



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 06:14 AM JST

PDB ID : 6L4U / pdb_00006l4u
EMDB ID : EMD-0835
Title : Structure of the PSI-FCPI supercomplex from diatom
Authors : Nagao, R.; Kato, K.; Miyazaki, N.; Akita, F.; Shen, J.R.
Deposited on : 2019-10-21
Resolution : 2.40 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:

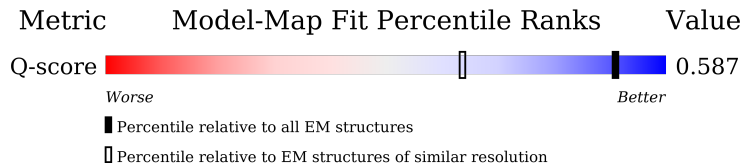
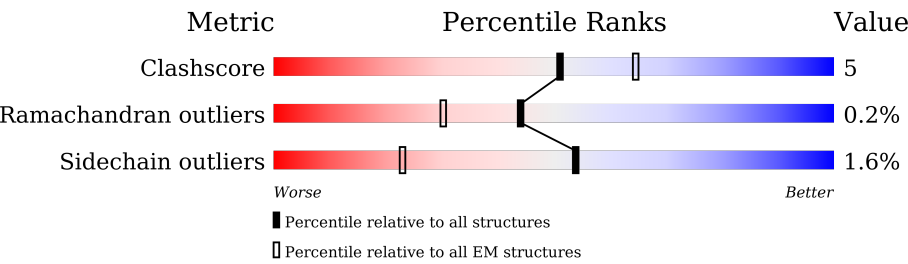
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 Å.

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



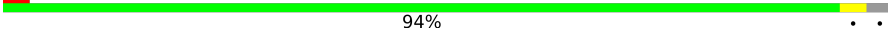
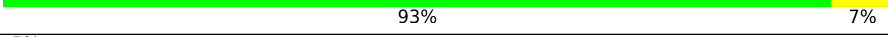
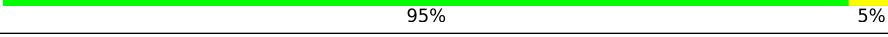
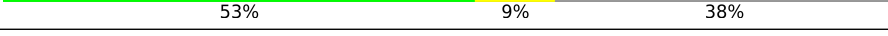
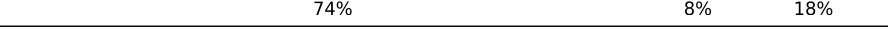
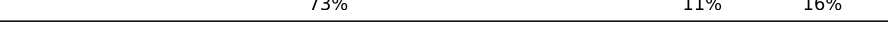
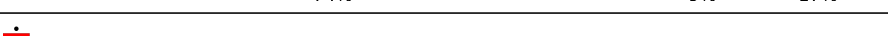
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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 <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	
2	B	733	
3	C	81	
4	D	139	

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Mol	Chain	Length	Quality of chain
5	E	67	
6	F	185	
7	I	36	
8	J	41	
9	L	151	
10	M	30	
11	1u	130	
12	2u	121	
13	1	227	
14	2	205	
15	3	200	
16	4	215	
17	5	266	
18	6	208	
19	7	296	
20	8	270	
21	9	214	
22	10	207	
23	11	229	
24	12	204	
25	13	244	
26	14	249	
27	15	281	
28	16	218	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 62199 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5841	3816	991	1005	29		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5801	3814	977	992	18		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			599	368	103	118	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	131	Total	C	N	O	S	0	0
			1037	663	177	194	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	60	Total	C	N	O	0	0
			478	302	86	90		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	161	Total	C	N	O	S	0	0
			1257	806	213	234	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	35	Total	C	N	O	S	0	0
			273	190	37	44	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			344	236	50	55	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	137	Total	C	N	O	S	0	0
			1030	680	169	179	2		

- Molecule 10 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	30	Total	C	N	O	S	0	0
			227	151	35	40	1		

- Molecule 11 is a protein called Unknown protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1u	130	Total	C	N	O	S	0	0
			650	390	130	130			

- Molecule 12 is a protein called Photosystem I reaction center subunit Ps28.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2u	89	Total	C	N	O	S	0	0
			674	438	110	120	6		

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	141	Total	C	N	O	S	0	0
			1086	692	184	201	9		

- Molecule 14 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	172	Total	C	N	O	S	0	0
			1310	846	216	238	10		

- Molecule 15 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	164	Total	C	N	O	S	0	0
			1275	825	213	232	5		

- Molecule 16 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	179	Total	C	N	O	S	0	0
			1368	878	227	250	13		

- Molecule 17 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	169	Total	C	N	O	S	0	0
			1304	834	222	236	12		

- Molecule 18 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	174	Total	C	N	O	S	0	0
			1354	884	216	246	8		

- Molecule 19 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	7	188	Total	C	N	O	S	0	0
			1416	894	240	266	16		

- Molecule 20 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	8	213	Total	C	N	O	S	0	0
			1660	1075	274	302	9		

- Molecule 21 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcf6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	9	163	Total	C	N	O	S	0	0
			1267	816	211	233	7		

- Molecule 22 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	10	169	Total	C	N	O	S	0	0
			1302	849	212	233	8		

- Molecule 23 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	11	191	Total	C	N	O	S	0	0
			1479	958	243	270	8		

- Molecule 24 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	12	173	Total	C	N	O	S	0	0
			1274	814	209	243	8		

- Molecule 25 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	13	150	Total	C	N	O	S	0	0
			1148	736	203	204	5		

- Molecule 26 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq10.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	14	208	Total	C	N	O	S	0	0
			1609	1049	262	292	6		

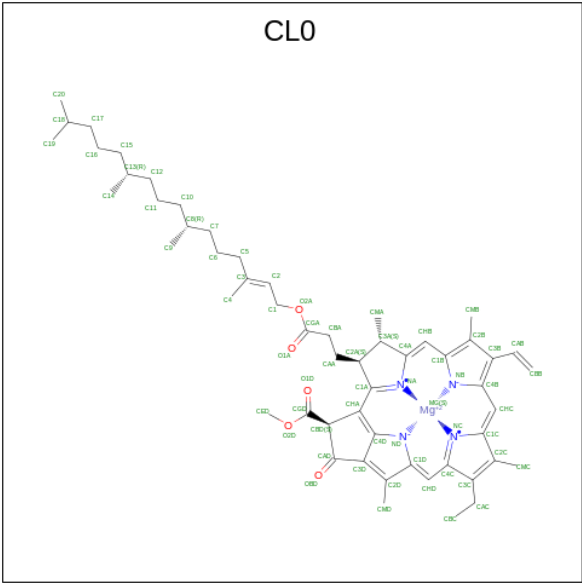
- Molecule 27 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	15	211	Total	C	N	O	S	0	0
			1654	1077	273	298	6		

- Molecule 28 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	16	174	Total	C	N	O	S	0	0
			1313	846	217	242	8		

- Molecule 29 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
30	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	F	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	2u	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	2	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	3	1	Total 62	C 52	Mg 1	N 4	O 5	0
30	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	4	1	Total 49	C 39	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	7	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	8	1	Total 58	C 48	Mg 1	N 4	O 5	0
30	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	8	1	Total 47	C 37	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 51	C 41	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	10	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 55	C 45	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	12	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0

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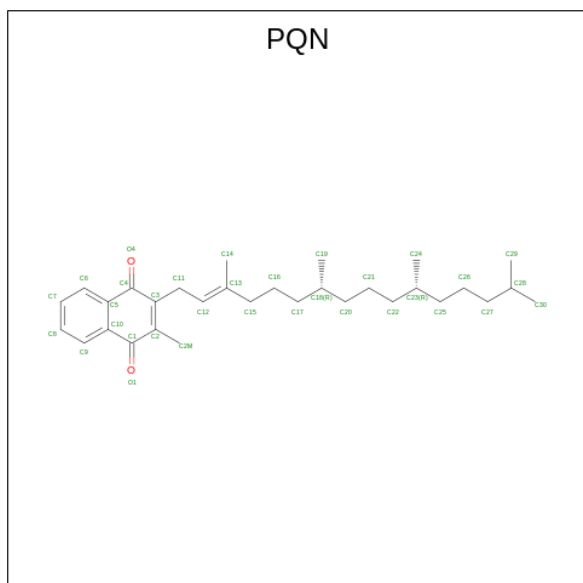
Mol	Chain	Residues	Atoms					AltConf
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 57	C 47	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 46	C 36	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 60	C 50	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	15	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
30	15	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 31 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



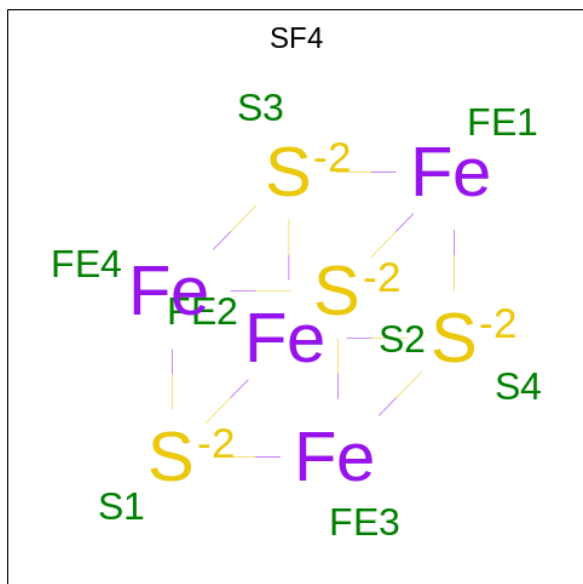
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			33	31	2	

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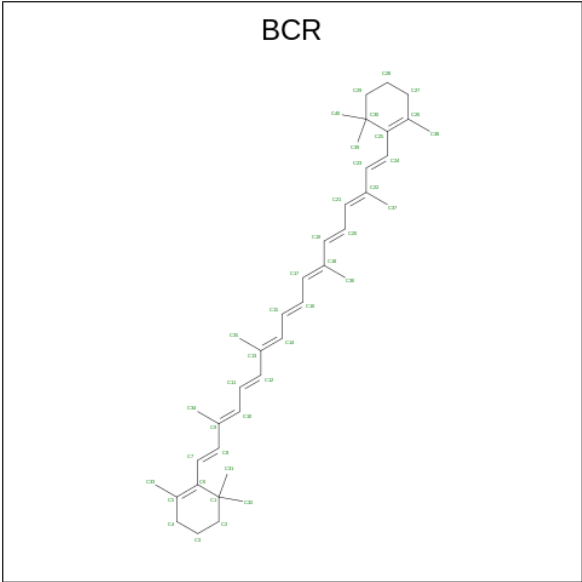
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			33	31	2	

- Molecule 32 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	
32	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 33 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



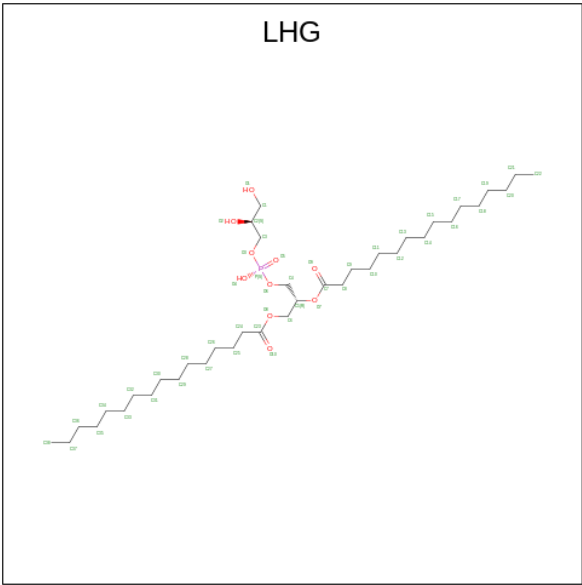
Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	F	1	Total	C	0
			40	40	
33	I	1	Total	C	0
			40	40	
33	J	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms		AltConf
33	J	1	Total	C	0
			40	40	
33	L	1	Total	C	0
			40	40	
33	L	1	Total	C	0
			40	40	
33	L	1	Total	C	0
			40	40	
33	M	1	Total	C	0
			40	40	
33	2u	1	Total	C	0
			40	40	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



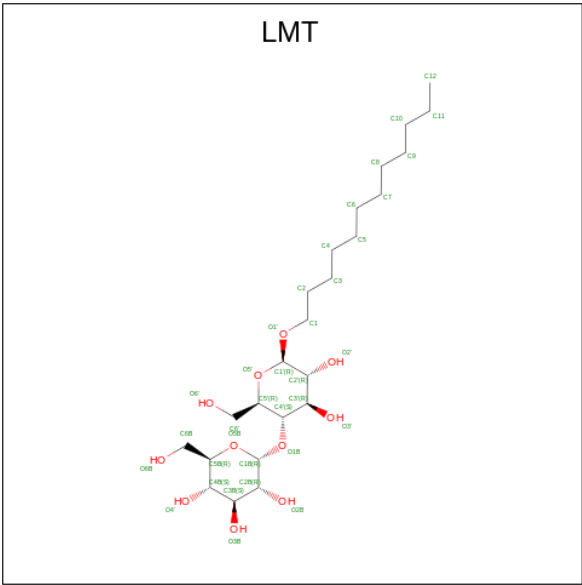
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	P	0
			49	38	10	1	
34	A	1	Total	C	O	P	0
			27	16	10	1	
34	B	1	Total	C	O	P	0
			27	16	10	1	
34	2	1	Total	C	O	P	0
			27	16	10	1	
34	5	1	Total	C	O	P	0
			27	16	10	1	

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Mol	Chain	Residues	Atoms				AltConf
34	6	1	Total	C	O	P	0
			27	16	10	1	
34	9	1	Total	C	O	P	0
			34	23	10	1	

- Molecule 35 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



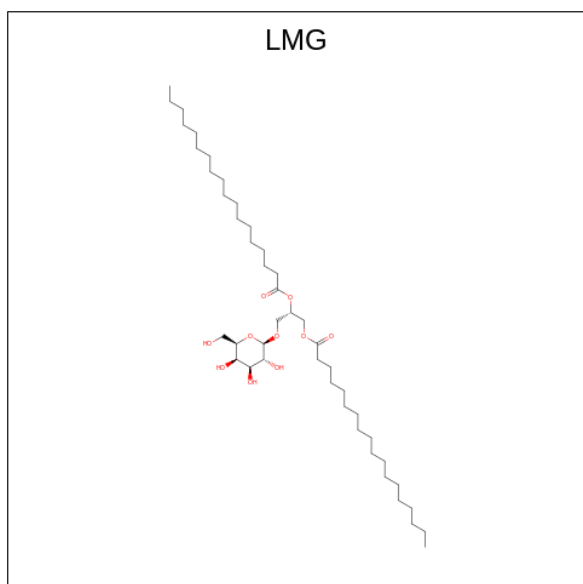
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O		0
			35	24	11		
35	A	1	Total	C	O		0
			35	24	11		
35	A	1	Total	C	O		0
			35	24	11		
35	B	1	Total	C	O		0
			35	24	11		
35	B	1	Total	C	O		0
			35	24	11		
35	1	1	Total	C	O		0
			35	24	11		
35	6	1	Total	C	O		0
			31	20	11		
35	7	1	Total	C	O		0
			35	24	11		
35	7	1	Total	C	O		0
			35	24	11		

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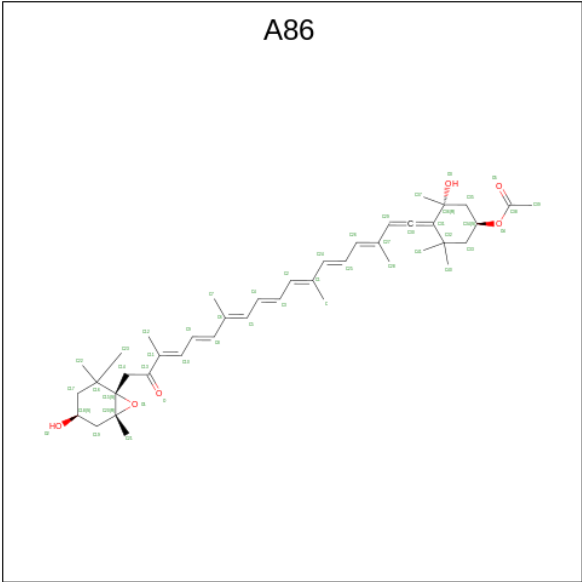
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	8	1	35	24	11	0
35	9	1	32	21	11	0
35	11	1	35	24	11	0
35	11	1	35	24	11	0
35	11	1	35	24	11	0
35	11	1	35	24	11	0
35	12	1	35	24	11	0
35	12	1	35	24	11	0
35	12	1	35	24	11	0
35	12	1	35	24	11	0
35	15	1	35	24	11	0
35	16	1	35	24	11	0

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



Mol	Chain	Residues	Atoms			AltConf
36	A	1	Total	C	O	0
			34	24	10	
36	B	1	Total	C	O	0
			55	45	10	
36	B	1	Total	C	O	0
			43	33	10	
36	F	1	Total	C	O	0
			27	17	10	
36	2u	1	Total	C	O	0
			31	21	10	
36	3	1	Total	C	O	0
			37	27	10	
36	5	1	Total	C	O	0
			33	23	10	
36	6	1	Total	C	O	0
			33	23	10	
36	7	1	Total	C	O	0
			37	27	10	
36	8	1	Total	C	O	0
			37	27	10	
36	8	1	Total	C	O	0
			42	32	10	
36	8	1	Total	C	O	0
			29	19	10	
36	14	1	Total	C	O	0
			38	28	10	

- Molecule 37 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
37	2u	1	Total	C	O	0
			48	42	6	
37	2u	1	Total	C	O	0
			48	42	6	
37	1	1	Total	C	O	0
			48	42	6	
37	2	1	Total	C	O	0
			48	42	6	
37	2	1	Total	C	O	0
			48	42	6	
37	2	1	Total	C	O	0
			48	42	6	
37	3	1	Total	C	O	0
			48	42	6	
37	3	1	Total	C	O	0
			48	42	6	
37	4	1	Total	C	O	0
			48	42	6	
37	4	1	Total	C	O	0
			48	42	6	
37	4	1	Total	C	O	0
			48	42	6	
37	4	1	Total	C	O	0
			48	42	6	
37	5	1	Total	C	O	0
			48	42	6	
37	5	1	Total	C	O	0
			48	42	6	

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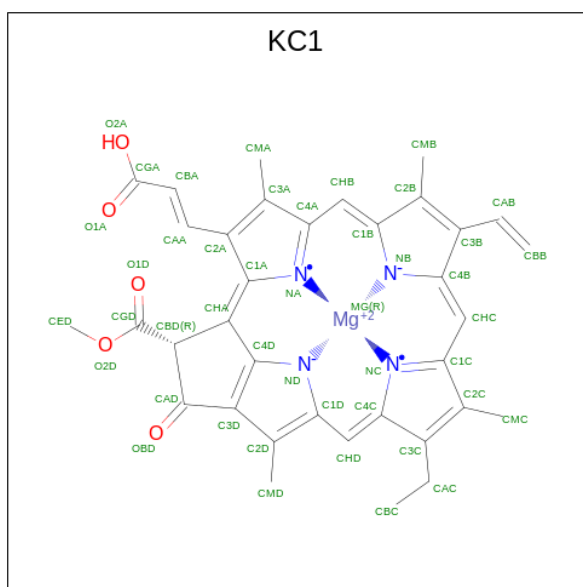
Mol	Chain	Residues	Atoms			AltConf
37	5	1	Total	C	O	0
			48	42	6	
37	6	1	Total	C	O	0
			48	42	6	
37	7	1	Total	C	O	0
			48	42	6	
37	7	1	Total	C	O	0
			48	42	6	
37	7	1	Total	C	O	0
			48	42	6	
37	8	1	Total	C	O	0
			48	42	6	
37	8	1	Total	C	O	0
			48	42	6	
37	9	1	Total	C	O	0
			48	42	6	
37	9	1	Total	C	O	0
			48	42	6	
37	9	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	10	1	Total	C	O	0
			48	42	6	
37	11	1	Total	C	O	0
			48	42	6	
37	11	1	Total	C	O	0
			48	42	6	
37	11	1	Total	C	O	0
			48	42	6	
37	11	1	Total	C	O	0
			48	42	6	
37	12	1	Total	C	O	0
			48	42	6	
37	12	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
37	13	1	Total	C	O	0
			45	40	5	
37	13	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	14	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	15	1	Total	C	O	0
			48	42	6	
37	16	1	Total	C	O	0
			48	42	6	
37	16	1	Total	C	O	0
			48	42	6	

- Molecule 38 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
38	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
38	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
38	10	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
38	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	11	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	12	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	13	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	14	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	16	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 39 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
39	1	1	Total 43	C 40	O 3	0
39	2	1	Total 43	C 40	O 3	0
39	2	1	Total 43	C 40	O 3	0
39	2	1	Total 43	C 40	O 3	0
39	3	1	Total 43	C 40	O 3	0
39	3	1	Total 43	C 40	O 3	0
39	3	1	Total 43	C 40	O 3	0
39	4	1	Total 43	C 40	O 3	0
39	4	1	Total 43	C 40	O 3	0
39	5	1	Total 43	C 40	O 3	0
39	5	1	Total 43	C 40	O 3	0
39	6	1	Total 43	C 40	O 3	0
39	6	1	Total 43	C 40	O 3	0
39	6	1	Total 43	C 40	O 3	0

Continued on next page...

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Mol	Chain	Residues	Atoms			AltConf
39	6	1	Total	C	O	0
			43	40	3	
39	7	1	Total	C	O	0
			43	40	3	
39	7	1	Total	C	O	0
			43	40	3	
39	7	1	Total	C	O	0
			43	40	3	
39	7	1	Total	C	O	0
			43	40	3	
39	8	1	Total	C	O	0
			43	40	3	
39	8	1	Total	C	O	0
			43	40	3	
39	9	1	Total	C	O	0
			43	40	3	
39	10	1	Total	C	O	0
			43	40	3	
39	10	1	Total	C	O	0
			43	40	3	
39	11	1	Total	C	O	0
			43	40	3	
39	12	1	Total	C	O	0
			43	40	3	
39	12	1	Total	C	O	0
			43	40	3	
39	13	1	Total	C	O	0
			43	40	3	
39	15	1	Total	C	O	0
			43	40	3	
39	15	1	Total	C	O	0
			43	40	3	
39	16	1	Total	C	O	0
			43	40	3	

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	A	42	Total	O	0
			42	42	
40	B	53	Total	O	0
			53	53	

Continued on next page...

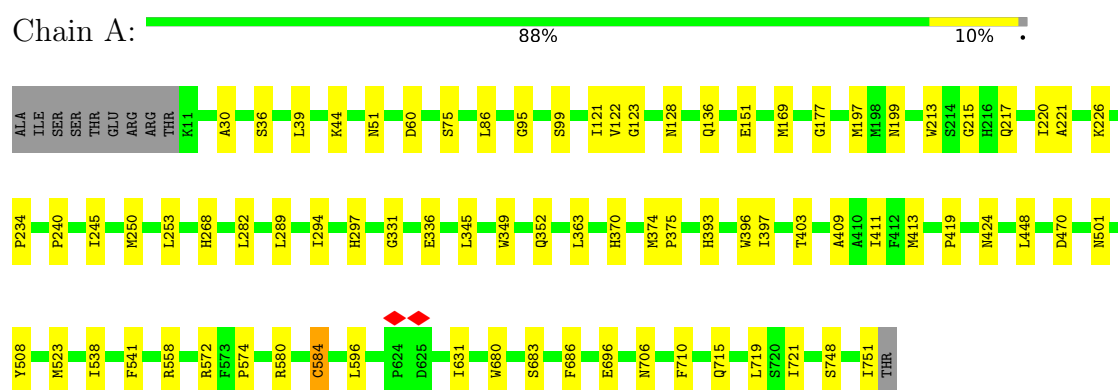
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
40	C	15	Total 15	O 15	0
40	D	13	Total 13	O 13	0
40	E	3	Total 3	O 3	0
40	F	3	Total 3	O 3	0
40	I	1	Total 1	O 1	0
40	L	8	Total 8	O 8	0
40	1	1	Total 1	O 1	0
40	2	2	Total 2	O 2	0
40	3	1	Total 1	O 1	0
40	5	1	Total 1	O 1	0
40	6	2	Total 2	O 2	0
40	7	2	Total 2	O 2	0
40	8	4	Total 4	O 4	0
40	9	1	Total 1	O 1	0
40	10	1	Total 1	O 1	0
40	11	1	Total 1	O 1	0
40	12	2	Total 2	O 2	0

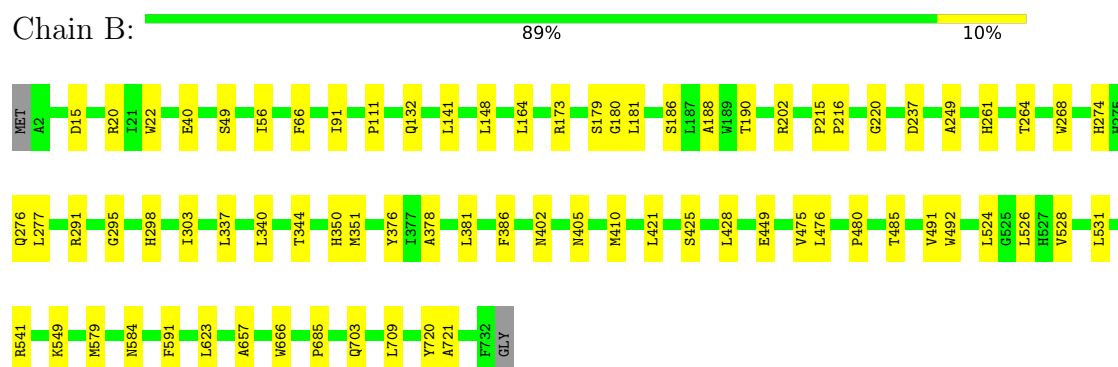
3 Residue-property plots [i](#)

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

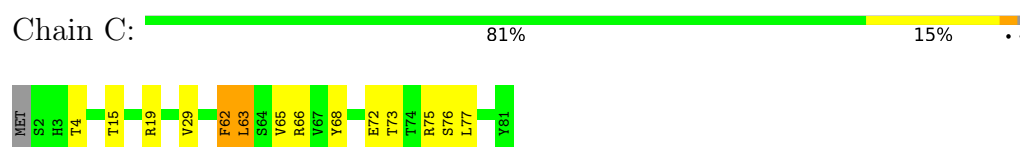
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



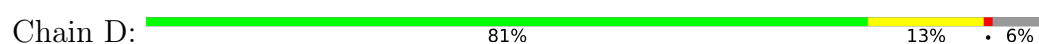
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II





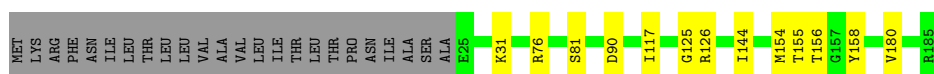
- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 85% 10%



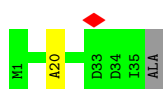
- Molecule 6: Photosystem I reaction center subunit III

Chain F: 80% 7% 13%



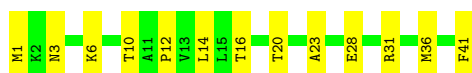
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 94%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 68% 32%



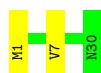
- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 84% 7% 9%



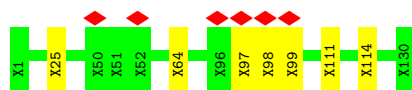
- Molecule 10: Photosystem I reaction center subunit XII

Chain M: 93% 7%



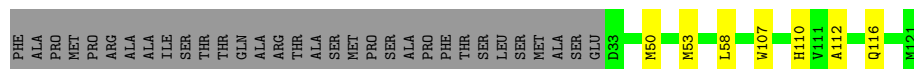
- Molecule 11: Unknown protein 1

Chain 1u: 5% 95% 5%



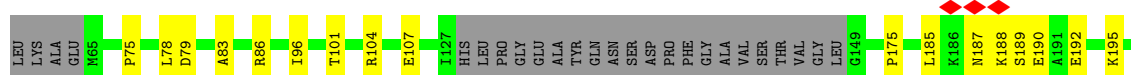
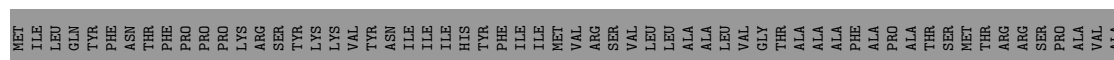
- Molecule 12: Photosystem I reaction center subunit Psa28

Chain 2u: 68% 6% 26%



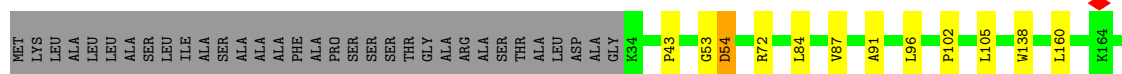
- Molecule 13: Fucoxanthin chlorophyll a/c-binding protein Lhcr15

Chain 1: 53% 9% 38%



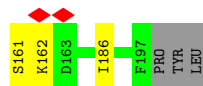
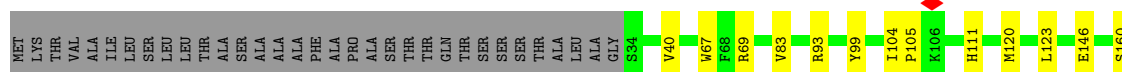
- Molecule 14: Fucoxanthin chlorophyll a/c-binding protein Lhcr8

Chain 2: 77% 7% 16%



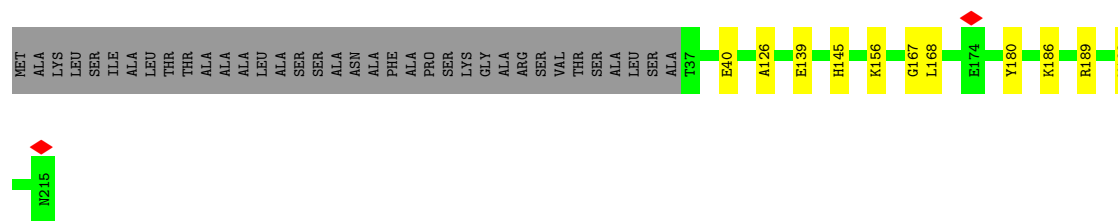
- Molecule 15: Fucoxanthin chlorophyll a/c-binding protein Lhcr2

Chain 3: 74% 8% 18%



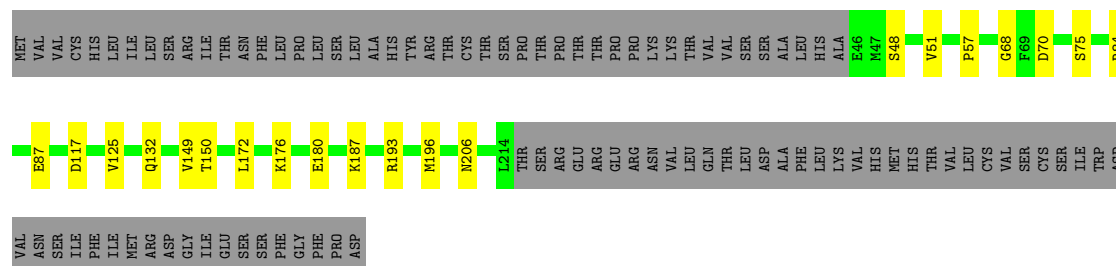
- Molecule 16: Fucoxanthin chlorophyll a/c-binding protein Lhcr9

Chain 4: 78% 5% 17%



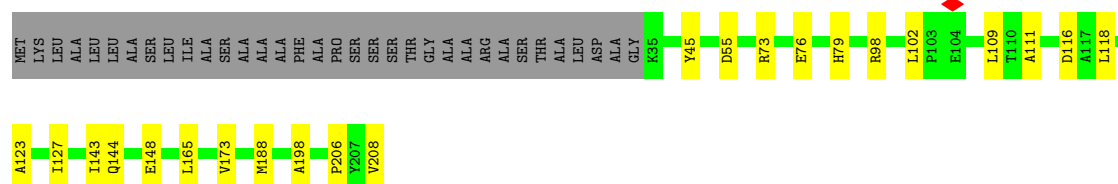
- Molecule 17: Fucoxanthin chlorophyll a/c-binding protein Lher11

Chain 5: 56% 8% 36%



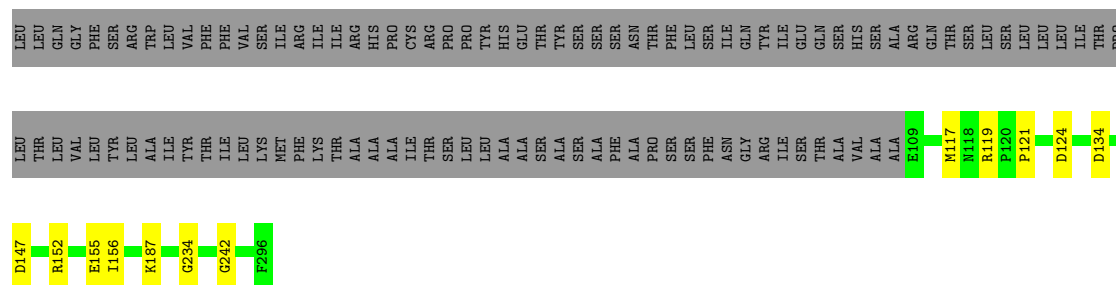
- Molecule 18: Fucoxanthin chlorophyll a/c-binding protein Lher12

Chain 6: 73% 11% 16%



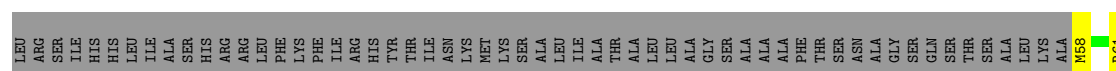
- Molecule 19: Fucoxanthin chlorophyll a/c-binding protein Lher10

Chain 7: 59% 36% 5%



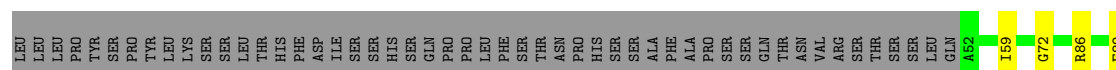
- Molecule 20: Fucoxanthin chlorophyll a/c-binding protein Lher4

Chain 8: 69% 10% 21%

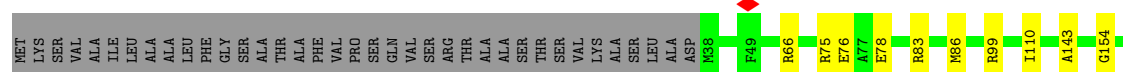
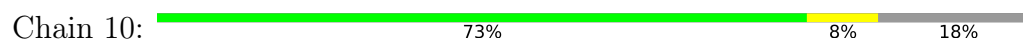




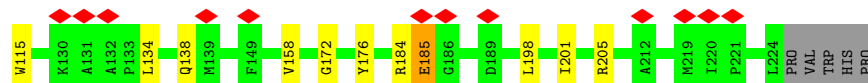
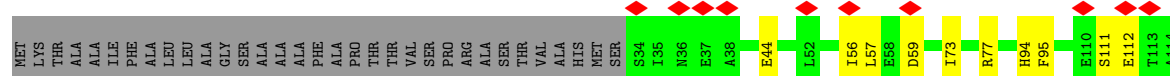
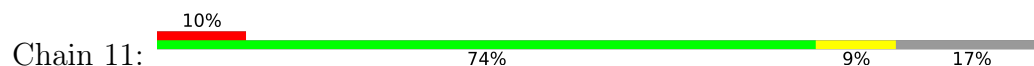
- Molecule 21: Fucoxanthin chlorophyll a/c-binding protein Lhcf6



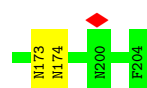
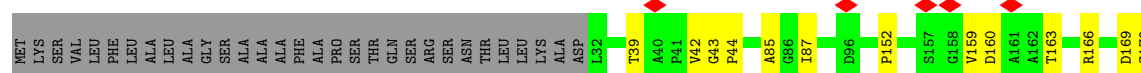
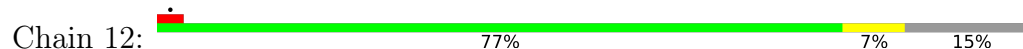
- Molecule 22: Fucoxanthin chlorophyll a/c-binding protein Lhcr3



- Molecule 23: Fucoxanthin chlorophyll a/c-binding protein Lhcq13

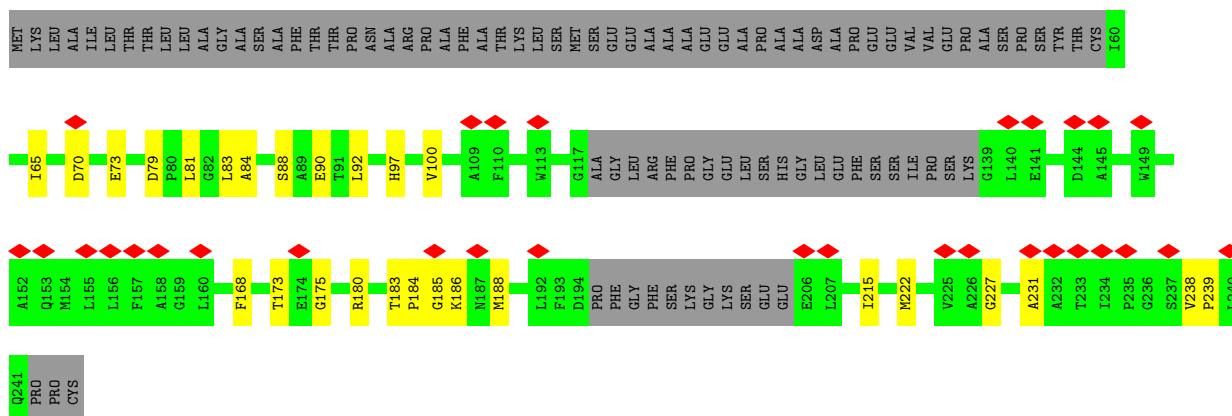


- Molecule 24: Fucoxanthin chlorophyll a/c-binding protein Lhcq3

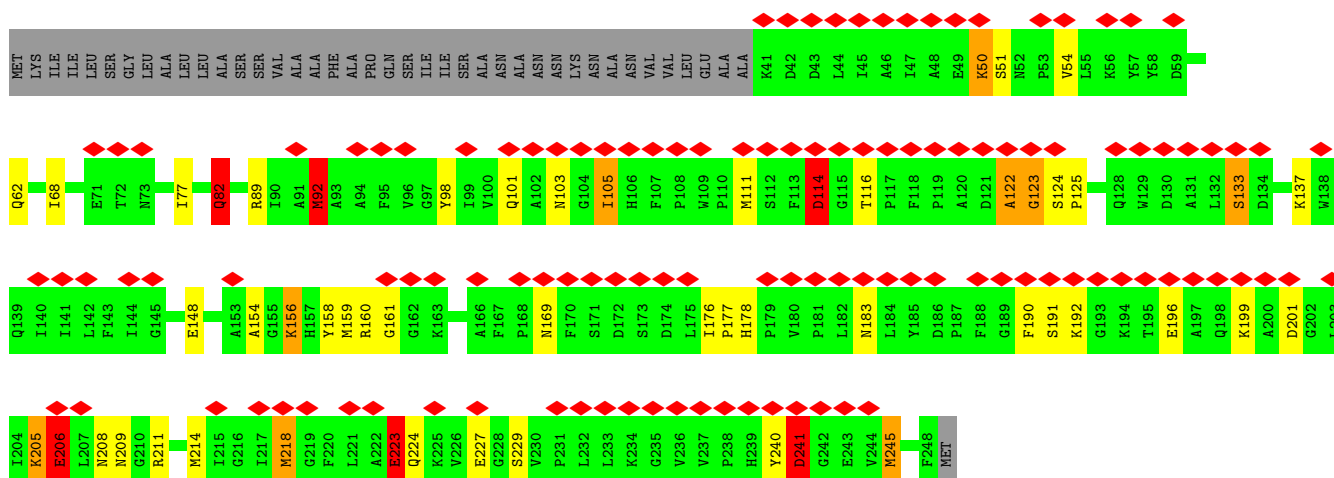


- Molecule 25: Fucoxanthin chlorophyll a/c-binding protein Lhcq11

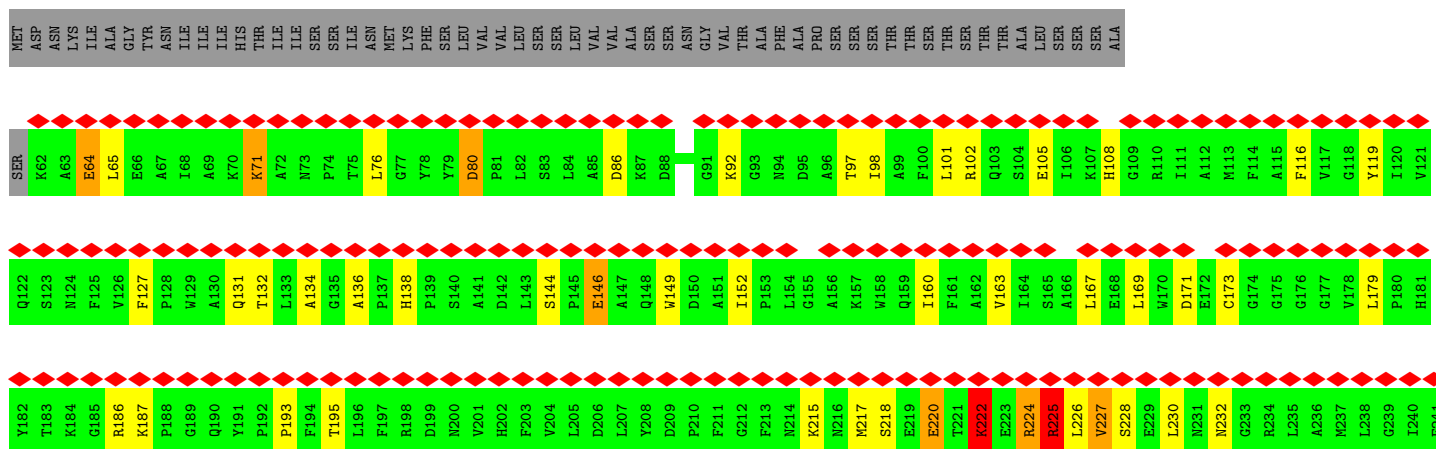
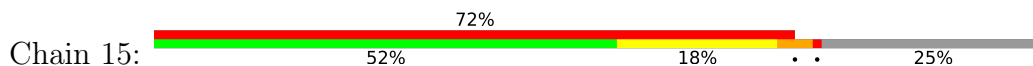


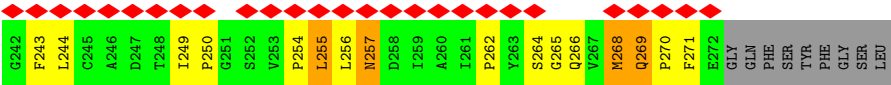


- Molecule 26: Fucoxanthin chlorophyll a/c-binding protein Lhcq10

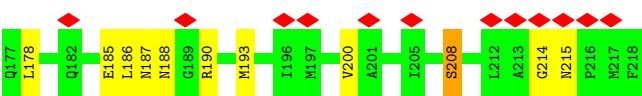
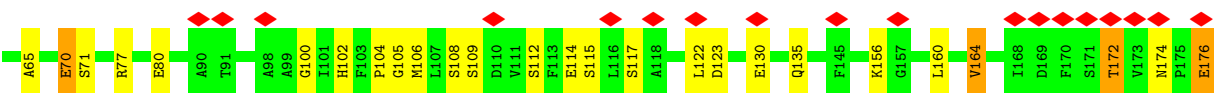
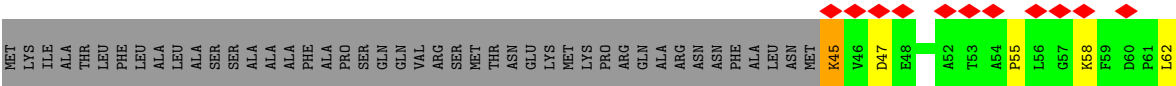


- Molecule 27: Fucoxanthin chlorophyll a/c-binding protein Lhcq8





• Molecule 28: 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
Maximum map value	0.401	Depositor
Minimum map value	-0.141	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.045	Depositor
Map size ($\text{\AA}$)	560.952, 560.952, 560.952	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.113, 1.113, 1.113	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: CLA, DD6, BCR, SF4, LHG, KC1, LMT, CL0, A86, PQN, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/6039	0.47	0/8220
2	B	0.33	0/6011	0.50	2/8209 (0.0%)
3	C	0.36	0/609	0.67	3/826 (0.4%)
4	D	0.32	0/1064	0.67	2/1437 (0.1%)
5	E	0.26	0/486	0.45	0/656
6	F	0.29	0/1287	0.47	0/1745
7	I	0.32	0/281	0.58	0/383
8	J	0.27	0/355	0.52	0/480
9	L	0.28	0/1054	0.48	0/1432
10	M	0.24	0/229	0.42	0/313
12	2u	0.26	0/696	0.40	0/948
13	1	0.21	0/1106	0.40	0/1490
14	2	0.28	0/1344	0.58	2/1818 (0.1%)
15	3	0.25	0/1309	0.55	0/1767
16	4	0.26	0/1404	0.48	0/1897
17	5	0.25	0/1336	0.49	0/1804
18	6	0.27	0/1391	0.47	0/1886
19	7	0.27	0/1445	0.48	0/1952
20	8	0.29	0/1706	0.50	0/2310
21	9	0.25	0/1302	0.52	0/1769
22	10	0.27	0/1344	0.52	0/1824
23	11	0.23	0/1522	0.56	2/2070 (0.1%)
24	12	0.29	0/1305	0.51	0/1776
25	13	0.23	0/1177	0.56	2/1592 (0.1%)
26	14	0.50	2/1660 (0.1%)	1.32	31/2255 (1.4%)
27	15	0.57	3/1705 (0.2%)	1.38	31/2319 (1.3%)
28	16	0.39	0/1347	0.98	8/1833 (0.4%)
All	All	0.32	5/40514 (0.0%)	0.64	83/55011 (0.2%)

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	D	0	1
11	1u	0	1
16	4	0	1
21	9	0	2
22	10	0	1
26	14	0	7
27	15	0	8
28	16	0	1
All	All	0	22

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	15	146	GLU	CB-CG	-6.90	1.31	1.52
26	14	245	MET	CB-CG	-6.32	1.33	1.52
26	14	50	LYS	CD-CE	-5.91	1.34	1.52
27	15	224	ARG	CD-NE	-5.43	1.38	1.46
27	15	224	ARG	CB-CG	-5.18	1.36	1.52

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	92	MET	CA-CB-CG	21.25	156.60	114.10
27	15	146	GLU	CA-CB-CG	17.81	149.72	114.10
27	15	224	ARG	NE-CZ-NH2	13.84	131.65	119.20
26	14	92	MET	CB-CG-SD	13.72	153.87	112.70
27	15	224	ARG	NE-CZ-NH1	-13.17	108.33	121.50

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1u	97	UNK	Peptide
16	4	145	HIS	Sidechain
21	9	109	GLY	Peptide
21	9	113	ALA	Peptide
4	D	91	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5841	0	5666	63	0
2	B	5801	0	5614	52	0
3	C	599	0	579	7	0
4	D	1037	0	1023	12	0
5	E	478	0	473	2	0
6	F	1257	0	1259	12	0
7	I	273	0	285	1	0
8	J	344	0	351	13	0
9	L	1030	0	1063	10	0
10	M	227	0	247	2	0
11	1u	650	0	138	4	0
12	2u	674	0	658	6	0
13	1	1086	0	1089	13	0
14	2	1310	0	1287	12	0
15	3	1275	0	1239	9	0
16	4	1368	0	1344	8	0
17	5	1304	0	1286	12	0
18	6	1354	0	1328	14	0
19	7	1416	0	1379	9	0
20	8	1660	0	1625	18	0
21	9	1267	0	1210	12	0
22	10	1302	0	1274	10	0
23	11	1479	0	1452	17	0
24	12	1274	0	1267	10	0
25	13	1148	0	1130	19	0
26	14	1609	0	1568	25	0
27	15	1654	0	1613	20	0
28	16	1313	0	1310	23	0
29	A	65	0	72	3	0
30	1	390	0	425	12	0
30	10	435	0	465	6	0
30	11	315	0	337	12	0
30	12	566	0	604	11	0
30	13	350	0	354	11	0
30	14	468	0	400	8	0
30	15	685	0	589	14	0
30	16	478	0	429	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	2	620	0	649	16	0
30	2u	65	0	72	3	0
30	3	472	0	474	7	0
30	4	484	0	495	12	0
30	5	455	0	499	12	0
30	6	620	0	656	10	0
30	7	566	0	609	13	0
30	8	420	0	427	7	0
30	9	486	0	503	12	0
30	A	2614	0	2694	85	0
30	B	2465	0	2570	85	0
30	F	175	0	177	7	0
30	J	45	0	33	1	0
30	L	110	0	105	6	0
31	A	33	0	46	5	0
31	B	33	0	46	1	0
32	A	8	0	0	0	0
32	C	16	0	0	0	0
33	2u	40	0	56	3	0
33	A	200	0	280	12	0
33	B	240	0	336	11	0
33	F	40	0	56	3	0
33	I	40	0	56	2	0
33	J	80	0	112	7	0
33	L	120	0	168	10	0
33	M	40	0	56	3	0
34	2	27	0	24	0	0
34	5	27	0	24	1	0
34	6	27	0	24	0	0
34	9	34	0	38	0	0
34	A	76	0	98	2	0
34	B	27	0	24	0	0
35	1	35	0	46	0	0
35	11	140	0	184	4	0
35	12	140	0	184	4	0
35	15	35	0	46	0	0
35	16	35	0	46	0	0
35	6	31	0	35	2	0
35	7	70	0	91	2	0
35	8	35	0	46	0	0
35	9	32	0	37	0	0
35	A	105	0	138	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	70	0	92	1	0
36	14	38	0	46	2	0
36	2u	31	0	31	0	0
36	3	37	0	44	2	0
36	5	33	0	36	0	0
36	6	33	0	34	0	0
36	7	37	0	44	0	0
36	8	108	0	123	1	0
36	A	34	0	38	3	0
36	B	98	0	141	3	0
36	F	27	0	24	0	0
37	1	48	0	0	0	0
37	10	240	0	0	0	0
37	11	192	0	0	1	0
37	12	96	0	0	0	0
37	13	93	0	0	0	0
37	14	384	0	0	2	0
37	15	336	0	0	0	0
37	16	96	0	0	0	0
37	2	144	0	0	0	0
37	2u	96	0	0	0	0
37	3	96	0	0	0	0
37	4	192	0	0	1	0
37	5	144	0	0	1	0
37	6	48	0	0	0	0
37	7	144	0	0	1	0
37	8	96	0	0	1	0
37	9	144	0	0	1	0
38	1	90	0	0	0	0
38	10	135	0	0	0	0
38	11	180	0	0	0	0
38	12	180	0	0	1	0
38	13	270	0	0	0	0
38	14	135	0	0	0	0
38	16	90	0	0	1	0
38	2	135	0	0	0	0
38	3	135	0	0	1	0
38	4	135	0	0	1	0
38	5	180	0	0	2	0
38	6	180	0	0	0	0
38	7	90	0	0	0	0
38	8	315	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	9	180	0	0	0	0
39	1	43	0	0	0	0
39	10	86	0	0	1	0
39	11	43	0	0	0	0
39	12	86	0	0	0	0
39	13	43	0	0	1	0
39	15	86	0	0	0	0
39	16	43	0	0	0	0
39	2	129	0	0	0	0
39	3	129	0	0	0	0
39	4	86	0	0	0	0
39	5	86	0	0	0	0
39	6	172	0	0	3	0
39	7	172	0	0	0	0
39	8	86	0	0	0	0
39	9	43	0	0	0	0
40	1	1	0	0	0	0
40	10	1	0	0	0	0
40	11	1	0	0	0	0
40	12	2	0	0	0	0
40	2	2	0	0	0	0
40	3	1	0	0	0	0
40	5	1	0	0	0	0
40	6	2	0	0	0	0
40	7	2	0	0	0	0
40	8	4	0	0	0	0
40	9	1	0	0	0	0
40	A	42	0	0	2	0
40	B	53	0	0	0	0
40	C	15	0	0	0	0
40	D	13	0	0	0	0
40	E	3	0	0	0	0
40	F	3	0	0	0	0
40	I	1	0	0	0	0
40	L	8	0	0	0	0
All	All	62199	0	55345	644	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 644 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)
26:14:101:GLN:OE1	30:14:303:CLA:NA	2.01	0.94
23:11:44:GLU:OE1	30:11:310:CLA:NC	2.10	0.84
25:13:73:GLU:OE1	30:13:307:CLA:NC	2.11	0.83
27:15:105:GLU:OE1	30:15:302:CLA:NB	2.21	0.74
30:B:815:CLA:HBB1	33:B:841:BCR:H333	1.74	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	712 (96%)	25 (3%)	2 (0%)	36	50
2	B	729/733 (100%)	699 (96%)	29 (4%)	1 (0%)	48	64
3	C	78/81 (96%)	73 (94%)	3 (4%)	2 (3%)	4	4
4	D	129/139 (93%)	109 (84%)	18 (14%)	2 (2%)	7	11
5	E	58/67 (87%)	55 (95%)	3 (5%)	0	100	100
6	F	159/185 (86%)	152 (96%)	7 (4%)	0	100	100
7	I	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	L	133/151 (88%)	128 (96%)	5 (4%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
12	2u	87/121 (72%)	87 (100%)	0	0	100	100
13	1	137/227 (60%)	130 (95%)	7 (5%)	0	100	100
14	2	170/205 (83%)	151 (89%)	19 (11%)	0	100	100
15	3	162/200 (81%)	151 (93%)	9 (6%)	2 (1%)	10	16
16	4	177/215 (82%)	167 (94%)	10 (6%)	0	100	100
17	5	167/266 (63%)	157 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	6	172/208 (83%)	167 (97%)	5 (3%)	0	100	100
19	7	186/296 (63%)	179 (96%)	7 (4%)	0	100	100
20	8	211/270 (78%)	203 (96%)	8 (4%)	0	100	100
21	9	161/214 (75%)	149 (92%)	12 (8%)	0	100	100
22	10	167/207 (81%)	157 (94%)	8 (5%)	2 (1%)	10	16
23	11	189/229 (82%)	173 (92%)	16 (8%)	0	100	100
24	12	171/204 (84%)	160 (94%)	11 (6%)	0	100	100
25	13	144/244 (59%)	133 (92%)	11 (8%)	0	100	100
26	14	206/249 (83%)	177 (86%)	29 (14%)	0	100	100
27	15	209/281 (74%)	171 (82%)	37 (18%)	1 (0%)	24	37
28	16	172/218 (79%)	157 (91%)	15 (9%)	0	100	100
All	All	5013/6068 (83%)	4694 (94%)	307 (6%)	12 (0%)	44	58

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
4	D	92	VAL
2	B	492	TRP
3	C	62	PHE
3	C	63	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	602/611 (98%)	601 (100%)	1 (0%)	87	94
2	B	592/593 (100%)	589 (100%)	3 (0%)	81	91
3	C	69/70 (99%)	67 (97%)	2 (3%)	37	60
4	D	111/119 (93%)	111 (100%)	0	100	100
5	E	51/58 (88%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	132/153 (86%)	132 (100%)	0	100	100
7	I	29/29 (100%)	29 (100%)	0	100	100
8	J	37/37 (100%)	37 (100%)	0	100	100
9	L	107/121 (88%)	107 (100%)	0	100	100
10	M	24/24 (100%)	24 (100%)	0	100	100
12	2u	69/94 (73%)	69 (100%)	0	100	100
13	1	114/183 (62%)	112 (98%)	2 (2%)	51	73
14	2	134/154 (87%)	133 (99%)	1 (1%)	76	88
15	3	128/154 (83%)	128 (100%)	0	100	100
16	4	142/165 (86%)	142 (100%)	0	100	100
17	5	137/228 (60%)	135 (98%)	2 (2%)	57	77
18	6	140/160 (88%)	140 (100%)	0	100	100
19	7	143/236 (61%)	143 (100%)	0	100	100
20	8	171/215 (80%)	171 (100%)	0	100	100
21	9	126/175 (72%)	125 (99%)	1 (1%)	73	86
22	10	133/161 (83%)	133 (100%)	0	100	100
23	11	154/181 (85%)	154 (100%)	0	100	100
24	12	136/159 (86%)	135 (99%)	1 (1%)	76	88
25	13	112/184 (61%)	112 (100%)	0	100	100
26	14	166/196 (85%)	148 (89%)	18 (11%)	6	9
27	15	171/231 (74%)	148 (86%)	23 (14%)	4	5
28	16	139/174 (80%)	126 (91%)	13 (9%)	8	13
All	All	4069/4865 (84%)	4002 (98%)	67 (2%)	54	76

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	16	70	GLU
28	16	115	SER
28	16	178	LEU
26	14	196	GLU
26	14	192	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
13	1	151	ASN
27	15	216	ASN
15	3	193	ASN
27	15	94	ASN
28	16	215	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](#)

427 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	$\# Z > 2$
30	CLA	4	305	16	69,73,73	1.99	20 (28%)	83,113,113	2.80	30 (36%)
30	CLA	10	307	22	69,73,73	1.98	20 (28%)	83,113,113	2.73	30 (36%)
30	CLA	3	301	15	69,73,73	1.97	19 (27%)	83,113,113	2.80	28 (33%)
37	A86	14	314	-	44,50,50	4.09	22 (50%)	51,76,76	8.27	21 (41%)
30	CLA	B	837	40	69,73,73	1.96	19 (27%)	83,113,113	2.77	28 (33%)
30	CLA	B	830	2	69,73,73	1.95	20 (28%)	83,113,113	2.97	31 (37%)
38	KC1	13	312	25	49,53,53	3.11	26 (53%)	63,89,89	4.02	35 (55%)
33	BCR	M	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.27	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	6	316	40	59,63,73	2.19	20 (33%)	71,101,113	2.91	27 (38%)
38	KC1	5	310	17	49,53,53	3.02	24 (48%)	63,89,89	4.12	36 (57%)
37	A86	5	315	-	44,50,50	4.05	23 (52%)	51,76,76	8.37	18 (35%)
30	CLA	10	309	22	69,73,73	2.04	20 (28%)	83,113,113	2.74	27 (32%)
35	LMT	A	854	-	36,36,36	0.45	0	47,47,47	1.19	5 (10%)
30	CLA	3	303	15	69,73,73	2.08	21 (30%)	83,113,113	2.88	31 (37%)
30	CLA	B	821	2	59,63,73	2.14	19 (32%)	71,101,113	2.90	29 (40%)
30	CLA	F	201	40	69,73,73	1.94	19 (27%)	83,113,113	2.74	29 (34%)
33	BCR	A	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	9 (16%)
30	CLA	8	308	20	59,63,73	2.17	18 (30%)	71,101,113	3.04	30 (42%)
30	CLA	A	836	1	58,62,73	2.15	19 (32%)	69,99,113	2.91	31 (44%)
30	CLA	12	312	24	69,73,73	2.01	20 (28%)	83,113,113	2.77	29 (34%)
30	CLA	A	829	30,1	69,73,73	1.98	20 (28%)	83,113,113	2.88	28 (33%)
30	CLA	A	843	40	69,73,73	1.96	18 (26%)	83,113,113	2.67	30 (36%)
30	CLA	A	828	1	69,73,73	1.91	19 (27%)	83,113,113	2.93	31 (37%)
38	KC1	11	311	23	49,53,53	3.08	25 (51%)	63,89,89	4.05	35 (55%)
37	A86	7	315	-	44,50,50	3.90	23 (52%)	51,76,76	7.79	20 (39%)
30	CLA	12	308	40	69,73,73	2.01	21 (30%)	83,113,113	2.70	29 (34%)
38	KC1	1	306	13	49,53,53	3.05	25 (51%)	63,89,89	4.08	36 (57%)
37	A86	2	302	-	44,50,50	4.10	23 (52%)	51,76,76	8.41	18 (35%)
33	BCR	A	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.24	7 (12%)
39	DD6	12	315	30	39,45,45	6.70	22 (56%)	52,67,67	6.85	26 (50%)
30	CLA	A	833	1	69,73,73	2.02	20 (28%)	83,113,113	2.78	28 (33%)
30	CLA	12	307	24	50,54,73	2.30	18 (36%)	60,90,113	3.14	27 (45%)
37	A86	14	317	-	44,50,50	4.03	23 (52%)	51,76,76	8.75	18 (35%)
30	CLA	2	311	14	69,73,73	2.06	19 (27%)	83,113,113	2.74	26 (31%)
38	KC1	11	312	-	49,53,53	3.04	23 (46%)	63,89,89	3.84	35 (55%)
30	CLA	B	814	2	59,63,73	2.13	19 (32%)	71,101,113	2.93	29 (40%)
30	CLA	B	822	2,30	69,73,73	1.98	20 (28%)	83,113,113	2.96	34 (40%)
30	CLA	5	311	17,40	69,73,73	2.04	20 (28%)	83,113,113	2.90	29 (34%)
34	LHG	B	848	30	26,26,48	0.93	1 (3%)	29,32,54	1.39	4 (13%)
30	CLA	4	303	16	69,73,73	2.00	20 (28%)	83,113,113	2.75	28 (33%)
30	CLA	13	307	25	69,73,73	2.08	20 (28%)	83,113,113	2.80	30 (36%)
37	A86	9	316	30	44,50,50	4.22	22 (50%)	51,76,76	8.44	16 (31%)
37	A86	2u	203	30	44,50,50	3.98	24 (54%)	51,76,76	8.18	21 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	6	309	18	69,73,73	2.00	17 (24%)	83,113,113	2.75	33 (39%)
38	KC1	5	305	17	49,53,53	3.03	24 (48%)	63,89,89	4.04	35 (55%)
34	LHG	2	320	30	26,26,48	0.87	1 (3%)	29,32,54	1.30	3 (10%)
38	KC1	8	314	40,38	49,53,53	3.02	24 (48%)	63,89,89	3.95	35 (55%)
36	LMG	8	320	-	42,42,55	0.90	3 (7%)	50,50,63	1.31	5 (10%)
37	A86	6	320	-	44,50,50	3.90	23 (52%)	51,76,76	7.09	20 (39%)
30	CLA	2	310	14	69,73,73	2.00	19 (27%)	83,113,113	4.59	30 (36%)
39	DD6	3	313	-	39,45,45	6.73	23 (58%)	52,67,67	6.66	24 (46%)
38	KC1	9	304	21	49,53,53	3.01	23 (46%)	63,89,89	4.03	36 (57%)
39	DD6	12	317	-	39,45,45	6.67	22 (56%)	52,67,67	7.20	28 (53%)
33	BCR	F	204	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	8 (14%)
32	SF4	C	101	3	0,12,12	-	-	-	-	-
38	KC1	11	305	23	49,53,53	3.02	24 (48%)	63,89,89	4.09	36 (57%)
38	KC1	6	308	18	49,53,53	2.98	22 (44%)	63,89,89	4.05	34 (53%)
37	A86	9	313	21	44,50,50	3.98	23 (52%)	51,76,76	7.51	20 (39%)
30	CLA	B	813	2	69,73,73	1.98	20 (28%)	83,113,113	2.78	29 (34%)
30	CLA	10	311	-	49,53,73	2.42	21 (42%)	59,89,113	3.23	26 (44%)
30	CLA	B	836	2	51,55,73	2.26	19 (37%)	61,91,113	3.30	28 (45%)
30	CLA	B	807	2	69,73,73	1.95	19 (27%)	83,113,113	2.85	32 (38%)
30	CLA	B	817	2	63,67,73	2.08	19 (30%)	75,105,113	3.04	28 (37%)
39	DD6	2	315	-	39,45,45	6.74	23 (58%)	52,67,67	6.78	27 (51%)
30	CLA	16	310	28	49,53,73	2.41	22 (44%)	59,89,113	3.26	29 (49%)
30	CLA	12	303	24	69,73,73	2.01	21 (30%)	83,113,113	2.75	28 (33%)
30	CLA	15	303	30,37,27	64,68,73	2.12	20 (31%)	77,107,113	3.00	30 (38%)
37	A86	3	315	-	44,50,50	4.12	24 (54%)	51,76,76	8.24	16 (31%)
30	CLA	1	302	30,13	69,73,73	2.00	19 (27%)	83,113,113	2.78	29 (34%)
30	CLA	F	202	40	69,73,73	1.99	20 (28%)	83,113,113	2.76	29 (34%)
30	CLA	13	301	25	69,73,73	2.00	20 (28%)	83,113,113	2.85	29 (34%)
30	CLA	B	810	2	69,73,73	1.96	20 (28%)	83,113,113	2.78	30 (36%)
30	CLA	6	317	-	69,73,73	2.03	21 (30%)	83,113,113	2.79	28 (33%)
30	CLA	A	810	1	69,73,73	1.97	20 (28%)	83,113,113	2.80	33 (39%)
37	A86	12	316	-	44,50,50	4.08	23 (52%)	51,76,76	8.38	17 (33%)
30	CLA	1	304	13	69,73,73	1.99	19 (27%)	83,113,113	2.66	29 (34%)
38	KC1	12	309	24	49,53,53	3.04	23 (46%)	63,89,89	3.98	36 (57%)
38	KC1	14	306	26	49,53,53	3.05	26 (53%)	63,89,89	4.06	36 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMT	11	303	-	36,36,36	0.40	0	47,47,47	0.84	0
30	CLA	B	833	30,40	69,73,73	1.99	21 (30%)	83,113,113	2.74	29 (34%)
30	CLA	16	301	28	69,73,73	2.00	18 (26%)	83,113,113	2.82	31 (37%)
30	CLA	B	831	2	62,66,73	2.10	19 (30%)	74,104,113	3.12	30 (40%)
39	DD6	15	318	-	39,45,45	6.78	21 (53%)	52,67,67	6.98	31 (59%)
30	CLA	B	838	2	69,73,73	1.97	18 (26%)	83,113,113	2.78	28 (33%)
30	CLA	10	303	22	69,73,73	2.01	18 (26%)	83,113,113	2.76	28 (33%)
30	CLA	12	321	24,26	69,73,73	2.04	20 (28%)	83,113,113	2.75	31 (37%)
30	CLA	A	817	36,40	53,57,73	2.27	18 (33%)	62,93,113	3.17	24 (38%)
30	CLA	11	310	23	69,73,73	2.09	21 (30%)	83,113,113	2.79	30 (36%)
30	CLA	A	809	30,1	69,73,73	1.95	21 (30%)	83,113,113	2.77	29 (34%)
30	CLA	A	823	1	53,57,73	2.24	19 (35%)	62,93,113	3.22	29 (46%)
30	CLA	1	305	40	69,73,73	2.06	21 (30%)	83,113,113	2.74	29 (34%)
39	DD6	10	313	-	39,45,45	6.78	24 (61%)	52,67,67	7.12	30 (57%)
30	CLA	14	302	26	69,73,73	2.05	20 (28%)	83,113,113	2.85	33 (39%)
30	CLA	A	821	1	65,69,73	2.00	19 (29%)	78,108,113	2.77	32 (41%)
30	CLA	14	309	26	49,53,73	2.46	20 (40%)	59,89,113	3.20	27 (45%)
30	CLA	B	829	2	69,73,73	1.97	18 (26%)	83,113,113	2.78	29 (34%)
30	CLA	A	802	40	69,73,73	1.96	18 (26%)	83,113,113	2.83	31 (37%)
30	CLA	6	310	34	69,73,73	2.03	21 (30%)	83,113,113	2.72	27 (32%)
35	LMT	A	857	-	36,36,36	0.37	0	47,47,47	0.78	0
36	LMG	F	205	-	27,27,55	1.02	1 (3%)	35,35,63	1.25	5 (14%)
37	A86	2	319	-	44,50,50	3.89	22 (50%)	51,76,76	7.61	18 (35%)
37	A86	11	315	-	44,50,50	3.99	22 (50%)	51,76,76	7.49	22 (43%)
38	KC1	12	305	24	49,53,53	3.04	24 (48%)	63,89,89	4.04	36 (57%)
30	CLA	7	311	19	69,73,73	2.01	19 (27%)	83,113,113	2.70	29 (34%)
37	A86	11	314	-	44,50,50	4.09	23 (52%)	51,76,76	8.59	18 (35%)
30	CLA	B	801	2	69,73,73	1.90	18 (26%)	83,113,113	2.88	34 (40%)
39	DD6	7	314	-	39,45,45	6.64	21 (53%)	52,67,67	7.34	28 (53%)
37	A86	15	321	27	44,50,50	4.11	23 (52%)	51,76,76	8.63	19 (37%)
30	CLA	12	310	40	69,73,73	1.99	18 (26%)	83,113,113	2.78	29 (34%)
30	CLA	7	307	19	69,73,73	1.98	20 (28%)	83,113,113	2.78	27 (32%)
30	CLA	3	307	15	69,73,73	2.09	21 (30%)	83,113,113	2.75	30 (36%)
37	A86	2u	205	-	44,50,50	4.13	23 (52%)	51,76,76	7.47	22 (43%)
30	CLA	L	202	9	69,73,73	1.94	20 (28%)	83,113,113	2.91	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	KC1	16	311	28	49,53,53	3.08	23 (46%)	63,89,89	3.91	32 (50%)
30	CLA	B	805	2	69,73,73	1.99	21 (30%)	83,113,113	2.87	30 (36%)
30	CLA	7	312	19	50,54,73	2.40	20 (40%)	60,90,113	3.21	27 (45%)
30	CLA	9	305	-	69,73,73	2.01	20 (28%)	83,113,113	2.91	32 (38%)
30	CLA	B	839	34	69,73,73	1.96	19 (27%)	83,113,113	2.99	30 (36%)
30	CLA	15	310	27	49,53,73	2.46	20 (40%)	59,89,113	3.28	26 (44%)
30	CLA	14	304	26	49,53,73	2.44	20 (40%)	59,89,113	3.25	25 (42%)
30	CLA	B	825	2	69,73,73	1.98	19 (27%)	83,113,113	2.84	30 (36%)
34	LHG	A	853	30	26,26,48	0.91	1 (3%)	29,32,54	1.29	3 (10%)
37	A86	12	314	-	44,50,50	4.02	22 (50%)	51,76,76	8.11	18 (35%)
33	BCR	J	103	-	41,41,41	1.15	3 (7%)	56,56,56	1.16	5 (8%)
30	CLA	7	304	19	69,73,73	1.97	20 (28%)	83,113,113	2.78	30 (36%)
30	CLA	B	806	2	69,73,73	1.98	17 (24%)	83,113,113	2.78	30 (36%)
30	CLA	A	813	1	69,73,73	2.00	20 (28%)	83,113,113	2.77	30 (36%)
36	LMG	2u	204	12	31,31,55	1.12	3 (9%)	39,39,63	1.18	4 (10%)
30	CLA	11	306	40	59,63,73	2.18	20 (33%)	71,101,113	3.10	33 (46%)
39	DD6	5	314	-	39,45,45	6.56	24 (61%)	52,67,67	7.17	30 (57%)
30	CLA	15	307	27	54,58,73	2.30	21 (38%)	65,95,113	3.07	30 (46%)
37	A86	16	314	-	44,50,50	4.12	23 (52%)	51,76,76	8.52	19 (37%)
35	LMT	11	317	-	36,36,36	0.43	0	47,47,47	0.89	1 (2%)
37	A86	14	320	-	44,50,50	4.14	23 (52%)	51,76,76	7.22	21 (41%)
38	KC1	13	305	25	49,53,53	3.05	26 (53%)	63,89,89	4.07	37 (58%)
37	A86	9	315	-	44,50,50	4.10	23 (52%)	51,76,76	7.06	19 (37%)
30	CLA	7	305	19,40	69,73,73	2.08	21 (30%)	83,113,113	2.89	32 (38%)
31	PQN	B	840	-	34,34,34	1.50	2 (5%)	42,45,45	1.09	4 (9%)
30	CLA	15	314	30,27	49,53,73	2.38	19 (38%)	59,89,113	3.36	27 (45%)
37	A86	1	309	-	44,50,50	3.96	23 (52%)	51,76,76	8.68	21 (41%)
29	CL0	A	801	1	69,73,73	1.93	19 (27%)	83,113,113	2.79	33 (39%)
33	BCR	B	841	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	8 (14%)
38	KC1	5	306	17	49,53,53	3.02	23 (46%)	63,89,89	4.32	36 (57%)
33	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.19	6 (10%)
39	DD6	3	316	-	39,45,45	6.75	24 (61%)	52,67,67	6.80	26 (50%)
39	DD6	8	317	-	39,45,45	6.64	22 (56%)	52,67,67	7.04	29 (55%)
38	KC1	13	310	25	49,53,53	3.06	25 (51%)	63,89,89	4.07	35 (55%)
37	A86	13	313	25	41,47,50	4.31	22 (53%)	49,72,76	8.60	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	10	304	22	69,73,73	2.01	21 (30%)	83,113,113	2.72	28 (33%)
34	LHG	5	317	30	26,26,48	0.84	1 (3%)	29,32,54	1.35	3 (10%)
30	CLA	12	304	39,24	69,73,73	2.03	21 (30%)	83,113,113	3.00	32 (38%)
38	KC1	3	304	15	49,53,53	3.03	24 (48%)	63,89,89	4.12	38 (60%)
30	CLA	9	303	21	69,73,73	1.97	19 (27%)	83,113,113	2.78	28 (33%)
39	DD6	11	313	-	39,45,45	6.77	23 (58%)	52,67,67	6.83	29 (55%)
30	CLA	B	828	2	69,73,73	1.99	20 (28%)	83,113,113	2.75	29 (34%)
38	KC1	16	304	28	49,53,53	3.10	23 (46%)	63,89,89	3.83	32 (50%)
30	CLA	14	303	26	61,65,73	2.18	20 (32%)	73,103,113	3.01	32 (43%)
30	CLA	10	308	22	69,73,73	2.02	20 (28%)	83,113,113	2.77	29 (34%)
30	CLA	14	305	26	54,58,73	2.30	20 (37%)	65,95,113	3.14	30 (46%)
30	CLA	B	835	2	69,73,73	1.98	19 (27%)	83,113,113	2.85	31 (37%)
30	CLA	16	306	28	56,60,73	2.24	20 (35%)	67,97,113	2.99	30 (44%)
30	CLA	16	307	-	50,54,73	2.40	20 (40%)	60,90,113	3.17	26 (43%)
30	CLA	A	840	1	51,55,73	2.29	19 (37%)	61,91,113	3.32	29 (47%)
30	CLA	A	808	1	55,59,73	2.22	20 (36%)	66,96,113	3.13	28 (42%)
38	KC1	9	310	21	49,53,53	2.98	24 (48%)	63,89,89	4.15	34 (53%)
34	LHG	9	318	-	33,33,48	0.70	0	36,39,54	1.25	4 (11%)
30	CLA	16	302	28	69,73,73	1.99	20 (28%)	83,113,113	2.77	28 (33%)
37	A86	15	317	30	44,50,50	4.15	23 (52%)	51,76,76	8.44	15 (29%)
39	DD6	15	319	30	39,45,45	6.79	22 (56%)	52,67,67	6.92	30 (57%)
32	SF4	A	846	2,1	0,12,12	-	-	-	-	-
30	CLA	14	307	38	69,73,73	2.04	20 (28%)	83,113,113	2.91	27 (32%)
37	A86	10	301	22	44,50,50	3.86	23 (52%)	51,76,76	7.28	23 (45%)
36	LMG	3	317	-	37,37,55	0.97	2 (5%)	45,45,63	1.42	7 (15%)
30	CLA	4	301	2,16	53,57,73	2.23	20 (37%)	62,93,113	3.21	27 (43%)
30	CLA	15	313	27	69,73,73	2.07	20 (28%)	83,113,113	2.82	30 (36%)
30	CLA	2	305	40	69,73,73	2.00	19 (27%)	83,113,113	2.85	30 (36%)
30	CLA	6	306	40	69,73,73	2.01	19 (27%)	83,113,113	2.81	29 (34%)
30	CLA	4	302	16	69,73,73	1.98	19 (27%)	83,113,113	2.72	27 (32%)
30	CLA	4	309	-	69,73,73	2.08	21 (30%)	83,113,113	2.81	31 (37%)
39	DD6	6	321	-	39,45,45	6.60	23 (58%)	52,67,67	6.79	28 (53%)
33	BCR	L	204	-	41,41,41	1.09	1 (2%)	56,56,56	1.44	8 (14%)
30	CLA	9	302	21,9	55,59,73	2.28	20 (36%)	66,96,113	3.23	30 (45%)
30	CLA	9	309	21,40	69,73,73	1.99	18 (26%)	83,113,113	2.64	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	KC1	6	311	18	49,53,53	2.98	23 (46%)	63,89,89	4.20	36 (57%)
32	SF4	C	102	3	0,12,12	-	-	-		
38	KC1	9	311	21	49,53,53	3.05	25 (51%)	63,89,89	4.14	37 (58%)
30	CLA	A	803	-	69,73,73	1.96	19 (27%)	83,113,113	2.81	32 (38%)
37	A86	4	317	-	44,50,50	3.99	23 (52%)	51,76,76	7.58	20 (39%)
30	CLA	15	302	30,27	69,73,73	2.07	20 (28%)	83,113,113	2.98	30 (36%)
30	CLA	2	304	14	69,73,73	2.00	20 (28%)	83,113,113	2.86	29 (34%)
35	LMT	B	852	-	36,36,36	0.36	0	47,47,47	1.12	2 (4%)
30	CLA	9	306	37,21	49,53,73	2.43	20 (40%)	59,89,113	3.29	28 (47%)
30	CLA	5	302	17	69,73,73	1.99	18 (26%)	83,113,113	2.76	29 (34%)
37	A86	15	315	27	44,50,50	4.30	23 (52%)	51,76,76	8.22	28 (54%)
30	CLA	5	309	34	69,73,73	2.01	20 (28%)	83,113,113	2.74	29 (34%)
33	BCR	B	842	-	41,41,41	1.07	2 (4%)	56,56,56	1.19	5 (8%)
37	A86	11	316	-	44,50,50	4.05	23 (52%)	51,76,76	8.21	16 (31%)
36	LMG	B	847	-	55,55,55	0.80	1 (1%)	63,63,63	1.37	8 (12%)
33	BCR	B	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	6 (10%)
30	CLA	F	203	6	49,53,73	2.38	20 (40%)	59,89,113	3.25	28 (47%)
38	KC1	6	312	18	49,53,53	3.00	25 (51%)	63,89,89	3.98	36 (57%)
37	A86	10	315	-	44,50,50	4.10	22 (50%)	51,76,76	8.25	16 (31%)
30	CLA	15	306	-	49,53,73	2.42	20 (40%)	59,89,113	3.34	26 (44%)
38	KC1	8	311	40	49,53,53	3.00	23 (46%)	63,89,89	4.05	35 (55%)
38	KC1	4	308	16	49,53,53	3.08	23 (46%)	63,89,89	3.86	35 (55%)
30	CLA	A	806	1	69,73,73	1.96	19 (27%)	83,113,113	3.02	32 (38%)
39	DD6	8	316	-	39,45,45	6.57	22 (56%)	52,67,67	6.80	30 (57%)
30	CLA	3	310	15	49,53,73	2.38	19 (38%)	59,89,113	3.28	27 (45%)
35	LMT	11	302	-	36,36,36	0.34	0	47,47,47	0.77	2 (4%)
30	CLA	9	307	21	69,73,73	2.00	19 (27%)	83,113,113	2.79	28 (33%)
30	CLA	A	815	1	69,73,73	2.01	21 (30%)	83,113,113	2.80	30 (36%)
35	LMT	12	318	-	36,36,36	0.41	0	47,47,47	0.76	0
37	A86	4	312	-	44,50,50	3.92	23 (52%)	51,76,76	8.64	21 (41%)
39	DD6	6	303	30	39,45,45	6.78	23 (58%)	52,67,67	6.69	28 (53%)
38	KC1	4	307	16	49,53,53	3.04	24 (48%)	63,89,89	3.94	35 (55%)
38	KC1	8	312	38	49,53,53	3.04	24 (48%)	63,89,89	3.67	34 (53%)
30	CLA	B	816	2	59,63,73	2.11	18 (30%)	71,101,113	3.09	30 (42%)
30	CLA	B	808	2	69,73,73	1.95	18 (26%)	83,113,113	2.83	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	A86	2	318	-	44,50,50	4.04	23 (52%)	51,76,76	7.66	23 (45%)
30	CLA	7	303	19	69,73,73	1.97	19 (27%)	83,113,113	2.79	31 (37%)
30	CLA	1	303	30,13	69,73,73	2.01	21 (30%)	83,113,113	2.80	30 (36%)
37	A86	10	316	-	44,50,50	3.92	24 (54%)	51,76,76	8.13	21 (41%)
38	KC1	14	311	26	49,53,53	3.04	24 (48%)	63,89,89	4.05	35 (55%)
30	CLA	9	308	21	69,73,73	2.00	18 (26%)	83,113,113	2.94	34 (40%)
30	CLA	A	822	40	69,73,73	1.99	19 (27%)	83,113,113	2.58	28 (33%)
30	CLA	5	304	17	69,73,73	2.07	21 (30%)	83,113,113	2.83	31 (37%)
30	CLA	A	824	1	55,59,73	2.23	20 (36%)	66,96,113	3.11	28 (42%)
38	KC1	10	306	22	49,53,53	2.98	23 (46%)	63,89,89	4.12	36 (57%)
38	KC1	6	313	18	49,53,53	3.01	23 (46%)	63,89,89	4.01	35 (55%)
38	KC1	8	306	40	49,53,53	3.00	22 (44%)	63,89,89	4.05	33 (52%)
30	CLA	A	814	1	64,68,73	2.05	19 (29%)	77,107,113	2.88	29 (37%)
30	CLA	11	304	23	69,73,73	2.04	20 (28%)	83,113,113	2.81	27 (32%)
37	A86	15	316	30	44,50,50	4.14	24 (54%)	51,76,76	7.80	17 (33%)
30	CLA	A	837	1	49,53,73	2.41	21 (42%)	59,89,113	3.24	28 (47%)
35	LMT	A	855	-	36,36,36	0.39	0	47,47,47	0.89	3 (6%)
30	CLA	16	305	28	54,58,73	2.26	22 (40%)	65,95,113	3.06	29 (44%)
37	A86	15	320	-	44,50,50	4.24	24 (54%)	51,76,76	8.23	19 (37%)
30	CLA	B	826	2	69,73,73	1.94	20 (28%)	83,113,113	2.81	31 (37%)
30	CLA	12	302	24	69,73,73	1.99	20 (28%)	83,113,113	2.85	33 (39%)
30	CLA	B	812	2	69,73,73	2.01	20 (28%)	83,113,113	2.68	28 (33%)
35	LMT	7	301	30	36,36,36	0.41	0	47,47,47	0.80	1 (2%)
30	CLA	6	307	39,18	69,73,73	2.01	17 (24%)	83,113,113	2.64	33 (39%)
39	DD6	1	310	-	39,45,45	6.70	23 (58%)	52,67,67	6.71	24 (46%)
39	DD6	4	316	-	39,45,45	6.68	23 (58%)	52,67,67	7.33	26 (50%)
33	BCR	2u	201	-	41,41,41	1.22	4 (9%)	56,56,56	1.38	7 (12%)
35	LMT	6	302	-	32,32,36	0.36	0	43,43,47	0.92	1 (2%)
30	CLA	5	307	17	69,73,73	1.97	21 (30%)	83,113,113	2.75	30 (36%)
31	PQN	A	845	-	34,34,34	1.52	2 (5%)	42,45,45	1.10	3 (7%)
33	BCR	B	846	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	5 (8%)
30	CLA	B	823	40	58,62,73	2.14	19 (32%)	69,99,113	2.99	29 (42%)
37	A86	14	316	-	44,50,50	4.03	23 (52%)	51,76,76	8.16	18 (35%)
35	LMT	11	318	-	36,36,36	0.43	0	47,47,47	0.88	2 (4%)
37	A86	5	316	-	44,50,50	4.04	22 (50%)	51,76,76	8.02	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMT	16	315	-	36,36,36	0.41	0	47,47,47	0.65	0
30	CLA	A	816	35,1	69,73,73	1.97	19 (27%)	83,113,113	2.77	30 (36%)
30	CLA	A	819	1	58,62,73	2.18	20 (34%)	69,99,113	3.05	30 (43%)
30	CLA	8	302	20	69,73,73	1.99	20 (28%)	83,113,113	2.84	29 (34%)
30	CLA	13	304	25	49,53,73	2.46	20 (40%)	59,89,113	3.30	28 (47%)
37	A86	14	318	-	44,50,50	4.10	22 (50%)	51,76,76	8.48	16 (31%)
30	CLA	2	303	14	59,63,73	2.41	20 (33%)	71,101,113	3.06	34 (47%)
38	KC1	3	311	40	49,53,53	3.05	23 (46%)	63,89,89	4.19	33 (52%)
35	LMT	15	301	-	36,36,36	0.51	0	47,47,47	1.13	3 (6%)
30	CLA	15	304	39,30,27	69,73,73	2.09	20 (28%)	83,113,113	2.88	30 (36%)
39	DD6	7	318	-	39,45,45	6.70	21 (53%)	52,67,67	6.91	29 (55%)
30	CLA	5	308	17	69,73,73	2.00	20 (28%)	83,113,113	2.80	30 (36%)
30	CLA	5	303	17	69,73,73	1.99	19 (27%)	83,113,113	2.73	30 (36%)
33	BCR	I	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	5 (8%)
30	CLA	A	825	1	63,67,73	2.10	19 (30%)	75,105,113	2.88	30 (40%)
38	KC1	12	313	24	49,53,53	3.06	22 (44%)	63,89,89	4.64	35 (55%)
30	CLA	1	307	13	69,73,73	2.05	21 (30%)	83,113,113	2.82	29 (34%)
35	LMT	12	319	-	36,36,36	0.40	0	47,47,47	0.86	0
38	KC1	2	312	14	49,53,53	3.04	24 (48%)	63,89,89	3.99	35 (55%)
36	LMG	8	319	36,20	37,37,55	0.93	0	45,45,63	1.28	5 (11%)
30	CLA	8	309	20	51,55,73	2.36	20 (39%)	61,91,113	3.12	26 (42%)
30	CLA	13	303	-	69,73,73	2.07	21 (30%)	83,113,113	2.85	31 (37%)
30	CLA	A	826	40	69,73,73	1.95	21 (30%)	83,113,113	2.81	28 (33%)
39	DD6	7	317	-	39,45,45	6.70	20 (51%)	52,67,67	6.69	29 (55%)
35	LMT	1	311	-	36,36,36	0.40	0	47,47,47	0.78	2 (4%)
30	CLA	A	831	1	69,73,73	1.97	19 (27%)	83,113,113	2.85	30 (36%)
30	CLA	A	820	1	69,73,73	2.03	19 (27%)	83,113,113	2.75	31 (37%)
30	CLA	8	304	20	62,66,73	2.08	18 (29%)	74,104,113	3.06	34 (45%)
30	CLA	7	310	19	69,73,73	2.03	20 (28%)	83,113,113	2.82	29 (34%)
30	CLA	16	303	28	69,73,73	2.01	19 (27%)	83,113,113	2.95	30 (36%)
30	CLA	12	306	24	69,73,73	1.98	20 (28%)	83,113,113	2.69	30 (36%)
39	DD6	6	319	-	39,45,45	6.71	23 (58%)	52,67,67	6.51	31 (59%)
34	LHG	6	322	30	26,26,48	0.88	1 (3%)	29,32,54	1.36	3 (10%)
30	CLA	B	815	2	49,53,73	2.34	19 (38%)	59,89,113	3.26	27 (45%)
30	CLA	4	304	-	64,68,73	2.08	18 (28%)	77,107,113	2.90	31 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	A86	3	314	-	44,50,50	4.05	23 (52%)	51,76,76	8.17	19 (37%)
37	A86	14	301	26	44,50,50	4.10	23 (52%)	51,76,76	8.08	17 (33%)
30	CLA	13	309	-	49,53,73	2.44	20 (40%)	59,89,113	3.29	26 (44%)
35	LMT	B	850	-	36,36,36	0.39	0	47,47,47	0.92	3 (6%)
30	CLA	8	305	20	69,73,73	1.96	20 (28%)	83,113,113	4.66	34 (40%)
30	CLA	B	827	2	69,73,73	1.95	18 (26%)	83,113,113	2.68	30 (36%)
30	CLA	B	803	-	69,73,73	1.91	20 (28%)	83,113,113	2.83	31 (37%)
30	CLA	B	824	40	69,73,73	2.01	20 (28%)	83,113,113	4.60	31 (37%)
30	CLA	2u	202	12	69,73,73	1.97	19 (27%)	83,113,113	2.81	33 (39%)
33	BCR	B	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.38	8 (14%)
30	CLA	A	818	1	58,62,73	2.12	20 (34%)	69,99,113	3.10	29 (42%)
30	CLA	A	842	1	69,73,73	1.98	20 (28%)	83,113,113	2.82	32 (38%)
30	CLA	1	301	13	69,73,73	2.01	19 (27%)	83,113,113	2.74	27 (32%)
35	LMT	9	317	-	33,33,36	0.49	0	44,44,47	1.11	5 (11%)
39	DD6	10	314	-	39,45,45	6.73	23 (58%)	52,67,67	6.78	28 (53%)
30	CLA	15	305	37,27	49,53,73	2.43	20 (40%)	59,89,113	3.26	29 (49%)
35	LMT	12	320	-	36,36,36	0.39	0	47,47,47	0.71	0
30	CLA	14	313	26	50,54,73	2.39	20 (40%)	60,90,113	3.30	29 (48%)
37	A86	8	315	-	44,50,50	3.75	22 (50%)	51,76,76	8.45	20 (39%)
30	CLA	2	307	14	69,73,73	1.98	19 (27%)	83,113,113	2.73	31 (37%)
30	CLA	B	802	30,40	69,73,73	1.90	20 (28%)	83,113,113	2.91	30 (36%)
30	CLA	10	305	40	69,73,73	2.00	19 (27%)	83,113,113	2.88	33 (39%)
38	KC1	13	306	25	49,53,53	3.06	25 (51%)	63,89,89	4.00	34 (53%)
37	A86	15	323	-	44,50,50	4.19	23 (52%)	51,76,76	8.39	17 (33%)
30	CLA	3	302	15	64,68,73	2.05	19 (29%)	77,107,113	2.86	32 (41%)
30	CLA	2	308	14	69,73,73	2.02	17 (24%)	83,113,113	2.79	29 (34%)
30	CLA	J	101	8	49,53,73	2.39	21 (42%)	59,89,113	3.19	27 (45%)
33	BCR	A	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.25	6 (10%)
37	A86	4	315	-	44,50,50	4.00	23 (52%)	51,76,76	7.94	19 (37%)
30	CLA	A	811	1	69,73,73	1.96	19 (27%)	83,113,113	2.79	28 (33%)
30	CLA	11	309	23	69,73,73	2.03	20 (28%)	83,113,113	2.78	29 (34%)
30	CLA	A	841	1	69,73,73	2.01	19 (27%)	83,113,113	2.76	31 (37%)
33	BCR	L	205	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	5 (8%)
38	KC1	11	307	23	49,53,53	3.05	25 (51%)	63,89,89	4.04	36 (57%)
30	CLA	B	809	2	69,73,73	1.92	17 (24%)	83,113,113	2.60	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LMG	8	321	36	29,29,55	1.11	2 (6%)	37,37,63	1.27	5 (13%)
36	LMG	14	321	-	38,38,55	1.03	3 (7%)	46,46,63	1.20	3 (6%)
30	CLA	16	308	28	49,53,73	2.43	20 (40%)	59,89,113	3.29	27 (45%)
37	A86	11	301	-	44,50,50	4.04	23 (52%)	51,76,76	8.20	21 (41%)
30	CLA	B	819	40	69,73,73	2.00	18 (26%)	83,113,113	2.52	31 (37%)
30	CLA	13	302	25	69,73,73	2.02	20 (28%)	83,113,113	2.71	29 (34%)
30	CLA	14	312	37,26	49,53,73	2.43	20 (40%)	59,89,113	3.22	26 (44%)
30	CLA	8	303	40	69,73,73	1.96	18 (26%)	83,113,113	2.68	29 (34%)
30	CLA	A	839	1	69,73,73	1.97	18 (26%)	83,113,113	2.91	33 (39%)
36	LMG	6	301	30	33,33,55	0.95	1 (3%)	41,41,63	1.21	4 (9%)
39	DD6	2	317	-	39,45,45	6.77	22 (56%)	52,67,67	6.58	28 (53%)
38	KC1	9	312	21	49,53,53	3.04	24 (48%)	63,89,89	4.00	34 (53%)
30	CLA	B	820	2	49,53,73	2.40	20 (40%)	59,89,113	3.43	25 (42%)
38	KC1	10	310	22	49,53,53	3.02	25 (51%)	63,89,89	4.15	36 (57%)
30	CLA	A	832	1	54,58,73	2.21	19 (35%)	65,95,113	3.13	30 (46%)
30	CLA	8	301	20	69,73,73	1.99	20 (28%)	83,113,113	2.82	31 (37%)
39	DD6	4	313	-	39,45,45	6.71	22 (56%)	52,67,67	6.72	26 (50%)
37	A86	14	315	26	44,50,50	3.99	23 (52%)	51,76,76	8.87	22 (43%)
30	CLA	6	314	18	69,73,73	1.98	18 (26%)	83,113,113	2.90	34 (40%)
30	CLA	6	315	18	49,53,73	2.42	20 (40%)	59,89,113	3.23	27 (45%)
30	CLA	3	306	15	69,73,73	2.02	18 (26%)	83,113,113	2.77	30 (36%)
30	CLA	4	306	16	69,73,73	2.00	19 (27%)	83,113,113	2.77	30 (36%)
37	A86	7	319	-	44,50,50	4.10	23 (52%)	51,76,76	8.25	22 (43%)
30	CLA	7	309	19	69,73,73	1.96	19 (27%)	83,113,113	2.72	28 (33%)
30	CLA	2	301	2,14	69,73,73	1.94	19 (27%)	83,113,113	2.90	29 (34%)
37	A86	5	301	-	44,50,50	4.06	24 (54%)	51,76,76	7.93	21 (41%)
30	CLA	11	308	23	69,73,73	2.03	21 (30%)	83,113,113	2.80	30 (36%)
37	A86	10	317	-	44,50,50	4.19	23 (52%)	51,76,76	8.16	15 (29%)
30	CLA	A	838	1	55,59,73	2.22	20 (36%)	66,96,113	3.17	29 (43%)
33	BCR	A	850	-	41,41,41	1.13	2 (4%)	56,56,56	1.34	9 (16%)
33	BCR	L	201	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	5 (8%)
30	CLA	B	811	2,30	69,73,73	1.96	20 (28%)	83,113,113	2.69	32 (38%)
37	A86	16	312	28	44,50,50	4.06	23 (52%)	51,76,76	8.15	23 (45%)
38	KC1	13	308	25	49,53,53	3.07	25 (51%)	63,89,89	4.11	35 (55%)
30	CLA	3	305	15	66,70,73	2.05	21 (31%)	79,109,113	2.83	33 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	A	804	1	69,73,73	1.96	18 (26%)	83,113,113	2.82	31 (37%)
38	KC1	8	310	20	49,53,53	2.97	21 (42%)	63,89,89	4.00	35 (55%)
39	DD6	7	302	-	39,45,45	6.75	24 (61%)	52,67,67	6.58	28 (53%)
39	DD6	13	314	-	39,45,45	6.78	22 (56%)	52,67,67	7.25	31 (59%)
30	CLA	4	311	16	54,58,73	2.31	21 (38%)	65,95,113	3.26	32 (49%)
30	CLA	A	844	-	69,73,73	2.06	20 (28%)	83,113,113	2.72	32 (38%)
37	A86	10	302	-	44,50,50	4.06	23 (52%)	51,76,76	8.39	17 (33%)
30	CLA	2	313	14	49,53,73	2.43	20 (40%)	59,89,113	3.27	27 (45%)
39	DD6	3	312	-	39,45,45	6.71	23 (58%)	52,67,67	6.79	26 (50%)
38	KC1	2	306	14	49,53,53	3.04	24 (48%)	63,89,89	4.13	37 (58%)
38	KC1	4	310	16	49,53,53	3.05	24 (48%)	63,89,89	4.09	35 (55%)
30	CLA	A	812	30,1	69,73,73	1.94	20 (28%)	83,113,113	2.87	28 (33%)
39	DD6	9	314	-	39,45,45	6.65	22 (56%)	52,67,67	7.29	26 (50%)
38	KC1	7	308	40	49,53,53	3.03	22 (44%)	63,89,89	3.94	34 (53%)
38	KC1	1	308	13	49,53,53	3.04	24 (48%)	63,89,89	4.03	34 (53%)
30	CLA	15	309	27	69,73,73	2.07	21 (30%)	83,113,113	2.81	28 (33%)
37	A86	14	319	30	44,50,50	4.09	22 (50%)	51,76,76	8.30	17 (33%)
37	A86	15	322	30	44,50,50	4.28	24 (54%)	51,76,76	8.43	21 (41%)
38	KC1	3	308	15	49,53,53	2.99	23 (46%)	63,89,89	4.03	34 (53%)
38	KC1	5	312	17	49,53,53	3.00	22 (44%)	63,89,89	3.97	34 (53%)
33	BCR	B	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	6 (10%)
30	CLA	6	304	18	69,73,73	2.00	19 (27%)	83,113,113	2.84	32 (38%)
30	CLA	B	804	2	56,60,73	2.18	20 (35%)	67,97,113	3.13	31 (46%)
33	BCR	A	848	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	4 (7%)
39	DD6	6	318	-	39,45,45	6.65	23 (58%)	52,67,67	6.55	29 (55%)
30	CLA	B	832	37,40	69,73,73	2.01	21 (30%)	83,113,113	2.82	31 (37%)
36	LMG	5	318	-	33,33,55	0.92	0	41,41,63	1.22	5 (12%)
30	CLA	A	835	1	69,73,73	2.00	20 (28%)	83,113,113	2.91	30 (36%)
38	KC1	8	313	20	49,53,53	2.97	21 (42%)	63,89,89	4.04	34 (53%)
30	CLA	2	309	14,34	69,73,73	2.03	20 (28%)	83,113,113	2.76	30 (36%)
37	A86	13	315	-	44,50,50	4.18	23 (52%)	51,76,76	8.50	18 (35%)
30	CLA	A	827	40	69,73,73	1.94	19 (27%)	83,113,113	2.96	31 (37%)
30	CLA	15	311	37	49,53,73	2.45	20 (40%)	59,89,113	3.24	26 (44%)
30	CLA	B	834	2	64,68,73	2.08	20 (31%)	77,107,113	2.89	29 (37%)
36	LMG	7	320	-	37,37,55	1.00	3 (8%)	45,45,63	1.25	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMT	7	321	-	36,36,36	0.32	0	47,47,47	0.75	2 (4%)
30	CLA	A	807	1	69,73,73	1.97	19 (27%)	83,113,113	2.83	31 (37%)
30	CLA	L	203	40	49,53,73	2.38	20 (40%)	59,89,113	3.23	25 (42%)
38	KC1	10	312	22	49,53,53	3.05	24 (48%)	63,89,89	4.07	34 (53%)
30	CLA	15	312	27	49,53,73	2.43	20 (40%)	59,89,113	3.38	31 (52%)
30	CLA	B	851	2,14	69,73,73	1.99	19 (27%)	83,113,113	2.79	32 (38%)
38	KC1	14	308	30,26	49,53,53	3.07	24 (48%)	63,89,89	3.92	36 (57%)
34	LHG	A	852	-	48,48,48	0.64	1 (2%)	51,54,54	1.20	5 (9%)
37	A86	8	318	-	44,50,50	3.98	24 (54%)	51,76,76	10.85	23 (45%)
38	KC1	2	314	40	49,53,53	3.05	24 (48%)	63,89,89	4.06	36 (57%)
39	DD6	16	313	-	39,45,45	6.75	21 (53%)	52,67,67	7.13	30 (57%)
30	CLA	3	309	15	49,53,73	2.44	20 (40%)	59,89,113	3.28	26 (44%)
30	CLA	A	834	1	69,73,73	1.97	19 (27%)	83,113,113	2.82	34 (40%)
30	CLA	6	305	18	69,73,73	2.03	20 (28%)	83,113,113	2.79	28 (33%)
37	A86	7	316	-	44,50,50	3.75	22 (50%)	51,76,76	7.71	27 (52%)
36	LMG	A	856	-	34,34,55	0.99	1 (2%)	42,42,63	1.19	3 (7%)
36	LMG	B	849	2	43,43,55	0.95	2 (4%)	51,51,63	1.18	3 (5%)
30	CLA	9	301	34	69,73,73	1.95	20 (28%)	83,113,113	2.89	30 (36%)
30	CLA	7	306	19	69,73,73	1.98	22 (31%)	83,113,113	2.69	31 (37%)
38	KC1	8	307	20	49,53,53	2.97	23 (46%)	63,89,89	4.12	36 (57%)
30	CLA	16	309	28	49,53,73	2.44	20 (40%)	59,89,113	3.32	27 (45%)
30	CLA	15	308	30,27	49,53,73	2.42	20 (40%)	59,89,113	3.18	29 (49%)
35	LMT	8	322	-	36,36,36	0.40	0	47,47,47	0.73	1 (2%)
38	KC1	7	313	-	49,53,53	2.98	22 (44%)	63,89,89	4.07	36 (57%)
38	KC1	12	311	24	49,53,53	3.05	24 (48%)	63,89,89	4.15	40 (63%)
30	CLA	B	818	2	64,68,73	2.04	18 (28%)	77,107,113	2.99	32 (41%)
39	DD6	2	316	-	39,45,45	6.62	22 (56%)	52,67,67	6.70	28 (53%)
30	CLA	A	805	30,1	63,67,73	2.10	19 (30%)	75,105,113	2.99	32 (42%)
39	DD6	5	313	-	39,45,45	6.74	23 (58%)	52,67,67	6.85	25 (48%)
38	KC1	13	311	25	49,53,53	3.07	25 (51%)	63,89,89	3.92	35 (55%)
35	LMT	12	301	-	36,36,36	0.43	0	47,47,47	0.76	0
37	A86	4	314	-	44,50,50	4.10	22 (50%)	51,76,76	8.17	22 (43%)
30	CLA	14	310	-	54,58,73	2.31	20 (37%)	65,95,113	3.21	29 (44%)
30	CLA	A	830	1	69,73,73	1.94	18 (26%)	83,113,113	2.69	32 (38%)

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
30	CLA	4	305	16	-	9/39/115/115	-
30	CLA	10	307	22	-	12/39/115/115	-
30	CLA	3	301	15	-	9/39/115/115	-
37	A86	14	314	-	-	13/34/90/90	0/3/3/3
30	CLA	B	837	40	-	5/39/115/115	-
30	CLA	B	830	2	-	12/39/115/115	-
38	KC1	13	312	25	-	9/15/71/71	-
33	BCR	M	101	-	-	11/29/63/63	0/2/2/2
30	CLA	6	316	40	-	9/27/103/115	-
38	KC1	5	310	17	-	6/15/71/71	-
37	A86	5	315	-	-	6/34/90/90	0/3/3/3
30	CLA	10	309	22	-	12/39/115/115	-
35	LMT	A	854	-	-	15/21/61/61	0/2/2/2
30	CLA	3	303	15	-	16/39/115/115	-
30	CLA	B	821	2	-	16/27/103/115	-
30	CLA	F	201	40	-	10/39/115/115	-
33	BCR	A	849	-	-	12/29/63/63	0/2/2/2
30	CLA	8	308	20	-	11/27/103/115	-
30	CLA	A	836	1	-	9/26/102/115	-
30	CLA	12	312	24	-	14/39/115/115	-
30	CLA	A	829	30,1	-	14/39/115/115	-
30	CLA	A	843	40	-	9/39/115/115	-
30	CLA	A	828	1	-	15/39/115/115	-
38	KC1	11	311	23	-	10/15/71/71	-
37	A86	7	315	-	-	15/34/90/90	0/3/3/3
30	CLA	12	308	40	-	11/39/115/115	-
38	KC1	1	306	13	-	8/15/71/71	-
37	A86	2	302	-	-	11/34/90/90	0/3/3/3
33	BCR	A	847	-	-	12/29/63/63	0/2/2/2
39	DD6	12	315	30	-	9/26/80/80	0/3/3/3
30	CLA	A	833	1	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	12	307	24	-	6/17/93/115	-
37	A86	14	317	-	-	15/34/90/90	0/3/3/3
30	CLA	2	311	14	-	13/39/115/115	-
38	KC1	11	312	-	-	5/15/71/71	-
30	CLA	B	814	2	-	5/27/103/115	-
30	CLA	B	822	2,30	-	14/39/115/115	-
30	CLA	5	311	17,40	-	17/39/115/115	-
34	LHG	B	848	30	-	18/31/31/53	-
30	CLA	4	303	16	-	5/39/115/115	-
30	CLA	13	307	25	-	9/39/115/115	-
37	A86	9	316	30	-	11/34/90/90	0/3/3/3
37	A86	2u	203	30	-	15/34/90/90	0/3/3/3
30	CLA	6	309	18	-	14/39/115/115	-
38	KC1	5	305	17	-	5/15/71/71	-
34	LHG	2	320	30	-	12/31/31/53	-
38	KC1	8	314	40,38	-	7/15/71/71	-
36	LMG	8	320	-	-	20/37/57/70	0/1/1/1
37	A86	6	320	-	-	9/34/90/90	0/3/3/3
30	CLA	2	310	14	-	6/39/115/115	-
39	DD6	3	313	-	-	9/26/80/80	0/3/3/3
38	KC1	9	304	21	-	6/15/71/71	-
39	DD6	12	317	-	-	13/26/80/80	0/3/3/3
33	BCR	F	204	-	-	10/29/63/63	0/2/2/2
32	SF4	C	101	3	-	-	0/6/5/5
38	KC1	11	305	23	-	7/15/71/71	-
38	KC1	6	308	18	-	6/15/71/71	-
37	A86	9	313	21	-	8/34/90/90	0/3/3/3
30	CLA	B	813	2	-	23/39/115/115	-
30	CLA	10	311	-	-	9/15/91/115	-
30	CLA	B	836	2	-	3/18/94/115	-
30	CLA	B	807	2	-	11/39/115/115	-
30	CLA	B	817	2	-	6/32/108/115	-
39	DD6	2	315	-	-	13/26/80/80	0/3/3/3
30	CLA	16	310	28	-	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	12	303	24	-	6/39/115/115	-
30	CLA	15	303	30,37,27	-	9/33/109/115	-
37	A86	3	315	-	-	14/34/90/90	0/3/3/3
30	CLA	1	302	30,13	-	10/39/115/115	-
30	CLA	F	202	40	-	18/39/115/115	-
30	CLA	13	301	25	-	17/39/115/115	-
30	CLA	B	810	2	-	10/39/115/115	-
30	CLA	6	317	-	-	16/39/115/115	-
30	CLA	A	810	1	-	12/39/115/115	-
37	A86	12	316	-	-	16/34/90/90	0/3/3/3
30	CLA	1	304	13	-	13/39/115/115	-
38	KC1	12	309	24	-	8/15/71/71	-
38	KC1	14	306	26	-	7/15/71/71	-
35	LMT	11	303	-	-	11/21/61/61	0/2/2/2
30	CLA	B	833	30,40	-	11/39/115/115	-
30	CLA	16	301	28	-	14/39/115/115	-
30	CLA	B	831	2	-	10/31/107/115	-
39	DD6	15	318	-	-	13/26/80/80	0/3/3/3
30	CLA	B	838	2	-	17/39/115/115	-
30	CLA	10	303	22	-	15/39/115/115	-
30	CLA	12	321	24,26	-	4/39/115/115	-
30	CLA	A	817	36,40	-	6/20/96/115	-
30	CLA	11	310	23	-	17/39/115/115	-
30	CLA	A	809	30,1	-	15/39/115/115	-
30	CLA	A	823	1	-	6/20/96/115	-
30	CLA	1	305	40	-	11/39/115/115	-
39	DD6	10	313	-	-	11/26/80/80	0/3/3/3
30	CLA	14	302	26	-	16/39/115/115	-
30	CLA	A	821	1	-	11/35/111/115	-
30	CLA	14	309	26	-	3/15/91/115	-
30	CLA	B	829	2	-	13/39/115/115	-
30	CLA	A	802	40	-	6/39/115/115	-
30	CLA	6	310	34	-	8/39/115/115	-
35	LMT	A	857	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMG	F	205	-	-	14/21/41/70	0/1/1/1
37	A86	2	319	-	-	12/34/90/90	0/3/3/3
37	A86	11	315	-	-	13/34/90/90	0/3/3/3
38	KC1	12	305	24	-	7/15/71/71	-
30	CLA	7	311	19	-	14/39/115/115	-
37	A86	11	314	-	-	14/34/90/90	0/3/3/3
30	CLA	B	801	2	-	10/39/115/115	-
39	DD6	7	314	-	-	11/26/80/80	0/3/3/3
37	A86	15	321	27	-	13/34/90/90	0/3/3/3
30	CLA	12	310	40	-	10/39/115/115	-
30	CLA	7	307	19	-	21/39/115/115	-
30	CLA	3	307	15	-	14/39/115/115	-
37	A86	2u	205	-	-	11/34/90/90	0/3/3/3
30	CLA	L	202	9	-	9/39/115/115	-
38	KC1	16	311	28	-	6/15/71/71	-
30	CLA	B	805	2	-	11/39/115/115	-
30	CLA	7	312	19	-	8/17/93/115	-
30	CLA	9	305	-	-	15/39/115/115	-
30	CLA	B	839	34	-	4/39/115/115	-
30	CLA	15	310	27	-	6/15/91/115	-
30	CLA	14	304	26	-	6/15/91/115	-
30	CLA	B	825	2	-	9/39/115/115	-
34	LHG	A	853	30	-	9/31/31/53	-
37	A86	12	314	-	-	13/34/90/90	0/3/3/3
33	BCR	J	103	-	-	9/29/63/63	0/2/2/2
30	CLA	7	304	19	-	9/39/115/115	-
30	CLA	B	806	2	-	11/39/115/115	-
30	CLA	A	813	1	-	13/39/115/115	-
36	LMG	2u	204	12	-	14/26/46/70	0/1/1/1
30	CLA	11	306	40	-	10/27/103/115	-
39	DD6	5	314	-	-	10/26/80/80	0/3/3/3
30	CLA	15	307	27	-	7/21/97/115	-
37	A86	16	314	-	-	11/34/90/90	0/3/3/3
35	LMT	11	317	-	-	2/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	14	320	-	-	9/34/90/90	0/3/3/3
38	KC1	13	305	25	-	8/15/71/71	-
37	A86	9	315	-	-	10/34/90/90	0/3/3/3
30	CLA	7	305	19,40	-	9/39/115/115	-
31	PQN	B	840	-	-	6/23/43/43	0/2/2/2
30	CLA	15	314	30,27	-	6/15/91/115	-
37	A86	1	309	-	-	8/34/90/90	0/3/3/3
29	CL0	A	801	1	-	6/39/115/115	-
33	BCR	B	841	-	-	10/29/63/63	0/2/2/2
38	KC1	5	306	17	-	10/15/71/71	-
33	BCR	J	102	-	-	12/29/63/63	0/2/2/2
39	DD6	3	316	-	-	12/26/80/80	0/3/3/3
39	DD6	8	317	-	-	10/26/80/80	0/3/3/3
38	KC1	13	310	25	-	5/15/71/71	-
37	A86	13	313	25	-	11/30/86/90	0/3/3/3
30	CLA	10	304	22	-	3/39/115/115	-
34	LHG	5	317	30	-	4/31/31/53	-
30	CLA	12	304	39,24	-	16/39/115/115	-
38	KC1	3	304	15	-	6/15/71/71	-
30	CLA	9	303	21	-	9/39/115/115	-
39	DD6	11	313	-	-	11/26/80/80	0/3/3/3
30	CLA	B	828	2	-	14/39/115/115	-
38	KC1	16	304	28	-	8/15/71/71	-
30	CLA	14	303	26	-	9/30/106/115	-
30	CLA	10	308	22	-	13/39/115/115	-
30	CLA	14	305	26	-	4/21/97/115	-
30	CLA	B	835	2	-	8/39/115/115	-
30	CLA	16	306	28	-	15/24/100/115	-
30	CLA	16	307	-	-	9/17/93/115	-
30	CLA	A	840	1	-	5/18/94/115	-
30	CLA	A	808	1	-	3/23/99/115	-
38	KC1	9	310	21	-	7/15/71/71	-
34	LHG	9	318	-	-	21/38/38/53	-
30	CLA	16	302	28	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	15	317	30	-	16/34/90/90	0/3/3/3
39	DD6	15	319	30	-	13/26/80/80	0/3/3/3
32	SF4	A	846	2,1	-	-	0/6/5/5
30	CLA	14	307	38	-	12/39/115/115	-
37	A86	10	301	22	-	6/34/90/90	0/3/3/3
36	LMG	3	317	-	-	18/32/52/70	0/1/1/1
30	CLA	4	301	2,16	-	9/20/96/115	-
30	CLA	15	313	27	-	11/39/115/115	-
30	CLA	2	305	40	-	11/39/115/115	-
30	CLA	6	306	40	-	11/39/115/115	-
30	CLA	4	302	16	-	12/39/115/115	-
30	CLA	4	309	-	-	11/39/115/115	-
39	DD6	6	321	-	-	12/26/80/80	0/3/3/3
33	BCR	L	204	-	-	11/29/63/63	0/2/2/2
30	CLA	9	302	21,9	-	8/23/99/115	-
30	CLA	9	309	21,40	-	11/39/115/115	-
38	KC1	6	311	18	-	10/15/71/71	-
32	SF4	C	102	3	-	-	0/6/5/5
38	KC1	9	311	21	-	8/15/71/71	-
30	CLA	A	803	-	-	8/39/115/115	-
37	A86	4	317	-	-	6/34/90/90	0/3/3/3
30	CLA	15	302	30,27	-	17/39/115/115	-
30	CLA	2	304	14	-	13/39/115/115	-
35	LMT	B	852	-	-	8/21/61/61	0/2/2/2
30	CLA	9	306	37,21	-	8/15/91/115	-
30	CLA	5	302	17	-	15/39/115/115	-
37	A86	15	315	27	-	9/34/90/90	0/3/3/3
30	CLA	5	309	34	-	11/39/115/115	-
33	BCR	B	842	-	-	10/29/63/63	0/2/2/2
37	A86	11	316	-	-	12/34/90/90	0/3/3/3
36	LMG	B	847	-	-	25/50/70/70	0/1/1/1
33	BCR	B	845	-	-	13/29/63/63	0/2/2/2
30	CLA	F	203	6	-	8/15/91/115	-
38	KC1	6	312	18	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	10	315	-	-	13/34/90/90	0/3/3/3
30	CLA	15	306	-	-	8/15/91/115	-
38	KC1	8	311	40	-	5/15/71/71	-
38	KC1	4	308	16	-	2/15/71/71	-
30	CLA	A	806	1	-	15/39/115/115	-
39	DD6	8	316	-	-	13/26/80/80	0/3/3/3
30	CLA	3	310	15	-	6/15/91/115	-
35	LMT	11	302	-	-	0/21/61/61	0/2/2/2
30	CLA	9	307	21	-	11/39/115/115	-
30	CLA	A	815	1	-	7/39/115/115	-
35	LMT	12	318	-	-	3/21/61/61	0/2/2/2
37	A86	4	312	-	-	11/34/90/90	0/3/3/3
39	DD6	6	303	30	-	10/26/80/80	0/3/3/3
38	KC1	4	307	16	-	6/15/71/71	-
38	KC1	8	312	38	-	9/15/71/71	-
30	CLA	B	816	2	-	9/27/103/115	-
30	CLA	B	808	2	-	16/39/115/115	-
37	A86	2	318	-	-	8/34/90/90	0/3/3/3
30	CLA	7	303	19	-	13/39/115/115	-
30	CLA	1	303	30,13	-	15/39/115/115	-
37	A86	10	316	-	-	11/34/90/90	0/3/3/3
38	KC1	14	311	26	-	5/15/71/71	-
30	CLA	9	308	21	-	18/39/115/115	-
30	CLA	A	822	40	-	10/39/115/115	-
30	CLA	5	304	17	-	14/39/115/115	-
30	CLA	A	824	1	-	3/23/99/115	-
38	KC1	10	306	22	-	8/15/71/71	-
38	KC1	6	313	18	-	5/15/71/71	-
38	KC1	8	306	40	-	8/15/71/71	-
30	CLA	A	814	1	-	12/33/109/115	-
30	CLA	11	304	23	-	11/39/115/115	-
37	A86	15	316	30	-	14/34/90/90	0/3/3/3
30	CLA	A	837	1	-	7/15/91/115	-
35	LMT	A	855	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	16	305	28	-	3/21/97/115	-
37	A86	15	320	-	-	15/34/90/90	0/3/3/3
30	CLA	B	826	2	-	16/39/115/115	-
30	CLA	12	302	24	-	15/39/115/115	-
30	CLA	B	812	2	-	8/39/115/115	-
35	LMT	7	301	30	-	3/21/61/61	0/2/2/2
30	CLA	6	307	39,18	-	13/39/115/115	-
39	DD6	1	310	-	-	13/26/80/80	0/3/3/3
39	DD6	4	316	-	-	14/26/80/80	0/3/3/3
33	BCR	2u	201	-	-	11/29/63/63	0/2/2/2
35	LMT	6	302	-	-	3/17/57/61	0/2/2/2
30	CLA	5	307	17	-	14/39/115/115	-
31	PQN	A	845	-	-	7/23/43/43	0/2/2/2
33	BCR	B	846	-	-	7/29/63/63	0/2/2/2
30	CLA	B	823	40	-	5/26/102/115	-
37	A86	14	316	-	-	11/34/90/90	0/3/3/3
35	LMT	11	318	-	-	1/21/61/61	0/2/2/2
37	A86	5	316	-	-	6/34/90/90	0/3/3/3
35	LMT	16	315	-	-	5/21/61/61	0/2/2/2
30	CLA	A	816	35,1	-	19/39/115/115	-
30	CLA	A	819	1	-	7/26/102/115	-
30	CLA	8	302	20	-	8/39/115/115	-
30	CLA	13	304	25	-	9/15/91/115	-
37	A86	14	318	-	-	17/34/90/90	0/3/3/3
30	CLA	2	303	14	-	15/27/103/115	-
38	KC1	3	311	40	-	6/15/71/71	-
35	LMT	15	301	-	-	6/21/61/61	0/2/2/2
30	CLA	15	304	39,30,27	-	21/39/115/115	-
39	DD6	7	318	-	-	13/26/80/80	0/3/3/3
30	CLA	5	308	17	-	16/39/115/115	-
30	CLA	5	303	17	-	8/39/115/115	-
33	BCR	I	101	-	-	5/29/63/63	0/2/2/2
30	CLA	A	825	1	-	15/32/108/115	-
38	KC1	12	313	24	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	1	307	13	-	17/39/115/115	-
35	LMT	12	319	-	-	0/21/61/61	0/2/2/2
38	KC1	2	312	14	-	2/15/71/71	-
36	LMG	8	319	36,20	-	17/32/52/70	0/1/1/1
30	CLA	8	309	20	-	3/18/94/115	-
30	CLA	13	303	-	-	10/39/115/115	-
30	CLA	A	826	40	-	14/39/115/115	-
39	DD6	7	317	-	-	10/26/80/80	0/3/3/3
35	LMT	1	311	-	-	4/21/61/61	0/2/2/2
30	CLA	A	831	1	-	9/39/115/115	-
30	CLA	A	820	1	-	18/39/115/115	-
30	CLA	8	304	20	-	11/31/107/115	-
30	CLA	7	310	19	-	13/39/115/115	-
30	CLA	16	303	28	-	21/39/115/115	-
30	CLA	12	306	24	-	7/39/115/115	-
39	DD6	6	319	-	-	11/26/80/80	0/3/3/3
34	LHG	6	322	30	-	12/31/31/53	-
30	CLA	B	815	2	-	3/15/91/115	-
30	CLA	4	304	-	-	11/33/109/115	-
37	A86	3	314	-	-	9/34/90/90	0/3/3/3
37	A86	14	301	26	-	8/34/90/90	0/3/3/3
30	CLA	13	309	-	-	10/15/91/115	-
35	LMT	B	850	-	-	1/21/61/61	0/2/2/2
30	CLA	8	305	20	-	13/39/115/115	-
30	CLA	B	827	2	-	7/39/115/115	-
30	CLA	B	803	-	-	8/39/115/115	-
30	CLA	B	824	40	-	7/39/115/115	-
30	CLA	2u	202	12	-	16/39/115/115	-
33	BCR	B	844	-	-	9/29/63/63	0/2/2/2
30	CLA	A	818	1	-	7/26/102/115	-
30	CLA	A	842	1	-	10/39/115/115	-
30	CLA	1	301	13	-	15/39/115/115	-
35	LMT	9	317	-	-	5/18/58/61	0/2/2/2
39	DD6	10	314	-	-	9/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	15	305	37,27	-	10/15/91/115	-
35	LMT	12	320	-	-	1/21/61/61	0/2/2/2
30	CLA	14	313	26	-	6/17/93/115	-
37	A86	8	315	-	-	7/34/90/90	0/3/3/3
30	CLA	2	307	14	-	9/39/115/115	-
30	CLA	B	802	30,40	-	10/39/115/115	-
30	CLA	10	305	40	-	12/39/115/115	-
38	KC1	13	306	25	-	9/15/71/71	-
37	A86	15	323	-	-	15/34/90/90	0/3/3/3
30	CLA	3	302	15	-	9/33/109/115	-
30	CLA	2	308	14	-	11/39/115/115	-
30	CLA	J	101	8	-	5/15/91/115	-
33	BCR	A	851	-	-	7/29/63/63	0/2/2/2
37	A86	4	315	-	-	5/34/90/90	0/3/3/3
30	CLA	A	811	1	-	14/39/115/115	-
30	CLA	11	309	23	-	16/39/115/115	-
30	CLA	A	841	1	-	12/39/115/115	-
33	BCR	L	205	-	-	8/29/63/63	0/2/2/2
38	KC1	11	307	23	-	10/15/71/71	-
30	CLA	B	809	2	-	12/39/115/115	-
36	LMG	8	321	36	-	5/24/44/70	0/1/1/1
36	LMG	14	321	-	-	13/33/53/70	0/1/1/1
30	CLA	16	308	28	-	8/15/91/115	-
37	A86	11	301	-	-	14/34/90/90	0/3/3/3
30	CLA	B	819	40	-	11/39/115/115	-
30	CLA	13	302	25	-	18/39/115/115	-
30	CLA	14	312	37,26	-	9/15/91/115	-
30	CLA	8	303	40	-	10/39/115/115	-
30	CLA	A	839	1	-	16/39/115/115	-
36	LMG	6	301	30	-	16/28/48/70	0/1/1/1
39	DD6	2	317	-	-	14/26/80/80	0/3/3/3
38	KC1	9	312	21	-	6/15/71/71	-
30	CLA	B	820	2	-	2/15/91/115	-
38	KC1	10	310	22	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	A	832	1	-	7/21/97/115	-
30	CLA	8	301	20	-	20/39/115/115	-
39	DD6	4	313	-	-	14/26/80/80	0/3/3/3
37	A86	14	315	26	-	11/34/90/90	0/3/3/3
30	CLA	6	314	18	-	18/39/115/115	-
30	CLA	6	315	18	-	5/15/91/115	-
30	CLA	3	306	15	-	10/39/115/115	-
30	CLA	4	306	16	-	12/39/115/115	-
37	A86	7	319	-	-	10/34/90/90	0/3/3/3
30	CLA	7	309	19	-	12/39/115/115	-
30	CLA	2	301	2,14	-	12/39/115/115	-
37	A86	5	301	-	-	11/34/90/90	0/3/3/3
30	CLA	11	308	23	-	12/39/115/115	-
37	A86	10	317	-	-	12/34/90/90	0/3/3/3
30	CLA	A	838	1	-	4/23/99/115	-
33	BCR	A	850	-	-	11/29/63/63	0/2/2/2
33	BCR	L	201	-	-	12/29/63/63	0/2/2/2
30	CLA	B	811	2,30	-	11/39/115/115	-
37	A86	16	312	28	-	13/34/90/90	0/3/3/3
38	KC1	13	308	25	-	10/15/71/71	-
30	CLA	3	305	15	-	14/36/112/115	-
30	CLA	A	804	1	-	11/39/115/115	-
38	KC1	8	310	20	-	6/15/71/71	-
39	DD6	7	302	-	-	12/26/80/80	0/3/3/3
39	DD6	13	314	-	-	13/26/80/80	0/3/3/3
30	CLA	4	311	16	-	3/21/97/115	-
30	CLA	A	844	-	-	14/39/115/115	-
37	A86	10	302	-	-	13/34/90/90	0/3/3/3
30	CLA	2	313	14	-	5/15/91/115	-
39	DD6	3	312	-	-	12/26/80/80	0/3/3/3
38	KC1	2	306	14	-	6/15/71/71	-
38	KC1	4	310	16	-	4/15/71/71	-
30	CLA	A	812	30,1	-	16/39/115/115	-
39	DD6	9	314	-	-	11/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC1	7	308	40	-	7/15/71/71	-
38	KC1	1	308	13	-	5/15/71/71	-
30	CLA	15	309	27	-	12/39/115/115	-
37	A86	14	319	30	-	11/34/90/90	0/3/3/3
37	A86	15	322	30	-	15/34/90/90	0/3/3/3
38	KC1	3	308	15	-	8/15/71/71	-
38	KC1	5	312	17	-	4/15/71/71	-
33	BCR	B	843	-	-	9/29/63/63	0/2/2/2
30	CLA	6	304	18	-	12/39/115/115	-
30	CLA	B	804	2	-	7/24/100/115	-
33	BCR	A	848	-	-	10/29/63/63	0/2/2/2
39	DD6	6	318	-	-	11/26/80/80	0/3/3/3
30	CLA	B	832	37,40	-	7/39/115/115	-
36	LMG	5	318	-	-	10/28/48/70	0/1/1/1
30	CLA	A	835	1	-	11/39/115/115	-
38	KC1	8	313	20	-	5/15/71/71	-
30	CLA	2	309	14,34	-	13/39/115/115	-
37	A86	13	315	-	-	13/34/90/90	0/3/3/3
30	CLA	A	827	40	-	7/39/115/115	-
30	CLA	15	311	37	-	7/15/91/115	-
30	CLA	B	834	2	-	8/33/109/115	-
36	LMG	7	320	-	-	14/32/52/70	0/1/1/1
35	LMT	7	321	-	-	4/21/61/61	0/2/2/2
30	CLA	A	807	1	-	15/39/115/115	-
30	CLA	L	203	40	-	2/15/91/115	-
38	KC1	10	312	22	-	5/15/71/71	-
30	CLA	15	312	27	-	7/15/91/115	-
30	CLA	B	851	2,14	-	16/39/115/115	-
38	KC1	14	308	30,26	-	9/15/71/71	-
34	LHG	A	852	-	-	25/53/53/53	-
37	A86	8	318	-	-	15/34/90/90	0/3/3/3
38	KC1	2	314	40	-	7/15/71/71	-
39	DD6	16	313	-	-	13/26/80/80	0/3/3/3
30	CLA	3	309	15	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	A	834	1	-	12/39/115/115	-
30	CLA	6	305	18	-	5/39/115/115	-
37	A86	7	316	-	-	7/34/90/90	0/3/3/3
36	LMG	A	856	-	-	15/29/49/70	0/1/1/1
36	LMG	B	849	2	-	15/38/58/70	0/1/1/1
30	CLA	9	301	34	-	10/39/115/115	-
30	CLA	7	306	19	-	8/39/115/115	-
38	KC1	8	307	20	-	8/15/71/71	-
30	CLA	16	309	28	-	6/15/91/115	-
30	CLA	15	308	30,27	-	9/15/91/115	-
35	LMT	8	322	-	-	3/21/61/61	0/2/2/2
38	KC1	7	313	-	-	4/15/71/71	-
38	KC1	12	311	24	-	6/15/71/71	-
30	CLA	B	818	2	-	8/33/109/115	-
39	DD6	2	316	-	-	12/26/80/80	0/3/3/3
30	CLA	A	805	30,1	-	9/32/108/115	-
39	DD6	5	313	-	-	9/26/80/80	0/3/3/3
38	KC1	13	311	25	-	3/15/71/71	-
35	LMT	12	301	-	-	4/21/61/61	0/2/2/2
37	A86	4	314	-	-	11/34/90/90	0/3/3/3
30	CLA	14	310	-	-	7/21/97/115	-
30	CLA	A	830	1	-	9/39/115/115	-

The worst 5 of 7637 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	2	315	DD6	C10-C11	26.29	1.70	1.35
39	11	313	DD6	C10-C11	25.97	1.70	1.35
39	6	303	DD6	C10-C11	25.93	1.70	1.35
39	15	318	DD6	C10-C11	25.83	1.70	1.35
39	10	313	DD6	C10-C11	25.83	1.70	1.35

The worst 5 of 10634 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	14	315	A86	O1-C20-C19	58.15	157.06	113.38
37	14	317	A86	O1-C20-C19	57.25	156.39	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	15	321	A86	O1-C20-C19	57.05	156.24	113.38
37	8	318	A86	O1-C20-C19	56.85	156.09	113.38
37	4	312	A86	O1-C20-C19	56.56	155.87	113.38

There are no chirality outliers.

