



wwPDB EM Validation Summary Report ⓘ

Aug 7, 2026 – 06:06 AM JST

PDB ID : 9WYP / pdb_00009wyp
EMDB ID : EMD-66373
Title : The PSI-ACPI supercomplex from the cryptophyte Chroomonas placoidea
Authors : Li, X.Y.; Mao, Z.Y.; Han, G.Y.
Deposited on : 2025-09-27
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

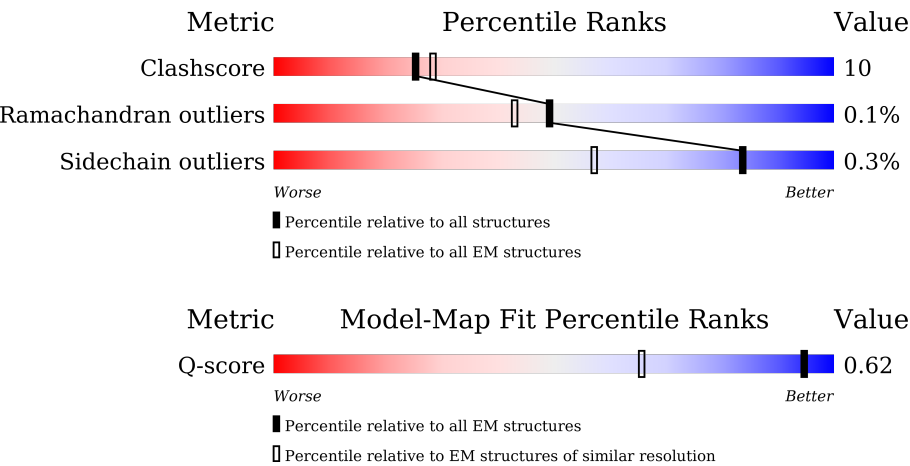
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.25 Å.

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



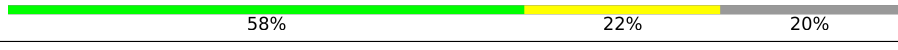
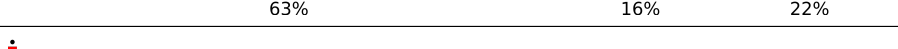
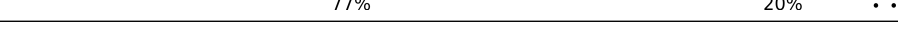
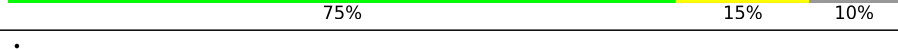
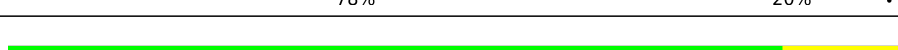
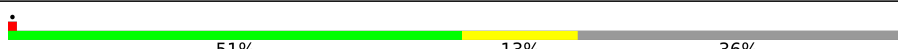
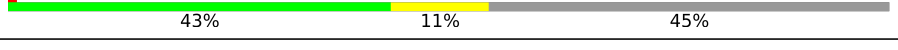
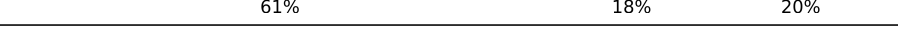
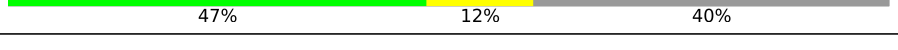
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3458 (1.75 - 2.75)

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

Mol	Chain	Length	Quality of chain
1	1	222	61%18%21%
2	2	216	62%16%22%
3	3	235	63%19%19%
4	4	217	71%10%19%

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Mol	Chain	Length	Quality of chain
5	5	229	
6	6	215	
7	7	230	
8	8	227	
9	9	220	
10	A	752	
11	B	734	
12	C	81	
13	D	141	
14	E	64	
15	F	183	
16	I	36	
17	J	42	
18	K	87	
19	L	153	
20	M	30	
21	O	155	
22	R	139	
23	Z	279	
24	a	215	
24	d	215	
25	b	218	
26	c	257	
27	e	208	
28	X	241	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 61306 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 ACPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	175	Total	C	N	O	S	0	0
			1316	848	222	238	8		

- Molecule 2 is a protein called ACPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	168	Total	C	N	O	S	0	0
			1320	872	215	230	3		

- Molecule 3 is a protein called ACPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	191	Total	C	N	O	S	0	0
			1433	920	243	259	11		

- Molecule 4 is a protein called ACPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	176	Total	C	N	O	S	0	0
			1366	891	224	245	6		

- Molecule 5 is a protein called ACPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	188	Total	C	N	O	S	0	0
			1403	908	234	253	8		

- Molecule 6 is a protein called ACPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	173	Total	C	N	O	S	0	0
			1305	846	217	232	10		

- Molecule 7 is a protein called ACPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	180	Total	C	N	O	S	0	0
			1358	874	234	242	8		

- Molecule 8 is a protein called ACPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	175	Total	C	N	O	S	0	0
			1313	852	219	237	5		

- Molecule 9 is a protein called ACPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	180	Total	C	N	O	S	0	0
			1349	864	230	243	12		

- Molecule 10 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	741	Total	C	N	O	S	0	0
			5824	3804	992	1000	28		

- Molecule 11 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	731	Total	C	N	O	S	0	0
			5828	3847	982	984	15		

- Molecule 12 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	80	Total	C	N	O	S	0	0
			591	361	103	115	12		

- Molecule 13 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	137	Total	C	N	O	S	0	0
			1070	685	184	198	3		

- Molecule 14 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	E	61	Total	C	N	O	0	0
			491	312	85	94		

- Molecule 15 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	160	Total	C	N	O	S	0	0
			1258	814	214	228	2		

- Molecule 16 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	33	Total	C	N	O	S	0	0
			258	180	34	42	2		

- Molecule 17 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	42	Total	C	N	O	S	0	0
			342	232	49	58	3		

- Molecule 18 is a protein called Photosystem I reaction center subunit Psak.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	78	Total	C	N	O	S	0	0
			553	358	90	102	3		

- Molecule 19 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	150	Total	C	N	O	S	0	0
			1143	746	184	211	2		

- Molecule 20 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	30	Total	C	N	O	S	0	0
			227	152	35	39	1		

- Molecule 21 is a protein called Psao.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	99	Total	C	N	O	S	0	0
			766	518	113	134	1		

- Molecule 22 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	92	Total	C	N	O	S	0	0
			680	439	112	127	2		

- Molecule 23 is a protein called CCPI-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	153	Total	C	N	O	S	0	0
			1130	721	188	211	10		

- Molecule 24 is a protein called ACPI-13/10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	171	Total	C	N	O	S	0	0
			1271	823	207	231	10		
24	d	171	Total	C	N	O	S	0	0
			1271	823	207	231	10		

- Molecule 25 is a protein called ACPI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	176	Total	C	N	O	S	0	0
			1368	891	224	244	9		

- Molecule 26 is a protein called ACPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	215	Total	C	N	O	S	0	0
			1615	1053	265	283	14		

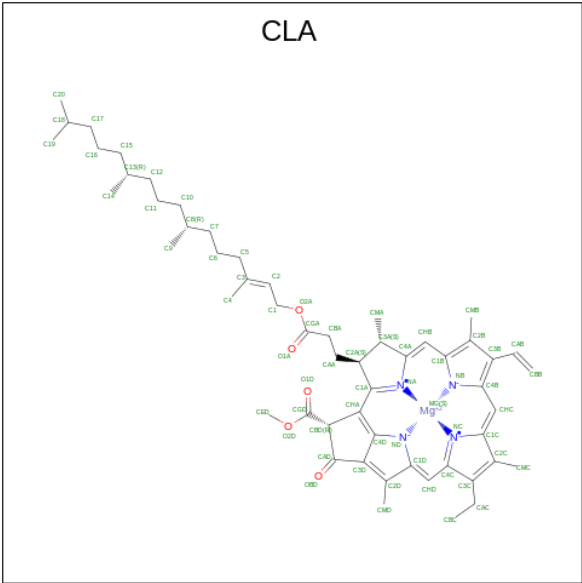
- Molecule 27 is a protein called ACPI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	168	Total	C	N	O	S	0	0
			1288	840	209	227	12		

- Molecule 28 is a protein called PsaQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	145	Total	C	N	O	S	0	0
			1034	655	176	199	4		

- Molecule 29 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	2	1	Total 59	C 49	Mg 1	N 4	O 5	0
29	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	3	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	4	1	Total 59	C 49	Mg 1	N 4	O 5	0
29	4	1	Total 54	C 44	Mg 1	N 4	O 5	0
29	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	5	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	7	1	Total 53	C 43	Mg 1	N 4	O 5	0
29	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	7	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 57	C 47	Mg 1	N 4	O 5	0
29	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	9	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
29	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	J	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	L	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
29	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	b	1	Total 64	C 54	Mg 1	N 4	O 5	0
29	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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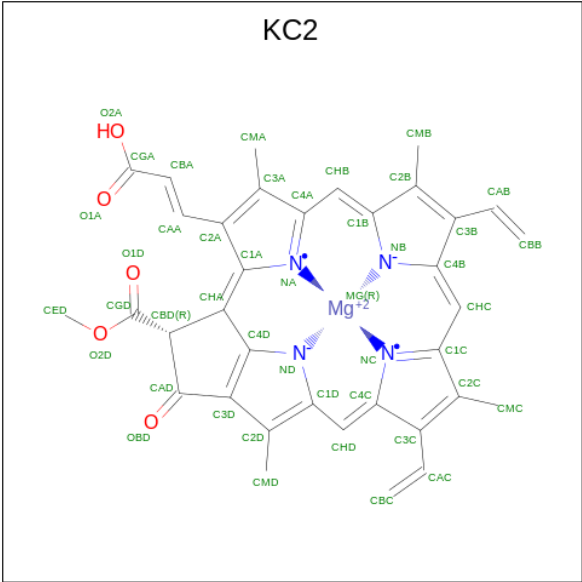
Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	d	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	e	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	X	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 30 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



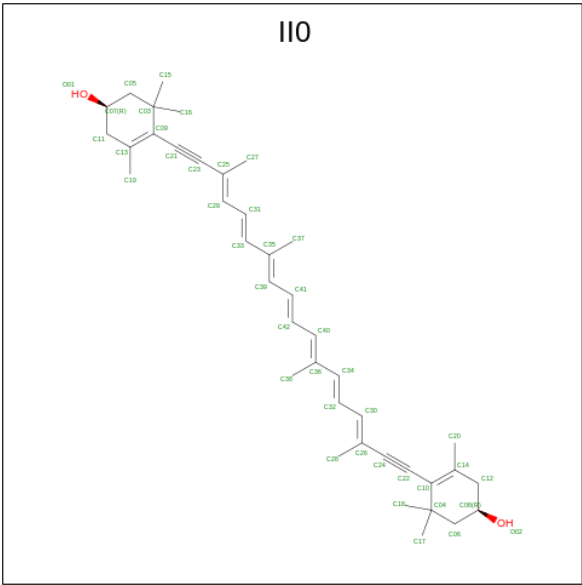
Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
30	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 31 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
31	2	1	Total 42	C 40	O 2	0
31	2	1	Total 42	C 40	O 2	0
31	2	1	Total 42	C 40	O 2	0
31	3	1	Total 42	C 40	O 2	0
31	3	1	Total 42	C 40	O 2	0
31	3	1	Total 42	C 40	O 2	0
31	3	1	Total 42	C 40	O 2	0
31	3	1	Total 42	C 40	O 2	0
31	4	1	Total 42	C 40	O 2	0
31	4	1	Total 42	C 40	O 2	0
31	4	1	Total 42	C 40	O 2	0
31	4	1	Total 42	C 40	O 2	0
31	4	1	Total 42	C 40	O 2	0
31	5	1	Total 42	C 40	O 2	0
31	5	1	Total 42	C 40	O 2	0
31	5	1	Total 42	C 40	O 2	0
31	5	1	Total 42	C 40	O 2	0
31	5	1	Total 42	C 40	O 2	0
31	6	1	Total 42	C 40	O 2	0
31	6	1	Total 42	C 40	O 2	0
31	7	1	Total 42	C 40	O 2	0
31	7	1	Total 42	C 40	O 2	0

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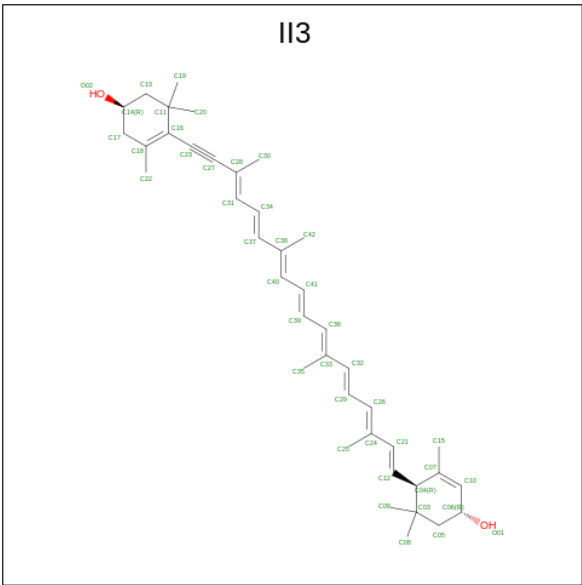
Mol	Chain	Residues	Atoms			AltConf
31	7	1	Total 42	C 40	O 2	0
31	7	1	Total 42	C 40	O 2	0
31	7	1	Total 42	C 40	O 2	0
31	8	1	Total 42	C 40	O 2	0
31	8	1	Total 42	C 40	O 2	0
31	8	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	J	1	Total 42	C 40	O 2	0
31	O	1	Total 42	C 40	O 2	0
31	O	1	Total 42	C 40	O 2	0
31	R	1	Total 42	C 40	O 2	0
31	R	1	Total 42	C 40	O 2	0
31	a	1	Total 42	C 40	O 2	0
31	a	1	Total 42	C 40	O 2	0
31	a	1	Total 42	C 40	O 2	0
31	a	1	Total 42	C 40	O 2	0
31	b	1	Total 42	C 40	O 2	0

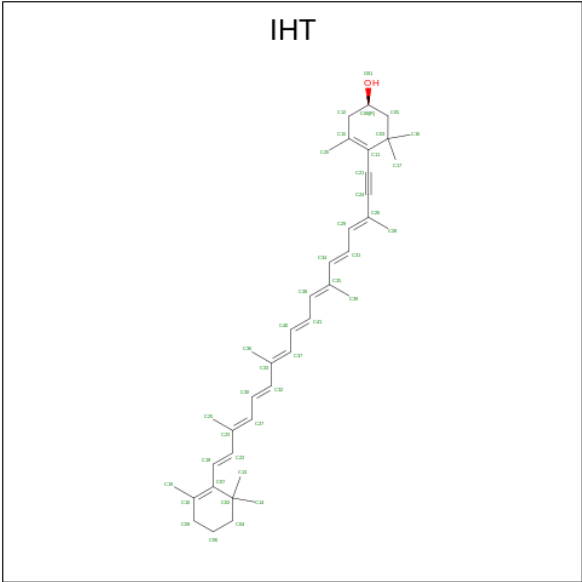
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Mol	Chain	Residues	Atoms			AltConf
31	b	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	d	1	Total	C	O	0
			42	40	2	
31	d	1	Total	C	O	0
			42	40	2	
31	d	1	Total	C	O	0
			42	40	2	
31	d	1	Total	C	O	0
			42	40	2	
31	e	1	Total	C	O	0
			42	40	2	
31	e	1	Total	C	O	0
			42	40	2	
31	e	1	Total	C	O	0
			42	40	2	

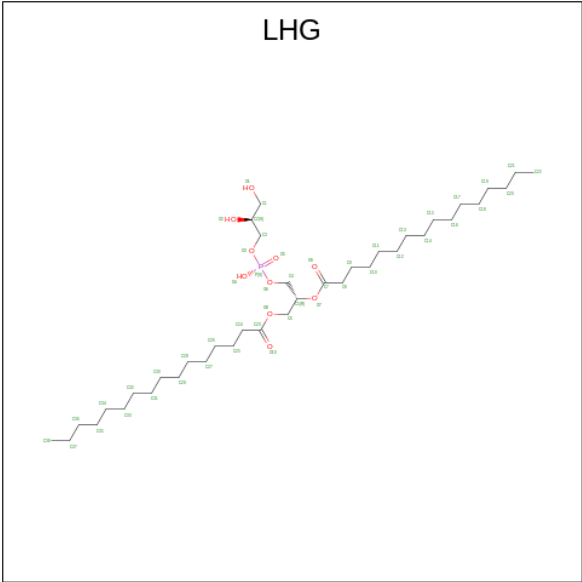
- Molecule 32 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: II3) (formula: C₄₀H₅₄O₂) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			AltConf
33	1	1	Total	C	O	0
			41	40	1	
33	2	1	Total	C	O	0
			41	40	1	
33	5	1	Total	C	O	0
			41	40	1	
33	6	1	Total	C	O	0
			41	40	1	
33	8	1	Total	C	O	0
			41	40	1	
33	9	1	Total	C	O	0
			41	40	1	
33	K	1	Total	C	O	0
			41	40	1	
33	L	1	Total	C	O	0
			41	40	1	
33	Z	1	Total	C	O	0
			41	40	1	
33	a	1	Total	C	O	0
			41	40	1	
33	c	1	Total	C	O	0
			41	40	1	
33	d	1	Total	C	O	0
			41	40	1	

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



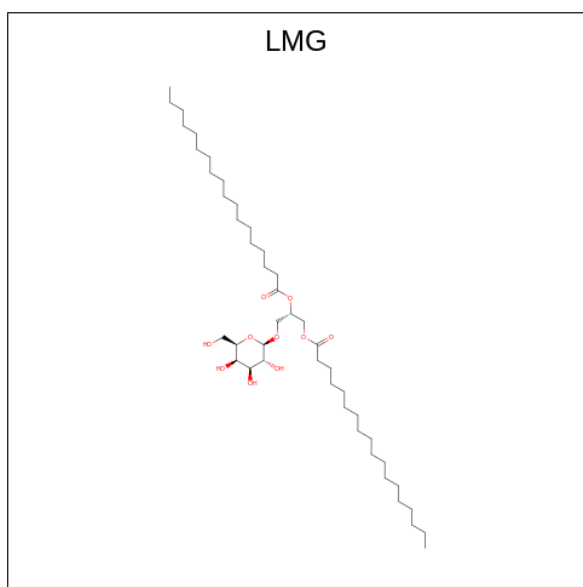
Mol	Chain	Residues	Atoms				AltConf
34	1	1	Total	C	O	P	0
			35	24	10	1	
34	2	1	Total	C	O	P	0
			22	12	9	1	
34	2	1	Total	C	O	P	0
			39	28	10	1	
34	3	1	Total	C	O	P	0
			42	31	10	1	
34	3	1	Total	C	O	P	0
			49	38	10	1	
34	4	1	Total	C	O	P	0
			49	38	10	1	
34	4	1	Total	C	O	P	0
			49	38	10	1	
34	4	1	Total	C	O	P	0
			45	34	10	1	
34	4	1	Total	C	O	P	0
			45	34	10	1	
34	5	1	Total	C	O	P	0
			23	12	10	1	
34	5	1	Total	C	O	P	0
			35	24	10	1	
34	7	1	Total	C	O	P	0
			39	28	10	1	
34	7	1	Total	C	O	P	0
			31	20	10	1	
34	8	1	Total	C	O	P	0
			33	22	10	1	

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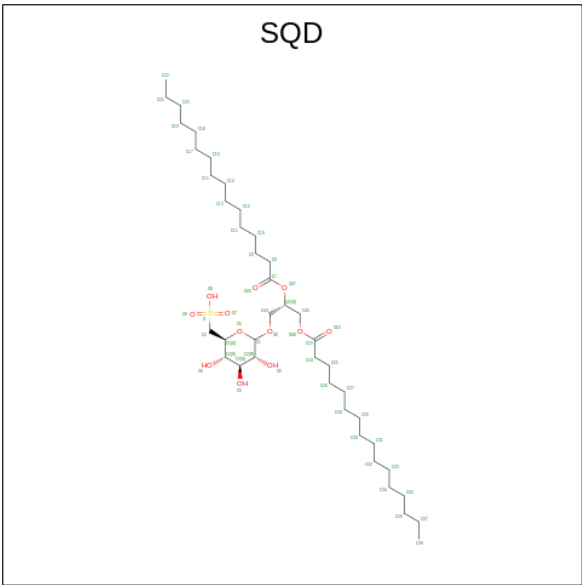
Mol	Chain	Residues	Atoms				AltConf
34	8	1	Total	C	O	P	0
			49	38	10	1	
34	9	1	Total	C	O	P	0
			36	27	8	1	
34	A	1	Total	C	O	P	0
			49	38	10	1	
34	A	1	Total	C	O	P	0
			39	28	10	1	
34	A	1	Total	C	O	P	0
			23	14	8	1	
34	B	1	Total	C	O	P	0
			40	31	8	1	
34	J	1	Total	C	O	P	0
			34	23	10	1	
34	L	1	Total	C	O	P	0
			22	16	5	1	
34	L	1	Total	C	O	P	0
			33	23	9	1	
34	L	1	Total	C	O	P	0
			34	23	10	1	
34	M	1	Total	C	O	P	0
			24	15	8	1	
34	O	1	Total	C	O	P	0
			40	31	8	1	
34	Z	1	Total	C	O	P	0
			40	31	8	1	
34	Z	1	Total	C	O	P	0
			46	35	10	1	
34	a	1	Total	C	O	P	0
			27	16	10	1	
34	b	1	Total	C	O	P	0
			30	19	10	1	
34	c	1	Total	C	O	P	0
			21	11	9	1	
34	c	1	Total	C	O	P	0
			35	24	10	1	
34	e	1	Total	C	O	P	0
			28	17	10	1	

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
35	2	1	Total	C	O	0
			36	26	10	
35	3	1	Total	C	O	0
			30	20	10	
35	6	1	Total	C	O	0
			32	22	10	
35	8	1	Total	C	O	0
			52	42	10	
35	F	1	Total	C	O	0
			32	22	10	
35	Z	1	Total	C	O	0
			48	38	10	
35	X	1	Total	C	O	0
			34	24	10	

- Molecule 36 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
36	3	1	Total	C	O	S	0
			36	23	12	1	
36	3	1	Total	C	O	S	0
			36	23	12	1	
36	7	1	Total	C	O	S	0
			36	23	12	1	
36	9	1	Total	C	O	S	0
			30	17	12	1	
36	B	1	Total	C	O	S	0
			33	20	12	1	
36	O	1	Total	C	O	S	0
			29	16	12	1	
36	a	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 37 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).

