



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 04:15 PM JST

PDB ID : 6L4T / pdb_00006l4t
EMDB ID : EMD-0834
Title : Structure of the peripheral FCPI from diatom
Authors : Nagao, R.; Kato, K.; Miyazaki, N.; Akita, F.; Shen, J.R.
Deposited on : 2019-10-21
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

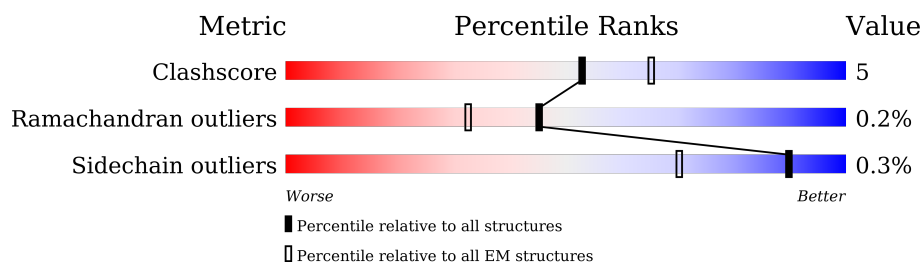
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

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




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	6	208	72% 12% 16%
2	7	296	59% 36%
3	8	270	69% 10% 21%
4	10	207	77% 18%
5	11	229	77% 6% 17%
6	12	204	79% 6% 15%
7	13	244	52% 9% 39%
8	14	249	74% 10% 16%
9	15	281	62% 12% 25%

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Mol	Chain	Length	Quality of chain
10	16	218	

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
11	CLA	10	304	X	-	-	-
11	CLA	10	305	X	-	-	-
11	CLA	10	307	X	-	-	-
11	CLA	10	308	X	-	-	-
11	CLA	10	309	X	-	-	-
11	CLA	11	305	X	-	-	-
11	CLA	11	307	X	-	-	-
11	CLA	11	309	X	-	-	-
11	CLA	12	303	X	-	-	-
11	CLA	12	304	X	-	-	-
11	CLA	12	306	X	-	-	-
11	CLA	12	307	X	-	-	-
11	CLA	12	308	X	-	-	-
11	CLA	12	312	X	-	-	-
11	CLA	12	321	X	-	-	-
11	CLA	13	302	X	-	-	-
11	CLA	13	307	X	-	-	-
11	CLA	13	309	X	-	-	-
11	CLA	14	302	X	-	-	-
11	CLA	14	303	X	-	-	-
11	CLA	14	304	X	-	-	-
11	CLA	14	305	X	-	-	-
11	CLA	14	309	X	-	-	-
11	CLA	14	310	X	-	-	-
11	CLA	14	313	X	-	-	-
11	CLA	15	303	X	-	-	-
11	CLA	15	304	X	-	-	-
11	CLA	15	305	X	-	-	-
11	CLA	15	306	X	-	-	-
11	CLA	15	307	X	-	-	-
11	CLA	15	308	X	-	-	-
11	CLA	15	309	X	-	-	-
11	CLA	15	310	X	-	-	-
11	CLA	15	311	X	-	-	-
11	CLA	15	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	16	302	X	-	-	-
11	CLA	16	303	X	-	-	-
11	CLA	16	305	X	-	-	-
11	CLA	16	306	X	-	-	-
11	CLA	16	307	X	-	-	-
11	CLA	16	308	X	-	-	-
11	CLA	16	310	X	-	-	-
11	CLA	6	301	X	-	-	-
11	CLA	6	302	X	-	-	-
11	CLA	6	303	X	-	-	-
11	CLA	6	304	X	-	-	-
11	CLA	6	306	X	-	-	-
11	CLA	6	307	X	-	-	-
11	CLA	6	312	X	-	-	-
11	CLA	6	313	X	-	-	-
11	CLA	6	314	X	-	-	-
11	CLA	7	302	X	-	-	-
11	CLA	7	303	X	-	-	-
11	CLA	7	304	X	-	-	-
11	CLA	7	305	X	-	-	-
11	CLA	7	308	X	-	-	-
11	CLA	7	309	X	-	-	-
11	CLA	7	310	X	-	-	-
11	CLA	8	301	X	-	-	-
11	CLA	8	302	X	-	-	-
11	CLA	8	303	X	-	-	-
11	CLA	8	304	X	-	-	-
11	CLA	8	308	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 23863 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 Fucoxanthin chlorophyll a/c-binding protein Lhcr12.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	6	174	Total	C	N	O	S	0	0
			1354	884	216	246	8		

- Molecule 2 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	188	Total	C	N	O	S	0	0
			1416	894	240	266	16		

- Molecule 3 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	213	Total	C	N	O	S	0	0
			1660	1075	274	302	9		

- Molecule 4 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	10	169	Total	C	N	O	S	0	0
			1302	849	212	233	8		

- Molecule 5 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	11	191	Total	C	N	O	S	0	0
			1479	958	243	270	8		

- Molecule 6 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	12	173	Total	C	N	O	S	0	0
			1274	814	209	243	8		

- Molecule 7 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	13	150	Total	C	N	O	S	0	0
			1148	736	203	204	5		

- Molecule 8 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	14	208	Total	C	N	O	S	0	0
			1609	1049	262	292	6		

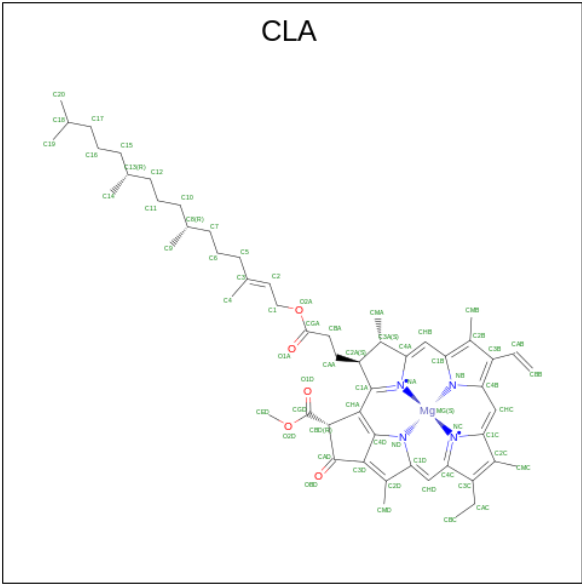
- Molecule 9 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	15	211	Total	C	N	O	S	0	0
			1654	1077	273	298	6		

- Molecule 10 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	16	174	Total	C	N	O	S	0	0
			1313	846	217	242	8		

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
11	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
11	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
11	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
11	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	8	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
11	8	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	8	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	10	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	11	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	12	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	13	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	14	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 12 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).

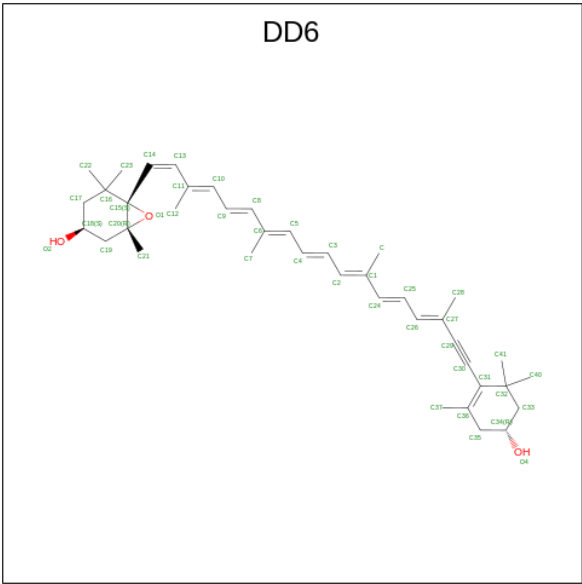


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Mol	Chain	Residues	Atoms					AltConf
12	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	12	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	16	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 13 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).



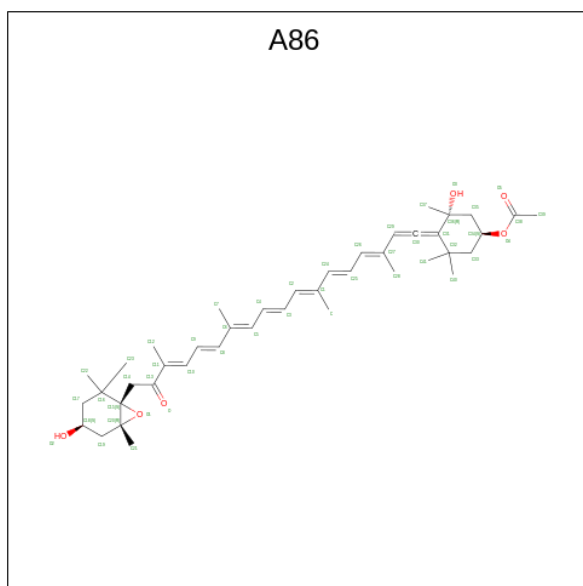
Mol	Chain	Residues	Atoms			AltConf
13	6	1	Total	C	O	0
			43	40	3	
13	6	1	Total	C	O	0
			43	40	3	
13	6	1	Total	C	O	0
			43	40	3	
13	7	1	Total	C	O	0
			43	40	3	
13	7	1	Total	C	O	0
			43	40	3	
13	7	1	Total	C	O	0
			43	40	3	
13	7	1	Total	C	O	0
			43	40	3	
13	8	1	Total	C	O	0
			43	40	3	
13	8	1	Total	C	O	0
			43	40	3	
13	10	1	Total	C	O	0
			43	40	3	
13	10	1	Total	C	O	0
			43	40	3	
13	11	1	Total	C	O	0
			43	40	3	

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Mol	Chain	Residues	Atoms			AltConf
13	12	1	Total	C	O	0
			43	40	3	
13	12	1	Total	C	O	0
			43	40	3	
13	13	1	Total	C	O	0
			43	40	3	
13	15	1	Total	C	O	0
			43	40	3	
13	15	1	Total	C	O	0
			43	40	3	
13	16	1	Total	C	O	0
			43	40	3	

- Molecule 14 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
14	6	1	Total	C	O	0
			48	42	6	
14	7	1	Total	C	O	0
			48	42	6	
14	7	1	Total	C	O	0
			48	42	6	
14	7	1	Total	C	O	0
			48	42	6	
14	8	1	Total	C	O	0
			48	42	6	

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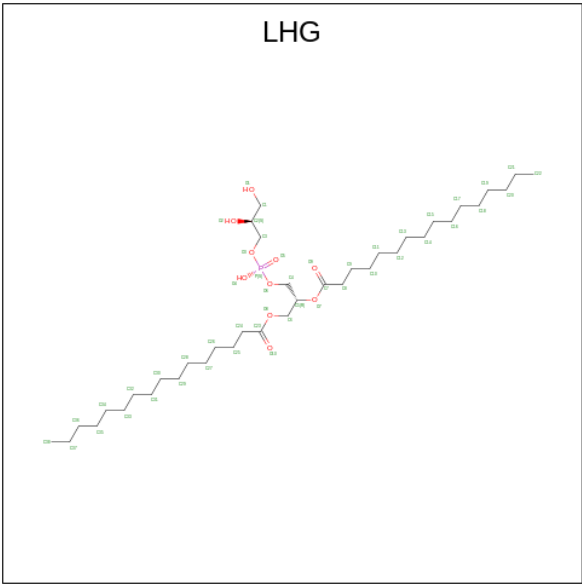
Mol	Chain	Residues	Atoms			AltConf
14	8	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	10	1	Total	C	O	0
			48	42	6	
14	11	1	Total	C	O	0
			48	42	6	
14	11	1	Total	C	O	0
			48	42	6	
14	11	1	Total	C	O	0
			48	42	6	
14	11	1	Total	C	O	0
			48	42	6	
14	12	1	Total	C	O	0
			48	42	6	
14	12	1	Total	C	O	0
			48	42	6	
14	13	1	Total	C	O	0
			45	40	5	
14	13	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	
14	14	1	Total	C	O	0
			48	42	6	

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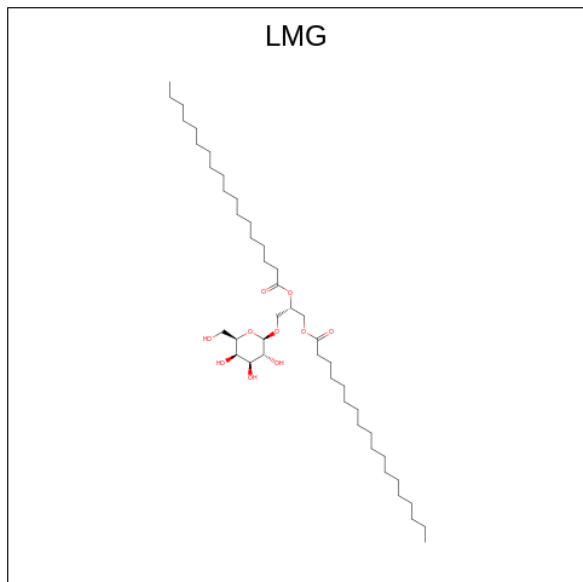
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
14	14	1	48	42	6	0
14	14	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	15	1	48	42	6	0
14	16	1	48	42	6	0
14	16	1	48	42	6	0

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).

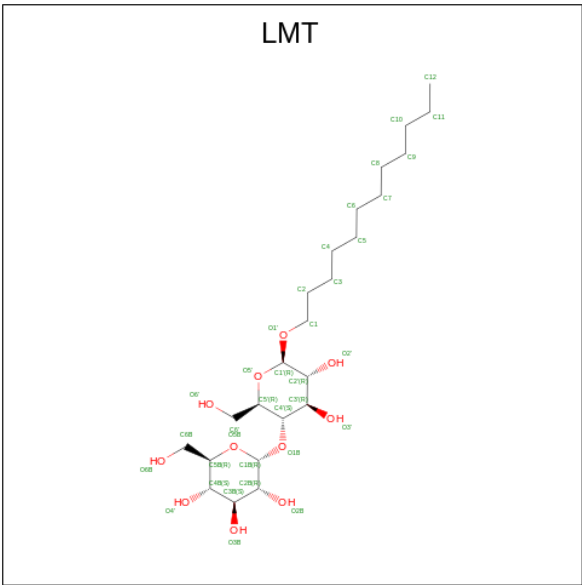


- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
16	7	1	Total	C	O	0
			37	27	10	
16	8	1	Total	C	O	0
			37	27	10	
16	8	1	Total	C	O	0
			42	32	10	
16	8	1	Total	C	O	0
			29	19	10	
16	14	1	Total	C	O	0
			38	28	10	

- Molecule 17 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
17	7	1	Total	C	O	0
			35	24	11	
17	8	1	Total	C	O	0
			35	24	11	
17	8	1	Total	C	O	0
			35	24	11	
17	8	1	Total	C	O	0
			35	24	11	
17	11	1	Total	C	O	0
			35	24	11	
17	11	1	Total	C	O	0
			35	24	11	
17	12	1	Total	C	O	0
			35	24	11	
17	12	1	Total	C	O	0
			35	24	11	
17	12	1	Total	C	O	0
			35	24	11	
17	12	1	Total	C	O	0
			35	24	11	
17	12	1	Total	C	O	0
			35	24	11	
17	15	1	Total	C	O	0
			35	24	11	
17	16	1	Total	C	O	0
			35	24	11	

- Molecule 18 is water.

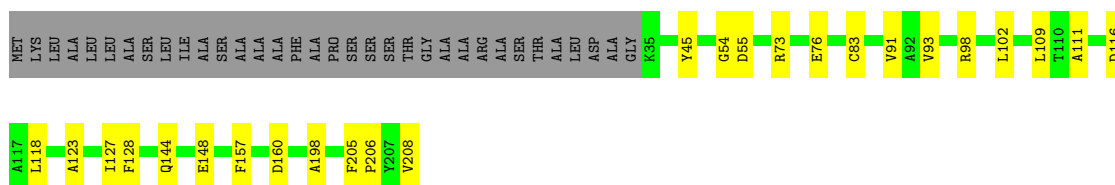
Mol	Chain	Residues	Atoms		AltConf
18	6	2	Total 2	O 2	0
18	7	2	Total 2	O 2	0
18	8	4	Total 4	O 4	0
18	10	1	Total 1	O 1	0
18	11	1	Total 1	O 1	0
18	12	2	Total 2	O 2	0

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

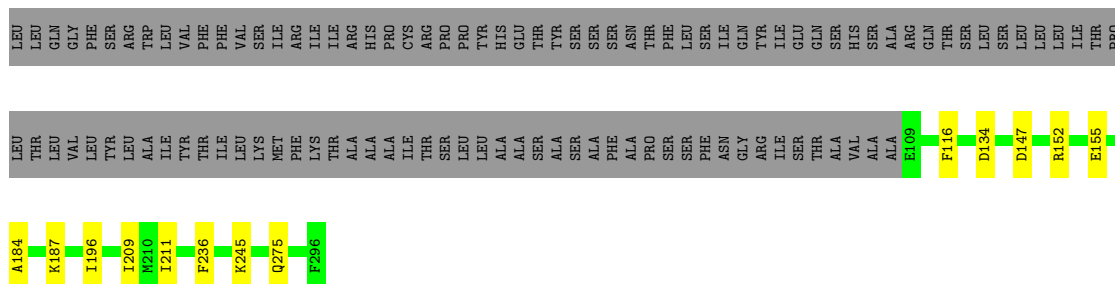
- Molecule 1: Fucoxanthin chlorophyll a/c-binding protein Lhcr12

Chain 6: 



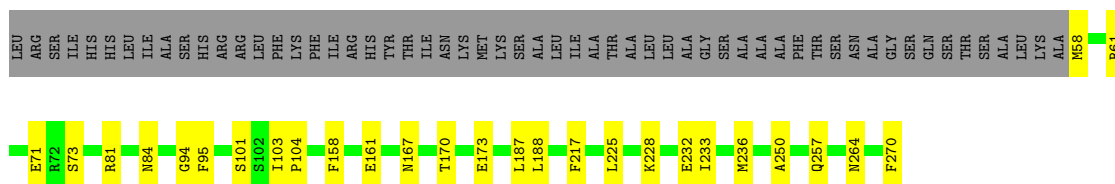
- Molecule 2: Fucoxanthin chlorophyll a/c-binding protein Lhcr10

Chain 7: 




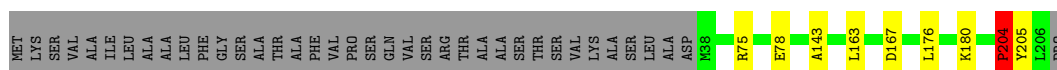
- Molecule 3: Fucoxanthin chlorophyll a/c-binding protein Lhcr4

Chain 8: 




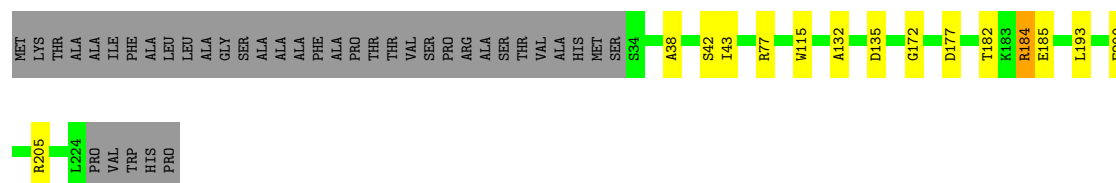
- Molecule 4: Fucoxanthin chlorophyll a/c-binding protein Lhcr3

Chain 10: 




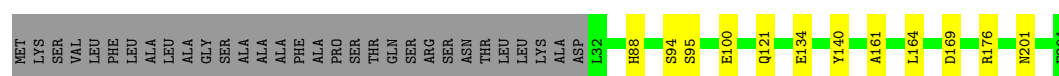
- Molecule 5: Fucoxanthin chlorophyll a/c-binding protein Lhcq13

Chain 11:  77% 6% 17%



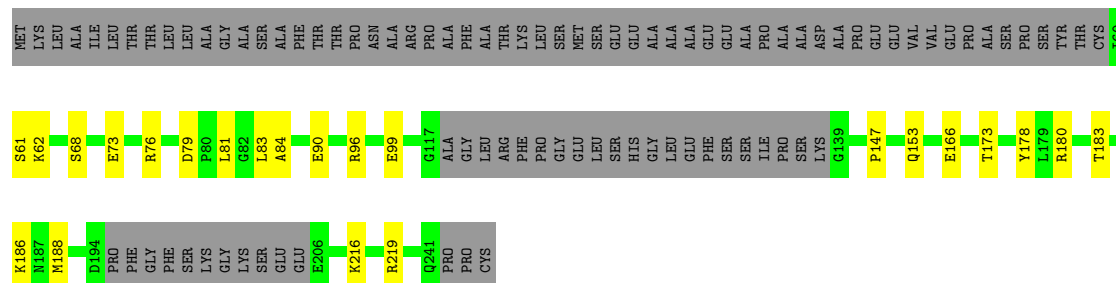
- Molecule 6: Fucoxanthin chlorophyll a/c-binding protein Lhcq3

Chain 12:  79% 6% 15%



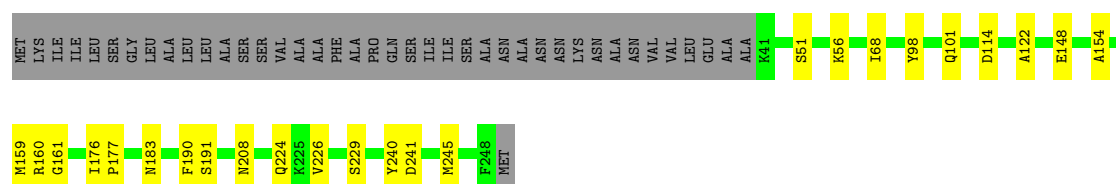
- Molecule 7: Fucoxanthin chlorophyll a/c-binding protein Lhcq11

Chain 13:  52% 9% 39%



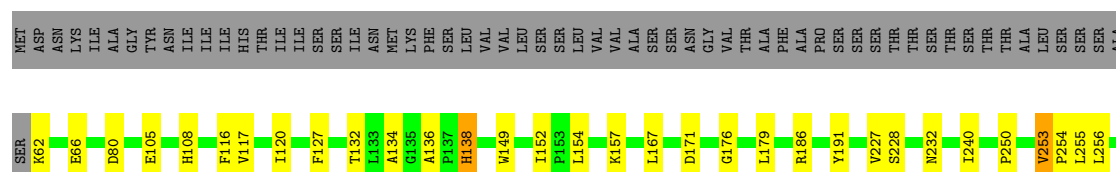
- Molecule 8: Fucoxanthin chlorophyll a/c-binding protein Lhcq10

Chain 14:  74% 10% 16%



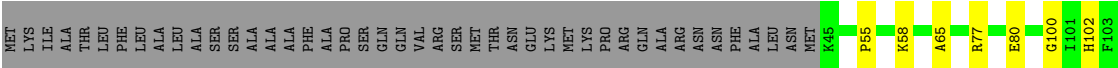
- Molecule 9: Fucoxanthin chlorophyll a/c-binding protein Lhcq8

Chain 15:  62% 12% 25%





● Molecule 10: Fucoxanthin chlorophyll a/c-binding protein Lhcq5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	470801	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DD6, A86, LMT, CLA, KC1, 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	6	0.37	1/1391 (0.1%)	0.48	0/1886
2	7	0.34	0/1445	0.46	0/1952
3	8	0.38	0/1706	0.49	0/2310
4	10	0.35	0/1344	0.52	0/1824
5	11	0.33	0/1522	0.49	0/2070
6	12	0.35	0/1305	0.51	1/1776 (0.1%)
7	13	0.30	0/1177	0.51	0/1592
8	14	0.32	0/1660	0.60	2/2255 (0.1%)
9	15	0.33	0/1705	0.68	3/2319 (0.1%)
10	16	0.31	0/1347	0.59	2/1833 (0.1%)
All	All	0.34	1/14602 (0.0%)	0.54	8/19817 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	10	0	1
8	14	0	2
9	15	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6	83	CYS	CB-SG	-5.02	1.73	1.81

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	16	169	ASP	CB-CG-OD1	10.03	127.32	118.30
9	15	152	ILE	C-N-CD	-5.65	108.17	120.60
8	14	241	ASP	CB-CG-OD1	5.59	123.33	118.30
6	12	176	ARG	NE-CZ-NH2	-5.51	117.55	120.30
8	14	122	ALA	C-N-CA	5.21	133.24	122.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	10	204	PRO	Peptide
8	14	154	ALA	Peptide
8	14	161	GLY	Peptide
9	15	136	ALA	Peptide
9	15	264	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6	1354	0	1328	17	0
2	7	1416	0	1379	11	0
3	8	1660	0	1625	20	0
4	10	1302	0	1274	6	0
5	11	1479	0	1452	10	0
6	12	1274	0	1267	7	0
7	13	1148	0	1130	16	0
8	14	1609	0	1568	17	0
9	15	1654	0	1613	21	0
10	16	1313	0	1310	20	0
11	10	435	0	465	9	0
11	11	315	0	337	6	0
11	12	566	0	604	13	0
11	13	350	0	354	10	0
11	14	468	0	400	9	0
11	15	685	0	589	17	0
11	16	478	0	429	16	0
11	6	620	0	658	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	7	566	0	609	14	0
11	8	420	0	427	14	0
12	10	135	0	0	0	0
12	11	180	0	0	0	0
12	12	180	0	0	0	0
12	13	270	0	0	1	0
12	14	135	0	0	0	0
12	16	90	0	0	1	0
12	6	180	0	0	0	0
12	7	90	0	0	0	0
12	8	315	0	0	1	0
13	10	86	0	0	1	0
13	11	43	0	0	1	0
13	12	86	0	0	0	0
13	13	43	0	0	1	0
13	15	86	0	0	0	0
13	16	43	0	0	0	0
13	6	129	0	0	4	0
13	7	172	0	0	1	0
13	8	86	0	0	0	0
14	10	240	0	0	0	0
14	11	192	0	0	1	0
14	12	96	0	0	0	0
14	13	93	0	0	0	0
14	14	432	0	0	2	0
14	15	288	0	0	0	0
14	16	96	0	0	0	0
14	6	48	0	0	0	0
14	7	144	0	0	1	0
14	8	96	0	0	1	0
15	6	27	0	24	0	0
16	14	38	0	46	1	0
16	7	37	0	44	1	0
16	8	108	0	123	2	0
17	11	70	0	92	2	0
17	12	175	0	230	6	0
17	15	35	0	46	0	0
17	16	35	0	46	0	0
17	7	35	0	46	0	0
17	8	105	0	138	1	0
18	10	1	0	0	0	0
18	11	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	12	2	0	0	0	0
18	6	2	0	0	0	0
18	7	2	0	0	0	0
18	8	4	0	0	0	0
All	All	23863	0	19653	223	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 5.

The worst 5 of 223 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)
8:14:101:GLN:OE1	11:14:303:CLA:NA	2.01	0.94
9:15:105:GLU:OE1	11:15:302:CLA:NB	2.22	0.72
7:13:73:GLU:OE1	11:13:307:CLA:NC	2.23	0.71
1:6:127:ILE:HB	11:6:311:CLA:HBC1	1.77	0.66
9:15:127:PHE:O	9:15:138:HIS:NE2	2.33	0.62

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	6	172/208 (83%)	170 (99%)	2 (1%)	0	100	100
2	7	186/296 (63%)	178 (96%)	8 (4%)	0	100	100
3	8	211/270 (78%)	205 (97%)	6 (3%)	0	100	100
4	10	167/207 (81%)	152 (91%)	13 (8%)	2 (1%)	11	24
5	11	189/229 (82%)	171 (90%)	18 (10%)	0	100	100
6	12	171/204 (84%)	160 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	13	144/244 (59%)	136 (94%)	8 (6%)	0	100	100
8	14	206/249 (83%)	177 (86%)	29 (14%)	0	100	100
9	15	209/281 (74%)	173 (83%)	35 (17%)	1 (0%)	25	47
10	16	172/218 (79%)	156 (91%)	16 (9%)	0	100	100
All	All	1827/2406 (76%)	1678 (92%)	146 (8%)	3 (0%)	45	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	15	250	PRO
4	10	205	TYR
4	10	204	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	6	140/160 (88%)	140 (100%)	0	100	100
2	7	143/236 (61%)	143 (100%)	0	100	100
3	8	171/215 (80%)	171 (100%)	0	100	100
4	10	133/161 (83%)	133 (100%)	0	100	100
5	11	154/181 (85%)	153 (99%)	1 (1%)	84	94
6	12	136/159 (86%)	136 (100%)	0	100	100
7	13	112/184 (61%)	111 (99%)	1 (1%)	75	90
8	14	166/196 (85%)	166 (100%)	0	100	100
9	15	171/231 (74%)	168 (98%)	3 (2%)	54	77
10	16	139/174 (80%)	139 (100%)	0	100	100
All	All	1465/1897 (77%)	1460 (100%)	5 (0%)	90	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	11	184	ARG
7	13	76	ARG
9	15	138	HIS
9	15	253	VAL
9	15	271	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
10	16	177	GLN
9	15	200	ASN
8	14	183	ASN
8	14	82	GLN
8	14	209	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

192 ligands are modelled in this entry.

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
12	KC1	14	311	8	48,53,53	3.43	24 (50%)	55,89,89	3.80	30 (54%)
16	LMG	14	322	-	38,38,55	0.97	3 (7%)	46,46,63	1.20	3 (6%)
17	LMT	12	301	-	36,36,36	0.39	0	47,47,47	0.79	0
11	CLA	11	307	5	65,73,73	2.00	15 (23%)	76,113,113	2.68	27 (35%)
14	A86	14	321	-	44,50,50	4.17	23 (52%)	51,76,76	8.40	16 (31%)
17	LMT	12	322	-	36,36,36	0.43	0	47,47,47	0.87	1 (2%)
12	KC1	8	314	18,12	48,53,53	3.39	25 (52%)	55,89,89	3.71	29 (52%)
12	KC1	6	310	1	48,53,53	3.40	23 (47%)	55,89,89	3.76	30 (54%)
13	DD6	6	315	-	39,45,45	6.65	24 (61%)	52,67,67	6.62	27 (51%)
14	A86	12	316	-	44,50,50	4.02	23 (52%)	51,76,76	8.31	17 (33%)
17	LMT	8	324	-	36,36,36	0.40	0	47,47,47	0.70	0
11	CLA	6	302	1	65,73,73	2.03	17 (26%)	76,113,113	2.64	28 (36%)
14	A86	8	318	-	44,50,50	3.96	24 (54%)	51,76,76	10.85	22 (43%)
13	DD6	10	314	-	39,45,45	6.63	23 (58%)	52,67,67	6.73	29 (55%)
11	CLA	11	308	5	65,73,73	2.00	15 (23%)	76,113,113	2.73	29 (38%)
11	CLA	12	308	18	65,73,73	2.00	18 (27%)	76,113,113	2.62	25 (32%)
11	CLA	15	311	14	45,53,73	2.48	16 (35%)	52,89,113	3.16	24 (46%)
12	KC1	16	311	10	48,53,53	3.47	25 (52%)	55,89,89	3.71	26 (47%)
17	LMT	12	320	-	36,36,36	0.35	0	47,47,47	0.71	0
11	CLA	6	312	1	45,53,73	2.49	17 (37%)	52,89,113	3.11	23 (44%)
13	DD6	7	317	-	39,45,45	6.75	21 (53%)	52,67,67	6.90	28 (53%)
14	A86	7	315	-	44,50,50	3.75	22 (50%)	51,76,76	7.73	24 (47%)
11	CLA	8	309	3	47,55,73	2.35	16 (34%)	54,91,113	3.04	24 (44%)
11	CLA	15	303	9,14,11	60,68,73	2.09	17 (28%)	70,107,113	2.87	28 (40%)
14	A86	15	321	9	44,50,50	4.09	23 (52%)	51,76,76	8.65	19 (37%)
11	CLA	16	308	10	45,53,73	2.46	17 (37%)	52,89,113	3.23	24 (46%)
11	CLA	13	307	7	65,73,73	2.06	18 (27%)	76,113,113	2.67	28 (36%)
11	CLA	7	309	2	65,73,73	2.01	16 (24%)	76,113,113	2.65	26 (34%)
13	DD6	10	313	-	39,45,45	6.76	23 (58%)	52,67,67	7.06	28 (53%)
11	CLA	6	304	1	65,73,73	2.04	17 (26%)	76,113,113	2.66	27 (35%)
13	DD6	12	315	11	39,45,45	6.61	23 (58%)	52,67,67	6.92	26 (50%)
14	A86	7	318	-	44,50,50	4.01	23 (52%)	51,76,76	7.94	25 (49%)
11	CLA	15	306	-	45,53,73	2.46	17 (37%)	52,89,113	3.29	24 (46%)
14	A86	14	301	8	44,50,50	4.06	23 (52%)	51,76,76	8.05	19 (37%)
11	CLA	12	306	6	65,73,73	1.97	16 (24%)	76,113,113	2.59	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	A86	10	301	4	44,50,50	3.84	23 (52%)	51,76,76	7.25	24 (47%)
17	LMT	8	322	-	36,36,36	0.37	0	47,47,47	0.71	0
12	KC1	10	310	4	48,53,53	3.44	24 (50%)	55,89,89	3.94	30 (54%)
12	KC1	12	313	6	48,53,53	3.42	23 (47%)	55,89,89	4.51	28 (50%)
12	KC1	6	305	1	48,53,53	3.39	24 (50%)	55,89,89	3.82	27 (49%)
11	CLA	16	303	10	65,73,73	2.00	16 (24%)	76,113,113	2.85	28 (36%)
11	CLA	7	310	2	65,73,73	1.98	16 (24%)	76,113,113	2.60	26 (34%)
11	CLA	12	307	6	46,54,73	2.32	16 (34%)	53,90,113	3.21	26 (49%)
12	KC1	6	309	1	48,53,53	3.42	24 (50%)	55,89,89	3.79	30 (54%)
13	DD6	6	318	-	39,45,45	6.55	23 (58%)	52,67,67	6.75	28 (53%)
14	A86	11	314	-	44,50,50	4.00	22 (50%)	51,76,76	7.45	23 (45%)
14	A86	14	319	11	44,50,50	4.08	23 (52%)	51,76,76	8.28	17 (33%)
11	CLA	8	308	3	55,63,73	2.16	15 (27%)	64,101,113	2.91	26 (40%)
11	CLA	15	313	9	65,73,73	2.05	17 (26%)	76,113,113	2.73	28 (36%)
16	LMG	8	321	-	42,42,55	0.93	2 (4%)	50,50,63	1.33	4 (8%)
12	KC1	11	311	-	48,53,53	3.41	24 (50%)	55,89,89	3.55	29 (52%)
12	KC1	8	306	18	48,53,53	3.35	22 (45%)	55,89,89	3.71	33 (60%)
11	CLA	11	309	5	65,73,73	2.07	17 (26%)	76,113,113	2.64	26 (34%)
17	LMT	15	301	-	36,36,36	0.44	0	47,47,47	1.04	3 (6%)
13	DD6	12	317	-	39,45,45	6.69	22 (56%)	52,67,67	7.11	28 (53%)
13	DD6	15	319	11	39,45,45	6.77	22 (56%)	52,67,67	6.93	30 (57%)
14	A86	14	320	-	44,50,50	4.12	23 (52%)	51,76,76	7.23	21 (41%)
12	KC1	8	313	3	48,53,53	3.34	22 (45%)	55,89,89	3.88	30 (54%)
11	CLA	14	303	8	57,65,73	2.19	16 (28%)	66,103,113	2.86	29 (43%)
12	KC1	6	308	1	48,53,53	3.37	23 (47%)	55,89,89	3.98	28 (50%)
12	KC1	11	310	5	48,53,53	3.45	26 (54%)	55,89,89	3.82	29 (52%)
14	A86	15	316	11	44,50,50	4.09	23 (52%)	51,76,76	7.82	17 (33%)
12	KC1	7	307	18	48,53,53	3.41	22 (45%)	55,89,89	3.70	28 (50%)
11	CLA	14	305	8	50,58,73	2.31	16 (32%)	58,95,113	3.03	27 (46%)
17	LMT	8	319	-	36,36,36	0.39	0	47,47,47	0.85	1 (2%)
13	DD6	11	312	-	39,45,45	6.71	23 (58%)	52,67,67	7.00	29 (55%)
17	LMT	16	315	-	36,36,36	0.41	0	47,47,47	0.64	0
11	CLA	6	303	18	65,73,73	2.01	17 (26%)	76,113,113	2.72	27 (35%)
12	KC1	11	306	5	48,53,53	3.46	26 (54%)	55,89,89	3.84	29 (52%)
11	CLA	16	310	10	45,53,73	2.45	19 (42%)	52,89,113	3.17	26 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	13	302	7	65,73,73	2.02	17 (26%)	76,113,113	2.62	28 (36%)
12	KC1	12	305	6	48,53,53	3.41	24 (50%)	55,89,89	3.79	27 (49%)
11	CLA	7	308	2	65,73,73	1.92	17 (26%)	76,113,113	2.67	24 (31%)
11	CLA	13	303	-	65,73,73	2.07	16 (24%)	76,113,113	2.77	29 (38%)
12	KC1	14	308	8,11	48,53,53	3.44	25 (52%)	55,89,89	3.77	29 (52%)
13	DD6	15	318	-	39,45,45	6.74	21 (53%)	52,67,67	6.97	31 (59%)
11	CLA	14	302	8	65,73,73	2.03	17 (26%)	76,113,113	2.74	31 (40%)
11	CLA	10	305	18	65,73,73	1.99	16 (24%)	76,113,113	2.78	27 (35%)
11	CLA	10	309	4	65,73,73	2.03	18 (27%)	76,113,113	2.65	27 (35%)
11	CLA	15	309	9	65,73,73	2.09	16 (24%)	76,113,113	2.70	25 (32%)
11	CLA	8	301	3	65,73,73	2.00	17 (26%)	76,113,113	2.75	27 (35%)
11	CLA	16	301	10	65,73,73	1.98	16 (24%)	76,113,113	2.74	28 (36%)
11	CLA	7	305	2	65,73,73	1.99	17 (26%)	76,113,113	2.61	27 (35%)
13	DD6	6	316	-	39,45,45	6.69	23 (58%)	52,67,67	6.50	30 (57%)
11	CLA	12	303	6	65,73,73	2.06	18 (27%)	76,113,113	2.63	27 (35%)
14	A86	14	316	-	44,50,50	3.99	23 (52%)	51,76,76	8.18	17 (33%)
14	A86	14	317	-	44,50,50	4.03	23 (52%)	51,76,76	8.74	18 (35%)
14	A86	8	315	-	44,50,50	3.65	22 (50%)	51,76,76	8.21	21 (41%)
11	CLA	14	304	8	45,53,73	2.46	16 (35%)	52,89,113	3.18	23 (44%)
11	CLA	15	312	9	45,53,73	2.46	16 (35%)	52,89,113	3.32	28 (53%)
12	KC1	13	312	7	48,53,53	3.52	27 (56%)	55,89,89	3.78	29 (52%)
12	KC1	7	312	-	48,53,53	3.36	22 (45%)	55,89,89	3.81	29 (52%)
11	CLA	15	305	9,14	45,53,73	2.46	17 (37%)	52,89,113	3.16	26 (50%)
12	KC1	12	311	6	48,53,53	3.43	24 (50%)	55,89,89	3.93	31 (56%)
13	DD6	7	316	-	39,45,45	6.72	21 (53%)	52,67,67	6.71	29 (55%)
11	CLA	12	302	6	65,73,73	1.97	17 (26%)	76,113,113	2.82	30 (39%)
11	CLA	8	303	18	65,73,73	1.97	15 (23%)	76,113,113	2.64	27 (35%)
12	KC1	12	309	6	48,53,53	3.40	23 (47%)	55,89,89	3.73	31 (56%)
12	KC1	8	311	18	48,53,53	3.37	23 (47%)	55,89,89	3.79	29 (52%)
11	CLA	14	309	8	45,53,73	2.50	16 (35%)	52,89,113	3.09	24 (46%)
11	CLA	6	311	1	65,73,73	1.96	15 (23%)	76,113,113	2.76	28 (36%)
11	CLA	16	309	10	45,53,73	2.47	17 (37%)	52,89,113	3.26	24 (46%)
14	A86	15	317	11	44,50,50	4.15	23 (52%)	51,76,76	8.46	15 (29%)
12	KC1	13	306	7	48,53,53	3.40	24 (50%)	55,89,89	3.76	30 (54%)
14	A86	13	313	7	41,47,50	4.23	22 (53%)	49,72,76	8.48	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	14	310	-	50,58,73	2.32	16 (32%)	58,95,113	3.10	26 (44%)
11	CLA	8	302	3	65,73,73	2.03	17 (26%)	76,113,113	2.78	25 (32%)
13	DD6	16	313	-	39,45,45	6.74	20 (51%)	52,67,67	7.14	30 (57%)
11	CLA	7	302	2	65,73,73	1.95	15 (23%)	76,113,113	2.71	30 (39%)
12	KC1	10	306	4	48,53,53	3.34	25 (52%)	55,89,89	3.95	32 (58%)
14	A86	11	313	-	44,50,50	3.99	23 (52%)	51,76,76	8.39	18 (35%)
14	A86	6	317	-	44,50,50	4.01	24 (54%)	51,76,76	7.16	21 (41%)
13	DD6	8	317	-	39,45,45	6.63	22 (56%)	52,67,67	6.94	29 (55%)
14	A86	14	318	-	44,50,50	4.09	23 (52%)	51,76,76	8.48	17 (33%)
11	CLA	12	321	8,6	65,73,73	2.02	17 (26%)	76,113,113	2.62	27 (35%)
11	CLA	10	304	4	65,73,73	2.02	18 (27%)	76,113,113	2.65	26 (34%)
16	LMG	7	319	-	37,37,55	0.98	3 (8%)	45,45,63	1.27	4 (8%)
12	KC1	13	311	7	48,53,53	3.47	26 (54%)	55,89,89	3.53	28 (50%)
17	LMT	11	316	-	36,36,36	0.40	0	47,47,47	1.00	5 (10%)
11	CLA	13	309	-	45,53,73	2.49	17 (37%)	52,89,113	3.13	26 (50%)
11	CLA	14	312	8,14	45,53,73	2.46	17 (37%)	52,89,113	3.15	24 (46%)
11	CLA	13	301	7	65,73,73	1.97	18 (27%)	76,113,113	2.75	30 (39%)
11	CLA	7	303	2	65,73,73	1.96	16 (24%)	76,113,113	2.70	28 (36%)
12	KC1	10	312	4	48,53,53	3.42	24 (50%)	55,89,89	3.91	29 (52%)
11	CLA	7	304	18,2	65,73,73	2.12	18 (27%)	76,113,113	2.82	28 (36%)
14	A86	10	317	-	44,50,50	4.17	23 (52%)	51,76,76	8.20	17 (33%)
14	A86	11	315	-	44,50,50	3.94	23 (52%)	51,76,76	8.40	18 (35%)
11	CLA	10	311	-	45,53,73	2.45	17 (37%)	52,89,113	3.16	22 (42%)
12	KC1	8	307	3	48,53,53	3.32	22 (45%)	55,89,89	3.85	30 (54%)
11	CLA	15	308	9,11	45,53,73	2.42	16 (35%)	52,89,113	3.13	27 (51%)
11	CLA	16	302	10	65,73,73	1.98	18 (27%)	76,113,113	2.68	27 (35%)
11	CLA	16	307	-	46,54,73	2.42	17 (36%)	53,90,113	3.11	24 (45%)
14	A86	13	315	-	44,50,50	4.17	23 (52%)	51,76,76	8.46	19 (37%)
14	A86	15	322	11	44,50,50	4.26	23 (52%)	51,76,76	8.45	22 (43%)
13	DD6	7	301	-	39,45,45	6.75	22 (56%)	52,67,67	6.70	28 (53%)
11	CLA	15	304	9,11,13	65,73,73	2.06	17 (26%)	76,113,113	2.74	27 (35%)
12	KC1	11	304	5	48,53,53	3.39	25 (52%)	55,89,89	3.82	30 (54%)
14	A86	14	314	-	44,50,50	4.08	23 (52%)	51,76,76	8.24	22 (43%)
17	LMT	12	318	-	36,36,36	0.40	0	47,47,47	0.79	1 (2%)
11	CLA	10	303	4	65,73,73	2.00	16 (24%)	76,113,113	2.69	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	DD6	13	314	-	39,45,45	6.72	22 (56%)	52,67,67	7.10	32 (61%)
17	LMT	12	319	-	36,36,36	0.37	0	47,47,47	0.80	0
11	CLA	13	304	7	45,53,73	2.50	16 (35%)	52,89,113	3.20	25 (48%)
16	LMG	8	323	16	29,29,55	1.14	2 (6%)	37,37,63	1.27	5 (13%)
14	A86	10	302	-	44,50,50	4.08	23 (52%)	51,76,76	8.60	20 (39%)
11	CLA	8	305	3	65,73,73	1.99	18 (27%)	76,113,113	4.73	30 (39%)
11	CLA	6	307	15	65,73,73	2.02	17 (26%)	76,113,113	2.58	28 (36%)
14	A86	14	315	8	44,50,50	3.95	23 (52%)	51,76,76	8.88	21 (41%)
11	CLA	7	311	2	46,54,73	2.42	17 (36%)	53,90,113	3.10	24 (45%)
17	LMT	7	320	-	36,36,36	0.30	0	47,47,47	0.71	1 (2%)
11	CLA	10	307	4	65,73,73	1.96	18 (27%)	76,113,113	2.64	29 (38%)
14	A86	12	314	-	44,50,50	3.95	23 (52%)	51,76,76	8.15	19 (37%)
11	CLA	6	306	1	65,73,73	2.01	16 (24%)	76,113,113	2.72	32 (42%)
11	CLA	15	310	9	45,53,73	2.52	16 (35%)	52,89,113	3.21	24 (46%)
11	CLA	12	310	18	65,73,73	1.98	18 (27%)	76,113,113	2.72	25 (32%)
11	CLA	14	307	12	65,73,73	2.06	17 (26%)	76,113,113	2.79	24 (31%)
11	CLA	6	301	1	65,73,73	1.97	15 (23%)	76,113,113	2.70	28 (36%)
11	CLA	11	303	5	65,73,73	2.01	16 (24%)	76,113,113	2.72	25 (32%)
15	LHG	6	319	11	26,26,48	0.91	1 (3%)	29,32,54	1.39	3 (10%)
11	CLA	15	307	9	50,58,73	2.29	18 (36%)	58,95,113	2.99	26 (44%)
11	CLA	12	304	6,13	65,73,73	2.03	18 (27%)	76,113,113	2.88	29 (38%)
11	CLA	6	313	18	55,63,73	2.19	17 (30%)	64,101,113	2.83	25 (39%)
12	KC1	13	310	7	48,53,53	3.45	24 (50%)	55,89,89	3.77	29 (52%)
12	KC1	16	304	10	48,53,53	3.48	24 (50%)	55,89,89	3.57	27 (49%)
11	CLA	11	305	18	55,63,73	2.20	16 (29%)	64,101,113	3.03	27 (42%)
13	DD6	7	313	-	39,45,45	6.57	22 (56%)	52,67,67	7.25	29 (55%)
14	A86	15	315	9	44,50,50	4.30	23 (52%)	51,76,76	8.24	27 (52%)
11	CLA	6	314	-	65,73,73	2.08	17 (26%)	76,113,113	2.64	27 (35%)
11	CLA	7	306	2	65,73,73	1.98	15 (23%)	76,113,113	2.75	26 (34%)
11	CLA	8	304	3	58,66,73	2.07	15 (25%)	67,104,113	2.99	31 (46%)
11	CLA	15	302	9,11	65,73,73	2.05	16 (24%)	76,113,113	2.94	29 (38%)
14	A86	15	320	-	44,50,50	4.24	24 (54%)	51,76,76	8.22	19 (37%)
11	CLA	16	305	10	50,58,73	2.26	17 (34%)	58,95,113	3.00	27 (46%)
12	KC1	14	306	8	48,53,53	3.43	24 (50%)	55,89,89	3.86	30 (54%)
12	KC1	13	305	7	48,53,53	3.44	26 (54%)	55,89,89	3.76	29 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	DD6	8	316	-	39,45,45	6.55	22 (56%)	52,67,67	6.81	30 (57%)
14	A86	7	314	-	44,50,50	3.85	23 (52%)	51,76,76	7.93	18 (35%)
11	CLA	14	313	8	46,54,73	2.42	16 (34%)	53,90,113	3.25	26 (49%)
16	LMG	8	320	16,3	37,37,55	0.98	1 (2%)	45,45,63	1.24	4 (8%)
14	A86	11	301	-	44,50,50	3.98	23 (52%)	51,76,76	8.34	19 (37%)
14	A86	16	314	-	44,50,50	4.10	24 (54%)	51,76,76	8.52	21 (41%)
12	KC1	13	308	7	48,53,53	3.45	25 (52%)	55,89,89	3.87	29 (52%)
14	A86	10	316	-	44,50,50	3.92	23 (52%)	51,76,76	7.96	23 (45%)
11	CLA	16	306	10	52,60,73	2.26	18 (34%)	60,97,113	2.95	28 (46%)
17	LMT	11	302	-	36,36,36	0.32	0	47,47,47	0.79	2 (4%)
11	CLA	10	308	4	65,73,73	2.00	15 (23%)	76,113,113	2.73	29 (38%)
11	CLA	12	312	6	65,73,73	2.01	18 (27%)	76,113,113	2.70	27 (35%)
11	CLA	15	314	9,11	45,53,73	2.40	17 (37%)	52,89,113	3.32	23 (44%)
12	KC1	8	310	3	48,53,53	3.31	22 (45%)	55,89,89	3.78	28 (50%)
14	A86	16	312	10	44,50,50	4.02	24 (54%)	51,76,76	8.20	22 (43%)
12	KC1	8	312	12	48,53,53	3.40	24 (50%)	55,89,89	3.39	28 (50%)
14	A86	10	315	-	44,50,50	4.12	22 (50%)	51,76,76	8.21	18 (35%)

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
12	KC1	14	311	8	-	5/15/71/71	-
16	LMG	14	322	-	-	14/33/53/70	0/1/1/1
17	LMT	12	301	-	-	3/21/61/61	0/2/2/2
11	CLA	11	307	5	1/1/15/20	10/37/115/115	-
14	A86	14	321	-	-	15/34/90/90	0/3/3/3
17	LMT	12	322	-	-	1/21/61/61	0/2/2/2
12	KC1	8	314	18,12	-	6/15/71/71	-
12	KC1	6	310	1	-	6/15/71/71	-
13	DD6	6	315	-	-	10/26/80/80	0/3/3/3
14	A86	12	316	-	-	14/34/90/90	0/3/3/3
17	LMT	8	324	-	-	5/21/61/61	0/2/2/2
11	CLA	6	302	1	1/1/15/20	4/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	A86	8	318	-	-	14/34/90/90	0/3/3/3
13	DD6	10	314	-	-	9/26/80/80	0/3/3/3
11	CLA	11	308	5	-	15/37/115/115	-
11	CLA	12	308	18	1/1/15/20	9/37/115/115	-
11	CLA	15	311	14	1/1/11/20	8/13/91/115	-
12	KC1	16	311	10	-	6/15/71/71	-
17	LMT	12	320	-	-	1/21/61/61	0/2/2/2
11	CLA	6	312	1	1/1/11/20	4/13/91/115	-
13	DD6	7	317	-	-	15/26/80/80	0/3/3/3
14	A86	7	315	-	-	9/34/90/90	0/3/3/3
11	CLA	8	309	3	-	3/16/94/115	-
11	CLA	15	303	9,14,11	1/1/14/20	9/31/109/115	-
14	A86	15	321	9	-	13/34/90/90	0/3/3/3
11	CLA	16	308	10	1/1/11/20	6/13/91/115	-
11	CLA	13	307	7	1/1/15/20	10/37/115/115	-
11	CLA	7	309	2	1/1/15/20	14/37/115/115	-
13	DD6	10	313	-	-	10/26/80/80	0/3/3/3
11	CLA	6	304	1	1/1/15/20	18/37/115/115	-
13	DD6	12	315	11	-	9/26/80/80	0/3/3/3
14	A86	7	318	-	-	9/34/90/90	0/3/3/3
11	CLA	15	306	-	1/1/11/20	6/13/91/115	-
14	A86	14	301	8	-	8/34/90/90	0/3/3/3
11	CLA	12	306	6	1/1/15/20	6/37/115/115	-
14	A86	10	301	4	-	9/34/90/90	0/3/3/3
17	LMT	8	322	-	-	1/21/61/61	0/2/2/2
12	KC1	10	310	4	-	8/15/71/71	-
12	KC1	12	313	6	-	7/15/71/71	-
12	KC1	6	305	1	-	6/15/71/71	-
11	CLA	16	303	10	1/1/15/20	19/37/115/115	-
11	CLA	7	310	2	1/1/15/20	12/37/115/115	-
11	CLA	12	307	6	1/1/11/20	7/15/93/115	-
12	KC1	6	309	1	-	5/15/71/71	-
13	DD6	6	318	-	-	9/26/80/80	0/3/3/3
14	A86	11	314	-	-	18/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	A86	14	319	11	-	11/34/90/90	0/3/3/3
11	CLA	8	308	3	1/1/13/20	10/25/103/115	-
11	CLA	15	313	9	-	11/37/115/115	-
16	LMG	8	321	-	-	22/37/57/70	0/1/1/1
12	KC1	11	311	-	-	9/15/71/71	-
12	KC1	8	306	18	-	5/15/71/71	-
11	CLA	11	309	5	1/1/15/20	15/37/115/115	-
17	LMT	15	301	-	-	7/21/61/61	0/2/2/2
13	DD6	12	317	-	-	12/26/80/80	0/3/3/3
13	DD6	15	319	11	-	13/26/80/80	0/3/3/3
14	A86	14	320	-	-	9/34/90/90	0/3/3/3
12	KC1	8	313	3	-	8/15/71/71	-
11	CLA	14	303	8	1/1/13/20	7/28/106/115	-
12	KC1	6	308	1	-	8/15/71/71	-
12	KC1	11	310	5	-	6/15/71/71	-
14	A86	15	316	11	-	14/34/90/90	0/3/3/3
12	KC1	7	307	18	-	7/15/71/71	-
11	CLA	14	305	8	1/1/12/20	2/19/97/115	-
17	LMT	8	319	-	-	10/21/61/61	0/2/2/2
13	DD6	11	312	-	-	11/26/80/80	0/3/3/3
17	LMT	16	315	-	-	5/21/61/61	0/2/2/2
11	CLA	6	303	18	1/1/15/20	7/37/115/115	-
12	KC1	11	306	5	-	10/15/71/71	-
11	CLA	16	310	10	1/1/11/20	7/13/91/115	-
11	CLA	13	302	7	1/1/15/20	11/37/115/115	-
12	KC1	12	305	6	-	7/15/71/71	-
11	CLA	7	308	2	1/1/15/20	8/37/115/115	-
11	CLA	13	303	-	-	16/37/115/115	-
12	KC1	14	308	8,11	-	9/15/71/71	-
13	DD6	15	318	-	-	13/26/80/80	0/3/3/3
11	CLA	14	302	8	1/1/15/20	14/37/115/115	-
11	CLA	10	305	18	1/1/15/20	8/37/115/115	-
11	CLA	10	309	4	1/1/15/20	12/37/115/115	-
11	CLA	15	309	9	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	8	301	3	1/1/15/20	15/37/115/115	-
11	CLA	16	301	10	-	13/37/115/115	-
11	CLA	7	305	2	1/1/15/20	6/37/115/115	-
13	DD6	6	316	-	-	11/26/80/80	0/3/3/3
11	CLA	12	303	6	1/1/15/20	7/37/115/115	-
14	A86	14	316	-	-	12/34/90/90	0/3/3/3
14	A86	14	317	-	-	15/34/90/90	0/3/3/3
14	A86	8	315	-	-	7/34/90/90	0/3/3/3
11	CLA	14	304	8	1/1/11/20	4/13/91/115	-
11	CLA	15	312	9	1/1/11/20	5/13/91/115	-
12	KC1	13	312	7	-	7/15/71/71	-
12	KC1	7	312	-	-	4/15/71/71	-
11	CLA	15	305	9,14	1/1/11/20	8/13/91/115	-
12	KC1	12	311	6	-	6/15/71/71	-
13	DD6	7	316	-	-	10/26/80/80	0/3/3/3
11	CLA	12	302	6	-	14/37/115/115	-
11	CLA	8	303	18	1/1/15/20	10/37/115/115	-
12	KC1	12	309	6	-	7/15/71/71	-
12	KC1	8	311	18	-	8/15/71/71	-
11	CLA	14	309	8	1/1/11/20	3/13/91/115	-
11	CLA	6	311	1	-	14/37/115/115	-
11	CLA	16	309	10	-	4/13/91/115	-
14	A86	15	317	11	-	16/34/90/90	0/3/3/3
12	KC1	13	306	7	-	11/15/71/71	-
14	A86	13	313	7	-	11/30/86/90	0/3/3/3
11	CLA	14	310	-	1/1/12/20	5/19/97/115	-
11	CLA	8	302	3	1/1/15/20	6/37/115/115	-
13	DD6	16	313	-	-	13/26/80/80	0/3/3/3
11	CLA	7	302	2	1/1/15/20	13/37/115/115	-
12	KC1	10	306	4	-	8/15/71/71	-
14	A86	11	313	-	-	13/34/90/90	0/3/3/3
14	A86	6	317	-	-	8/34/90/90	0/3/3/3
13	DD6	8	317	-	-	11/26/80/80	0/3/3/3
14	A86	14	318	-	-	17/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	12	321	8,6	1/1/15/20	4/37/115/115	-
11	CLA	10	304	4	1/1/15/20	2/37/115/115	-
16	LMG	7	319	-	-	12/32/52/70	0/1/1/1
12	KC1	13	311	7	-	6/15/71/71	-
17	LMT	11	316	-	-	1/21/61/61	0/2/2/2
11	CLA	13	309	-	1/1/11/20	6/13/91/115	-
11	CLA	14	312	8,14	-	7/13/91/115	-
11	CLA	13	301	7	-	16/37/115/115	-
11	CLA	7	303	2	1/1/15/20	6/37/115/115	-
12	KC1	10	312	4	-	5/15/71/71	-
11	CLA	7	304	18,2	1/1/15/20	8/37/115/115	-
14	A86	10	317	-	-	10/34/90/90	0/3/3/3
14	A86	11	315	-	-	15/34/90/90	0/3/3/3
11	CLA	10	311	-	-	7/13/91/115	-
12	KC1	8	307	3	-	8/15/71/71	-
11	CLA	15	308	9,11	1/1/11/20	6/13/91/115	-
11	CLA	16	302	10	1/1/15/20	9/37/115/115	-
11	CLA	16	307	-	1/1/11/20	7/15/93/115	-
14	A86	13	315	-	-	16/34/90/90	0/3/3/3
14	A86	15	322	11	-	15/34/90/90	0/3/3/3
13	DD6	7	301	-	-	11/26/80/80	0/3/3/3
11	CLA	15	304	9,11,13	1/1/15/20	21/37/115/115	-
12	KC1	11	304	5	-	7/15/71/71	-
14	A86	14	314	-	-	13/34/90/90	0/3/3/3
17	LMT	12	318	-	-	1/21/61/61	0/2/2/2
11	CLA	10	303	4	-	12/37/115/115	-
13	DD6	13	314	-	-	13/26/80/80	0/3/3/3
17	LMT	12	319	-	-	0/21/61/61	0/2/2/2
11	CLA	13	304	7	-	6/13/91/115	-
16	LMG	8	323	16	-	5/24/44/70	0/1/1/1
14	A86	10	302	-	-	13/34/90/90	0/3/3/3
11	CLA	8	305	3	-	13/37/115/115	-
11	CLA	6	307	15	1/1/15/20	10/37/115/115	-
14	A86	14	315	8	-	11/34/90/90	0/3/3/3
11	CLA	7	311	2	-	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LMT	7	320	-	-	4/21/61/61	0/2/2/2
11	CLA	10	307	4	1/1/15/20	11/37/115/115	-
14	A86	12	314	-	-	12/34/90/90	0/3/3/3
11	CLA	6	306	1	1/1/15/20	12/37/115/115	-
11	CLA	15	310	9	1/1/11/20	6/13/91/115	-
11	CLA	12	310	18	-	9/37/115/115	-
11	CLA	14	307	12	-	9/37/115/115	-
11	CLA	6	301	1	1/1/15/20	12/37/115/115	-
11	CLA	11	303	5	-	10/37/115/115	-
15	LHG	6	319	11	-	13/31/31/53	-
11	CLA	12	304	6,13	1/1/15/20	14/37/115/115	-
11	CLA	6	313	18	1/1/13/20	5/25/103/115	-
11	CLA	15	307	9	1/1/12/20	7/19/97/115	-
12	KC1	13	310	7	-	5/15/71/71	-
12	KC1	16	304	10	-	8/15/71/71	-
11	CLA	11	305	18	1/1/13/20	8/25/103/115	-
13	DD6	7	313	-	-	11/26/80/80	0/3/3/3
14	A86	15	315	9	-	9/34/90/90	0/3/3/3
11	CLA	6	314	-	1/1/15/20	6/37/115/115	-
11	CLA	7	306	2	-	21/37/115/115	-
11	CLA	8	304	3	1/1/13/20	11/29/107/115	-
11	CLA	15	302	9,11	-	15/37/115/115	-
14	A86	15	320	-	-	15/34/90/90	0/3/3/3
11	CLA	16	305	10	1/1/12/20	3/19/97/115	-
12	KC1	14	306	8	-	7/15/71/71	-
12	KC1	13	305	7	-	10/15/71/71	-
13	DD6	8	316	-	-	11/26/80/80	0/3/3/3
14	A86	7	314	-	-	16/34/90/90	0/3/3/3
11	CLA	14	313	8	1/1/11/20	4/15/93/115	-
16	LMG	8	320	16,3	-	17/32/52/70	0/1/1/1
14	A86	11	301	-	-	12/34/90/90	0/3/3/3
14	A86	16	314	-	-	11/34/90/90	0/3/3/3
12	KC1	13	308	7	-	10/15/71/71	-
14	A86	10	316	-	-	11/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	16	306	10	1/1/12/20	13/22/100/115	-
17	LMT	11	302	-	-	0/21/61/61	0/2/2/2
11	CLA	10	308	4	1/1/15/20	10/37/115/115	-
11	CLA	12	312	6	1/1/15/20	12/37/115/115	-
11	CLA	15	314	9,11	-	4/13/91/115	-
12	KC1	8	310	3	-	7/15/71/71	-
14	A86	16	312	10	-	12/34/90/90	0/3/3/3
12	KC1	8	312	12	-	7/15/71/71	-
14	A86	10	315	-	-	15/34/90/90	0/3/3/3

The worst 5 of 3477 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	11	312	DD6	C10-C11	26.03	1.70	1.35
13	10	313	DD6	C10-C11	25.96	1.70	1.35
13	7	317	DD6	C10-C11	25.86	1.70	1.35
13	15	318	DD6	C10-C11	25.75	1.69	1.35
13	10	314	DD6	C10-C11	25.68	1.69	1.35

The worst 5 of 4528 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	14	315	A86	O1-C20-C19	58.19	157.09	113.38
14	14	317	A86	O1-C20-C19	57.22	156.37	113.38
14	15	321	A86	O1-C20-C19	57.11	156.29	113.38
14	8	318	A86	O1-C20-C19	56.82	156.07	113.38
14	16	314	A86	O1-C20-C19	56.19	155.59	113.38

5 of 63 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	6	301	CLA	ND
11	6	302	CLA	ND
11	6	303	CLA	ND
11	6	304	CLA	ND
11	6	306	CLA	ND

5 of 1794 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	6	301	CLA	C1A-C2A-CAA-CBA
11	6	301	CLA	C3A-C2A-CAA-CBA
11	6	304	CLA	C2-C3-C5-C6
11	6	304	CLA	C4-C3-C5-C6
11	6	306	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

88 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	14	322	LMG	1	0
17	12	301	LMT	1	0
11	11	307	CLA	1	0
17	12	322	LMT	1	0
13	6	315	DD6	2	0
17	8	324	LMT	1	0
11	6	302	CLA	1	0
11	11	308	CLA	1	0
11	12	308	CLA	3	0
17	12	320	LMT	2	0
11	8	309	CLA	1	0
11	15	303	CLA	3	0
11	13	307	CLA	4	0
11	7	309	CLA	1	0
13	10	313	DD6	1	0
11	6	304	CLA	2	0
11	12	306	CLA	2	0
11	16	303	CLA	3	0
11	7	310	CLA	2	0
13	6	318	DD6	1	0
14	11	314	A86	1	0
11	8	308	CLA	2	0
11	15	313	CLA	4	0
16	8	321	LMG	1	0
14	14	320	A86	1	0
12	8	313	KC1	1	0
11	14	303	CLA	3	0
11	14	305	CLA	1	0
13	11	312	DD6	1	0
11	6	303	CLA	1	0
11	16	310	CLA	2	0
11	13	302	CLA	2	0
11	7	308	CLA	4	0

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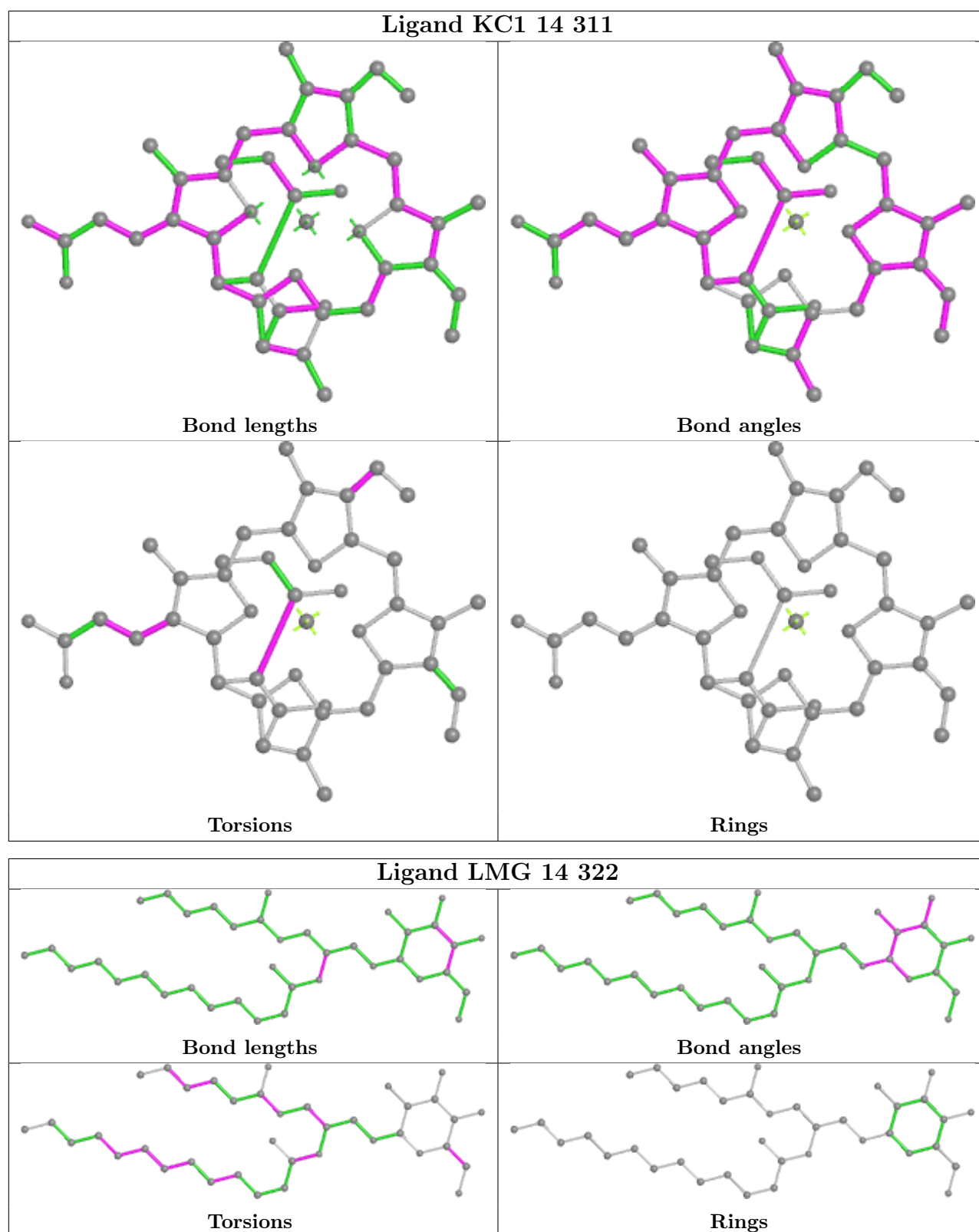
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	13	303	CLA	1	0
11	14	302	CLA	2	0
11	10	305	CLA	2	0
11	10	309	CLA	1	0
11	15	309	CLA	2	0
11	8	301	CLA	1	0
11	16	301	CLA	7	0
11	7	305	CLA	2	0
13	6	316	DD6	1	0
11	12	303	CLA	3	0
14	14	317	A86	1	0
14	8	315	A86	1	0
11	15	312	CLA	1	0
11	12	302	CLA	1	0
11	8	303	CLA	5	0
11	6	311	CLA	3	0
11	8	302	CLA	2	0
11	7	302	CLA	1	0
11	12	321	CLA	1	0
11	10	304	CLA	3	0
16	7	319	LMG	1	0
17	11	316	LMT	2	0
11	14	312	CLA	1	0
11	13	301	CLA	2	0
11	7	303	CLA	1	0
11	15	308	CLA	1	0
11	16	302	CLA	1	0
11	16	307	CLA	2	0
11	15	304	CLA	1	0
11	10	303	CLA	3	0
13	13	314	DD6	1	0
17	12	319	LMT	3	0
11	13	304	CLA	2	0
16	8	323	LMG	1	0
11	8	305	CLA	2	0
11	10	307	CLA	2	0
11	6	306	CLA	3	0
11	12	310	CLA	2	0
11	14	307	CLA	2	0
11	6	301	CLA	2	0
11	11	303	CLA	4	0
11	15	307	CLA	2	0