5 of 4277 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	A	804	CLA	C3A-C2A-CAA-CBA
30	A	806	CLA	C1A-C2A-CAA-CBA
30	A	806	CLA	C3A-C2A-CAA-CBA
30	A	807	CLA	C1A-C2A-CAA-CBA
30	A	807	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

229 monomers are involved in 407 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	4	305	CLA	1	0
30	10	307	CLA	1	0
30	3	301	CLA	1	0
30	B	837	CLA	2	0
30	B	830	CLA	2	0
33	M	101	BCR	3	0
30	6	316	CLA	3	0
38	5	310	KC1	1	0
37	5	315	A86	1	0
30	10	309	CLA	2	0
30	3	303	CLA	2	0
30	B	821	CLA	4	0
30	F	201	CLA	4	0
33	A	849	BCR	4	0
30	8	308	CLA	1	0
30	A	836	CLA	2	0
30	12	312	CLA	1	0
30	A	829	CLA	7	0
30	A	843	CLA	2	0
30	A	828	CLA	1	0
37	7	315	A86	1	0
30	12	308	CLA	4	0
33	A	847	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	833	CLA	6	0
37	14	317	A86	1	0
30	2	311	CLA	1	0
30	B	822	CLA	3	0
30	13	307	CLA	4	0
37	9	316	A86	1	0
30	6	309	CLA	2	0
30	2	310	CLA	2	0
33	F	204	BCR	3	0
30	B	813	CLA	7	0
30	B	836	CLA	3	0
30	B	807	CLA	2	0
30	B	817	CLA	3	0
30	16	310	CLA	1	0
30	12	303	CLA	2	0
30	15	303	CLA	3	0
30	1	302	CLA	3	0
30	F	202	CLA	3	0
30	13	301	CLA	5	0
30	A	810	CLA	4	0
30	1	304	CLA	2	0
38	12	309	KC1	1	0
35	11	303	LMT	1	0
30	B	833	CLA	1	0
30	16	301	CLA	6	0
30	B	831	CLA	1	0
30	B	838	CLA	7	0
30	10	303	CLA	3	0
30	12	321	CLA	2	0
30	A	817	CLA	3	0
30	11	310	CLA	4	0
30	A	809	CLA	1	0
39	10	313	DD6	1	0
30	14	302	CLA	2	0
30	A	821	CLA	3	0
30	A	802	CLA	2	0
35	A	857	LMT	1	0
37	11	315	A86	1	0
30	7	311	CLA	2	0
30	B	801	CLA	4	0
30	12	310	CLA	1	0
30	7	307	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	L	202	CLA	4	0
30	B	805	CLA	2	0
30	9	305	CLA	2	0
30	B	839	CLA	1	0
30	B	825	CLA	1	0
34	A	853	LHG	1	0
33	J	103	BCR	4	0
30	7	304	CLA	1	0
30	B	806	CLA	6	0
30	A	813	CLA	3	0
30	11	306	CLA	2	0
30	15	307	CLA	1	0
35	11	317	LMT	2	0
37	14	320	A86	1	0
31	B	840	PQN	1	0
29	A	801	CL0	3	0
33	B	841	BCR	1	0
33	J	102	BCR	3	0
30	10	304	CLA	1	0
34	5	317	LHG	1	0
38	3	304	KC1	1	0
30	B	828	CLA	4	0
38	16	304	KC1	1	0
30	14	303	CLA	3	0
30	14	305	CLA	1	0
30	B	835	CLA	4	0
30	16	306	CLA	1	0
30	16	307	CLA	2	0
30	16	302	CLA	1	0
30	14	307	CLA	1	0
36	3	317	LMG	2	0
30	4	301	CLA	3	0
30	15	313	CLA	3	0
30	2	305	CLA	2	0
30	6	306	CLA	2	0
30	4	302	CLA	1	0
30	4	309	CLA	1	0
39	6	321	DD6	1	0
33	L	204	BCR	4	0
30	9	302	CLA	1	0
30	A	803	CLA	1	0
30	15	302	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	2	304	CLA	1	0
35	B	852	LMT	1	0
30	9	306	CLA	2	0
30	5	302	CLA	3	0
33	B	842	BCR	1	0
36	B	847	LMG	2	0
33	B	845	BCR	1	0
30	A	806	CLA	3	0
30	3	310	CLA	2	0
30	9	307	CLA	4	0
30	B	816	CLA	2	0
30	B	808	CLA	3	0
30	7	303	CLA	1	0
30	1	303	CLA	3	0
30	9	308	CLA	2	0
30	A	822	CLA	2	0
30	5	304	CLA	2	0
30	A	824	CLA	1	0
30	A	814	CLA	1	0
30	11	304	CLA	3	0
30	A	837	CLA	1	0
35	A	855	LMT	1	0
30	B	826	CLA	5	0
30	12	302	CLA	1	0
30	B	812	CLA	2	0
35	7	301	LMT	1	0
30	6	307	CLA	1	0
33	2u	201	BCR	3	0
35	6	302	LMT	2	0
30	5	307	CLA	2	0
31	A	845	PQN	5	0
33	B	846	BCR	4	0
30	B	823	CLA	1	0
35	11	318	LMT	1	0
30	A	816	CLA	4	0
30	A	819	CLA	3	0
30	8	302	CLA	1	0
30	2	303	CLA	4	0
30	15	304	CLA	2	0
30	5	308	CLA	2	0
30	5	303	CLA	4	0
33	I	101	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	1	307	CLA	2	0
35	12	319	LMT	1	0
36	8	319	LMG	1	0
30	A	826	CLA	4	0
30	A	831	CLA	4	0
30	A	820	CLA	6	0
39	6	319	DD6	1	0
30	B	815	CLA	2	0
30	8	305	CLA	2	0
30	B	827	CLA	5	0
30	B	803	CLA	2	0
30	B	824	CLA	3	0
30	2u	202	CLA	3	0
33	B	844	BCR	2	0
30	A	818	CLA	1	0
30	A	842	CLA	3	0
30	1	301	CLA	2	0
35	12	320	LMT	1	0
37	8	315	A86	1	0
30	2	307	CLA	2	0
30	B	802	CLA	2	0
30	3	302	CLA	1	0
30	2	308	CLA	1	0
30	J	101	CLA	1	0
33	A	851	BCR	2	0
37	4	315	A86	1	0
30	A	811	CLA	3	0
30	11	309	CLA	1	0
30	A	841	CLA	1	0
33	L	205	BCR	4	0
30	B	809	CLA	6	0
36	8	321	LMG	1	0
36	14	321	LMG	2	0
30	B	819	CLA	1	0
30	13	302	CLA	2	0
30	14	312	CLA	1	0
30	8	303	CLA	2	0
30	A	839	CLA	4	0
30	B	820	CLA	1	0
30	A	832	CLA	1	0
30	8	301	CLA	1	0
30	6	314	CLA	2	0

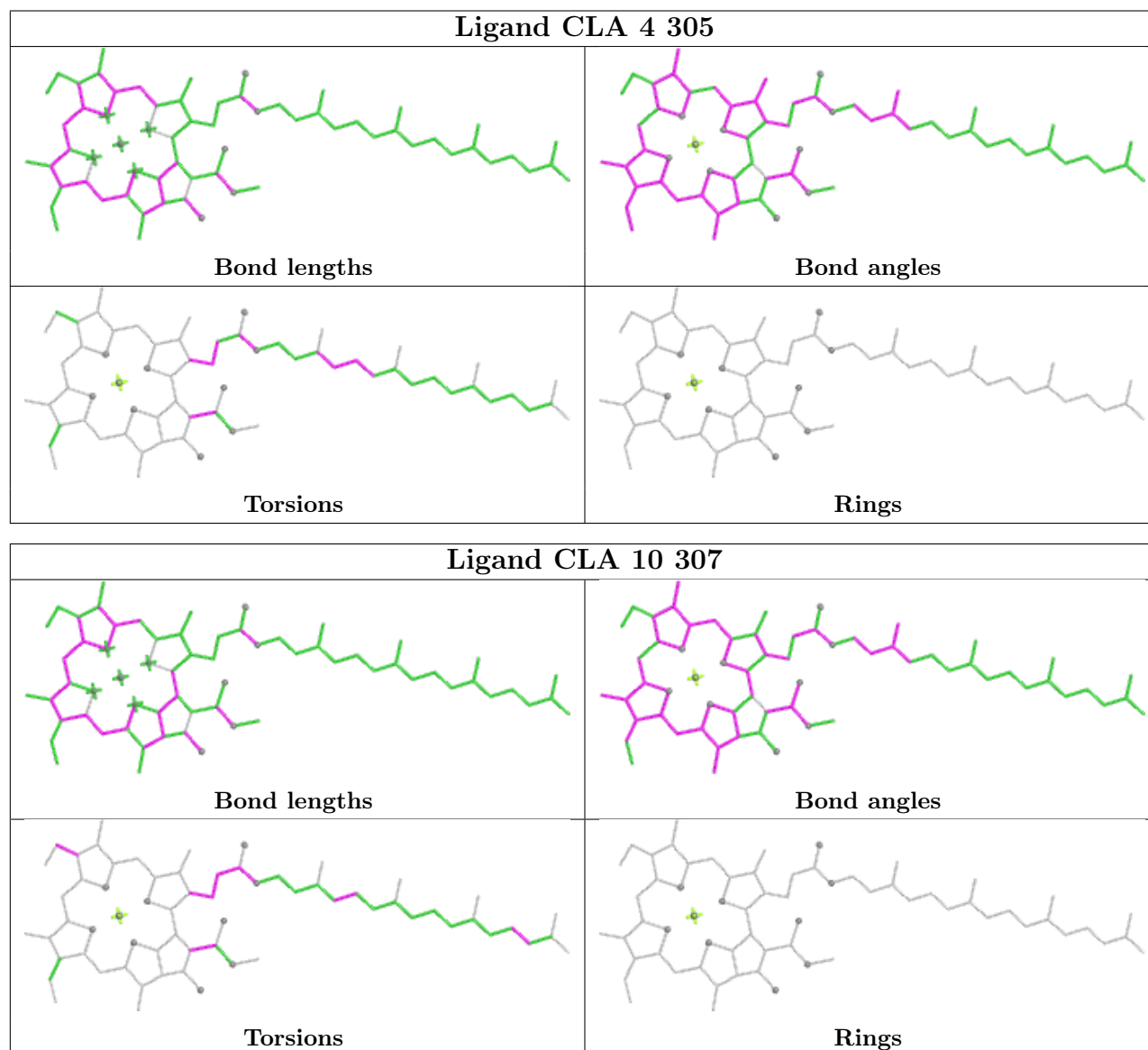
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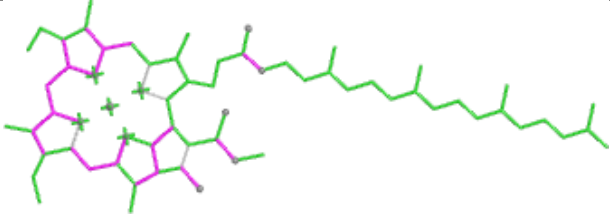
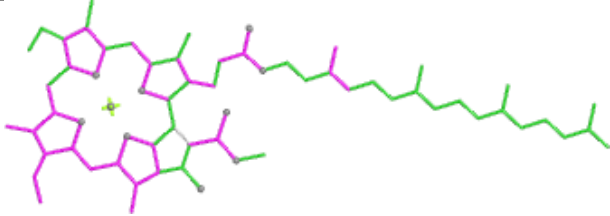
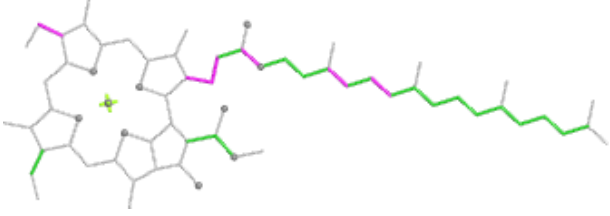
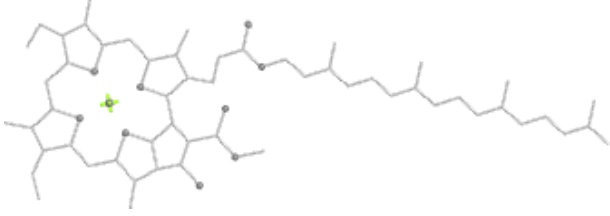
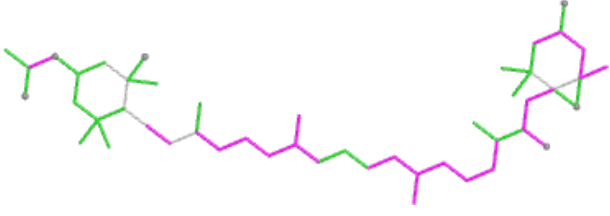
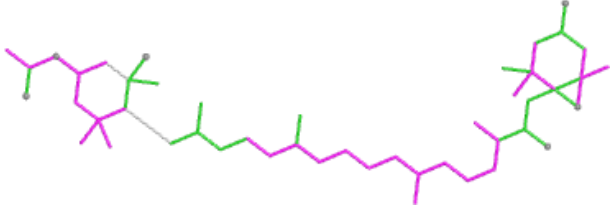
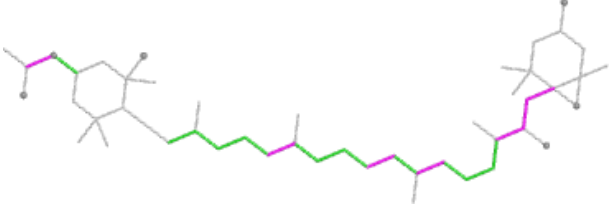
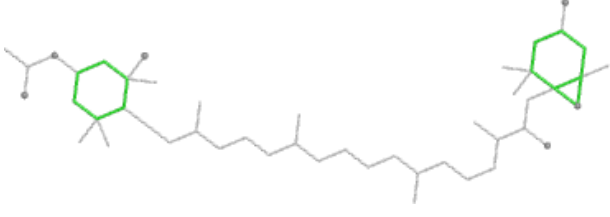
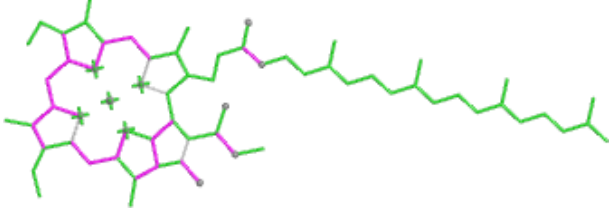
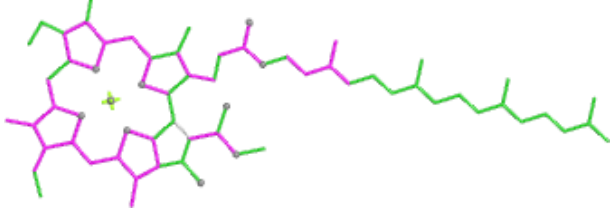
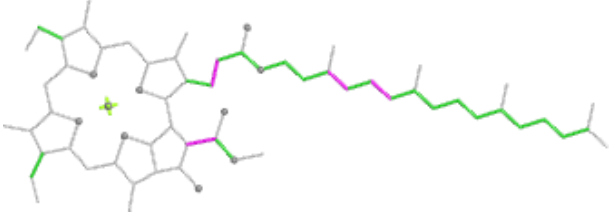
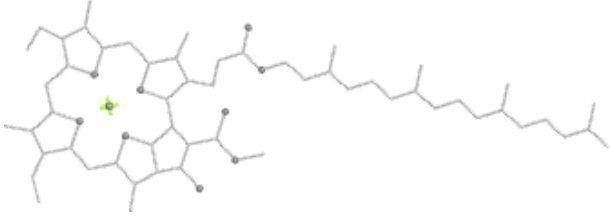
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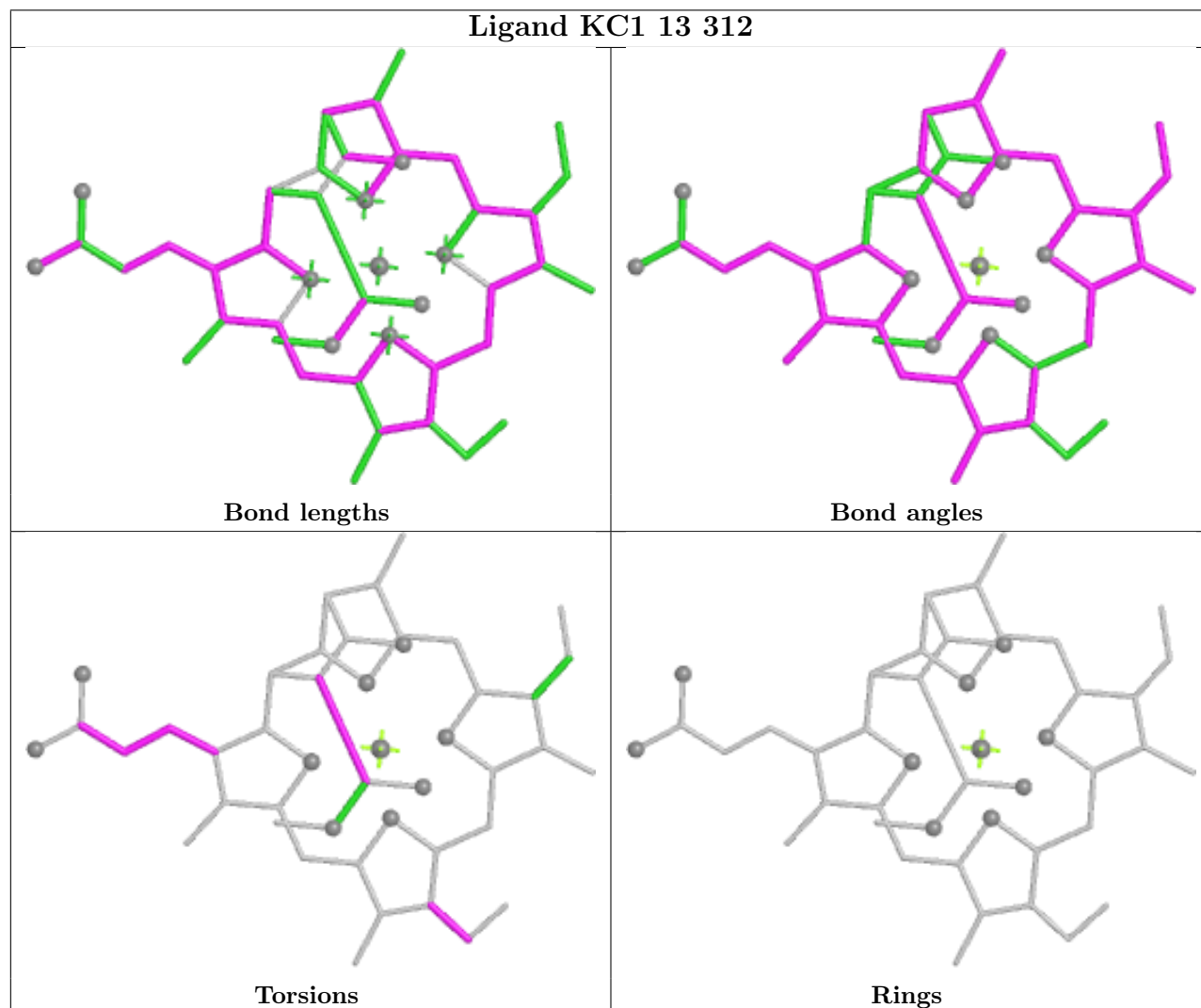
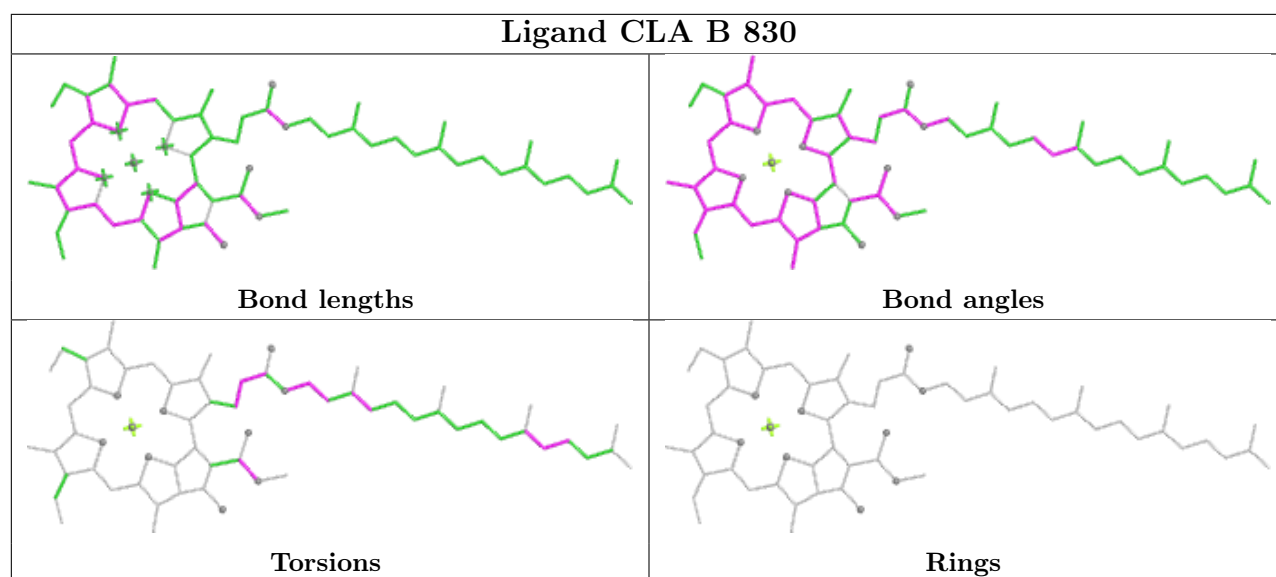
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	3	306	CLA	1	0
30	4	306	CLA	4	0
30	7	309	CLA	6	0
30	2	301	CLA	1	0
30	11	308	CLA	2	0
33	A	850	BCR	2	0
33	L	201	BCR	2	0
30	B	811	CLA	4	0
30	3	305	CLA	1	0
30	A	804	CLA	3	0
39	13	314	DD6	1	0
30	4	311	CLA	2	0
30	A	844	CLA	1	0
38	4	310	KC1	1	0
30	A	812	CLA	4	0
30	15	309	CLA	2	0
38	5	312	KC1	1	0
33	B	843	BCR	2	0
30	B	804	CLA	2	0
33	A	848	BCR	2	0
39	6	318	DD6	1	0
30	A	835	CLA	2	0
30	2	309	CLA	3	0
35	7	321	LMT	1	0
30	A	807	CLA	1	0
30	L	203	CLA	2	0
30	B	851	CLA	1	0
34	A	852	LHG	1	0
30	A	834	CLA	2	0
36	A	856	LMG	3	0
36	B	849	LMG	1	0
30	9	301	CLA	1	0
30	7	306	CLA	2	0
30	16	309	CLA	1	0
30	B	818	CLA	1	0
30	A	805	CLA	2	0
35	12	301	LMT	2	0
30	A	830	CLA	4	0

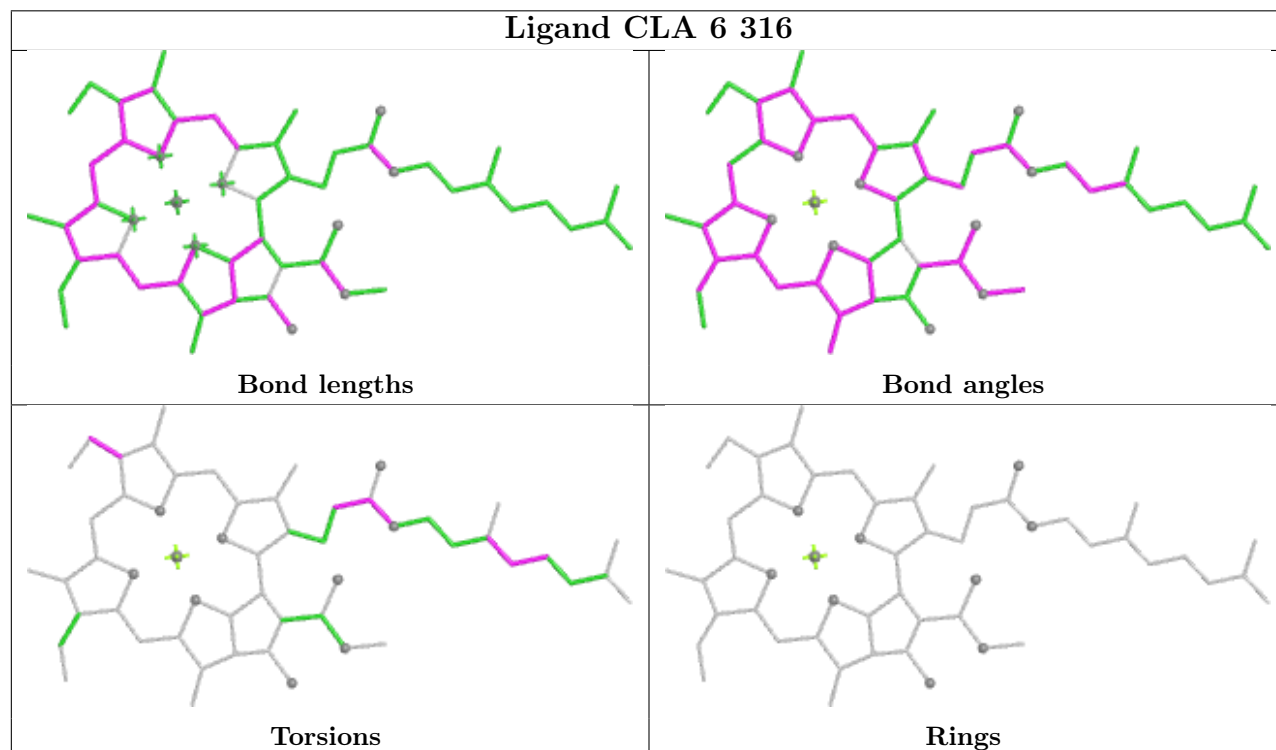
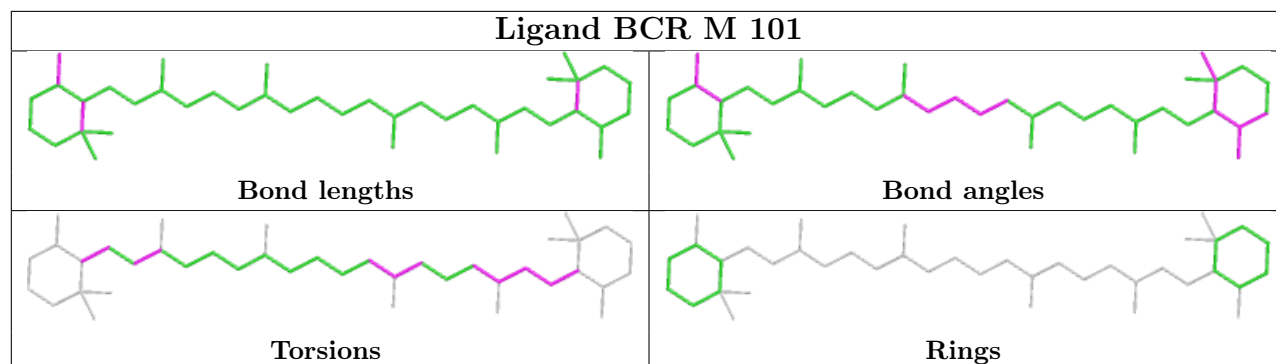
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

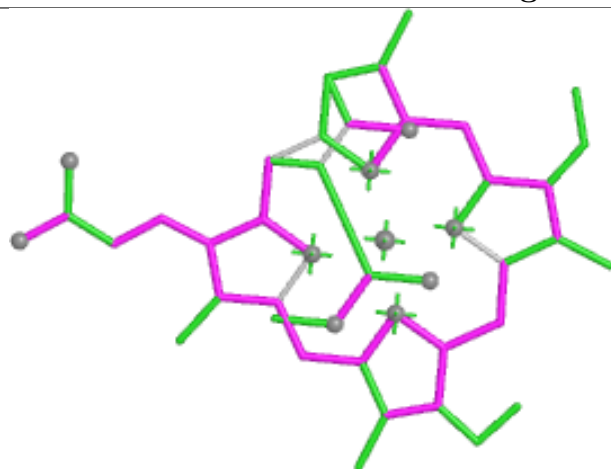


Ligand CLA 3 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand A86 14 314	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

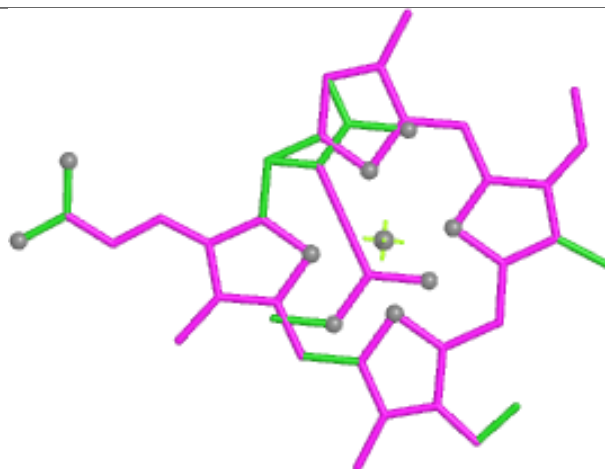




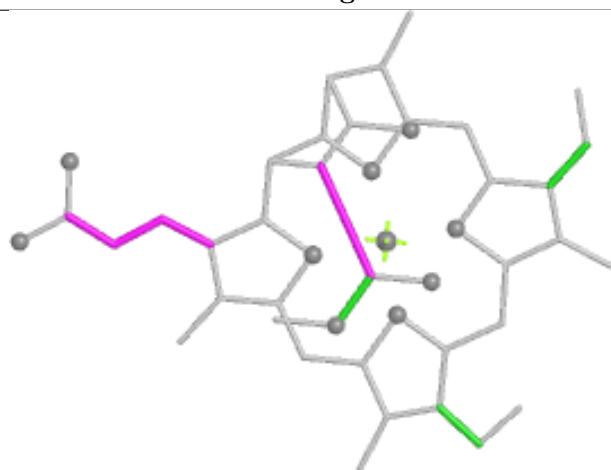
Ligand KC1 5 310



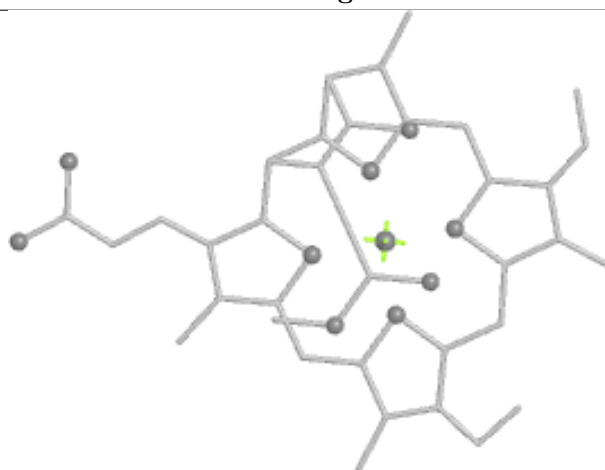
Bond lengths



Bond angles

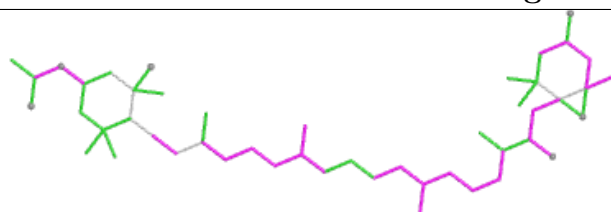


Torsions

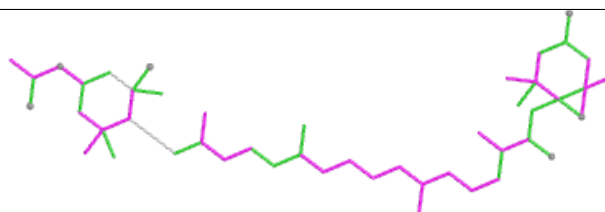


Rings

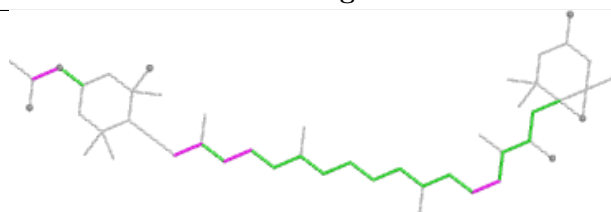
Ligand A86 5 315



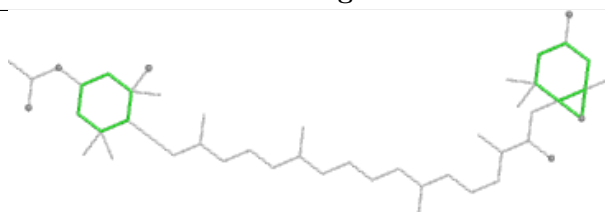
Bond lengths



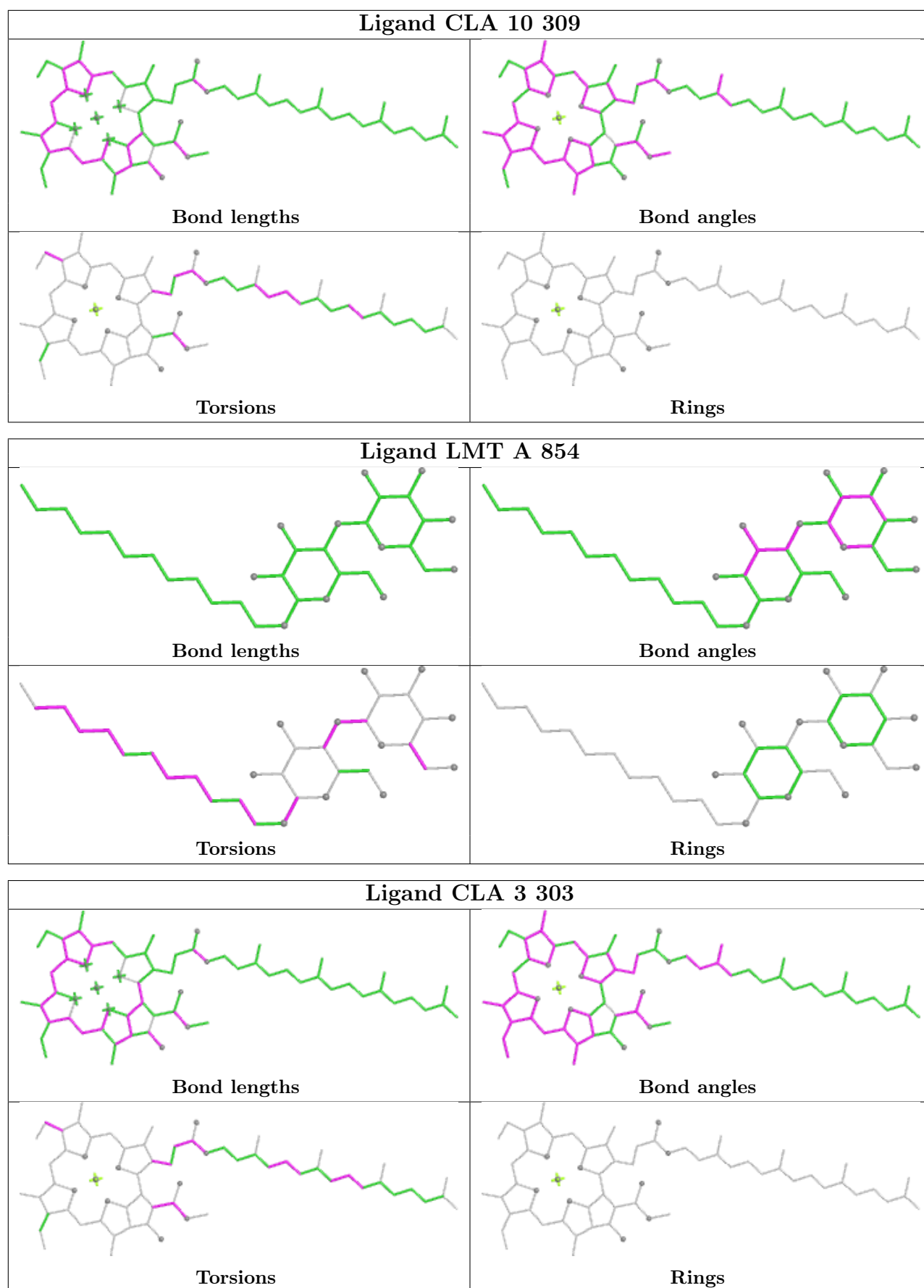
Bond angles

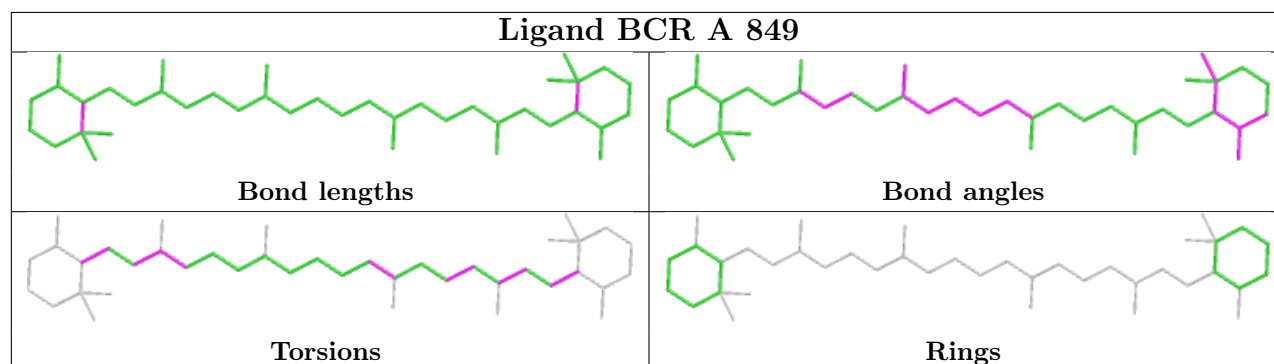
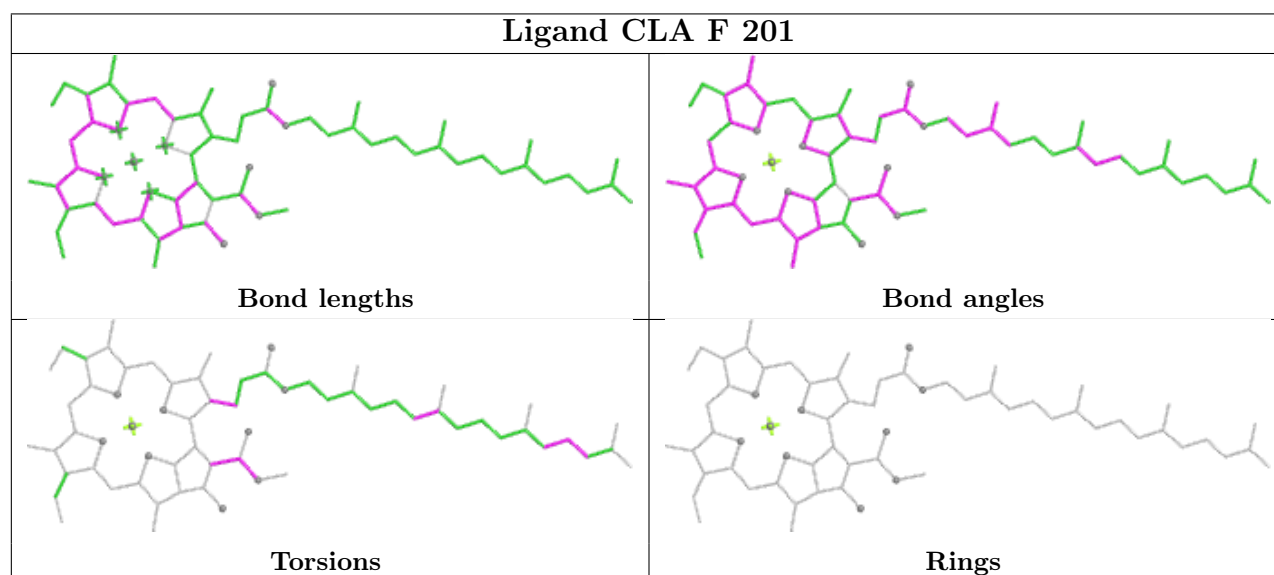
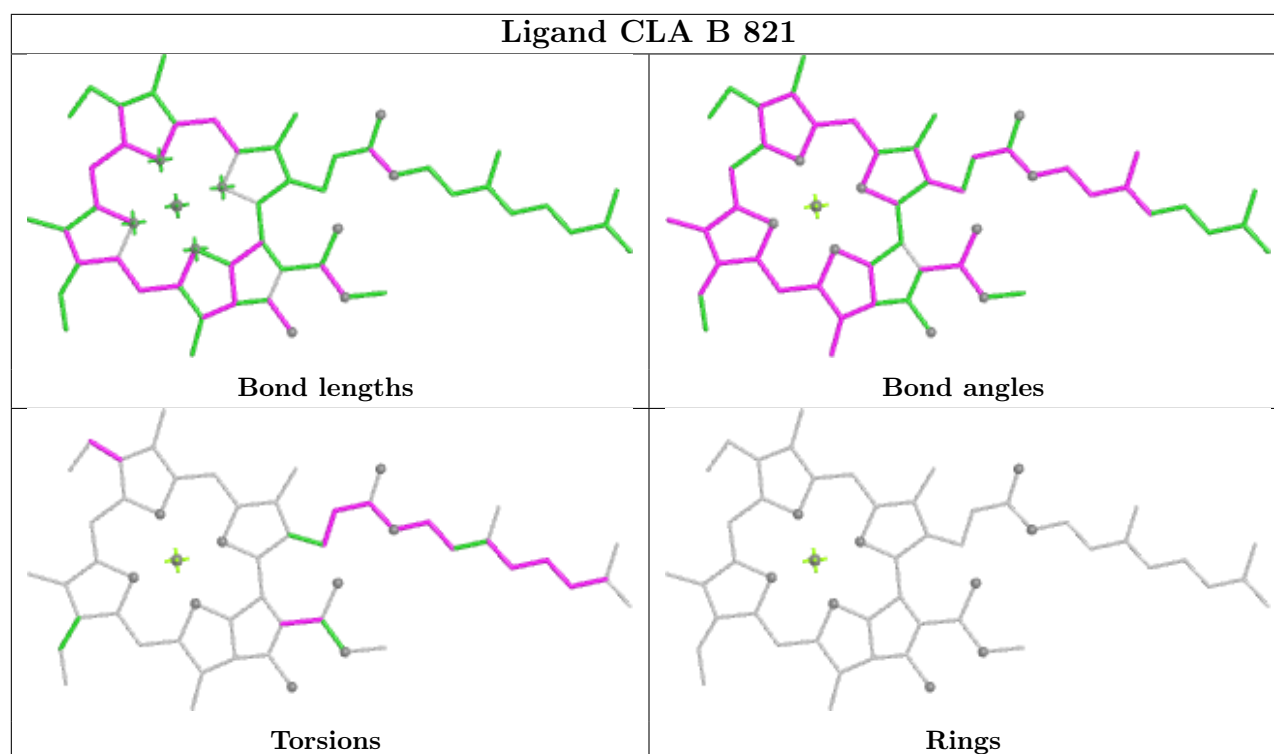


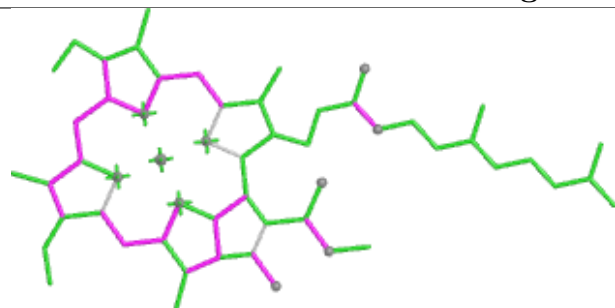
Torsions



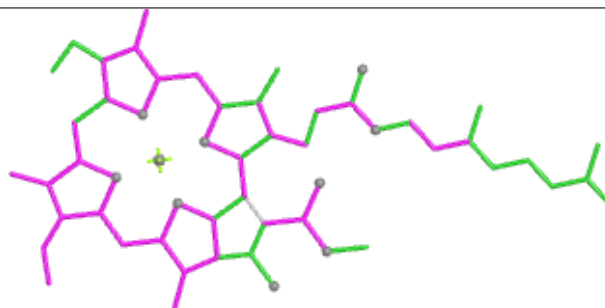
Rings



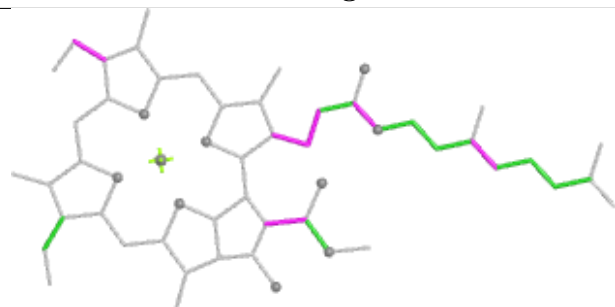


Ligand CLA 8 308

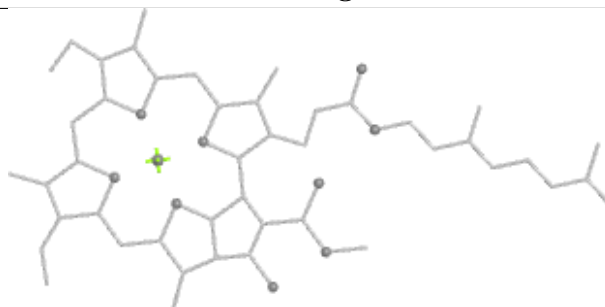
Bond lengths



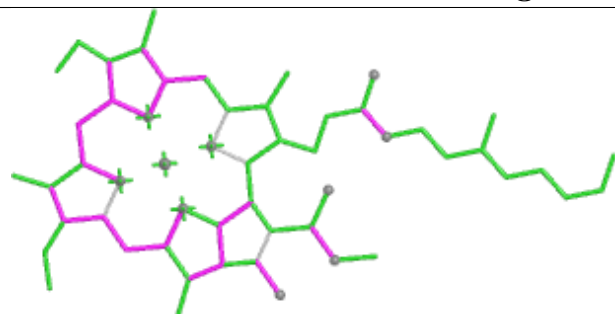
Bond angles



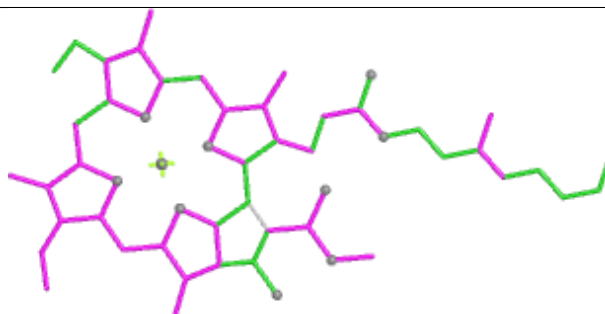
Torsions



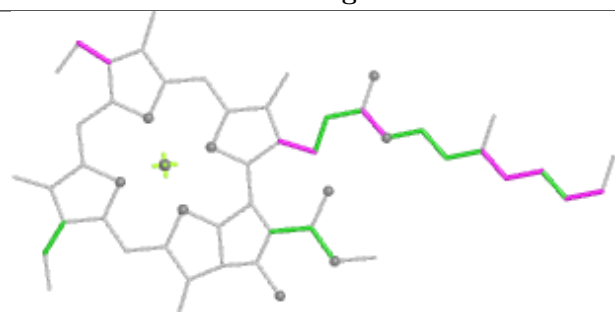
Rings

Ligand CLA A 836

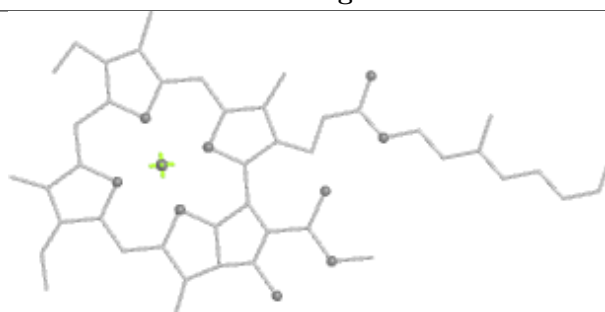
Bond lengths



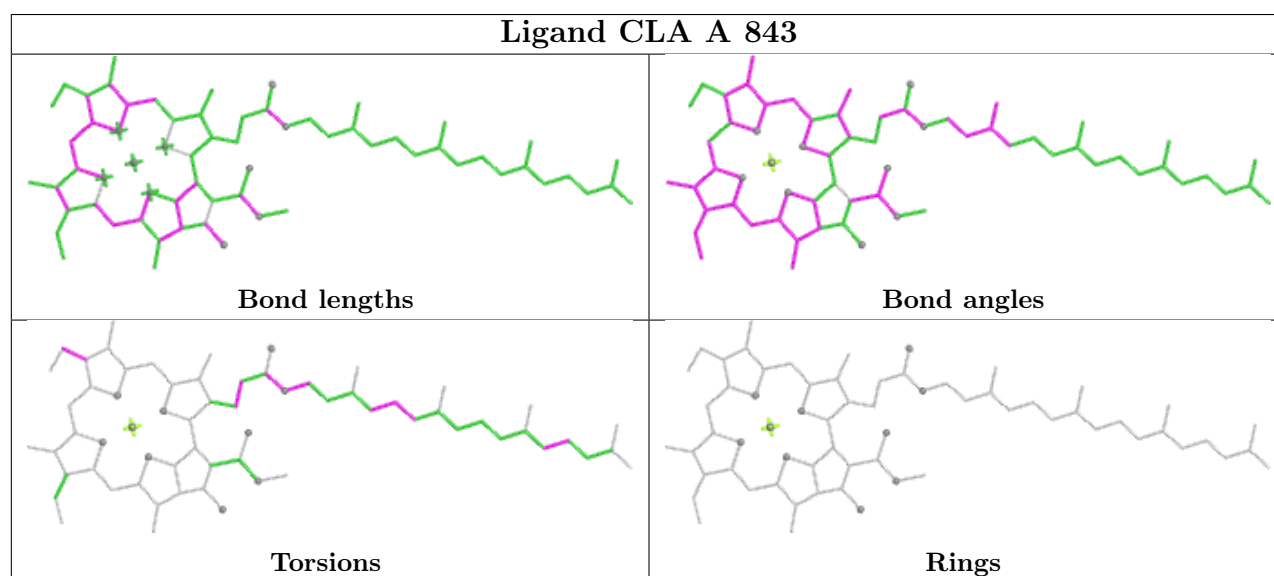
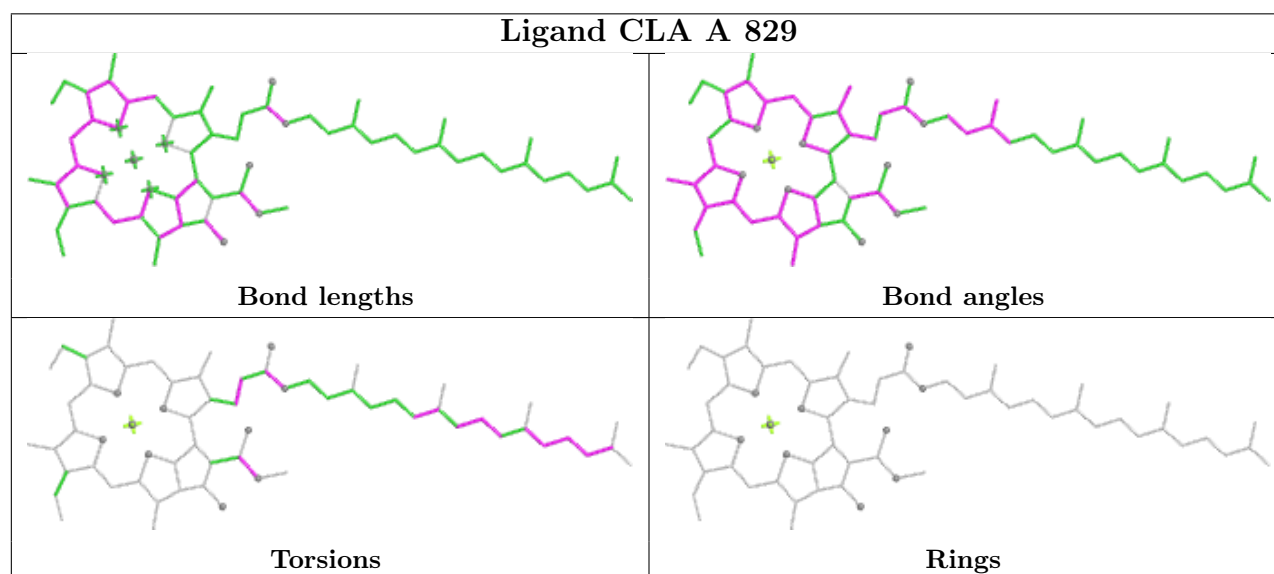
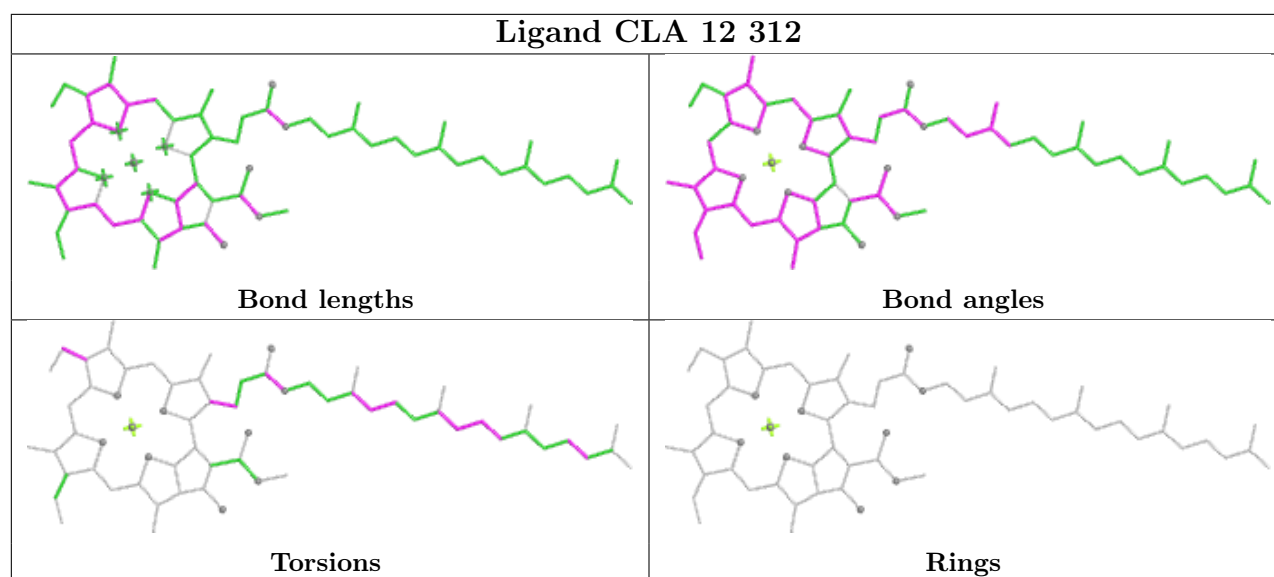
Bond angles

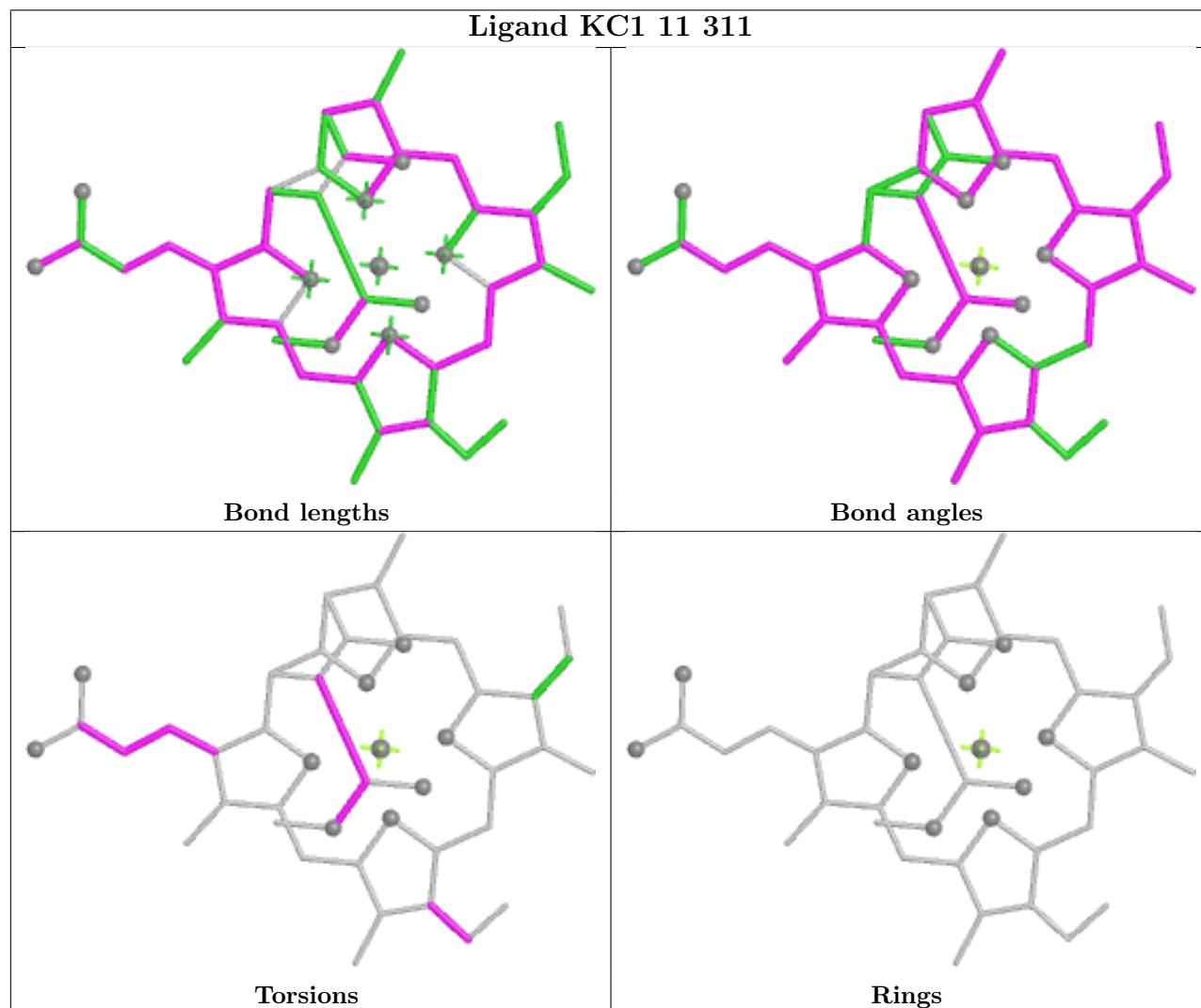
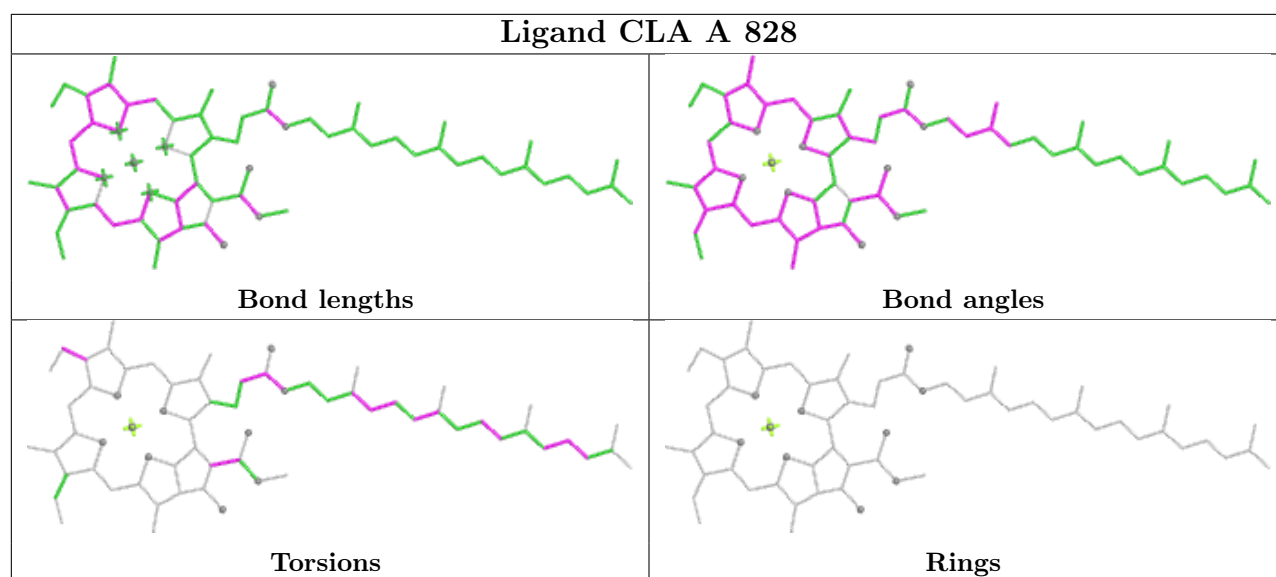


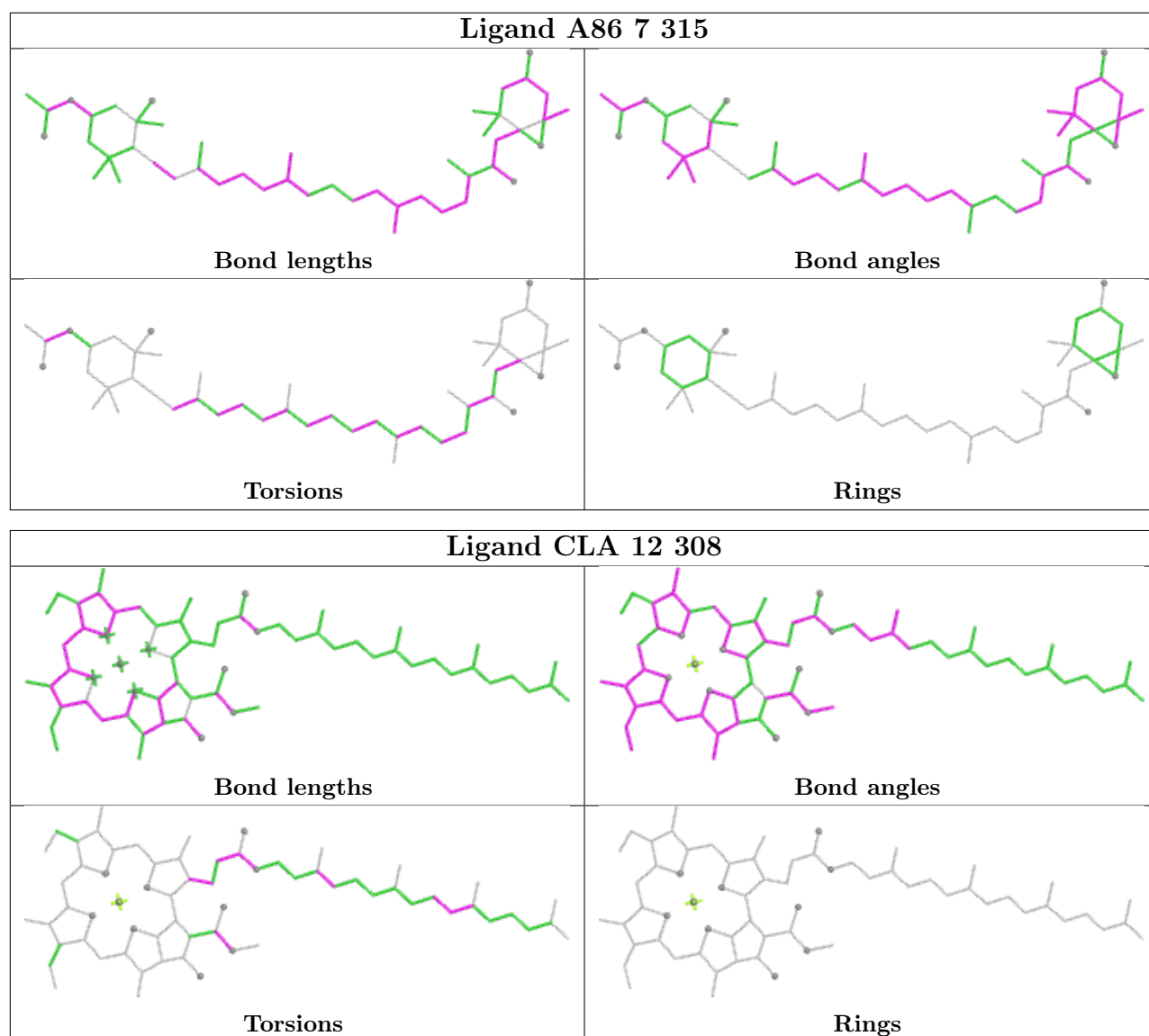
Torsions



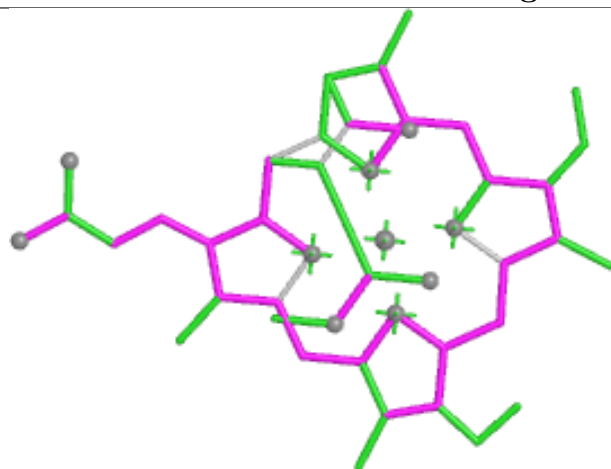
Rings



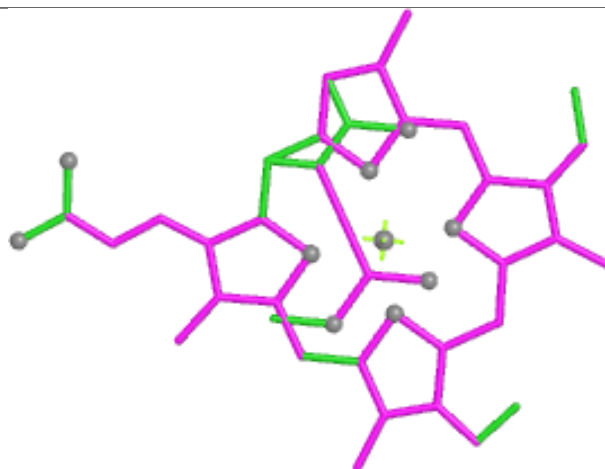




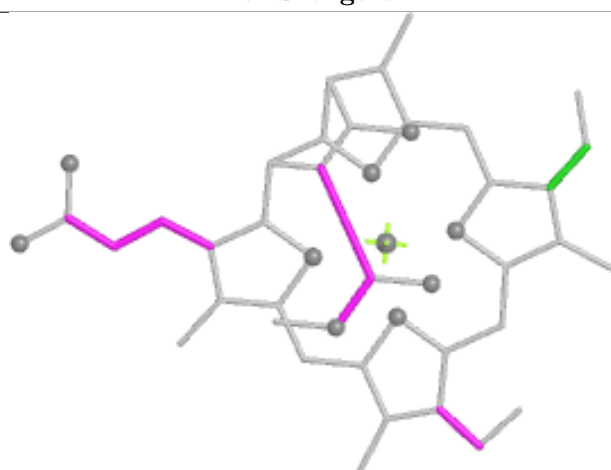
Ligand KC1 1 306



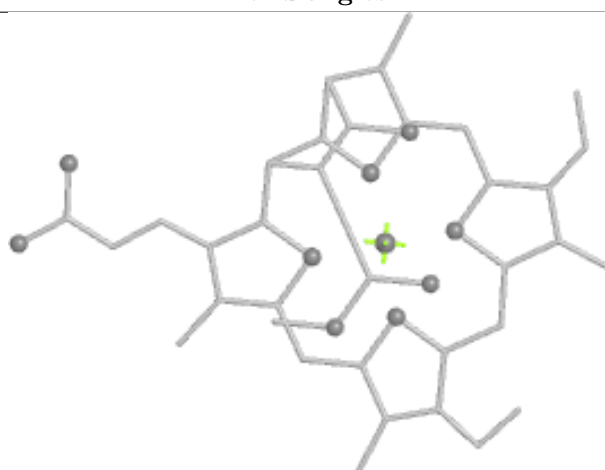
Bond lengths



Bond angles

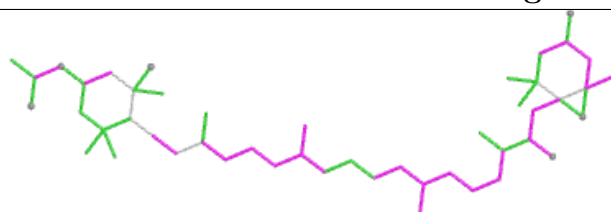


Torsions

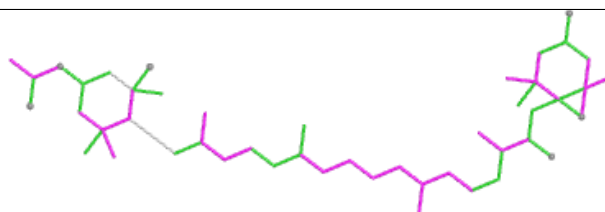


Rings

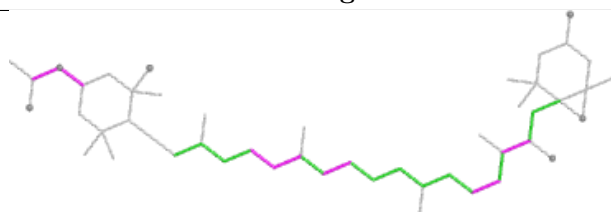
Ligand A86 2 302



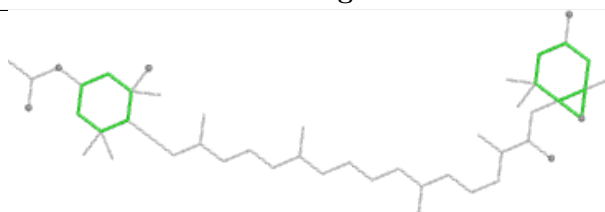
Bond lengths



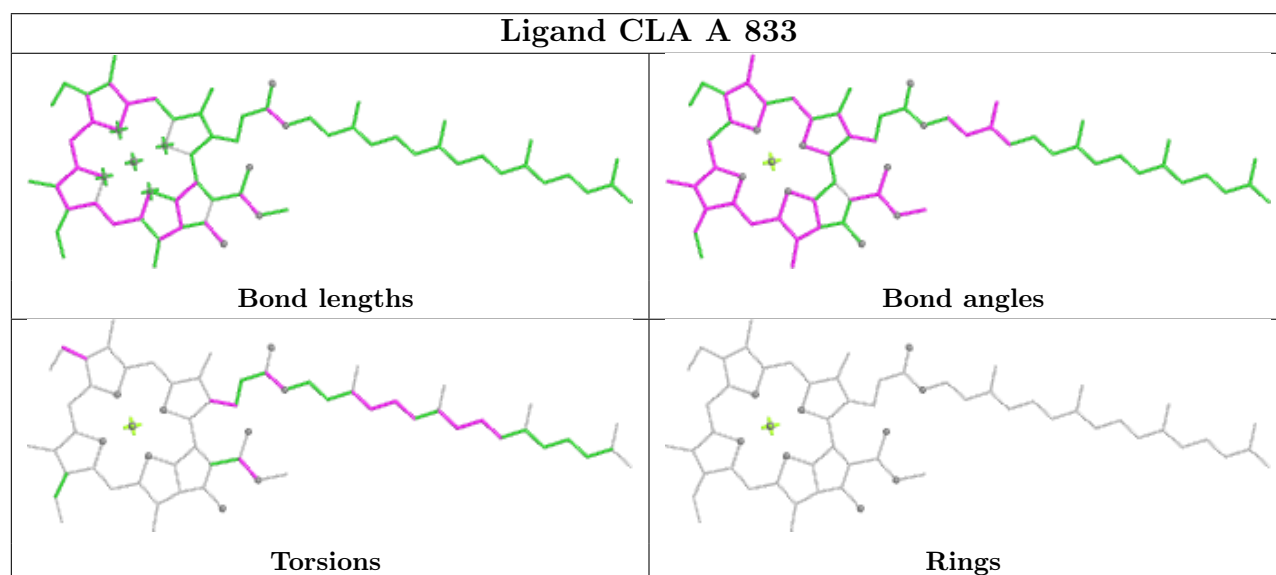
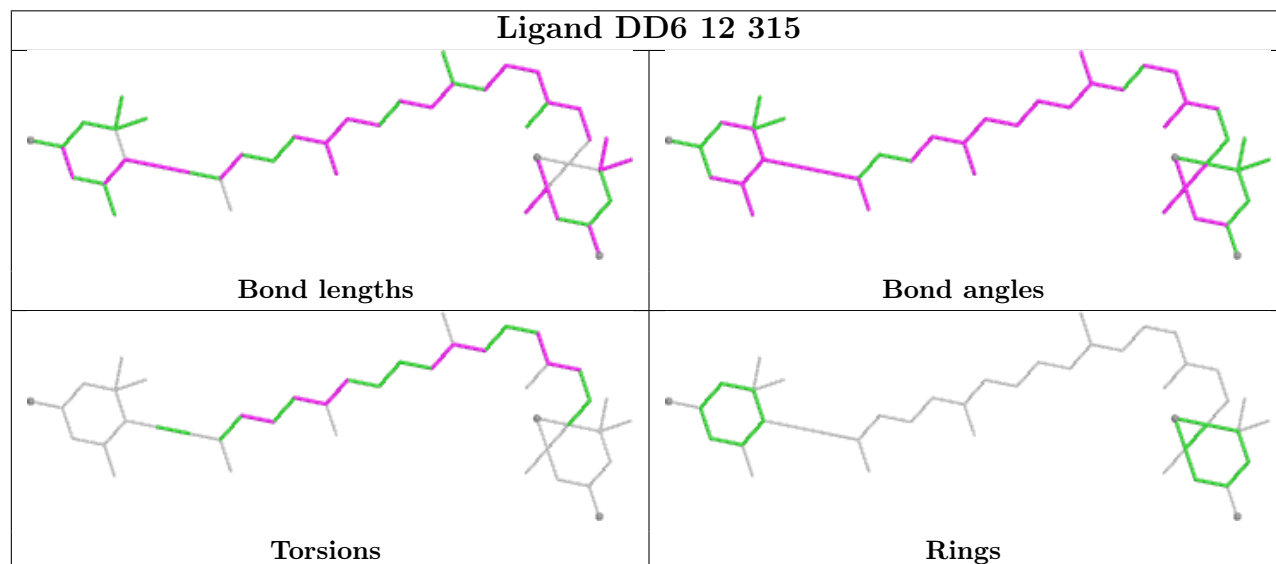
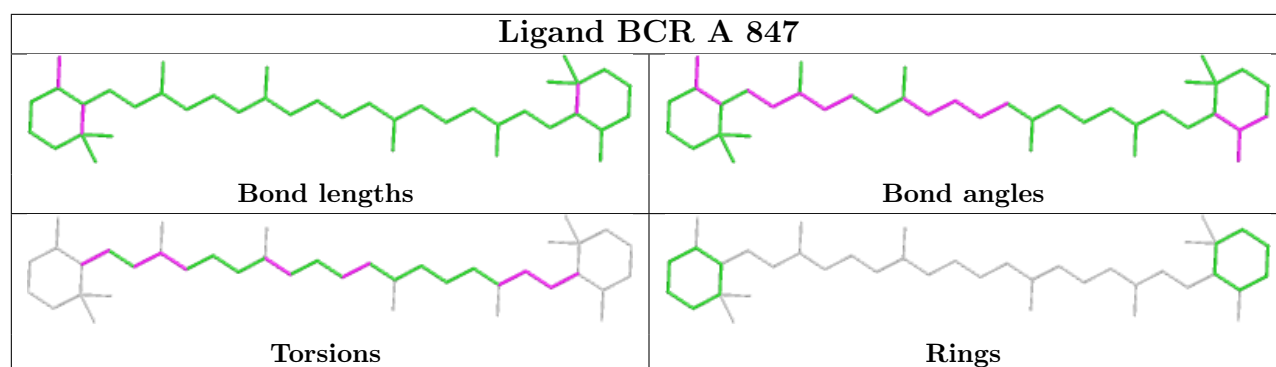
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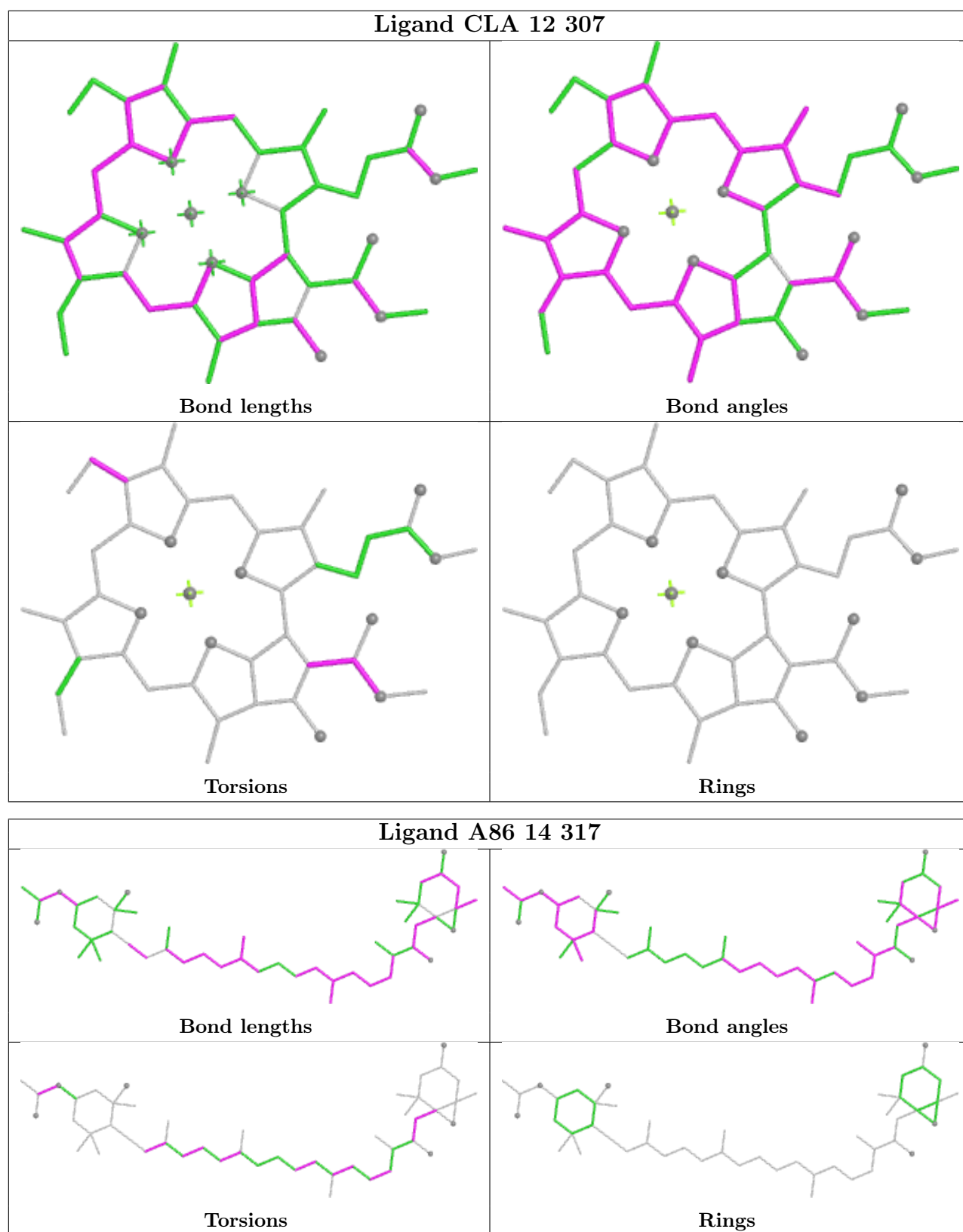


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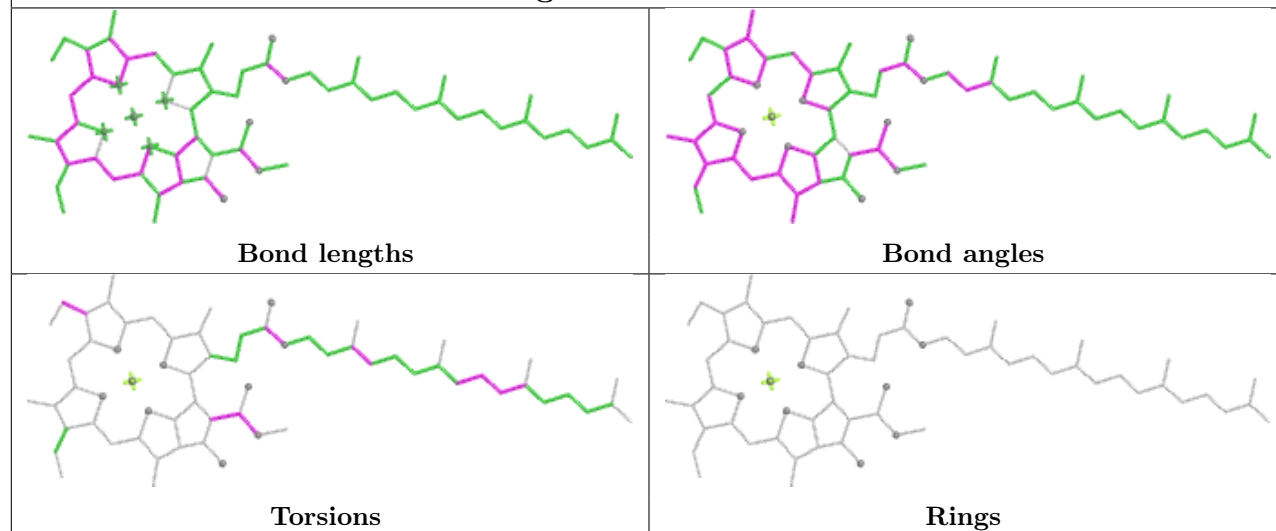


Rings

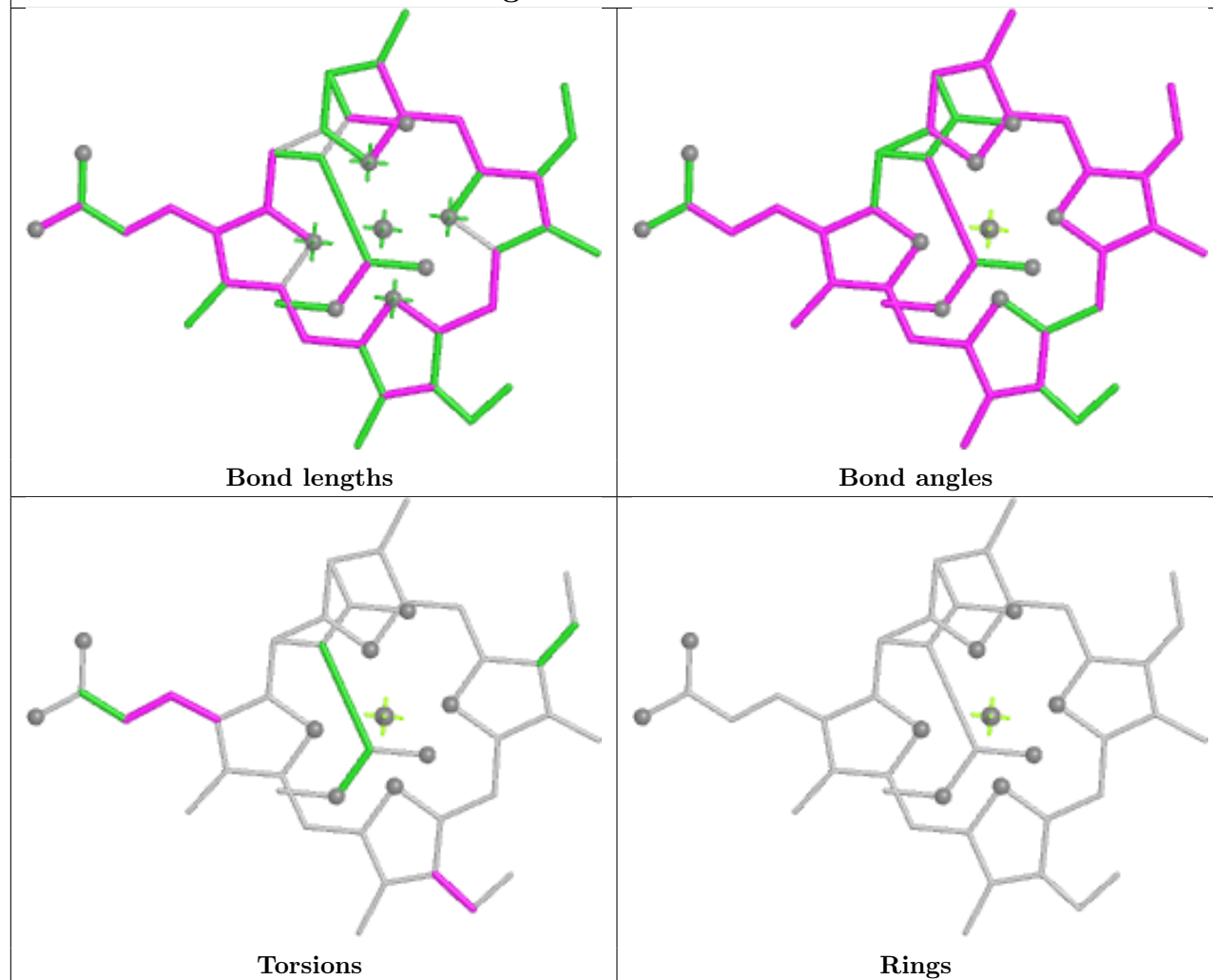


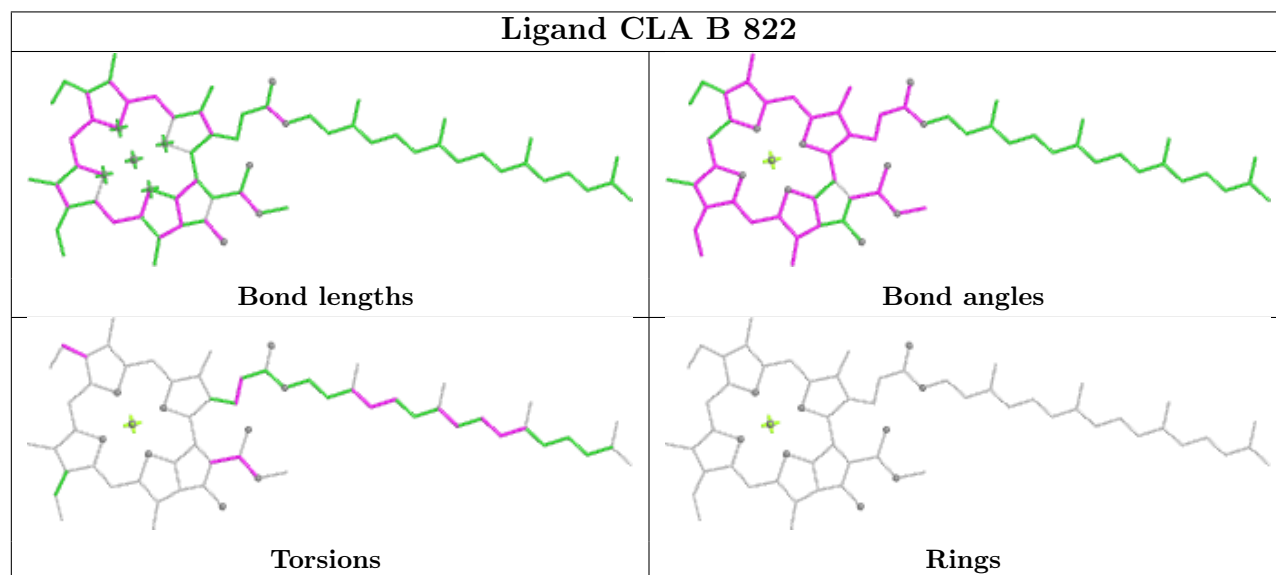
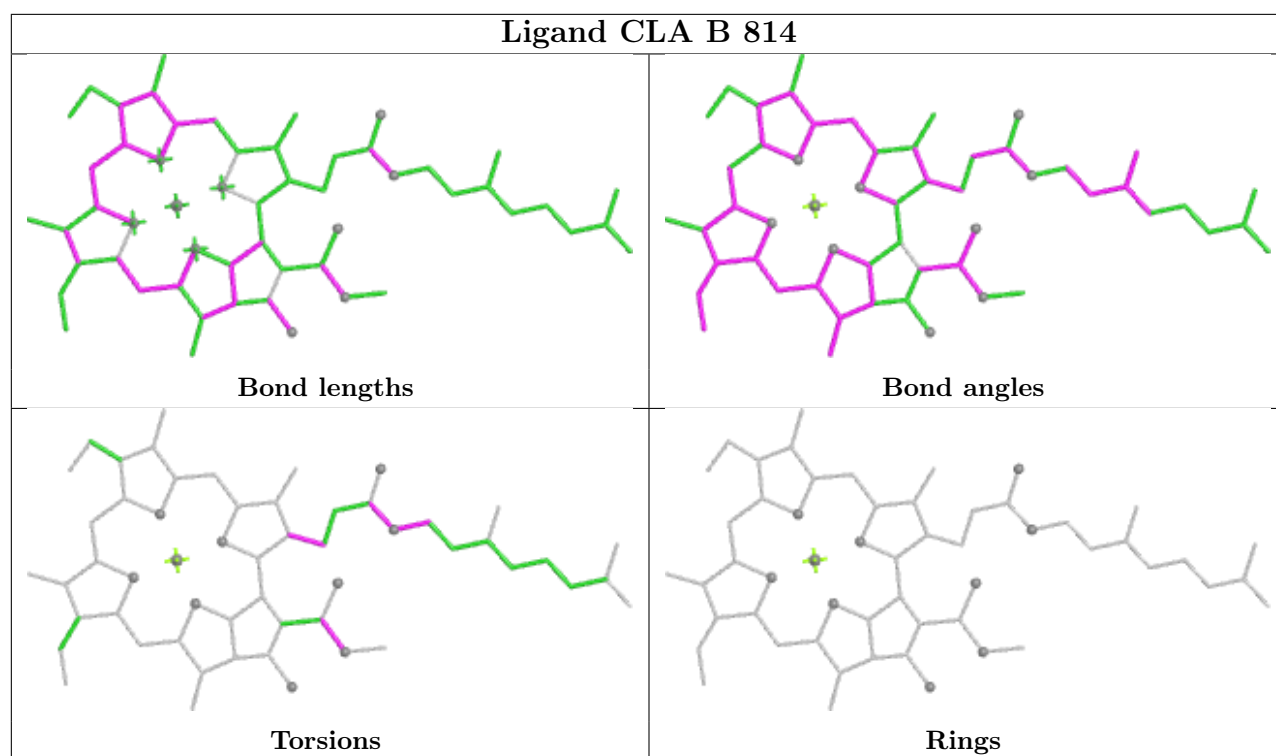


Ligand CLA 2 311

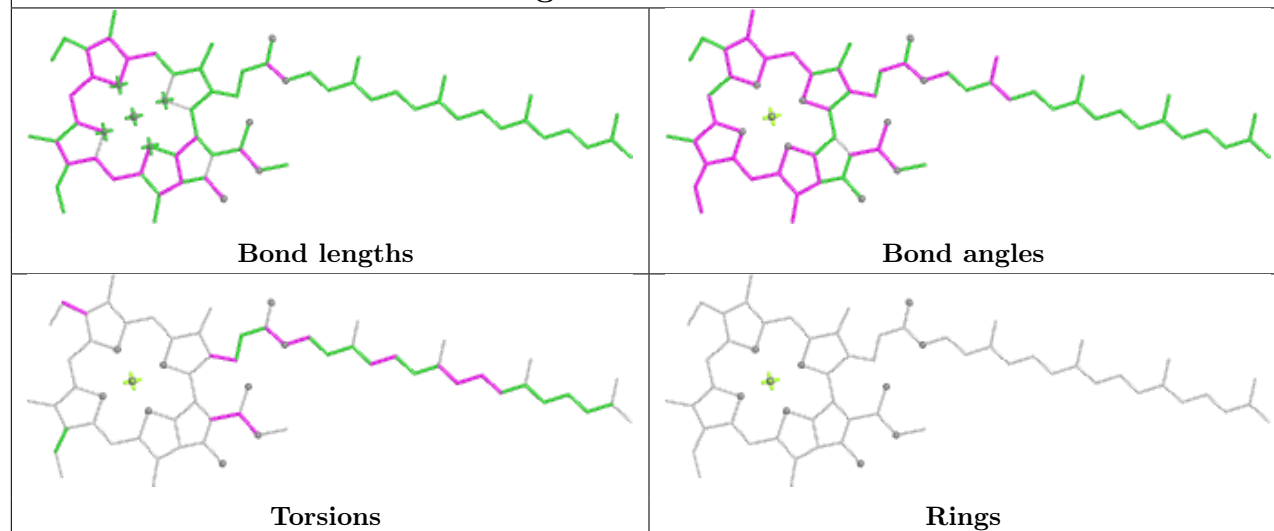


Ligand KC1 11 312

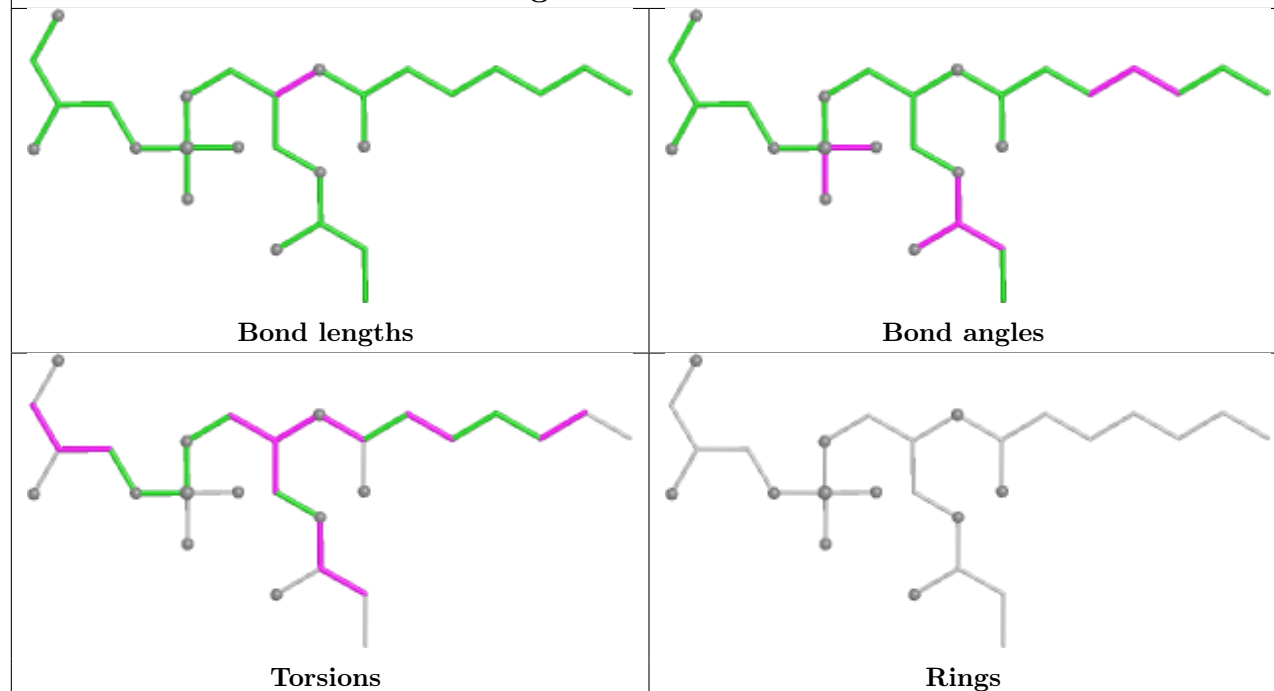


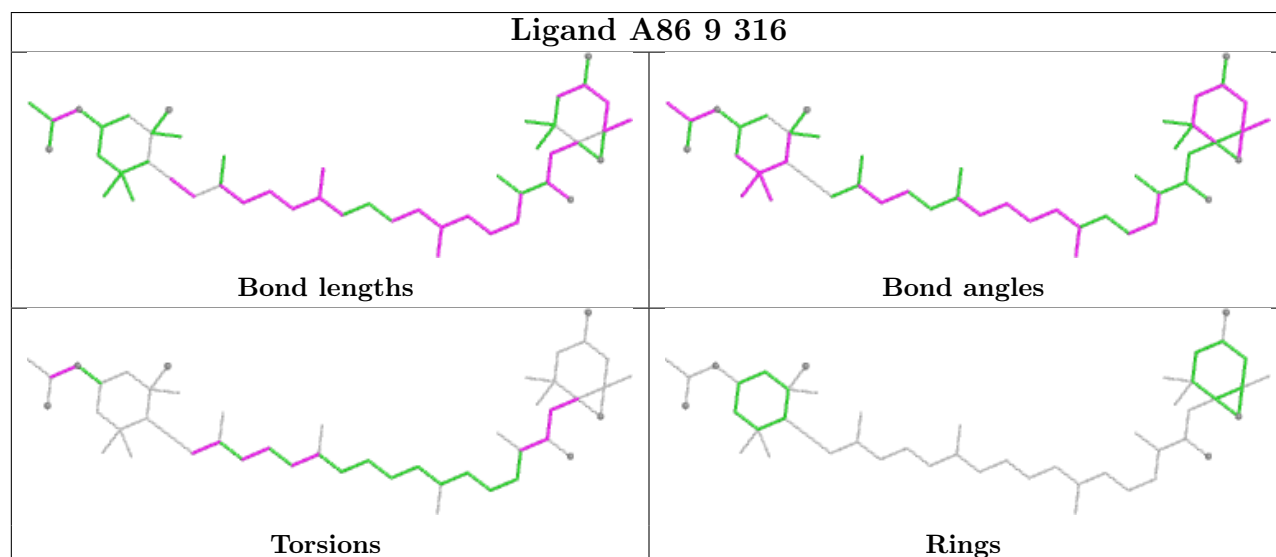
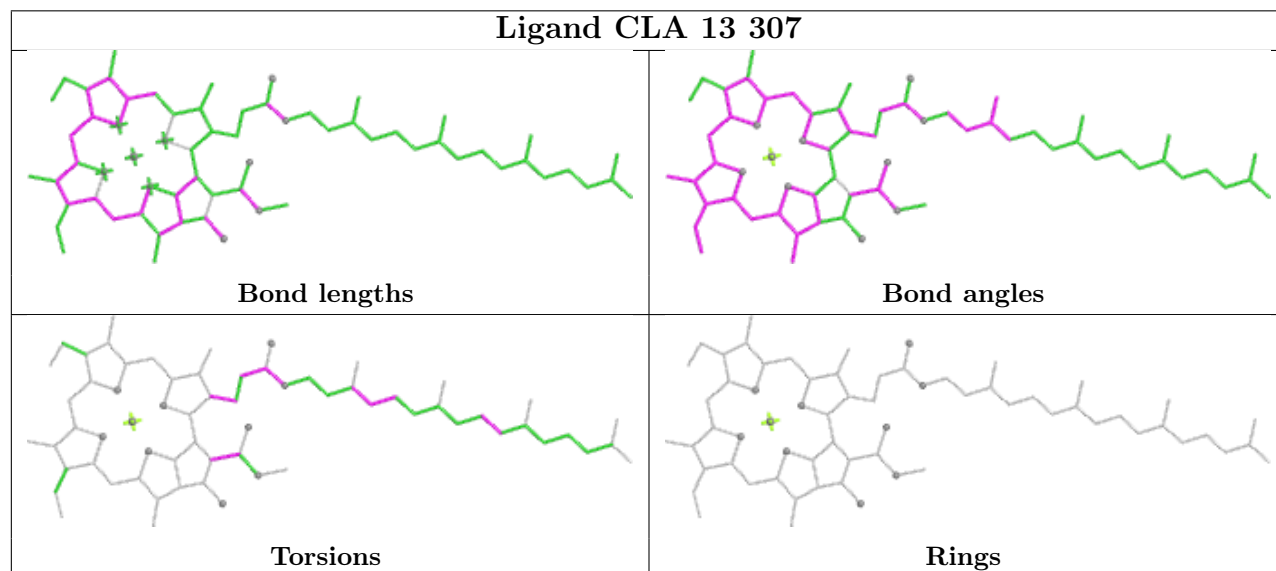
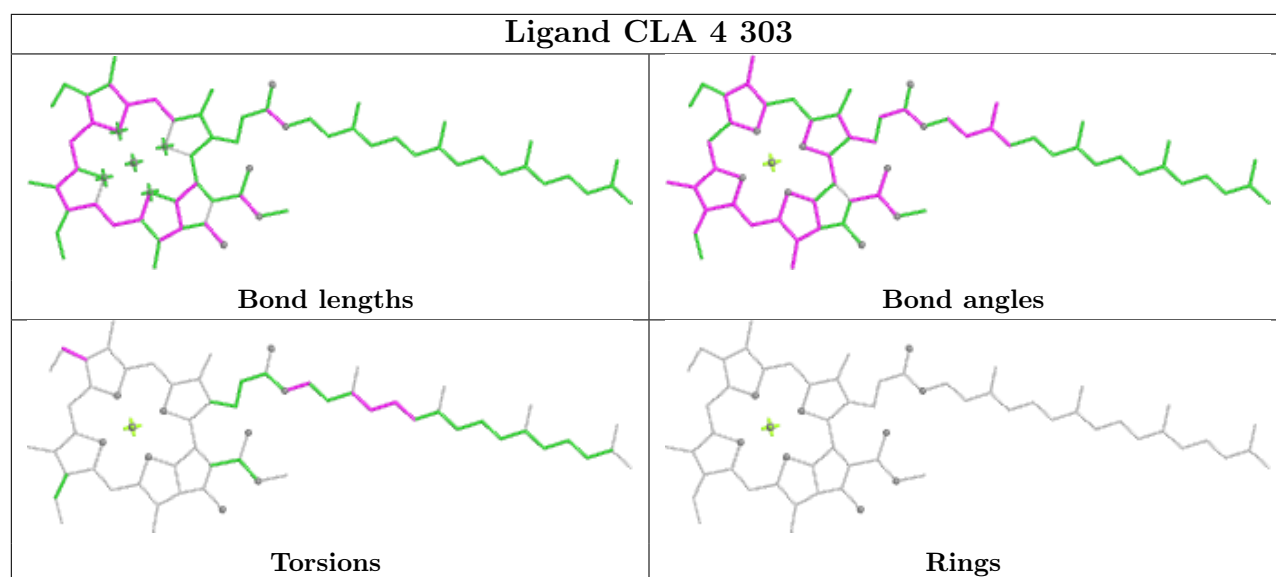


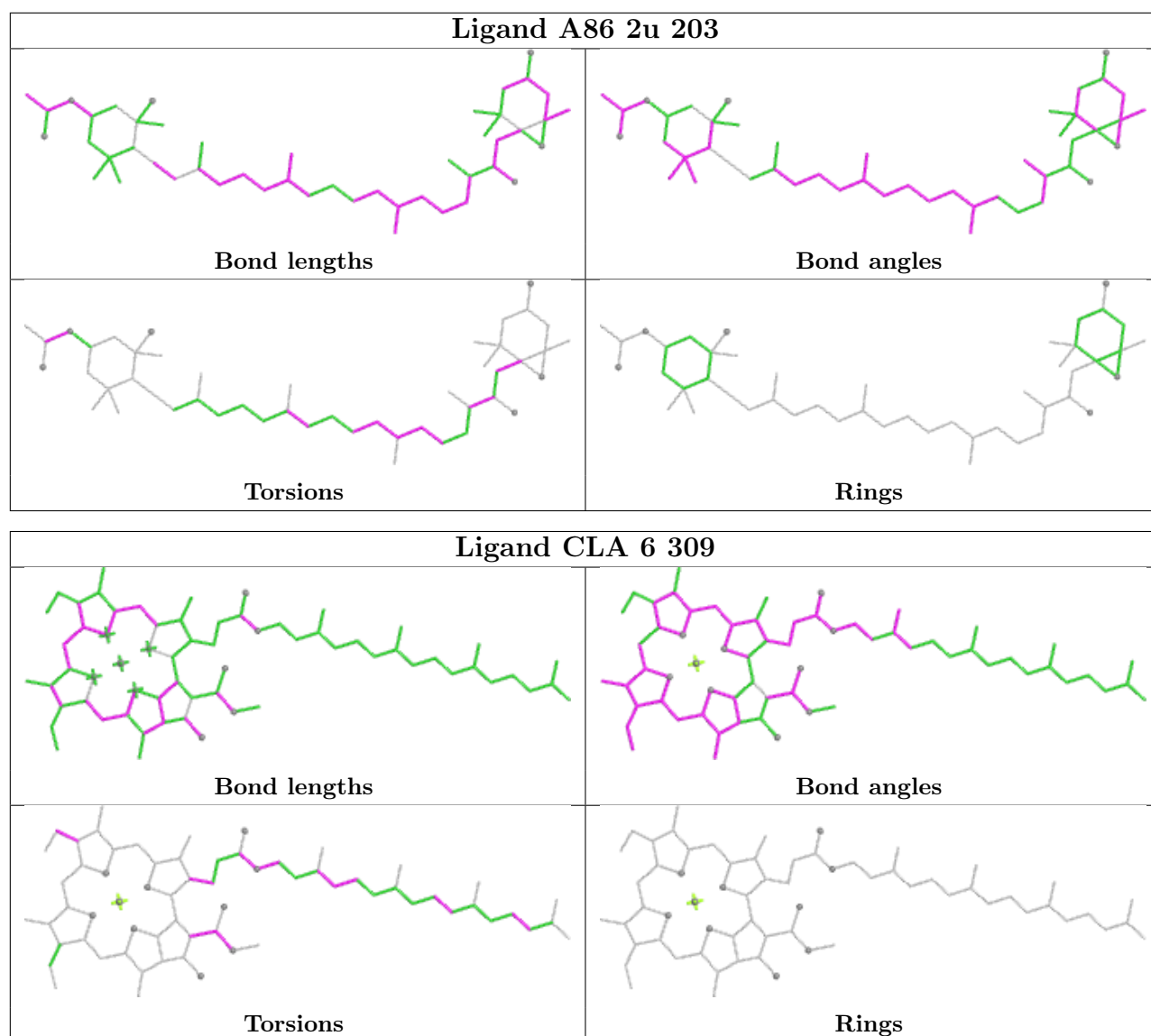
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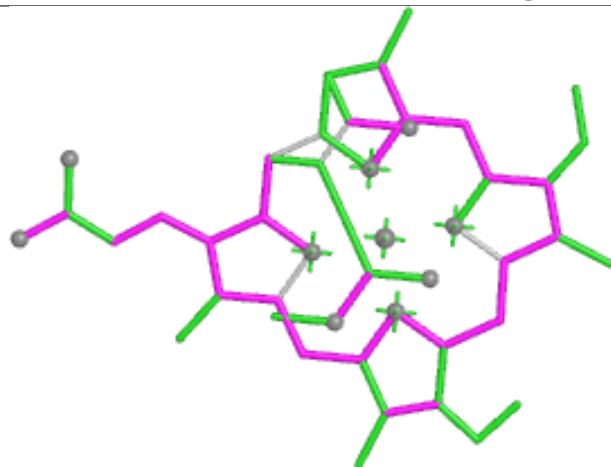
Ligand LHG B 848



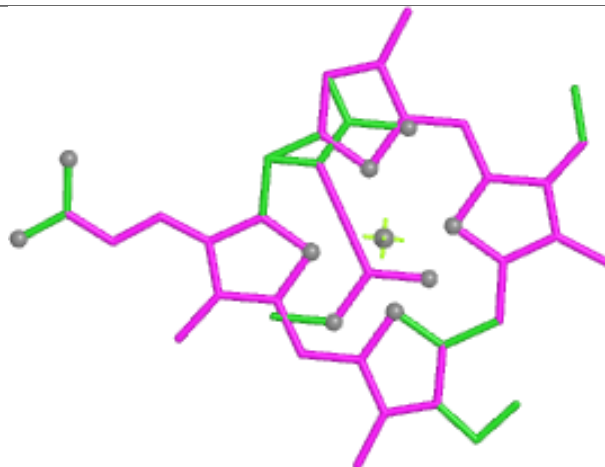




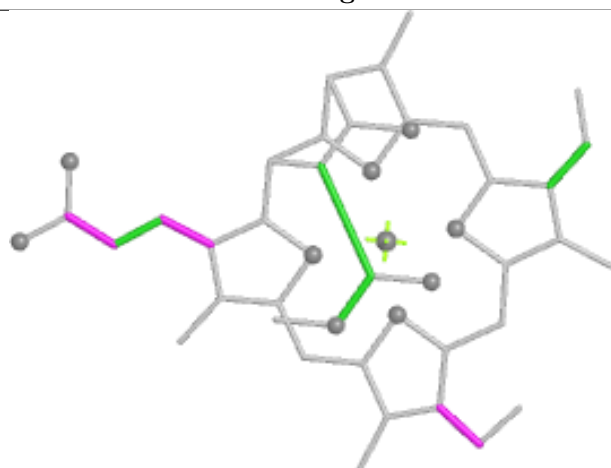
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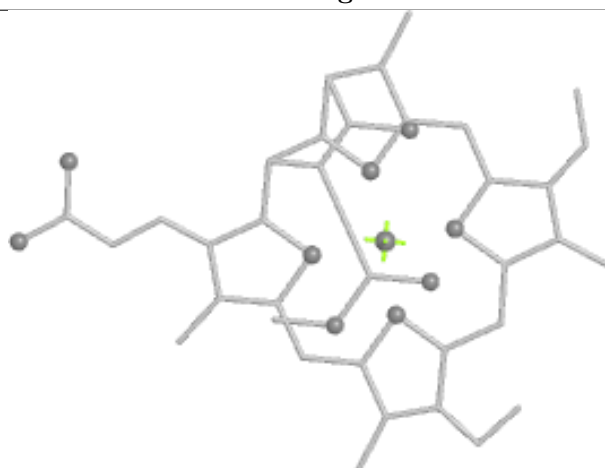
Bond lengths



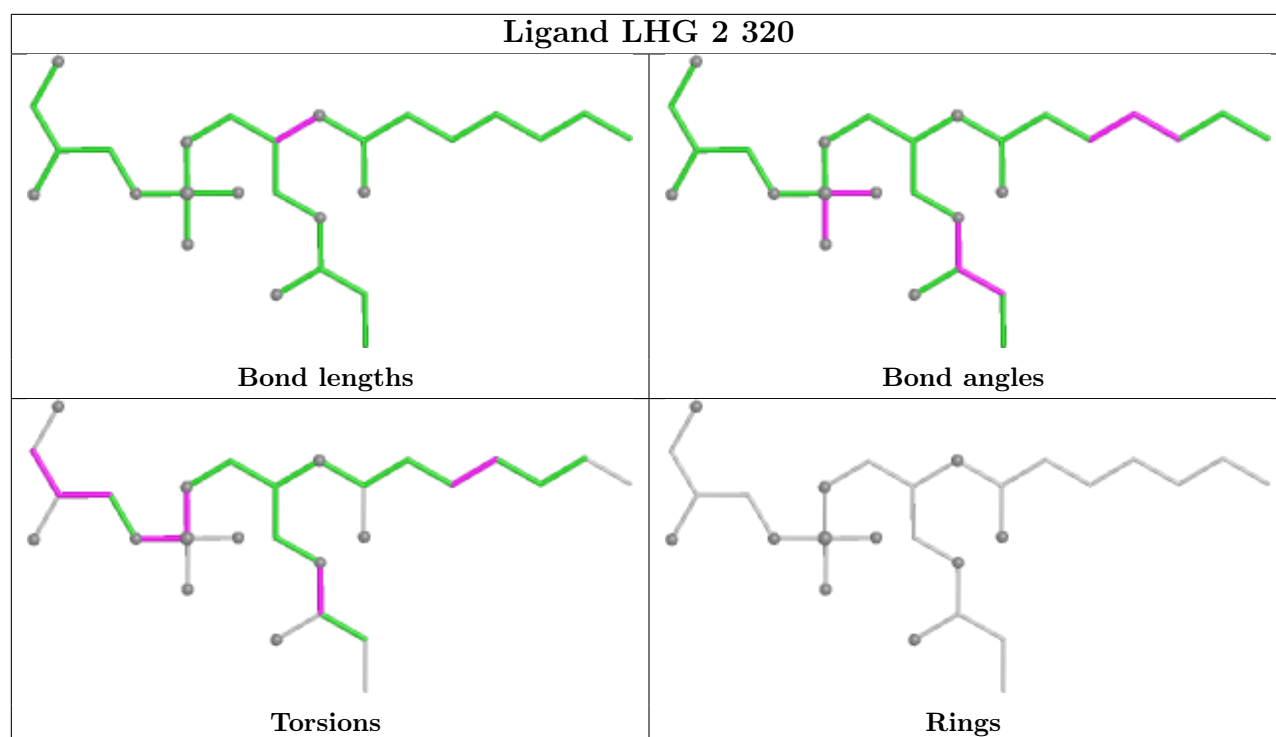
Bond angles



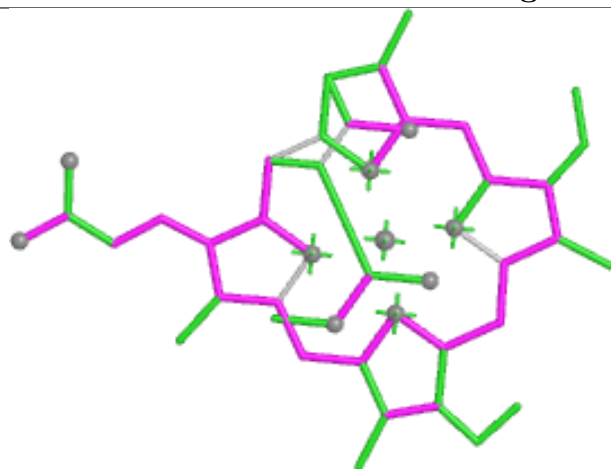
Torsions



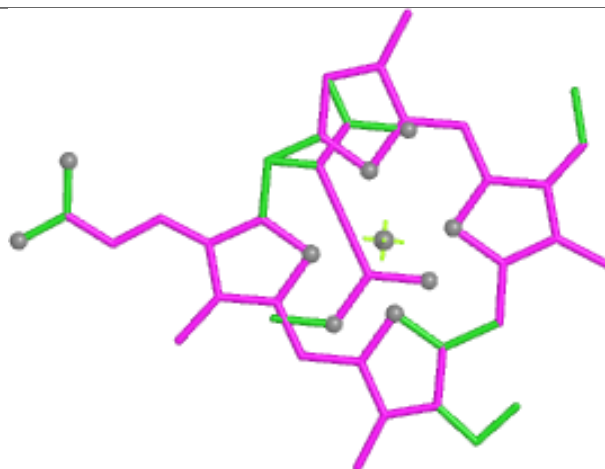
Rings



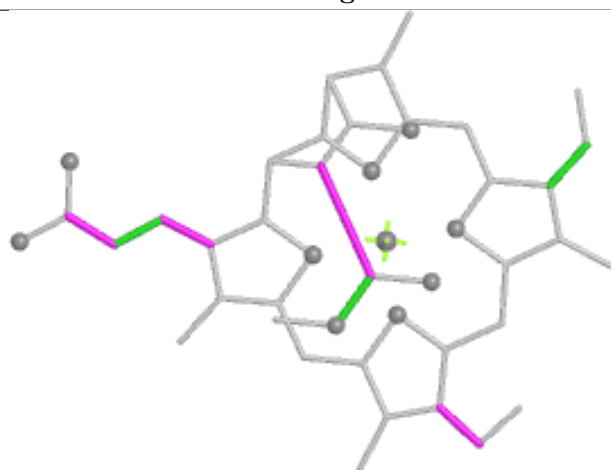
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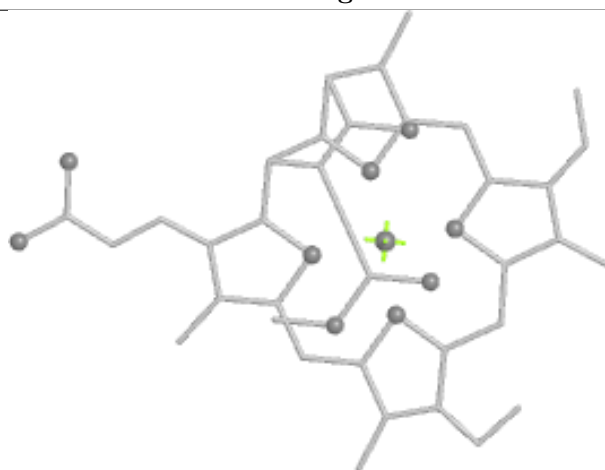
Bond lengths



Bond angles

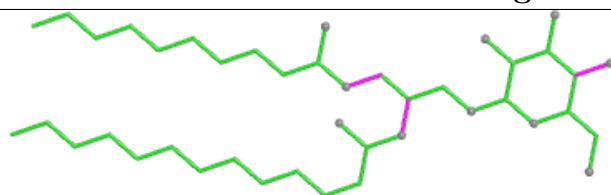


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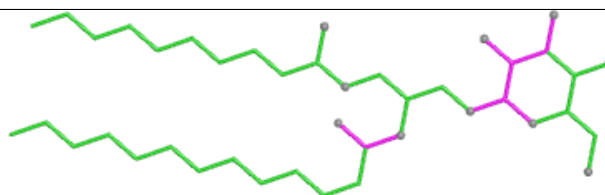


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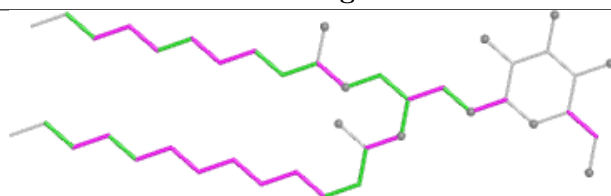
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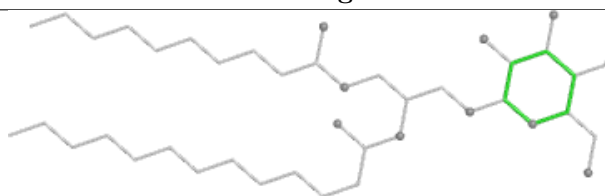
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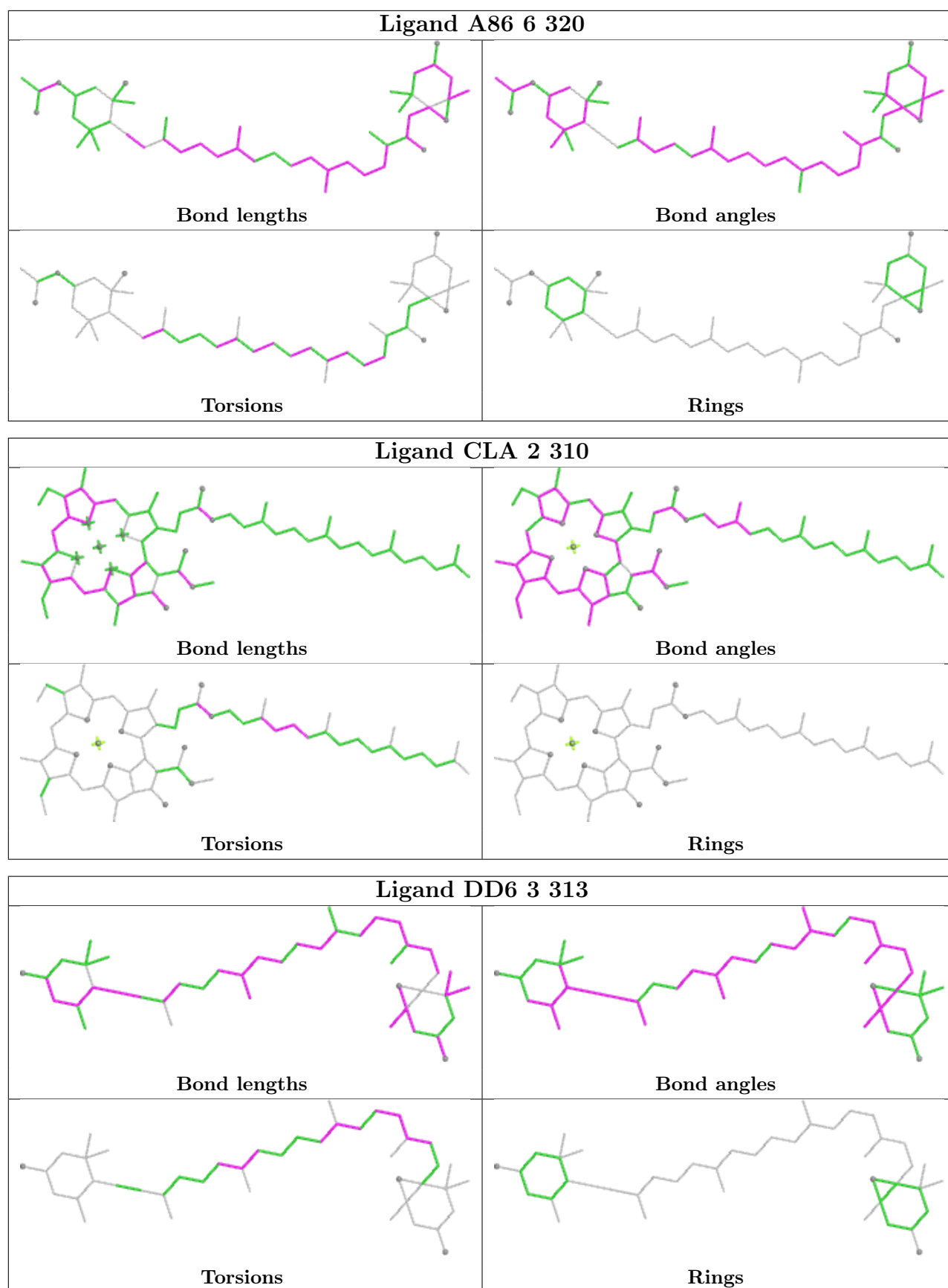
Bond angles



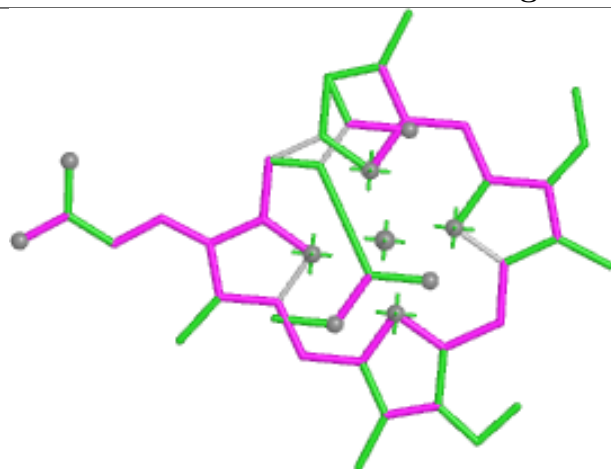
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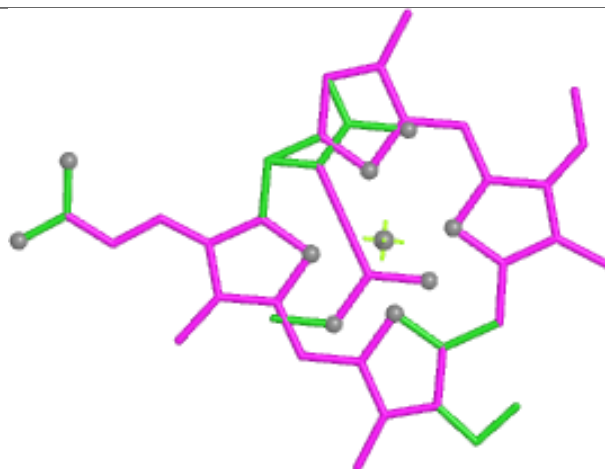
Rings



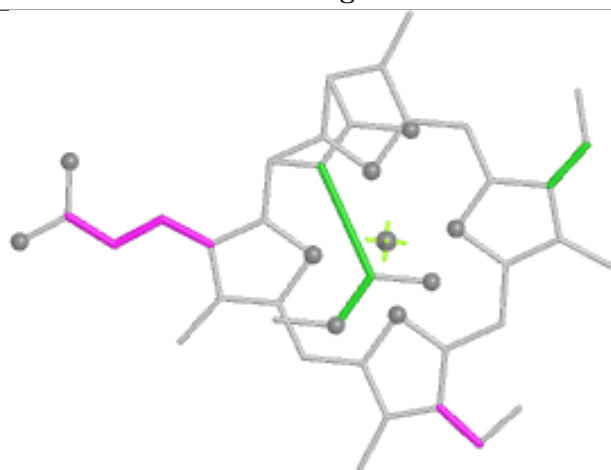
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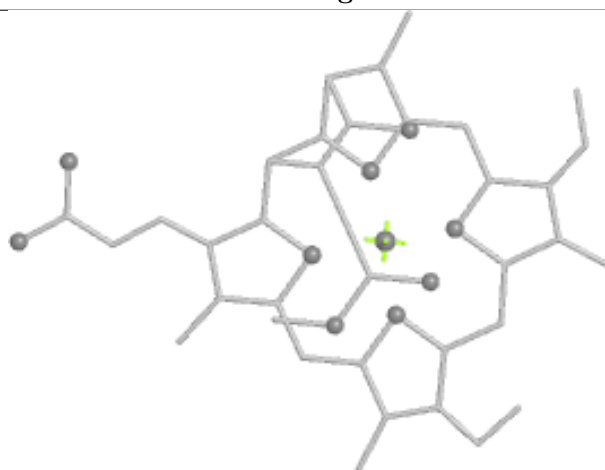
Bond lengths



Bond angles

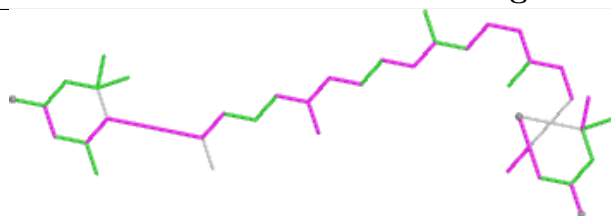


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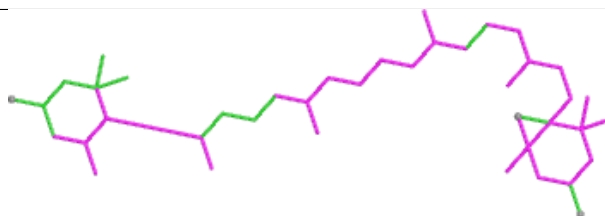


Rings

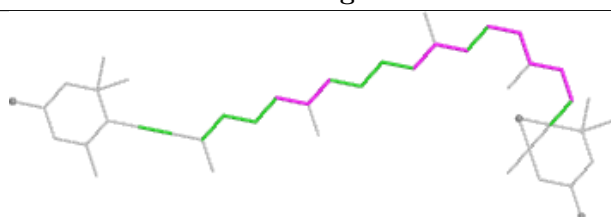
Ligand DD6 12 317



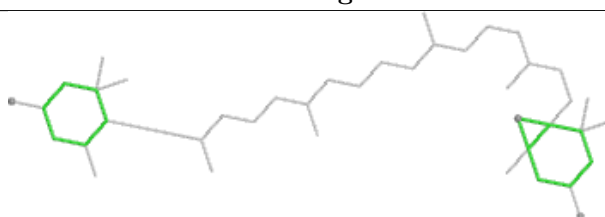
Bond lengths



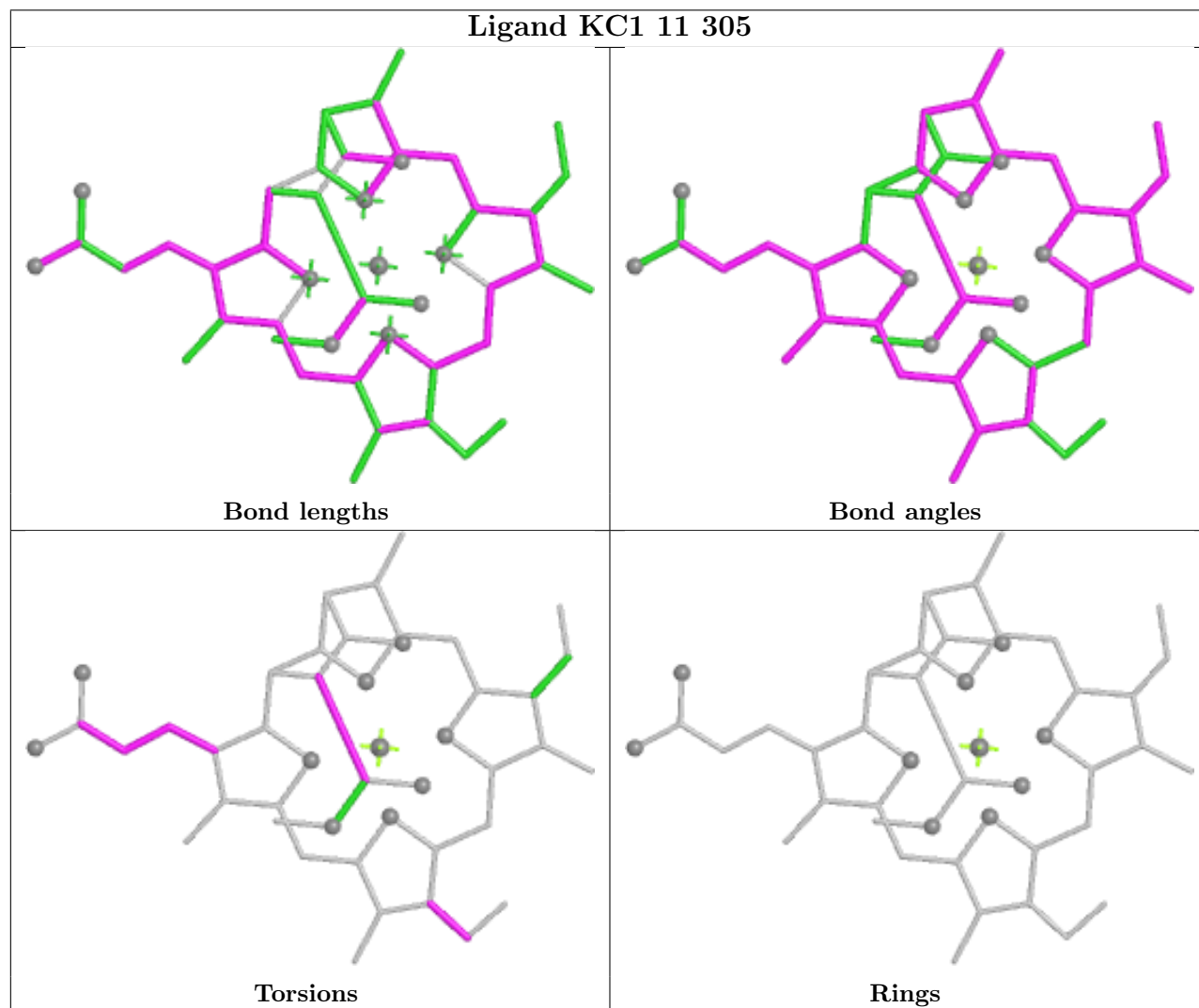
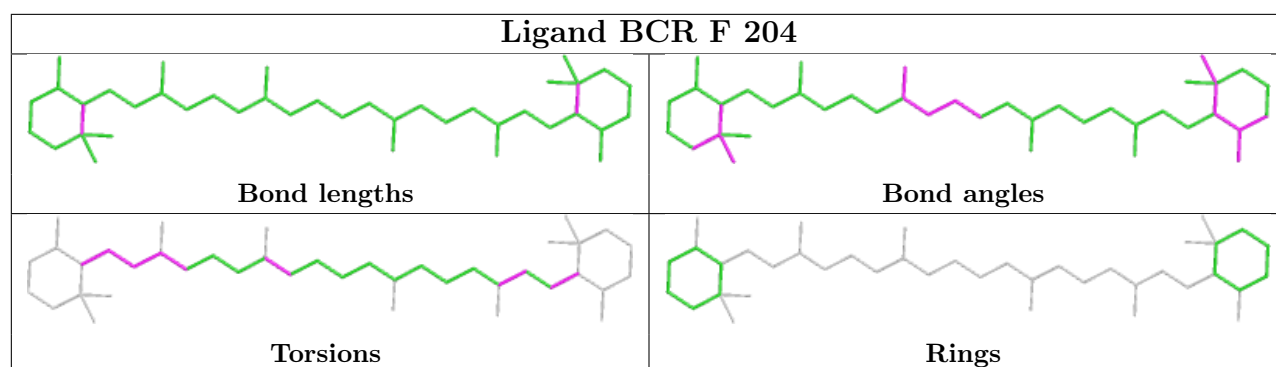
Bond angles



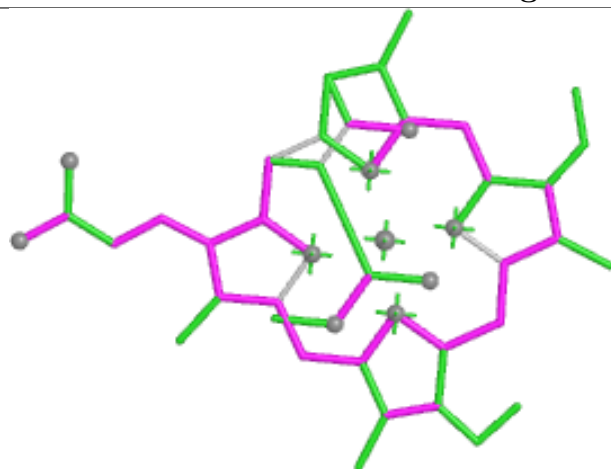
Torsions



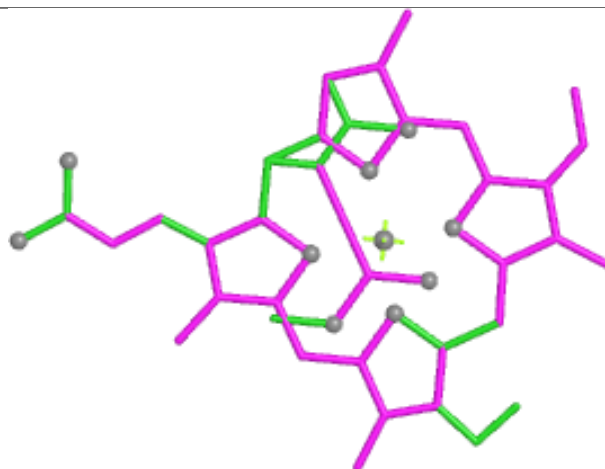
Rings



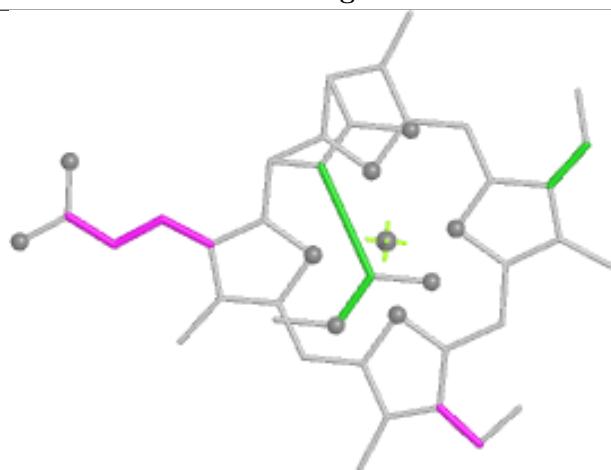
Ligand KC1 6 308



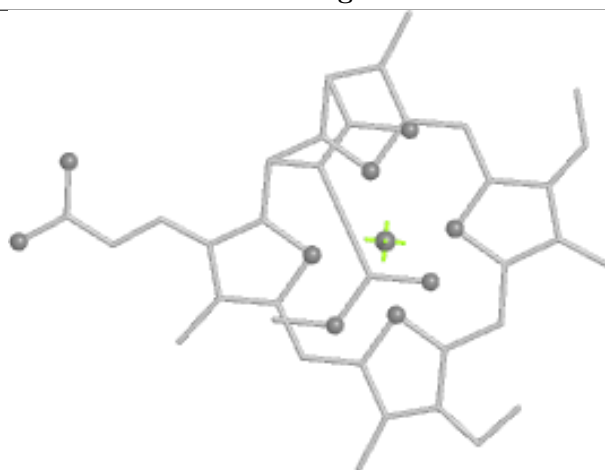
Bond lengths



Bond angles

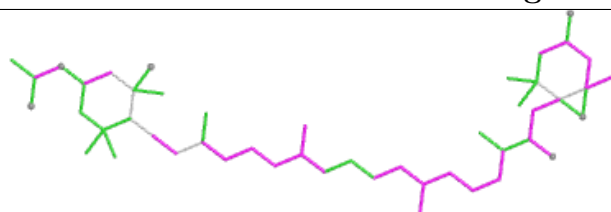


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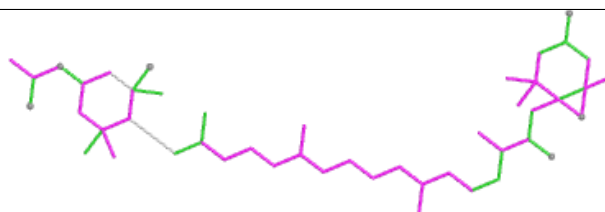


Rings

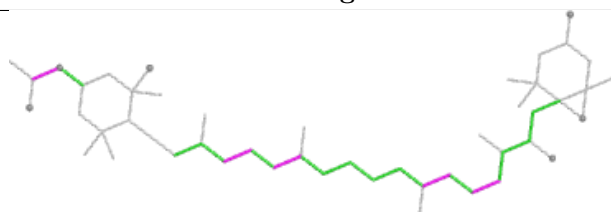
Ligand A86 9 313



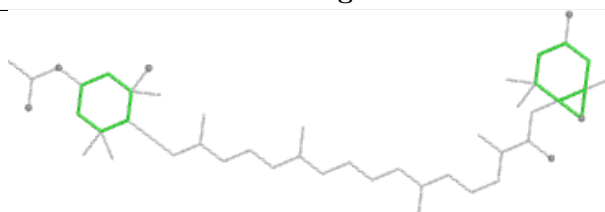
Bond lengths



Bond angles

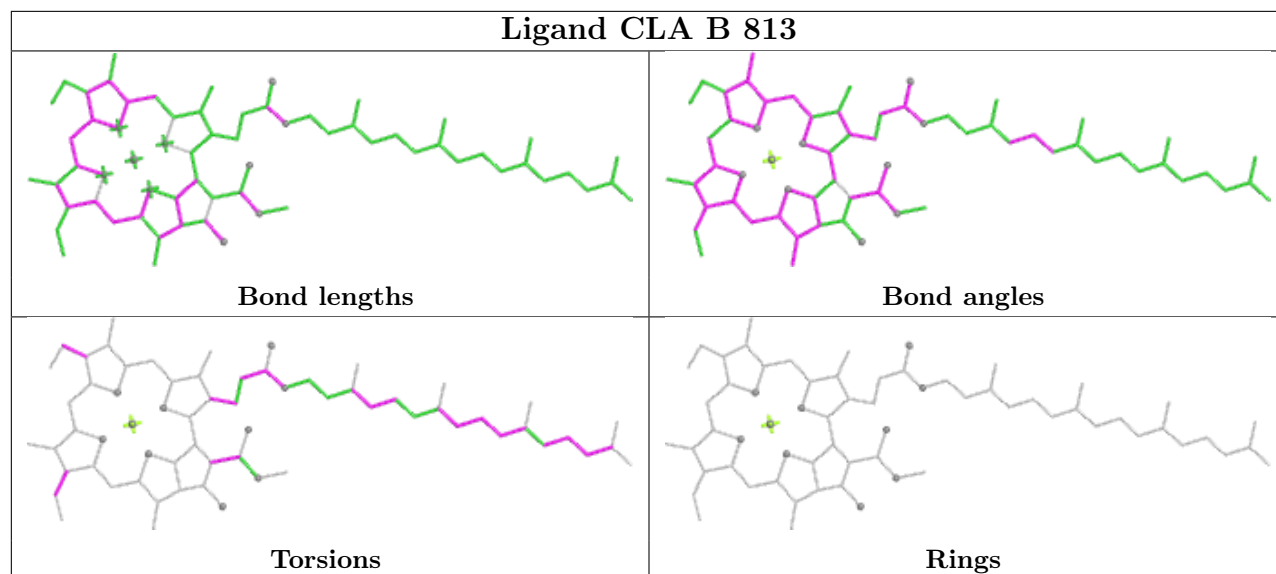


Torsions

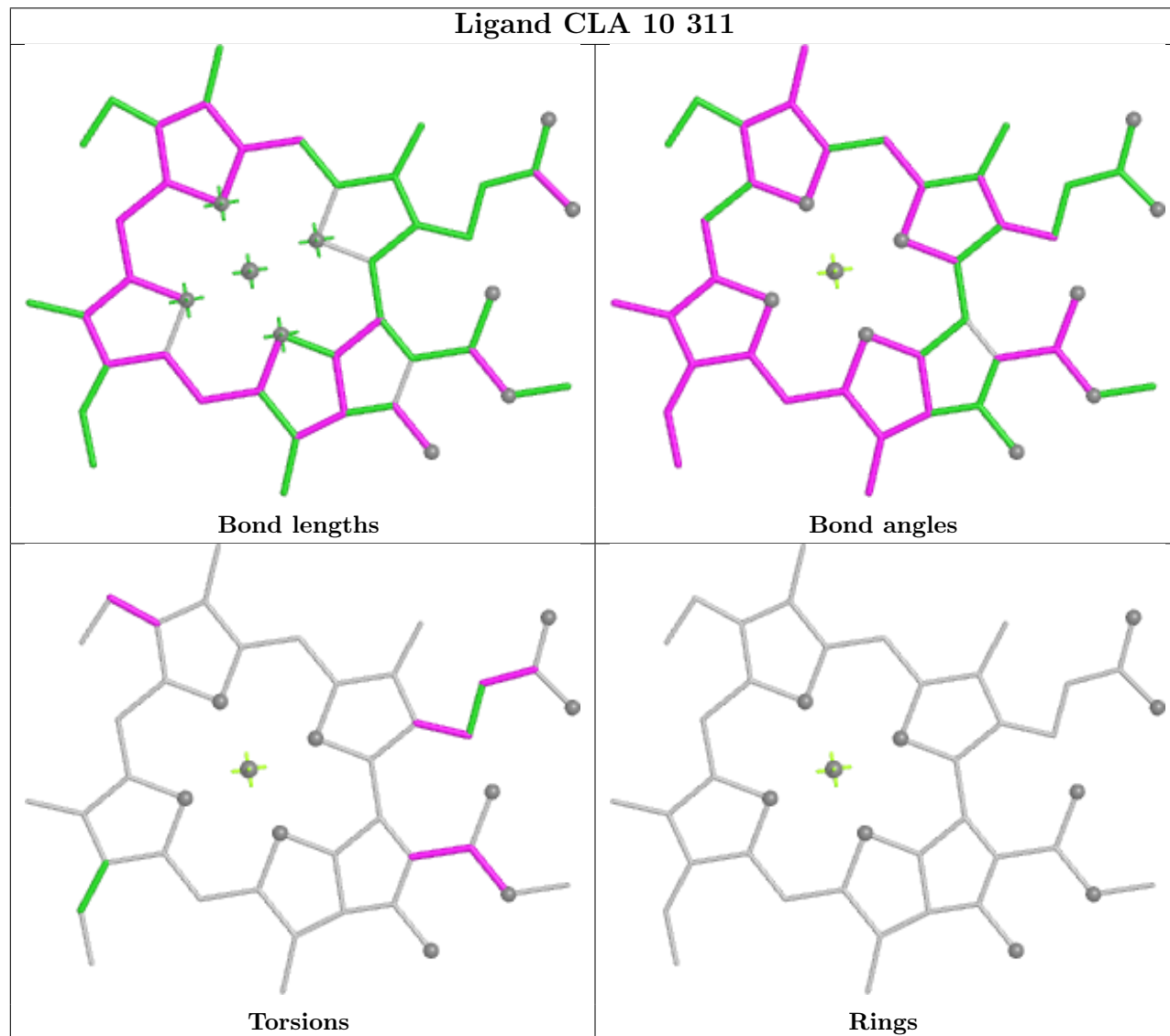


Rings

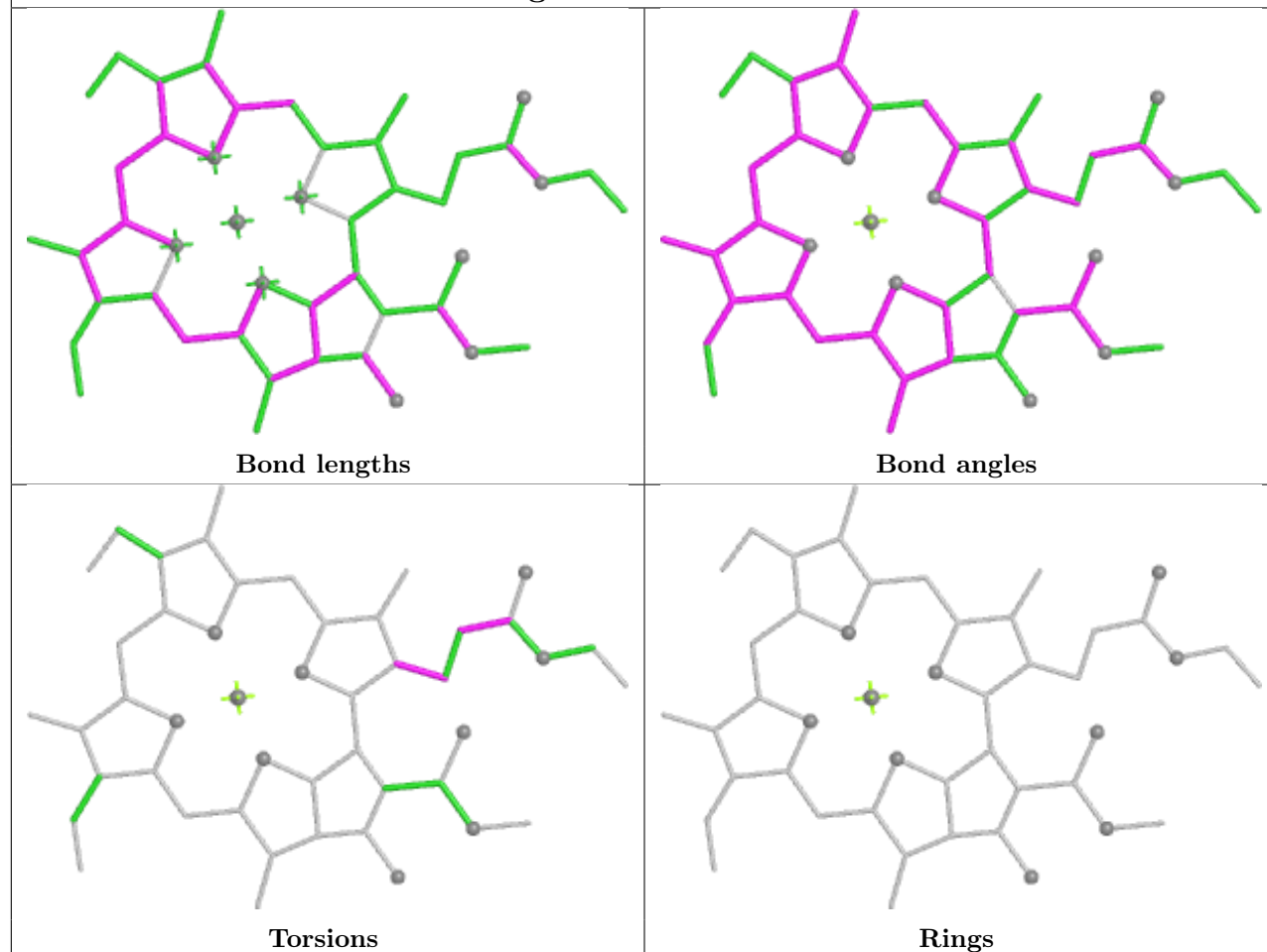
Ligand CLA B 813



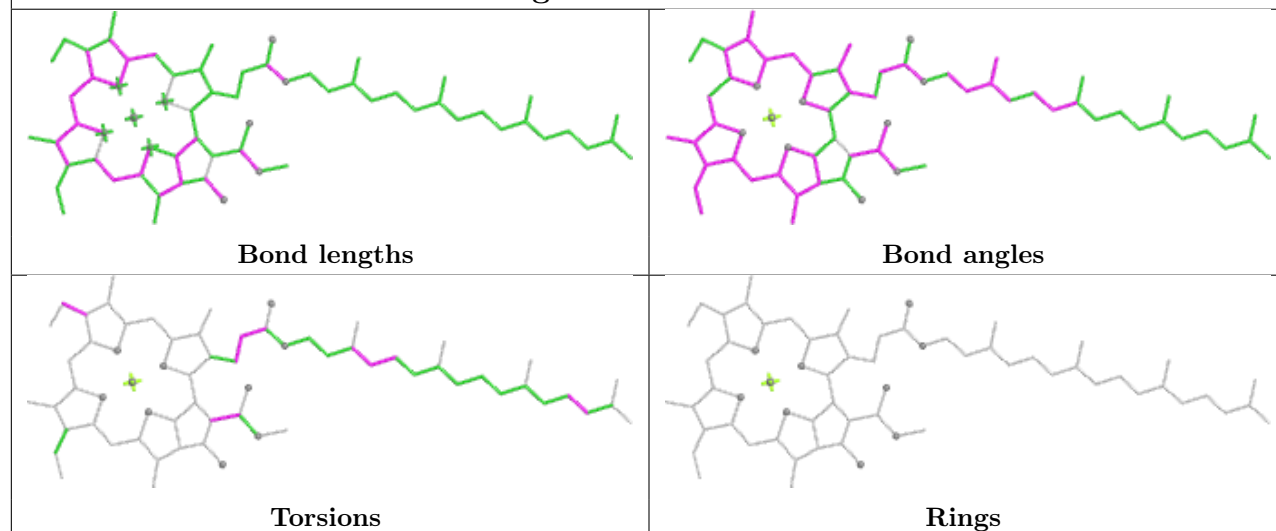
Ligand CLA 10 311

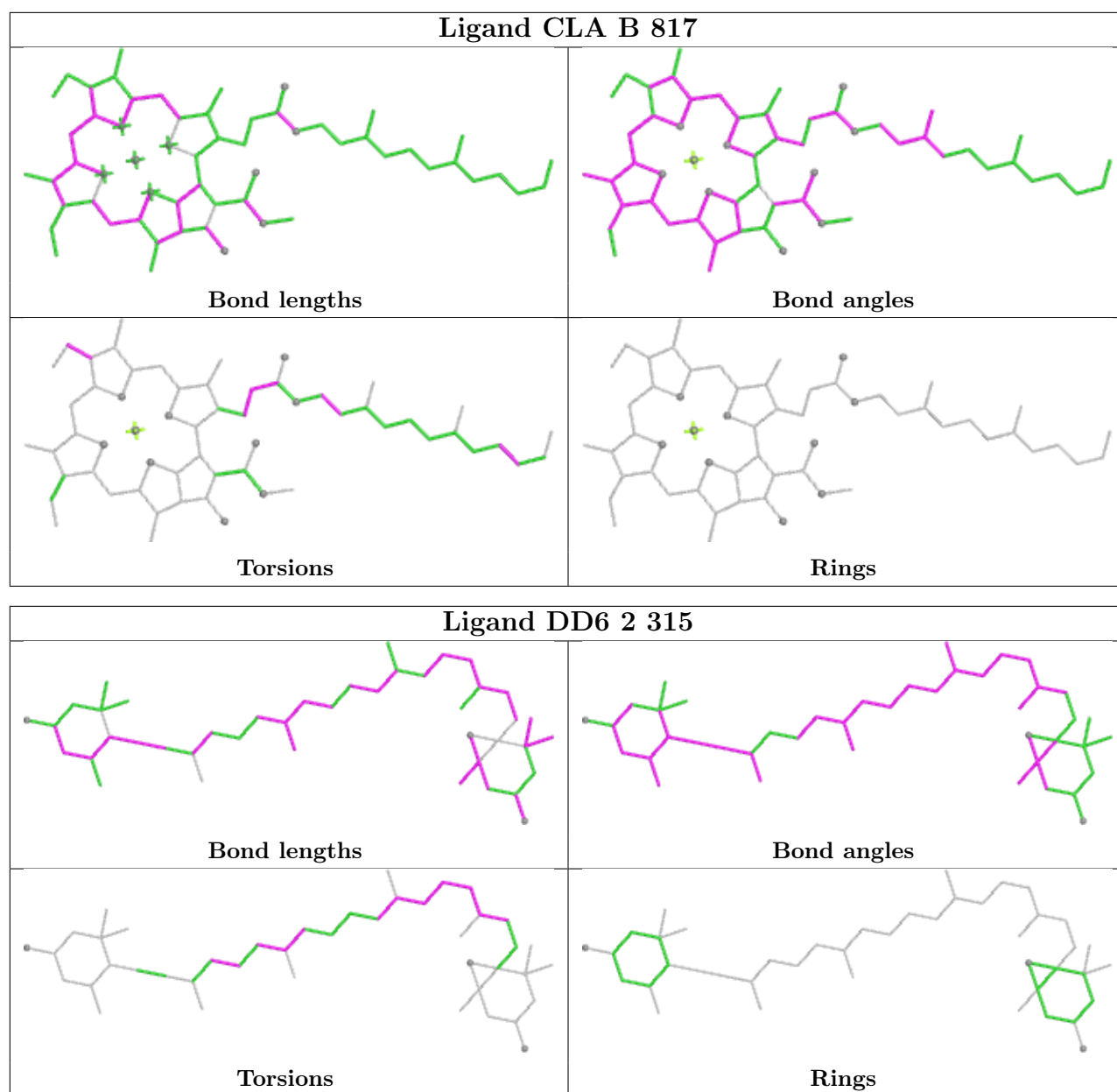


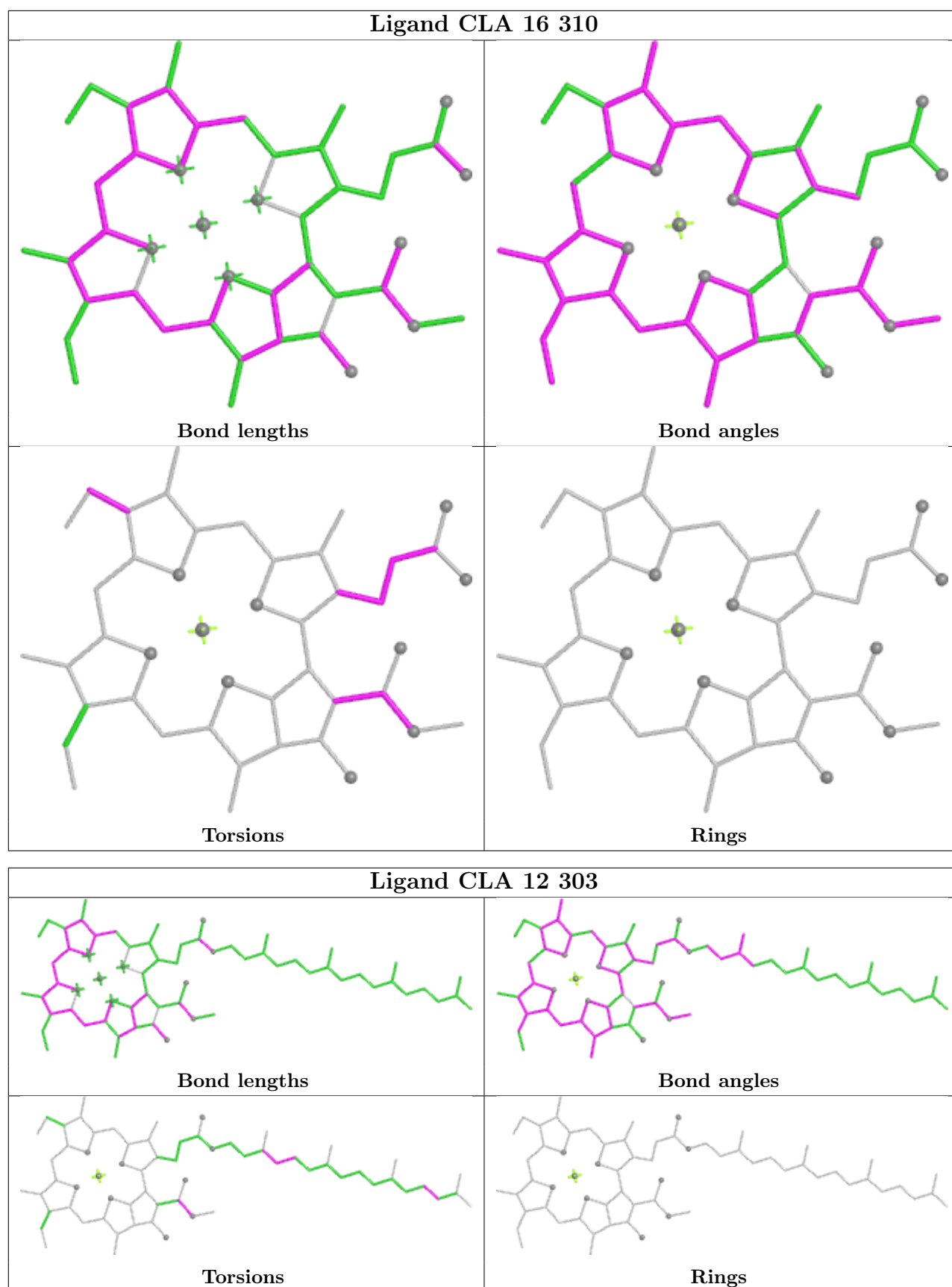
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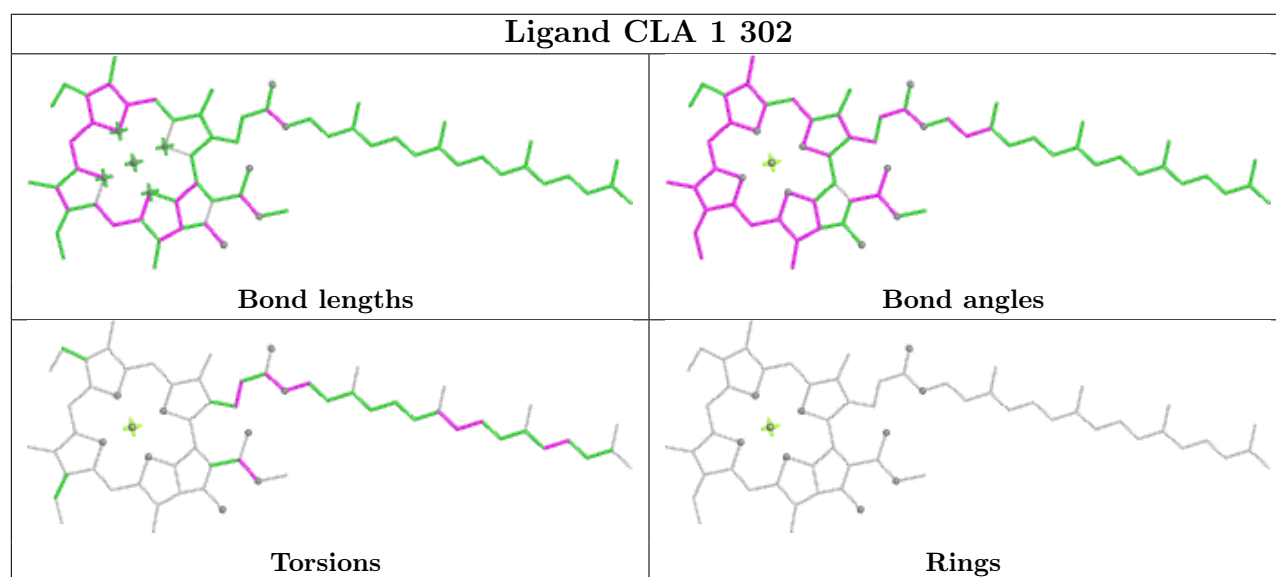
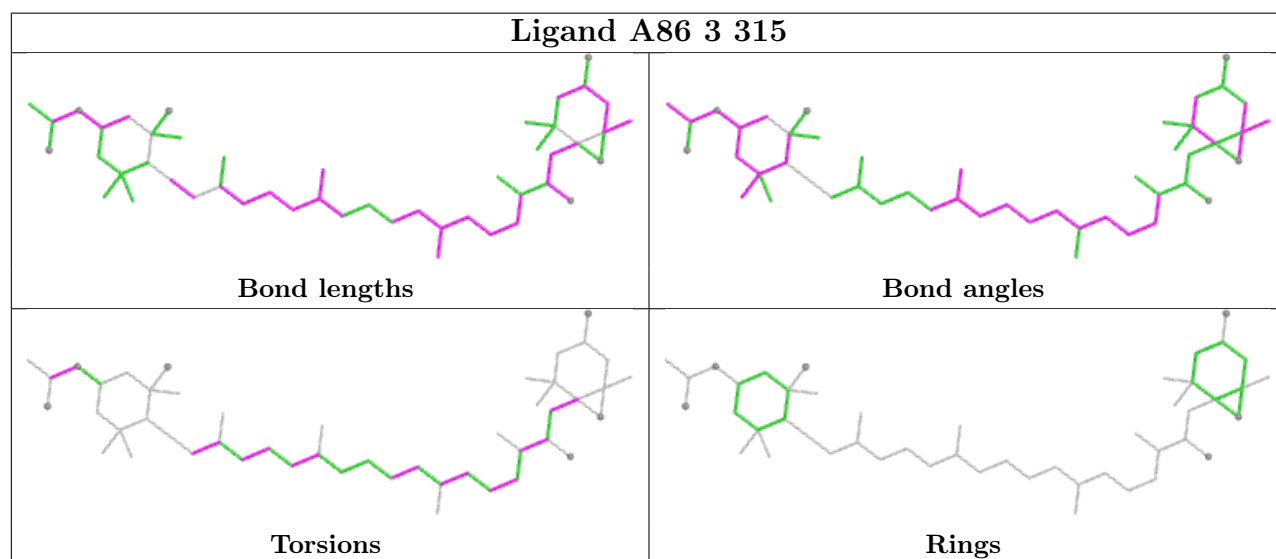
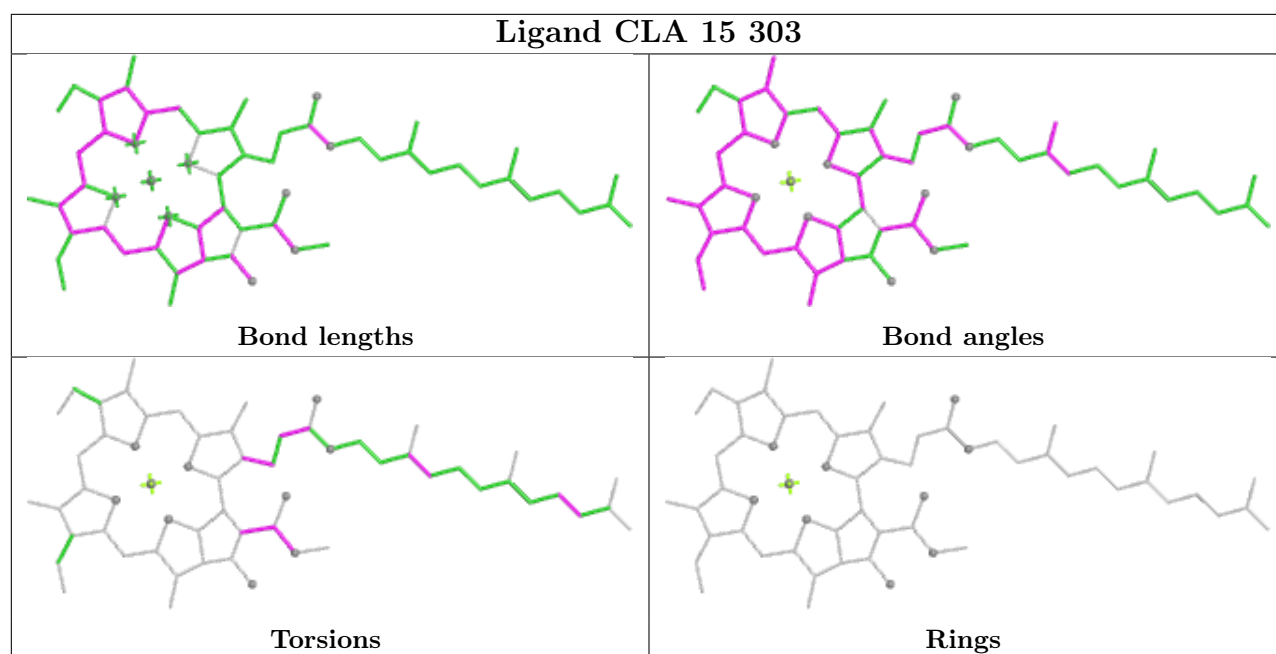