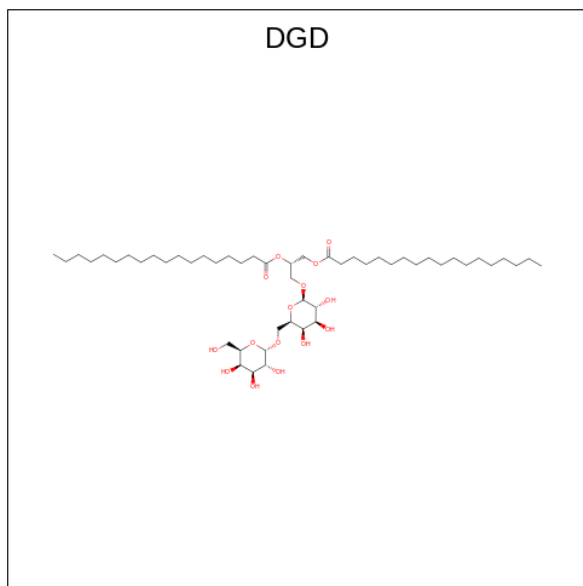


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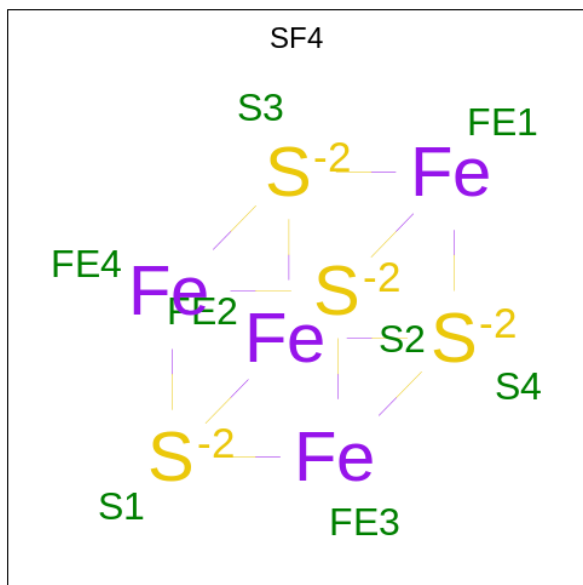
Mol	Chain	Residues	Atoms	AltConf
37	F	1	Total C 40 40	0
37	I	1	Total C 40 40	0
37	J	1	Total C 40 40	0
37	K	1	Total C 40 40	0
37	L	1	Total C 40 40	0
37	M	1	Total C 40 40	0
37	R	1	Total C 40 40	0
37	Z	1	Total C 40 40	0
37	Z	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	e	1	Total C 40 40	0

- Molecule 38 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
38	9	1	Total	C	O	0
			60	45	15	
38	B	1	Total	C	O	0
			59	44	15	

- Molecule 39 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 40 is PHYLLOQUINONE (CCD ID: PQN) (formula: $\text{C}_{31}\text{H}_{46}\text{O}_2$).

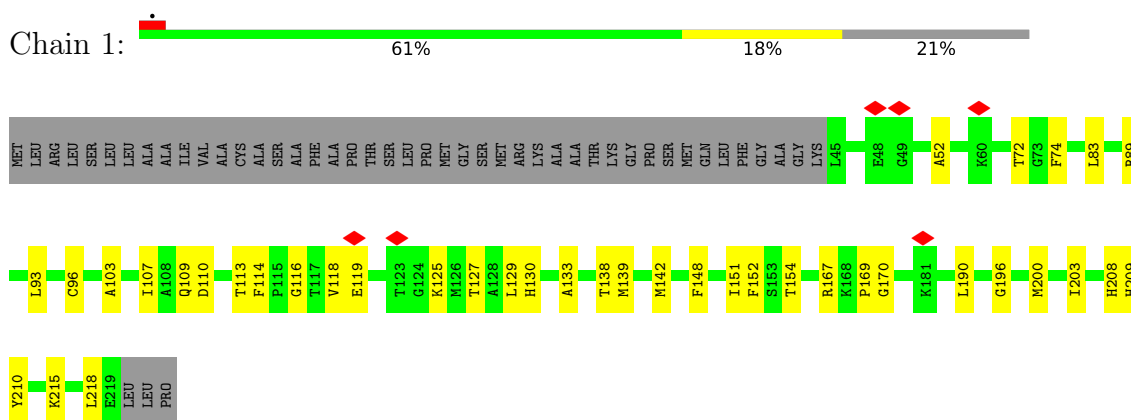


Mol	Chain	Residues	Atoms			AltConf
40	A	1	Total 33	C 31	O 2	0
40	B	1	Total 33	C 31	O 2	0

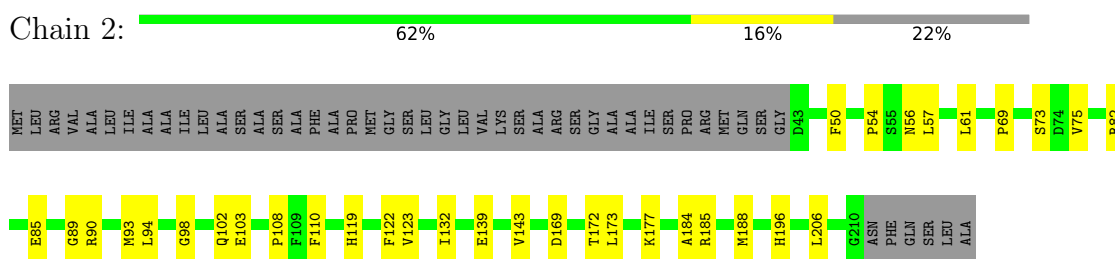
3 Residue-property plots

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

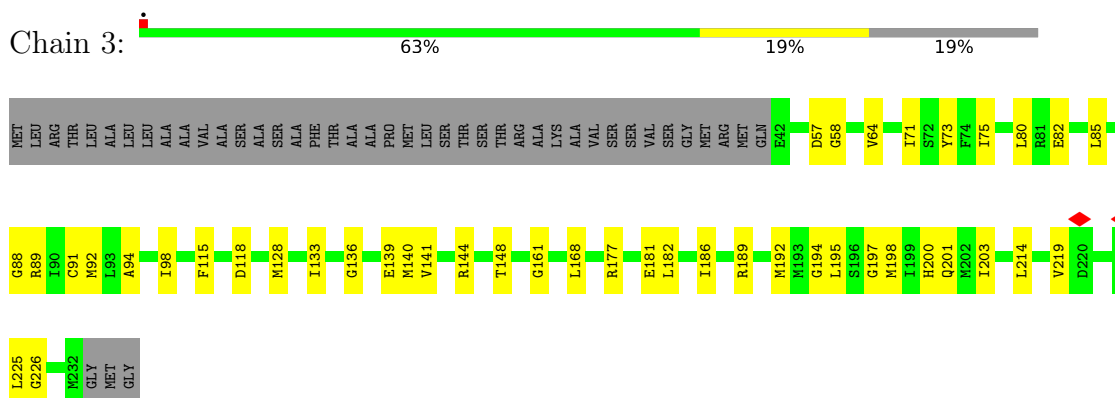
• Molecule 1: ACPI-1



• Molecule 2: ACPI-2

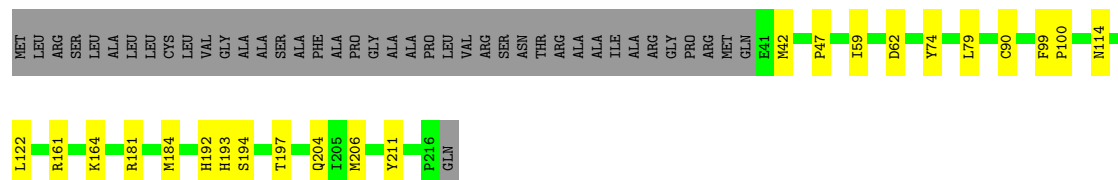


• Molecule 3: ACPI-3



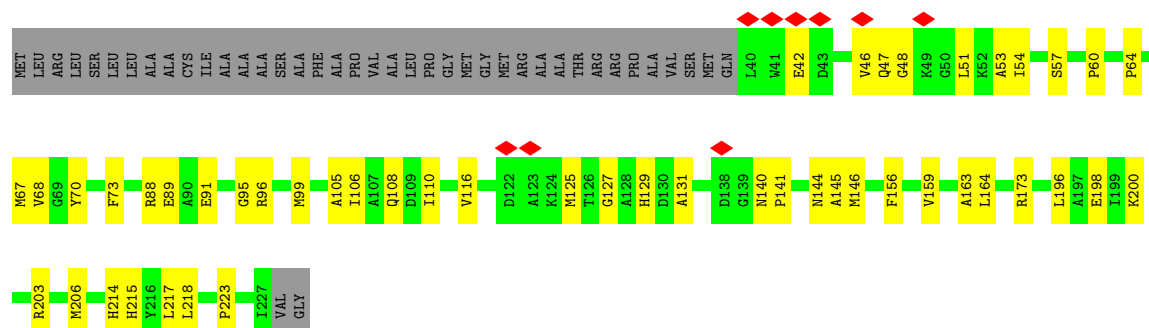
- Molecule 4: ACPI-4

Chain 4:  71% 10% 19%



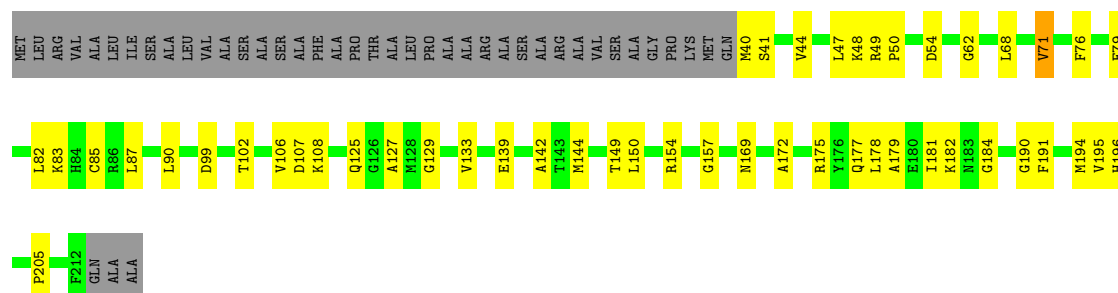
- Molecule 5: ACPI-5

Chain 5:  61% 21% 18%



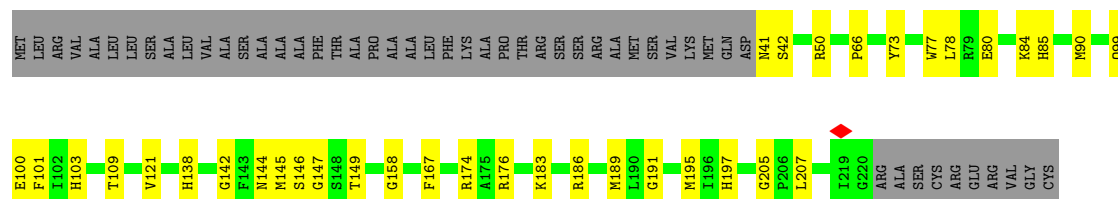
- Molecule 6: ACPI-6

Chain 6:  58% 22% 20%



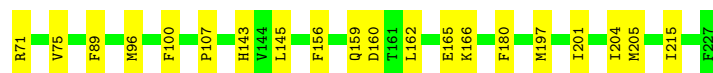
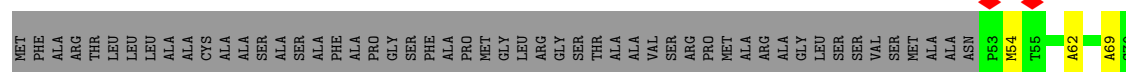
- Molecule 7: ACPI-7

Chain 7:  63% 16% 22%



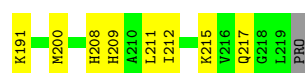
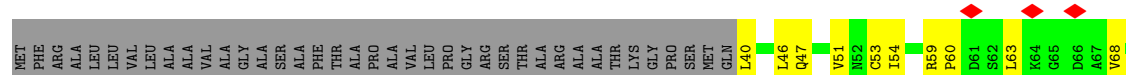
- Molecule 8: ACPI-8

Chain 8:  67% 10% 23%



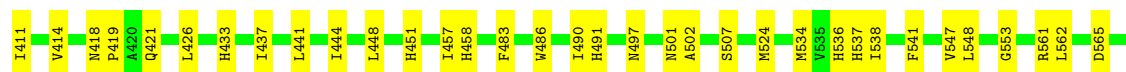
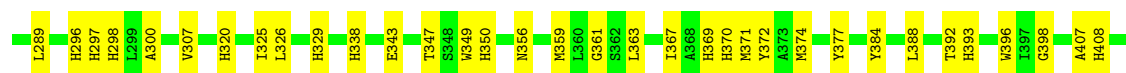
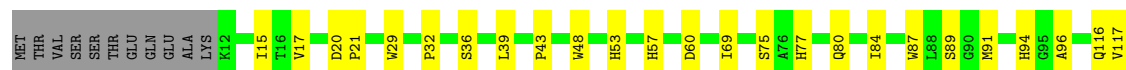
• Molecule 9: ACPI-12

Chain 9:  59% 23% 18%



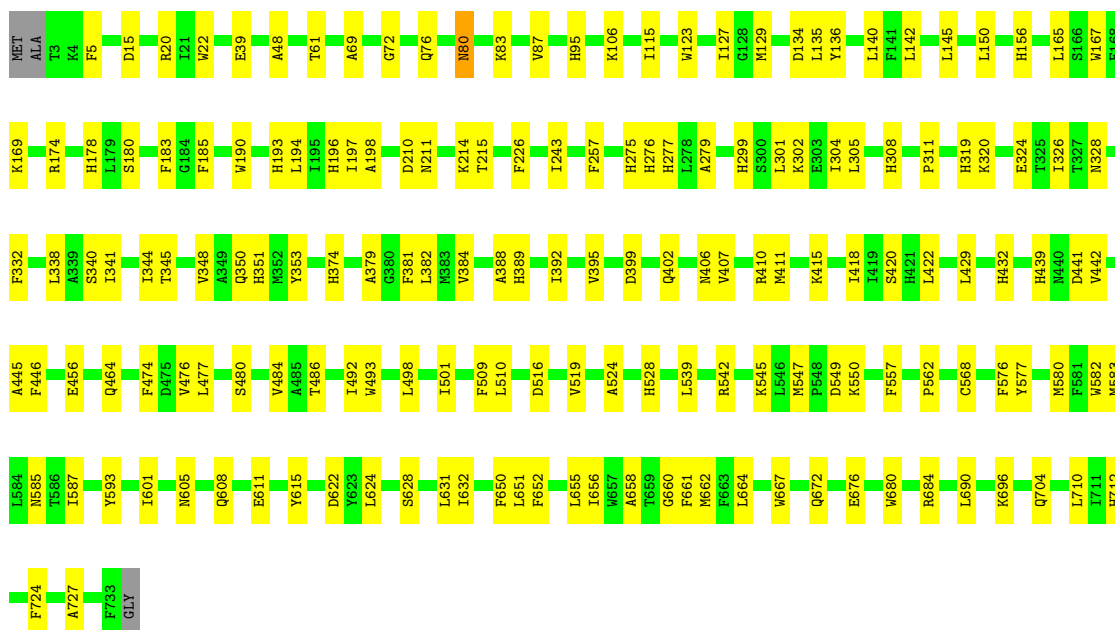
• Molecule 10: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:  77% 22%



• Molecule 11: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  77% 23%



- Molecule 12: Photosystem I iron-sulfur center

Chain C: 89% 10% .



- Molecule 13: Photosystem I reaction center subunit II

Chain D: 77% 20% ..



- Molecule 14: Photosystem I reaction center subunit IV

Chain E: 83% 12% 5%



- Molecule 15: Photosystem I reaction center subunit III

Chain F: 72% 15% 13%



- Molecule 16: Photosystem I reaction center subunit VIII

Chain I:  69% 22% 8%



- Molecule 17: Photosystem I reaction center subunit IX

Chain J:  81% 19%



- Molecule 18: Photosystem I reaction center subunit PsaK

Chain K:  75% 15% 10%



- Molecule 19: Photosystem I reaction center subunit XI

Chain L:  78% 20%



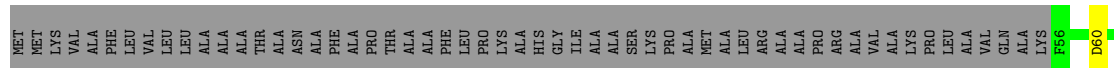
- Molecule 20: Photosystem I reaction center subunit XII

Chain M:  87% 13%



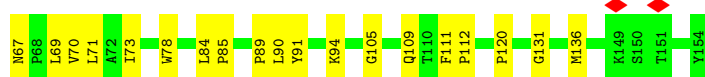
- Molecule 21: PsaO

Chain O:  51% 13% 36%



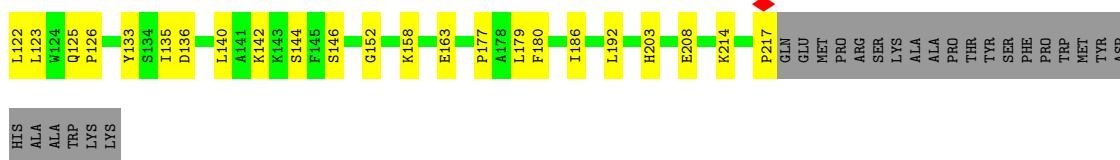
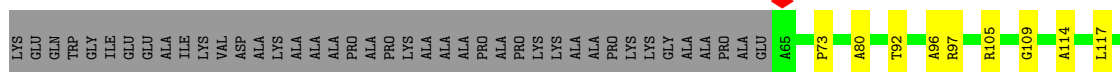
- Molecule 22: PsaR

Chain R:  51% 15% 34%





Chain Z: 43% 11% 45%



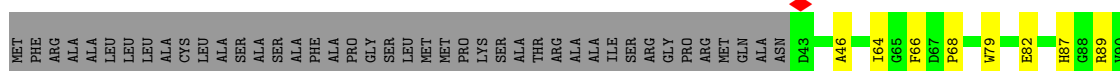
Chain a: 61% 18% 20%



Chain d: 60% 19% 20%

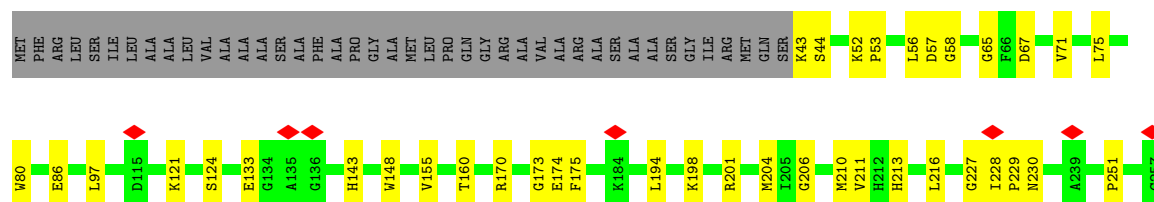


Chain b: 62% 19% 19%

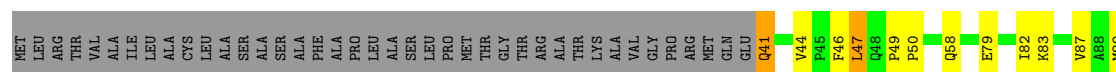




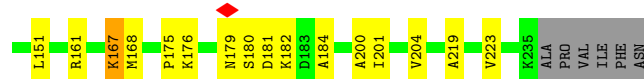
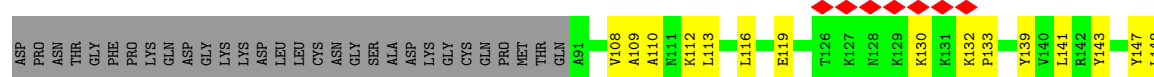
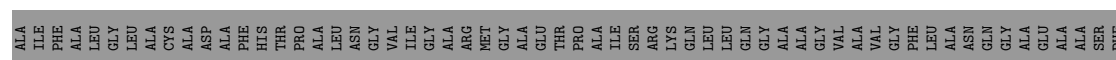
• Molecule 26: ACPI-9



