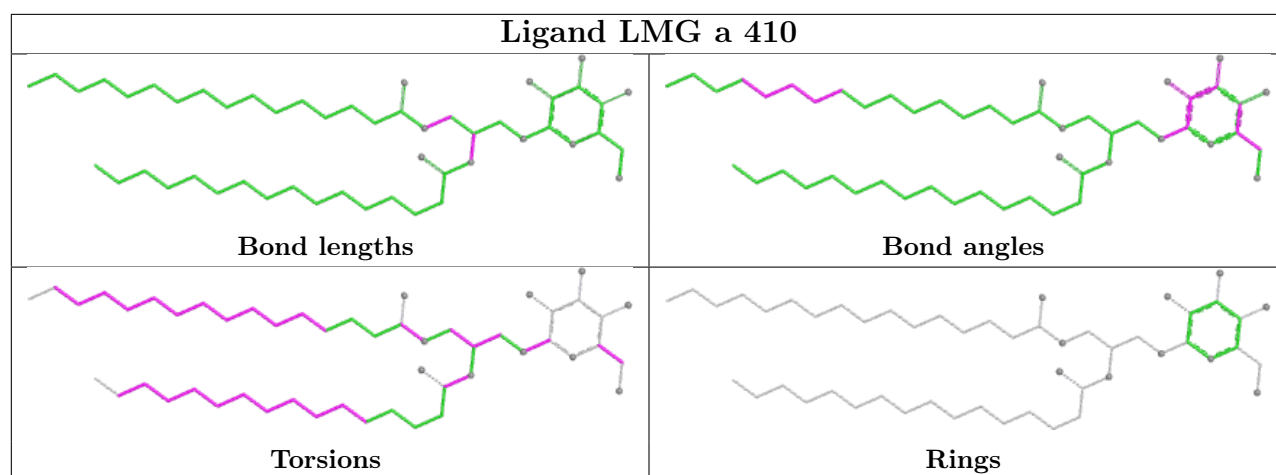


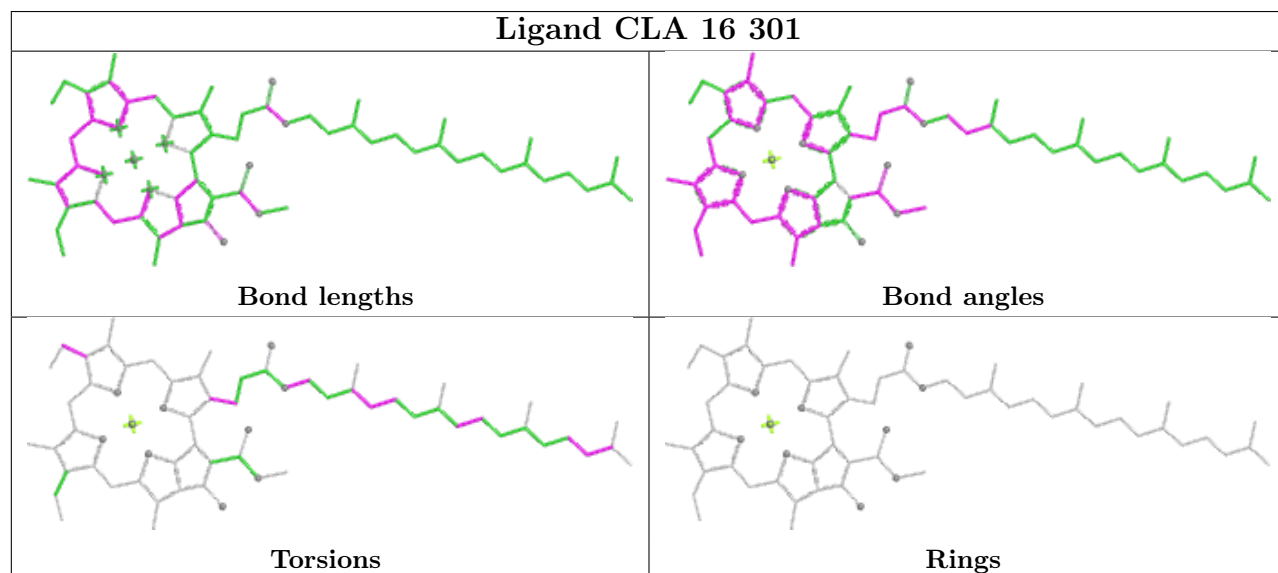
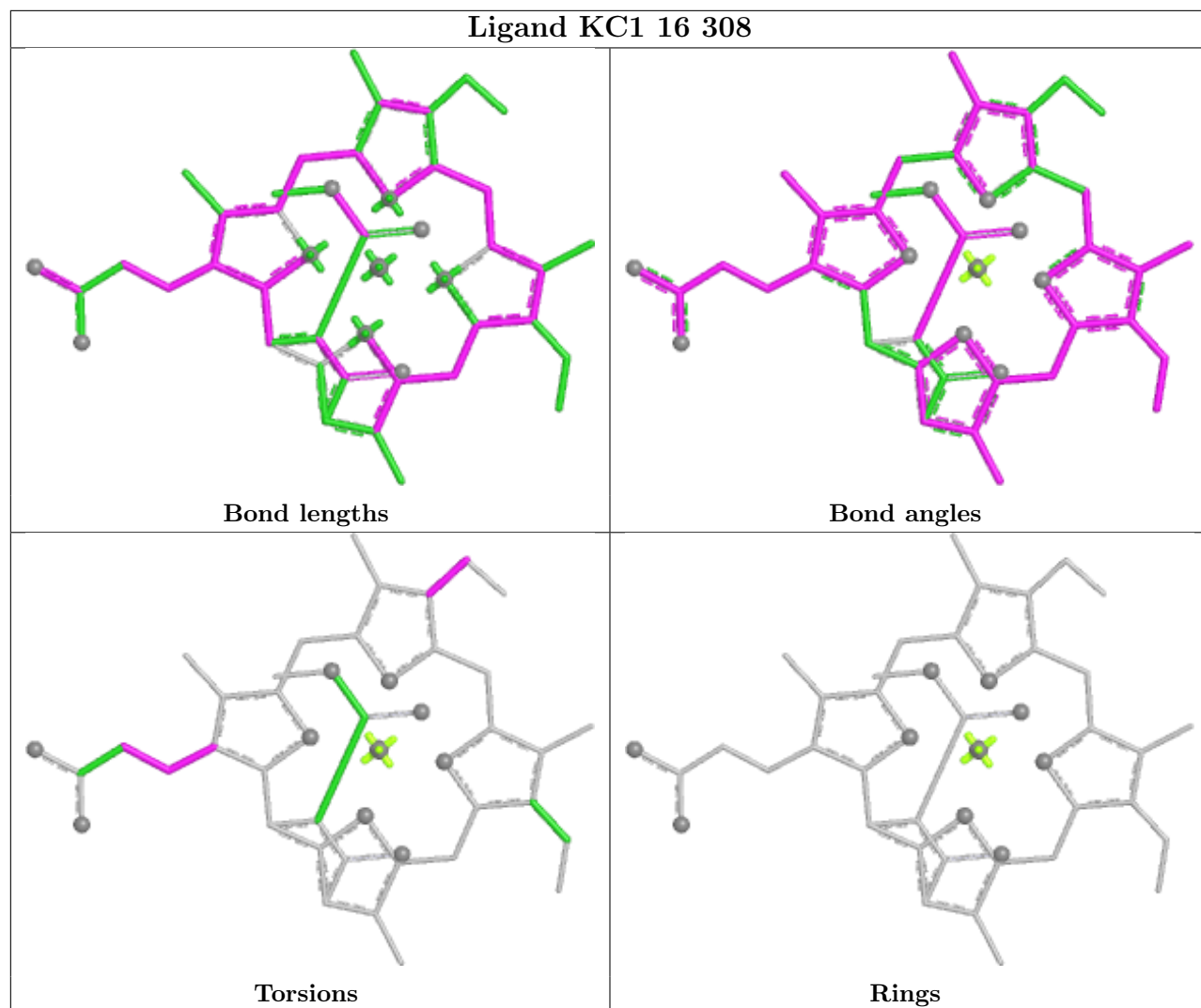


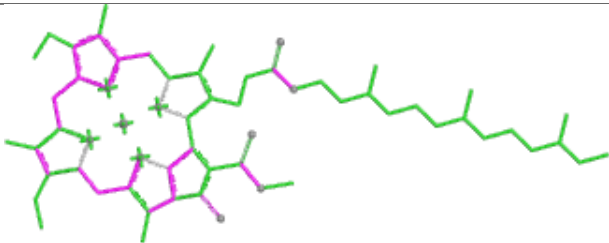
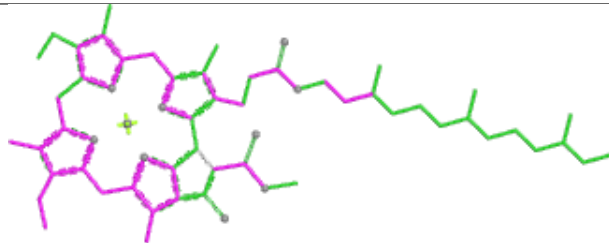
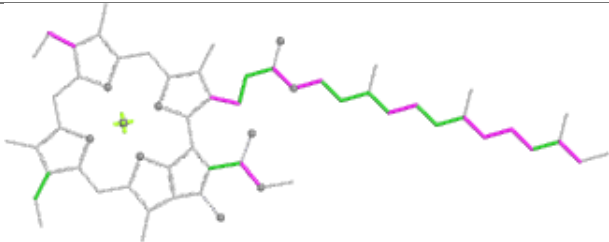
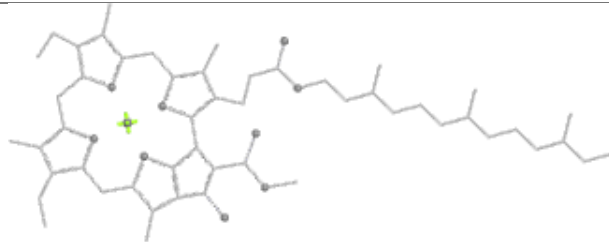


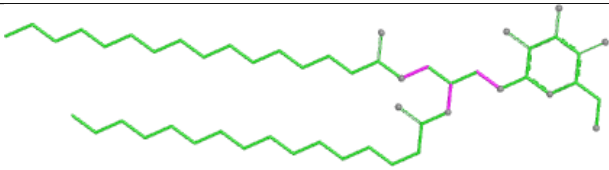
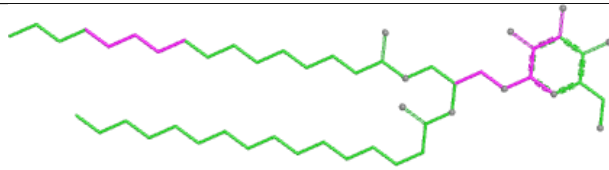
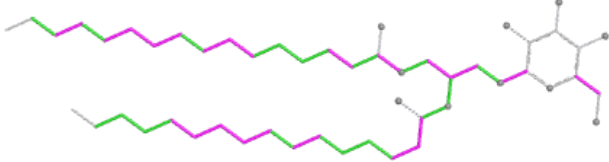
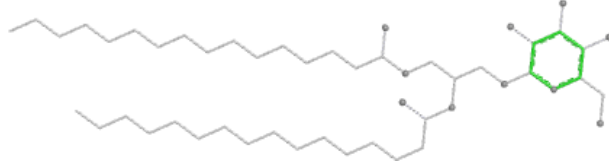


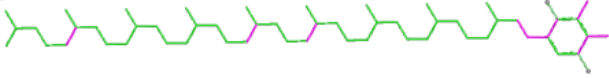
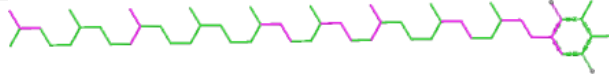
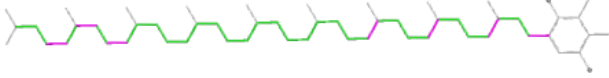
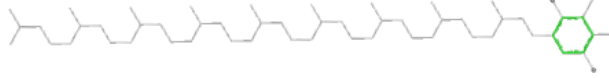


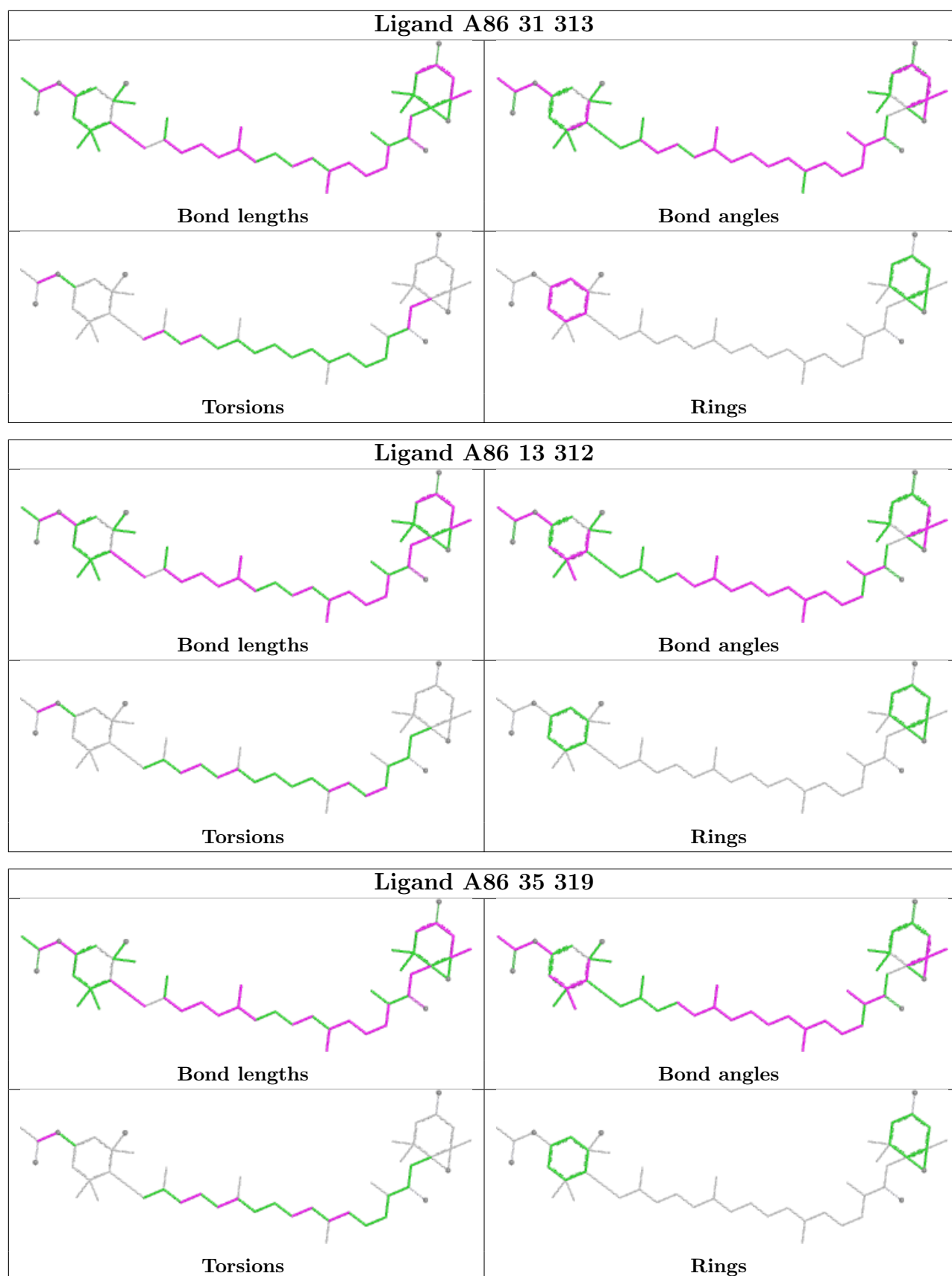


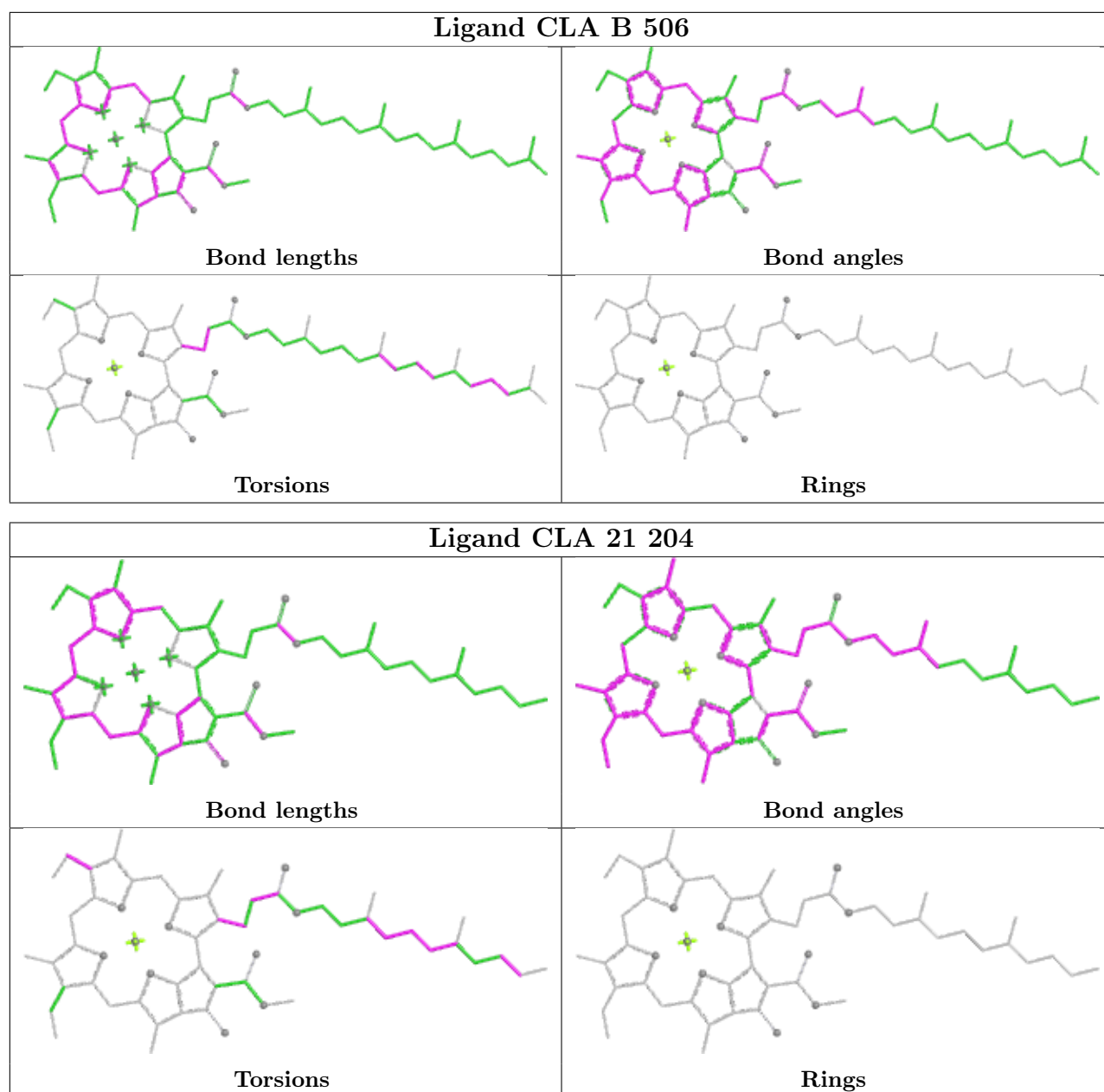


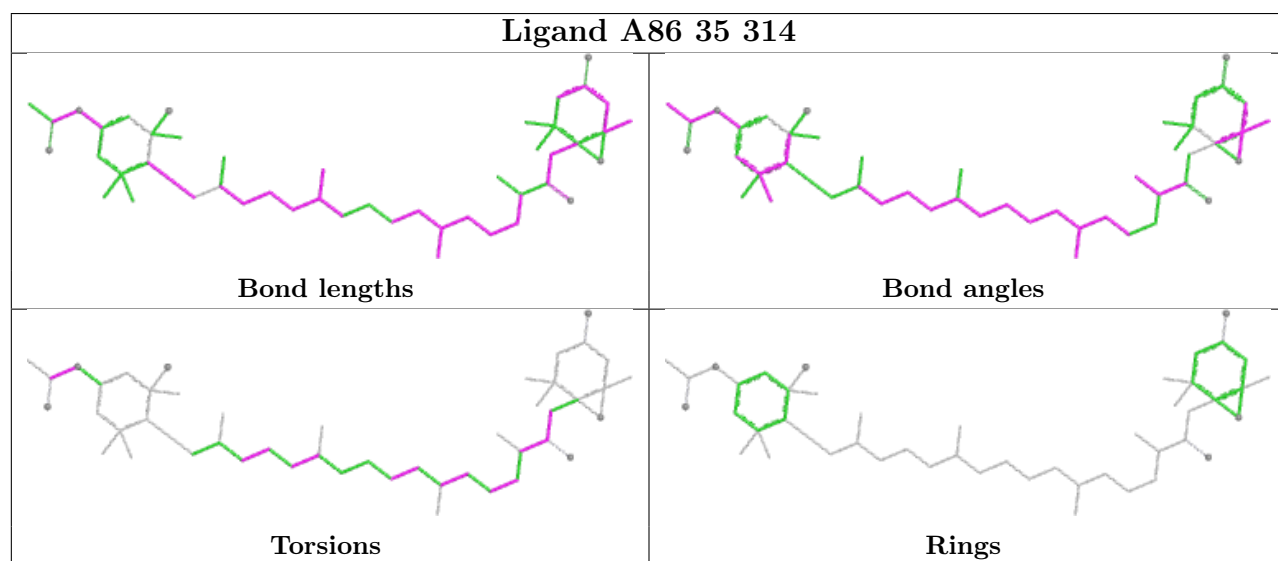
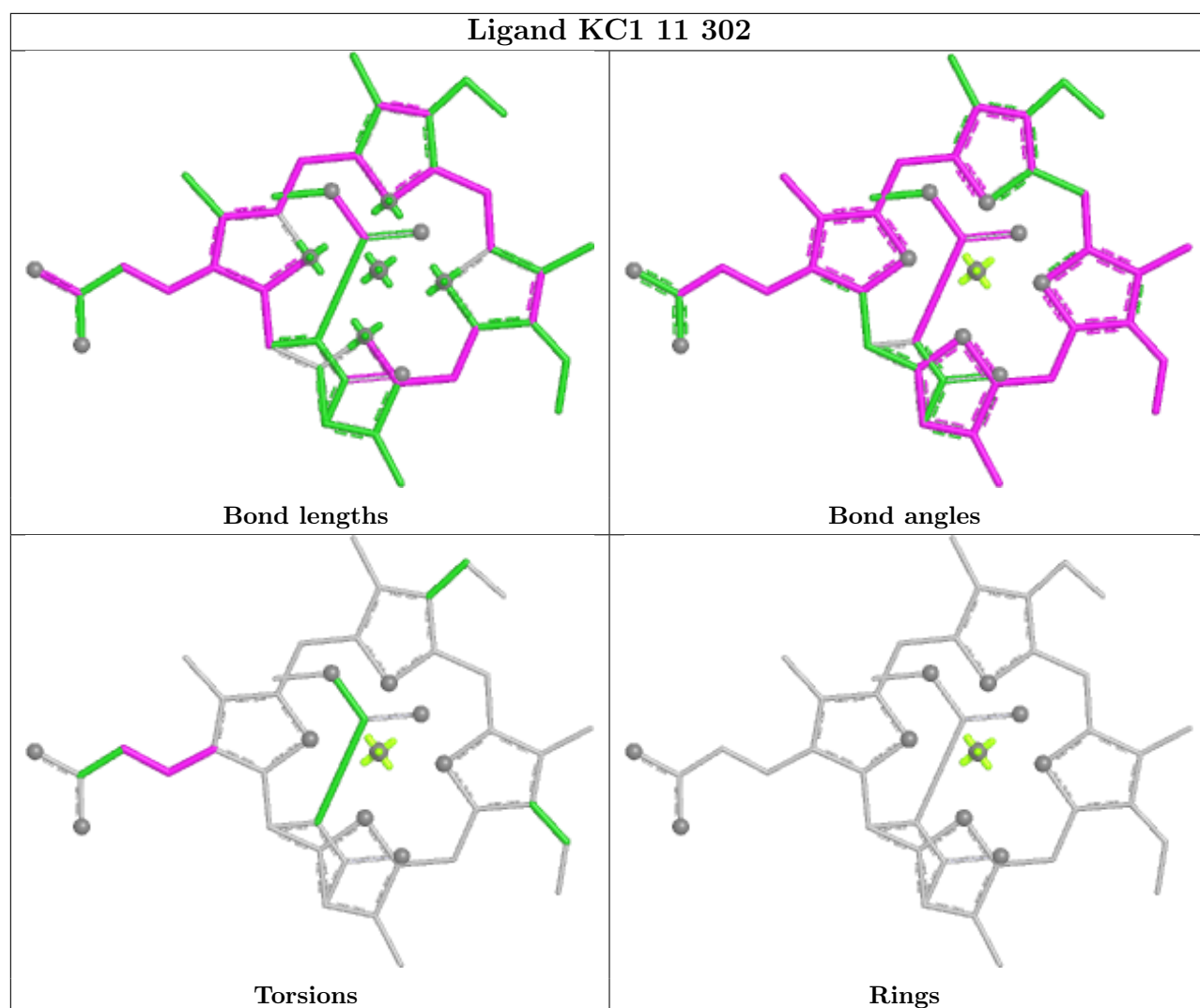
Ligand CLA 36 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

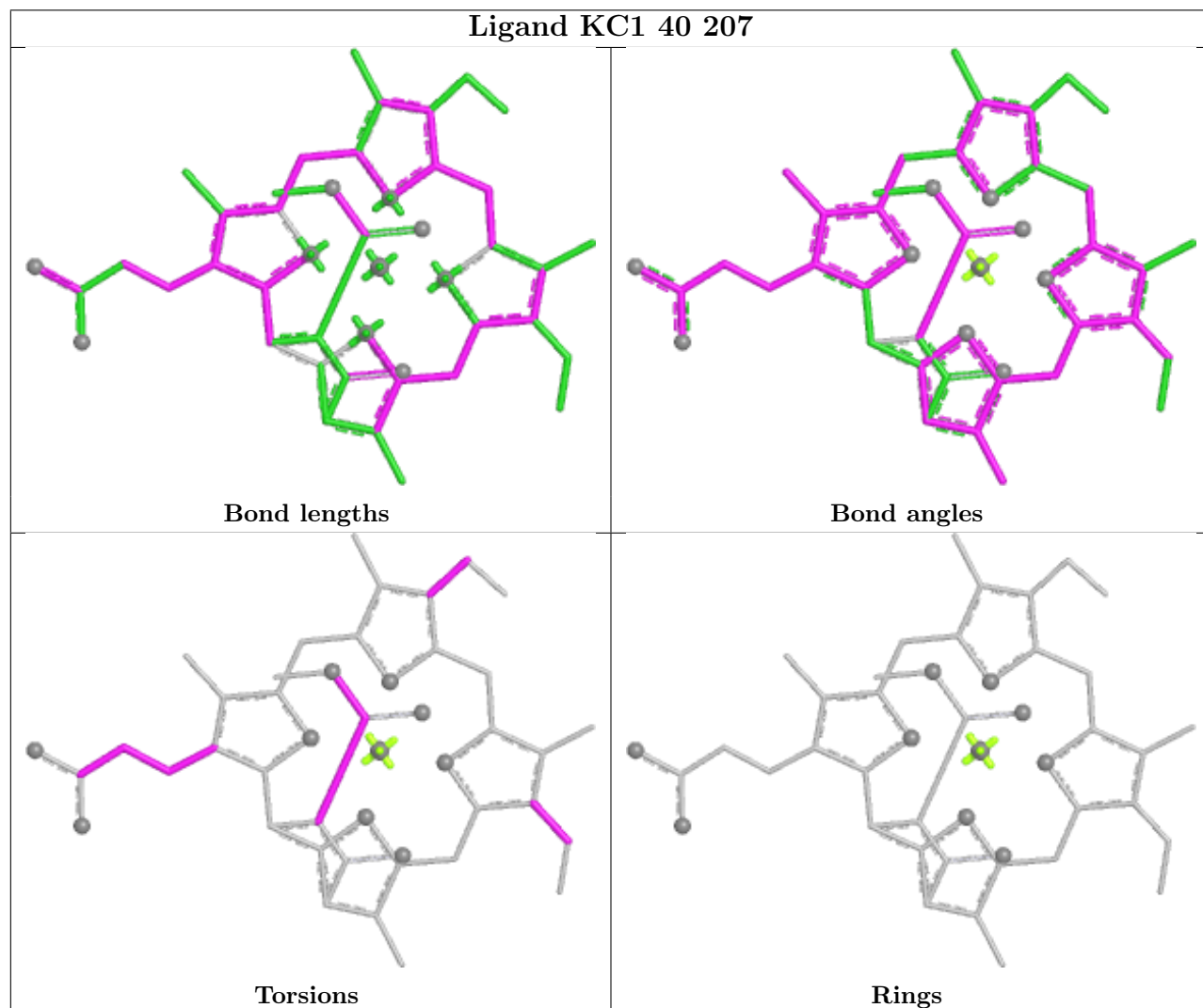
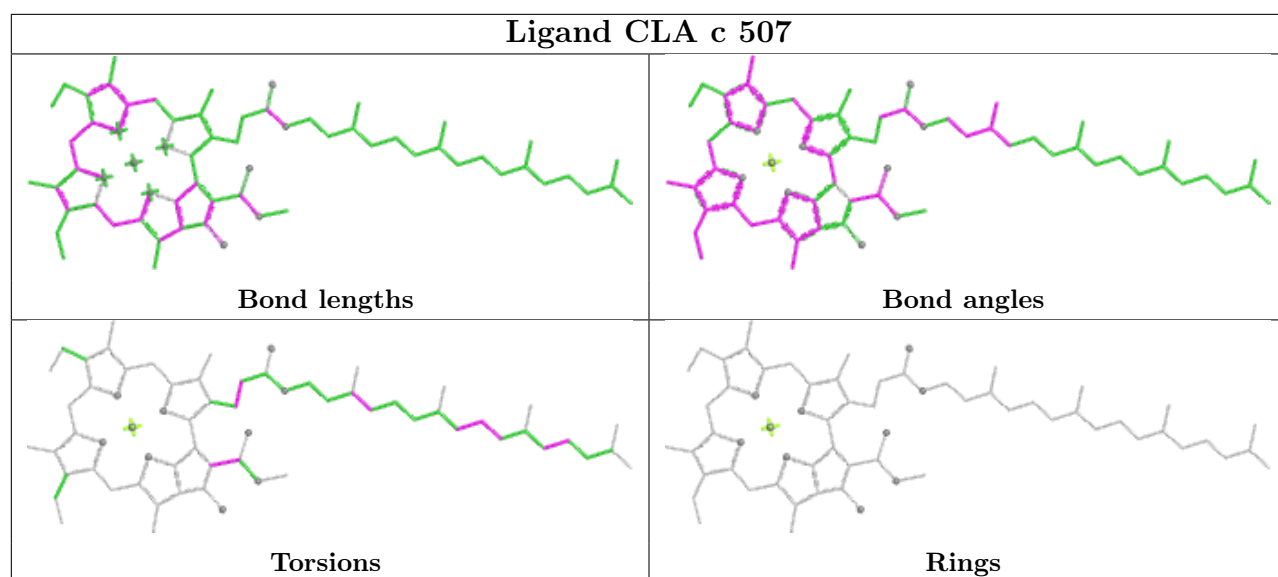
Ligand LMG c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

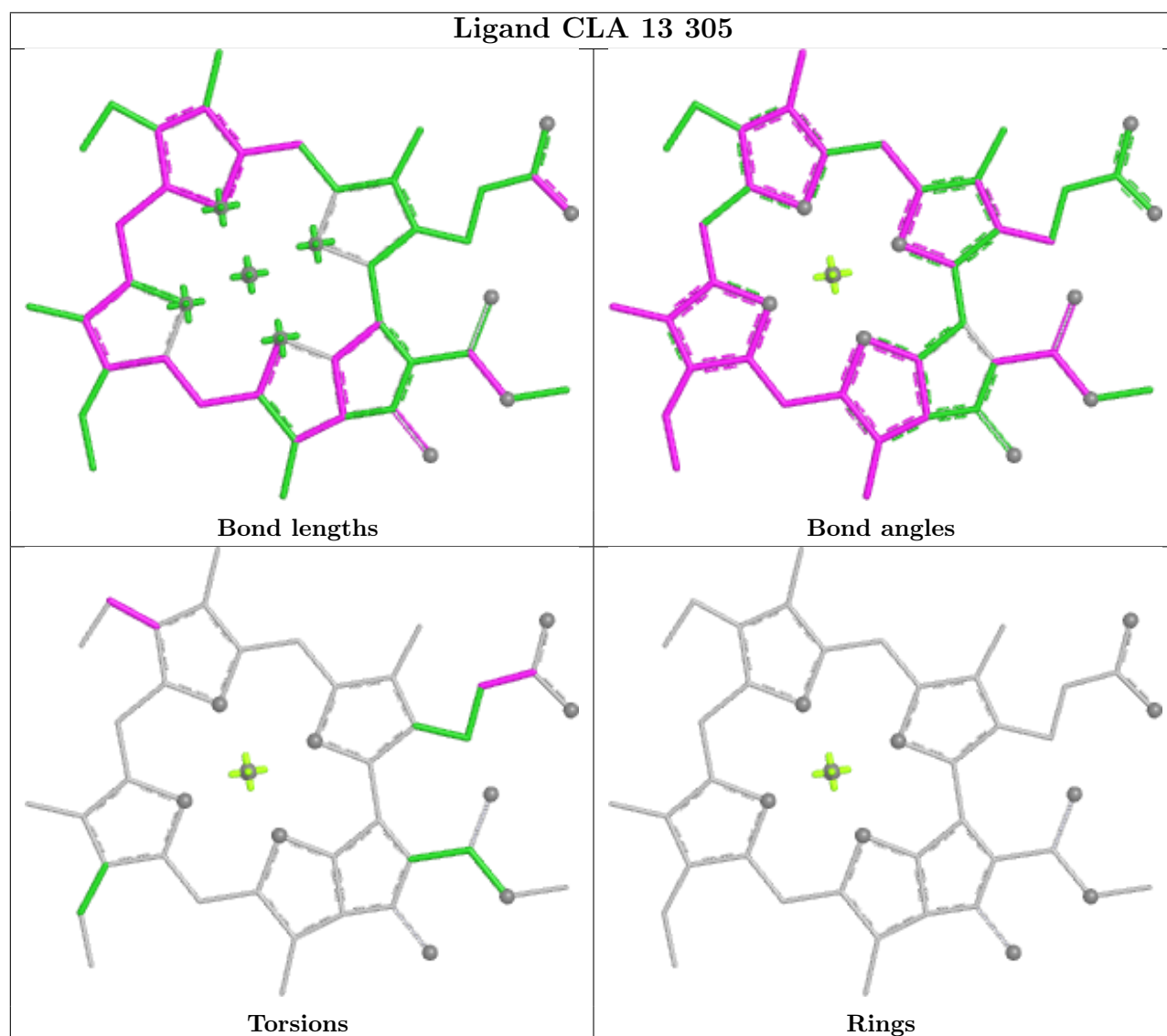
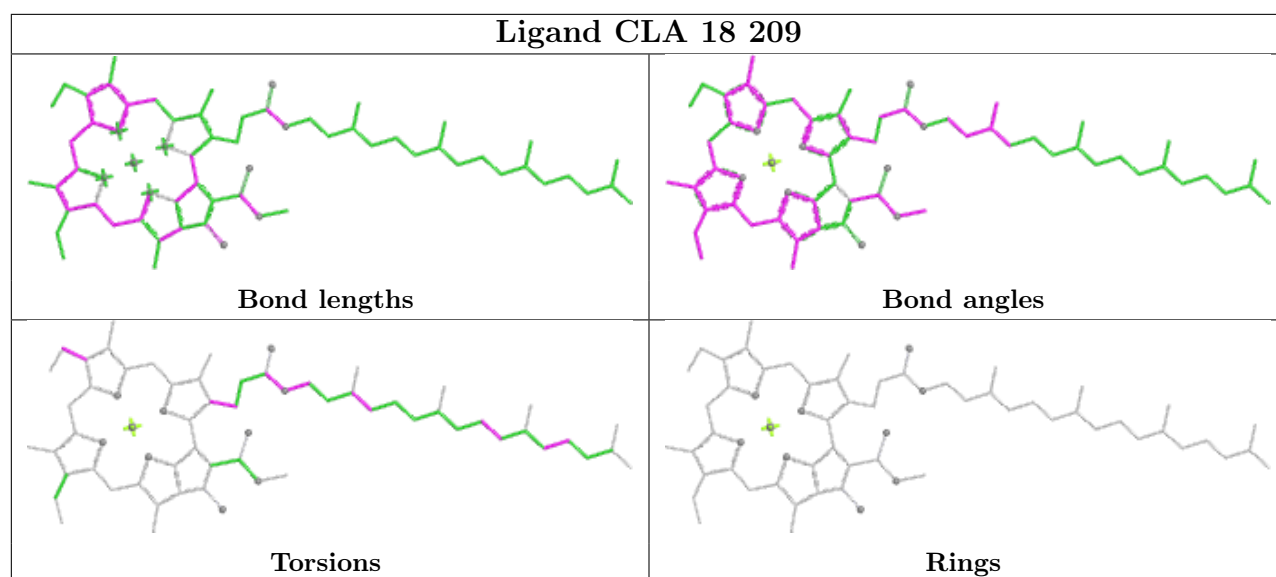
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Bond lengths	Bond angles
	
Torsions	Rings

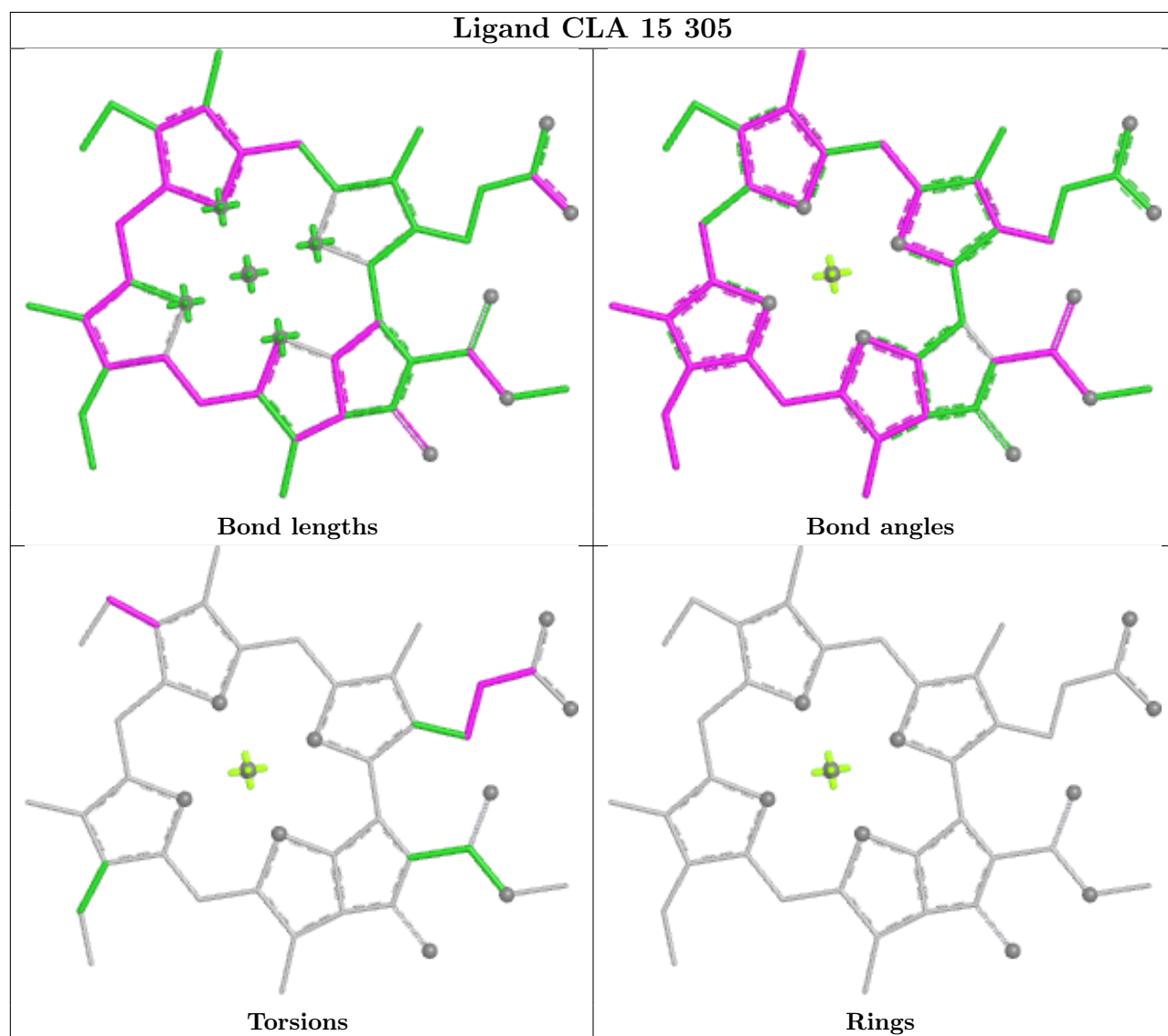
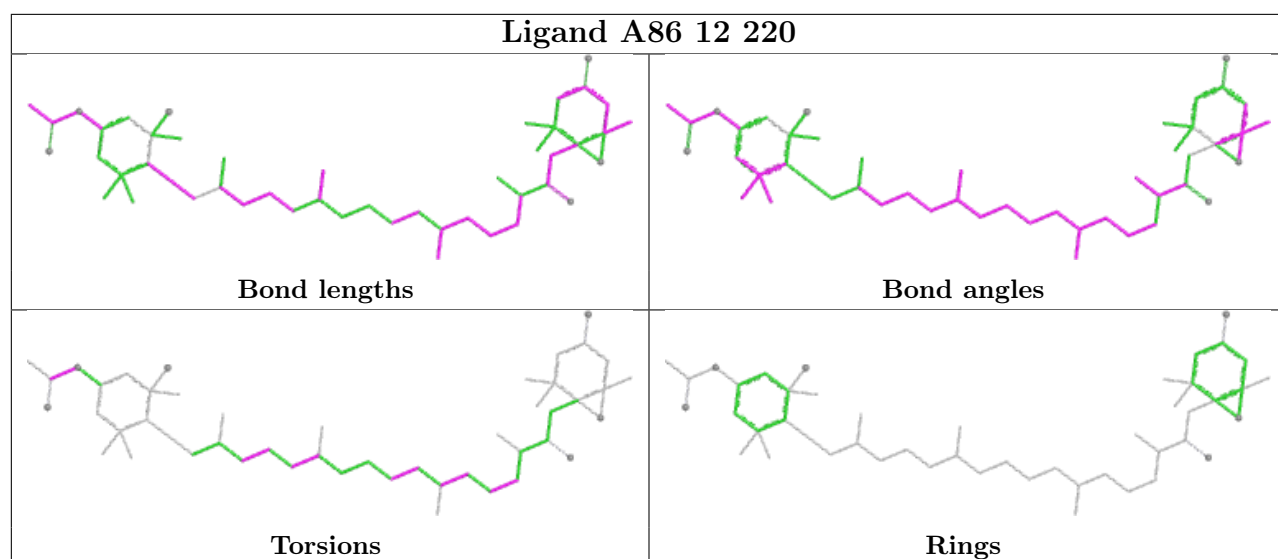


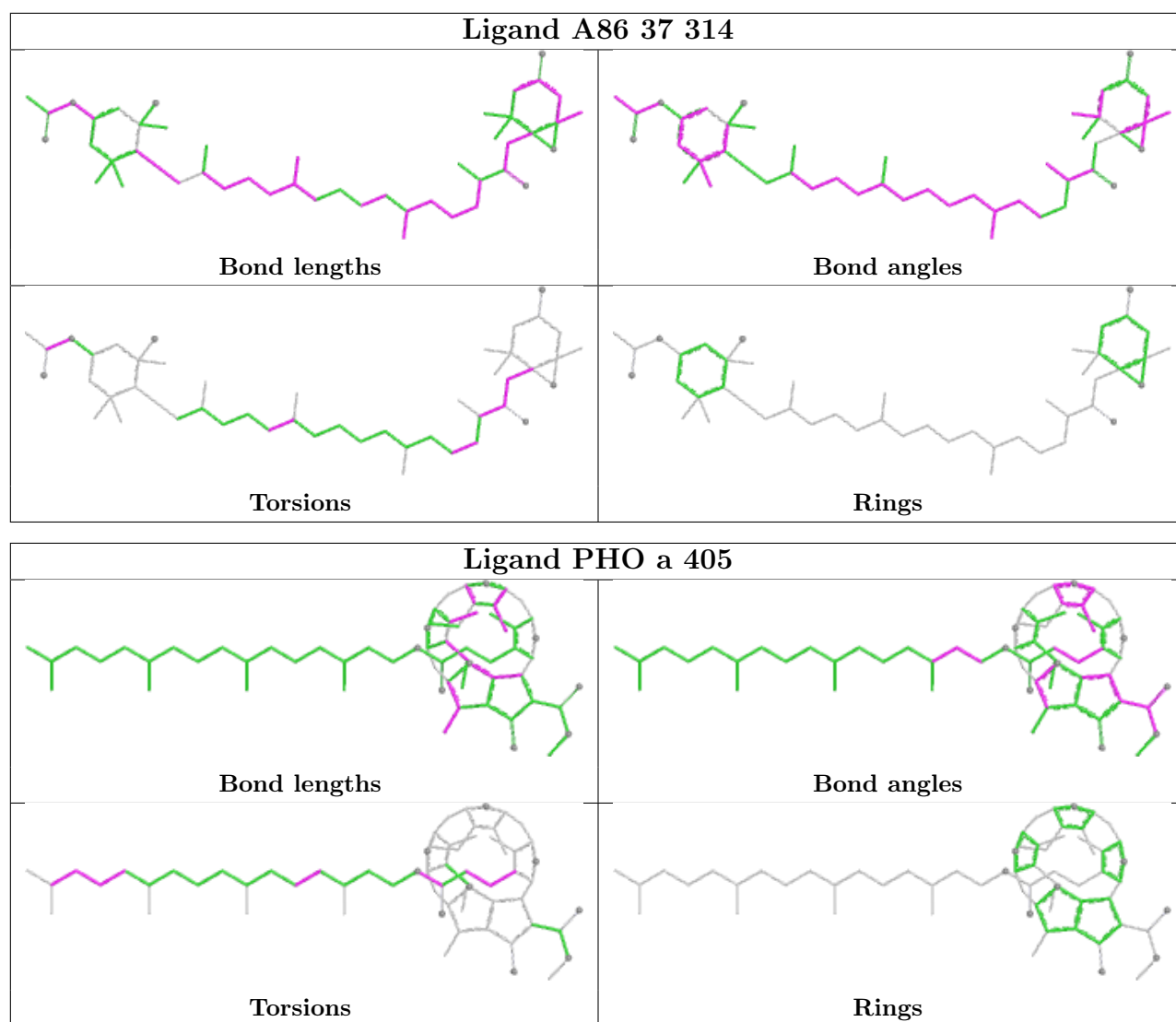


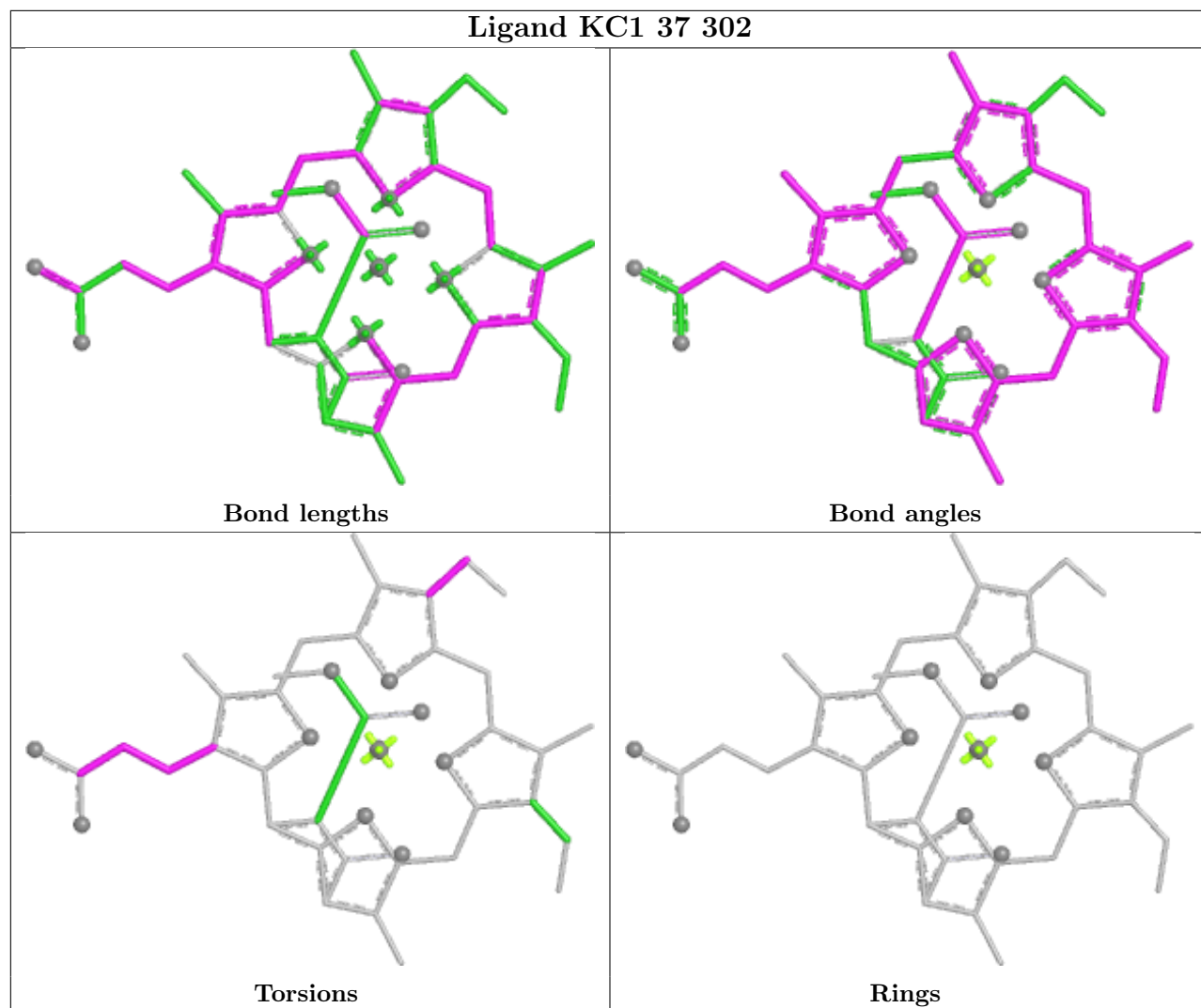


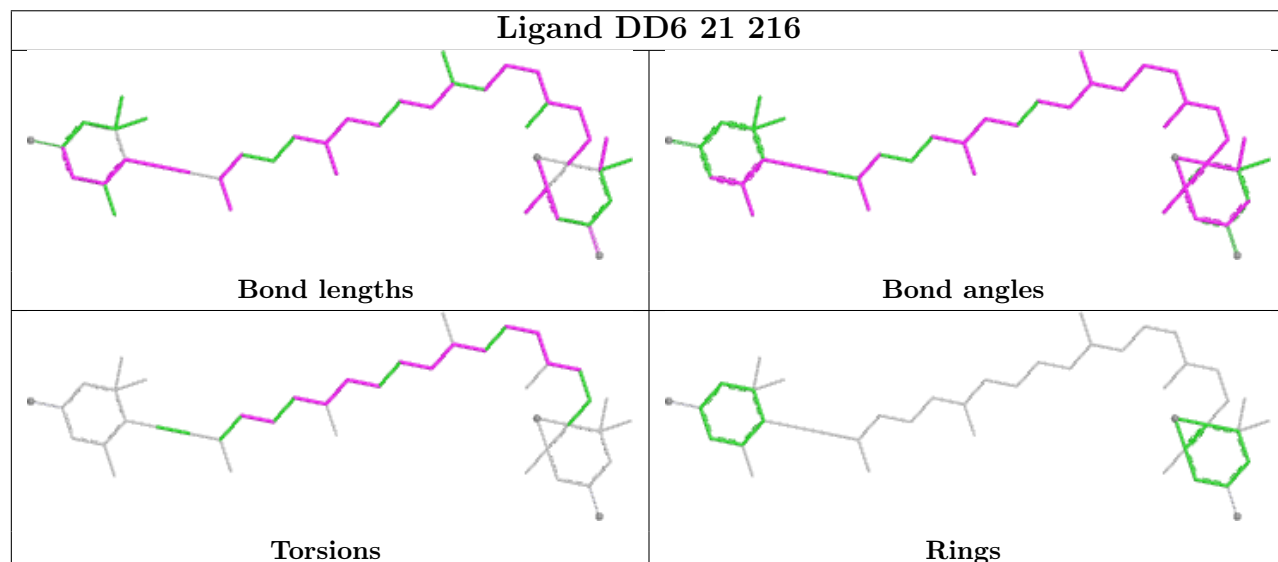
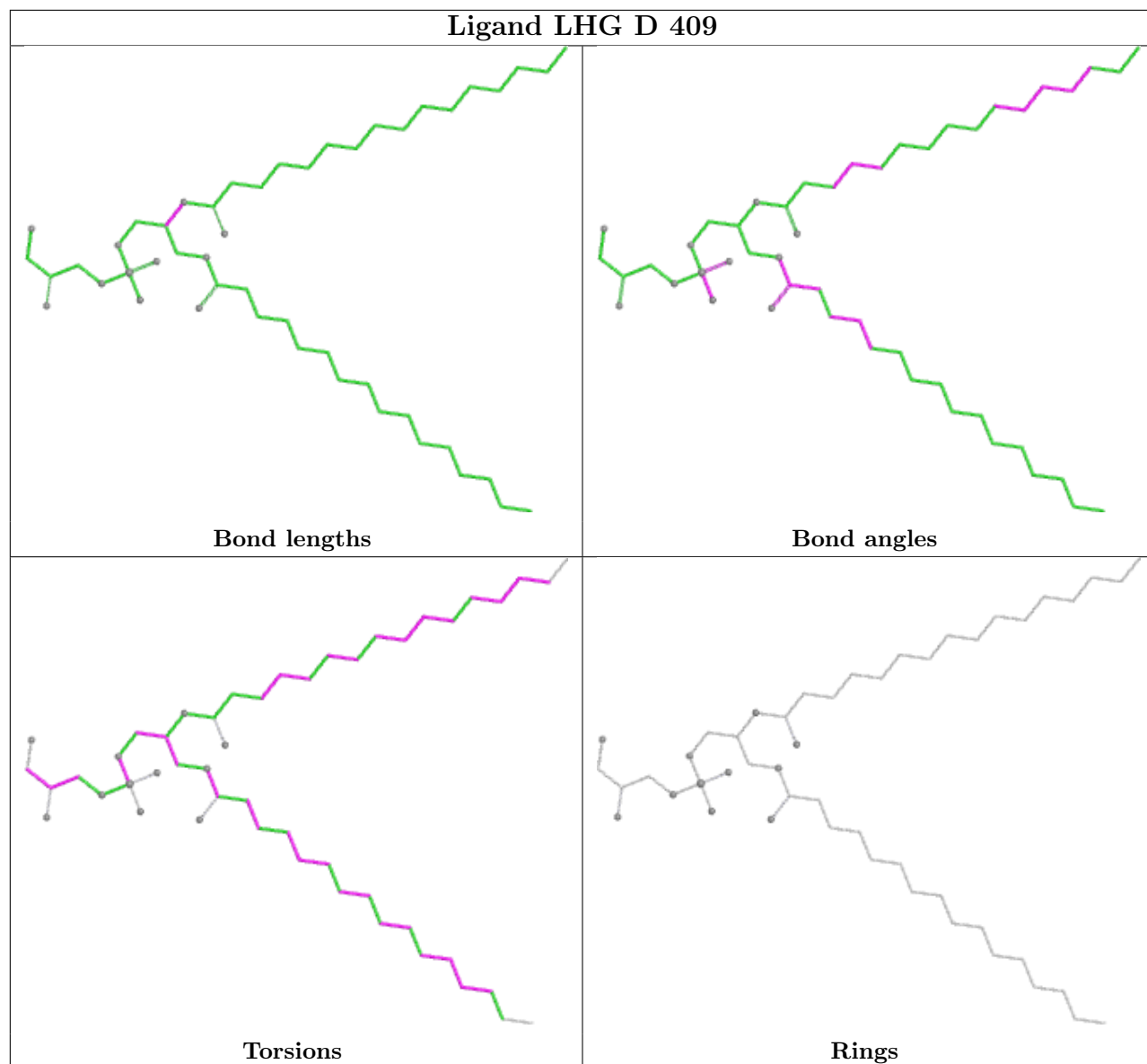