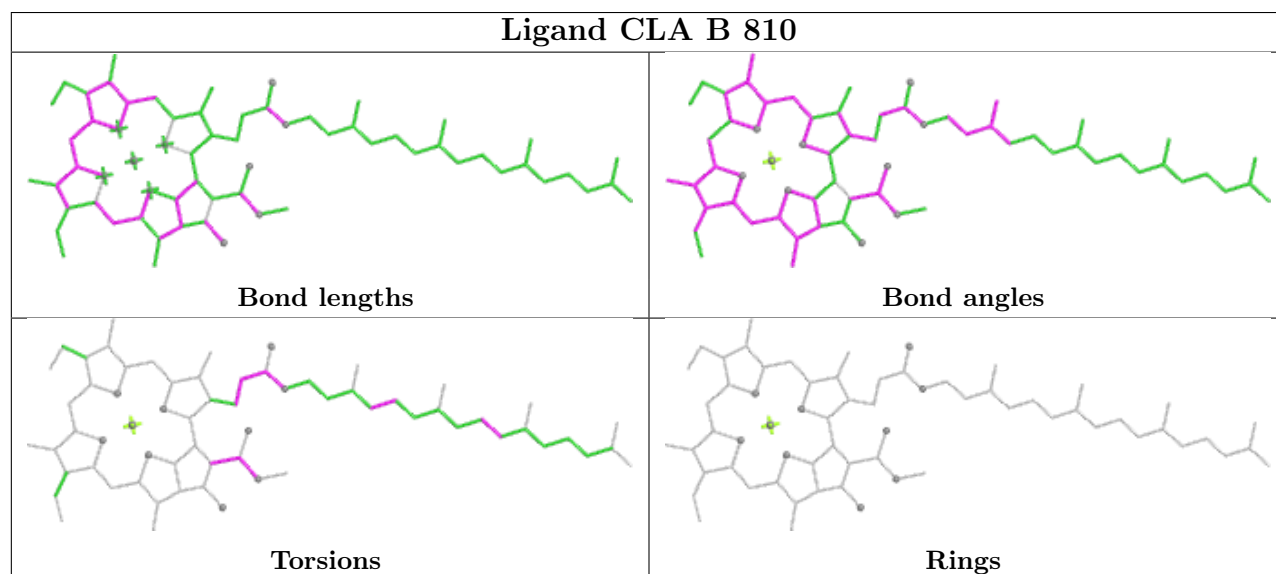
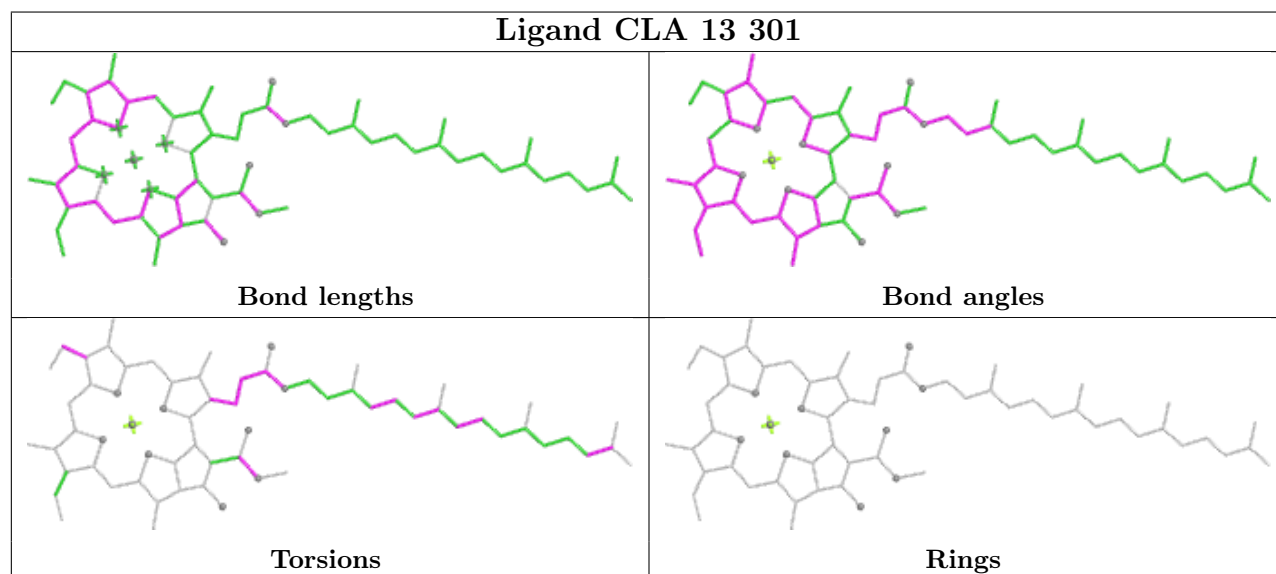
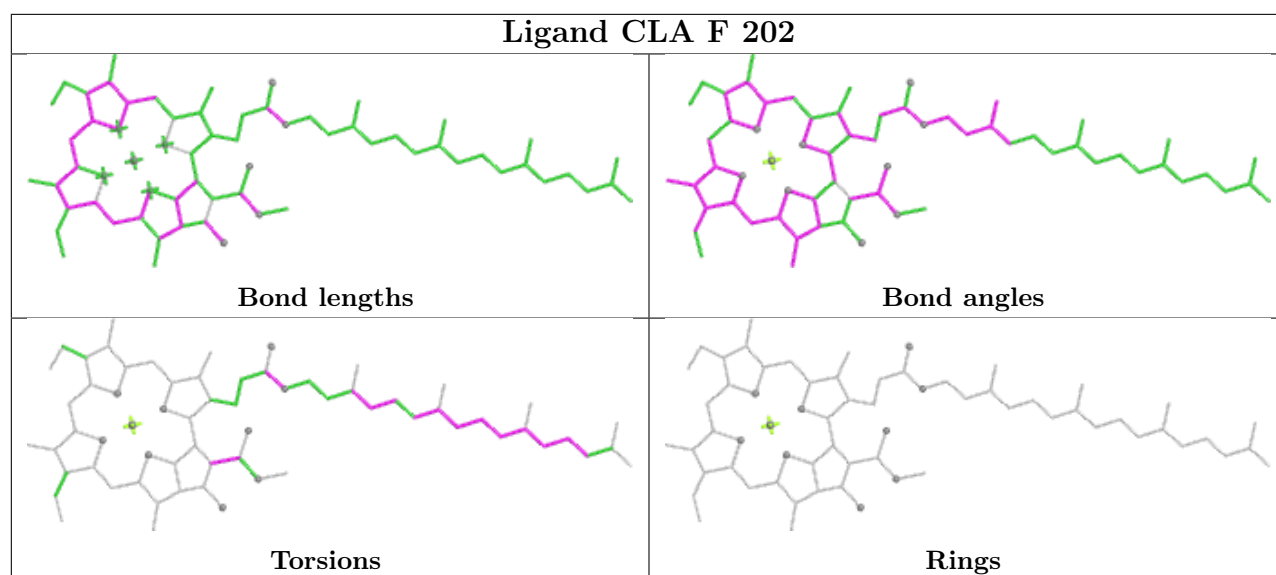
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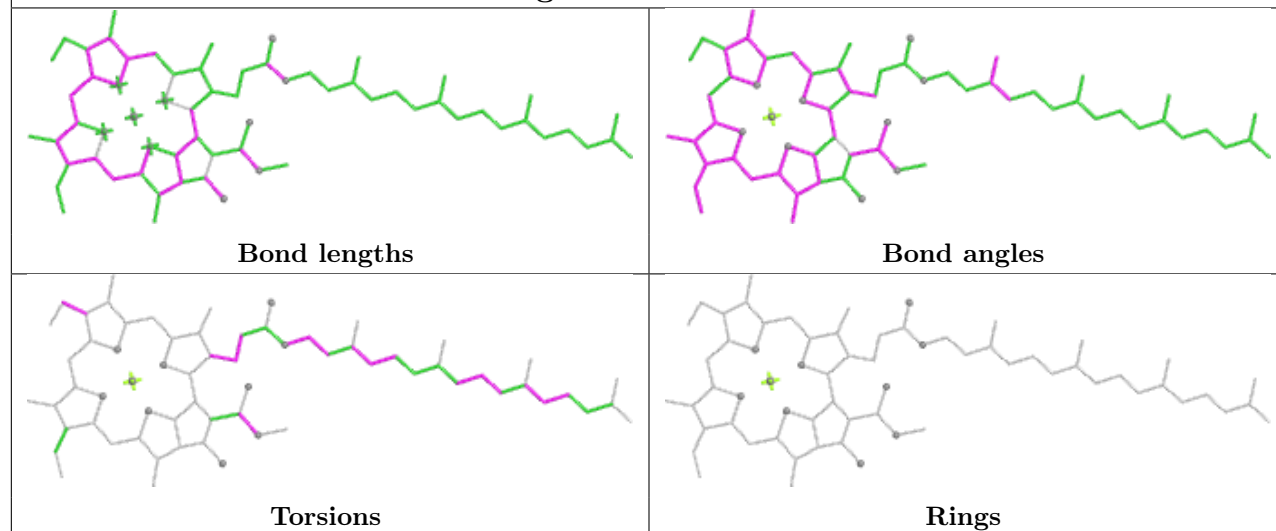
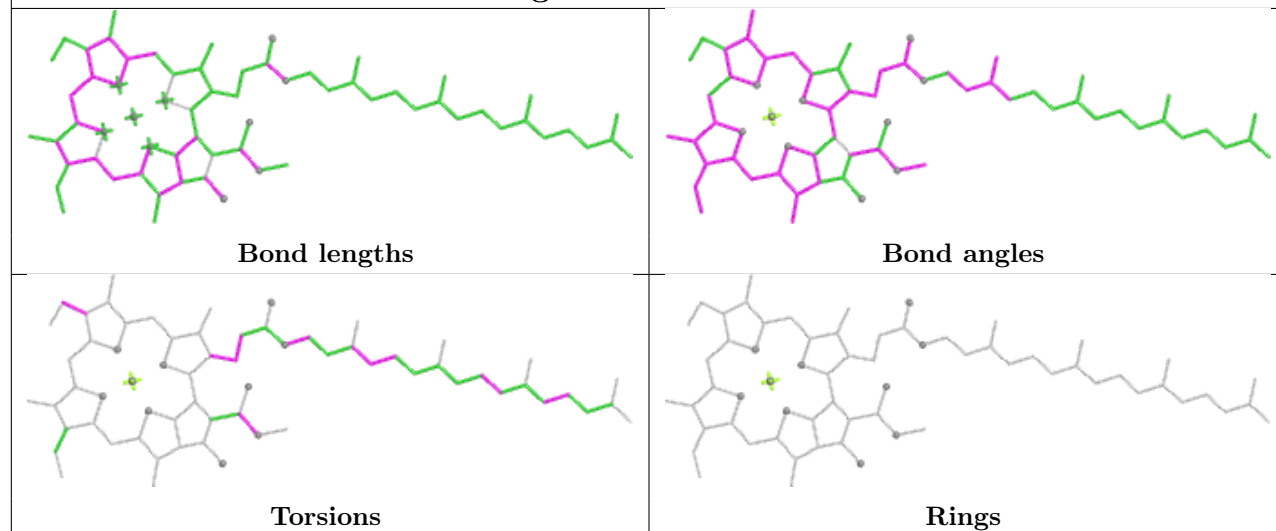
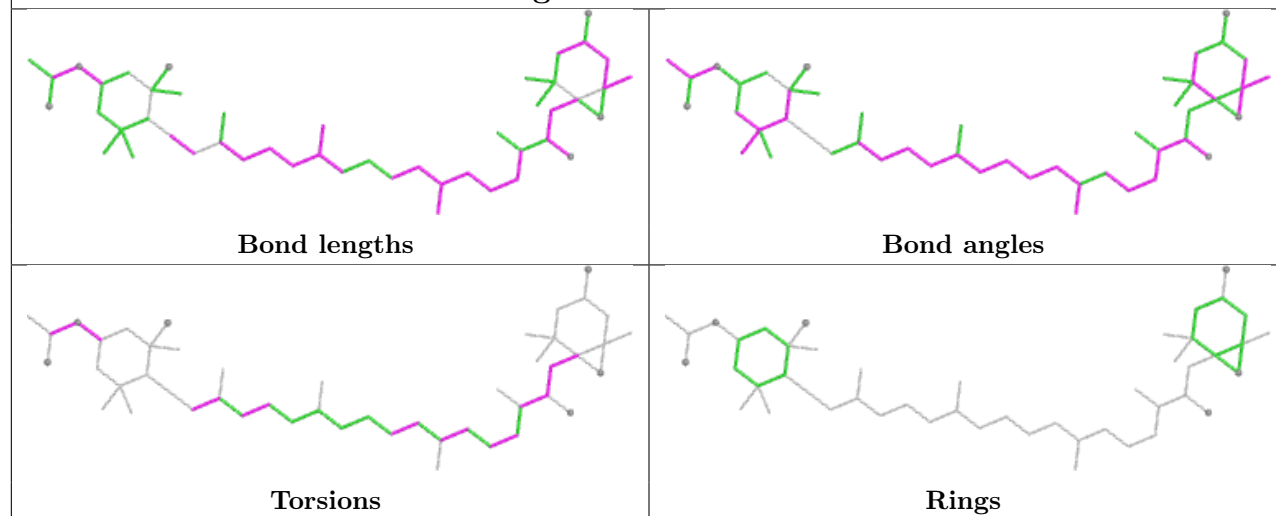




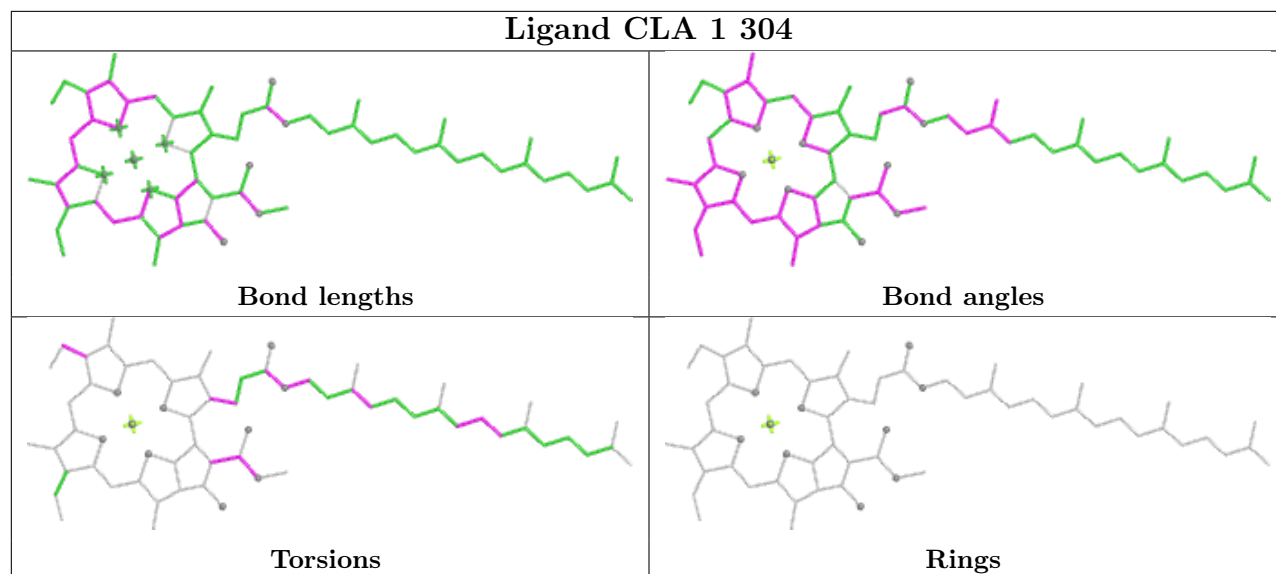




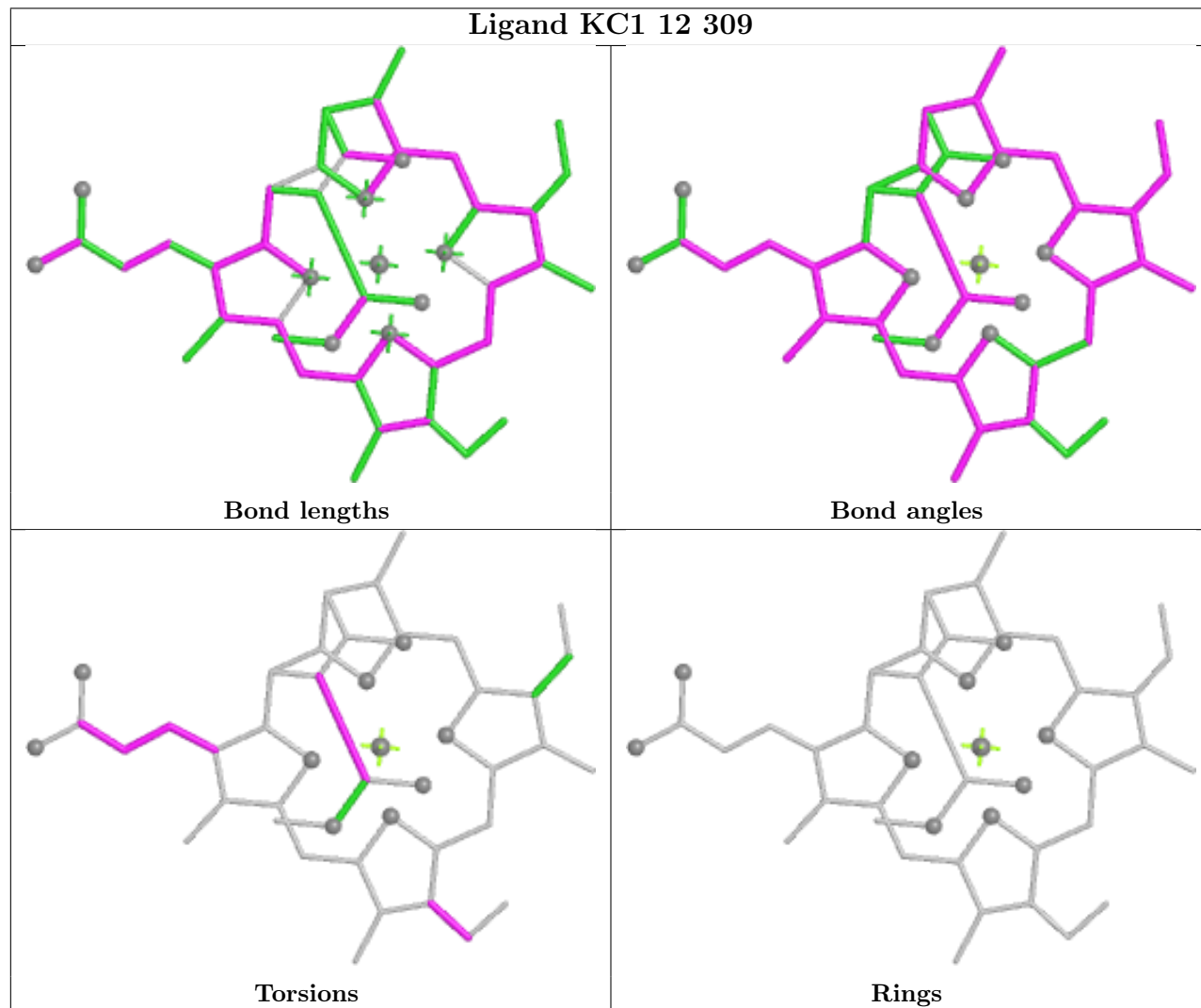


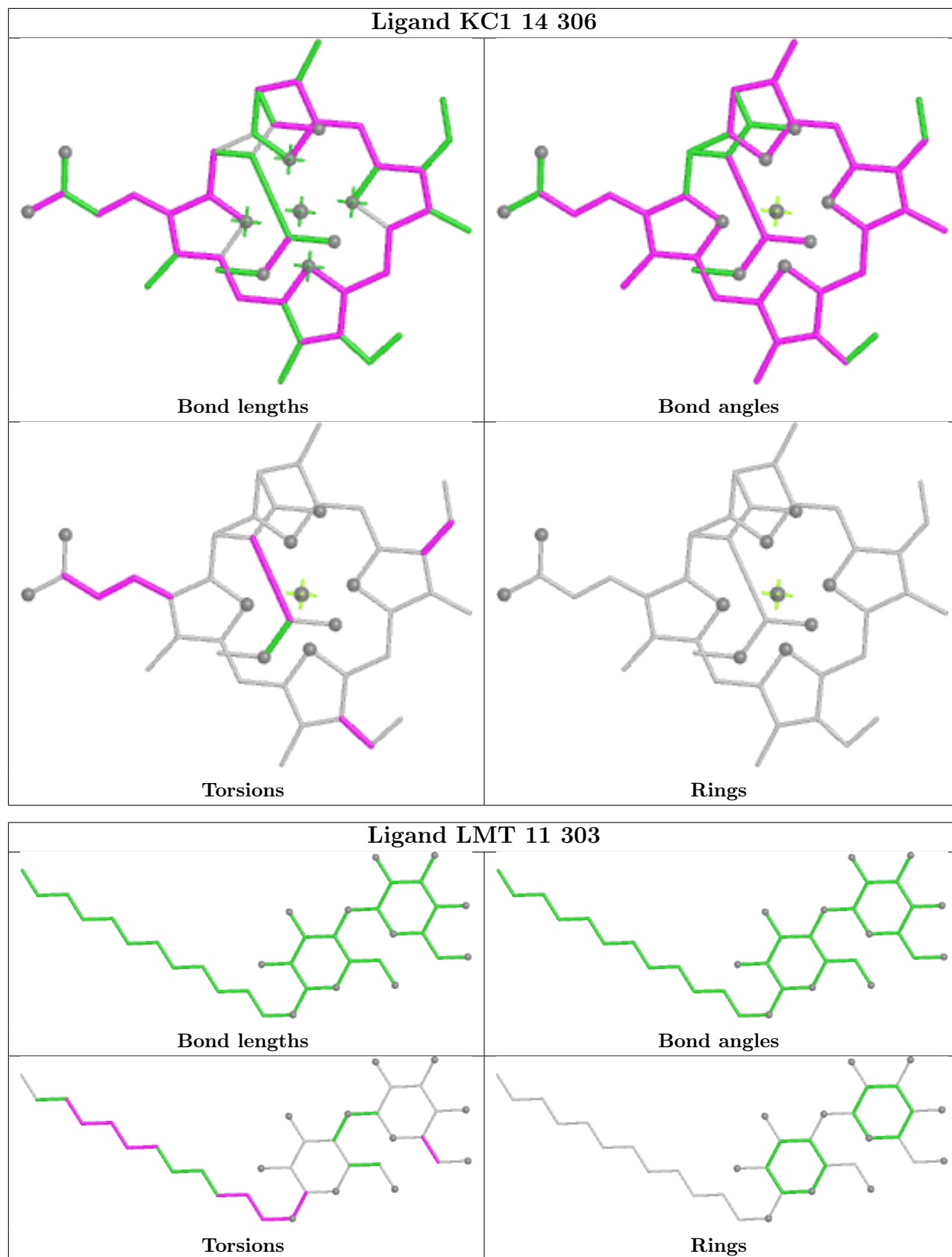
Ligand CLA 6 317**Ligand CLA A 810****Ligand A86 12 316**

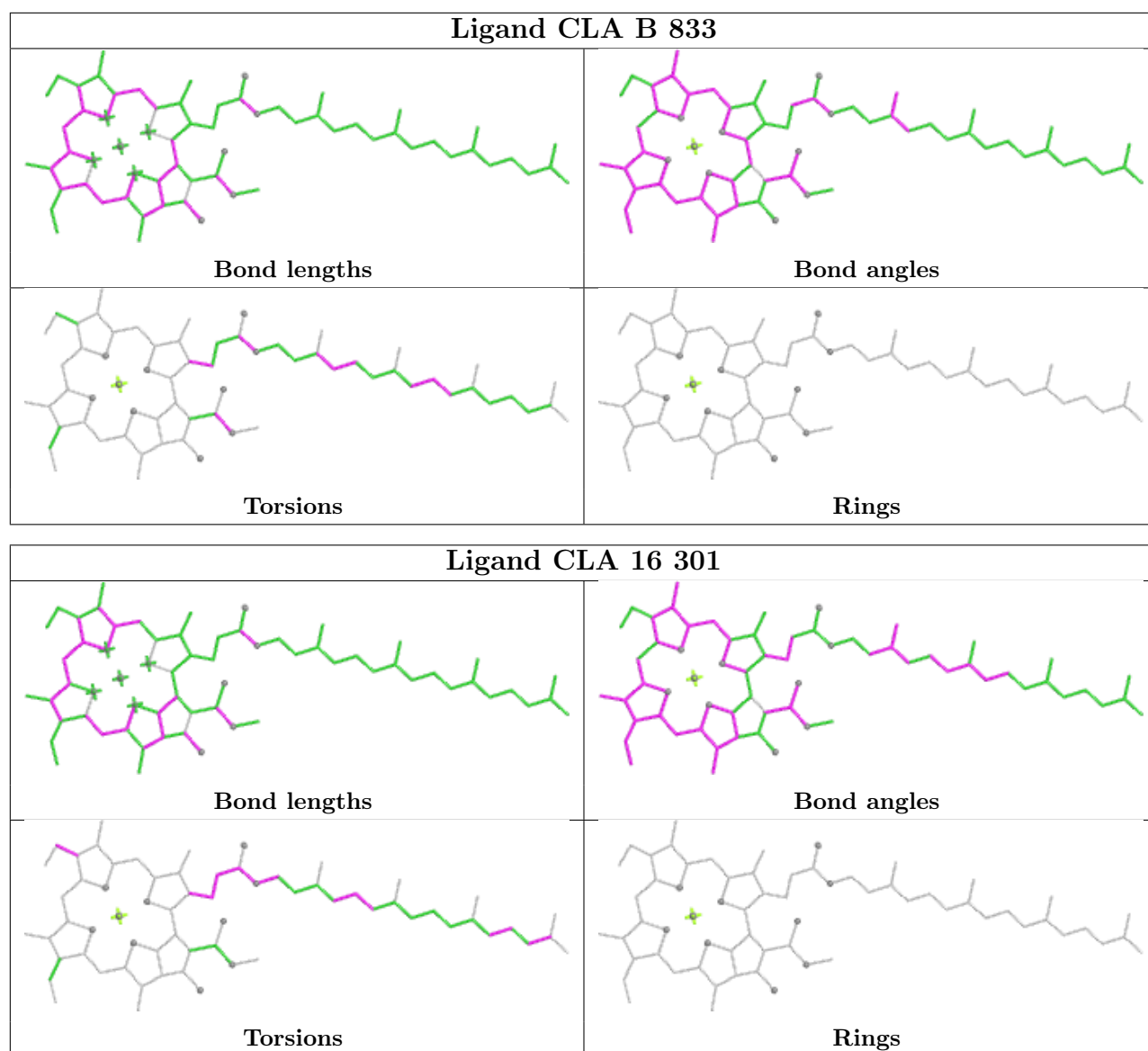
Ligand CLA 1 304

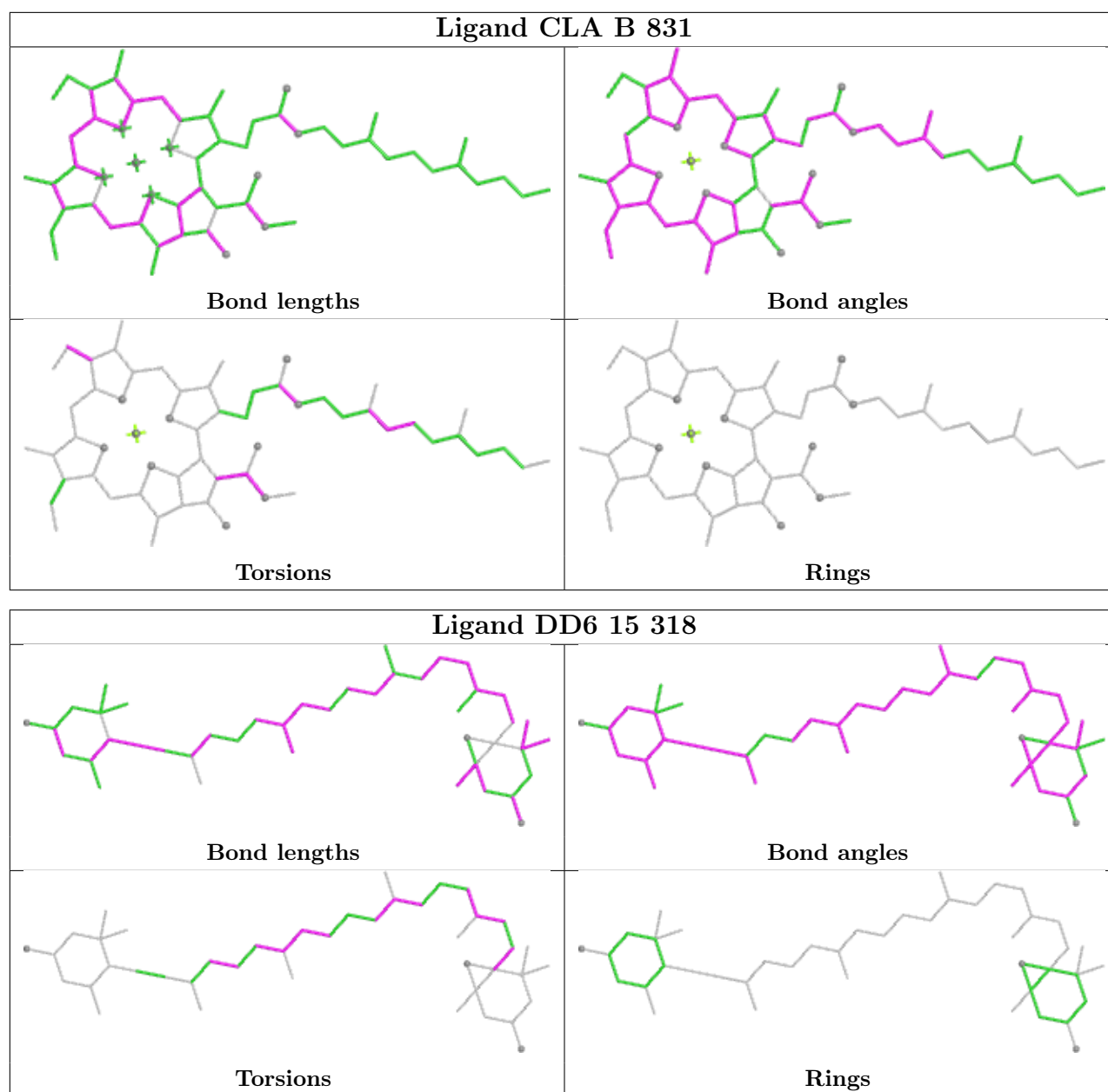


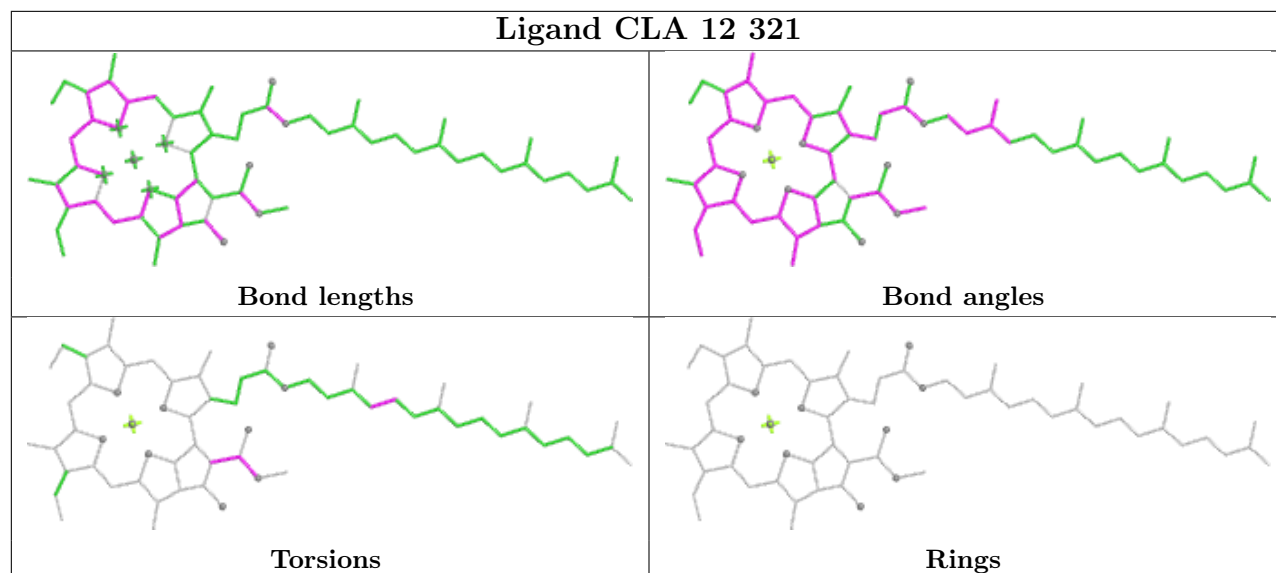
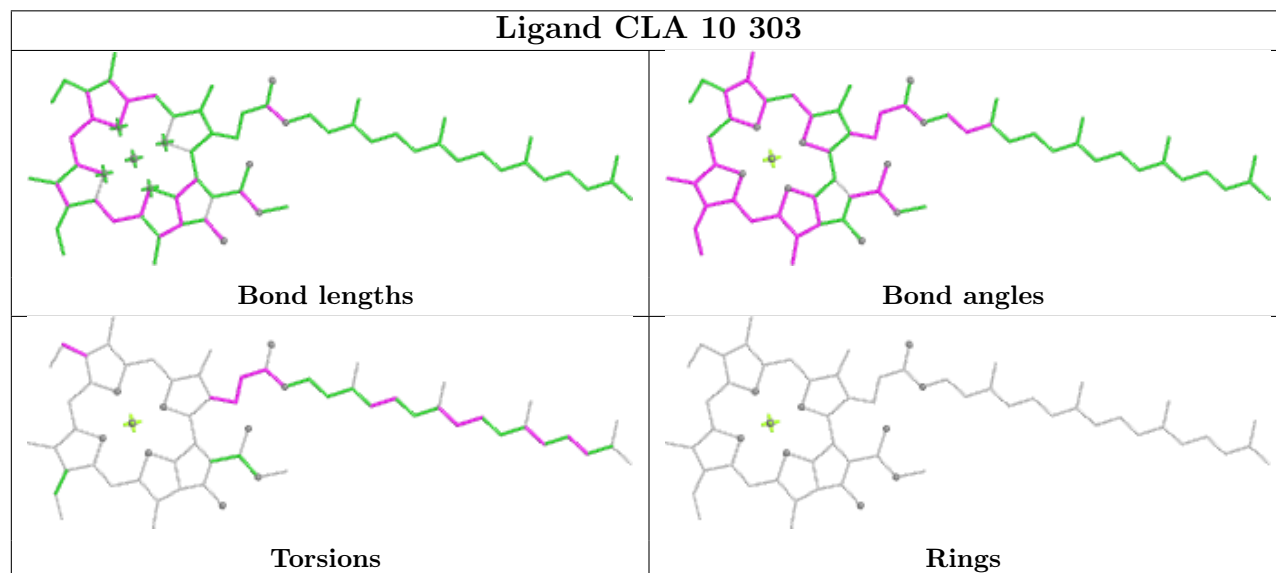
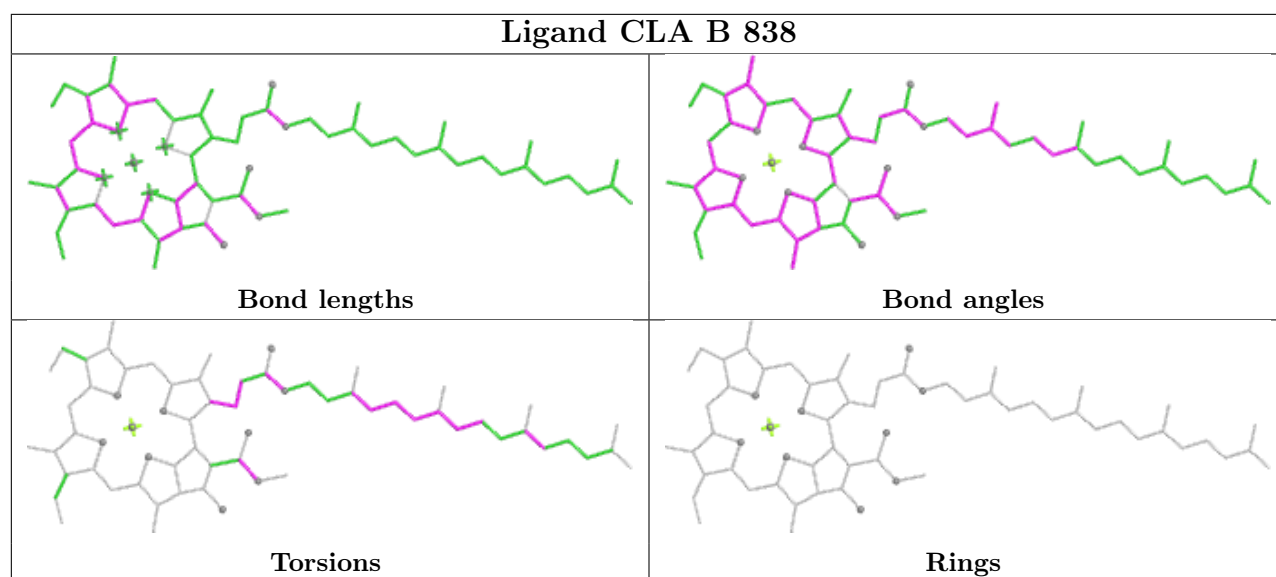
Ligand KC1 12 309



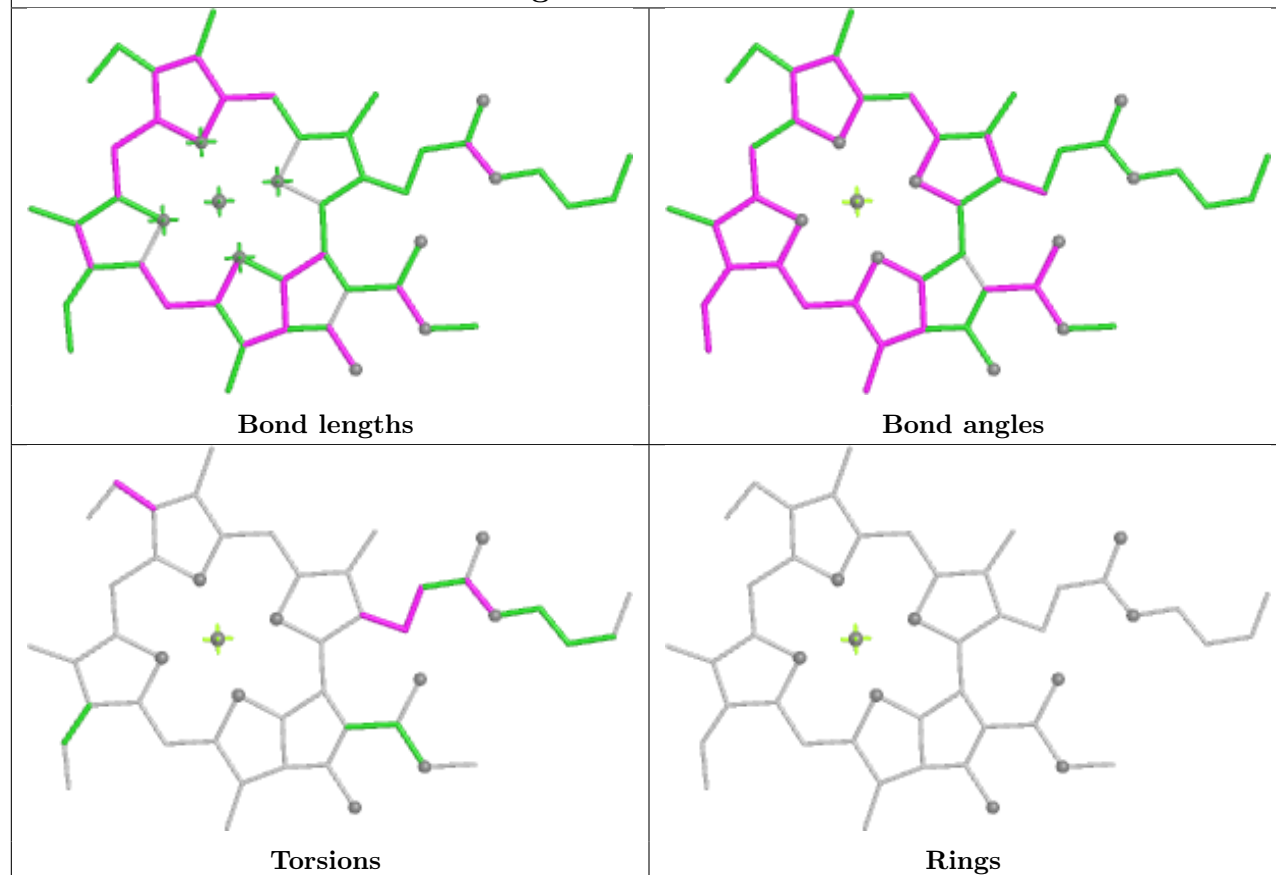




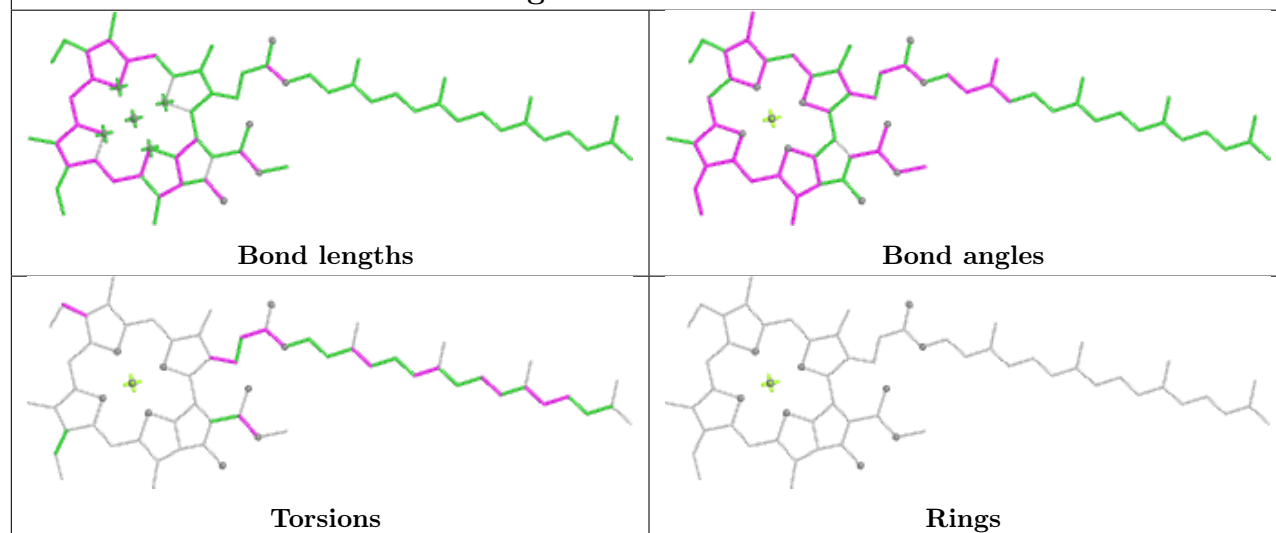


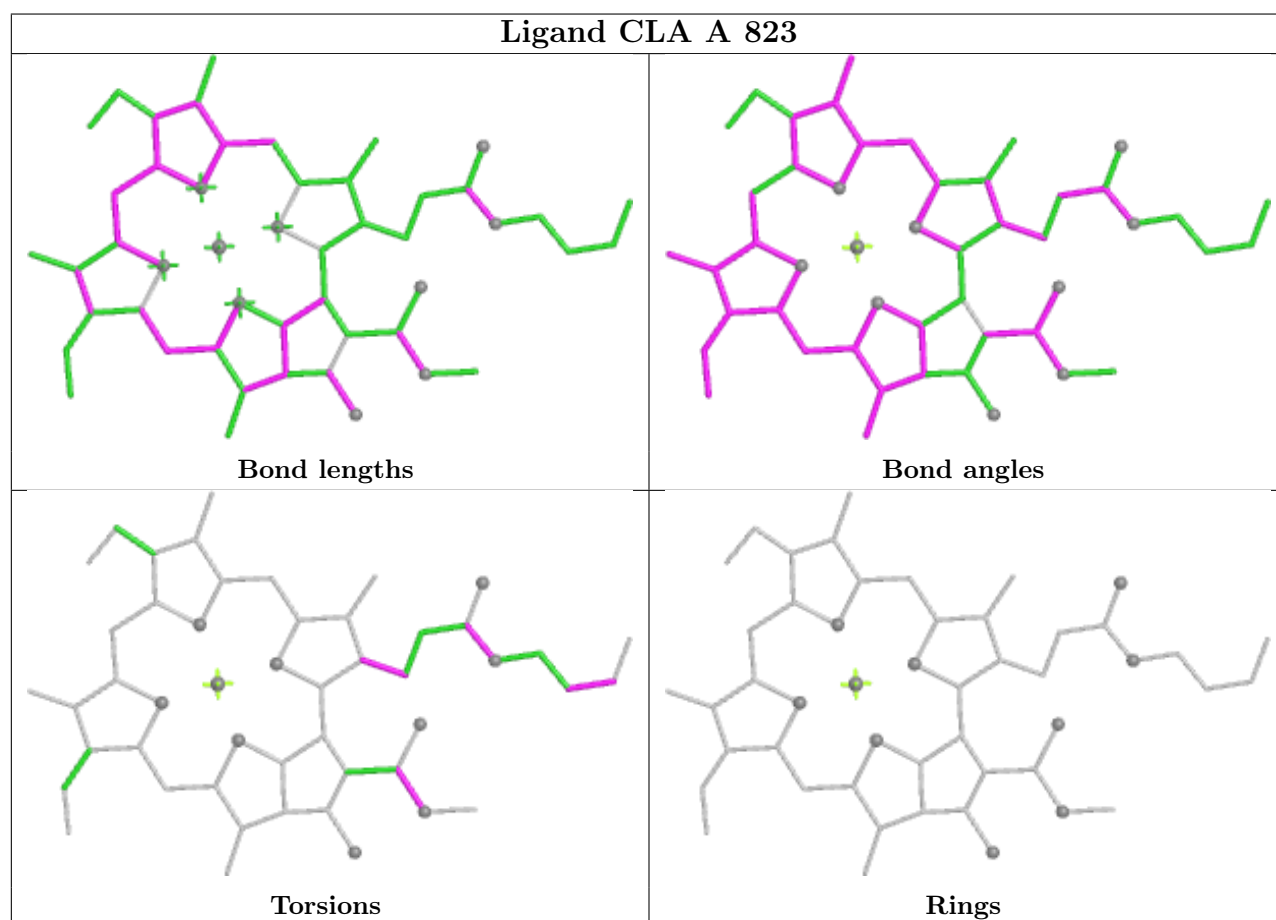
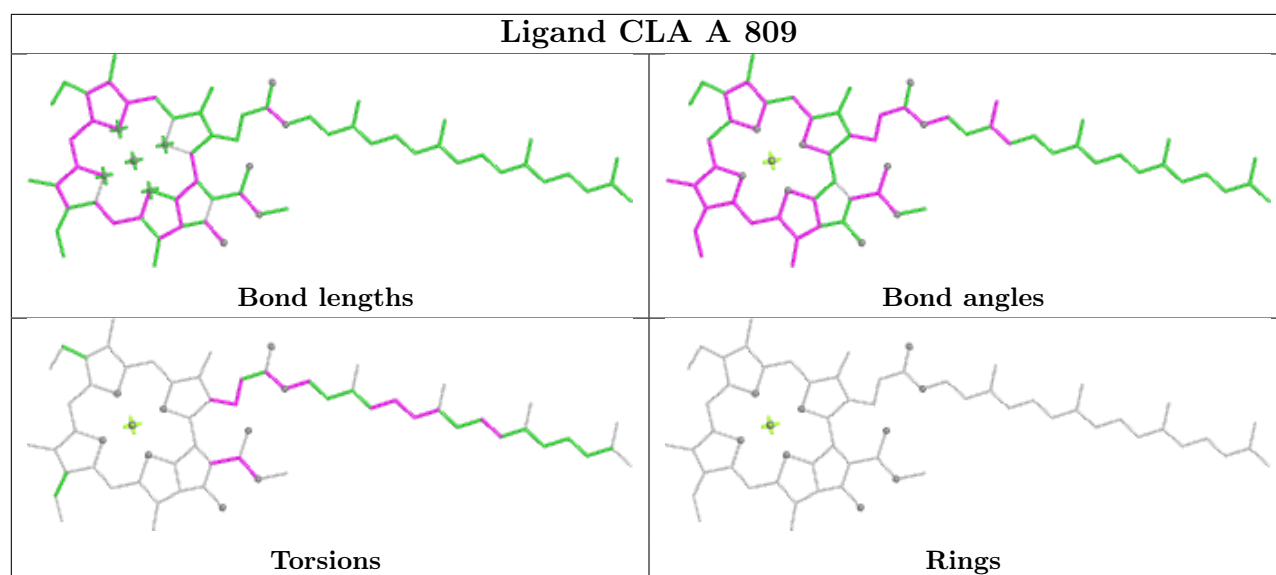


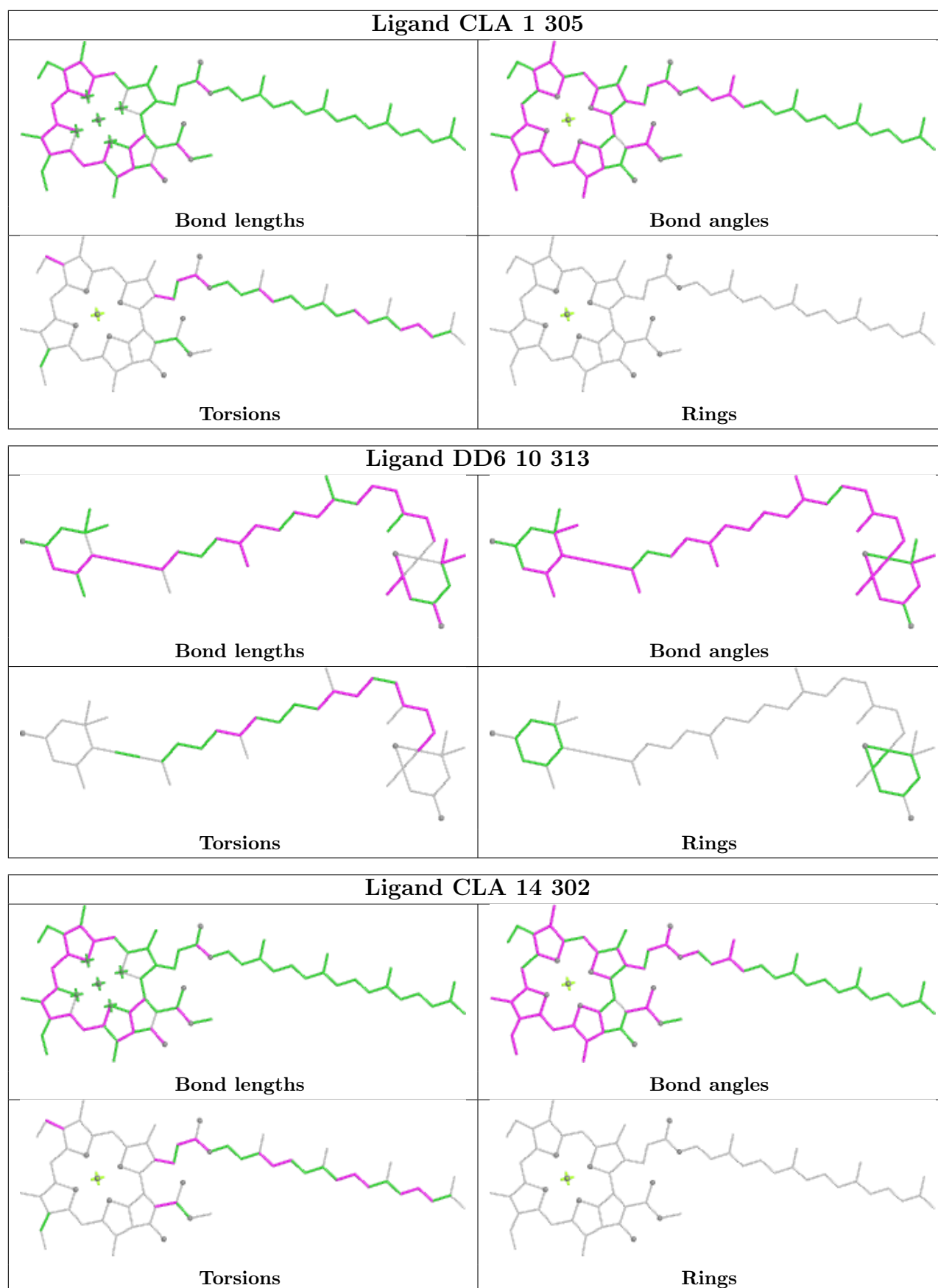
Ligand CLA A 817



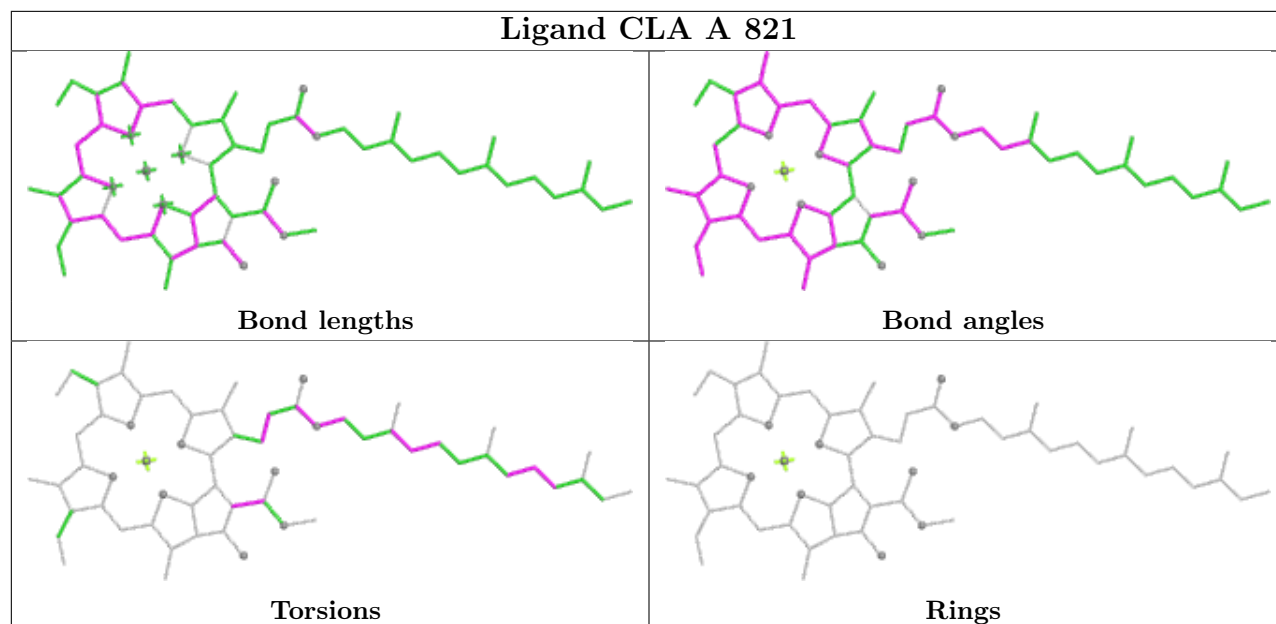
Ligand CLA 11 310



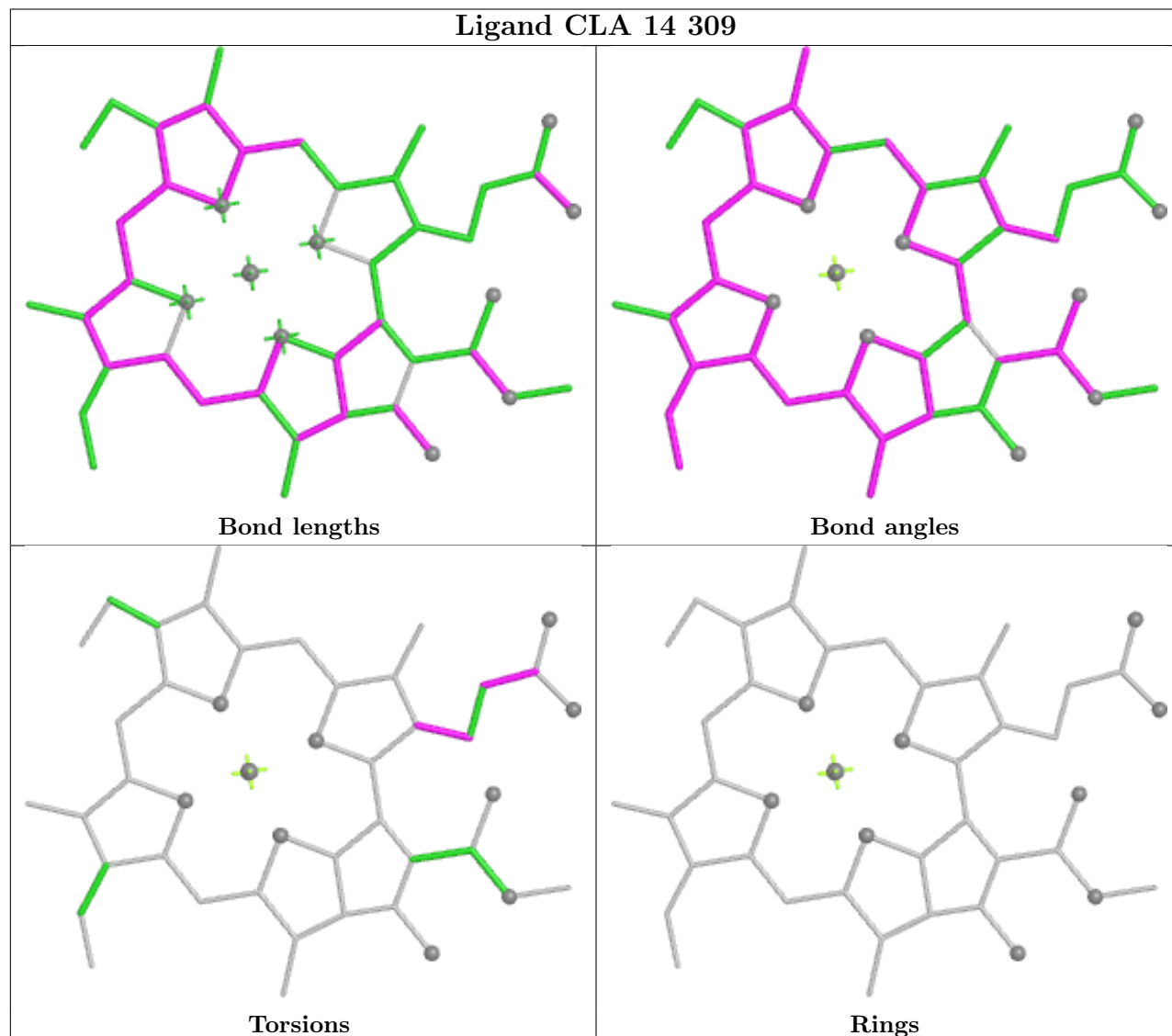


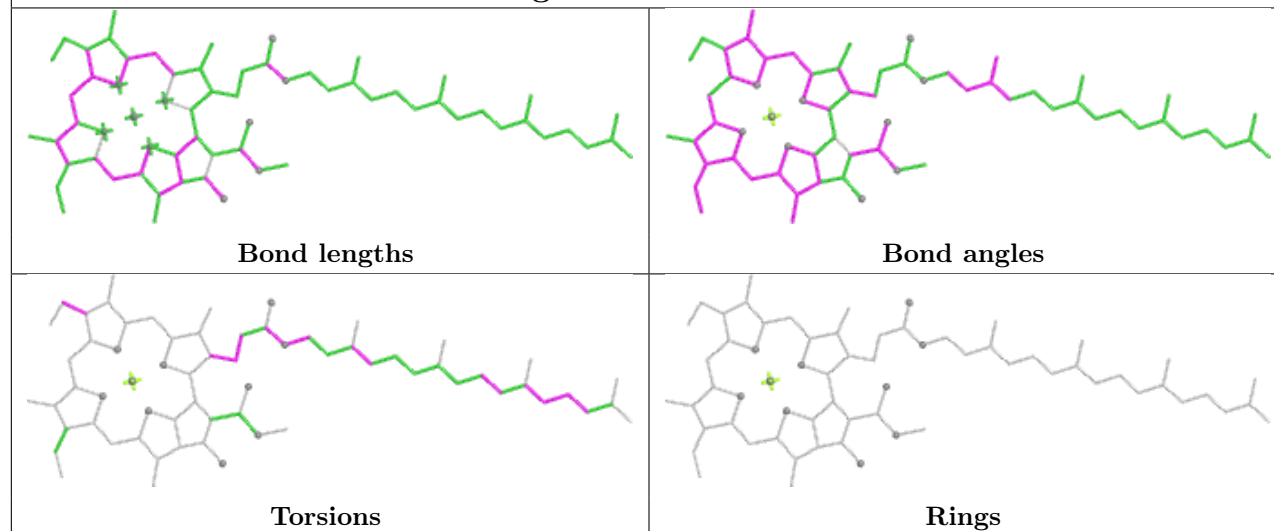
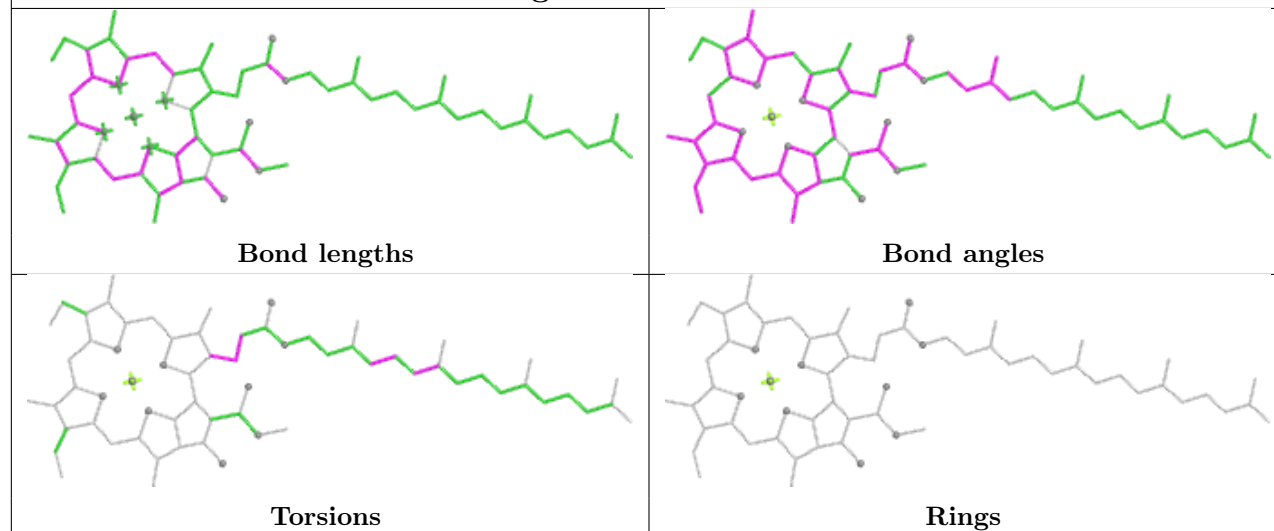
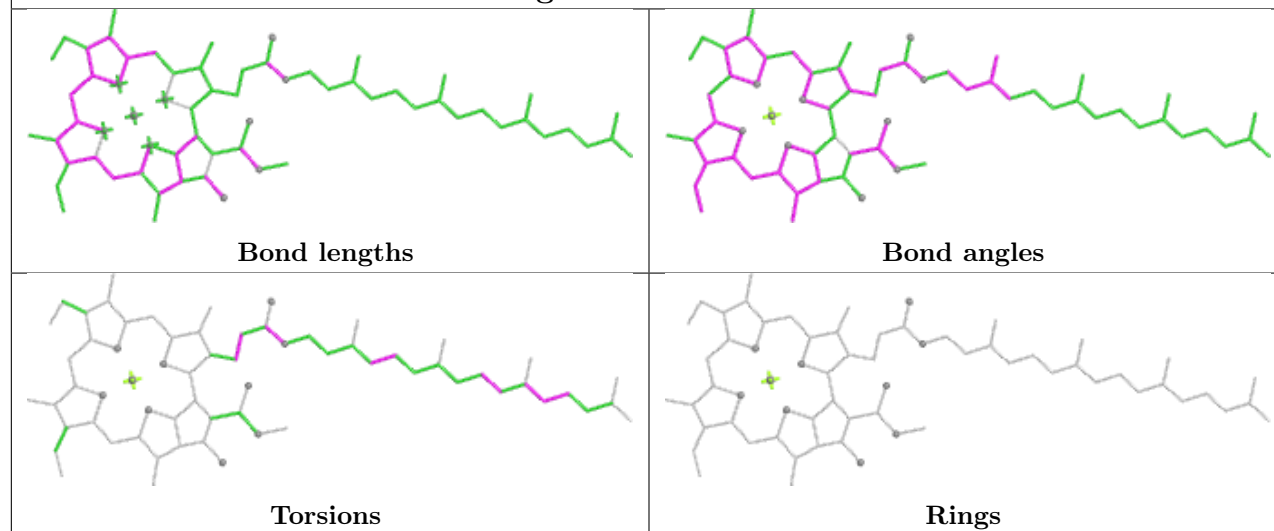


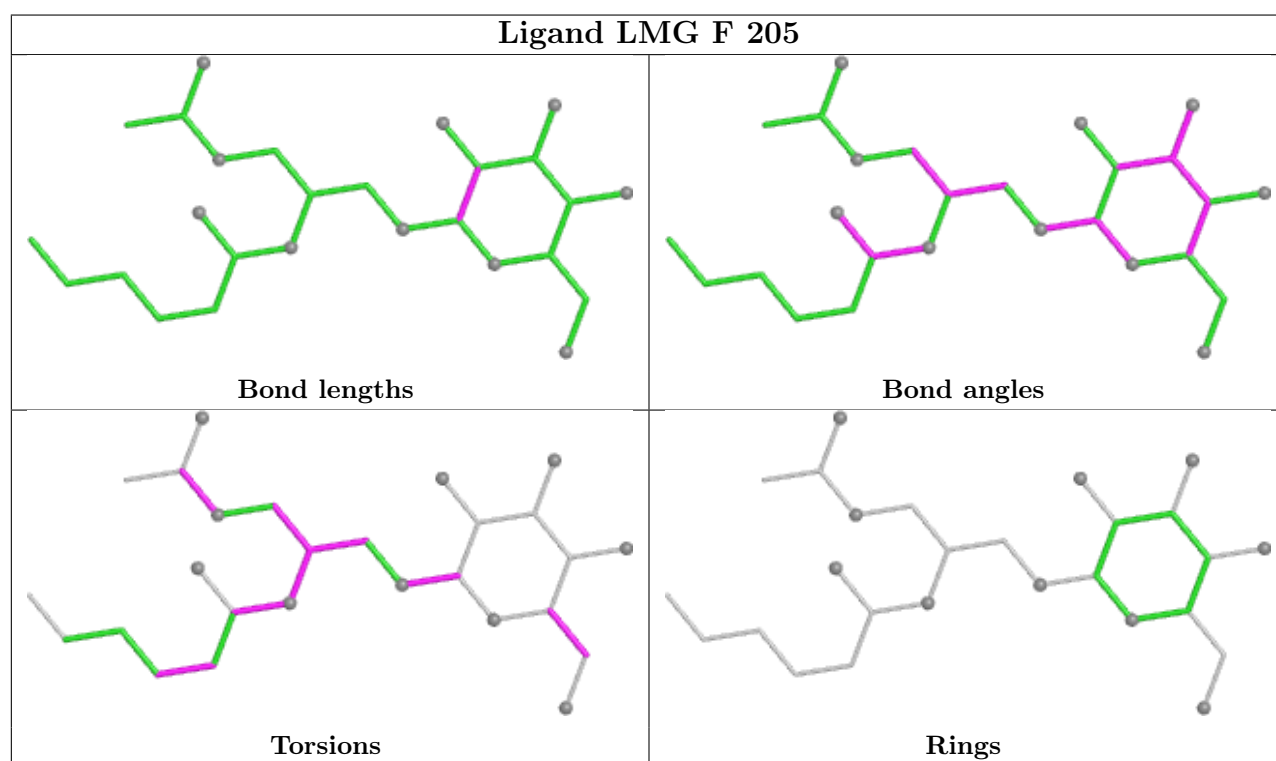
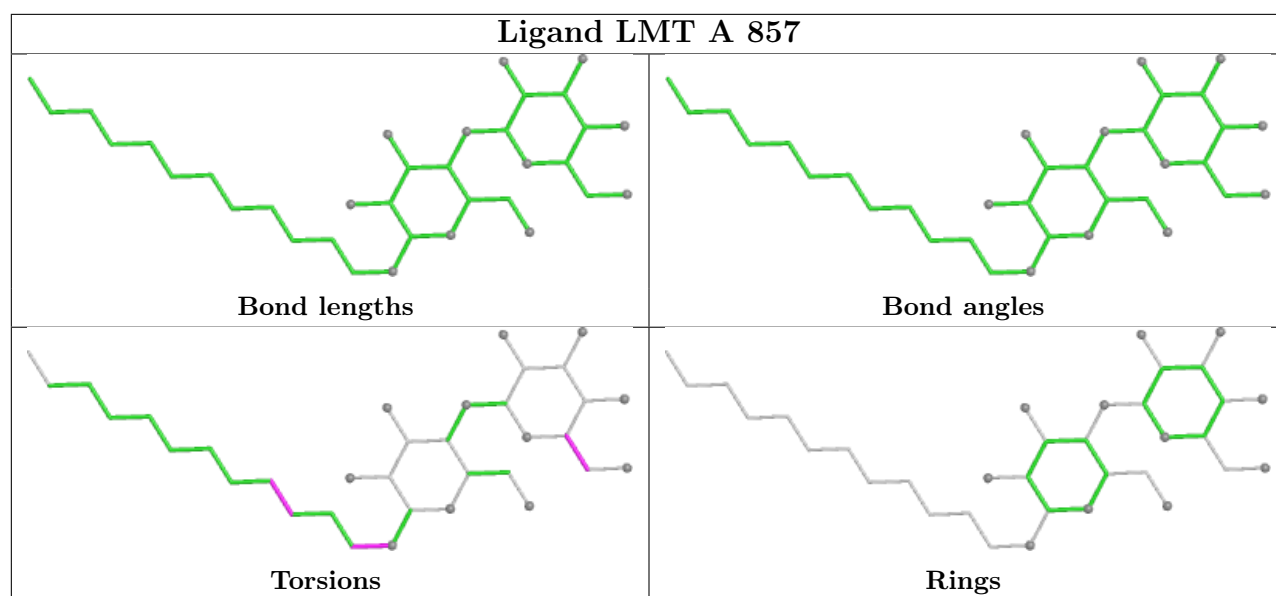
Ligand CLA A 821

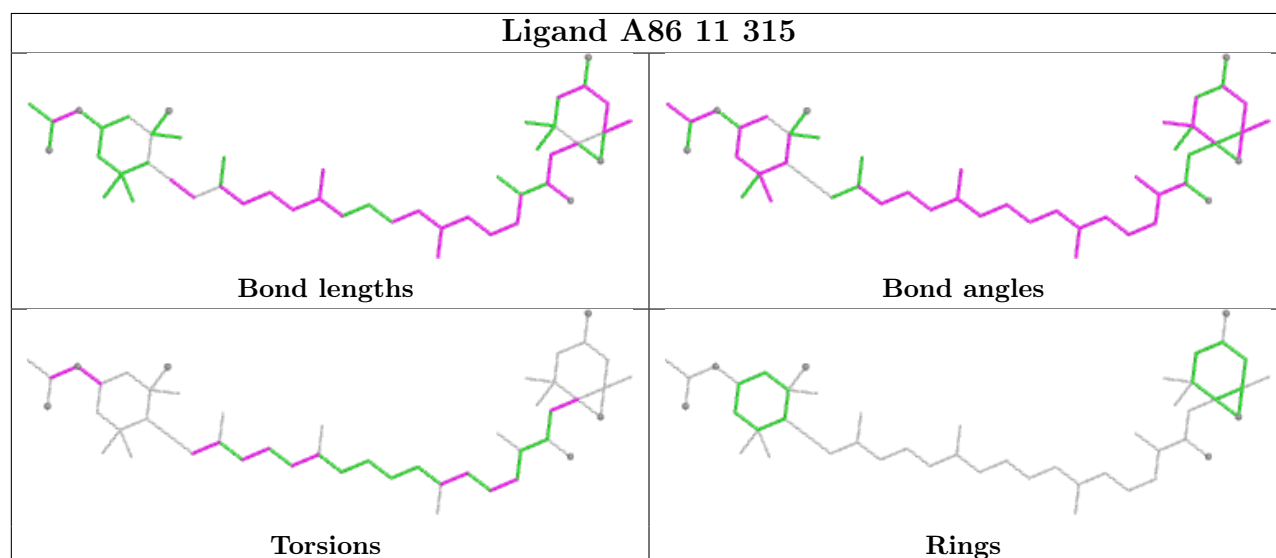
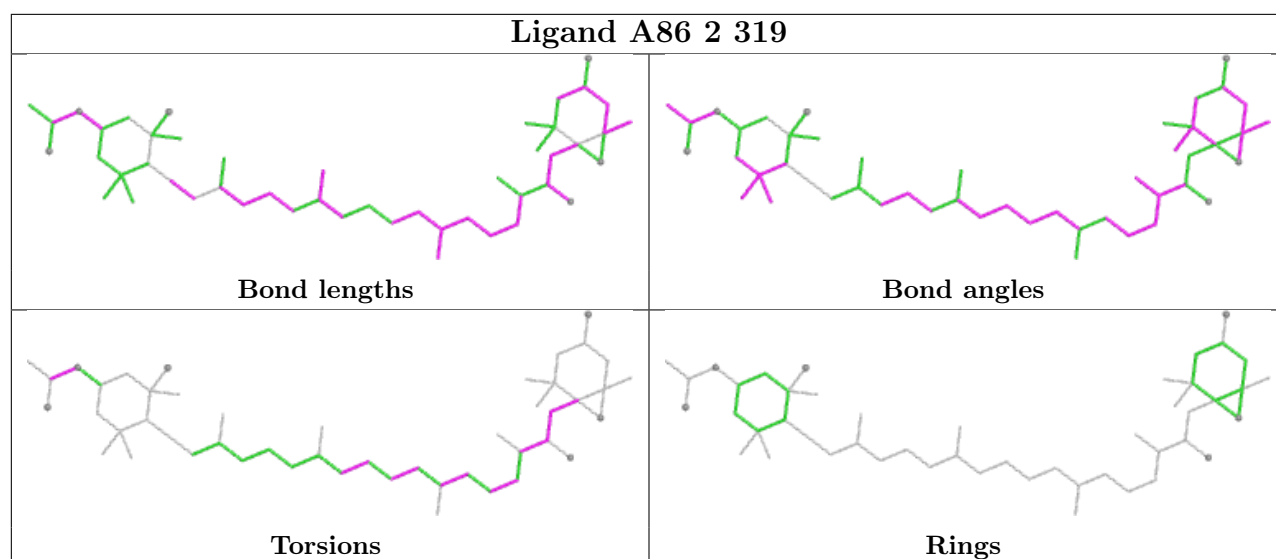


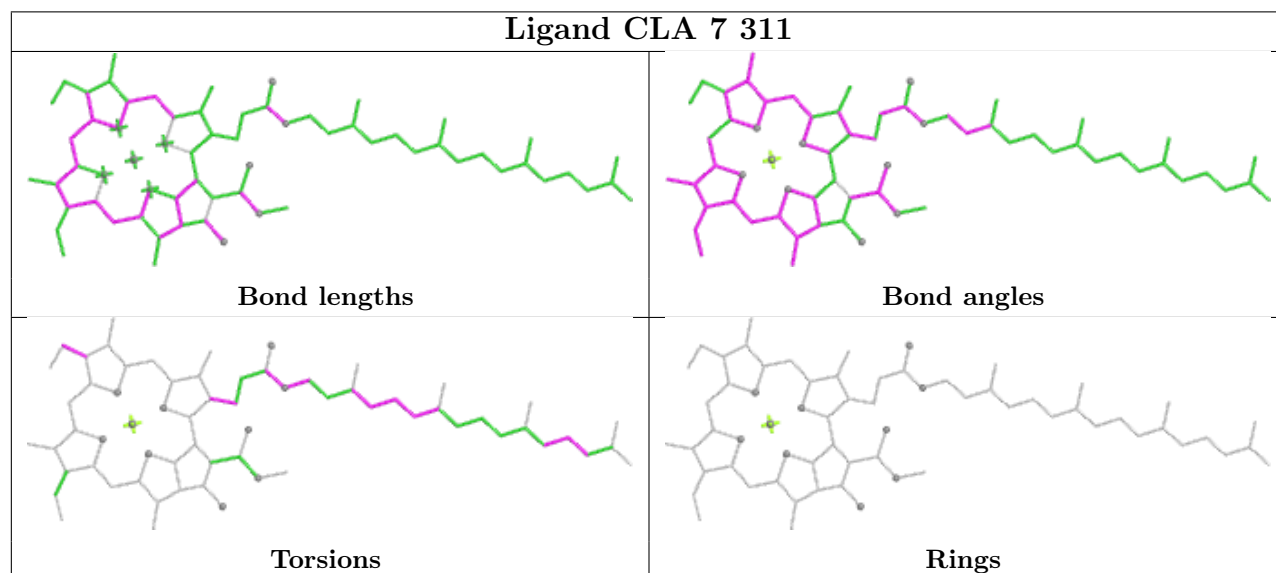
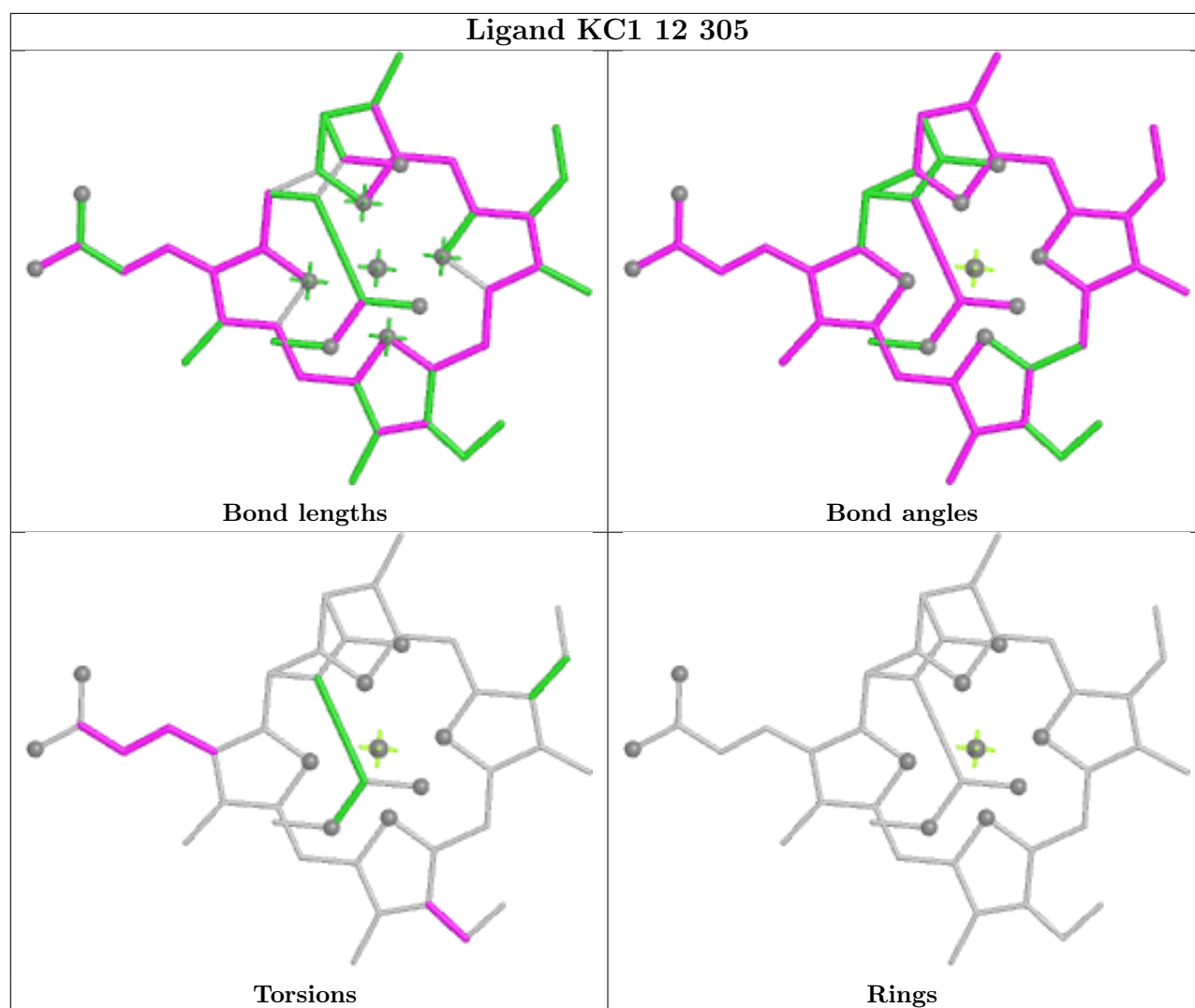
Ligand CLA 14 309

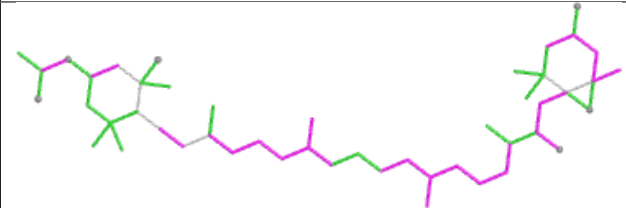
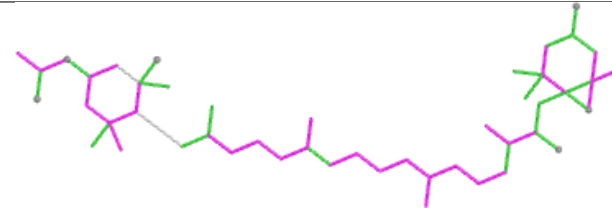
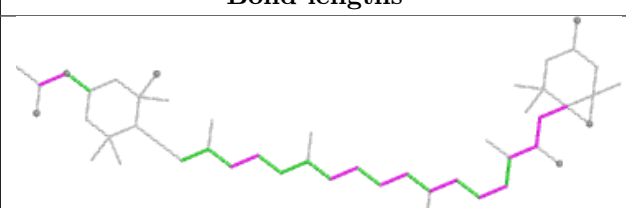
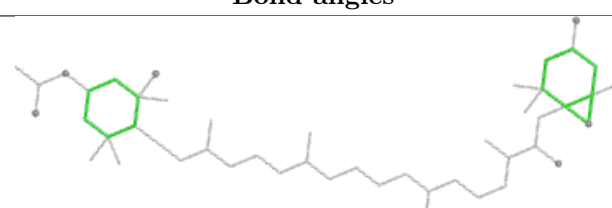


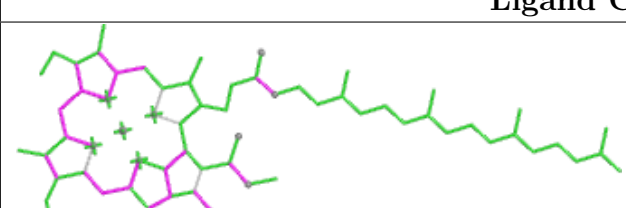
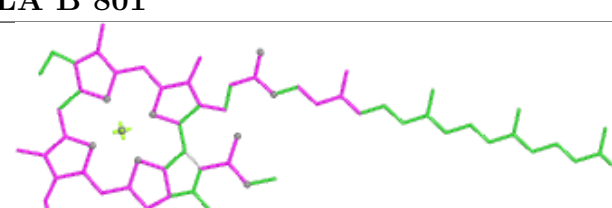
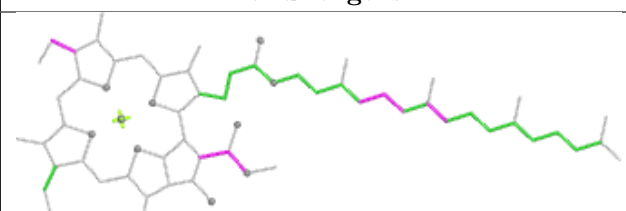
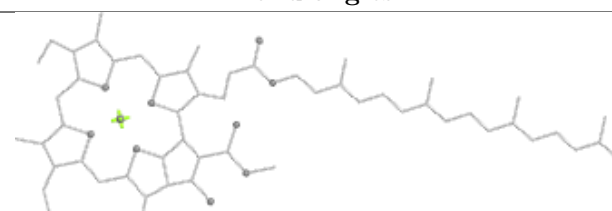
Ligand CLA B 829**Ligand CLA A 802****Ligand CLA 6 310**

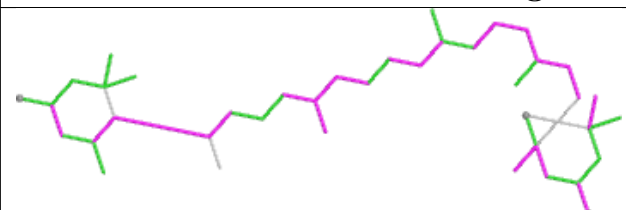
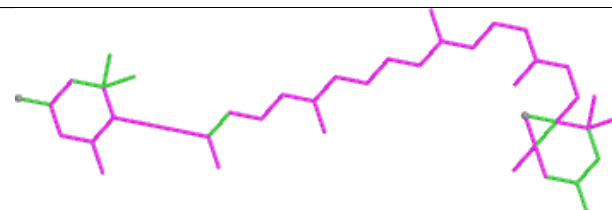
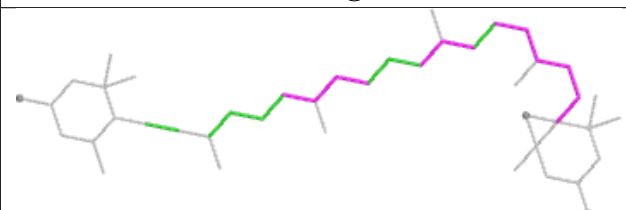
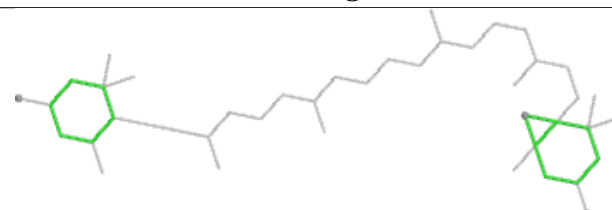


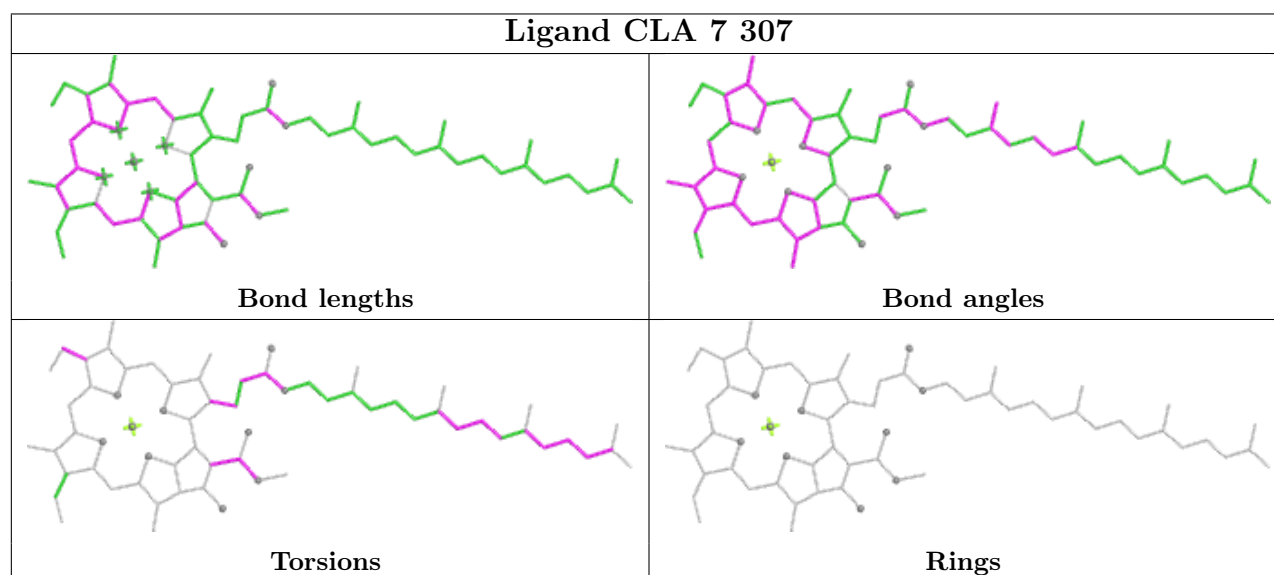
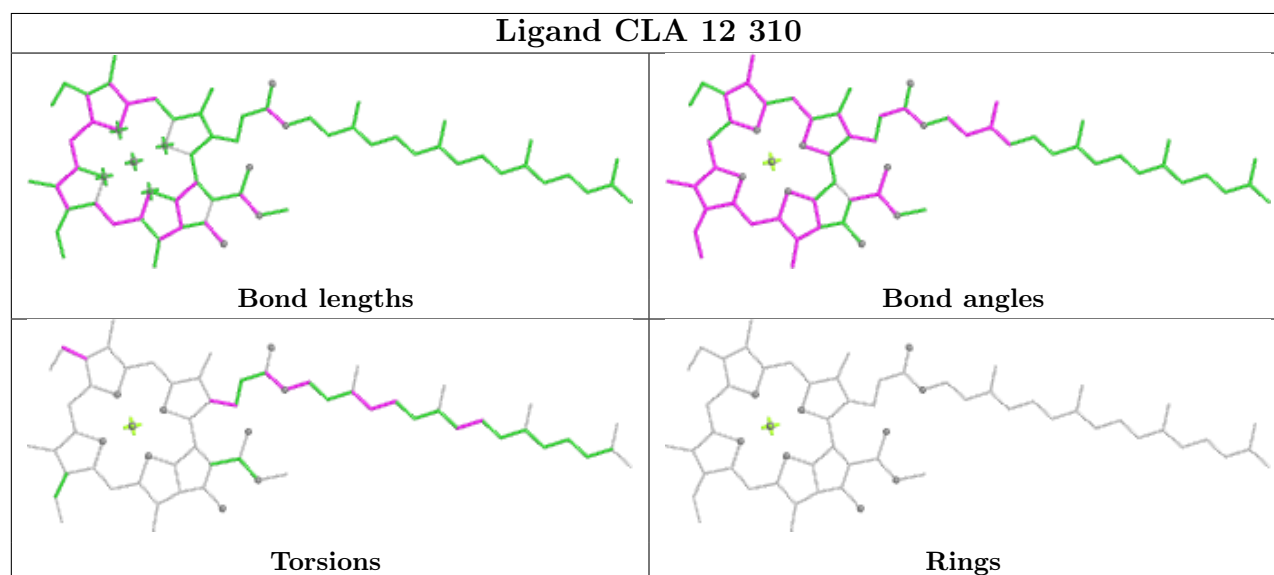
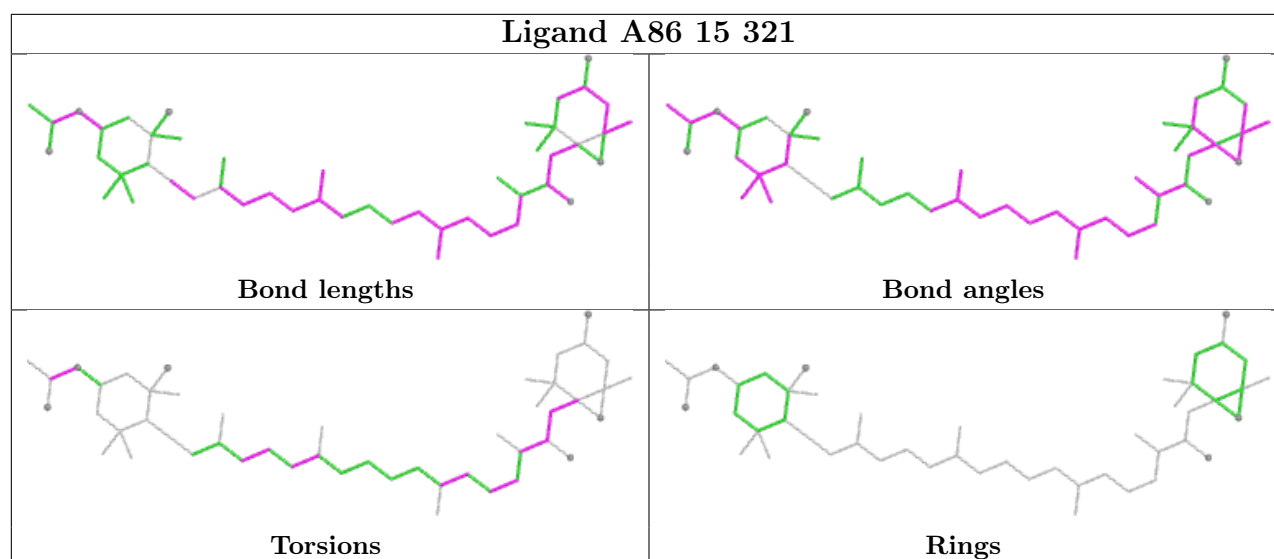


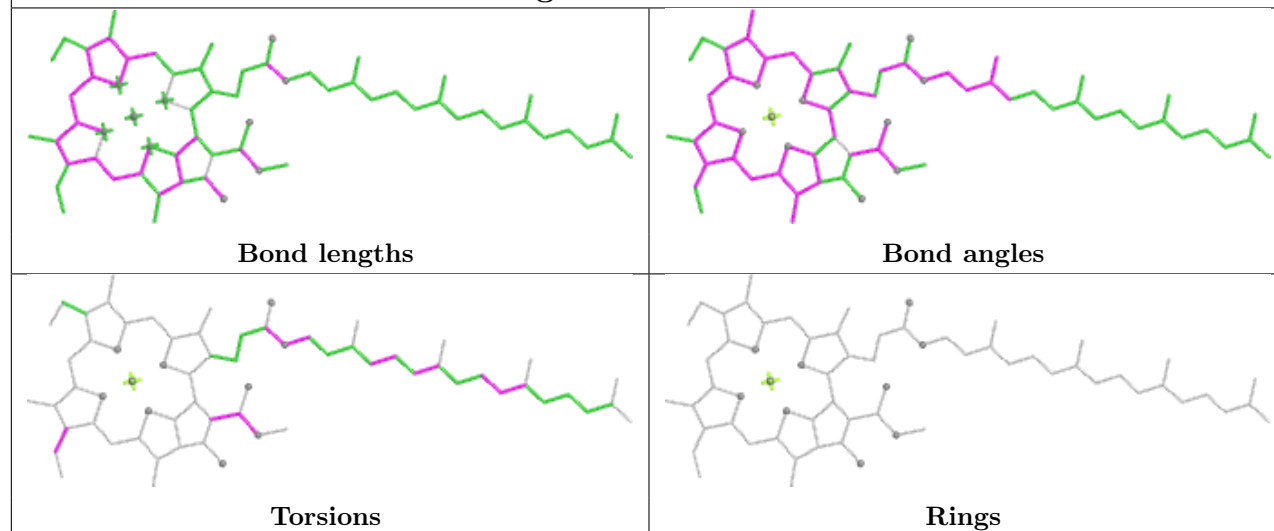
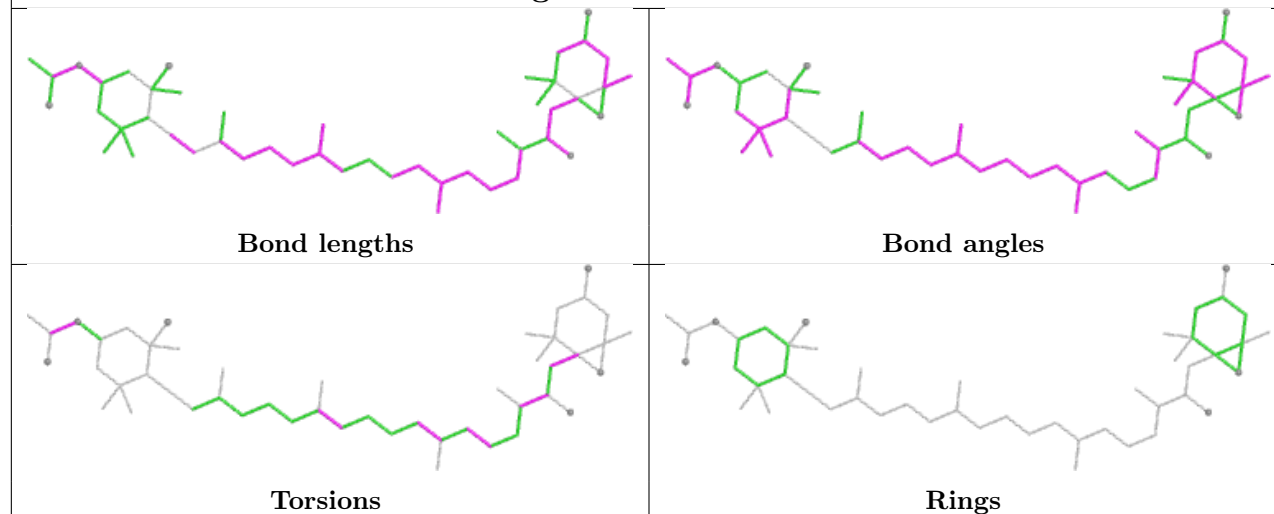
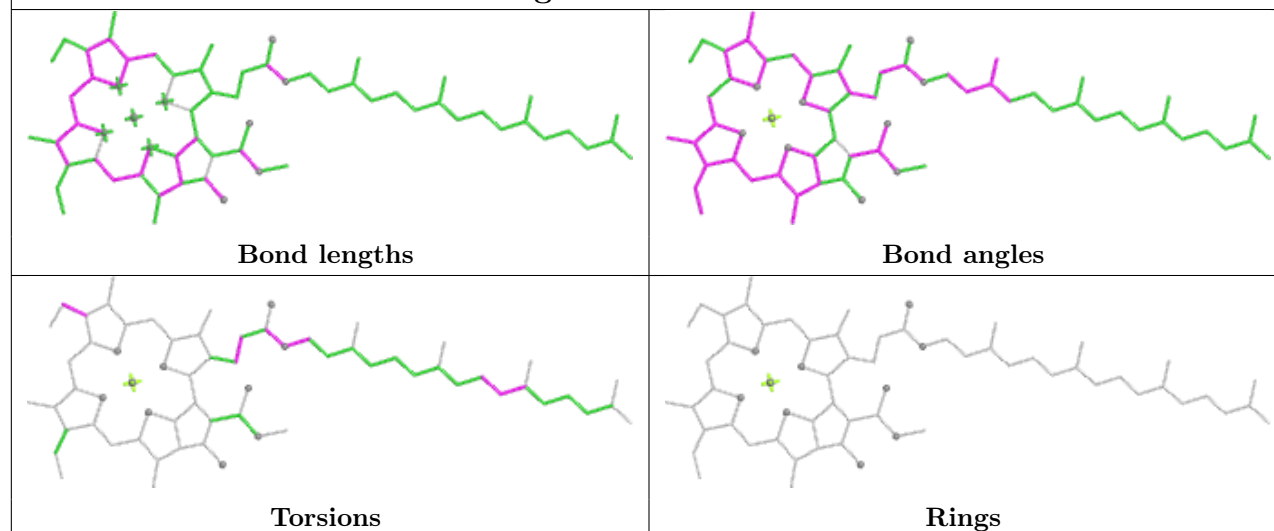


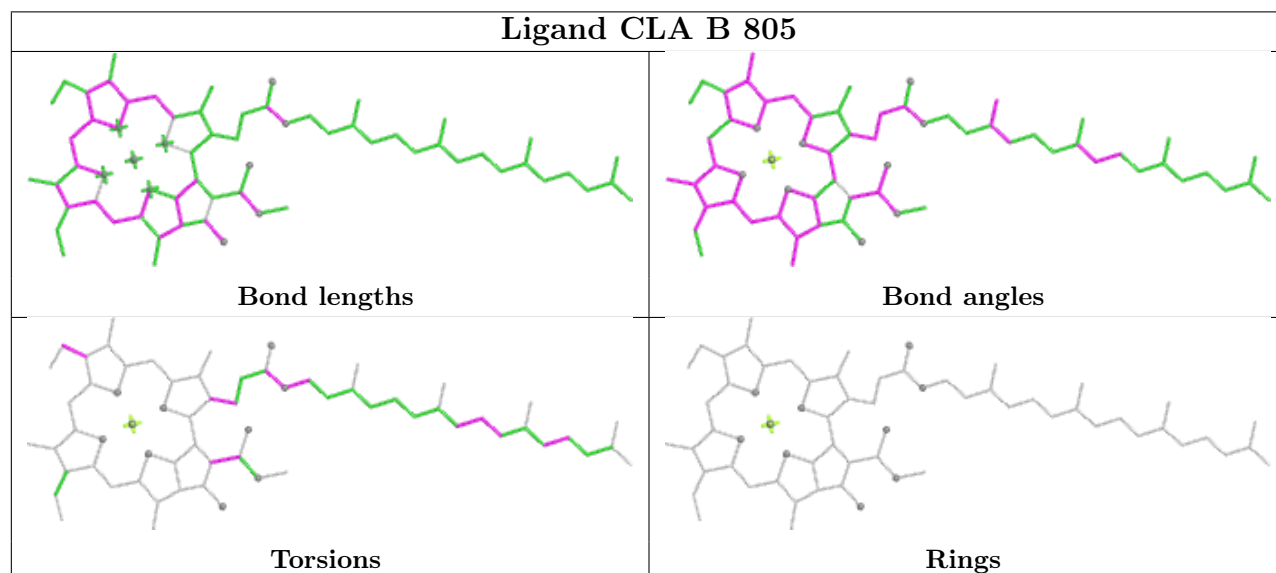
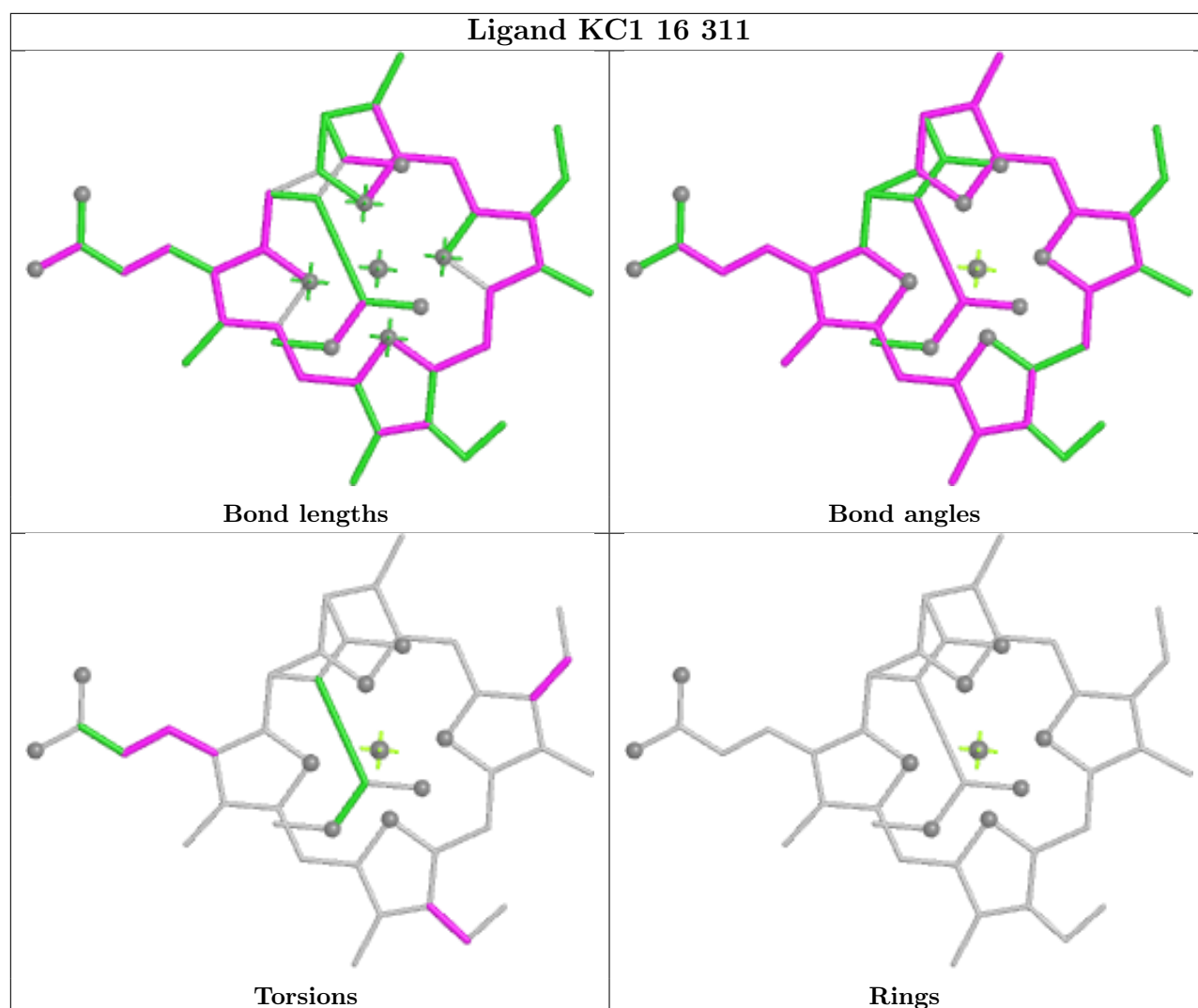
Ligand A86 11 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

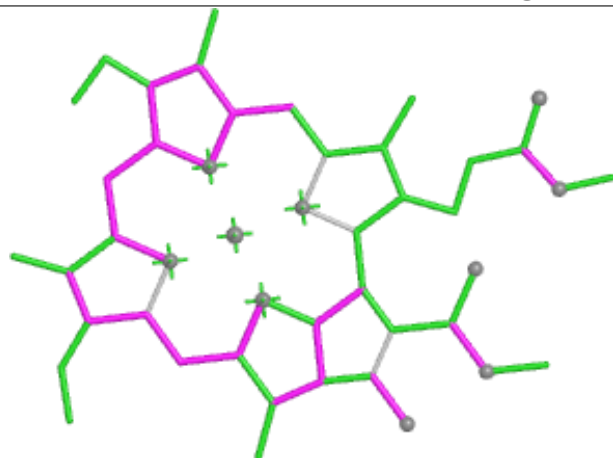
Ligand DD6 7 314	
	
Bond lengths	Bond angles
	
Torsions	Rings



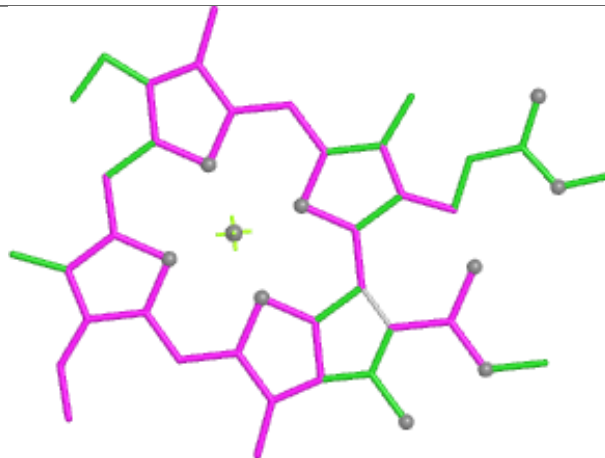
Ligand CLA 3 307**Ligand A86 2u 205****Ligand CLA L 202**



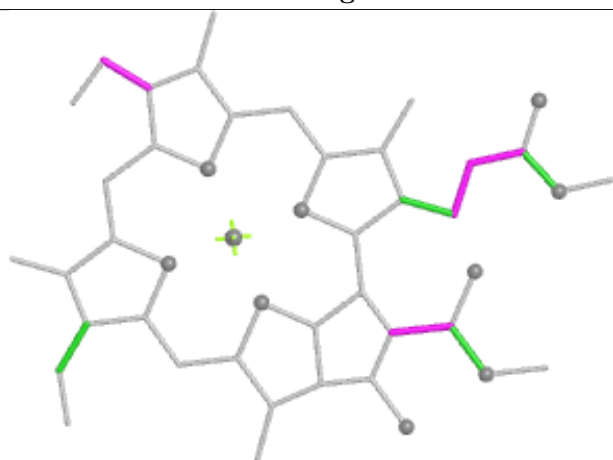
Ligand CLA 7 312



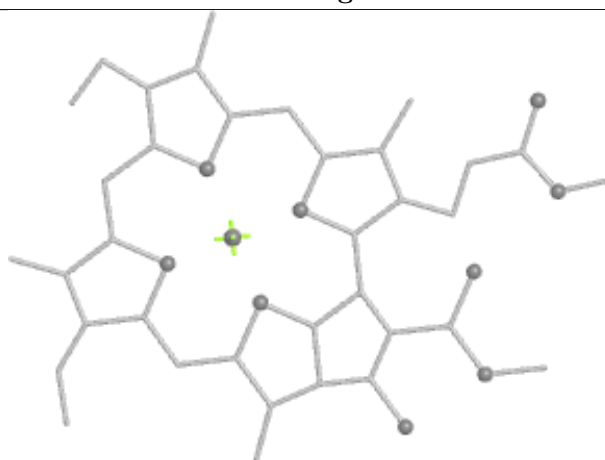
Bond lengths



Bond angles

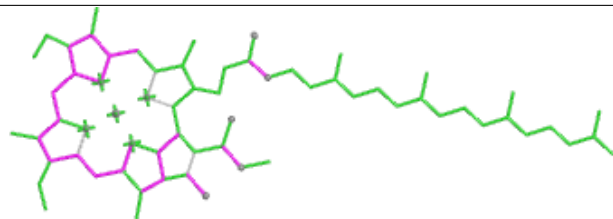


Torsions

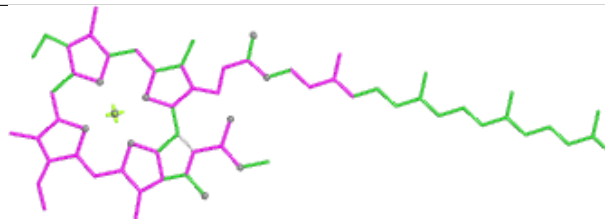


Rings

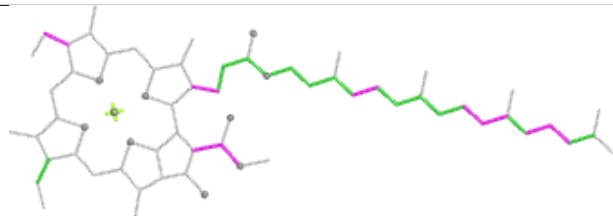
Ligand CLA 9 305



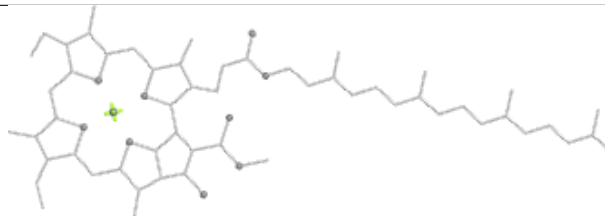
Bond lengths



Bond angles

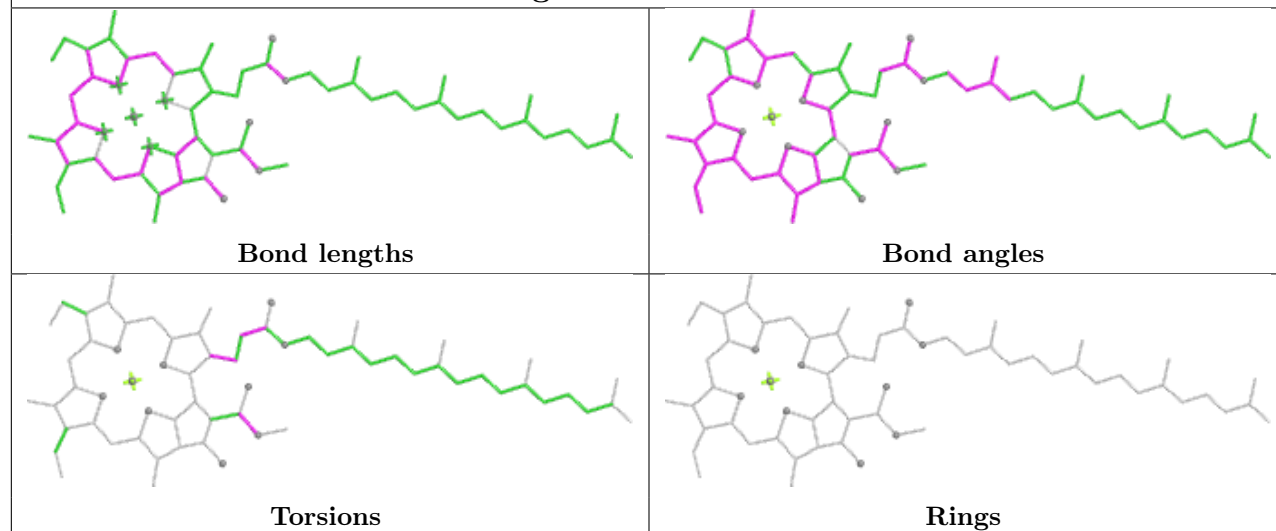


Torsions

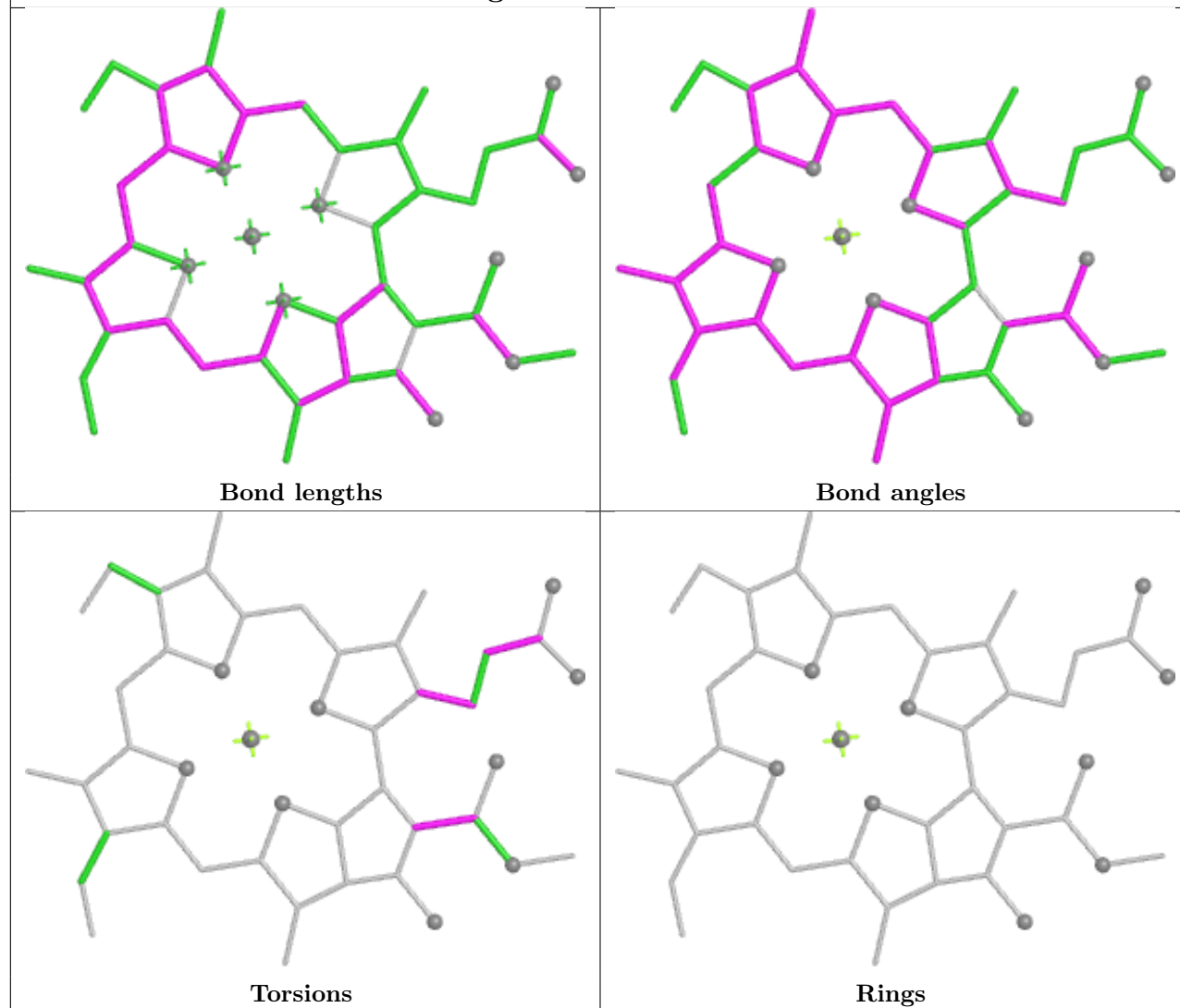


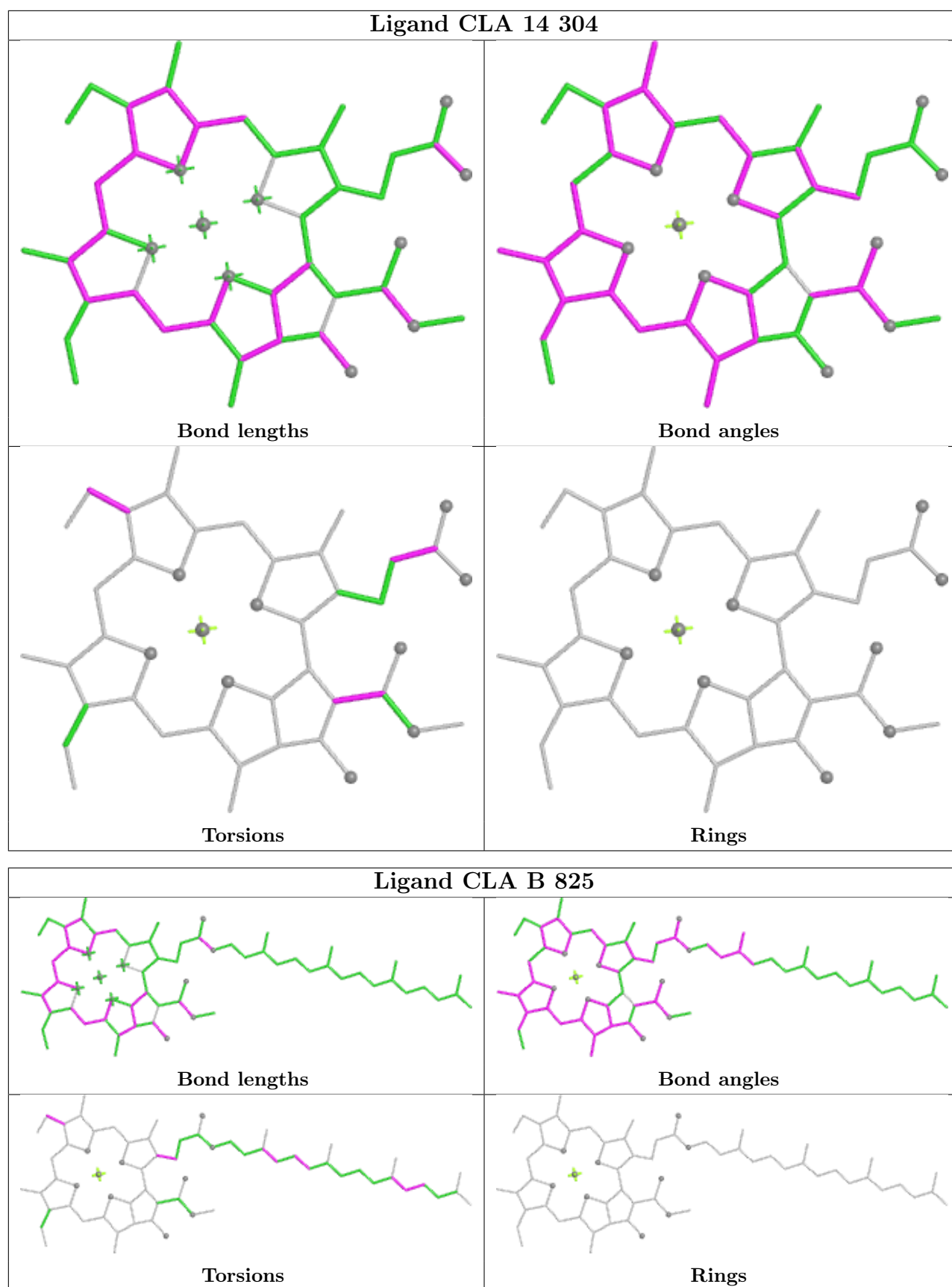
Rings

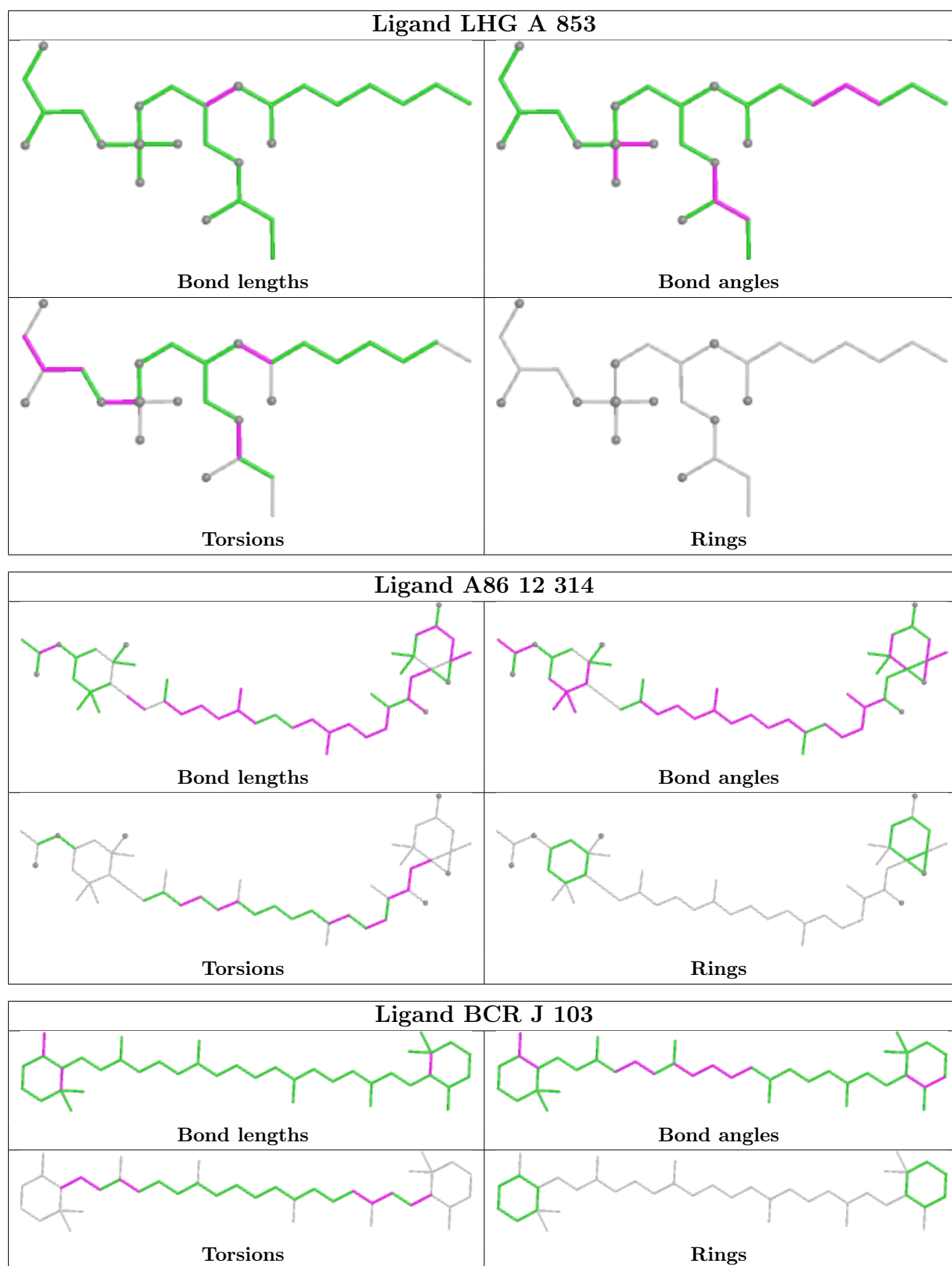
Ligand CLA B 839

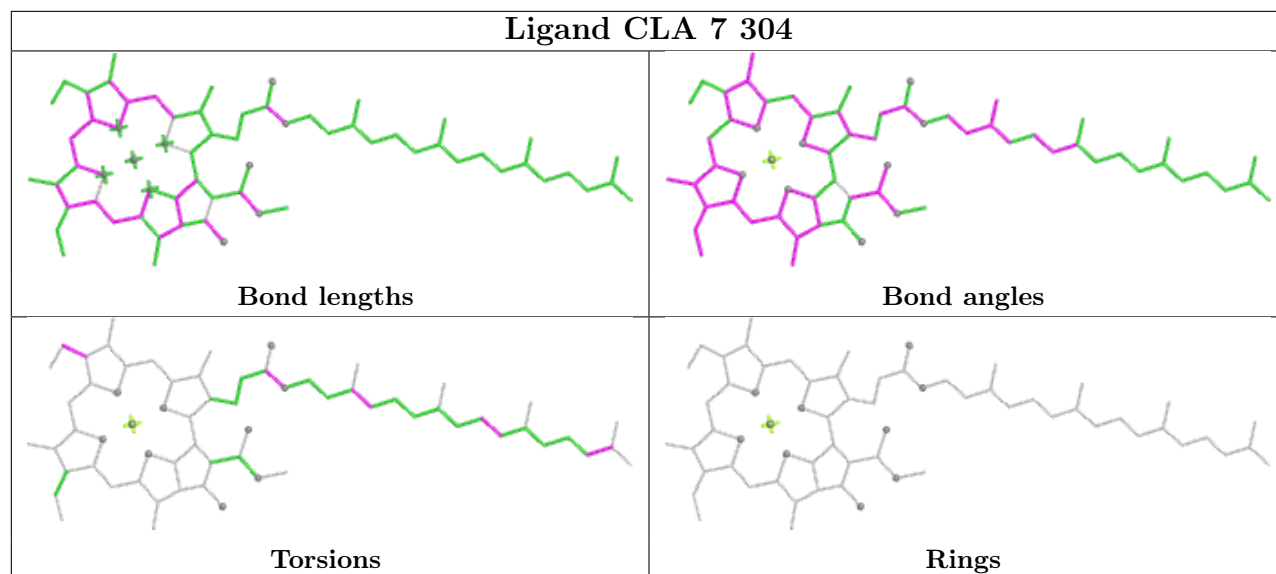
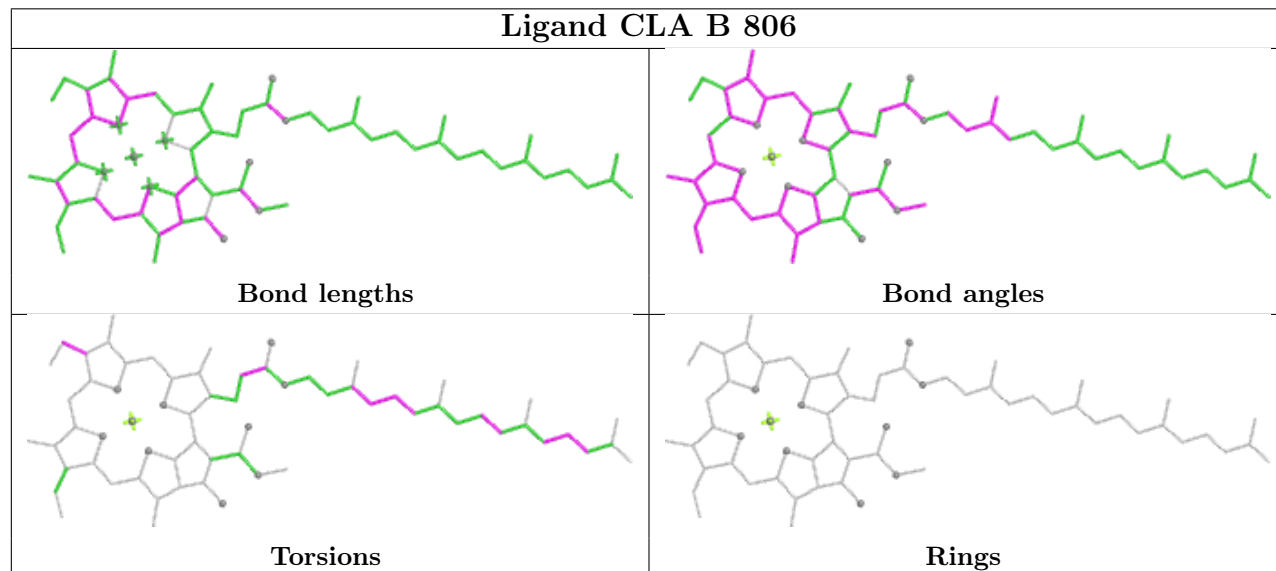
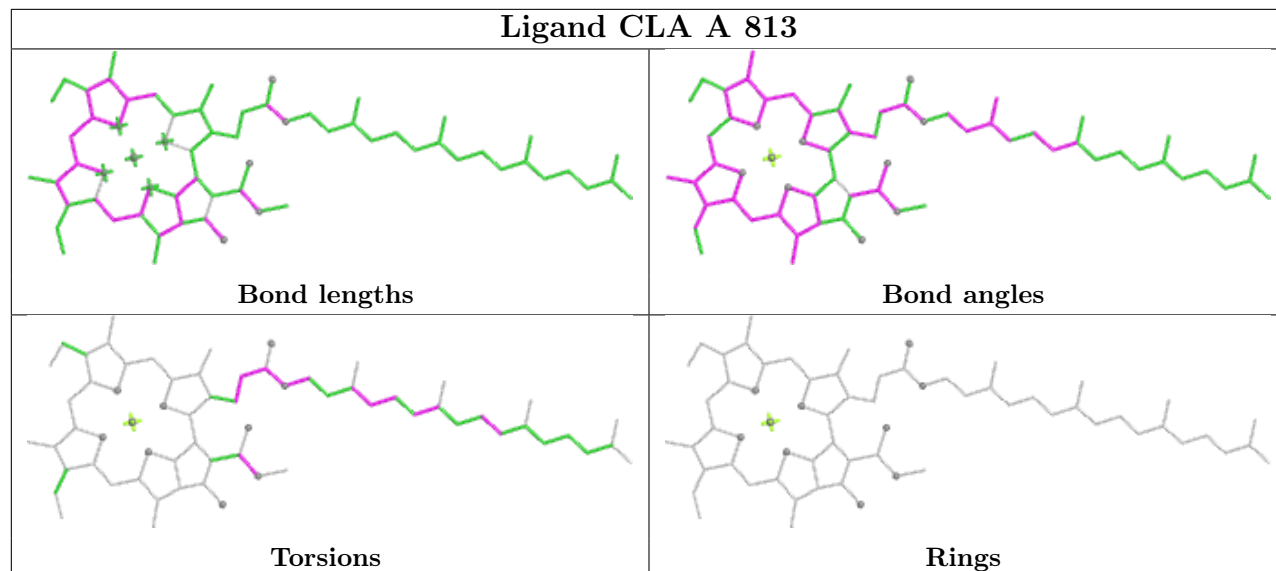


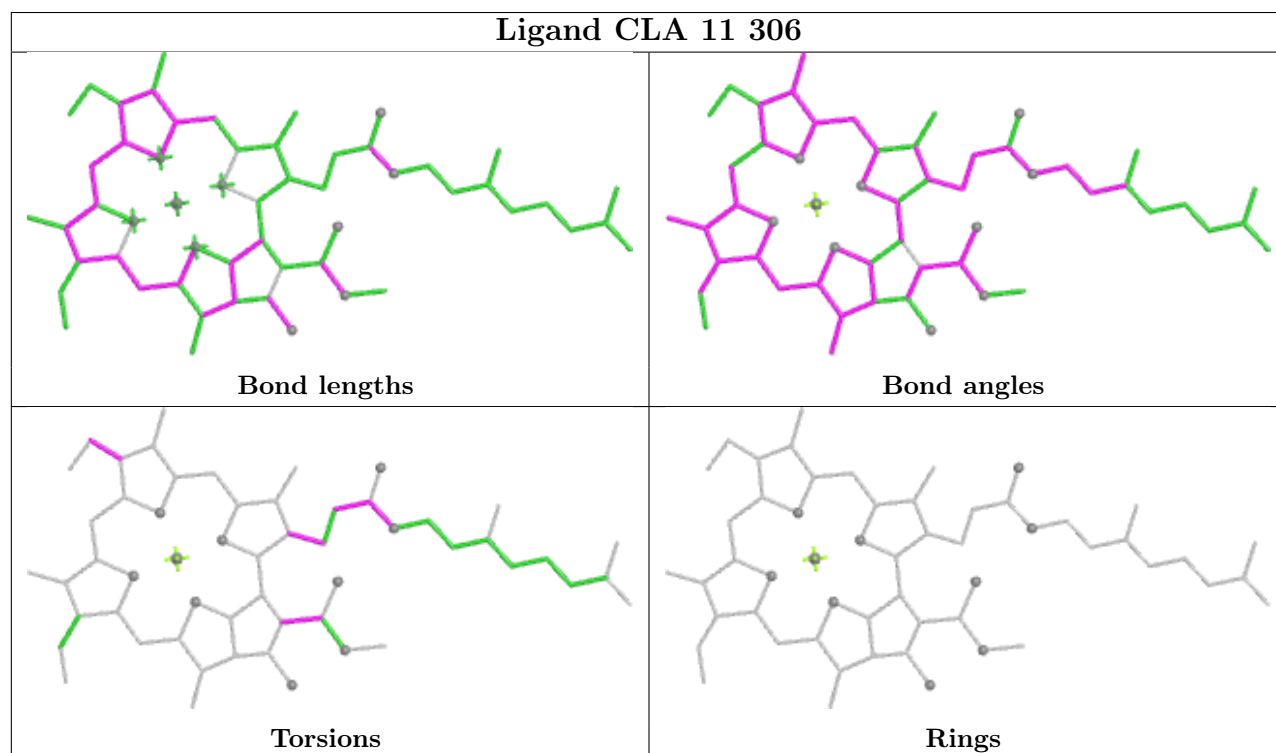
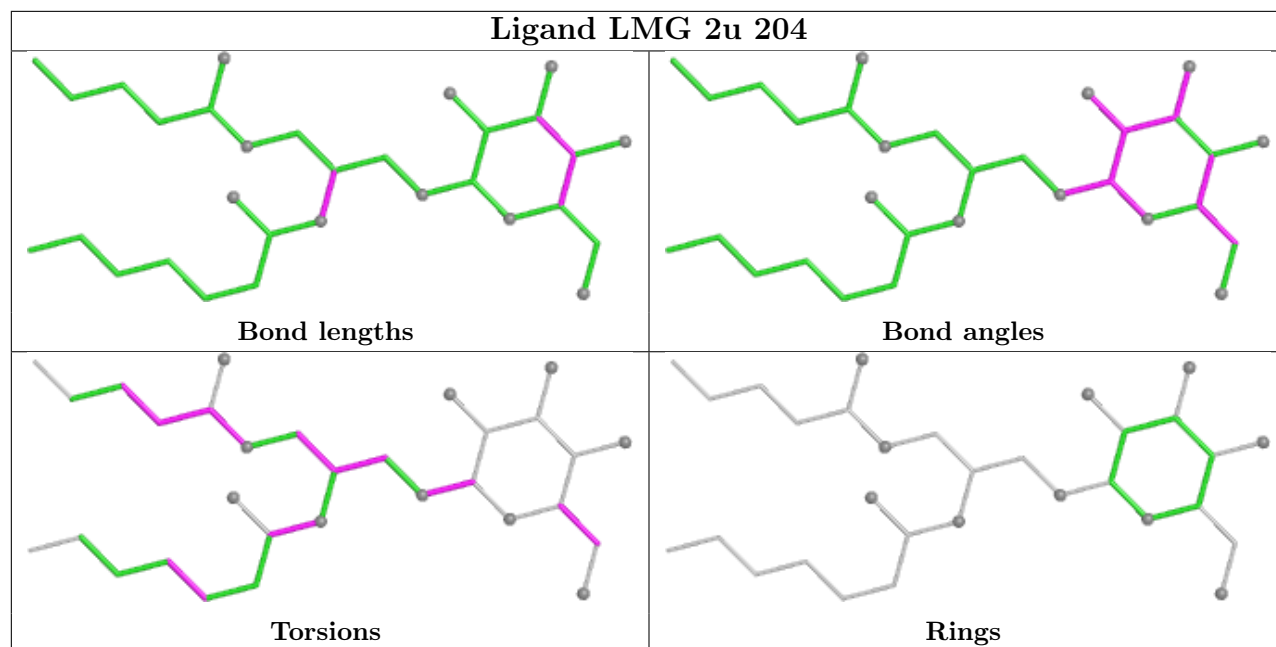
Ligand CLA 15 310

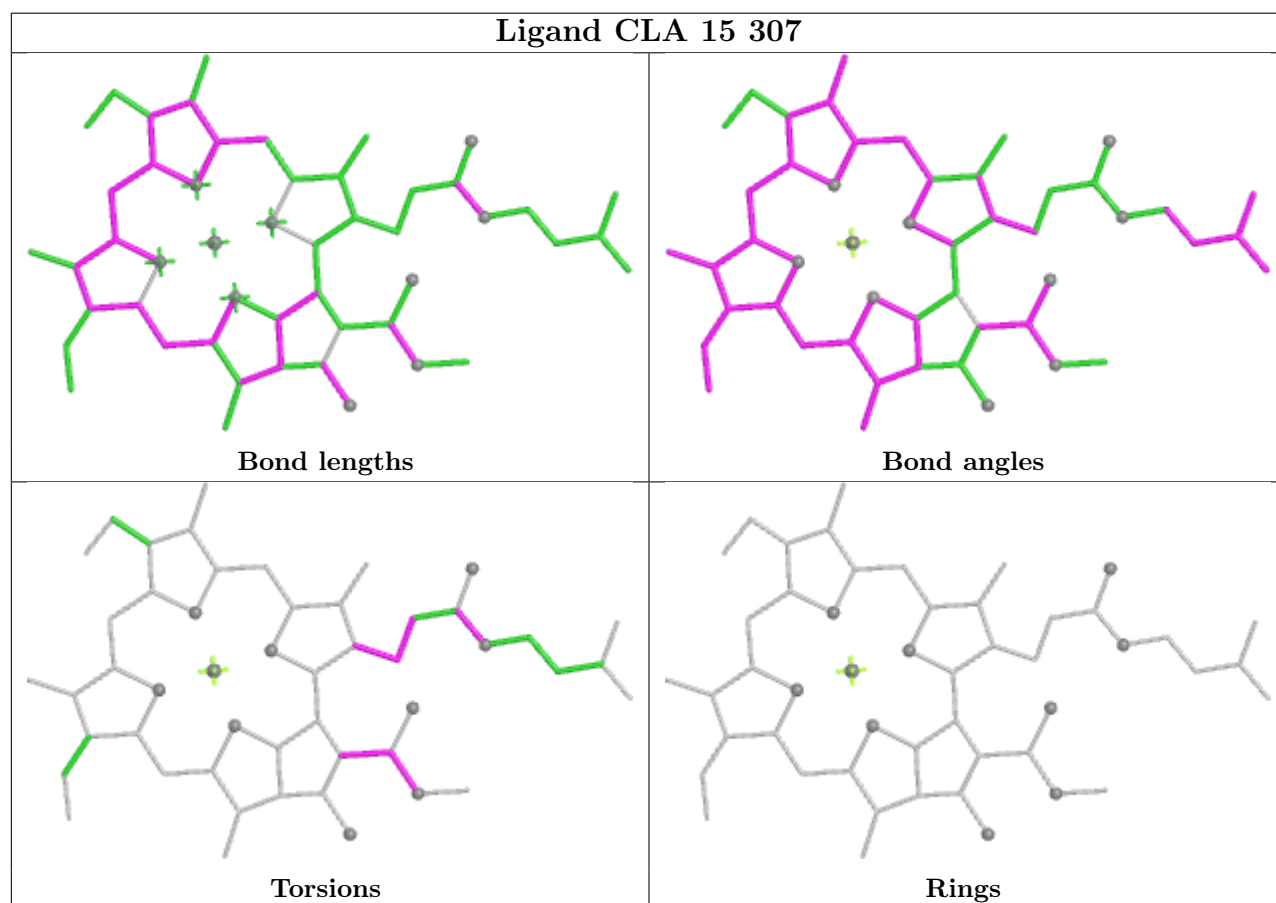
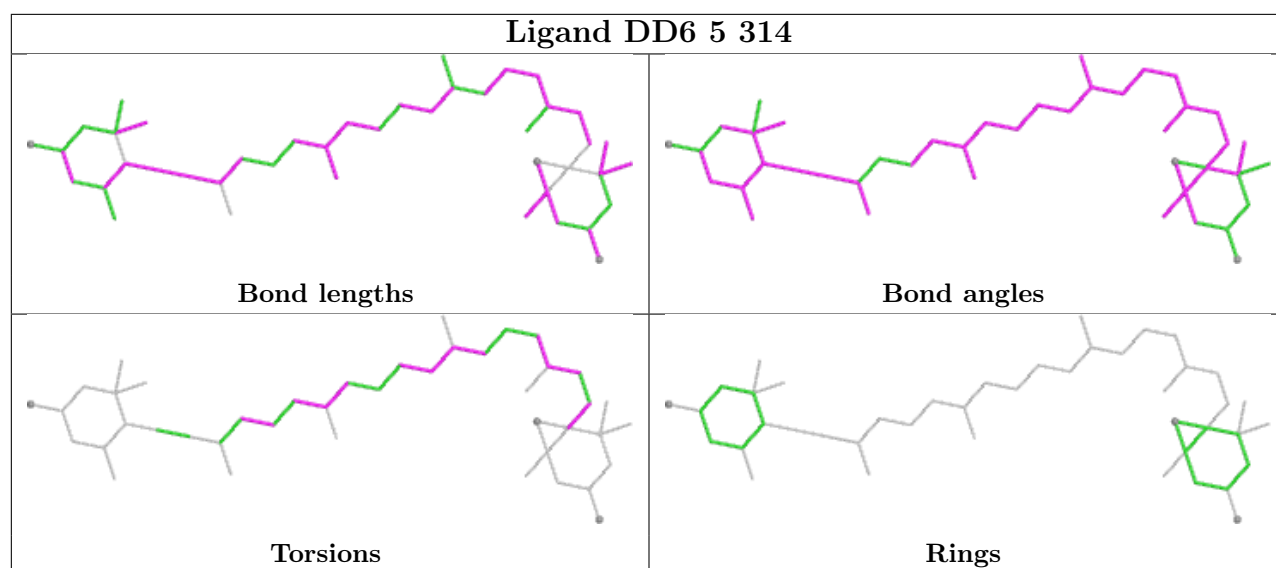


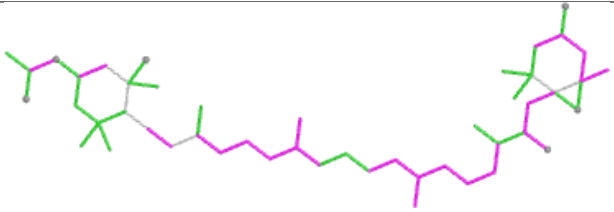
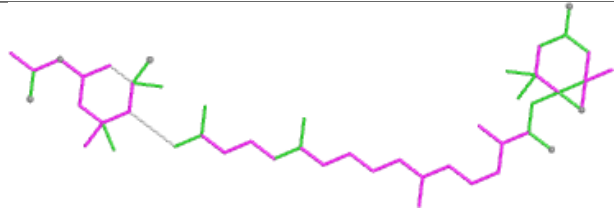
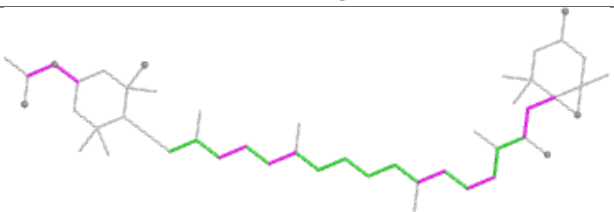
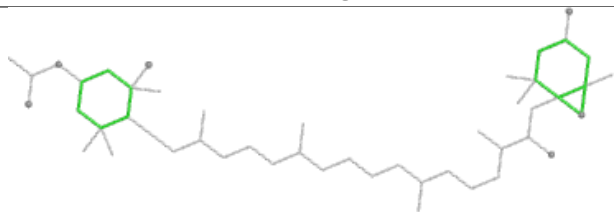
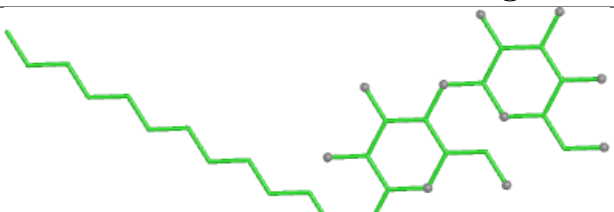
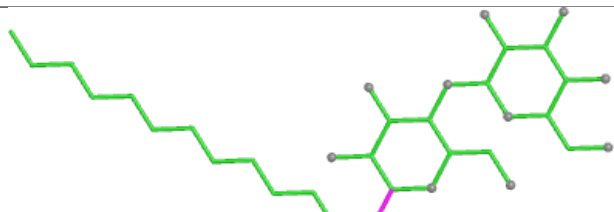
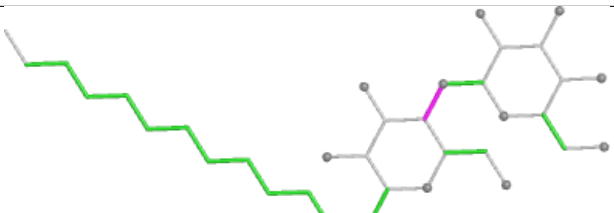
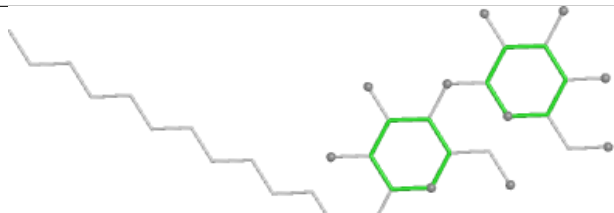
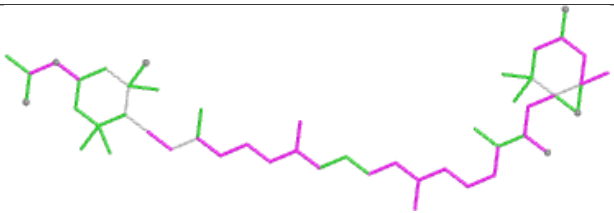
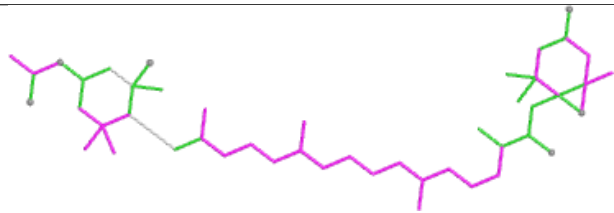
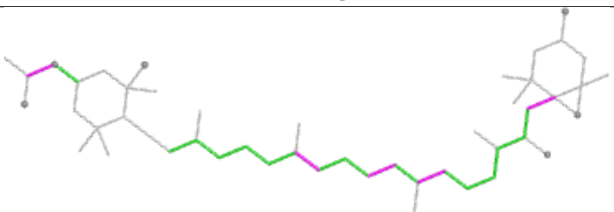
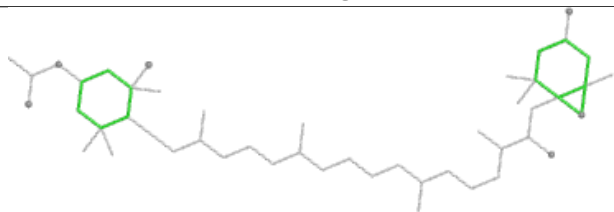