• Molecule 27: ACPI-11



• Molecule 28: PsaQ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171764	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.00	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.709	Depositor
Minimum map value	-0.190	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	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: KC2, 8CT, IHT, II0, SQD, SF4, LHG, II3, DGD, PQN, CLA, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.18	0/1349	0.39	0/1826
2	2	0.17	0/1356	0.30	0/1835
3	3	0.18	0/1464	0.38	0/1978
4	4	0.16	0/1406	0.30	0/1900
5	5	0.19	0/1438	0.44	0/1940
6	6	0.25	0/1334	0.39	0/1796
7	7	0.17	0/1394	0.38	0/1886
8	8	0.19	0/1342	0.33	0/1825
9	9	0.21	0/1376	0.37	0/1846
10	A	0.20	0/6019	0.37	0/8204
11	B	0.24	0/6046	0.41	0/8254
12	C	0.16	0/600	0.37	0/812
13	D	0.31	0/1094	0.47	0/1476
14	E	0.19	0/499	0.31	0/677
15	F	0.18	0/1290	0.40	0/1745
16	I	0.20	0/266	0.39	0/362
17	J	0.14	0/353	0.29	0/481
18	K	0.19	0/563	0.33	0/768
19	L	0.15	0/1171	0.34	0/1594
20	M	0.14	0/228	0.23	0/310
21	O	0.14	0/796	0.29	0/1091
22	R	0.37	0/700	0.52	0/963
23	Z	0.15	0/1163	0.35	0/1572
24	a	0.18	0/1299	0.37	0/1747
24	d	0.17	0/1299	0.31	0/1747
25	b	0.15	0/1404	0.33	0/1902
26	c	0.15	0/1658	0.33	0/2241
27	e	0.14	0/1325	0.32	0/1793
28	X	0.30	0/1046	0.49	0/1413
All	All	0.20	0/41278	0.38	0/55984

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1	1316	0	1305	30	0
2	2	1320	0	1309	28	0
3	3	1433	0	1462	37	0
4	4	1366	0	1349	19	0
5	5	1403	0	1398	37	0
6	6	1305	0	1324	35	0
7	7	1358	0	1339	27	0
8	8	1313	0	1339	20	0
9	9	1349	0	1358	38	0
10	A	5824	0	5672	149	0
11	B	5828	0	5626	172	0
12	C	591	0	567	10	0
13	D	1070	0	1076	27	0
14	E	491	0	491	6	0
15	F	1258	0	1266	21	0
16	I	258	0	268	8	0
17	J	342	0	344	8	0
18	K	553	0	581	15	0
19	L	1143	0	1145	28	0
20	M	227	0	257	4	0
21	O	766	0	752	15	0
22	R	680	0	674	17	0
23	Z	1130	0	1088	28	0
24	a	1271	0	1279	32	0
24	d	1271	0	1281	32	0
25	b	1368	0	1346	32	0
26	c	1615	0	1646	28	0
27	e	1288	0	1282	24	0
28	X	1034	0	1090	29	0
29	1	584	0	476	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	2	552	0	462	15	0
29	3	625	0	596	25	0
29	4	598	0	597	25	0
29	5	563	0	442	23	0
29	6	581	0	514	19	0
29	7	509	0	431	19	0
29	8	496	0	471	25	0
29	9	635	0	524	35	0
29	A	2794	0	2881	168	0
29	B	2404	0	2454	139	0
29	F	100	0	82	3	0
29	J	41	0	29	0	0
29	K	120	0	121	4	0
29	L	161	0	139	9	0
29	O	206	0	176	5	0
29	R	55	0	49	3	0
29	X	52	0	43	2	0
29	Z	225	0	206	9	0
29	a	645	0	632	21	0
29	b	523	0	508	20	0
29	c	666	0	632	25	0
29	d	589	0	538	18	0
29	e	472	0	414	17	0
30	1	45	0	0	1	0
30	2	45	0	0	0	0
30	3	45	0	0	1	0
30	4	45	0	0	0	0
30	5	45	0	0	0	0
30	6	90	0	0	1	0
30	7	90	0	0	1	0
30	9	45	0	0	0	0
30	Z	45	0	0	1	0
30	a	45	0	0	0	0
30	b	90	0	0	4	0
30	c	135	0	0	1	0
30	d	45	0	0	0	0
30	e	90	0	0	0	0
31	1	168	0	0	1	0
31	2	126	0	0	1	0
31	3	210	0	0	0	0
31	4	168	0	0	0	0
31	5	210	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	6	84	0	0	1	0
31	7	210	0	0	1	0
31	8	126	0	0	0	0
31	9	210	0	0	0	0
31	J	42	0	0	0	0
31	O	84	0	0	0	0
31	R	84	0	0	2	0
31	a	168	0	0	0	0
31	b	84	0	0	0	0
31	c	210	0	0	2	0
31	d	168	0	0	1	0
31	e	126	0	0	0	0
32	1	42	0	0	0	0
32	8	42	0	0	2	0
32	b	42	0	0	1	0
32	e	42	0	0	2	0
33	1	41	0	0	0	0
33	2	41	0	0	0	0
33	5	41	0	0	0	0
33	6	41	0	0	0	0
33	8	41	0	0	0	0
33	9	41	0	0	0	0
33	K	41	0	0	0	0
33	L	41	0	0	1	0
33	Z	41	0	0	0	0
33	a	41	0	0	1	0
33	c	41	0	0	1	0
33	d	41	0	0	0	0
34	1	35	0	39	2	0
34	2	61	0	68	1	0
34	3	91	0	131	4	0
34	4	188	0	271	15	0
34	5	58	0	56	4	0
34	7	70	0	83	5	0
34	8	82	0	110	1	0
34	9	36	0	45	1	0
34	A	111	0	139	5	0
34	B	40	0	56	3	0
34	J	34	0	38	2	0
34	L	89	0	96	4	0
34	M	24	0	21	2	0
34	O	40	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	Z	86	0	119	2	0
34	a	27	0	24	1	0
34	b	30	0	30	0	0
34	c	56	0	61	2	0
34	e	28	0	26	1	0
35	2	36	0	42	3	0
35	3	30	0	29	2	0
35	6	32	0	34	0	0
35	8	52	0	77	2	0
35	F	32	0	34	3	0
35	X	34	0	38	3	0
35	Z	48	0	69	1	0
36	3	72	0	72	3	0
36	7	36	0	36	2	0
36	9	30	0	24	1	0
36	B	33	0	30	1	0
36	O	29	0	22	0	0
36	a	42	0	48	3	0
37	4	40	0	0	1	0
37	7	40	0	0	1	0
37	A	160	0	0	0	0
37	B	320	0	0	3	0
37	F	40	0	0	1	0
37	I	40	0	0	0	0
37	J	40	0	0	0	0
37	K	40	0	0	0	0
37	L	40	0	0	0	0
37	M	40	0	0	1	0
37	R	40	0	0	0	0
37	Z	80	0	0	0	0
37	b	40	0	0	0	0
37	e	40	0	0	0	0
38	9	60	0	78	1	0
38	B	59	0	79	4	0
39	A	8	0	0	0	0
39	C	16	0	0	1	0
40	A	33	0	46	5	0
40	B	33	0	46	2	0
All	All	61306	0	55604	1221	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 10.

The worst 5 of 1221 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)
10:A:393:HIS:HE1	29:A:826:CLA:ND	1.69	0.91
18:K:24:MET:HE1	18:K:70:HIS:HA	1.54	0.90
10:A:408:HIS:HE1	29:A:828:CLA:NA	1.72	0.86
29:A:819:CLA:NB	29:A:825:CLA:H122	1.90	0.85
11:B:374:HIS:HE1	29:B:827:CLA:ND	1.76	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	173/222 (78%)	163 (94%)	10 (6%)	0	100	100
2	2	166/216 (77%)	164 (99%)	2 (1%)	0	100	100
3	3	189/235 (80%)	187 (99%)	2 (1%)	0	100	100
4	4	174/217 (80%)	173 (99%)	1 (1%)	0	100	100
5	5	186/229 (81%)	173 (93%)	13 (7%)	0	100	100
6	6	171/215 (80%)	165 (96%)	6 (4%)	0	100	100
7	7	178/230 (77%)	171 (96%)	7 (4%)	0	100	100
8	8	173/227 (76%)	169 (98%)	4 (2%)	0	100	100
9	9	178/220 (81%)	176 (99%)	2 (1%)	0	100	100
10	A	739/752 (98%)	714 (97%)	25 (3%)	0	100	100
11	B	729/734 (99%)	710 (97%)	19 (3%)	0	100	100
12	C	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
13	D	135/141 (96%)	126 (93%)	8 (6%)	1 (1%)	18	17
14	E	59/64 (92%)	59 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	F	158/183 (86%)	153 (97%)	5 (3%)	0	100	100
16	I	31/36 (86%)	28 (90%)	3 (10%)	0	100	100
17	J	40/42 (95%)	40 (100%)	0	0	100	100
18	K	76/87 (87%)	73 (96%)	3 (4%)	0	100	100
19	L	148/153 (97%)	143 (97%)	5 (3%)	0	100	100
20	M	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
21	O	97/155 (63%)	96 (99%)	1 (1%)	0	100	100
22	R	90/139 (65%)	89 (99%)	1 (1%)	0	100	100
23	Z	151/279 (54%)	143 (95%)	7 (5%)	1 (1%)	18	17
24	a	169/215 (79%)	166 (98%)	3 (2%)	0	100	100
24	d	169/215 (79%)	166 (98%)	3 (2%)	0	100	100
25	b	174/218 (80%)	174 (100%)	0	0	100	100
26	c	213/257 (83%)	202 (95%)	11 (5%)	0	100	100
27	e	166/208 (80%)	164 (99%)	1 (1%)	1 (1%)	21	21
28	X	143/241 (59%)	142 (99%)	1 (1%)	0	100	100
All	All	5181/6241 (83%)	5028 (97%)	150 (3%)	3 (0%)	49	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	D	99	HIS
23	Z	179	LEU
27	e	47	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	1	129/163 (79%)	128 (99%)	1 (1%)	73	80
2	2	134/167 (80%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	151/182 (83%)	151 (100%)	0	100	100
4	4	139/167 (83%)	139 (100%)	0	100	100
5	5	139/166 (84%)	138 (99%)	1 (1%)	76	82
6	6	134/160 (84%)	133 (99%)	1 (1%)	76	82
7	7	139/176 (79%)	138 (99%)	1 (1%)	76	82
8	8	136/169 (80%)	136 (100%)	0	100	100
9	9	138/164 (84%)	137 (99%)	1 (1%)	76	82
10	A	607/617 (98%)	606 (100%)	1 (0%)	87	92
11	B	592/593 (100%)	589 (100%)	3 (0%)	81	87
12	C	66/67 (98%)	66 (100%)	0	100	100
13	D	114/117 (97%)	114 (100%)	0	100	100
14	E	56/59 (95%)	55 (98%)	1 (2%)	51	63
15	F	133/154 (86%)	133 (100%)	0	100	100
16	I	27/29 (93%)	27 (100%)	0	100	100
17	J	38/38 (100%)	38 (100%)	0	100	100
18	K	62/69 (90%)	62 (100%)	0	100	100
19	L	126/128 (98%)	126 (100%)	0	100	100
20	M	25/25 (100%)	25 (100%)	0	100	100
21	O	81/116 (70%)	81 (100%)	0	100	100
22	R	74/111 (67%)	74 (100%)	0	100	100
23	Z	117/205 (57%)	117 (100%)	0	100	100
24	a	128/153 (84%)	128 (100%)	0	100	100
24	d	128/153 (84%)	128 (100%)	0	100	100
25	b	144/173 (83%)	144 (100%)	0	100	100
26	c	169/195 (87%)	169 (100%)	0	100	100
27	e	133/162 (82%)	132 (99%)	1 (1%)	73	80
28	X	100/166 (60%)	99 (99%)	1 (1%)	68	77
All	All	4159/4844 (86%)	4147 (100%)	12 (0%)	84	90

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	B	80	ASN

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Mol	Chain	Res	Type
11	B	83	LYS
28	X	167	LYS
14	E	56	ASP
7	7	42	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
11	B	80	ASN
13	D	6	ASN
28	X	179	ASN
11	B	608	GLN
15	F	67	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