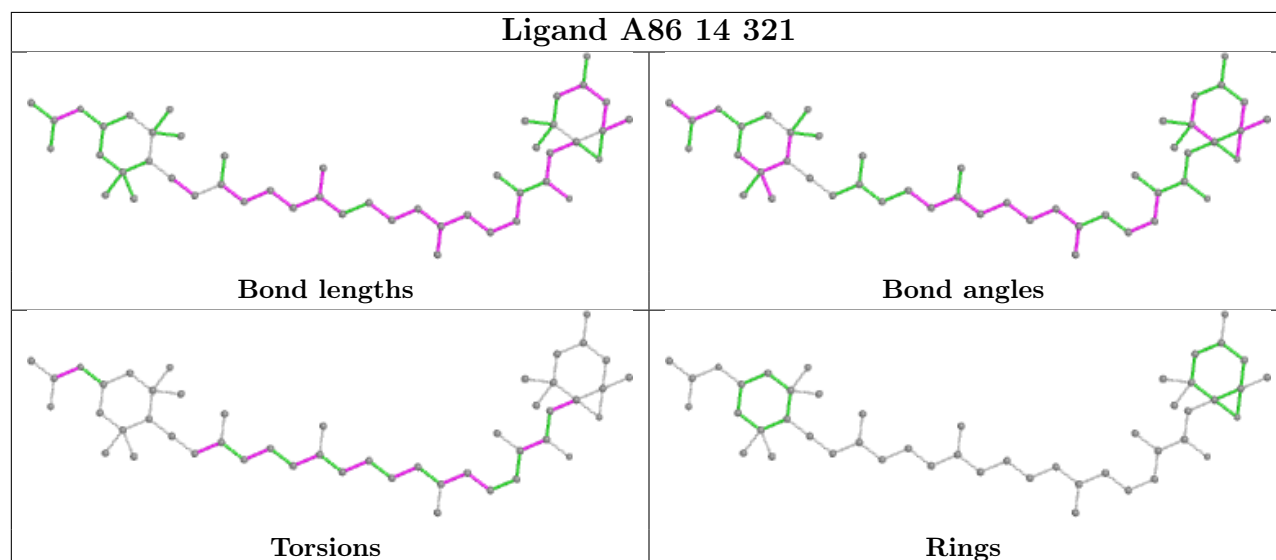
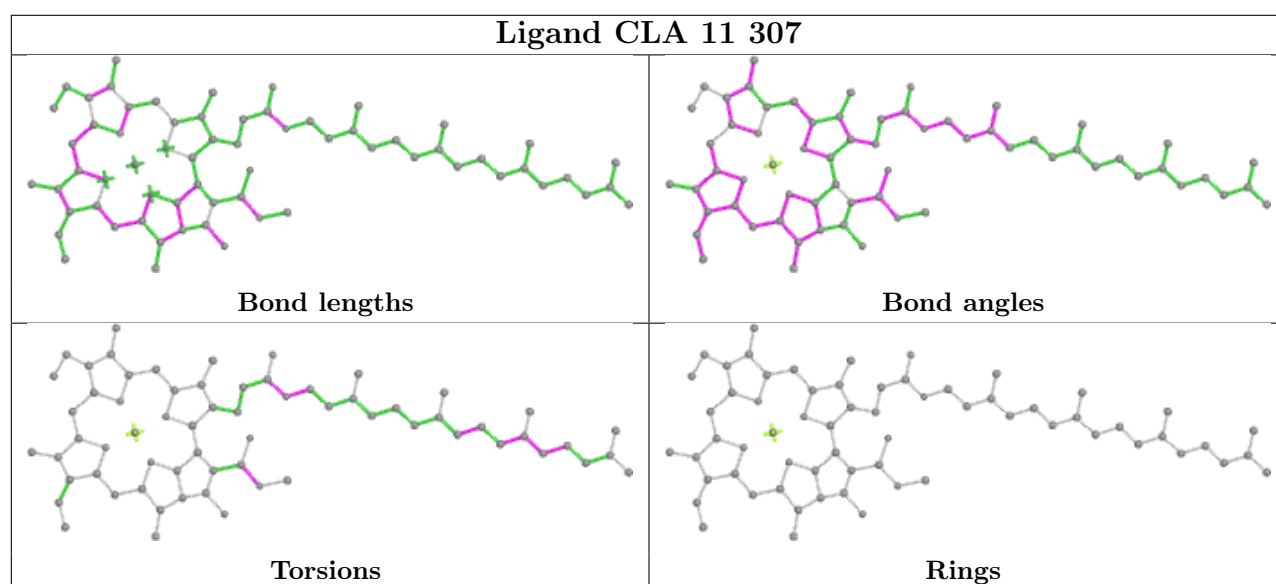
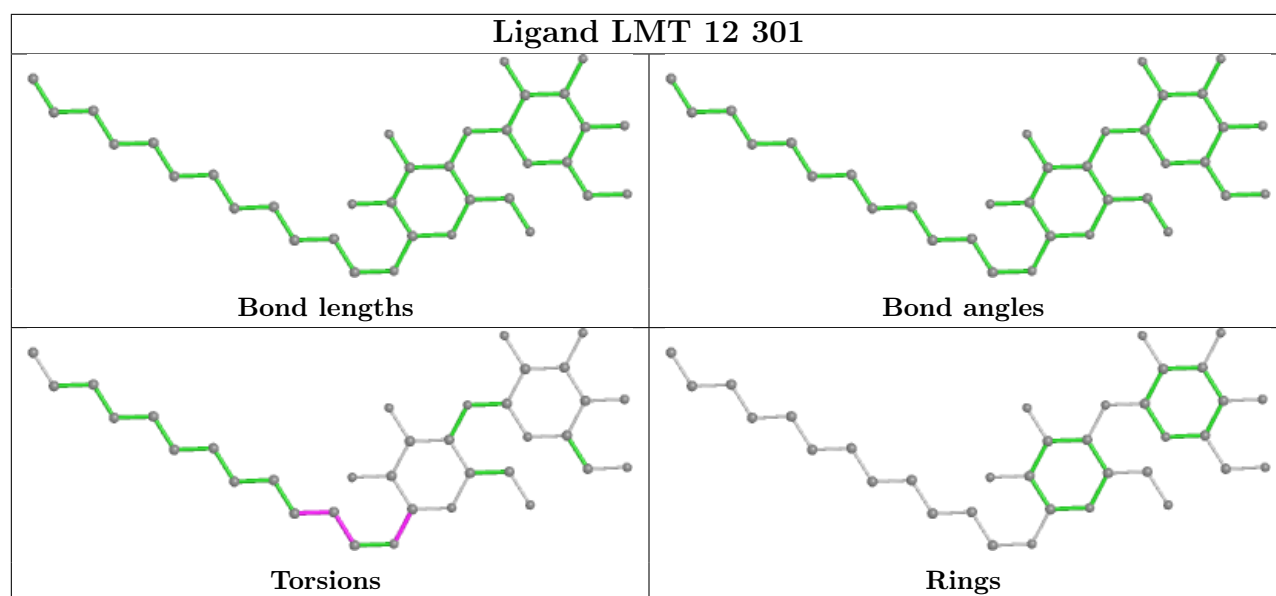
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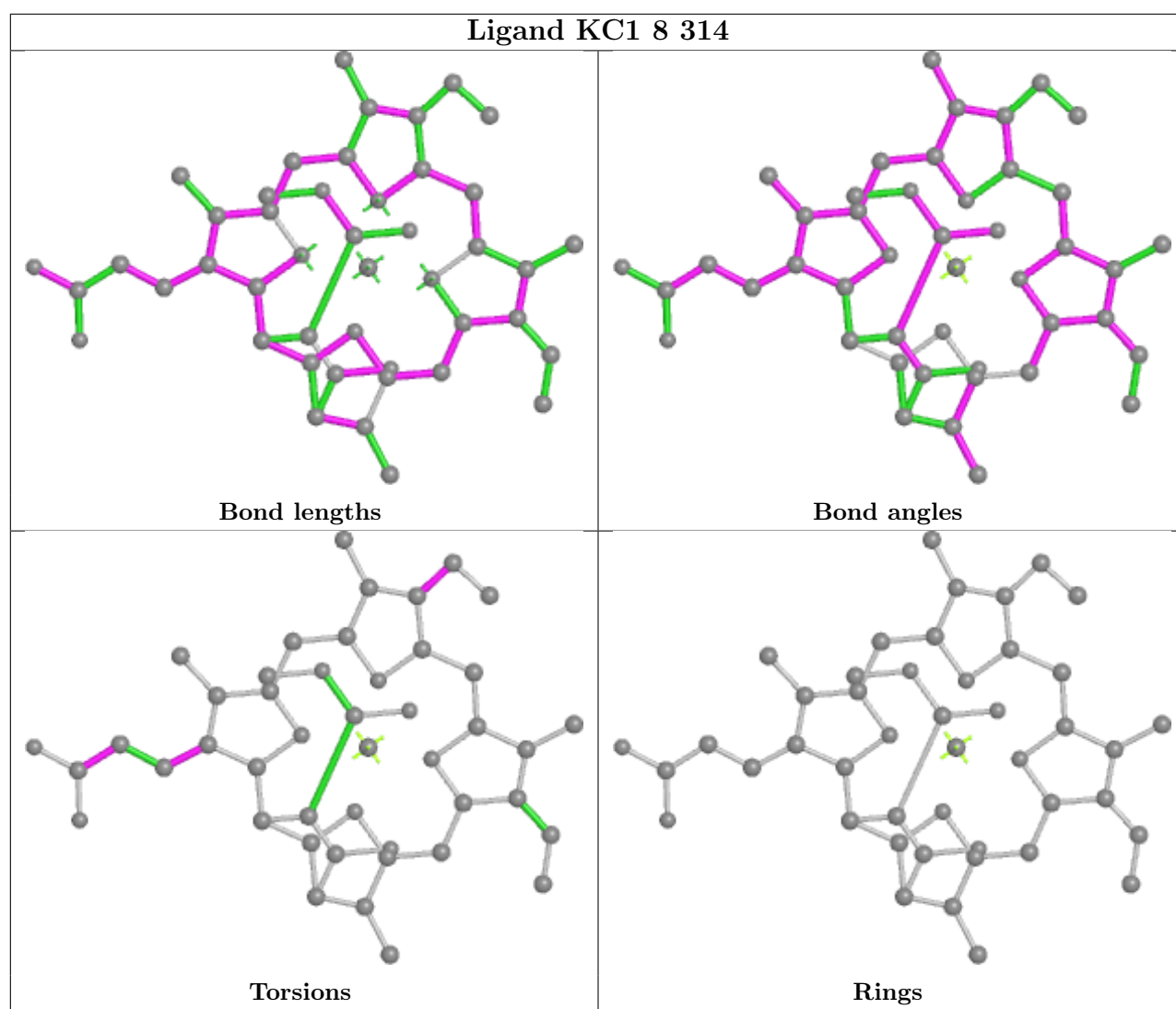
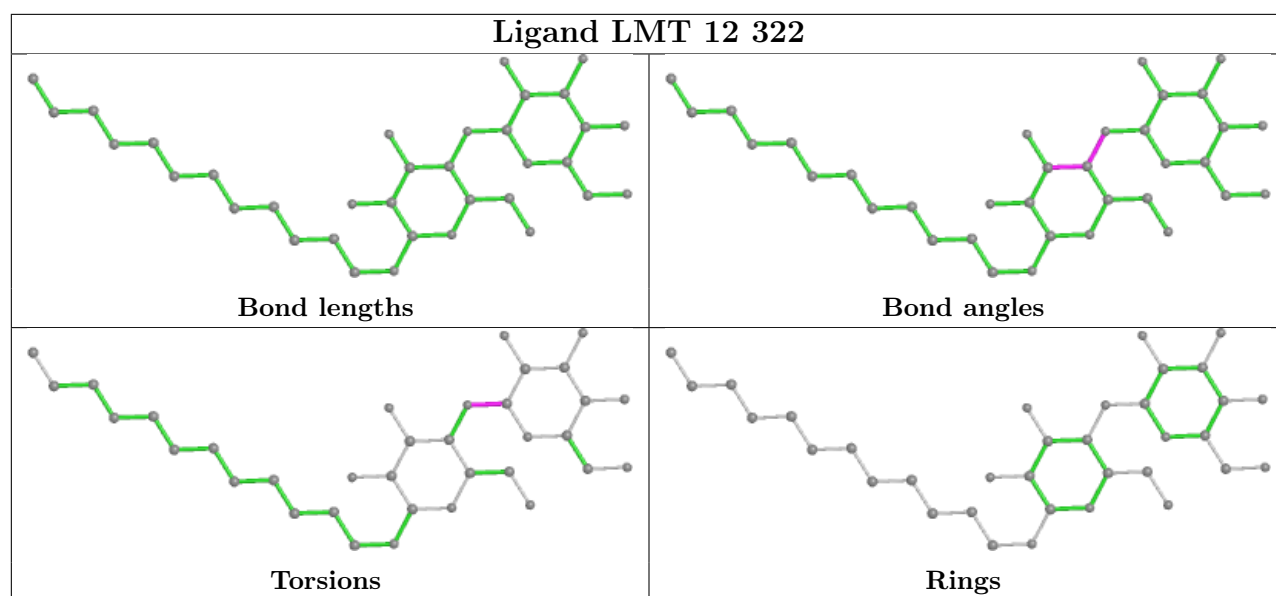
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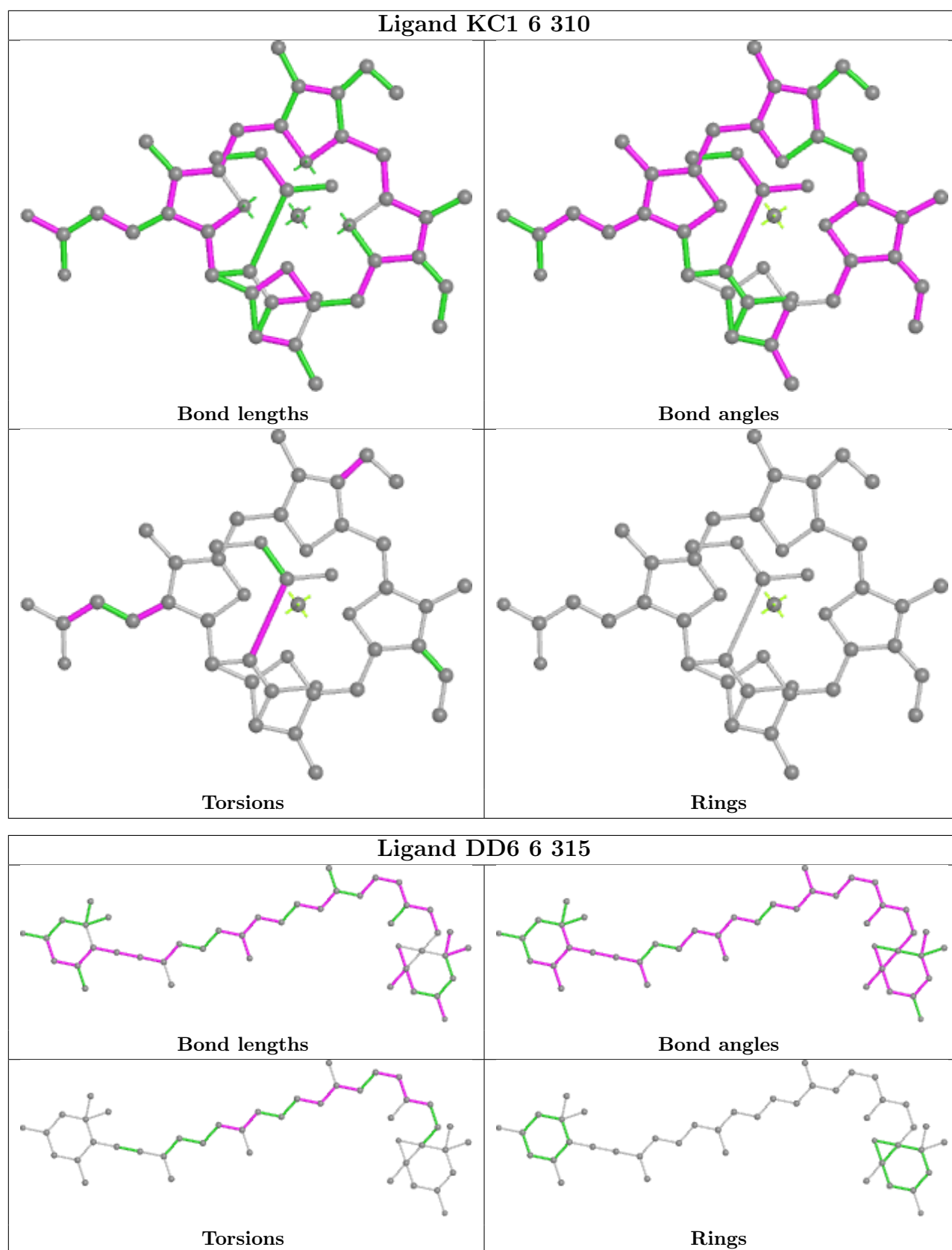
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	12	304	CLA	2	0
11	6	313	CLA	2	0
12	13	310	KC1	1	0
12	16	304	KC1	1	0
13	7	313	DD6	1	0
11	7	306	CLA	3	0
11	8	304	CLA	1	0
11	15	302	CLA	5	0
14	7	314	A86	1	0
16	8	320	LMG	1	0
11	16	306	CLA	1	0
11	10	308	CLA	3	0
11	12	312	CLA	1	0

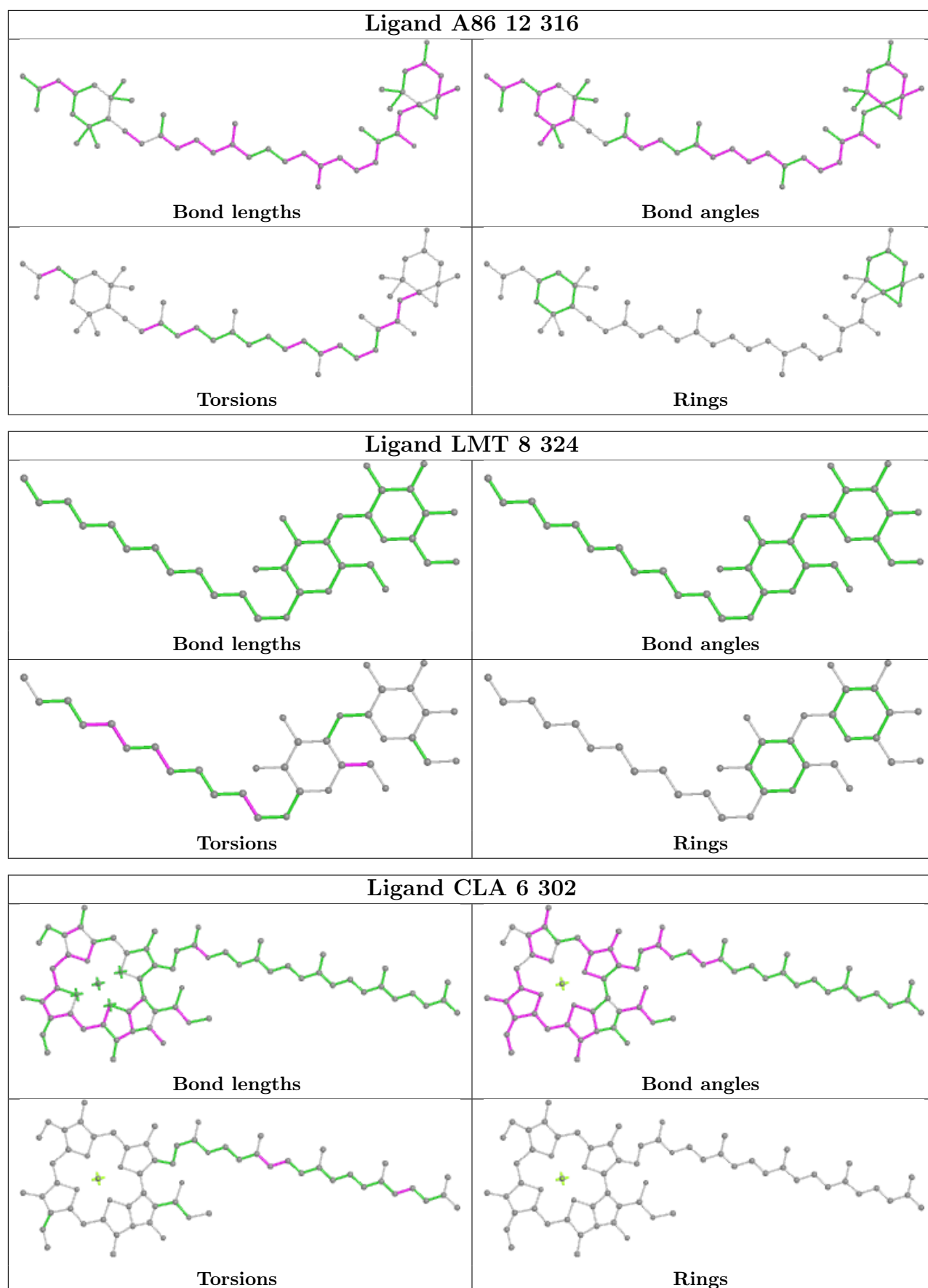
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

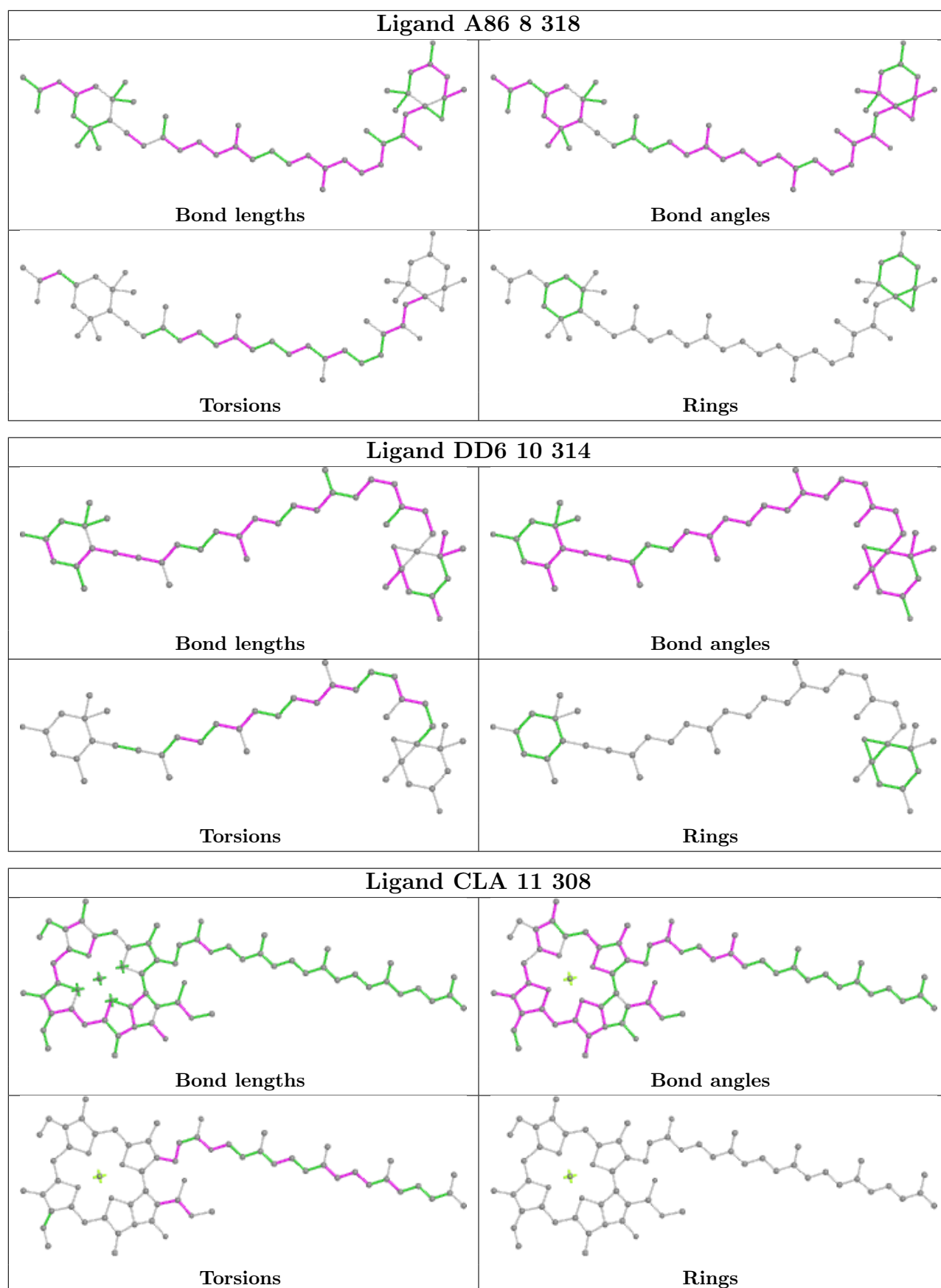


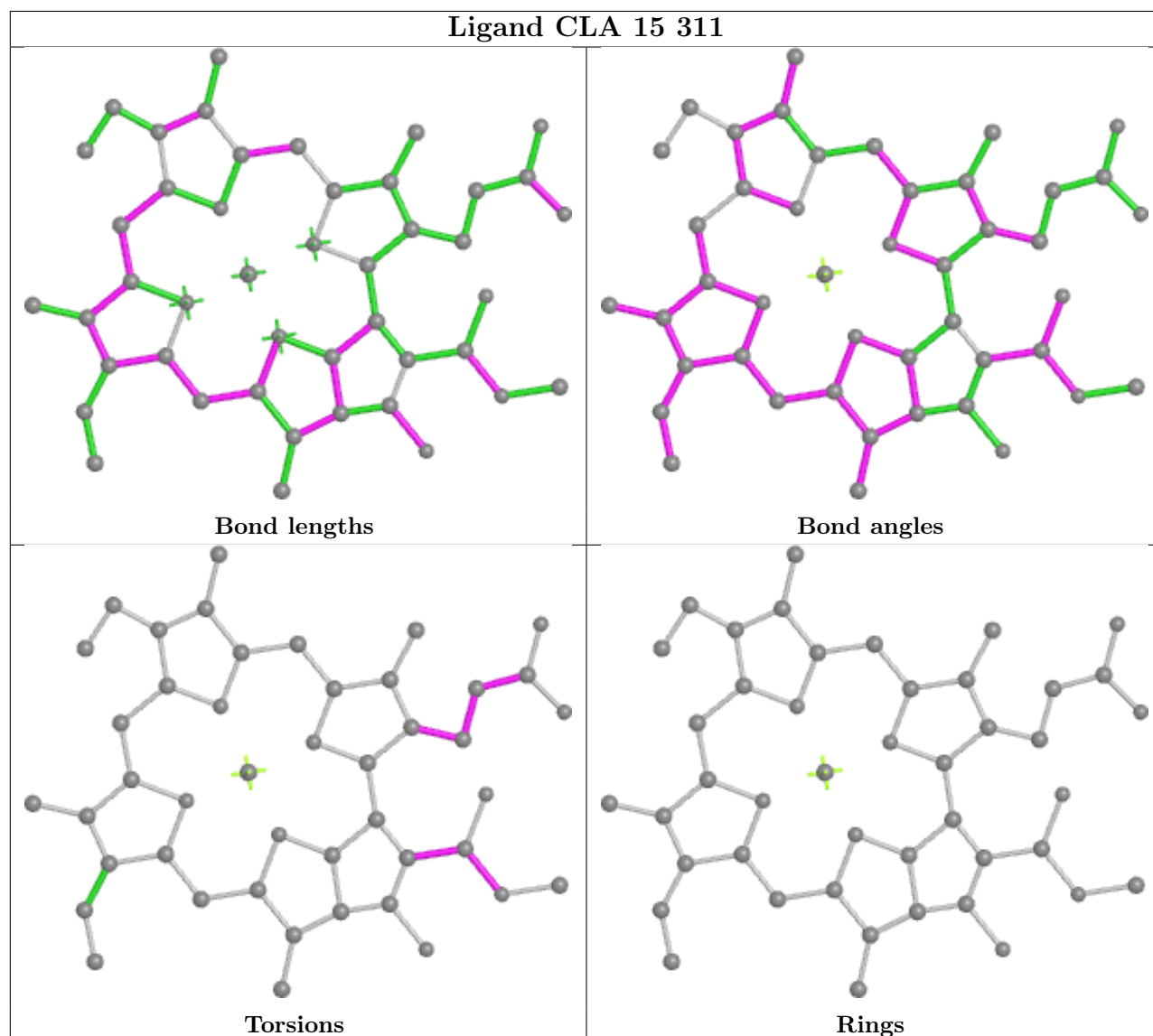
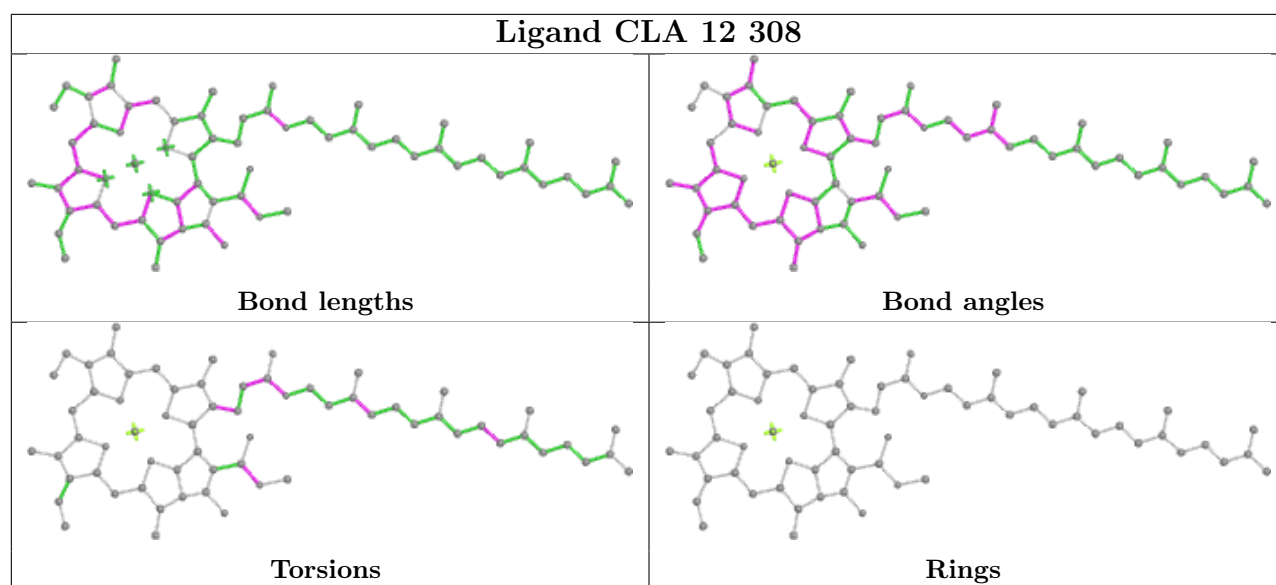


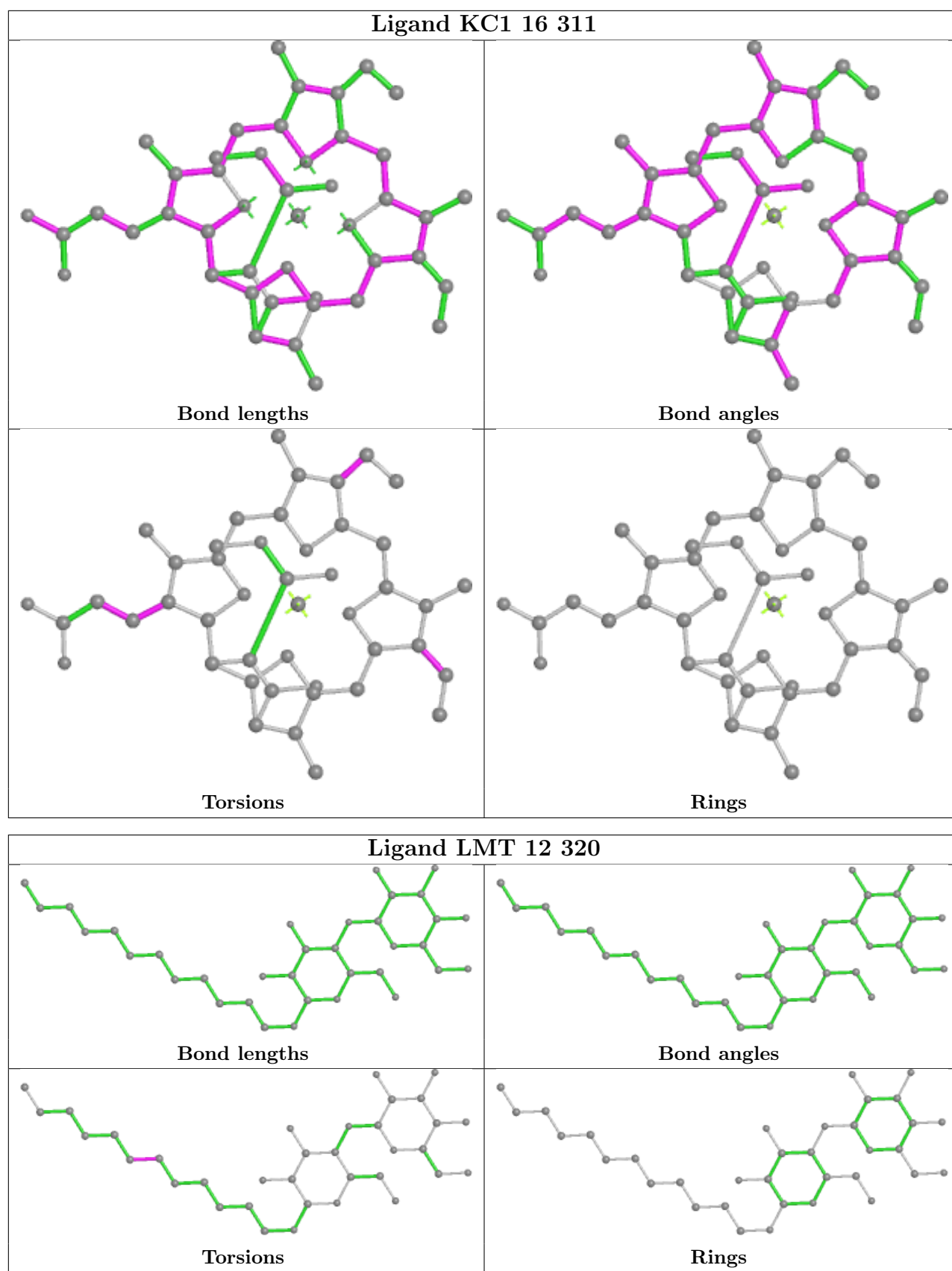




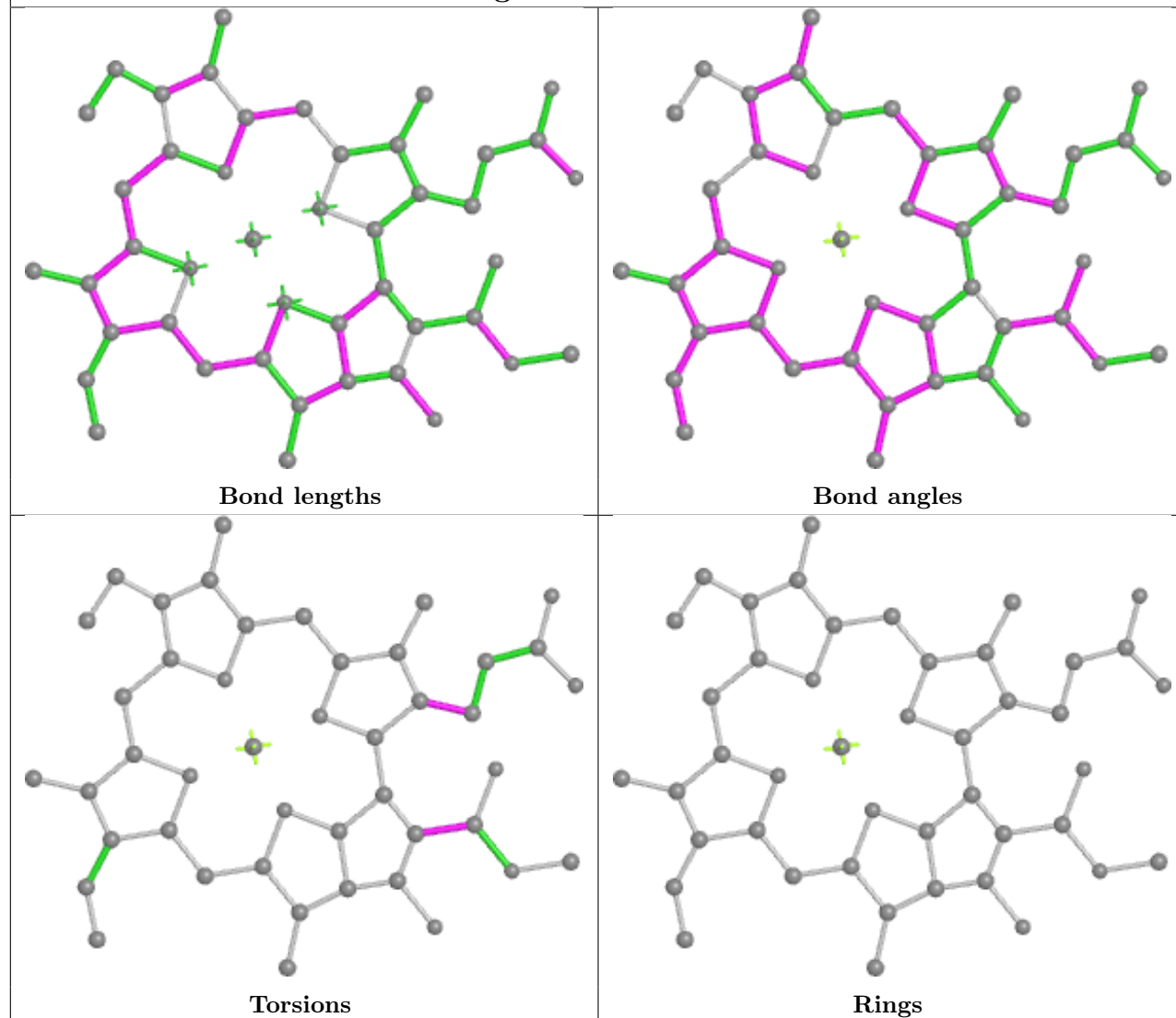




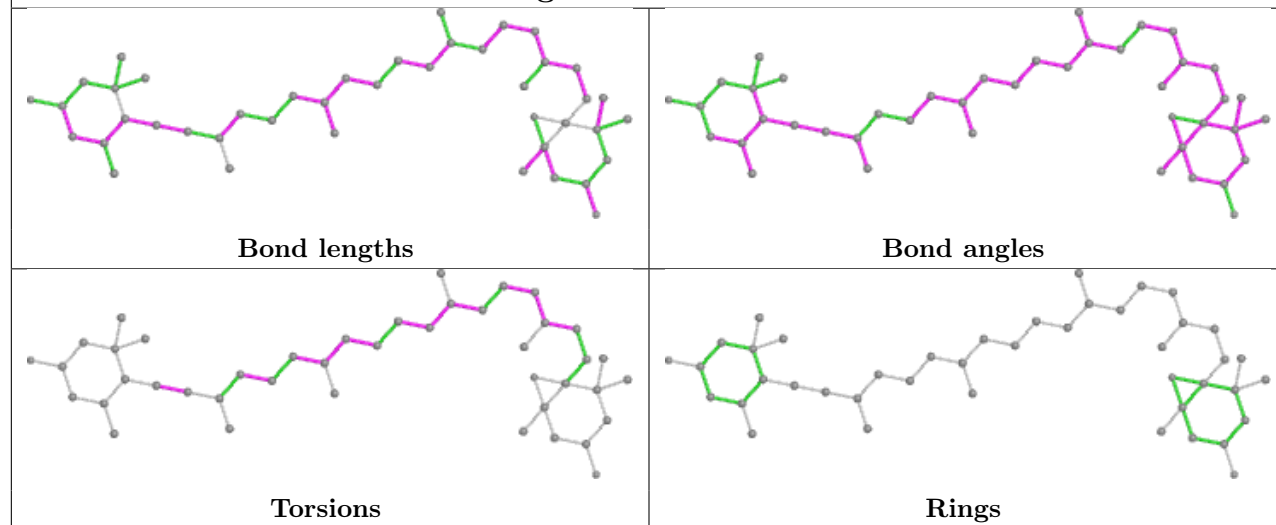


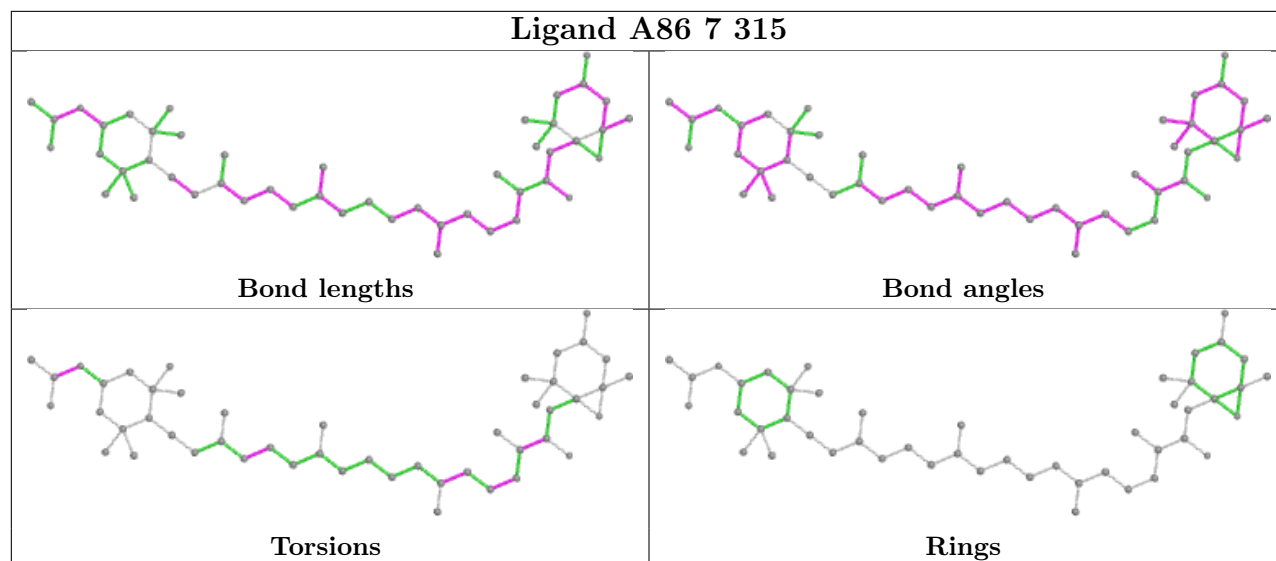
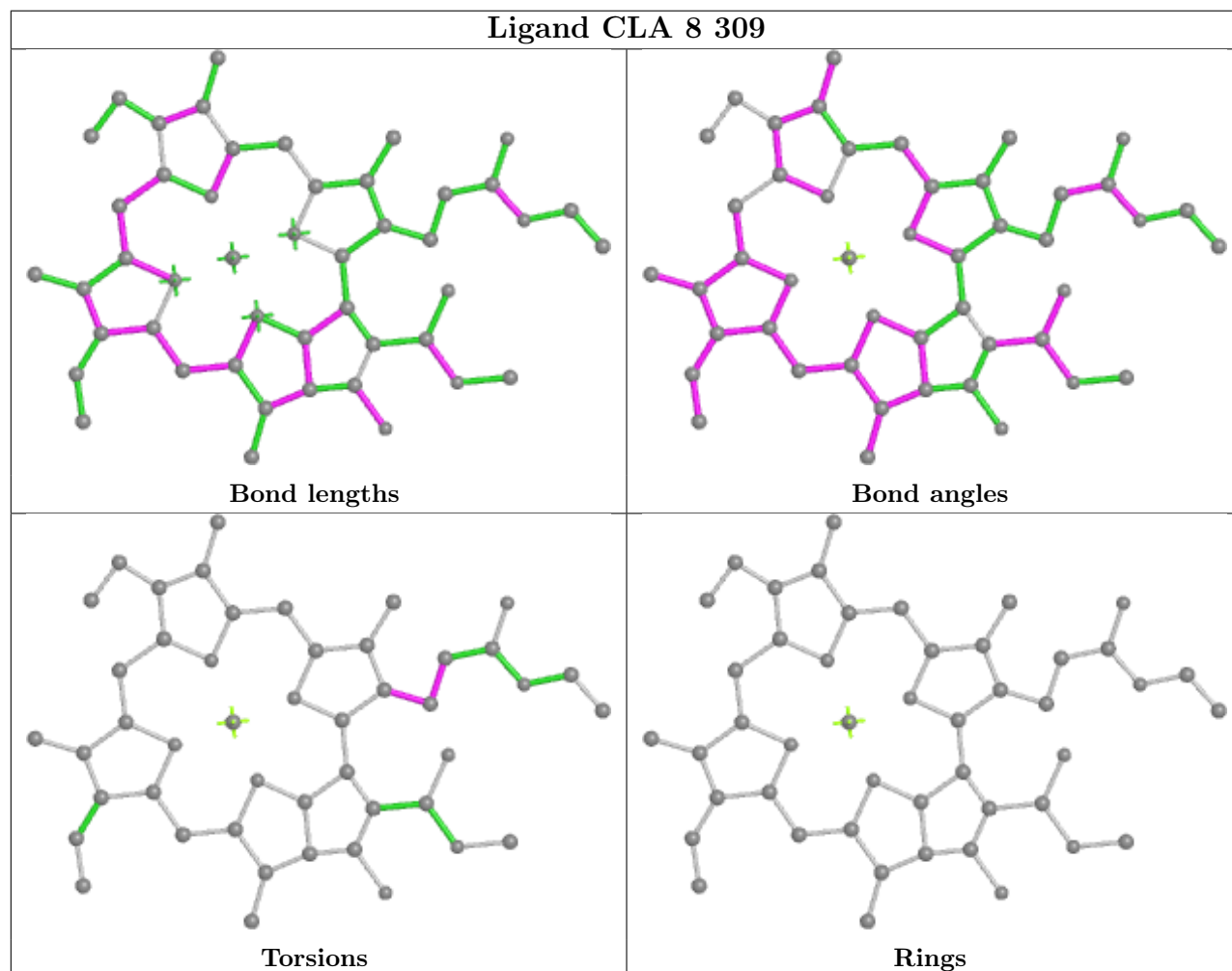


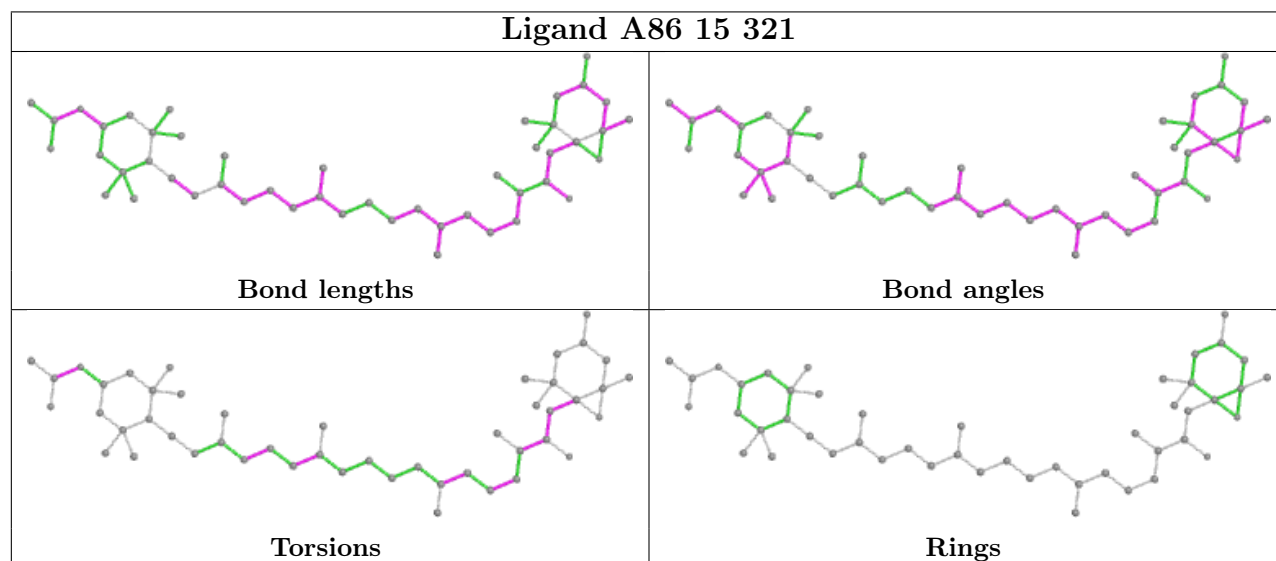
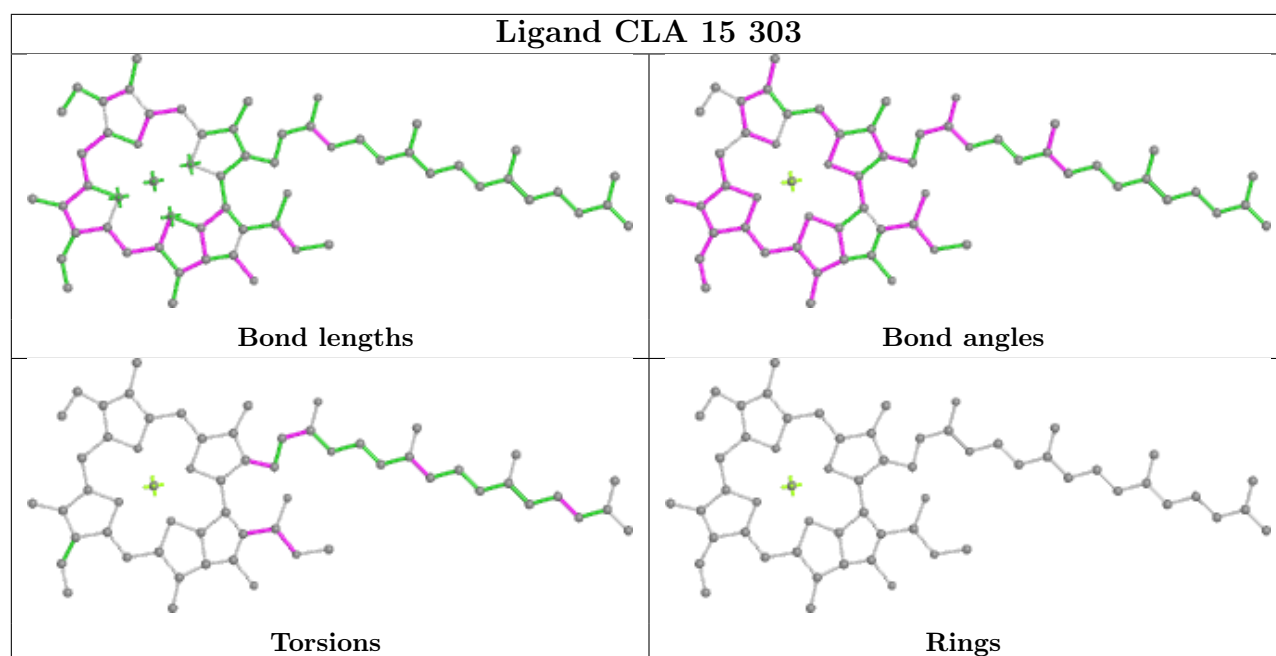
Ligand CLA 6 312

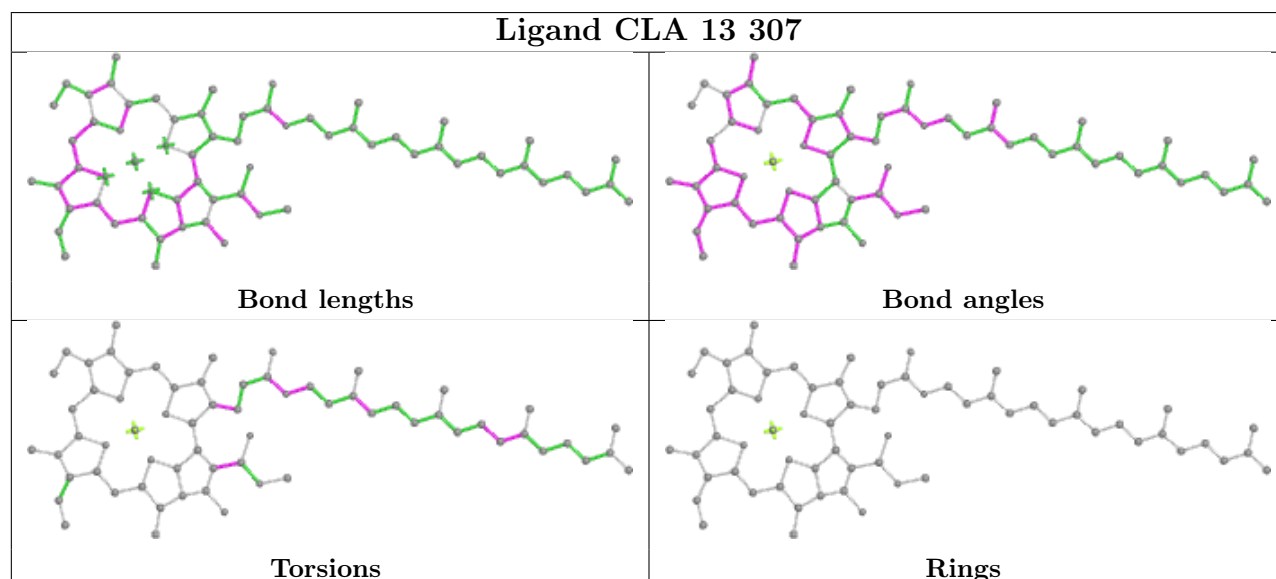
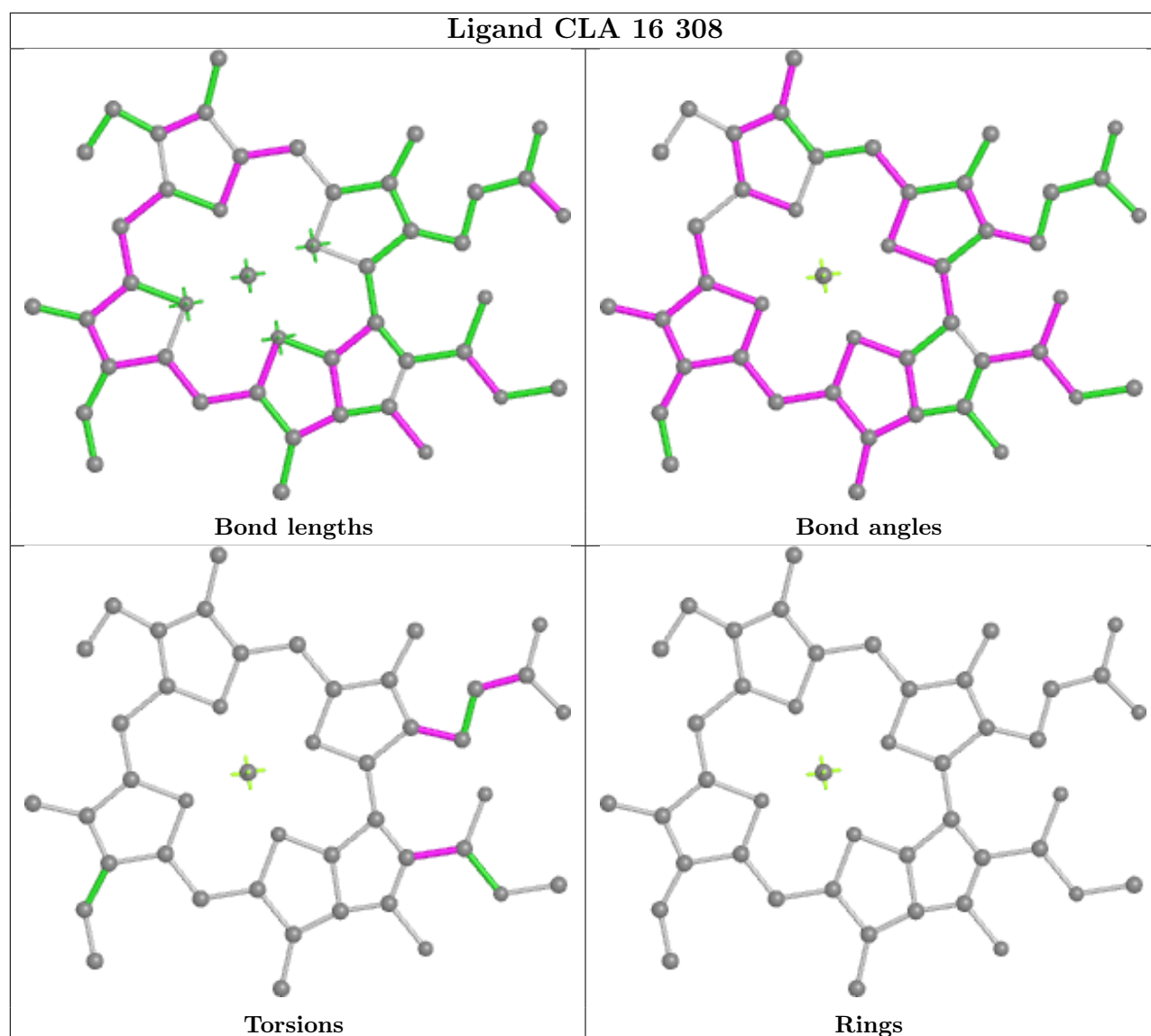


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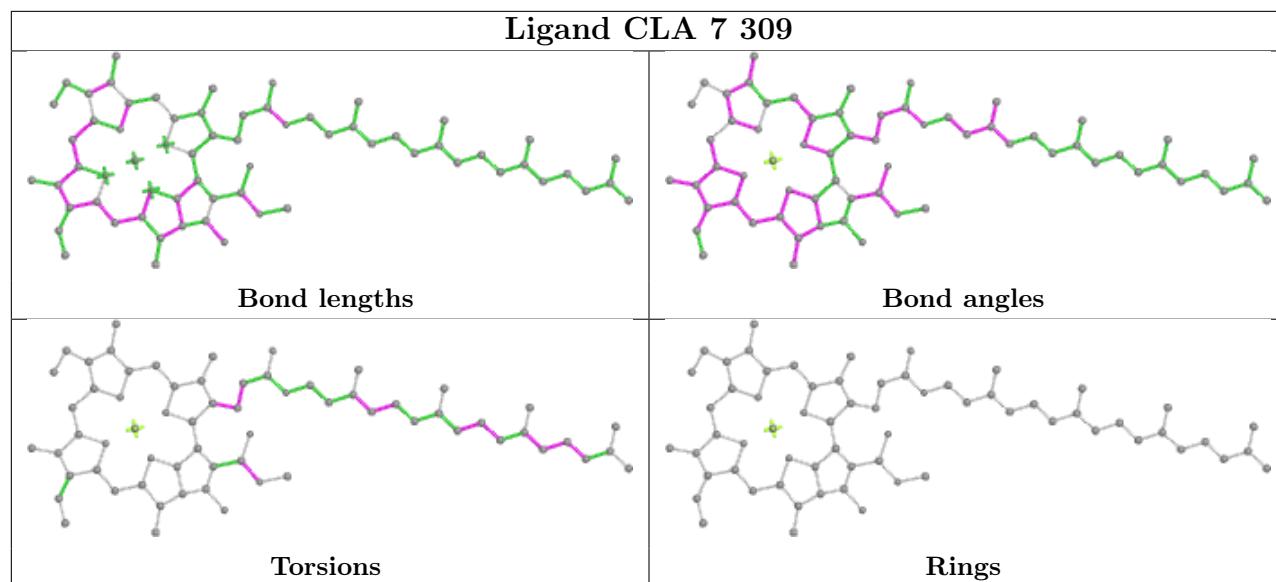


Ligand A86 7 315**Ligand CLA 8 309**

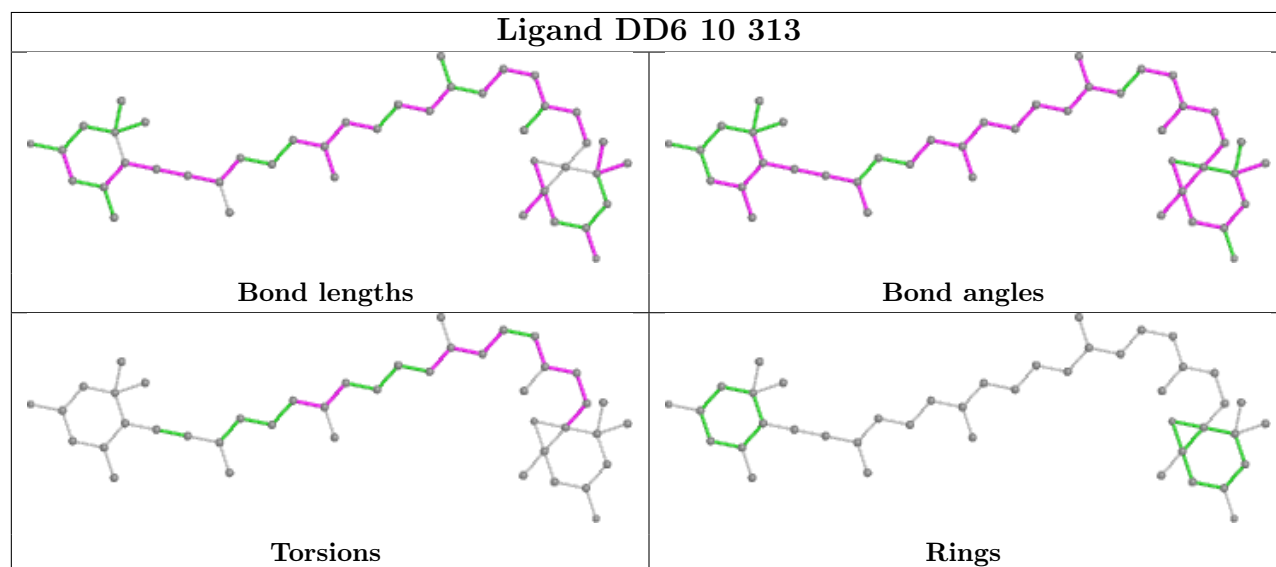




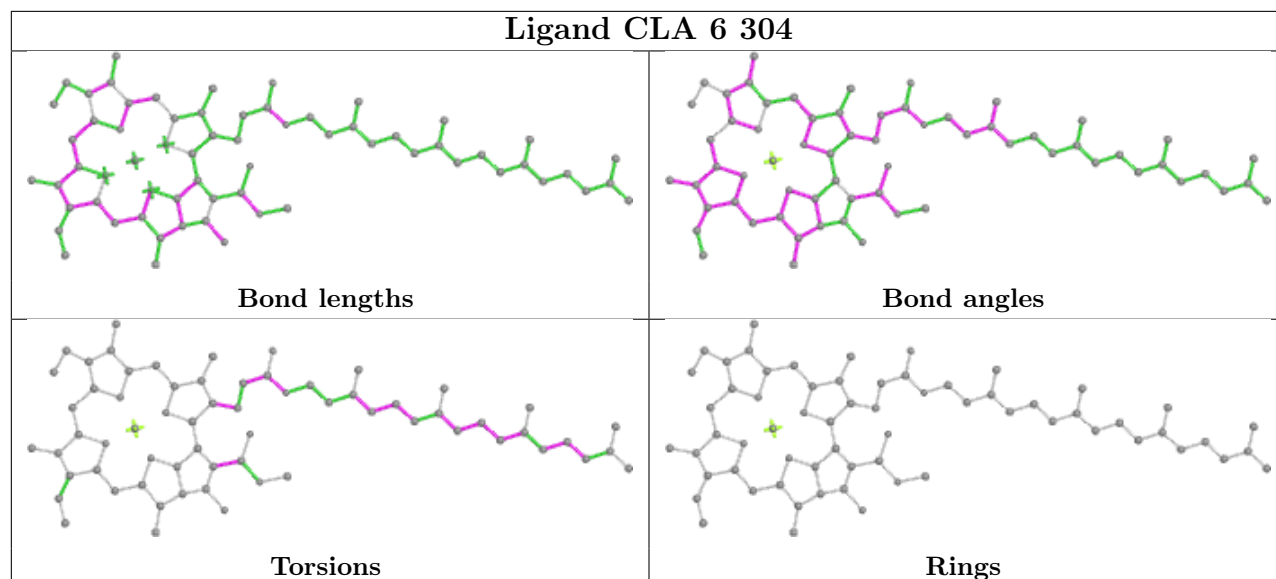
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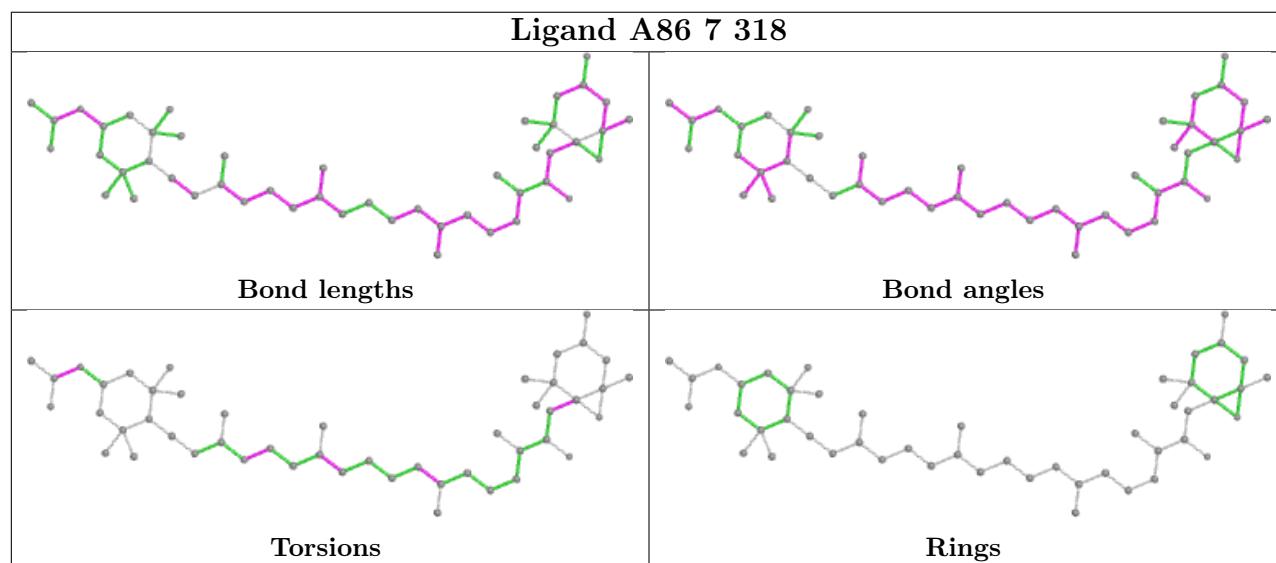
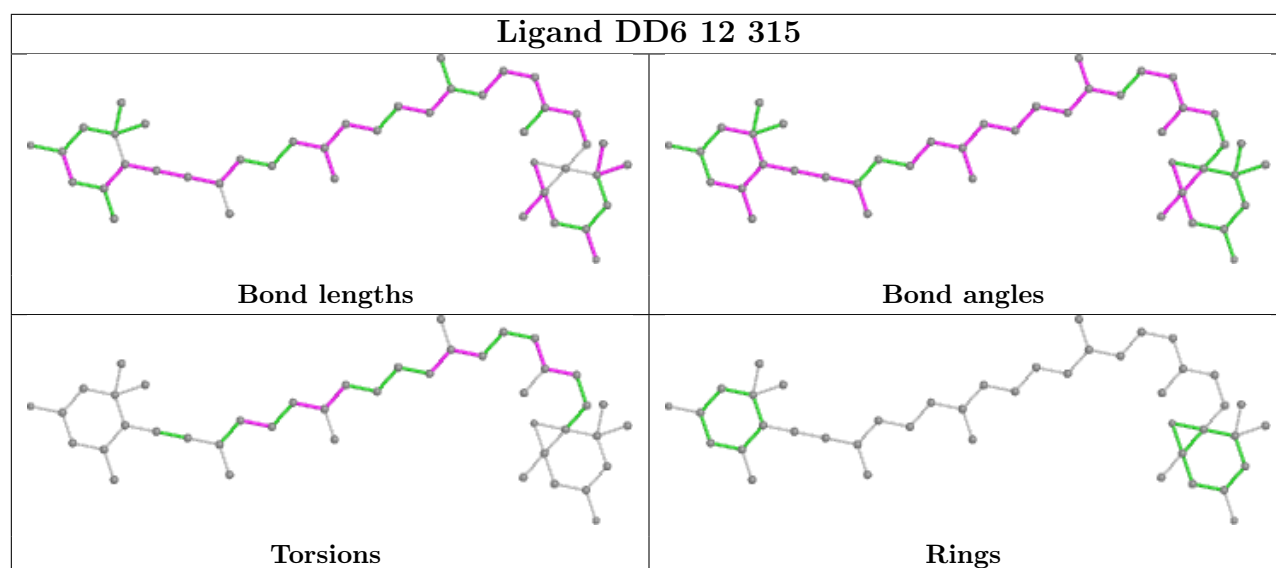