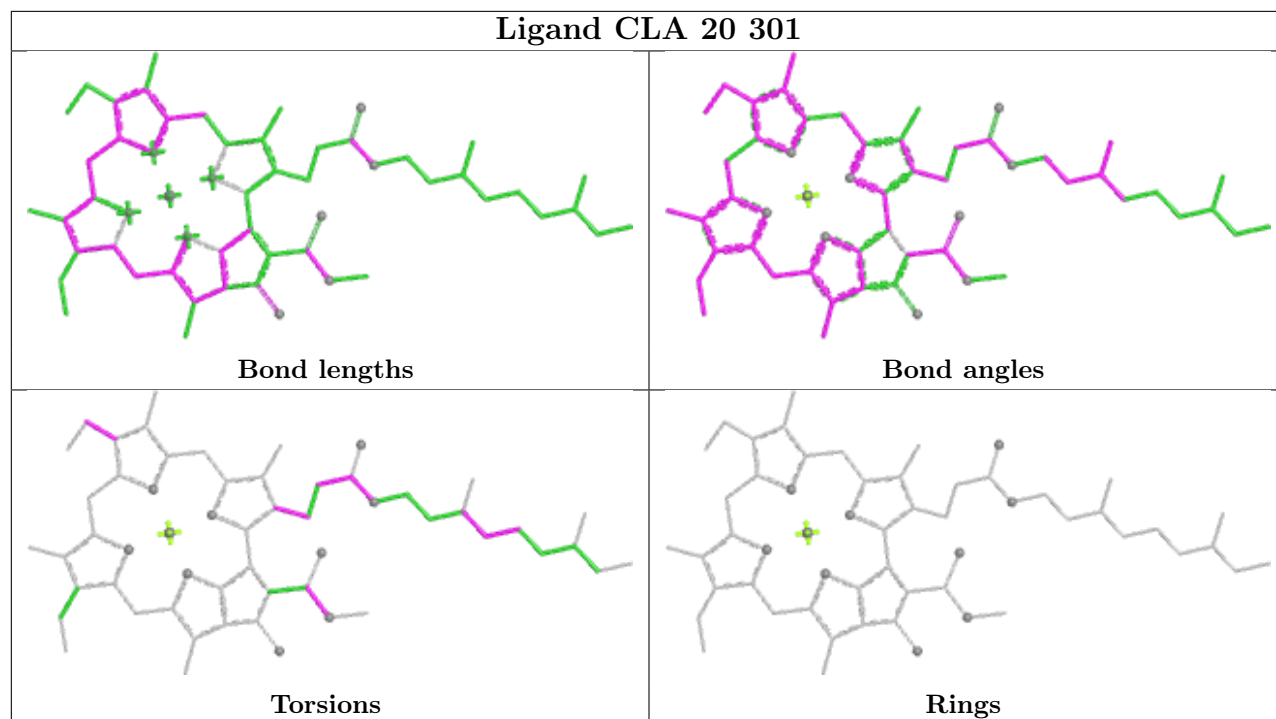


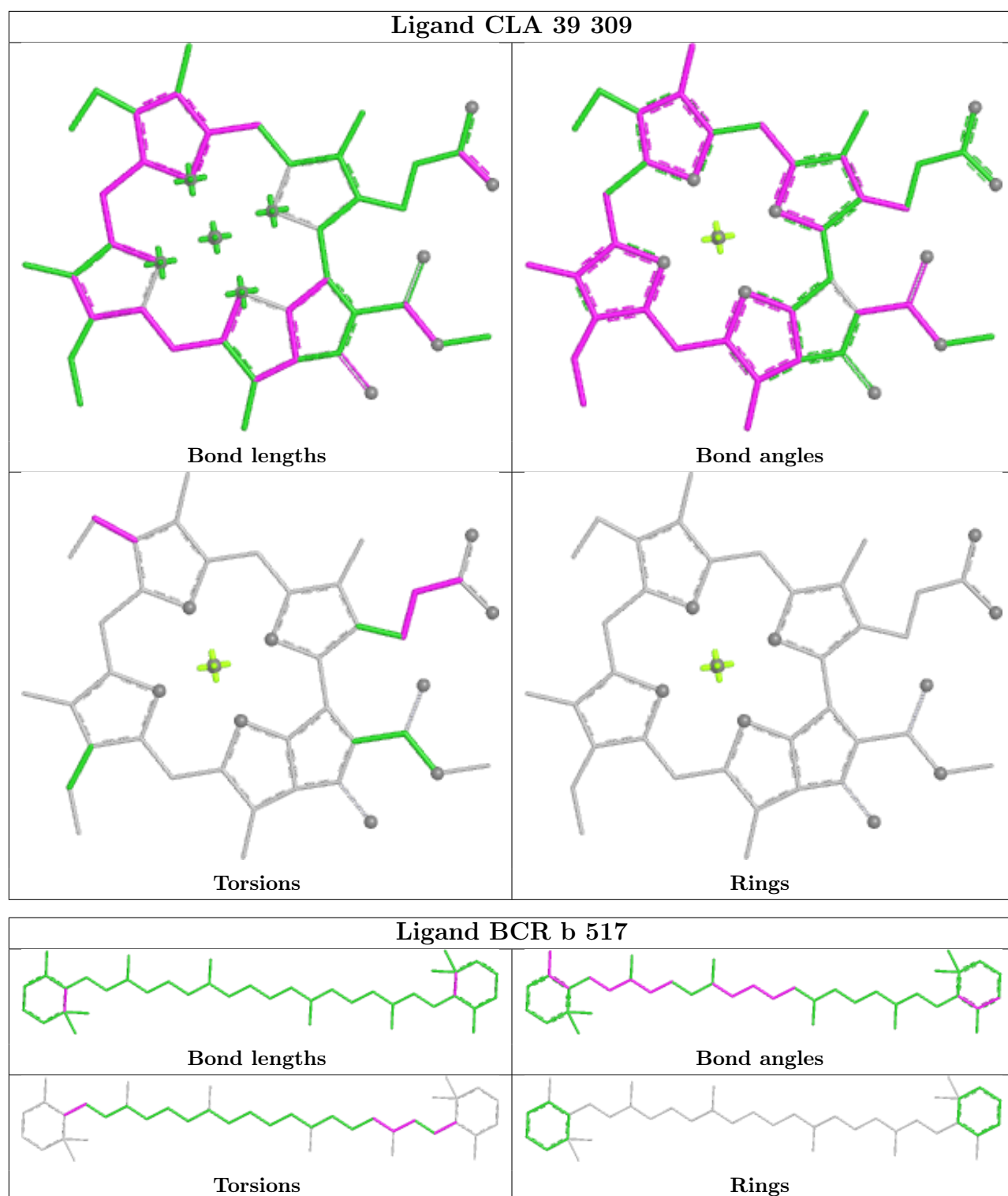


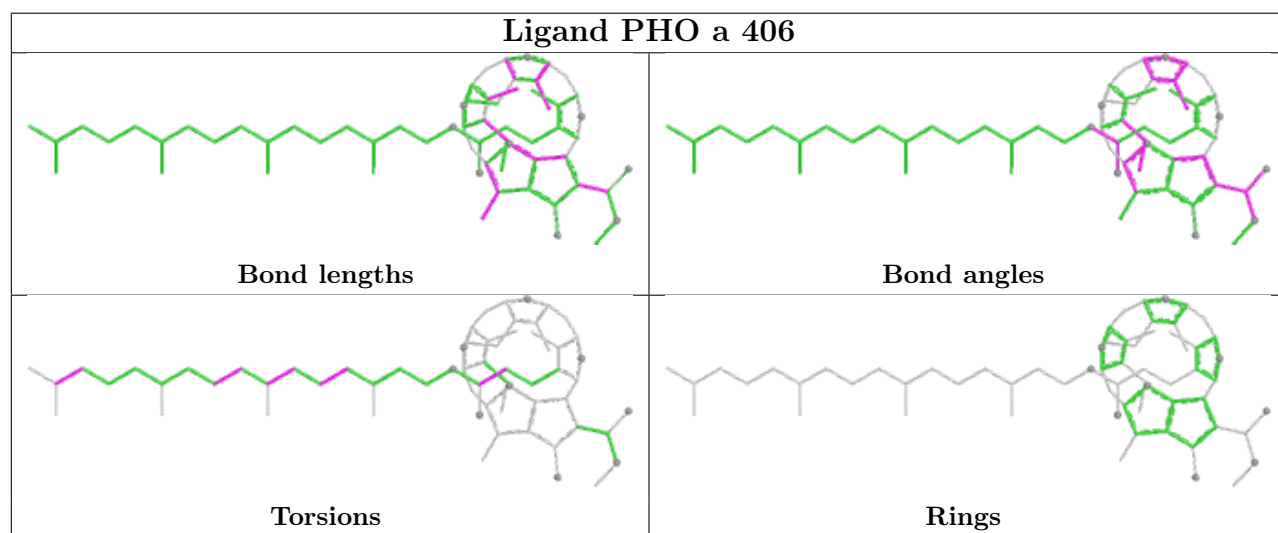
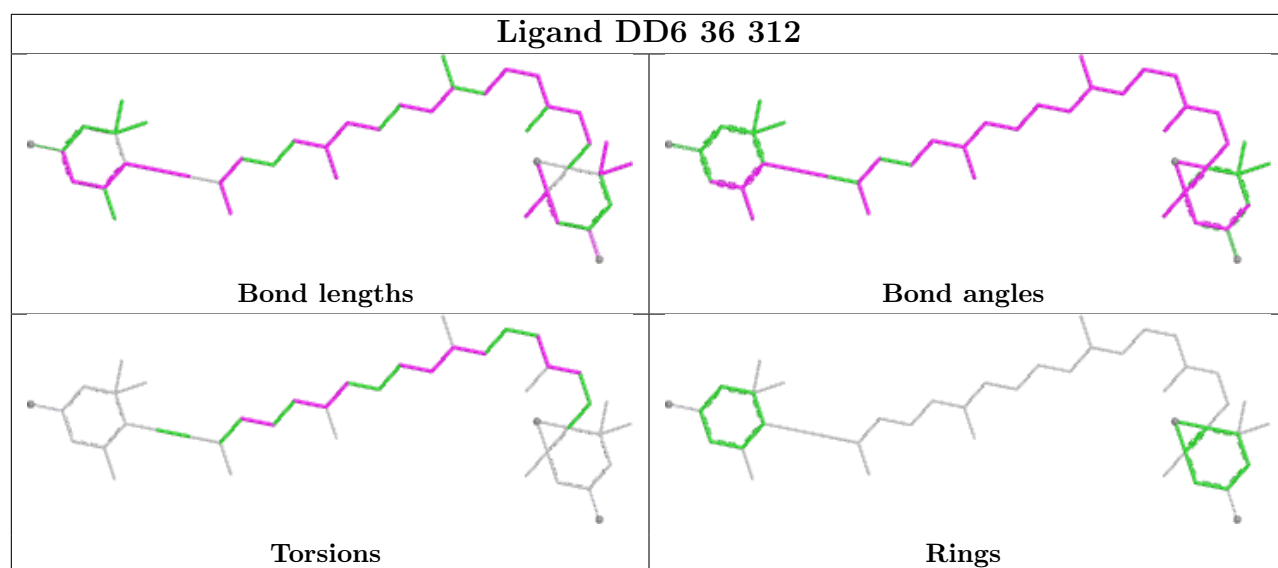


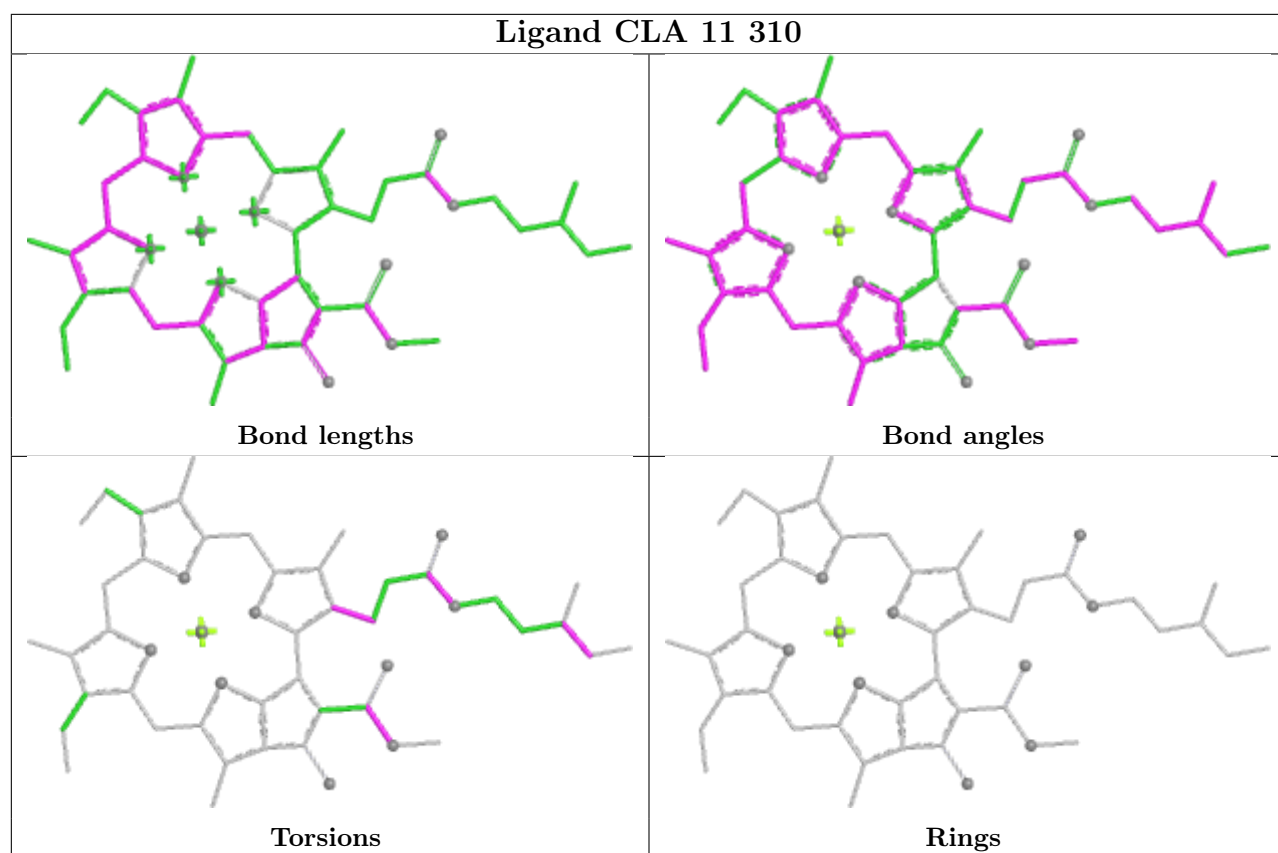


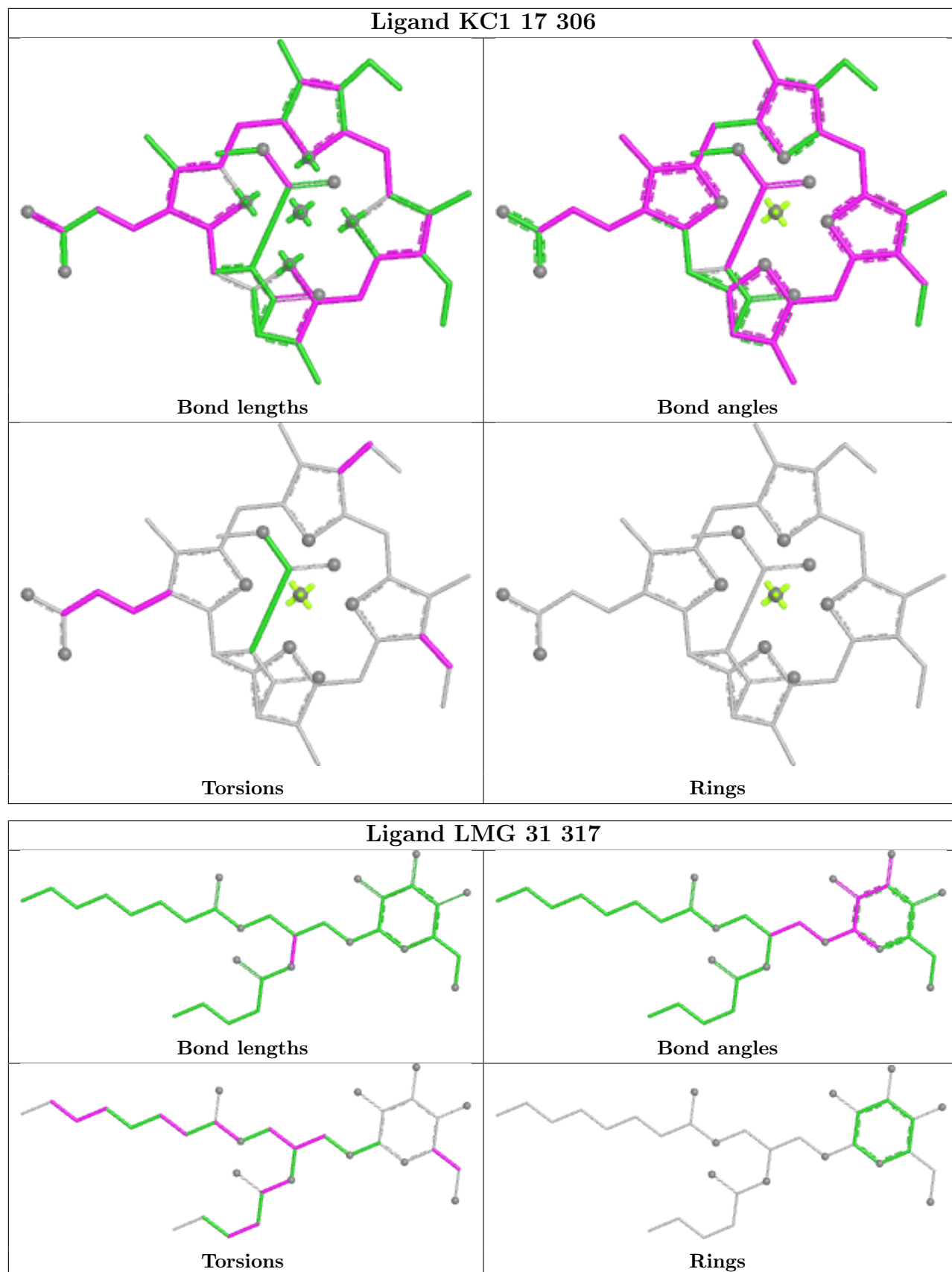


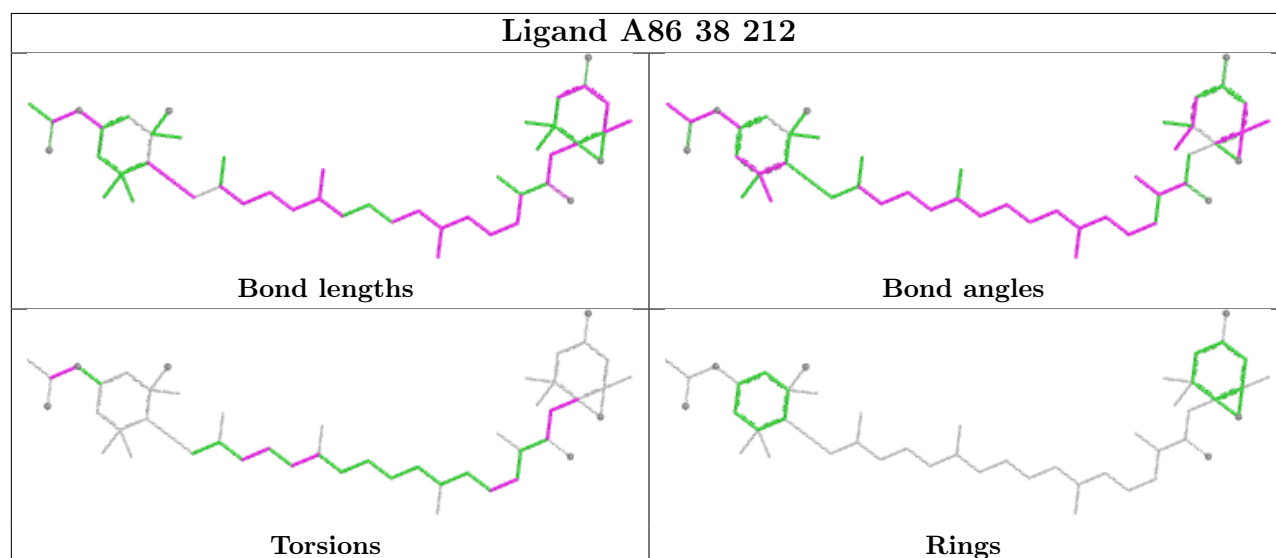
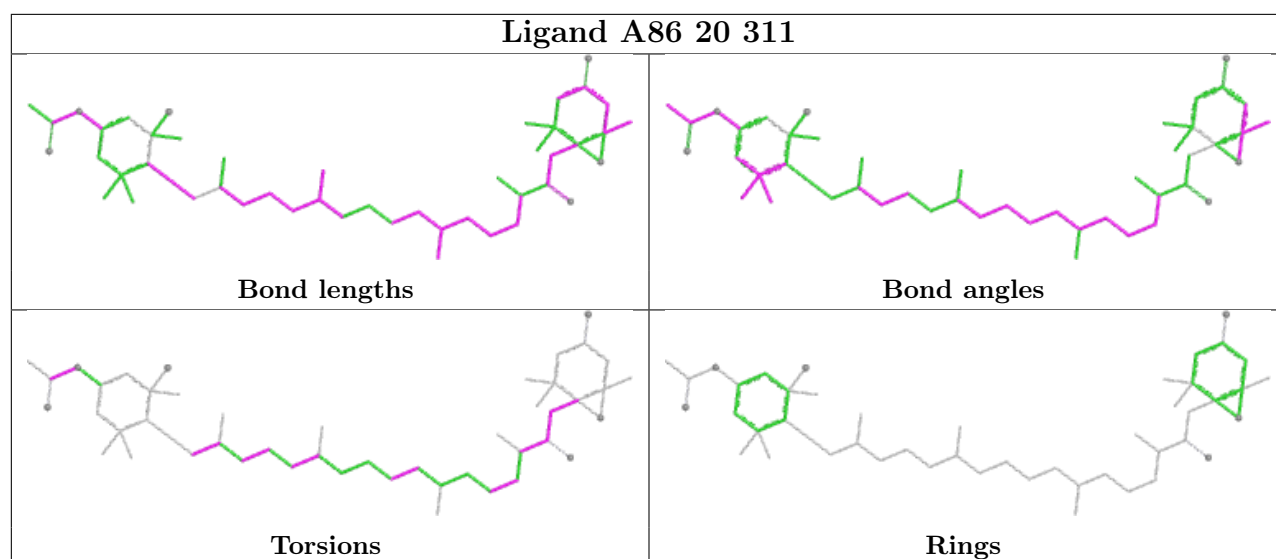


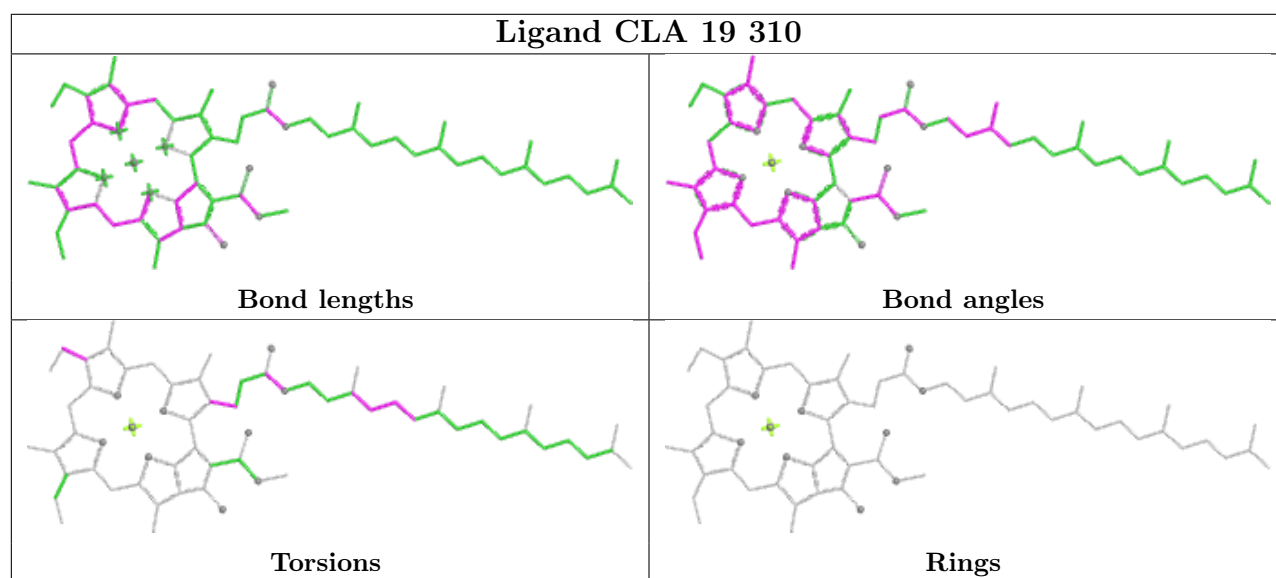
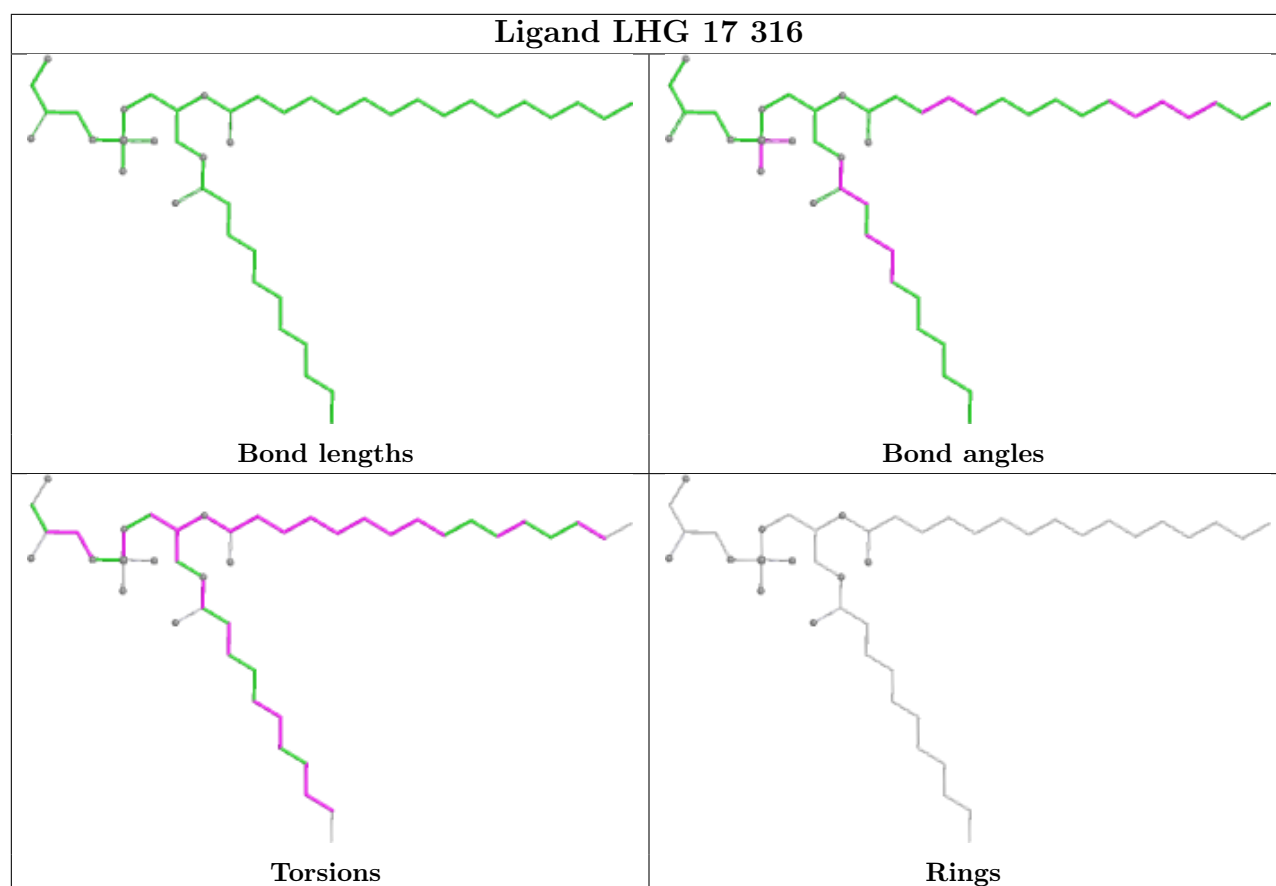


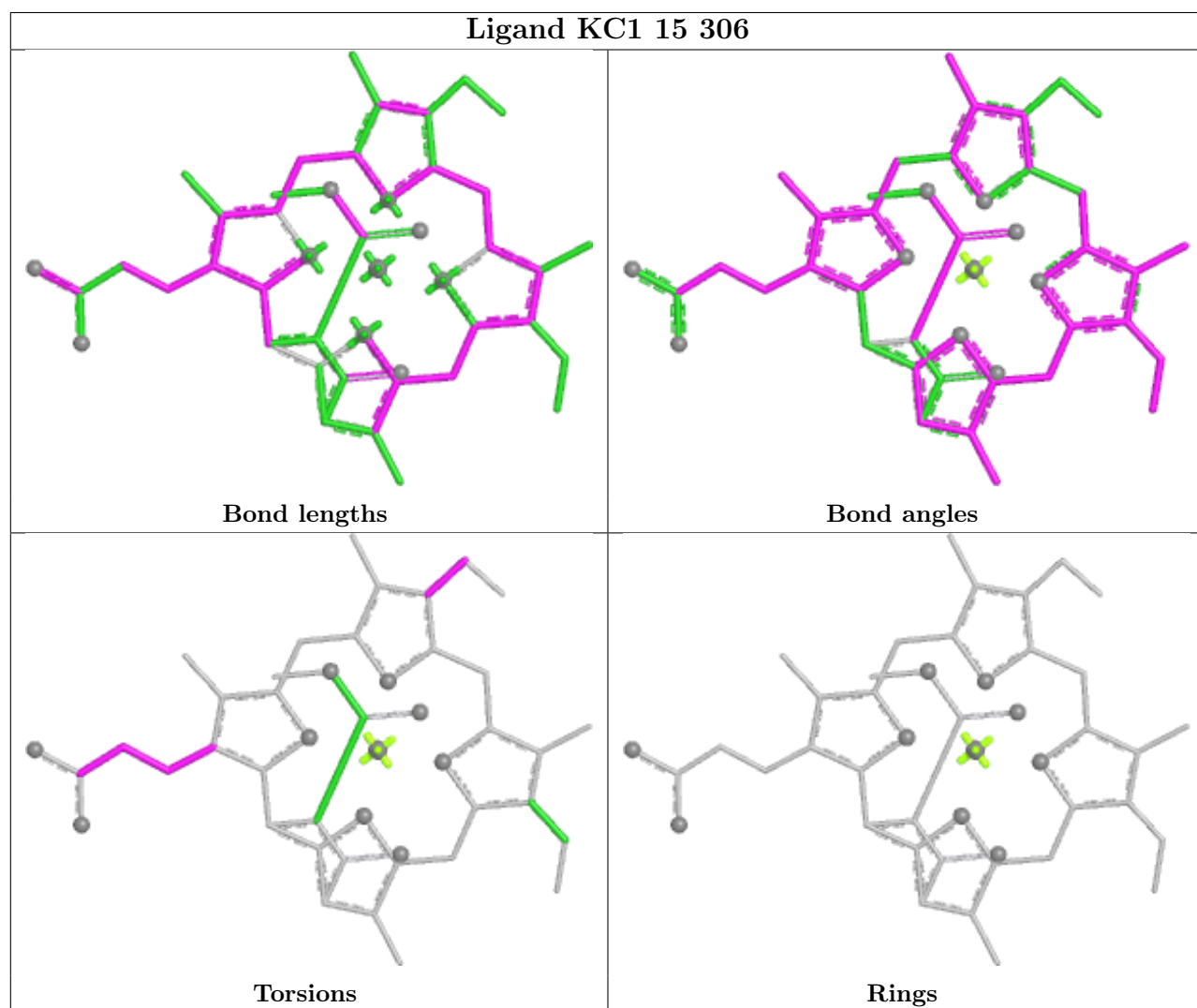
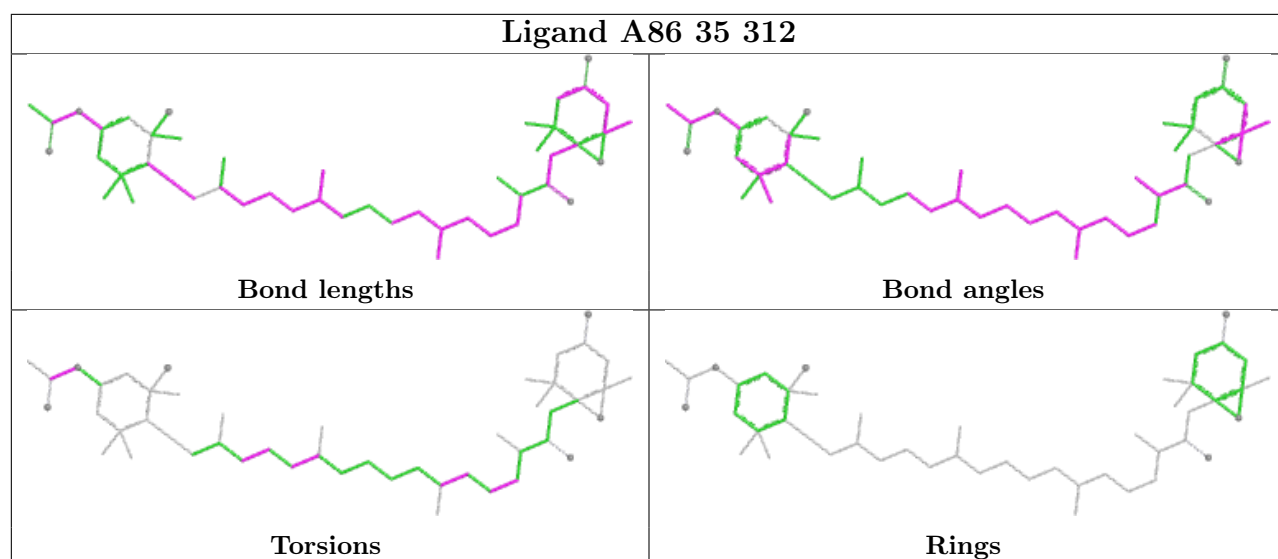


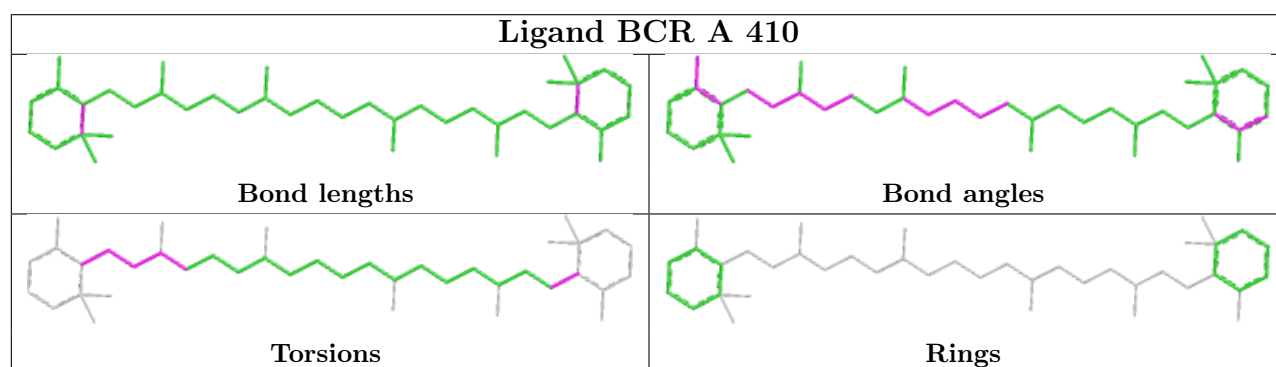
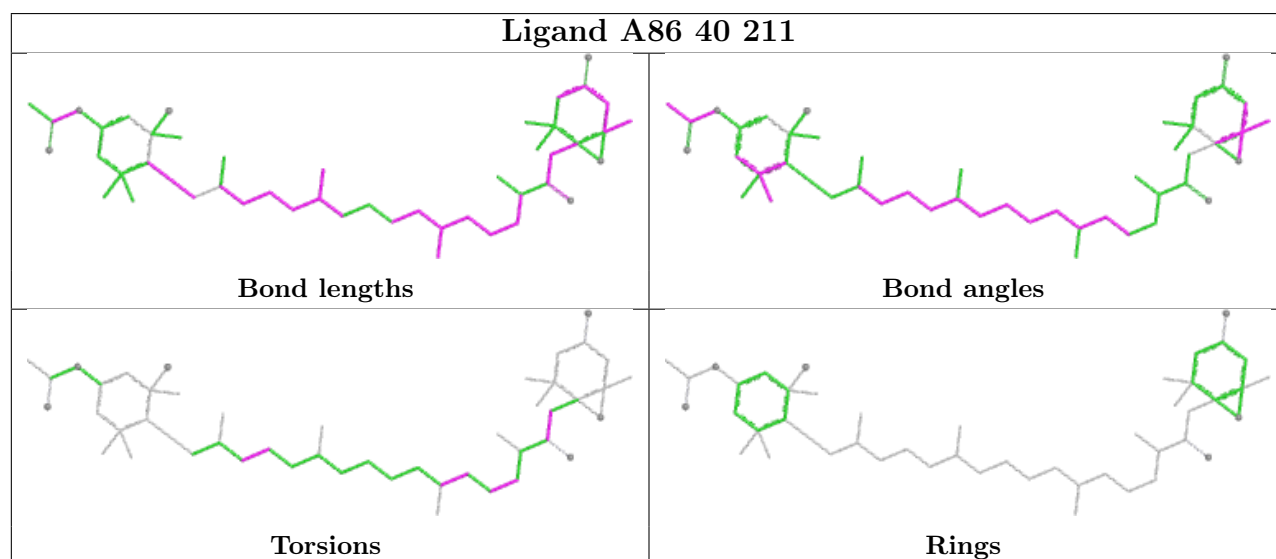
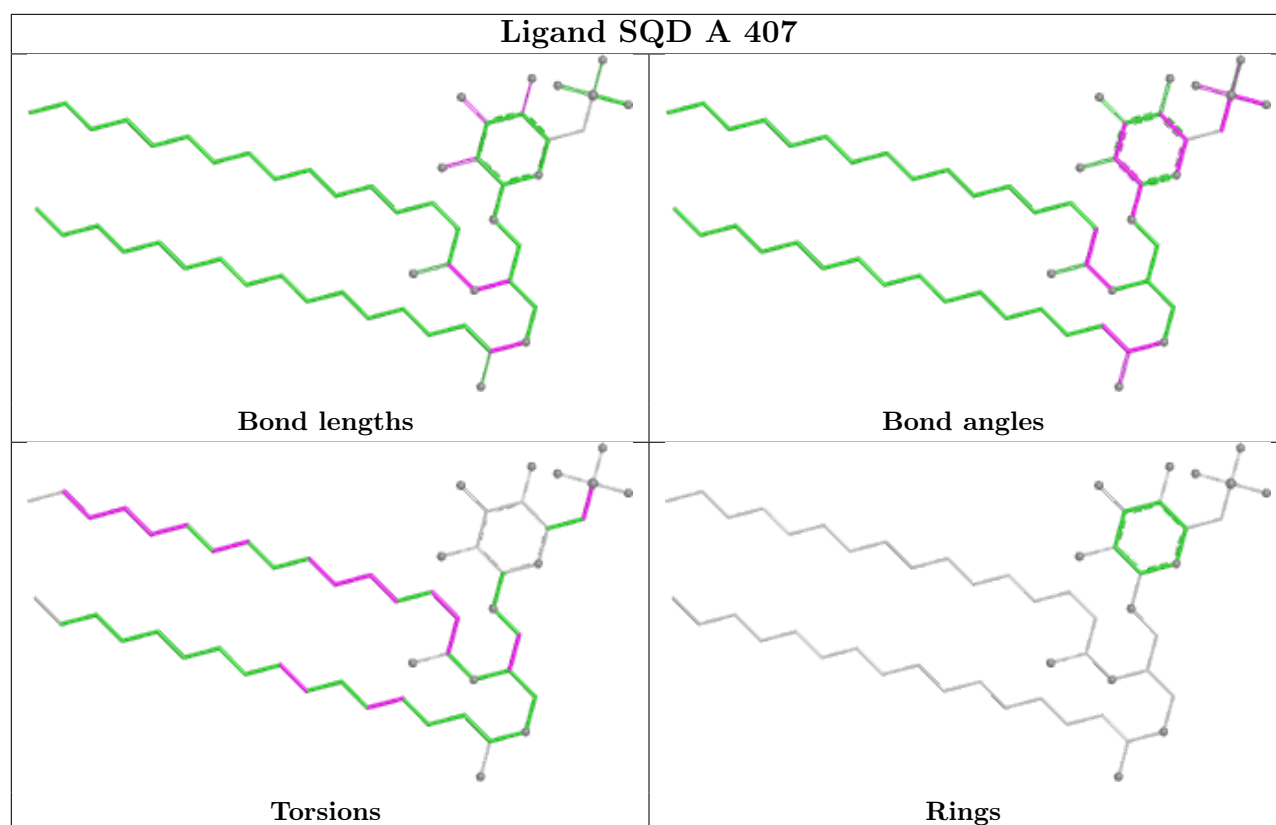


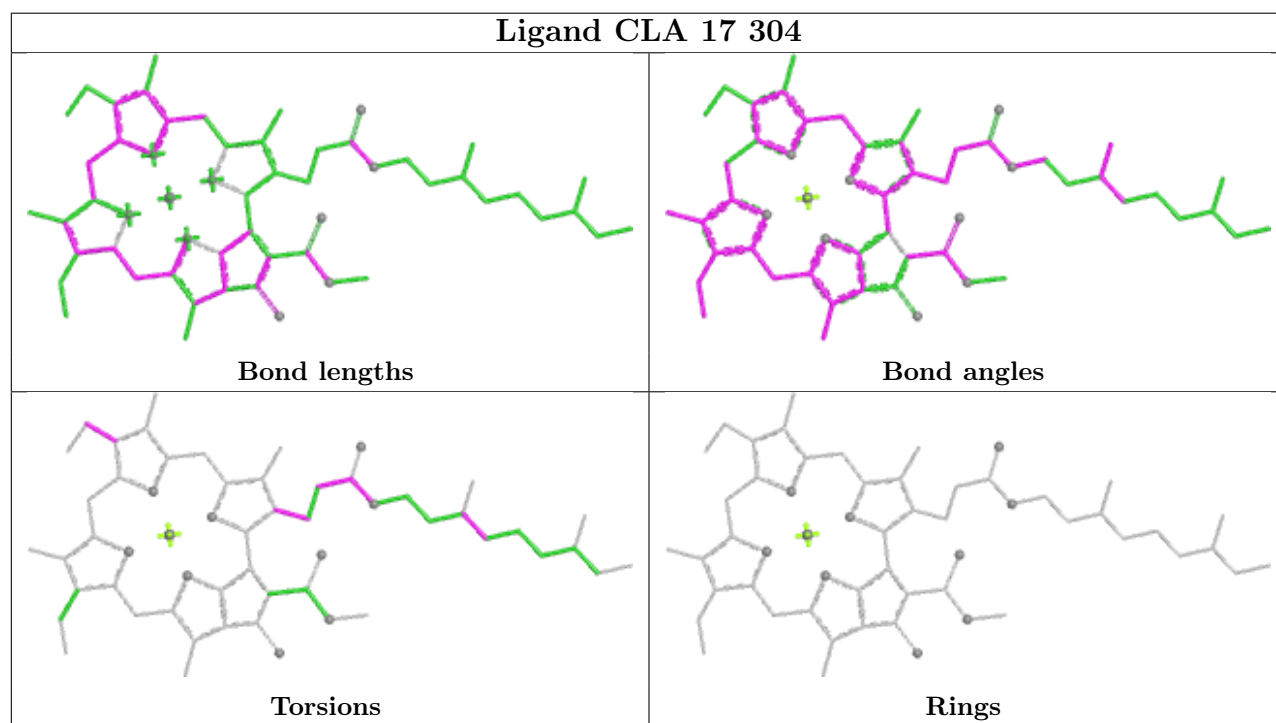
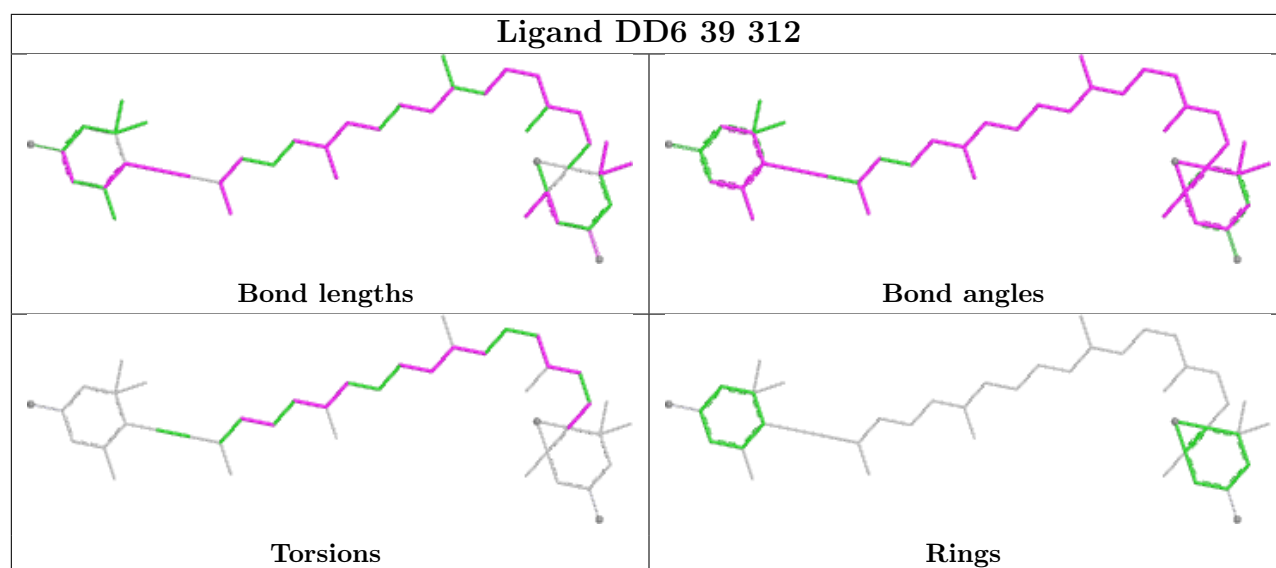


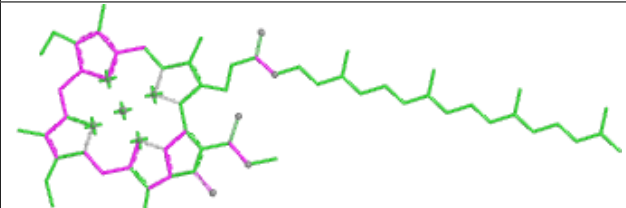
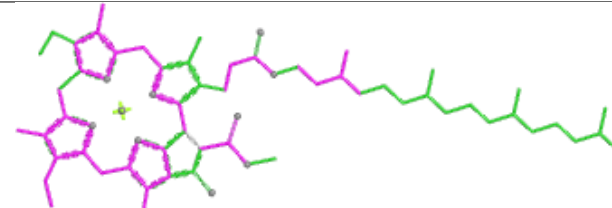
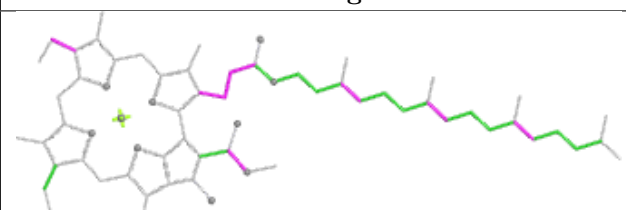
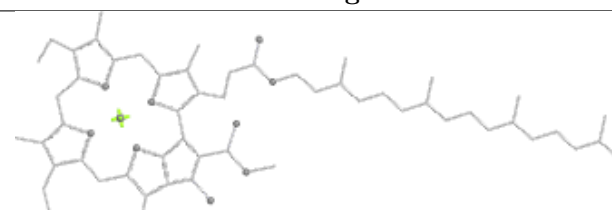


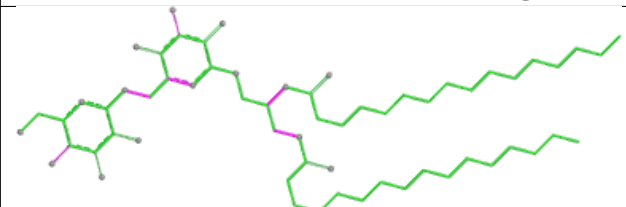
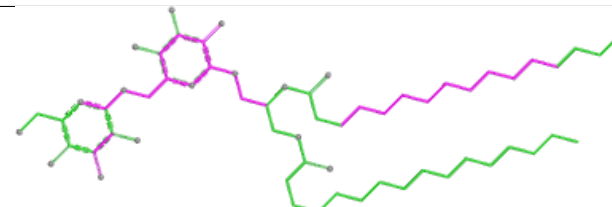
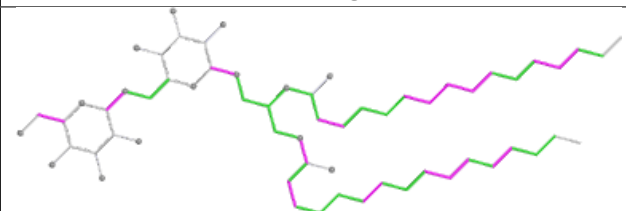
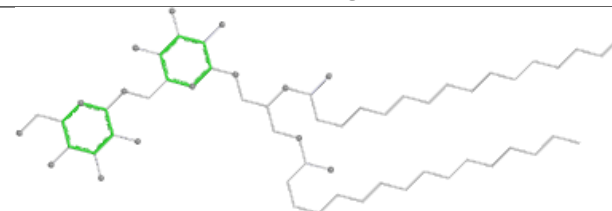