429 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
34	LHG	A	850	-	48,48,48	0.62	1 (2%)	51,54,54	1.25	5 (9%)
37	8CT	B	847	-	40,41,41	4.59	23 (57%)	50,56,56	2.86	25 (50%)
29	CLA	c	601	26	49,53,73	1.49	7 (14%)	59,89,113	1.45	5 (8%)
37	8CT	B	851	-	40,41,41	4.63	23 (57%)	50,56,56	2.79	18 (36%)
33	IHT	L	204	-	40,42,42	2.12	4 (10%)	53,58,58	1.84	16 (30%)
31	II0	7	316	-	39,43,43	2.80	4 (10%)	50,60,60	1.83	11 (22%)
29	CLA	L	202	19	64,68,73	1.28	8 (12%)	77,107,113	1.36	8 (10%)
31	II0	8	313	-	39,43,43	2.76	4 (10%)	50,60,60	1.36	6 (12%)
29	CLA	a	606	24	69,73,73	1.27	10 (14%)	83,113,113	1.21	7 (8%)
29	CLA	A	825	10	69,73,73	1.25	10 (14%)	83,113,113	1.31	5 (6%)
31	II0	O	205	-	39,43,43	2.89	4 (10%)	50,60,60	1.66	12 (24%)
29	CLA	d	607	24	69,73,73	1.26	9 (13%)	83,113,113	1.32	7 (8%)
33	IHT	2	616	-	40,42,42	2.07	3 (7%)	53,58,58	2.03	15 (28%)
29	CLA	3	306	29,3	59,63,73	1.35	7 (11%)	71,101,113	1.35	6 (8%)
29	CLA	5	608	5	64,68,73	1.29	9 (14%)	77,107,113	1.33	9 (11%)
29	CLA	d	602	24	68,72,73	1.25	8 (11%)	81,111,113	1.31	8 (9%)
29	CLA	c	602	26	69,73,73	1.24	8 (11%)	83,113,113	1.26	8 (9%)
30	KC2	1	610	1	49,53,53	1.76	10 (20%)	62,89,89	2.15	16 (25%)
29	CLA	A	854	-	69,73,73	1.24	8 (11%)	83,113,113	1.40	7 (8%)
29	CLA	A	834	10	59,63,73	1.35	7 (11%)	71,101,113	1.37	7 (9%)
39	SF4	C	101	12	0,12,12	-	-	-	-	-
29	CLA	d	608	24	69,73,73	1.25	8 (11%)	83,113,113	1.29	8 (9%)
29	CLA	A	803	10	69,73,73	1.23	8 (11%)	83,113,113	1.40	7 (8%)
29	CLA	8	304	8	54,58,73	1.40	7 (12%)	65,95,113	1.41	8 (12%)
31	II0	4	615	-	39,43,43	2.82	4 (10%)	50,60,60	1.79	13 (26%)
29	CLA	F	202	15	59,63,73	1.35	8 (13%)	71,101,113	1.35	7 (9%)
31	II0	3	314	-	39,43,43	2.65	4 (10%)	50,60,60	1.54	8 (16%)
29	CLA	8	302	8	69,73,73	1.26	9 (13%)	83,113,113	1.26	7 (8%)
29	CLA	4	602	4	63,67,73	1.30	8 (12%)	75,105,113	1.32	8 (10%)
35	LMG	3	319	29	30,30,55	1.04	0	38,38,63	1.22	5 (13%)
29	CLA	9	312	9	45,49,73	1.52	9 (20%)	54,84,113	1.51	7 (12%)
31	II0	c	616	-	39,43,43	2.75	4 (10%)	50,60,60	1.61	9 (18%)
29	CLA	O	204	-	59,63,73	1.35	8 (13%)	71,101,113	1.35	6 (8%)
29	CLA	1	609	34	45,49,73	1.53	8 (17%)	54,84,113	1.51	5 (9%)
29	CLA	8	308	-	69,73,73	1.24	9 (13%)	83,113,113	1.26	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	A	829	10	54,58,73	1.40	9 (16%)	65,95,113	1.45	8 (12%)
31	II0	d	614	-	39,43,43	2.73	4 (10%)	50,60,60	1.61	10 (20%)
29	CLA	B	829	11	69,73,73	1.27	7 (10%)	83,113,113	1.35	7 (8%)
31	II0	6	614	-	39,43,43	2.70	4 (10%)	50,60,60	1.67	10 (20%)
31	II0	R	201	-	39,43,43	2.86	4 (10%)	50,60,60	1.77	10 (20%)
29	CLA	A	842	10	69,73,73	1.23	7 (10%)	83,113,113	1.37	9 (10%)
29	CLA	B	833	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
31	II0	5	616	-	39,43,43	2.82	4 (10%)	50,60,60	1.81	14 (28%)
35	LMG	6	617	-	32,32,55	1.06	3 (9%)	40,40,63	1.27	5 (12%)
34	LHG	e	617	29	27,27,48	0.85	1 (3%)	30,33,54	1.23	2 (6%)
29	CLA	3	310	35	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
30	KC2	c	614	30	49,53,53	1.82	9 (18%)	62,89,89	2.01	15 (24%)
29	CLA	b	602	25	68,72,73	1.25	8 (11%)	81,111,113	1.34	10 (12%)
31	II0	2	615	-	39,43,43	2.77	5 (12%)	50,60,60	1.65	14 (28%)
31	II0	9	316	-	39,43,43	2.79	4 (10%)	50,60,60	1.70	10 (20%)
30	KC2	7	310	7	49,53,53	1.75	10 (20%)	62,89,89	2.18	18 (29%)
34	LHG	A	851	29	38,38,48	0.69	1 (2%)	41,44,54	1.30	5 (12%)
34	LHG	c	622	29	20,20,48	0.78	0	22,25,54	1.30	2 (9%)
29	CLA	B	813	11	69,73,73	1.26	10 (14%)	83,113,113	1.25	7 (8%)
29	CLA	a	604	24	64,68,73	1.30	9 (14%)	77,107,113	1.37	7 (9%)
37	8CT	B	843	-	40,41,41	4.60	23 (57%)	50,56,56	2.98	20 (40%)
29	CLA	a	605	24	59,63,73	1.36	8 (13%)	71,101,113	1.32	6 (8%)
29	CLA	B	807	11	69,73,73	1.24	9 (13%)	83,113,113	1.31	7 (8%)
29	CLA	c	607	26	69,73,73	1.26	8 (11%)	83,113,113	1.31	5 (6%)
29	CLA	A	833	10	69,73,73	1.25	8 (11%)	83,113,113	1.25	5 (6%)
29	CLA	e	610	-	55,59,73	1.41	8 (14%)	66,96,113	1.38	5 (7%)
29	CLA	7	311	-	59,63,73	1.35	8 (13%)	71,101,113	1.36	6 (8%)
34	LHG	8	315	-	32,32,48	0.75	1 (3%)	35,38,54	1.22	3 (8%)
33	IHT	1	618	-	40,42,42	2.03	3 (7%)	53,58,58	2.15	19 (35%)
29	CLA	c	603	31,26	69,73,73	1.25	8 (11%)	83,113,113	1.26	9 (10%)
30	KC2	d	610	24	49,53,53	1.76	10 (20%)	62,89,89	2.18	19 (30%)
29	CLA	A	802	29,10	59,63,73	1.35	8 (13%)	71,101,113	1.32	6 (8%)
31	II0	R	204	-	39,43,43	2.88	4 (10%)	50,60,60	1.65	10 (20%)
29	CLA	4	606	4	64,68,73	1.30	8 (12%)	77,107,113	1.27	6 (7%)
34	LHG	3	321	-	48,48,48	0.60	0	51,54,54	1.27	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	II0	2	613	-	39,43,43	2.71	4 (10%)	50,60,60	1.69	11 (22%)
29	CLA	A	813	10	46,50,73	1.48	7 (15%)	55,85,113	1.46	5 (9%)
29	CLA	A	836	10	59,63,73	1.36	8 (13%)	71,101,113	1.31	5 (7%)
33	IHT	6	616	-	40,42,42	1.99	2 (5%)	53,58,58	1.69	11 (20%)
29	CLA	8	305	8	59,63,73	1.35	9 (15%)	71,101,113	1.39	8 (11%)
29	CLA	d	611	-	54,58,73	1.42	8 (14%)	65,95,113	1.40	8 (12%)
29	CLA	a	607	24	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
29	CLA	A	826	10	69,73,73	1.25	7 (10%)	83,113,113	1.24	6 (7%)
37	8CT	Z	307	-	40,41,41	4.68	23 (57%)	50,56,56	2.26	19 (38%)
29	CLA	2	602	2	63,67,73	1.29	8 (12%)	75,105,113	1.36	6 (8%)
29	CLA	B	821	11	64,68,73	1.30	8 (12%)	77,107,113	1.36	8 (10%)
29	CLA	A	824	-	69,73,73	1.25	8 (11%)	83,113,113	1.31	8 (9%)
29	CLA	A	822	10	69,73,73	1.26	9 (13%)	83,113,113	1.25	6 (7%)
31	II0	7	317	-	39,43,43	2.83	4 (10%)	50,60,60	1.66	10 (20%)
33	IHT	c	620	-	40,42,42	2.20	3 (7%)	53,58,58	1.98	15 (28%)
29	CLA	3	309	3	64,68,73	1.31	10 (15%)	77,107,113	1.26	7 (9%)
29	CLA	e	604	-	64,68,73	1.30	8 (12%)	77,107,113	1.36	5 (6%)
29	CLA	B	839	11	69,73,73	1.25	8 (11%)	83,113,113	1.28	5 (6%)
31	II0	5	617	-	39,43,43	2.77	4 (10%)	50,60,60	1.60	9 (18%)
29	CLA	a	601	24	49,53,73	1.50	7 (14%)	59,89,113	1.41	4 (6%)
29	CLA	K	102	18	59,63,73	1.36	10 (16%)	71,101,113	1.32	5 (7%)
29	CLA	b	608	34	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
30	KC2	6	610	6	49,53,53	1.78	10 (20%)	62,89,89	2.21	19 (30%)
30	KC2	c	610	26	49,53,53	1.76	10 (20%)	62,89,89	2.15	20 (32%)
31	II0	7	315	-	39,43,43	2.64	4 (10%)	50,60,60	1.61	8 (16%)
31	II0	3	318	-	39,43,43	2.75	4 (10%)	50,60,60	1.67	11 (22%)
31	II0	c	618	-	39,43,43	2.74	4 (10%)	50,60,60	1.58	7 (14%)
29	CLA	a	603	24	64,68,73	1.29	8 (12%)	77,107,113	1.29	5 (6%)
29	CLA	4	610	4	69,73,73	1.25	8 (11%)	83,113,113	1.34	8 (9%)
29	CLA	6	611	-	59,63,73	1.35	8 (13%)	71,101,113	1.40	6 (8%)
29	CLA	1	606	1	49,53,73	1.48	8 (16%)	59,89,113	1.40	7 (11%)
29	CLA	Z	303	29,23	59,63,73	1.35	8 (13%)	71,101,113	1.34	6 (8%)
29	CLA	X	301	-	56,60,73	1.39	9 (16%)	67,97,113	1.35	5 (7%)
29	CLA	A	831	10	69,73,73	1.24	9 (13%)	83,113,113	1.28	6 (7%)
31	II0	c	619	-	39,43,43	2.86	4 (10%)	50,60,60	1.75	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	6	608	6	64,68,73	1.29	8 (12%)	77,107,113	1.32	7 (9%)
29	CLA	a	611	-	59,63,73	1.35	8 (13%)	71,101,113	1.37	5 (7%)
31	II0	a	614	-	39,43,43	2.75	4 (10%)	50,60,60	1.52	8 (16%)
29	CLA	1	603	1	56,60,73	1.38	8 (14%)	67,97,113	1.43	6 (8%)
29	CLA	8	307	8	45,49,73	1.52	8 (17%)	54,84,113	1.53	5 (9%)
29	CLA	e	606	27	64,68,73	1.28	8 (12%)	77,107,113	1.32	7 (9%)
37	8CT	A	847	-	40,41,41	4.57	23 (57%)	50,56,56	2.87	22 (44%)
37	8CT	7	318	-	40,41,41	1.64	8 (20%)	50,56,56	1.68	11 (22%)
30	KC2	6	613	6	49,53,53	1.76	10 (20%)	62,89,89	2.16	16 (25%)
31	II0	9	323	-	39,43,43	2.86	4 (10%)	50,60,60	1.67	9 (18%)
31	II0	c	621	29	39,43,43	2.82	5 (12%)	50,60,60	1.78	14 (28%)
31	II0	9	317	-	39,43,43	2.74	4 (10%)	50,60,60	1.63	11 (22%)
29	CLA	B	814	11	60,64,73	1.34	8 (13%)	72,102,113	1.38	5 (6%)
29	CLA	5	613	5	45,49,73	1.54	7 (15%)	54,84,113	1.46	5 (9%)
36	SQD	a	618	-	41,42,54	1.69	7 (17%)	50,53,65	1.48	6 (12%)
38	DGD	9	322	-	61,61,67	0.95	2 (3%)	75,75,81	1.36	9 (12%)
30	KC2	e	605	27	49,53,53	1.77	9 (18%)	62,89,89	2.17	18 (29%)
29	CLA	a	602	24	59,63,73	1.35	8 (13%)	71,101,113	1.33	6 (8%)
29	CLA	B	836	11	69,73,73	1.23	8 (11%)	83,113,113	1.39	8 (9%)
29	CLA	c	606	26	69,73,73	1.27	9 (13%)	83,113,113	1.25	7 (8%)
37	8CT	B	844	-	40,41,41	4.64	23 (57%)	50,56,56	2.83	20 (40%)
29	CLA	B	837	11	51,55,73	1.43	8 (15%)	61,91,113	1.48	7 (11%)
35	LMG	X	302	-	34,34,55	0.94	0	42,42,63	1.22	4 (9%)
29	CLA	3	304	3	64,68,73	1.29	8 (12%)	77,107,113	1.26	9 (11%)
29	CLA	B	805	11	69,73,73	1.23	6 (8%)	83,113,113	1.33	8 (9%)
37	8CT	Z	308	-	40,41,41	4.61	23 (57%)	50,56,56	2.67	20 (40%)
31	II0	d	616	-	39,43,43	2.76	4 (10%)	50,60,60	1.96	13 (26%)
32	II3	1	615	-	40,43,43	1.99	3 (7%)	47,60,60	1.63	9 (19%)
29	CLA	a	612	24	69,73,73	1.26	8 (11%)	83,113,113	1.26	9 (10%)
32	II3	e	613	-	40,43,43	2.03	2 (5%)	47,60,60	1.71	9 (19%)
29	CLA	9	302	9	49,53,73	1.49	6 (12%)	59,89,113	1.45	5 (8%)
29	CLA	A	837	10	69,73,73	1.27	9 (13%)	83,113,113	1.38	9 (10%)
29	CLA	e	611	27	69,73,73	1.26	8 (11%)	83,113,113	1.29	6 (7%)
34	LHG	O	208	-	39,39,48	0.74	1 (2%)	43,44,54	1.58	7 (16%)
37	8CT	M	101	-	40,41,41	4.61	23 (57%)	50,56,56	3.02	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	816	11	69,73,73	1.24	9 (13%)	83,113,113	1.29	9 (10%)
29	CLA	A	811	10	69,73,73	1.27	9 (13%)	83,113,113	1.29	8 (9%)
29	CLA	B	811	11	64,68,73	1.29	8 (12%)	77,107,113	1.24	6 (7%)
29	CLA	5	604	5	59,63,73	1.33	9 (15%)	71,101,113	1.39	9 (12%)
29	CLA	B	808	11	69,73,73	1.23	9 (13%)	83,113,113	1.43	8 (9%)
29	CLA	e	602	27	59,63,73	1.34	8 (13%)	71,101,113	1.38	8 (11%)
29	CLA	B	840	34	69,73,73	1.25	8 (11%)	83,113,113	1.31	10 (12%)
35	LMG	8	314	-	52,52,55	0.78	1 (1%)	60,60,63	1.36	7 (11%)
34	LHG	2	617	29	21,21,48	0.78	1 (4%)	23,26,54	1.25	2 (8%)
29	CLA	5	603	5	49,53,73	1.48	7 (14%)	59,89,113	1.41	6 (10%)
29	CLA	B	823	11	69,73,73	1.26	10 (14%)	83,113,113	1.28	5 (6%)
29	CLA	d	603	24	54,58,73	1.41	8 (14%)	65,95,113	1.39	7 (10%)
29	CLA	e	601	27	49,53,73	1.49	8 (16%)	59,89,113	1.43	4 (6%)
34	LHG	4	620	-	44,44,48	0.65	1 (2%)	47,50,54	1.23	4 (8%)
37	8CT	B	846	-	40,41,41	4.60	23 (57%)	50,56,56	2.80	19 (38%)
29	CLA	2	607	2	49,53,73	1.49	9 (18%)	59,89,113	1.40	6 (10%)
30	KC2	5	610	5	49,53,53	1.77	11 (22%)	62,89,89	2.17	18 (29%)
29	CLA	4	601	4	59,63,73	1.35	9 (15%)	71,101,113	1.40	8 (11%)
29	CLA	B	804	11	49,53,73	1.47	9 (18%)	59,89,113	1.52	6 (10%)
29	CLA	O	201	34	59,63,73	1.35	8 (13%)	71,101,113	1.38	8 (11%)
29	CLA	B	817	11	63,67,73	1.31	8 (12%)	75,105,113	1.33	7 (9%)
29	CLA	3	312	3	54,58,73	1.42	8 (14%)	65,95,113	1.50	7 (10%)
34	LHG	L	206	-	20,21,48	0.80	1 (5%)	22,23,54	1.22	2 (9%)
29	CLA	9	314	9	49,53,73	1.49	8 (16%)	59,89,113	1.45	6 (10%)
29	CLA	Z	302	-	64,68,73	1.29	8 (12%)	77,107,113	1.31	6 (7%)
31	II0	8	311	-	39,43,43	2.73	4 (10%)	50,60,60	1.69	13 (26%)
30	KC2	c	611	26,30	49,53,53	1.77	10 (20%)	62,89,89	2.09	15 (24%)
31	II0	2	614	-	39,43,43	2.66	4 (10%)	50,60,60	1.62	7 (14%)
39	SF4	C	102	12	0,12,12	-	-	-	-	-
29	CLA	B	824	-	69,73,73	1.25	10 (14%)	83,113,113	1.30	5 (6%)
29	CLA	2	608	2	64,68,73	1.29	10 (15%)	77,107,113	1.32	6 (7%)
37	8CT	K	103	-	40,41,41	4.62	23 (57%)	50,56,56	2.63	21 (42%)
29	CLA	B	838	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
29	CLA	3	311	3	69,73,73	1.24	8 (11%)	83,113,113	1.28	4 (4%)
29	CLA	4	611	4	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	II0	4	614	-	39,43,43	2.73	4 (10%)	50,60,60	1.67	9 (18%)
29	CLA	1	607	1	49,53,73	1.49	9 (18%)	59,89,113	1.44	6 (10%)
34	LHG	Z	311	-	45,45,48	0.63	1 (2%)	48,51,54	1.22	4 (8%)
36	SQD	3	320	-	35,36,54	1.76	7 (20%)	44,47,65	1.47	6 (13%)
31	II0	3	315	-	39,43,43	2.65	4 (10%)	50,60,60	1.53	8 (16%)
31	II0	1	614	-	39,43,43	2.63	4 (10%)	50,60,60	1.61	8 (16%)
29	CLA	6	606	6	59,63,73	1.36	8 (13%)	71,101,113	1.33	7 (9%)
29	CLA	Z	305	23	64,68,73	1.30	9 (14%)	77,107,113	1.29	4 (5%)
29	CLA	e	607	27	49,53,73	1.48	8 (16%)	59,89,113	1.46	7 (11%)
29	CLA	d	606	24	45,49,73	1.54	9 (20%)	54,84,113	1.42	7 (12%)
34	LHG	A	852	-	22,22,48	0.82	0	25,27,54	1.28	2 (8%)
30	KC2	2	610	2	49,53,53	1.78	10 (20%)	62,89,89	2.19	18 (29%)
31	II0	e	614	-	39,43,43	2.78	4 (10%)	50,60,60	1.69	8 (16%)
29	CLA	9	313	9	49,53,73	1.50	9 (18%)	59,89,113	1.38	4 (6%)
29	CLA	A	832	10	69,73,73	1.23	9 (13%)	83,113,113	1.28	9 (10%)
29	CLA	b	610	25	55,59,73	1.40	8 (14%)	66,96,113	1.43	7 (10%)
29	CLA	7	312	7	54,58,73	1.42	9 (16%)	65,95,113	1.46	7 (10%)
29	CLA	O	203	21	59,63,73	1.36	9 (15%)	71,101,113	1.37	7 (9%)
31	II0	e	615	-	39,43,43	2.77	4 (10%)	50,60,60	1.58	9 (18%)
29	CLA	B	819	-	64,68,73	1.30	9 (14%)	77,107,113	1.34	7 (9%)
37	8CT	L	205	-	40,41,41	4.60	23 (57%)	50,56,56	2.85	21 (42%)
29	CLA	5	612	5	49,53,73	1.49	7 (14%)	59,89,113	1.45	6 (10%)
33	IHT	5	618	-	40,42,42	2.00	2 (5%)	53,58,58	1.94	13 (24%)
29	CLA	A	807	10	54,58,73	1.38	7 (12%)	65,95,113	1.49	7 (10%)
33	IHT	a	616	-	40,42,42	2.05	3 (7%)	53,58,58	1.81	15 (28%)
29	CLA	1	611	1	49,53,73	1.48	8 (16%)	59,89,113	1.50	5 (8%)
35	LMG	2	618	-	36,36,55	0.84	0	44,44,63	1.35	6 (13%)
29	CLA	e	603	27	54,58,73	1.41	8 (14%)	65,95,113	1.42	9 (13%)
31	II0	a	619	-	39,43,43	2.82	4 (10%)	50,60,60	1.69	10 (20%)
34	LHG	c	623	-	34,34,48	0.73	1 (2%)	37,40,54	1.31	5 (13%)
36	SQD	3	322	-	35,36,54	1.76	7 (20%)	44,47,65	1.57	7 (15%)
29	CLA	R	202	22	59,63,73	1.36	8 (13%)	71,101,113	1.46	9 (12%)
32	II3	b	613	-	40,43,43	2.00	3 (7%)	47,60,60	1.67	12 (25%)
29	CLA	1	602	1	63,67,73	1.29	7 (11%)	75,105,113	1.34	6 (8%)
29	CLA	7	306	7	49,53,73	1.49	8 (16%)	59,89,113	1.44	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	d	604	24	64,68,73	1.30	7 (10%)	77,107,113	1.31	7 (9%)
31	II0	8	310	-	39,43,43	2.75	4 (10%)	50,60,60	1.68	11 (22%)
29	CLA	A	828	10	69,73,73	1.24	10 (14%)	83,113,113	1.24	7 (8%)
34	LHG	4	617	29	48,48,48	0.64	1 (2%)	51,54,54	1.33	8 (15%)
30	KC2	7	313	-	49,53,53	1.76	10 (20%)	62,89,89	2.12	18 (29%)
29	CLA	B	809	11	69,73,73	1.25	9 (13%)	83,113,113	1.36	9 (10%)
29	CLA	B	834	-	49,53,73	1.48	9 (18%)	59,89,113	1.49	7 (11%)
29	CLA	7	309	34	45,49,73	1.52	7 (15%)	54,84,113	1.50	5 (9%)
29	CLA	L	201	19	55,59,73	1.39	8 (14%)	66,96,113	1.41	6 (9%)
34	LHG	L	207	-	32,32,48	0.72	1 (3%)	35,37,54	1.34	5 (14%)
31	II0	J	102	-	39,43,43	2.73	4 (10%)	50,60,60	1.66	9 (18%)
29	CLA	1	604	1	49,53,73	1.48	7 (14%)	59,89,113	1.49	5 (8%)
29	CLA	1	605	1	45,50,73	1.53	9 (20%)	53,85,113	1.38	4 (7%)
29	CLA	B	828	11	69,73,73	1.24	9 (13%)	83,113,113	1.21	8 (9%)
