



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 07:31 PM 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.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

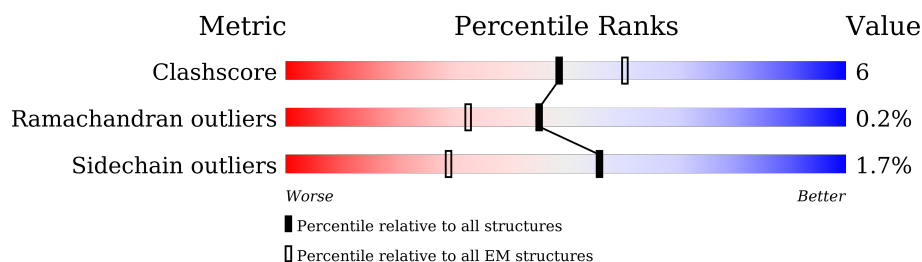
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	751	
2	B	733	
3	C	81	
4	D	139	
5	E	67	
6	F	185	
7	I	36	
8	J	41	
9	L	151	

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Mol	Chain	Length	Quality of chain
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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CL0	A	801	X	-	-	-
30	CLA	1	301	X	-	-	-
30	CLA	1	302	X	-	-	-
30	CLA	1	303	X	-	-	-
30	CLA	1	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	1	305	X	-	-	-
30	CLA	10	303	X	-	-	-
30	CLA	10	304	X	-	-	-
30	CLA	10	305	X	-	-	-
30	CLA	10	307	X	-	-	-
30	CLA	10	308	X	-	-	-
30	CLA	10	309	X	-	-	-
30	CLA	11	304	X	-	-	-
30	CLA	11	306	X	-	-	-
30	CLA	11	308	X	-	-	-
30	CLA	11	310	X	-	-	-
30	CLA	12	303	X	-	-	-
30	CLA	12	304	X	-	-	-
30	CLA	12	306	X	-	-	-
30	CLA	12	307	X	-	-	-
30	CLA	12	308	X	-	-	-
30	CLA	12	312	X	-	-	-
30	CLA	12	321	X	-	-	-
30	CLA	13	301	X	-	-	-
30	CLA	13	302	X	-	-	-
30	CLA	13	307	X	-	-	-
30	CLA	13	309	X	-	-	-
30	CLA	14	302	X	-	-	-
30	CLA	14	303	X	-	-	-
30	CLA	14	304	X	-	-	-
30	CLA	14	305	X	-	-	-
30	CLA	14	309	X	-	-	-
30	CLA	14	310	X	-	-	-
30	CLA	14	313	X	-	-	-
30	CLA	15	303	X	-	-	-
30	CLA	15	304	X	-	-	-
30	CLA	15	305	X	-	-	-
30	CLA	15	306	X	-	-	-
30	CLA	15	307	X	-	-	-
30	CLA	15	308	X	-	-	-
30	CLA	15	310	X	-	-	-
30	CLA	15	311	X	-	-	-
30	CLA	15	312	X	-	-	-
30	CLA	16	302	X	-	-	-
30	CLA	16	303	X	-	-	-
30	CLA	16	305	X	-	-	-
30	CLA	16	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	16	307	X	-	-	-
30	CLA	16	308	X	-	-	-
30	CLA	16	310	X	-	-	-
30	CLA	2	301	X	-	-	-
30	CLA	2	304	X	-	-	-
30	CLA	2	305	X	-	-	-
30	CLA	2	307	X	-	-	-
30	CLA	2	309	X	-	-	-
30	CLA	2	310	X	-	-	-
30	CLA	2u	202	X	-	-	-
30	CLA	3	301	X	-	-	-
30	CLA	3	302	X	-	-	-
30	CLA	3	303	X	-	-	-
30	CLA	3	305	X	-	-	-
30	CLA	3	306	X	-	-	-
30	CLA	3	307	X	-	-	-
30	CLA	4	301	X	-	-	-
30	CLA	4	302	X	-	-	-
30	CLA	4	303	X	-	-	-
30	CLA	4	304	X	-	-	-
30	CLA	4	305	X	-	-	-
30	CLA	4	306	X	-	-	-
30	CLA	4	309	X	-	-	-
30	CLA	4	311	X	-	-	-
30	CLA	5	302	X	-	-	-
30	CLA	5	303	X	-	-	-
30	CLA	5	304	X	-	-	-
30	CLA	5	307	X	-	-	-
30	CLA	5	309	X	-	-	-
30	CLA	5	311	X	-	-	-
30	CLA	6	304	X	-	-	-
30	CLA	6	305	X	-	-	-
30	CLA	6	306	X	-	-	-
30	CLA	6	307	X	-	-	-
30	CLA	6	309	X	-	-	-
30	CLA	6	310	X	-	-	-
30	CLA	6	315	X	-	-	-
30	CLA	6	316	X	-	-	-
30	CLA	6	317	X	-	-	-
30	CLA	7	303	X	-	-	-
30	CLA	7	304	X	-	-	-
30	CLA	7	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	7	306	X	-	-	-
30	CLA	7	309	X	-	-	-
30	CLA	7	311	X	-	-	-
30	CLA	7	312	X	-	-	-
30	CLA	8	301	X	-	-	-
30	CLA	8	302	X	-	-	-
30	CLA	8	304	X	-	-	-
30	CLA	8	308	X	-	-	-
30	CLA	9	301	X	-	-	-
30	CLA	9	302	X	-	-	-
30	CLA	9	305	X	-	-	-
30	CLA	9	306	X	-	-	-
30	CLA	9	307	X	-	-	-
30	CLA	9	308	X	-	-	-
30	CLA	9	309	X	-	-	-
30	CLA	A	802	X	-	-	-
30	CLA	A	803	X	-	-	-
30	CLA	A	804	X	-	-	-
30	CLA	A	805	X	-	-	-
30	CLA	A	806	X	-	-	-
30	CLA	A	807	X	-	-	-
30	CLA	A	808	X	-	-	-
30	CLA	A	809	X	-	-	-
30	CLA	A	810	X	-	-	-
30	CLA	A	811	X	-	-	-
30	CLA	A	812	X	-	-	-
30	CLA	A	813	X	-	-	-
30	CLA	A	814	X	-	-	-
30	CLA	A	815	X	-	-	-
30	CLA	A	816	X	-	-	-
30	CLA	A	820	X	-	-	-
30	CLA	A	821	X	-	-	-
30	CLA	A	822	X	-	-	-
30	CLA	A	824	X	-	-	-
30	CLA	A	825	X	-	-	-
30	CLA	A	826	X	-	-	-
30	CLA	A	827	X	-	-	-
30	CLA	A	828	X	-	-	-
30	CLA	A	829	X	-	-	-
30	CLA	A	830	X	-	-	-
30	CLA	A	831	X	-	-	-
30	CLA	A	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	A	834	X	-	-	-
30	CLA	A	835	X	-	-	-
30	CLA	A	836	X	-	-	-
30	CLA	A	837	X	-	-	-
30	CLA	A	838	X	-	-	-
30	CLA	A	839	X	-	-	-
30	CLA	A	840	X	-	-	-
30	CLA	A	841	X	-	-	-
30	CLA	A	842	X	-	-	-
30	CLA	A	843	X	-	-	-
30	CLA	A	844	X	-	-	-
30	CLA	B	801	X	-	-	-
30	CLA	B	802	X	-	-	-
30	CLA	B	803	X	-	-	-
30	CLA	B	804	X	-	-	-
30	CLA	B	805	X	-	-	-
30	CLA	B	806	X	-	-	-
30	CLA	B	807	X	-	-	-
30	CLA	B	808	X	-	-	-
30	CLA	B	809	X	-	-	-
30	CLA	B	810	X	-	-	-
30	CLA	B	811	X	-	-	-
30	CLA	B	812	X	-	-	-
30	CLA	B	813	X	-	-	-
30	CLA	B	814	X	-	-	-
30	CLA	B	815	X	-	-	-
30	CLA	B	817	X	-	-	-
30	CLA	B	818	X	-	-	-
30	CLA	B	819	X	-	-	-
30	CLA	B	821	X	-	-	-
30	CLA	B	823	X	-	-	-
30	CLA	B	824	X	-	-	-
30	CLA	B	825	X	-	-	-
30	CLA	B	826	X	-	-	-
30	CLA	B	827	X	-	-	-
30	CLA	B	828	X	-	-	-
30	CLA	B	829	X	-	-	-
30	CLA	B	830	X	-	-	-
30	CLA	B	832	X	-	-	-
30	CLA	B	833	X	-	-	-
30	CLA	B	834	X	-	-	-
30	CLA	B	835	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CLA	B	836	X	-	-	-
30	CLA	B	837	X	-	-	-
30	CLA	B	838	X	-	-	-
30	CLA	B	839	X	-	-	-
30	CLA	F	201	X	-	-	-
30	CLA	F	202	X	-	-	-
30	CLA	F	203	X	-	-	-
30	CLA	J	101	X	-	-	-
30	CLA	L	202	X	-	-	-
30	CLA	L	203	X	-	-	-

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		0	0
			650	390	130	130			

- Molecule 12 is a protein called Photosystem I reaction center subunit Psu28.

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 Lhc15.

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 Lhc8.

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		

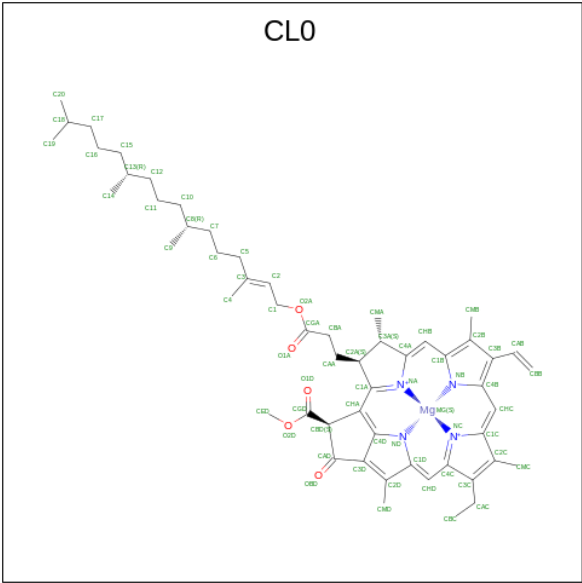
- Molecule 27 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

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.

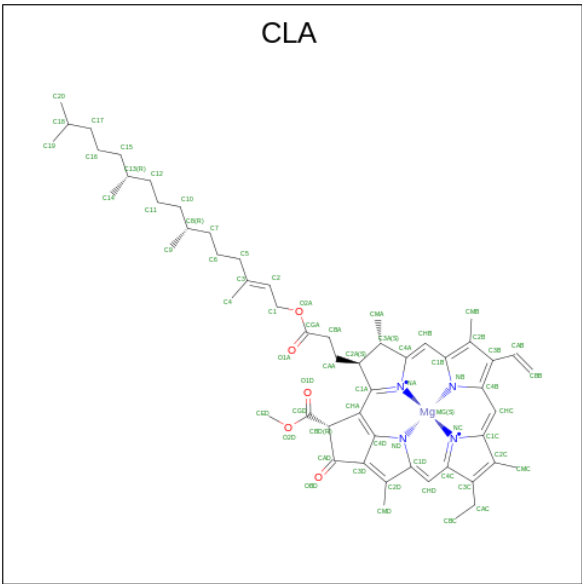
Mol	Chain	Residues	Atoms					AltConf	Trace
28	16	174	Total	C	N	O	S	0	0
			1313	846	217	242	8		

- Molecule 29 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 30 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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 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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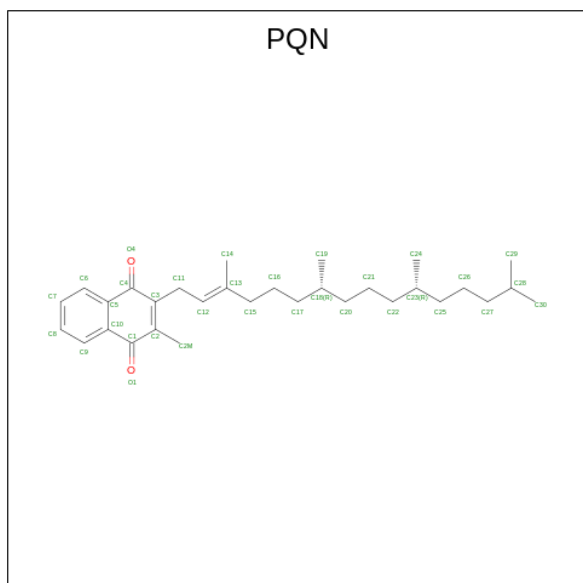
Mol	Chain	Residues	Atoms					AltConf
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 57	C 47	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	14	1	Total 65	C 55	Mg 1	N 4	O 5	0
30	14	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	14	1	Total 50	C 40	Mg 1	N 4	O 5	0
30	14	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: $C_{31}H_{46}O_2$).



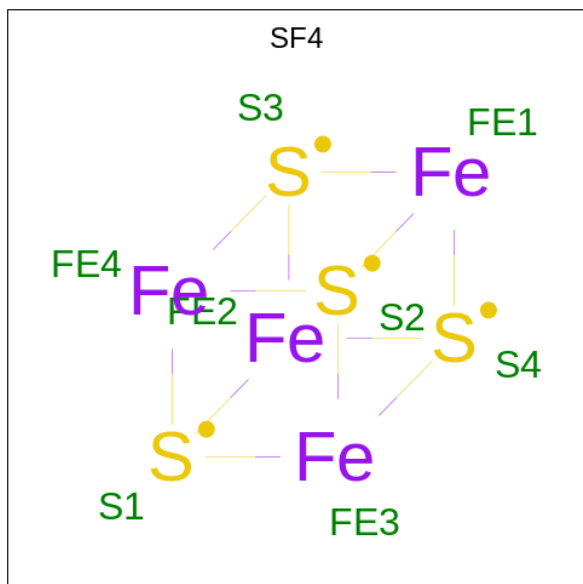
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			33	31	2	

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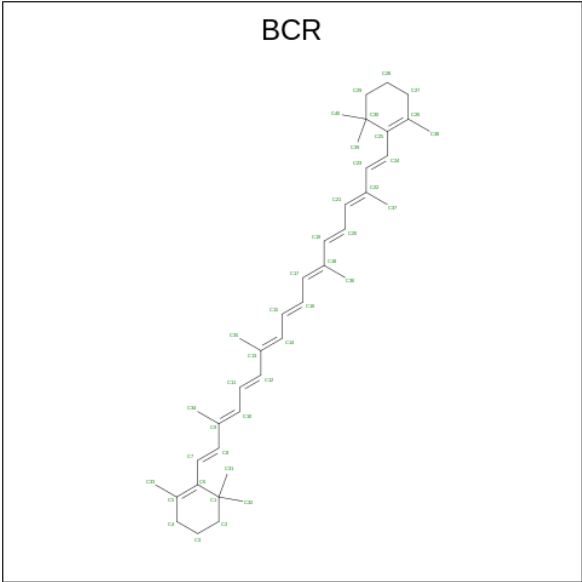
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			33	31	2	

- 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: $\text{C}_{40}\text{H}_{56}$).



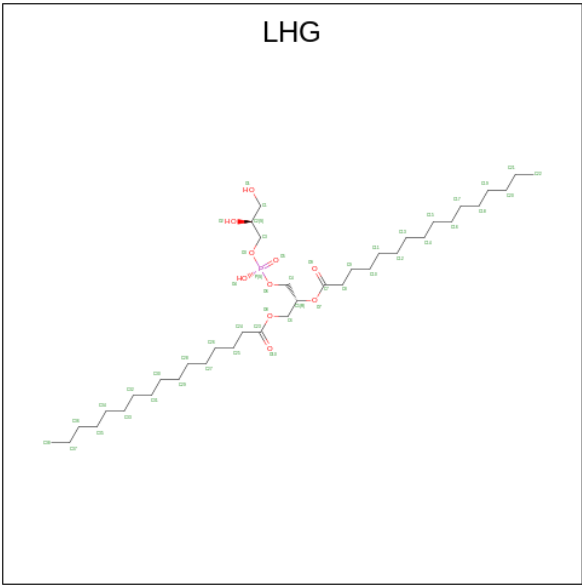
Mol	Chain	Residues	Atoms		AltConf
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
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).



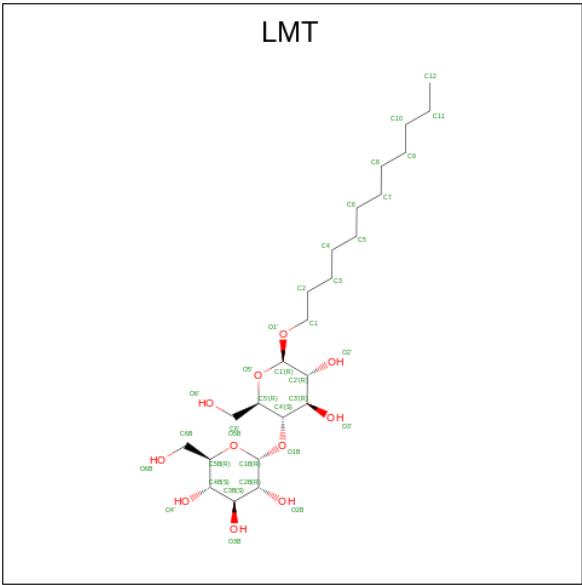
Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	O	P	0
			49	38	10	1	
34	A	1	Total	C	O	P	0
			27	16	10	1	
34	B	1	Total	C	O	P	0
			27	16	10	1	
34	2	1	Total	C	O	P	0
			27	16	10	1	
34	5	1	Total	C	O	P	0
			27	16	10	1	

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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).



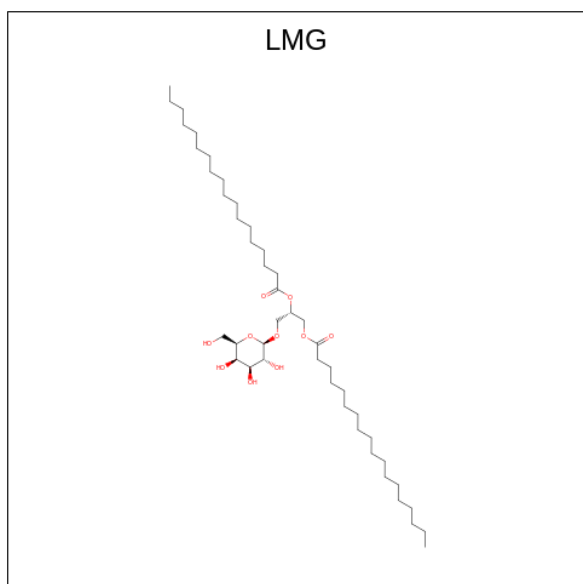
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O		0
			35	24	11		
35	A	1	Total	C	O		0
			35	24	11		
35	A	1	Total	C	O		0
			35	24	11		
35	B	1	Total	C	O		0
			35	24	11		
35	B	1	Total	C	O		0
			35	24	11		
35	1	1	Total	C	O		0
			35	24	11		
35	6	1	Total	C	O		0
			31	20	11		
35	7	1	Total	C	O		0
			35	24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

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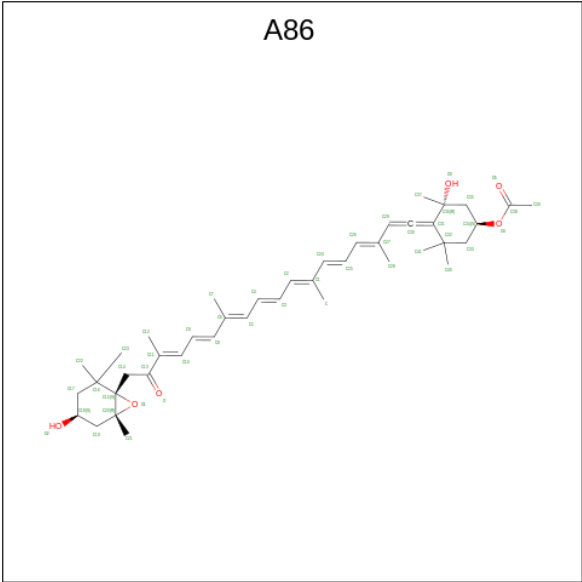
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	8	1	35	24	11	0
35	9	1	32	21	11	0
35	11	1	35	24	11	0
35	11	1	35	24	11	0
35	11	1	35	24	11	0
35	11	1	35	24	11	0
35	12	1	35	24	11	0
35	12	1	35	24	11	0
35	12	1	35	24	11	0
35	12	1	35	24	11	0
35	15	1	35	24	11	0
35	16	1	35	24	11	0

- 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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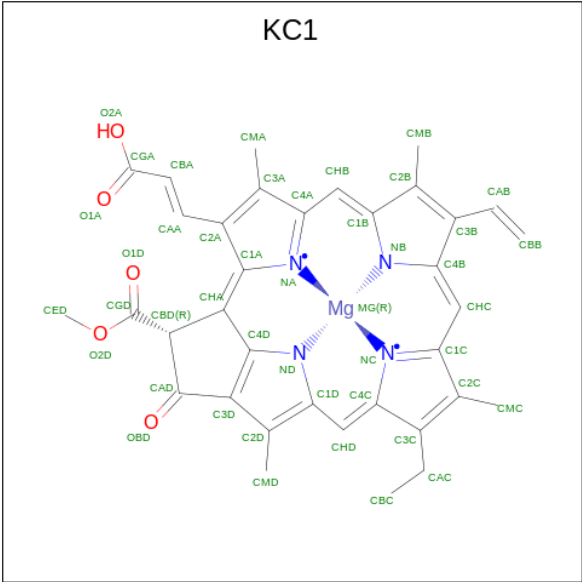
Mol	Chain	Residues	Atoms			AltConf
37	5	1	Total	C	O	0
			48	42	6	
37	6	1	Total	C	O	0
			48	42	6	
37	7	1	Total	C	O	0
			48	42	6	
37	7	1	Total	C	O	0
			48	42	6	
37	7	1	Total	C	O	0
			48	42	6	
37	8	1	Total	C	O	0
			48	42	6	
37	8	1	Total	C	O	0
			48	42	6	
37	9	1	Total	C	O	0
			48	42	6	
37	9	1	Total	C	O	0
			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	C	Mg	N	O	0
			45	35	1	4	5	
38	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
38	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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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).



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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	

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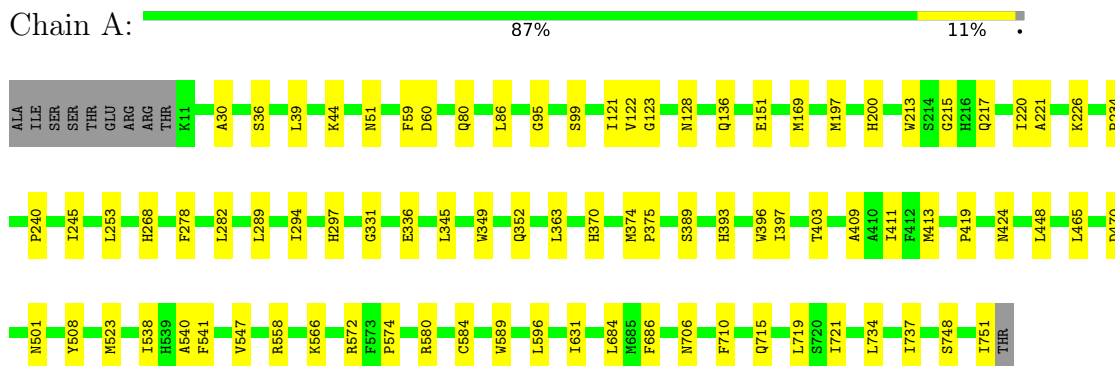
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Mol	Chain	Residues	Atoms		AltConf
40	C	15	Total 15	O 15	0
40	D	13	Total 13	O 13	0
40	E	3	Total 3	O 3	0
40	F	3	Total 3	O 3	0
40	I	1	Total 1	O 1	0
40	L	8	Total 8	O 8	0
40	1	1	Total 1	O 1	0
40	2	2	Total 2	O 2	0
40	3	1	Total 1	O 1	0
40	5	1	Total 1	O 1	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

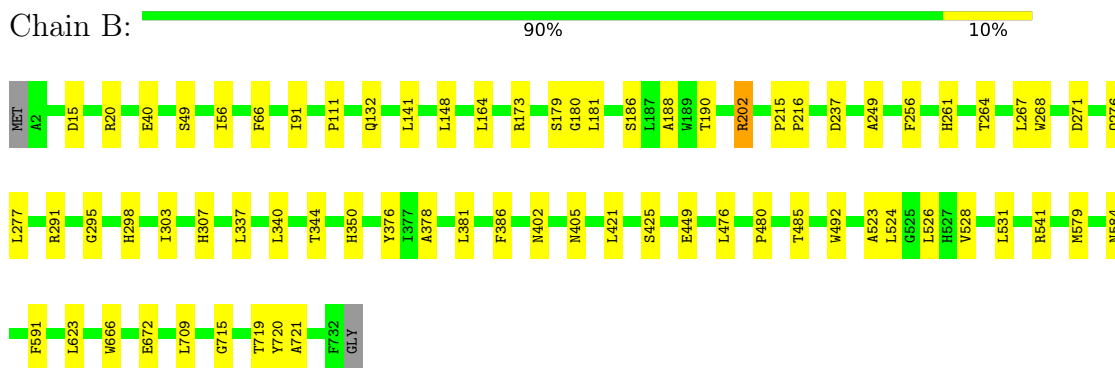
3 Residue-property plots

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

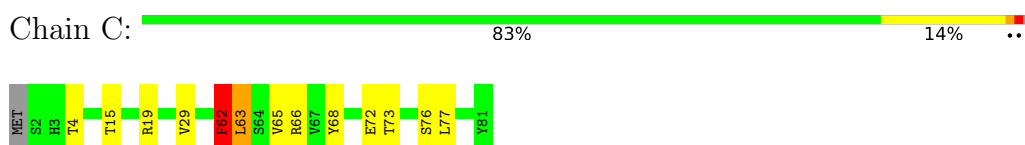
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



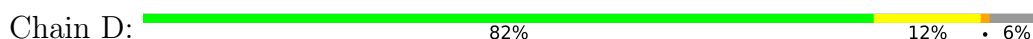
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



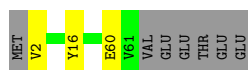
- Molecule 4: Photosystem I reaction center subunit II





- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 85% 10%



- Molecule 6: Photosystem I reaction center subunit III

Chain F: 81% 6% 13%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 94% . .



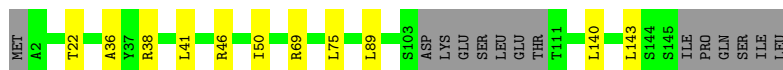
- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 76% 24%



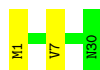
- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 83% 7% 9%



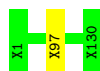
- Molecule 10: Photosystem I reaction center subunit XII

Chain M: 93% 7%



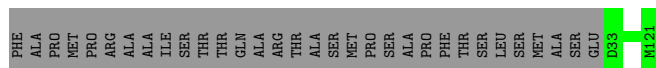
- Molecule 11: Unknown protein 1

Chain 1u: 99% .



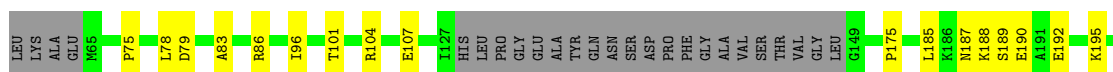
- Molecule 12: Photosystem I reaction center subunit Psa28

Chain 2u: 74% 26%



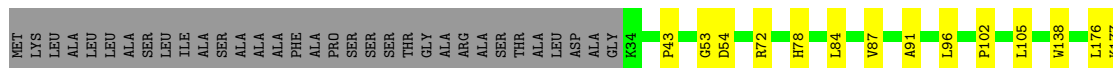
- Molecule 13: Fucoxanthin chlorophyll a/c-binding protein Lhcr15

Chain 1: 53% 9% 38%



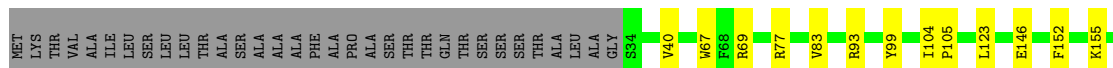
- Molecule 14: Fucoxanthin chlorophyll a/c-binding protein Lhcr8

Chain 2: 77% 7% 16%



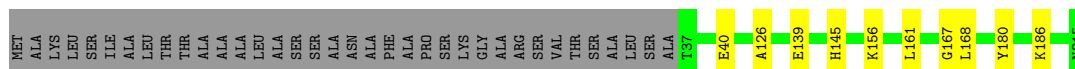
- Molecule 15: Fucoxanthin chlorophyll a/c-binding protein Lhcr2

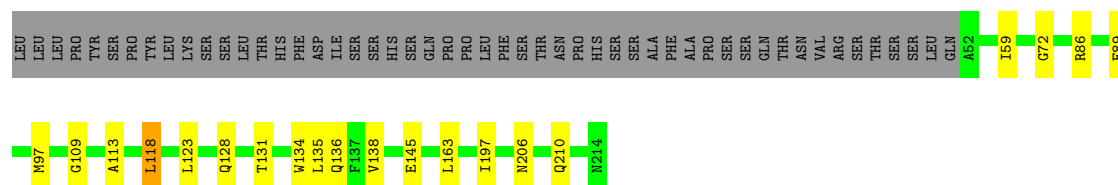
Chain 3: 74% 8% 18%



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

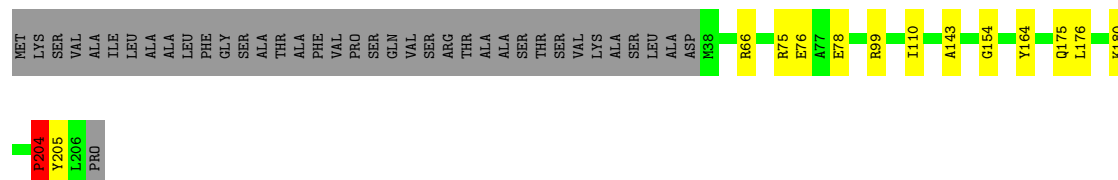
Chain 4: 79% 5% 17%





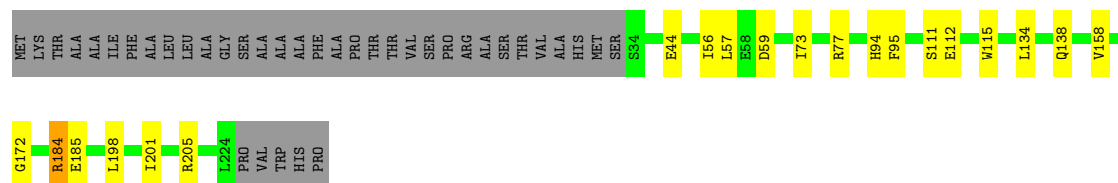
- Molecule 22: Fucoxanthin chlorophyll a/c-binding protein Lhcr3

Chain 10: 75% 6% 18%



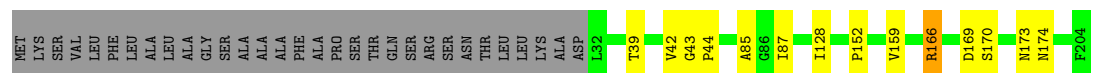
- Molecule 23: Fucoxanthin chlorophyll a/c-binding protein Lhcq13

Chain 11: 75% 8% 17%



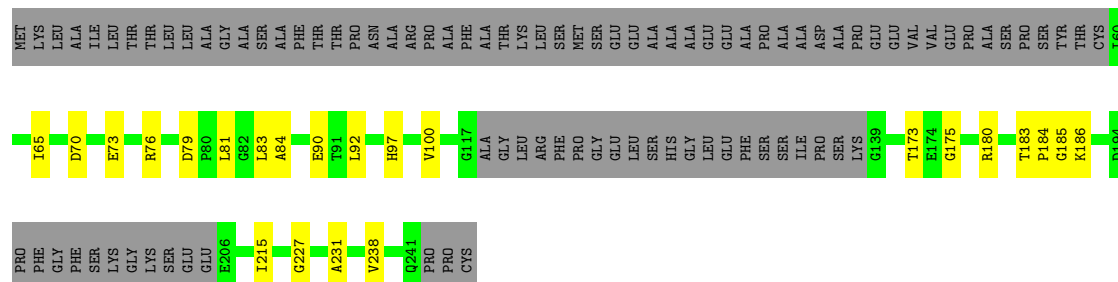
- Molecule 24: Fucoxanthin chlorophyll a/c-binding protein Lhcq3

Chain 12: 78% 6% 15%



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

Chain 13: 52% 9% 39%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	470801	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KC1, PQN, DD6, LMG, A86, LMT, CLA, BCR, SF4, CL0, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/6039	0.50	0/8220
2	B	0.38	0/6011	0.51	0/8209
3	C	0.44	0/609	0.63	1/826 (0.1%)
4	D	0.38	0/1064	0.62	0/1437
5	E	0.37	0/486	0.53	0/656
6	F	0.36	0/1287	0.50	0/1745
7	I	0.37	0/281	0.60	0/383
8	J	0.34	0/355	0.56	0/480
9	L	0.34	0/1054	0.49	0/1432
10	M	0.32	0/229	0.48	0/313
12	2u	0.32	0/696	0.45	0/948
13	1	0.30	0/1106	0.45	0/1490
14	2	0.35	0/1344	0.55	0/1818
15	3	0.32	0/1309	0.57	2/1767 (0.1%)
16	4	0.35	0/1404	0.51	0/1897
17	5	0.33	0/1336	0.52	0/1804
18	6	0.36	0/1391	0.48	0/1886
19	7	0.33	0/1445	0.48	0/1952
20	8	0.35	0/1706	0.49	0/2310
21	9	0.32	0/1302	0.54	1/1769 (0.1%)
22	10	0.32	0/1344	0.51	0/1824
23	11	0.30	0/1522	0.52	0/2070
24	12	0.32	0/1305	0.51	0/1776
25	13	0.31	0/1177	0.52	0/1592
26	14	0.55	4/1660 (0.2%)	1.29	23/2255 (1.0%)
27	15	0.61	2/1705 (0.1%)	1.46	33/2319 (1.4%)
28	16	0.48	1/1347 (0.1%)	0.98	12/1833 (0.7%)
All	All	0.38	7/40514 (0.0%)	0.65	72/55011 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
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

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	15	146	GLU	CB-CG	-10.73	1.31	1.52
28	16	70	GLU	CB-CG	-7.53	1.37	1.52
26	14	50	LYS	CD-CE	-6.61	1.34	1.51
26	14	206	GLU	CG-CD	-5.84	1.43	1.51
27	15	224	ARG	CB-CG	-5.79	1.36	1.52

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	92	MET	CA-CB-CG	25.47	156.60	113.30
27	15	224	ARG	NE-CZ-NH1	-23.93	108.33	120.30
27	15	224	ARG	NE-CZ-NH2	22.70	131.65	120.30
27	15	146	GLU	CA-CB-CG	16.51	149.72	113.40
26	14	92	MET	CB-CG-SD	13.82	153.87	112.40

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	71	0
2	B	5801	0	5614	50	0
3	C	599	0	579	6	0
4	D	1037	0	1023	10	0
5	E	478	0	473	2	0
6	F	1257	0	1259	11	0
7	I	273	0	285	1	0
8	J	344	0	351	10	0
9	L	1030	0	1063	11	0
10	M	227	0	247	2	0
11	1u	650	0	138	0	0
12	2u	674	0	658	0	0
13	1	1086	0	1089	13	0
14	2	1310	0	1287	13	0
15	3	1275	0	1239	9	0
16	4	1368	0	1344	8	0
17	5	1304	0	1286	10	0
18	6	1354	0	1328	13	0
19	7	1416	0	1379	8	0
20	8	1660	0	1625	16	0
21	9	1267	0	1210	12	0
22	10	1302	0	1274	8	0
23	11	1479	0	1452	16	0
24	12	1274	0	1267	10	0
25	13	1148	0	1130	16	0
26	14	1609	0	1568	22	0
27	15	1654	0	1613	21	0
28	16	1313	0	1309	22	0
29	A	65	0	72	3	0
30	1	390	0	425	12	0
30	10	435	0	465	7	0
30	11	315	0	337	11	0
30	12	566	0	604	12	0
30	13	350	0	354	11	0
30	14	468	0	400	8	0
30	15	685	0	589	16	0
30	16	478	0	429	13	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	0	0
30	3	472	0	474	8	0
30	4	484	0	495	14	0
30	5	455	0	499	12	0
30	6	620	0	656	13	0
30	7	566	0	609	14	0
30	8	420	0	427	8	0
30	9	486	0	503	12	0
30	A	2614	0	2694	105	0
30	B	2465	0	2570	91	0
30	F	175	0	177	9	0
30	J	45	0	33	1	0
30	L	110	0	105	7	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	0	0
33	A	200	0	280	13	0
33	B	240	0	336	12	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	5	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	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	70	0	92	0	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	1	0
36	7	37	0	44	0	0
36	8	108	0	123	1	0
36	A	34	0	38	2	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	2	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	55344	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 6.

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

5.3.1 Protein backbone

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%)	37	51
2	B	729/733 (100%)	699 (96%)	29 (4%)	1 (0%)	48	65
3	C	78/81 (96%)	73 (94%)	3 (4%)	2 (3%)	4	4
4	D	129/139 (93%)	109 (84%)	18 (14%)	2 (2%)	8	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%)	11	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%)	11	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%)	25	38
28	16	172/218 (79%)	157 (91%)	15 (9%)	0	100	100
All	All	5013/6068 (83%)	4694 (94%)	307 (6%)	12 (0%)	45	59

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%)	92	97
2	B	592/593 (100%)	589 (100%)	3 (0%)	86	94
3	C	69/70 (99%)	66 (96%)	3 (4%)	25	42
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%)	113 (99%)	1 (1%)	75	88
14	2	134/154 (87%)	134 (100%)	0	100	100
15	3	128/154 (83%)	127 (99%)	1 (1%)	79	90
16	4	142/165 (86%)	142 (100%)	0	100	100
17	5	137/228 (60%)	136 (99%)	1 (1%)	81	91
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%)	79	90
22	10	133/161 (83%)	133 (100%)	0	100	100
23	11	154/181 (85%)	153 (99%)	1 (1%)	84	92
24	12	136/159 (86%)	134 (98%)	2 (2%)	60	77
25	13	112/184 (61%)	111 (99%)	1 (1%)	75	88
26	14	166/196 (85%)	145 (87%)	21 (13%)	3	4
27	15	171/231 (74%)	151 (88%)	20 (12%)	4	6
28	16	139/174 (80%)	127 (91%)	12 (9%)	8	14
All	All	4069/4865 (84%)	4001 (98%)	68 (2%)	56	75

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	16	47	ASP
28	16	70	GLU
28	16	172	THR
26	14	156	LYS
26	14	133	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
22	10	175	GLN
28	16	177	GLN
22	10	201	HIS
26	14	183	ASN
2	B	632	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	A	813	1	65,73,73	2.03	18 (27%)	76,113,113	2.68	27 (35%)
33	BCR	B	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	6 (10%)
30	CLA	2	307	14	65,73,73	1.97	16 (24%)	76,113,113	2.62	27 (35%)
30	CLA	3	306	15	65,73,73	2.01	15 (23%)	76,113,113	2.65	29 (38%)
30	CLA	15	310	27	45,53,73	2.54	17 (37%)	52,89,113	3.22	23 (44%)
30	CLA	B	837	40	65,73,73	1.95	16 (24%)	76,113,113	2.68	26 (34%)
38	KC1	8	306	40	48,53,53	3.40	22 (45%)	55,89,89	3.75	27 (49%)
38	KC1	10	312	22	48,53,53	3.44	25 (52%)	55,89,89	3.83	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	12	310	40	65,73,73	1.98	16 (24%)	76,113,113	2.72	26 (34%)
38	KC1	2	314	40	48,53,53	3.43	24 (50%)	55,89,89	3.81	30 (54%)
30	CLA	A	824	1	51,59,73	2.23	17 (33%)	59,96,113	3.09	27 (45%)
38	KC1	2	312	14	48,53,53	3.42	25 (52%)	55,89,89	3.75	29 (52%)
30	CLA	7	310	19	65,73,73	2.02	16 (24%)	76,113,113	2.68	26 (34%)
39	DD6	9	314	-	39,45,45	6.65	22 (56%)	52,67,67	7.29	26 (50%)
30	CLA	A	834	1	65,73,73	1.96	17 (26%)	76,113,113	2.71	29 (38%)
30	CLA	A	843	40	65,73,73	1.94	16 (24%)	76,113,113	2.63	27 (35%)
30	CLA	14	302	26	65,73,73	2.05	16 (24%)	76,113,113	2.75	31 (40%)
39	DD6	12	315	30	39,45,45	6.70	22 (56%)	52,67,67	6.85	26 (50%)
39	DD6	2	316	-	39,45,45	6.62	22 (56%)	52,67,67	6.70	28 (53%)
30	CLA	1	301	13	65,73,73	2.00	17 (26%)	76,113,113	2.64	24 (31%)
37	A86	2	319	-	44,50,50	3.89	22 (50%)	51,76,76	7.61	18 (35%)
30	CLA	B	839	34	65,73,73	1.92	16 (24%)	76,113,113	2.86	27 (35%)
30	CLA	B	806	2	65,73,73	1.97	15 (23%)	76,113,113	2.67	27 (35%)
30	CLA	A	841	1	65,73,73	2.01	17 (26%)	76,113,113	2.62	28 (36%)
30	CLA	A	819	1	54,62,73	2.18	16 (29%)	62,99,113	2.95	27 (43%)
30	CLA	6	315	18	45,53,73	2.45	16 (35%)	52,89,113	3.17	24 (46%)
30	CLA	B	832	37,40	65,73,73	2.01	17 (26%)	76,113,113	2.69	28 (36%)
30	CLA	2	305	40	65,73,73	2.00	17 (26%)	76,113,113	2.77	28 (36%)
37	A86	5	301	-	44,50,50	4.06	24 (54%)	51,76,76	7.93	21 (41%)
39	DD6	3	312	-	39,45,45	6.71	23 (58%)	52,67,67	6.79	26 (50%)
33	BCR	L	204	-	41,41,41	1.09	1 (2%)	56,56,56	1.44	8 (14%)
34	LHG	5	317	30	26,26,48	0.84	1 (3%)	29,32,54	1.35	3 (10%)
38	KC1	12	313	24	48,53,53	3.45	22 (45%)	55,89,89	4.42	28 (50%)
30	CLA	J	101	8	45,53,73	2.42	17 (37%)	52,89,113	3.10	24 (46%)
37	A86	15	322	30	44,50,50	4.28	24 (54%)	51,76,76	8.43	21 (41%)
38	KC1	13	305	25	48,53,53	3.47	27 (56%)	55,89,89	3.85	31 (56%)
37	A86	2u	203	30	44,50,50	3.98	24 (54%)	51,76,76	8.18	21 (41%)
30	CLA	A	830	1	65,73,73	1.91	15 (23%)	76,113,113	2.61	29 (38%)
31	PQN	A	845	-	34,34,34	1.52	2 (5%)	42,45,45	1.10	3 (7%)
30	CLA	A	811	1	65,73,73	1.96	15 (23%)	76,113,113	2.70	25 (32%)
30	CLA	11	309	23	65,73,73	2.05	17 (26%)	76,113,113	2.70	28 (36%)
37	A86	16	314	-	44,50,50	4.12	23 (52%)	51,76,76	8.52	19 (37%)
30	CLA	A	802	40	65,73,73	1.97	15 (23%)	76,113,113	2.78	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	KC1	4	307	16	48,53,53	3.46	25 (52%)	55,89,89	3.70	29 (52%)
37	A86	14	301	26	44,50,50	4.10	23 (52%)	51,76,76	8.08	17 (33%)
38	KC1	13	306	25	48,53,53	3.47	26 (54%)	55,89,89	3.73	29 (52%)
30	CLA	14	312	37,26	45,53,73	2.47	16 (35%)	52,89,113	3.14	23 (44%)
30	CLA	A	842	1	65,73,73	1.97	17 (26%)	76,113,113	2.75	28 (36%)
30	CLA	B	810	2	65,73,73	1.95	17 (26%)	76,113,113	2.69	27 (35%)
38	KC1	5	312	17	48,53,53	3.38	23 (47%)	55,89,89	3.78	28 (50%)
30	CLA	1	305	40	65,73,73	2.06	18 (27%)	76,113,113	2.64	27 (35%)
33	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.19	6 (10%)
30	CLA	A	803	-	65,73,73	1.97	16 (24%)	76,113,113	2.68	30 (39%)
39	DD6	6	318	-	39,45,45	6.65	23 (58%)	52,67,67	6.55	29 (55%)
30	CLA	3	305	15	62,70,73	2.06	17 (27%)	72,109,113	2.74	30 (41%)
38	KC1	13	308	25	48,53,53	3.48	27 (56%)	55,89,89	3.91	29 (52%)
30	CLA	6	307	39,18	65,73,73	2.01	16 (24%)	76,113,113	2.57	30 (39%)
32	SF4	C	101	3	0,12,12	-	-	-	-	-
30	CLA	6	310	34	65,73,73	2.04	17 (26%)	76,113,113	2.62	26 (34%)
30	CLA	7	305	40,19	65,73,73	2.12	18 (27%)	76,113,113	2.78	29 (38%)
34	LHG	9	318	-	33,33,48	0.70	0	36,39,54	1.25	4 (11%)
30	CLA	12	304	24,39	65,73,73	2.04	18 (27%)	76,113,113	2.90	29 (38%)
30	CLA	16	307	-	46,54,73	2.44	17 (36%)	53,90,113	3.11	24 (45%)
39	DD6	5	313	-	39,45,45	6.74	23 (58%)	52,67,67	6.85	25 (48%)
37	A86	1	309	-	44,50,50	3.96	23 (52%)	51,76,76	8.68	21 (41%)
37	A86	7	315	-	44,50,50	3.90	23 (52%)	51,76,76	7.79	20 (39%)
30	CLA	A	814	1	60,68,73	2.06	16 (26%)	70,107,113	2.76	26 (37%)
35	LMT	11	303	-	36,36,36	0.40	0	47,47,47	0.84	0
39	DD6	8	317	-	39,45,45	6.64	22 (56%)	52,67,67	7.04	29 (55%)
33	BCR	L	201	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	5 (8%)
30	CLA	A	826	40	65,73,73	1.99	18 (27%)	76,113,113	2.72	26 (34%)
30	CLA	14	305	26	50,58,73	2.32	16 (32%)	58,95,113	3.02	27 (46%)
38	KC1	8	312	38	48,53,53	3.43	24 (50%)	55,89,89	3.29	28 (50%)
30	CLA	12	302	24	65,73,73	2.00	17 (26%)	76,113,113	2.76	31 (40%)
30	CLA	B	831	2	58,66,73	2.10	16 (27%)	67,104,113	2.98	27 (40%)
37	A86	11	315	-	44,50,50	3.99	22 (50%)	51,76,76	7.49	22 (43%)
38	KC1	7	308	40	48,53,53	3.43	24 (50%)	55,89,89	3.70	28 (50%)
30	CLA	A	825	1	59,67,73	2.09	17 (28%)	68,105,113	2.76	26 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	BCR	M	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.27	6 (10%)
39	DD6	7	314	-	39,45,45	6.64	21 (53%)	52,67,67	7.34	28 (53%)
30	CLA	9	301	34	65,73,73	1.99	17 (26%)	76,113,113	2.83	27 (35%)
30	CLA	A	829	30,1	65,73,73	1.99	17 (26%)	76,113,113	2.75	27 (35%)
35	LMT	A	854	-	36,36,36	0.45	0	47,47,47	1.19	5 (10%)
36	LMG	A	856	-	34,34,55	0.99	1 (2%)	42,42,63	1.19	3 (7%)
30	CLA	B	820	2	45,53,73	2.42	16 (35%)	52,89,113	3.39	22 (42%)
30	CLA	A	823	1	49,57,73	2.28	17 (34%)	55,93,113	3.16	26 (47%)
30	CLA	3	302	15	60,68,73	2.06	17 (28%)	70,107,113	2.78	30 (42%)
30	CLA	8	308	20	55,63,73	2.17	15 (27%)	64,101,113	2.92	27 (42%)
37	A86	2	318	-	44,50,50	4.04	23 (52%)	51,76,76	7.66	23 (45%)
30	CLA	7	303	19	65,73,73	1.95	15 (23%)	76,113,113	2.72	29 (38%)
30	CLA	B	830	2	65,73,73	1.93	17 (26%)	76,113,113	2.87	27 (35%)
34	LHG	6	322	30	26,26,48	0.88	1 (3%)	29,32,54	1.36	3 (10%)
30	CLA	B	816	2	55,63,73	2.12	16 (29%)	64,101,113	3.01	26 (40%)
37	A86	3	314	-	44,50,50	4.05	23 (52%)	51,76,76	8.17	19 (37%)
37	A86	14	319	30	44,50,50	4.09	22 (50%)	51,76,76	8.30	17 (33%)
30	CLA	A	805	30,1	59,67,73	2.11	15 (25%)	68,105,113	2.87	29 (42%)
30	CLA	3	303	15	65,73,73	2.09	18 (27%)	76,113,113	2.78	29 (38%)
39	DD6	1	310	-	39,45,45	6.70	23 (58%)	52,67,67	6.71	24 (46%)
38	KC1	6	308	18	48,53,53	3.36	23 (47%)	55,89,89	3.84	28 (50%)
30	CLA	10	309	22	65,73,73	2.05	17 (26%)	76,113,113	2.64	25 (32%)
30	CLA	A	809	30,1	65,73,73	1.97	17 (26%)	76,113,113	2.69	28 (36%)
30	CLA	14	313	26	46,54,73	2.42	16 (34%)	53,90,113	3.25	26 (49%)
30	CLA	4	311	16	50,58,73	2.33	17 (34%)	58,95,113	3.23	30 (51%)
33	BCR	B	842	-	41,41,41	1.07	2 (4%)	56,56,56	1.19	5 (8%)
37	A86	4	314	-	44,50,50	4.10	22 (50%)	51,76,76	8.17	22 (43%)
36	LMG	3	317	-	37,37,55	0.97	2 (5%)	45,45,63	1.42	7 (15%)
30	CLA	10	304	22	65,73,73	2.01	18 (27%)	76,113,113	2.66	26 (34%)
30	CLA	A	821	1	61,69,73	1.98	17 (27%)	71,108,113	2.73	28 (39%)
30	CLA	A	832	1	50,58,73	2.22	17 (34%)	58,95,113	3.05	28 (48%)
30	CLA	1	303	30,13	65,73,73	2.00	16 (24%)	76,113,113	2.69	27 (35%)
39	DD6	7	317	-	39,45,45	6.70	20 (51%)	52,67,67	6.69	29 (55%)
30	CLA	9	303	21	65,73,73	1.99	16 (24%)	76,113,113	2.69	27 (35%)
39	DD6	15	319	30	39,45,45	6.79	22 (56%)	52,67,67	6.92	30 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	DD6	6	321	-	39,45,45	6.60	23 (58%)	52,67,67	6.79	28 (53%)
30	CLA	10	303	22	65,73,73	2.01	15 (23%)	76,113,113	2.64	26 (34%)
30	CLA	B	817	2	59,67,73	2.07	16 (27%)	68,105,113	2.94	26 (38%)
38	KC1	3	311	40	48,53,53	3.44	24 (50%)	55,89,89	3.97	27 (49%)
30	CLA	B	807	2	65,73,73	1.93	18 (27%)	76,113,113	2.77	28 (36%)
30	CLA	12	306	24	65,73,73	1.97	17 (26%)	76,113,113	2.59	27 (35%)
30	CLA	11	310	23	65,73,73	2.10	17 (26%)	76,113,113	2.66	28 (36%)
30	CLA	A	827	40	65,73,73	1.93	18 (27%)	76,113,113	2.90	29 (38%)
30	CLA	12	312	24	65,73,73	2.02	16 (24%)	76,113,113	2.69	27 (35%)
37	A86	4	317	-	44,50,50	3.99	23 (52%)	51,76,76	7.58	20 (39%)
38	KC1	9	311	21	48,53,53	3.47	25 (52%)	55,89,89	3.90	31 (56%)
39	DD6	7	302	-	39,45,45	6.75	24 (61%)	52,67,67	6.58	28 (53%)
37	A86	10	315	-	44,50,50	4.10	22 (50%)	51,76,76	8.25	16 (31%)
30	CLA	B	838	2	65,73,73	1.96	14 (21%)	76,113,113	2.72	26 (34%)
30	CLA	5	307	17	65,73,73	2.00	19 (29%)	76,113,113	2.68	30 (39%)
30	CLA	7	312	19	46,54,73	2.44	17 (36%)	53,90,113	3.12	24 (45%)
30	CLA	2	308	14	65,73,73	2.02	15 (23%)	76,113,113	2.71	27 (35%)
30	CLA	B	802	30,40	65,73,73	1.92	17 (26%)	76,113,113	2.87	29 (38%)
30	CLA	A	828	1	65,73,73	1.92	16 (24%)	76,113,113	2.84	28 (36%)
35	LMT	12	301	-	36,36,36	0.43	0	47,47,47	0.76	0
30	CLA	13	304	25	45,53,73	2.50	16 (35%)	52,89,113	3.22	25 (48%)
30	CLA	B	821	2	55,63,73	2.16	15 (27%)	64,101,113	2.84	27 (42%)
37	A86	14	320	-	44,50,50	4.14	23 (52%)	51,76,76	7.22	21 (41%)
30	CLA	7	311	19	65,73,73	2.00	17 (26%)	76,113,113	2.60	26 (34%)
37	A86	9	313	21	44,50,50	3.98	23 (52%)	51,76,76	7.51	20 (39%)
33	BCR	J	103	-	41,41,41	1.15	3 (7%)	56,56,56	1.16	5 (8%)
38	KC1	6	311	18	48,53,53	3.36	23 (47%)	55,89,89	3.98	30 (54%)
39	DD6	6	303	30	39,45,45	6.78	23 (58%)	52,67,67	6.69	28 (53%)
30	CLA	A	844	-	65,73,73	2.06	16 (24%)	76,113,113	2.61	29 (38%)
38	KC1	7	313	-	48,53,53	3.36	22 (45%)	55,89,89	3.79	30 (54%)
39	DD6	13	314	-	39,45,45	6.78	22 (56%)	52,67,67	7.25	31 (59%)
30	CLA	8	304	20	58,66,73	2.08	16 (27%)	67,104,113	3.00	32 (47%)
30	CLA	A	804	1	65,73,73	1.95	16 (24%)	76,113,113	2.74	28 (36%)
39	DD6	15	318	-	39,45,45	6.78	21 (53%)	52,67,67	6.98	31 (59%)
30	CLA	13	309	-	45,53,73	2.48	16 (35%)	52,89,113	3.22	24 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	B	828	2	65,73,73	2.02	18 (27%)	76,113,113	2.74	28 (36%)
30	CLA	15	307	27	50,58,73	2.32	18 (36%)	58,95,113	3.02	26 (44%)
30	CLA	A	808	1	51,59,73	2.22	16 (31%)	59,96,113	3.06	26 (44%)
30	CLA	10	308	22	65,73,73	2.01	16 (24%)	76,113,113	2.63	26 (34%)
30	CLA	12	308	40	65,73,73	2.02	18 (27%)	76,113,113	2.63	27 (35%)
30	CLA	9	307	21	65,73,73	1.99	16 (24%)	76,113,113	2.68	26 (34%)
30	CLA	14	304	26	45,53,73	2.48	16 (35%)	52,89,113	3.19	23 (44%)
30	CLA	B	823	40	54,62,73	2.16	17 (31%)	62,99,113	2.93	27 (43%)
30	CLA	B	826	2	65,73,73	1.96	18 (27%)	76,113,113	2.74	28 (36%)
30	CLA	1	307	13	65,73,73	2.05	18 (27%)	76,113,113	2.73	27 (35%)
38	KC1	11	312	-	48,53,53	3.44	24 (50%)	55,89,89	3.58	29 (52%)
30	CLA	15	303	30,37,27	60,68,73	2.11	17 (28%)	70,107,113	2.88	27 (38%)
30	CLA	B	803	-	65,73,73	1.91	17 (26%)	76,113,113	2.69	28 (36%)
33	BCR	B	841	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	8 (14%)
30	CLA	3	310	15	45,53,73	2.40	17 (37%)	52,89,113	3.21	24 (46%)
30	CLA	8	302	20	65,73,73	2.02	18 (27%)	76,113,113	2.76	26 (34%)
30	CLA	8	305	20	65,73,73	1.99	18 (27%)	76,113,113	4.76	31 (40%)
30	CLA	A	815	1	65,73,73	2.03	16 (24%)	76,113,113	2.72	28 (36%)
37	A86	2	302	-	44,50,50	4.10	23 (52%)	51,76,76	8.41	18 (35%)
30	CLA	6	306	40	65,73,73	2.01	16 (24%)	76,113,113	2.70	27 (35%)
38	KC1	8	307	20	48,53,53	3.36	23 (47%)	55,89,89	3.88	30 (54%)
39	DD6	16	313	-	39,45,45	6.75	21 (53%)	52,67,67	7.13	30 (57%)
30	CLA	B	819	40	65,73,73	1.97	16 (24%)	76,113,113	2.43	28 (36%)
30	CLA	11	308	23	65,73,73	2.03	16 (24%)	76,113,113	2.66	27 (35%)
34	LHG	A	853	30	26,26,48	0.91	1 (3%)	29,32,54	1.29	3 (10%)
30	CLA	3	307	15	65,73,73	2.10	18 (27%)	76,113,113	2.64	26 (34%)
30	CLA	4	305	16	65,73,73	1.97	16 (24%)	76,113,113	2.69	27 (35%)
39	DD6	12	317	-	39,45,45	6.67	22 (56%)	52,67,67	7.20	28 (53%)
30	CLA	F	203	6	45,53,73	2.41	17 (37%)	52,89,113	3.19	26 (50%)
37	A86	15	315	27	44,50,50	4.30	23 (52%)	51,76,76	8.22	28 (54%)
38	KC1	11	305	23	48,53,53	3.42	25 (52%)	55,89,89	3.86	30 (54%)
30	CLA	15	311	37	45,53,73	2.49	16 (35%)	52,89,113	3.17	24 (46%)
30	CLA	A	833	1	65,73,73	2.02	19 (29%)	76,113,113	2.65	26 (34%)
30	CLA	14	309	26	45,53,73	2.50	17 (37%)	52,89,113	3.10	24 (46%)
30	CLA	2u	202	12	65,73,73	1.95	17 (26%)	76,113,113	2.73	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	BCR	A	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.24	7 (12%)
38	KC1	16	311	28	48,53,53	3.48	25 (52%)	55,89,89	3.70	26 (47%)
30	CLA	6	317	-	65,73,73	2.04	17 (26%)	76,113,113	2.69	26 (34%)
38	KC1	13	311	25	48,53,53	3.48	27 (56%)	55,89,89	3.61	29 (52%)
39	DD6	3	316	-	39,45,45	6.75	24 (61%)	52,67,67	6.80	26 (50%)
34	LHG	B	848	30	26,26,48	0.93	1 (3%)	29,32,54	1.39	4 (13%)
38	KC1	5	310	17	48,53,53	3.42	24 (50%)	55,89,89	3.91	30 (54%)
36	LMG	F	205	-	27,27,55	1.02	1 (3%)	35,35,63	1.25	5 (14%)
30	CLA	13	303	-	65,73,73	2.07	17 (26%)	76,113,113	2.76	29 (38%)
36	LMG	8	319	36,20	37,37,55	0.93	0	45,45,63	1.28	5 (11%)
37	A86	4	315	-	44,50,50	4.00	23 (52%)	51,76,76	7.94	19 (37%)
30	CLA	15	305	37,27	45,53,73	2.48	16 (35%)	52,89,113	3.16	26 (50%)
30	CLA	2	311	14	65,73,73	2.06	17 (26%)	76,113,113	2.64	24 (31%)
30	CLA	6	314	18	65,73,73	1.96	15 (23%)	76,113,113	2.78	30 (39%)
36	LMG	5	318	-	33,33,55	0.92	0	41,41,63	1.22	5 (12%)
30	CLA	B	827	2	65,73,73	1.95	16 (24%)	76,113,113	2.60	28 (36%)
30	CLA	4	303	16	65,73,73	1.99	17 (26%)	76,113,113	2.68	26 (34%)
38	KC1	14	306	26	48,53,53	3.44	27 (56%)	55,89,89	3.84	30 (54%)
30	CLA	2	304	14	65,73,73	2.02	16 (24%)	76,113,113	2.74	28 (36%)
38	KC1	4	308	16	48,53,53	3.48	24 (50%)	55,89,89	3.60	29 (52%)
38	KC1	8	311	40	48,53,53	3.36	23 (47%)	55,89,89	3.75	29 (52%)
38	KC1	9	312	21	48,53,53	3.43	25 (52%)	55,89,89	3.75	28 (50%)
37	A86	15	316	30	44,50,50	4.14	24 (54%)	51,76,76	7.80	17 (33%)
30	CLA	8	303	40	65,73,73	1.97	16 (24%)	76,113,113	2.64	28 (36%)
35	LMT	11	318	-	36,36,36	0.43	0	47,47,47	0.88	2 (4%)
37	A86	9	315	-	44,50,50	4.10	23 (52%)	51,76,76	7.06	19 (37%)
36	LMG	7	320	-	37,37,55	1.00	3 (8%)	45,45,63	1.25	5 (11%)
38	KC1	9	310	21	48,53,53	3.37	24 (50%)	55,89,89	3.92	28 (50%)
39	DD6	3	313	-	39,45,45	6.73	23 (58%)	52,67,67	6.66	24 (46%)
38	KC1	8	314	40,38	48,53,53	3.43	25 (52%)	55,89,89	3.72	29 (52%)
38	KC1	12	309	24	48,53,53	3.45	24 (50%)	55,89,89	3.72	30 (54%)
37	A86	12	314	-	44,50,50	4.02	22 (50%)	51,76,76	8.11	18 (35%)
30	CLA	B	829	2	65,73,73	1.94	15 (23%)	76,113,113	2.65	25 (32%)
30	CLA	L	202	9	65,73,73	1.94	16 (24%)	76,113,113	2.84	27 (35%)
30	CLA	A	810	1	65,73,73	1.98	18 (27%)	76,113,113	2.70	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	B	813	2	65,73,73	1.98	17 (26%)	76,113,113	2.67	26 (34%)
30	CLA	L	203	40	45,53,73	2.46	18 (40%)	52,89,113	3.19	23 (44%)
38	KC1	10	310	22	48,53,53	3.42	26 (54%)	55,89,89	3.93	30 (54%)
35	LMT	12	318	-	36,36,36	0.41	0	47,47,47	0.76	0
37	A86	16	312	28	44,50,50	4.06	23 (52%)	51,76,76	8.15	23 (45%)
30	CLA	B	822	30,2	65,73,73	1.97	17 (26%)	76,113,113	2.87	30 (39%)
35	LMT	9	317	-	33,33,36	0.49	0	44,44,47	1.11	5 (11%)
39	DD6	4	313	-	39,45,45	6.71	22 (56%)	52,67,67	6.72	26 (50%)
30	CLA	9	305	-	65,73,73	2.02	17 (26%)	76,113,113	2.85	30 (39%)
37	A86	12	316	-	44,50,50	4.08	23 (52%)	51,76,76	8.38	17 (33%)
37	A86	14	317	-	44,50,50	4.03	23 (52%)	51,76,76	8.75	18 (35%)
30	CLA	7	306	19	65,73,73	1.97	18 (27%)	76,113,113	2.60	28 (36%)
35	LMT	B	850	-	36,36,36	0.39	0	47,47,47	0.92	3 (6%)
37	A86	3	315	-	44,50,50	4.12	24 (54%)	51,76,76	8.24	16 (31%)
35	LMT	16	315	-	36,36,36	0.41	0	47,47,47	0.65	0
37	A86	4	312	-	44,50,50	3.92	23 (52%)	51,76,76	8.64	21 (41%)
30	CLA	16	301	28	65,73,73	2.00	16 (24%)	76,113,113	2.76	28 (36%)
38	KC1	10	306	22	48,53,53	3.39	25 (52%)	55,89,89	3.95	31 (56%)
39	DD6	11	313	-	39,45,45	6.77	23 (58%)	52,67,67	6.83	29 (55%)
35	LMT	8	322	-	36,36,36	0.40	0	47,47,47	0.73	1 (2%)
38	KC1	6	312	18	48,53,53	3.39	25 (52%)	55,89,89	3.69	30 (54%)
30	CLA	9	309	40,21	65,73,73	1.99	16 (24%)	76,113,113	2.59	27 (35%)
30	CLA	10	311	-	45,53,73	2.45	18 (40%)	52,89,113	3.19	24 (46%)
30	CLA	B	824	40	65,73,73	2.01	17 (26%)	76,113,113	4.67	29 (38%)
30	CLA	3	309	15	45,53,73	2.48	17 (37%)	52,89,113	3.24	24 (46%)
33	BCR	B	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	6 (10%)
37	A86	13	313	25	41,47,50	4.31	22 (53%)	49,72,76	8.60	17 (34%)
38	KC1	8	313	20	48,53,53	3.34	23 (47%)	55,89,89	3.80	29 (52%)
38	KC1	12	305	24	48,53,53	3.44	25 (52%)	55,89,89	3.81	30 (54%)
30	CLA	9	308	21	65,73,73	2.00	16 (24%)	76,113,113	2.83	31 (40%)
39	DD6	4	316	-	39,45,45	6.68	23 (58%)	52,67,67	7.33	26 (50%)
30	CLA	6	305	18	65,73,73	2.05	18 (27%)	76,113,113	2.69	27 (35%)
38	KC1	12	311	24	48,53,53	3.46	25 (52%)	55,89,89	3.91	34 (61%)
30	CLA	A	807	1	65,73,73	1.96	16 (24%)	76,113,113	2.75	29 (38%)
36	LMG	B	847	-	55,55,55	0.80	1 (1%)	63,63,63	1.37	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	KC1	6	313	18	48,53,53	3.41	23 (47%)	55,89,89	3.78	29 (52%)
30	CLA	2	303	14	55,63,73	2.42	16 (29%)	64,101,113	2.89	28 (43%)
37	A86	5	316	-	44,50,50	4.04	22 (50%)	51,76,76	8.02	17 (33%)
30	CLA	B	804	2	52,60,73	2.21	17 (32%)	60,97,113	3.07	29 (48%)
30	CLA	15	314	30,27	45,53,73	2.40	16 (35%)	52,89,113	3.30	24 (46%)
37	A86	10	316	-	44,50,50	3.92	24 (54%)	51,76,76	8.13	21 (41%)
37	A86	14	318	-	44,50,50	4.10	22 (50%)	51,76,76	8.48	16 (31%)
30	CLA	B	835	2	65,73,73	1.96	16 (24%)	76,113,113	2.74	29 (38%)
32	SF4	C	102	3	0,12,12	-	-	-	-	-
30	CLA	2	301	14,2	65,73,73	1.94	16 (24%)	76,113,113	2.83	26 (34%)
30	CLA	7	309	19	65,73,73	1.94	17 (26%)	76,113,113	2.65	24 (31%)
30	CLA	9	302	9,21	51,59,73	2.30	17 (33%)	59,96,113	3.16	28 (47%)
30	CLA	14	310	-	50,58,73	2.33	16 (32%)	58,95,113	3.09	26 (44%)
36	LMG	2u	204	12	31,31,55	1.12	3 (9%)	39,39,63	1.18	4 (10%)
38	KC1	3	304	15	48,53,53	3.43	26 (54%)	55,89,89	3.89	32 (58%)
30	CLA	A	835	1	65,73,73	1.99	17 (26%)	76,113,113	2.77	26 (34%)
38	KC1	1	306	13	48,53,53	3.45	25 (52%)	55,89,89	3.83	30 (54%)
38	KC1	16	304	28	48,53,53	3.50	25 (52%)	55,89,89	3.59	27 (49%)
33	BCR	B	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.38	8 (14%)
30	CLA	4	302	16	65,73,73	1.98	17 (26%)	76,113,113	2.63	25 (32%)
30	CLA	A	822	40	65,73,73	1.97	16 (24%)	76,113,113	2.52	27 (35%)
35	LMT	6	302	-	32,32,36	0.36	0	43,43,47	0.92	1 (2%)
30	CLA	5	309	34	65,73,73	2.01	17 (26%)	76,113,113	2.63	27 (35%)
30	CLA	13	307	25	65,73,73	2.09	17 (26%)	76,113,113	2.69	27 (35%)
30	CLA	B	815	2	45,53,73	2.37	16 (35%)	52,89,113	3.17	24 (46%)
30	CLA	A	820	1	65,73,73	2.02	17 (26%)	76,113,113	2.69	29 (38%)
35	LMT	7	321	-	36,36,36	0.32	0	47,47,47	0.75	2 (4%)
30	CLA	B	836	2	47,55,73	2.27	17 (36%)	54,91,113	3.25	25 (46%)
30	CLA	15	313	27	65,73,73	2.07	17 (26%)	76,113,113	2.74	28 (36%)
30	CLA	B	809	2	65,73,73	1.90	15 (23%)	76,113,113	2.60	24 (31%)
37	A86	10	317	-	44,50,50	4.19	23 (52%)	51,76,76	8.16	15 (29%)
33	BCR	A	850	-	41,41,41	1.13	2 (4%)	56,56,56	1.34	9 (16%)
36	LMG	B	849	2	43,43,55	0.95	2 (4%)	51,51,63	1.18	3 (5%)
30	CLA	7	304	19	65,73,73	1.97	16 (24%)	76,113,113	2.70	28 (36%)
35	LMT	11	317	-	36,36,36	0.43	0	47,47,47	0.89	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	A86	14	314	-	44,50,50	4.09	22 (50%)	51,76,76	8.27	21 (41%)
35	LMT	15	301	-	36,36,36	0.51	0	47,47,47	1.13	3 (6%)
38	KC1	11	307	23	48,53,53	3.46	25 (52%)	55,89,89	3.79	30 (54%)
38	KC1	13	312	25	48,53,53	3.54	27 (56%)	55,89,89	3.77	29 (52%)
36	LMG	8	320	-	42,42,55	0.90	3 (7%)	50,50,63	1.31	5 (10%)
38	KC1	14	308	30,26	48,53,53	3.45	26 (54%)	55,89,89	3.77	30 (54%)
30	CLA	12	307	24	46,54,73	2.33	16 (34%)	53,90,113	3.17	25 (47%)
39	DD6	7	318	-	39,45,45	6.70	21 (53%)	52,67,67	6.91	29 (55%)
33	BCR	F	204	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	8 (14%)
37	A86	13	315	-	44,50,50	4.18	23 (52%)	51,76,76	8.50	18 (35%)
30	CLA	A	816	1,35	65,73,73	1.96	17 (26%)	76,113,113	2.68	26 (34%)
30	CLA	B	834	2	60,68,73	2.11	18 (30%)	70,107,113	2.85	27 (38%)
39	DD6	6	319	-	39,45,45	6.71	23 (58%)	52,67,67	6.51	31 (59%)
30	CLA	3	301	15	65,73,73	1.97	17 (26%)	76,113,113	2.74	27 (35%)
30	CLA	1	302	30,13	65,73,73	2.00	16 (24%)	76,113,113	2.69	26 (34%)
30	CLA	A	839	1	65,73,73	1.96	15 (23%)	76,113,113	2.83	30 (39%)
30	CLA	12	303	24	65,73,73	2.04	19 (29%)	76,113,113	2.66	26 (34%)
37	A86	8	315	-	44,50,50	3.75	22 (50%)	51,76,76	8.45	20 (39%)
30	CLA	15	308	30,27	45,53,73	2.43	18 (40%)	52,89,113	3.11	26 (50%)
37	A86	14	316	-	44,50,50	4.03	23 (52%)	51,76,76	8.16	18 (35%)
30	CLA	B	825	2	65,73,73	1.99	18 (27%)	76,113,113	2.77	29 (38%)
30	CLA	11	306	40	55,63,73	2.19	16 (29%)	64,101,113	3.02	30 (46%)
30	CLA	A	806	1	65,73,73	1.98	17 (26%)	76,113,113	2.92	29 (38%)
35	LMT	11	302	-	36,36,36	0.34	0	47,47,47	0.77	2 (4%)
37	A86	11	301	-	44,50,50	4.04	23 (52%)	51,76,76	8.20	21 (41%)
30	CLA	B	805	2	65,73,73	2.00	17 (26%)	76,113,113	2.72	27 (35%)
36	LMG	8	321	36	29,29,55	1.11	2 (6%)	37,37,63	1.27	5 (13%)
30	CLA	B	801	2	65,73,73	1.87	17 (26%)	76,113,113	2.81	31 (40%)
35	LMT	7	301	30	36,36,36	0.41	0	47,47,47	0.80	1 (2%)
39	DD6	2	315	-	39,45,45	6.74	23 (58%)	52,67,67	6.78	27 (51%)
30	CLA	B	808	2	65,73,73	1.94	16 (24%)	76,113,113	2.75	28 (36%)
37	A86	15	320	-	44,50,50	4.24	24 (54%)	51,76,76	8.23	19 (37%)
38	KC1	2	306	14	48,53,53	3.44	26 (54%)	55,89,89	3.90	31 (56%)
38	KC1	13	310	25	48,53,53	3.47	25 (52%)	55,89,89	3.83	29 (52%)
30	CLA	F	202	40	65,73,73	2.01	18 (27%)	76,113,113	2.70	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	LMG	14	321	-	38,38,55	1.03	3 (7%)	46,46,63	1.20	3 (6%)
30	CLA	A	817	40,36	49,57,73	2.30	15 (30%)	55,93,113	3.15	23 (41%)
38	KC1	9	304	21	48,53,53	3.40	23 (47%)	55,89,89	3.79	30 (54%)
30	CLA	2	310	14	65,73,73	2.03	16 (24%)	76,113,113	4.67	29 (38%)
30	CLA	16	305	28	50,58,73	2.28	19 (38%)	58,95,113	3.00	27 (46%)
30	CLA	10	305	40	65,73,73	1.99	16 (24%)	76,113,113	2.80	30 (39%)
38	KC1	8	310	20	48,53,53	3.35	23 (47%)	55,89,89	3.74	29 (52%)
33	BCR	B	846	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	5 (8%)
30	CLA	A	838	1	51,59,73	2.27	17 (33%)	59,96,113	3.10	26 (44%)
35	LMT	A	857	-	36,36,36	0.37	0	47,47,47	0.78	0
30	CLA	B	833	30,40	65,73,73	1.97	18 (27%)	76,113,113	2.64	26 (34%)
37	A86	7	319	-	44,50,50	4.10	23 (52%)	51,76,76	8.25	22 (43%)
38	KC1	4	310	16	48,53,53	3.46	26 (54%)	55,89,89	3.91	29 (52%)
30	CLA	15	304	30,39,27	65,73,73	2.09	16 (24%)	76,113,113	2.75	26 (34%)
35	LMT	12	319	-	36,36,36	0.40	0	47,47,47	0.86	0
30	CLA	B	818	2	60,68,73	2.04	14 (23%)	70,107,113	2.88	29 (41%)
30	CLA	1	304	13	65,73,73	1.99	16 (24%)	76,113,113	2.59	27 (35%)
38	KC1	14	311	26	48,53,53	3.44	25 (52%)	55,89,89	3.80	29 (52%)
30	CLA	9	306	37,21	45,53,73	2.48	15 (33%)	52,89,113	3.21	26 (50%)
38	KC1	5	306	17	48,53,53	3.41	24 (50%)	55,89,89	4.11	30 (54%)
30	CLA	8	309	20	47,55,73	2.38	17 (36%)	54,91,113	3.05	24 (44%)
37	A86	10	301	22	44,50,50	3.86	23 (52%)	51,76,76	7.28	23 (45%)
37	A86	15	321	27	44,50,50	4.11	23 (52%)	51,76,76	8.63	19 (37%)
30	CLA	6	316	40	55,63,73	2.22	17 (30%)	64,101,113	2.80	25 (39%)
30	CLA	5	311	40,17	65,73,73	2.05	18 (27%)	76,113,113	2.80	26 (34%)
30	CLA	A	836	1	54,62,73	2.17	16 (29%)	62,99,113	2.85	29 (46%)
34	LHG	2	320	30	26,26,48	0.87	1 (3%)	29,32,54	1.30	3 (10%)
39	DD6	5	314	-	39,45,45	6.56	24 (61%)	52,67,67	7.17	30 (57%)
32	SF4	A	846	1,2	0,12,12	-	-	-	-	-
30	CLA	B	811	30,2	65,73,73	1.97	17 (26%)	76,113,113	2.62	31 (40%)
30	CLA	10	307	22	65,73,73	1.96	17 (26%)	76,113,113	2.61	27 (35%)
33	BCR	A	848	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	4 (7%)
35	LMT	A	855	-	36,36,36	0.39	0	47,47,47	0.89	3 (6%)
30	CLA	5	304	17	65,73,73	2.08	18 (27%)	76,113,113	2.72	29 (38%)
35	LMT	1	311	-	36,36,36	0.40	0	47,47,47	0.78	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	15	302	30,27	65,73,73	2.06	16 (24%)	76,113,113	2.93	29 (38%)
30	CLA	5	303	17	65,73,73	1.98	17 (26%)	76,113,113	2.64	28 (36%)
35	LMT	B	852	-	36,36,36	0.36	0	47,47,47	1.12	2 (4%)
38	KC1	1	308	13	48,53,53	3.44	26 (54%)	55,89,89	3.81	28 (50%)
30	CLA	15	309	27	65,73,73	2.09	17 (26%)	76,113,113	2.68	26 (34%)
38	KC1	5	305	17	48,53,53	3.42	25 (52%)	55,89,89	3.80	29 (52%)
30	CLA	F	201	40	65,73,73	1.92	17 (26%)	76,113,113	2.65	27 (35%)
30	CLA	2	313	14	45,53,73	2.47	16 (35%)	52,89,113	3.21	25 (48%)
37	A86	6	320	-	44,50,50	3.90	23 (52%)	51,76,76	7.09	20 (39%)
37	A86	10	302	-	44,50,50	4.06	23 (52%)	51,76,76	8.39	17 (33%)
30	CLA	A	831	1	65,73,73	1.98	16 (24%)	76,113,113	2.83	28 (36%)
33	BCR	A	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	9 (16%)
37	A86	11	314	-	44,50,50	4.09	23 (52%)	51,76,76	8.59	18 (35%)
39	DD6	2	317	-	39,45,45	6.77	22 (56%)	52,67,67	6.58	28 (53%)
30	CLA	16	302	28	65,73,73	1.99	17 (26%)	76,113,113	2.69	26 (34%)
37	A86	7	316	-	44,50,50	3.75	22 (50%)	51,76,76	7.71	27 (52%)
39	DD6	10	313	-	39,45,45	6.78	24 (61%)	52,67,67	7.12	30 (57%)
30	CLA	14	307	38	65,73,73	2.05	16 (24%)	76,113,113	2.81	24 (31%)
30	CLA	B	814	2	55,63,73	2.16	17 (30%)	64,101,113	2.84	27 (42%)
30	CLA	11	304	23	65,73,73	2.04	16 (24%)	76,113,113	2.69	25 (32%)
30	CLA	16	309	28	45,53,73	2.48	17 (37%)	52,89,113	3.26	24 (46%)
39	DD6	10	314	-	39,45,45	6.73	23 (58%)	52,67,67	6.78	28 (53%)
38	KC1	3	308	15	48,53,53	3.38	25 (52%)	55,89,89	3.81	29 (52%)
30	CLA	16	308	28	45,53,73	2.47	17 (37%)	52,89,113	3.21	25 (48%)
30	CLA	16	310	28	45,53,73	2.46	18 (40%)	52,89,113	3.21	26 (50%)
30	CLA	6	304	18	65,73,73	1.98	16 (24%)	76,113,113	2.75	28 (36%)
37	A86	2u	205	-	44,50,50	4.13	23 (52%)	51,76,76	7.47	22 (43%)
37	A86	9	316	30	44,50,50	4.22	22 (50%)	51,76,76	8.44	16 (31%)
30	CLA	16	303	28	65,73,73	2.01	15 (23%)	76,113,113	2.86	28 (36%)
30	CLA	5	308	17	65,73,73	2.00	16 (24%)	76,113,113	2.70	28 (36%)
30	CLA	4	304	-	60,68,73	2.08	15 (25%)	70,107,113	2.78	28 (40%)
30	CLA	B	851	14,2	65,73,73	1.98	17 (26%)	76,113,113	2.67	30 (39%)
30	CLA	16	306	28	52,60,73	2.26	18 (34%)	60,97,113	2.95	28 (46%)
33	BCR	L	205	-	41,41,41	1.06	2 (4%)	56,56,56	1.24	5 (8%)
30	CLA	12	321	24,26	65,73,73	2.04	17 (26%)	76,113,113	2.63	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CLA	15	306	-	45,53,73	2.47	17 (37%)	52,89,113	3.29	23 (44%)
37	A86	15	317	30	44,50,50	4.15	23 (52%)	51,76,76	8.44	15 (29%)
30	CLA	4	301	16,2	49,57,73	2.25	18 (36%)	55,93,113	3.13	24 (43%)
29	CL0	A	801	1	65,73,73	1.92	17 (26%)	76,113,113	2.76	29 (38%)
30	CLA	14	303	26	57,65,73	2.19	16 (28%)	66,103,113	2.88	29 (43%)
30	CLA	8	301	20	65,73,73	2.00	17 (26%)	76,113,113	2.71	29 (38%)
33	BCR	2u	201	-	41,41,41	1.22	4 (9%)	56,56,56	1.38	7 (12%)
30	CLA	6	309	18	65,73,73	2.00	15 (23%)	76,113,113	2.68	31 (40%)
30	CLA	15	312	27	45,53,73	2.47	16 (35%)	52,89,113	3.33	28 (53%)
30	CLA	A	837	1	45,53,73	2.43	17 (37%)	52,89,113	3.15	24 (46%)
30	CLA	A	840	1	47,55,73	2.31	17 (36%)	54,91,113	3.27	26 (48%)
30	CLA	5	302	17	65,73,73	1.98	16 (24%)	76,113,113	2.66	27 (35%)
30	CLA	B	812	2	65,73,73	2.05	17 (26%)	76,113,113	2.57	26 (34%)
37	A86	8	318	-	44,50,50	3.98	24 (54%)	51,76,76	10.85	23 (45%)
30	CLA	13	301	25	65,73,73	1.99	16 (24%)	76,113,113	2.81	26 (34%)
30	CLA	4	309	-	65,73,73	2.09	17 (26%)	76,113,113	2.70	28 (36%)
33	BCR	I	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	5 (8%)
37	A86	14	315	26	44,50,50	3.99	23 (52%)	51,76,76	8.87	22 (43%)
34	LHG	A	852	-	48,48,48	0.64	1 (2%)	51,54,54	1.20	5 (9%)
36	LMG	6	301	30	33,33,55	0.95	1 (3%)	41,41,63	1.21	4 (9%)
30	CLA	A	812	30,1	65,73,73	1.93	18 (27%)	76,113,113	2.79	26 (34%)
38	KC1	11	311	23	48,53,53	3.49	26 (54%)	55,89,89	3.81	29 (52%)
37	A86	15	323	-	44,50,50	4.19	23 (52%)	51,76,76	8.39	17 (33%)
30	CLA	13	302	25	65,73,73	2.03	17 (26%)	76,113,113	2.62	27 (35%)
33	BCR	A	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.25	6 (10%)
37	A86	11	316	-	44,50,50	4.05	23 (52%)	51,76,76	8.21	16 (31%)
30	CLA	7	307	19	65,73,73	1.97	16 (24%)	76,113,113	2.69	25 (32%)
30	CLA	4	306	16	65,73,73	2.00	16 (24%)	76,113,113	2.68	28 (36%)
31	PQN	B	840	-	34,34,34	1.50	2 (5%)	42,45,45	1.09	4 (9%)
35	LMT	12	320	-	36,36,36	0.39	0	47,47,47	0.71	0
30	CLA	A	818	1	54,62,73	2.11	16 (29%)	62,99,113	3.04	27 (43%)
37	A86	5	315	-	44,50,50	4.05	23 (52%)	51,76,76	8.37	18 (35%)
39	DD6	8	316	-	39,45,45	6.57	22 (56%)	52,67,67	6.80	30 (57%)
30	CLA	2	309	14,34	65,73,73	2.03	17 (26%)	76,113,113	2.67	28 (36%)

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	A	813	1	1/1/15/20	13/37/115/115	-
33	BCR	B	843	-	-	9/29/63/63	0/2/2/2
30	CLA	2	307	14	1/1/15/20	7/37/115/115	-
30	CLA	3	306	15	1/1/15/20	8/37/115/115	-
30	CLA	15	310	27	1/1/11/20	6/13/91/115	-
30	CLA	B	837	40	1/1/15/20	5/37/115/115	-
38	KC1	8	306	40	-	8/15/71/71	-
38	KC1	10	312	22	-	5/15/71/71	-
30	CLA	12	310	40	-	8/37/115/115	-
38	KC1	2	314	40	-	7/15/71/71	-
30	CLA	A	824	1	1/1/12/20	3/21/99/115	-
38	KC1	2	312	14	-	2/15/71/71	-
30	CLA	7	310	19	-	11/37/115/115	-
39	DD6	9	314	-	-	11/26/80/80	0/3/3/3
30	CLA	A	834	1	1/1/15/20	10/37/115/115	-
30	CLA	A	843	40	1/1/15/20	7/37/115/115	-
30	CLA	14	302	26	1/1/15/20	14/37/115/115	-
39	DD6	12	315	30	-	9/26/80/80	0/3/3/3
39	DD6	2	316	-	-	12/26/80/80	0/3/3/3
30	CLA	1	301	13	1/1/15/20	13/37/115/115	-
37	A86	2	319	-	-	12/34/90/90	0/3/3/3
30	CLA	B	839	34	1/1/15/20	4/37/115/115	-
30	CLA	B	806	2	1/1/15/20	9/37/115/115	-
30	CLA	A	841	1	1/1/15/20	10/37/115/115	-
30	CLA	A	819	1	-	6/24/102/115	-
30	CLA	6	315	18	1/1/11/20	3/13/91/115	-
30	CLA	B	832	37,40	1/1/15/20	5/37/115/115	-
30	CLA	2	305	40	1/1/15/20	9/37/115/115	-
37	A86	5	301	-	-	11/34/90/90	0/3/3/3
39	DD6	3	312	-	-	12/26/80/80	0/3/3/3
33	BCR	L	204	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LHG	5	317	30	-	4/31/31/53	-
38	KC1	12	313	24	-	7/15/71/71	-
30	CLA	J	101	8	1/1/11/20	3/13/91/115	-
37	A86	15	322	30	-	15/34/90/90	0/3/3/3
38	KC1	13	305	25	-	8/15/71/71	-
37	A86	2u	203	30	-	15/34/90/90	0/3/3/3
30	CLA	A	830	1	1/1/15/20	9/37/115/115	-
31	PQN	A	845	-	-	7/23/43/43	0/2/2/2
30	CLA	A	811	1	1/1/15/20	12/37/115/115	-
30	CLA	11	309	23	-	16/37/115/115	-
37	A86	16	314	-	-	11/34/90/90	0/3/3/3
30	CLA	A	802	40	1/1/15/20	6/37/115/115	-
38	KC1	4	307	16	-	6/15/71/71	-
37	A86	14	301	26	-	8/34/90/90	0/3/3/3
38	KC1	13	306	25	-	9/15/71/71	-
30	CLA	14	312	37,26	-	7/13/91/115	-
30	CLA	A	842	1	1/1/15/20	10/37/115/115	-
30	CLA	B	810	2	1/1/15/20	10/37/115/115	-
38	KC1	5	312	17	-	4/15/71/71	-
30	CLA	1	305	40	1/1/15/20	9/37/115/115	-
33	BCR	J	102	-	-	12/29/63/63	0/2/2/2
30	CLA	A	803	-	1/1/15/20	8/37/115/115	-
39	DD6	6	318	-	-	11/26/80/80	0/3/3/3
30	CLA	3	305	15	1/1/14/20	12/34/112/115	-
38	KC1	13	308	25	-	10/15/71/71	-
30	CLA	6	307	39,18	1/1/15/20	11/37/115/115	-
32	SF4	C	101	3	-	-	0/6/5/5
30	CLA	6	310	34	1/1/15/20	8/37/115/115	-
30	CLA	7	305	40,19	1/1/15/20	8/37/115/115	-
34	LHG	9	318	-	-	21/38/38/53	-
30	CLA	12	304	24,39	1/1/15/20	14/37/115/115	-
30	CLA	16	307	-	1/1/11/20	7/15/93/115	-
39	DD6	5	313	-	-	9/26/80/80	0/3/3/3
37	A86	1	309	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	A86	7	315	-	-	15/34/90/90	0/3/3/3
30	CLA	A	814	1	1/1/14/20	10/31/109/115	-
35	LMT	11	303	-	-	11/21/61/61	0/2/2/2
39	DD6	8	317	-	-	10/26/80/80	0/3/3/3
33	BCR	L	201	-	-	12/29/63/63	0/2/2/2
30	CLA	A	826	40	1/1/15/20	14/37/115/115	-
30	CLA	14	305	26	1/1/12/20	2/19/97/115	-
38	KC1	8	312	38	-	9/15/71/71	-
30	CLA	12	302	24	-	13/37/115/115	-
30	CLA	B	831	2	-	8/29/107/115	-
37	A86	11	315	-	-	13/34/90/90	0/3/3/3
38	KC1	7	308	40	-	7/15/71/71	-
30	CLA	A	825	1	1/1/13/20	13/30/108/115	-
33	BCR	M	101	-	-	11/29/63/63	0/2/2/2
39	DD6	7	314	-	-	11/26/80/80	0/3/3/3
30	CLA	9	301	34	1/1/15/20	10/37/115/115	-
30	CLA	A	829	30,1	1/1/15/20	14/37/115/115	-
35	LMT	A	854	-	-	15/21/61/61	0/2/2/2
36	LMG	A	856	-	-	15/29/49/70	0/1/1/1
30	CLA	B	820	2	-	2/13/91/115	-
30	CLA	3	302	15	1/1/14/20	7/31/109/115	-
30	CLA	A	823	1	-	6/18/96/115	-
30	CLA	8	308	20	1/1/13/20	10/25/103/115	-
37	A86	2	318	-	-	8/34/90/90	0/3/3/3
30	CLA	7	303	19	1/1/15/20	11/37/115/115	-
30	CLA	B	830	2	1/1/15/20	12/37/115/115	-
34	LHG	6	322	30	-	12/31/31/53	-
30	CLA	B	816	2	-	7/25/103/115	-
37	A86	3	314	-	-	9/34/90/90	0/3/3/3
37	A86	14	319	30	-	11/34/90/90	0/3/3/3
30	CLA	A	805	30,1	1/1/13/20	9/30/108/115	-
30	CLA	3	303	15	1/1/15/20	14/37/115/115	-
39	DD6	1	310	-	-	13/26/80/80	0/3/3/3
38	KC1	6	308	18	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	10	309	22	1/1/15/20	10/37/115/115	-
30	CLA	A	809	30,1	1/1/15/20	15/37/115/115	-
30	CLA	14	313	26	1/1/11/20	4/15/93/115	-
30	CLA	4	311	16	1/1/12/20	1/19/97/115	-
33	BCR	B	842	-	-	10/29/63/63	0/2/2/2
37	A86	4	314	-	-	11/34/90/90	0/3/3/3
36	LMG	3	317	-	-	18/32/52/70	0/1/1/1
30	CLA	10	304	22	1/1/15/20	3/37/115/115	-
30	CLA	A	821	1	1/1/14/20	11/33/111/115	-
30	CLA	A	832	1	-	5/19/97/115	-
30	CLA	1	303	30,13	1/1/15/20	13/37/115/115	-
39	DD6	7	317	-	-	10/26/80/80	0/3/3/3
30	CLA	9	303	21	-	9/37/115/115	-
39	DD6	15	319	30	-	13/26/80/80	0/3/3/3
39	DD6	6	321	-	-	12/26/80/80	0/3/3/3
30	CLA	10	303	22	1/1/15/20	13/37/115/115	-
30	CLA	B	817	2	1/1/13/20	5/30/108/115	-
38	KC1	3	311	40	-	6/15/71/71	-
30	CLA	B	807	2	1/1/15/20	9/37/115/115	-
30	CLA	12	306	24	1/1/15/20	6/37/115/115	-
30	CLA	11	310	23	1/1/15/20	15/37/115/115	-
30	CLA	A	827	40	1/1/15/20	5/37/115/115	-
30	CLA	12	312	24	1/1/15/20	12/37/115/115	-
37	A86	4	317	-	-	6/34/90/90	0/3/3/3
38	KC1	9	311	21	-	8/15/71/71	-
39	DD6	7	302	-	-	12/26/80/80	0/3/3/3
37	A86	10	315	-	-	13/34/90/90	0/3/3/3
30	CLA	B	838	2	1/1/15/20	17/37/115/115	-
30	CLA	5	307	17	1/1/15/20	14/37/115/115	-
30	CLA	7	312	19	1/1/11/20	6/15/93/115	-
30	CLA	2	308	14	-	9/37/115/115	-
30	CLA	B	802	30,40	1/1/15/20	10/37/115/115	-
30	CLA	A	828	1	1/1/15/20	13/37/115/115	-
35	LMT	12	301	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	13	304	25	-	7/13/91/115	-
30	CLA	B	821	2	1/1/13/20	14/25/103/115	-
37	A86	14	320	-	-	9/34/90/90	0/3/3/3
30	CLA	7	311	19	1/1/15/20	12/37/115/115	-
37	A86	9	313	21	-	8/34/90/90	0/3/3/3
33	BCR	J	103	-	-	9/29/63/63	0/2/2/2
38	KC1	6	311	18	-	10/15/71/71	-
39	DD6	6	303	30	-	10/26/80/80	0/3/3/3
30	CLA	A	844	-	1/1/15/20	12/37/115/115	-
38	KC1	7	313	-	-	4/15/71/71	-
39	DD6	13	314	-	-	13/26/80/80	0/3/3/3
30	CLA	8	304	20	1/1/13/20	9/29/107/115	-
30	CLA	A	804	1	1/1/15/20	11/37/115/115	-
39	DD6	15	318	-	-	13/26/80/80	0/3/3/3
30	CLA	13	309	-	1/1/11/20	8/13/91/115	-
30	CLA	B	828	2	1/1/15/20	14/37/115/115	-
30	CLA	15	307	27	1/1/12/20	7/19/97/115	-
30	CLA	A	808	1	1/1/12/20	3/21/99/115	-
30	CLA	10	308	22	1/1/15/20	11/37/115/115	-
30	CLA	12	308	40	1/1/15/20	11/37/115/115	-
30	CLA	9	307	21	1/1/15/20	9/37/115/115	-
30	CLA	14	304	26	1/1/11/20	4/13/91/115	-
30	CLA	B	823	40	1/1/12/20	3/24/102/115	-
30	CLA	B	826	2	1/1/15/20	14/37/115/115	-
30	CLA	1	307	13	-	17/37/115/115	-
38	KC1	11	312	-	-	5/15/71/71	-
30	CLA	15	303	30,37,27	1/1/14/20	9/31/109/115	-
30	CLA	B	803	-	1/1/15/20	6/37/115/115	-
33	BCR	B	841	-	-	10/29/63/63	0/2/2/2
30	CLA	8	302	20	1/1/15/20	8/37/115/115	-
30	CLA	3	310	15	-	4/13/91/115	-
30	CLA	8	305	20	-	13/37/115/115	-
30	CLA	A	815	1	1/1/15/20	7/37/115/115	-
37	A86	2	302	-	-	11/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	6	306	40	1/1/15/20	9/37/115/115	-
38	KC1	8	307	20	-	8/15/71/71	-
39	DD6	16	313	-	-	13/26/80/80	0/3/3/3
30	CLA	B	819	40	1/1/15/20	9/37/115/115	-
30	CLA	11	308	23	1/1/15/20	10/37/115/115	-
34	LHG	A	853	30	-	9/31/31/53	-
30	CLA	3	307	15	1/1/15/20	14/37/115/115	-
30	CLA	4	305	16	1/1/15/20	9/37/115/115	-
39	DD6	12	317	-	-	13/26/80/80	0/3/3/3
30	CLA	F	203	6	1/1/11/20	6/13/91/115	-
37	A86	15	315	27	-	9/34/90/90	0/3/3/3
38	KC1	11	305	23	-	7/15/71/71	-
30	CLA	15	311	37	1/1/11/20	7/13/91/115	-
30	CLA	A	833	1	1/1/15/20	13/37/115/115	-
30	CLA	14	309	26	1/1/11/20	3/13/91/115	-
30	CLA	2u	202	12	1/1/15/20	14/37/115/115	-
33	BCR	A	847	-	-	12/29/63/63	0/2/2/2
38	KC1	16	311	28	-	6/15/71/71	-
30	CLA	6	317	-	1/1/15/20	14/37/115/115	-
38	KC1	13	311	25	-	3/15/71/71	-
39	DD6	3	316	-	-	12/26/80/80	0/3/3/3
34	LHG	B	848	30	-	18/31/31/53	-
38	KC1	5	310	17	-	6/15/71/71	-
36	LMG	F	205	-	-	14/21/41/70	0/1/1/1
30	CLA	13	303	-	-	8/37/115/115	-
36	LMG	8	319	36,20	-	17/32/52/70	0/1/1/1
37	A86	4	315	-	-	5/34/90/90	0/3/3/3
30	CLA	15	305	37,27	1/1/11/20	8/13/91/115	-
30	CLA	2	311	14	-	11/37/115/115	-
30	CLA	6	314	18	-	16/37/115/115	-
36	LMG	5	318	-	-	10/28/48/70	0/1/1/1
30	CLA	B	827	2	1/1/15/20	5/37/115/115	-
30	CLA	4	303	16	1/1/15/20	4/37/115/115	-
38	KC1	14	306	26	-	7/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	2	304	14	1/1/15/20	13/37/115/115	-
38	KC1	4	308	16	-	2/15/71/71	-
38	KC1	8	311	40	-	5/15/71/71	-
38	KC1	9	312	21	-	6/15/71/71	-
37	A86	15	316	30	-	14/34/90/90	0/3/3/3
30	CLA	8	303	40	-	10/37/115/115	-
35	LMT	11	318	-	-	1/21/61/61	0/2/2/2
37	A86	9	315	-	-	10/34/90/90	0/3/3/3
36	LMG	7	320	-	-	14/32/52/70	0/1/1/1
38	KC1	9	310	21	-	7/15/71/71	-
39	DD6	3	313	-	-	9/26/80/80	0/3/3/3
38	KC1	8	314	40,38	-	7/15/71/71	-
38	KC1	12	309	24	-	8/15/71/71	-
37	A86	12	314	-	-	13/34/90/90	0/3/3/3
30	CLA	B	829	2	1/1/15/20	11/37/115/115	-
30	CLA	L	202	9	1/1/15/20	7/37/115/115	-
30	CLA	A	810	1	1/1/15/20	10/37/115/115	-
30	CLA	B	813	2	1/1/15/20	21/37/115/115	-
30	CLA	L	203	40	1/1/11/20	2/13/91/115	-
38	KC1	10	310	22	-	7/15/71/71	-
35	LMT	12	318	-	-	3/21/61/61	0/2/2/2
37	A86	16	312	28	-	13/34/90/90	0/3/3/3
30	CLA	B	822	30,2	-	12/37/115/115	-
35	LMT	9	317	-	-	5/18/58/61	0/2/2/2
39	DD6	4	313	-	-	14/26/80/80	0/3/3/3
30	CLA	9	305	-	1/1/15/20	13/37/115/115	-
37	A86	12	316	-	-	16/34/90/90	0/3/3/3
37	A86	14	317	-	-	15/34/90/90	0/3/3/3
30	CLA	7	306	19	1/1/15/20	8/37/115/115	-
35	LMT	B	850	-	-	1/21/61/61	0/2/2/2
37	A86	3	315	-	-	14/34/90/90	0/3/3/3
35	LMT	16	315	-	-	5/21/61/61	0/2/2/2
37	A86	4	312	-	-	11/34/90/90	0/3/3/3
30	CLA	16	301	28	-	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC1	10	306	22	-	8/15/71/71	-
39	DD6	11	313	-	-	11/26/80/80	0/3/3/3
35	LMT	8	322	-	-	3/21/61/61	0/2/2/2
38	KC1	6	312	18	-	6/15/71/71	-
30	CLA	9	309	40,21	1/1/15/20	9/37/115/115	-
30	CLA	10	311	-	-	7/13/91/115	-
30	CLA	B	824	40	1/1/15/20	5/37/115/115	-
30	CLA	3	309	15	-	4/13/91/115	-
33	BCR	B	845	-	-	13/29/63/63	0/2/2/2
37	A86	13	313	25	-	11/30/86/90	0/3/3/3
38	KC1	8	313	20	-	5/15/71/71	-
38	KC1	12	305	24	-	7/15/71/71	-
30	CLA	9	308	21	1/1/15/20	16/37/115/115	-
39	DD6	4	316	-	-	14/26/80/80	0/3/3/3
30	CLA	6	305	18	1/1/15/20	5/37/115/115	-
38	KC1	12	311	24	-	6/15/71/71	-
30	CLA	A	807	1	1/1/15/20	13/37/115/115	-
36	LMG	B	847	-	-	25/50/70/70	0/1/1/1
38	KC1	6	313	18	-	5/15/71/71	-
30	CLA	2	303	14	-	13/25/103/115	-
37	A86	5	316	-	-	6/34/90/90	0/3/3/3
30	CLA	B	804	2	1/1/12/20	6/22/100/115	-
30	CLA	15	314	30,27	-	4/13/91/115	-
37	A86	10	316	-	-	11/34/90/90	0/3/3/3
37	A86	14	318	-	-	17/34/90/90	0/3/3/3
30	CLA	B	835	2	1/1/15/20	6/37/115/115	-
32	SF4	C	102	3	-	-	0/6/5/5
30	CLA	2	301	14,2	1/1/15/20	12/37/115/115	-
30	CLA	7	309	19	1/1/15/20	10/37/115/115	-
30	CLA	9	302	9,21	1/1/12/20	7/21/99/115	-
30	CLA	14	310	-	1/1/12/20	5/19/97/115	-
36	LMG	2u	204	12	-	14/26/46/70	0/1/1/1
38	KC1	3	304	15	-	6/15/71/71	-
30	CLA	A	835	1	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	KC1	1	306	13	-	8/15/71/71	-
38	KC1	16	304	28	-	8/15/71/71	-
33	BCR	B	844	-	-	9/29/63/63	0/2/2/2
30	CLA	4	302	16	1/1/15/20	10/37/115/115	-
30	CLA	A	822	40	1/1/15/20	8/37/115/115	-
35	LMT	6	302	-	-	3/17/57/61	0/2/2/2
30	CLA	5	309	34	1/1/15/20	9/37/115/115	-
30	CLA	13	307	25	1/1/15/20	9/37/115/115	-
30	CLA	B	815	2	1/1/11/20	1/13/91/115	-
30	CLA	A	820	1	1/1/15/20	16/37/115/115	-
35	LMT	7	321	-	-	4/21/61/61	0/2/2/2
30	CLA	B	836	2	1/1/11/20	3/16/94/115	-
30	CLA	15	313	27	-	11/37/115/115	-
30	CLA	B	809	2	1/1/15/20	10/37/115/115	-
37	A86	10	317	-	-	12/34/90/90	0/3/3/3
33	BCR	A	850	-	-	11/29/63/63	0/2/2/2
36	LMG	B	849	2	-	15/38/58/70	0/1/1/1
30	CLA	7	304	19	1/1/15/20	7/37/115/115	-
35	LMT	11	317	-	-	2/21/61/61	0/2/2/2
37	A86	14	314	-	-	13/34/90/90	0/3/3/3
35	LMT	15	301	-	-	6/21/61/61	0/2/2/2
38	KC1	11	307	23	-	10/15/71/71	-
38	KC1	13	312	25	-	9/15/71/71	-
36	LMG	8	320	-	-	20/37/57/70	0/1/1/1
38	KC1	14	308	30,26	-	9/15/71/71	-
30	CLA	12	307	24	1/1/11/20	4/15/93/115	-
39	DD6	7	318	-	-	13/26/80/80	0/3/3/3
33	BCR	F	204	-	-	10/29/63/63	0/2/2/2
37	A86	13	315	-	-	13/34/90/90	0/3/3/3
30	CLA	A	816	1,35	1/1/15/20	17/37/115/115	-
30	CLA	B	834	2	1/1/14/20	8/31/109/115	-
39	DD6	6	319	-	-	11/26/80/80	0/3/3/3
30	CLA	3	301	15	1/1/15/20	7/37/115/115	-
30	CLA	1	302	30,13	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	A	839	1	1/1/15/20	14/37/115/115	-
30	CLA	12	303	24	1/1/15/20	6/37/115/115	-
37	A86	8	315	-	-	7/34/90/90	0/3/3/3
30	CLA	15	308	30,27	1/1/11/20	7/13/91/115	-
37	A86	14	316	-	-	11/34/90/90	0/3/3/3
30	CLA	B	825	2	1/1/15/20	7/37/115/115	-
30	CLA	11	306	40	1/1/13/20	8/25/103/115	-
30	CLA	A	806	1	1/1/15/20	15/37/115/115	-
35	LMT	11	302	-	-	0/21/61/61	0/2/2/2
37	A86	11	301	-	-	14/34/90/90	0/3/3/3
30	CLA	B	805	2	1/1/15/20	9/37/115/115	-
36	LMG	8	321	36	-	5/24/44/70	0/1/1/1
30	CLA	B	801	2	1/1/15/20	8/37/115/115	-
35	LMT	7	301	30	-	3/21/61/61	0/2/2/2
39	DD6	2	315	-	-	13/26/80/80	0/3/3/3
30	CLA	B	808	2	1/1/15/20	14/37/115/115	-
37	A86	15	320	-	-	15/34/90/90	0/3/3/3
38	KC1	2	306	14	-	6/15/71/71	-
38	KC1	13	310	25	-	5/15/71/71	-
30	CLA	F	202	40	1/1/15/20	18/37/115/115	-
36	LMG	14	321	-	-	13/33/53/70	0/1/1/1
30	CLA	A	817	40,36	-	4/18/96/115	-
38	KC1	9	304	21	-	6/15/71/71	-
30	CLA	2	310	14	1/1/15/20	6/37/115/115	-
30	CLA	16	305	28	1/1/12/20	3/19/97/115	-
30	CLA	10	305	40	1/1/15/20	10/37/115/115	-
38	KC1	8	310	20	-	6/15/71/71	-
33	BCR	B	846	-	-	7/29/63/63	0/2/2/2
30	CLA	A	838	1	1/1/12/20	4/21/99/115	-
35	LMT	A	857	-	-	3/21/61/61	0/2/2/2
30	CLA	B	833	30,40	1/1/15/20	11/37/115/115	-
37	A86	7	319	-	-	10/34/90/90	0/3/3/3
38	KC1	4	310	16	-	4/15/71/71	-
30	CLA	15	304	30,39,27	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	12	319	-	-	0/21/61/61	0/2/2/2
30	CLA	B	818	2	1/1/14/20	6/31/109/115	-
30	CLA	1	304	13	1/1/15/20	11/37/115/115	-
38	KC1	14	311	26	-	5/15/71/71	-
30	CLA	9	306	37,21	1/1/11/20	6/13/91/115	-
38	KC1	5	306	17	-	10/15/71/71	-
30	CLA	8	309	20	-	3/16/94/115	-
37	A86	10	301	22	-	6/34/90/90	0/3/3/3
37	A86	15	321	27	-	13/34/90/90	0/3/3/3
30	CLA	6	316	40	1/1/13/20	7/25/103/115	-
30	CLA	5	311	40,17	1/1/15/20	15/37/115/115	-
30	CLA	A	836	1	1/1/12/20	7/24/102/115	-
34	LHG	2	320	30	-	12/31/31/53	-
39	DD6	5	314	-	-	10/26/80/80	0/3/3/3
32	SF4	A	846	1,2	-	-	0/6/5/5
30	CLA	B	811	30,2	1/1/15/20	10/37/115/115	-
30	CLA	10	307	22	1/1/15/20	10/37/115/115	-
33	BCR	A	848	-	-	10/29/63/63	0/2/2/2
35	LMT	A	855	-	-	4/21/61/61	0/2/2/2
30	CLA	5	304	17	1/1/15/20	12/37/115/115	-
35	LMT	1	311	-	-	4/21/61/61	0/2/2/2
30	CLA	15	302	30,27	-	15/37/115/115	-
30	CLA	5	303	17	1/1/15/20	6/37/115/115	-
35	LMT	B	852	-	-	8/21/61/61	0/2/2/2
38	KC1	1	308	13	-	5/15/71/71	-
30	CLA	15	309	27	-	10/37/115/115	-
38	KC1	5	305	17	-	5/15/71/71	-
30	CLA	F	201	40	1/1/15/20	10/37/115/115	-
30	CLA	2	313	14	-	3/13/91/115	-
37	A86	6	320	-	-	9/34/90/90	0/3/3/3
37	A86	10	302	-	-	13/34/90/90	0/3/3/3
30	CLA	A	831	1	1/1/15/20	9/37/115/115	-
33	BCR	A	849	-	-	12/29/63/63	0/2/2/2
37	A86	11	314	-	-	14/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	DD6	2	317	-	-	14/26/80/80	0/3/3/3
30	CLA	16	302	28	1/1/15/20	9/37/115/115	-
37	A86	7	316	-	-	7/34/90/90	0/3/3/3
39	DD6	10	313	-	-	11/26/80/80	0/3/3/3
30	CLA	14	307	38	-	10/37/115/115	-
30	CLA	B	814	2	1/1/13/20	5/25/103/115	-
30	CLA	11	304	23	1/1/15/20	9/37/115/115	-
30	CLA	16	309	28	-	4/13/91/115	-
39	DD6	10	314	-	-	9/26/80/80	0/3/3/3
38	KC1	3	308	15	-	8/15/71/71	-
30	CLA	16	308	28	1/1/11/20	6/13/91/115	-
30	CLA	16	310	28	1/1/11/20	7/13/91/115	-
30	CLA	6	304	18	1/1/15/20	10/37/115/115	-
37	A86	2u	205	-	-	11/34/90/90	0/3/3/3
37	A86	9	316	30	-	11/34/90/90	0/3/3/3
30	CLA	16	303	28	1/1/15/20	19/37/115/115	-
30	CLA	5	308	17	-	14/37/115/115	-
30	CLA	4	304	-	1/1/14/20	9/31/109/115	-
30	CLA	B	851	14,2	-	14/37/115/115	-
30	CLA	16	306	28	1/1/12/20	13/22/100/115	-
33	BCR	L	205	-	-	8/29/63/63	0/2/2/2
30	CLA	12	321	24,26	1/1/15/20	4/37/115/115	-
30	CLA	15	306	-	1/1/11/20	6/13/91/115	-
37	A86	15	317	30	-	16/34/90/90	0/3/3/3
30	CLA	4	301	16,2	1/1/11/20	7/18/96/115	-
29	CL0	A	801	1	3/3/20/25	4/37/135/135	-
30	CLA	14	303	26	1/1/13/20	7/28/106/115	-
30	CLA	8	301	20	1/1/15/20	20/37/115/115	-
33	BCR	2u	201	-	-	11/29/63/63	0/2/2/2
30	CLA	6	309	18	1/1/15/20	12/37/115/115	-
30	CLA	15	312	27	1/1/11/20	5/13/91/115	-
30	CLA	A	837	1	1/1/11/20	7/13/91/115	-
30	CLA	A	840	1	1/1/11/20	5/16/94/115	-
30	CLA	5	302	17	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CLA	B	812	2	1/1/15/20	8/37/115/115	-
37	A86	8	318	-	-	15/34/90/90	0/3/3/3
30	CLA	13	301	25	1/1/15/20	15/37/115/115	-
30	CLA	4	309	-	1/1/15/20	9/37/115/115	-
33	BCR	I	101	-	-	5/29/63/63	0/2/2/2
37	A86	14	315	26	-	11/34/90/90	0/3/3/3
34	LHG	A	852	-	-	25/53/53/53	-
36	LMG	6	301	30	-	16/28/48/70	0/1/1/1
30	CLA	A	812	30,1	1/1/15/20	14/37/115/115	-
38	KC1	11	311	23	-	10/15/71/71	-
37	A86	15	323	-	-	15/34/90/90	0/3/3/3
30	CLA	13	302	25	1/1/15/20	16/37/115/115	-
33	BCR	A	851	-	-	7/29/63/63	0/2/2/2
37	A86	11	316	-	-	12/34/90/90	0/3/3/3
30	CLA	7	307	19	-	19/37/115/115	-
30	CLA	4	306	16	1/1/15/20	10/37/115/115	-
31	PQN	B	840	-	-	6/23/43/43	0/2/2/2
35	LMT	12	320	-	-	1/21/61/61	0/2/2/2
30	CLA	A	818	1	-	7/24/102/115	-
37	A86	5	315	-	-	6/34/90/90	0/3/3/3
39	DD6	8	316	-	-	13/26/80/80	0/3/3/3
30	CLA	2	309	14,34	1/1/15/20	11/37/115/115	-

The worst 5 of 7031 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 9756 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

5 of 185 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	801	CL0	NA
29	A	801	CL0	ND
29	A	801	CL0	NC
30	A	802	CLA	ND
30	A	803	CLA	ND

5 of 3979 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.

235 monomers are involved in 440 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	813	CLA	3	0
33	B	843	BCR	2	0
30	2	307	CLA	3	0
30	3	306	CLA	2	0
30	B	837	CLA	2	0
30	12	310	CLA	2	0
30	A	824	CLA	1	0
30	A	834	CLA	2	0
30	A	843	CLA	2	0
30	14	302	CLA	2	0
30	1	301	CLA	2	0
30	B	839	CLA	3	0
30	B	806	CLA	7	0
30	A	841	CLA	2	0
30	A	819	CLA	3	0
30	2	305	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	L	204	BCR	4	0
34	5	317	LHG	1	0
30	J	101	CLA	1	0
30	A	830	CLA	4	0
31	A	845	PQN	5	0
30	A	811	CLA	3	0
30	A	802	CLA	3	0
30	14	312	CLA	1	0
30	A	842	CLA	4	0
38	5	312	KC1	1	0
33	J	102	BCR	3	0
30	A	803	CLA	2	0
39	6	318	DD6	1	0
30	3	305	CLA	1	0
30	6	307	CLA	1	0
30	16	307	CLA	2	0
37	7	315	A86	1	0
30	A	814	CLA	3	0
35	11	303	LMT	1	0
33	L	201	BCR	2	0
30	A	826	CLA	4	0
30	14	305	CLA	1	0
30	12	302	CLA	1	0
30	B	831	CLA	2	0
37	11	315	A86	1	0
33	M	101	BCR	3	0
30	9	301	CLA	1	0
30	A	829	CLA	10	0
36	A	856	LMG	2	0
30	B	820	CLA	2	0
30	A	823	CLA	1	0
30	3	302	CLA	1	0
30	8	308	CLA	1	0
30	7	303	CLA	1	0
30	B	830	CLA	2	0
30	B	816	CLA	2	0
30	A	805	CLA	3	0
30	3	303	CLA	2	0
30	10	309	CLA	2	0
30	A	809	CLA	1	0
30	4	311	CLA	2	0
33	B	842	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	3	317	LMG	2	0
30	10	304	CLA	1	0
30	A	821	CLA	2	0
30	A	832	CLA	1	0
30	1	303	CLA	3	0
39	6	321	DD6	1	0
30	10	303	CLA	3	0
30	B	817	CLA	5	0
30	B	807	CLA	2	0
30	11	310	CLA	4	0
30	12	312	CLA	1	0
30	B	838	CLA	7	0
30	5	307	CLA	2	0
30	2	308	CLA	1	0
30	B	802	CLA	2	0
30	A	828	CLA	2	0
35	12	301	LMT	2	0
30	B	821	CLA	2	0
37	14	320	A86	1	0
30	7	311	CLA	2	0
33	J	103	BCR	4	0
30	A	844	CLA	1	0
39	13	314	DD6	1	0
30	A	804	CLA	4	0
30	B	828	CLA	5	0
30	15	307	CLA	1	0
30	10	308	CLA	1	0
30	12	308	CLA	4	0
30	9	307	CLA	4	0
30	B	823	CLA	1	0
30	B	826	CLA	5	0
30	1	307	CLA	2	0
30	15	303	CLA	3	0
30	B	803	CLA	1	0
33	B	841	BCR	1	0
30	3	310	CLA	2	0
30	8	302	CLA	2	0
30	8	305	CLA	2	0
30	6	306	CLA	2	0
30	B	819	CLA	2	0
30	11	308	CLA	2	0
34	A	853	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	4	305	CLA	1	0
30	A	833	CLA	6	0
33	A	847	BCR	3	0
38	5	310	KC1	1	0
36	8	319	LMG	1	0
37	4	315	A86	1	0
30	2	311	CLA	1	0
30	6	314	CLA	2	0
30	B	827	CLA	5	0
30	2	304	CLA	1	0
30	8	303	CLA	2	0
35	11	318	LMT	2	0
38	12	309	KC1	1	0
30	L	202	CLA	5	0
30	A	810	CLA	5	0
30	B	813	CLA	7	0
30	L	203	CLA	2	0
30	B	822	CLA	2	0
30	9	305	CLA	2	0
37	14	317	A86	1	0
30	7	306	CLA	3	0
30	16	301	CLA	6	0
30	B	824	CLA	3	0
33	B	845	BCR	2	0
30	9	308	CLA	2	0
30	A	807	CLA	2	0
36	B	847	LMG	2	0
30	2	303	CLA	4	0
30	B	804	CLA	2	0
30	B	835	CLA	4	0
30	2	301	CLA	1	0
30	7	309	CLA	6	0
30	9	302	CLA	1	0
38	3	304	KC1	1	0
30	A	835	CLA	2	0
38	16	304	KC1	1	0
33	B	844	BCR	2	0
30	4	302	CLA	1	0
30	A	822	CLA	3	0
35	6	302	LMT	2	0
30	13	307	CLA	4	0
30	B	815	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	A	820	CLA	6	0
35	7	321	LMT	1	0
30	B	836	CLA	4	0
30	15	313	CLA	4	0
30	B	809	CLA	7	0
33	A	850	BCR	2	0
36	B	849	LMG	1	0
30	7	304	CLA	1	0
35	11	317	LMT	2	0
33	F	204	BCR	3	0
30	A	816	CLA	4	0
30	B	834	CLA	2	0
39	6	319	DD6	1	0
30	3	301	CLA	1	0
30	1	302	CLA	3	0
30	A	839	CLA	6	0
30	12	303	CLA	2	0
37	8	315	A86	1	0
30	15	308	CLA	1	0
30	B	825	CLA	1	0
30	11	306	CLA	2	0
30	A	806	CLA	5	0
30	B	805	CLA	2	0
36	8	321	LMG	1	0
30	B	801	CLA	4	0
35	7	301	LMT	1	0
30	B	808	CLA	2	0
30	F	202	CLA	3	0
36	14	321	LMG	2	0
30	A	817	CLA	3	0
30	2	310	CLA	1	0
30	10	305	CLA	1	0
33	B	846	BCR	4	0
30	A	838	CLA	1	0
35	A	857	LMT	1	0
30	B	833	CLA	1	0
38	4	310	KC1	1	0
30	15	304	CLA	2	0
35	12	319	LMT	1	0
30	B	818	CLA	1	0
30	1	304	CLA	2	0
30	9	306	CLA	2	0

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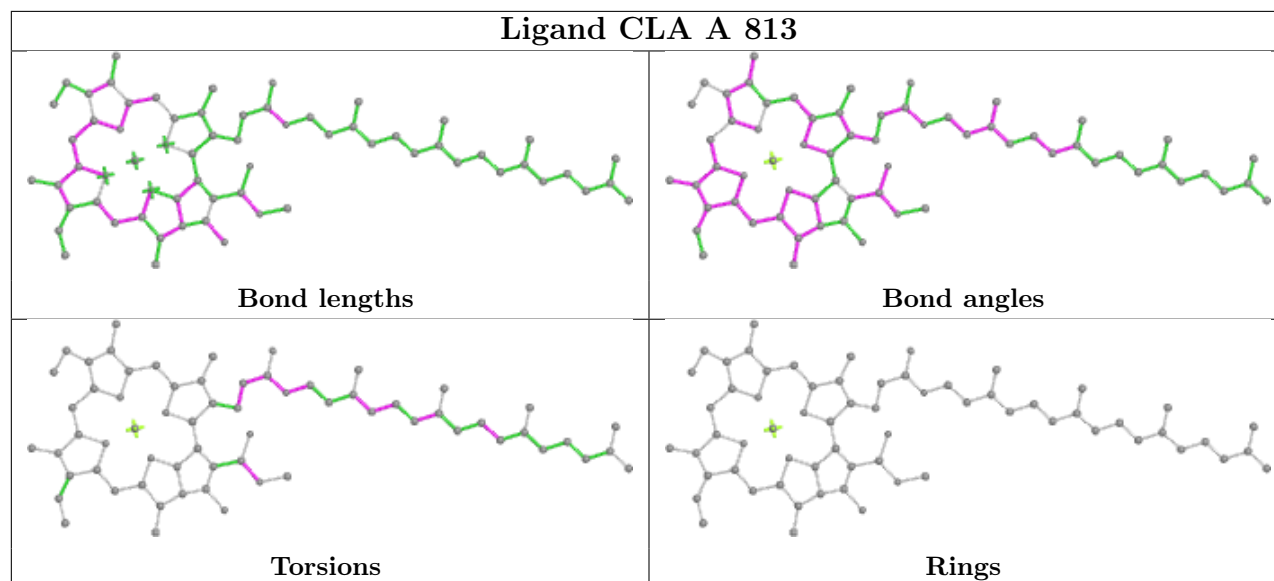
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30	A	836	CLA	3	0
30	B	811	CLA	4	0
30	10	307	CLA	1	0
33	A	848	BCR	2	0
35	A	855	LMT	2	0
30	5	304	CLA	2	0
30	15	302	CLA	4	0
30	5	303	CLA	4	0
30	15	309	CLA	2	0
30	F	201	CLA	6	0
30	A	831	CLA	5	0
33	A	849	BCR	4	0
30	16	302	CLA	1	0
39	10	313	DD6	1	0
30	14	307	CLA	1	0
30	11	304	CLA	3	0
30	16	309	CLA	1	0
30	16	310	CLA	1	0
37	9	316	A86	1	0
30	16	303	CLA	1	0
30	5	308	CLA	2	0
30	B	851	CLA	1	0
30	16	306	CLA	1	0
33	L	205	BCR	4	0
30	12	321	CLA	2	0
30	4	301	CLA	3	0
29	A	801	CL0	3	0
30	14	303	CLA	3	0
30	8	301	CLA	1	0
30	6	309	CLA	3	0
30	A	837	CLA	1	0
30	A	840	CLA	1	0
30	5	302	CLA	3	0
30	B	812	CLA	2	0
30	13	301	CLA	5	0
30	4	309	CLA	1	0
33	I	101	BCR	2	0
34	A	852	LHG	1	0
36	6	301	LMG	1	0
30	A	812	CLA	4	0
30	13	302	CLA	3	0

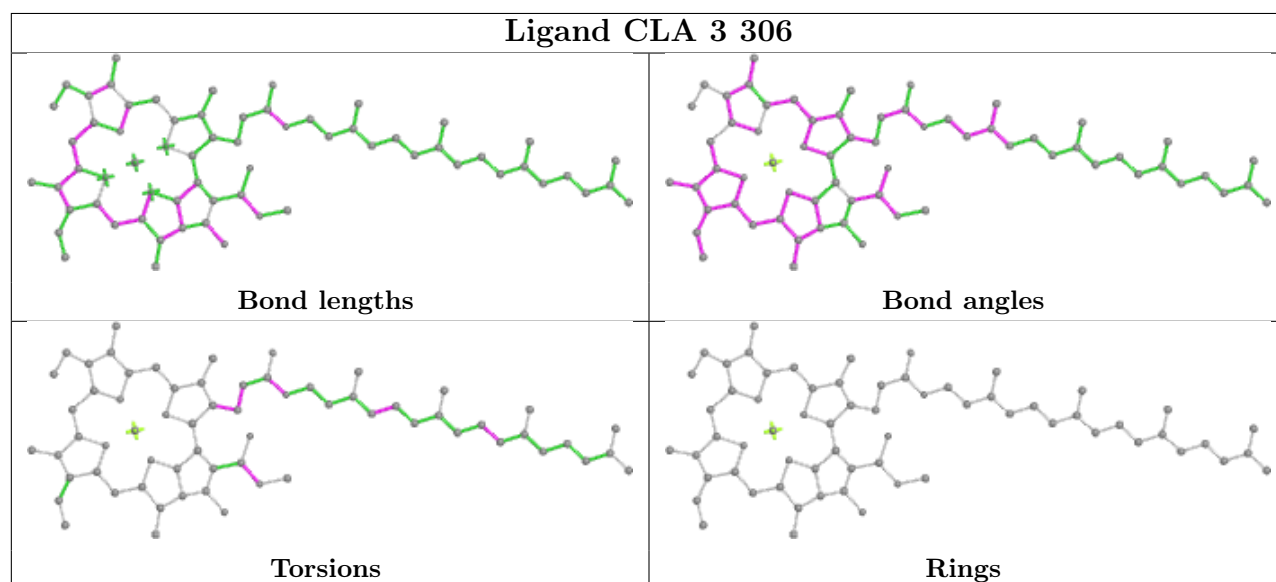
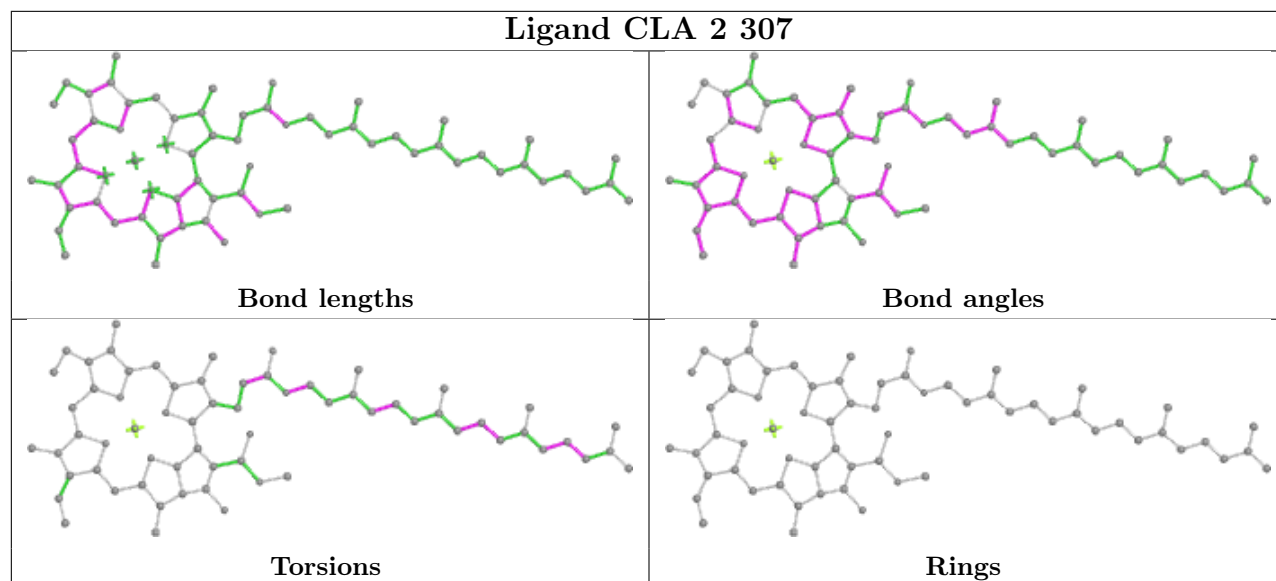
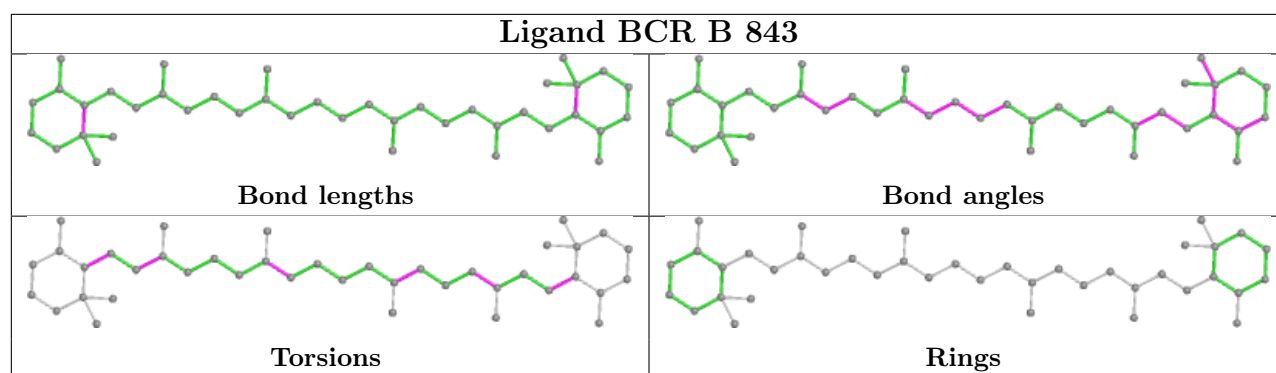
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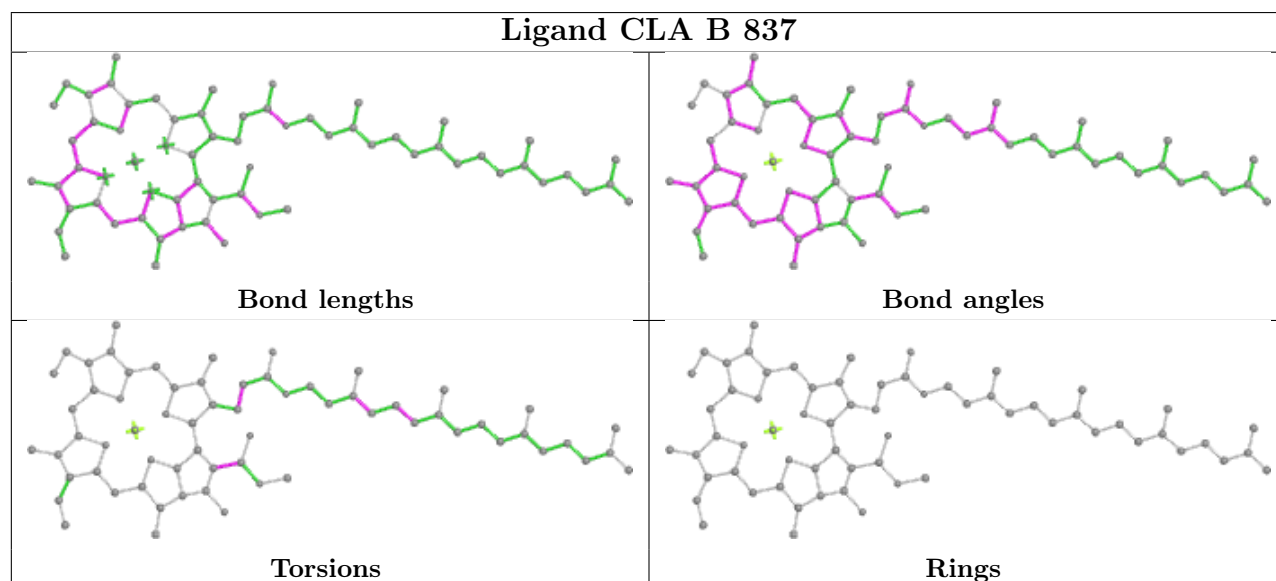
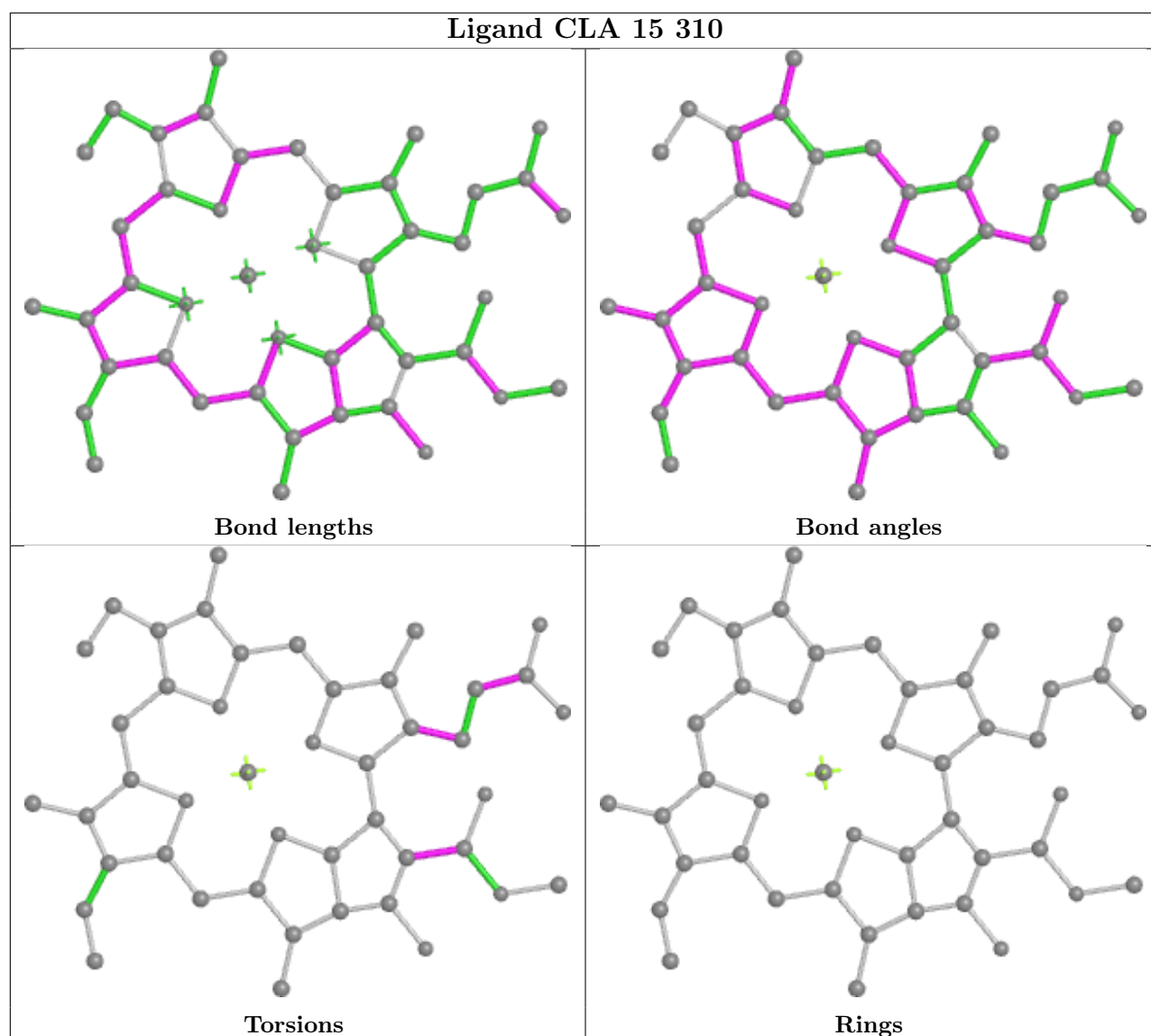
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	851	BCR	2	0
37	11	316	A86	1	0
30	7	307	CLA	2	0
30	4	306	CLA	6	0
31	B	840	PQN	1	0
35	12	320	LMT	1	0
30	A	818	CLA	1	0
37	5	315	A86	1	0
30	2	309	CLA	2	0

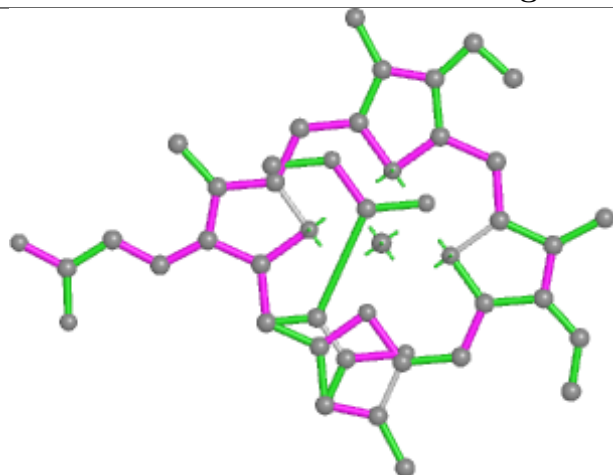
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