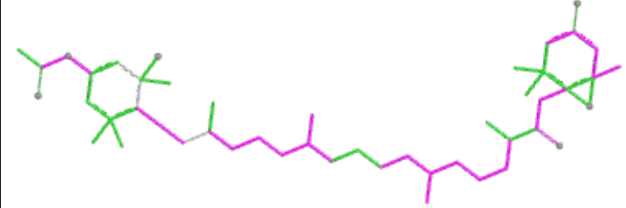
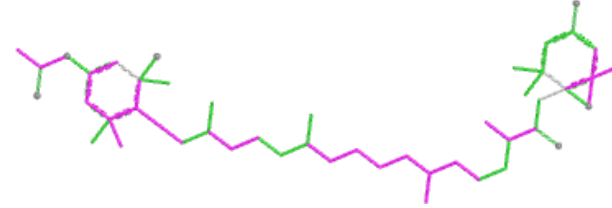
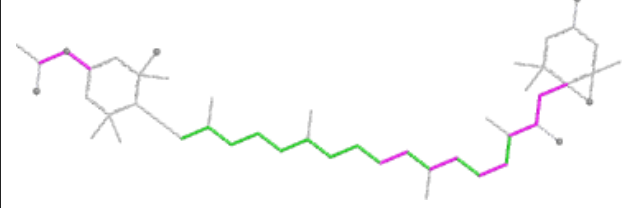
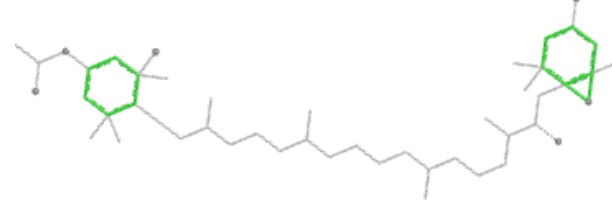


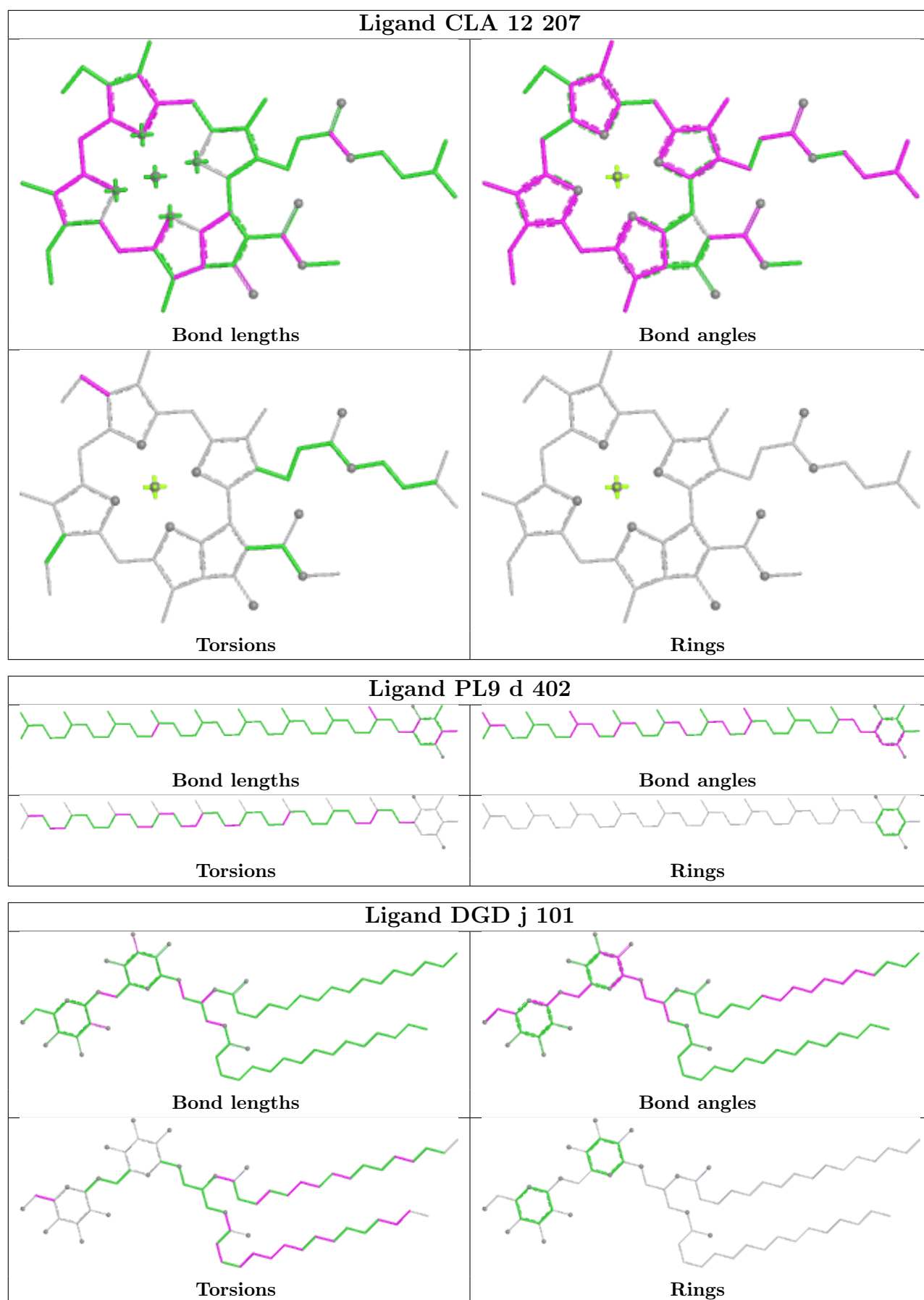


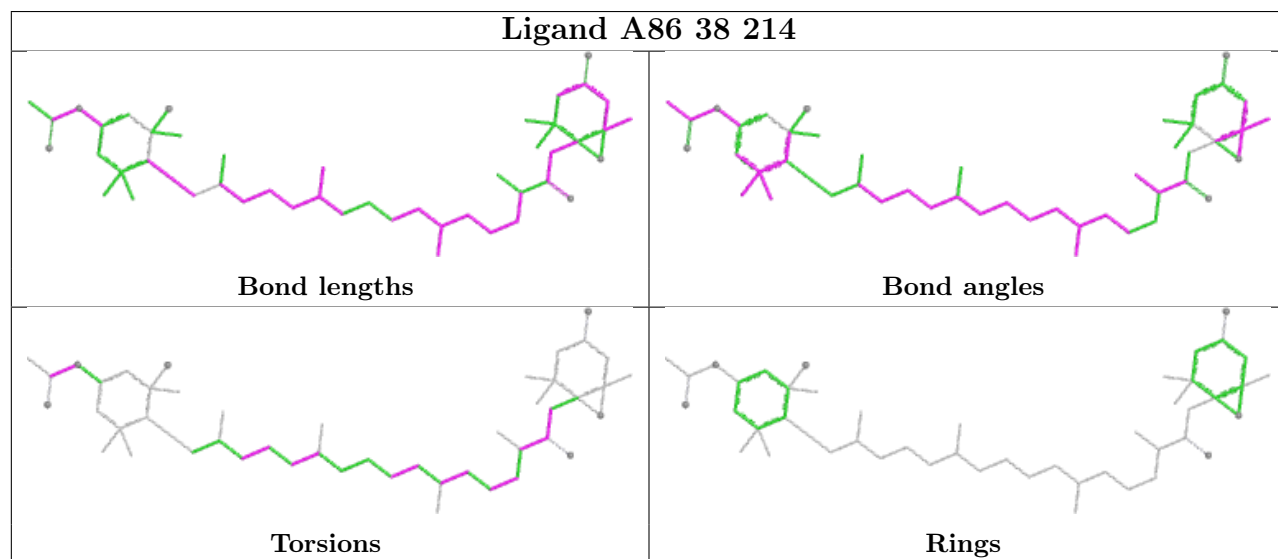
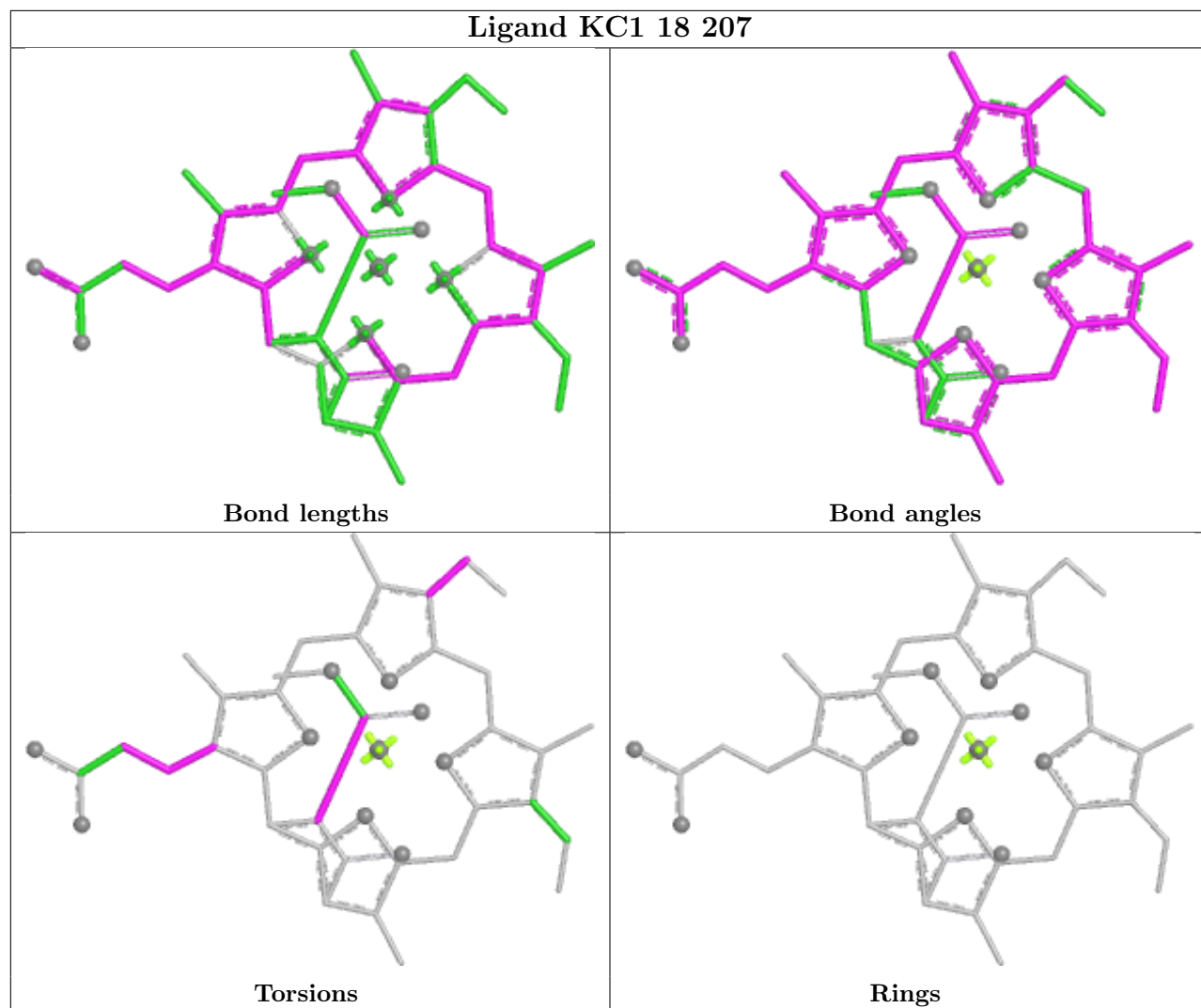


Ligand CLA 38 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

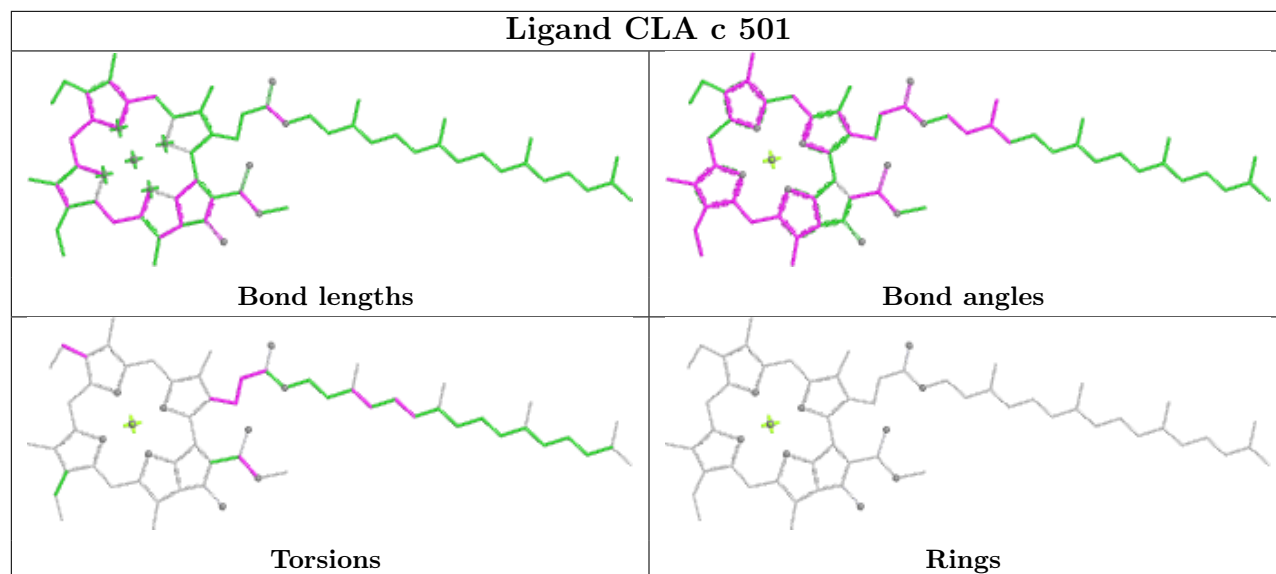
Ligand DGD C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A86 18 215	
	
Bond lengths	Bond angles
	
Torsions	Rings

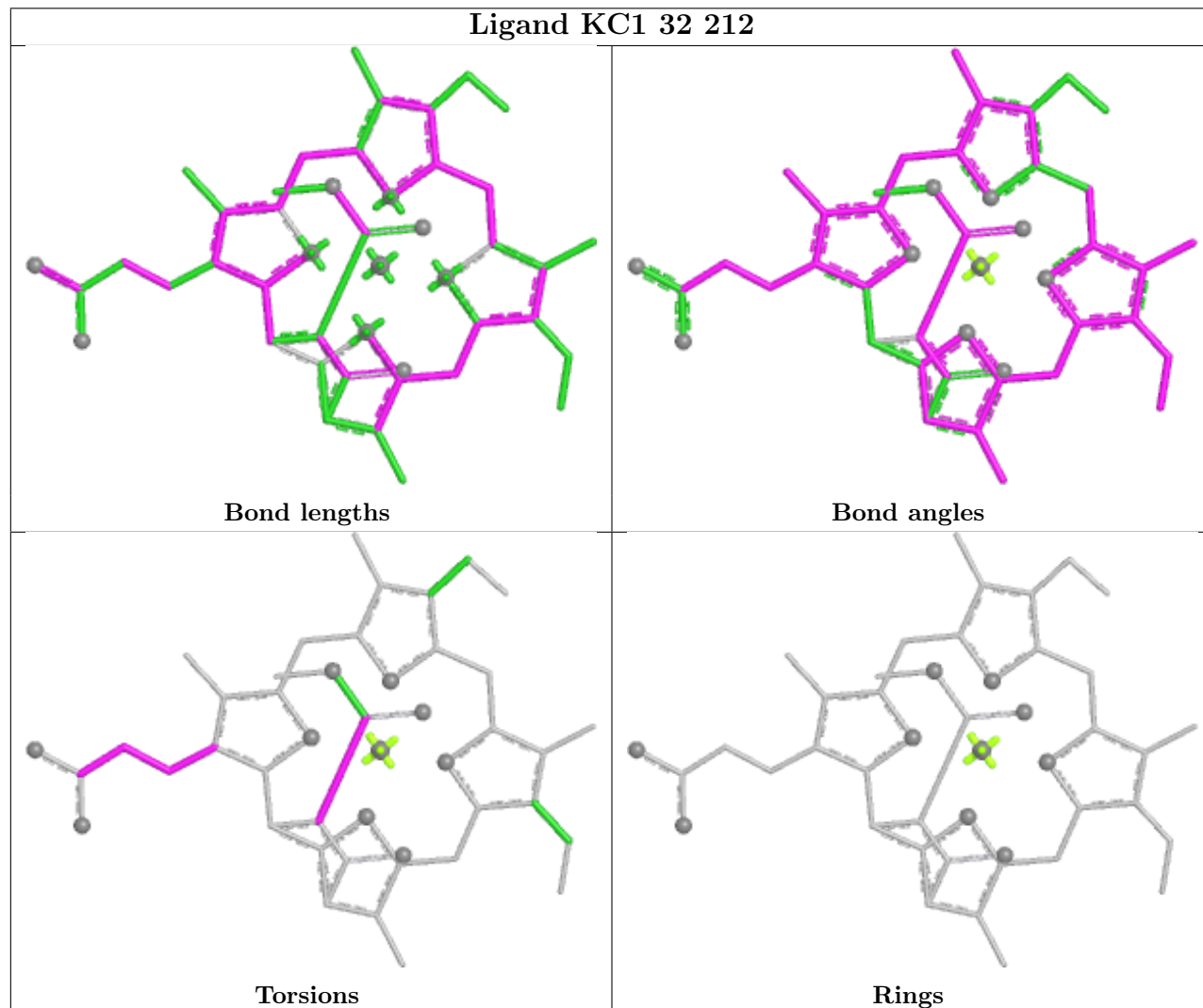


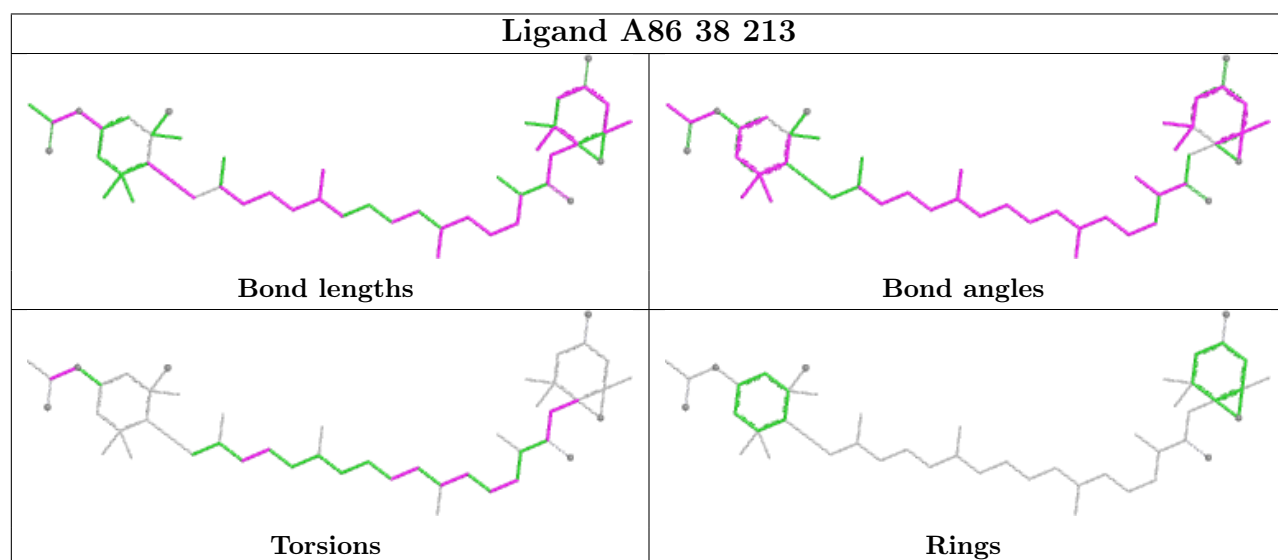
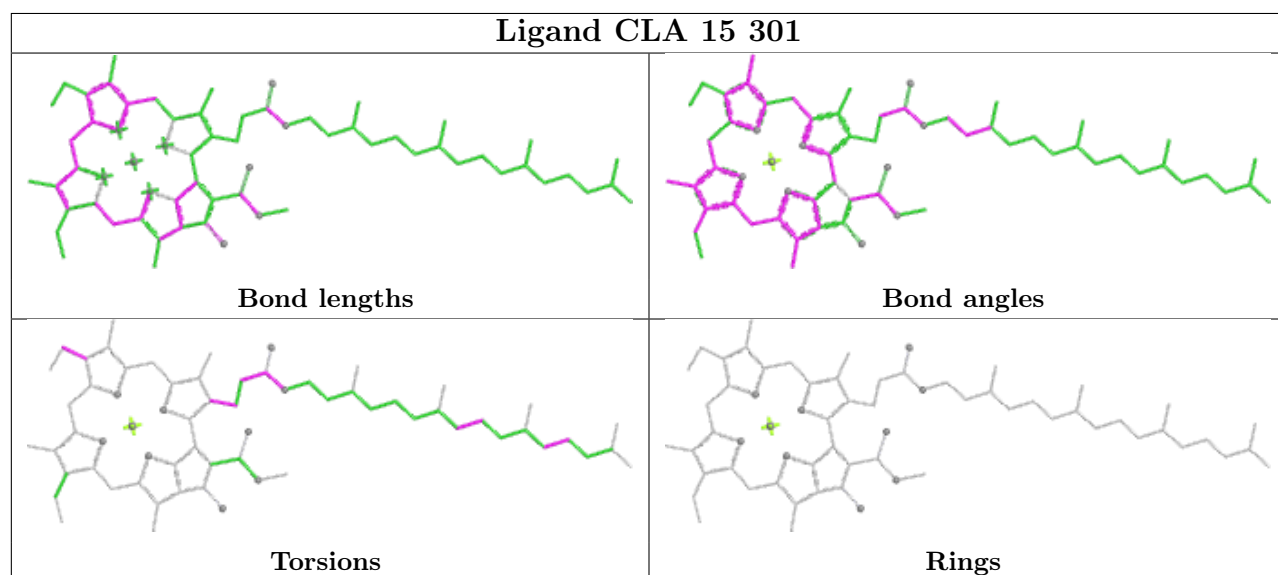
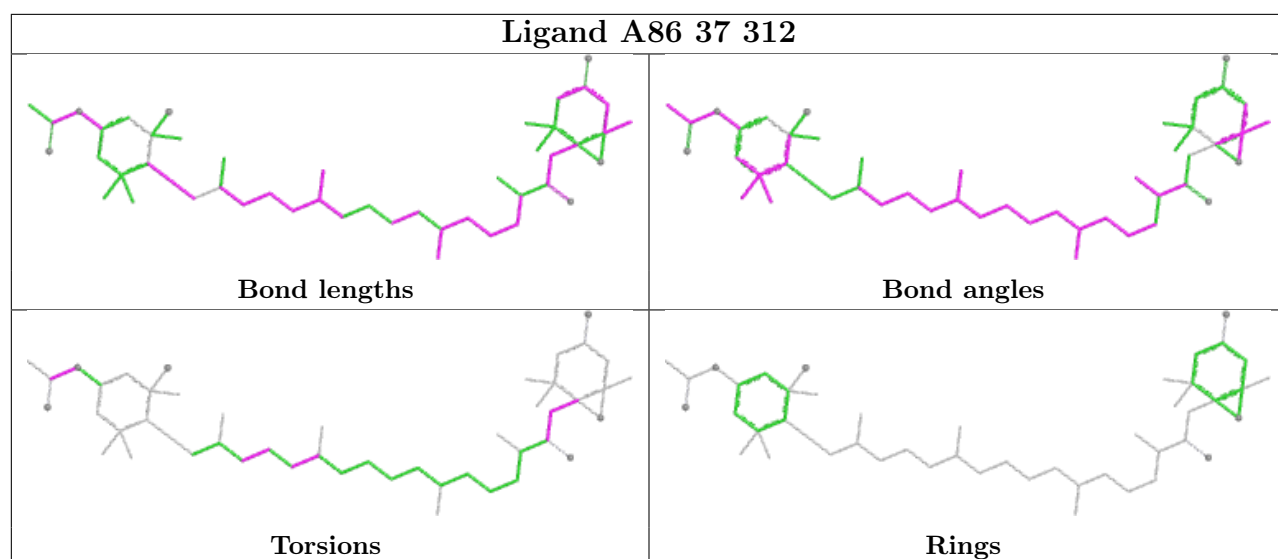


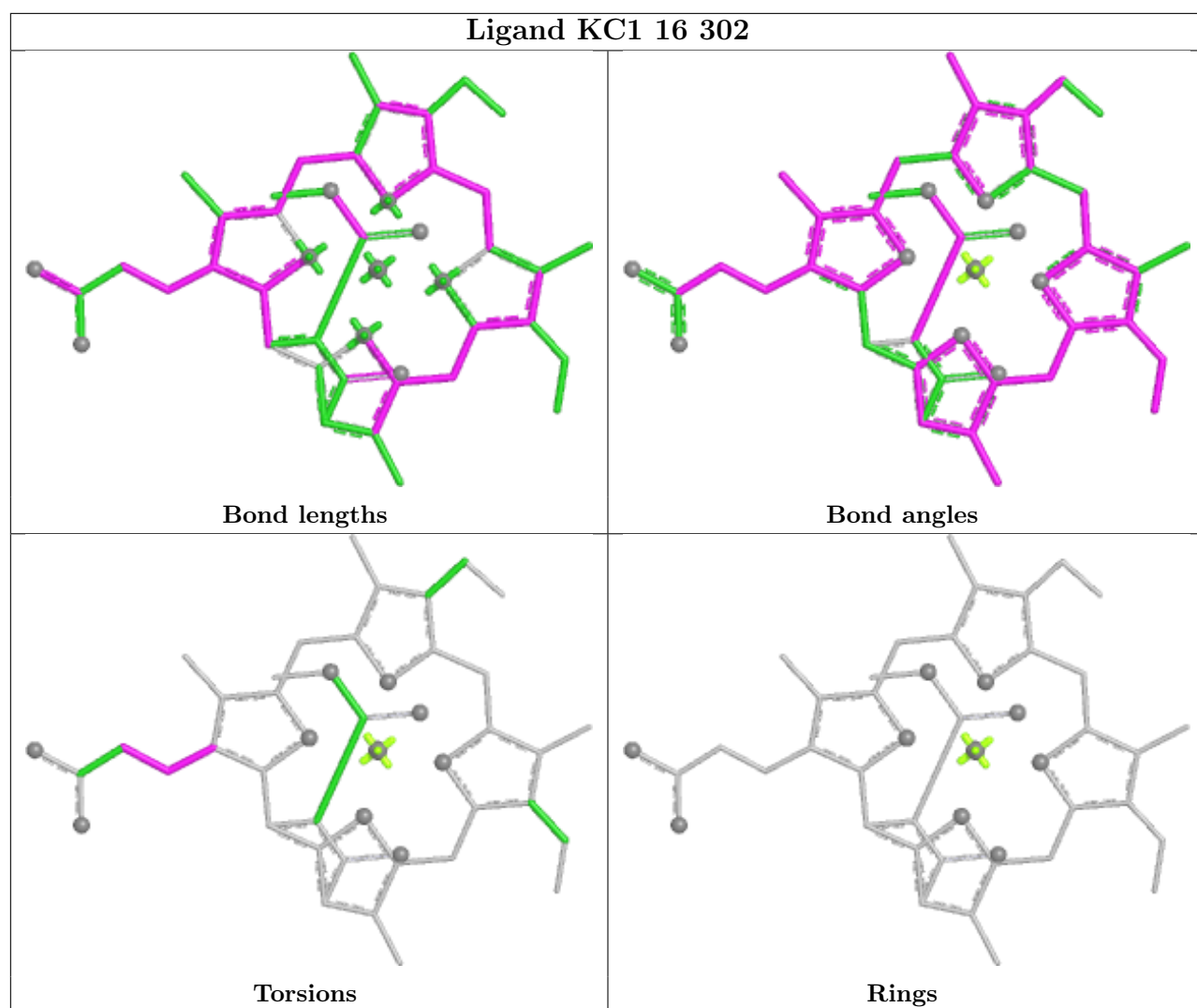
Ligand CLA c 501

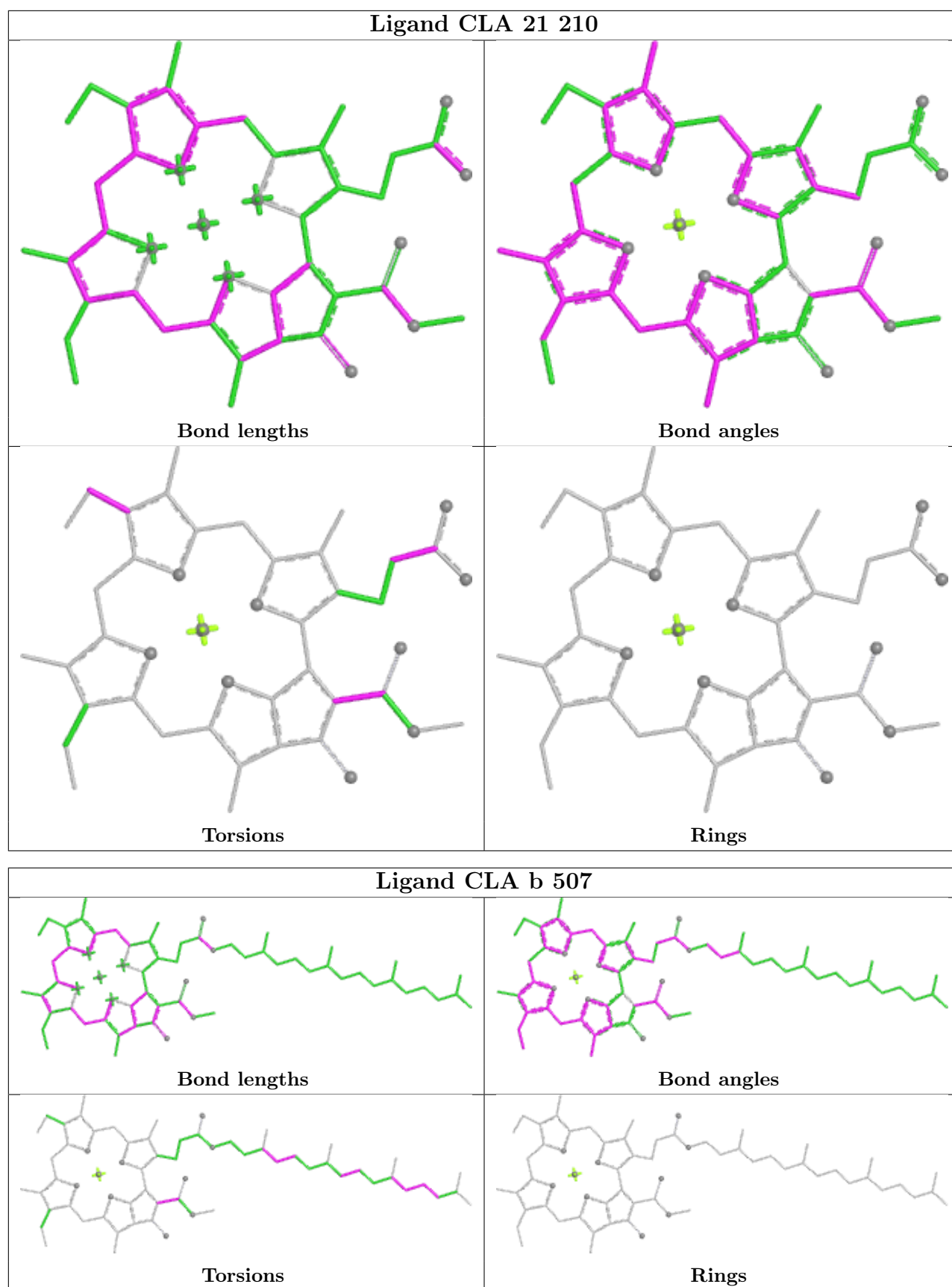


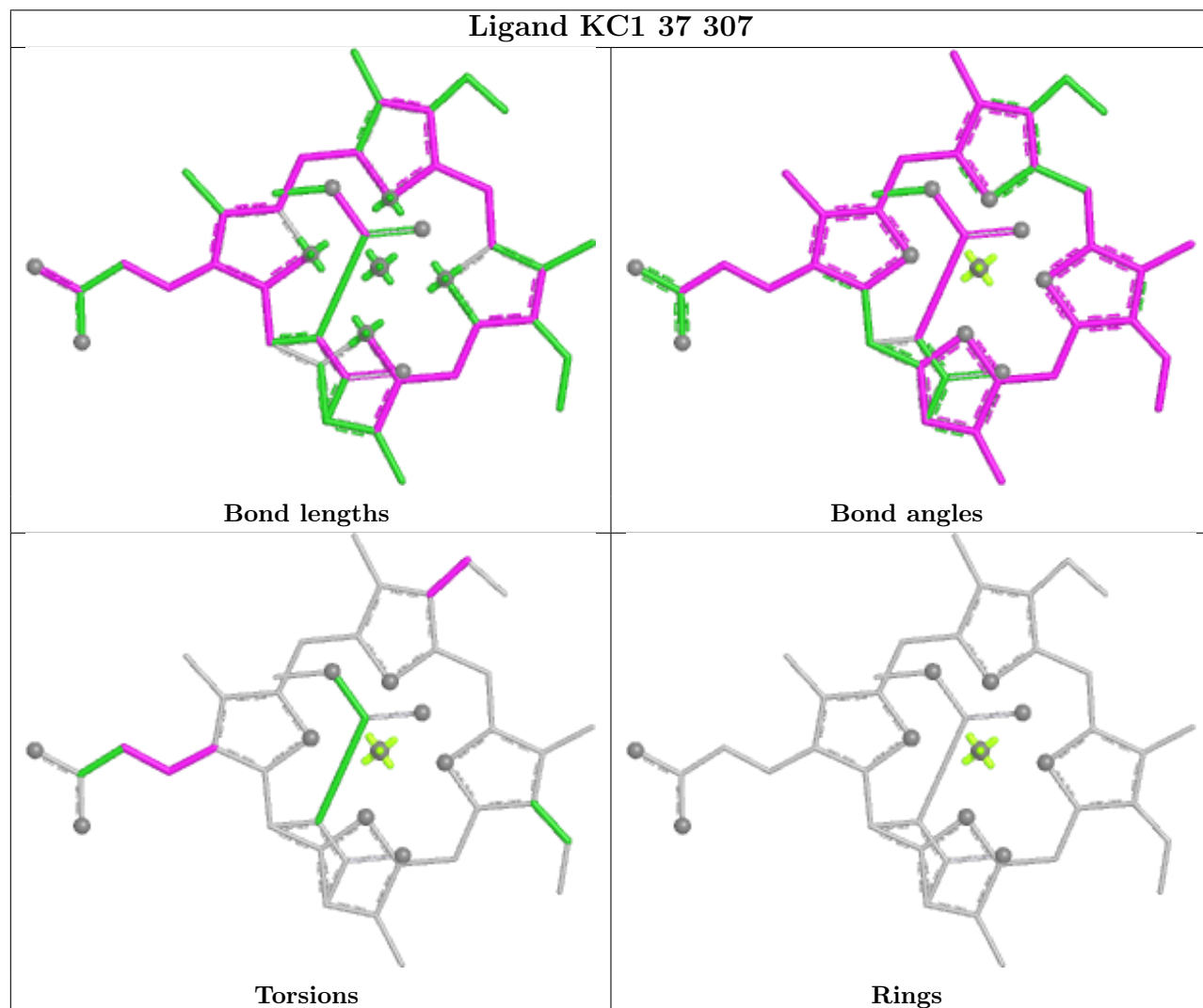
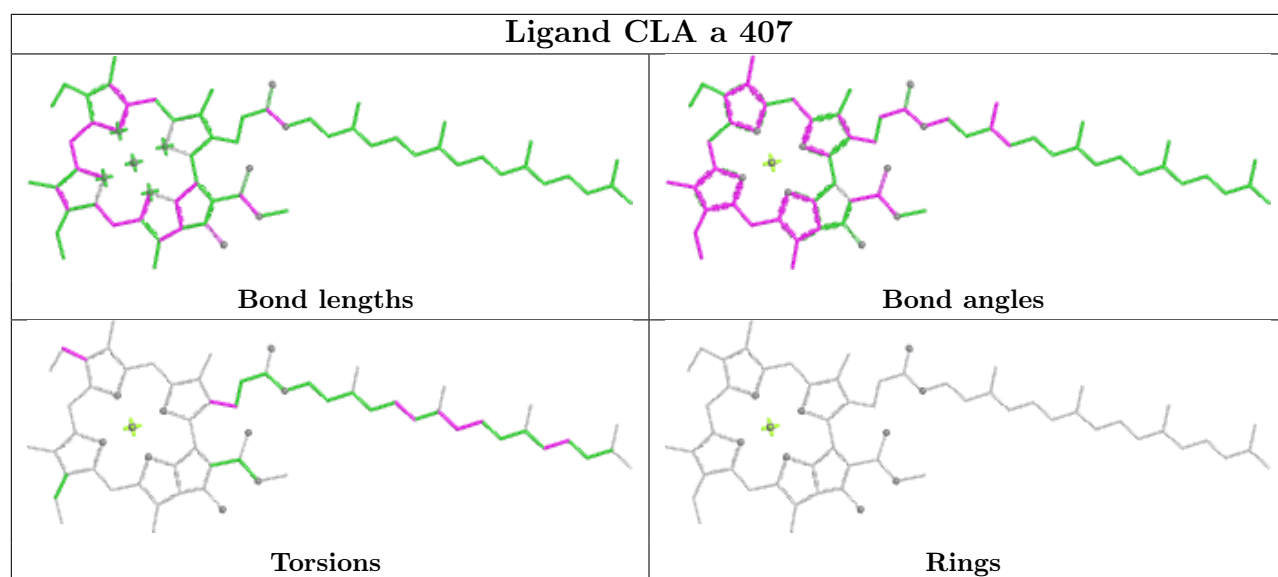
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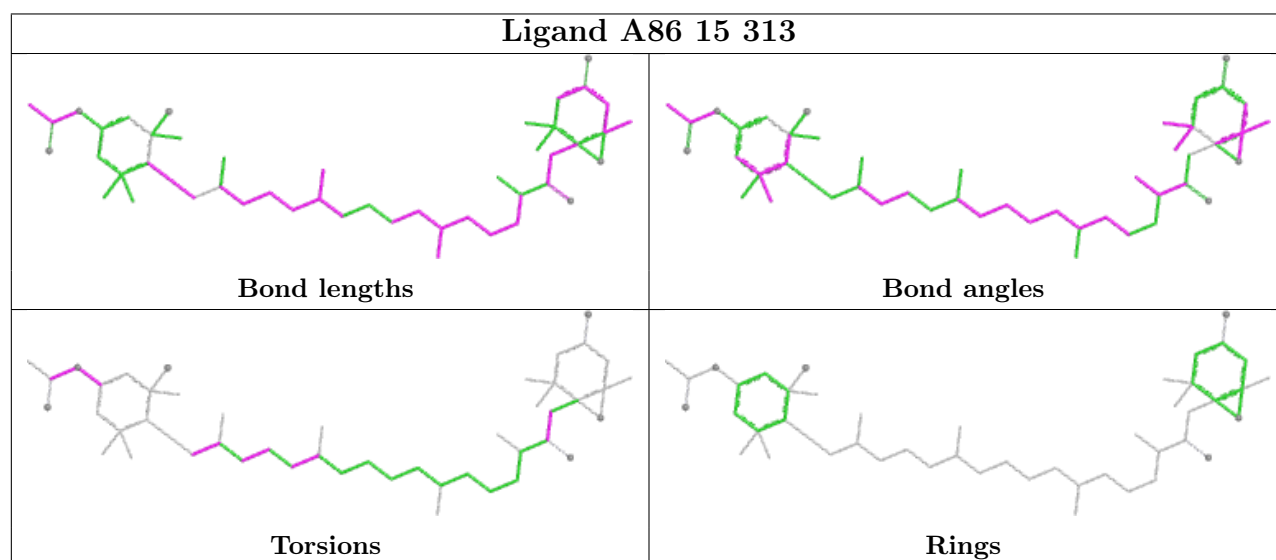
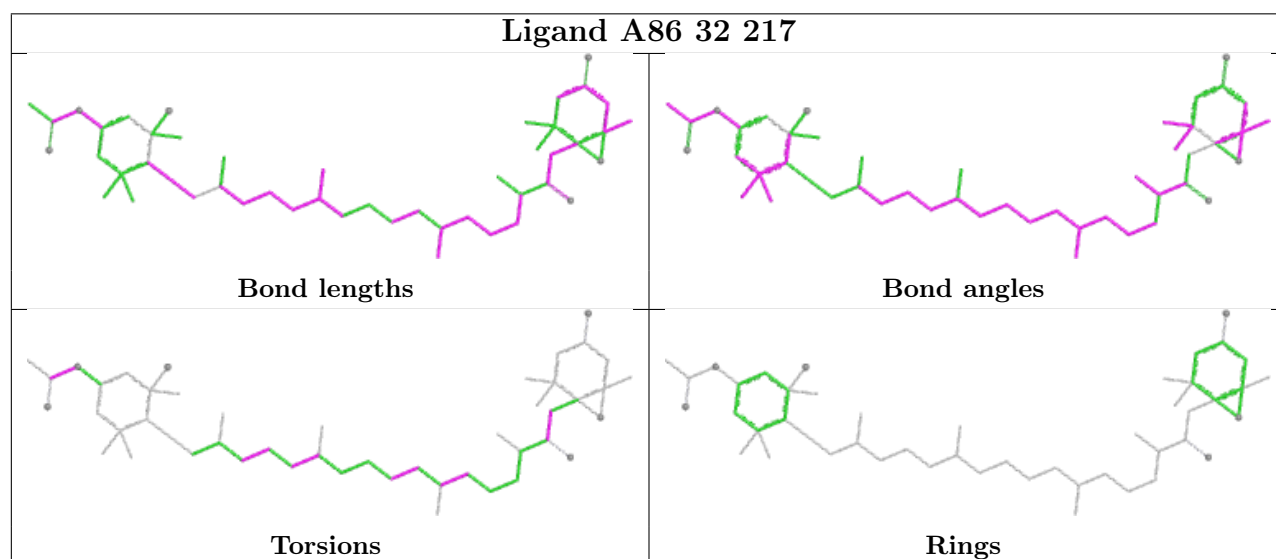
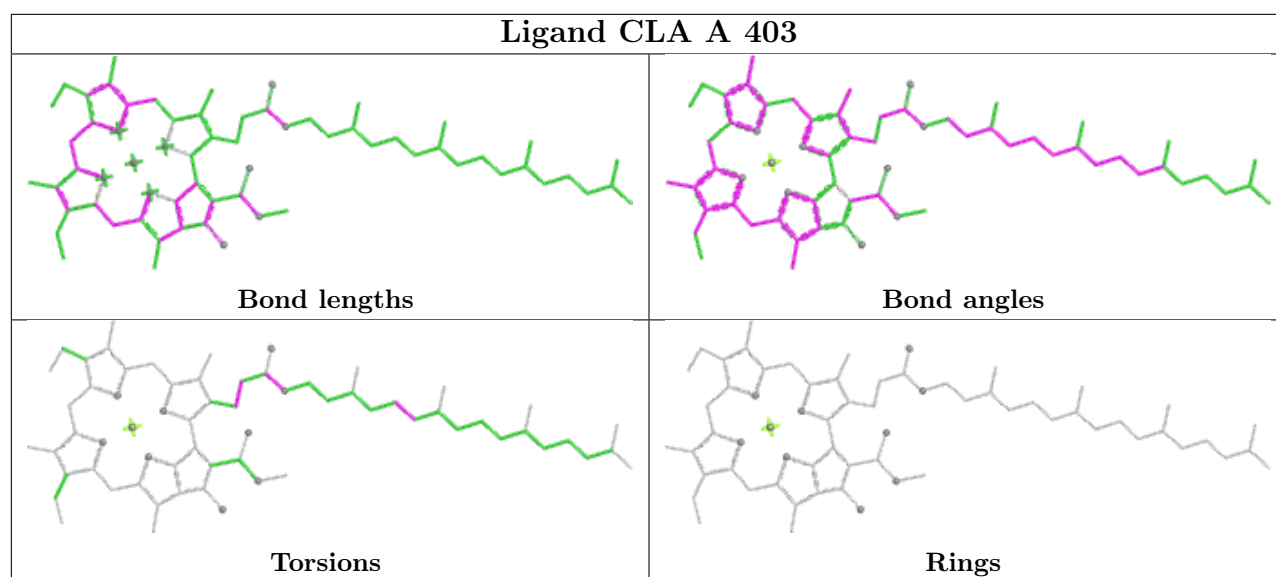


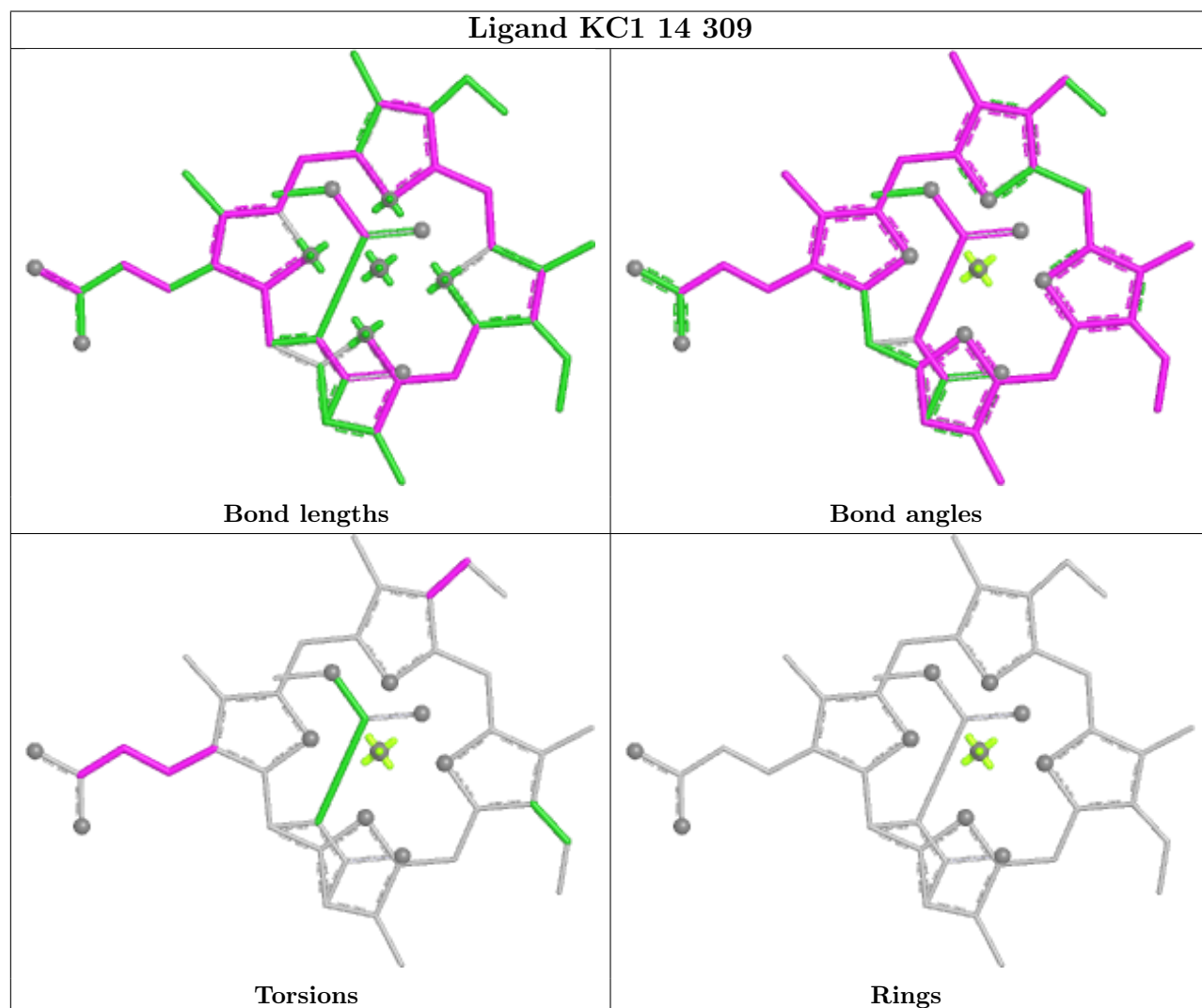
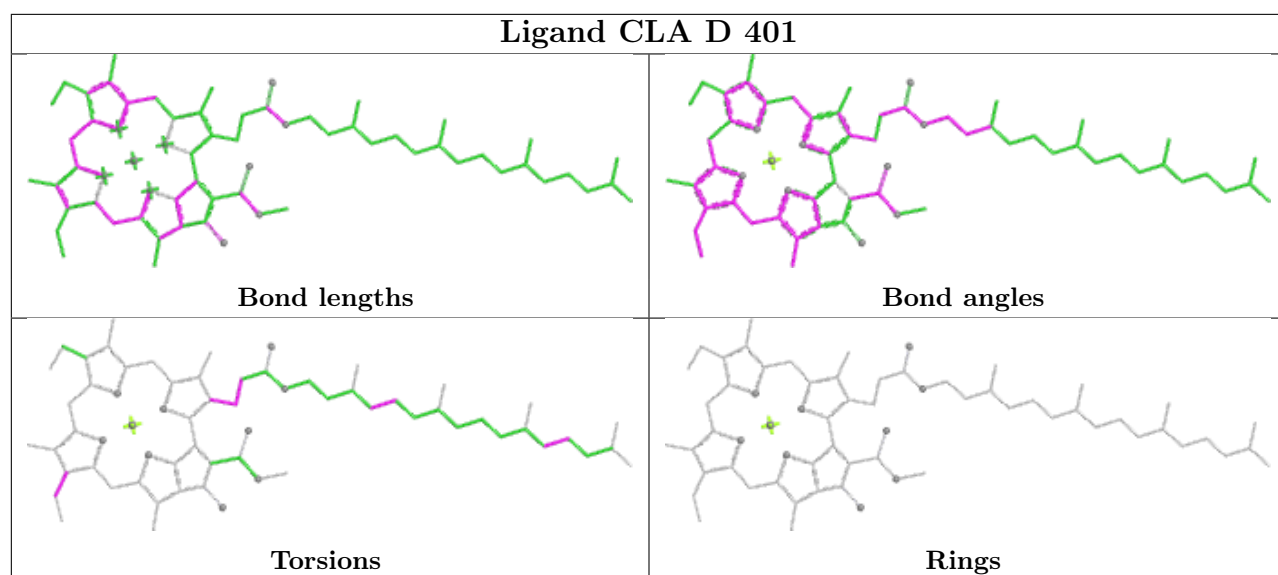


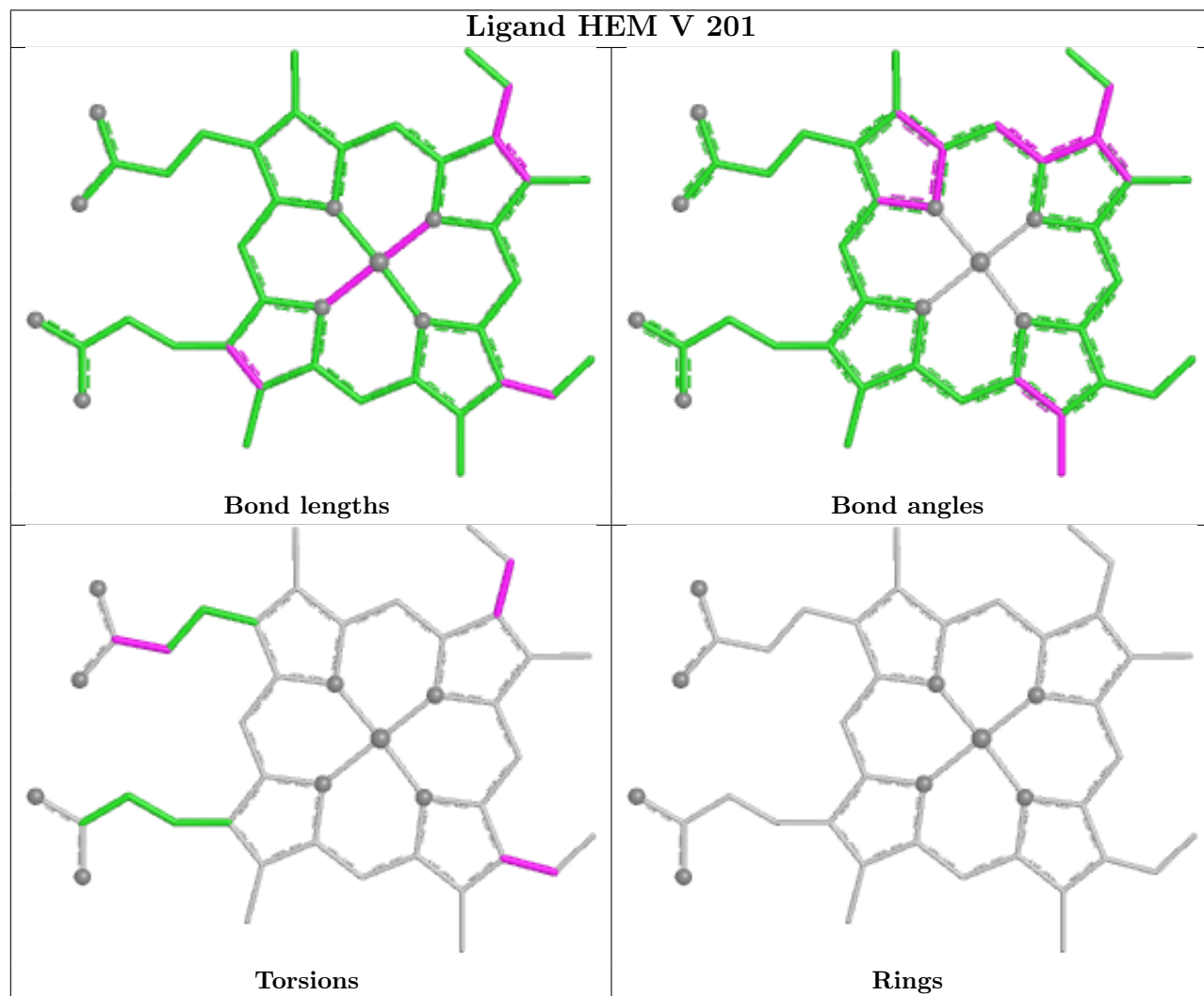
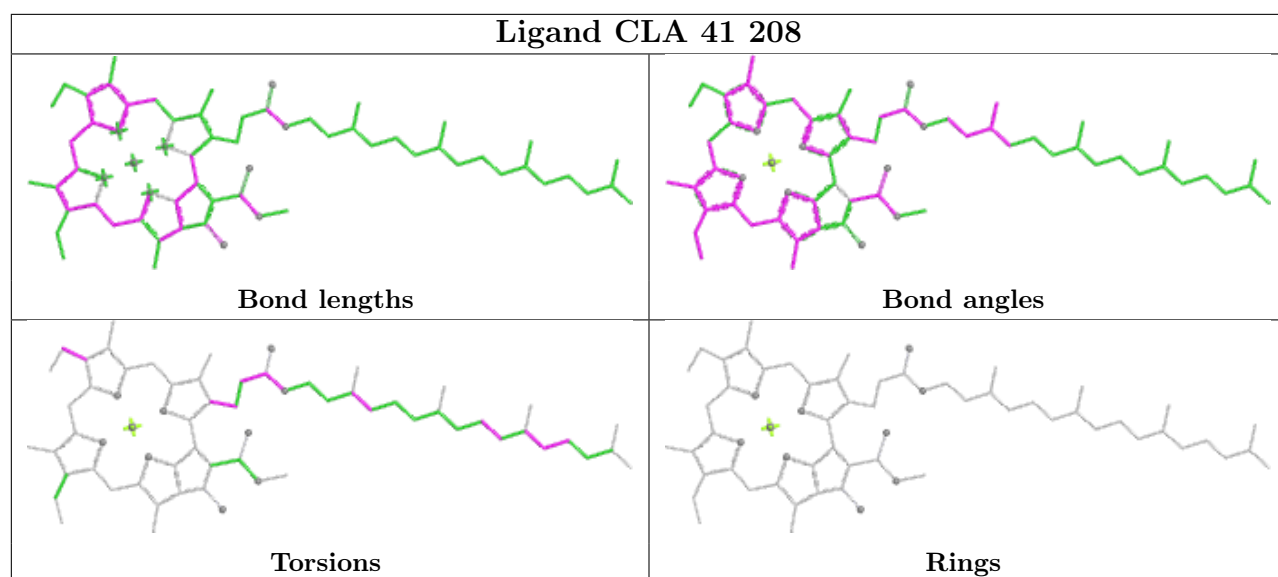