29	CLA	A	839	-	69,73,73	1.26	9 (13%)	83,113,113	1.25	7 (8%)
29	CLA	9	315	-	45,49,73	1.53	7 (15%)	54,84,113	1.51	6 (11%)
29	CLA	2	611	2	54,58,73	1.42	9 (16%)	65,95,113	1.40	7 (10%)
29	CLA	3	308	3	64,68,73	1.29	9 (14%)	77,107,113	1.39	6 (7%)
29	CLA	B	820	11	64,68,73	1.31	9 (14%)	77,107,113	1.31	8 (10%)
29	CLA	L	203	-	54,58,73	1.41	8 (14%)	65,95,113	1.42	7 (10%)
34	LHG	5	619	29	22,22,48	0.84	0	25,28,54	1.28	2 (8%)
29	CLA	9	306	9	49,53,73	1.50	9 (18%)	59,89,113	1.36	6 (10%)
29	CLA	1	612	1	64,68,73	1.31	8 (12%)	77,107,113	1.29	6 (7%)
31	II0	a	615	-	39,43,43	2.82	5 (12%)	50,60,60	1.69	9 (18%)
29	CLA	7	303	7	69,73,73	1.24	8 (11%)	83,113,113	1.31	10 (12%)
29	CLA	a	608	24	64,68,73	1.30	7 (10%)	77,107,113	1.33	9 (11%)
33	IHT	8	309	-	40,42,42	2.09	3 (7%)	53,58,58	2.11	16 (30%)
34	LHG	M	102	-	23,23,48	0.93	1 (4%)	27,28,54	1.77	3 (11%)
29	CLA	9	304	9	49,53,73	1.48	9 (18%)	59,89,113	1.42	7 (11%)
29	CLA	6	604	6	64,68,73	1.29	7 (10%)	77,107,113	1.34	7 (9%)
30	KC2	9	311	9	49,53,53	1.76	10 (20%)	62,89,89	2.14	17 (27%)
29	CLA	5	611	5	49,53,73	1.48	7 (14%)	59,89,113	1.45	5 (8%)
29	CLA	4	609	4	64,68,73	1.30	8 (12%)	77,107,113	1.34	4 (5%)
31	II0	b	612	-	39,43,43	2.69	4 (10%)	50,60,60	1.56	9 (18%)
37	8CT	J	104	-	40,41,41	4.60	23 (57%)	50,56,56	2.72	24 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	8CT	B	845	-	40,41,41	4.67	23 (57%)	50,56,56	2.46	18 (36%)
29	CLA	A	801	10	69,73,73	1.23	8 (11%)	83,113,113	1.32	8 (9%)
29	CLA	5	602	5	59,63,73	1.33	8 (13%)	71,101,113	1.36	6 (8%)
29	CLA	b	604	25	62,66,73	1.31	8 (12%)	74,104,113	1.39	6 (8%)
34	LHG	4	618	-	48,48,48	0.58	0	51,54,54	1.27	6 (11%)
29	CLA	1	608	1	64,68,73	1.30	7 (10%)	77,107,113	1.35	8 (10%)
29	CLA	B	822	11	64,68,73	1.28	8 (12%)	77,107,113	1.32	7 (9%)
29	CLA	e	608	34	45,49,73	1.53	9 (20%)	54,84,113	1.48	7 (12%)
29	CLA	7	302	7	49,53,73	1.48	8 (16%)	59,89,113	1.46	4 (6%)
34	LHG	B	801	-	39,39,48	0.73	1 (2%)	43,44,54	1.59	5 (11%)
29	CLA	b	607	25	64,68,73	1.30	7 (10%)	77,107,113	1.33	7 (9%)
29	CLA	c	613	26	49,53,73	1.50	7 (14%)	59,89,113	1.46	4 (6%)
29	CLA	A	810	10	69,73,73	1.26	8 (11%)	83,113,113	1.33	8 (9%)
29	CLA	9	305	-	59,63,73	1.35	9 (15%)	71,101,113	1.37	7 (9%)
29	CLA	9	310	-	45,49,73	1.52	7 (15%)	54,84,113	1.54	6 (11%)
31	II0	5	620	-	39,43,43	2.80	4 (10%)	50,60,60	1.89	14 (28%)
32	II3	8	312	-	40,43,43	2.05	2 (5%)	47,60,60	1.94	14 (29%)
29	CLA	B	810	11	69,73,73	1.26	9 (13%)	83,113,113	1.29	7 (8%)
29	CLA	B	825	-	64,68,73	1.28	8 (12%)	77,107,113	1.35	11 (14%)
29	CLA	A	816	10	64,68,73	1.28	8 (12%)	77,107,113	1.34	6 (7%)
29	CLA	Z	304	23	54,58,73	1.43	9 (16%)	65,95,113	1.40	6 (9%)
29	CLA	d	612	24	67,71,73	1.27	7 (10%)	80,110,113	1.32	6 (7%)
34	LHG	7	320	-	30,30,48	0.76	1 (3%)	33,36,54	1.18	3 (9%)
31	II0	1	616	-	39,43,43	2.79	4 (10%)	50,60,60	1.93	11 (22%)
29	CLA	1	601	1	49,53,73	1.50	7 (14%)	59,89,113	1.50	5 (8%)
29	CLA	8	301	8	49,53,73	1.48	9 (18%)	59,89,113	1.45	6 (10%)
29	CLA	B	827	11	69,73,73	1.24	8 (11%)	83,113,113	1.27	6 (7%)
29	CLA	B	818	11	64,68,73	1.30	9 (14%)	77,107,113	1.29	9 (11%)
36	SQD	B	850	-	32,33,54	1.85	8 (25%)	41,44,65	1.67	8 (19%)
34	LHG	9	321	-	35,35,48	0.78	2 (5%)	39,40,54	1.61	5 (12%)
37	8CT	R	203	-	40,41,41	4.61	23 (57%)	50,56,56	2.88	22 (44%)
29	CLA	2	604	2	59,63,73	1.37	8 (13%)	71,101,113	1.47	8 (11%)
31	II0	3	316	-	39,43,43	2.81	4 (10%)	50,60,60	2.05	14 (28%)
29	CLA	2	605	2	64,68,73	1.29	7 (10%)	77,107,113	1.36	5 (6%)
29	CLA	6	602	6	69,73,73	1.23	8 (11%)	83,113,113	1.29	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	PQN	A	849	-	34,34,34	1.58	2 (5%)	42,45,45	1.22	5 (11%)
29	CLA	3	305	3	69,73,73	1.24	8 (11%)	83,113,113	1.28	7 (8%)
29	CLA	4	608	34	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
29	CLA	6	612	6	49,53,73	1.50	8 (16%)	59,89,113	1.39	6 (10%)
29	CLA	a	609	34	64,68,73	1.31	8 (12%)	77,107,113	1.32	7 (9%)
33	IHT	d	617	-	40,42,42	2.08	3 (7%)	53,58,58	1.93	15 (28%)
29	CLA	8	317	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	6 (7%)
29	CLA	A	817	10	69,73,73	1.26	9 (13%)	83,113,113	1.27	8 (9%)
29	CLA	3	303	3	59,63,73	1.34	9 (15%)	71,101,113	1.38	8 (11%)
31	II0	7	314	-	39,43,43	2.65	4 (10%)	50,60,60	1.69	12 (24%)
29	CLA	B	815	11	46,50,73	1.48	9 (19%)	55,85,113	1.42	5 (9%)
29	CLA	9	309	9	59,63,73	1.35	8 (13%)	71,101,113	1.37	6 (8%)
31	II0	9	319	-	39,43,43	2.78	4 (10%)	50,60,60	1.46	6 (12%)
29	CLA	4	604	-	59,63,73	1.36	8 (13%)	71,101,113	1.42	10 (14%)
29	CLA	B	830	11	49,53,73	1.47	8 (16%)	59,89,113	1.44	6 (10%)
34	LHG	4	619	29	44,44,48	0.62	1 (2%)	47,50,54	1.26	5 (10%)
29	CLA	8	306	8	49,53,73	1.48	8 (16%)	59,89,113	1.48	4 (6%)
37	8CT	F	203	-	40,41,41	4.61	23 (57%)	50,56,56	2.95	22 (44%)
31	II0	9	318	-	39,43,43	2.84	4 (10%)	50,60,60	1.75	13 (26%)
29	CLA	5	605	5	49,53,73	1.49	7 (14%)	59,89,113	1.45	6 (10%)
29	CLA	A	815	10	66,70,73	1.25	8 (12%)	79,109,113	1.32	8 (10%)
29	CLA	5	601	5	45,49,73	1.53	8 (17%)	54,84,113	1.48	5 (9%)
29	CLA	b	603	25	64,68,73	1.30	7 (10%)	77,107,113	1.31	8 (10%)
34	LHG	b	616	29	29,29,48	0.74	1 (3%)	32,35,54	1.22	3 (9%)
29	CLA	b	611	25	59,63,73	1.35	8 (13%)	71,101,113	1.36	7 (9%)
34	LHG	5	621	29	34,34,48	0.74	2 (5%)	37,40,54	1.24	4 (10%)
29	CLA	d	605	24	49,53,73	1.48	8 (16%)	59,89,113	1.43	6 (10%)
29	CLA	2	601	2	46,50,73	1.51	9 (19%)	55,85,113	1.48	5 (9%)
29	CLA	A	808	10	59,63,73	1.34	9 (15%)	71,101,113	1.35	8 (11%)
29	CLA	d	609	-	45,49,73	1.52	7 (15%)	54,84,113	1.51	7 (12%)
29	CLA	A	812	10	59,63,73	1.37	9 (15%)	71,101,113	1.37	9 (12%)
29	CLA	A	819	-	69,73,73	1.28	8 (11%)	83,113,113	1.41	8 (9%)
29	CLA	c	612	26	59,63,73	1.37	7 (11%)	71,101,113	1.35	7 (9%)
29	CLA	A	827	10	69,73,73	1.24	8 (11%)	83,113,113	1.24	11 (13%)
29	CLA	9	307	9	61,65,73	1.33	8 (13%)	73,103,113	1.28	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	802	-	59,63,73	1.34	8 (13%)	71,101,113	1.30	6 (8%)
30	KC2	4	605	4	49,53,53	1.77	10 (20%)	62,89,89	2.14	17 (27%)
29	CLA	9	303	9	59,63,73	1.34	8 (13%)	71,101,113	1.37	5 (7%)
29	CLA	K	101	-	69,73,73	1.23	8 (11%)	83,113,113	1.37	9 (10%)
33	IHT	9	320	-	40,42,42	2.06	3 (7%)	53,58,58	2.06	13 (24%)
29	CLA	A	821	10	59,63,73	1.36	9 (15%)	71,101,113	1.35	7 (9%)
31	II0	c	617	-	39,43,43	2.70	4 (10%)	50,60,60	1.44	9 (18%)
34	LHG	3	301	29	41,41,48	0.66	1 (2%)	44,47,54	1.23	4 (9%)
36	SQD	O	207	-	28,29,54	1.91	7 (25%)	37,40,65	1.66	6 (16%)
29	CLA	A	843	-	69,73,73	1.26	9 (13%)	83,113,113	1.22	6 (7%)
29	CLA	B	806	11	69,73,73	1.25	8 (11%)	83,113,113	1.29	9 (10%)
29	CLA	6	603	6	49,53,73	1.48	9 (18%)	59,89,113	1.44	7 (11%)
34	LHG	1	619	29	34,34,48	0.66	0	37,40,54	1.27	4 (10%)
29	CLA	7	307	7	49,53,73	1.47	8 (16%)	59,89,113	1.50	4 (6%)
34	LHG	L	208	-	33,33,48	0.73	0	36,39,54	1.25	4 (11%)
29	CLA	c	609	34	45,49,73	1.51	7 (15%)	54,84,113	1.51	6 (11%)
31	II0	e	612	-	39,43,43	2.87	4 (10%)	50,60,60	1.75	15 (30%)
29	CLA	d	601	24	49,53,73	1.48	9 (18%)	59,89,113	1.43	4 (6%)
29	CLA	6	609	34	45,49,73	1.52	7 (15%)	54,84,113	1.53	7 (12%)
31	II0	4	612	-	39,43,43	2.65	4 (10%)	50,60,60	1.56	8 (16%)
31	II0	b	614	-	39,43,43	2.84	4 (10%)	50,60,60	1.50	9 (18%)
30	KC2	3	307	34	49,53,53	1.79	12 (24%)	62,89,89	2.19	19 (30%)
31	II0	O	206	-	39,43,43	2.76	4 (10%)	50,60,60	1.58	8 (16%)
34	LHG	8	316	-	48,48,48	0.60	0	51,54,54	1.25	6 (11%)
37	8CT	b	615	-	40,41,41	1.62	8 (20%)	50,56,56	1.52	9 (18%)
29	CLA	B	841	11	69,73,73	1.24	7 (10%)	83,113,113	1.32	9 (10%)
29	CLA	O	202	-	45,49,73	1.51	6 (13%)	54,84,113	1.52	7 (12%)
30	KC2	b	609	25	49,53,53	1.79	10 (20%)	62,89,89	2.19	19 (30%)
29	CLA	B	803	11	69,73,73	1.22	9 (13%)	83,113,113	1.37	6 (7%)
34	LHG	7	319	29	38,38,48	0.67	1 (2%)	41,44,54	1.17	3 (7%)
37	8CT	I	101	-	40,41,41	4.64	23 (57%)	50,56,56	2.57	19 (38%)
29	CLA	2	603	2	54,58,73	1.40	8 (14%)	65,95,113	1.46	11 (16%)
31	II0	5	615	-	39,43,43	2.81	4 (10%)	50,60,60	1.81	13 (26%)
29	CLA	3	302	3	49,53,73	1.48	8 (16%)	59,89,113	1.43	6 (10%)
37	8CT	4	616	-	40,41,41	1.68	8 (20%)	50,56,56	1.69	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	1	613	1	49,53,73	1.50	9 (18%)	59,89,113	1.44	6 (10%)
29	CLA	4	607	4	64,68,73	1.30	9 (14%)	77,107,113	1.33	9 (11%)
29	CLA	B	835	11	59,63,73	1.35	8 (13%)	71,101,113	1.33	9 (12%)
31	II0	7	301	-	39,43,43	2.72	4 (10%)	50,60,60	1.64	12 (24%)
29	CLA	A	805	10	54,58,73	1.42	8 (14%)	65,95,113	1.37	8 (12%)
36	SQD	7	321	-	35,36,54	1.78	7 (20%)	44,47,65	1.55	6 (13%)
30	KC2	a	610	24	49,53,53	1.75	10 (20%)	62,89,89	2.18	18 (29%)
29	CLA	4	603	4	58,62,73	1.35	7 (12%)	69,99,113	1.40	10 (14%)
35	LMG	F	204	-	32,32,55	0.94	1 (3%)	40,40,63	1.35	6 (15%)
31	II0	a	613	-	39,43,43	2.77	4 (10%)	50,60,60	1.72	12 (24%)
31	II0	d	613	-	39,43,43	2.73	4 (10%)	50,60,60	1.66	9 (18%)
30	KC2	e	609	27	49,53,53	1.76	10 (20%)	62,89,89	2.16	18 (29%)
31	II0	3	317	-	39,43,43	2.75	4 (10%)	50,60,60	1.58	8 (16%)
29	CLA	5	607	5	49,53,73	1.50	8 (16%)	59,89,113	1.47	5 (8%)
29	CLA	A	855	-	64,68,73	1.30	8 (12%)	77,107,113	1.31	7 (9%)
31	II0	6	615	-	39,43,43	2.79	4 (10%)	50,60,60	1.71	14 (28%)
39	SF4	A	848	11,10	0,12,12	-	-	-	-	-
29	CLA	B	826	11	69,73,73	1.24	9 (13%)	83,113,113	1.32	8 (9%)
37	8CT	A	845	-	40,41,41	4.61	23 (57%)	50,56,56	2.56	20 (40%)
29	CLA	7	308	7	59,63,73	1.34	8 (13%)	71,101,113	1.38	6 (8%)
29	CLA	A	835	10	64,68,73	1.28	8 (12%)	77,107,113	1.37	9 (11%)
38	DGD	B	849	-	60,60,67	0.93	2 (3%)	74,74,81	1.39	9 (12%)
29	CLA	F	201	-	49,53,73	1.47	9 (18%)	59,89,113	1.47	7 (11%)
29	CLA	c	615	-	59,63,73	1.36	9 (15%)	71,101,113	1.35	6 (8%)
29	CLA	A	838	10	69,73,73	1.24	8 (11%)	83,113,113	1.30	8 (9%)
29	CLA	A	840	-	69,73,73	1.25	10 (14%)	83,113,113	1.38	10 (12%)
29	CLA	7	304	7	59,63,73	1.35	8 (13%)	71,101,113	1.36	6 (8%)
31	II0	5	614	-	39,43,43	2.66	4 (10%)	50,60,60	1.76	12 (24%)
29	CLA	A	818	10	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
29	CLA	b	606	25	69,73,73	1.23	9 (13%)	83,113,113	1.40	9 (10%)
36	SQD	9	301	-	29,30,54	1.89	7 (24%)	38,41,65	1.63	6 (15%)
29	CLA	A	814	-	49,53,73	1.46	8 (16%)	59,89,113	1.50	8 (13%)
29	CLA	6	607	6	59,63,73	1.38	7 (11%)	71,101,113	1.32	7 (9%)
37	8CT	A	844	-	40,41,41	4.56	23 (57%)	50,56,56	2.88	19 (38%)
37	8CT	A	846	-	40,41,41	4.59	23 (57%)	50,56,56	2.83	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	A	809	29,10	64,68,73	1.29	8 (12%)	77,107,113	1.25	6 (7%)
34	LHG	J	101	30	33,33,48	0.74	1 (3%)	36,39,54	1.26	3 (8%)
29	CLA	c	608	26	64,68,73	1.29	7 (10%)	77,107,113	1.32	5 (6%)
29	CLA	A	804	10	69,73,73	1.24	7 (10%)	83,113,113	1.35	8 (9%)
35	LMG	Z	310	-	48,48,55	0.79	2 (4%)	56,56,63	1.38	8 (14%)
37	8CT	e	616	-	40,41,41	1.61	8 (20%)	50,56,56	1.53	10 (20%)
33	IHT	Z	301	-	40,42,42	2.00	2 (5%)	53,58,58	2.22	15 (28%)
29	CLA	6	605	6	59,63,73	1.36	8 (13%)	71,101,113	1.36	7 (9%)
29	CLA	A	823	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	9 (10%)
29	CLA	c	604	26	64,68,73	1.31	9 (14%)	77,107,113	1.31	7 (9%)
29	CLA	J	103	17	45,49,73	1.53	9 (20%)	54,84,113	1.49	6 (11%)
29	CLA	6	601	6	49,53,73	1.49	8 (16%)	59,89,113	1.43	6 (10%)
29	CLA	A	820	10	69,73,73	1.25	8 (11%)	83,113,113	1.34	10 (12%)
29	CLA	A	830	10	64,68,73	1.29	9 (14%)	77,107,113	1.31	9 (11%)
29	CLA	2	612	2	49,53,73	1.50	8 (16%)	59,89,113	1.46	4 (6%)
29	CLA	2	609	34	45,49,73	1.51	9 (20%)	54,84,113	1.51	6 (11%)
29	CLA	8	303	8	69,73,73	1.25	9 (13%)	83,113,113	1.23	7 (8%)
29	CLA	3	313	3	49,53,73	1.49	7 (14%)	59,89,113	1.47	4 (6%)
40	PQN	B	842	-	34,34,34	1.57	2 (5%)	42,45,45	1.13	3 (7%)
30	KC2	b	605	25	49,53,53	1.76	9 (18%)	62,89,89	2.17	17 (27%)
29	CLA	5	609	34	45,49,73	1.50	8 (17%)	54,84,113	1.53	5 (9%)
37	8CT	B	848	-	40,41,41	4.67	23 (57%)	50,56,56	2.64	20 (40%)
29	CLA	5	606	5	49,53,73	1.49	8 (16%)	59,89,113	1.39	5 (8%)
29	CLA	b	601	25	49,53,73	1.50	9 (18%)	59,89,113	1.47	5 (8%)
29	CLA	A	841	10	69,73,73	1.27	10 (14%)	83,113,113	1.31	7 (8%)
29	CLA	B	812	11	59,63,73	1.35	10 (16%)	71,101,113	1.36	7 (9%)
29	CLA	B	832	11	59,63,73	1.34	9 (15%)	71,101,113	1.47	10 (14%)
29	CLA	A	853	34	49,53,73	1.49	8 (16%)	59,89,113	1.59	6 (10%)
31	II0	4	613	-	39,43,43	2.68	4 (10%)	50,60,60	1.61	9 (18%)
29	CLA	9	308	-	69,73,73	1.27	9 (13%)	83,113,113	1.28	4 (4%)
31	II0	d	615	-	39,43,43	2.88	4 (10%)	50,60,60	1.73	11 (22%)
29	CLA	2	606	2	49,53,73	1.49	10 (20%)	59,89,113	1.43	4 (6%)
31	II0	1	617	-	39,43,43	2.80	4 (10%)	50,60,60	1.77	12 (24%)
30	KC2	Z	306	23	49,53,53	1.76	10 (20%)	62,89,89	2.19	19 (30%)
34	LHG	Z	309	-	39,39,48	0.64	1 (2%)	42,44,54	1.34	6 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	II0	1	620	-	39,43,43	2.89	6 (15%)	50,60,60	2.07	11 (22%)
29	CLA	B	831	11	64,68,73	1.27	8 (12%)	77,107,113	1.28	9 (11%)
34	LHG	a	617	29	26,26,48	0.81	1 (3%)	29,32,54	1.33	3 (10%)
37	8CT	B	852	-	40,41,41	4.58	23 (57%)	50,56,56	2.86	22 (44%)
33	IHT	K	104	-	40,42,42	2.16	3 (7%)	53,58,58	1.73	11 (20%)
29	CLA	c	605	26	49,53,73	1.48	9 (18%)	59,89,113	1.43	4 (6%)
29	CLA	7	305	7	57,61,73	1.39	8 (14%)	68,98,113	1.37	8 (11%)
29	CLA	A	806	10	69,73,73	1.23	8 (11%)	83,113,113	1.29	4 (4%)
34	LHG	2	619	-	38,38,48	0.68	1 (2%)	41,44,54	1.29	5 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LHG	A	850	-	-	23/53/53/53	-
37	8CT	B	847	-	-	4/29/63/63	0/2/2/2
29	CLA	c	601	26	-	8/15/91/115	-
37	8CT	B	851	-	-	12/29/63/63	0/2/2/2
33	IHT	L	204	-	-	0/25/65/65	0/2/2/2
31	II0	7	316	-	-	3/21/67/67	0/2/2/2
29	CLA	L	202	19	-	8/33/109/115	-
31	II0	8	313	-	-	4/21/67/67	0/2/2/2
29	CLA	a	606	24	-	10/39/115/115	-
29	CLA	A	825	10	-	14/39/115/115	-
31	II0	O	205	-	-	1/21/67/67	0/2/2/2
29	CLA	d	607	24	-	7/39/115/115	-
33	IHT	2	616	-	-	3/25/65/65	0/2/2/2
29	CLA	3	306	29,3	-	7/27/103/115	-
29	CLA	5	608	5	-	14/33/109/115	-
29	CLA	d	602	24	-	15/38/114/115	-
29	CLA	c	602	26	-	18/39/115/115	-
30	KC2	1	610	1	-	4/15/71/71	-
29	CLA	A	854	-	-	19/39/115/115	-
29	CLA	A	834	10	-	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	SF4	C	101	12	-	-	0/6/5/5
29	CLA	d	608	24	-	14/39/115/115	-
29	CLA	A	803	10	-	5/39/115/115	-
29	CLA	8	304	8	-	2/21/97/115	-
31	II0	4	615	-	-	3/21/67/67	0/2/2/2
29	CLA	F	202	15	-	9/27/103/115	-
31	II0	3	314	-	-	1/21/67/67	0/2/2/2
29	CLA	8	302	8	-	16/39/115/115	-
29	CLA	4	602	4	-	5/32/108/115	-