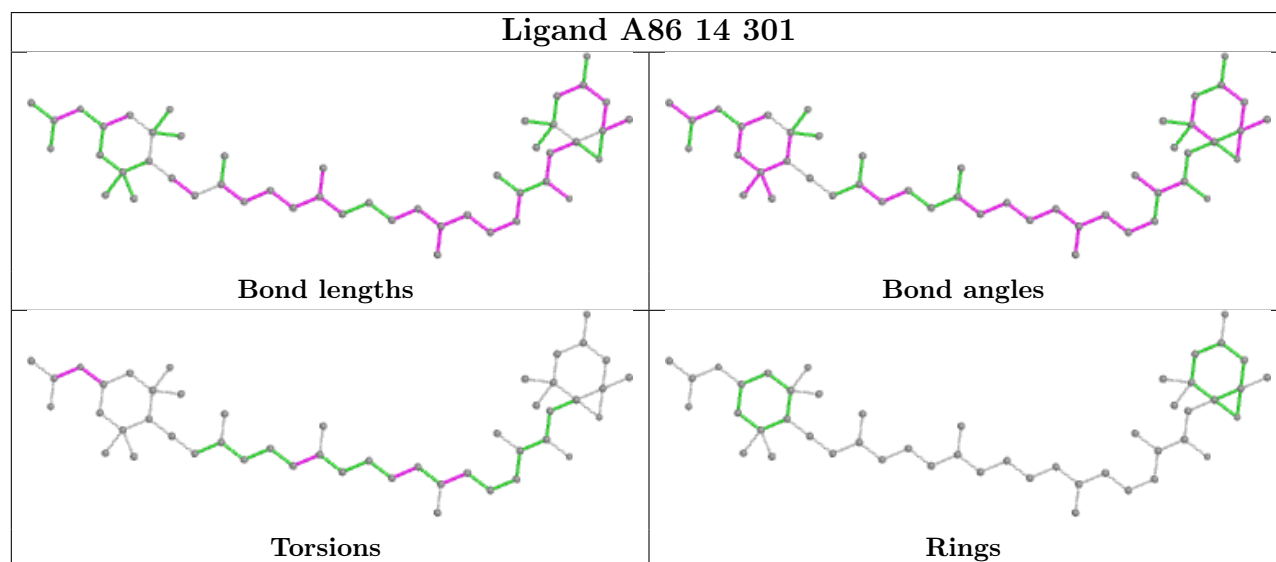
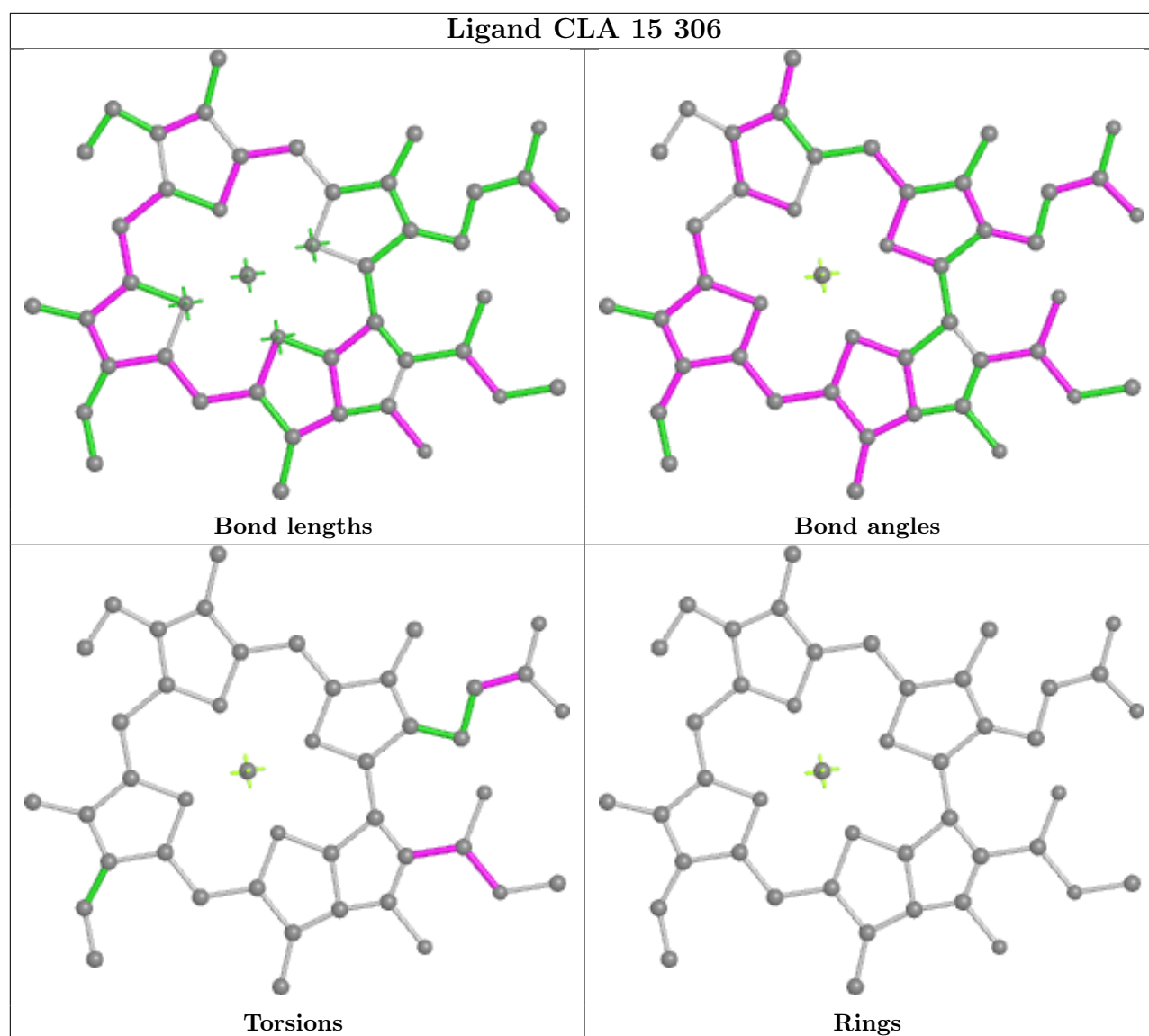
Ligand DD6 10 313

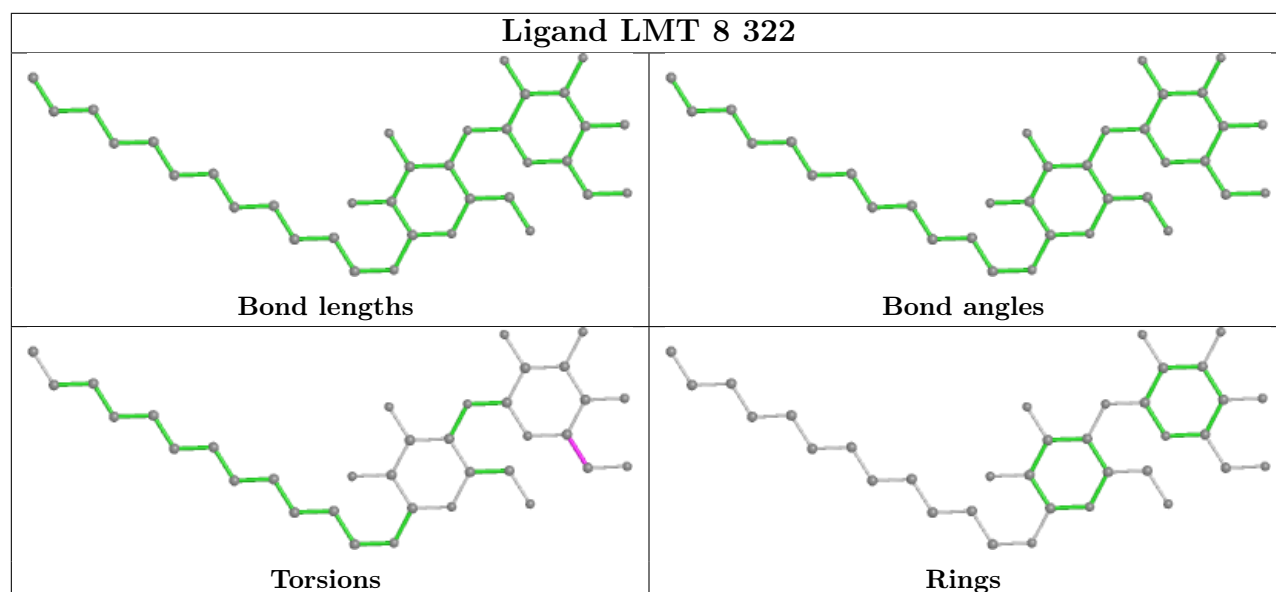
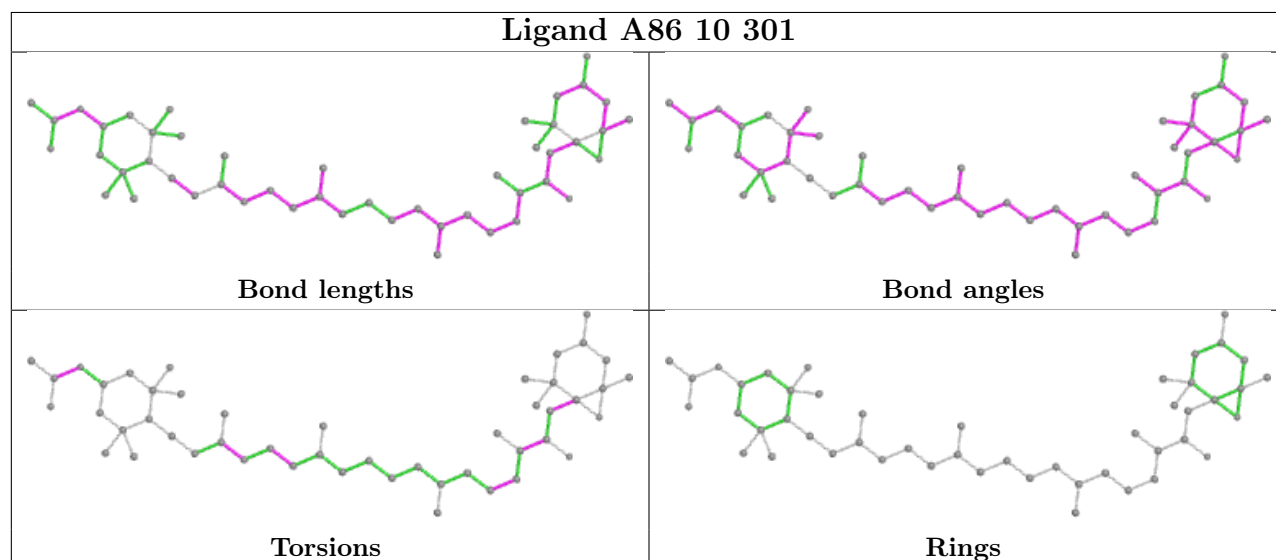
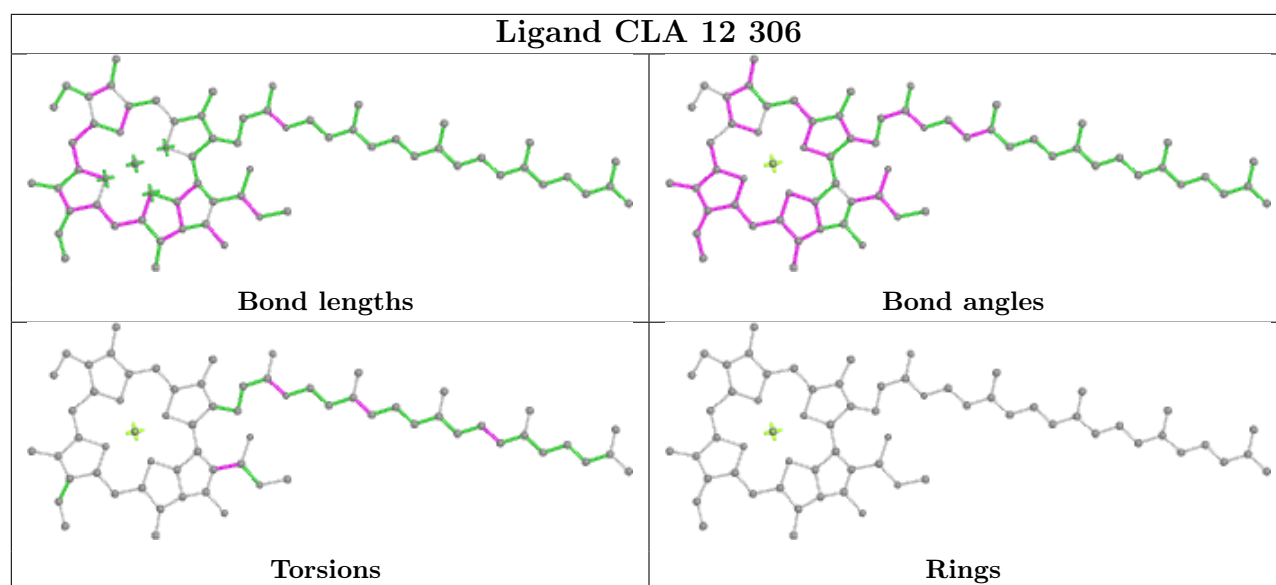


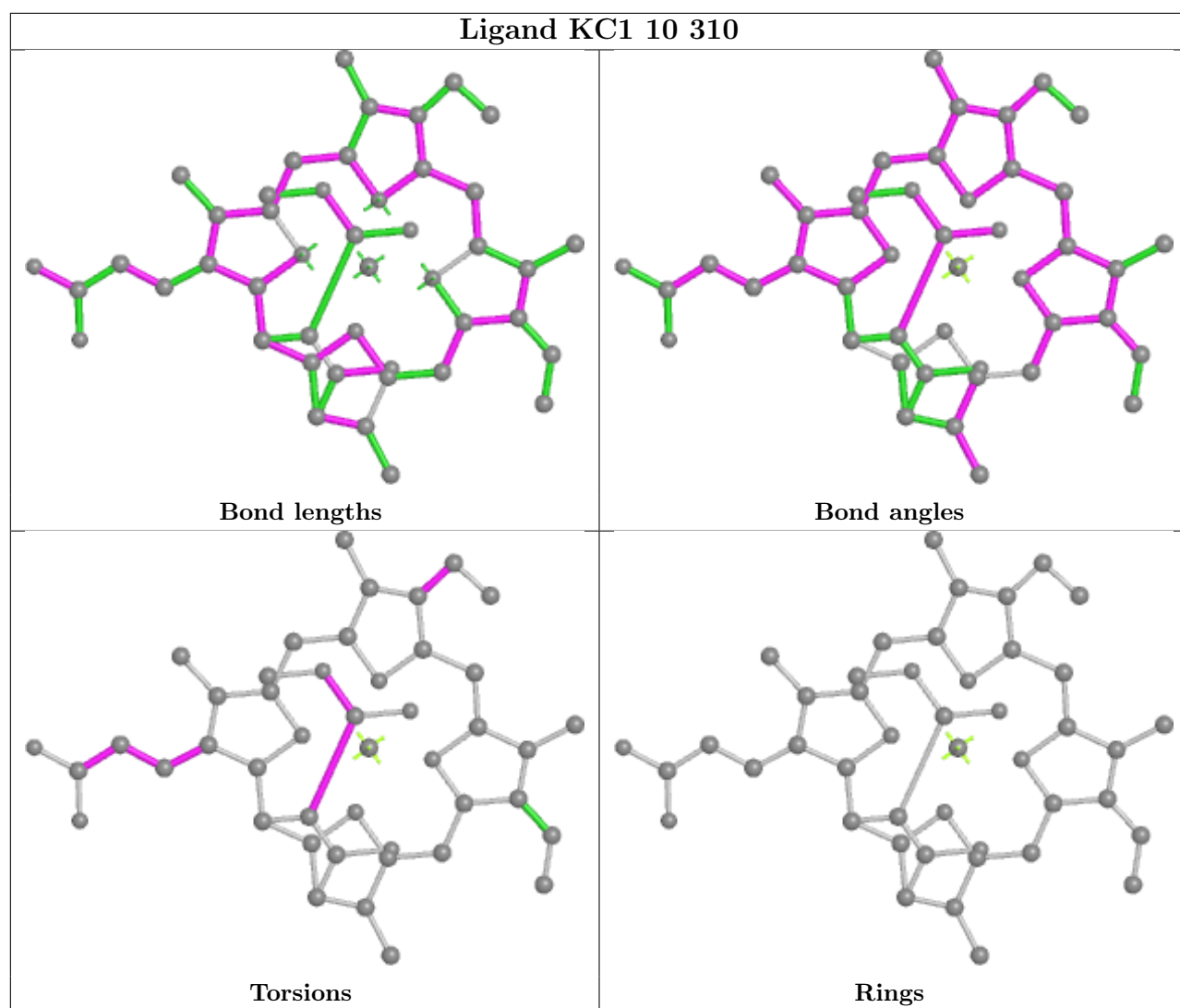
Ligand CLA 6 304

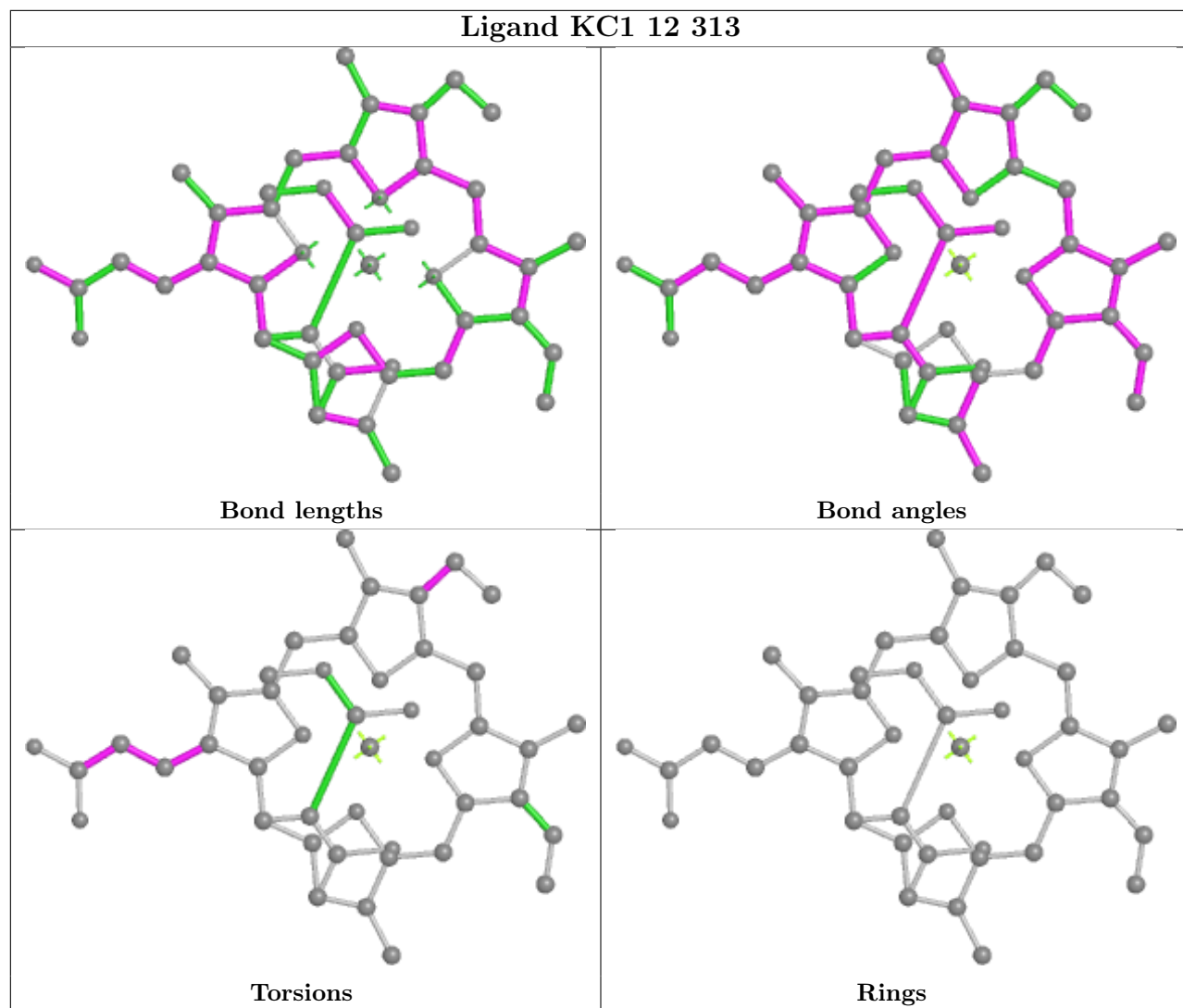




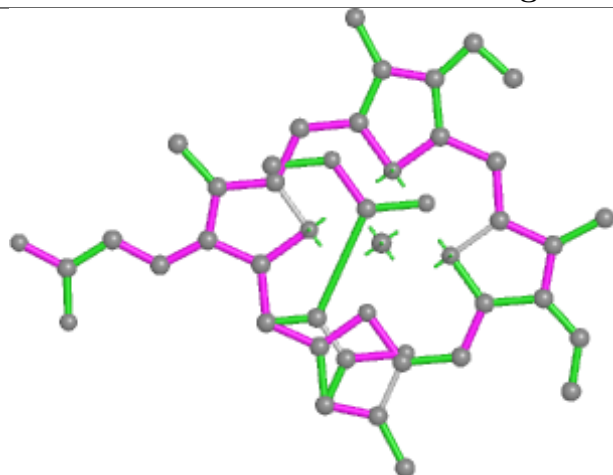




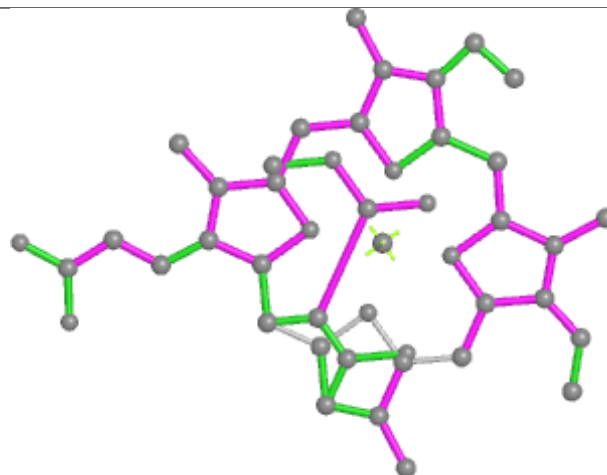




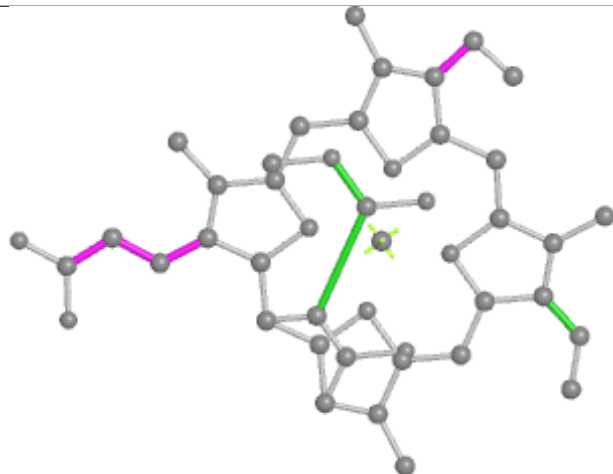
Ligand KC1 6 305



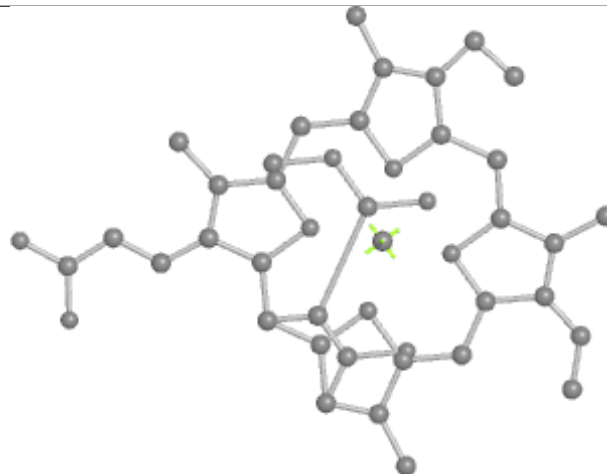
Bond lengths



Bond angles

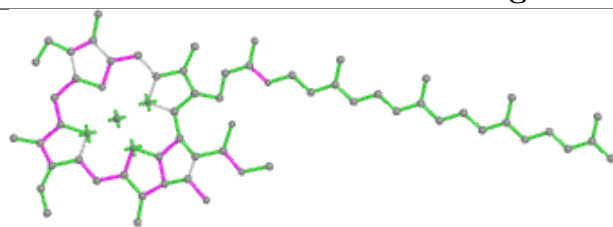


Torsions

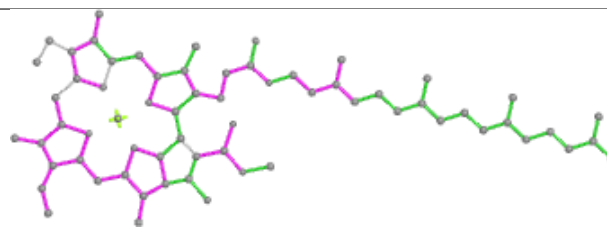


Rings

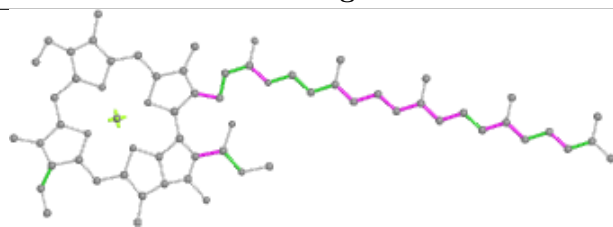
Ligand CLA 16 303



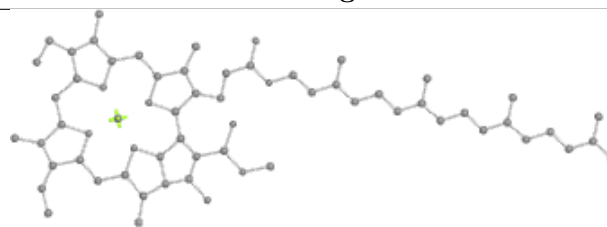
Bond lengths



Bond angles

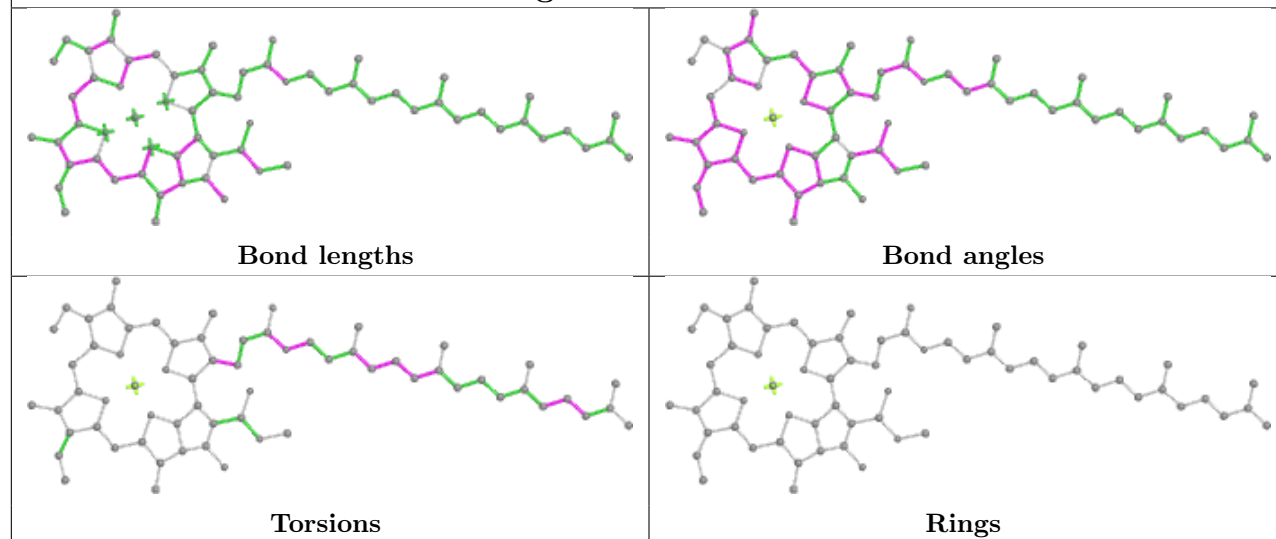


Torsions

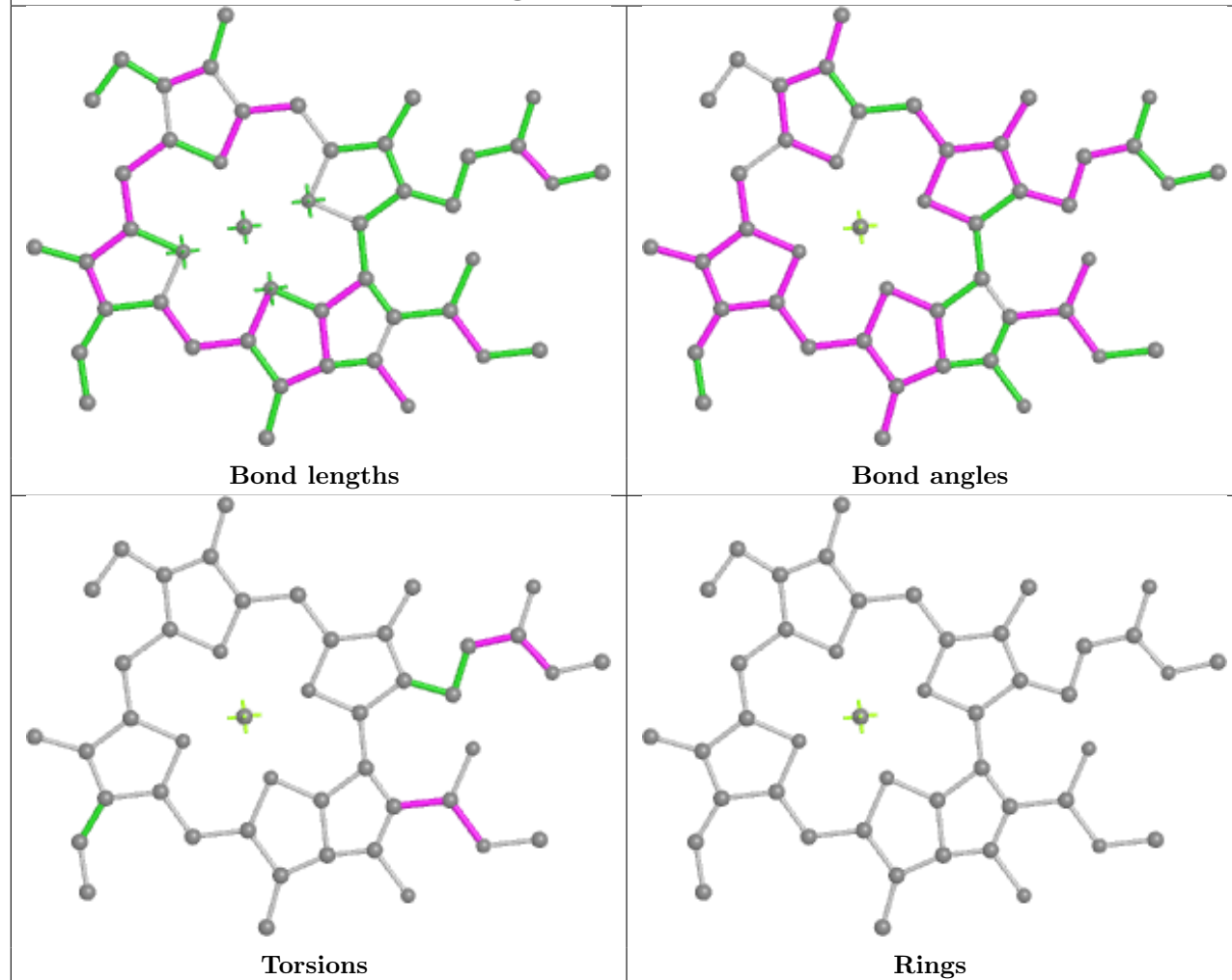


Rings

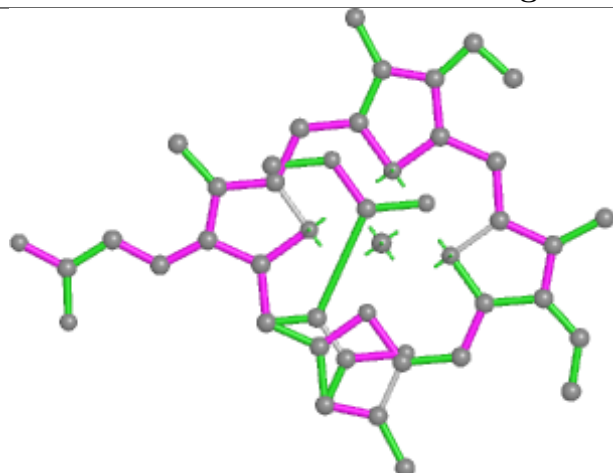
Ligand CLA 7 310



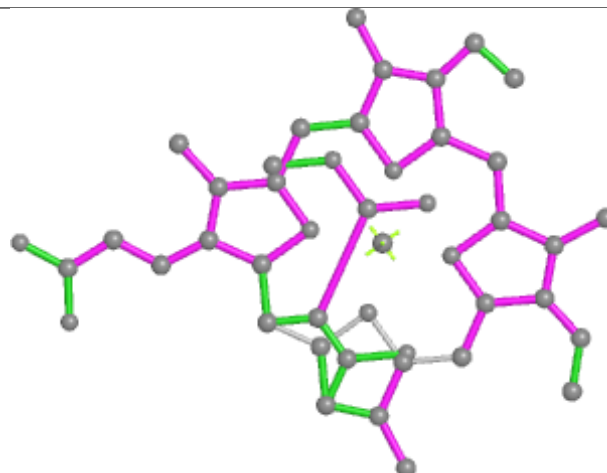
Ligand CLA 12 307



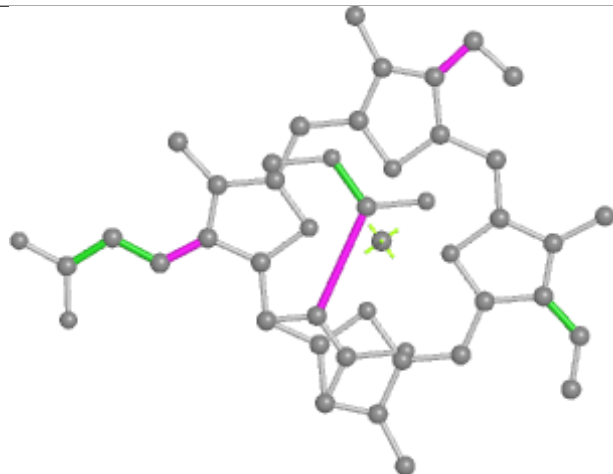
Ligand KC1 6 309



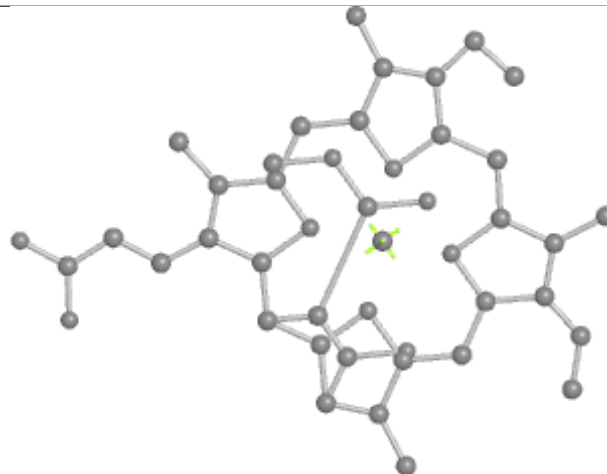
Bond lengths



Bond angles

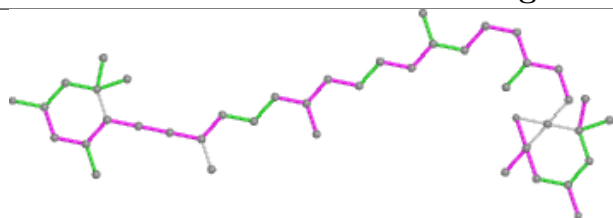


Torsions

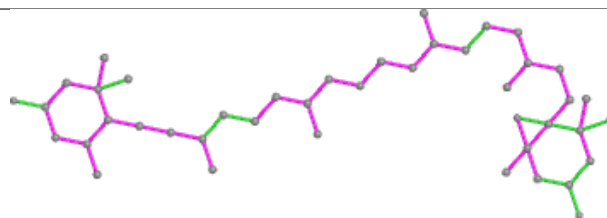


Rings

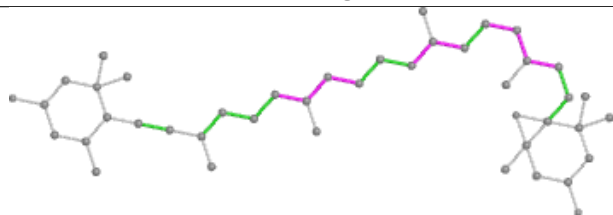
Ligand DD6 6 318



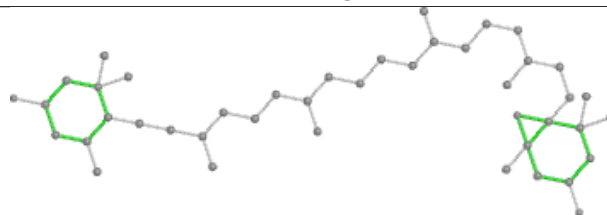
Bond lengths



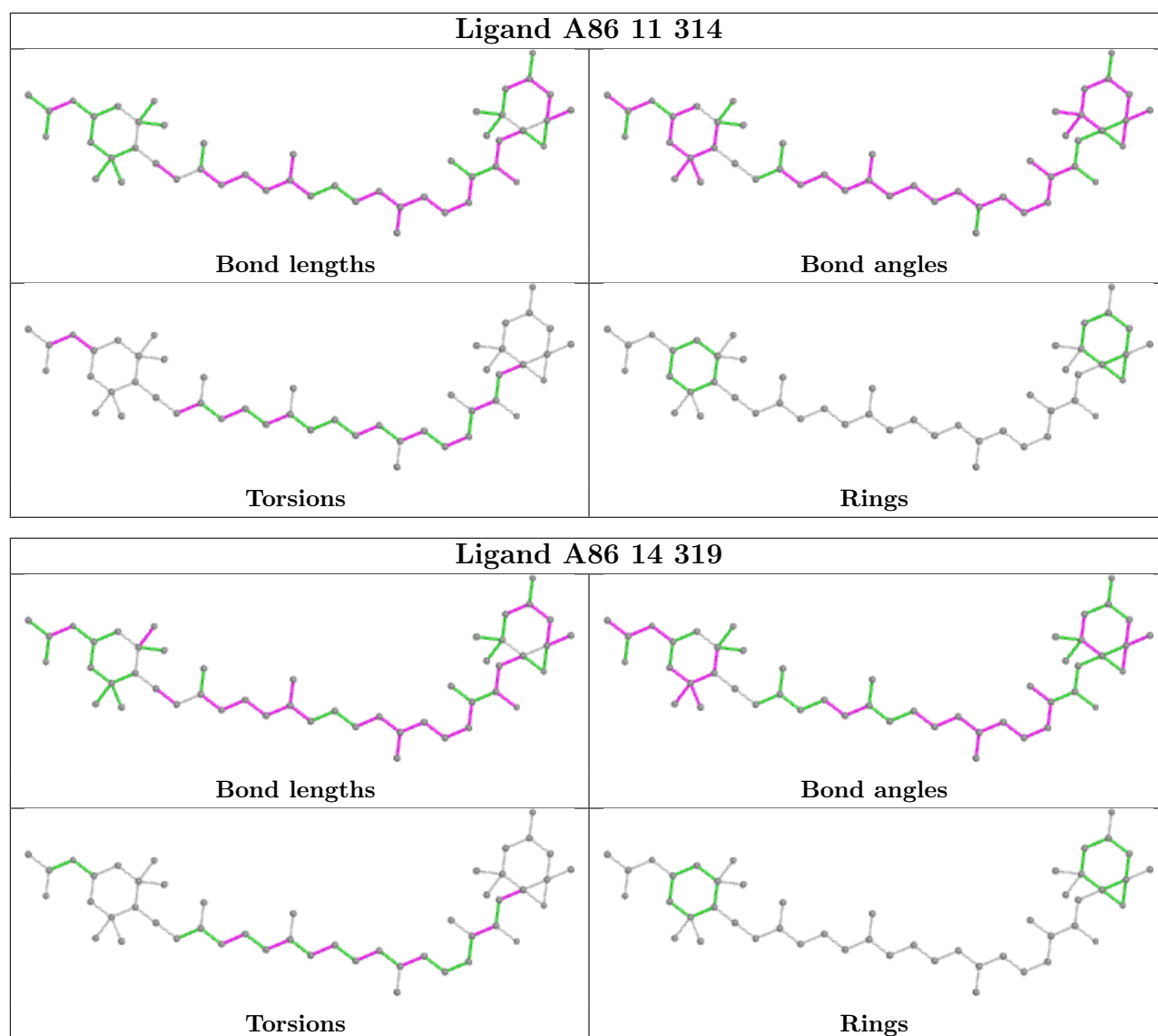
Bond angles

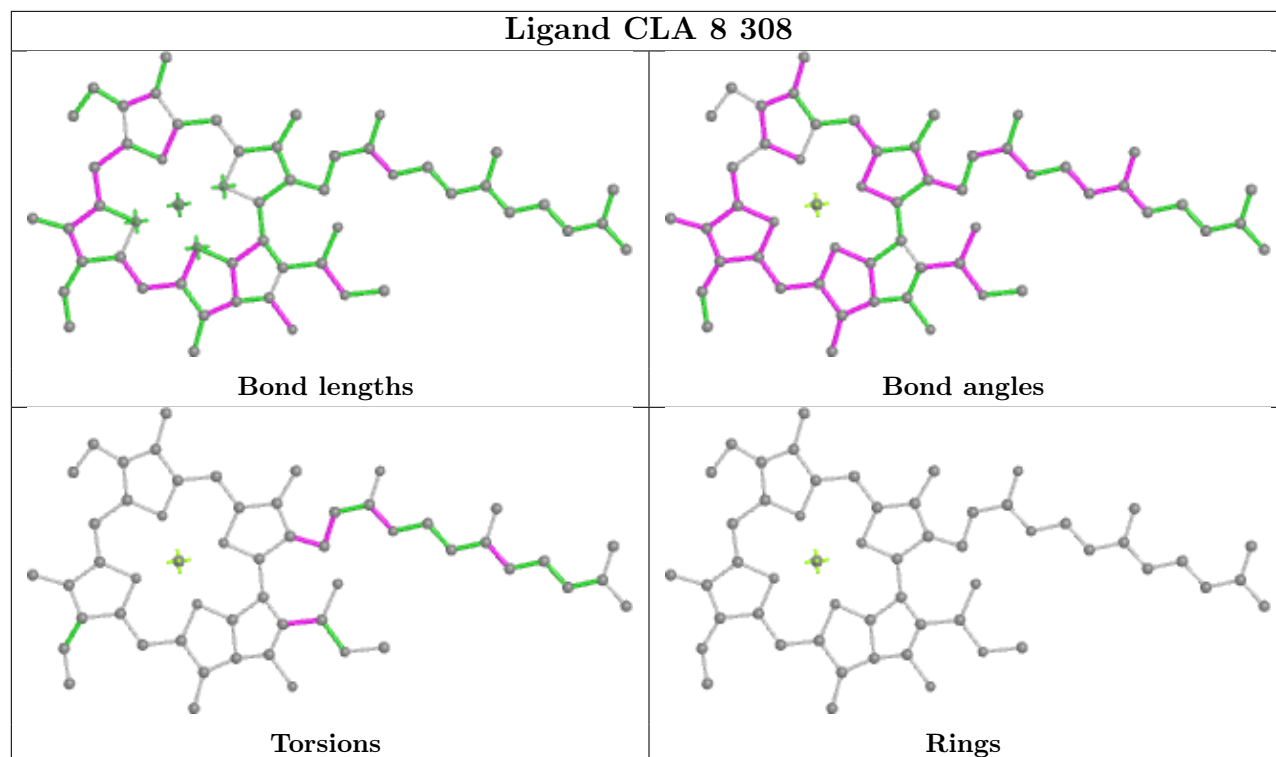
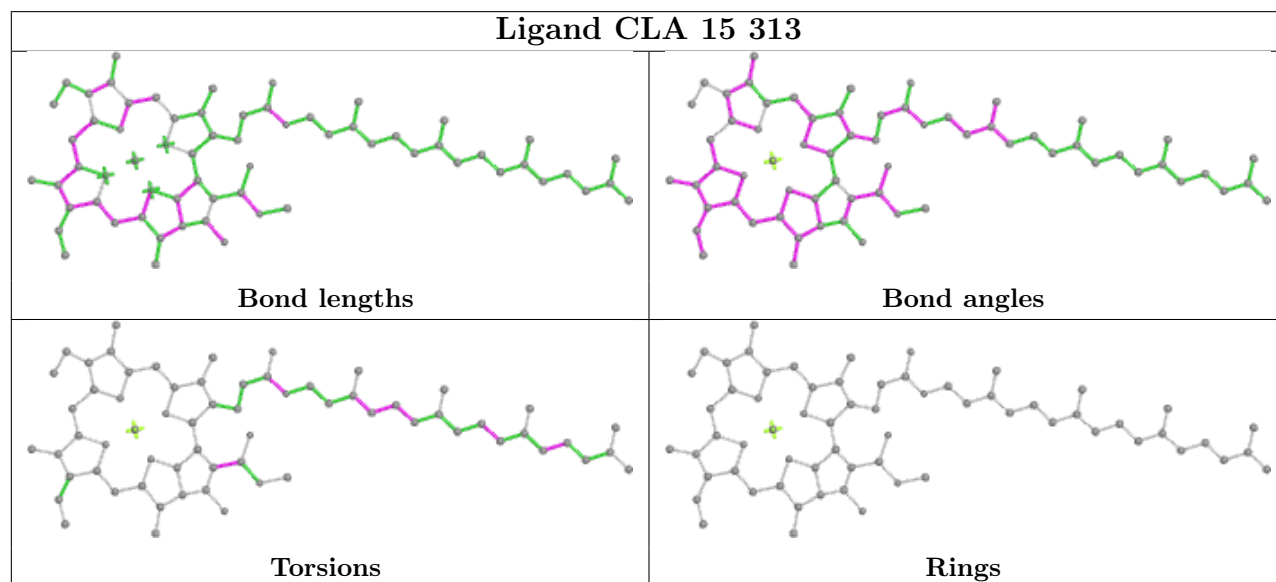


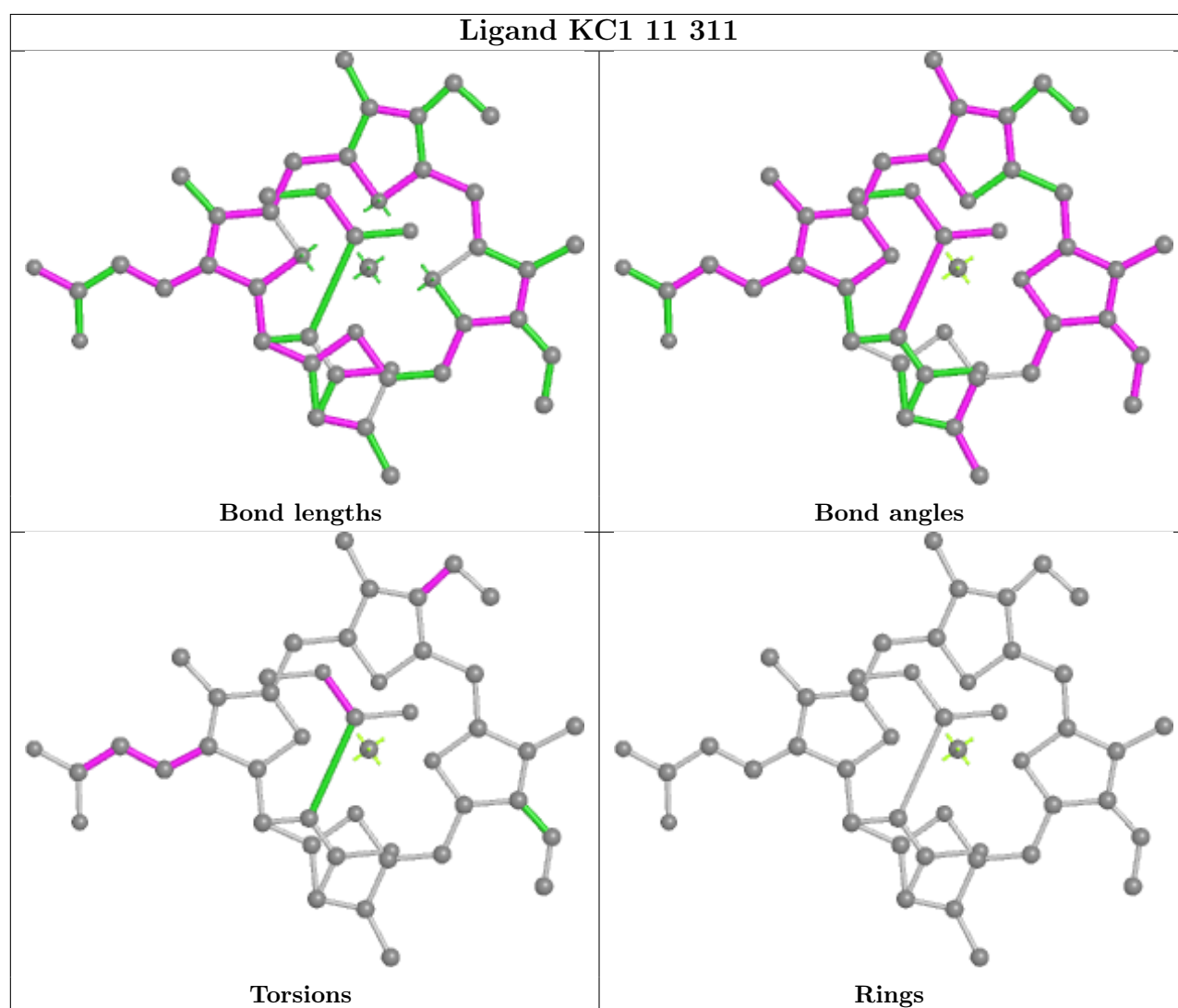
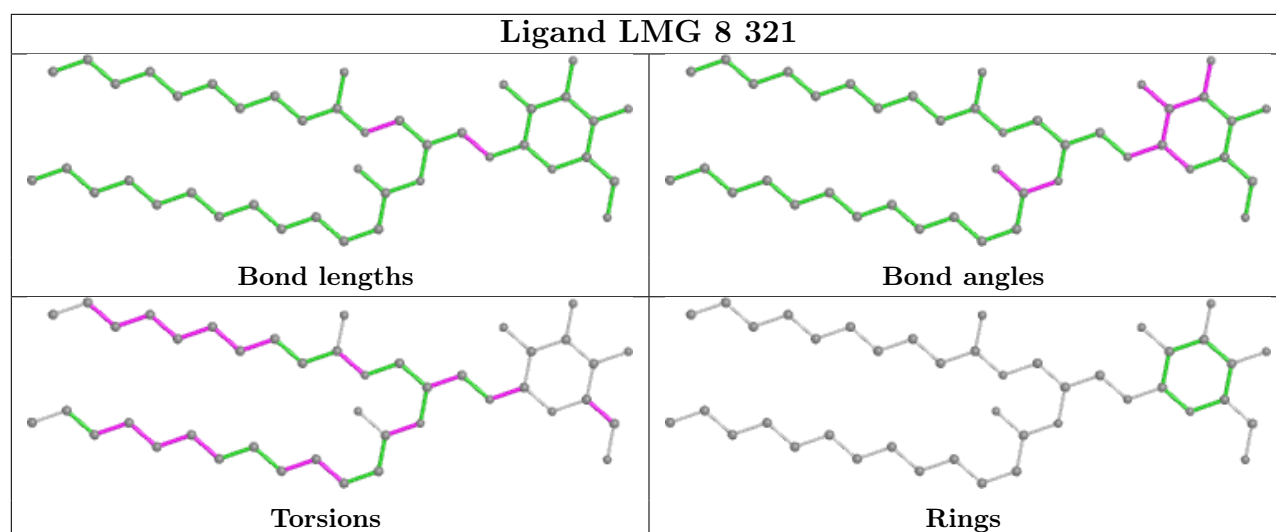
Torsions



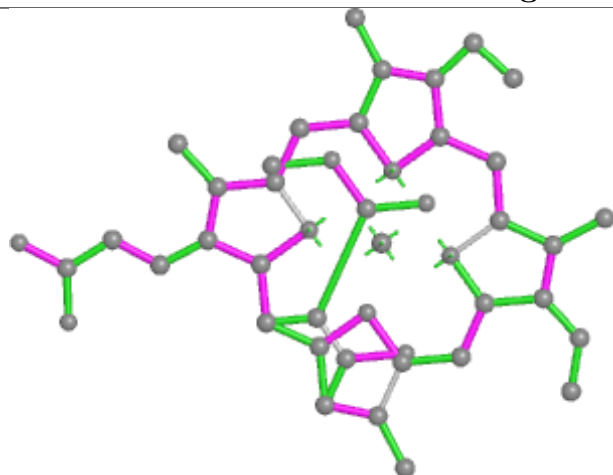
Rings



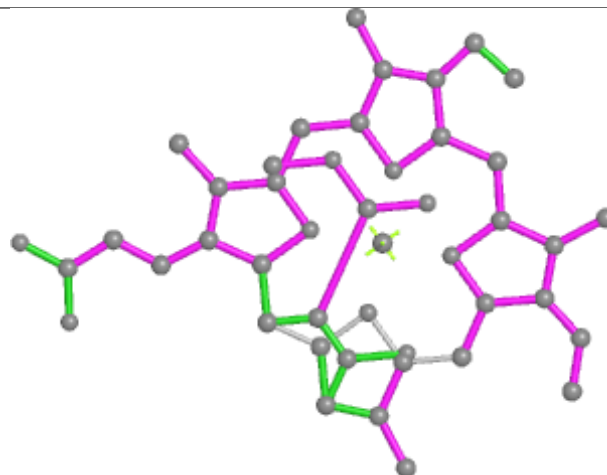
Ligand CLA 8 308**Ligand CLA 15 313**



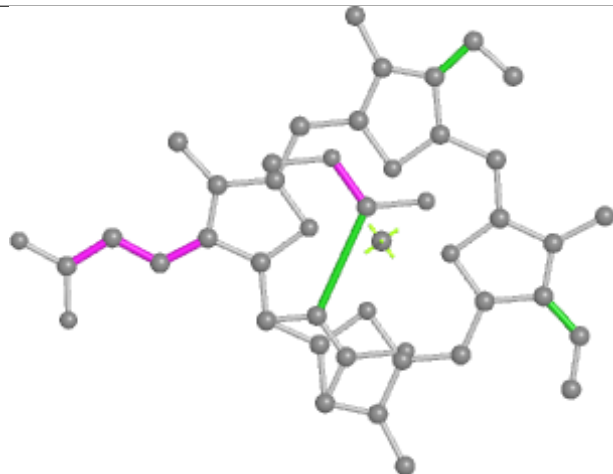
Ligand KC1 8 306



Bond lengths



Bond angles

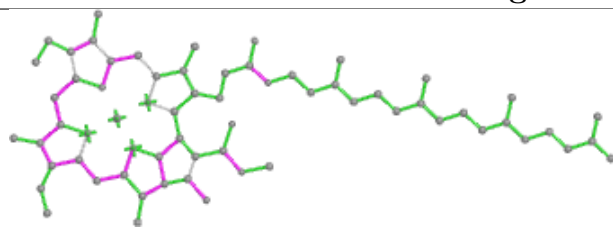


Torsions

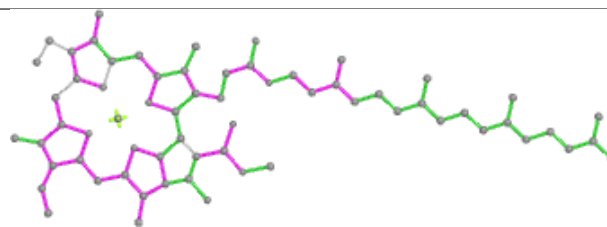


Rings

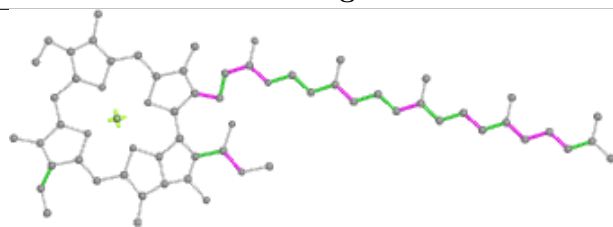
Ligand CLA 11 309



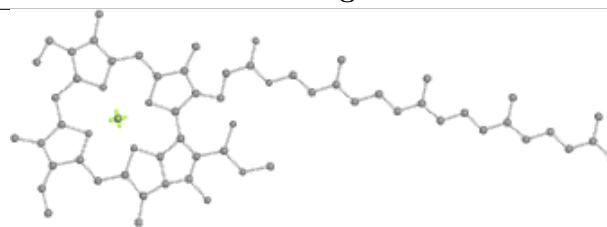
Bond lengths



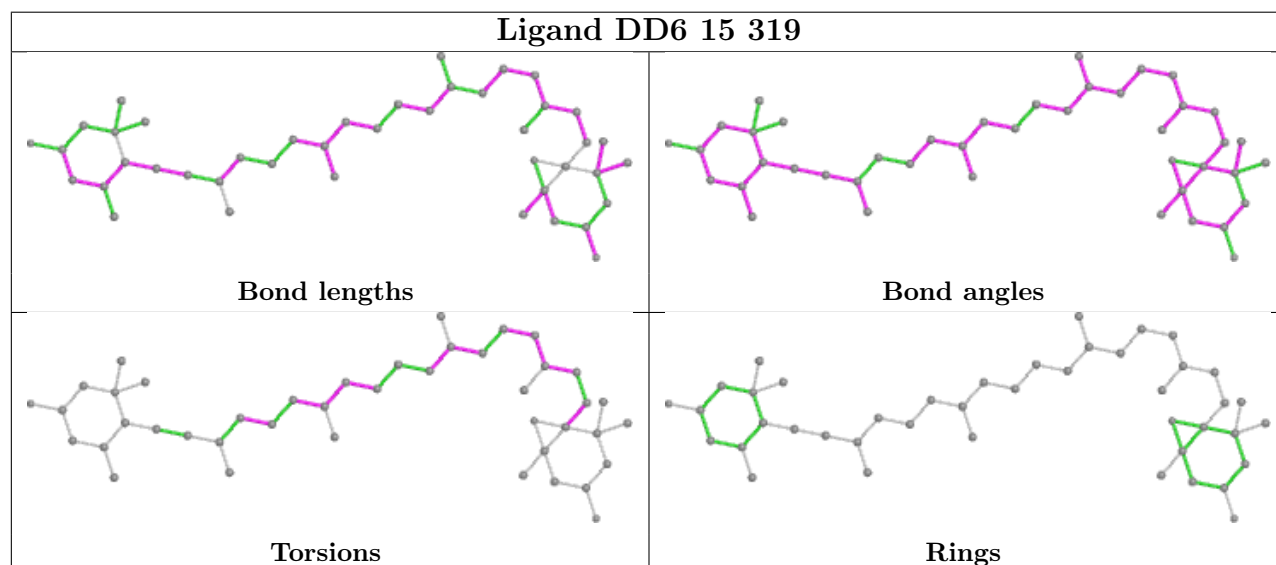
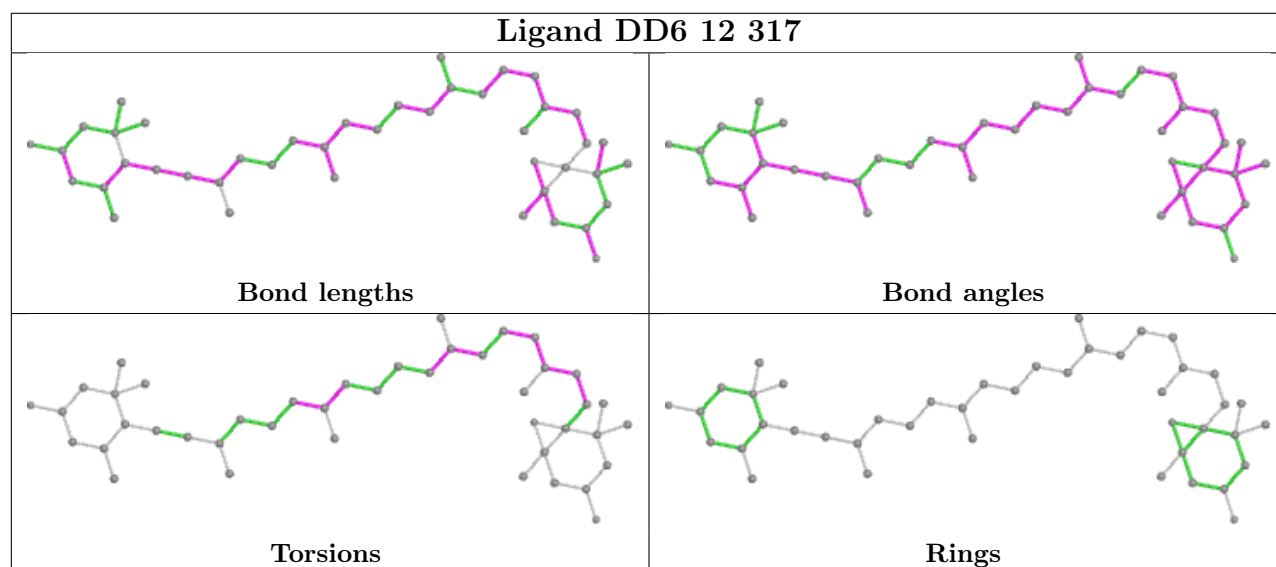
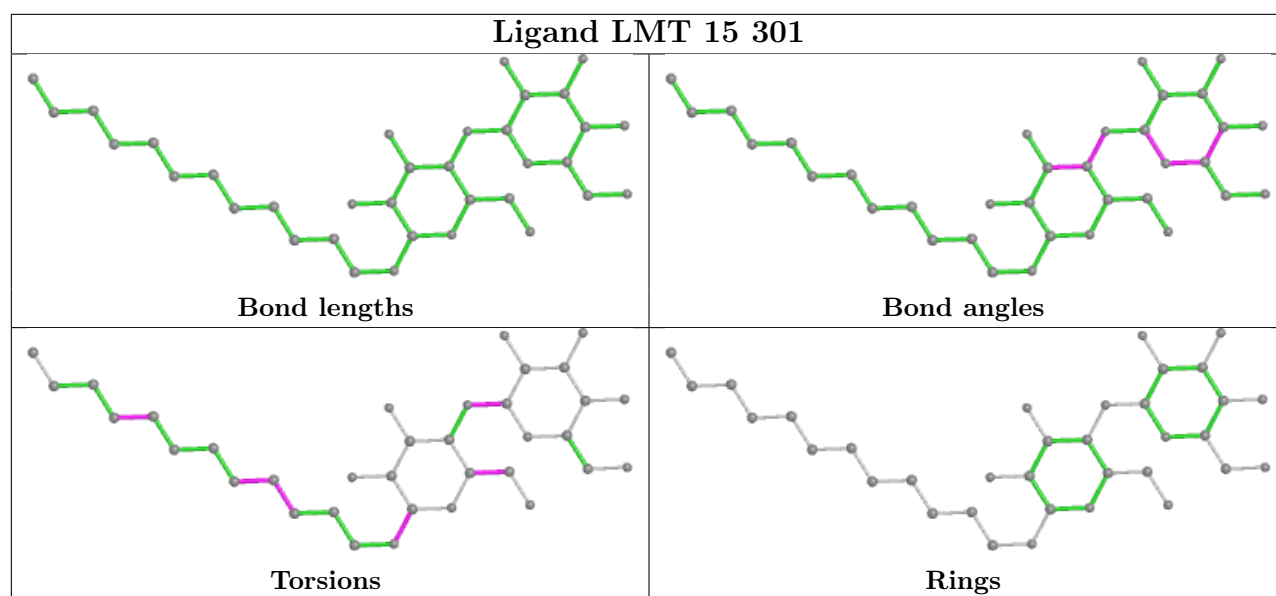
Bond angles