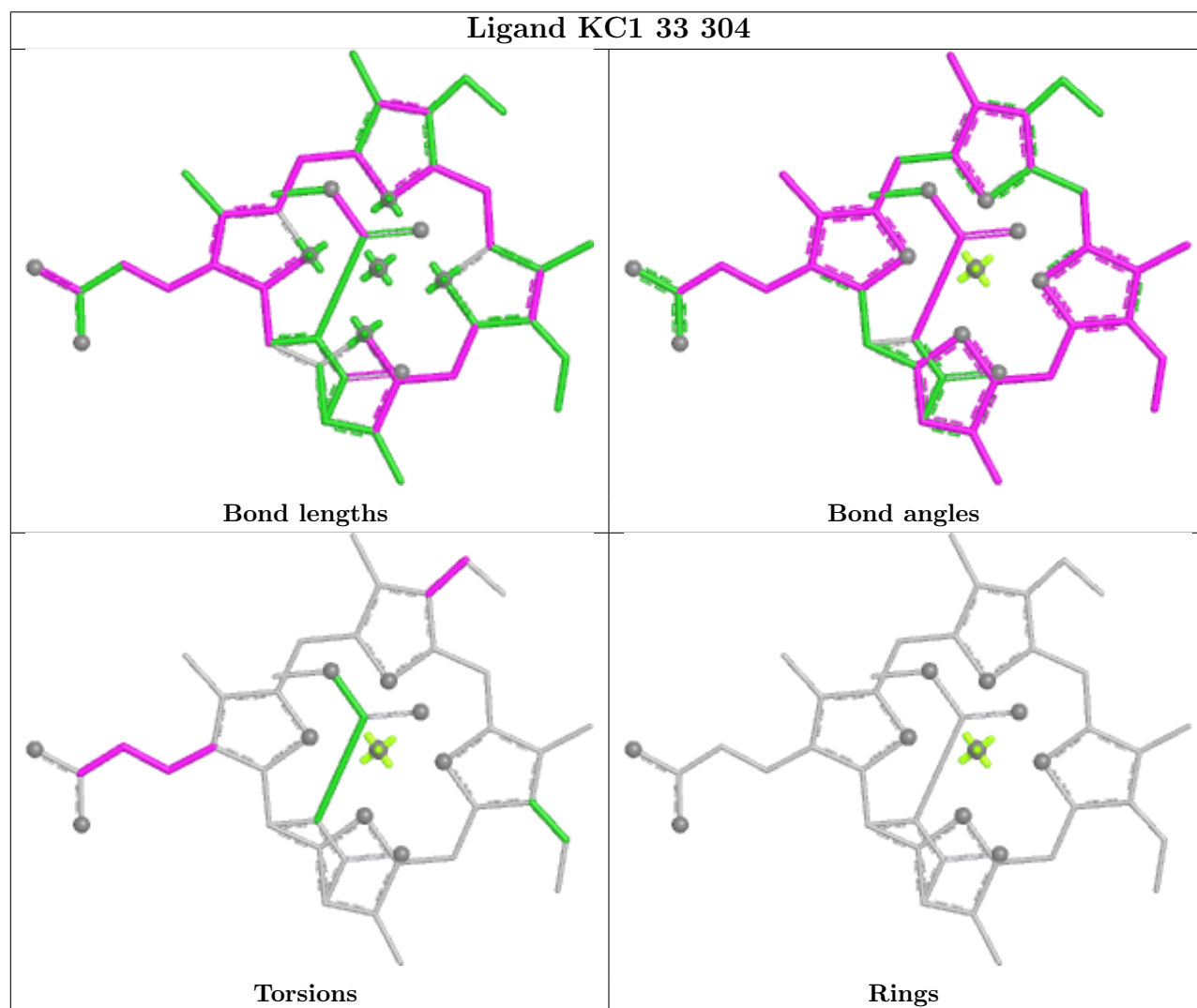
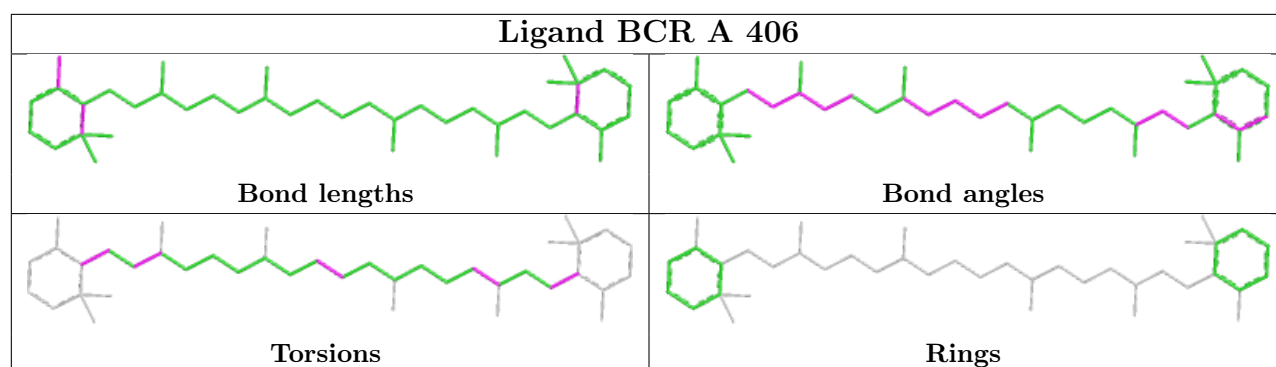


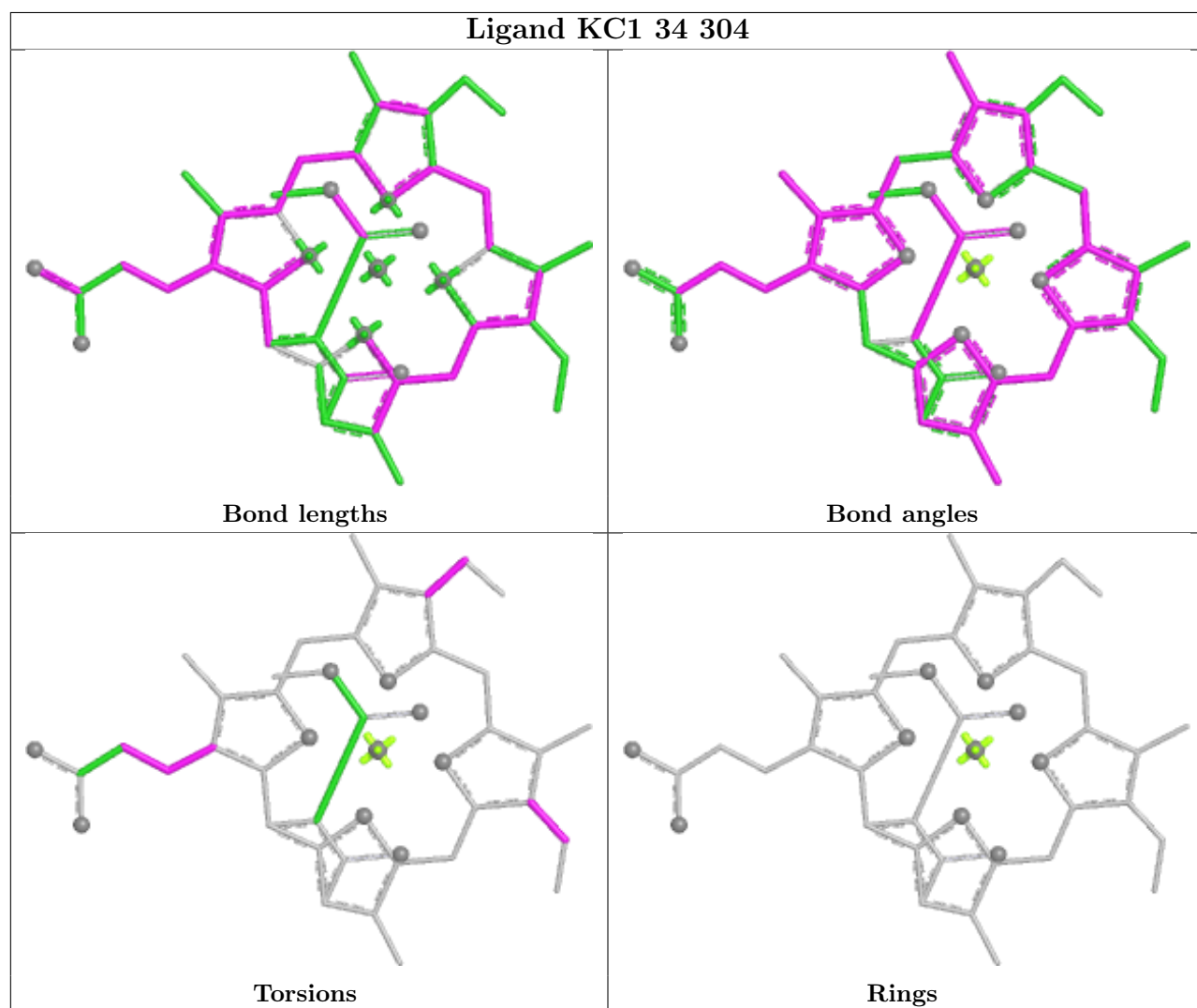
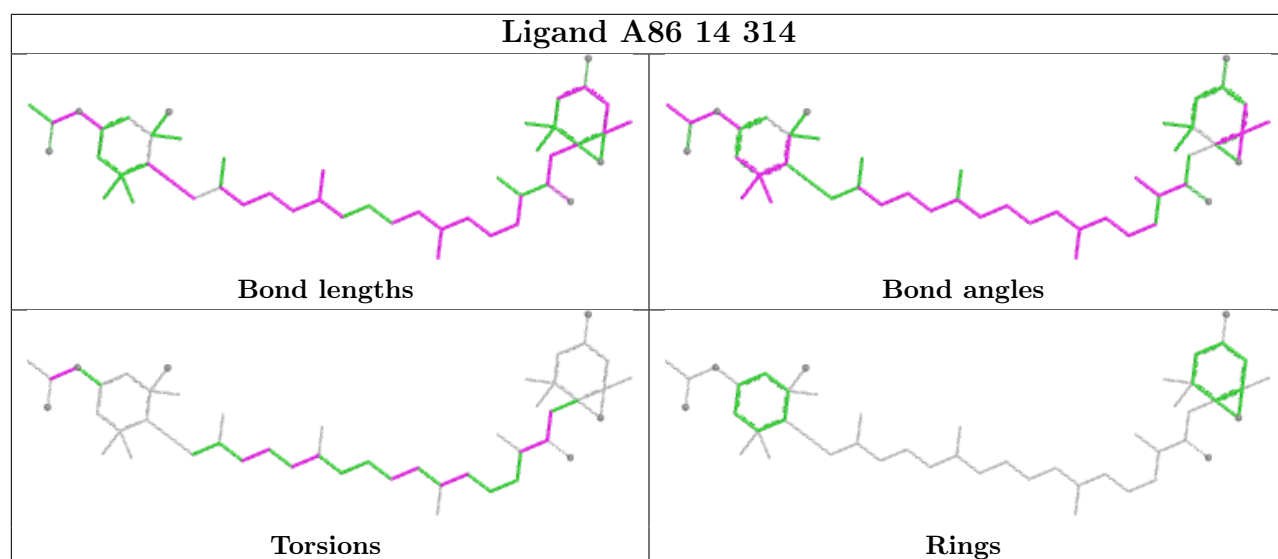


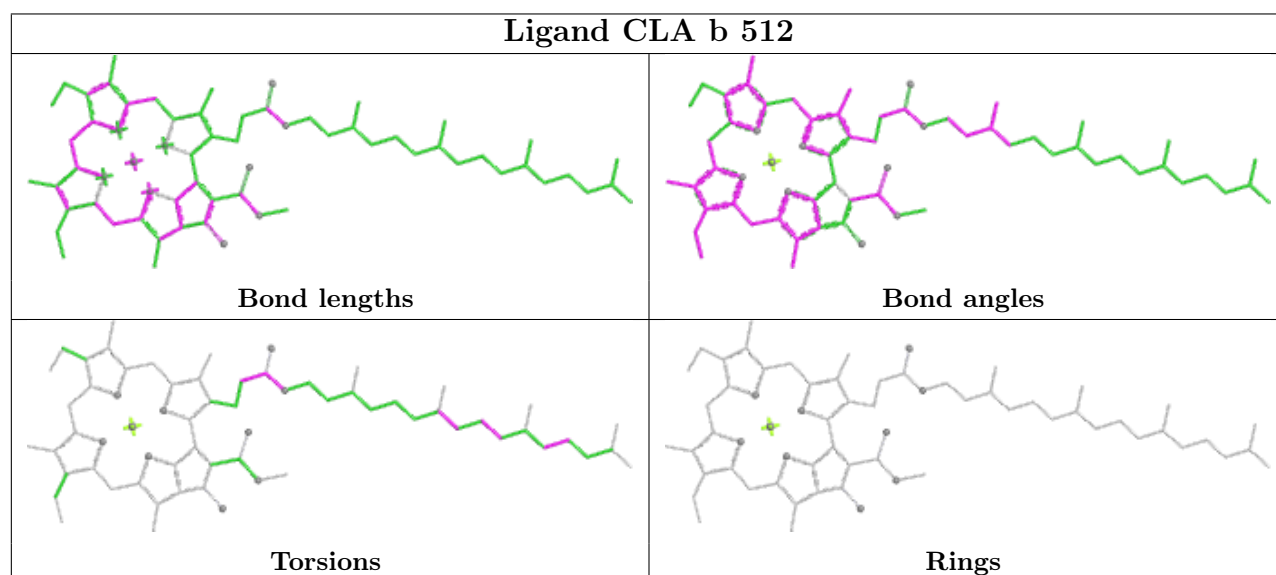
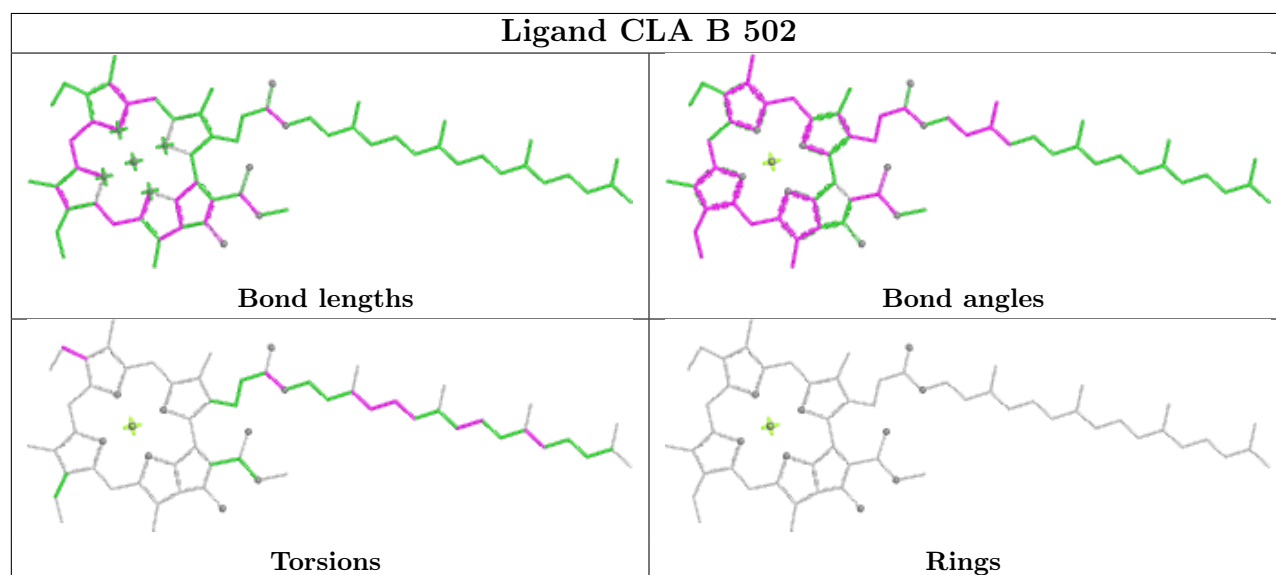
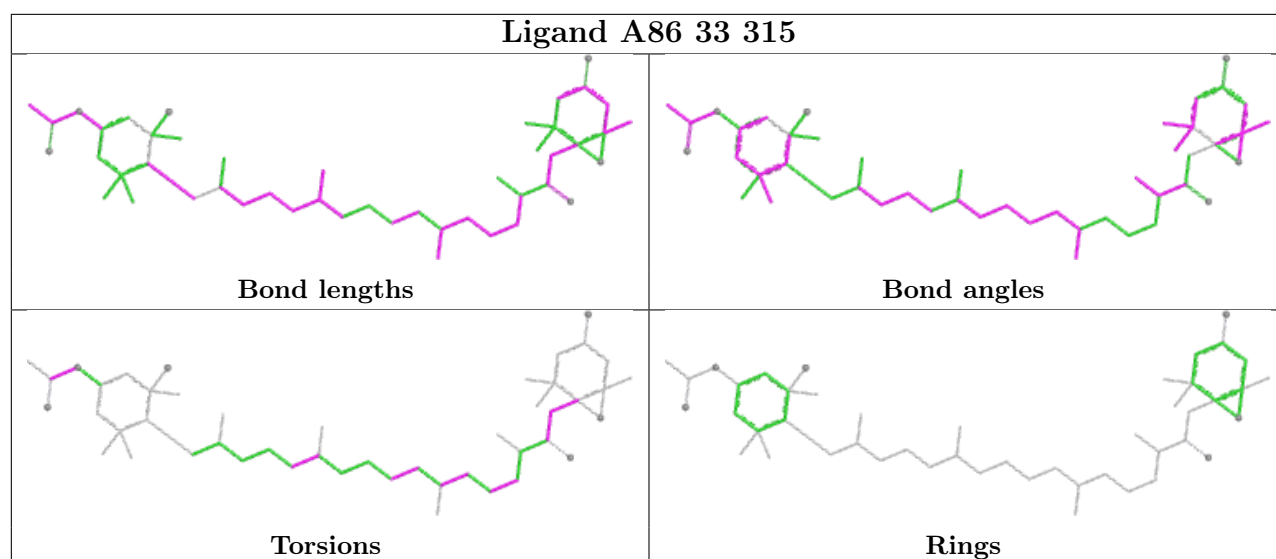


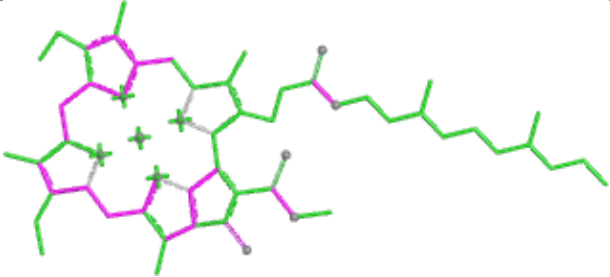
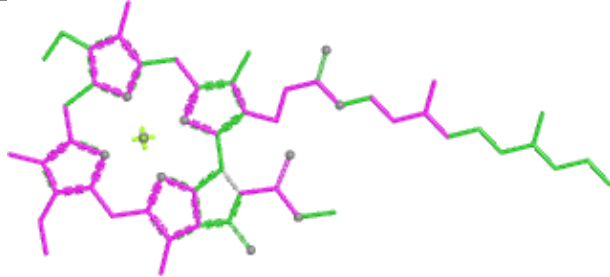
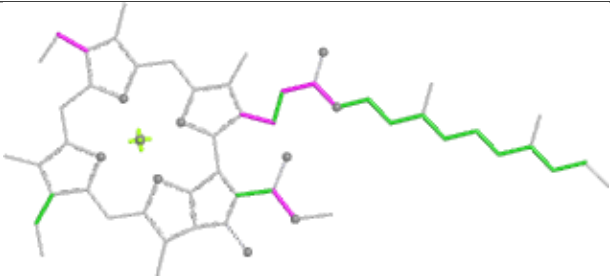
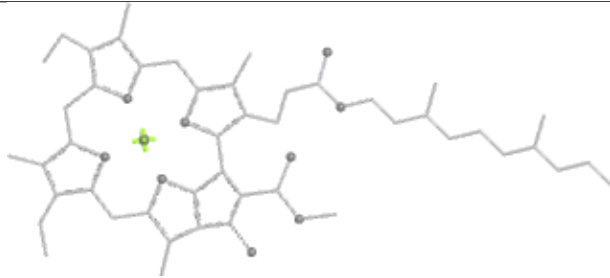
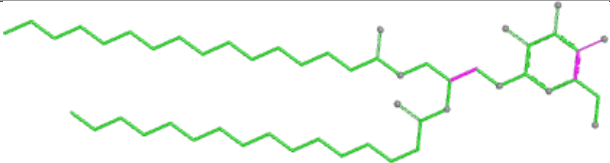
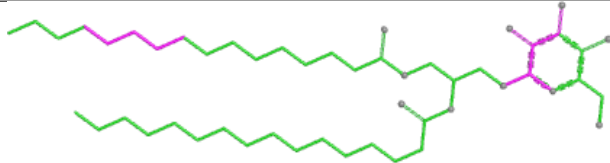
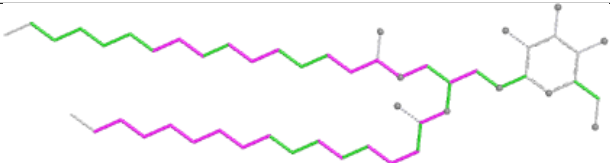
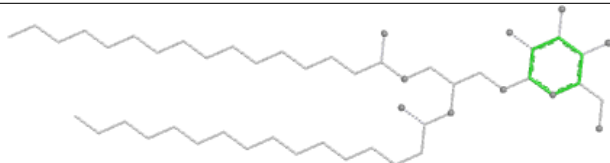
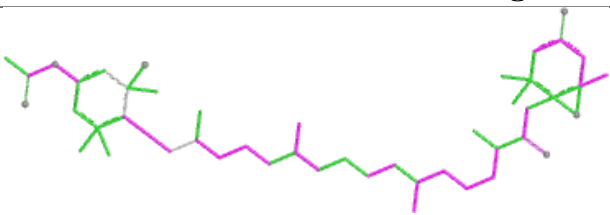
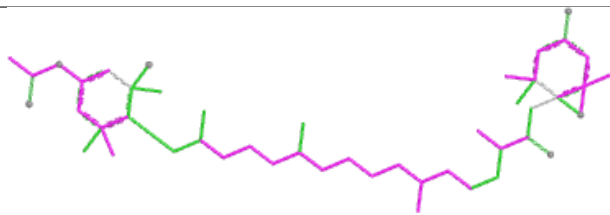
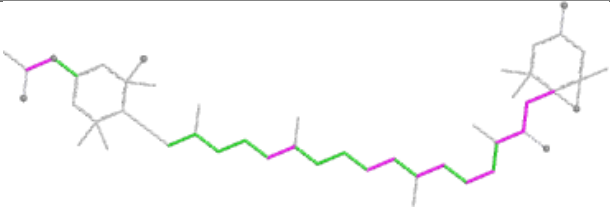
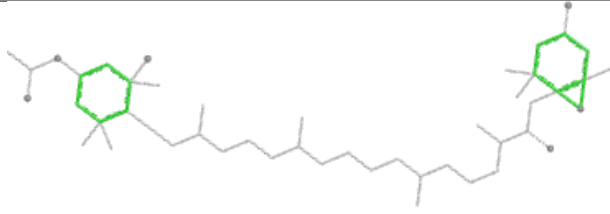


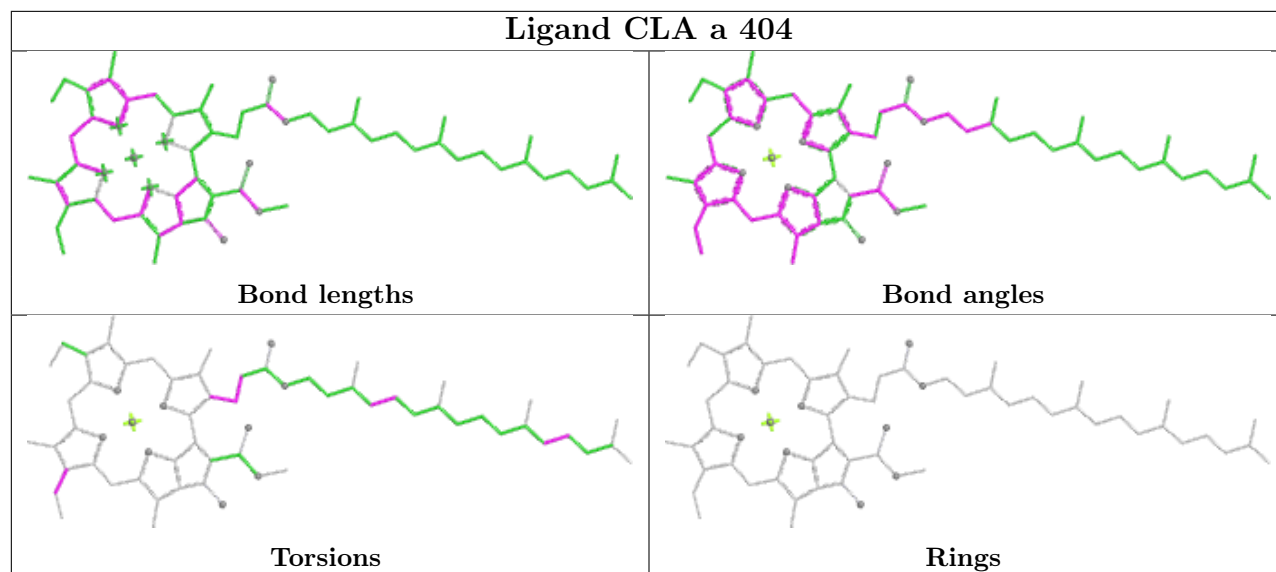
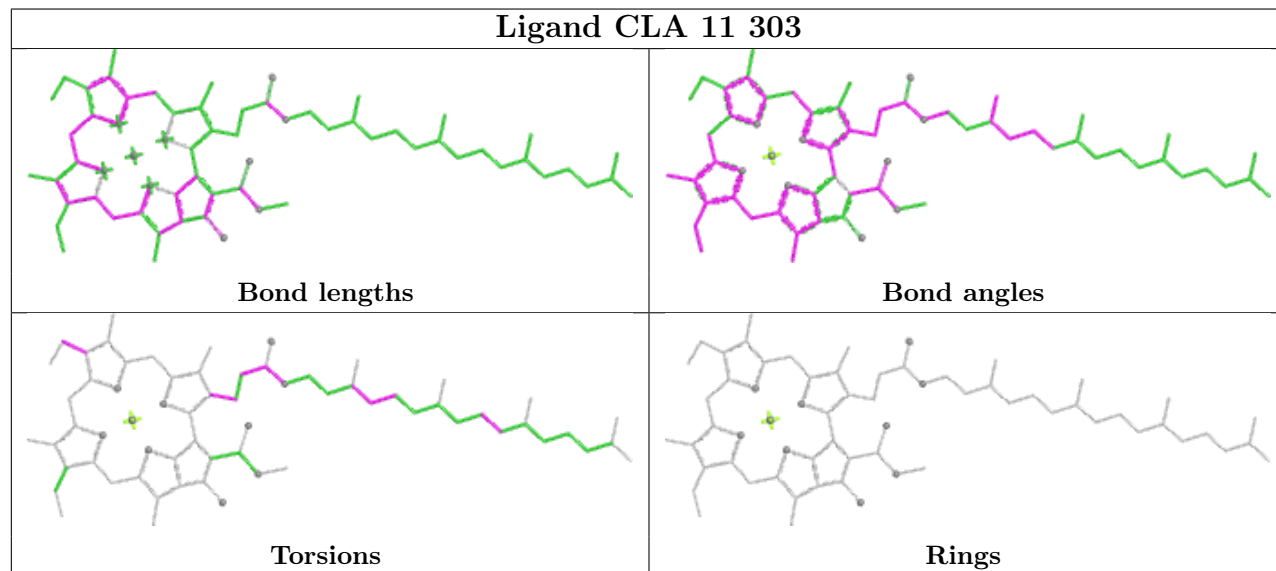


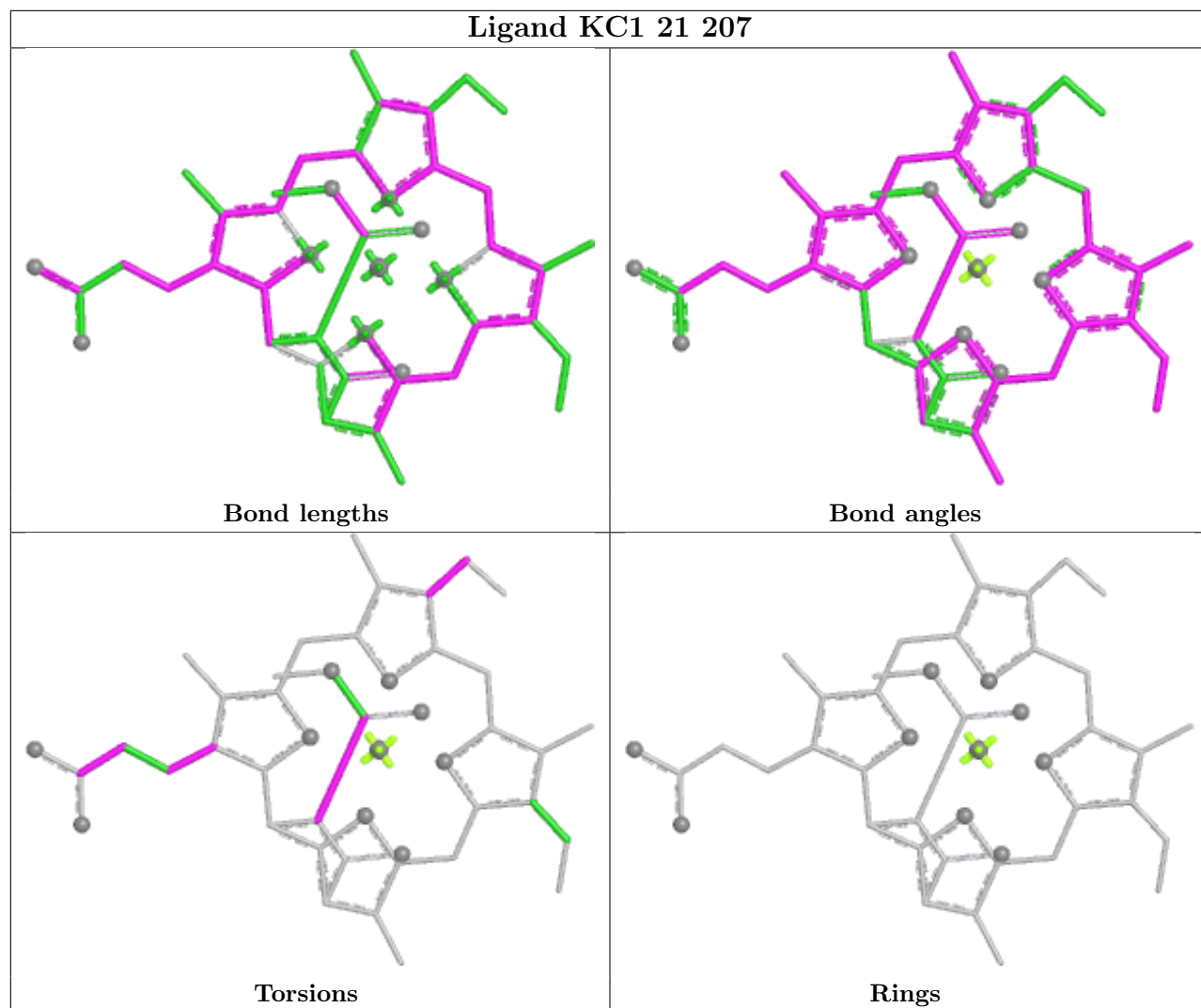


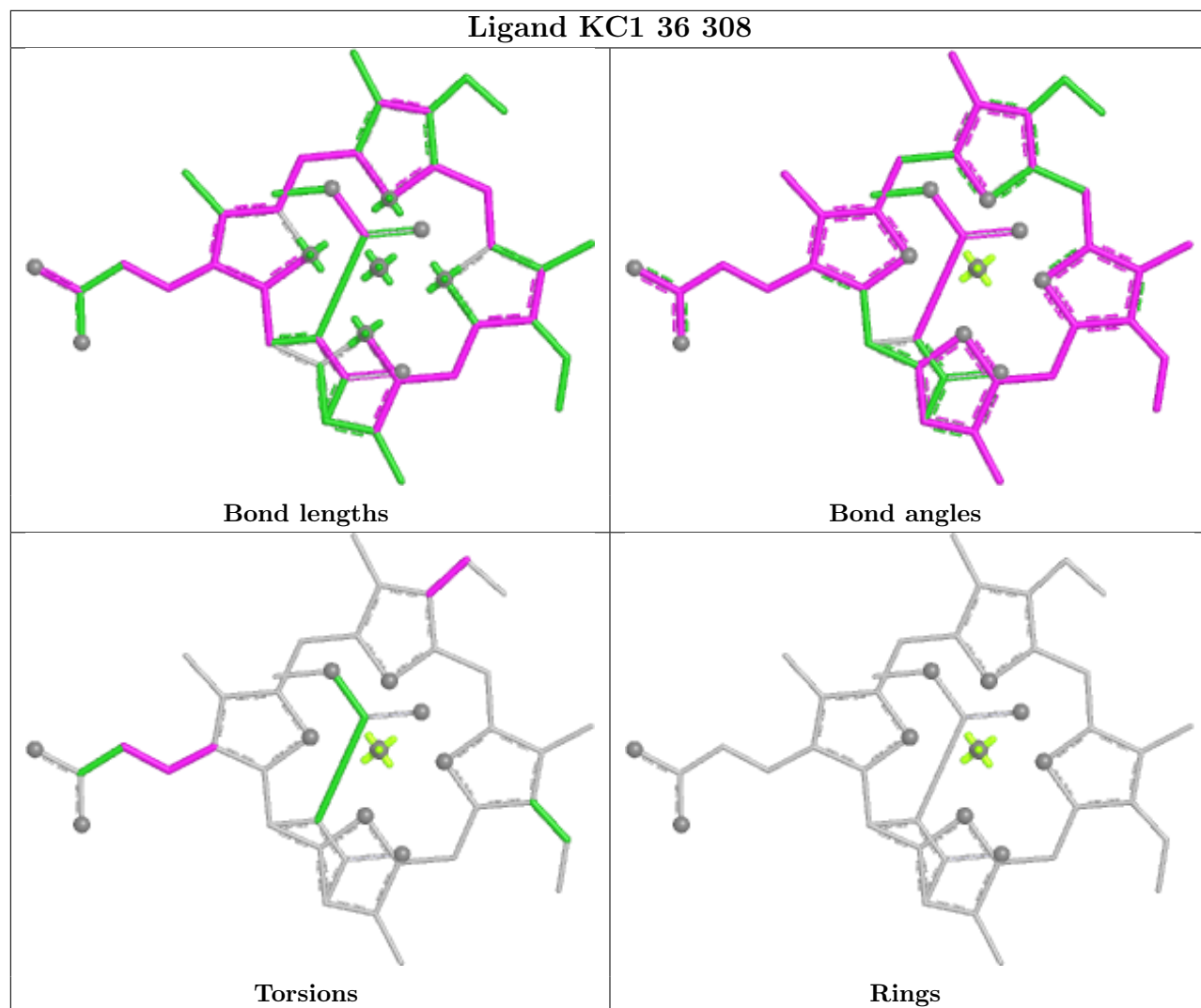


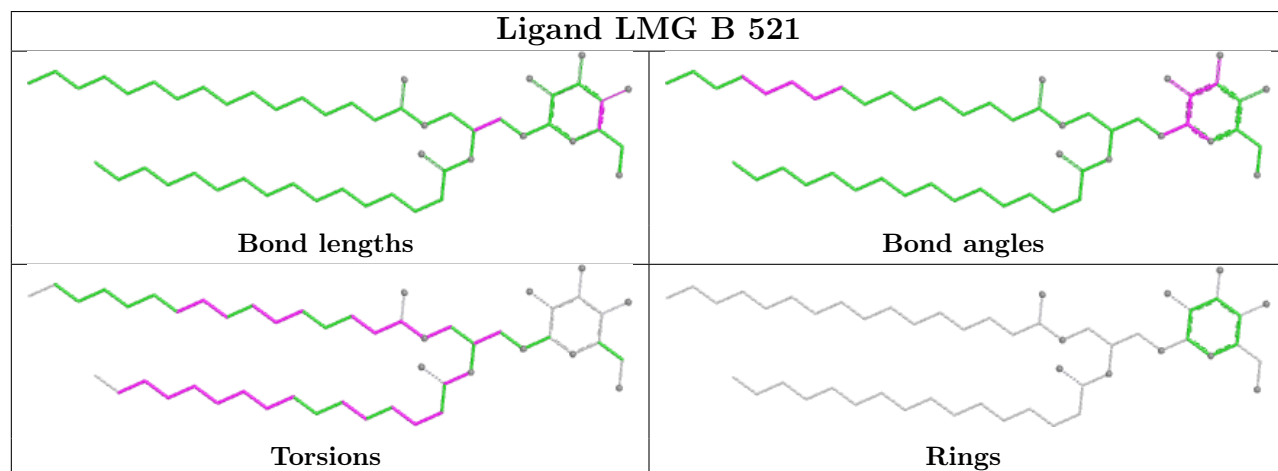
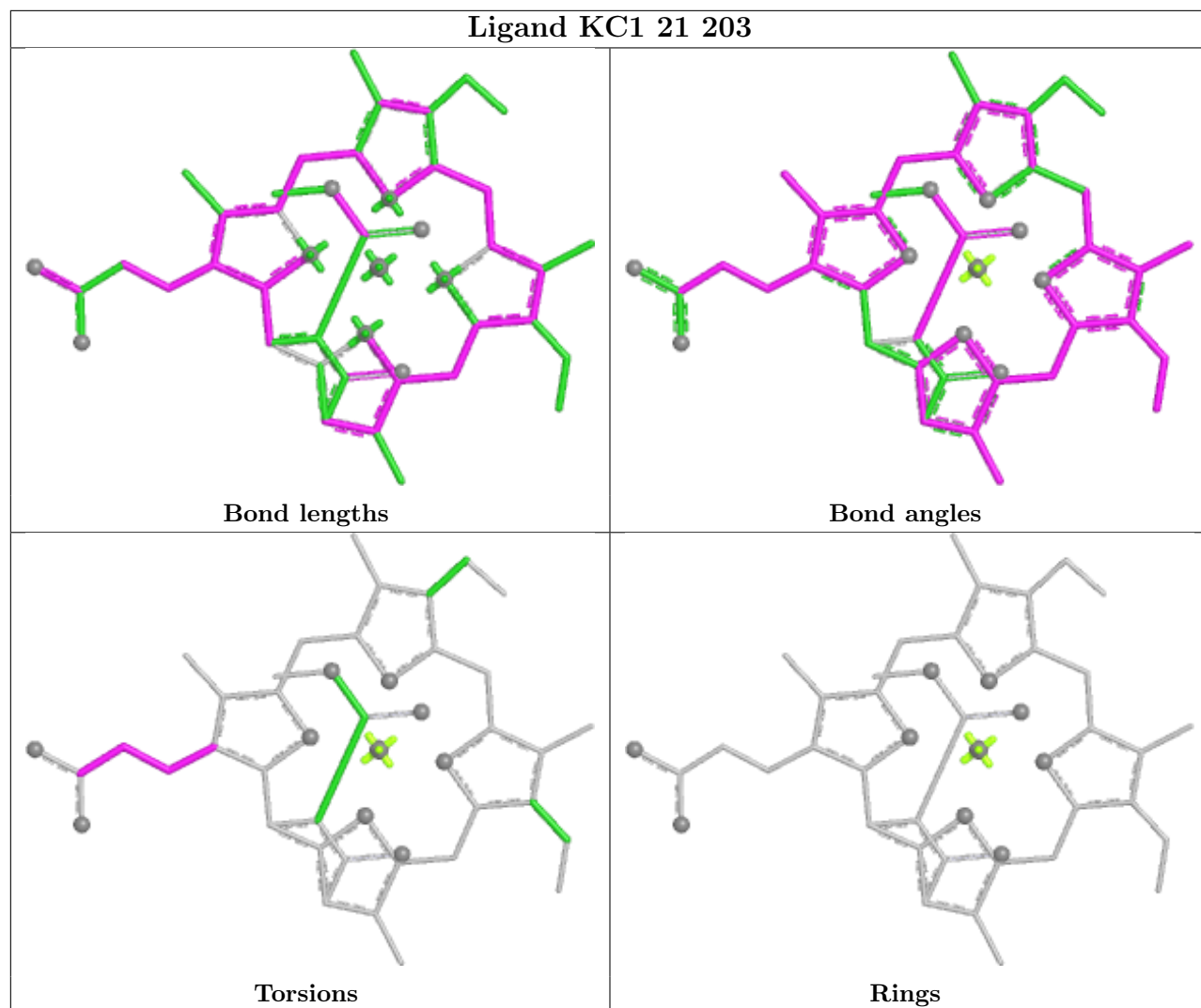


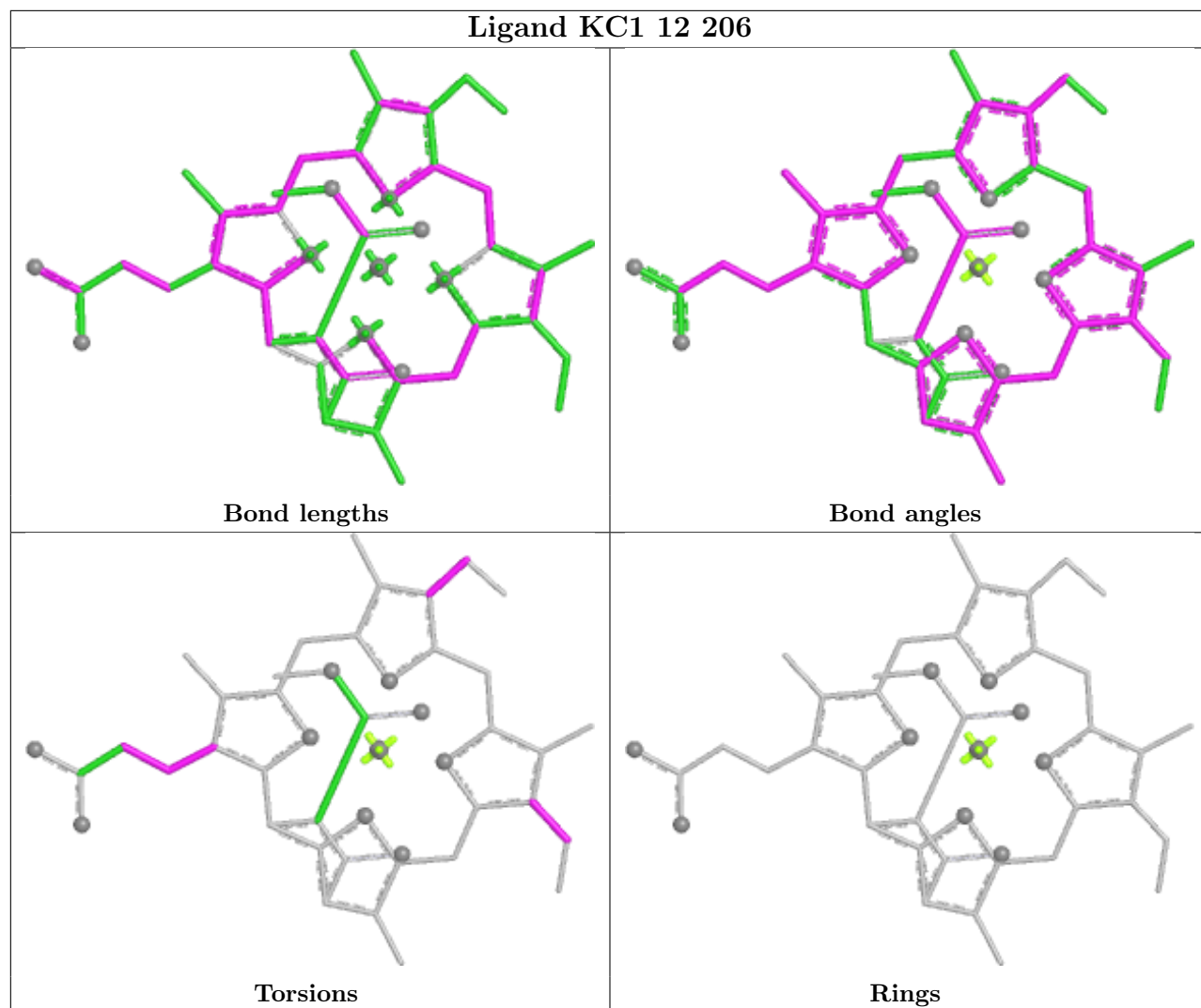
Ligand CLA 36 303	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG b 520	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A86 32 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

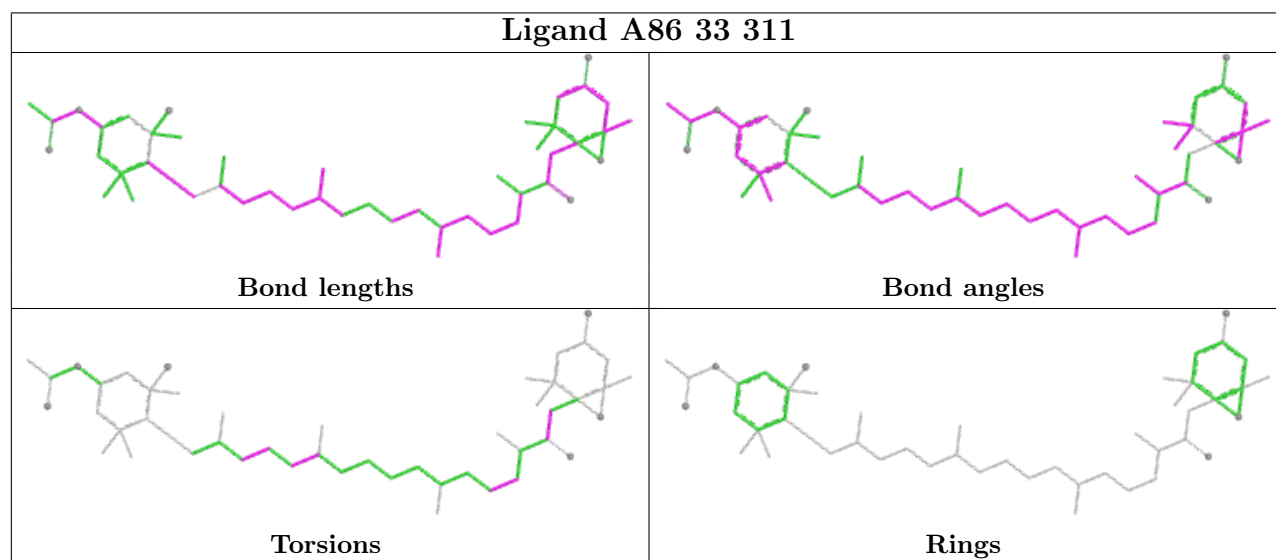
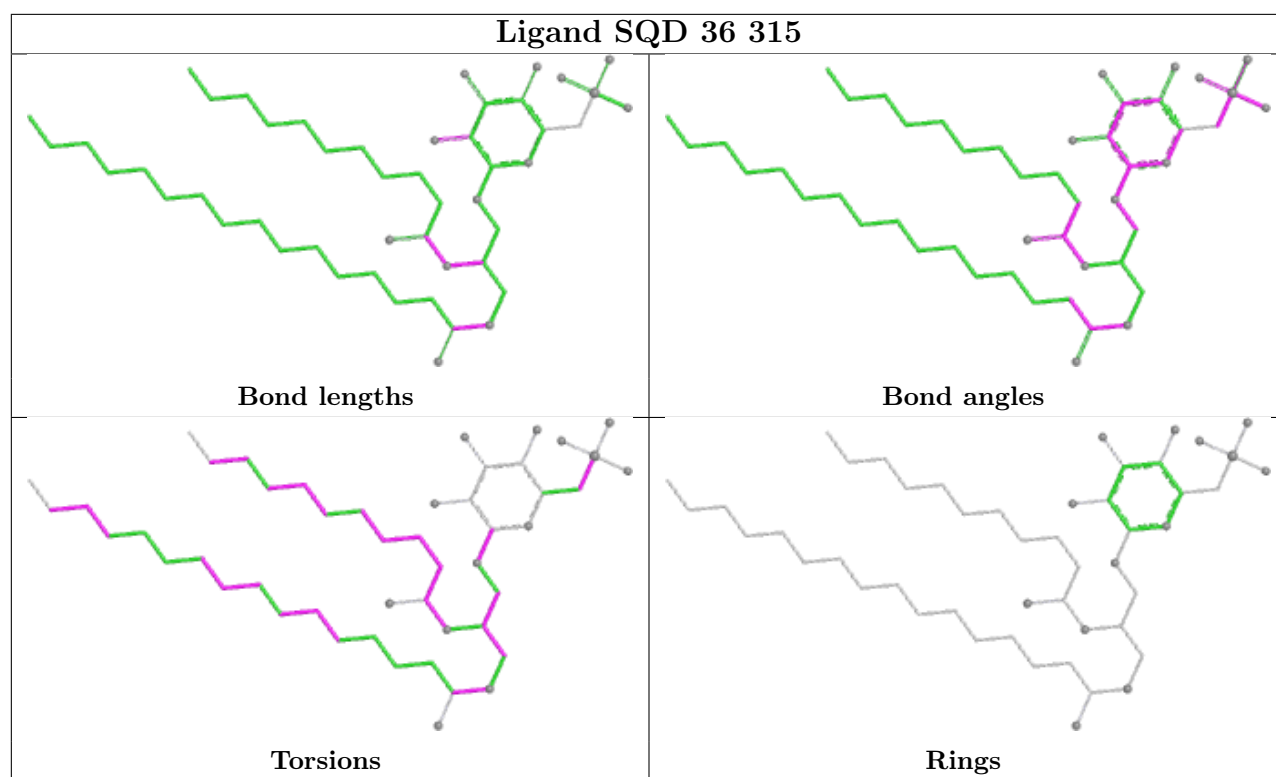
Ligand CLA a 404**Ligand CLA 11 303**