35	LMG	3	319	29	-	16/25/45/70	0/1/1/1
29	CLA	9	312	9	-	6/10/86/115	-
31	II0	c	616	-	-	1/21/67/67	0/2/2/2
29	CLA	O	204	-	-	7/27/103/115	-
29	CLA	1	609	34	-	5/10/86/115	-
29	CLA	8	308	-	-	6/39/115/115	-
29	CLA	A	829	10	-	6/21/97/115	-
31	II0	d	614	-	-	0/21/67/67	0/2/2/2
29	CLA	B	829	11	-	18/39/115/115	-
31	II0	6	614	-	-	0/21/67/67	0/2/2/2
31	II0	R	201	-	-	0/21/67/67	0/2/2/2
29	CLA	A	842	10	-	14/39/115/115	-
29	CLA	B	833	-	-	12/39/115/115	-
31	II0	5	616	-	-	1/21/67/67	0/2/2/2
35	LMG	6	617	-	-	10/27/47/70	0/1/1/1
34	LHG	e	617	29	-	17/32/32/53	-
29	CLA	3	310	35	-	5/39/115/115	-
30	KC2	c	614	30	-	7/15/71/71	-
29	CLA	b	602	25	-	17/38/114/115	-
31	II0	2	615	-	-	5/21/67/67	0/2/2/2
31	II0	9	316	-	-	0/21/67/67	0/2/2/2
30	KC2	7	310	7	-	10/15/71/71	-
34	LHG	A	851	29	-	19/43/43/53	-
34	LHG	c	622	29	-	13/23/23/53	-
29	CLA	B	813	11	-	15/39/115/115	-
29	CLA	a	604	24	-	10/33/109/115	-
37	8CT	B	843	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	a	605	24	-	10/27/103/115	-
29	CLA	B	807	11	-	7/39/115/115	-
29	CLA	c	607	26	-	13/39/115/115	-
29	CLA	A	833	10	-	6/39/115/115	-
29	CLA	e	610	-	-	5/23/99/115	-
29	CLA	7	311	-	-	7/27/103/115	-
34	LHG	8	315	-	-	23/37/37/53	-
33	IHT	1	618	-	-	3/25/65/65	0/2/2/2
29	CLA	c	603	31,26	-	14/39/115/115	-
30	KC2	d	610	24	-	11/15/71/71	-
29	CLA	A	802	29,10	-	6/27/103/115	-
31	II0	R	204	-	-	0/21/67/67	0/2/2/2
29	CLA	4	606	4	-	3/33/109/115	-
34	LHG	3	321	-	-	25/53/53/53	-
31	II0	2	613	-	-	3/21/67/67	0/2/2/2
29	CLA	A	813	10	-	3/12/88/115	-
29	CLA	A	836	10	-	7/27/103/115	-
33	IHT	6	616	-	-	6/25/65/65	0/2/2/2
29	CLA	8	305	8	-	8/27/103/115	-
29	CLA	d	611	-	-	6/21/97/115	-
29	CLA	a	607	24	-	8/39/115/115	-
29	CLA	A	826	10	-	11/39/115/115	-
37	8CT	Z	307	-	-	7/29/63/63	0/2/2/2
29	CLA	2	602	2	-	9/32/108/115	-
29	CLA	B	821	11	-	9/33/109/115	-
29	CLA	A	824	-	-	9/39/115/115	-
29	CLA	A	822	10	-	15/39/115/115	-
31	II0	7	317	-	-	3/21/67/67	0/2/2/2
33	IHT	c	620	-	-	4/25/65/65	0/2/2/2
29	CLA	3	309	3	-	6/33/109/115	-
29	CLA	e	604	-	-	8/33/109/115	-
29	CLA	B	839	11	-	5/39/115/115	-
31	II0	5	617	-	-	6/21/67/67	0/2/2/2
29	CLA	a	601	24	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	K	102	18	-	8/27/103/115	-
29	CLA	b	608	34	-	13/39/115/115	-
30	KC2	6	610	6	-	10/15/71/71	-
30	KC2	c	610	26	-	7/15/71/71	-
31	II0	7	315	-	-	0/21/67/67	0/2/2/2
31	II0	3	318	-	-	3/21/67/67	0/2/2/2
31	II0	c	618	-	-	1/21/67/67	0/2/2/2
29	CLA	a	603	24	-	10/33/109/115	-
29	CLA	4	610	4	-	14/39/115/115	-
29	CLA	6	611	-	-	2/27/103/115	-
29	CLA	1	606	1	-	4/15/91/115	-
29	CLA	Z	303	29,23	-	9/27/103/115	-
29	CLA	X	301	-	-	5/24/100/115	-
29	CLA	A	831	10	-	16/39/115/115	-
31	II0	c	619	-	-	4/21/67/67	0/2/2/2
29	CLA	6	608	6	-	5/33/109/115	-
29	CLA	a	611	-	-	10/27/103/115	-
31	II0	a	614	-	-	2/21/67/67	0/2/2/2
29	CLA	1	603	1	-	7/24/100/115	-
29	CLA	8	307	8	-	7/10/86/115	-
29	CLA	e	606	27	-	10/33/109/115	-
37	8CT	A	847	-	-	10/29/63/63	0/2/2/2
37	8CT	7	318	-	-	13/29/63/63	0/2/2/2
30	KC2	6	613	6	-	10/15/71/71	-
31	II0	9	323	-	-	4/21/67/67	0/2/2/2
31	II0	c	621	29	-	0/21/67/67	0/2/2/2
31	II0	9	317	-	-	0/21/67/67	0/2/2/2
29	CLA	B	814	11	-	12/29/105/115	-
29	CLA	5	613	5	-	8/10/86/115	-
36	SQD	a	618	-	-	17/37/57/69	0/1/1/1
38	DGD	9	322	-	-	20/49/89/95	0/2/2/2
30	KC2	e	605	27	-	7/15/71/71	-
29	CLA	a	602	24	-	11/27/103/115	-
29	CLA	B	836	11	-	14/39/115/115	-
29	CLA	c	606	26	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	8CT	B	844	-	-	9/29/63/63	0/2/2/2
29	CLA	B	837	11	-	0/18/94/115	-
35	LMG	X	302	-	-	9/29/49/70	0/1/1/1
29	CLA	3	304	3	-	8/33/109/115	-
29	CLA	B	805	11	-	13/39/115/115	-
37	8CT	Z	308	-	-	11/29/63/63	0/2/2/2
31	II0	d	616	-	-	3/21/67/67	0/2/2/2
32	II3	1	615	-	-	1/25/67/67	0/2/2/2
29	CLA	a	612	24	-	12/39/115/115	-
32	II3	e	613	-	-	1/25/67/67	0/2/2/2
29	CLA	9	302	9	-	4/15/91/115	-
29	CLA	A	837	10	-	13/39/115/115	-
29	CLA	e	611	27	-	15/39/115/115	-
34	LHG	O	208	-	-	17/41/41/53	-
37	8CT	M	101	-	-	7/29/63/63	0/2/2/2
29	CLA	B	816	11	-	11/39/115/115	-
29	CLA	A	811	10	-	13/39/115/115	-
29	CLA	B	811	11	-	8/33/109/115	-
29	CLA	5	604	5	-	15/27/103/115	-
29	CLA	B	808	11	-	22/39/115/115	-
29	CLA	e	602	27	-	8/27/103/115	-
29	CLA	B	840	34	-	7/39/115/115	-
35	LMG	8	314	-	-	17/47/67/70	0/1/1/1
34	LHG	2	617	29	-	11/24/24/53	-
29	CLA	5	603	5	-	3/15/91/115	-
29	CLA	B	823	11	-	15/39/115/115	-
29	CLA	d	603	24	-	4/21/97/115	-
29	CLA	e	601	27	-	4/15/91/115	-
34	LHG	4	620	-	-	23/49/49/53	-
37	8CT	B	846	-	-	9/29/63/63	0/2/2/2
29	CLA	2	607	2	-	6/15/91/115	-
30	KC2	5	610	5	-	9/15/71/71	-
29	CLA	4	601	4	-	4/27/103/115	-
29	CLA	B	804	11	-	6/15/91/115	-
29	CLA	O	201	34	-	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	817	11	-	14/32/108/115	-
29	CLA	3	312	3	-	7/21/97/115	-
34	LHG	L	206	-	-	8/22/23/53	-
29	CLA	9	314	9	-	7/15/91/115	-
29	CLA	Z	302	-	-	13/33/109/115	-
31	II0	8	311	-	-	6/21/67/67	0/2/2/2
30	KC2	c	611	26,30	-	4/15/71/71	-
31	II0	2	614	-	-	1/21/67/67	0/2/2/2
39	SF4	C	102	12	-	-	0/6/5/5
29	CLA	B	824	-	-	16/39/115/115	-
29	CLA	2	608	2	-	6/33/109/115	-
37	8CT	K	103	-	-	10/29/63/63	0/2/2/2
29	CLA	B	838	-	-	6/39/115/115	-
29	CLA	3	311	3	-	11/39/115/115	-
29	CLA	4	611	4	-	11/39/115/115	-
31	II0	4	614	-	-	4/21/67/67	0/2/2/2
29	CLA	1	607	1	-	6/15/91/115	-
34	LHG	Z	311	-	-	25/50/50/53	-
36	SQD	3	320	-	-	13/31/51/69	0/1/1/1
31	II0	3	315	-	-	1/21/67/67	0/2/2/2
31	II0	1	614	-	-	4/21/67/67	0/2/2/2
29	CLA	6	606	6	-	9/27/103/115	-
29	CLA	Z	305	23	-	14/33/109/115	-
29	CLA	e	607	27	-	2/15/91/115	-
29	CLA	d	606	24	-	1/10/86/115	-
34	LHG	A	852	-	-	12/26/26/53	-
30	KC2	2	610	2	-	10/15/71/71	-
31	II0	e	614	-	-	1/21/67/67	0/2/2/2
29	CLA	9	313	9	-	8/15/91/115	-
29	CLA	A	832	10	-	5/39/115/115	-
29	CLA	b	610	25	-	8/23/99/115	-
29	CLA	7	312	7	-	9/21/97/115	-
29	CLA	O	203	21	-	8/27/103/115	-
31	II0	e	615	-	-	4/21/67/67	0/2/2/2
29	CLA	B	819	-	-	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	8CT	L	205	-	-	11/29/63/63	0/2/2/2
29	CLA	5	612	5	-	8/15/91/115	-
33	IHT	5	618	-	-	1/25/65/65	0/2/2/2
29	CLA	A	807	10	-	5/21/97/115	-
33	IHT	a	616	-	-	4/25/65/65	0/2/2/2
29	CLA	1	611	1	-	7/15/91/115	-
35	LMG	2	618	-	-	9/31/51/70	0/1/1/1
29	CLA	e	603	27	-	7/21/97/115	-
31	II0	a	619	-	-	0/21/67/67	0/2/2/2
34	LHG	c	623	-	-	23/38/38/53	-
36	SQD	3	322	-	-	14/31/51/69	0/1/1/1
29	CLA	R	202	22	-	11/27/103/115	-
32	II3	b	613	-	-	2/25/67/67	0/2/2/2
29	CLA	1	602	1	-	3/32/108/115	-
29	CLA	7	306	7	-	6/15/91/115	-
29	CLA	d	604	24	-	9/33/109/115	-
31	II0	8	310	-	-	5/21/67/67	0/2/2/2
29	CLA	A	828	10	-	9/39/115/115	-
34	LHG	4	617	29	-	25/53/53/53	-
30	KC2	7	313	-	-	10/15/71/71	-
29	CLA	B	809	11	-	13/39/115/115	-
29	CLA	B	834	-	-	2/15/91/115	-
29	CLA	7	309	34	-	5/10/86/115	-
29	CLA	L	201	19	-	8/23/99/115	-
34	LHG	L	207	-	-	18/36/36/53	-
31	II0	J	102	-	-	6/21/67/67	0/2/2/2
29	CLA	1	604	1	-	3/15/91/115	-
29	CLA	1	605	1	-	4/11/87/115	-
29	CLA	B	828	11	-	6/39/115/115	-
29	CLA	A	839	-	-	16/39/115/115	-
29	CLA	9	315	-	-	4/10/86/115	-
29	CLA	2	611	2	-	6/21/97/115	-
29	CLA	3	308	3	-	19/33/109/115	-
29	CLA	B	820	11	-	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	L	203	-	-	5/21/97/115	-
34	LHG	5	619	29	-	12/26/26/53	-
29	CLA	9	306	9	-	0/15/91/115	-
29	CLA	1	612	1	-	7/33/109/115	-
31	II0	a	615	-	-	6/21/67/67	0/2/2/2
29	CLA	7	303	7	-	8/39/115/115	-
29	CLA	a	608	24	-	12/33/109/115	-
33	IHT	8	309	-	-	6/25/65/65	0/2/2/2
34	LHG	M	102	-	-	10/25/25/53	-
29	CLA	9	304	9	-	6/15/91/115	-
29	CLA	6	604	6	-	15/33/109/115	-
30	KC2	9	311	9	-	9/15/71/71	-
29	CLA	5	611	5	-	6/15/91/115	-
29	CLA	4	609	4	-	6/33/109/115	-
31	II0	b	612	-	-	5/21/67/67	0/2/2/2
37	8CT	J	104	-	-	9/29/63/63	0/2/2/2
37	8CT	B	845	-	-	6/29/63/63	0/2/2/2
29	CLA	A	801	10	-	20/39/115/115	-
29	CLA	5	602	5	-	2/27/103/115	-
29	CLA	b	604	25	-	9/31/107/115	-
34	LHG	4	618	-	-	30/53/53/53	-
29	CLA	1	608	1	-	10/33/109/115	-
29	CLA	B	822	11	-	9/33/109/115	-
29	CLA	e	608	34	-	4/10/86/115	-
29	CLA	7	302	7	-	3/15/91/115	-
34	LHG	B	801	-	-	24/41/41/53	-
29	CLA	b	607	25	-	5/33/109/115	-
29	CLA	c	613	26	-	10/15/91/115	-
29	CLA	A	810	10	-	16/39/115/115	-
29	CLA	9	305	-	-	5/27/103/115	-
29	CLA	9	310	-	-	5/10/86/115	-
31	II0	5	620	-	-	3/21/67/67	0/2/2/2
32	II3	8	312	-	-	8/25/67/67	0/2/2/2
29	CLA	B	810	11	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	825	-	-	6/33/109/115	-
29	CLA	A	816	10	-	19/33/109/115	-
29	CLA	Z	304	23	-	6/21/97/115	-
29	CLA	d	612	24	-	11/37/113/115	-
34	LHG	7	320	-	-	19/35/35/53	-
31	II0	1	616	-	-	5/21/67/67	0/2/2/2
29	CLA	1	601	1	-	8/15/91/115	-
29	CLA	8	301	8	-	7/15/91/115	-
29	CLA	B	827	11	-	13/39/115/115	-
29	CLA	B	818	11	-	4/33/109/115	-
36	SQD	B	850	-	-	15/28/48/69	0/1/1/1
34	LHG	9	321	-	-	19/37/37/53	-
37	8CT	R	203	-	-	4/29/63/63	0/2/2/2
29	CLA	2	604	2	-	8/27/103/115	-
31	II0	3	316	-	-	4/21/67/67	0/2/2/2
29	CLA	2	605	2	-	7/33/109/115	-
29	CLA	6	602	6	-	14/39/115/115	-
40	PQN	A	849	-	-	2/23/43/43	0/2/2/2
29	CLA	3	305	3	-	8/39/115/115	-
29	CLA	4	608	34	-	10/39/115/115	-
29	CLA	6	612	6	-	6/15/91/115	-
29	CLA	a	609	34	-	9/33/109/115	-
33	IHT	d	617	-	-	1/25/65/65	0/2/2/2
29	CLA	8	317	-	-	13/39/115/115	-
29	CLA	A	817	10	-	15/39/115/115	-
29	CLA	3	303	3	-	6/27/103/115	-
31	II0	7	314	-	-	1/21/67/67	0/2/2/2
29	CLA	B	815	11	-	3/12/88/115	-
29	CLA	9	309	9	-	11/27/103/115	-
31	II0	9	319	-	-	6/21/67/67	0/2/2/2
29	CLA	4	604	-	-	12/27/103/115	-
29	CLA	B	830	11	-	2/15/91/115	-
34	LHG	4	619	29	-	22/49/49/53	-
29	CLA	8	306	8	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	8CT	F	203	-	-	10/29/63/63	0/2/2/2
31	II0	9	318	-	-	3/21/67/67	0/2/2/2
29	CLA	5	605	5	-	7/15/91/115	-
29	CLA	A	815	10	-	4/36/112/115	-
29	CLA	5	601	5	-	5/10/86/115	-
29	CLA	b	603	25	-	6/33/109/115	-
34	LHG	b	616	29	-	17/34/34/53	-
29	CLA	b	611	25	-	5/27/103/115	-
34	LHG	5	621	29	-	14/39/39/53	-
29	CLA	d	605	24	-	4/15/91/115	-
29	CLA	2	601	2	-	5/12/88/115	-
29	CLA	A	808	10	-	8/27/103/115	-
29	CLA	d	609	-	-	2/10/86/115	-
29	CLA	A	812	10	-	2/27/103/115	-
29	CLA	A	819	-	-	5/39/115/115	-
29	CLA	c	612	26	-	9/27/103/115	-
29	CLA	A	827	10	-	8/39/115/115	-
29	CLA	9	307	9	-	8/30/106/115	-
29	CLA	B	802	-	-	4/27/103/115	-
30	KC2	4	605	4	-	7/15/71/71	-
29	CLA	9	303	9	-	10/27/103/115	-
29	CLA	K	101	-	-	11/39/115/115	-
33	IHT	9	320	-	-	7/25/65/65	0/2/2/2
29	CLA	A	821	10	-	5/27/103/115	-
31	II0	c	617	-	-	0/21/67/67	0/2/2/2
34	LHG	3	301	29	-	13/46/46/53	-
36	SQD	O	207	-	-	14/24/44/69	0/1/1/1
29	CLA	A	843	-	-	8/39/115/115	-
29	CLA	B	806	11	-	13/39/115/115	-
29	CLA	6	603	6	-	5/15/91/115	-
34	LHG	1	619	29	-	21/39/39/53	-
29	CLA	7	307	7	-	7/15/91/115	-
34	LHG	L	208	-	-	22/38/38/53	-
29	CLA	c	609	34	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	II0	e	612	-	-	6/21/67/67	0/2/2/2
29	CLA	d	601	24	-	9/15/91/115	-
29	CLA	6	609	34	-	1/10/86/115	-
31	II0	4	612	-	-	2/21/67/67	0/2/2/2
31	II0	b	614	-	-	3/21/67/67	0/2/2/2
30	KC2	3	307	34	-	9/15/71/71	-
31	II0	O	206	-	-	0/21/67/67	0/2/2/2
34	LHG	8	316	-	-	30/53/53/53	-
37	8CT	b	615	-	-	14/29/63/63	0/2/2/2
29	CLA	B	841	11	-	3/39/115/115	-
29	CLA	O	202	-	-	4/10/86/115	-
30	KC2	b	609	25	-	3/15/71/71	-
29	CLA	B	803	11	-	21/39/115/115	-
34	LHG	7	319	29	-	26/43/43/53	-
37	8CT	I	101	-	-	9/29/63/63	0/2/2/2
29	CLA	2	603	2	-	7/21/97/115	-
31	II0	5	615	-	-	3/21/67/67	0/2/2/2
29	CLA	3	302	3	-	6/15/91/115	-
37	8CT	4	616	-	-	13/29/63/63	0/2/2/2
29	CLA	1	613	1	-	10/15/91/115	-
29	CLA	4	607	4	-	9/33/109/115	-
29	CLA	B	835	11	-	4/27/103/115	-
31	II0	7	301	-	-	4/21/67/67	0/2/2/2
29	CLA	A	805	10	-	2/21/97/115	-
36	SQD	7	321	-	-	16/31/51/69	0/1/1/1
30	KC2	a	610	24	-	9/15/71/71	-
29	CLA	4	603	4	-	8/26/102/115	-
35	LMG	F	204	-	-	8/27/47/70	0/1/1/1
31	II0	a	613	-	-	1/21/67/67	0/2/2/2
31	II0	d	613	-	-	0/21/67/67	0/2/2/2
30	KC2	e	609	27	-	7/15/71/71	-
31	II0	3	317	-	-	3/21/67/67	0/2/2/2
29	CLA	5	607	5	-	8/15/91/115	-
29	CLA	A	855	-	-	9/33/109/115	-
31	II0	6	615	-	-	3/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	SF4	A	848	11,10	-	-	0/6/5/5
29	CLA	B	826	11	-	7/39/115/115	-
37	8CT	A	845	-	-	5/29/63/63	0/2/2/2
29	CLA	7	308	7	-	10/27/103/115	-
29	CLA	A	835	10	-	6/33/109/115	-
38	DGD	B	849	-	-	18/48/88/95	0/2/2/2
29	CLA	F	201	-	-	3/15/91/115	-
29	CLA	c	615	-	-	8/27/103/115	-
29	CLA	A	838	10	-	8/39/115/115	-
29	CLA	A	840	-	-	13/39/115/115	-
29	CLA	7	304	7	-	8/27/103/115	-
31	II0	5	614	-	-	1/21/67/67	0/2/2/2
29	CLA	A	818	10	-	12/39/115/115	-
29	CLA	b	606	25	-	16/39/115/115	-
36	SQD	9	301	-	-	10/25/45/69	0/1/1/1
29	CLA	A	814	-	-	10/15/91/115	-
29	CLA	6	607	6	-	12/27/103/115	-
37	8CT	A	844	-	-	7/29/63/63	0/2/2/2
37	8CT	A	846	-	-	8/29/63/63	0/2/2/2
29	CLA	A	809	29,10	-	7/33/109/115	-
34	LHG	J	101	30	-	13/38/38/53	-
29	CLA	c	608	26	-	8/33/109/115	-
29	CLA	A	804	10	-	16/39/115/115	-
35	LMG	Z	310	-	-	21/43/63/70	0/1/1/1
37	8CT	e	616	-	-	11/29/63/63	0/2/2/2
33	IHT	Z	301	-	-	7/25/65/65	0/2/2/2
29	CLA	6	605	6	-	9/27/103/115	-
29	CLA	A	823	-	-	11/39/115/115	-
29	CLA	c	604	26	-	11/33/109/115	-
29	CLA	J	103	17	-	3/10/86/115	-
29	CLA	6	601	6	-	7/15/91/115	-
29	CLA	A	820	10	-	12/39/115/115	-
29	CLA	A	830	10	-	7/33/109/115	-
29	CLA	2	612	2	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	2	609	34	-	5/10/86/115	-
29	CLA	8	303	8	-	19/39/115/115	-
29	CLA	3	313	3	-	7/15/91/115	-
40	PQN	B	842	-	-	3/23/43/43	0/2/2/2
30	KC2	b	605	25	-	7/15/71/71	-
29	CLA	5	609	34	-	3/10/86/115	-
37	8CT	B	848	-	-	8/29/63/63	0/2/2/2
29	CLA	5	606	5	-	5/15/91/115	-
29	CLA	b	601	25	-	2/15/91/115	-
29	CLA	A	841	10	-	12/39/115/115	-
29	CLA	B	812	11	-	5/27/103/115	-
29	CLA	B	832	11	-	11/27/103/115	-
29	CLA	A	853	34	-	10/15/91/115	-
31	II0	4	613	-	-	2/21/67/67	0/2/2/2
29	CLA	9	308	-	-	22/39/115/115	-
31	II0	d	615	-	-	1/21/67/67	0/2/2/2
29	CLA	2	606	2	-	6/15/91/115	-
31	II0	1	617	-	-	6/21/67/67	0/2/2/2
30	KC2	Z	306	23	-	3/15/71/71	-
34	LHG	Z	309	-	-	18/43/43/53	-
31	II0	1	620	-	-	5/21/67/67	0/2/2/2
29	CLA	B	831	11	-	12/33/109/115	-
34	LHG	a	617	29	-	17/31/31/53	-
37	8CT	B	852	-	-	14/29/63/63	0/2/2/2
33	IHT	K	104	-	-	4/25/65/65	0/2/2/2
29	CLA	c	605	26	-	10/15/91/115	-
29	CLA	7	305	7	-	6/25/101/115	-
29	CLA	A	806	10	-	15/39/115/115	-
34	LHG	2	619	-	-	22/43/43/53	-