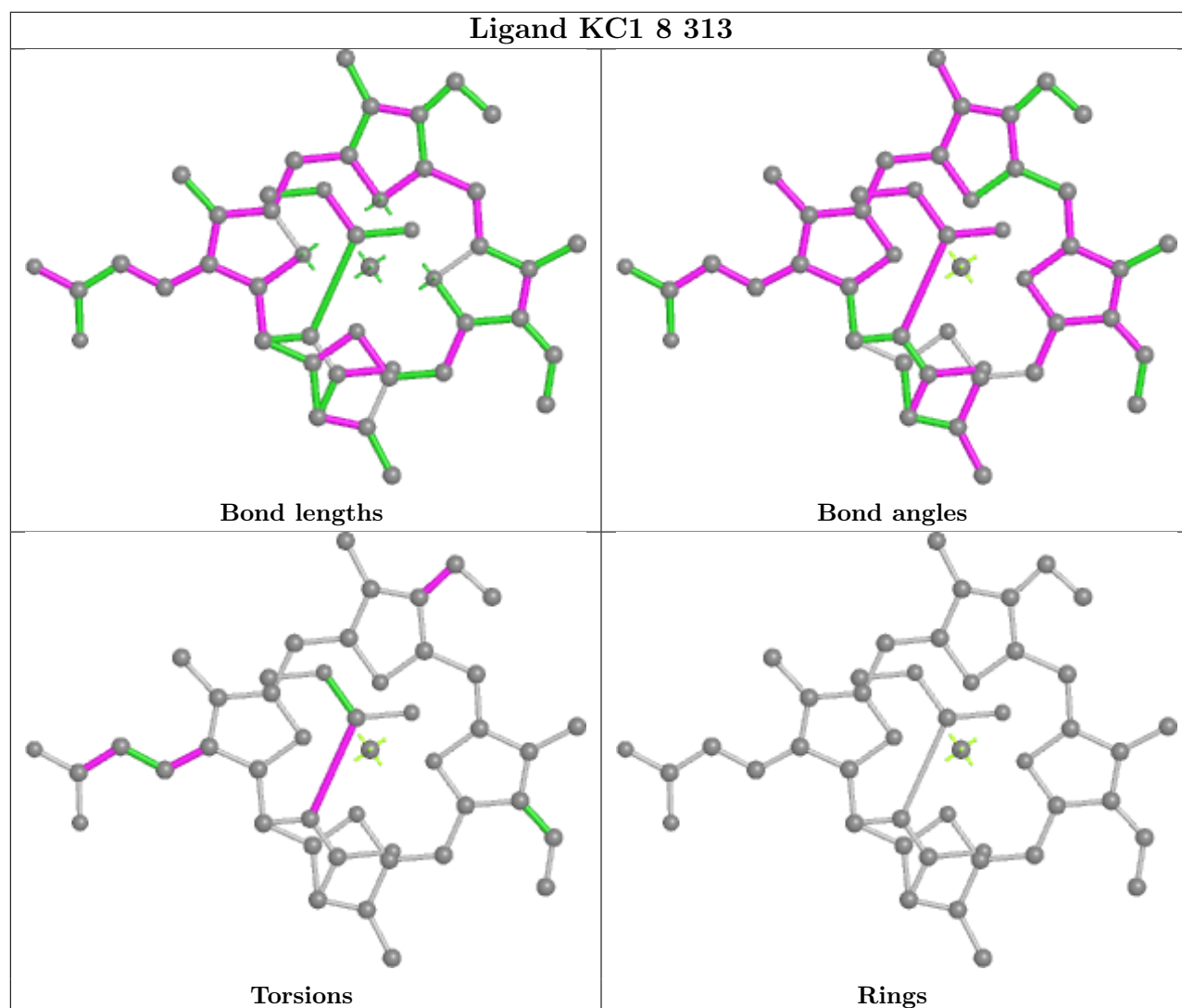
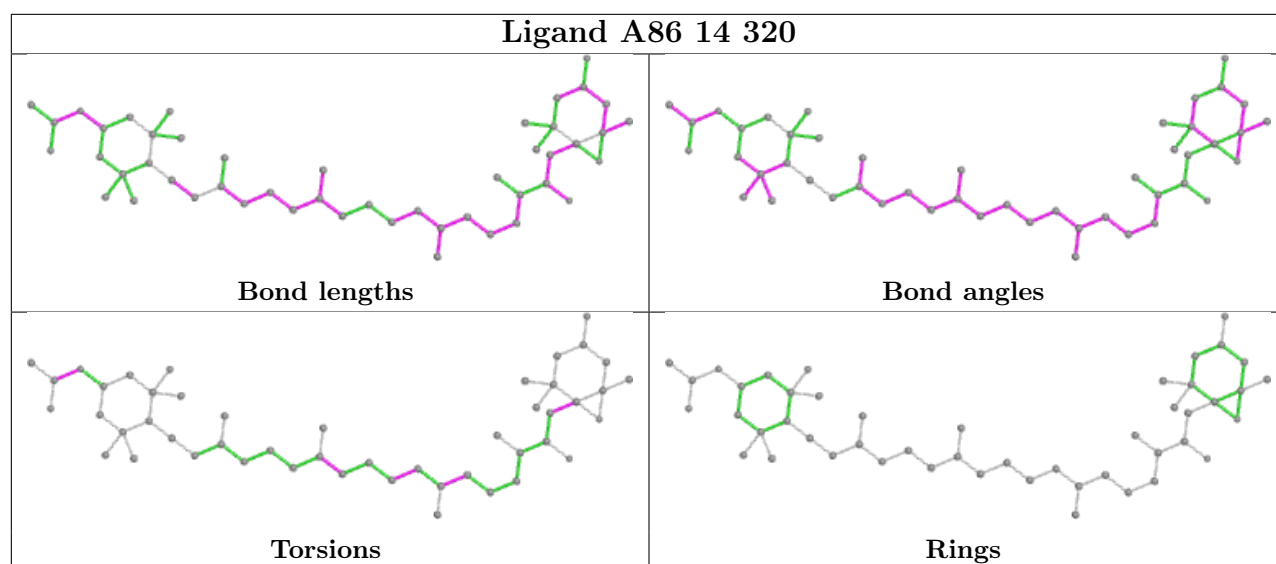


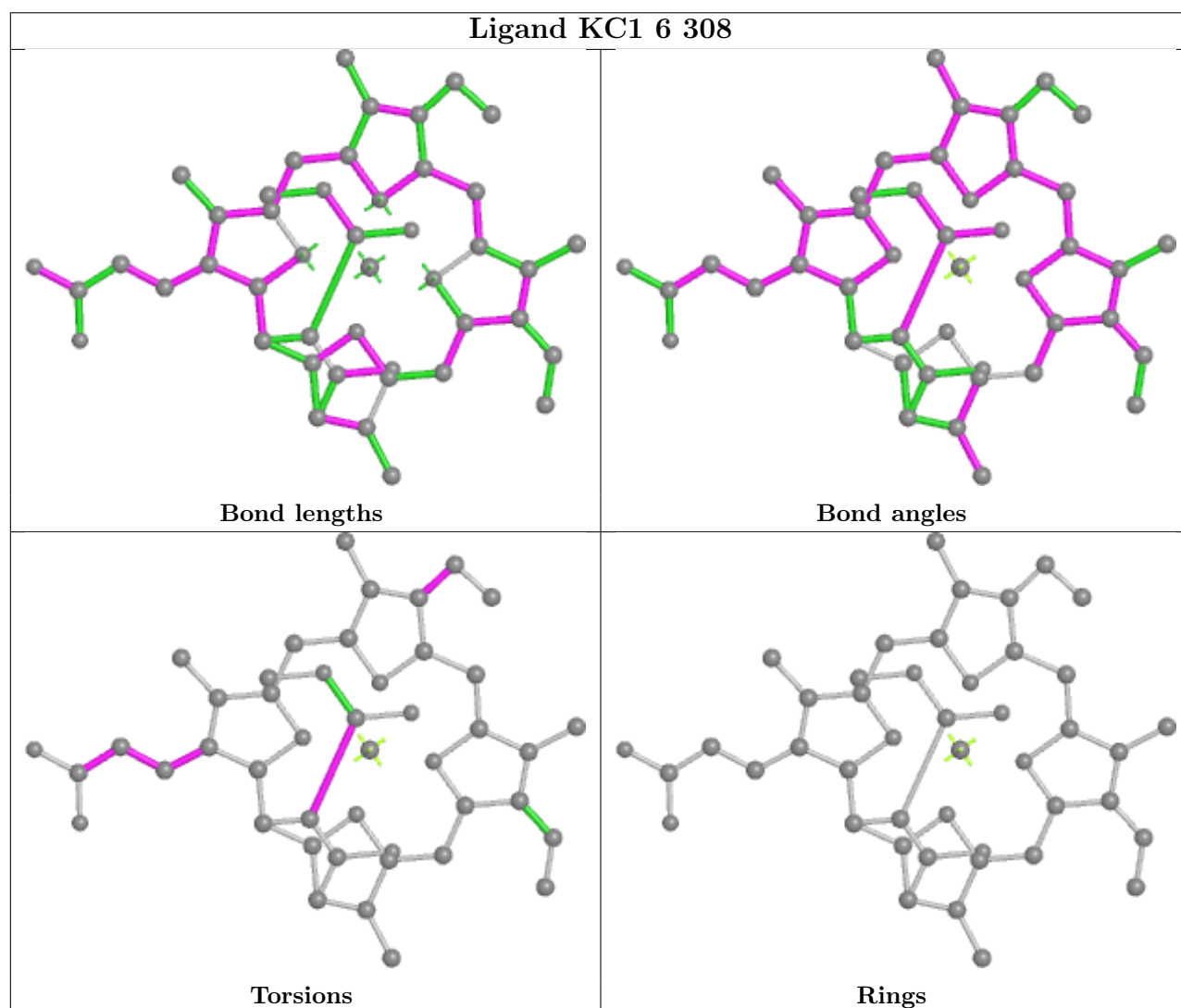
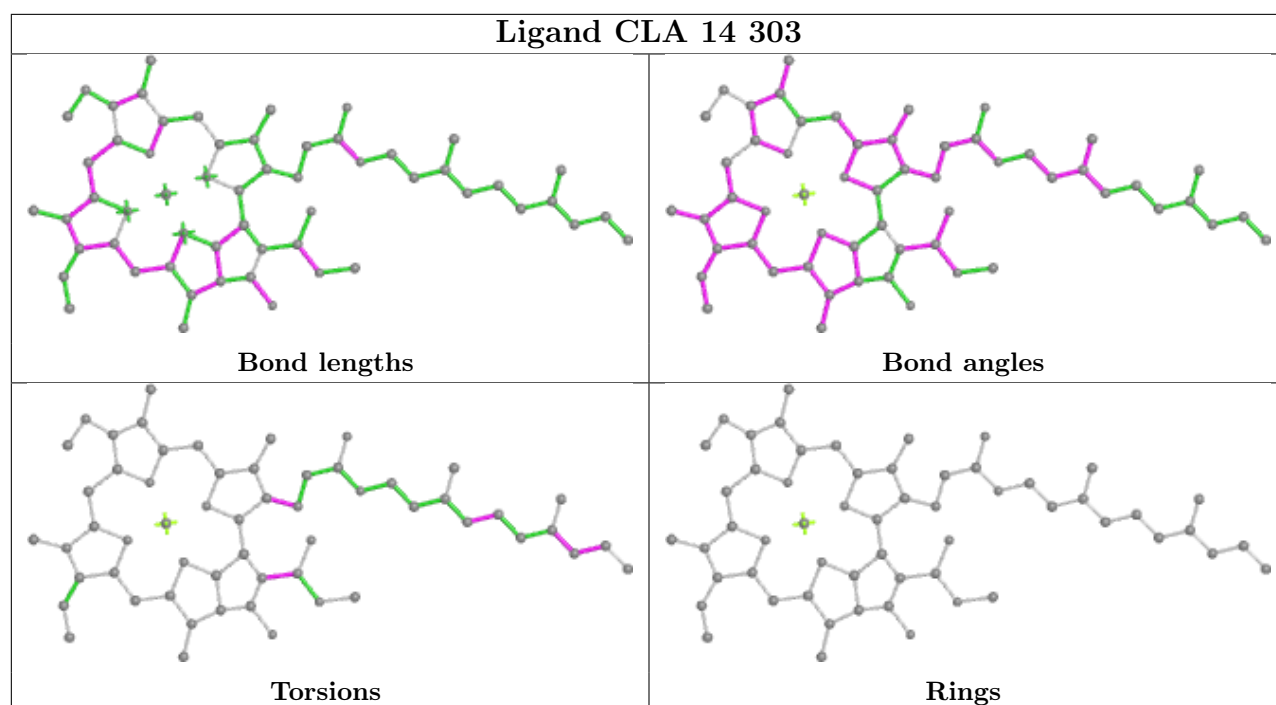
Torsions

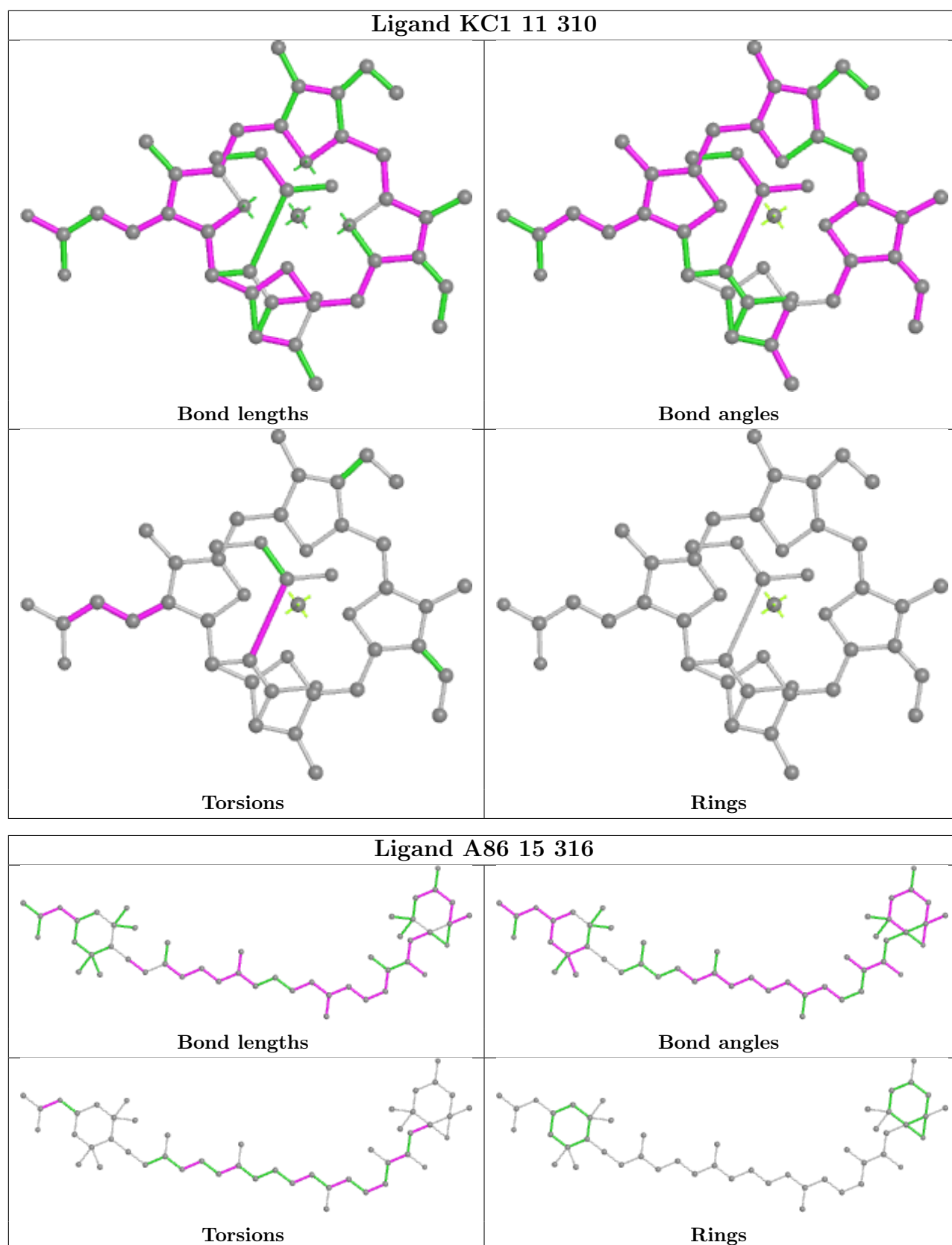


Rings

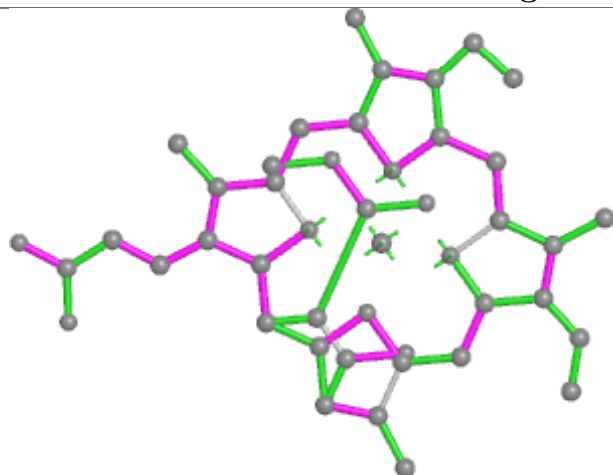




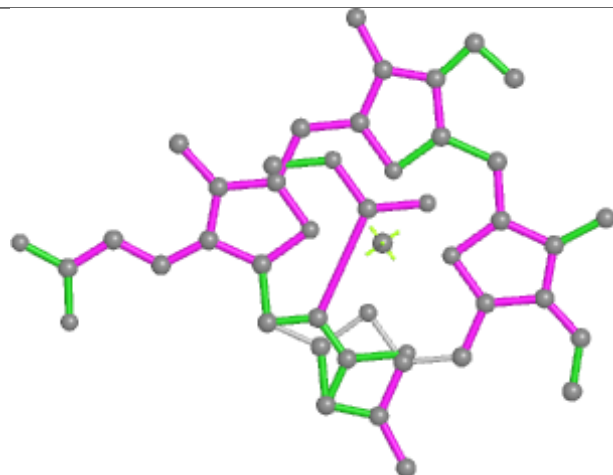




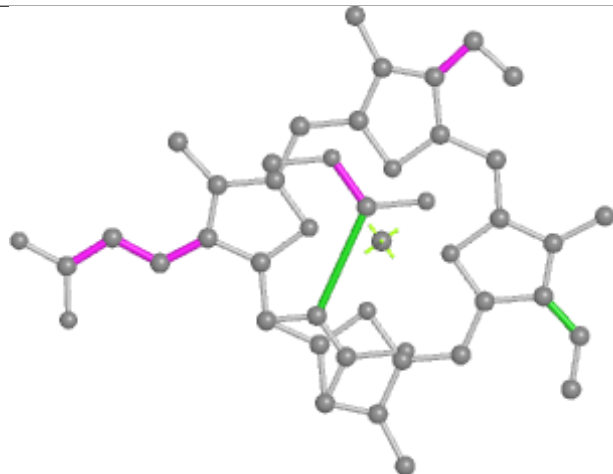
Ligand KC1 7 307



Bond lengths



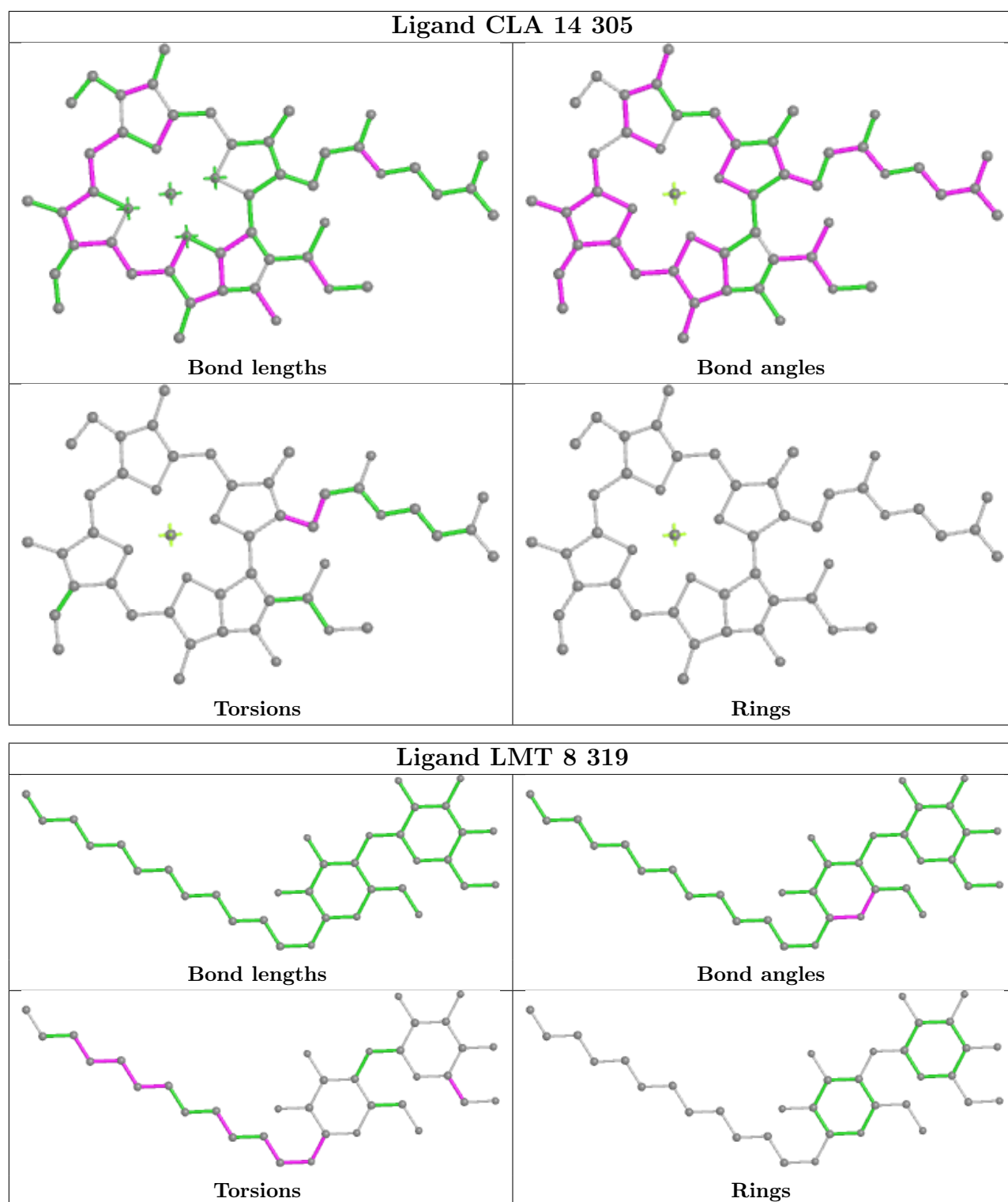
Bond angles

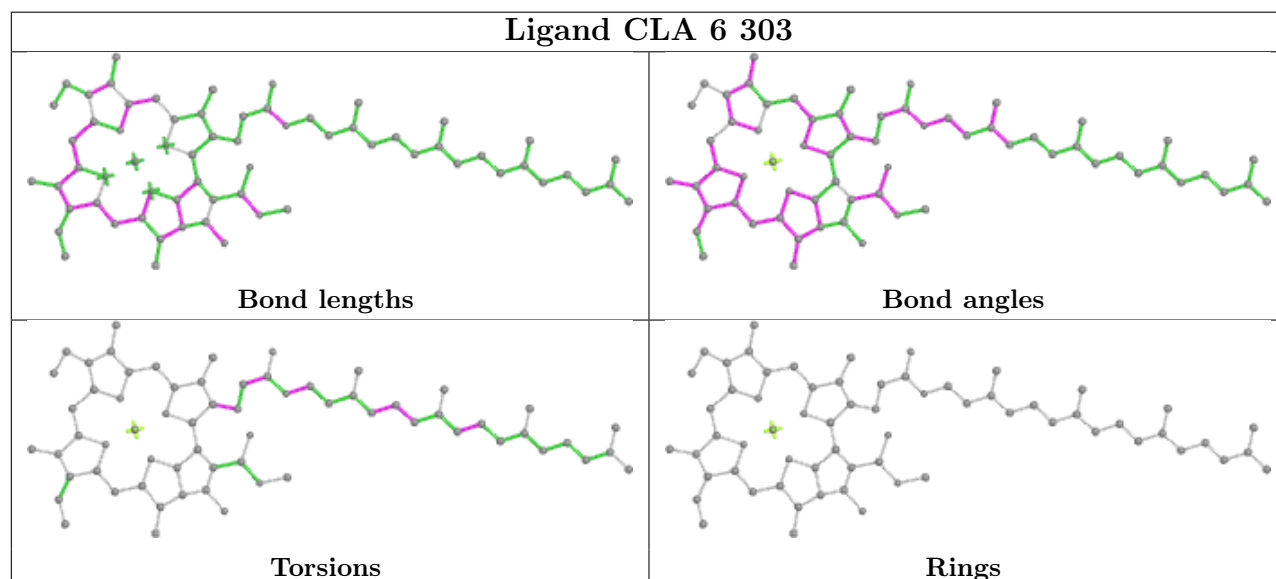
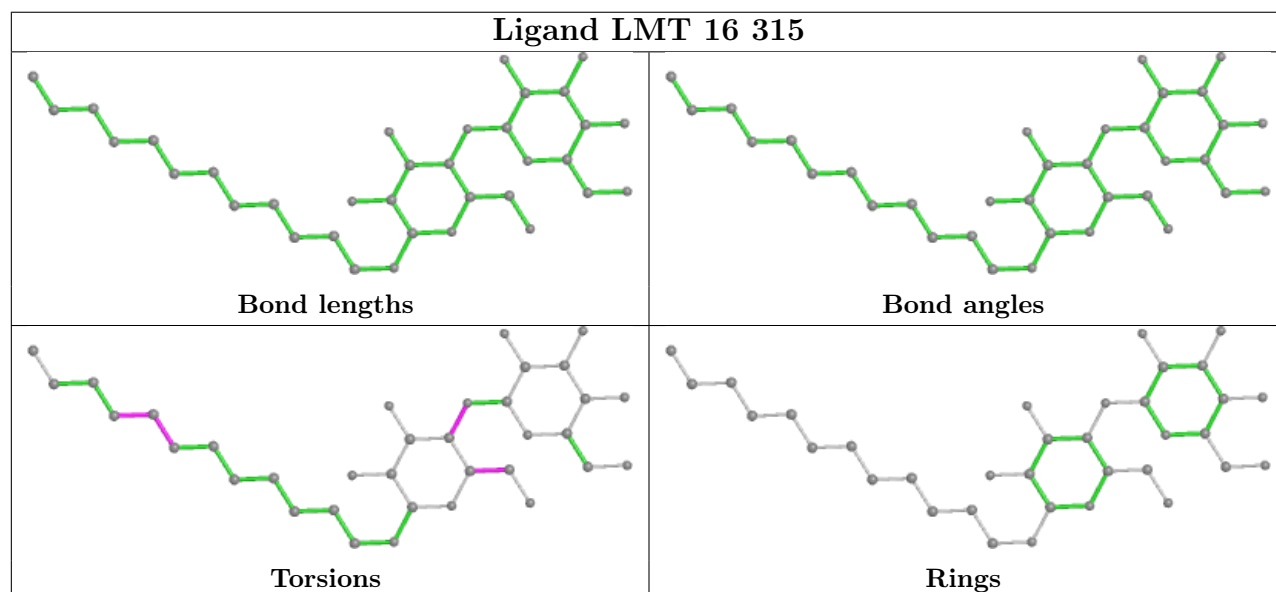
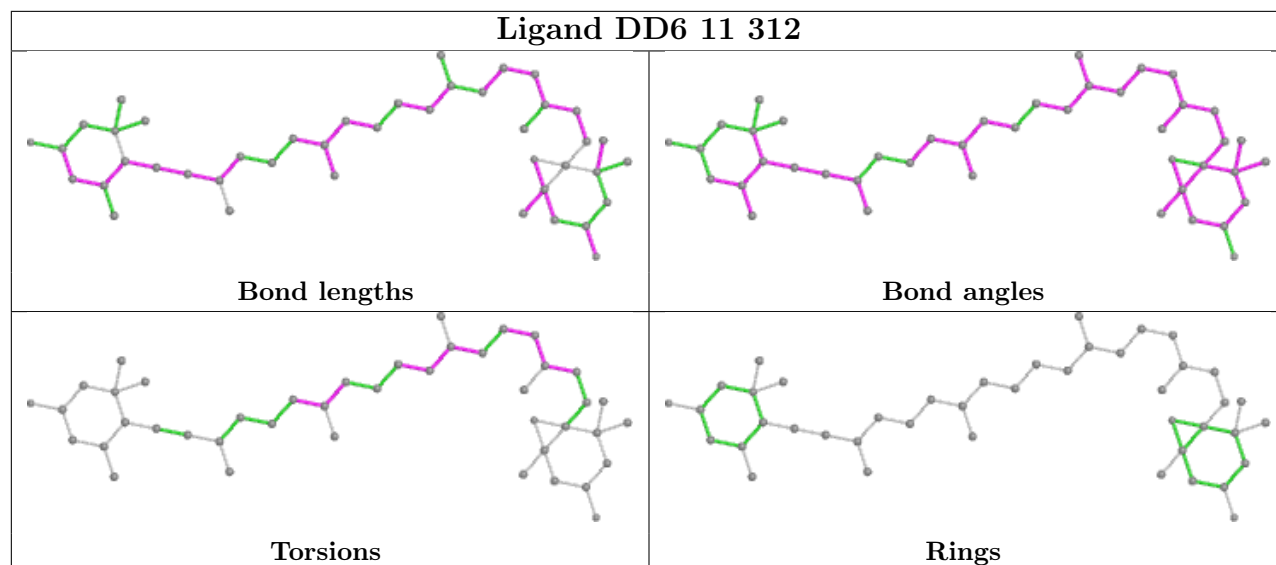


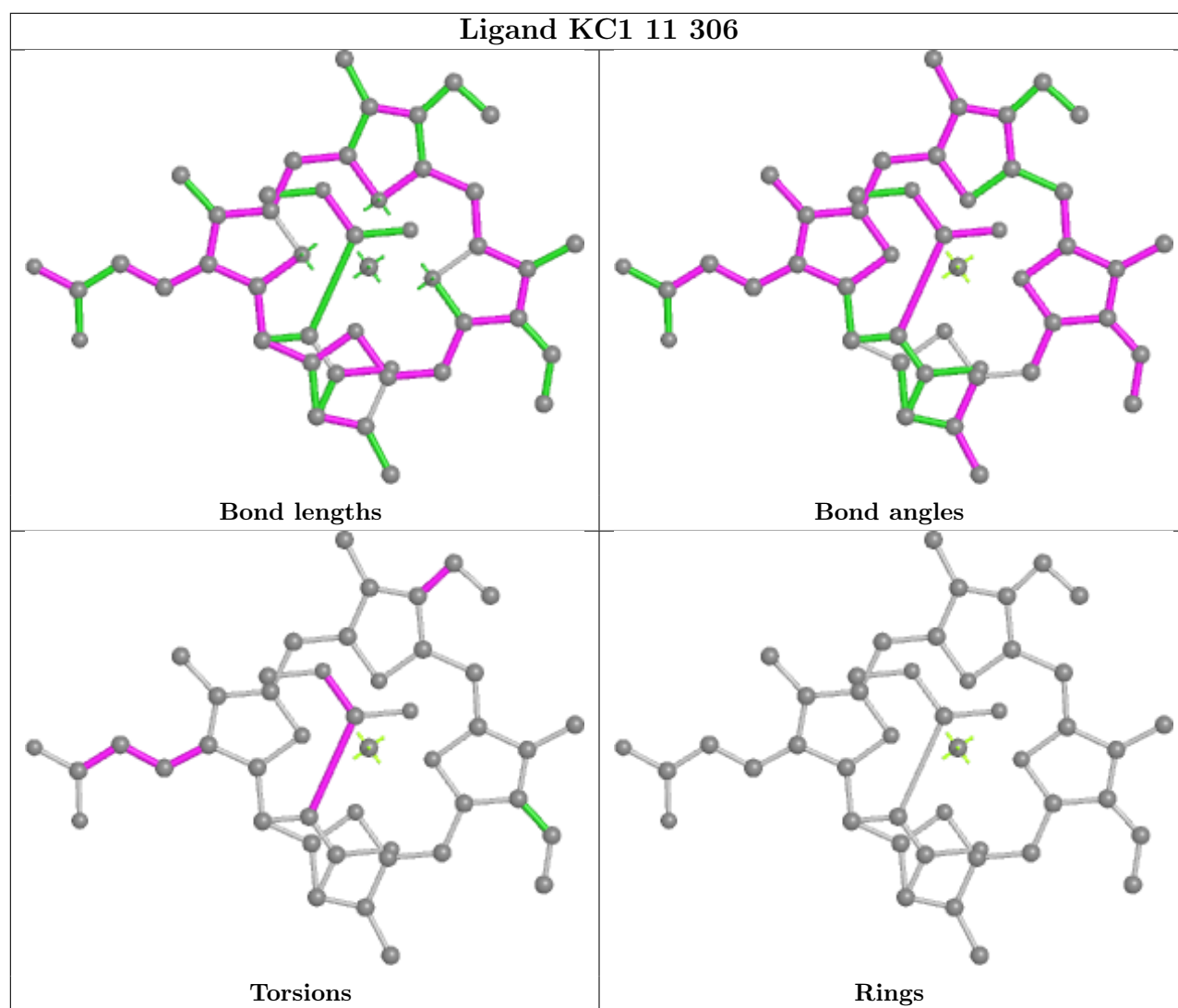
Torsions

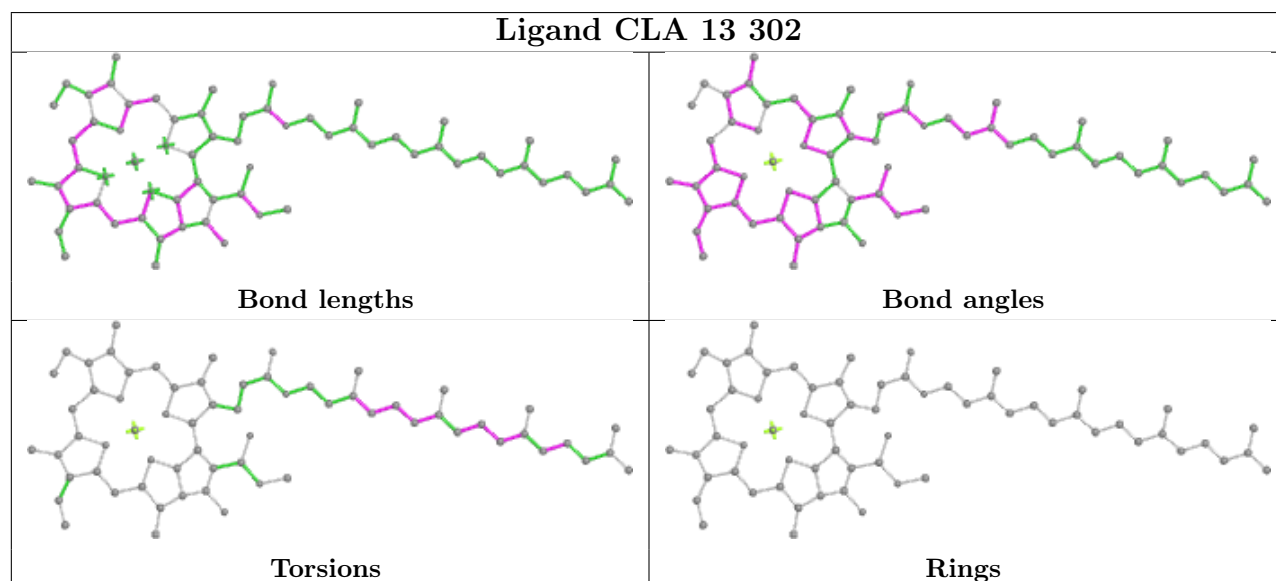
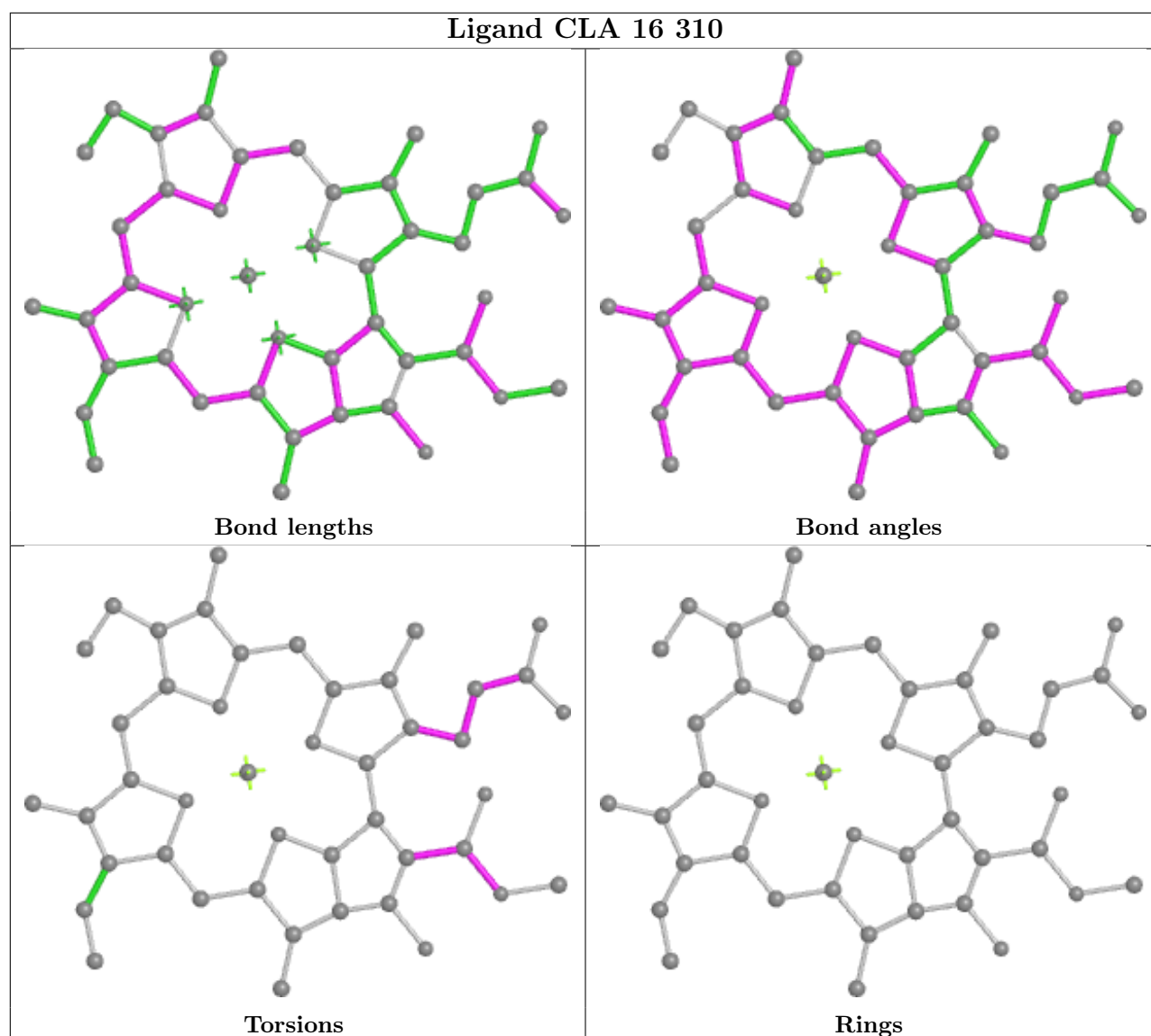


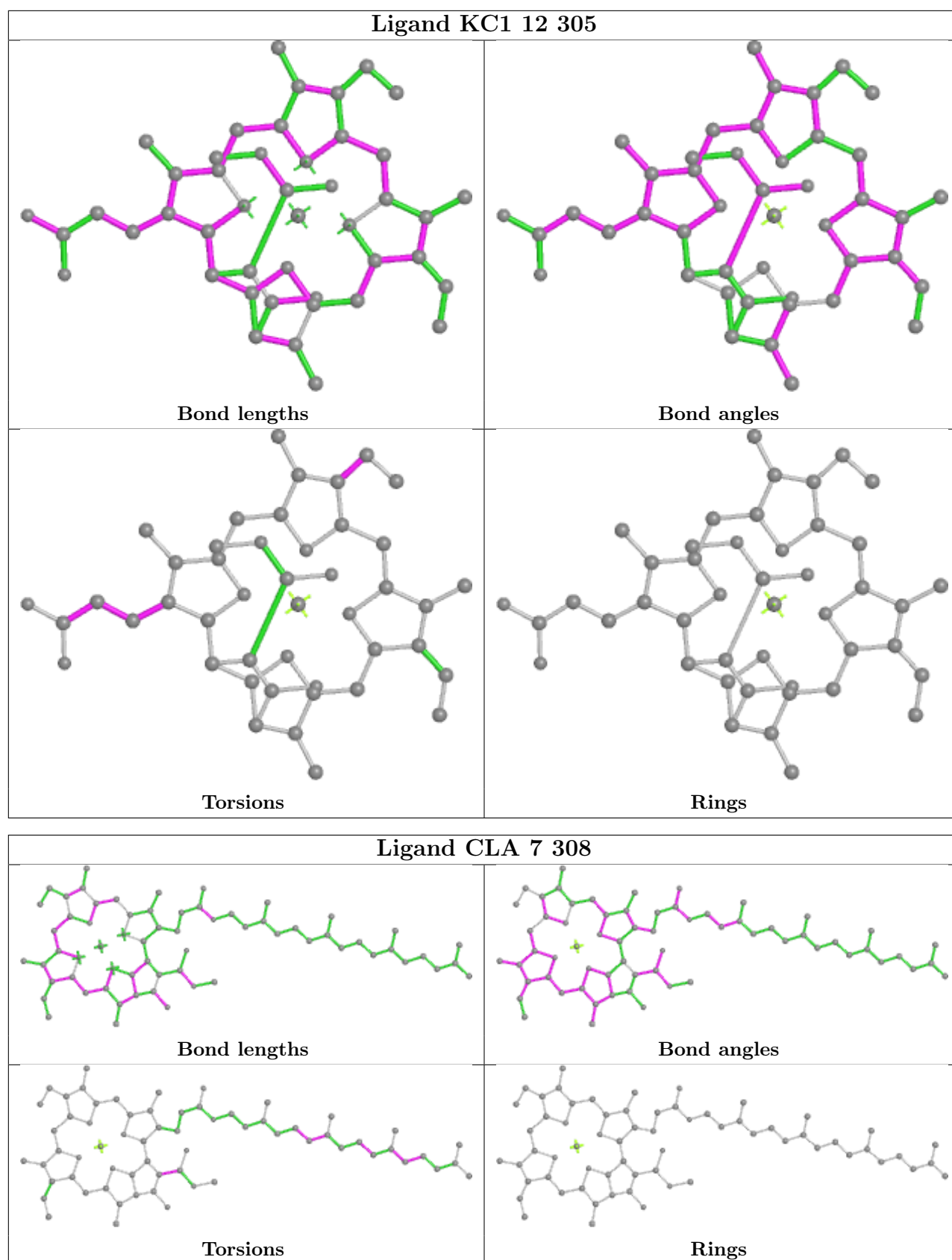
Rings

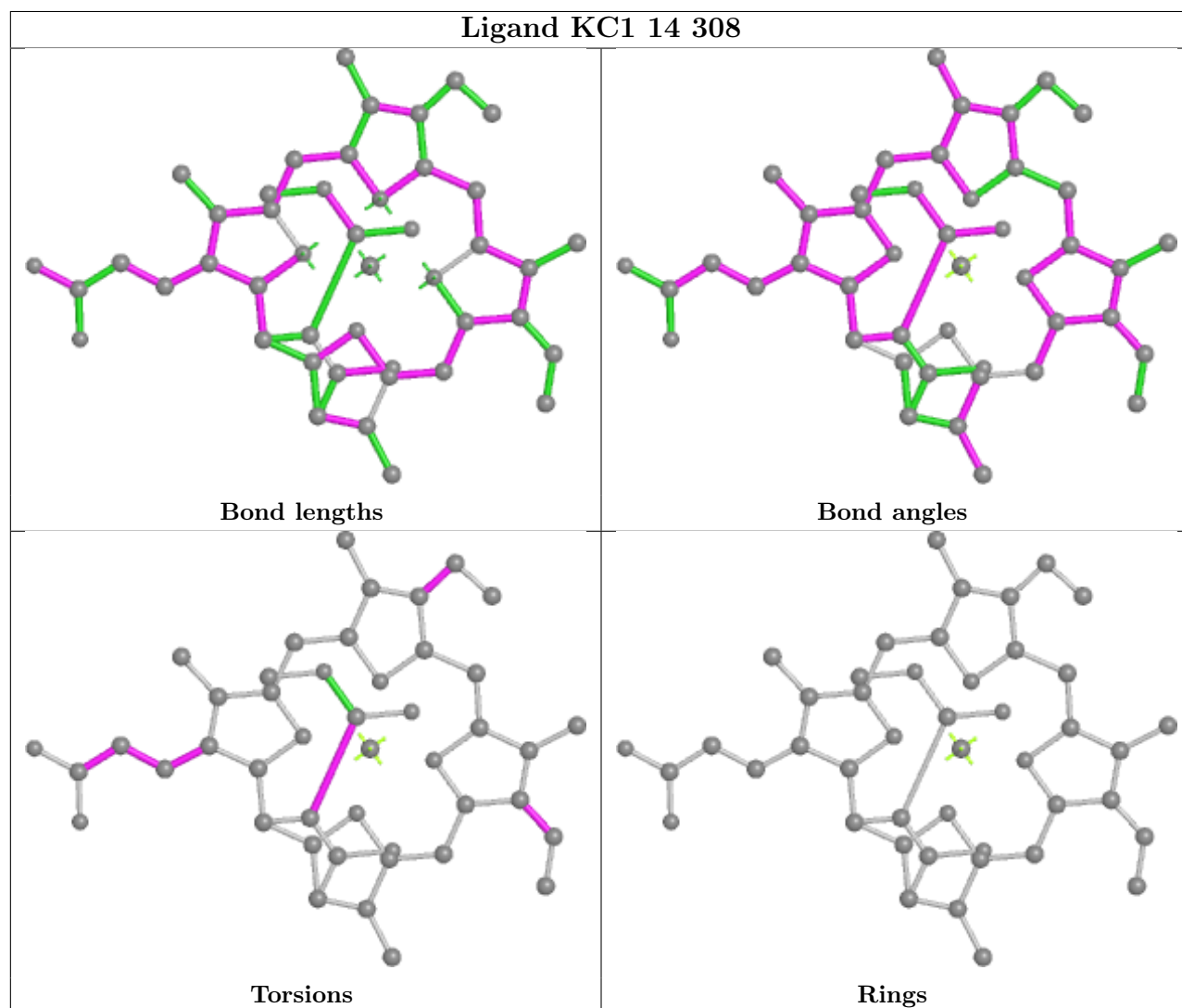
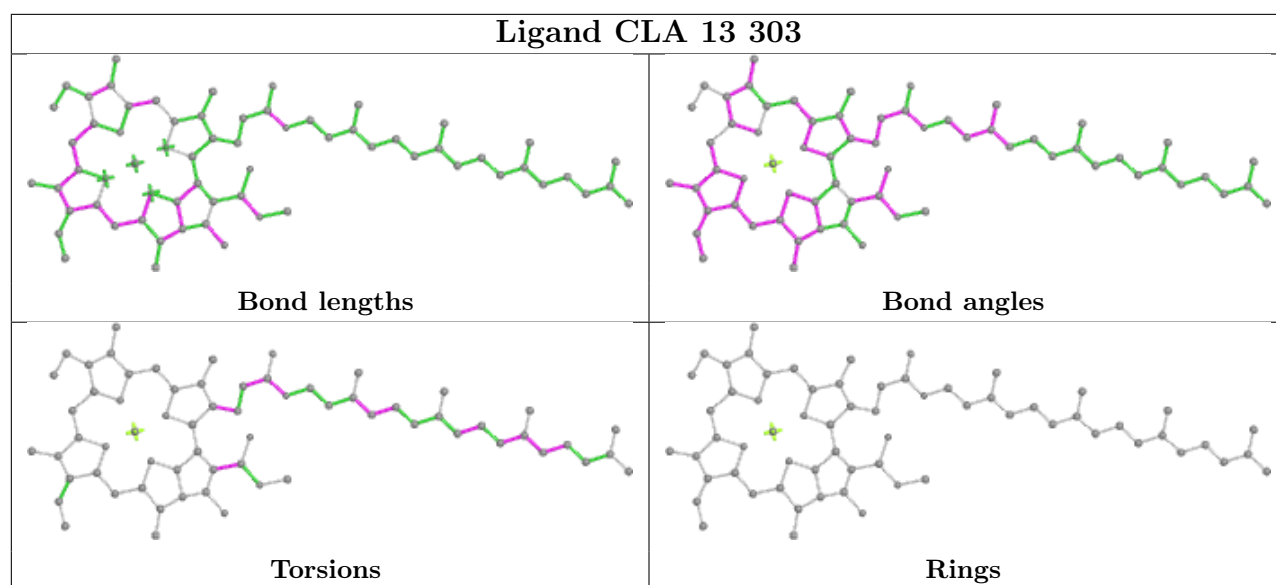


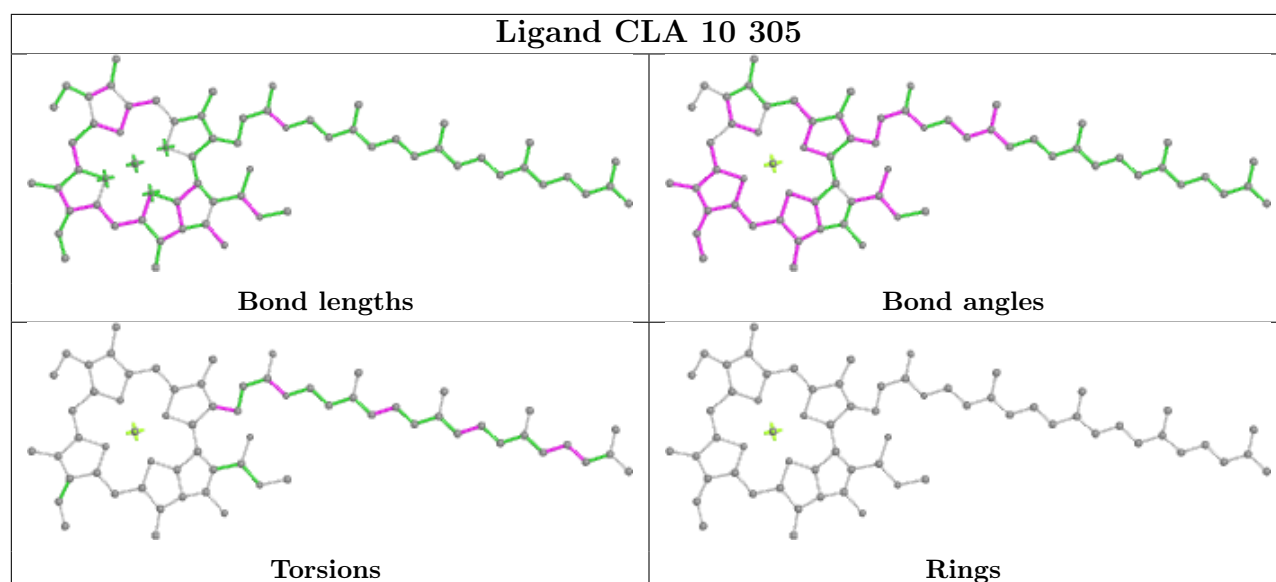
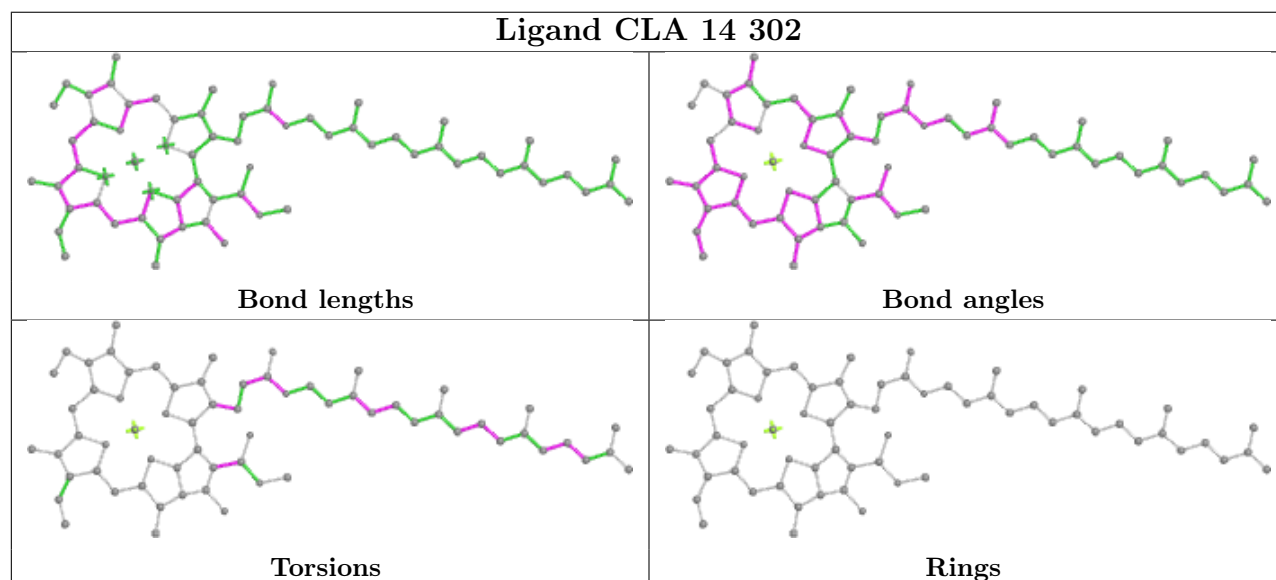
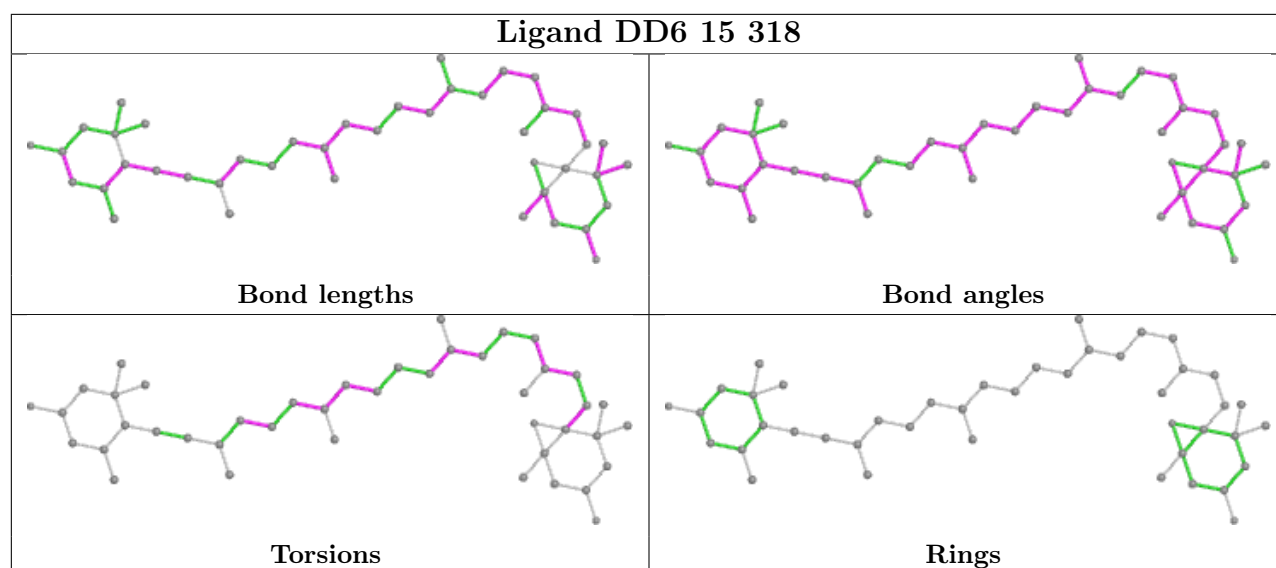


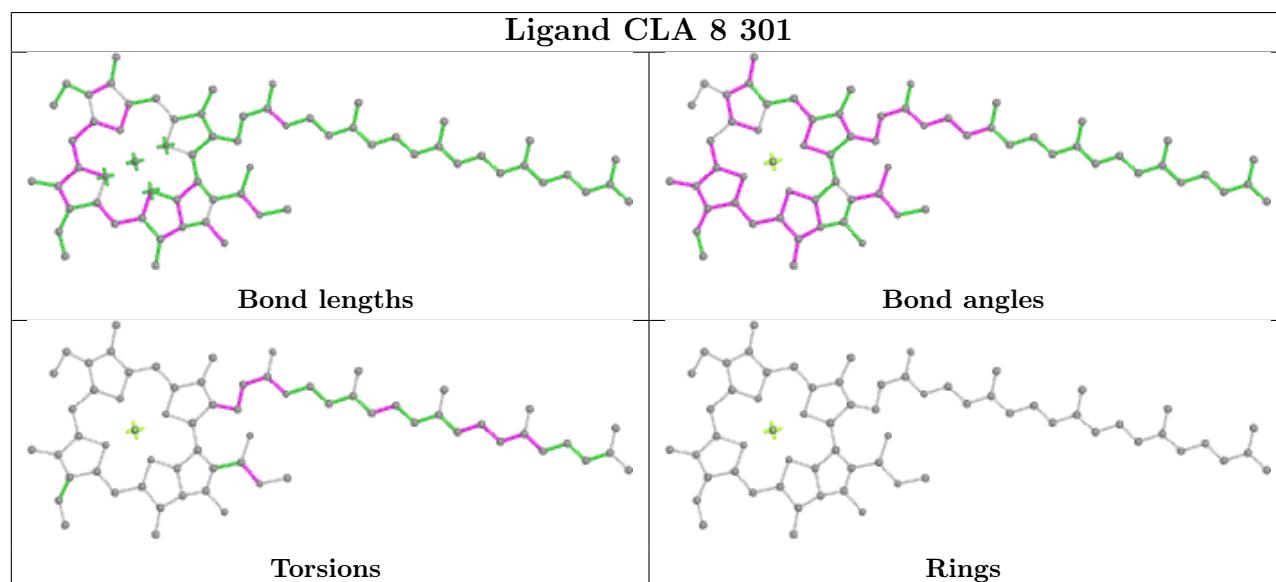
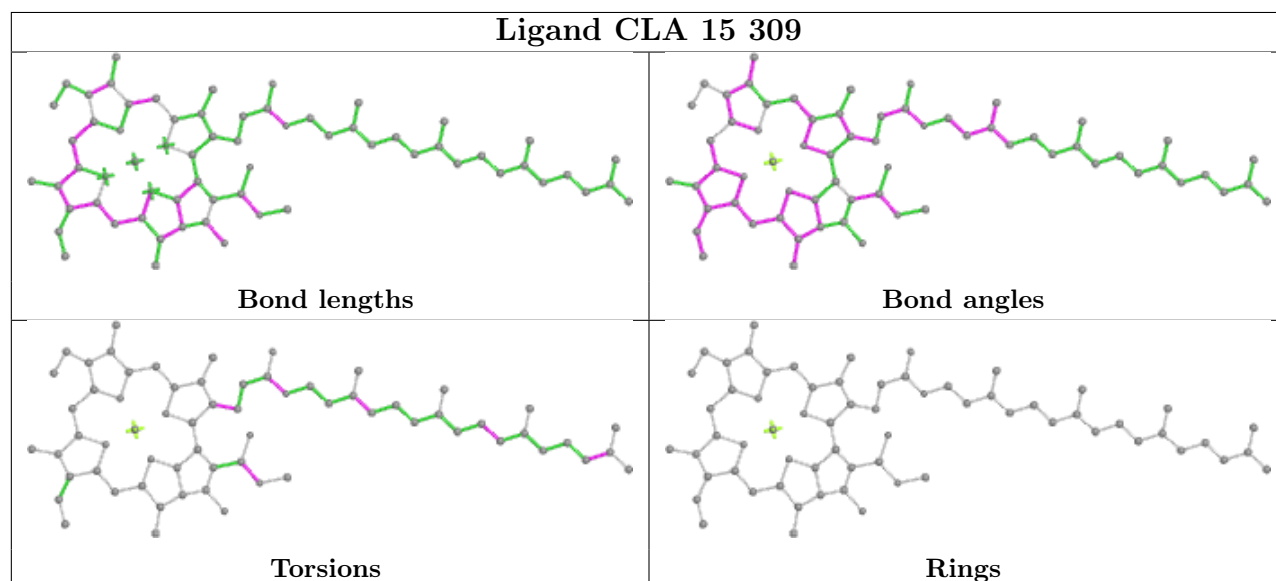
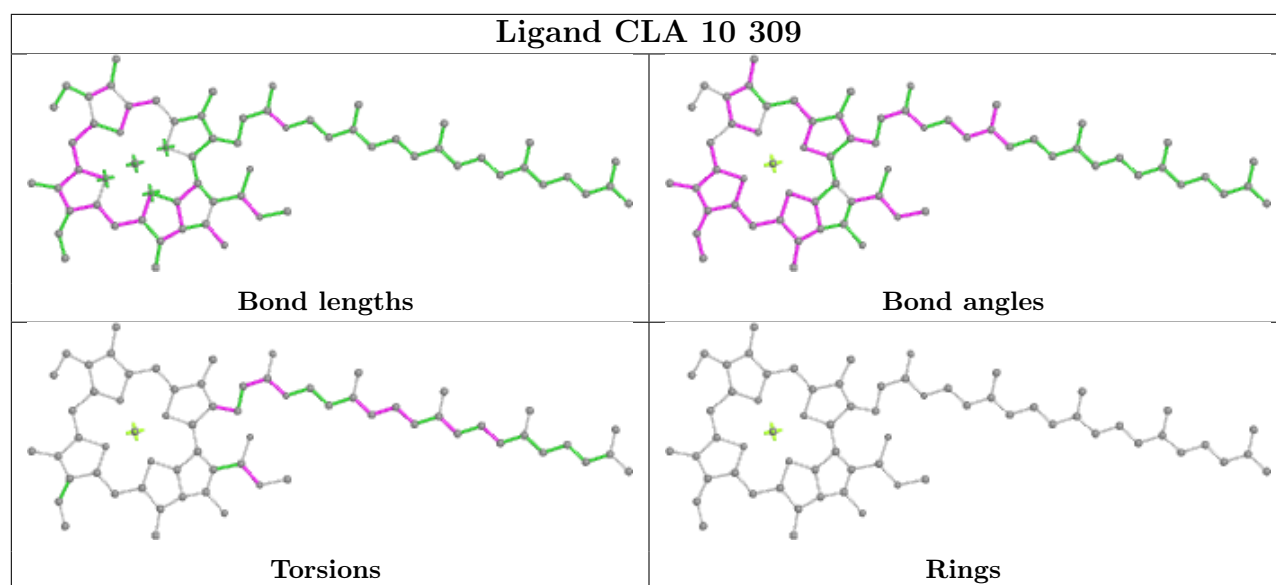


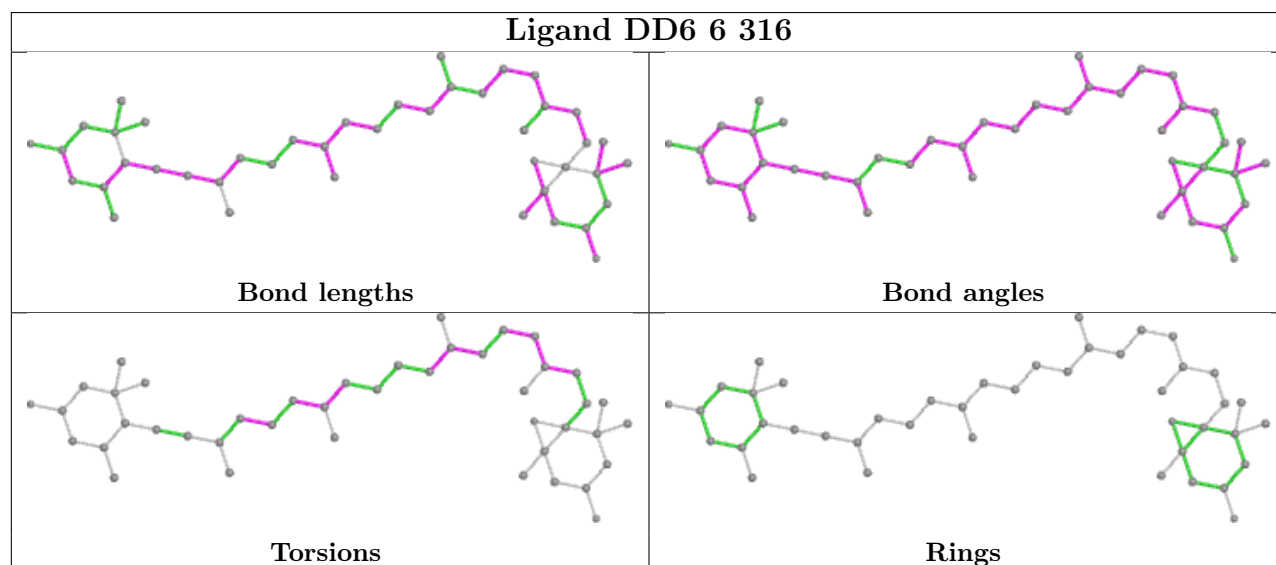
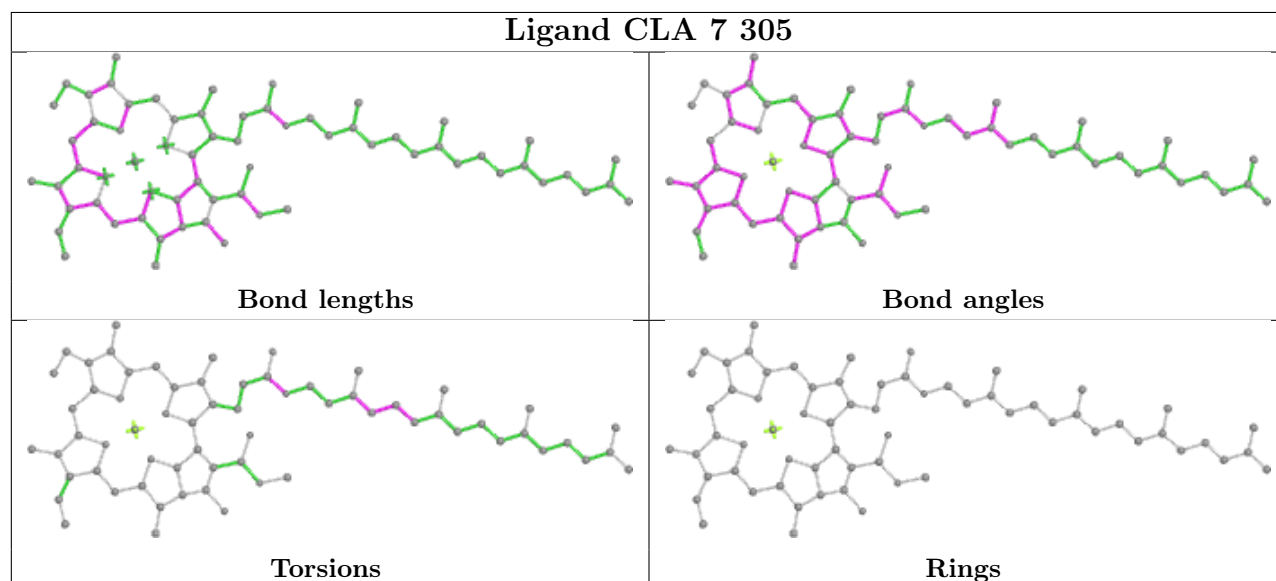
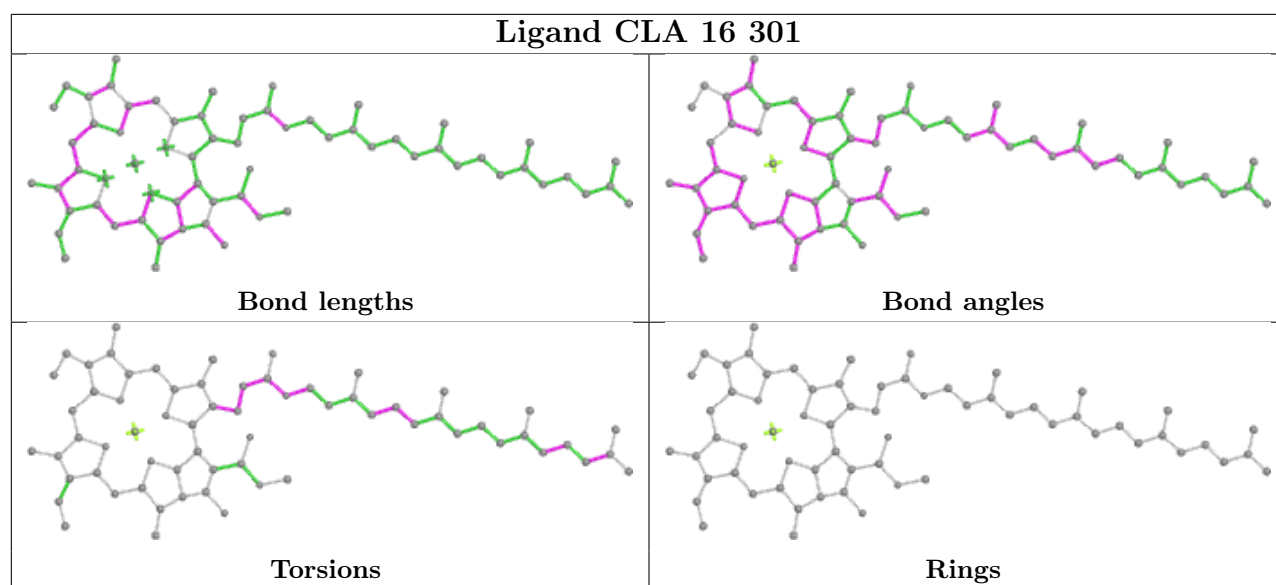