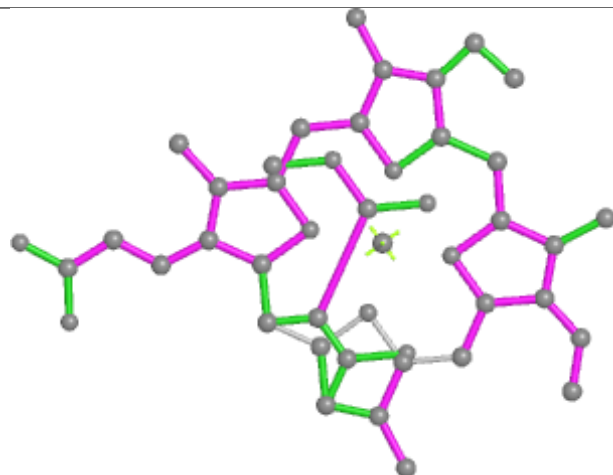




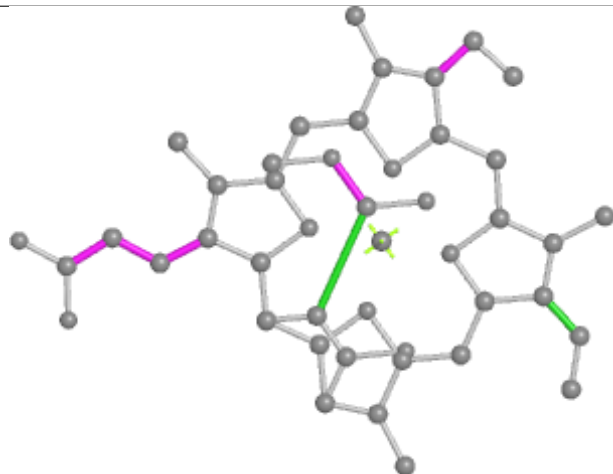
Ligand KC1 8 306



Bond lengths



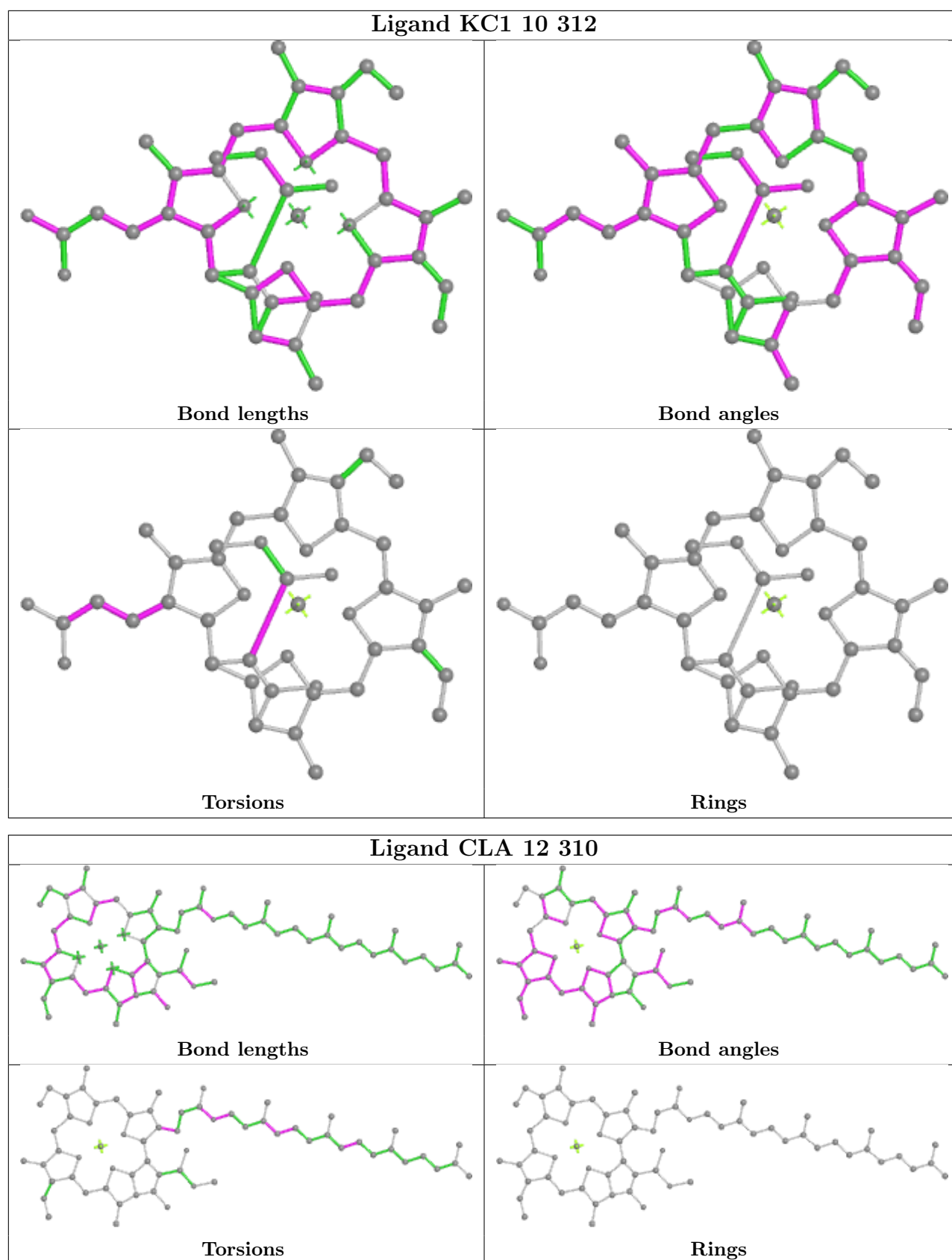
Bond angles



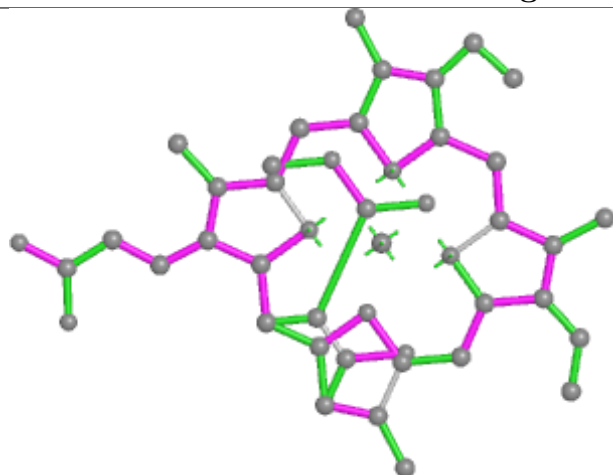
Torsions



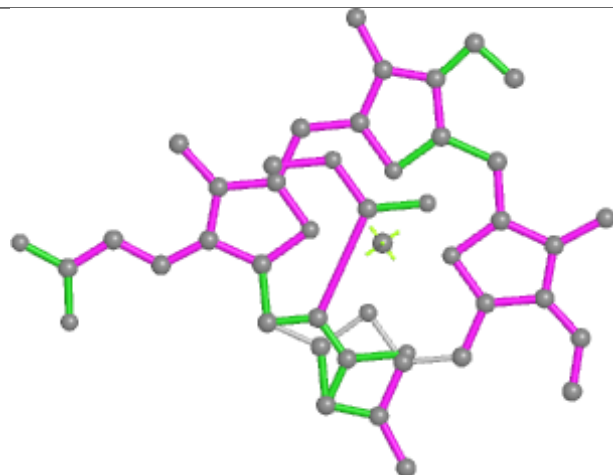
Rings



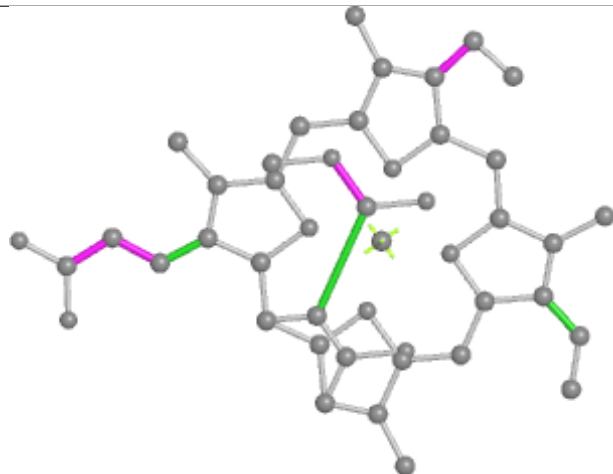
Ligand KC1 2 314



Bond lengths



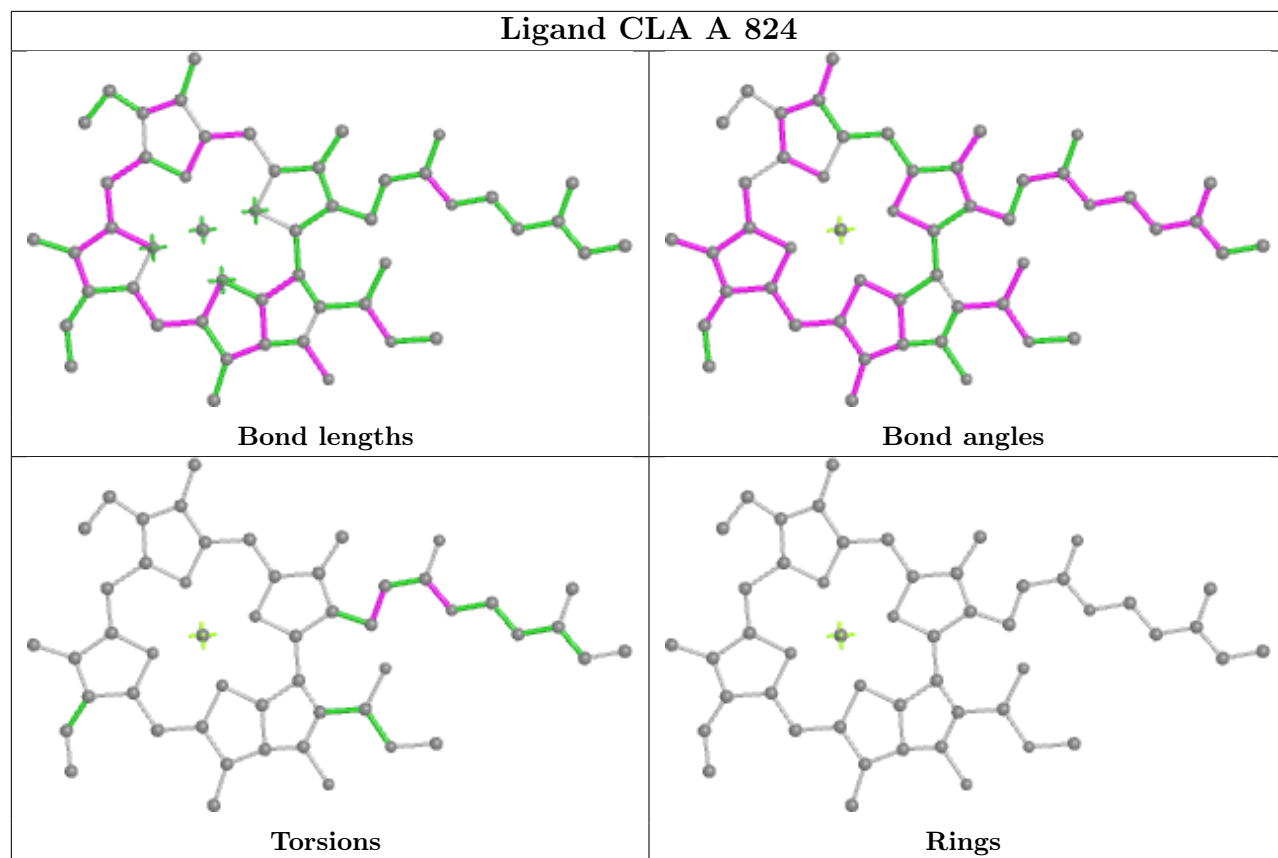
Bond angles



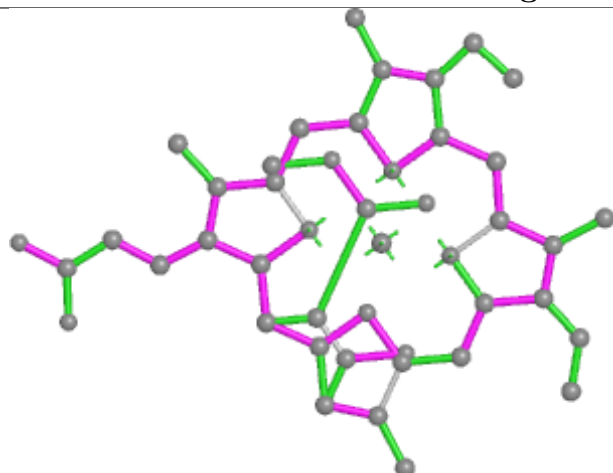
Torsions



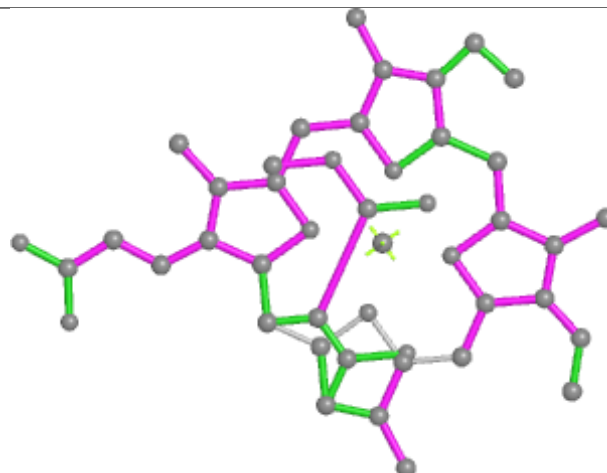
Rings



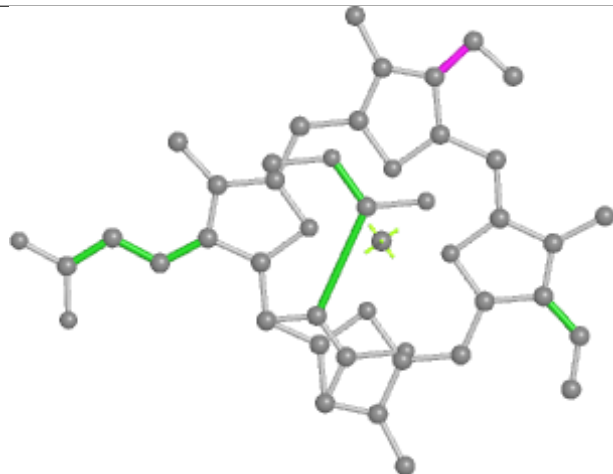
Ligand KC1 2 312



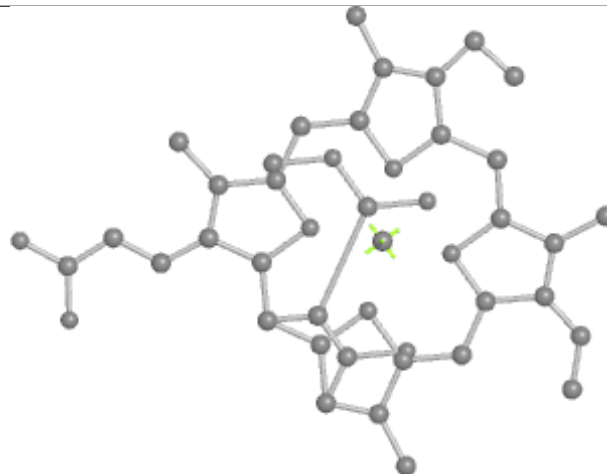
Bond lengths



Bond angles

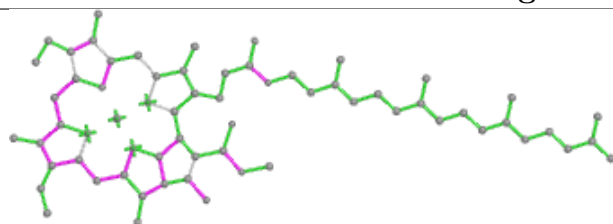


Torsions

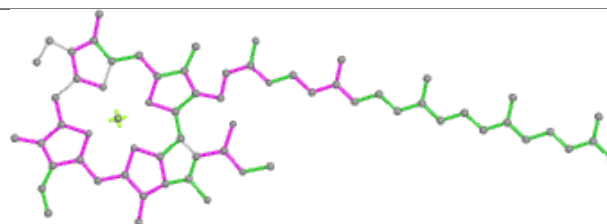


Rings

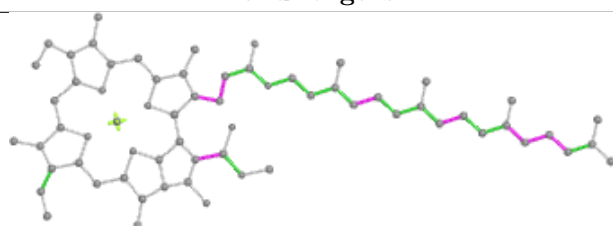
Ligand CLA 7 310



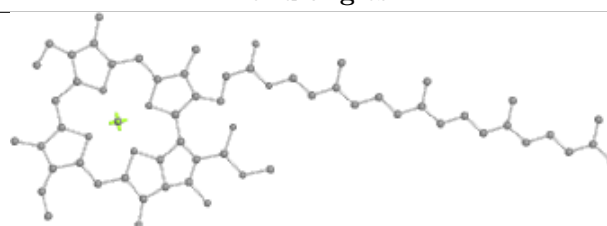
Bond lengths



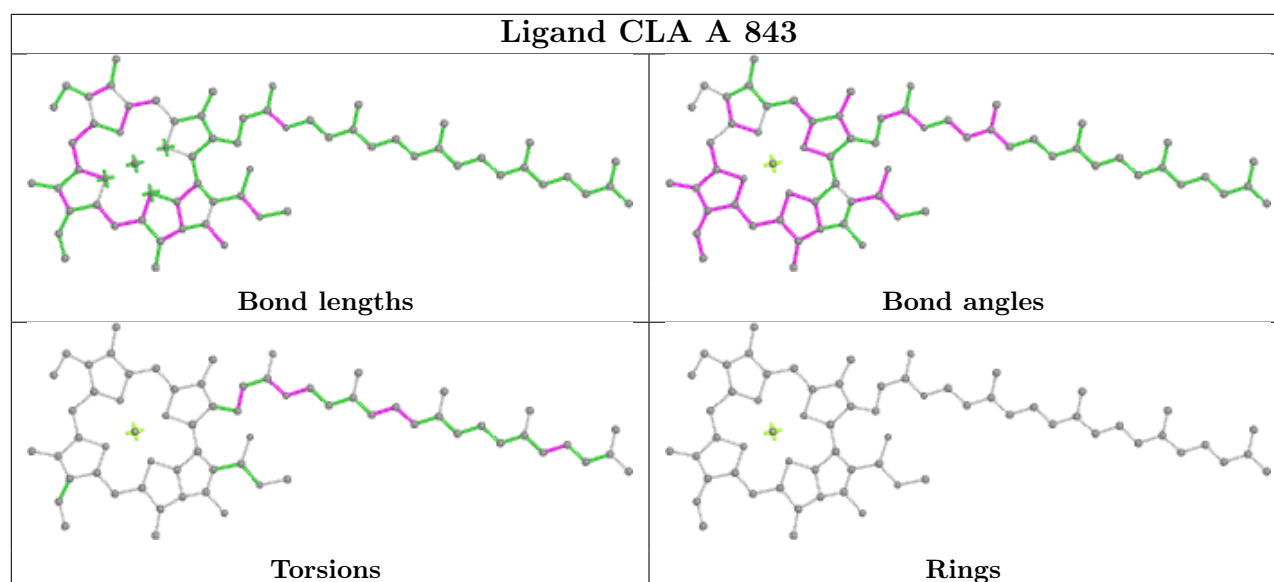
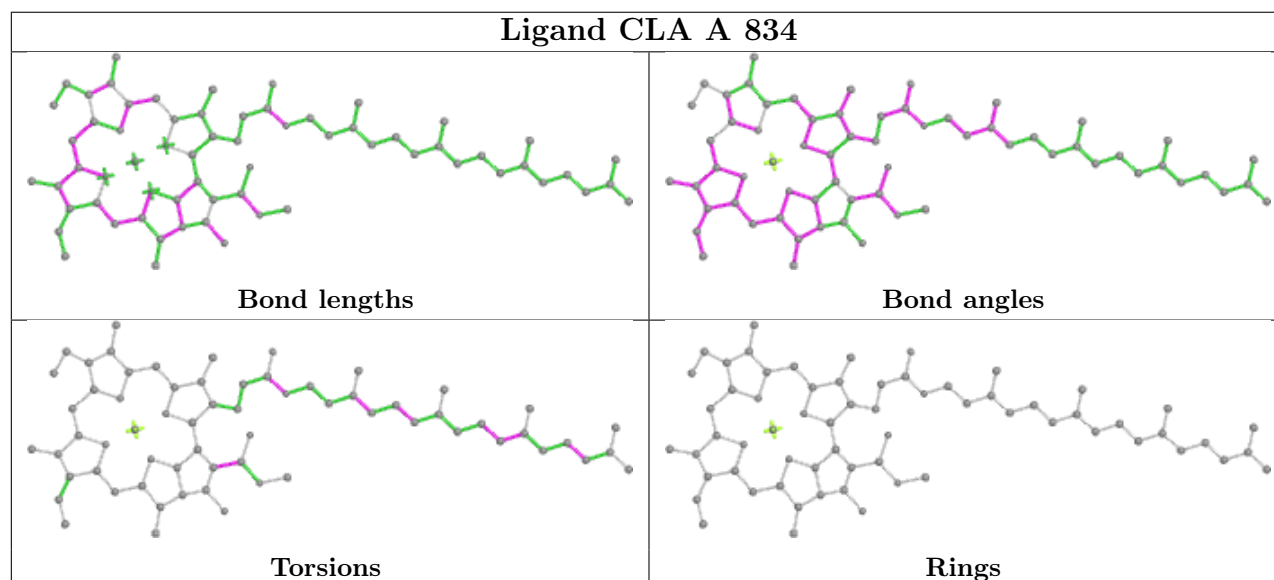
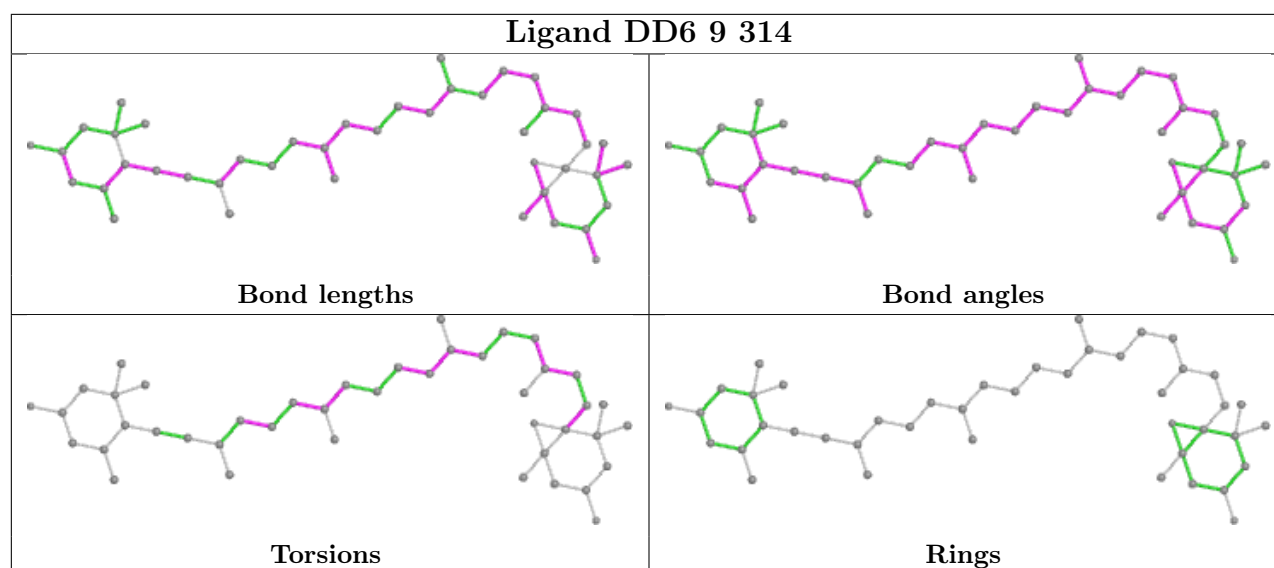
Bond angles

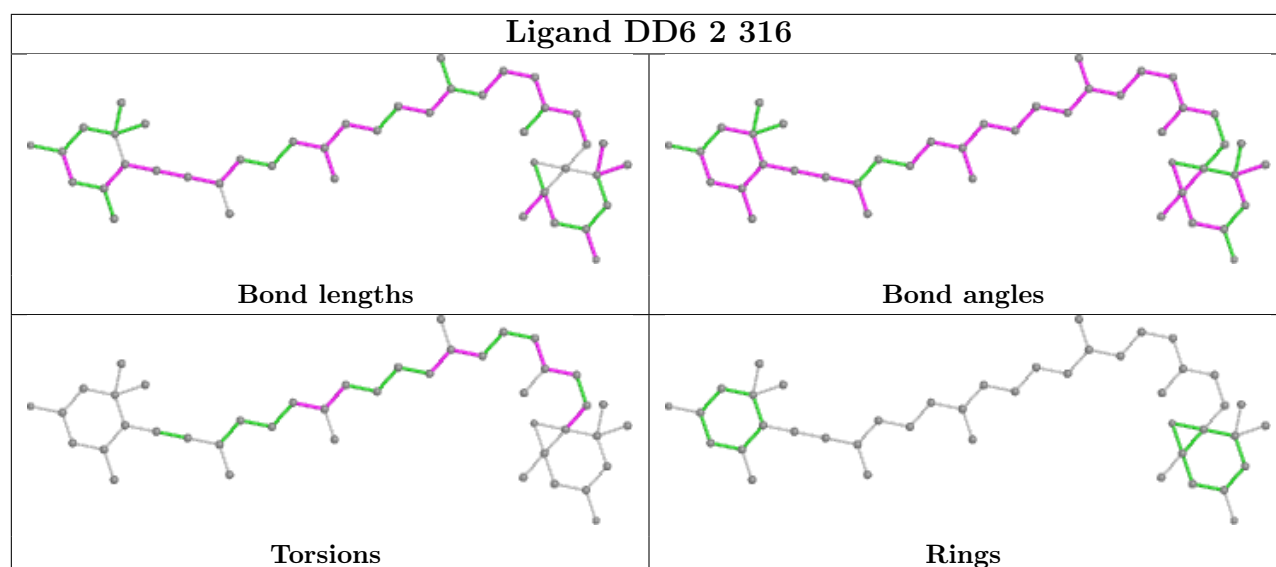
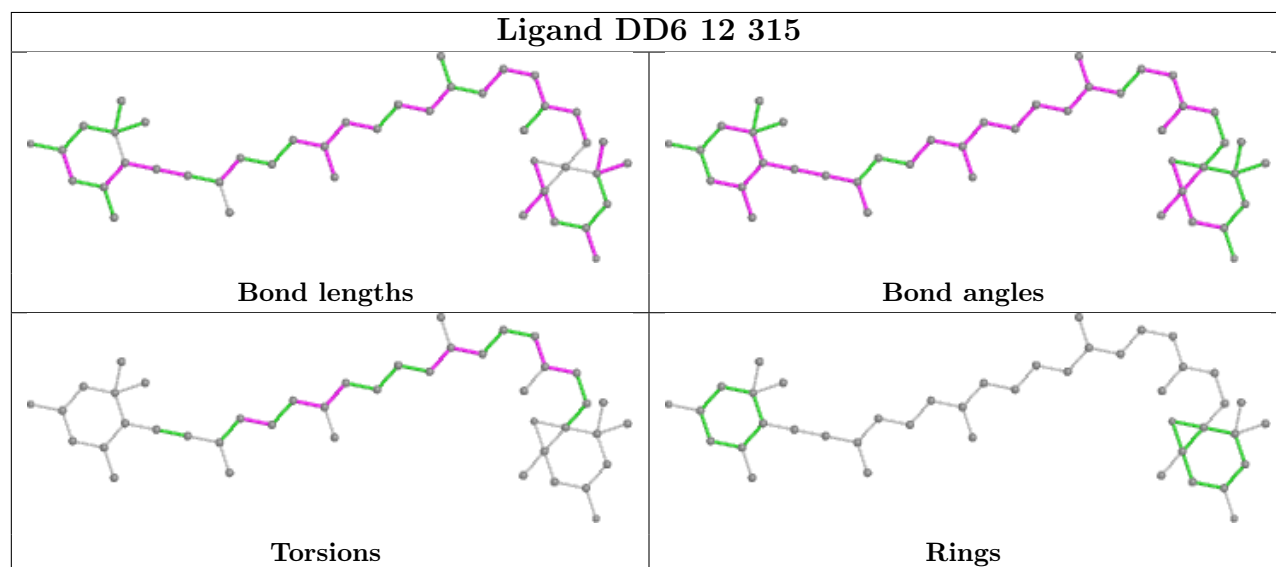
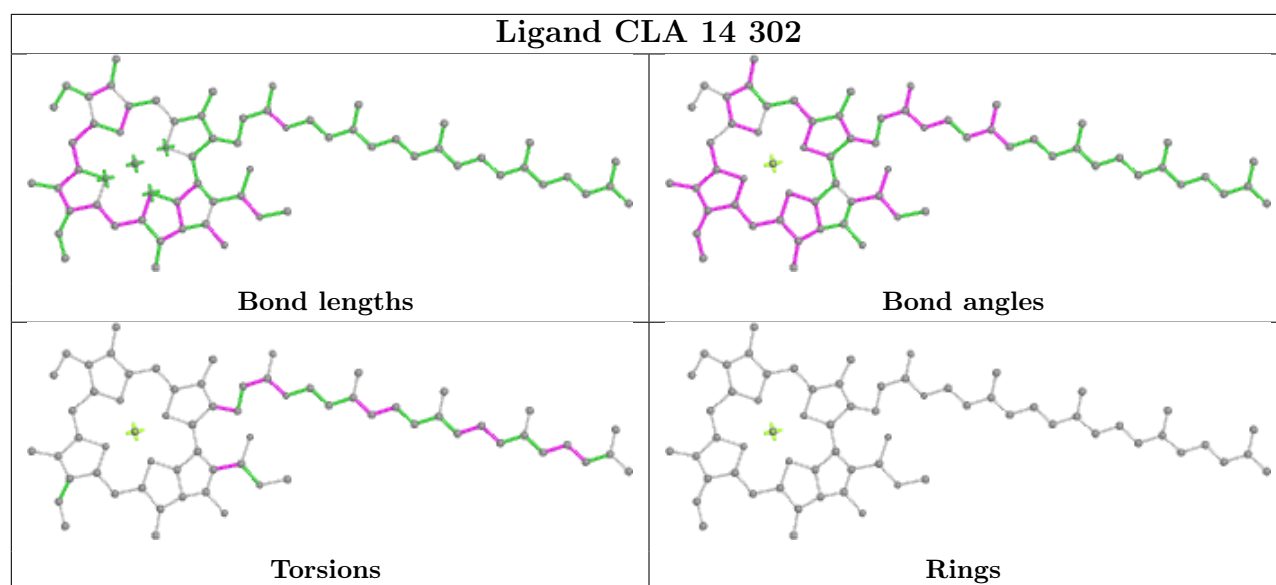


Torsions

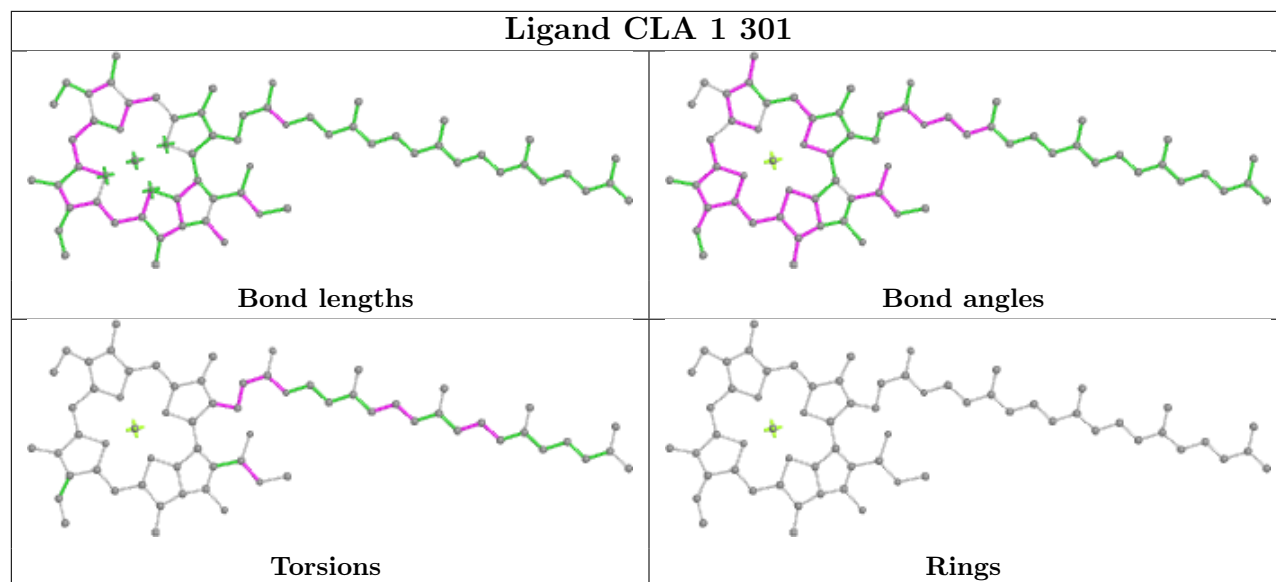


Rings

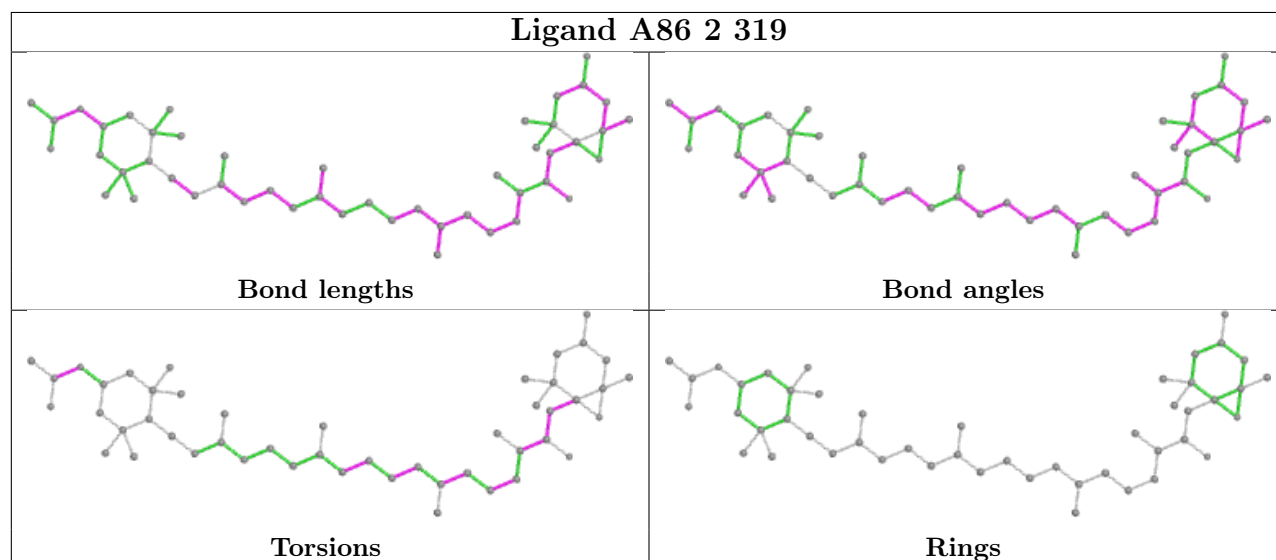




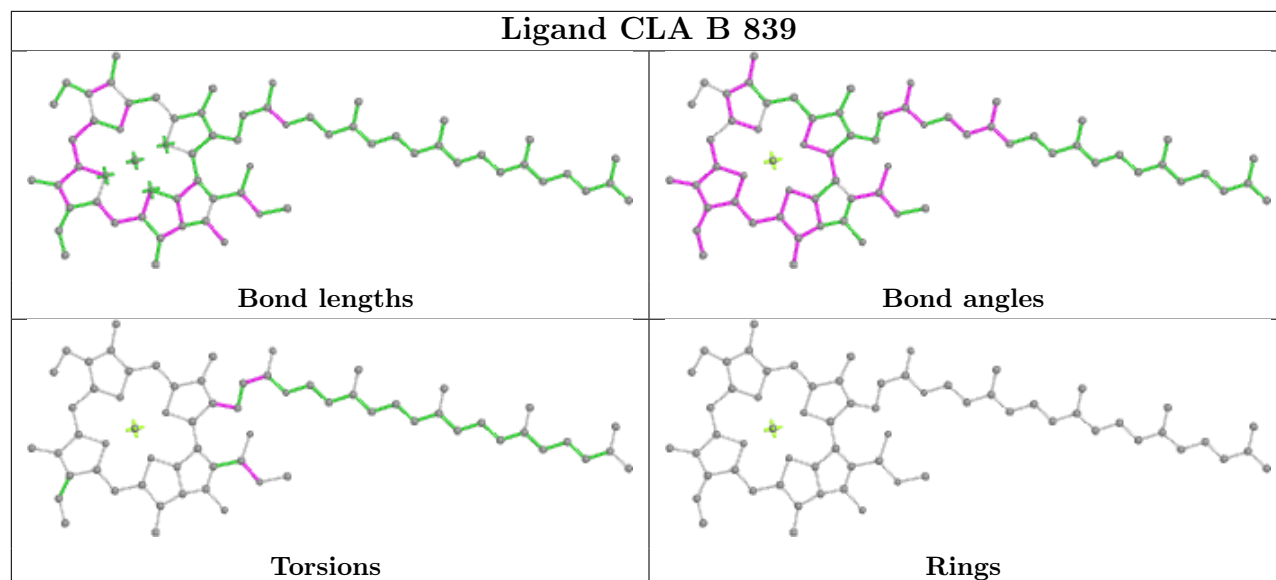
Ligand CLA 1 301

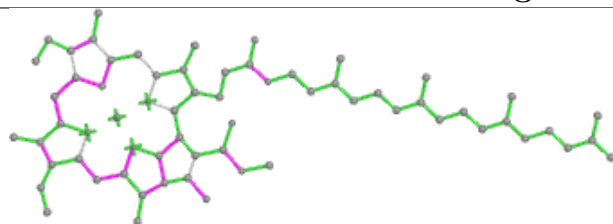
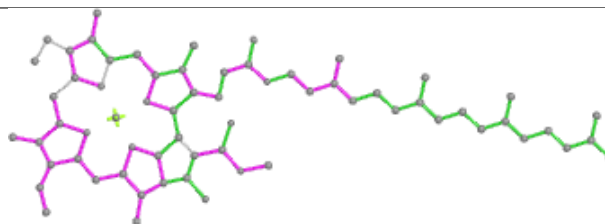
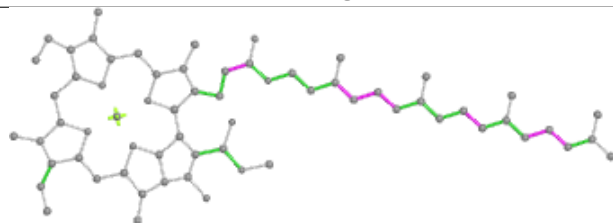
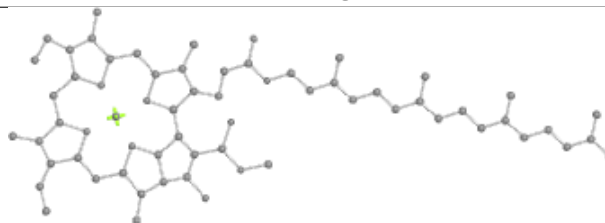
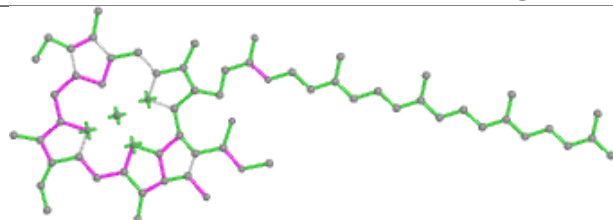
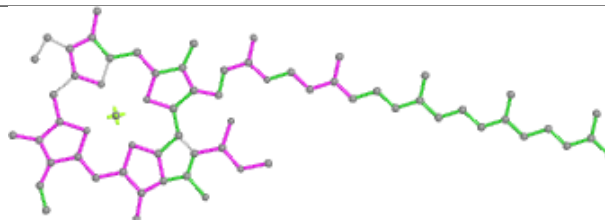
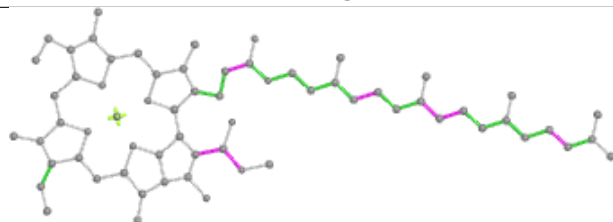
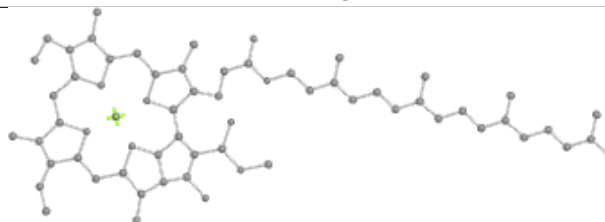


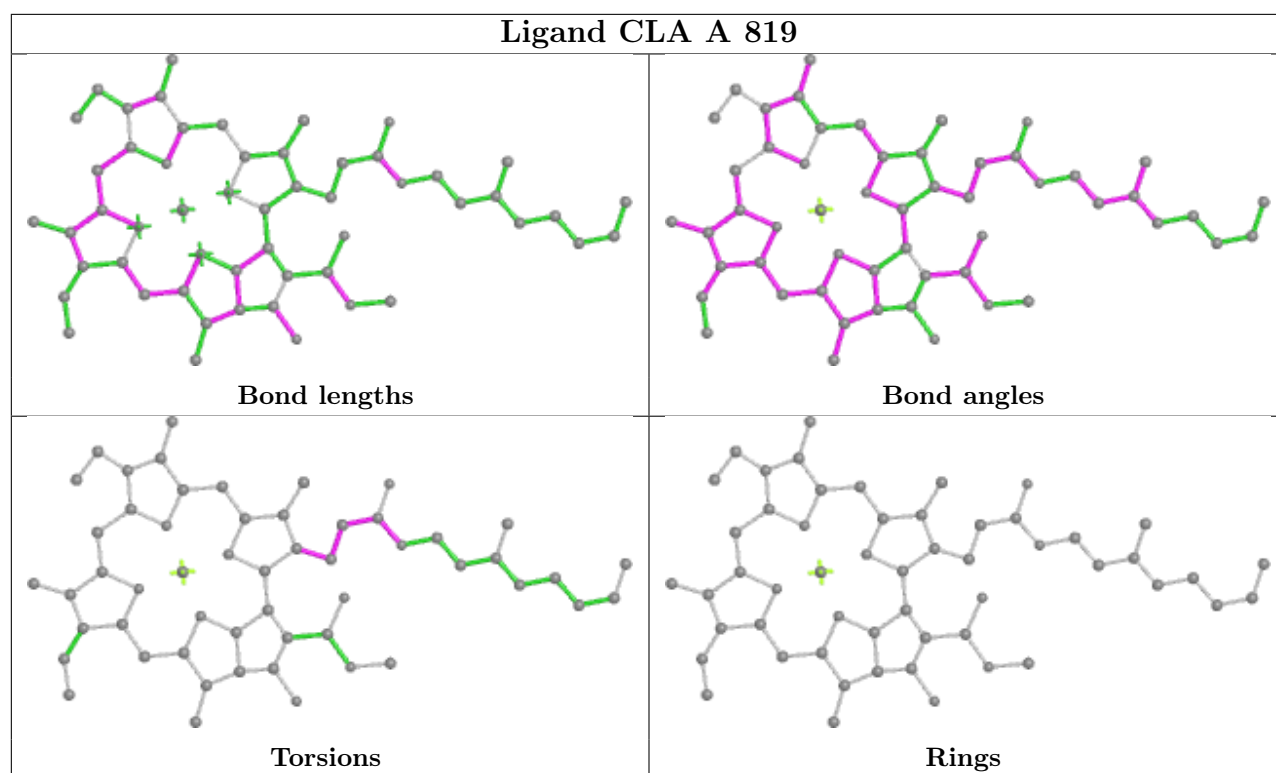
Ligand A86 2 319



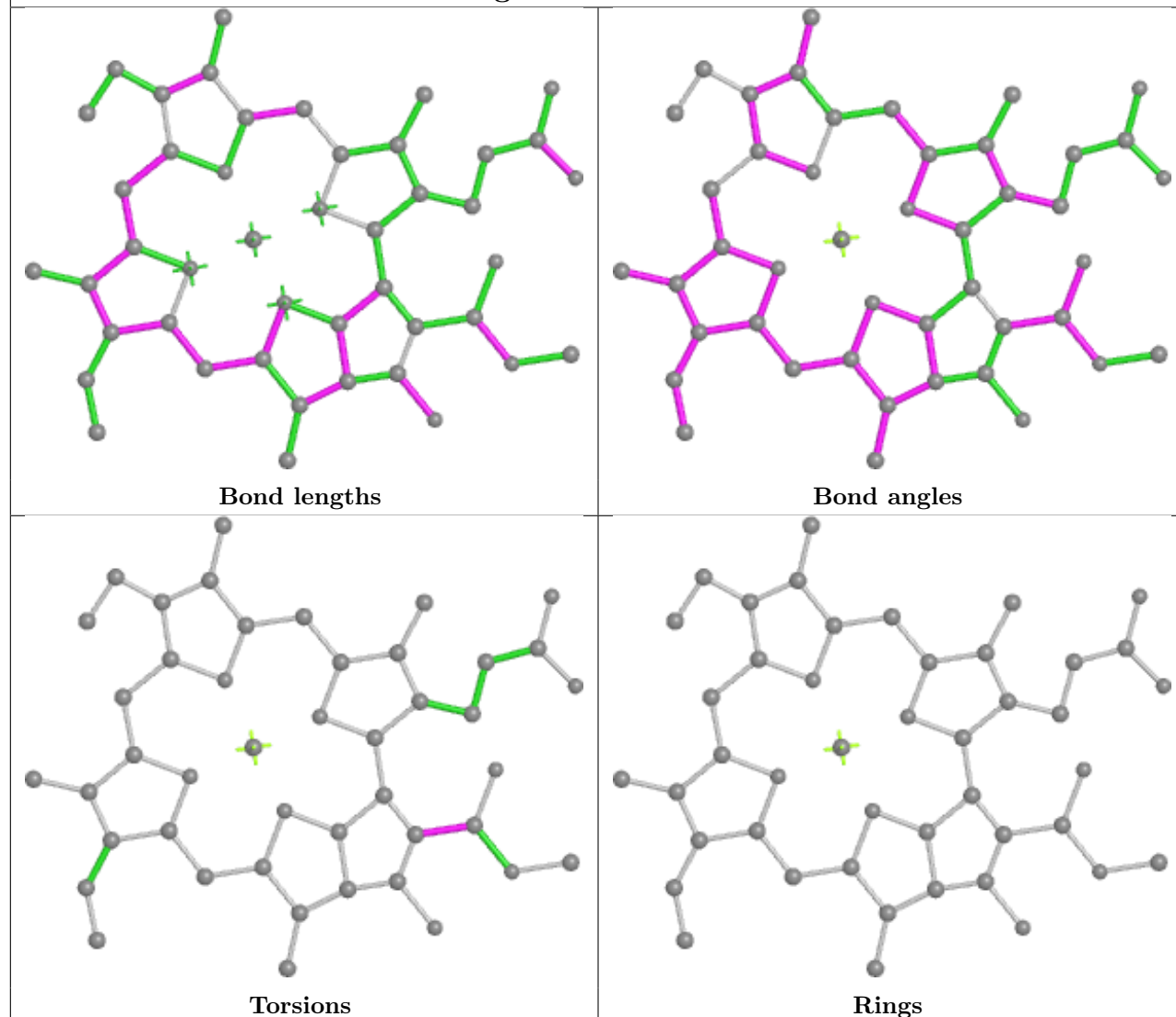
Ligand CLA B 839



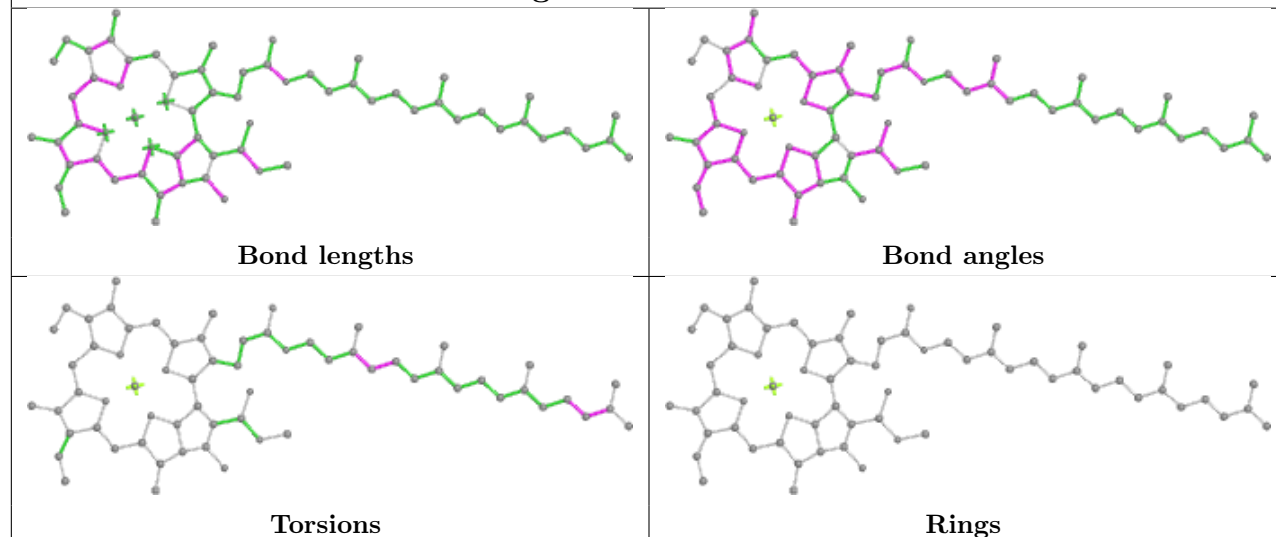
Ligand CLA B 806**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 841****Bond lengths****Bond angles****Torsions****Rings**

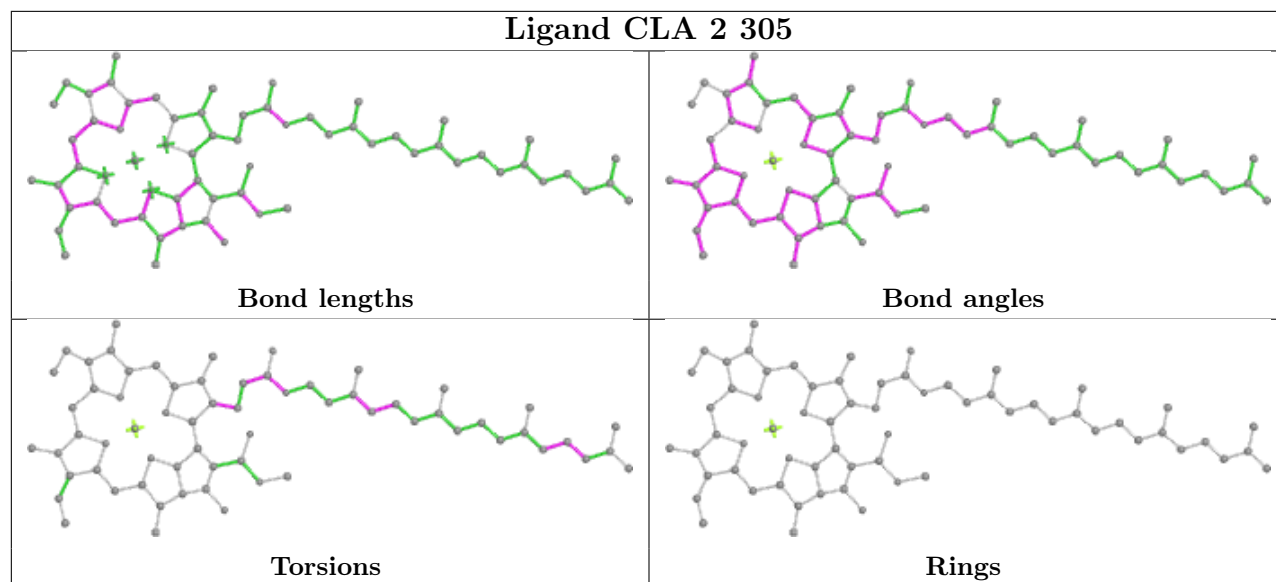
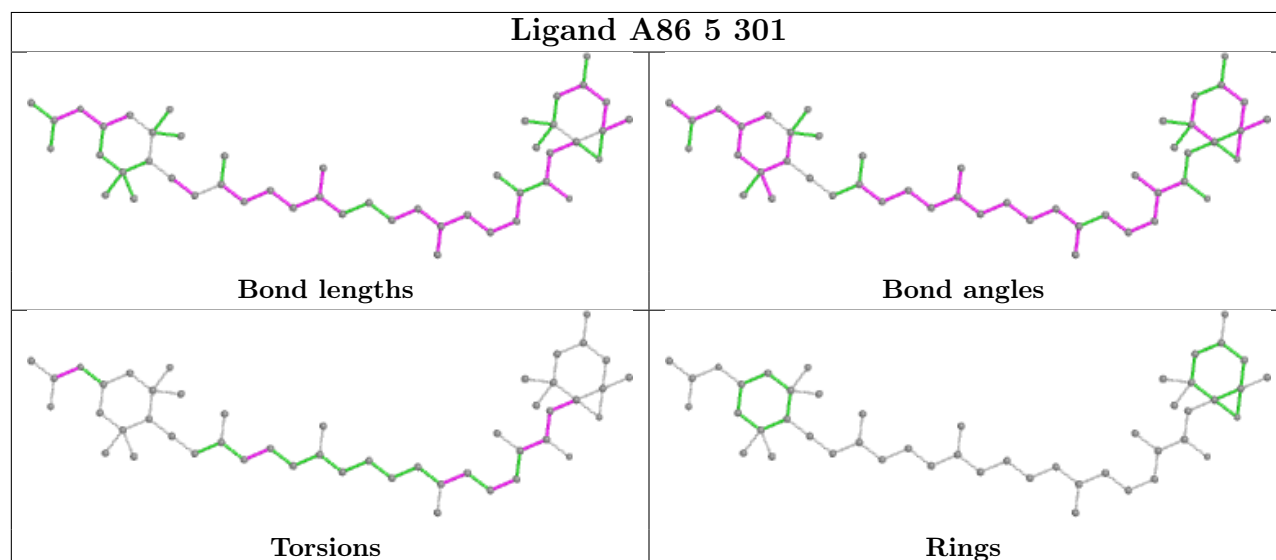
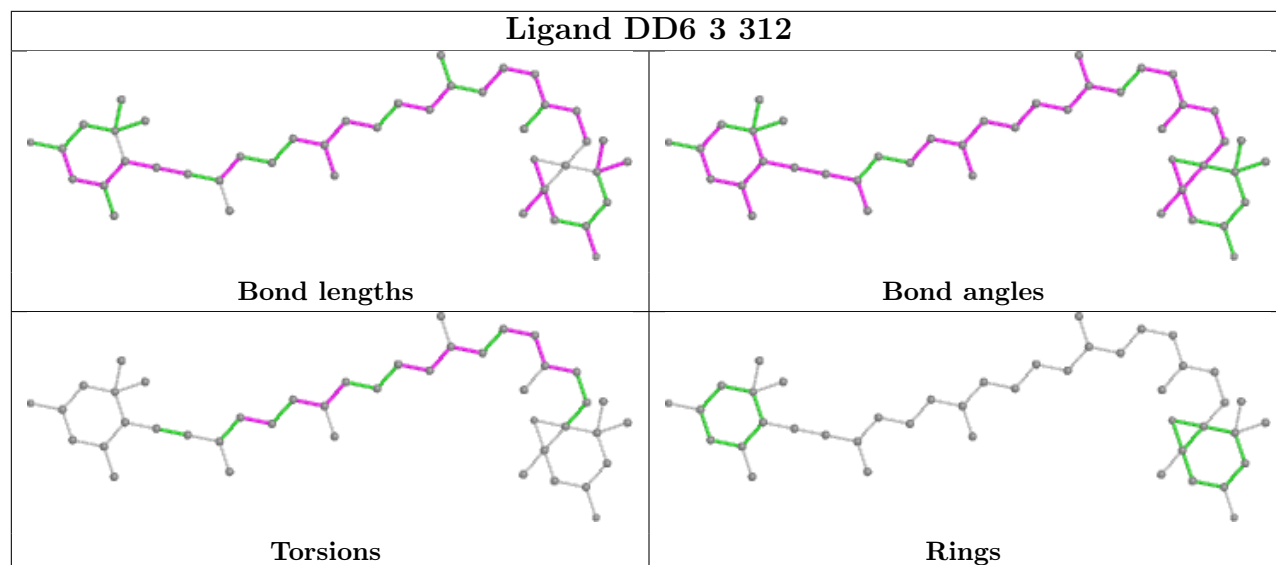


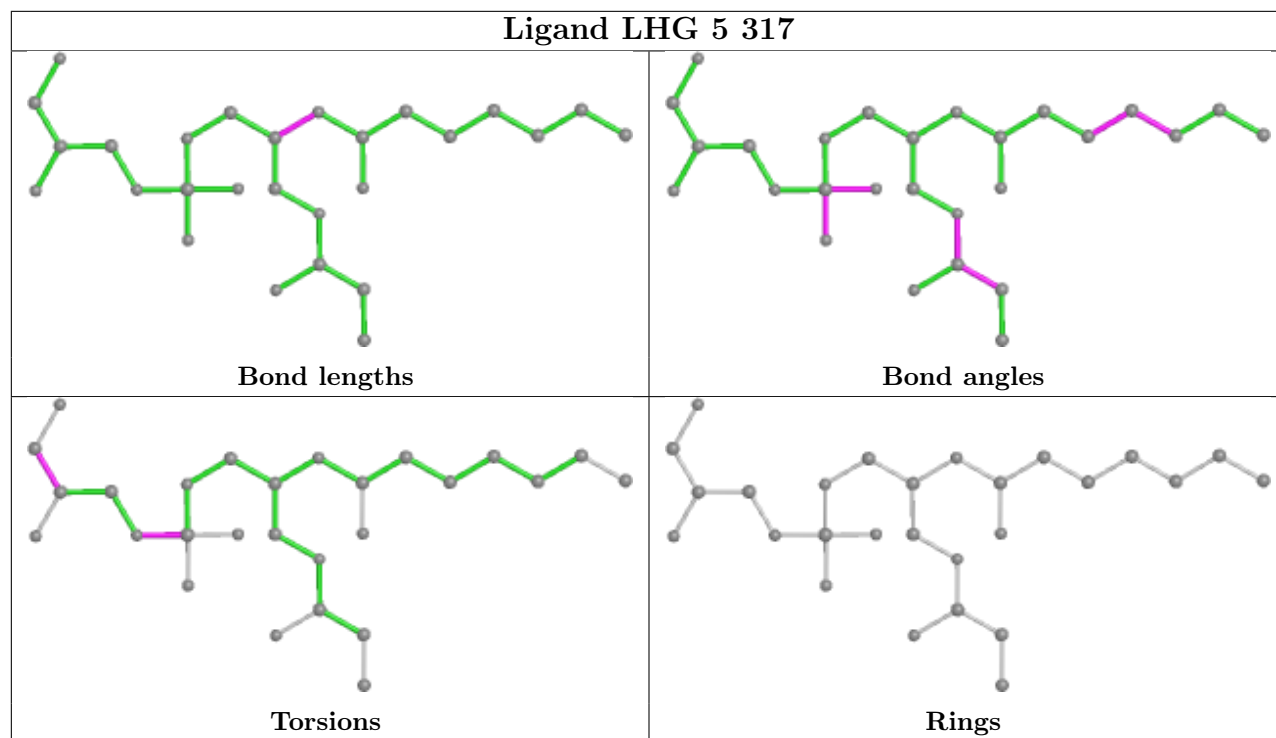
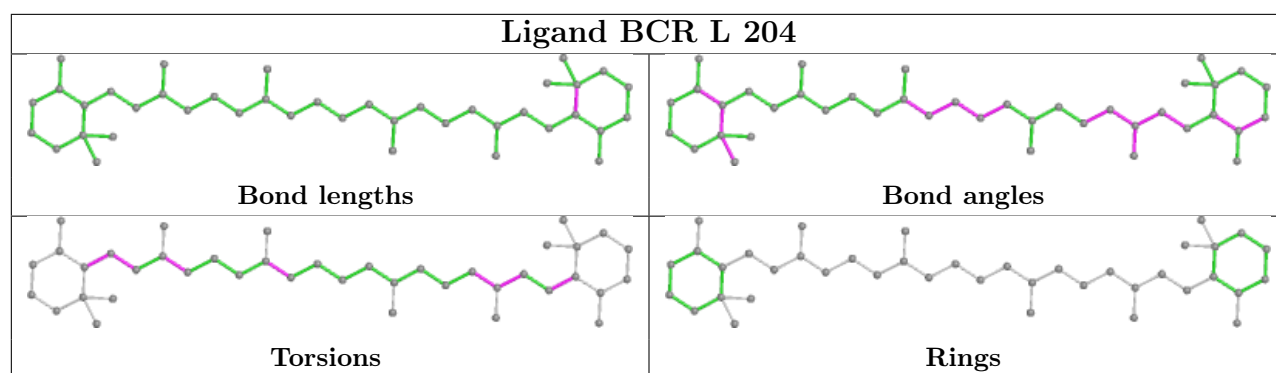
Ligand CLA 6 315

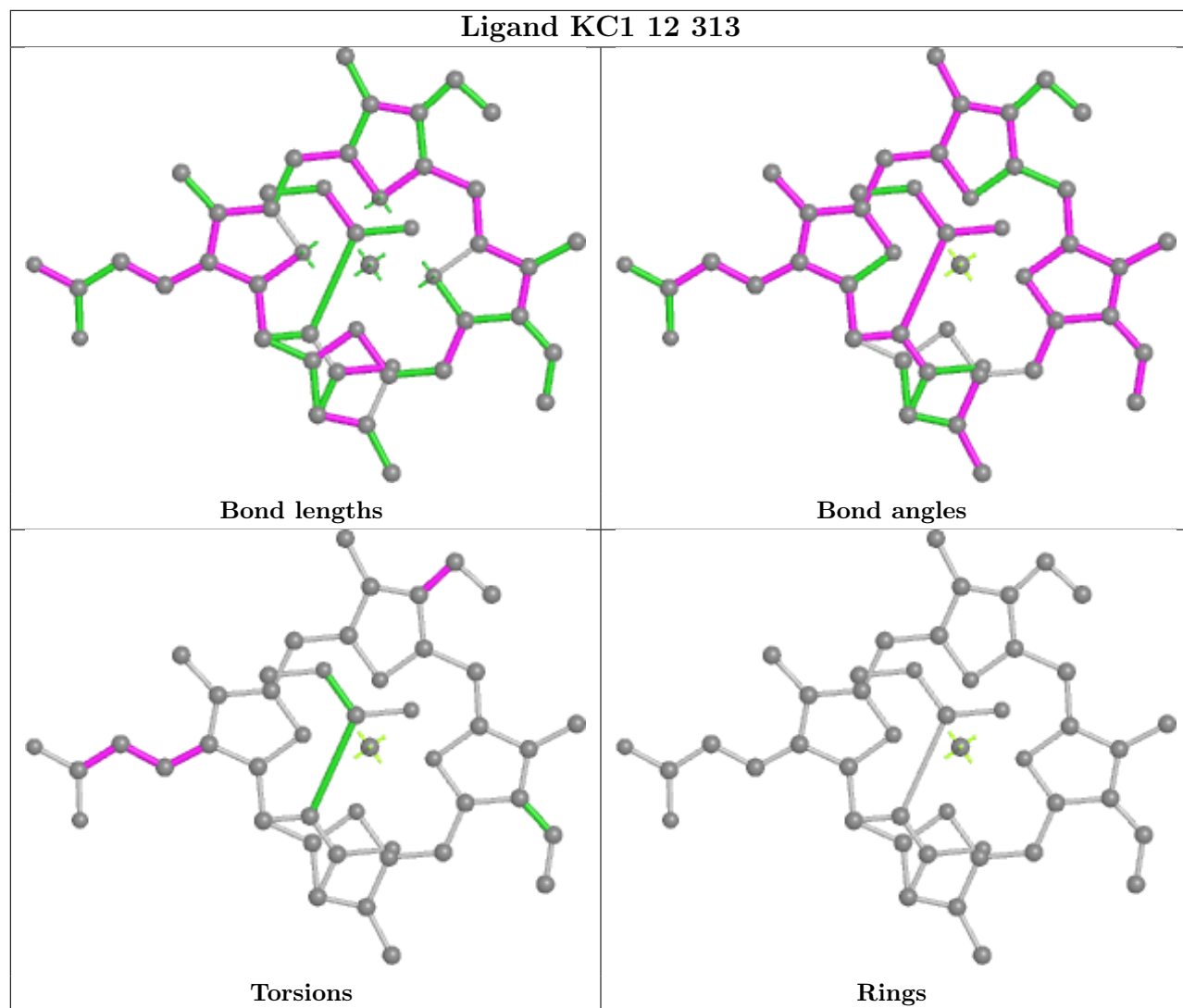


Ligand CLA B 832

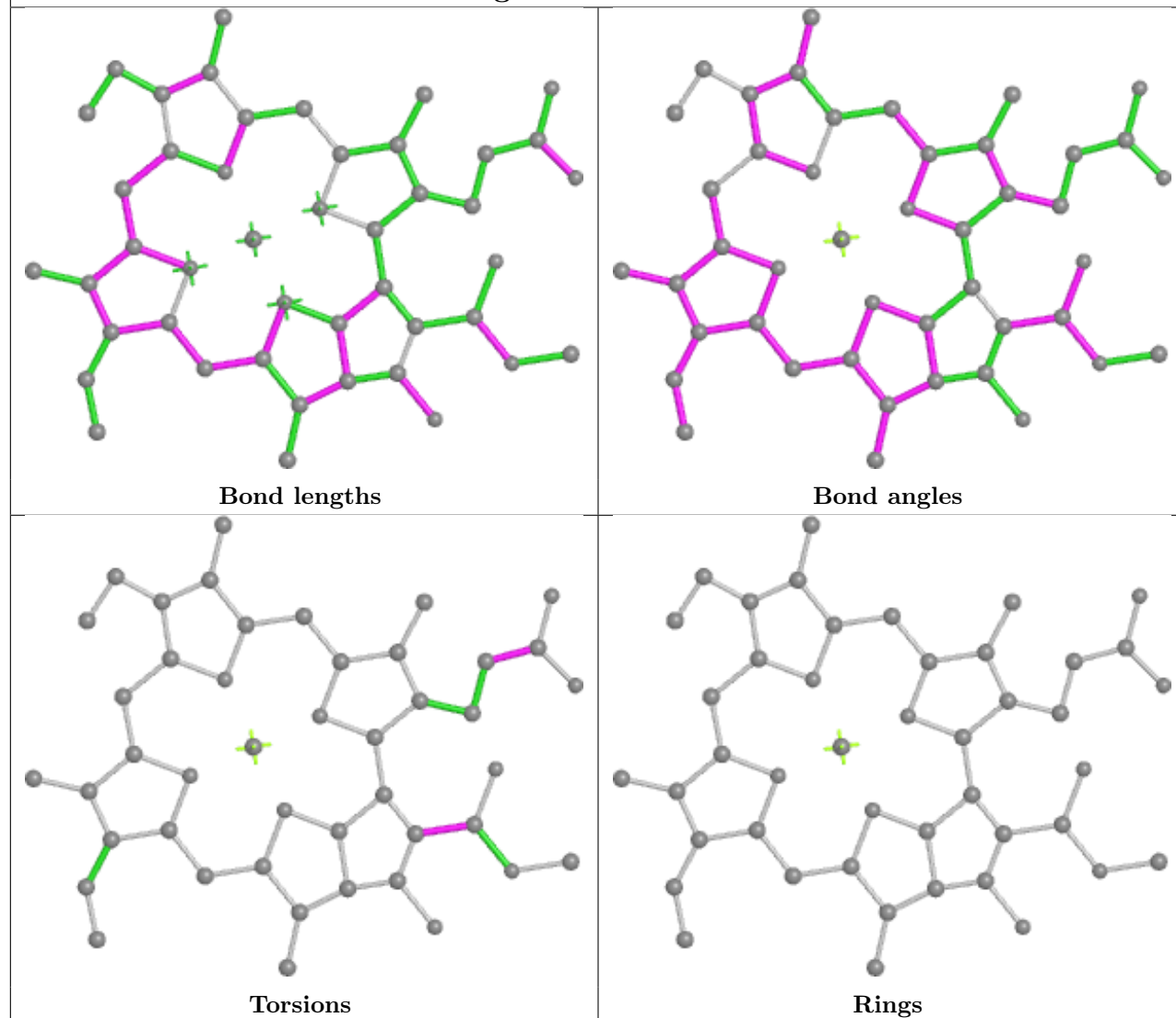


Ligand CLA 2 305**Ligand A86 5 301****Ligand DD6 3 312**

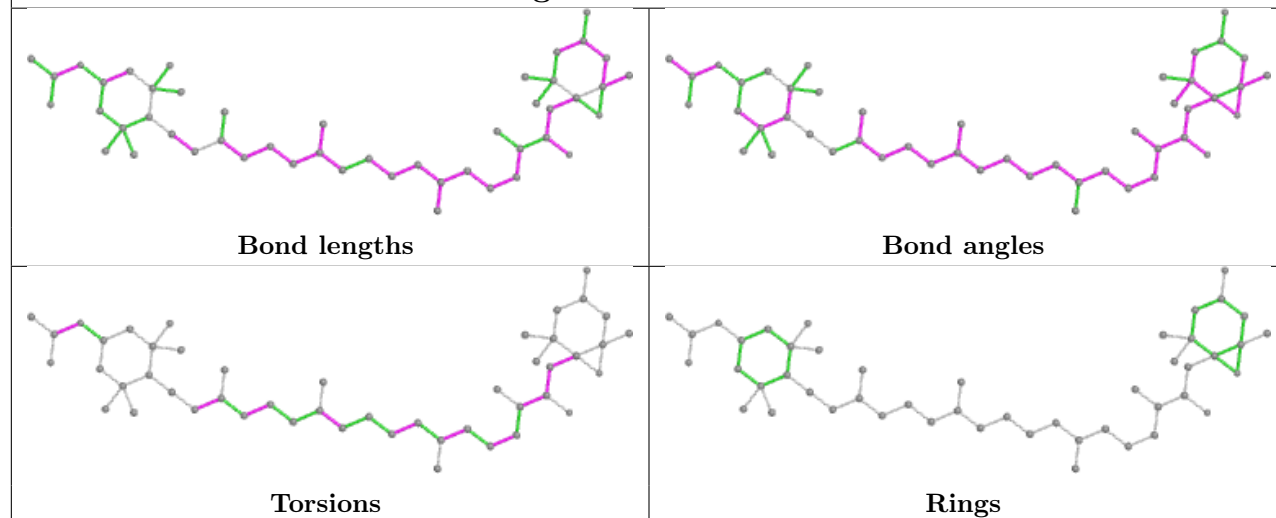


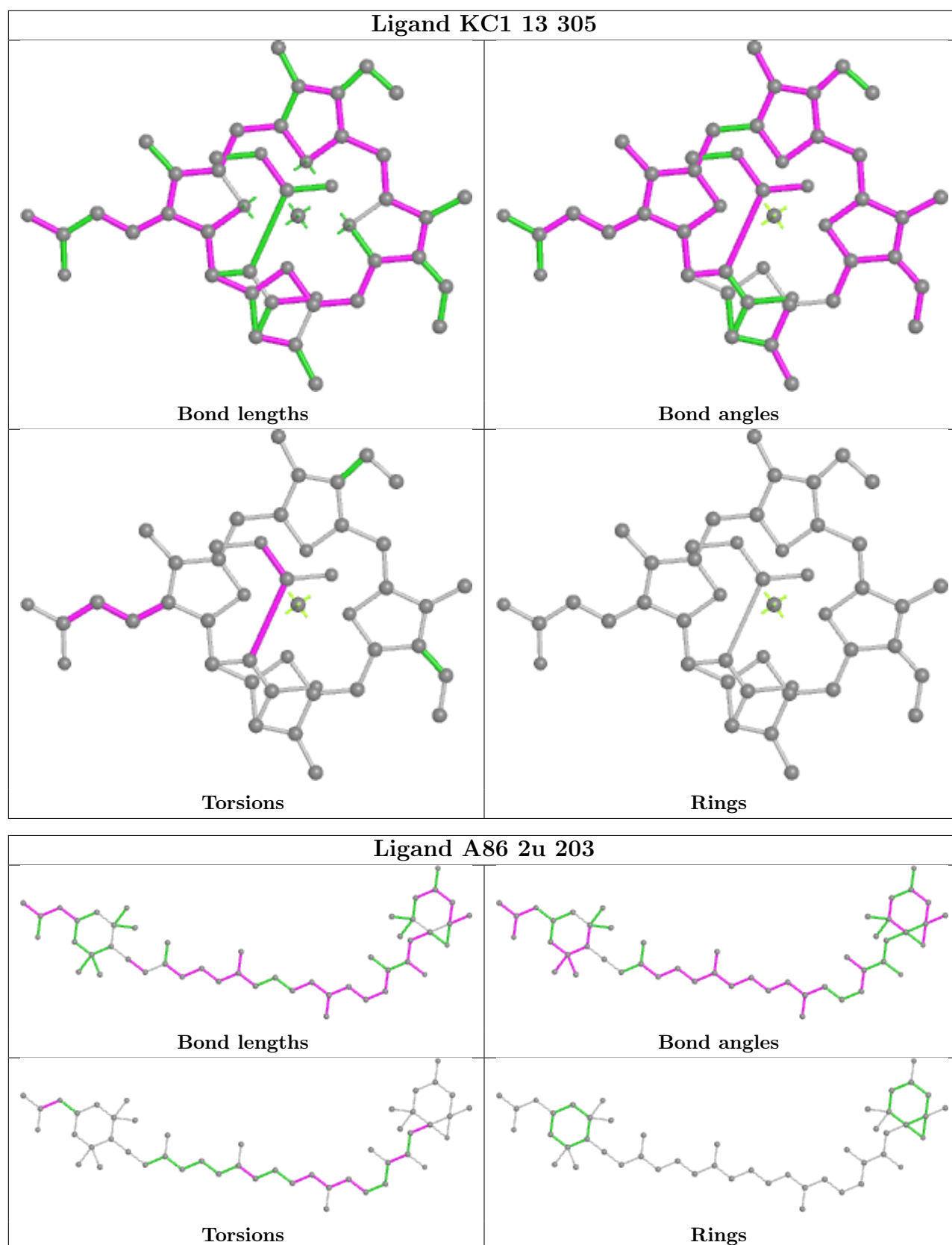


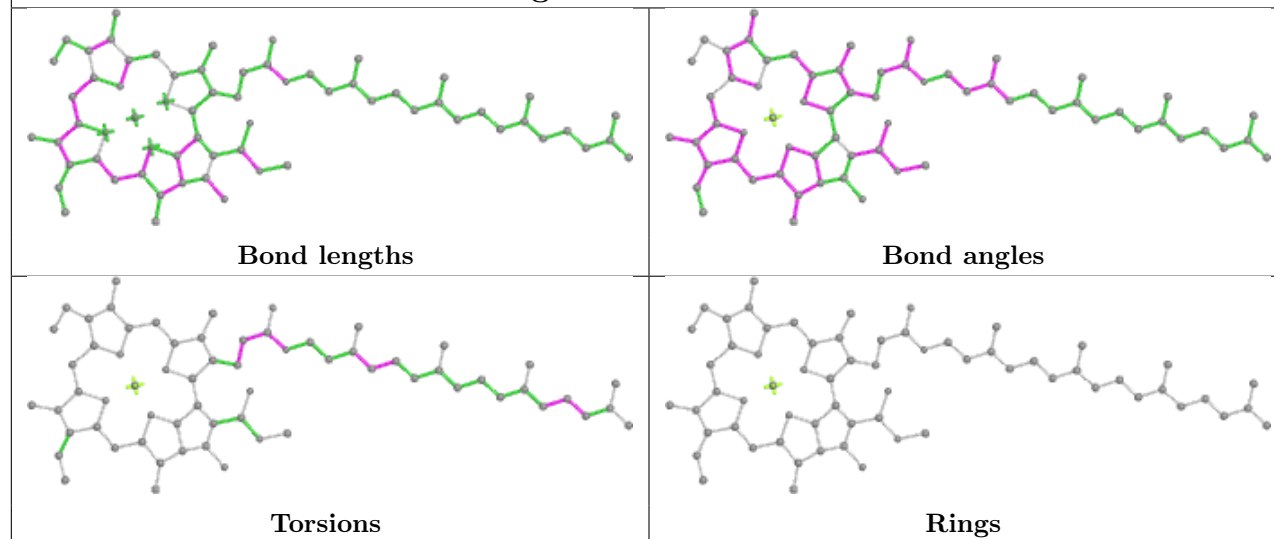
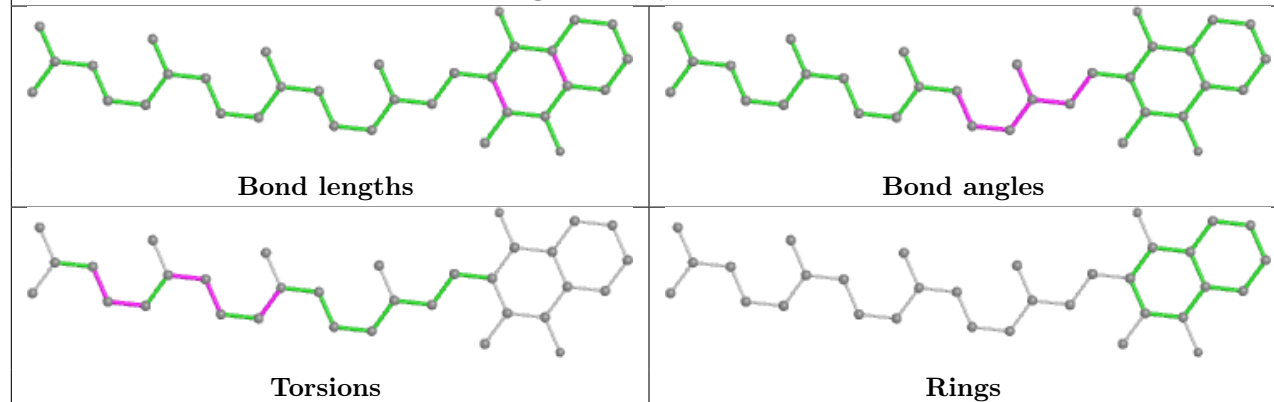
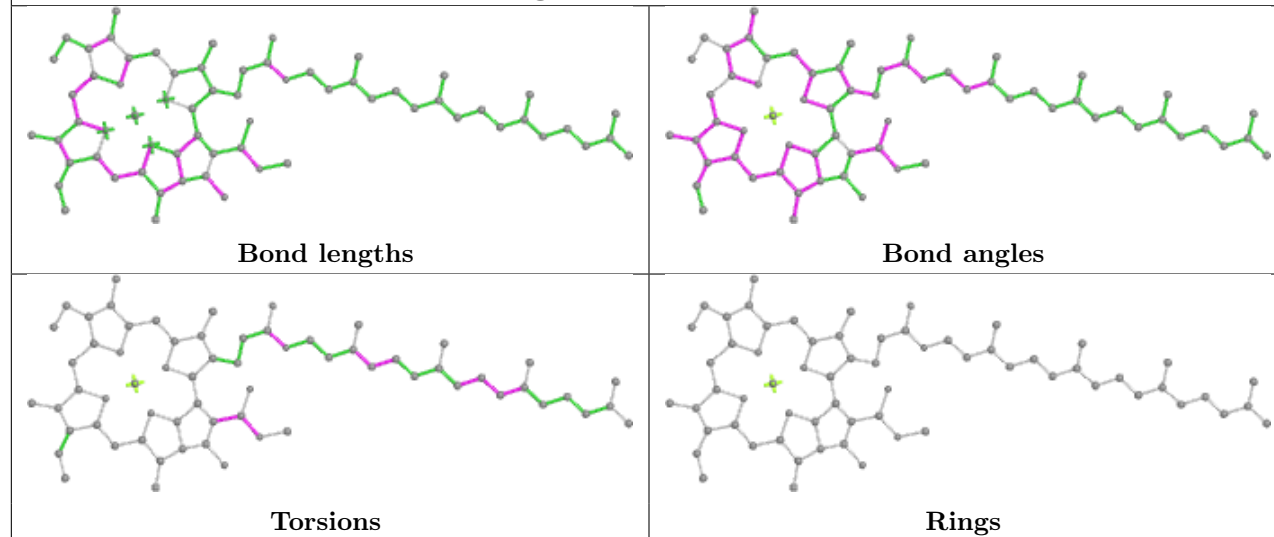
Ligand CLA J 101

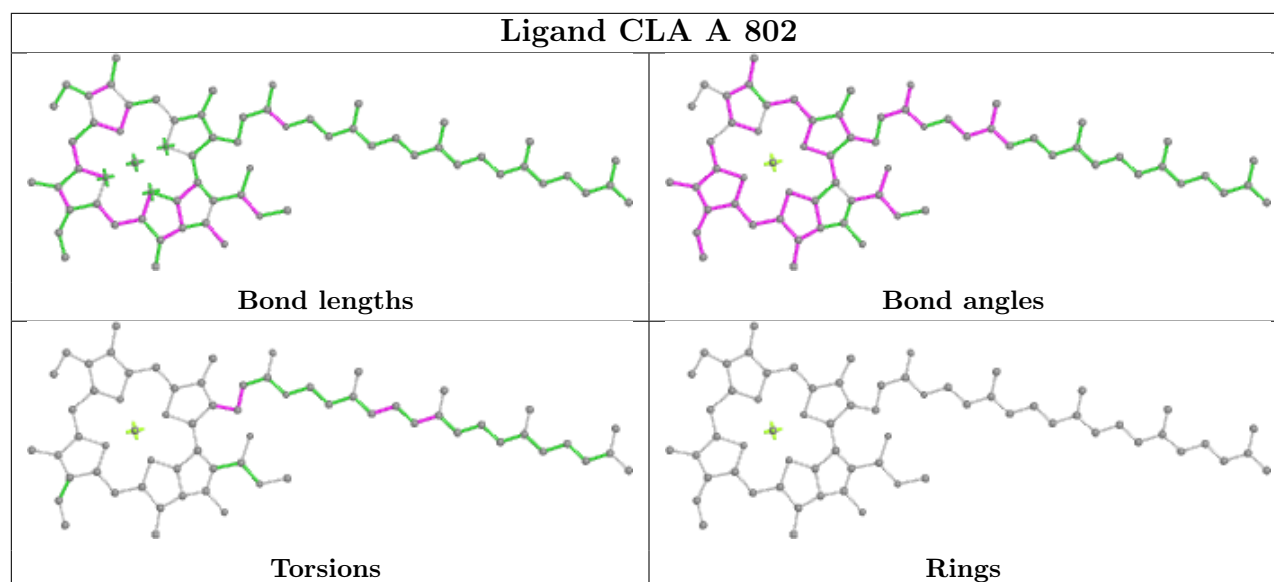
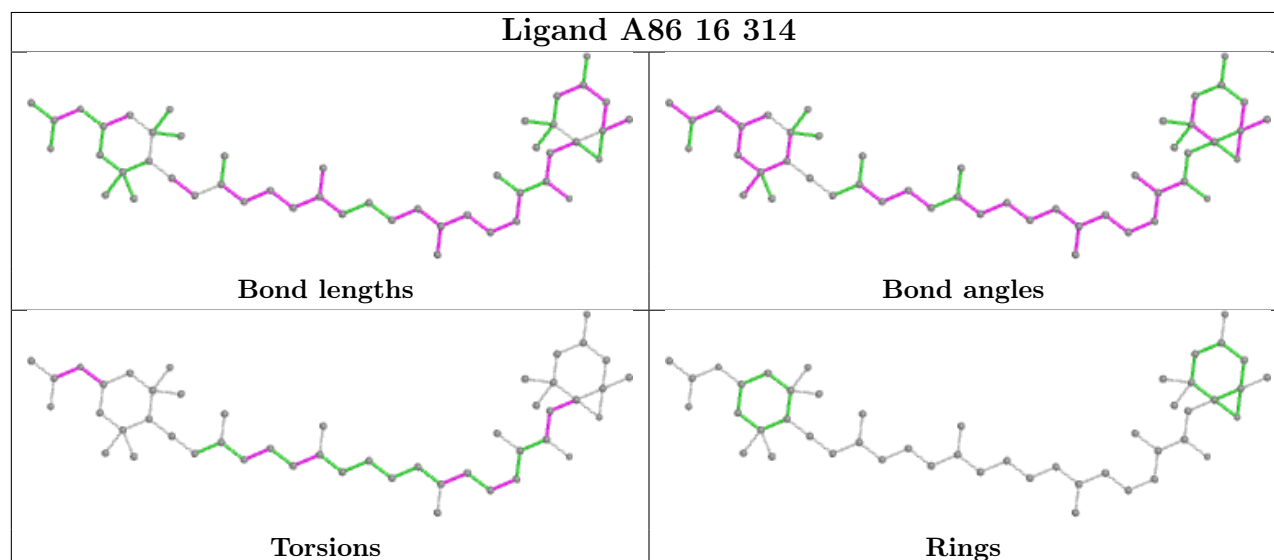
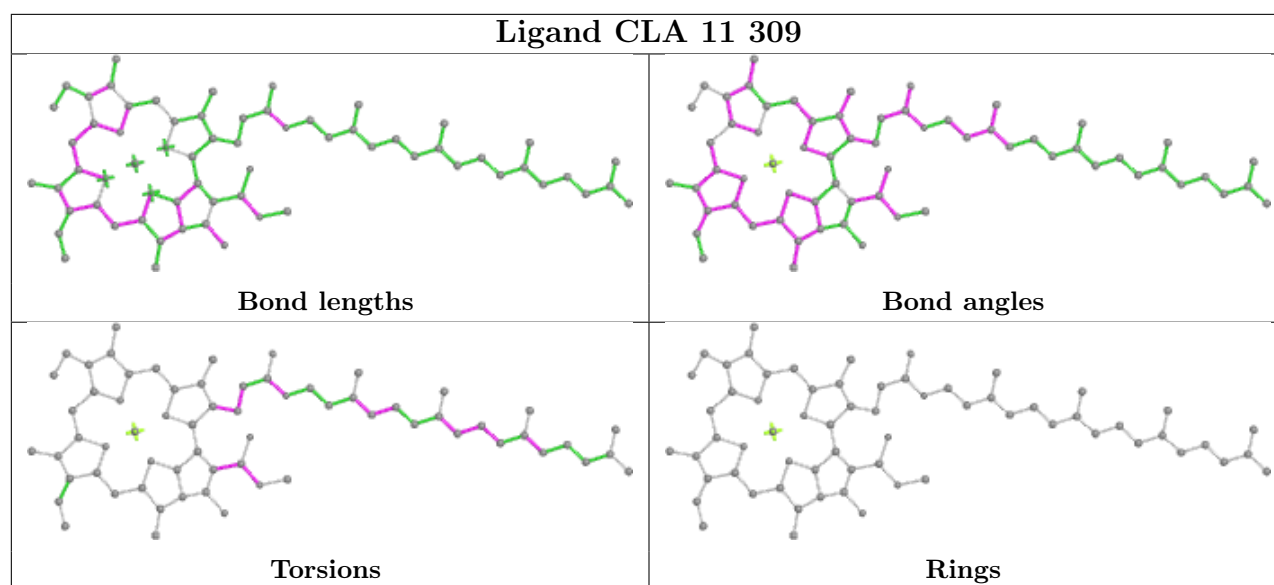


Ligand A86 15 322

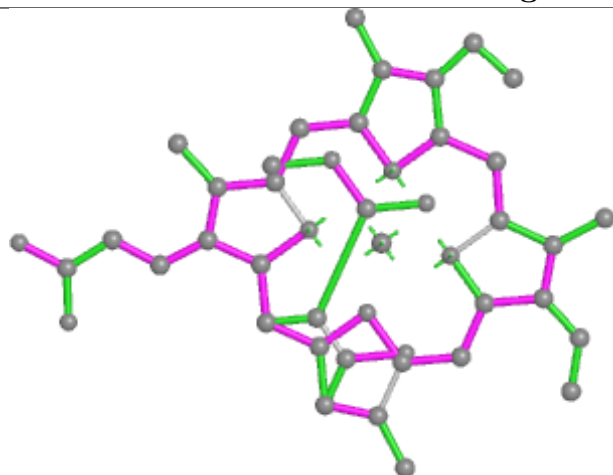




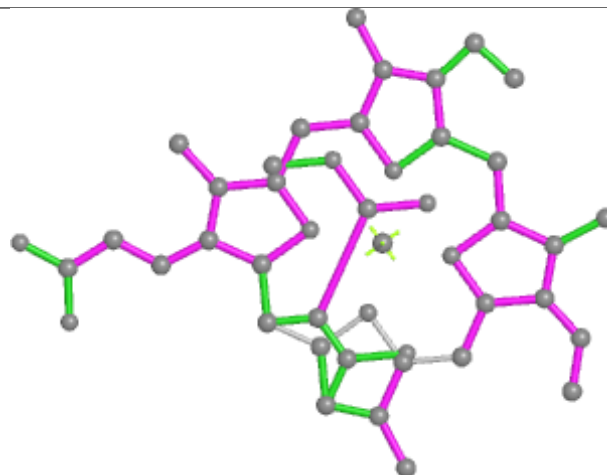
Ligand CLA A 830**Ligand PQN A 845****Ligand CLA A 811**



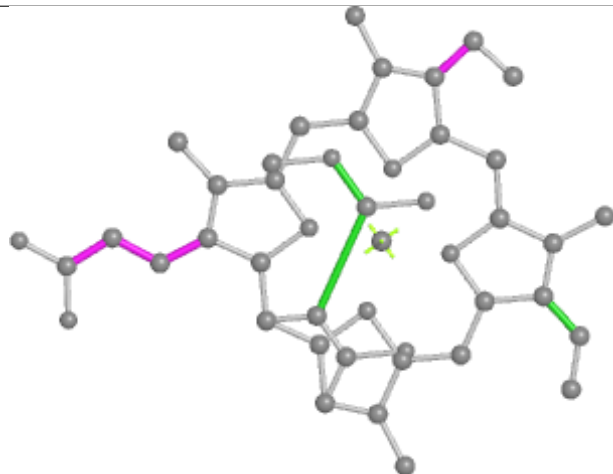
Ligand KC1 4 307



Bond lengths



Bond angles

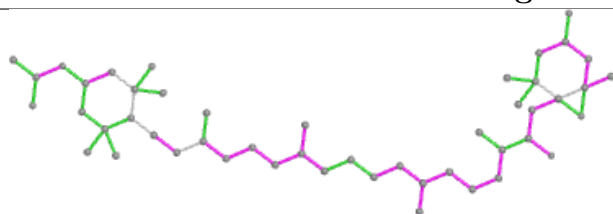


Torsions

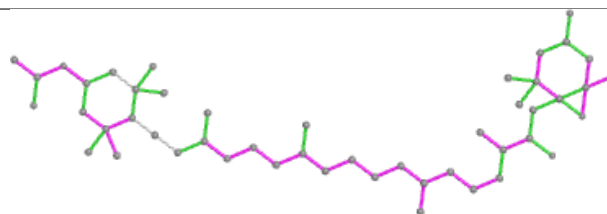


Rings

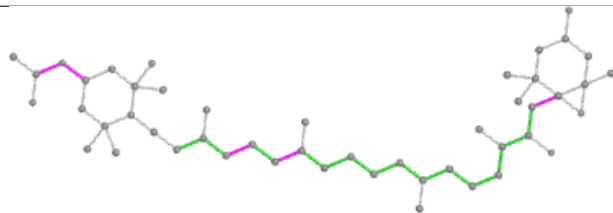
Ligand A86 14 301



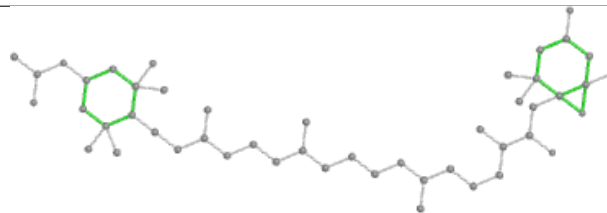
Bond lengths



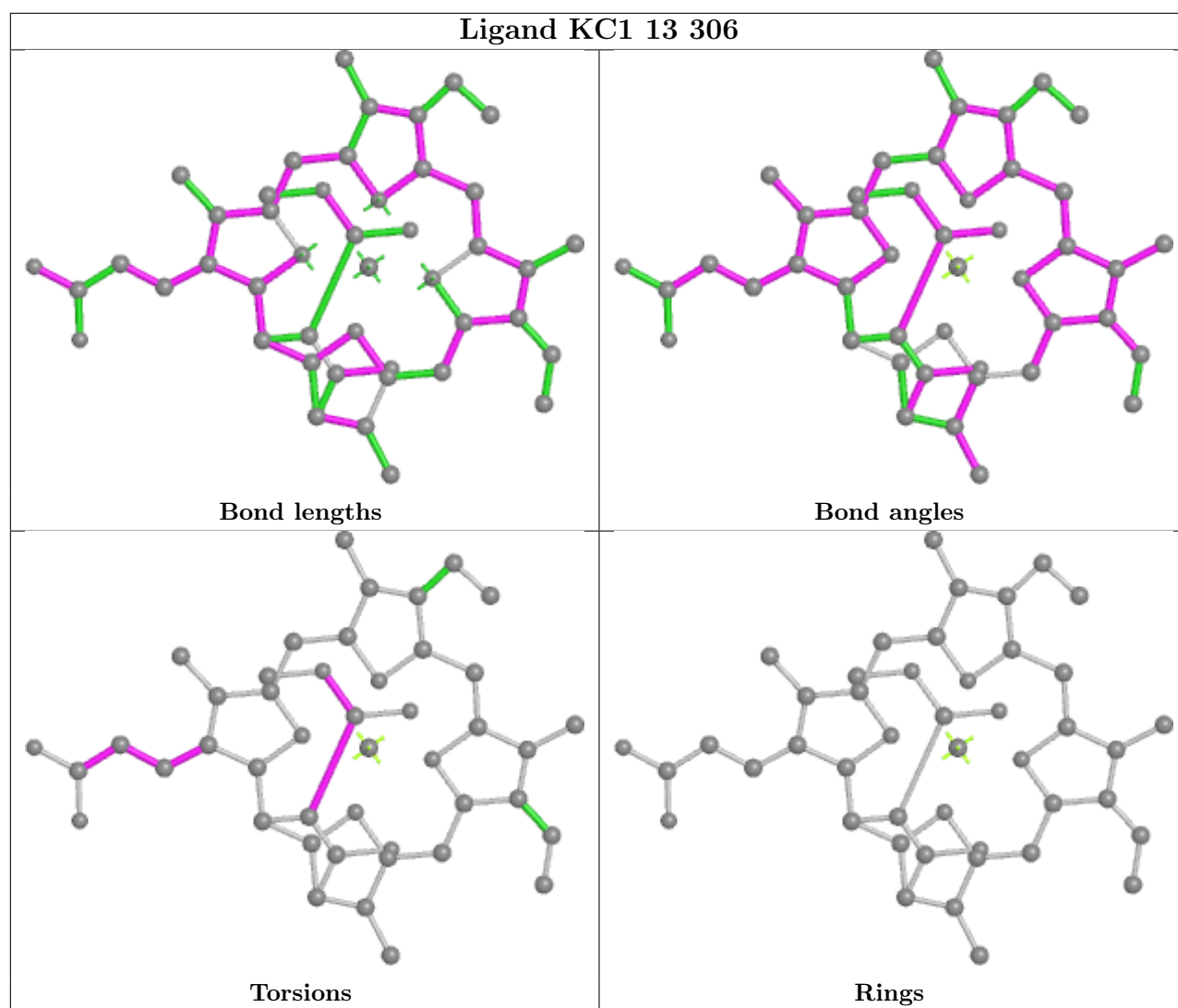
Bond angles

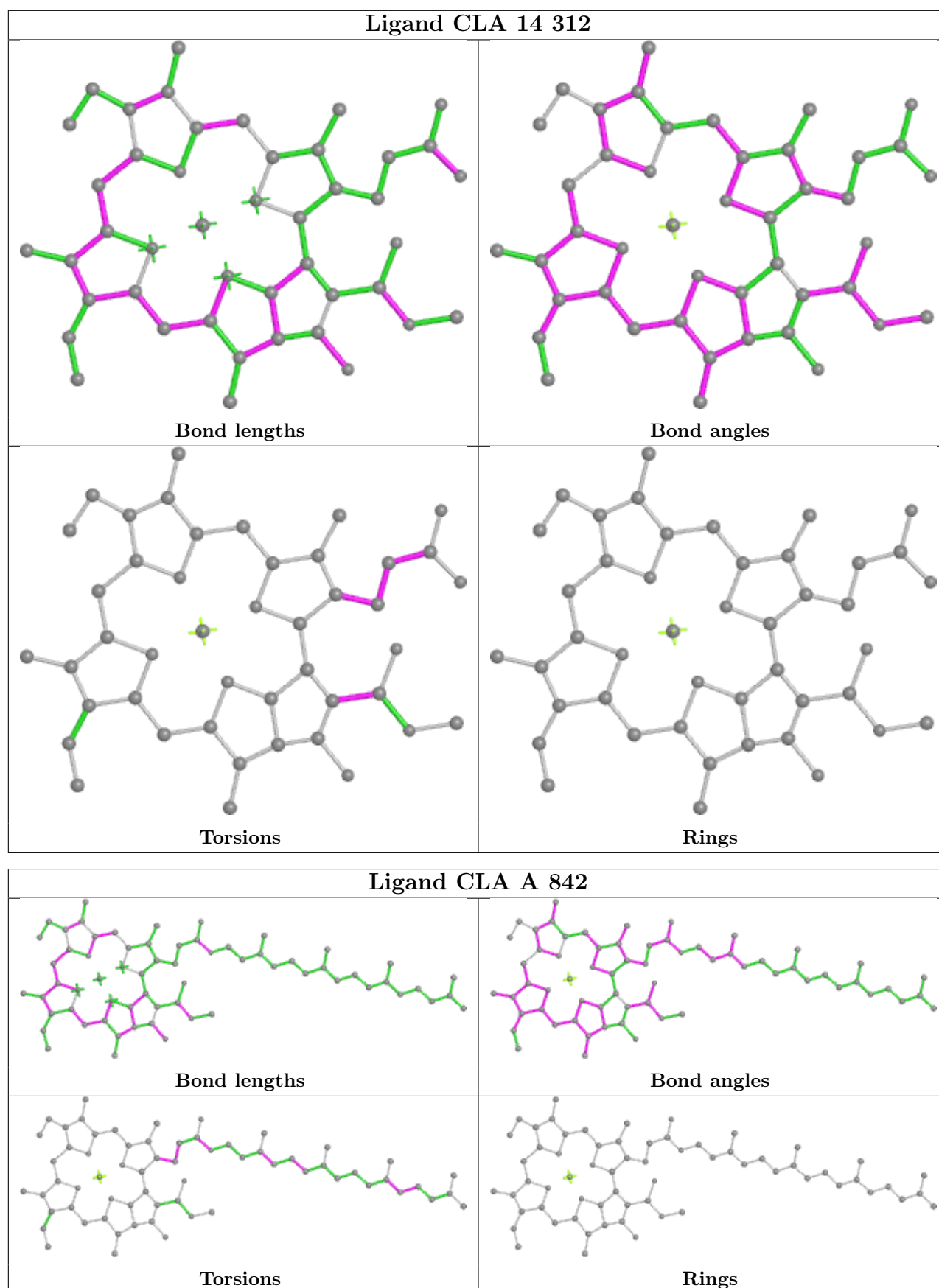


Torsions

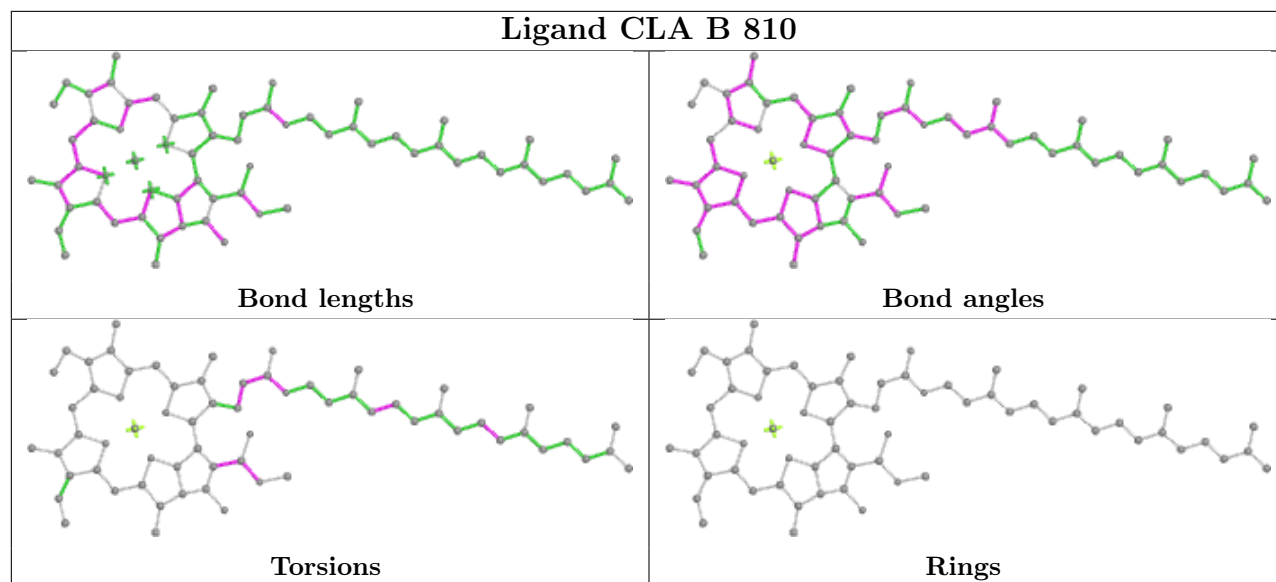


Rings

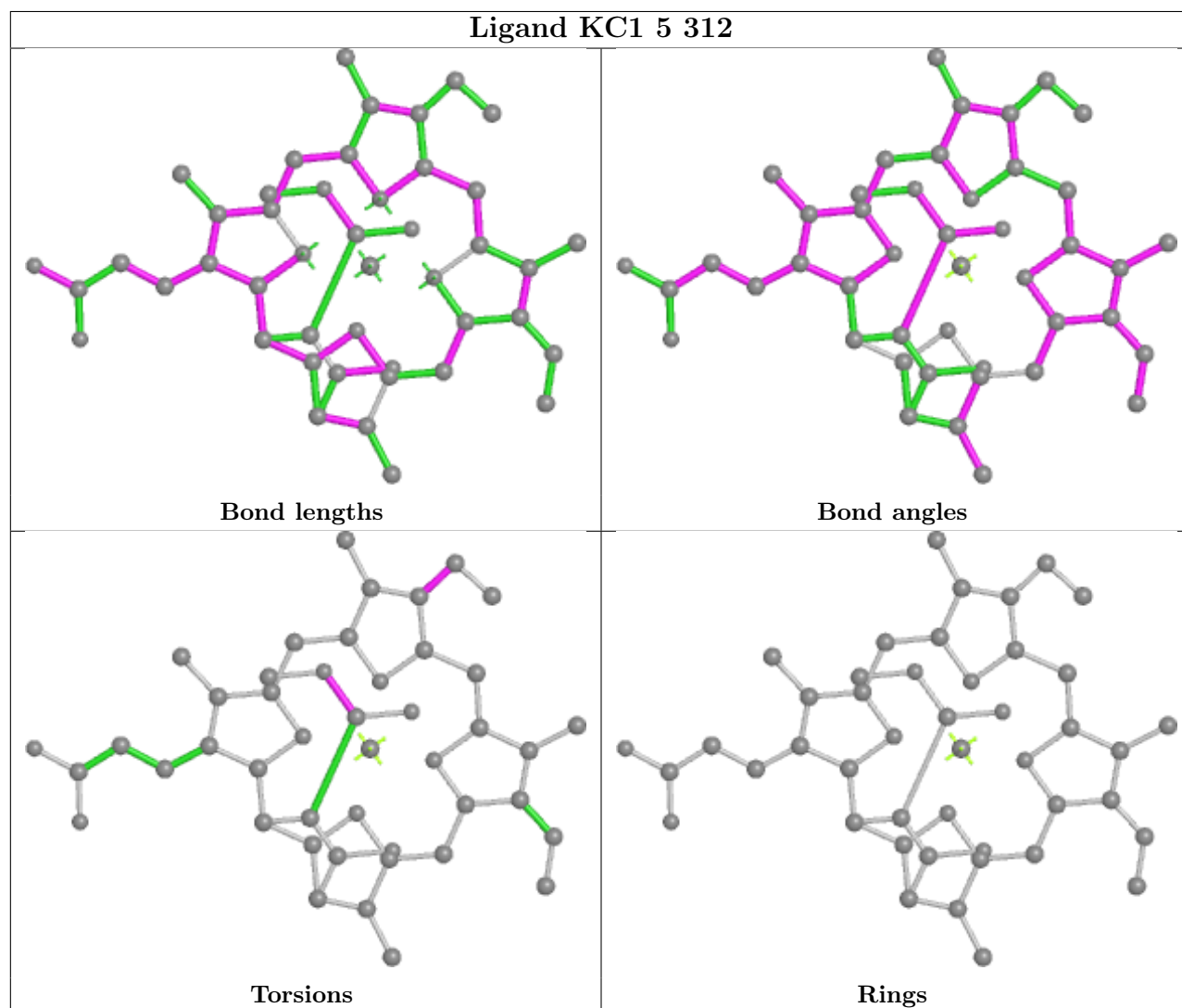


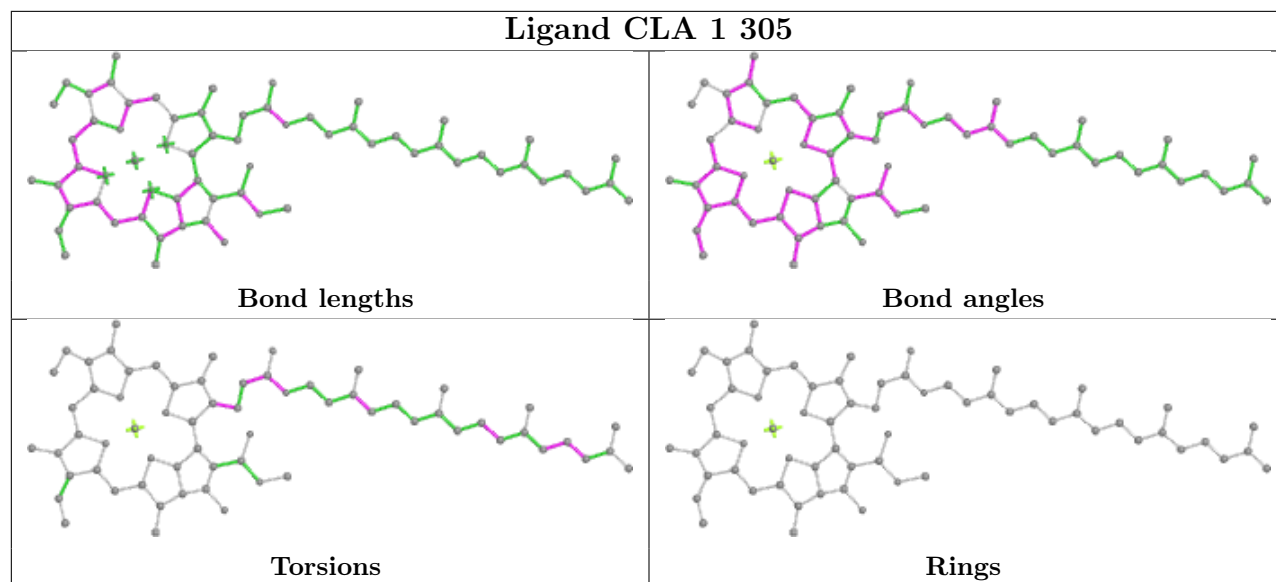
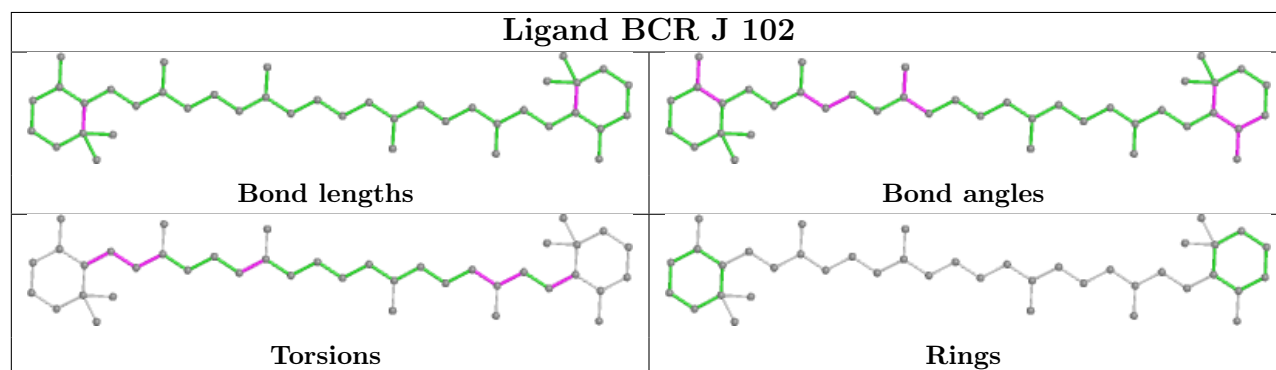
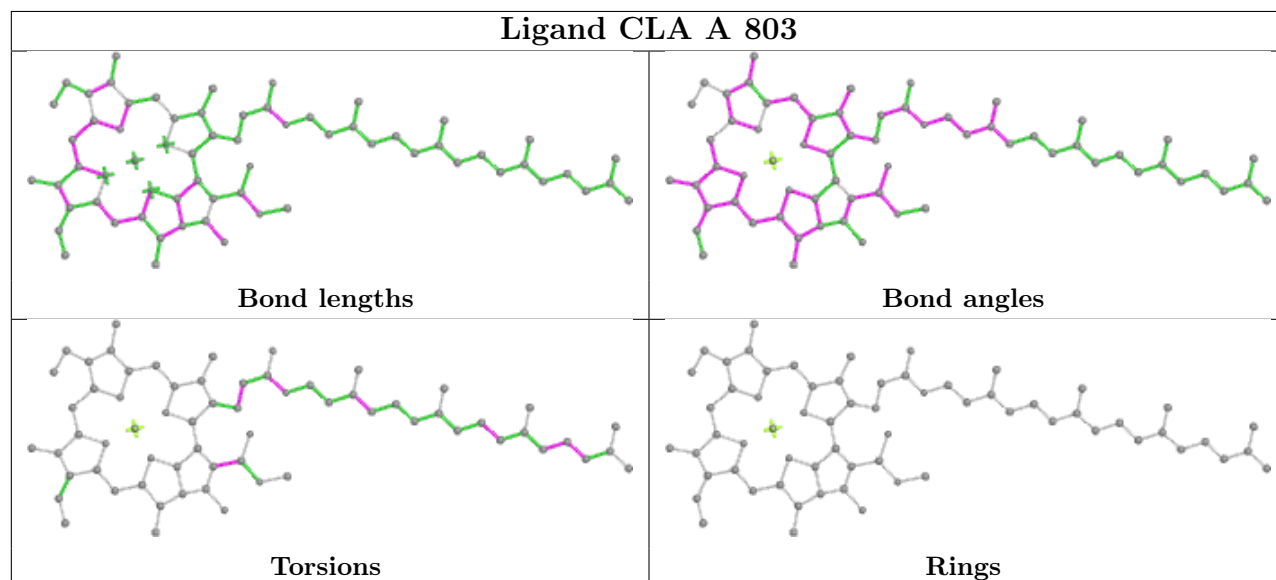


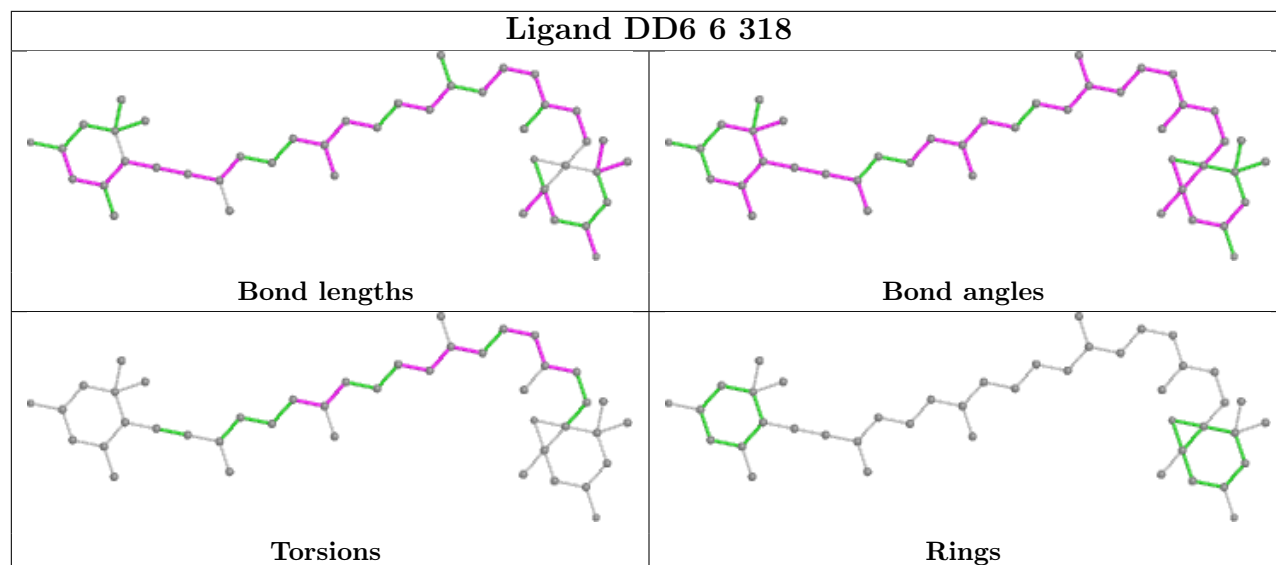
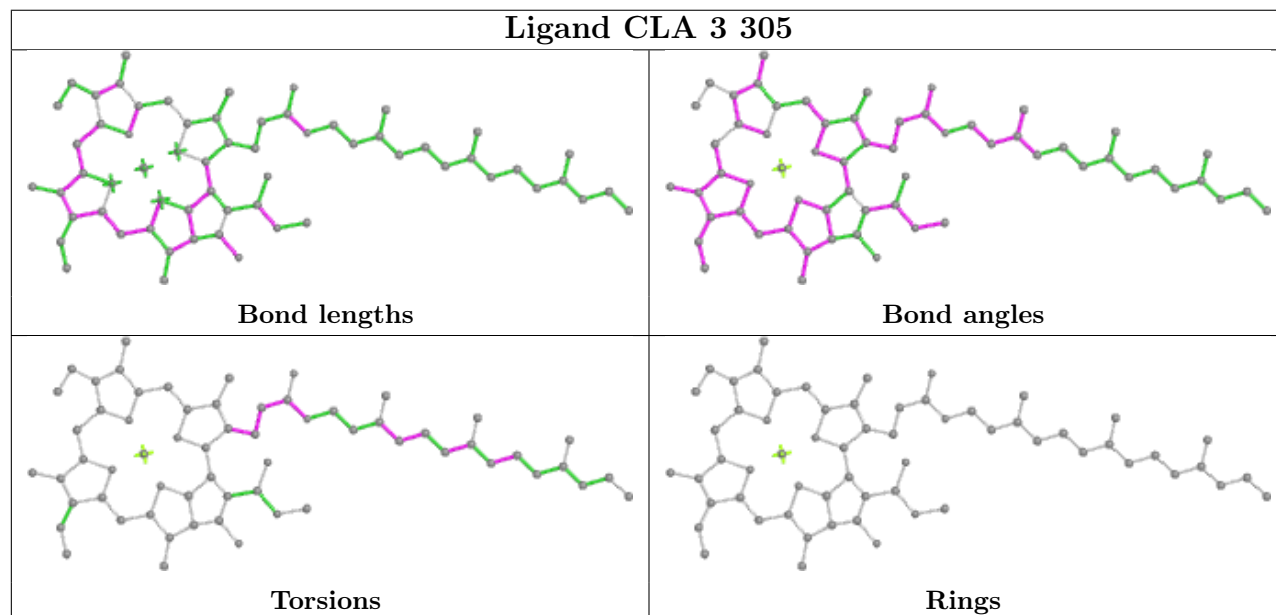
Ligand CLA B 810

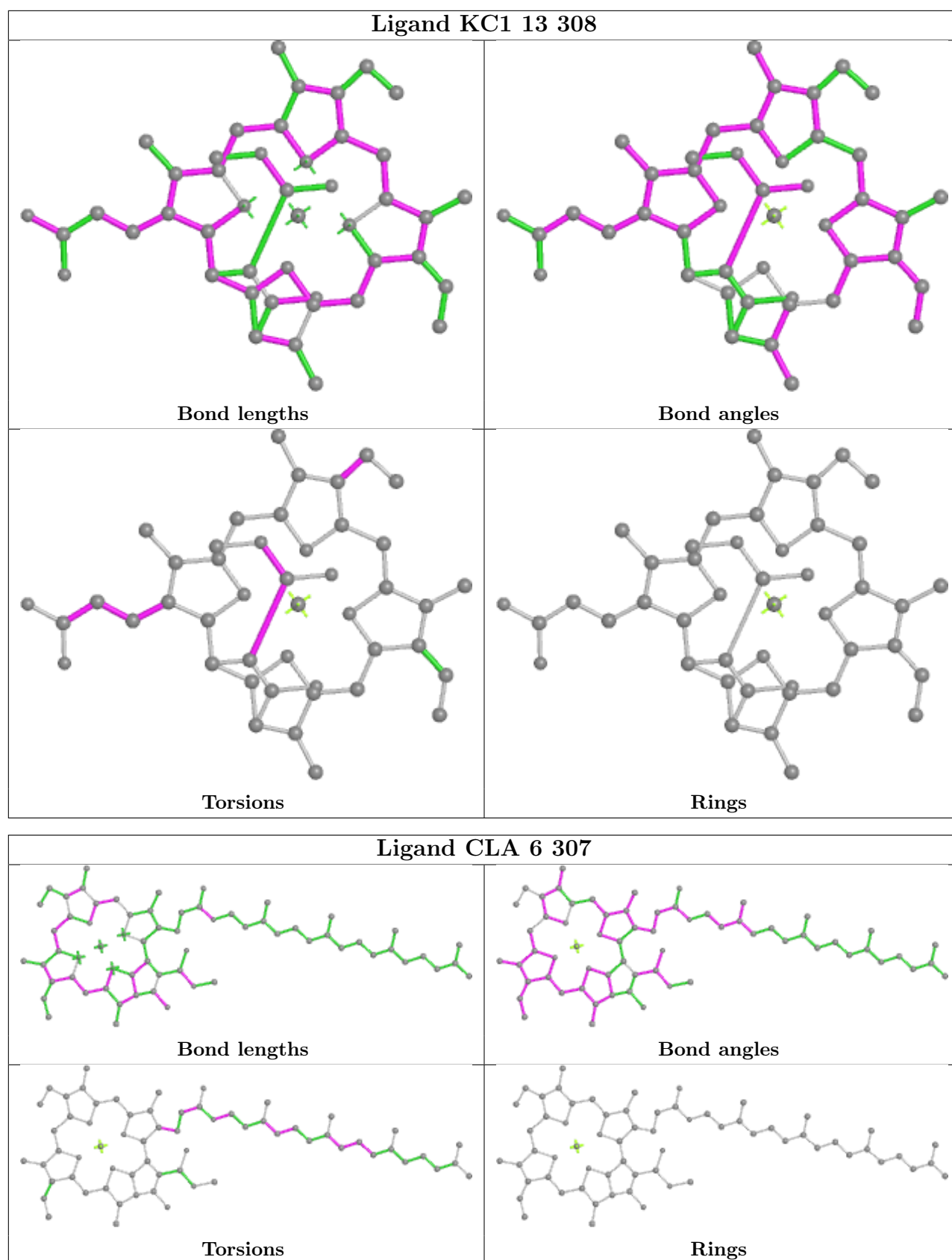


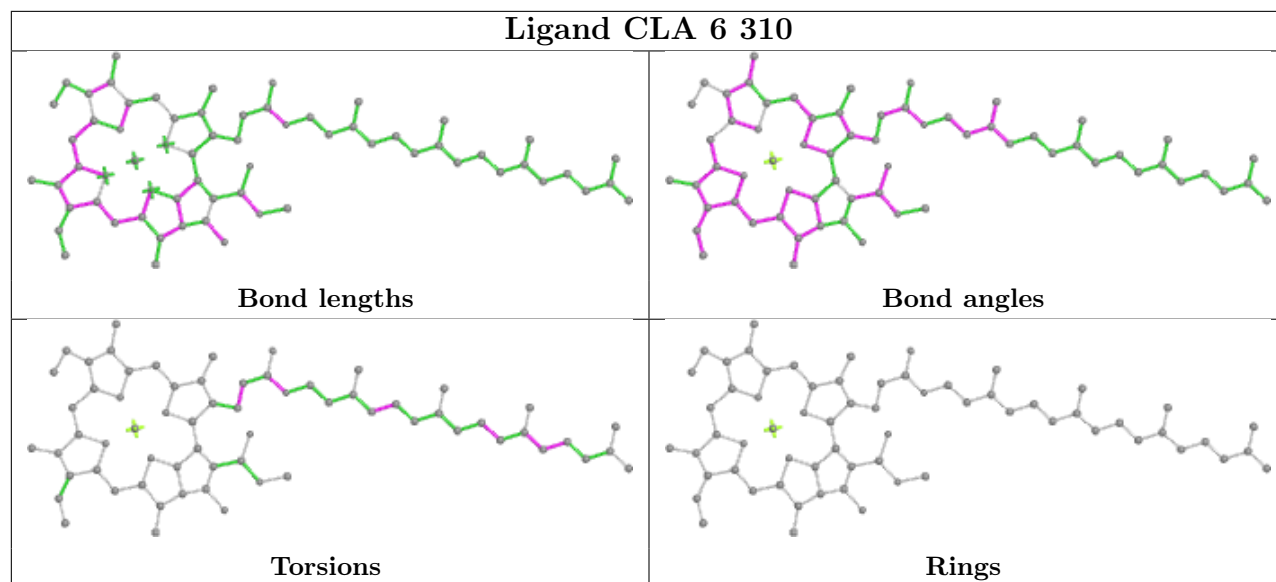
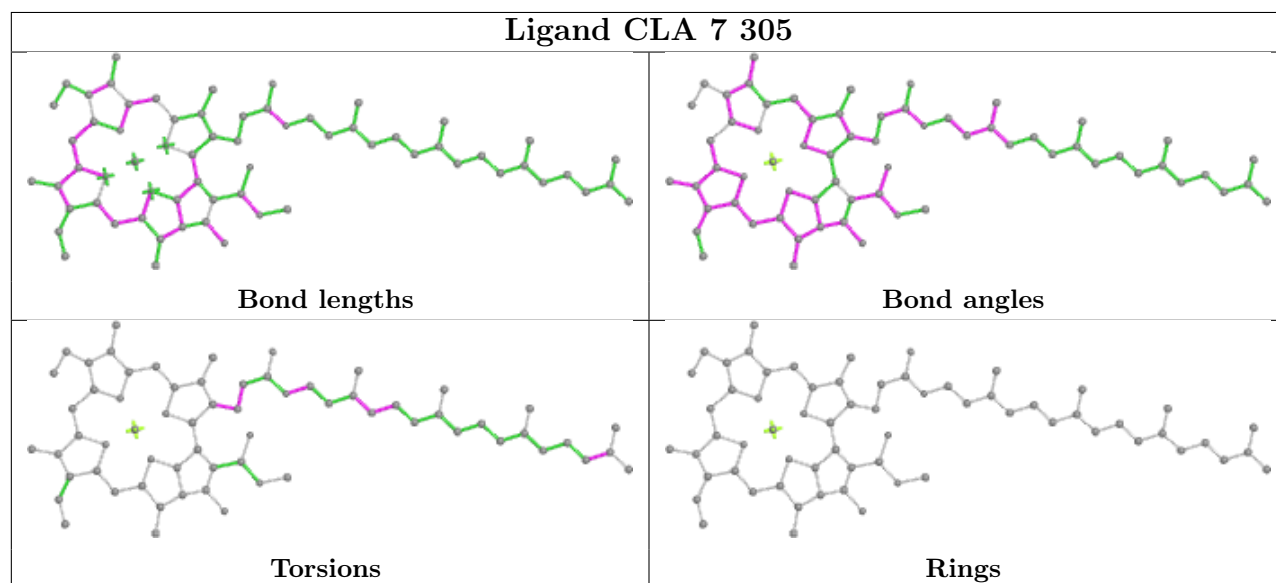
Ligand KC1 5 312



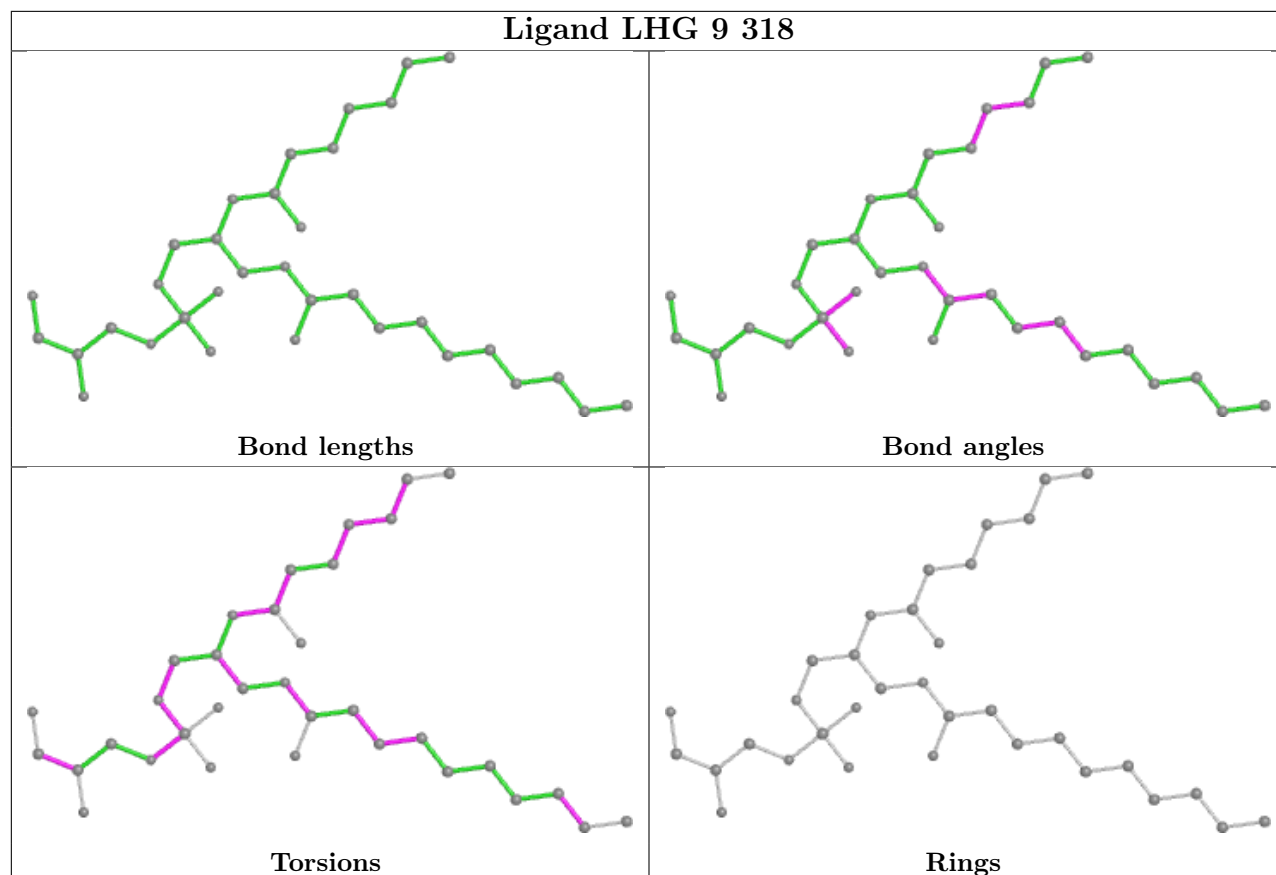
Ligand CLA 1 305**Ligand BCR J 102****Ligand CLA A 803**

Ligand DD6 6 318**Ligand CLA 3 305**

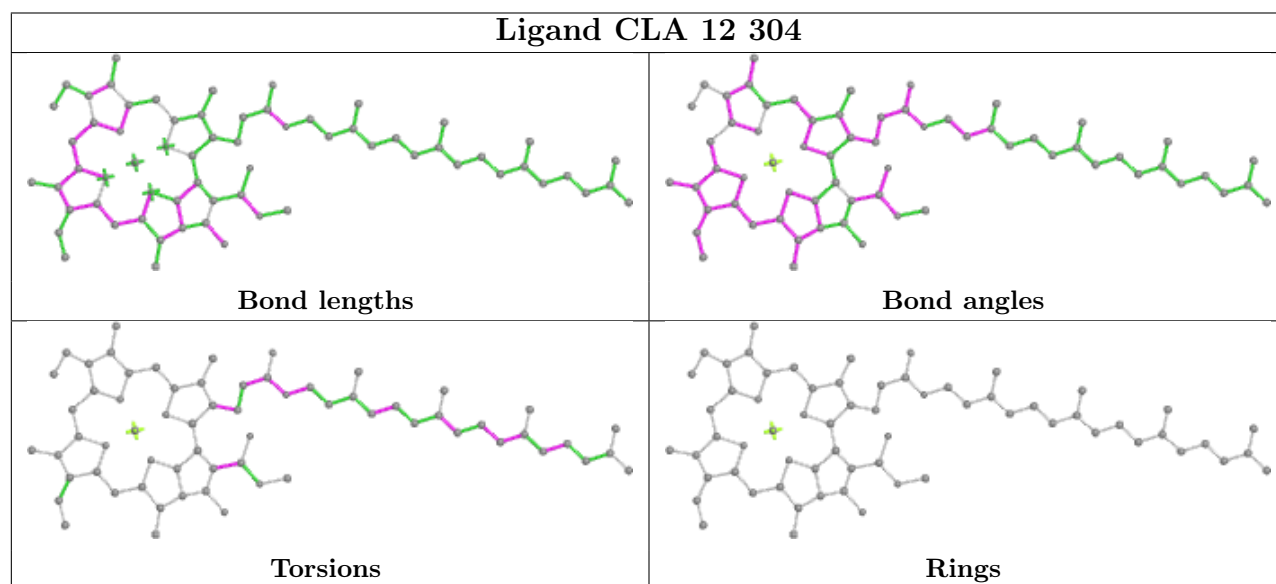


Ligand CLA 6 310**Ligand CLA 7 305**

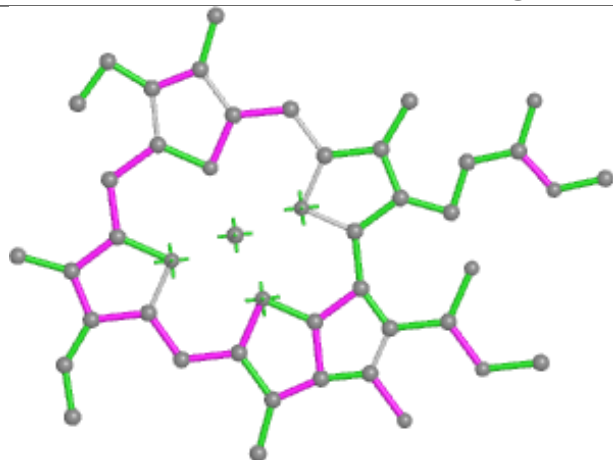
Ligand LHG 9 318



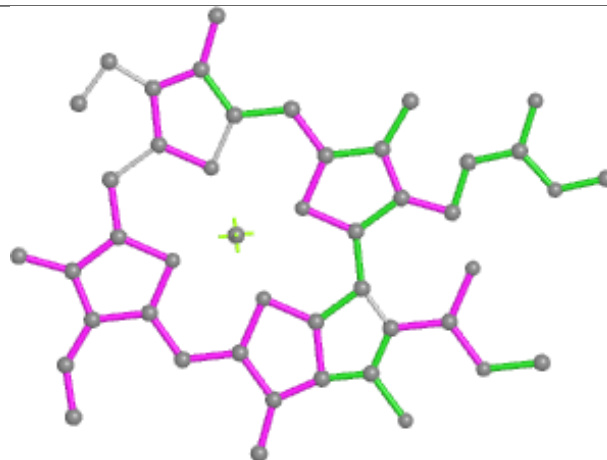
Ligand CLA 12 304



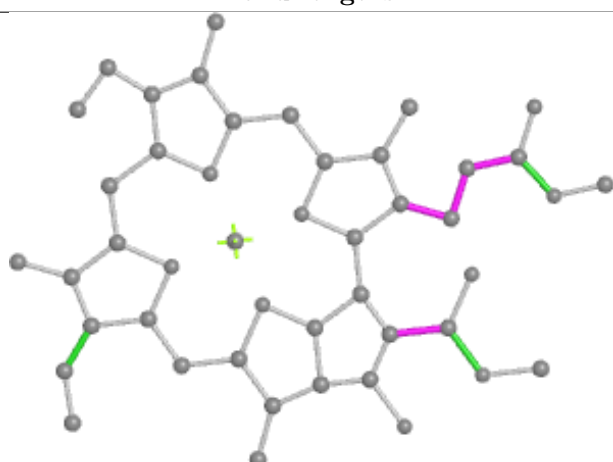
Ligand CLA 16 307



Bond lengths



Bond angles

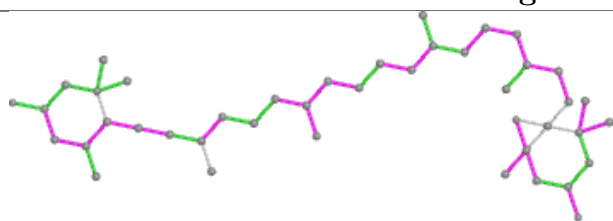


Torsions

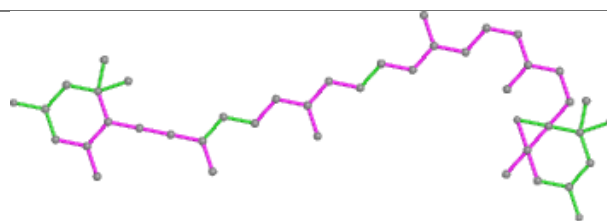


Rings

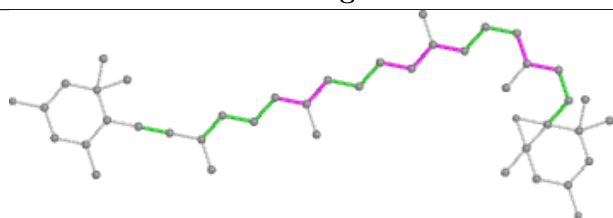
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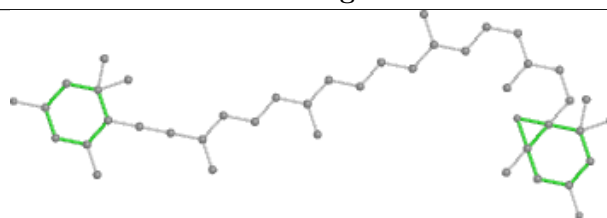
Bond lengths



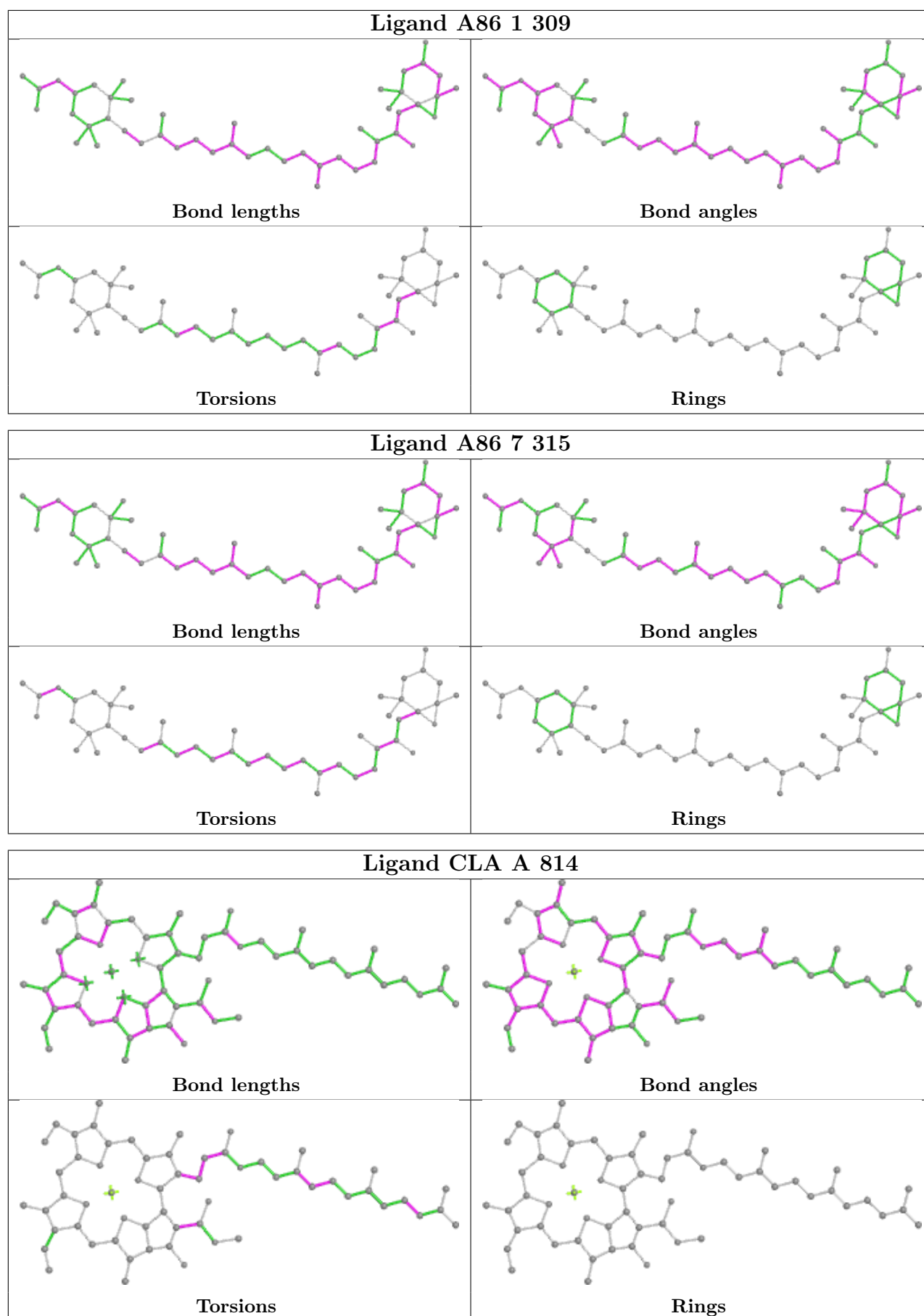
Bond angles

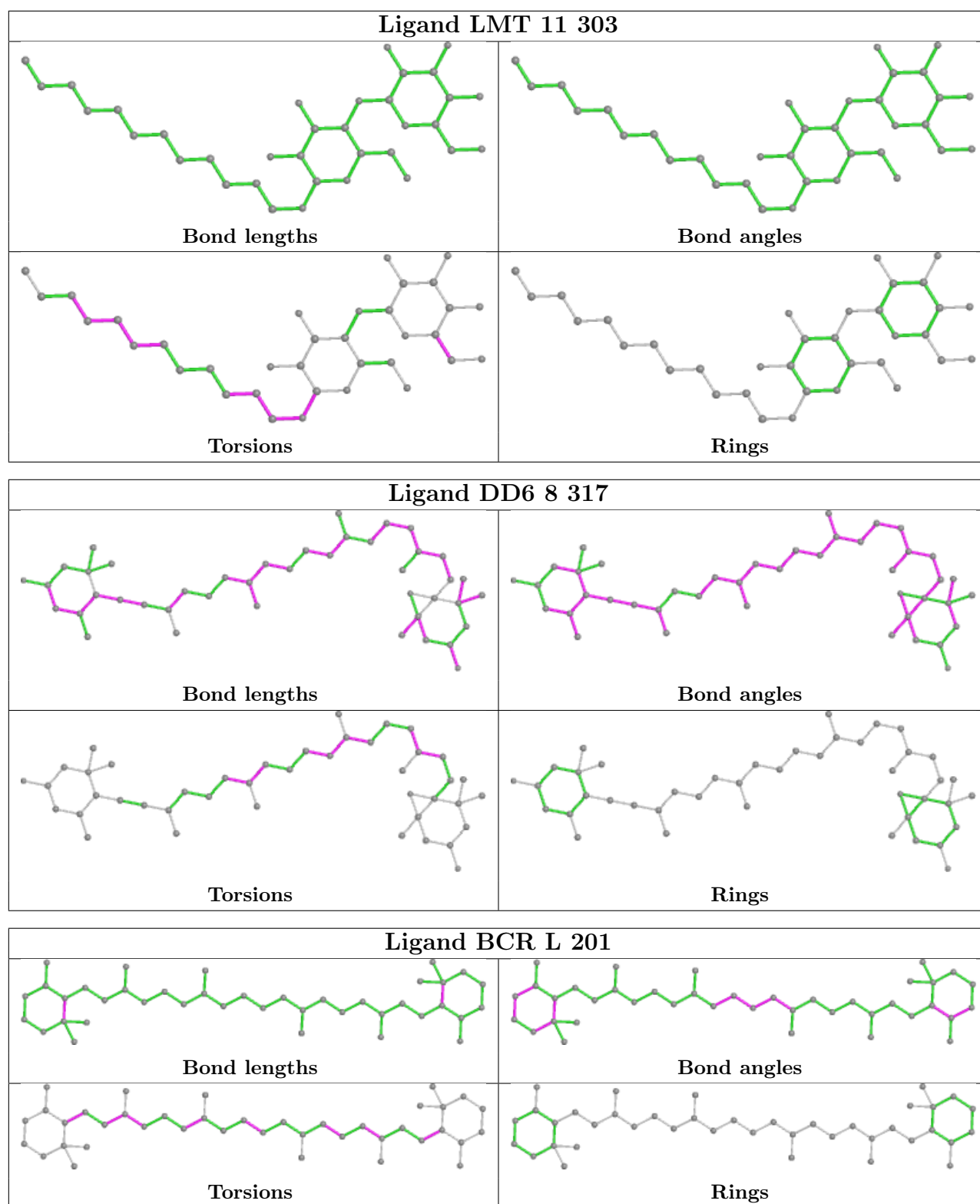


Torsions

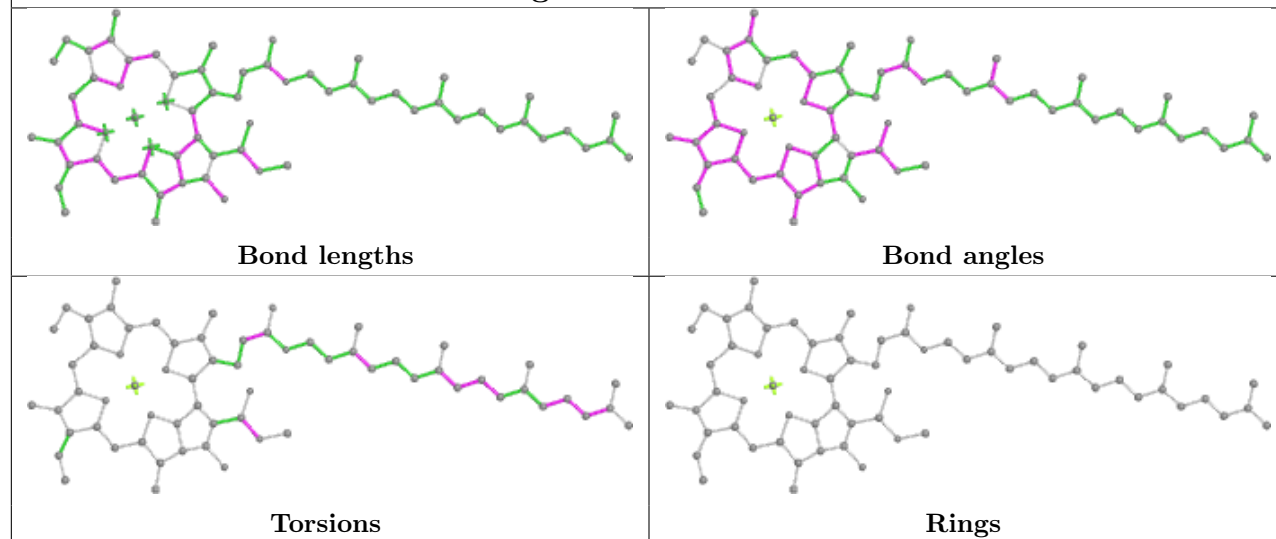


Rings

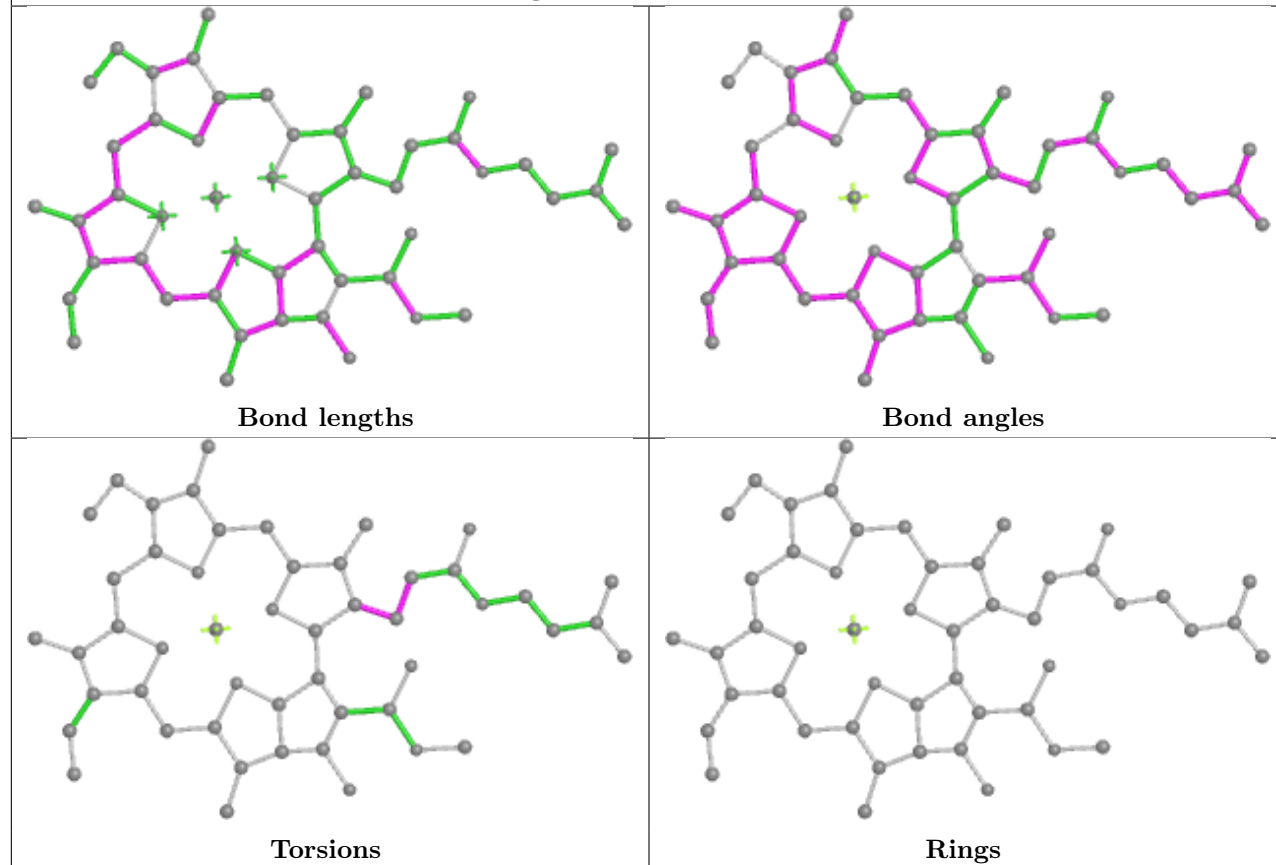




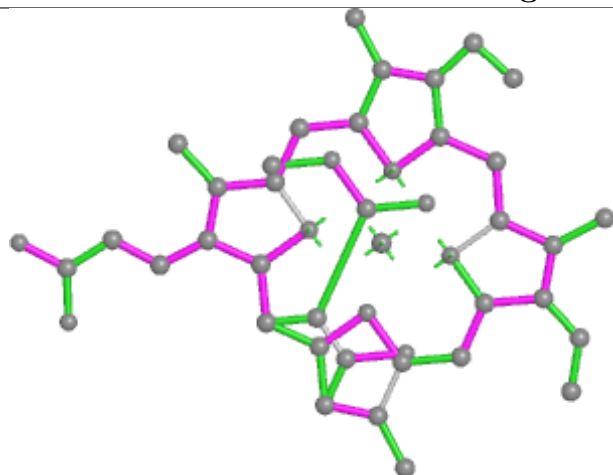
Ligand CLA A 826



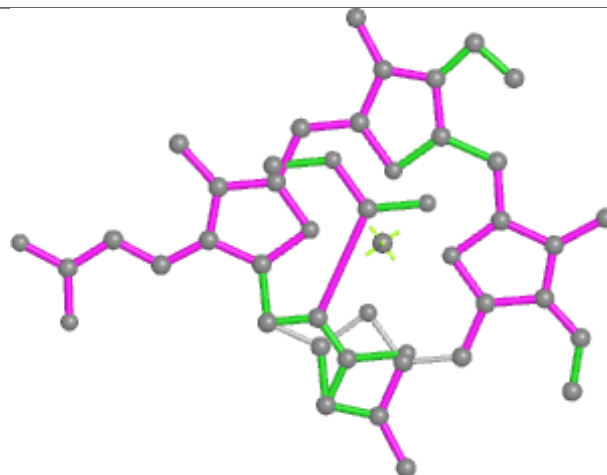
Ligand CLA 14 305



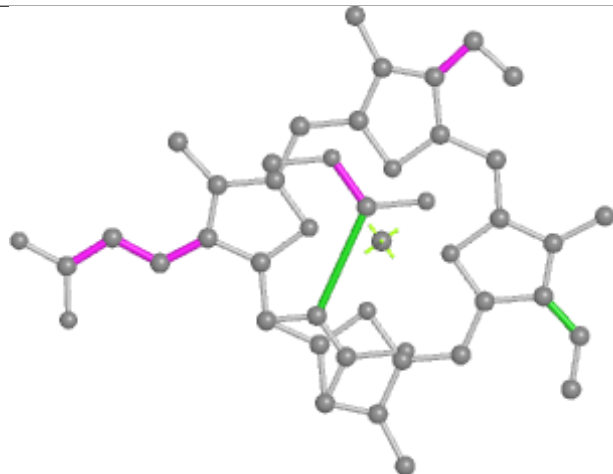
Ligand KC1 8 312



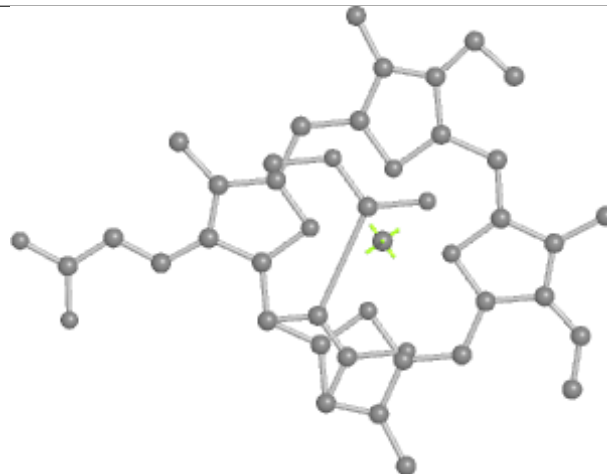
Bond lengths



Bond angles

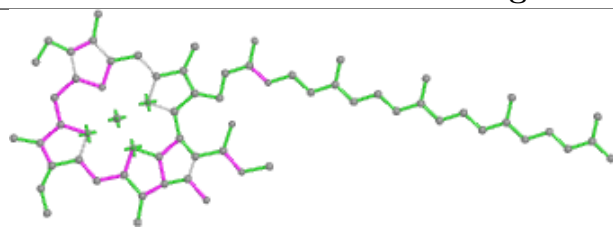


Torsions

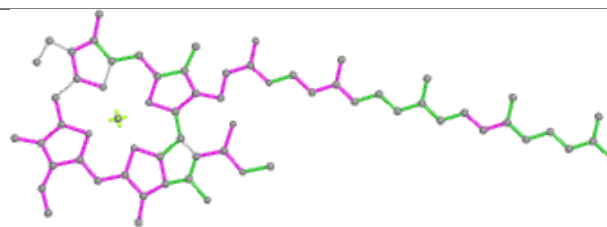


Rings

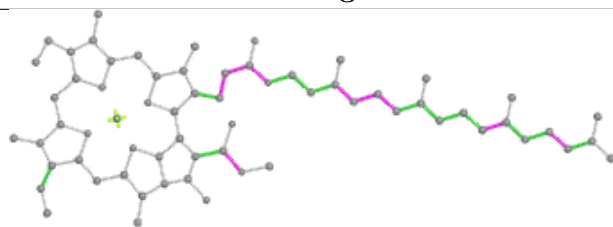
Ligand CLA 12 302



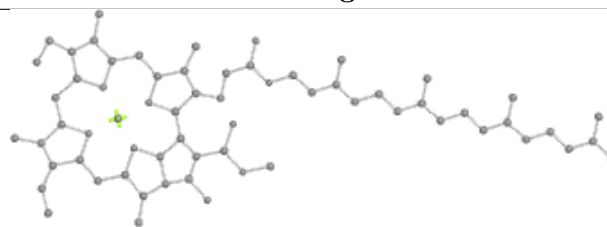
Bond lengths



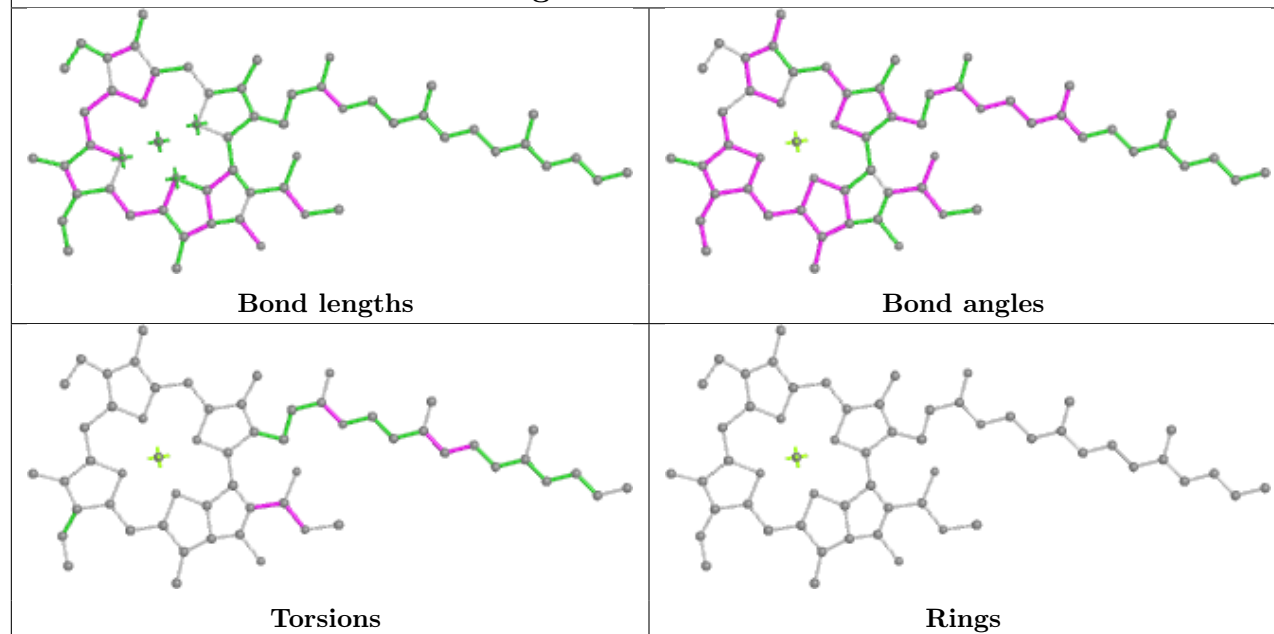
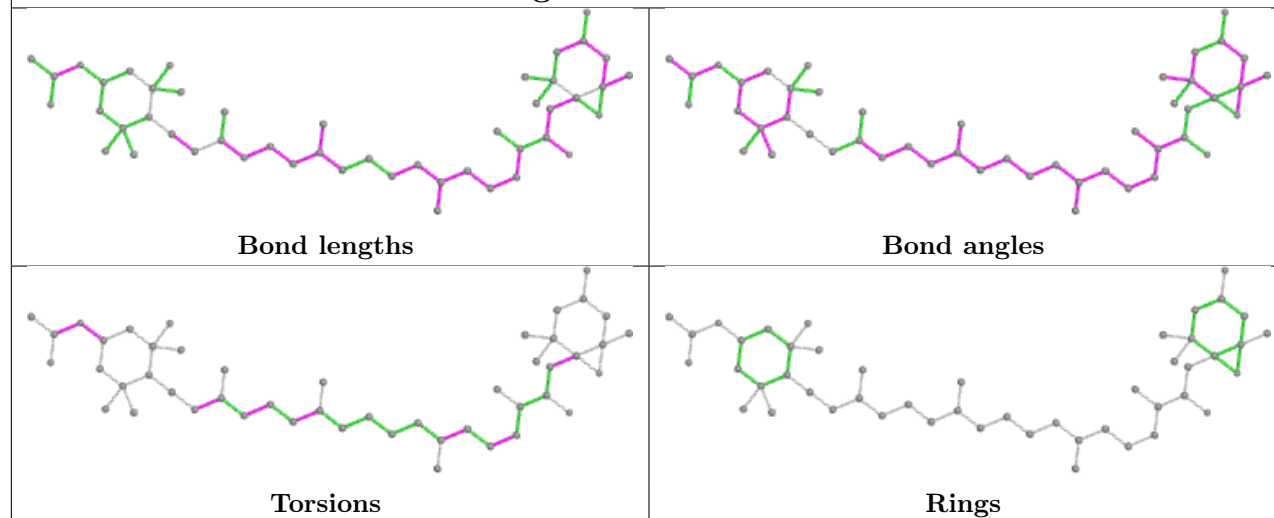
Bond angles