The worst 5 of 3186 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B	847	8CT	C02-C03	14.67	1.59	1.34
37	Z	307	8CT	C02-C03	14.59	1.59	1.34
37	B	845	8CT	C02-C03	14.47	1.59	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Z	308	8CT	C02-C03	14.40	1.59	1.34
37	I	101	8CT	C02-C03	14.37	1.59	1.34

The worst 5 of 3628 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B	843	8CT	C33-C32-C31	-12.07	113.28	124.85
37	L	205	8CT	C33-C32-C31	-12.05	113.30	124.85
37	A	844	8CT	C33-C32-C31	-11.82	113.51	124.85
37	A	846	8CT	C33-C32-C31	-11.68	113.66	124.85
37	M	101	8CT	C33-C32-C31	-11.65	113.68	124.85

There are no chirality outliers.

5 of 3638 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	1	607	CLA	C1A-C2A-CAA-CBA
29	1	608	CLA	C2-C3-C5-C6
29	1	608	CLA	C4-C3-C5-C6
29	1	611	CLA	CHA-CBD-CGD-O1D
29	1	611	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

297 monomers are involved in 691 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	850	LHG	2	0
29	c	601	CLA	1	0
37	B	851	8CT	1	0
33	L	204	IHT	1	0
29	L	202	CLA	3	0
29	a	606	CLA	2	0
29	A	825	CLA	7	0
29	d	607	CLA	2	0
29	3	306	CLA	1	0
29	5	608	CLA	2	0
29	d	602	CLA	4	0
29	c	602	CLA	5	0
30	1	610	KC2	1	0
29	A	854	CLA	9	0
29	A	834	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	d	608	CLA	2	0
29	A	803	CLA	5	0
29	8	304	CLA	6	0
29	F	202	CLA	1	0
29	8	302	CLA	5	0
29	4	602	CLA	1	0
35	3	319	LMG	2	0
29	9	312	CLA	1	0
31	c	616	II0	1	0
29	O	204	CLA	1	0
29	1	609	CLA	2	0
29	8	308	CLA	4	0
29	A	829	CLA	4	0
29	B	829	CLA	6	0
31	6	614	II0	1	0
29	A	842	CLA	6	0
34	e	617	LHG	1	0
29	3	310	CLA	4	0
29	b	602	CLA	3	0
30	7	310	KC2	1	0
34	A	851	LHG	2	0
29	B	813	CLA	4	0
29	a	604	CLA	2	0
29	a	605	CLA	2	0
29	B	807	CLA	2	0
29	c	607	CLA	6	0
29	A	833	CLA	5	0
29	7	311	CLA	1	0
29	c	603	CLA	4	0
29	A	802	CLA	3	0
31	R	204	II0	2	0
29	4	606	CLA	2	0
34	3	321	LHG	2	0
31	2	613	II0	1	0
29	A	813	CLA	1	0
29	A	836	CLA	5	0
29	8	305	CLA	1	0
29	a	607	CLA	3	0
29	A	826	CLA	6	0
29	2	602	CLA	2	0
29	B	821	CLA	3	0
29	A	824	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	822	CLA	4	0
33	c	620	IHT	1	0
29	3	309	CLA	2	0
29	e	604	CLA	2	0
29	B	839	CLA	4	0
29	a	601	CLA	3	0
29	K	102	CLA	4	0
29	b	608	CLA	3	0
29	a	603	CLA	1	0
29	4	610	CLA	4	0
29	1	606	CLA	1	0
29	Z	303	CLA	1	0
29	X	301	CLA	2	0
29	A	831	CLA	4	0
29	6	608	CLA	1	0
29	a	611	CLA	1	0
29	1	603	CLA	3	0
29	8	307	CLA	2	0
29	e	606	CLA	3	0
37	7	318	8CT	1	0
30	6	613	KC2	1	0
31	c	621	II0	1	0
29	B	814	CLA	8	0
29	5	613	CLA	1	0
36	a	618	SQD	3	0
38	9	322	DGD	1	0
29	a	602	CLA	2	0
29	B	836	CLA	3	0
29	c	606	CLA	3	0
37	B	844	8CT	1	0
29	B	837	CLA	7	0
35	X	302	LMG	3	0
29	3	304	CLA	1	0
29	B	805	CLA	2	0
29	a	612	CLA	5	0
32	e	613	II3	2	0
29	9	302	CLA	2	0
29	A	837	CLA	6	0
29	e	611	CLA	5	0
37	M	101	8CT	1	0
29	B	816	CLA	5	0
29	A	811	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	811	CLA	4	0
29	5	604	CLA	5	0
29	B	808	CLA	5	0
29	e	602	CLA	5	0
29	B	840	CLA	5	0
35	8	314	LMG	2	0
29	5	603	CLA	3	0
29	B	823	CLA	5	0
29	d	603	CLA	2	0
34	4	620	LHG	2	0
29	2	607	CLA	1	0
29	4	601	CLA	2	0
29	B	804	CLA	1	0
29	O	201	CLA	2	0
29	B	817	CLA	10	0
29	3	312	CLA	1	0
34	L	206	LHG	1	0
29	9	314	CLA	1	0
29	Z	302	CLA	4	0
30	c	611	KC2	1	0
39	C	102	SF4	1	0
29	B	824	CLA	8	0
29	2	608	CLA	2	0
29	B	838	CLA	1	0
29	3	311	CLA	2	0
29	4	611	CLA	7	0
29	1	607	CLA	1	0
36	3	320	SQD	2	0
31	1	614	II0	1	0
29	6	606	CLA	3	0
29	Z	305	CLA	3	0
29	e	607	CLA	1	0
29	d	606	CLA	1	0
34	A	852	LHG	1	0
29	9	313	CLA	3	0
29	A	832	CLA	4	0
29	b	610	CLA	1	0
29	7	312	CLA	4	0
29	B	819	CLA	1	0
29	5	612	CLA	2	0
29	A	807	CLA	3	0
33	a	616	IHT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	1	611	CLA	1	0
35	2	618	LMG	3	0
34	c	623	LHG	2	0
36	3	322	SQD	1	0
29	R	202	CLA	3	0
32	b	613	II3	1	0
29	d	604	CLA	2	0
29	A	828	CLA	4	0
34	4	617	LHG	5	0
29	B	809	CLA	4	0
29	B	834	CLA	3	0
29	7	309	CLA	1	0
29	L	201	CLA	3	0
34	L	207	LHG	2	0
29	1	604	CLA	2	0
29	1	605	CLA	2	0
29	B	828	CLA	1	0
29	A	839	CLA	3	0
29	3	308	CLA	8	0
29	B	820	CLA	4	0
29	L	203	CLA	4	0
29	1	612	CLA	1	0
29	7	303	CLA	1	0
34	M	102	LHG	2	0
29	9	304	CLA	3	0
29	6	604	CLA	1	0
29	5	611	CLA	3	0
29	4	609	CLA	1	0
29	A	801	CLA	2	0
29	5	602	CLA	2	0
29	b	604	CLA	1	0
34	4	618	LHG	6	0
29	1	608	CLA	1	0
29	B	822	CLA	6	0
29	e	608	CLA	1	0
34	B	801	LHG	3	0
29	A	810	CLA	4	0
29	9	305	CLA	2	0
29	9	310	CLA	4	0
32	8	312	II3	2	0
29	B	810	CLA	11	0
29	B	825	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	816	CLA	6	0
29	Z	304	CLA	1	0
29	d	612	CLA	2	0
34	7	320	LHG	3	0
29	1	601	CLA	3	0
29	8	301	CLA	1	0
29	B	827	CLA	8	0
29	B	818	CLA	3	0
36	B	850	SQD	1	0
34	9	321	LHG	1	0
29	2	604	CLA	2	0
29	2	605	CLA	2	0
29	6	602	CLA	4	0
40	A	849	PQN	5	0
29	3	305	CLA	1	0
29	4	608	CLA	5	0
29	6	612	CLA	1	0
29	8	317	CLA	4	0
29	A	817	CLA	5	0
29	3	303	CLA	2	0
31	7	314	II0	1	0
29	B	815	CLA	3	0
29	9	309	CLA	4	0
29	4	604	CLA	1	0
34	4	619	LHG	2	0
29	8	306	CLA	2	0
37	F	203	8CT	1	0
29	5	605	CLA	2	0
29	A	815	CLA	6	0
29	5	601	CLA	2	0
29	b	603	CLA	2	0
29	b	611	CLA	4	0
34	5	621	LHG	4	0
29	d	605	CLA	2	0
29	A	808	CLA	4	0
29	A	812	CLA	7	0
29	A	819	CLA	5	0
29	c	612	CLA	4	0
29	A	827	CLA	3	0
29	9	307	CLA	4	0
29	B	802	CLA	3	0
29	9	303	CLA	4	0

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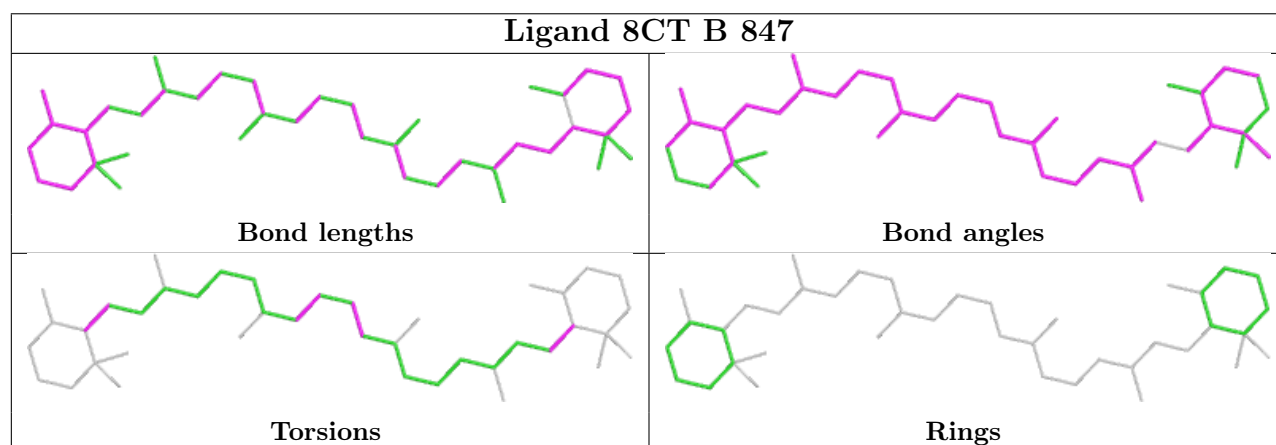
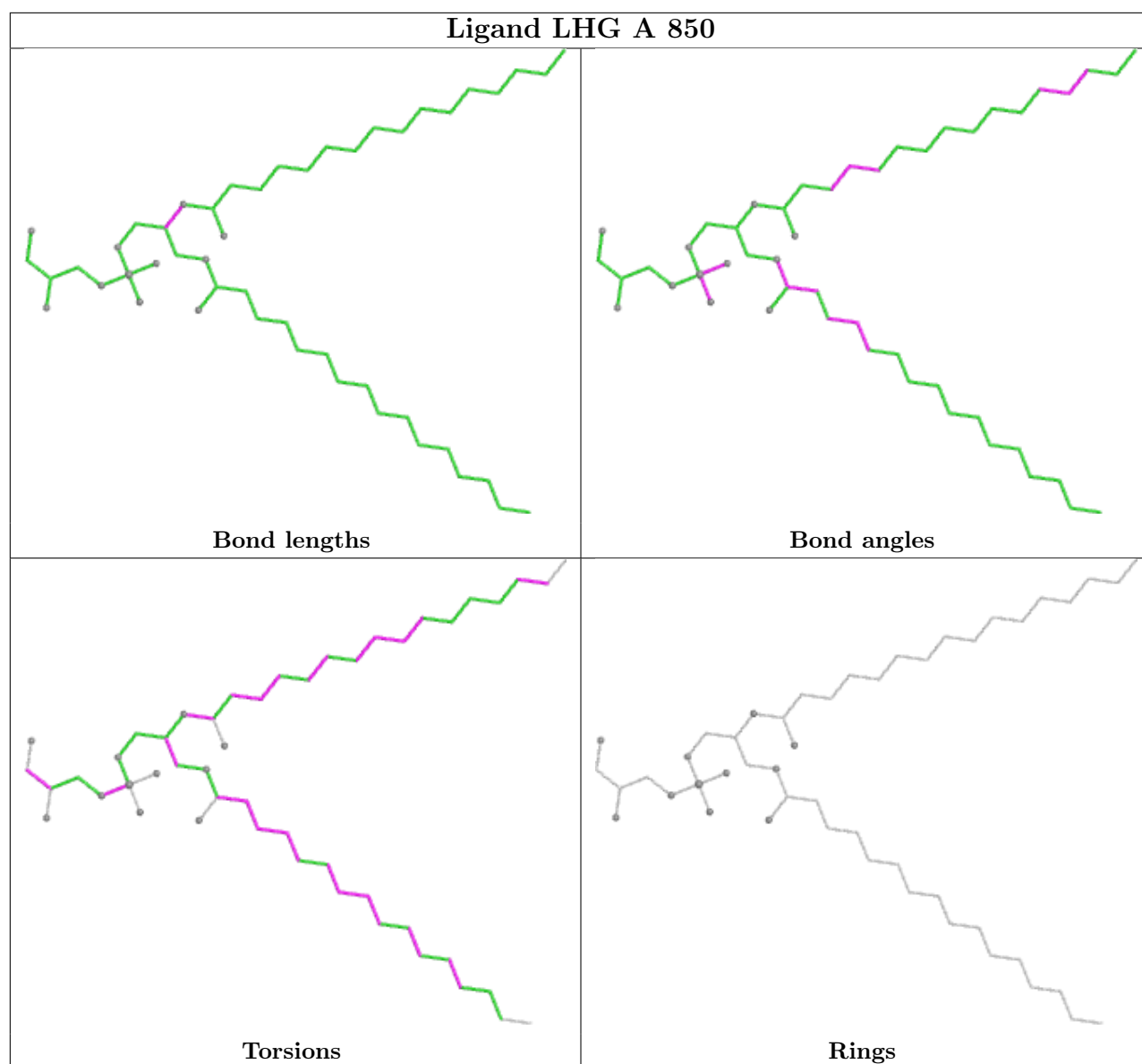
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	821	CLA	3	0
34	3	301	LHG	2	0
29	A	843	CLA	8	0
29	B	806	CLA	4	0
29	6	603	CLA	1	0
34	1	619	LHG	2	0
29	7	307	CLA	4	0
34	L	208	LHG	1	0
29	d	601	CLA	2	0
29	6	609	CLA	3	0
30	3	307	KC2	1	0
34	8	316	LHG	1	0
29	B	841	CLA	3	0
29	O	202	CLA	2	0
30	b	609	KC2	4	0
29	B	803	CLA	4	0
34	7	319	LHG	2	0
29	2	603	CLA	2	0
31	5	615	II0	1	0
29	3	302	CLA	2	0
37	4	616	8CT	1	0
29	4	607	CLA	1	0
29	A	805	CLA	2	0
36	7	321	SQD	2	0
29	4	603	CLA	2	0
35	F	204	LMG	3	0
29	5	607	CLA	2	0
29	A	855	CLA	1	0
29	B	826	CLA	4	0
29	7	308	CLA	5	0
29	A	835	CLA	4	0
38	B	849	DGD	4	0
29	F	201	CLA	2	0
29	c	615	CLA	1	0
29	A	838	CLA	6	0
29	A	840	CLA	5	0
29	7	304	CLA	4	0
29	A	818	CLA	5	0
29	b	606	CLA	4	0
36	9	301	SQD	1	0
29	A	814	CLA	1	0
29	6	607	CLA	4	0

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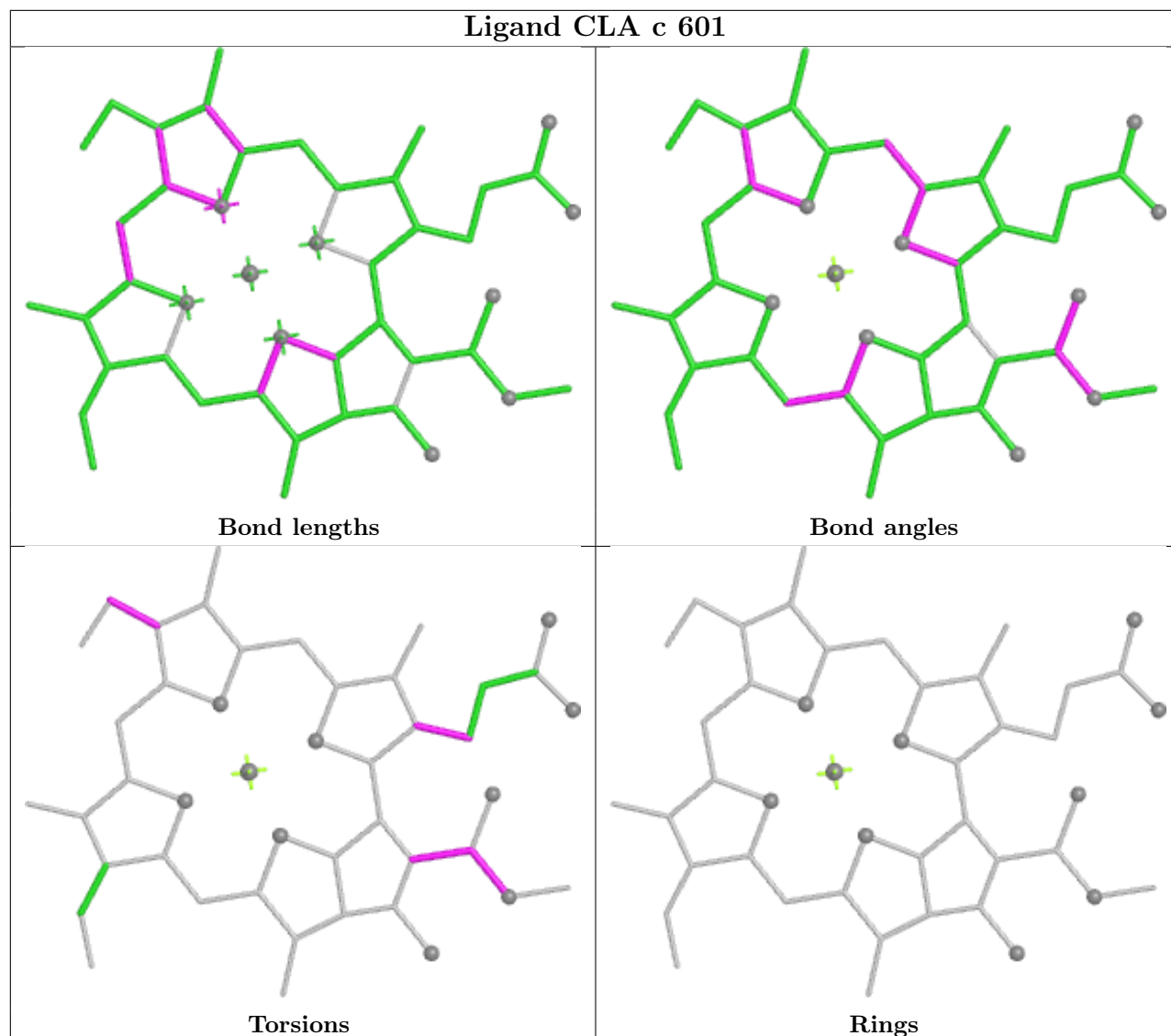
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	809	CLA	5	0
34	J	101	LHG	2	0
29	c	608	CLA	2	0
29	A	804	CLA	5	0
35	Z	310	LMG	1	0
29	A	823	CLA	1	0
29	c	604	CLA	1	0
29	6	601	CLA	2	0
29	A	820	CLA	4	0
29	A	830	CLA	3	0
29	2	612	CLA	1	0
29	8	303	CLA	2	0
29	3	313	CLA	2	0
40	B	842	PQN	2	0
29	5	606	CLA	2	0
29	b	601	CLA	2	0
29	A	841	CLA	5	0
29	B	832	CLA	5	0
29	A	853	CLA	5	0
29	9	308	CLA	9	0
31	d	615	II0	1	0
29	2	606	CLA	4	0
30	Z	306	KC2	1	0
34	Z	309	LHG	2	0
29	B	831	CLA	3	0
34	a	617	LHG	1	0
37	B	852	8CT	1	0
29	c	605	CLA	1	0
29	A	806	CLA	2	0
34	2	619	LHG	1	0

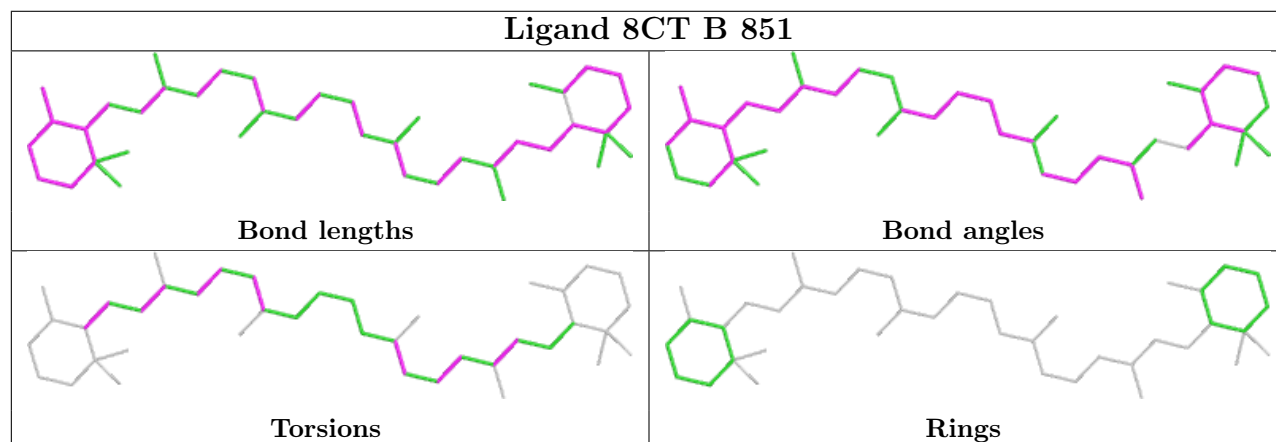
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