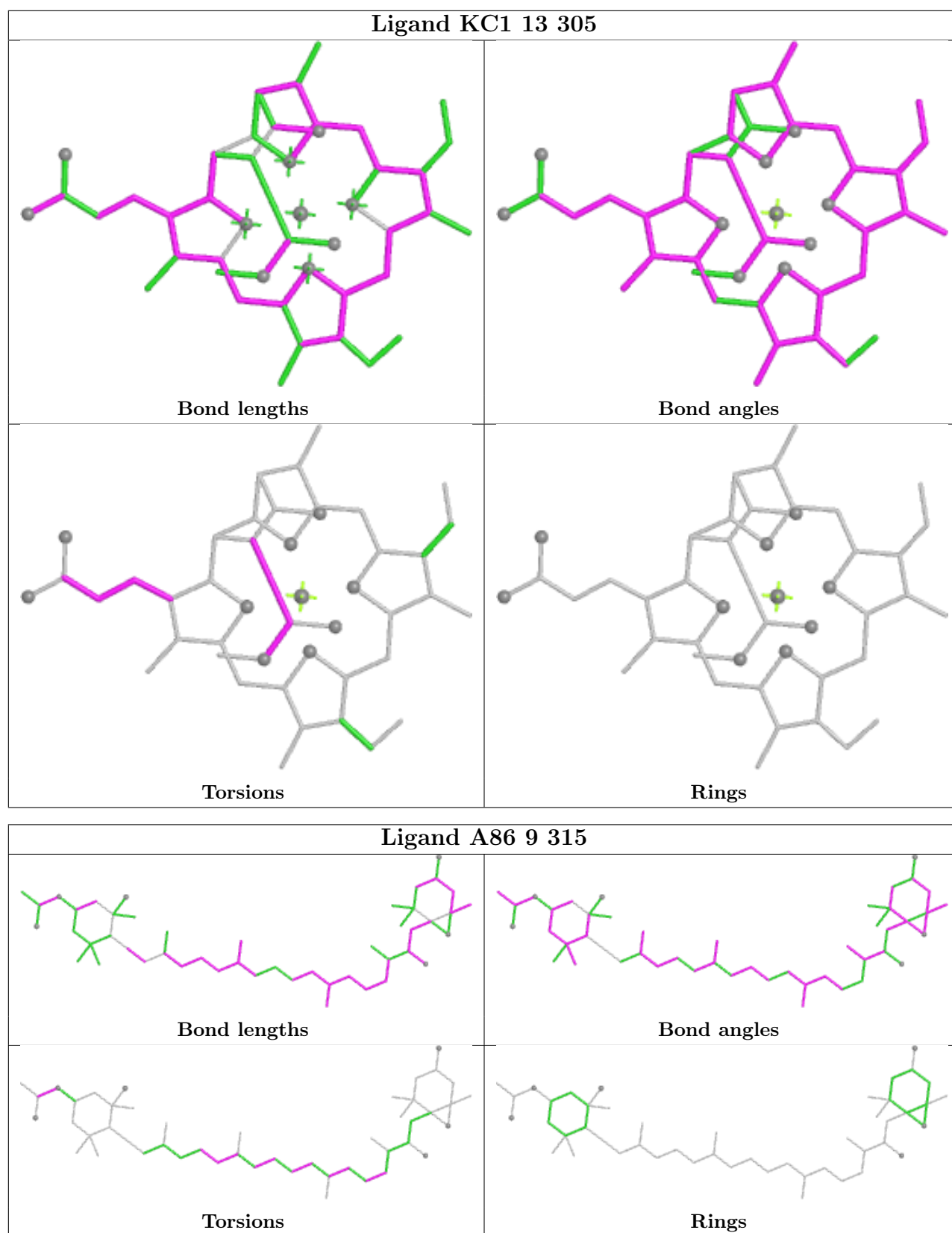


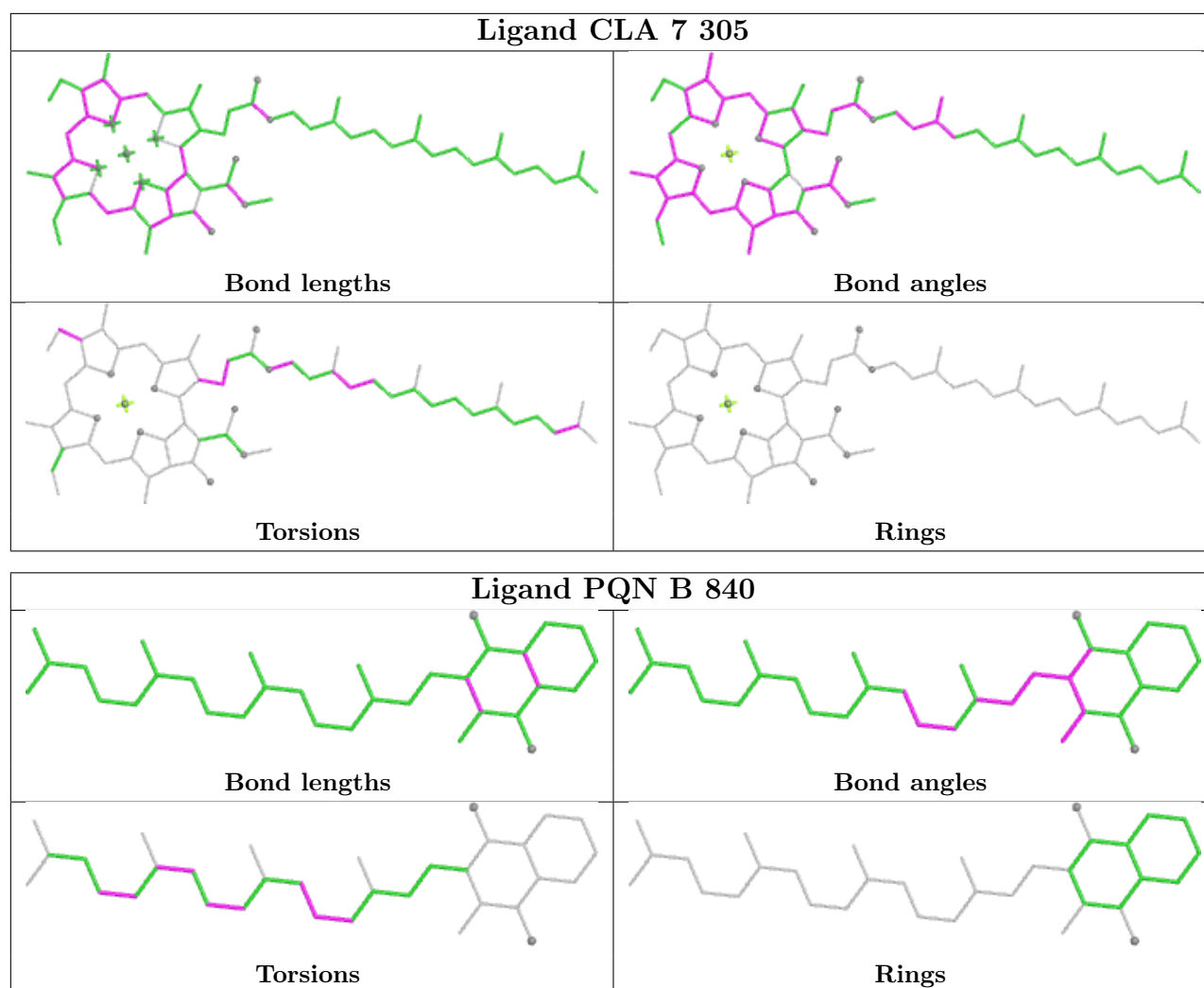
Ligand CLA 7 304**Ligand CLA B 806****Ligand CLA A 813**

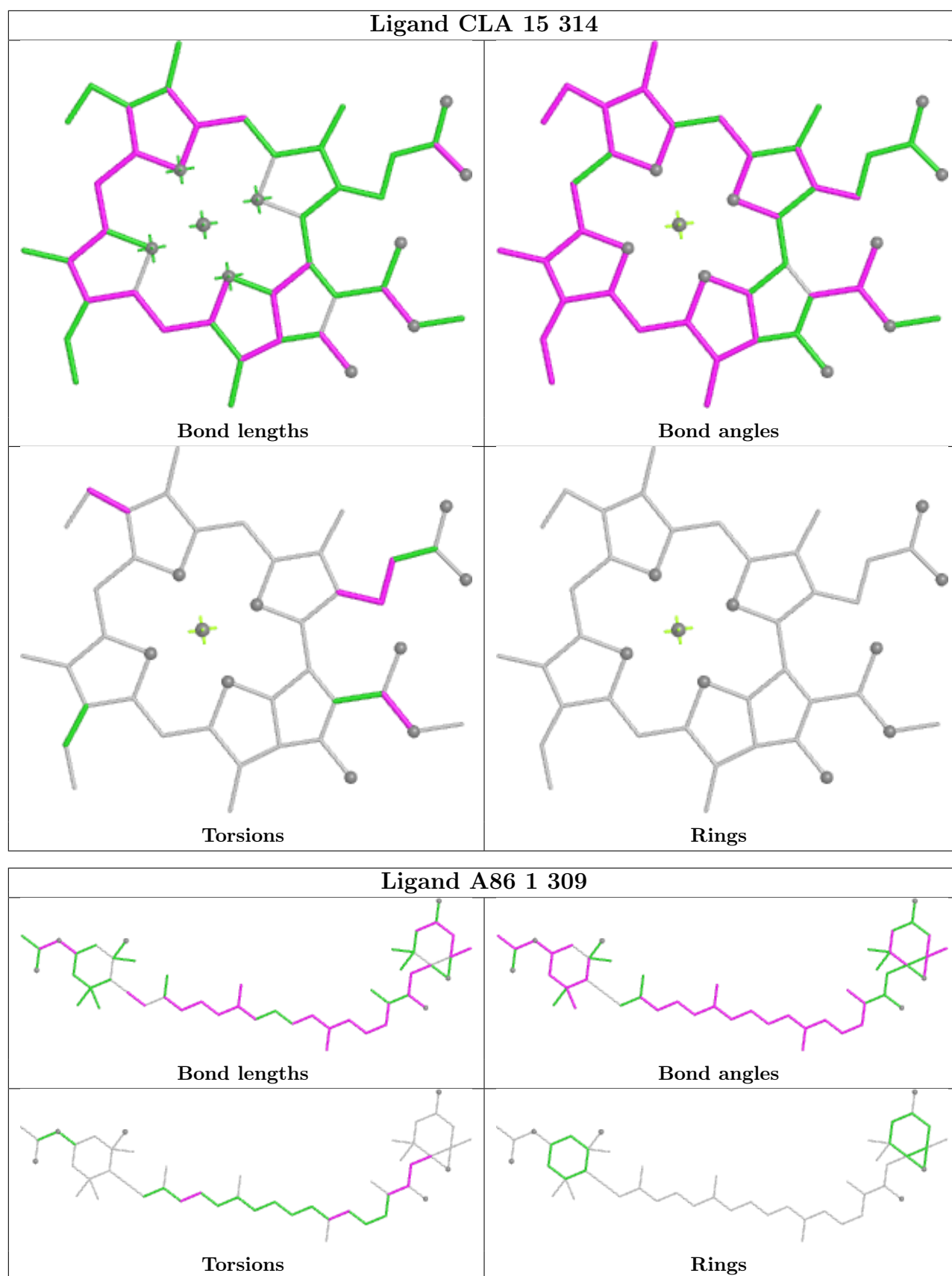


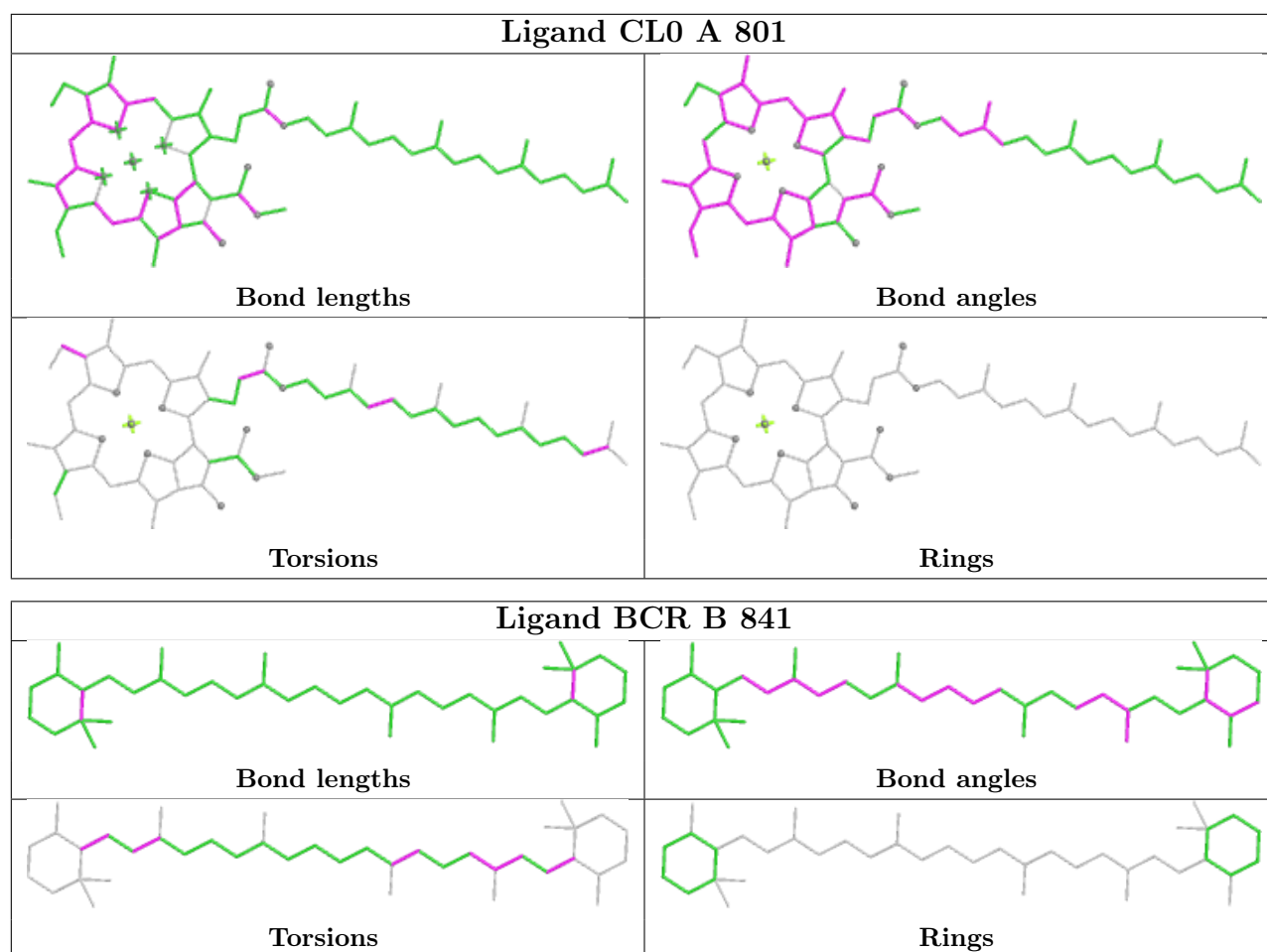


Ligand A86 16 314	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT 11 317	
 Bond lengths	 Bond angles
 Torsions	 Rings
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 Bond lengths	 Bond angles
 Torsions	 Rings

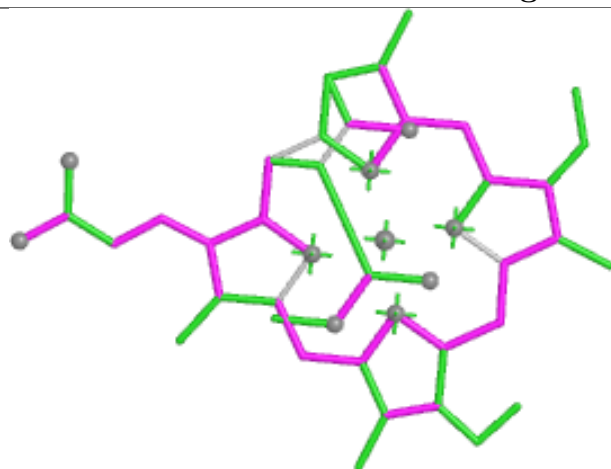




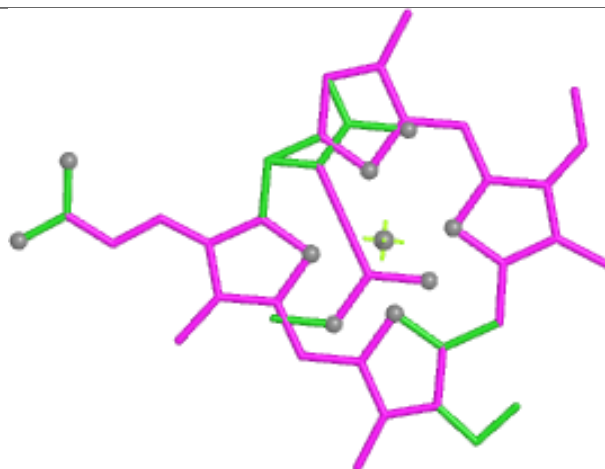




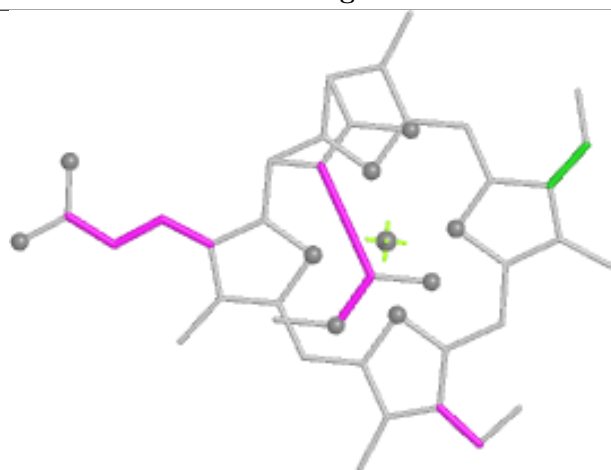
Ligand KC1 5 306



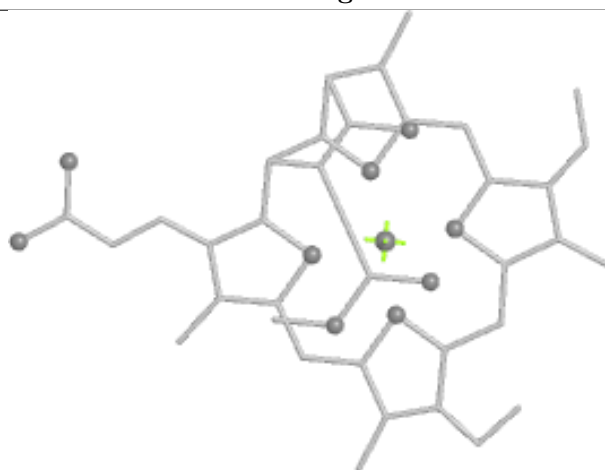
Bond lengths



Bond angles



Torsions

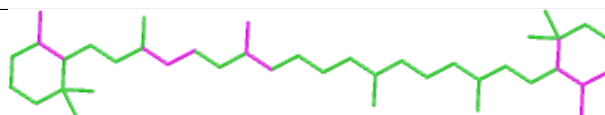


Rings

Ligand BCR J 102



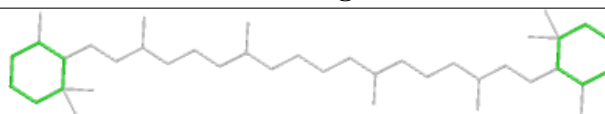
Bond lengths



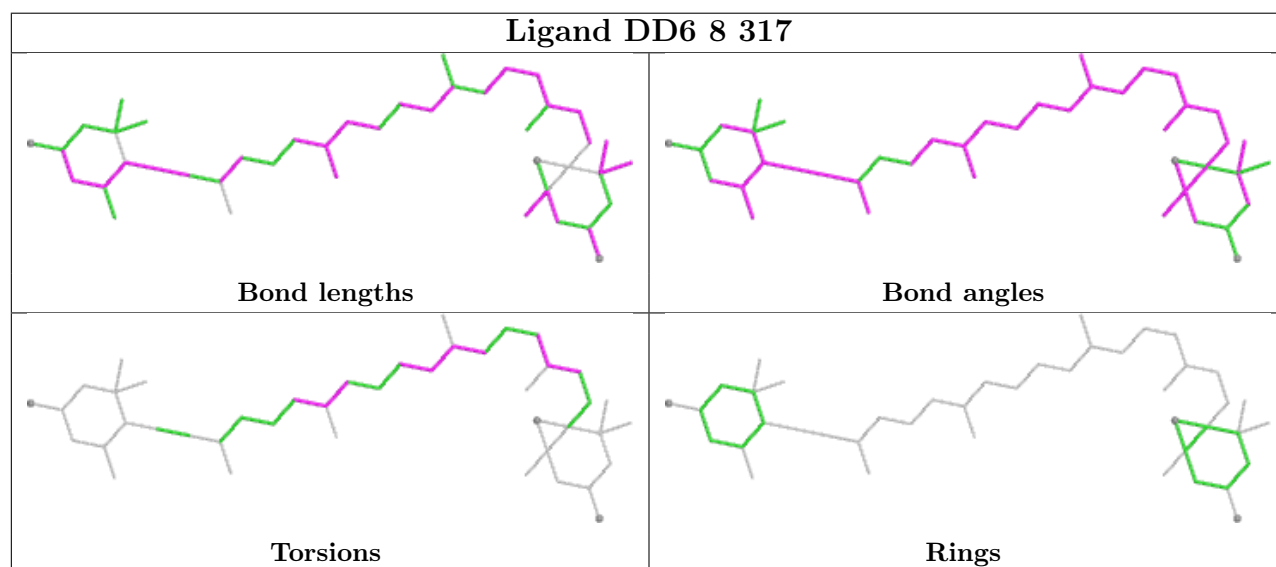
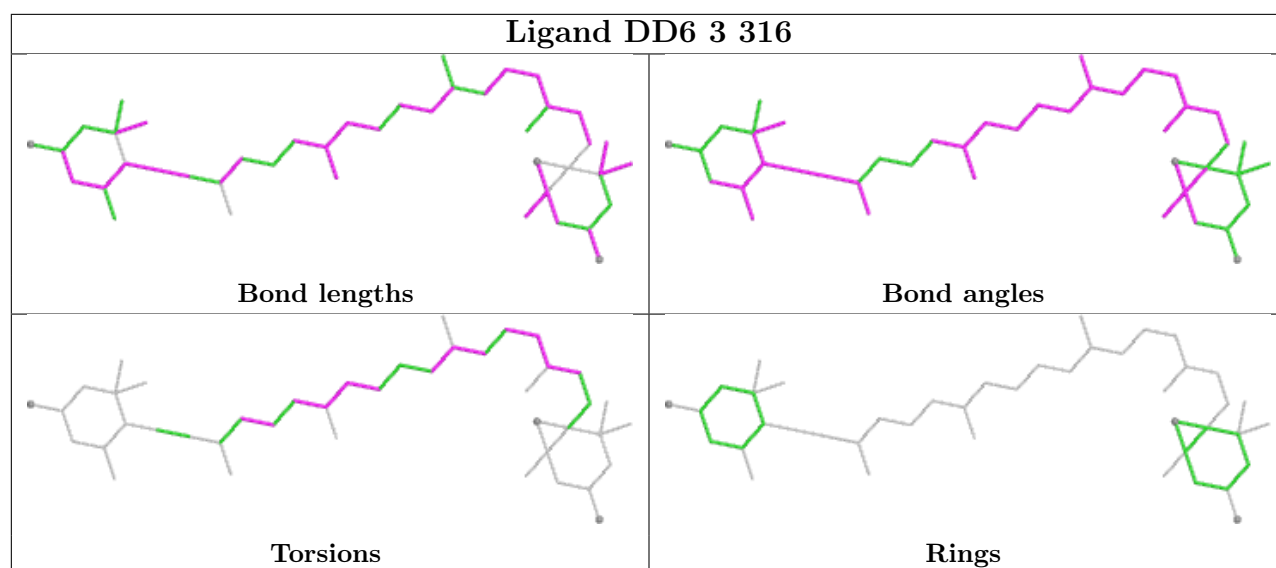
Bond angles

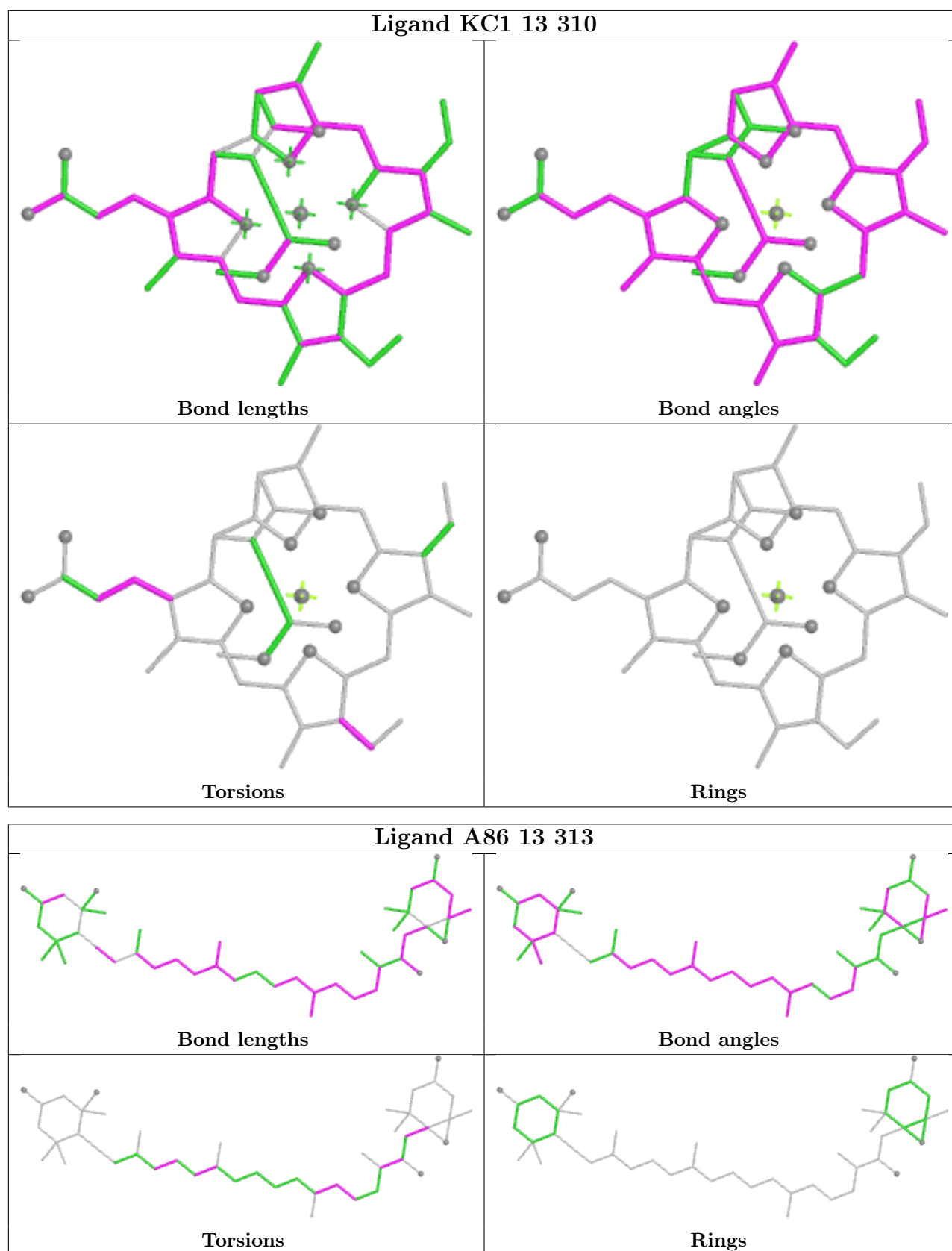


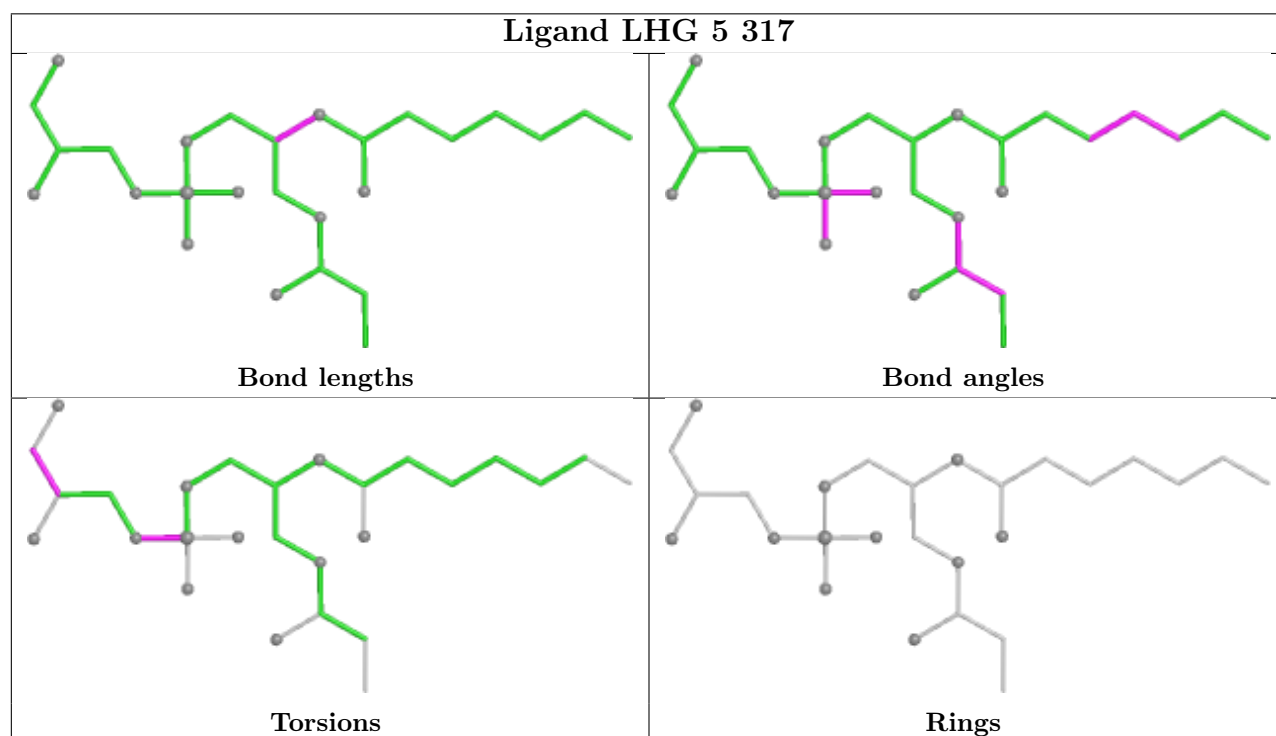
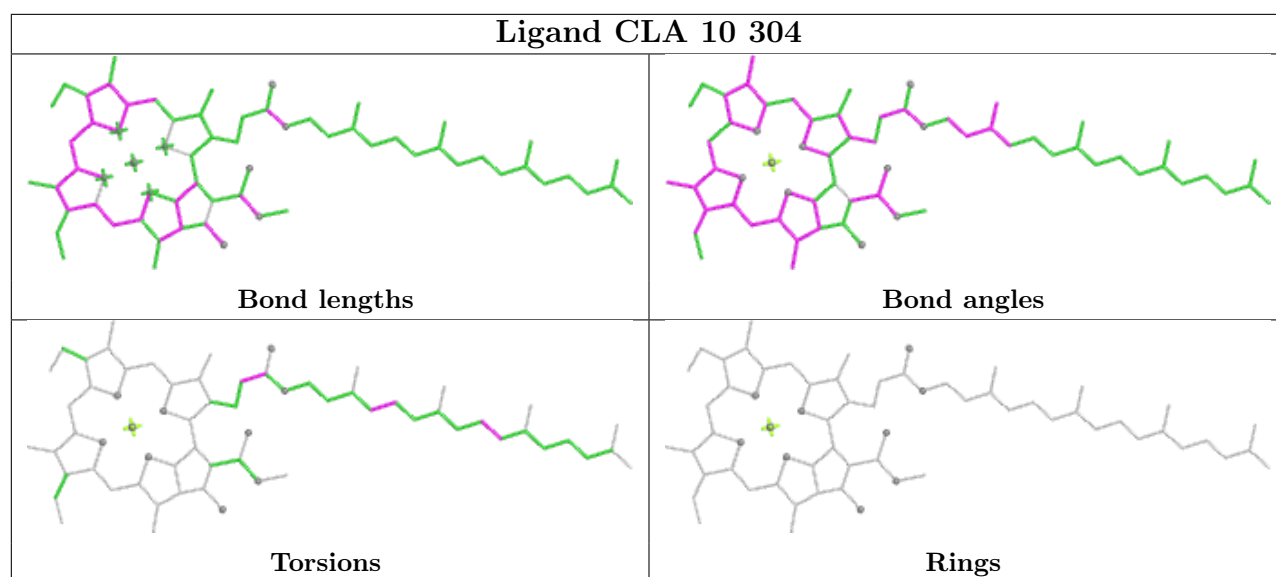
Torsions

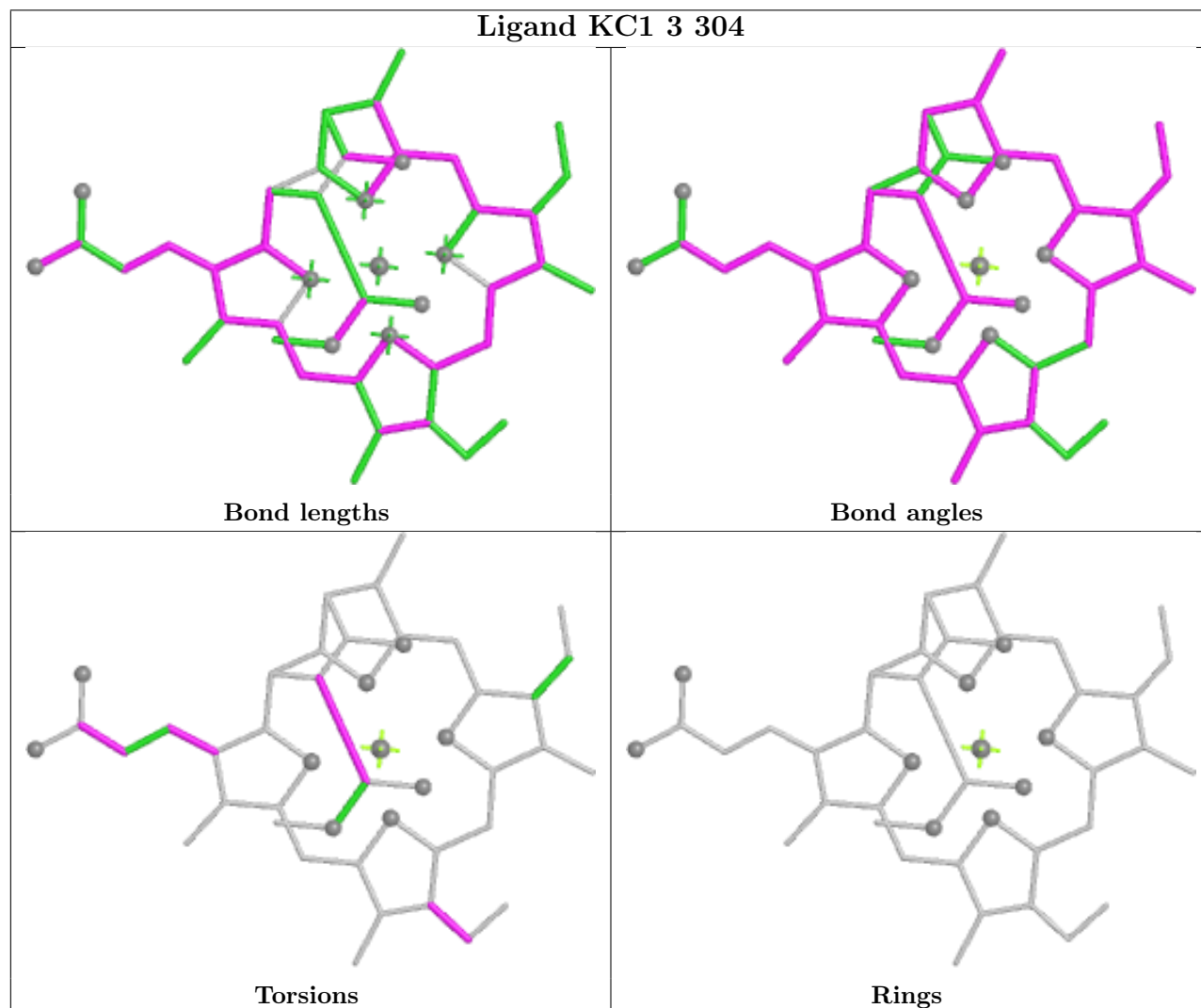
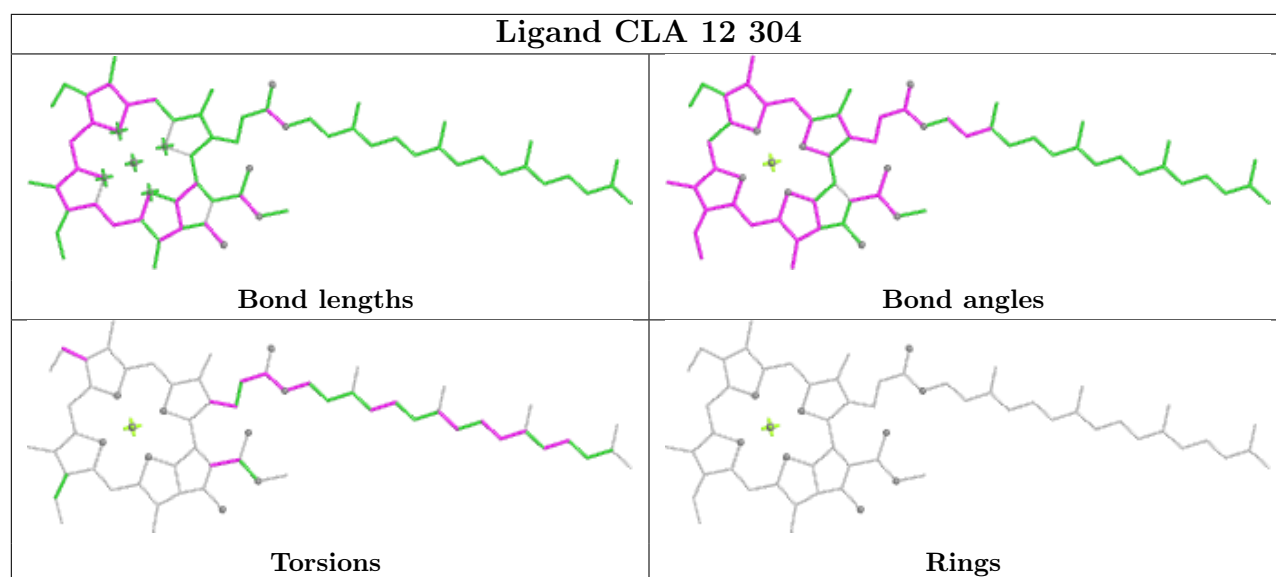


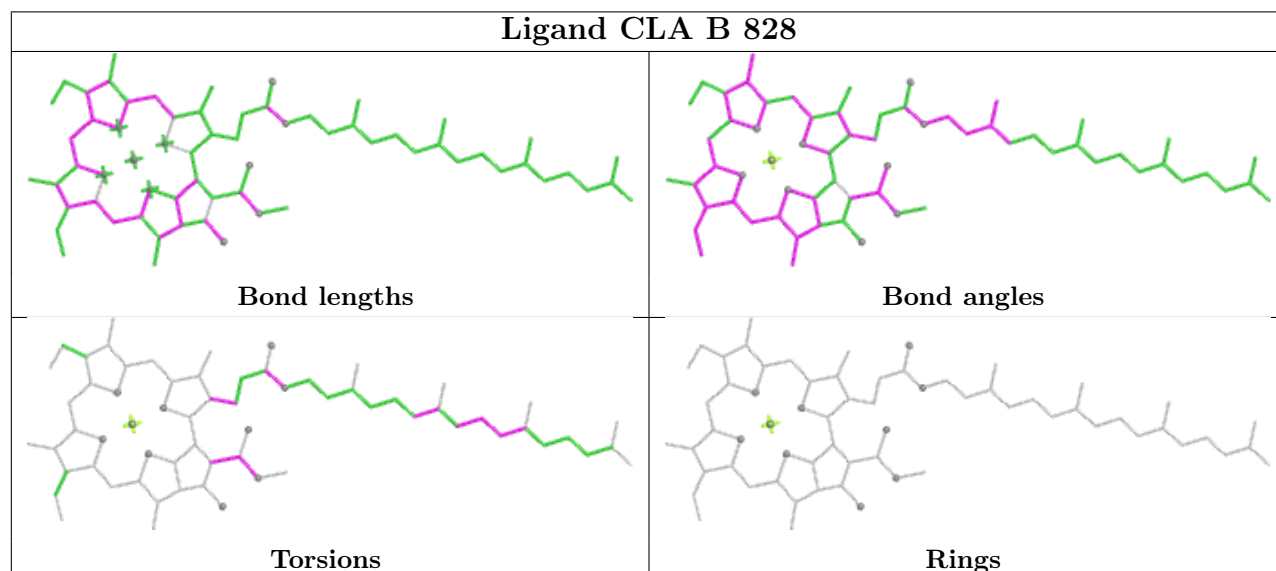
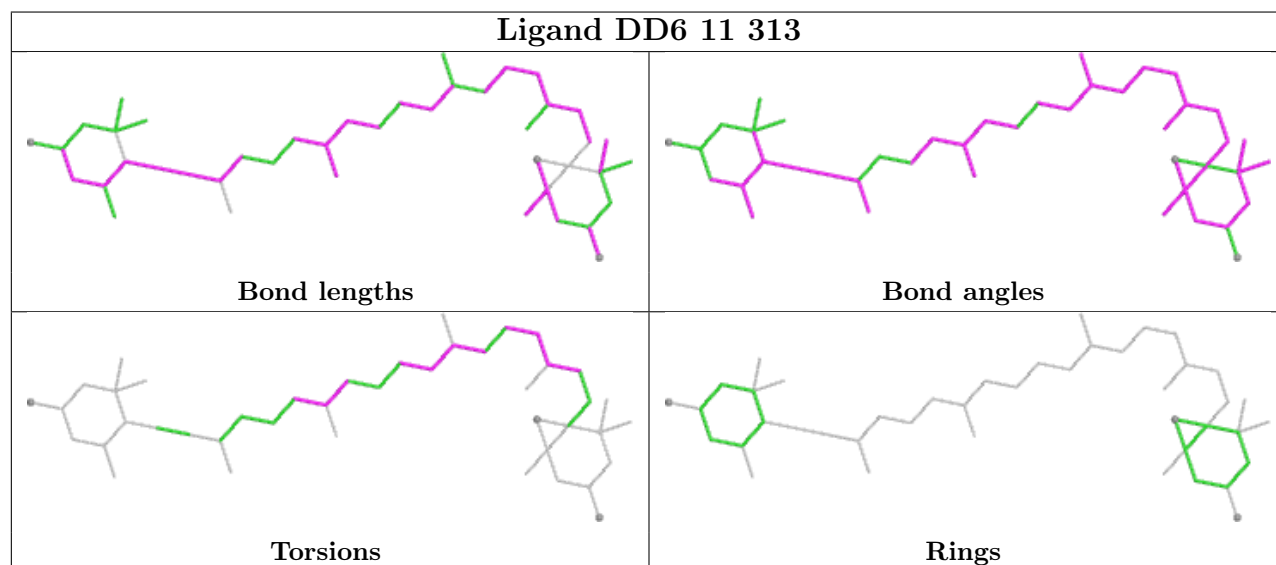
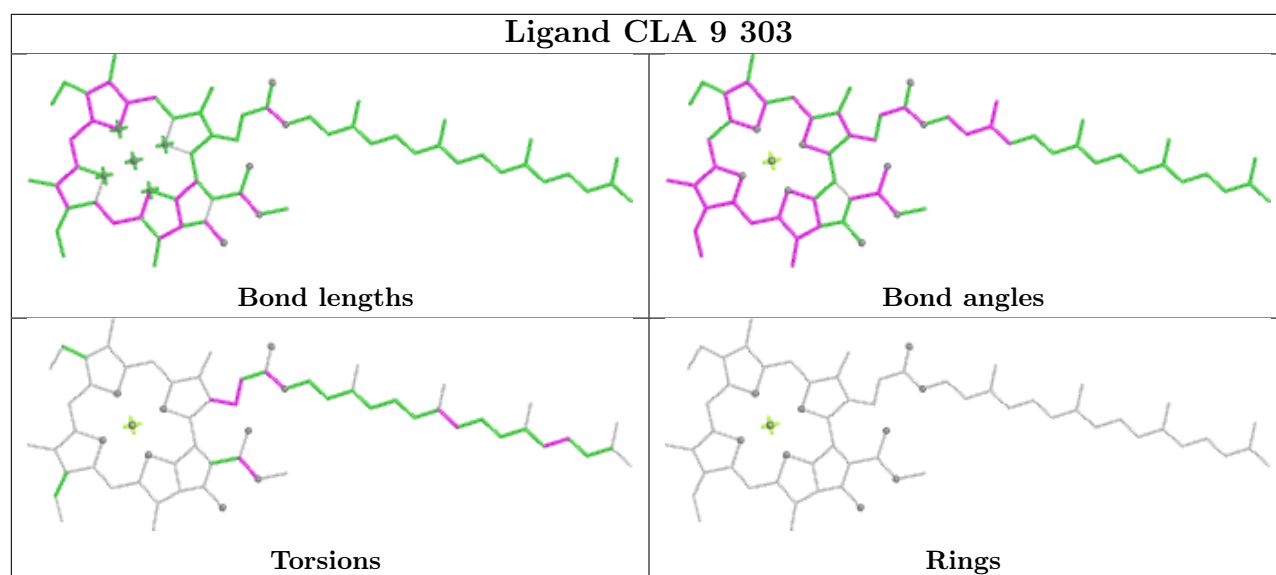
Rings

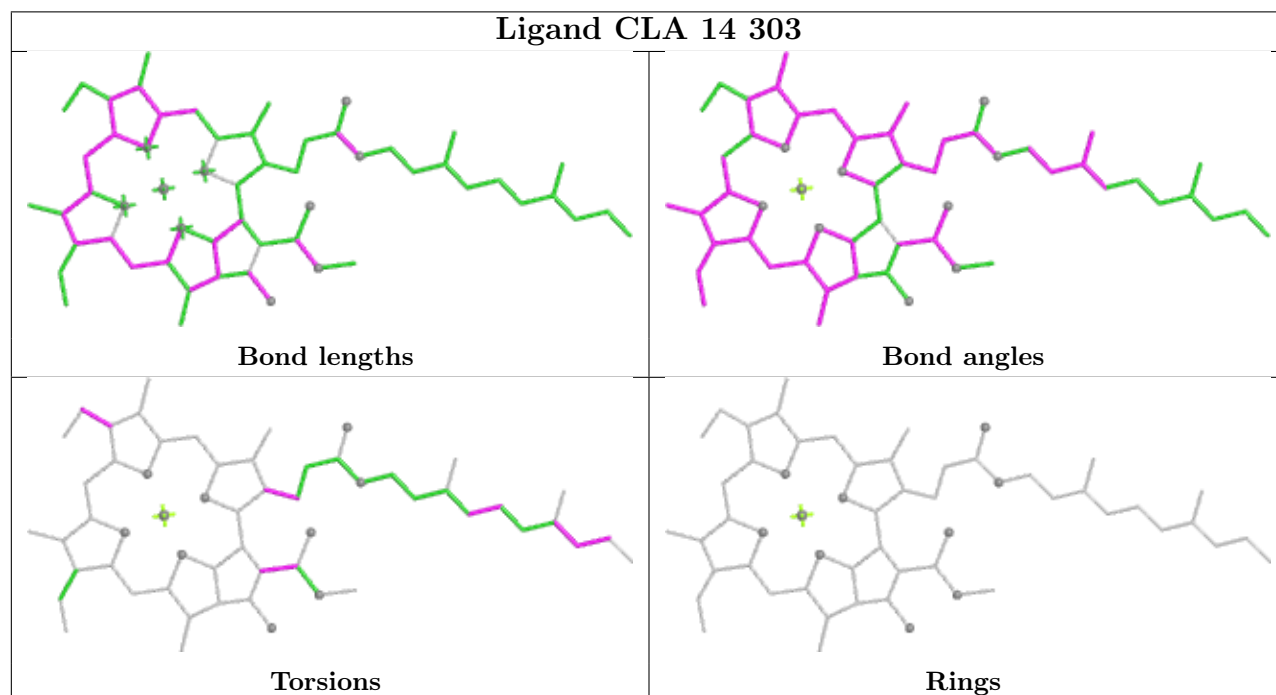
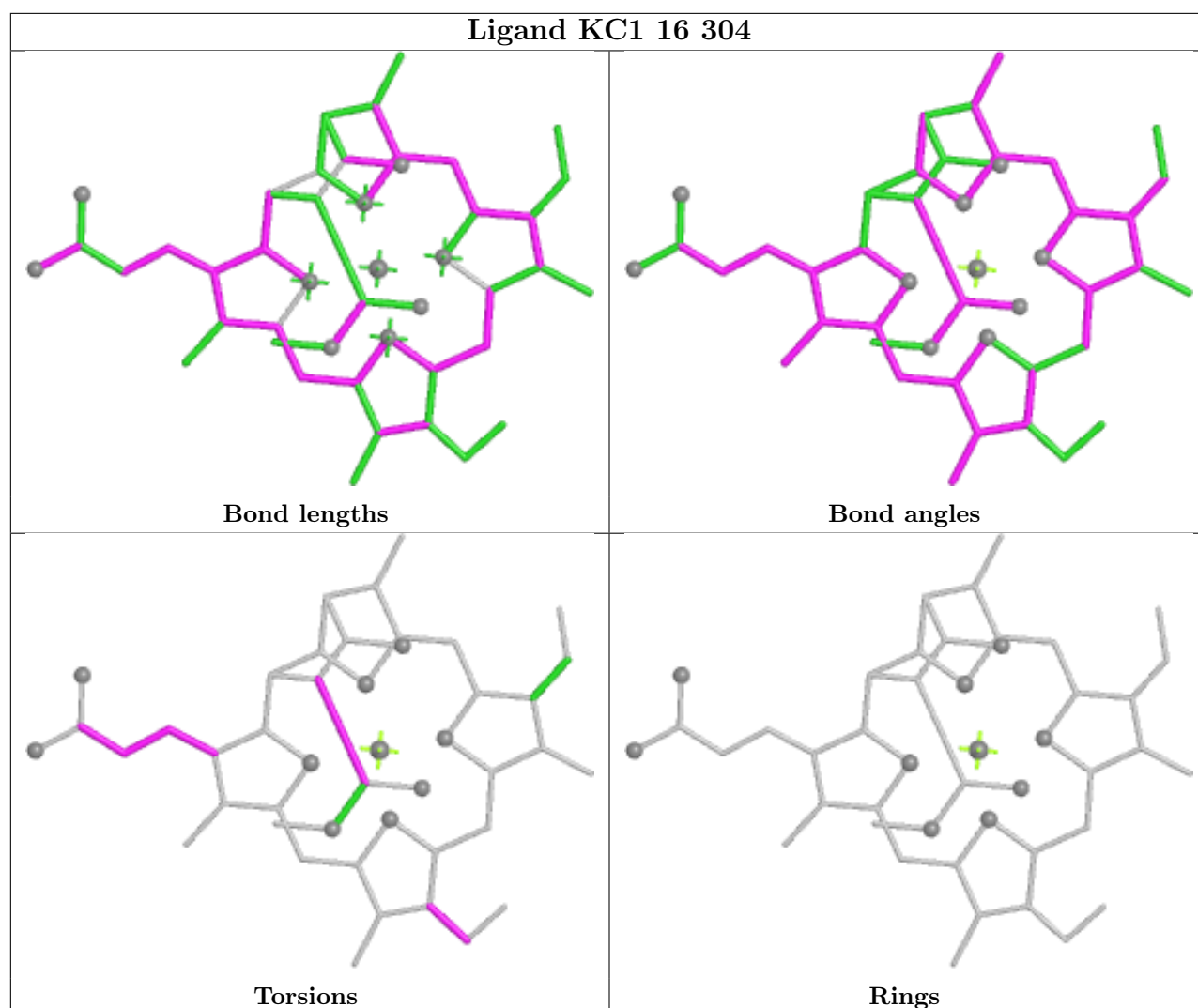


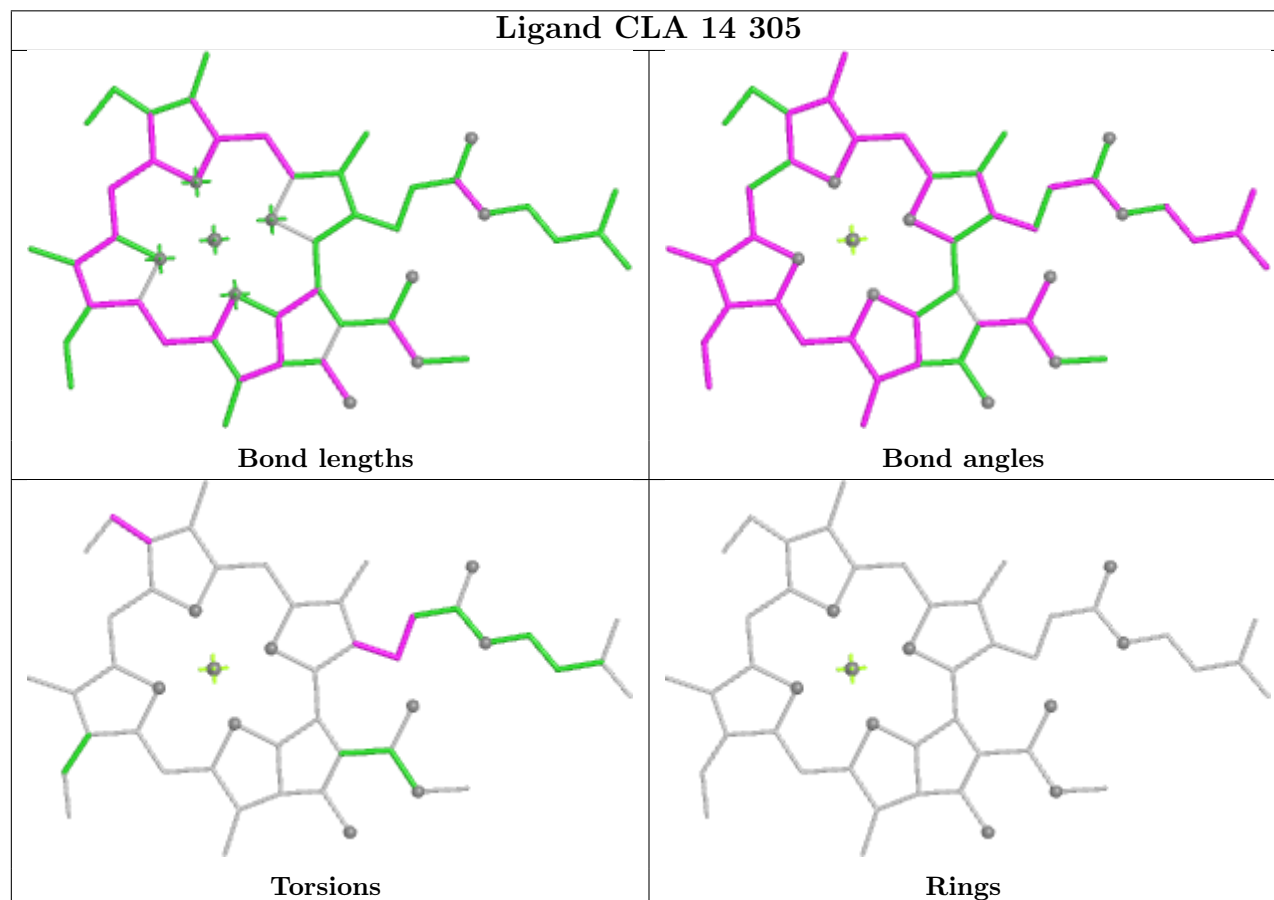
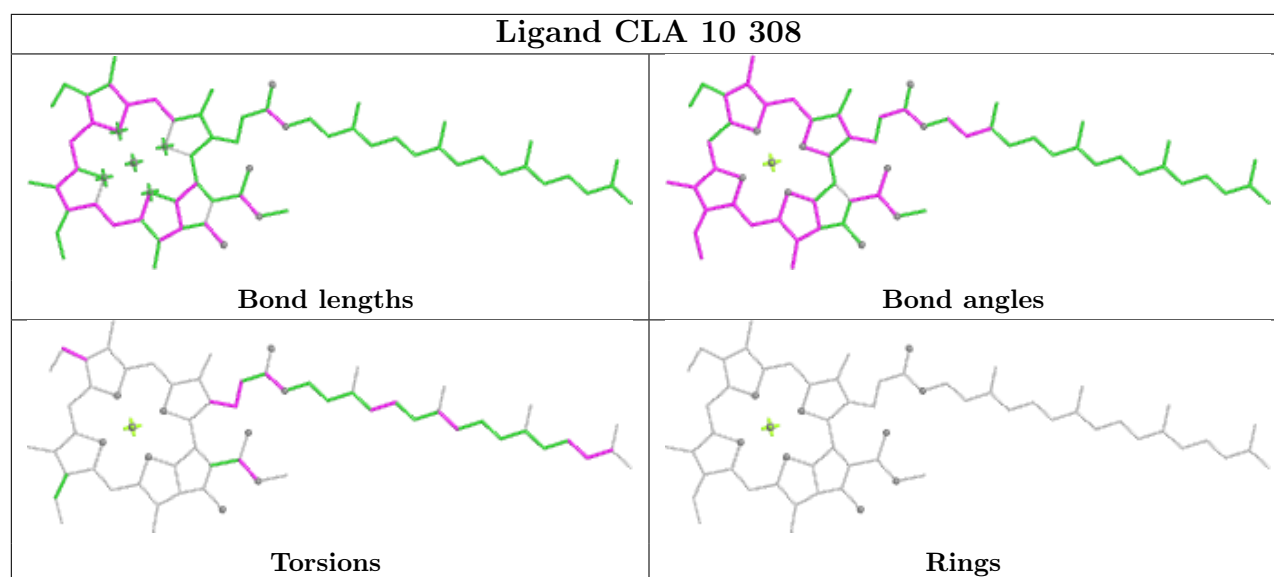


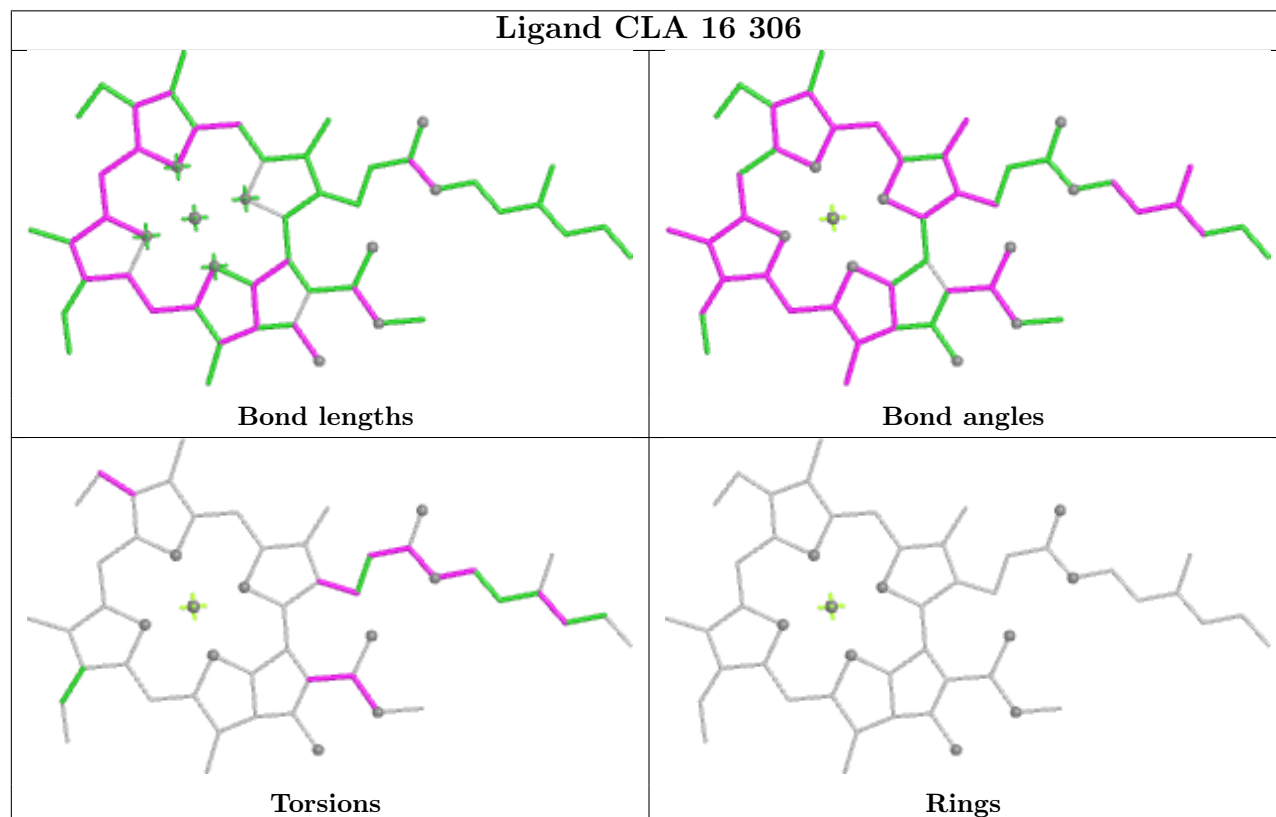
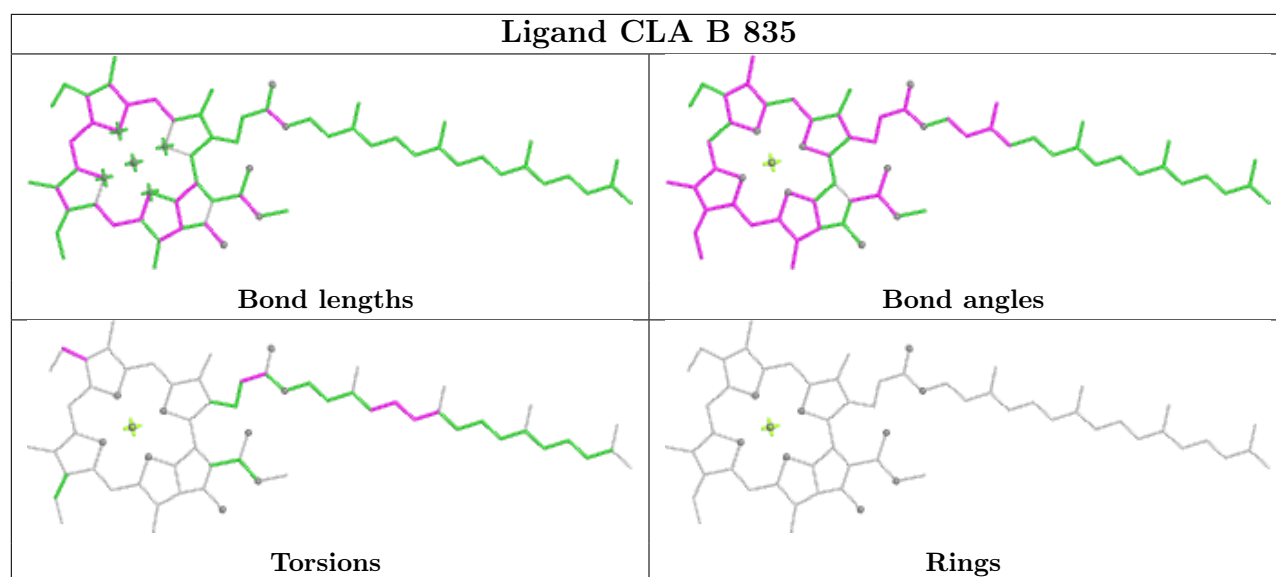


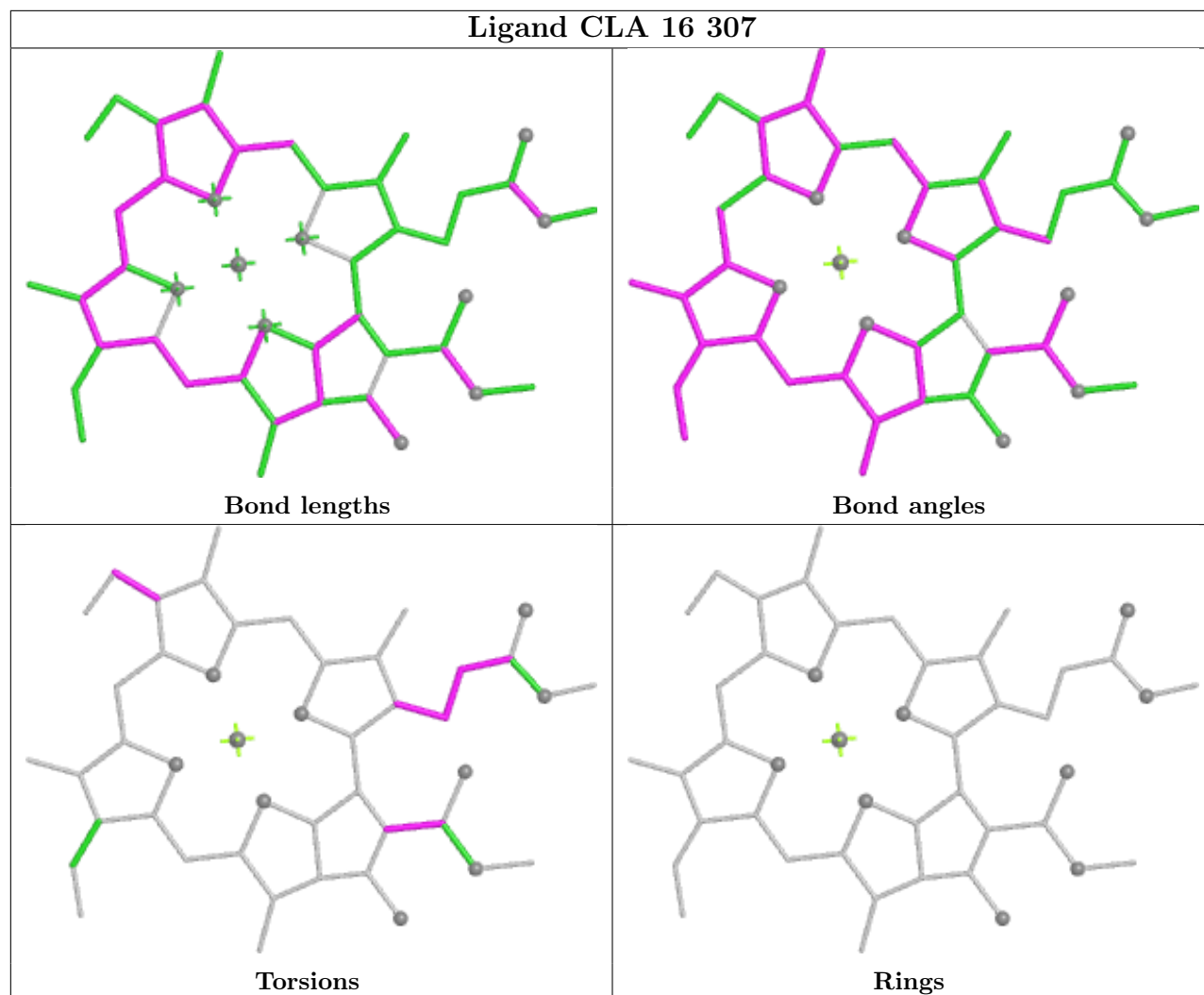




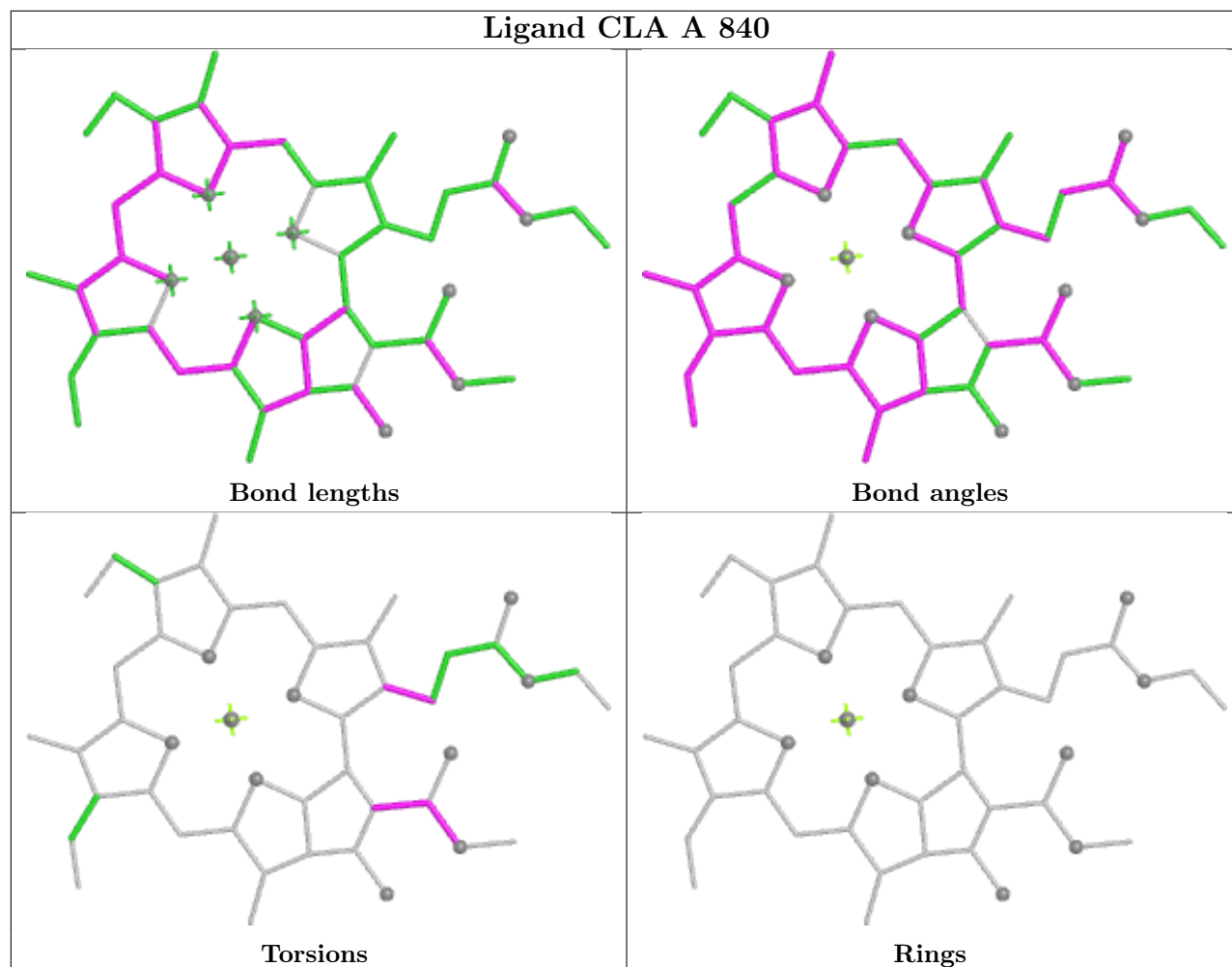


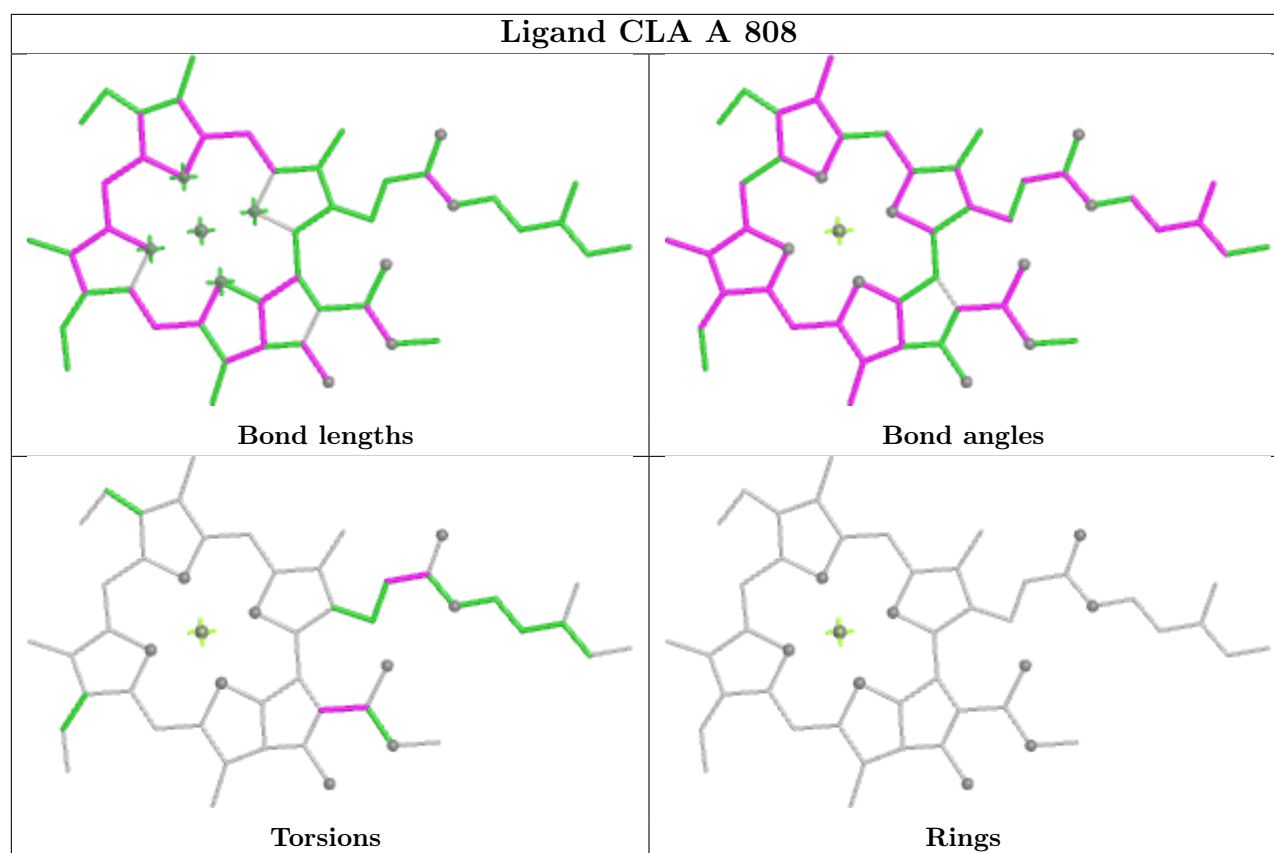




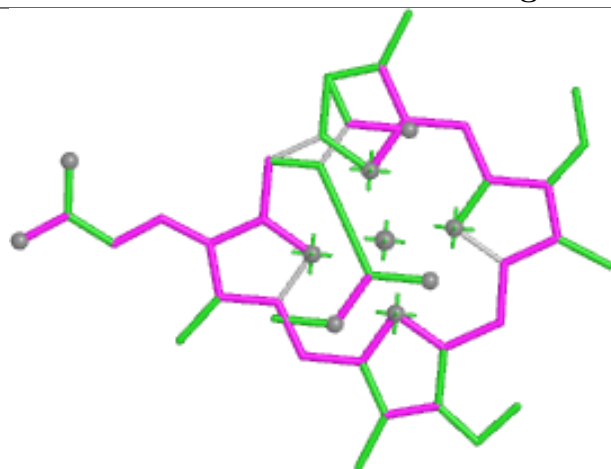


Ligand CLA A 840

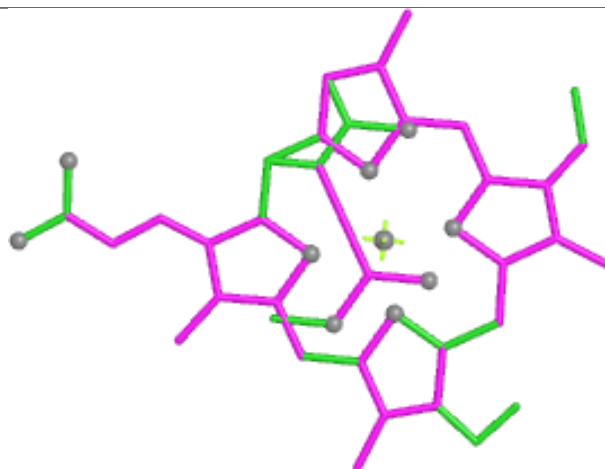




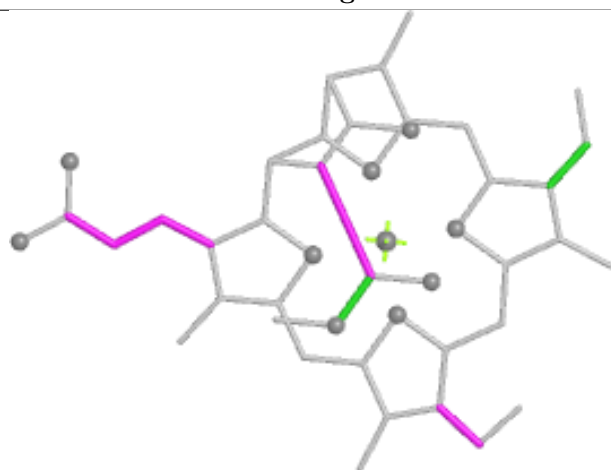
Ligand KC1 9 310



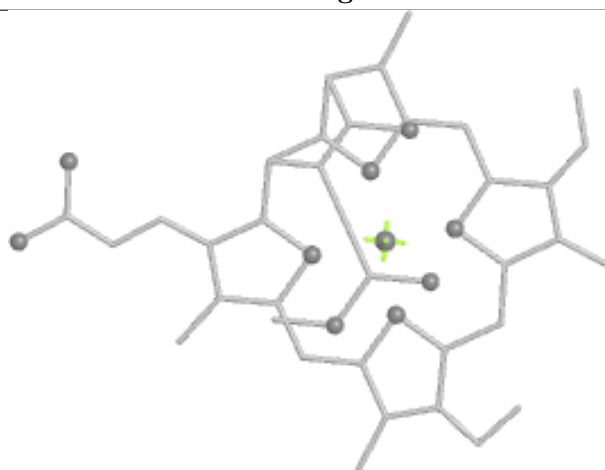
Bond lengths



Bond angles

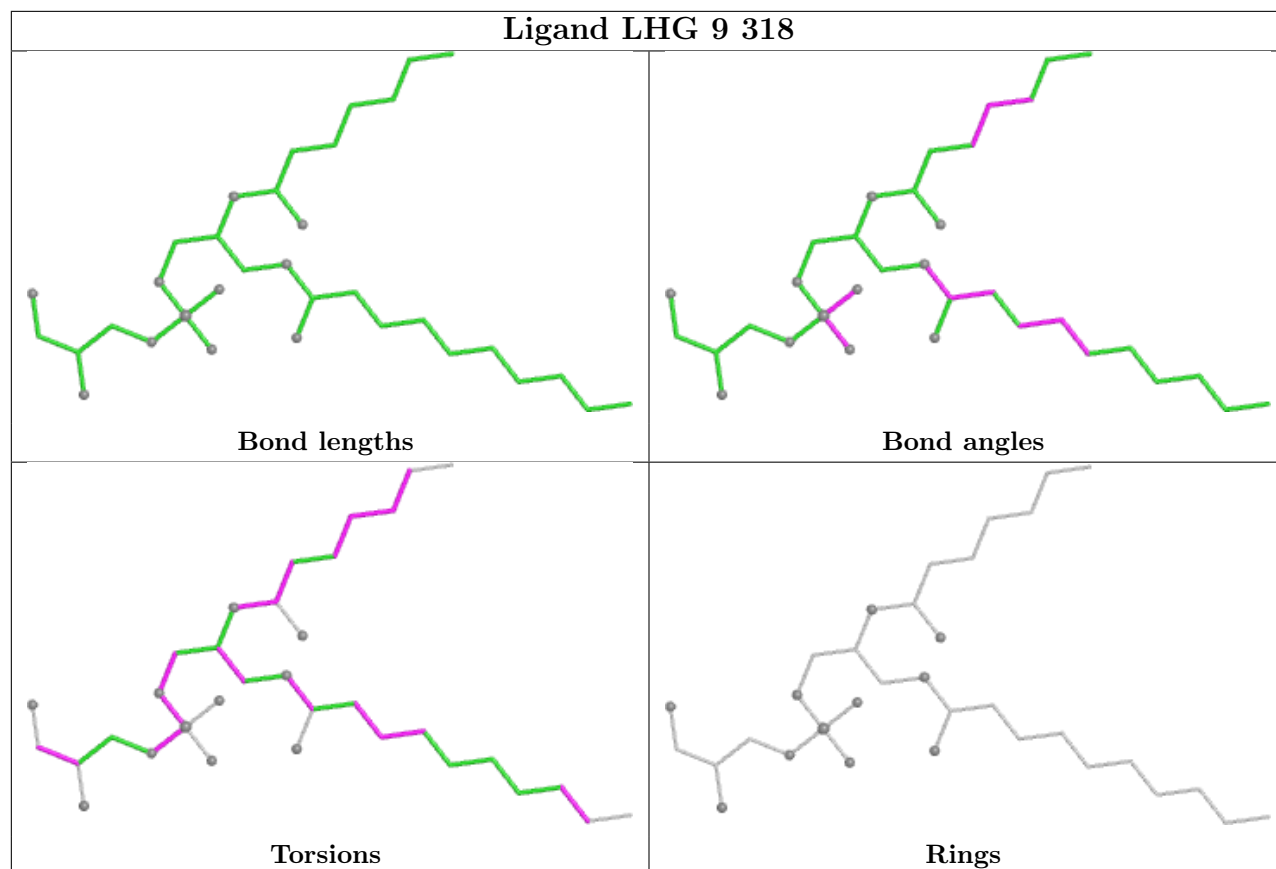


Torsions

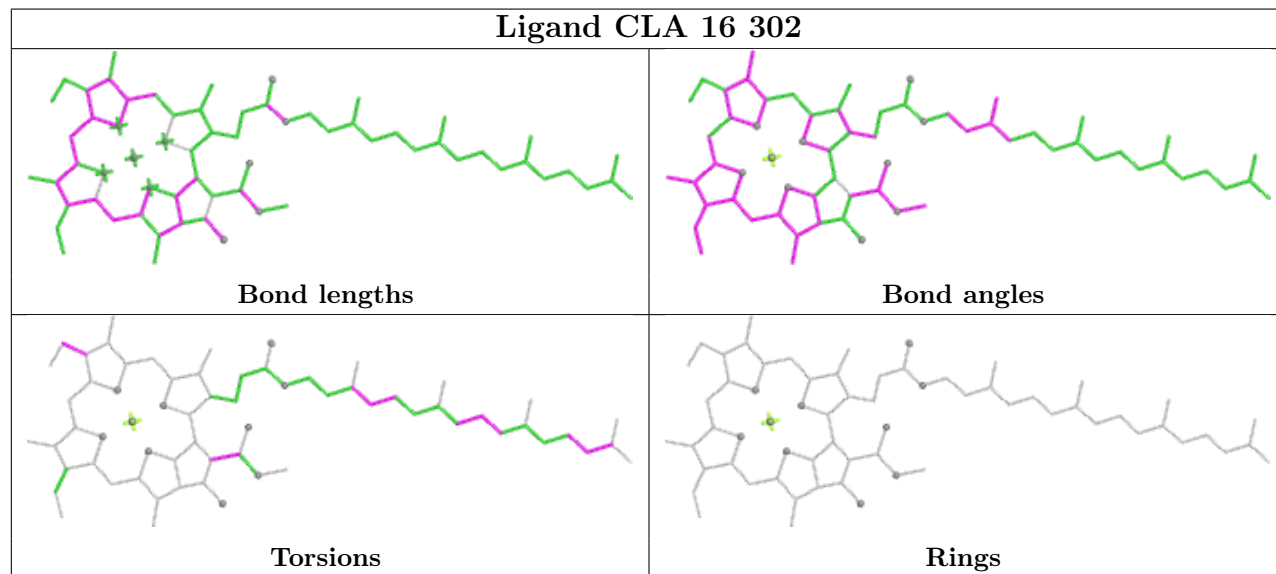


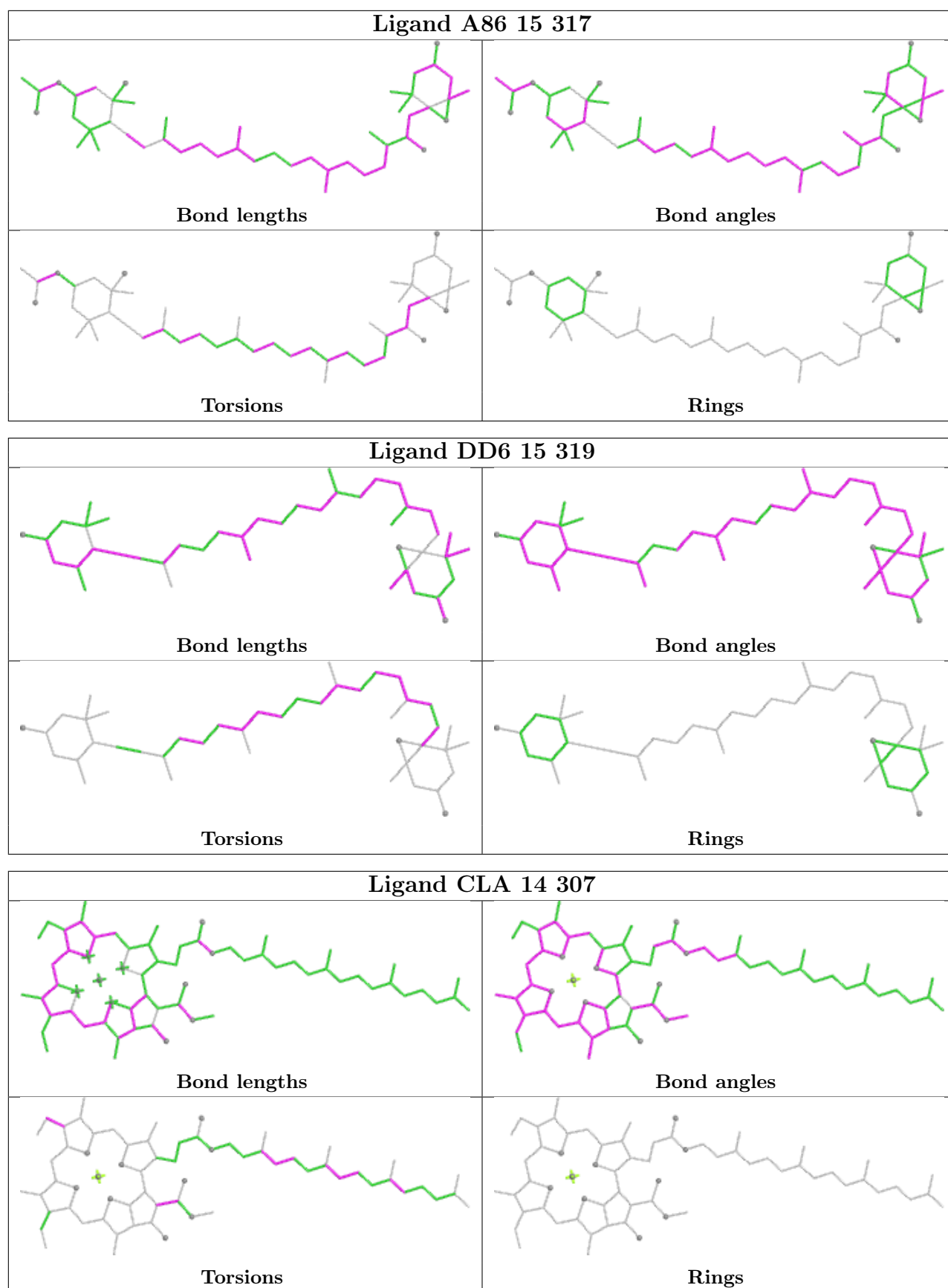
Rings

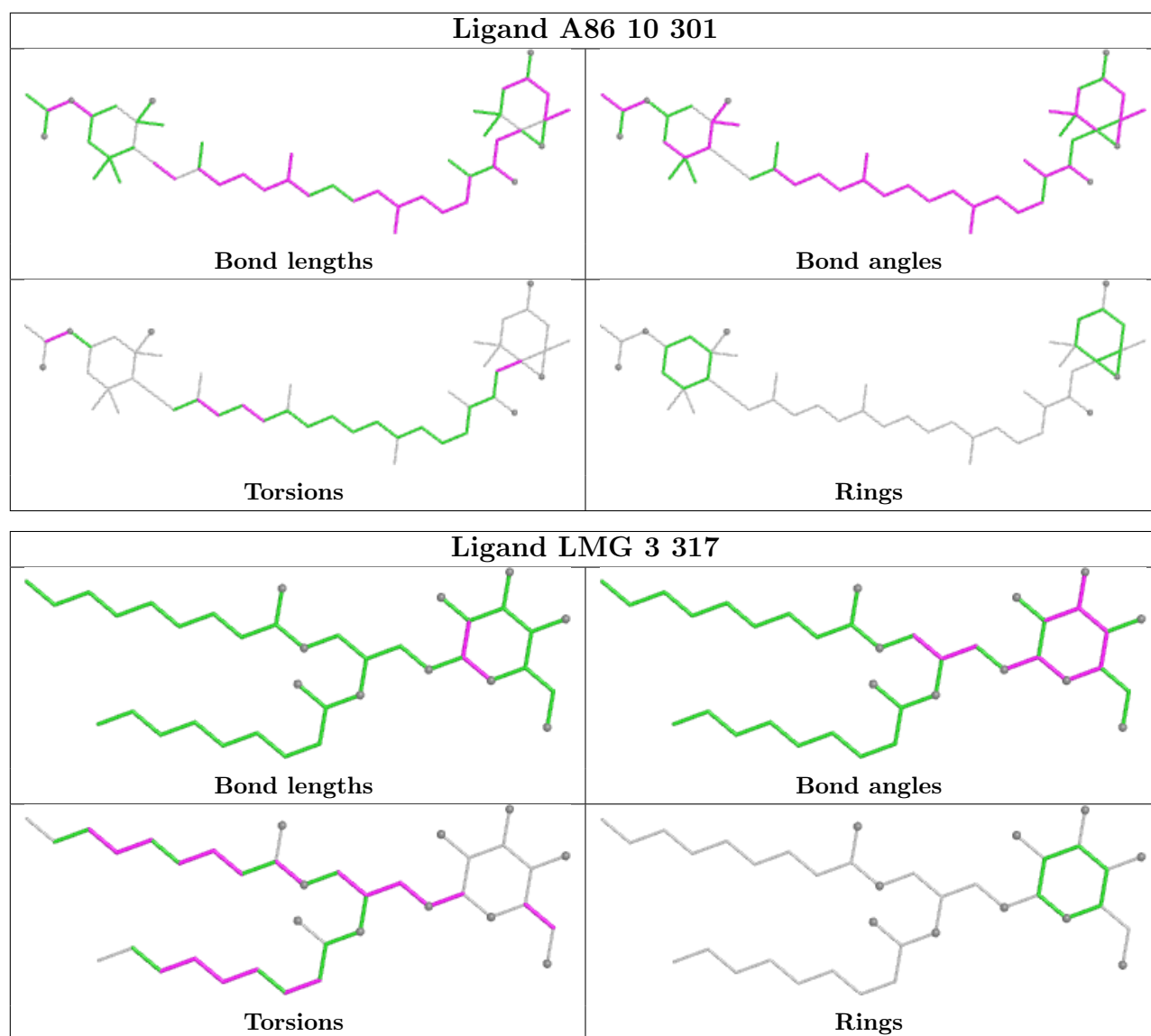
Ligand LHG 9 318



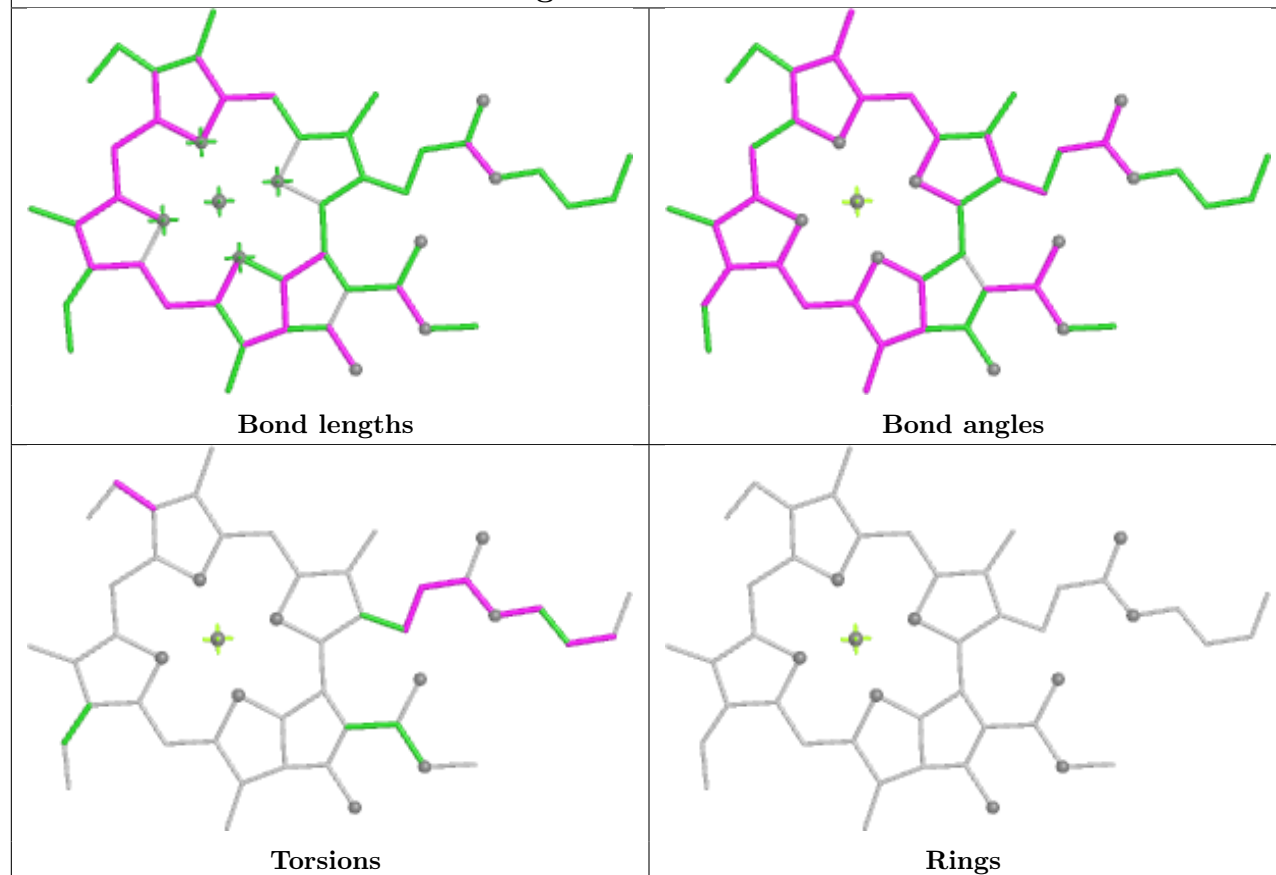
Ligand CLA 16 302



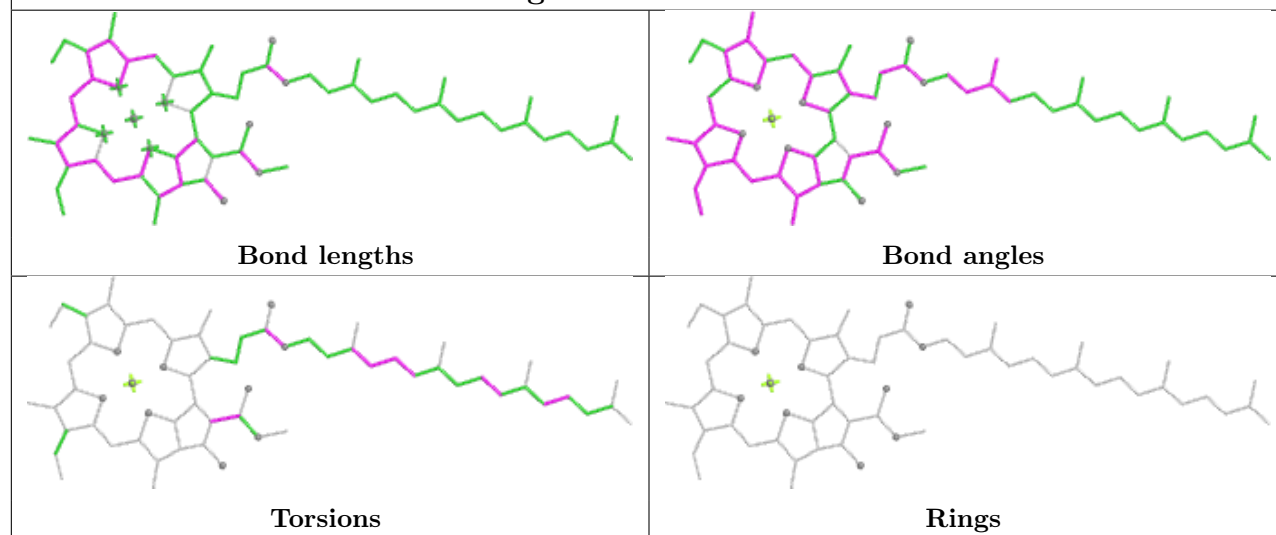


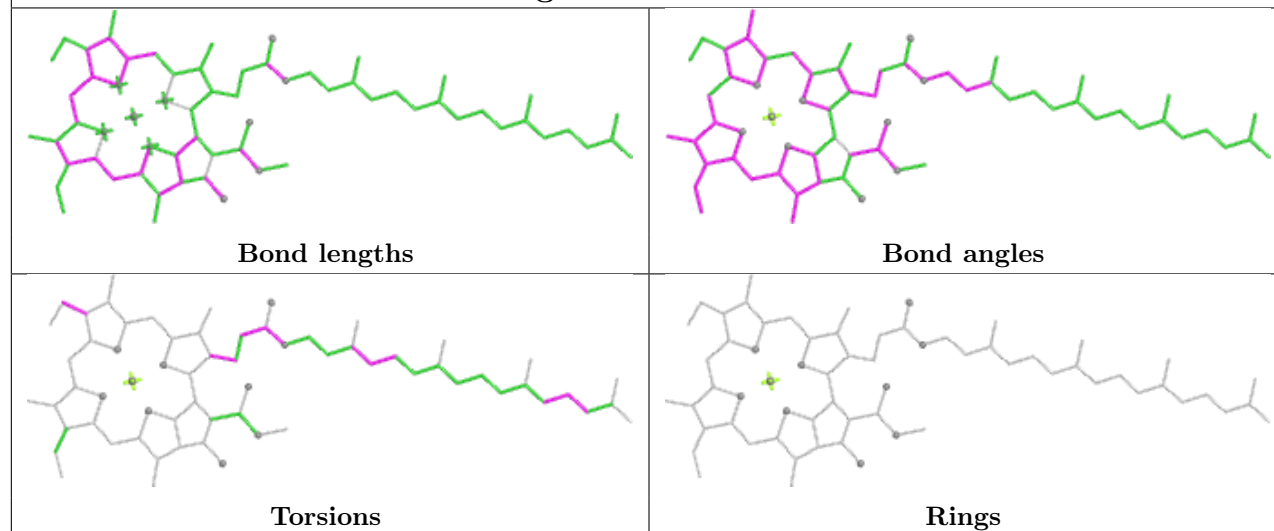
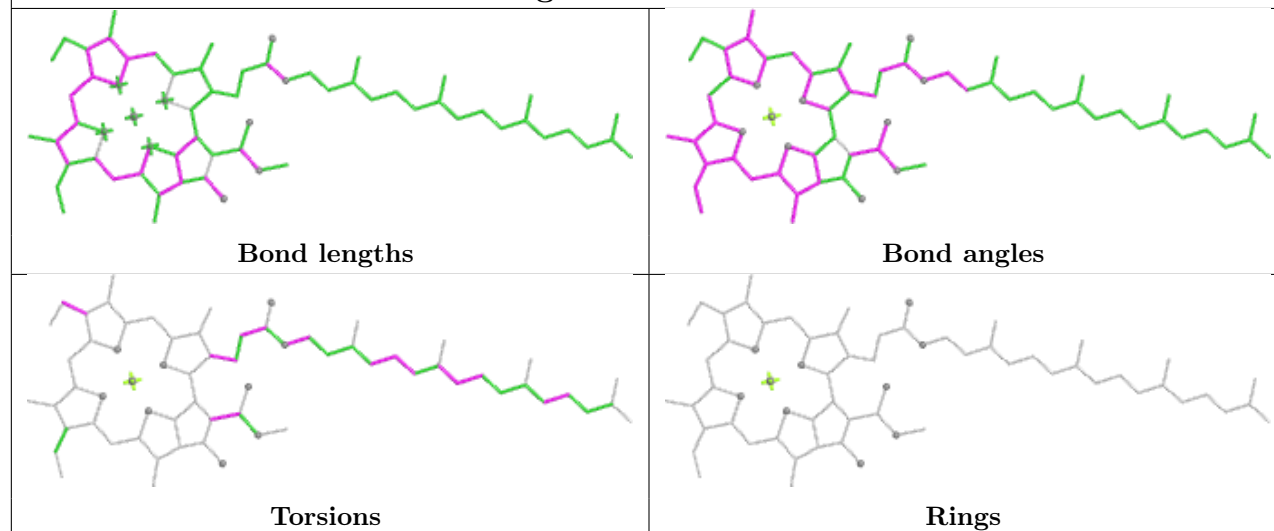
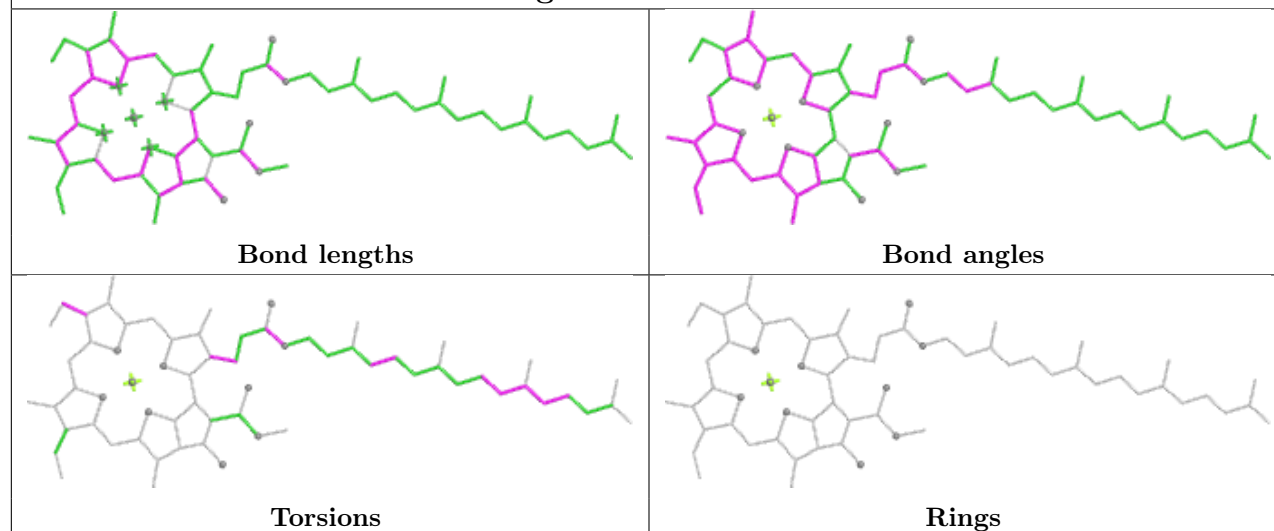


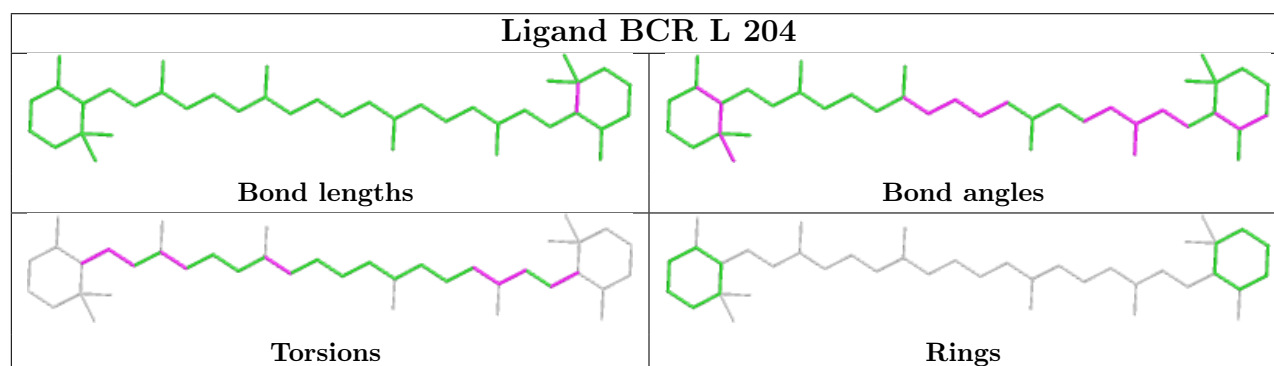
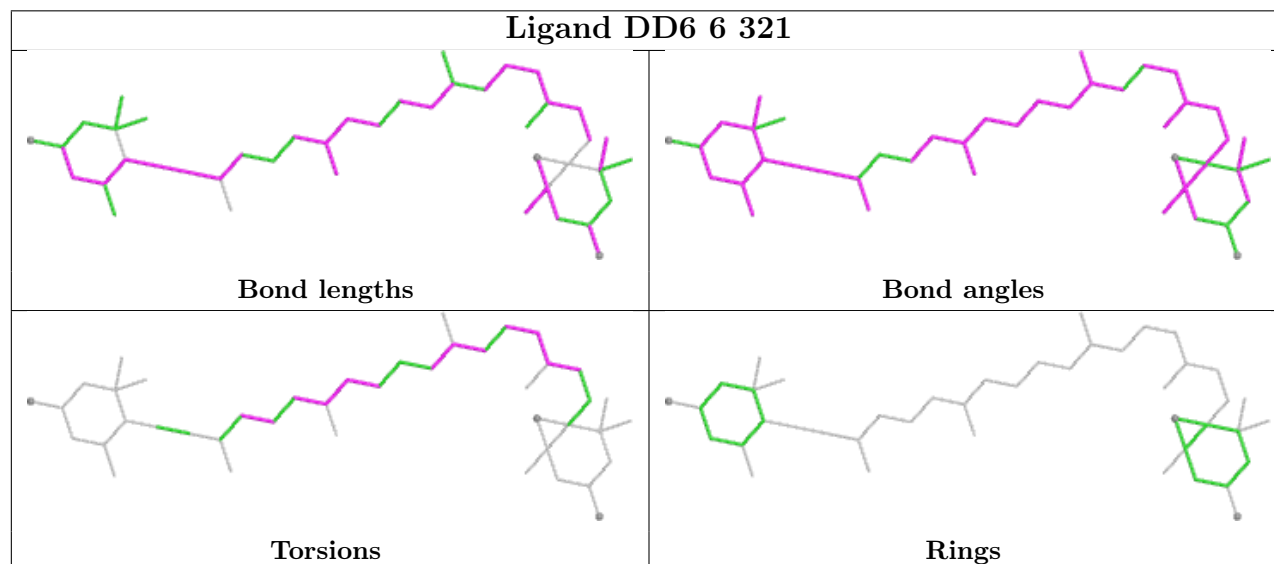
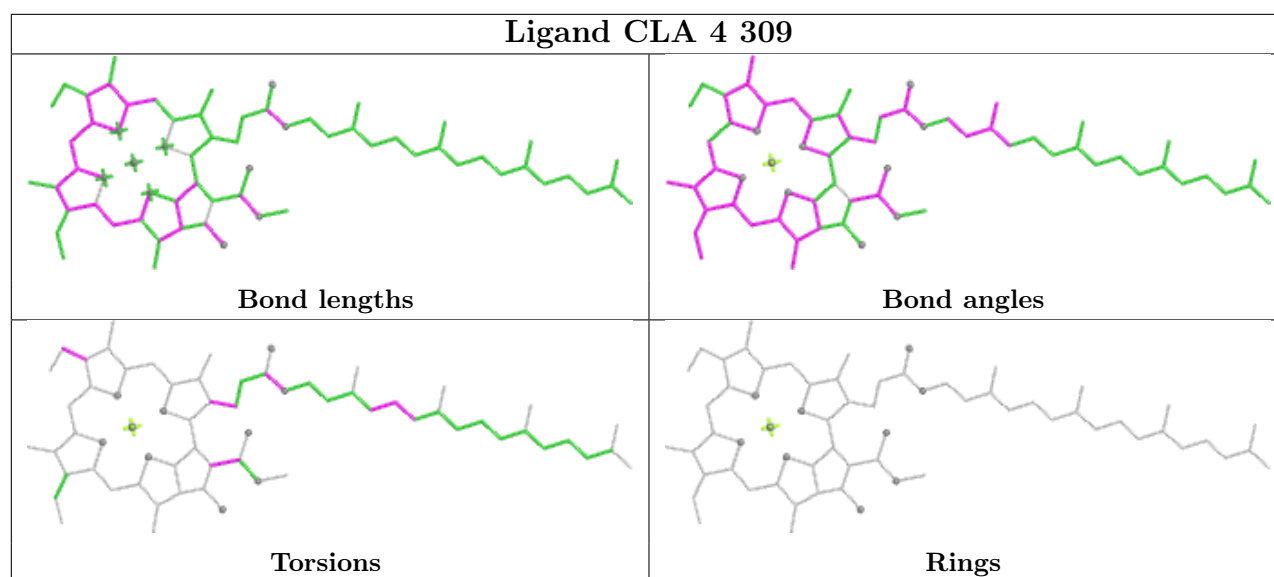
Ligand CLA 4 301



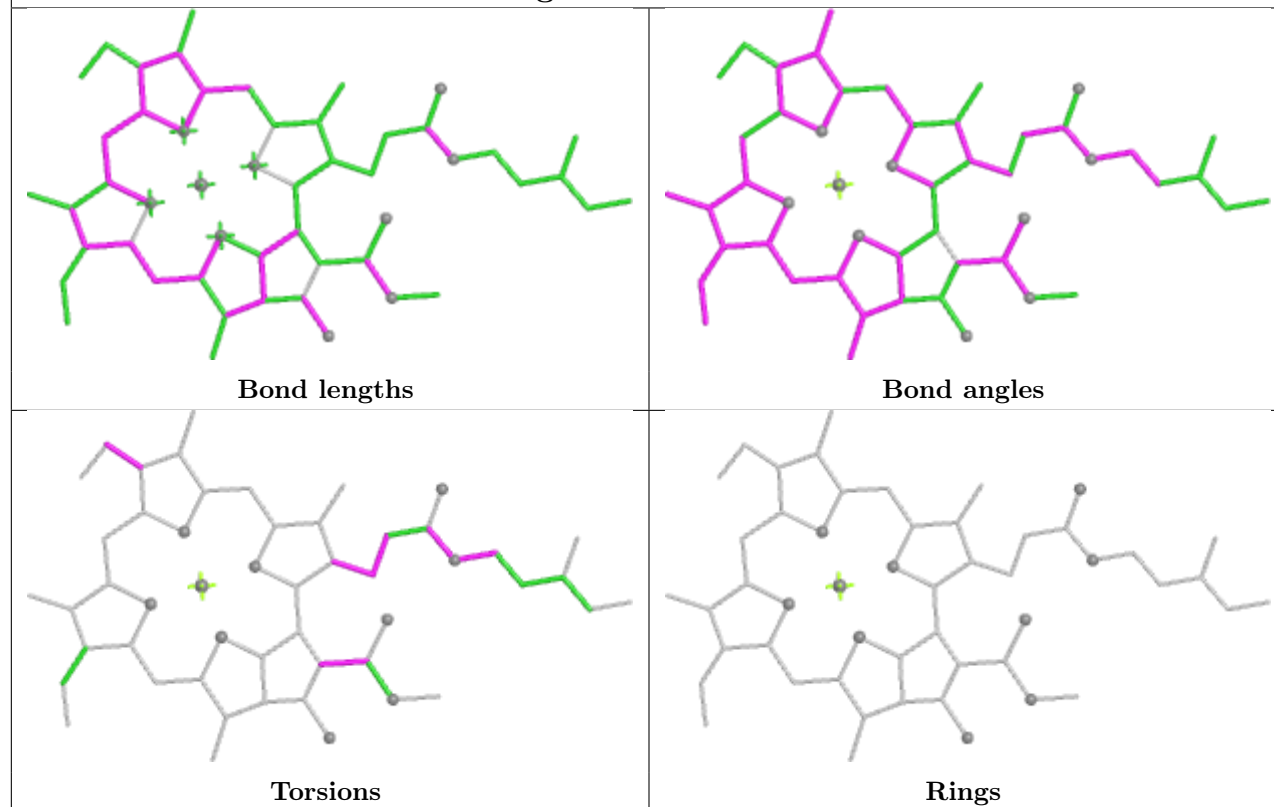
Ligand CLA 15 313



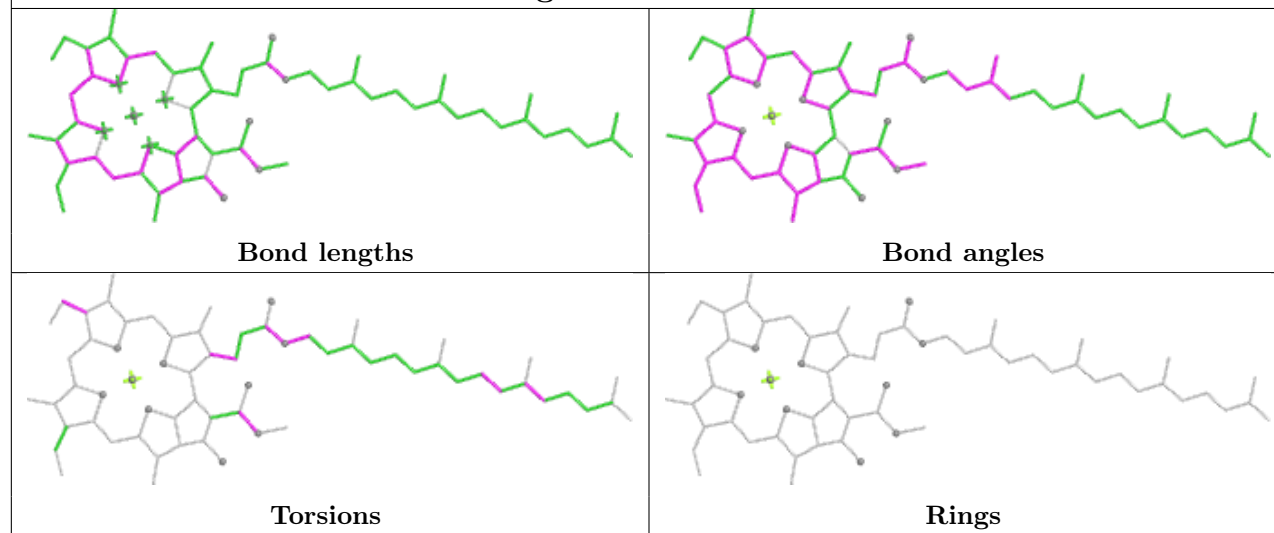
Ligand CLA 2 305**Ligand CLA 6 306****Ligand CLA 4 302**



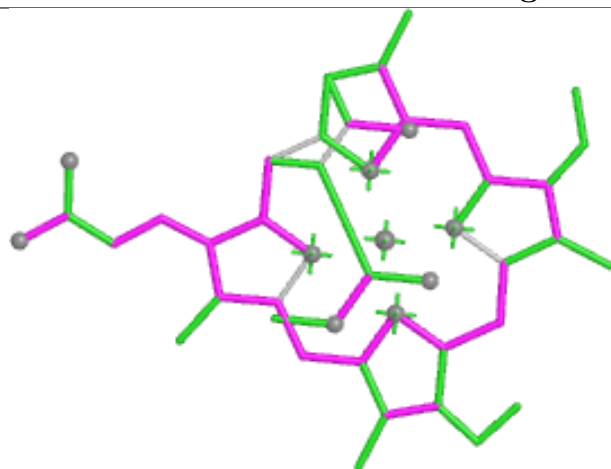
Ligand CLA 9 302



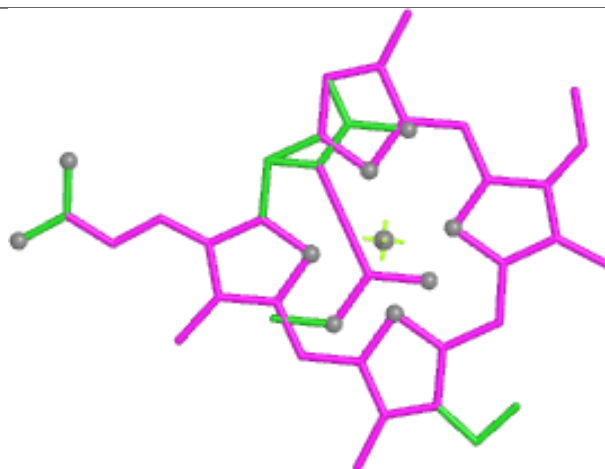
Ligand CLA 9 309



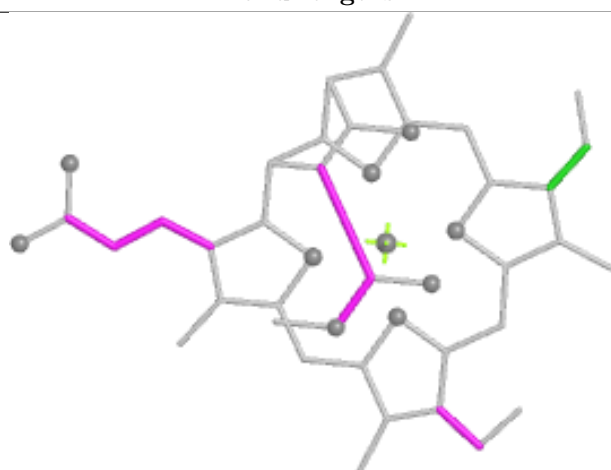
Ligand KC1 6 311



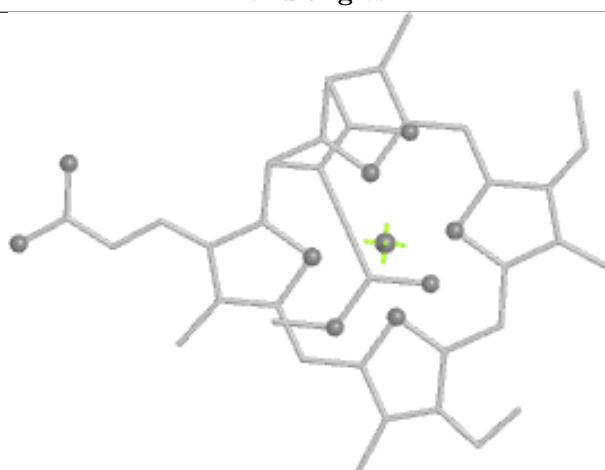
Bond lengths



Bond angles

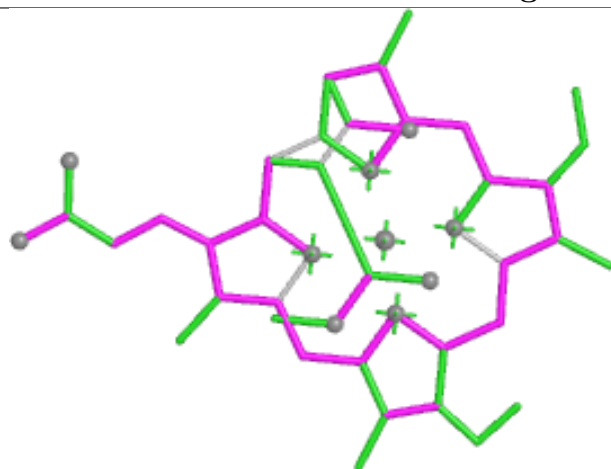


Torsions

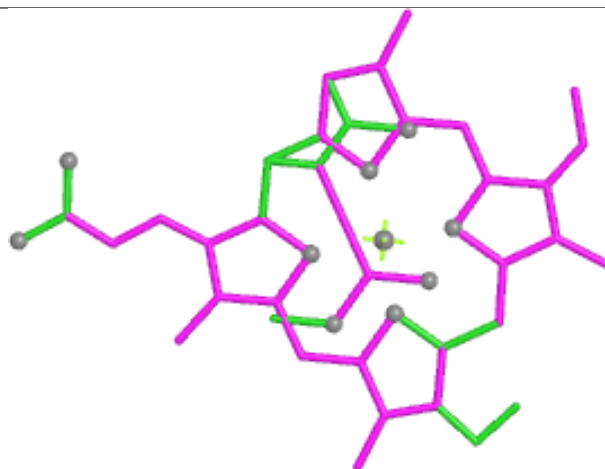


Rings

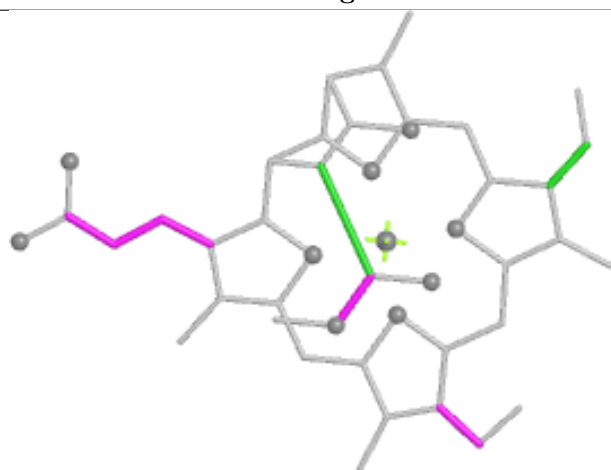
Ligand KC1 9 311



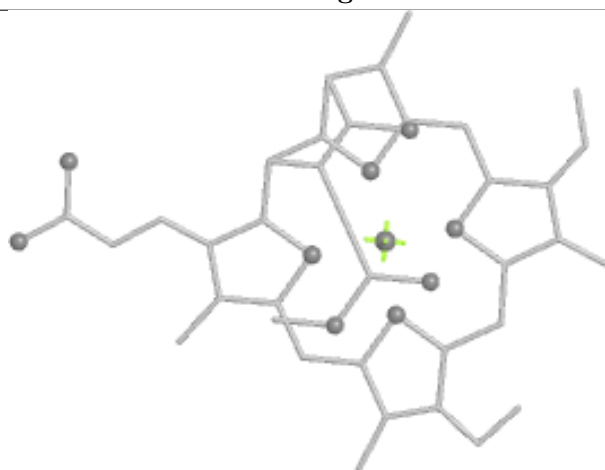
Bond lengths



Bond angles

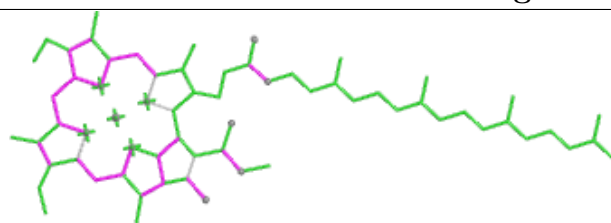


Torsions

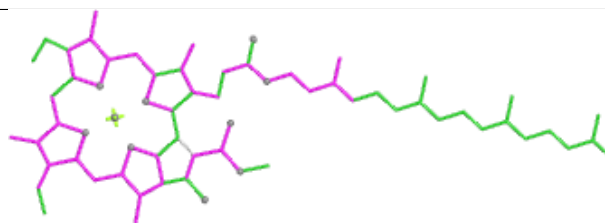


Rings

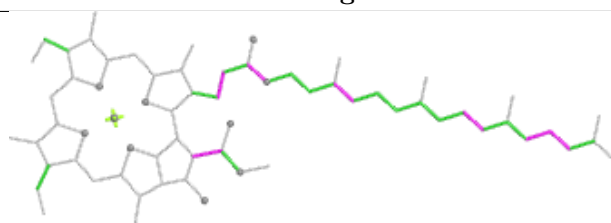
Ligand CLA A 803



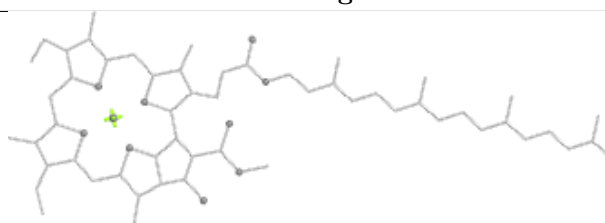
Bond lengths



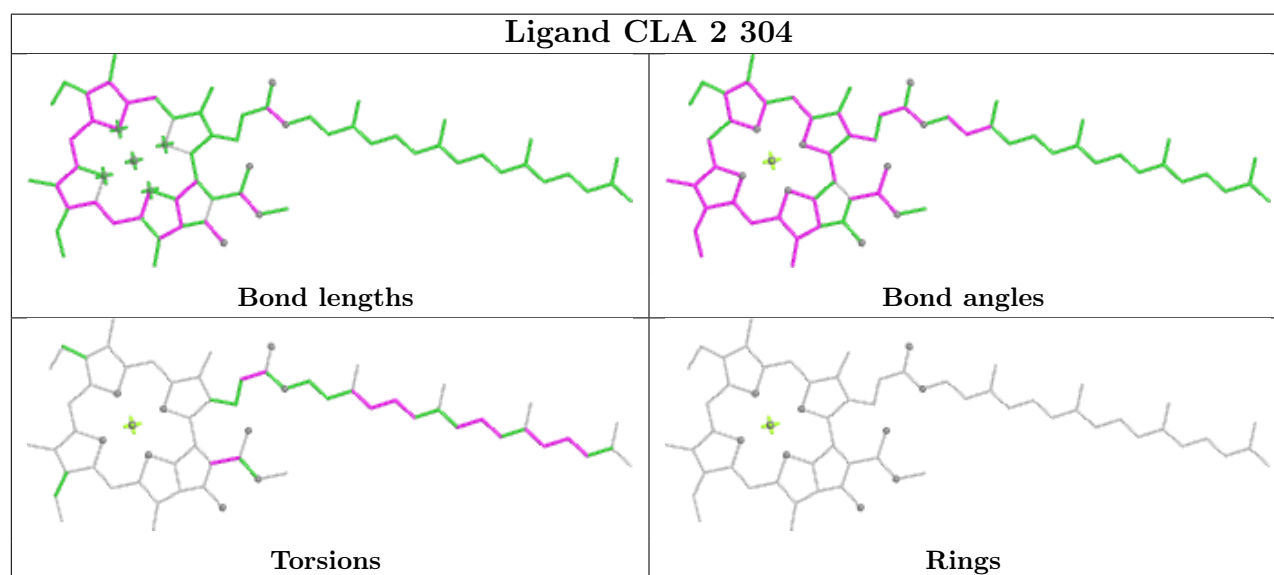
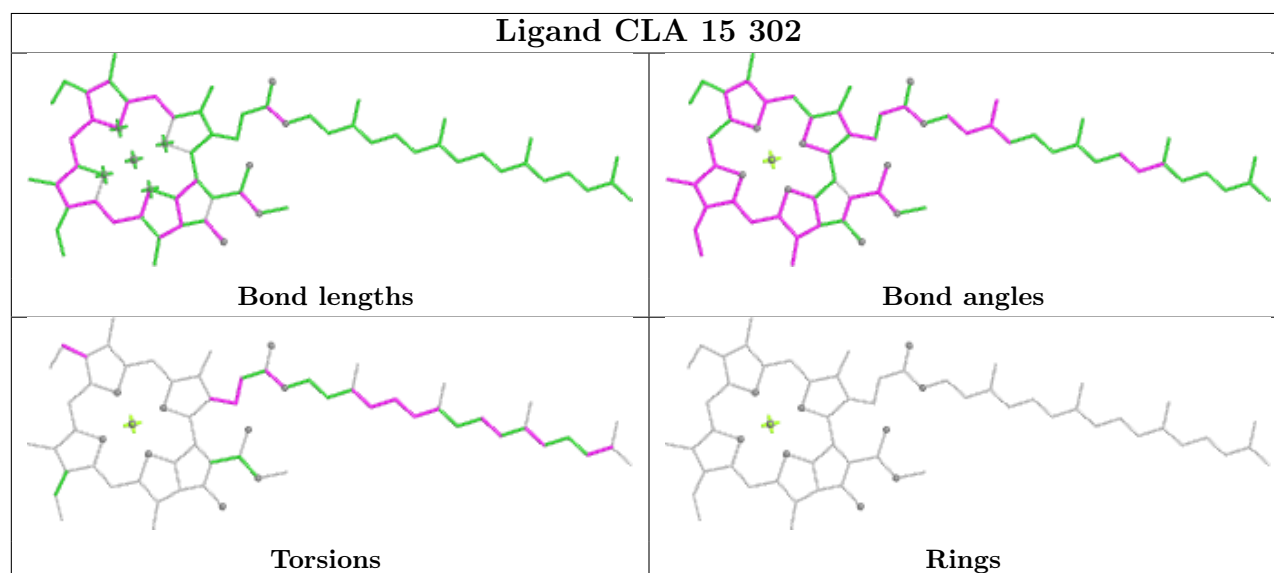
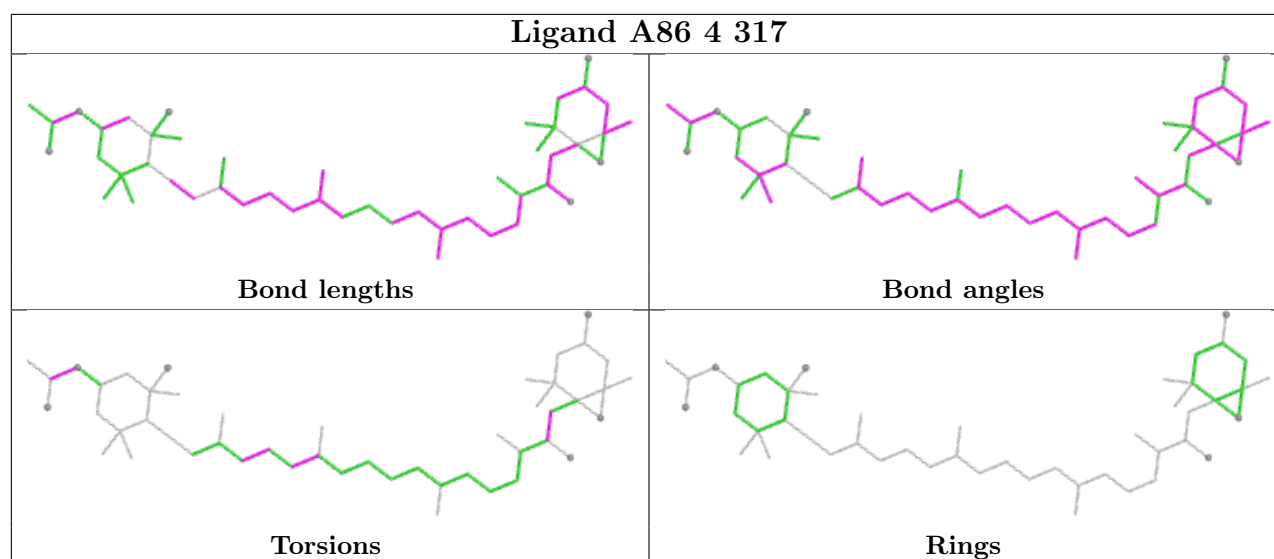
Bond angles

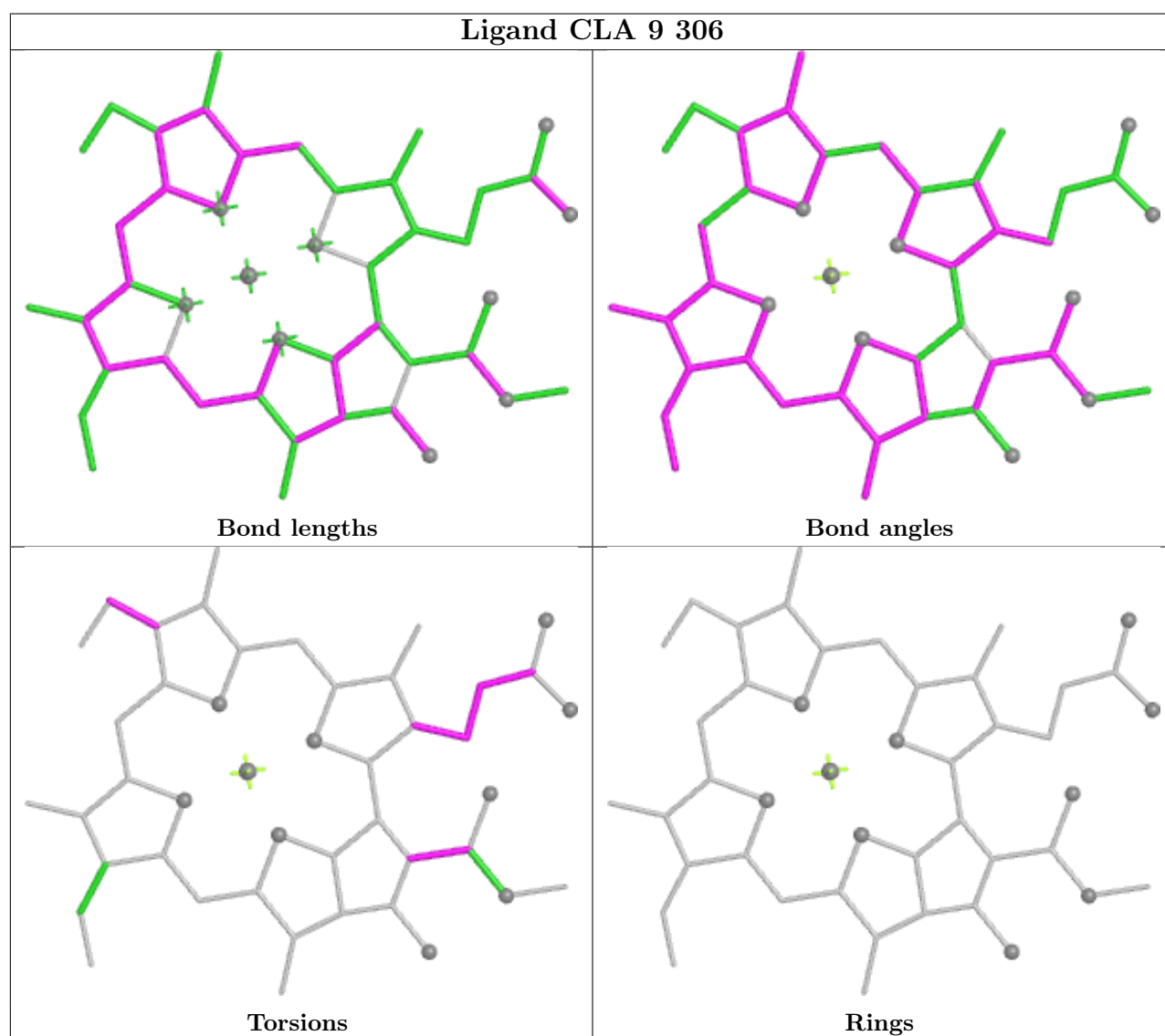
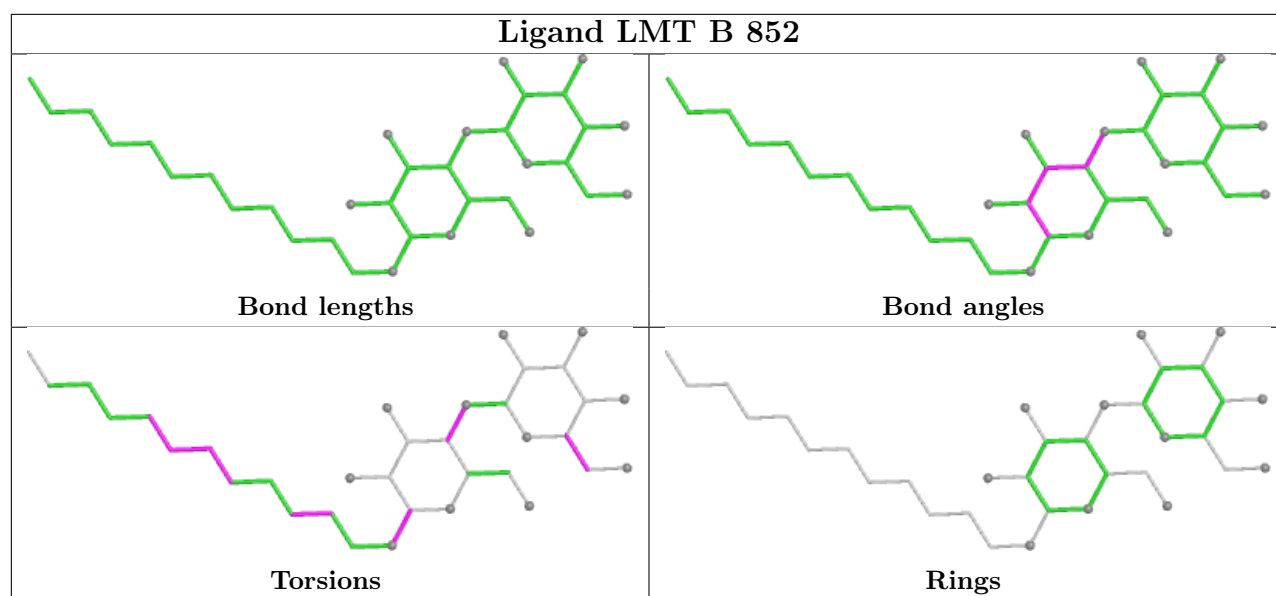


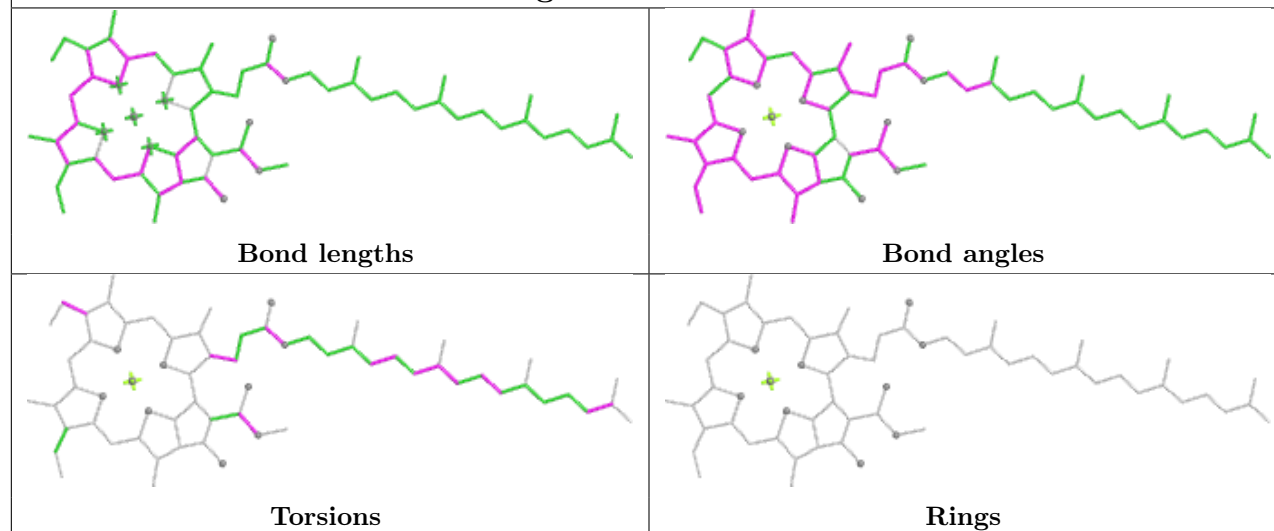
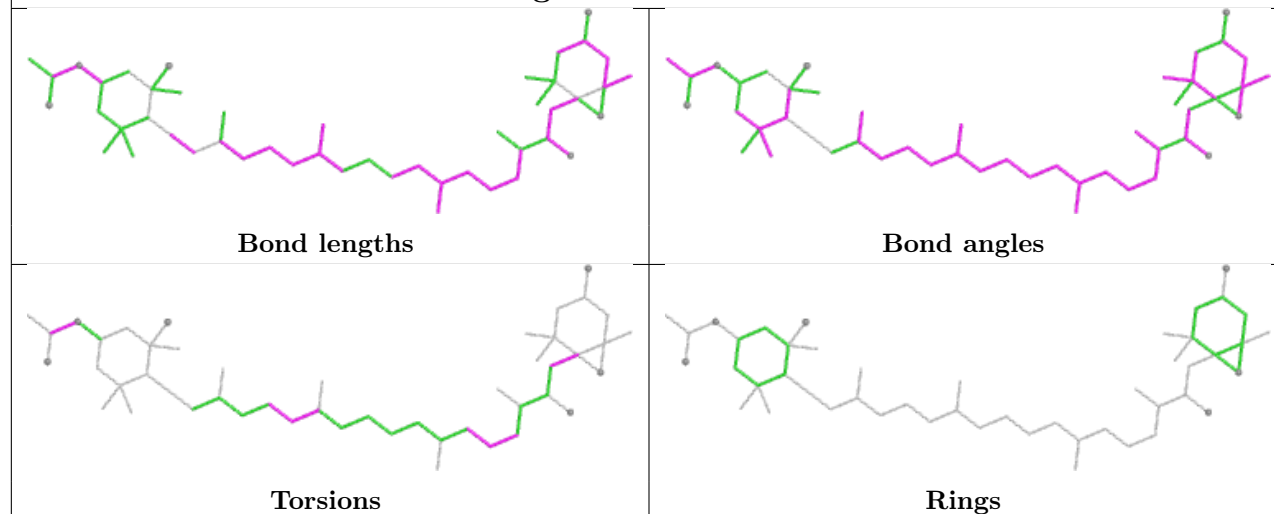
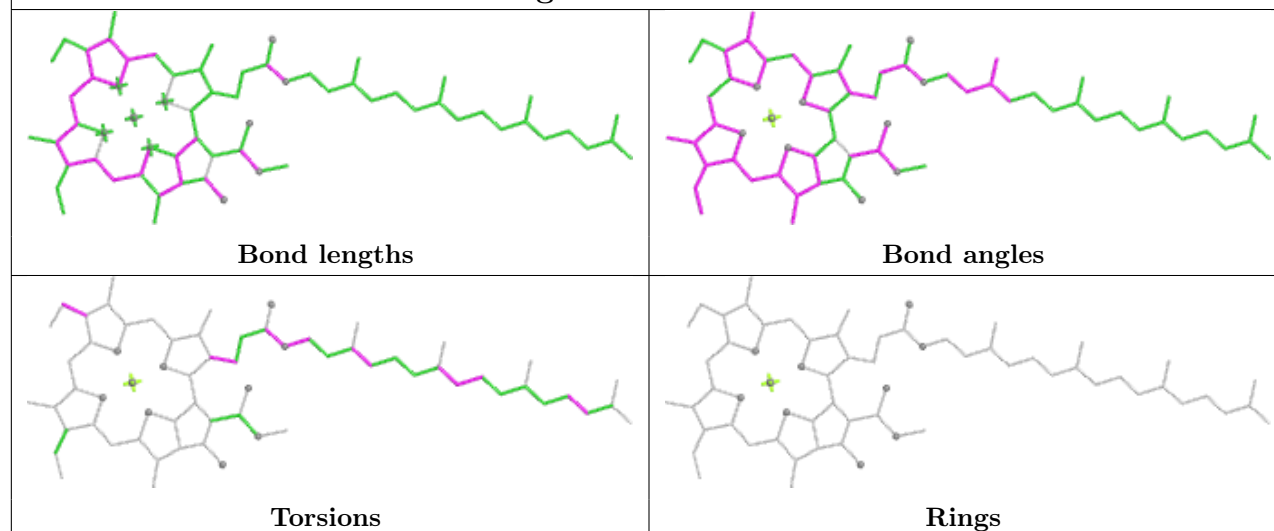
Torsions

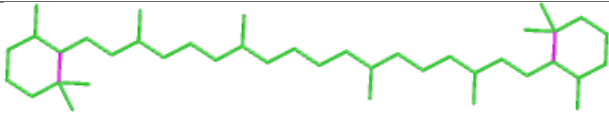
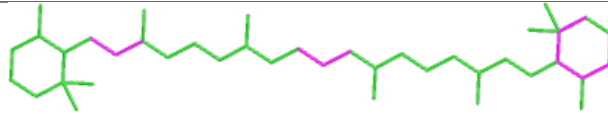
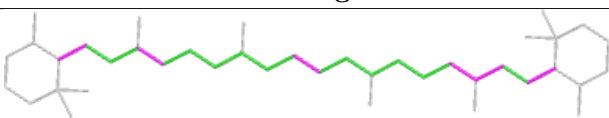
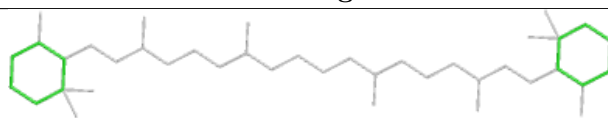


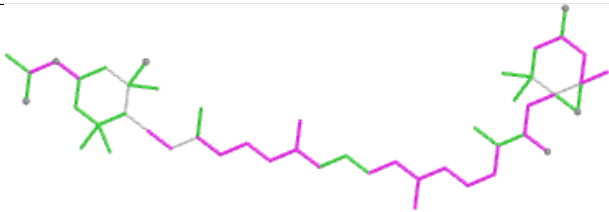
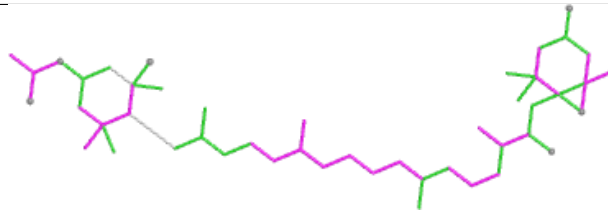
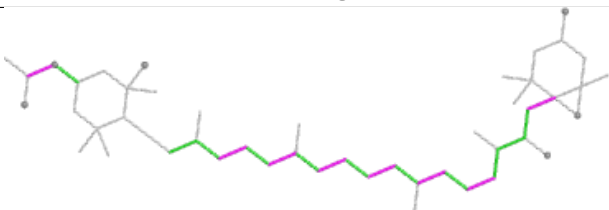
Rings

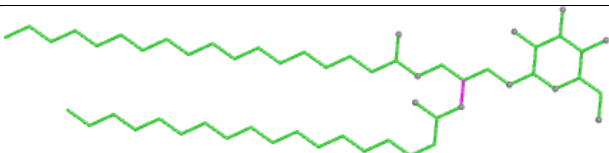
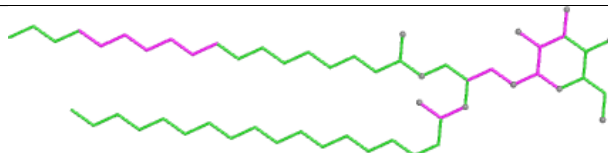
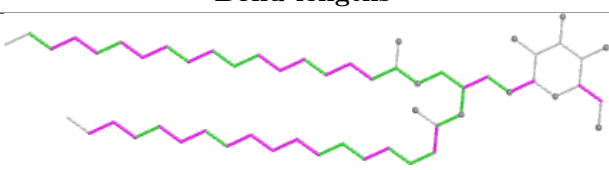
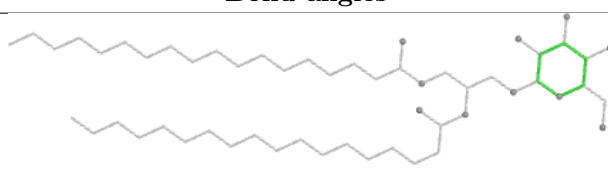


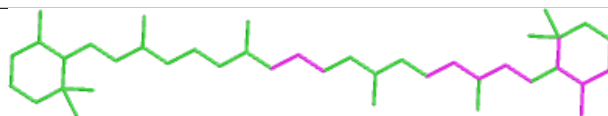
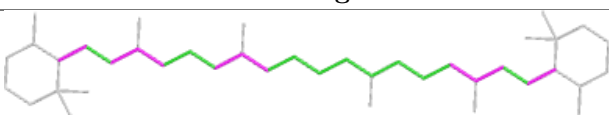
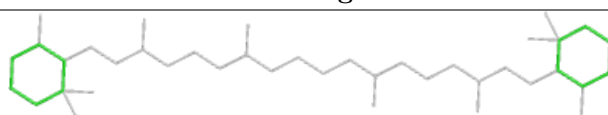