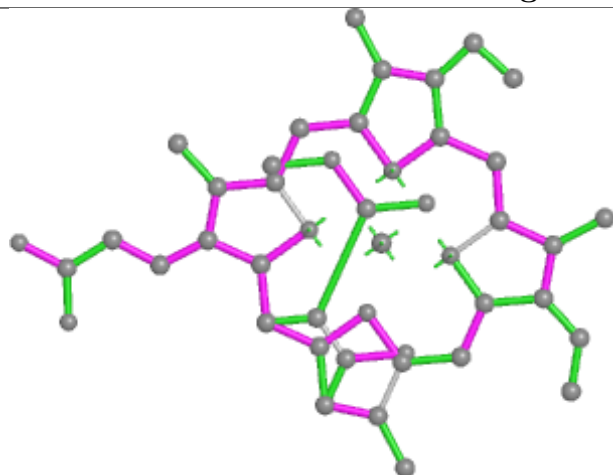
Torsions



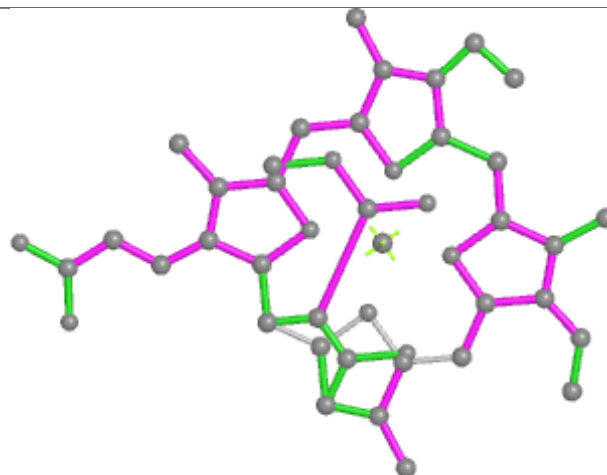
Rings

Ligand CLA B 831**Ligand A86 11 315**

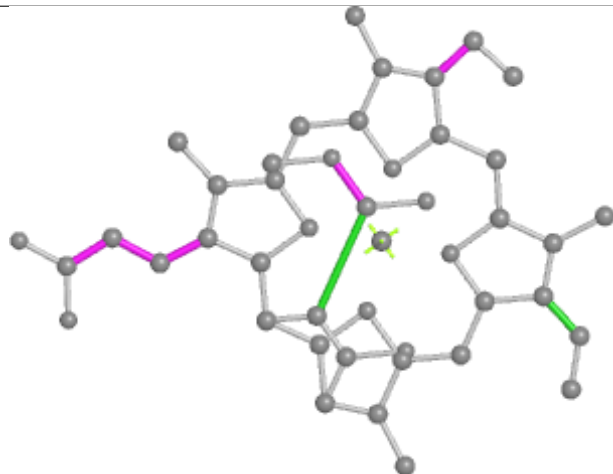
Ligand KC1 7 308



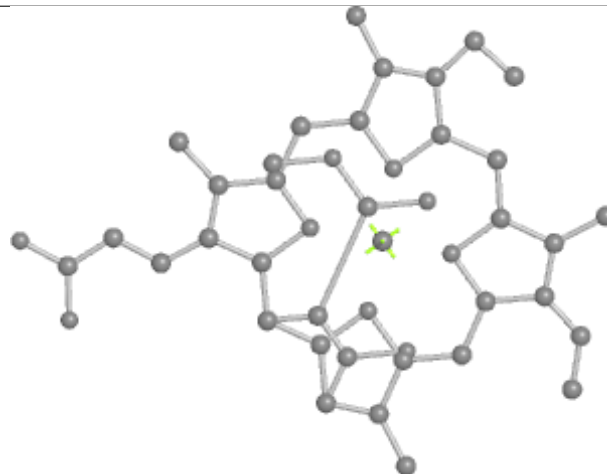
Bond lengths



Bond angles

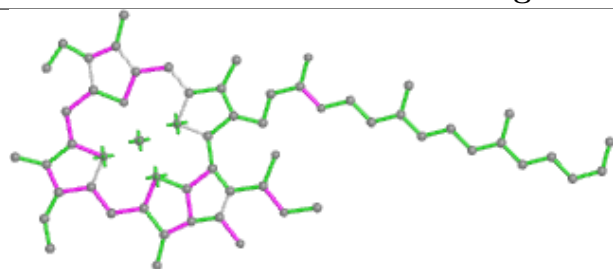


Torsions

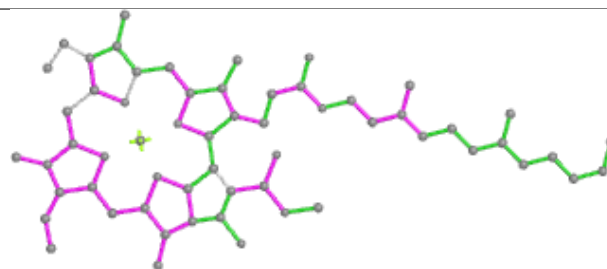


Rings

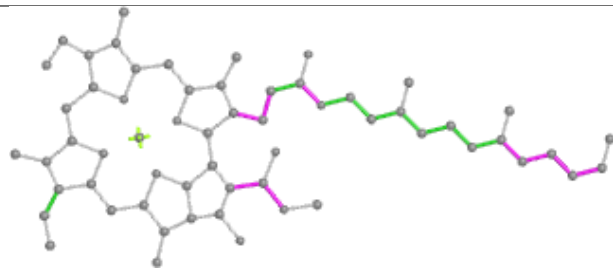
Ligand CLA A 825



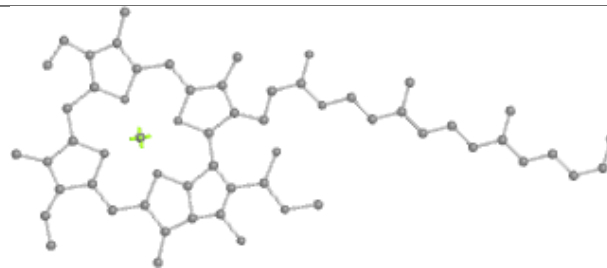
Bond lengths



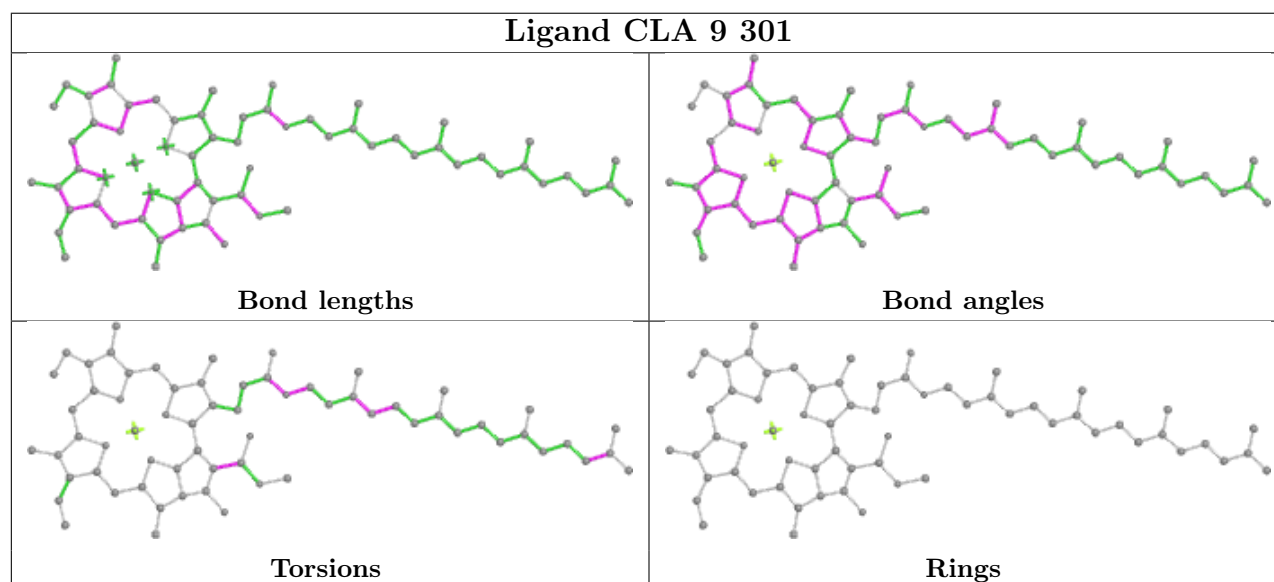
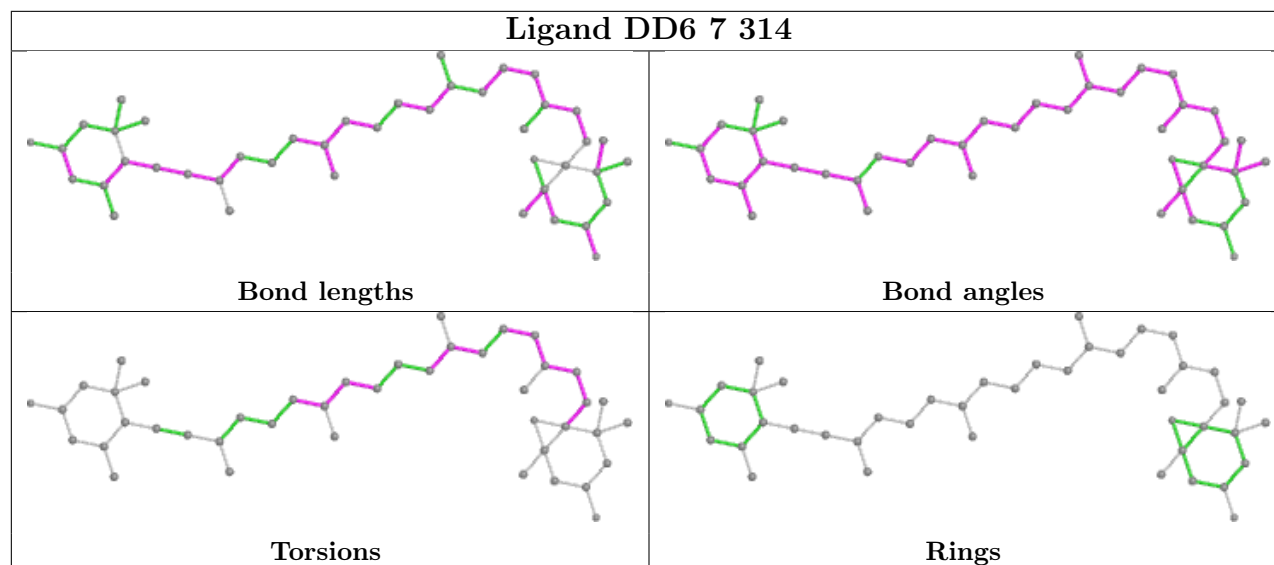
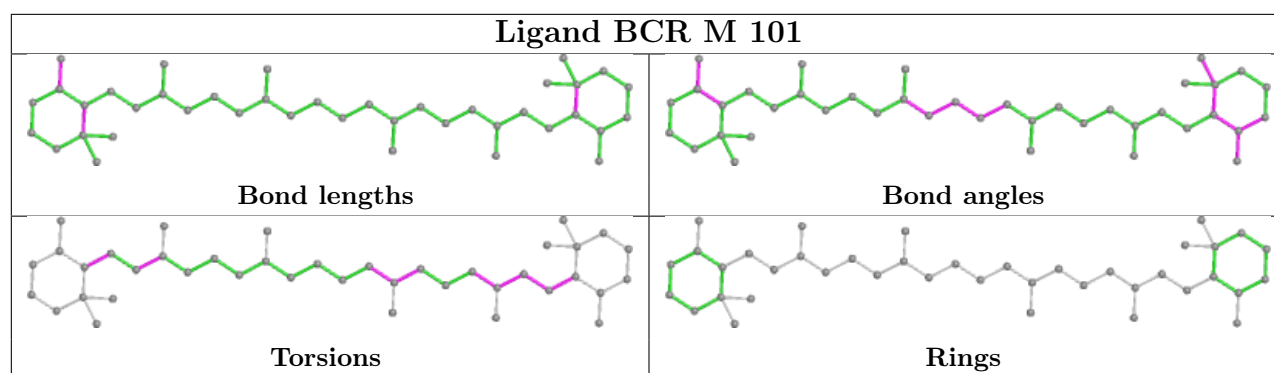
Bond angles

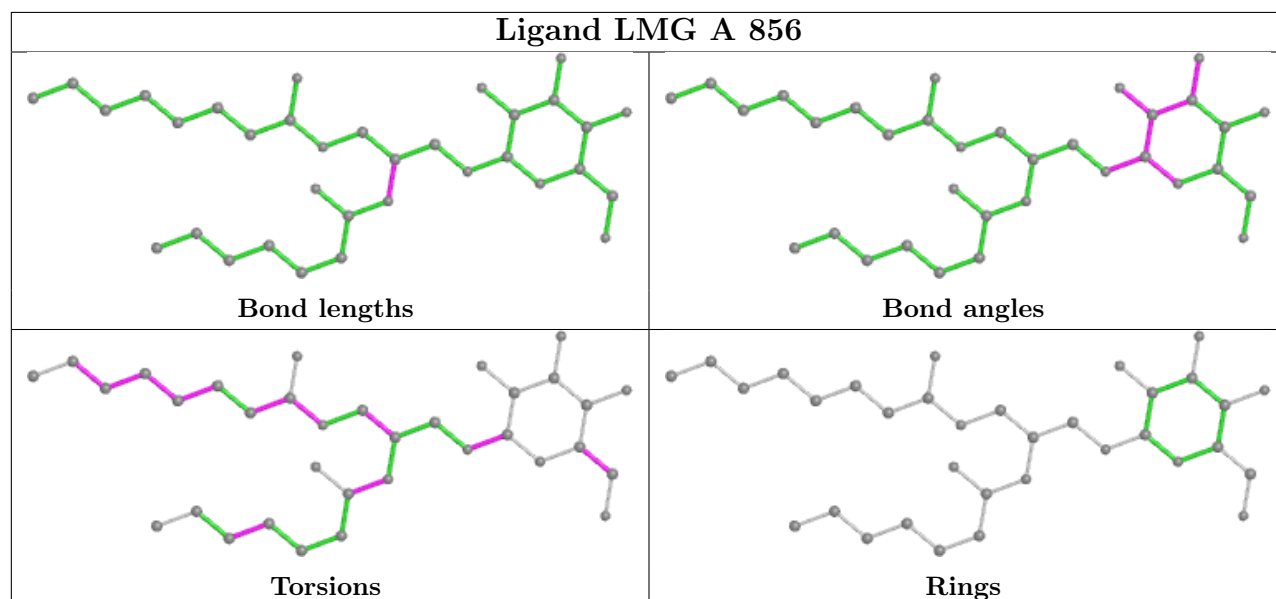
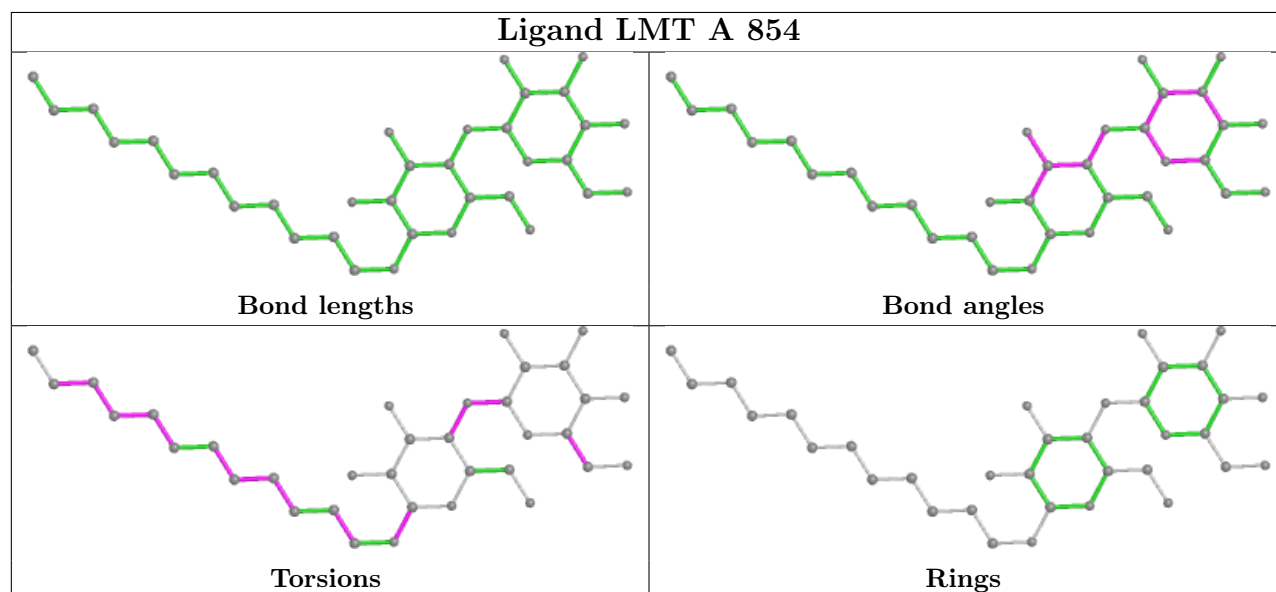
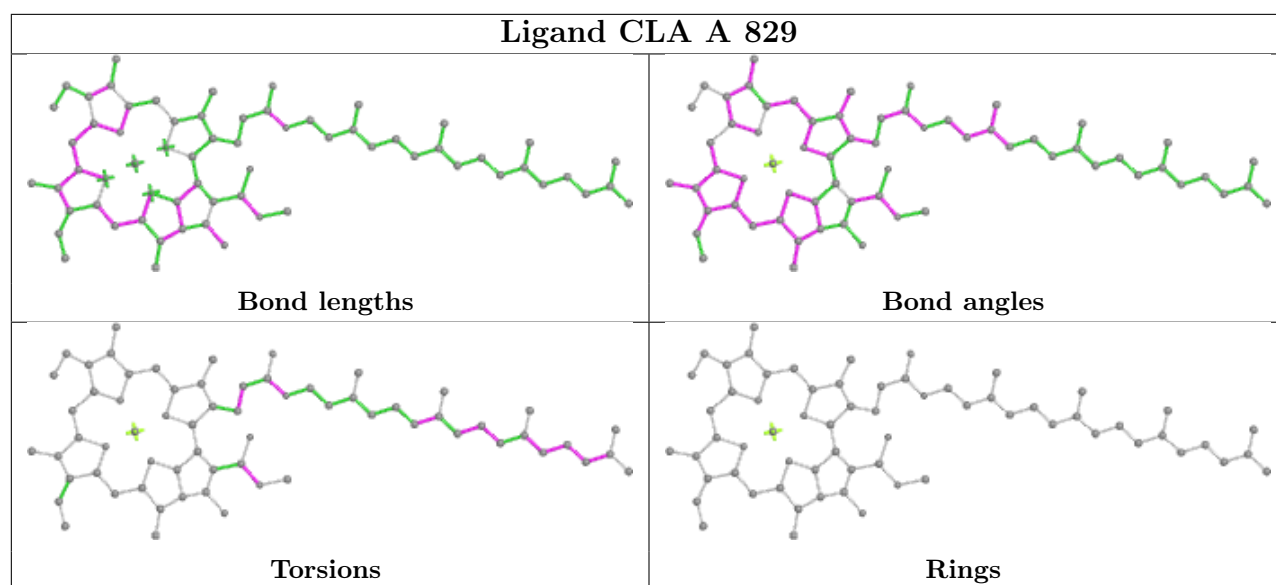


Torsions

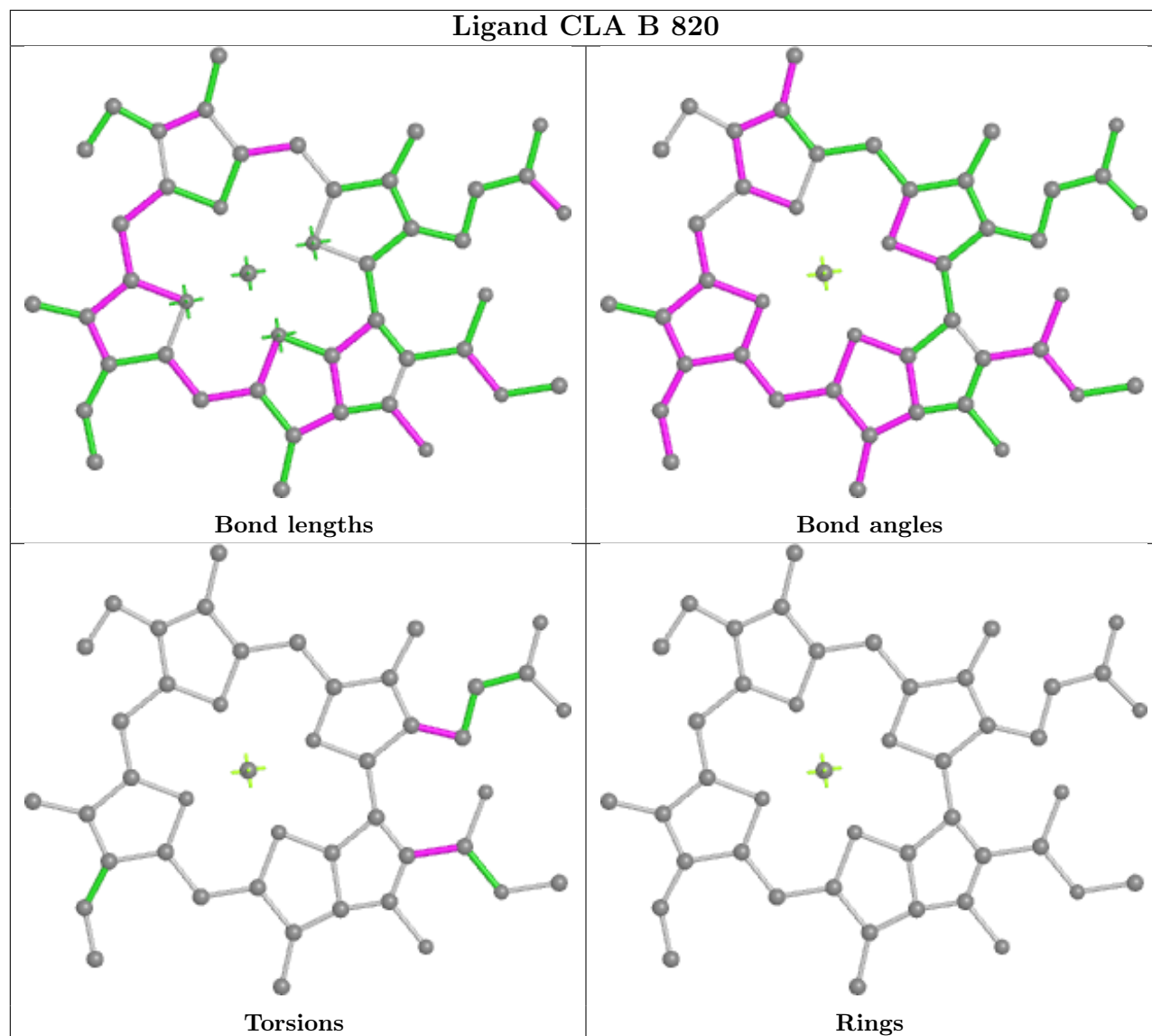


Rings

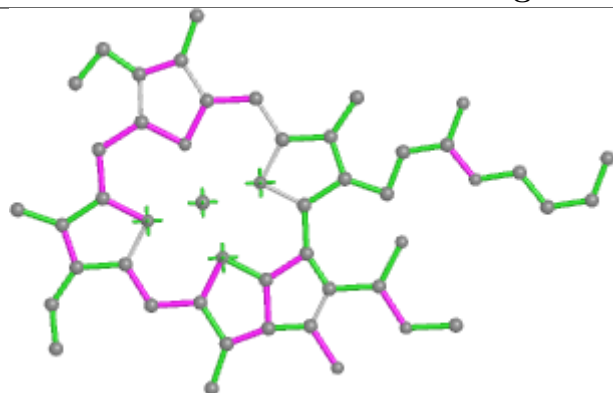




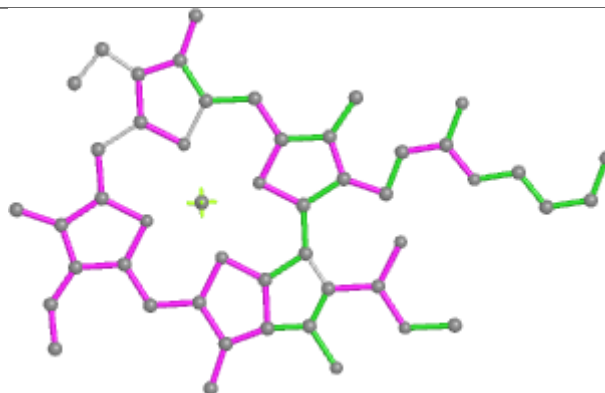
Ligand CLA B 820



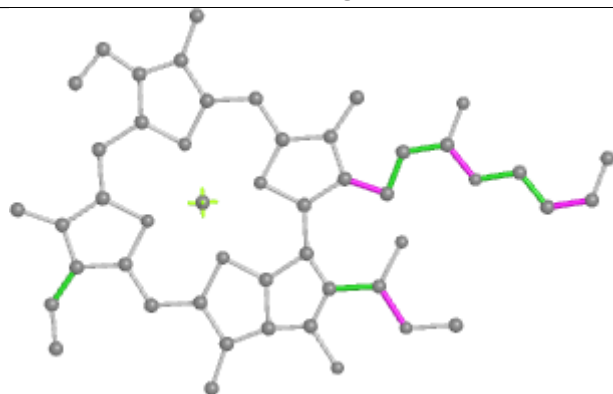
Ligand CLA A 823



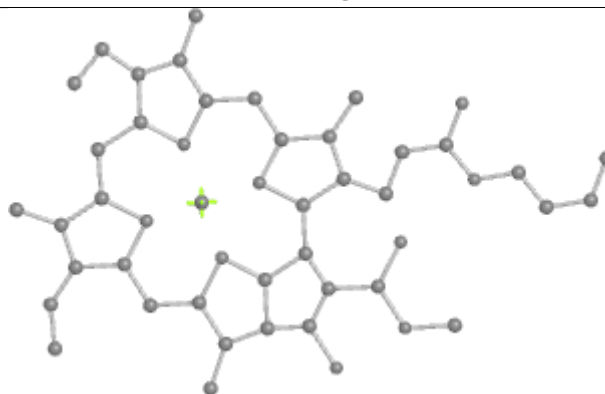
Bond lengths



Bond angles

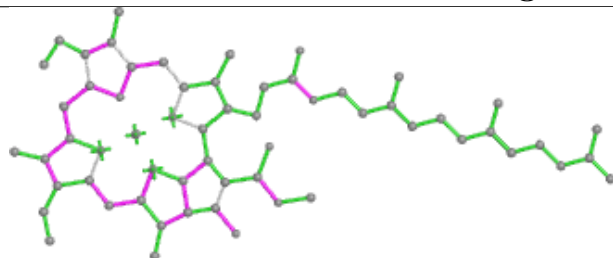


Torsions

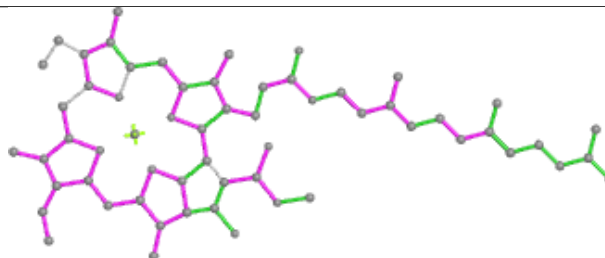


Rings

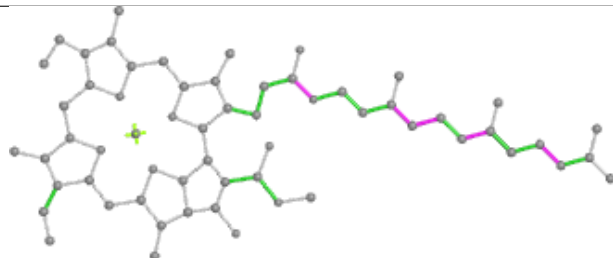
Ligand CLA 3 302



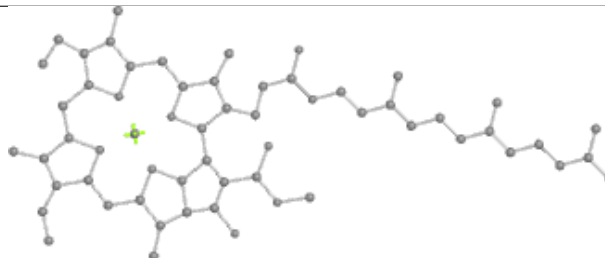
Bond lengths



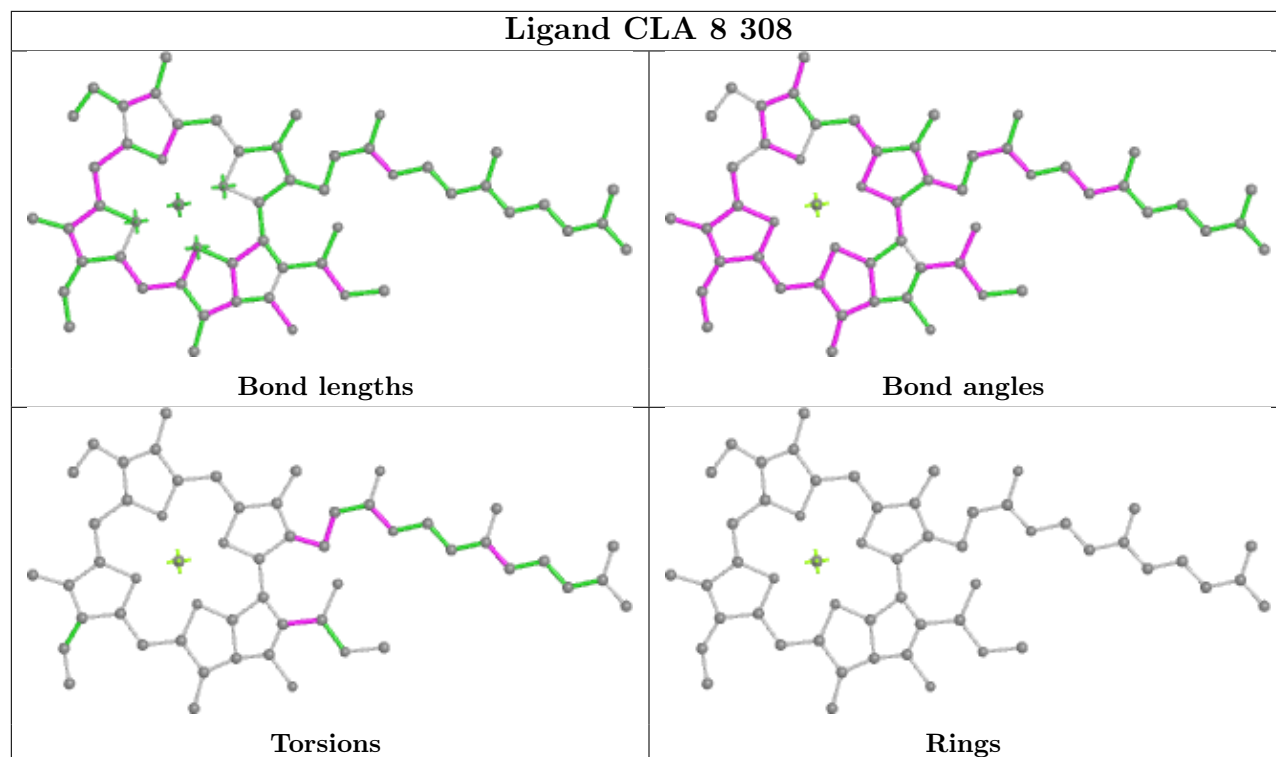
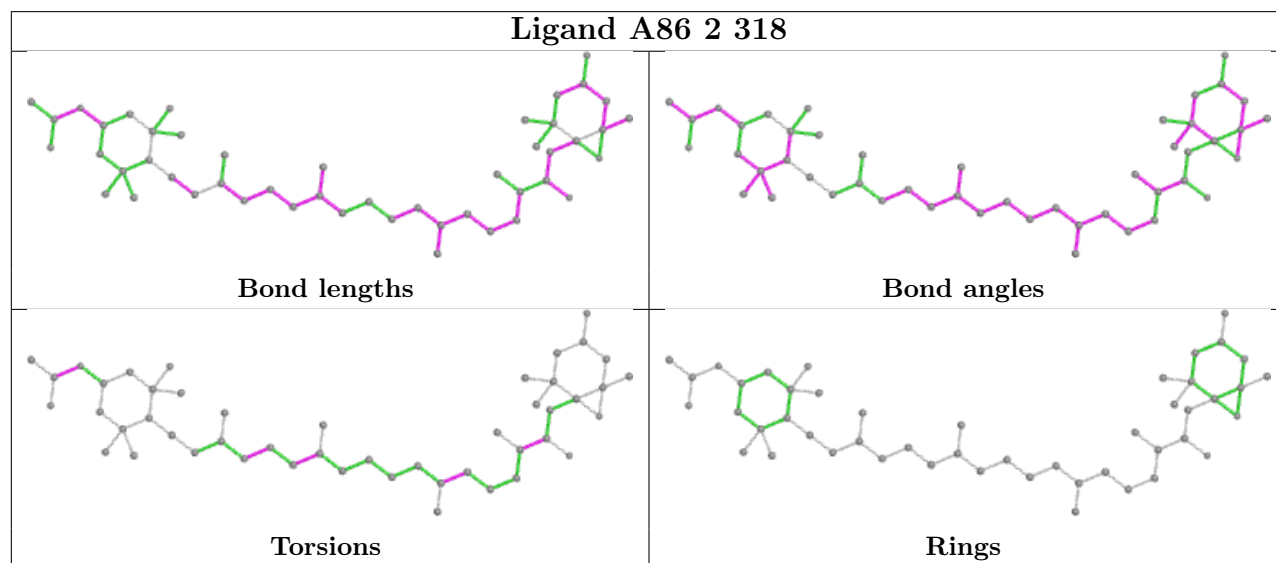
Bond angles

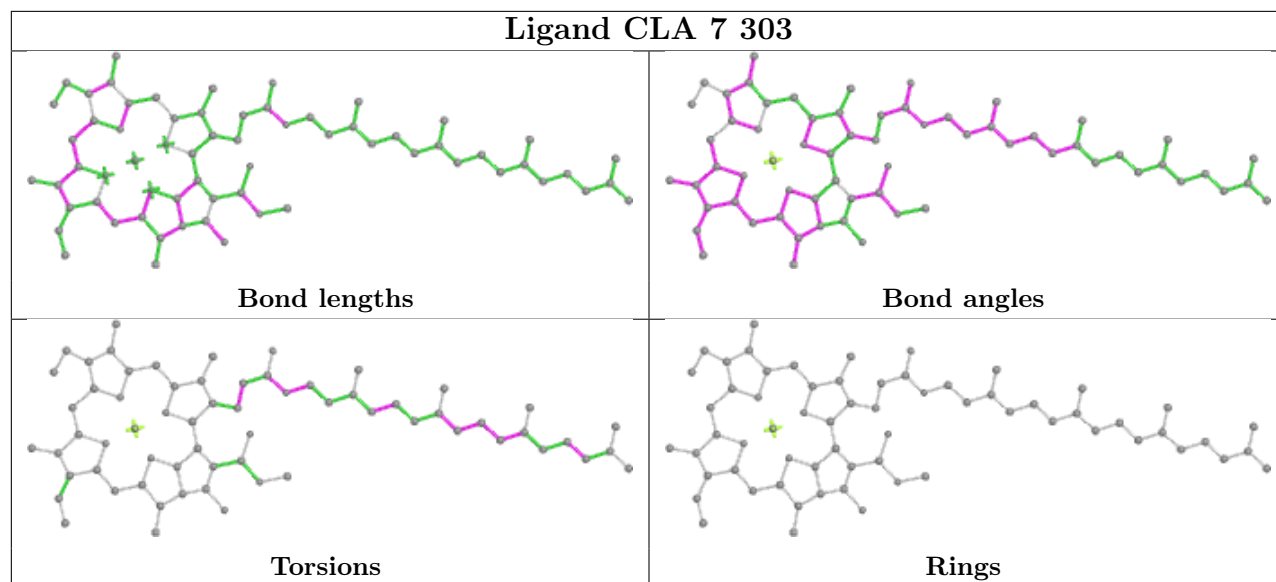
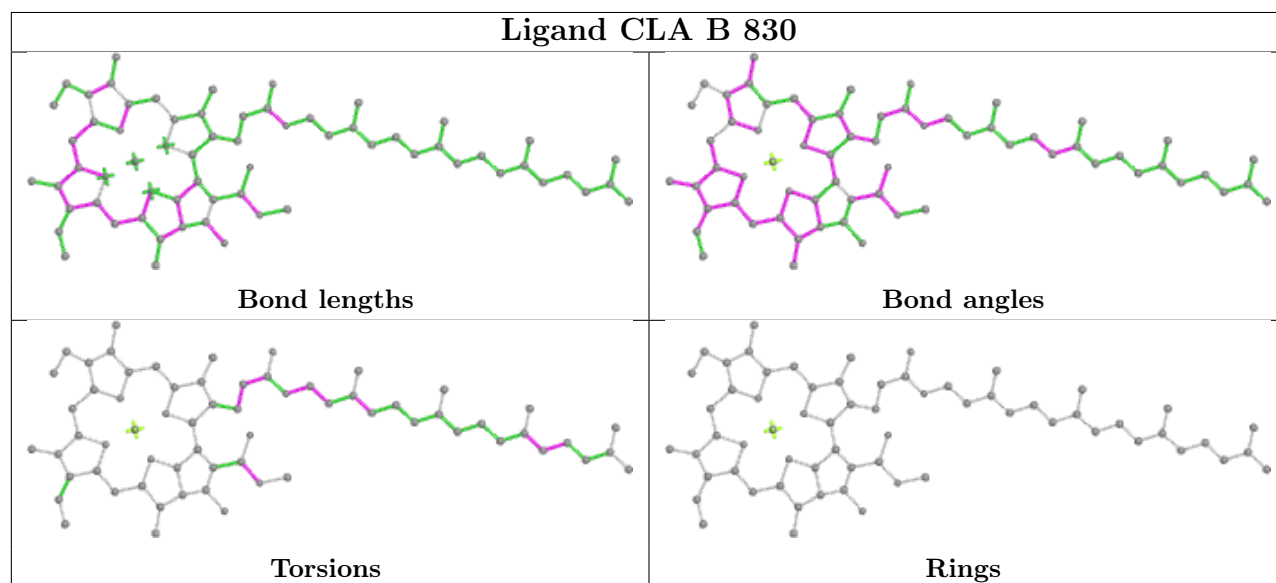


Torsions

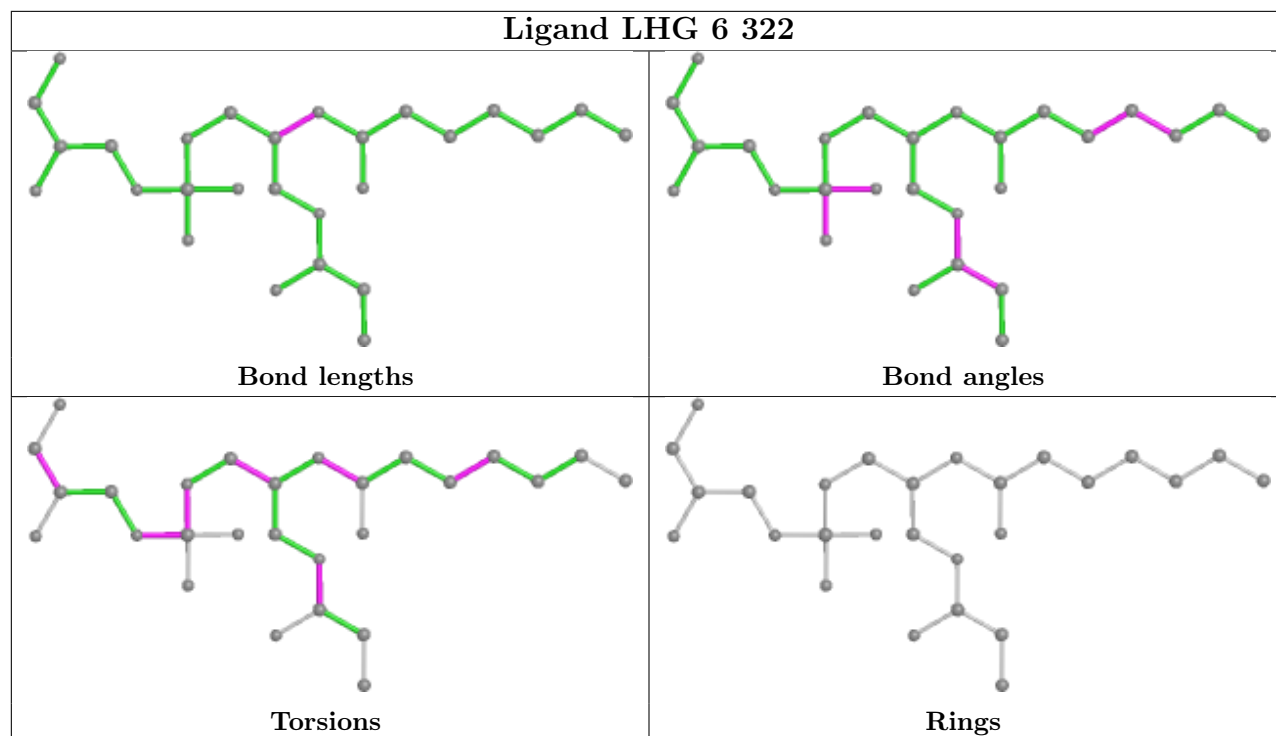


Rings

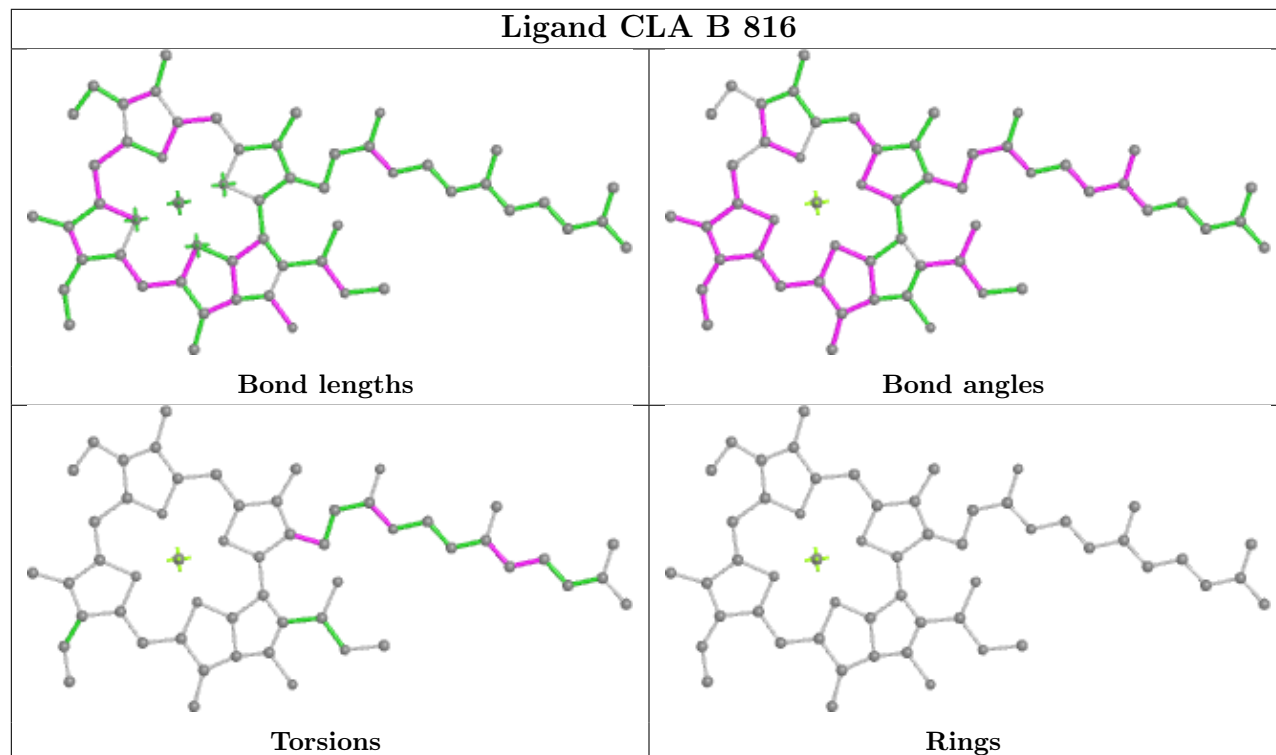
Ligand CLA 8 308**Ligand A86 2 318**

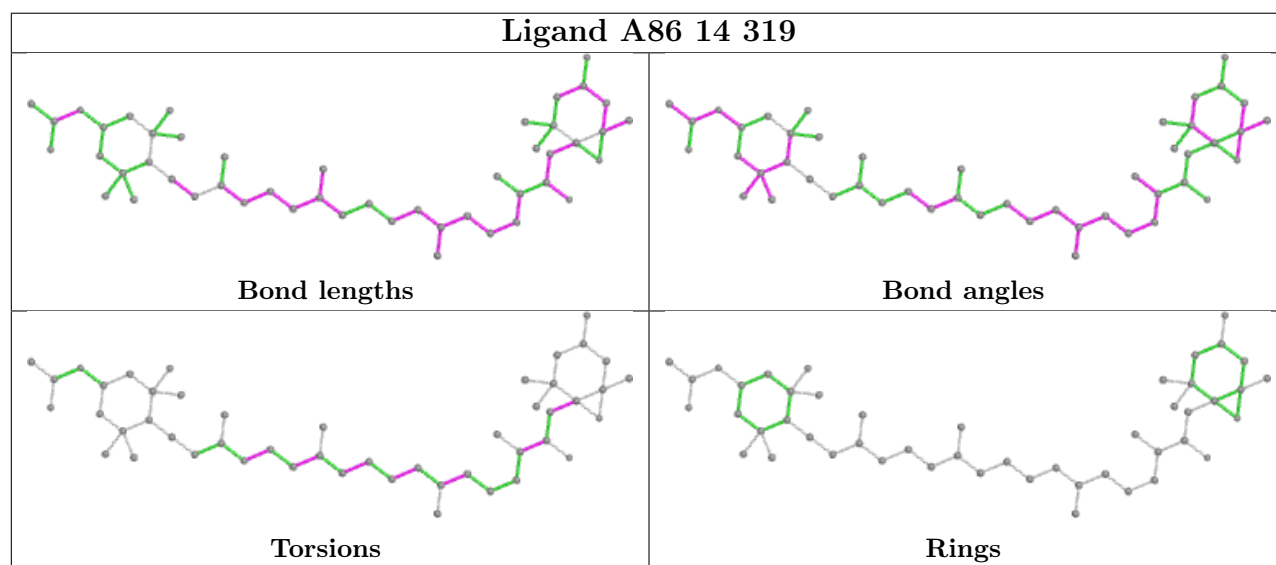
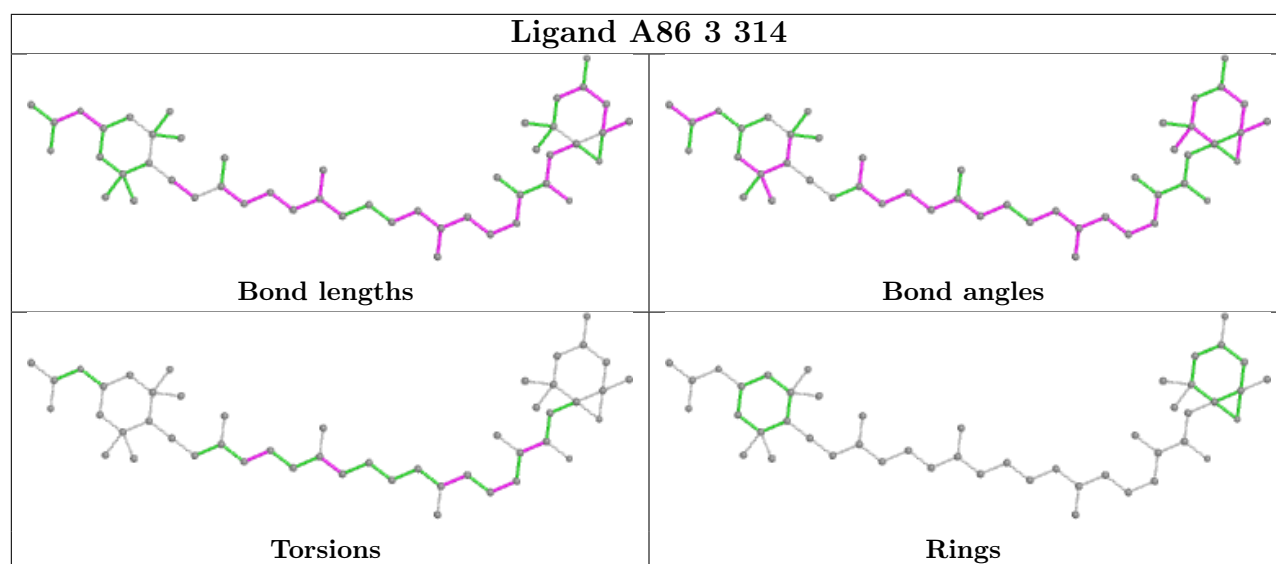
Ligand CLA 7 303**Ligand CLA B 830**

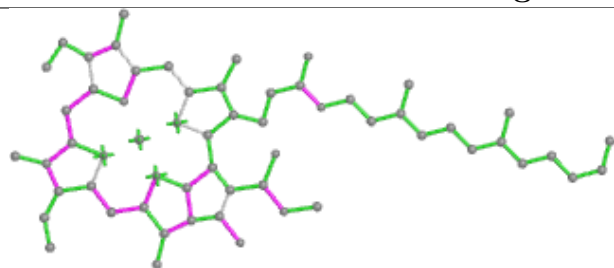
Ligand LHG 6 322



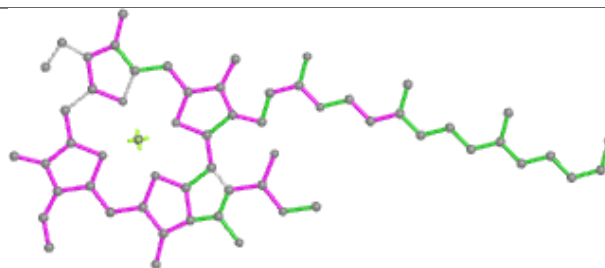
Ligand CLA B 816



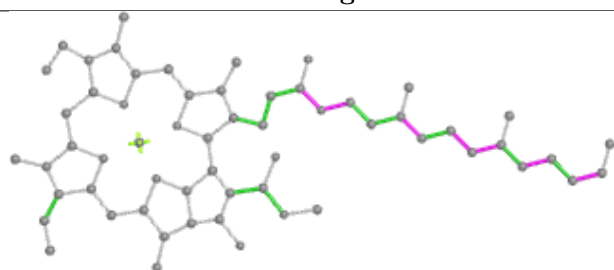


Ligand CLA A 805

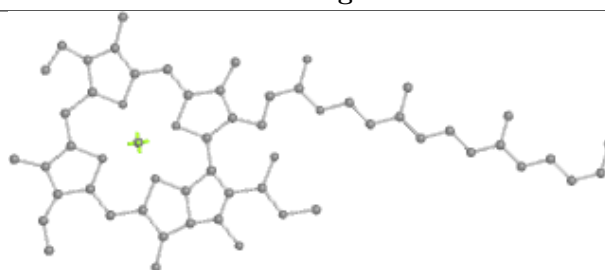
Bond lengths



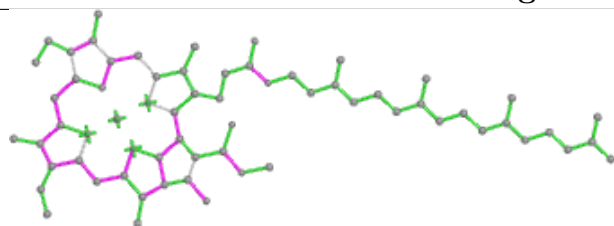
Bond angles



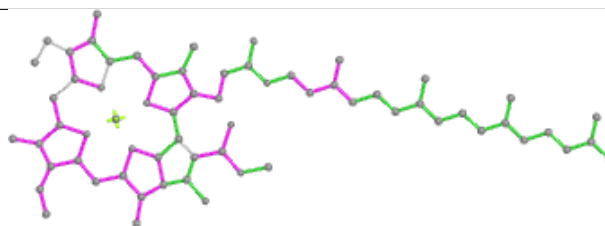
Torsions



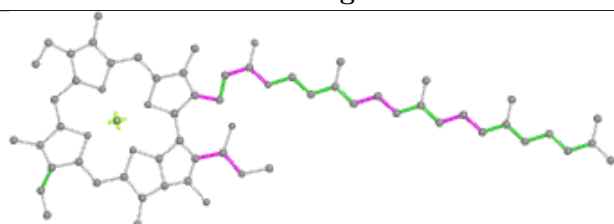
Rings

Ligand CLA 3 303

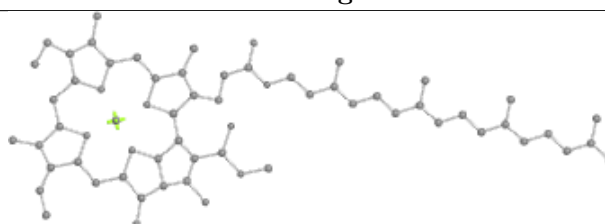
Bond lengths



Bond angles

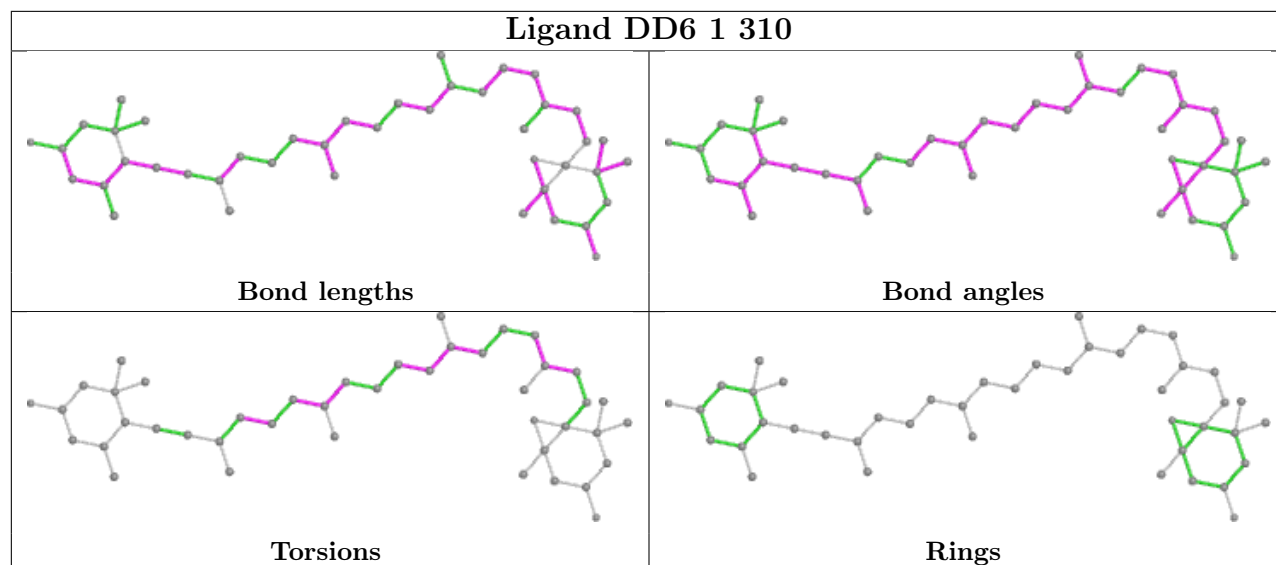


Torsions

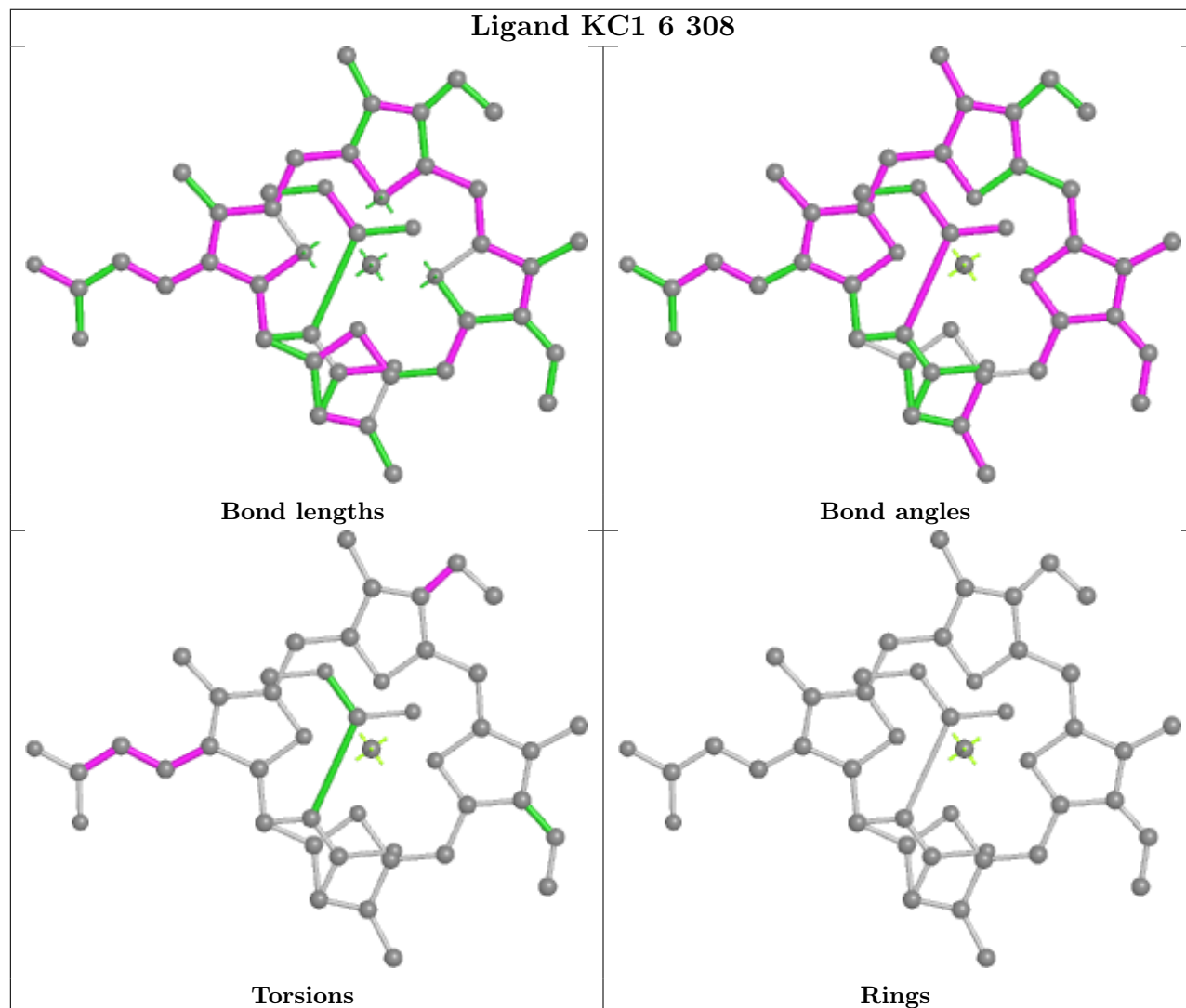


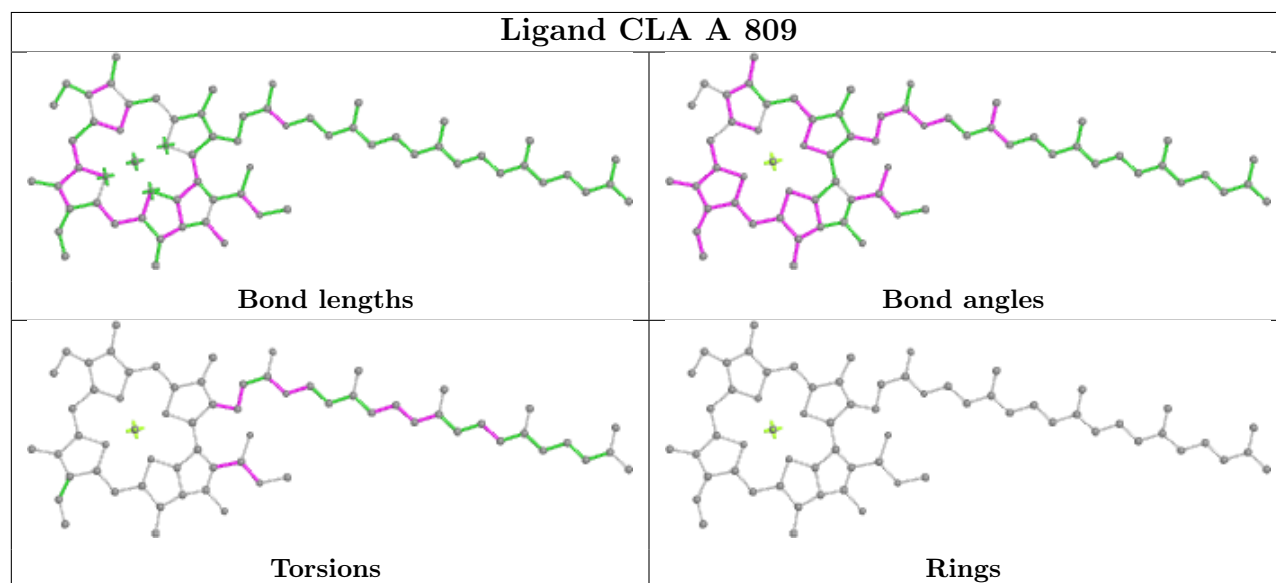
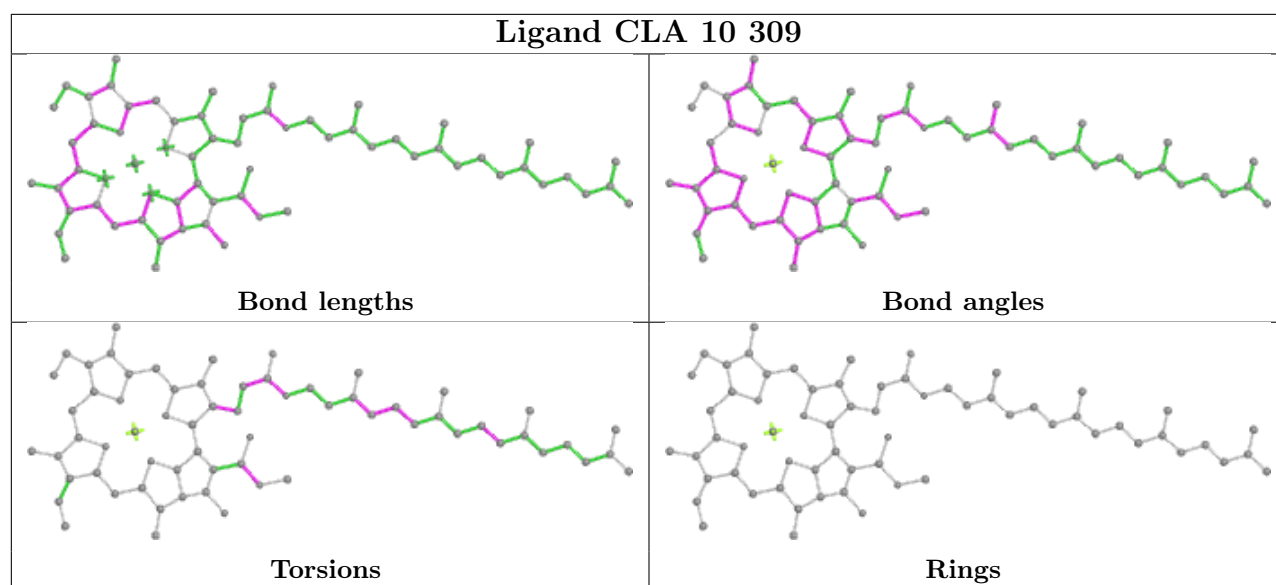
Rings

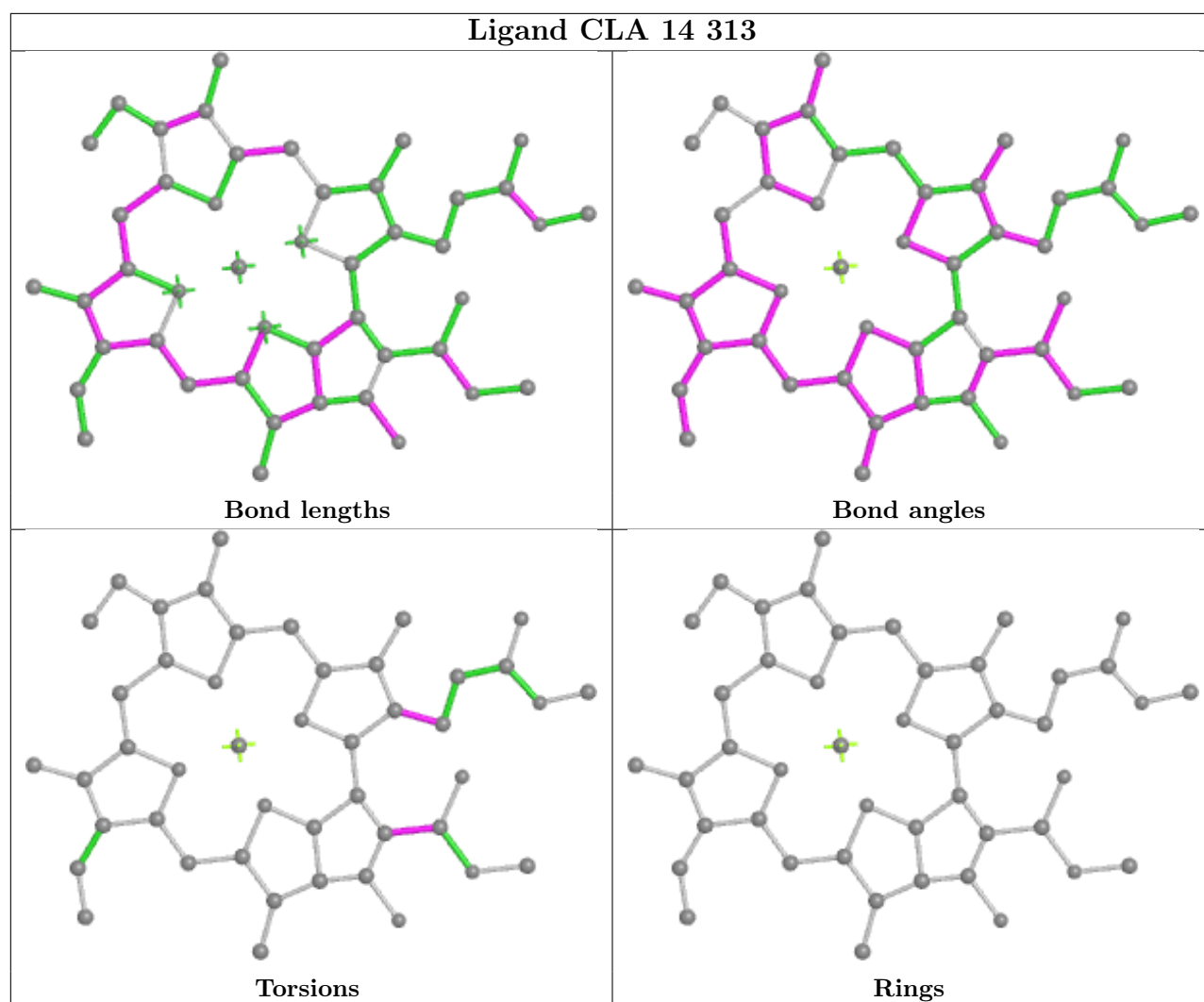
Ligand DD6 1 310



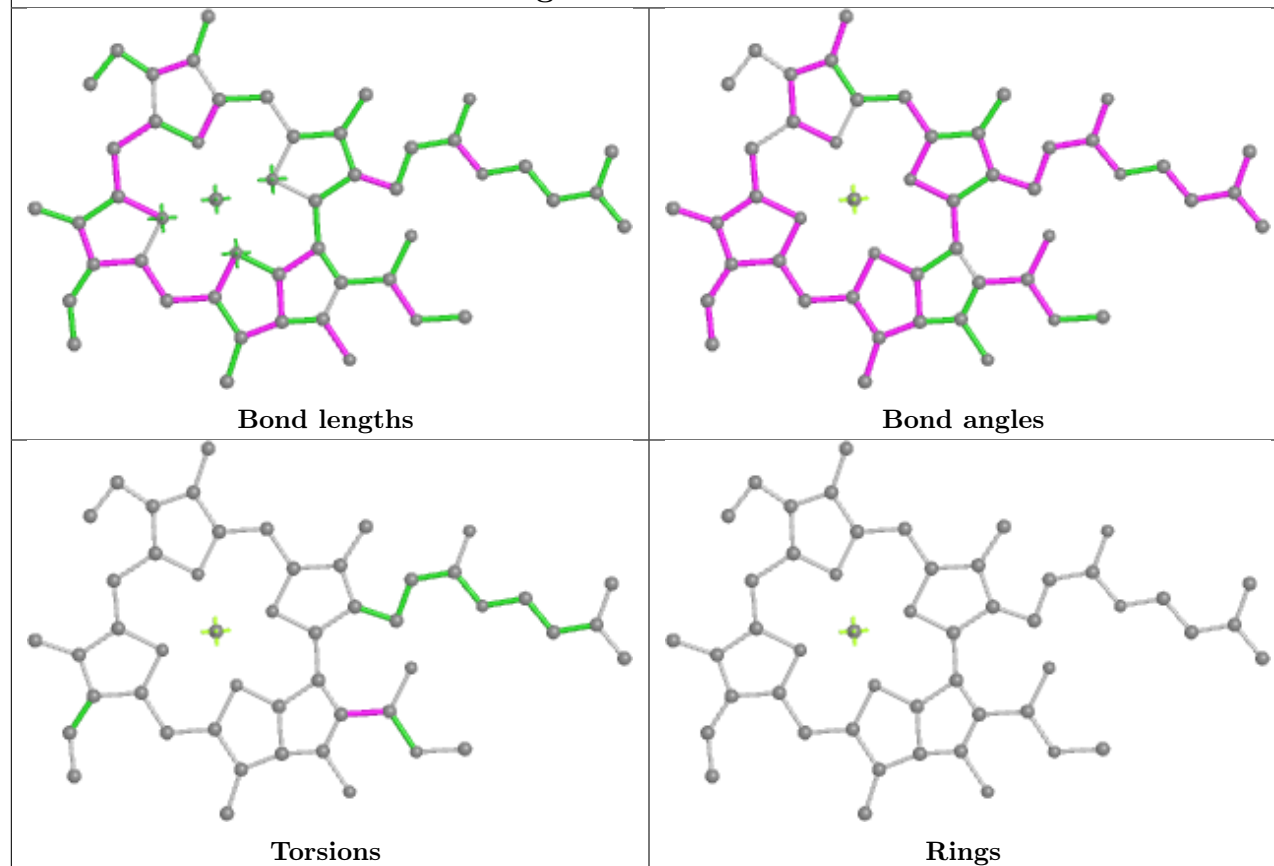
Ligand KC1 6 308



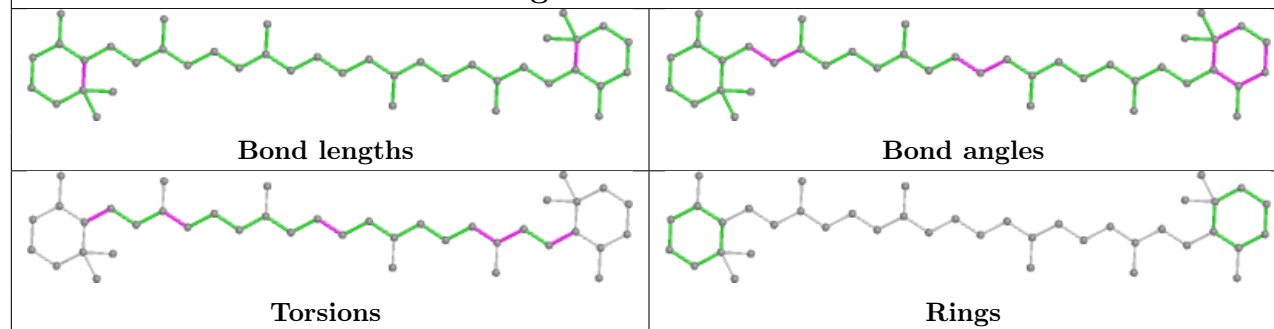


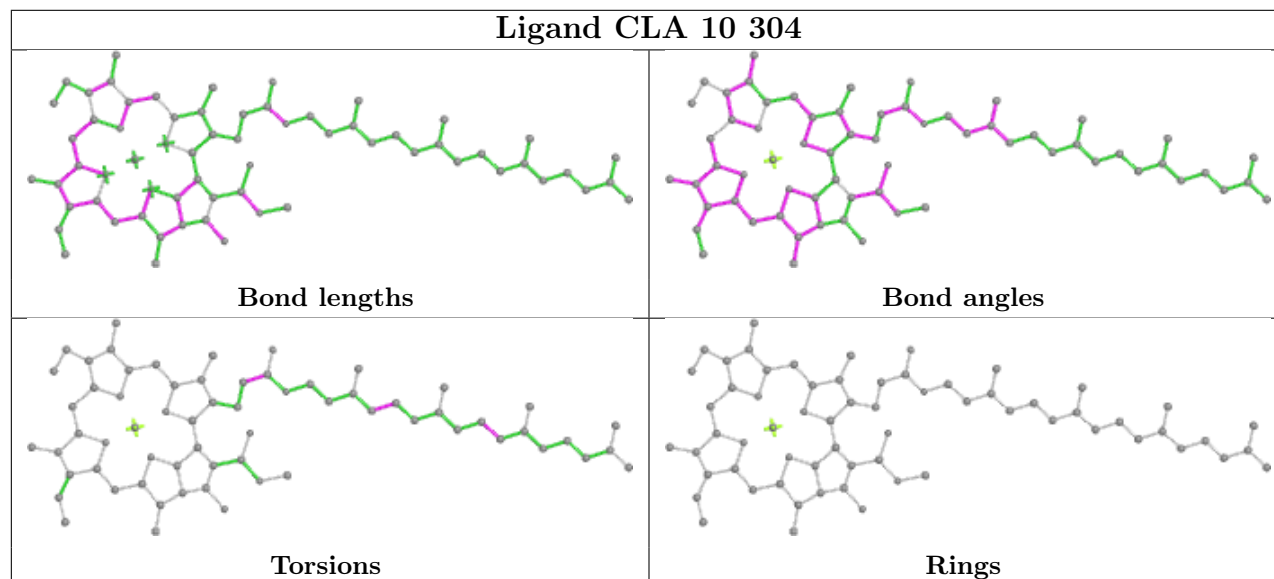
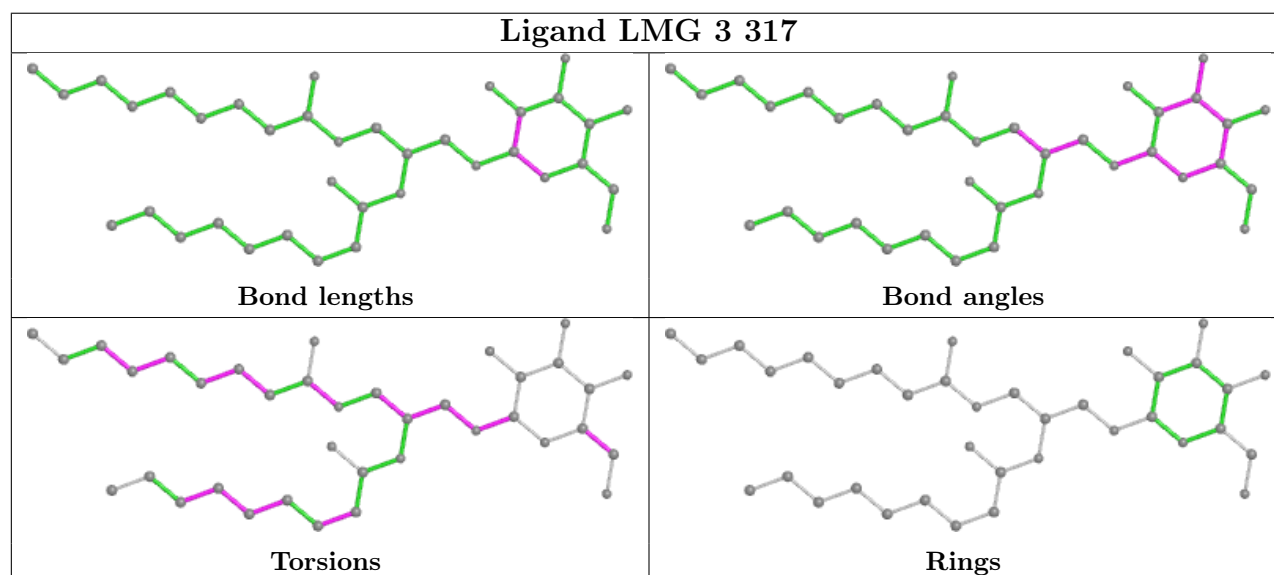
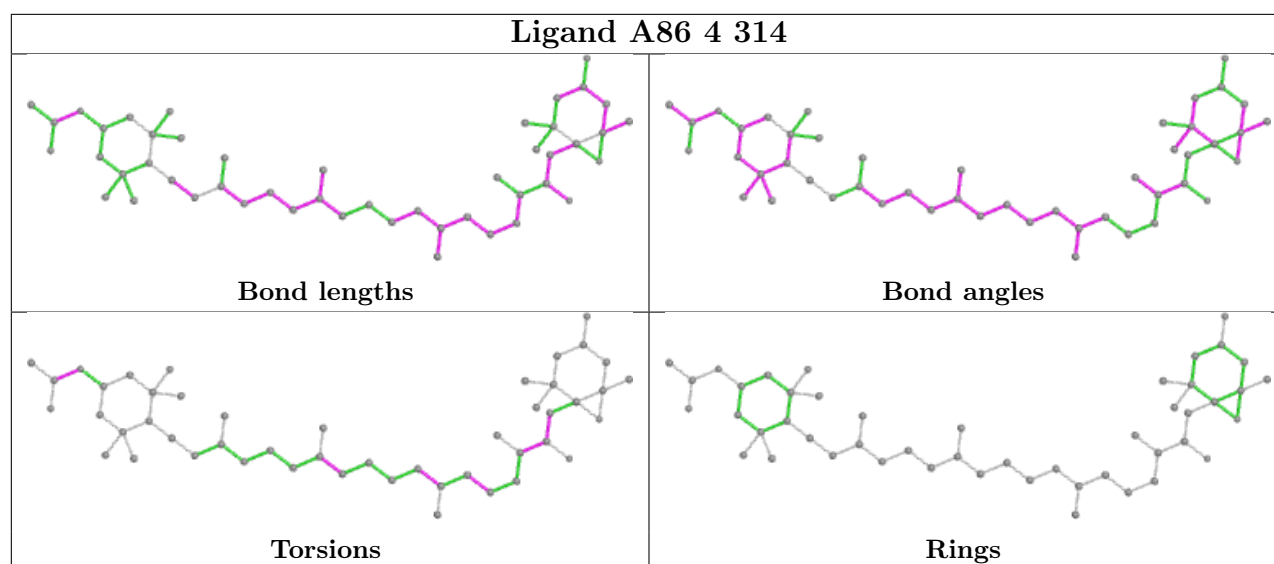


Ligand CLA 4 311

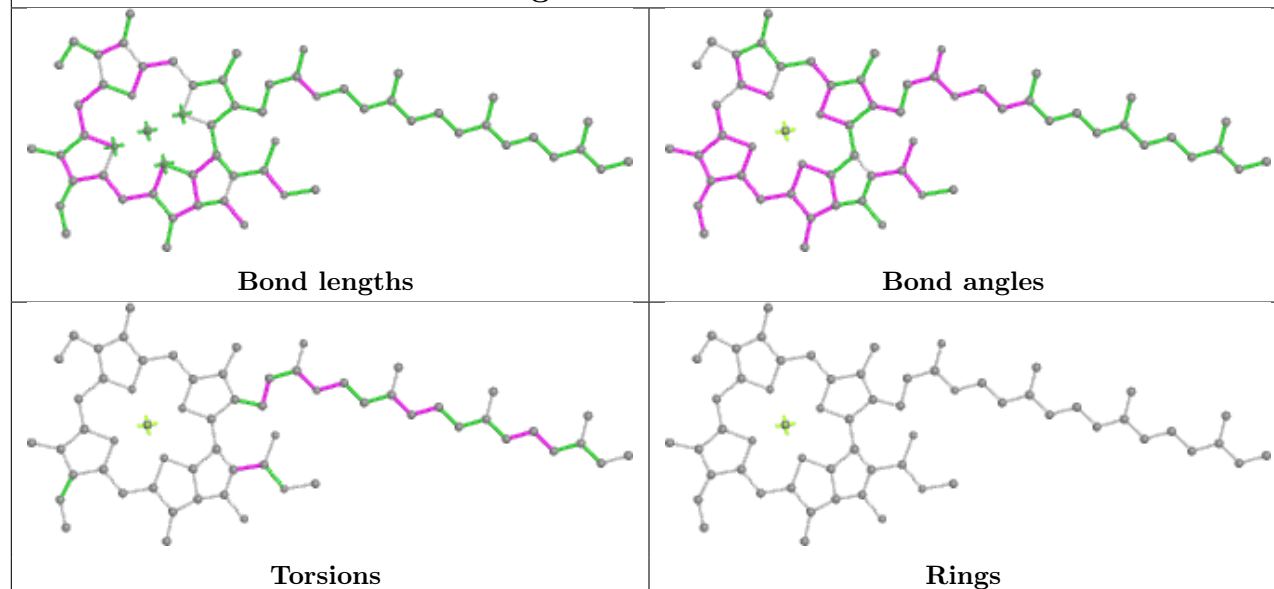


Ligand BCR B 842

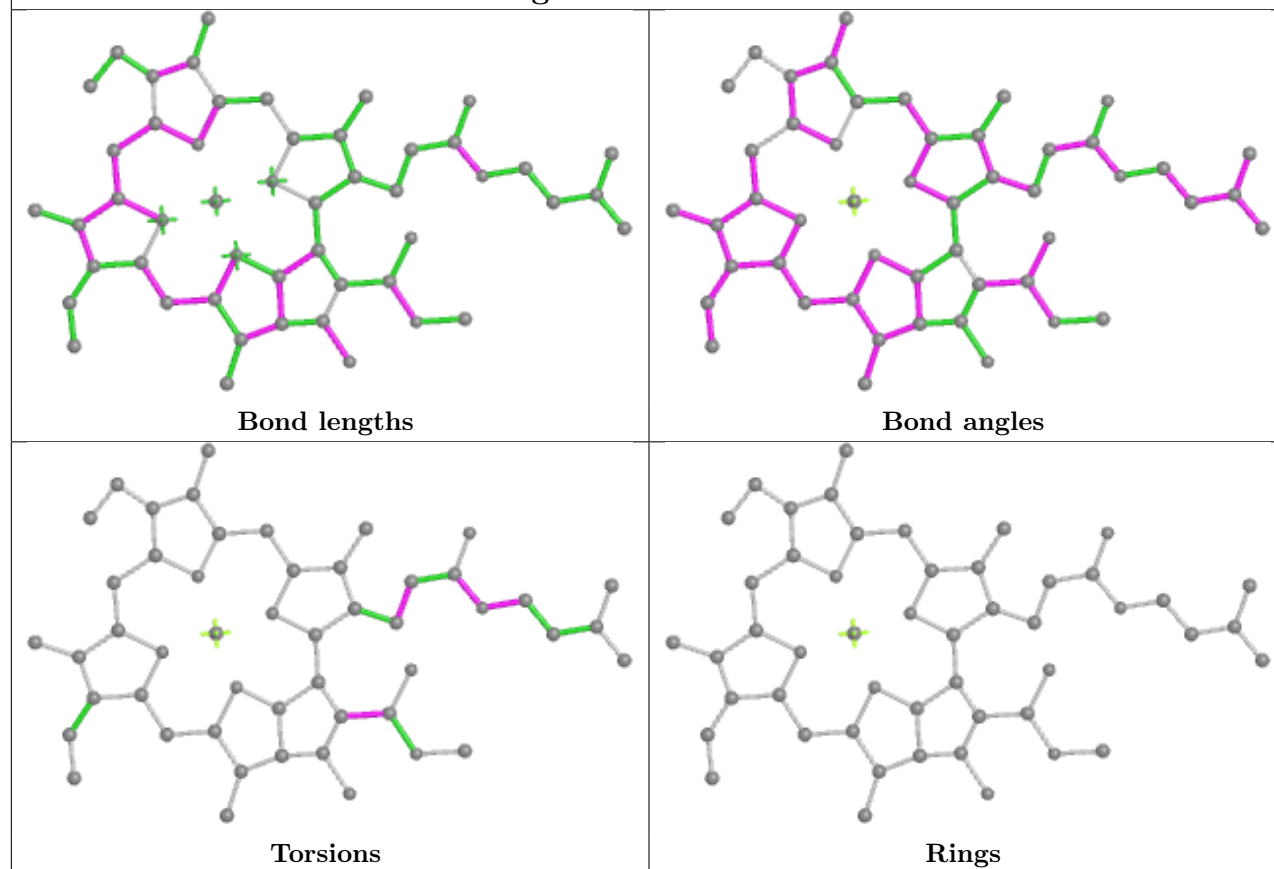


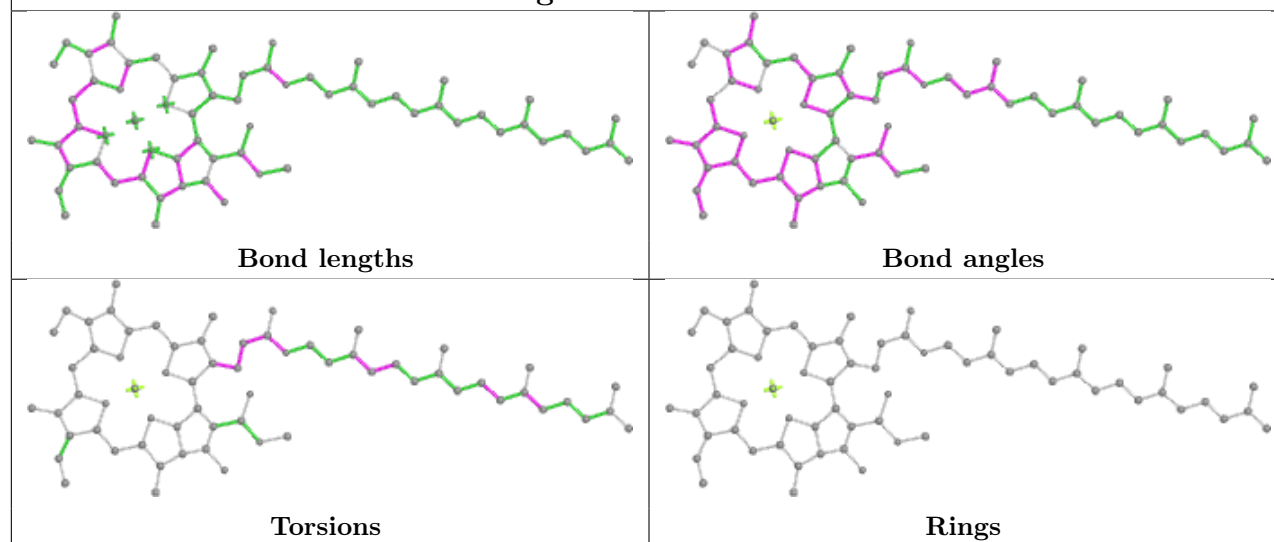
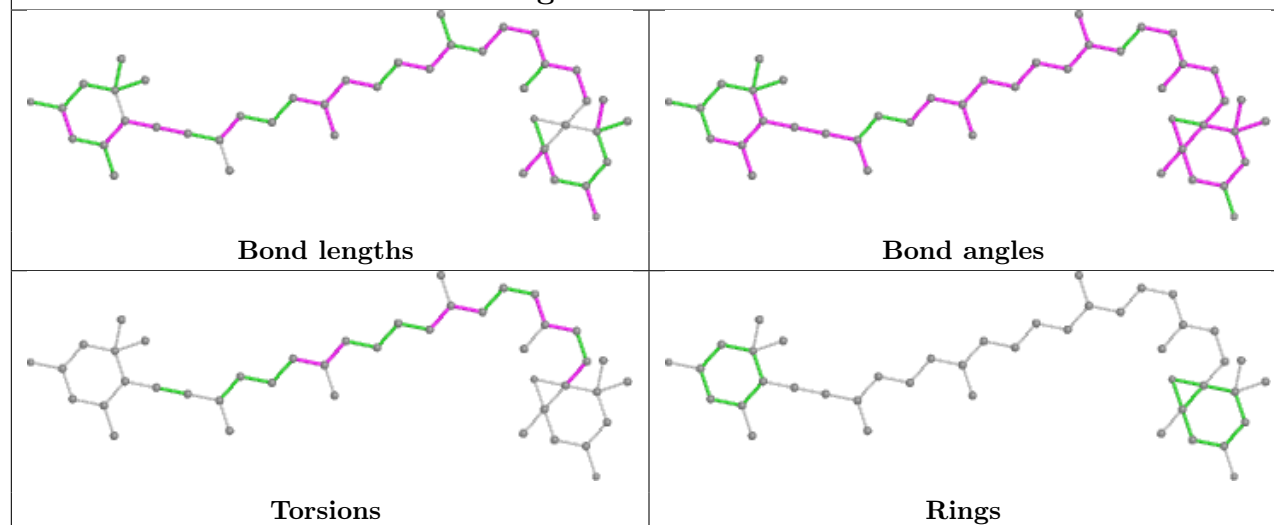
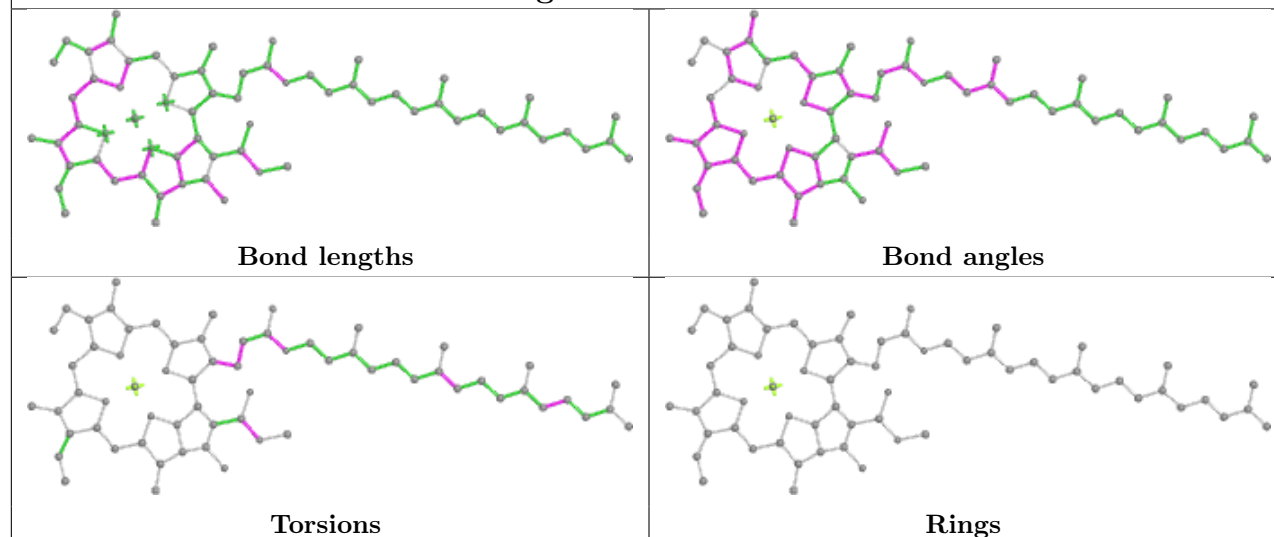


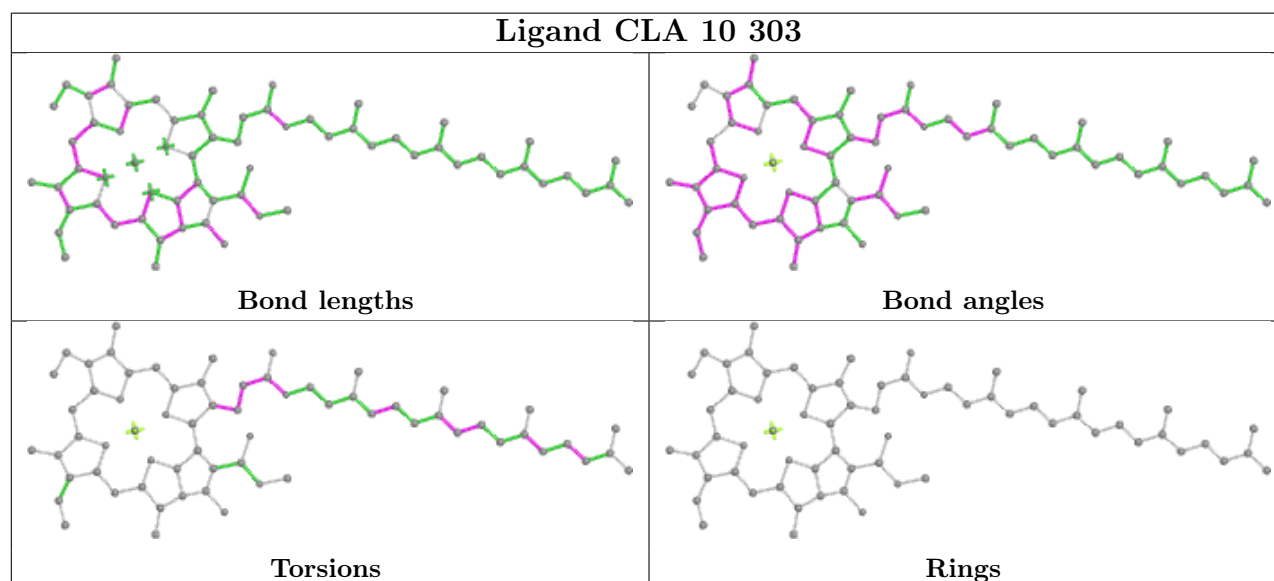
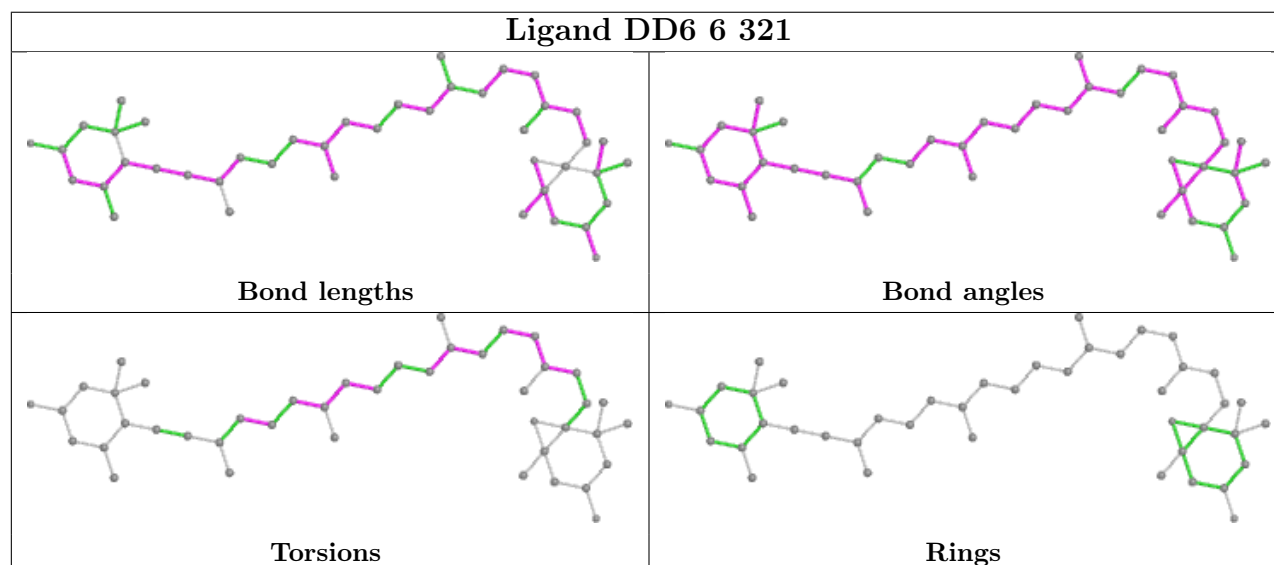
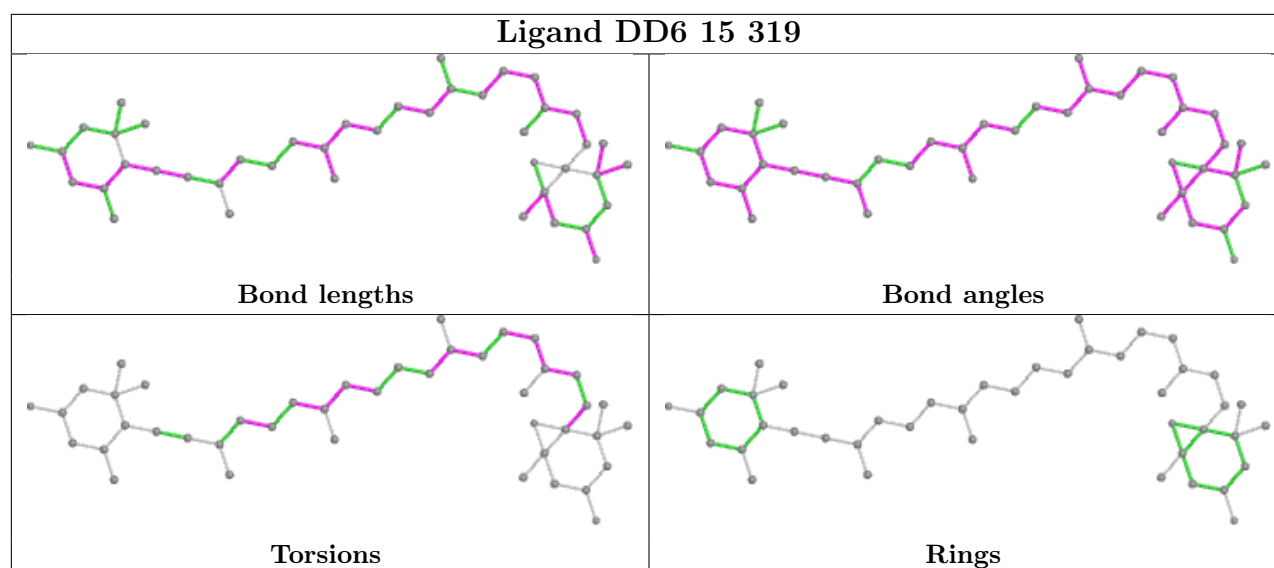
Ligand CLA A 821



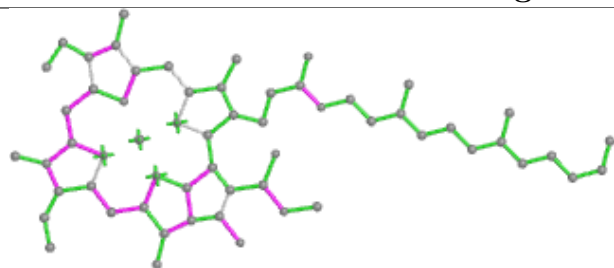
Ligand CLA A 832



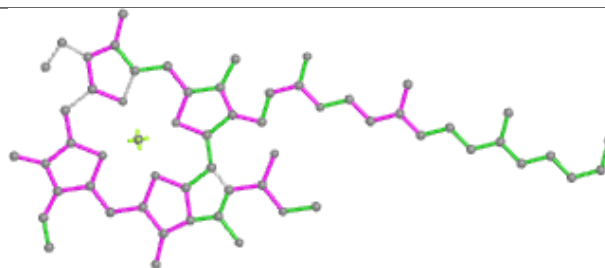
Ligand CLA 1 303**Ligand DD6 7 317****Ligand CLA 9 303**



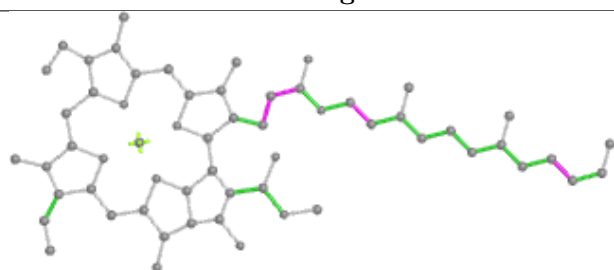
Ligand CLA B 817



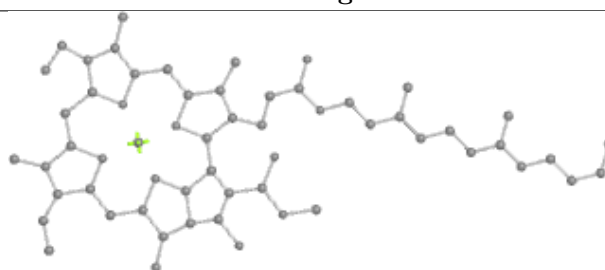
Bond lengths



Bond angles

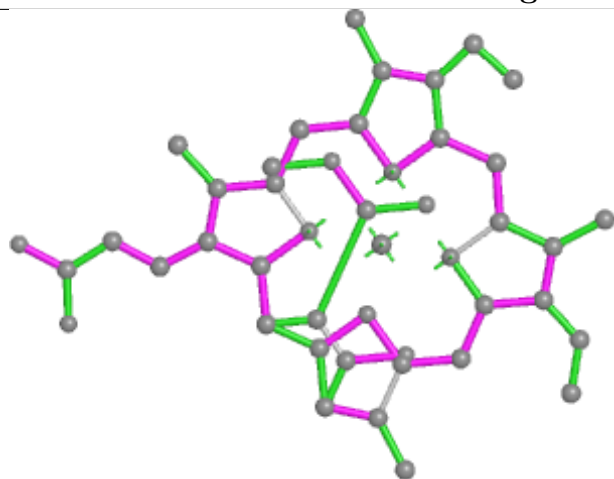


Torsions

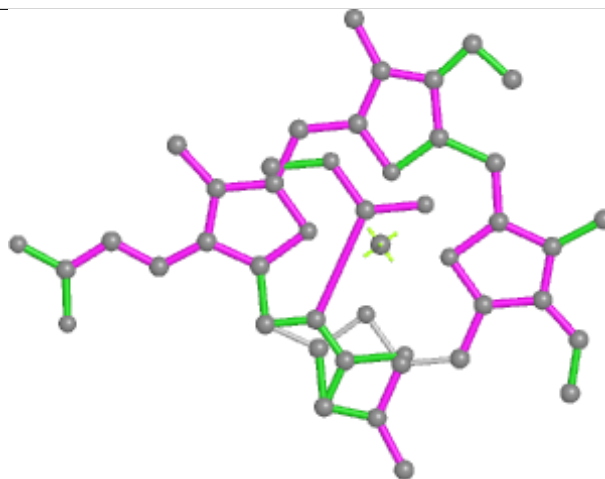


Rings

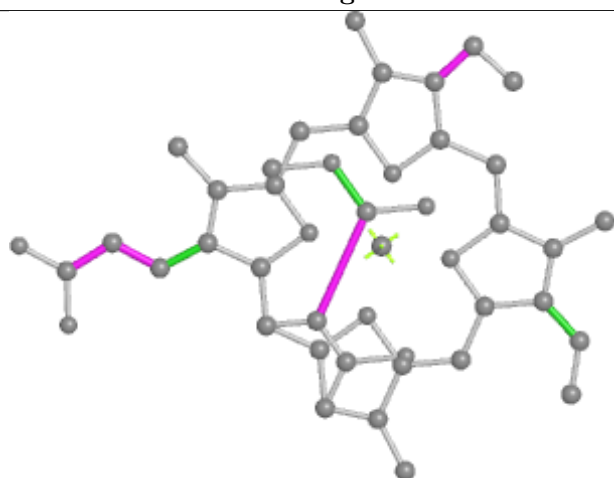
Ligand KC1 3 311



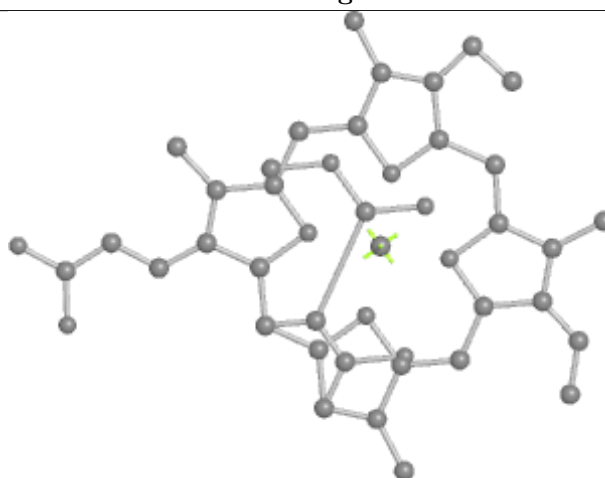
Bond lengths



Bond angles

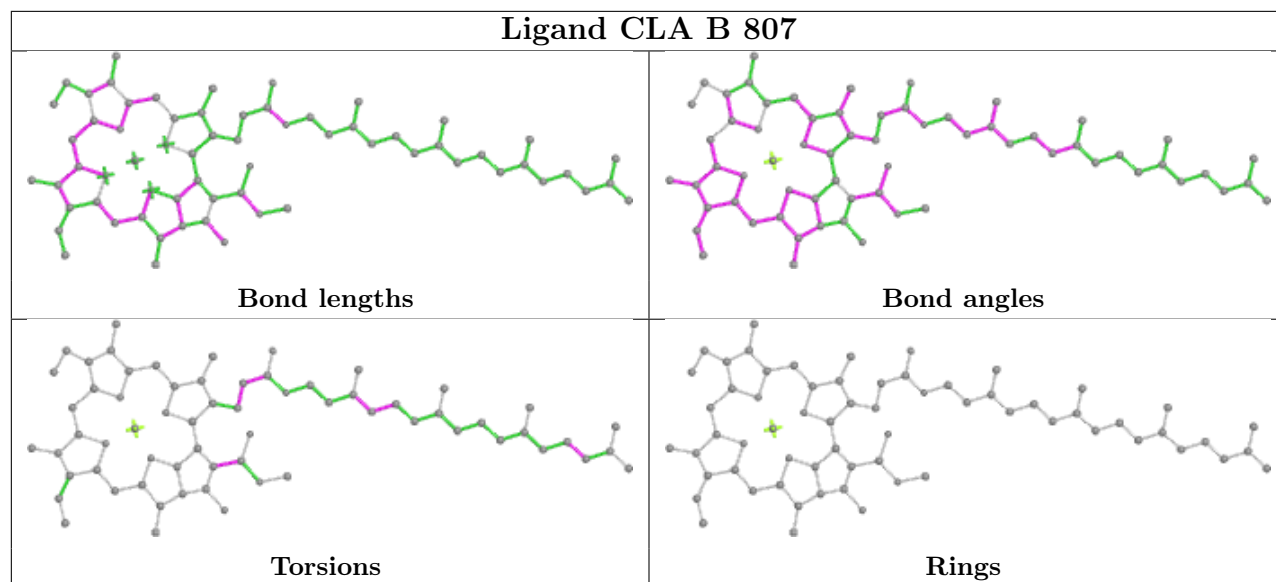


Torsions

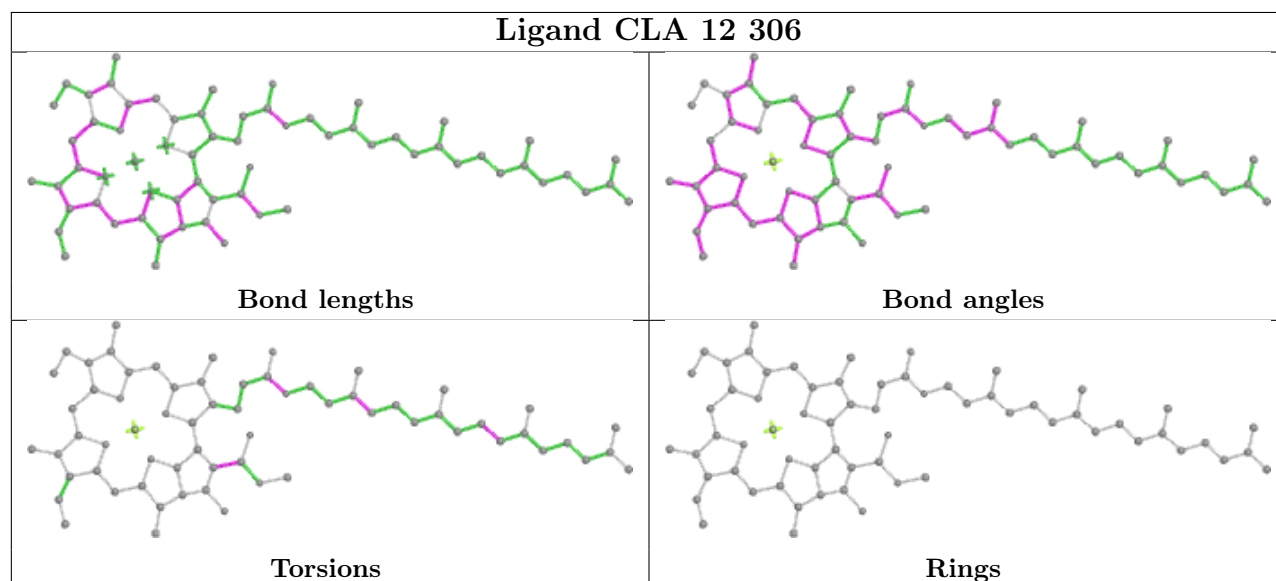


Rings

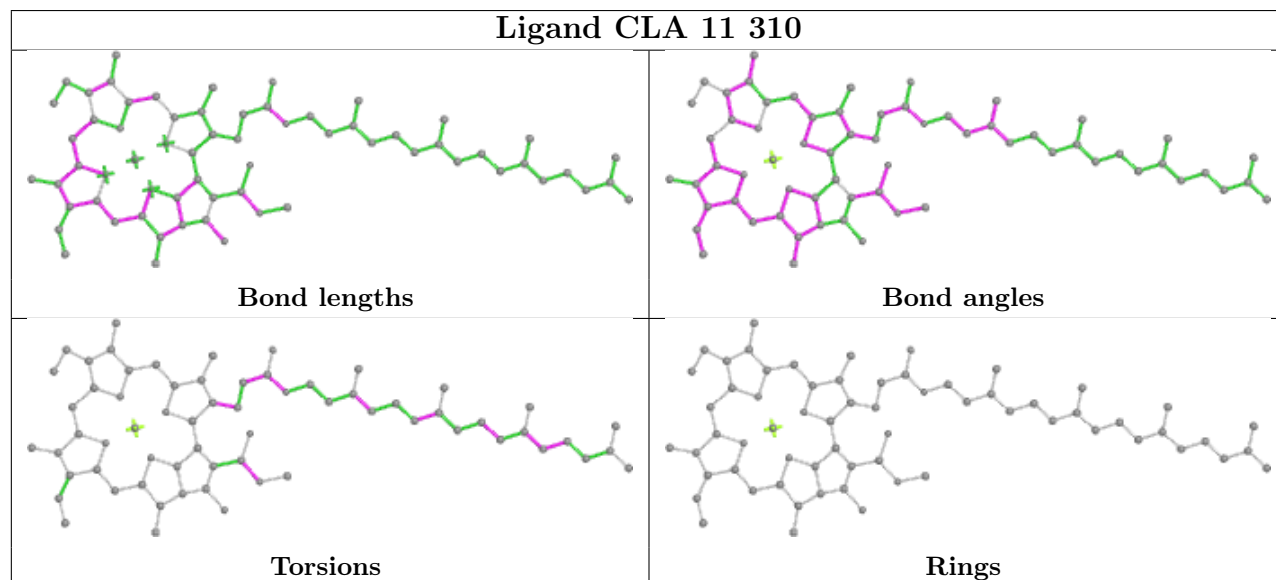
Ligand CLA B 807



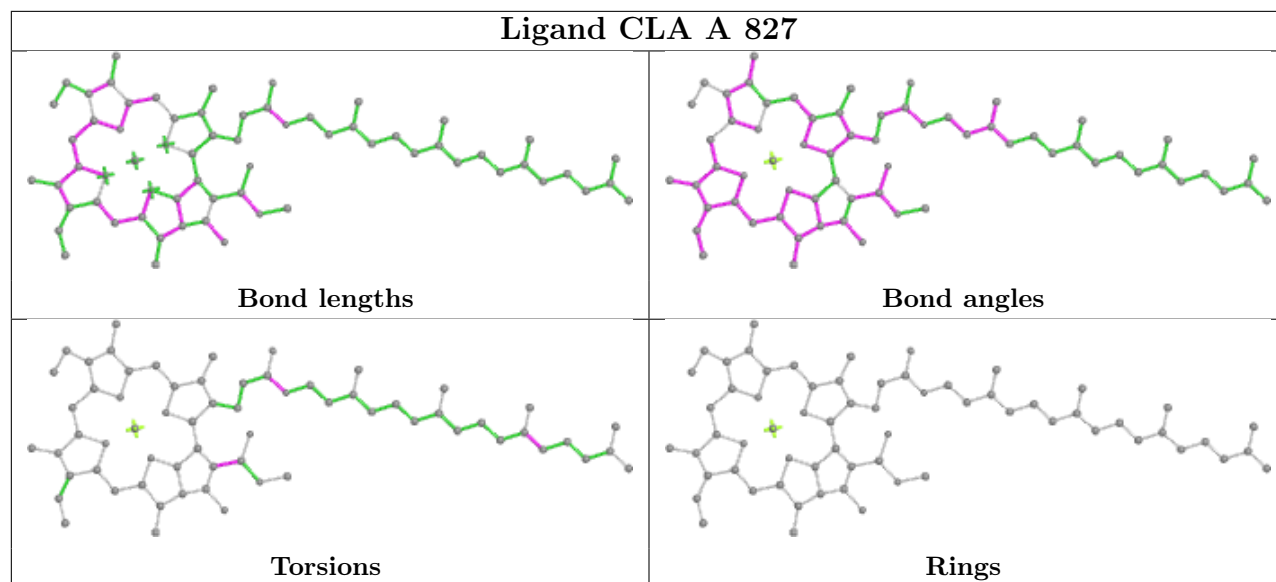
Ligand CLA 12 306



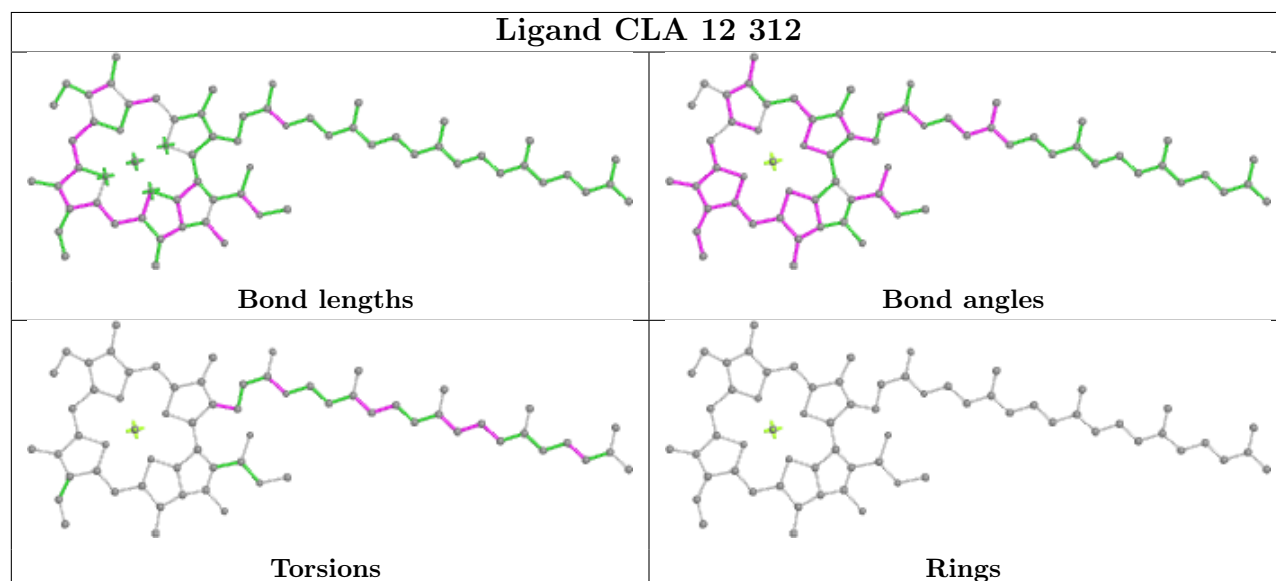
Ligand CLA 11 310



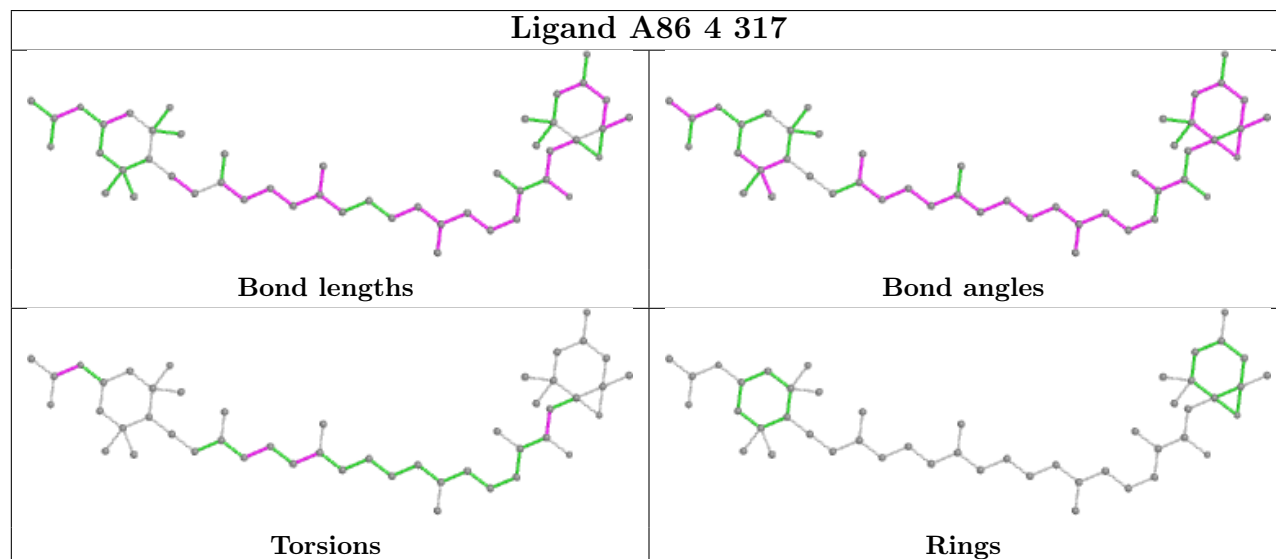
Ligand CLA A 827



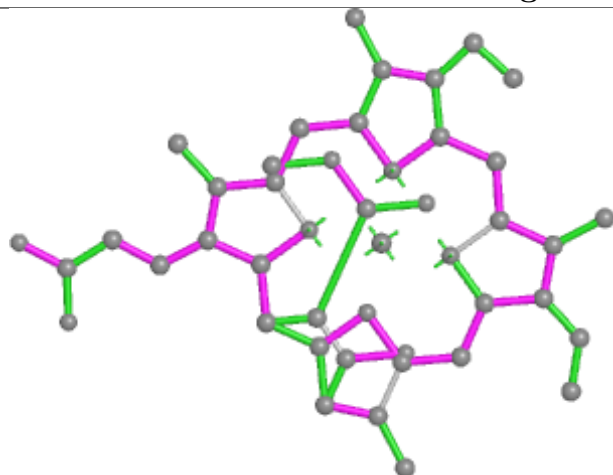
Ligand CLA 12 312



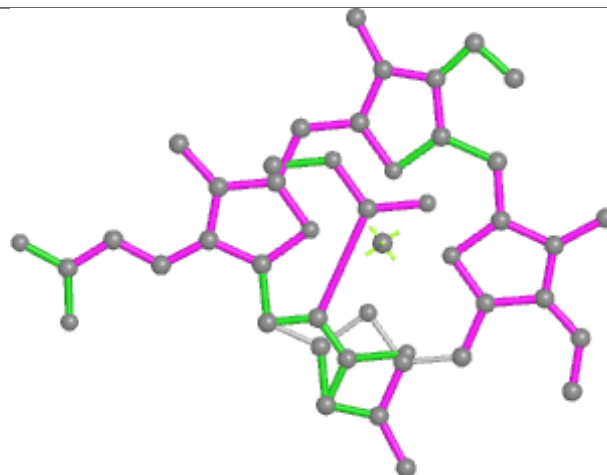
Ligand A86 4 317



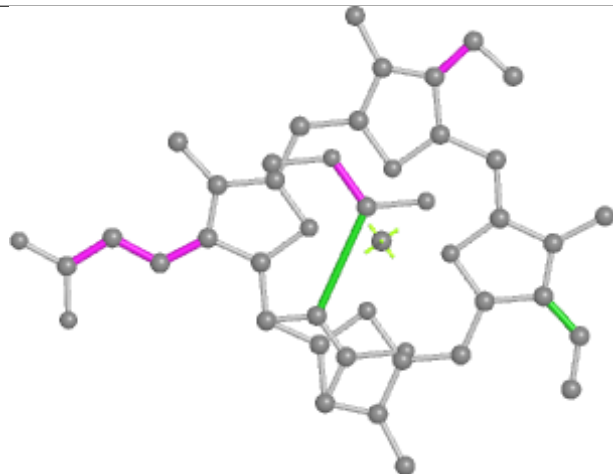
Ligand KC1 9 311



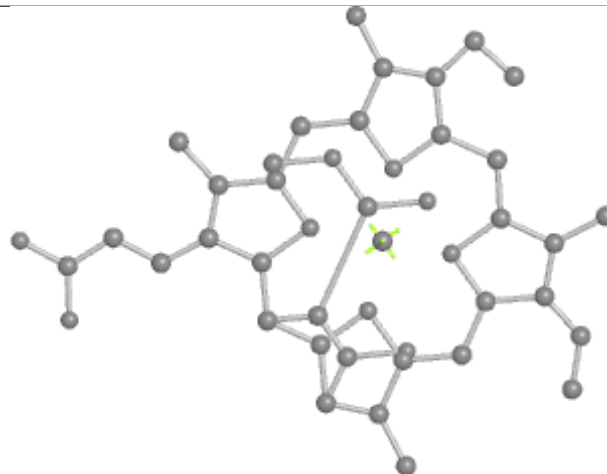
Bond lengths



Bond angles

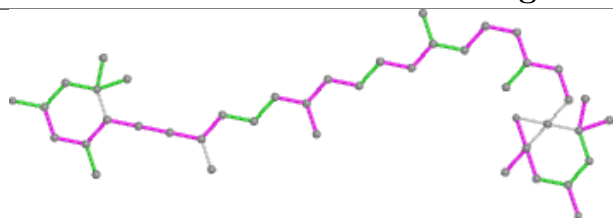


Torsions

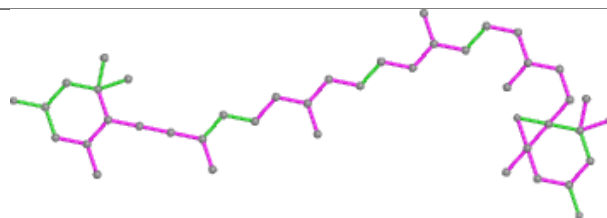


Rings

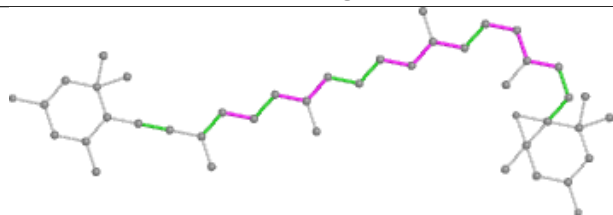
Ligand DD6 7 302



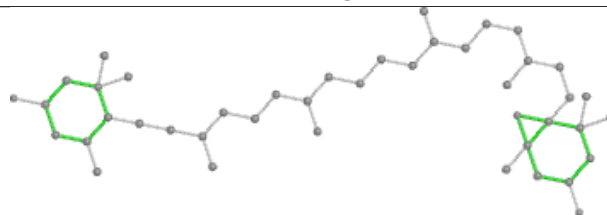
Bond lengths



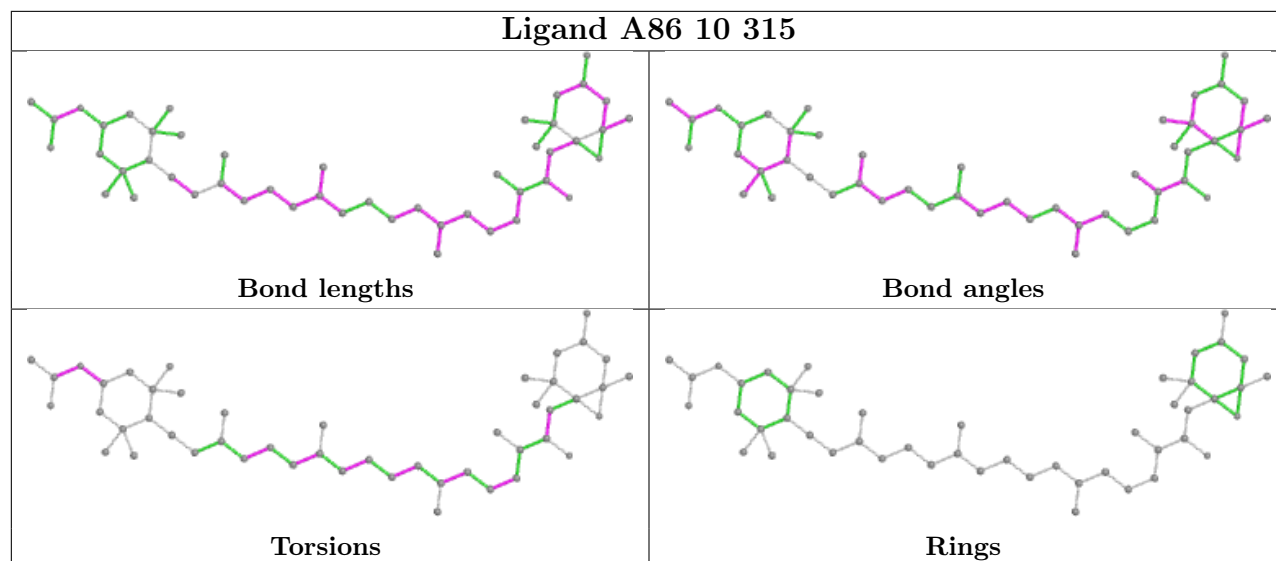
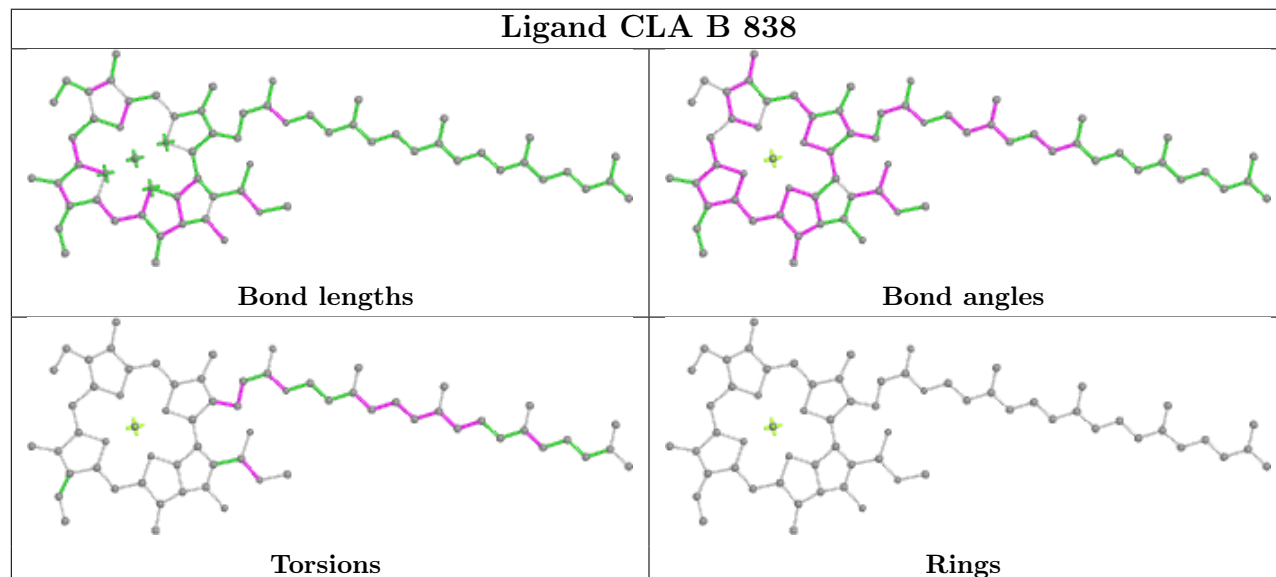
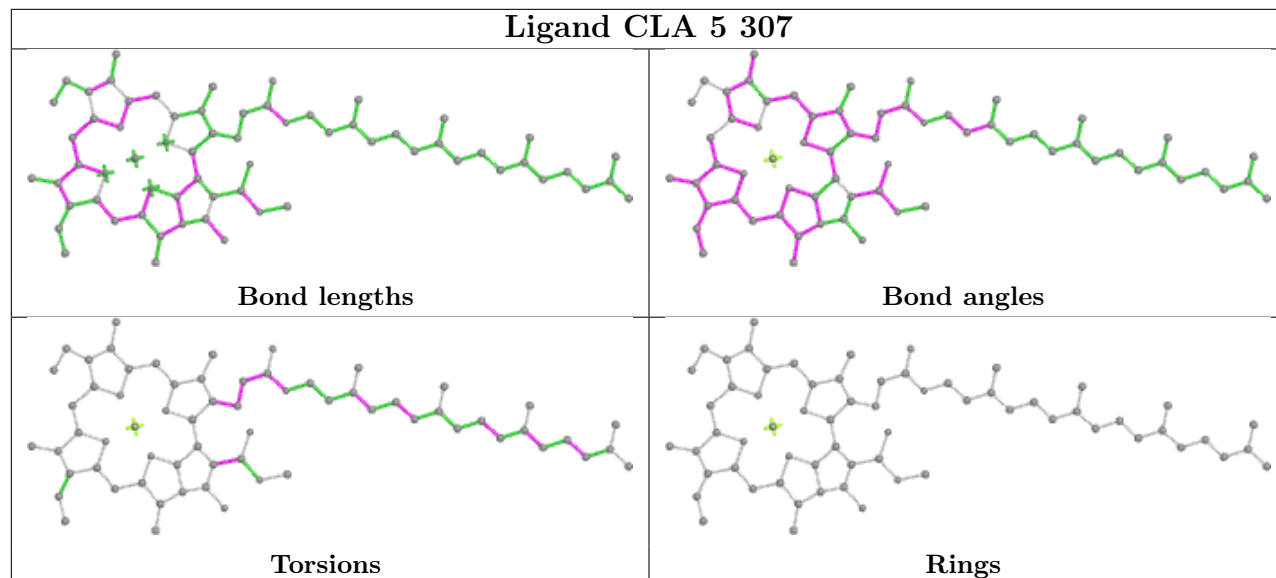
Bond angles