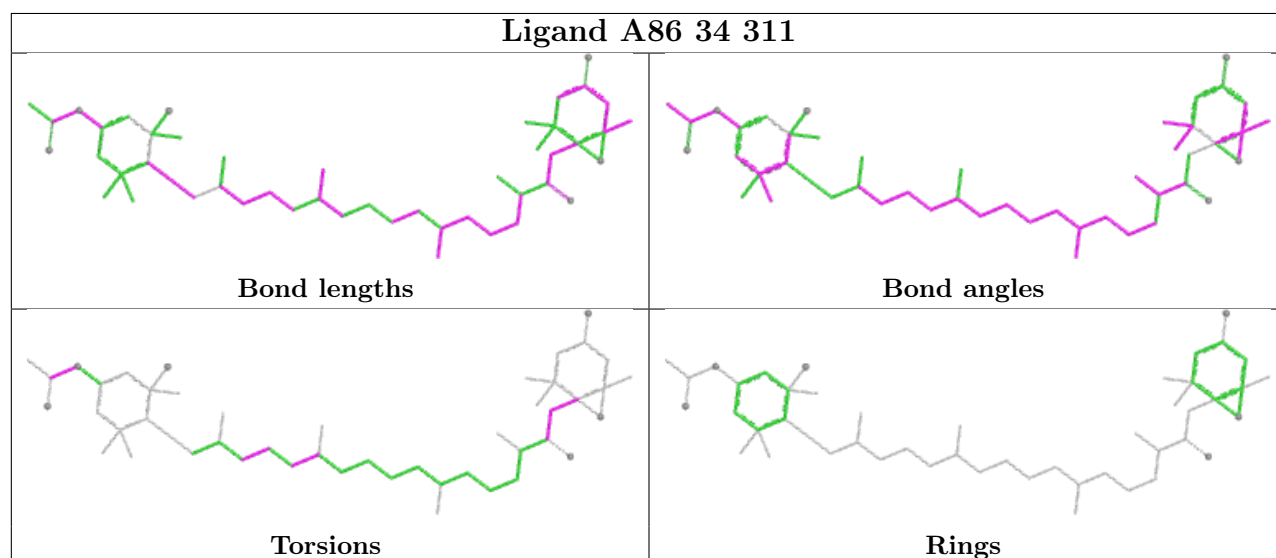
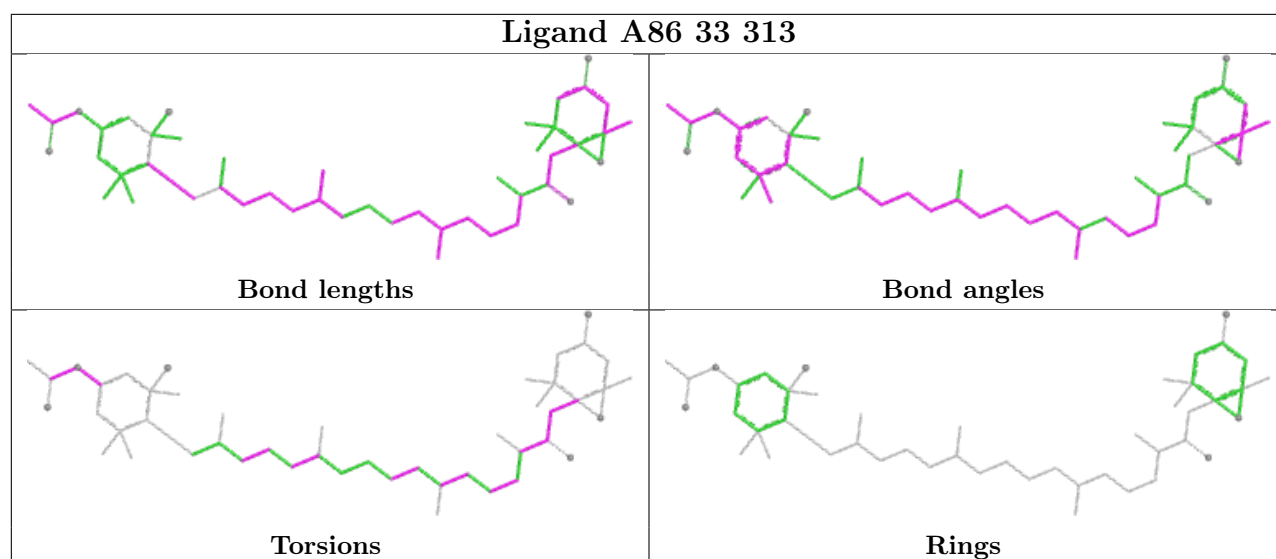


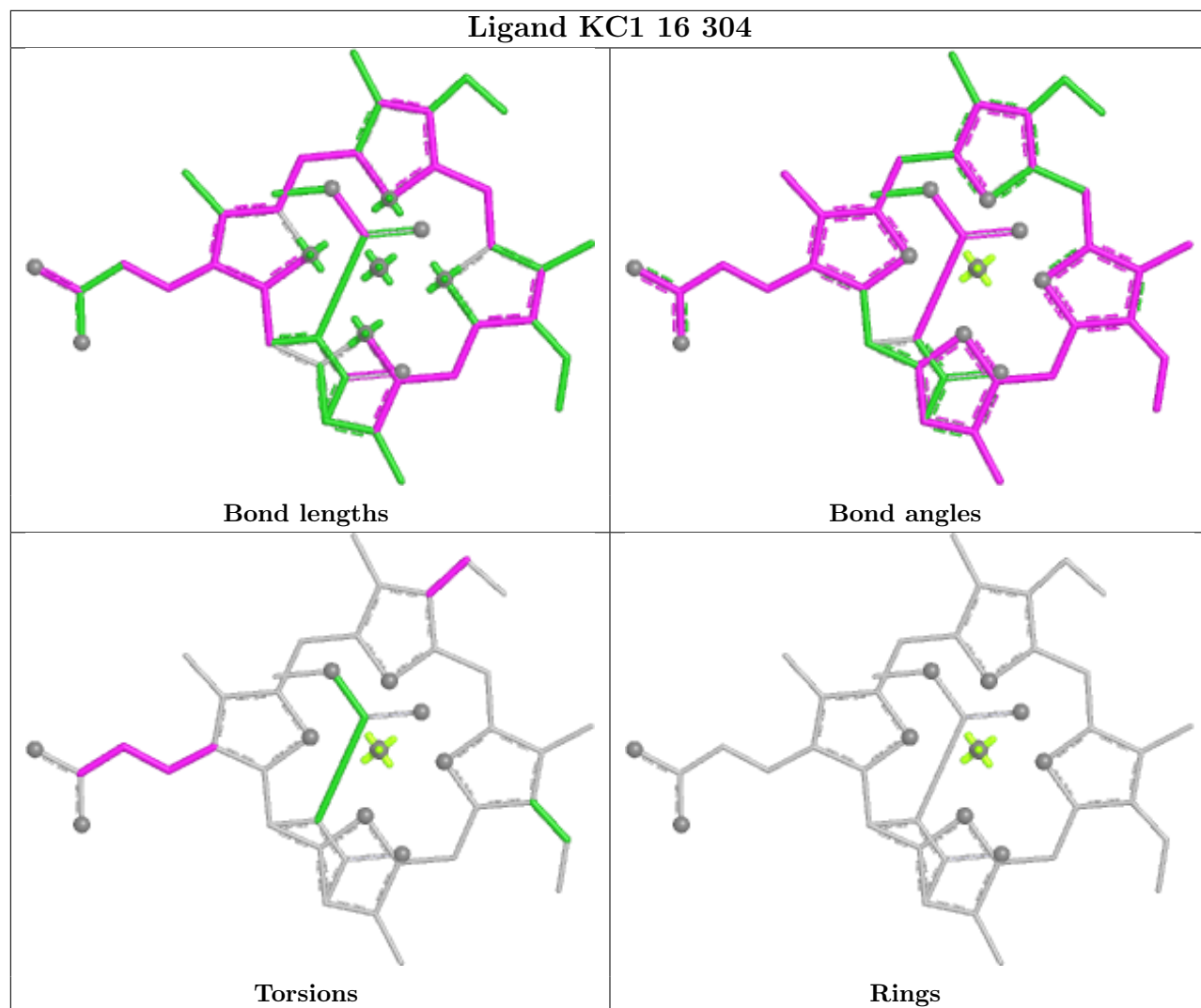


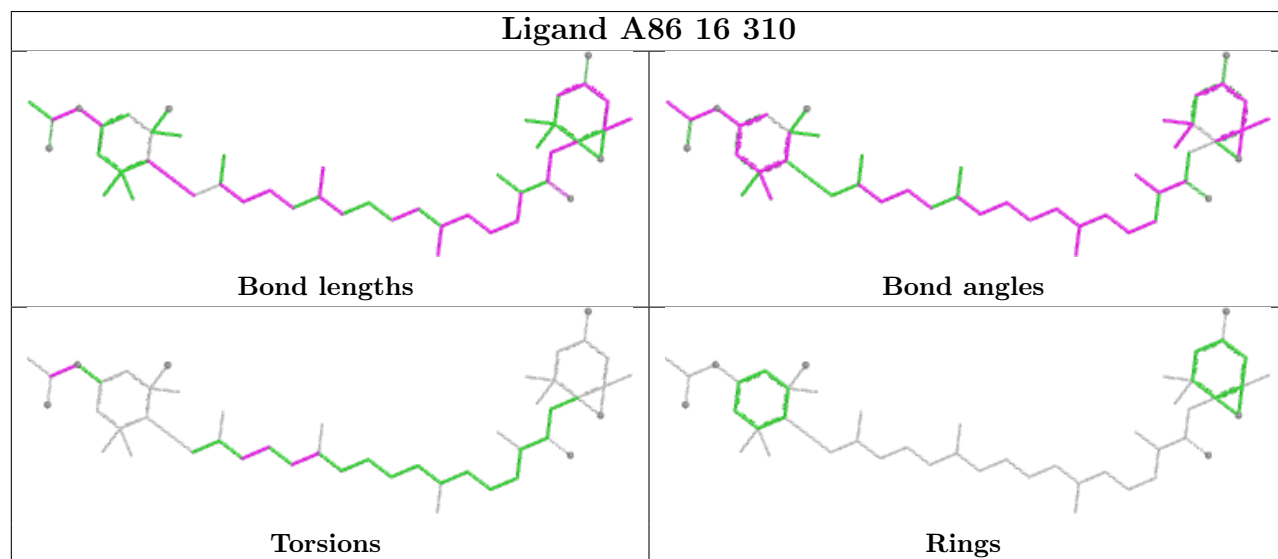
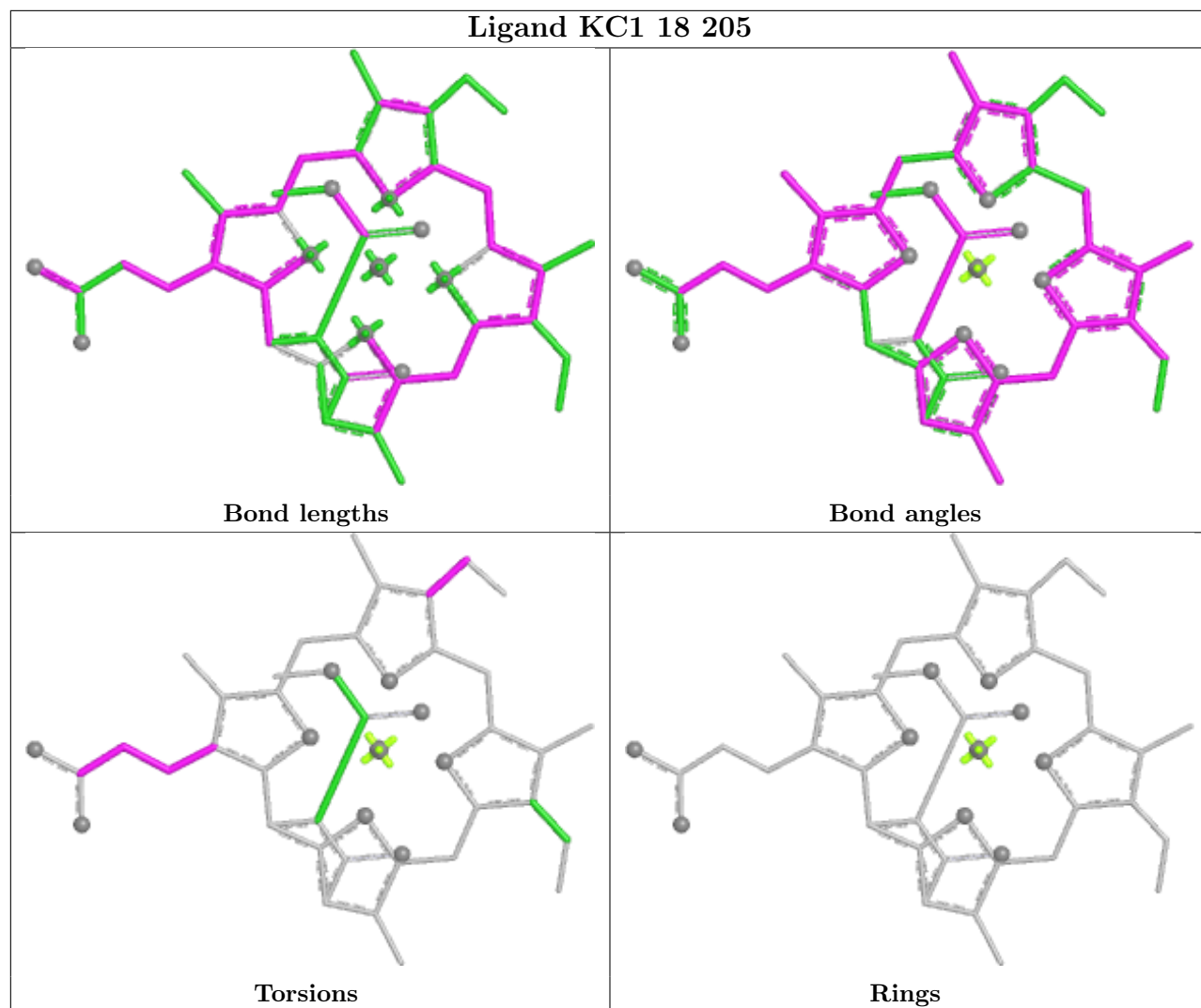


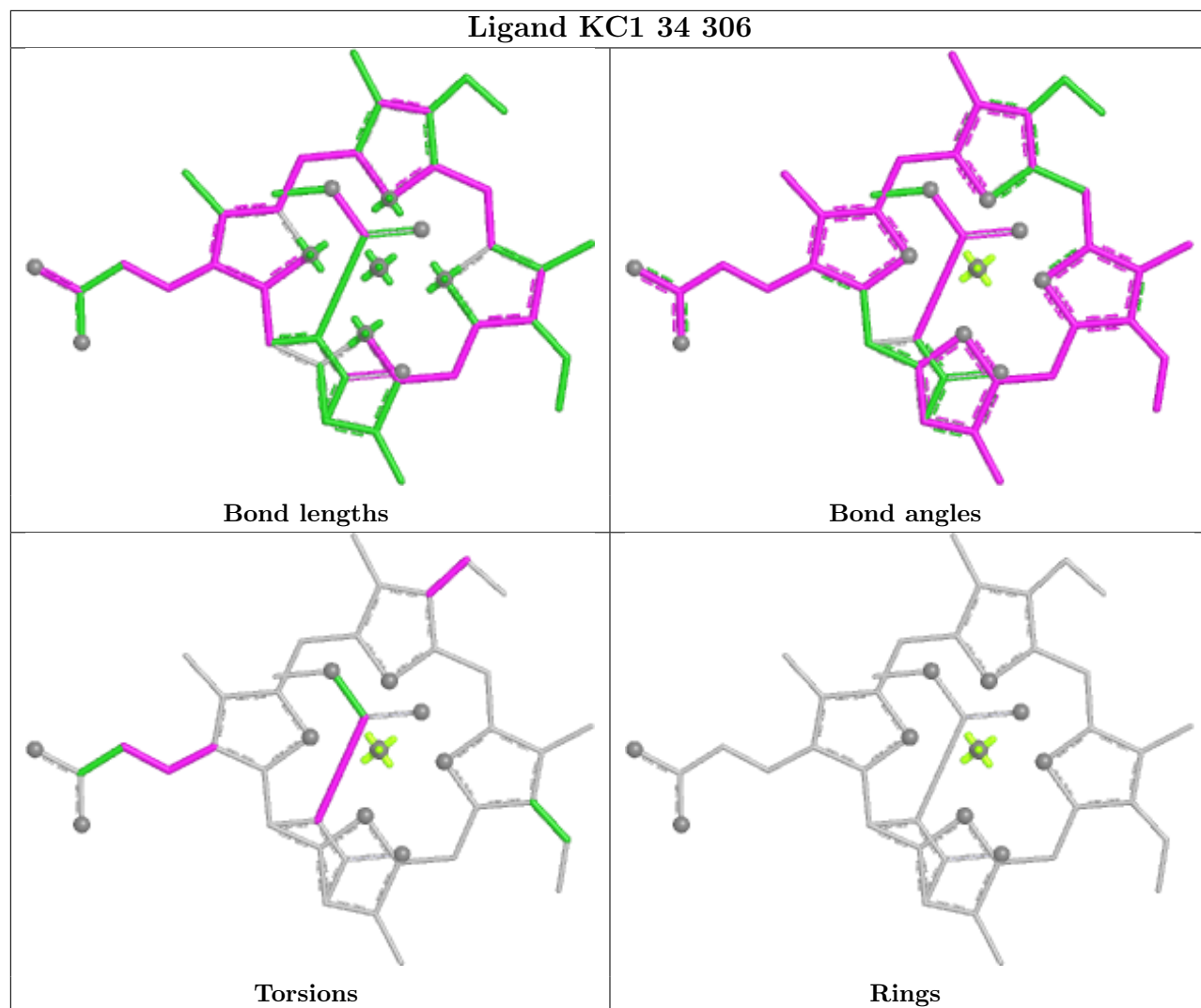


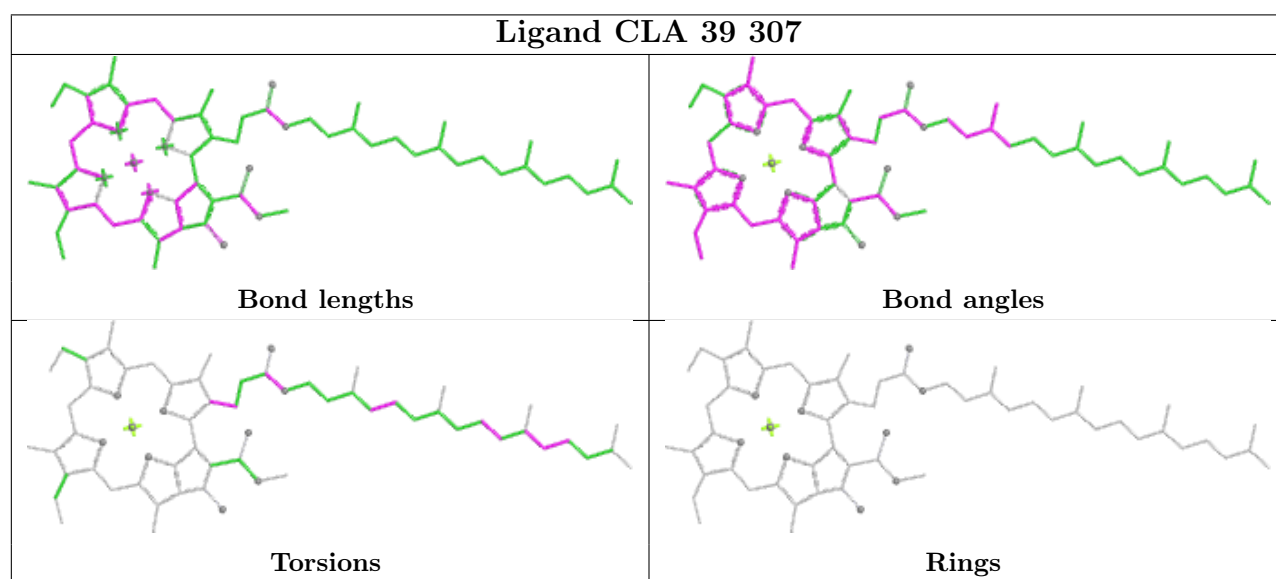
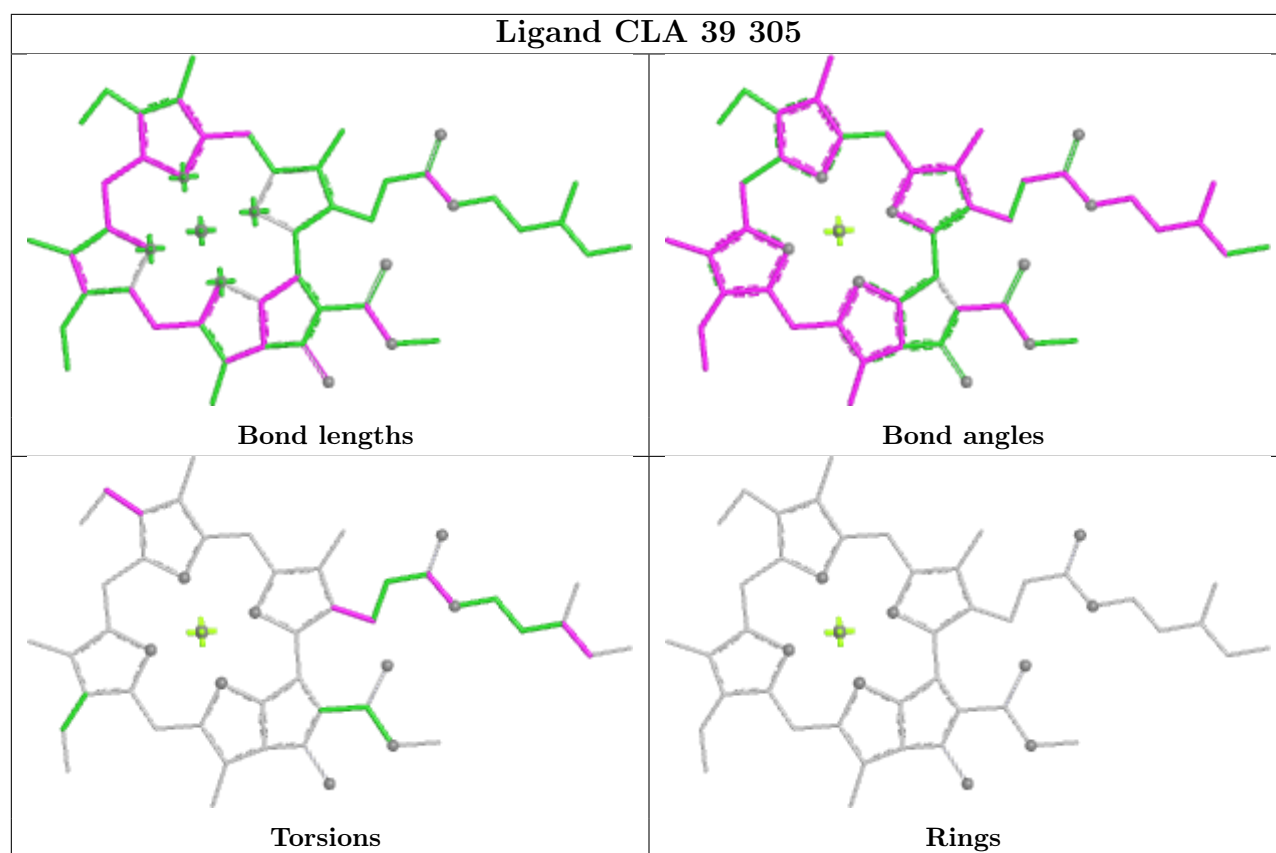


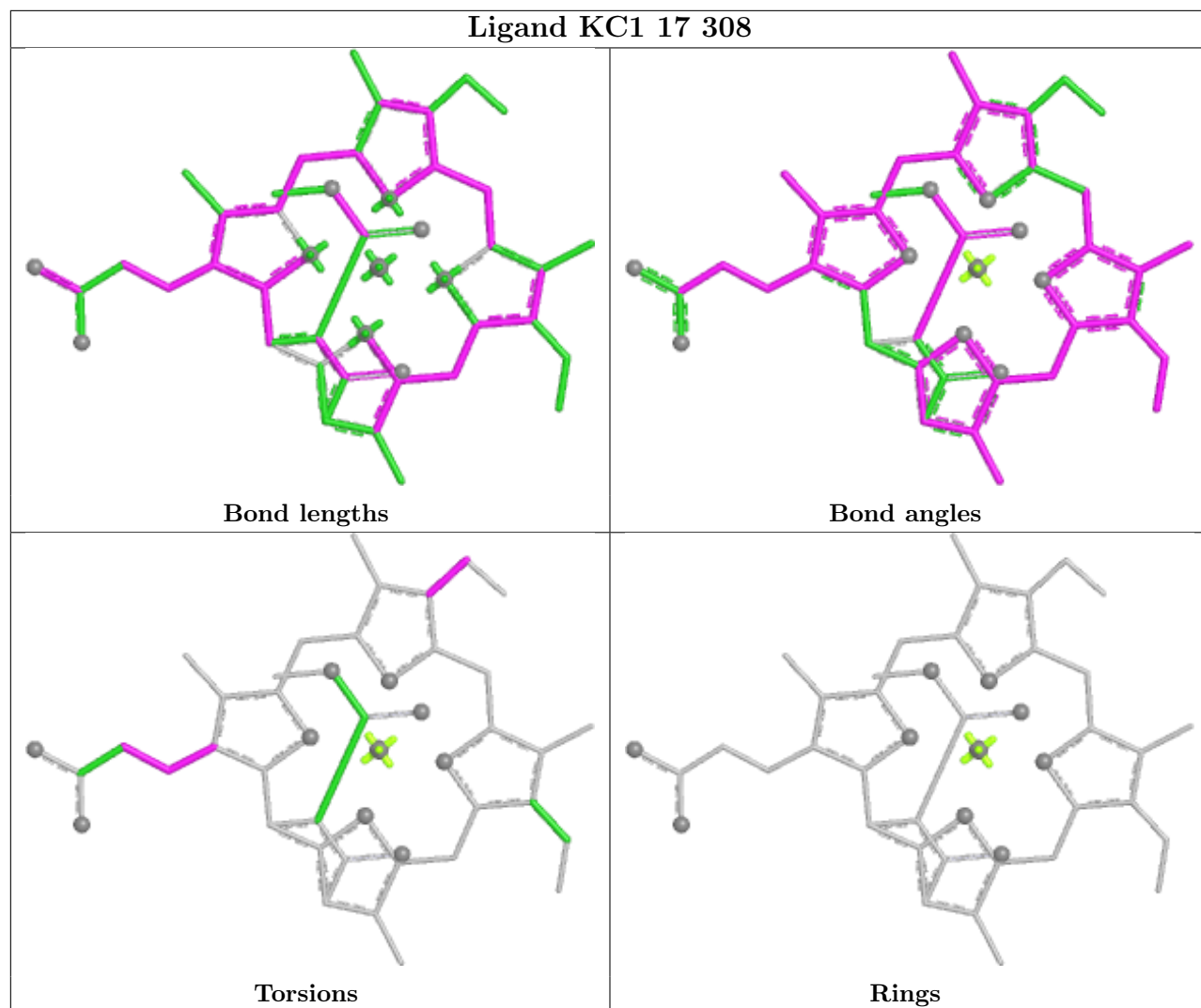


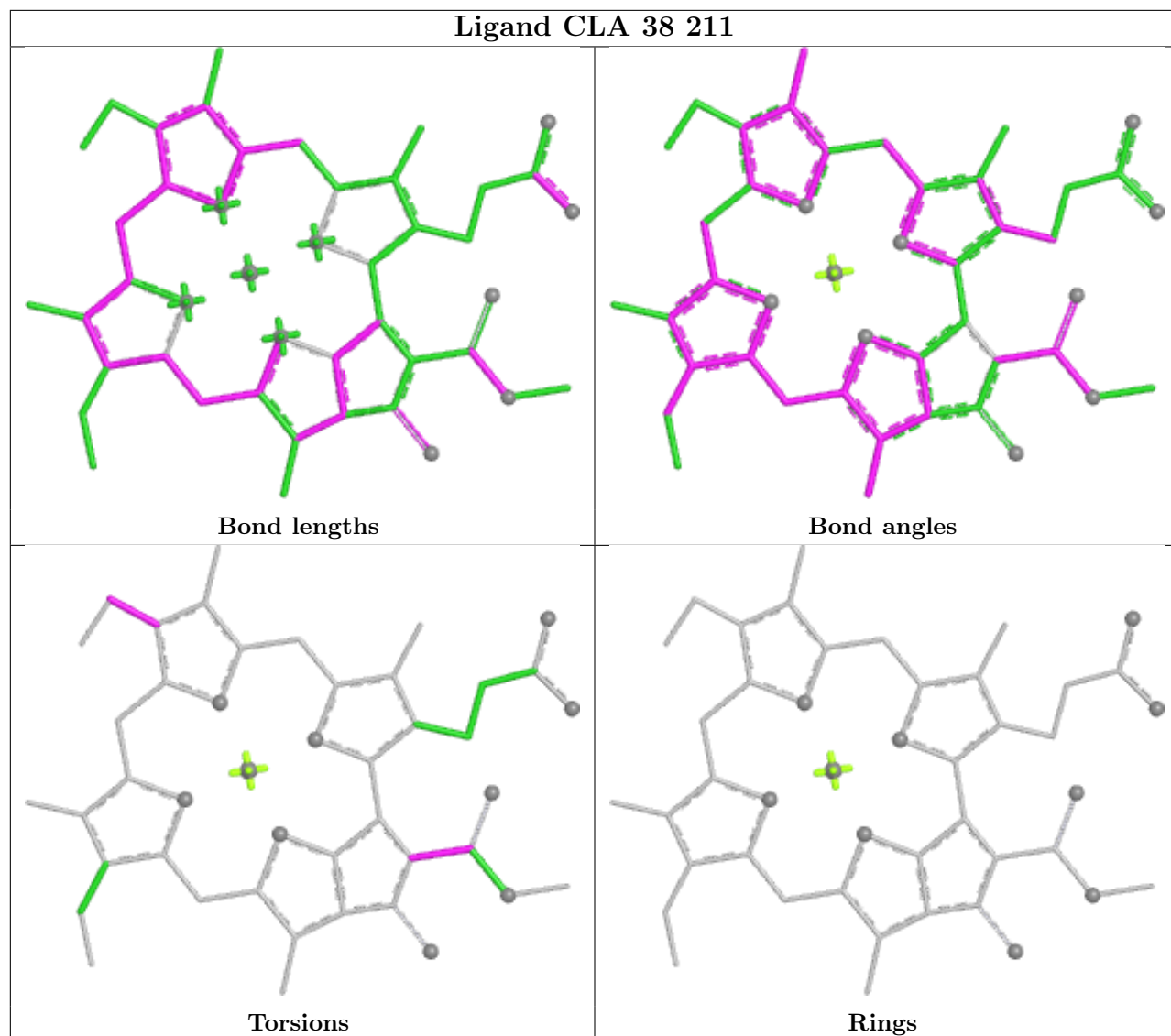


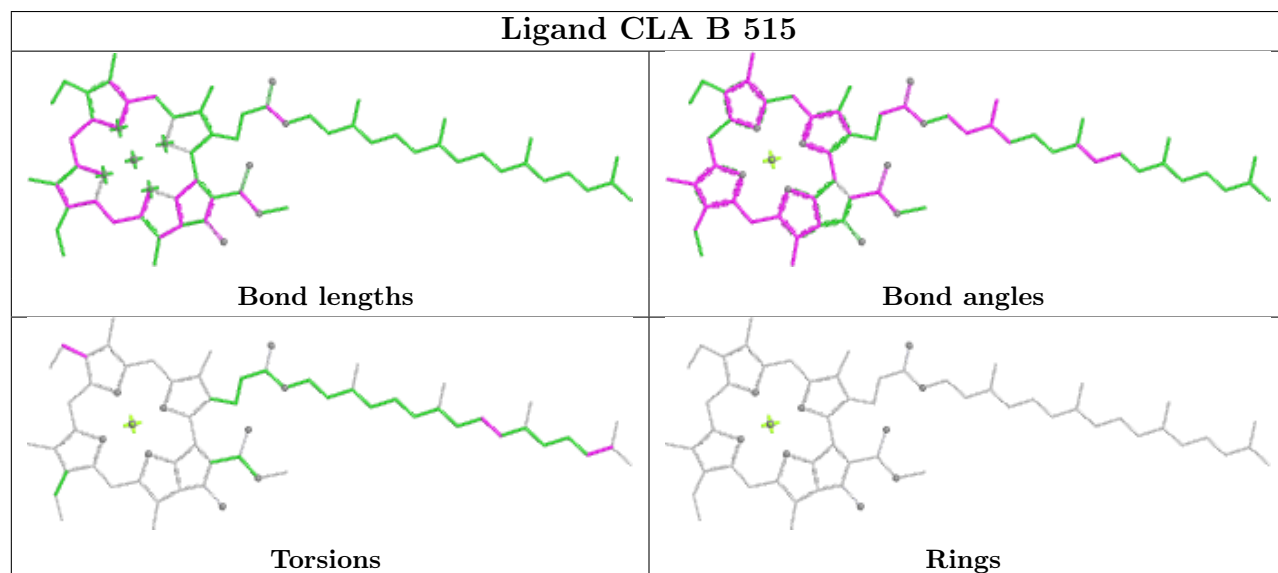
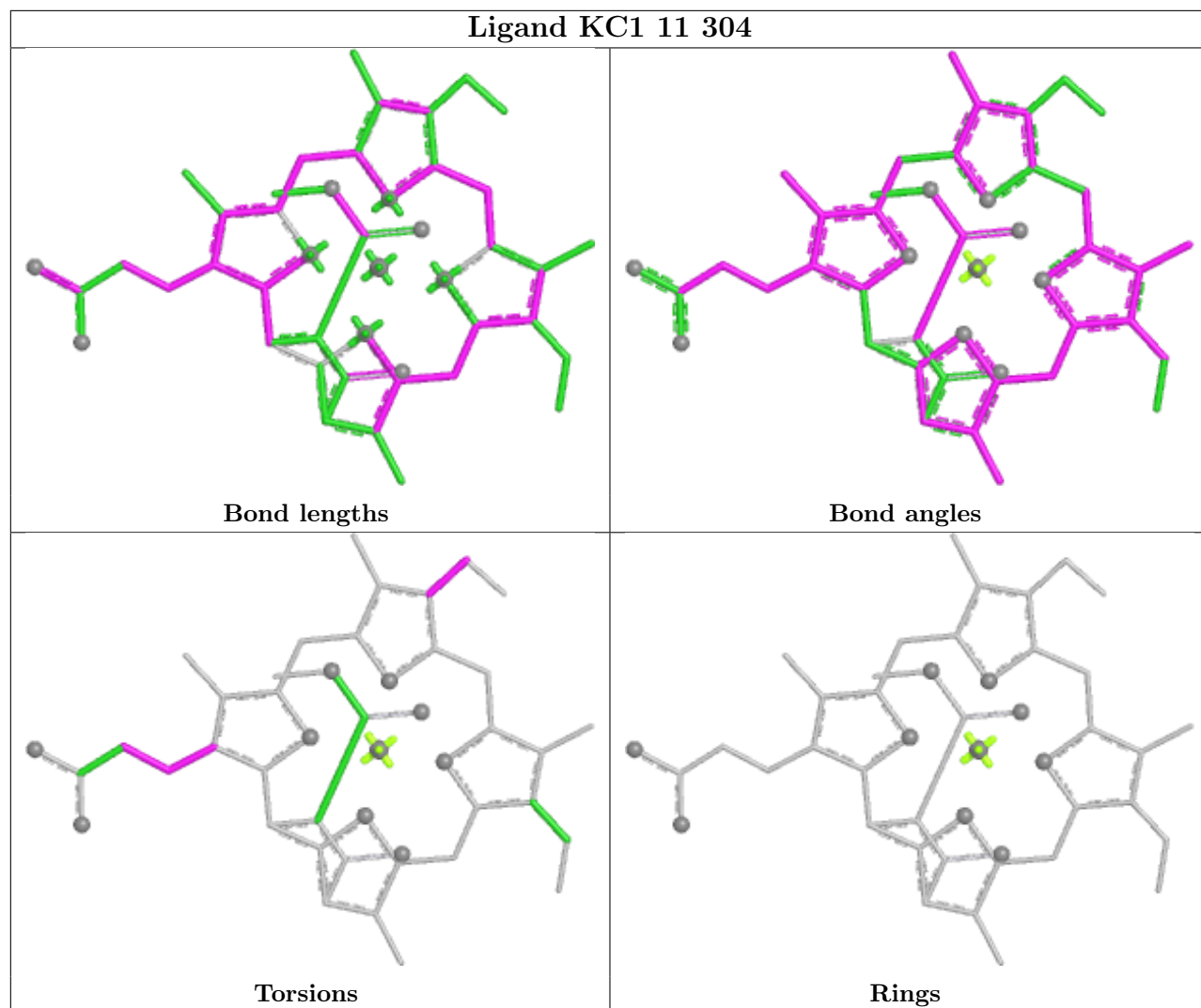


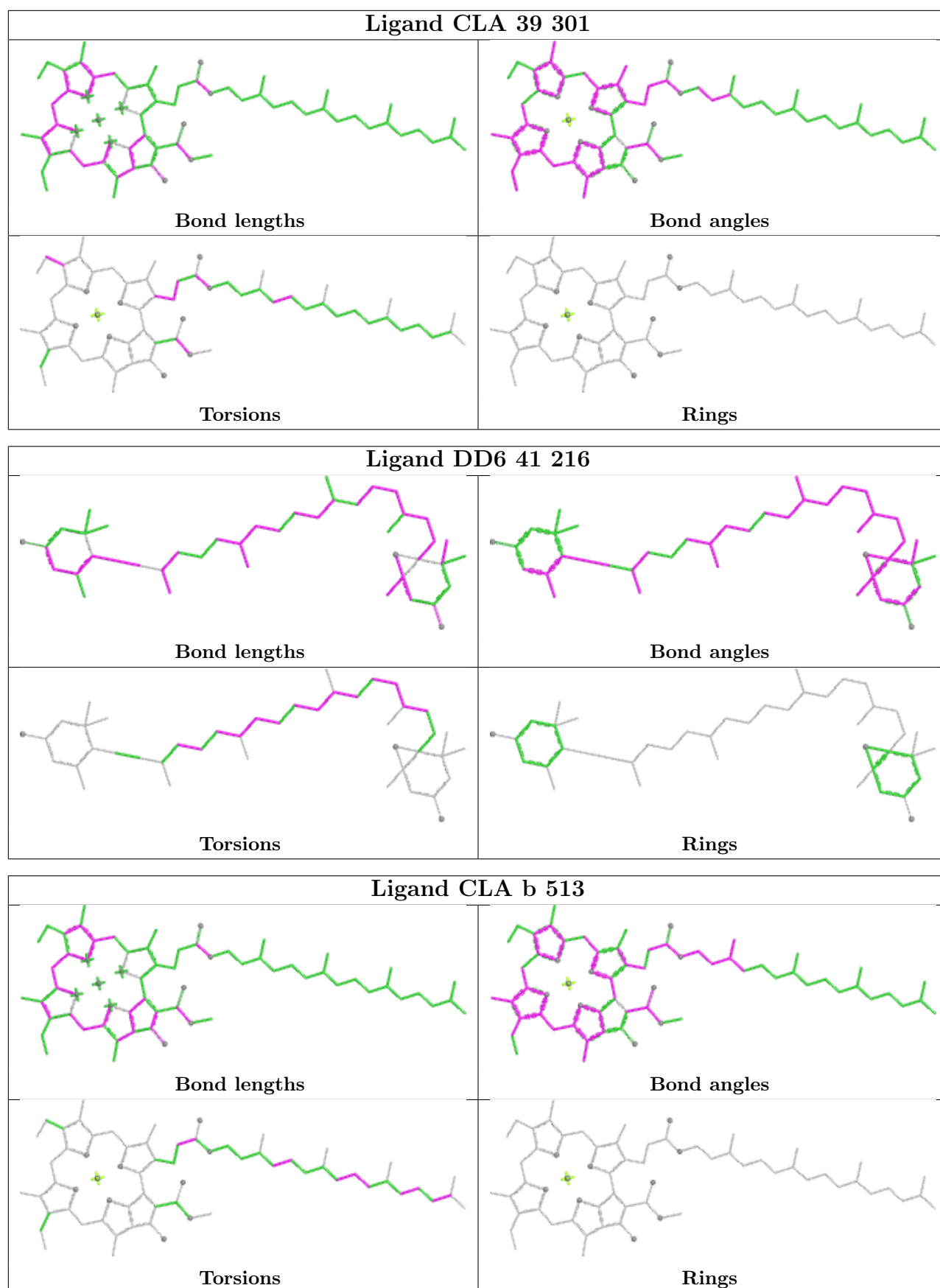


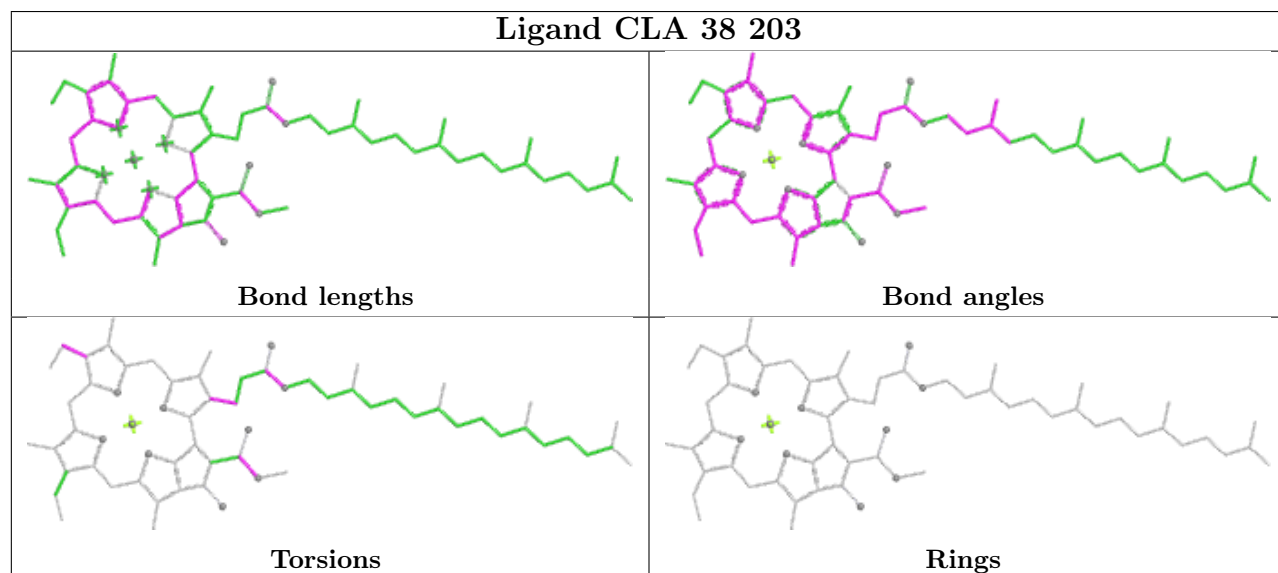
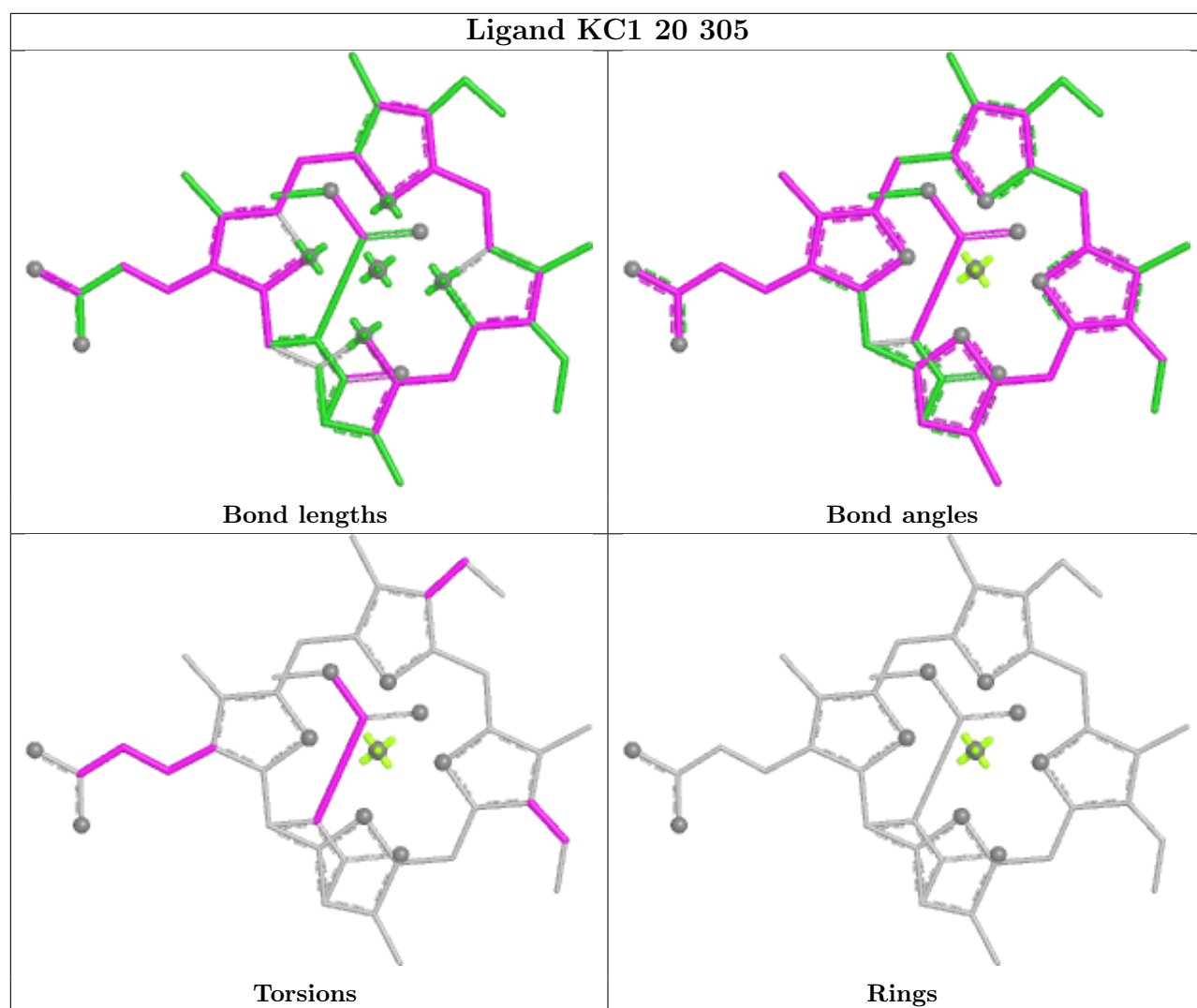


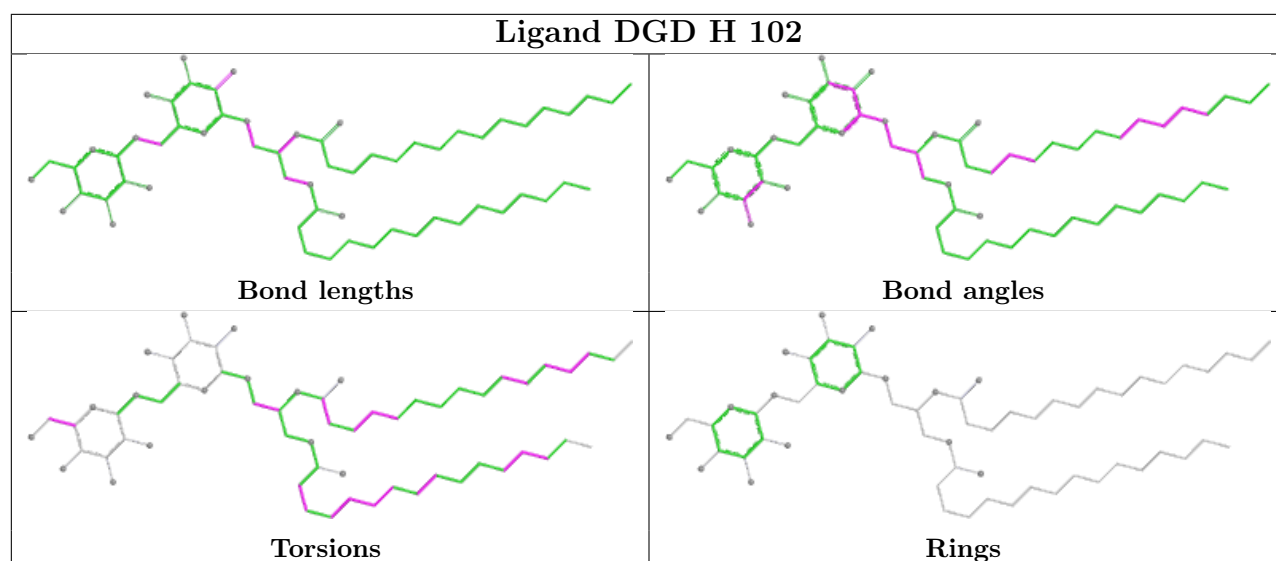
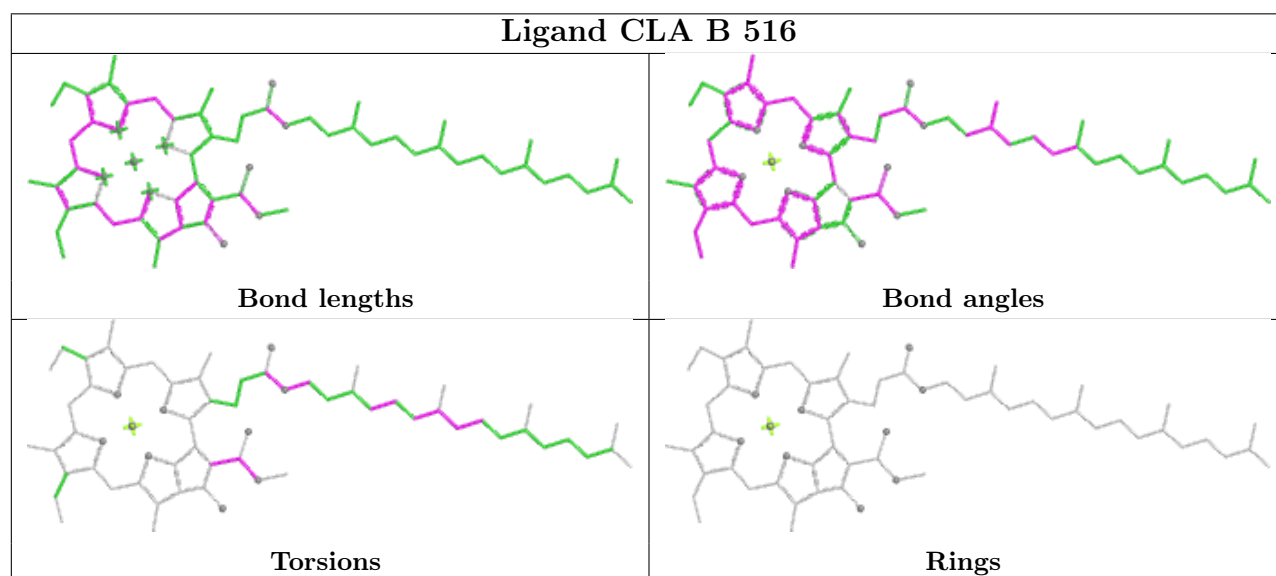
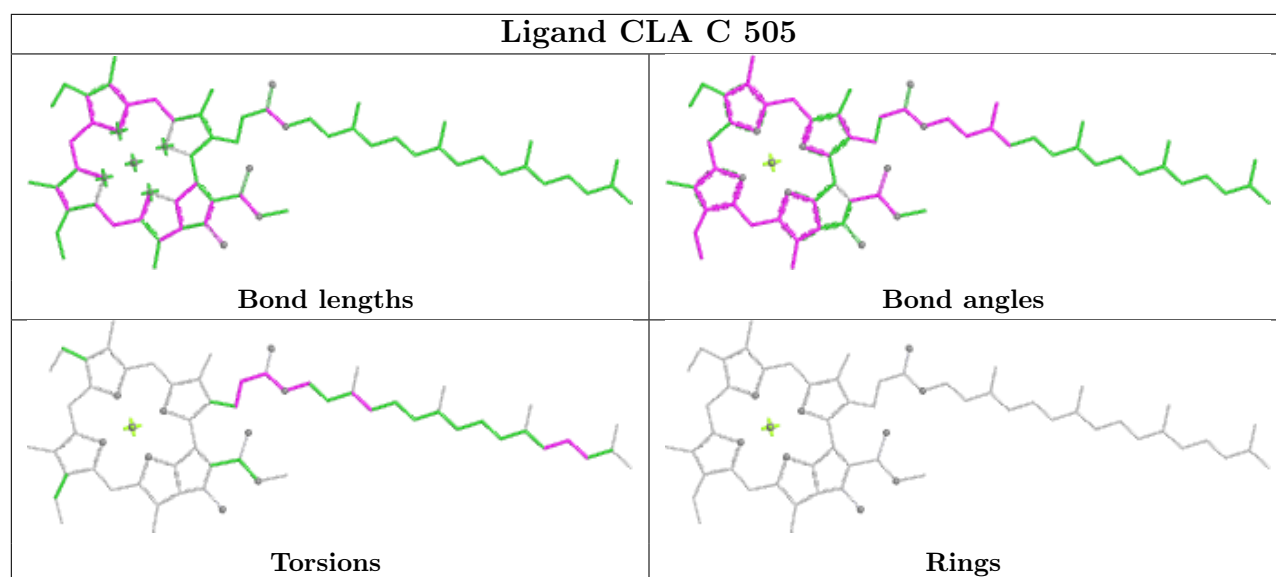