Ligand CLA 5 302**Ligand A86 15 315****Ligand CLA 5 309**

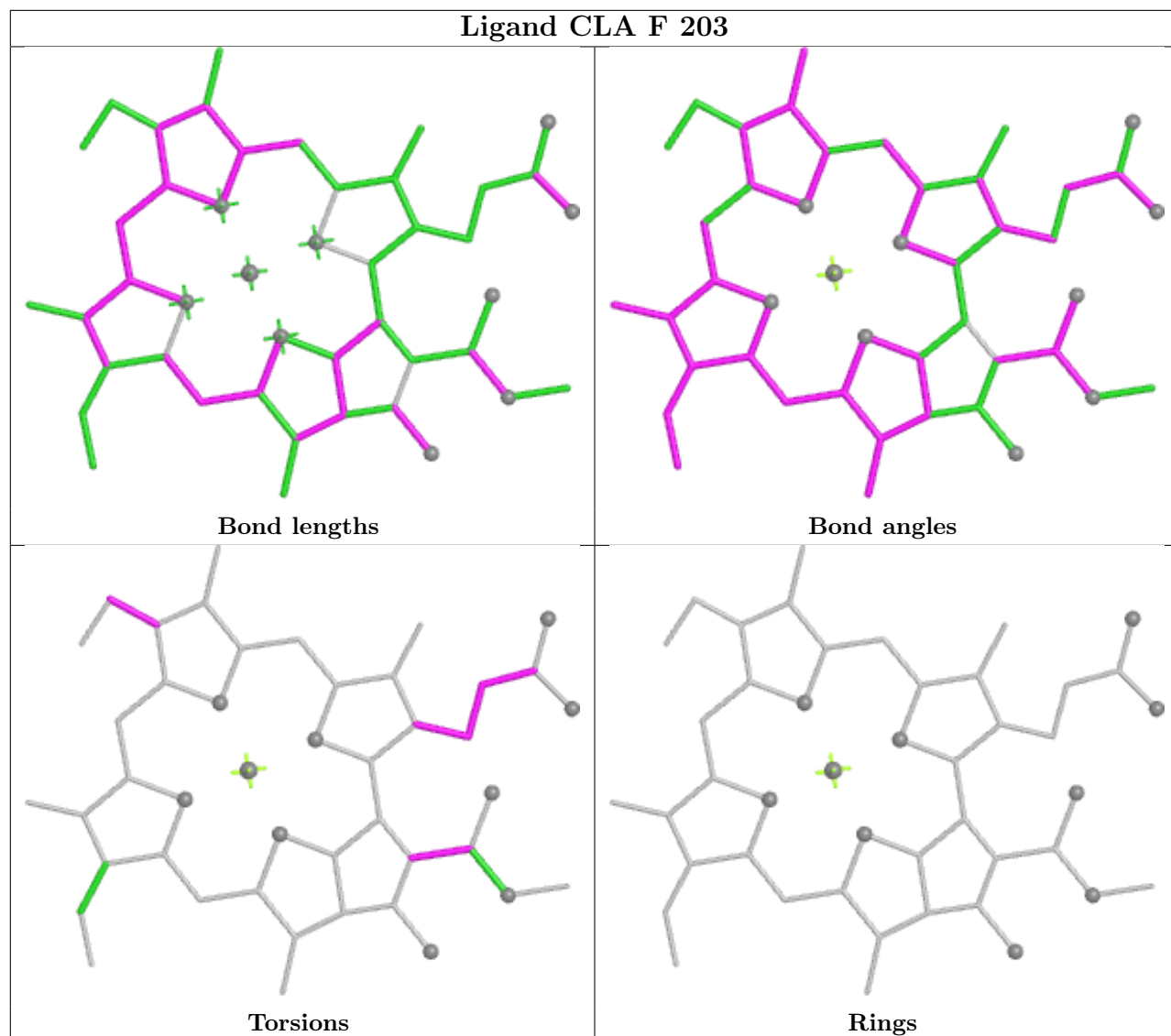
Ligand BCR B 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A86 11 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

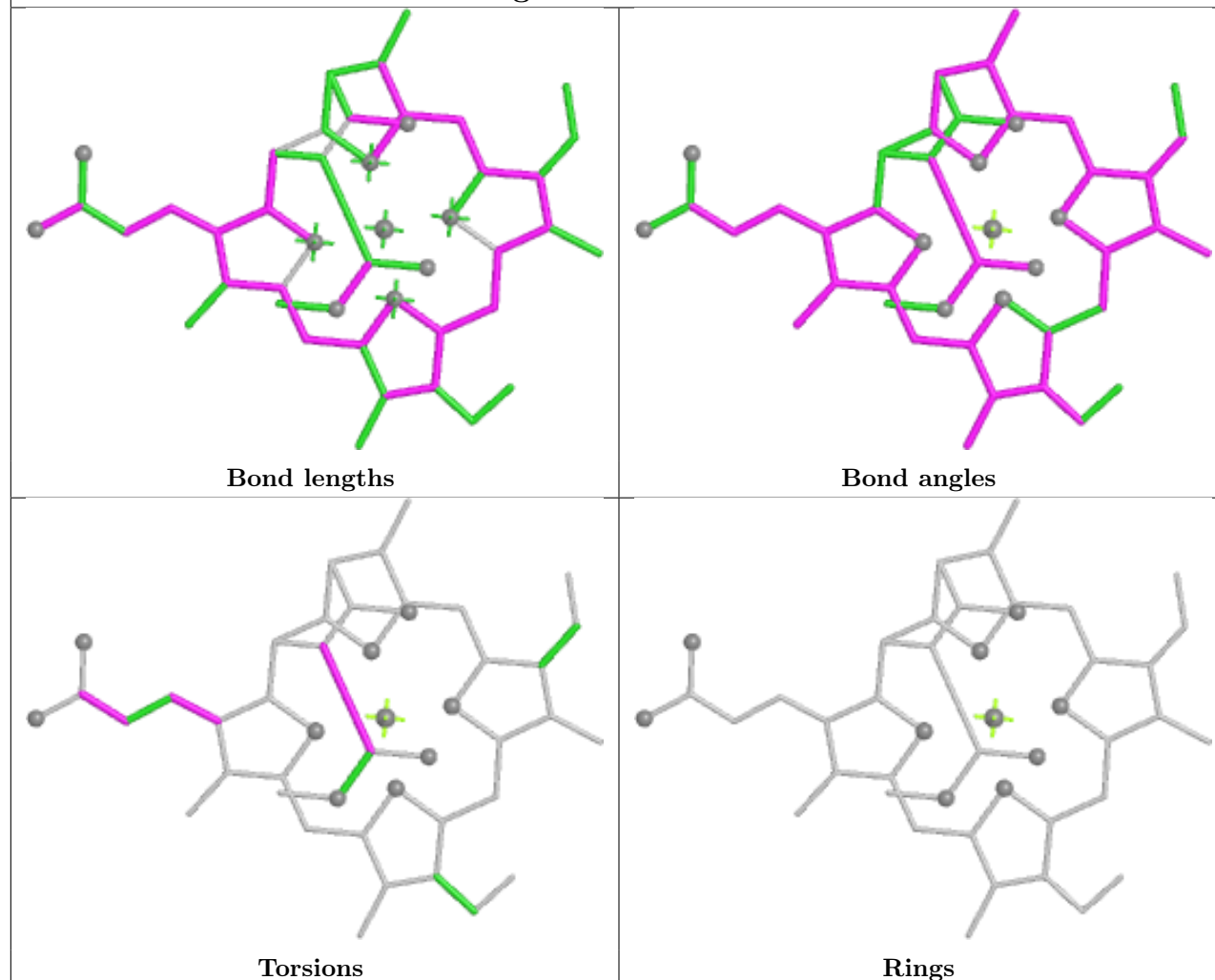
Ligand LMG B 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

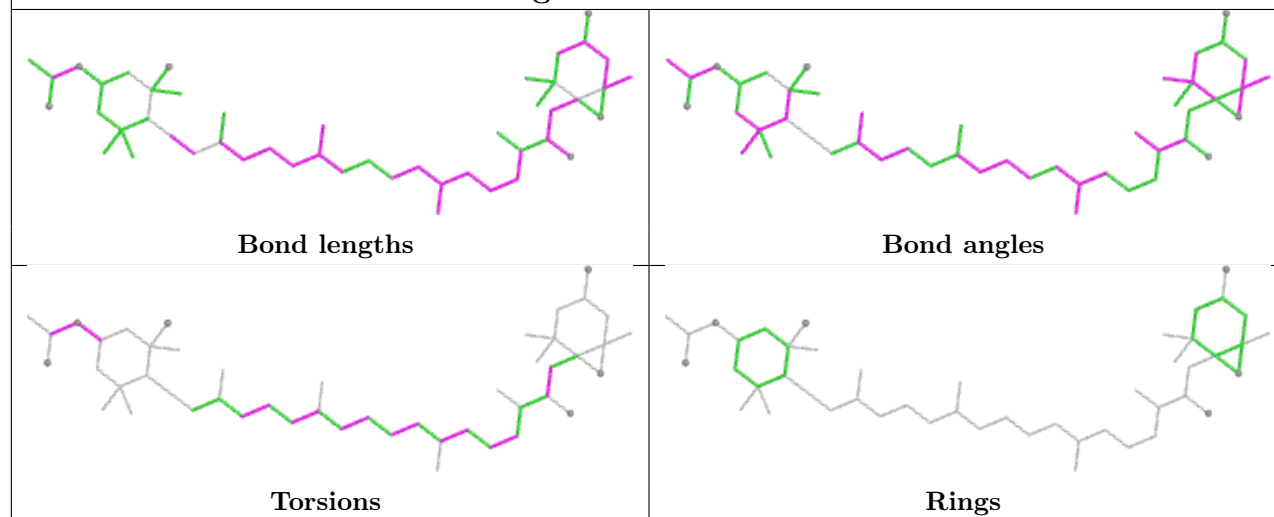
Ligand CLA F 203

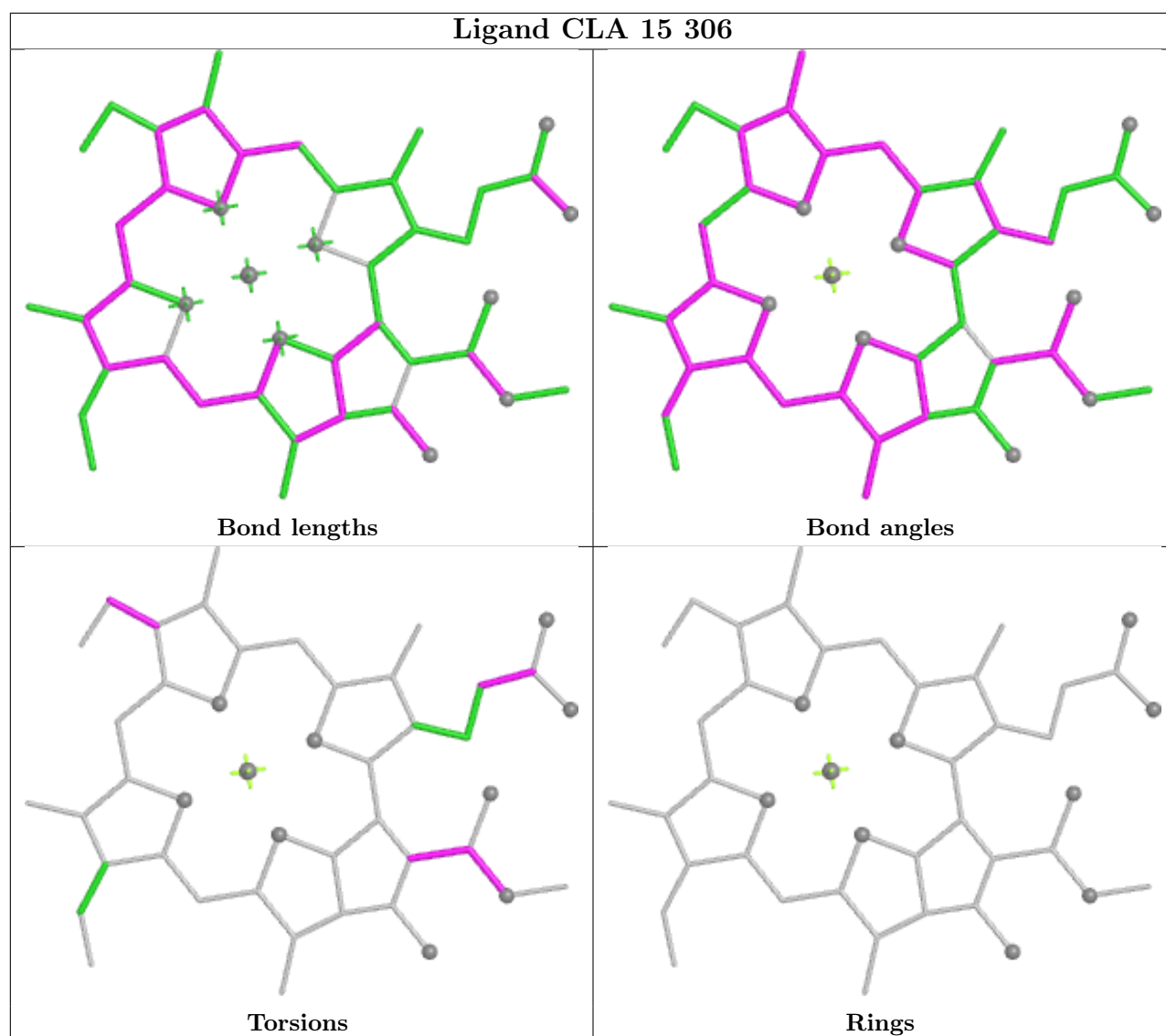


Ligand KC1 6 312

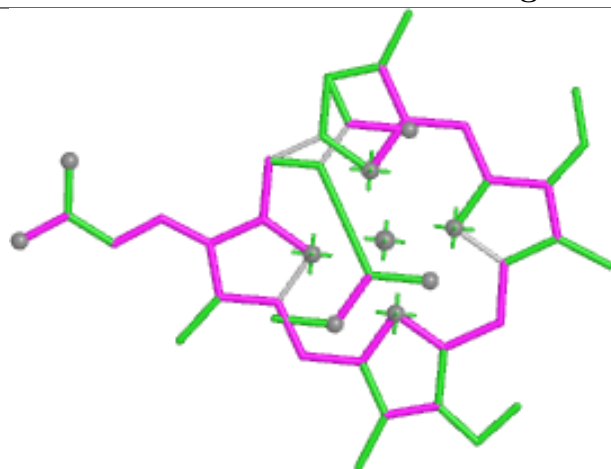


Ligand A86 10 315

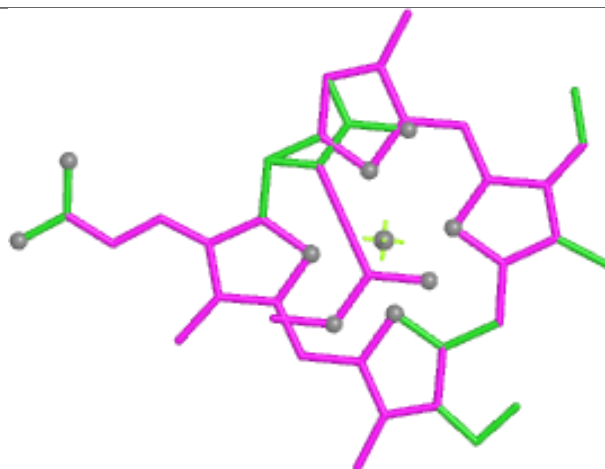




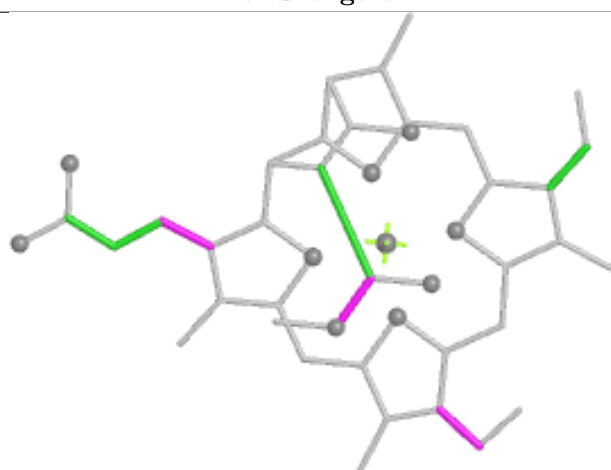
Ligand KC1 8 311



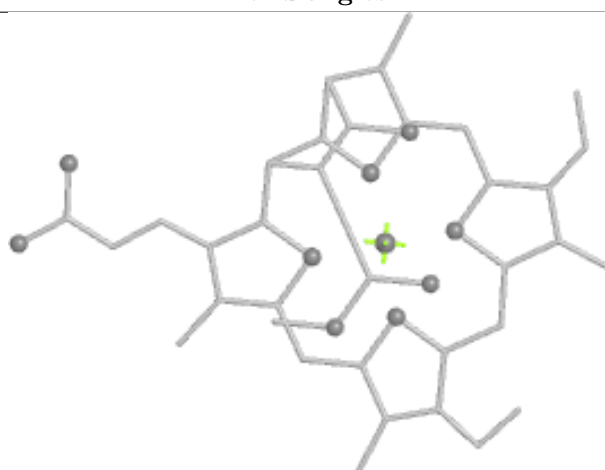
Bond lengths



Bond angles

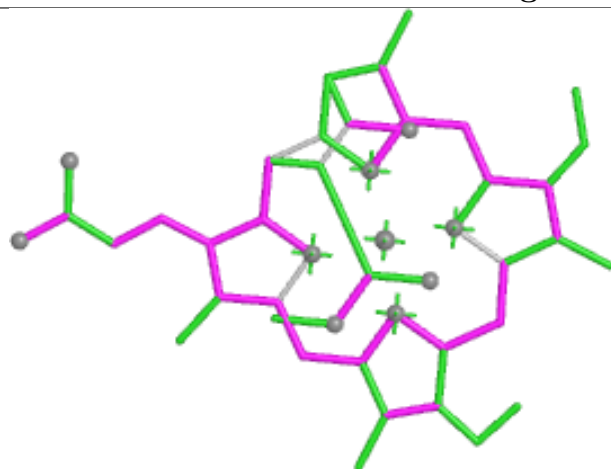


Torsions

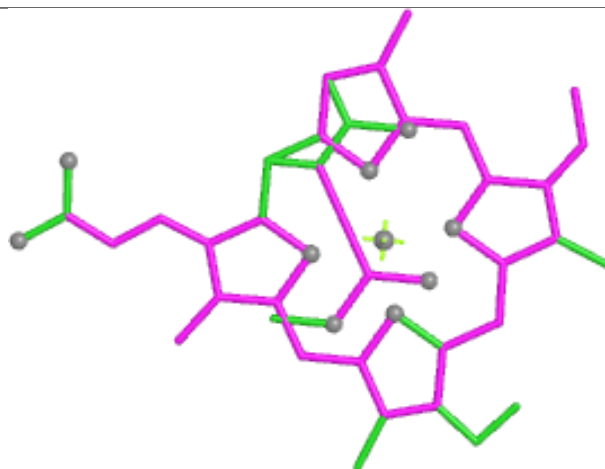


Rings

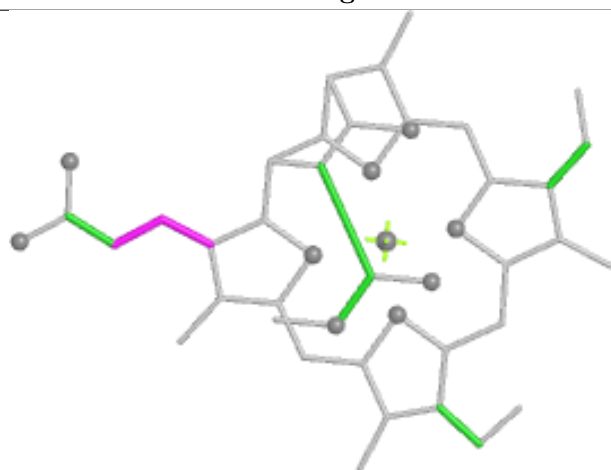
Ligand KC1 4 308



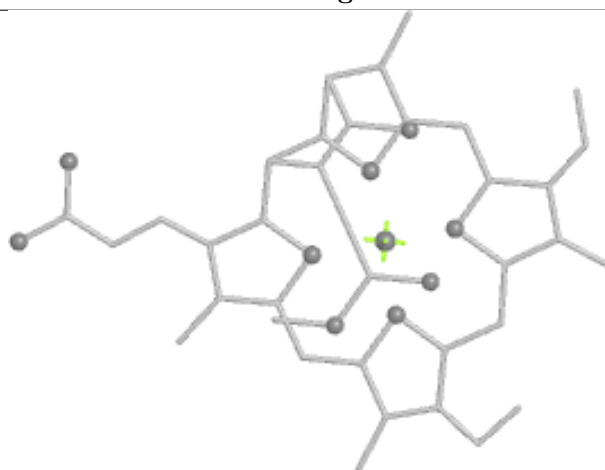
Bond lengths



Bond angles

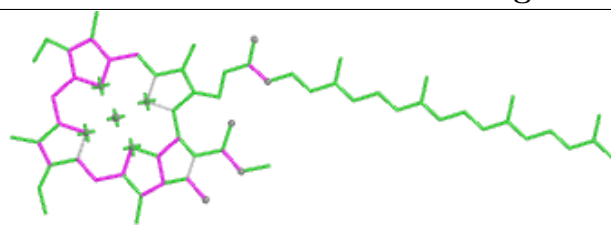


Torsions

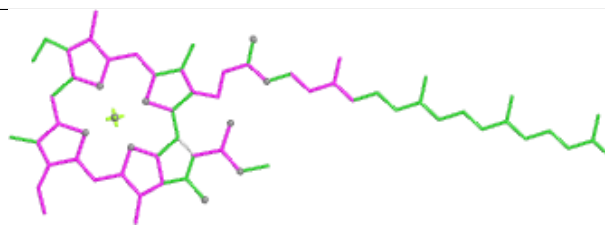


Rings

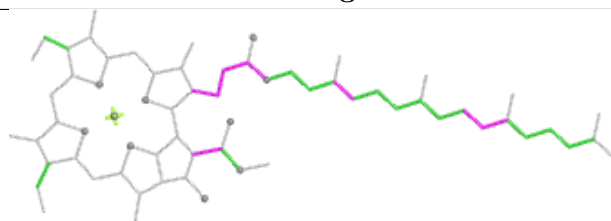
Ligand CLA A 806



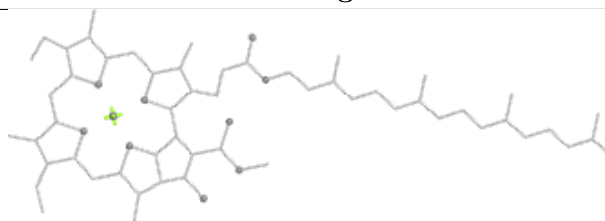
Bond lengths



Bond angles

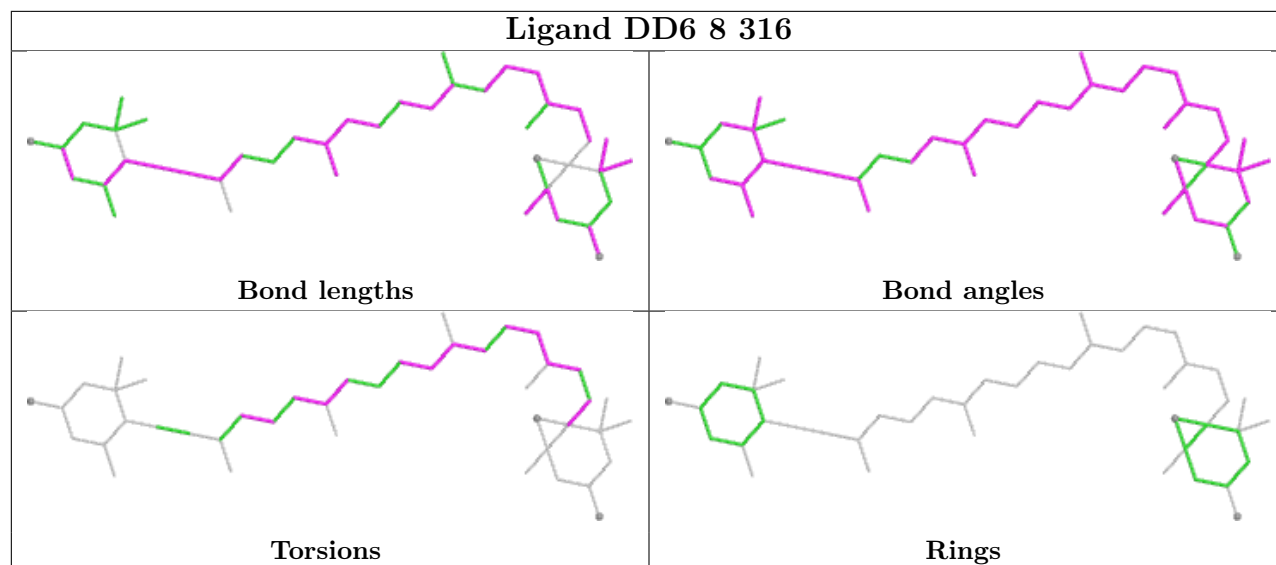


Torsions

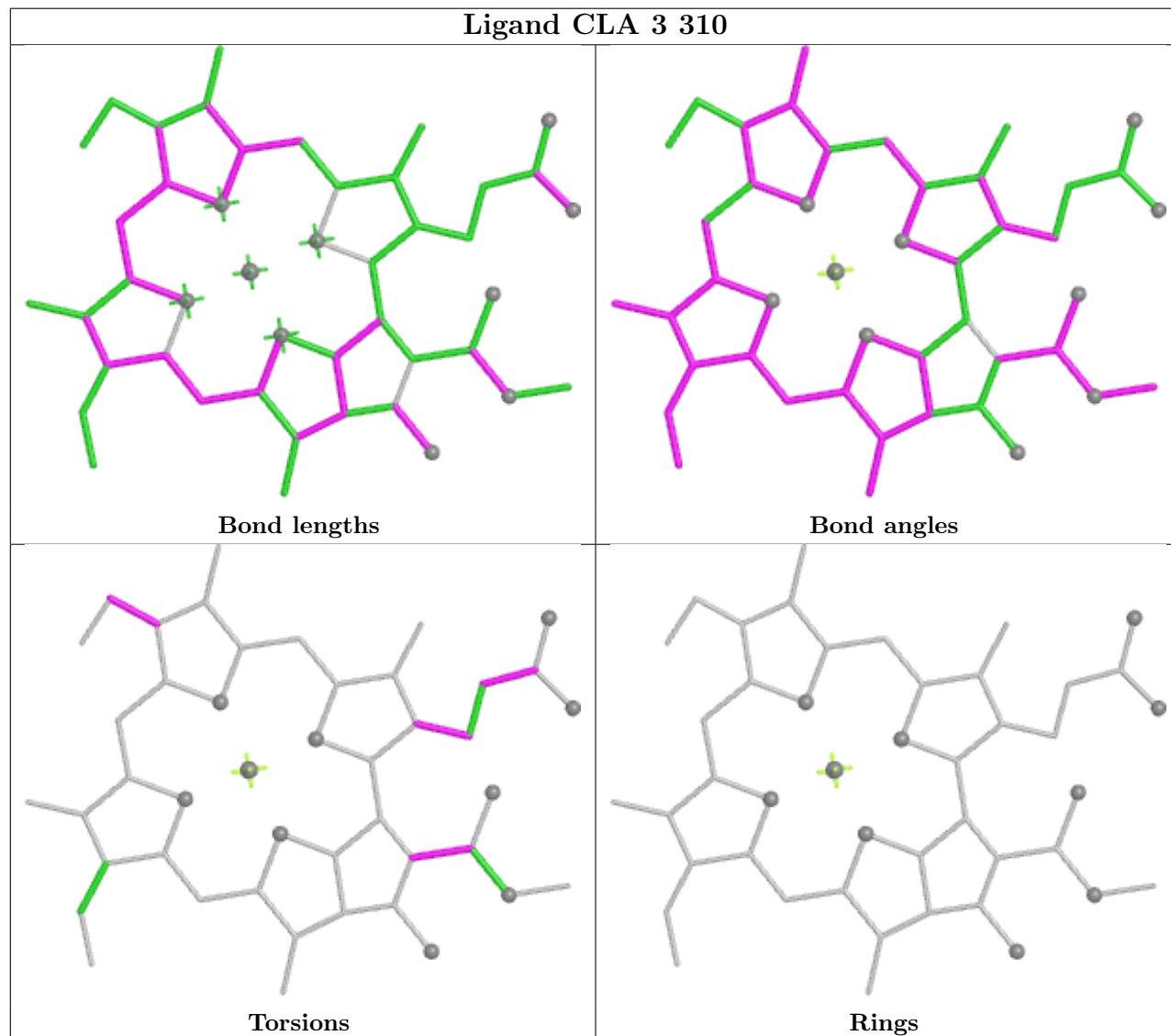


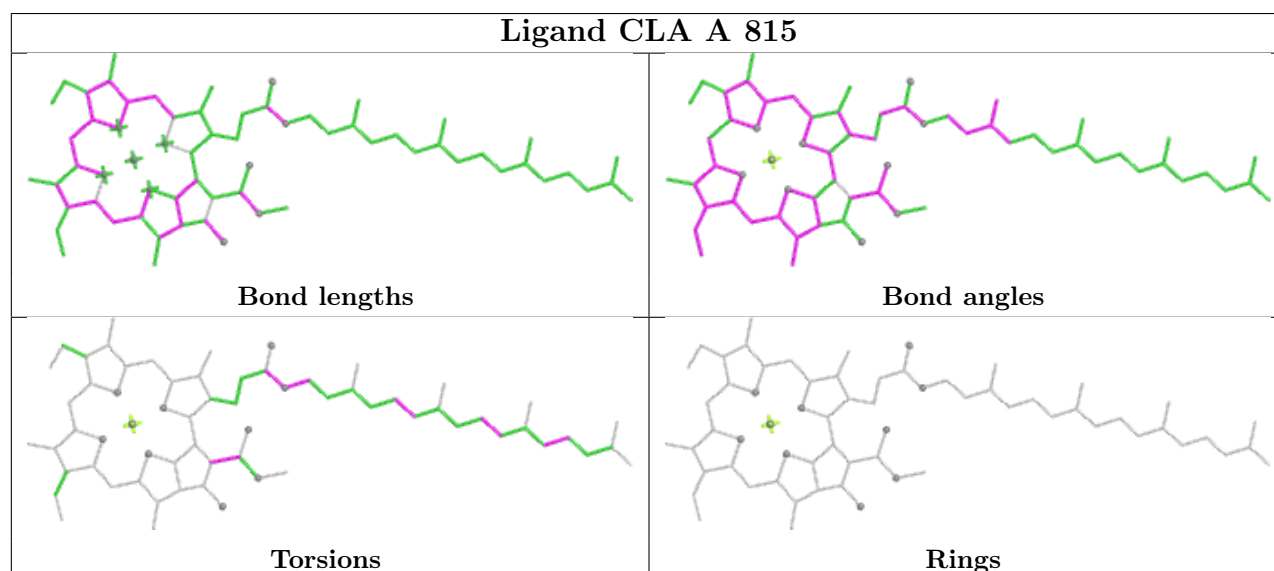
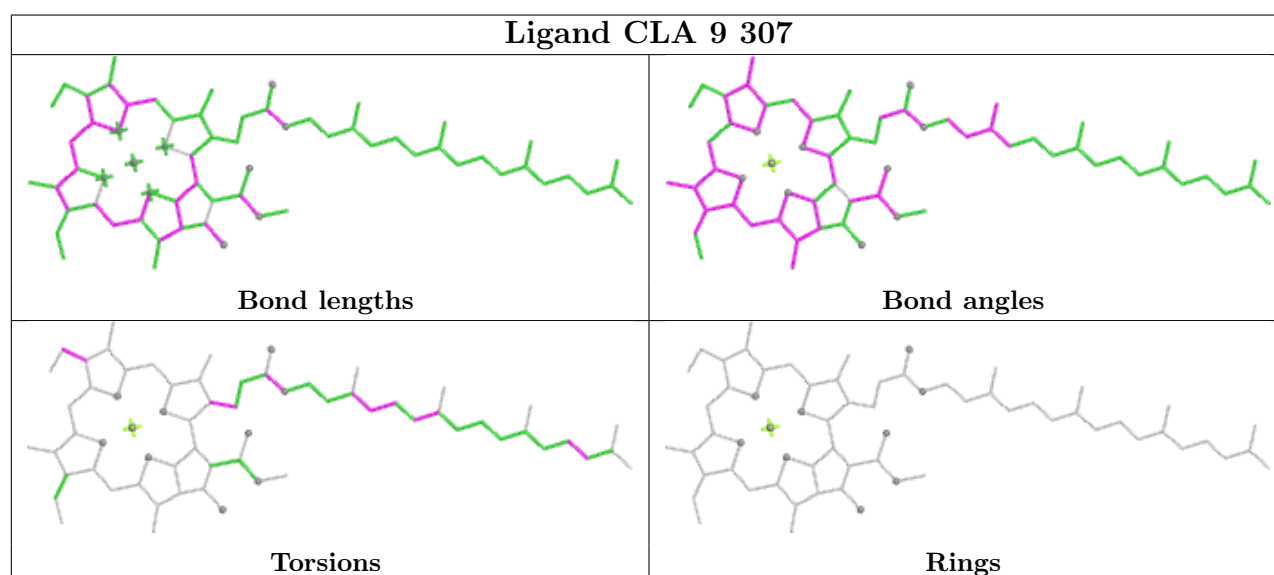
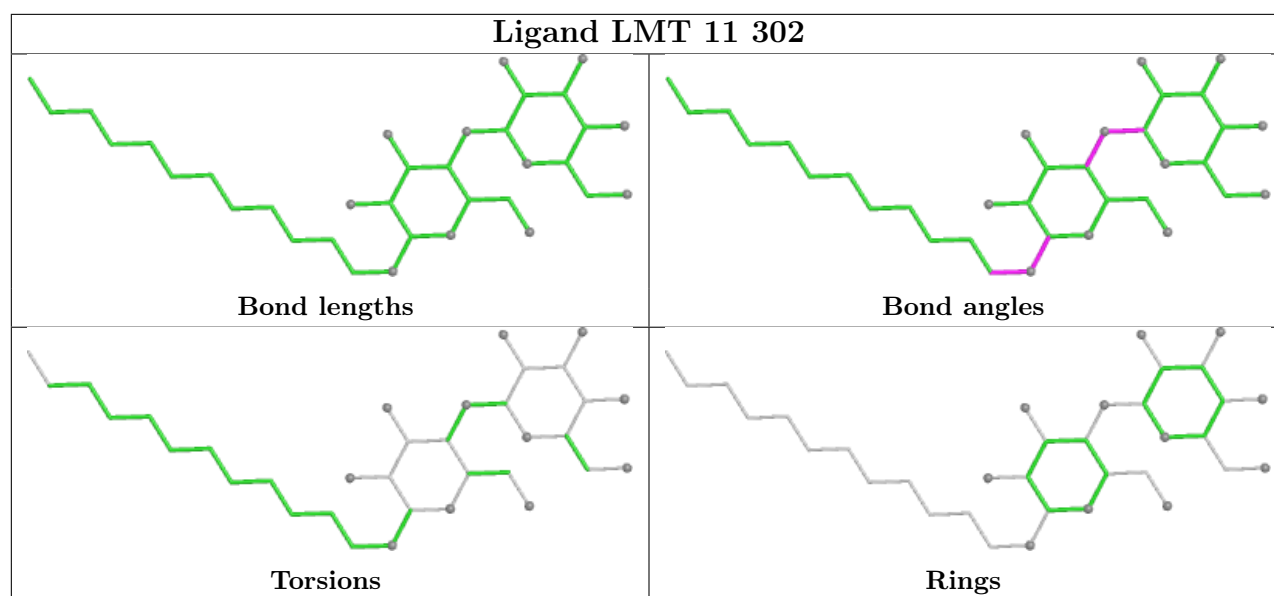
Rings

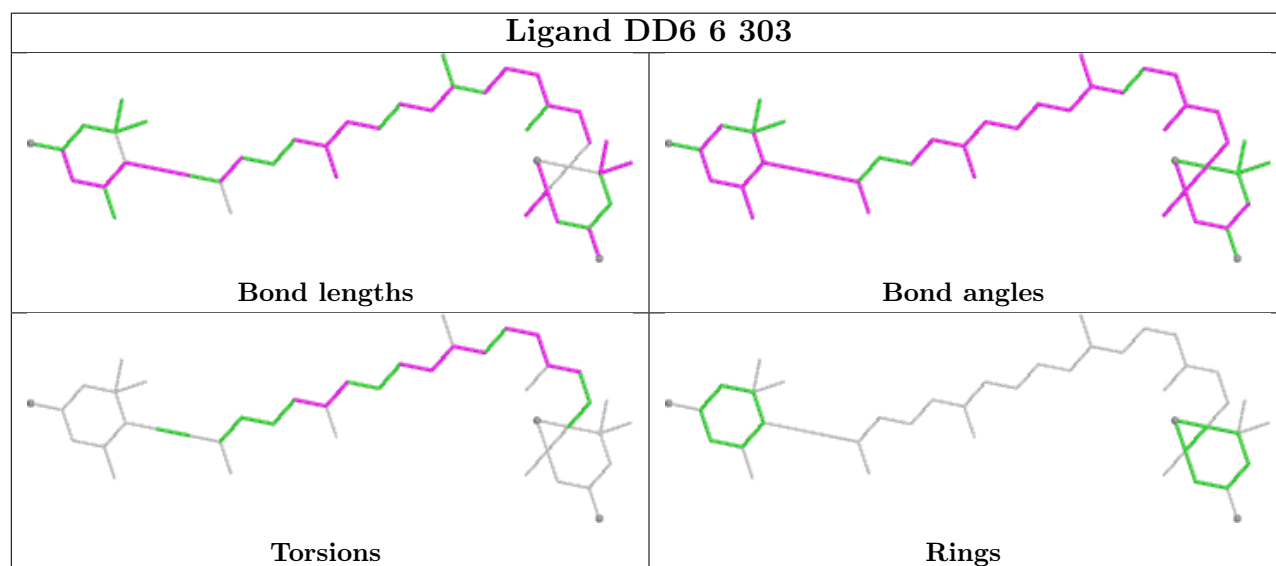
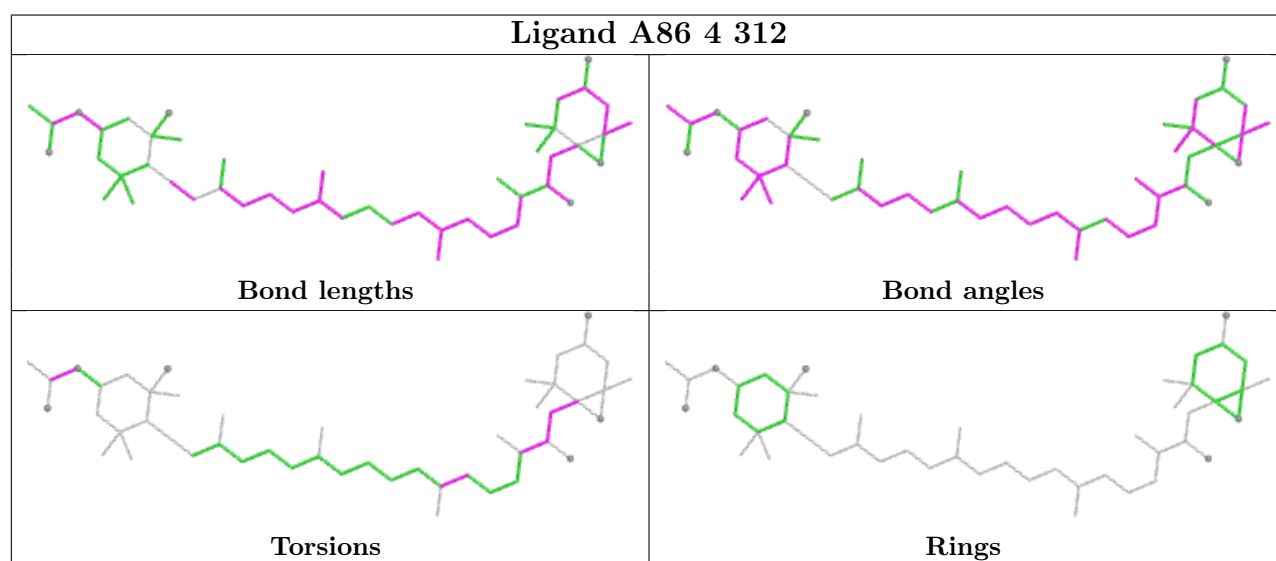
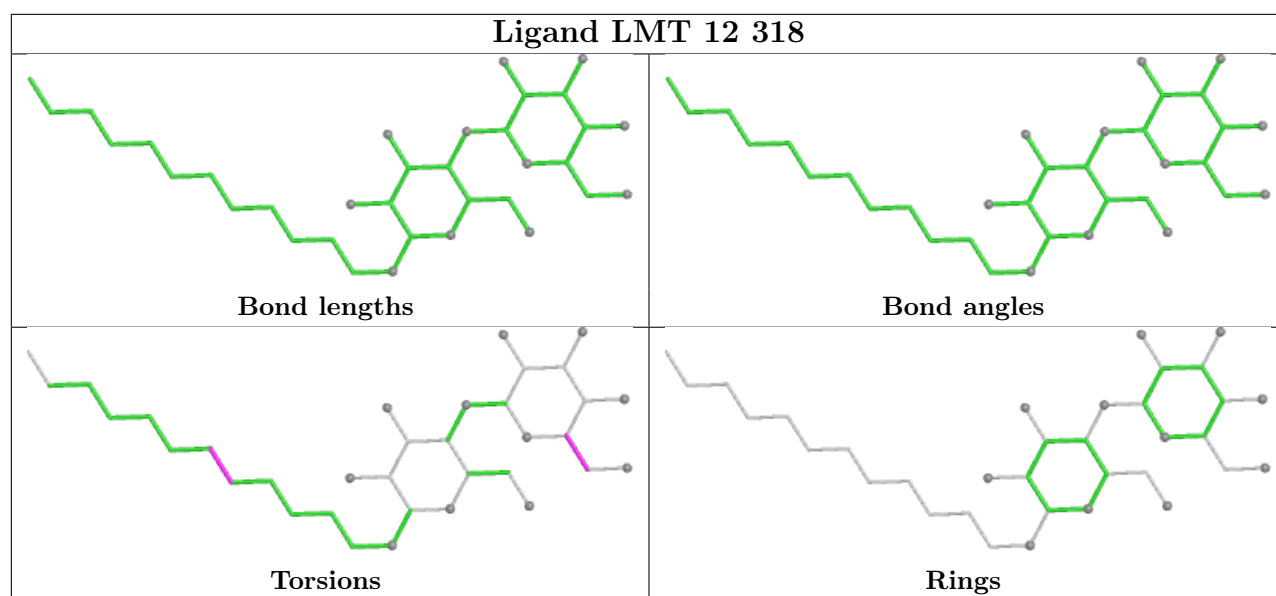
Ligand DD6 8 316



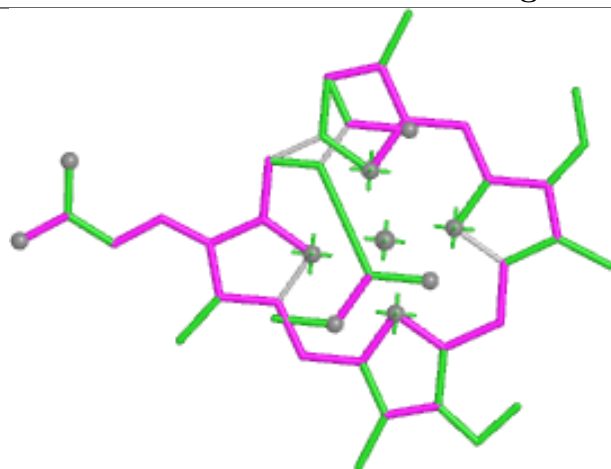
Ligand CLA 3 310



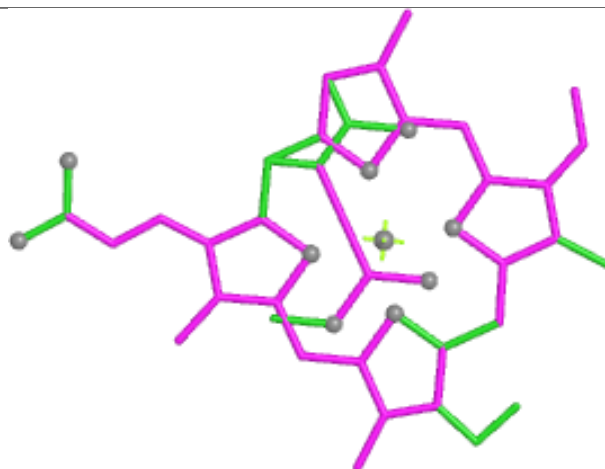




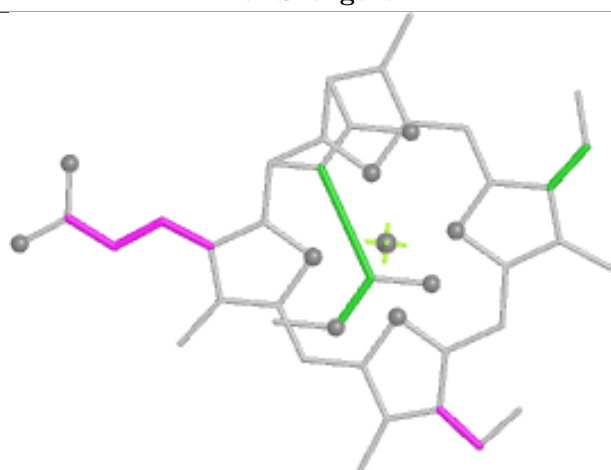
Ligand KC1 4 307



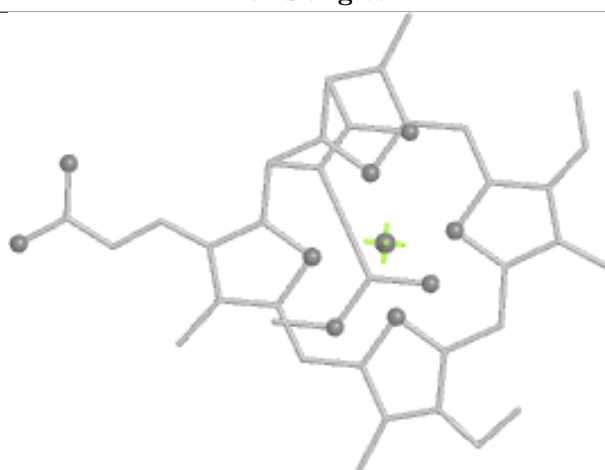
Bond lengths



Bond angles

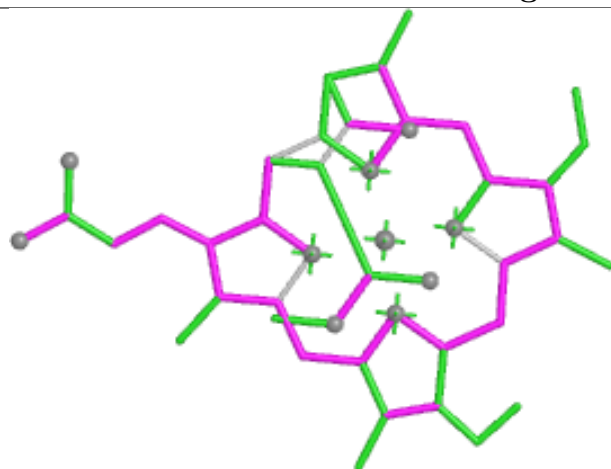


Torsions

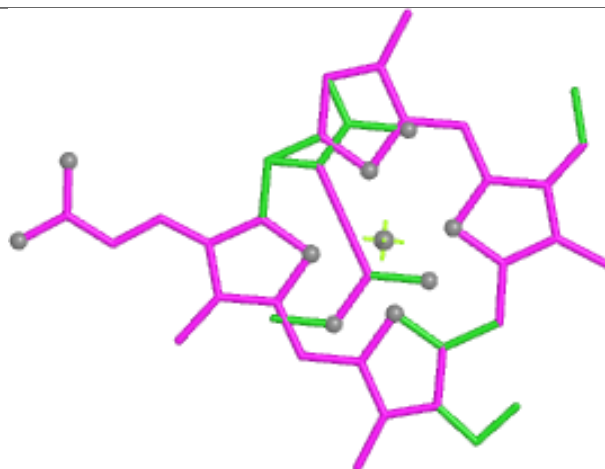


Rings

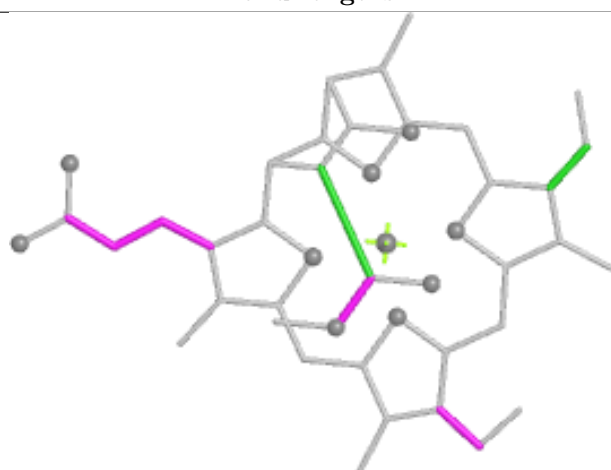
Ligand KC1 8 312



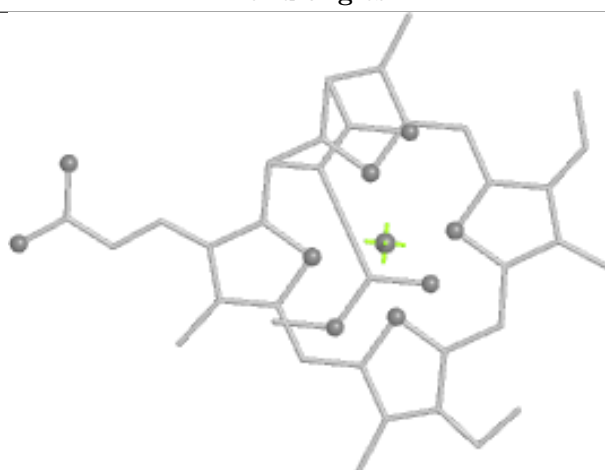
Bond lengths



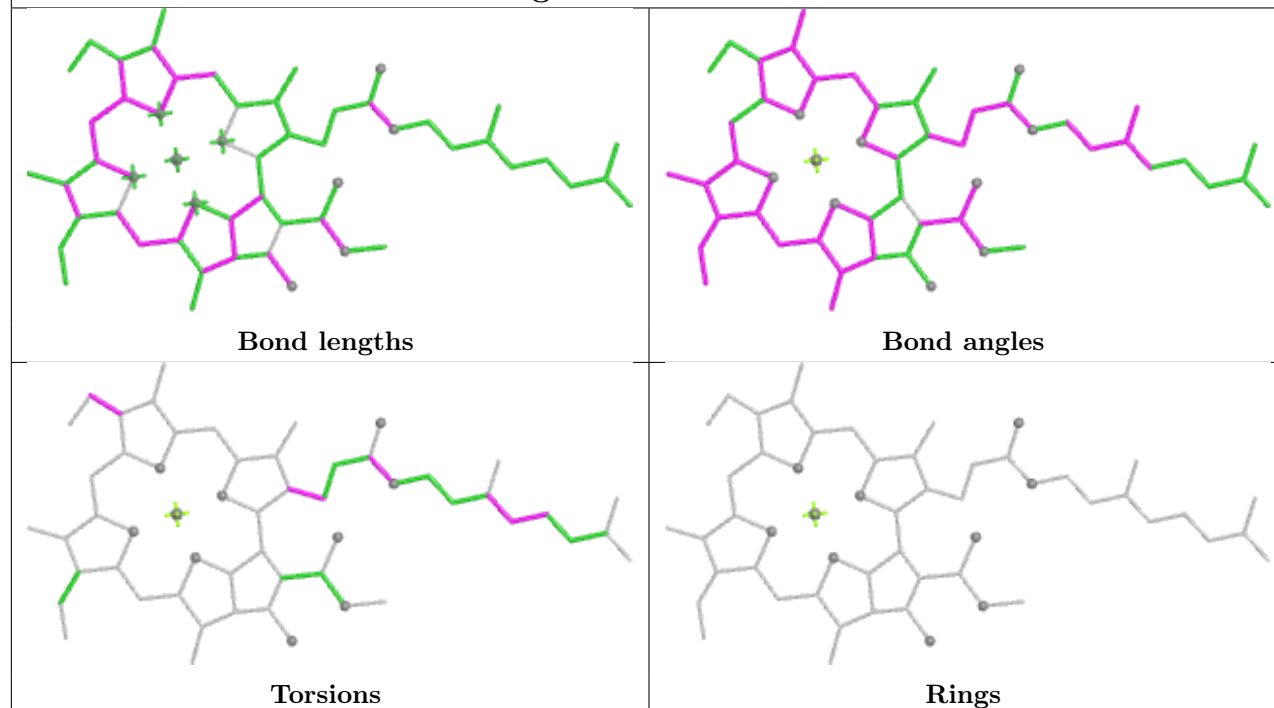
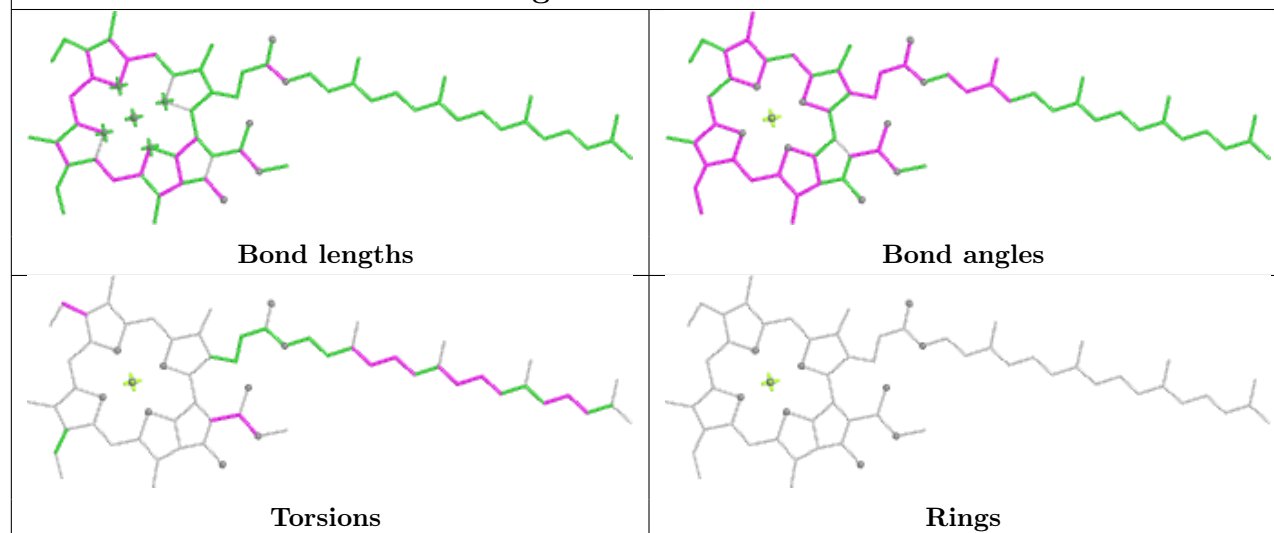
Bond angles

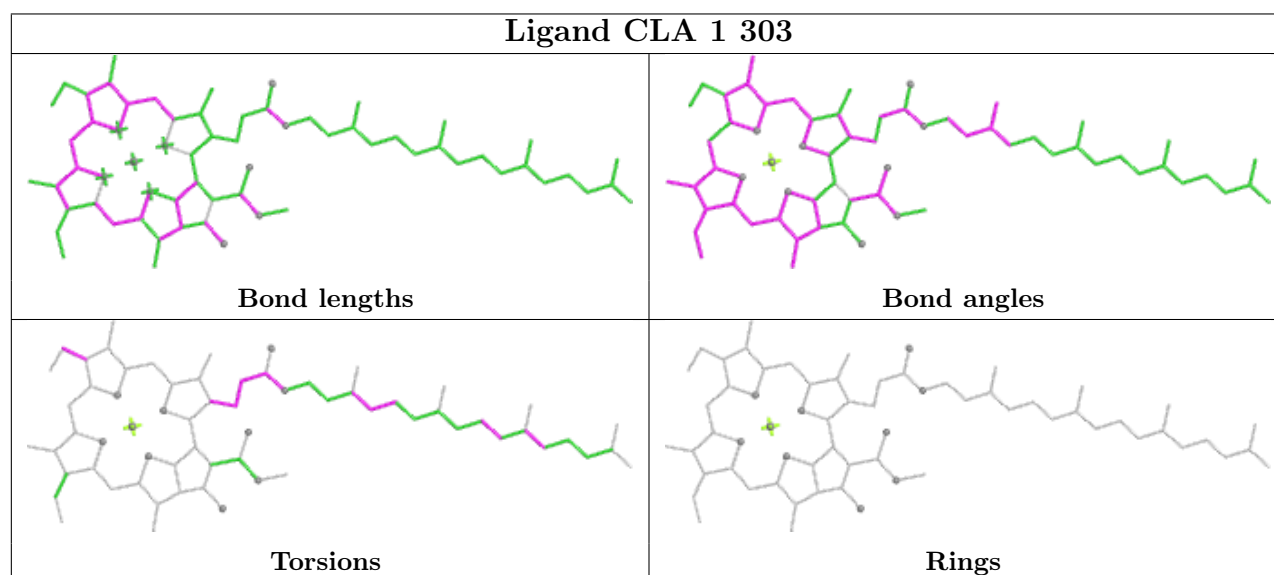
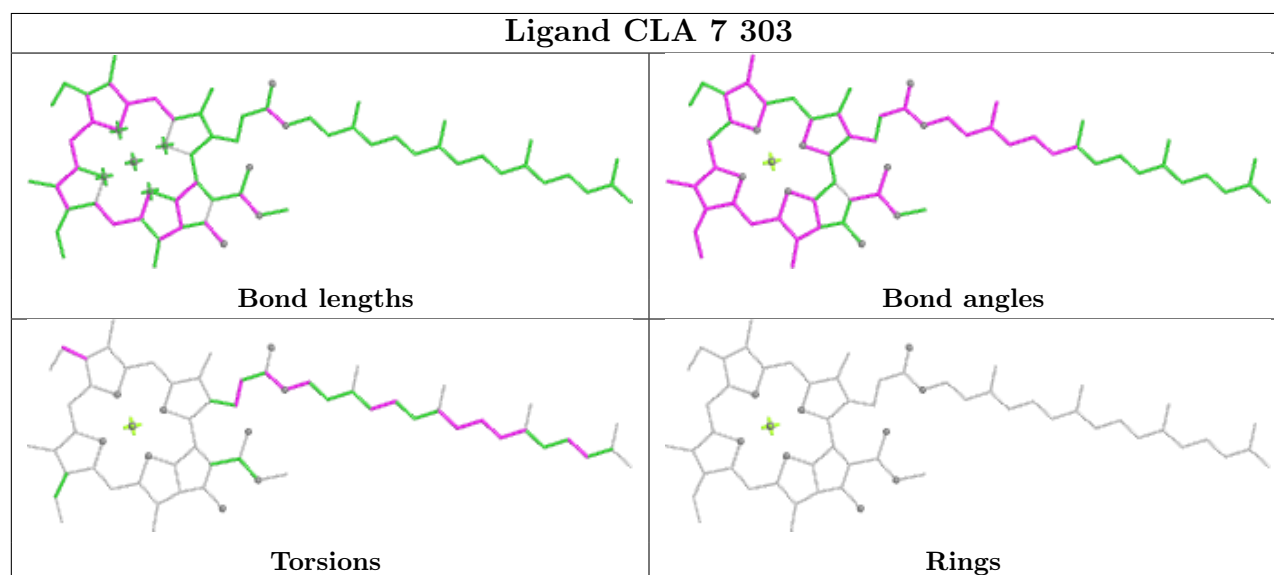
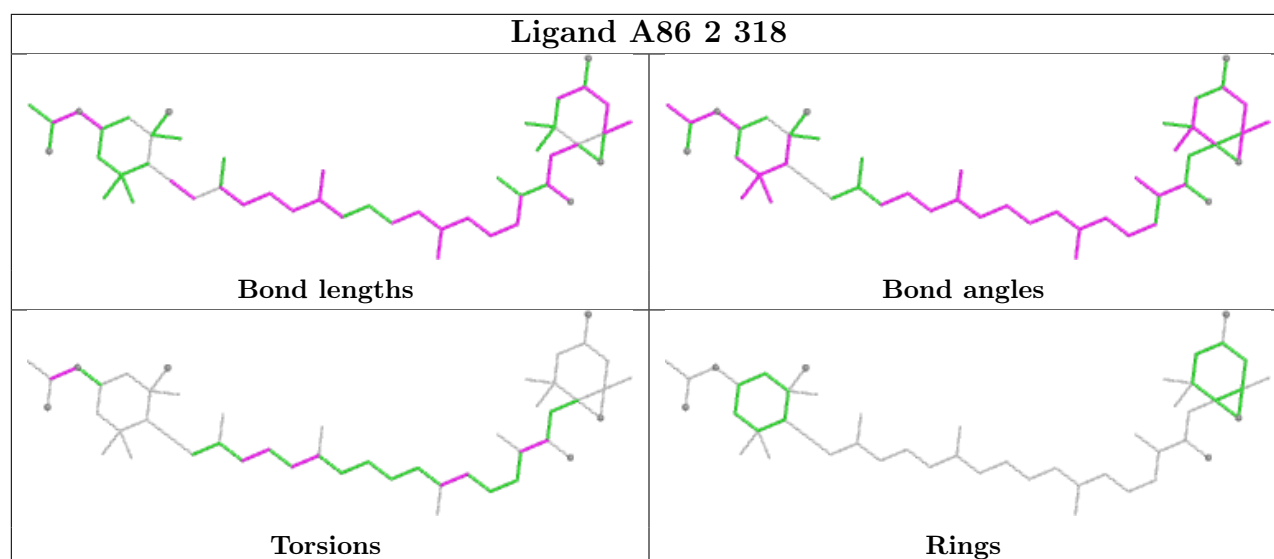


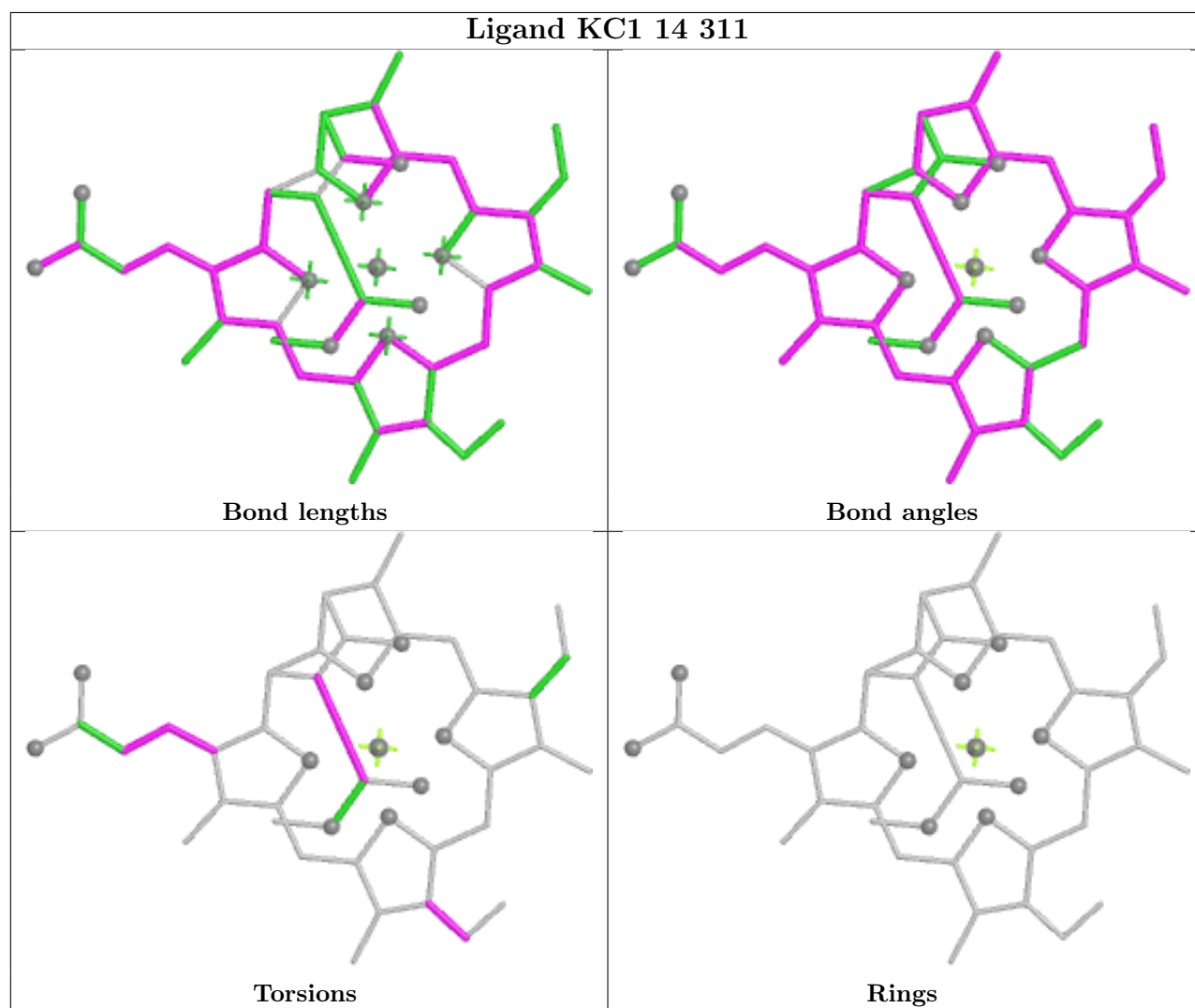
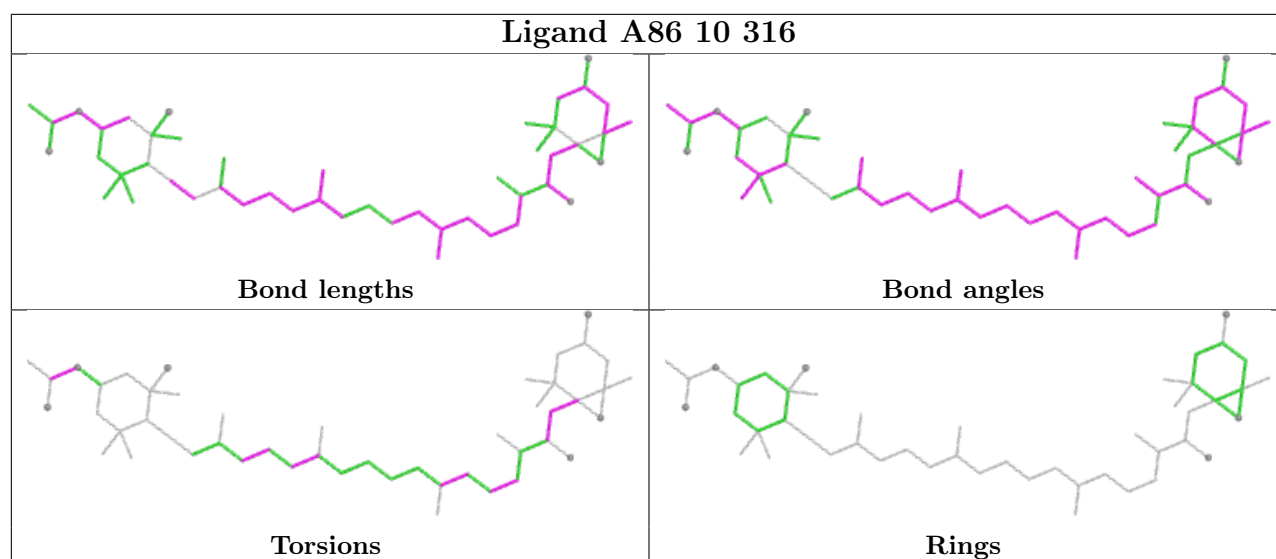
Torsions

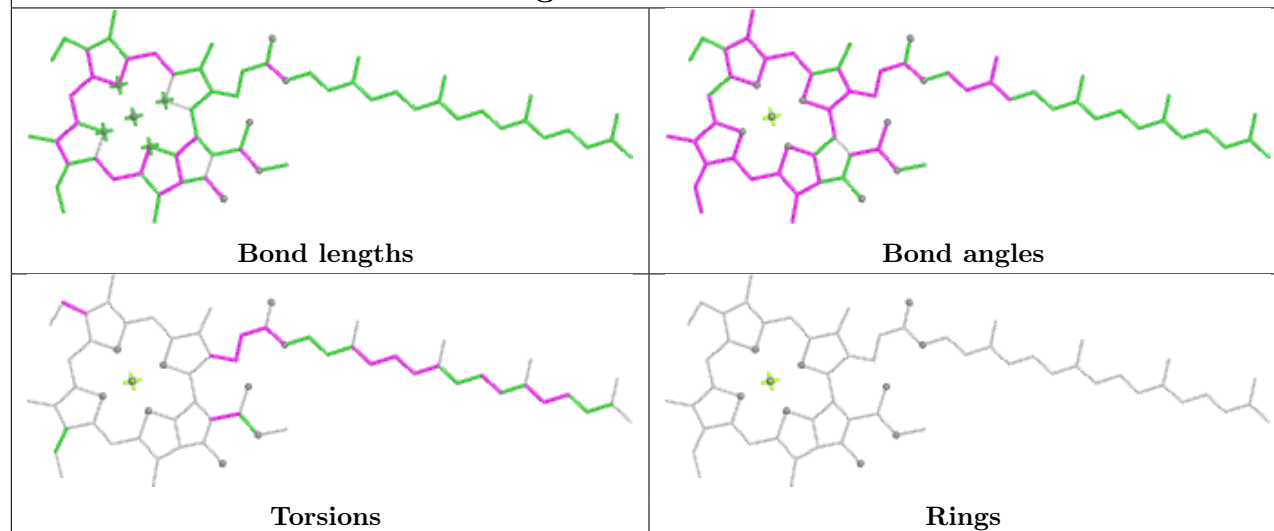
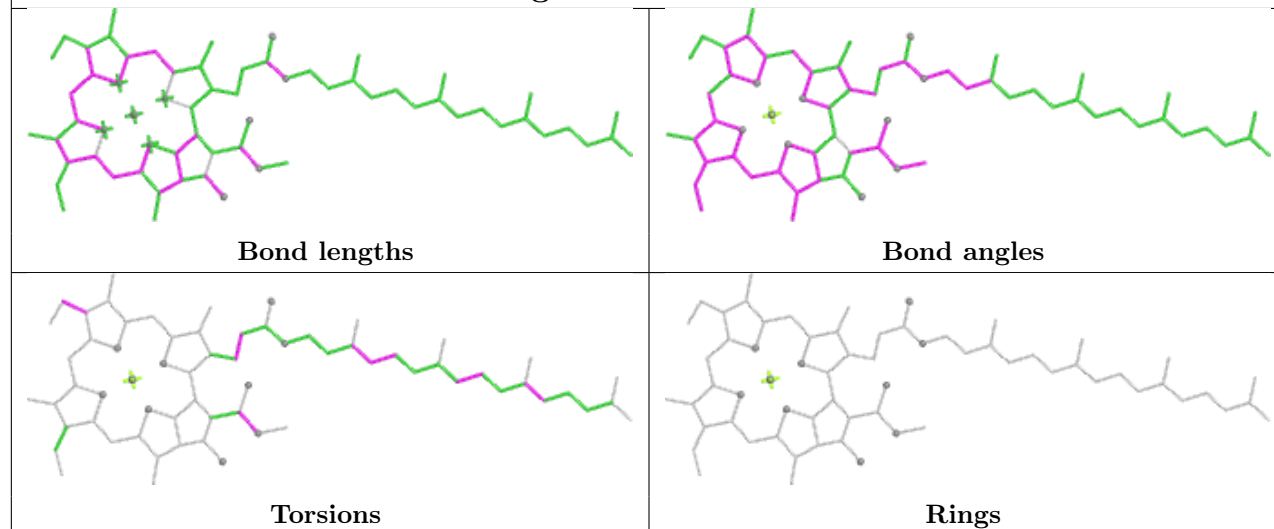
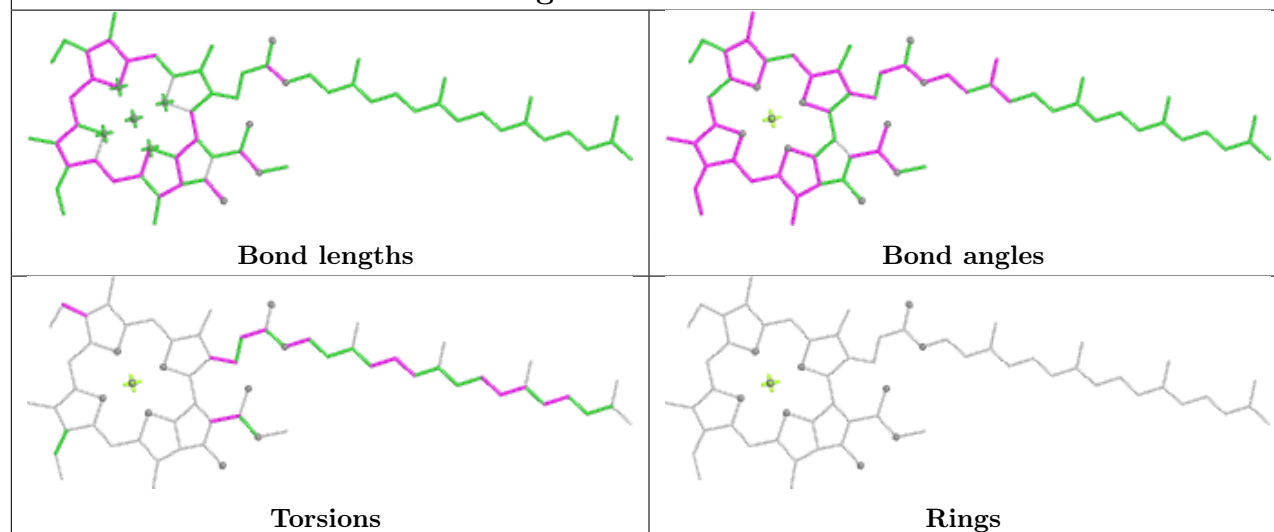


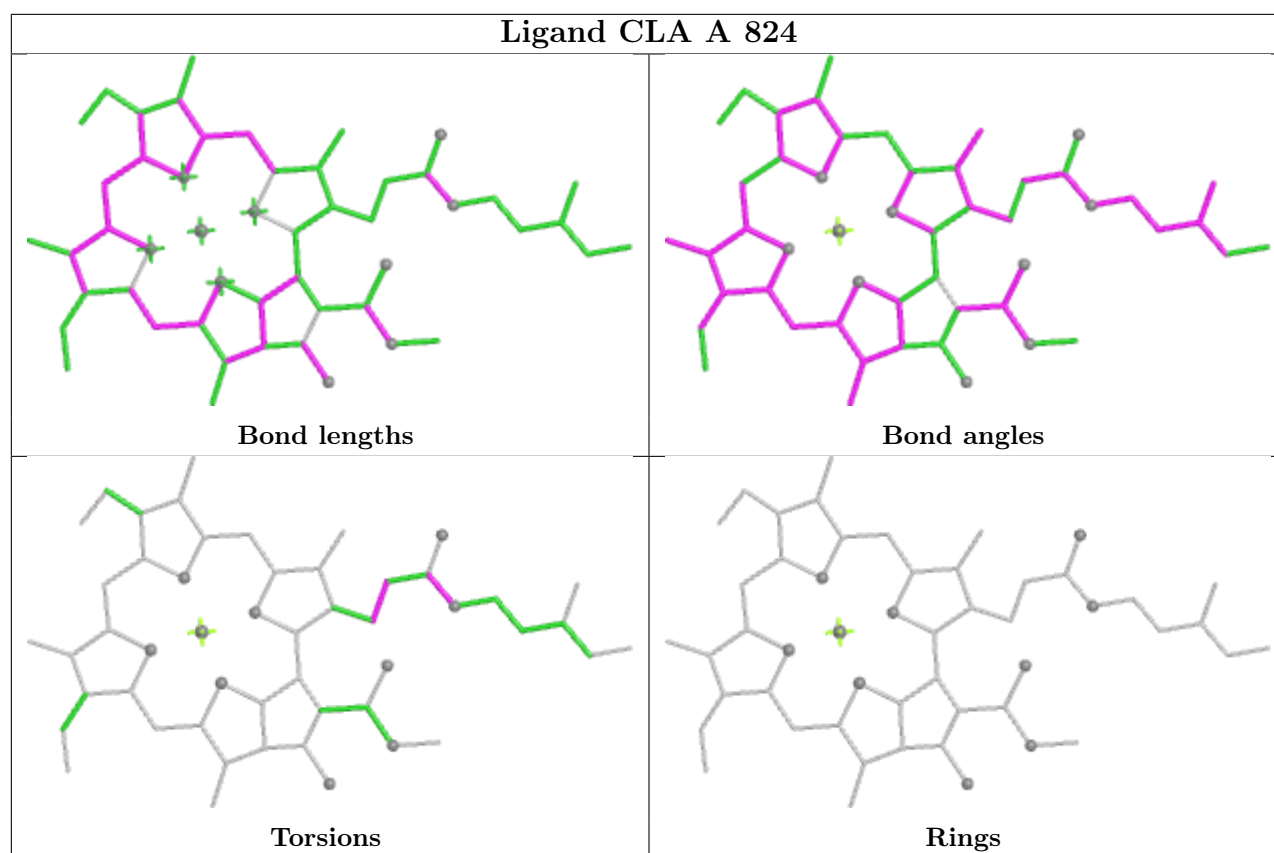
Rings

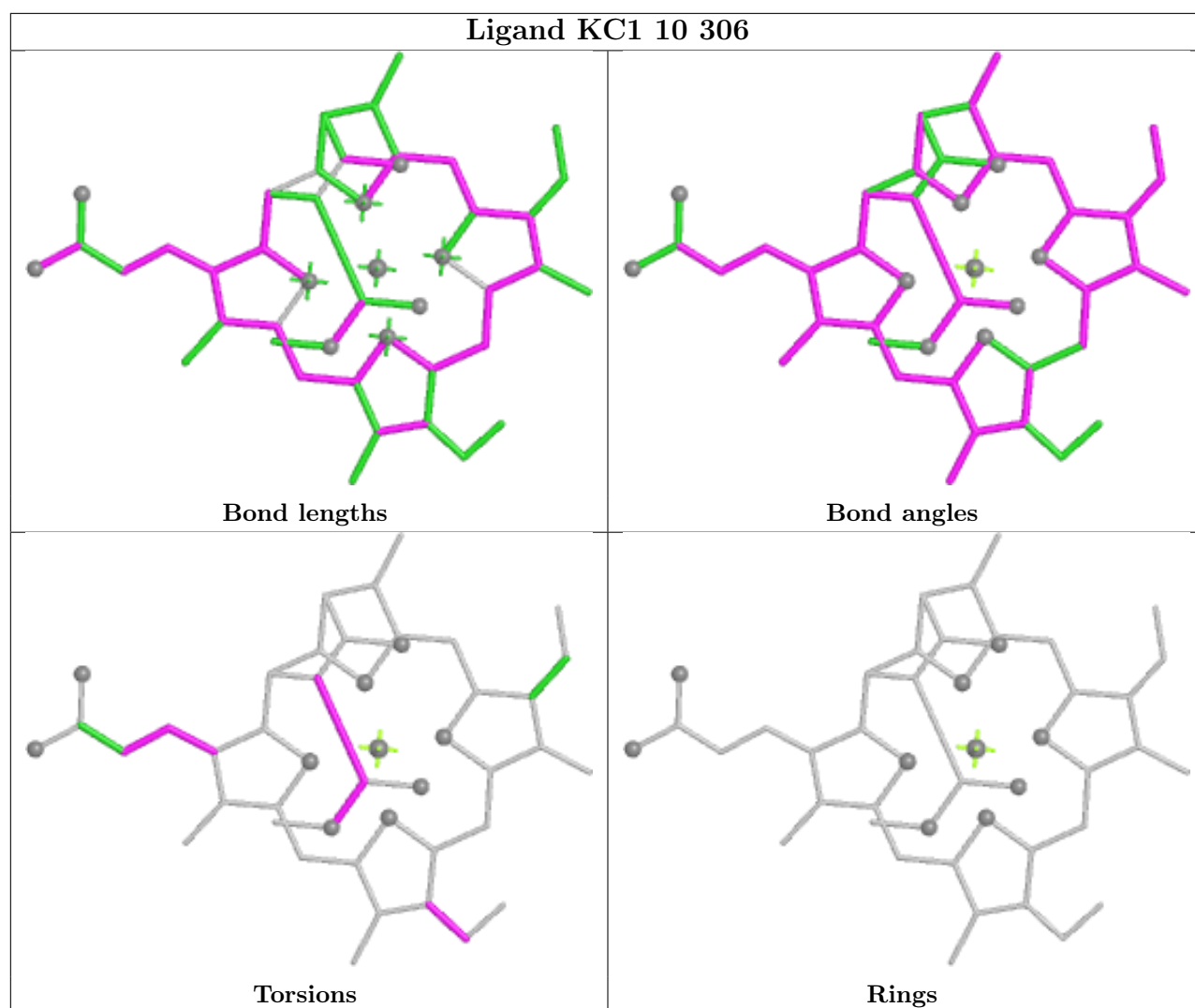
Ligand CLA B 816**Ligand CLA B 808**



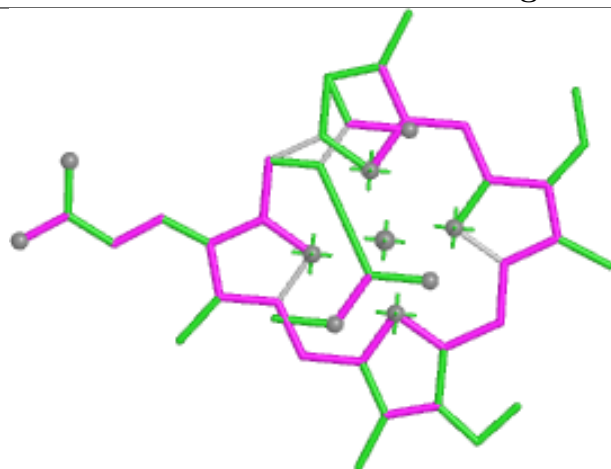


Ligand CLA 9 308**Ligand CLA A 822****Ligand CLA 5 304**

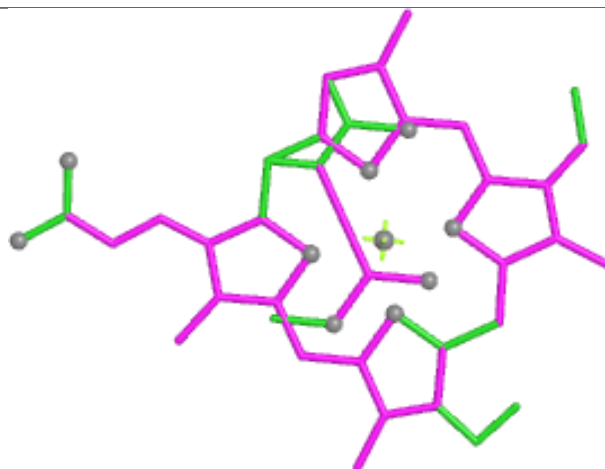




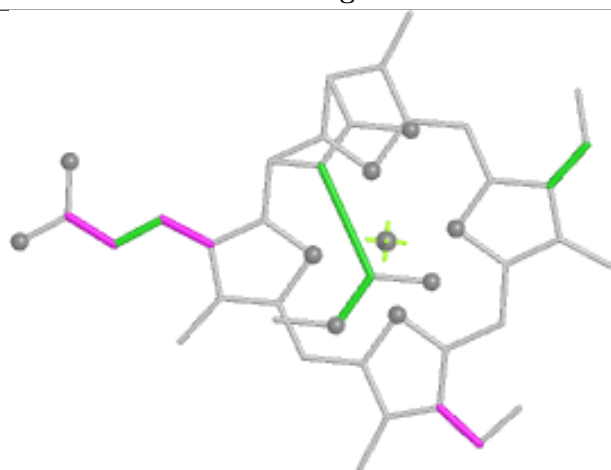
Ligand KC1 6 313



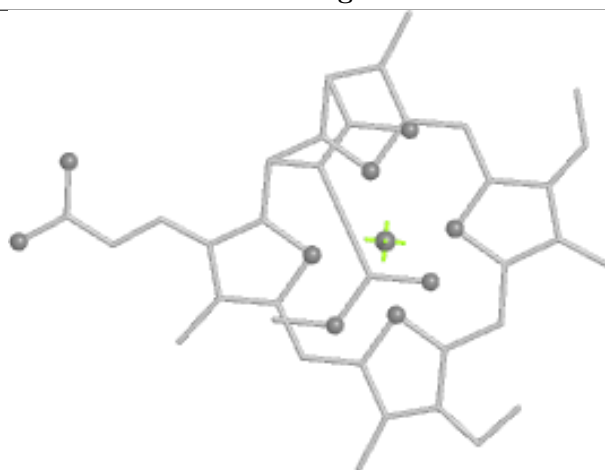
Bond lengths



Bond angles

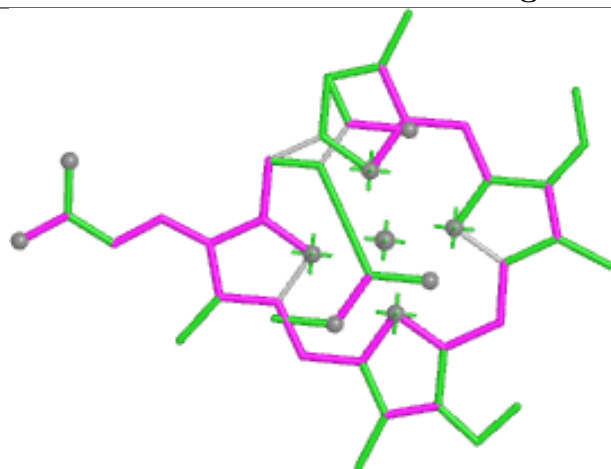


Torsions

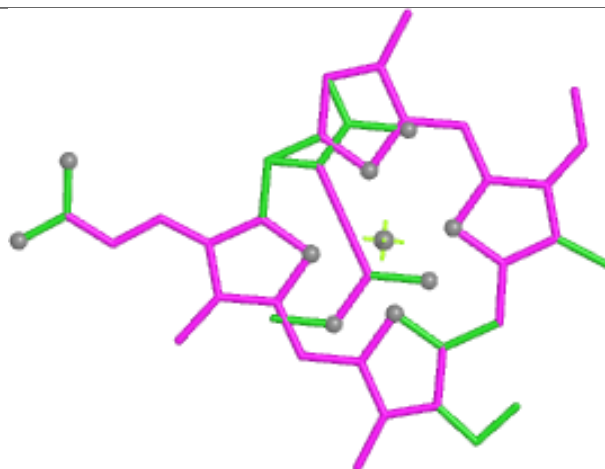


Rings

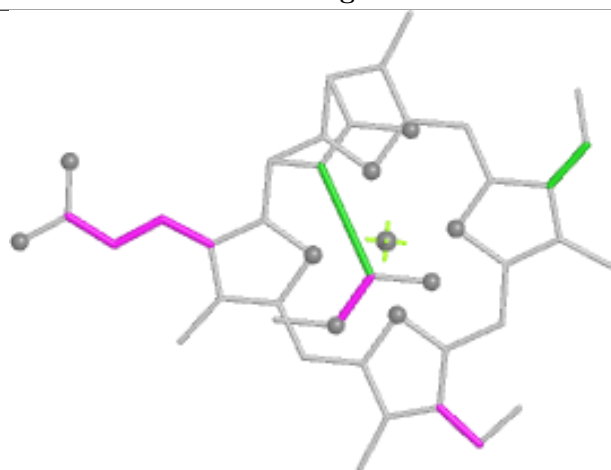
Ligand KC1 8 306



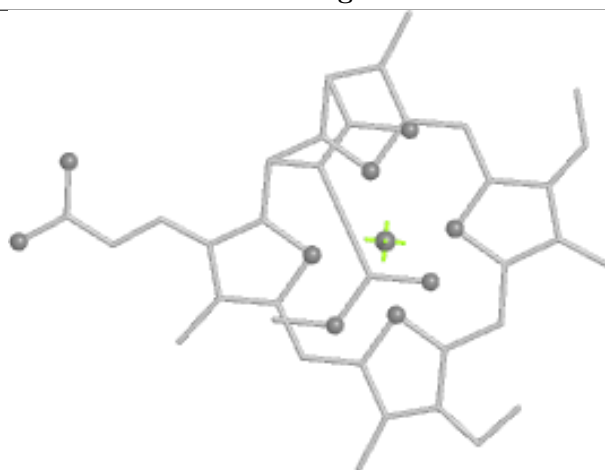
Bond lengths



Bond angles

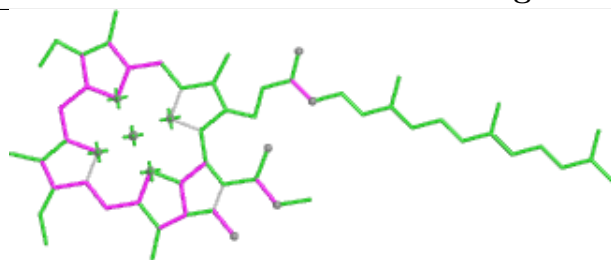


Torsions

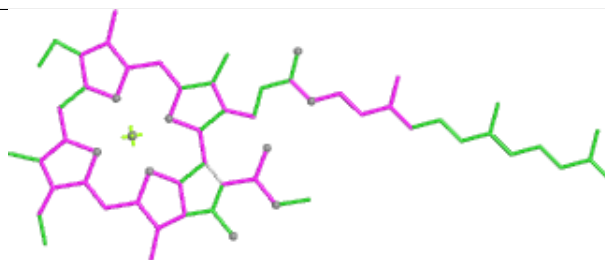


Rings

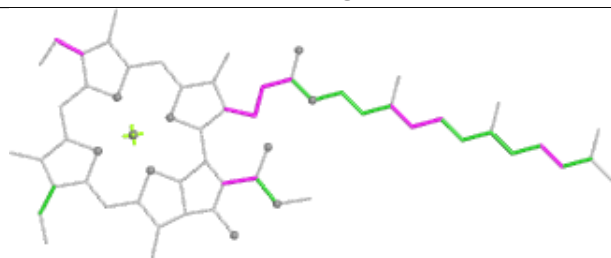
Ligand CLA A 814



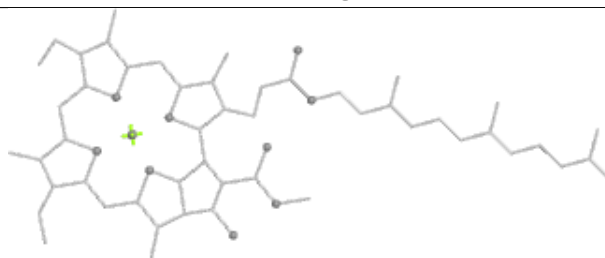
Bond lengths



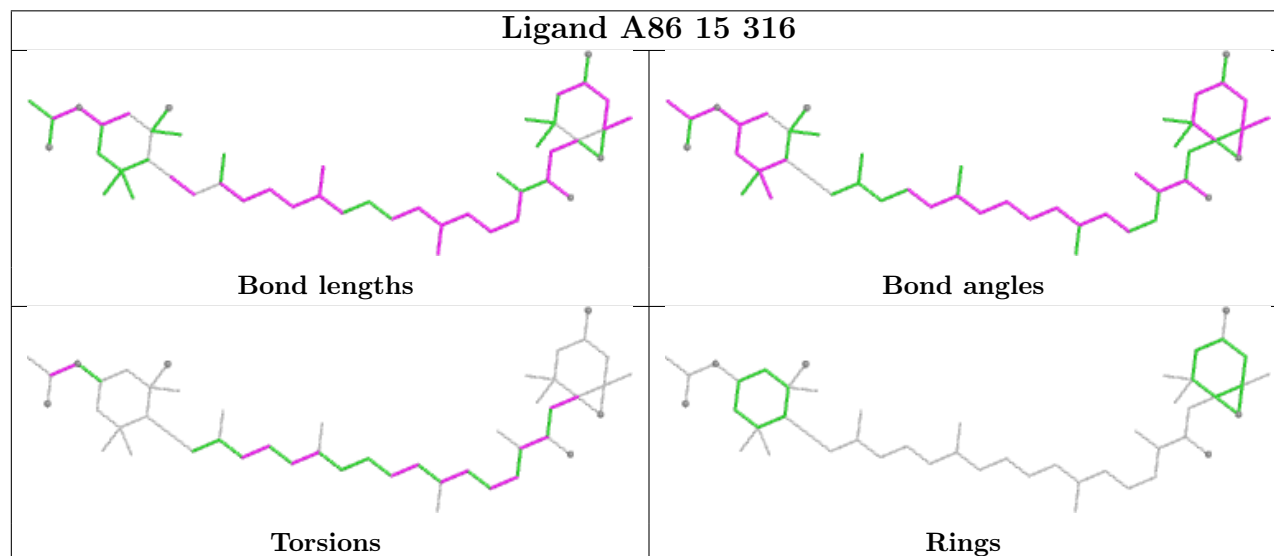
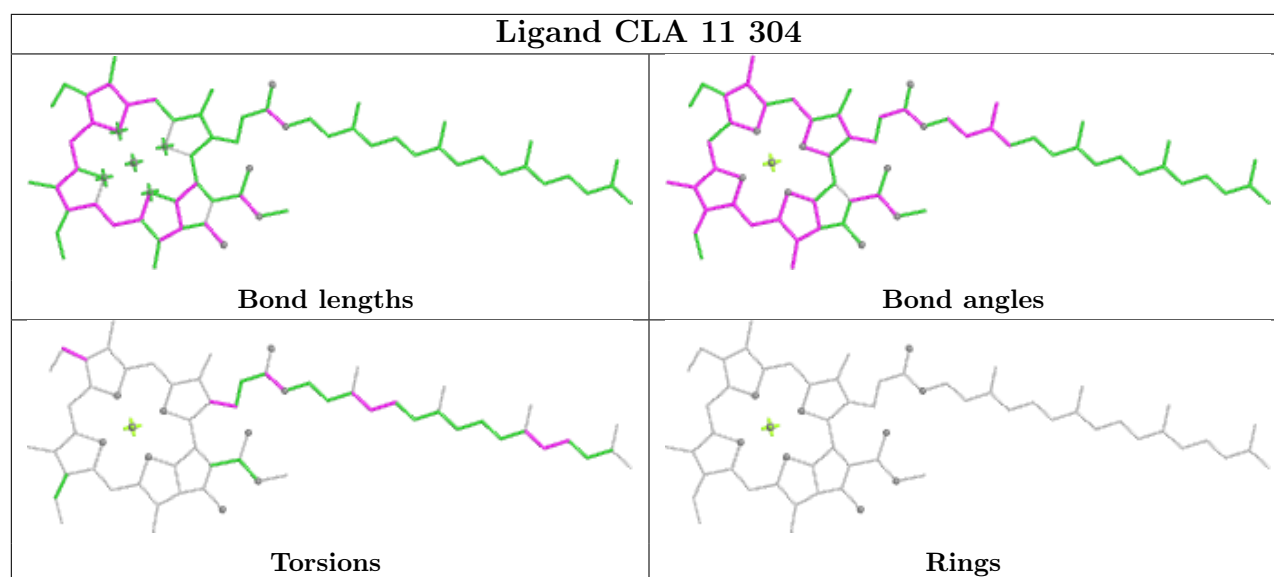
Bond angles

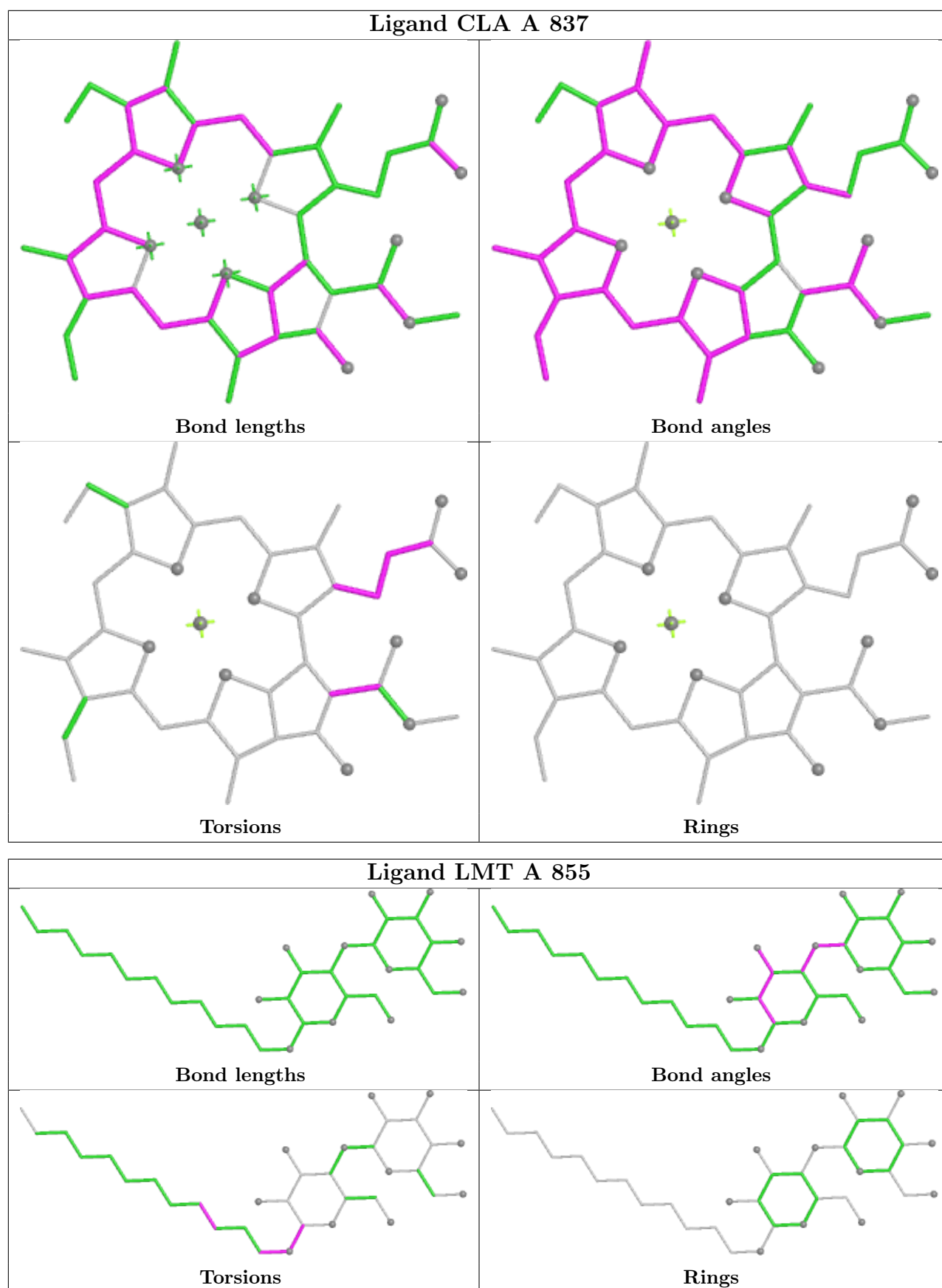


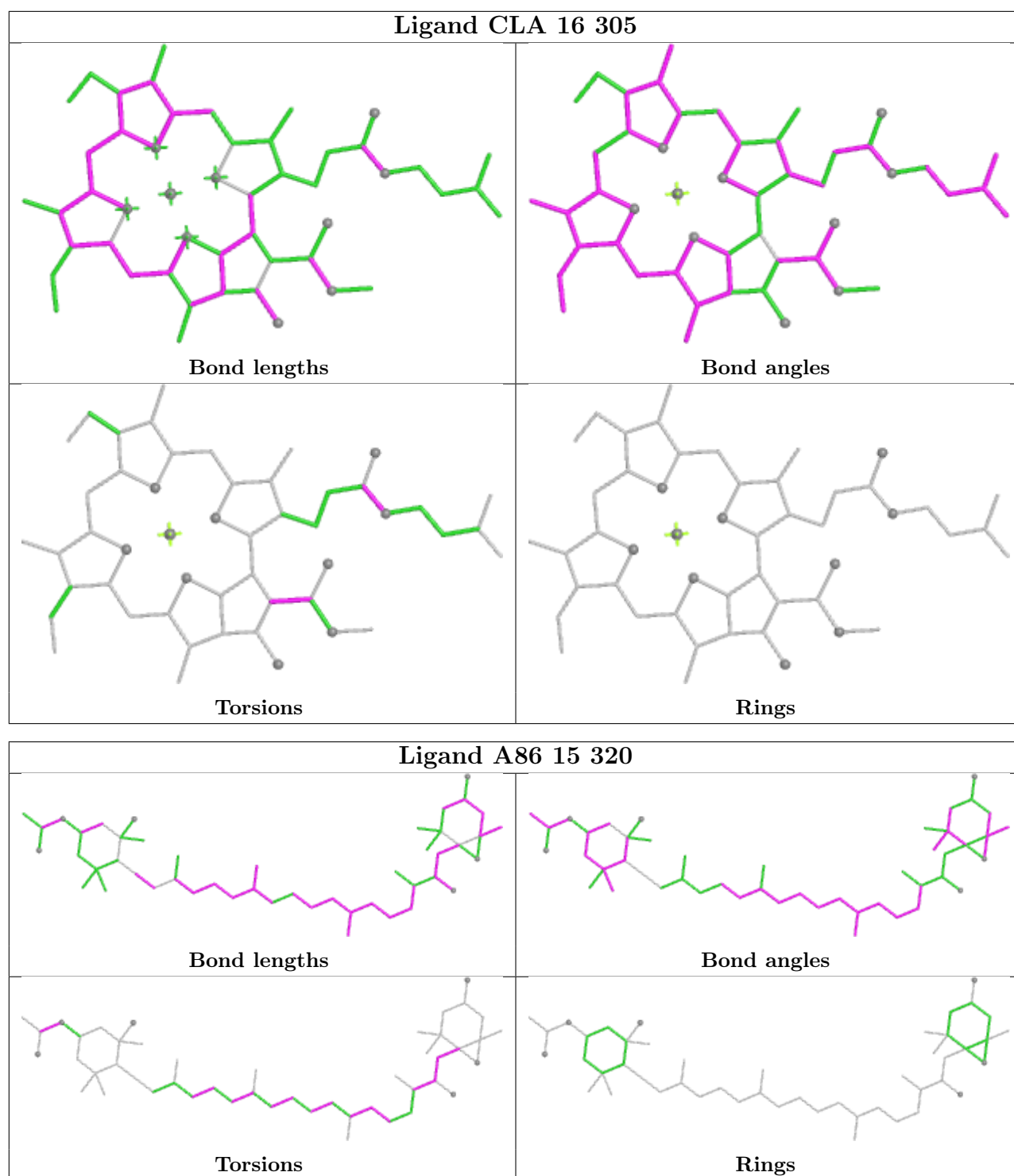
Torsions

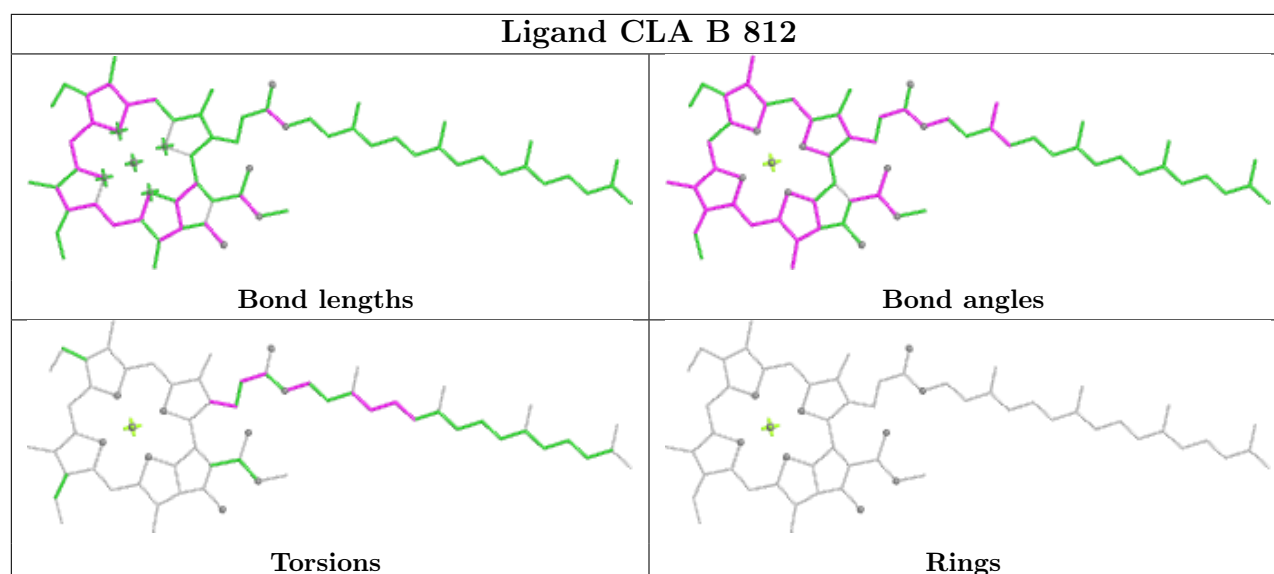
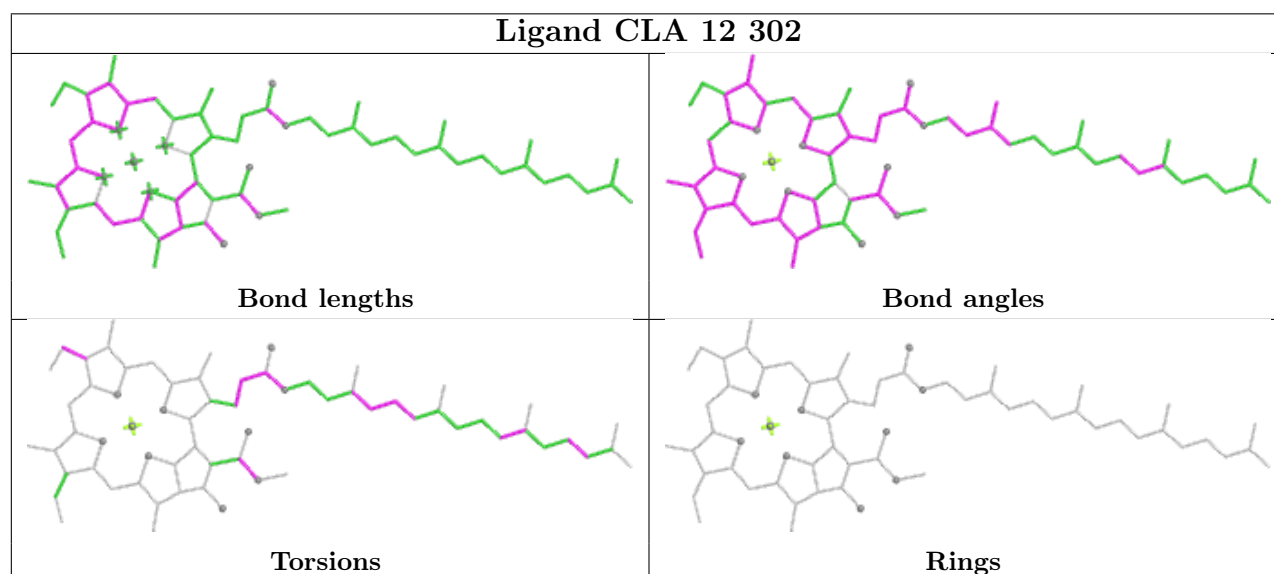
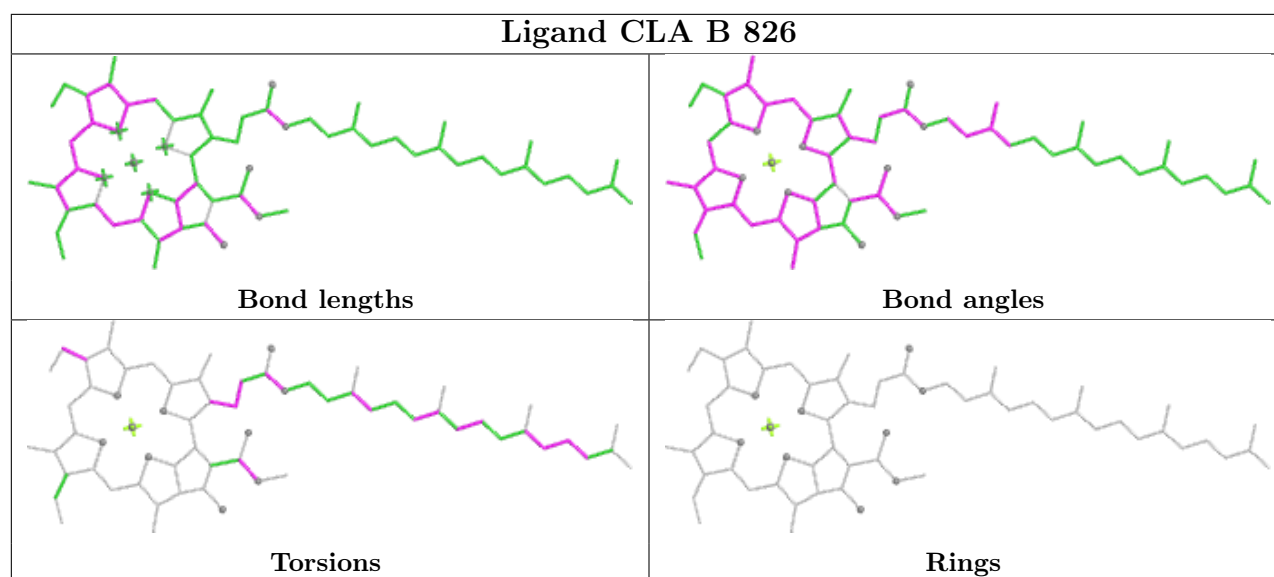


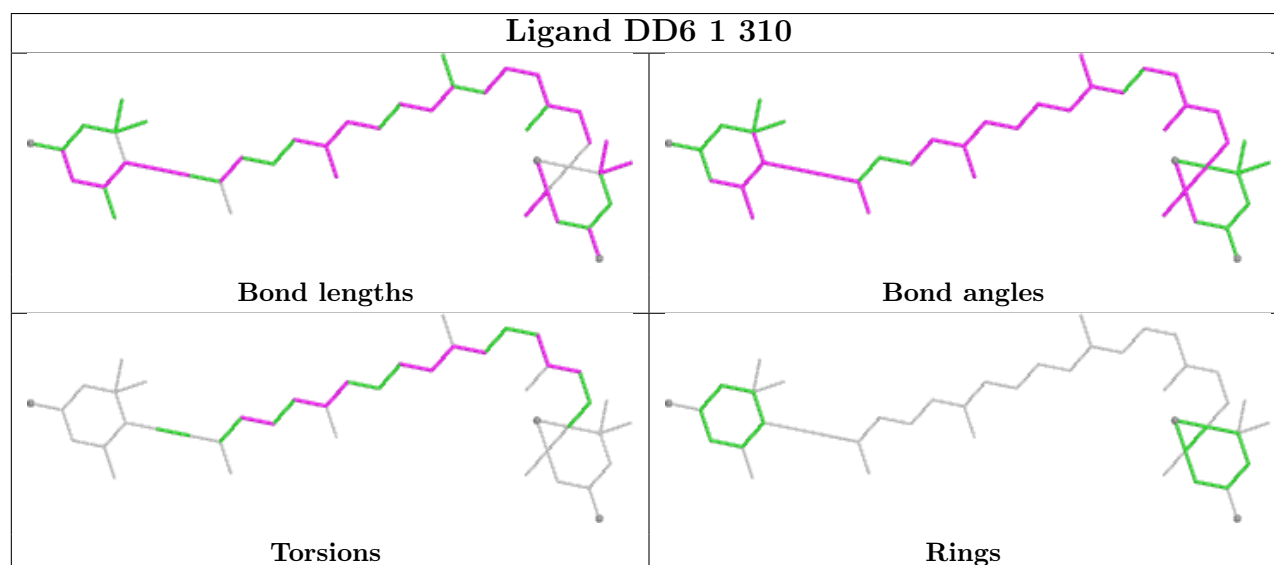
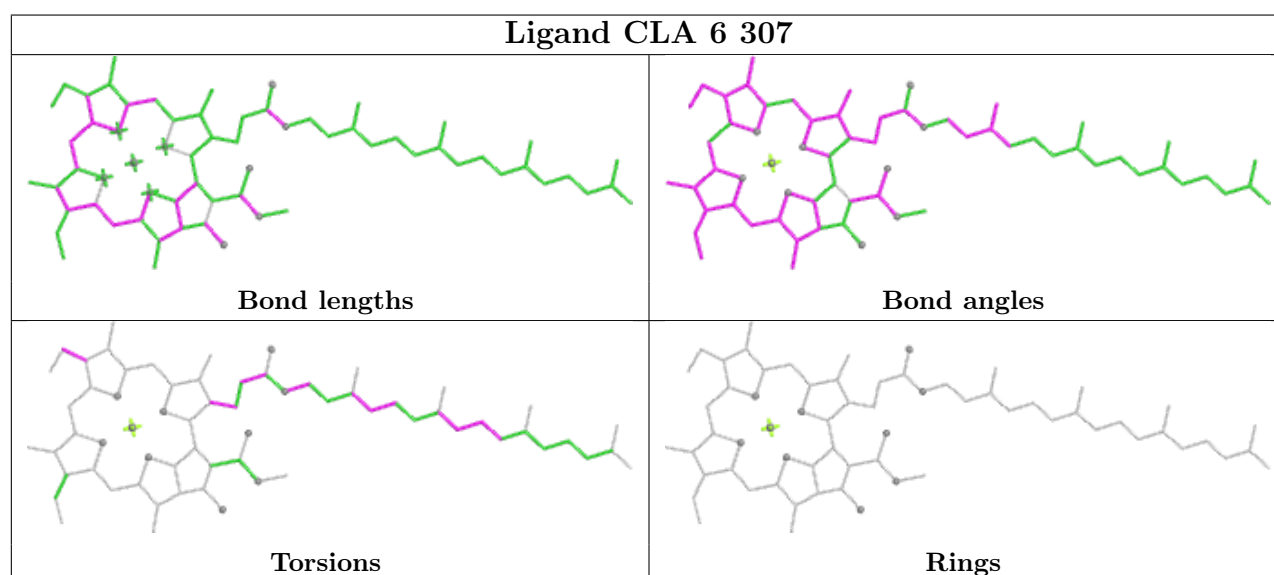
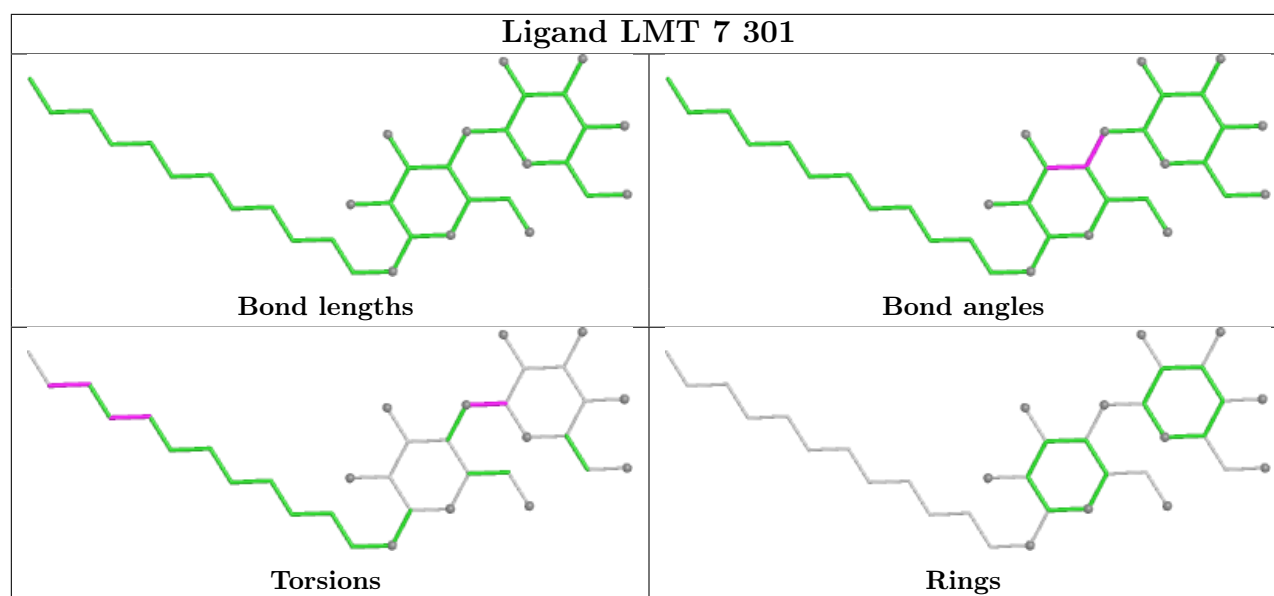
Rings

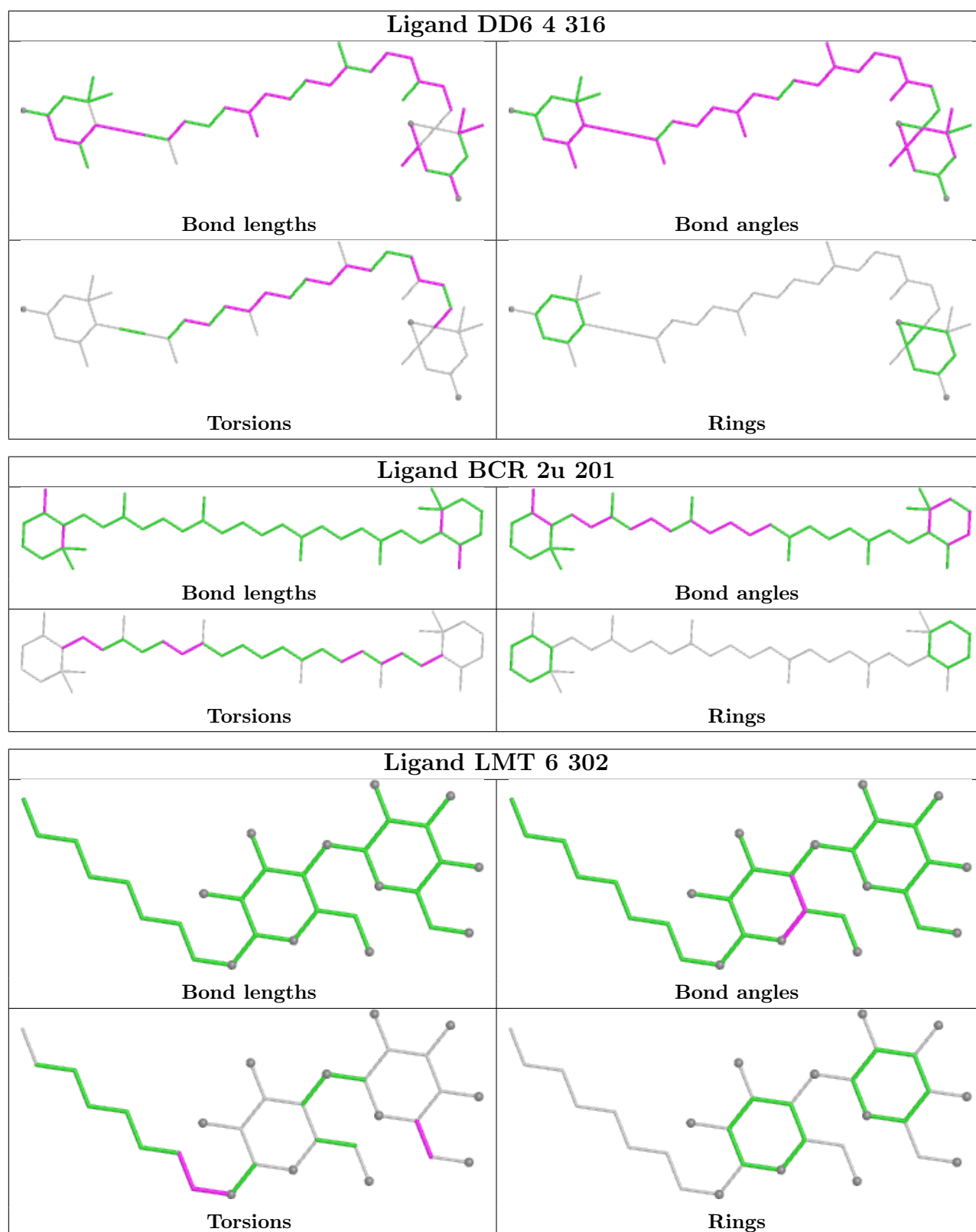


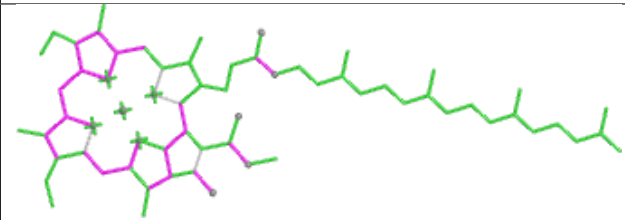
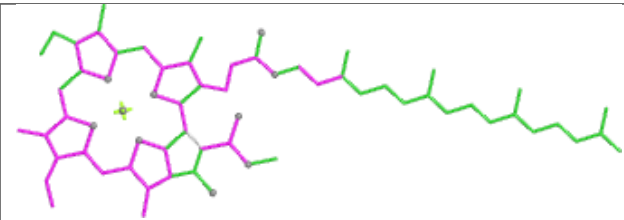
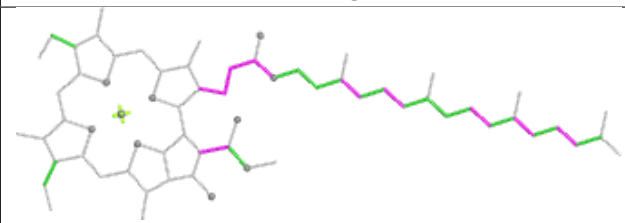
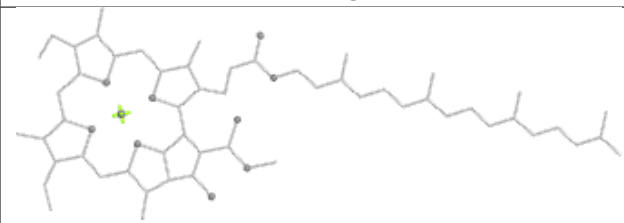


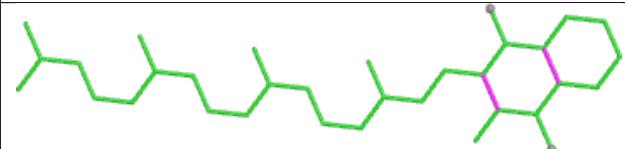
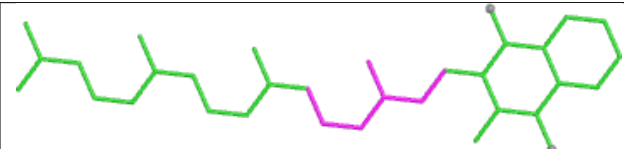
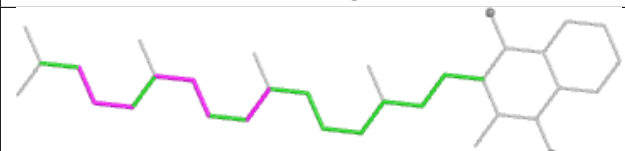
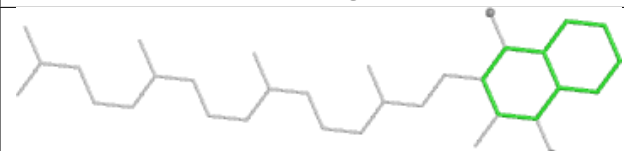


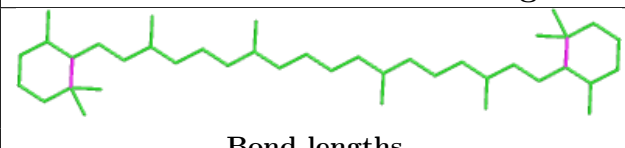
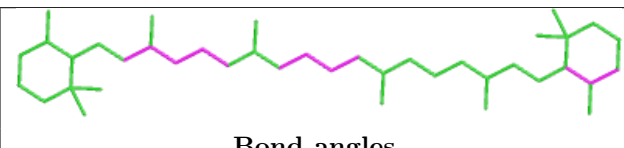
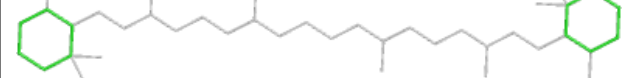


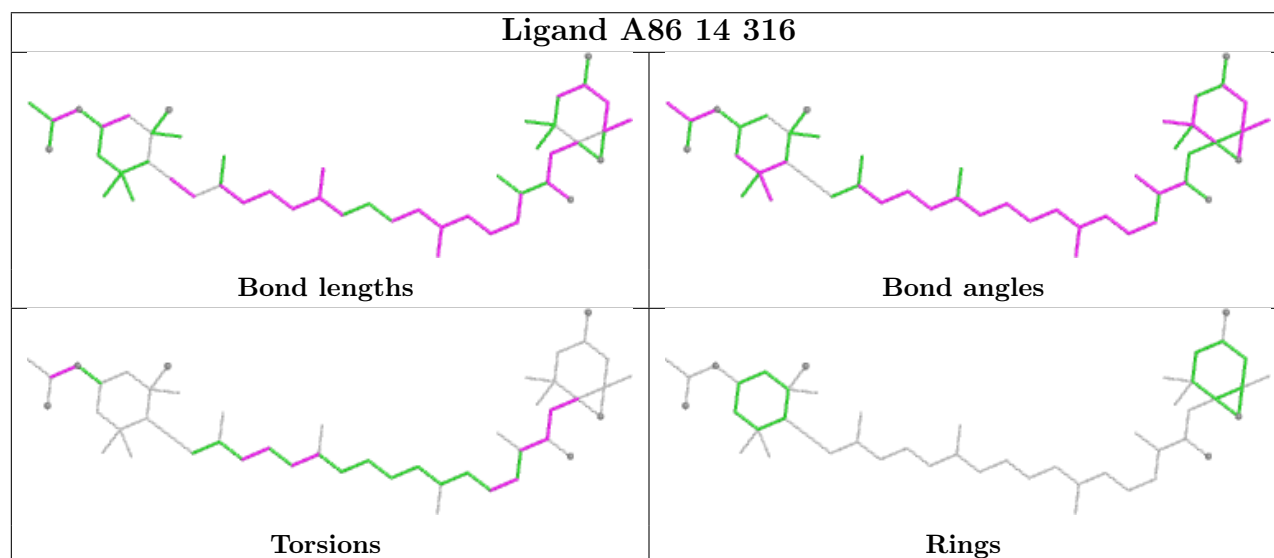
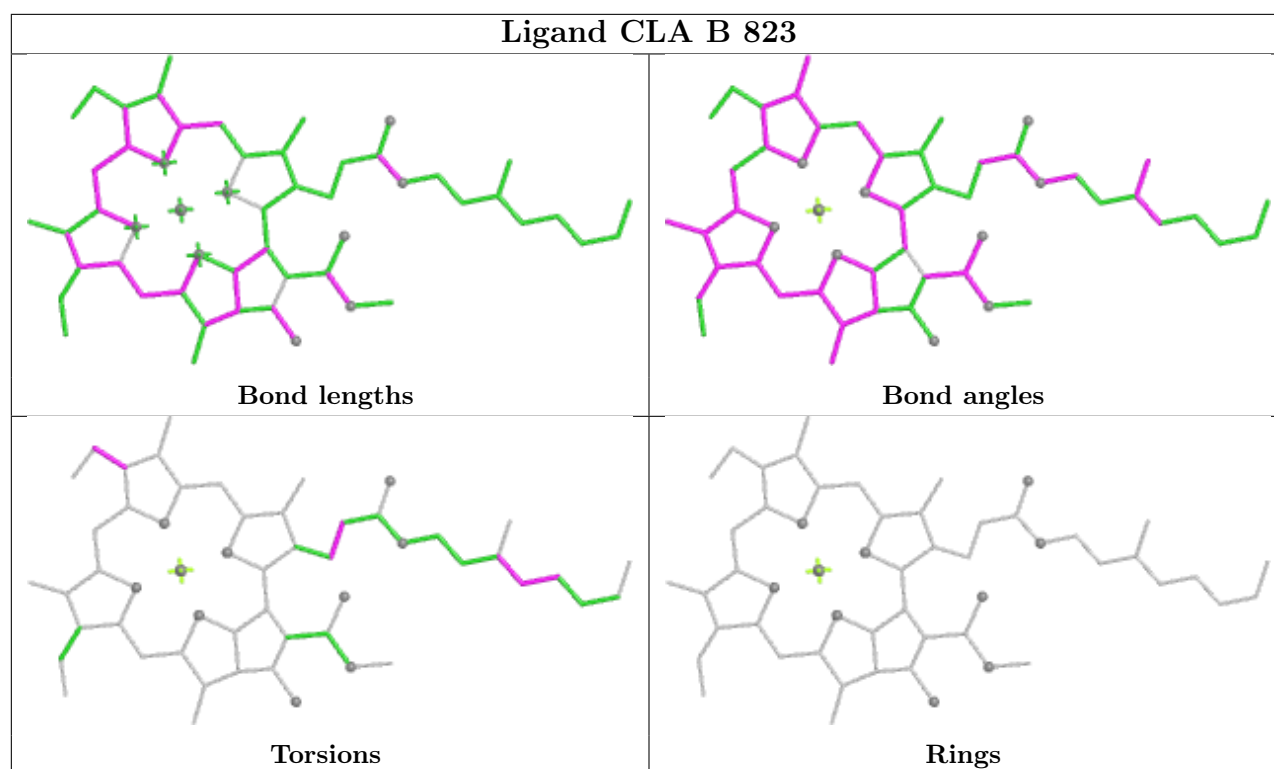


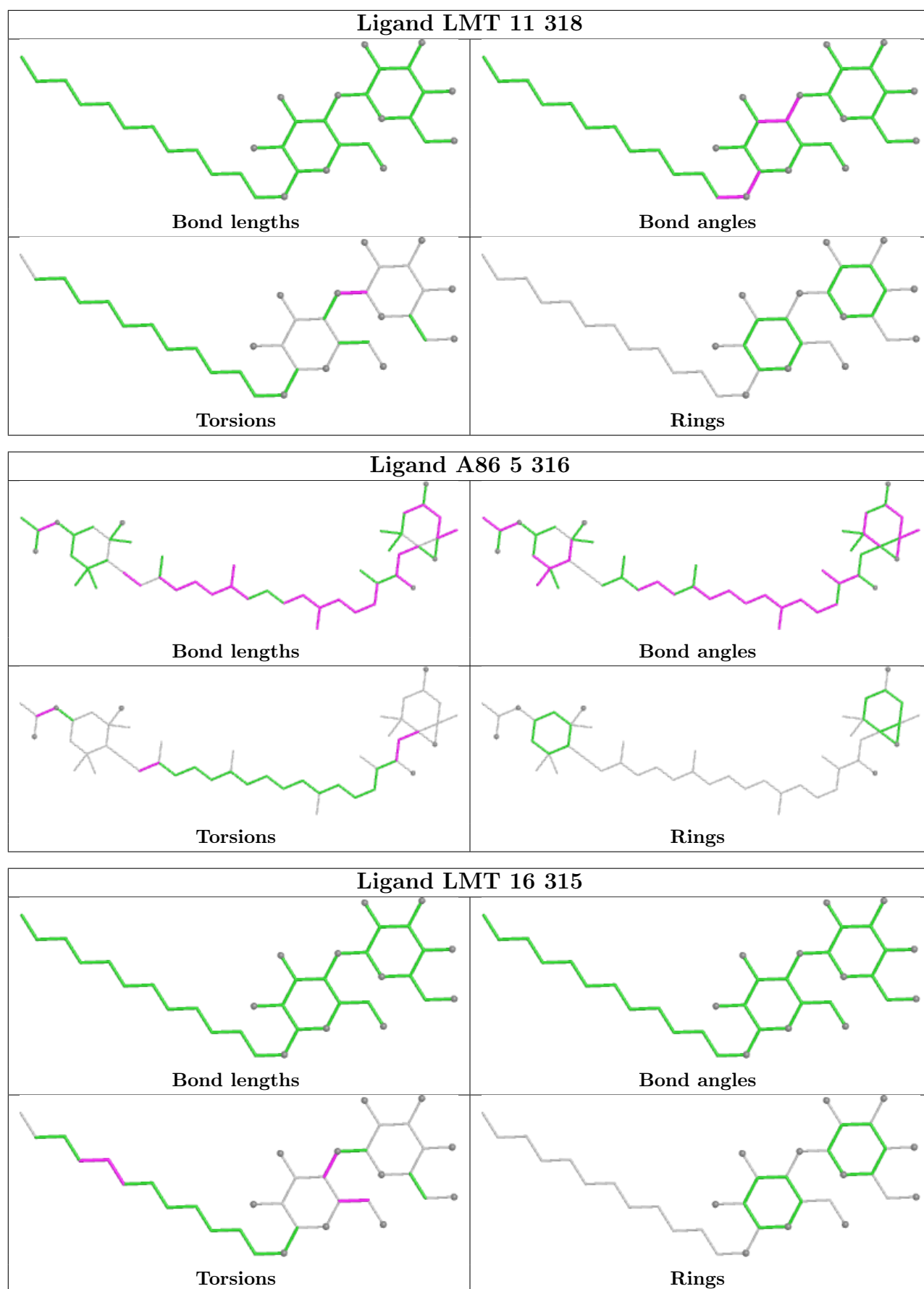


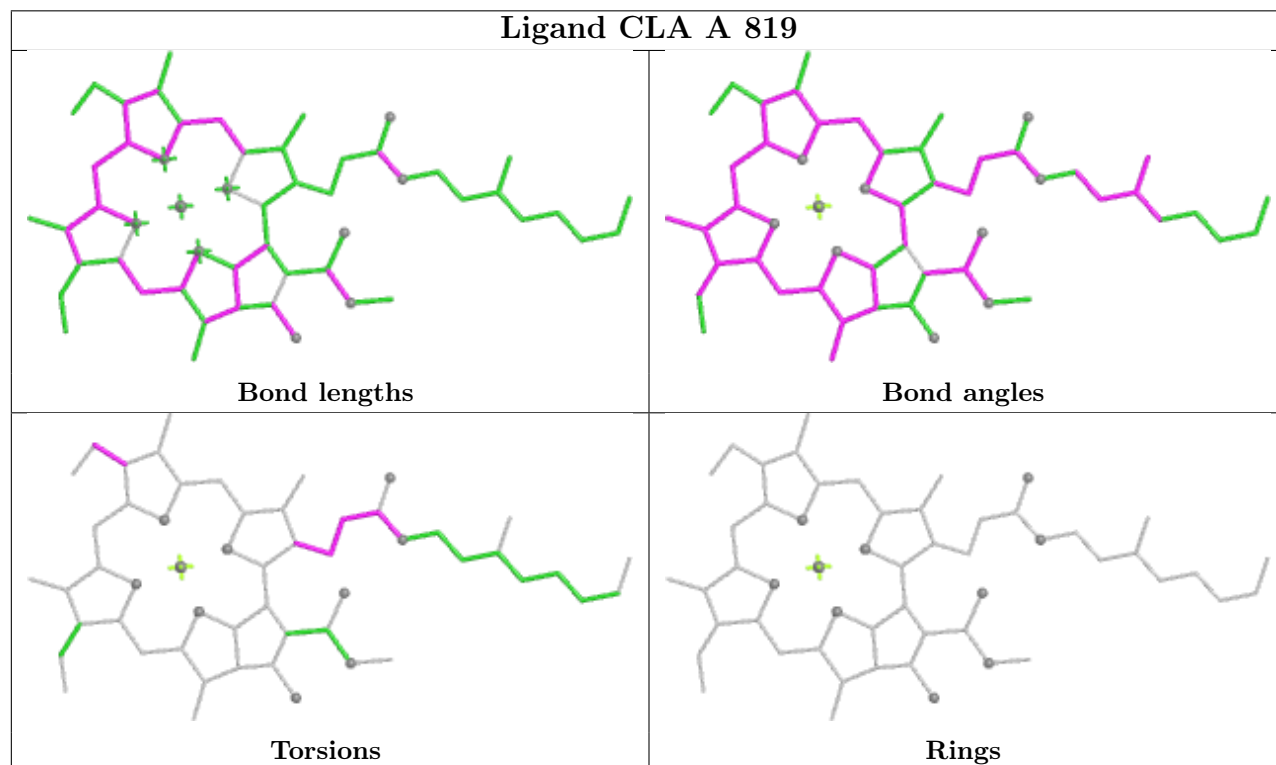
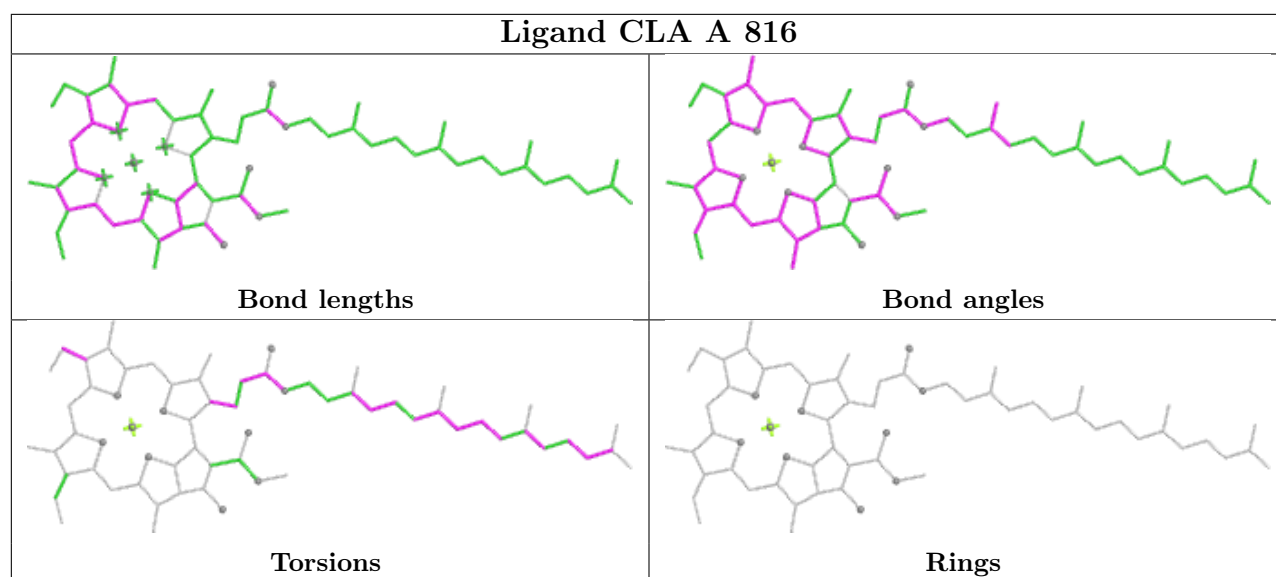
Ligand CLA 5 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PQN A 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

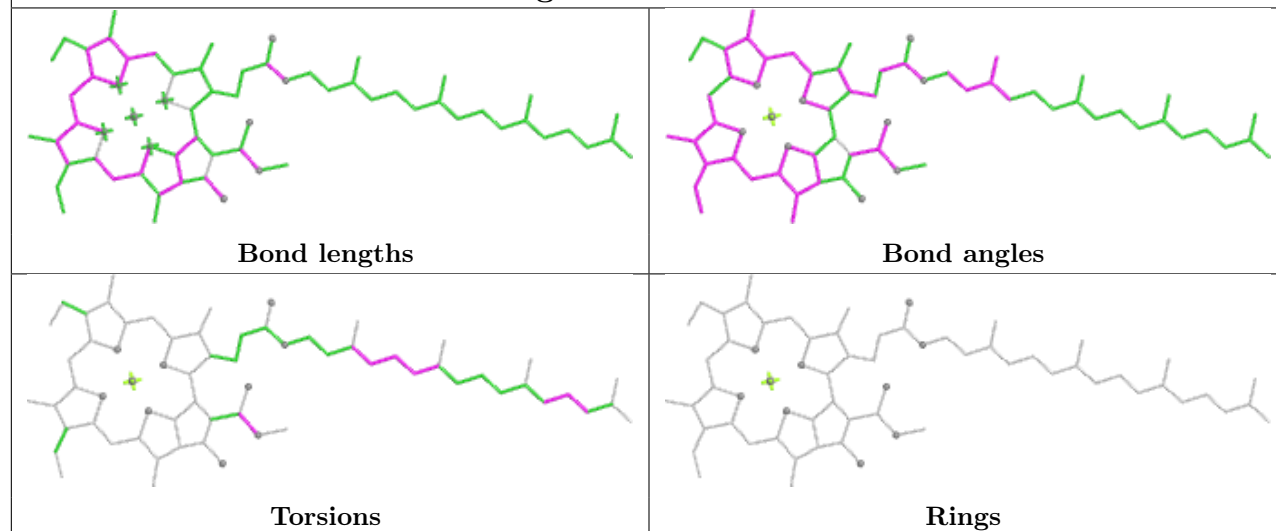
Ligand BCR B 846	
	
Bond lengths	Bond angles
	
Torsions	Rings



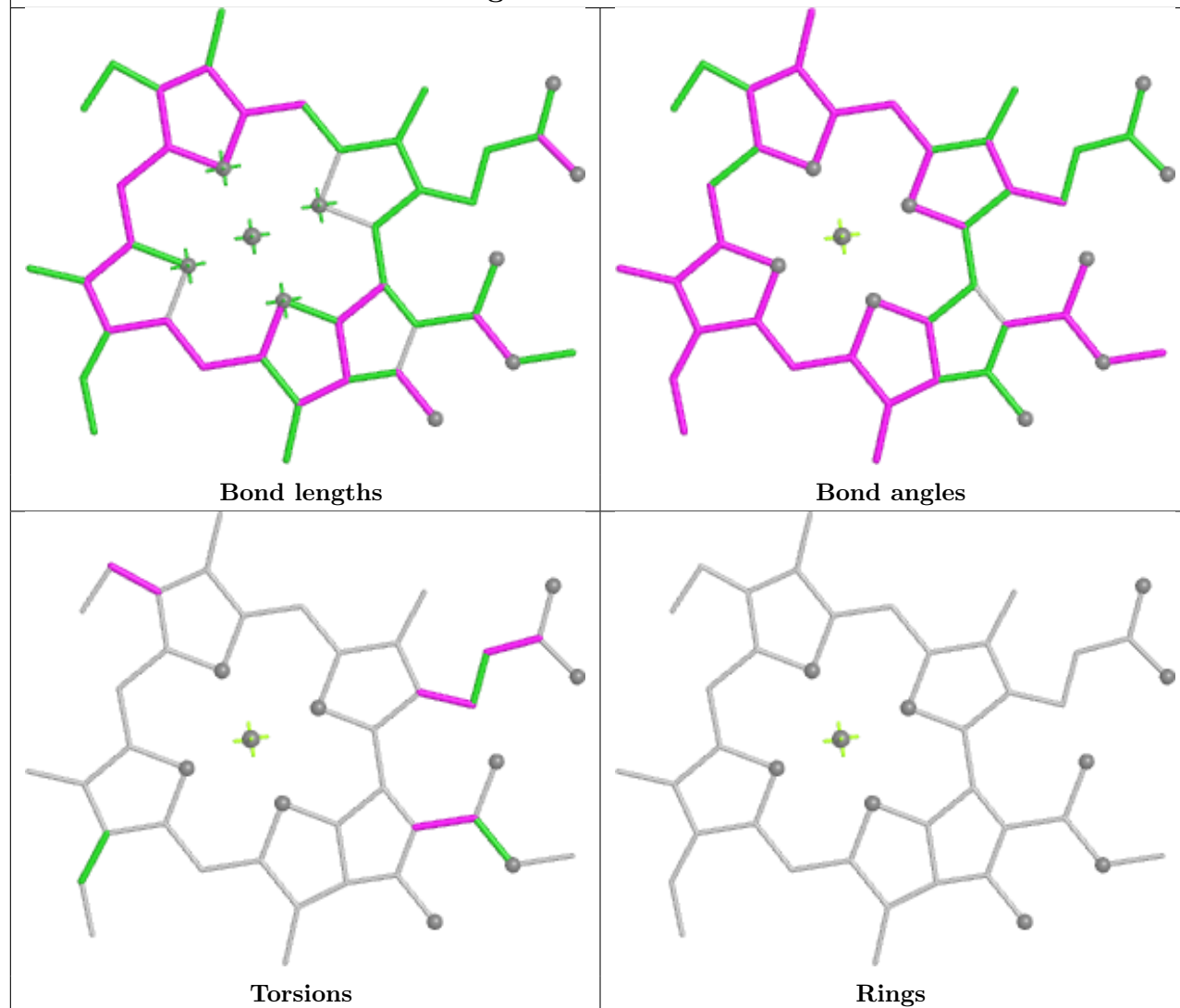


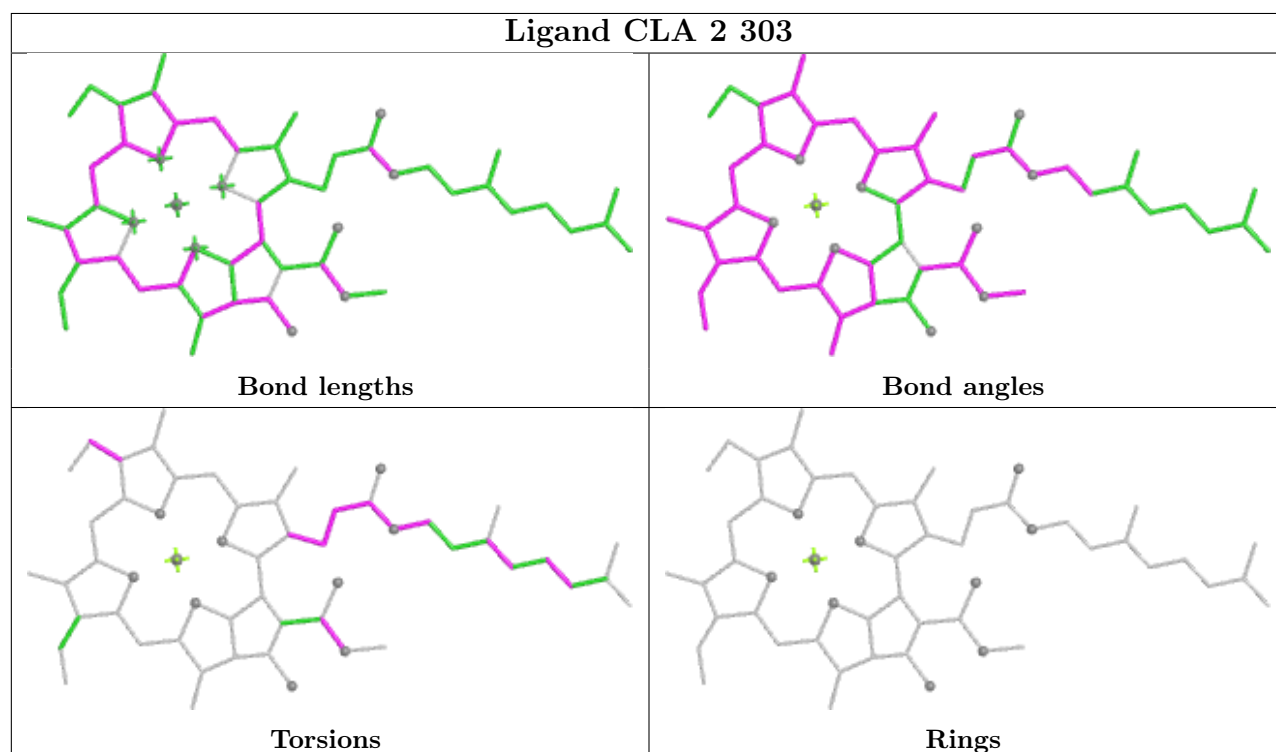
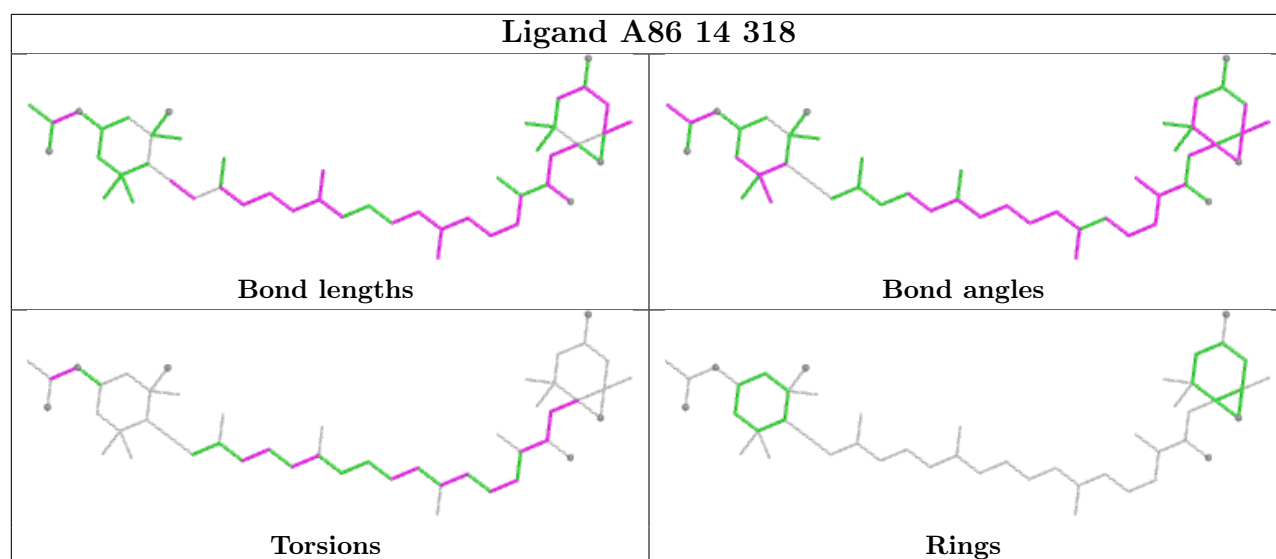