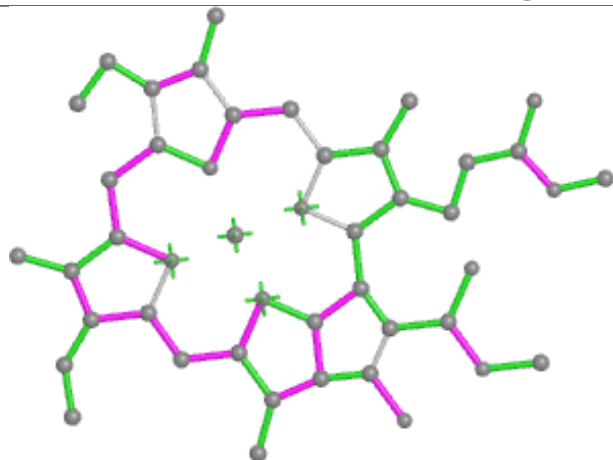
Torsions



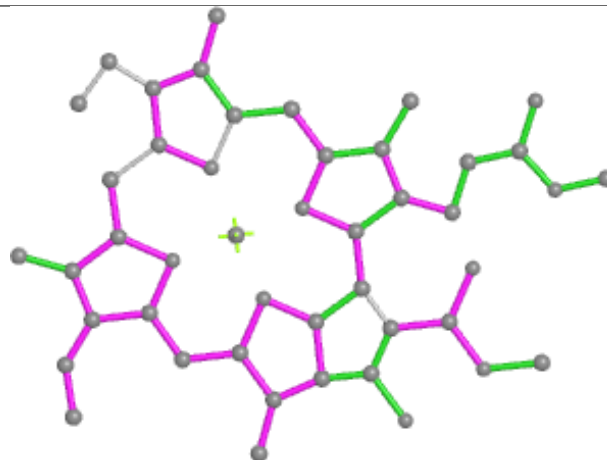
Rings

Ligand A86 10 315**Ligand CLA B 838****Ligand CLA 5 307**

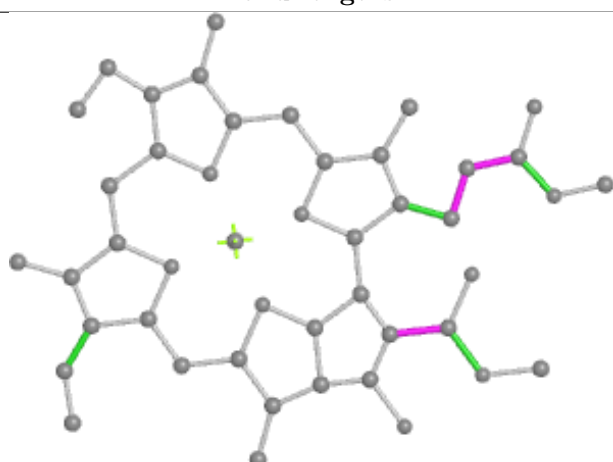
Ligand CLA 7 312



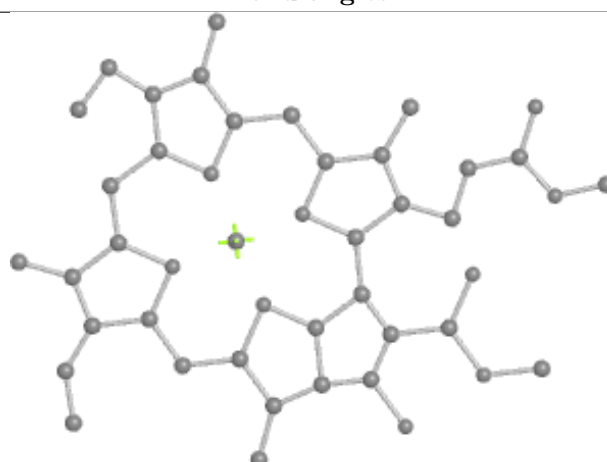
Bond lengths



Bond angles

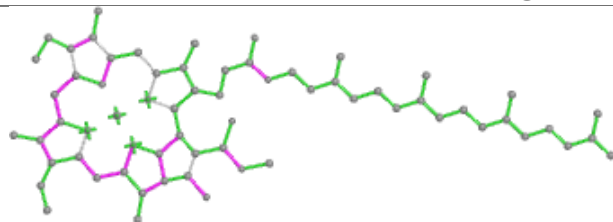


Torsions

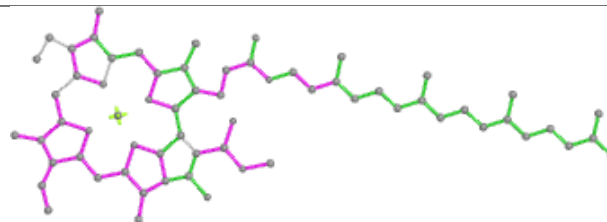


Rings

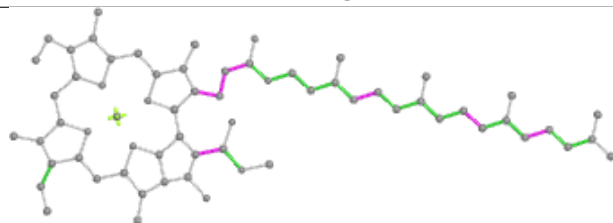
Ligand CLA 2 308



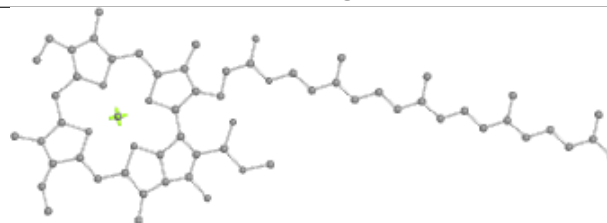
Bond lengths



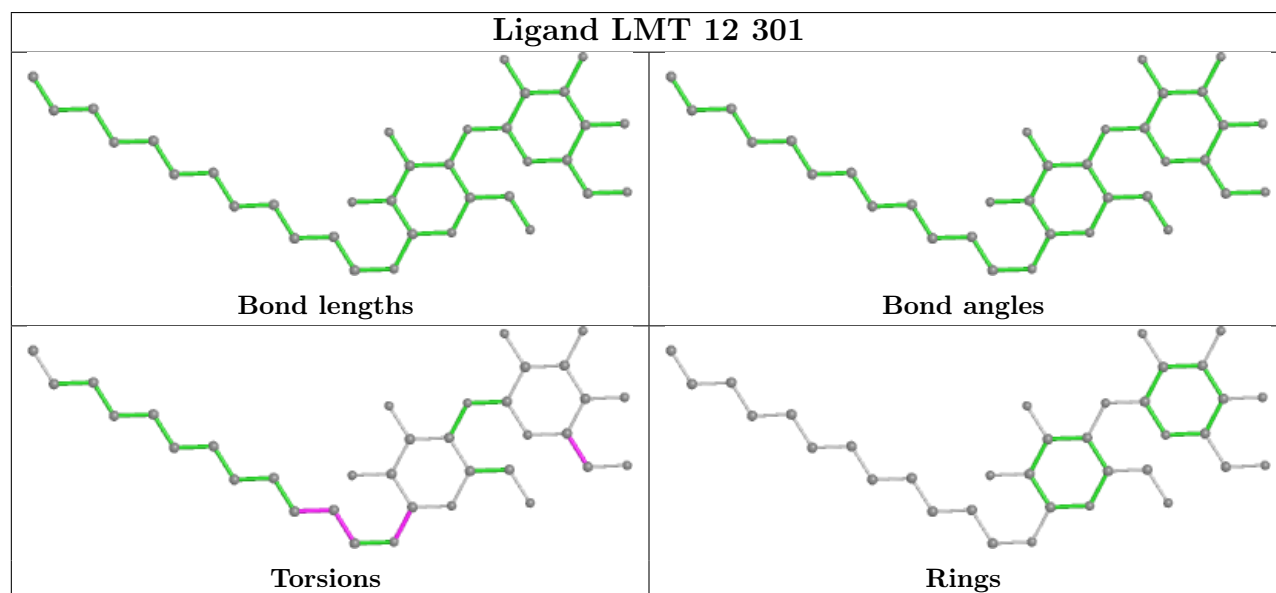
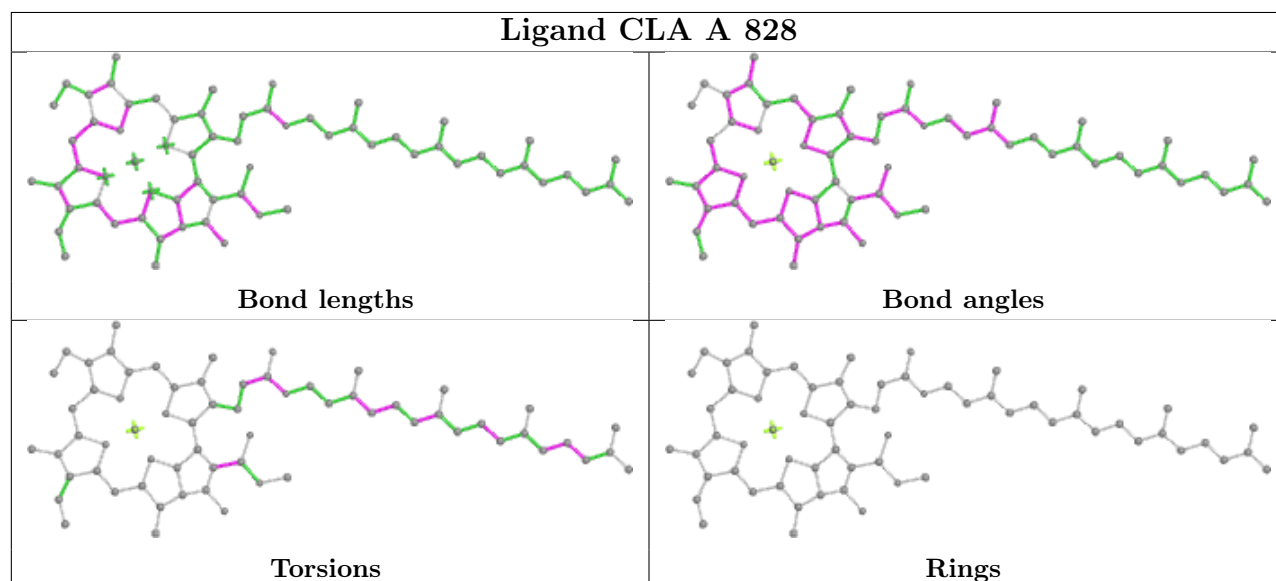
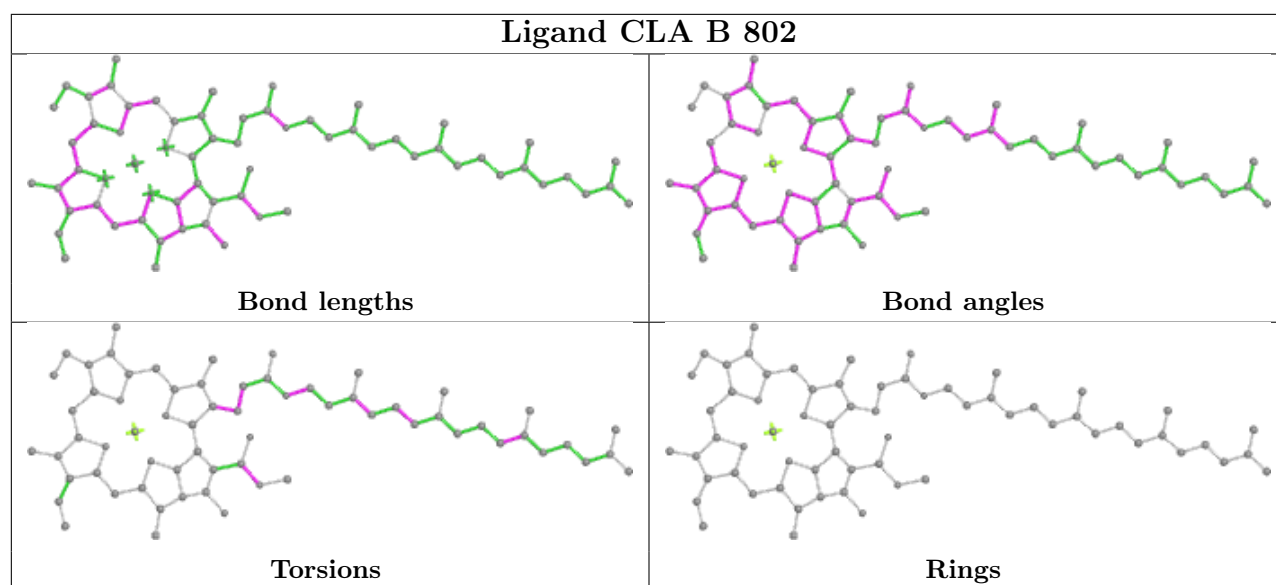
Bond angles

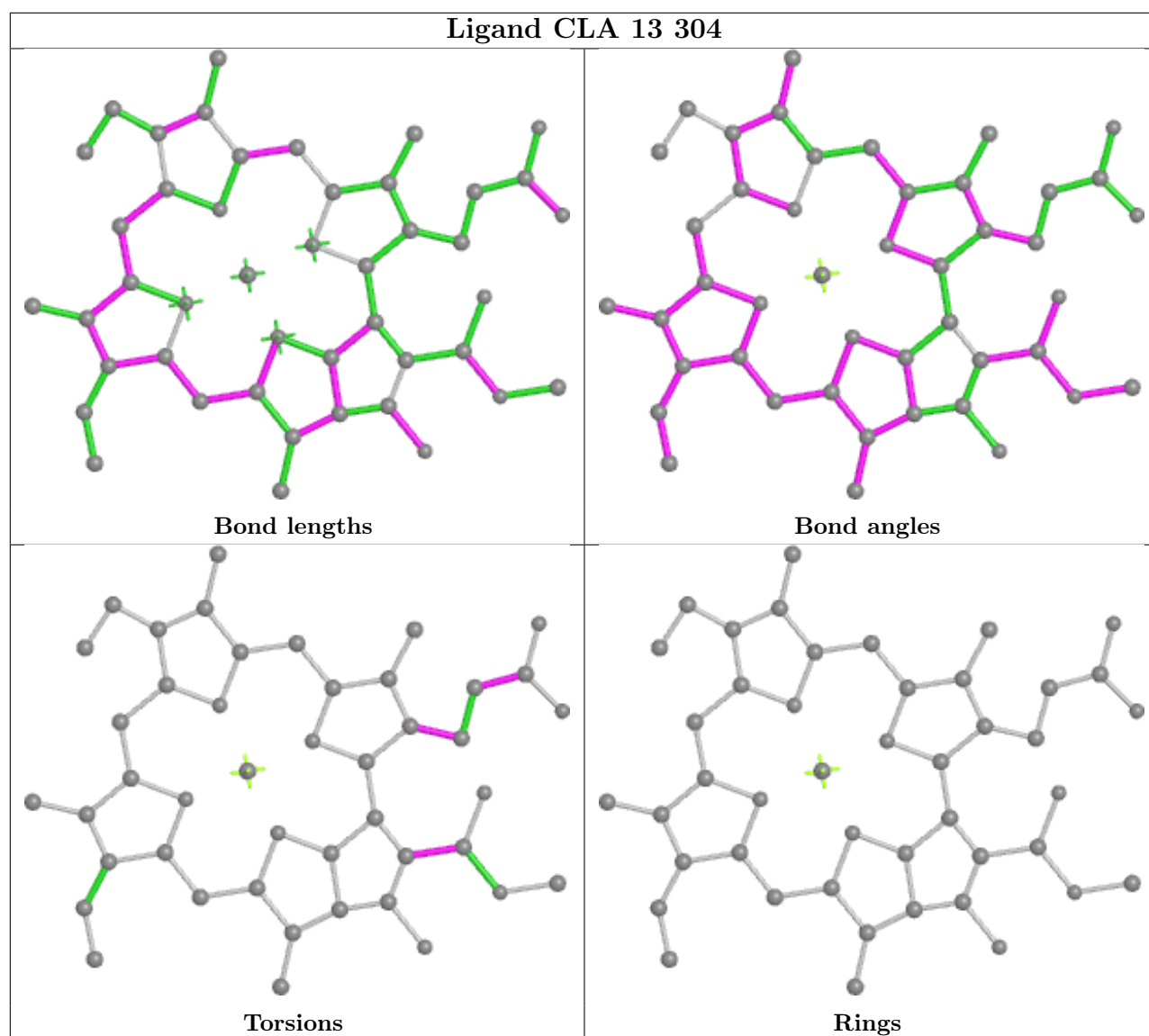


Torsions

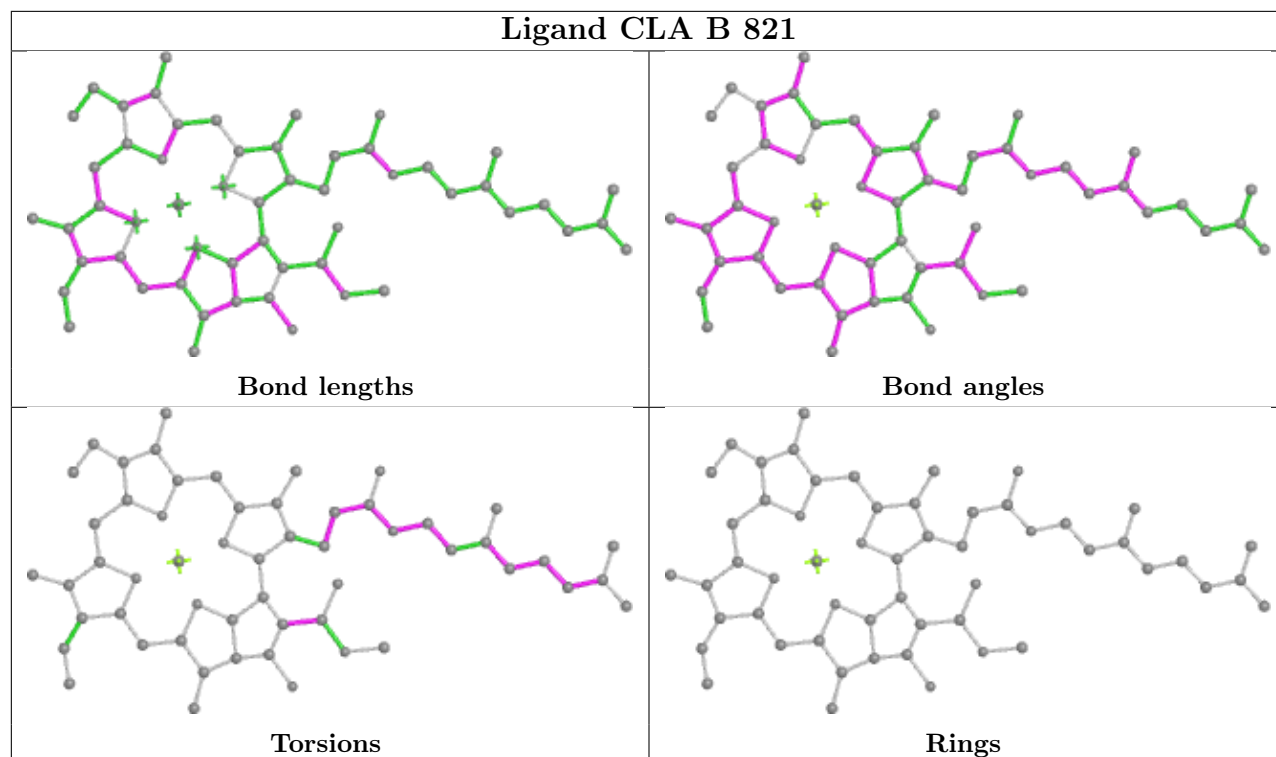


Rings

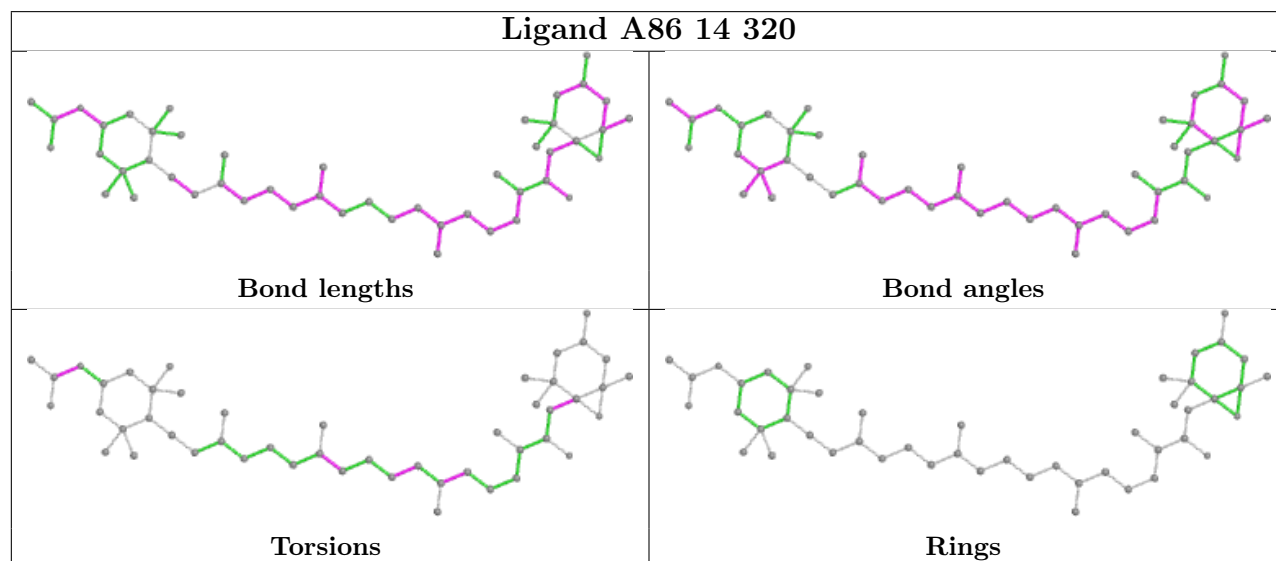


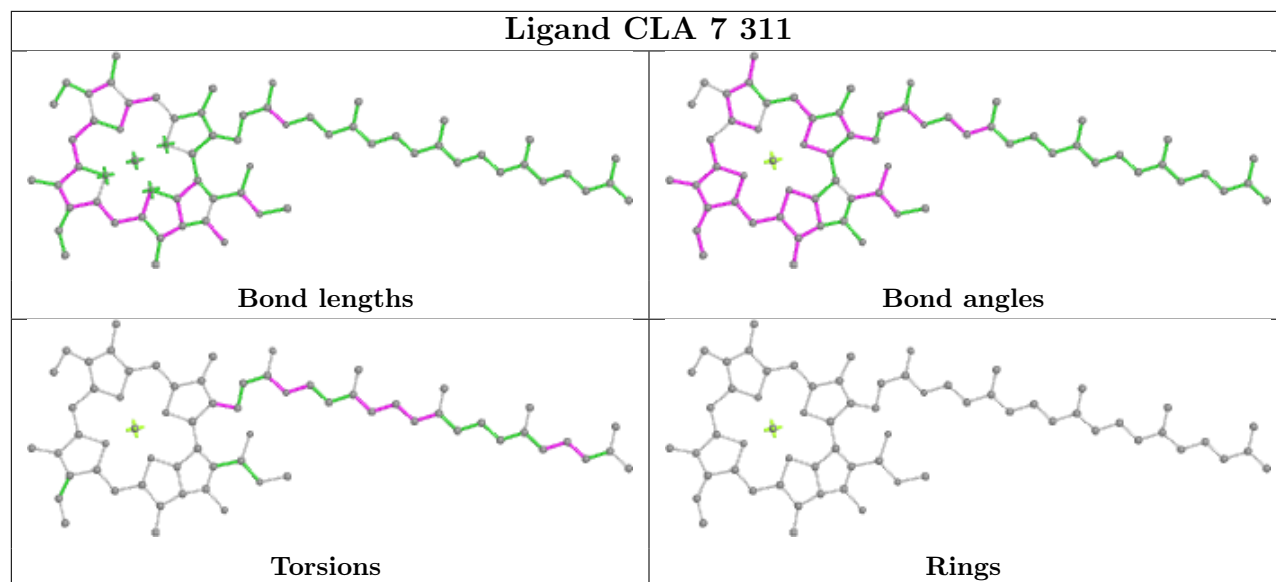
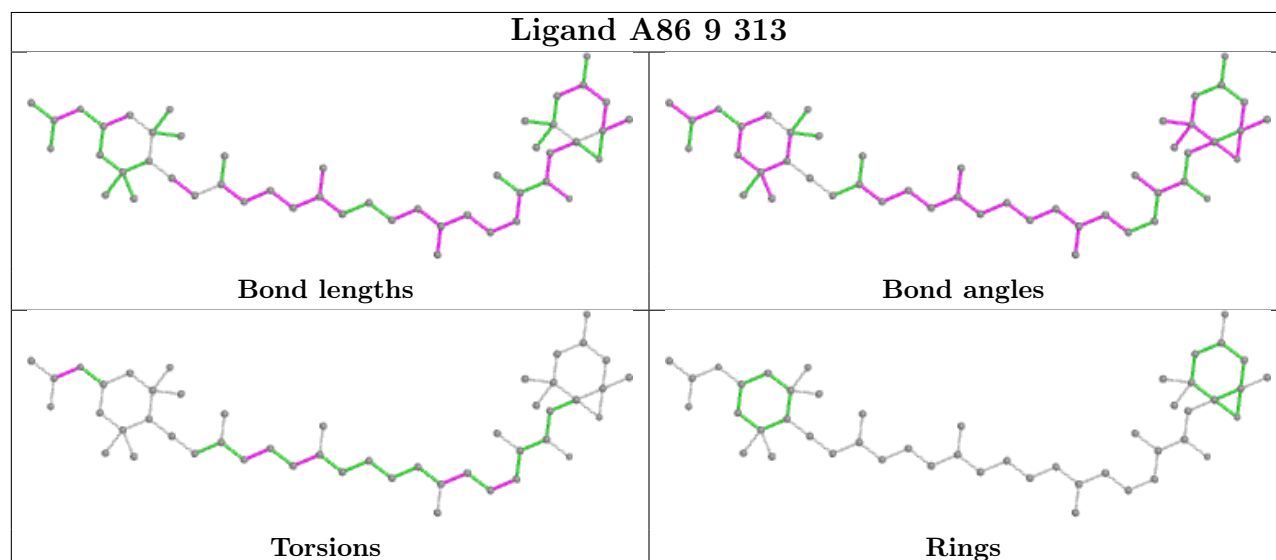
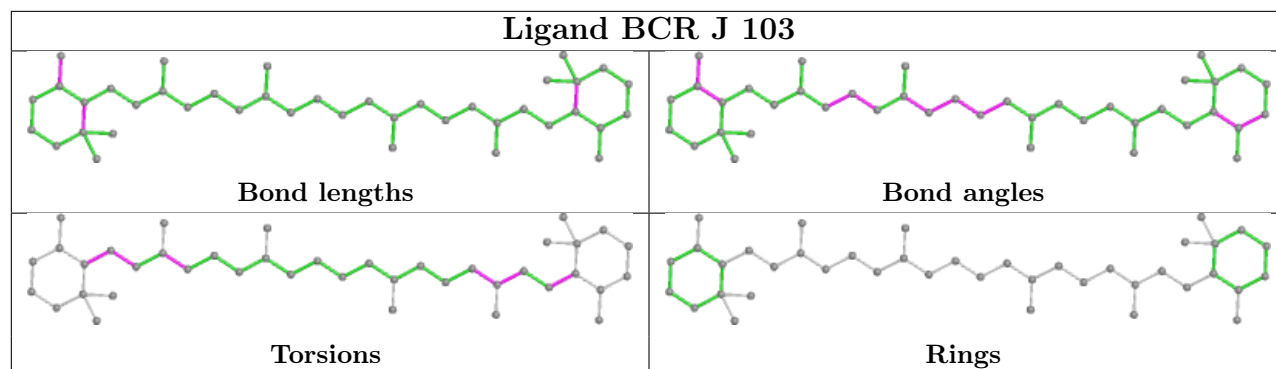


Ligand CLA B 821

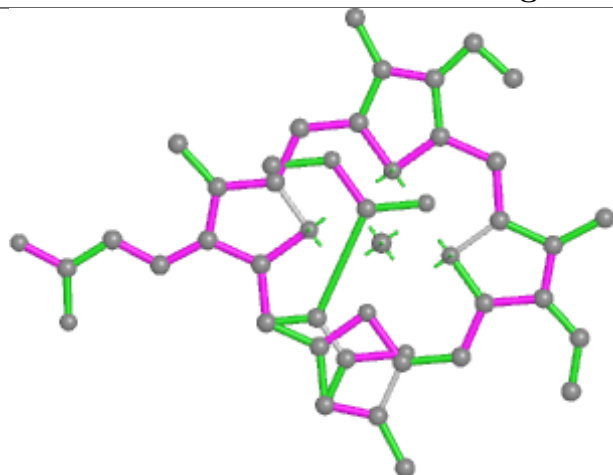


Ligand A86 14 320

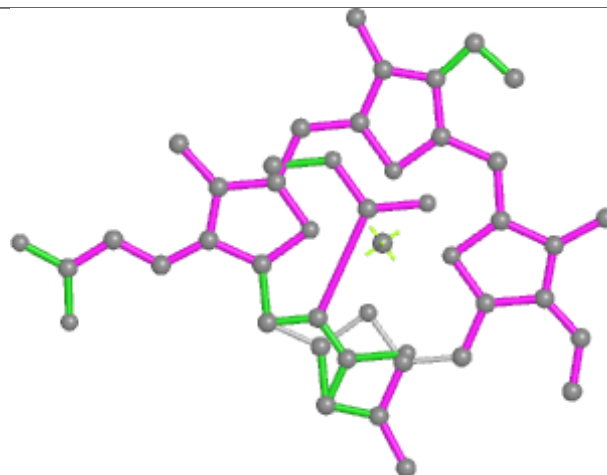


Ligand CLA 7 311**Ligand A86 9 313****Ligand BCR J 103**

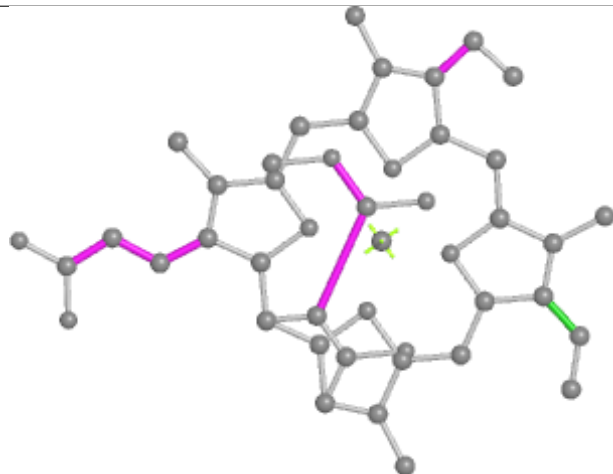
Ligand KC1 6 311



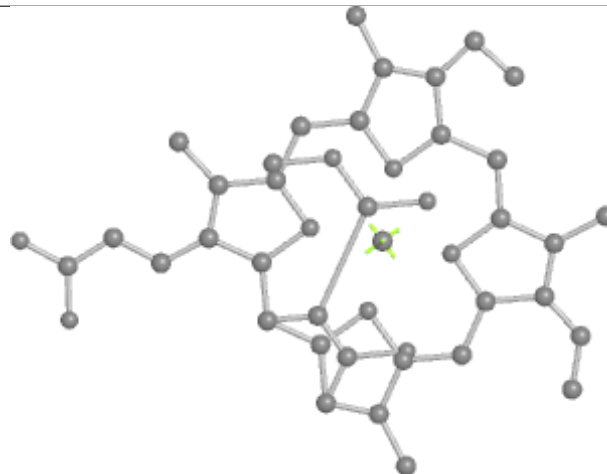
Bond lengths



Bond angles

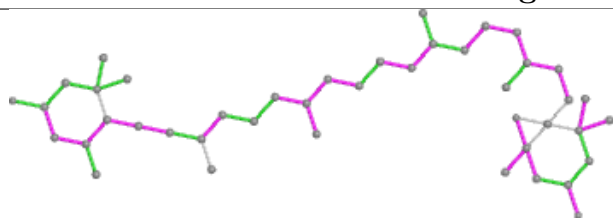


Torsions

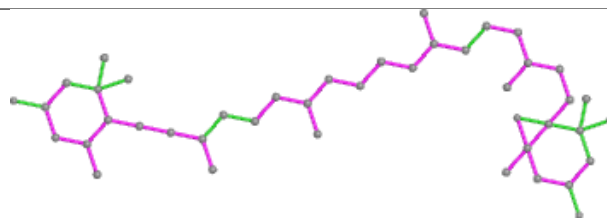


Rings

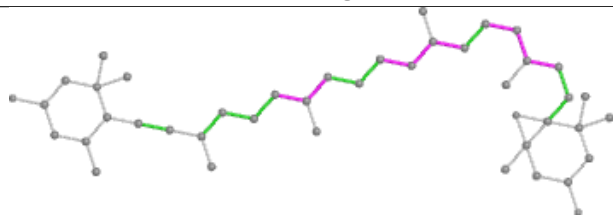
Ligand DD6 6 303



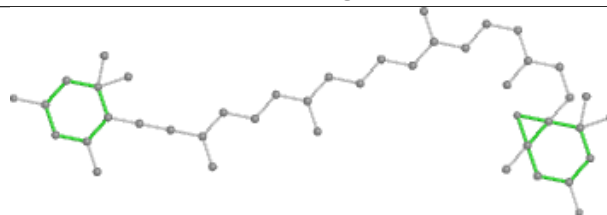
Bond lengths



Bond angles

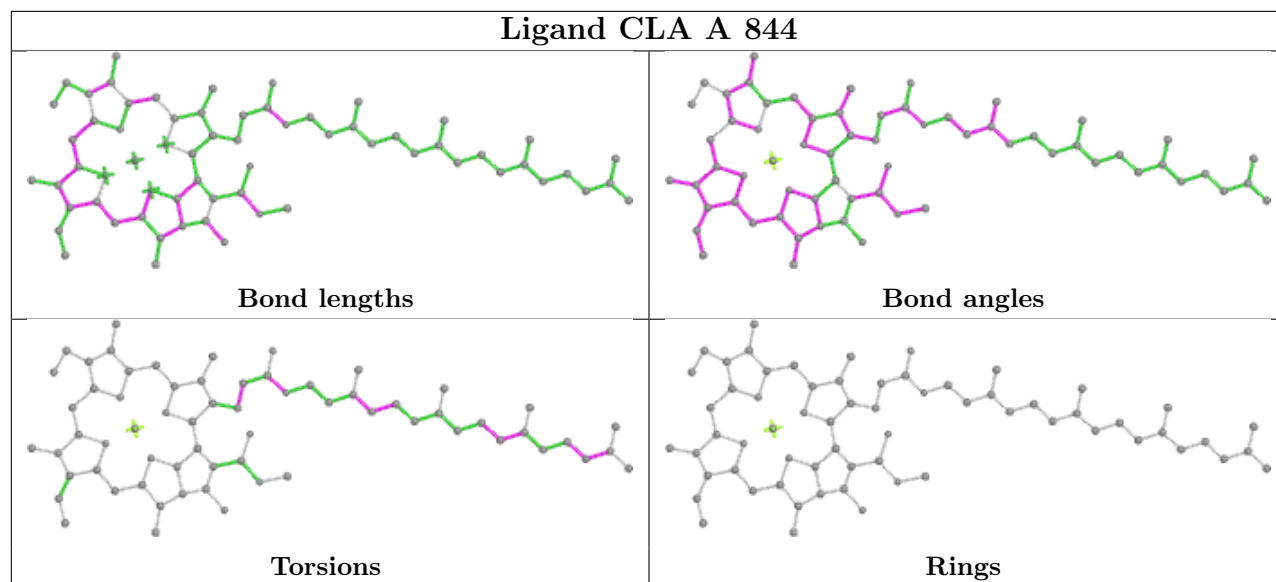


Torsions

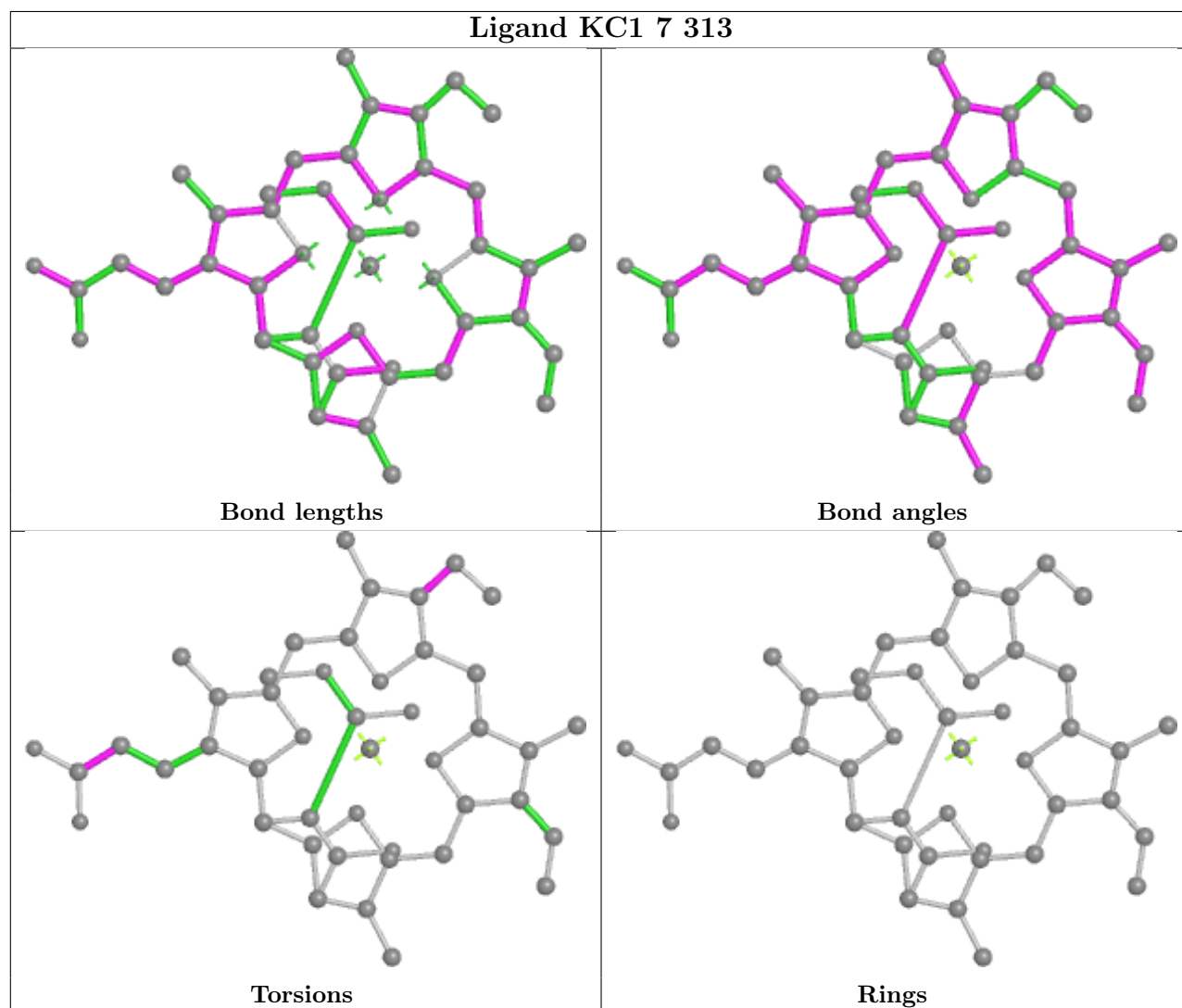


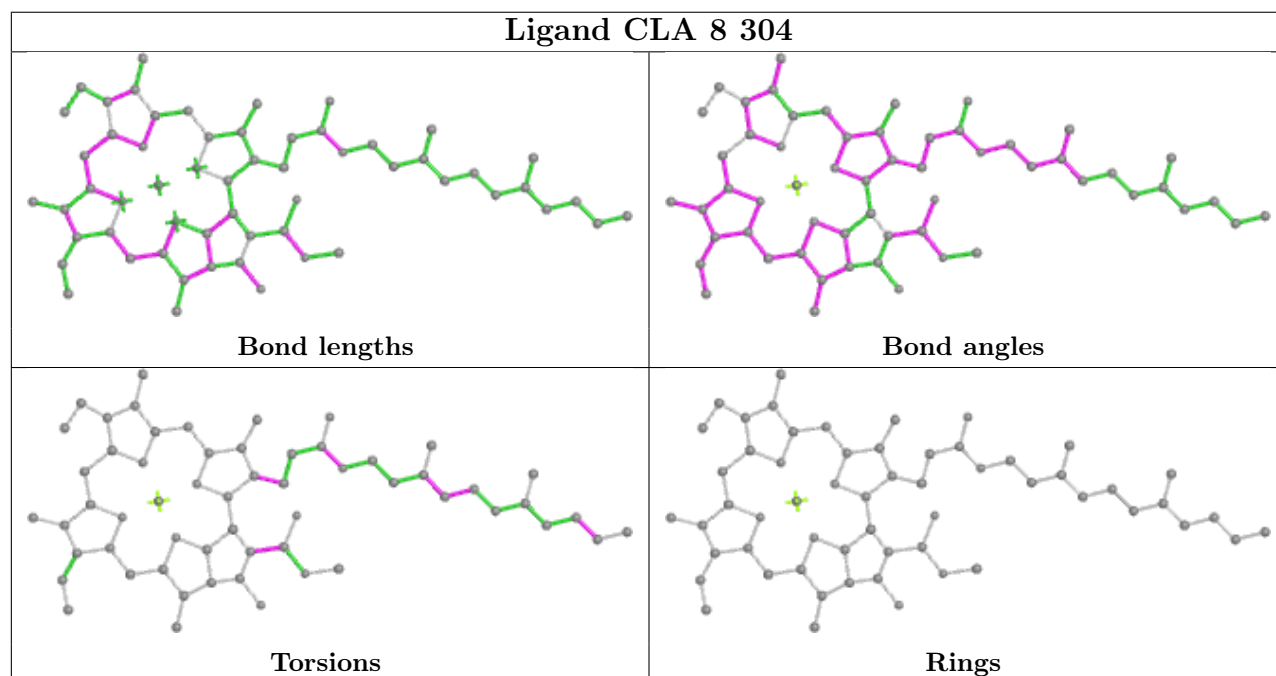
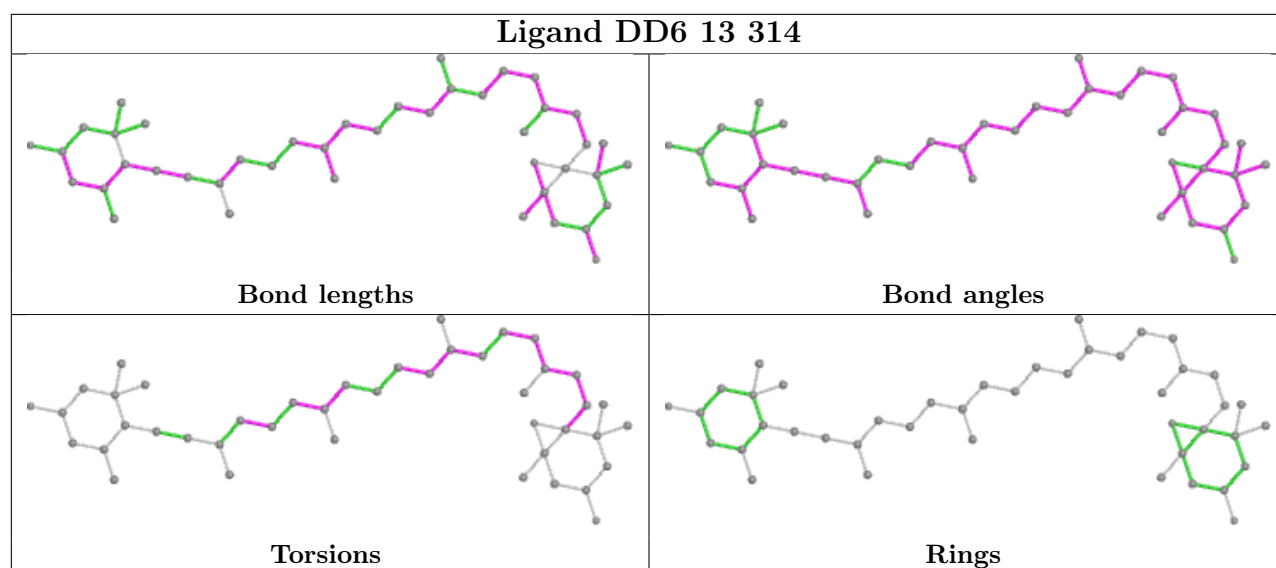
Rings

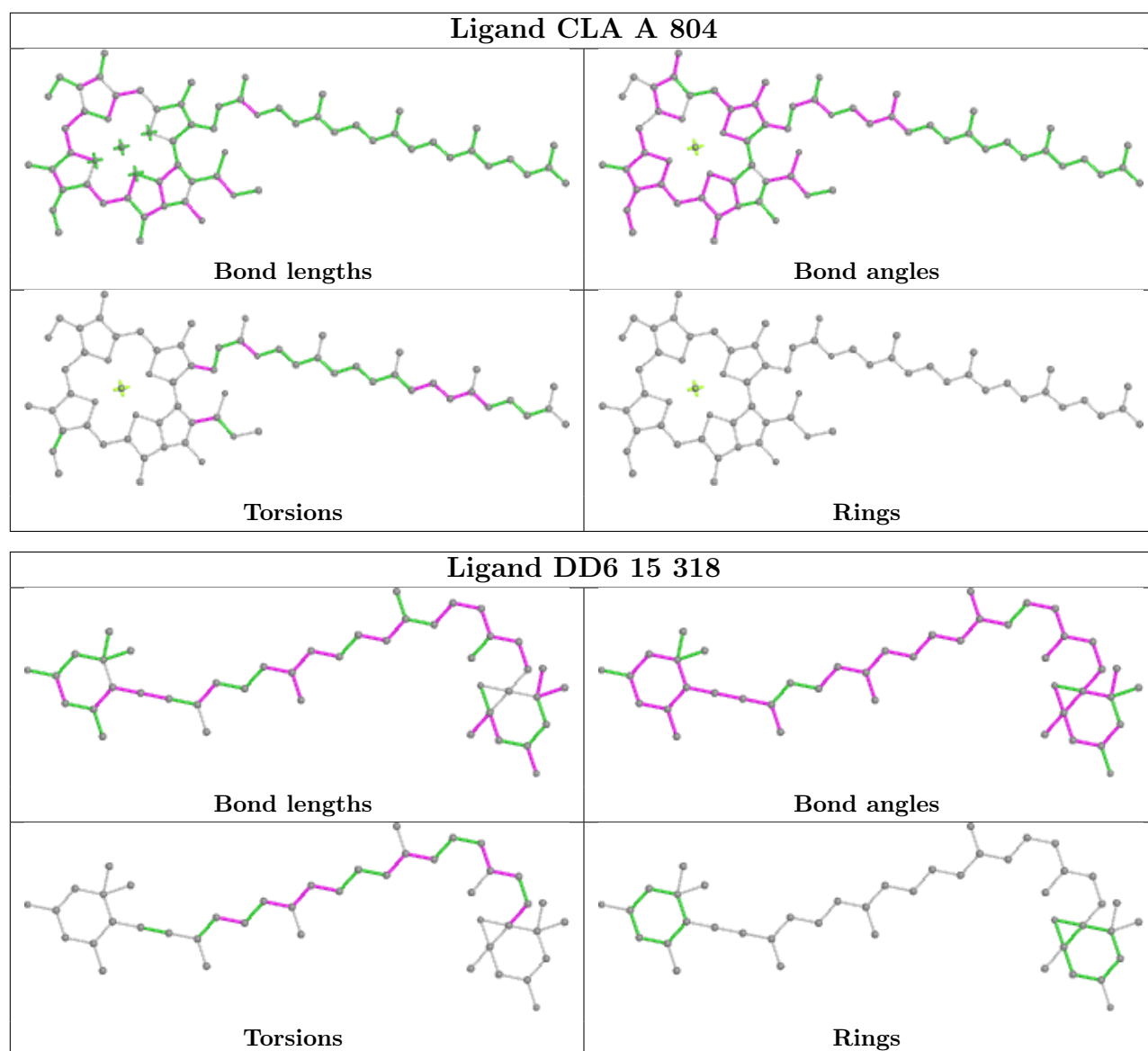
Ligand CLA A 844



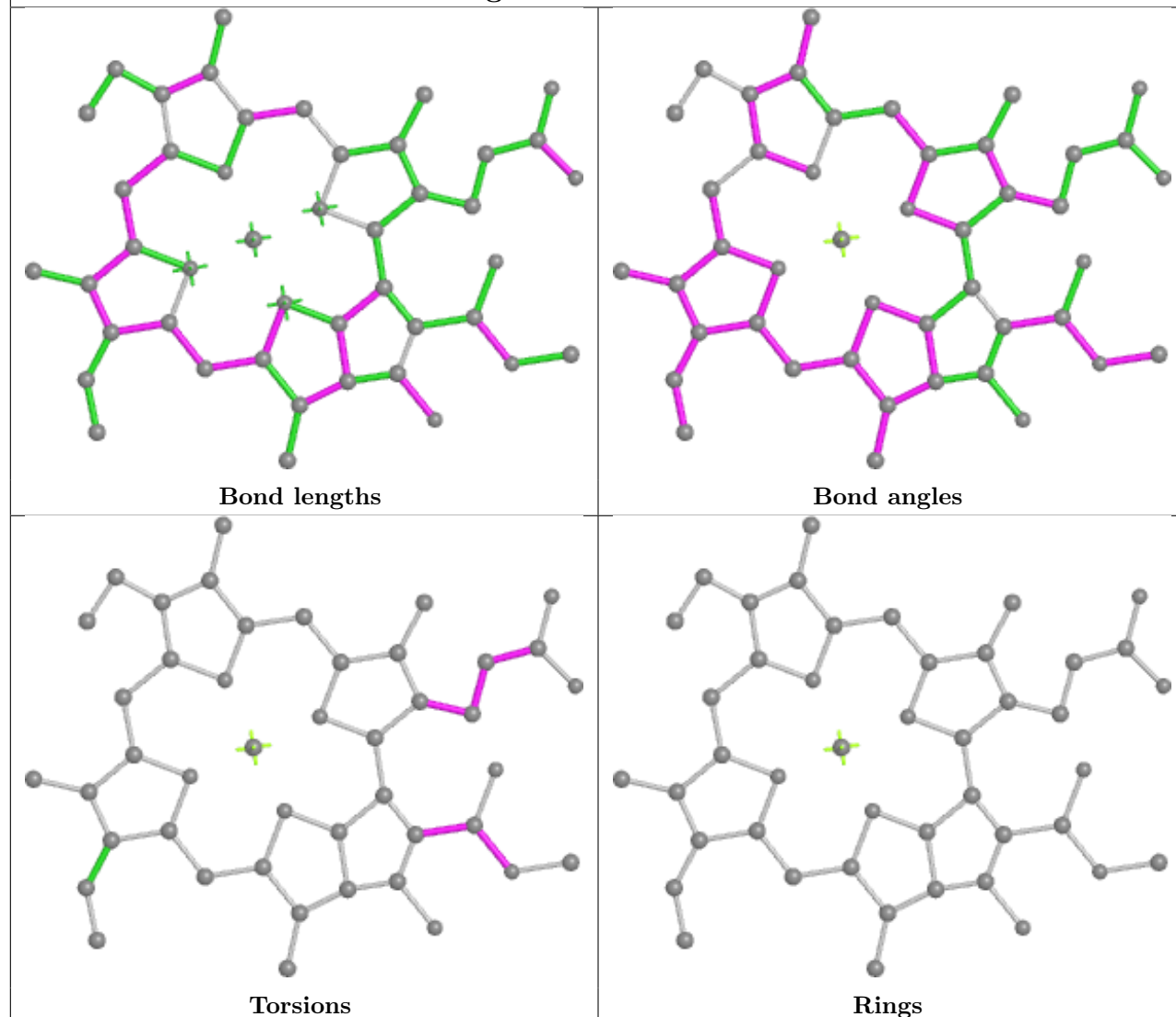
Ligand KC1 7 313



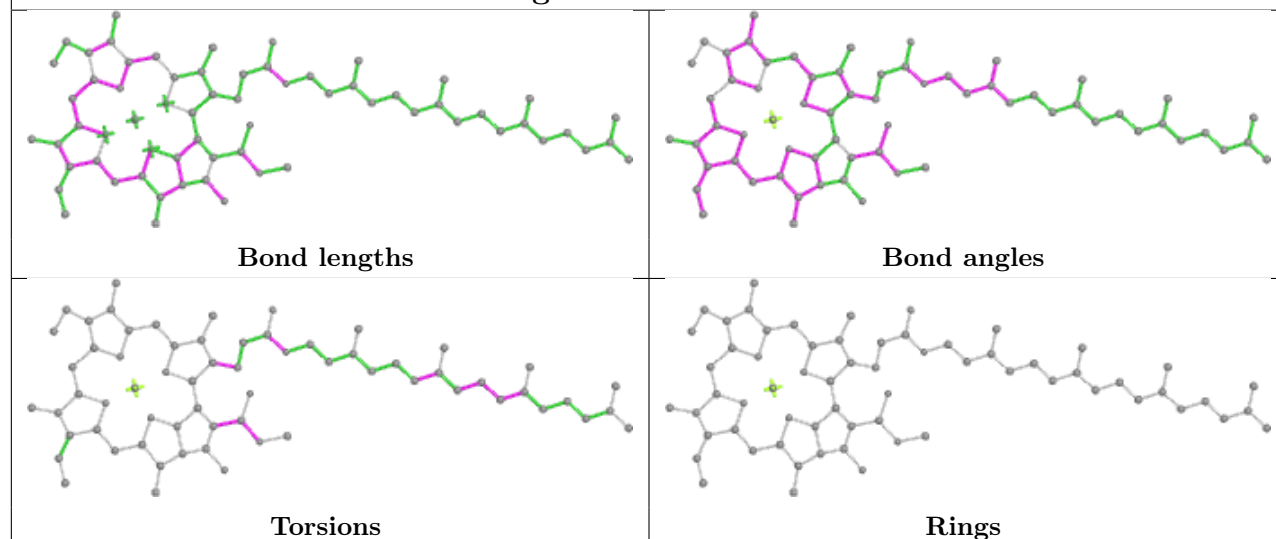




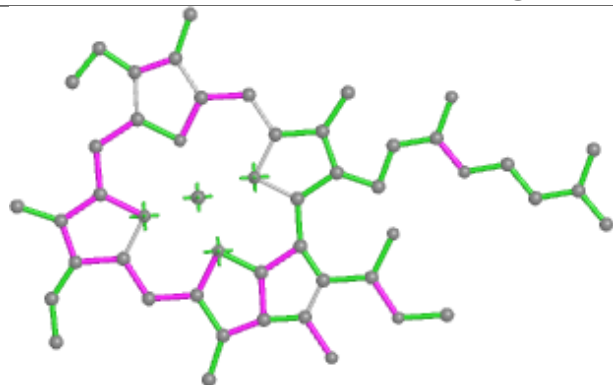
Ligand CLA 13 309



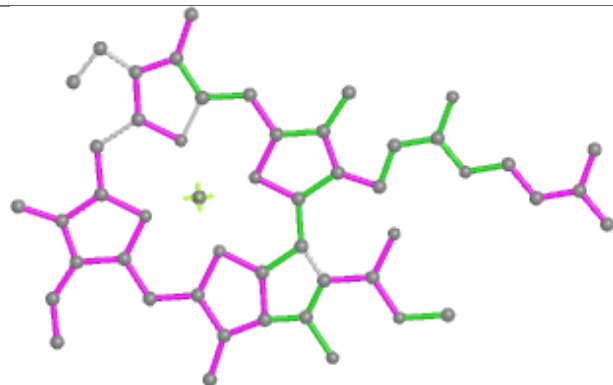
Ligand CLA B 828



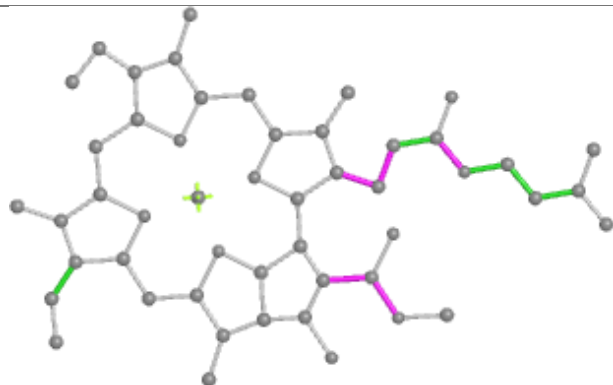
Ligand CLA 15 307



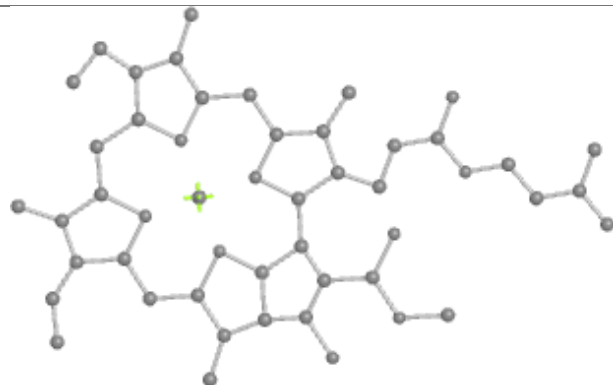
Bond lengths



Bond angles

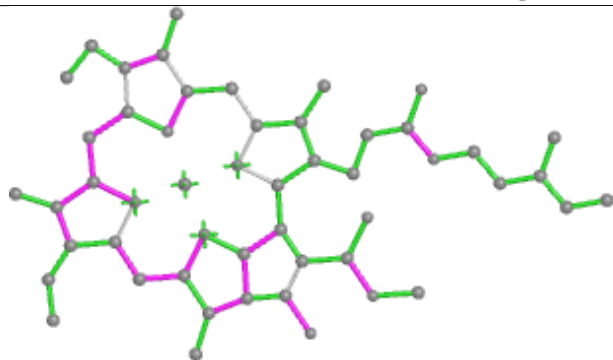


Torsions

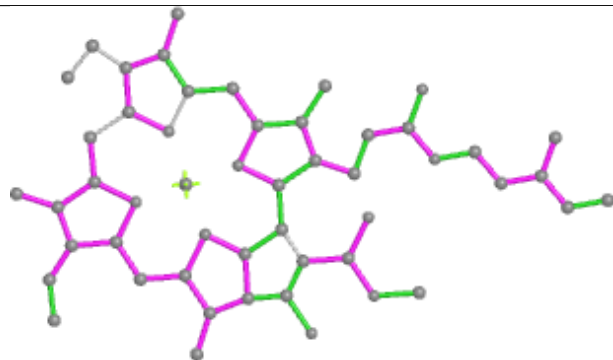


Rings

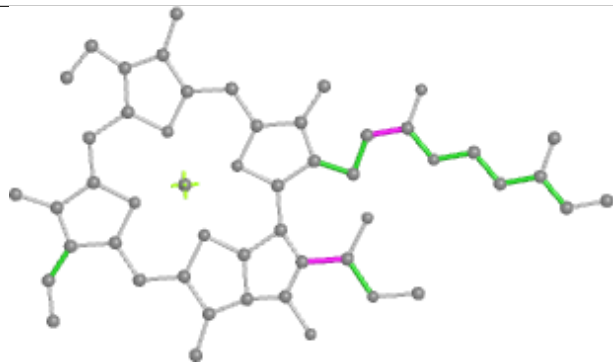
Ligand CLA A 808



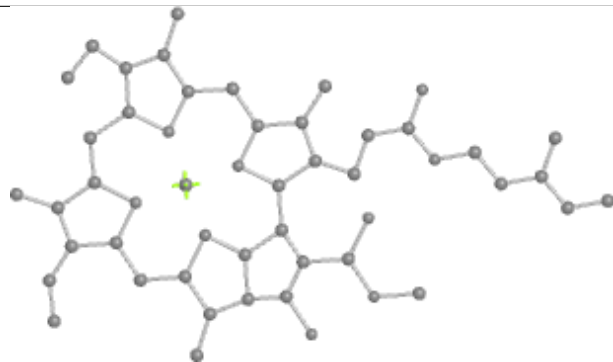
Bond lengths



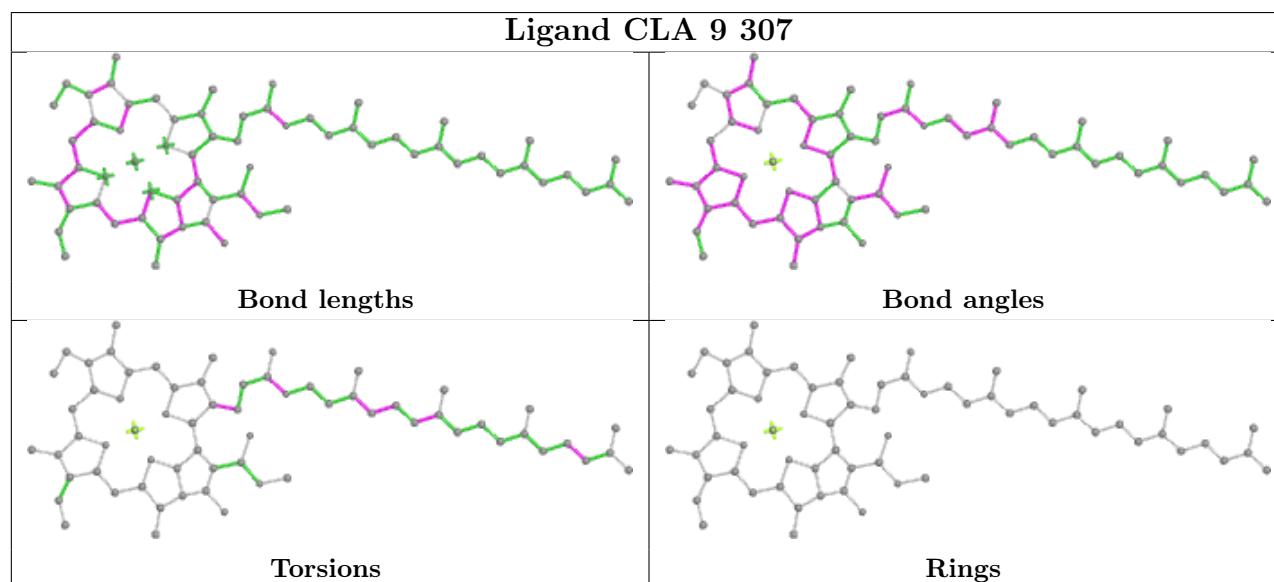
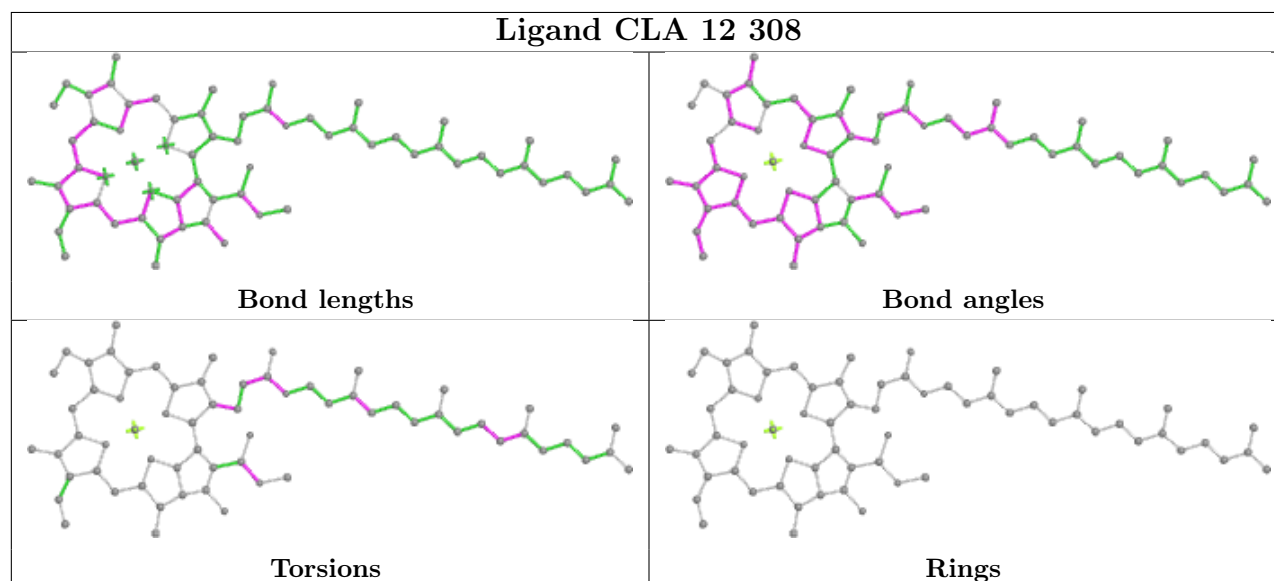
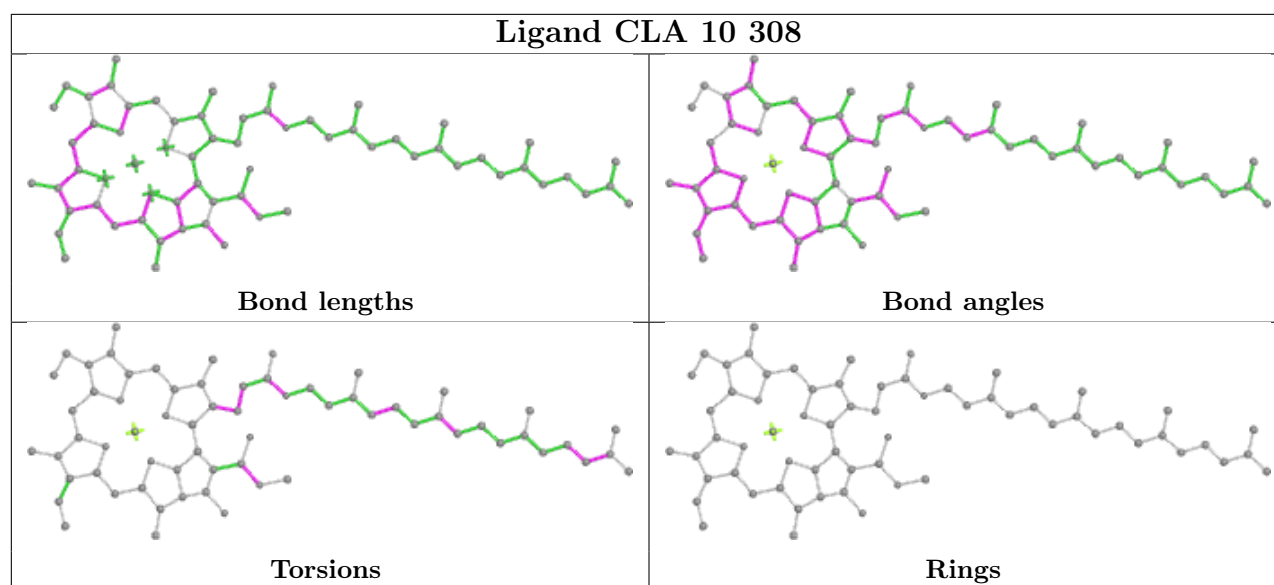
Bond angles

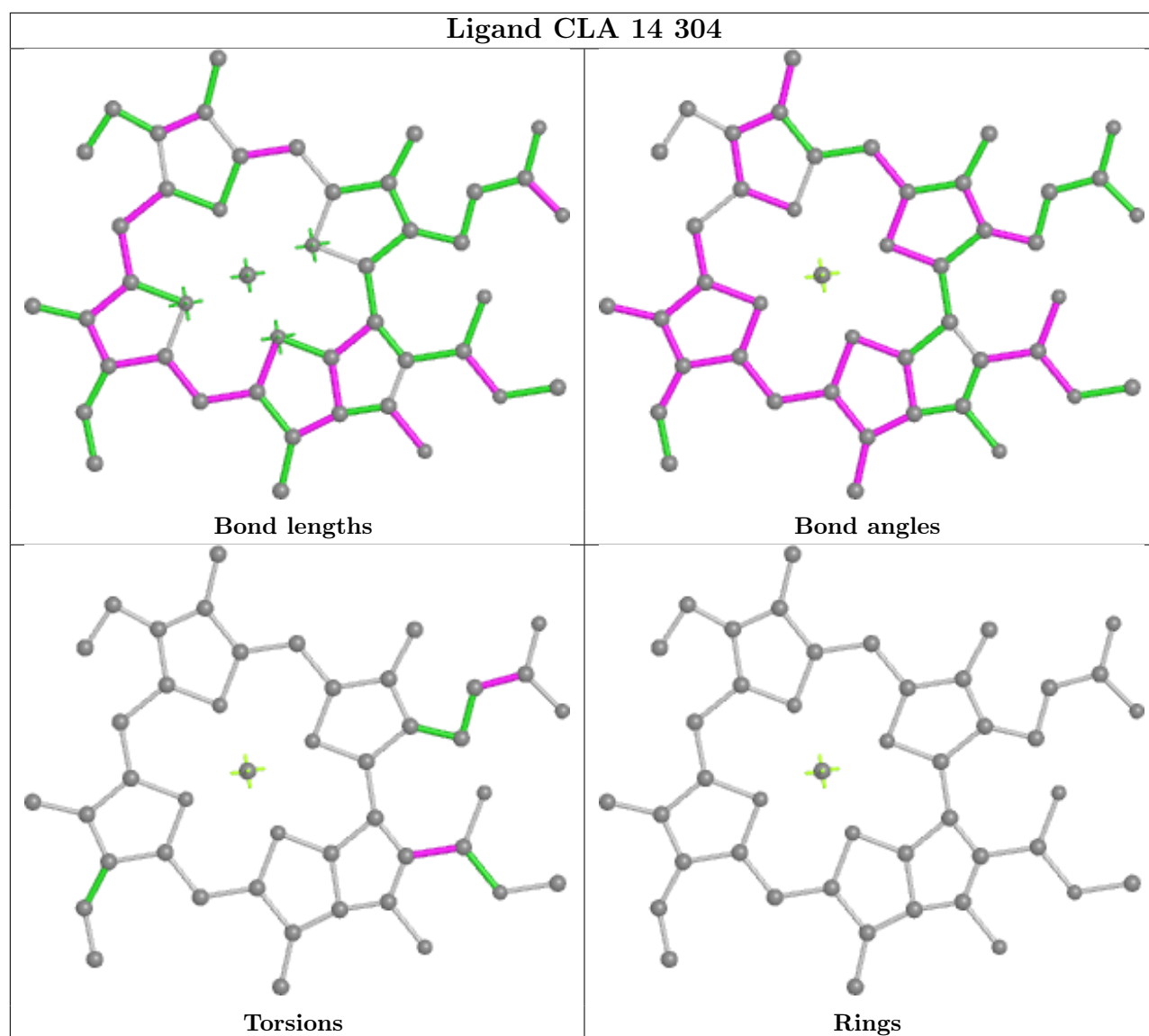


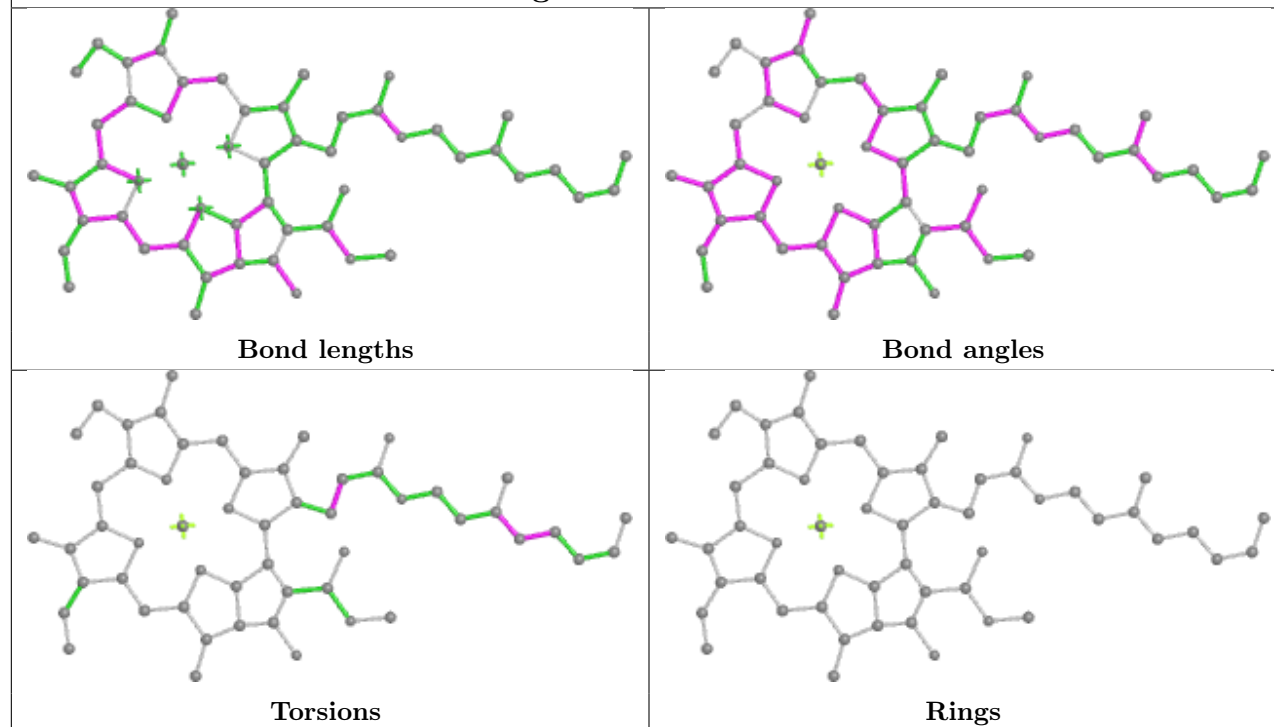
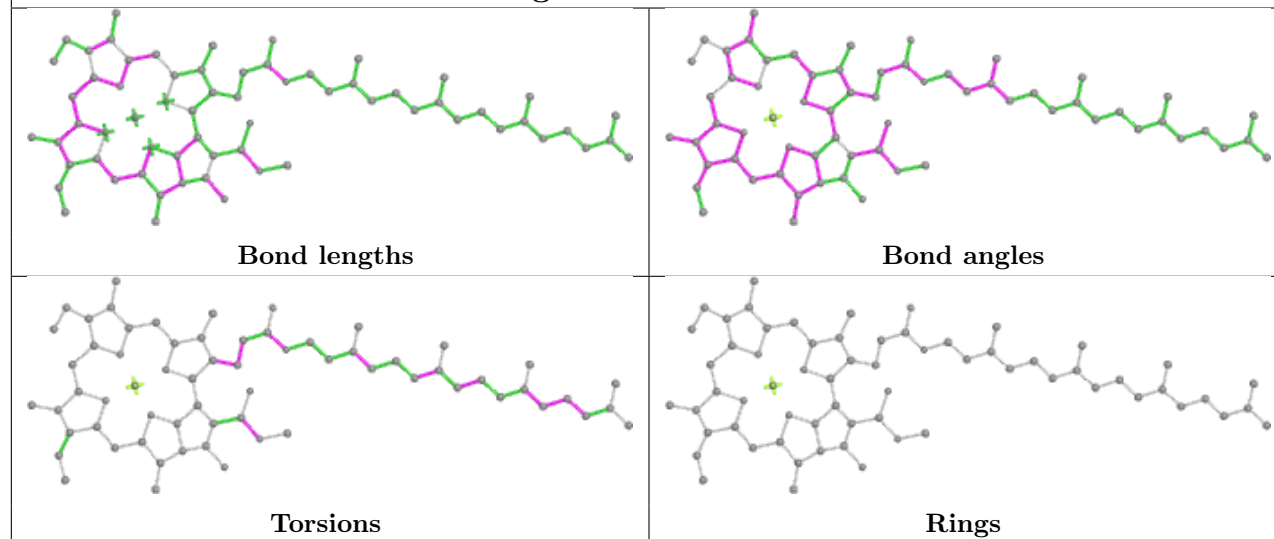
Torsions



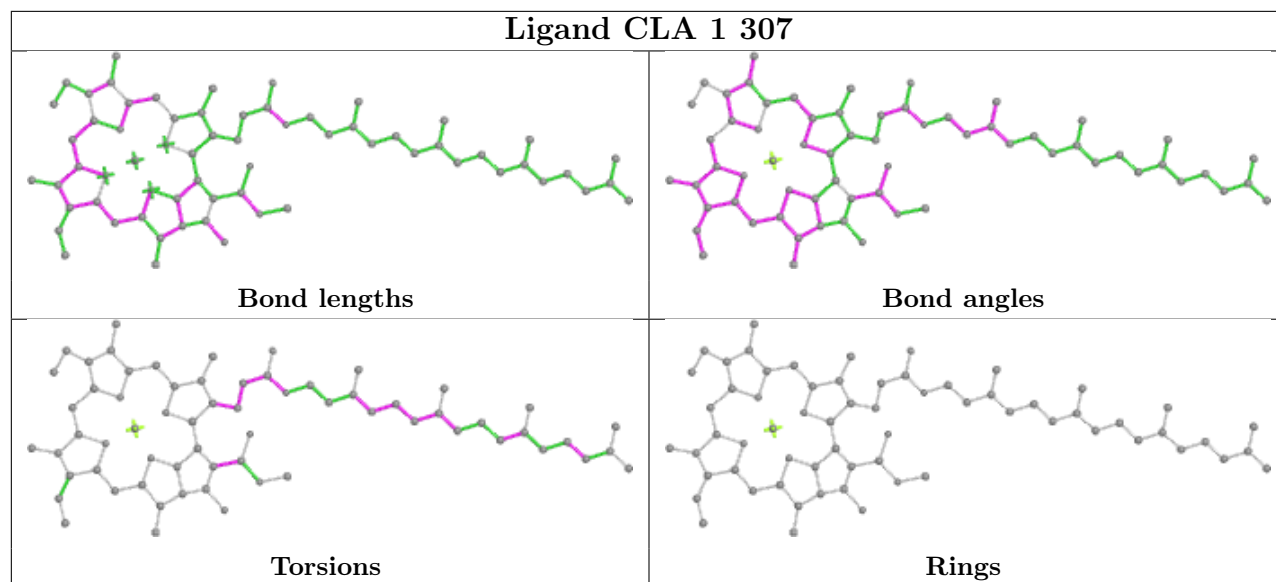
Rings



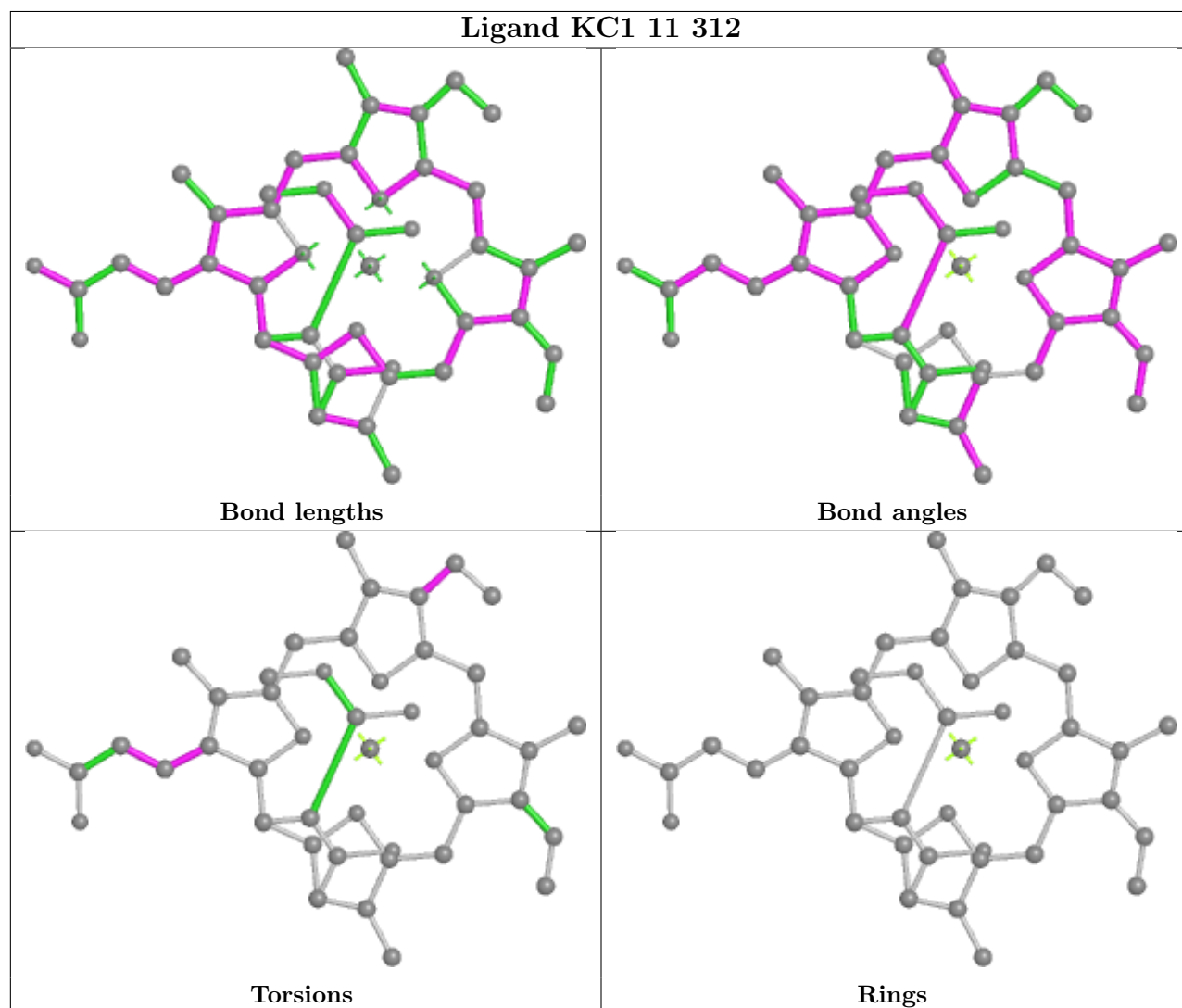


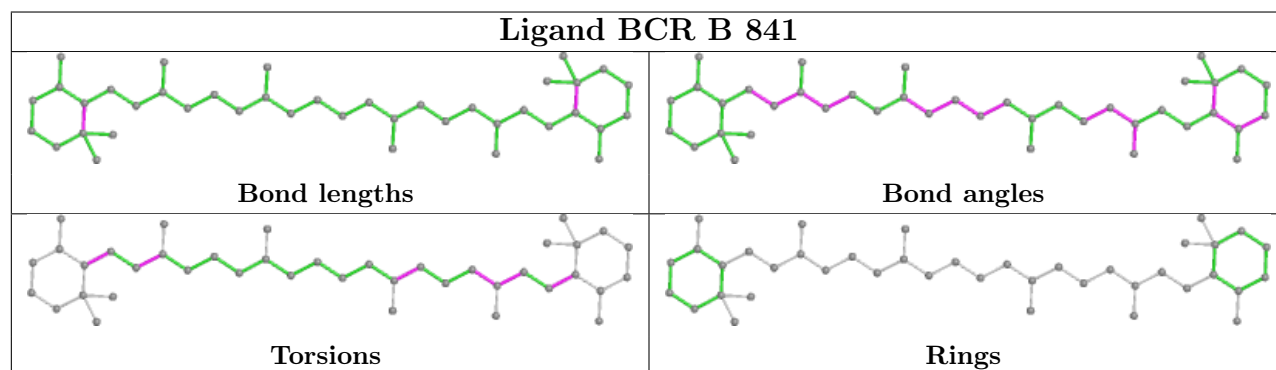
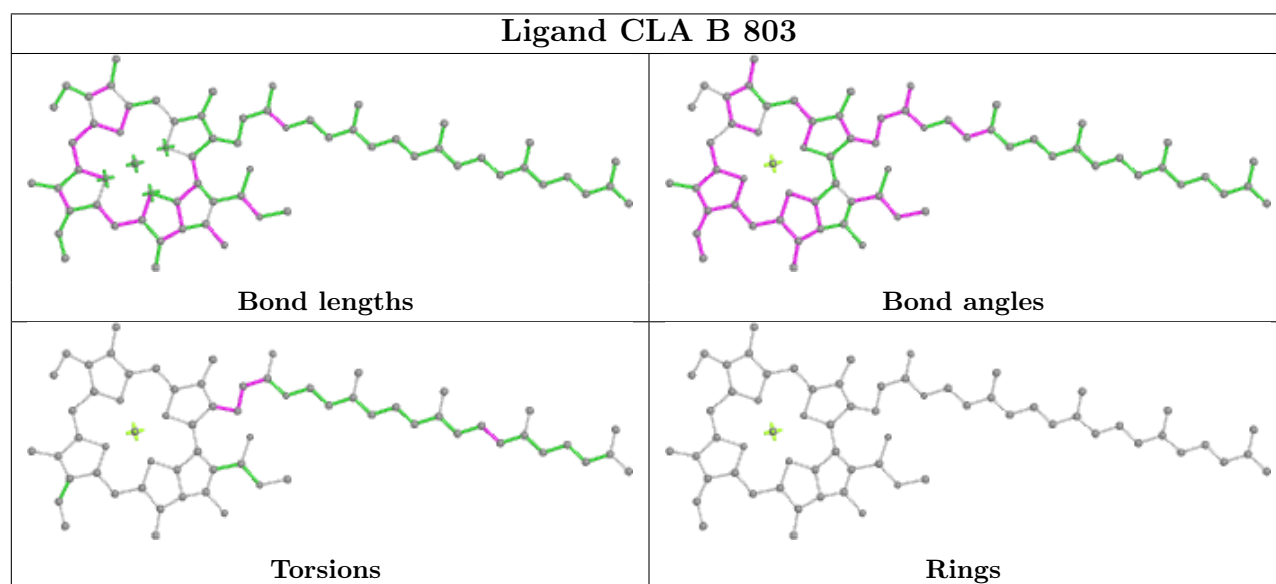
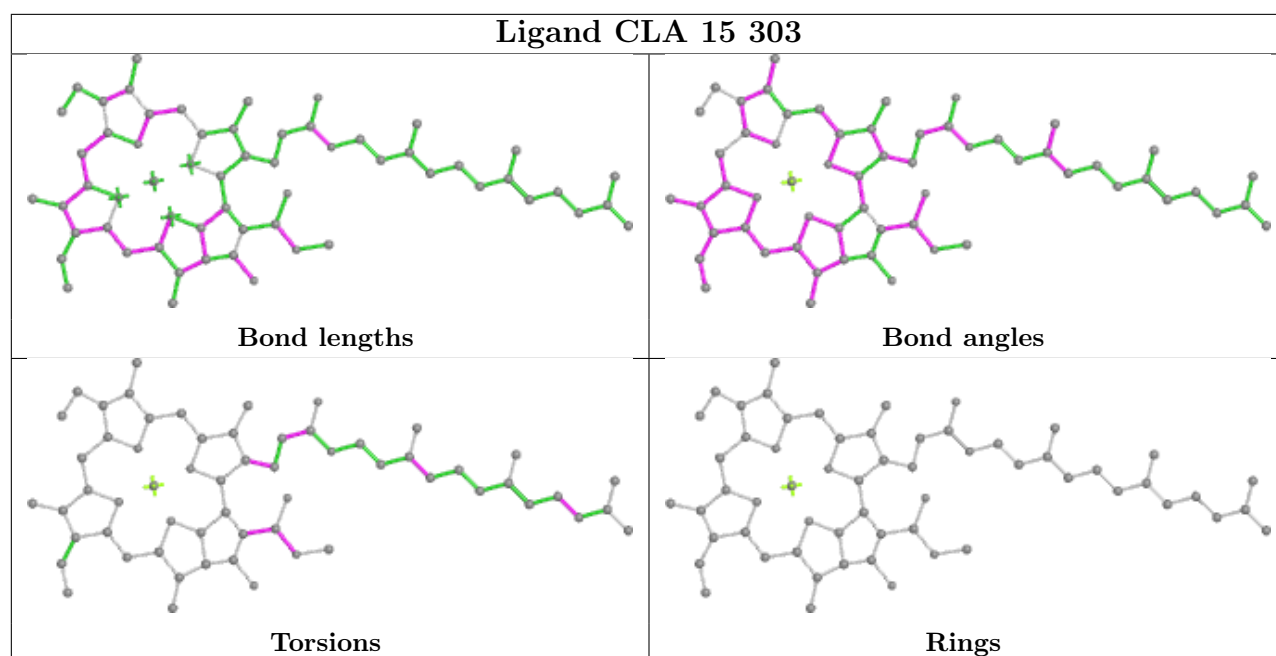
Ligand CLA B 823**Ligand CLA B 826**

Ligand CLA 1 307

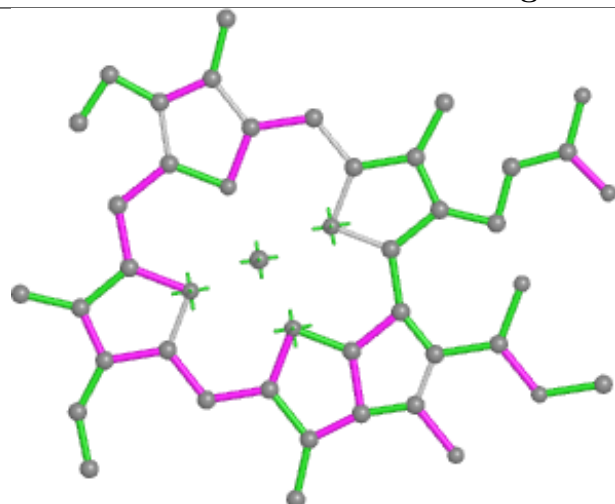


Ligand KC1 11 312

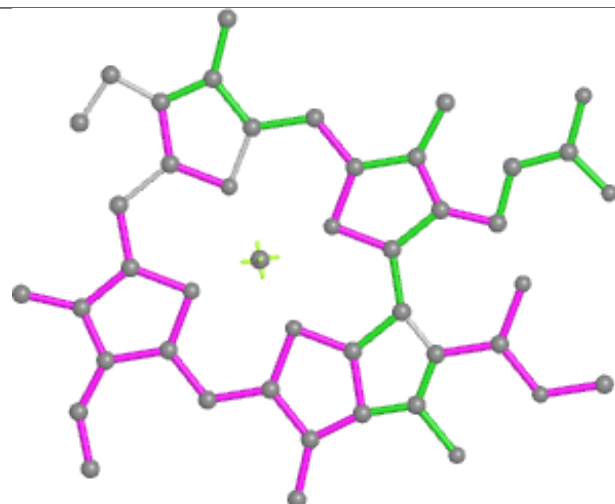




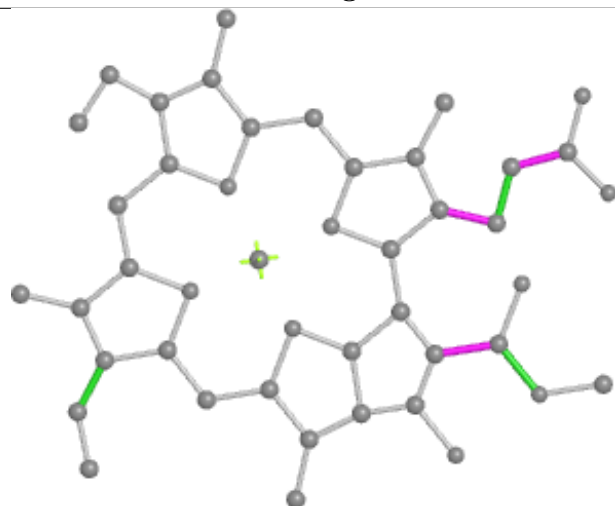
Ligand CLA 3 310



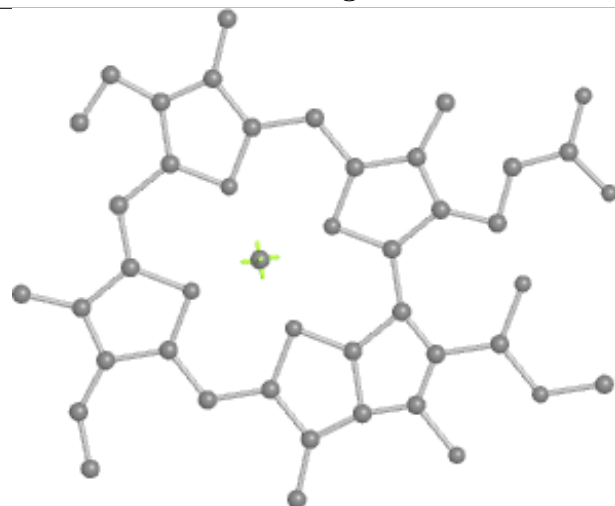
Bond lengths



Bond angles

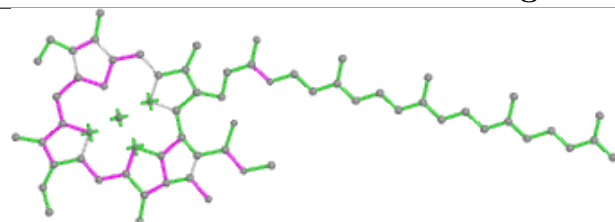


Torsions

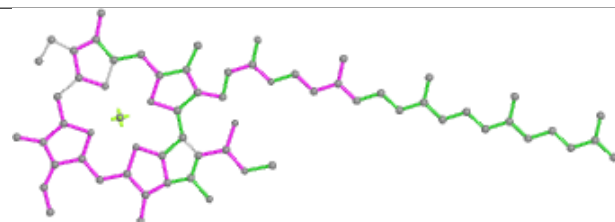


Rings

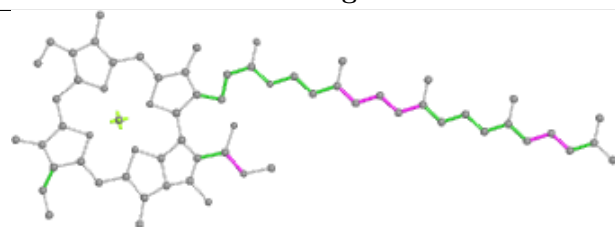
Ligand CLA 8 302



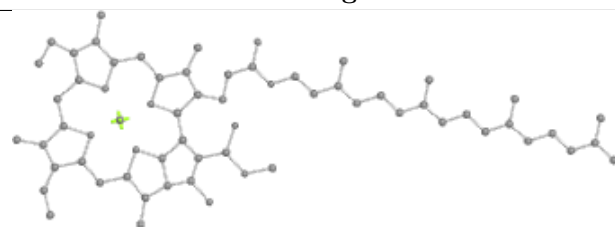
Bond lengths



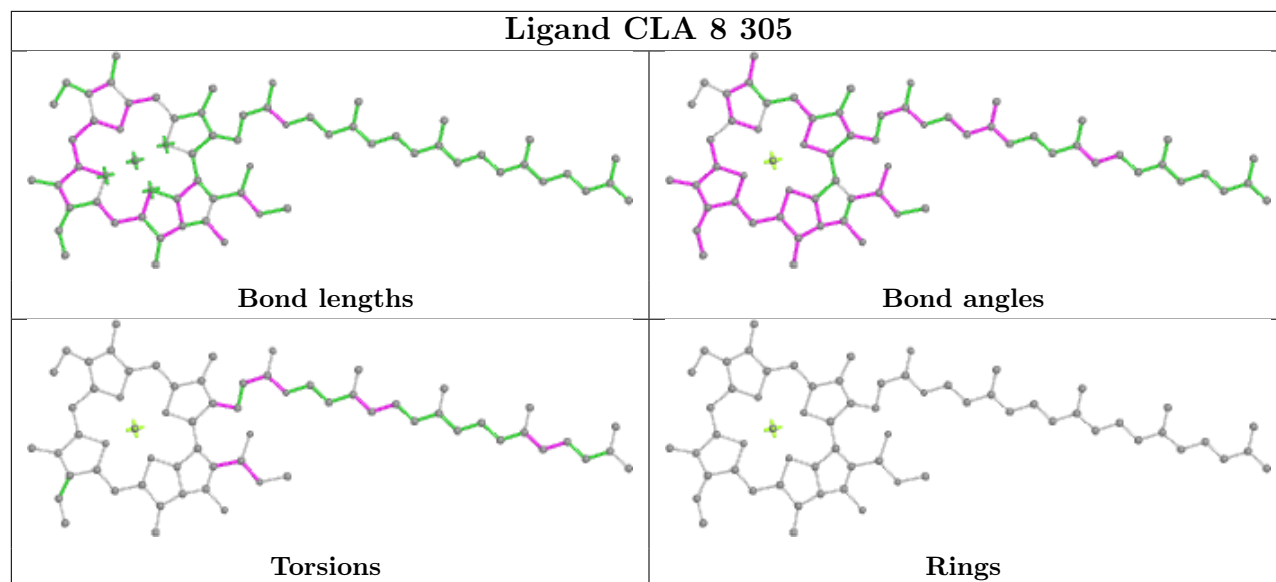
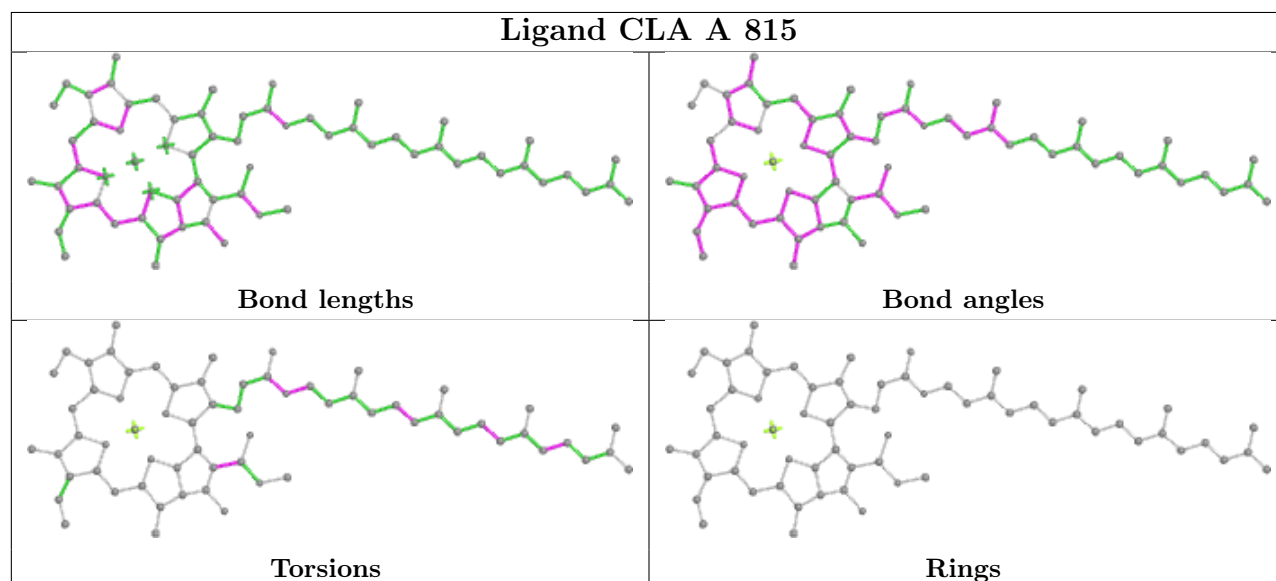
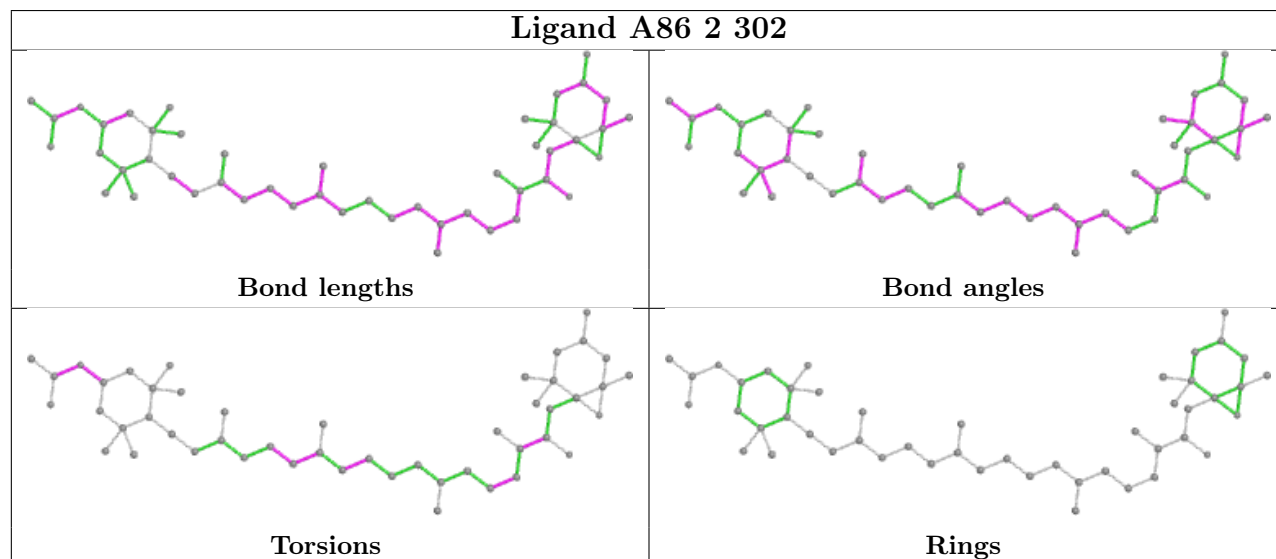
Bond angles



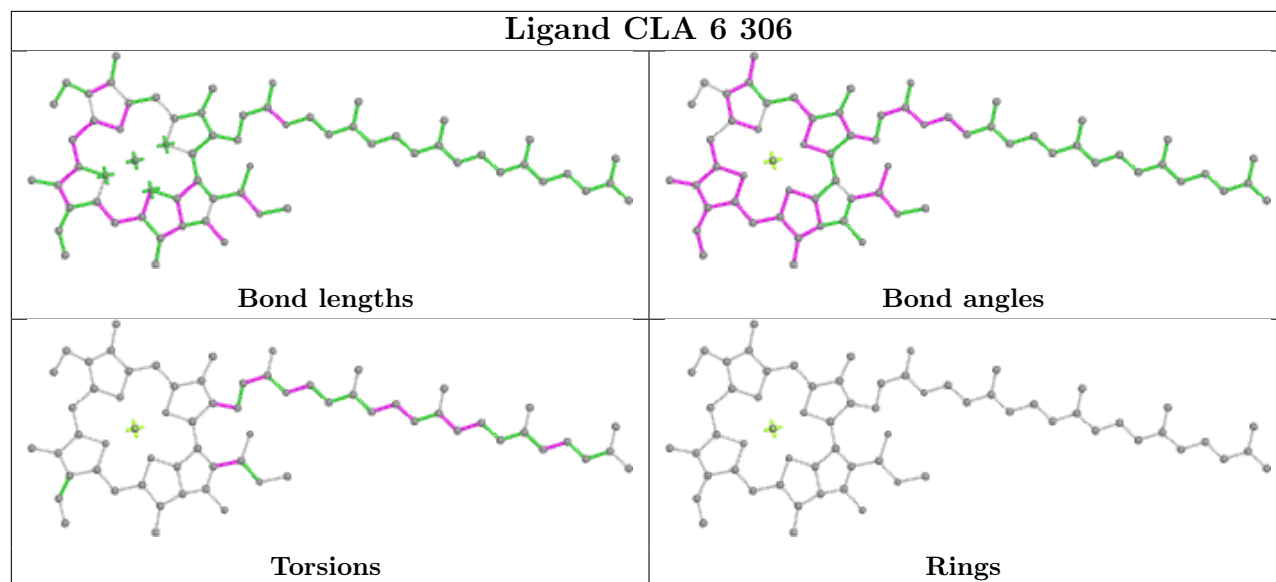
Torsions



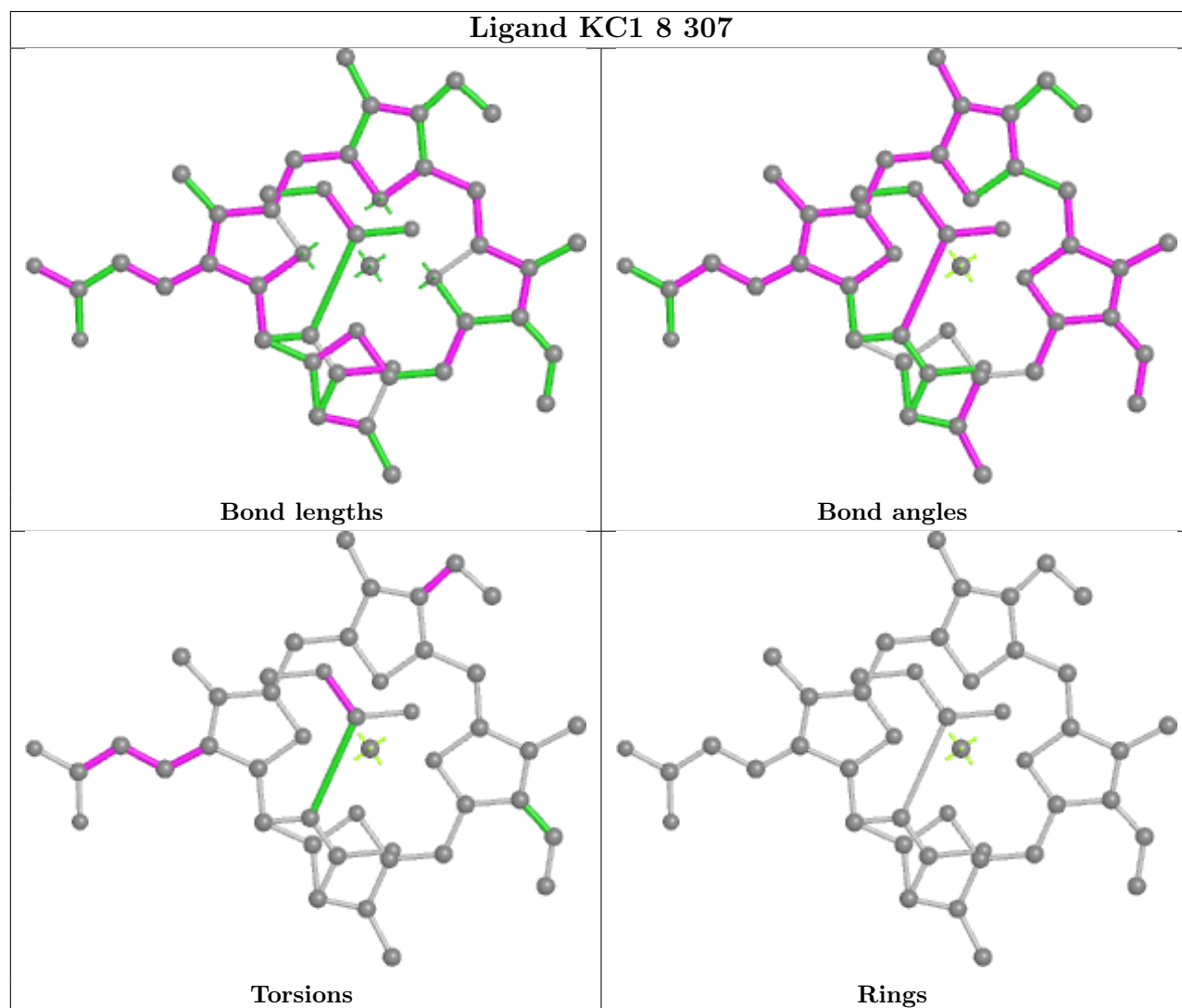
Rings

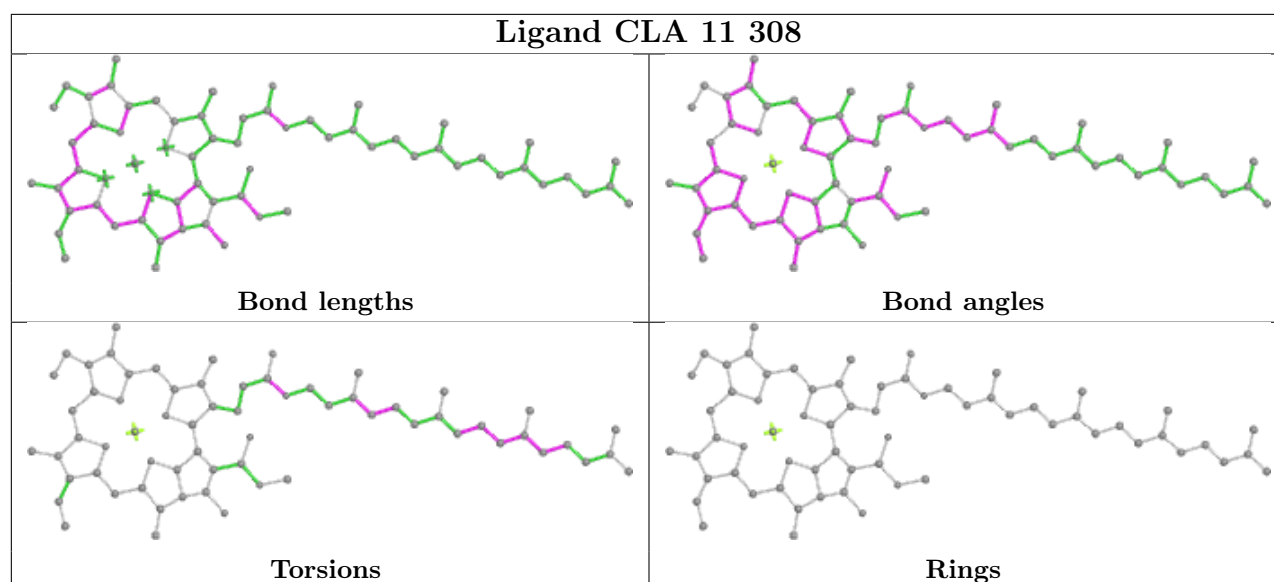
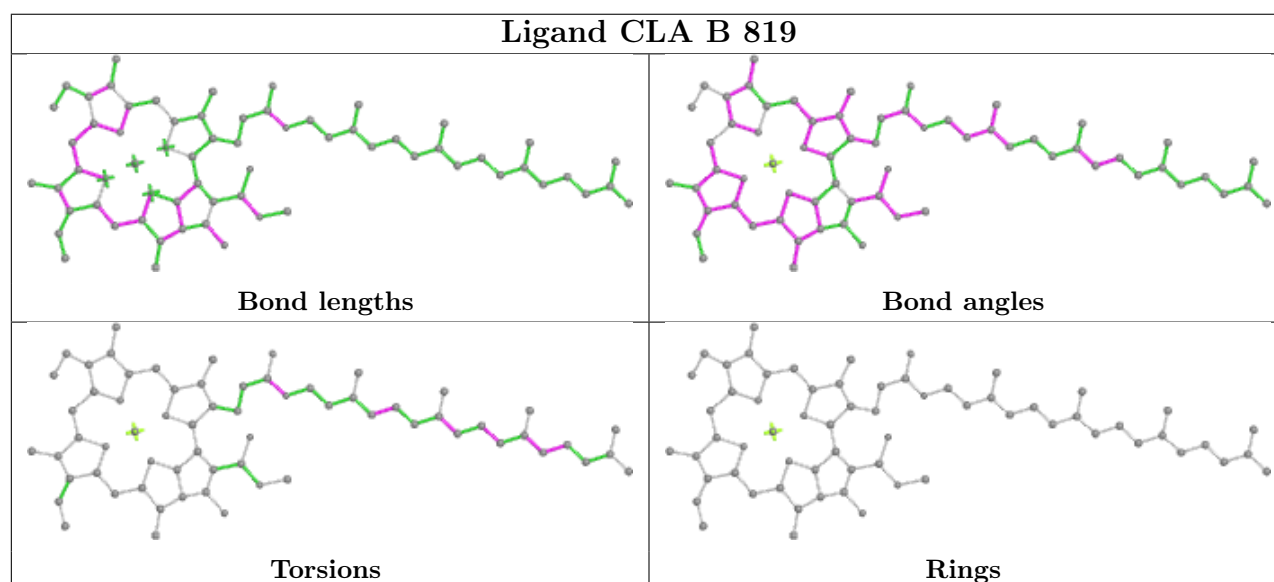
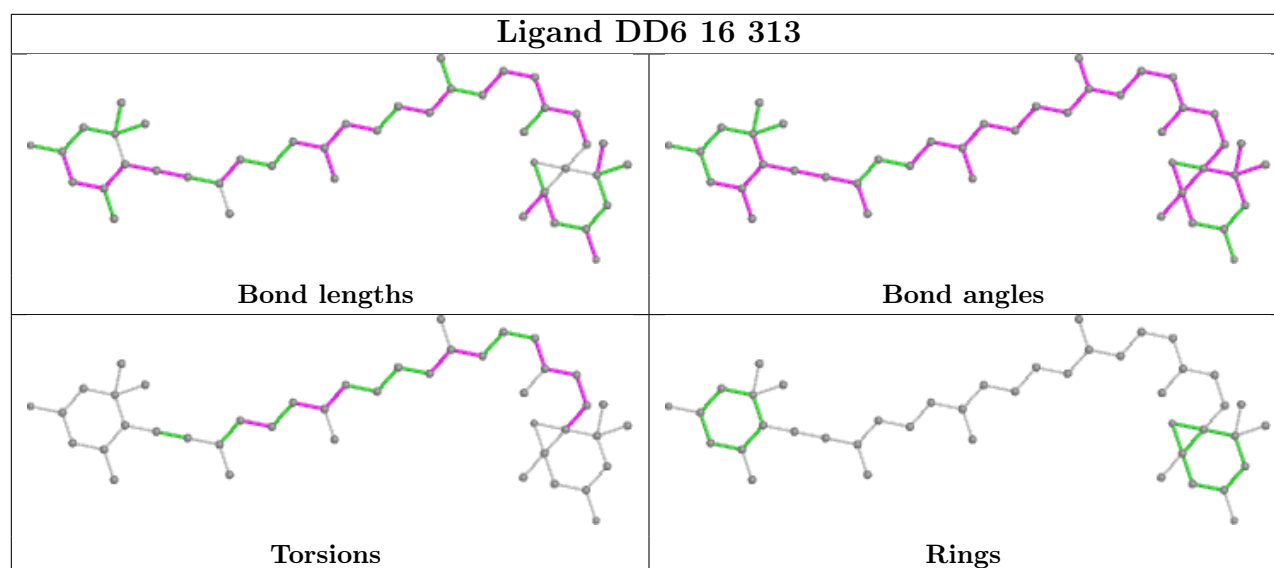
Ligand CLA 8 305**Ligand CLA A 815****Ligand A86 2 302**

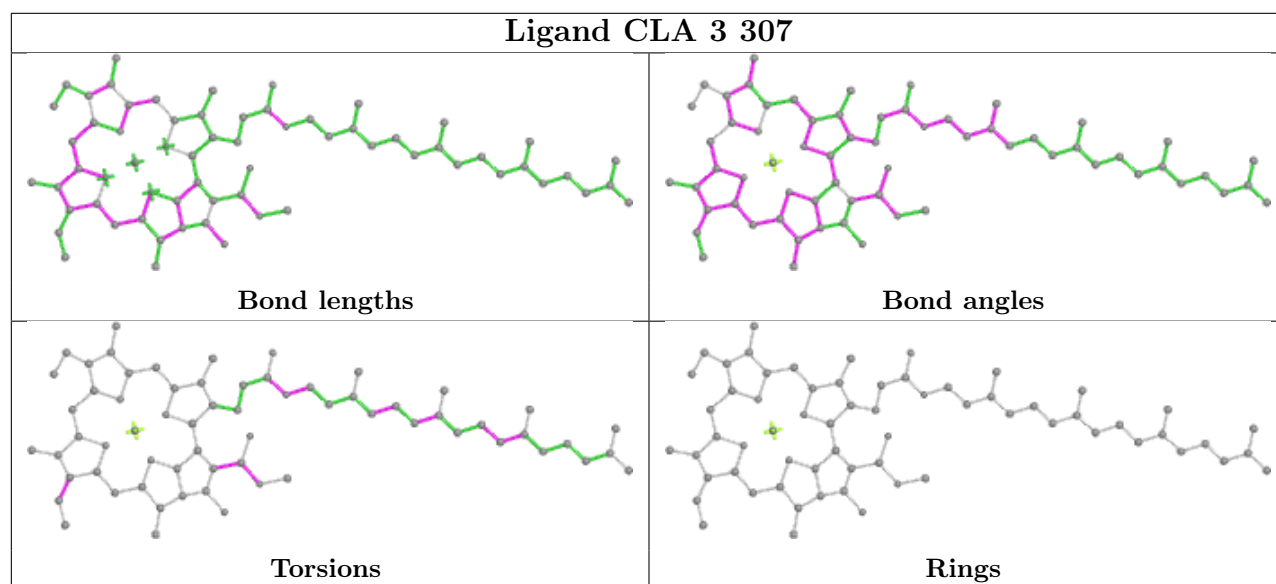
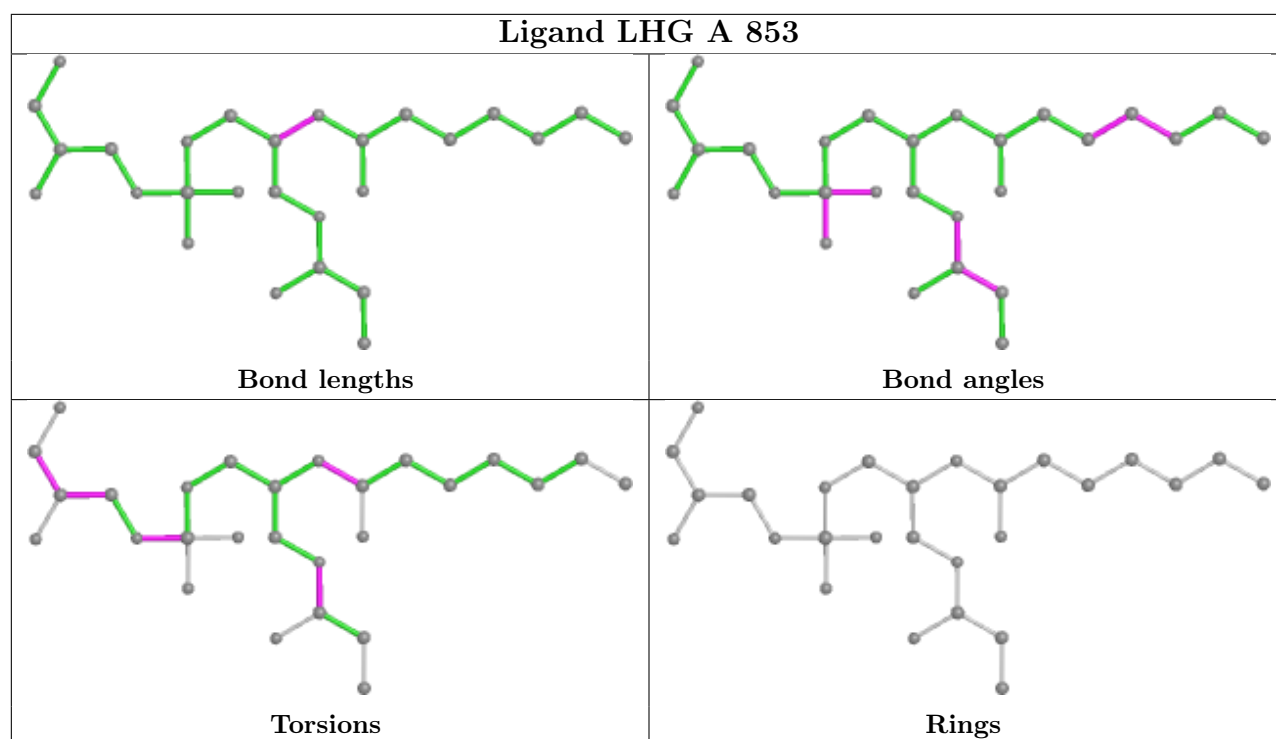
Ligand CLA 6 306

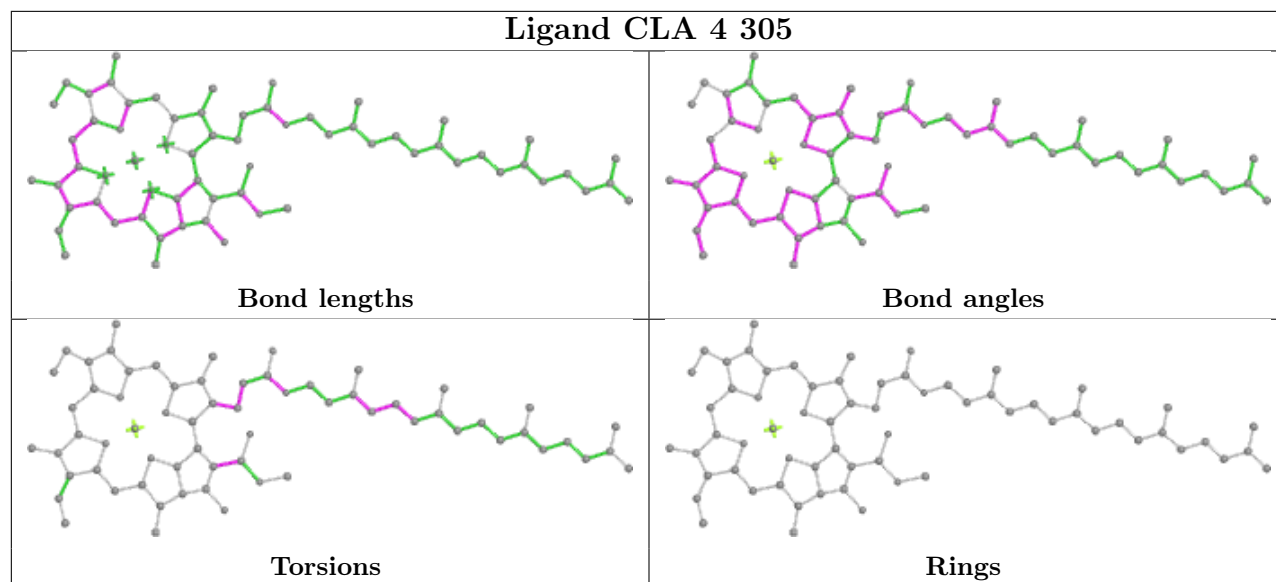
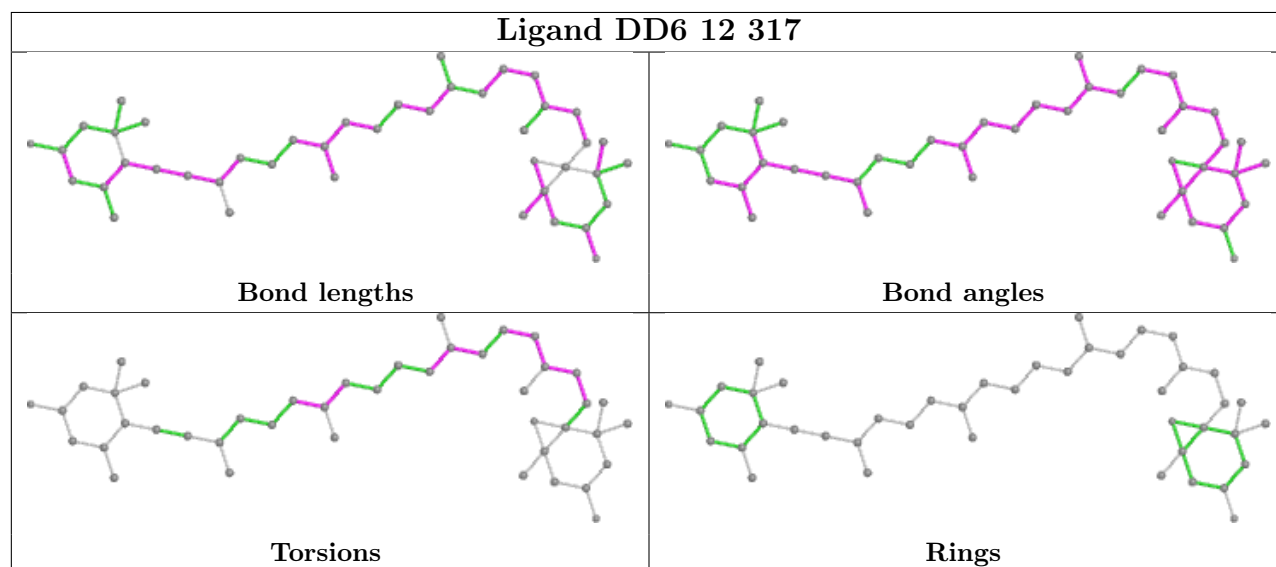


Ligand KC1 8 307

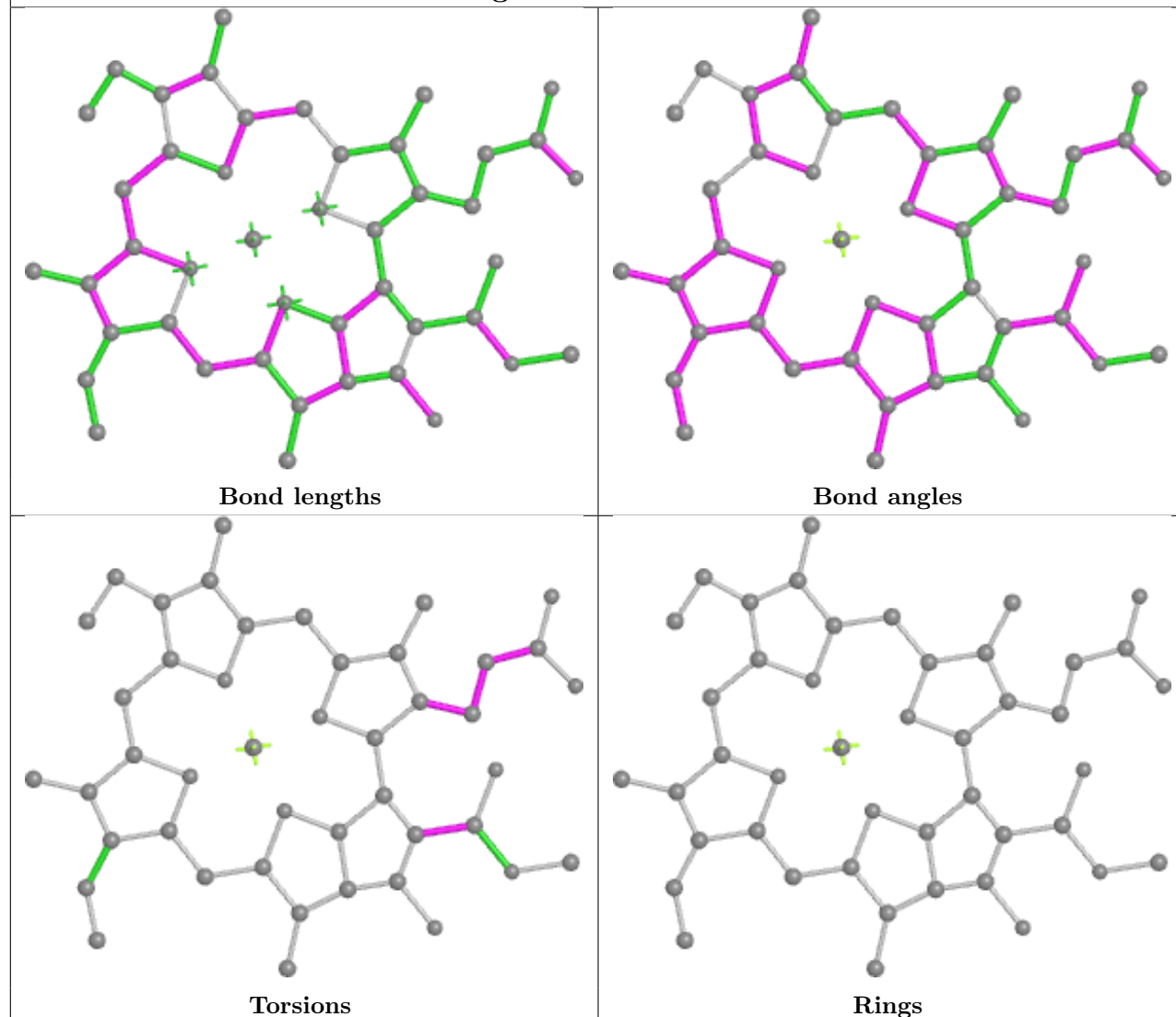




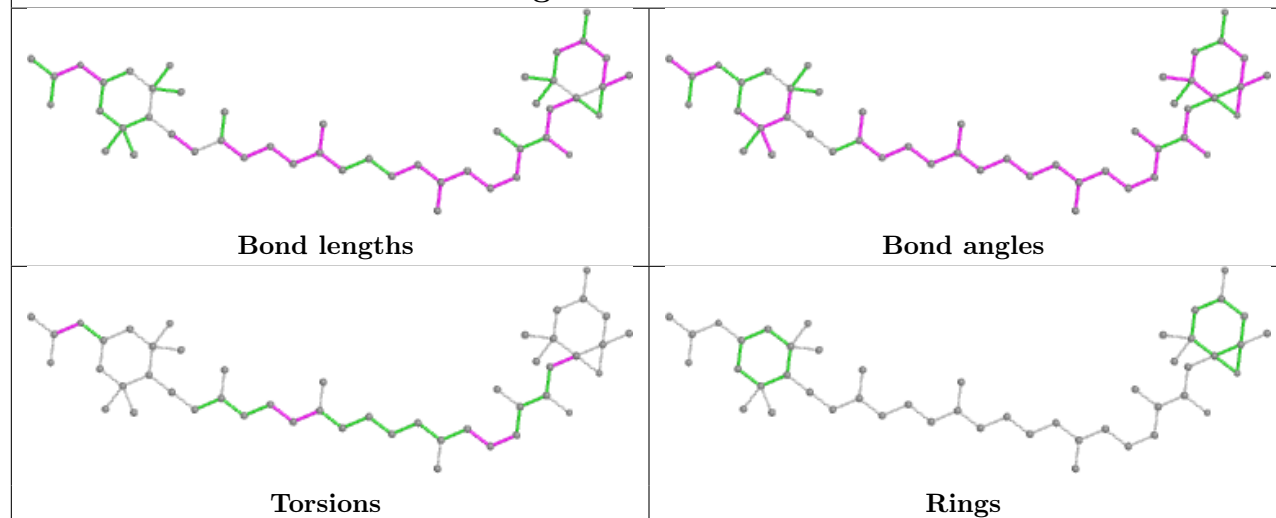


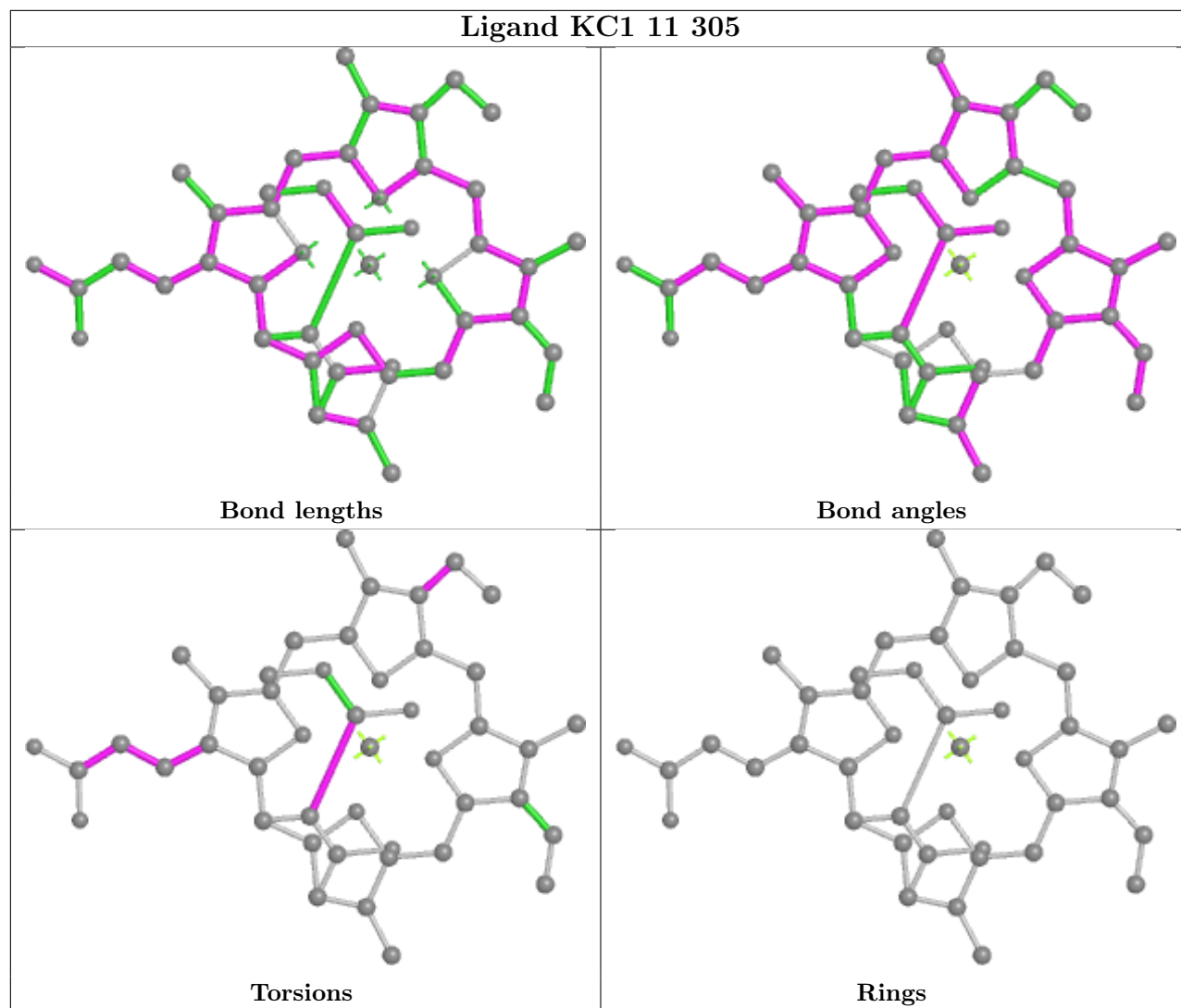
Ligand CLA 4 305**Ligand DD6 12 317**

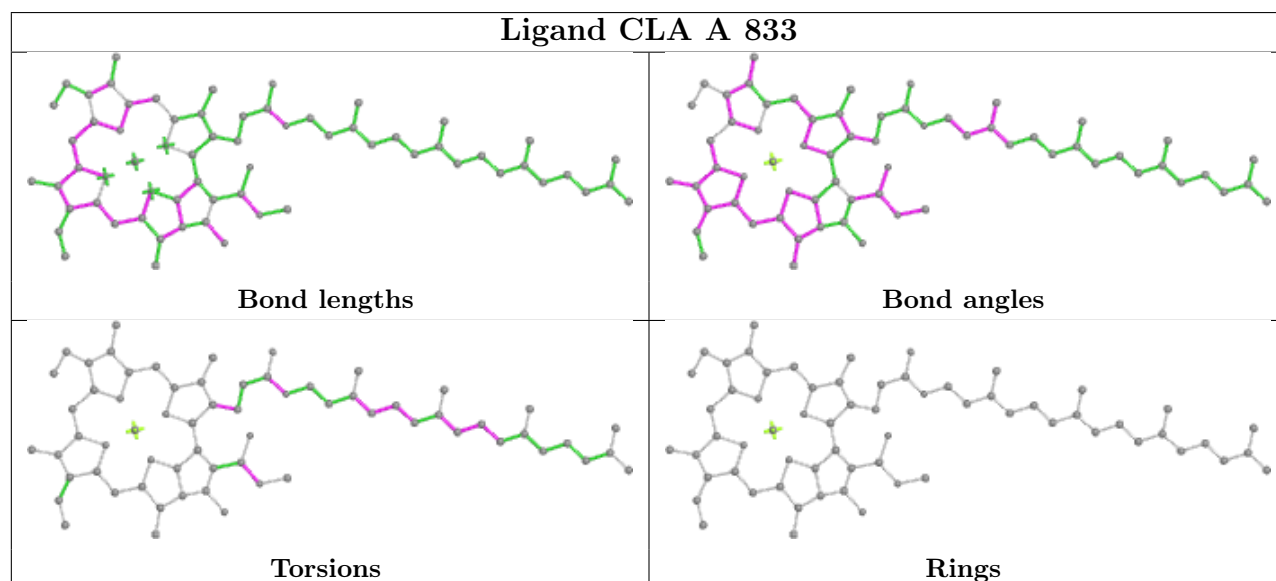
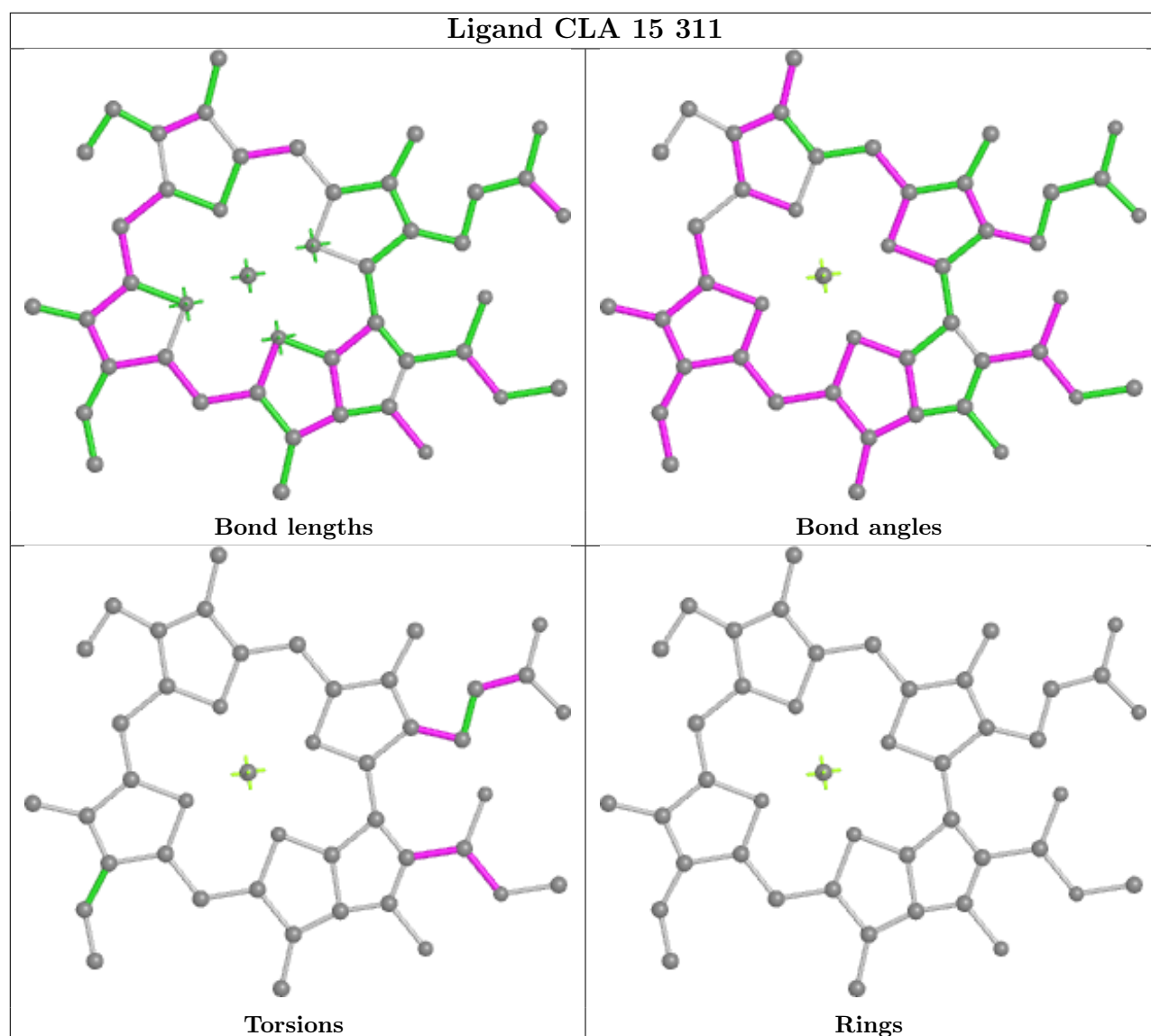
Ligand CLA F 203



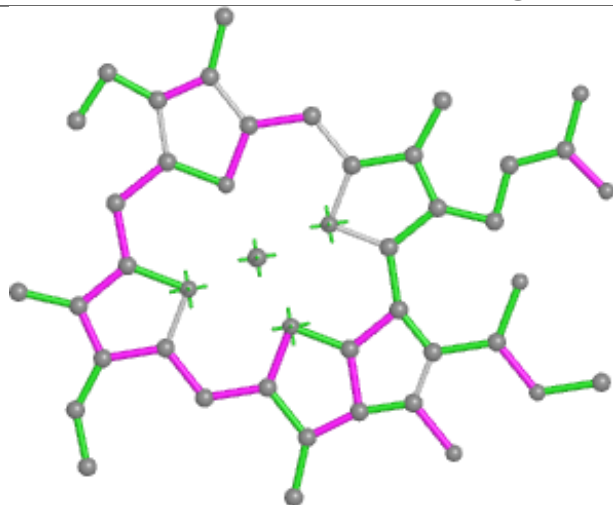
Ligand A86 15 315



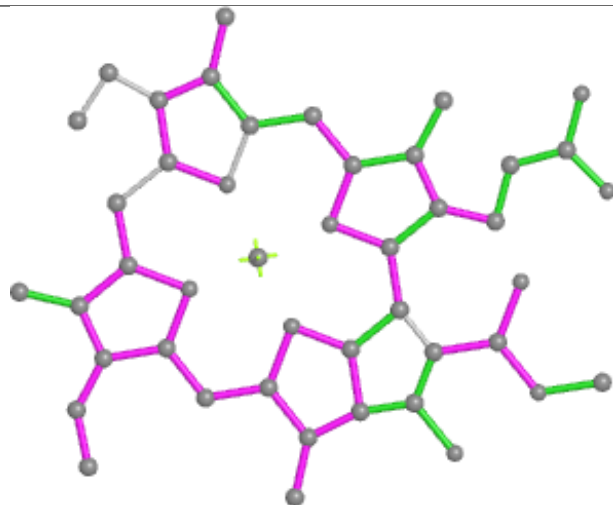




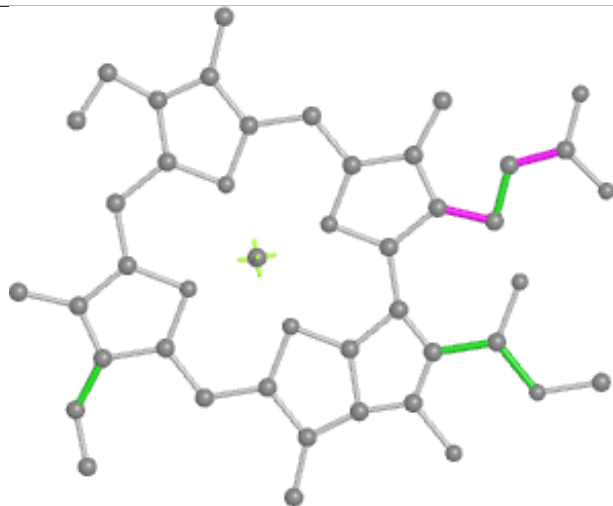
Ligand CLA 14 309



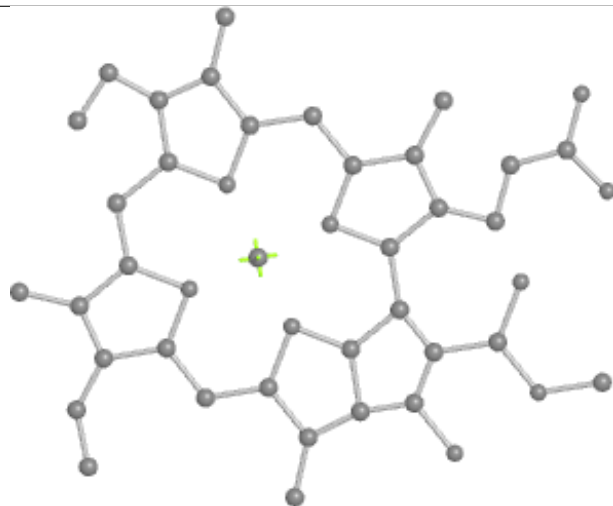
Bond lengths



Bond angles

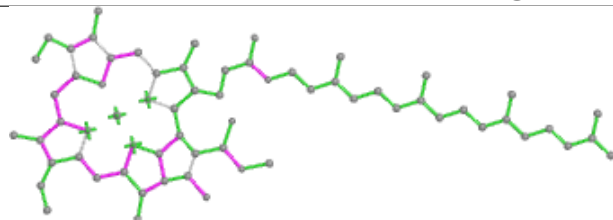


Torsions

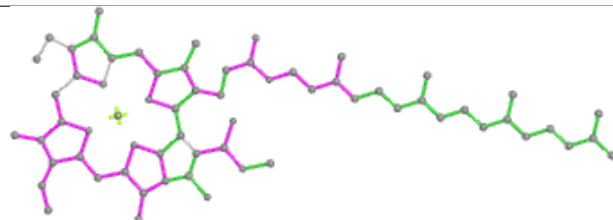


Rings

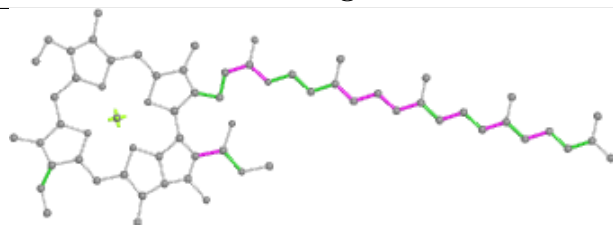
Ligand CLA 2u 202



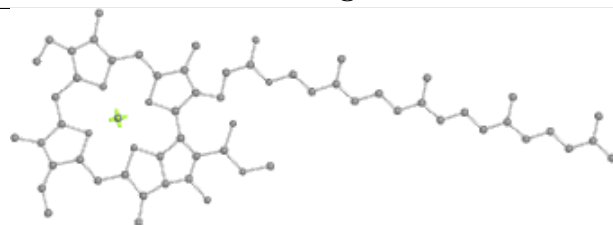
Bond lengths



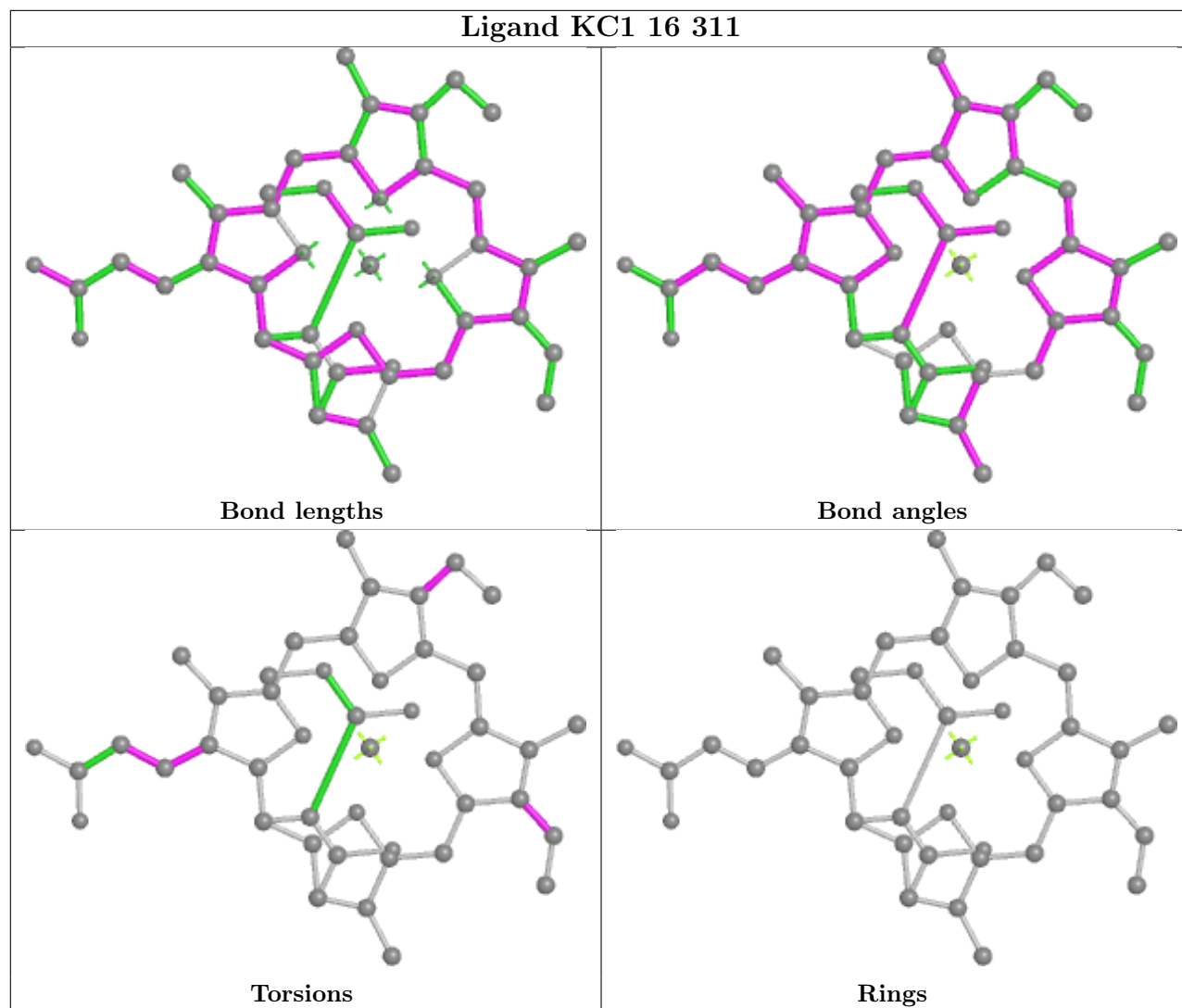
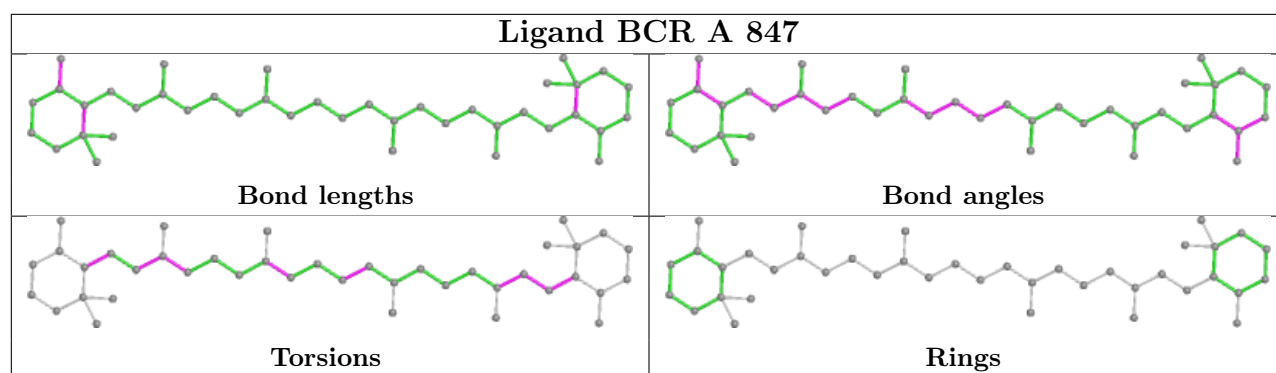
Bond angles