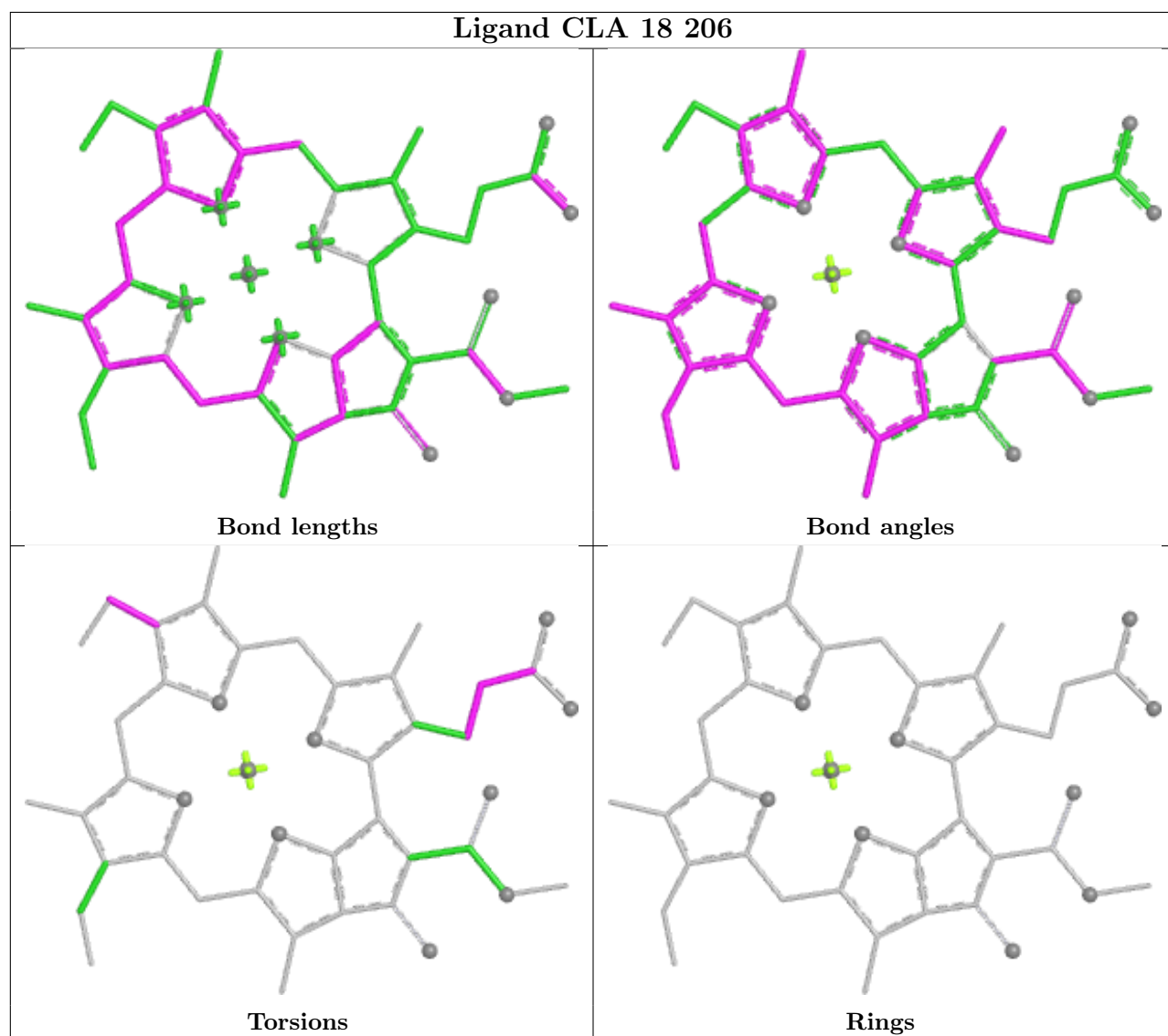
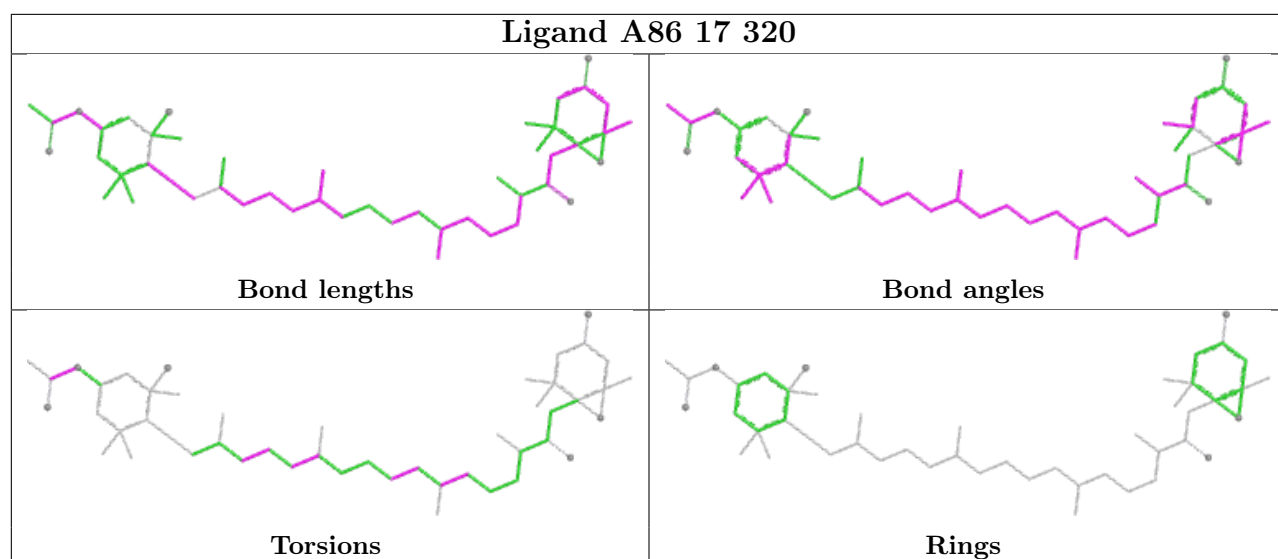


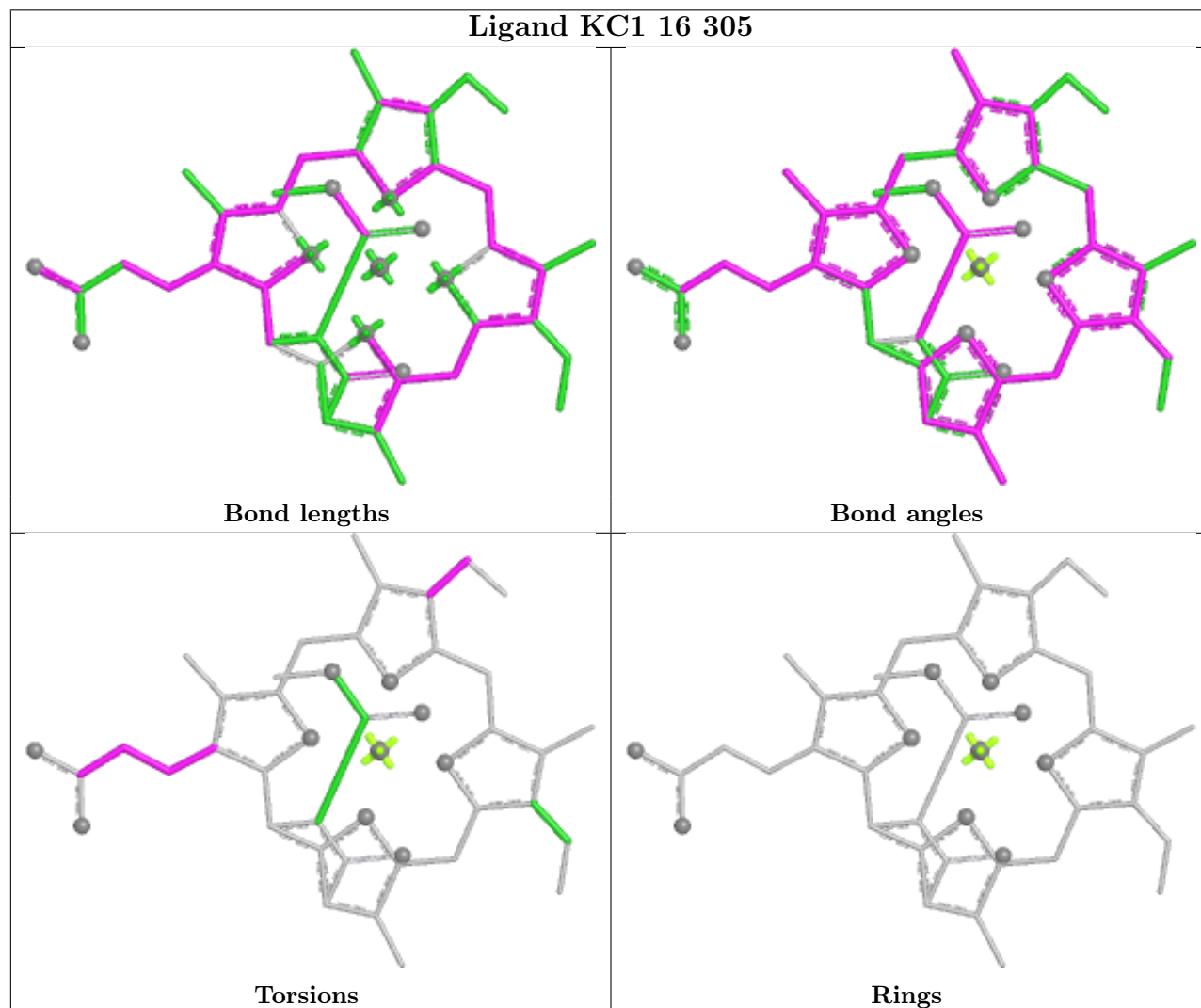
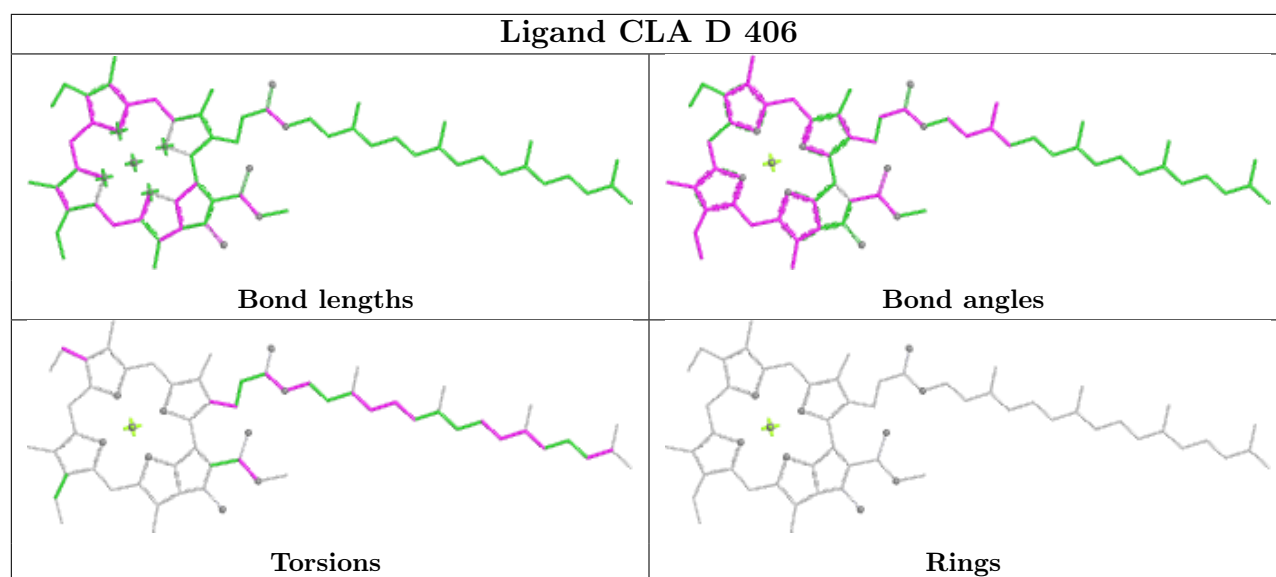


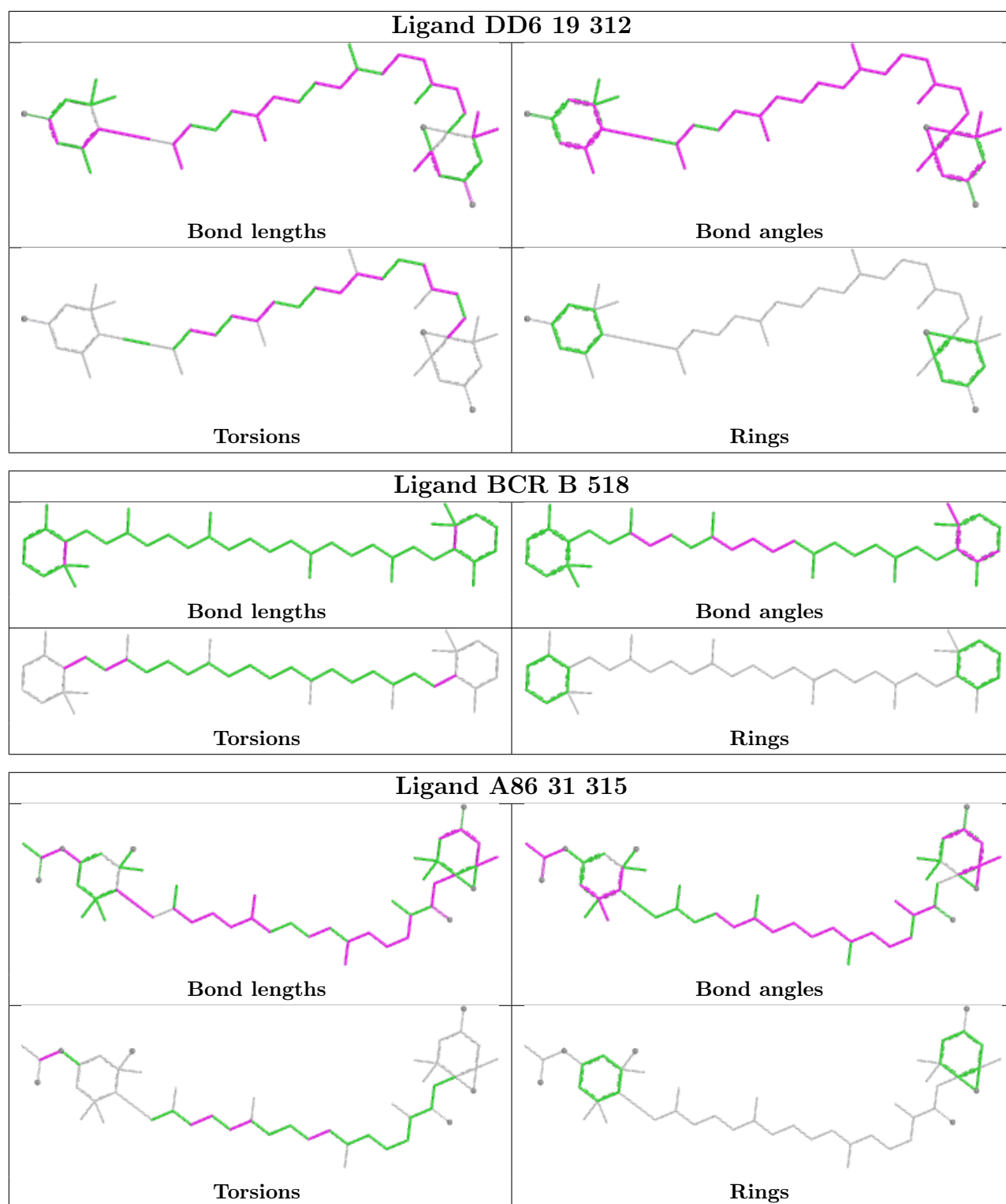


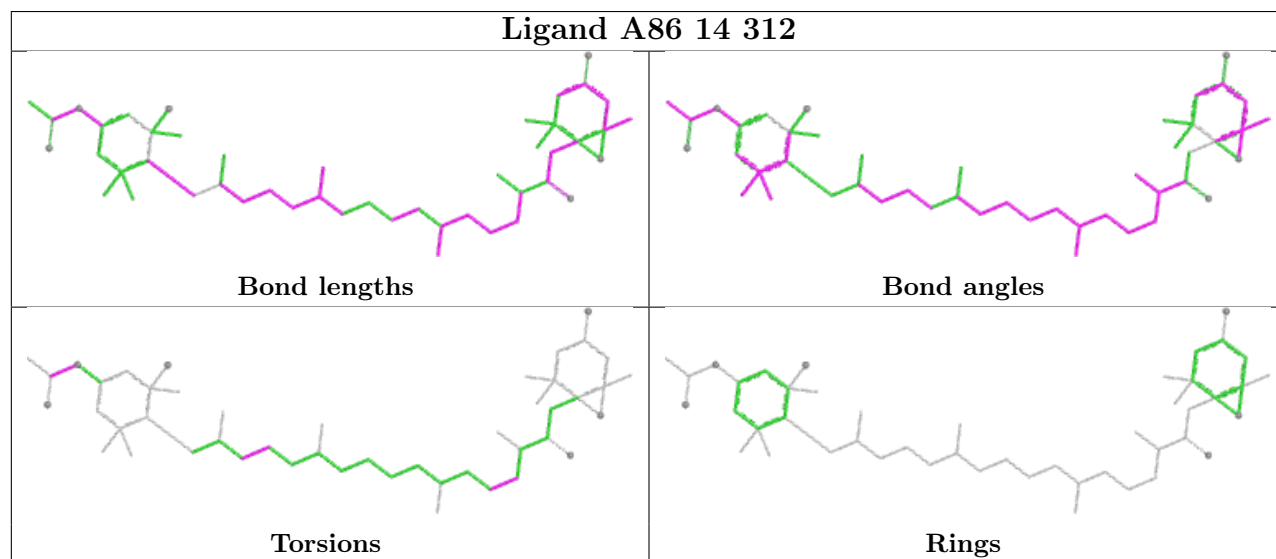
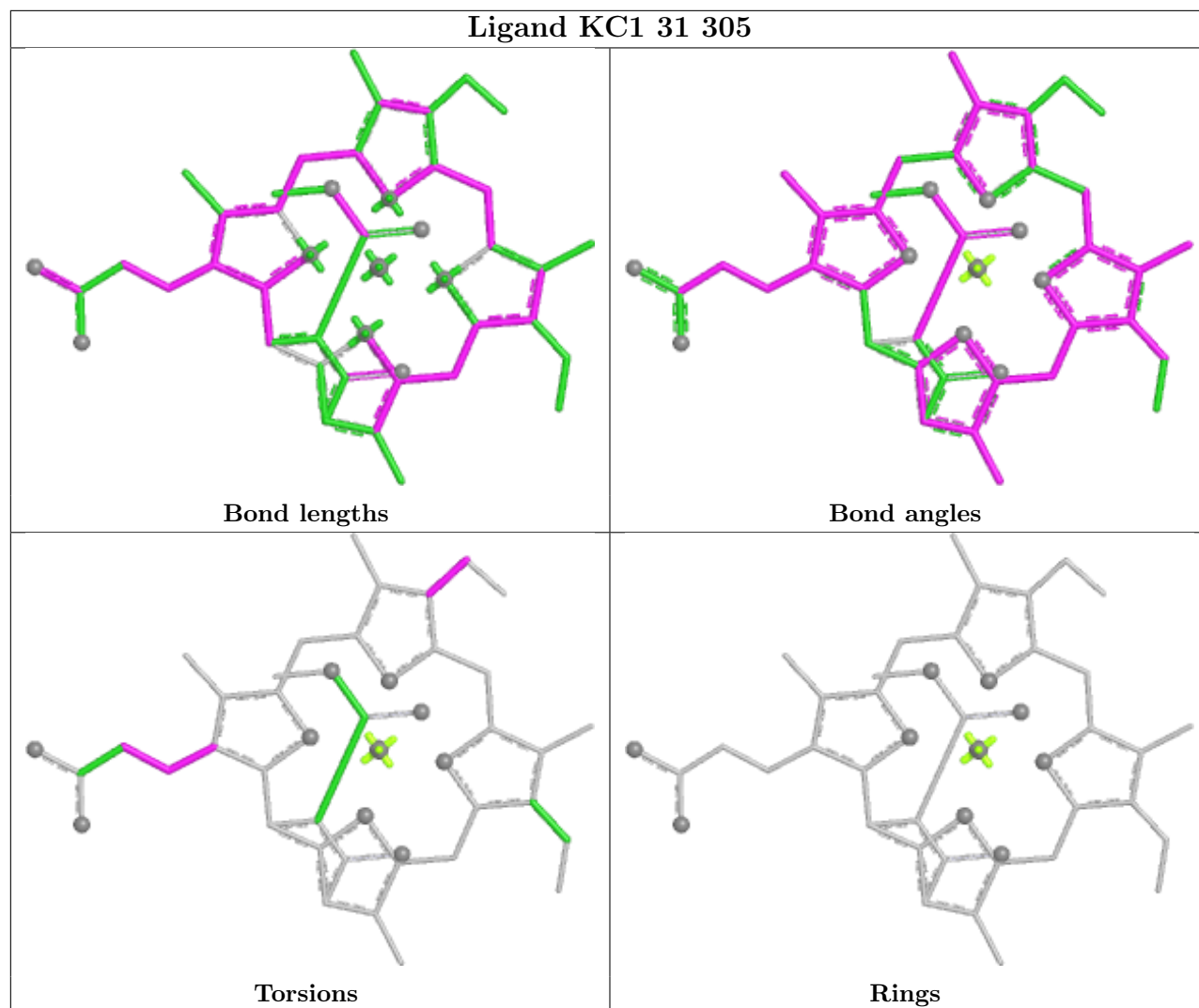


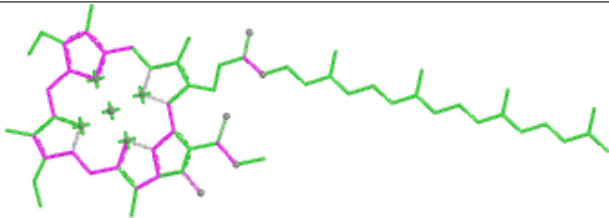
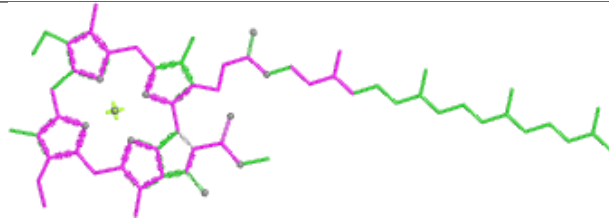
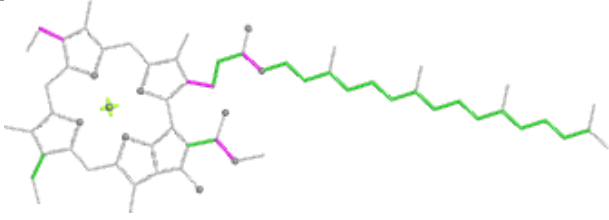
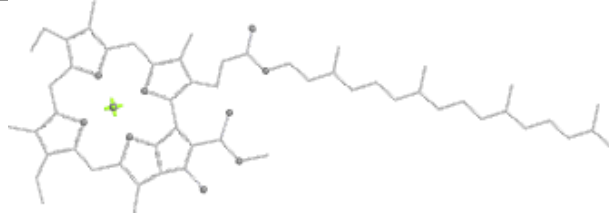


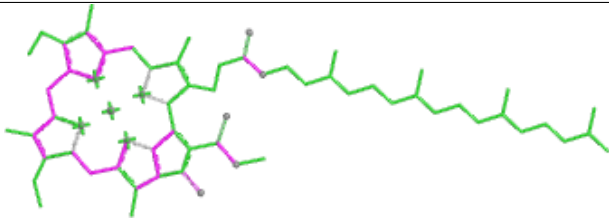
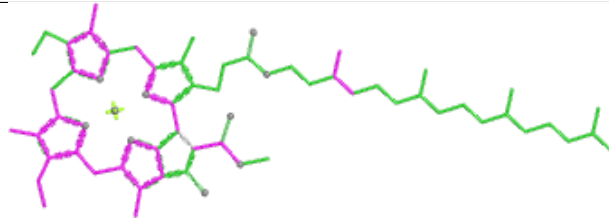
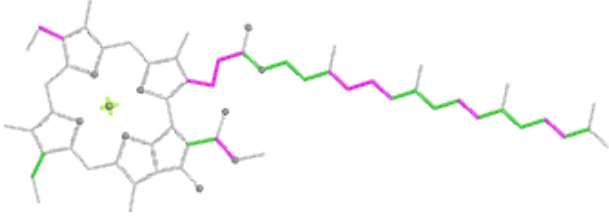
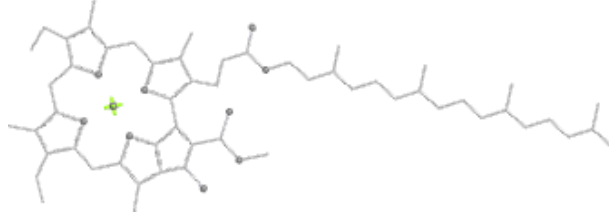


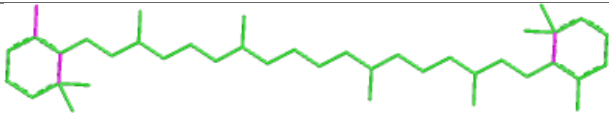
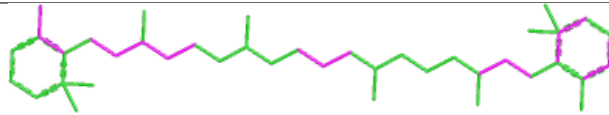
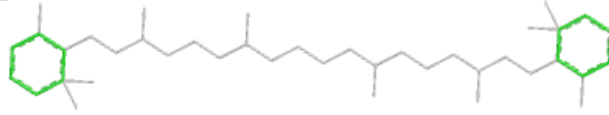


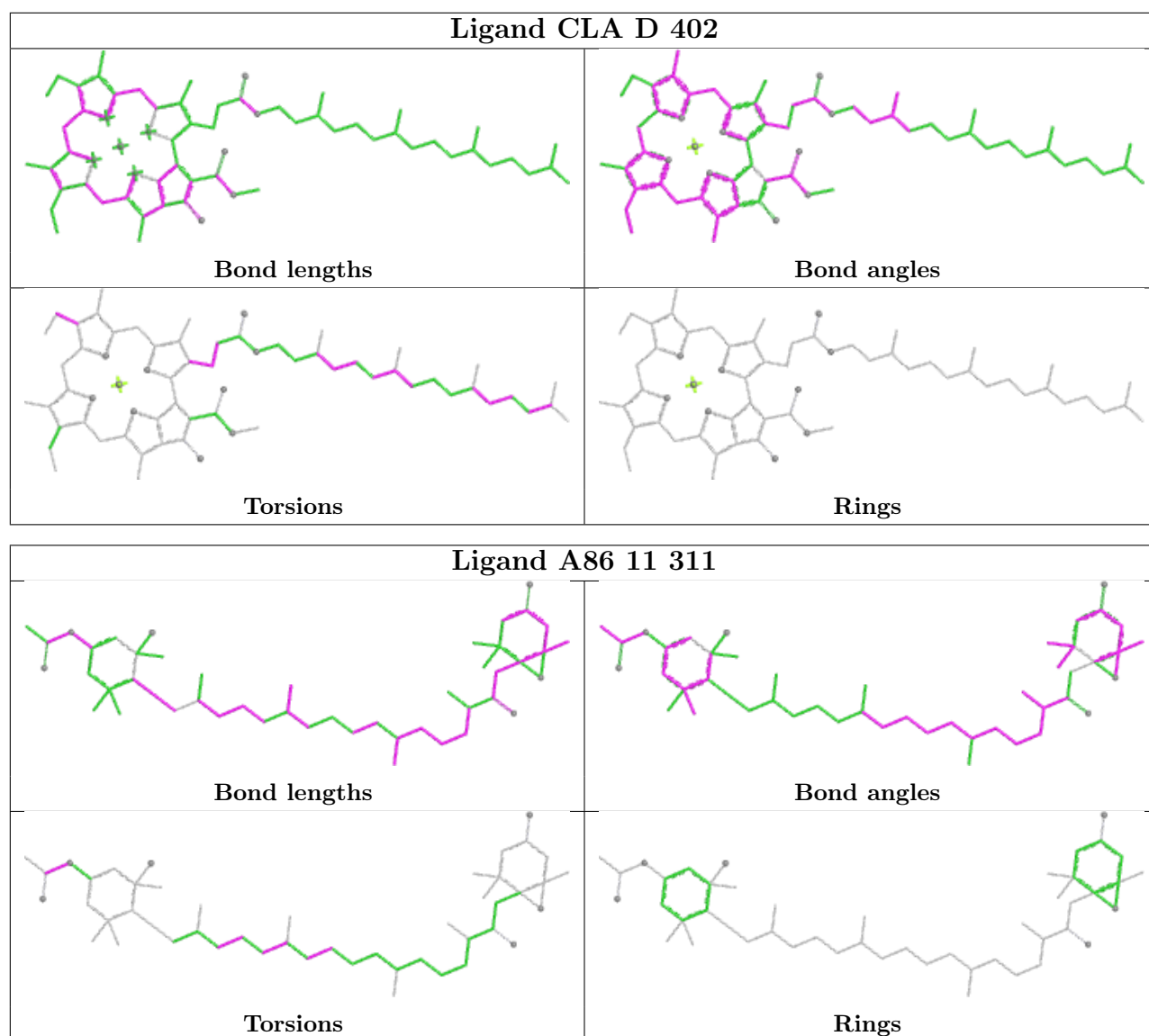


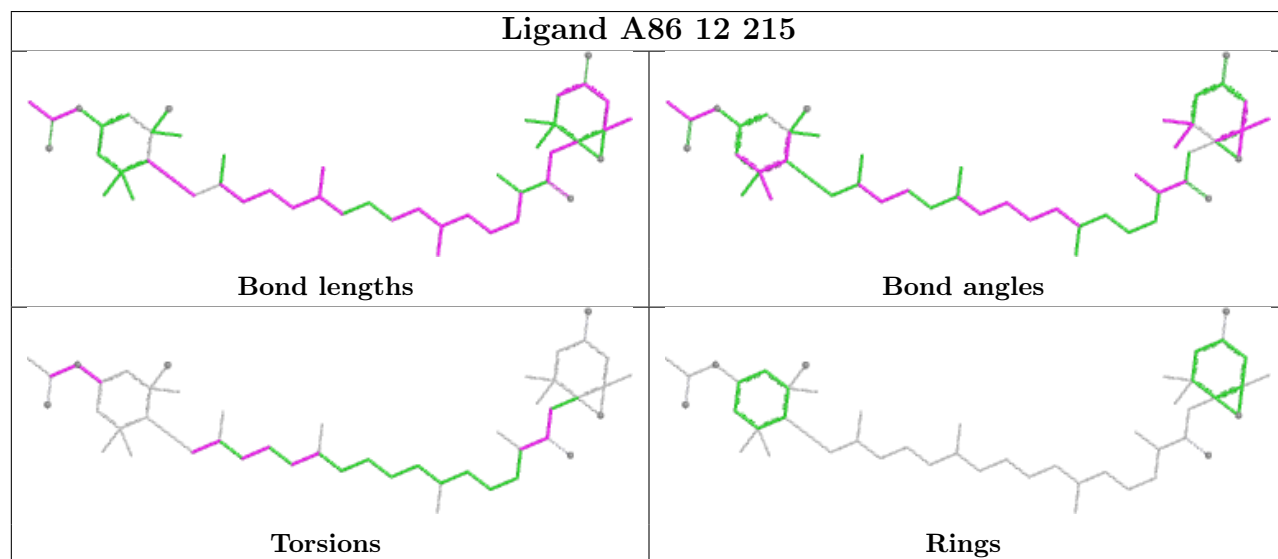
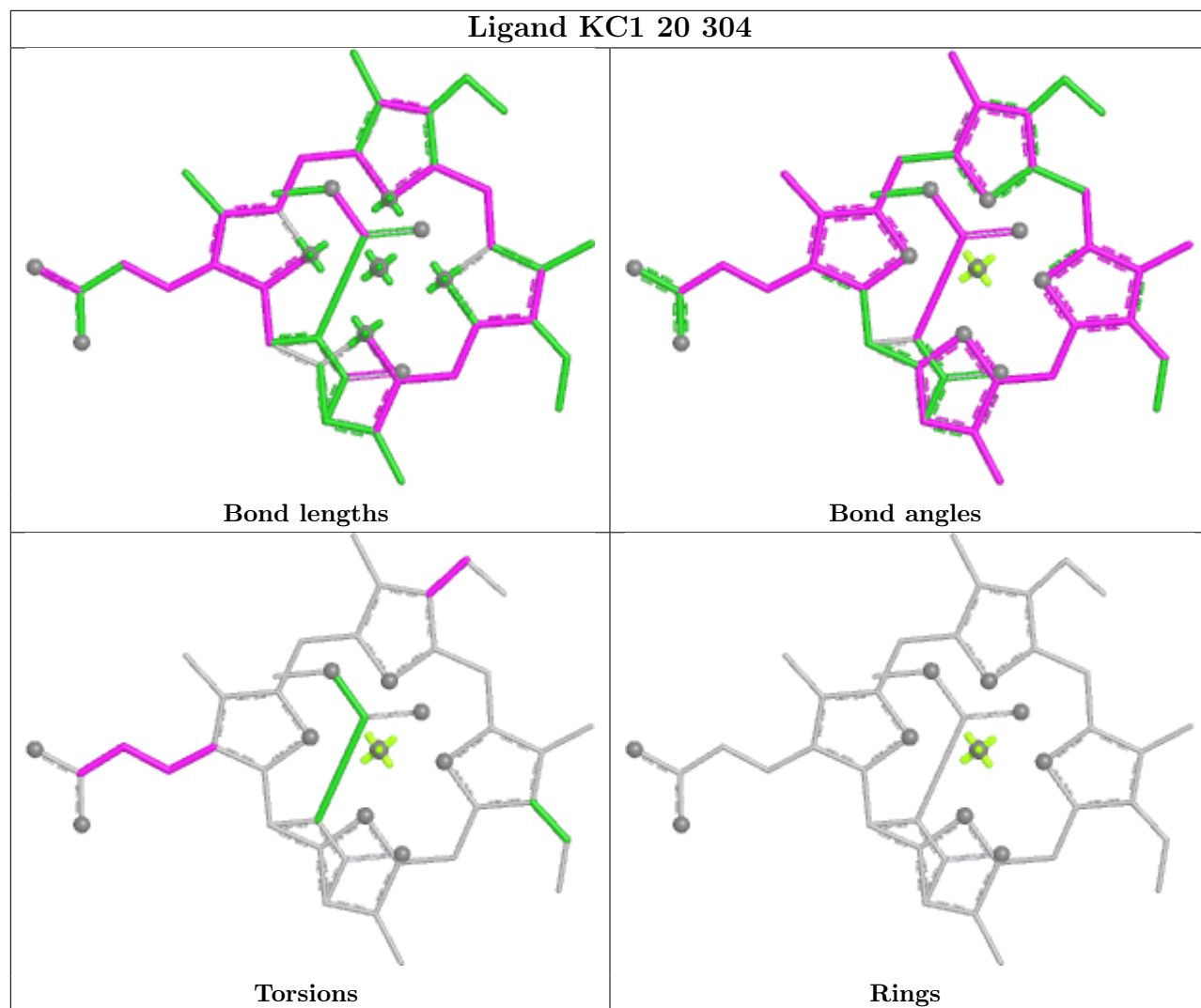


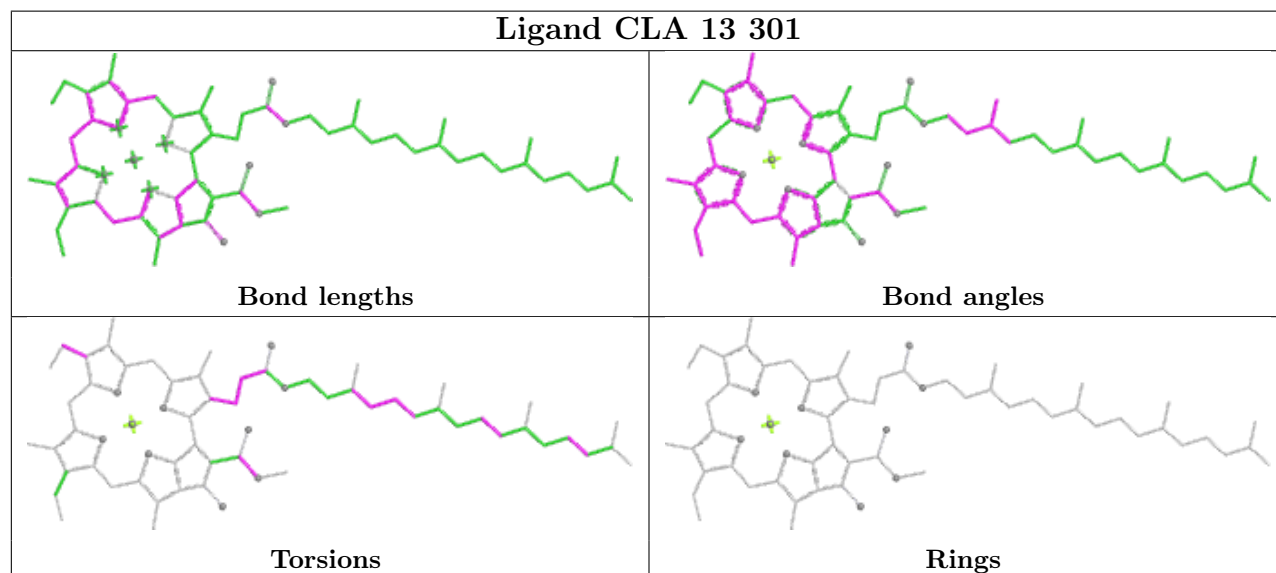
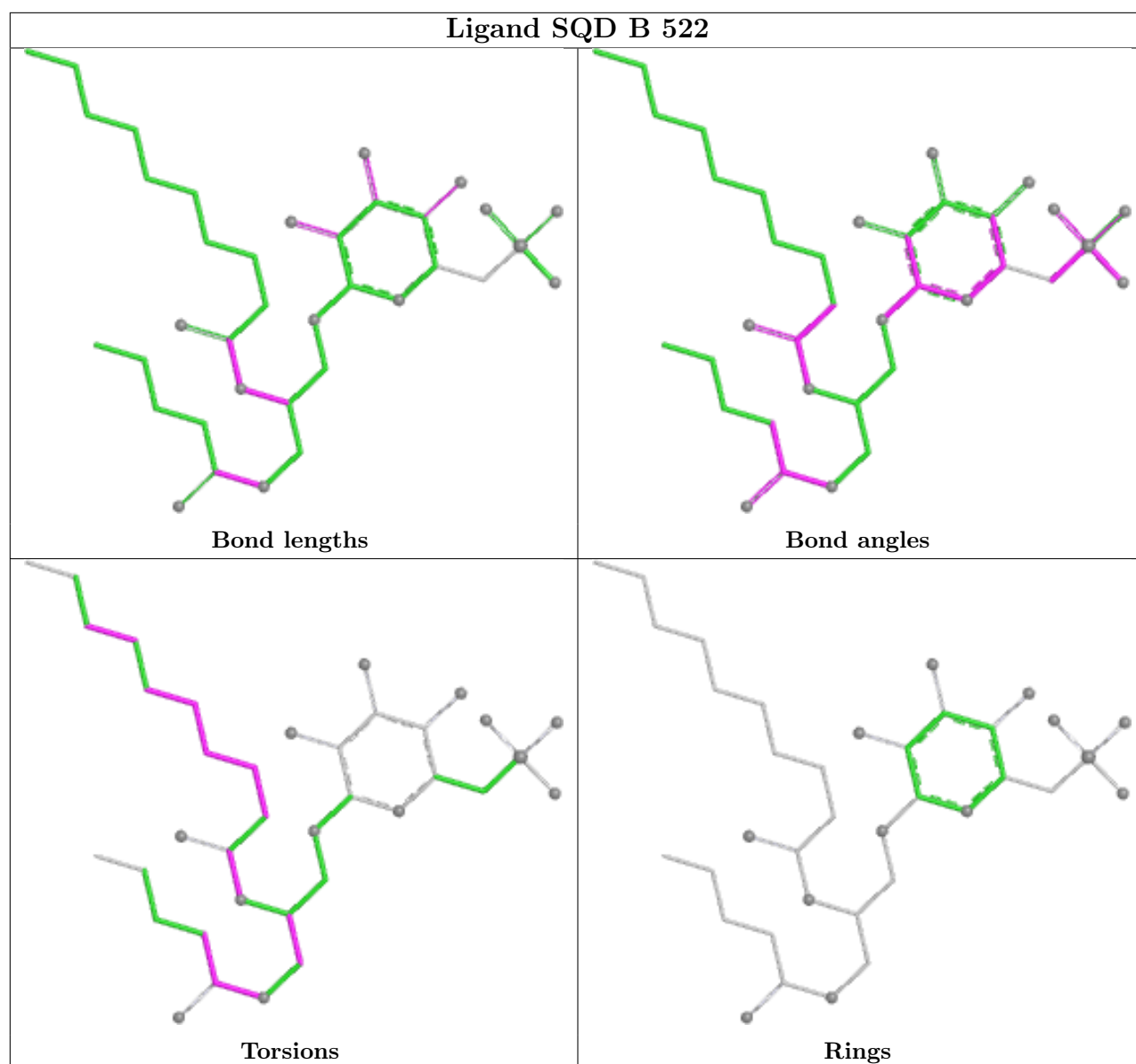
Ligand CLA 18 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

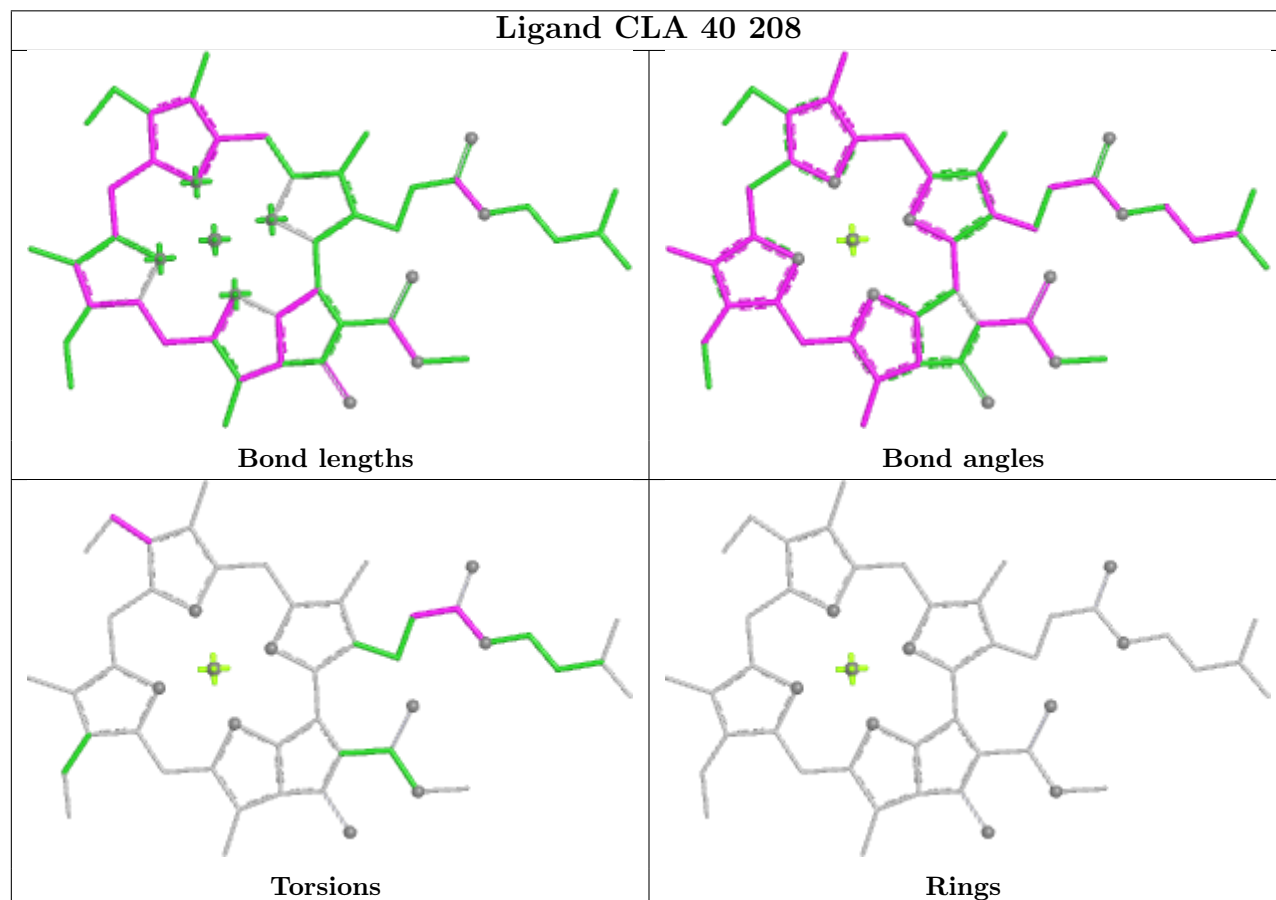
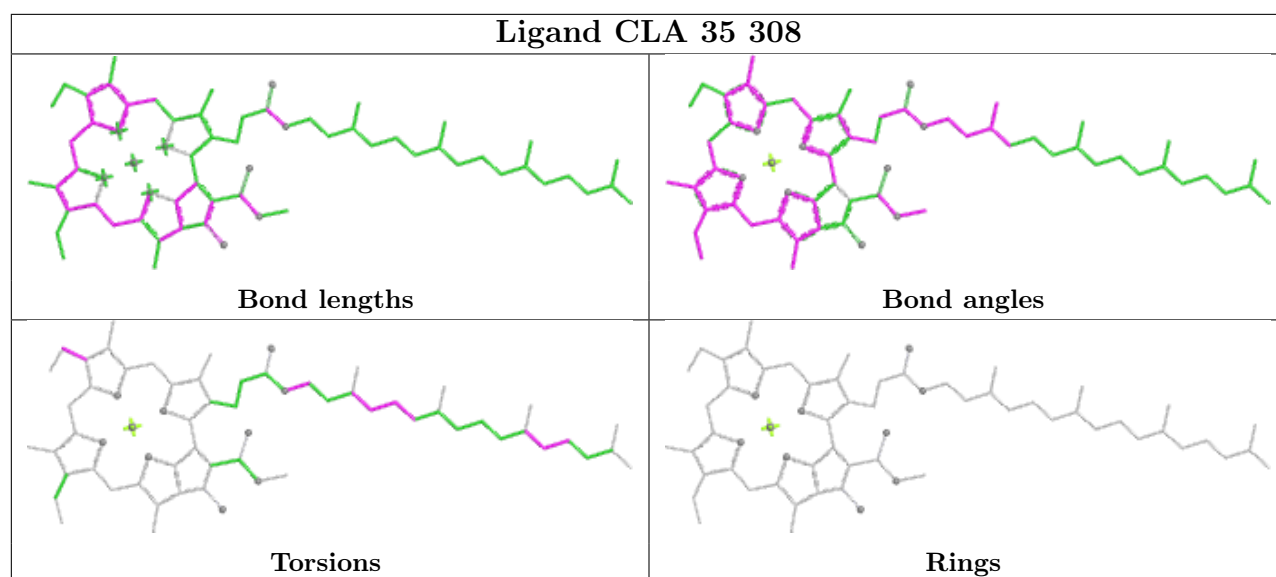
Ligand CLA 33 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

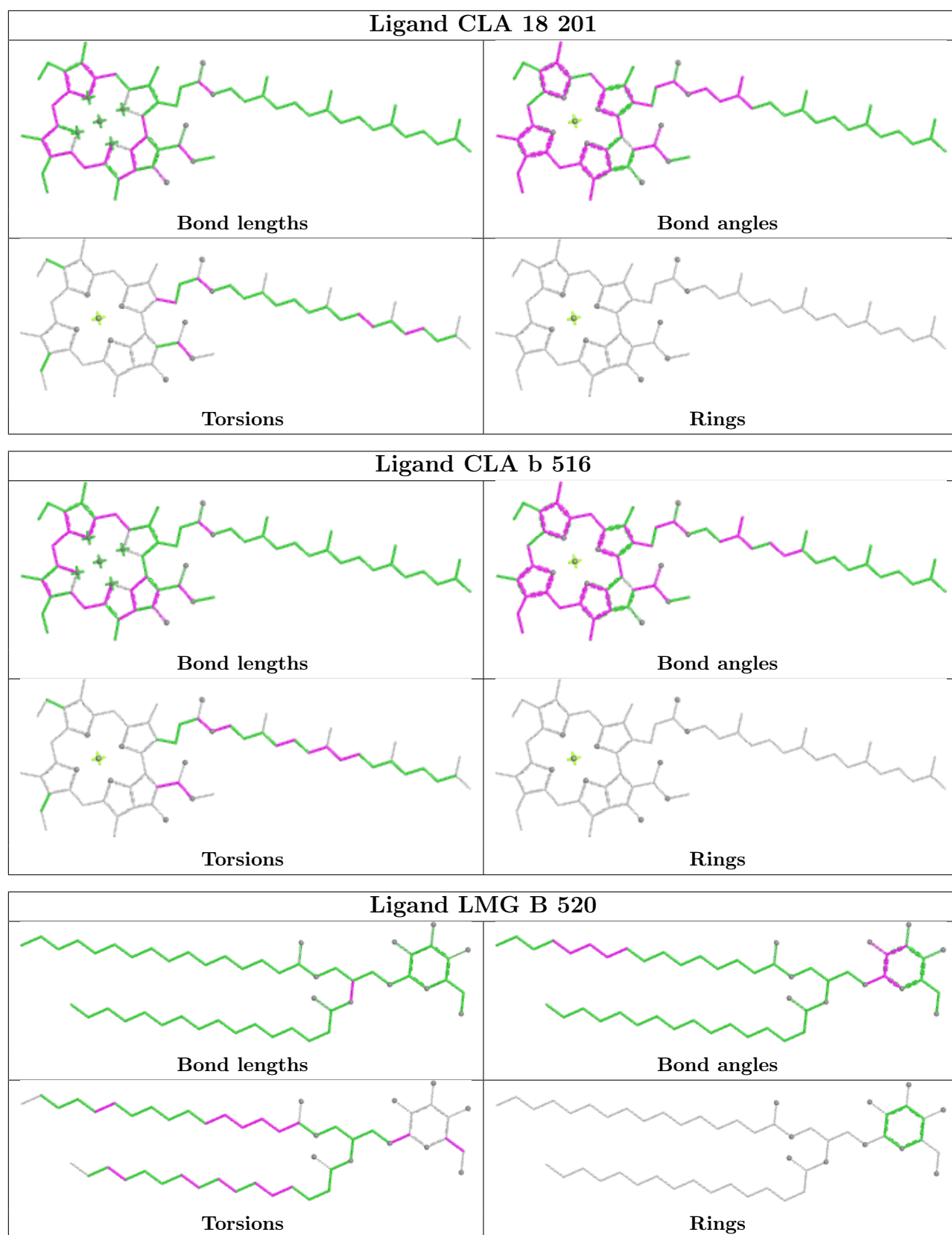
Ligand BCR d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