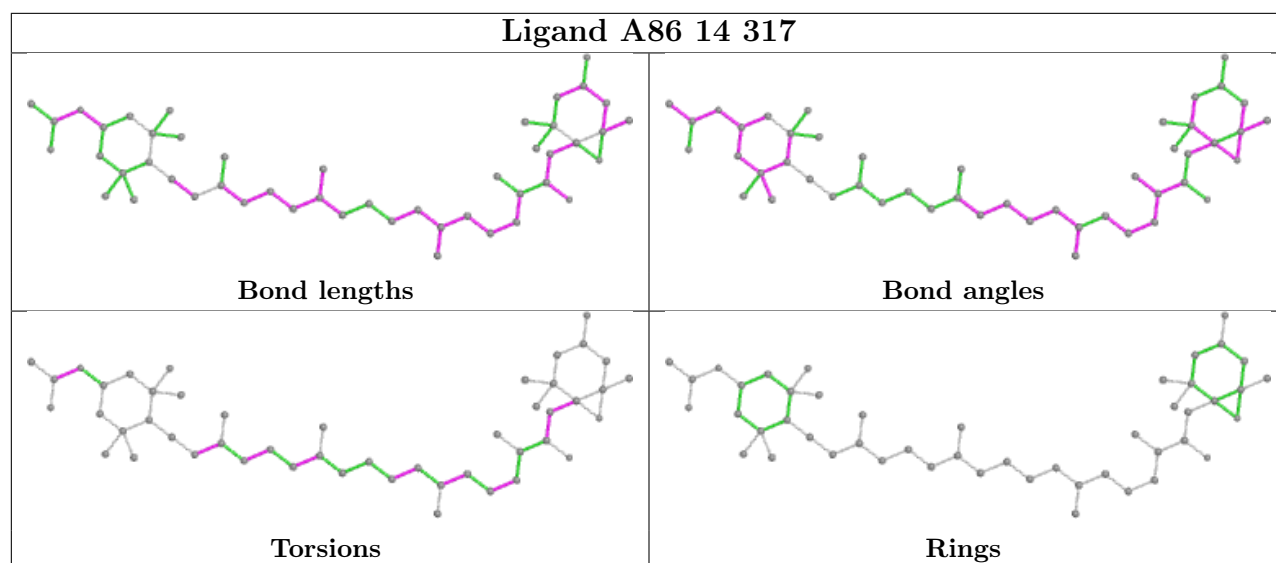
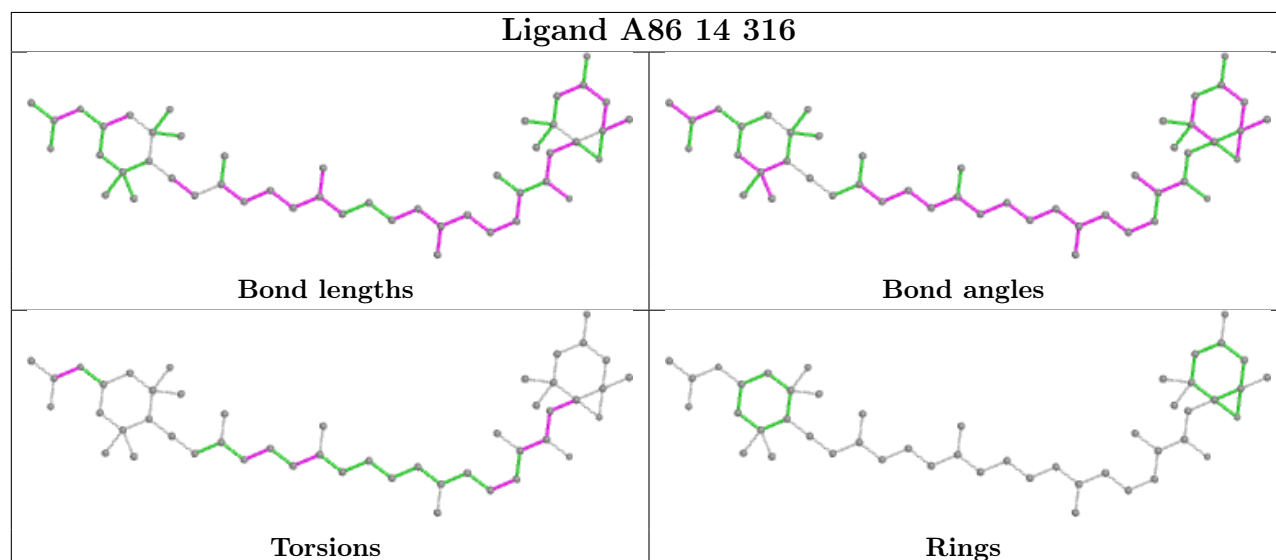
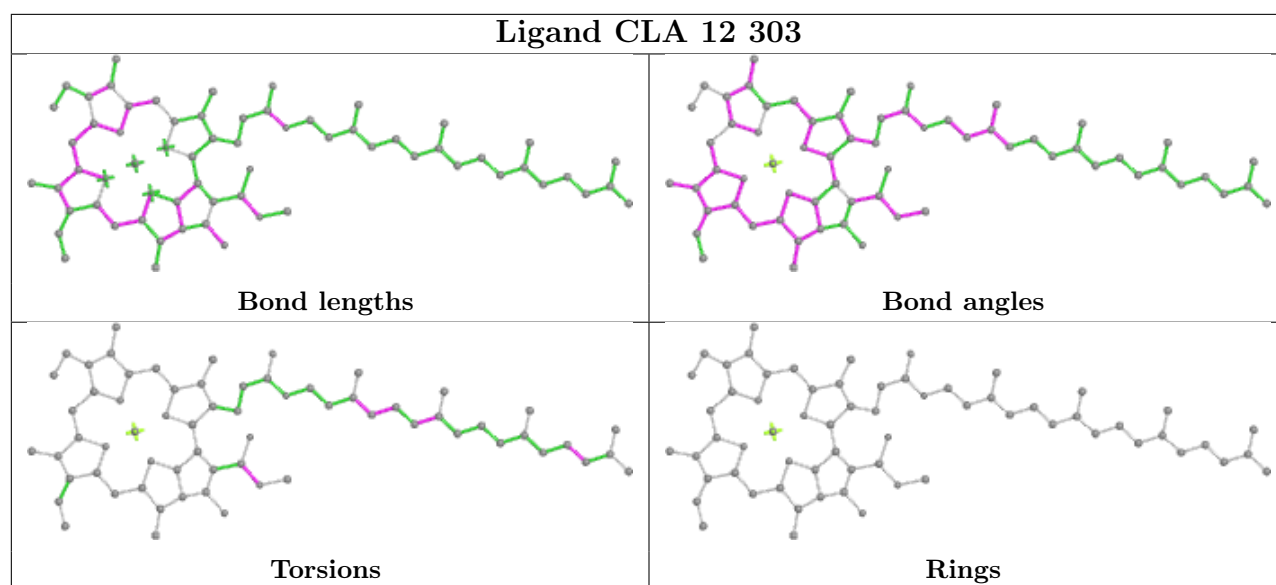




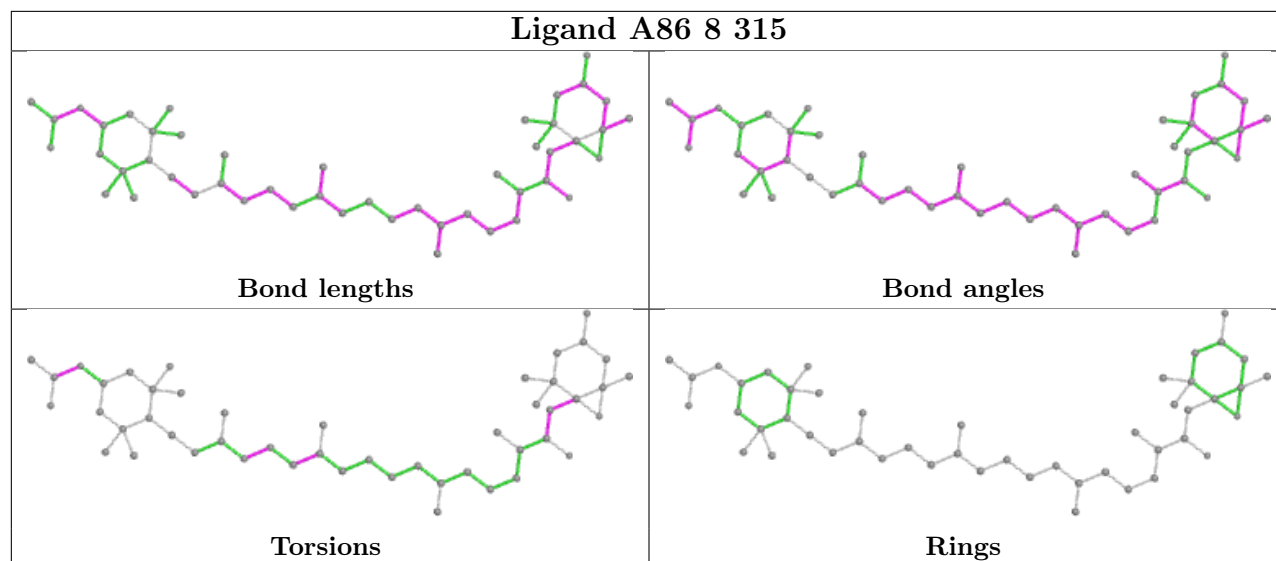




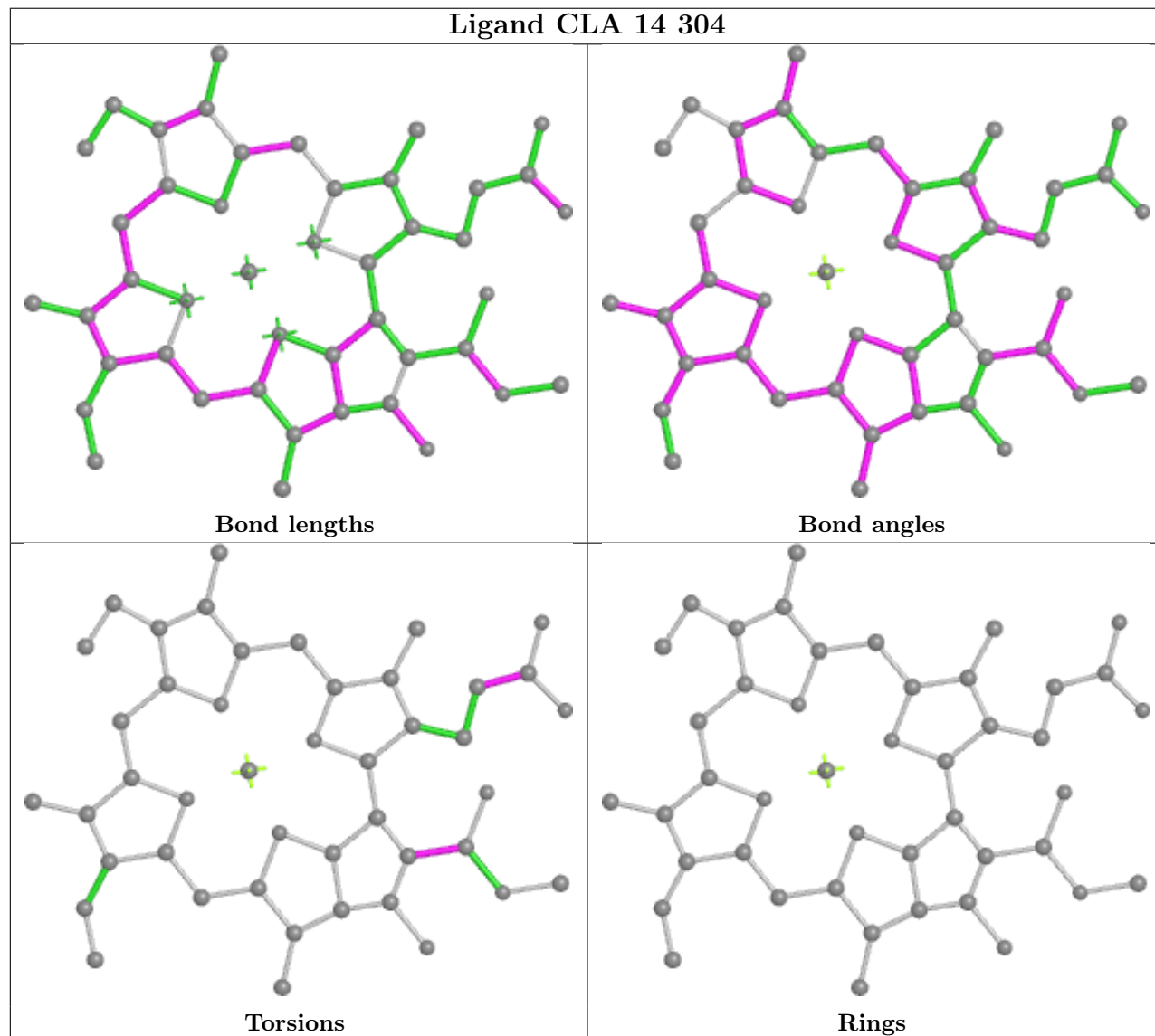


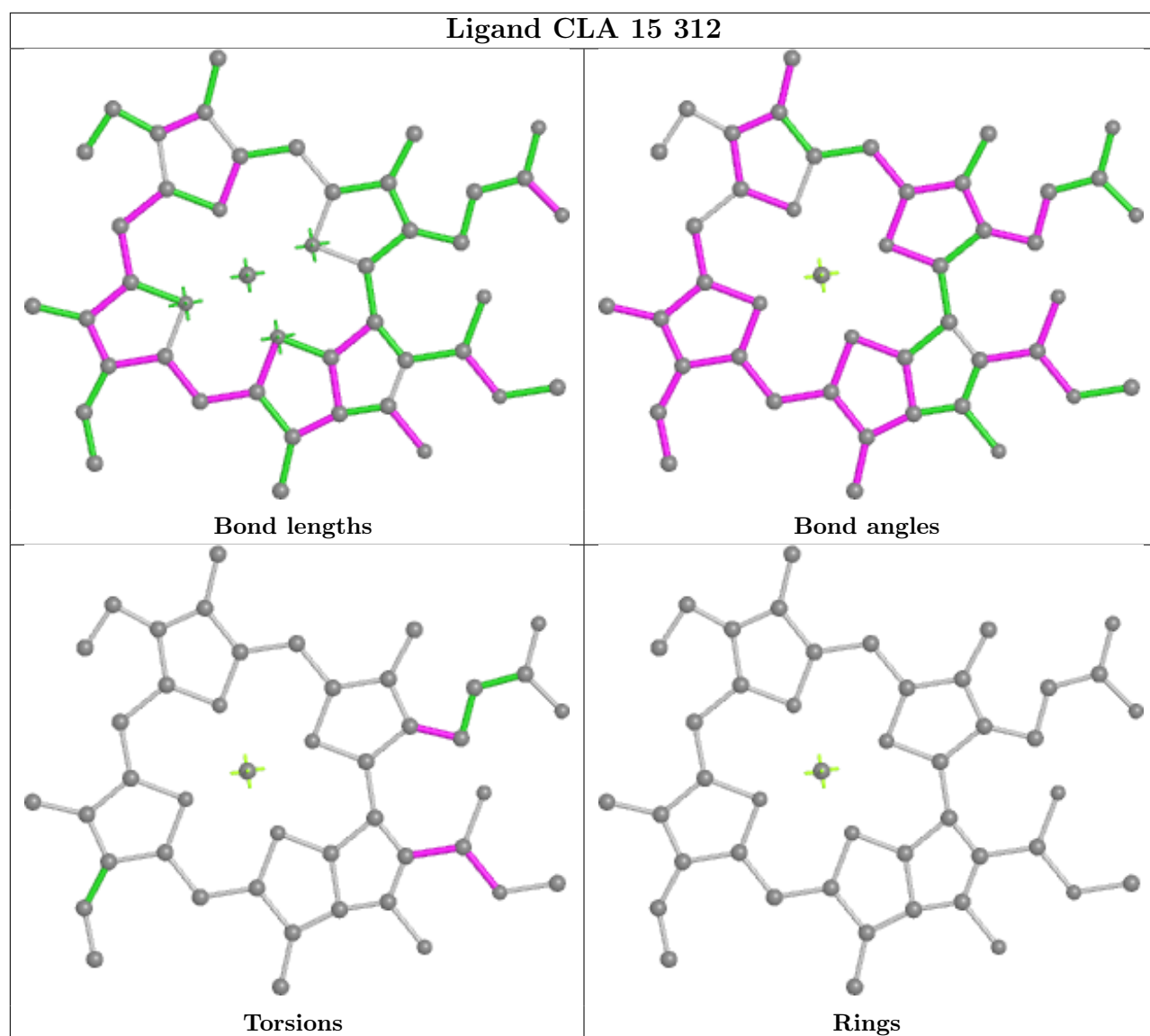


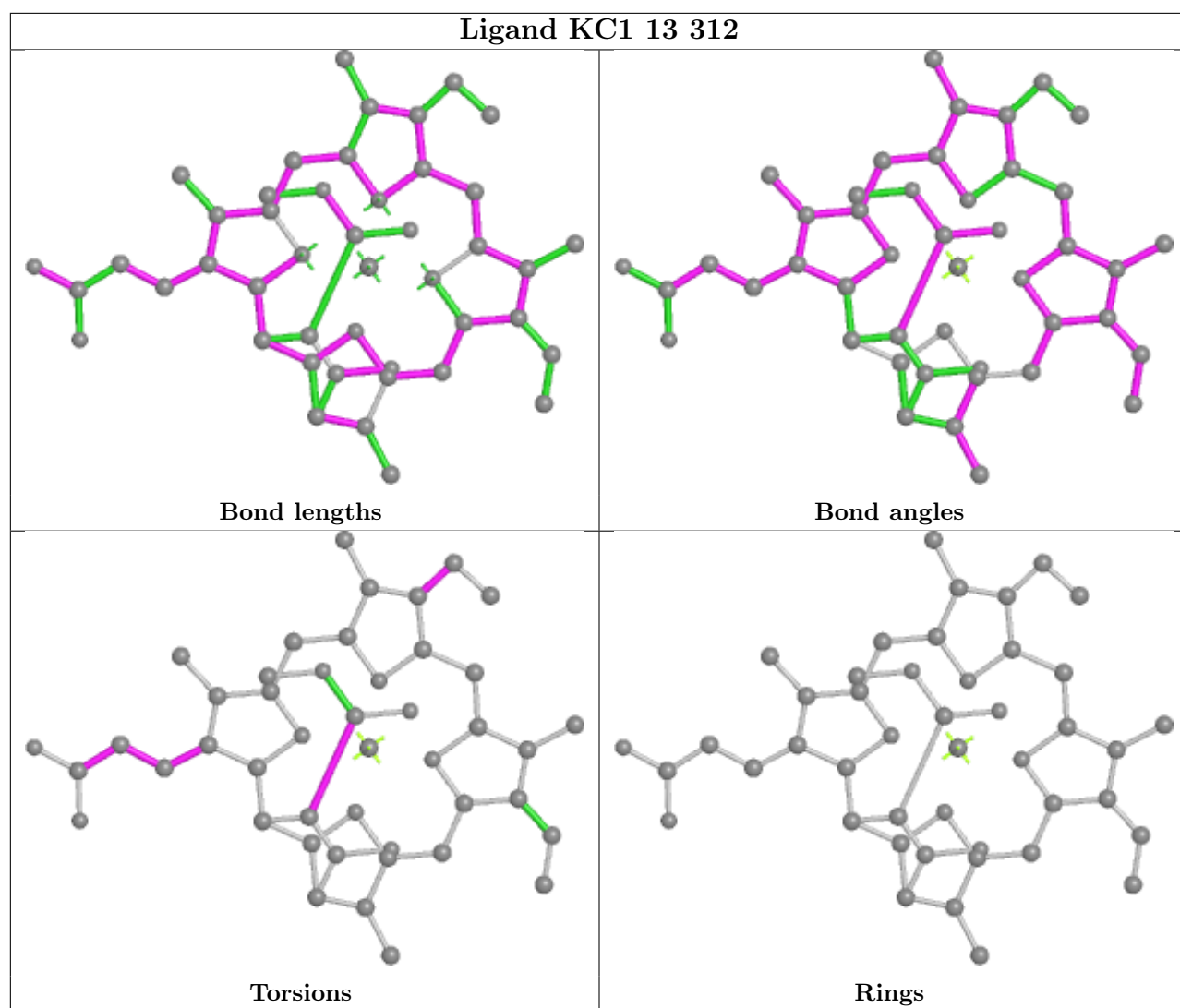
Ligand A86 8 315



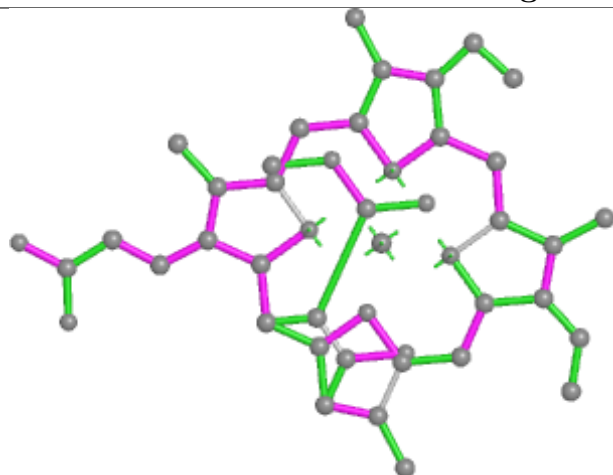
Ligand CLA 14 304



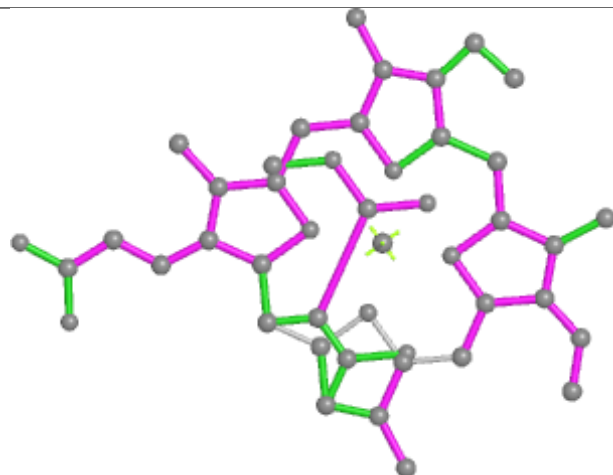




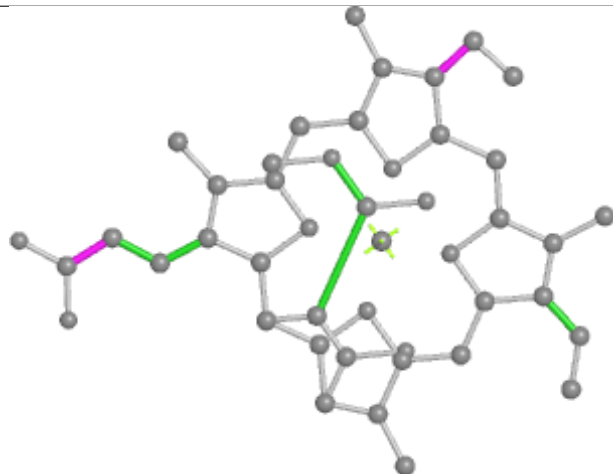
Ligand KC1 7 312



Bond lengths



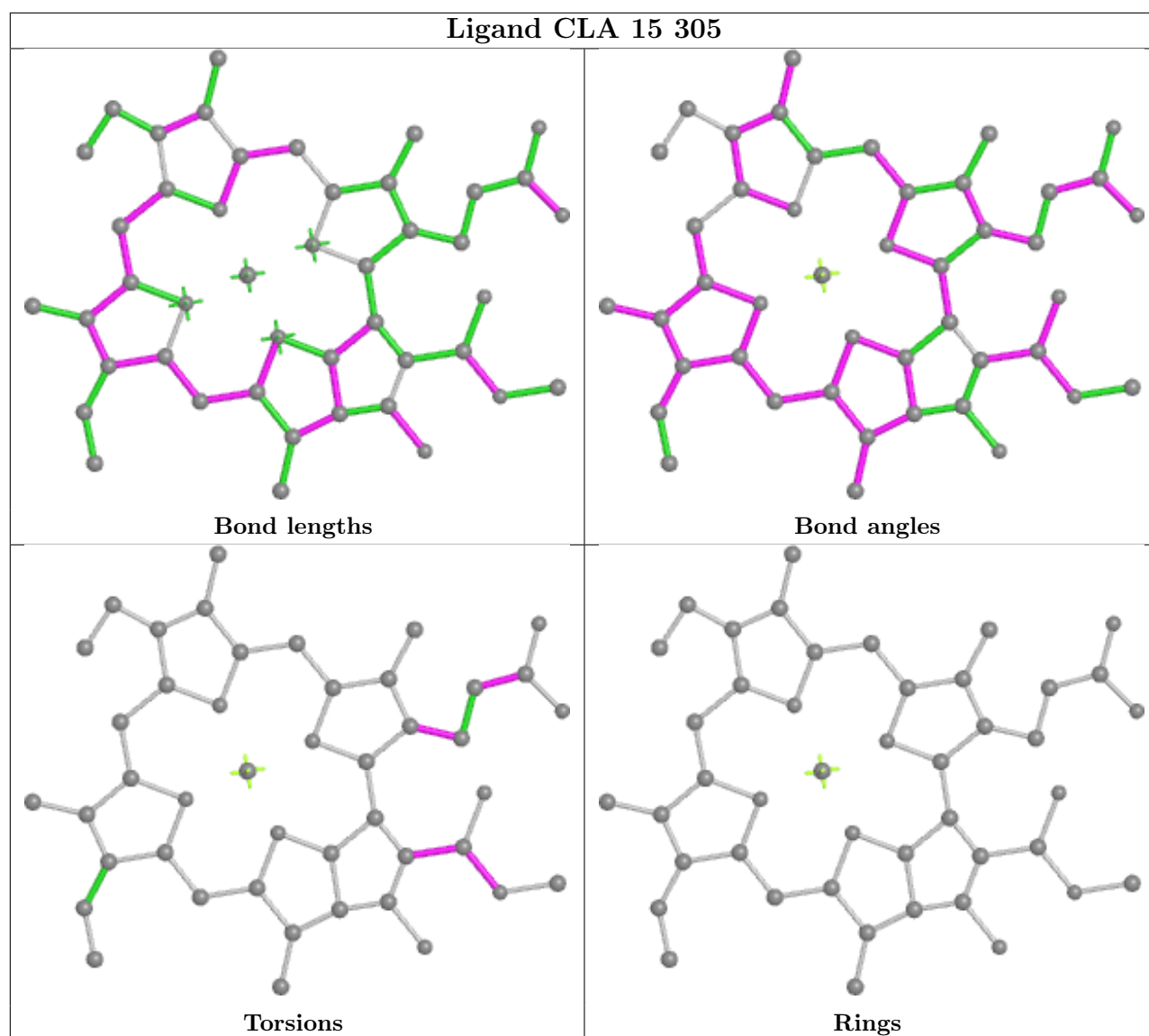
Bond angles

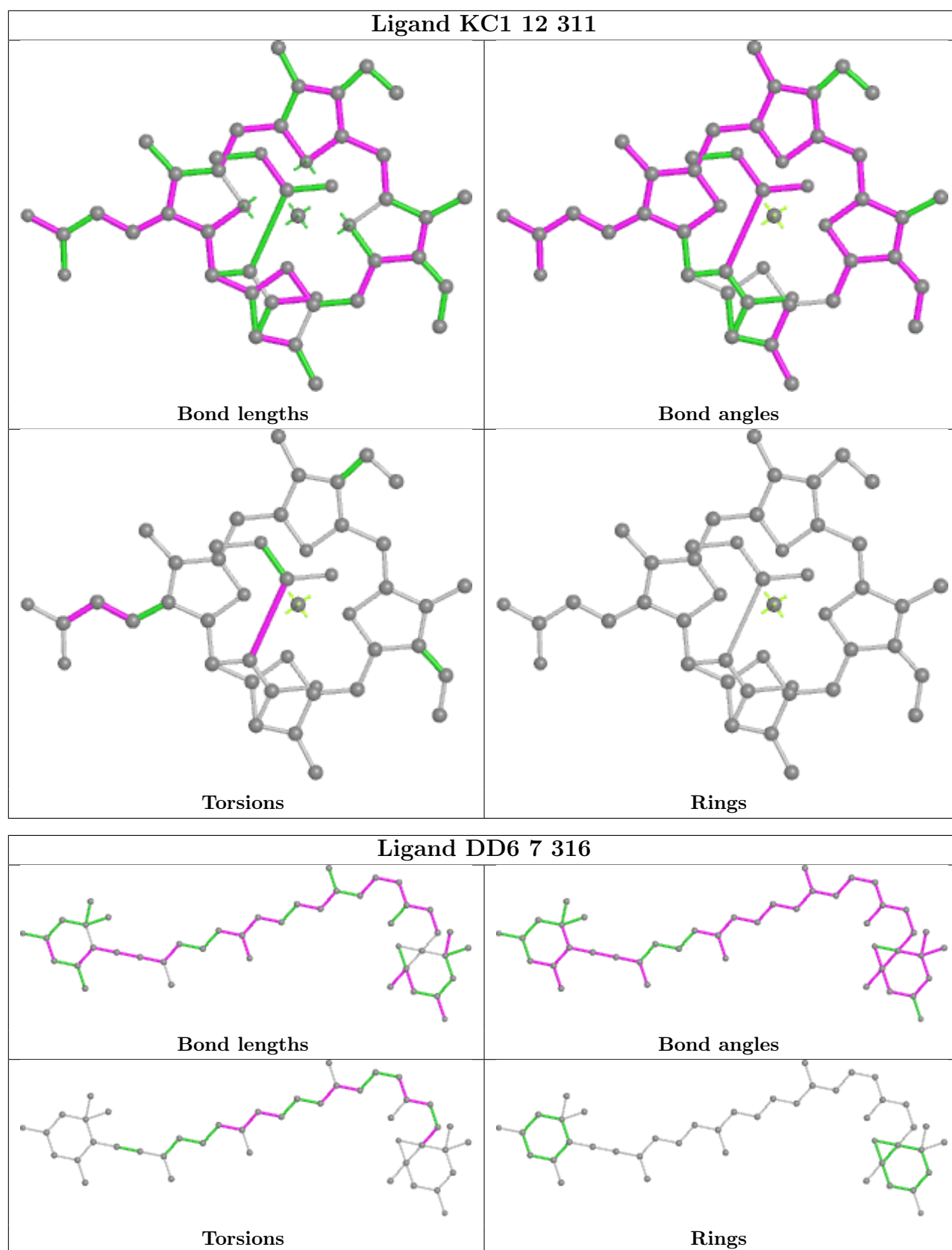


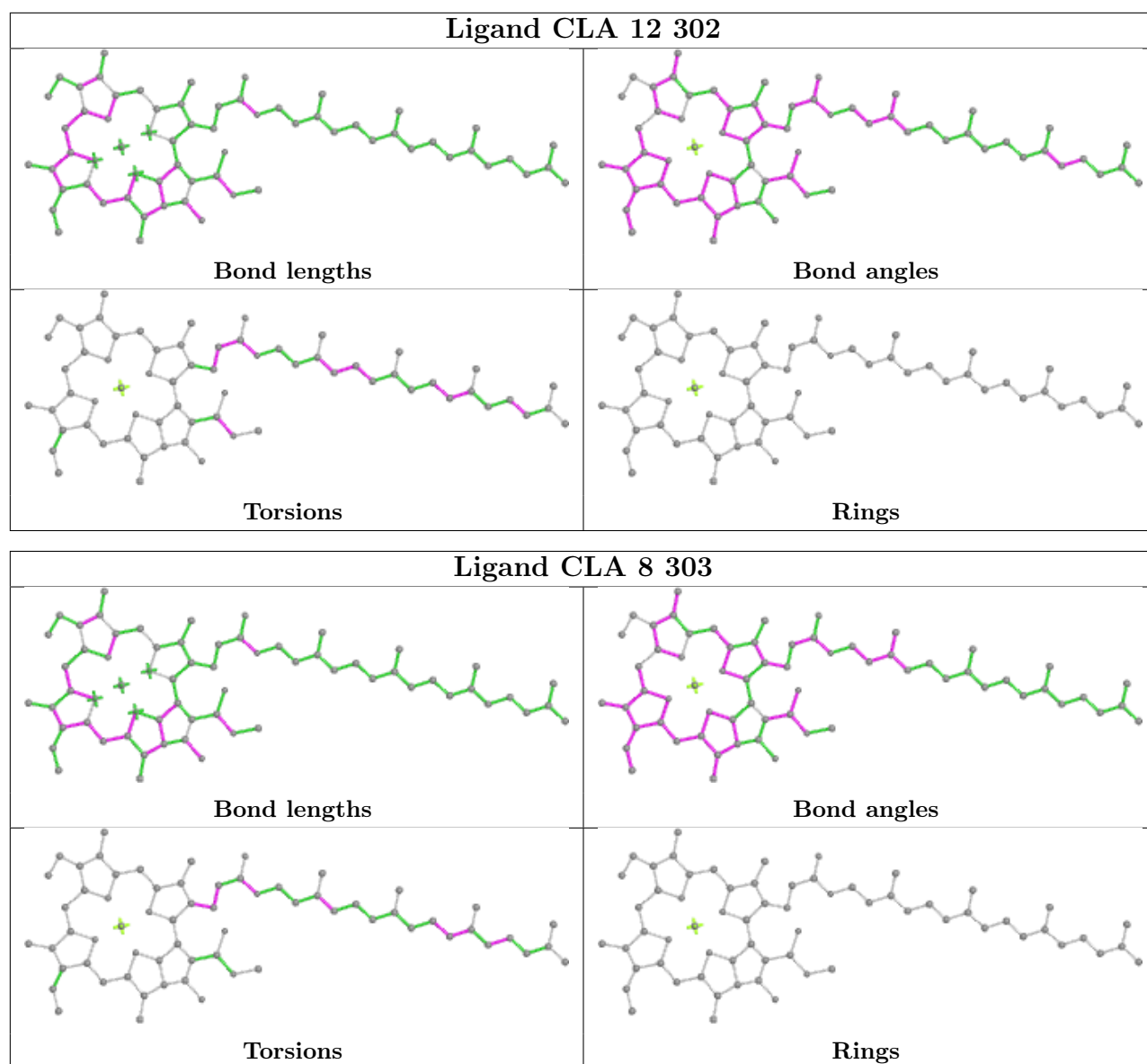
Torsions

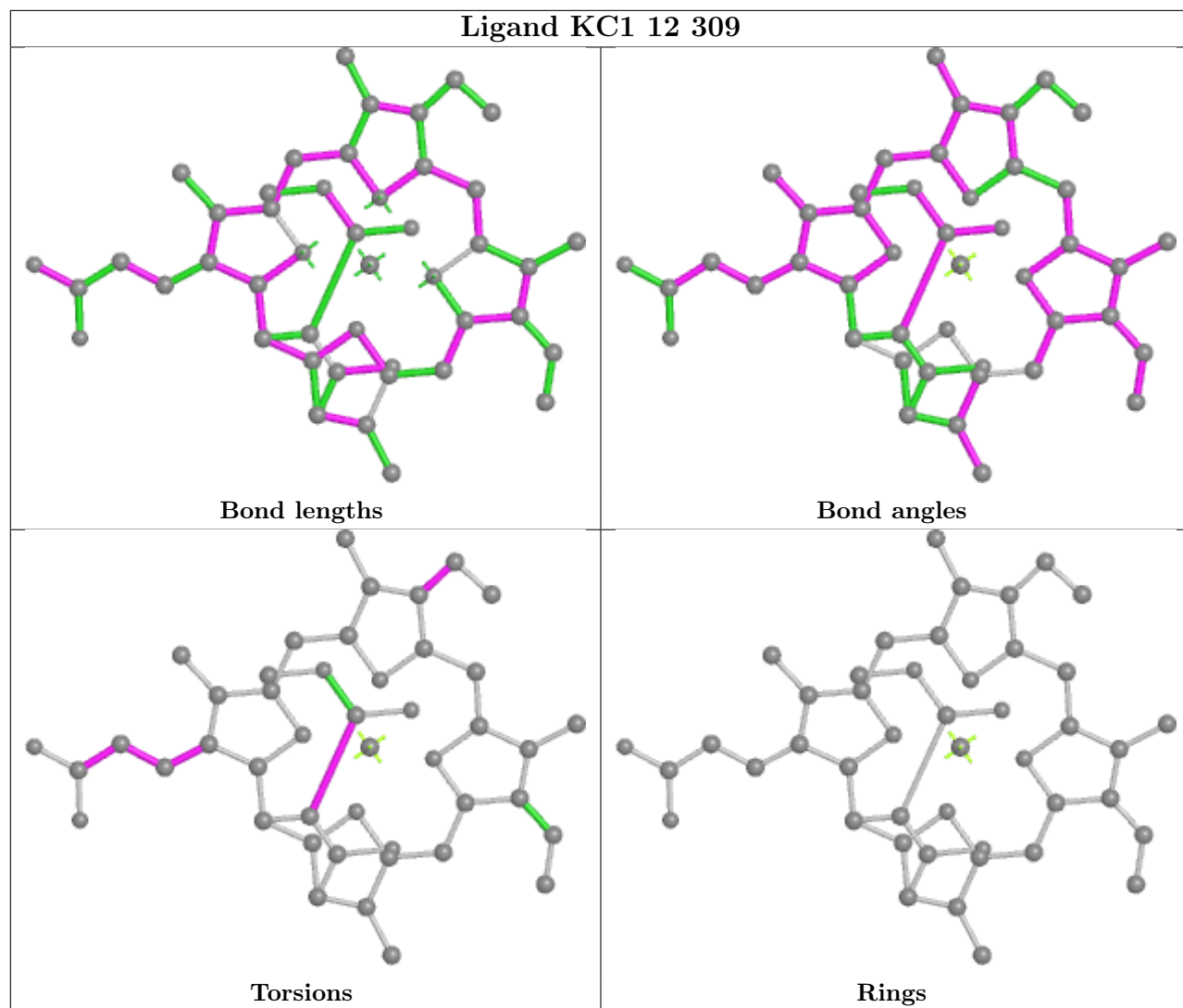


Rings

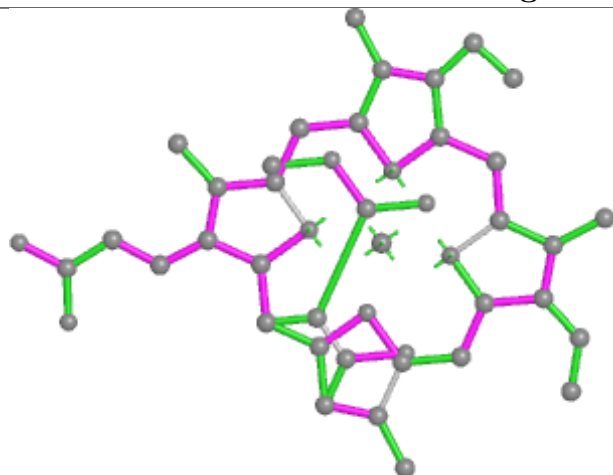




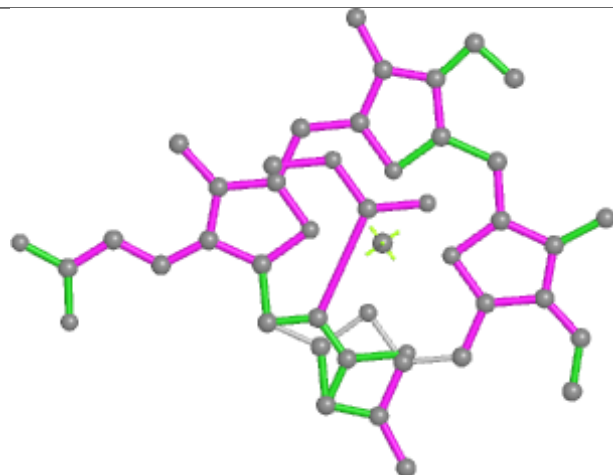




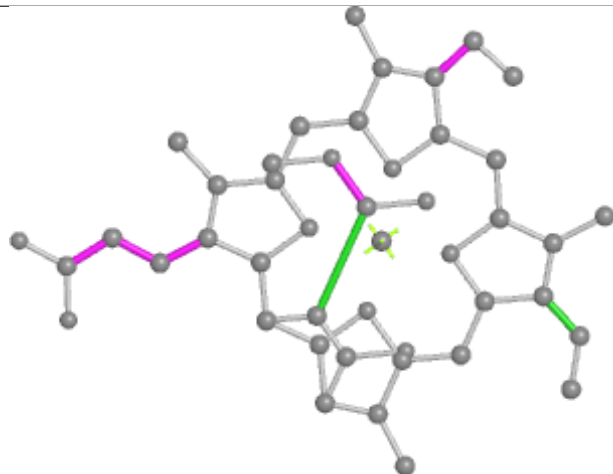
Ligand KC1 8 311



Bond lengths



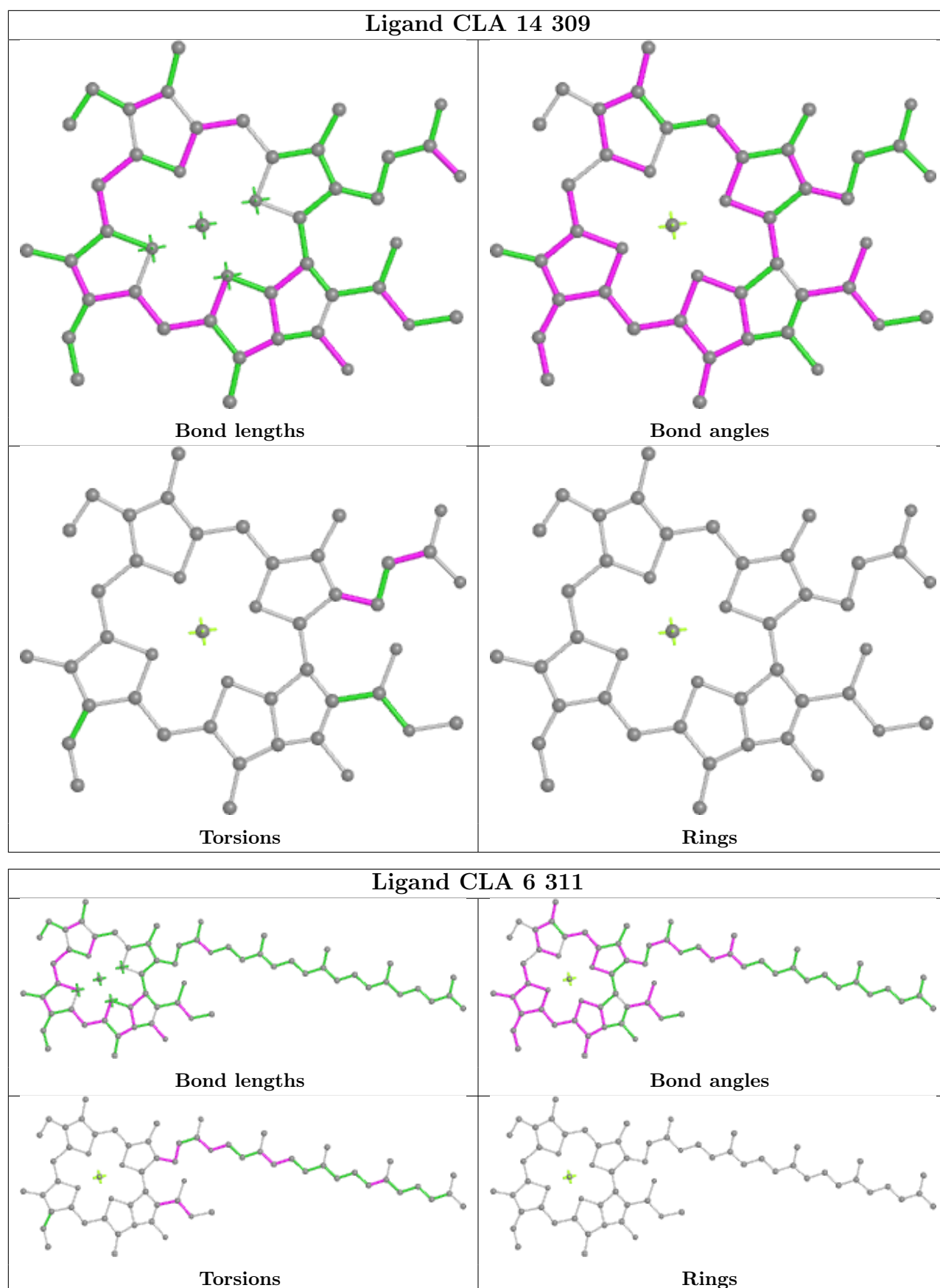
Bond angles

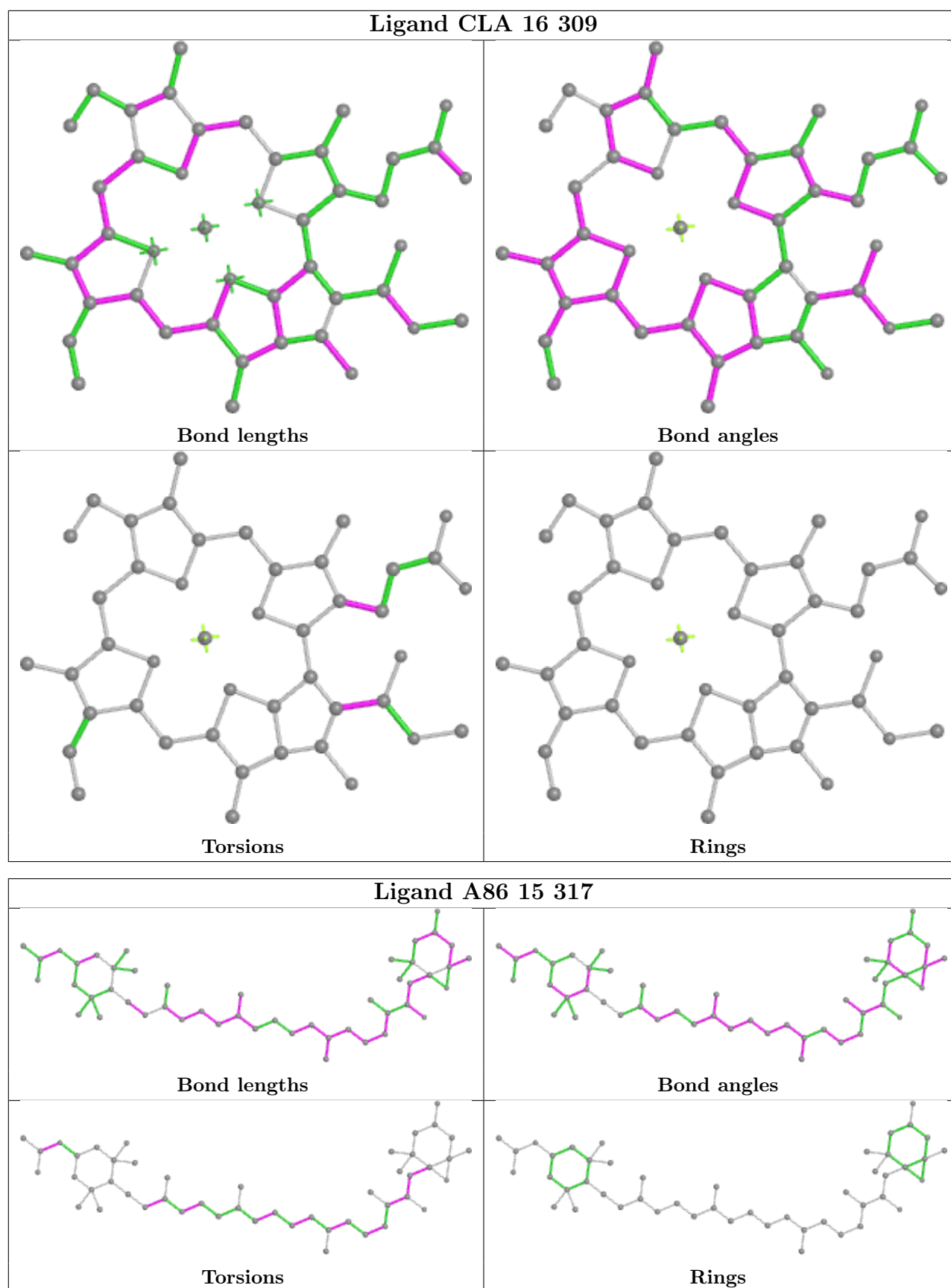


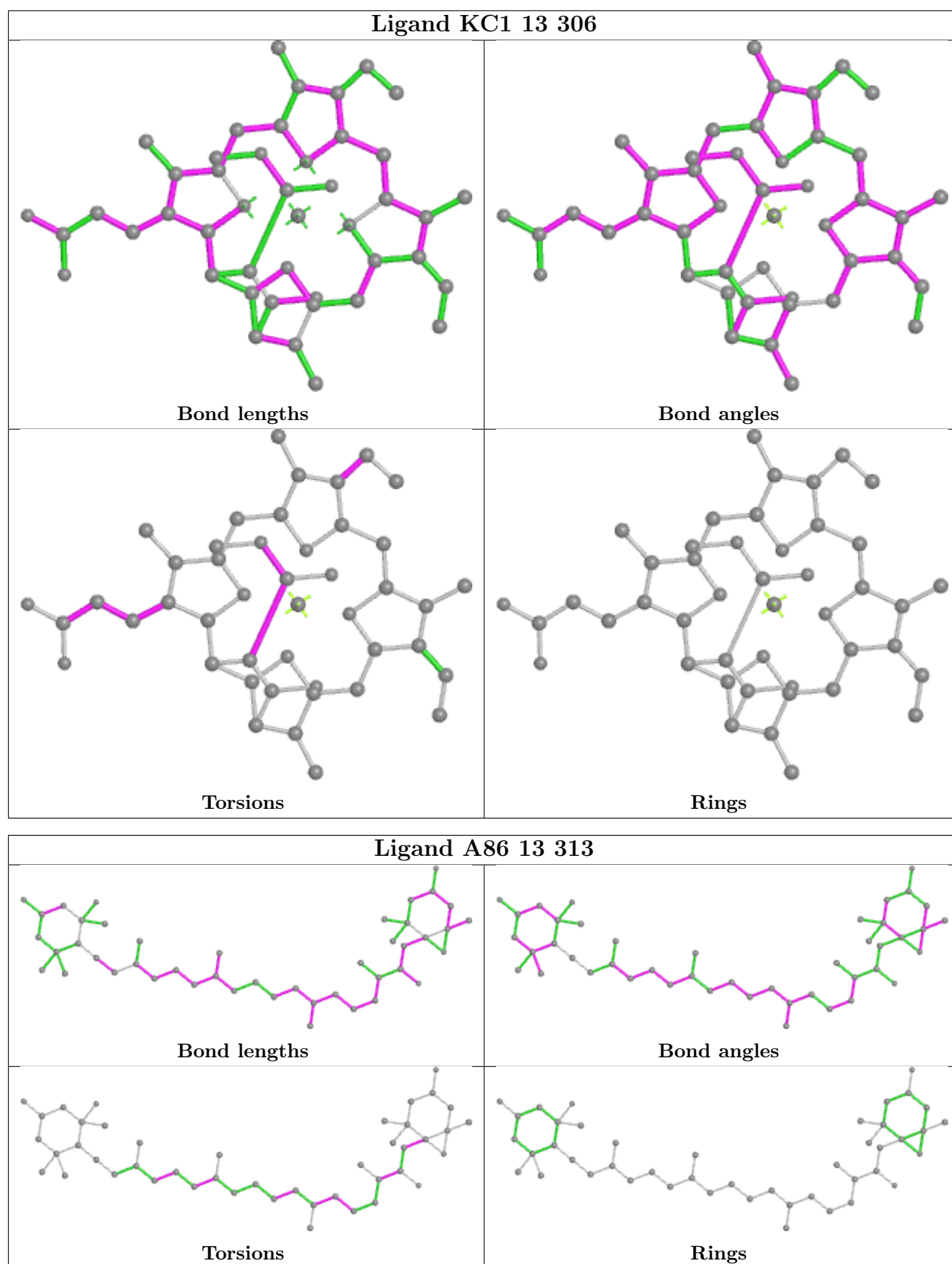
Torsions

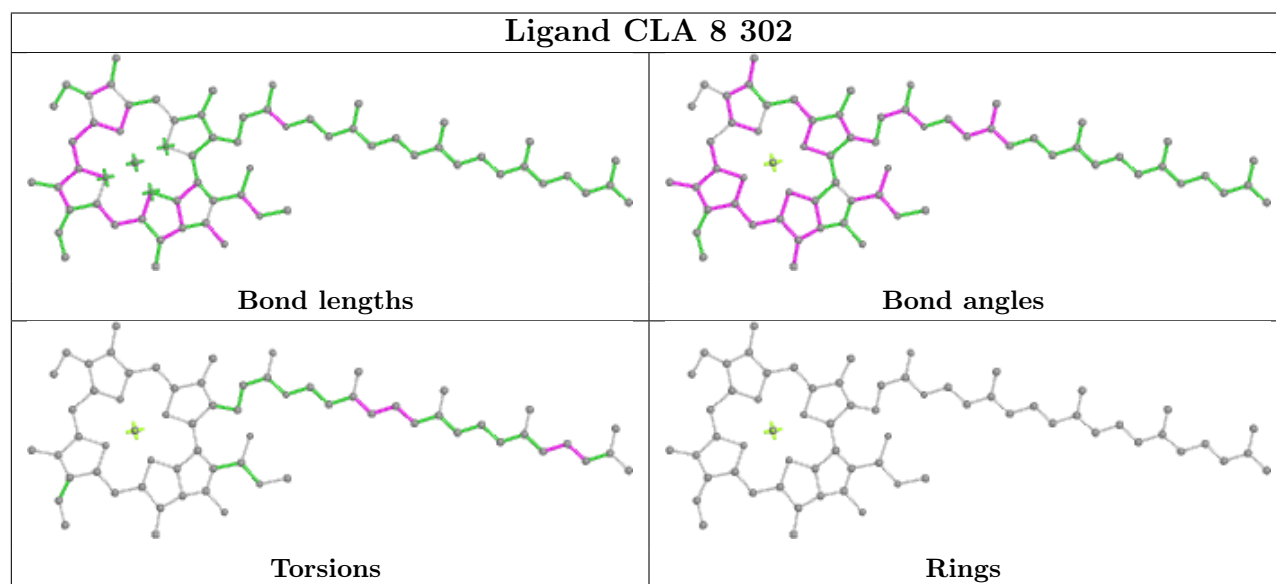
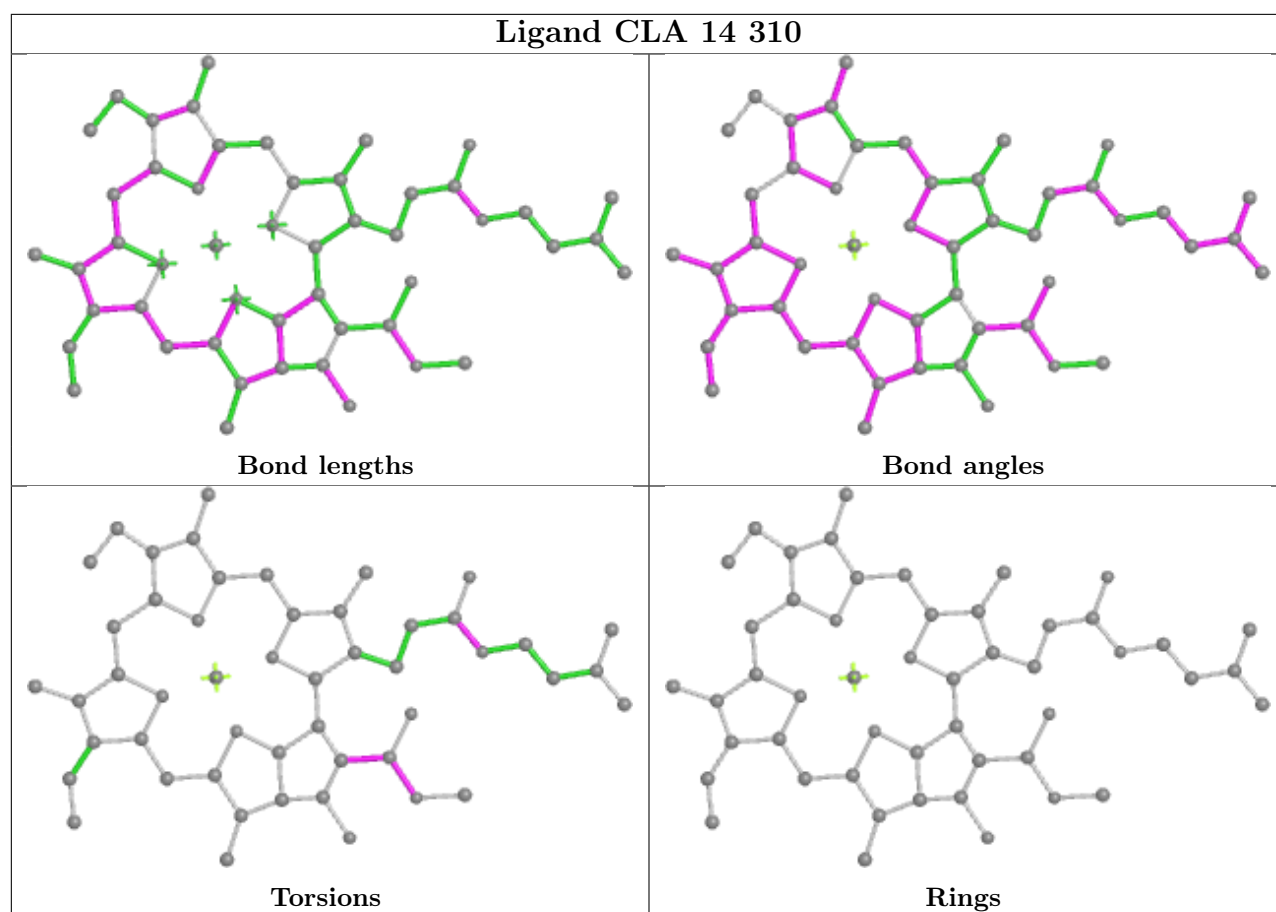


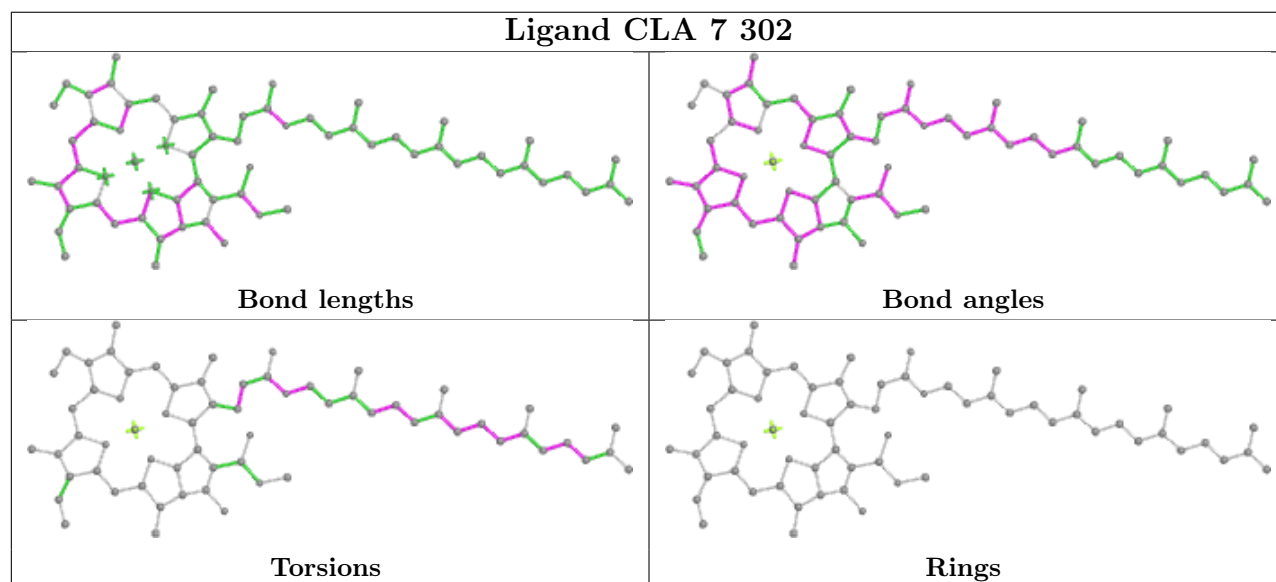
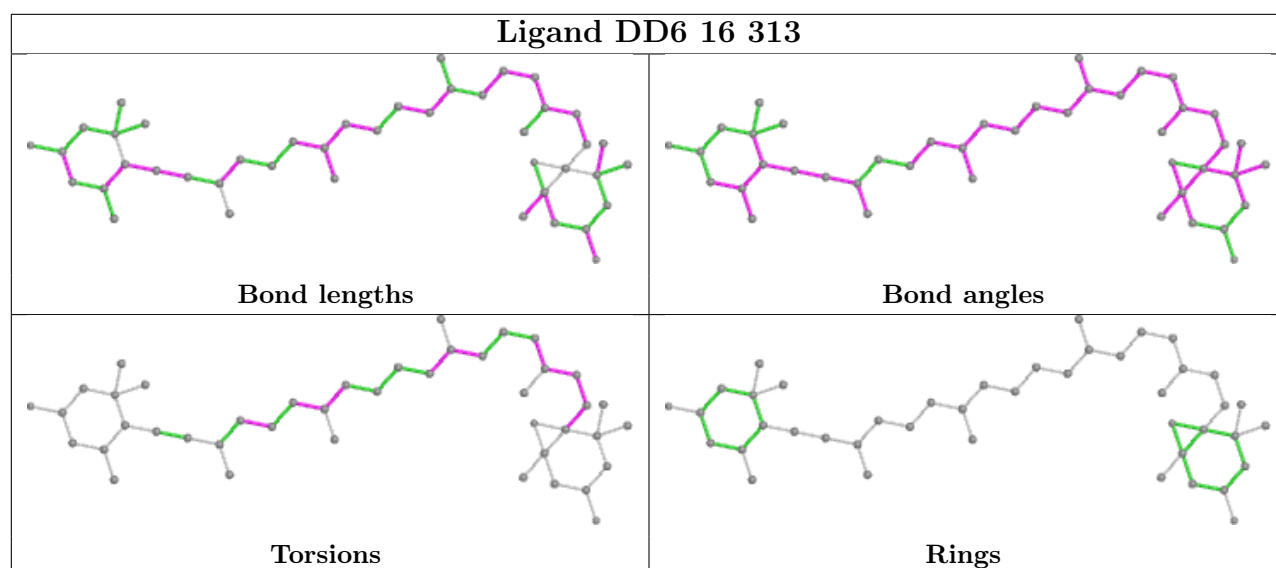
Rings