Ligand CLA 8 302

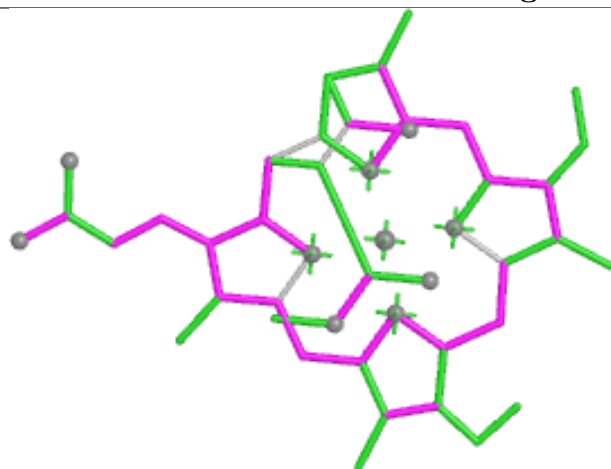


Ligand CLA 13 304

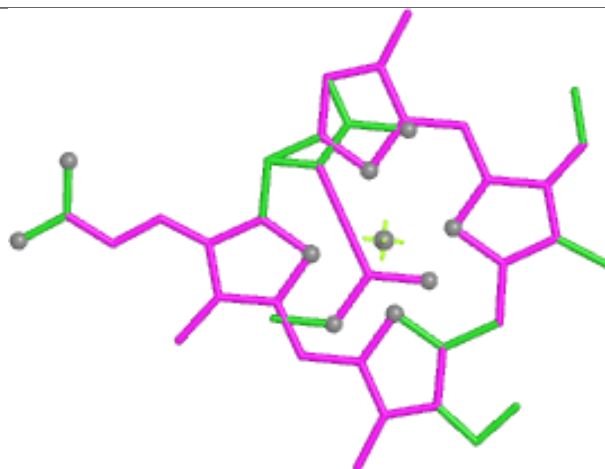




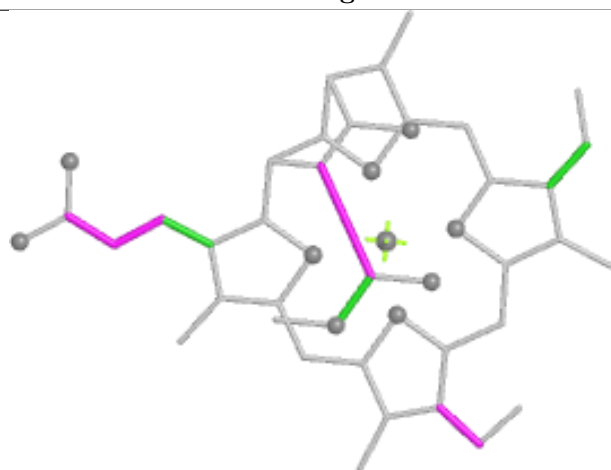
Ligand KC1 3 311



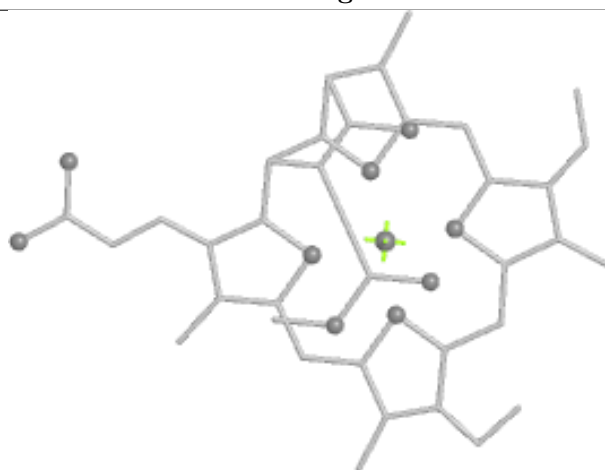
Bond lengths



Bond angles

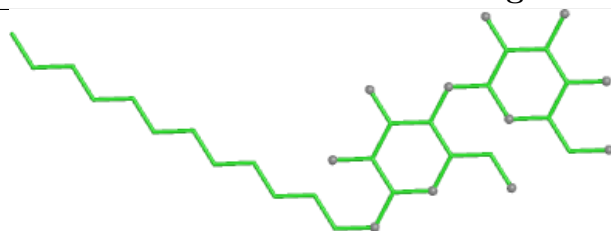


Torsions

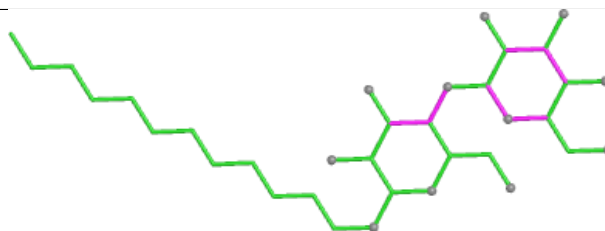


Rings

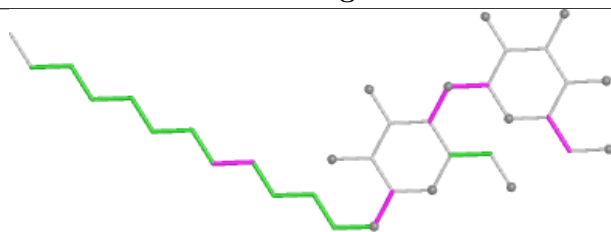
Ligand LMT 15 301



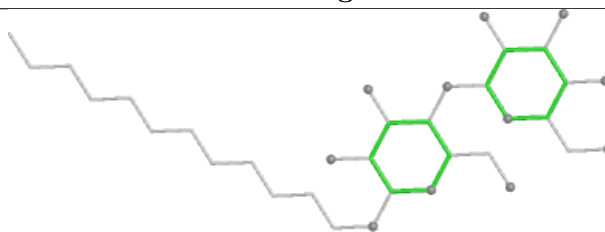
Bond lengths



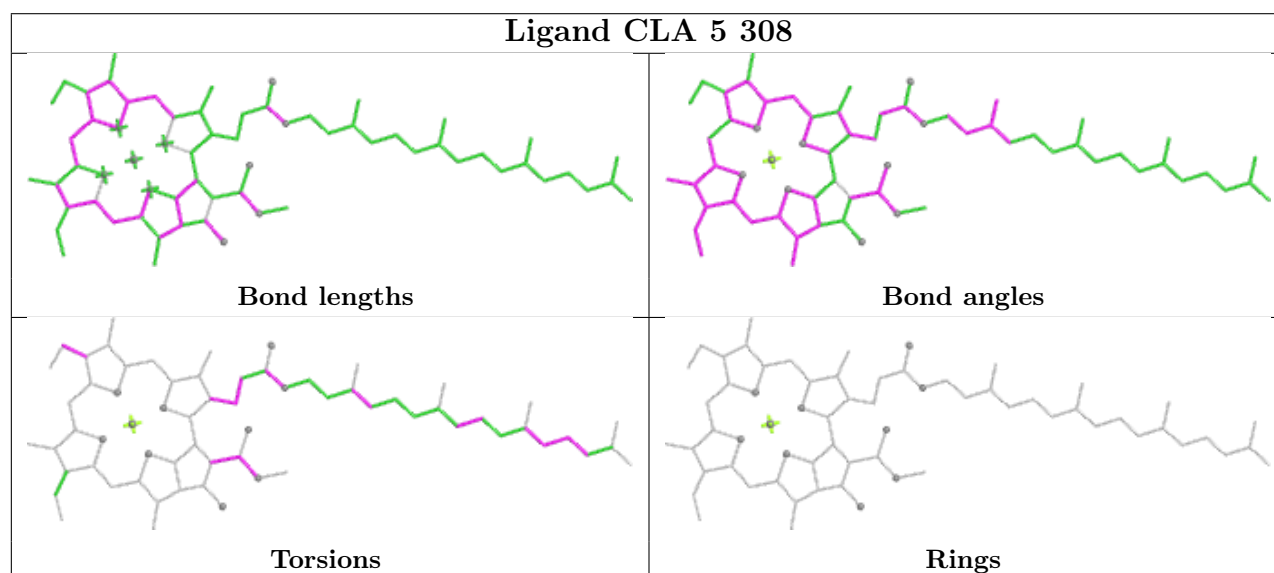
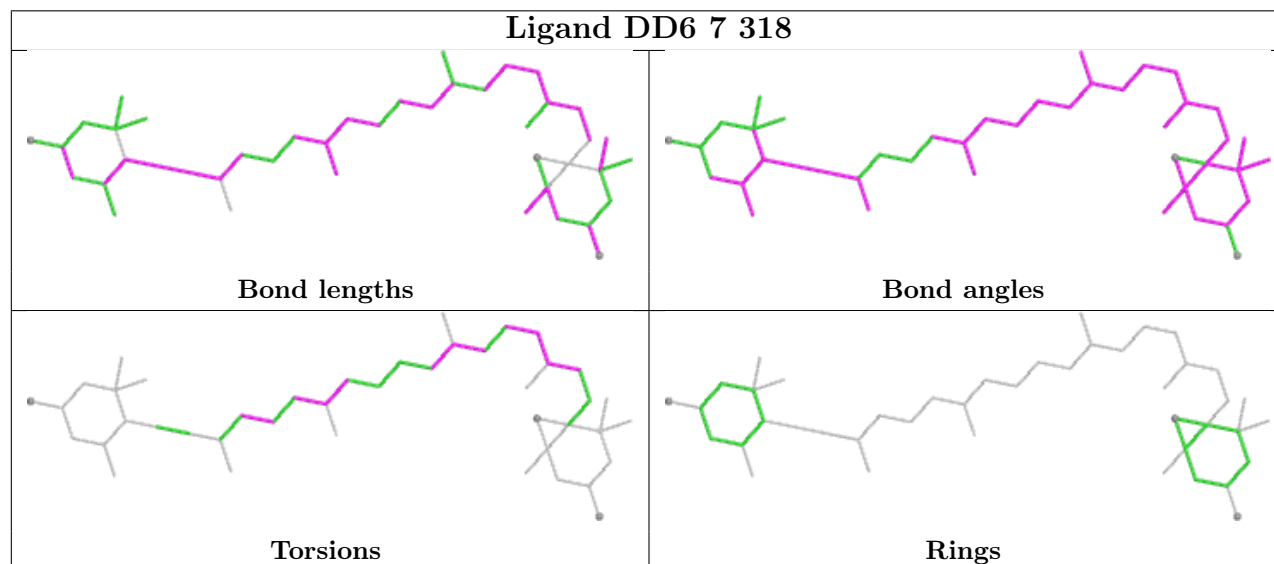
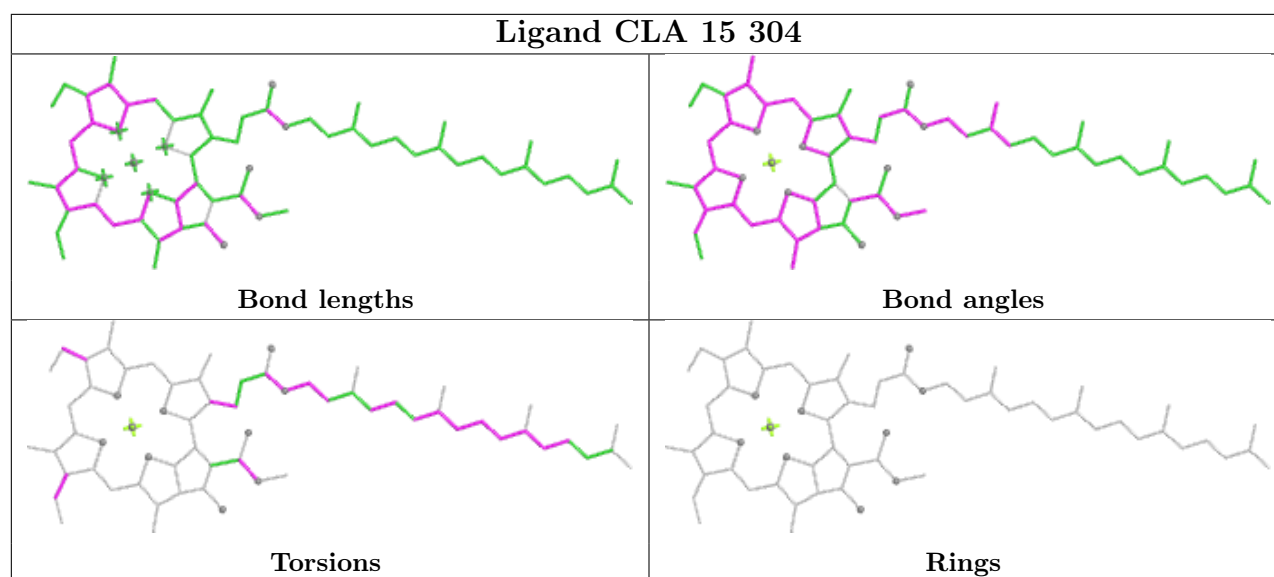
Bond angles

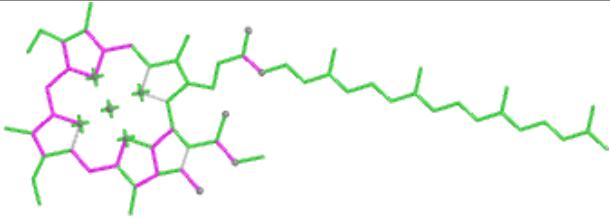
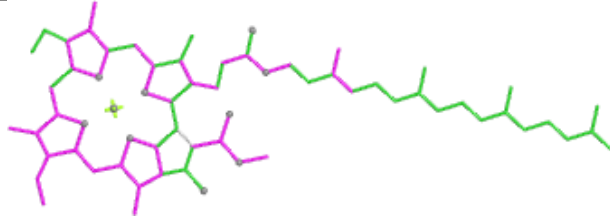
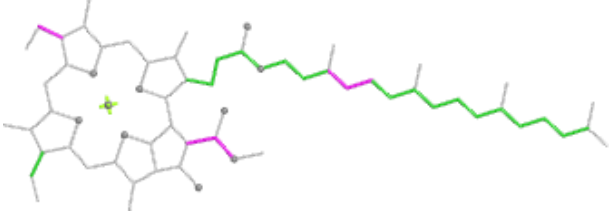
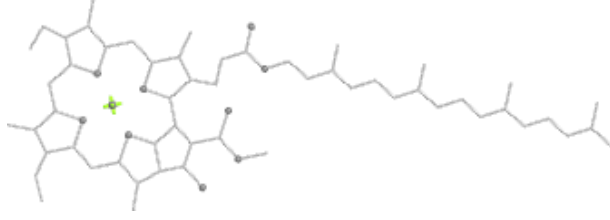
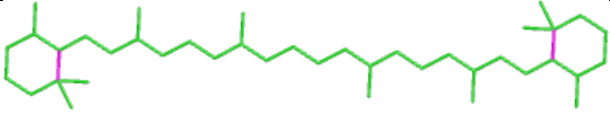
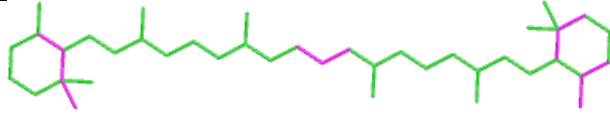
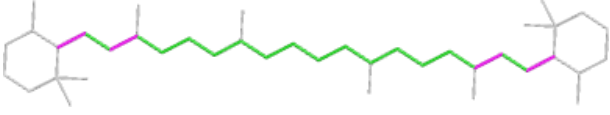
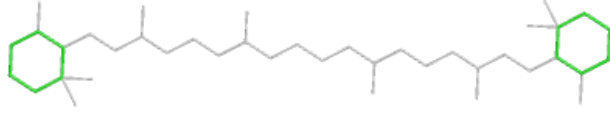
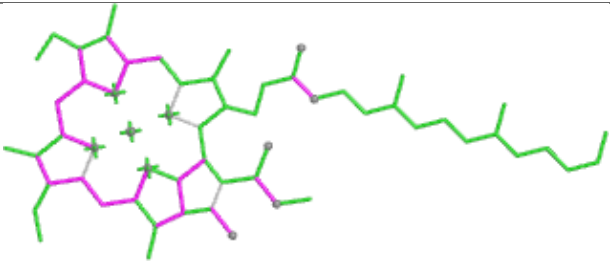
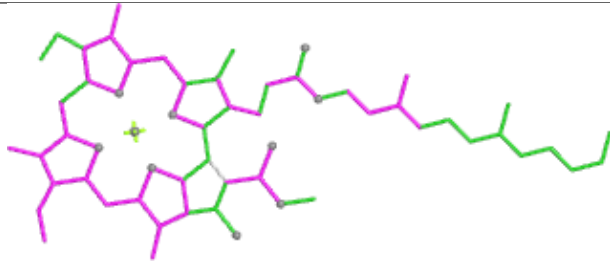
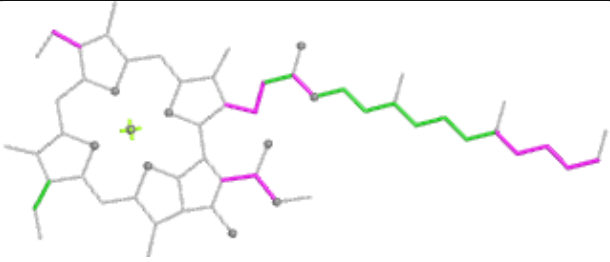
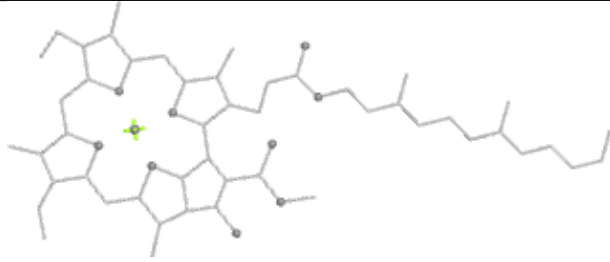


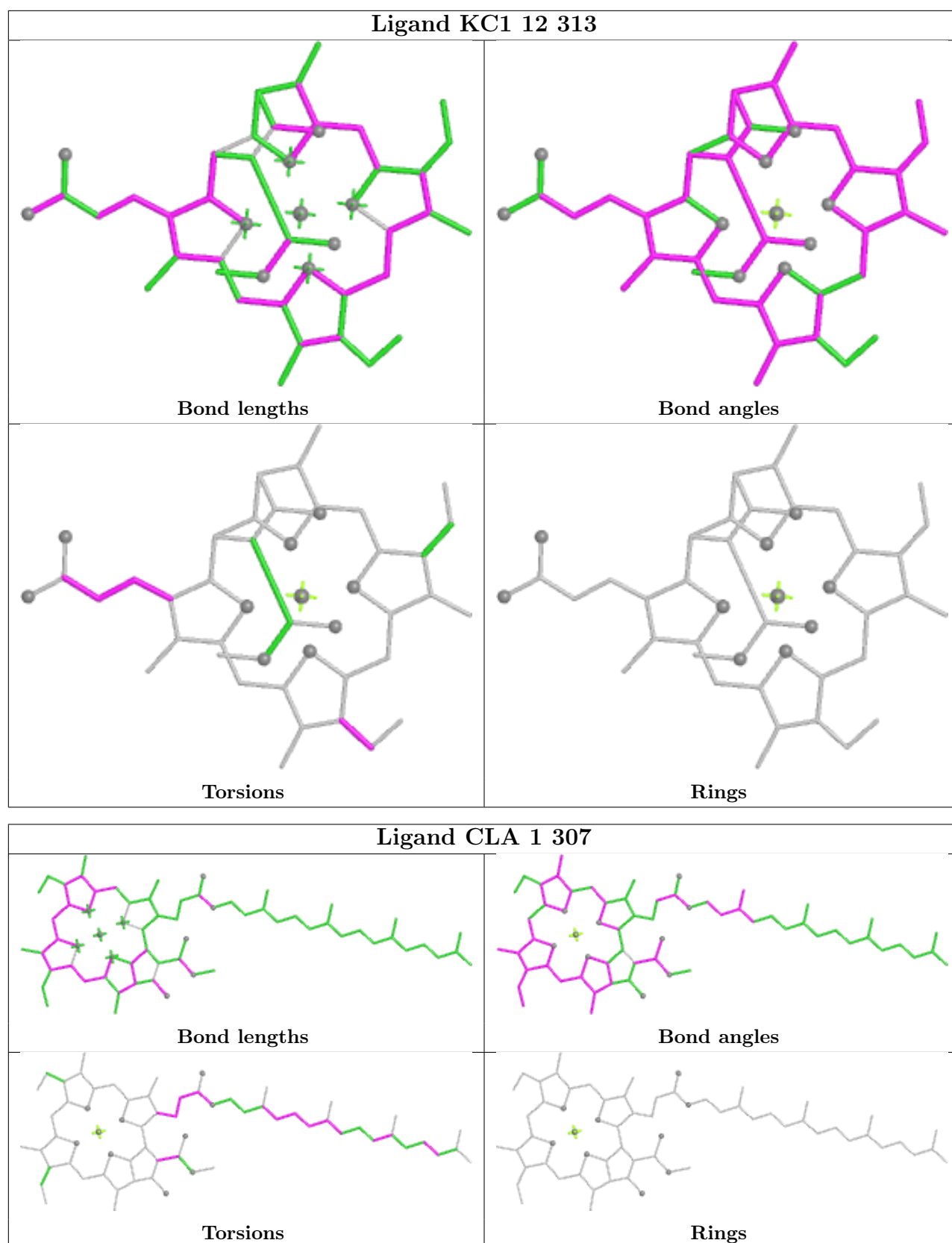
Torsions



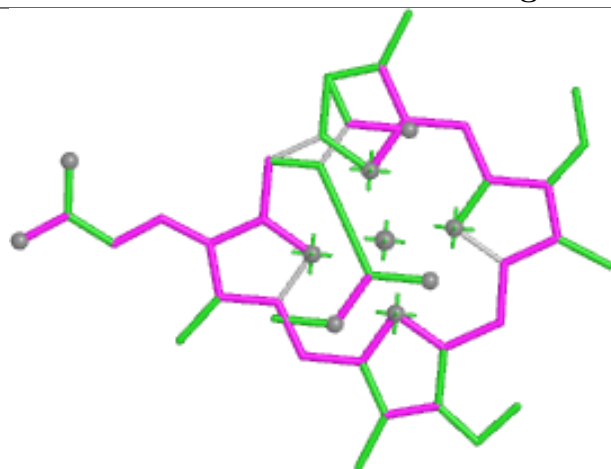
Rings



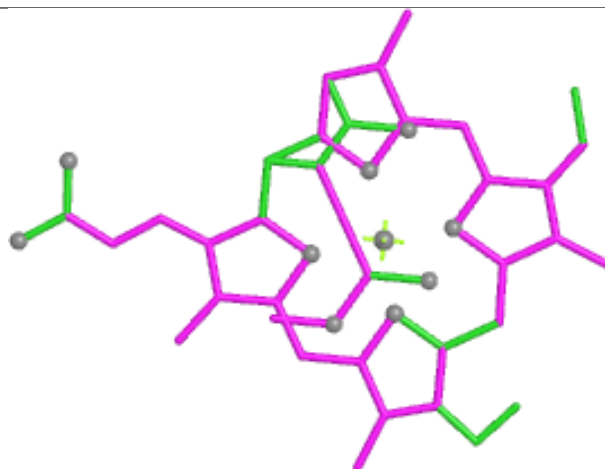
Ligand CLA 5 303	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 825	
 Bond lengths	 Bond angles
 Torsions	 Rings



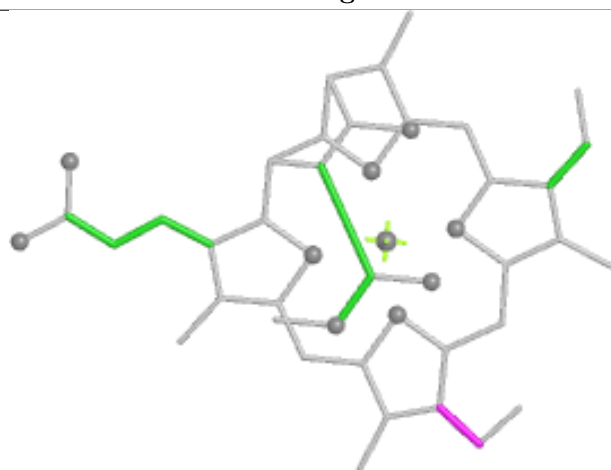
Ligand KC1 2 312



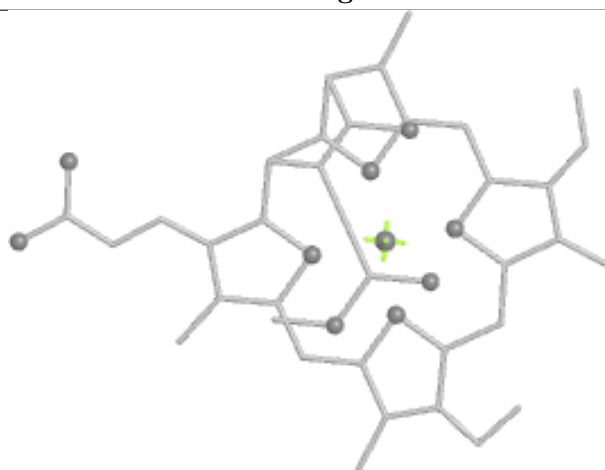
Bond lengths



Bond angles

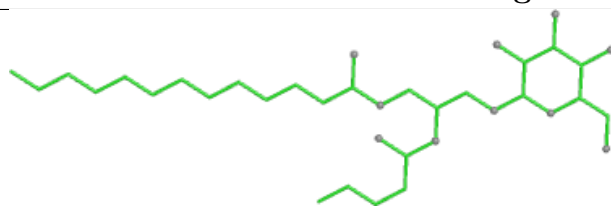


Torsions

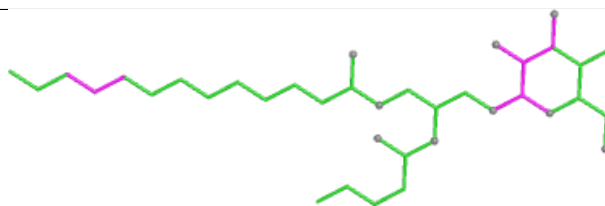


Rings

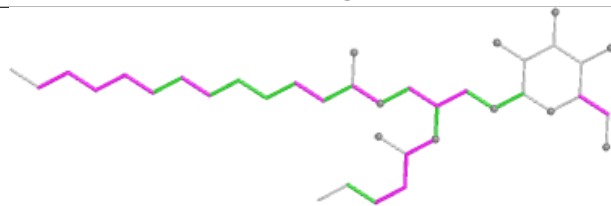
Ligand LMG 8 319



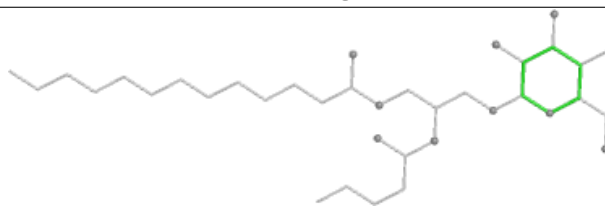
Bond lengths



Bond angles

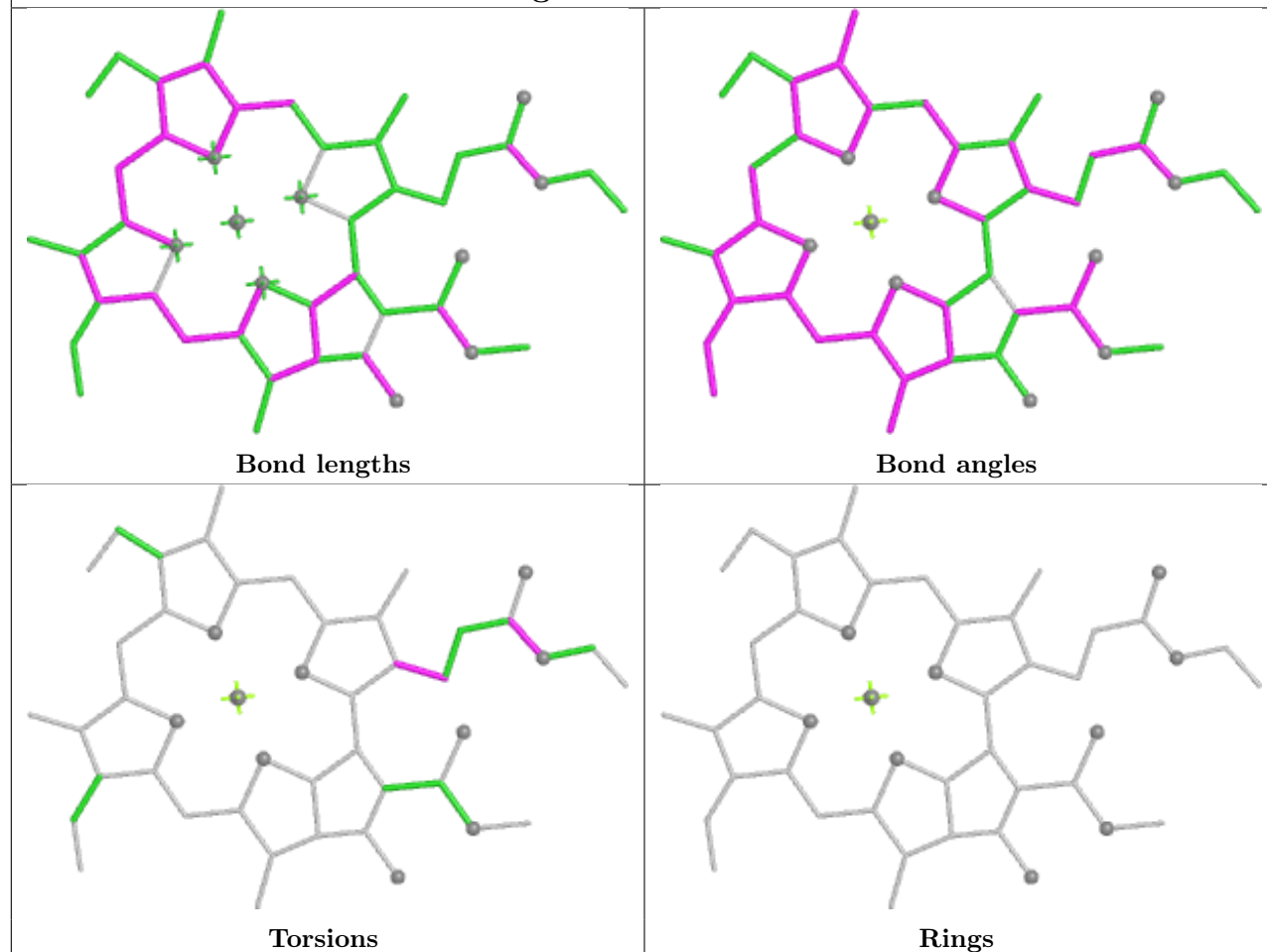


Torsions

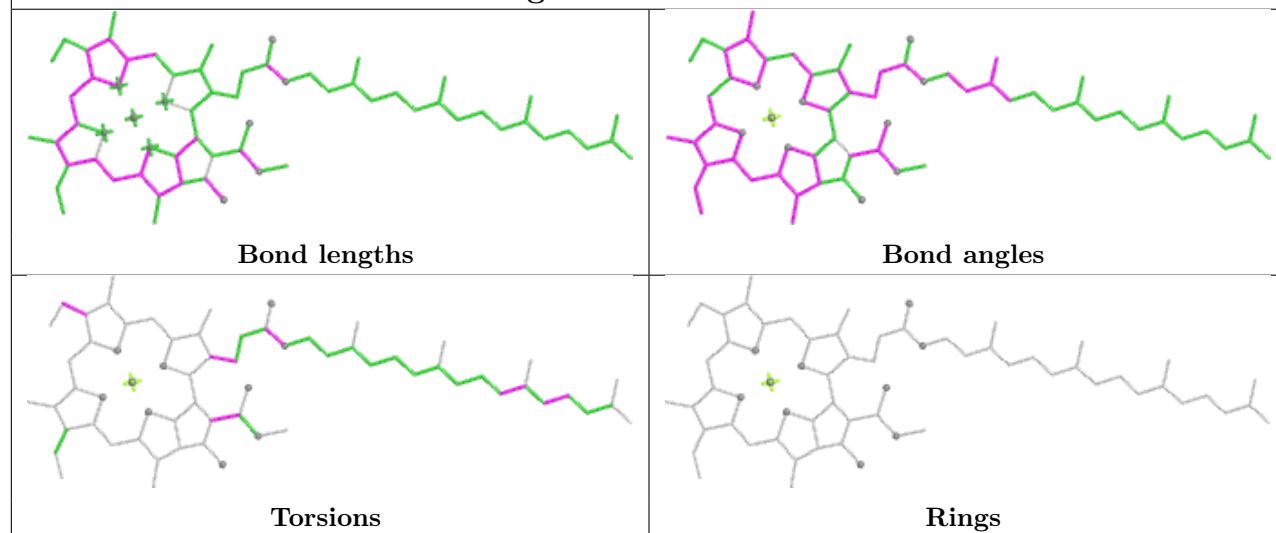


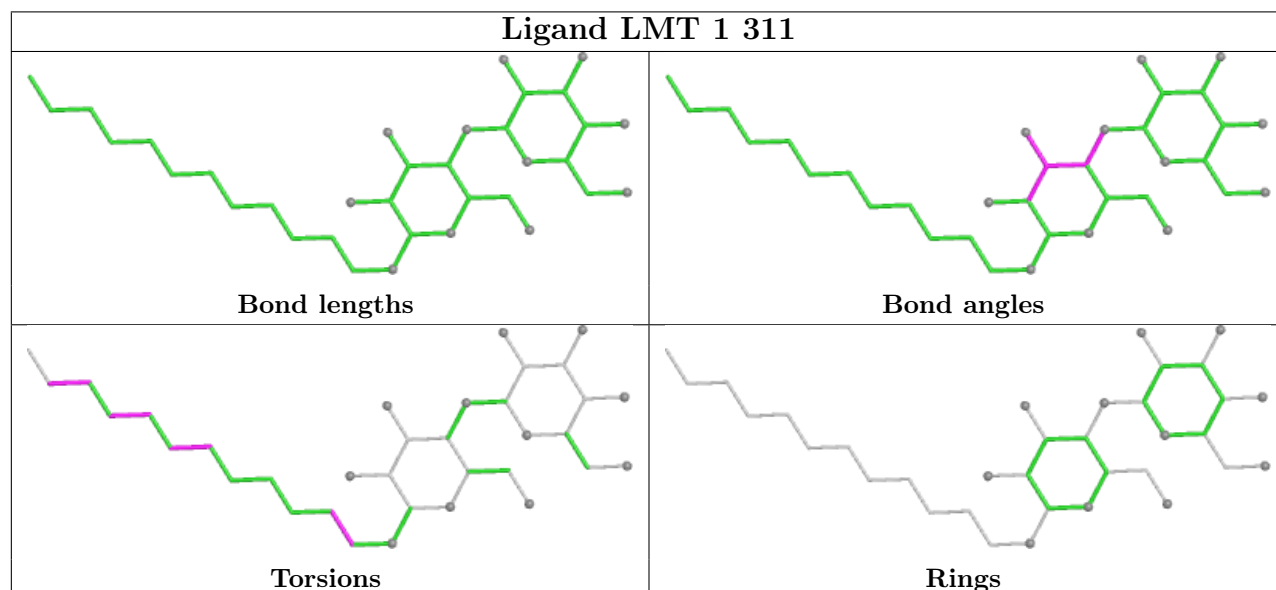
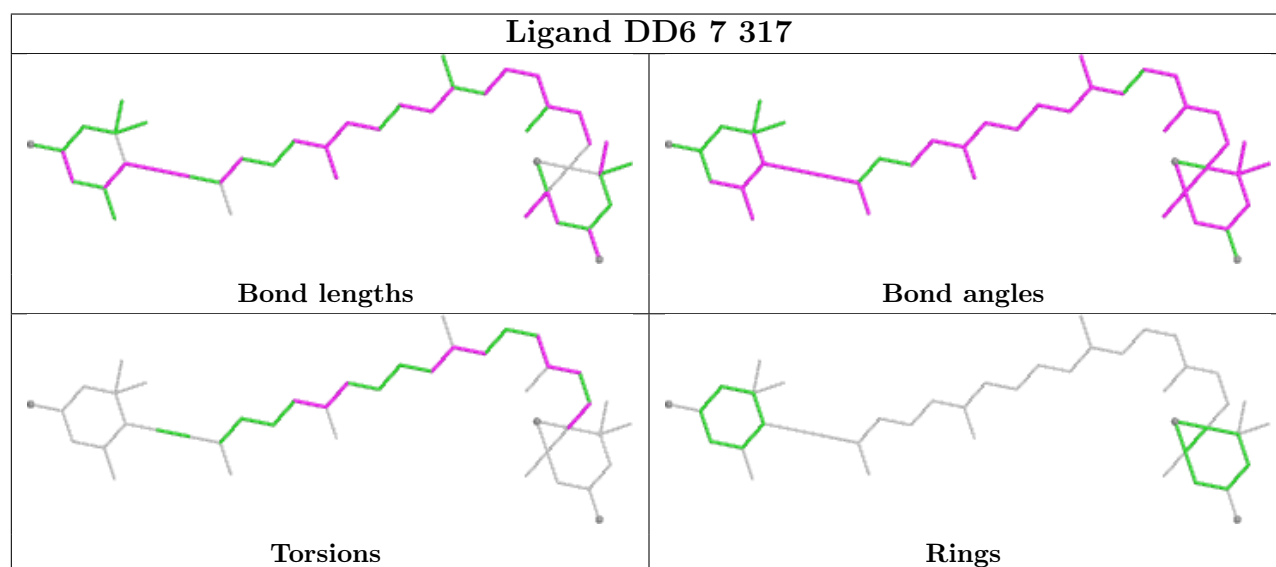
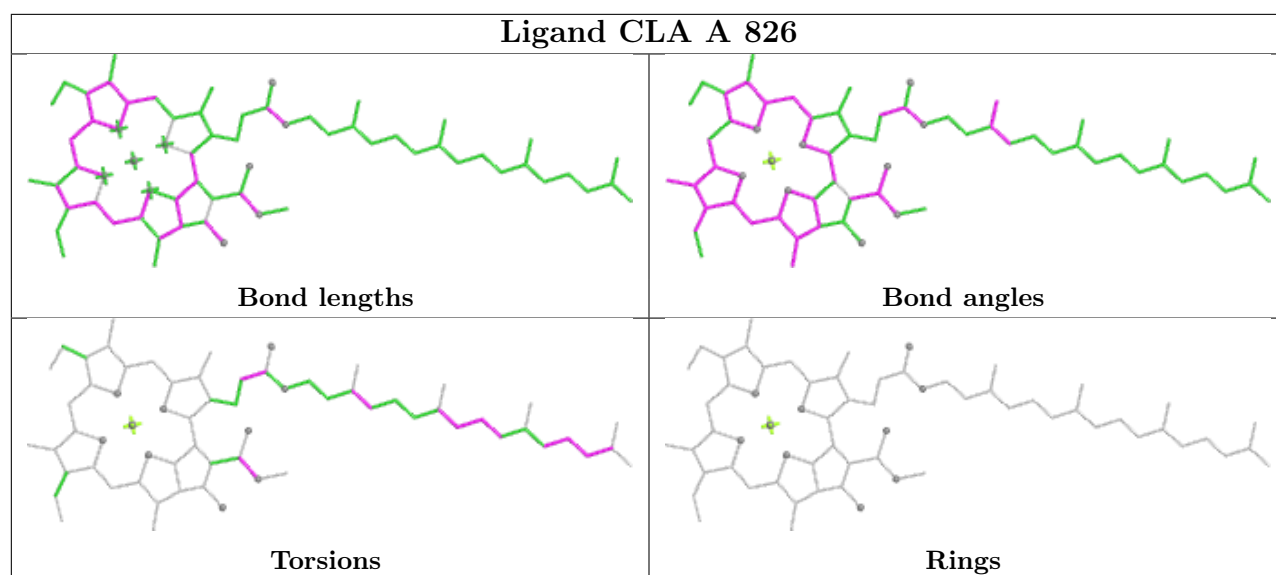
Rings

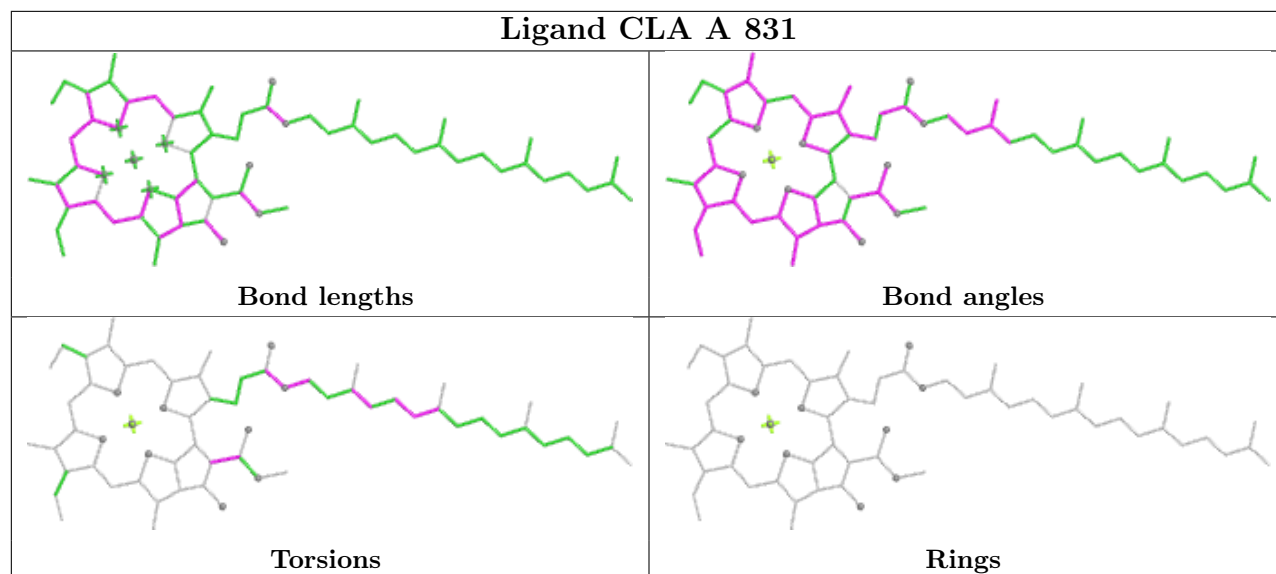
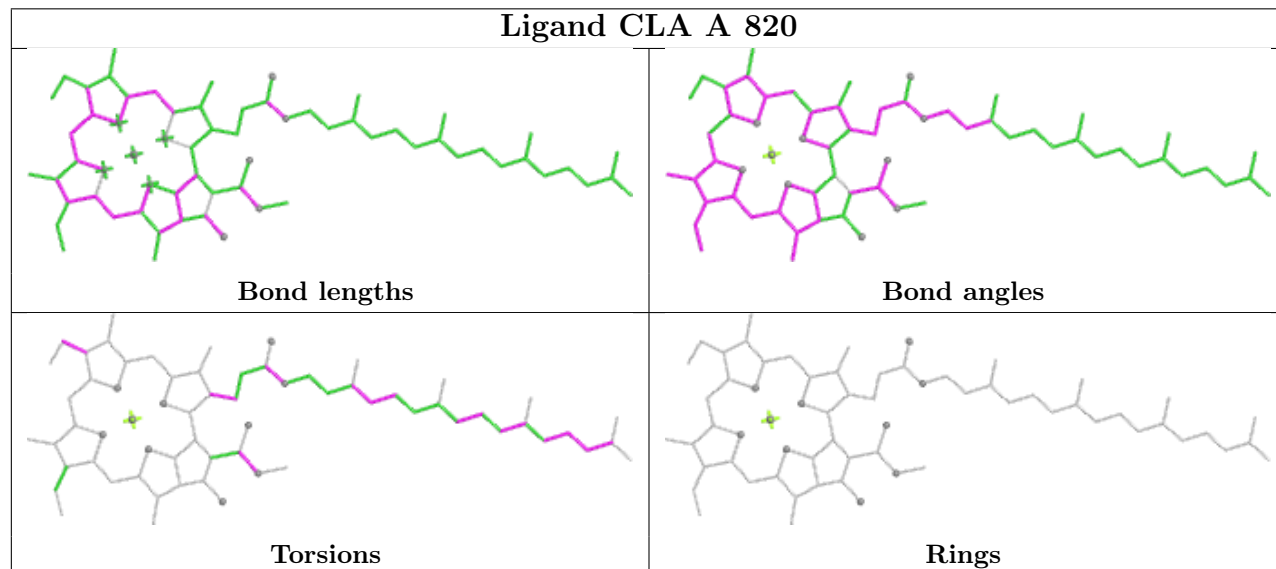
Ligand CLA 8 309

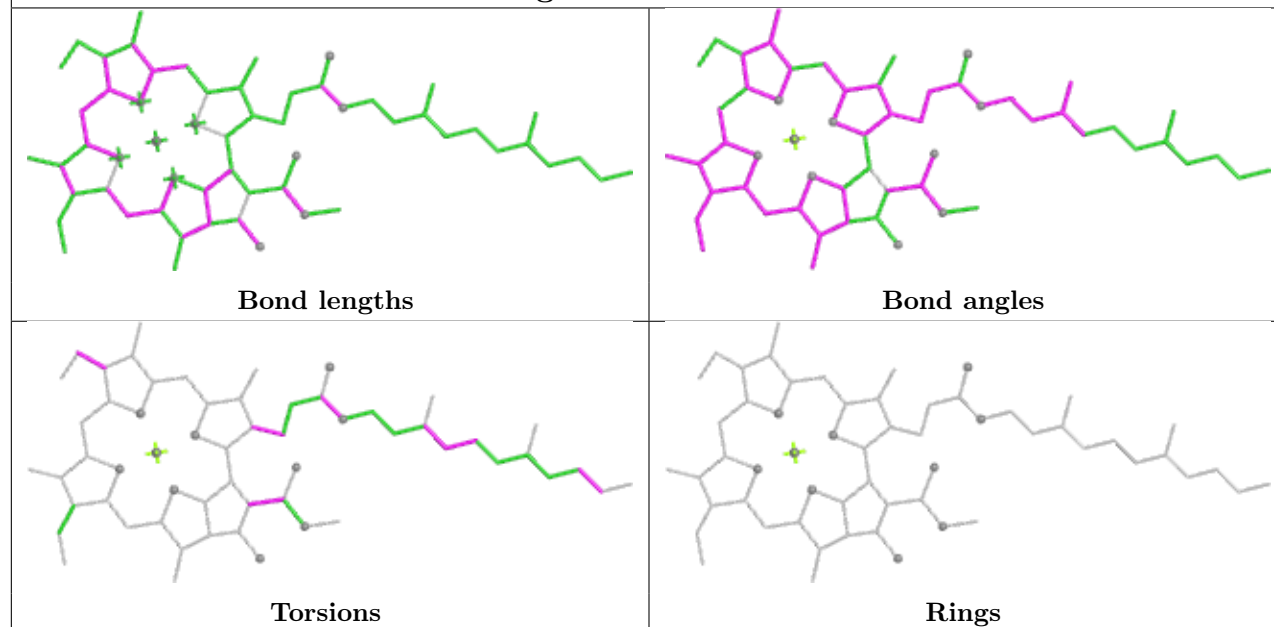
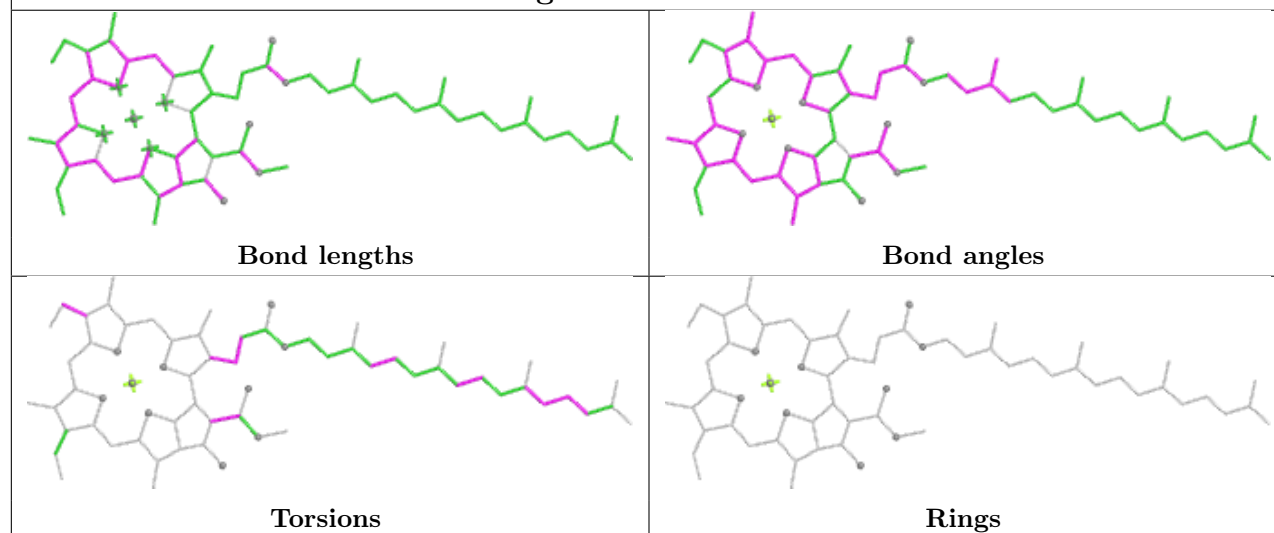


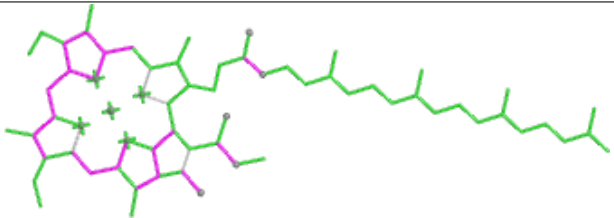
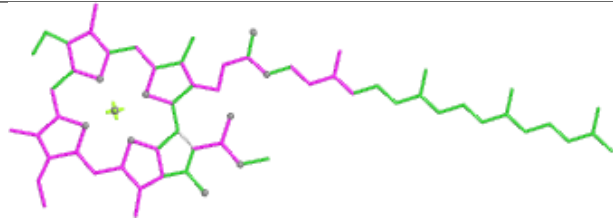
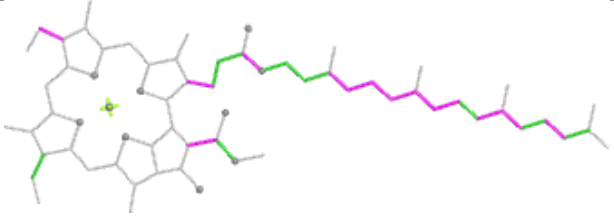
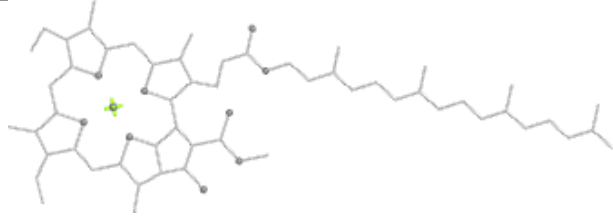
Ligand CLA 13 303

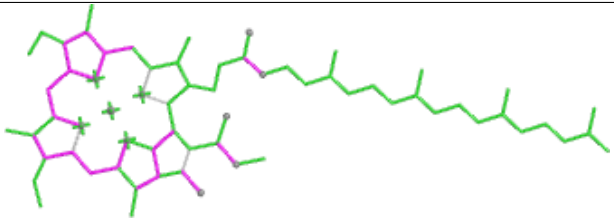
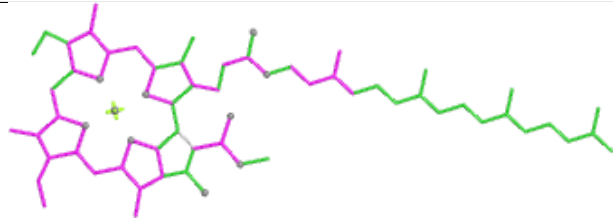
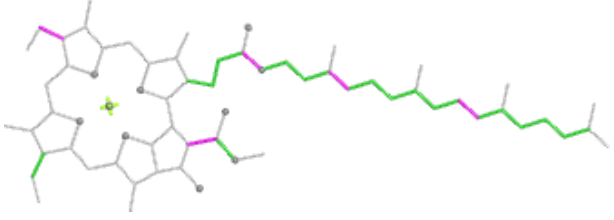
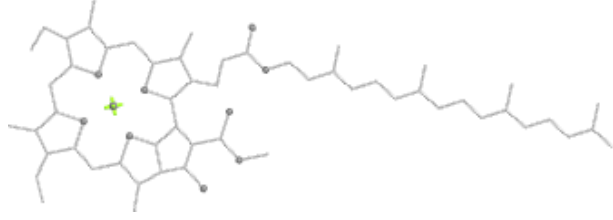


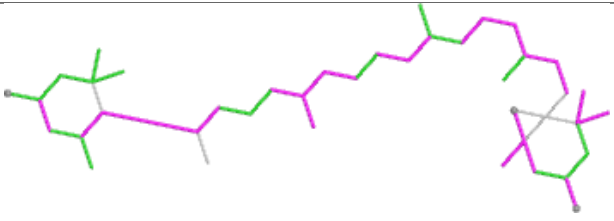
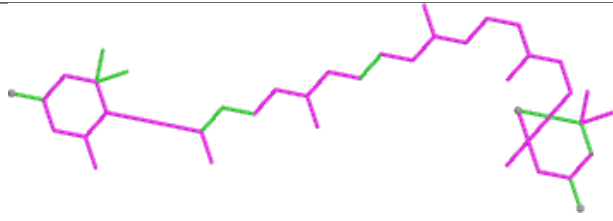
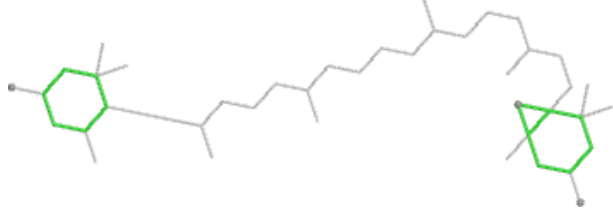


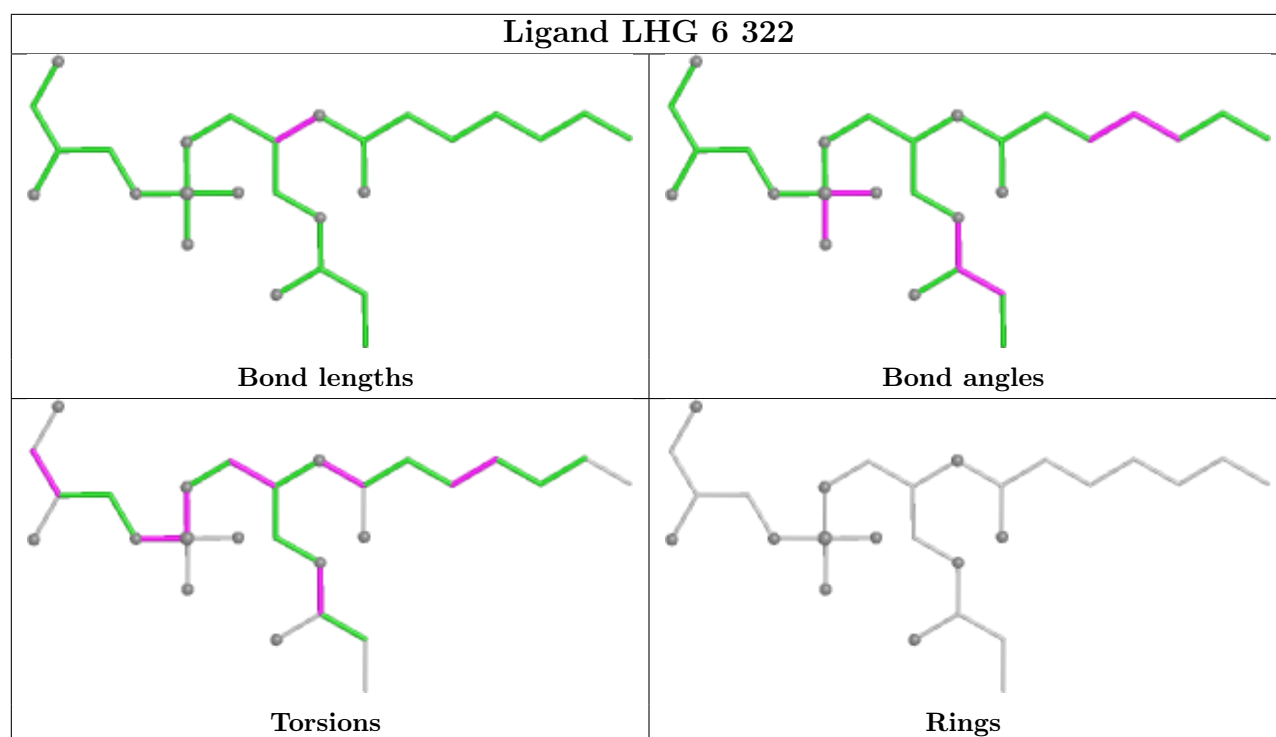
Ligand CLA A 831**Ligand CLA A 820**

Ligand CLA 8 304**Ligand CLA 7 310**

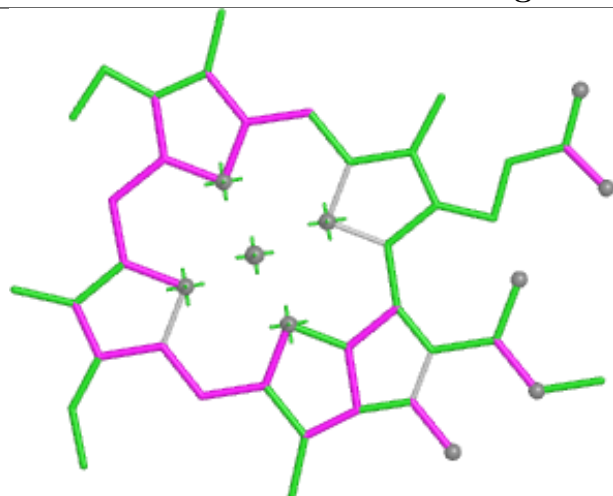
Ligand CLA 16 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 12 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

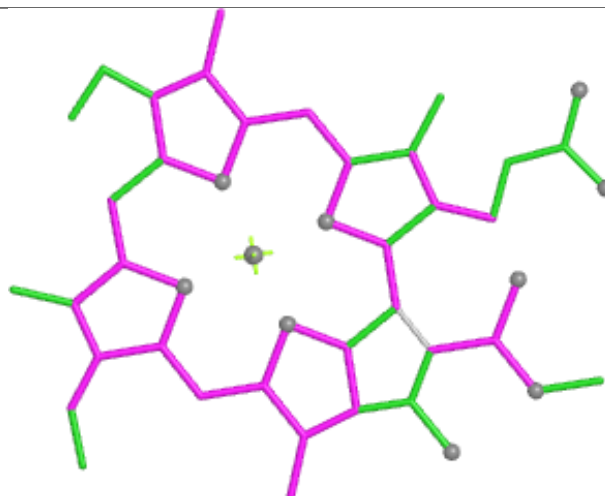
Ligand DD6 6 319	
	
Bond lengths	Bond angles
	
Torsions	Rings



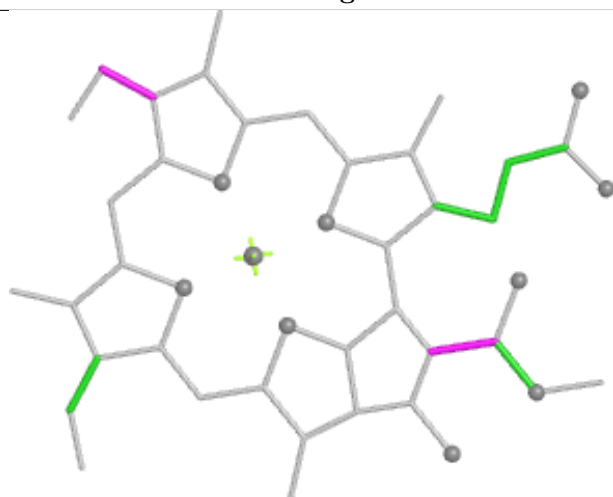
Ligand CLA B 815



Bond lengths



Bond angles

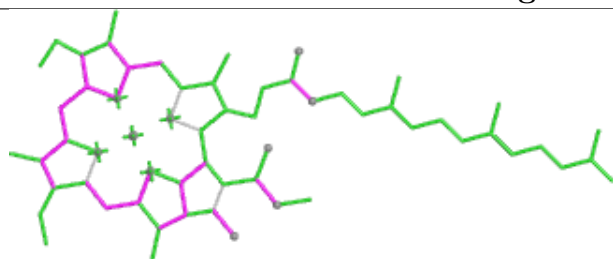


Torsions

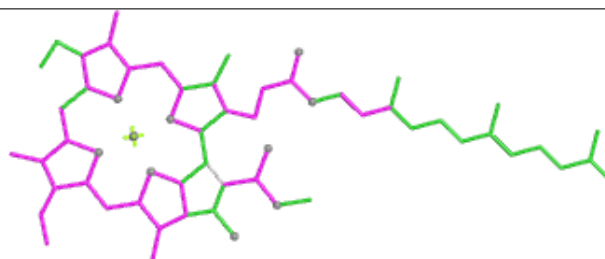


Rings

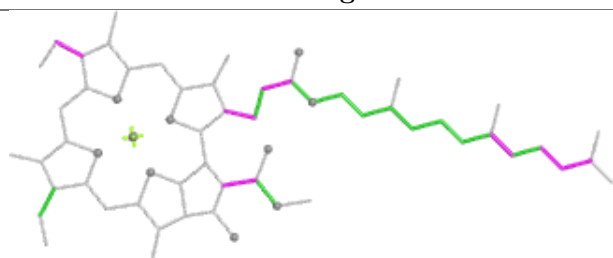
Ligand CLA 4 304



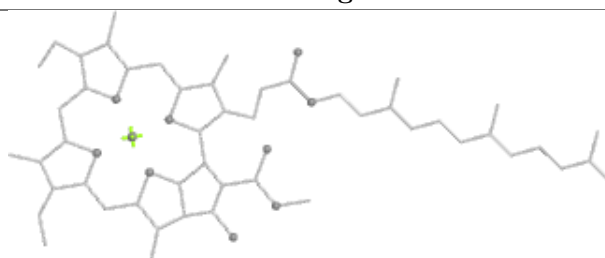
Bond lengths



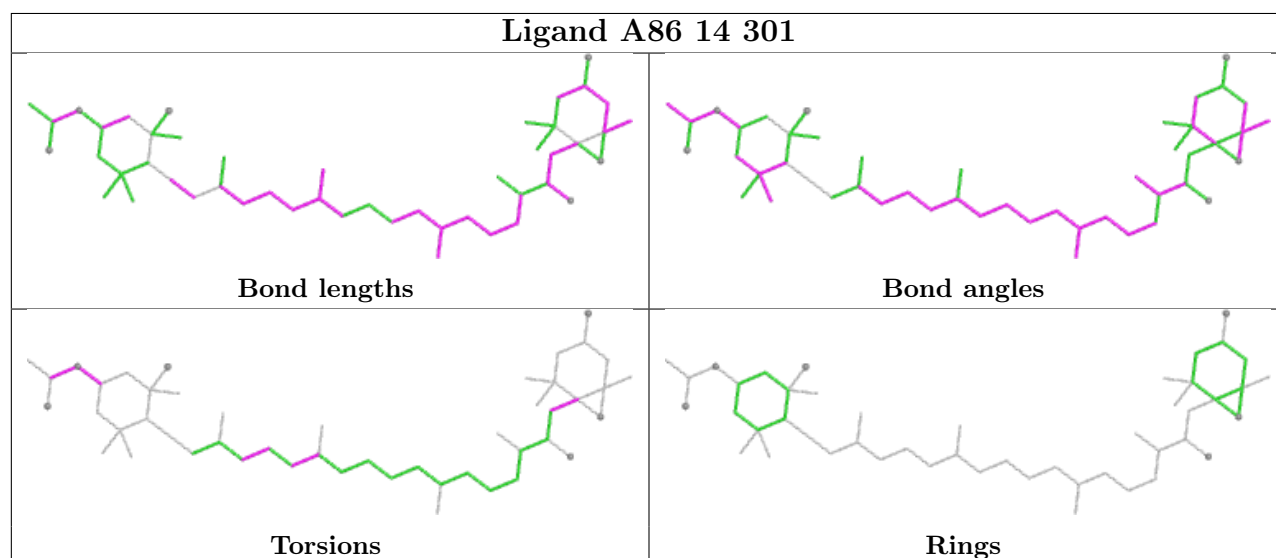
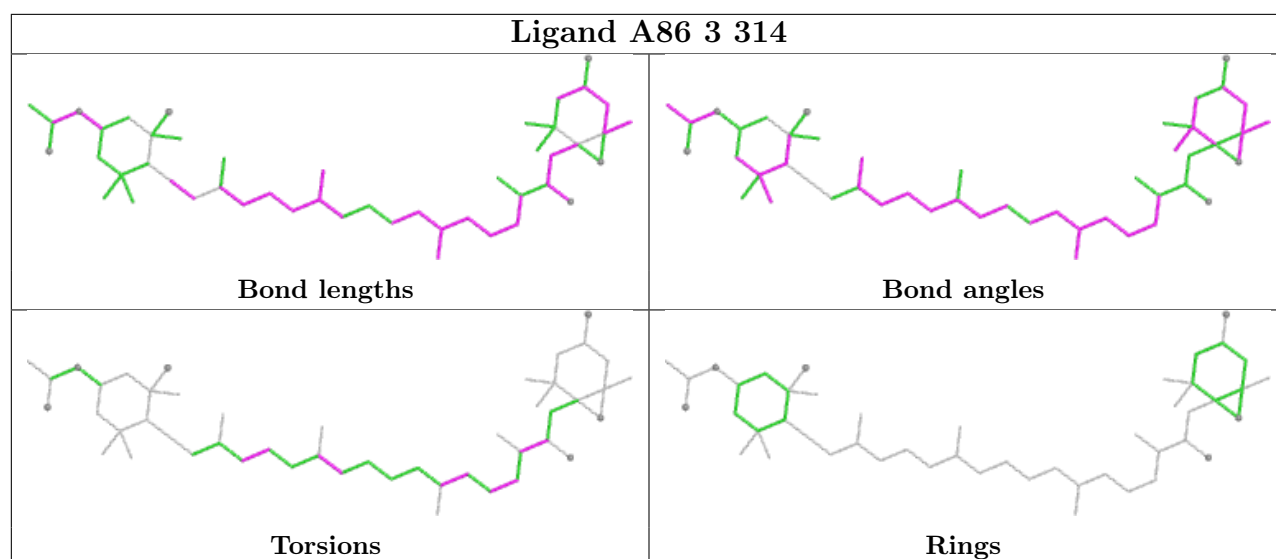
Bond angles

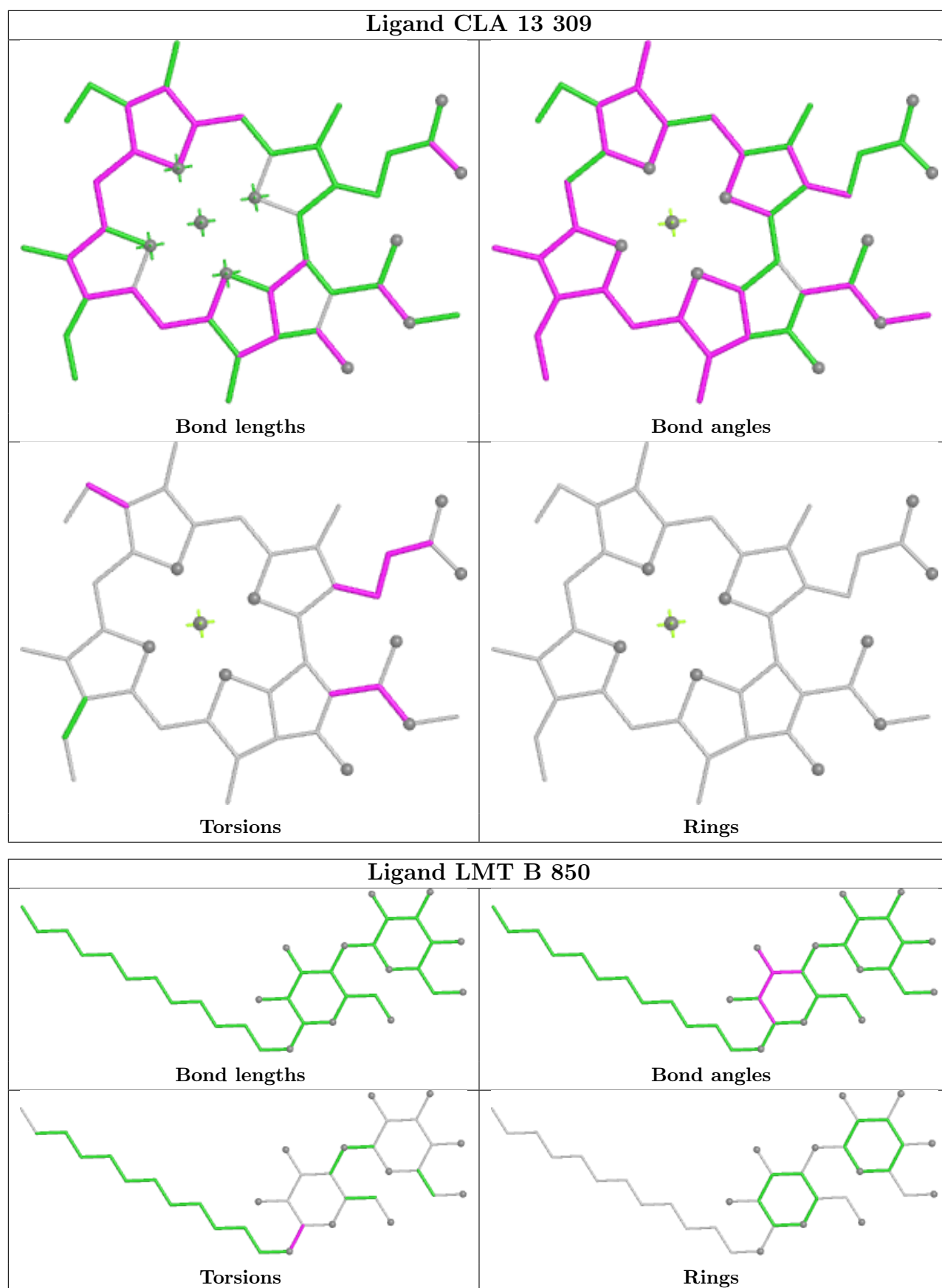


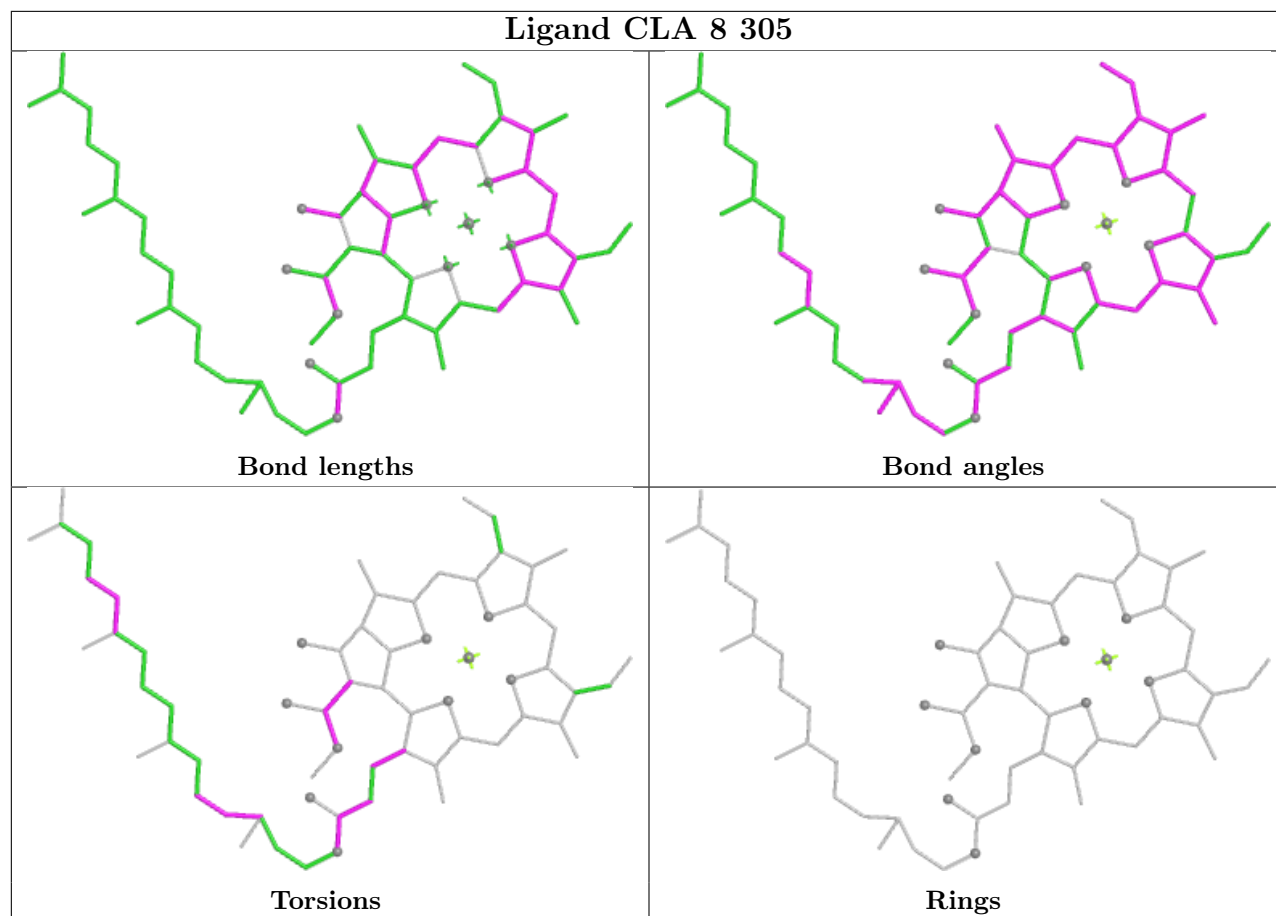
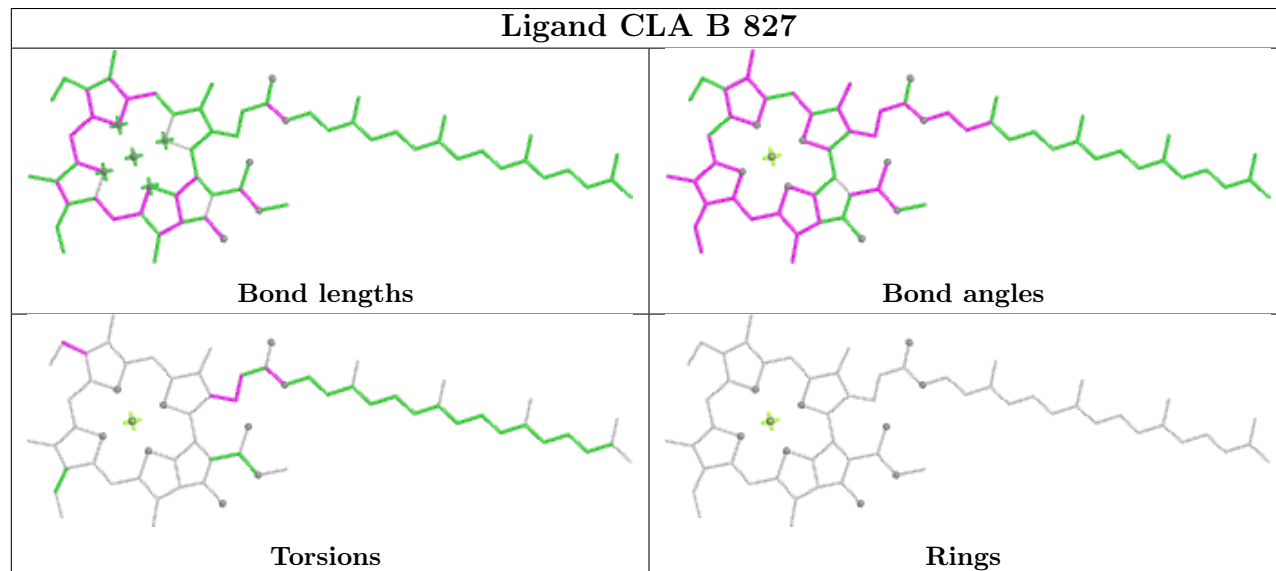
Torsions

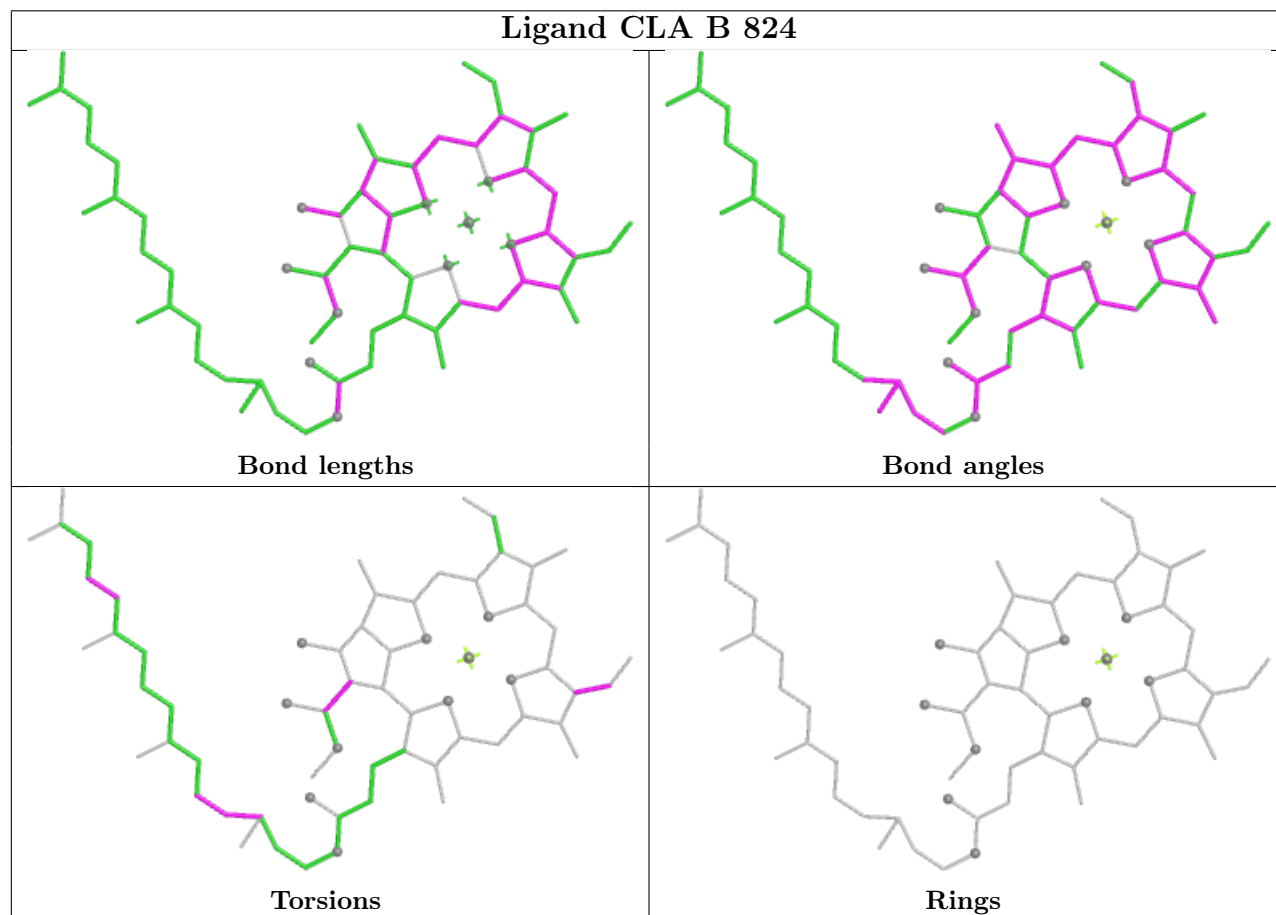
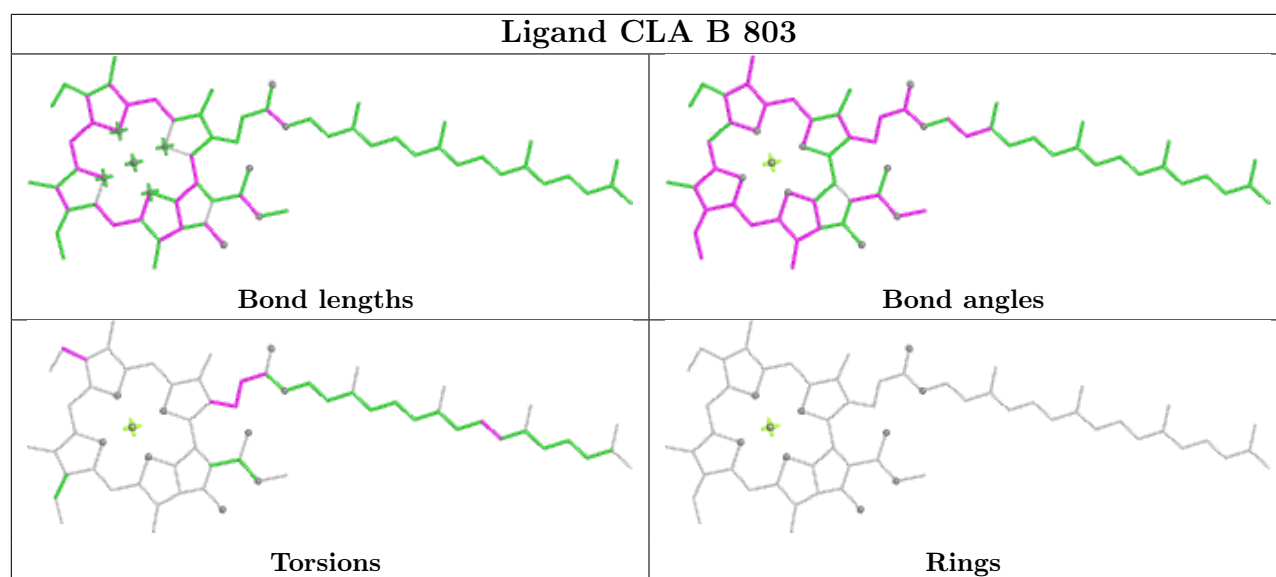


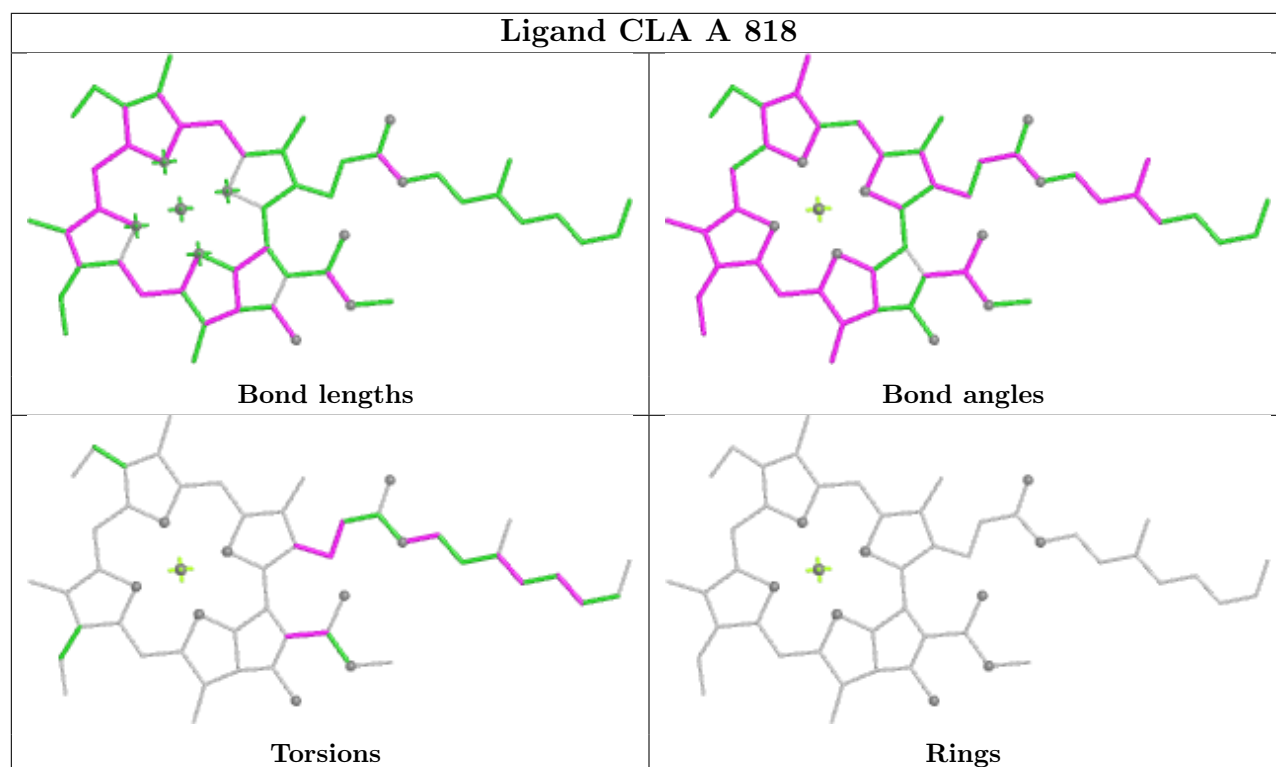
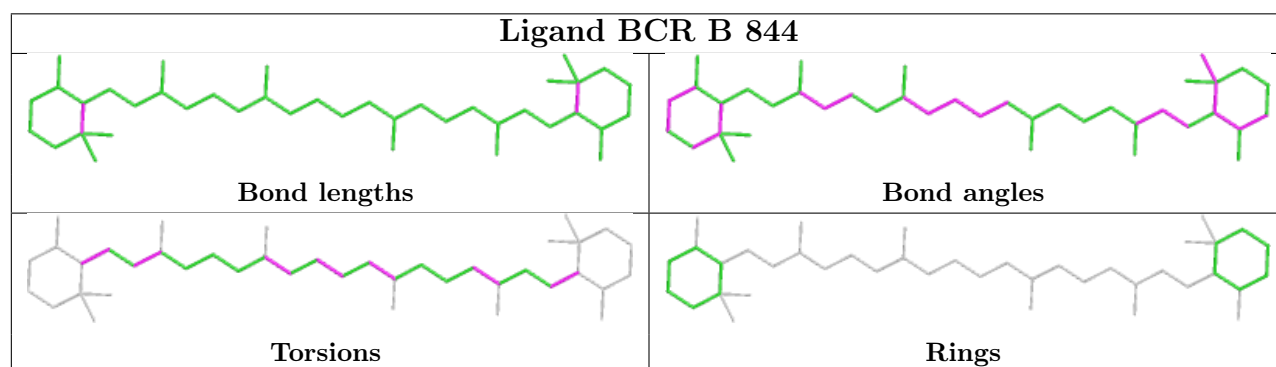
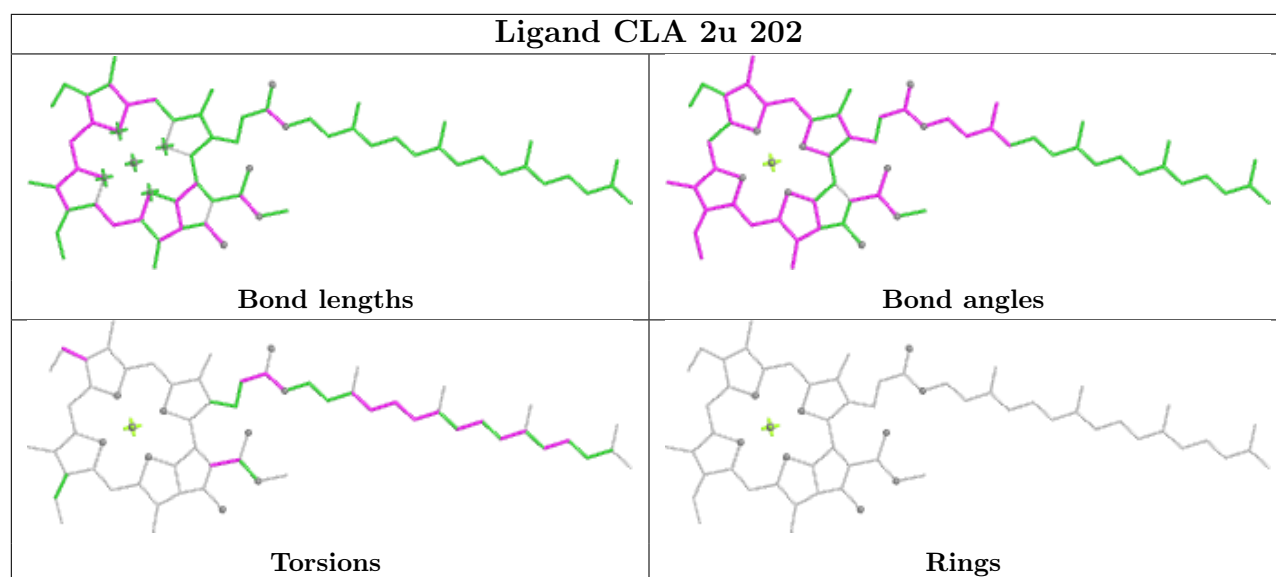
Rings

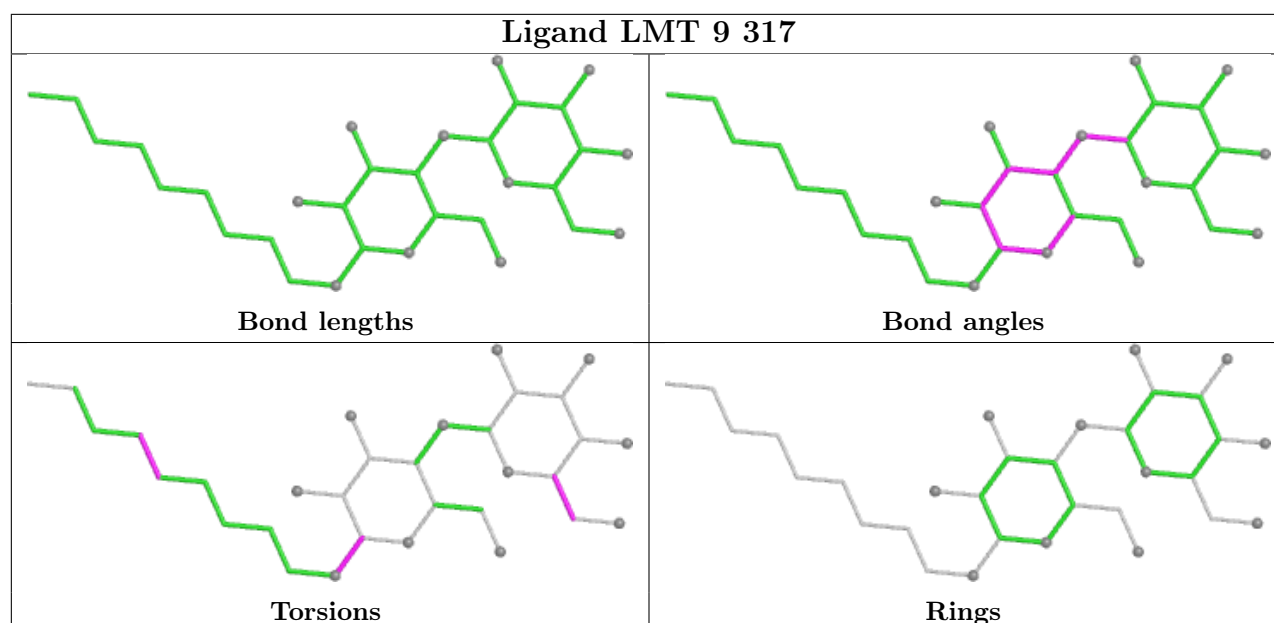
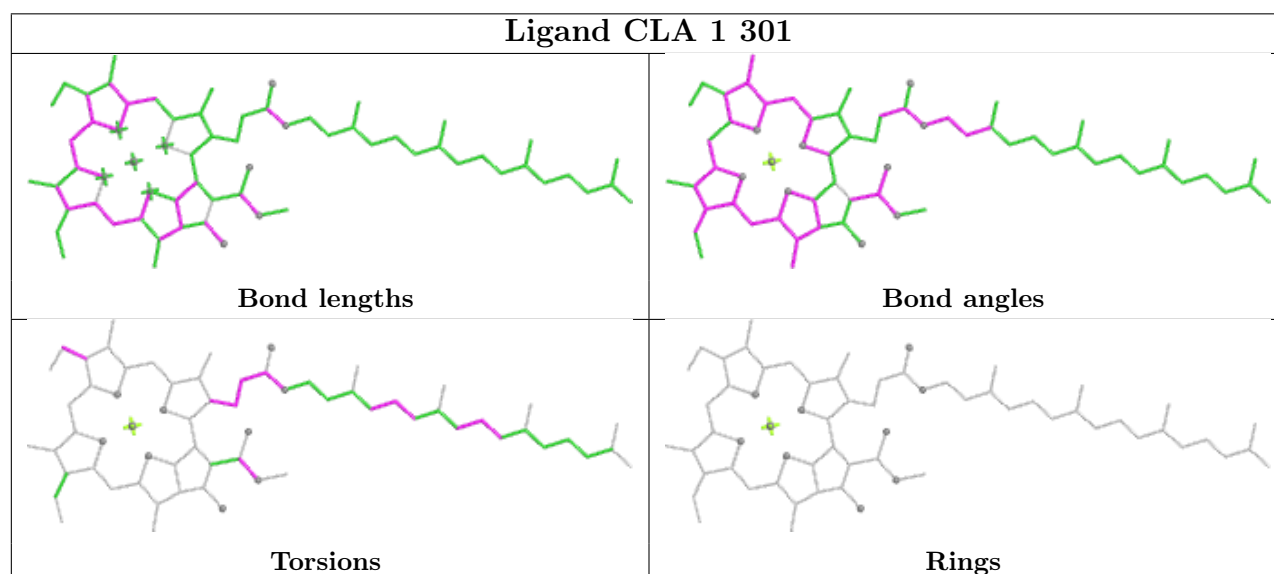
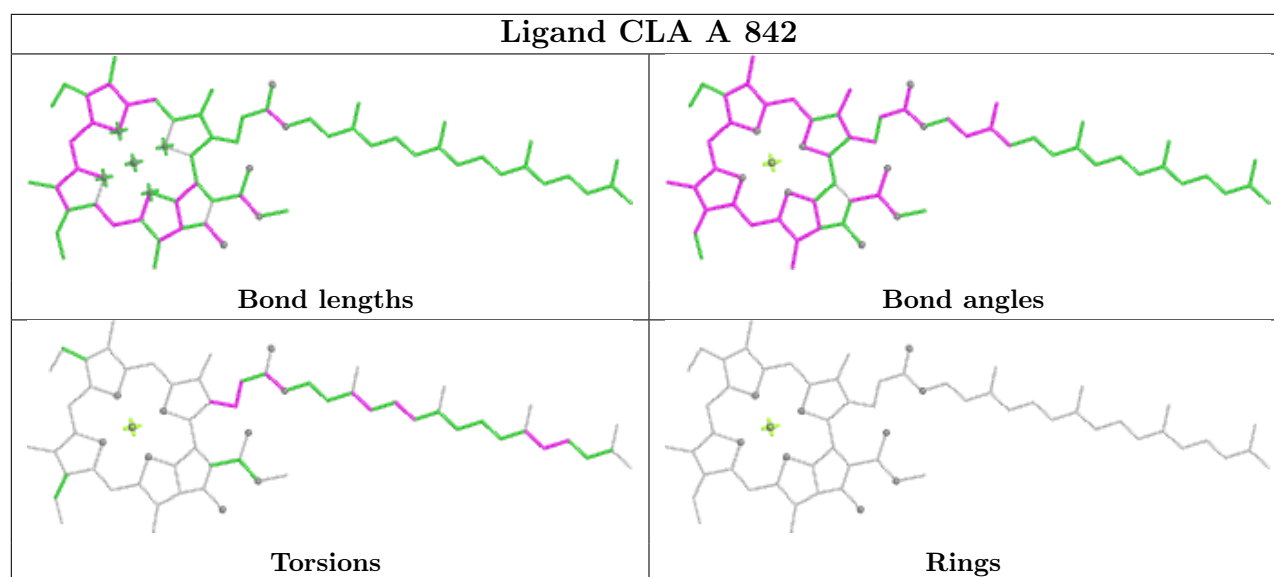


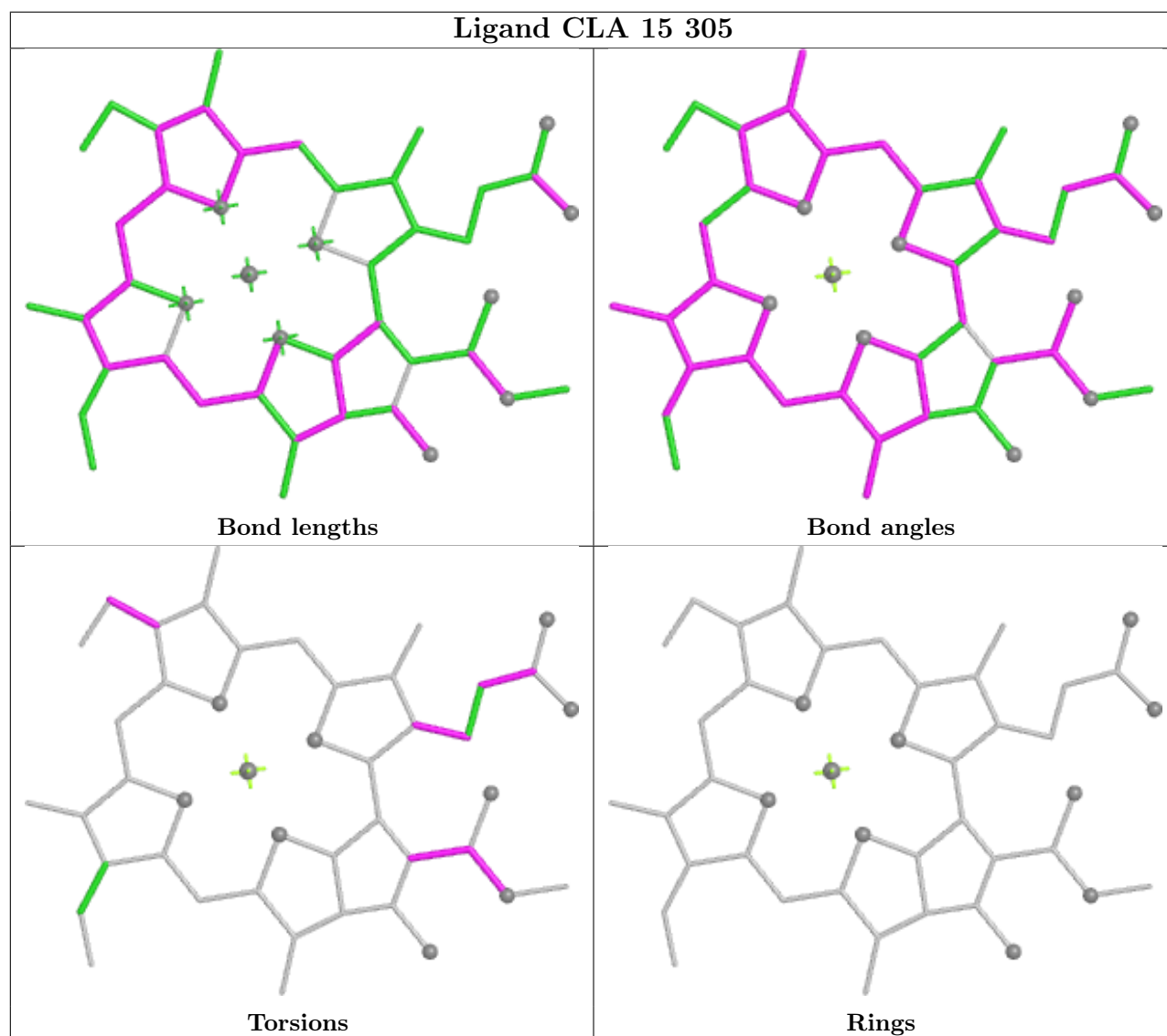
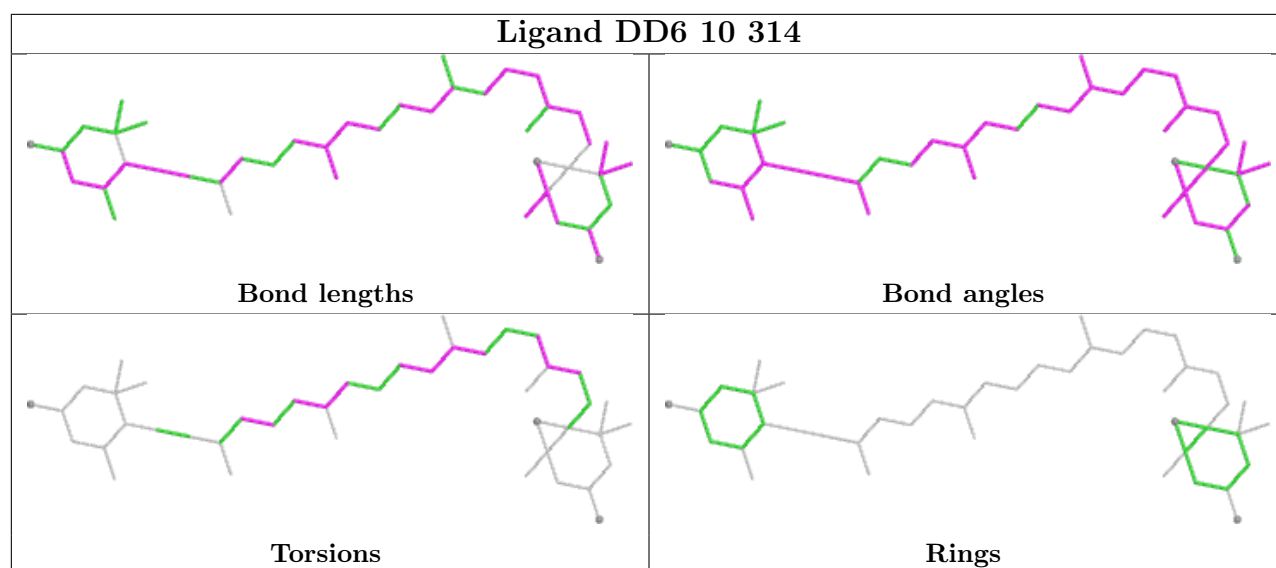


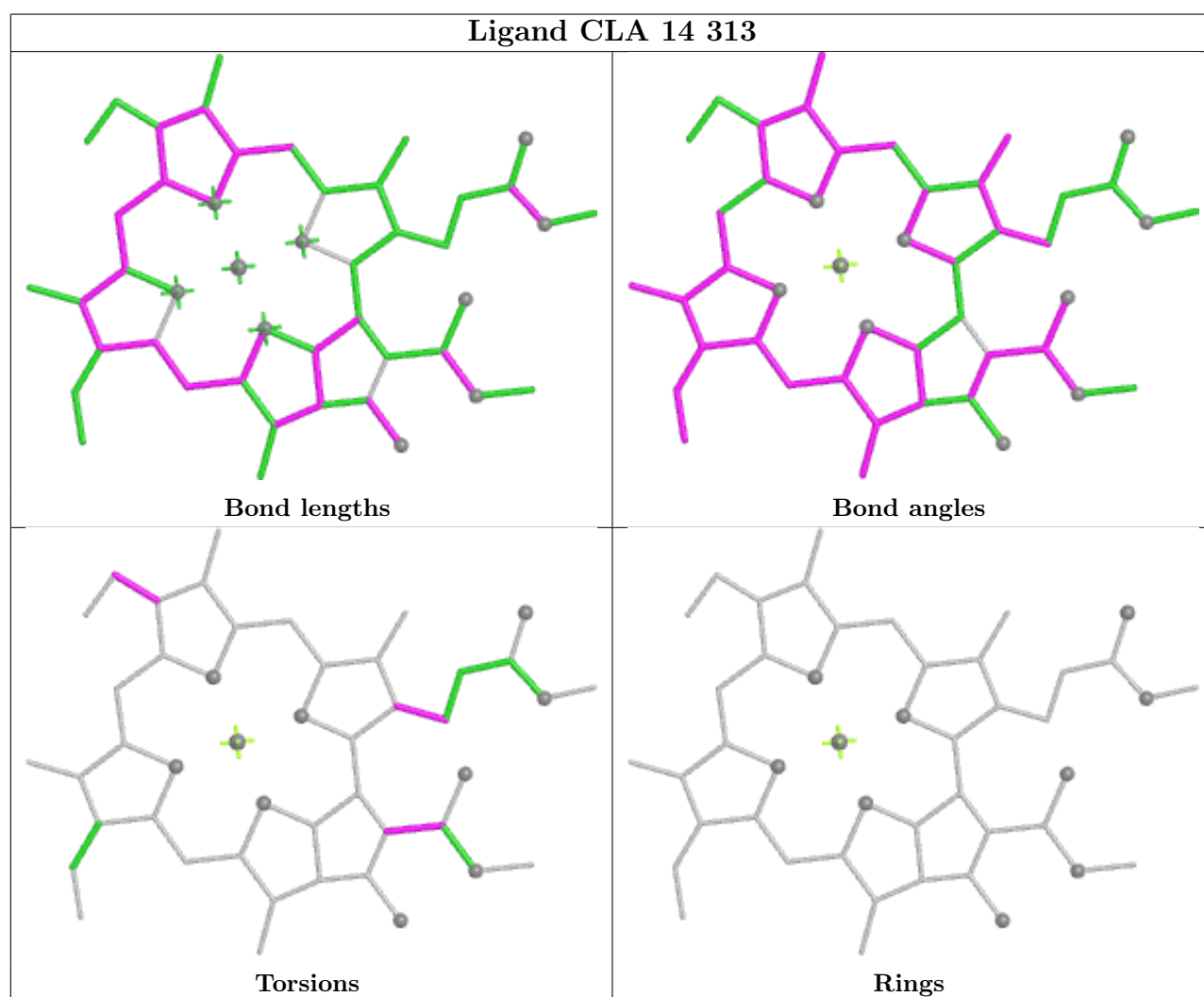
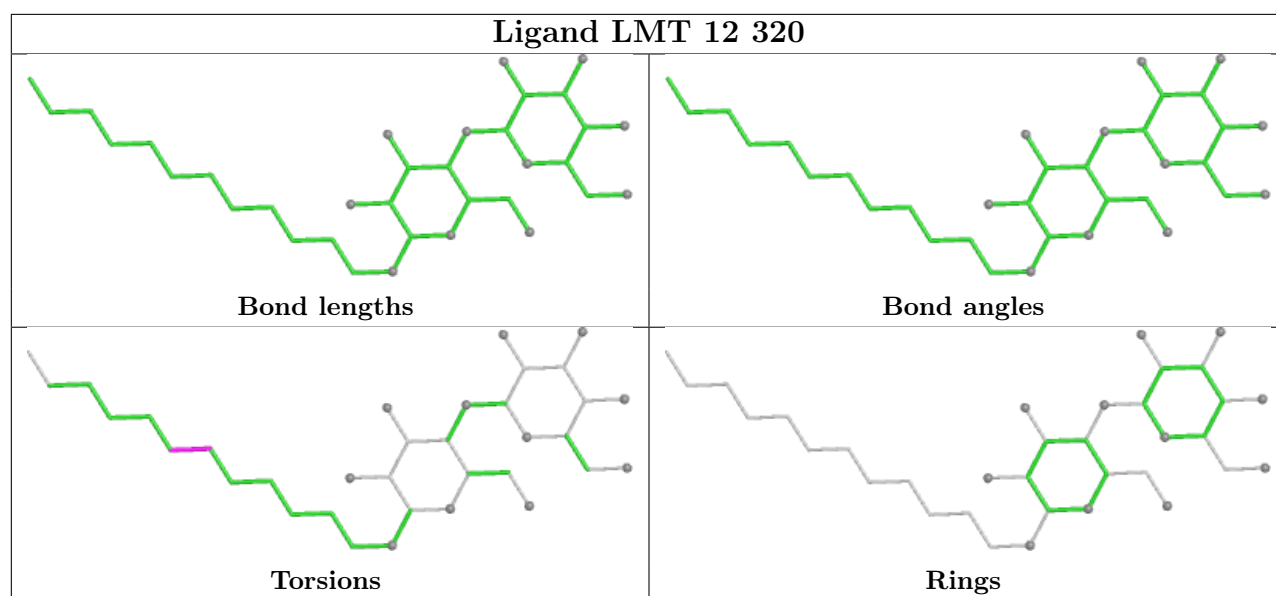
Ligand CLA 8 305**Ligand CLA B 827**

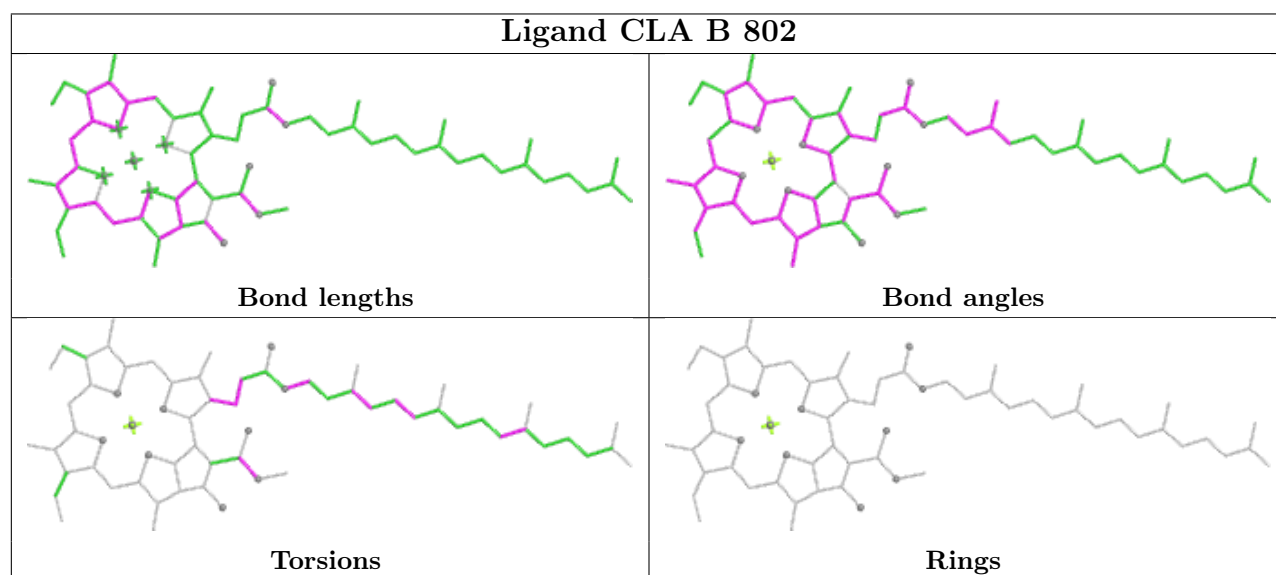
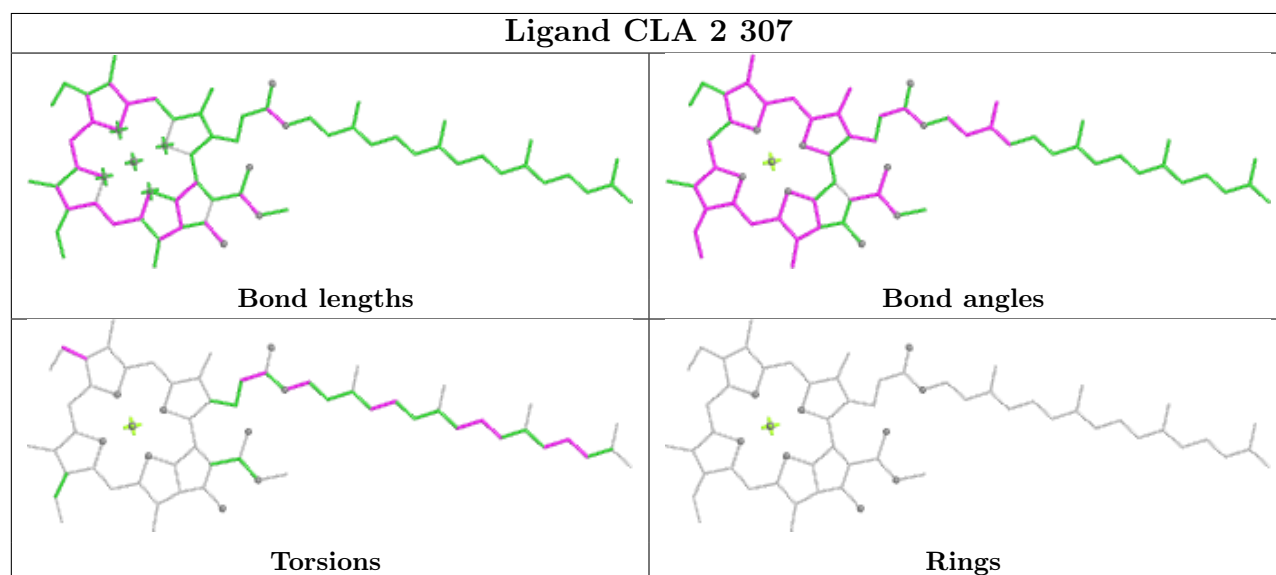
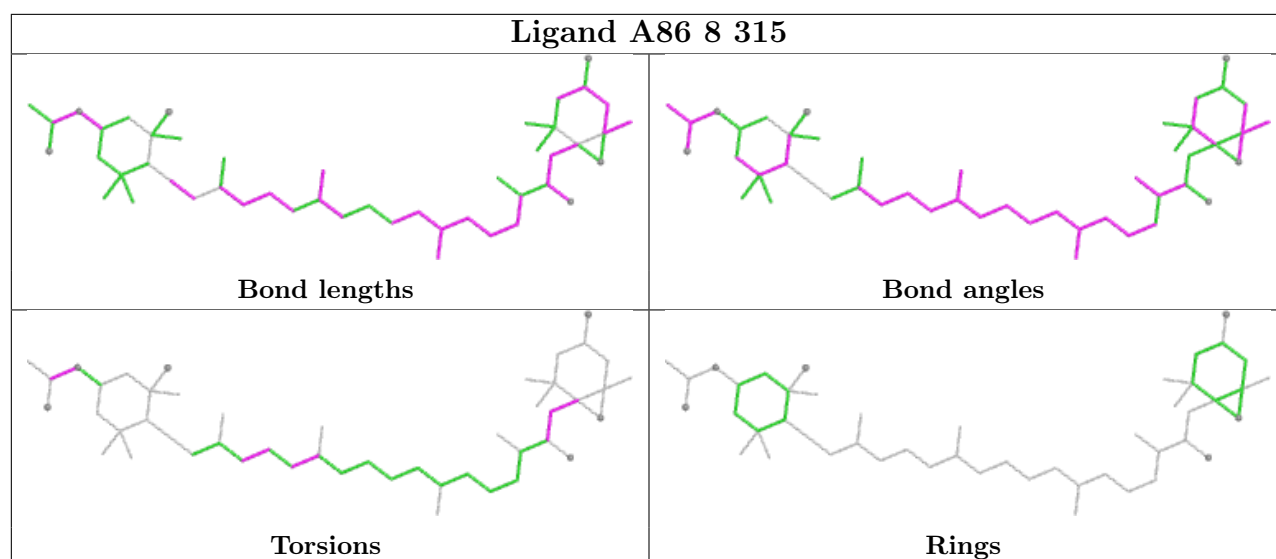


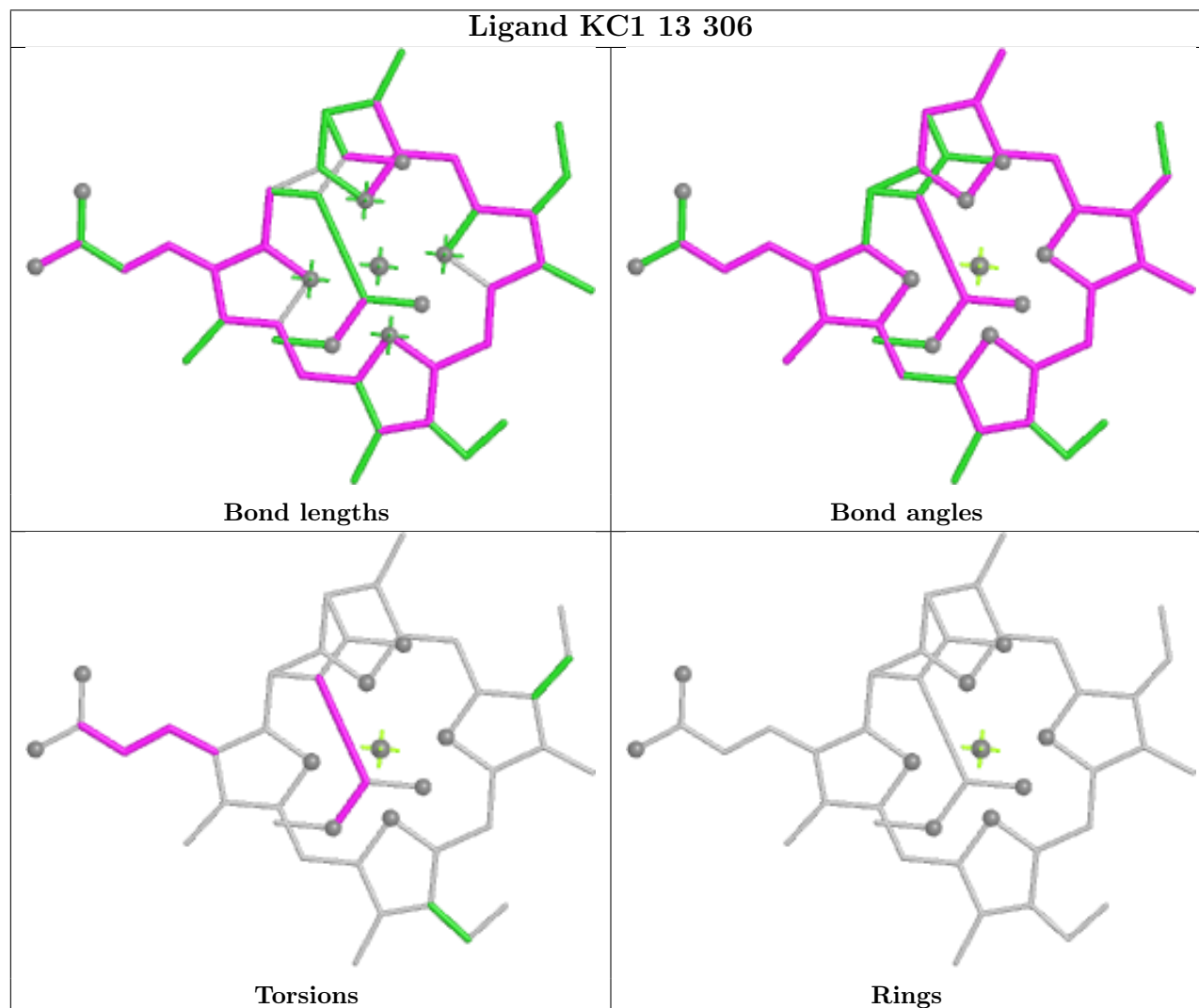
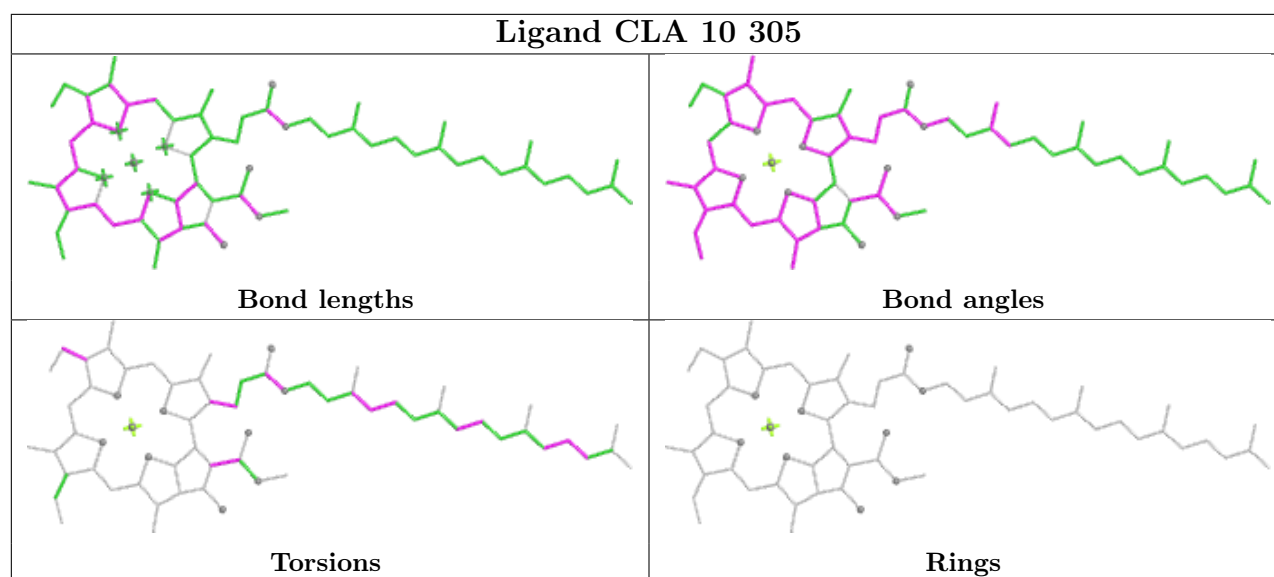


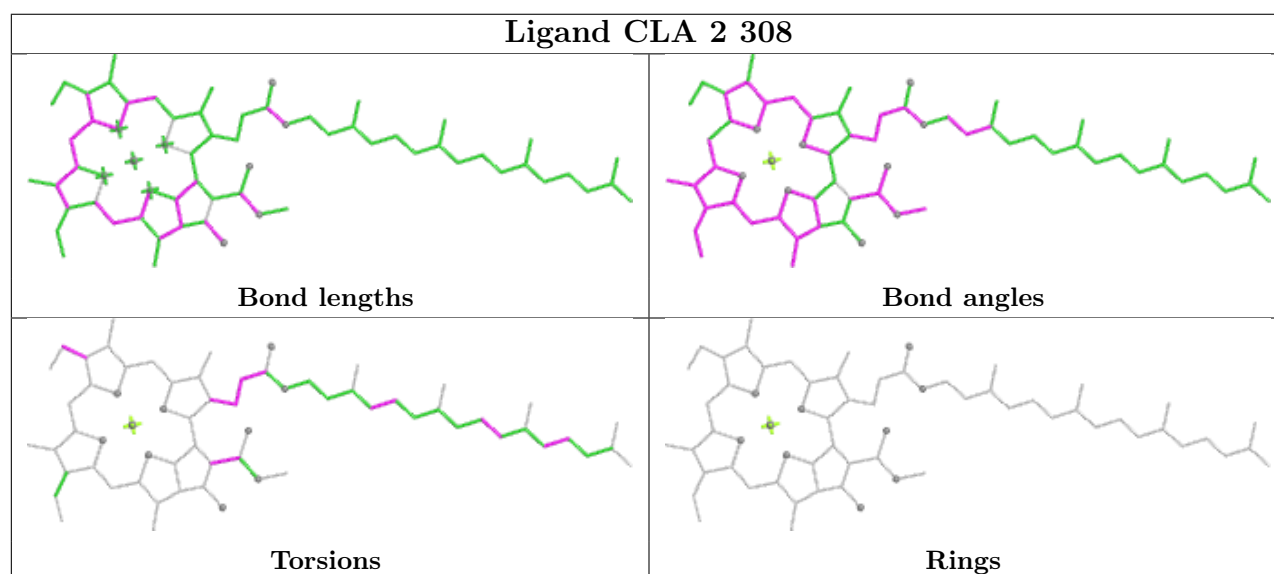
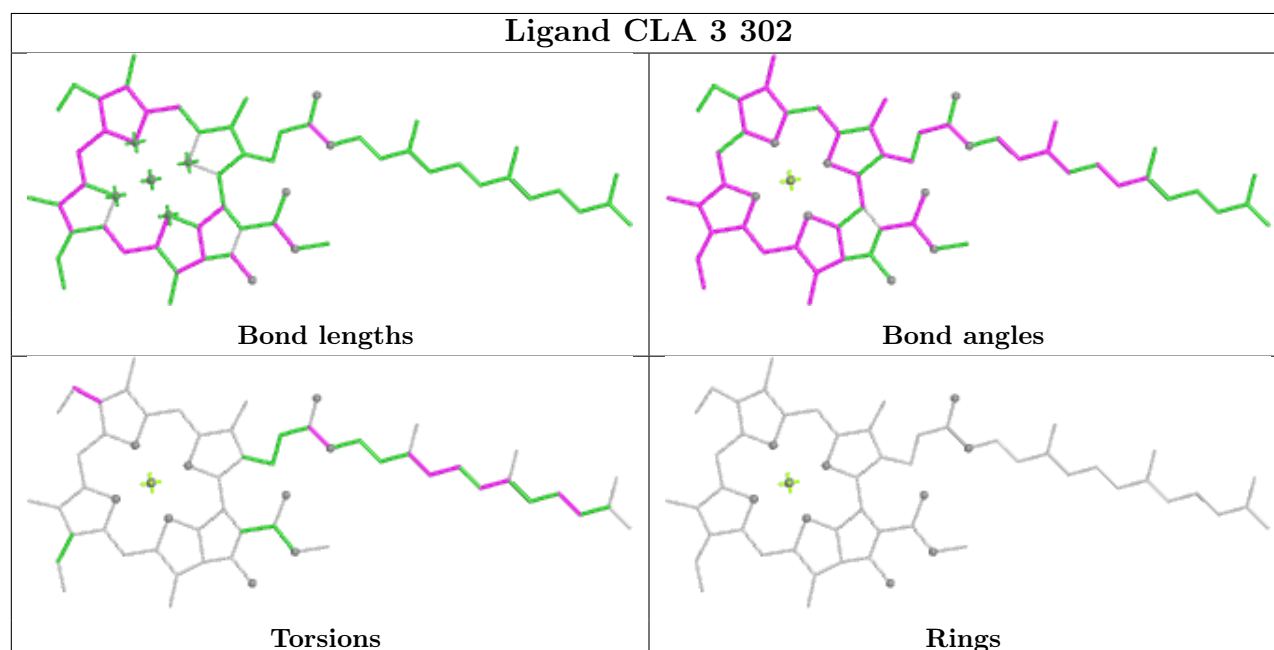
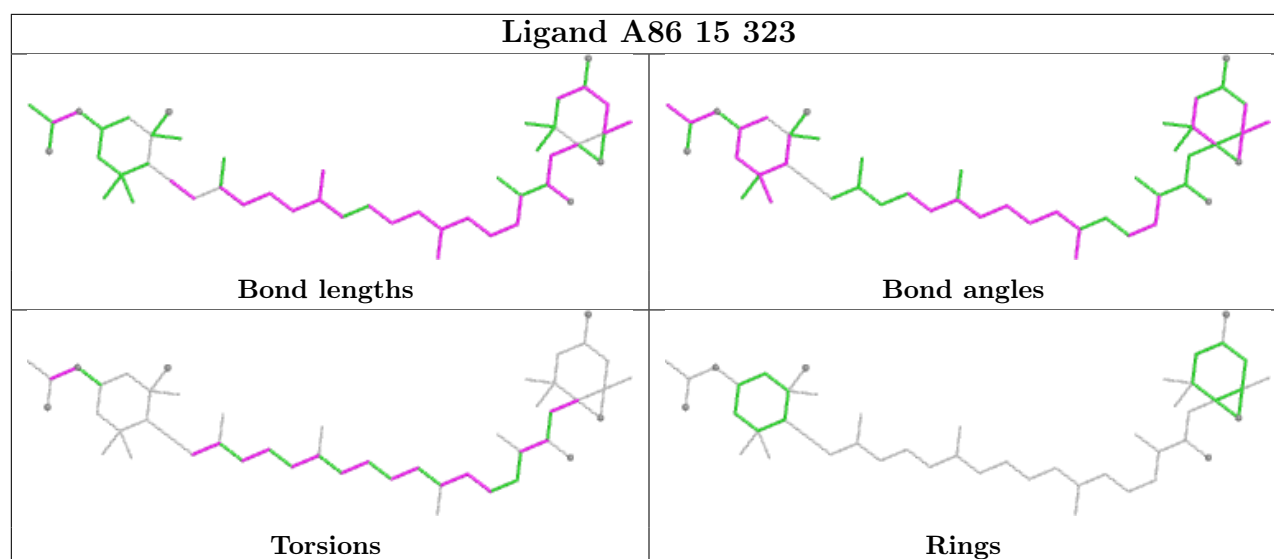




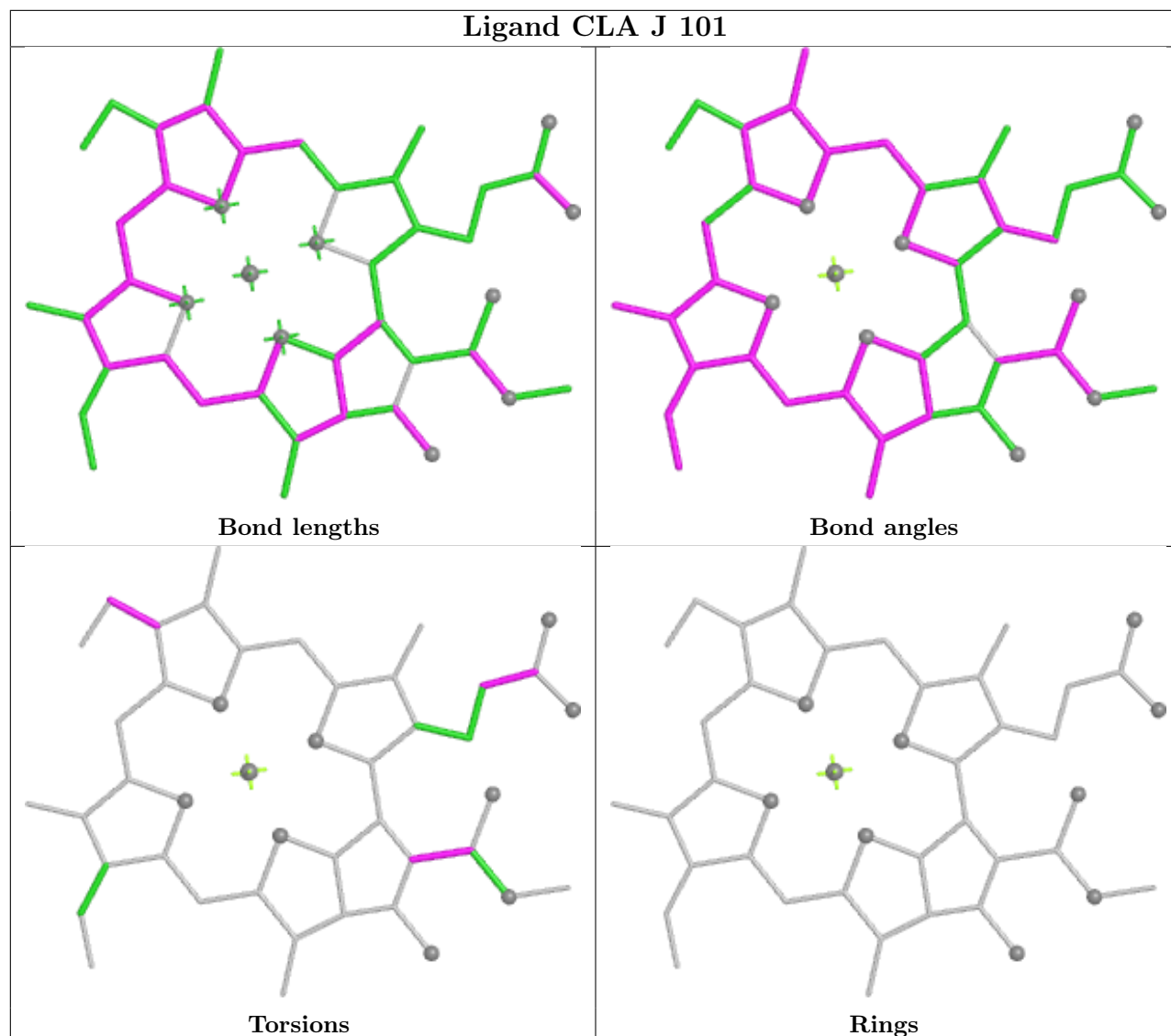




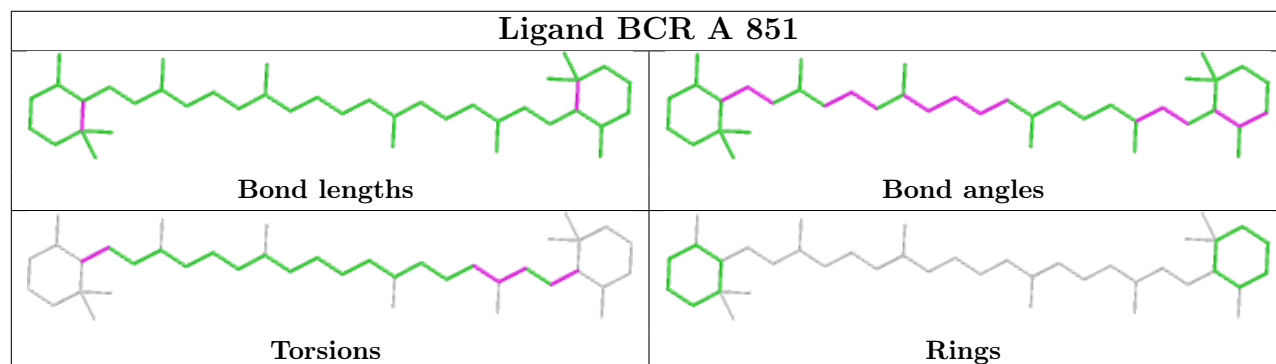


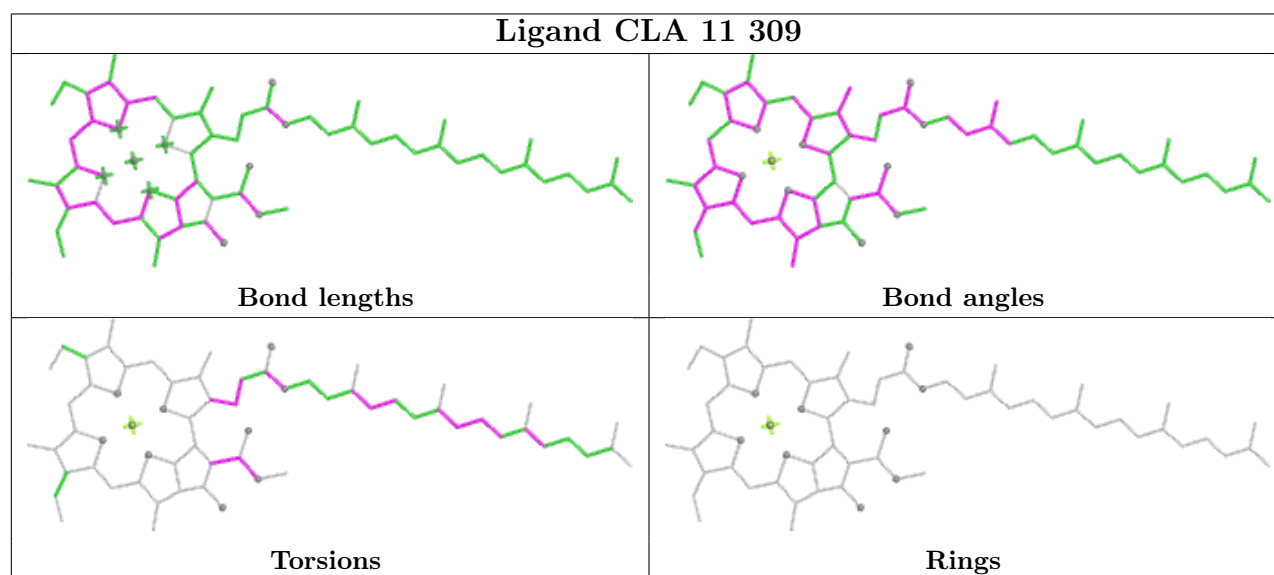
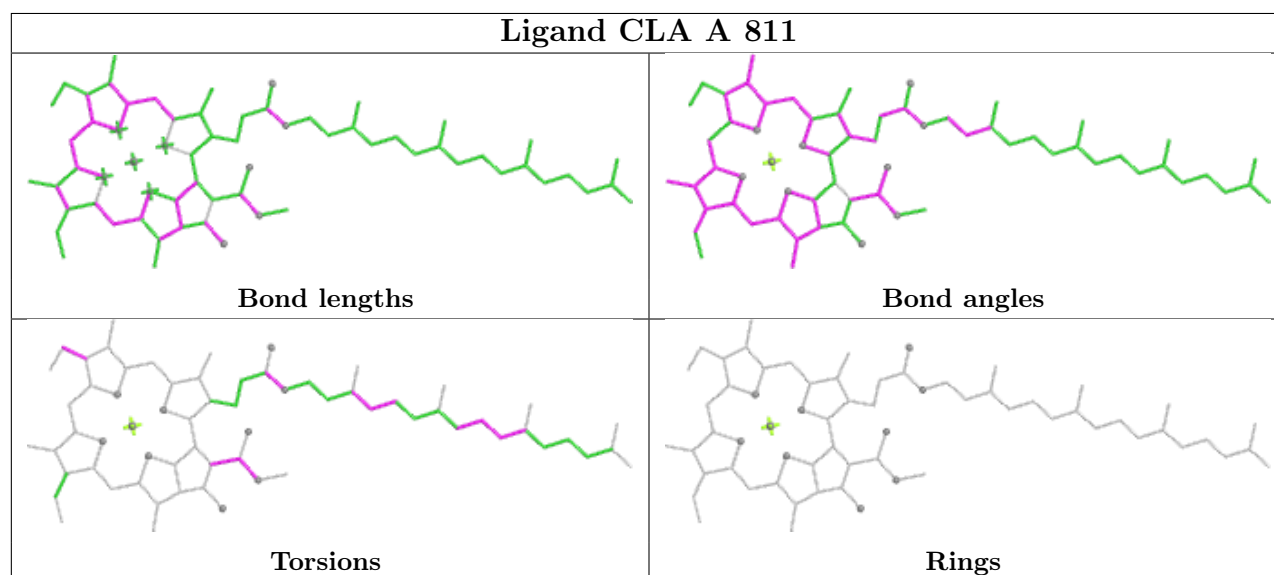
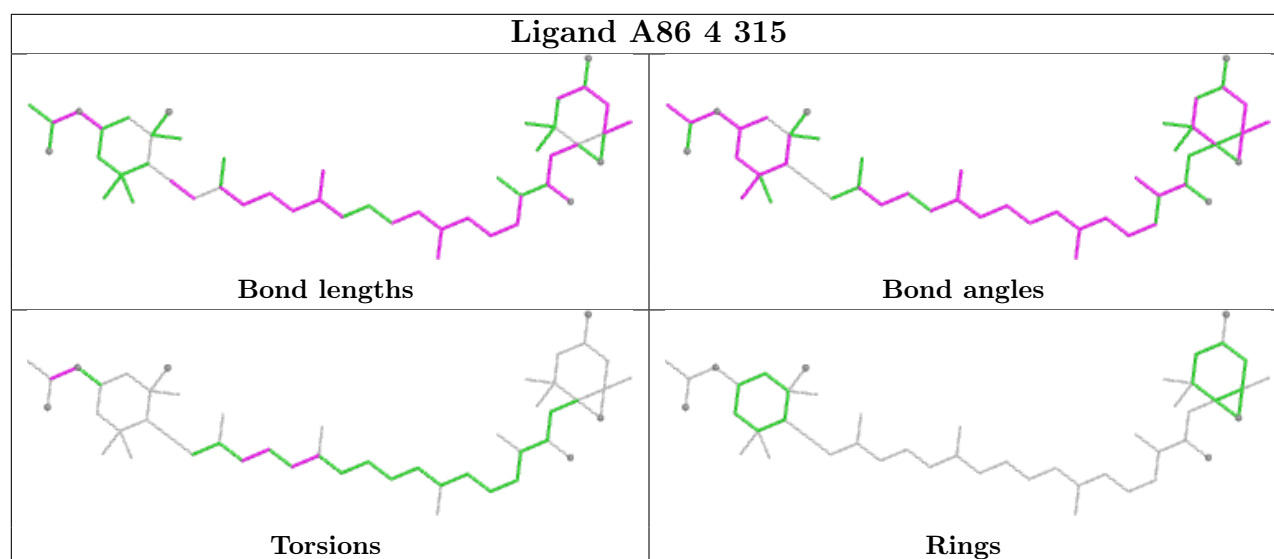


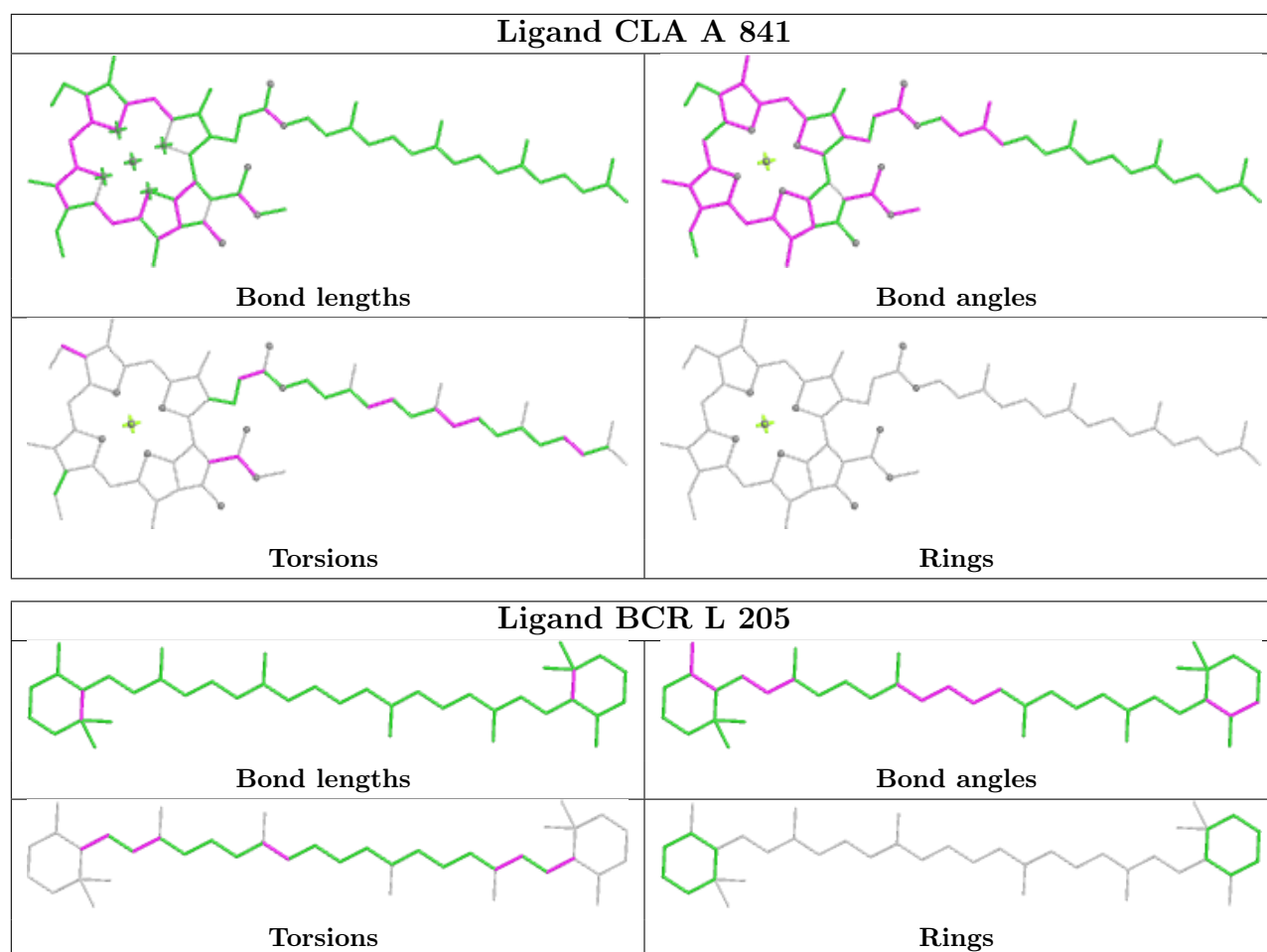
Ligand CLA J 101

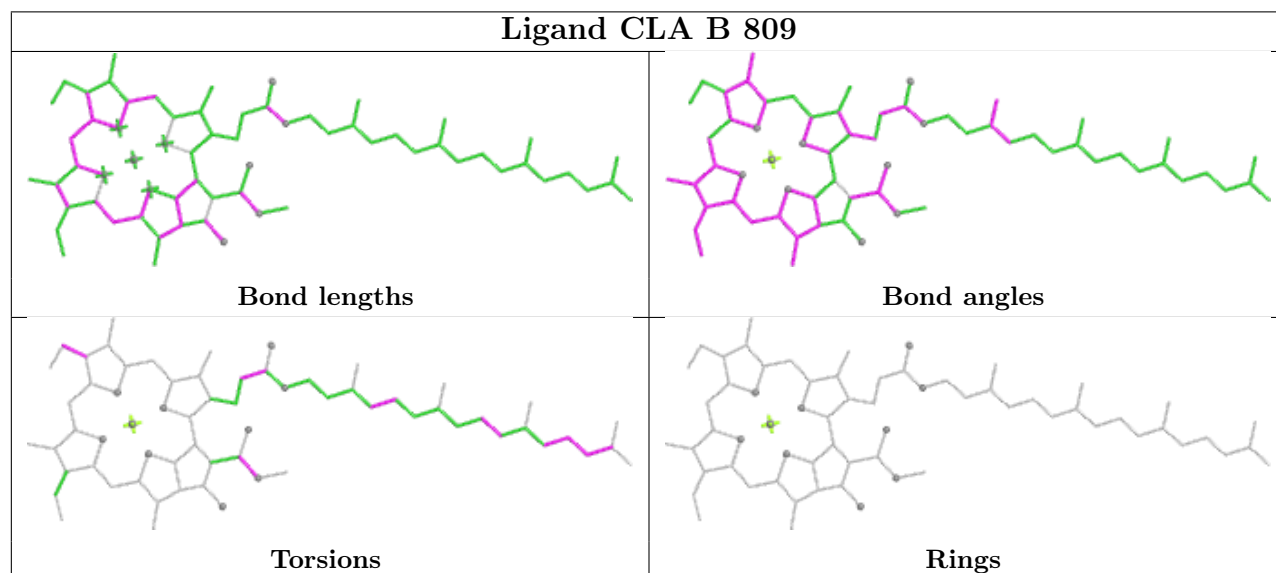
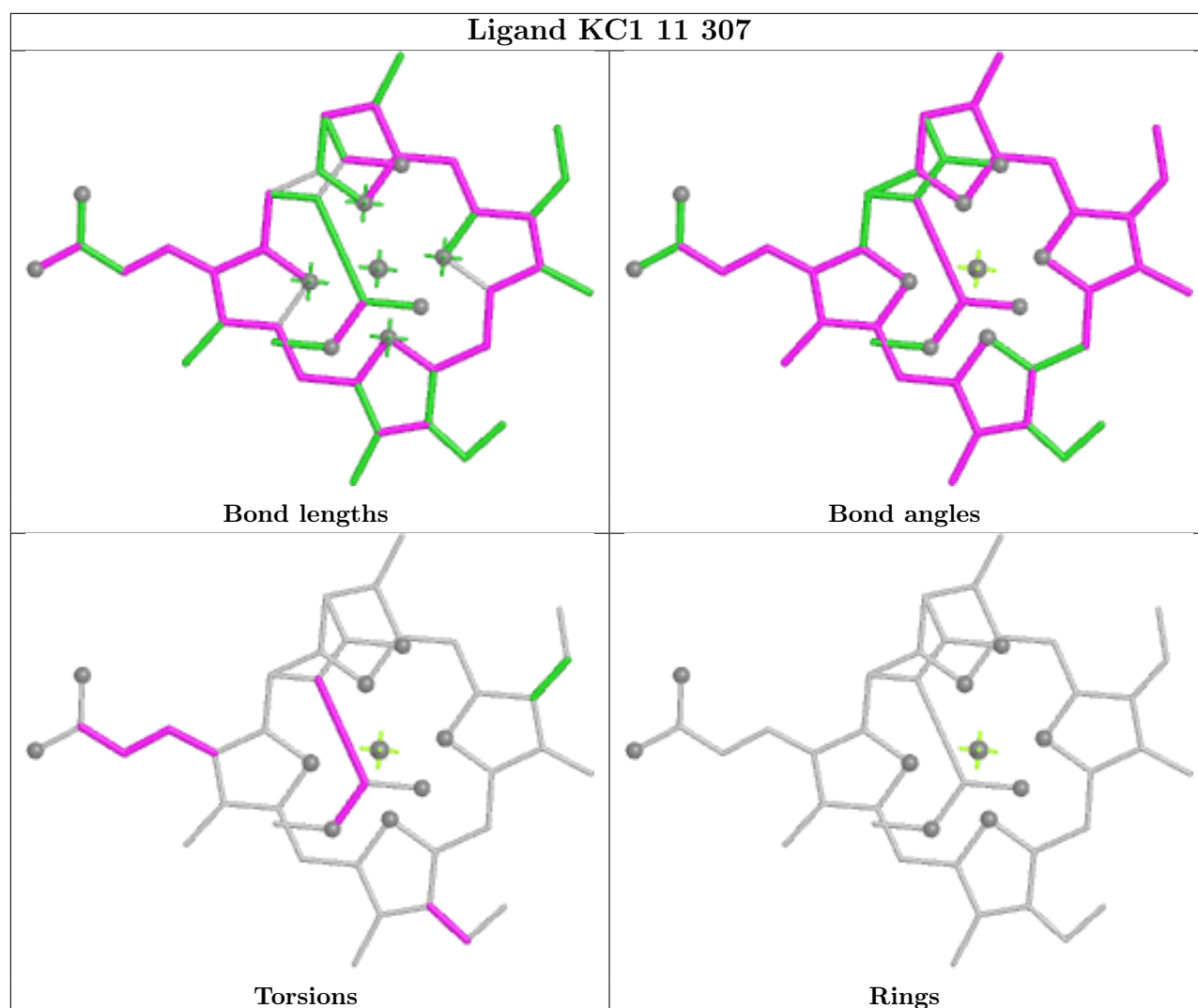