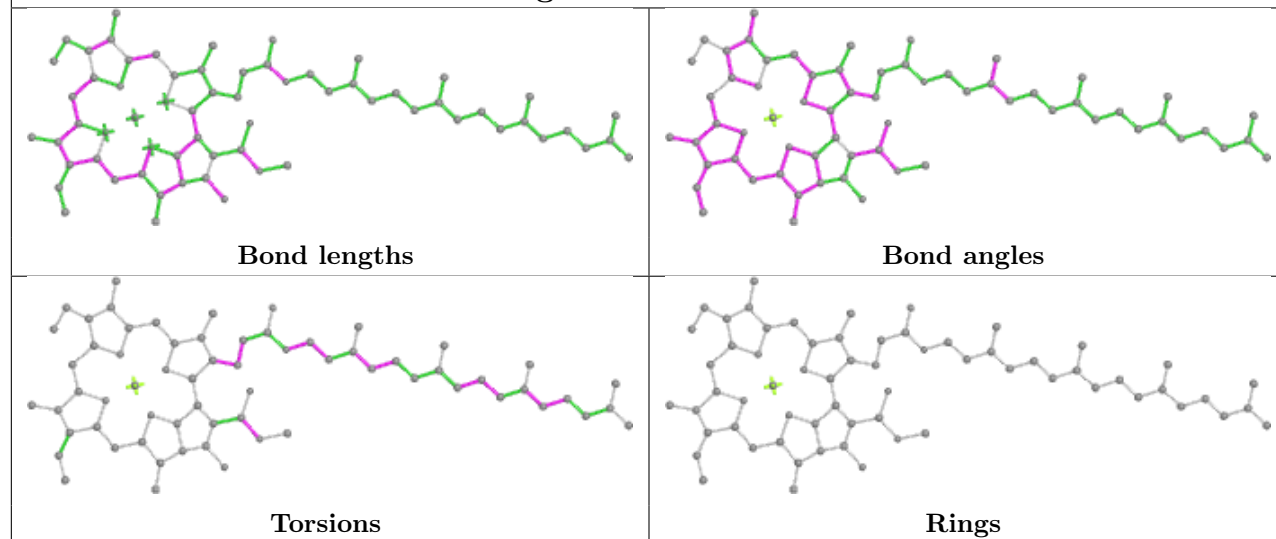
Torsions



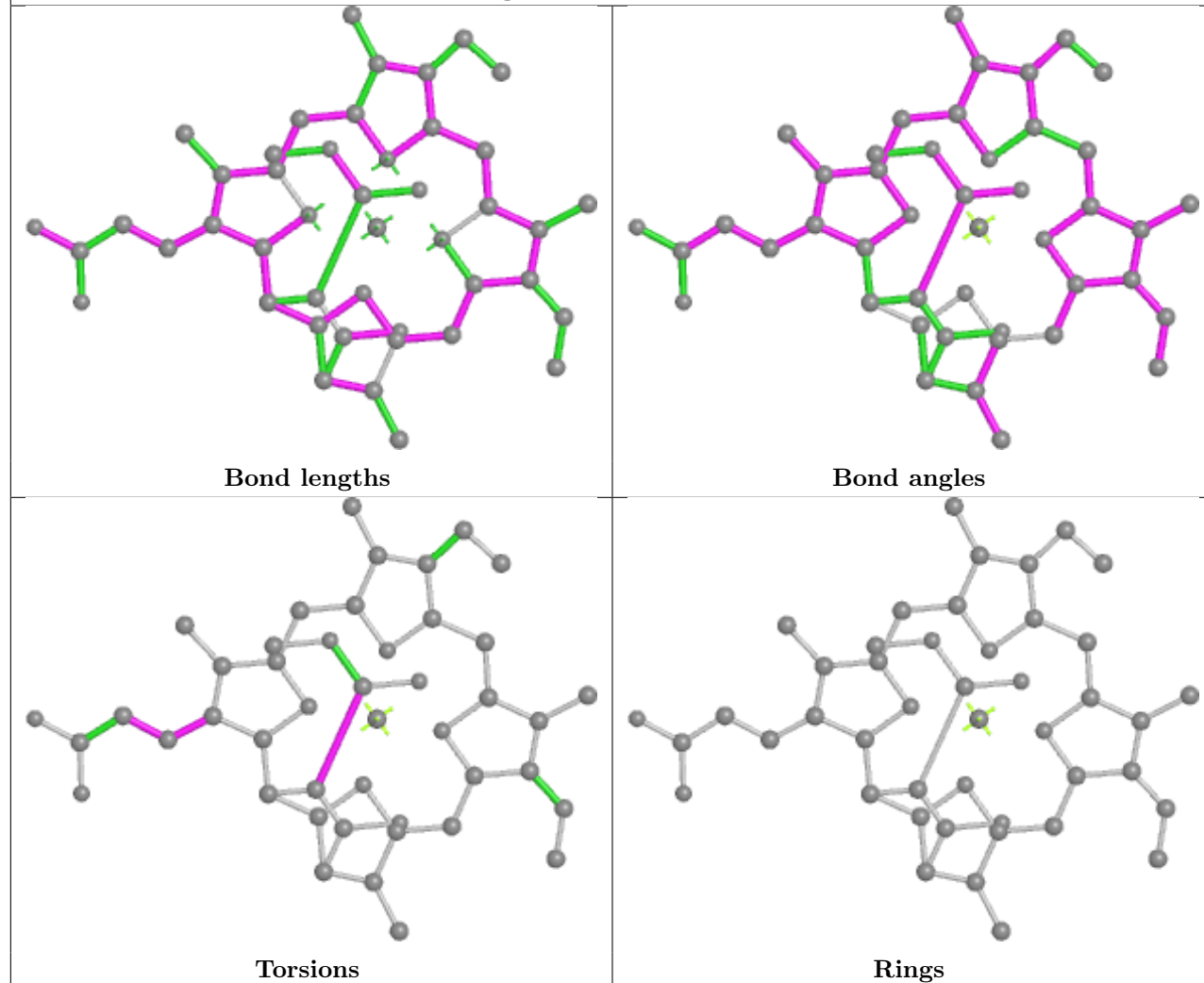
Rings

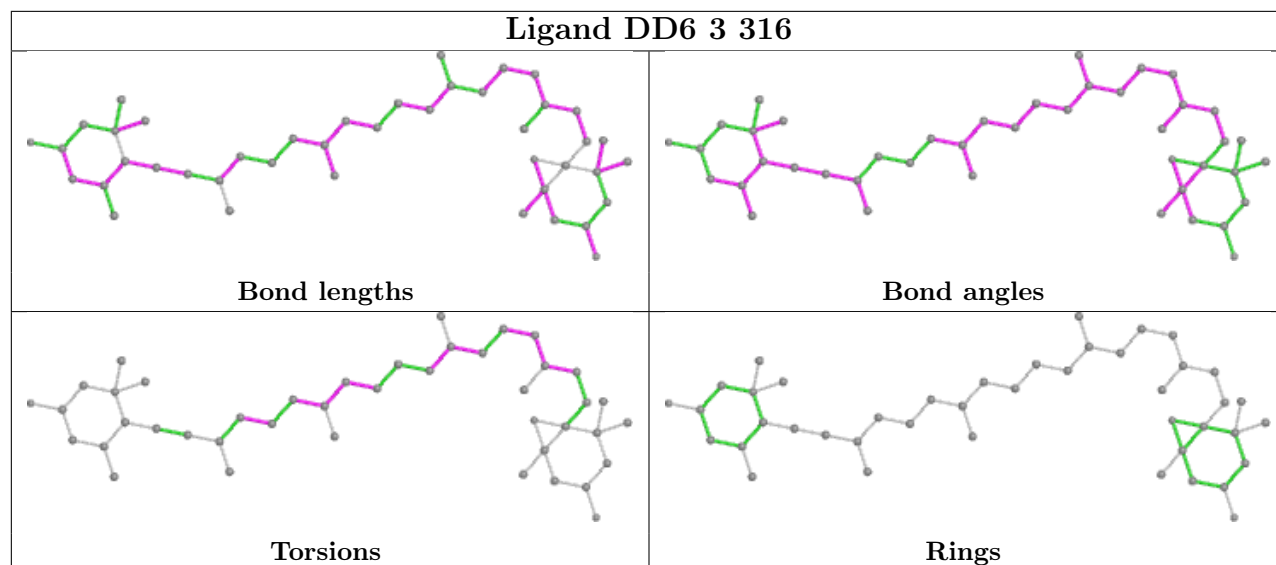
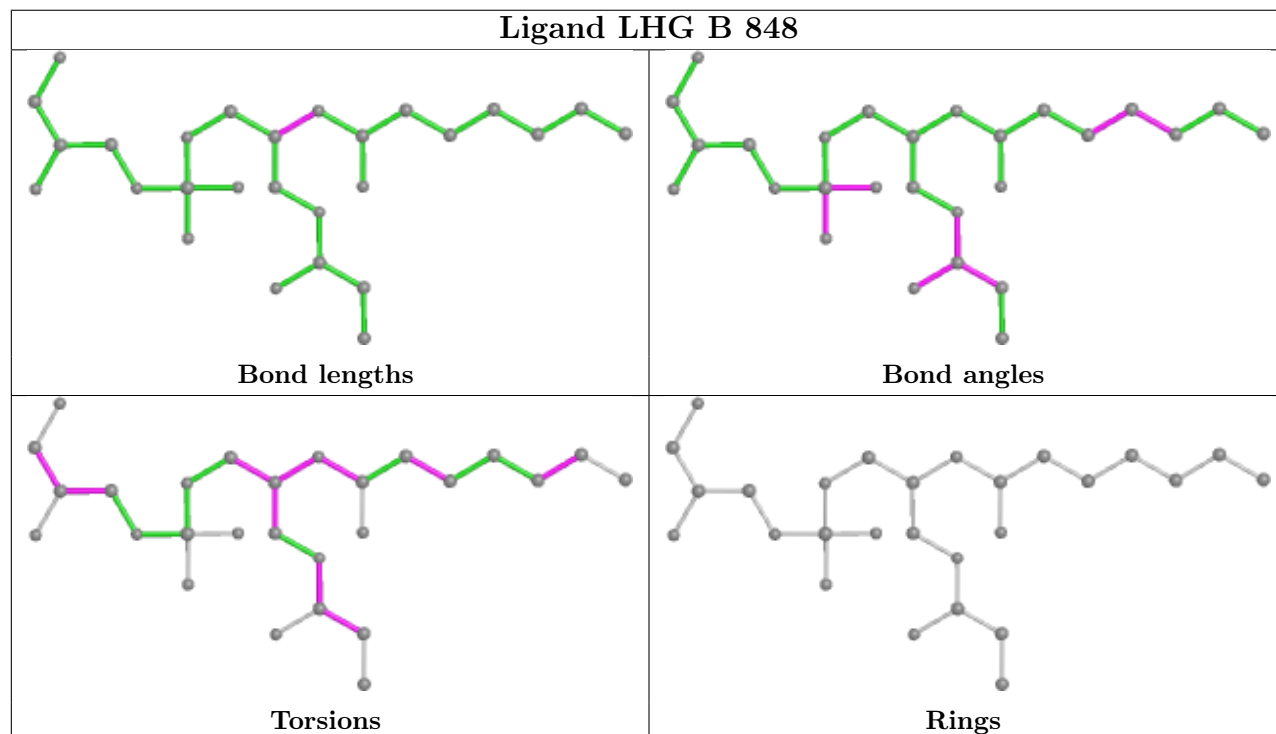


Ligand CLA 6 317

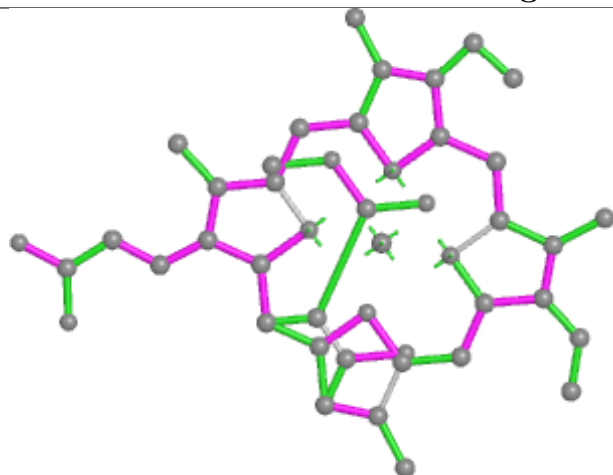


Ligand KC1 13 311

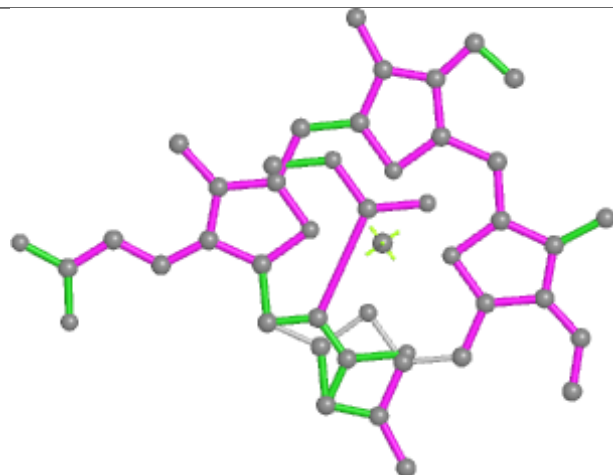


Ligand DD6 3 316**Ligand LHG B 848**

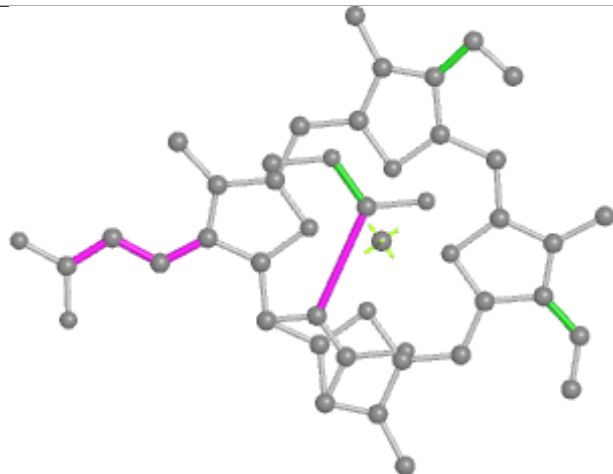
Ligand KC1 5 310



Bond lengths



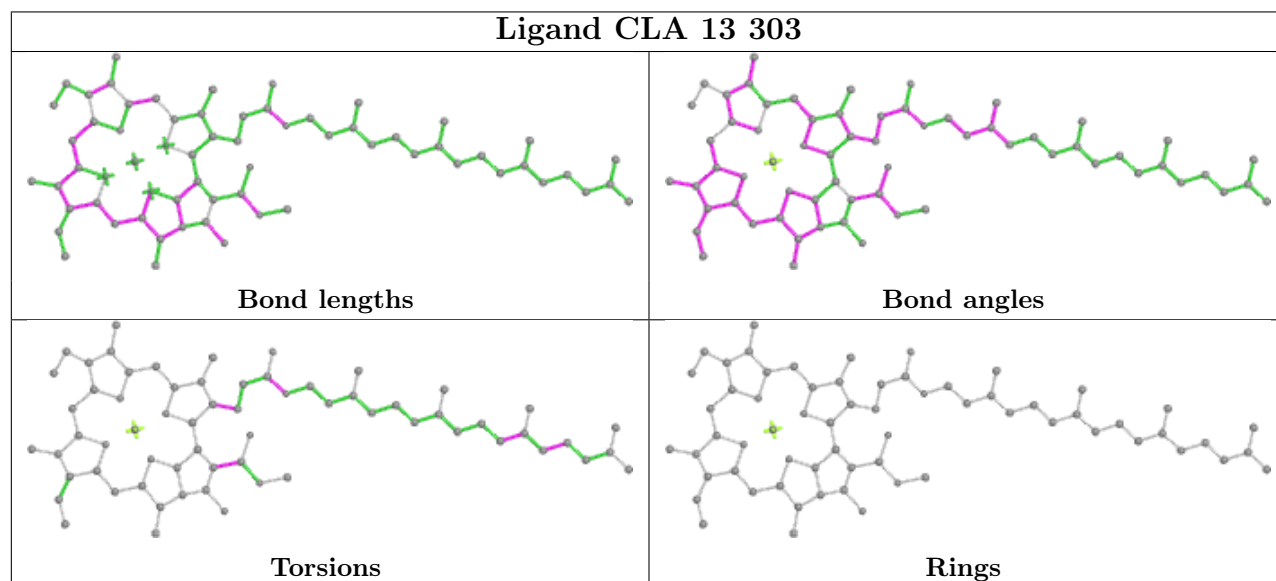
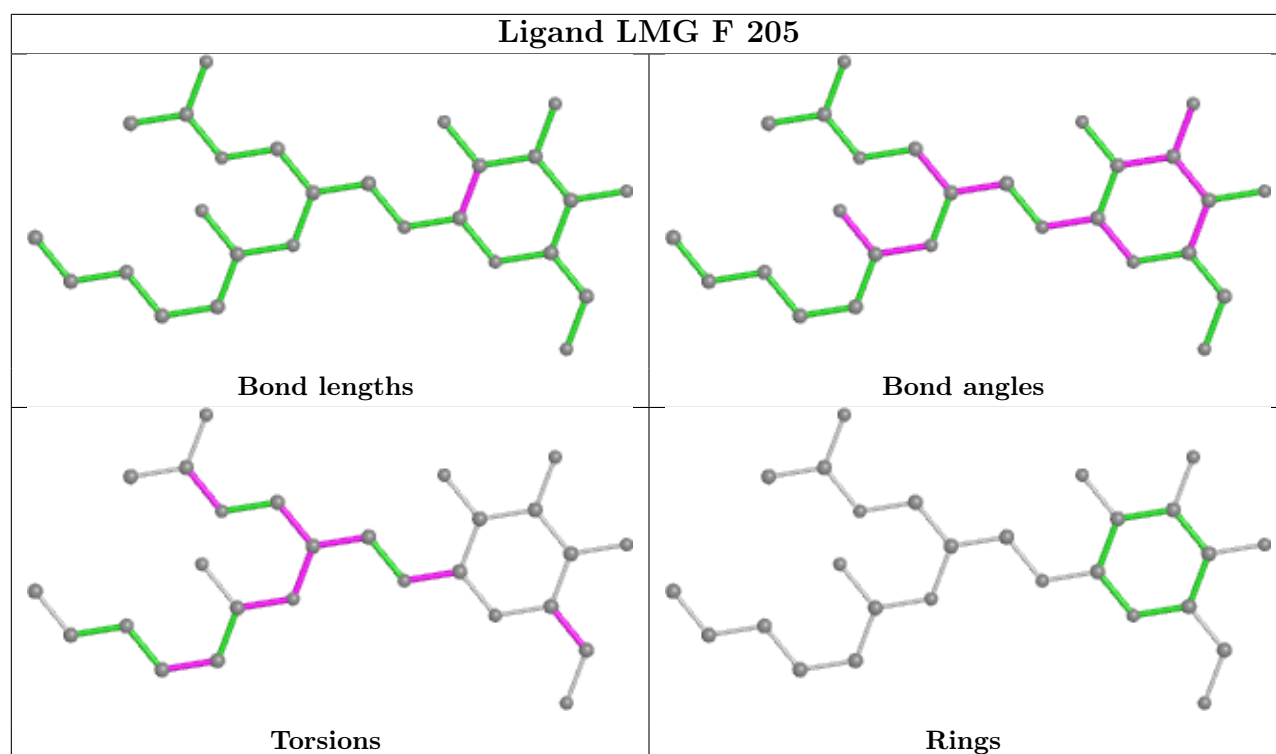
Bond angles

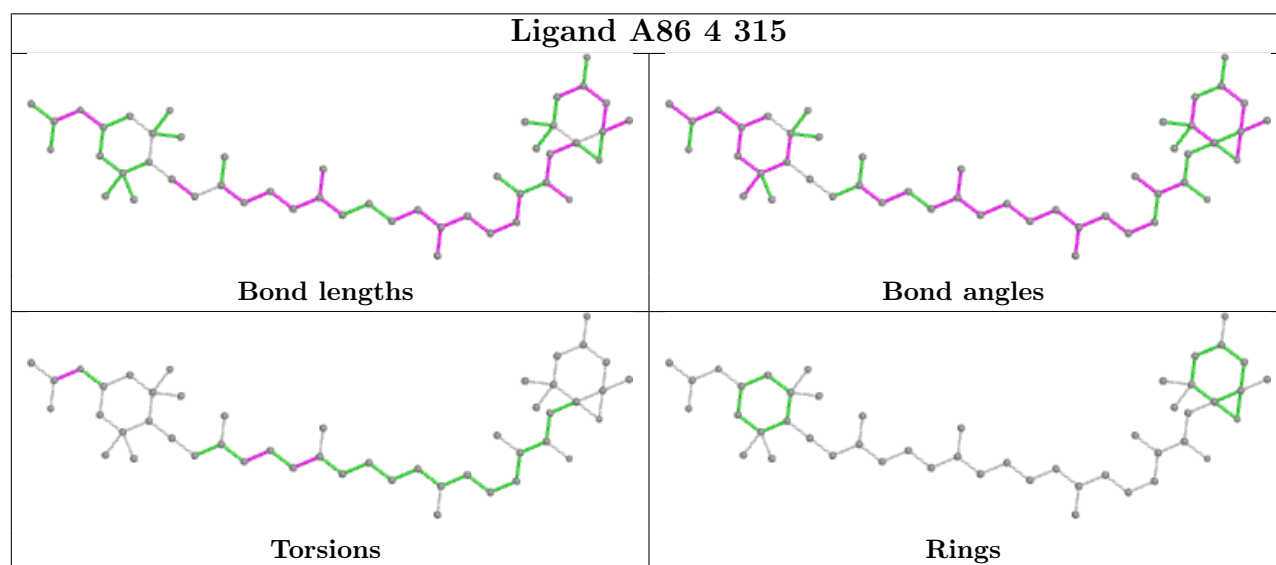
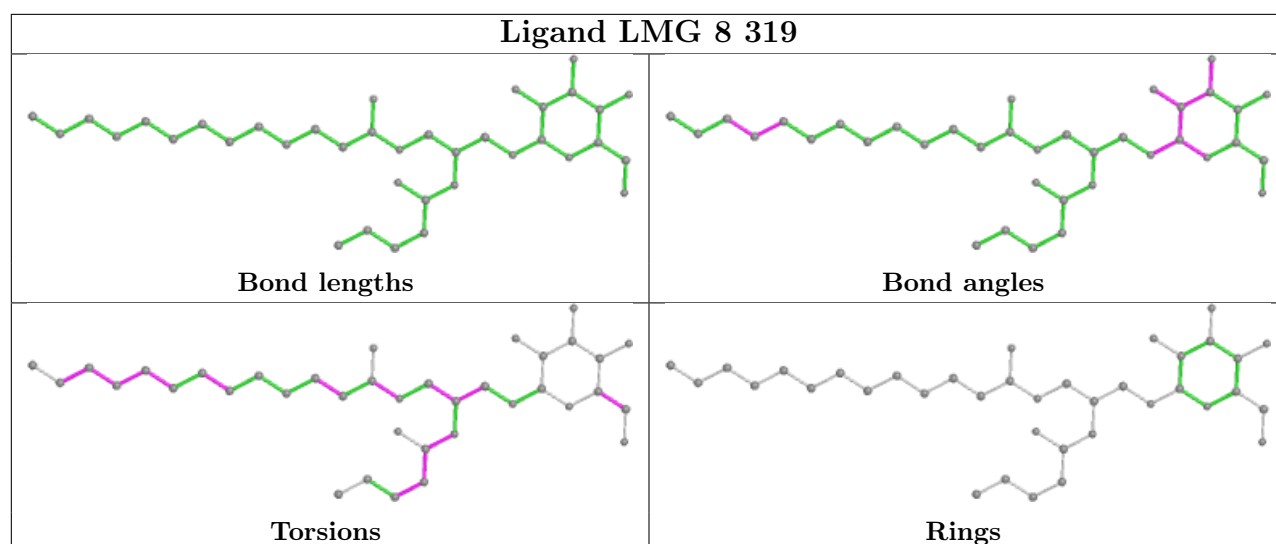


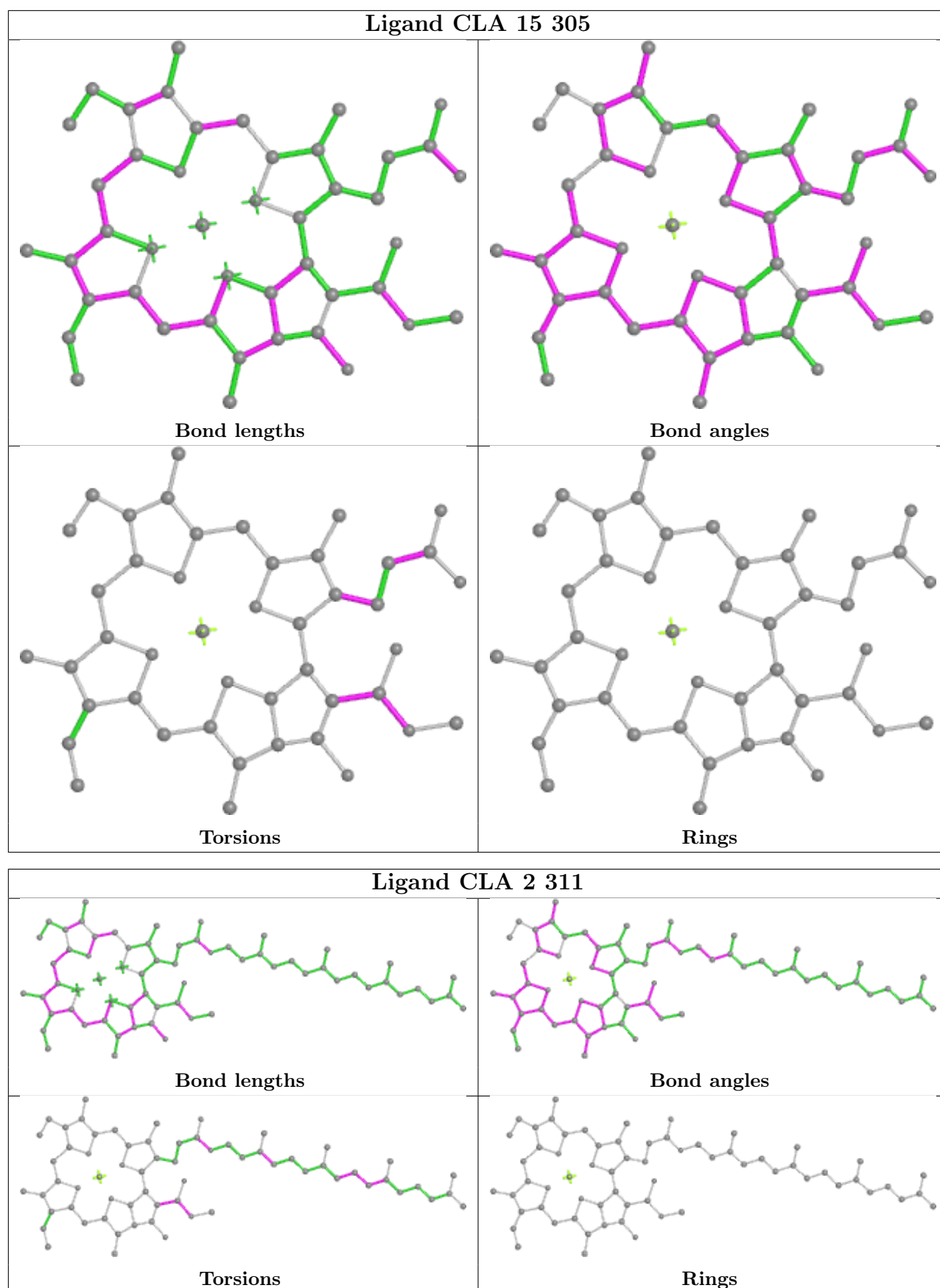
Torsions



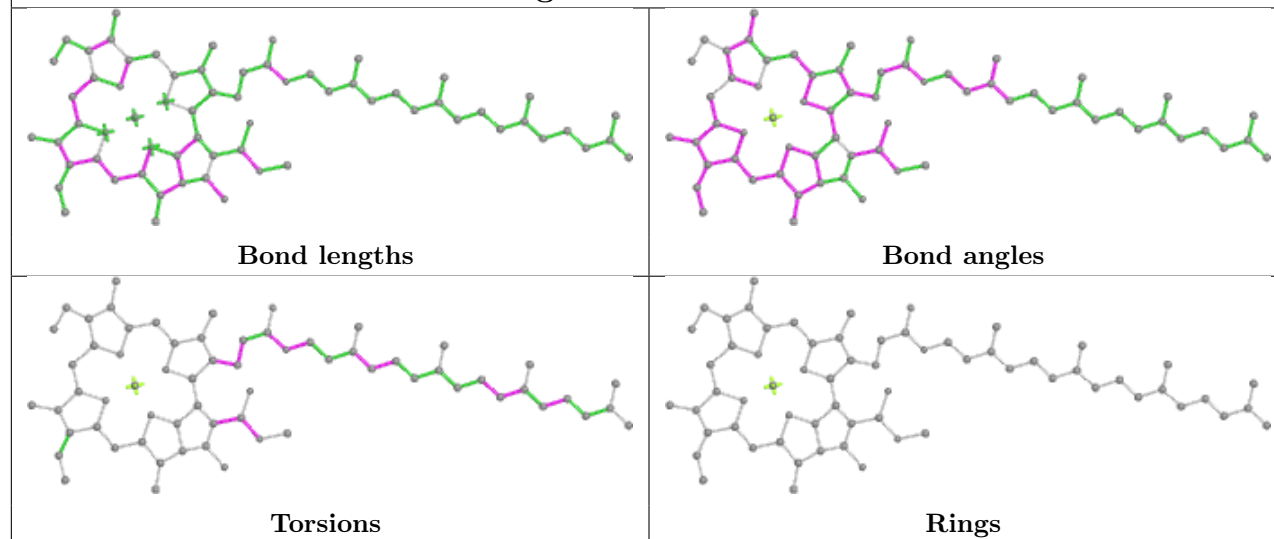
Rings



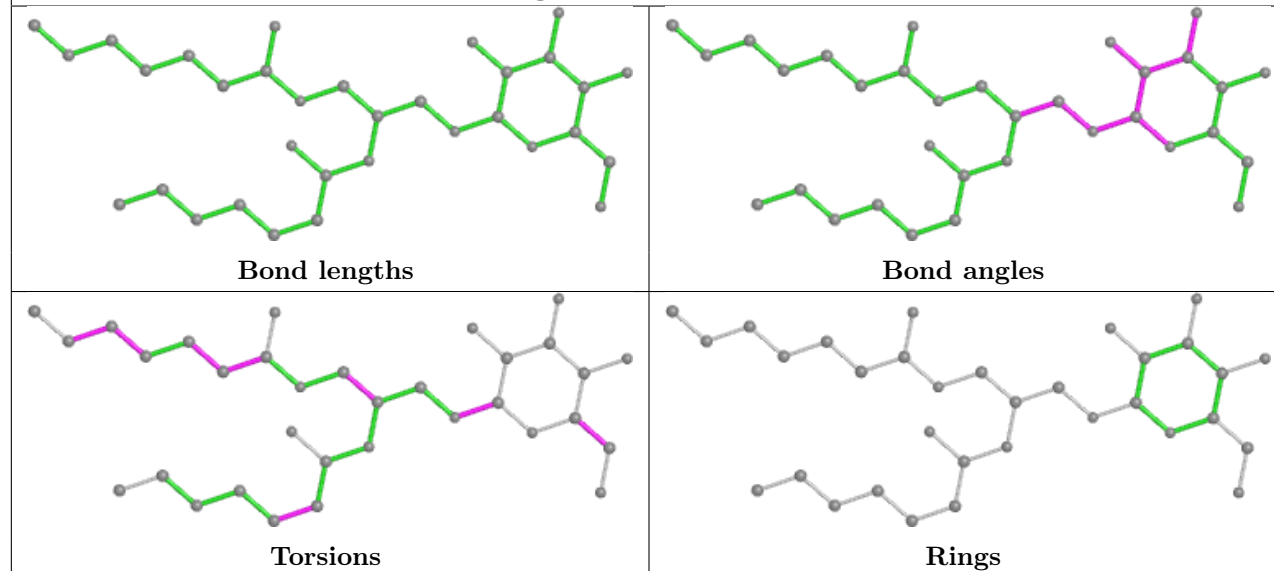




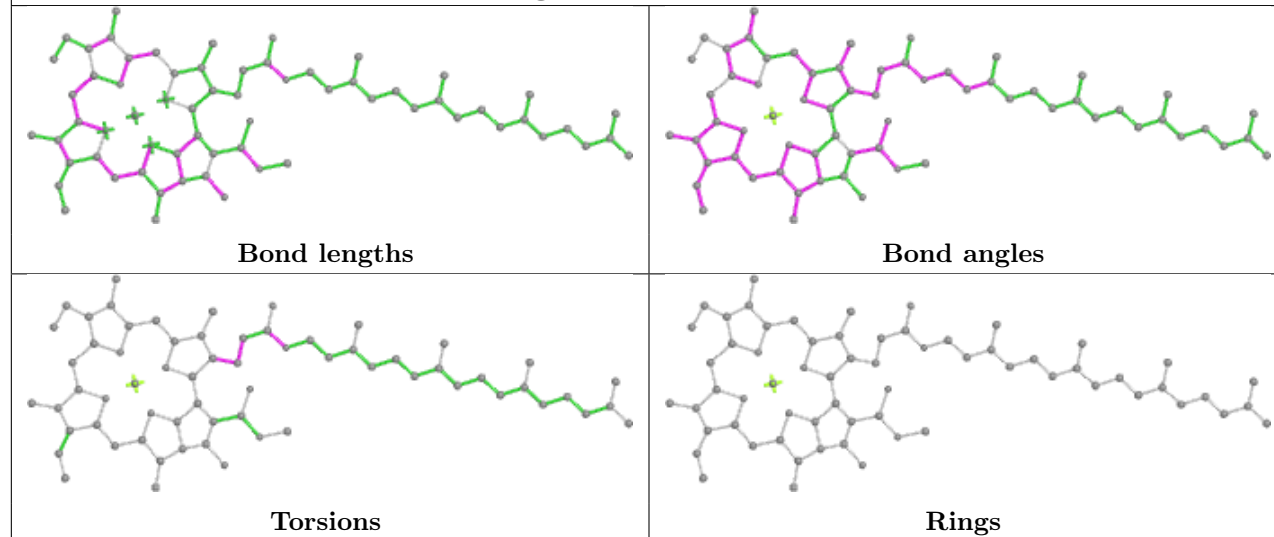
Ligand CLA 6 314



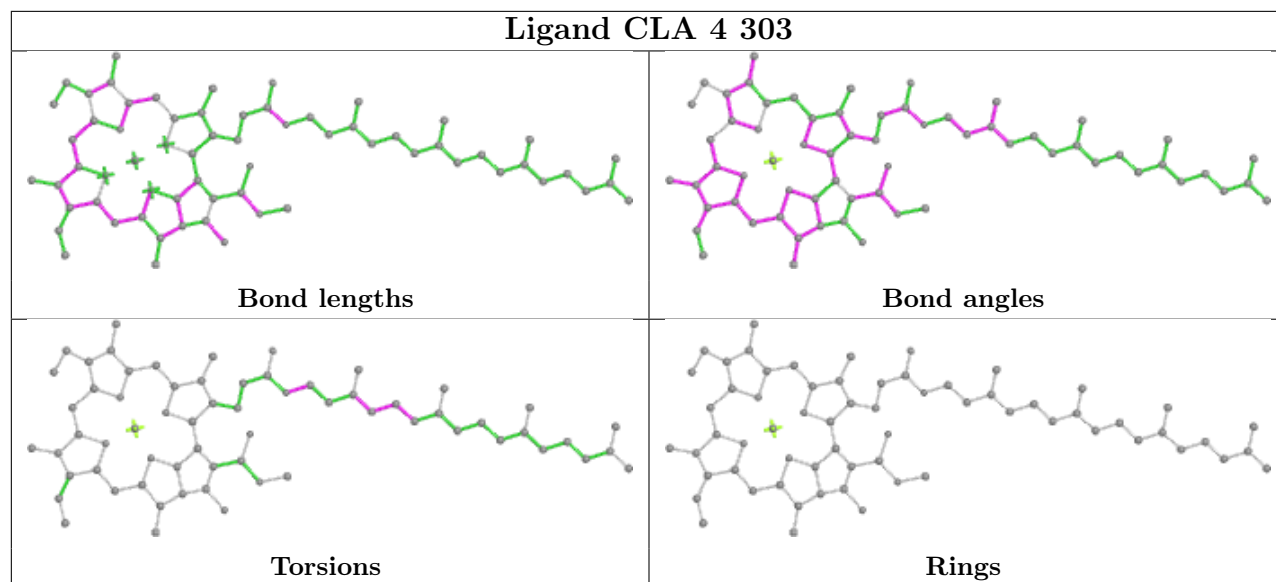
Ligand LMG 5 318



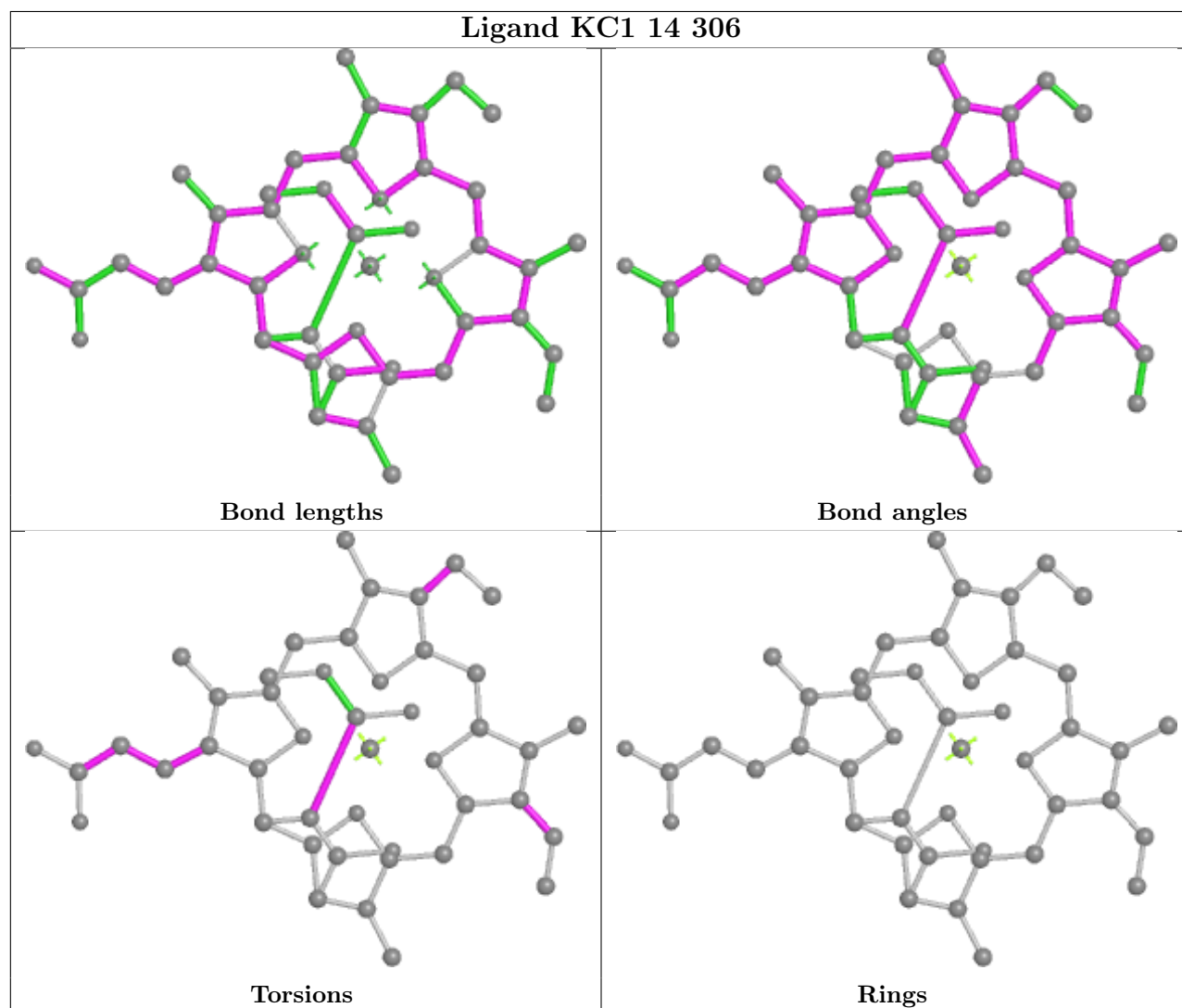
Ligand CLA B 827



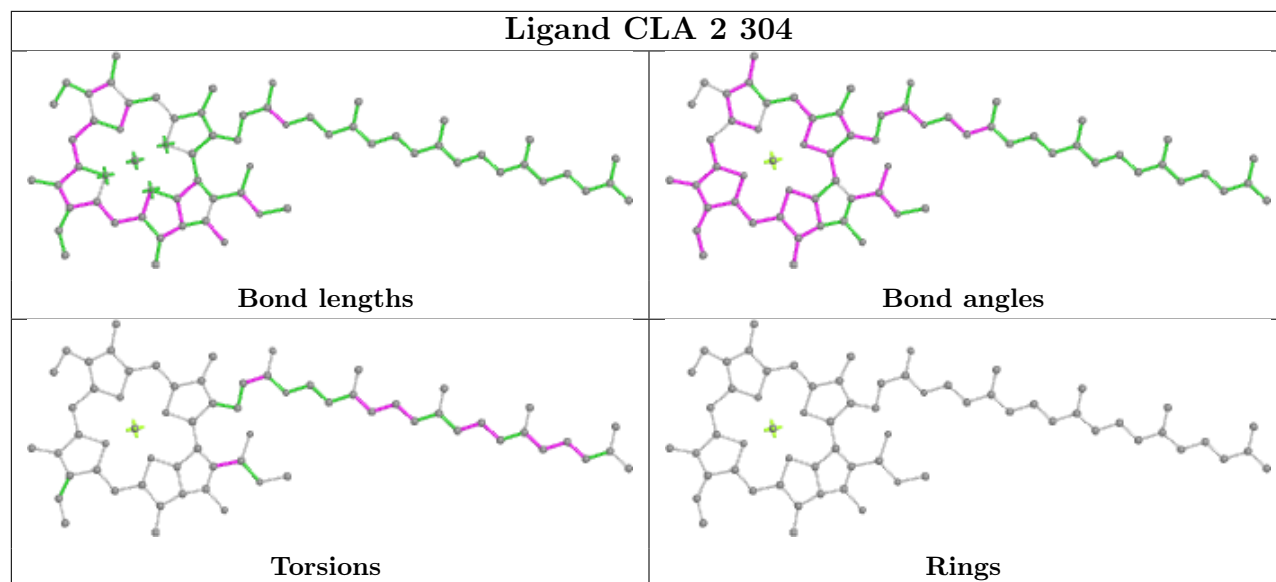
Ligand CLA 4 303



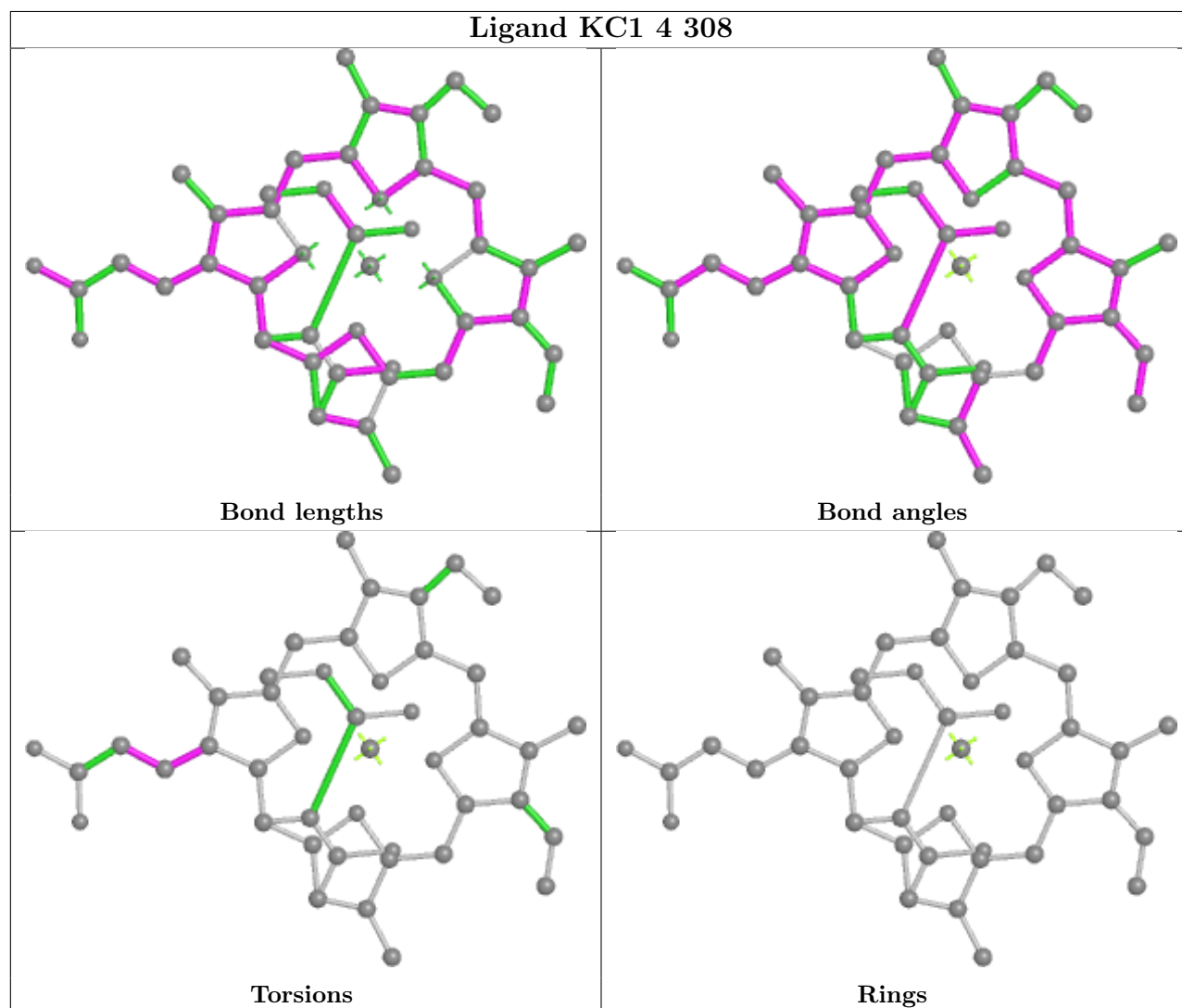
Ligand KC1 14 306



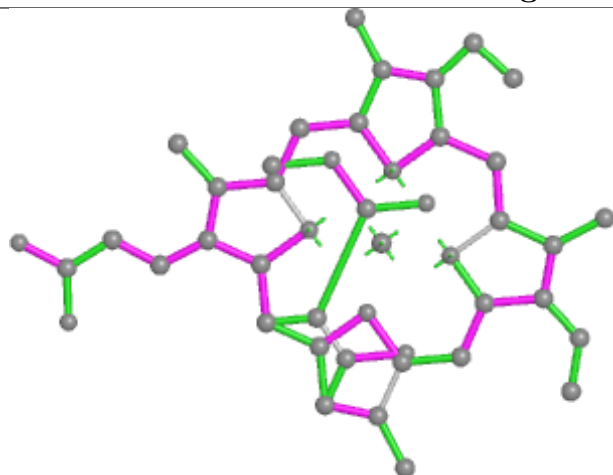
Ligand CLA 2 304



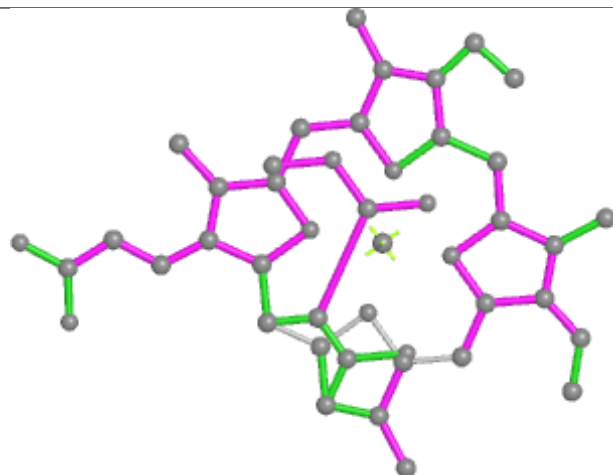
Ligand KC1 4 308



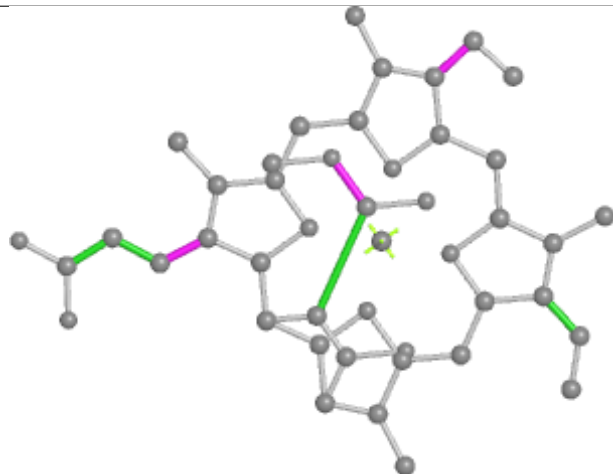
Ligand KC1 8 311



Bond lengths



Bond angles

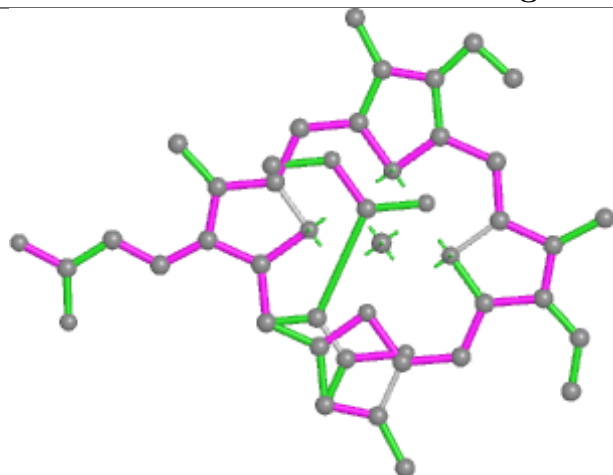


Torsions

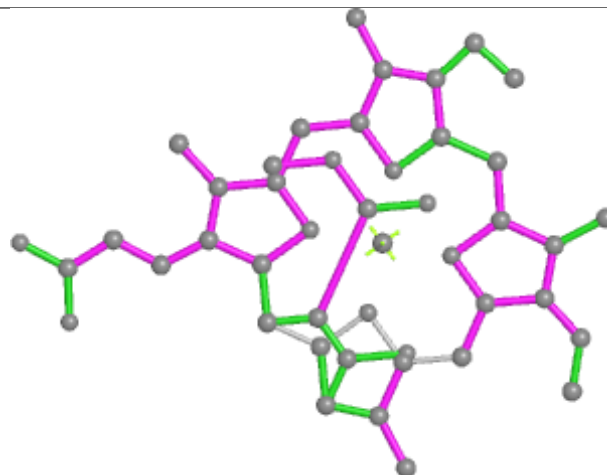


Rings

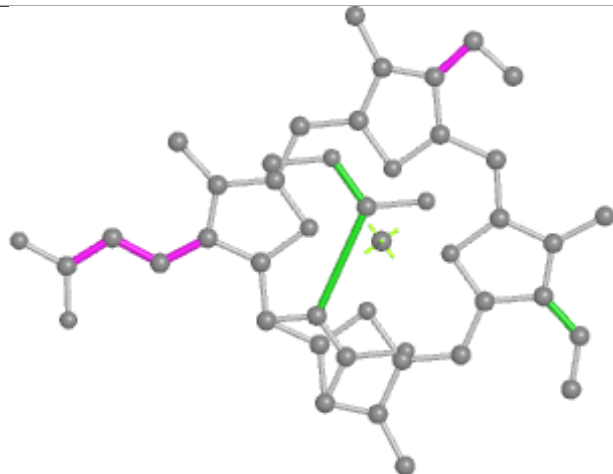
Ligand KC1 9 312



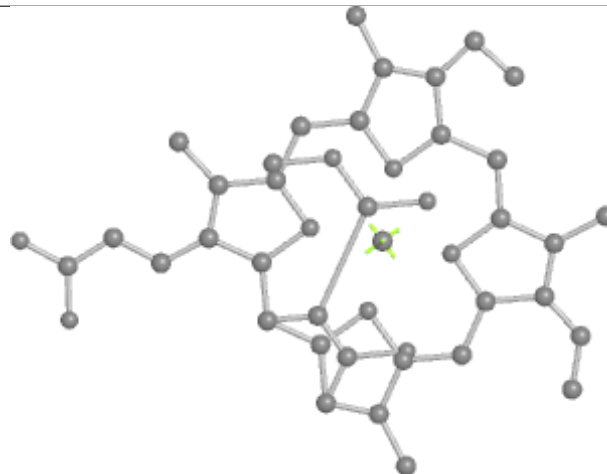
Bond lengths



Bond angles

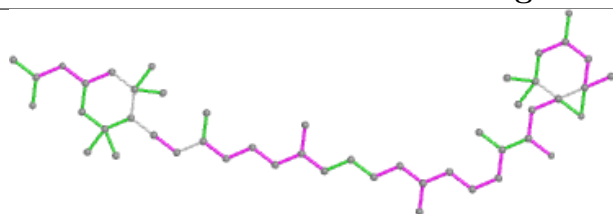


Torsions

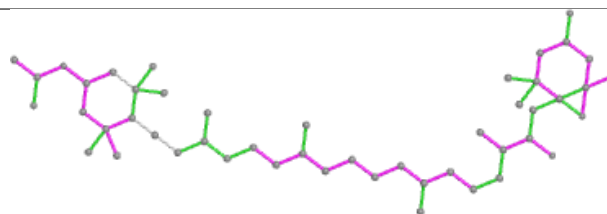


Rings

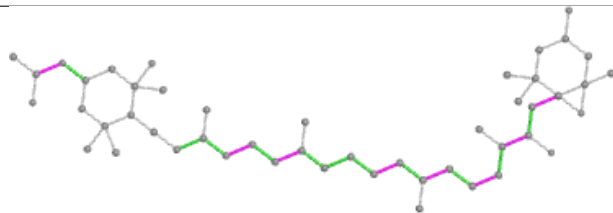
Ligand A86 15 316



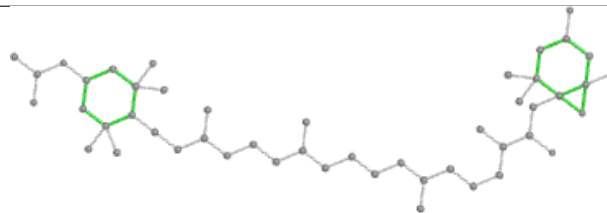
Bond lengths



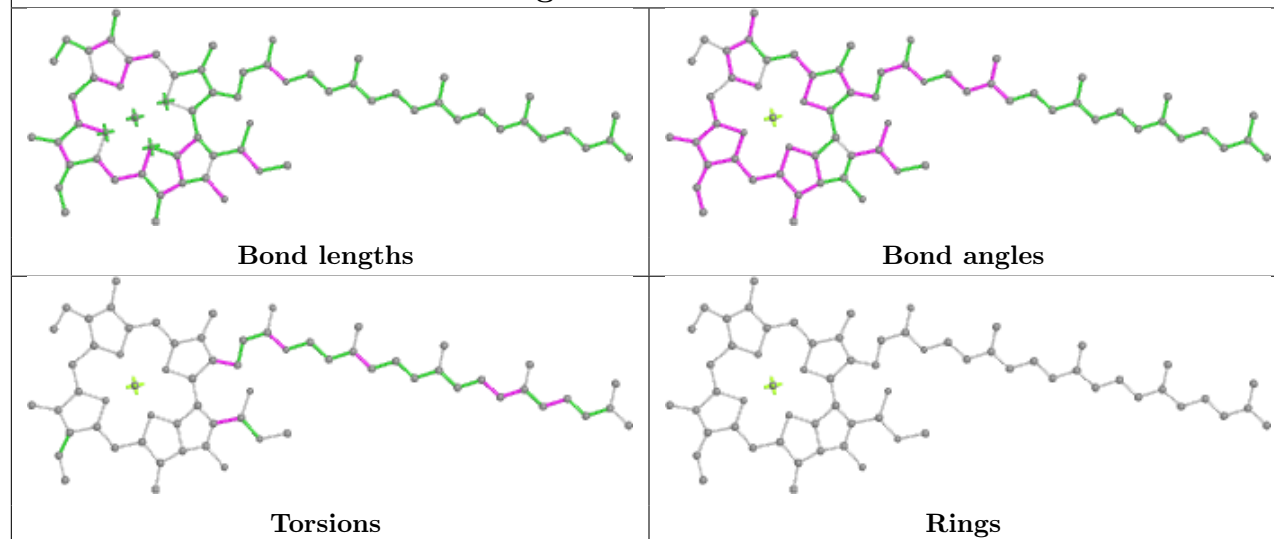
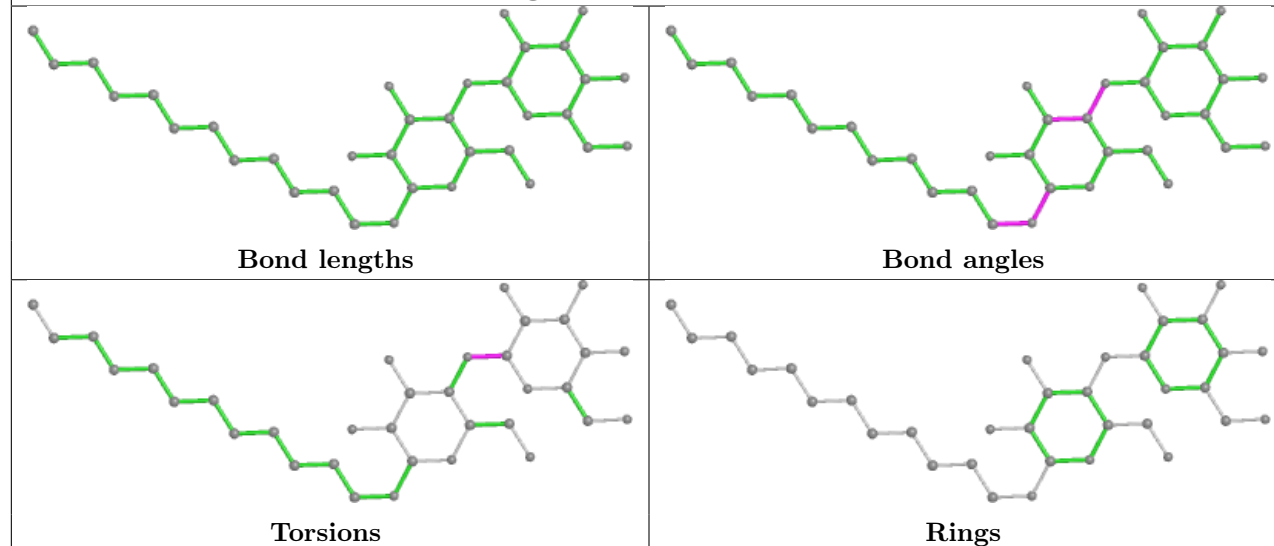
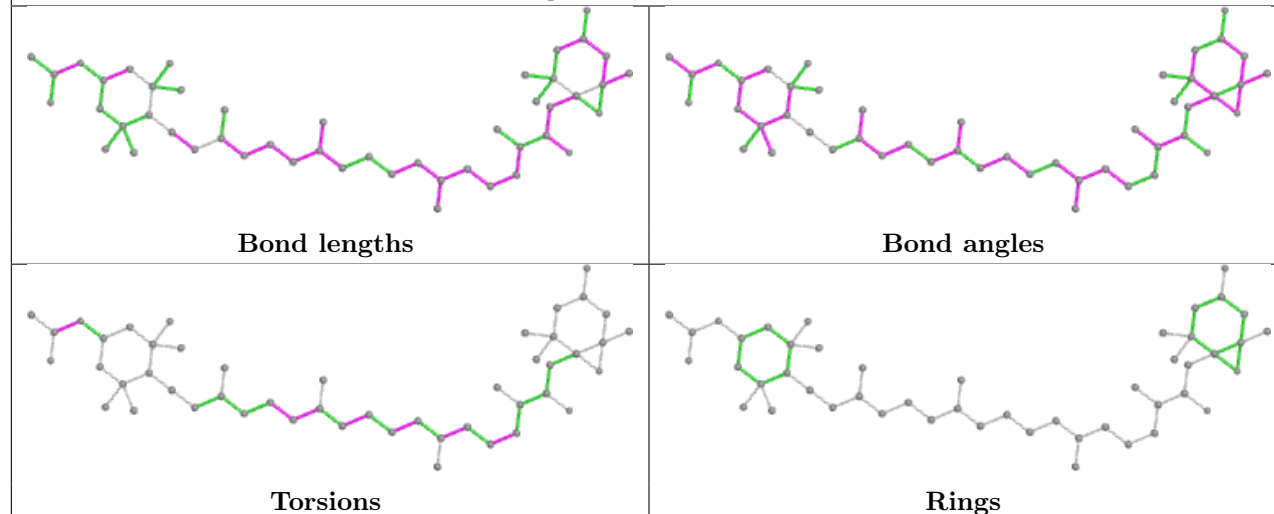
Bond angles

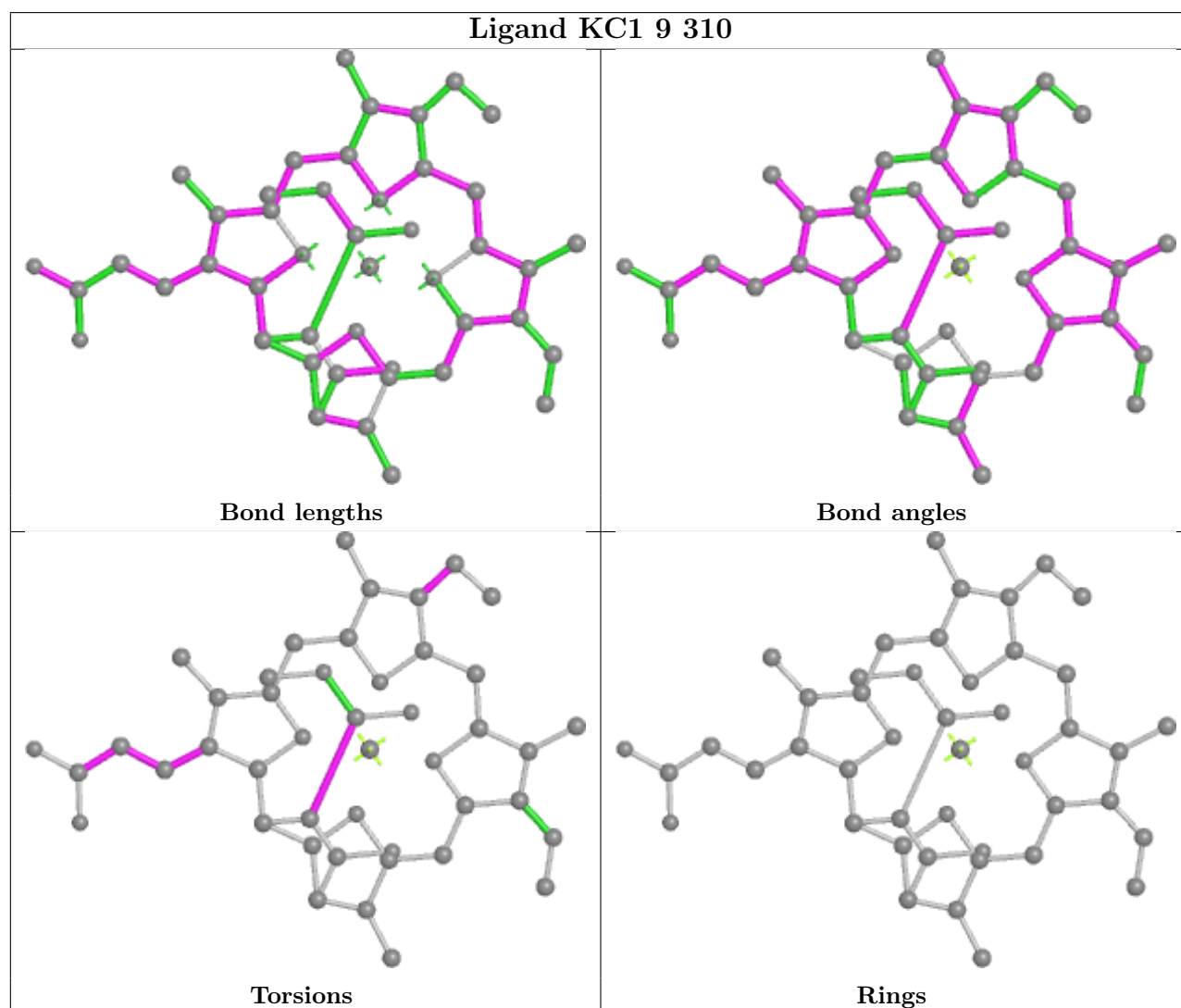
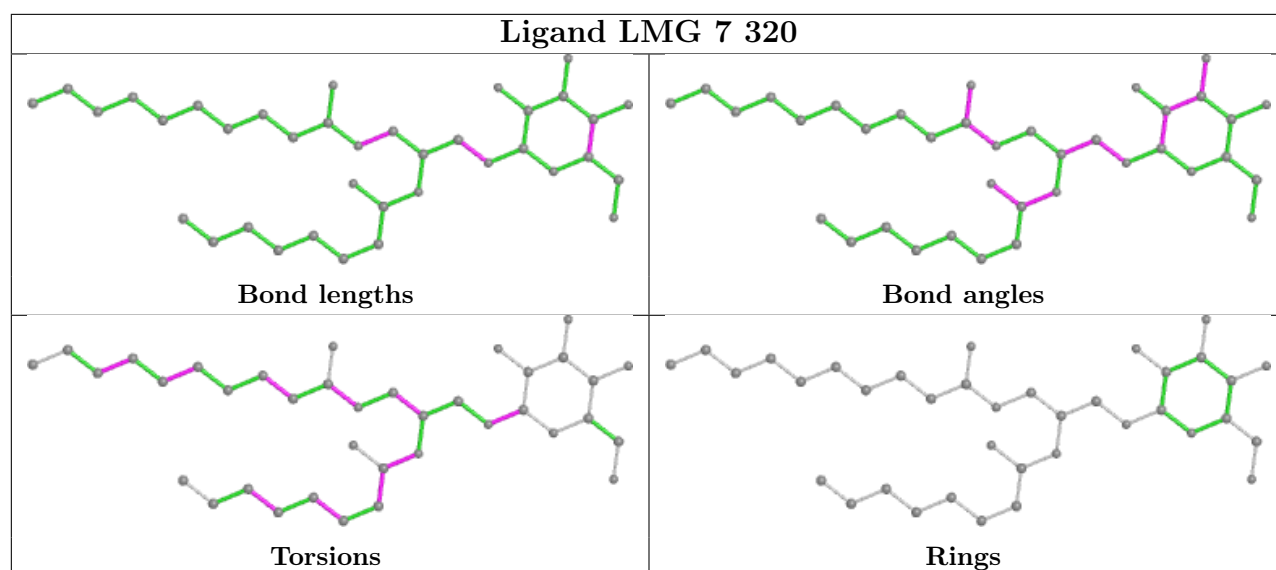


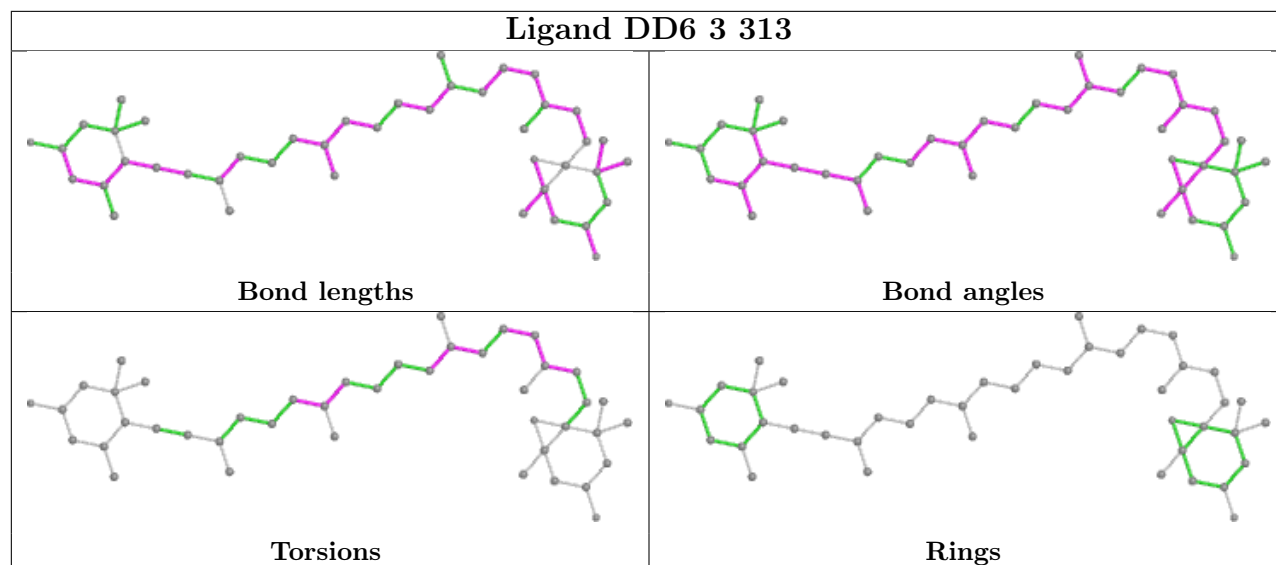
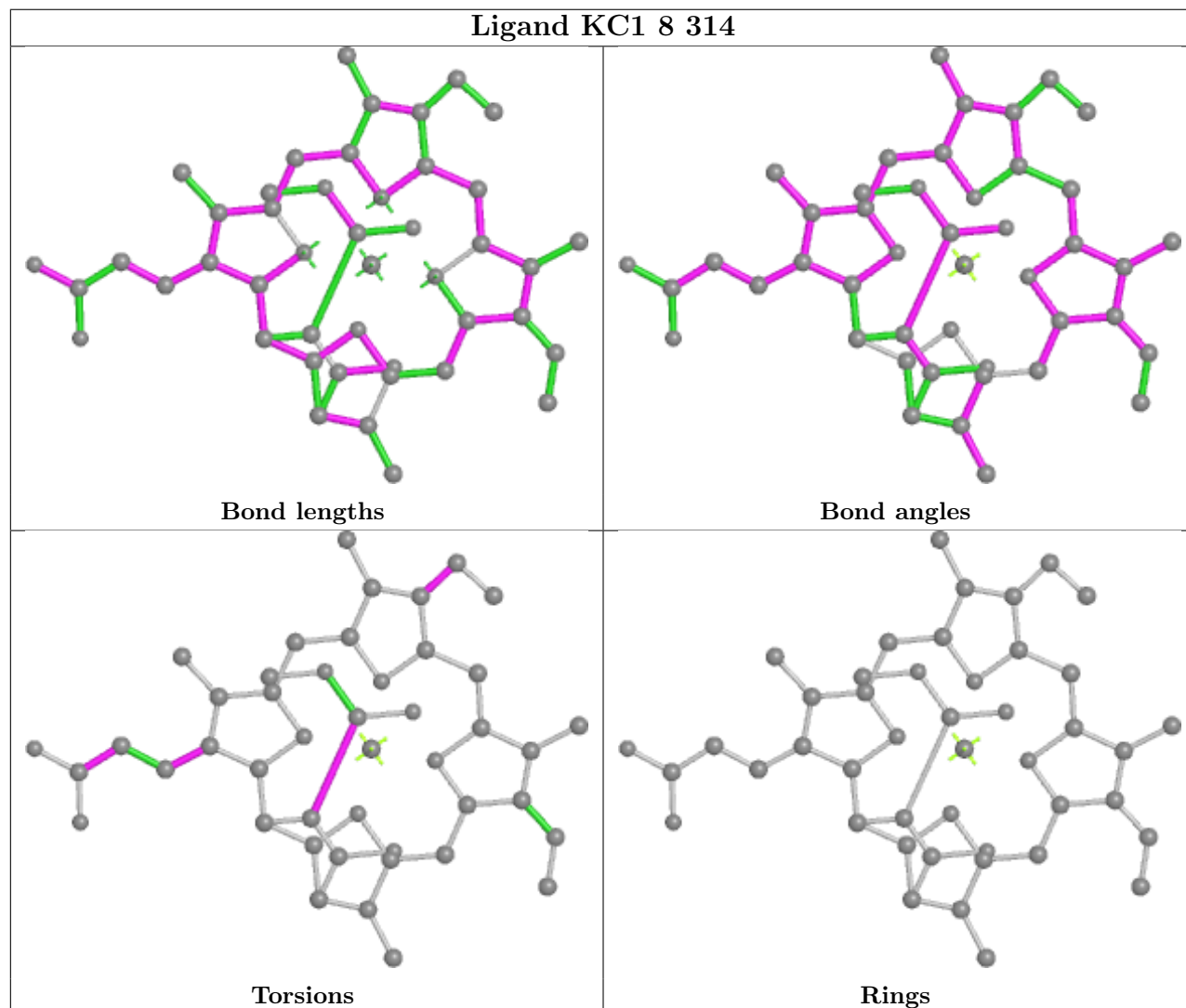
Torsions

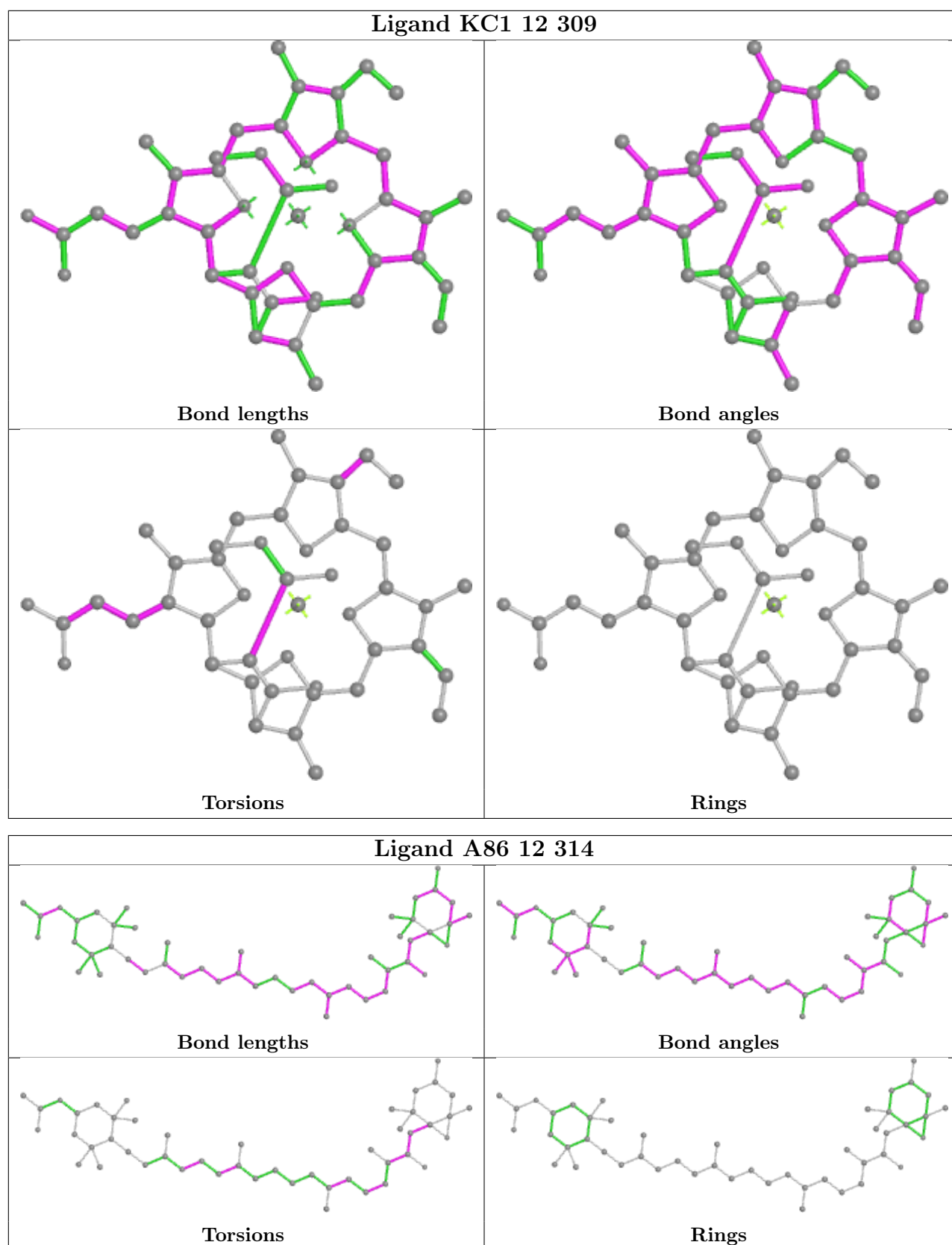


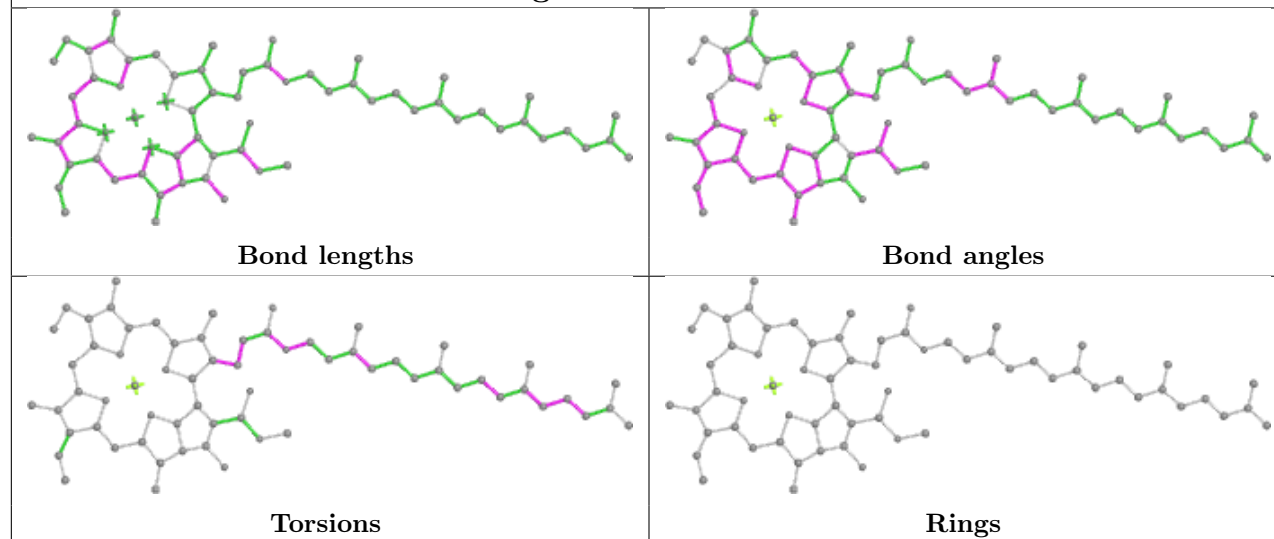
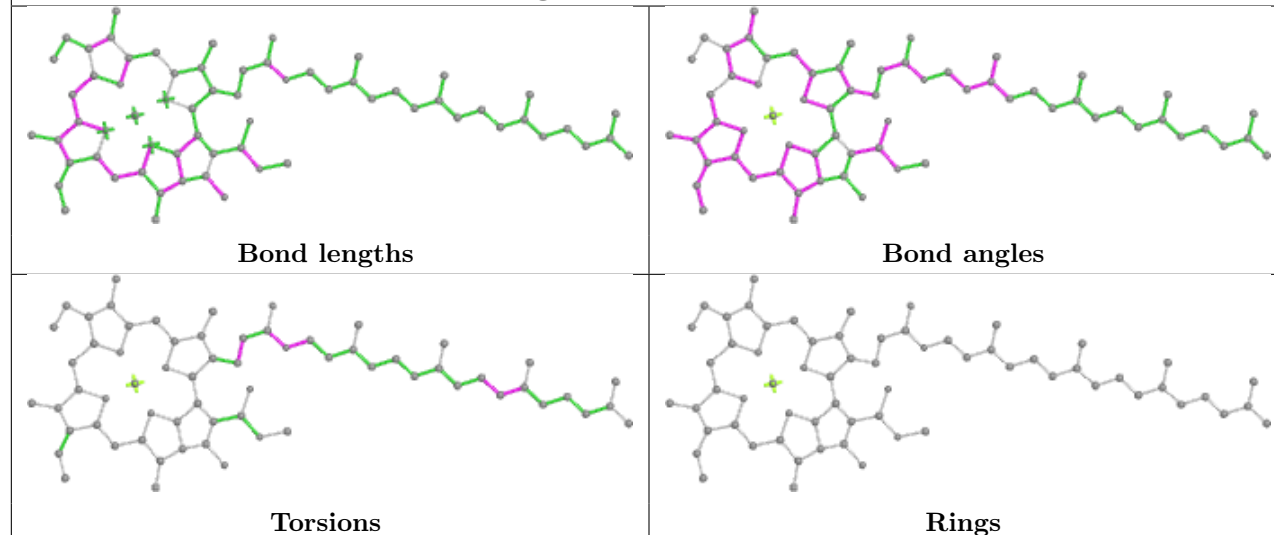
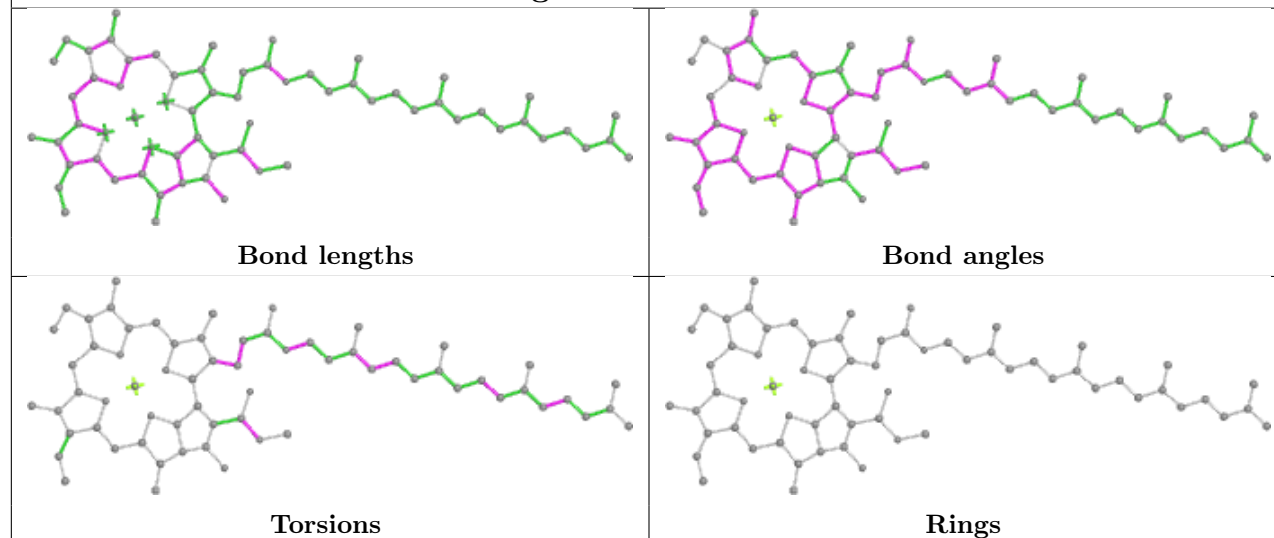
Rings

Ligand CLA 8 303**Ligand LMT 11 318****Ligand A86 9 315**

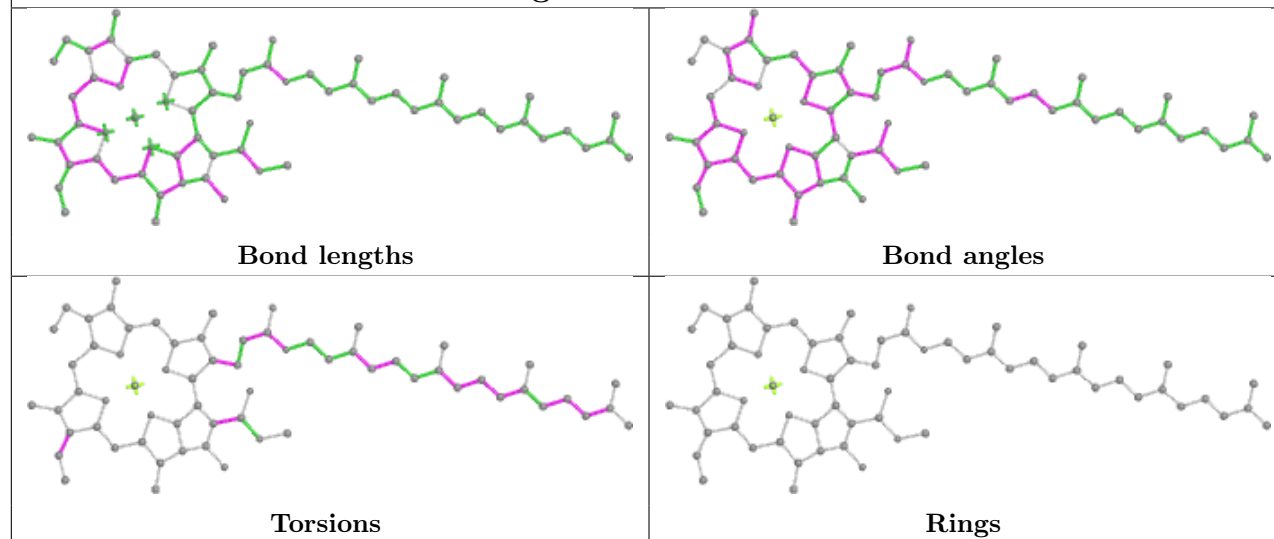


Ligand DD6 3 313**Ligand KC1 8 314**

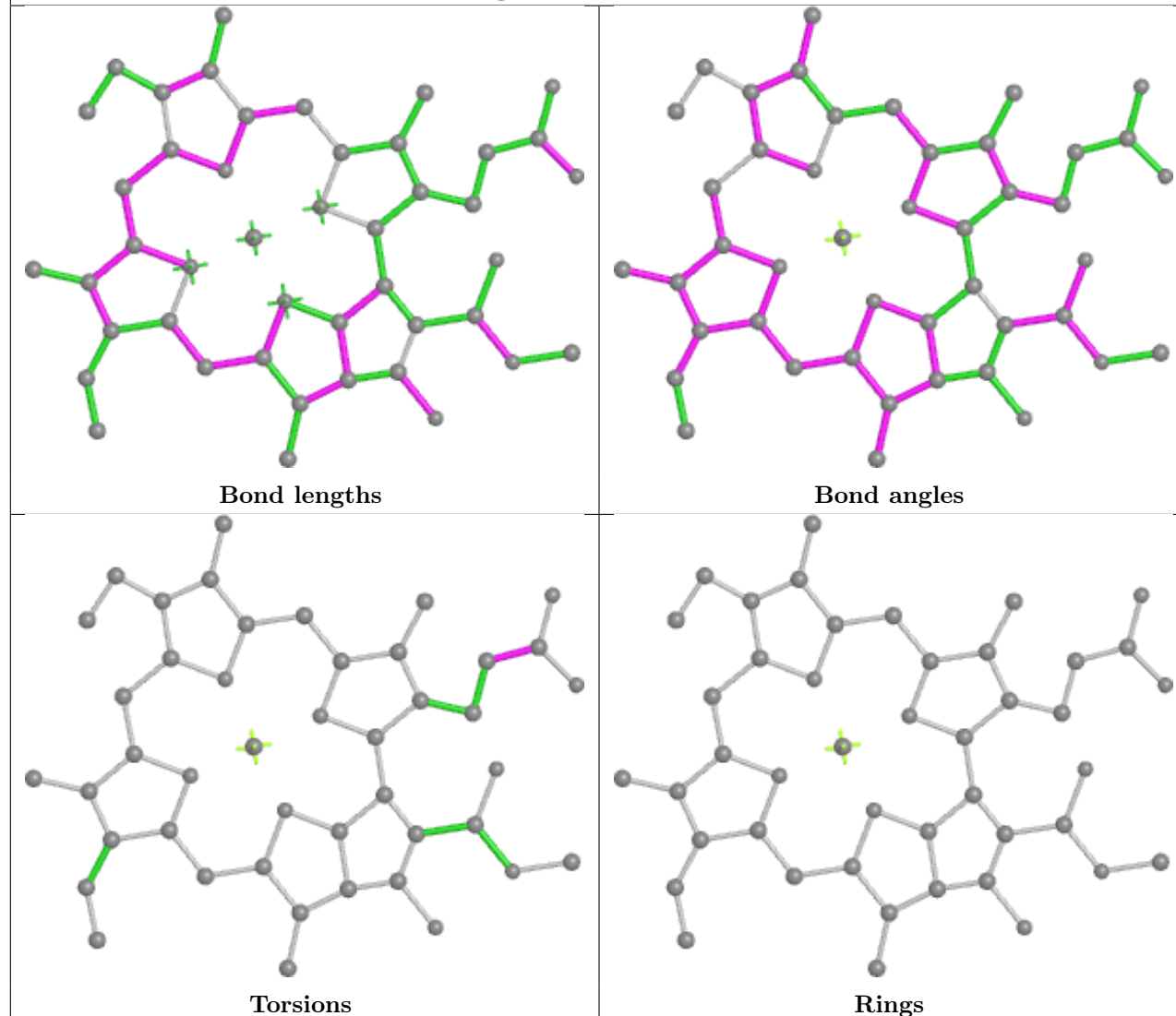


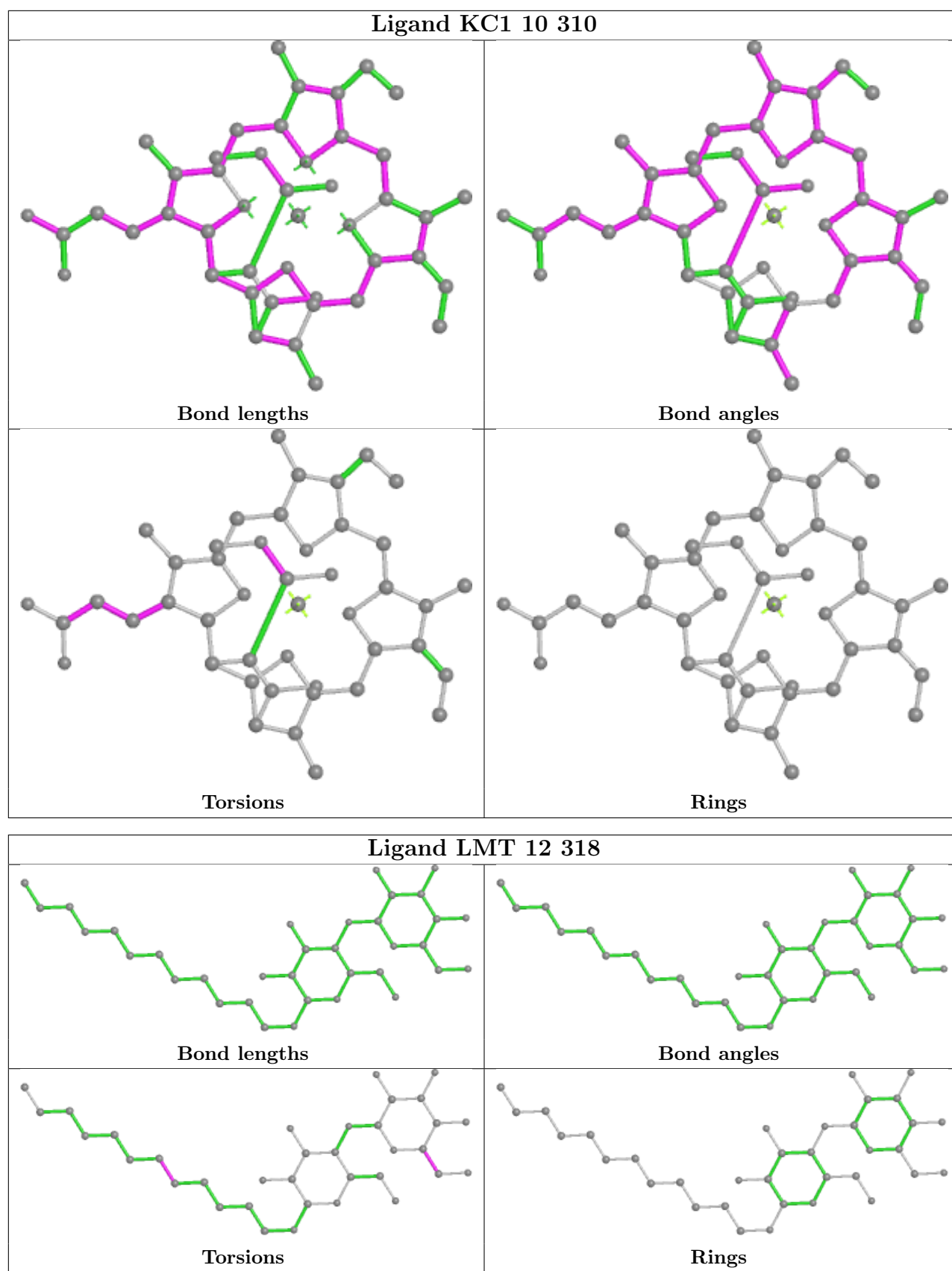
Ligand CLA B 829**Ligand CLA L 202****Ligand CLA A 810**

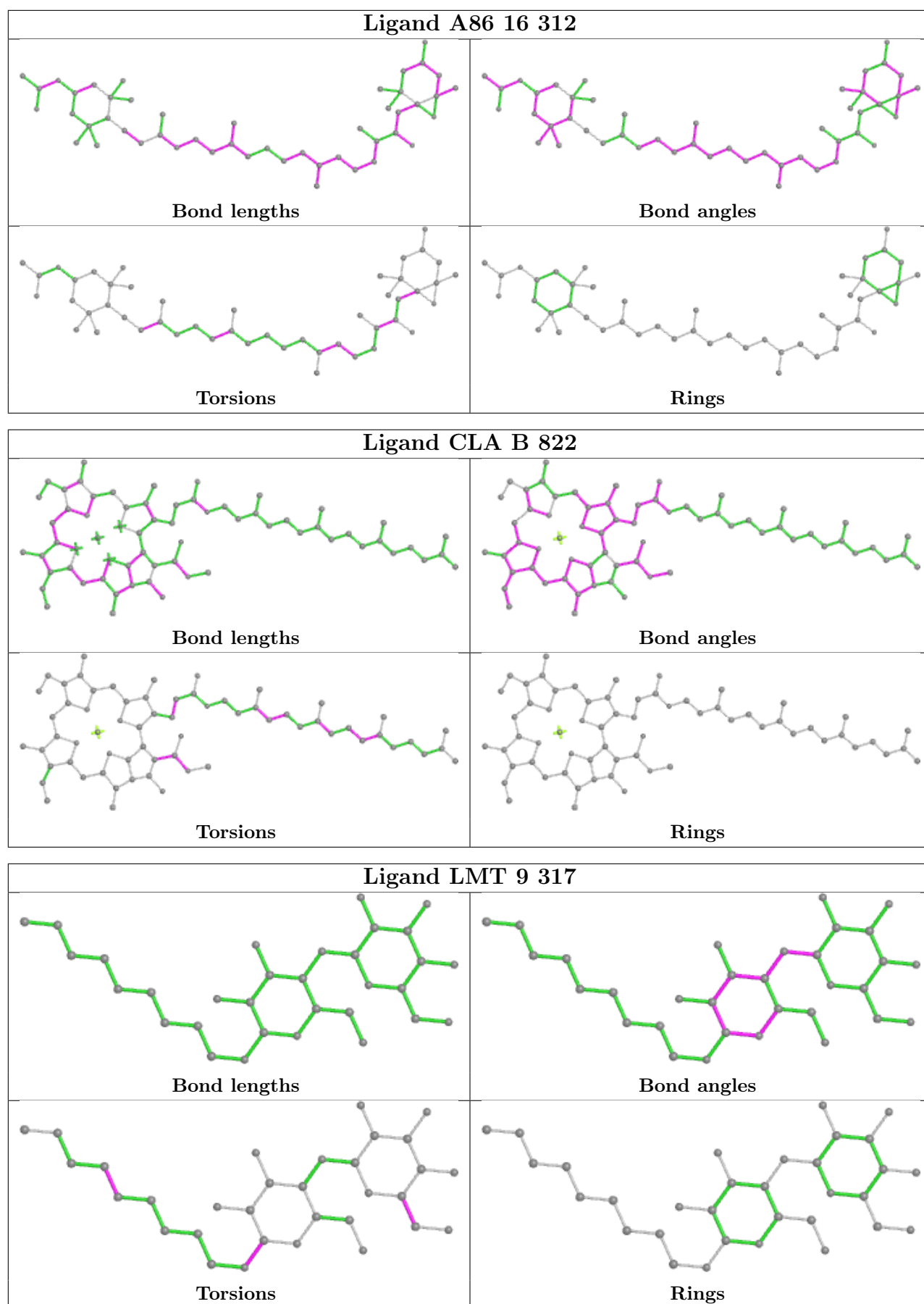
Ligand CLA B 813

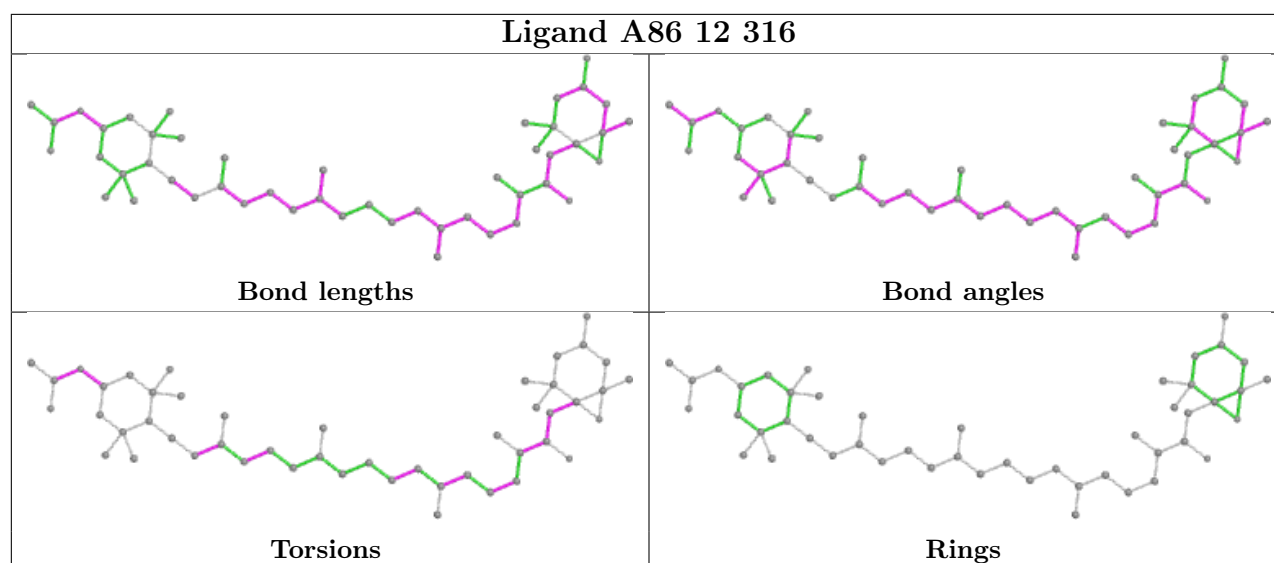
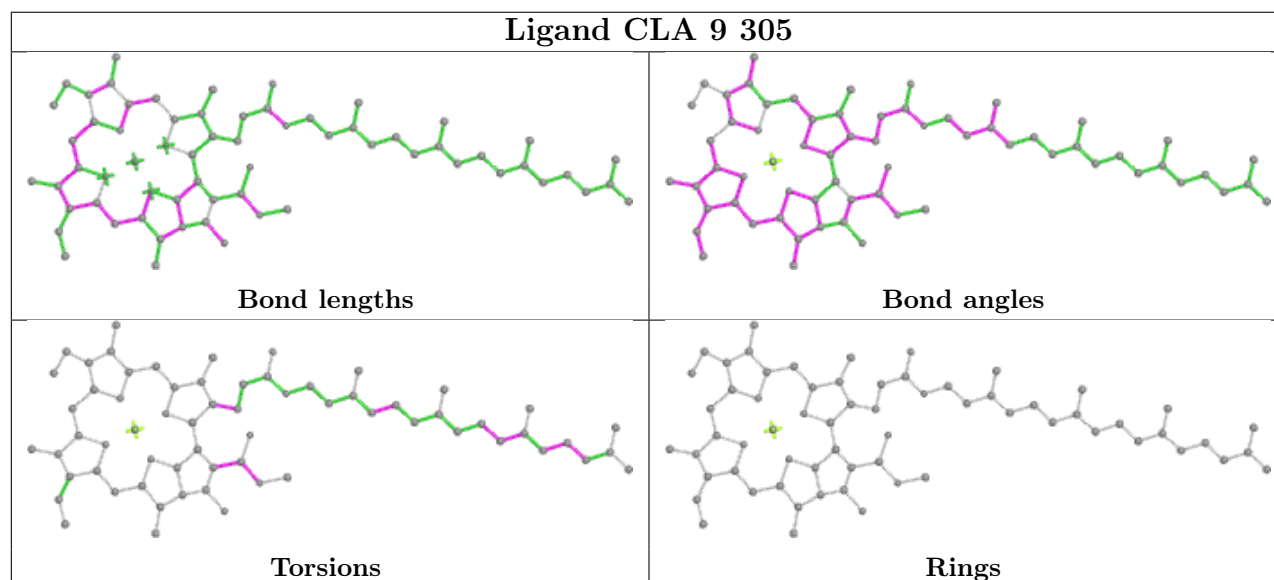
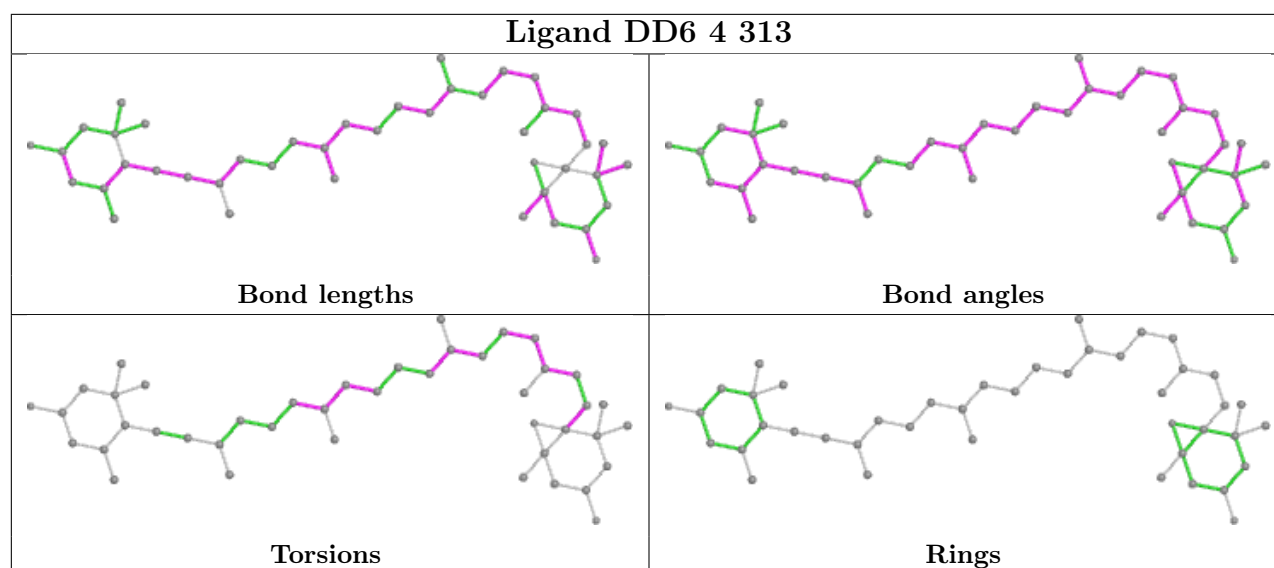


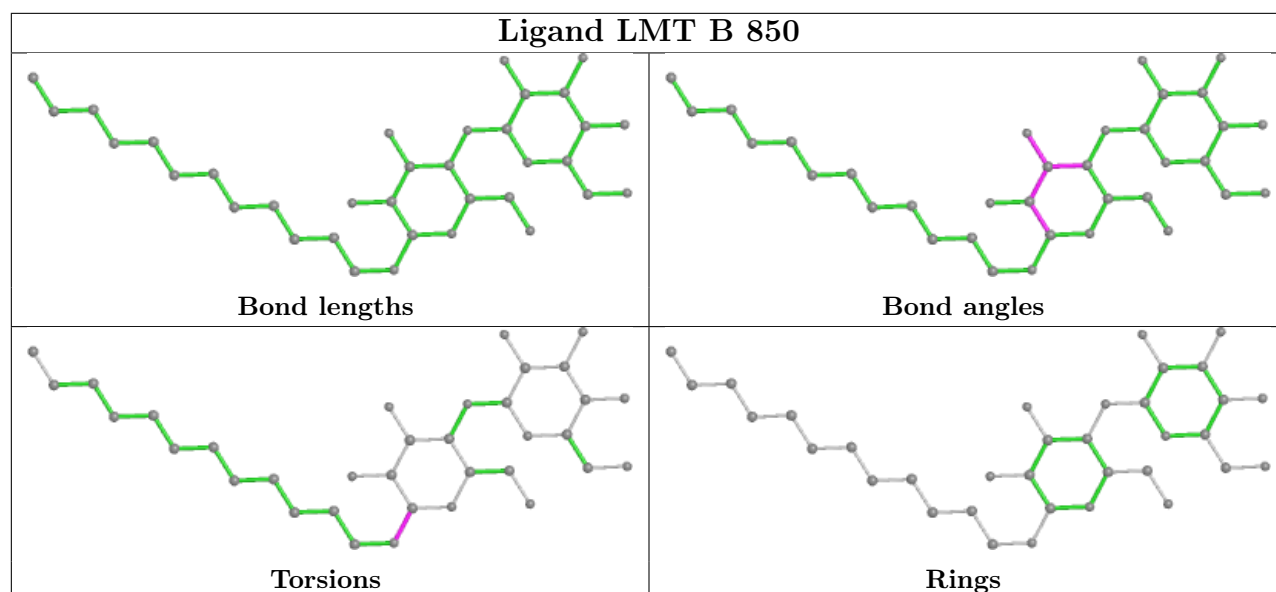
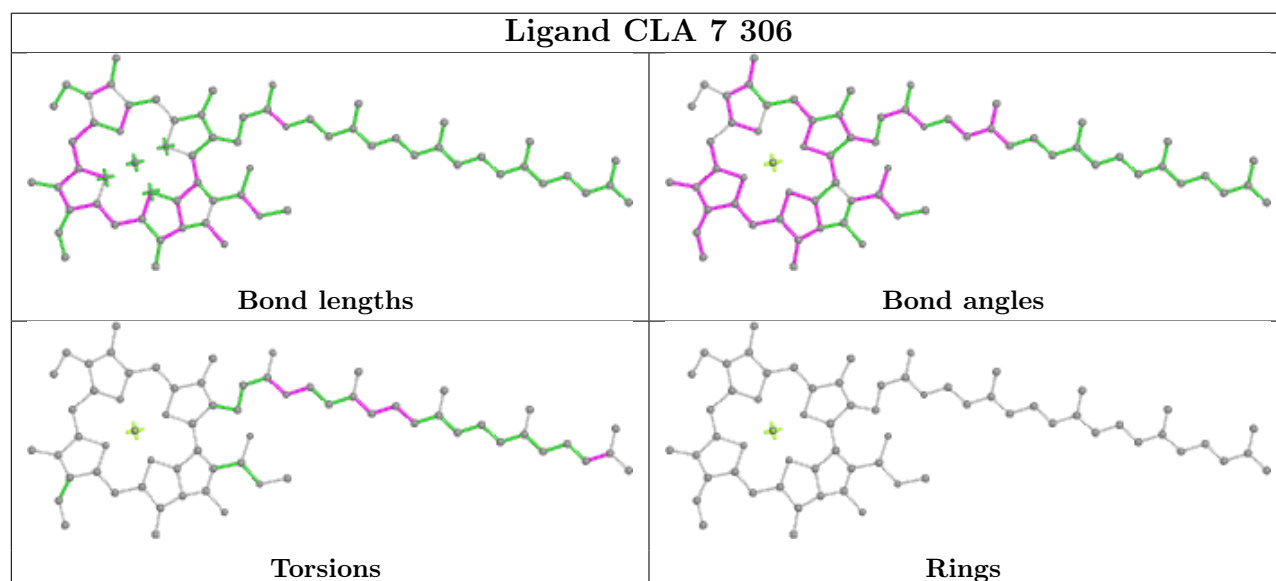
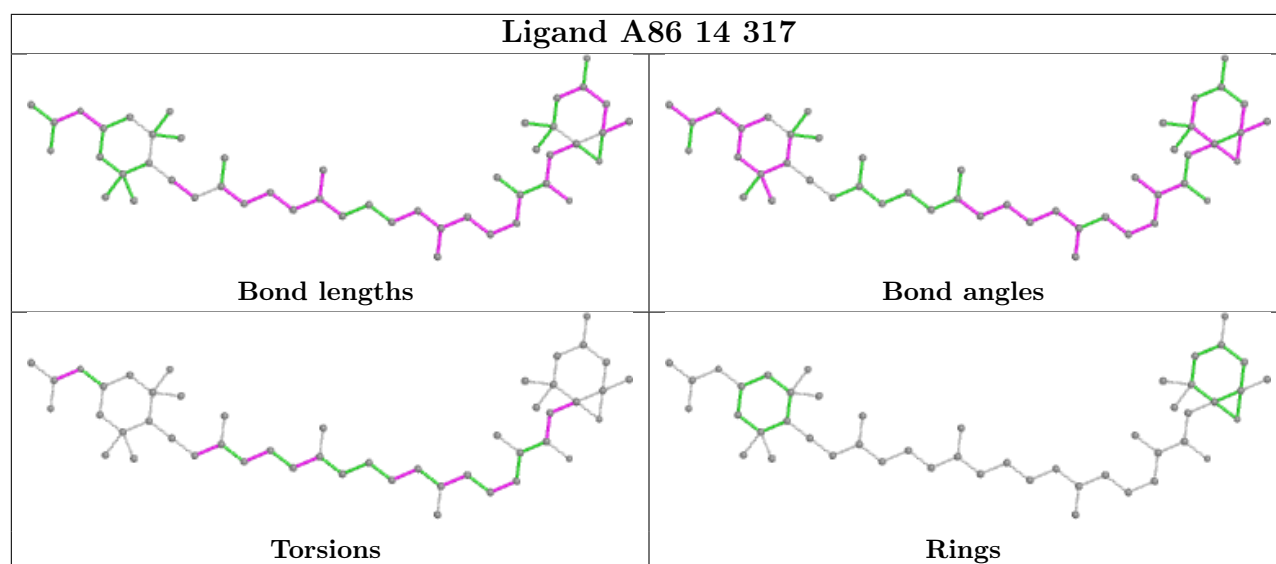
Ligand CLA L 203

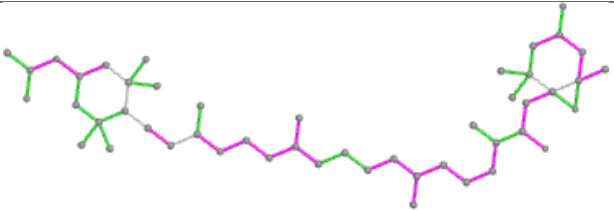
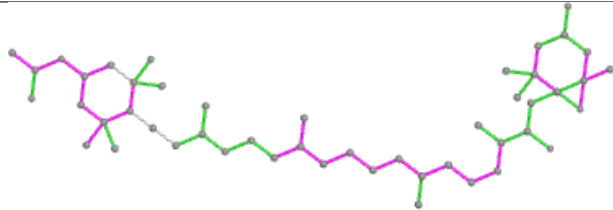
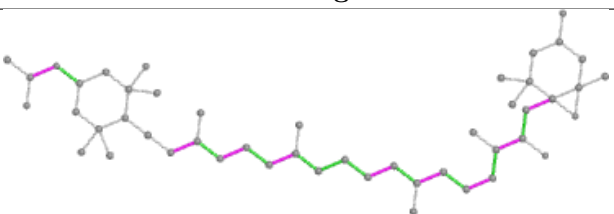
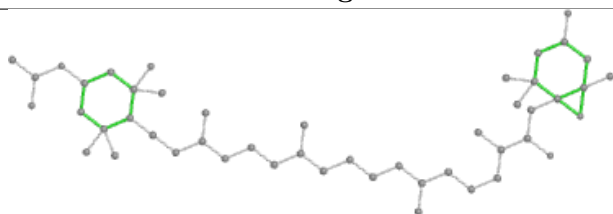


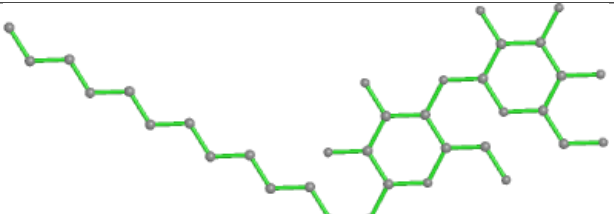
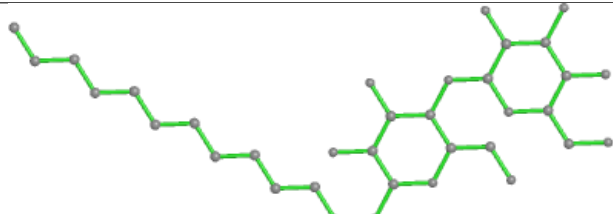
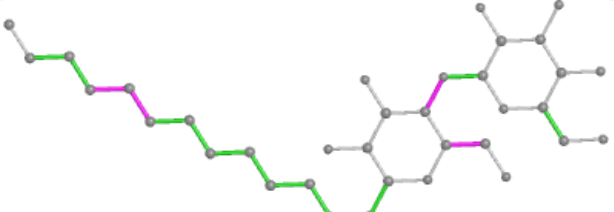
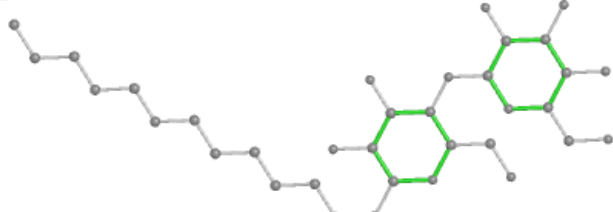


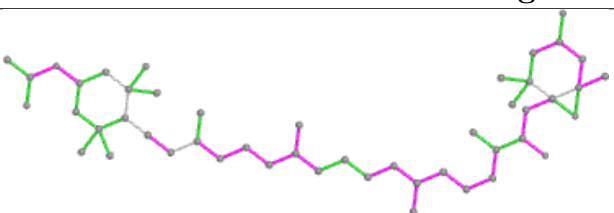
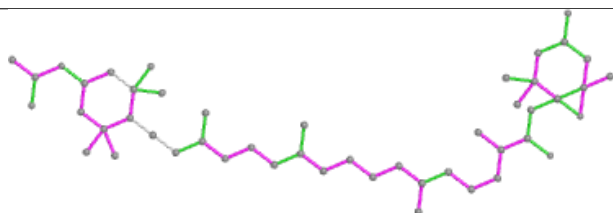
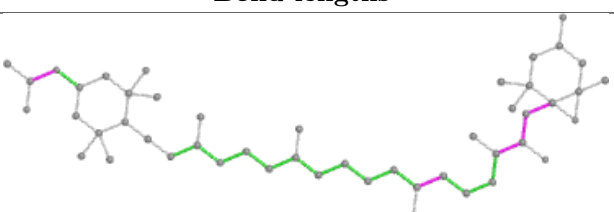
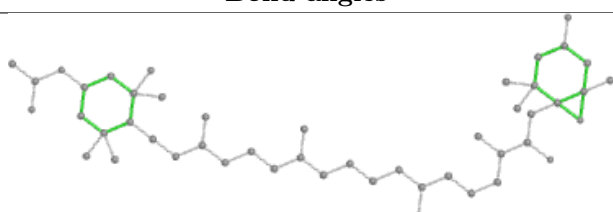


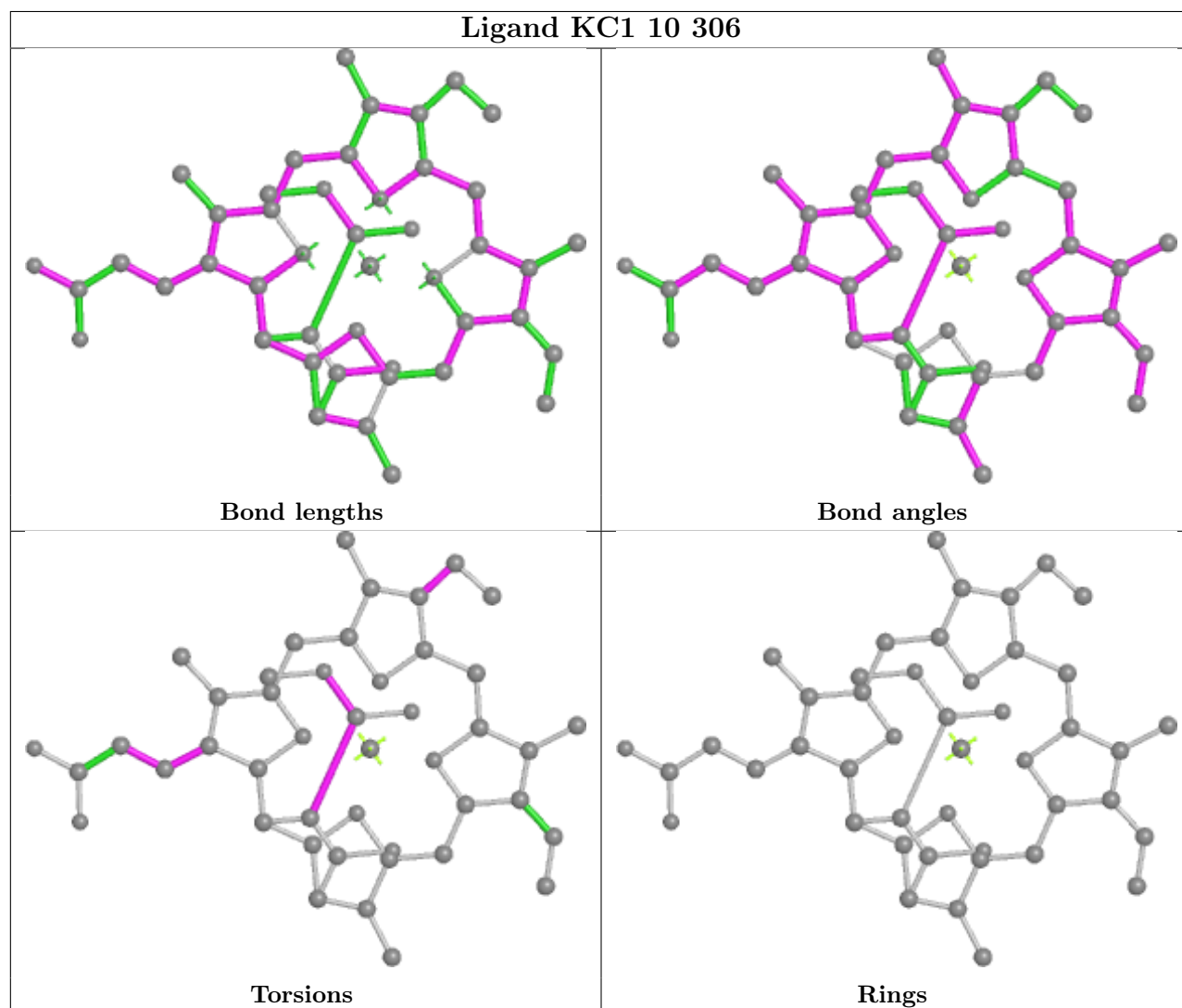
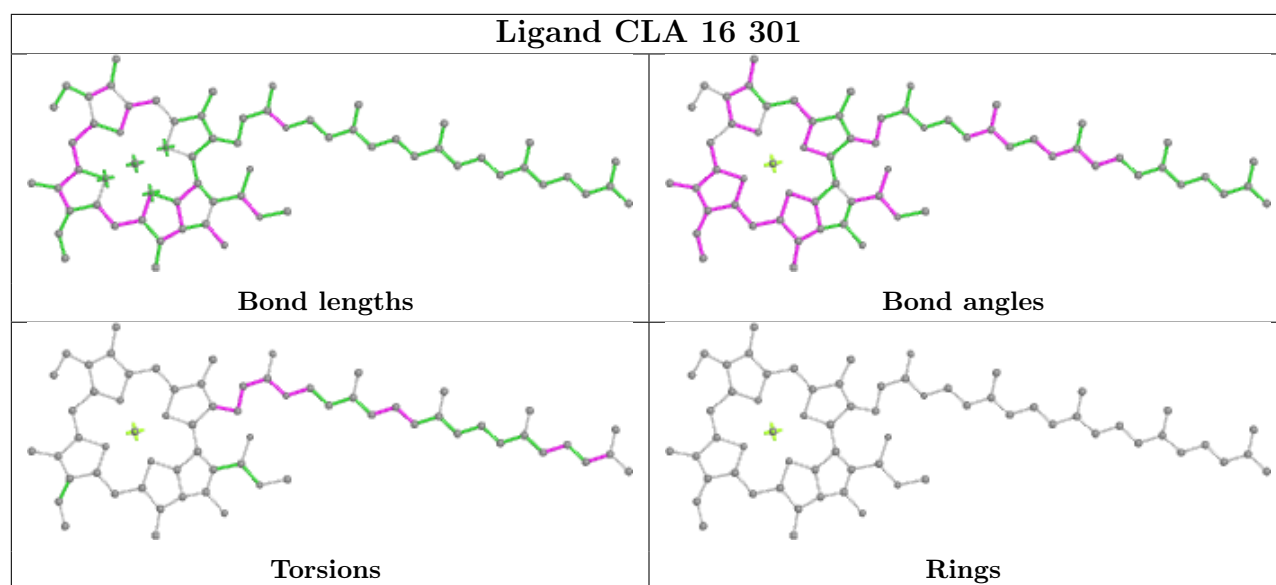


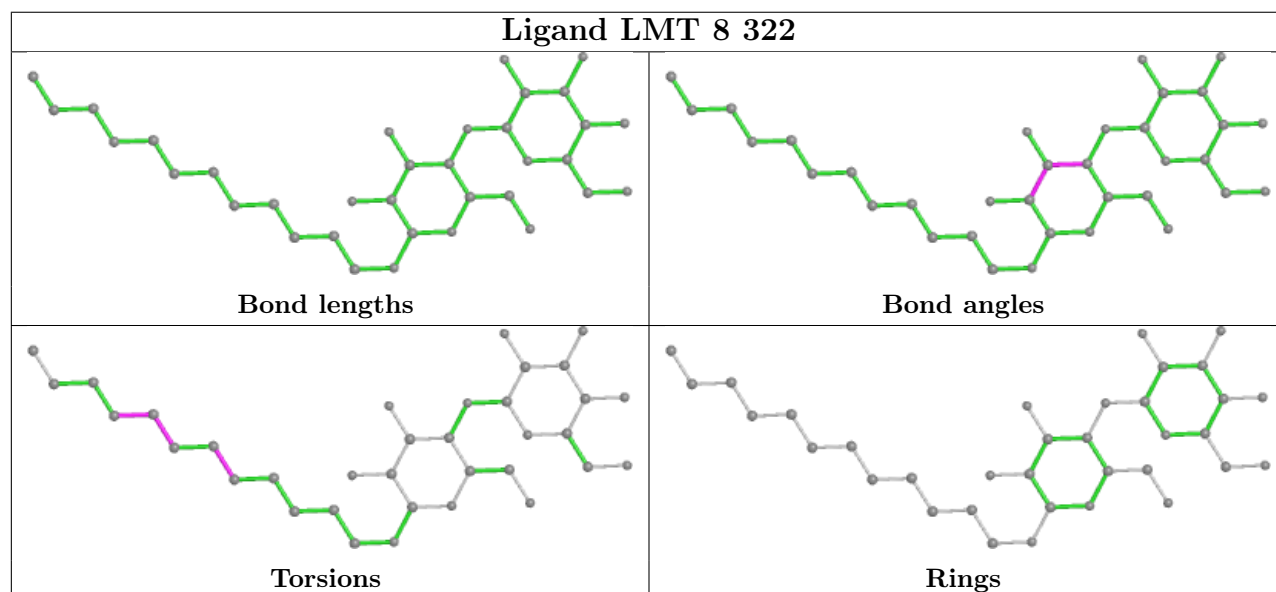
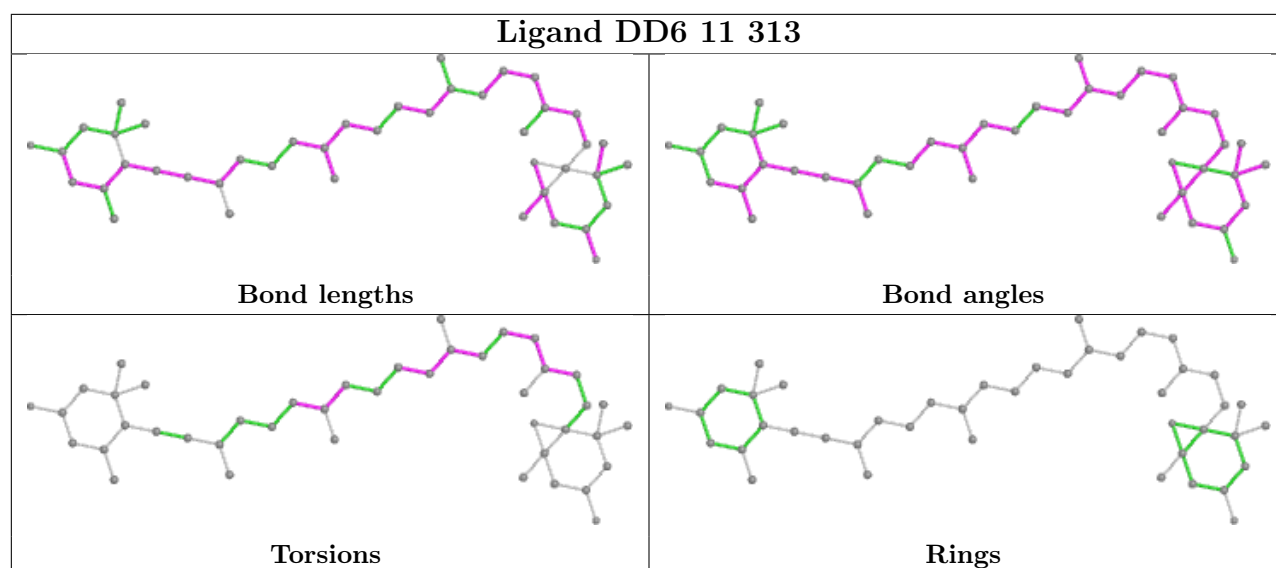


Ligand A86 3 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

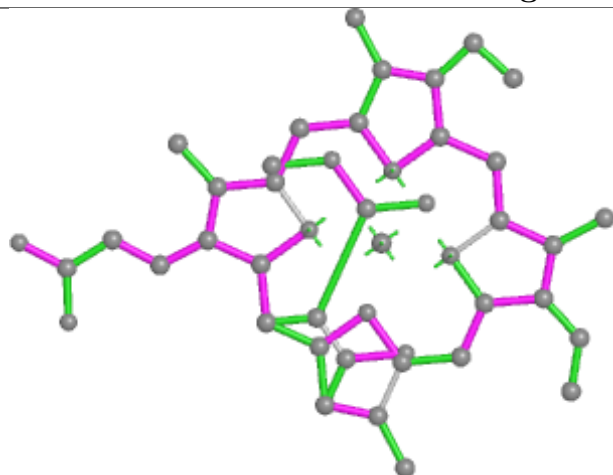
Ligand LMT 16 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand A86 4 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

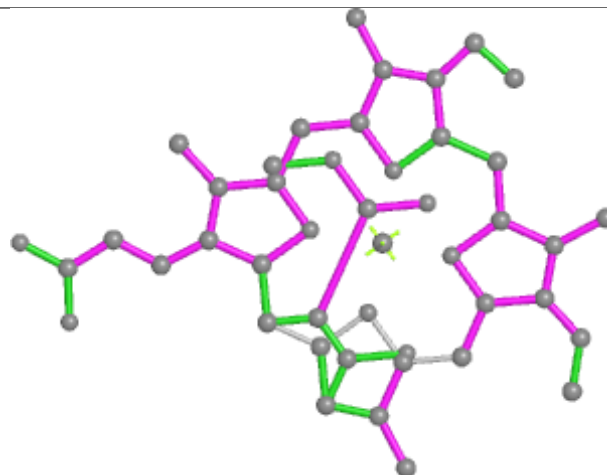




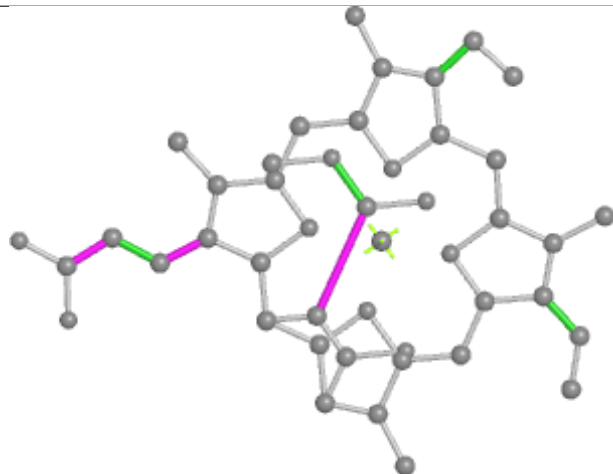
Ligand KC1 6 312



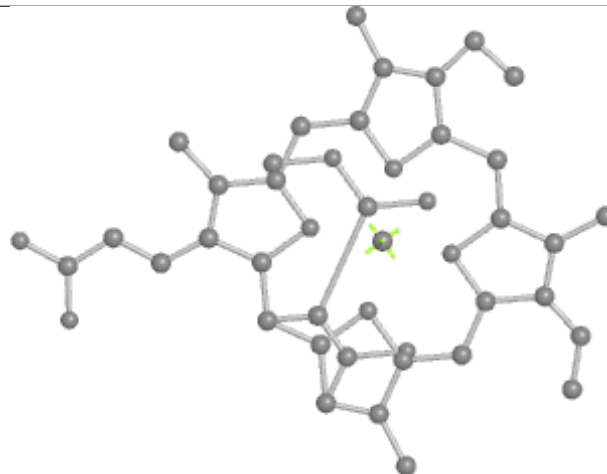
Bond lengths



Bond angles

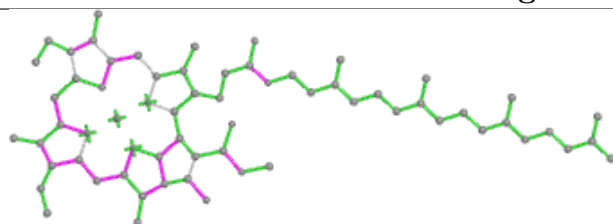


Torsions

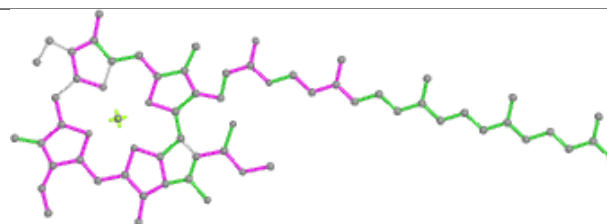


Rings

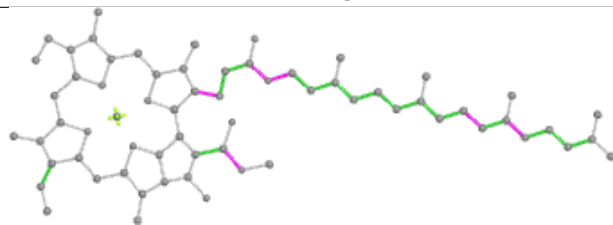
Ligand CLA 9 309



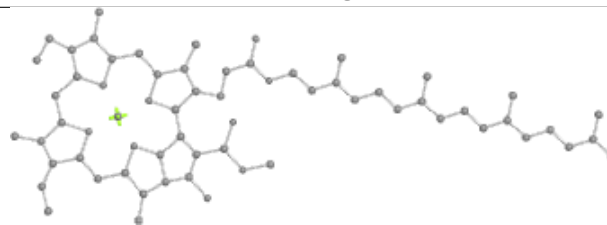
Bond lengths



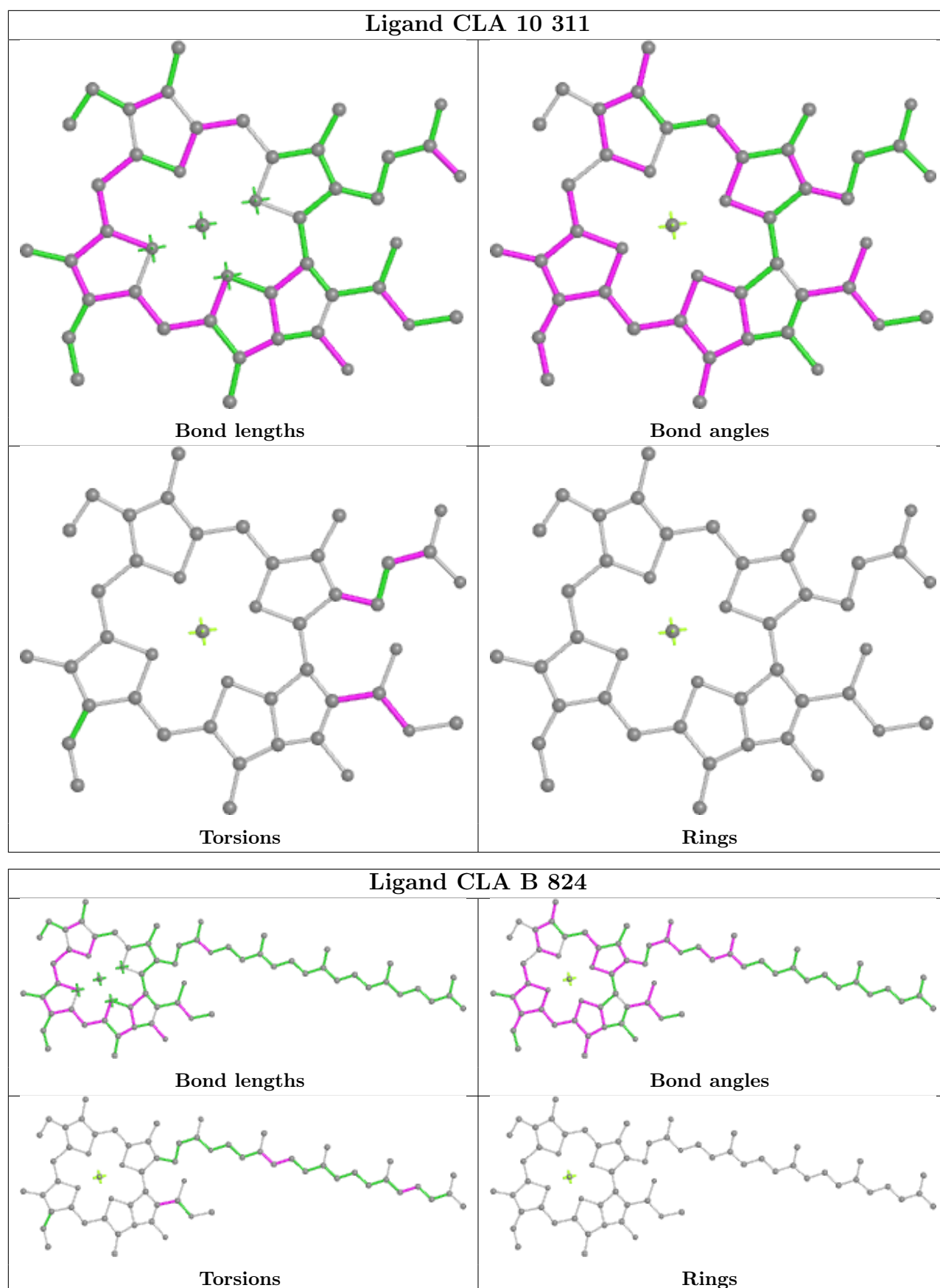
Bond angles



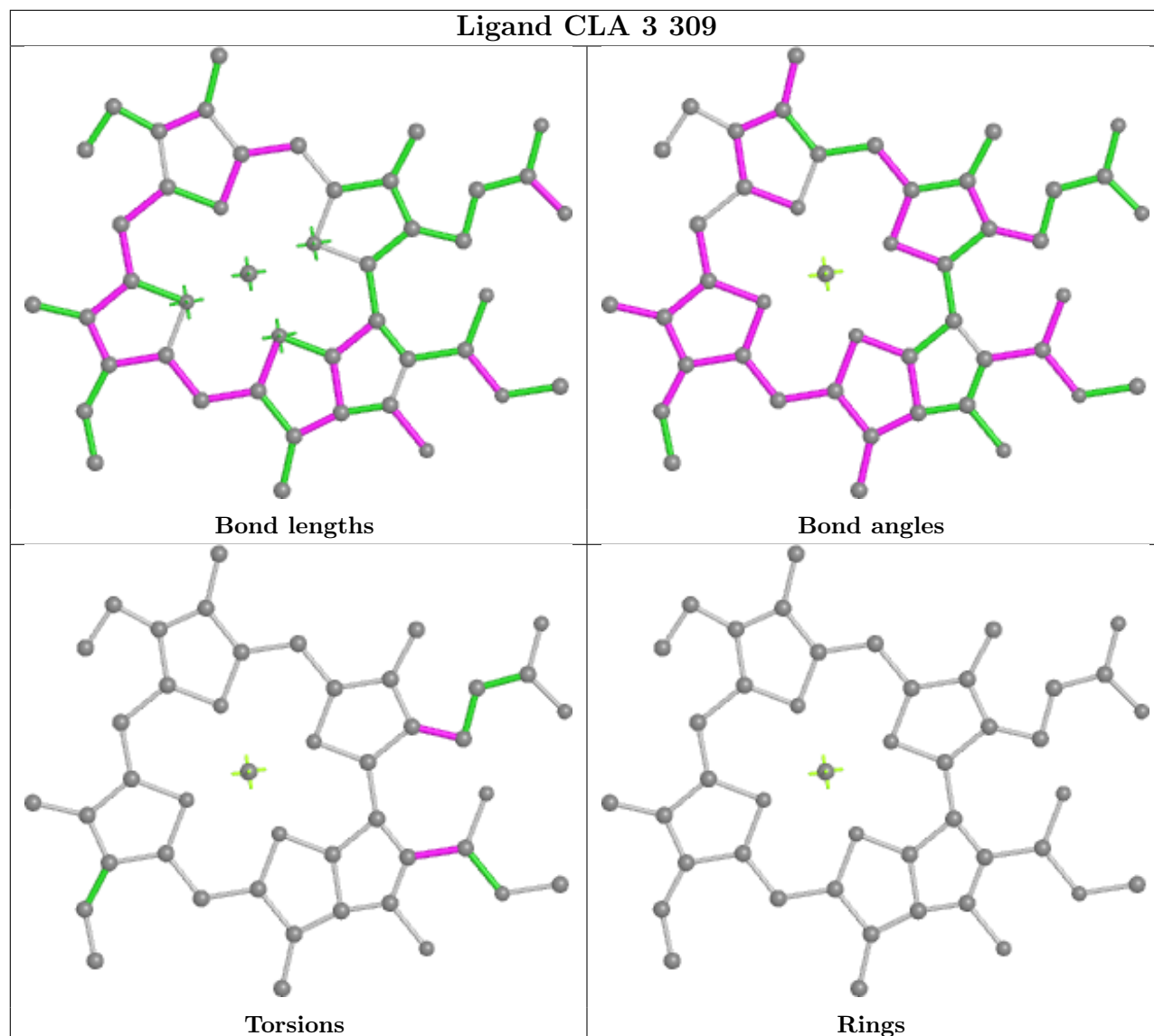
Torsions



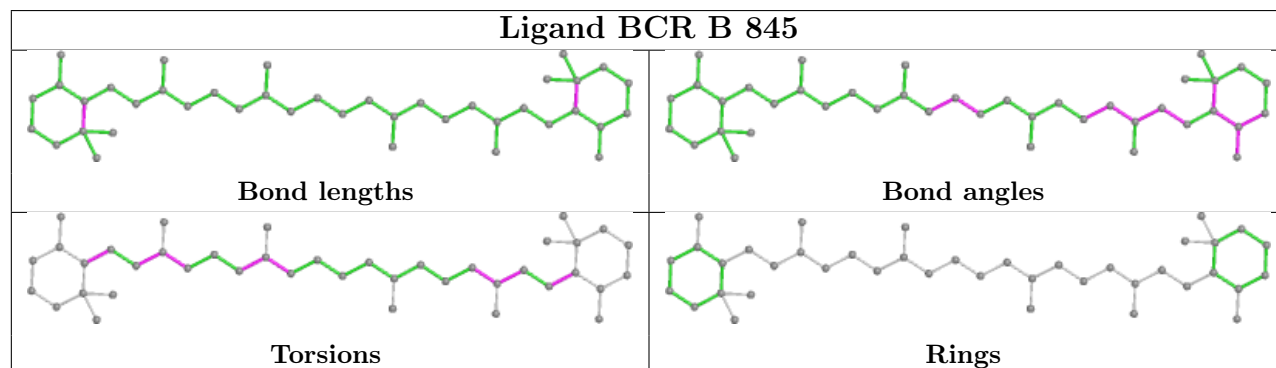
Rings

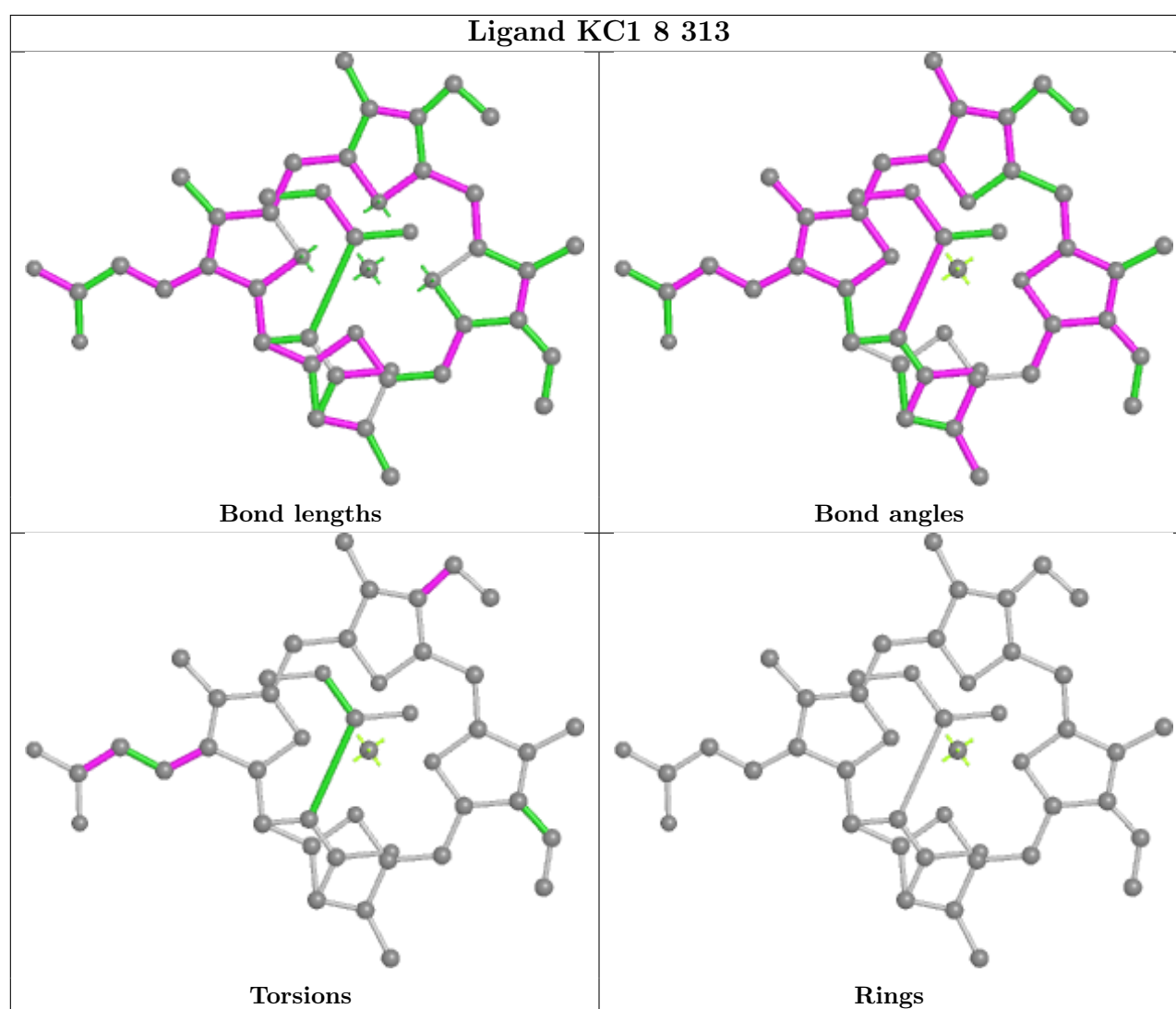
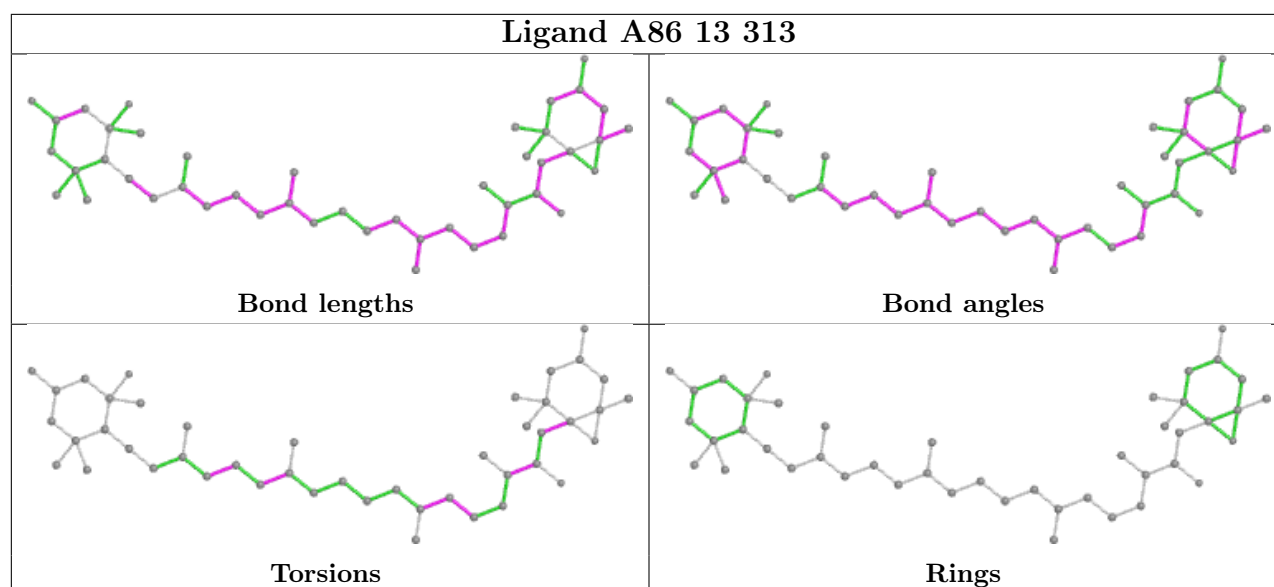