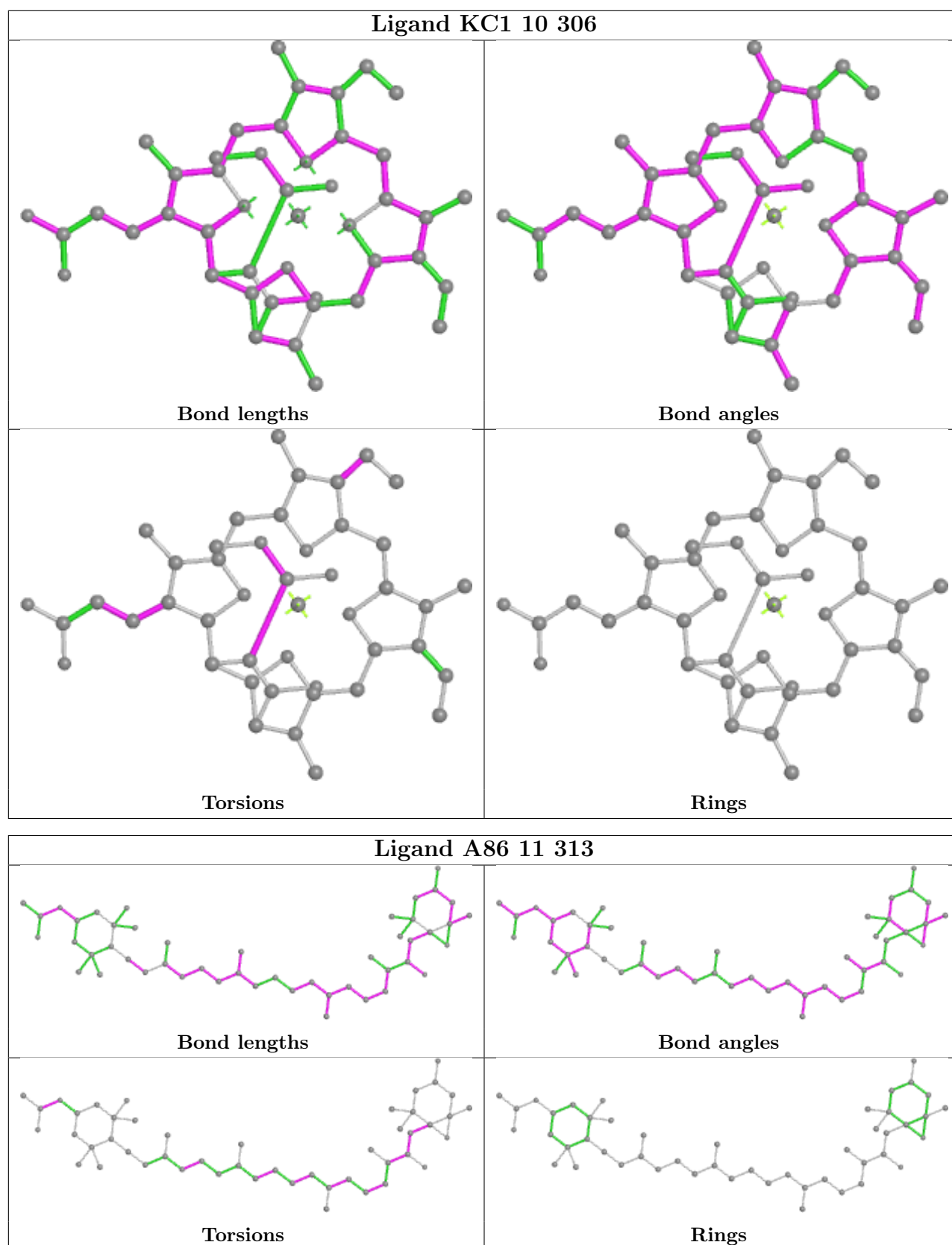


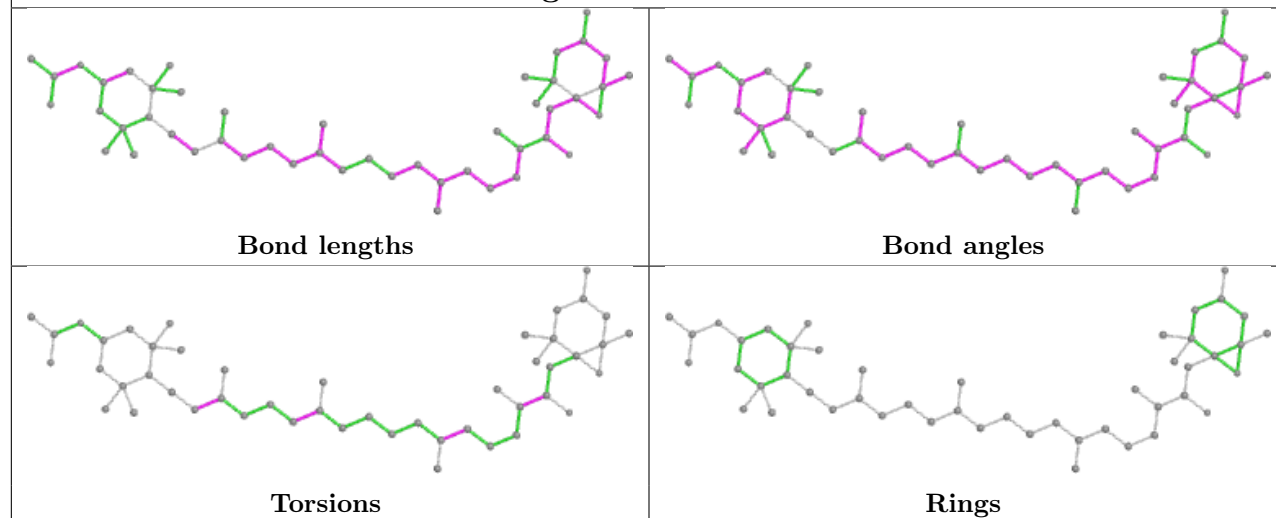
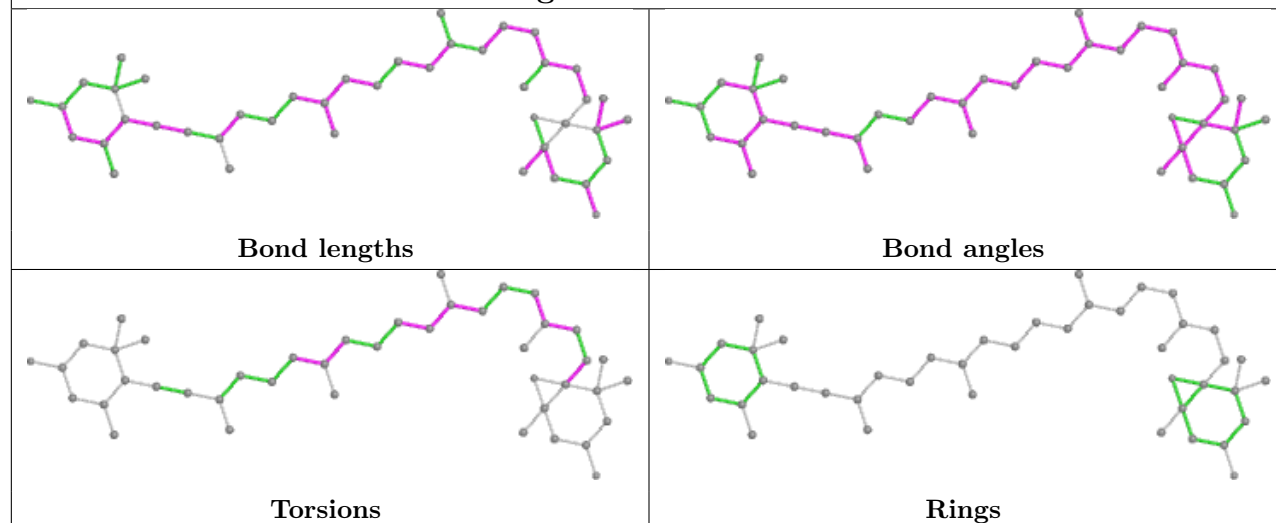
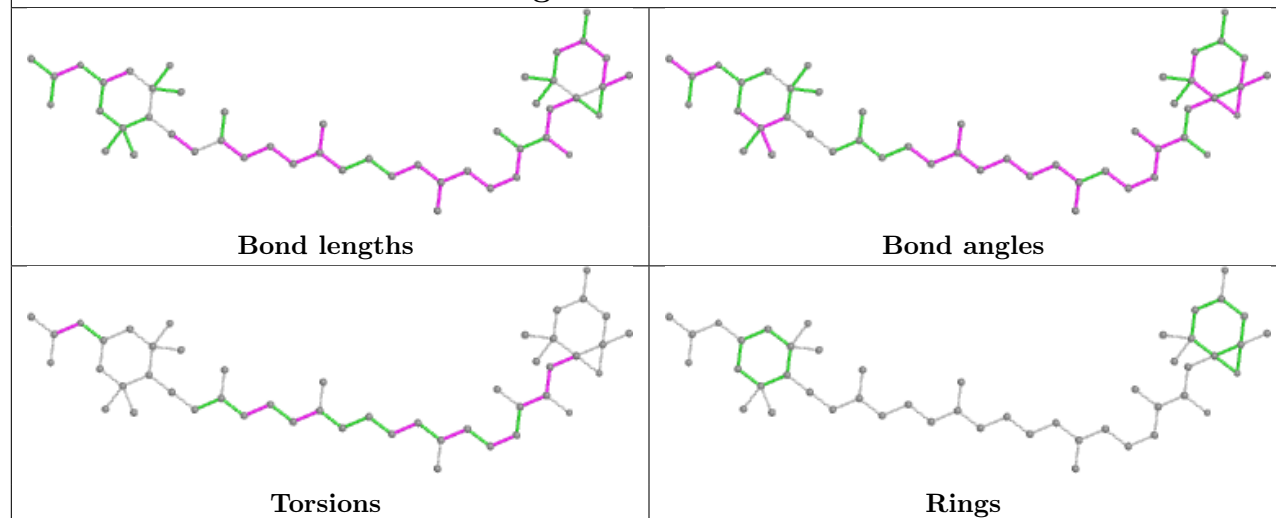


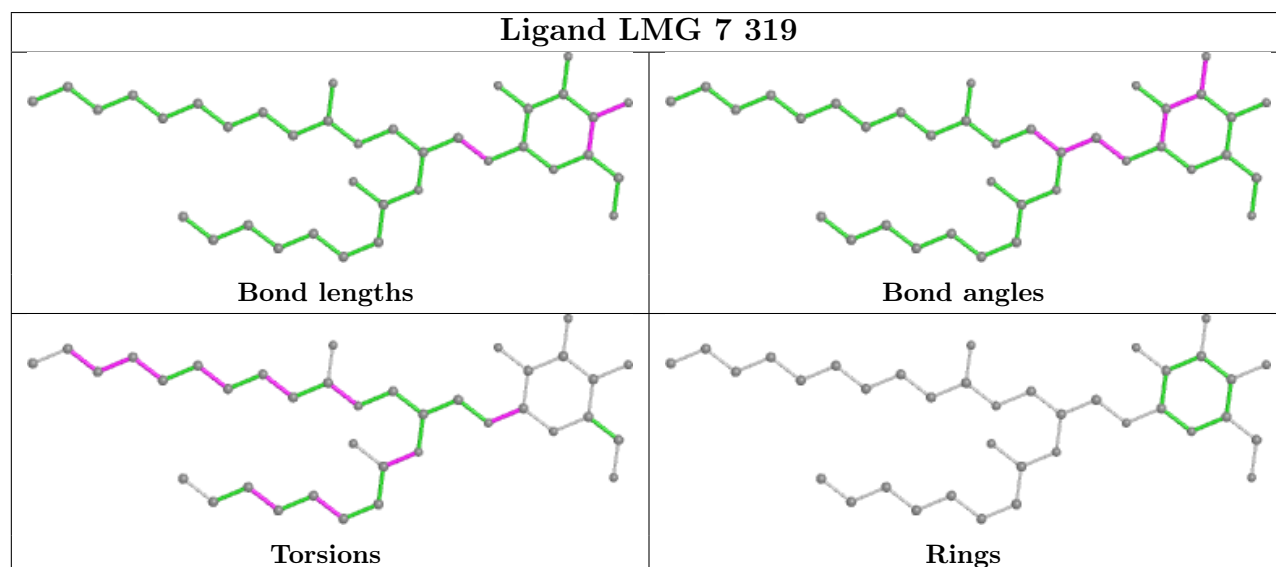
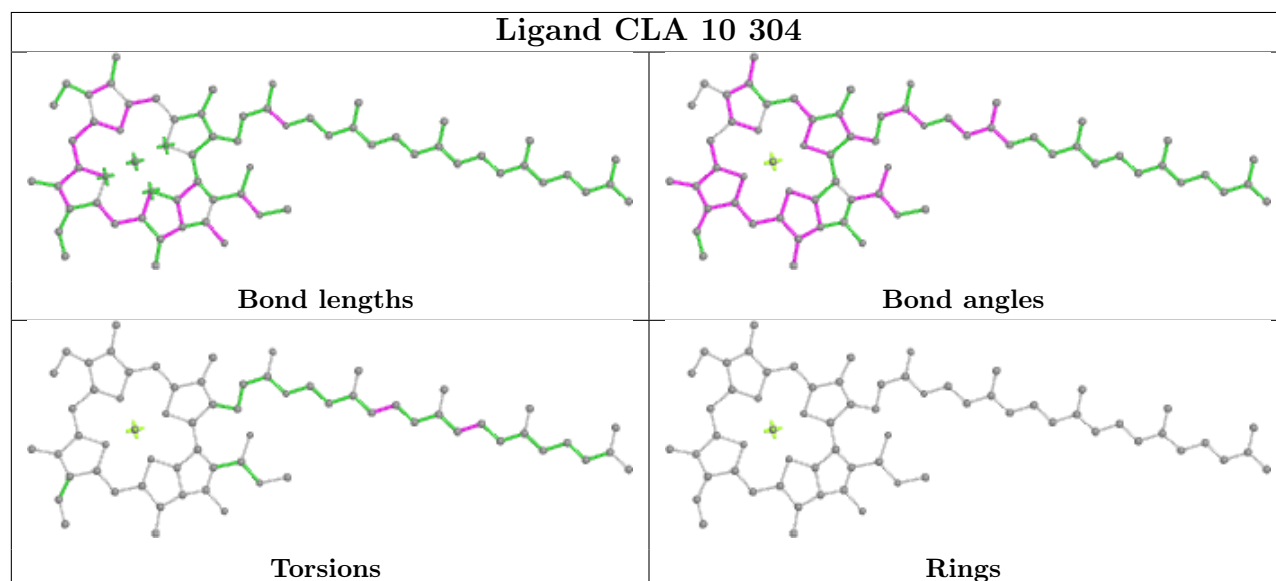
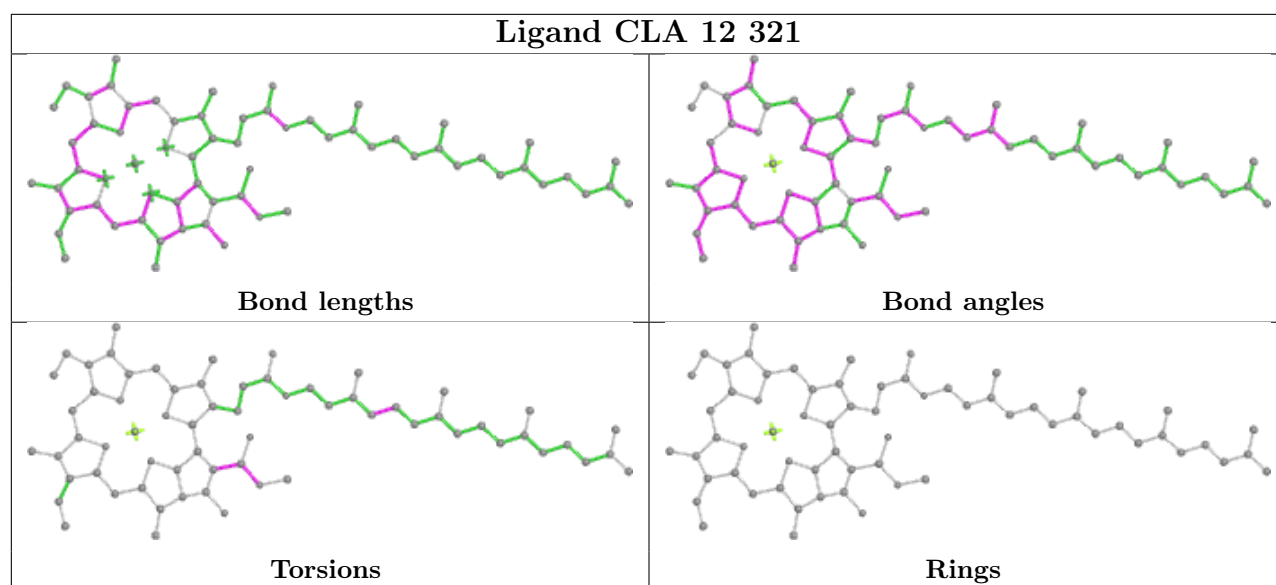


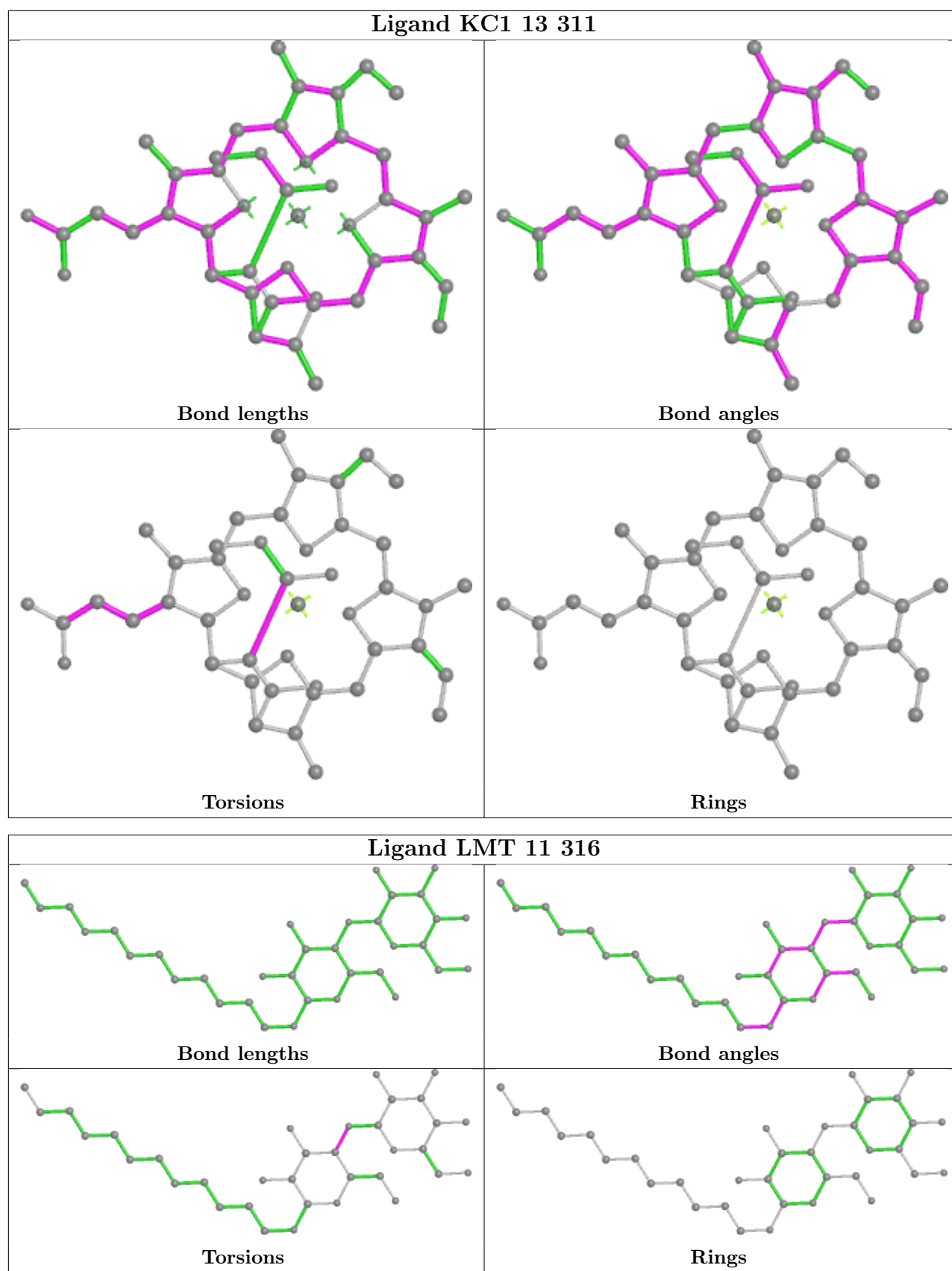


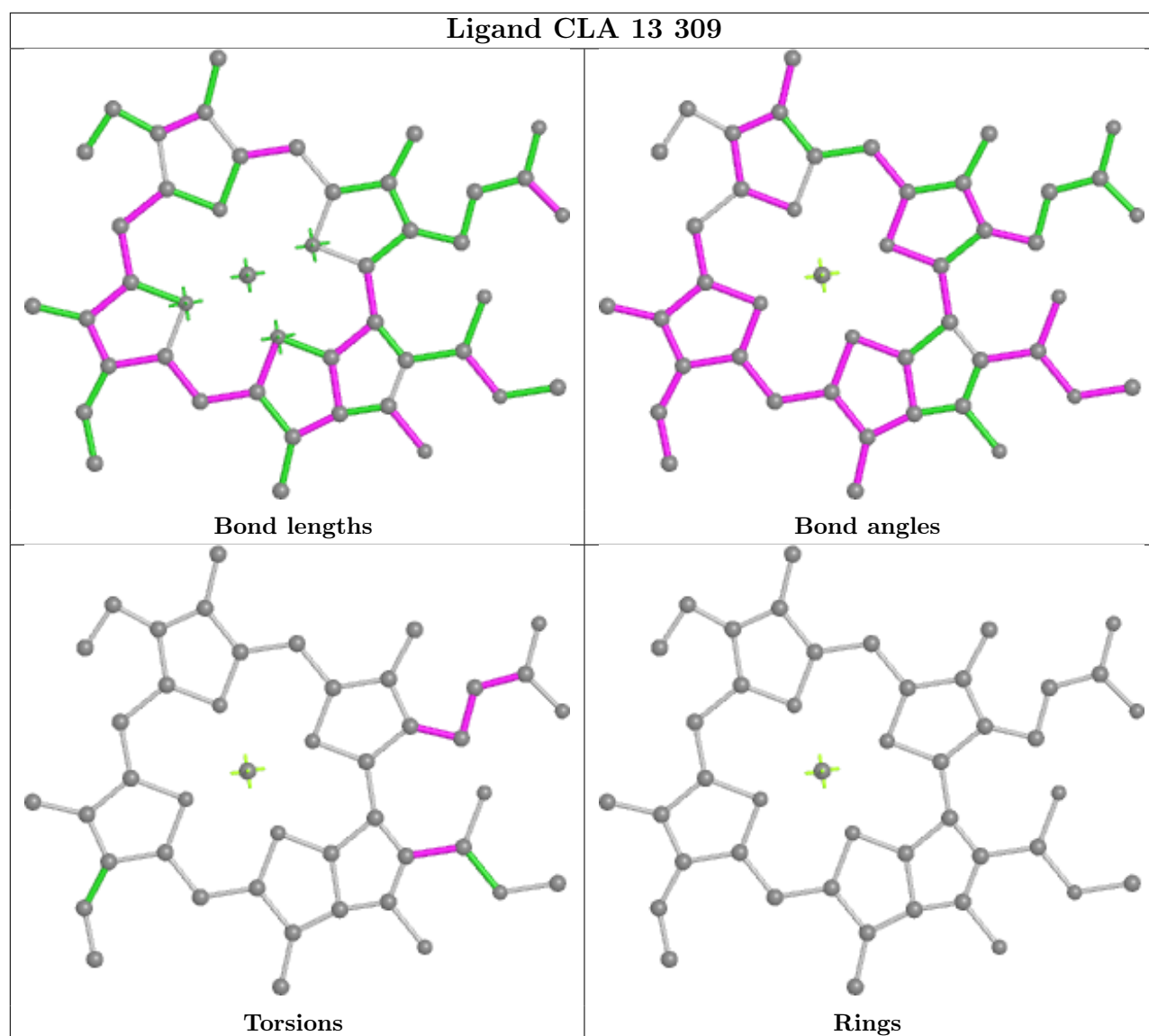


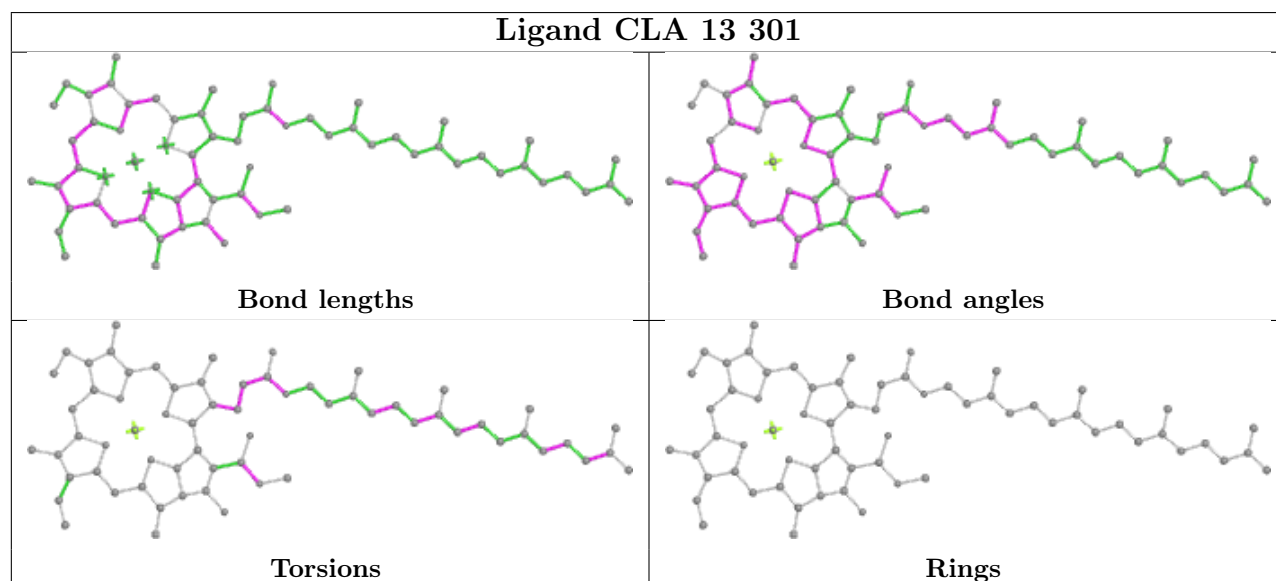
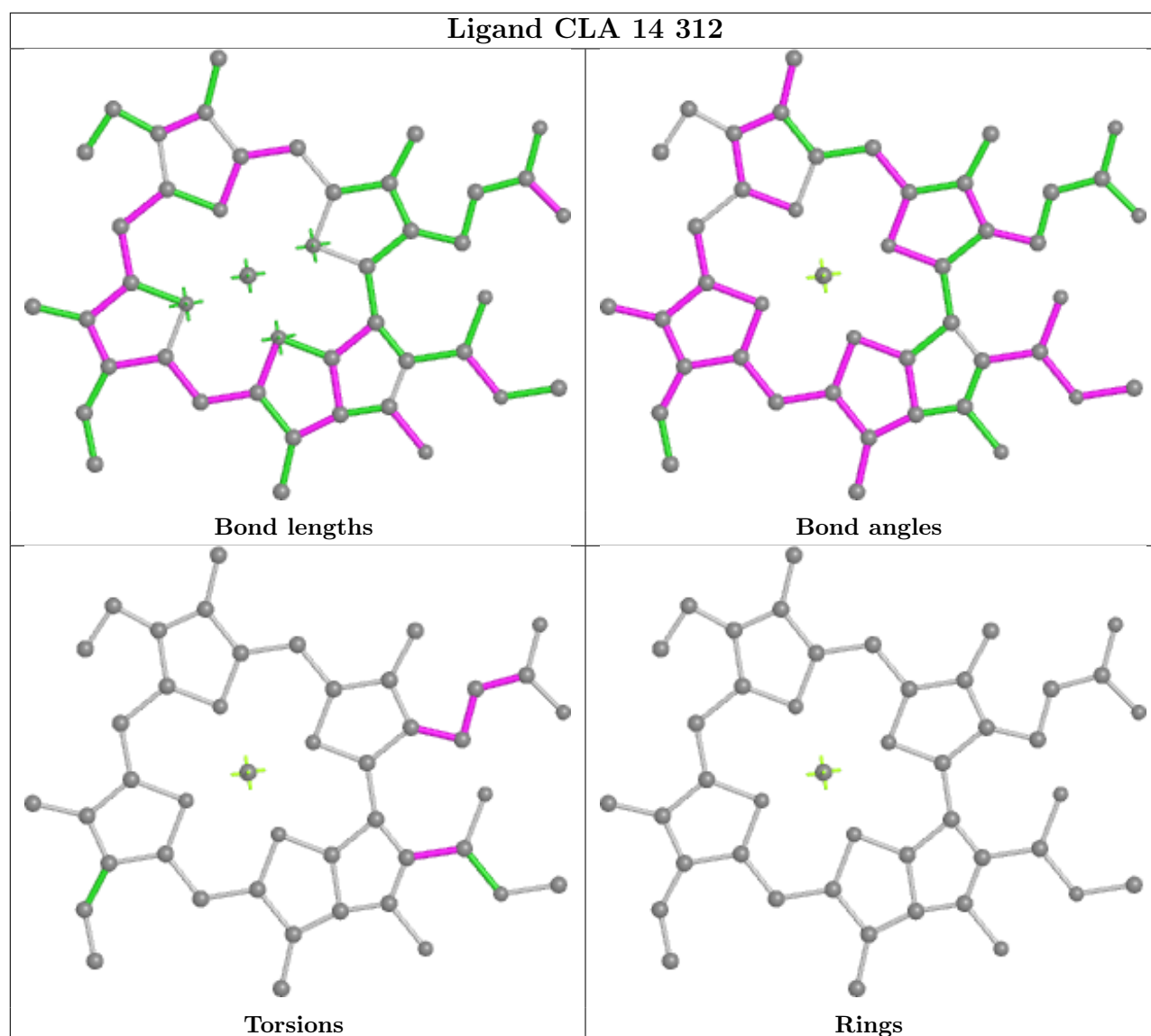


Ligand A86 6 317**Ligand DD6 8 317****Ligand A86 14 318**

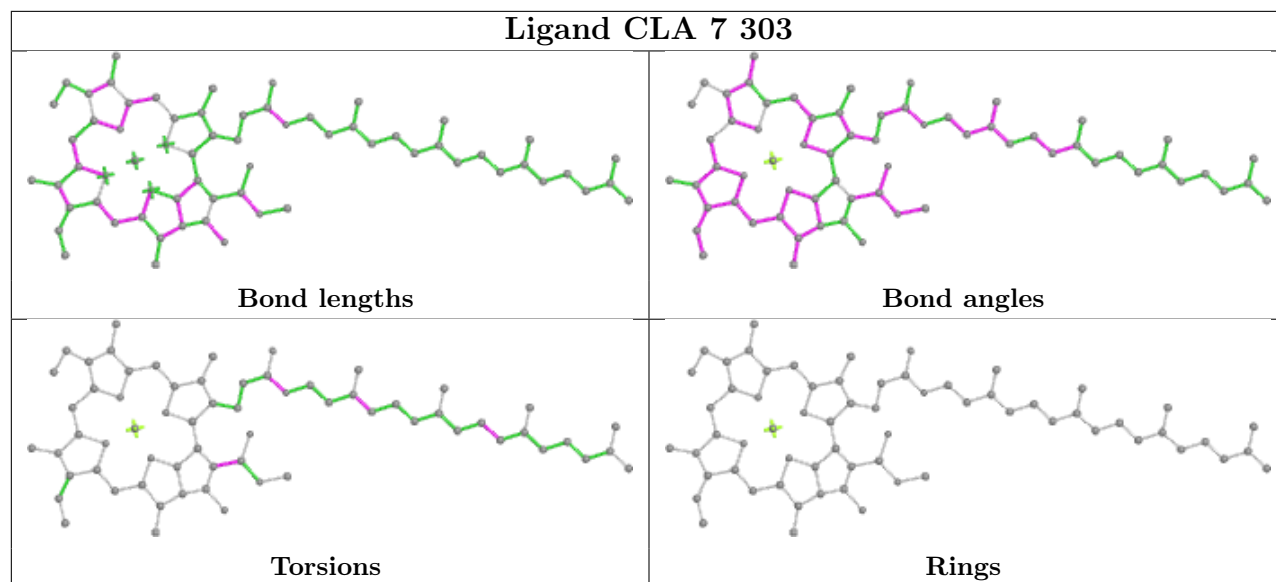




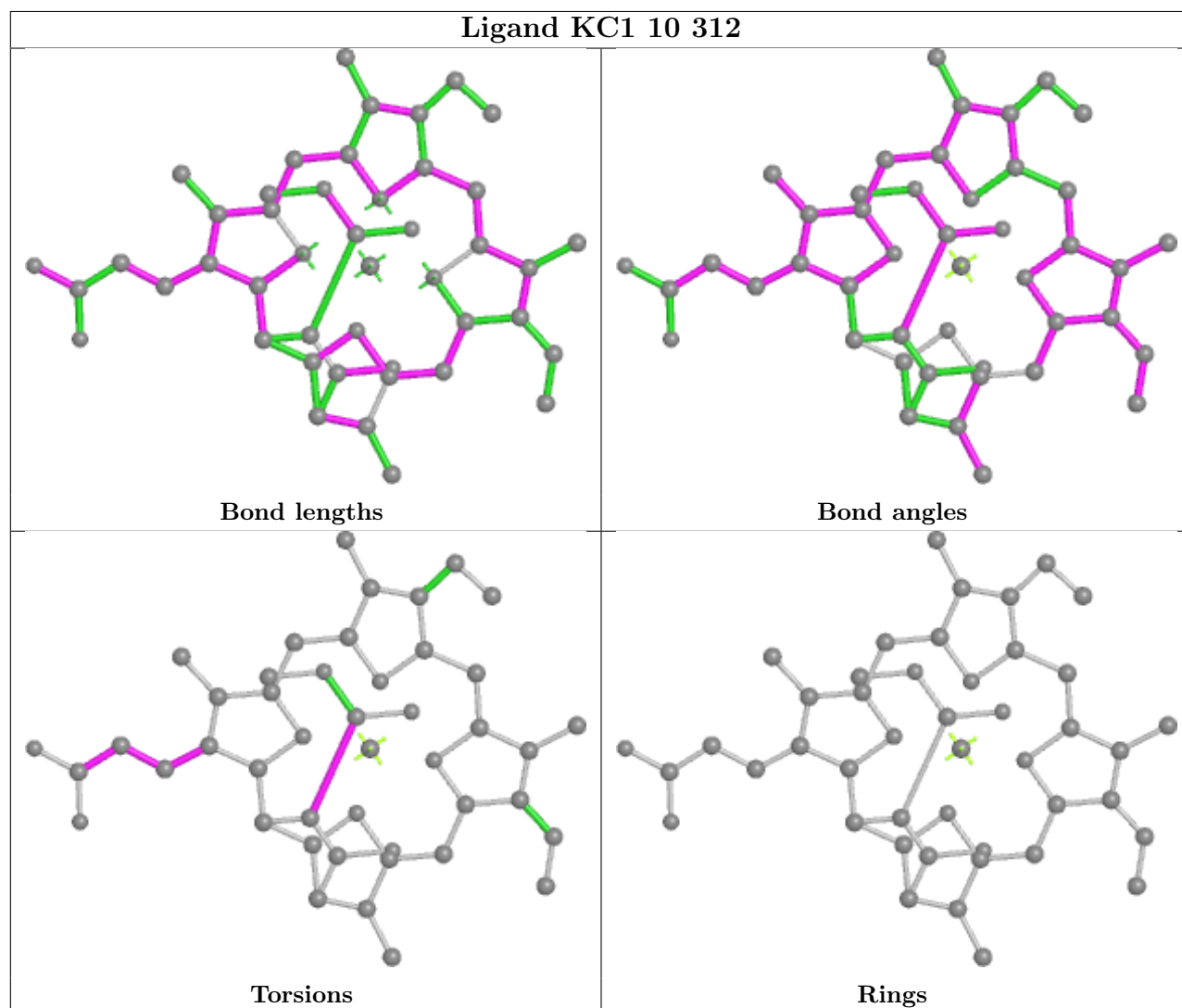




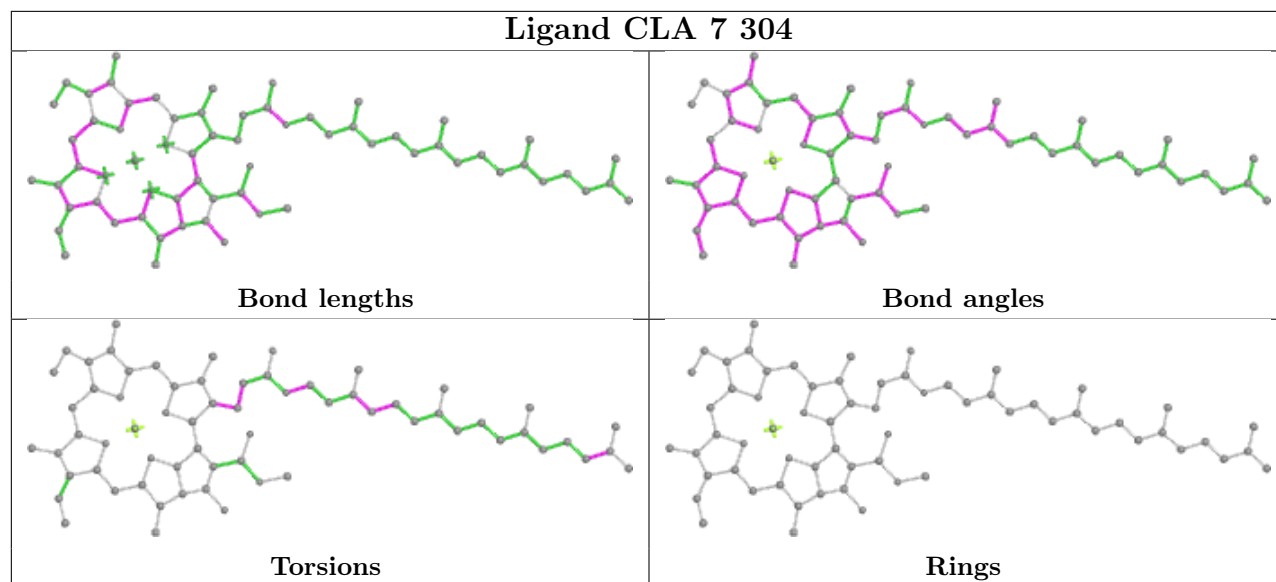
Ligand CLA 7 303



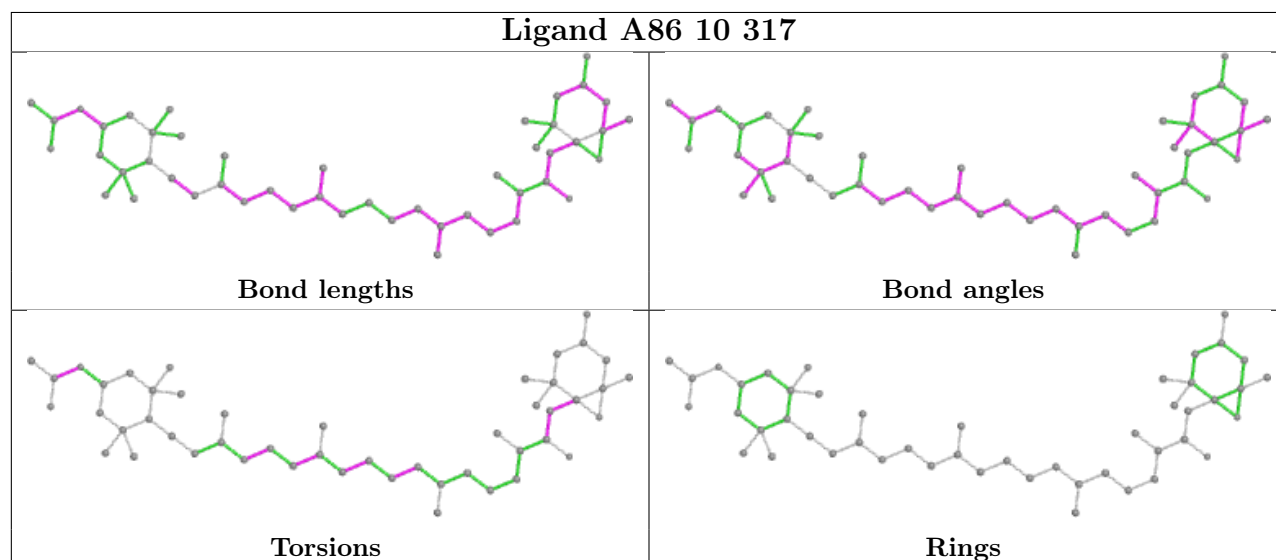
Ligand KC1 10 312



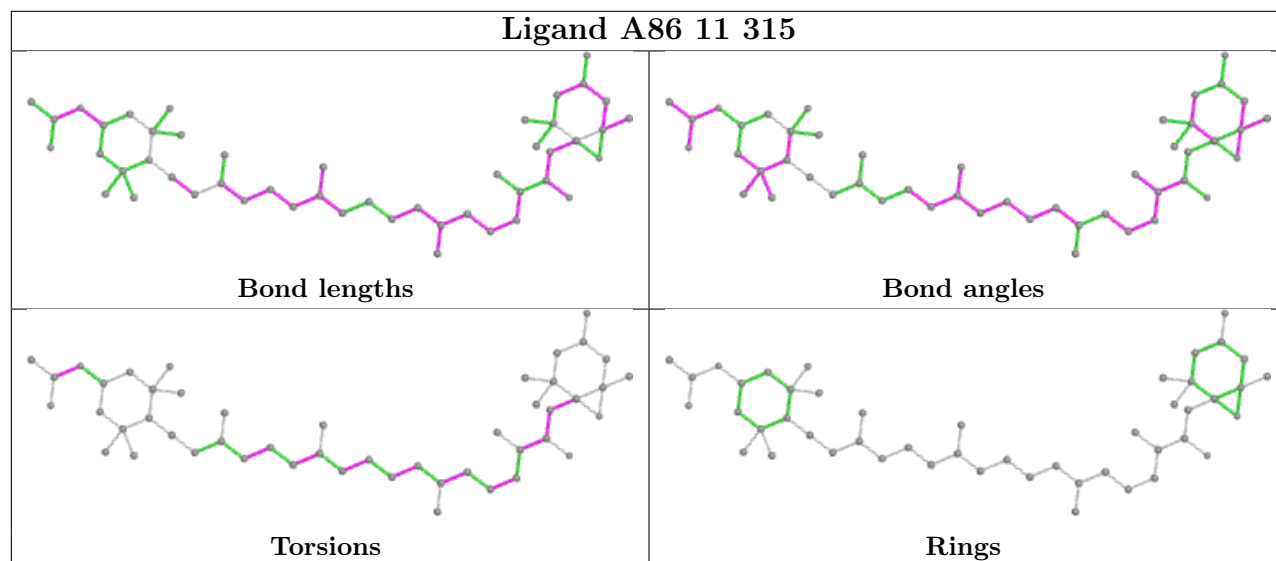
Ligand CLA 7 304

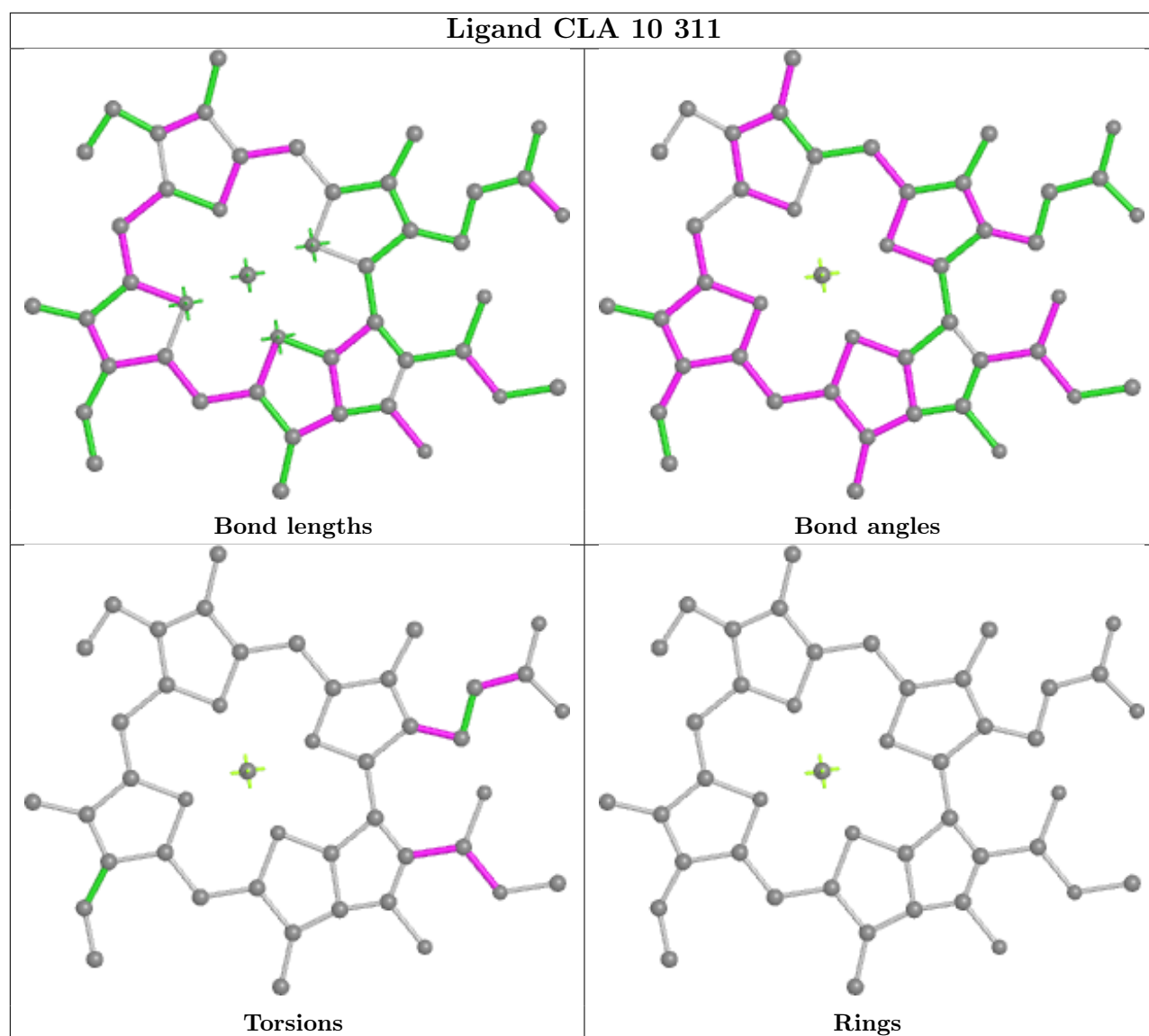


Ligand A86 10 317

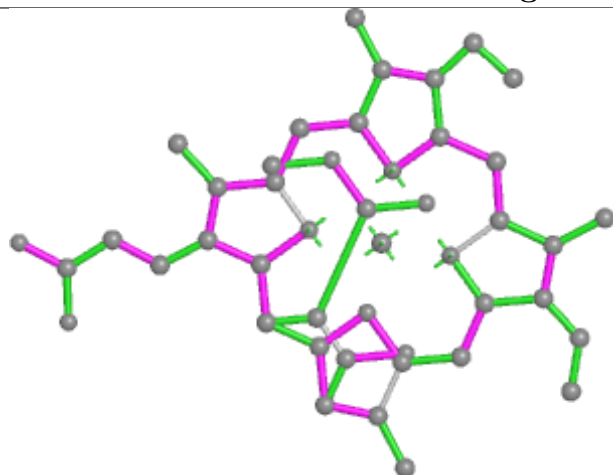


Ligand A86 11 315

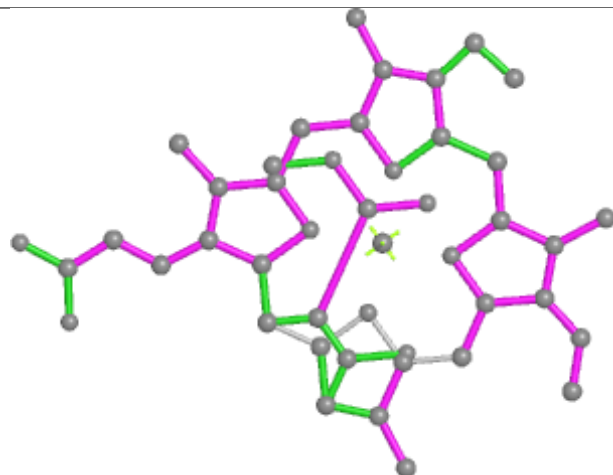




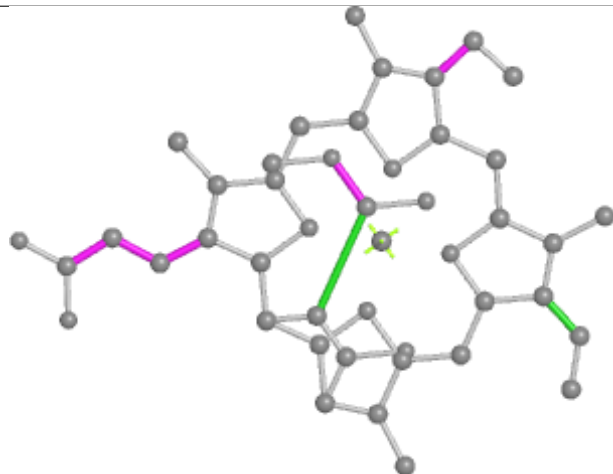
Ligand KC1 8 307



Bond lengths



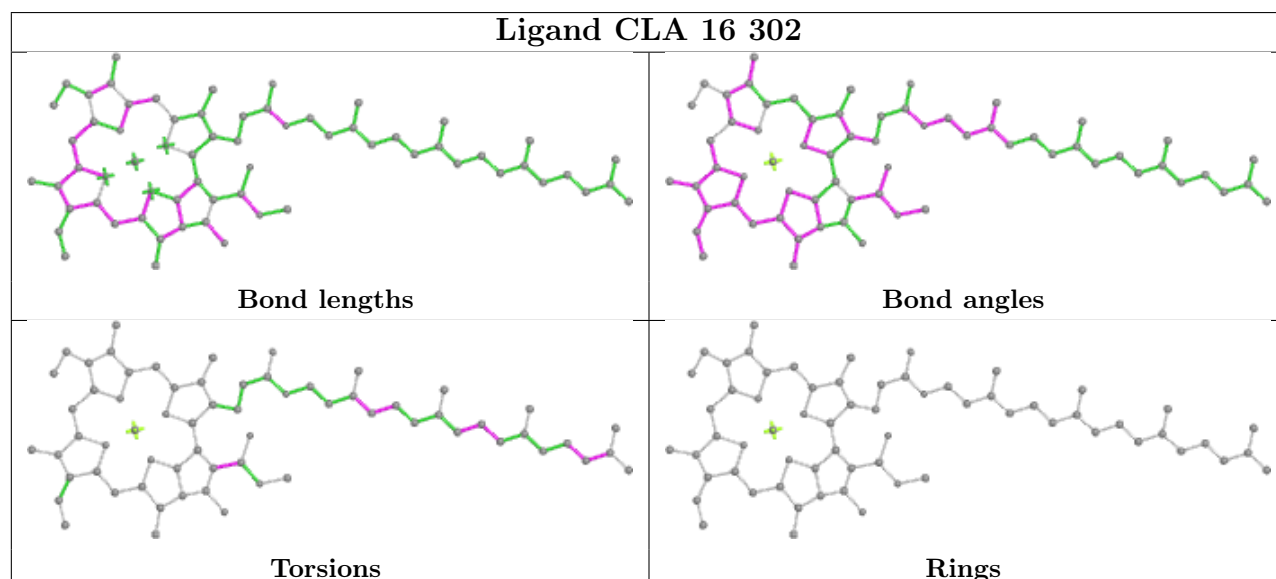
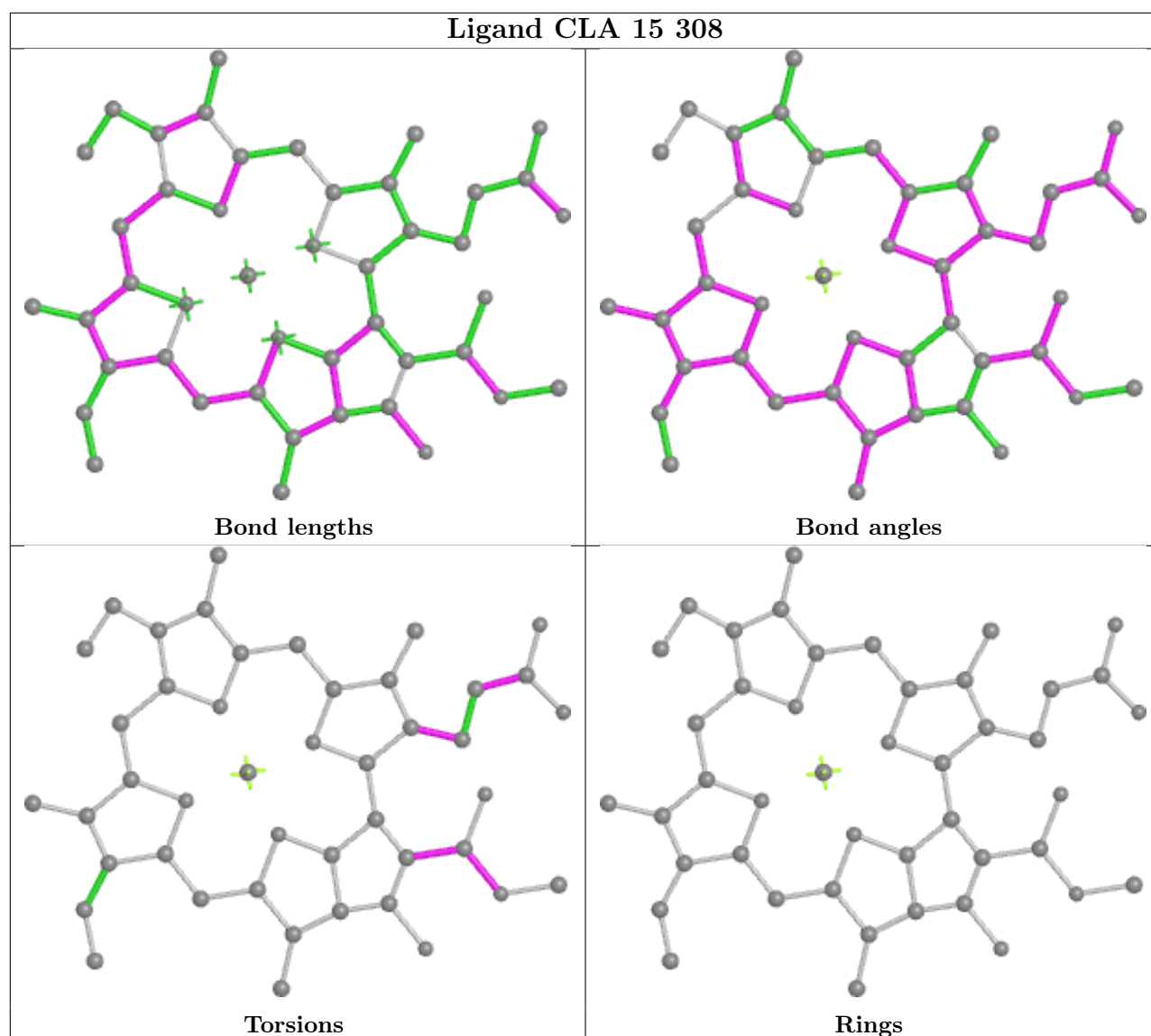
Bond angles

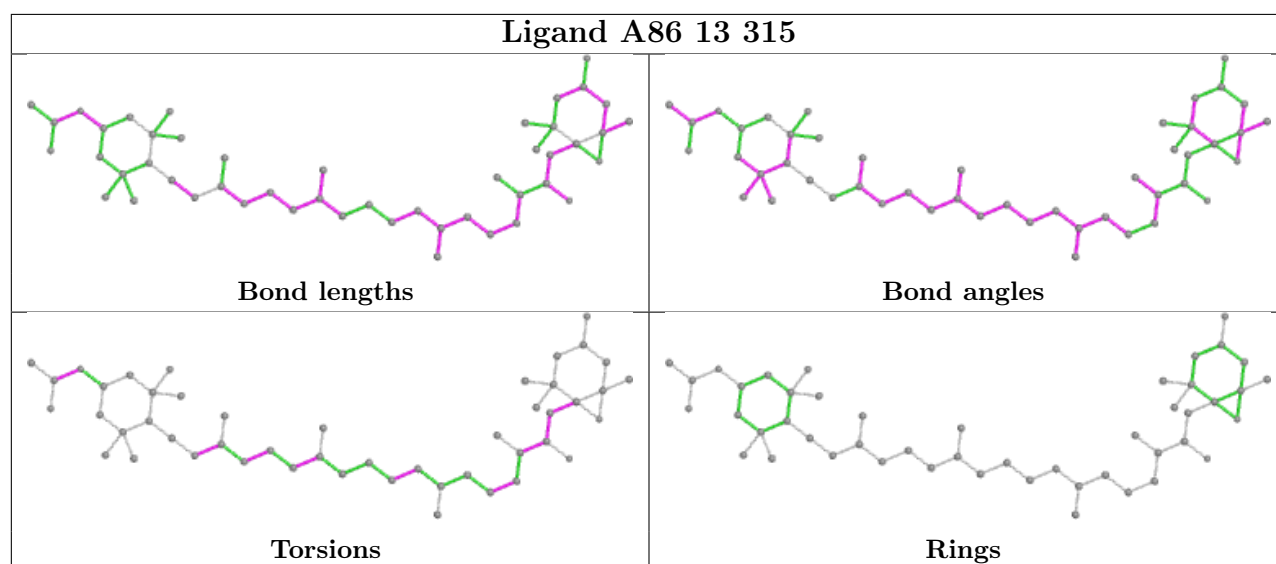
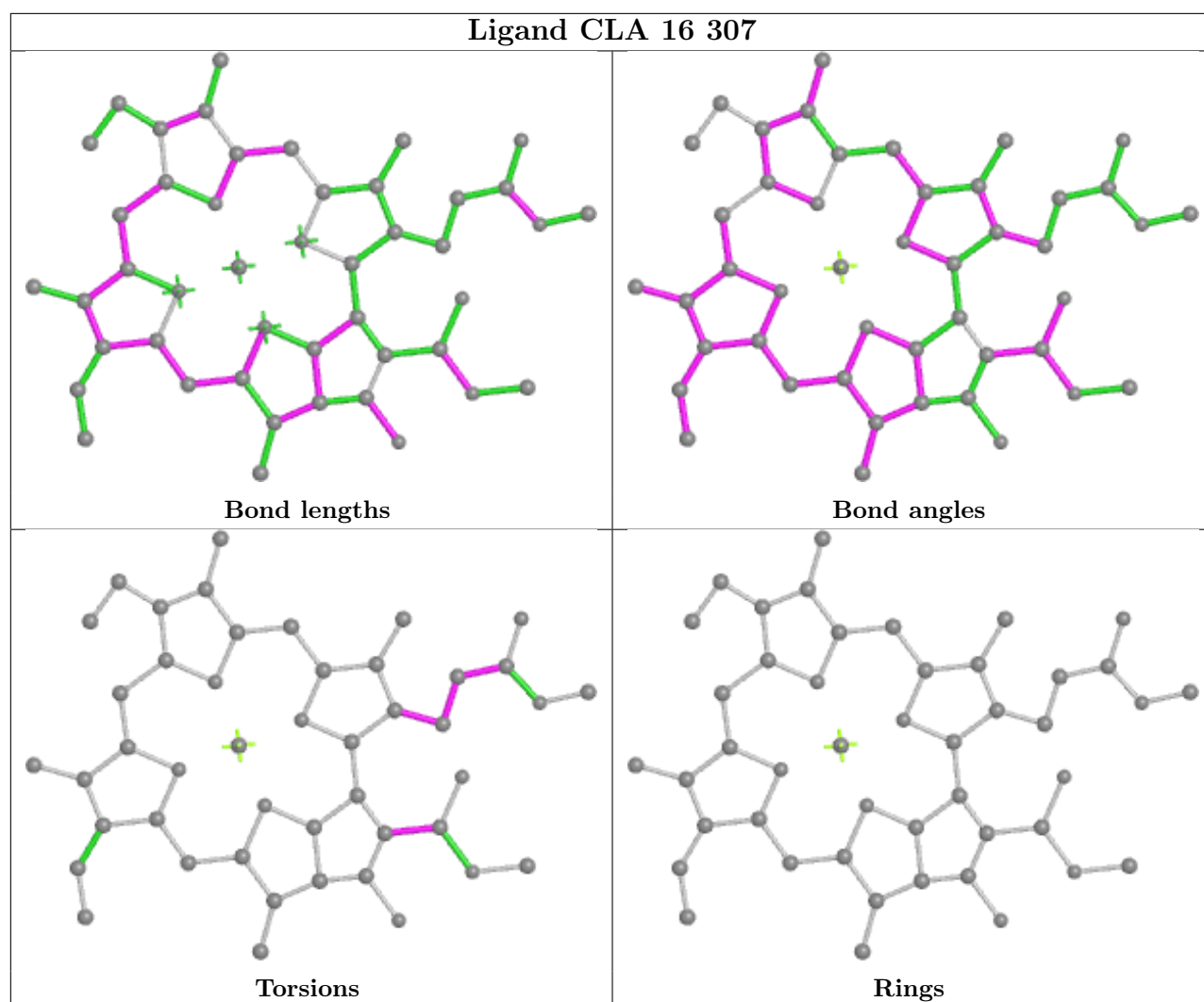


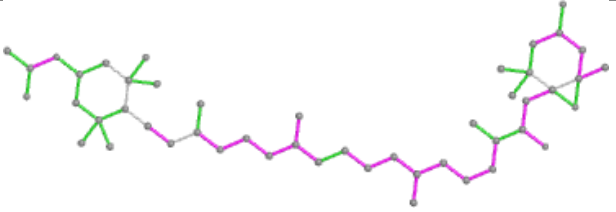
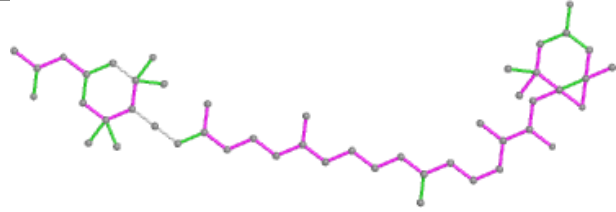
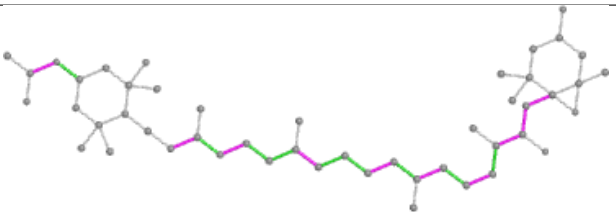
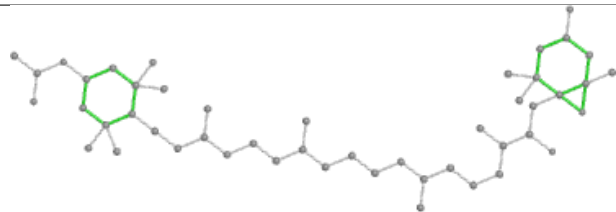
Torsions

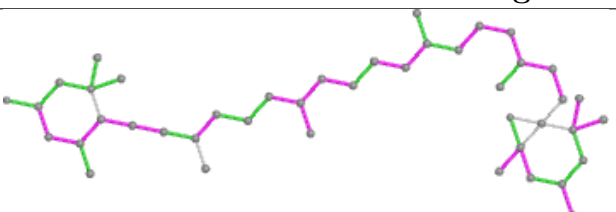
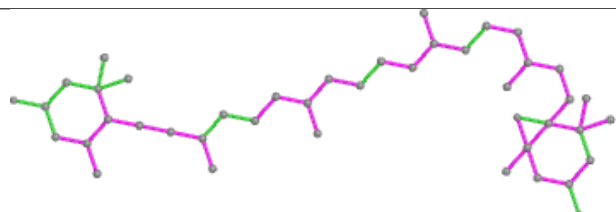
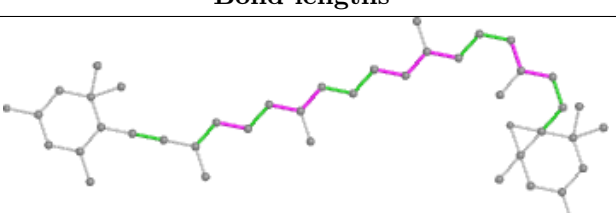
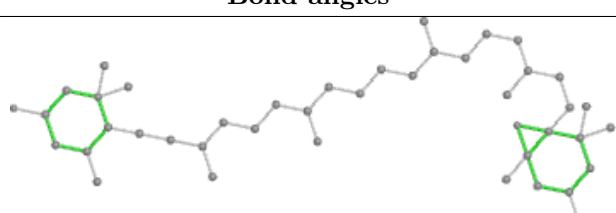


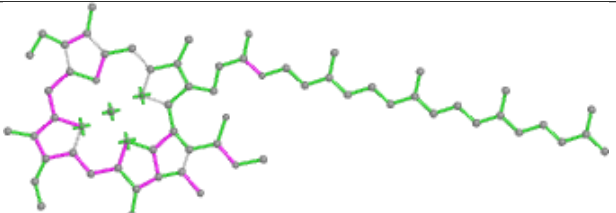
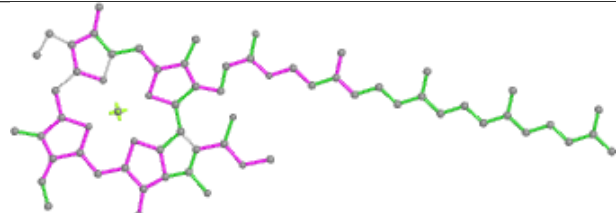
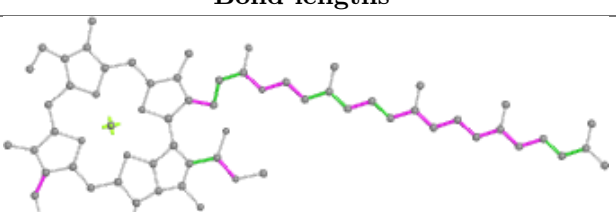
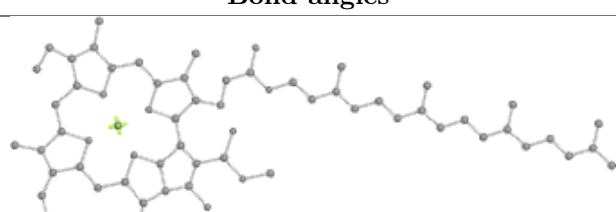
Rings