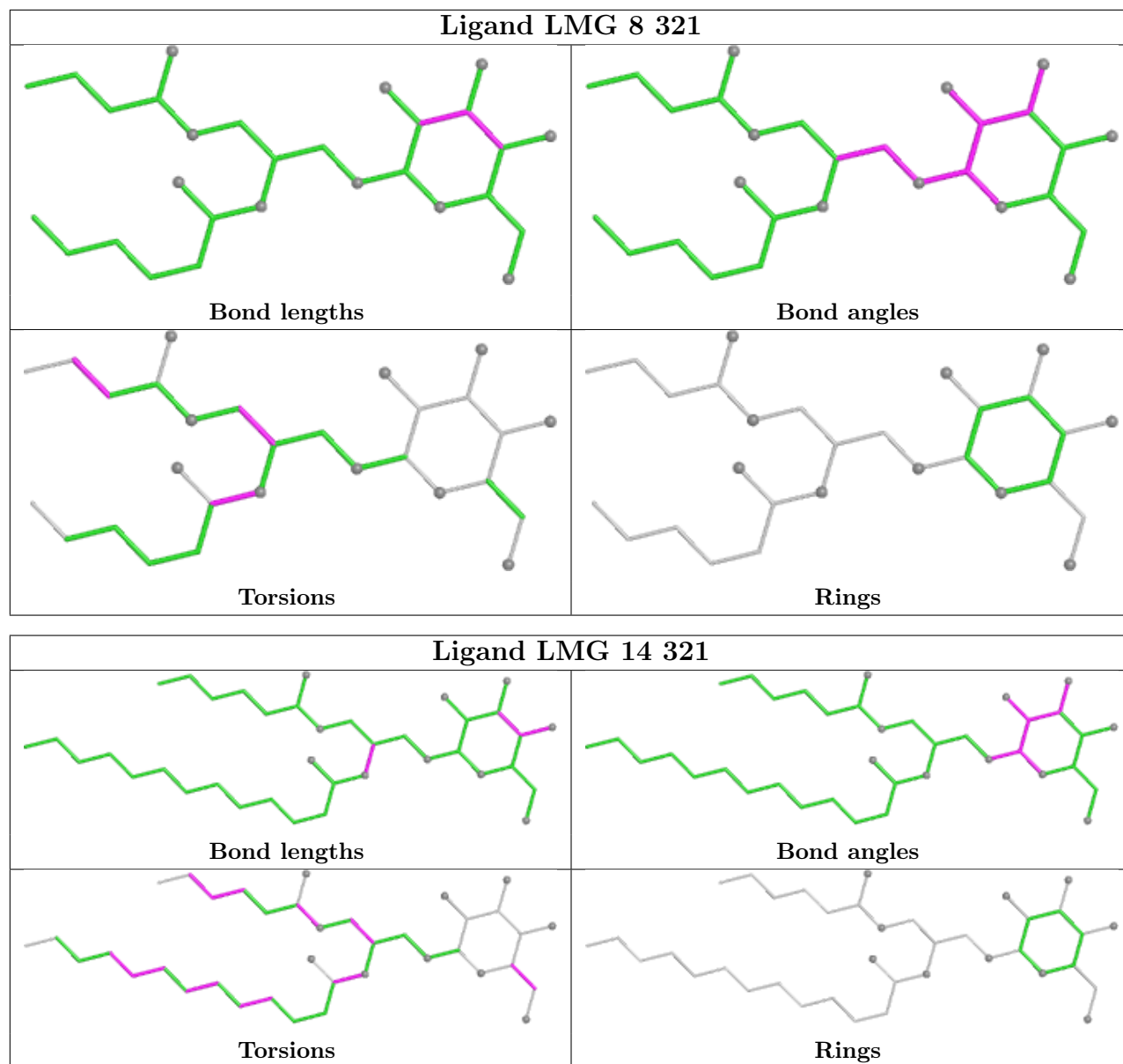
Ligand BCR A 851

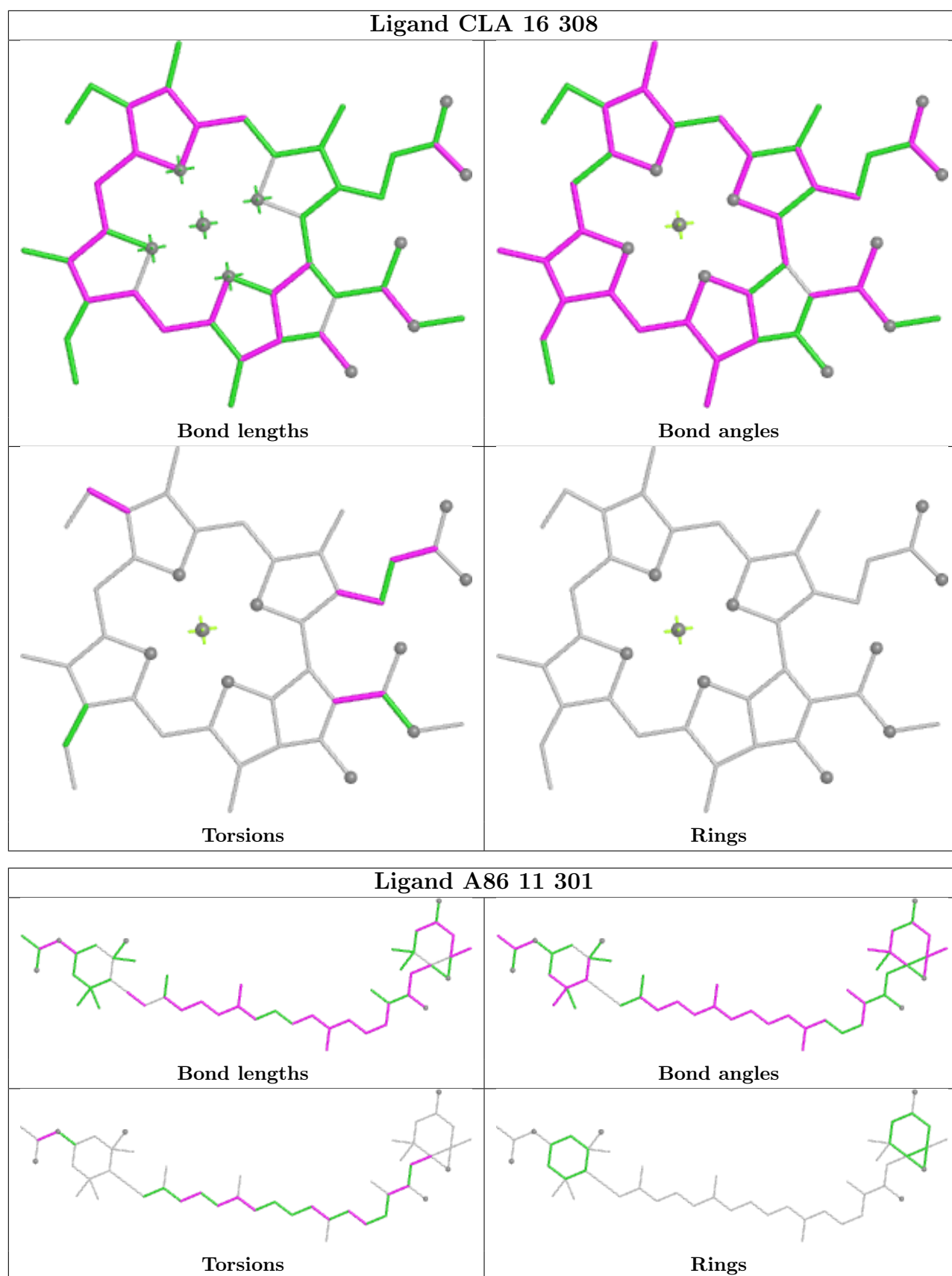


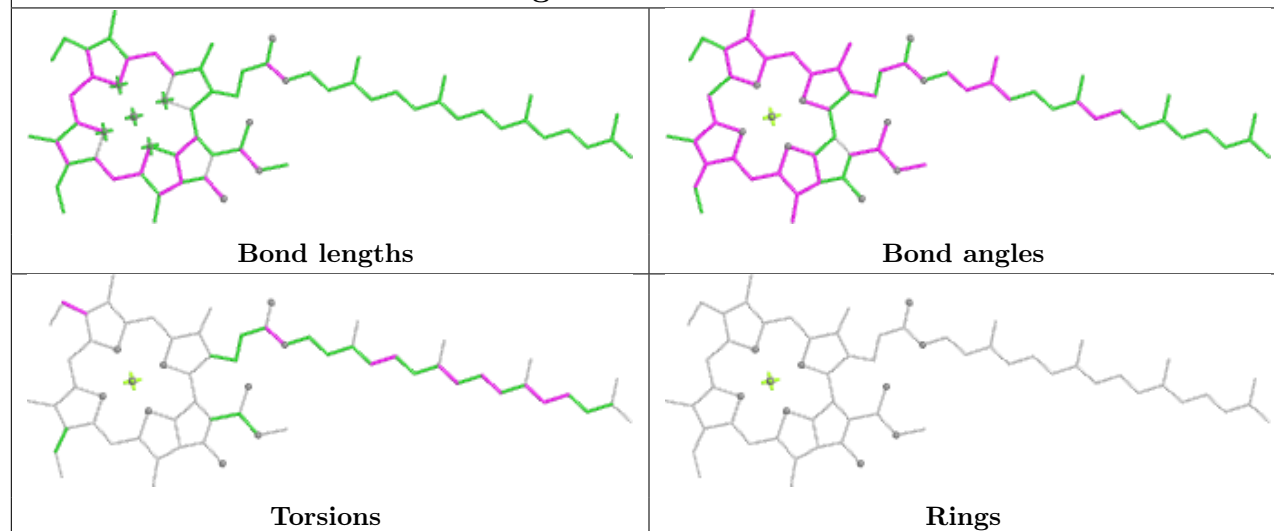
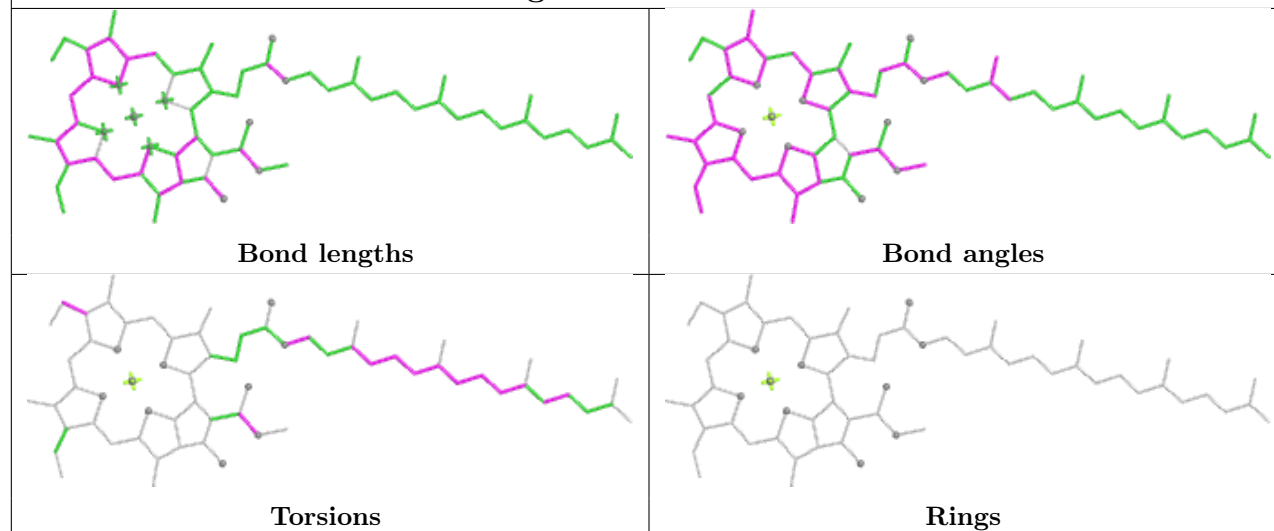


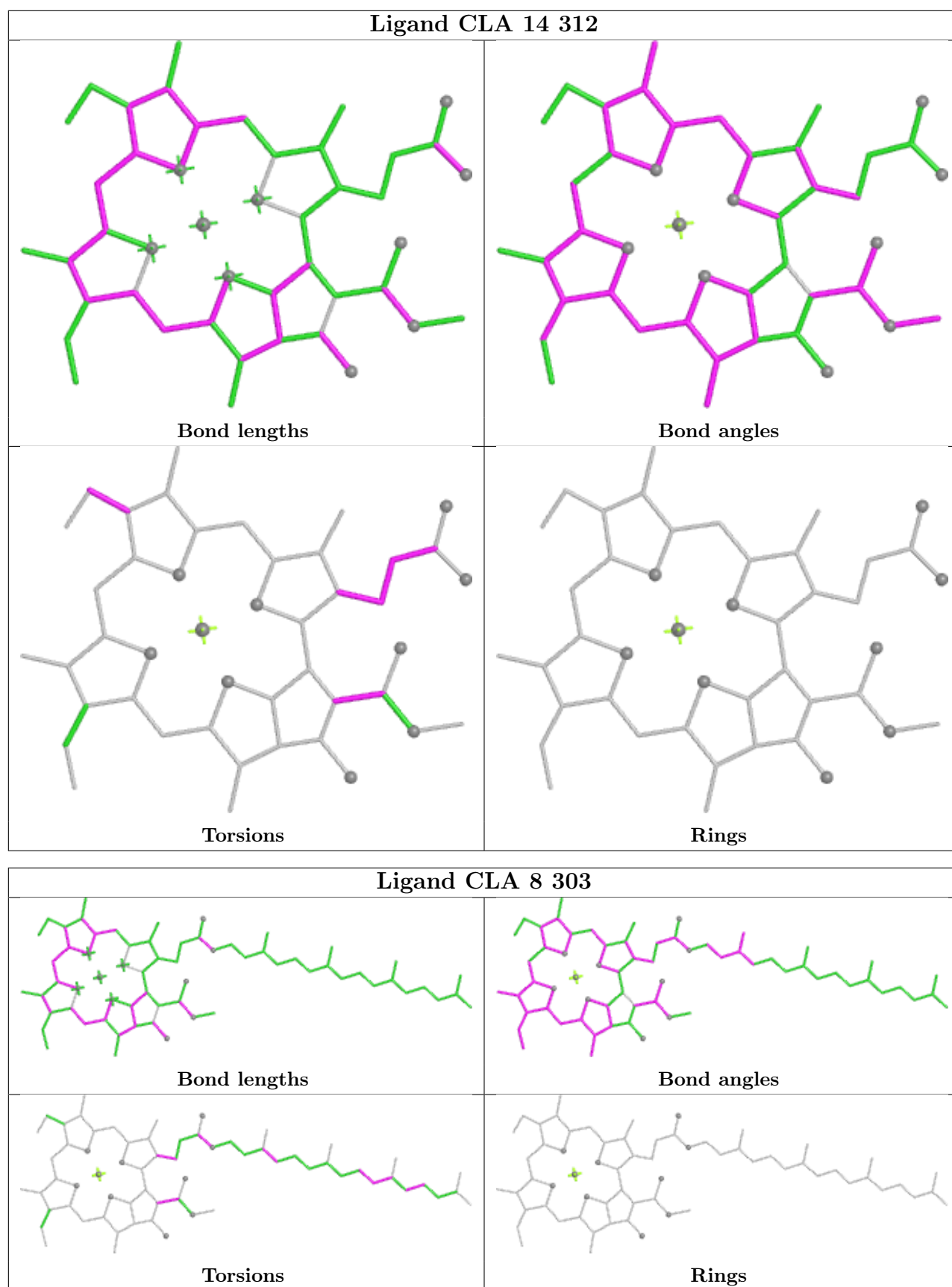


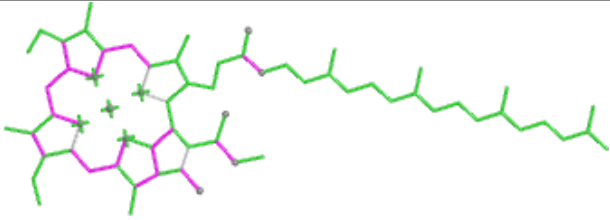
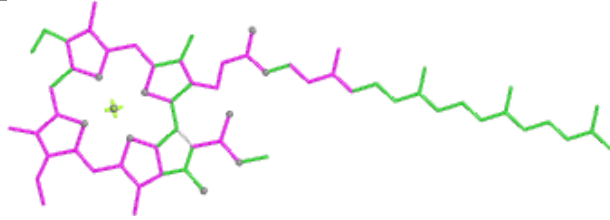
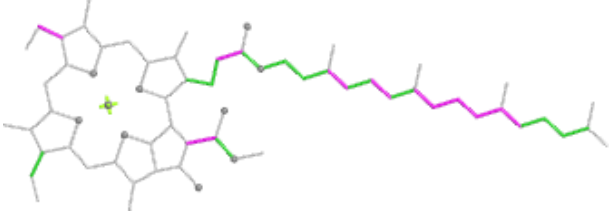
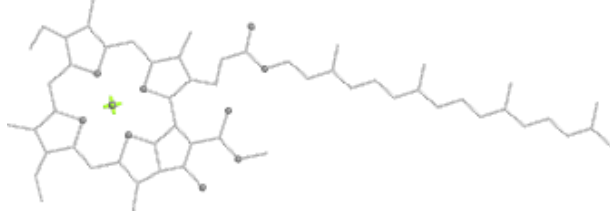
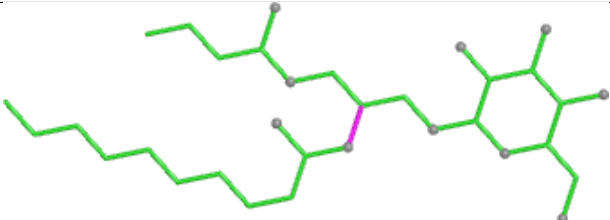
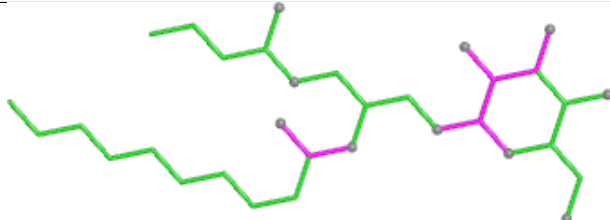
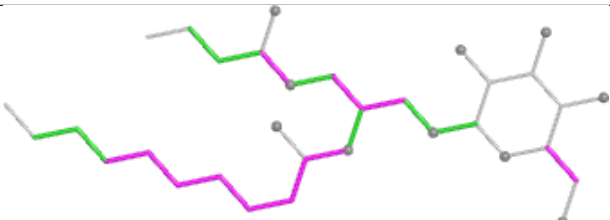
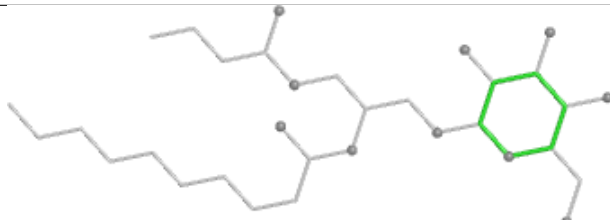
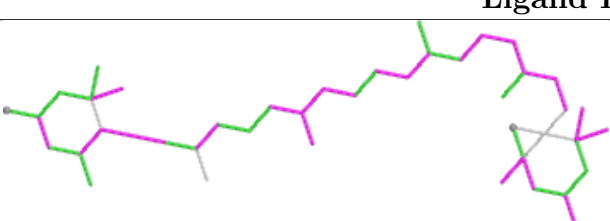
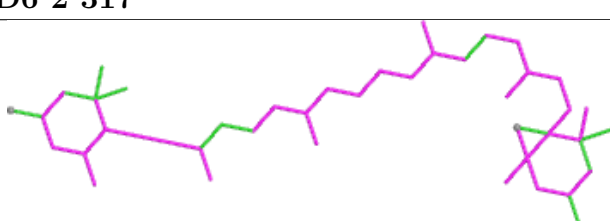
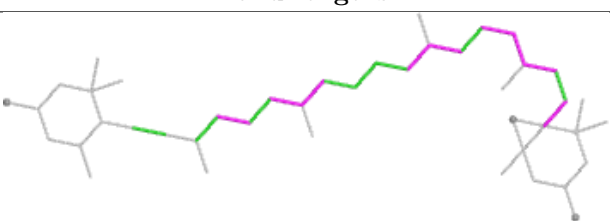
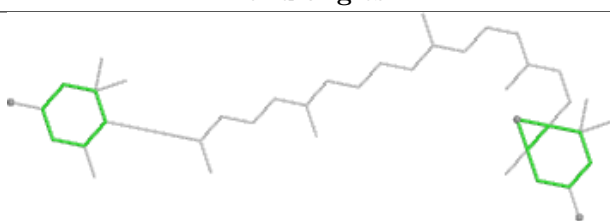




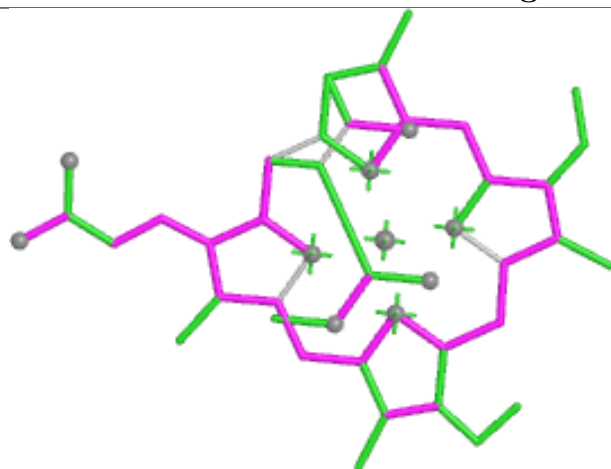


Ligand CLA B 819**Ligand CLA 13 302**

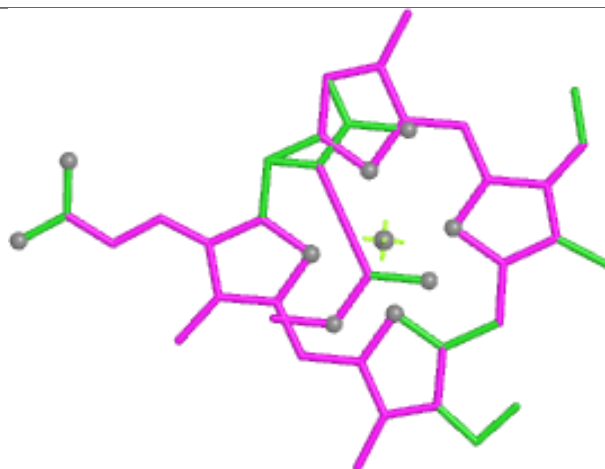


Ligand CLA A 839	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG 6 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DD6 2 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

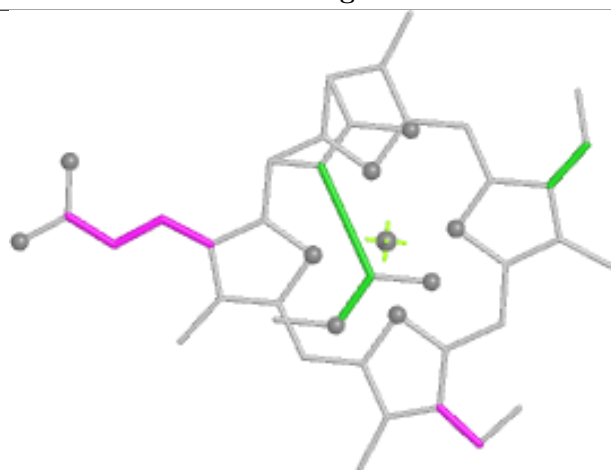
Ligand KC1 9 312



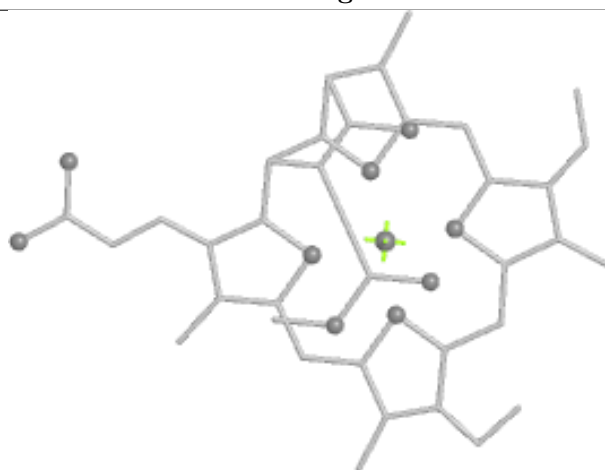
Bond lengths



Bond angles

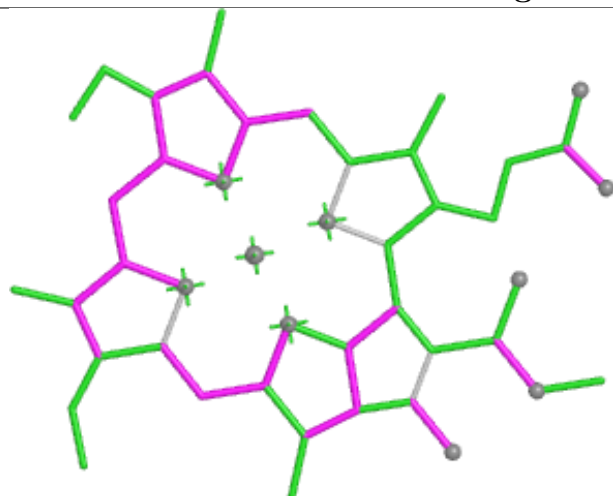


Torsions

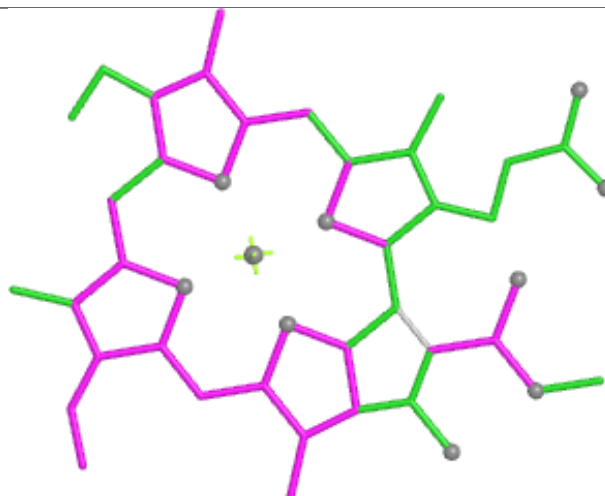


Rings

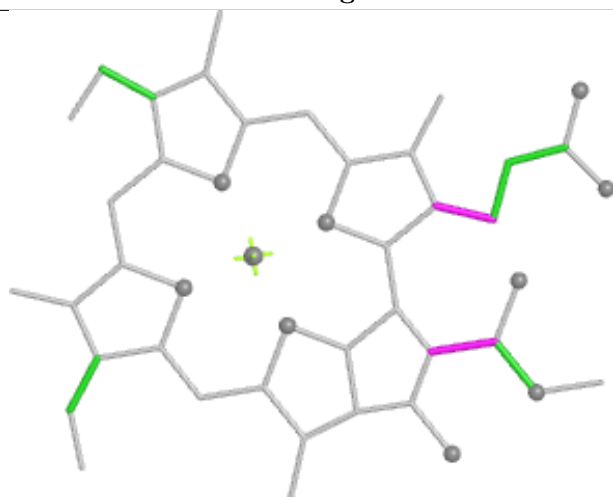
Ligand CLA B 820



Bond lengths



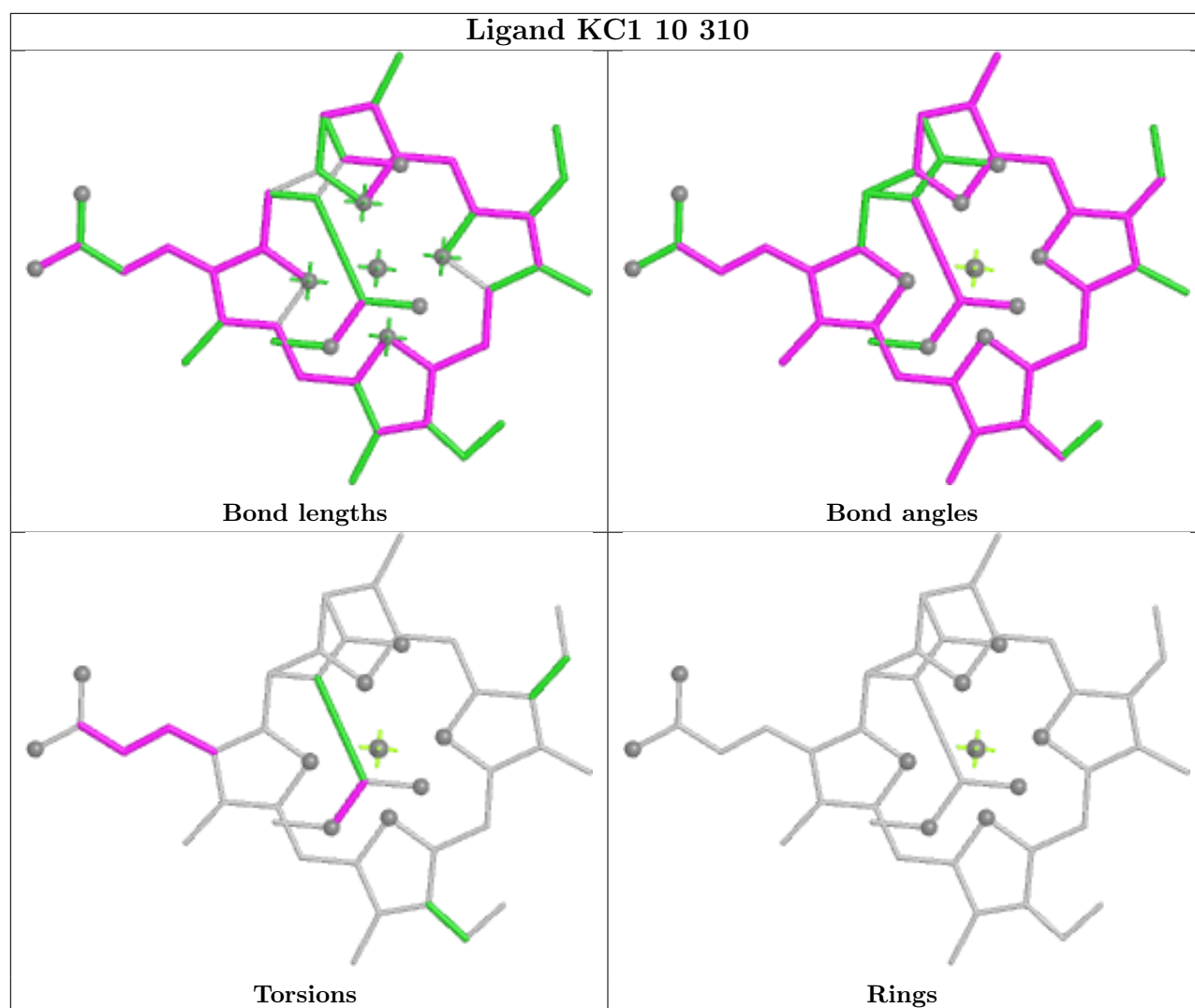
Bond angles



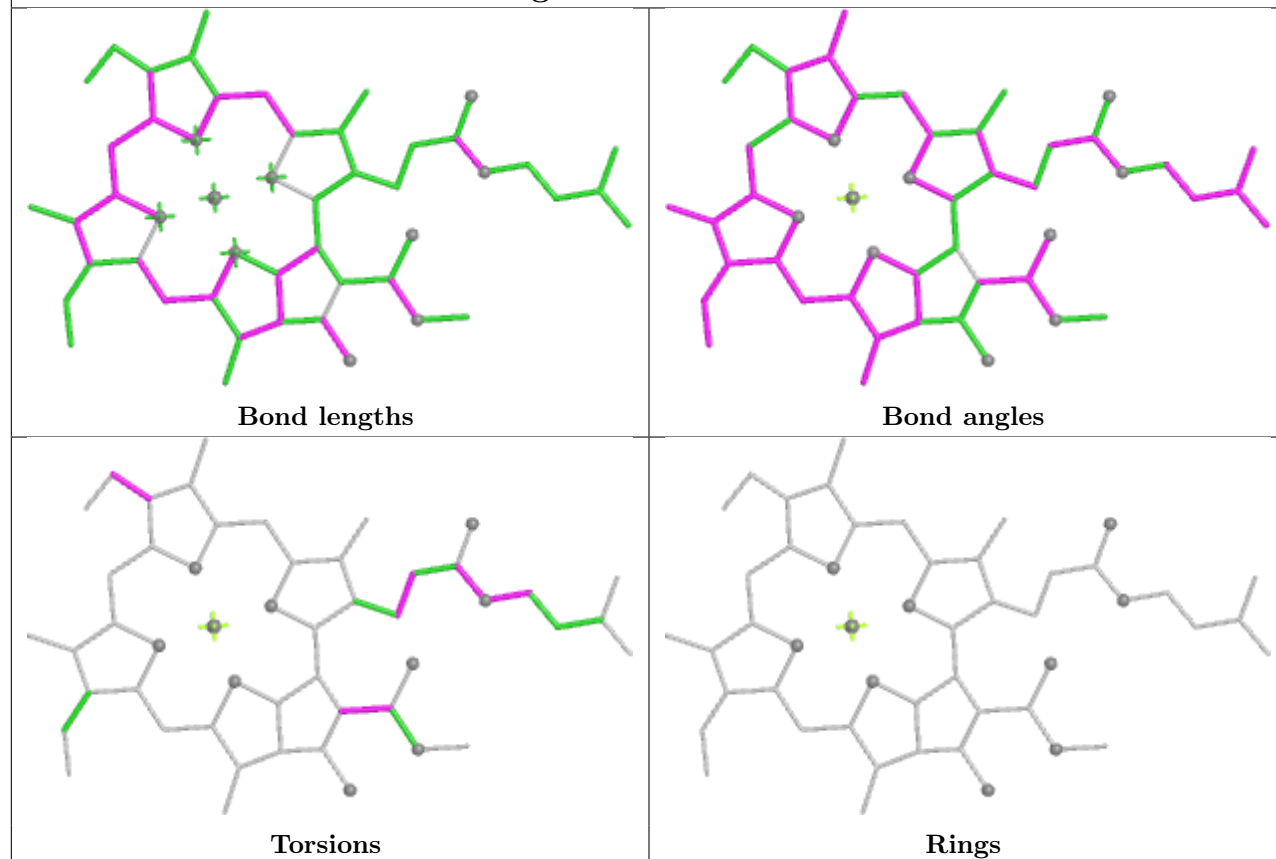
Torsions



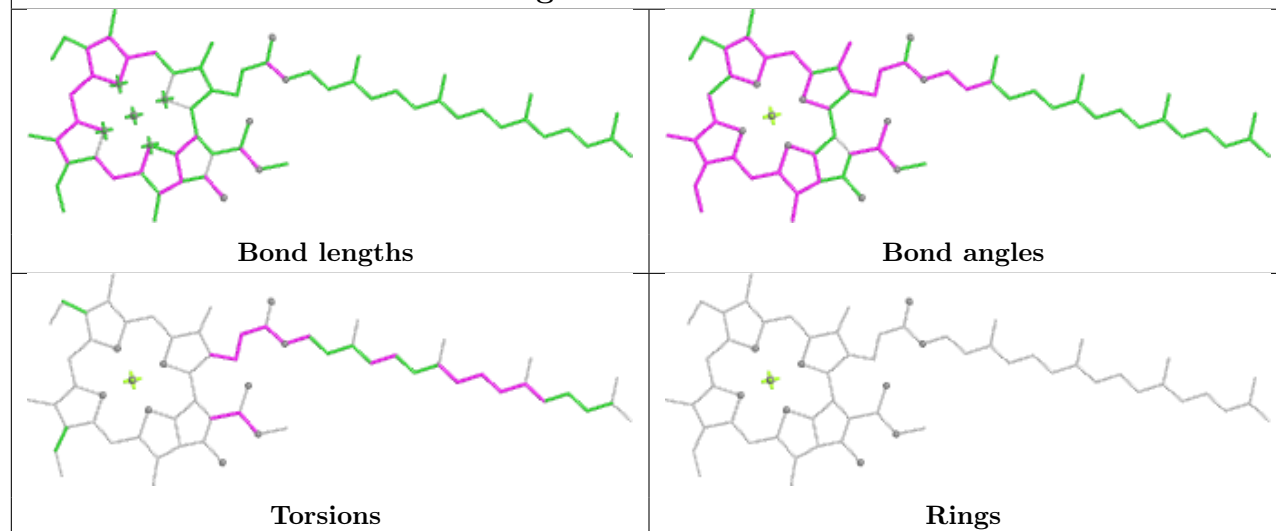
Rings

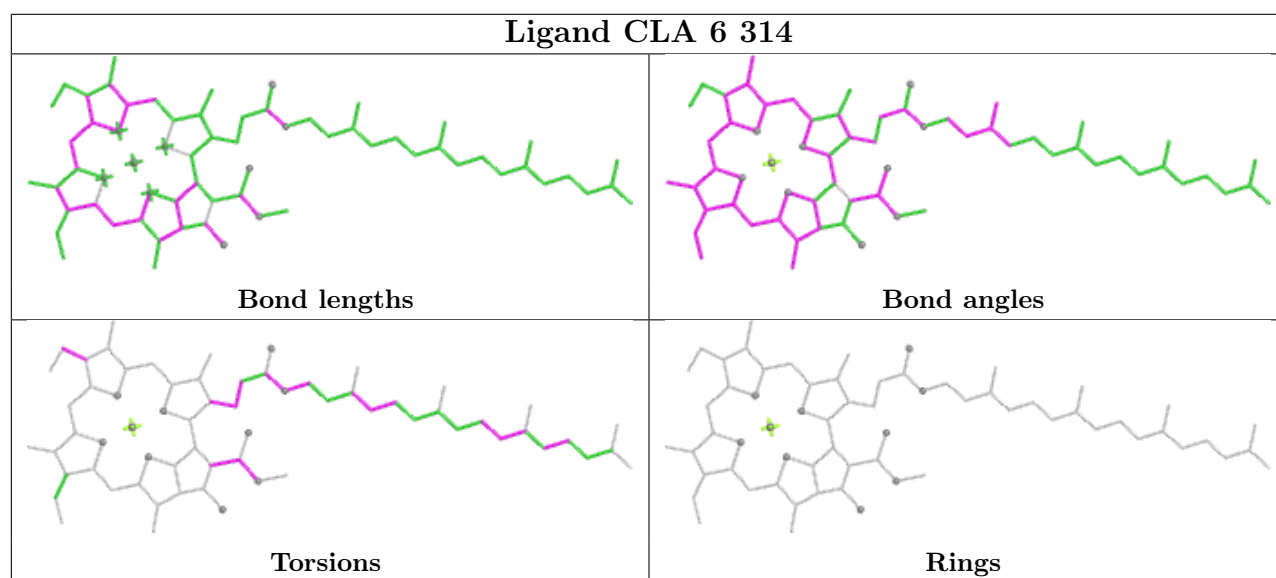
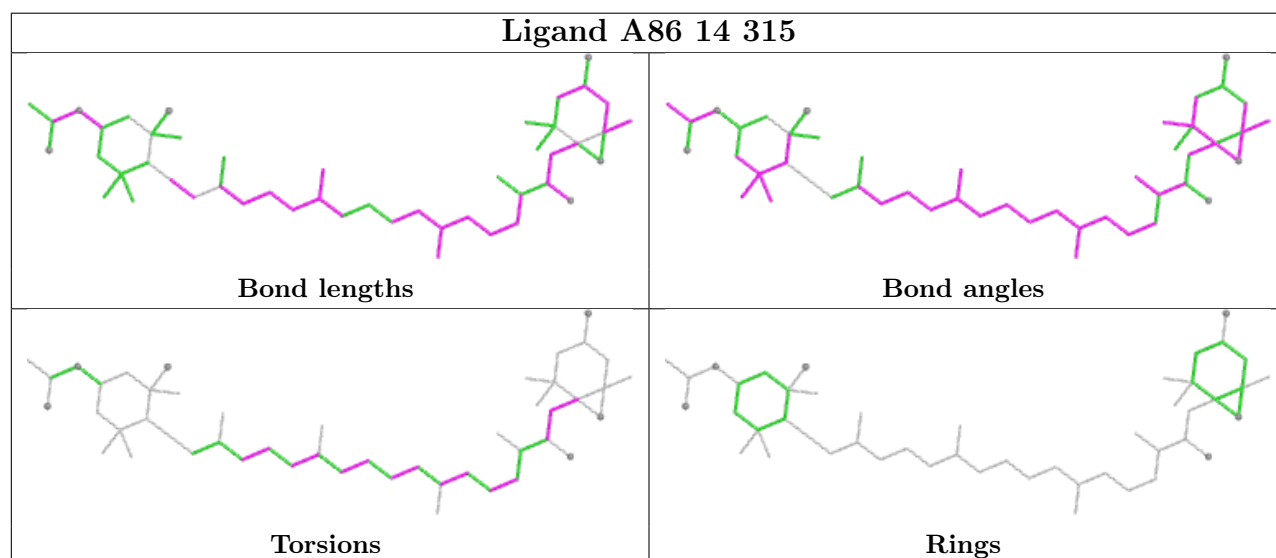
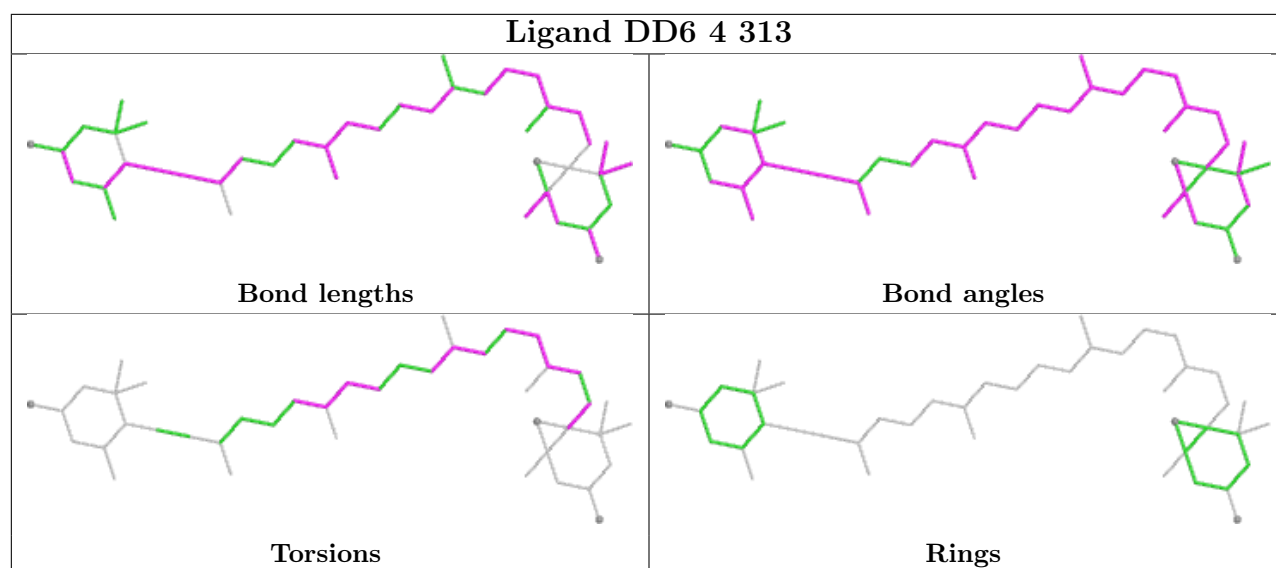


Ligand CLA A 832

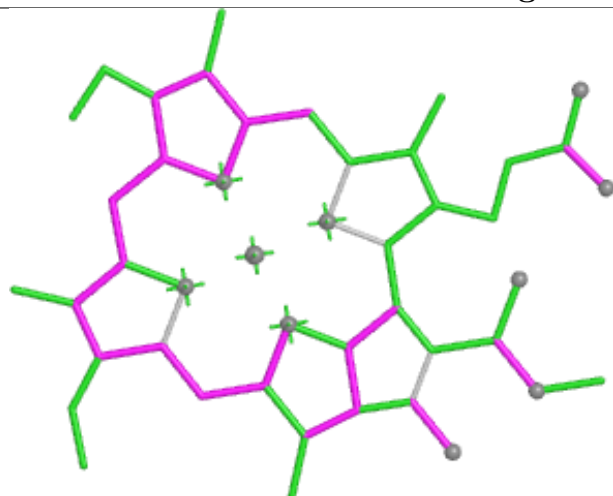


Ligand CLA 8 301

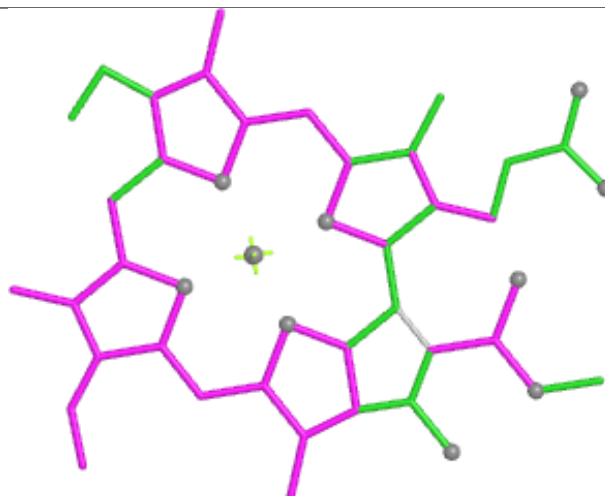




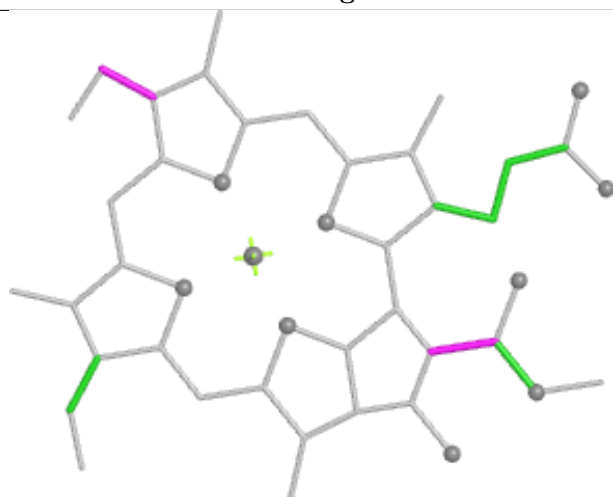
Ligand CLA 6 315



Bond lengths



Bond angles

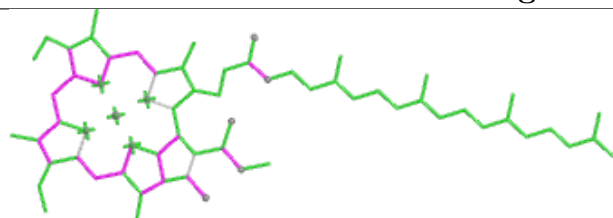


Torsions

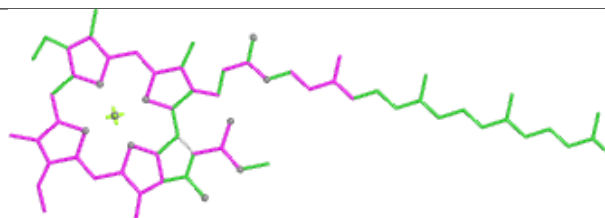


Rings

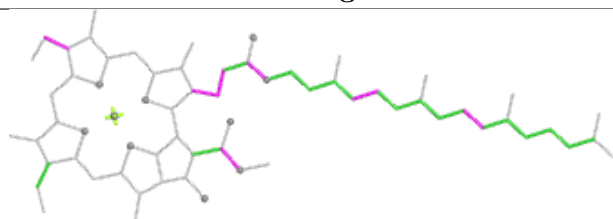
Ligand CLA 3 306



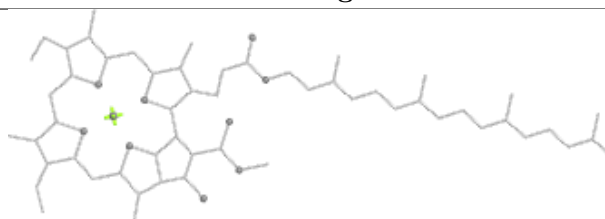
Bond lengths



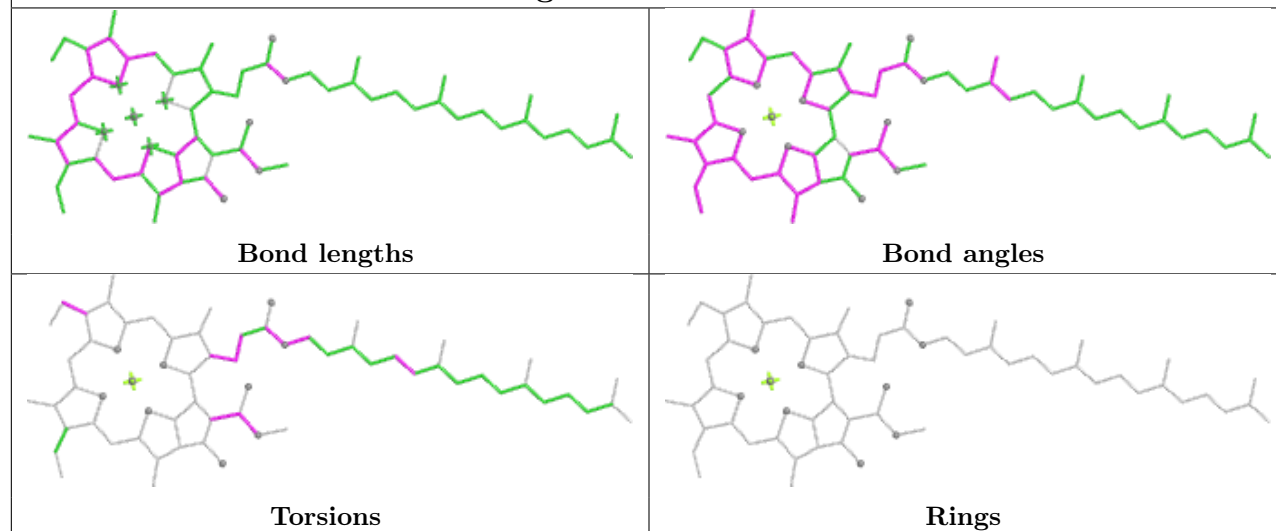
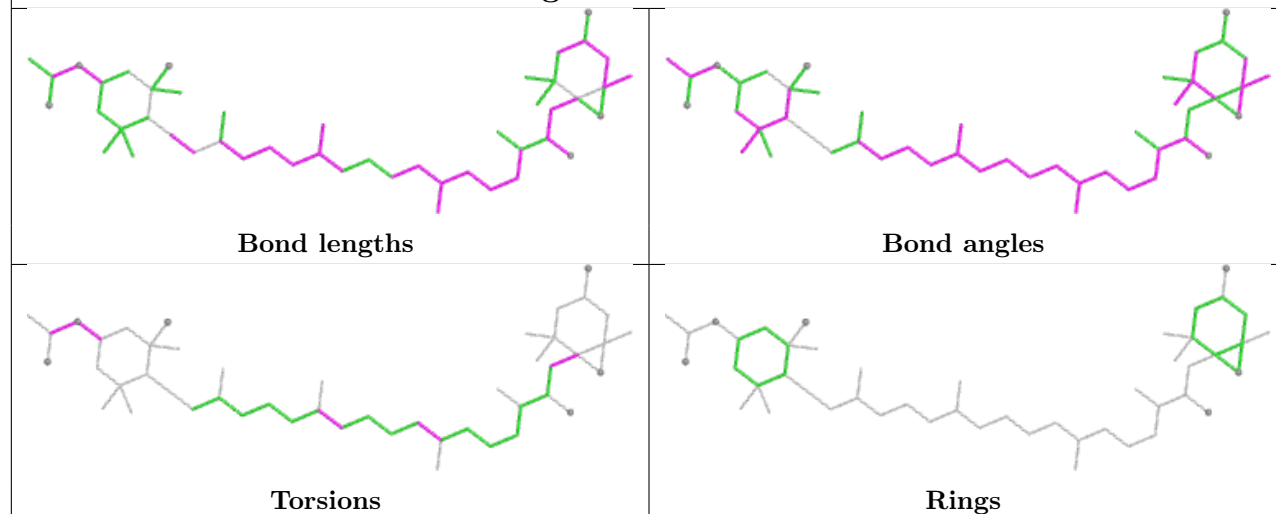
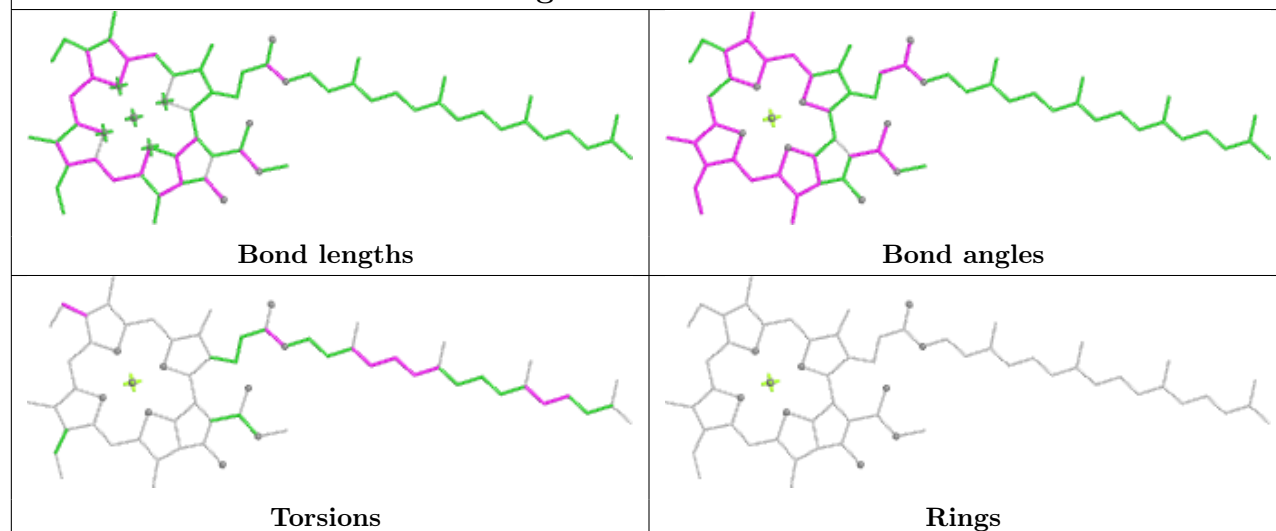
Bond angles



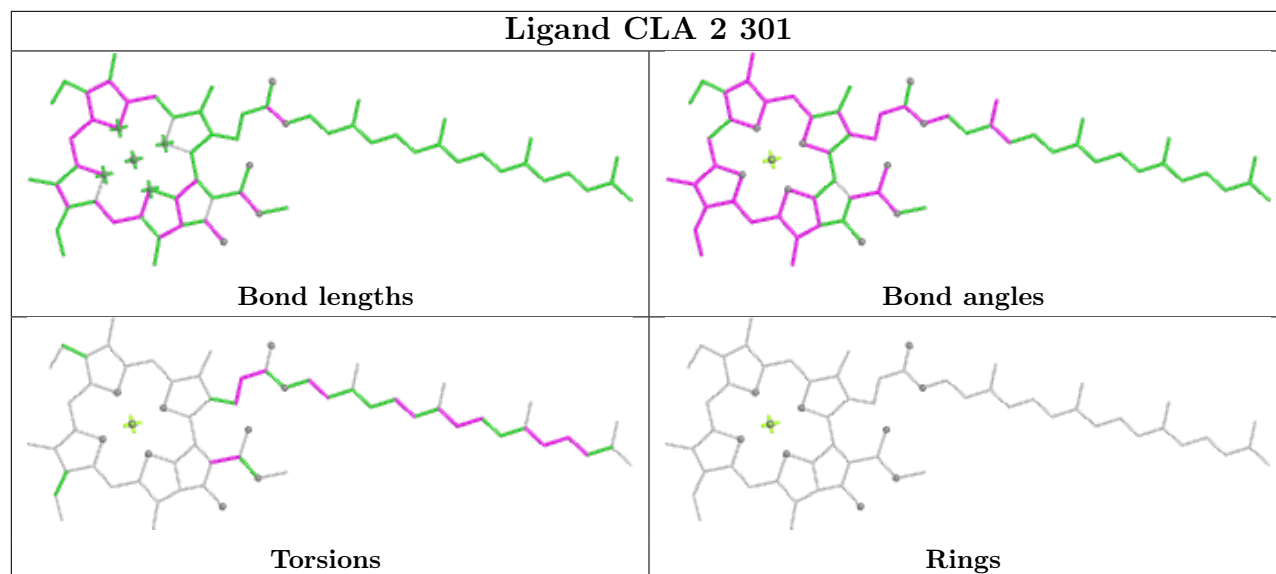
Torsions



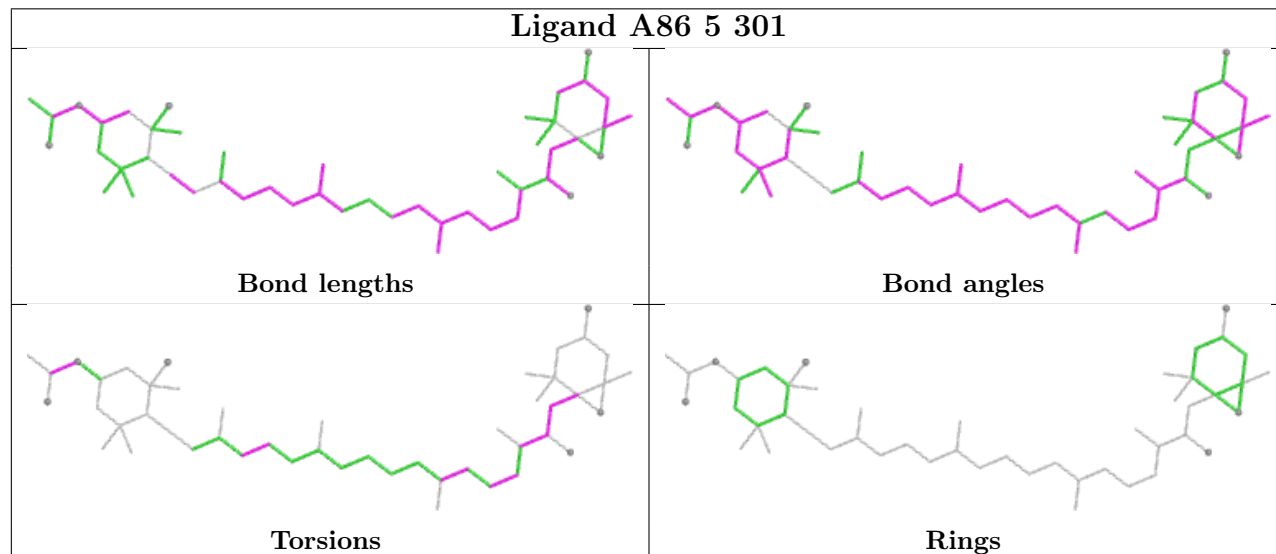
Rings

Ligand CLA 4 306**Ligand A86 7 319****Ligand CLA 7 309**

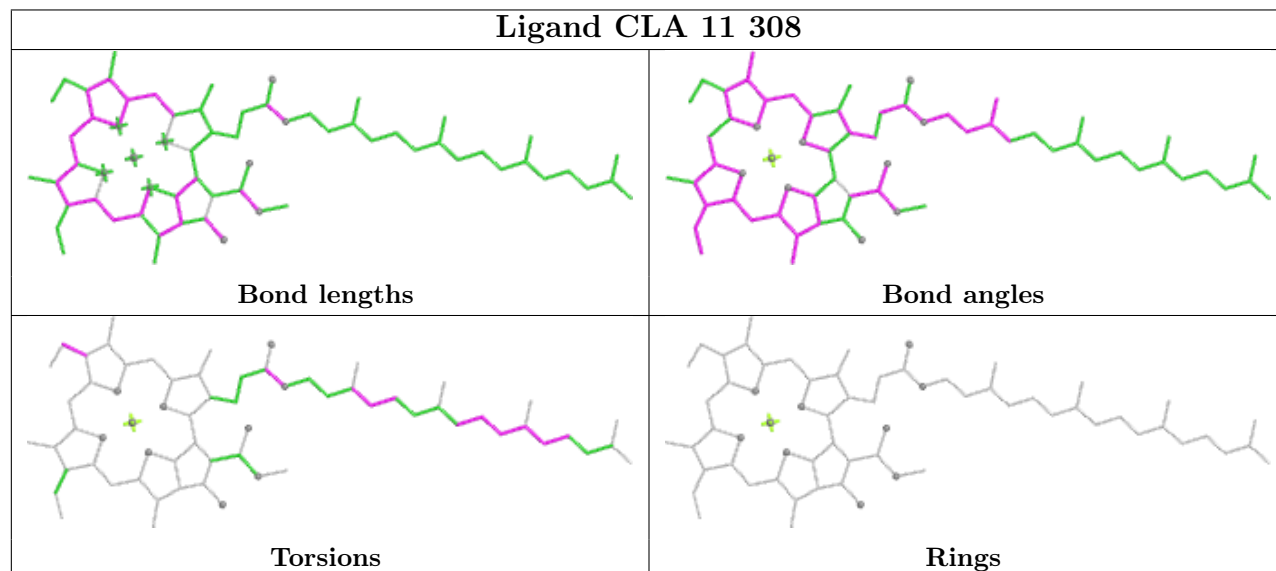
Ligand CLA 2 301

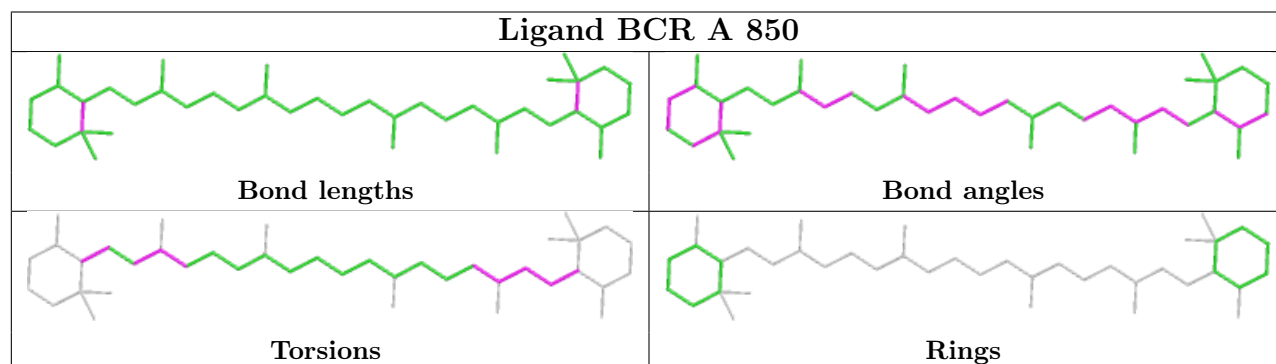
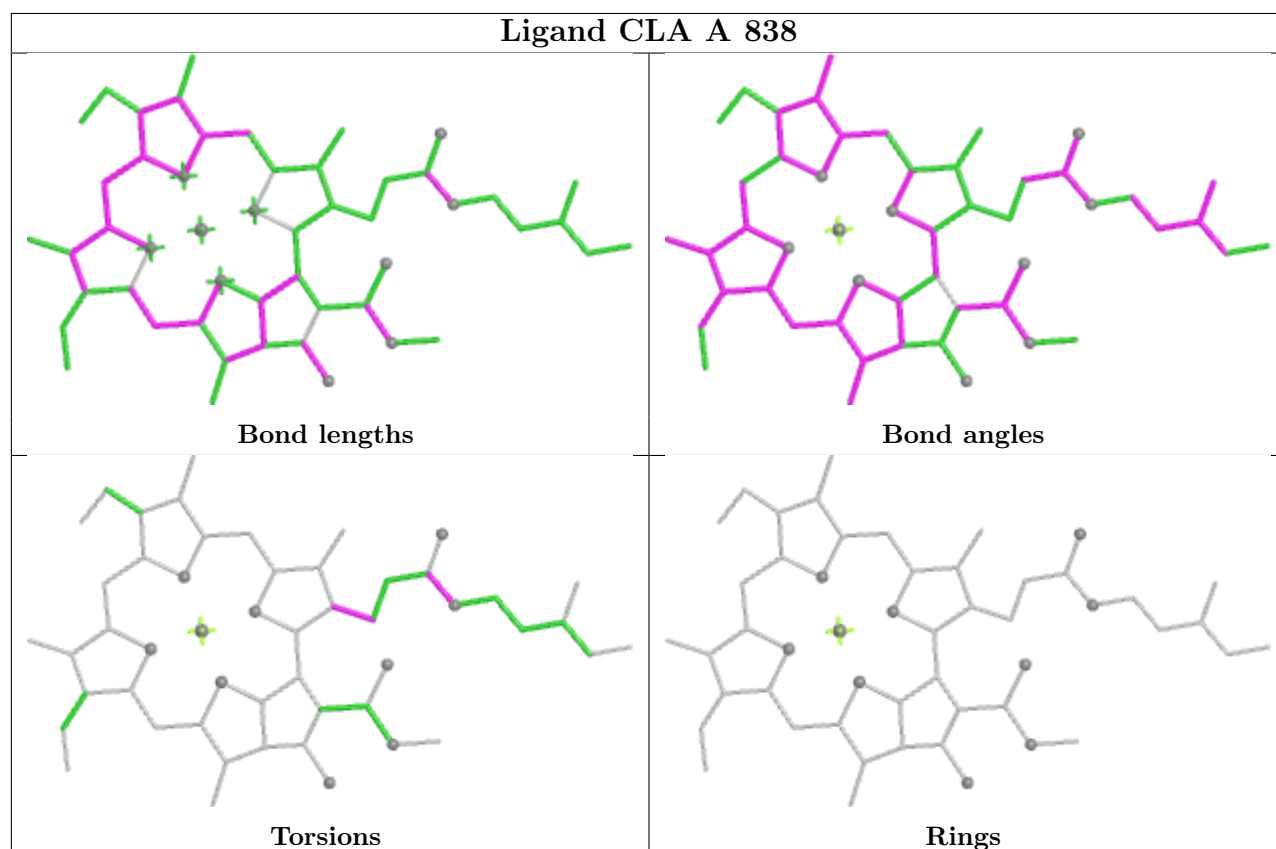
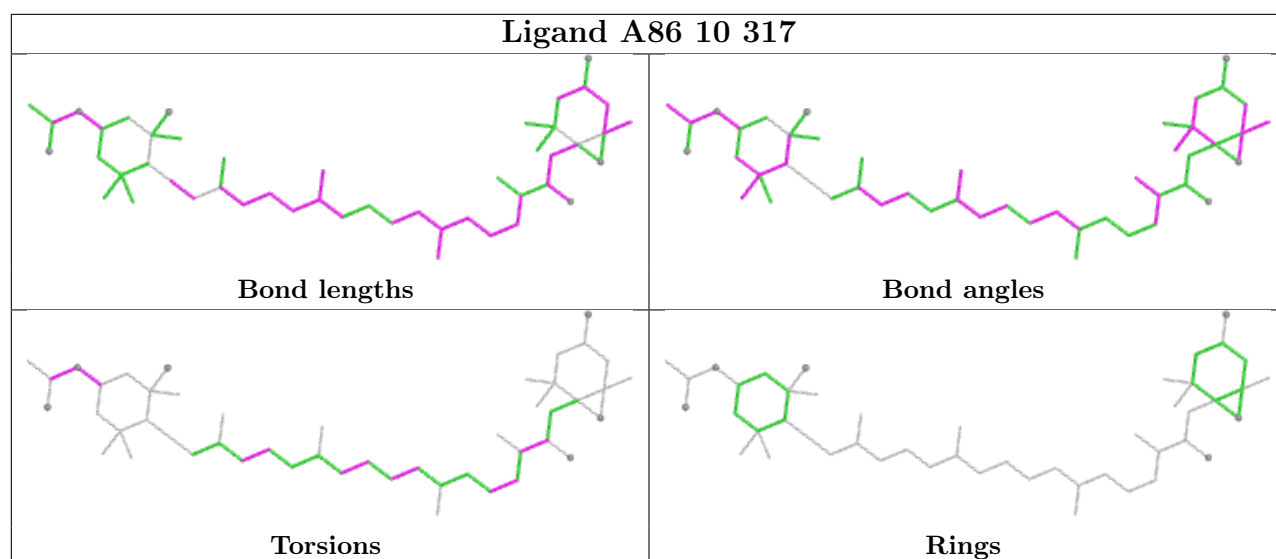


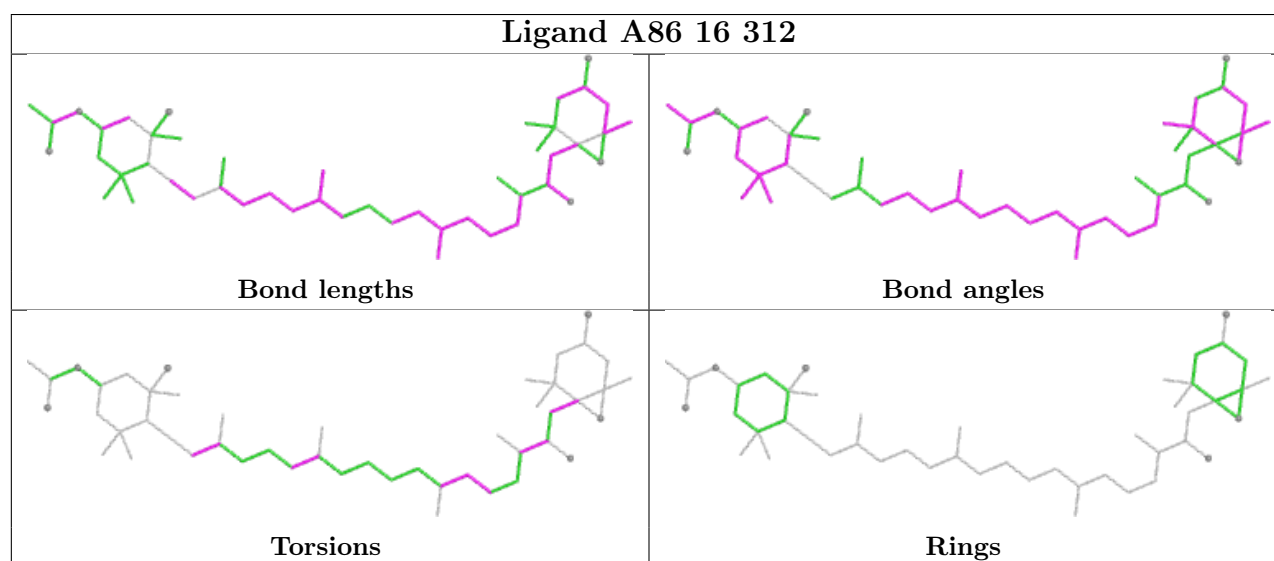
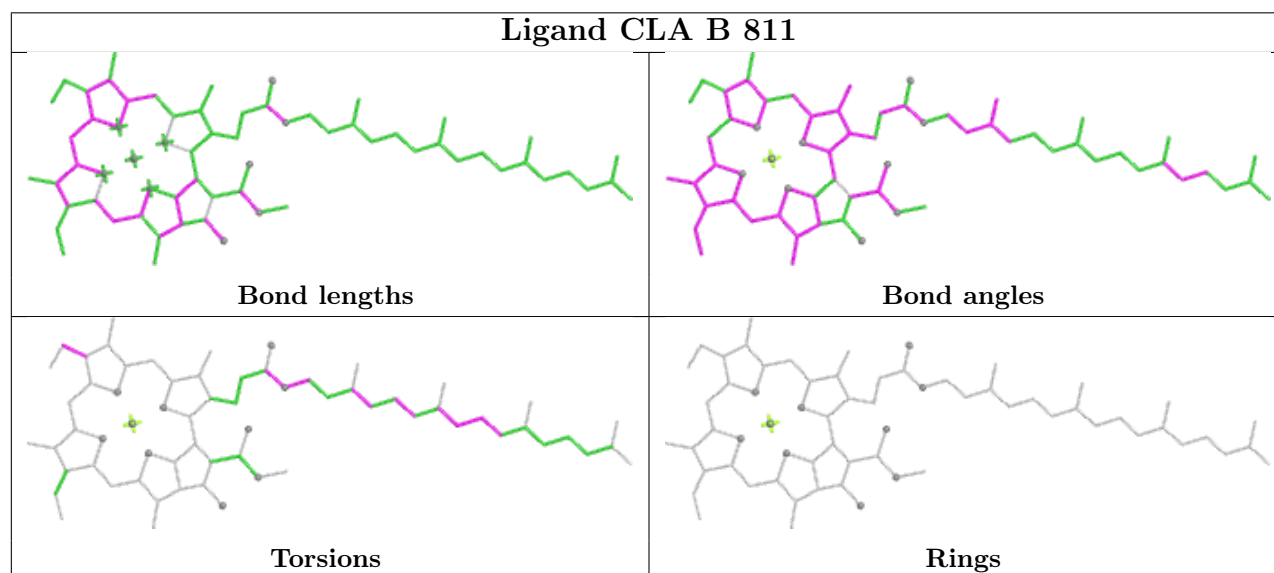
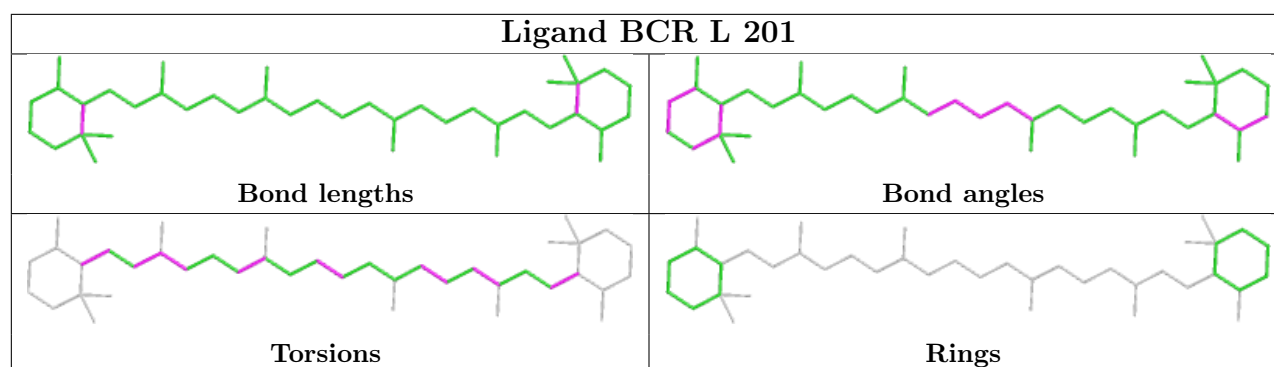
Ligand A86 5 301

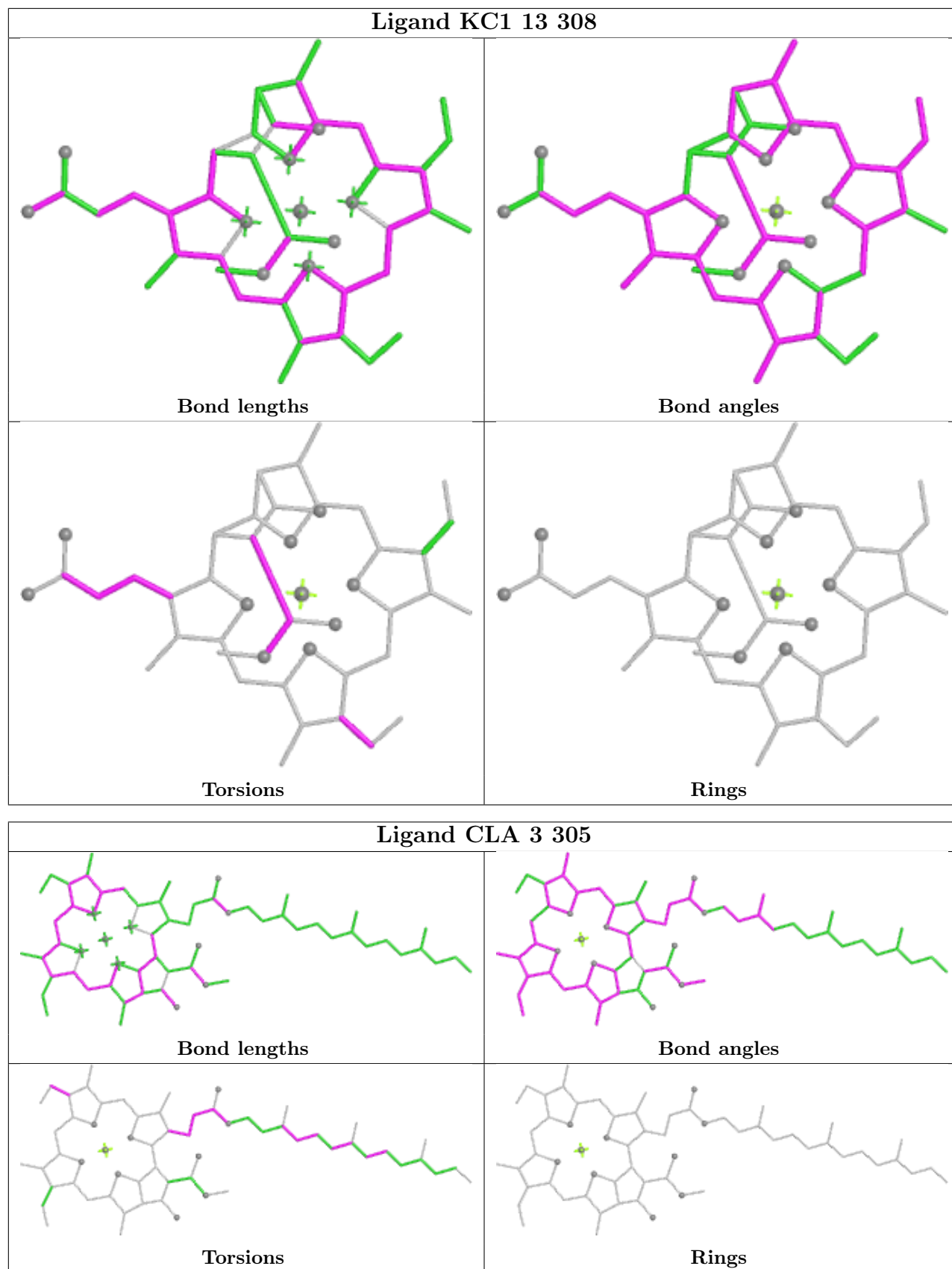


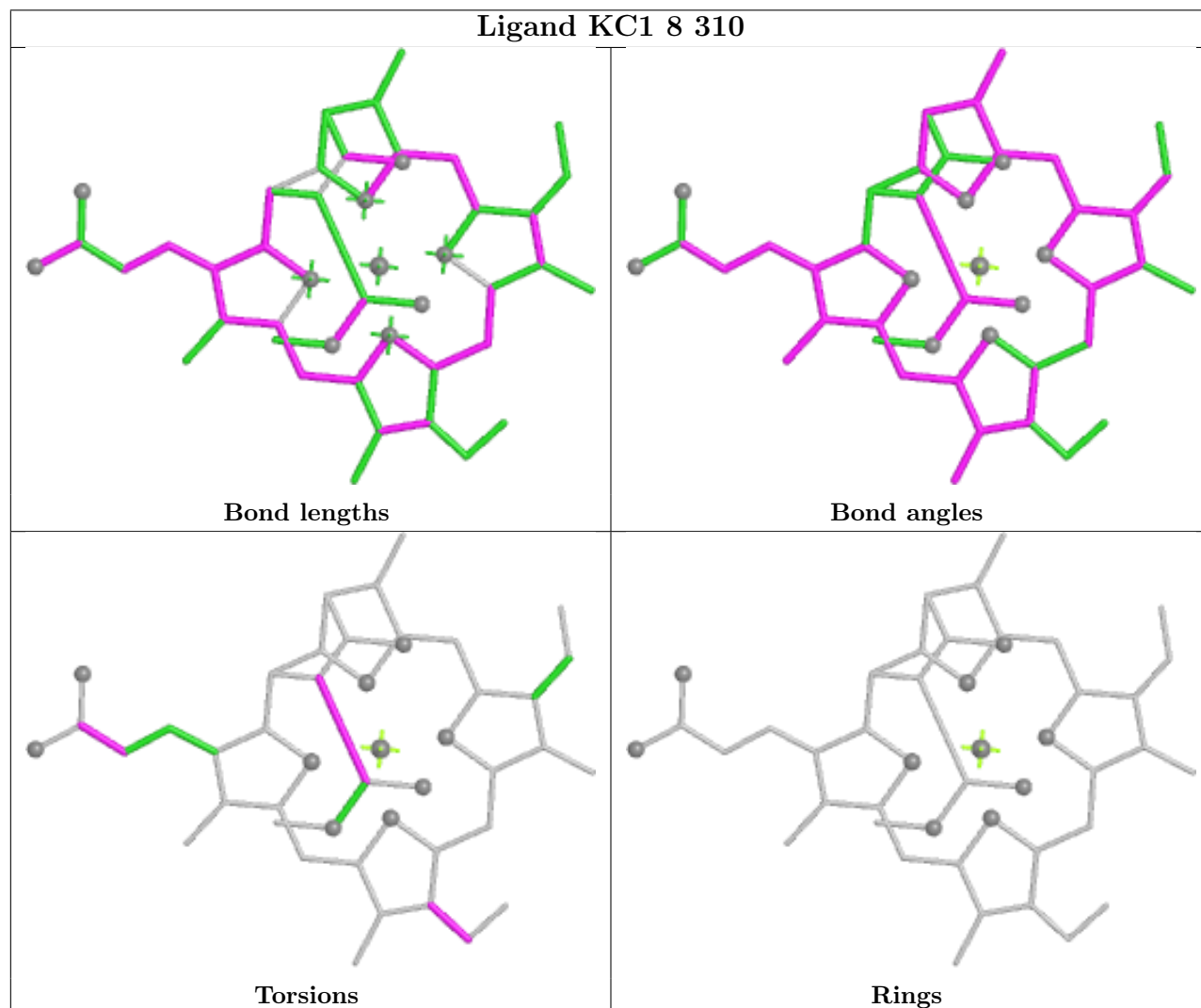
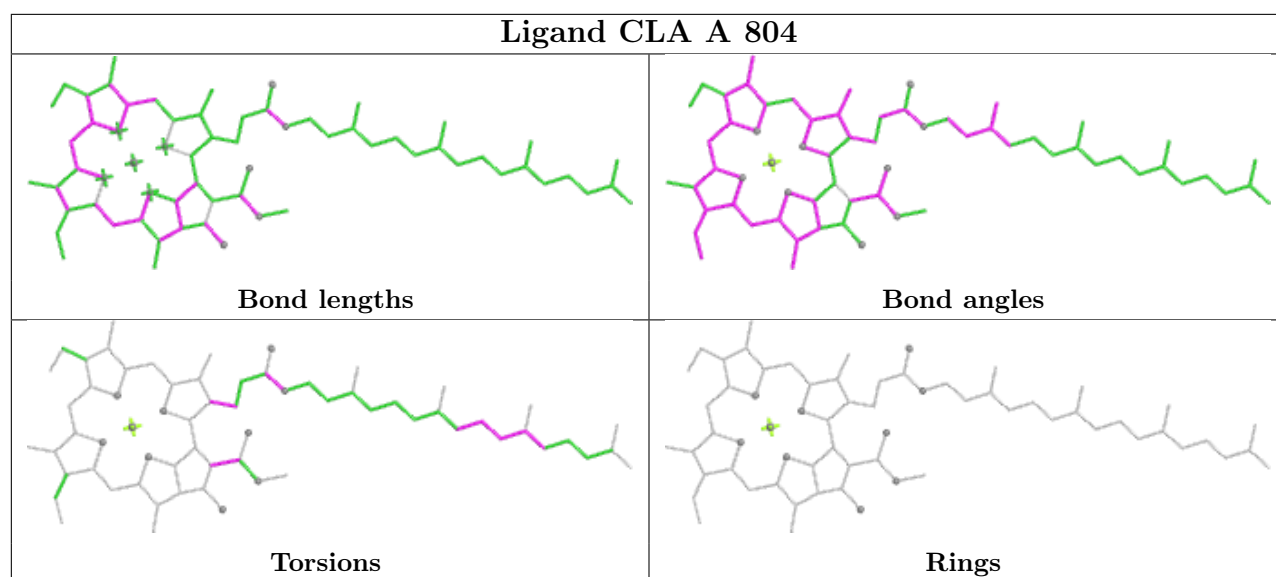
Ligand CLA 11 308

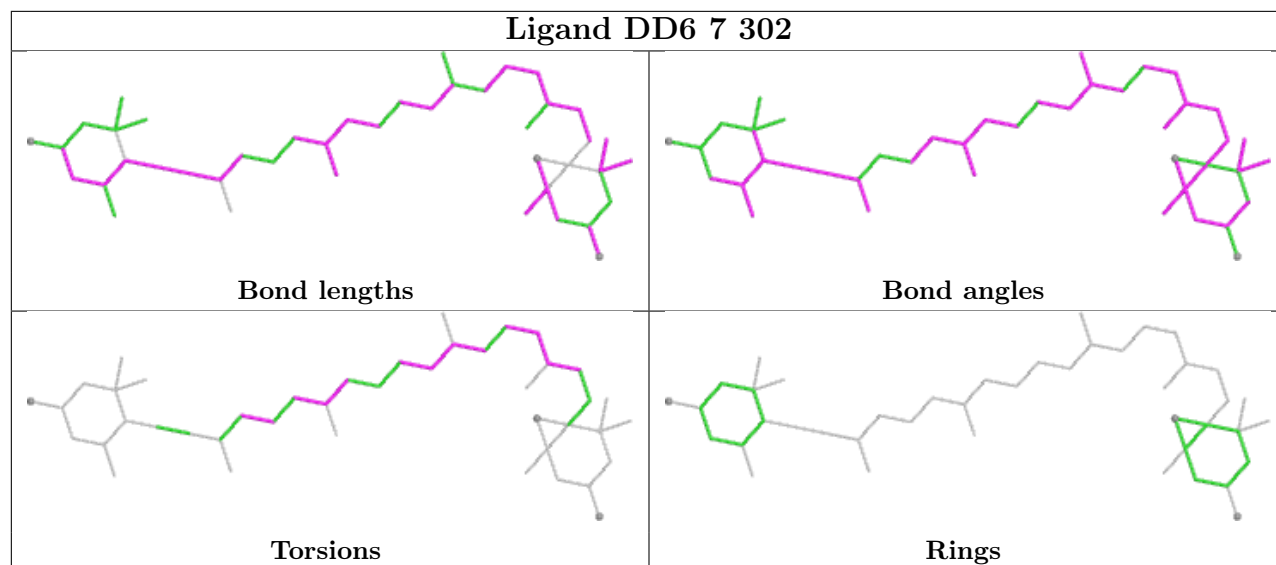
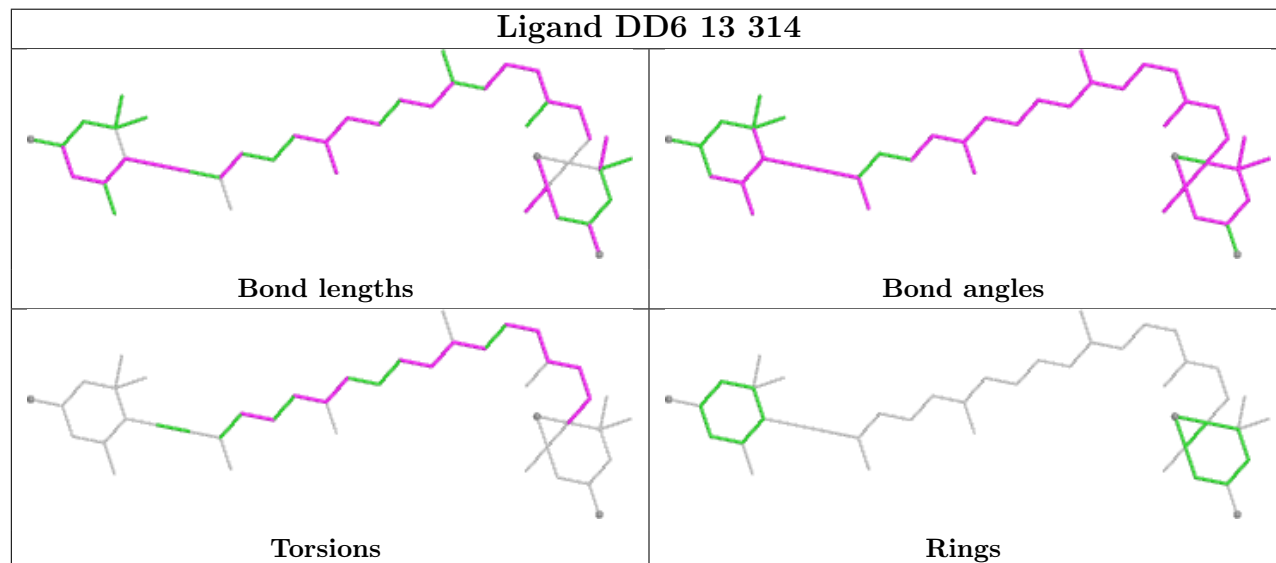




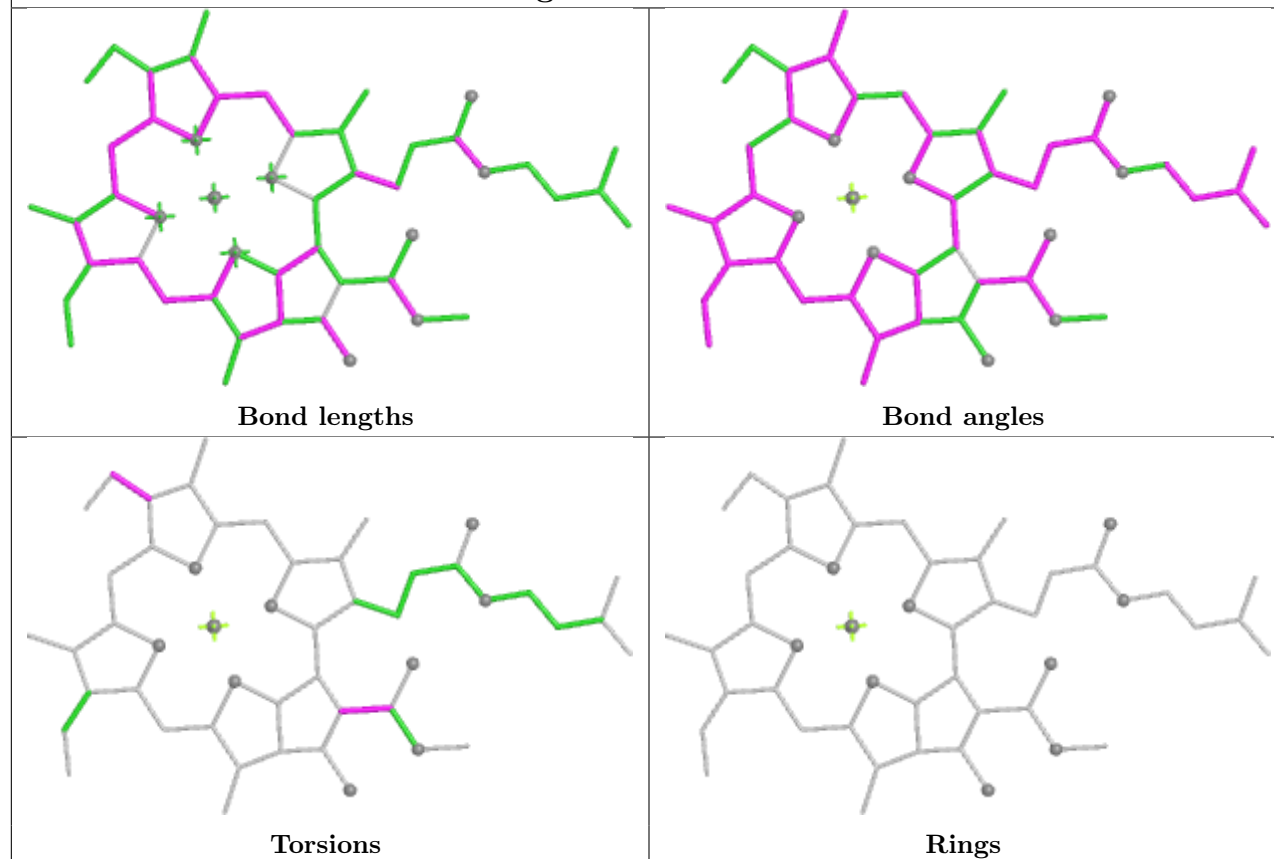




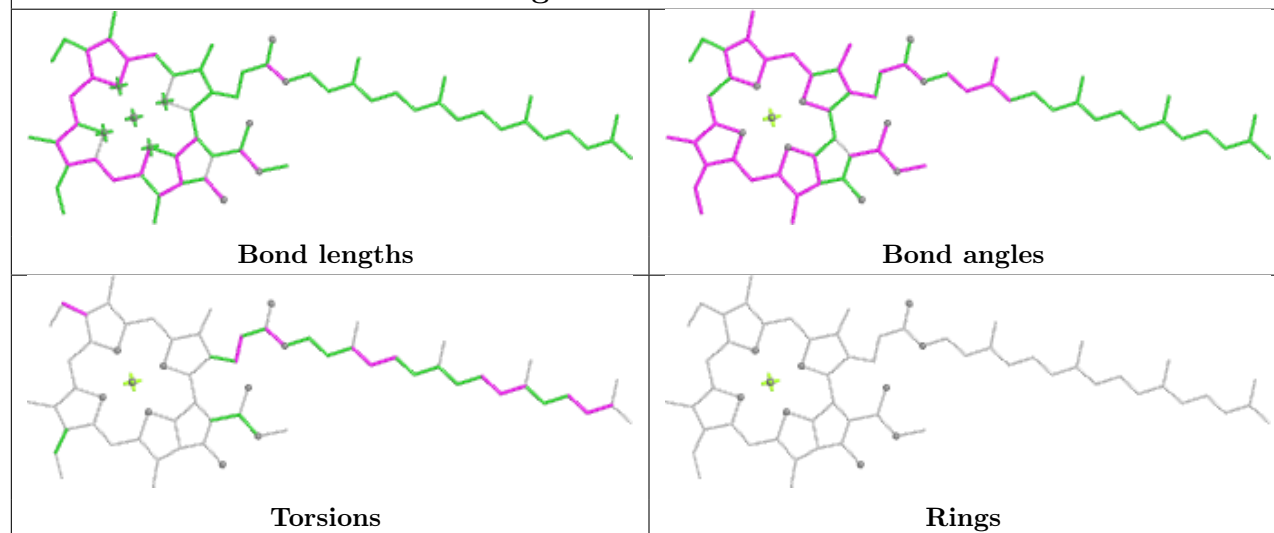


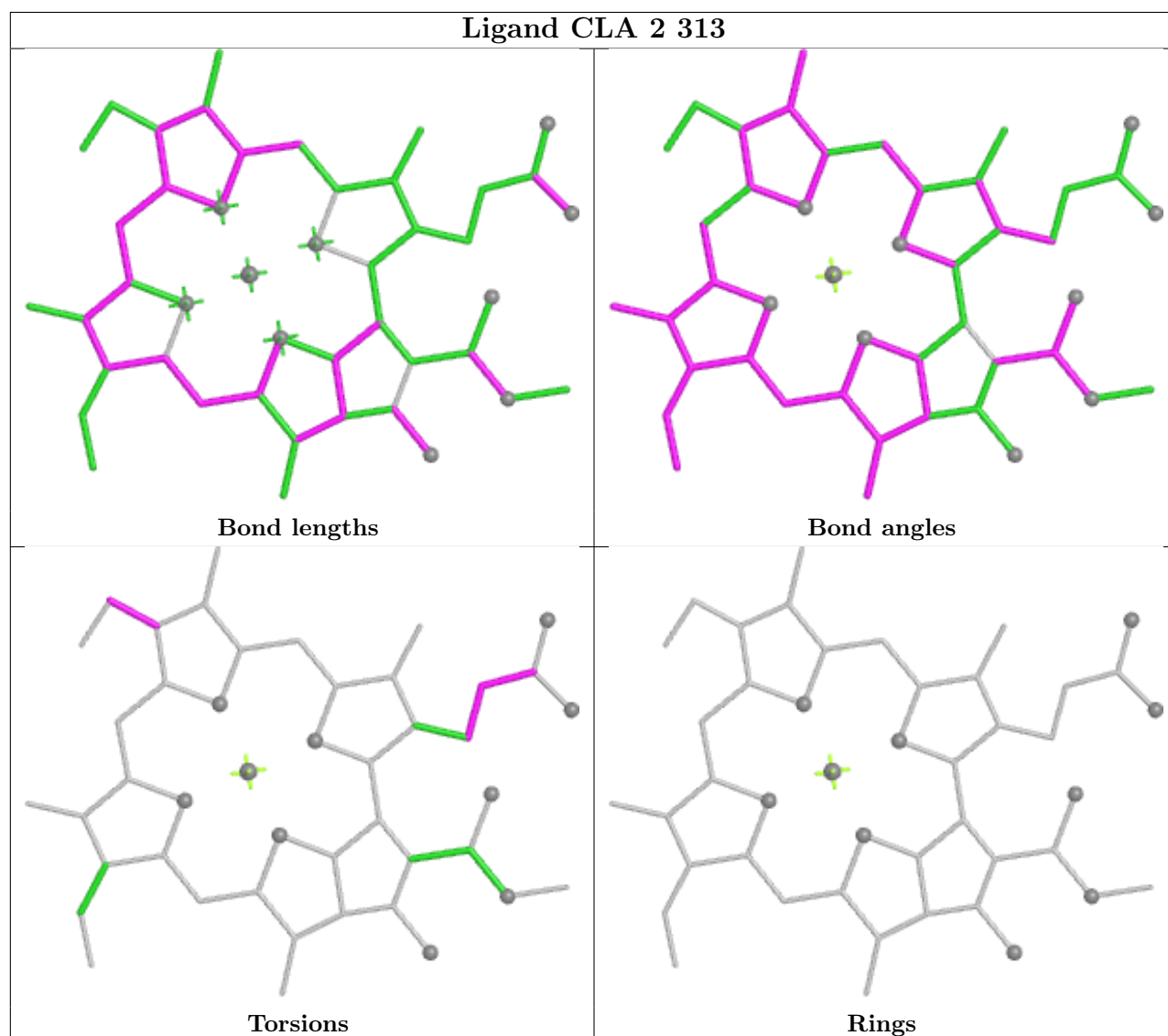
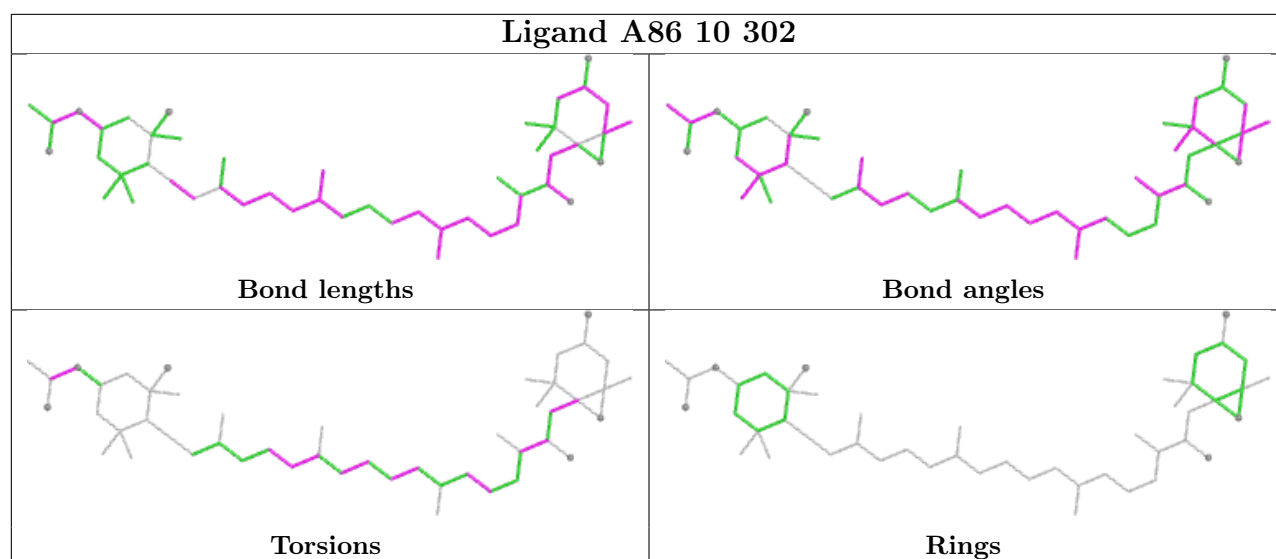
Ligand DD6 7 302**Ligand DD6 13 314**

Ligand CLA 4 311

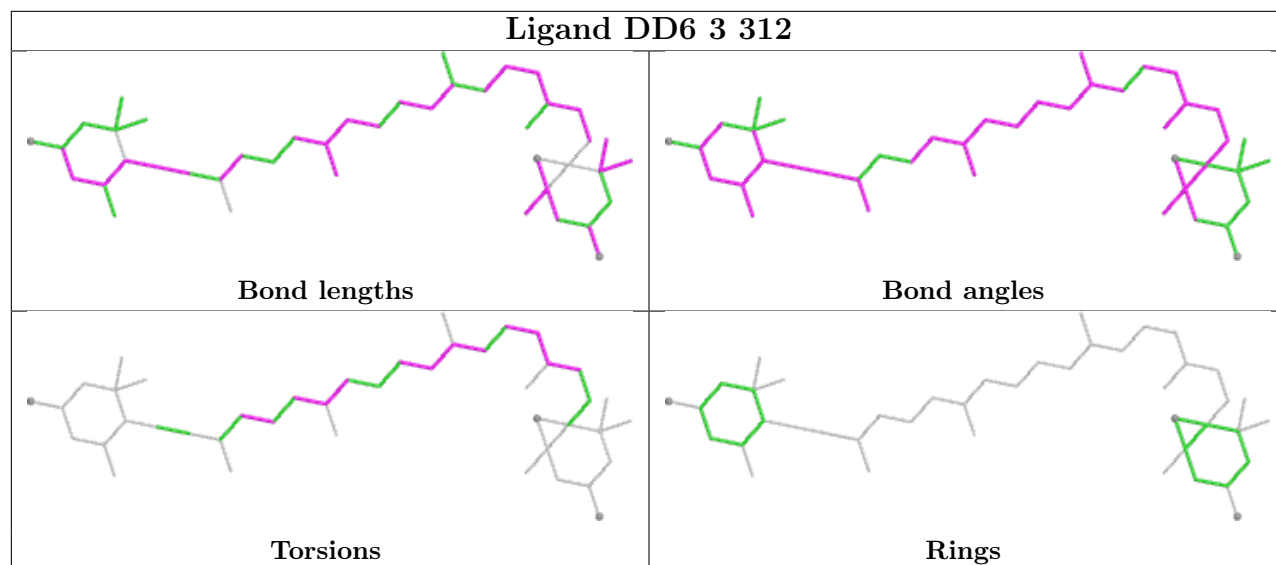


Ligand CLA A 844

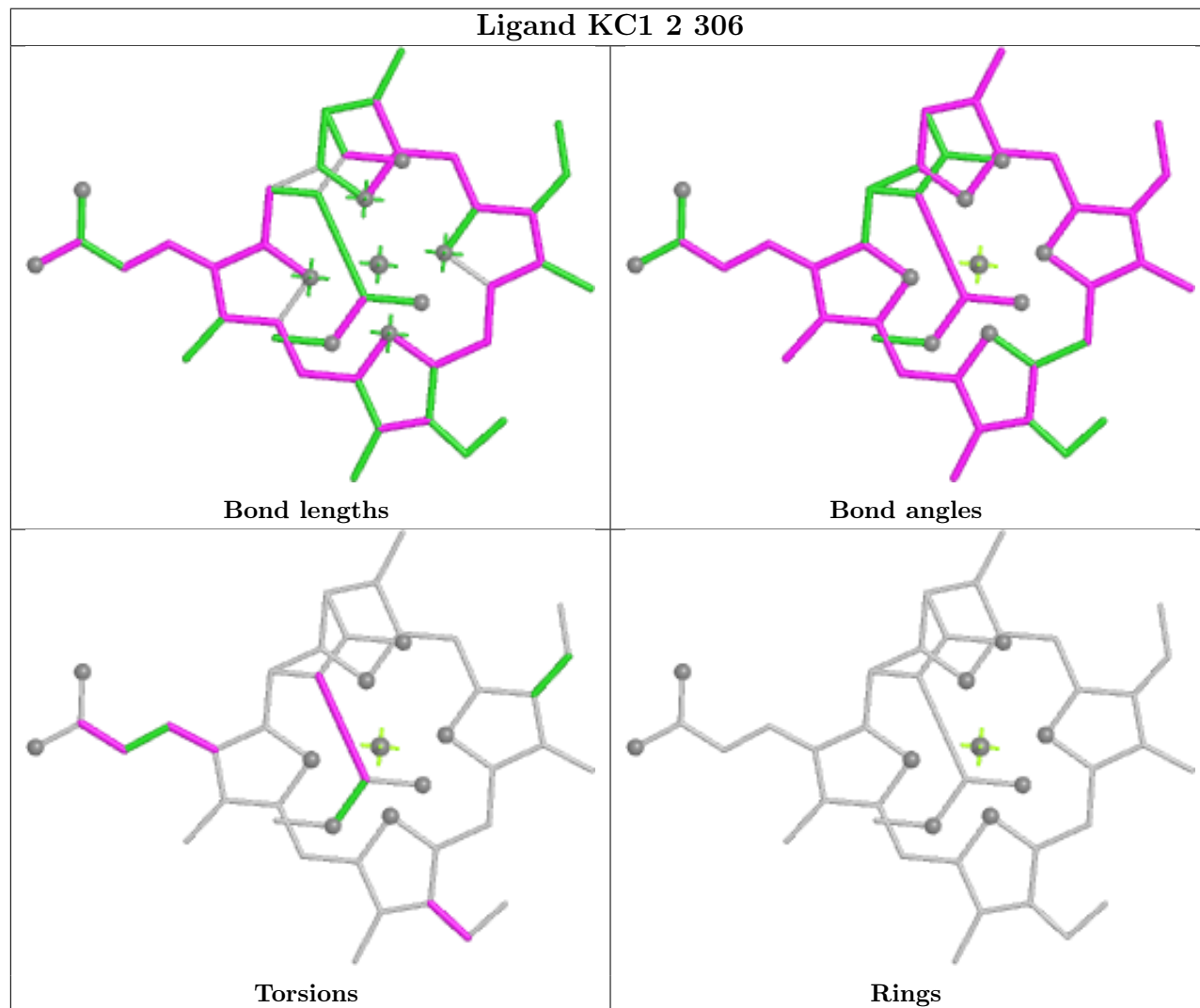




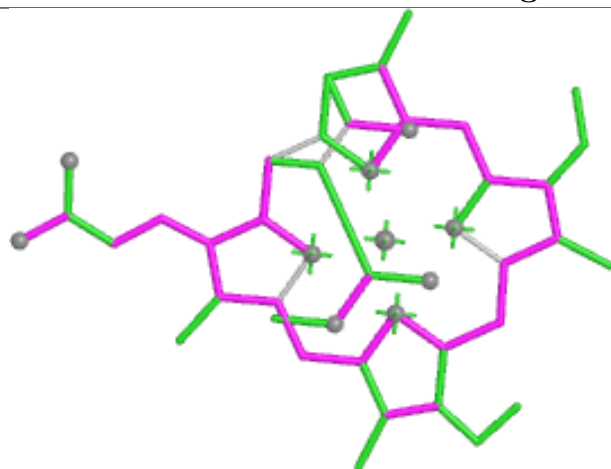
Ligand DD6 3 312



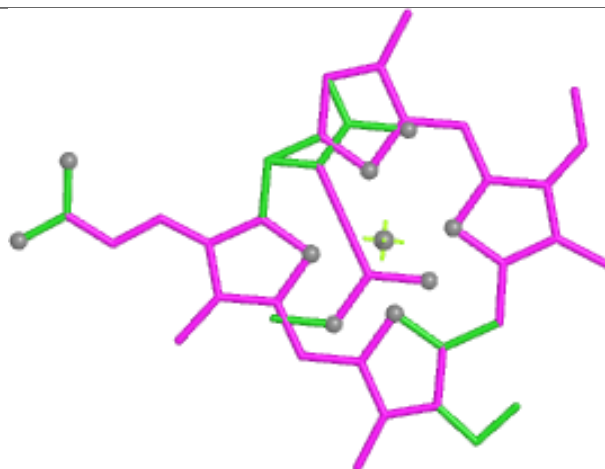
Ligand KC1 2 306



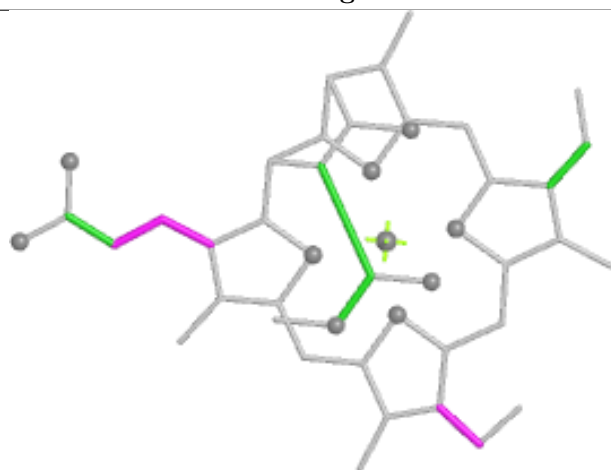
Ligand KC1 4 310



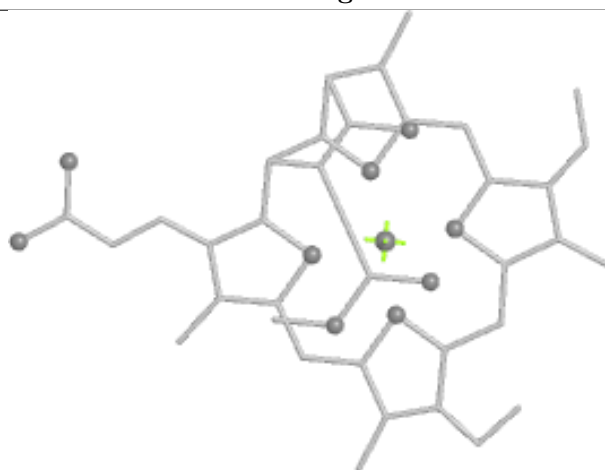
Bond lengths



Bond angles

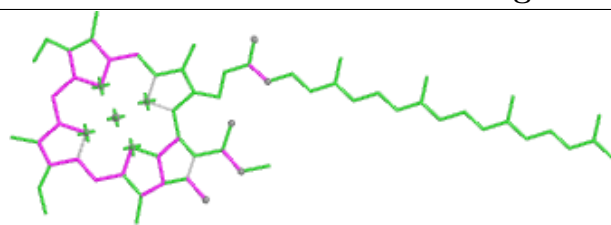


Torsions

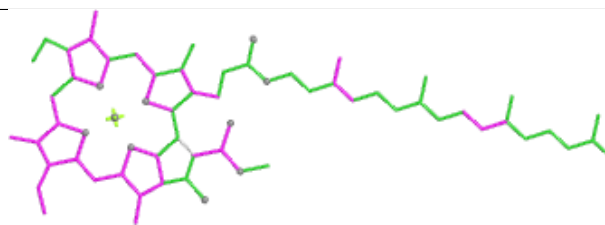


Rings

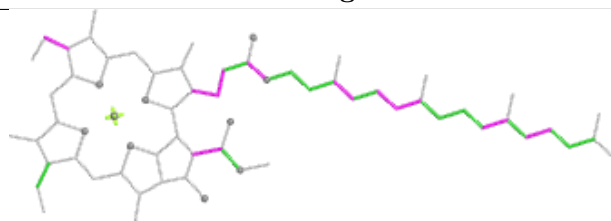
Ligand CLA A 812



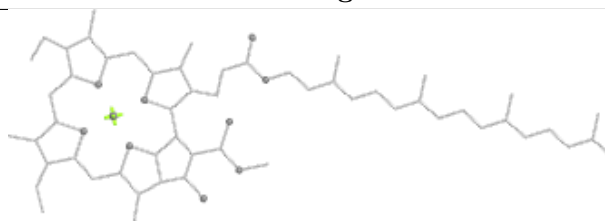
Bond lengths



Bond angles

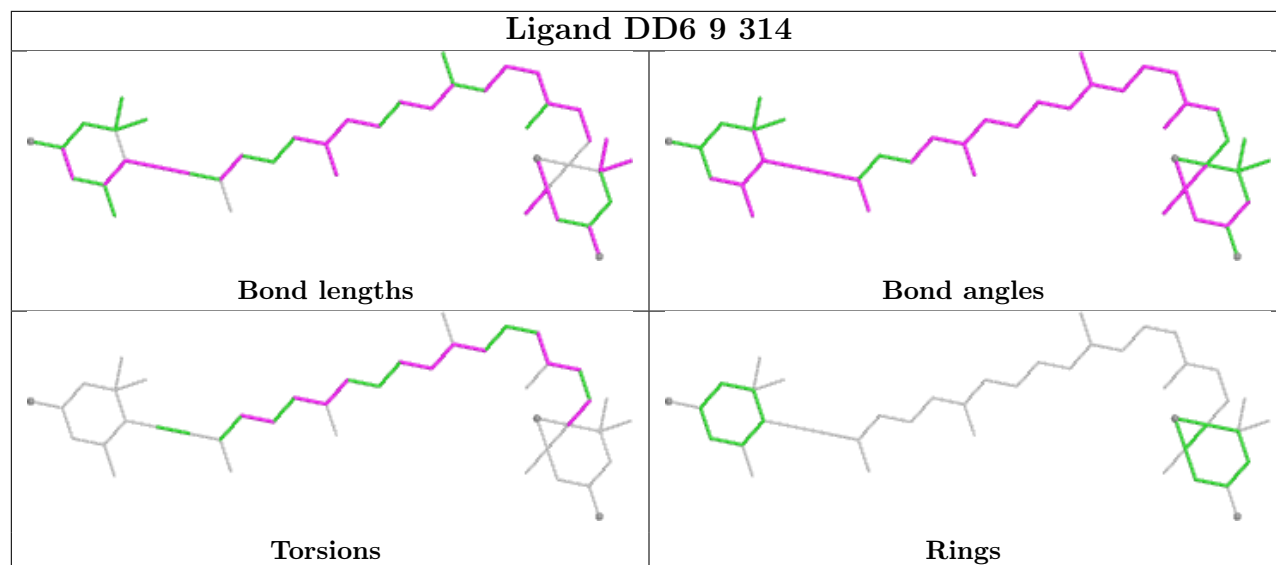


Torsions

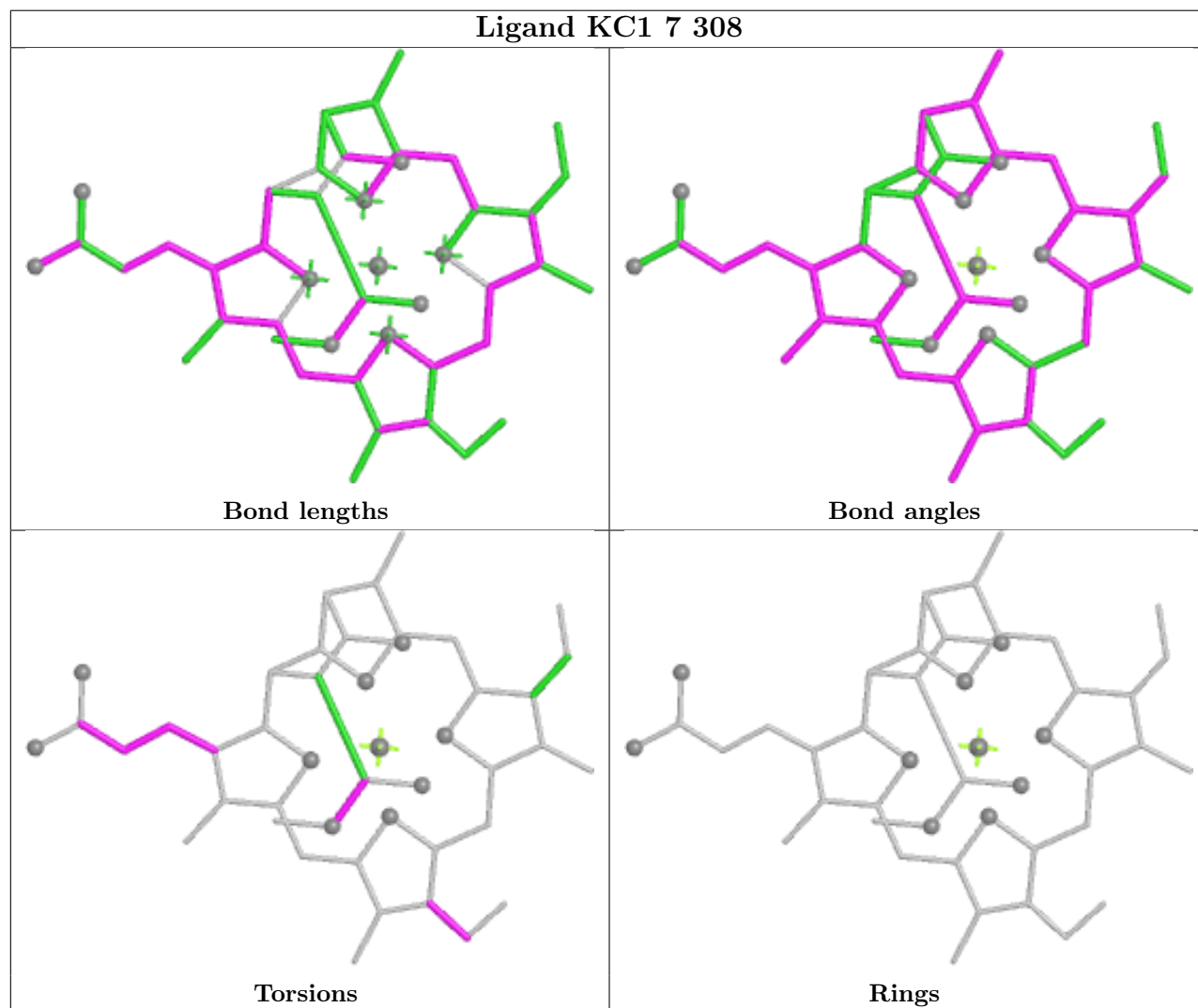


Rings

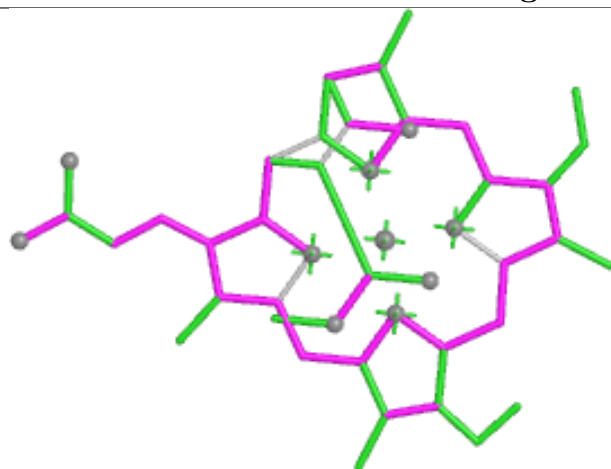
Ligand DD6 9 314



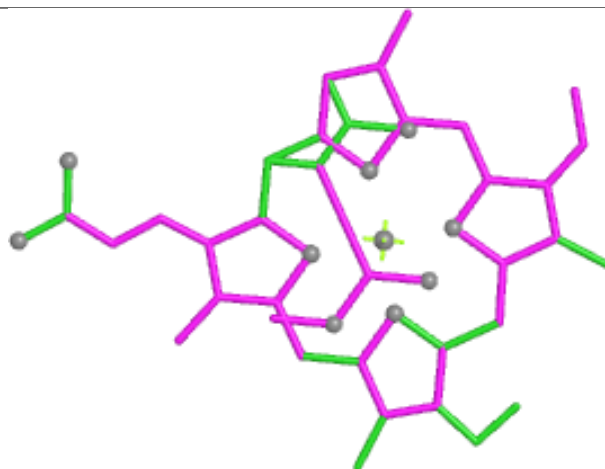
Ligand KC1 7 308



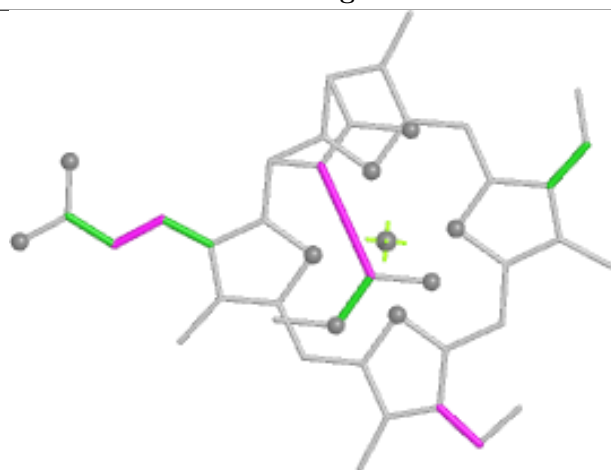
Ligand KC1 1 308



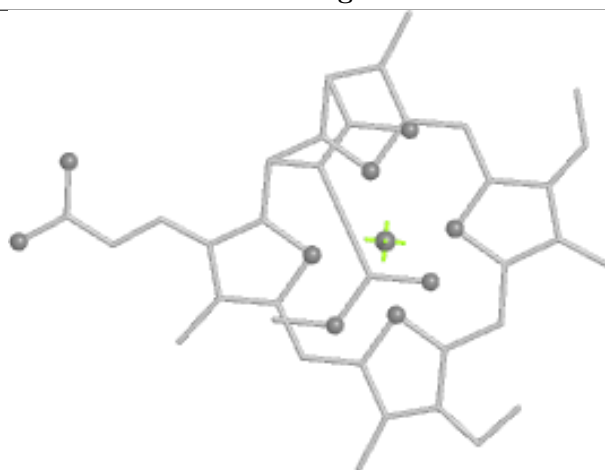
Bond lengths



Bond angles

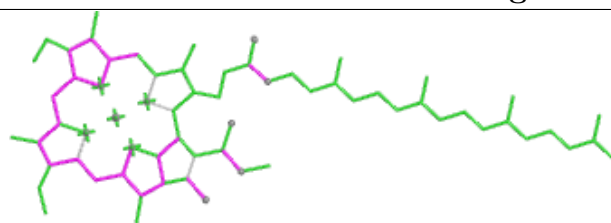


Torsions

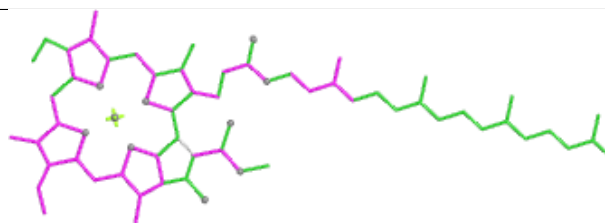


Rings

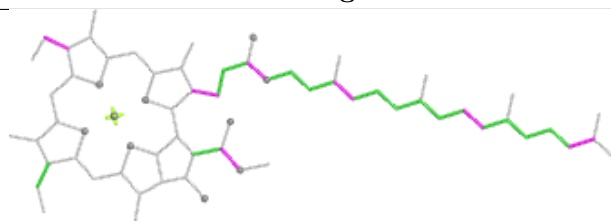
Ligand CLA 15 309



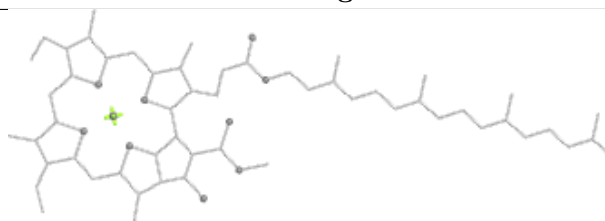
Bond lengths



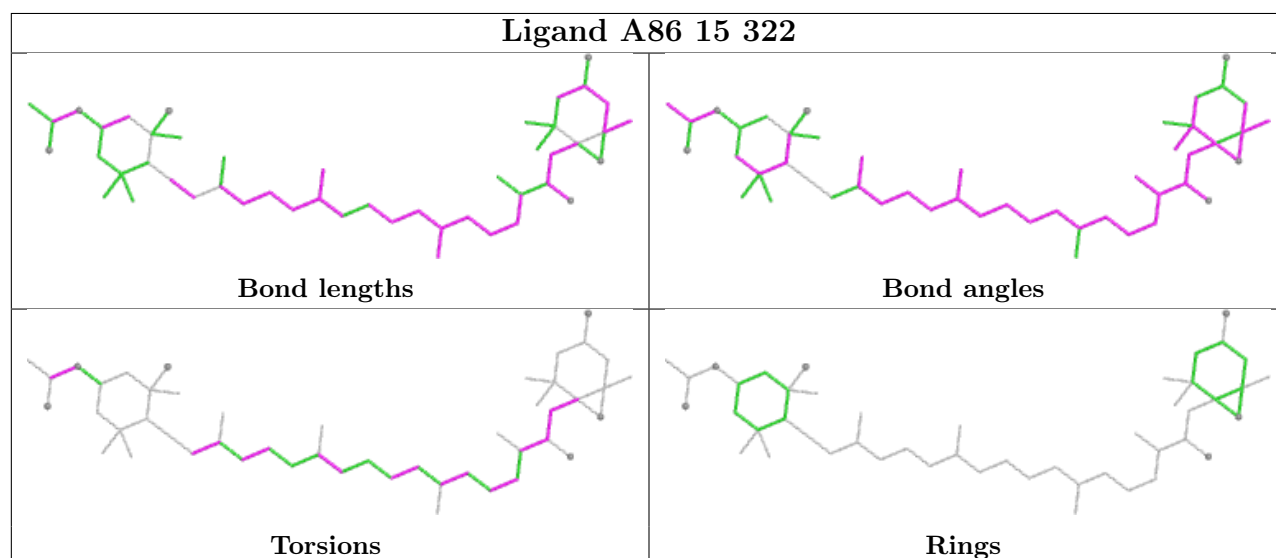
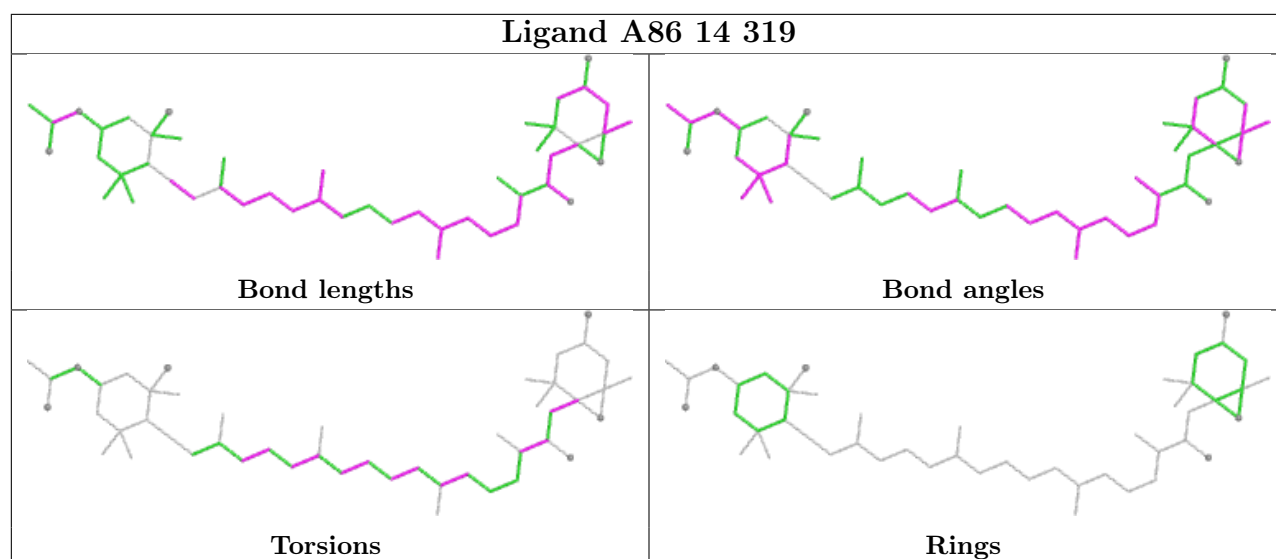
Bond angles



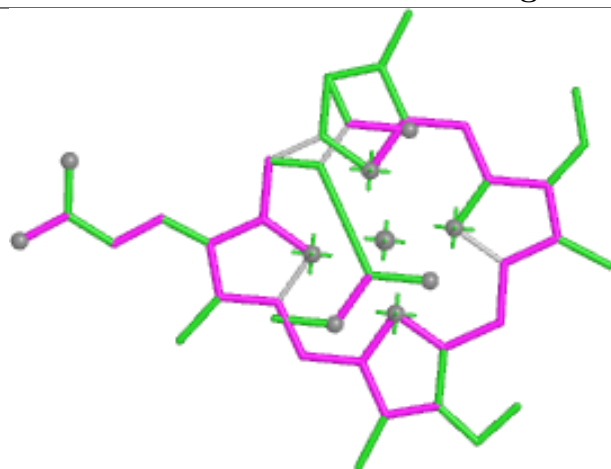
Torsions



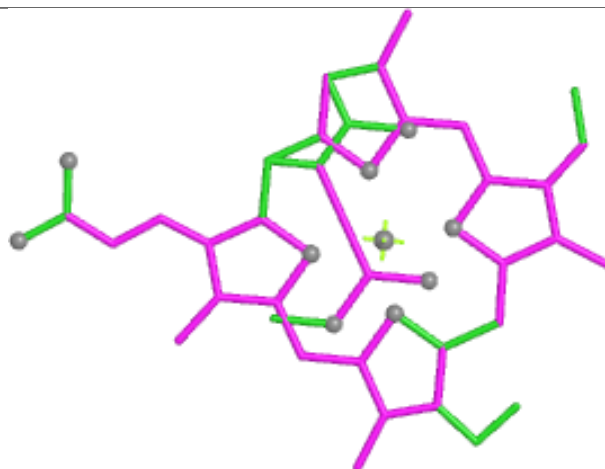
Rings



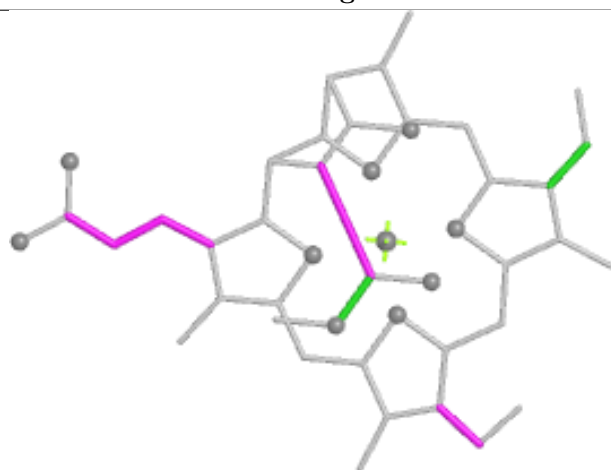
Ligand KC1 3 308



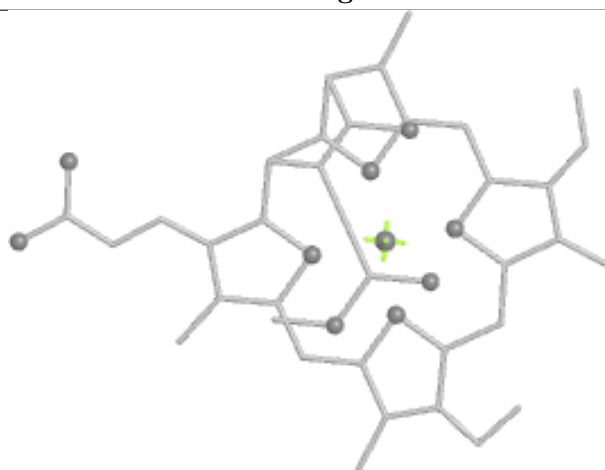
Bond lengths



Bond angles

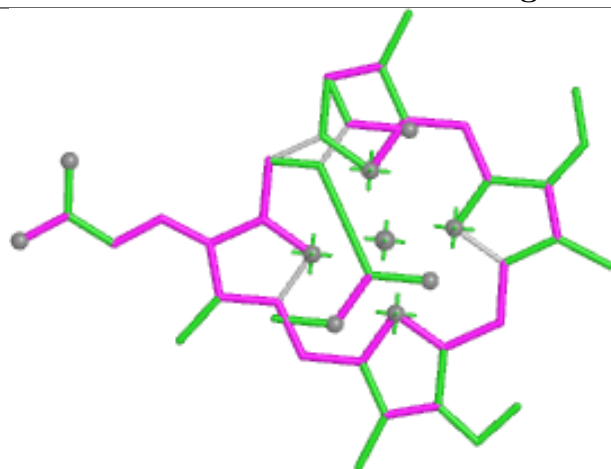


Torsions

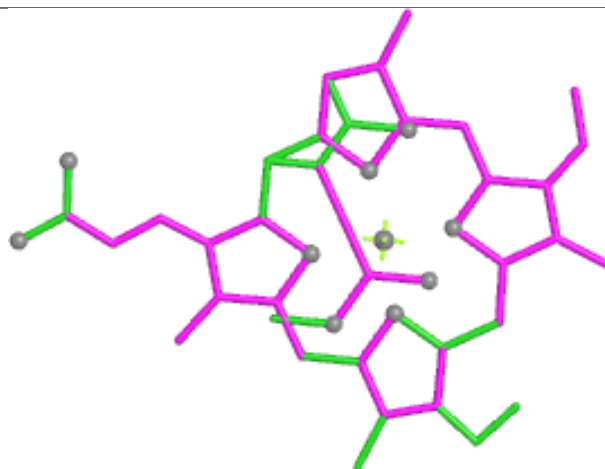


Rings

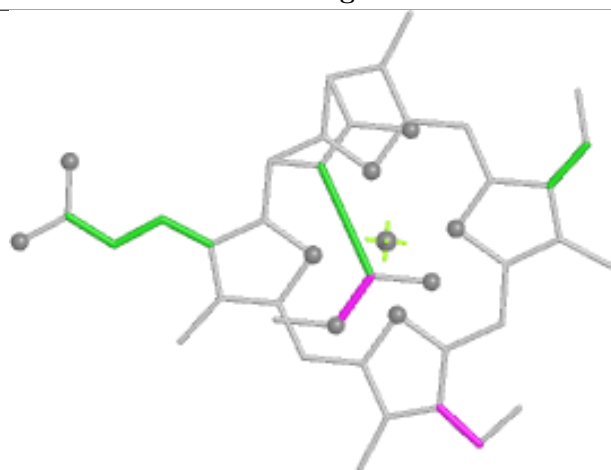
Ligand KC1 5 312



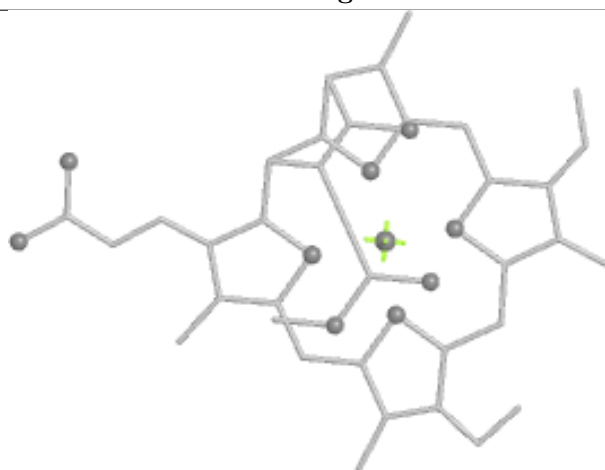
Bond lengths



Bond angles



Torsions

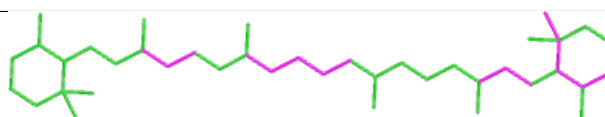


Rings

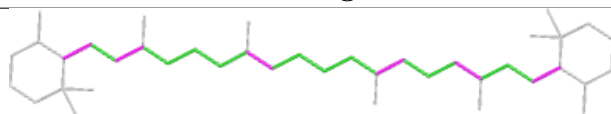
Ligand BCR B 843



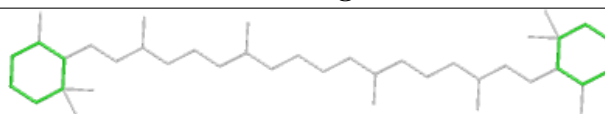
Bond lengths



Bond angles

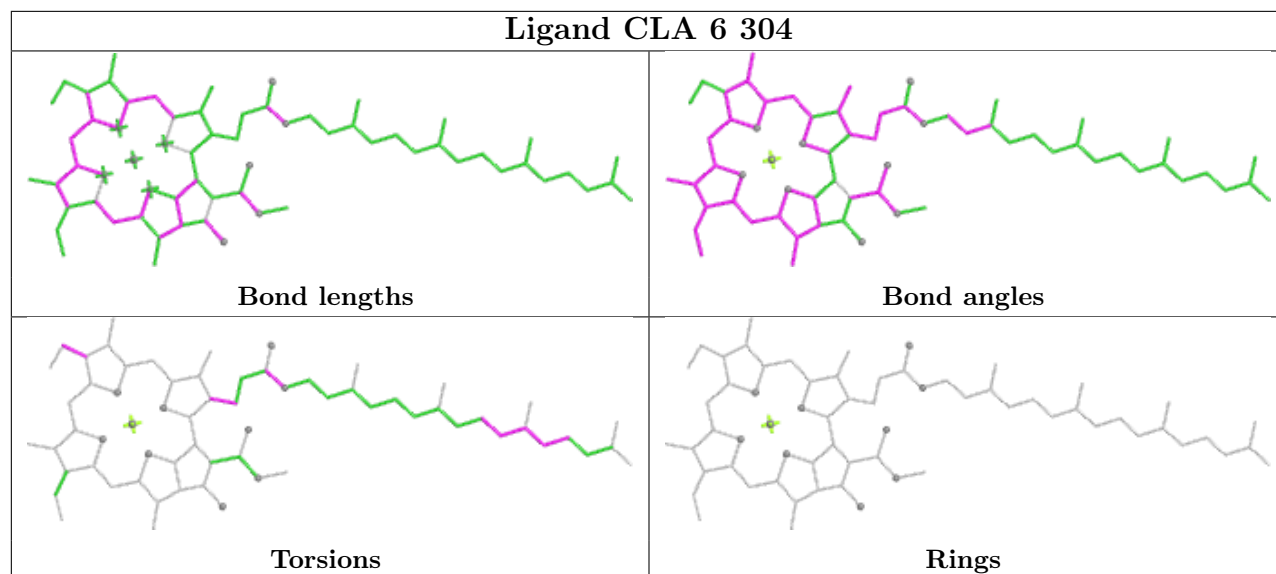


Torsions

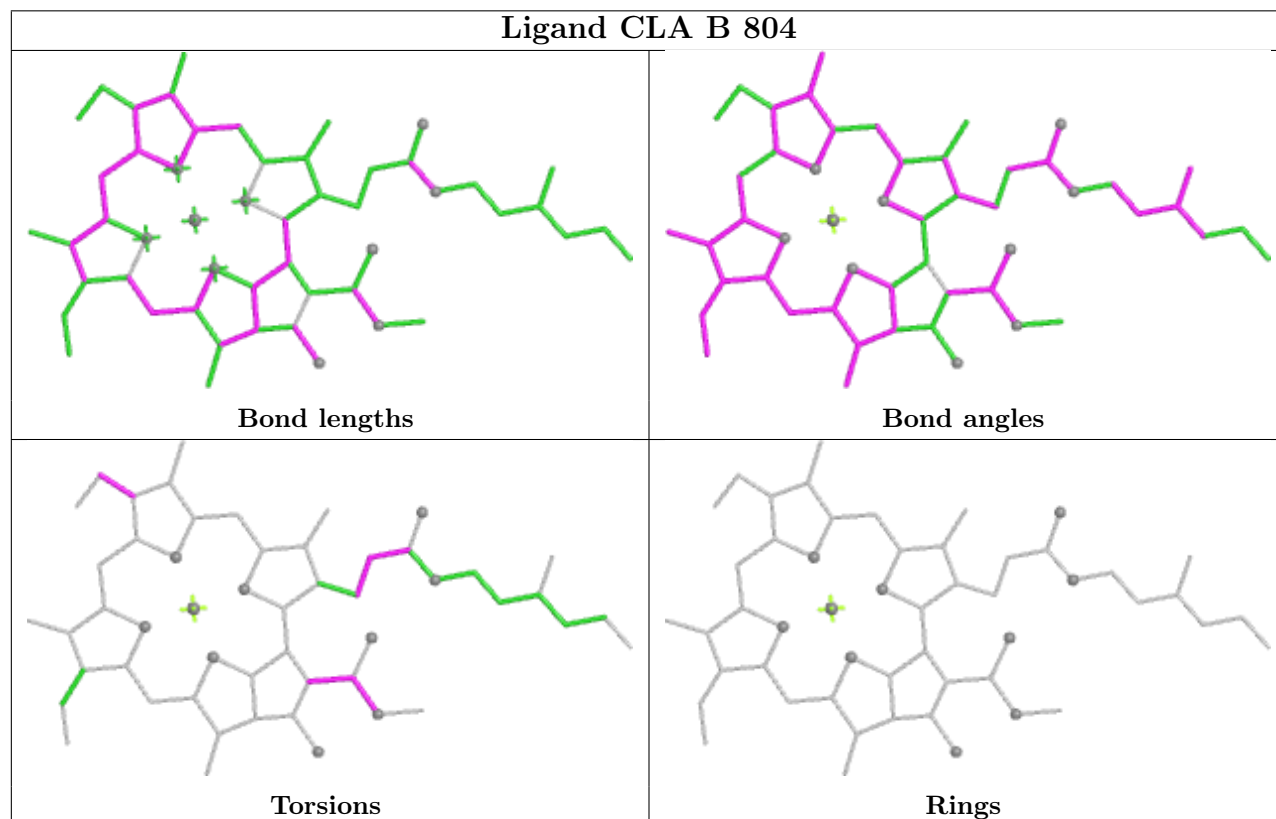


Rings

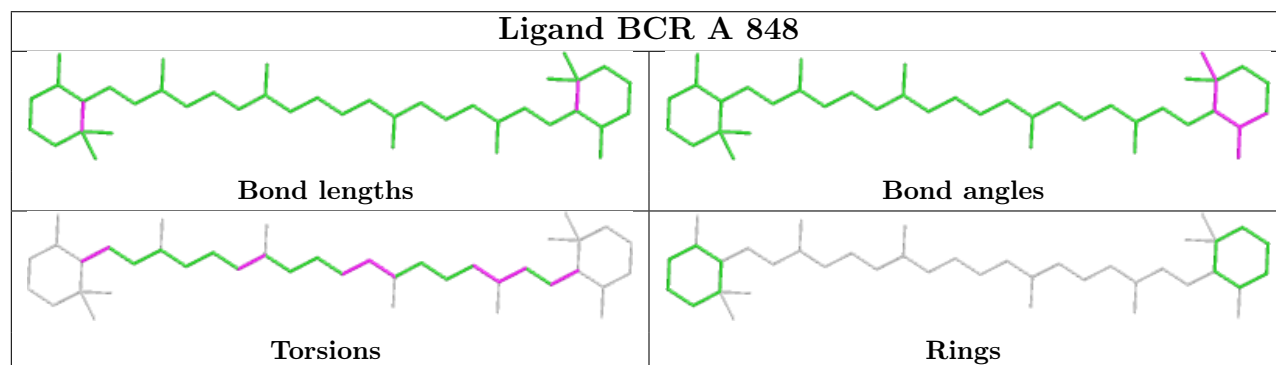
Ligand CLA 6 304

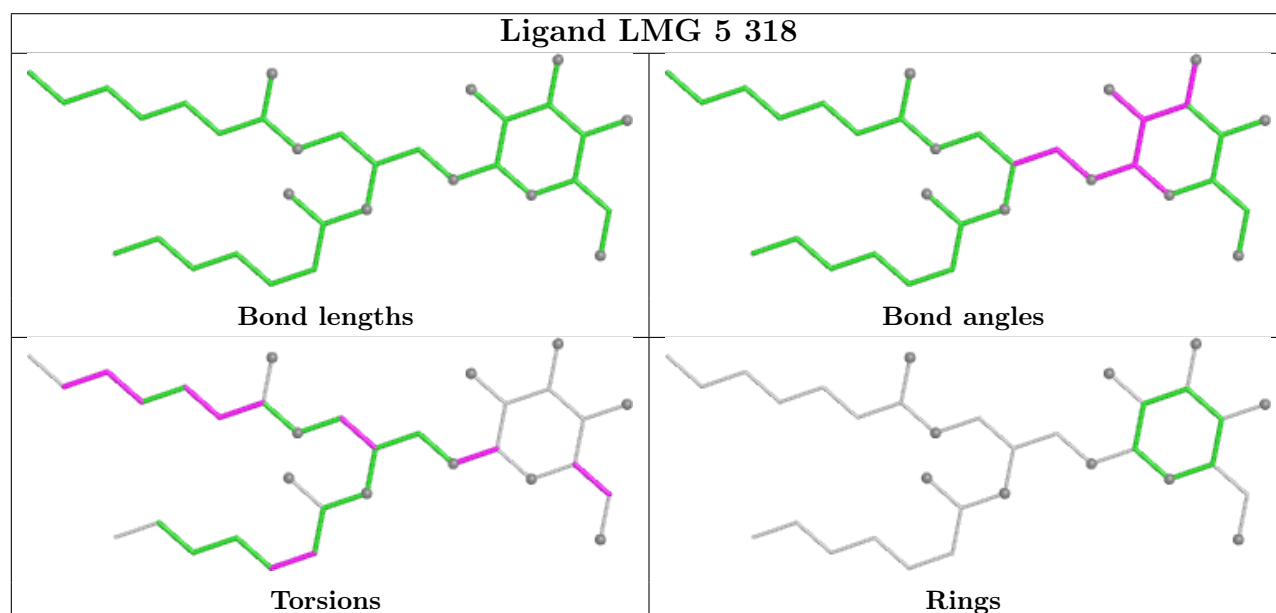
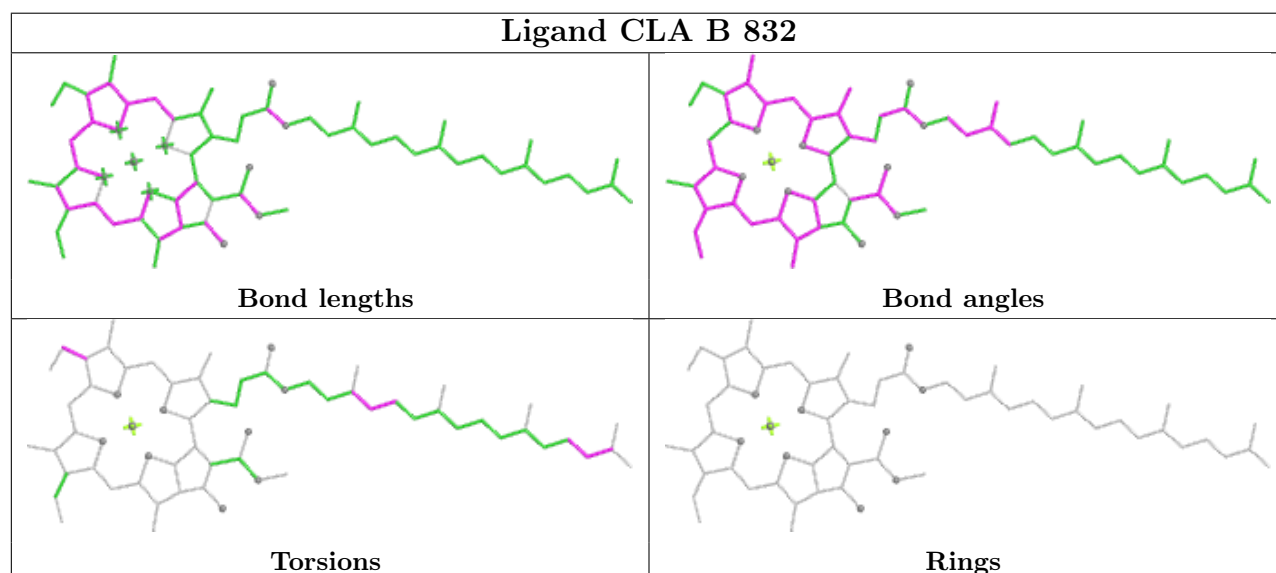
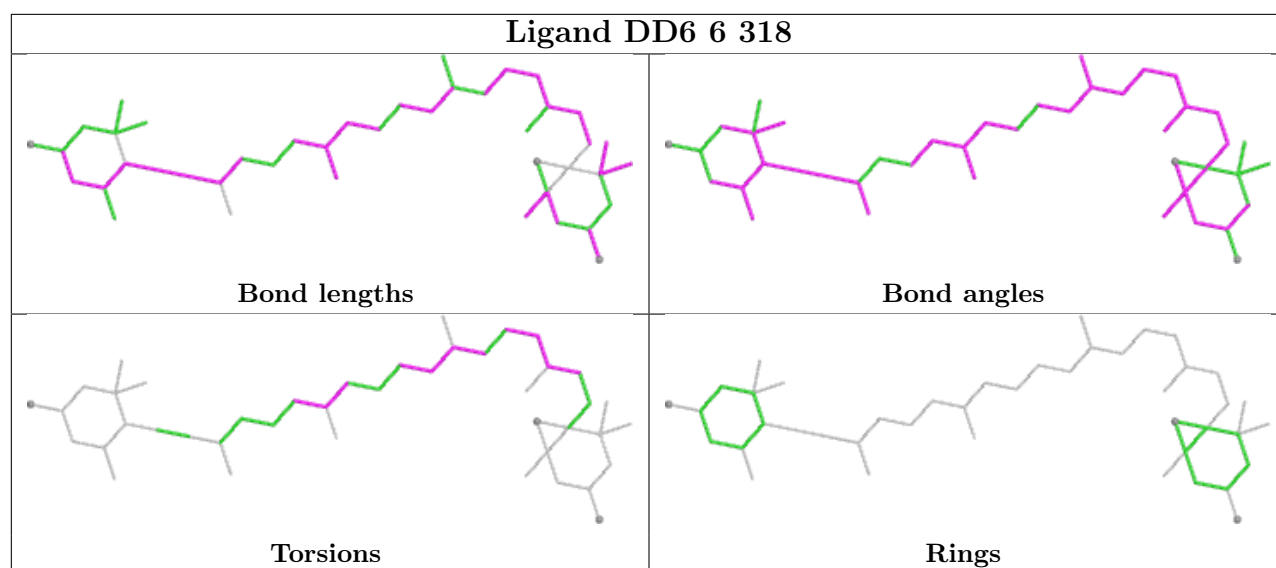