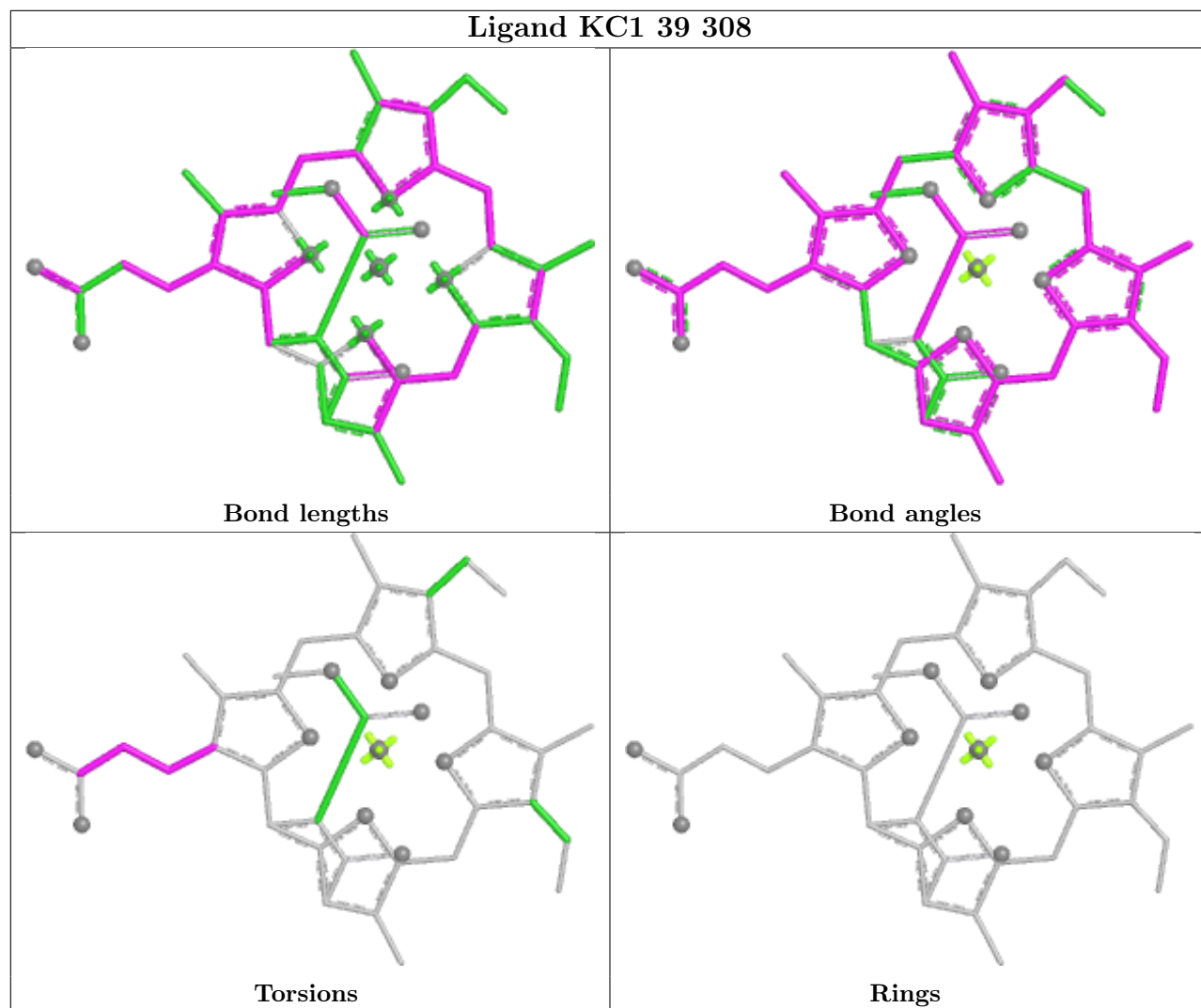


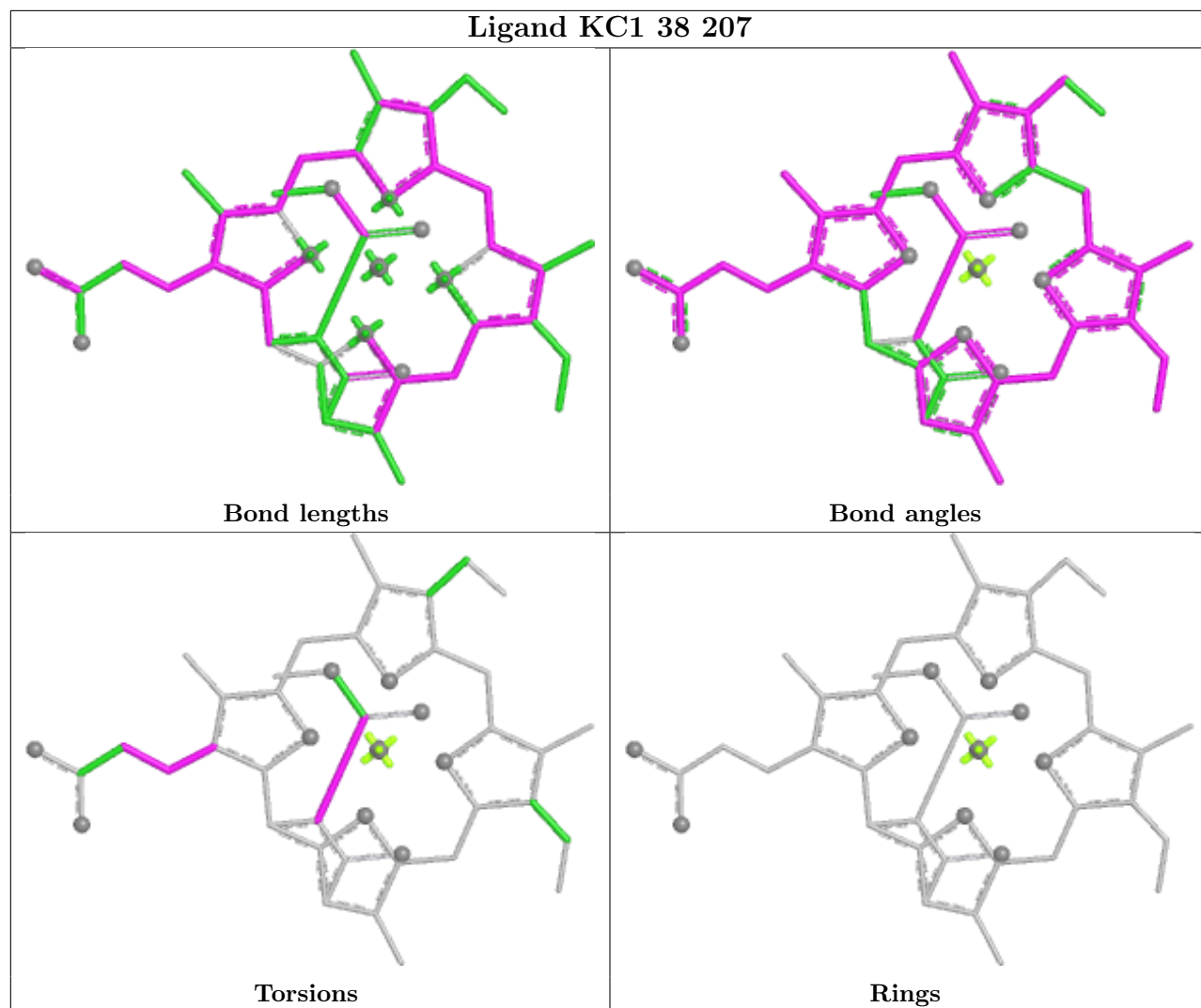


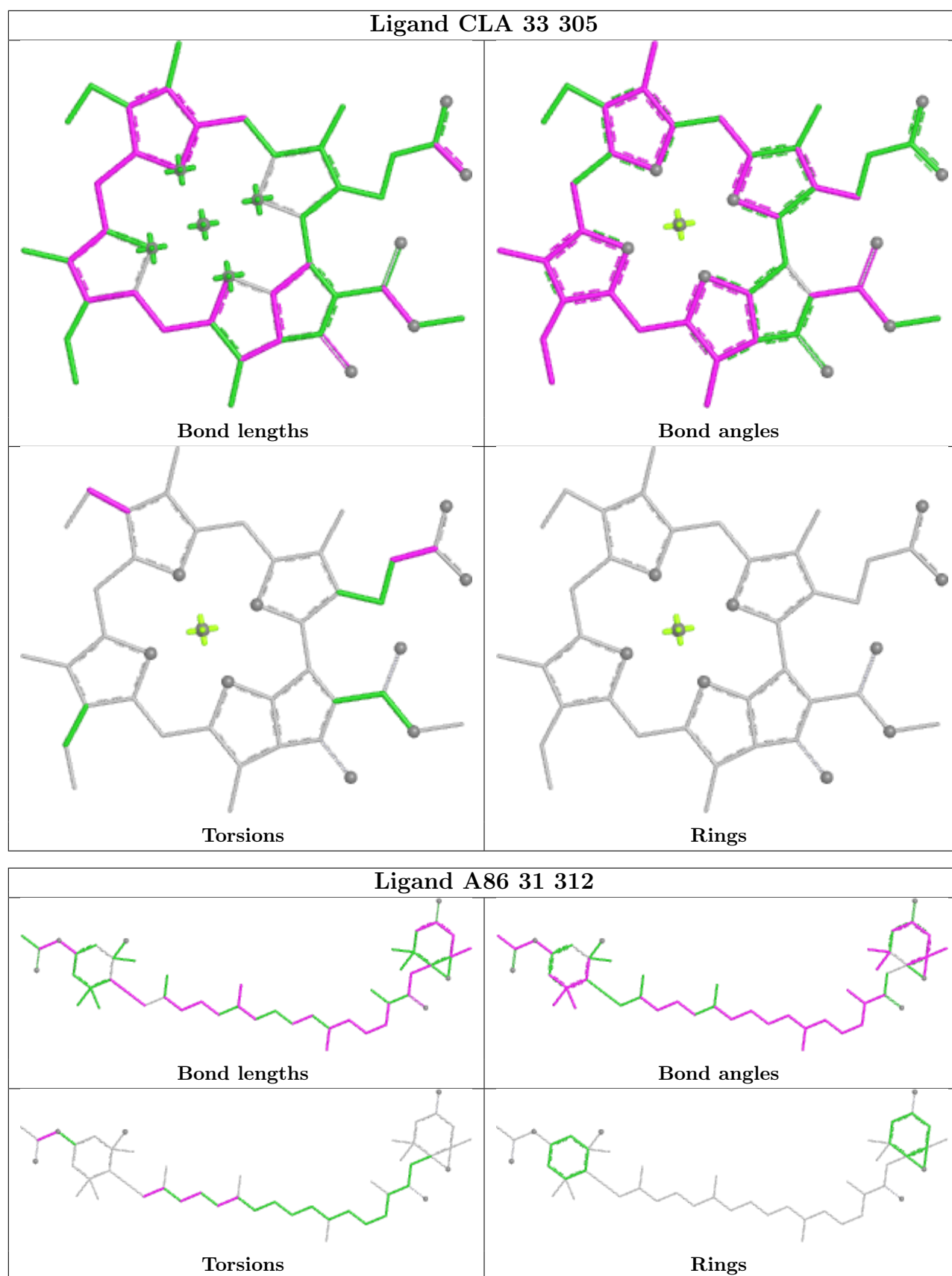


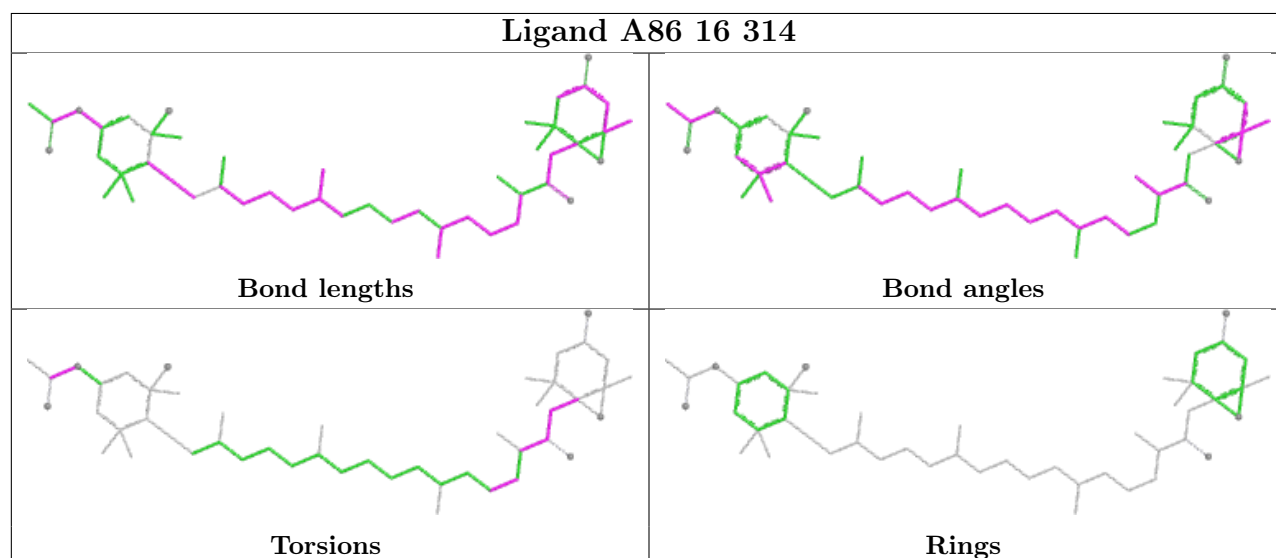
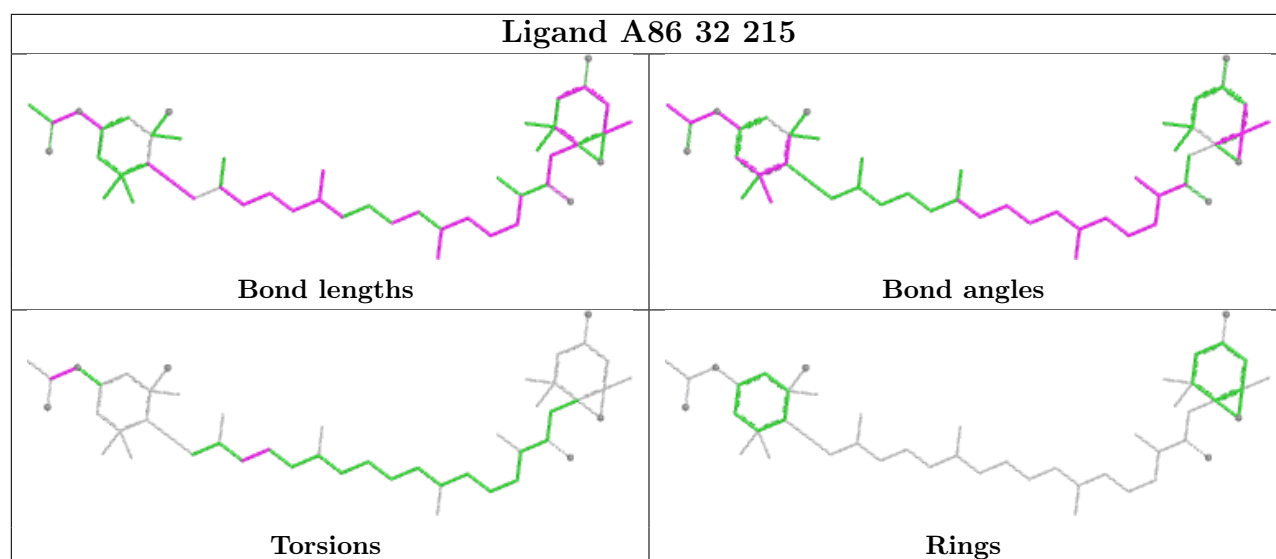


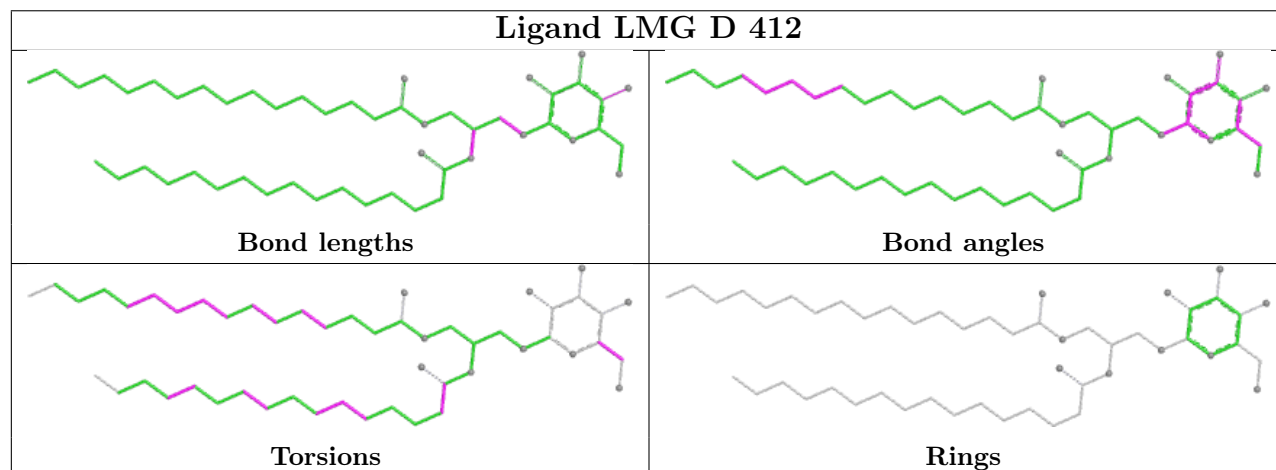
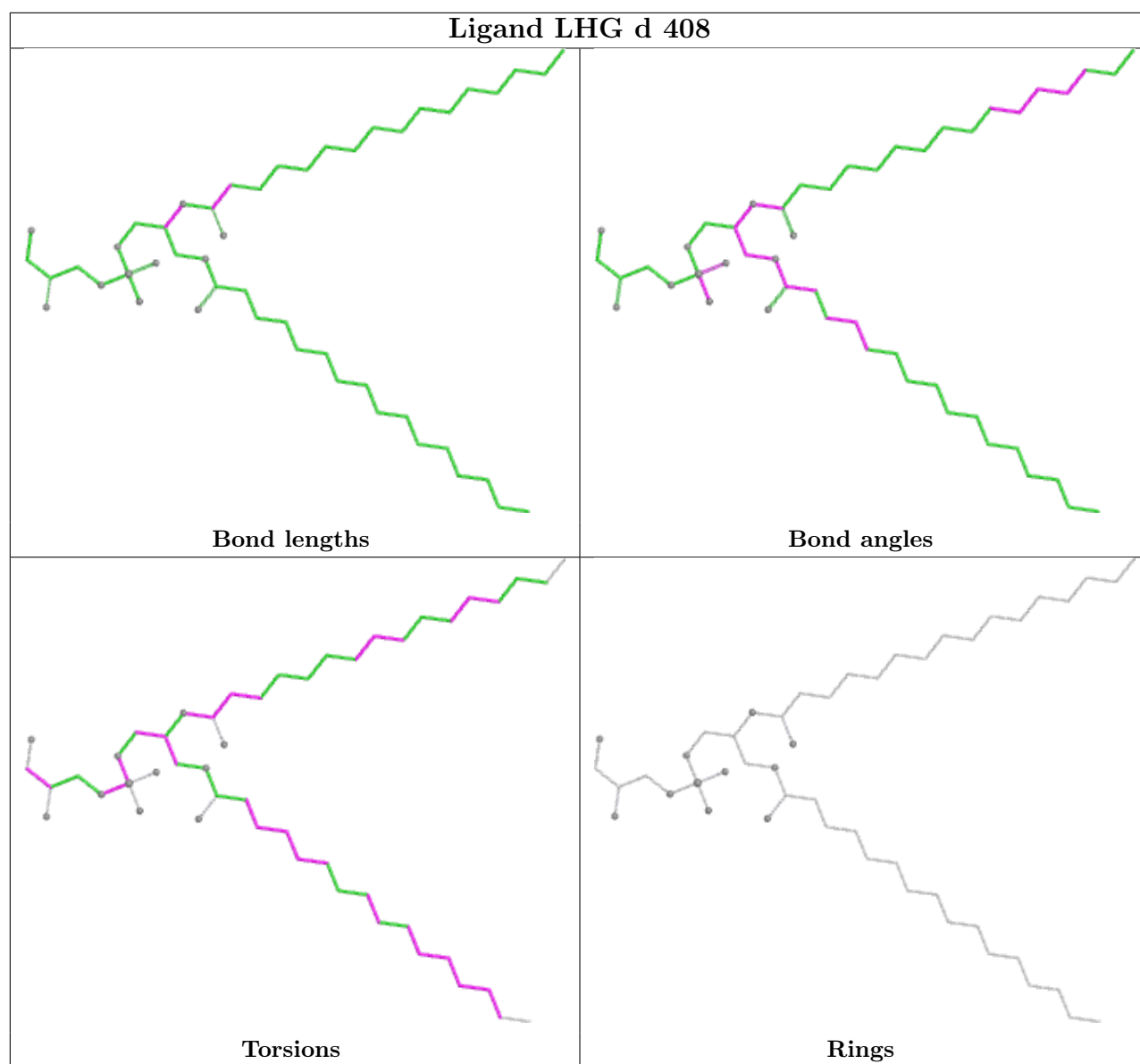


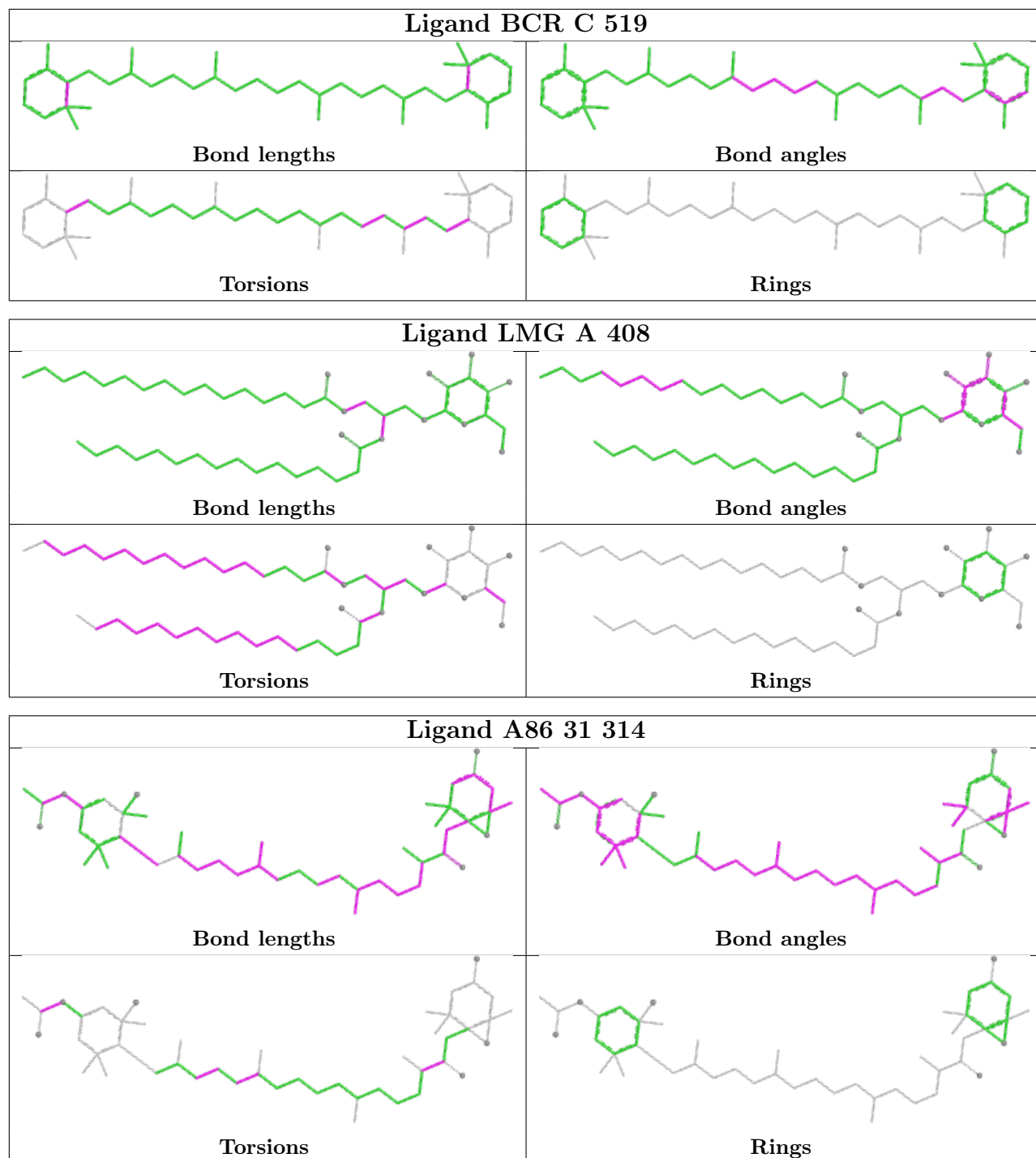


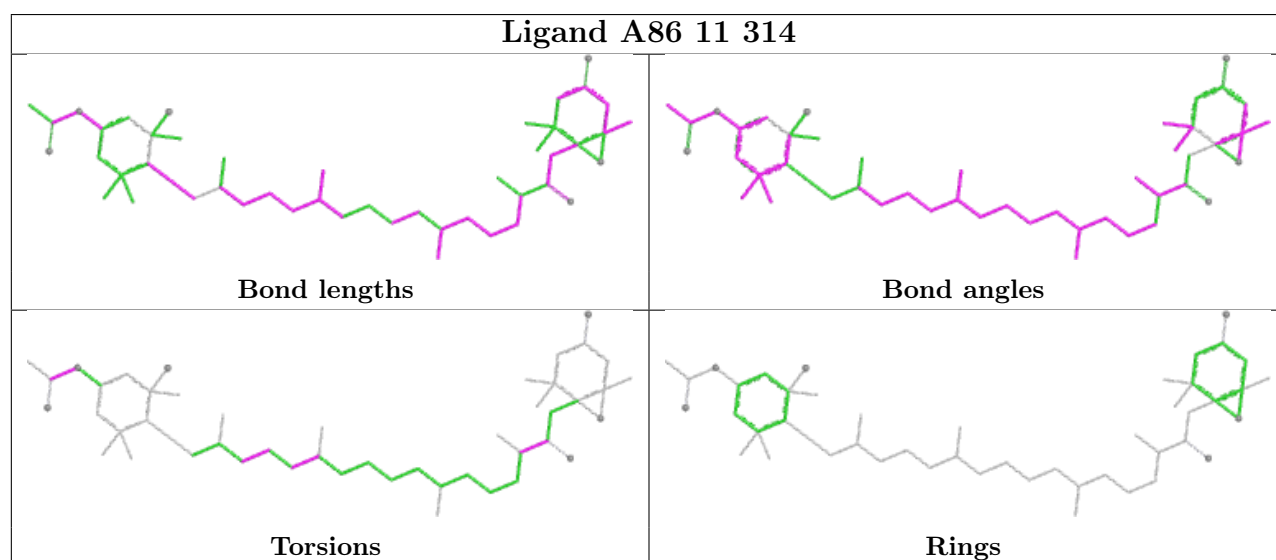
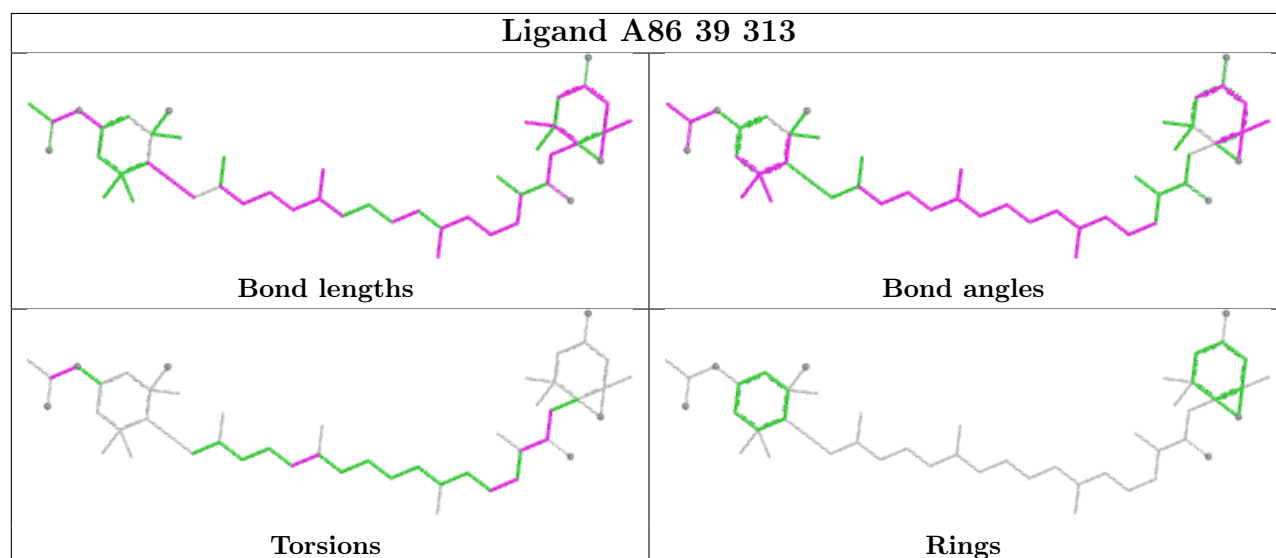
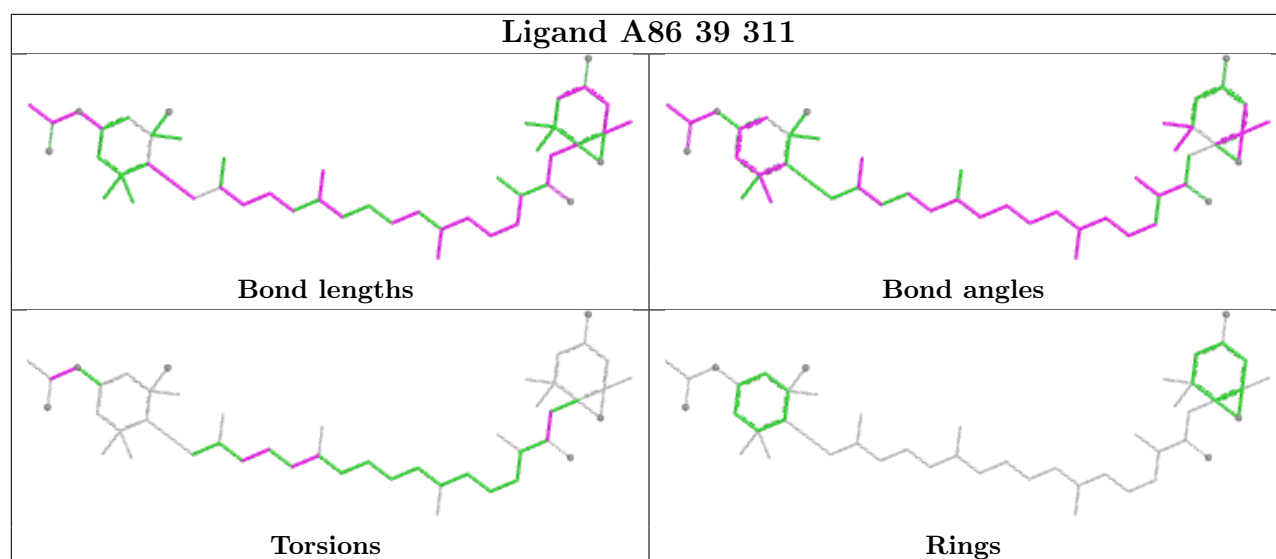


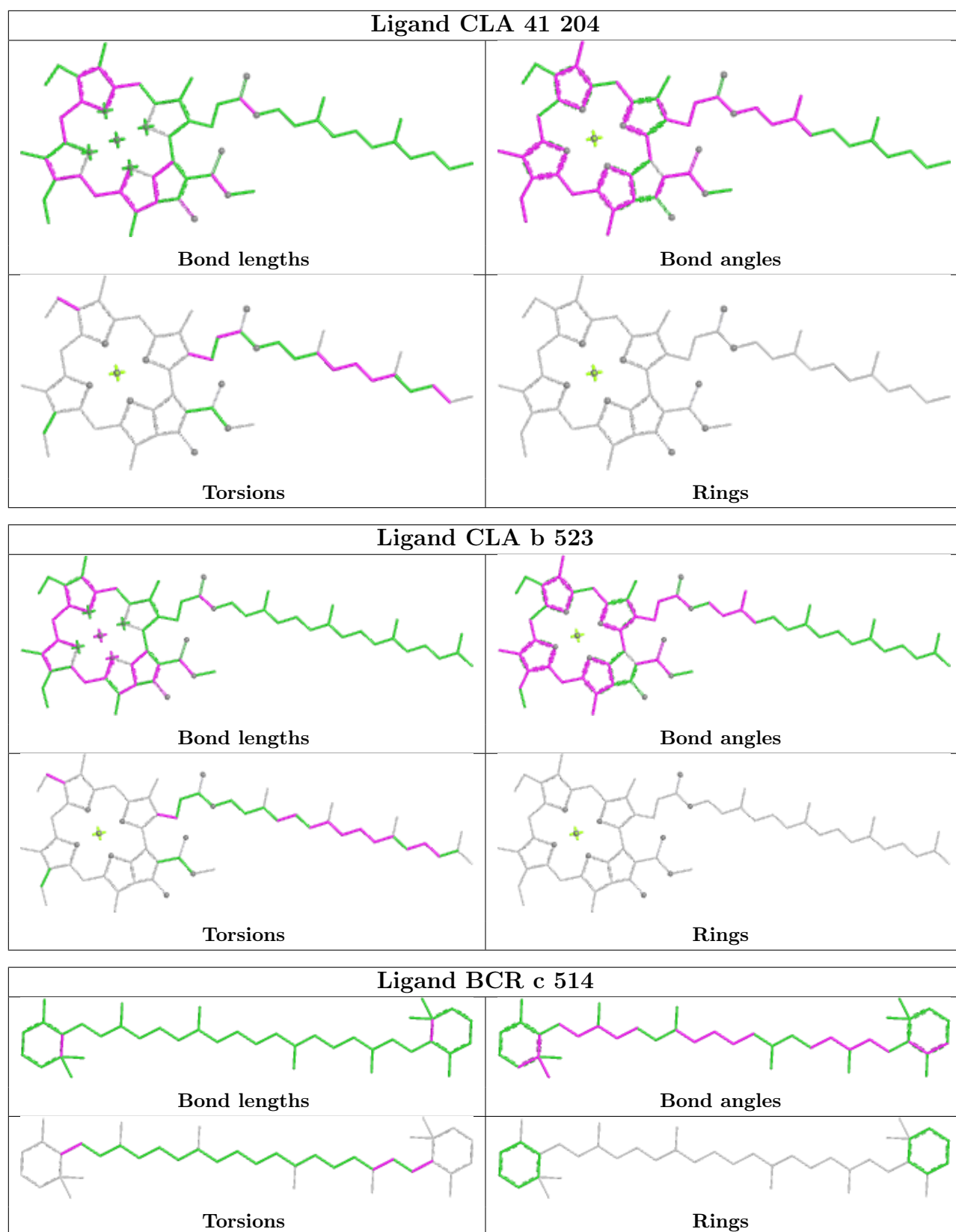


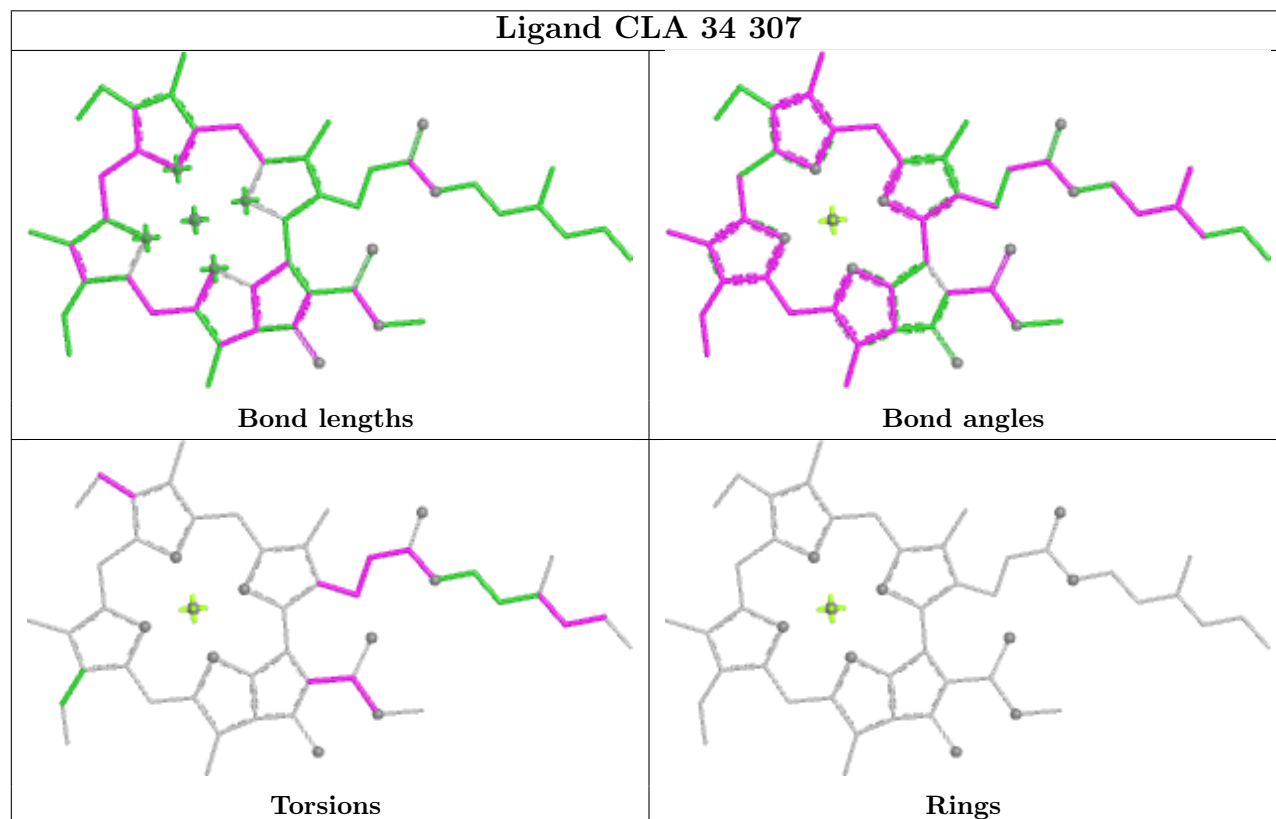
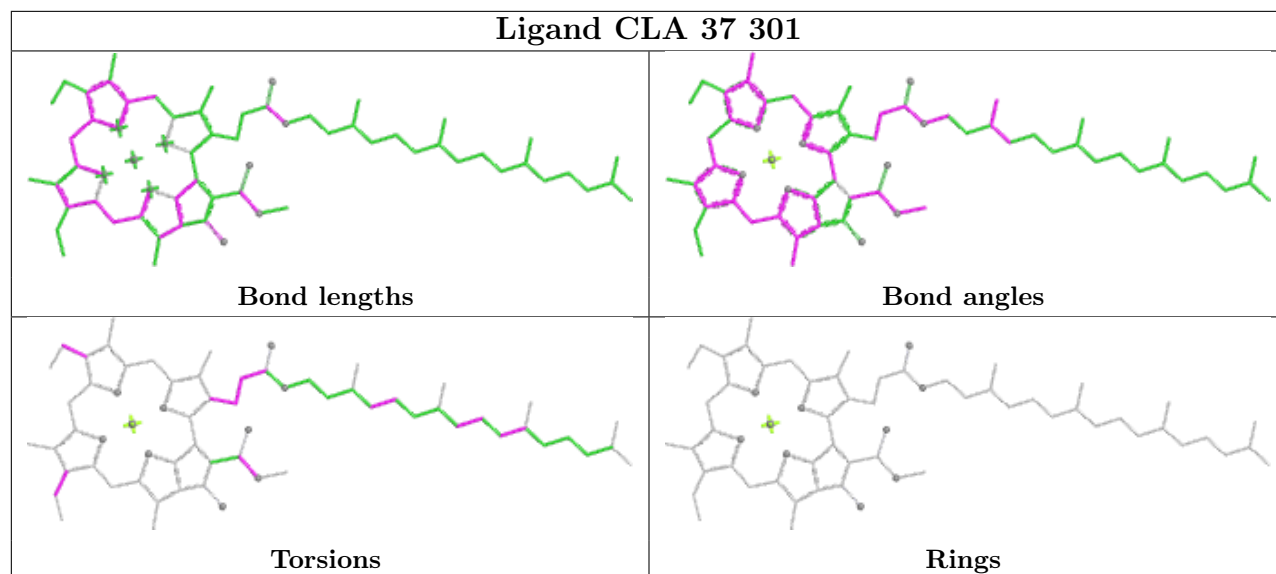


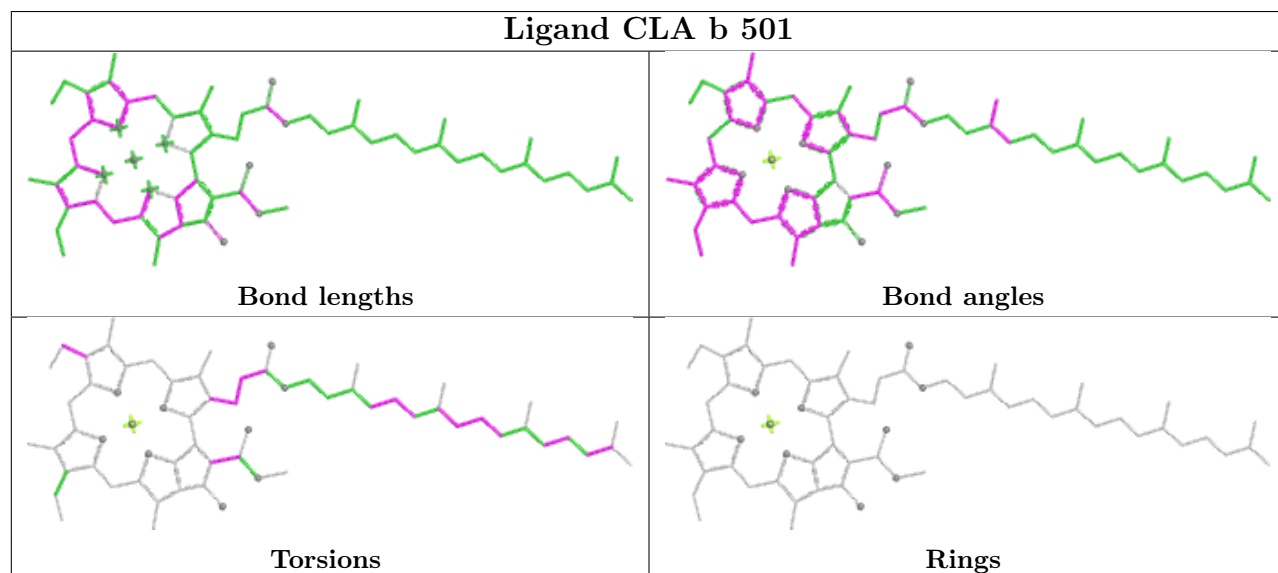
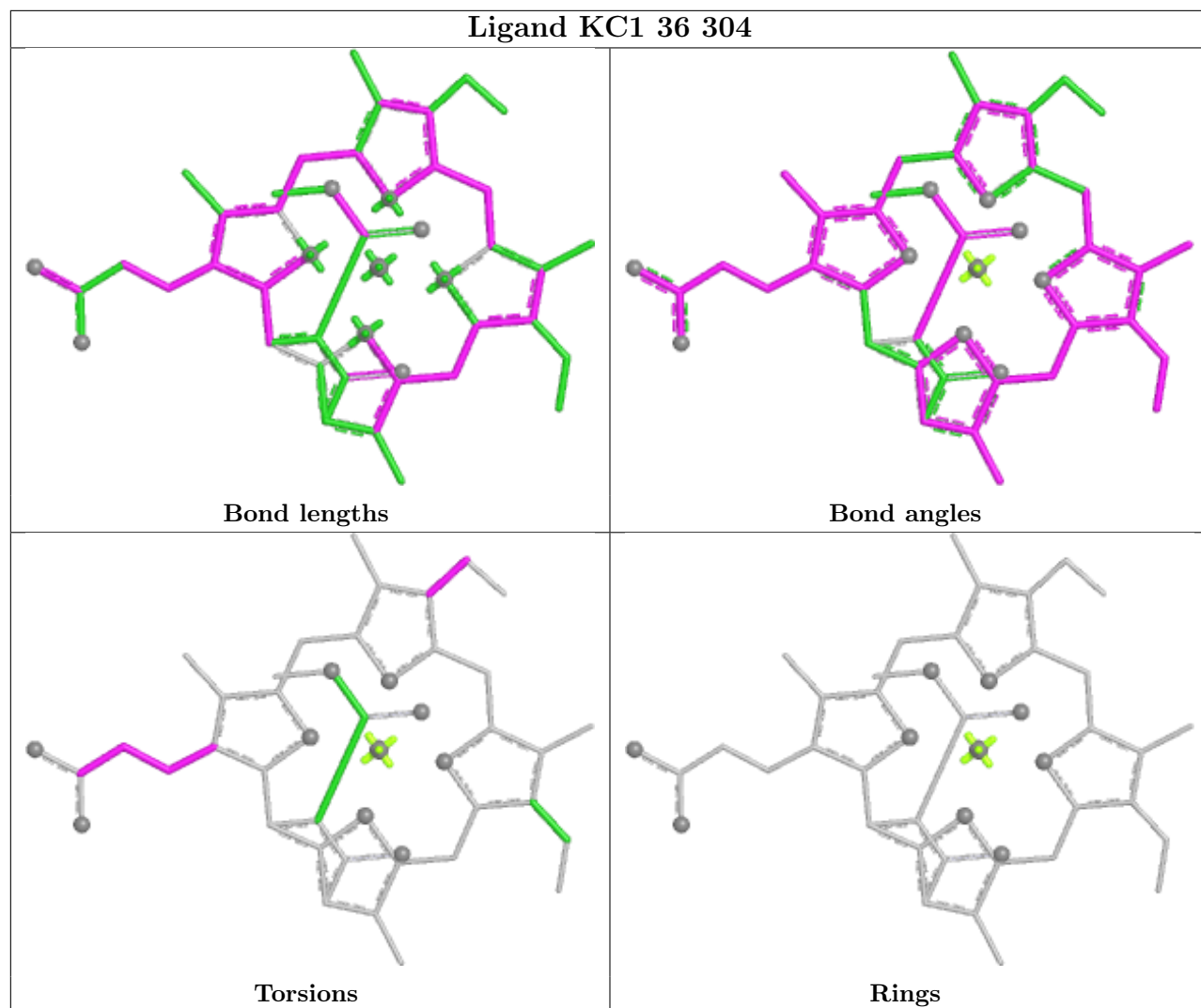


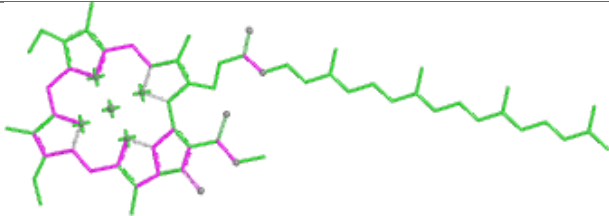
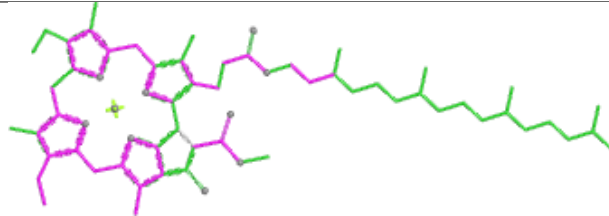
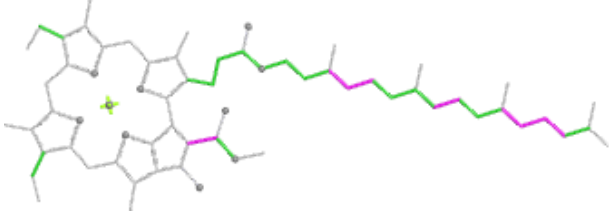
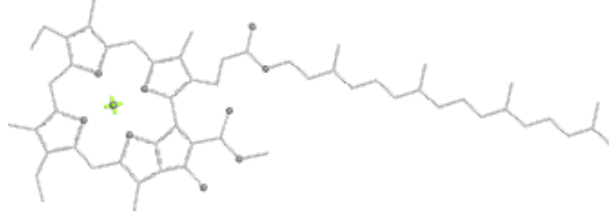


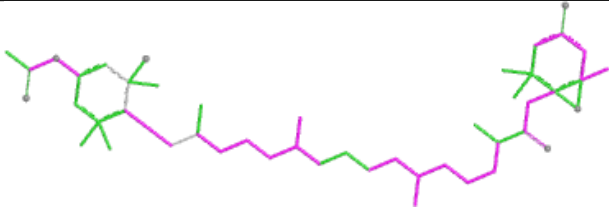
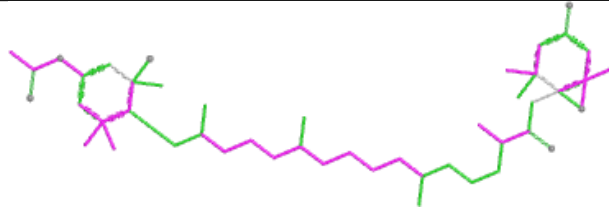
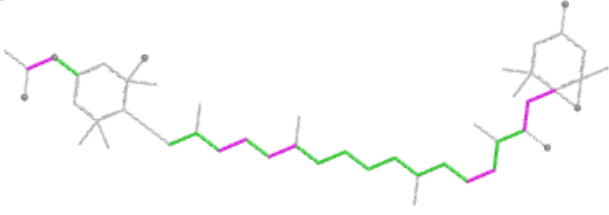
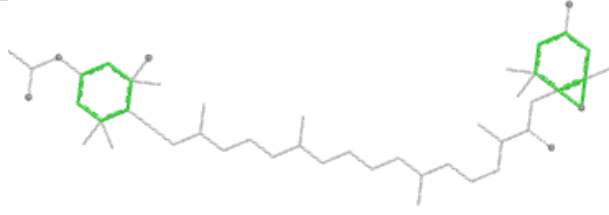


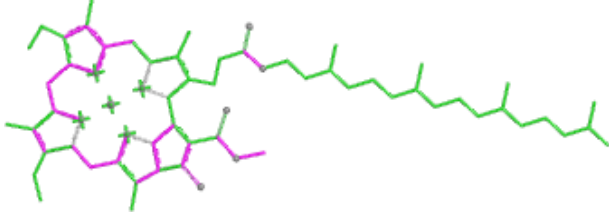
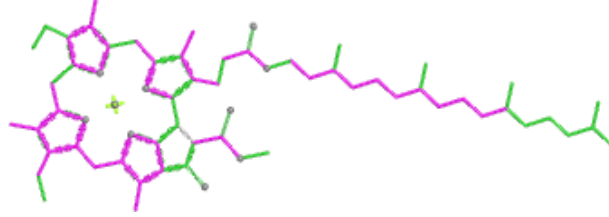
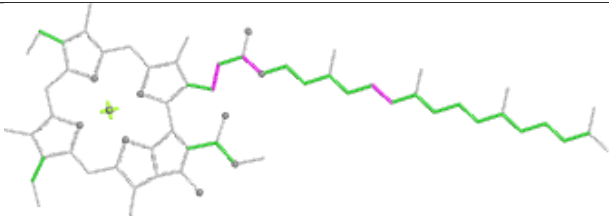
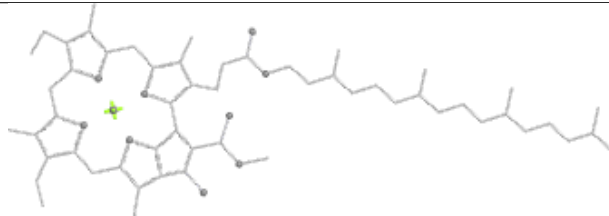


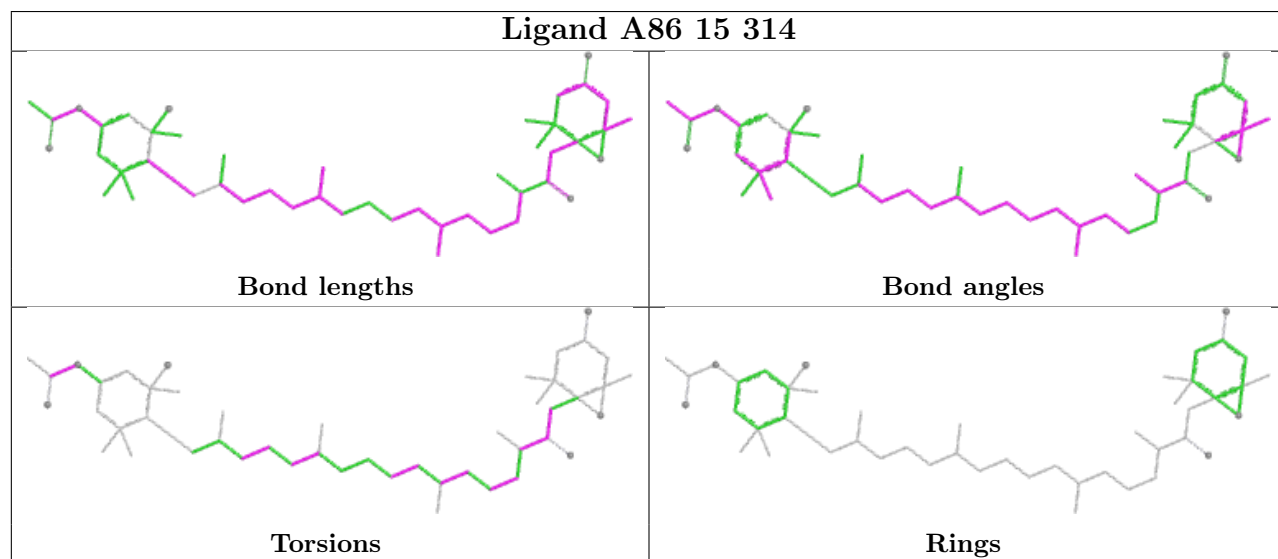
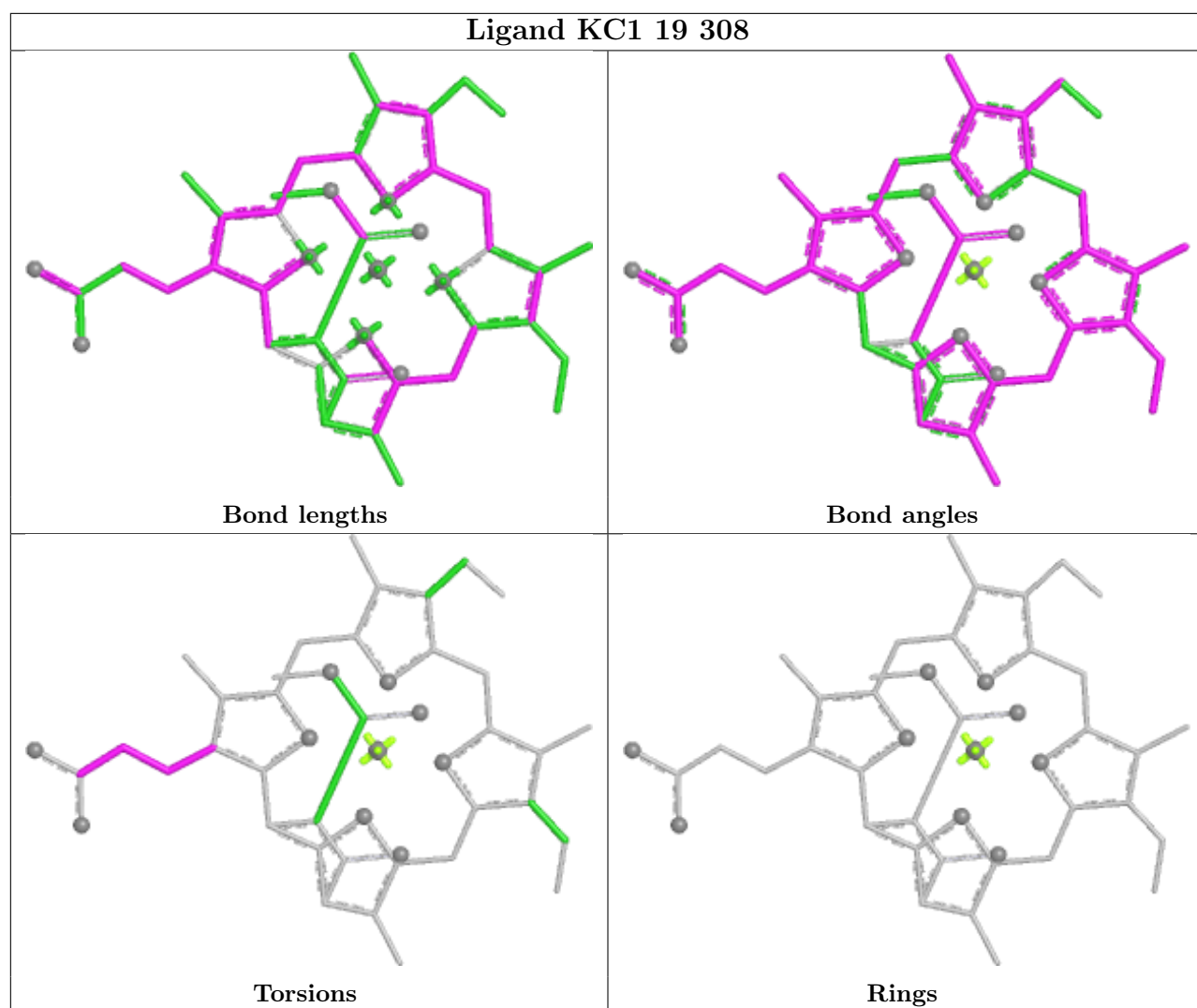