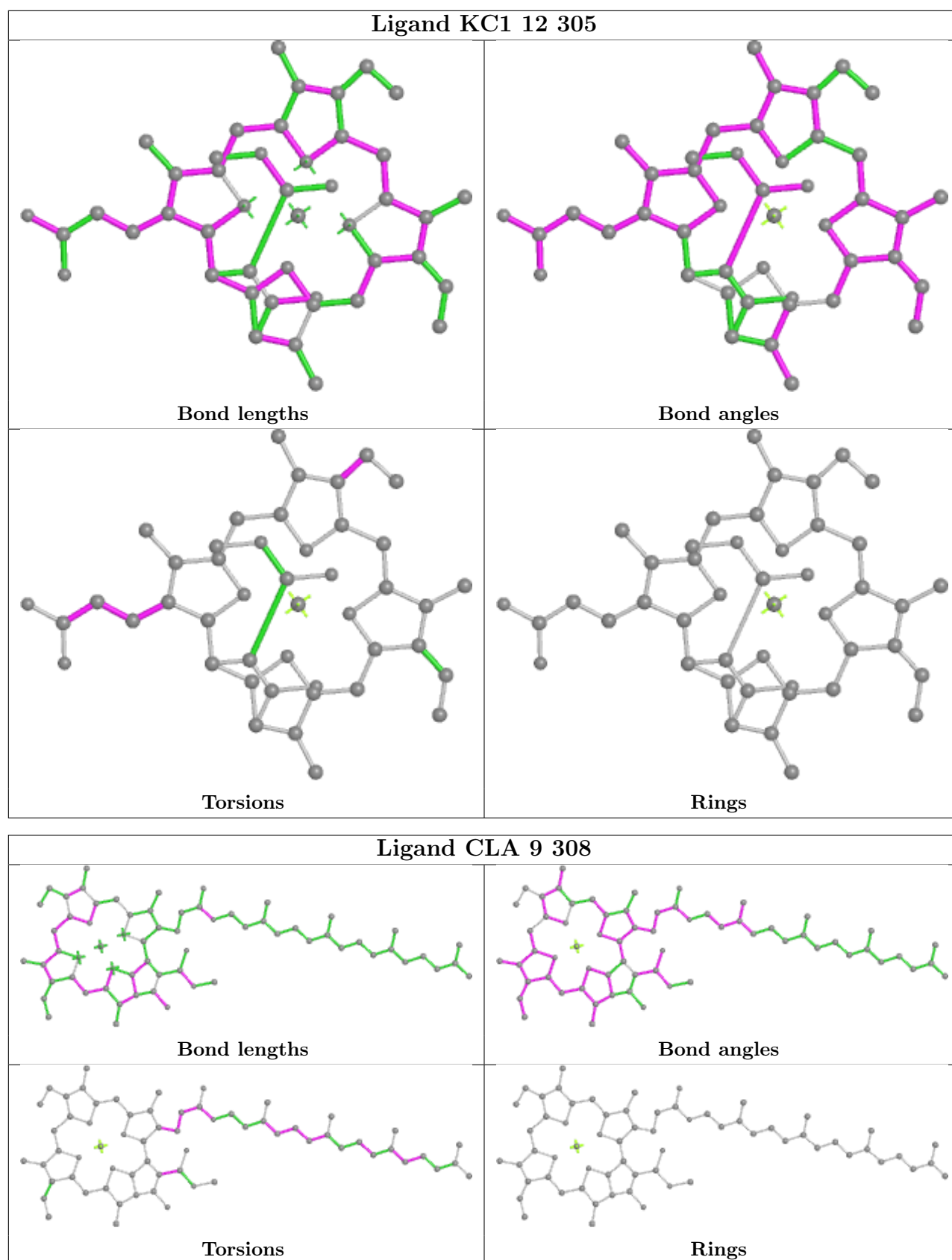
Ligand CLA 3 309

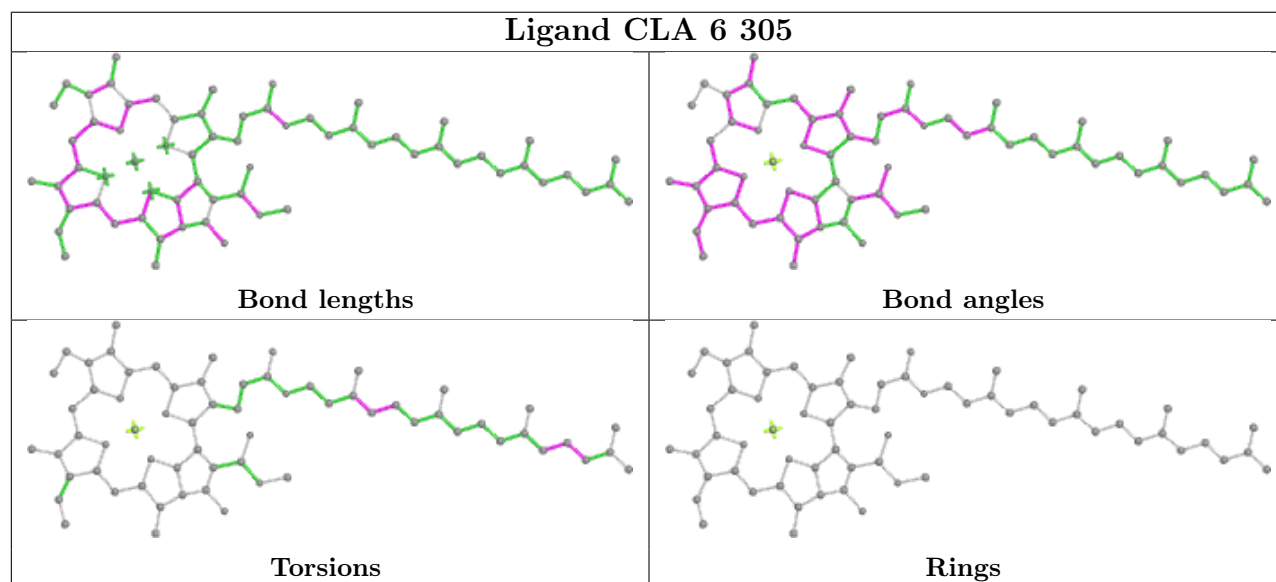
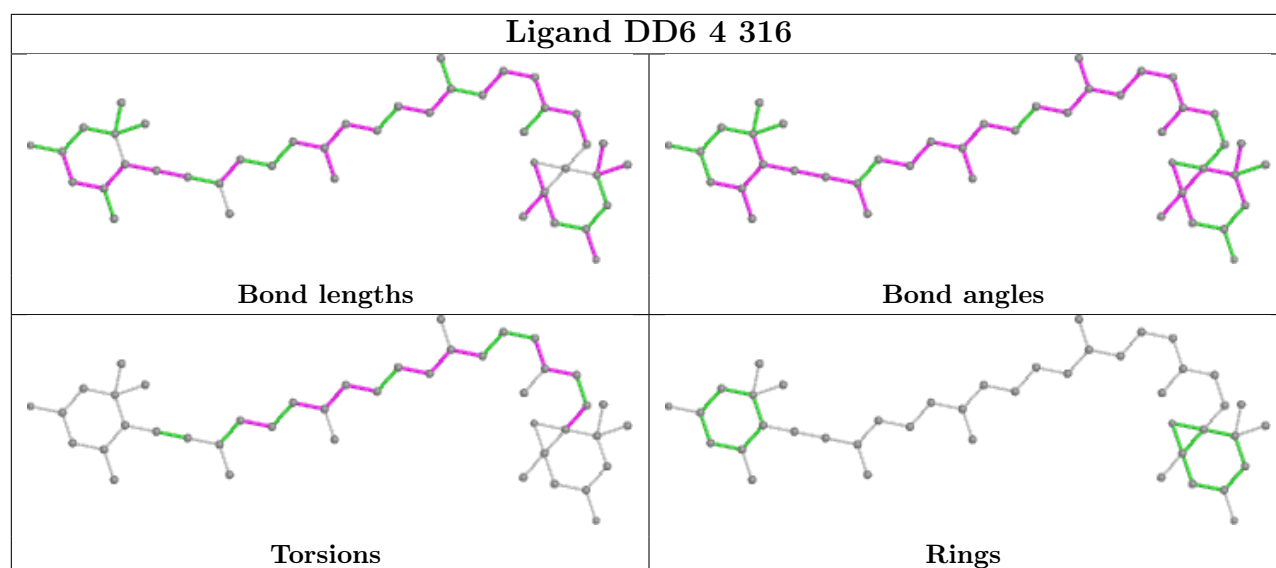


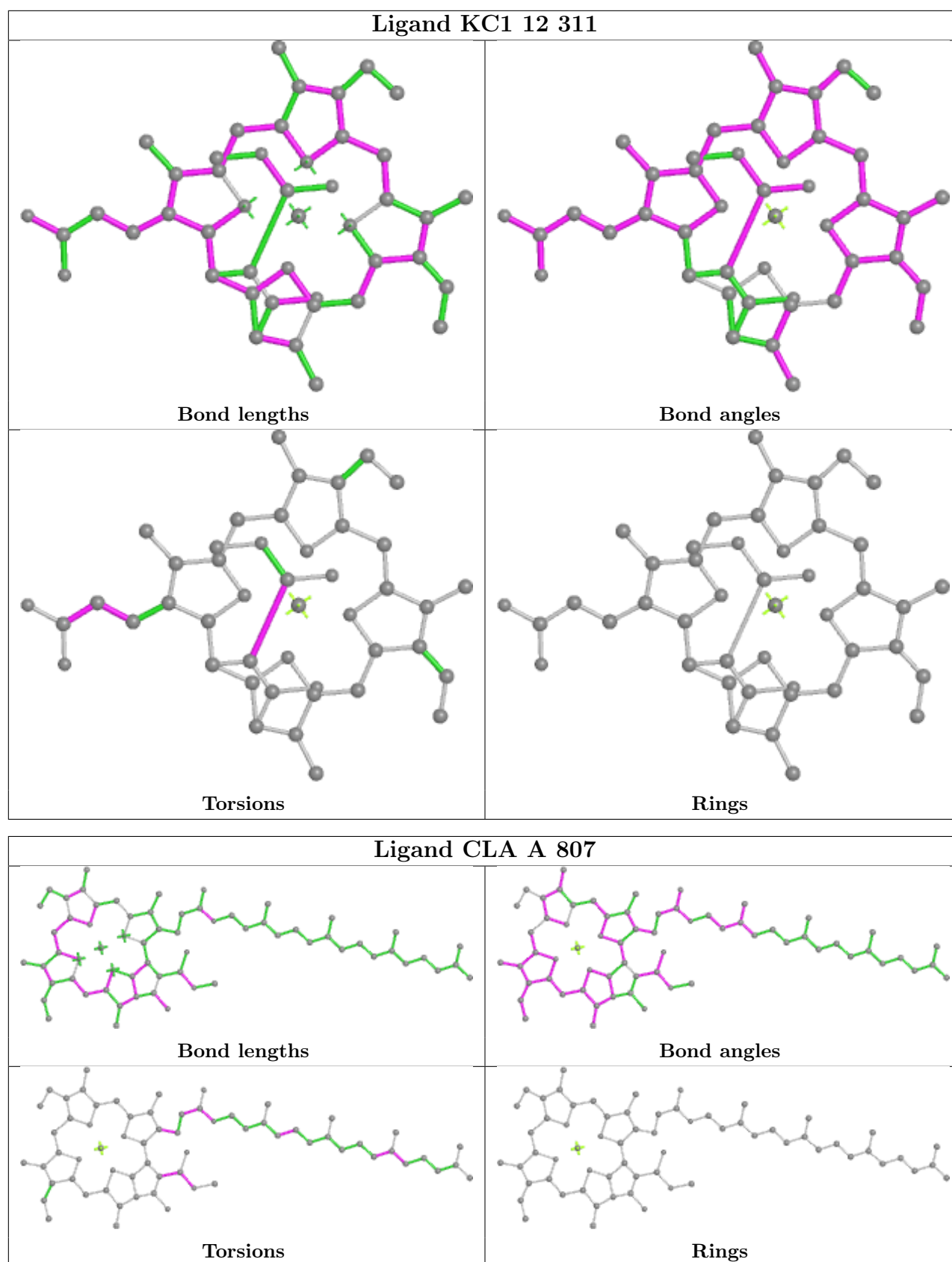
Ligand BCR B 845

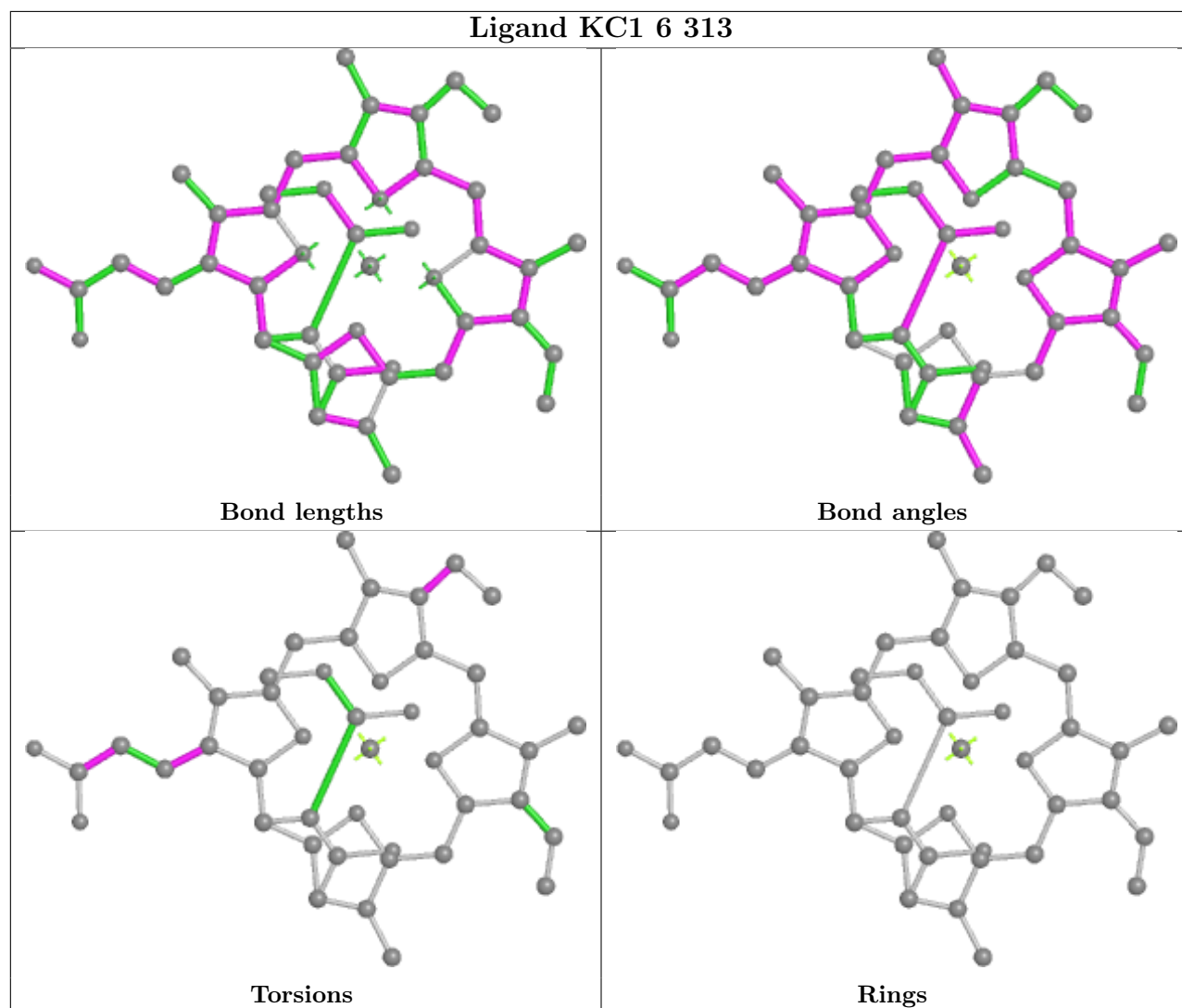
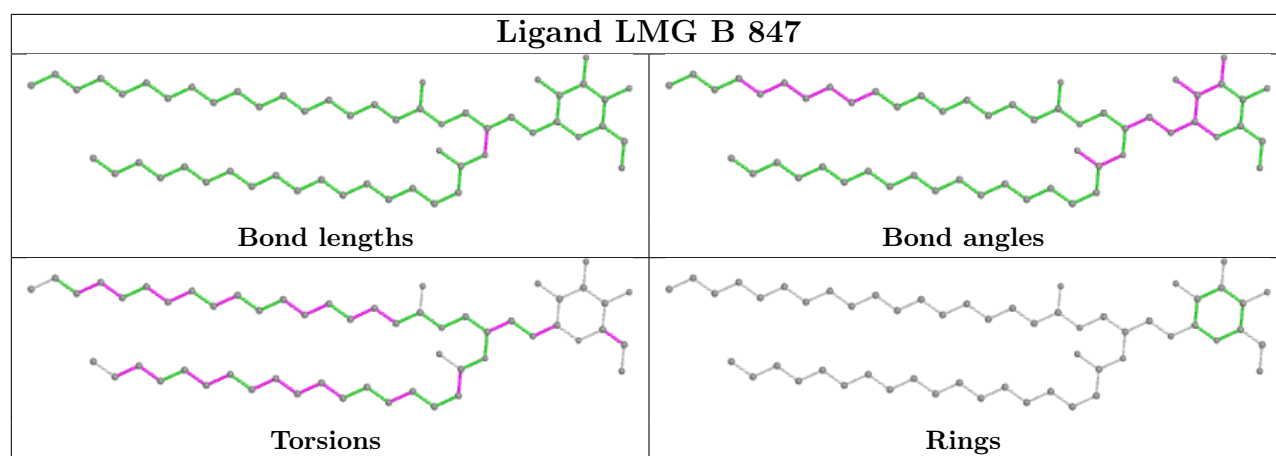


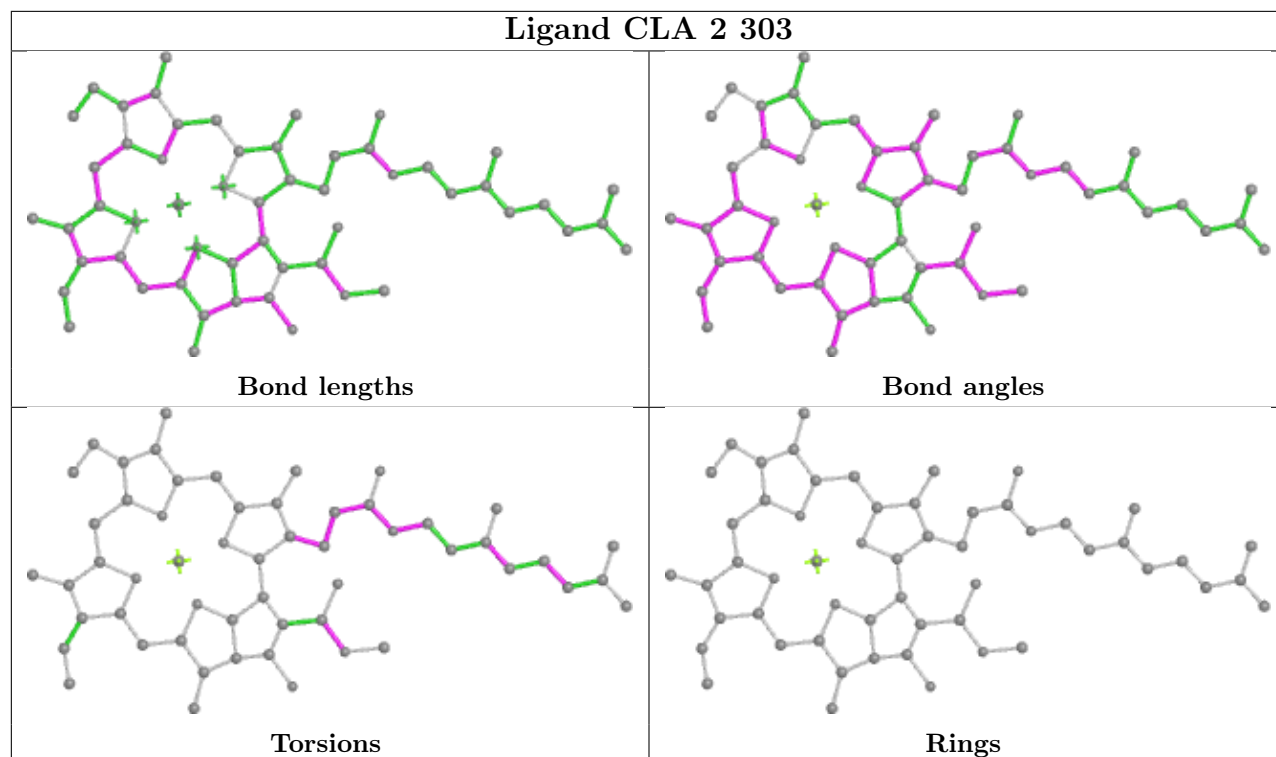
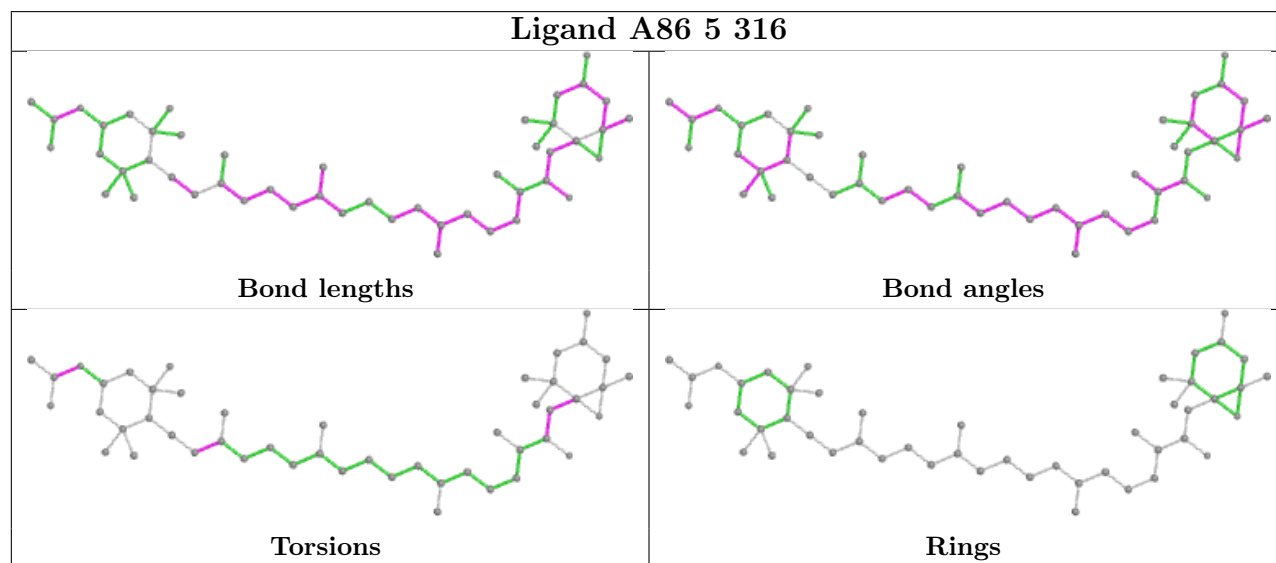


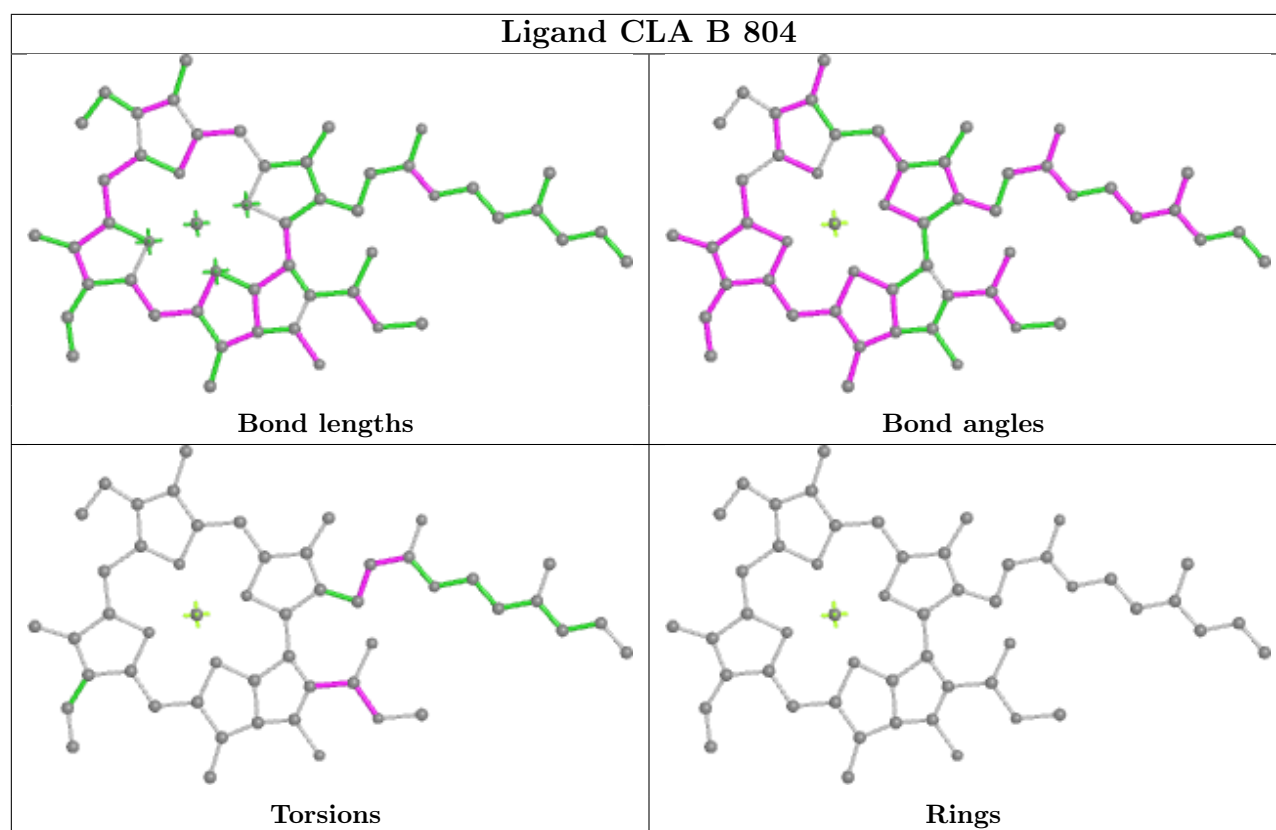


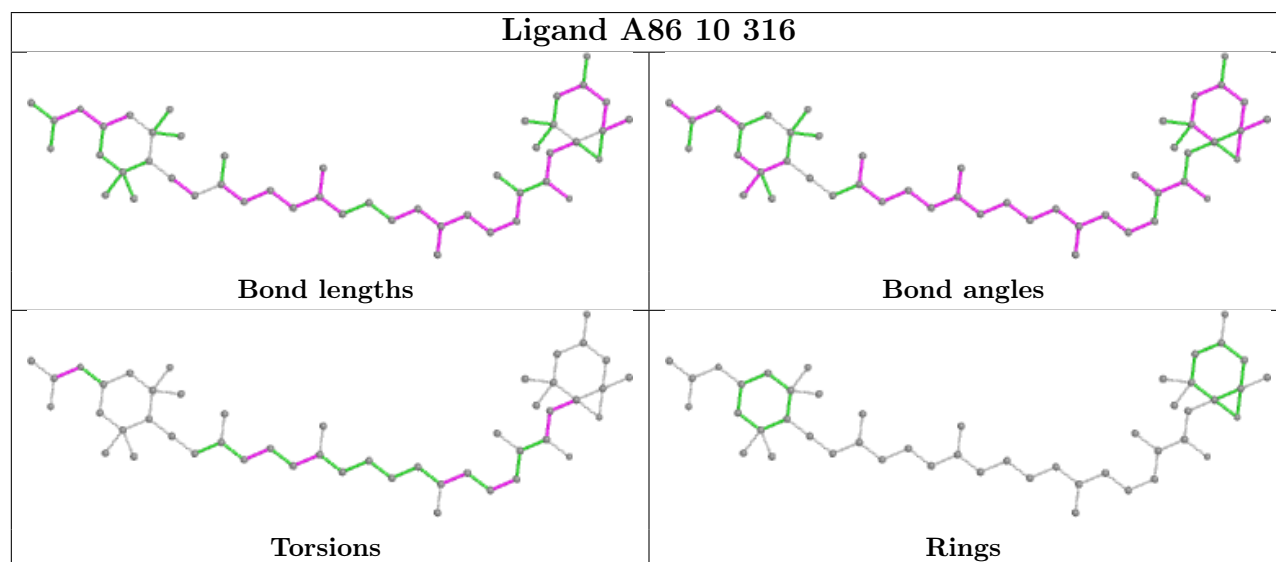
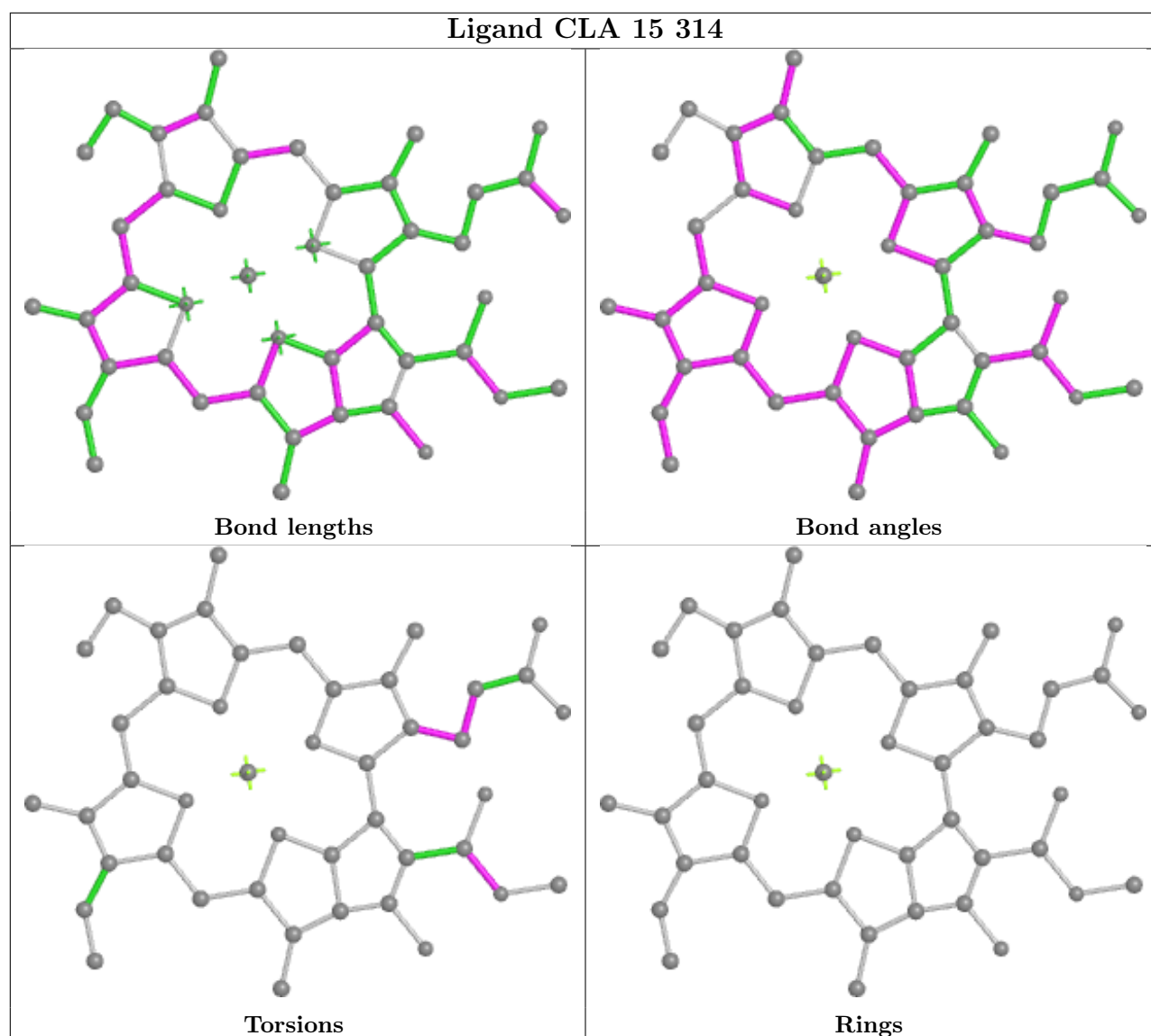


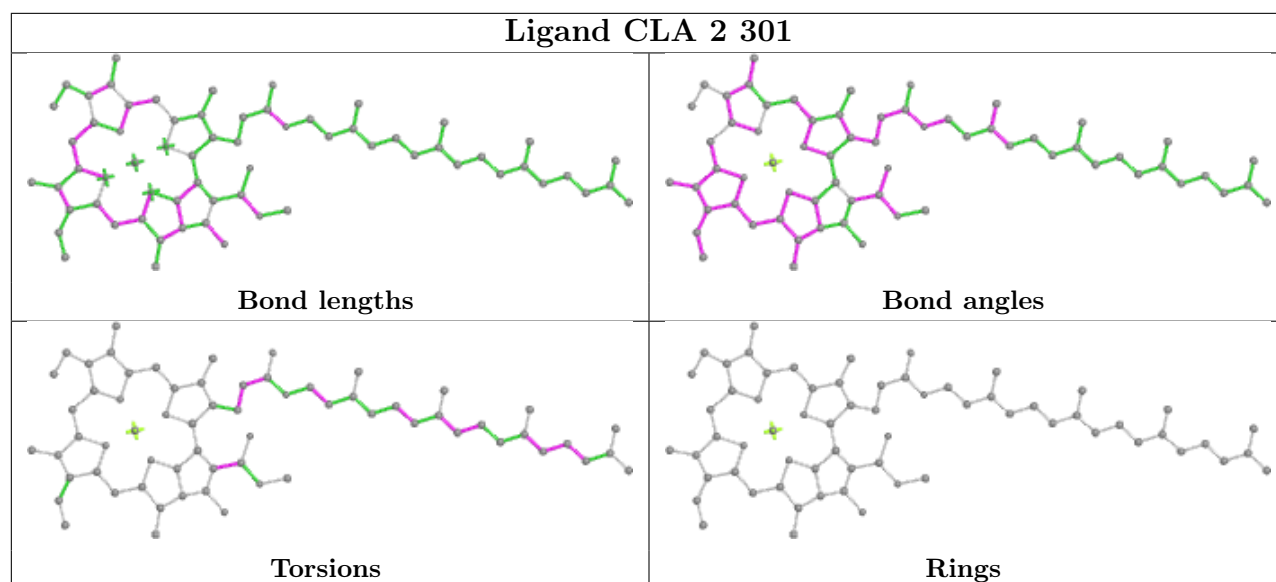
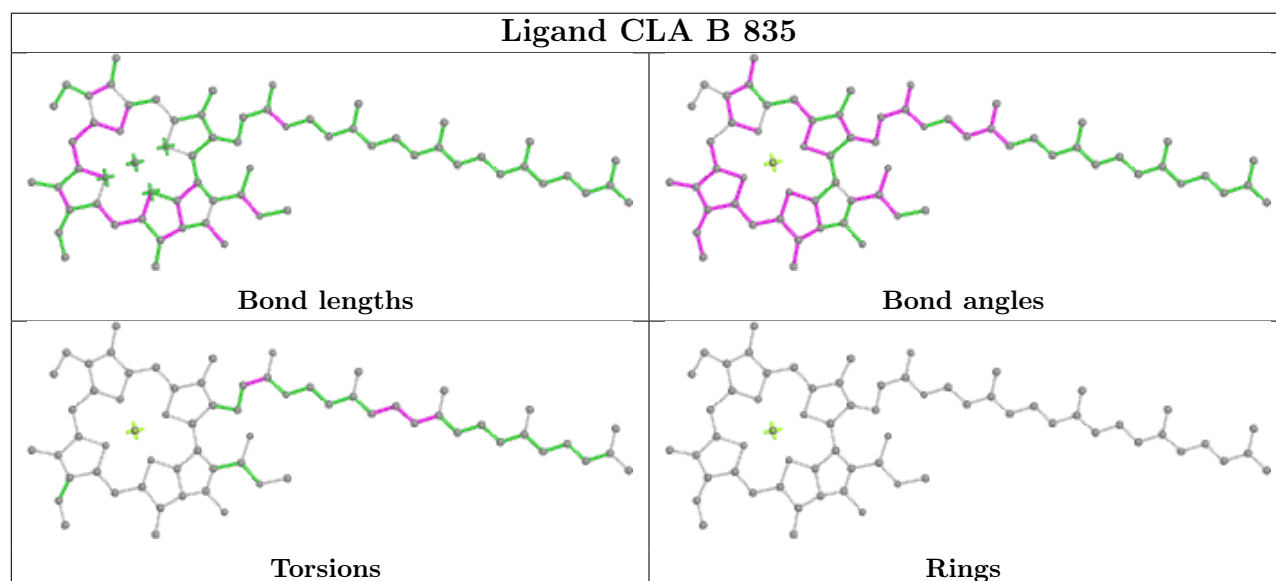
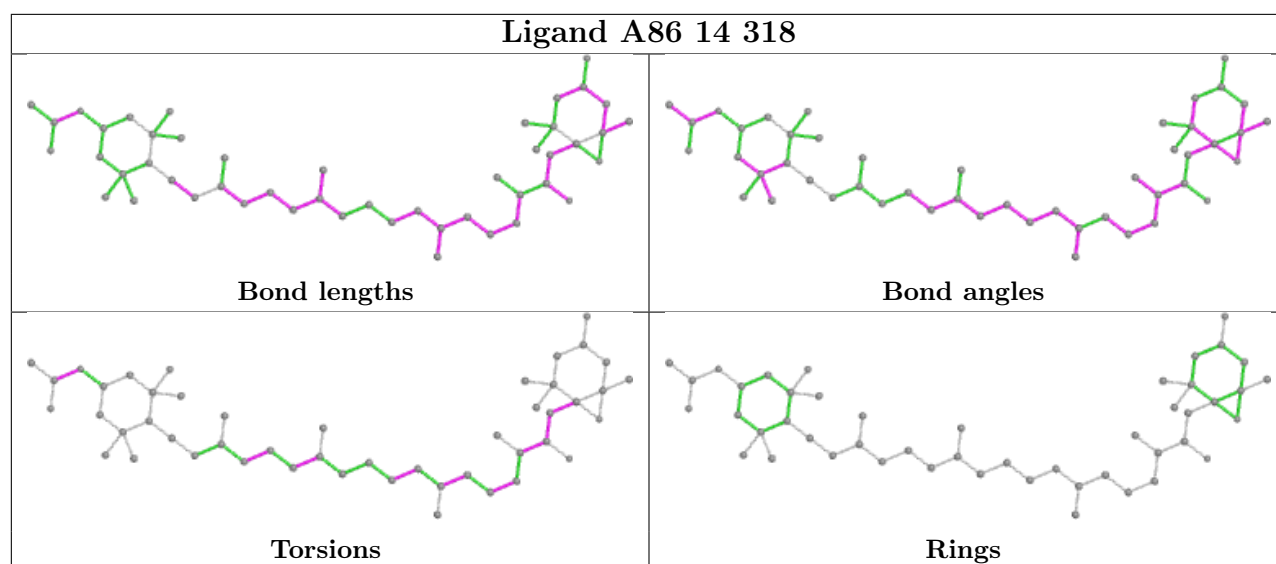




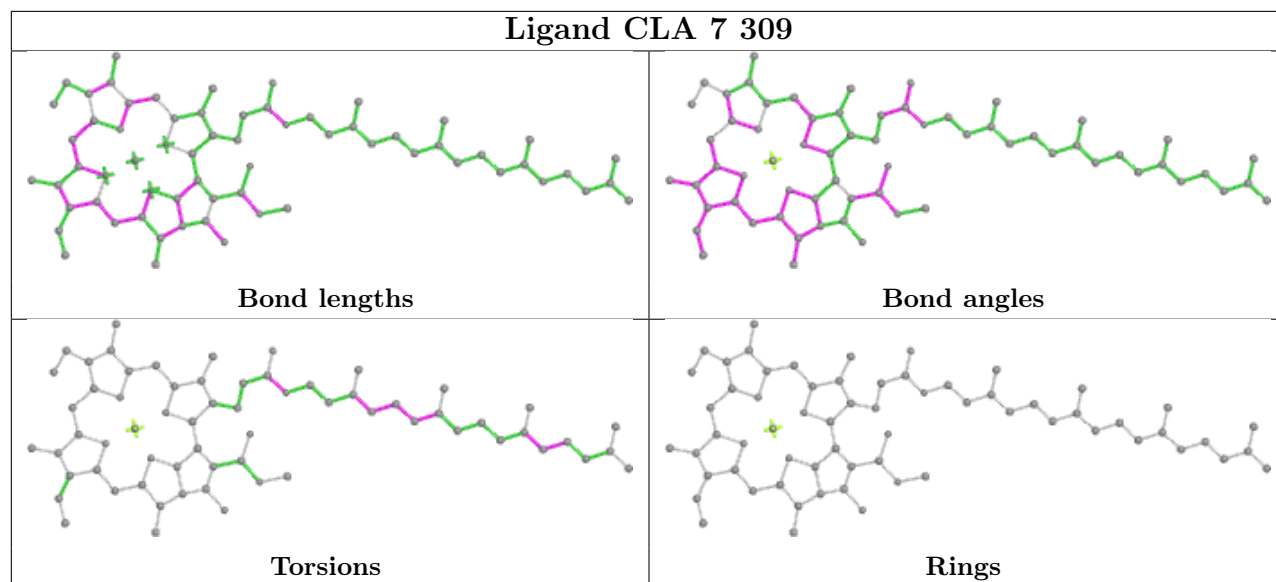
Ligand CLA 2 303**Ligand A86 5 316**



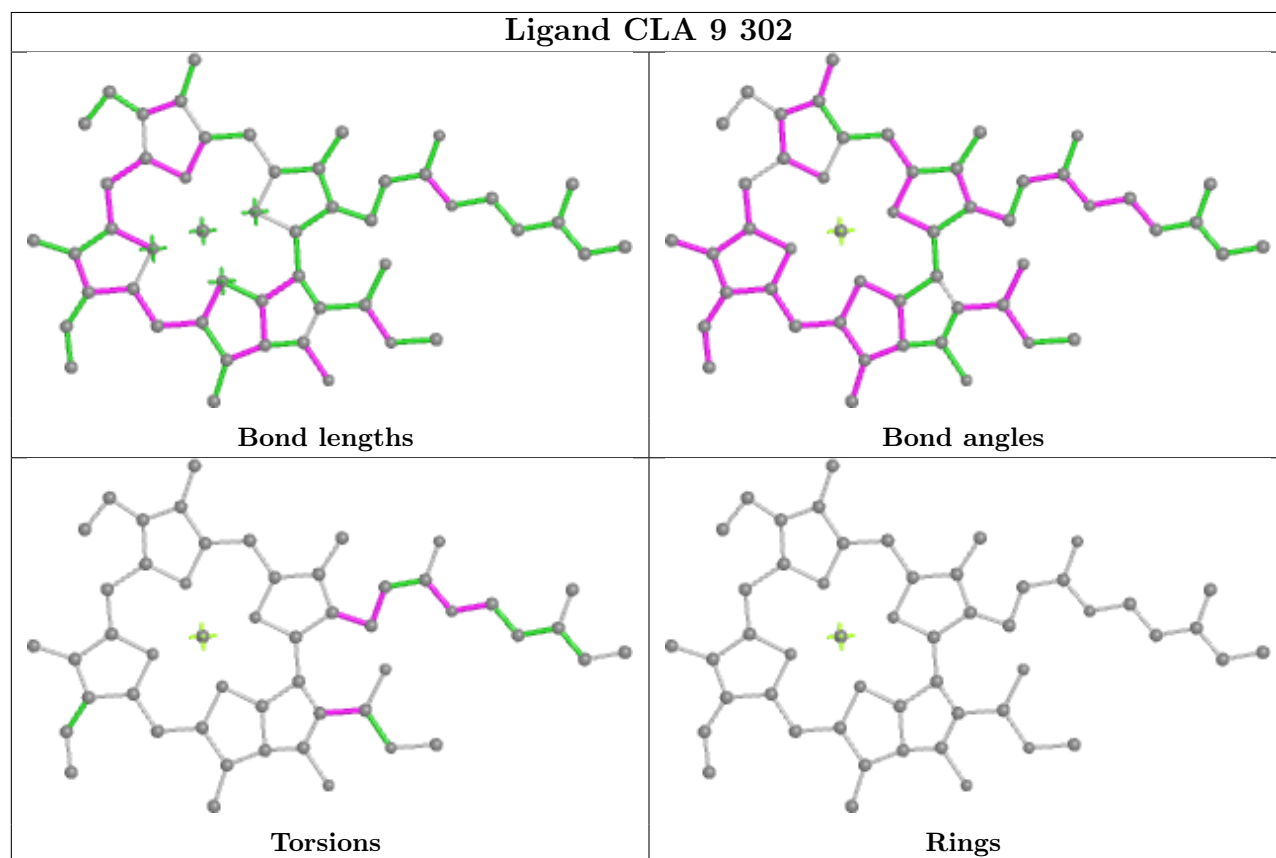


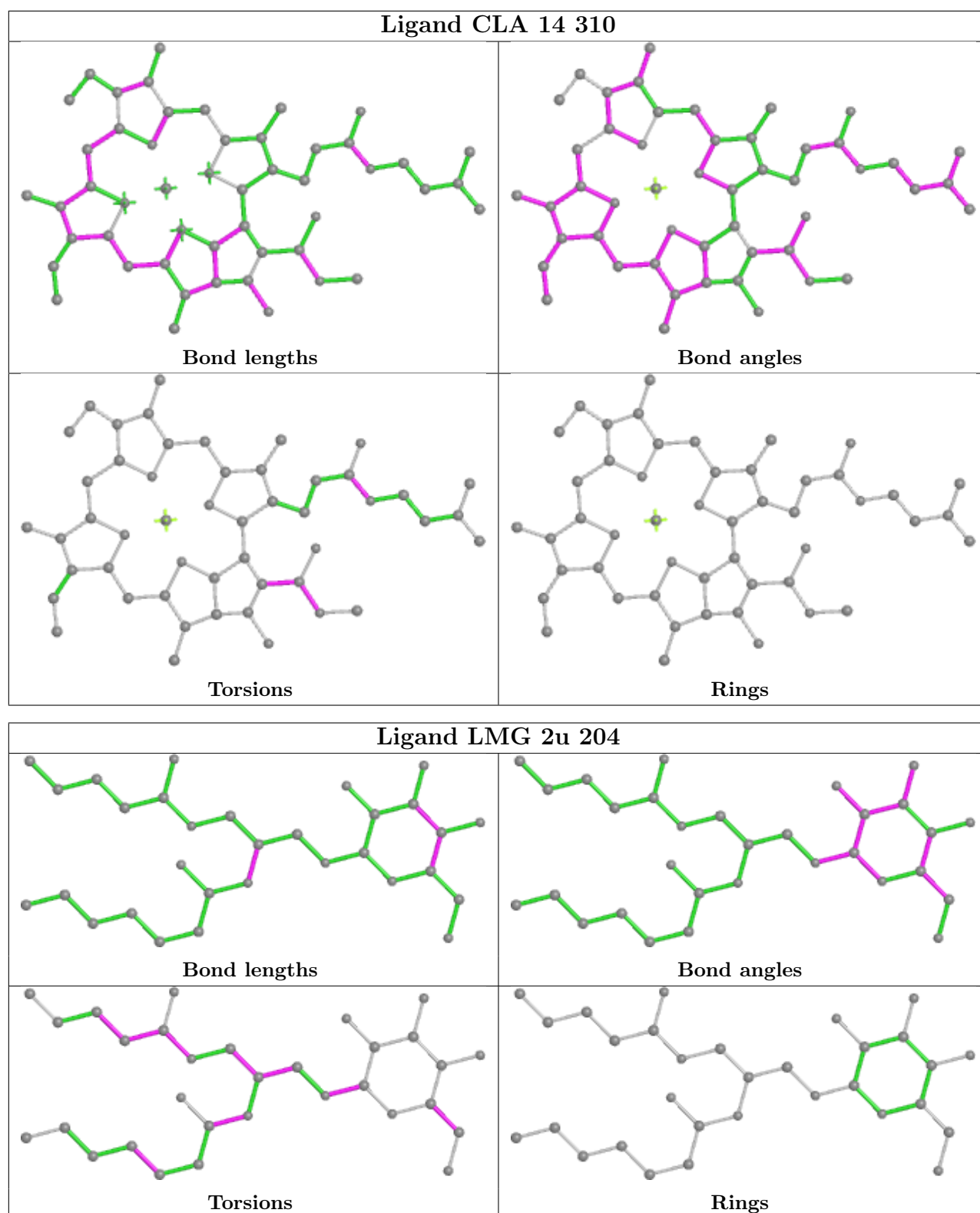


Ligand CLA 7 309

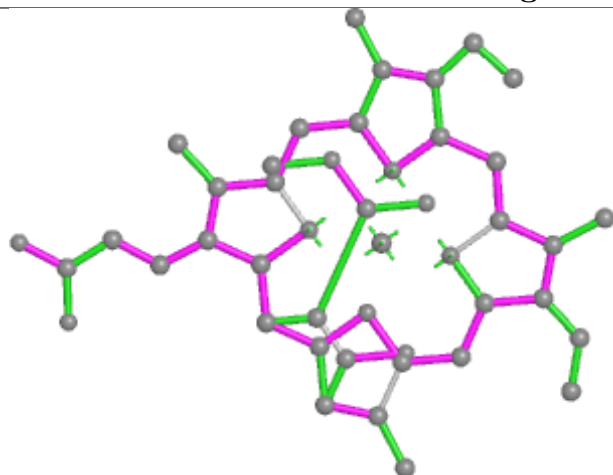


Ligand CLA 9 302

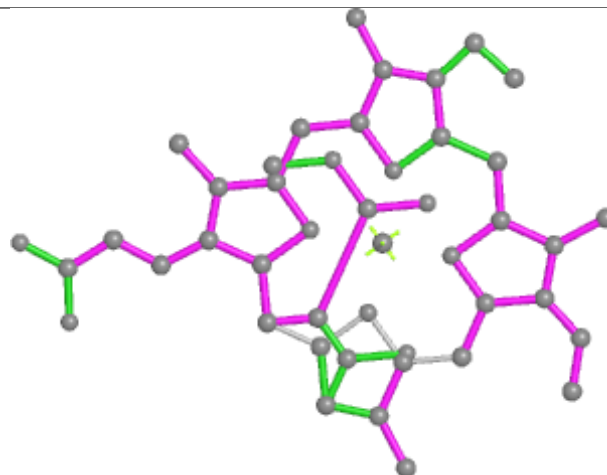




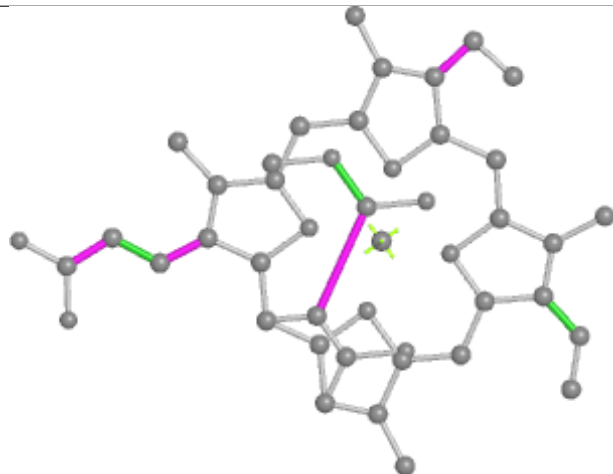
Ligand KC1 3 304



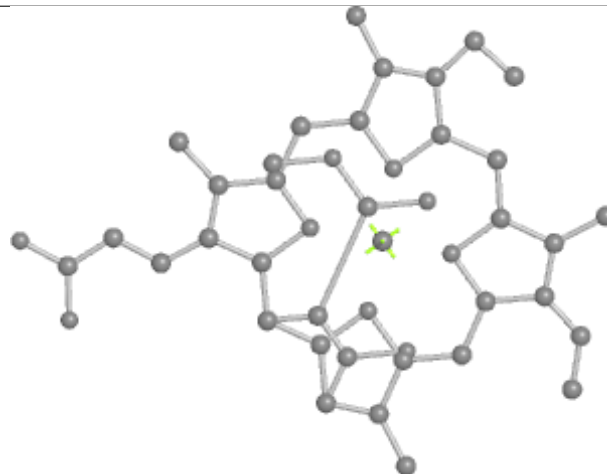
Bond lengths



Bond angles

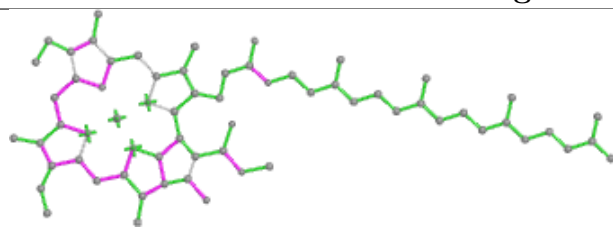


Torsions

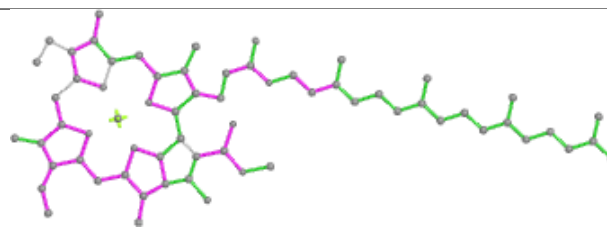


Rings

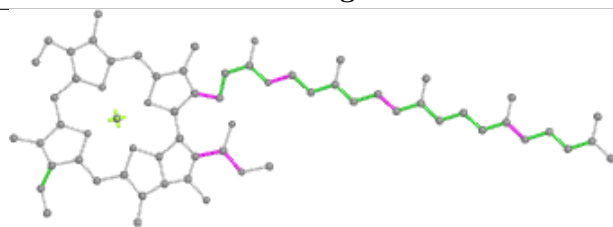
Ligand CLA A 835



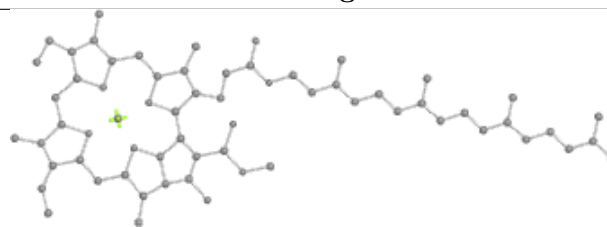
Bond lengths



Bond angles

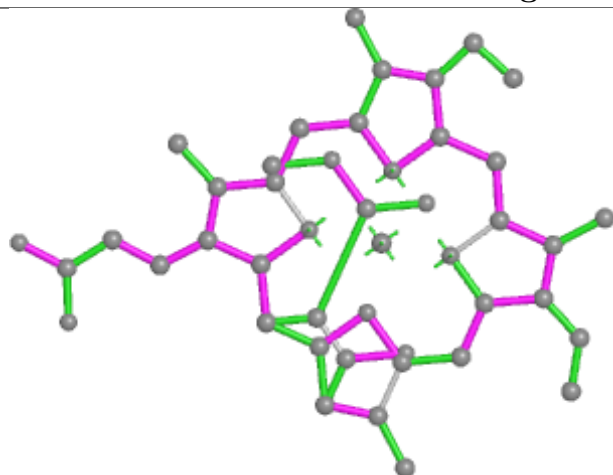


Torsions

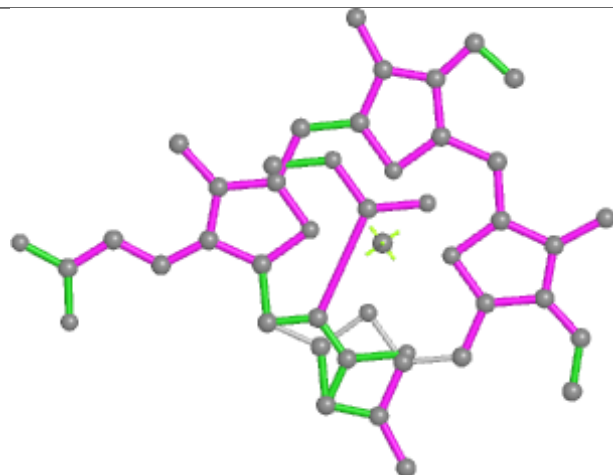


Rings

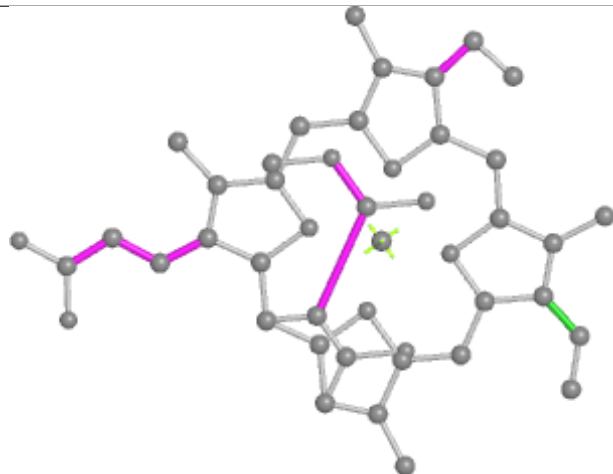
Ligand KC1 1 306



Bond lengths



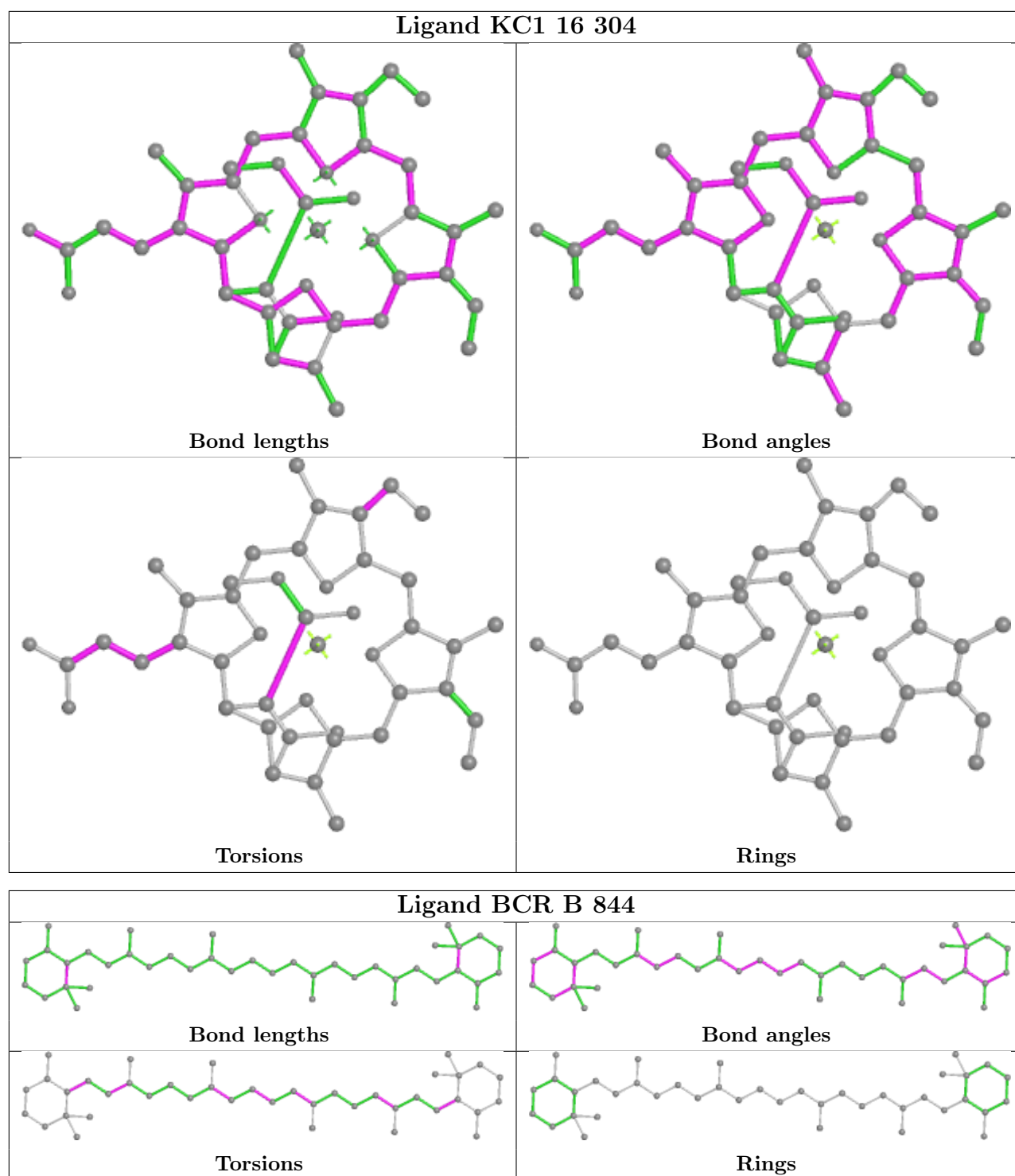
Bond angles

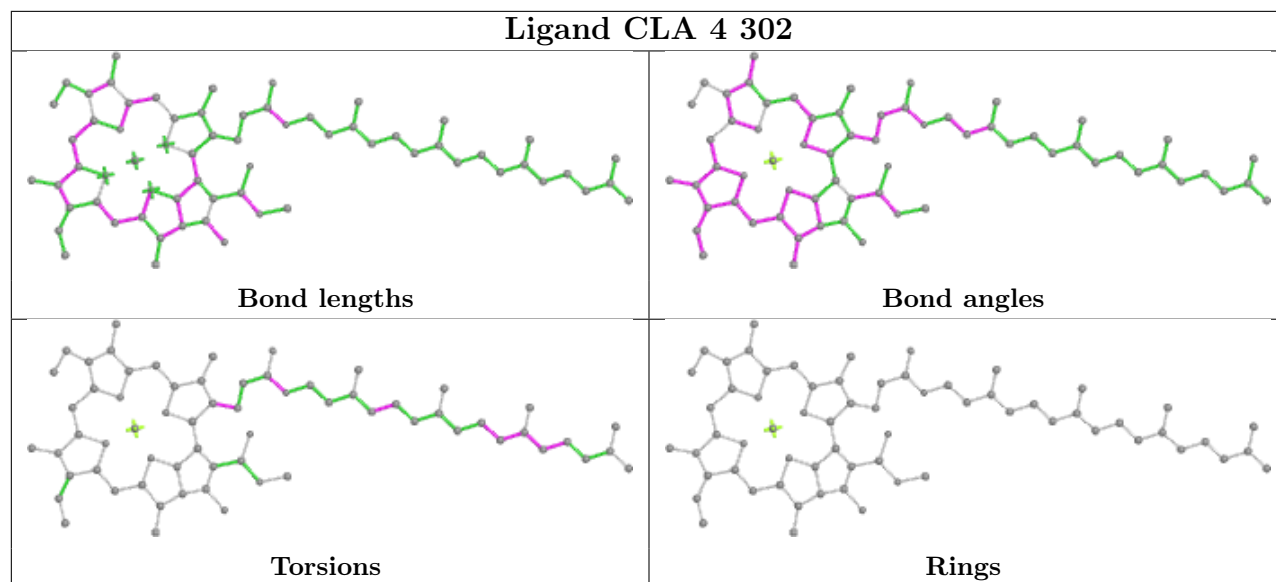
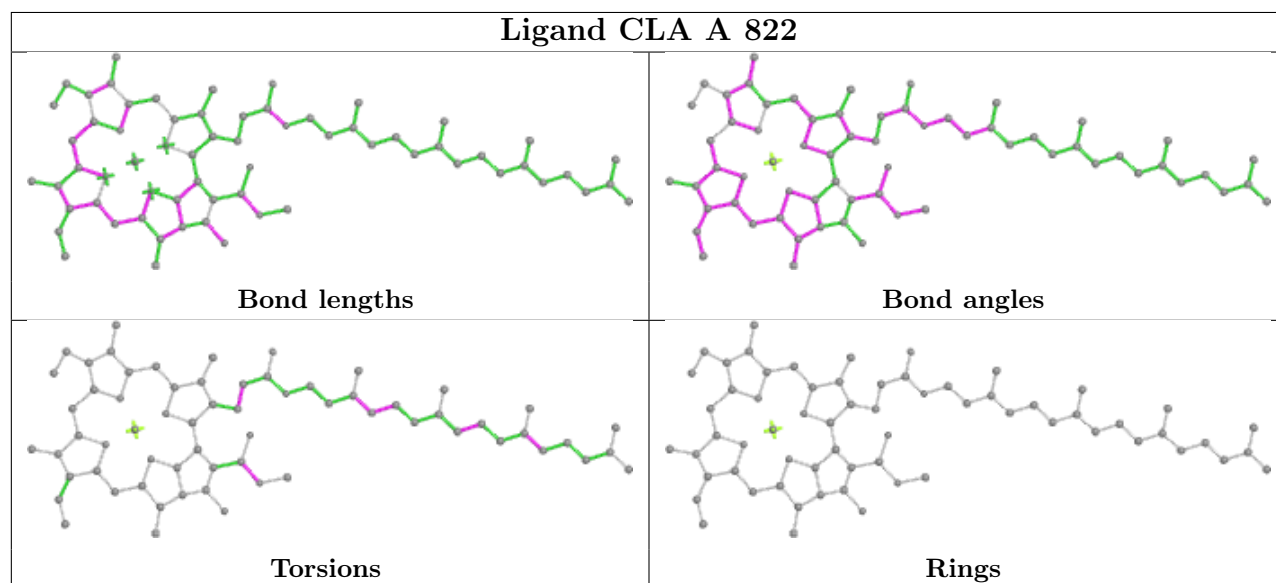


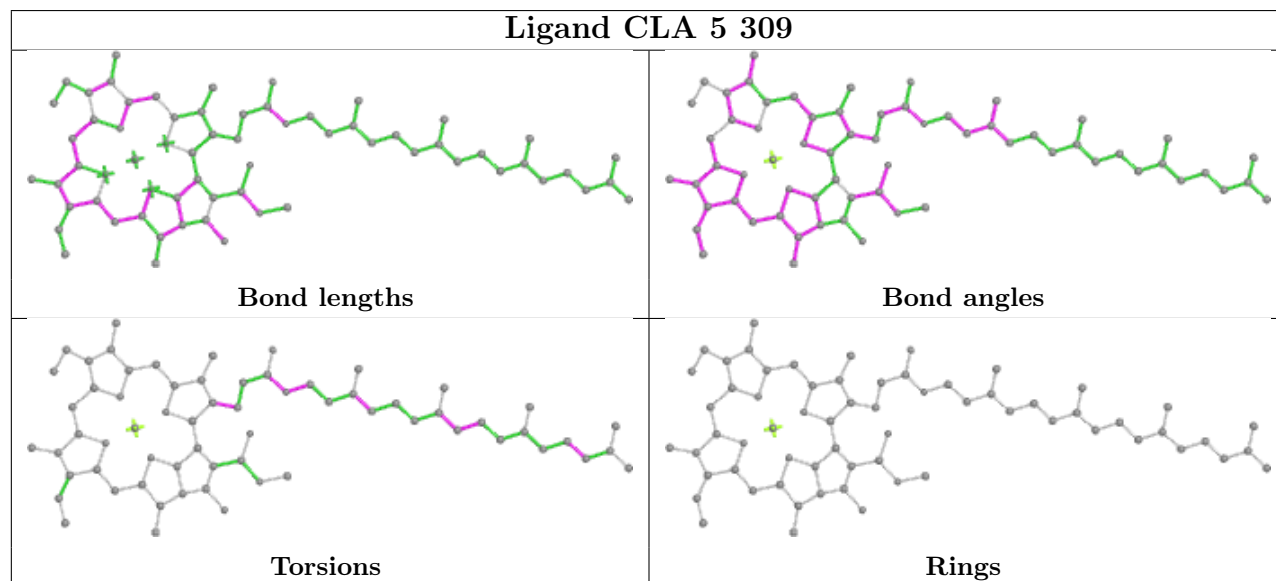
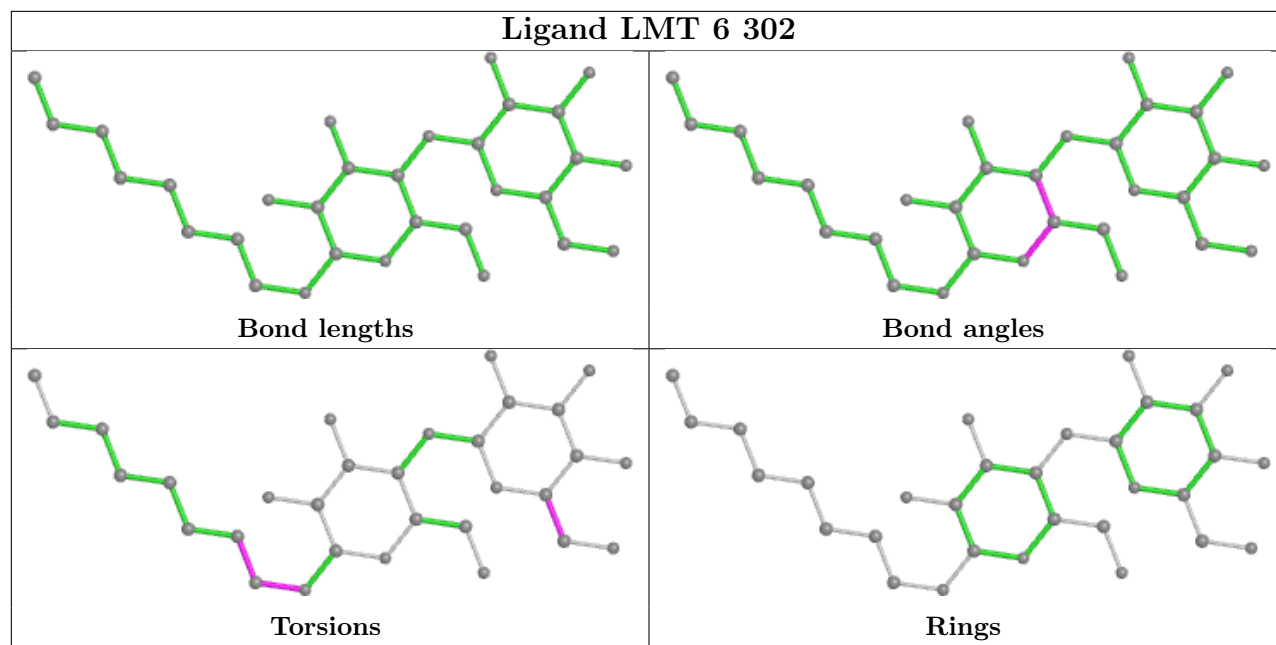
Torsions

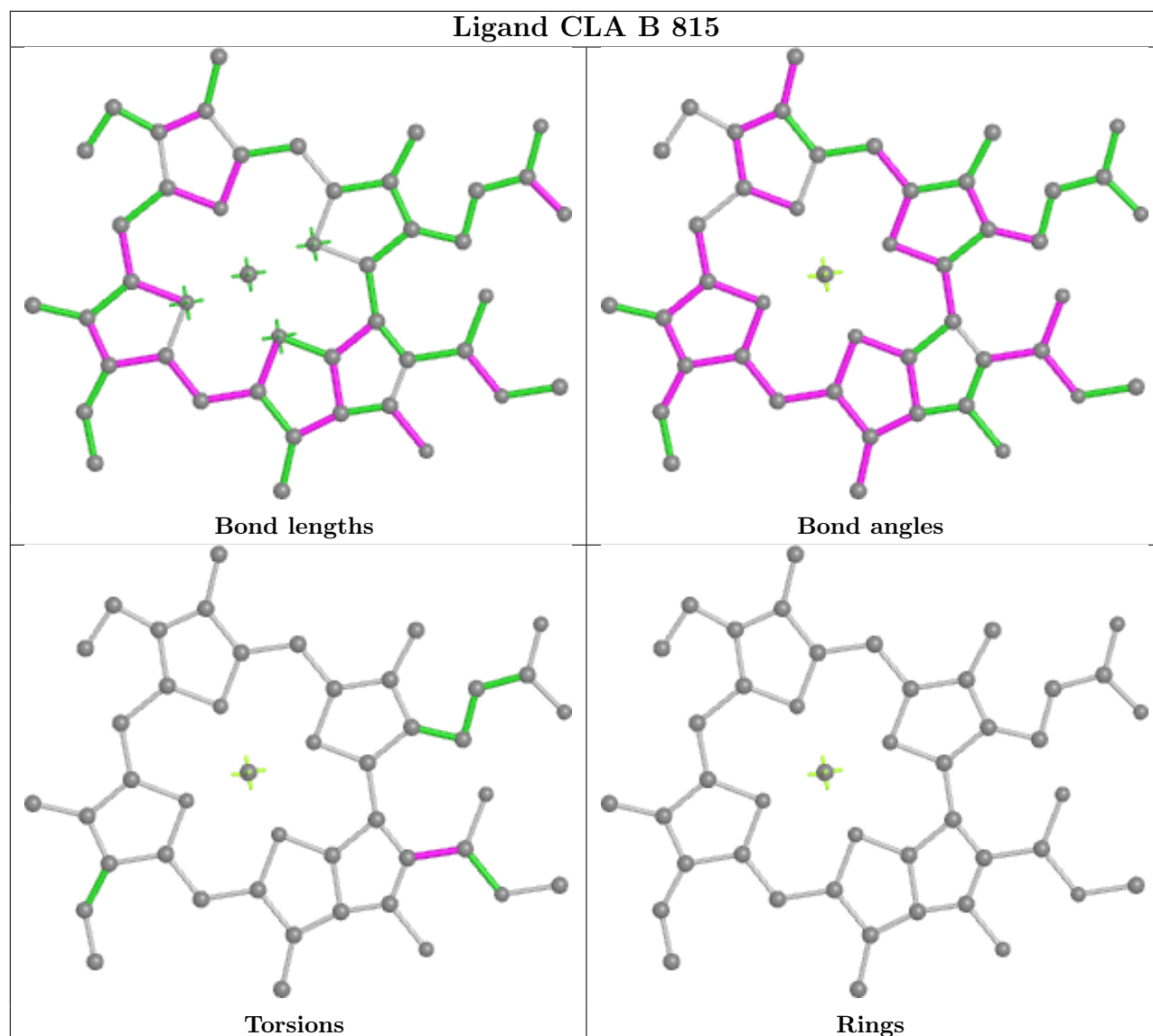
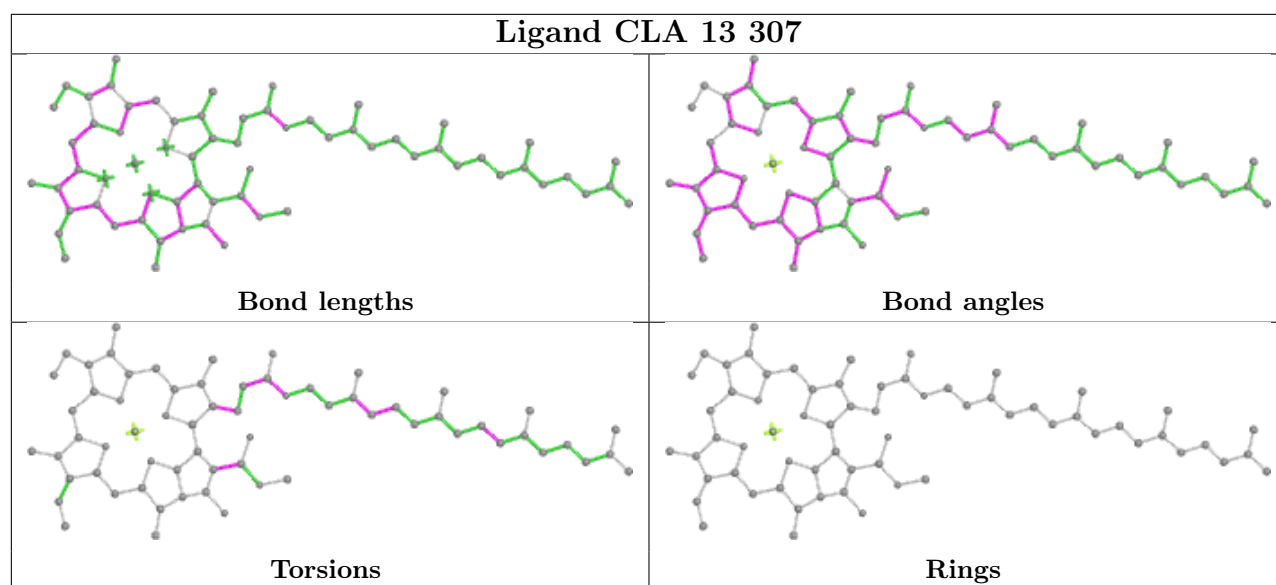


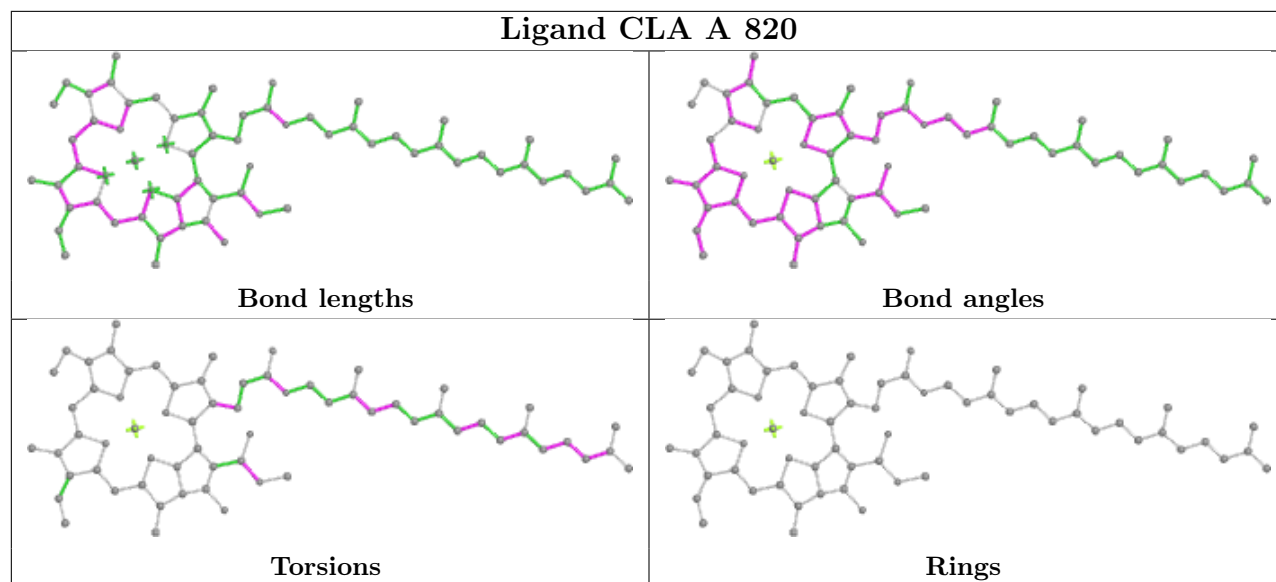
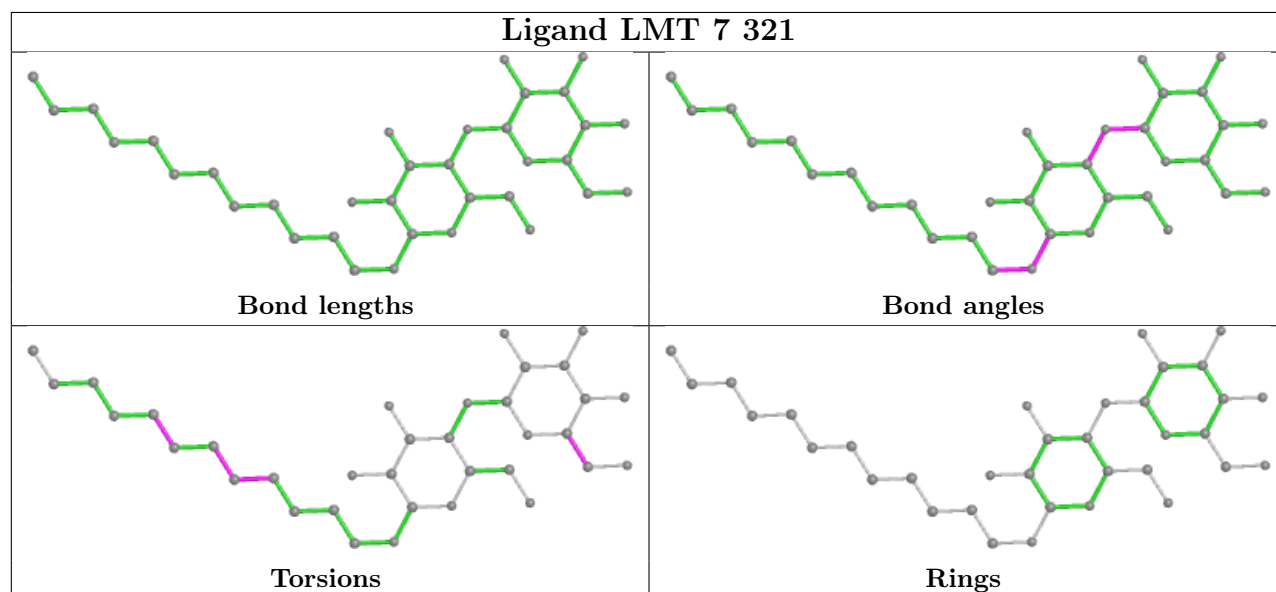
Rings



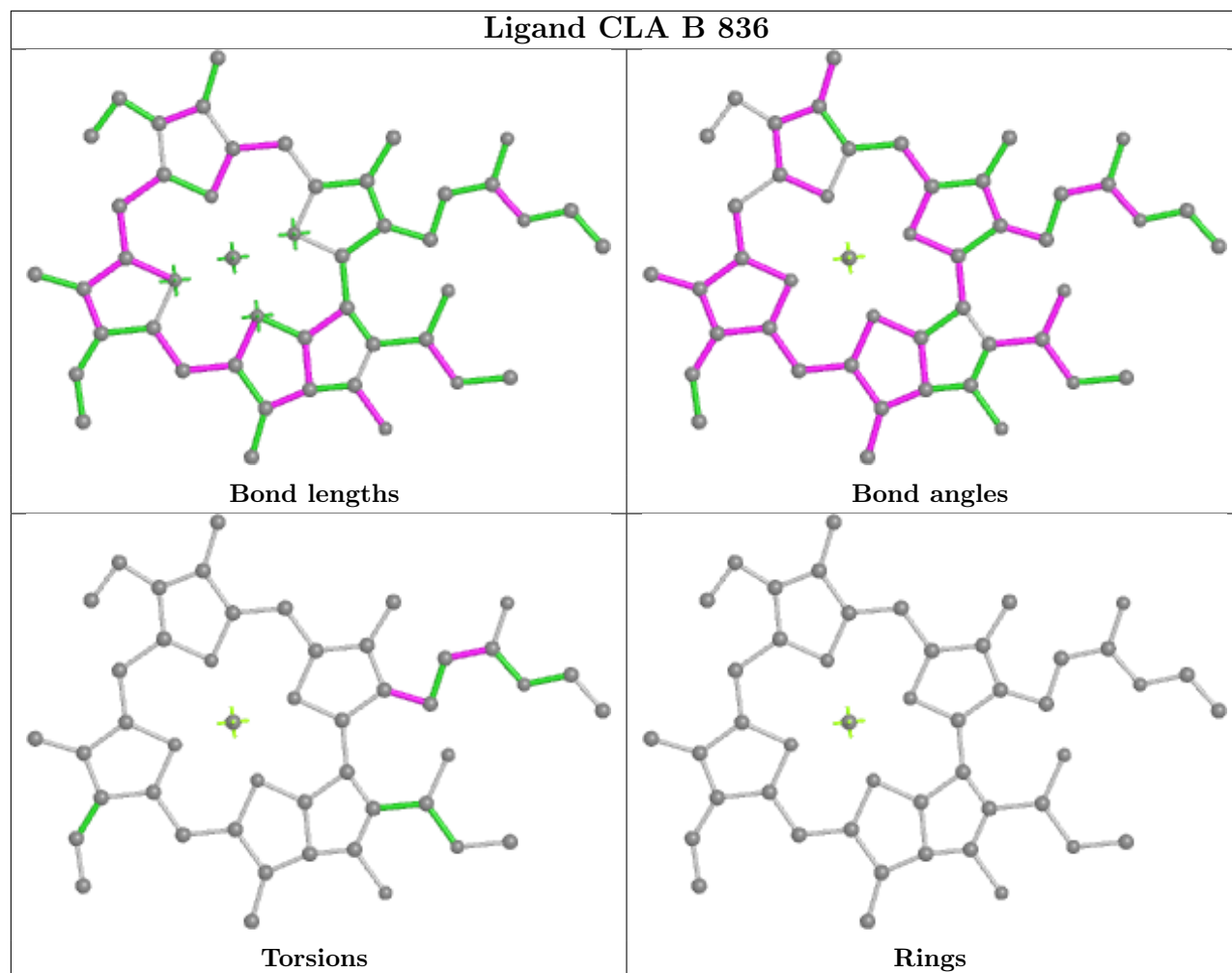
Ligand CLA 4 302**Ligand CLA A 822**



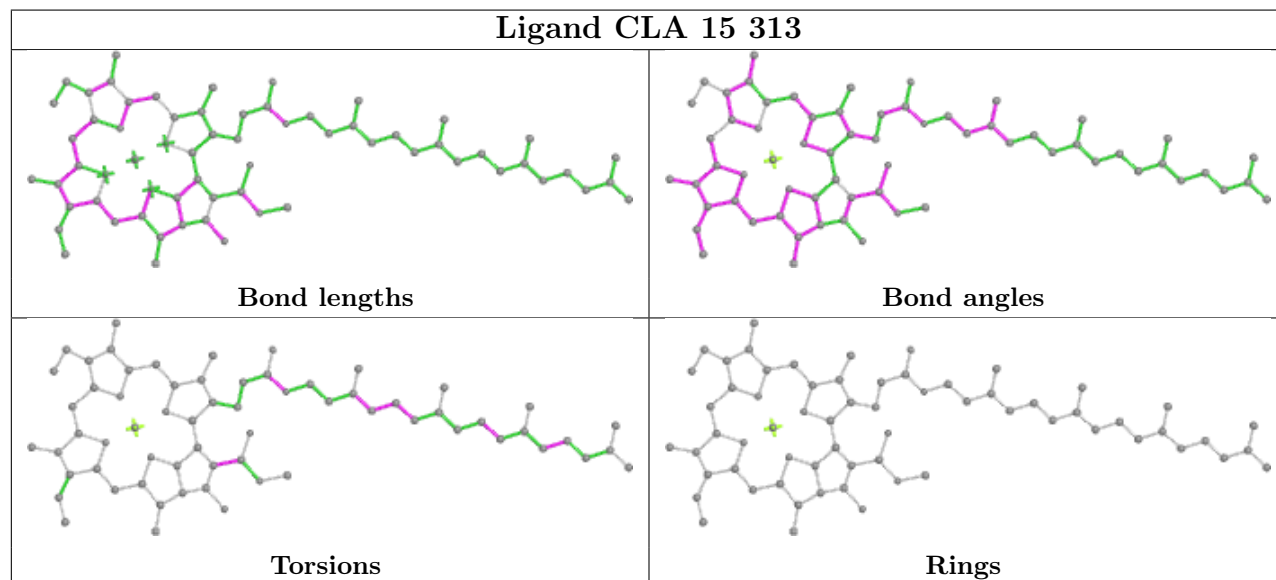


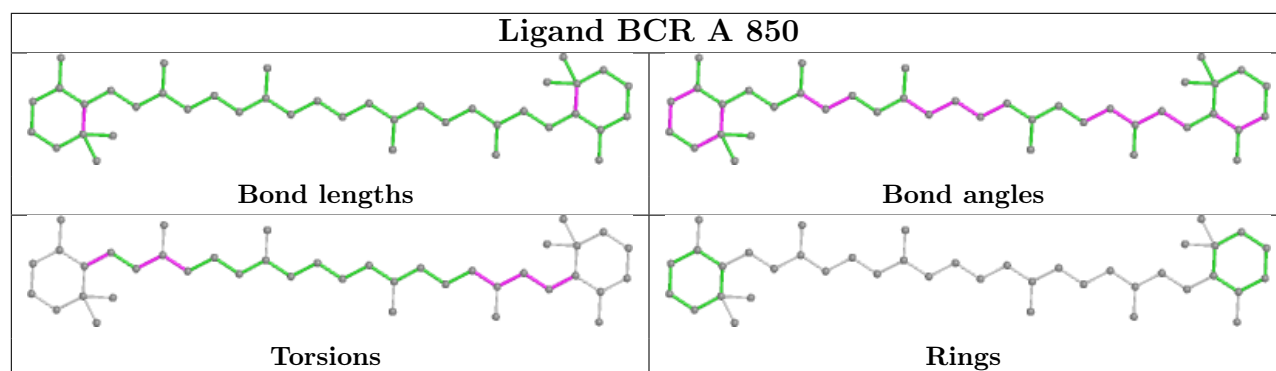
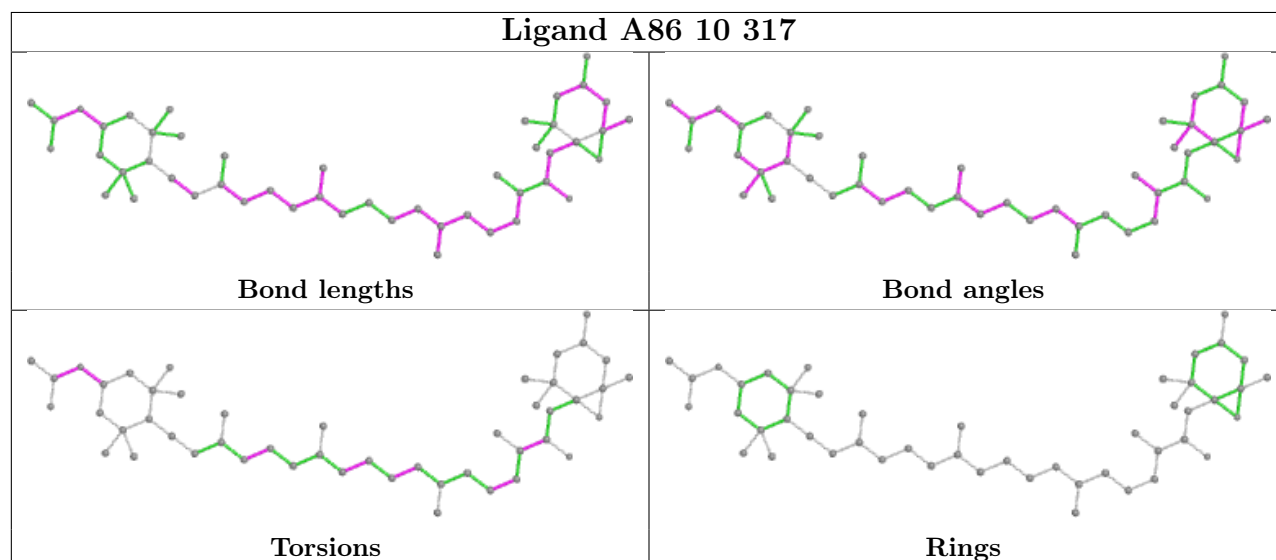
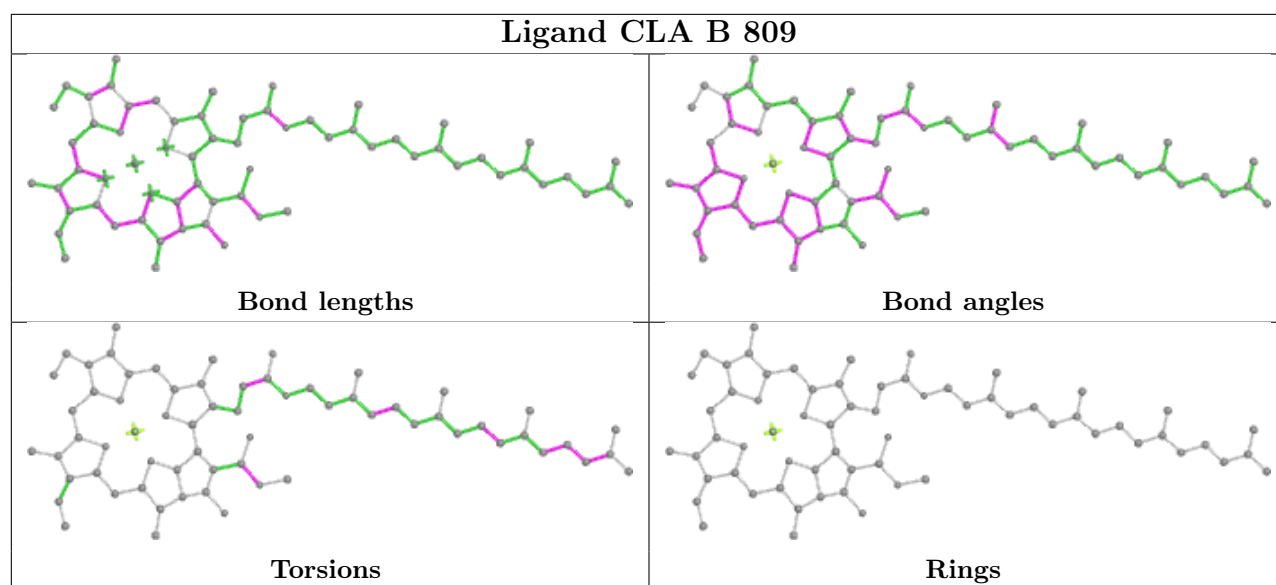
Ligand CLA A 820**Ligand LMT 7 321**

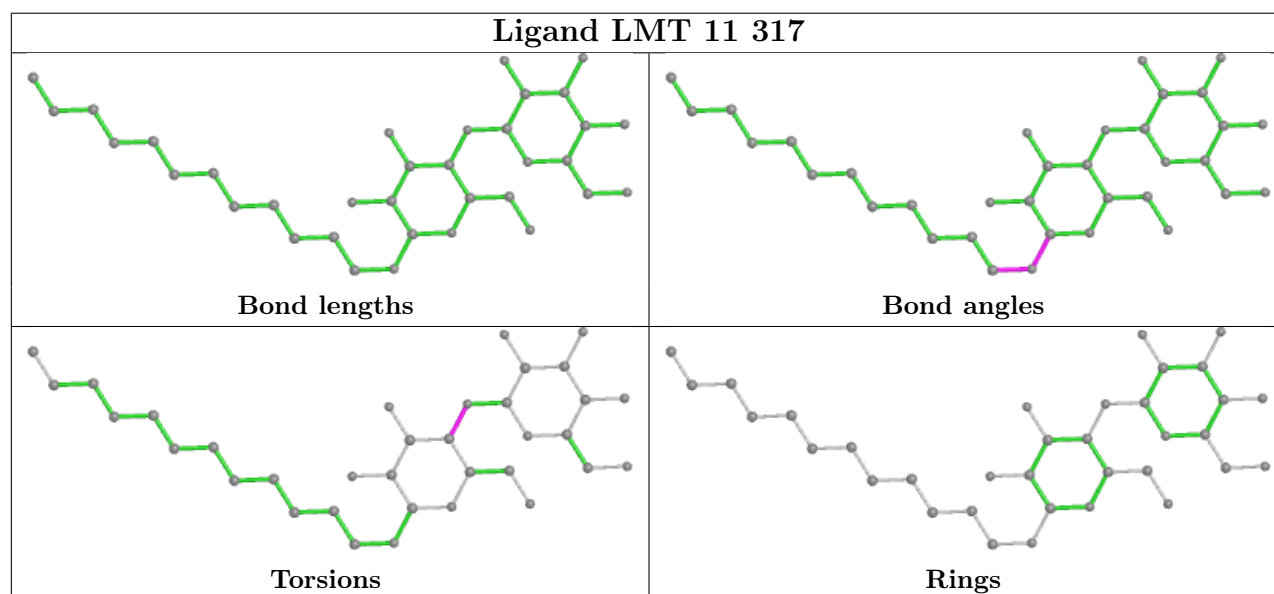
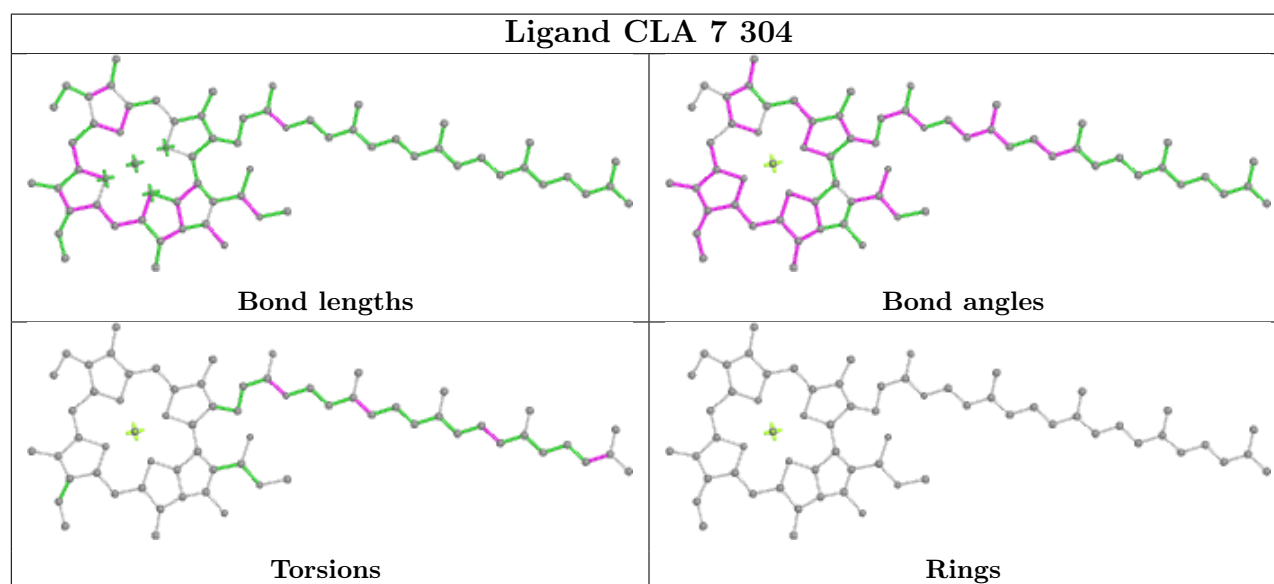
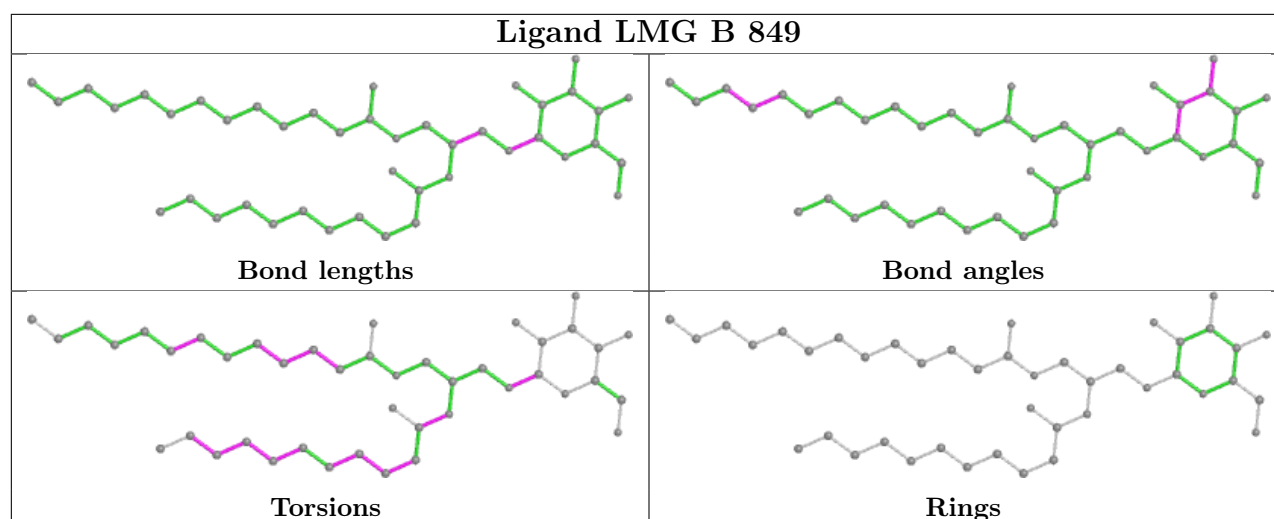
Ligand CLA B 836

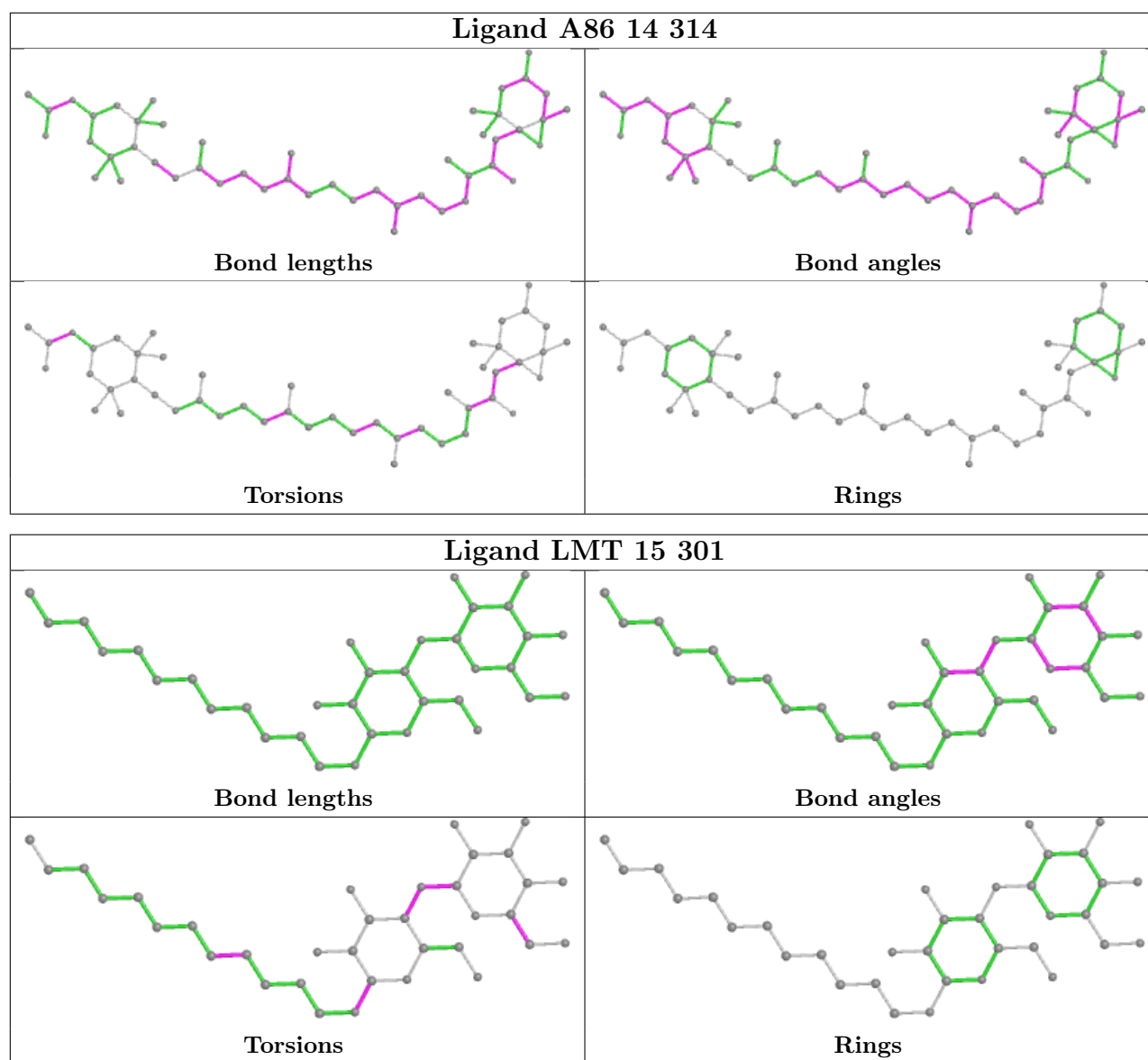


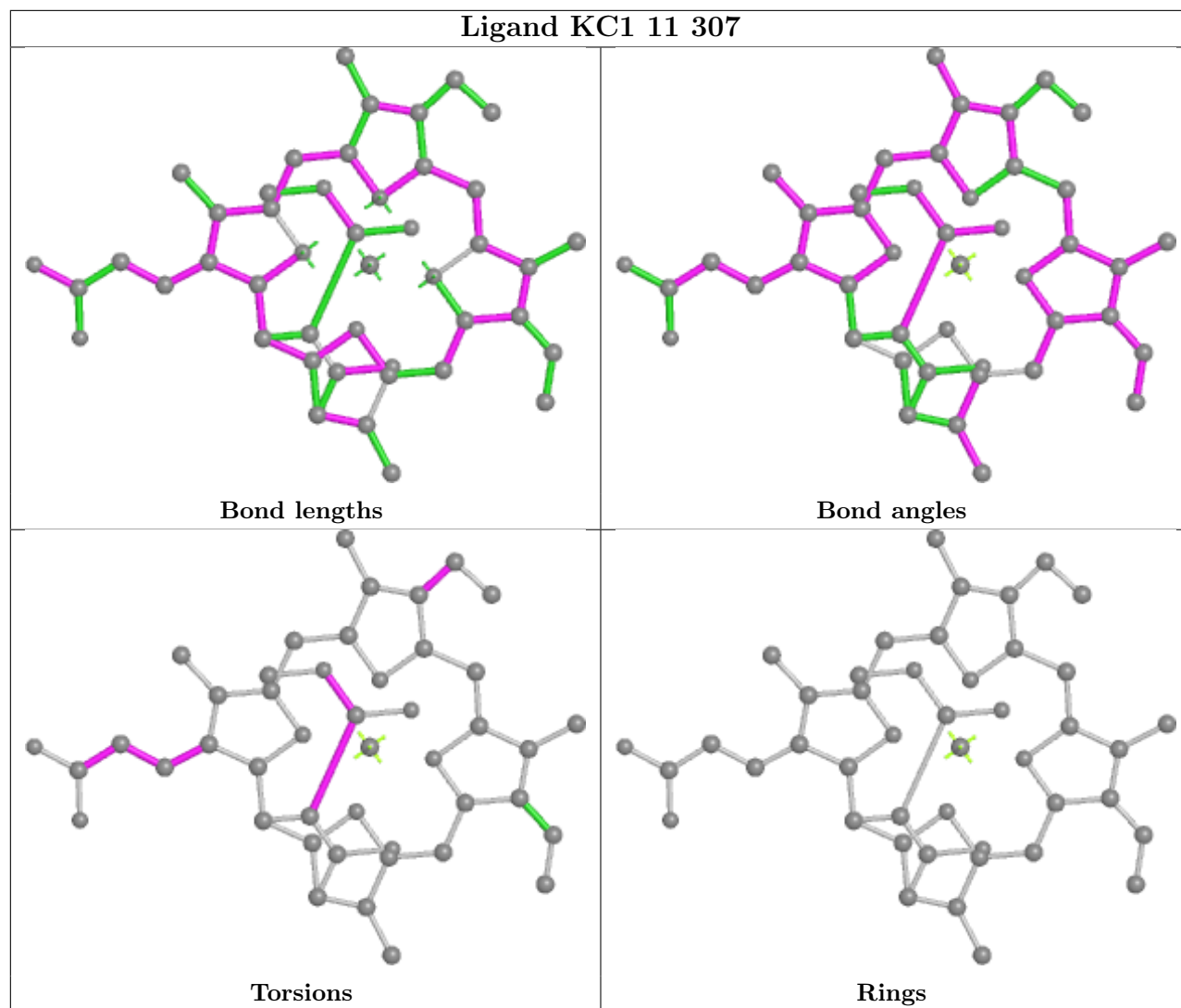
Ligand CLA 15 313

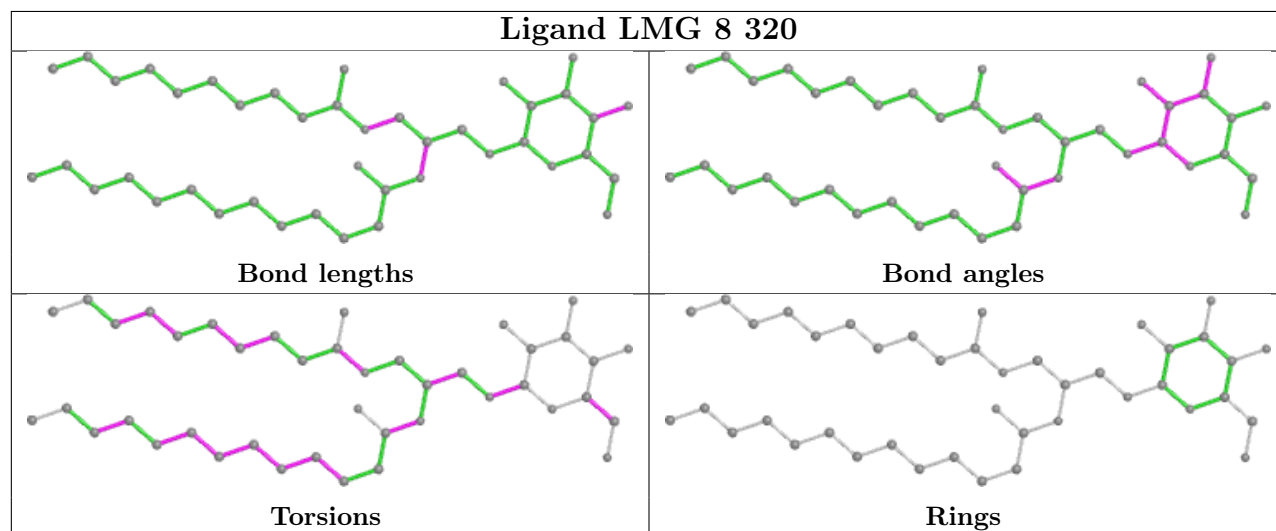
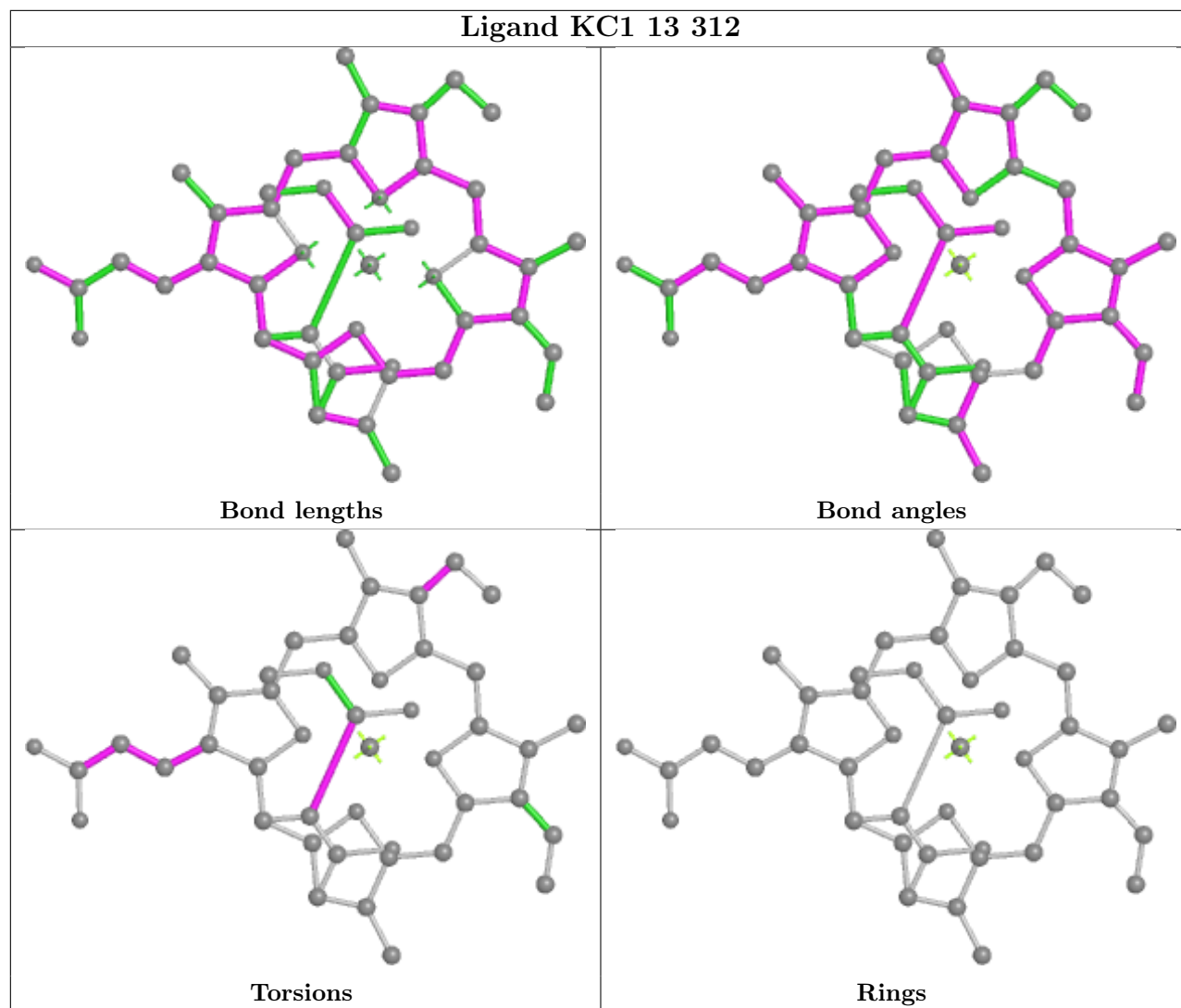


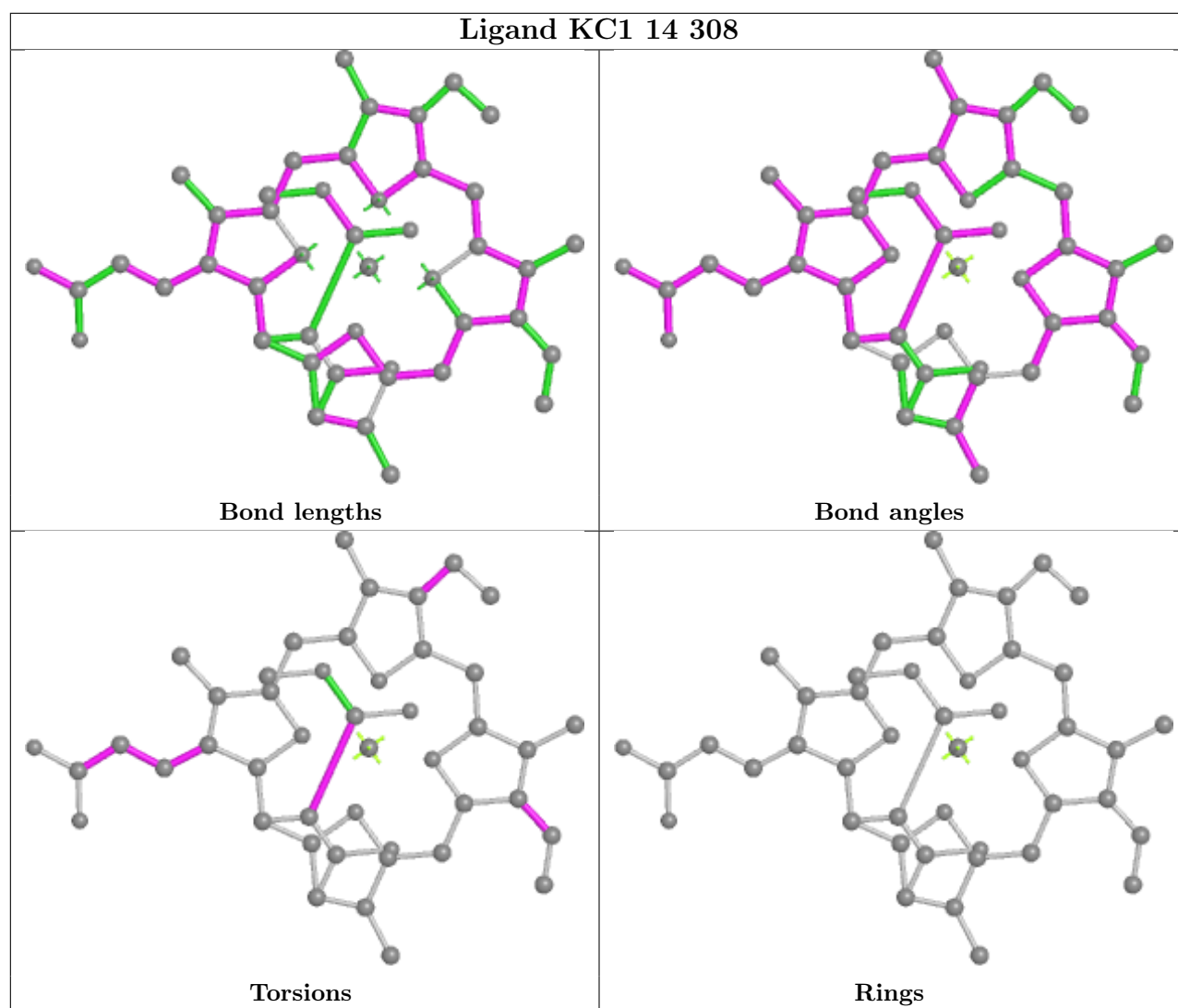


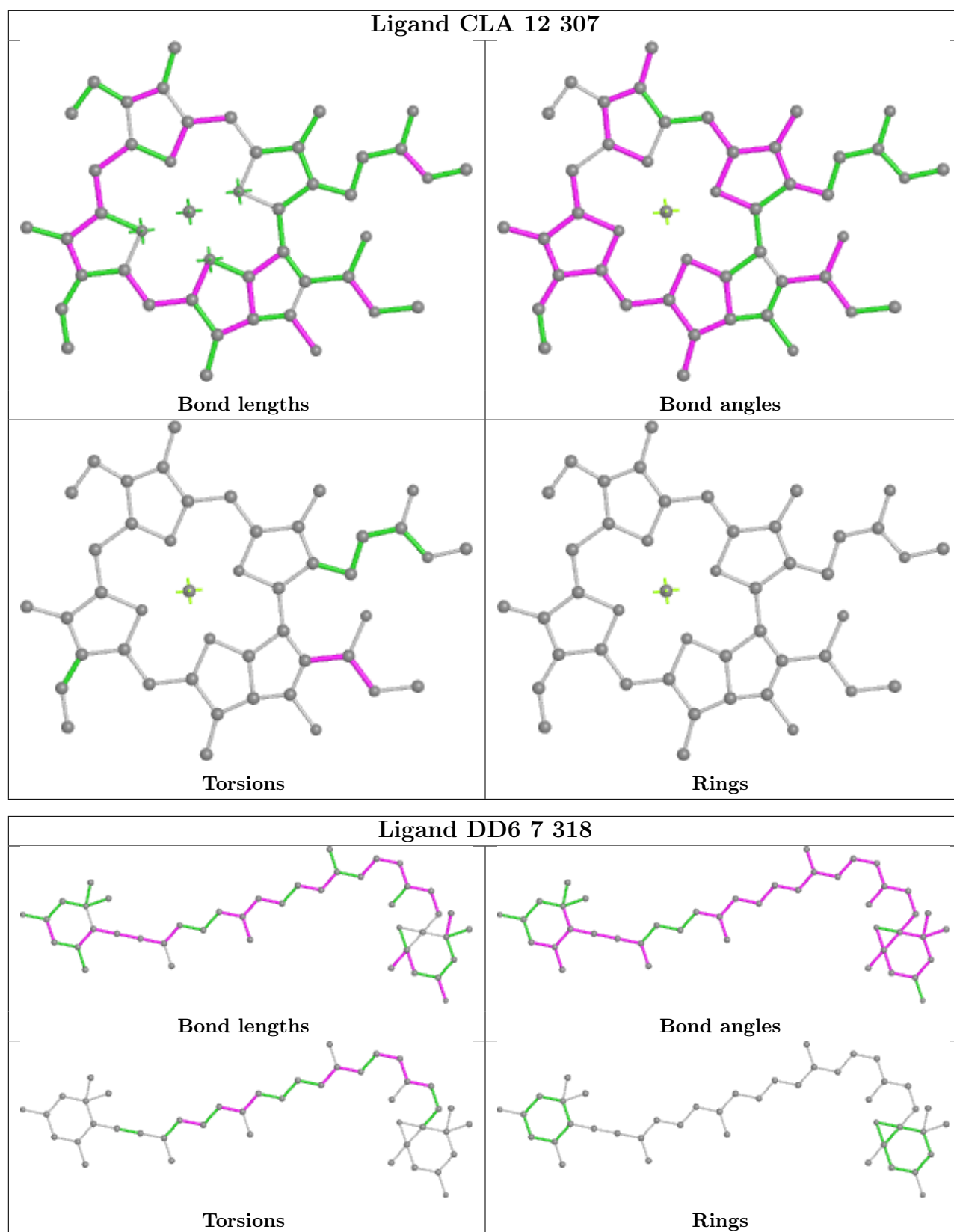


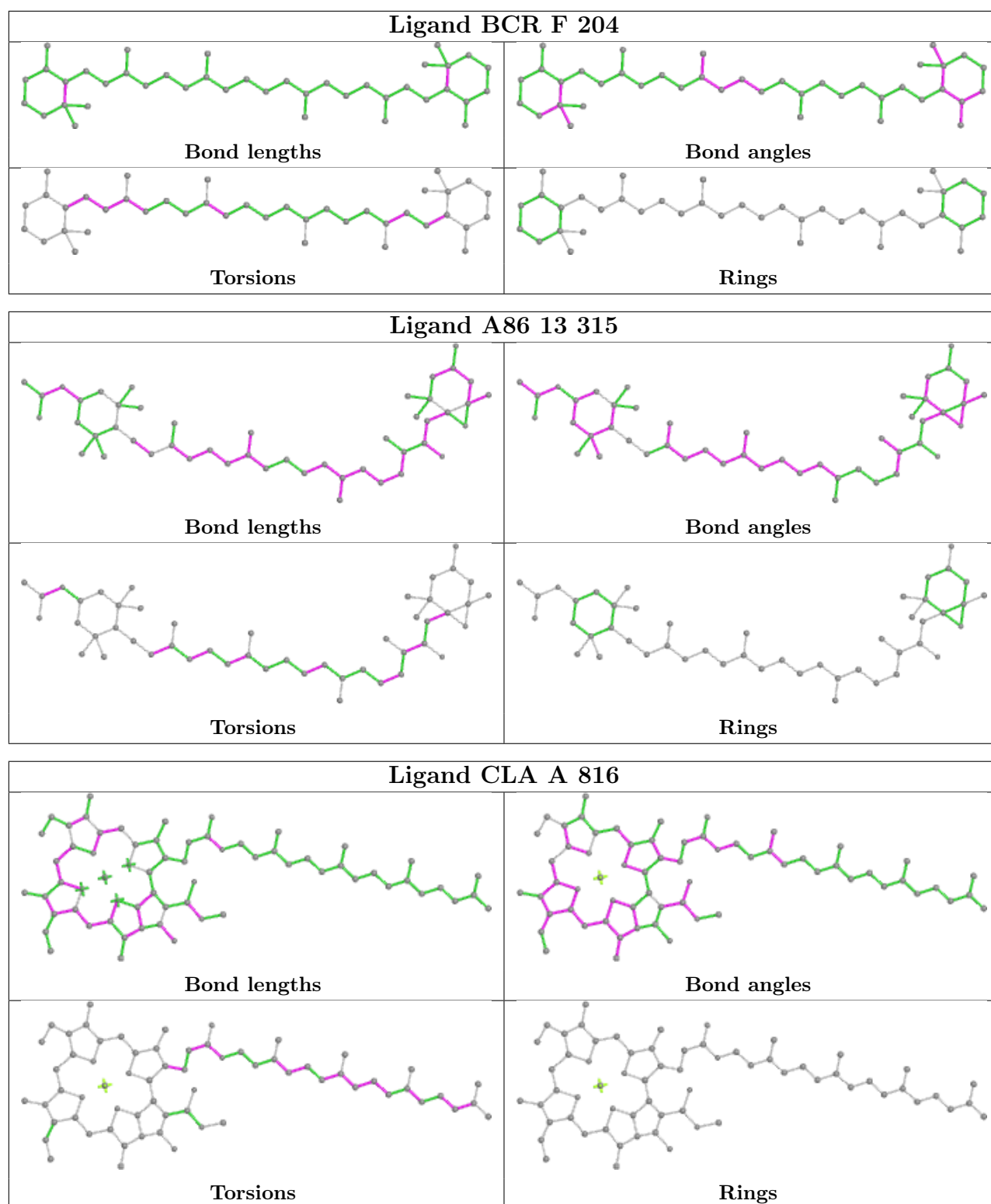


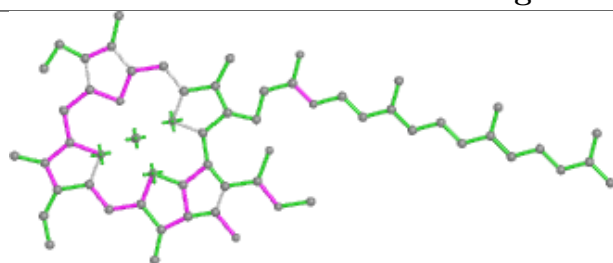
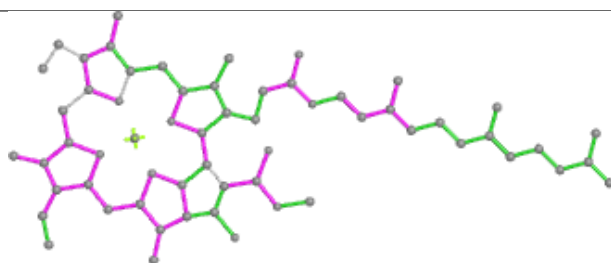
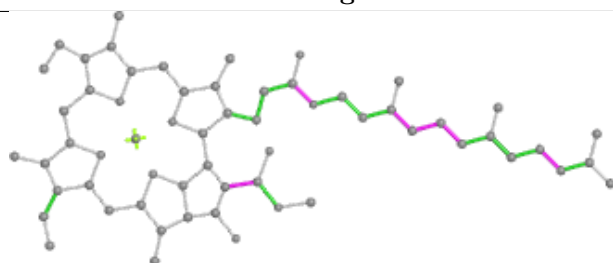
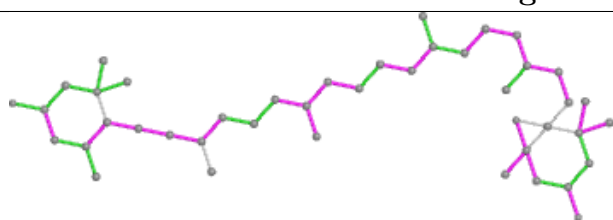
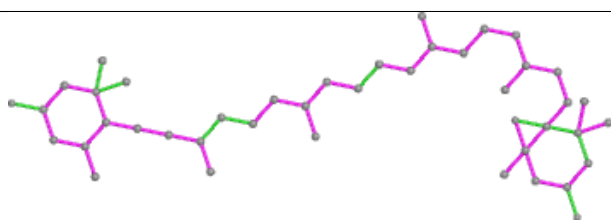
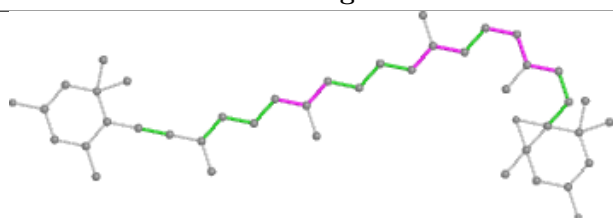
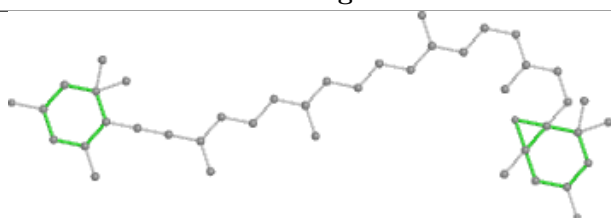


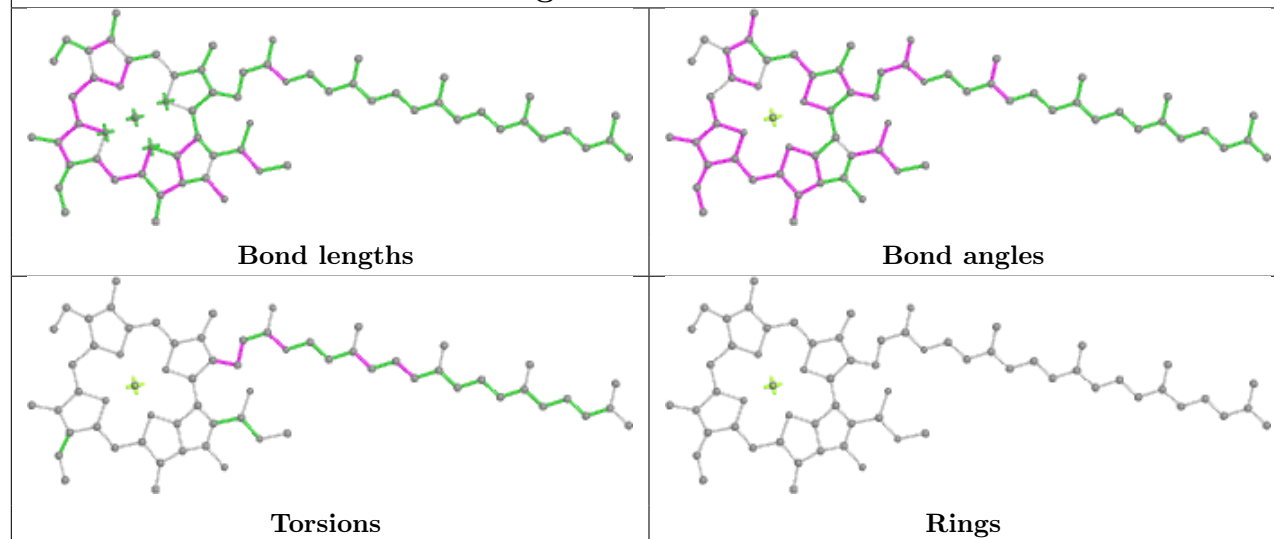
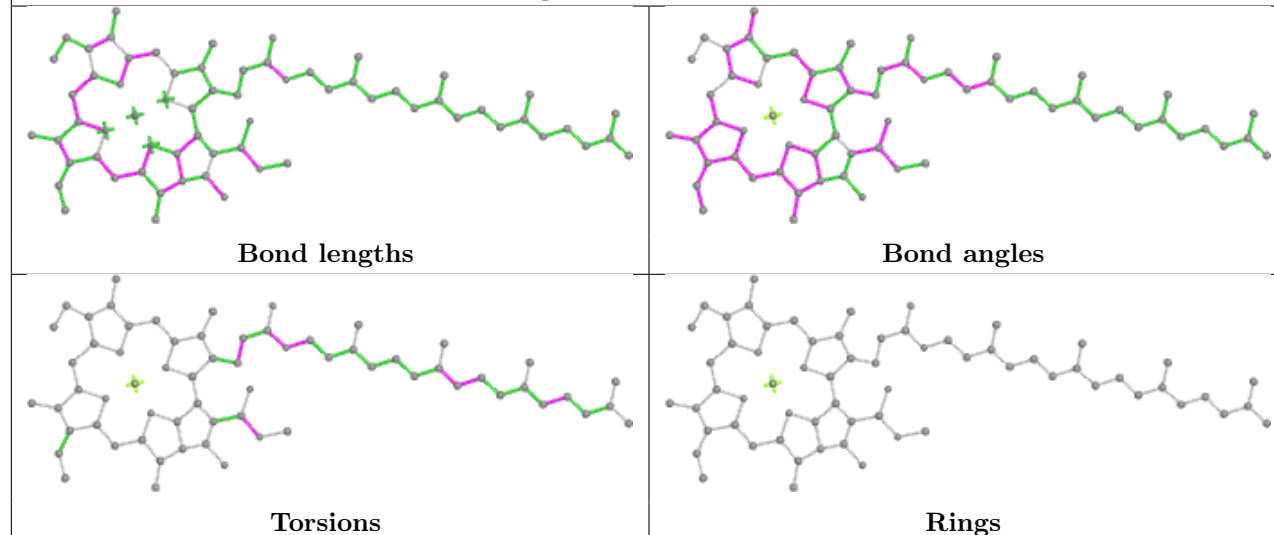
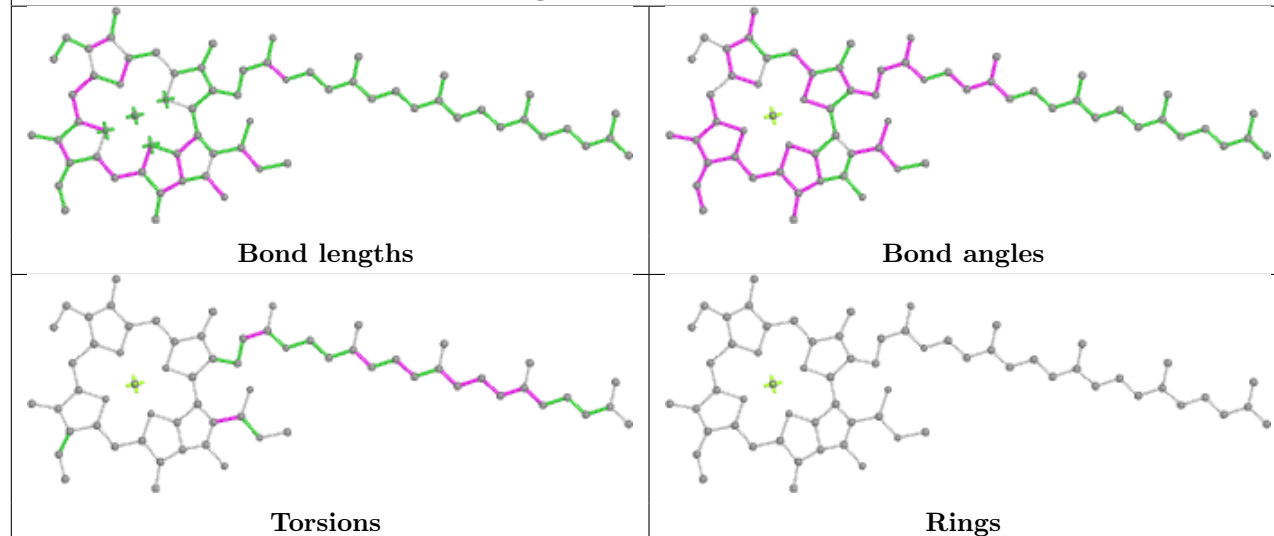


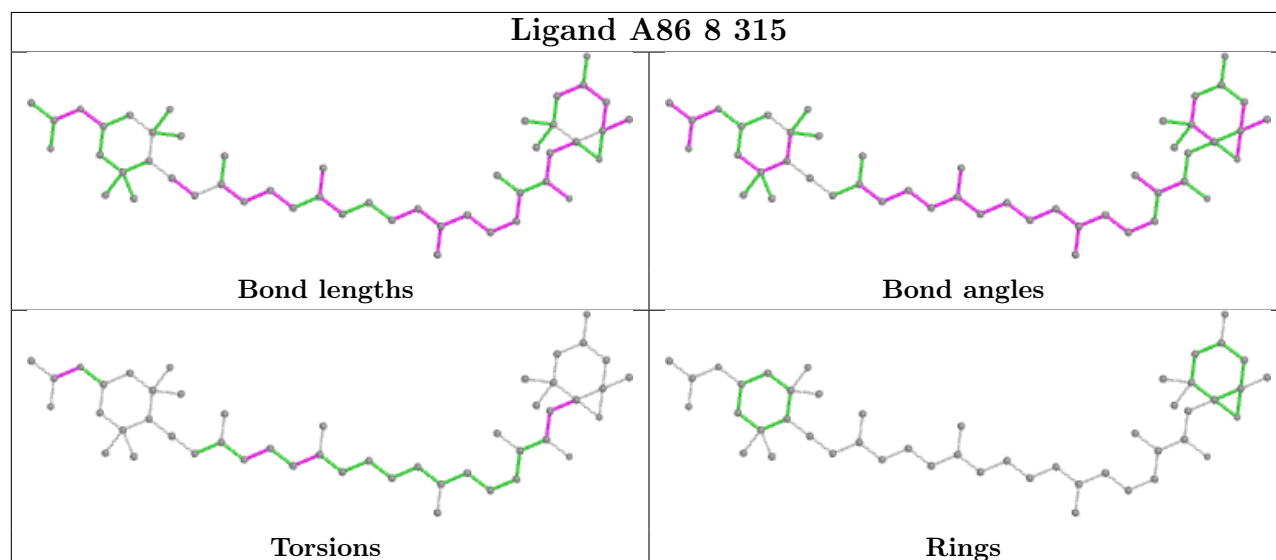
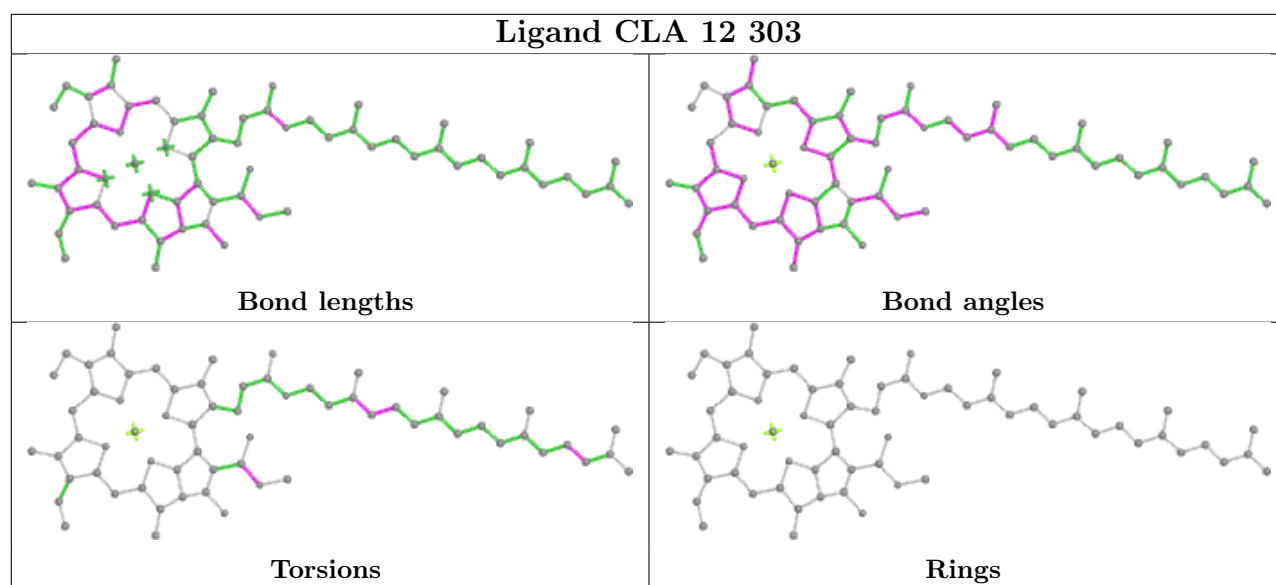