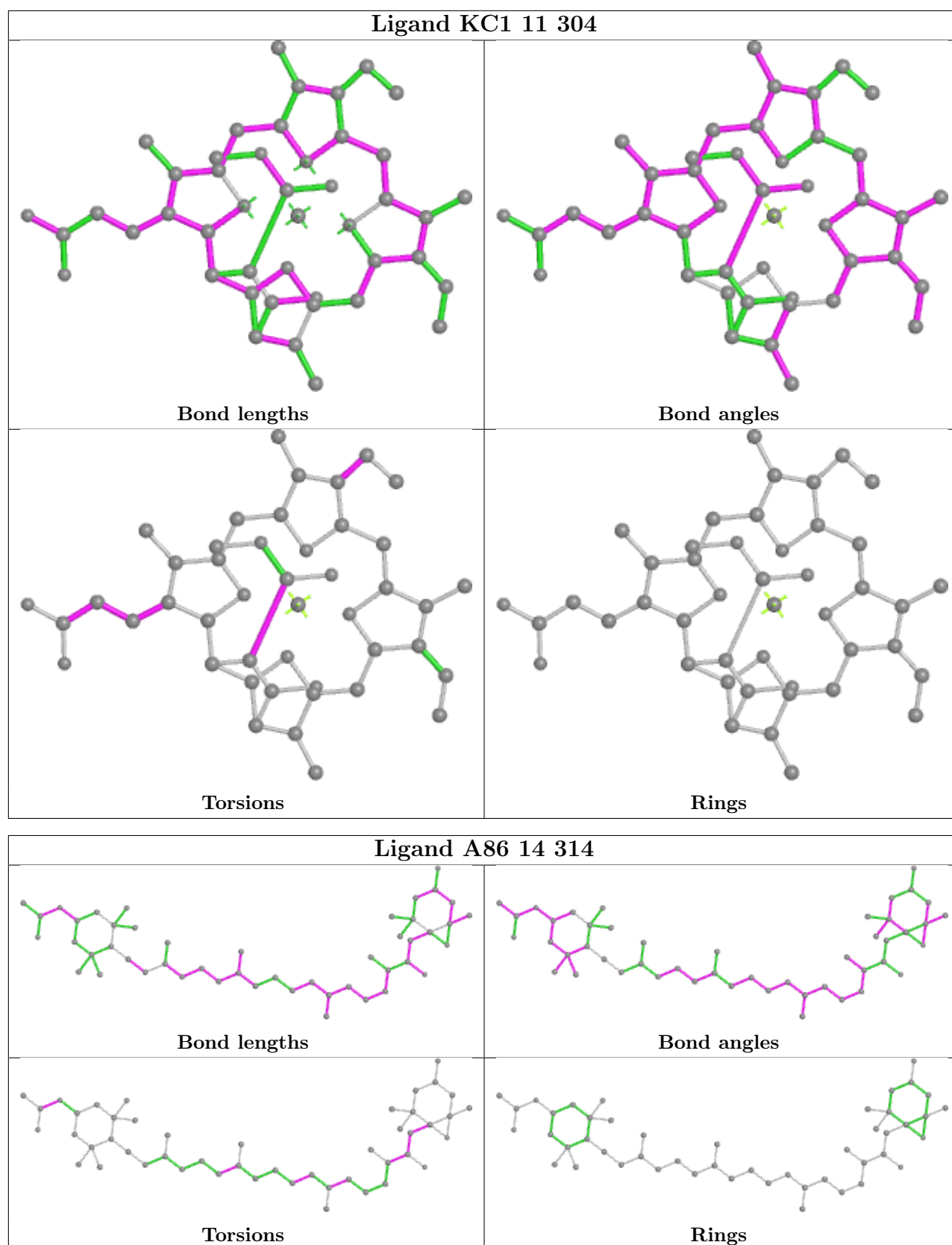


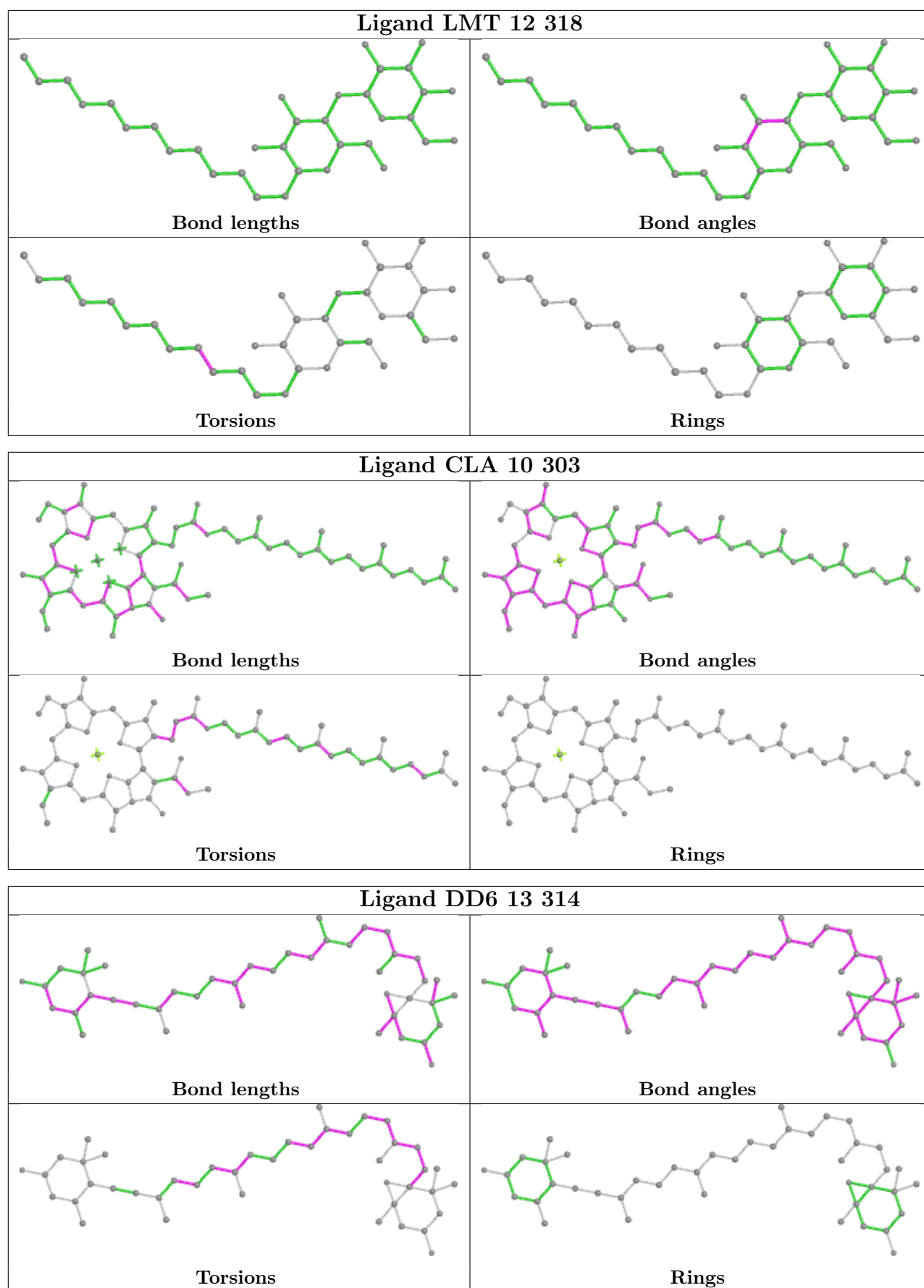


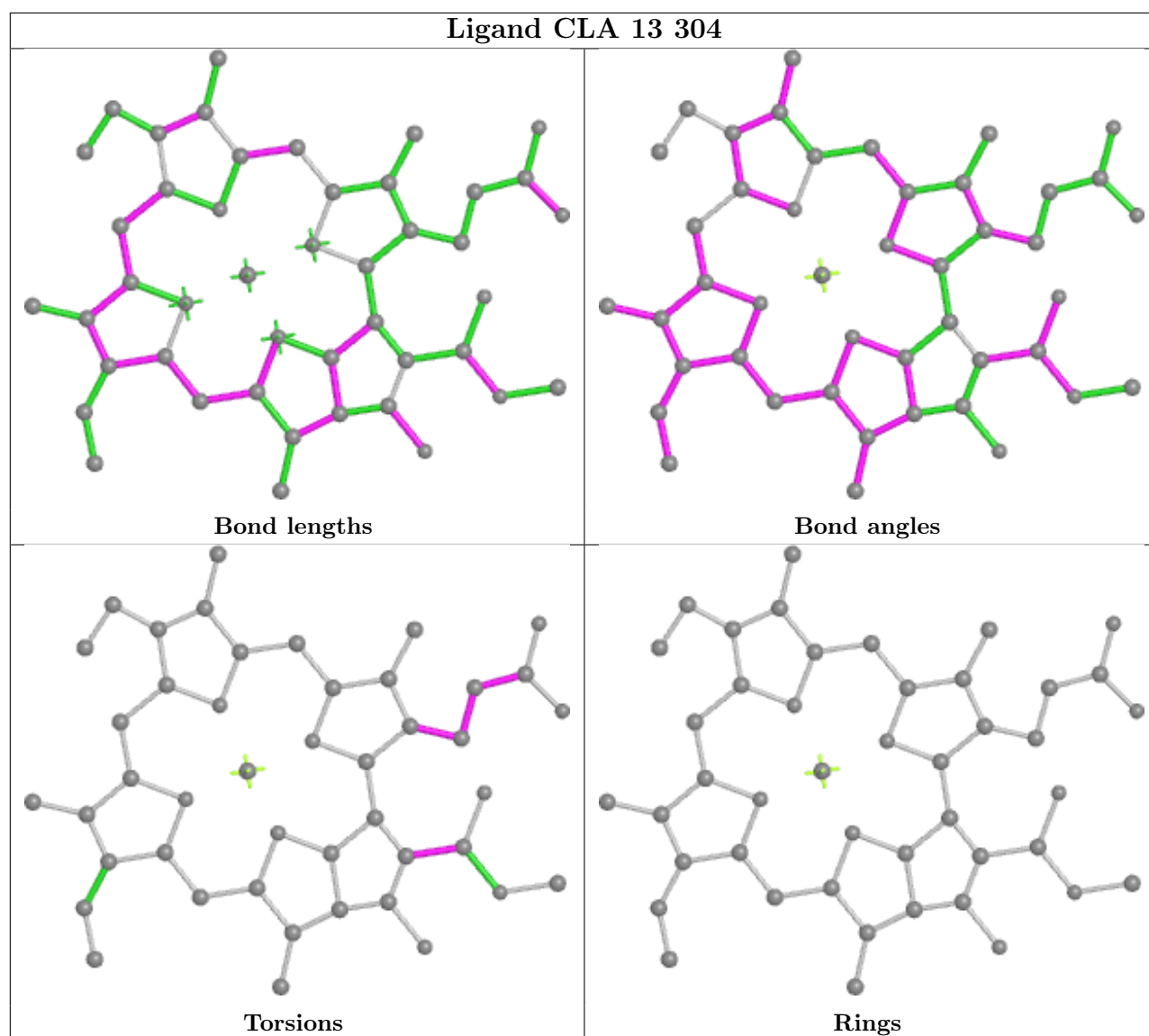
Ligand A86 15 322	
	
Bond lengths	Bond angles
	
Torsions	Rings

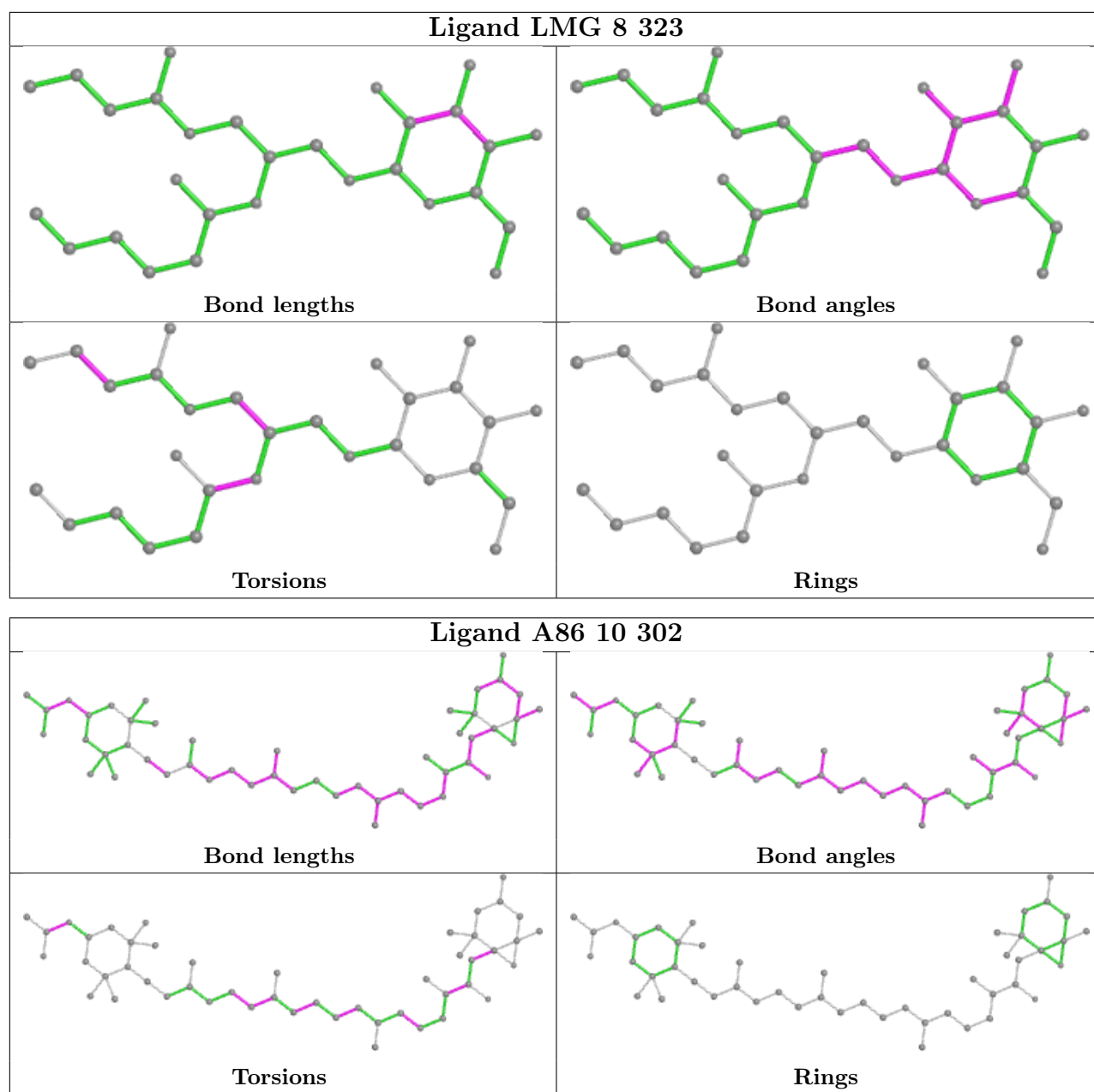
Ligand DD6 7 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

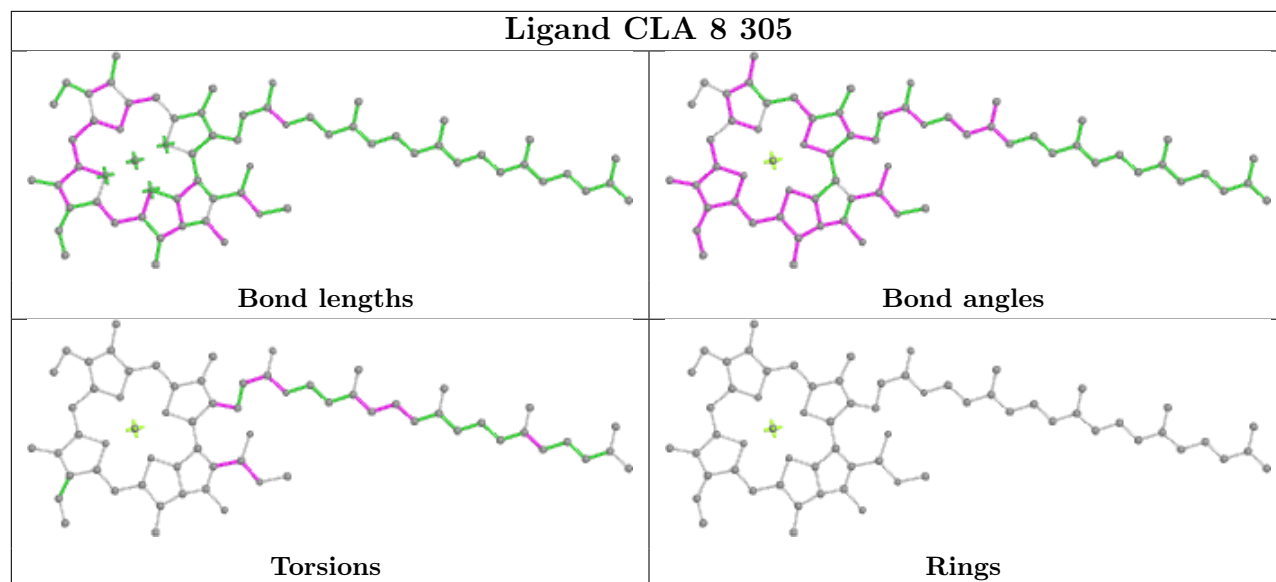
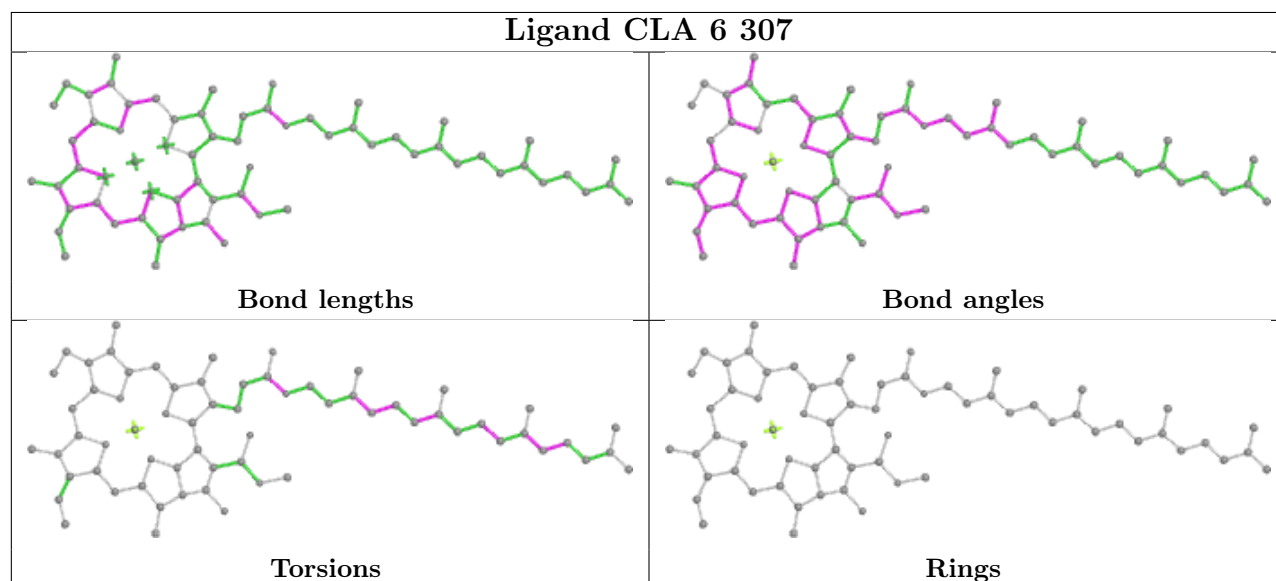
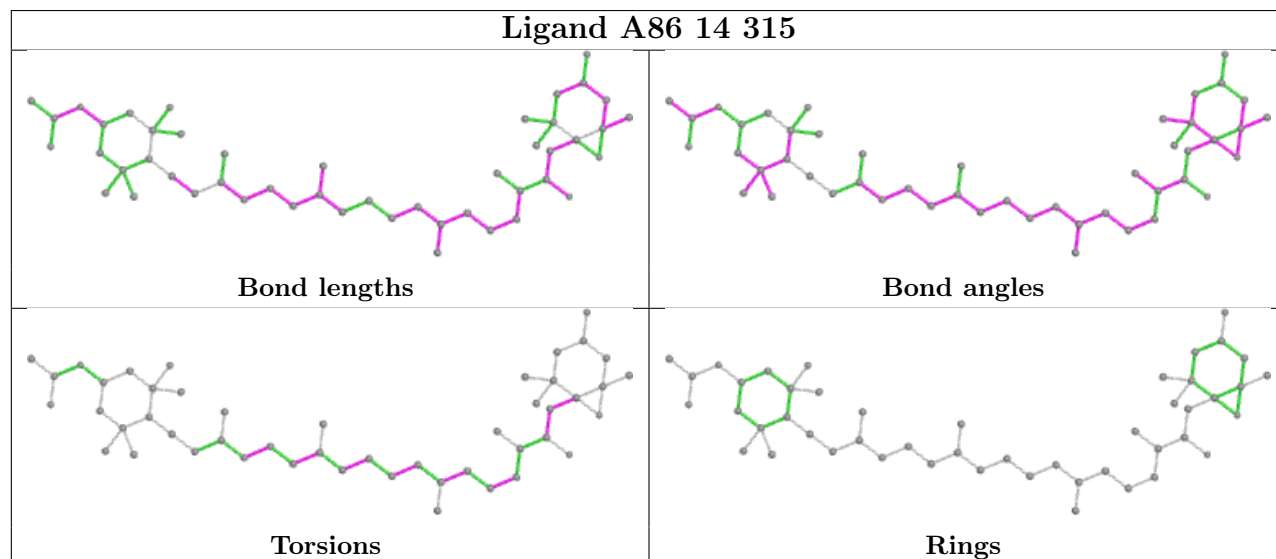
Ligand CLA 15 304	
	
Bond lengths	Bond angles
	
Torsions	Rings



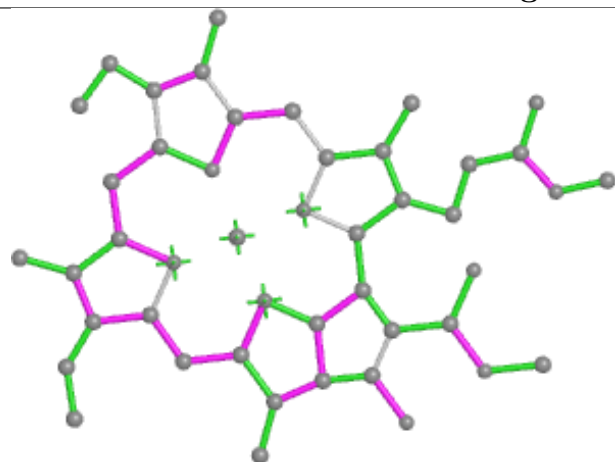




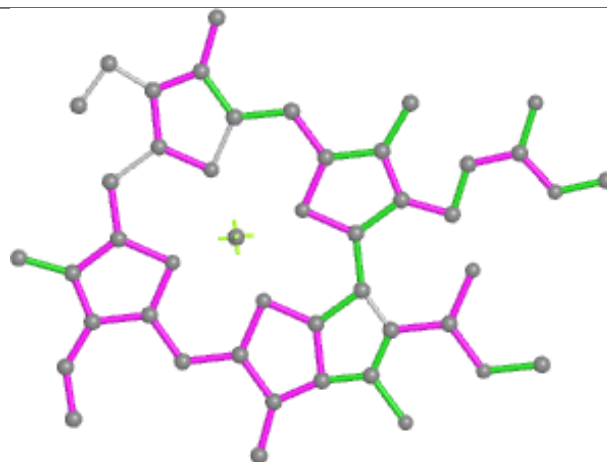


Ligand CLA 8 305**Ligand CLA 6 307****Ligand A86 14 315**

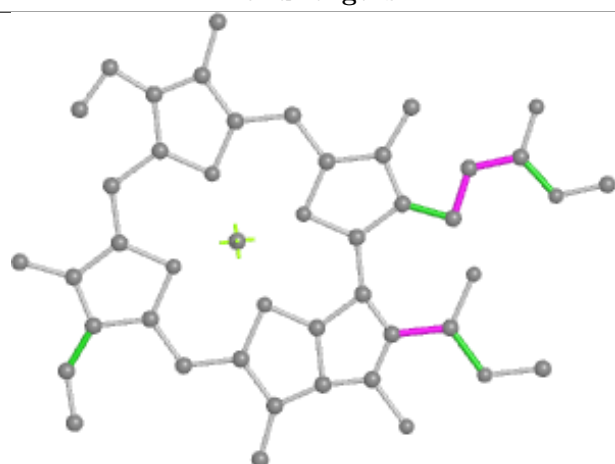
Ligand CLA 7 311



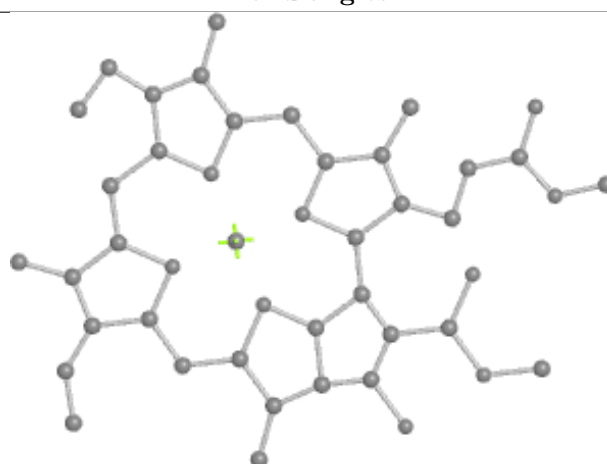
Bond lengths



Bond angles

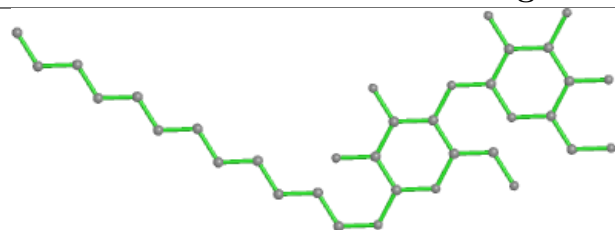


Torsions

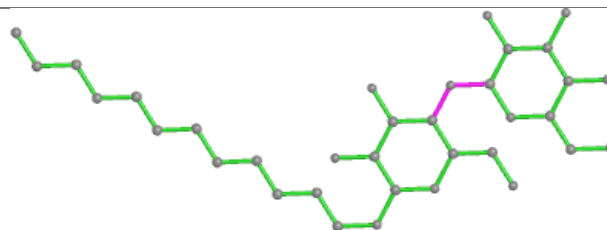


Rings

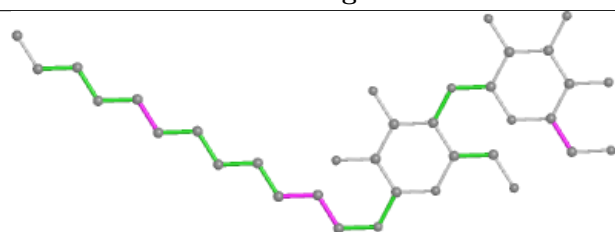
Ligand LMT 7 320



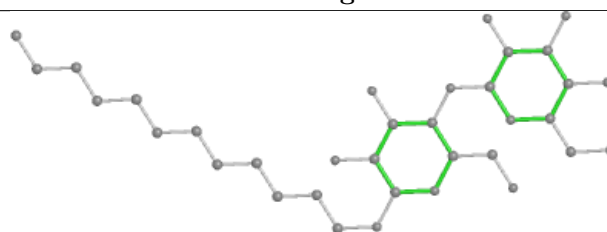
Bond lengths



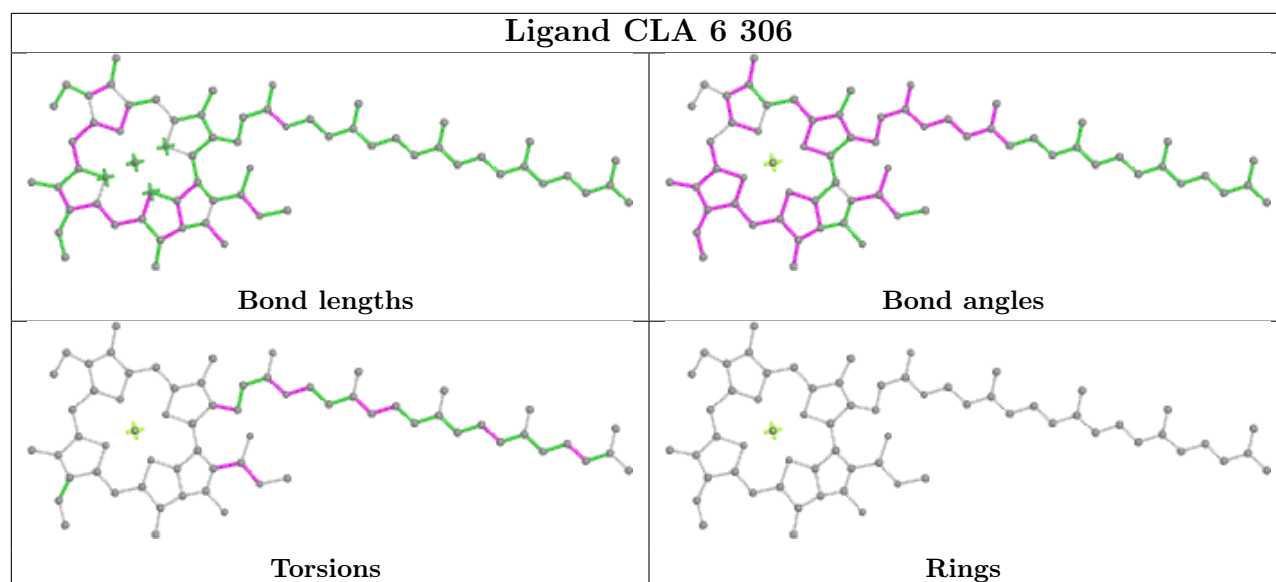
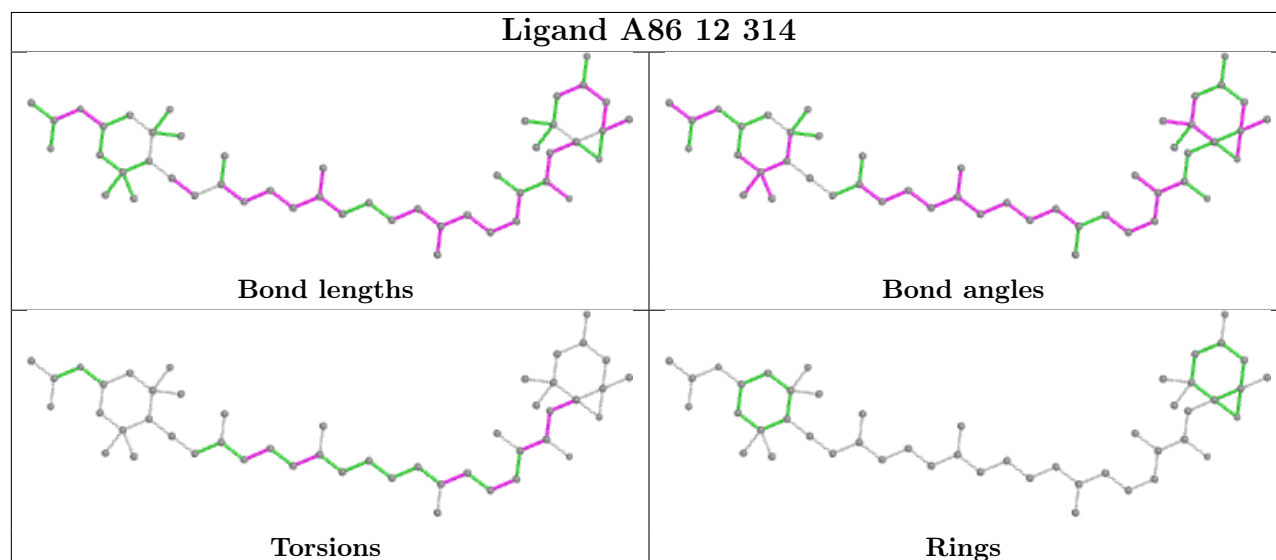
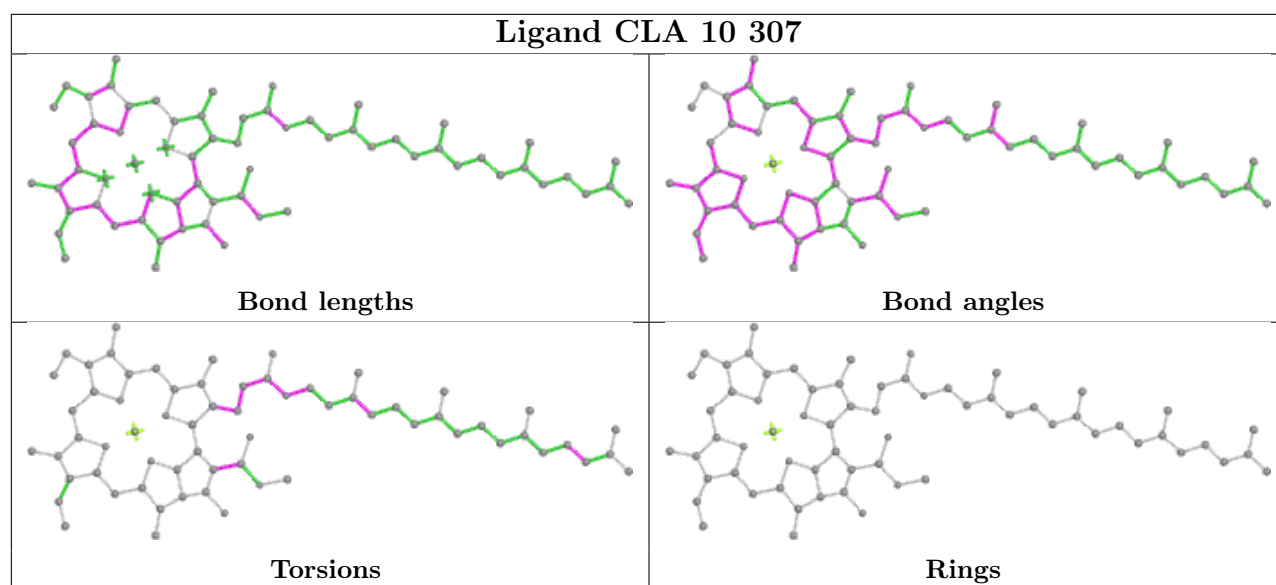
Bond angles

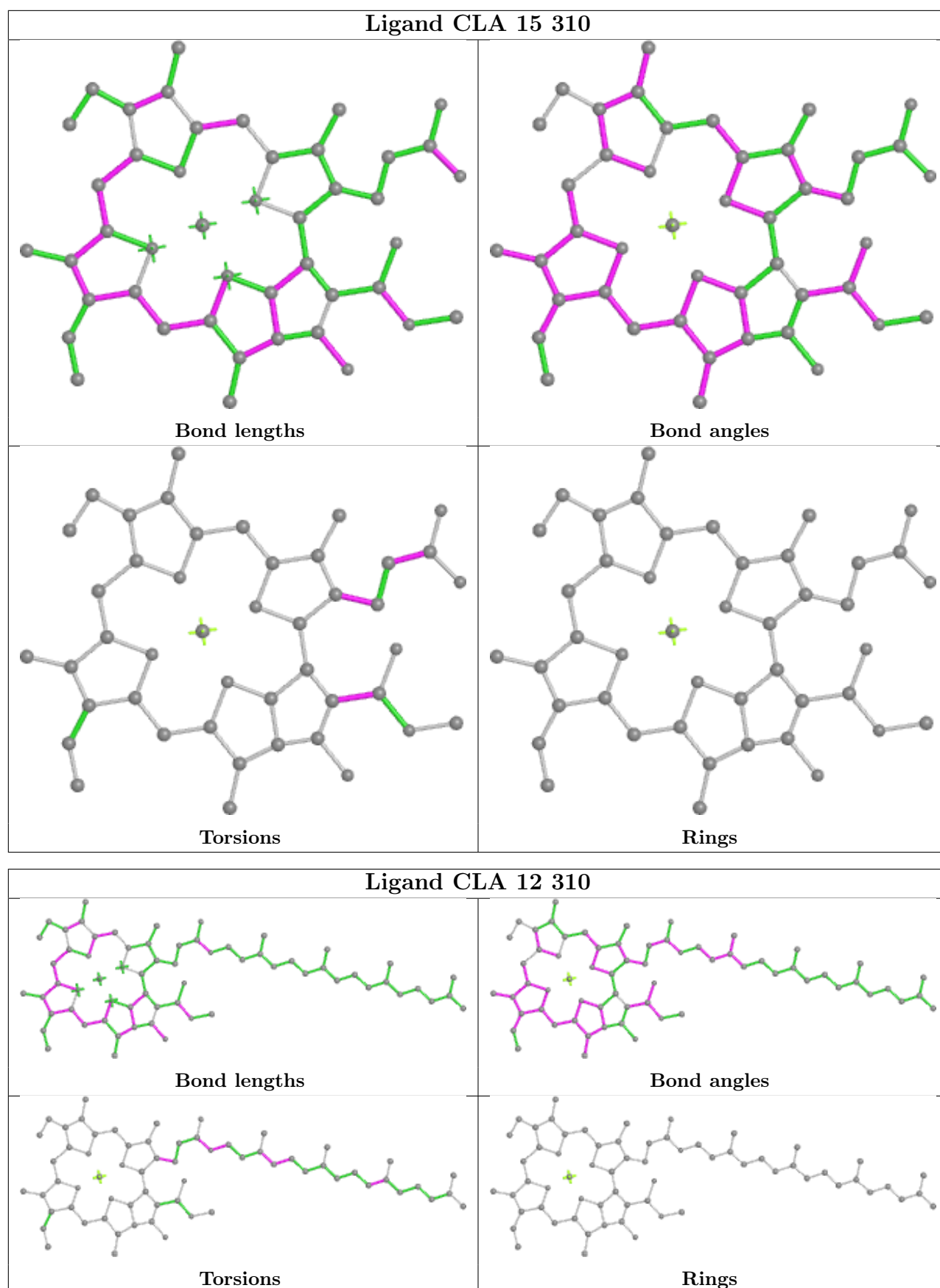


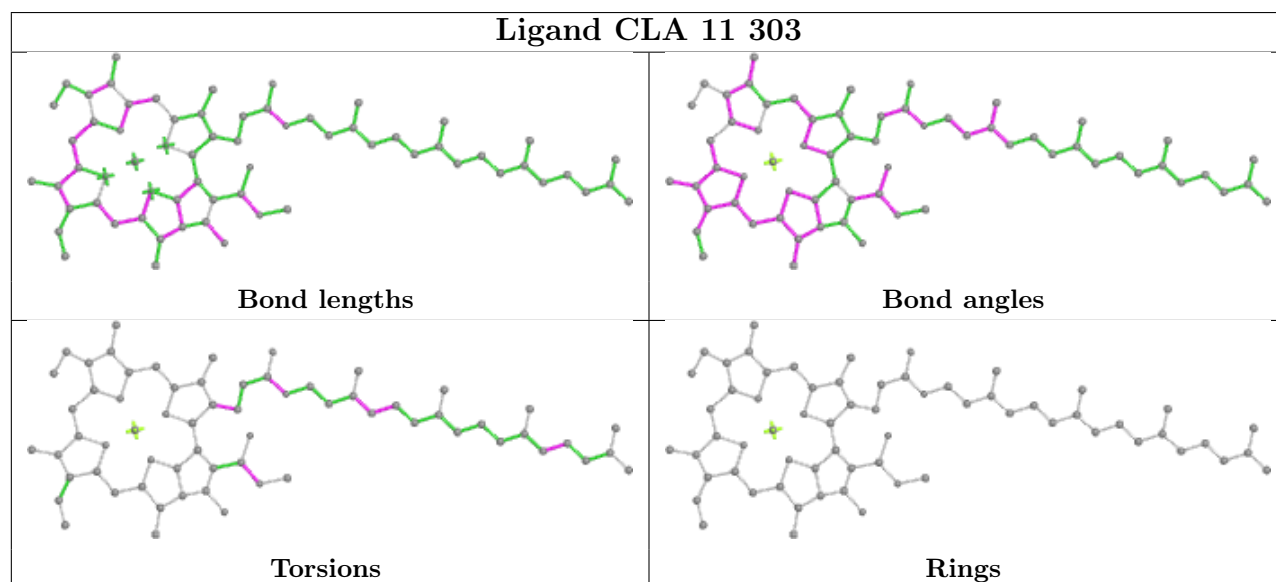
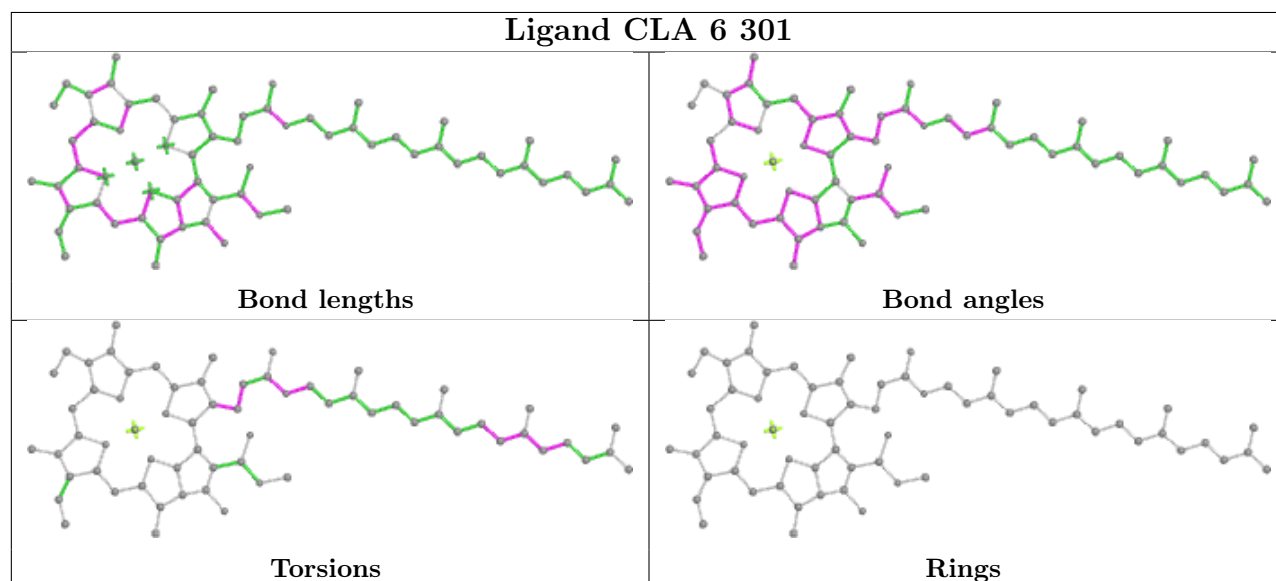
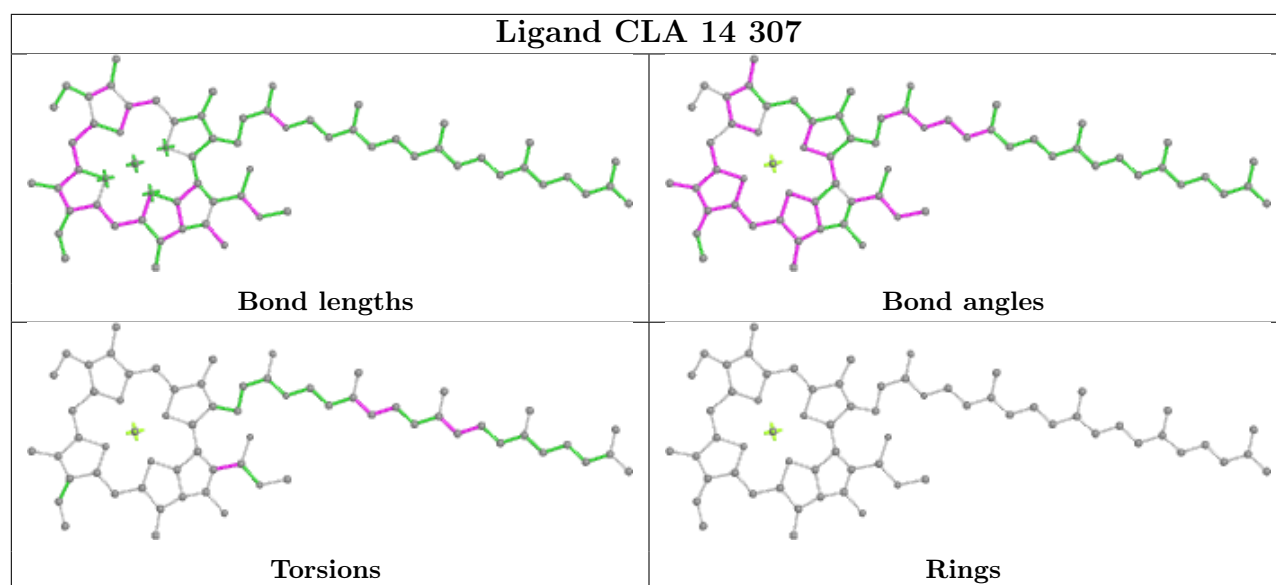
Torsions



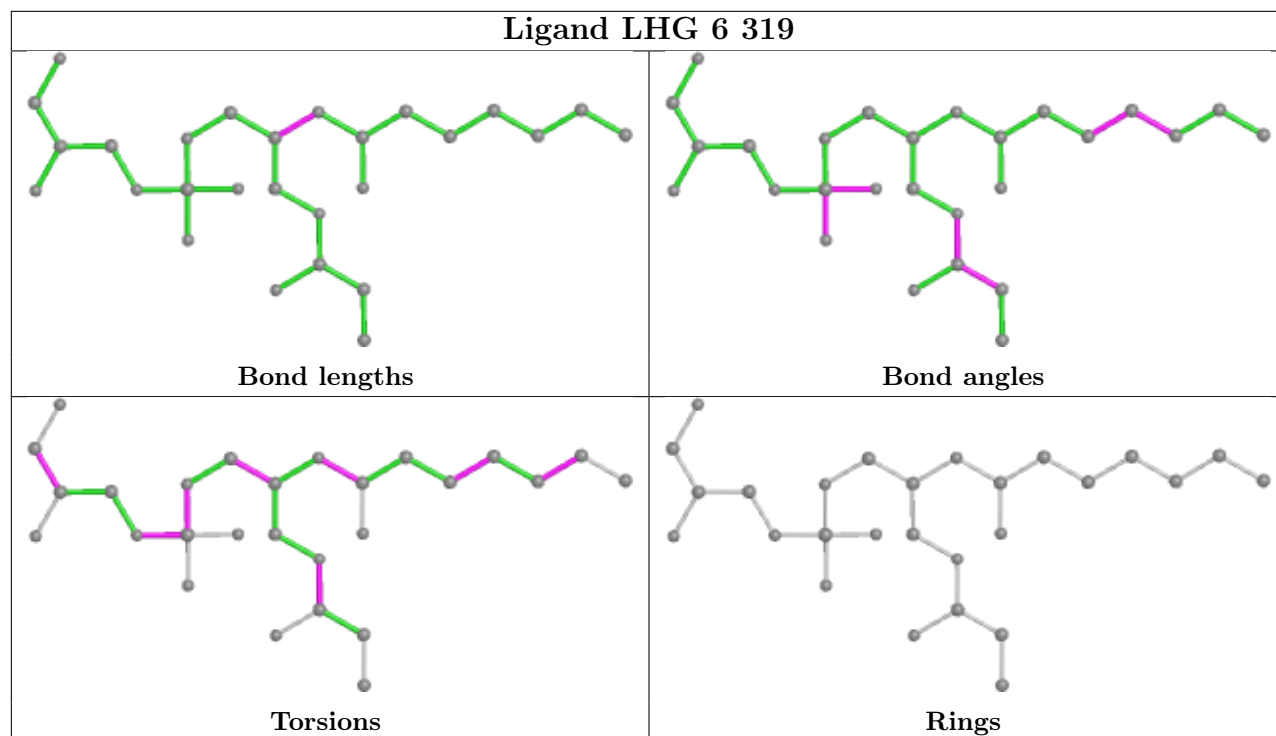
Rings



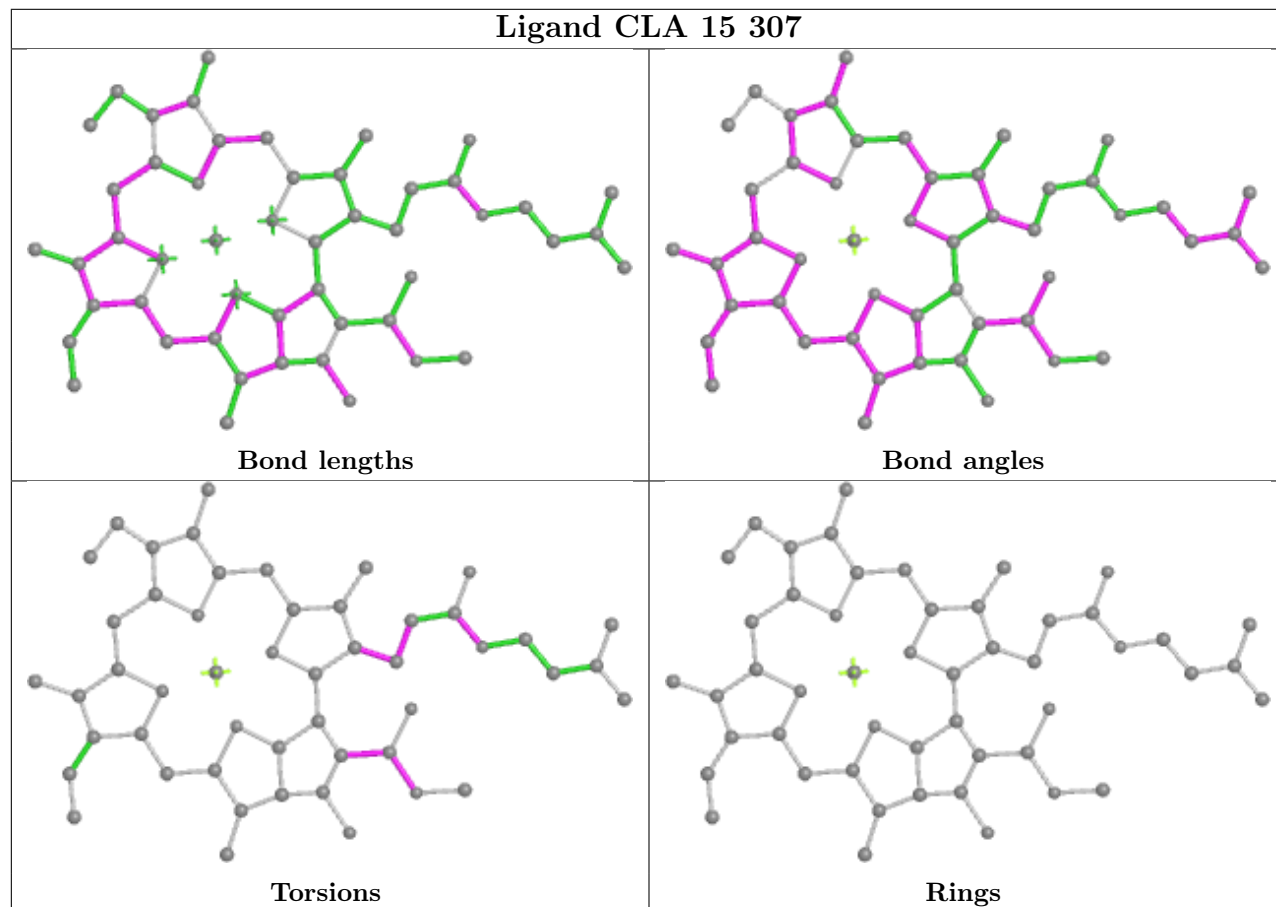


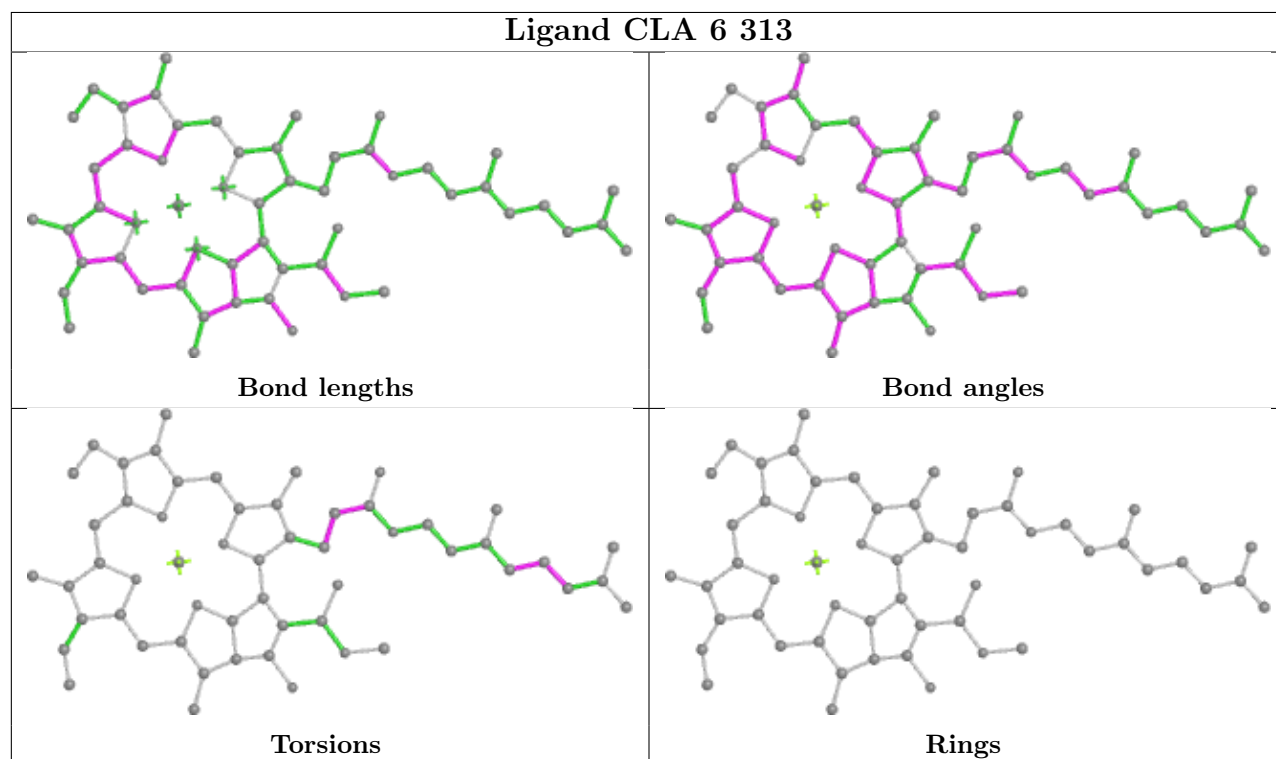
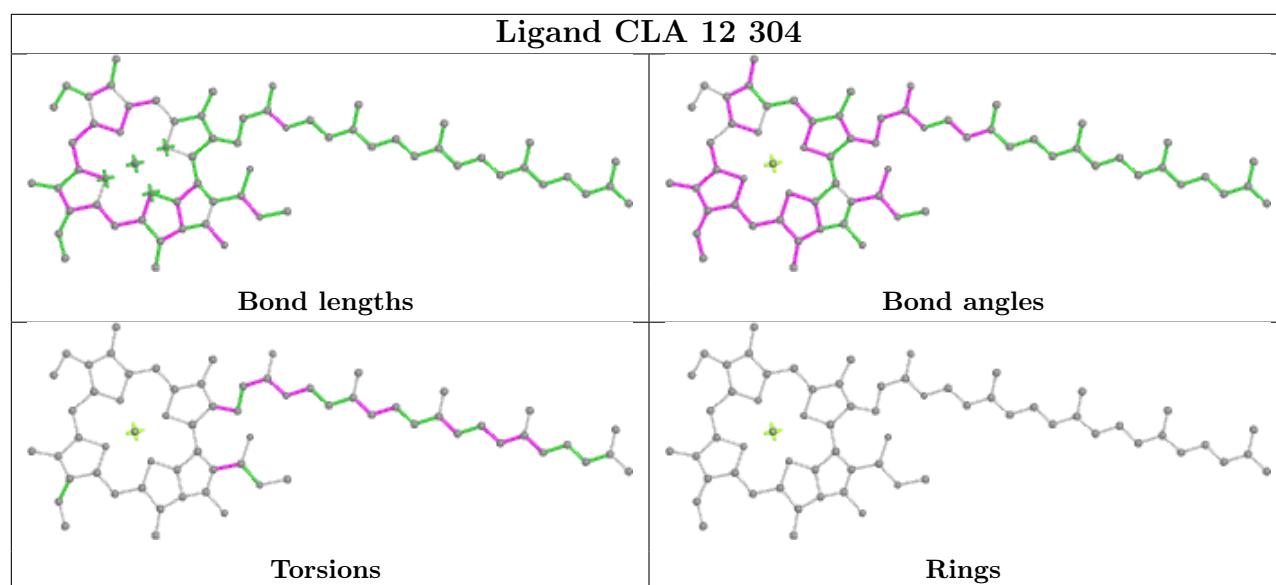


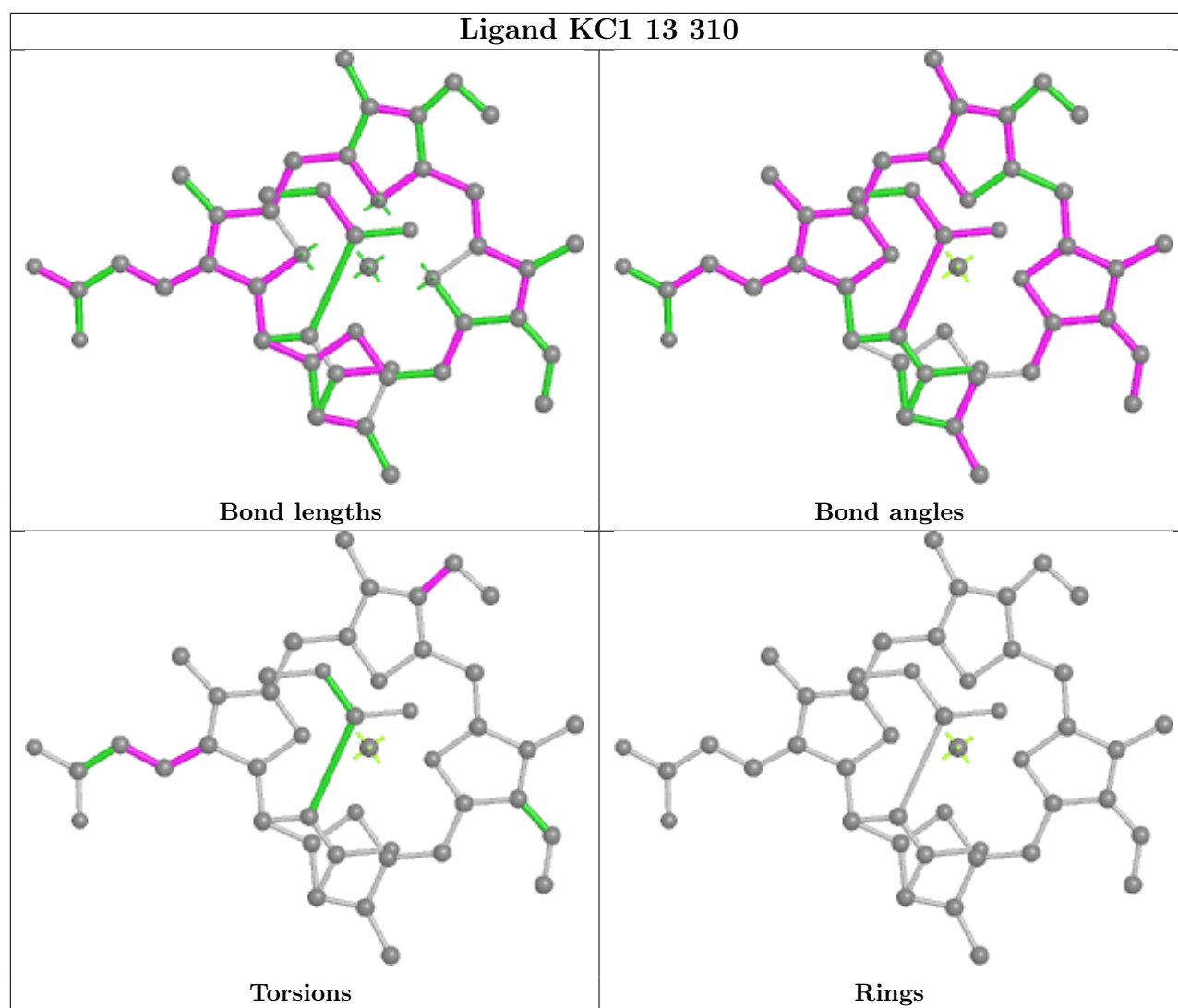
Ligand LHG 6 319

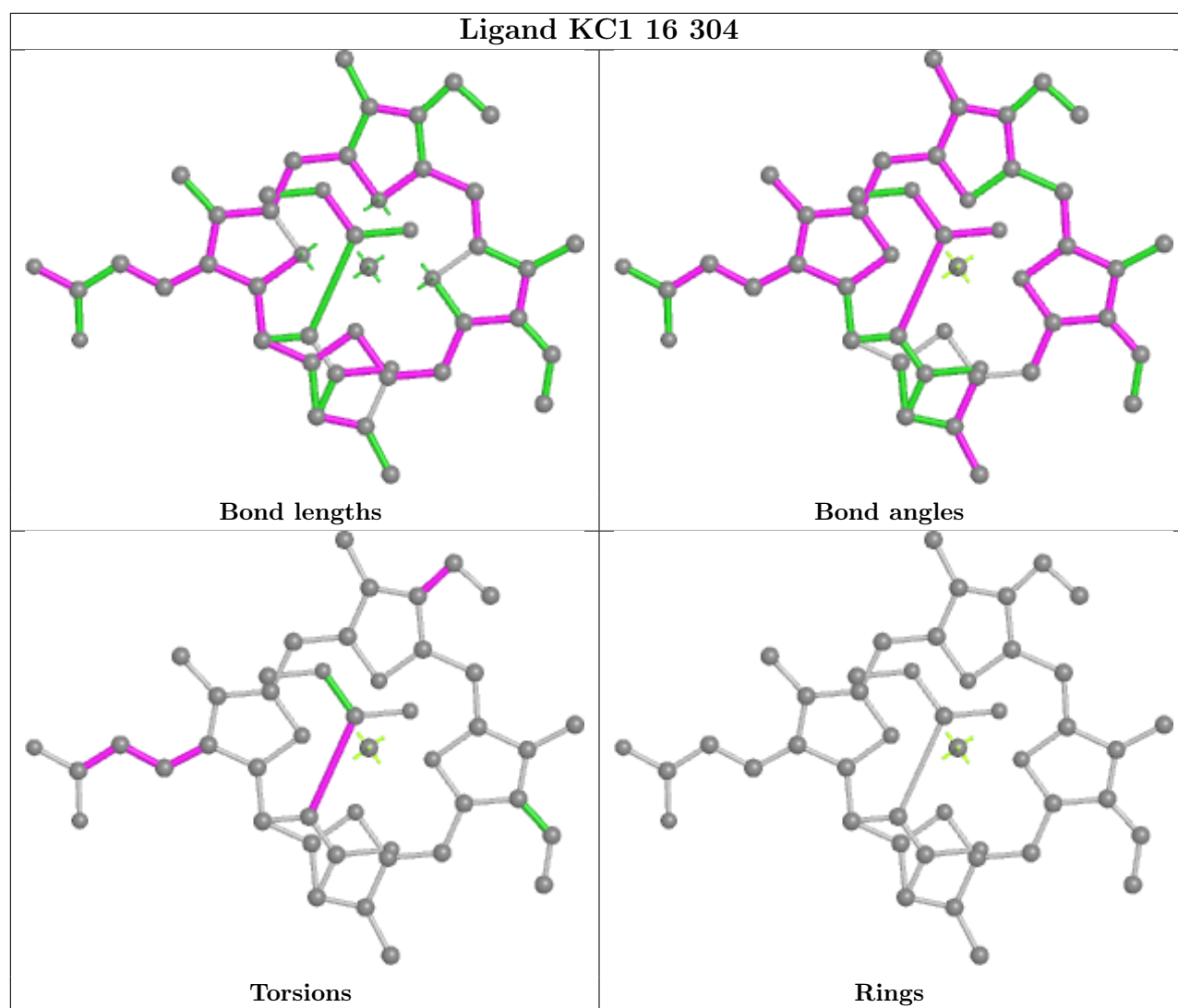


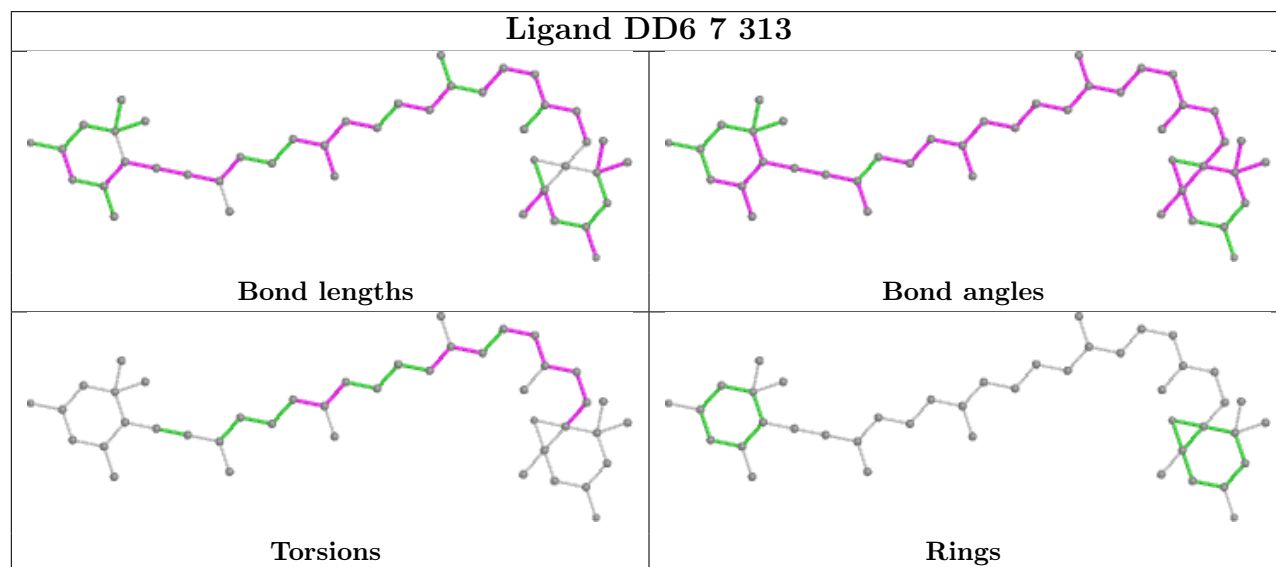
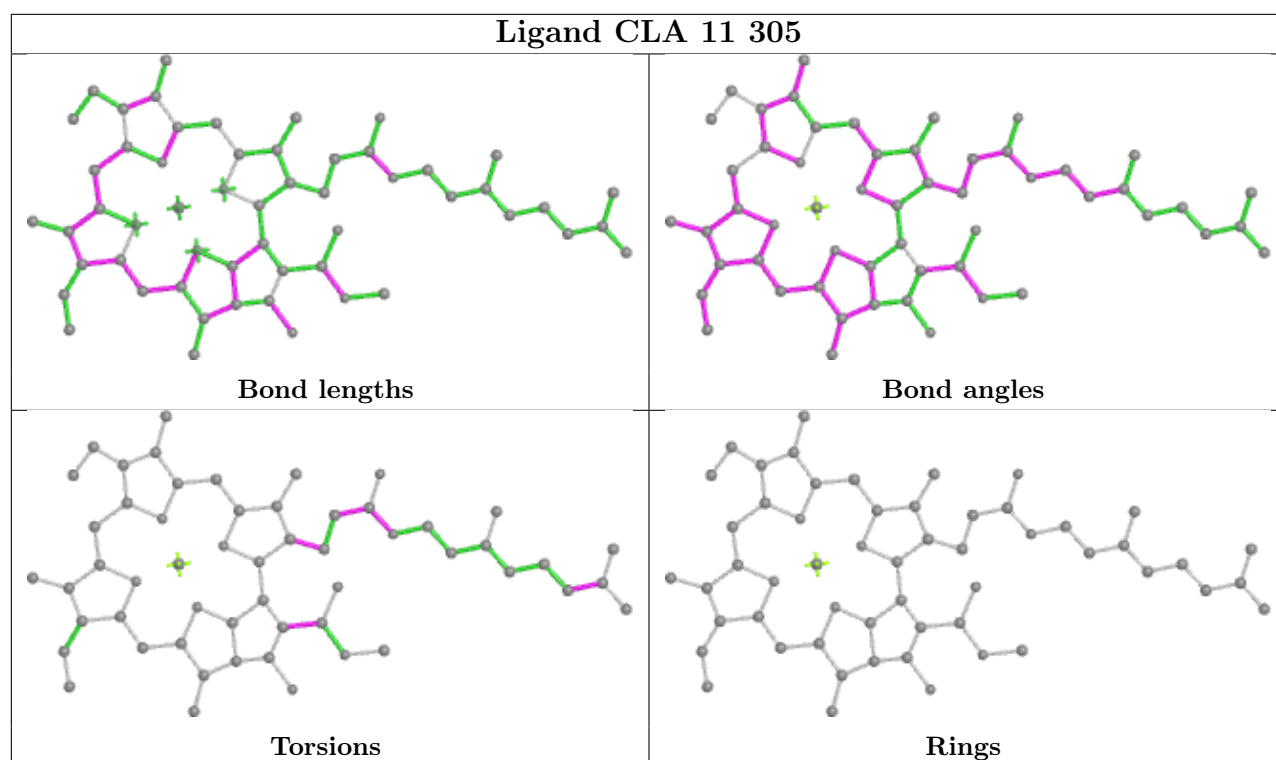
Ligand CLA 15 307