Ligand CLA B 804

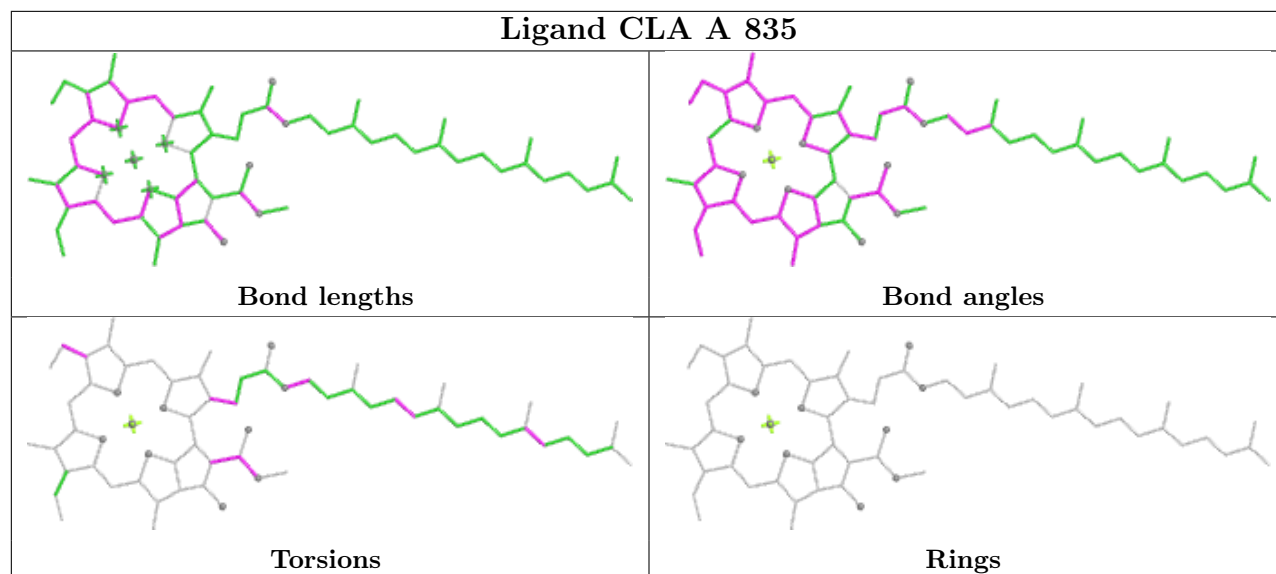


Ligand BCR A 848

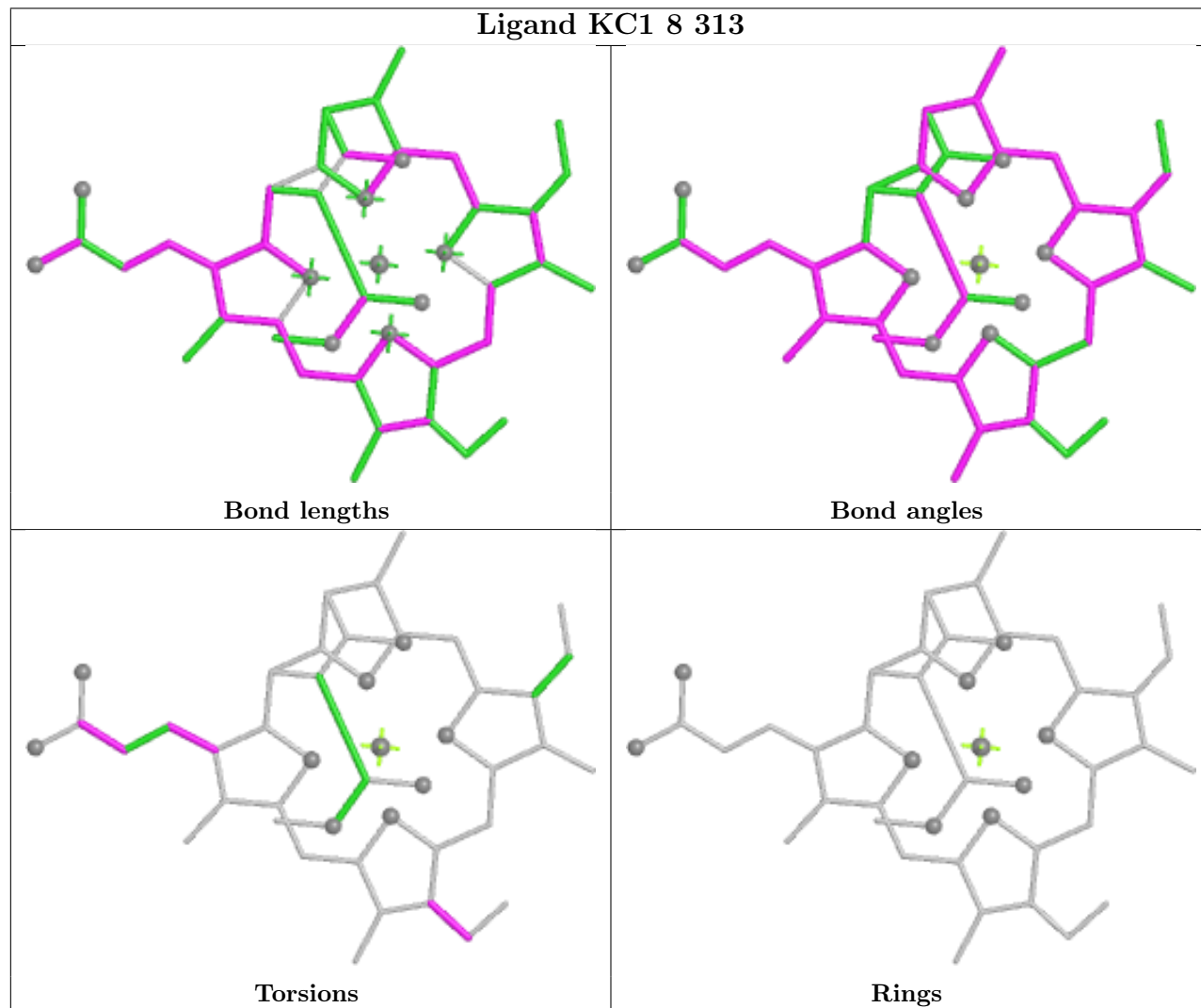




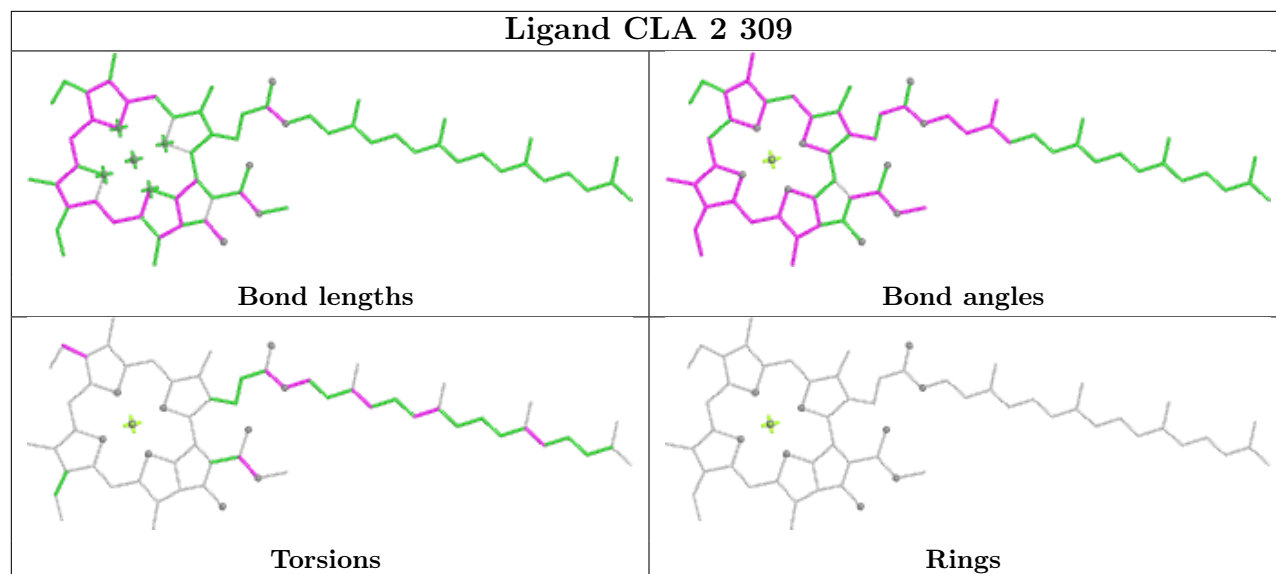
Ligand CLA A 835



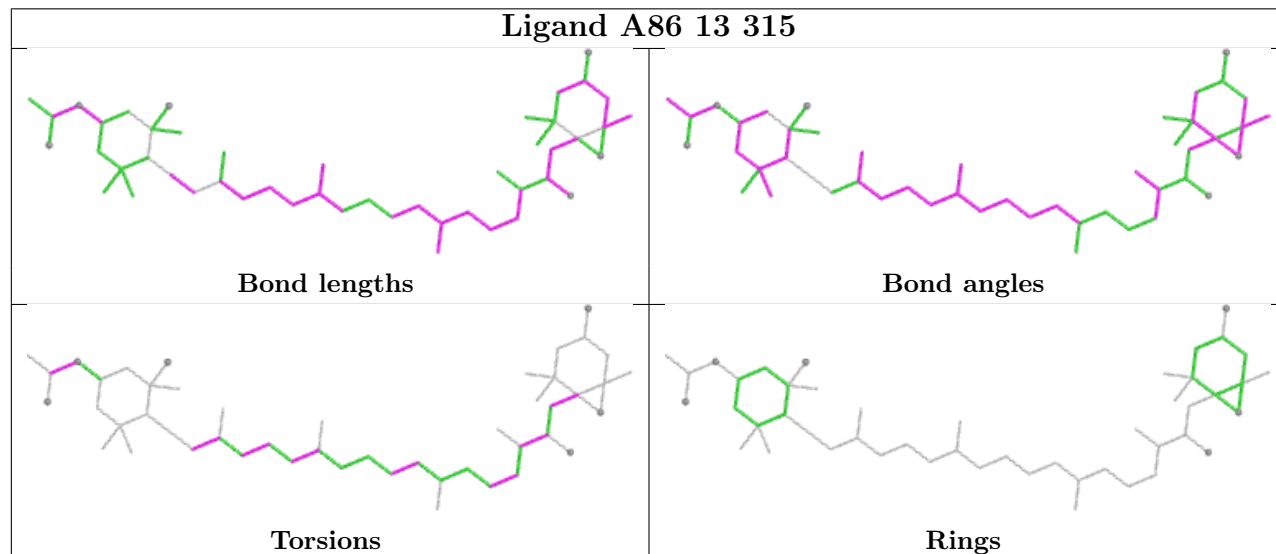
Ligand KC1 8 313



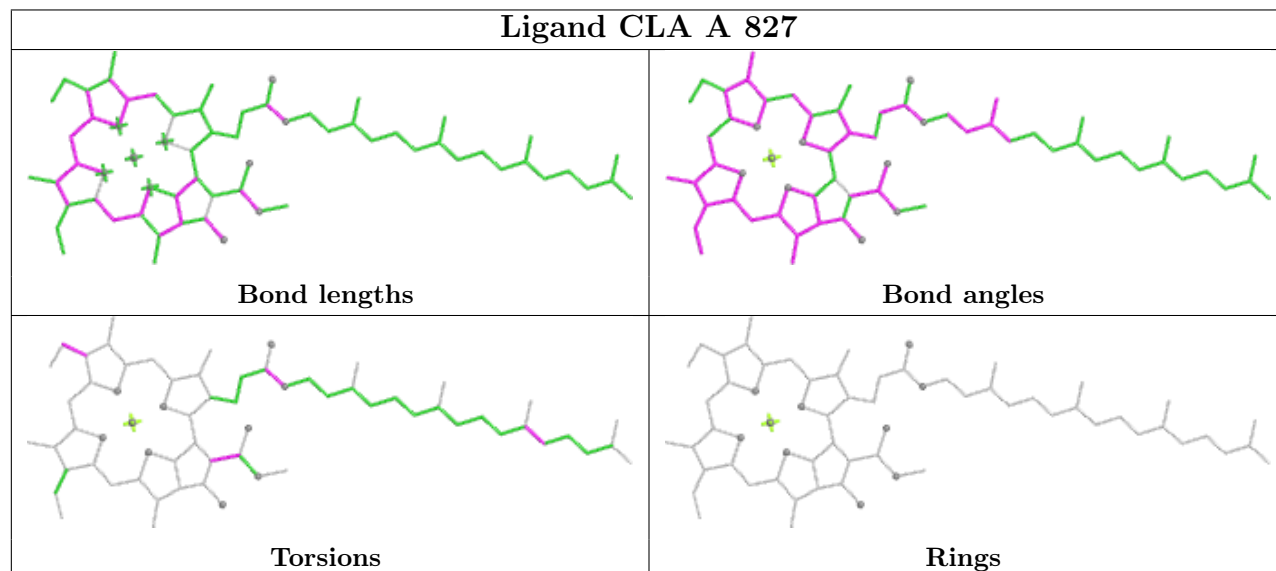
Ligand CLA 2 309

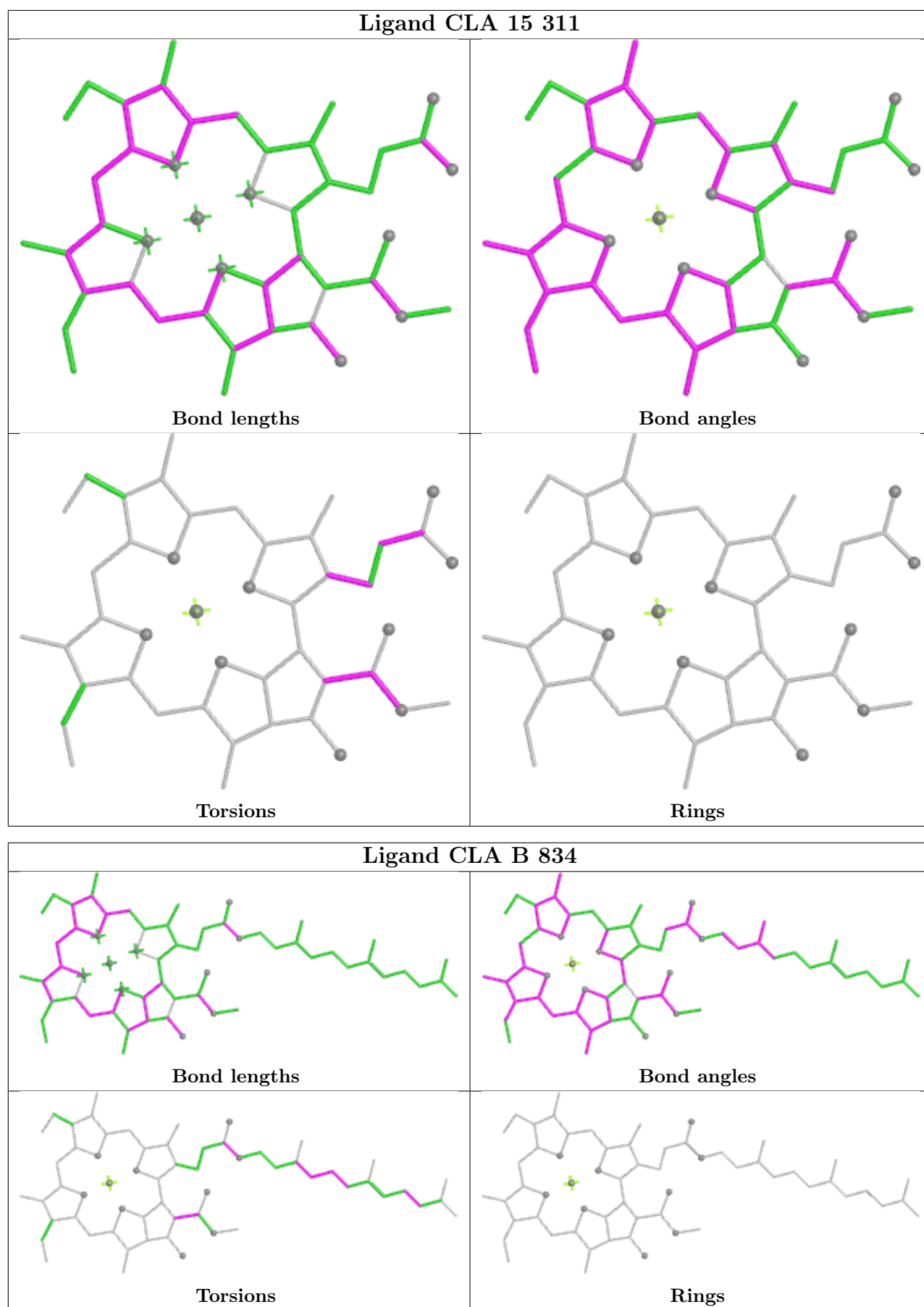


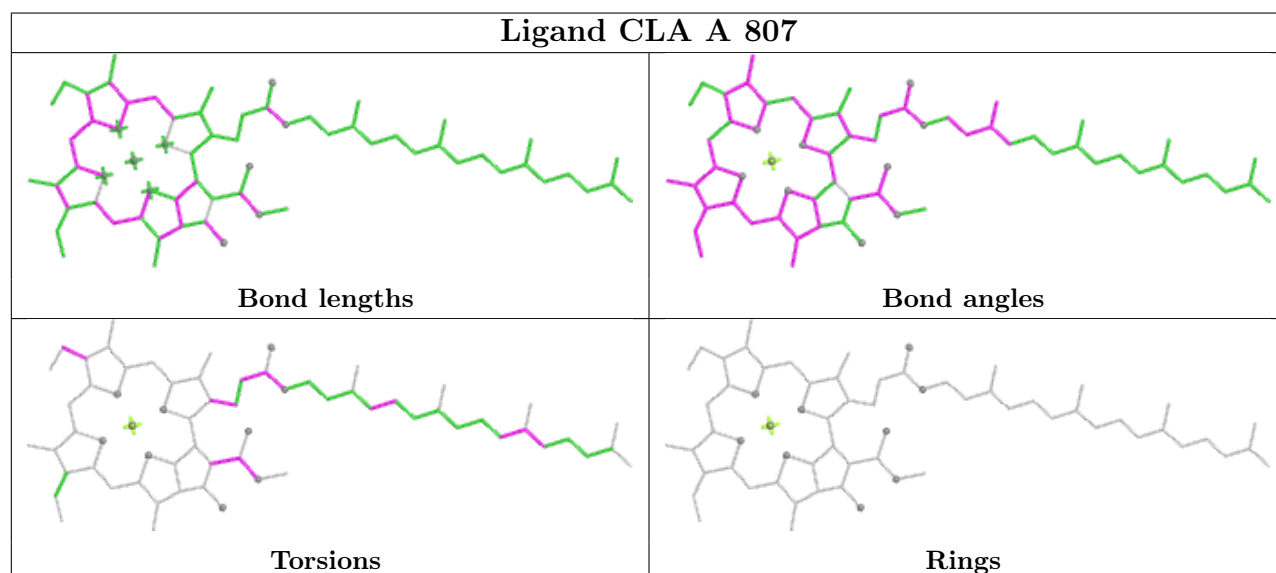
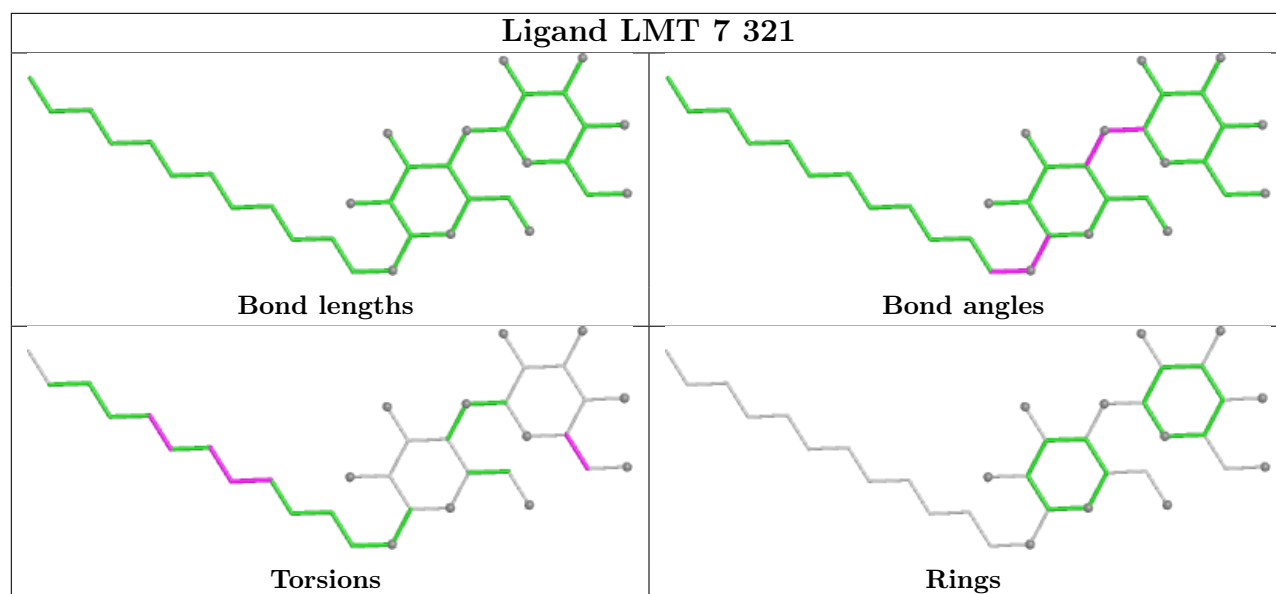
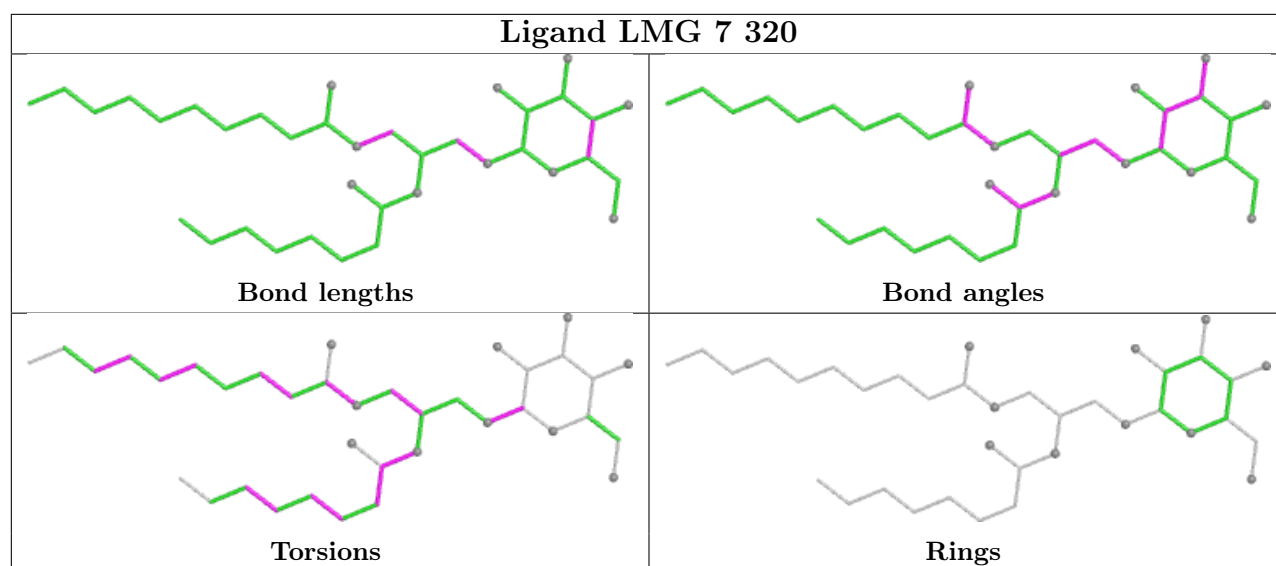
Ligand A86 13 315



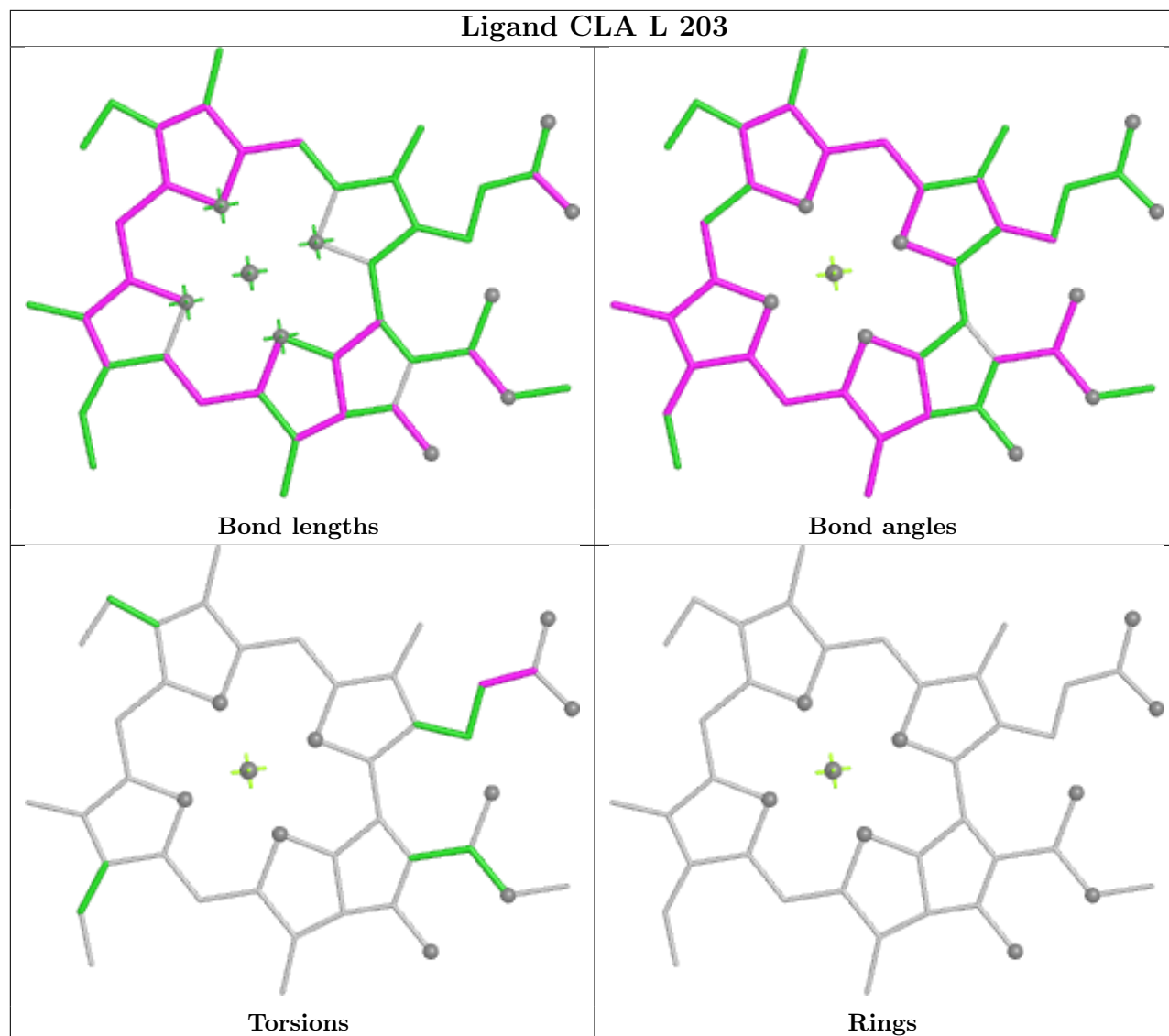
Ligand CLA A 827

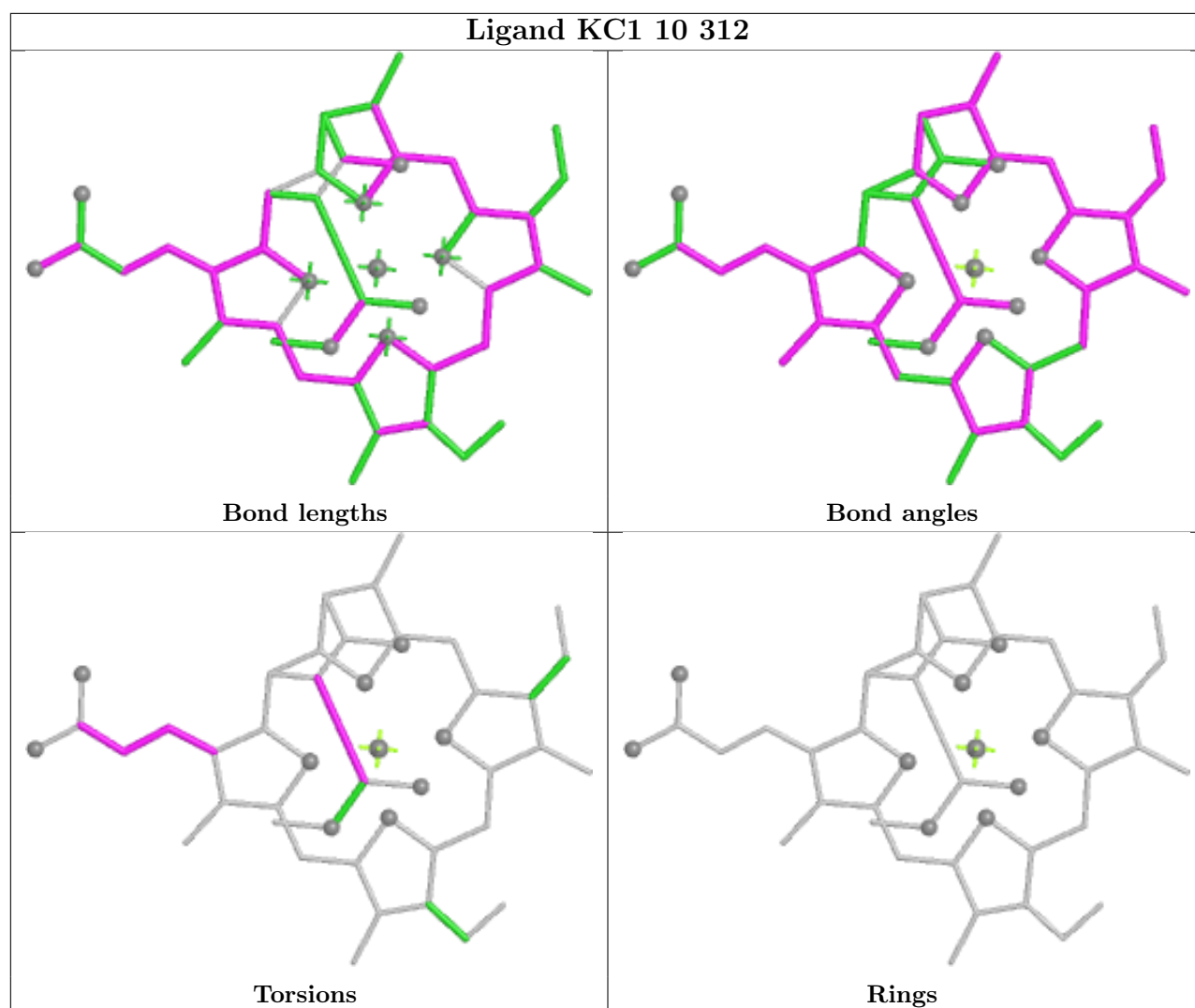


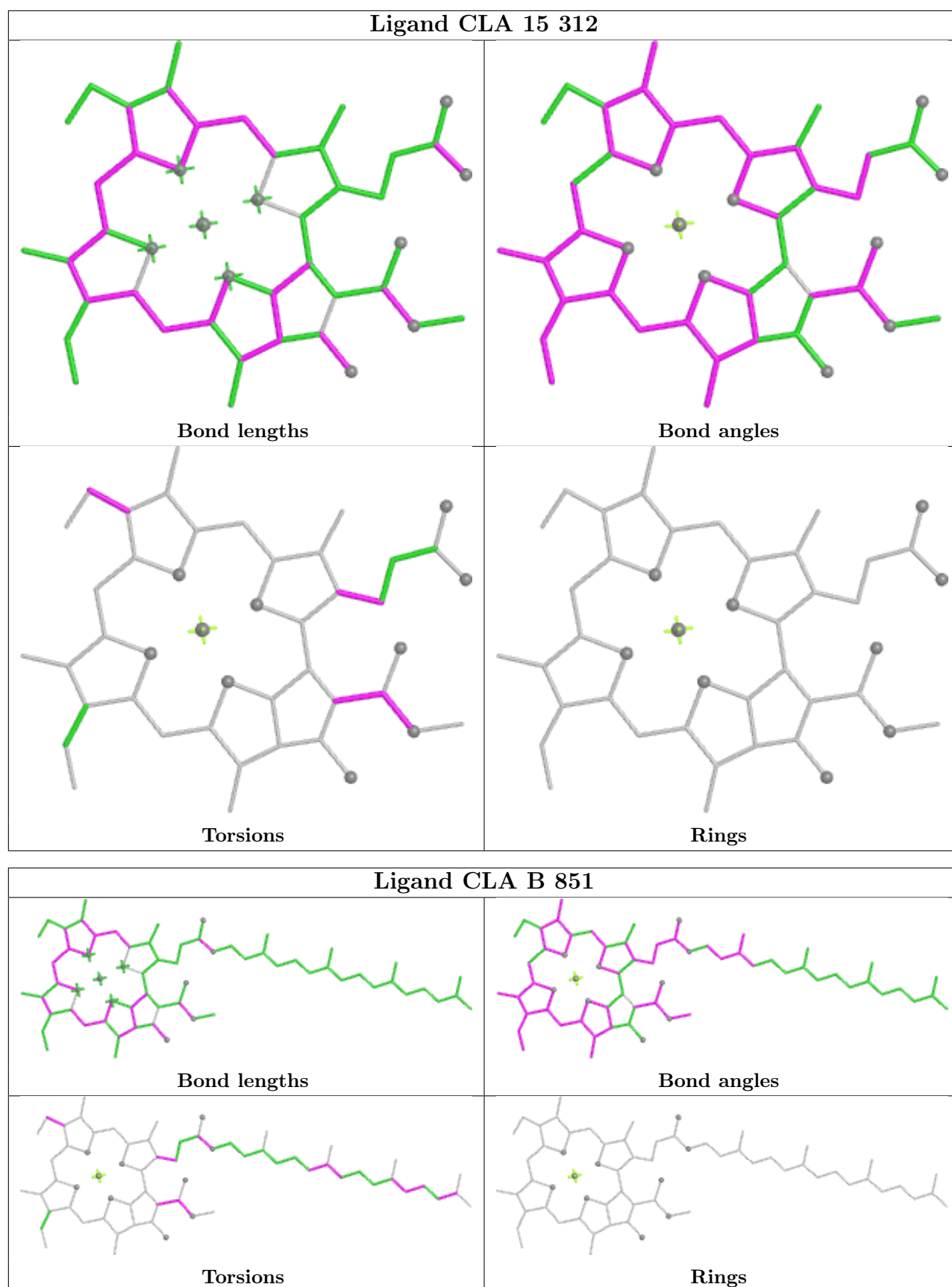


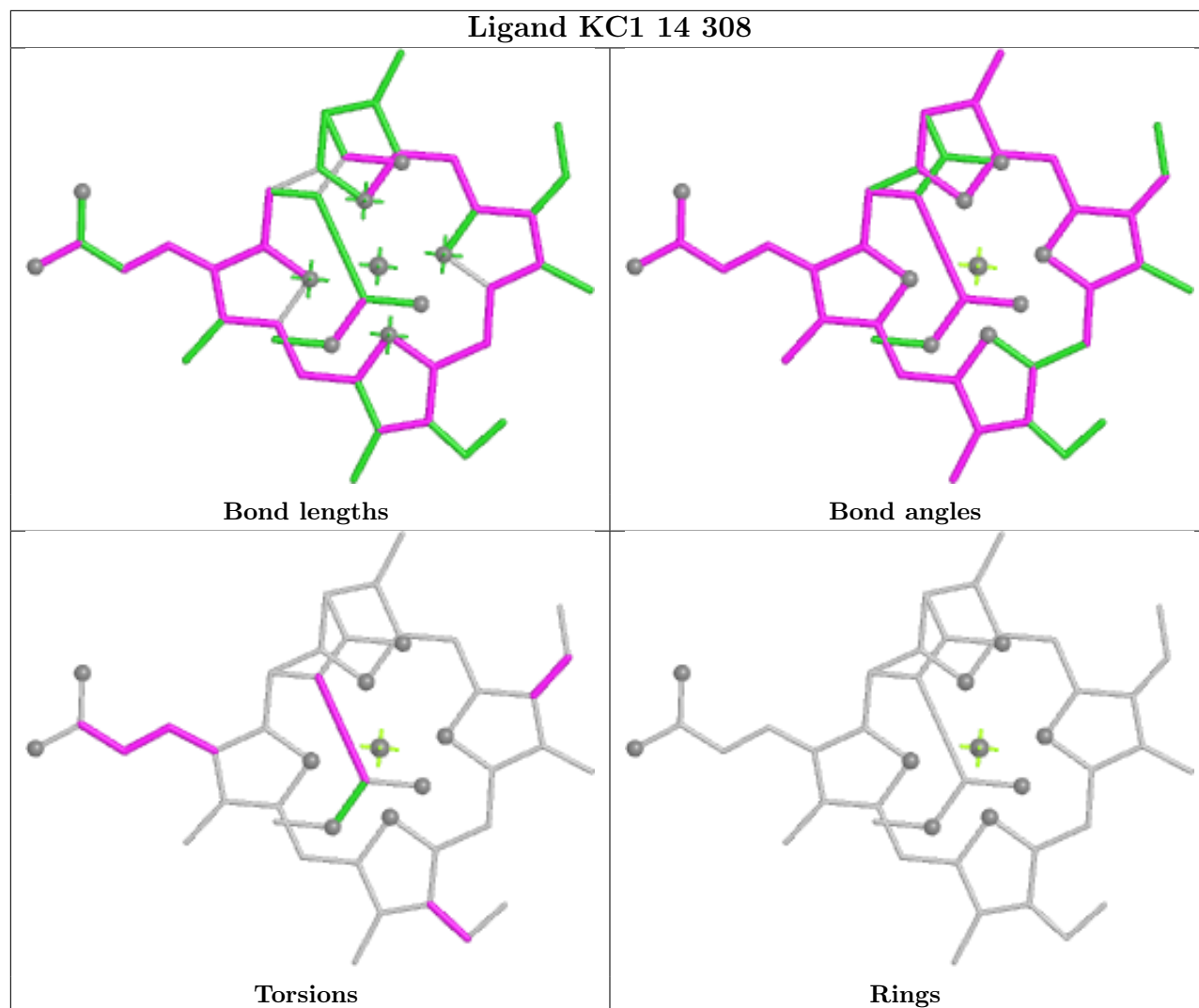


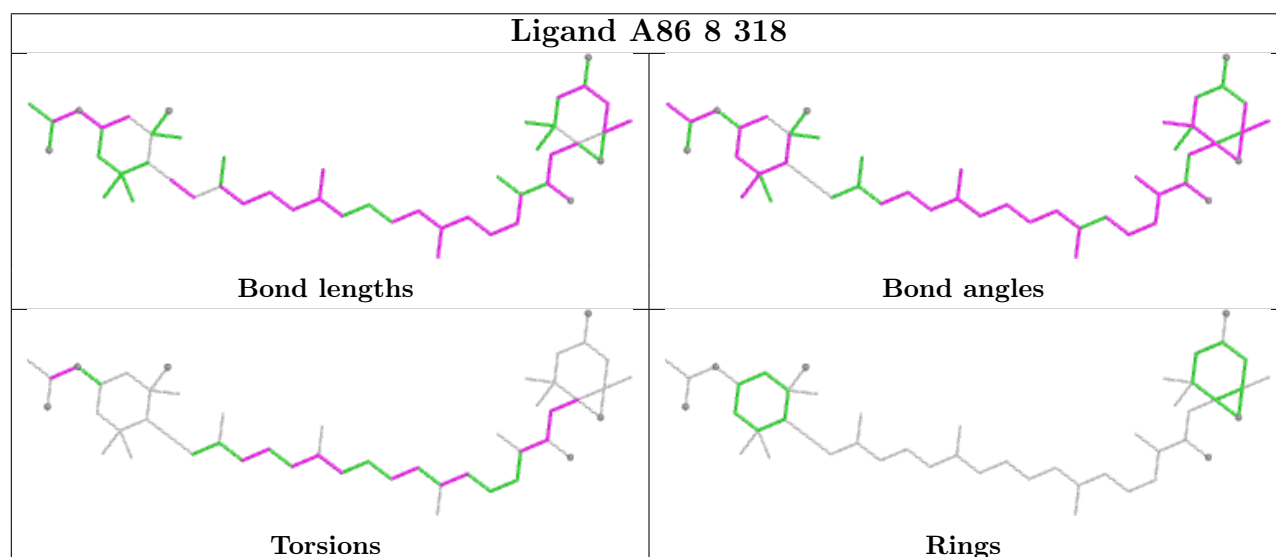
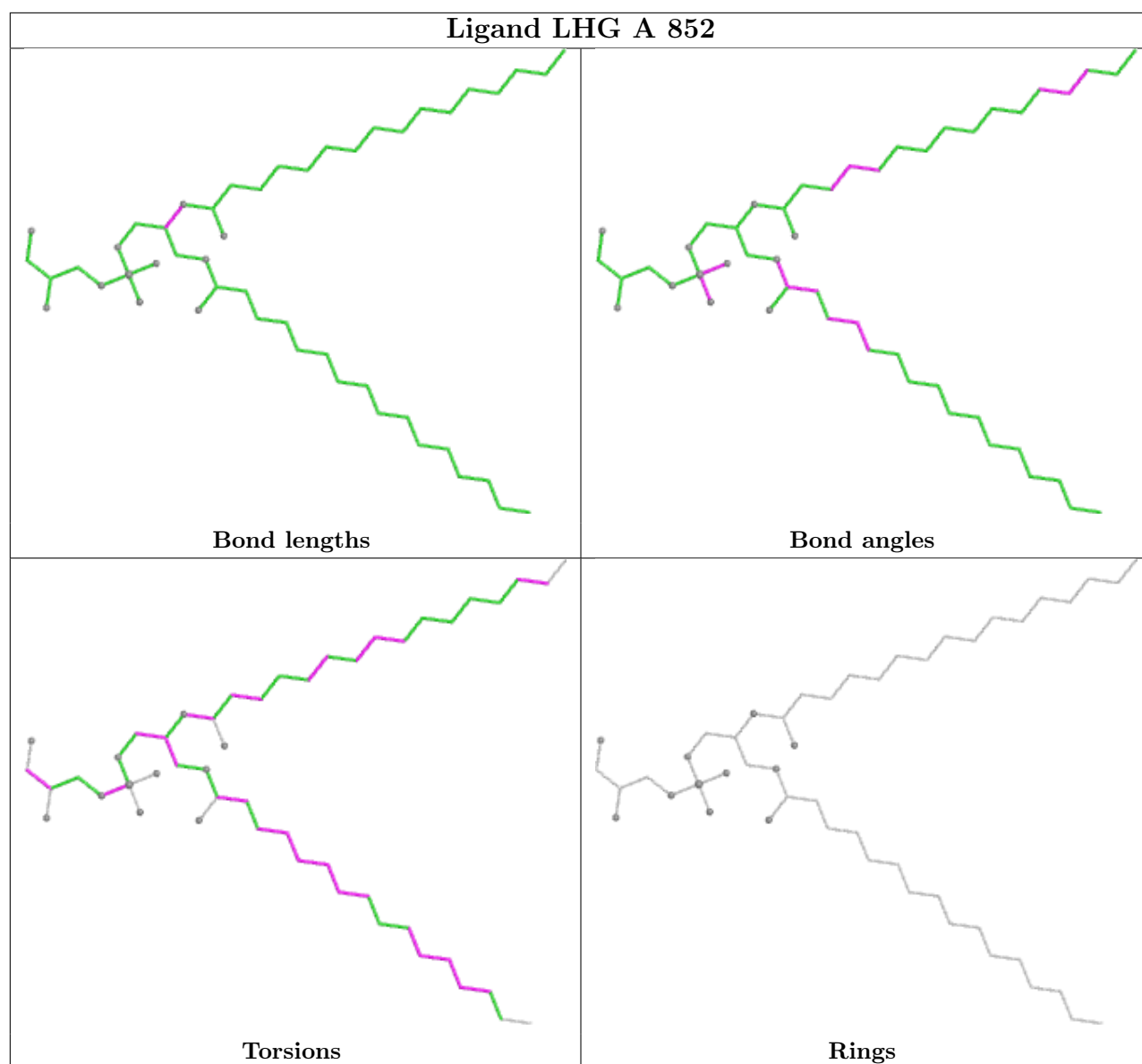
Ligand CLA L 203



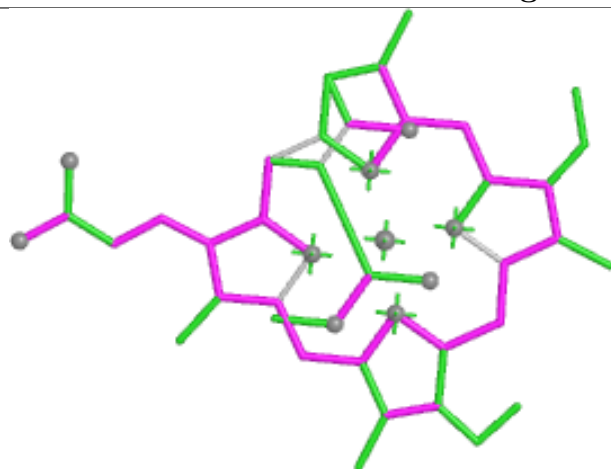




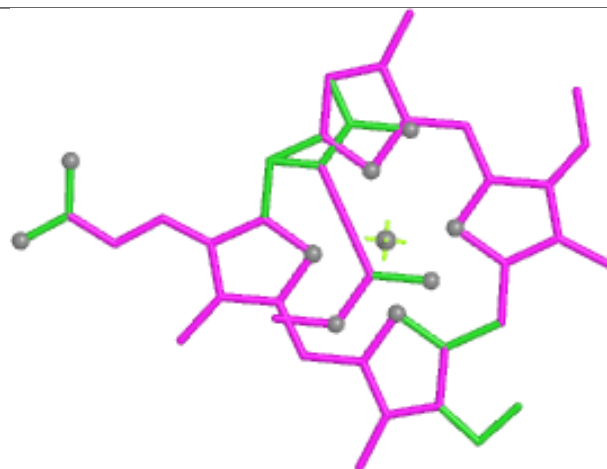




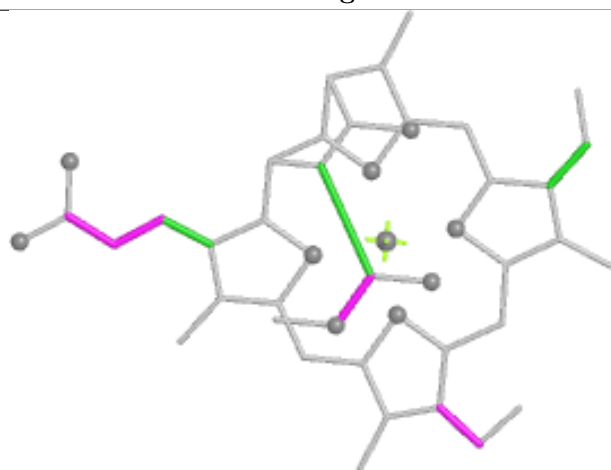
Ligand KC1 2 314



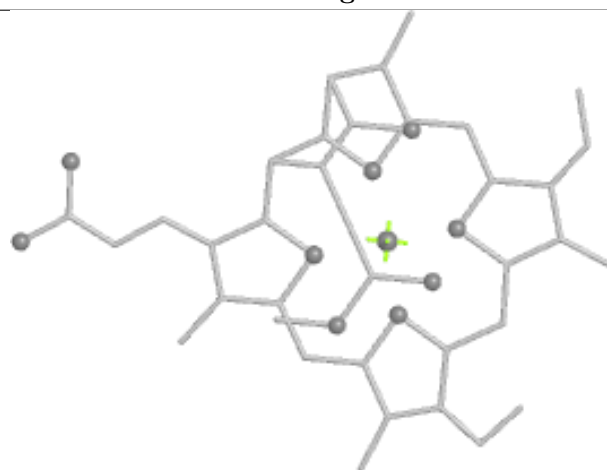
Bond lengths



Bond angles

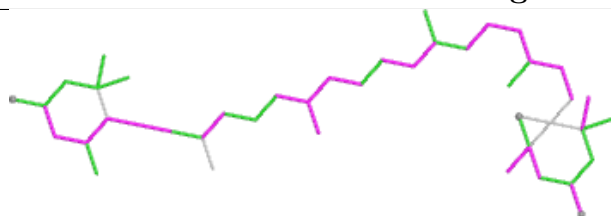


Torsions

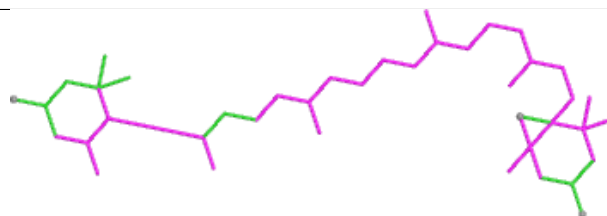


Rings

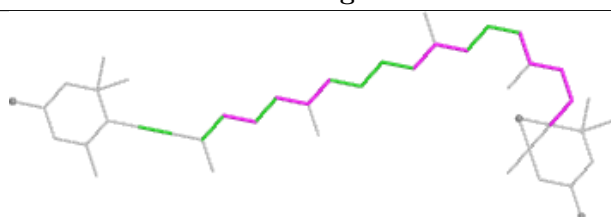
Ligand DD6 16 313



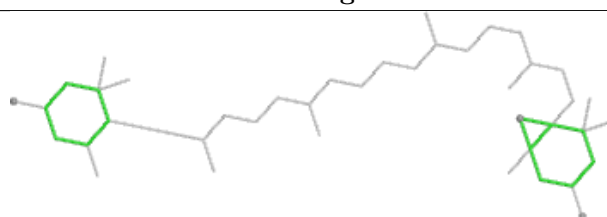
Bond lengths



Bond angles

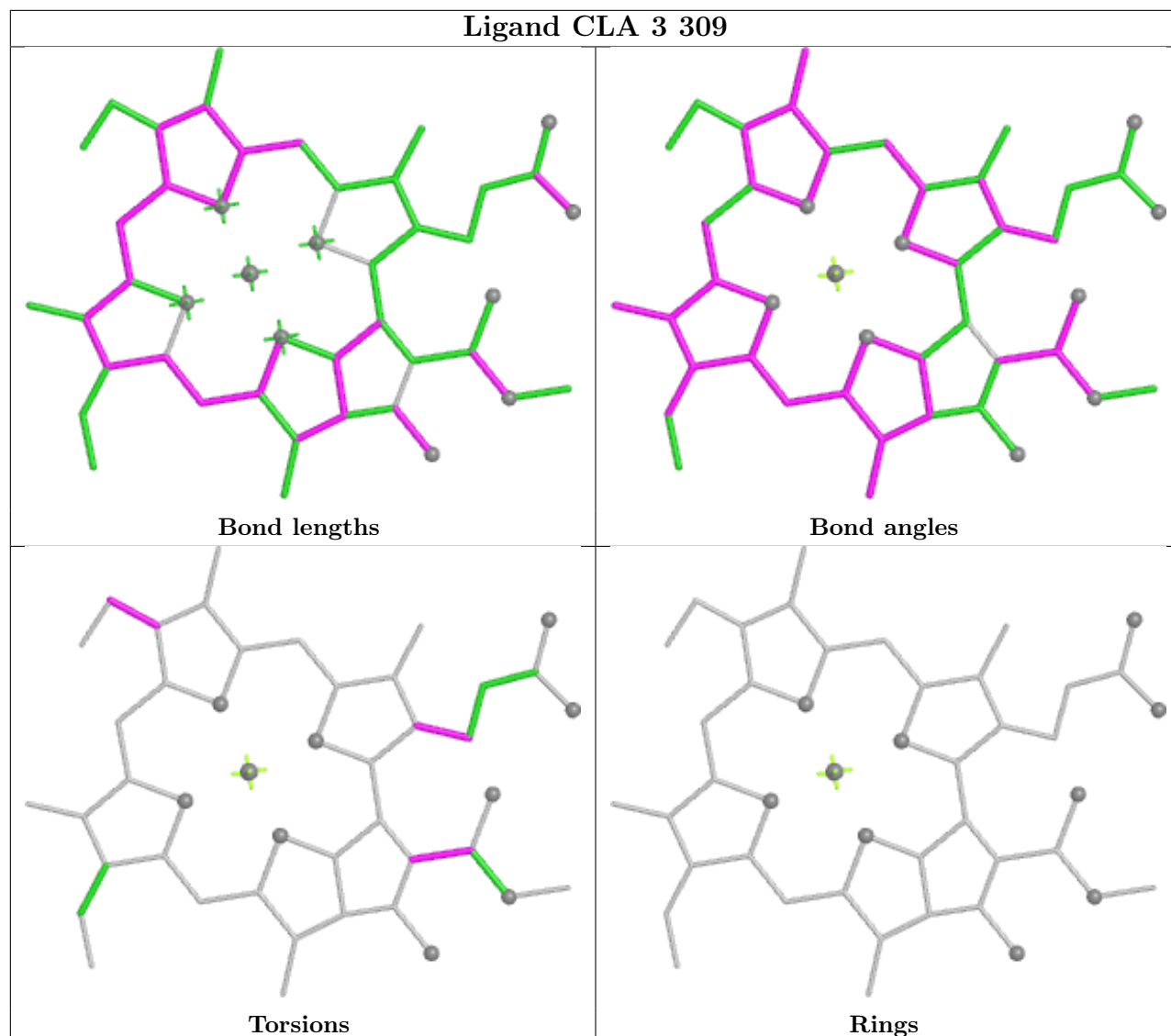


Torsions

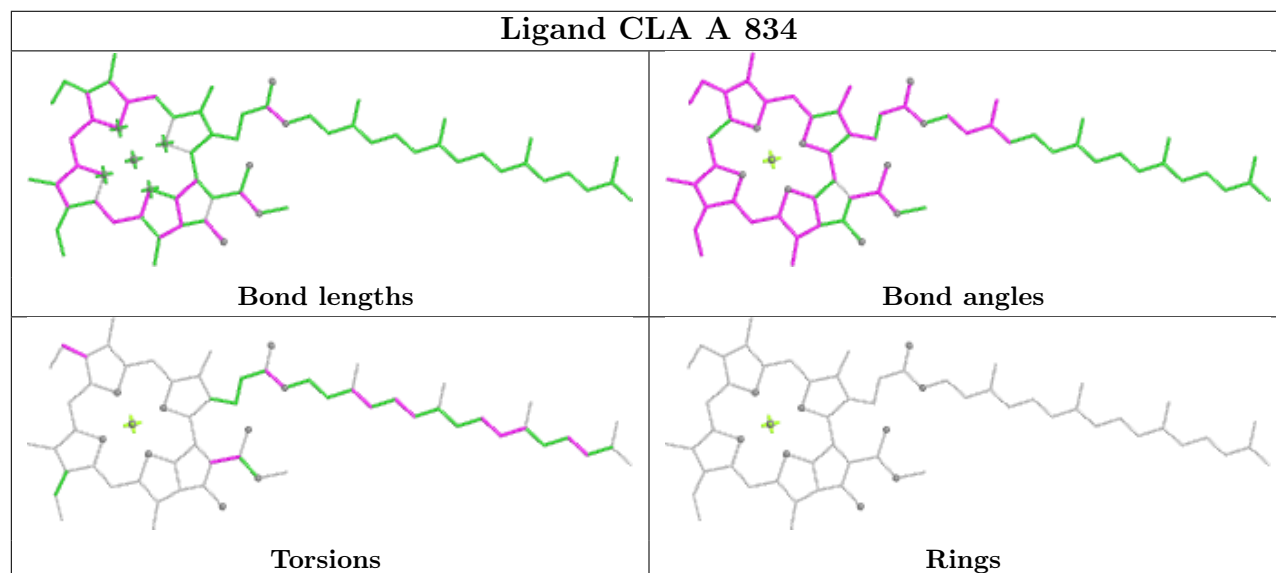


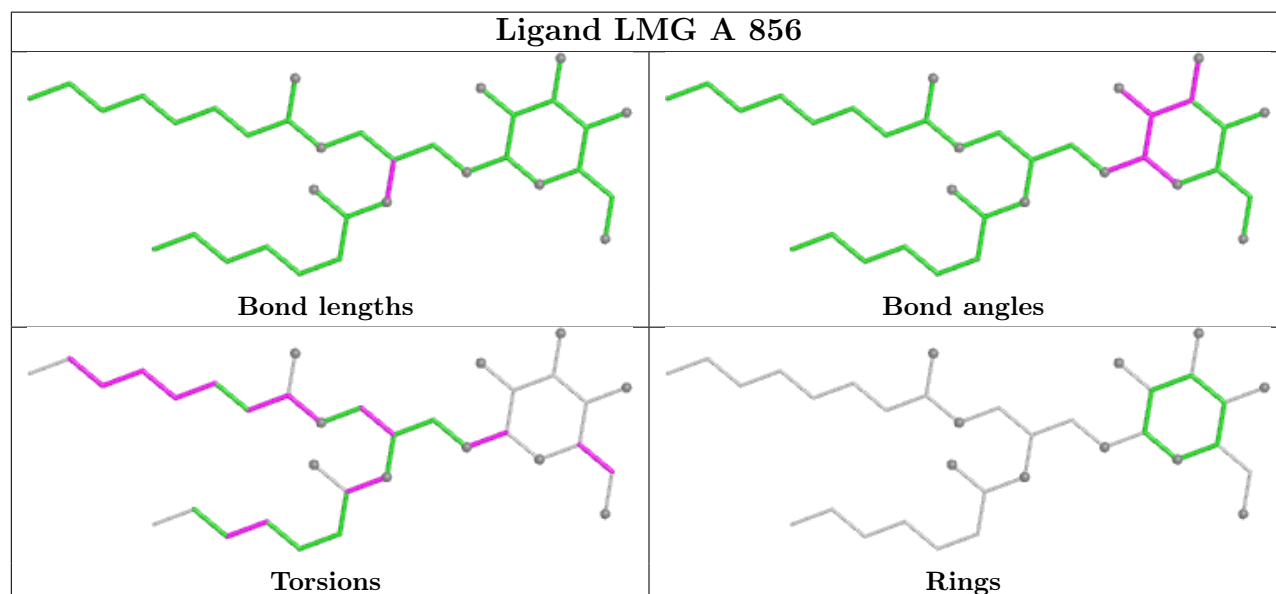
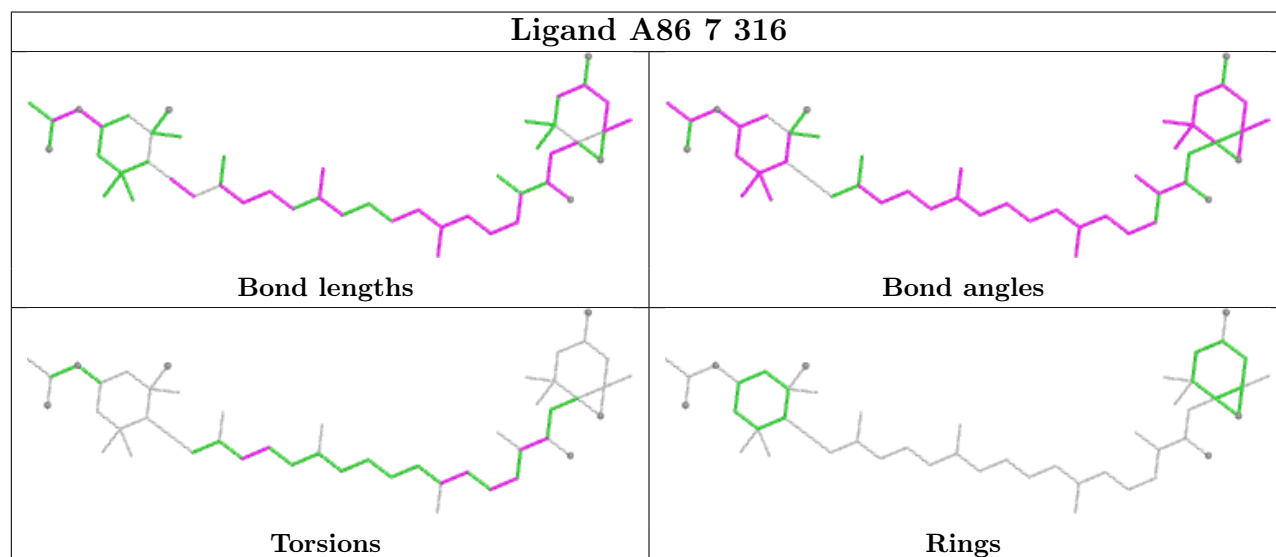
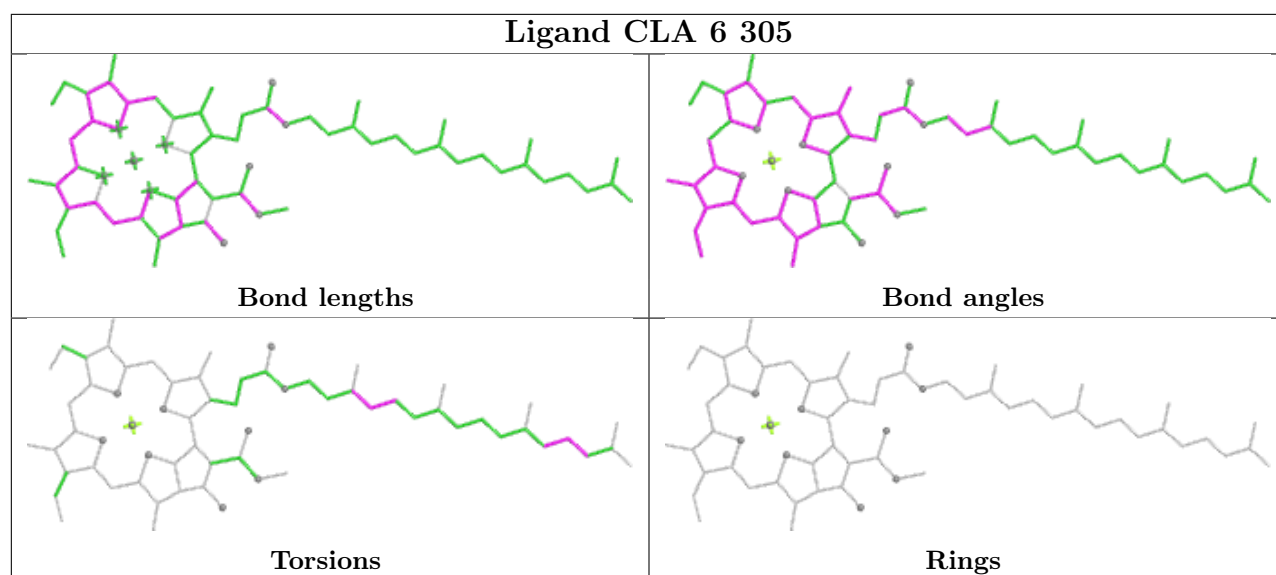
Rings

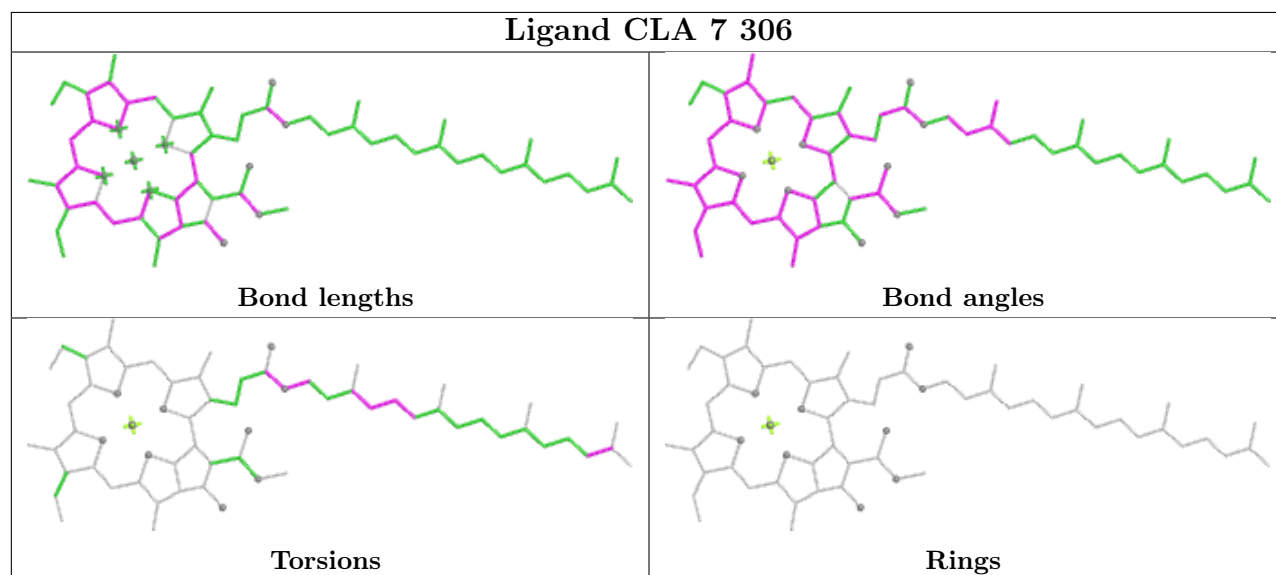
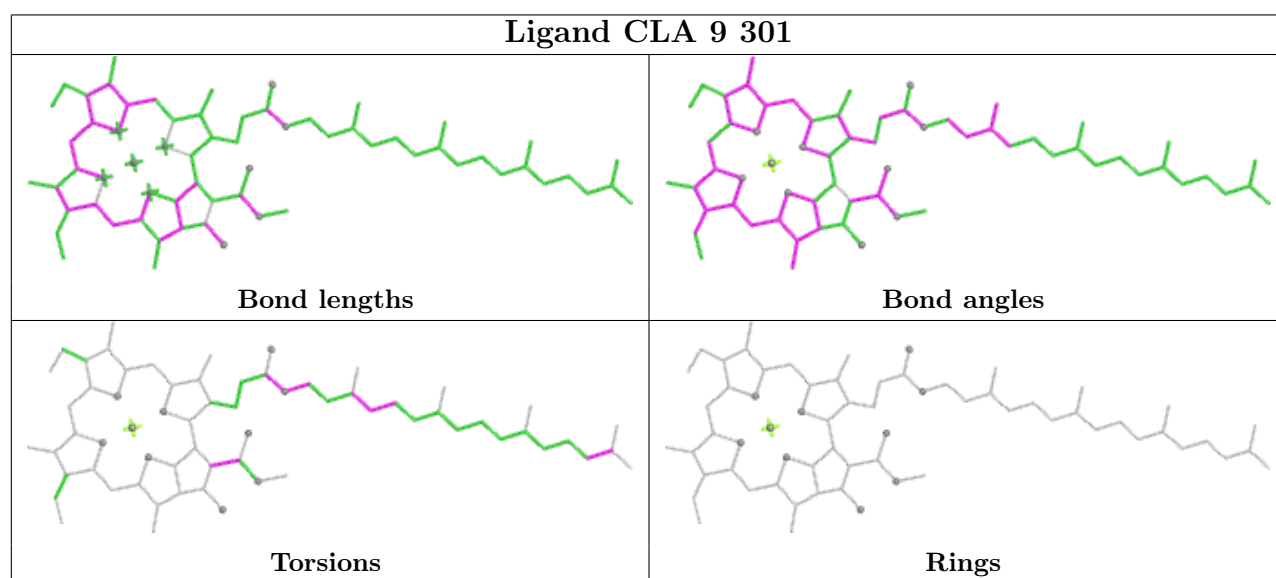
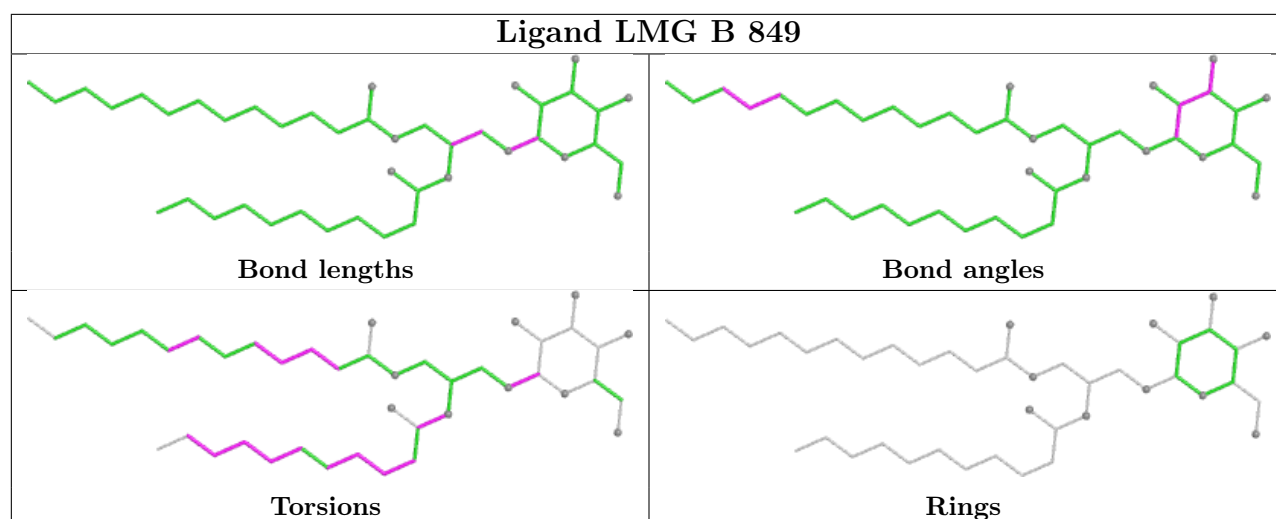
Ligand CLA 3 309



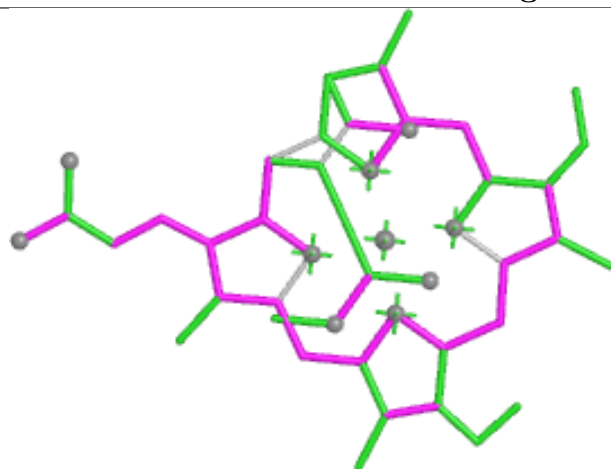
Ligand CLA A 834



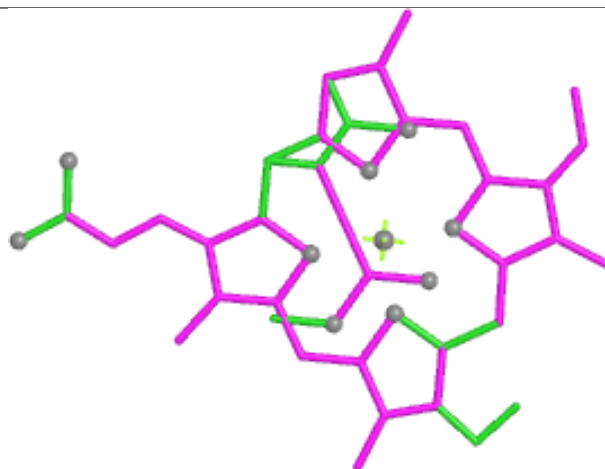




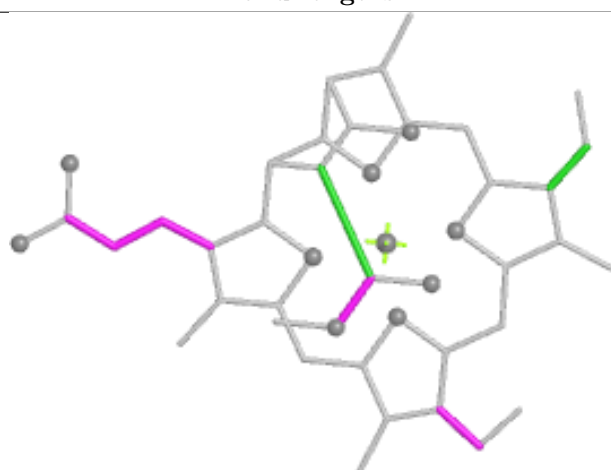
Ligand KC1 8 307



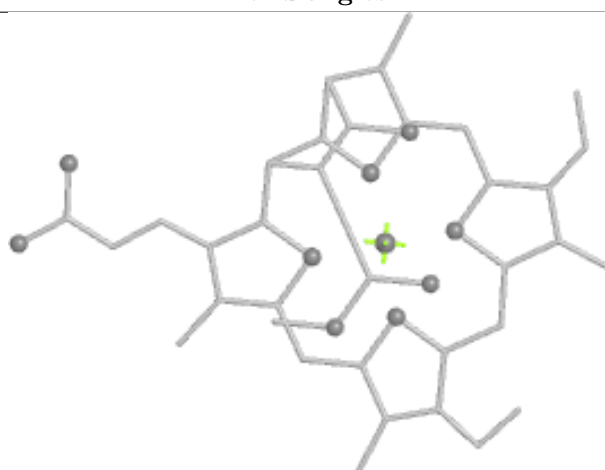
Bond lengths



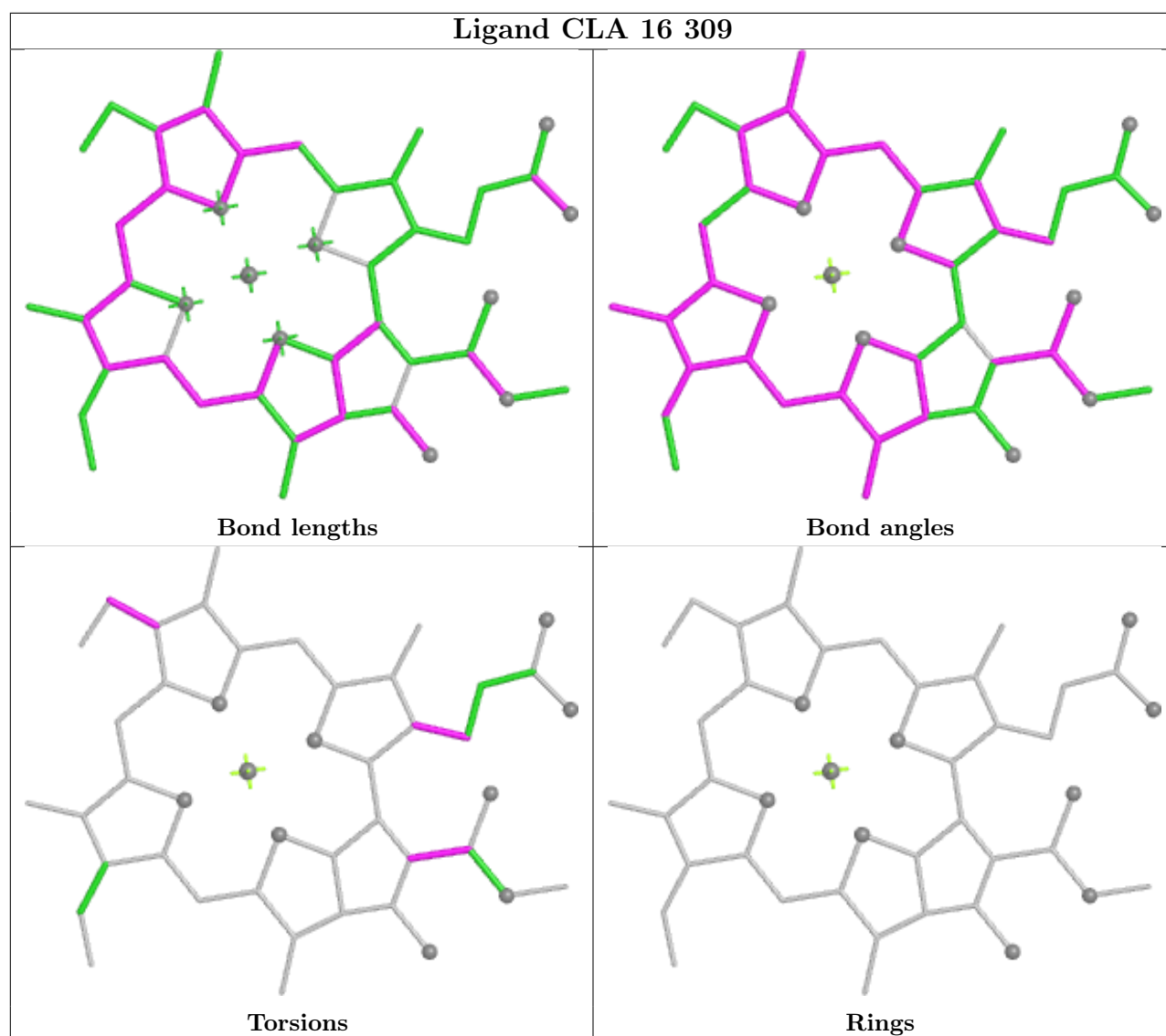
Bond angles

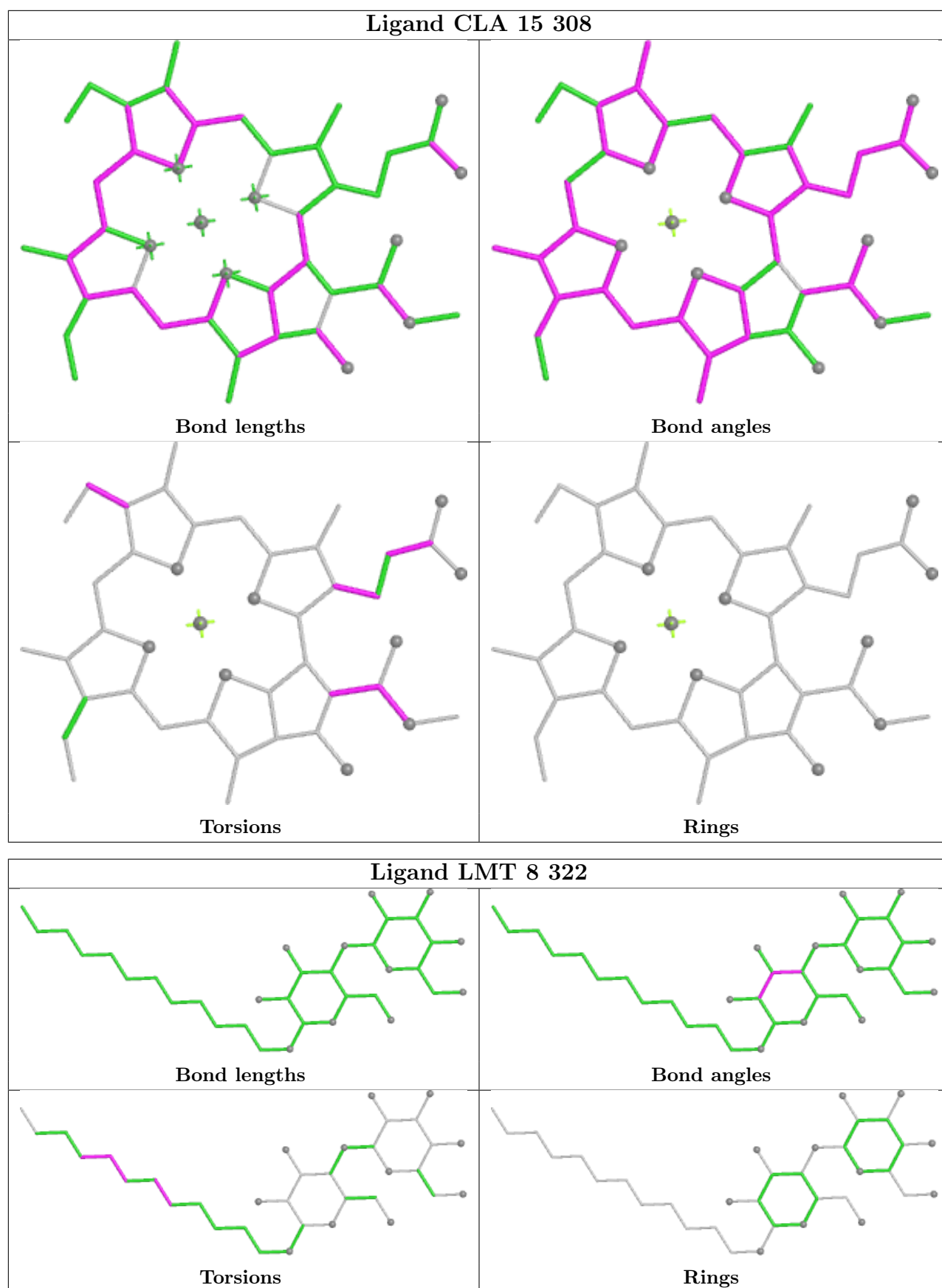


Torsions

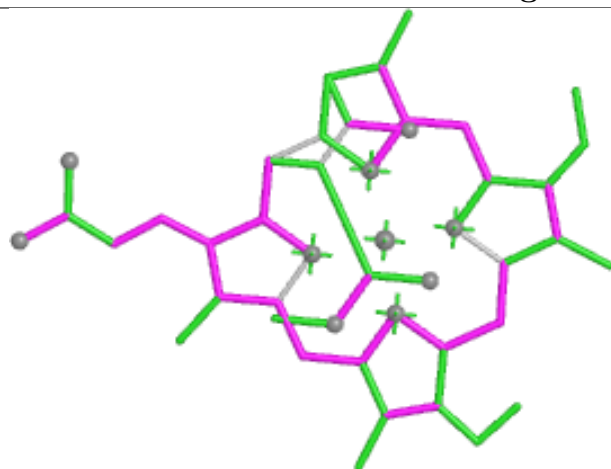


Rings

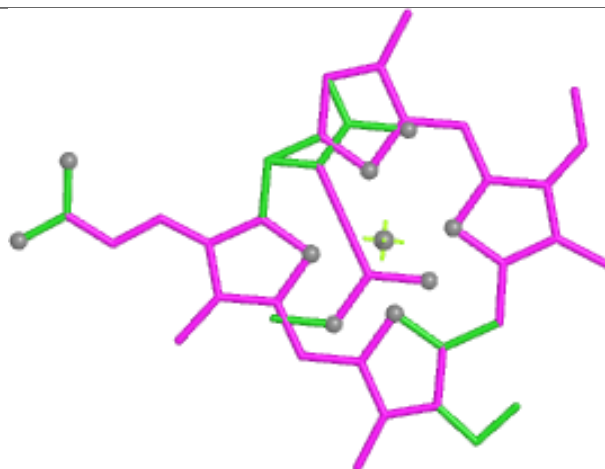




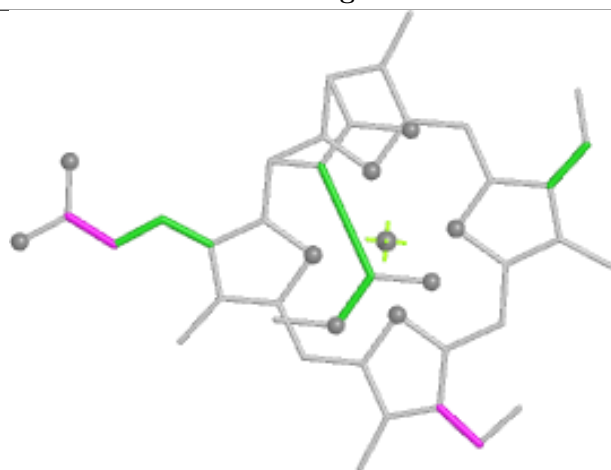
Ligand KC1 7 313



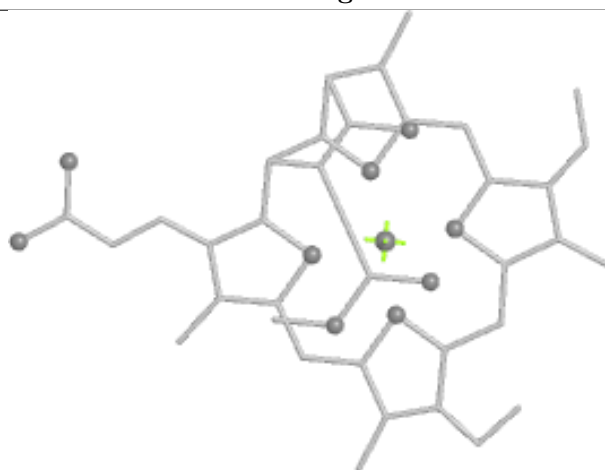
Bond lengths



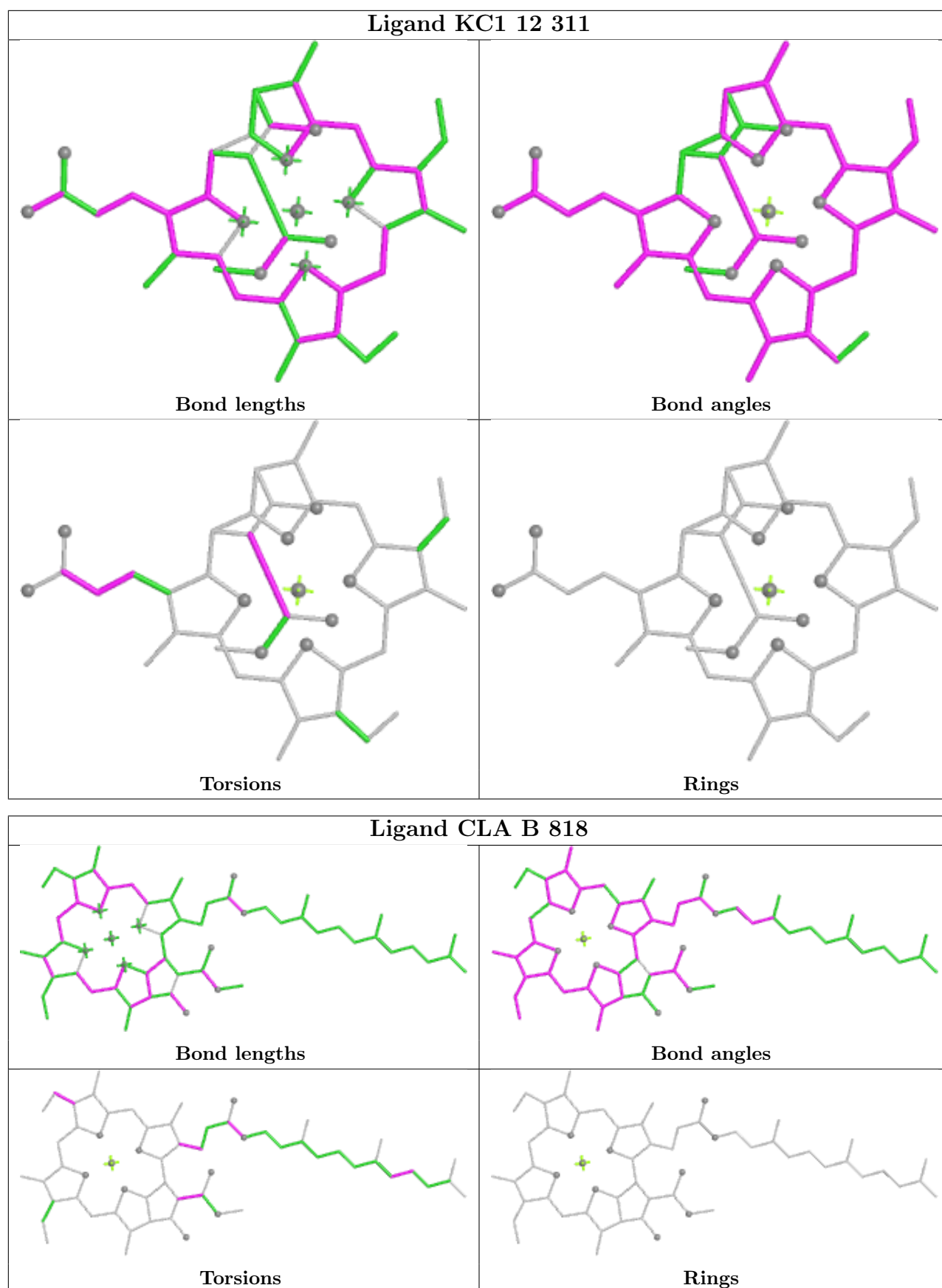
Bond angles

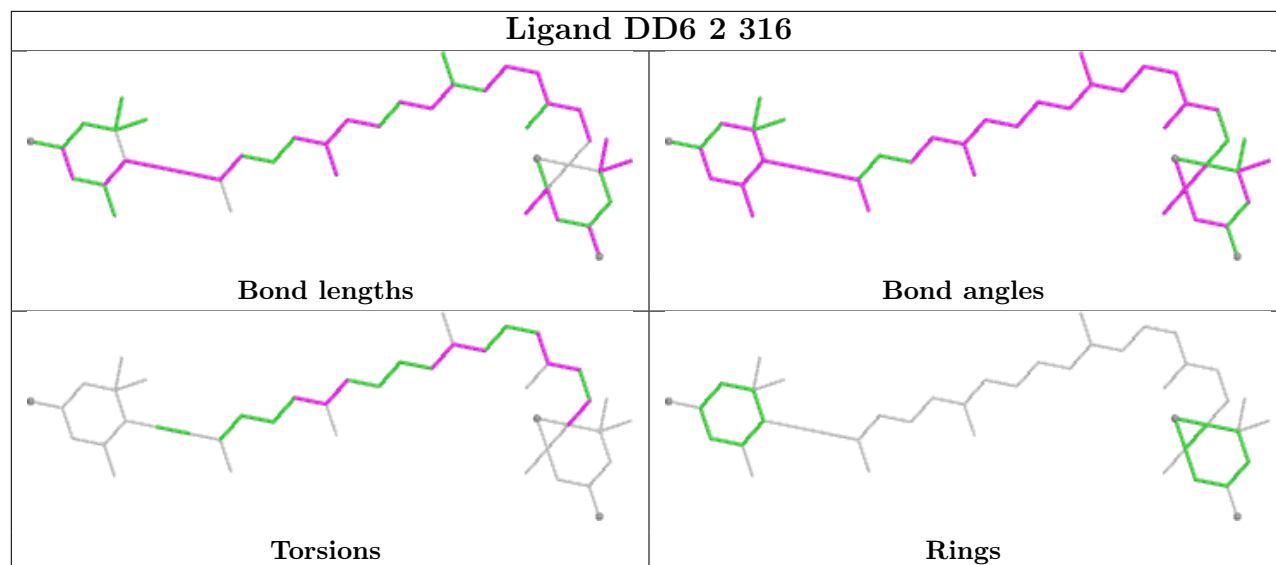
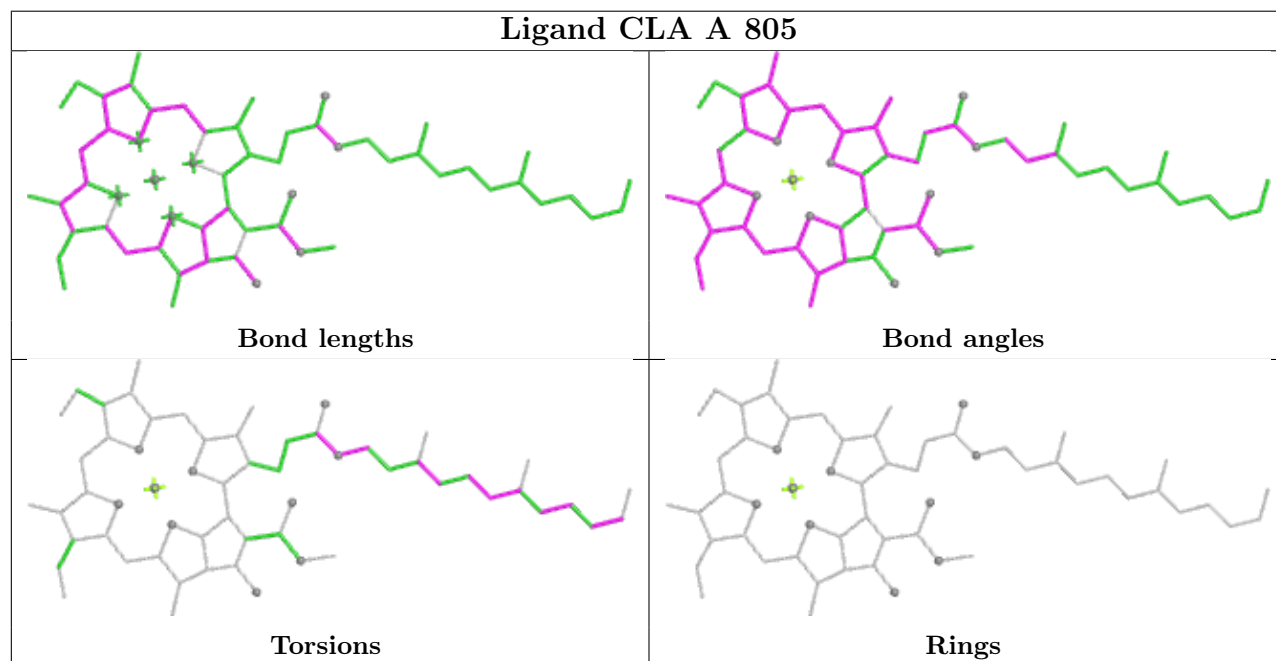


Torsions

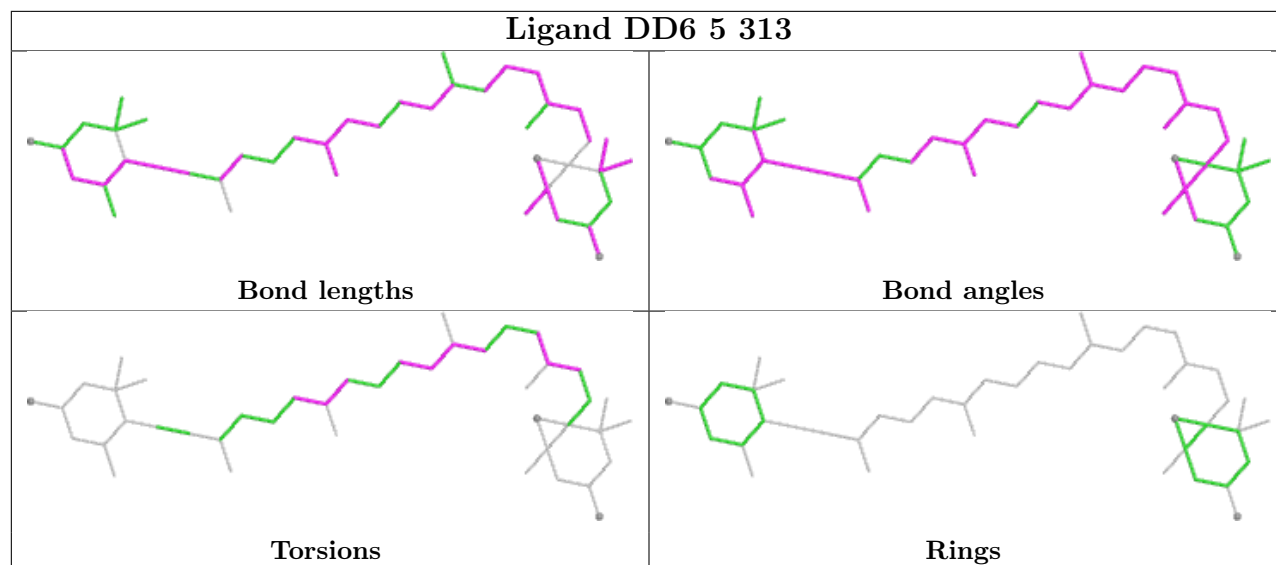


Rings

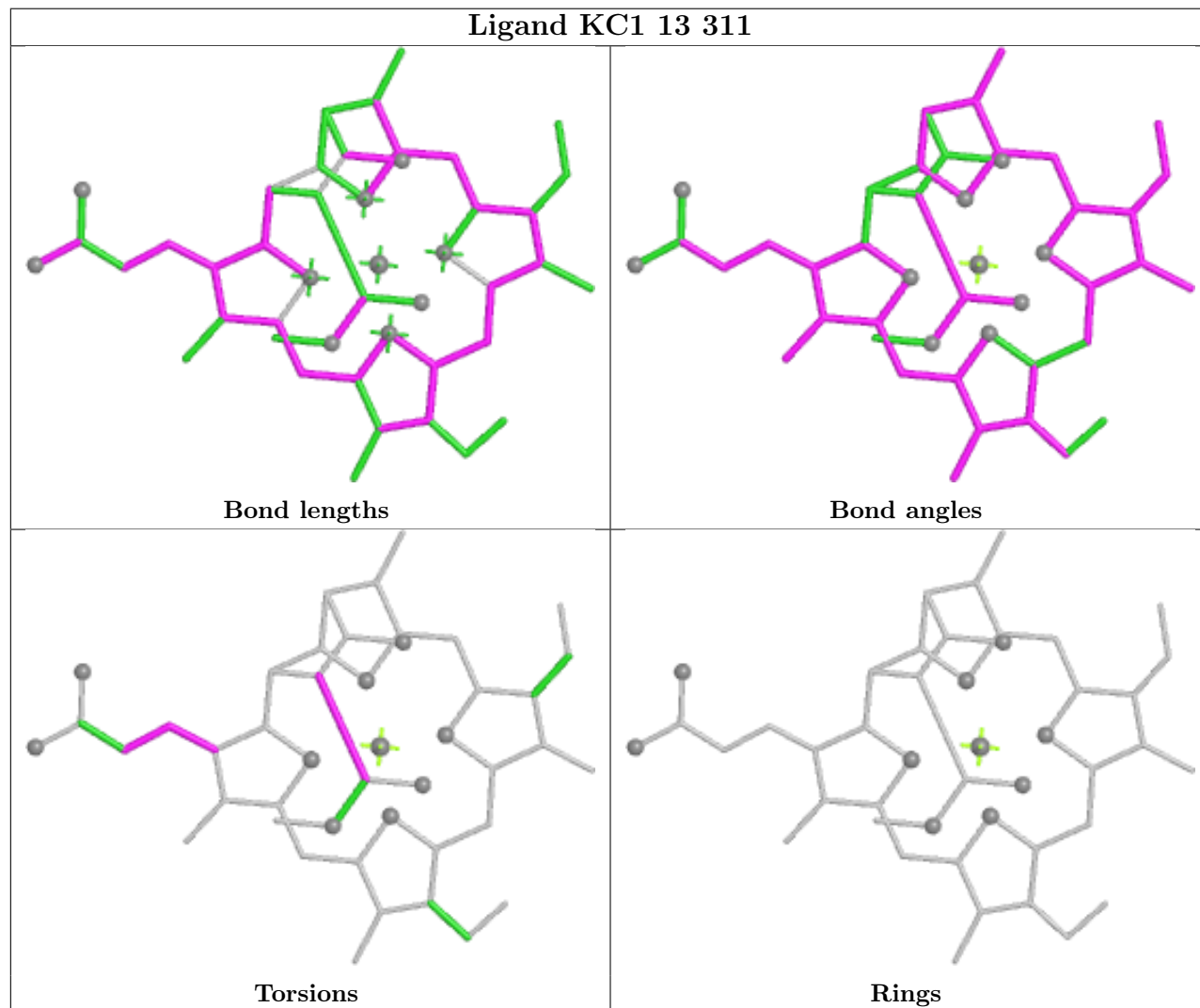


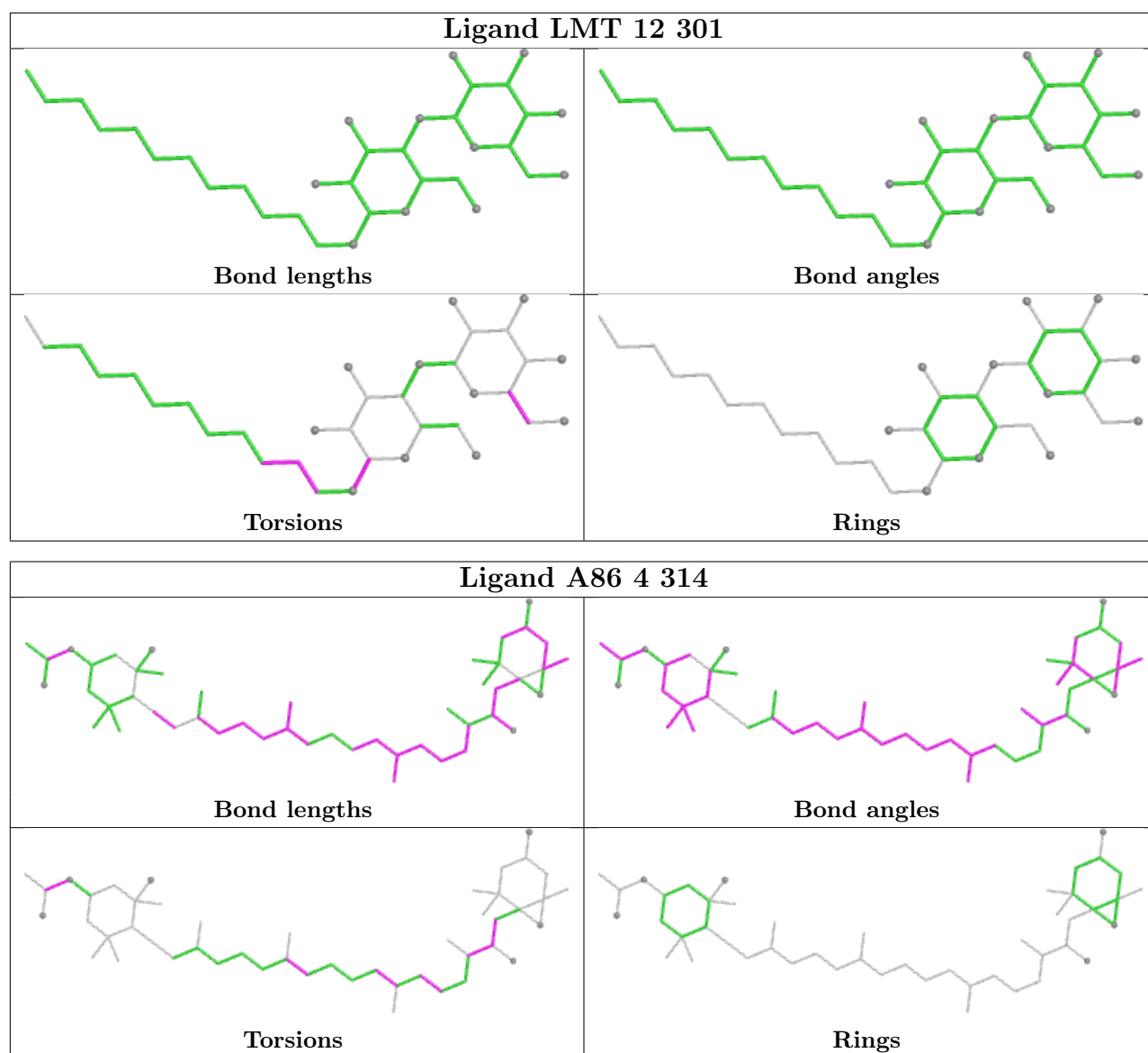
Ligand DD6 2 316**Ligand CLA A 805**

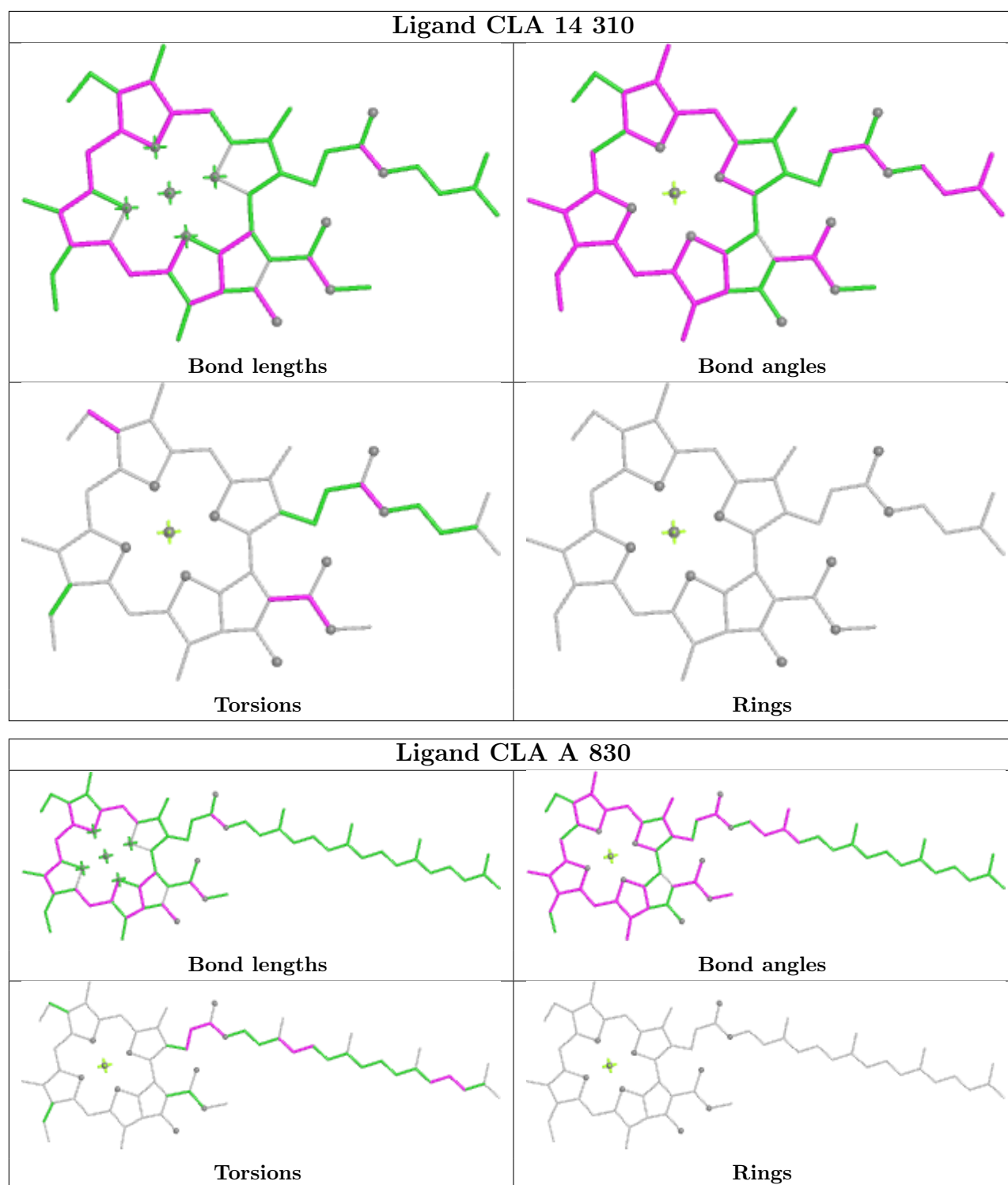
Ligand DD6 5 313



Ligand KC1 13 311







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

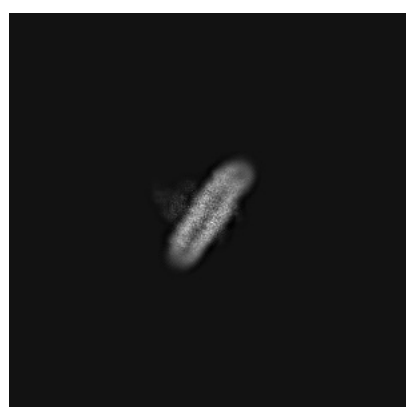
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0835. These allow visual inspection of the internal detail of the map and identification of artifacts.

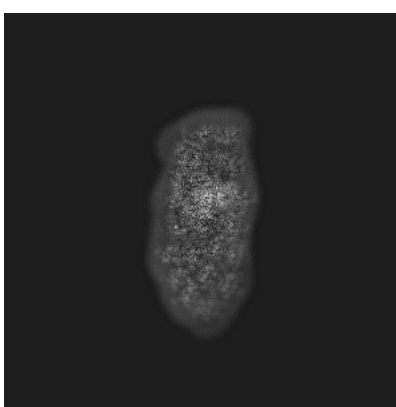
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

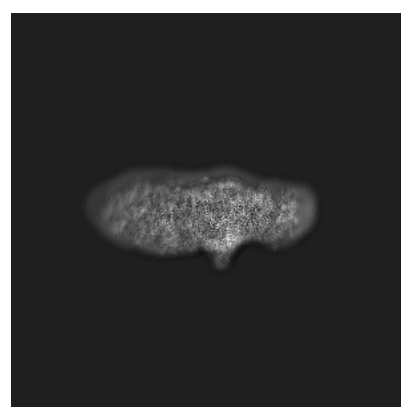
6.1.1 Primary map



X



Y

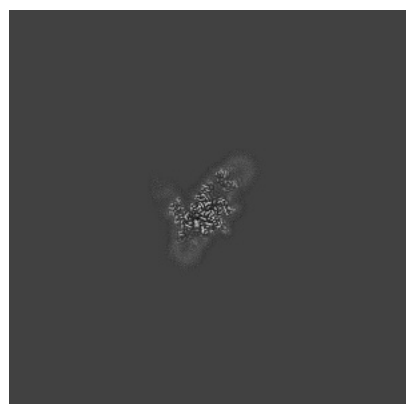


Z

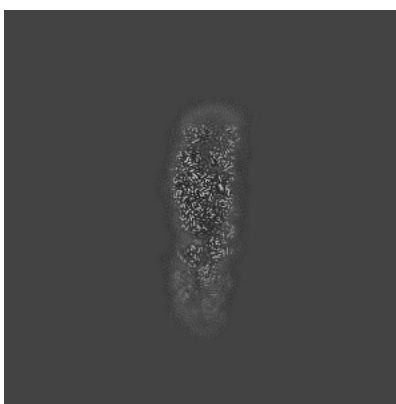
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

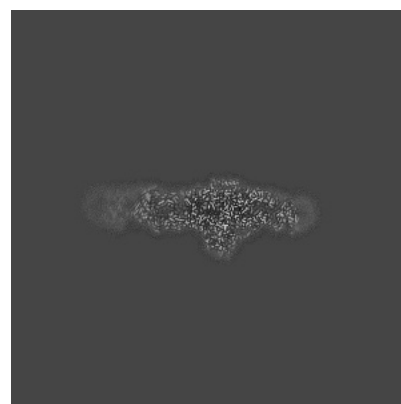
6.2.1 Primary map



X Index: 252



Y Index: 252

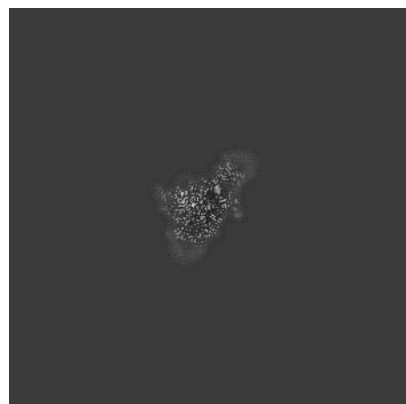


Z Index: 252

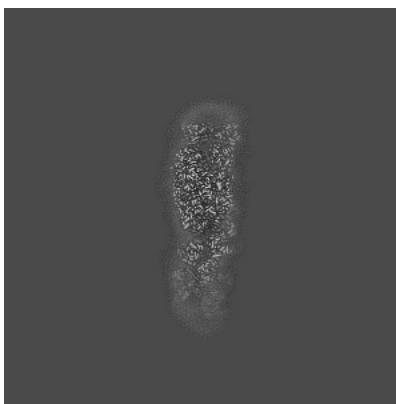
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

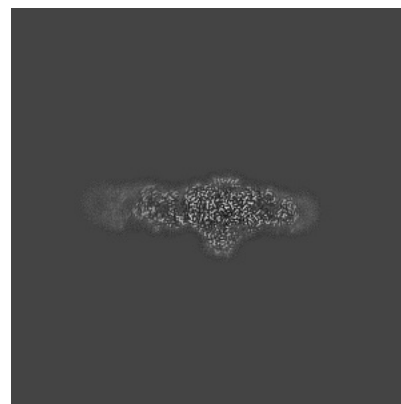
6.3.1 Primary map



X Index: 273



Y Index: 251

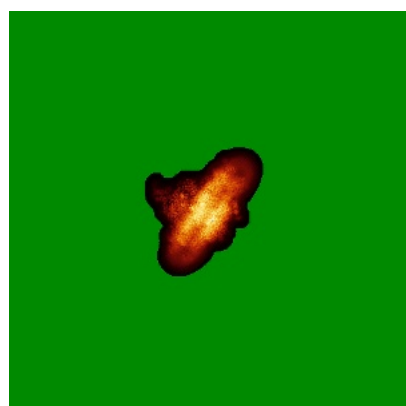


Z Index: 250

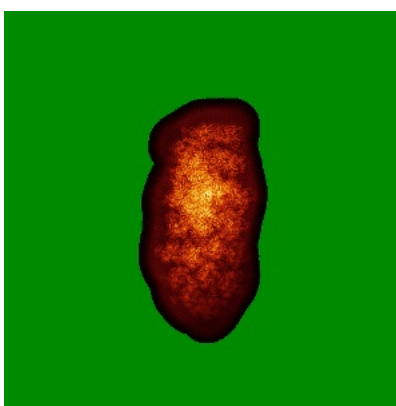
The images above show the largest variance slices of the map in three orthogonal directions.

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

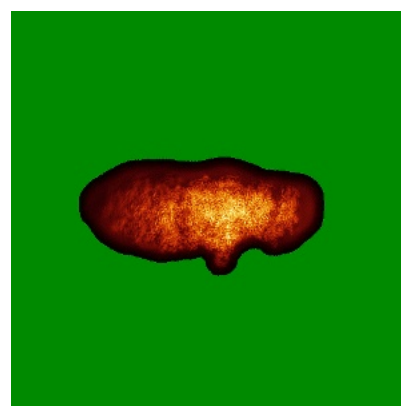
6.4.1 Primary map



X



Y

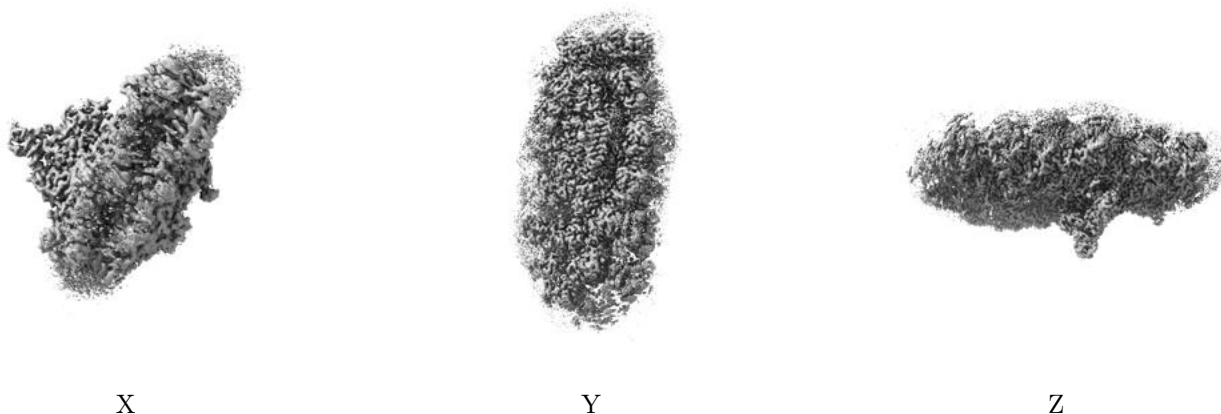


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

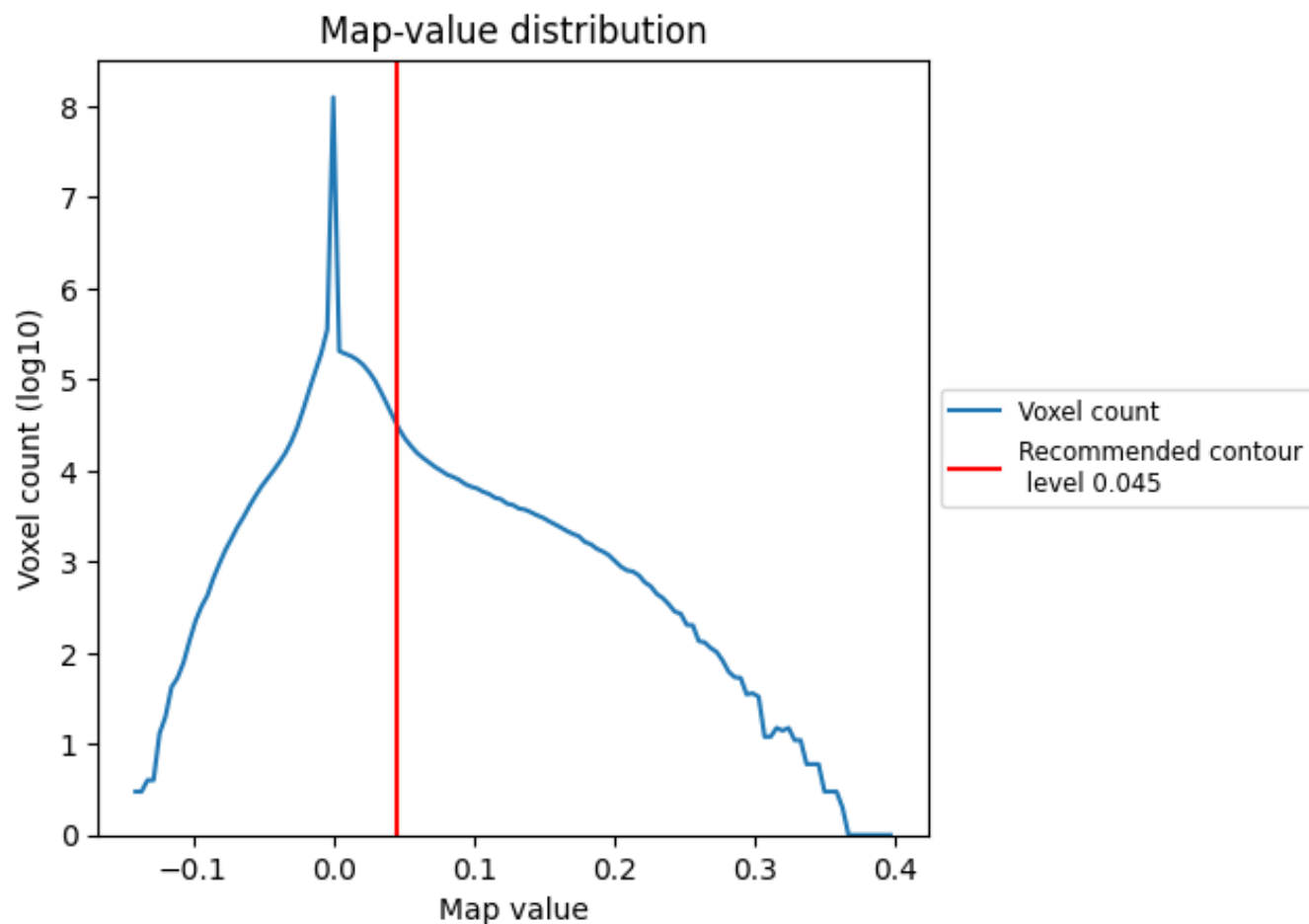
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

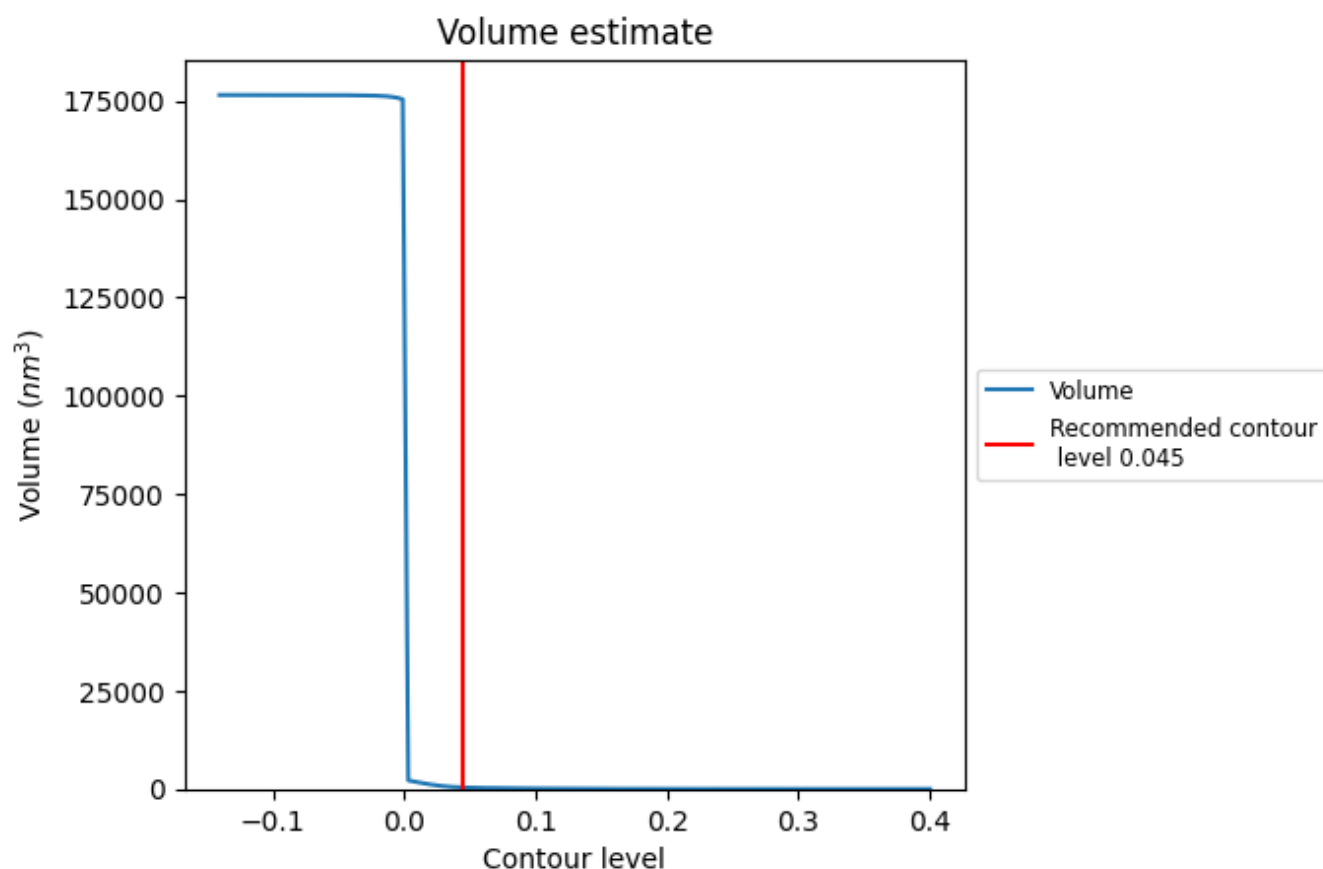
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

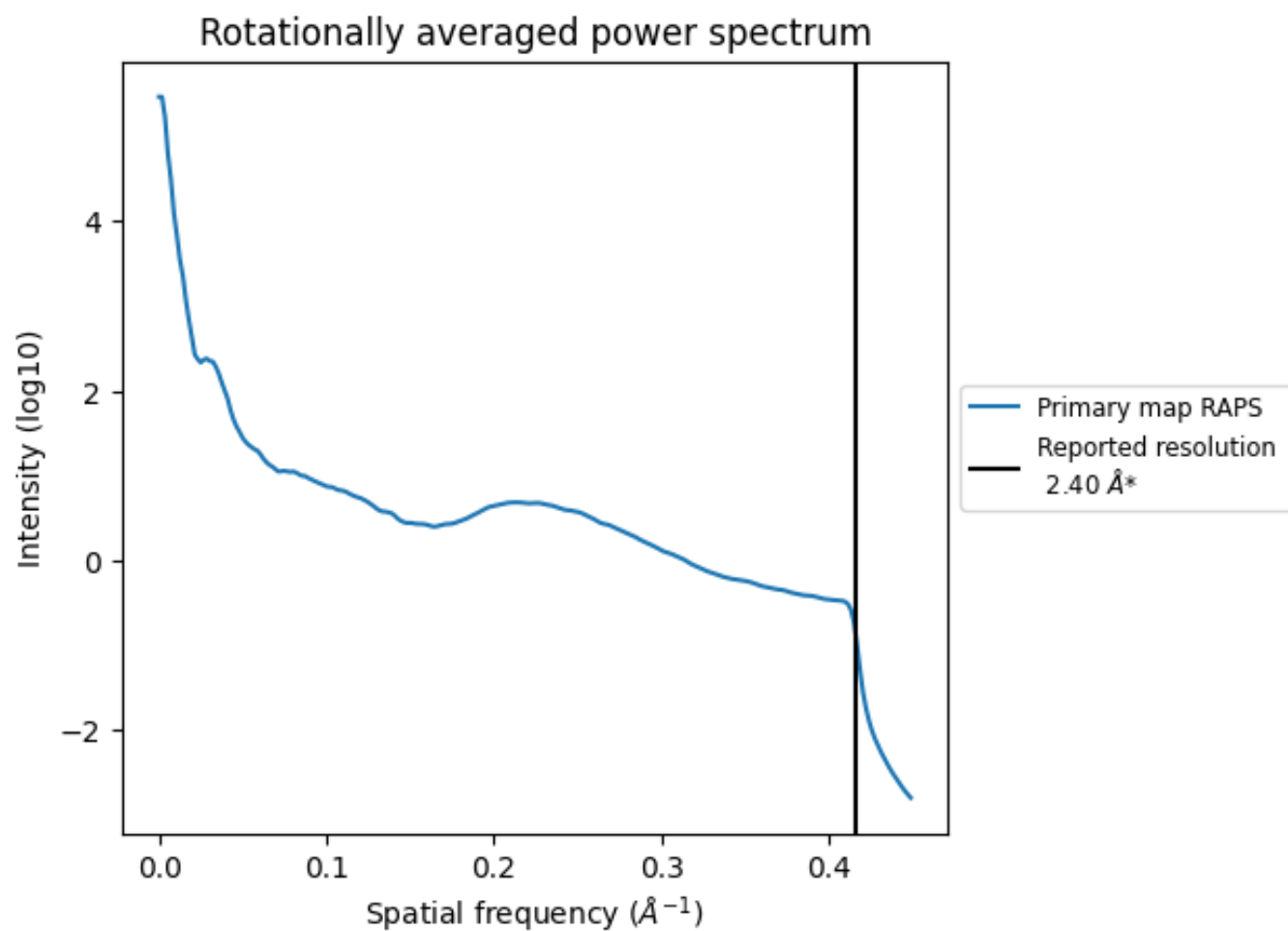
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 370 nm^3 ; this corresponds to an approximate mass of 334 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

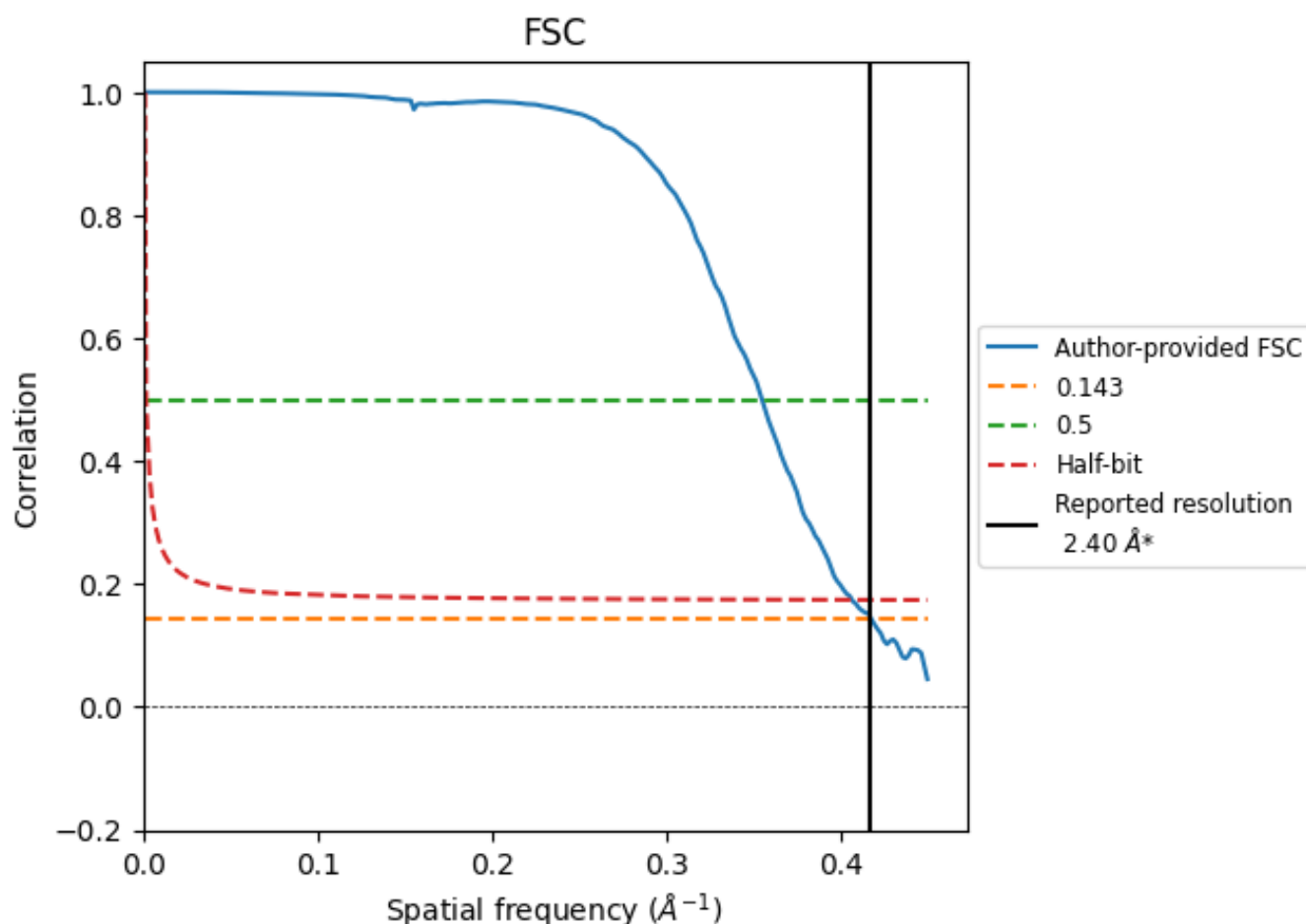


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

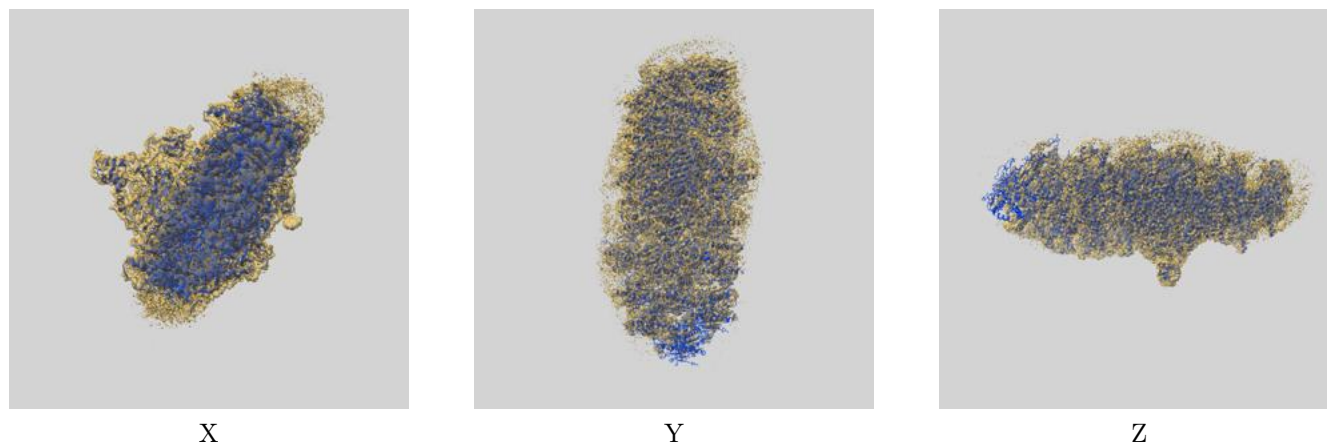
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.82	2.46
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

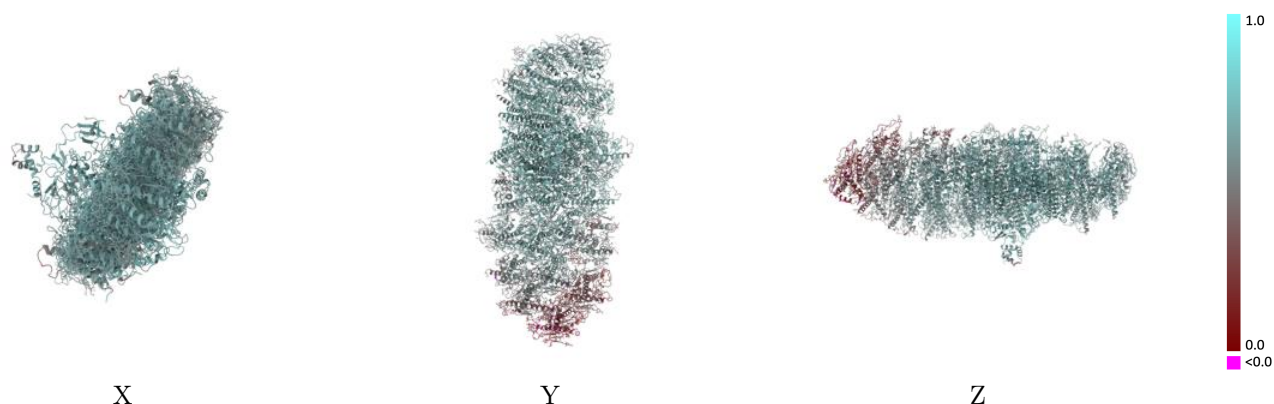
This section contains information regarding the fit between EMDB map EMD-0835 and PDB model 6L4U. Per-residue inclusion information can be found in section [3](#) on page [35](#).

9.1 Map-model overlay [i](#)



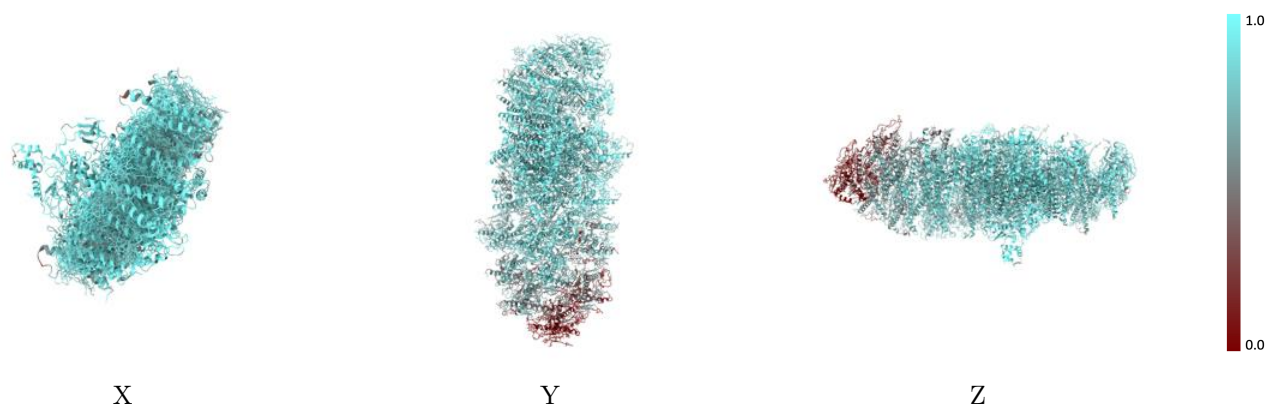
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



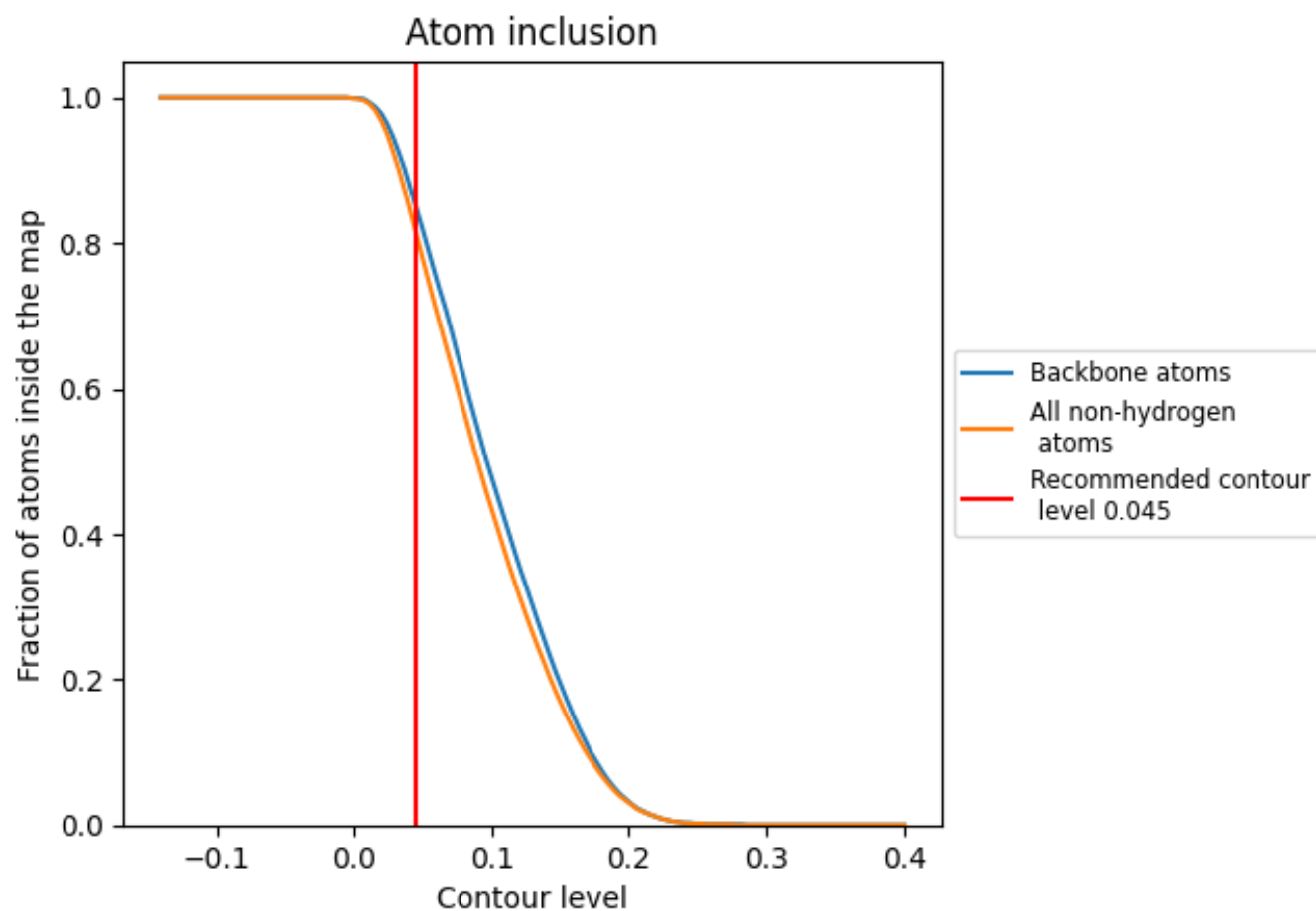
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion ⓘ



At the recommended contour level, 85% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8130	 0.5870
1	 0.8160	 0.5890
10	 0.8010	 0.5590
11	 0.6960	 0.5050
12	 0.7640	 0.5640
13	 0.6120	 0.4800
14	 0.3760	 0.3440
15	 0.1110	 0.2110
16	 0.5790	 0.4140
1u	 0.9010	 0.5810
2	 0.8680	 0.6050
2u	 0.9370	 0.6560
3	 0.8200	 0.5840
4	 0.8600	 0.6130
5	 0.8460	 0.6020
6	 0.8750	 0.6140
7	 0.8830	 0.6270
8	 0.9030	 0.6360
9	 0.8260	 0.5850
A	 0.9420	 0.6770
B	 0.9490	 0.6780
C	 0.9800	 0.6770
D	 0.9540	 0.6510
E	 0.9330	 0.6710
F	 0.9250	 0.6620
I	 0.9070	 0.6480
J	 0.9410	 0.6590
L	 0.9540	 0.6600
M	 0.9200	 0.6500