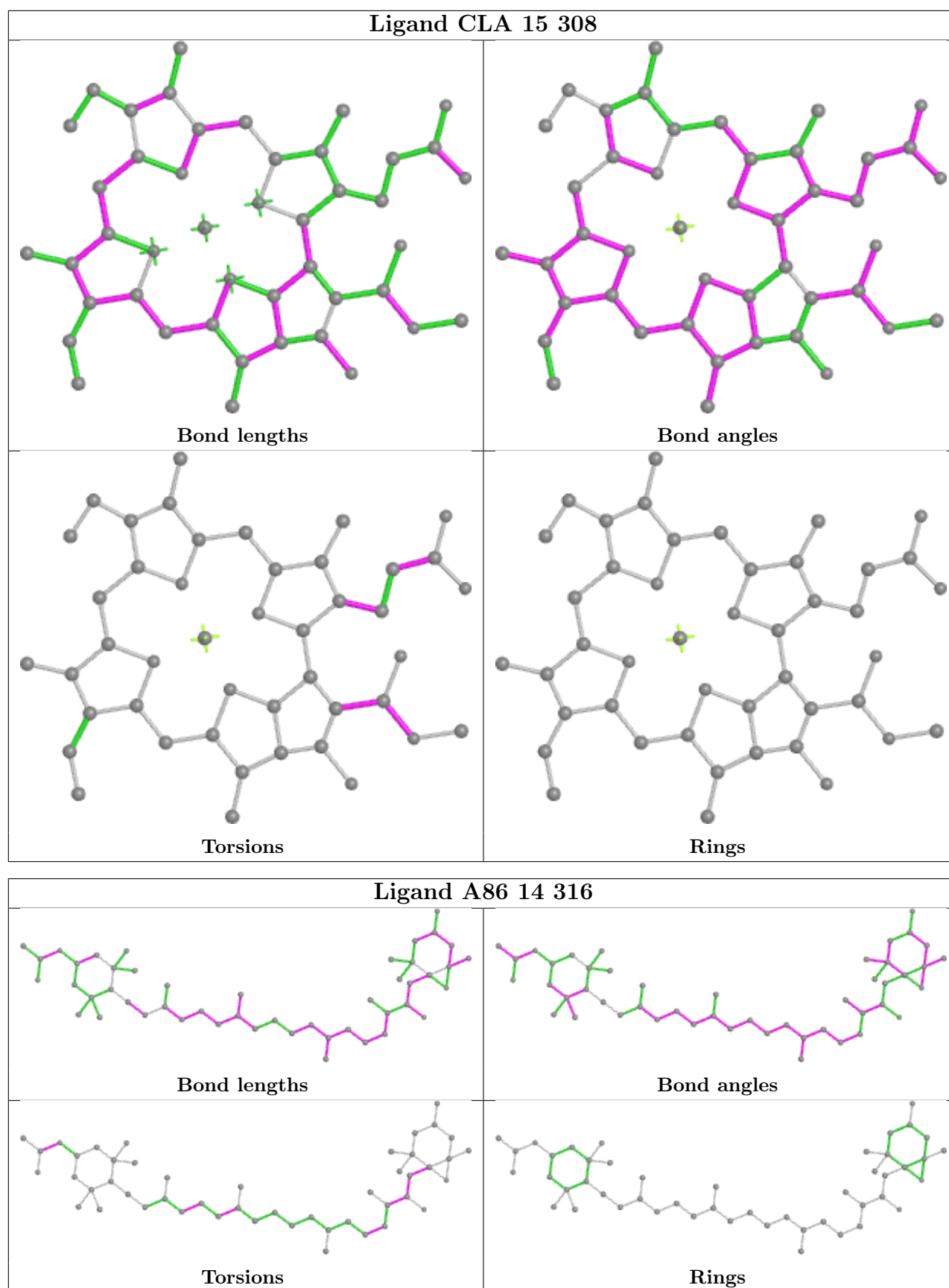


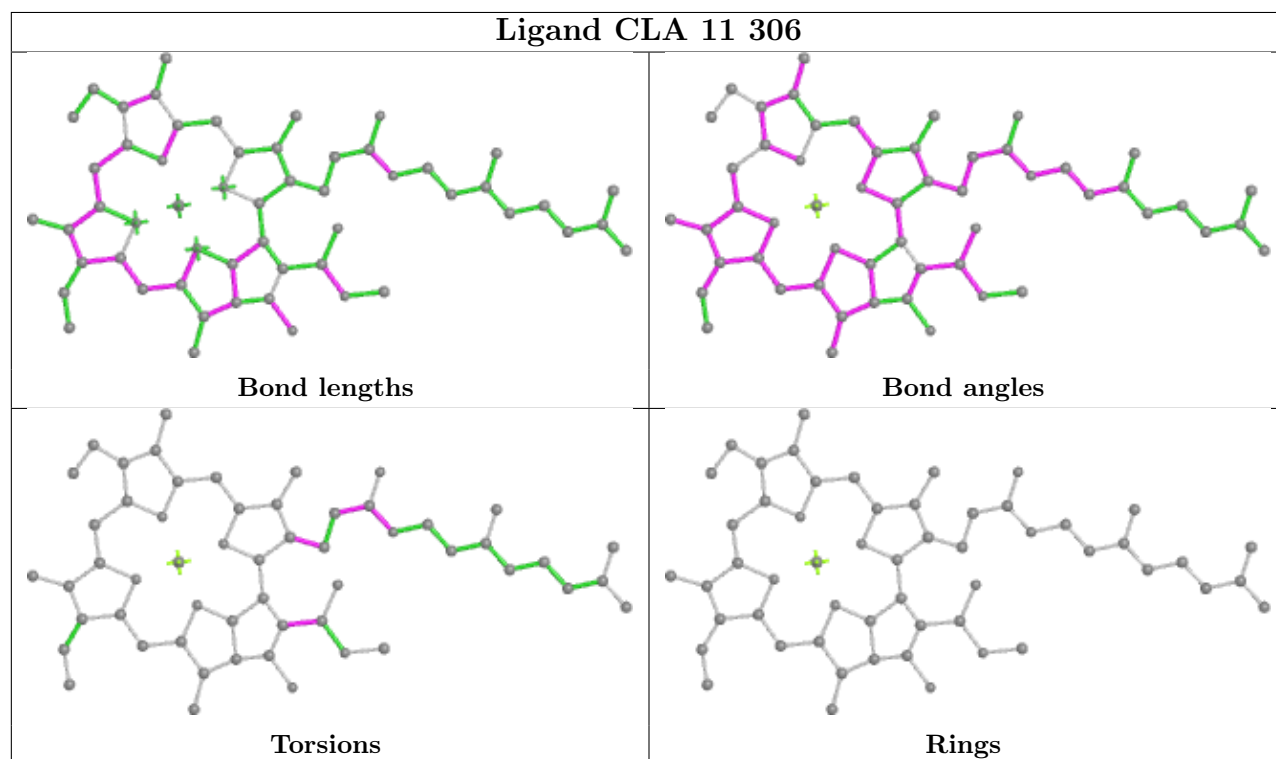
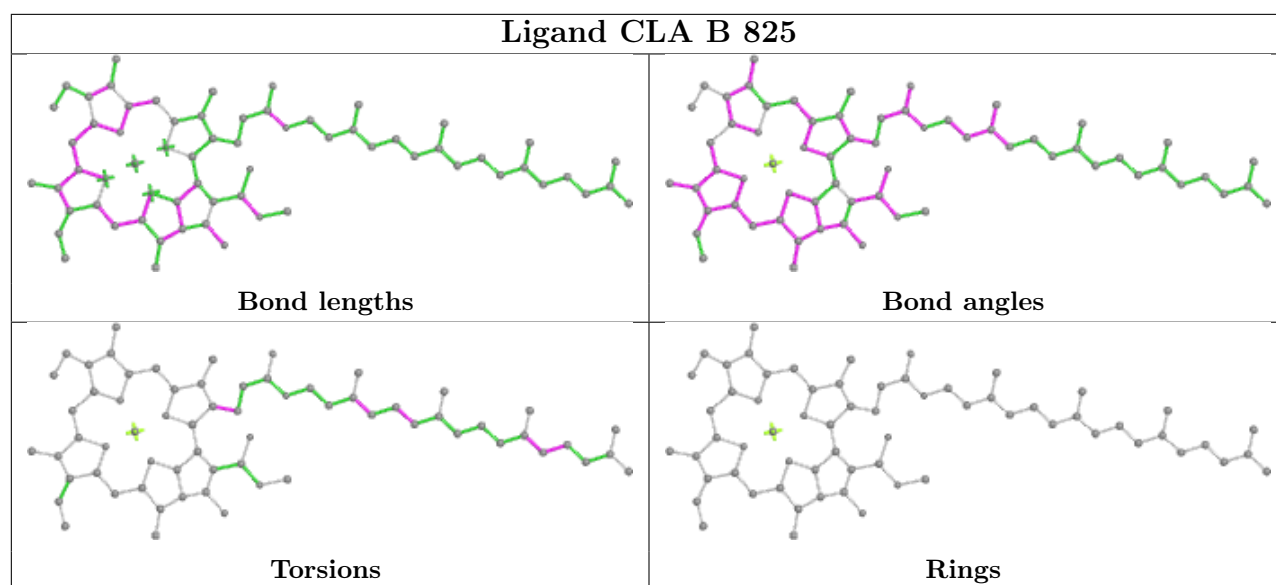


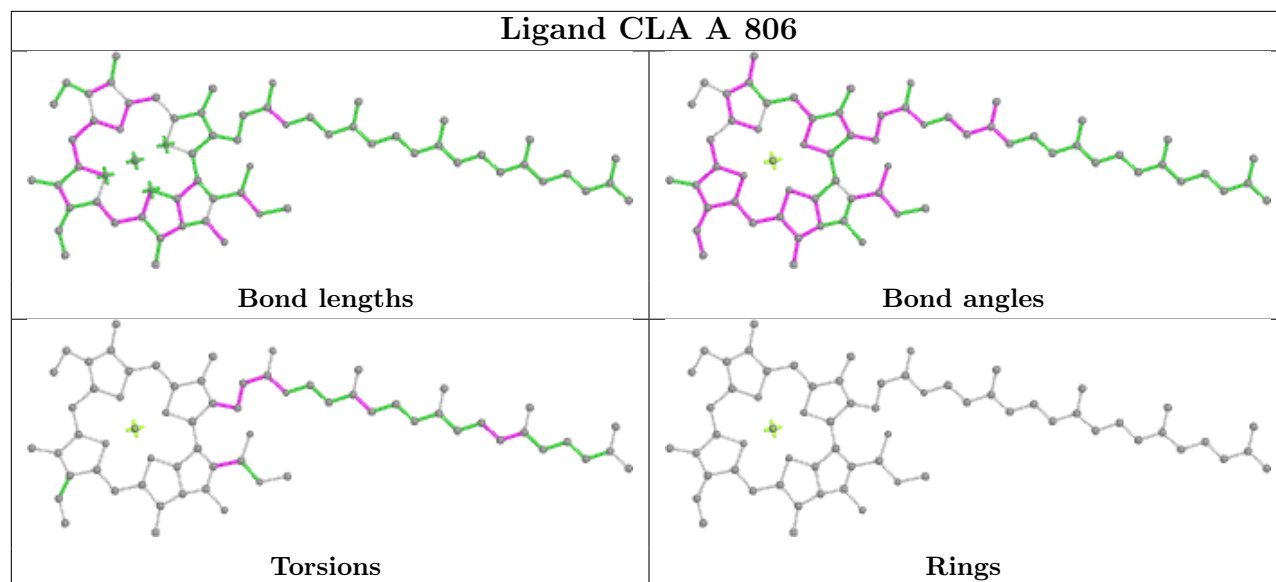
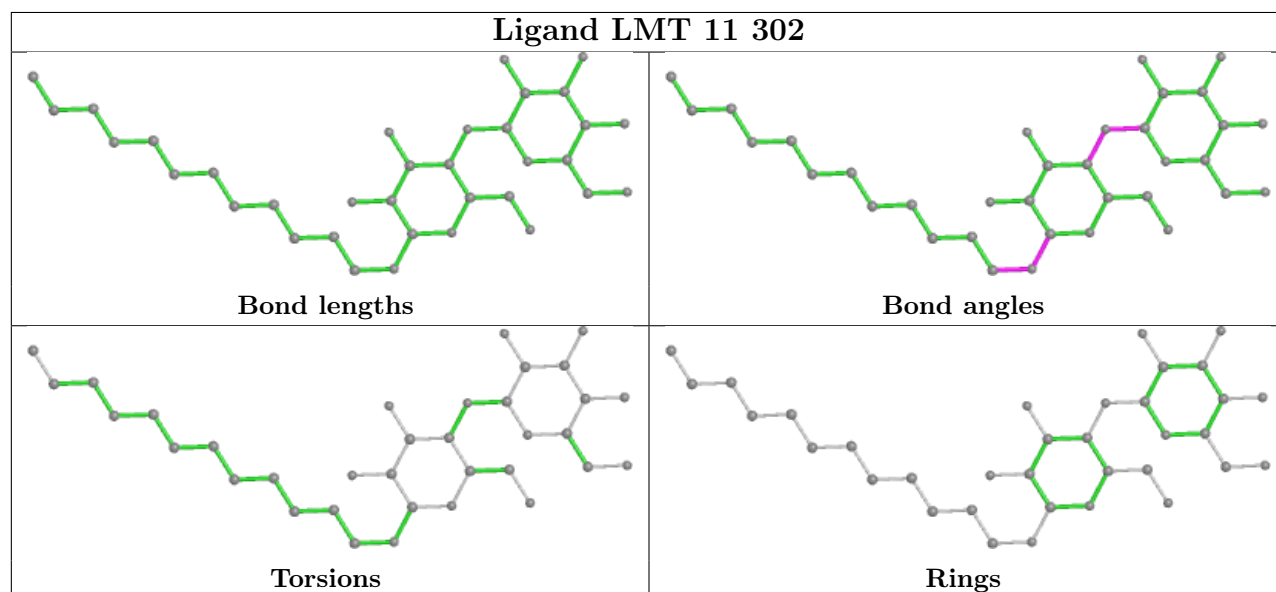
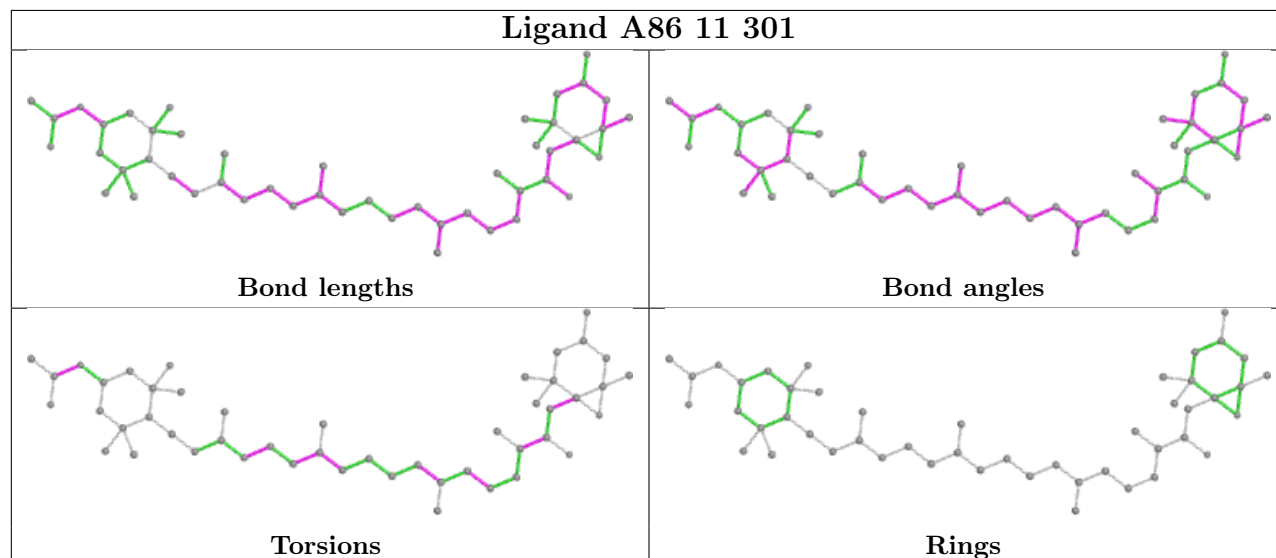
Ligand CLA B 834**Bond lengths****Bond angles****Torsions****Rings****Ligand DD6 6 319****Bond lengths****Bond angles****Torsions****Rings**

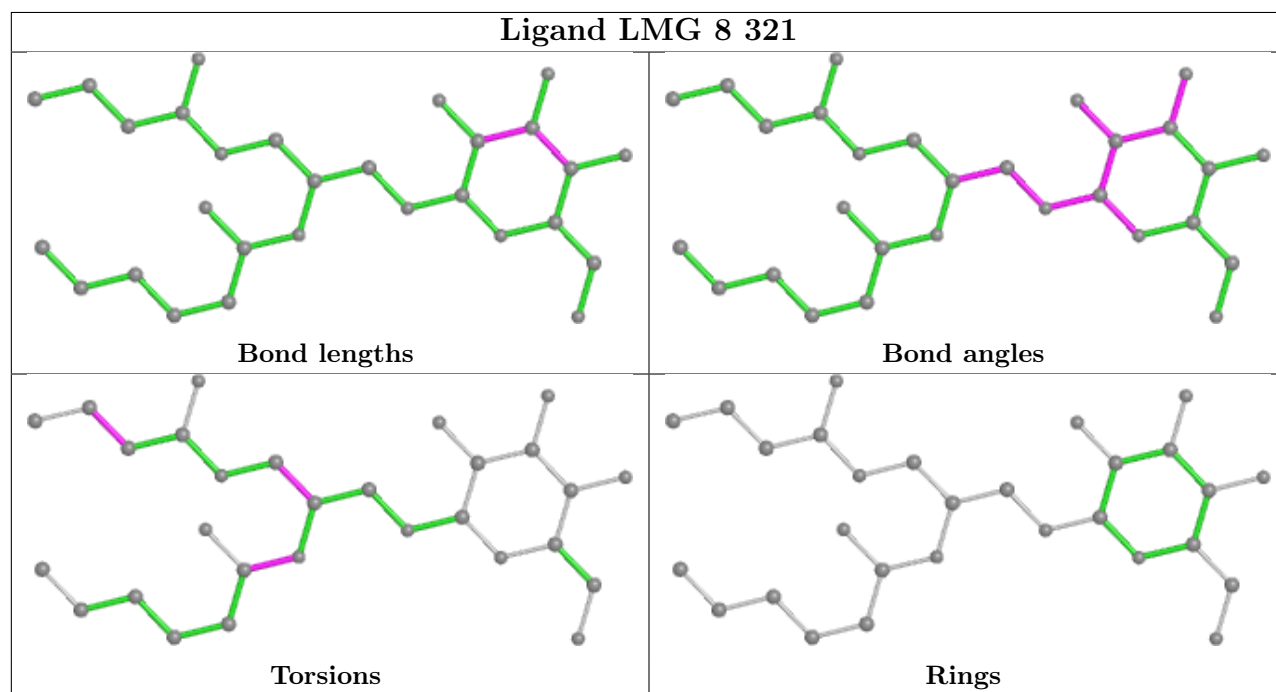
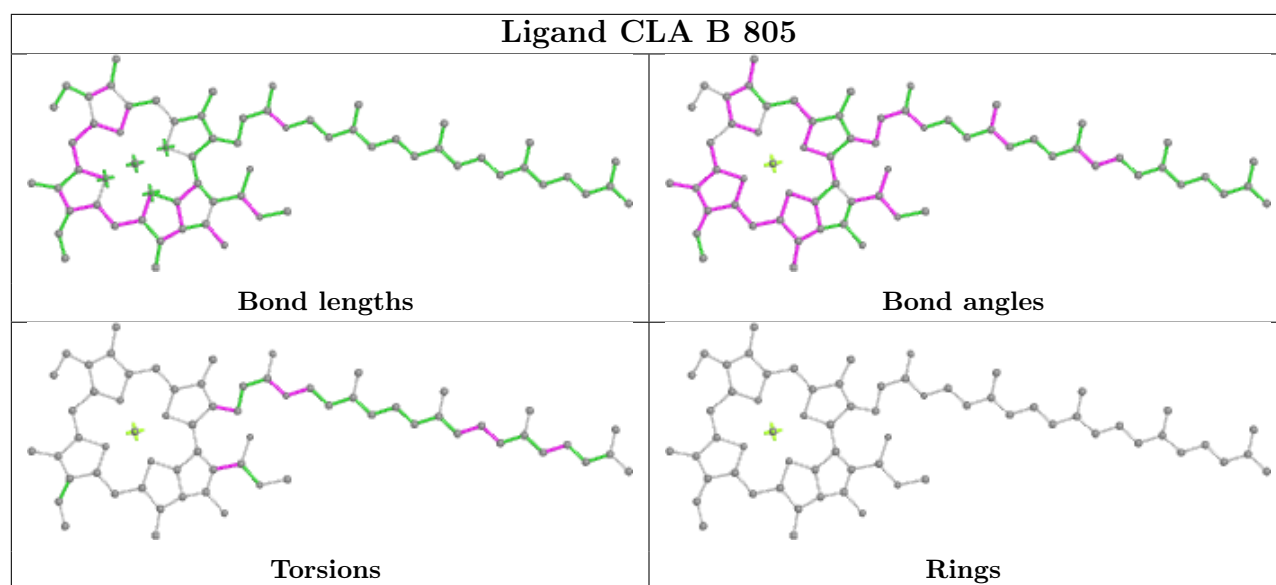
Ligand CLA 3 301**Ligand CLA 1 302****Ligand CLA A 839**

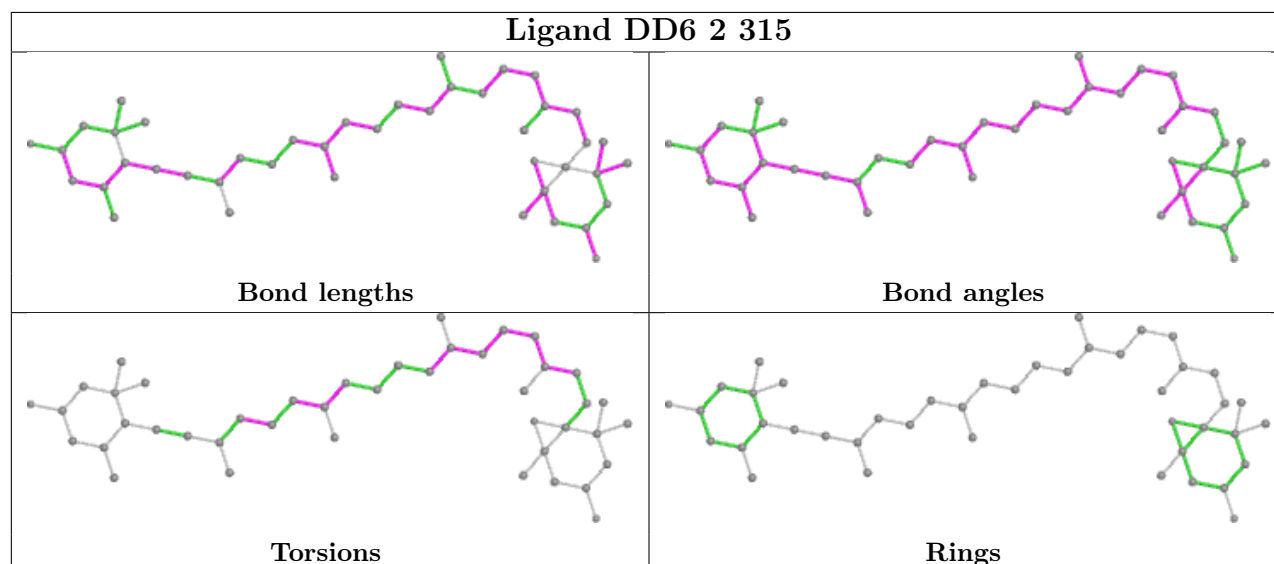
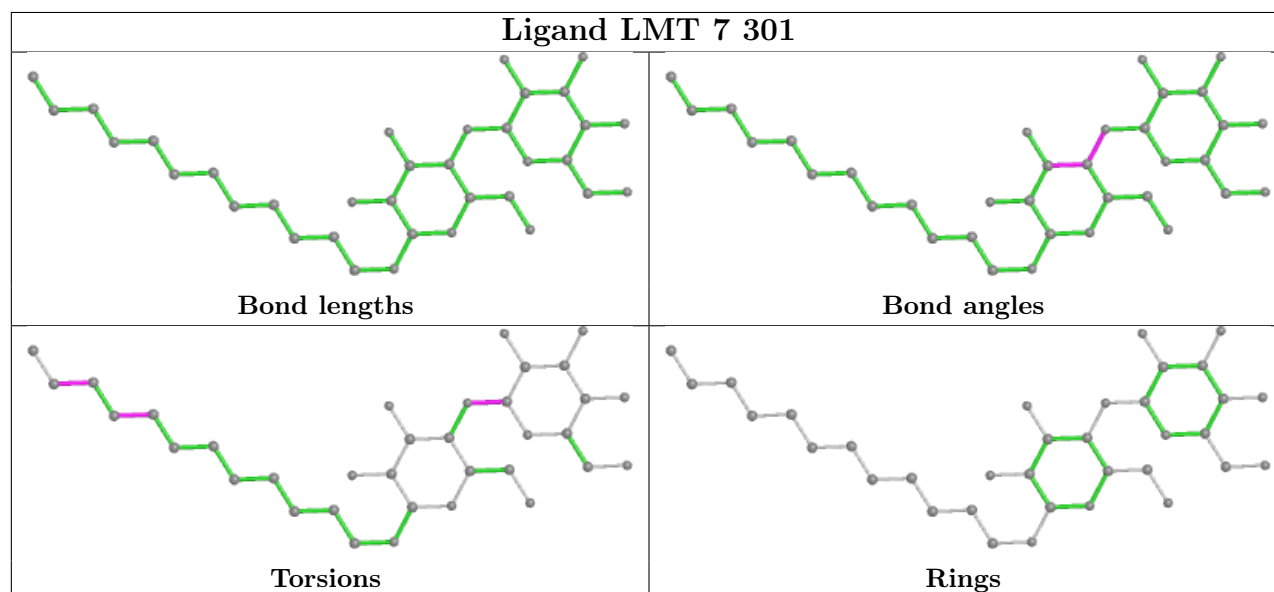
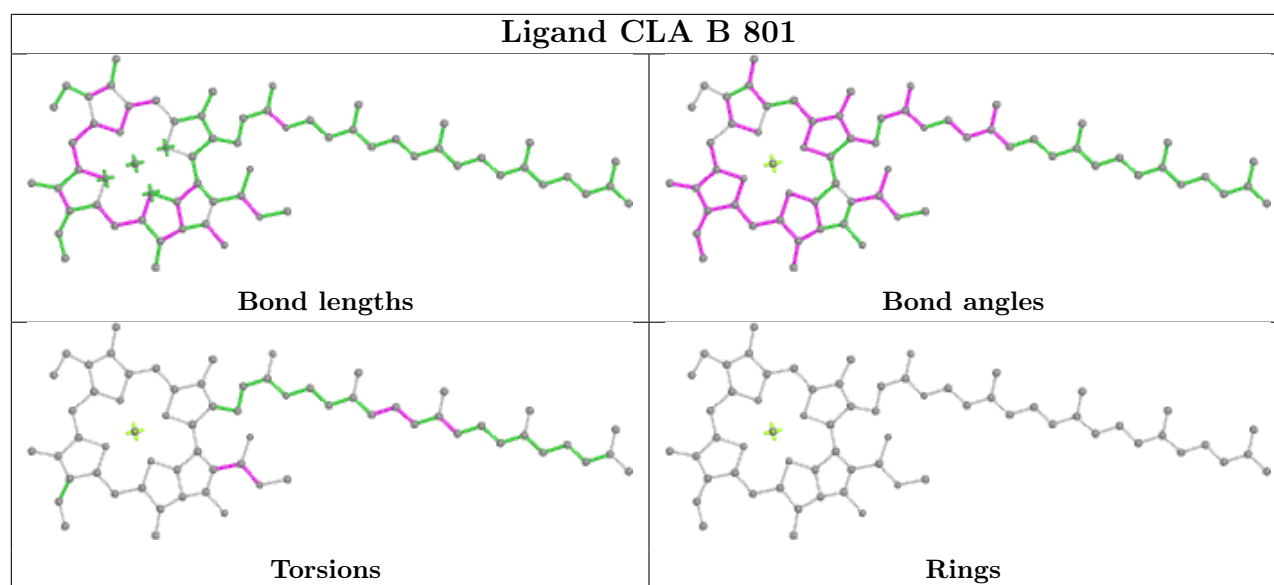


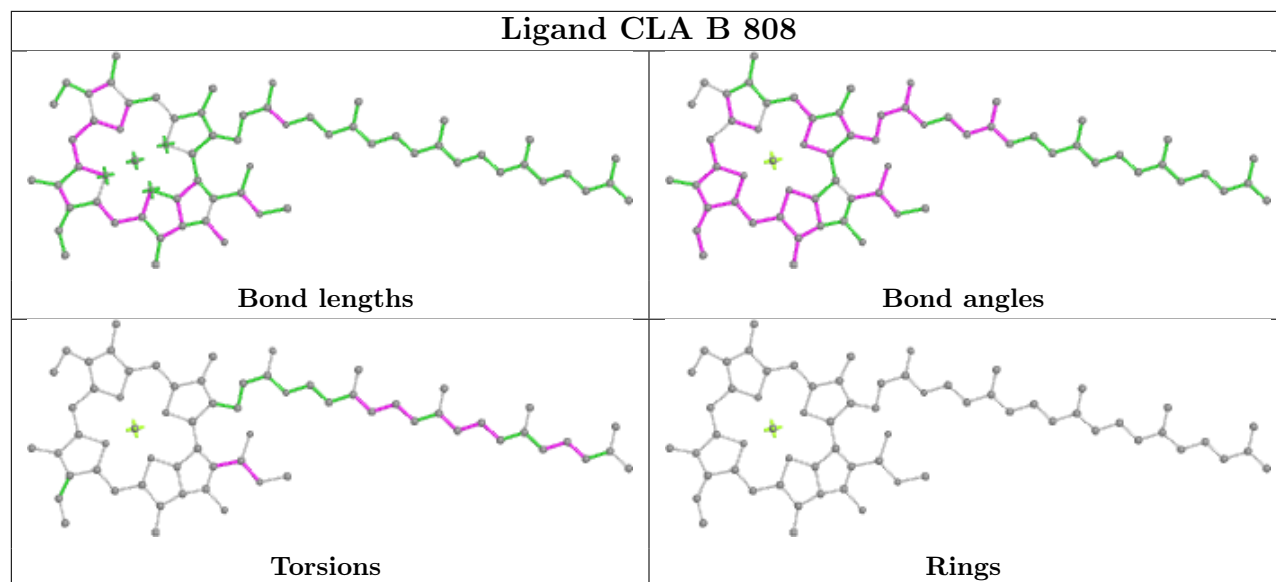
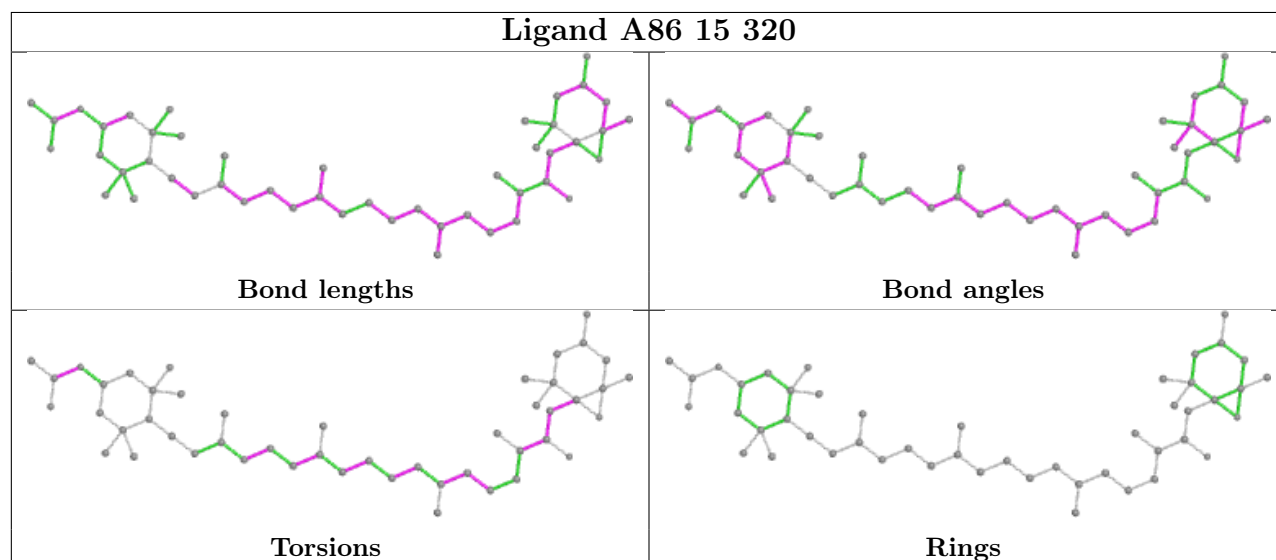




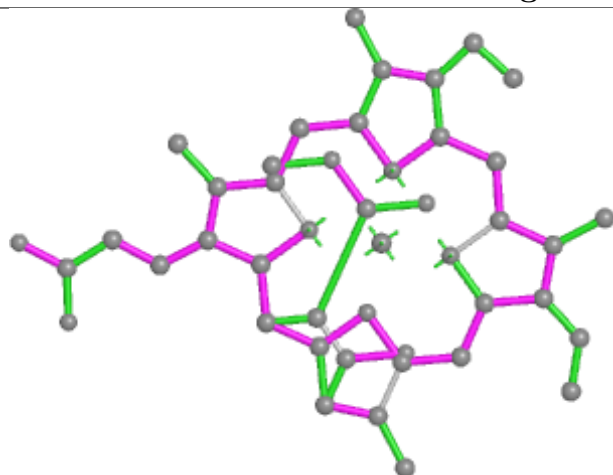
Ligand CLA A 806**Ligand LMT 11 302****Ligand A86 11 301**



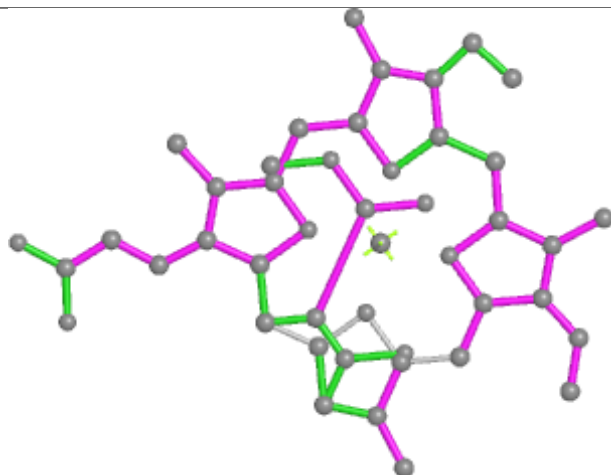


Ligand CLA B 808**Ligand A86 15 320**

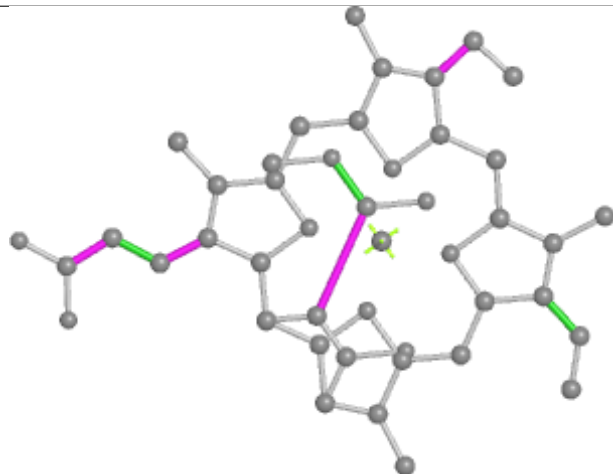
Ligand KC1 2 306



Bond lengths



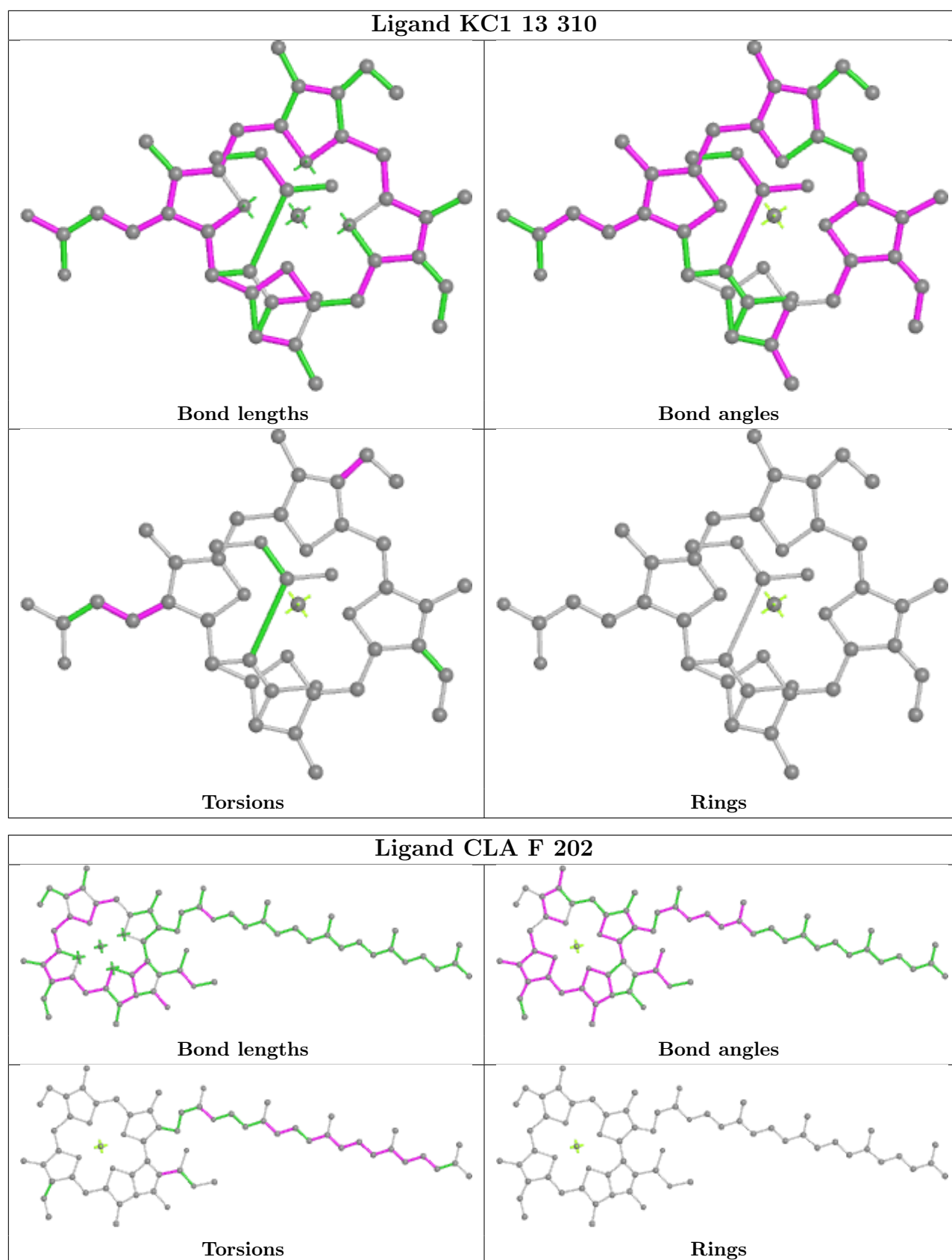
Bond angles



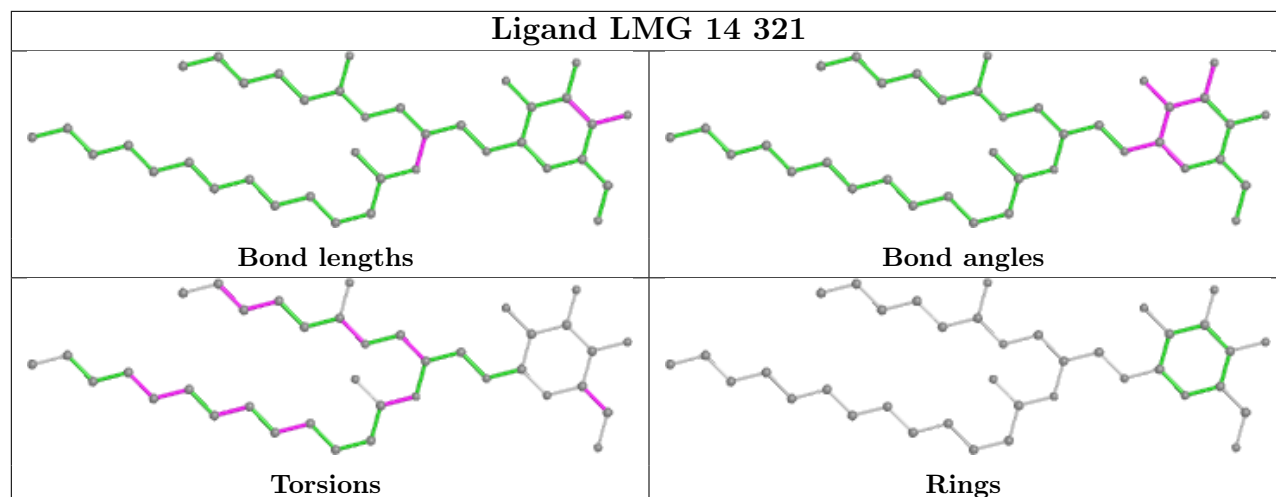
Torsions



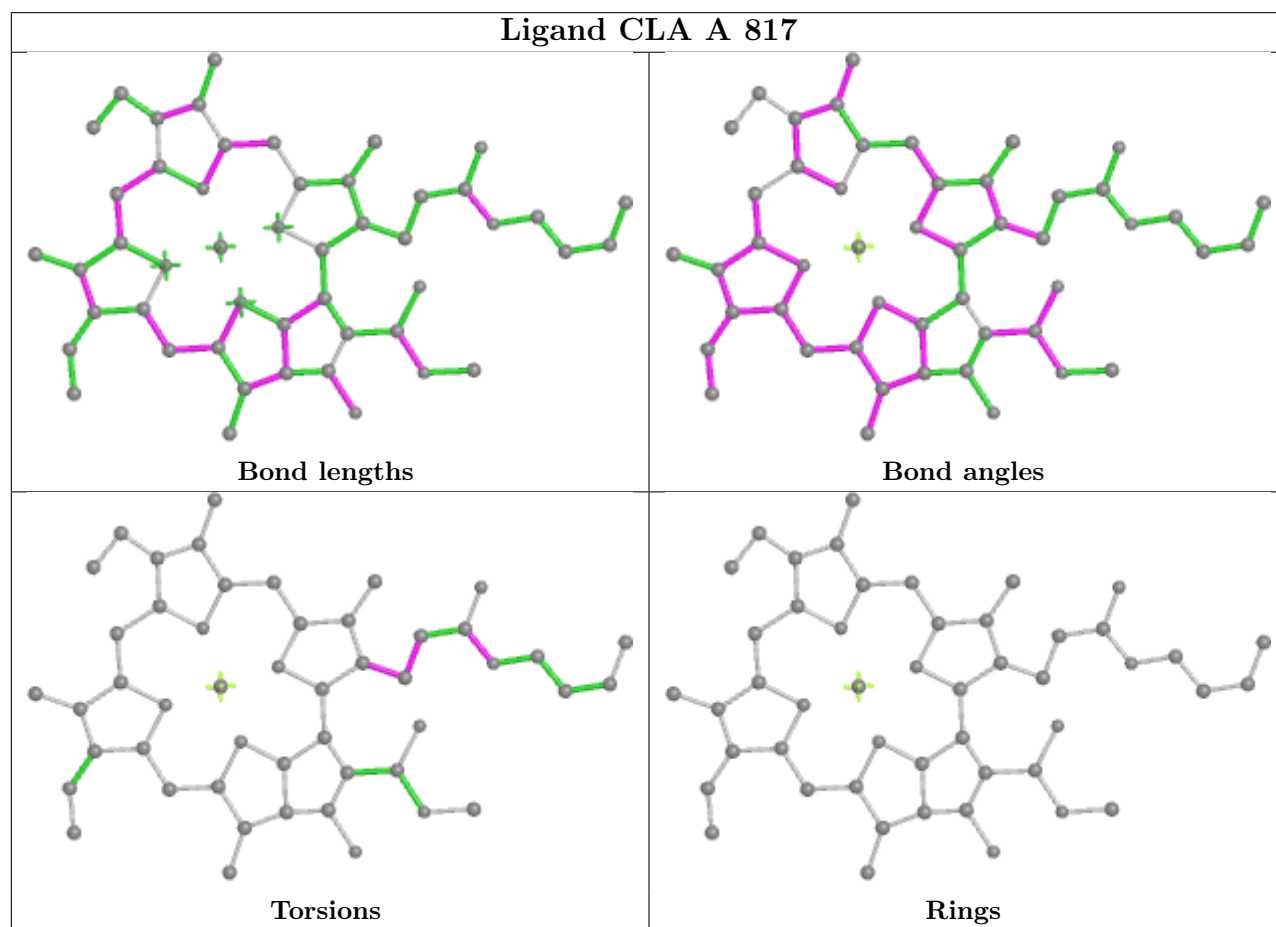
Rings



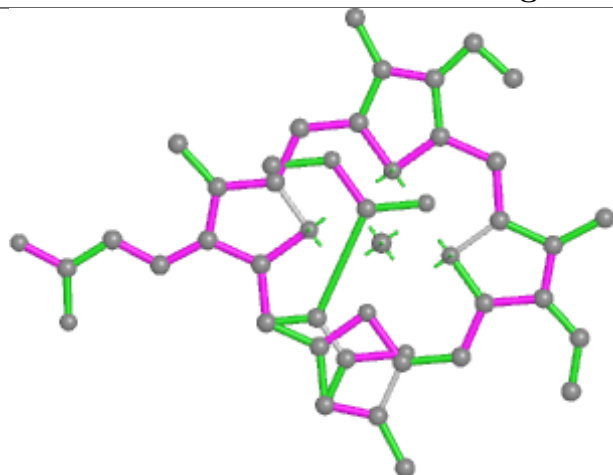
Ligand LMG 14 321



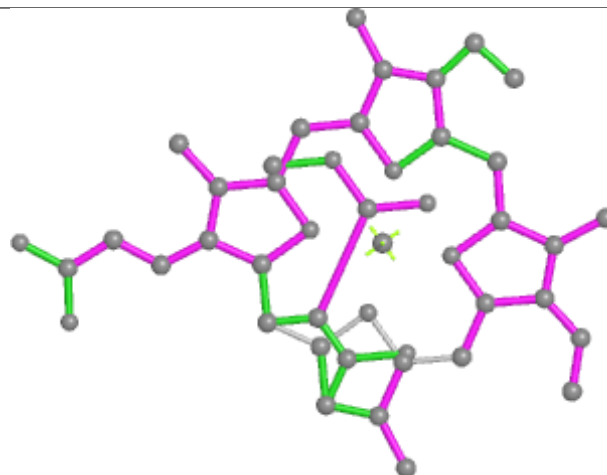
Ligand CLA A 817



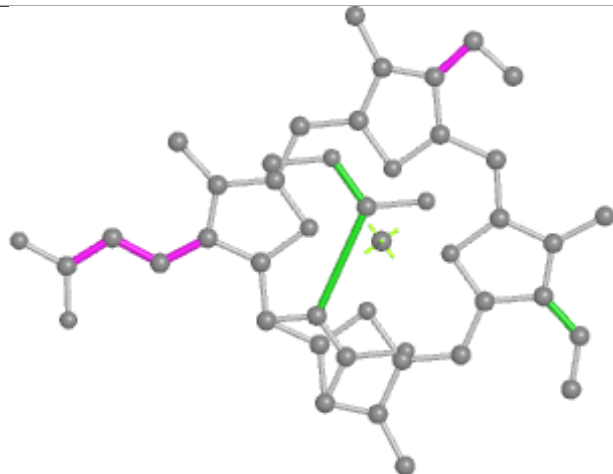
Ligand KC1 9 304



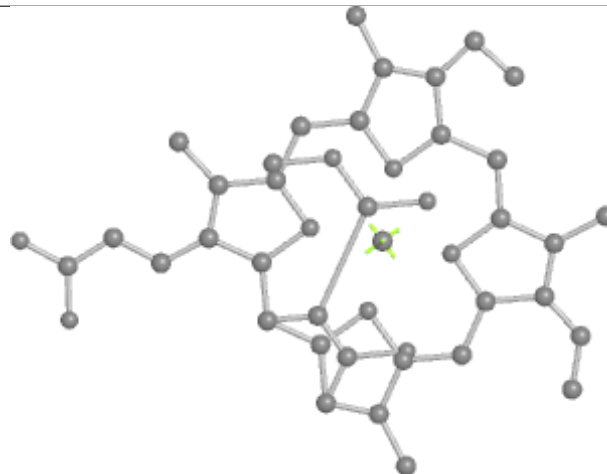
Bond lengths



Bond angles

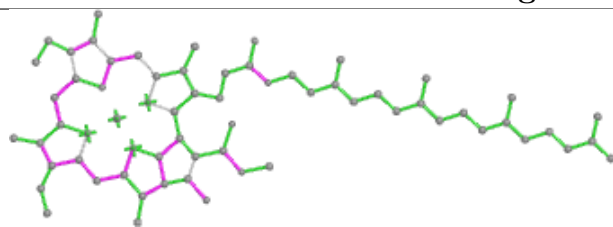


Torsions

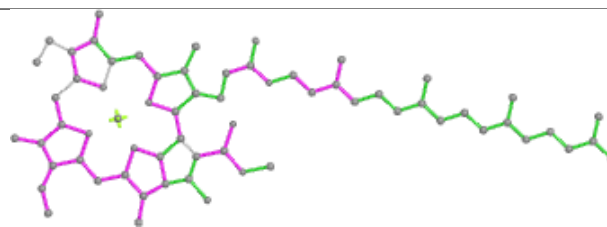


Rings

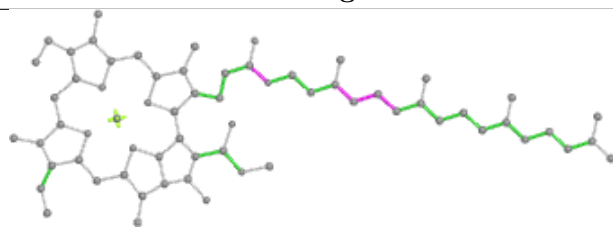
Ligand CLA 2 310



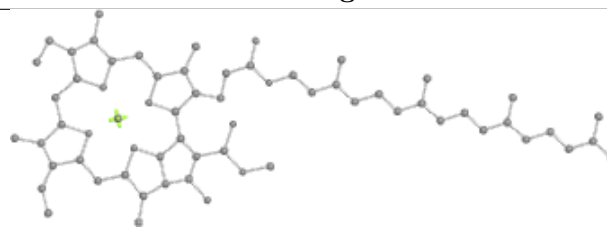
Bond lengths



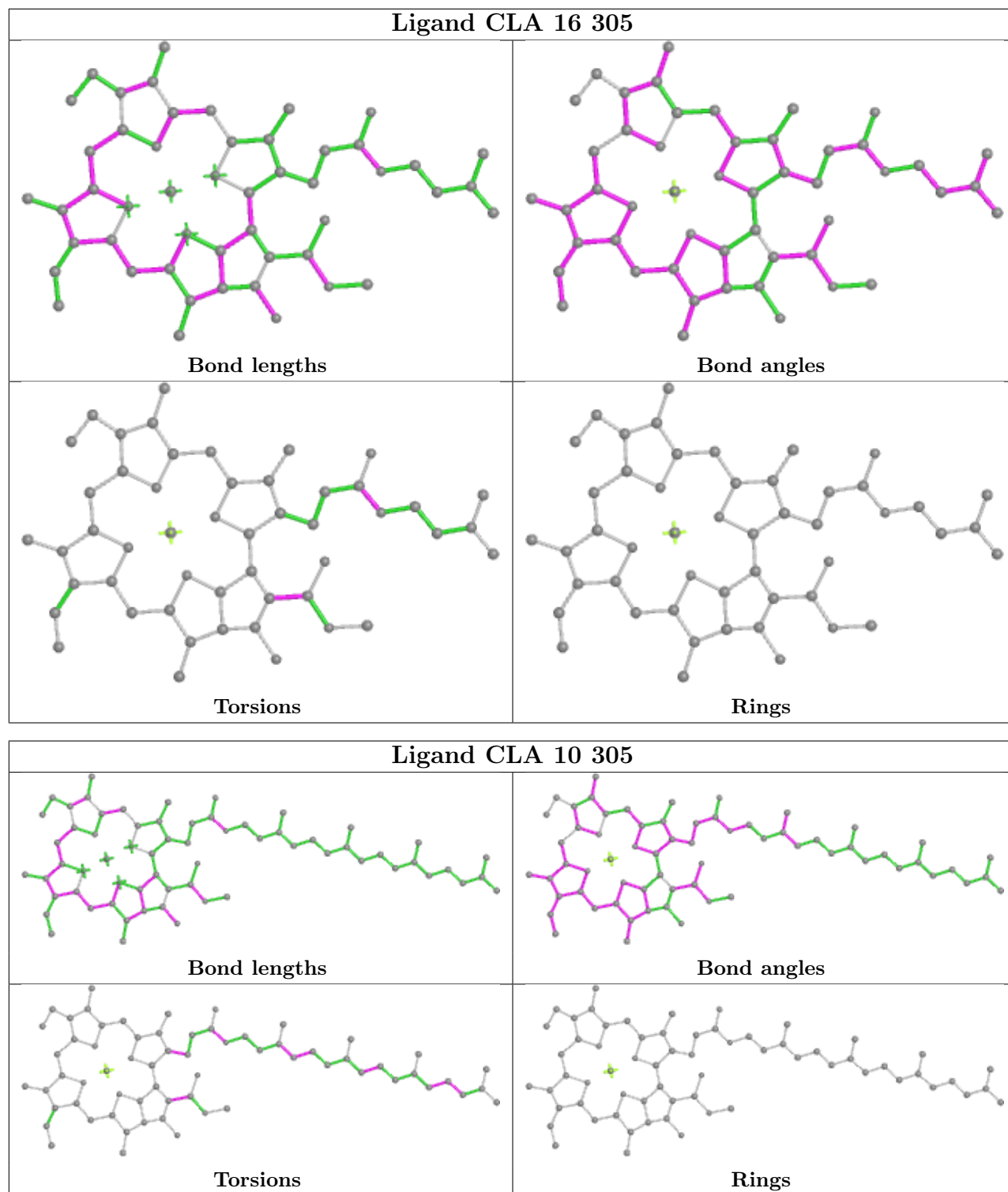
Bond angles



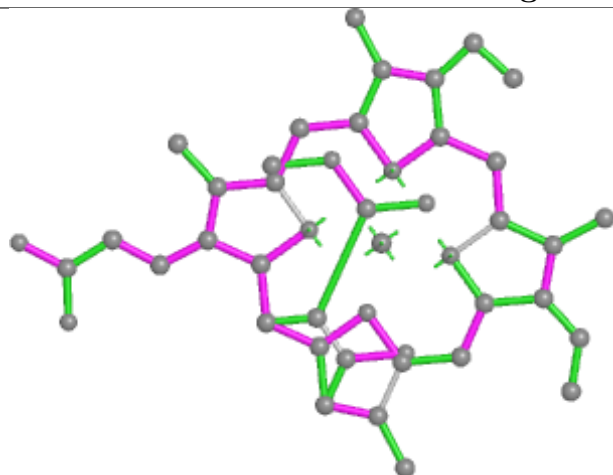
Torsions



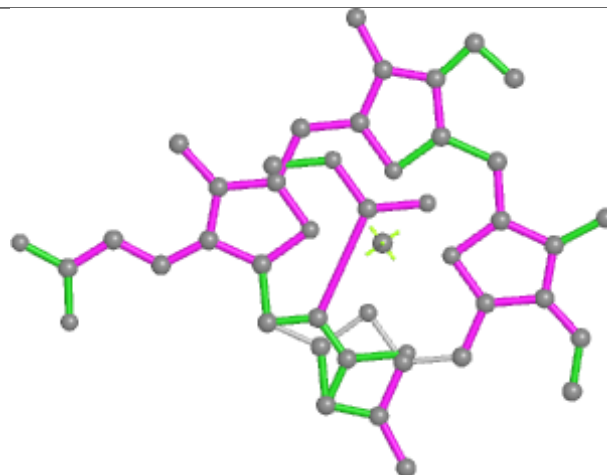
Rings



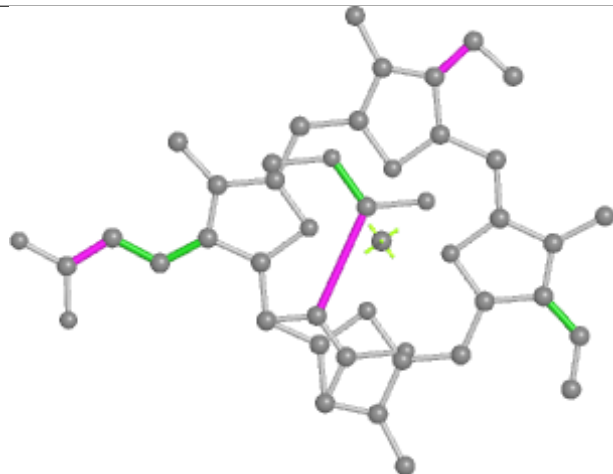
Ligand KC1 8 310



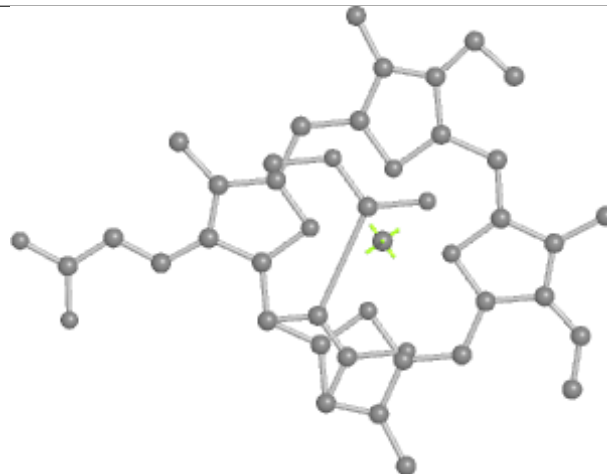
Bond lengths



Bond angles

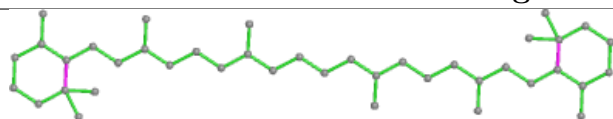


Torsions

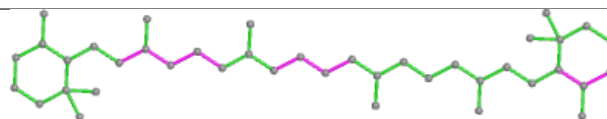


Rings

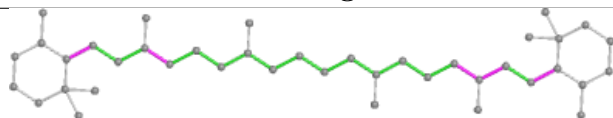
Ligand BCR B 846



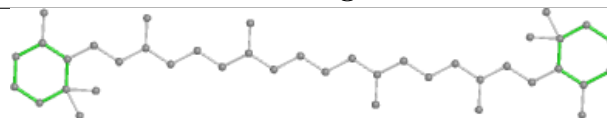
Bond lengths



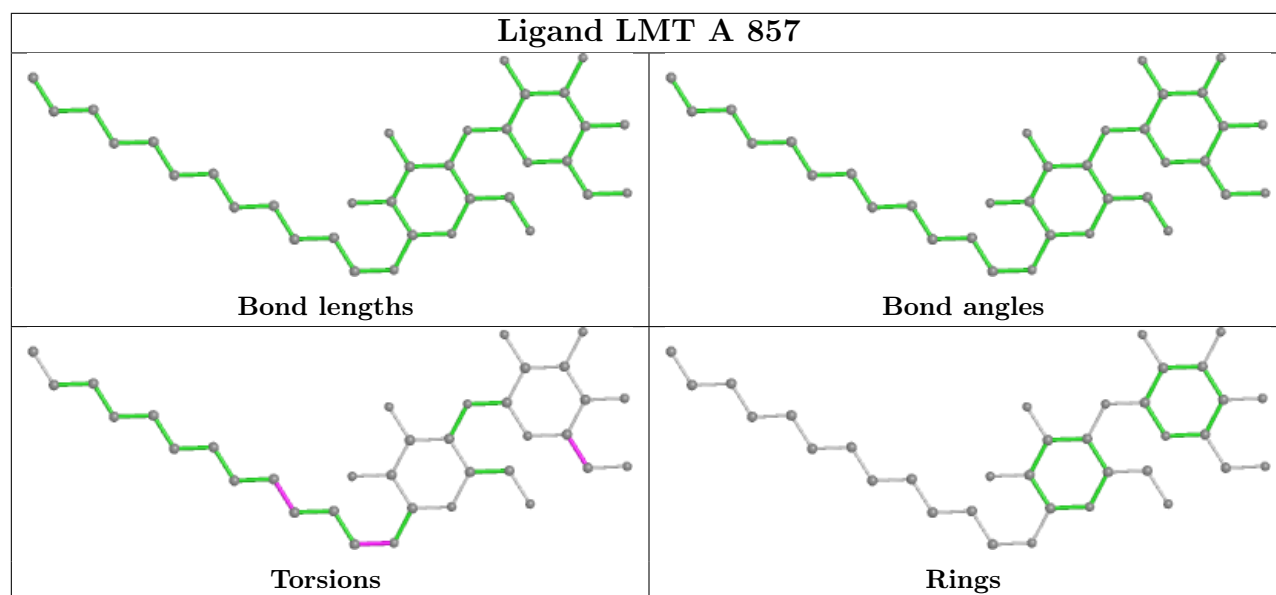
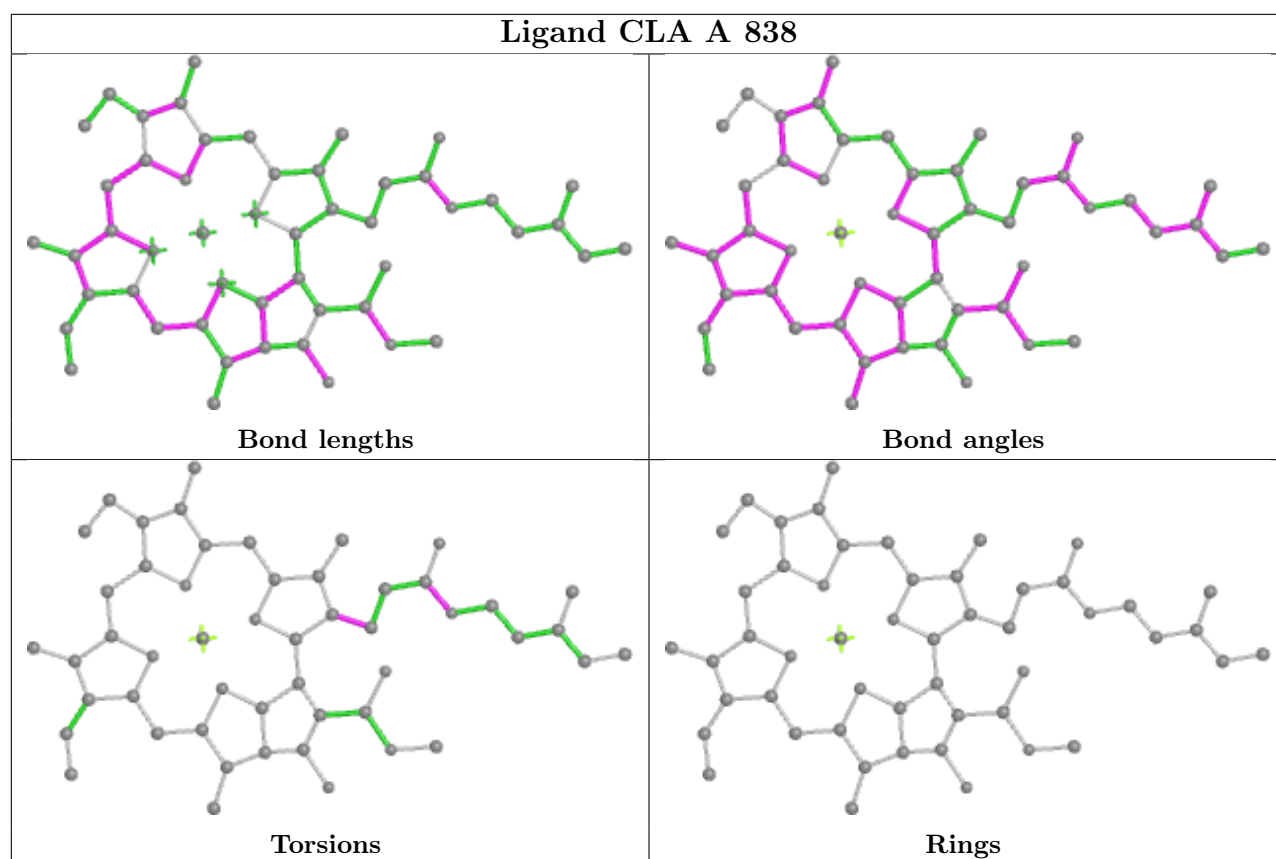
Bond angles

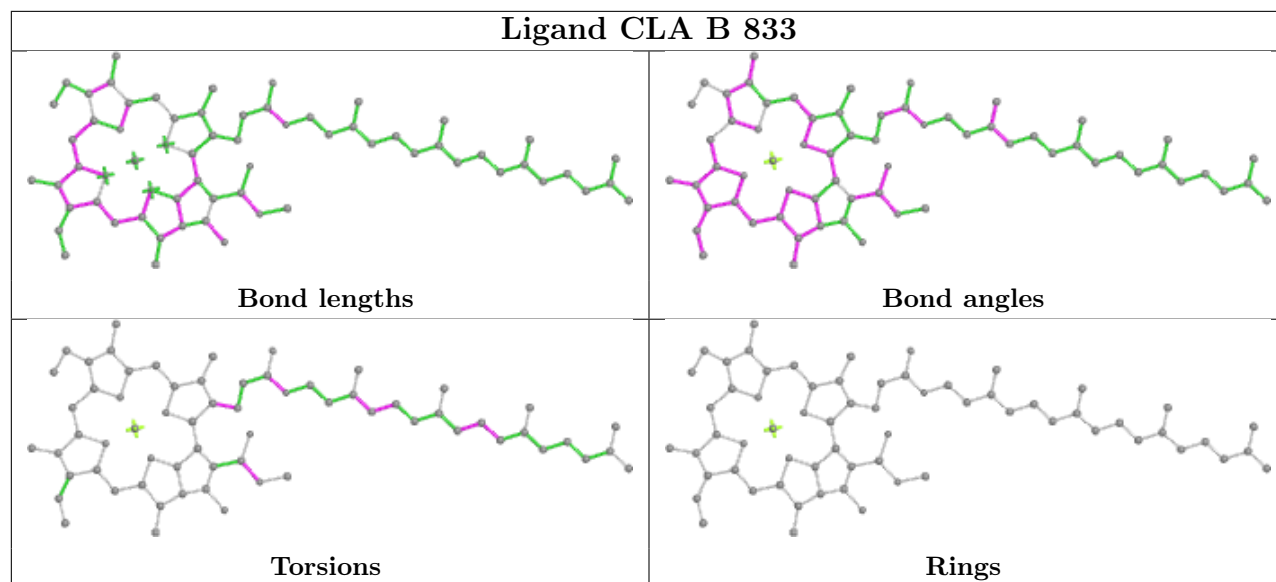
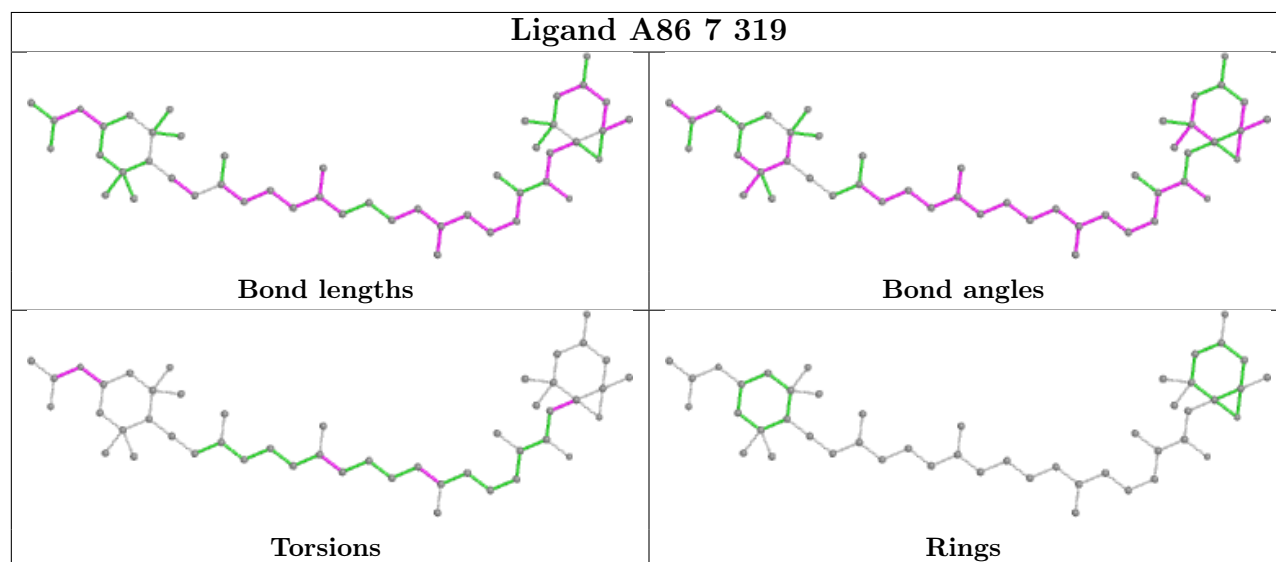


Torsions

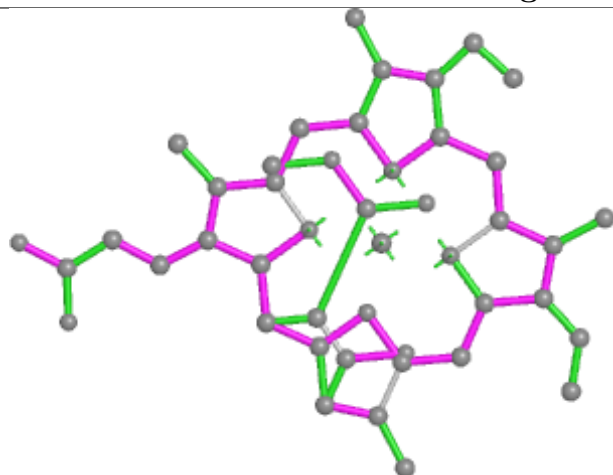


Rings

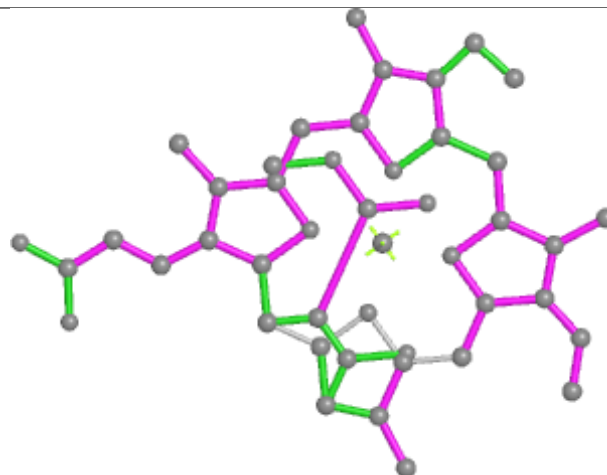


Ligand CLA B 833**Ligand A86 7 319**

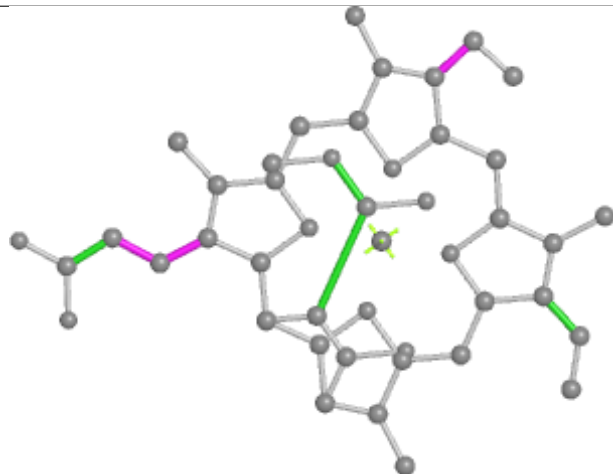
Ligand KC1 4 310



Bond lengths



Bond angles

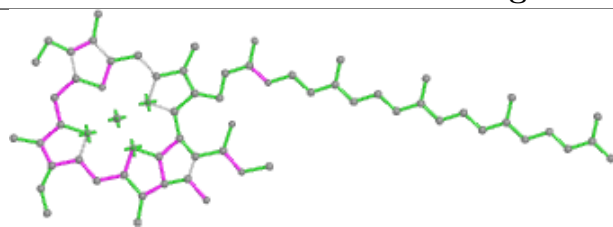


Torsions

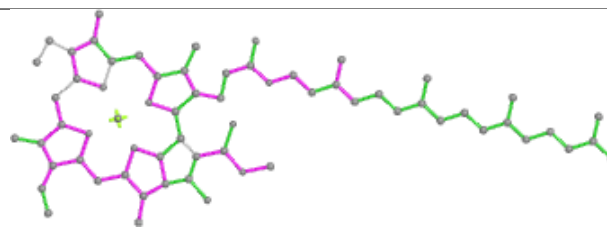


Rings

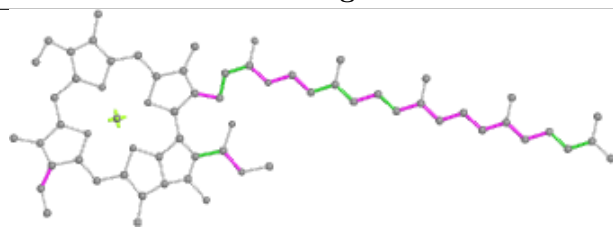
Ligand CLA 15 304



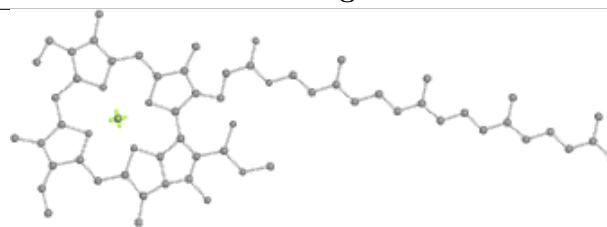
Bond lengths



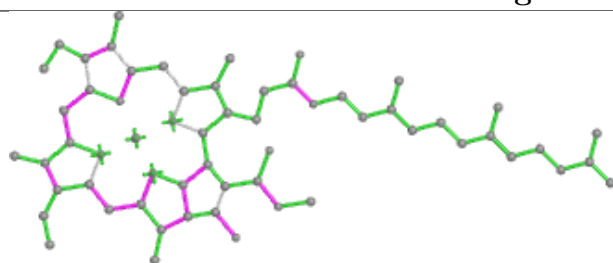
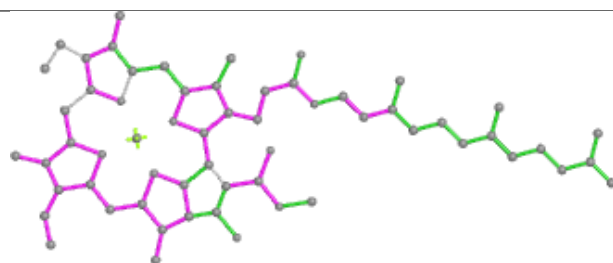
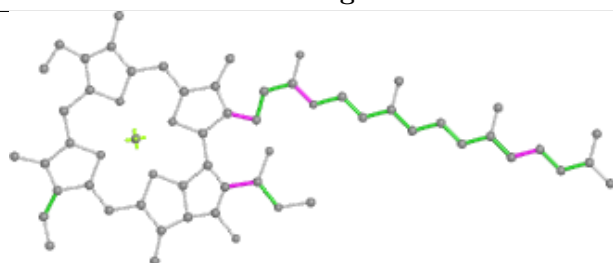
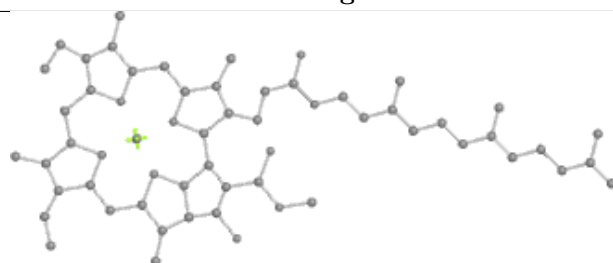
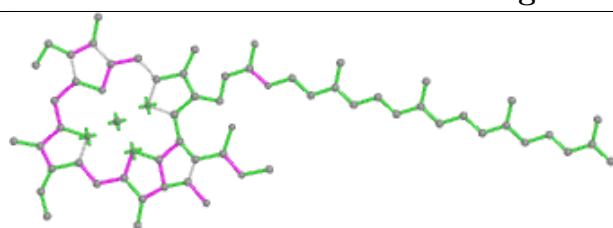
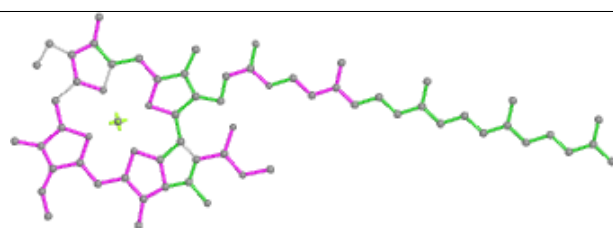
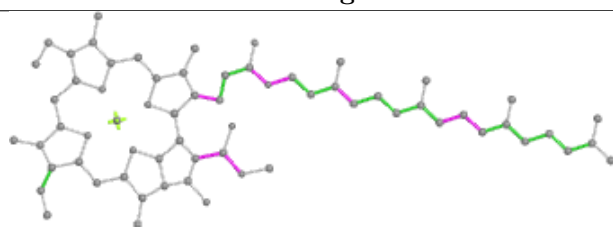
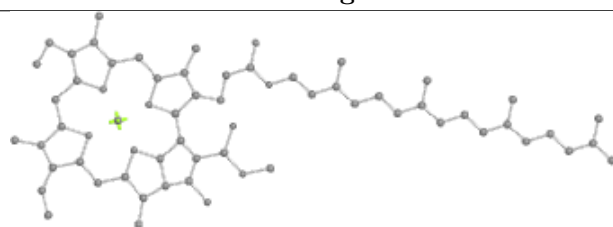
Bond angles

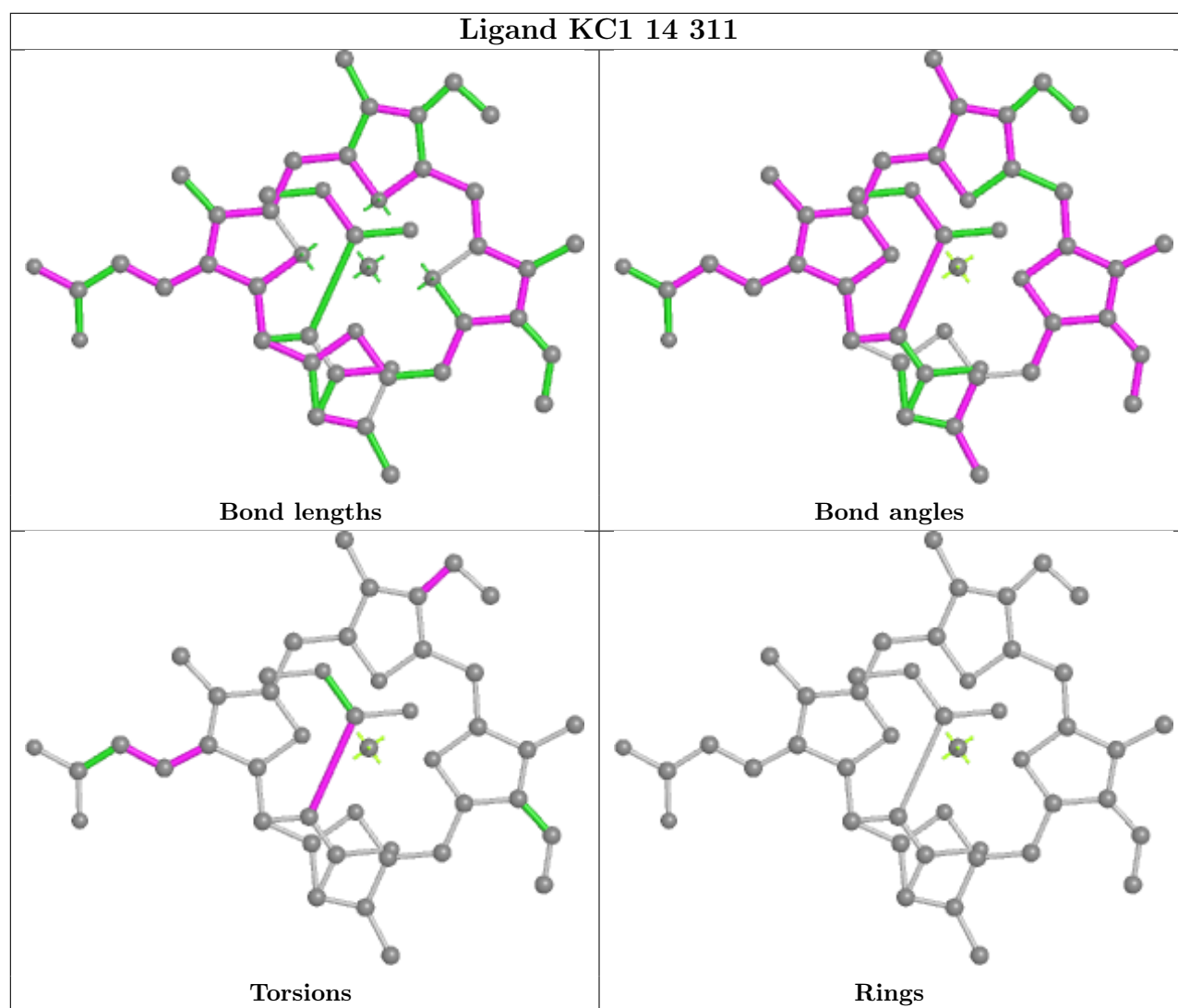


Torsions

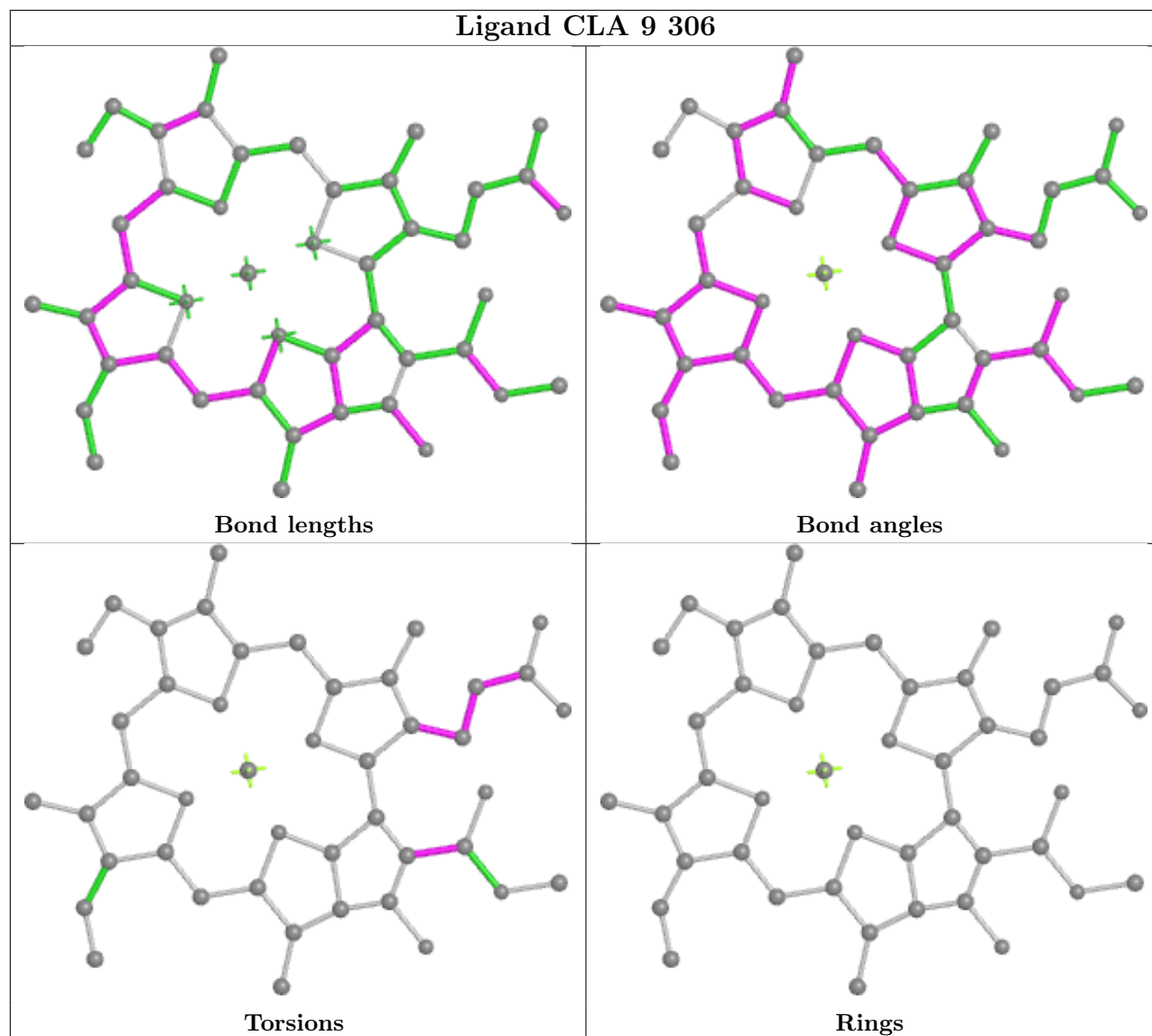


Rings

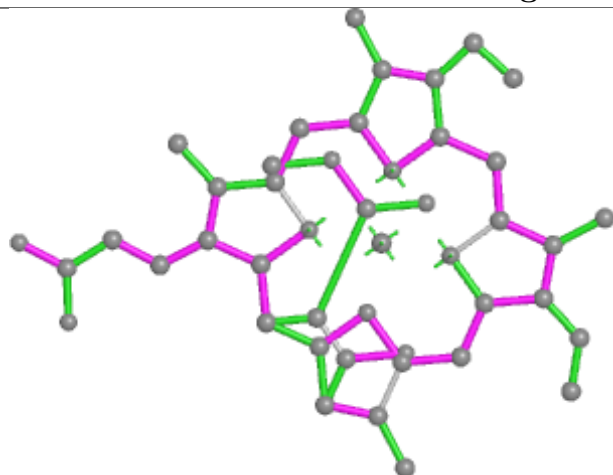
Ligand CLA B 818**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 1 304****Bond lengths****Bond angles****Torsions****Rings**



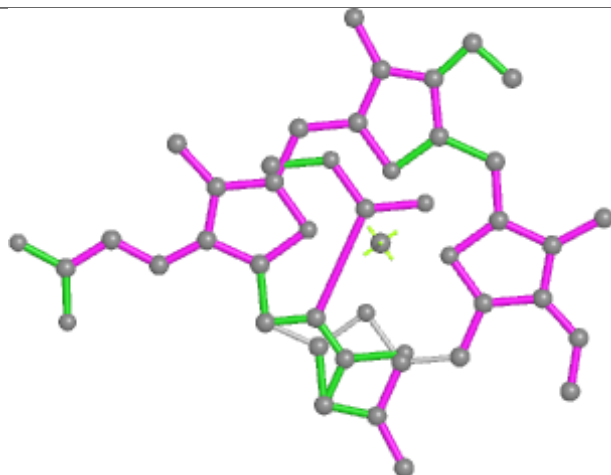
Ligand CLA 9 306



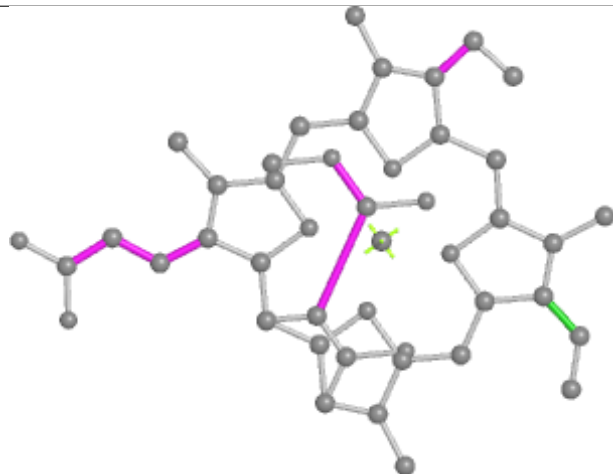
Ligand KC1 5 306



Bond lengths



Bond angles

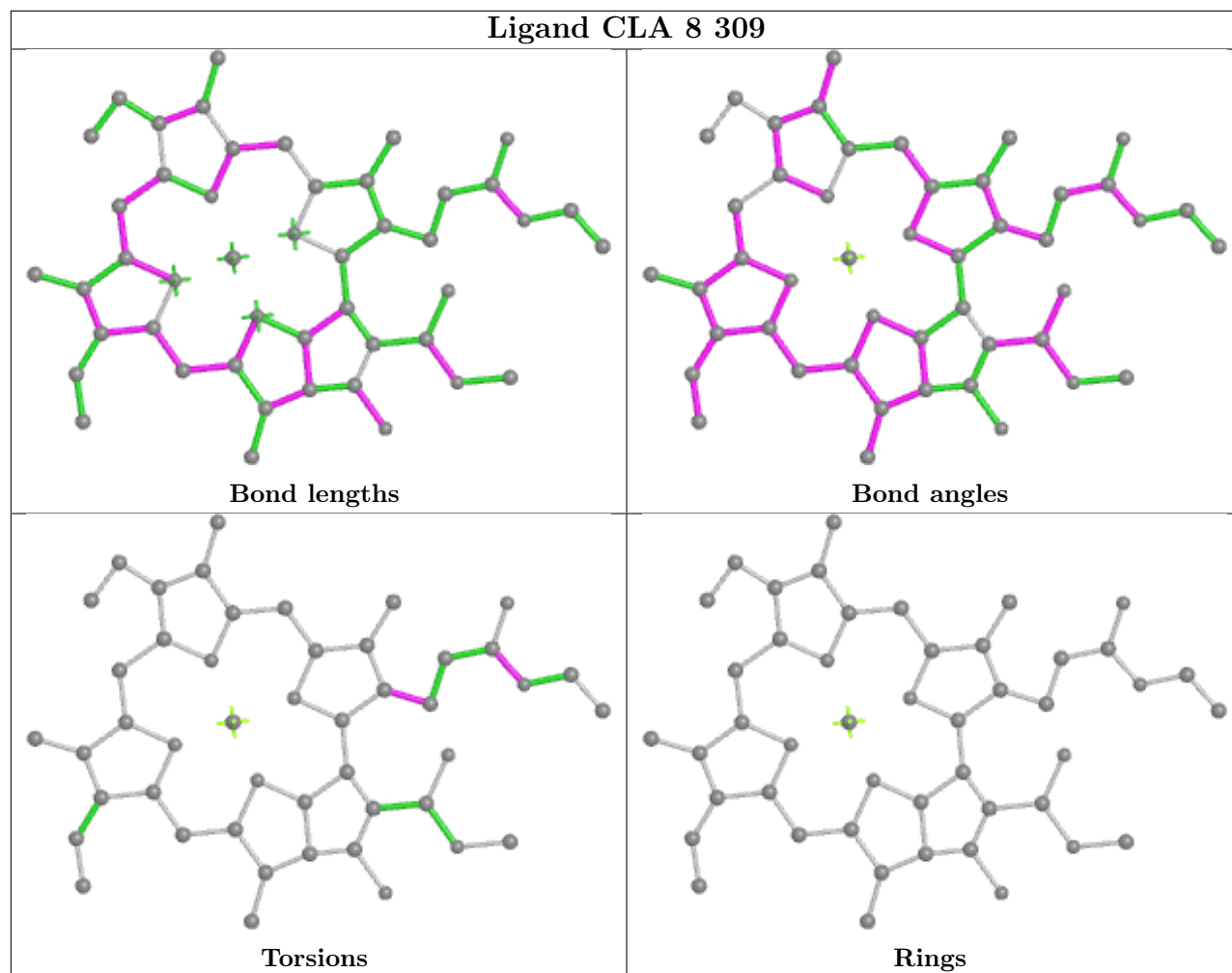


Torsions

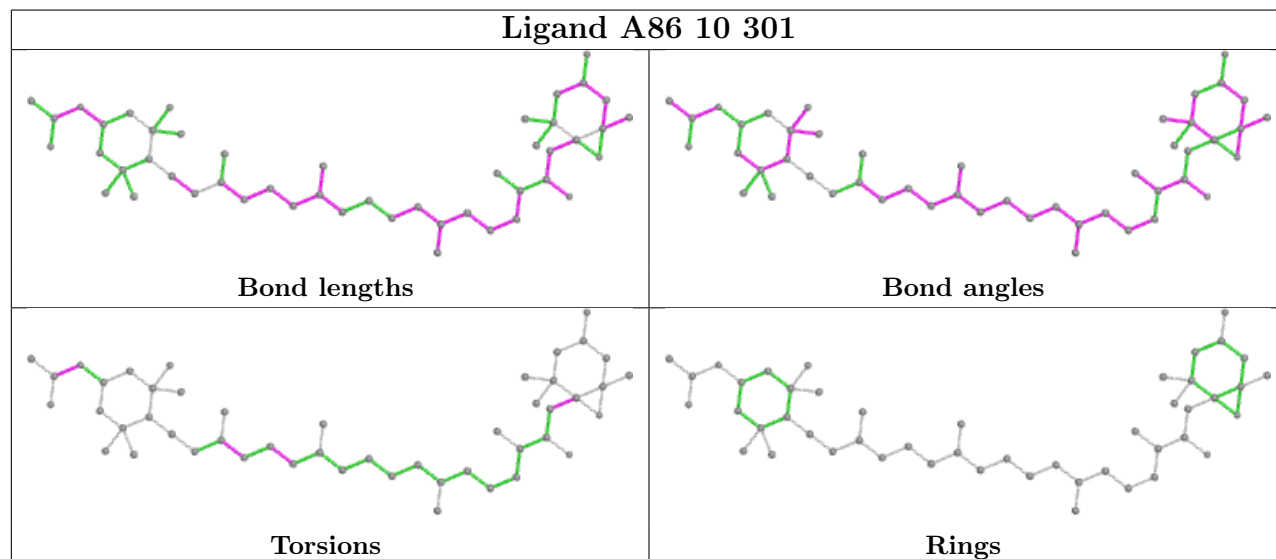


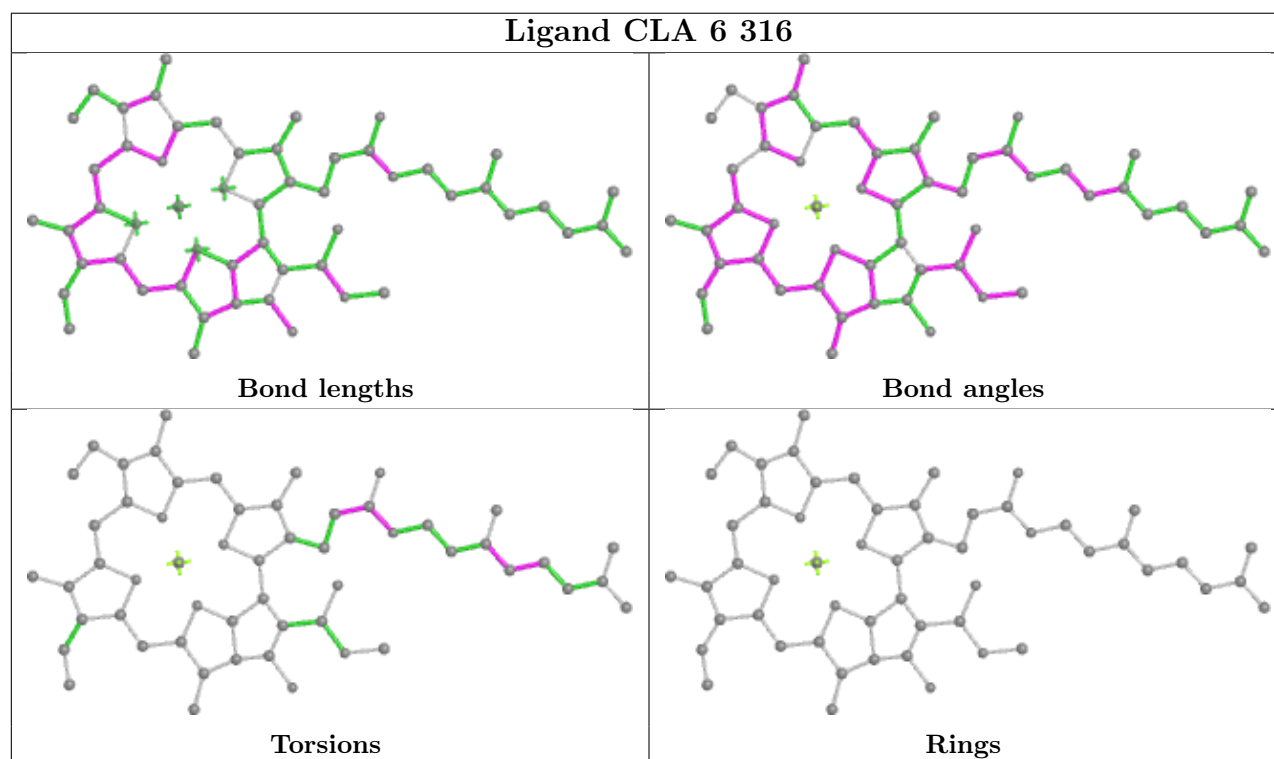
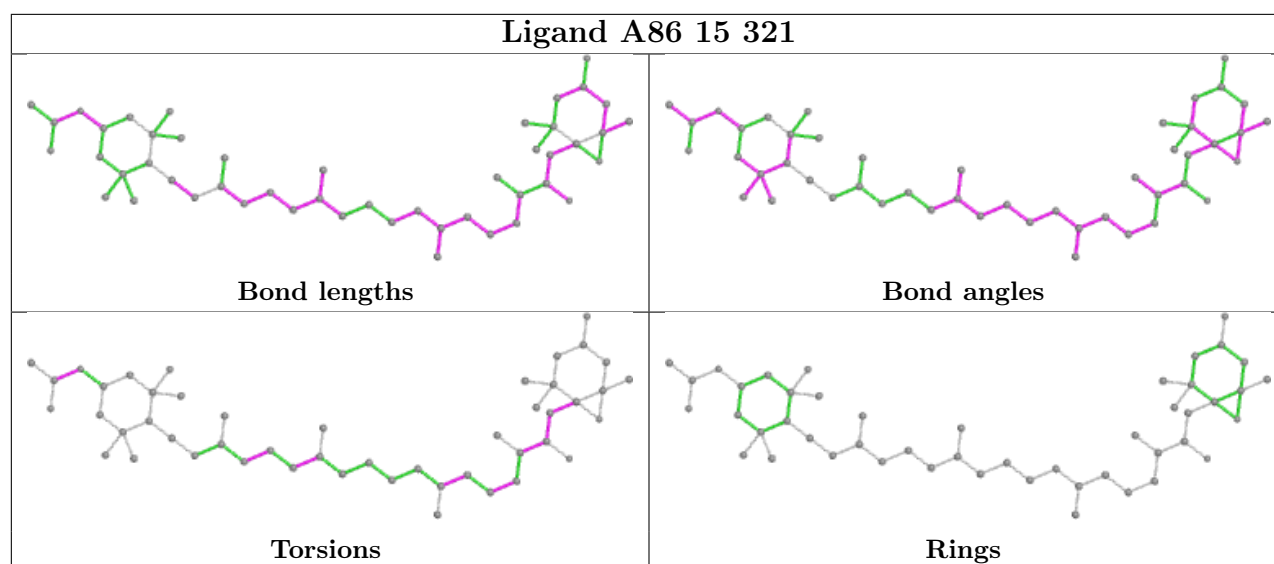
Rings

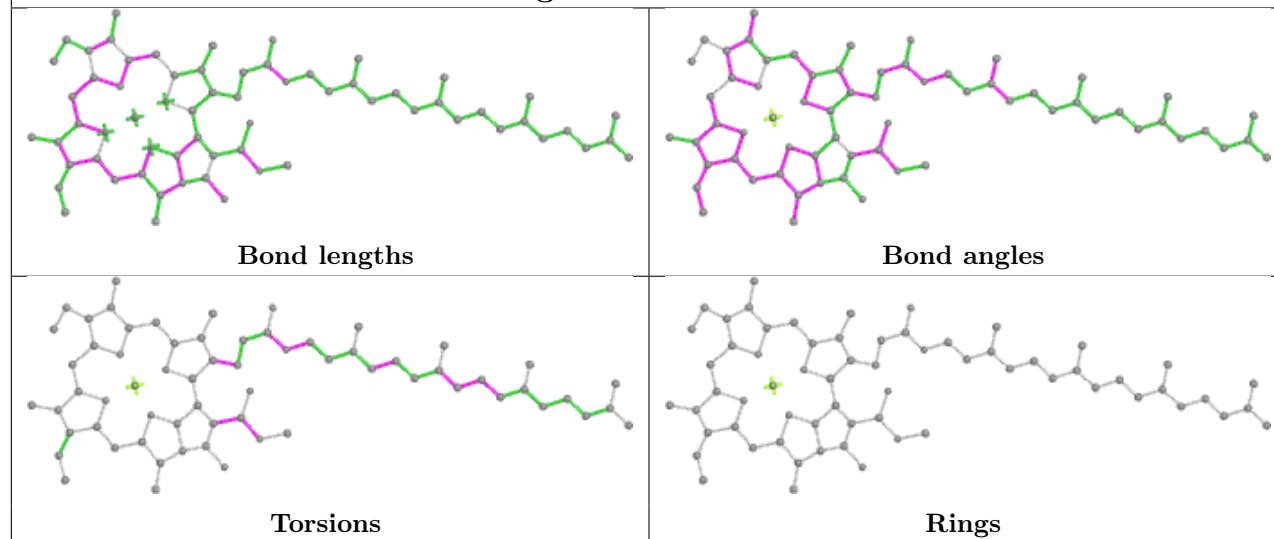
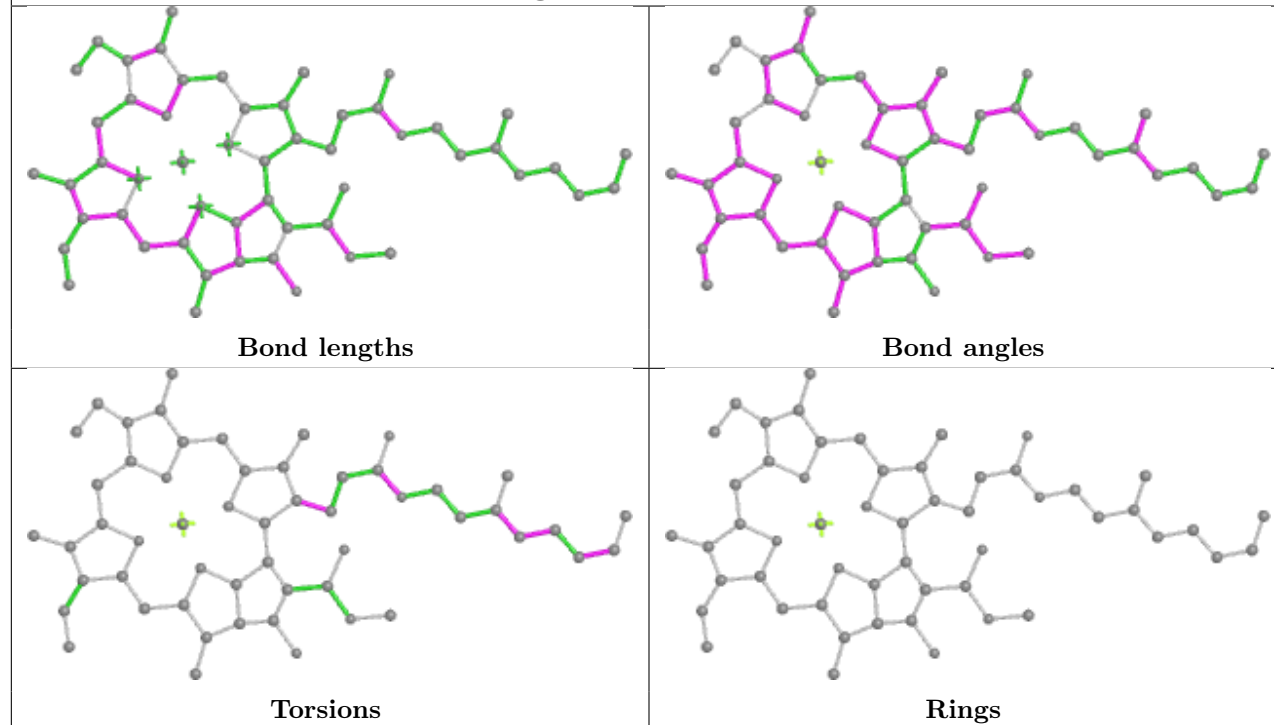
Ligand CLA 8 309

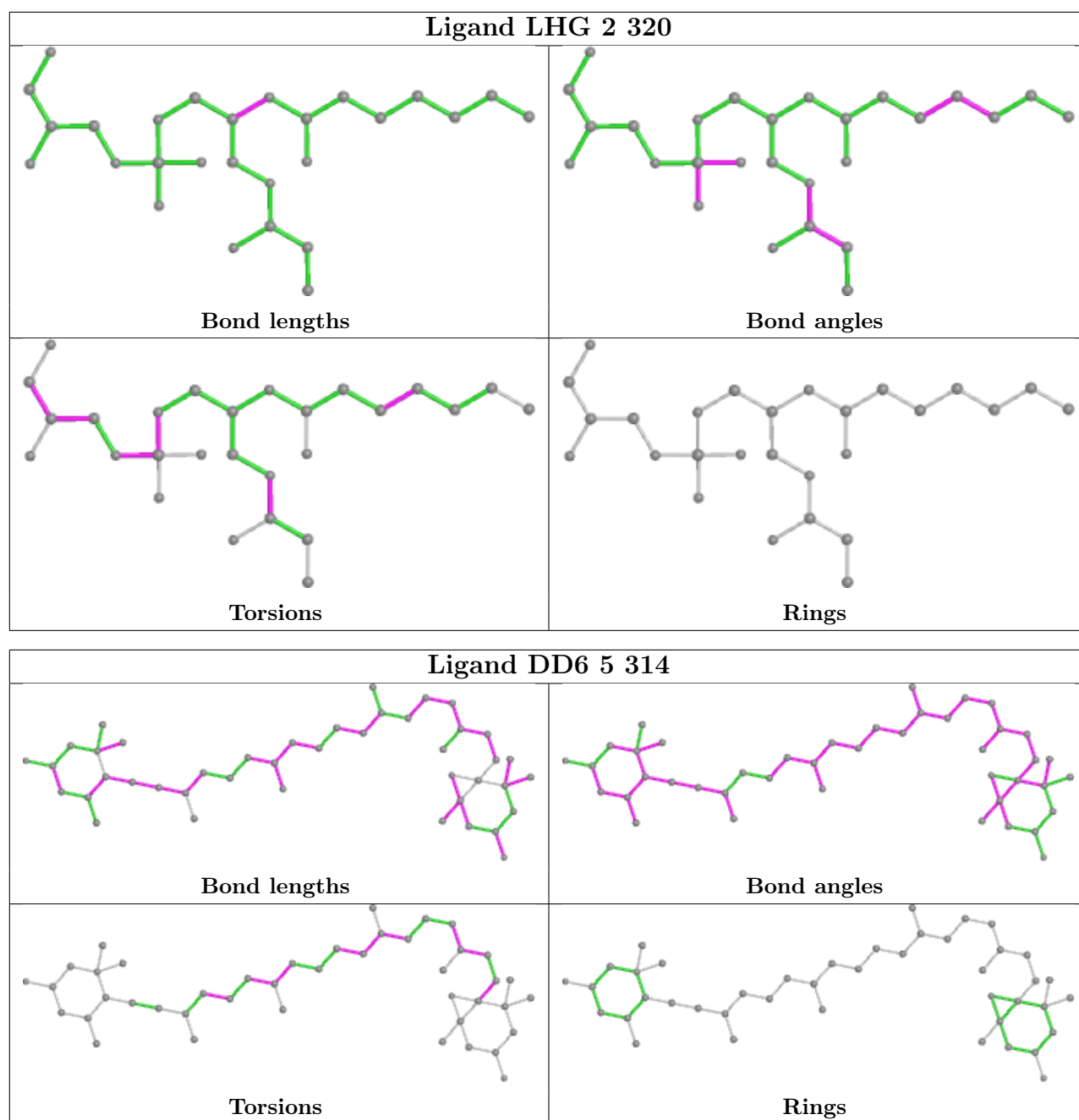


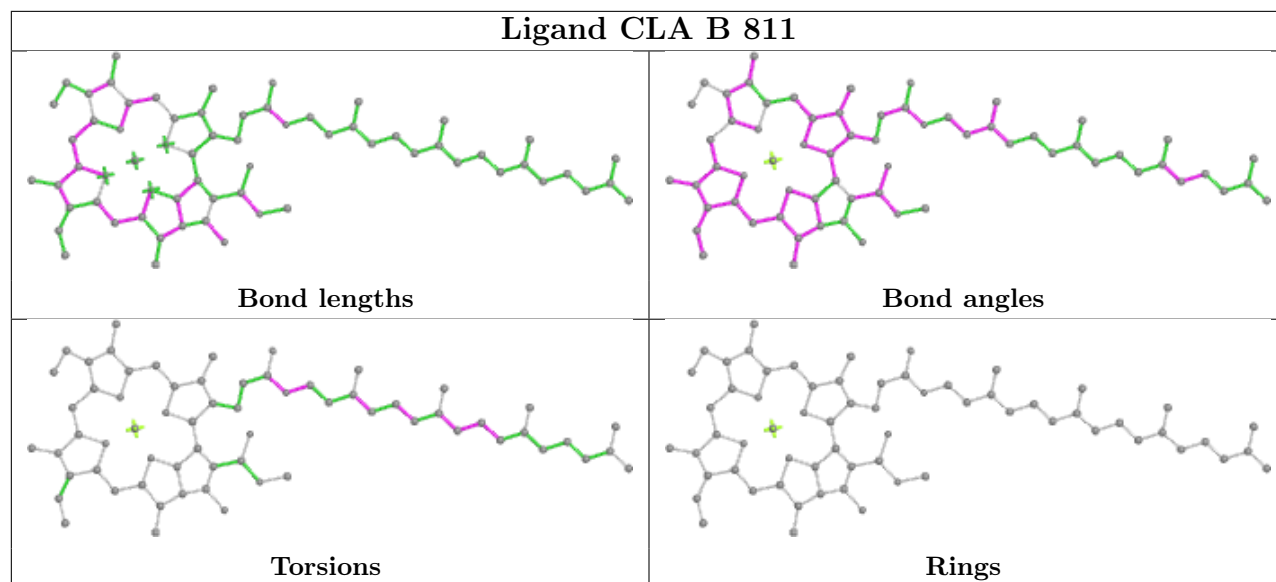
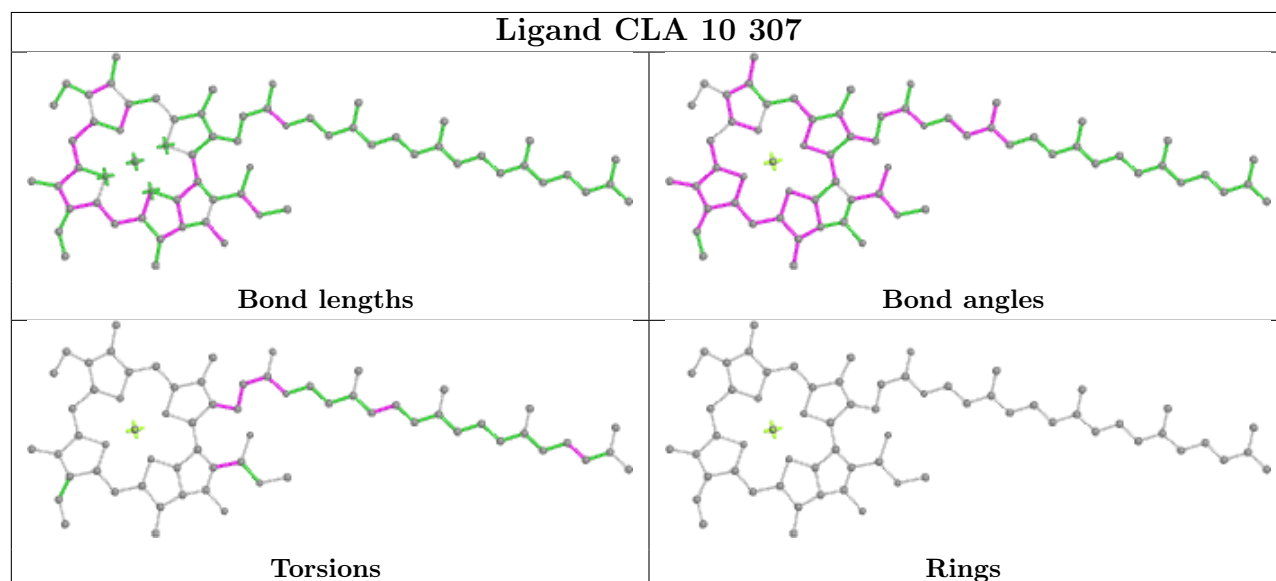
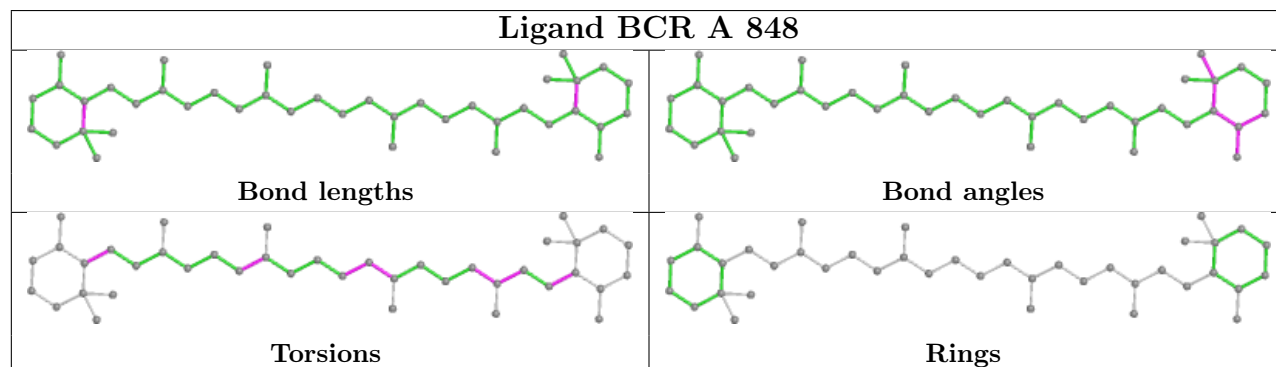
Ligand A86 10 301

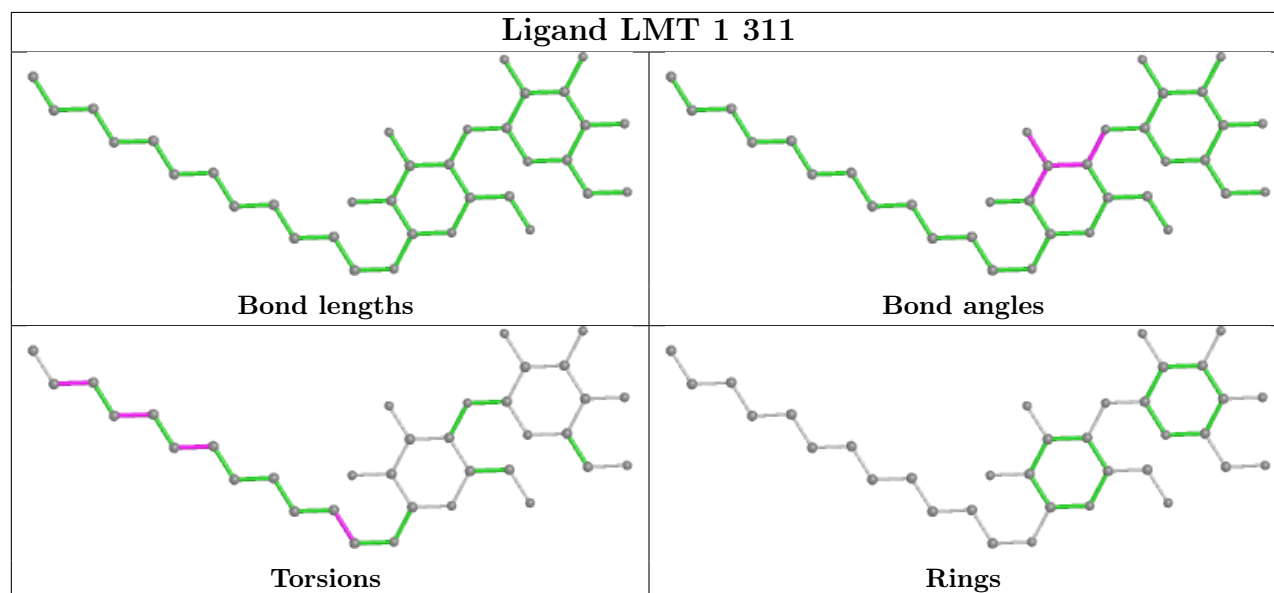
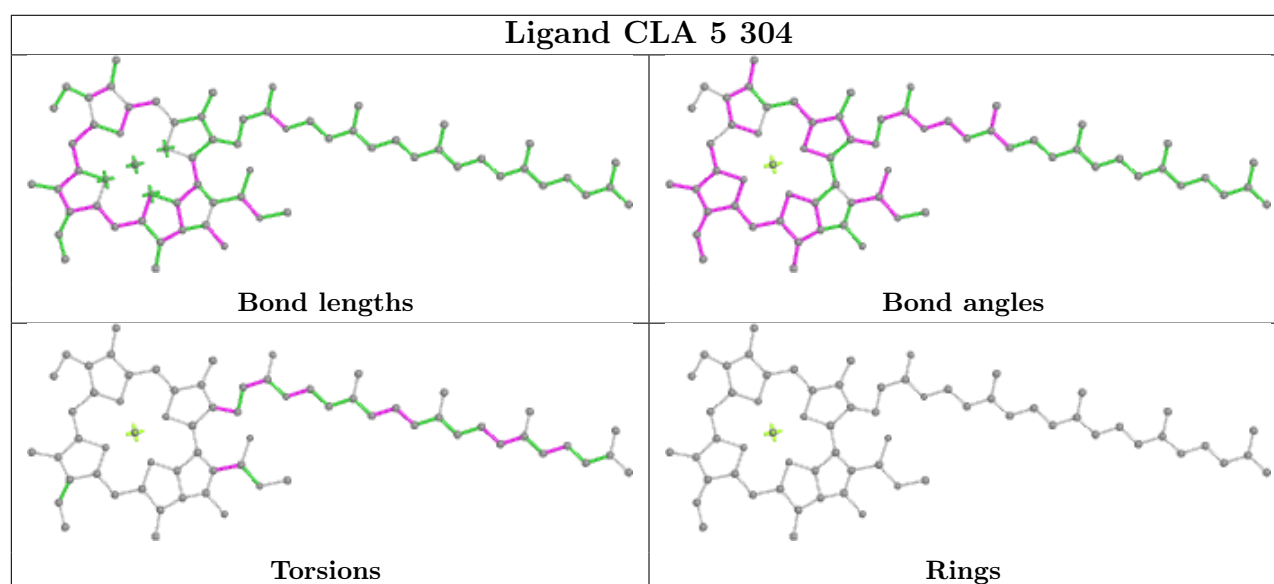
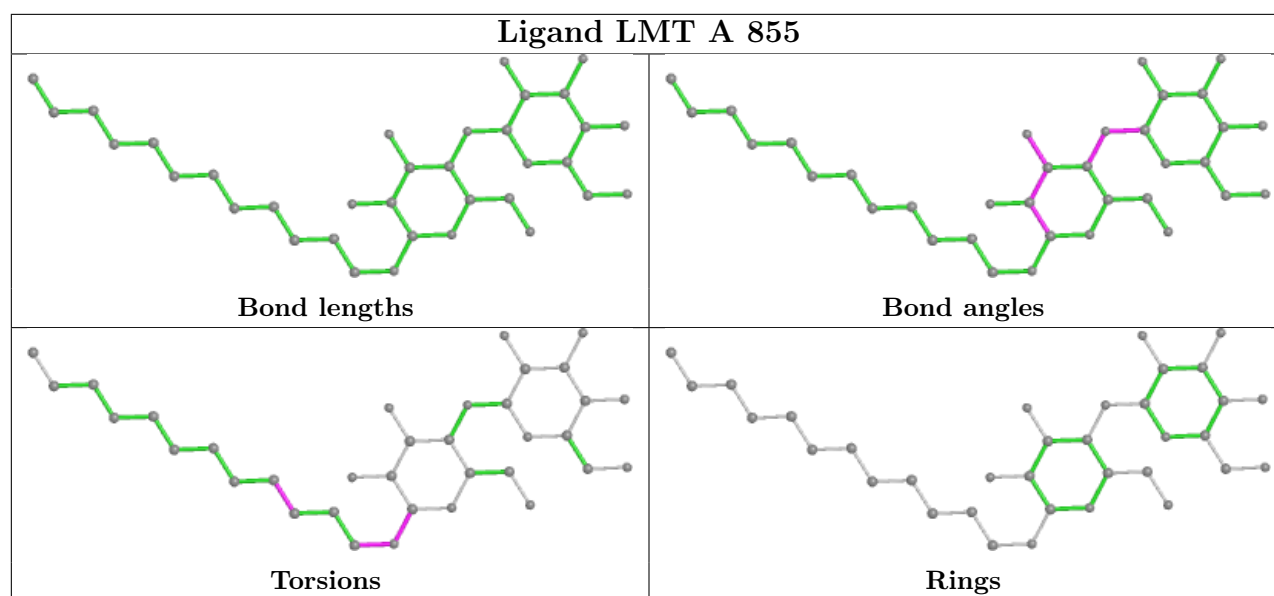


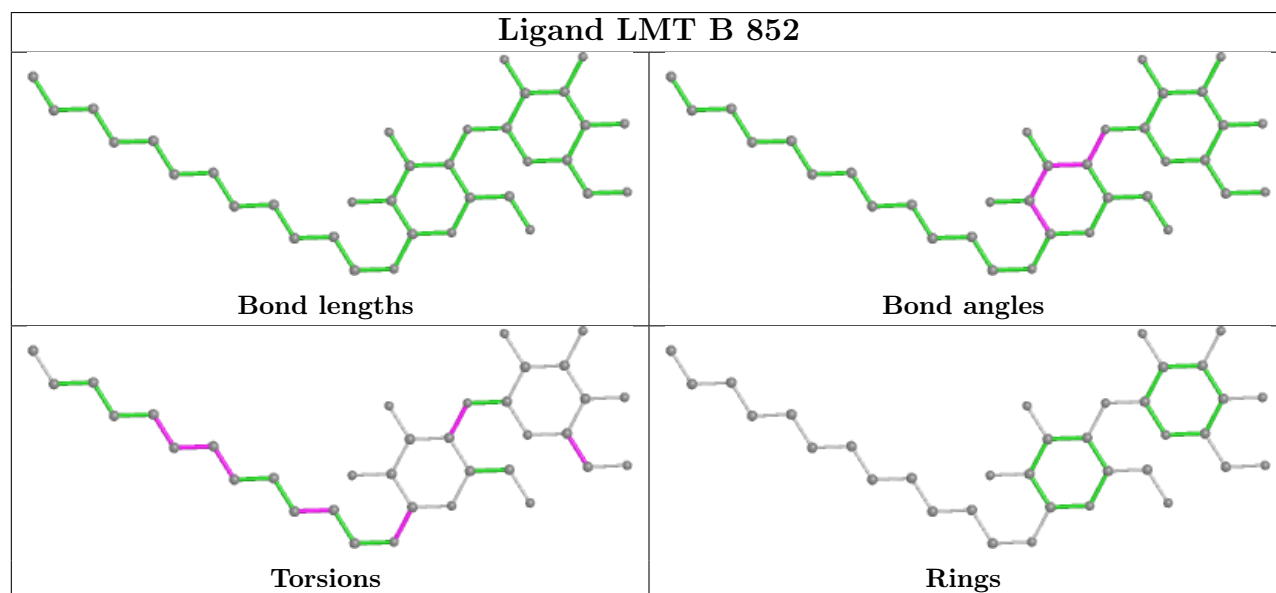
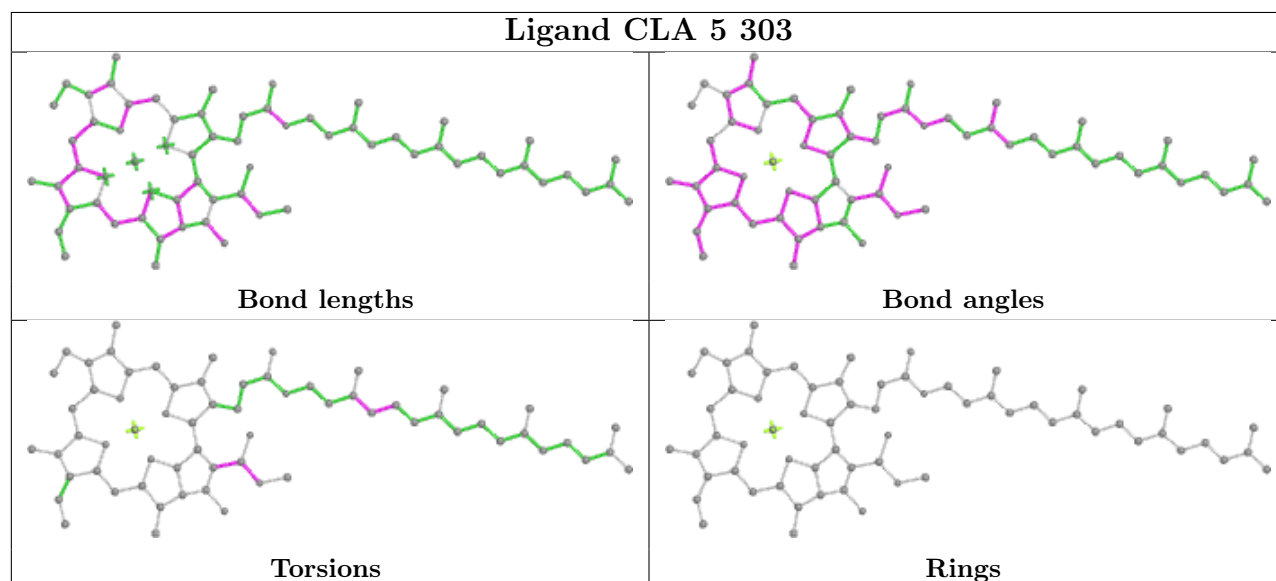
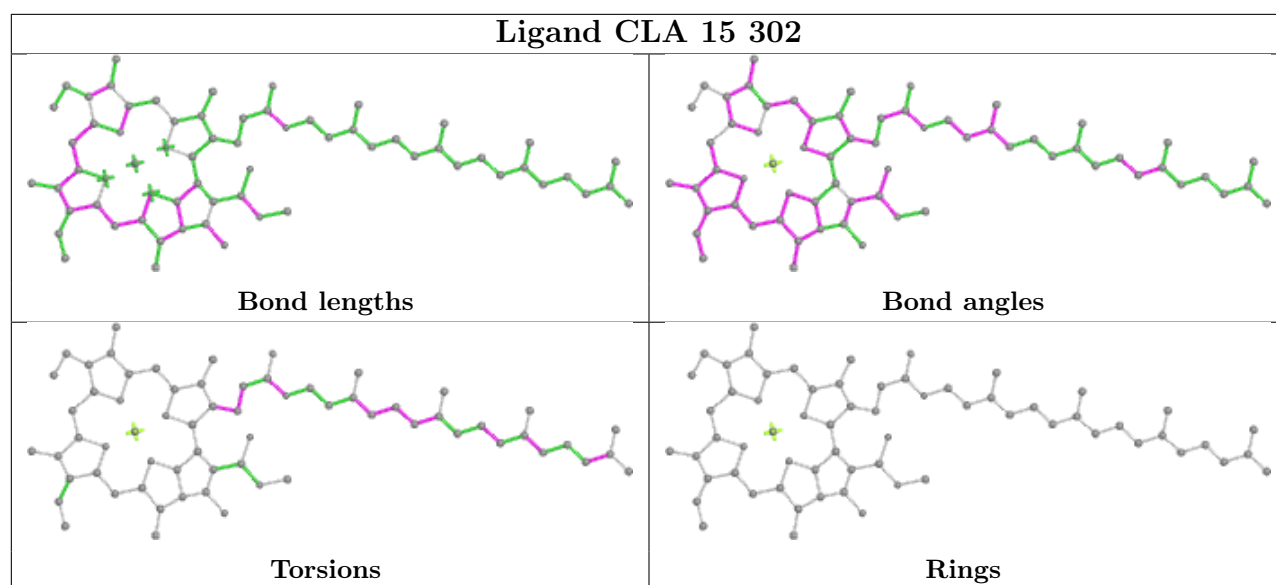


Ligand CLA 5 311**Ligand CLA A 836**

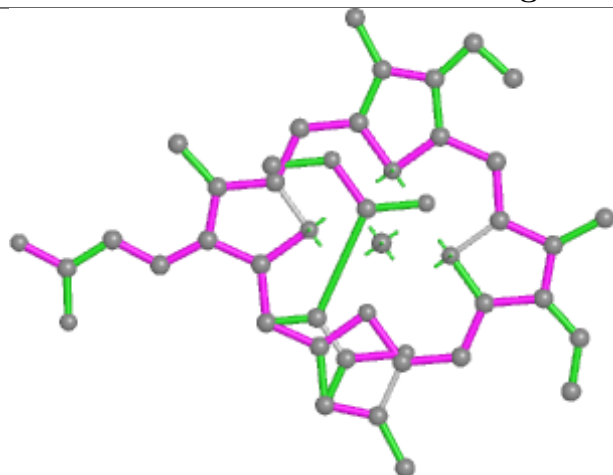


Ligand CLA B 811**Ligand CLA 10 307****Ligand BCR A 848**

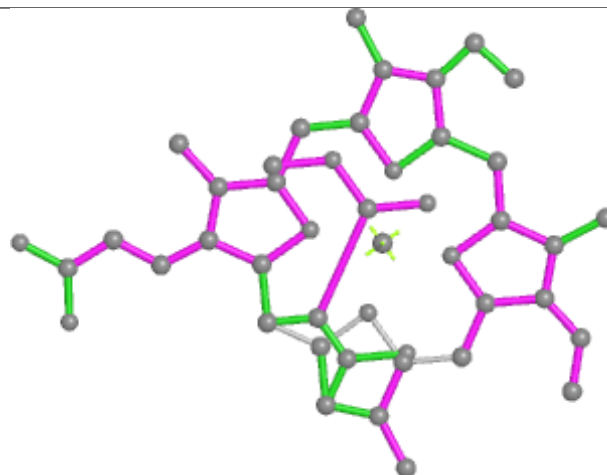




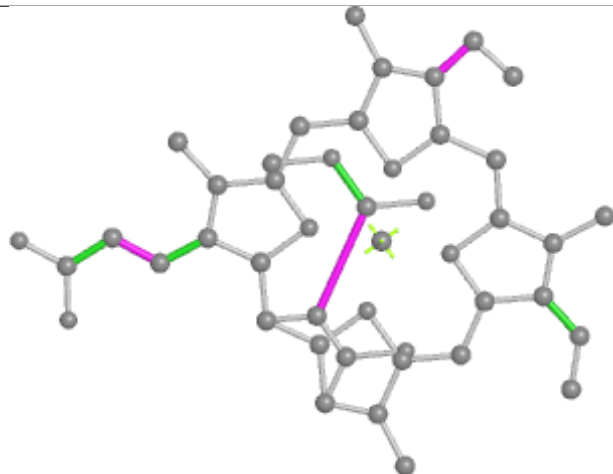
Ligand KC1 1 308



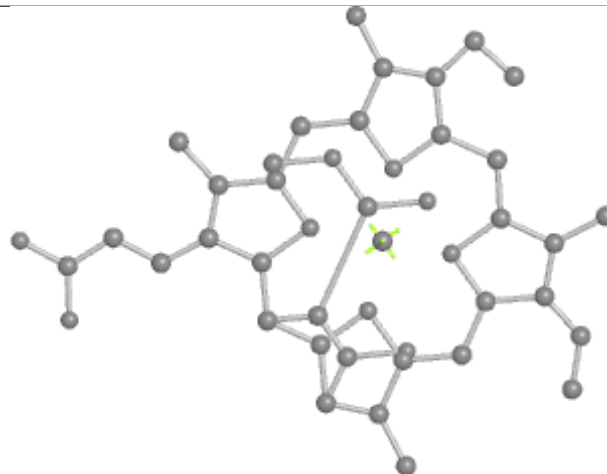
Bond lengths



Bond angles

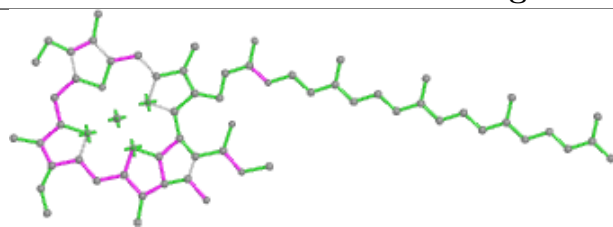


Torsions

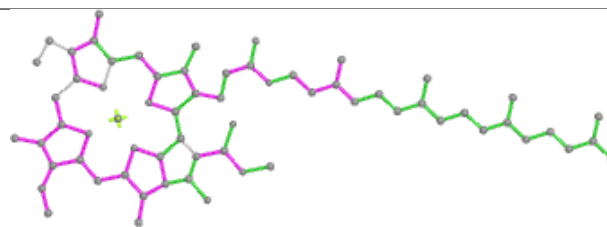


Rings

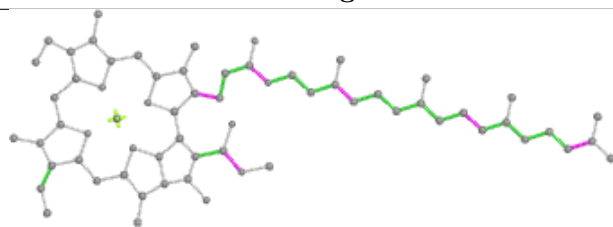
Ligand CLA 15 309



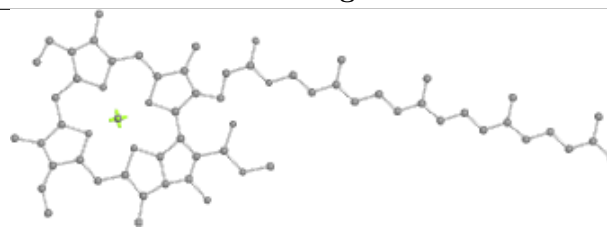
Bond lengths



Bond angles

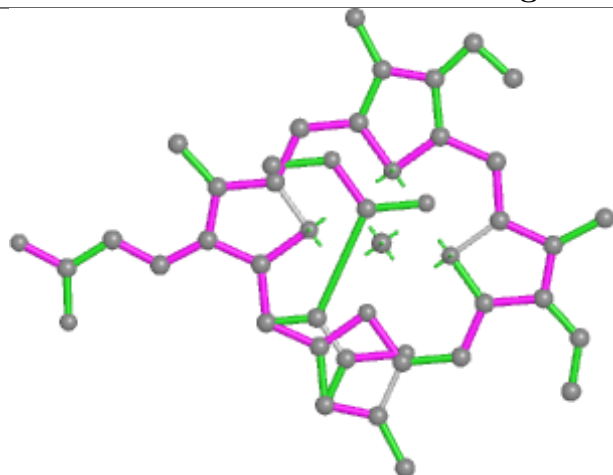


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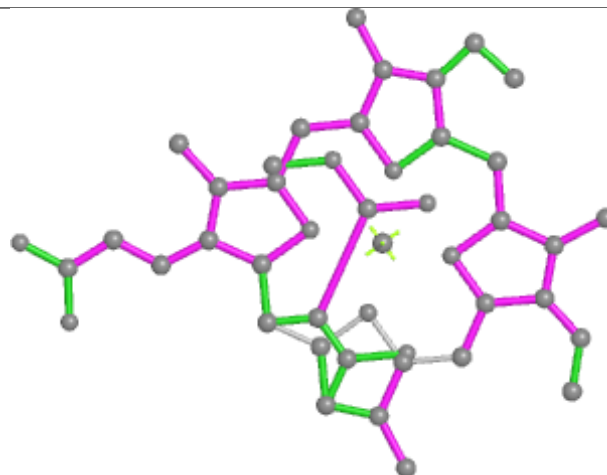