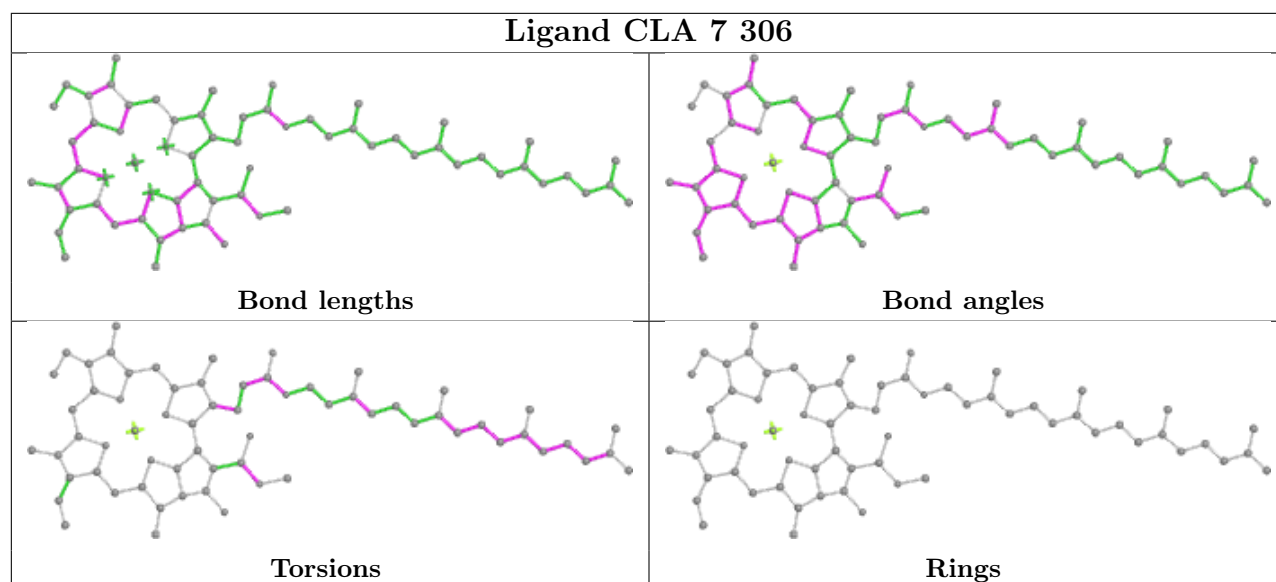
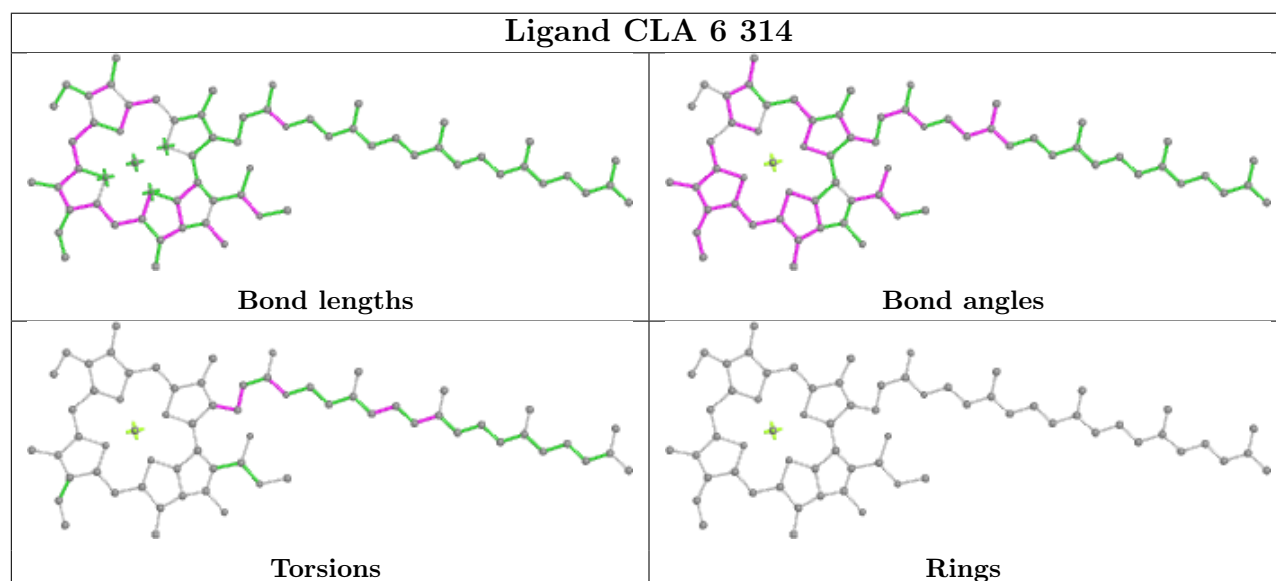
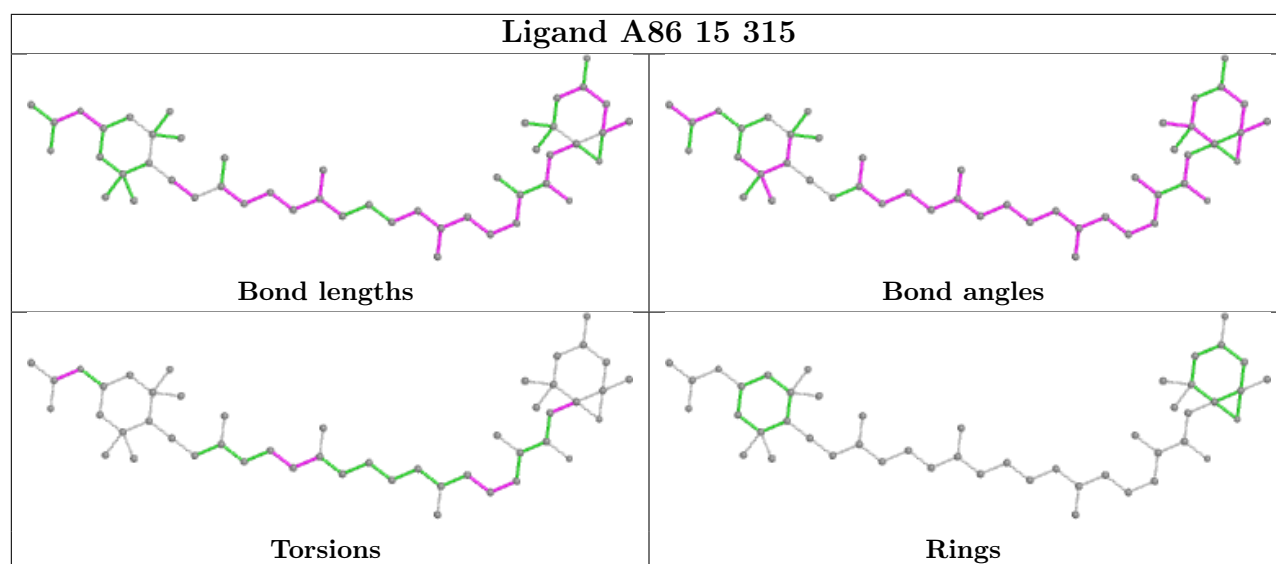


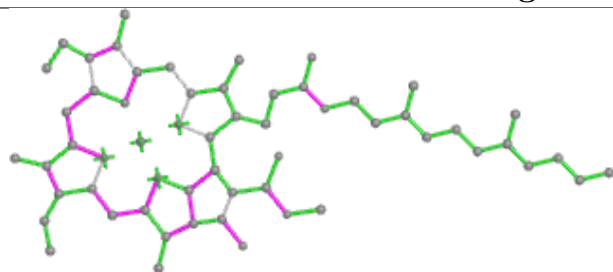
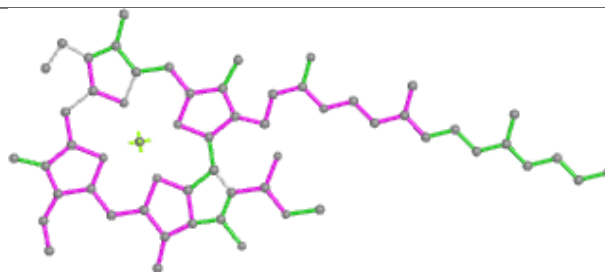
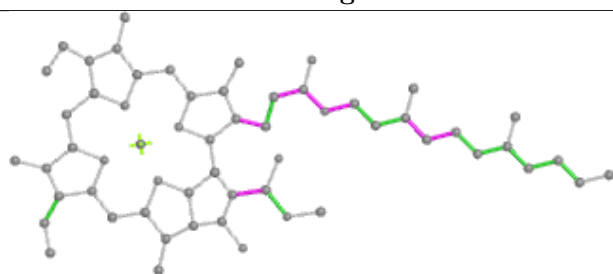
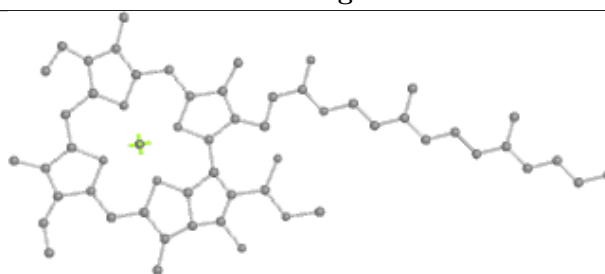
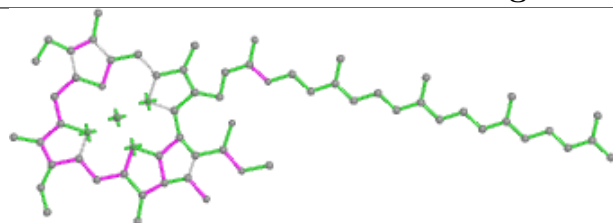
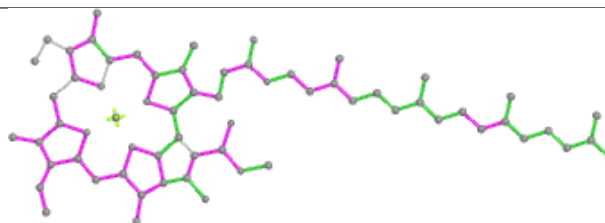
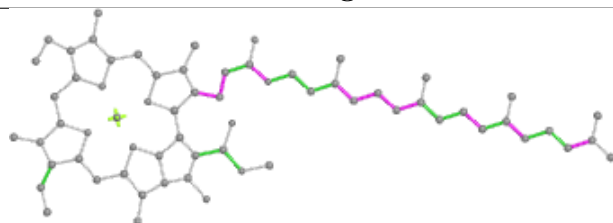
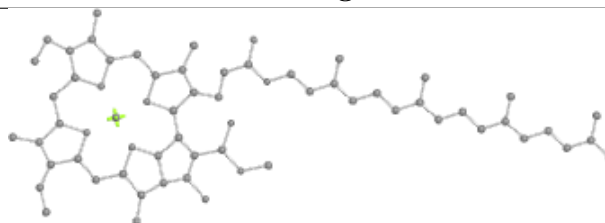


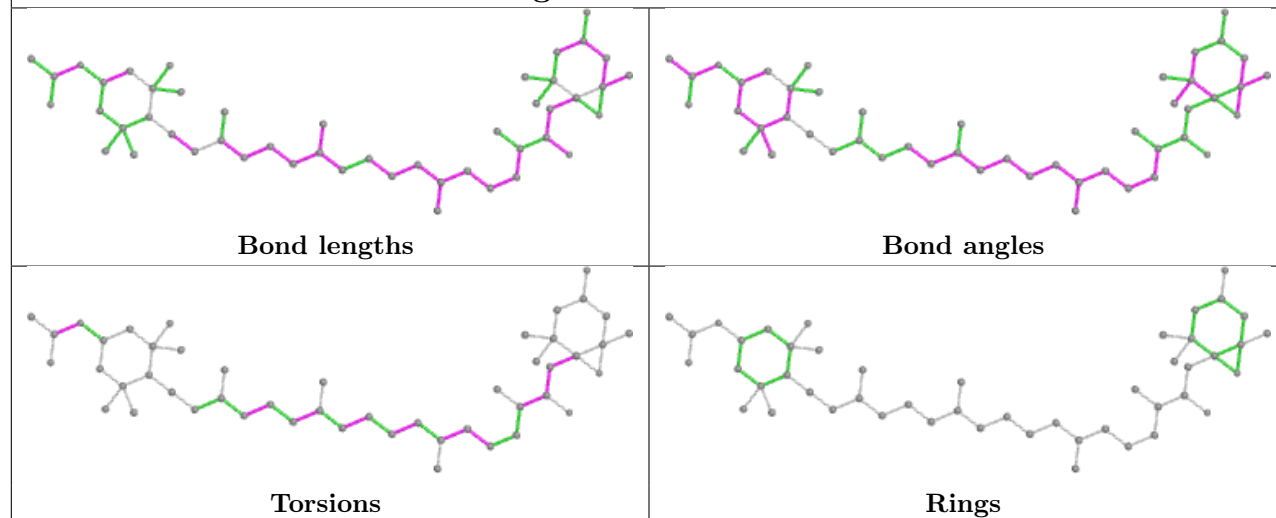
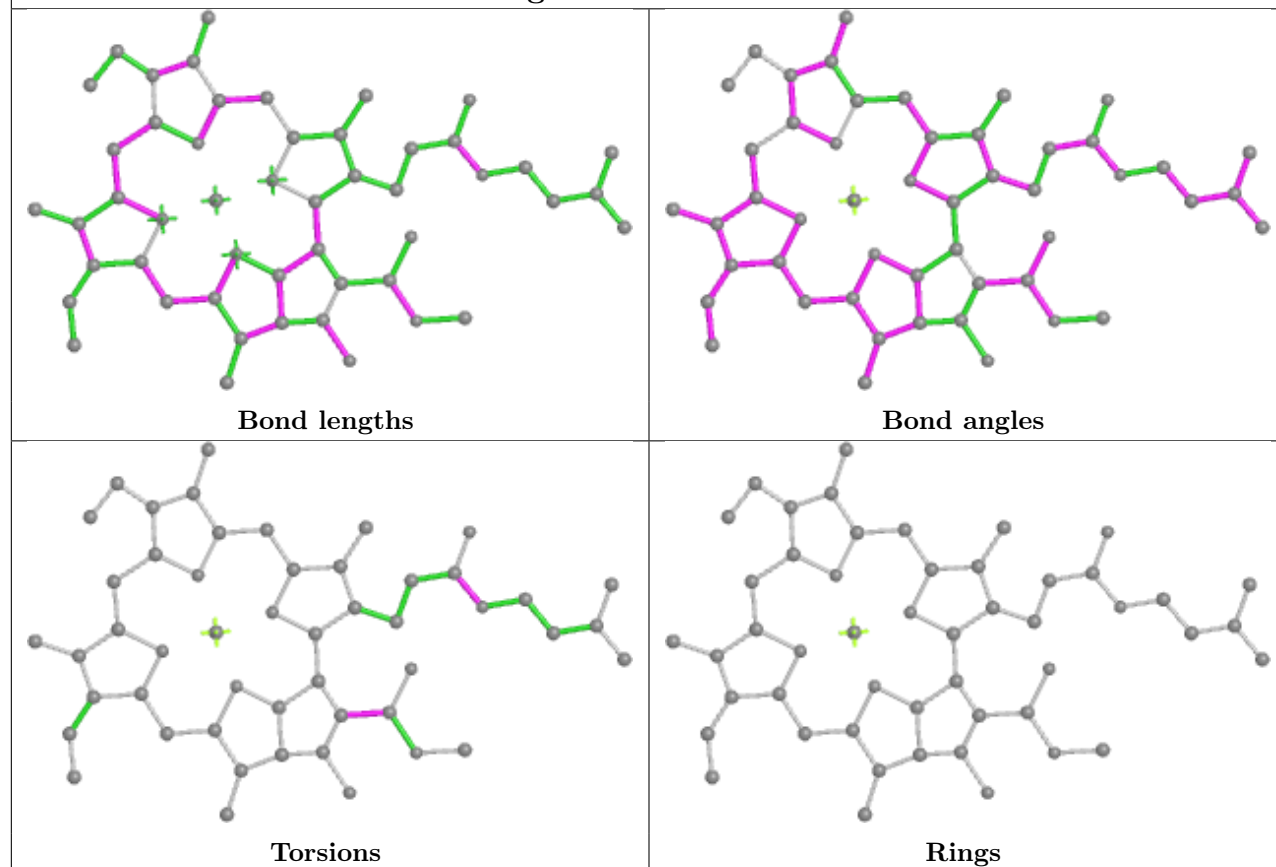


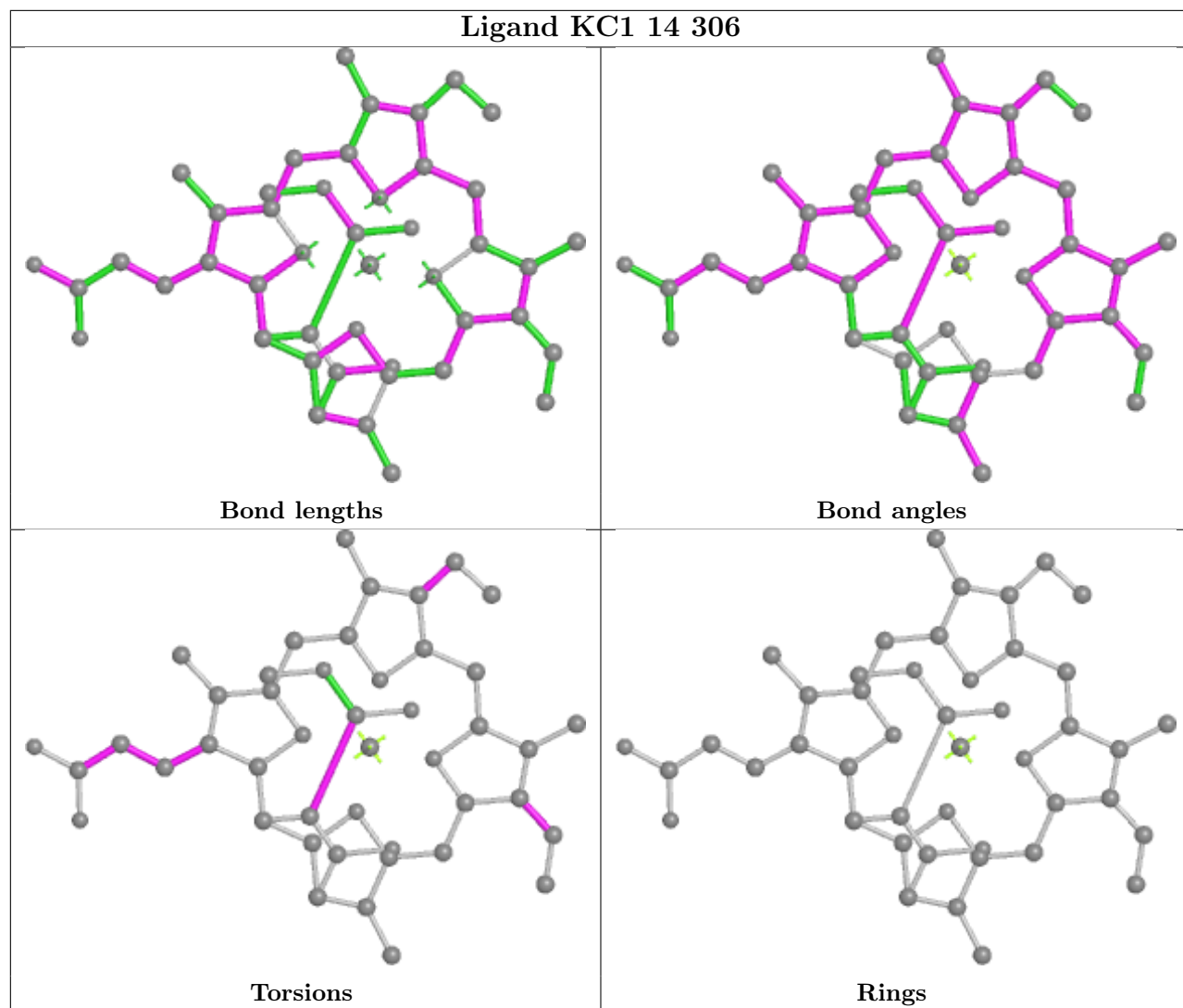


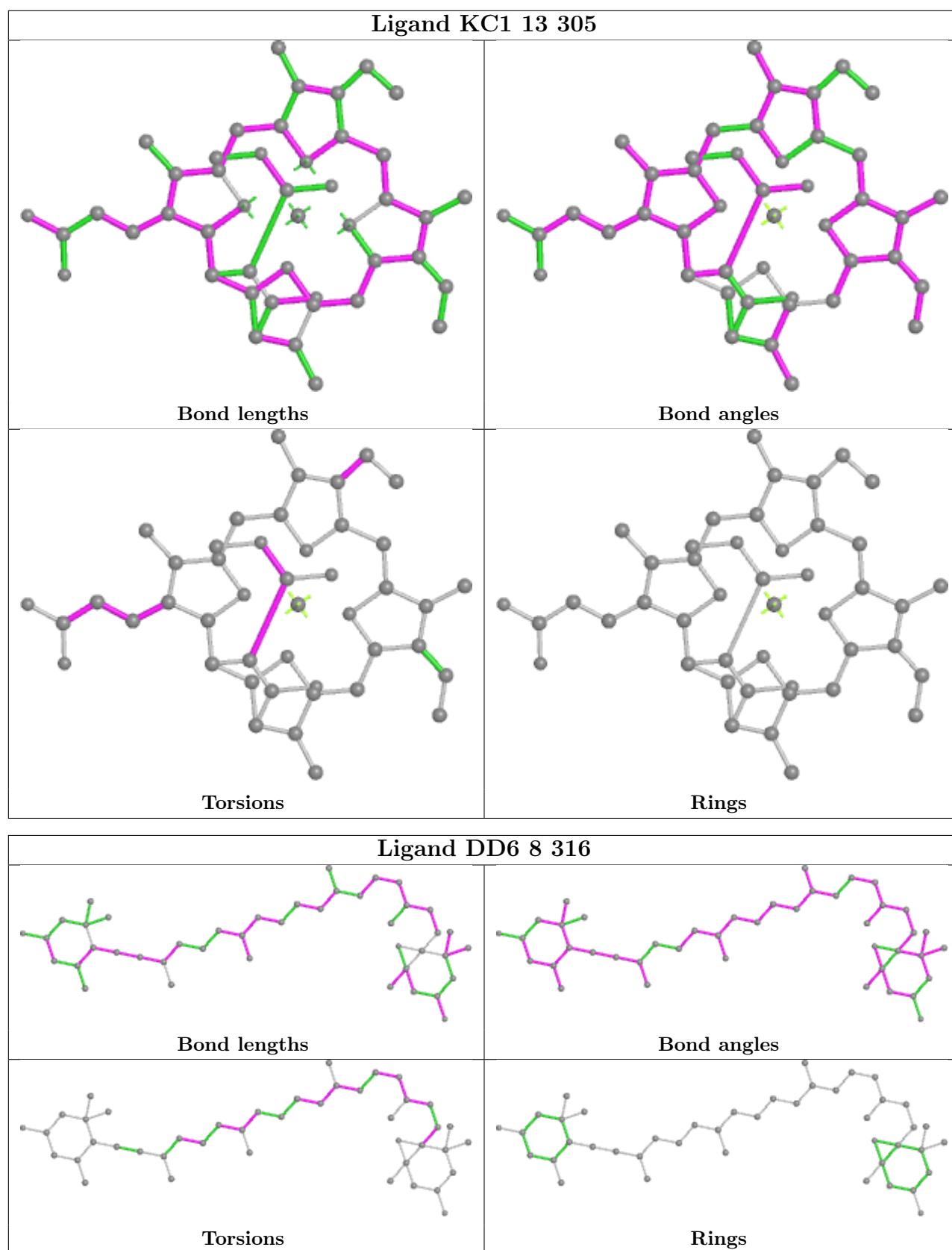


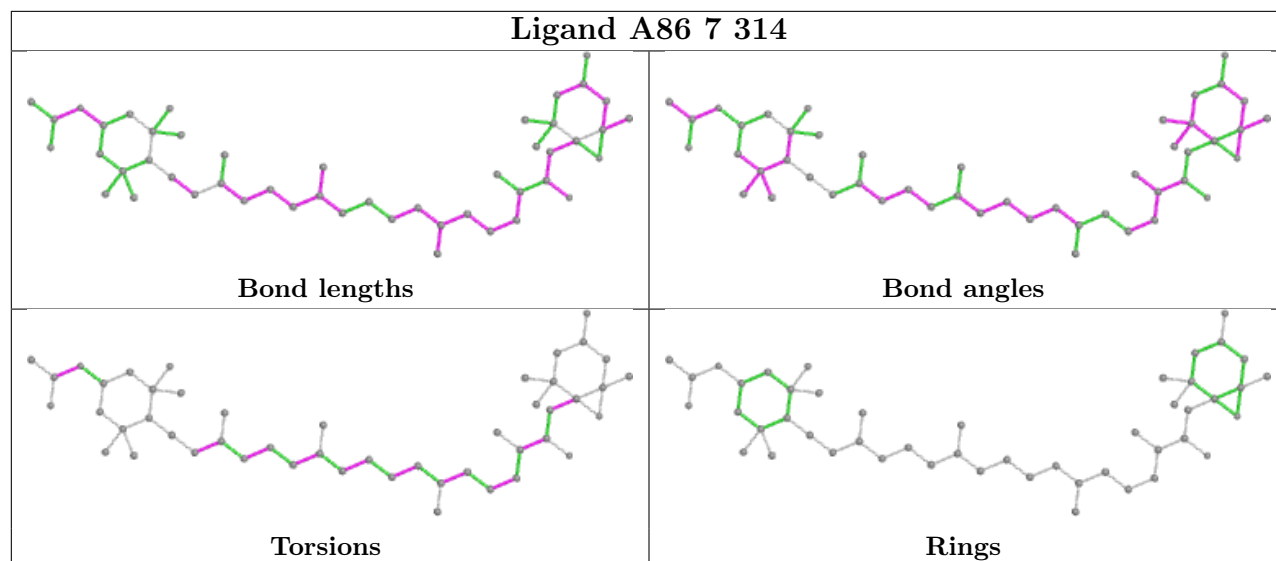
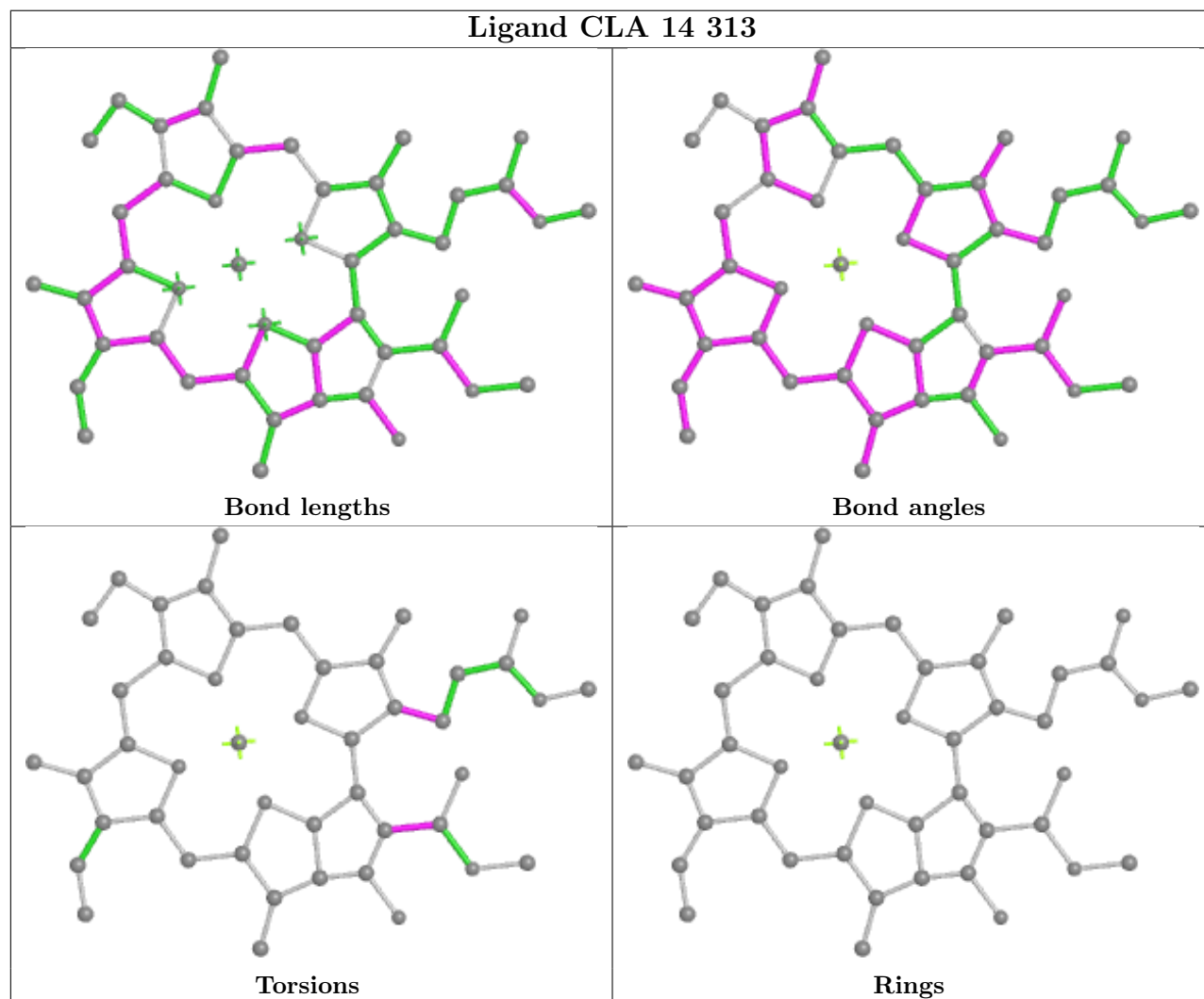


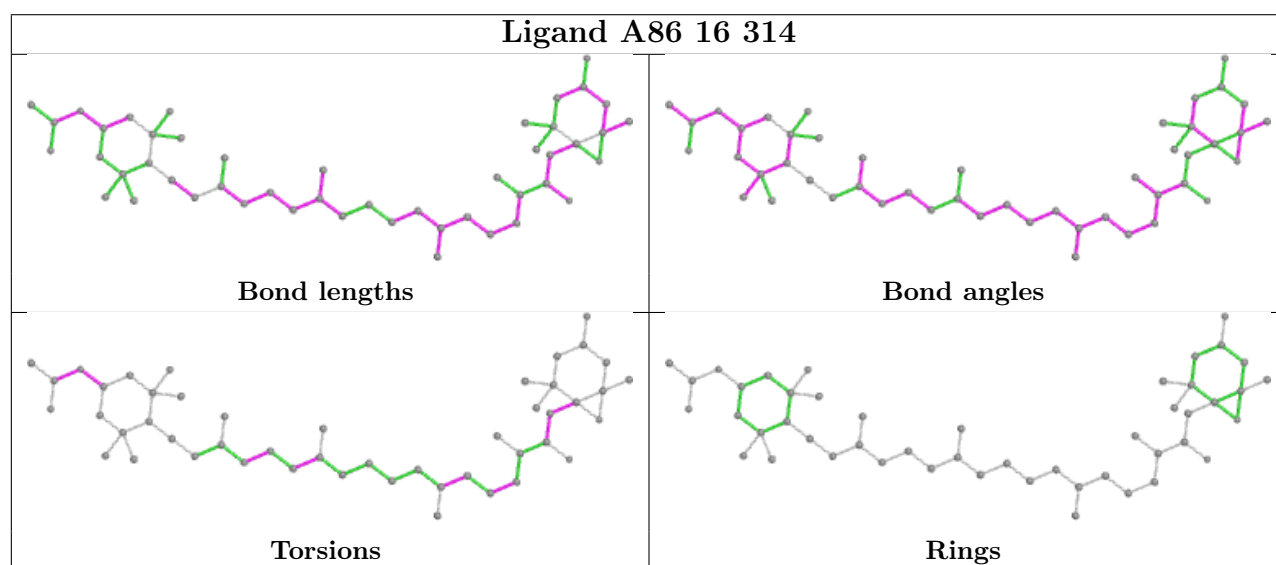
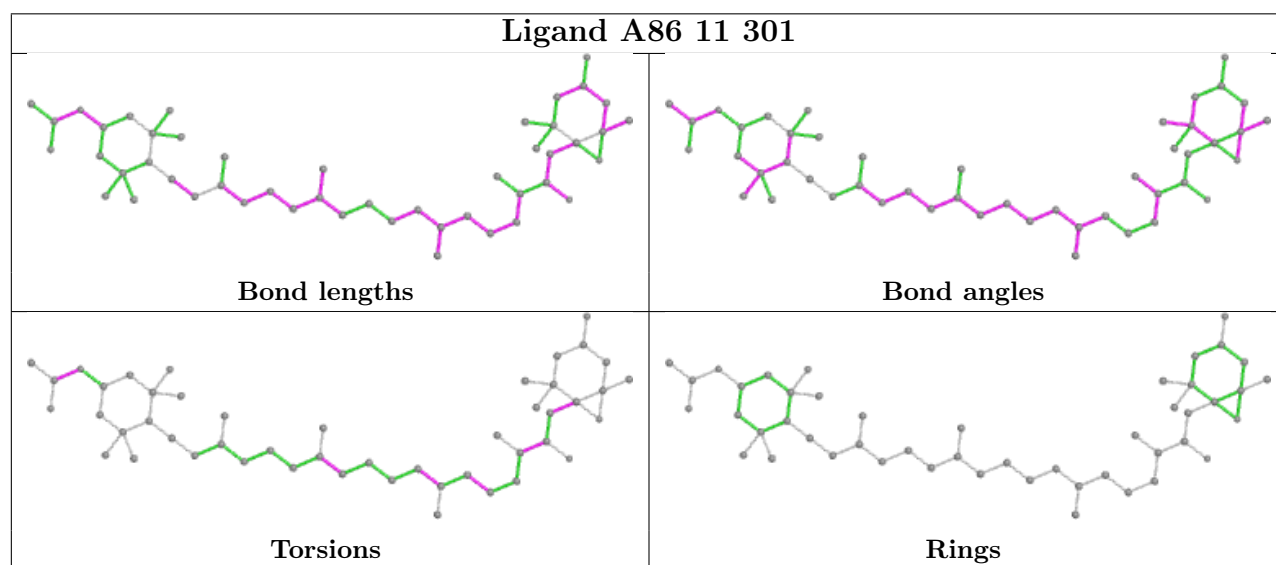
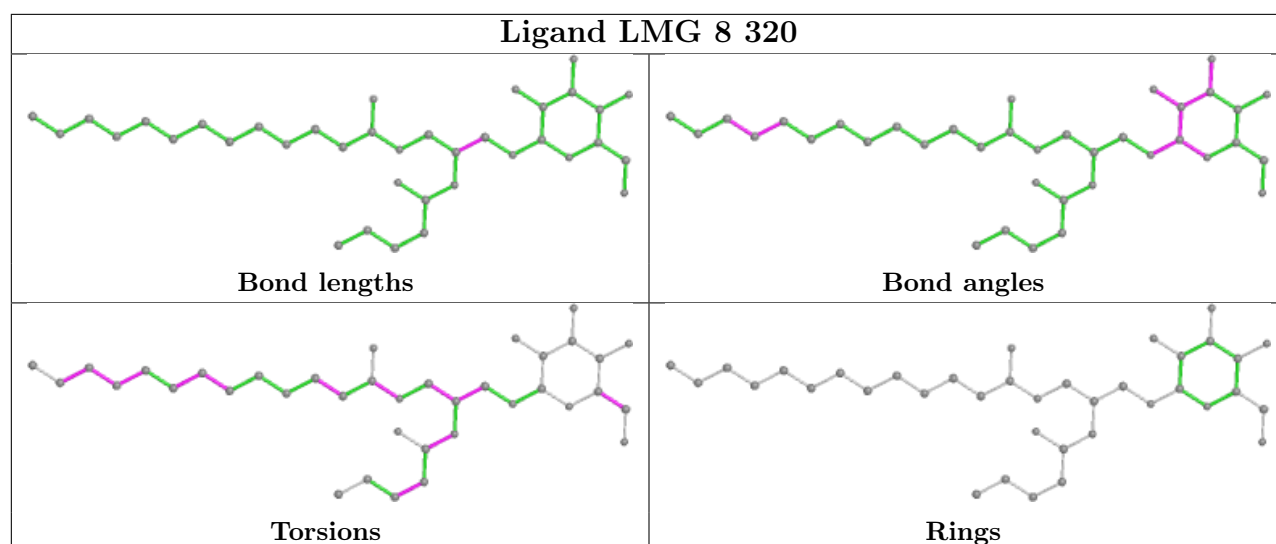
Ligand CLA 8 304**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 15 302****Bond lengths****Bond angles****Torsions****Rings**

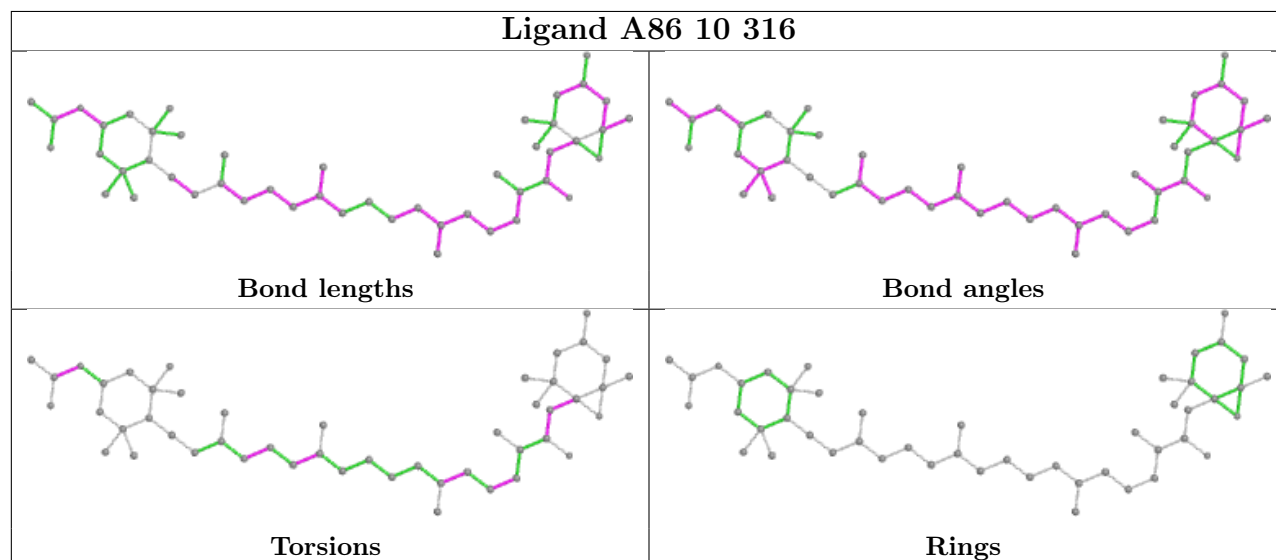
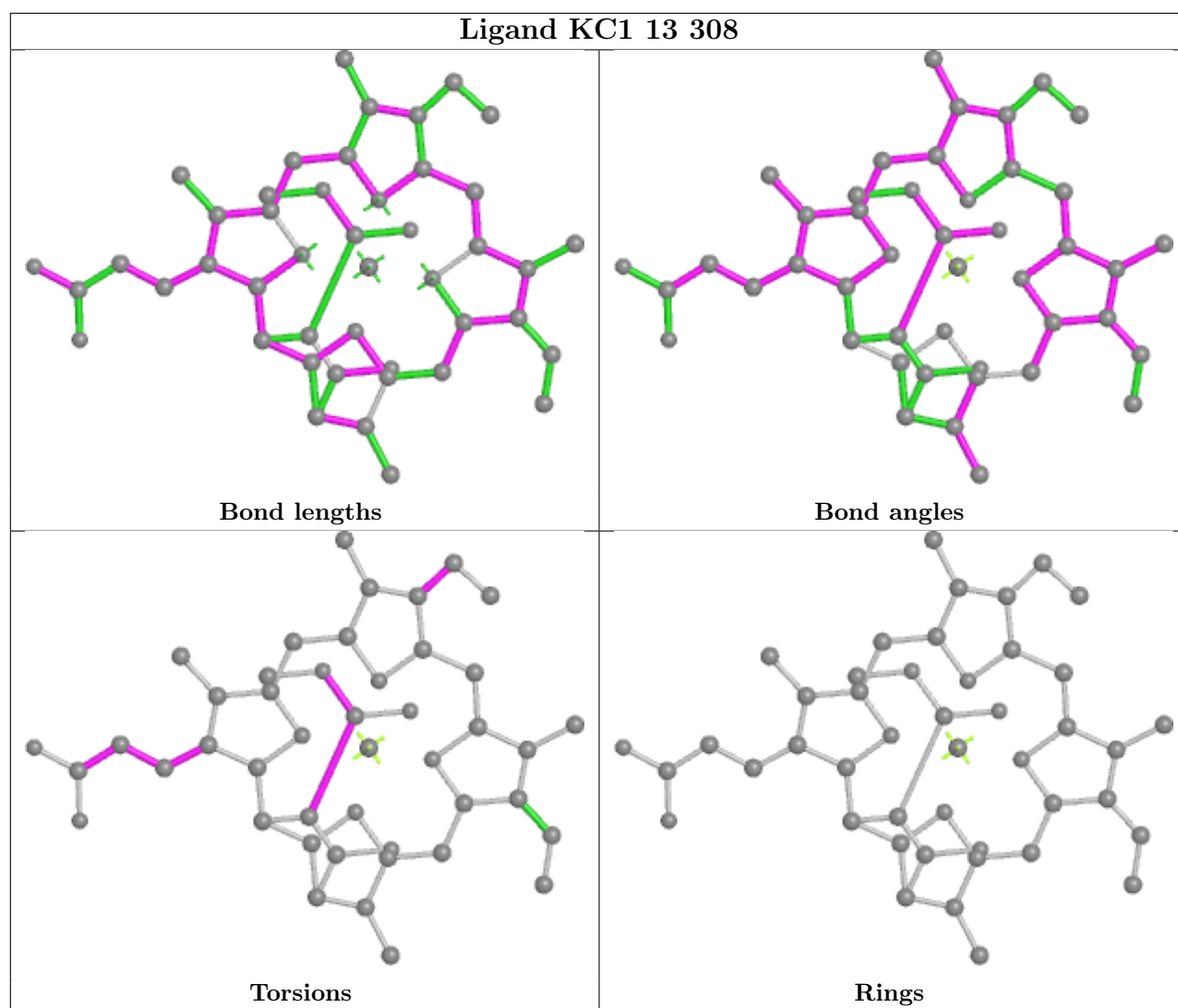
Ligand A86 15 320**Ligand CLA 16 305**

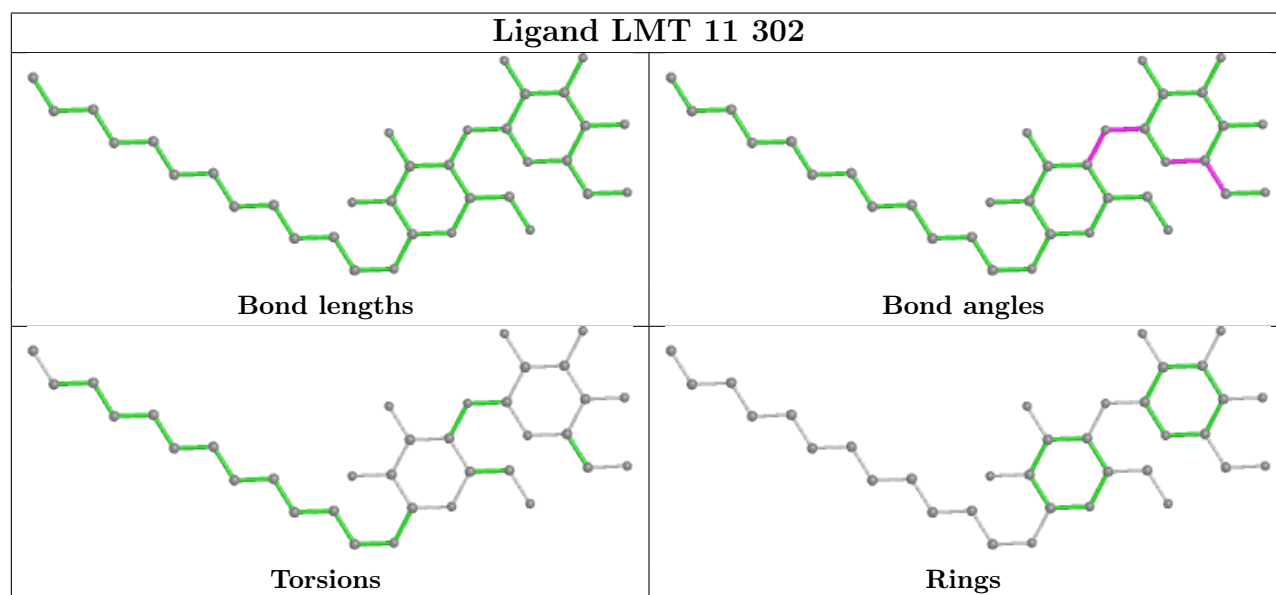
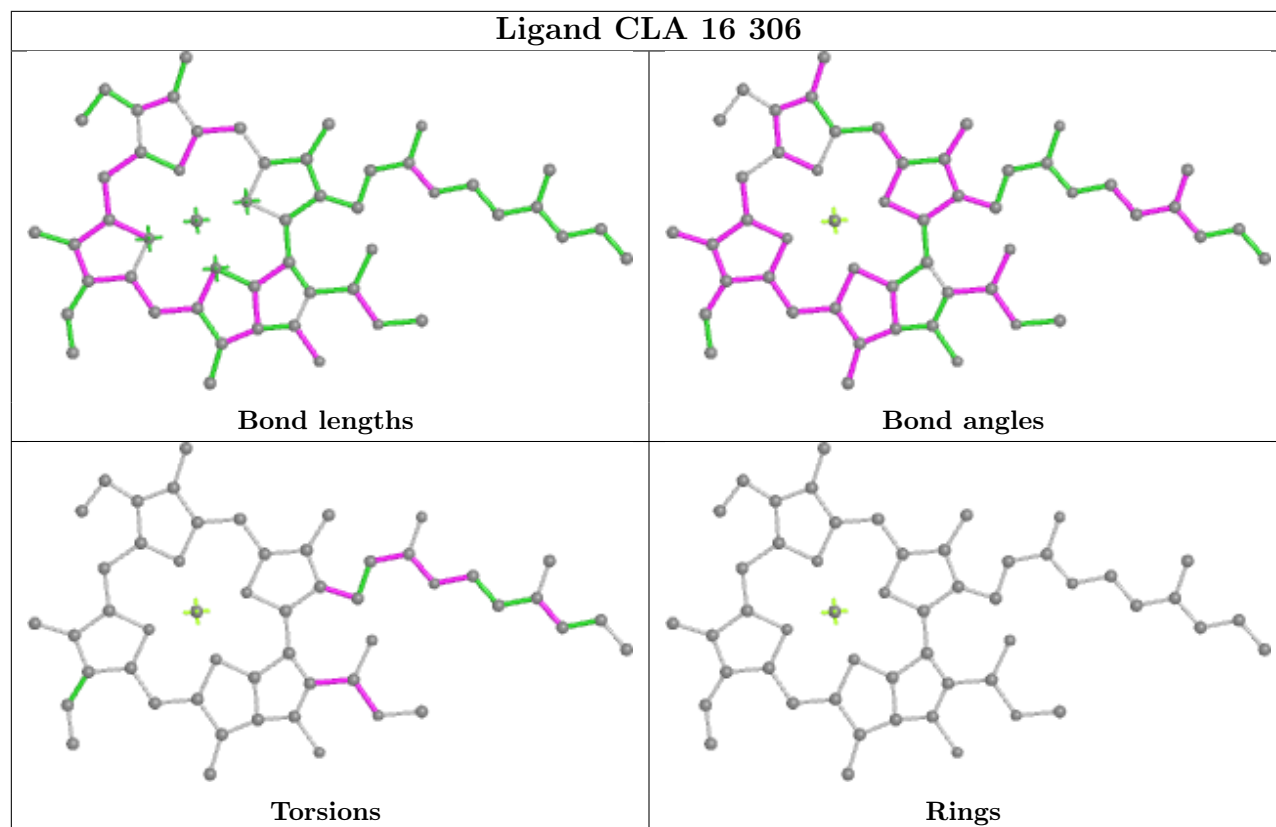


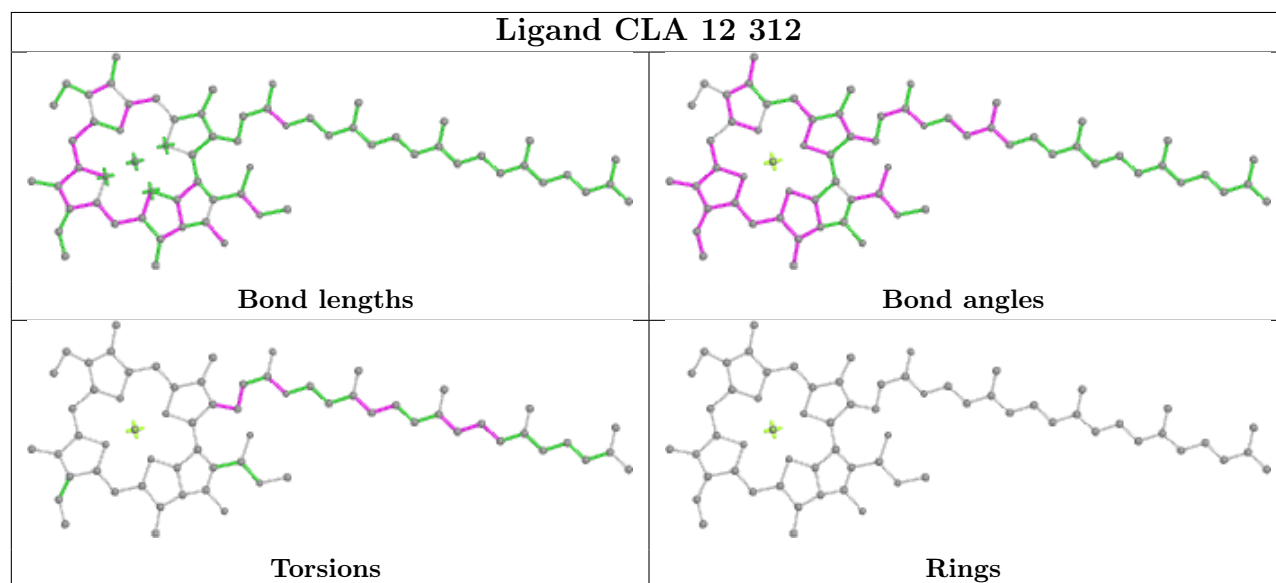
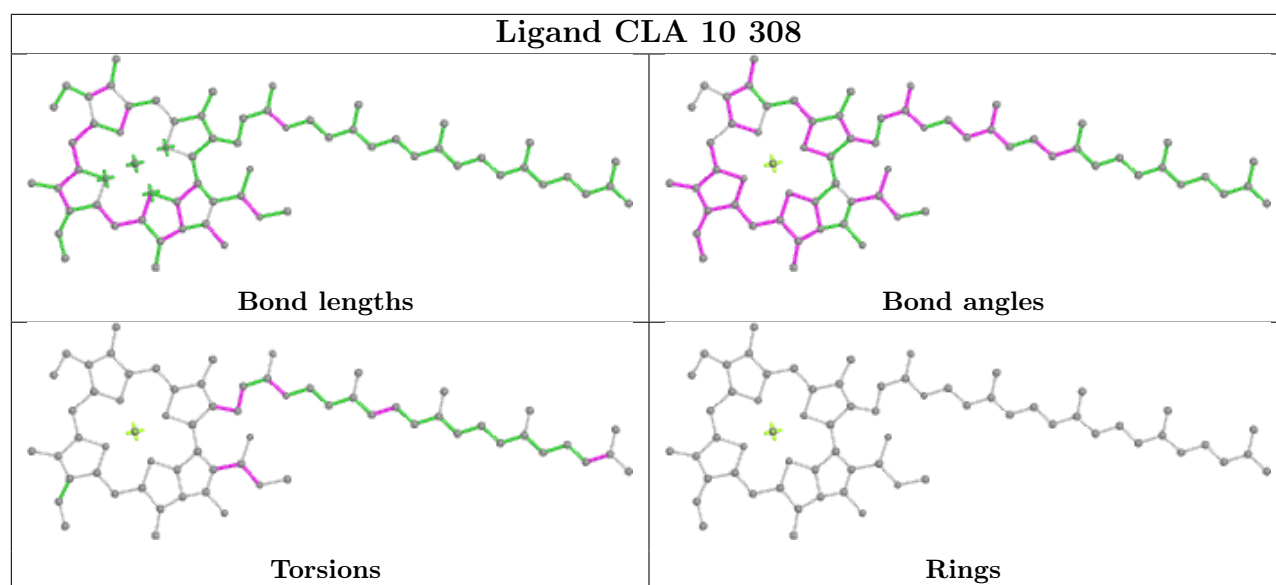


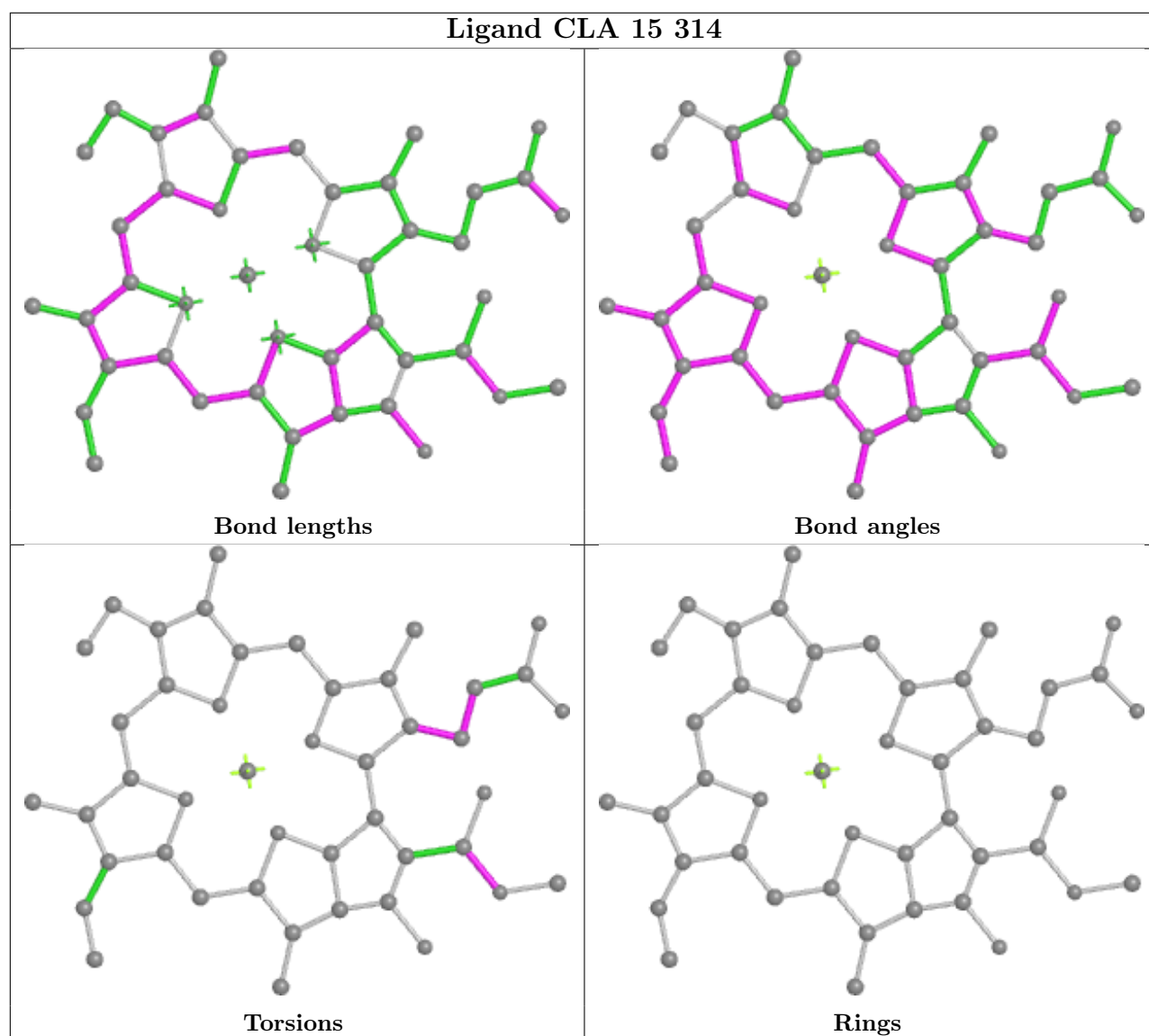
Ligand A86 7 314**Ligand CLA 14 313**



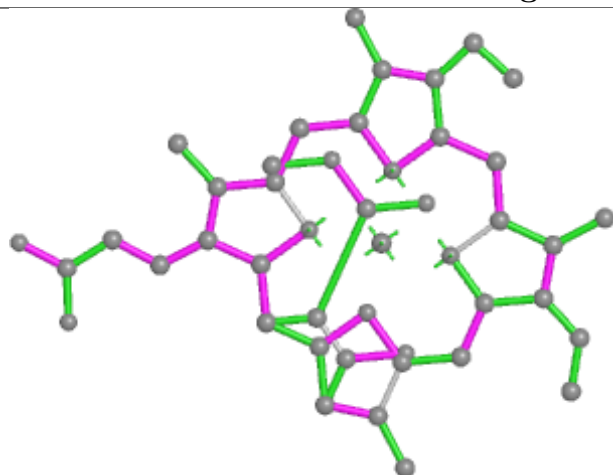




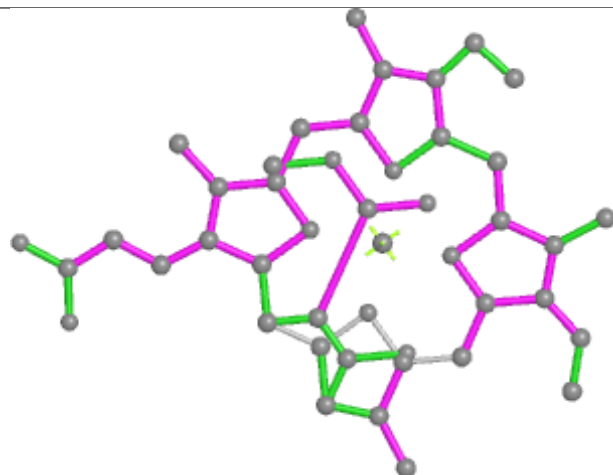




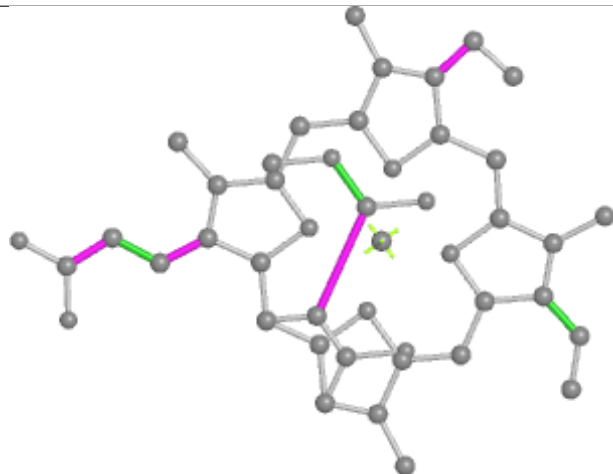
Ligand KC1 8 310



Bond lengths



Bond angles

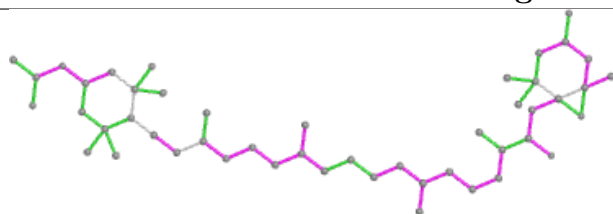


Torsions

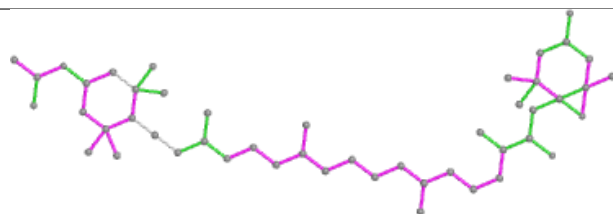


Rings

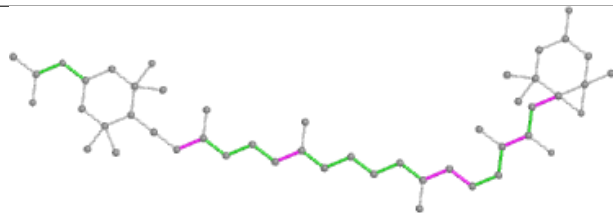
Ligand A86 16 312



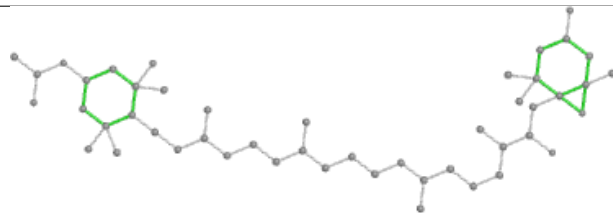
Bond lengths



Bond angles

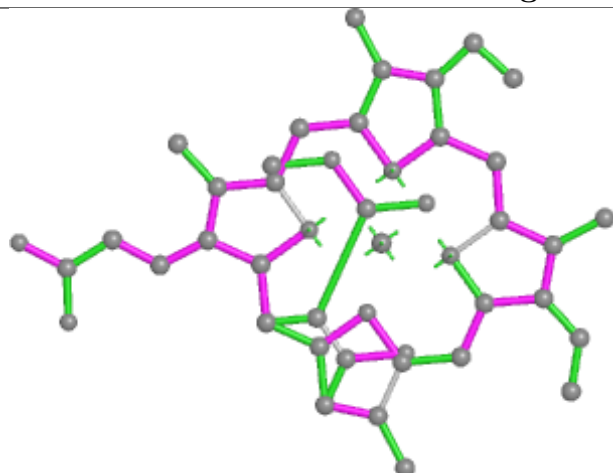


Torsions

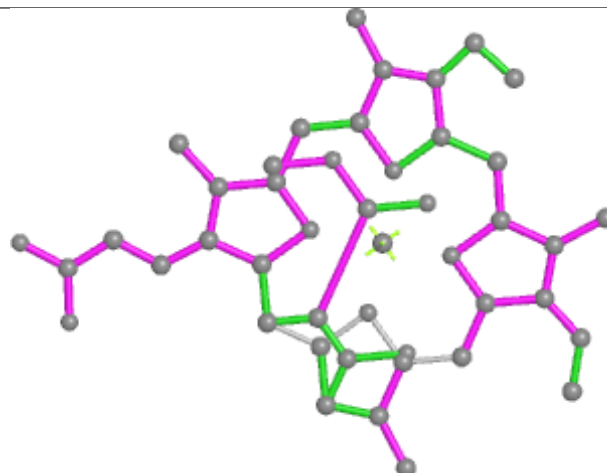


Rings

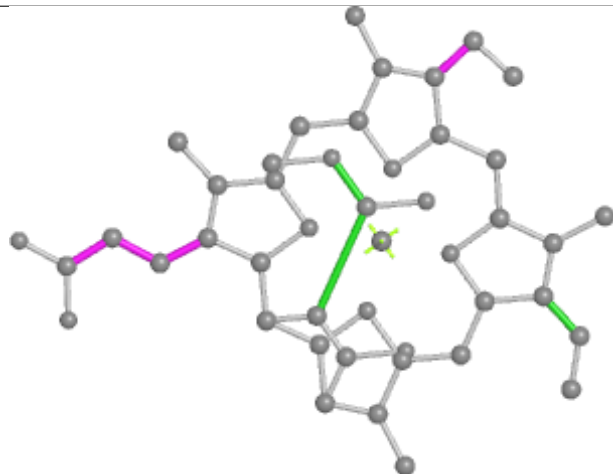
Ligand KC1 8 312



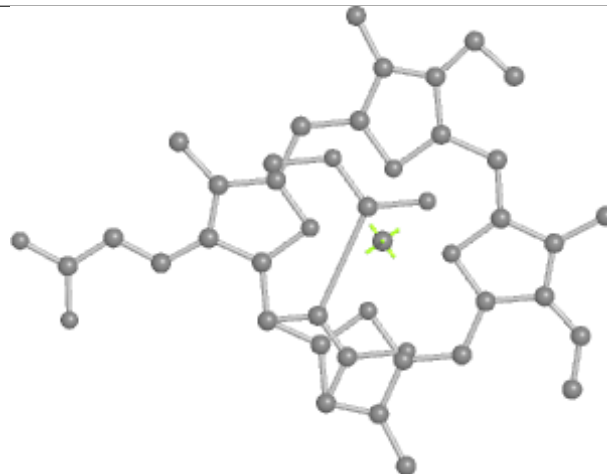
Bond lengths



Bond angles

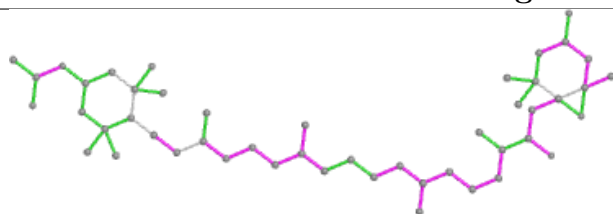


Torsions

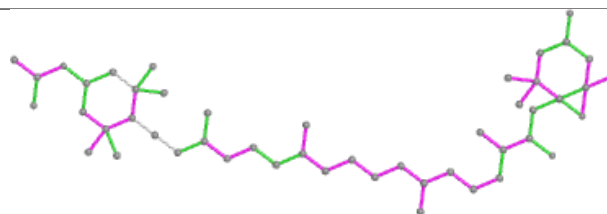


Rings

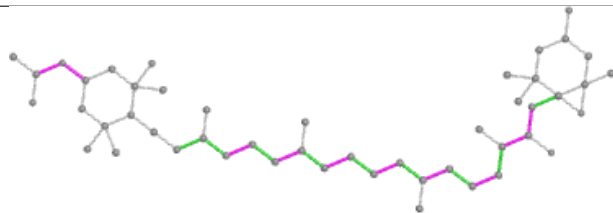
Ligand A86 10 315



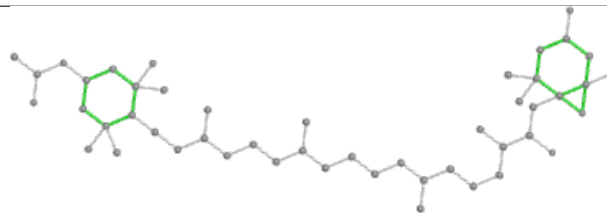
Bond lengths



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 ⓘ

This section contains visualisations of the EMDB entry EMD-0834. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ

This section was not generated.

6.2 Central slices ⓘ

This section was not generated.

6.3 Largest variance slices ⓘ

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

This section was not generated.

6.5 Orthogonal surface views ⓘ

This section was not generated.

6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.