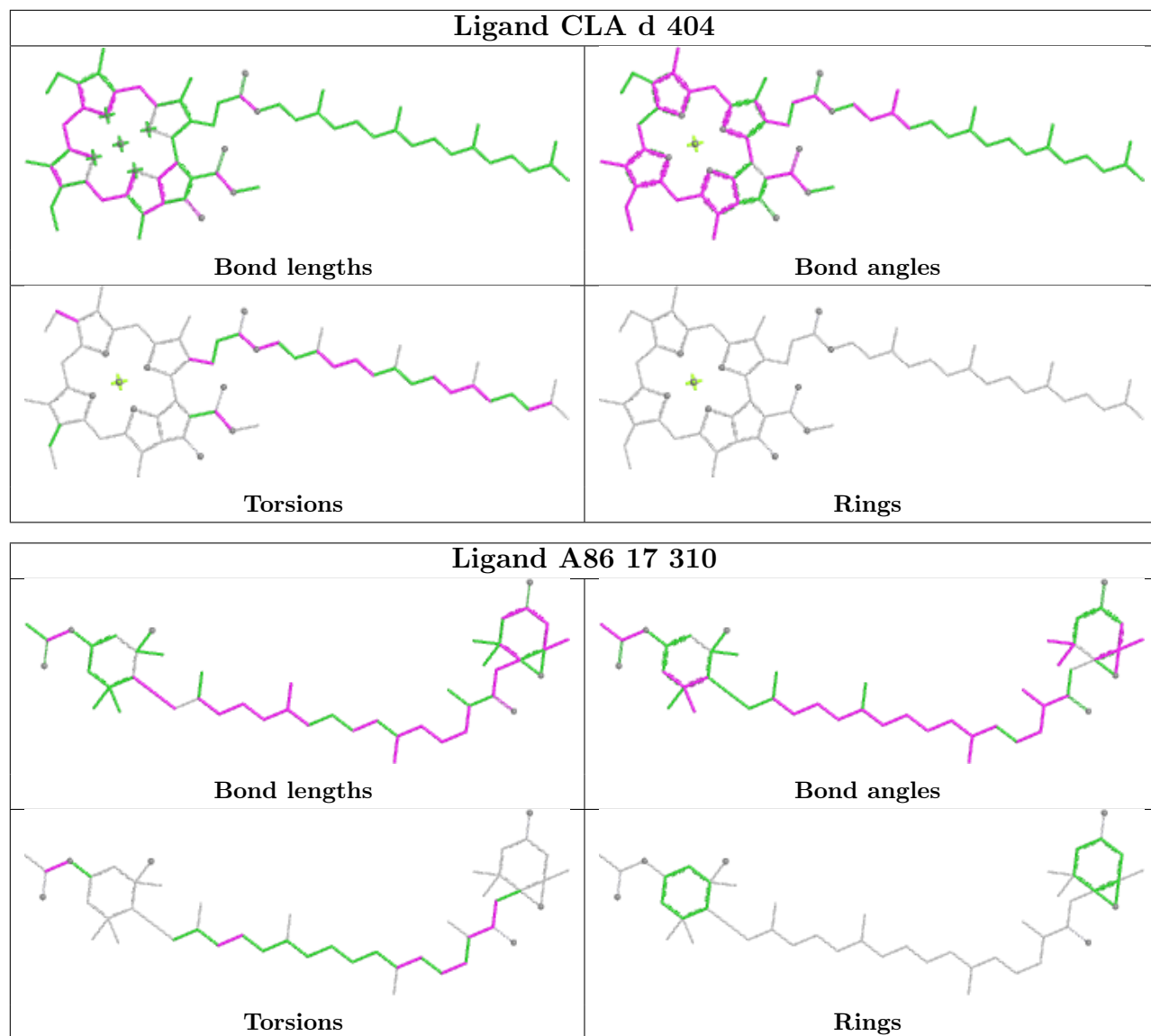


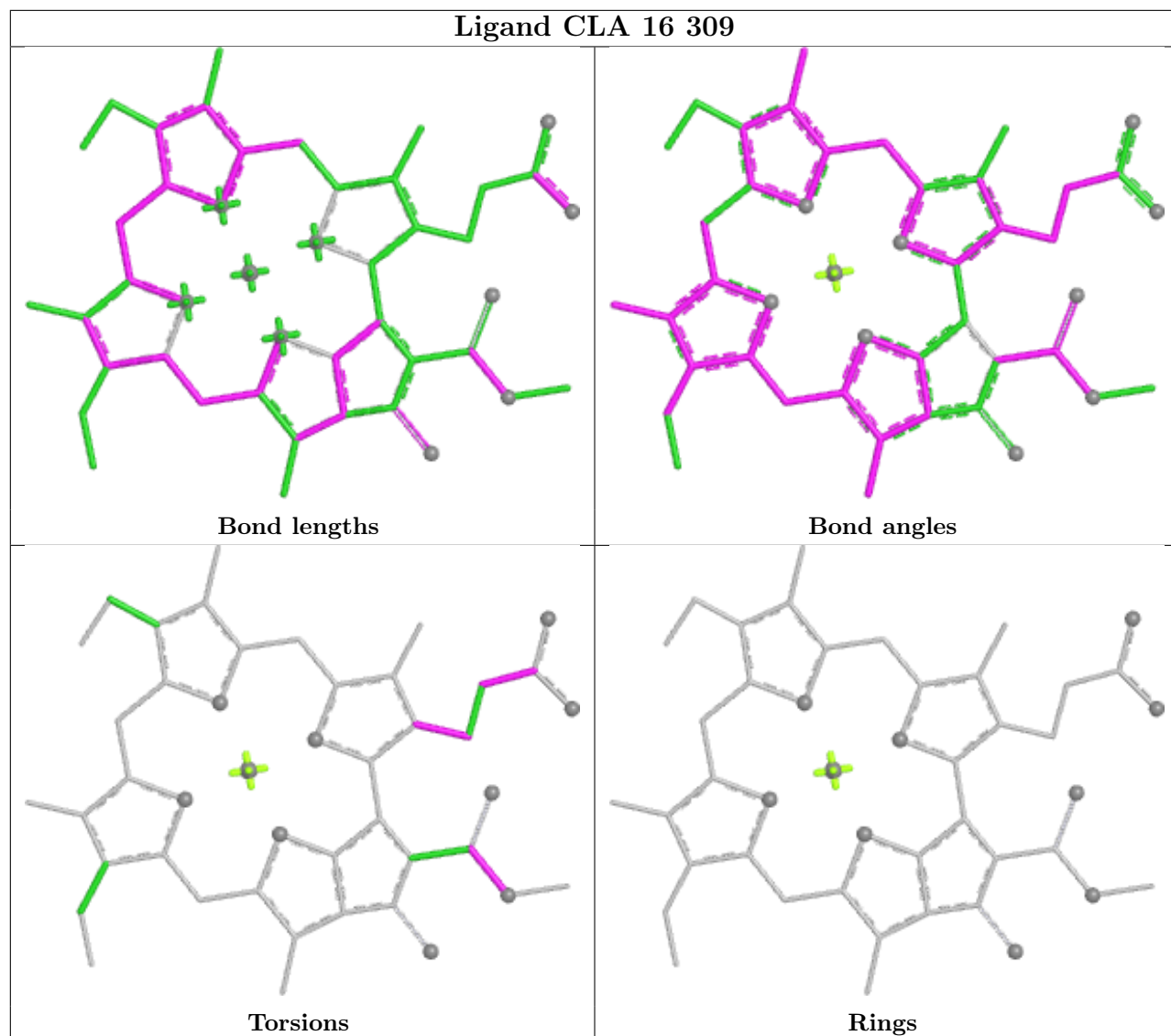
Ligand CLA B 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

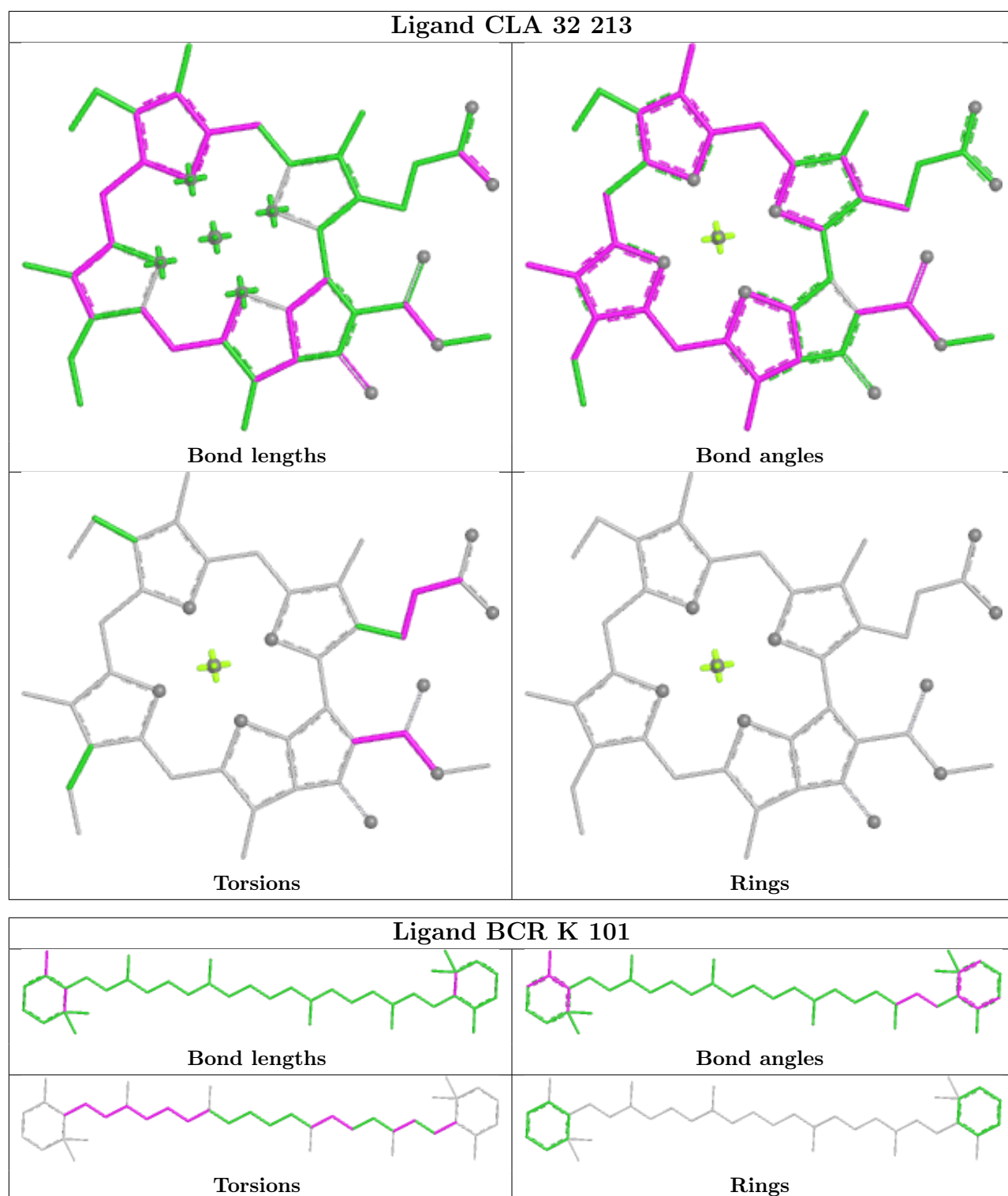
Ligand A86 13 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

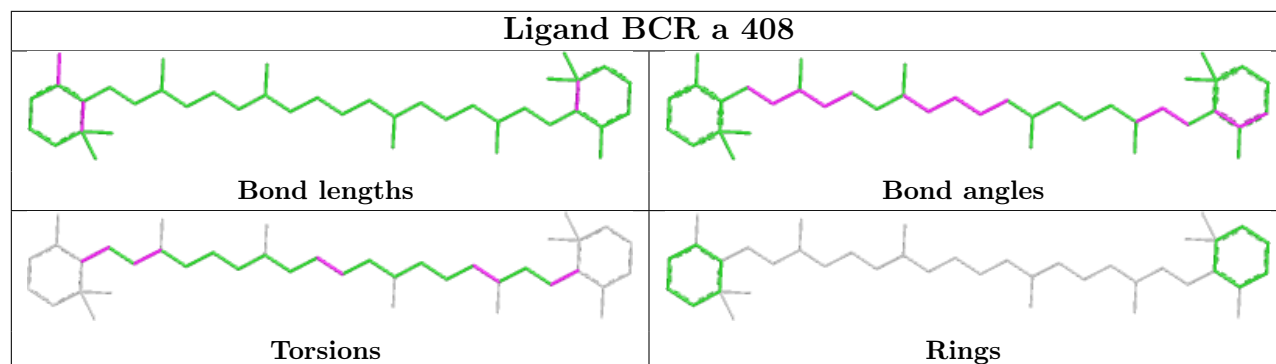
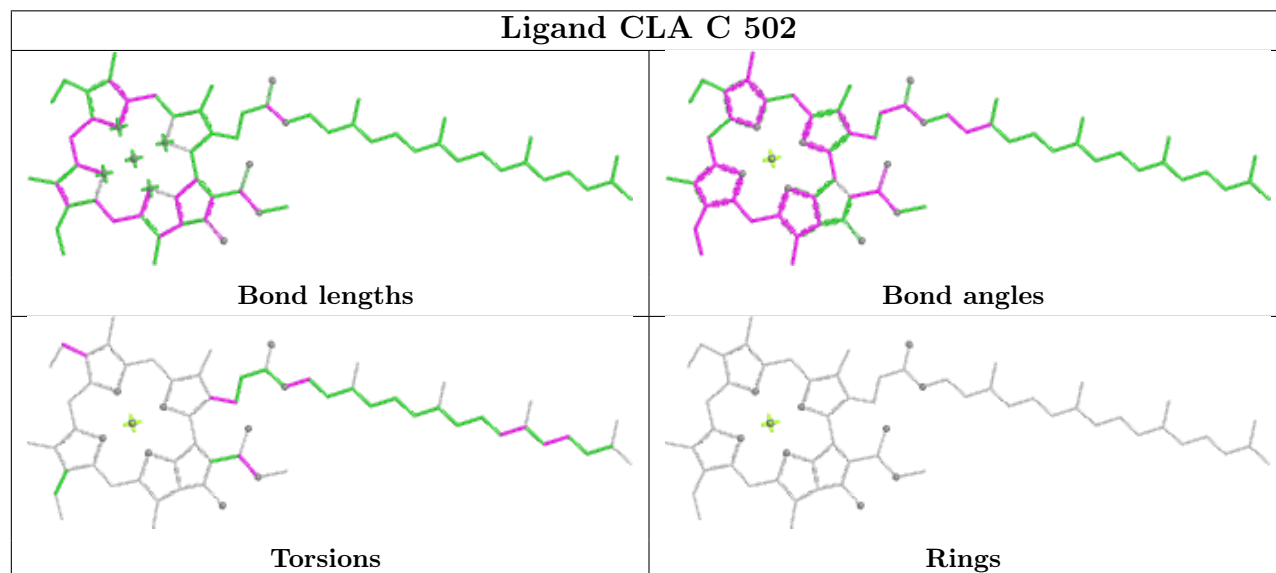
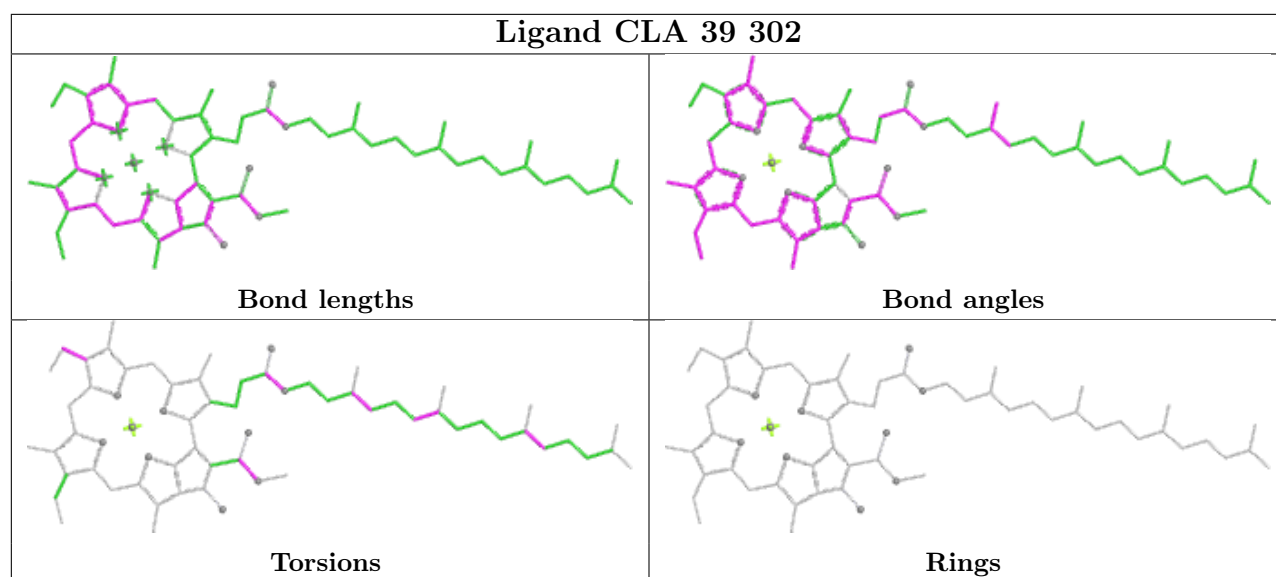
Ligand CLA a 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

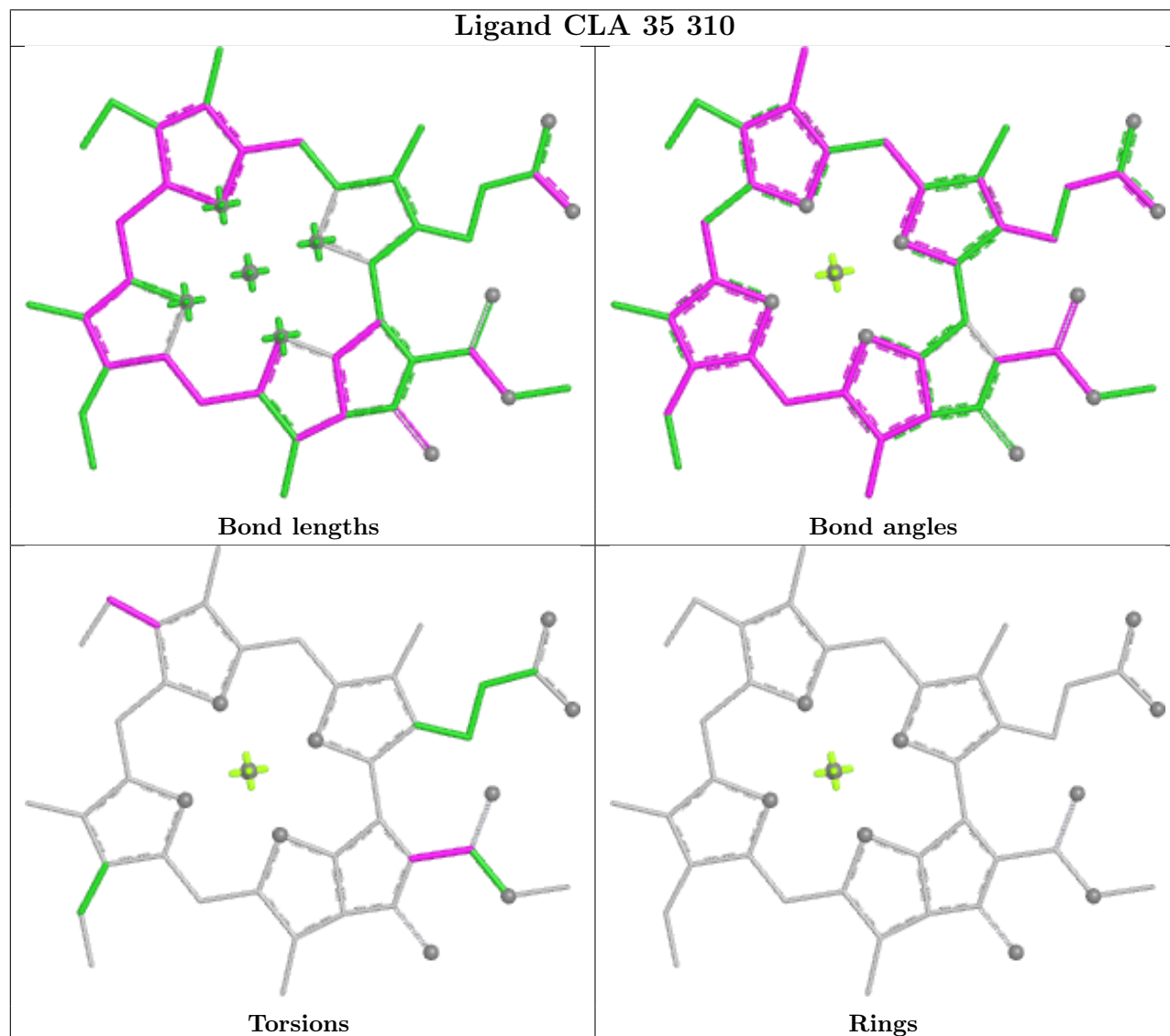
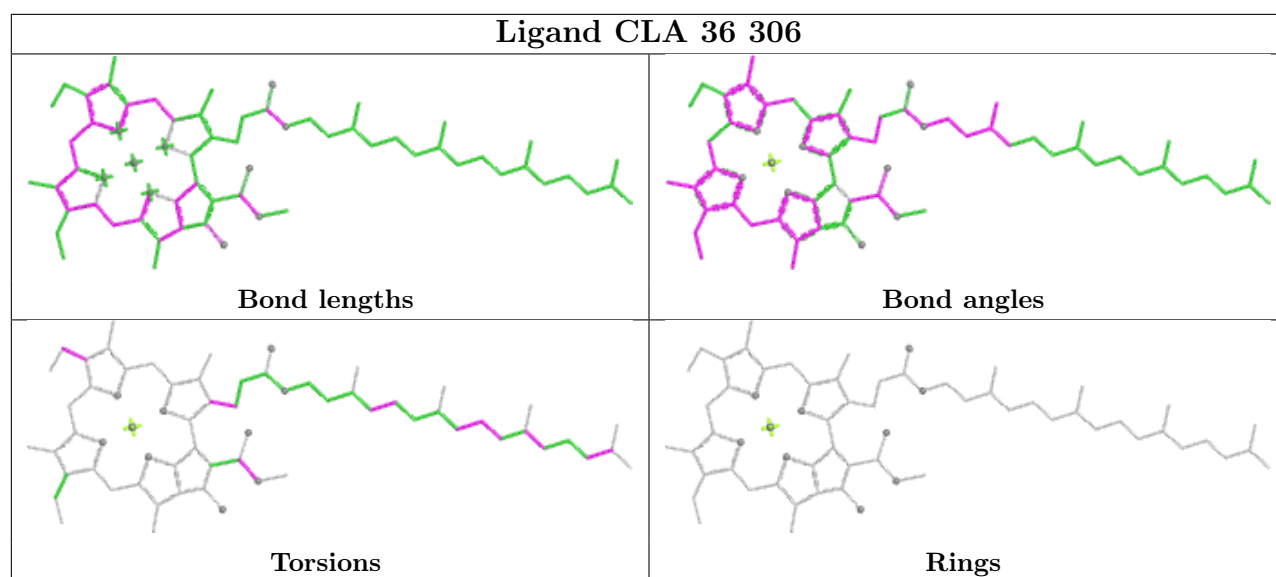


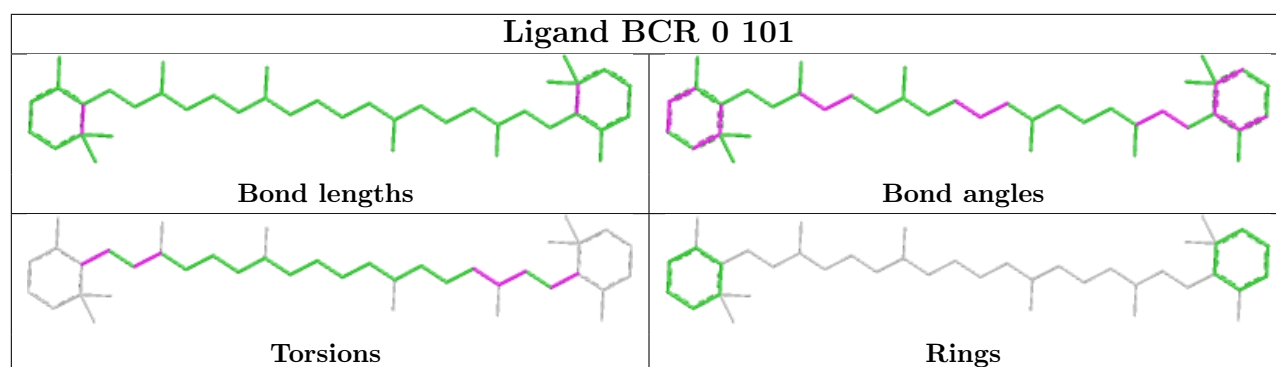












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

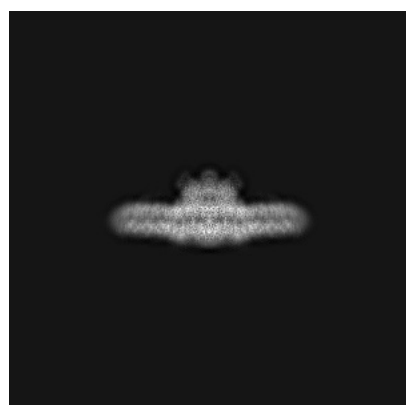
6 Map visualisation [i](#)

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

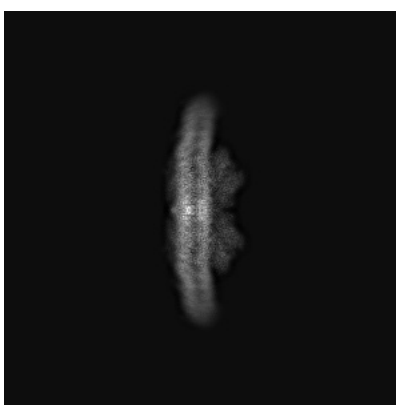
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

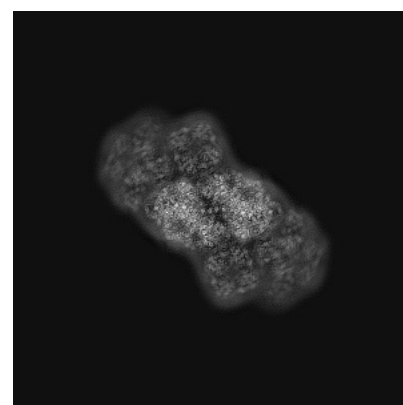
6.1.1 Primary map



X



Y

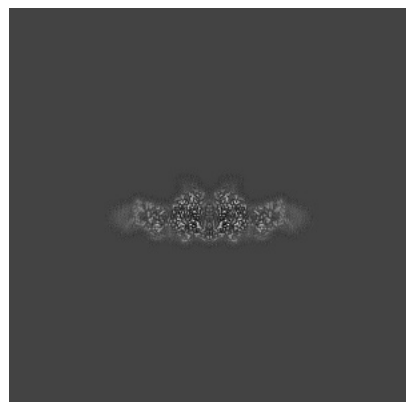


Z

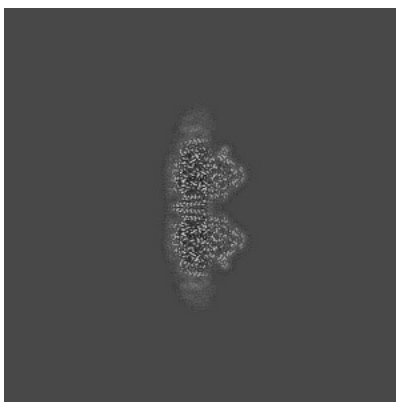
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

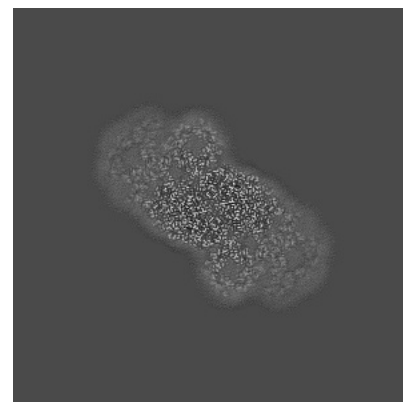
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

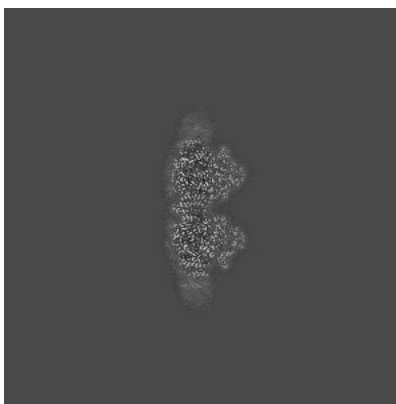
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

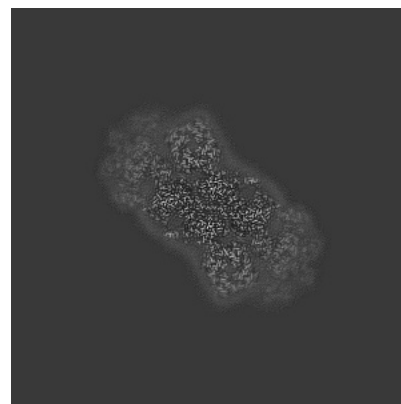
6.3.1 Primary map



X Index: 252



Y Index: 257

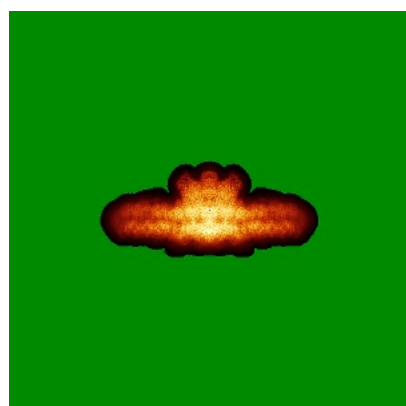


Z Index: 234

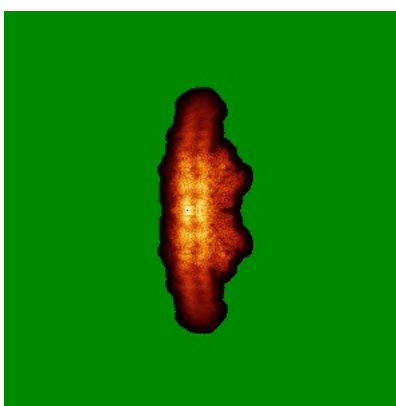
The images above show the largest variance slices of the map in three orthogonal directions.

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

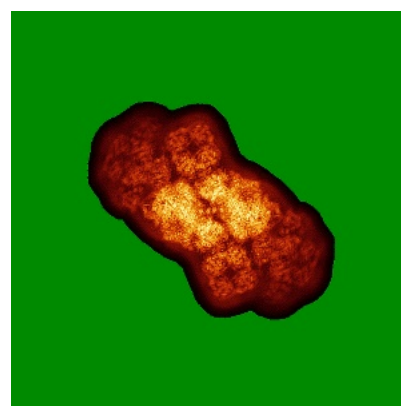
6.4.1 Primary map



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.

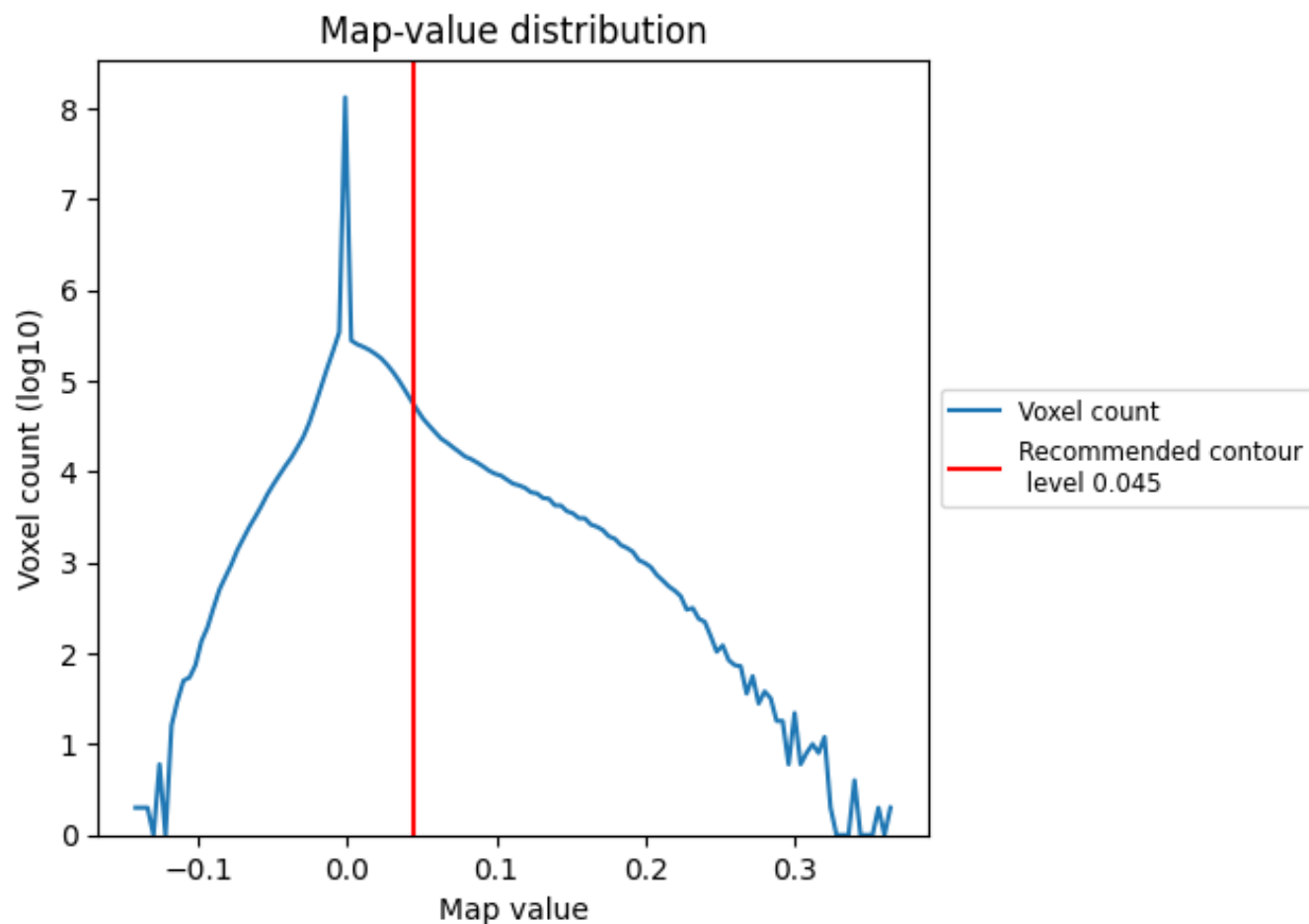
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

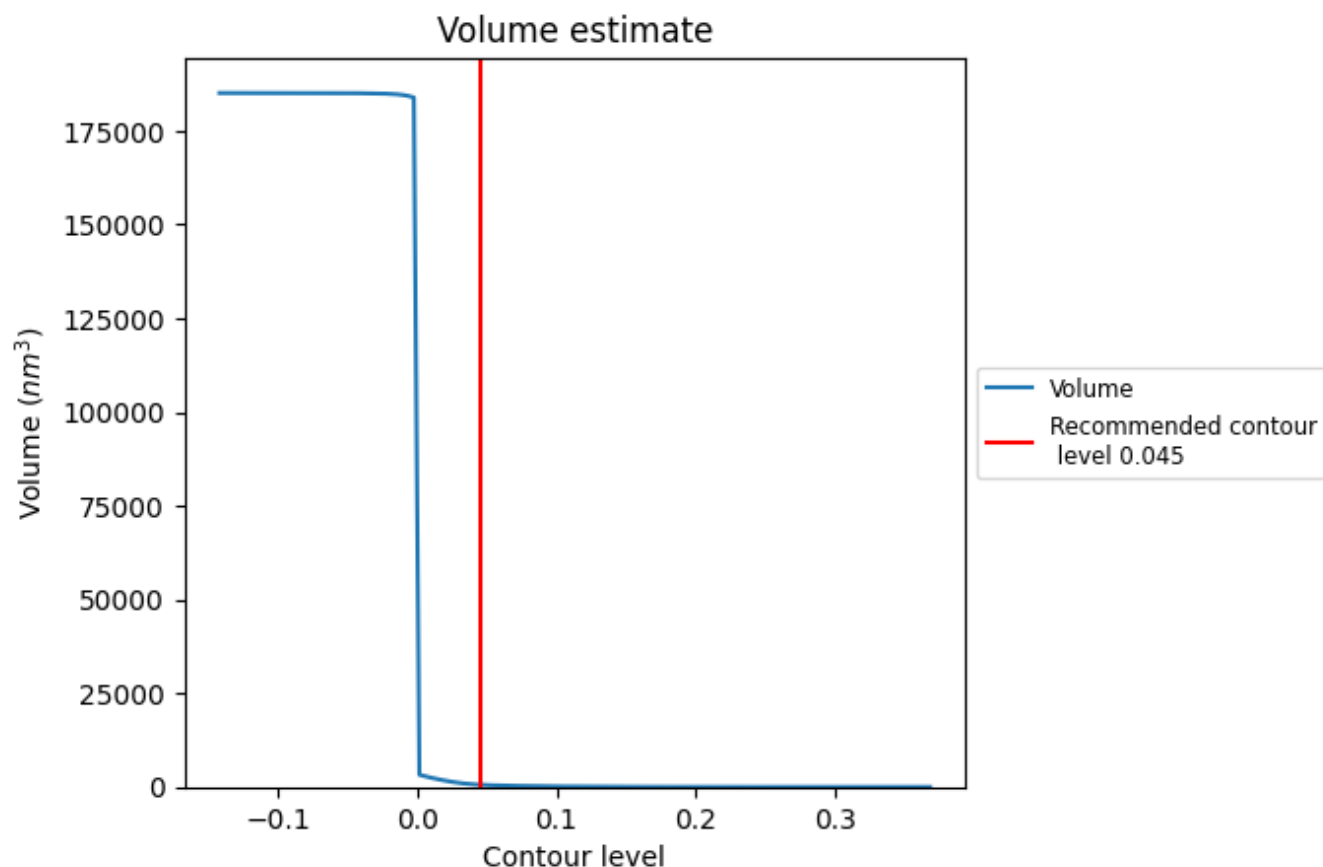
This section contains the results of statistical analysis of the map.

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.

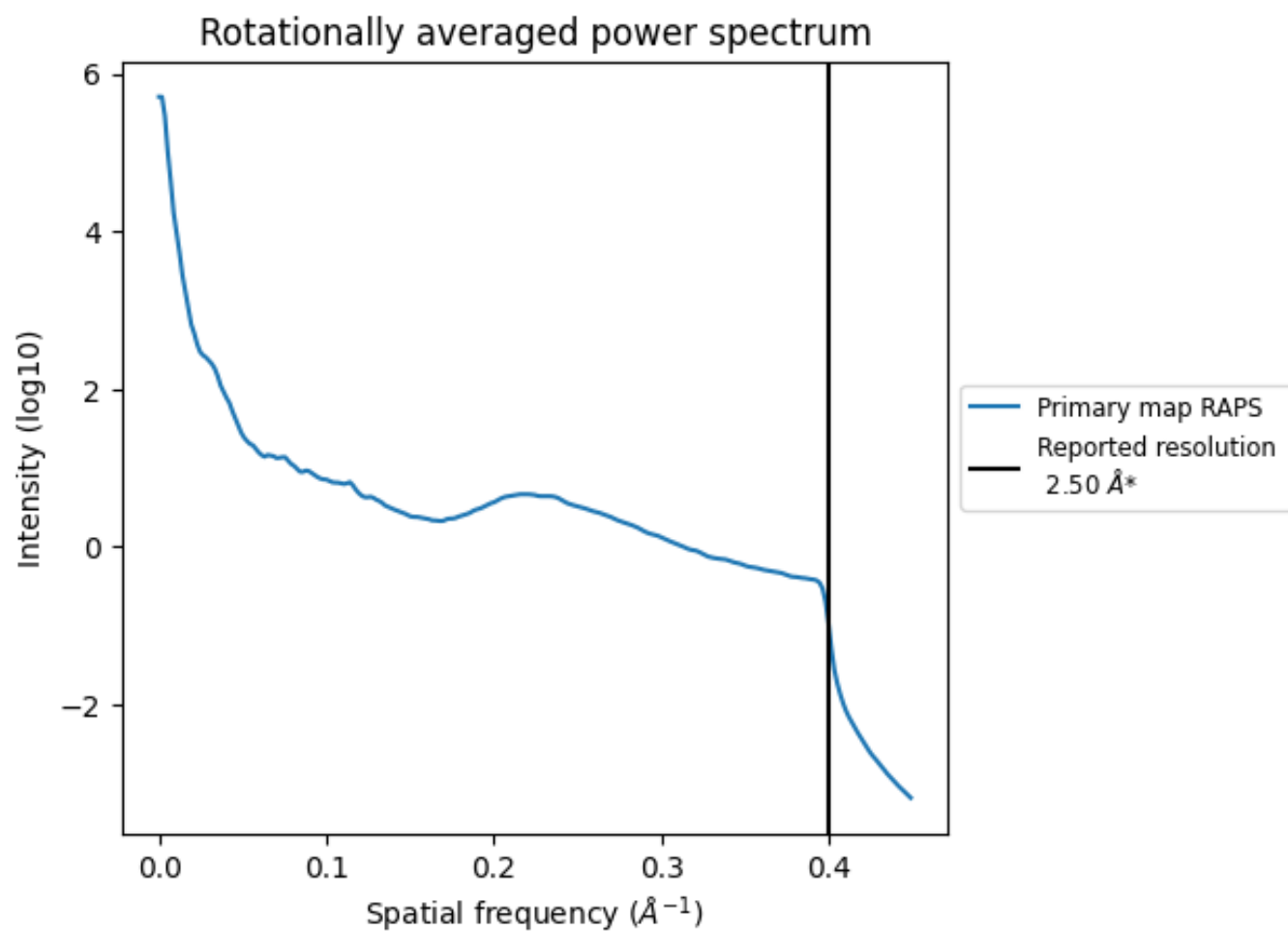
7.2 Volume estimate [i](#)



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 ⓘ

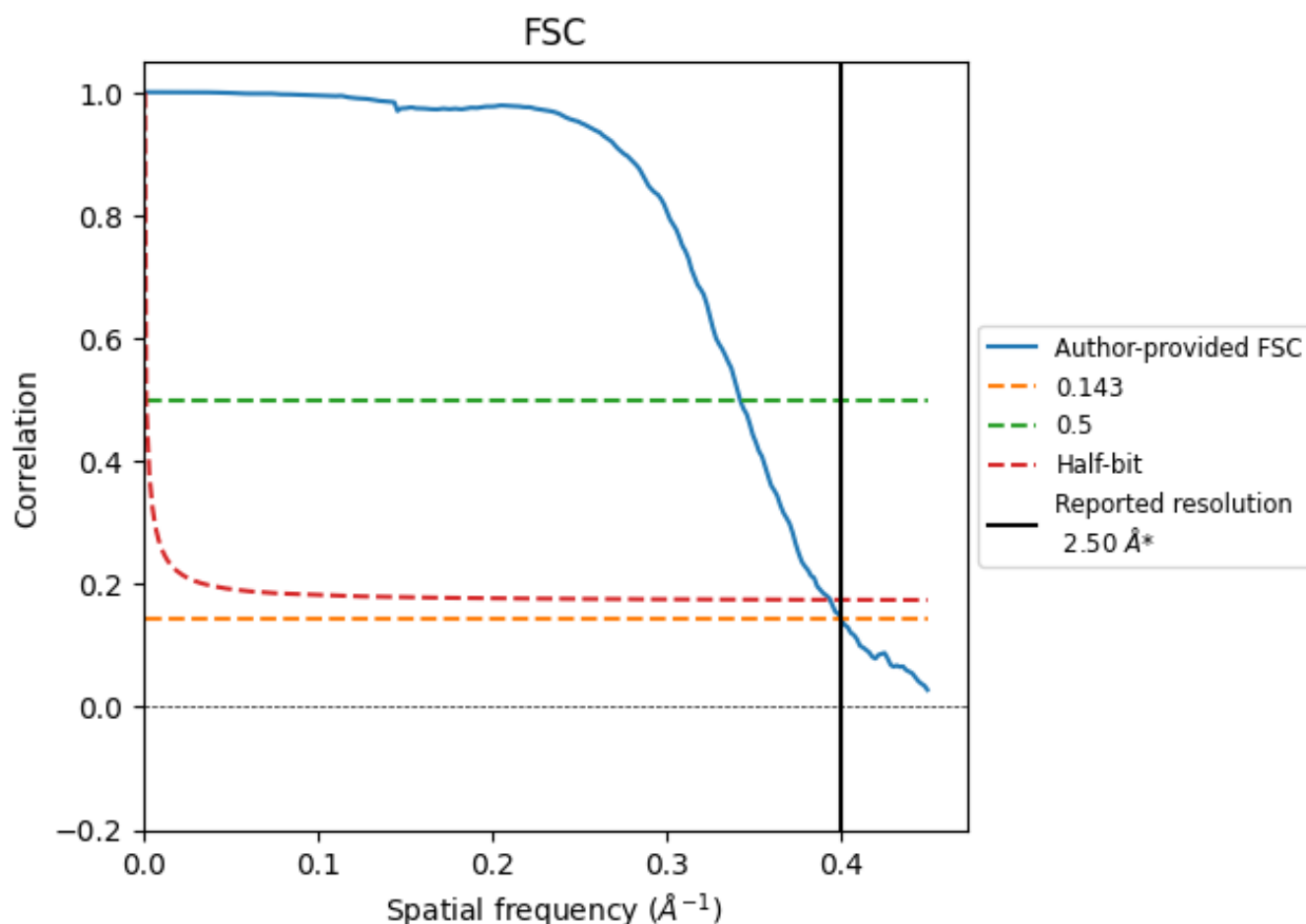


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

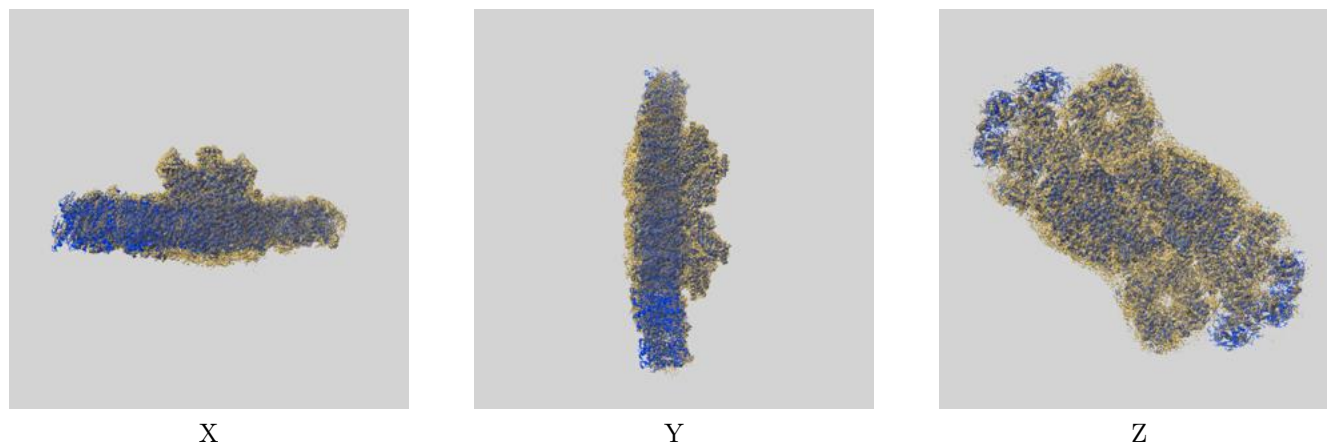
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.50	2.92	2.54
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

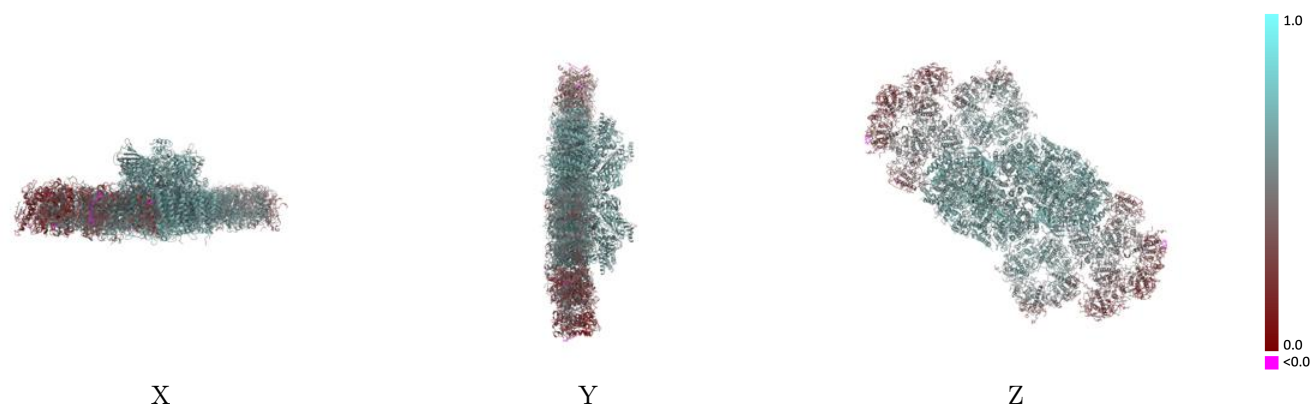
This section contains information regarding the fit between EMDB map EMD-31905 and PDB model 7VD5. Per-residue inclusion information can be found in section [3](#) on page [51](#).

9.1 Map-model overlay [i](#)



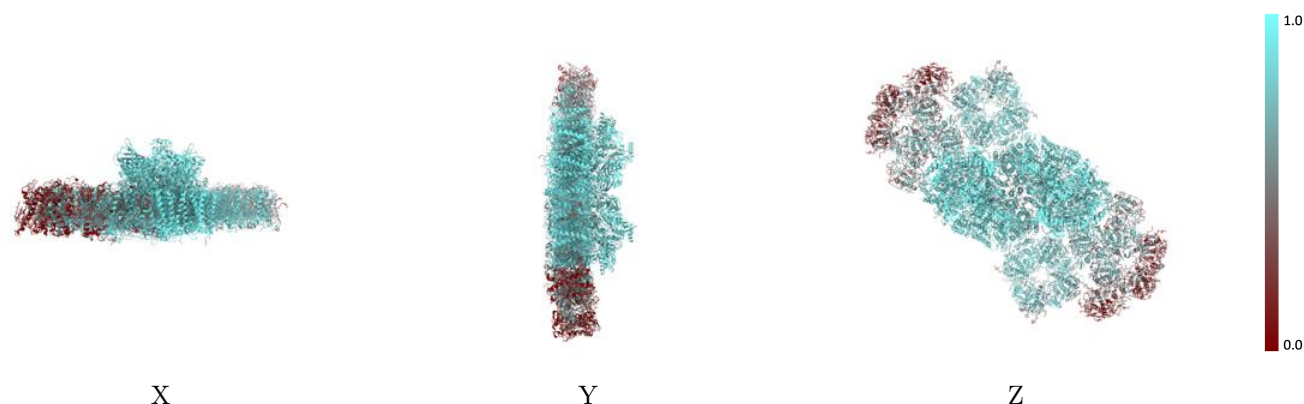
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



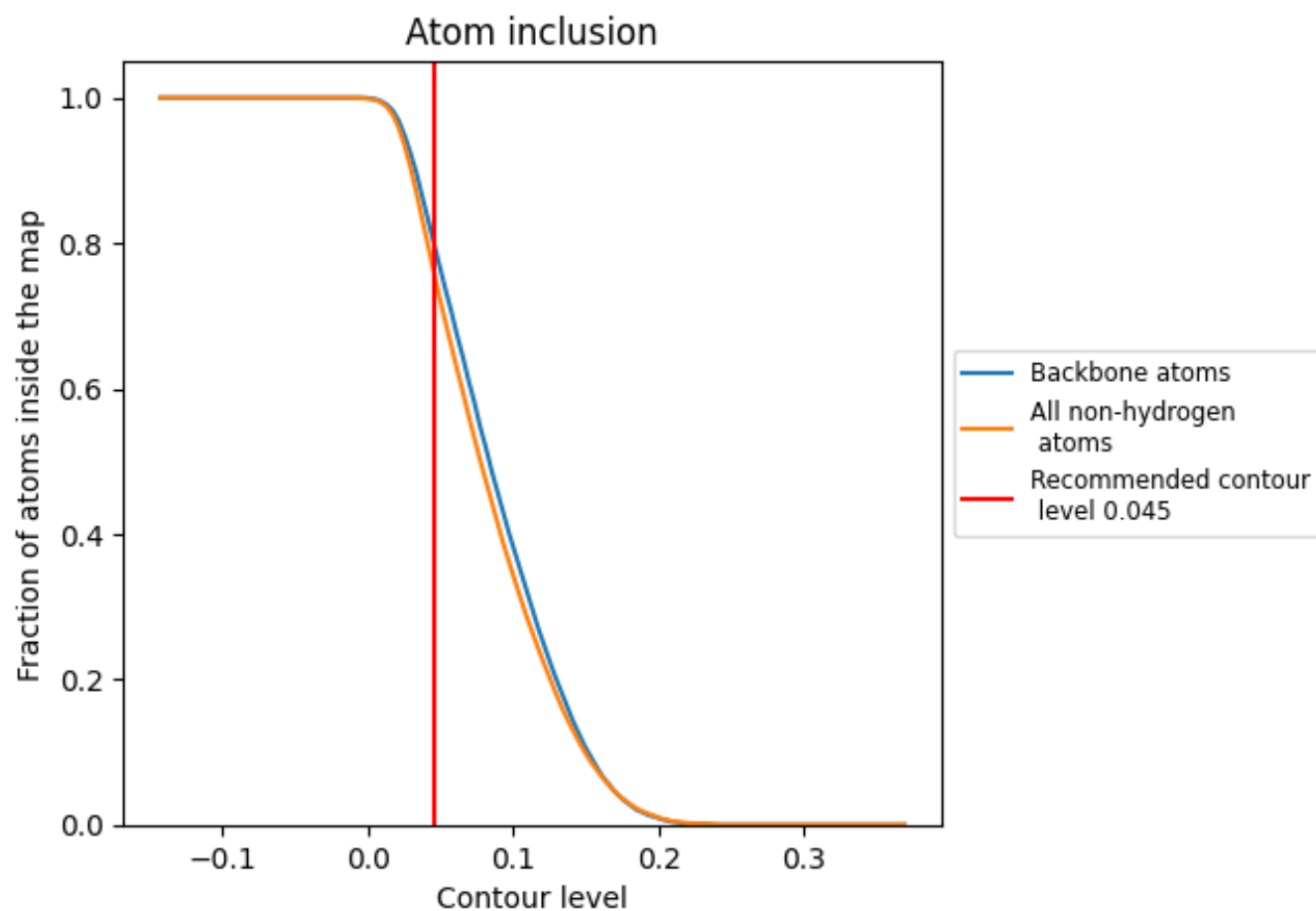
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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