Rings

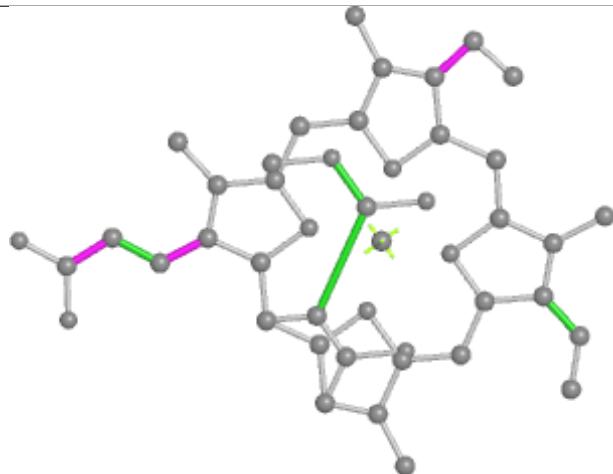
Ligand KC1 5 305



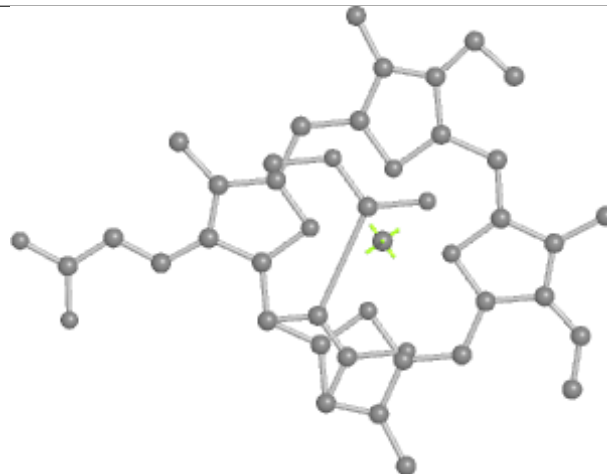
Bond lengths



Bond angles

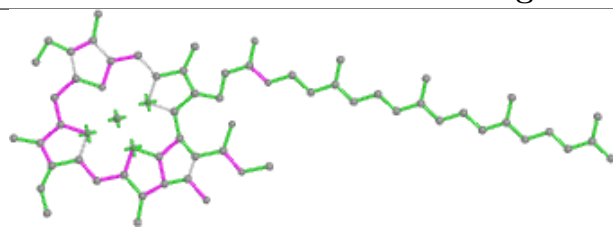


Torsions

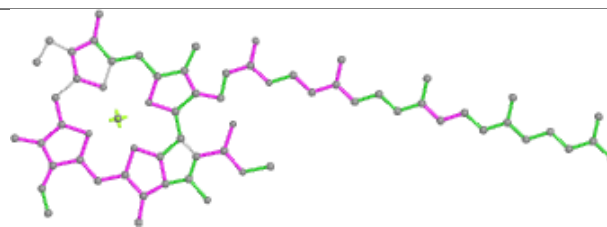


Rings

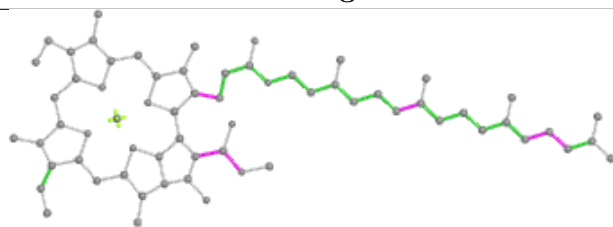
Ligand CLA F 201



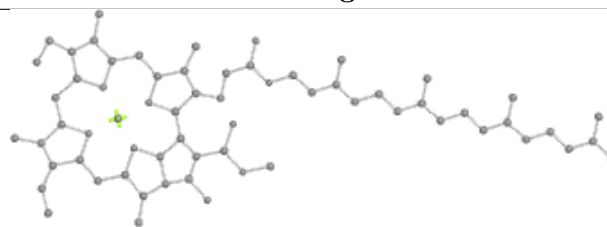
Bond lengths



Bond angles

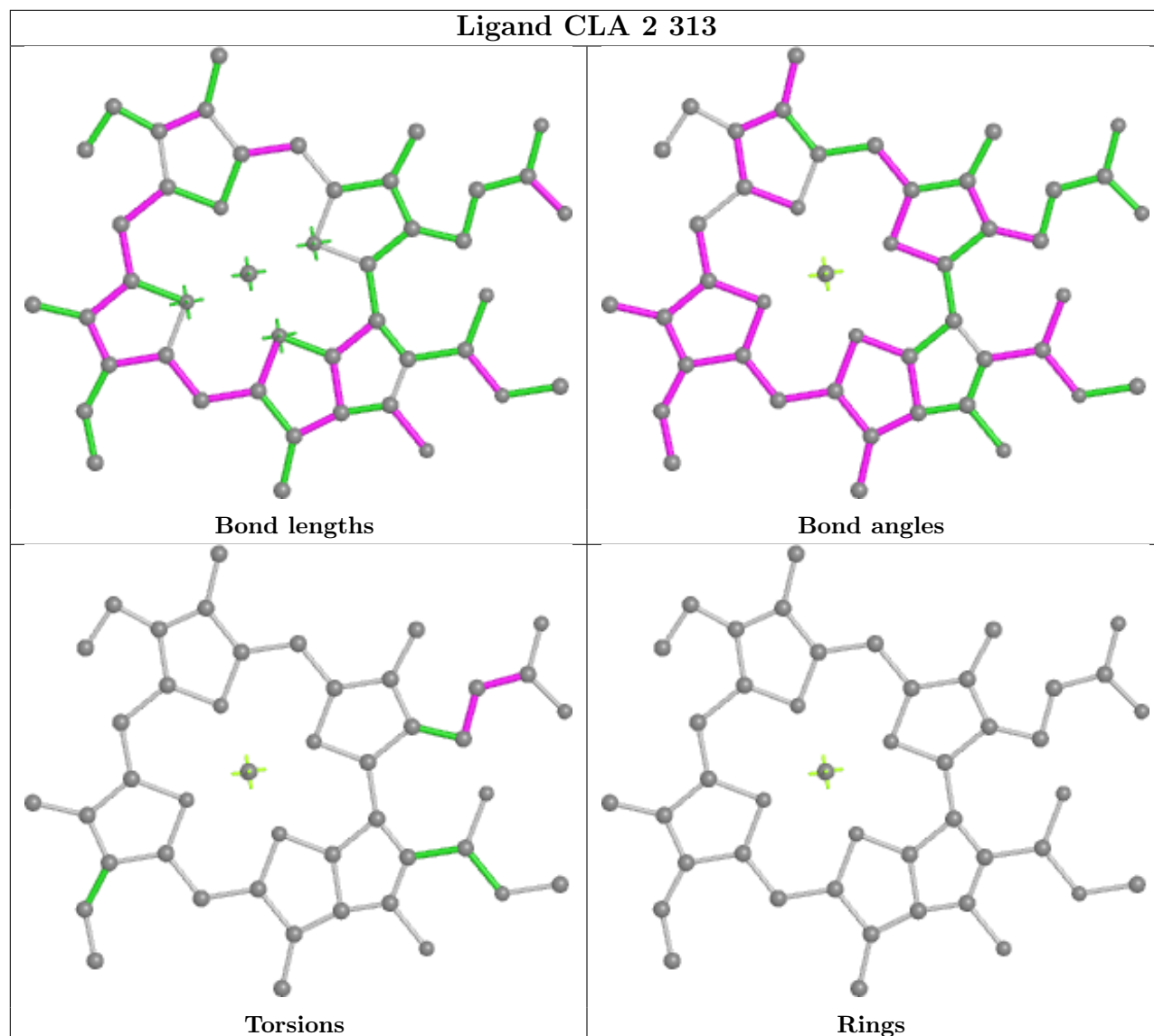


Torsions

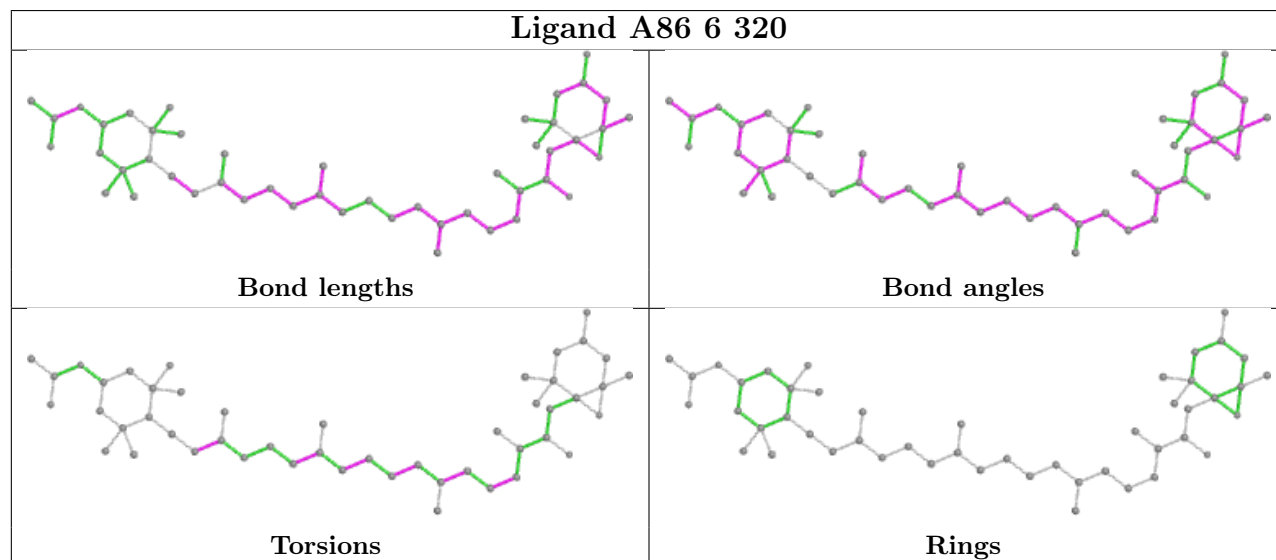


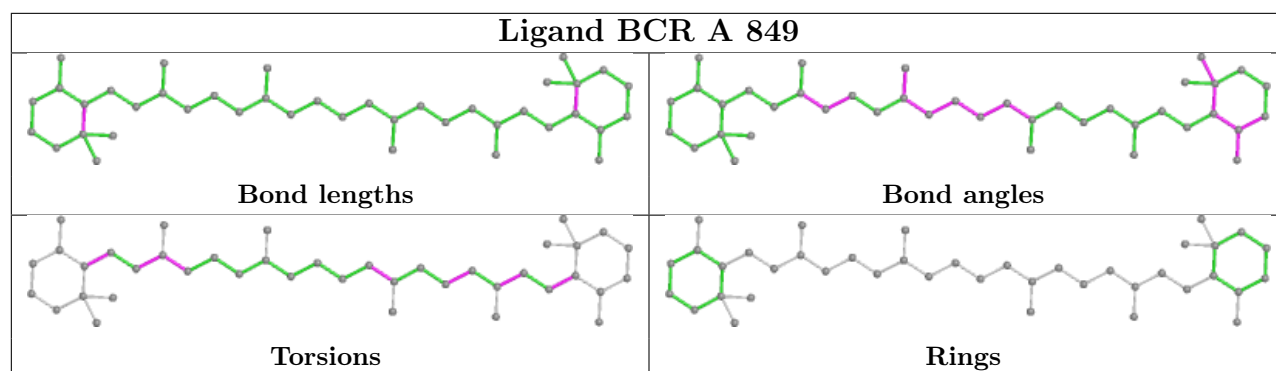
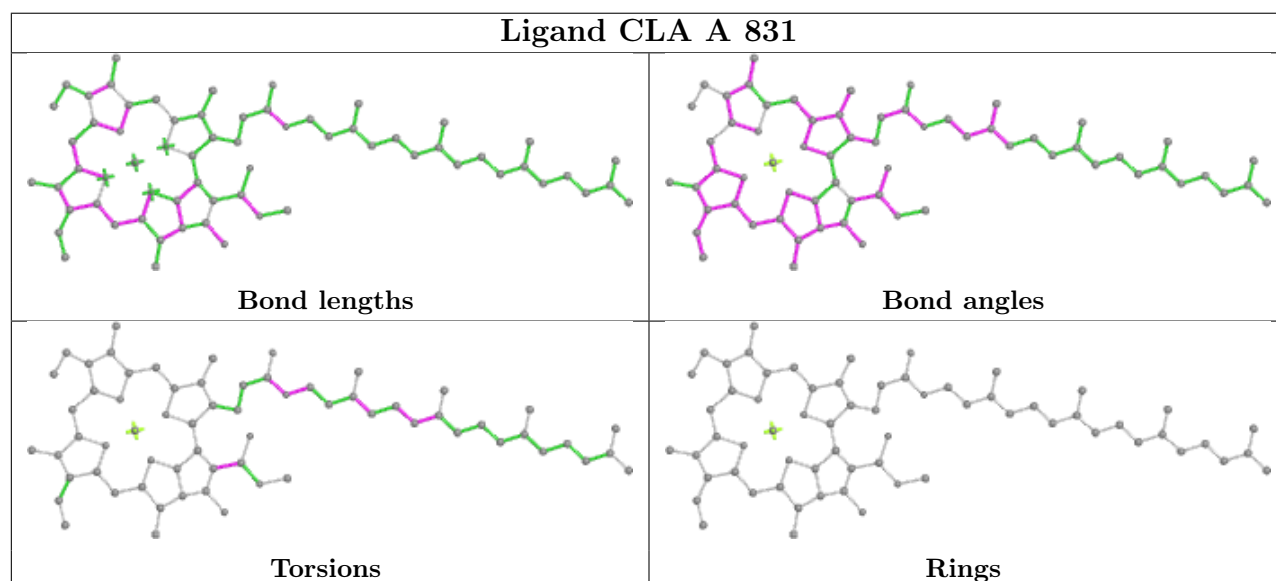
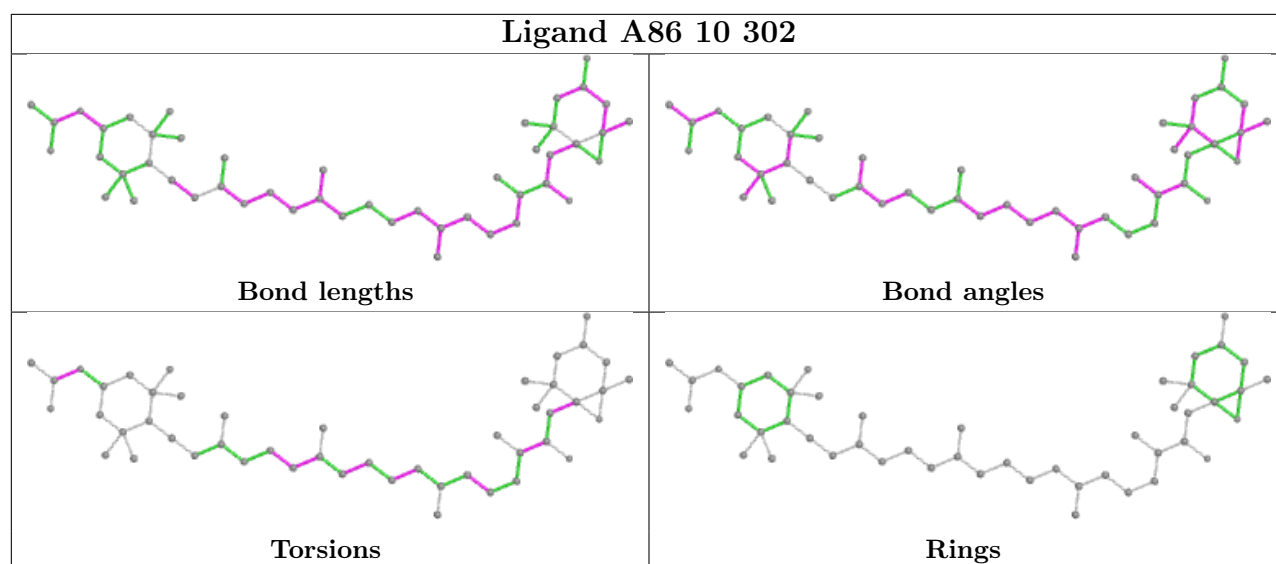
Rings

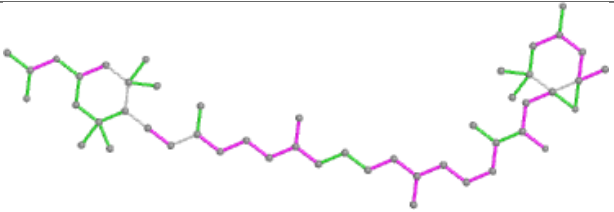
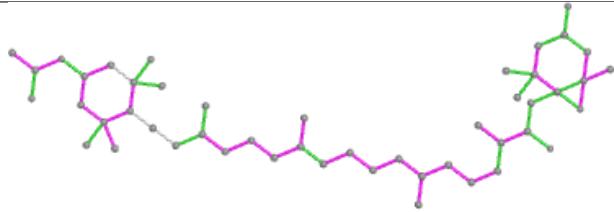
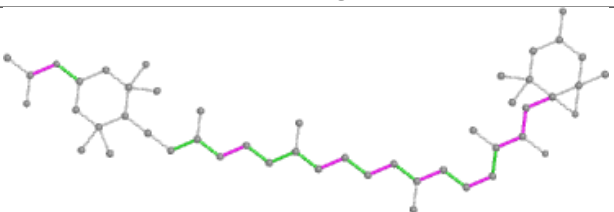
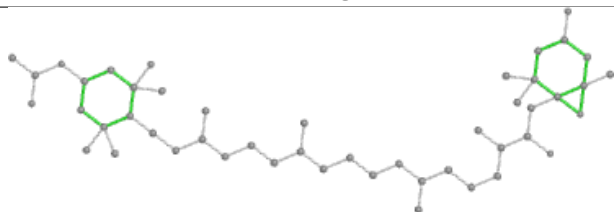
Ligand CLA 2 313

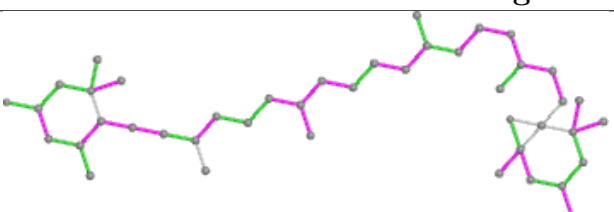
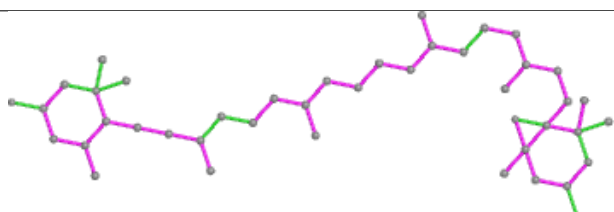
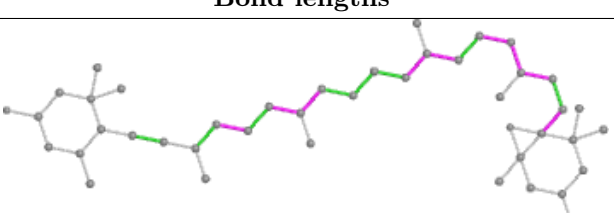
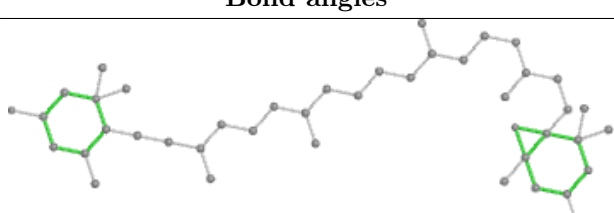


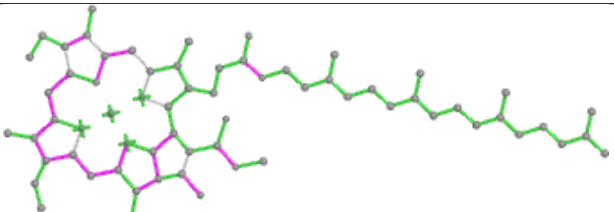
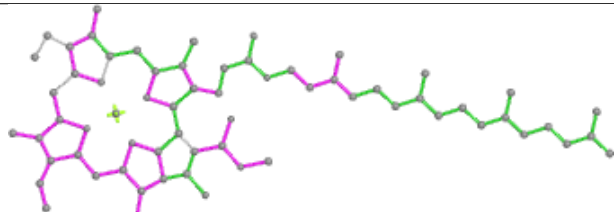
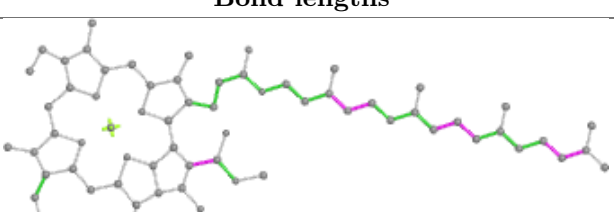
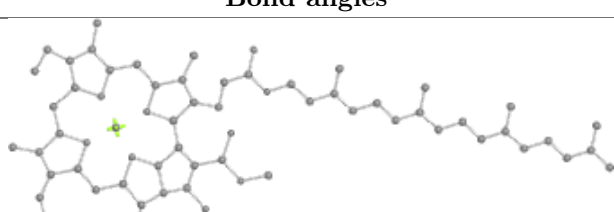
Ligand A86 6 320

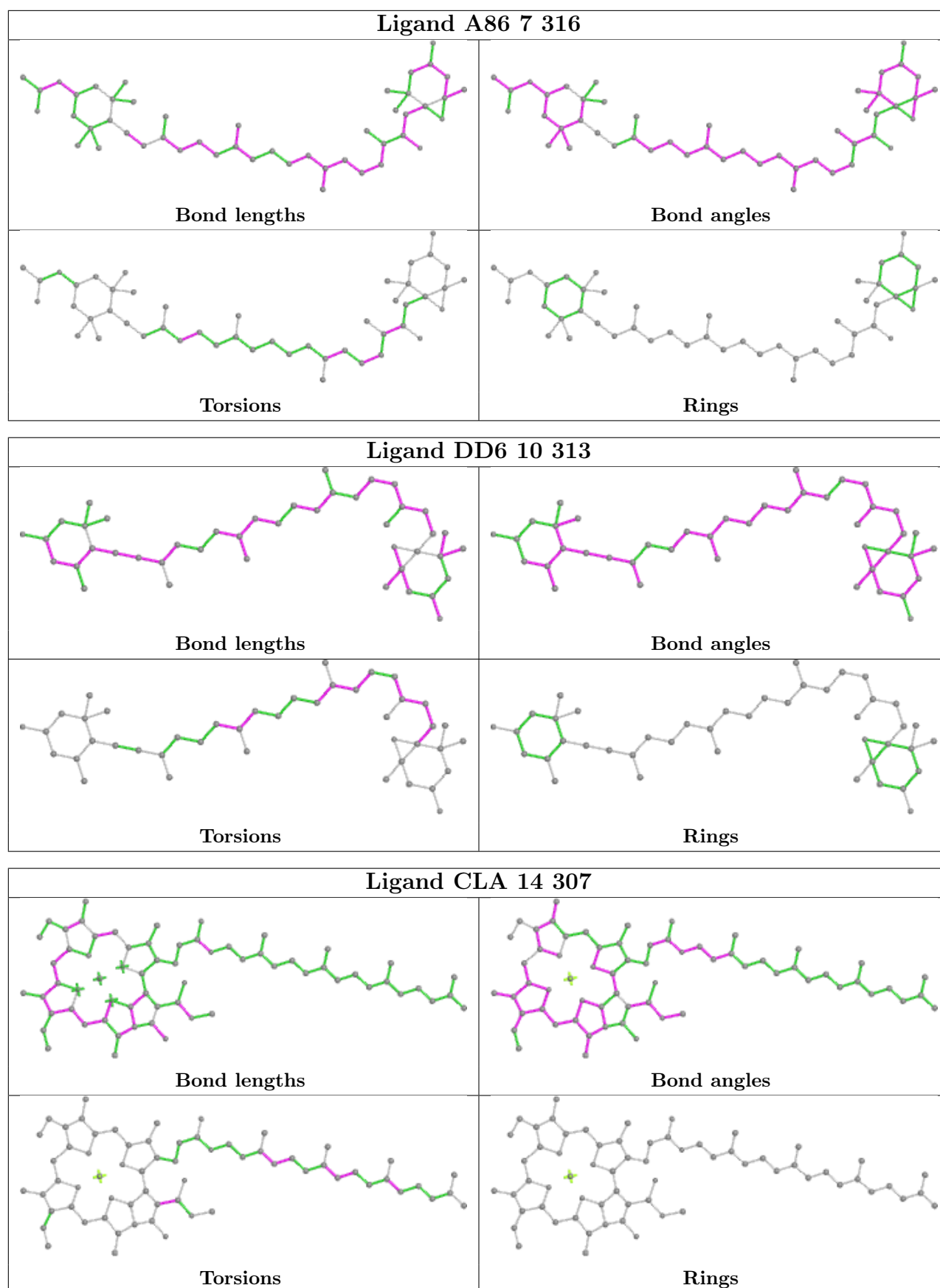




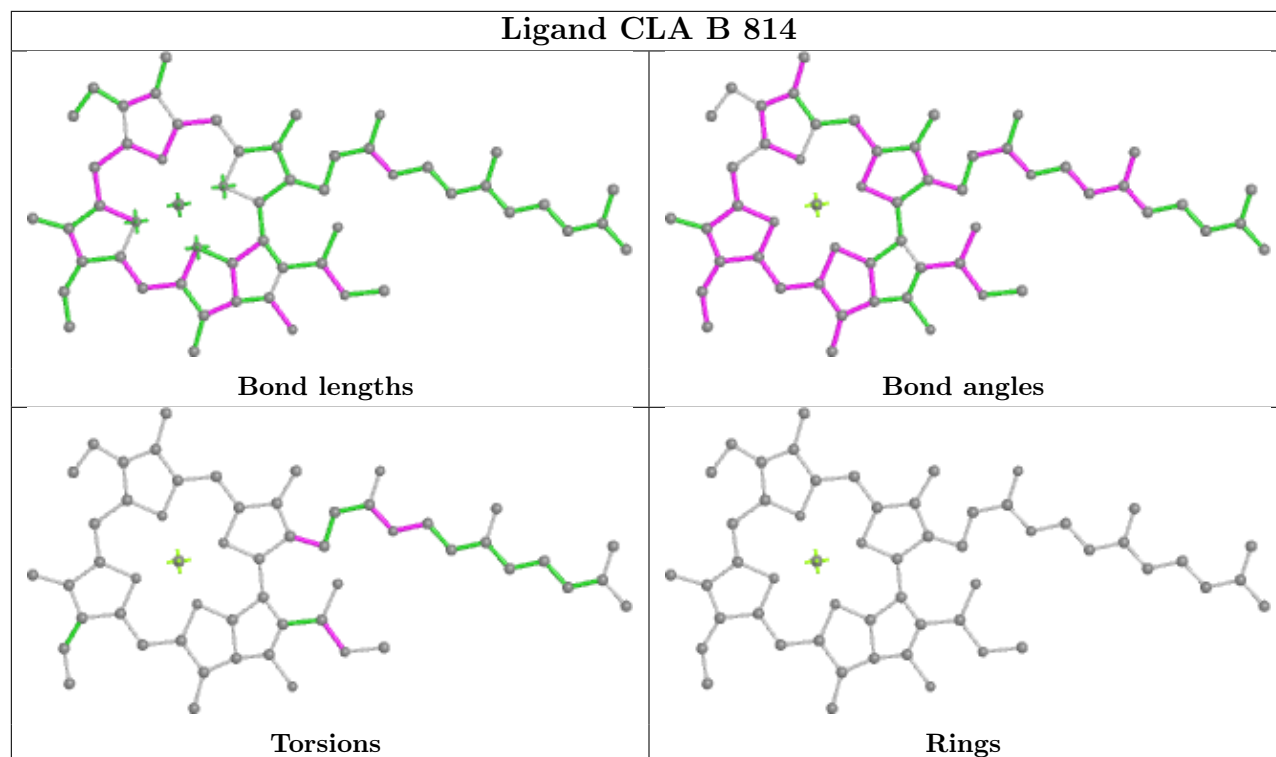
Ligand A86 11 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DD6 2 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

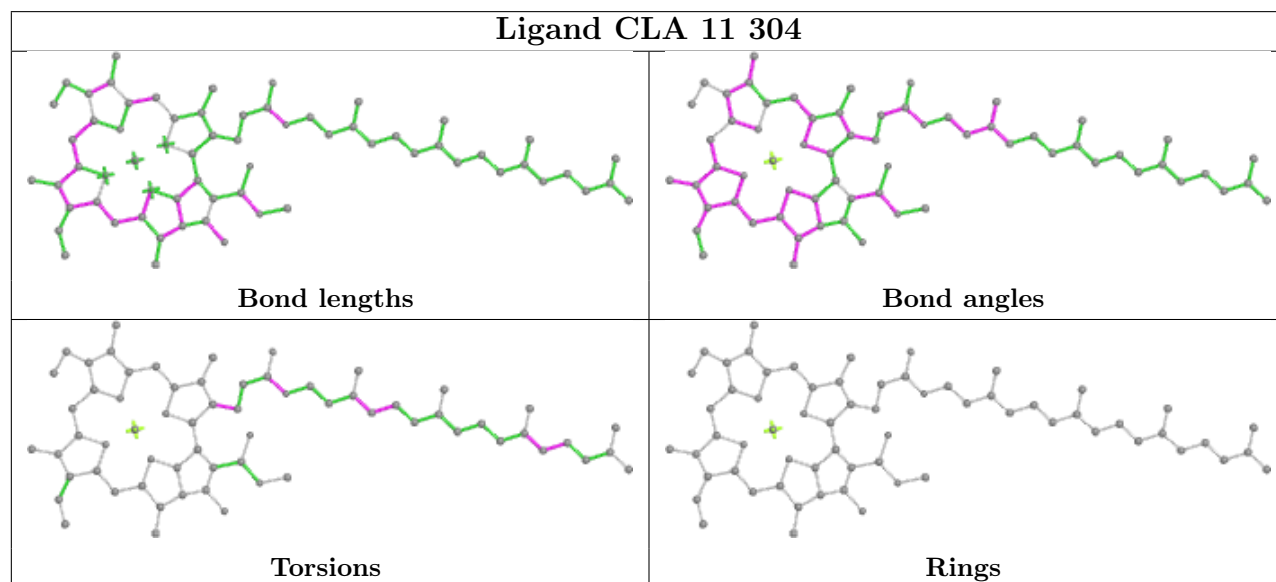
Ligand CLA 16 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

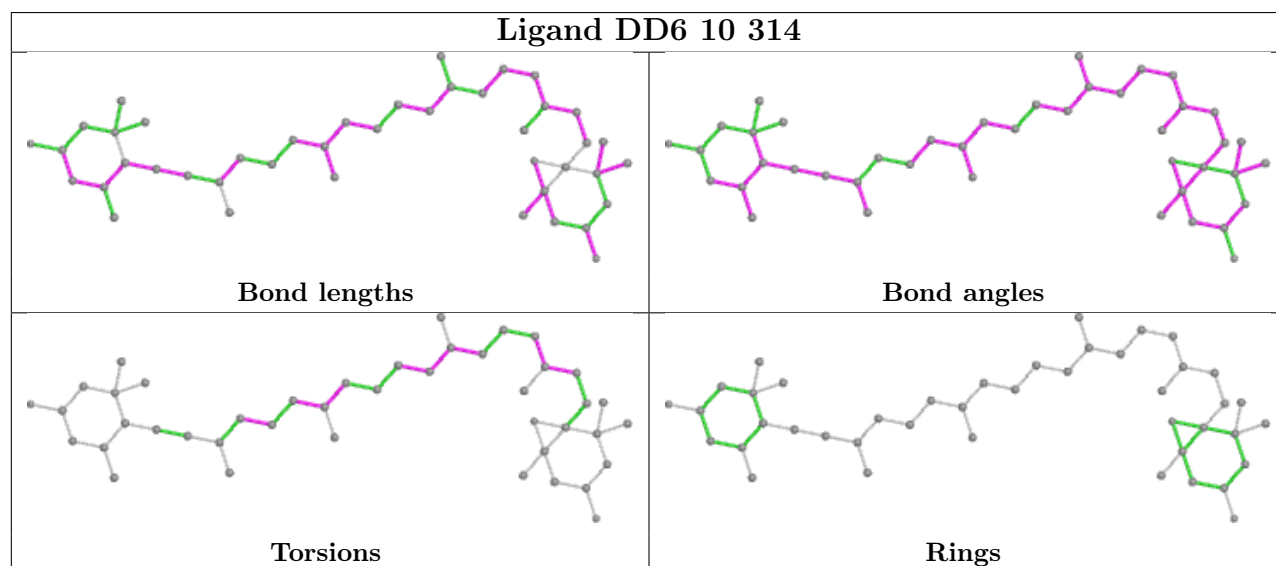
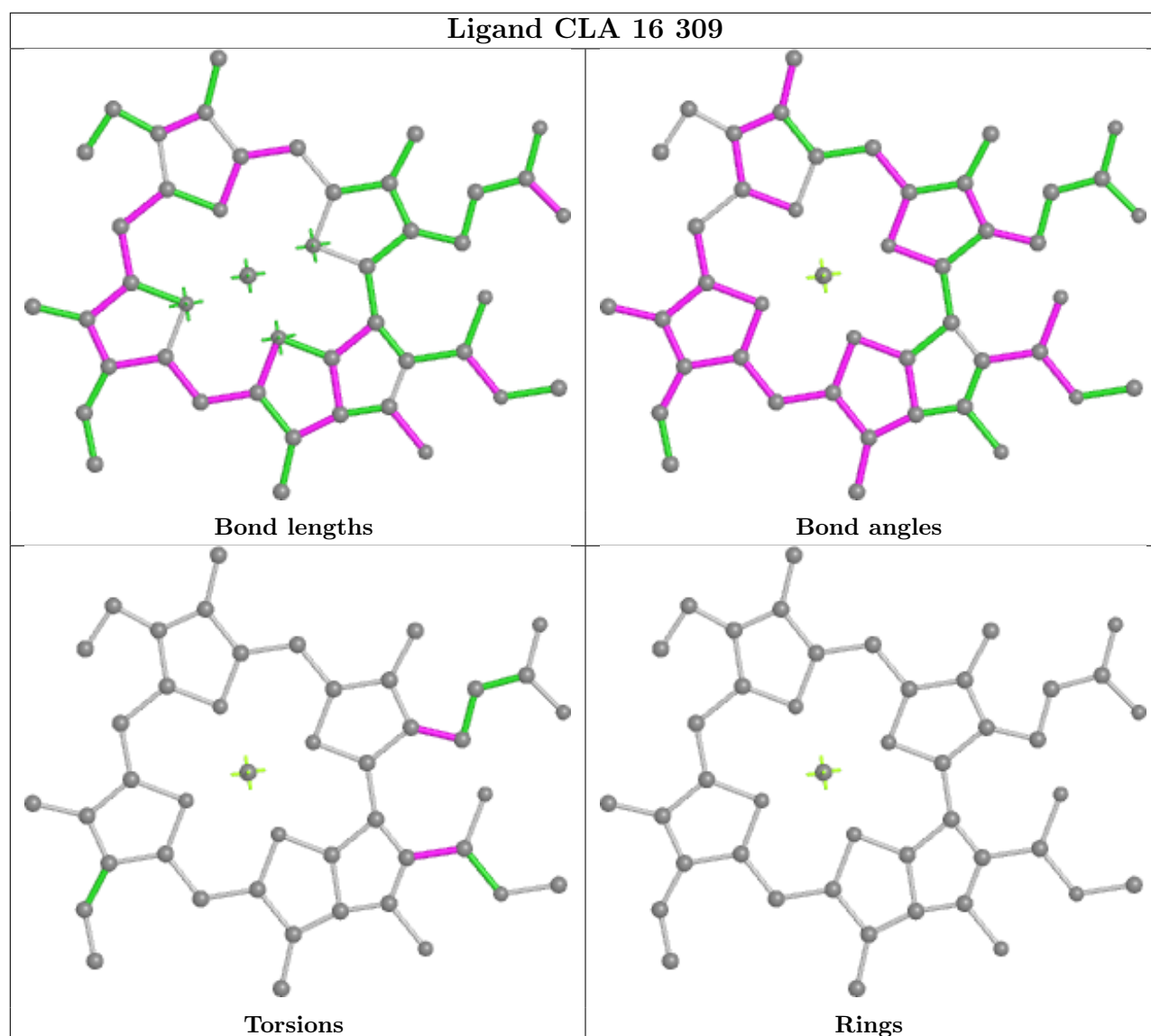


Ligand CLA B 814

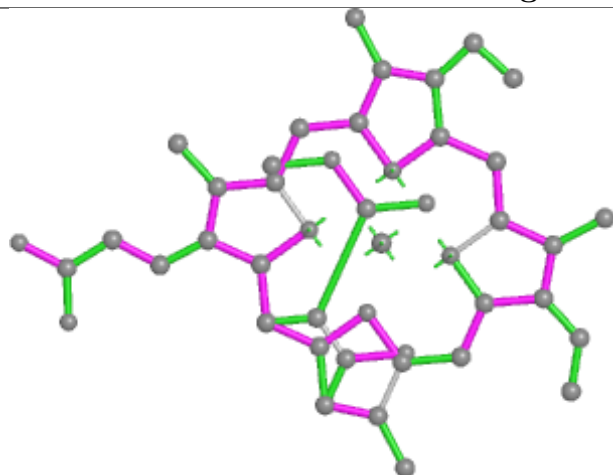


Ligand CLA 11 304

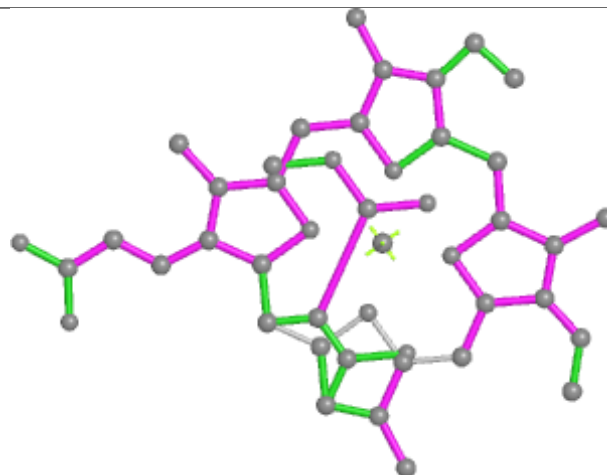




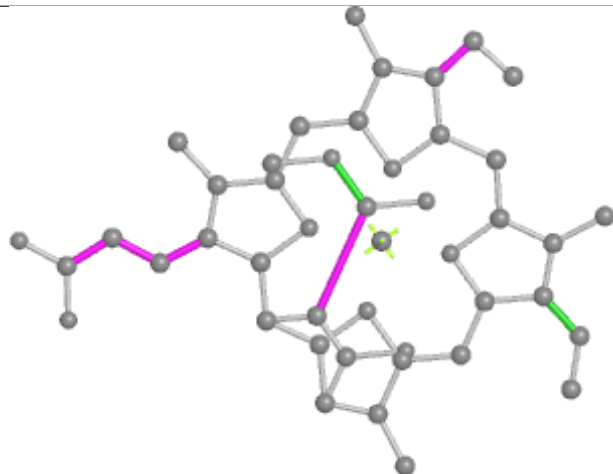
Ligand KC1 3 308



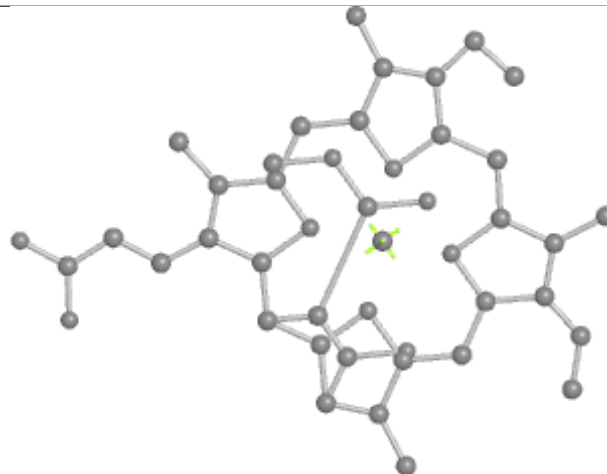
Bond lengths



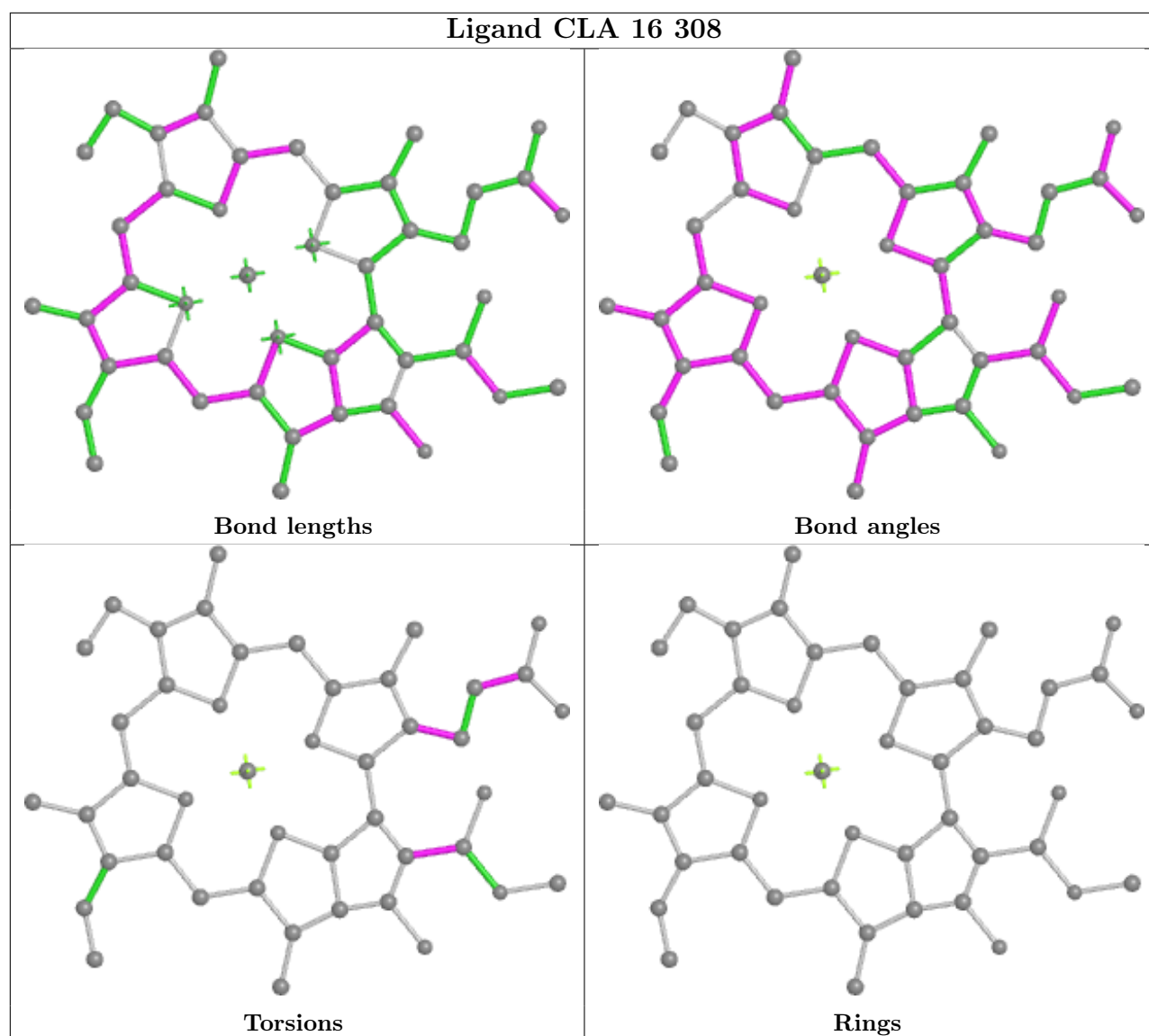
Bond angles

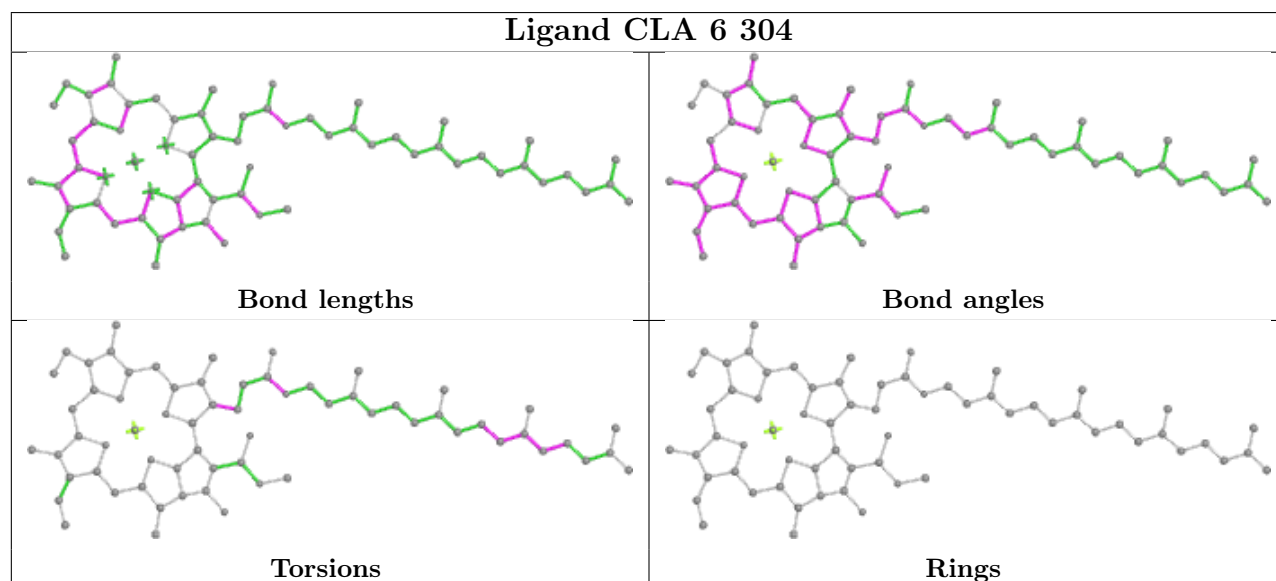
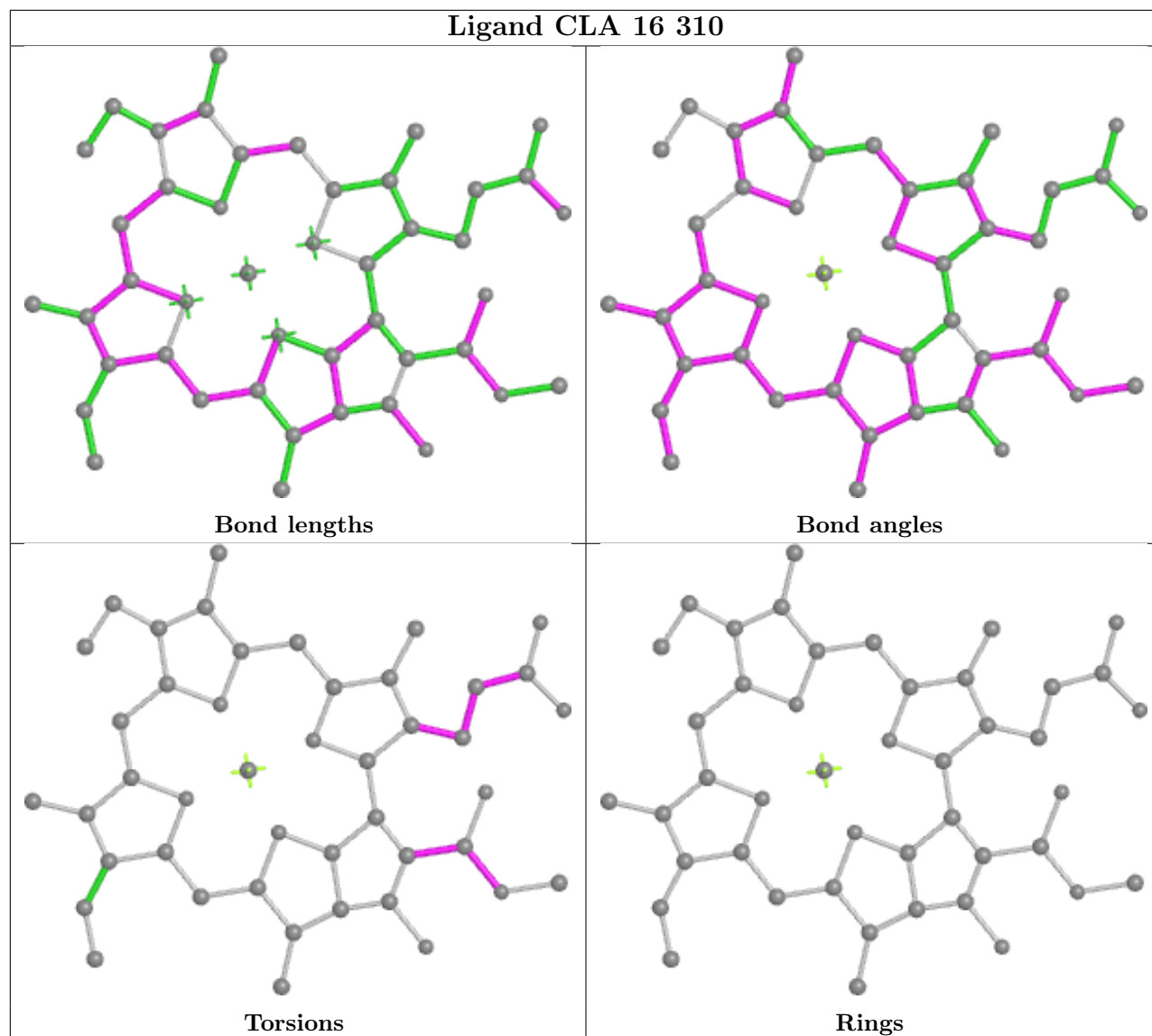


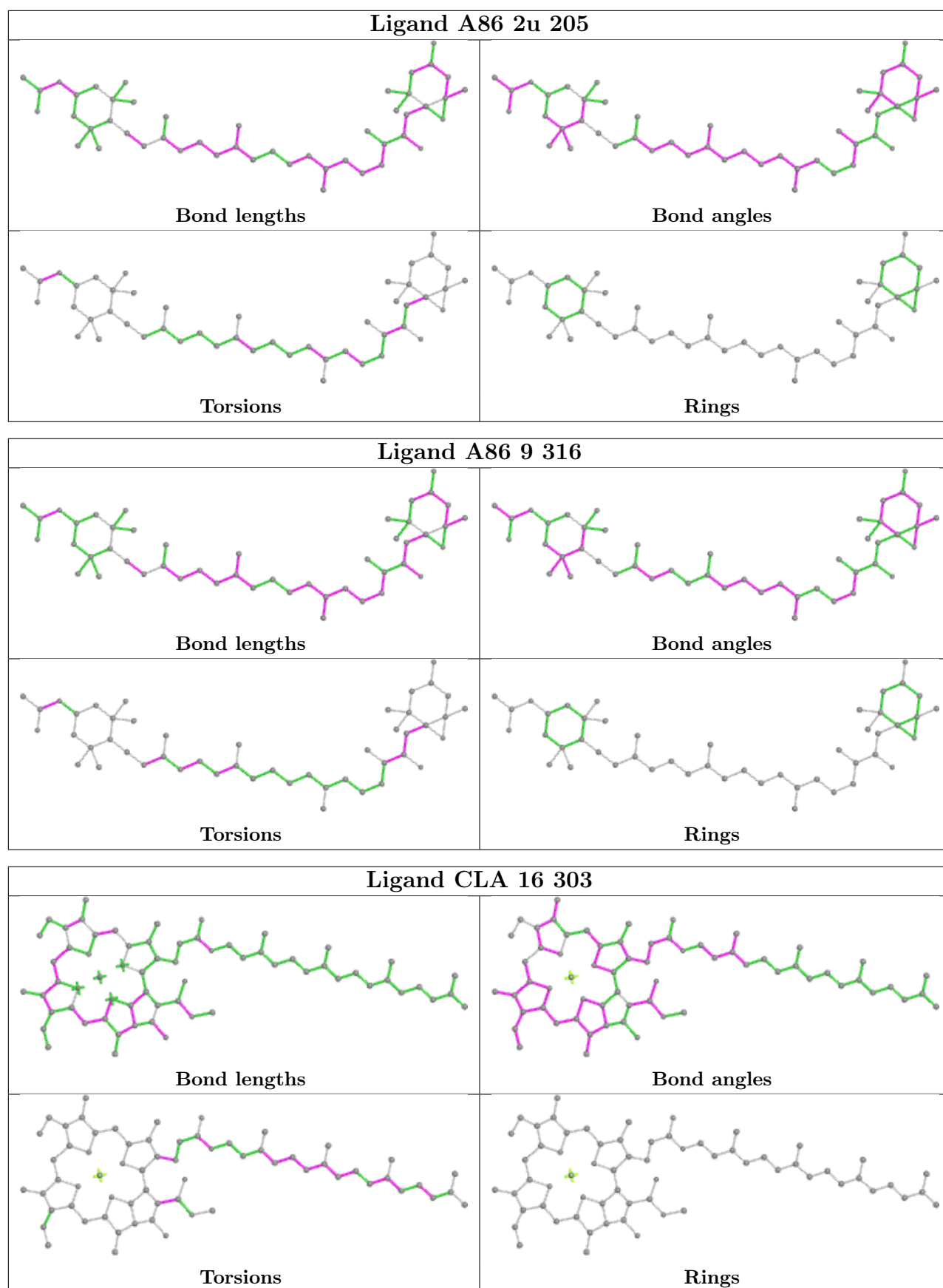
Torsions

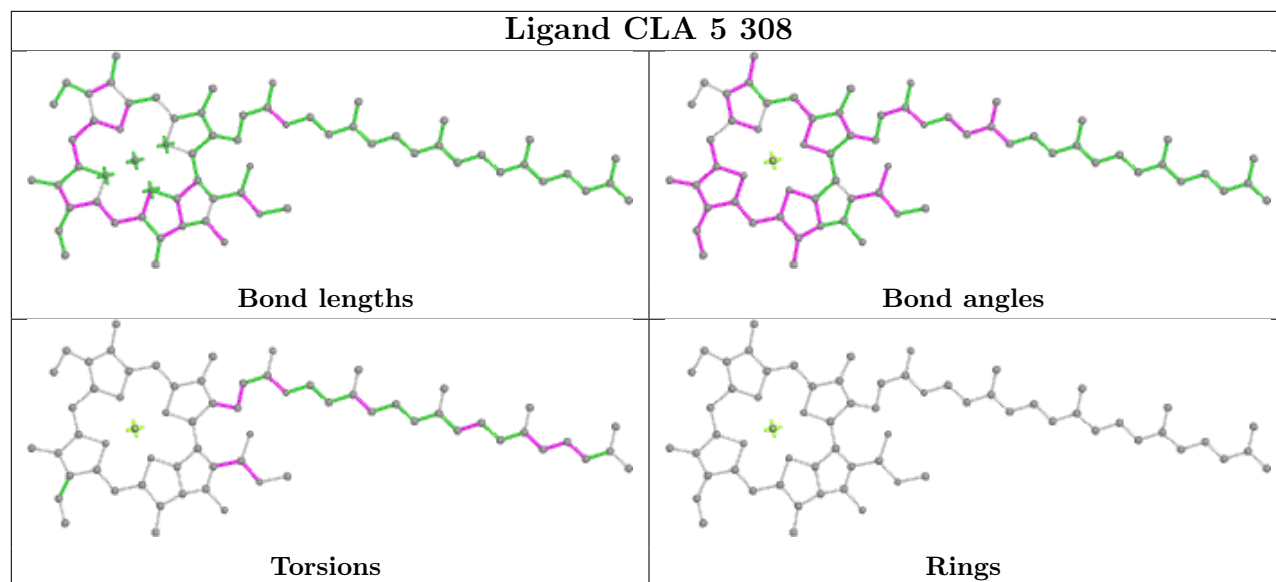
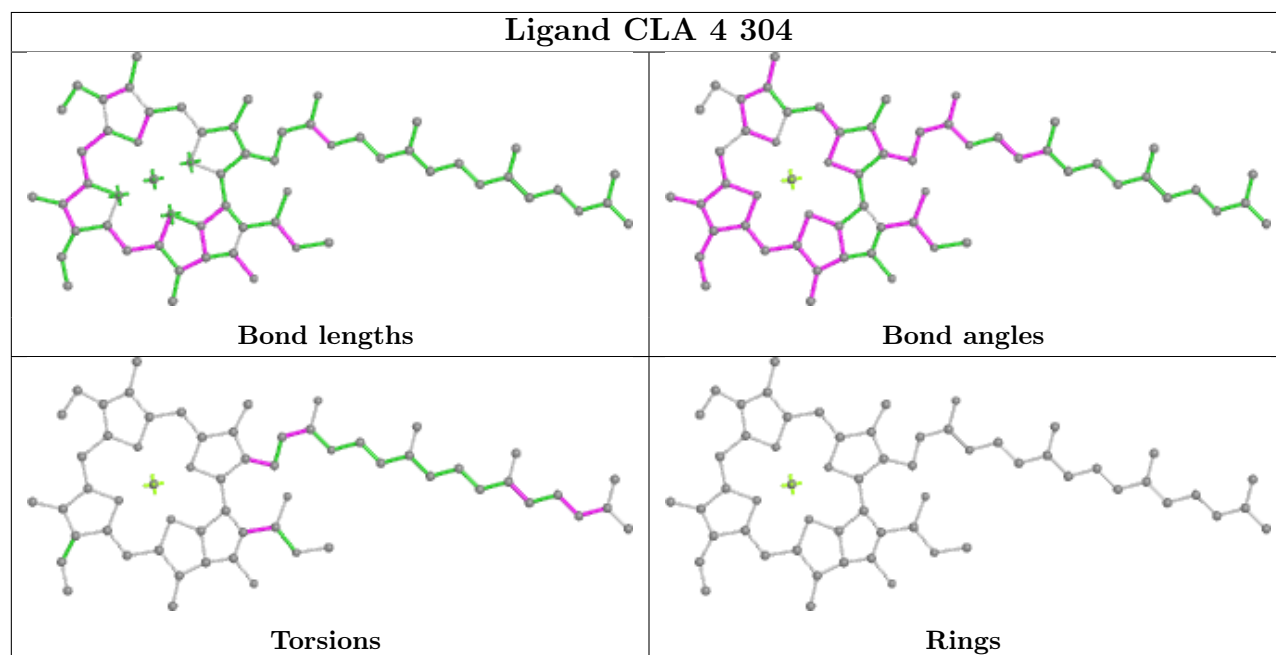


Rings

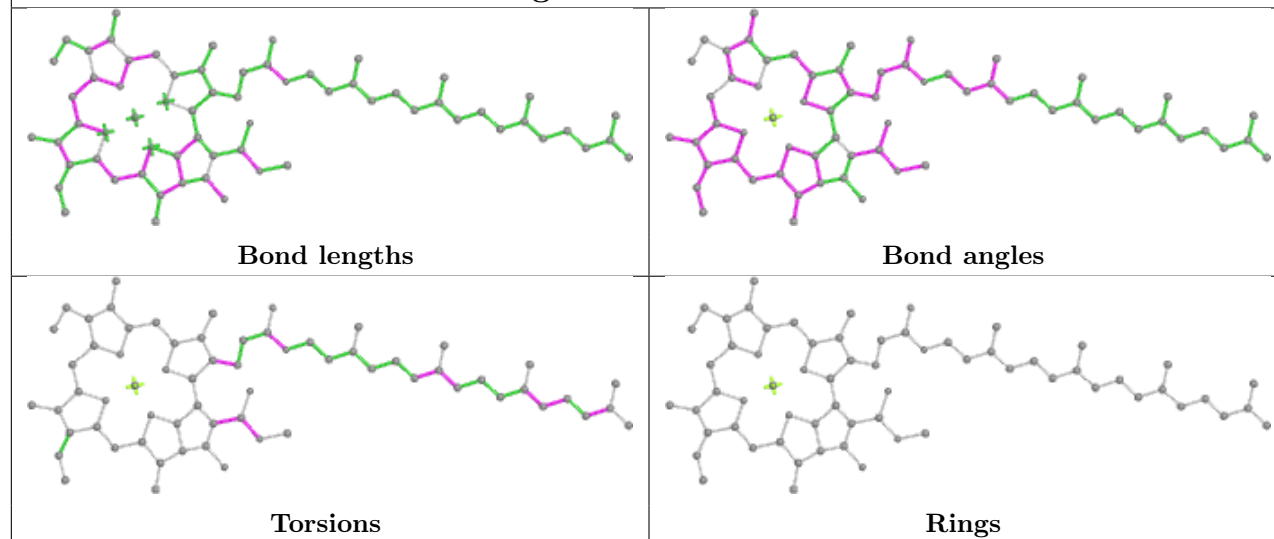




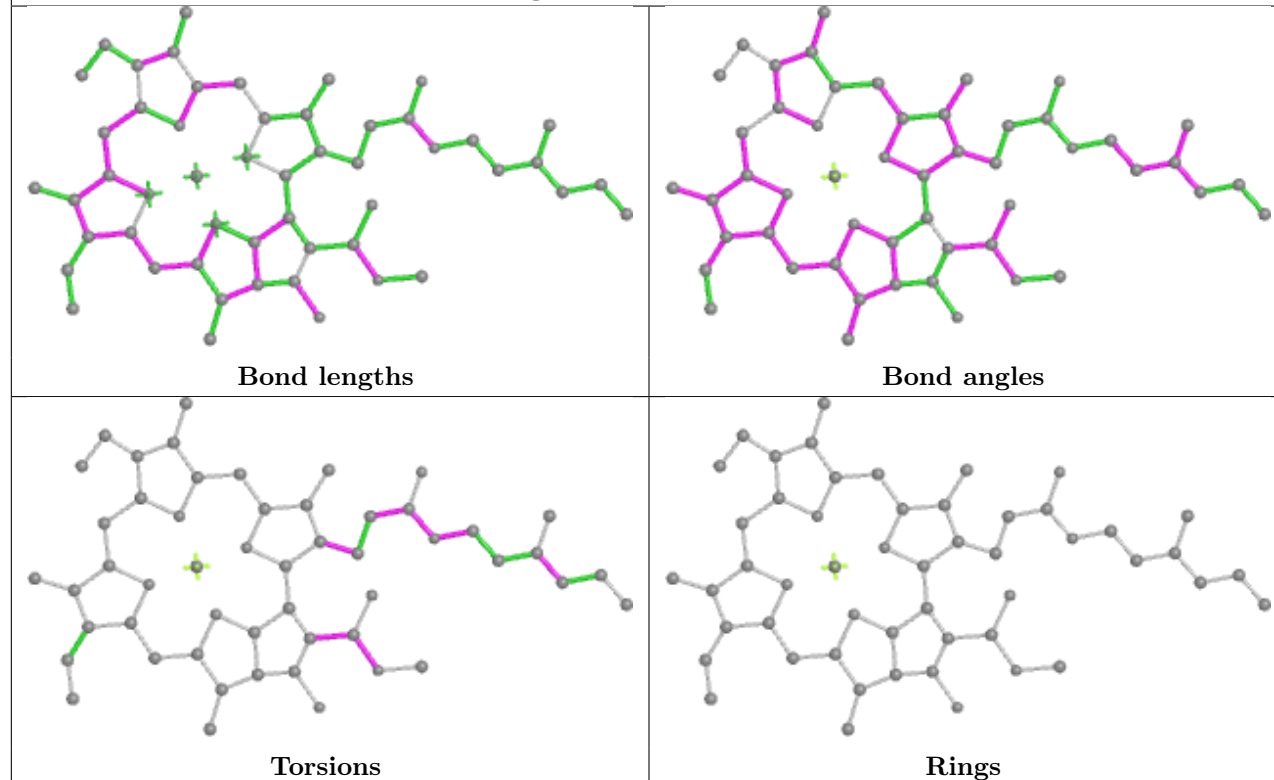


Ligand CLA 5 308**Ligand CLA 4 304**

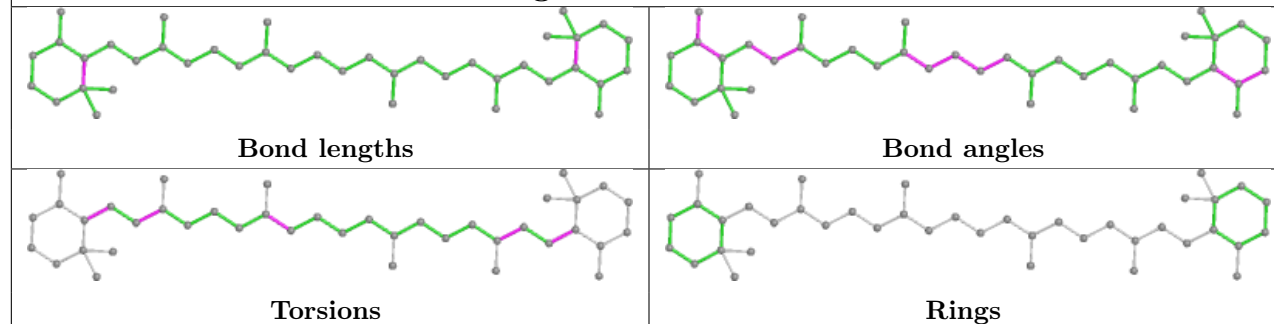
Ligand CLA B 851

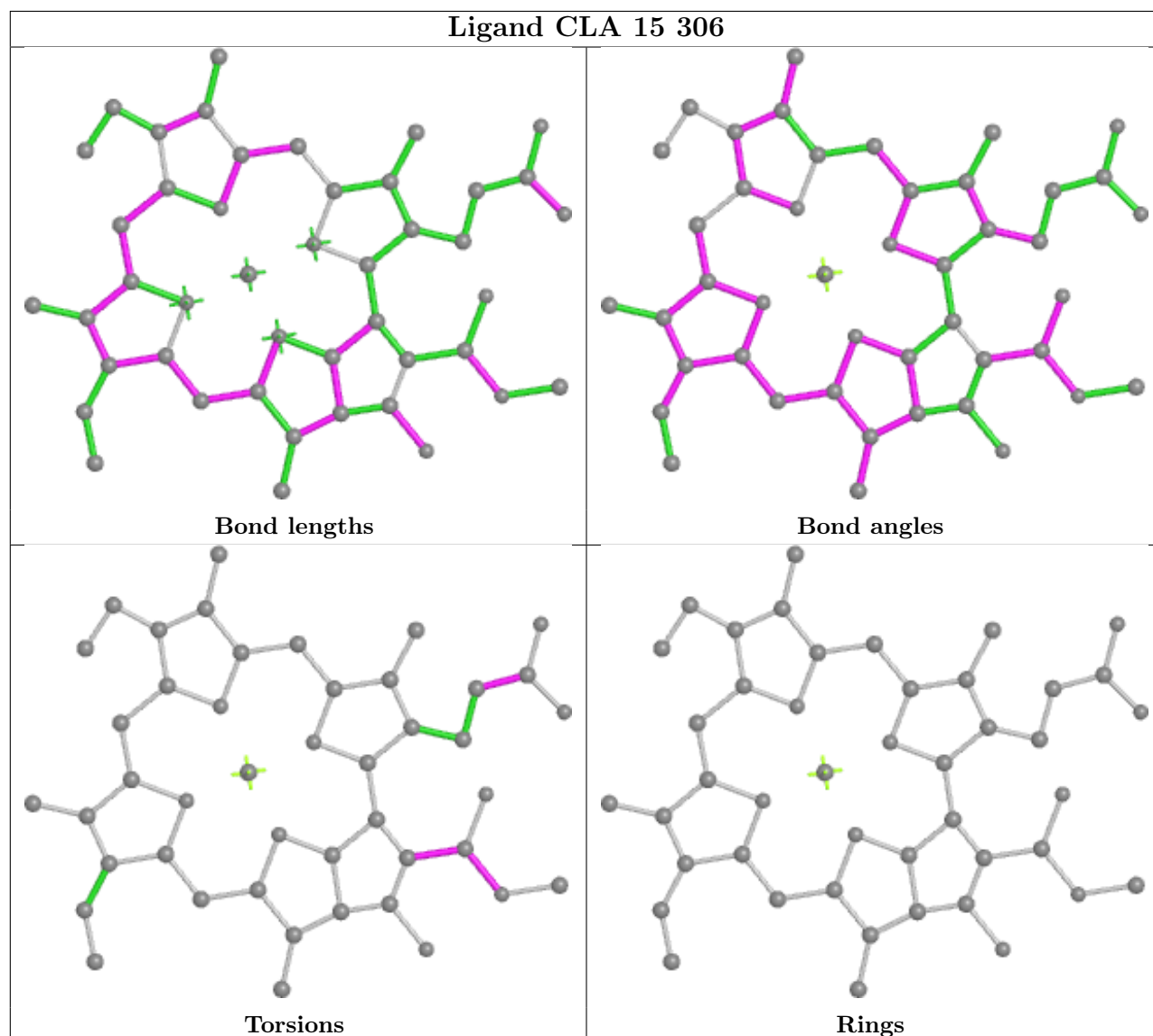
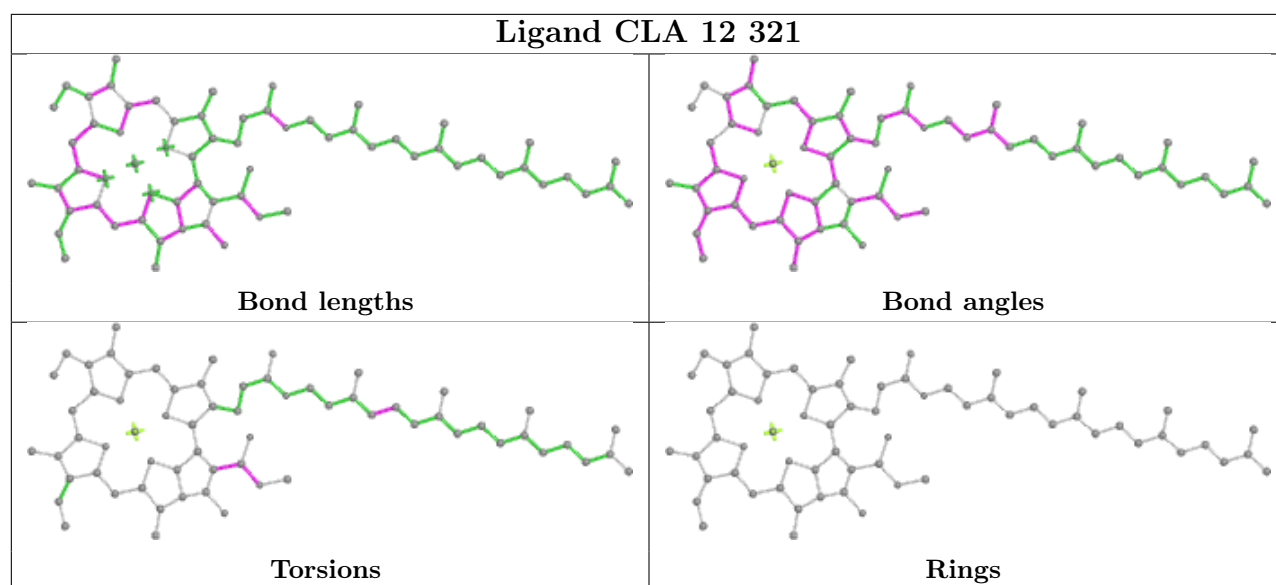


Ligand CLA 16 306

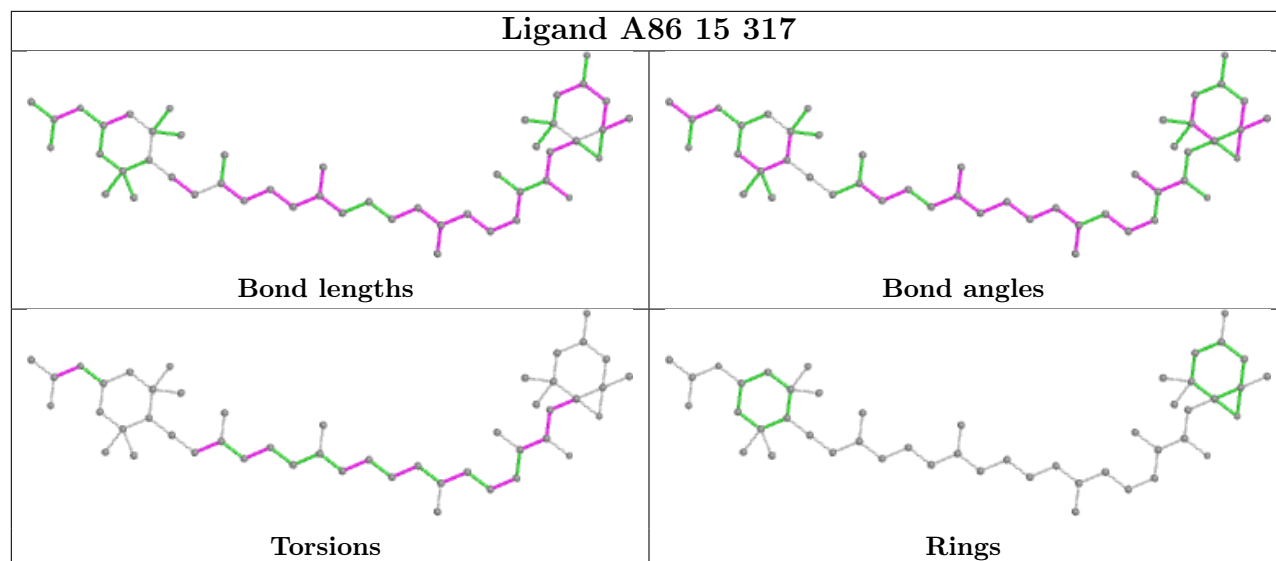


Ligand BCR L 205

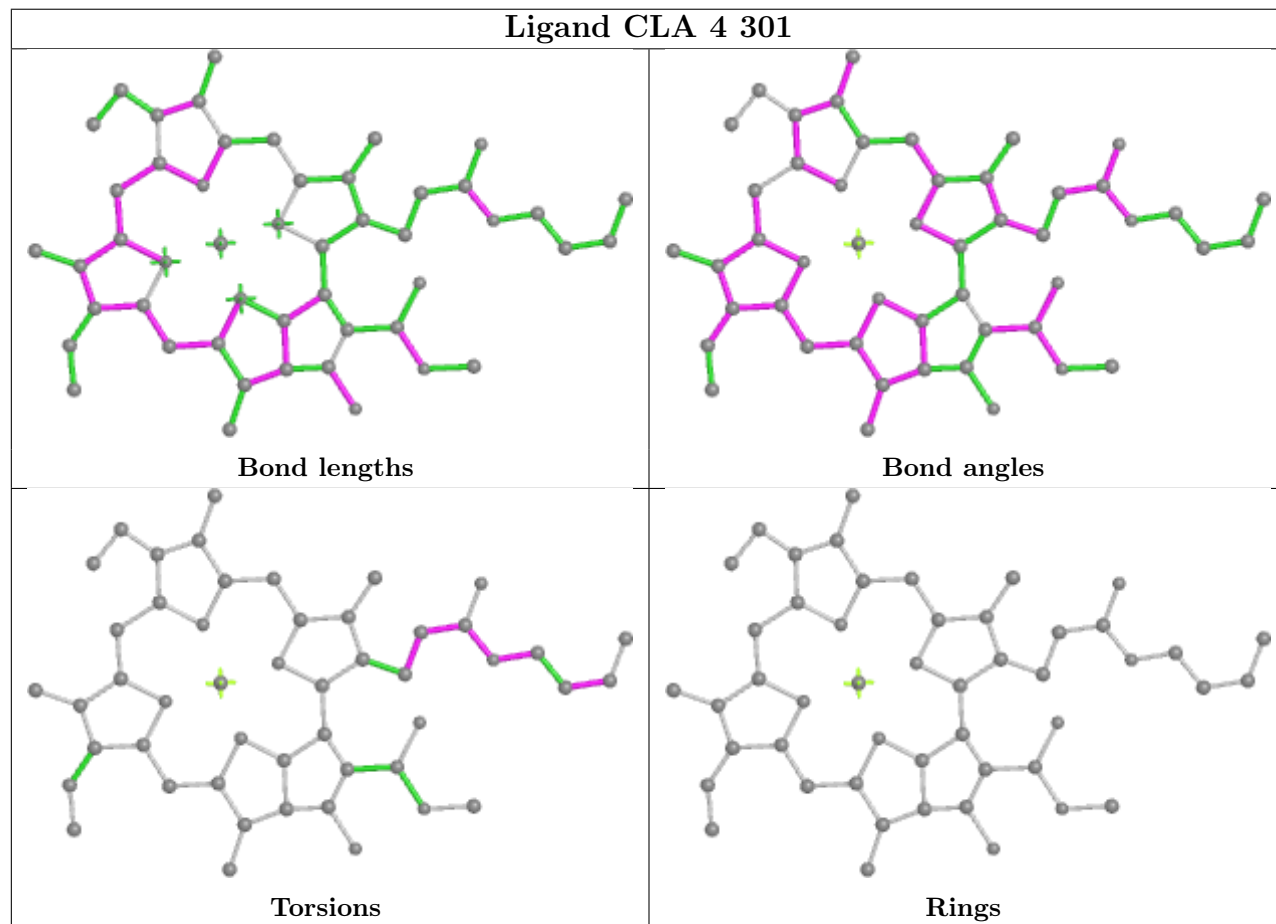




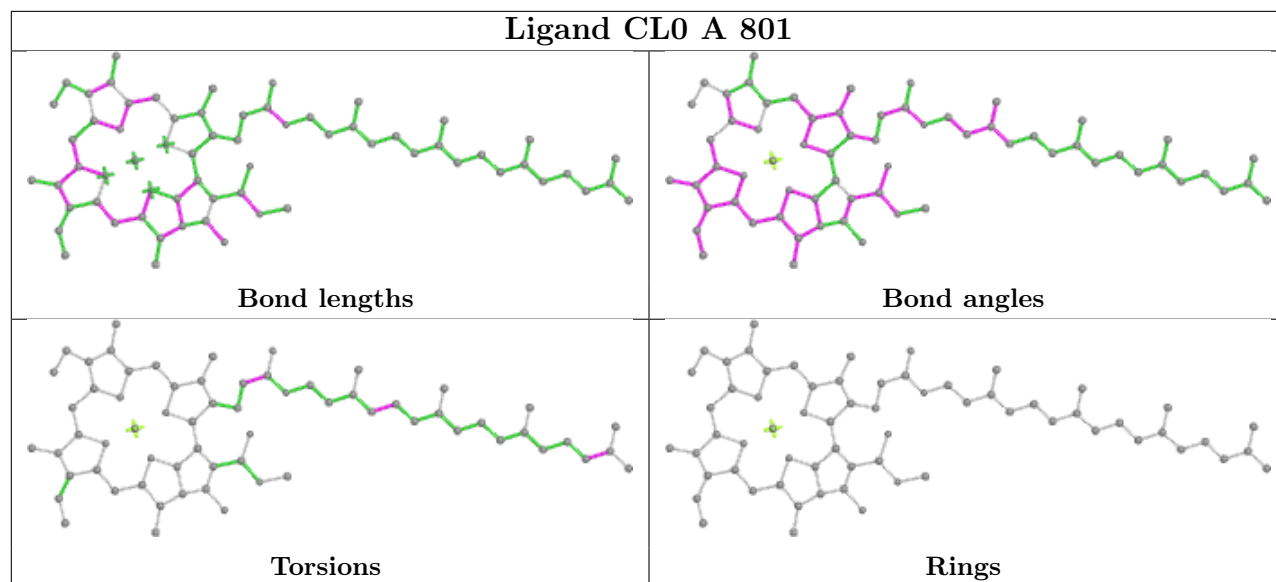
Ligand A86 15 317



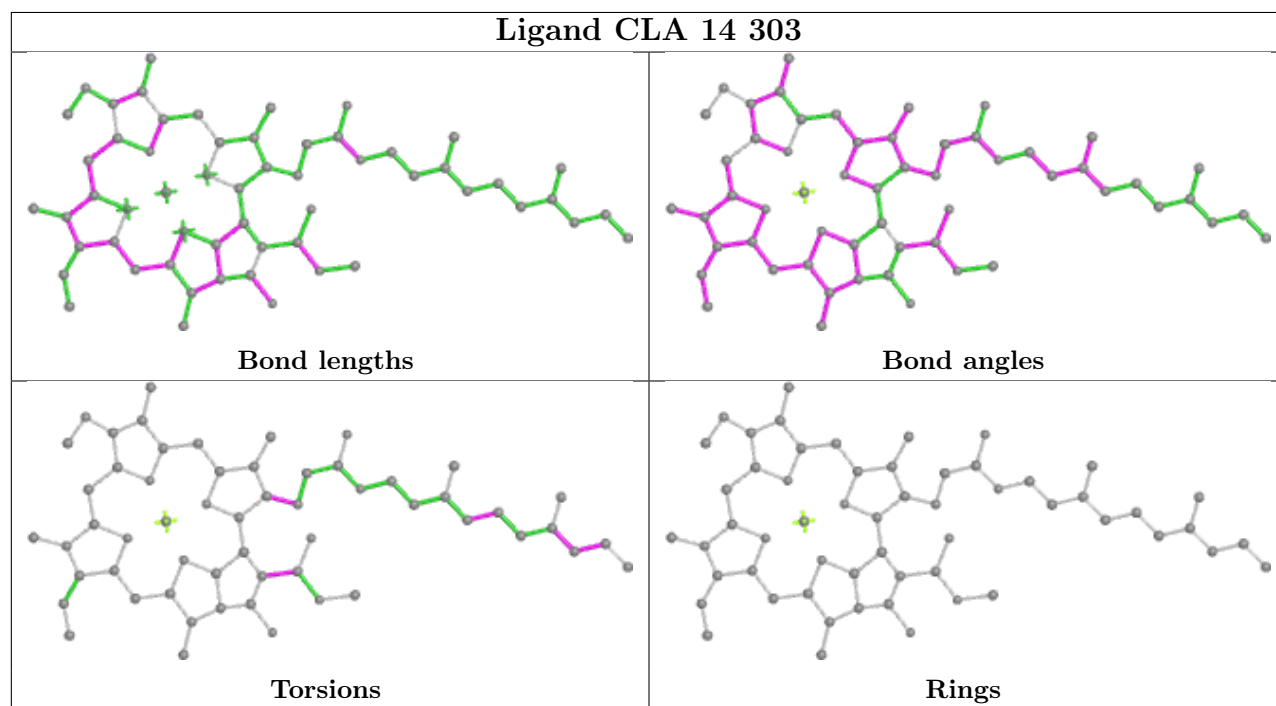
Ligand CLA 4 301

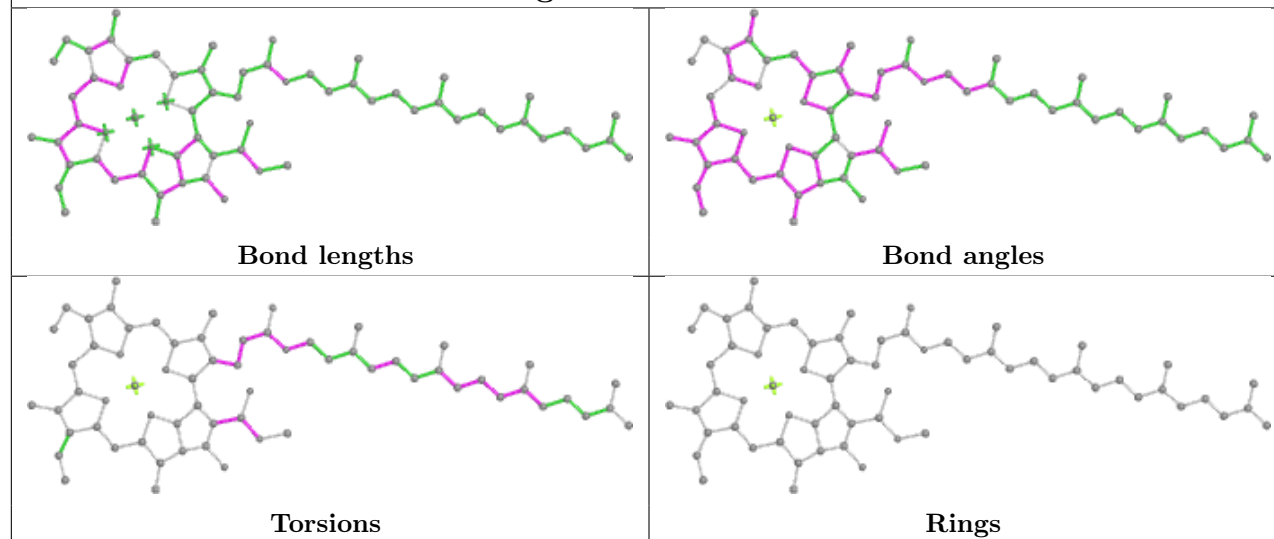
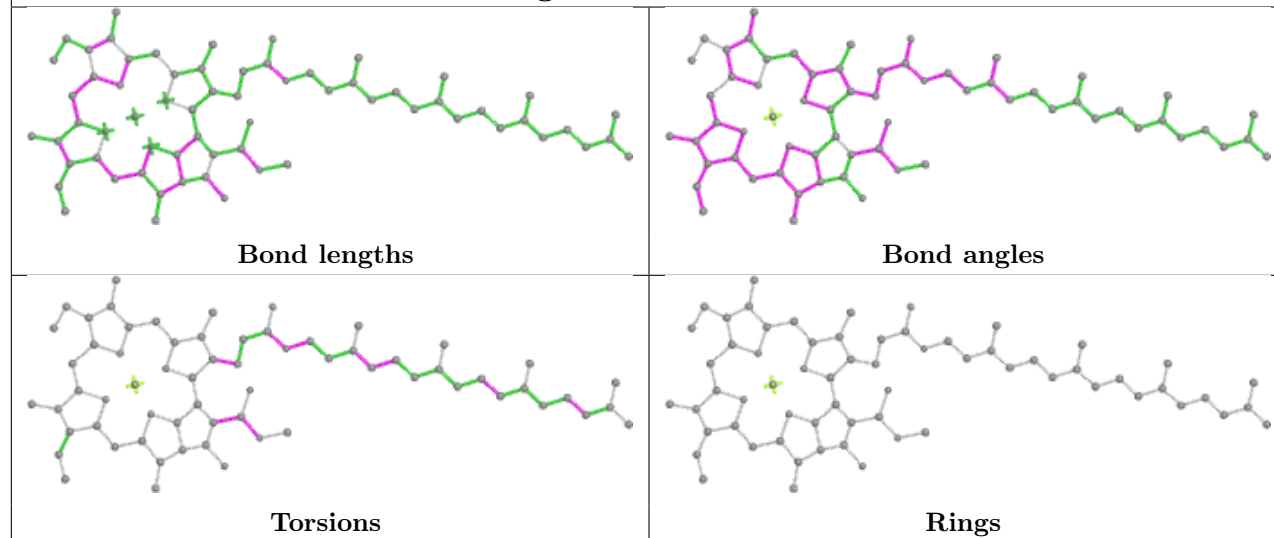


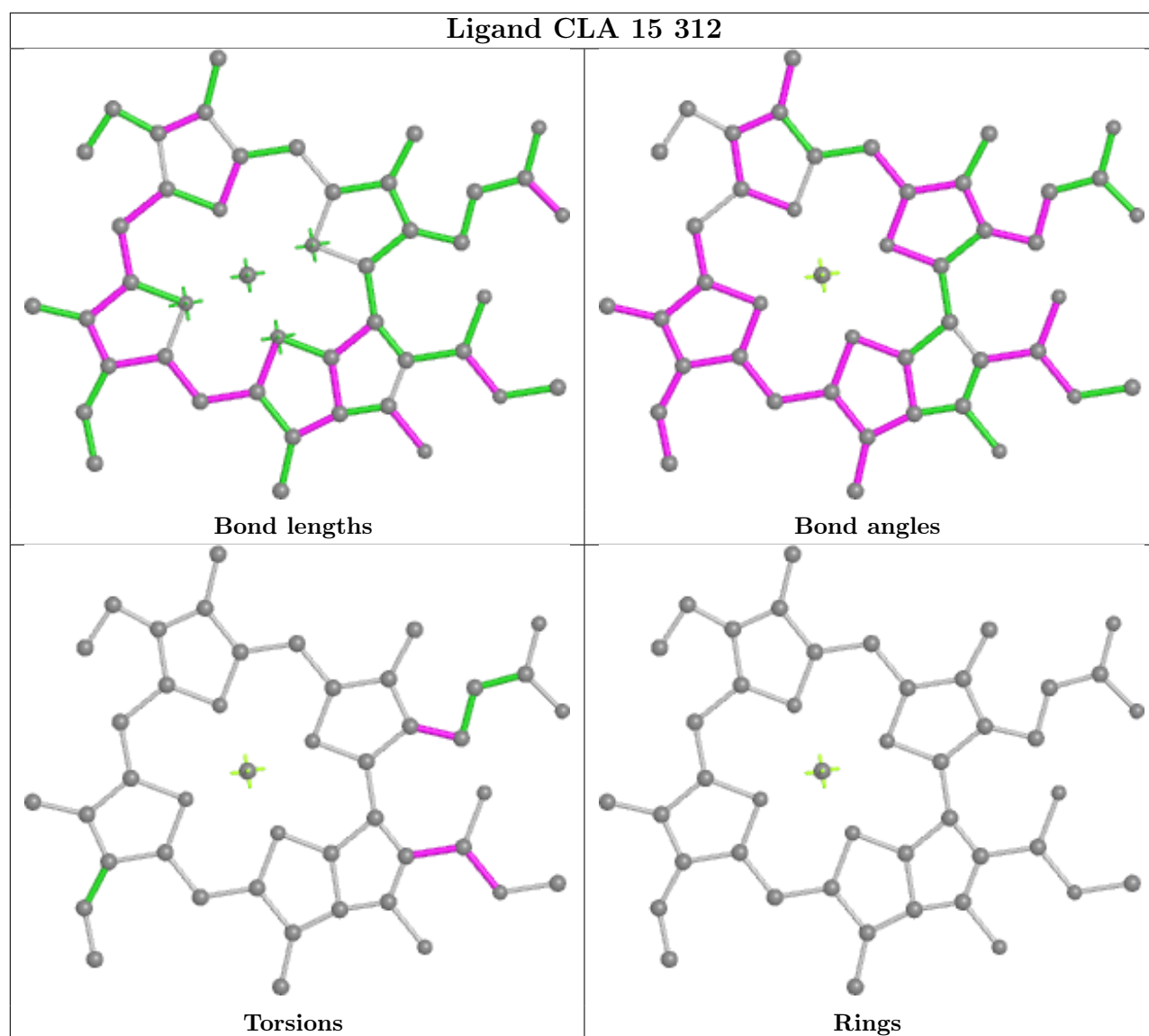
Ligand CL0 A 801



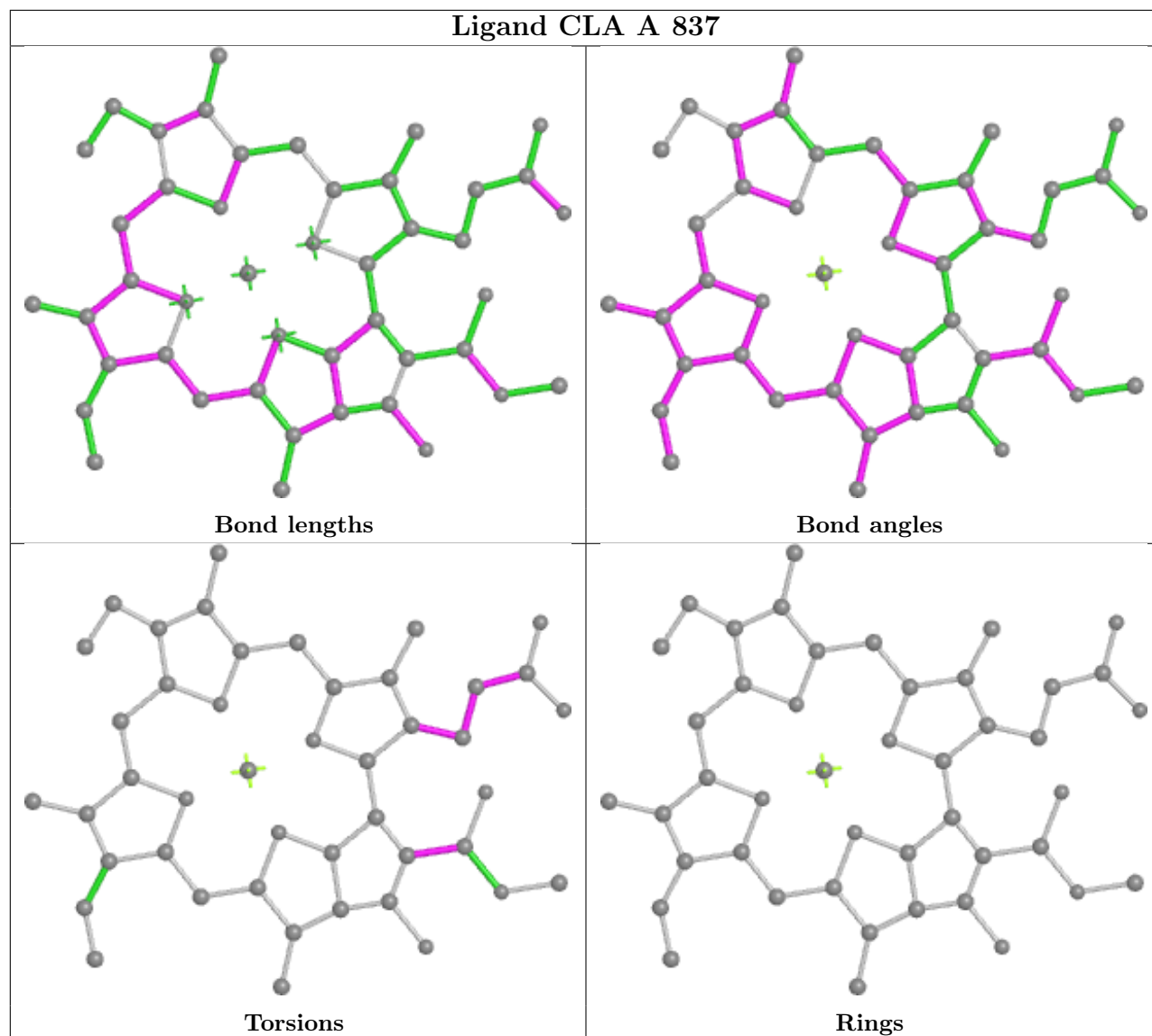
Ligand CLA 14 303



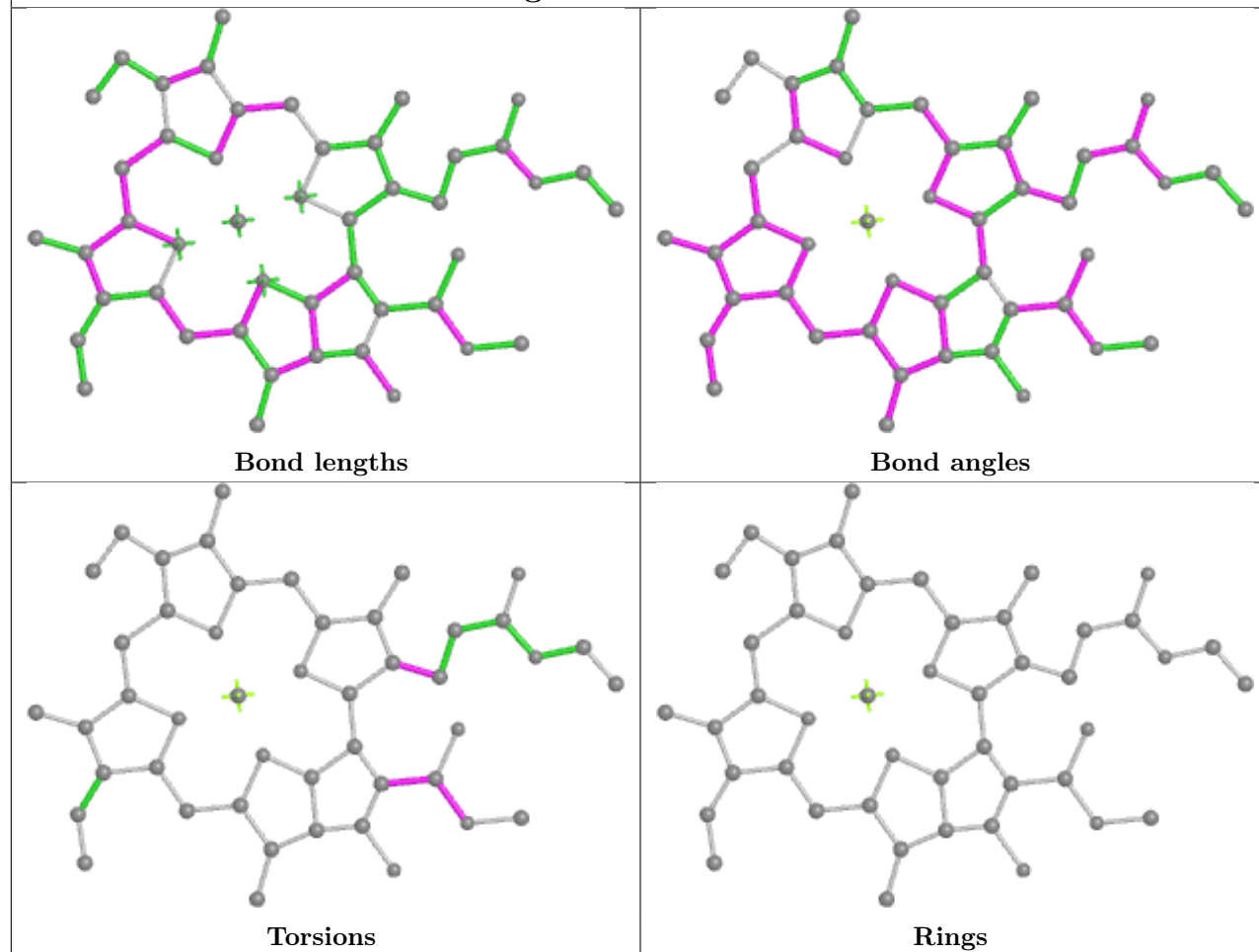
Ligand CLA 8 301**Ligand BCR 2u 201****Ligand CLA 6 309**



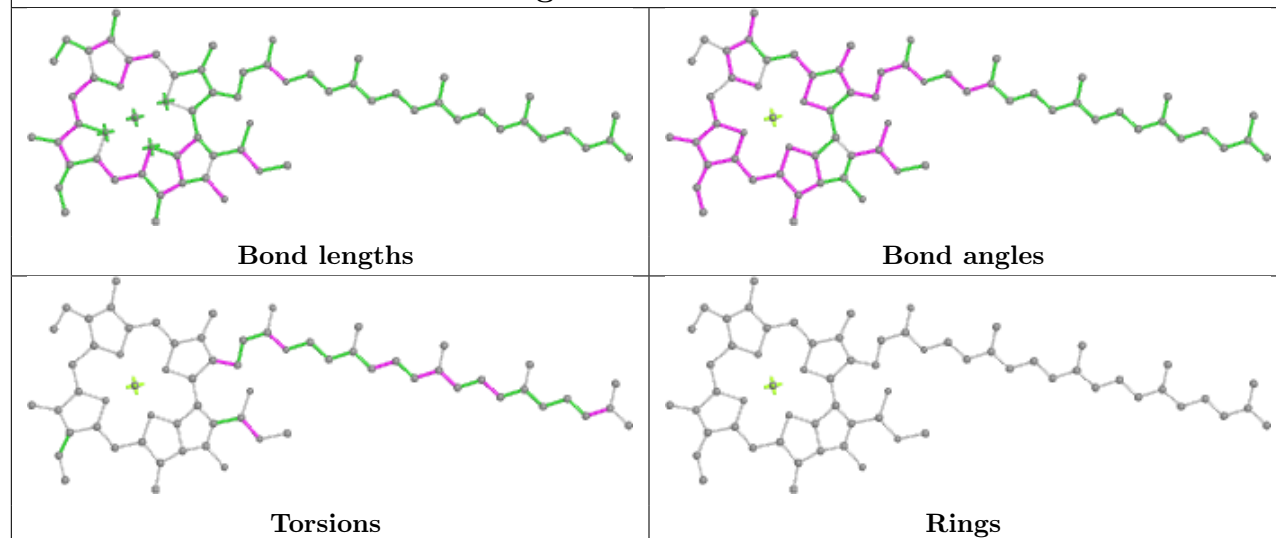
Ligand CLA A 837

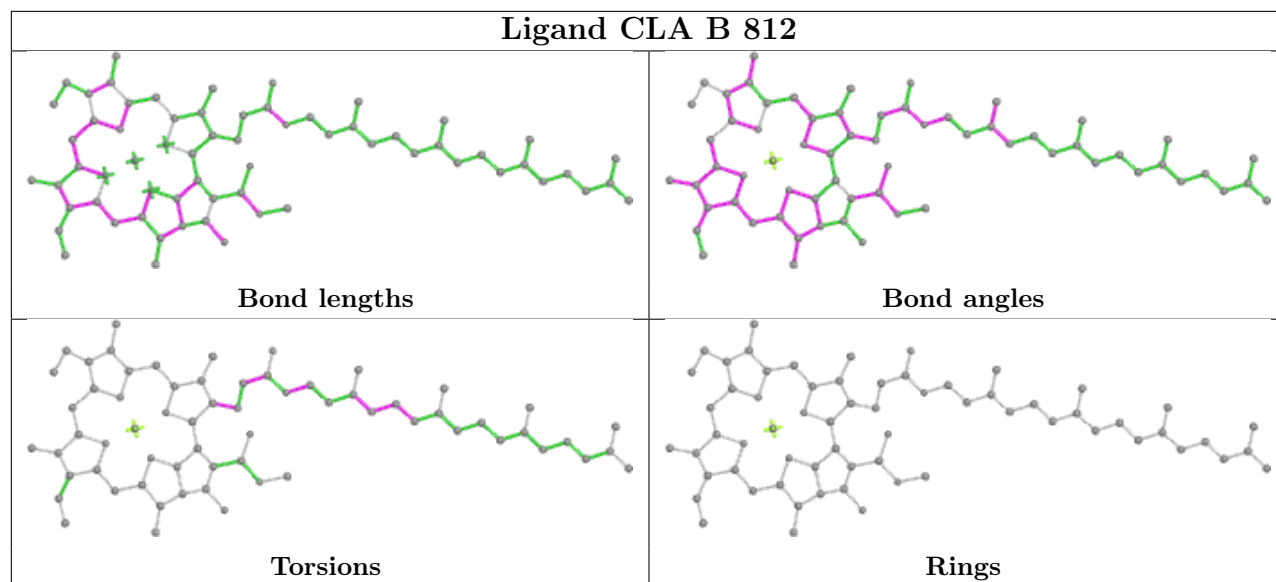
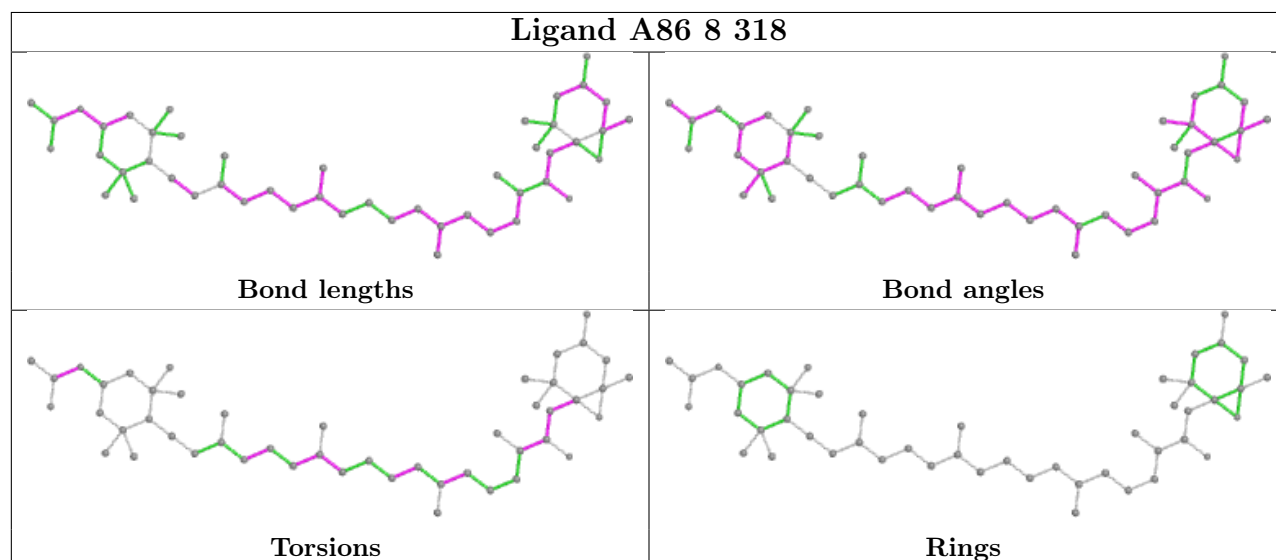
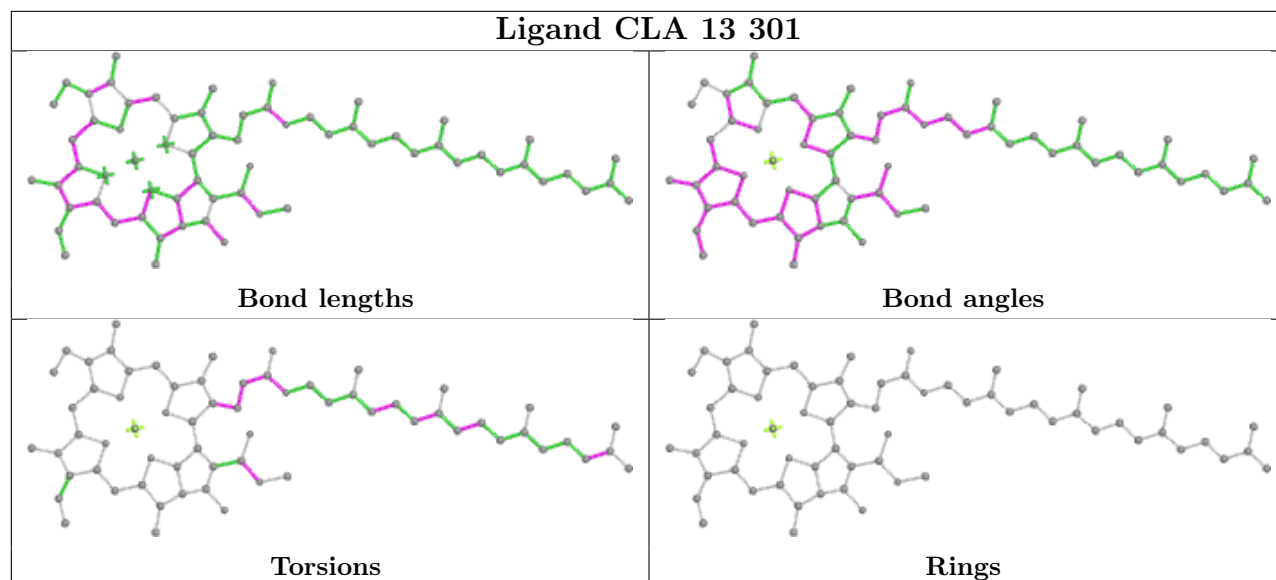


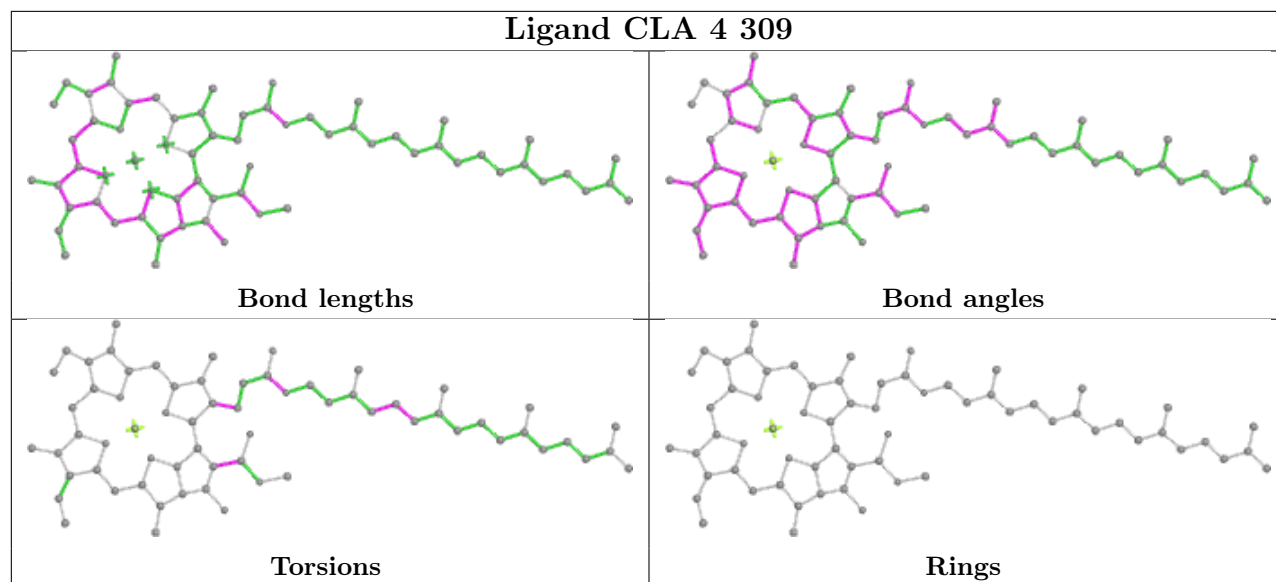
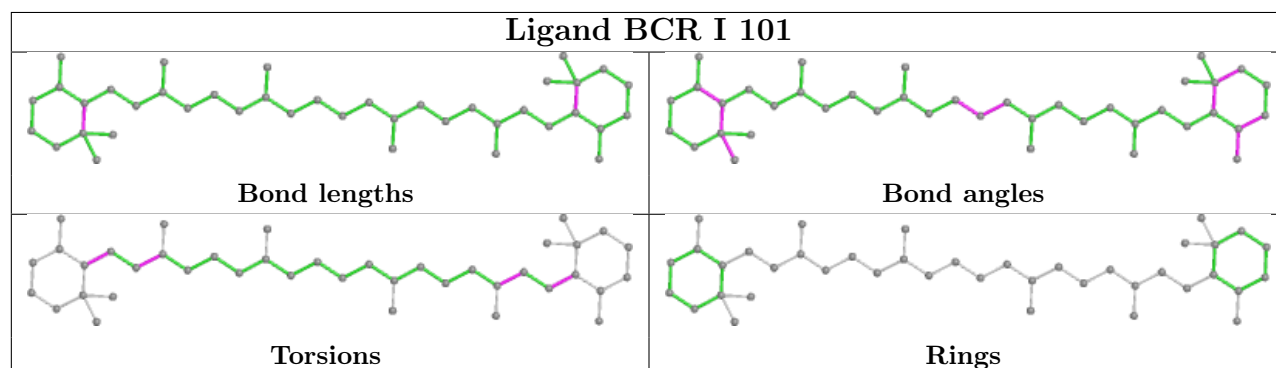
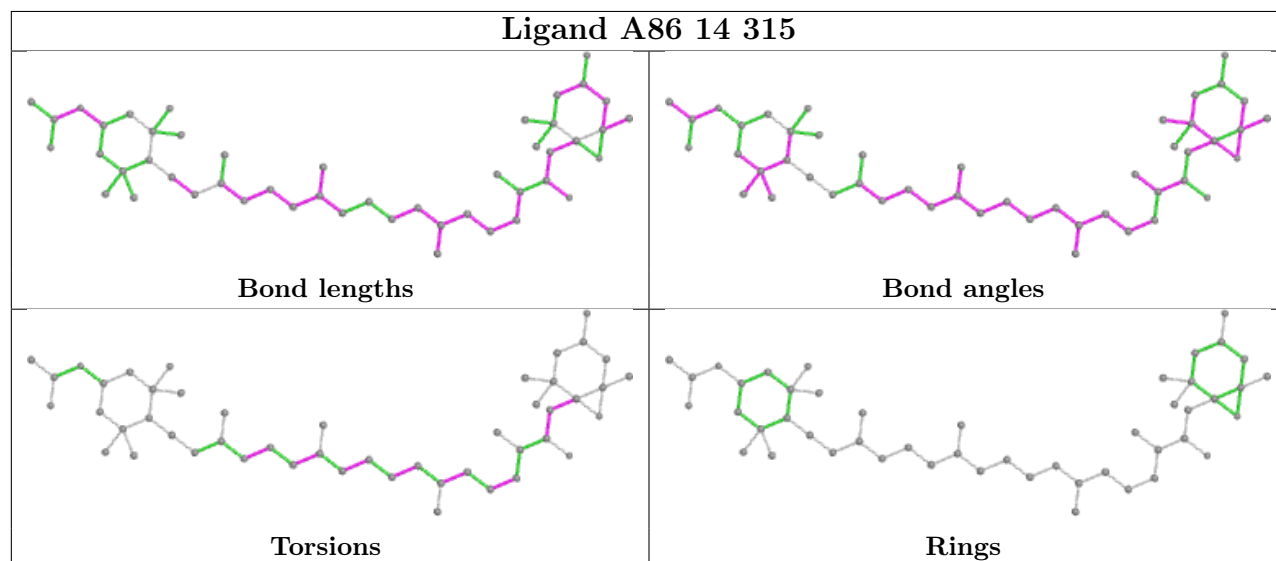
Ligand CLA A 840

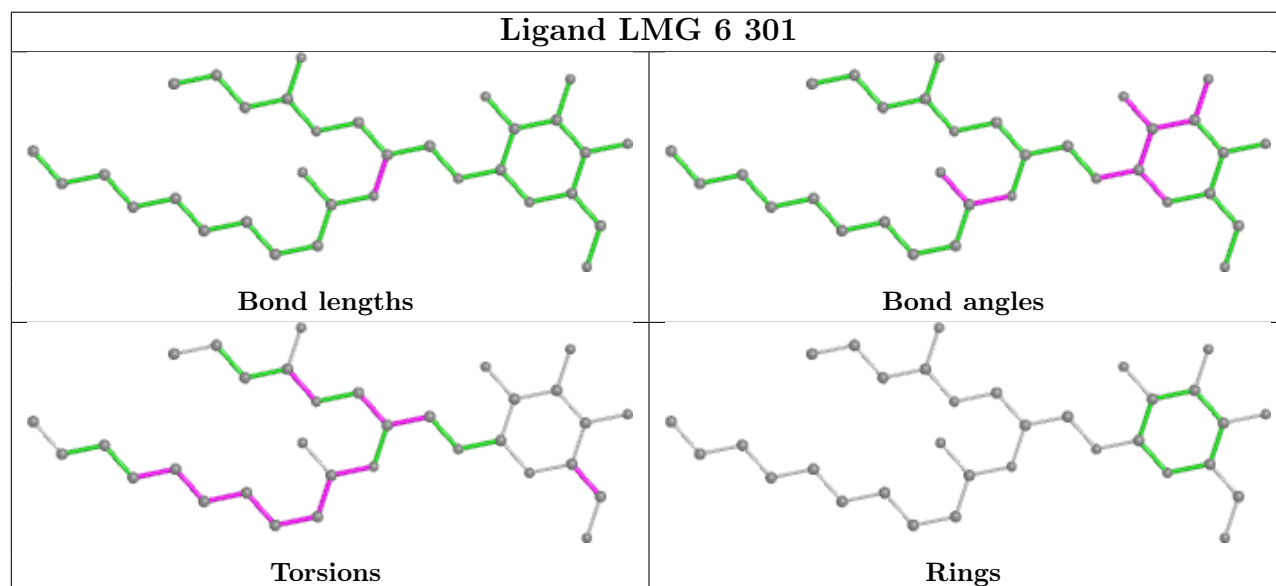
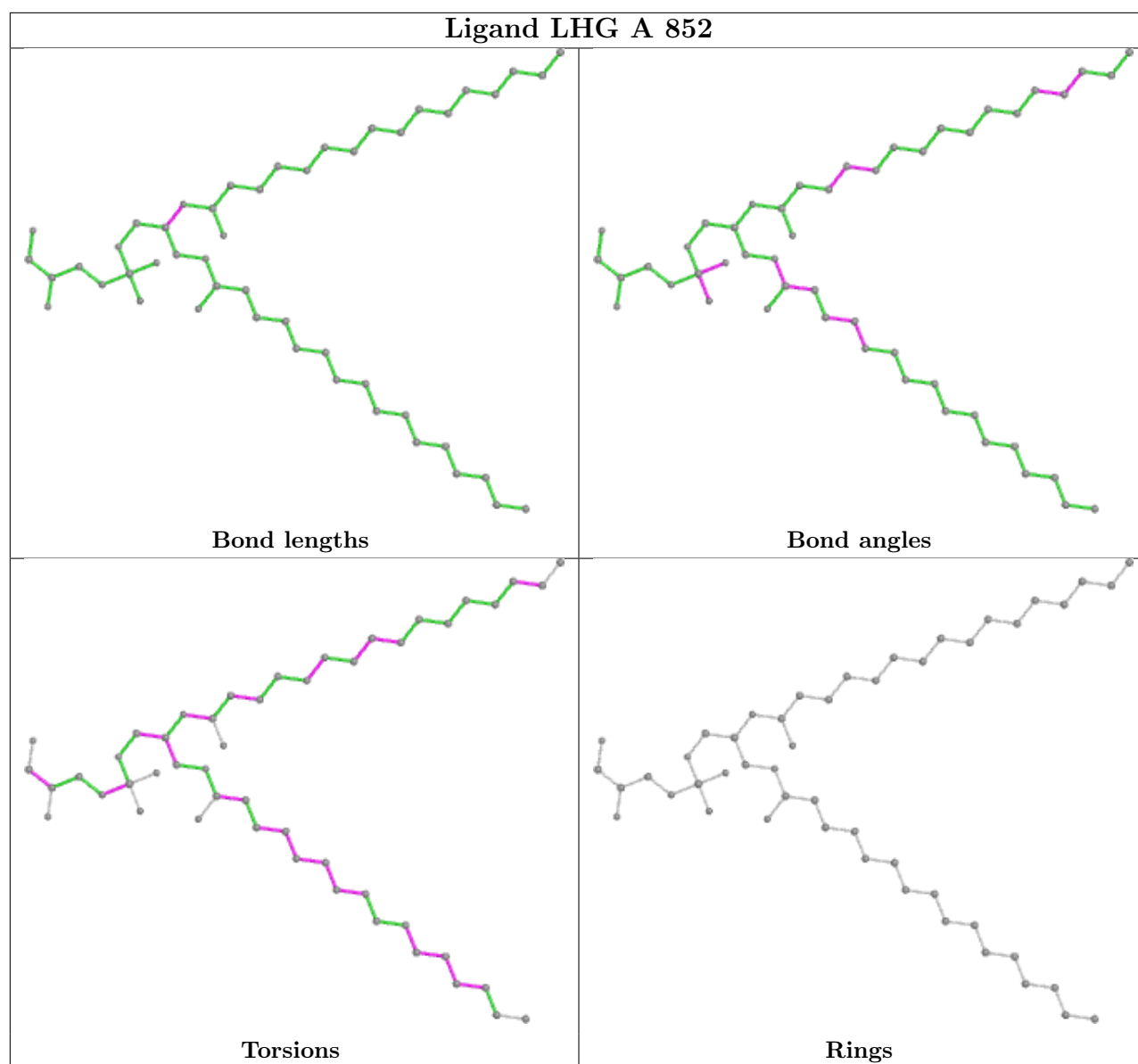


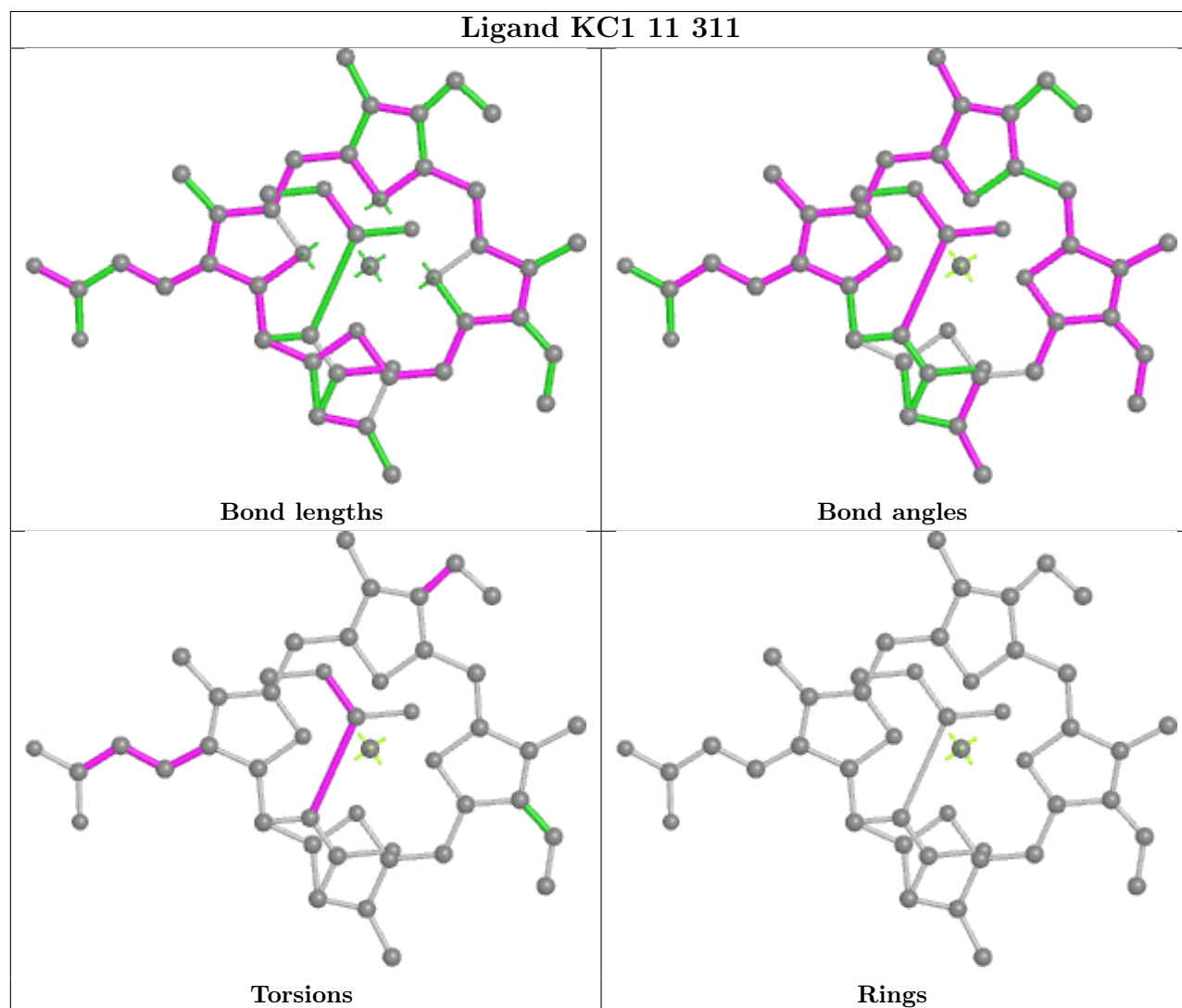
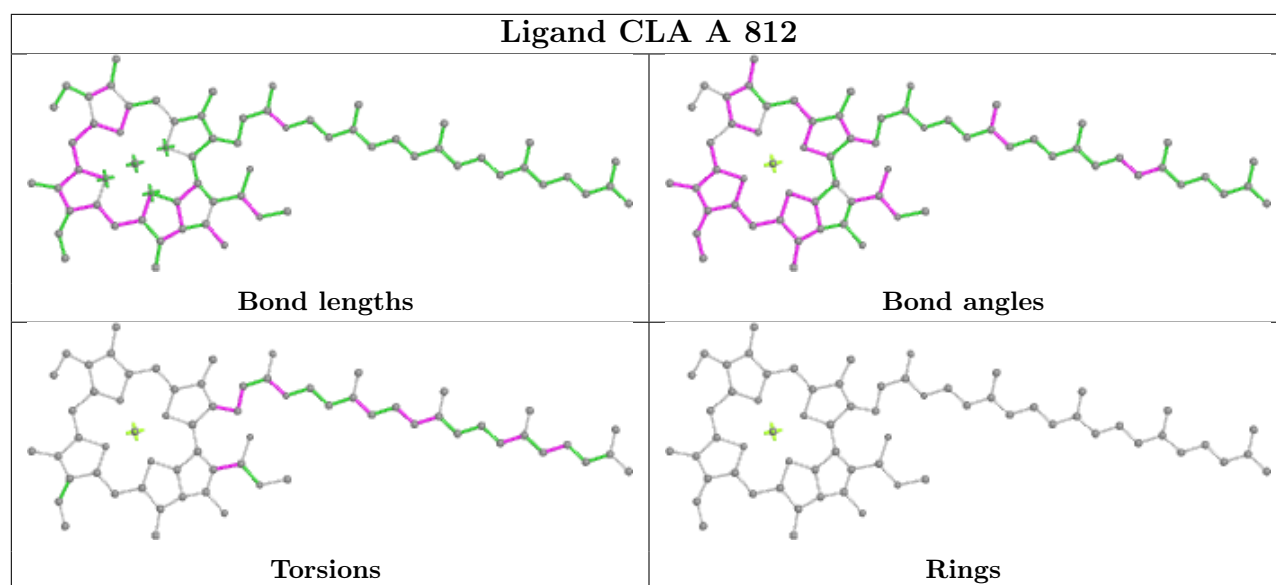
Ligand CLA 5 302

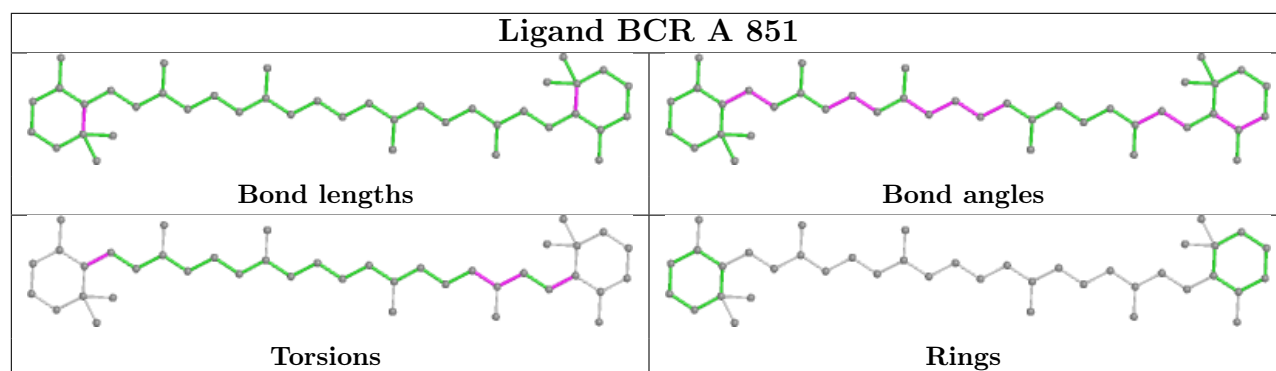
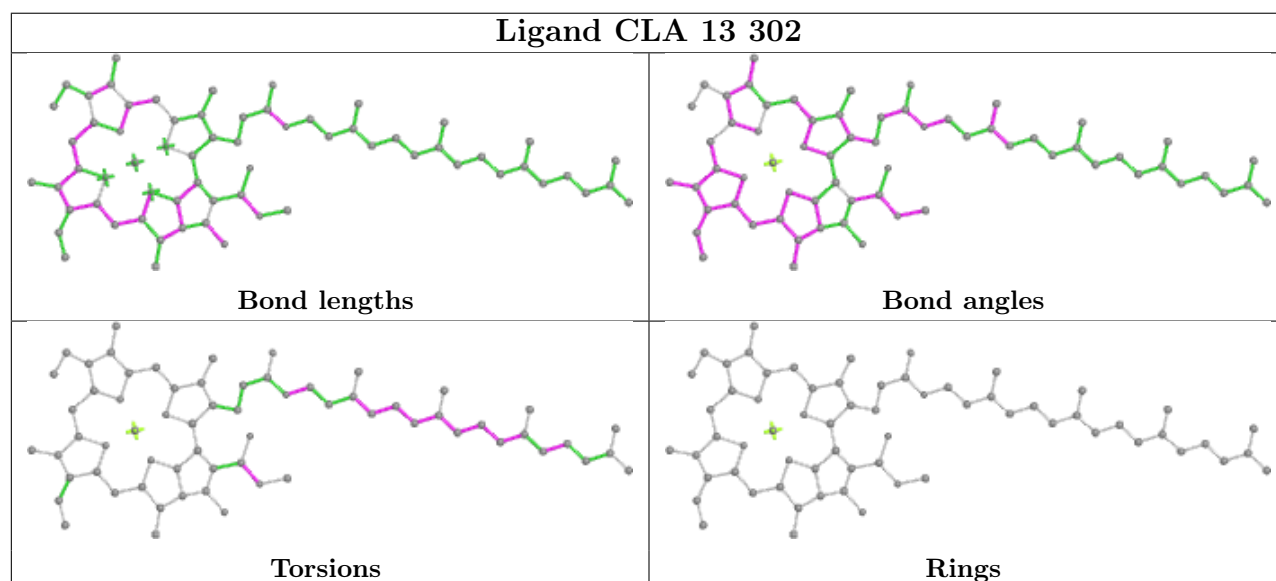
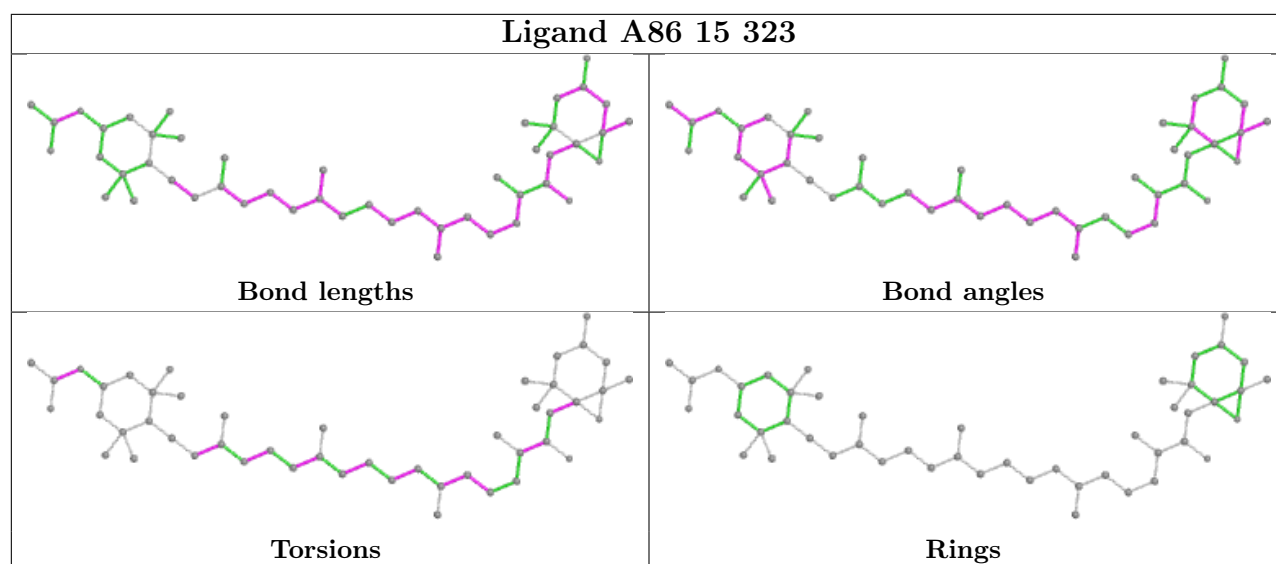


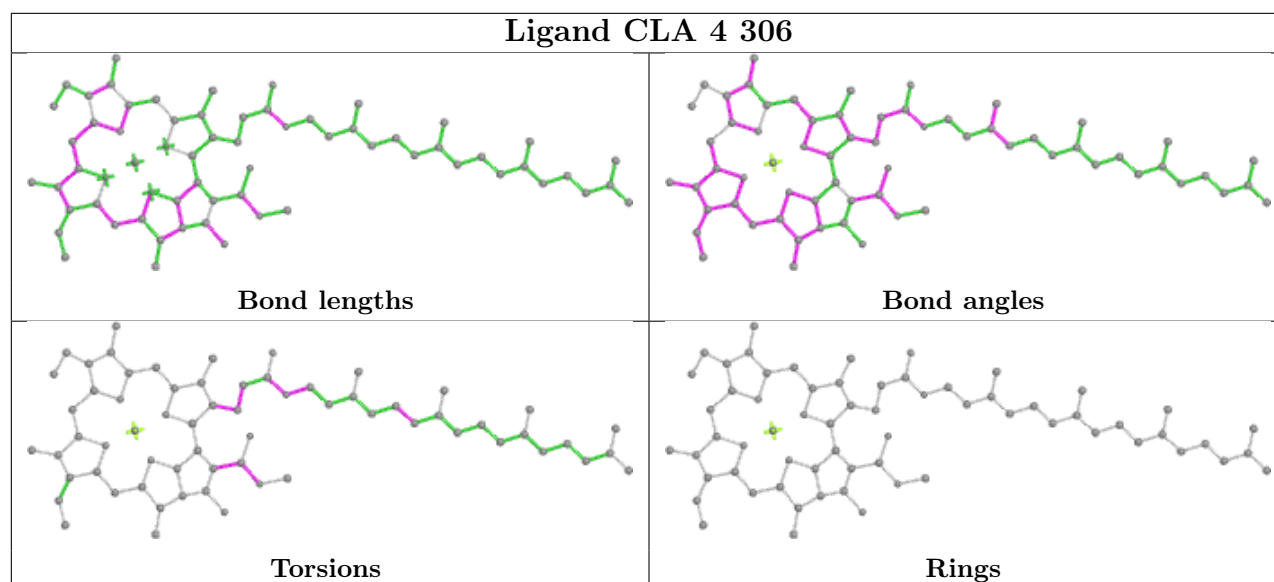
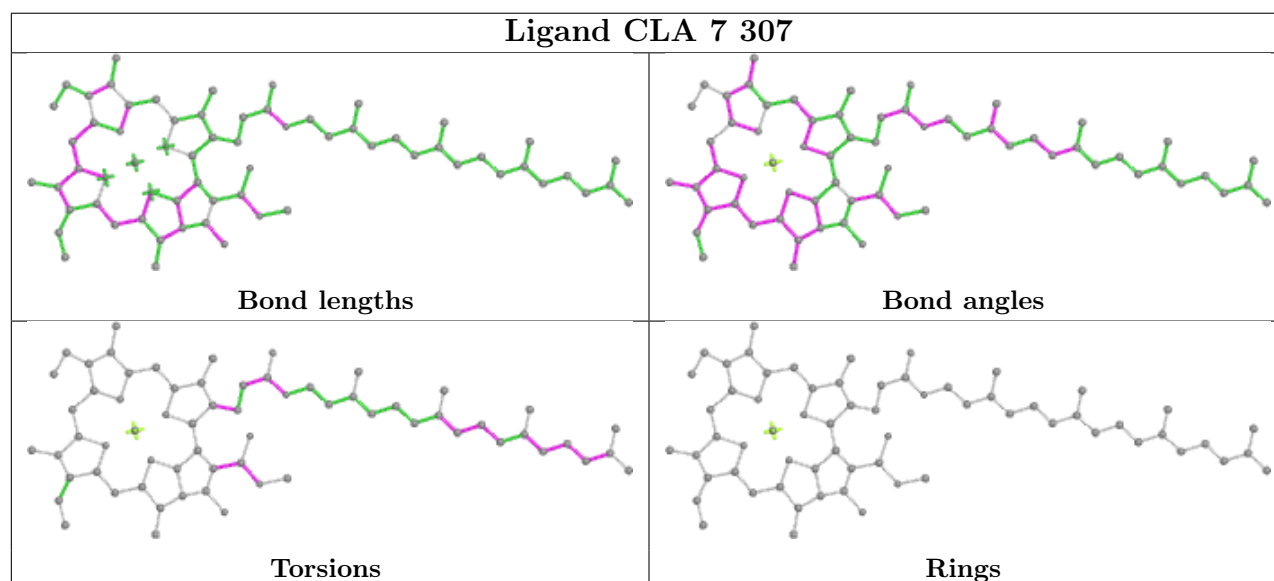
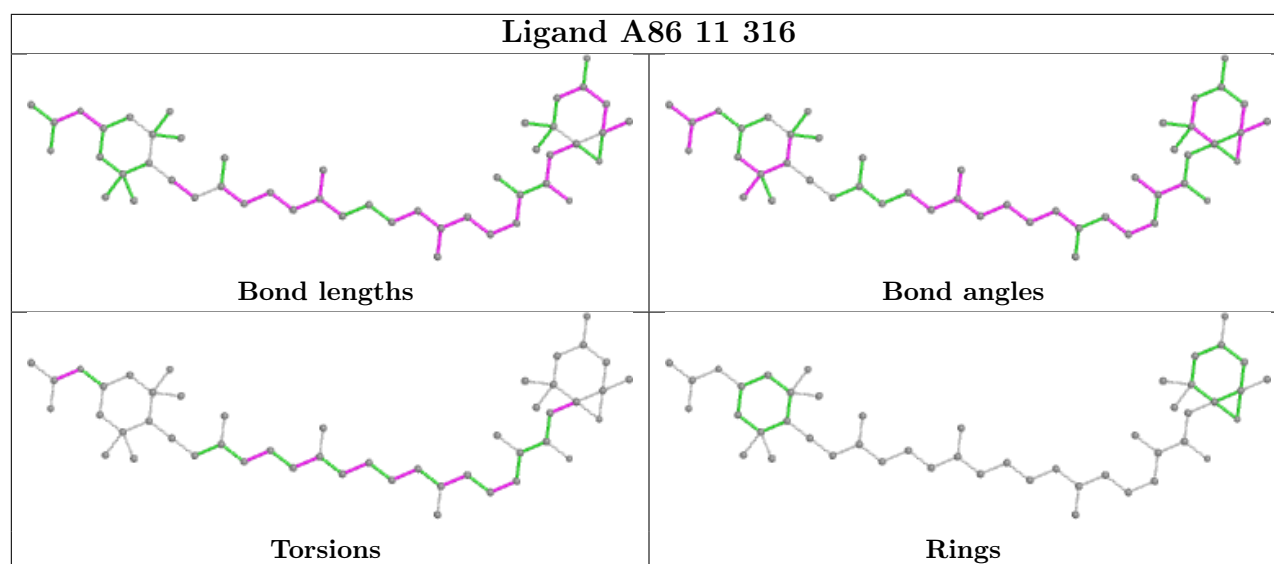
Ligand CLA B 812**Ligand A86 8 318****Ligand CLA 13 301**

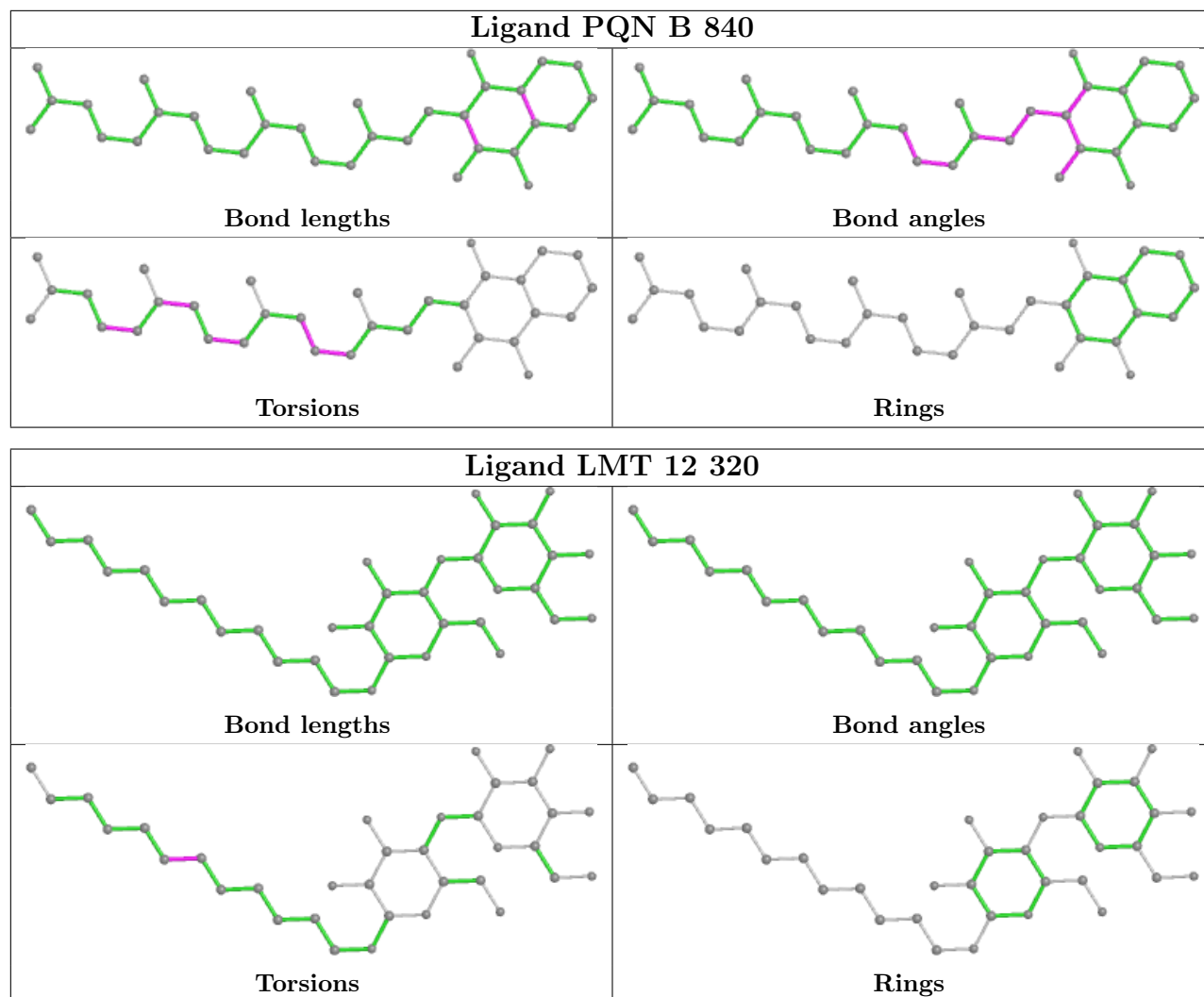
Ligand CLA 4 309**Ligand BCR I 101****Ligand A86 14 315**

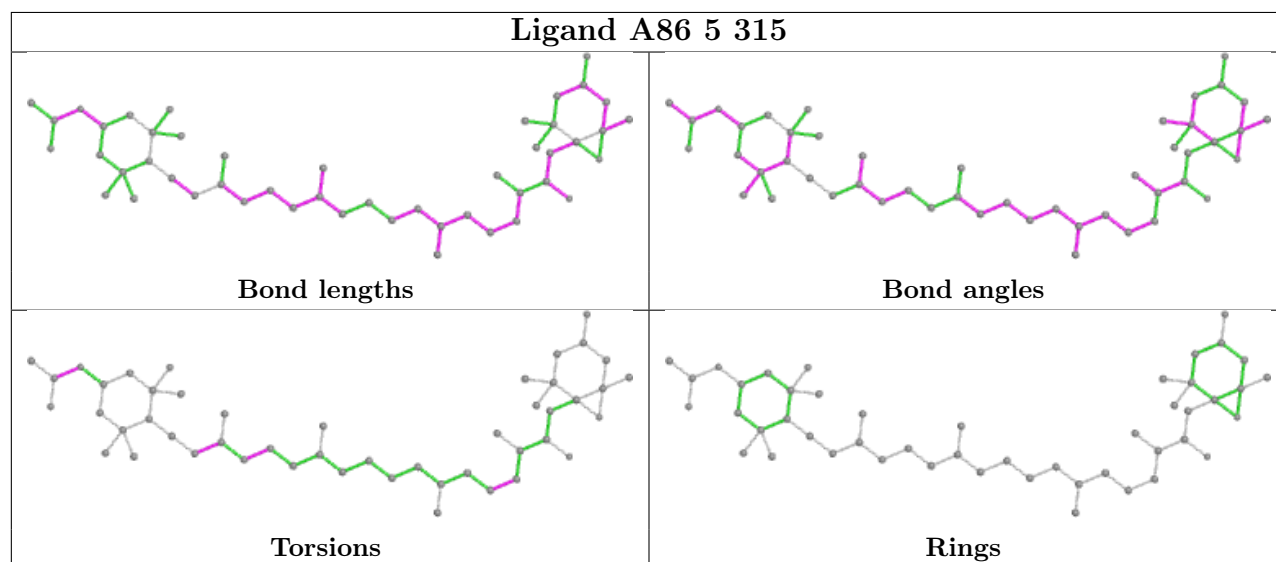
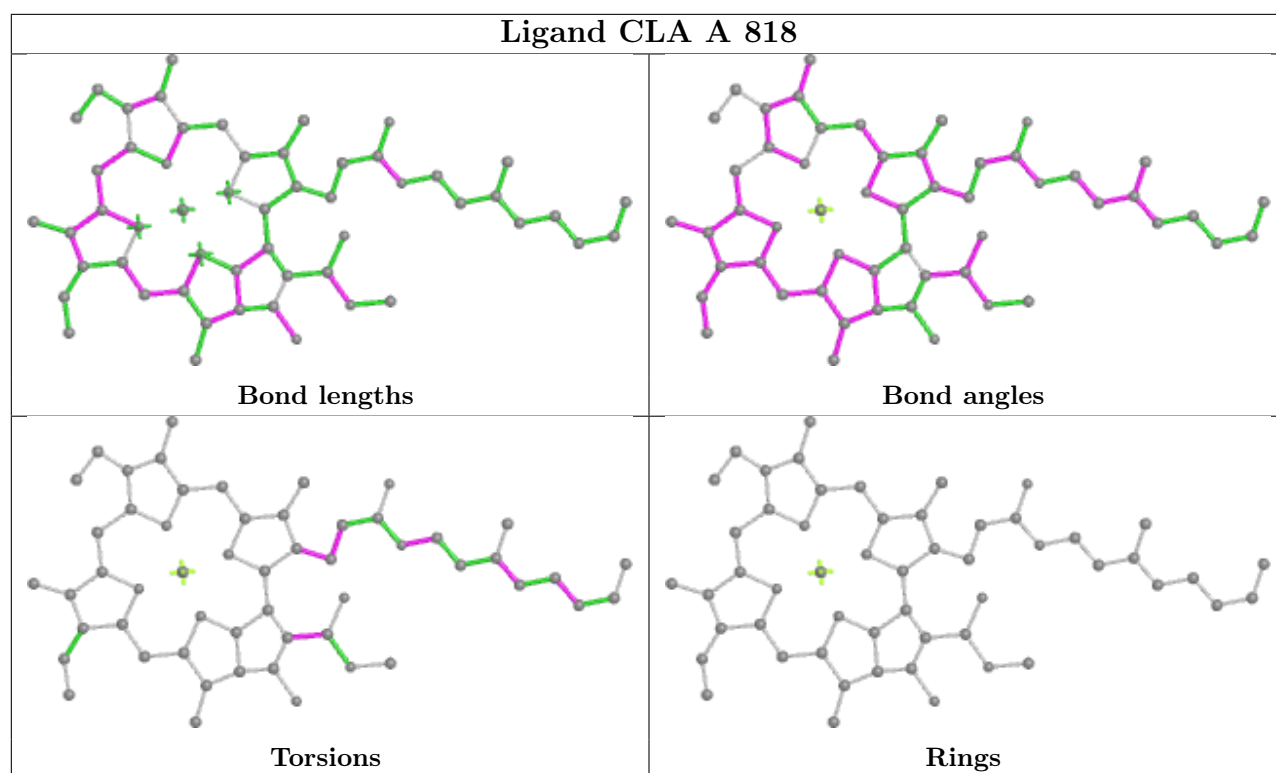


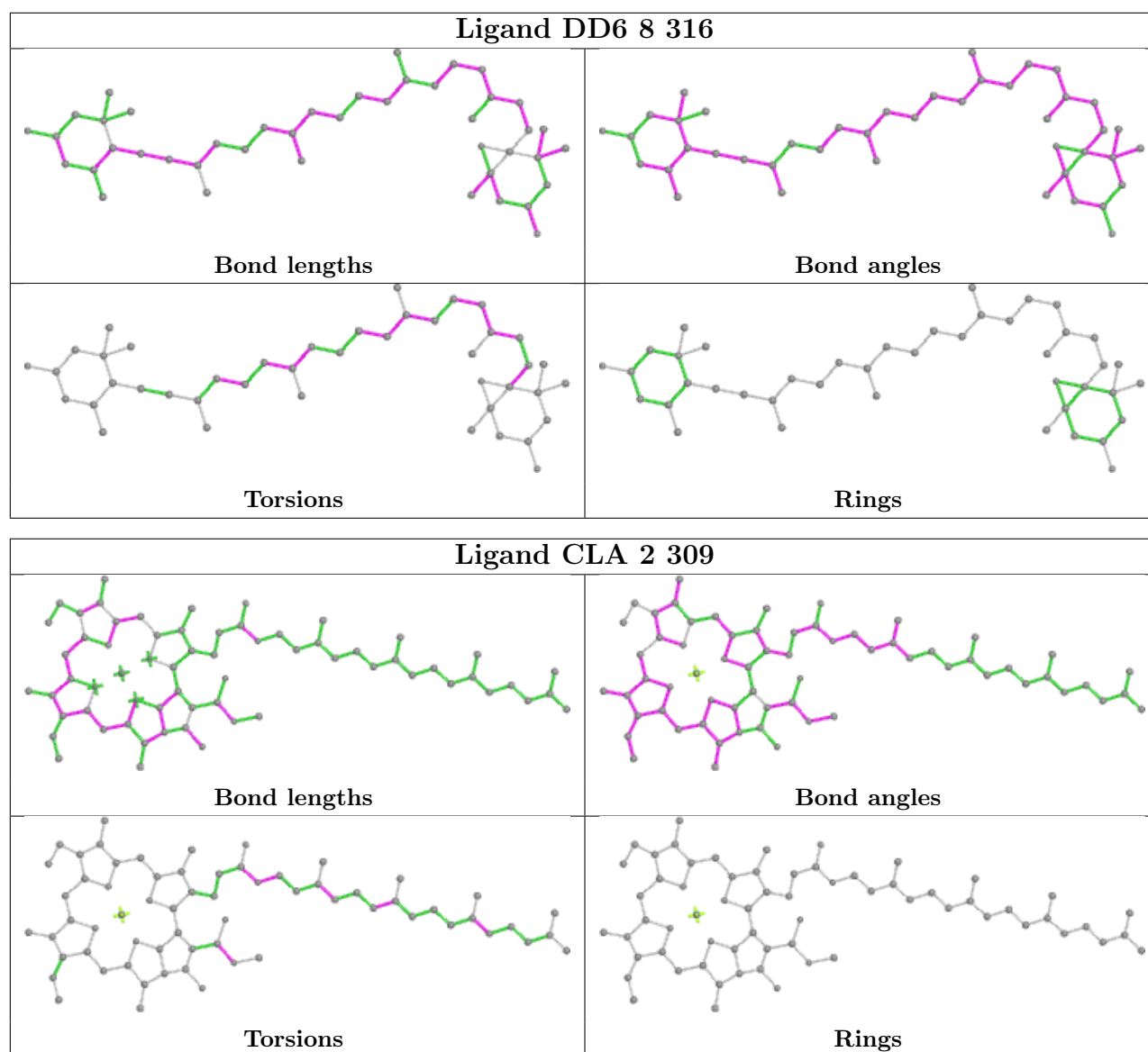












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.