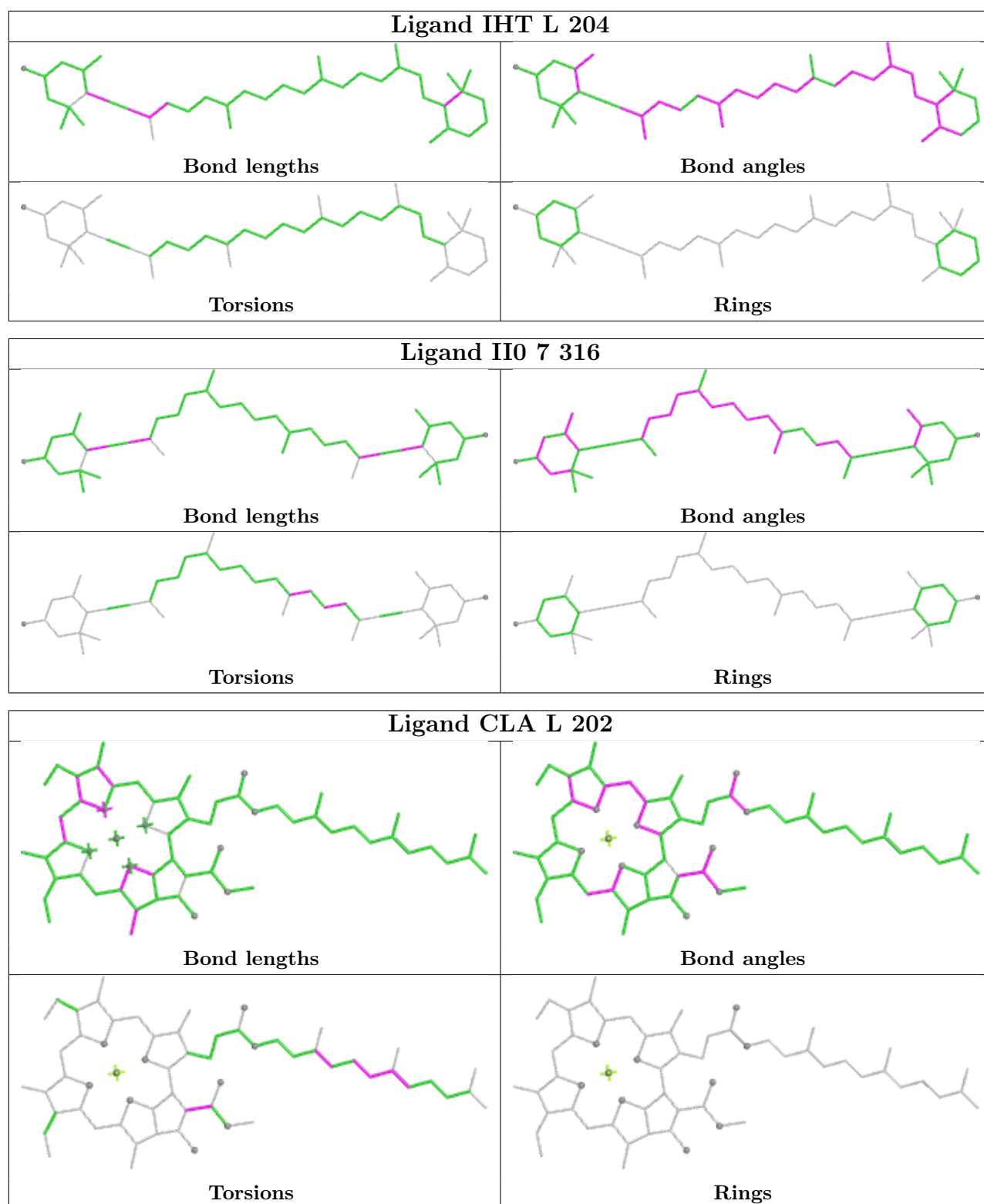


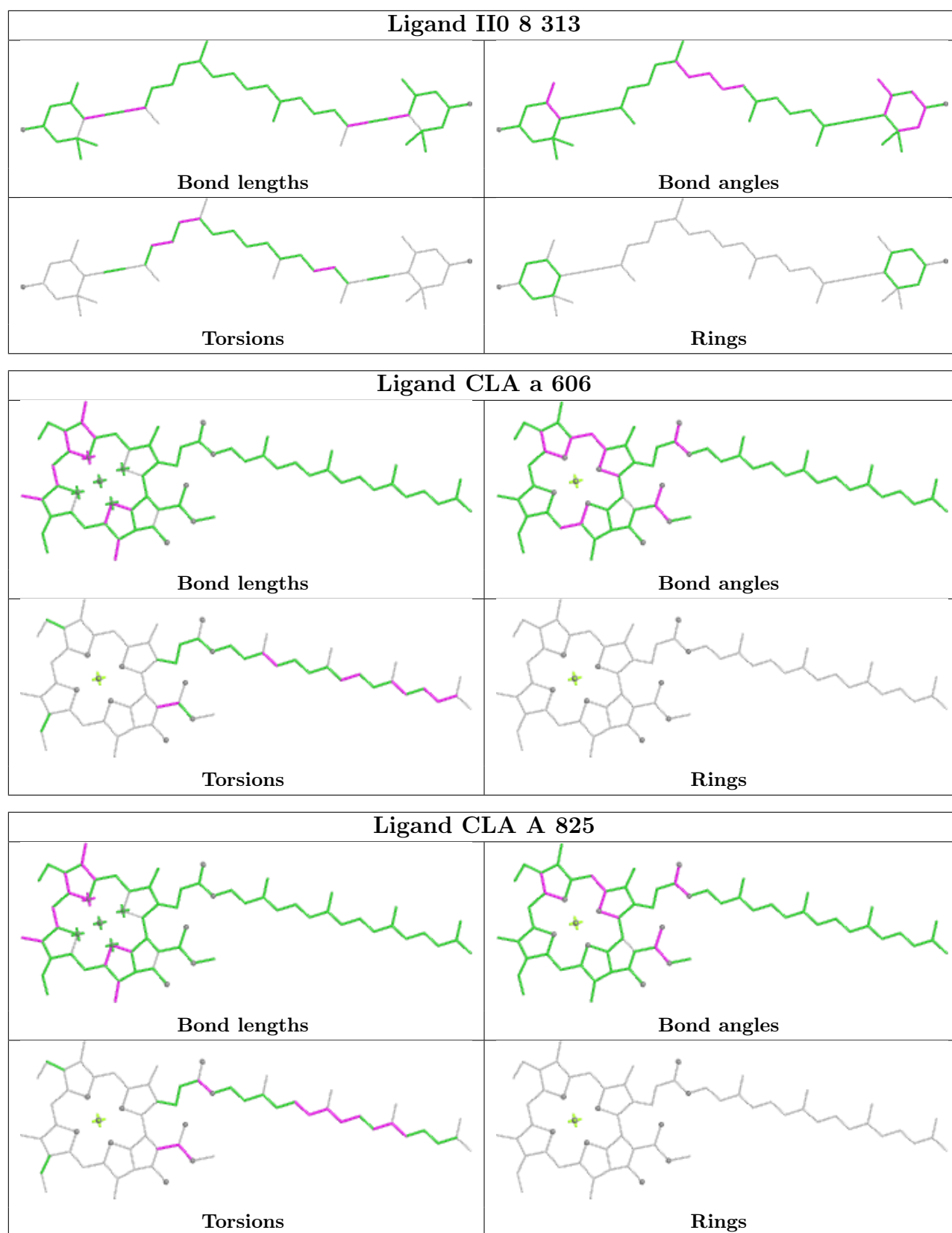
Ligand CLA c 601



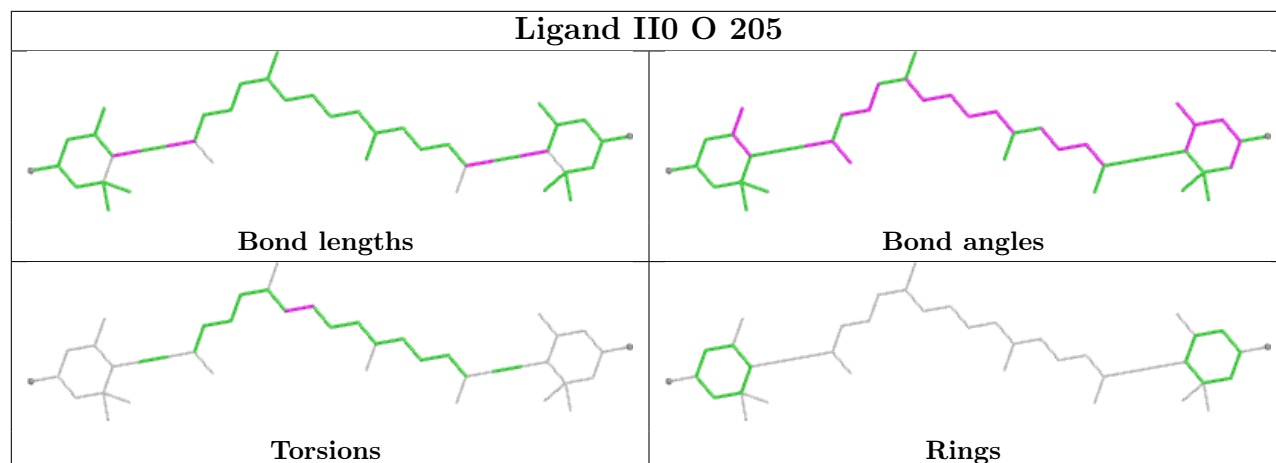
Ligand 8CT B 851



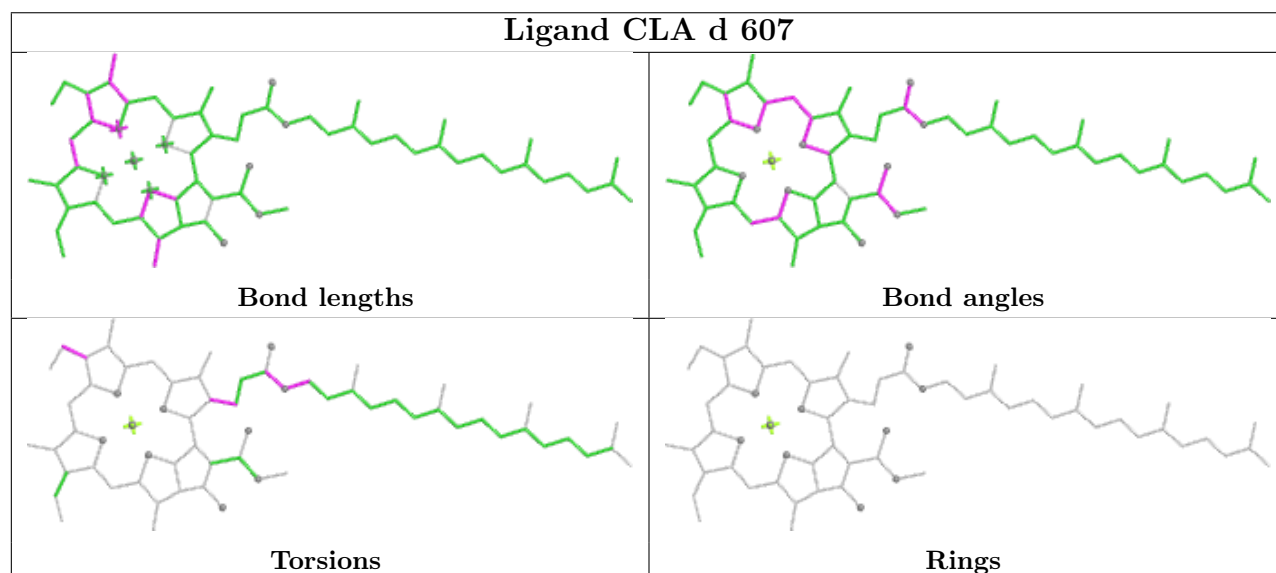




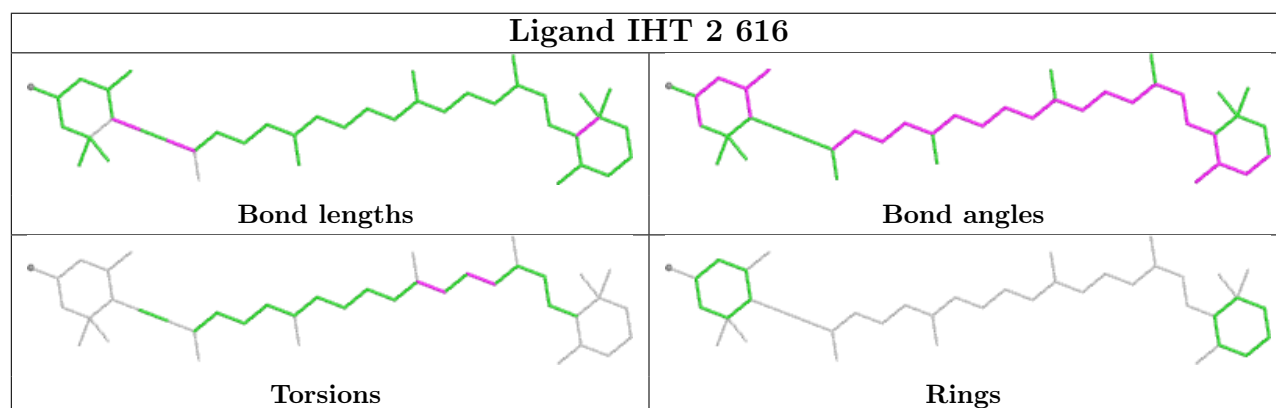
Ligand II0 O 205

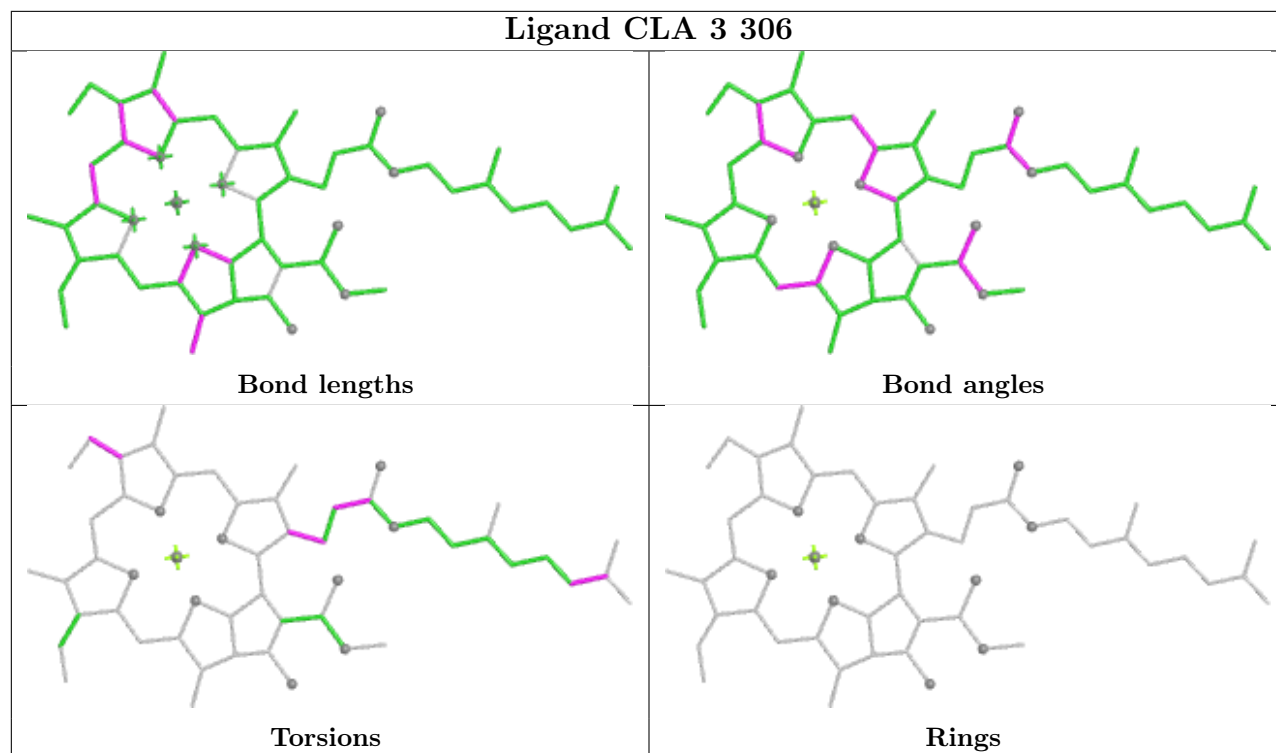
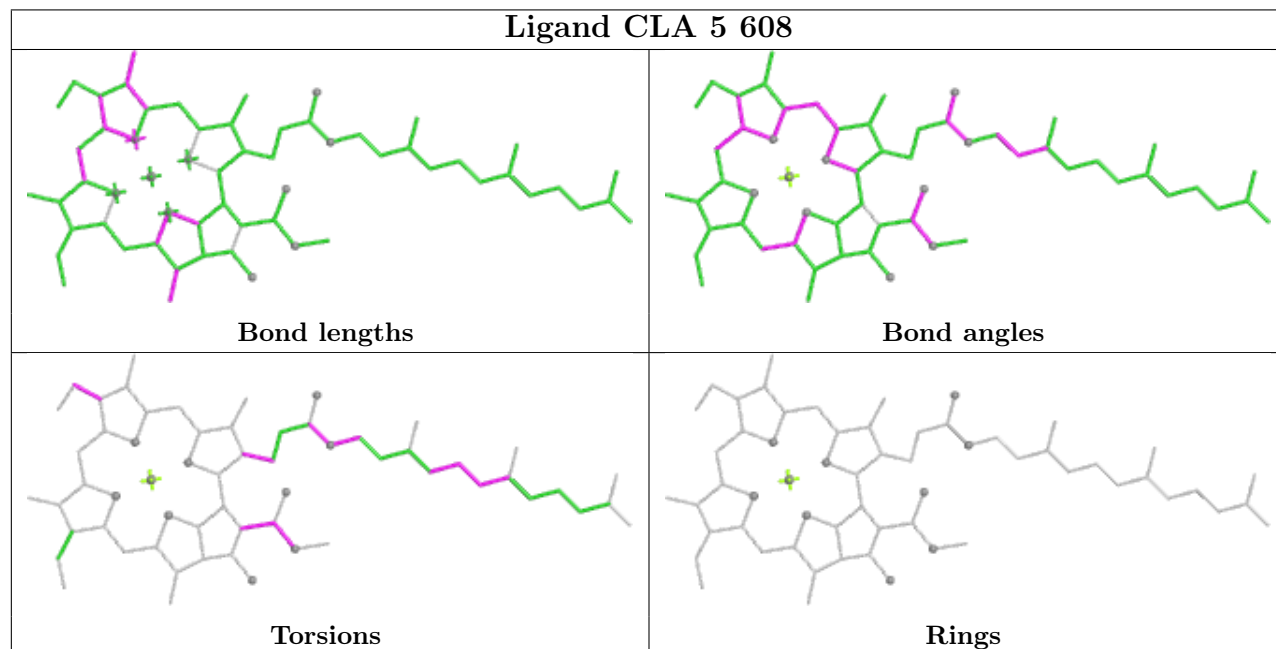


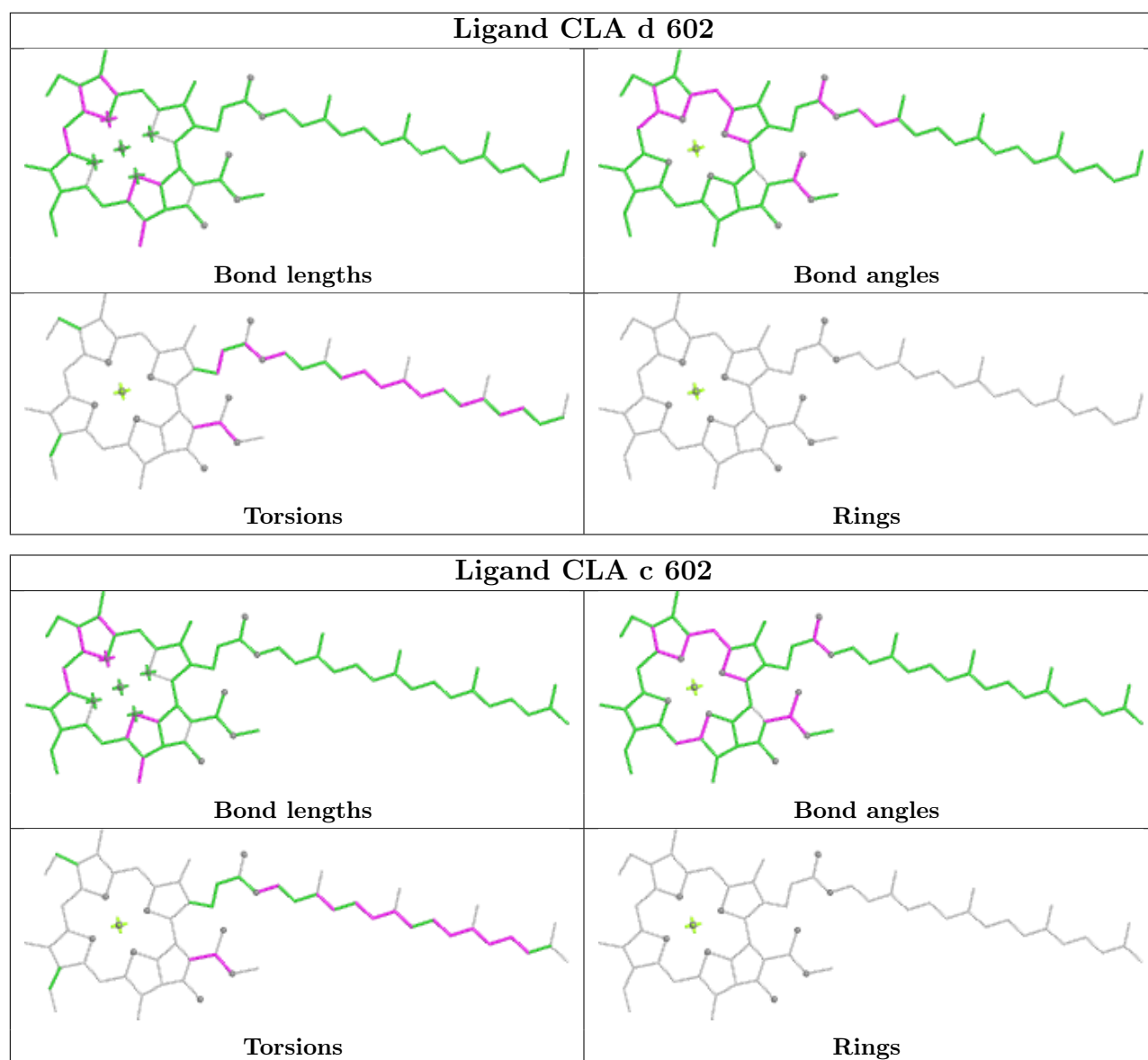
Ligand CLA d 607



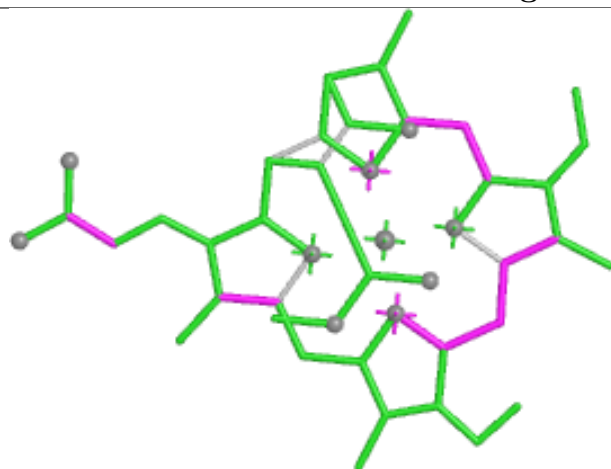
Ligand IHT 2 616



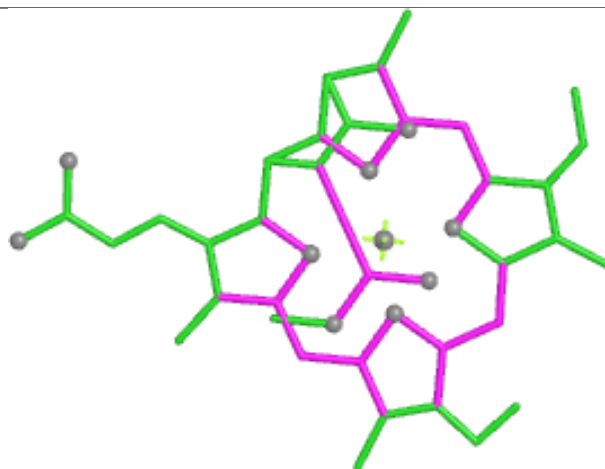
Ligand CLA 3 306**Ligand CLA 5 608**



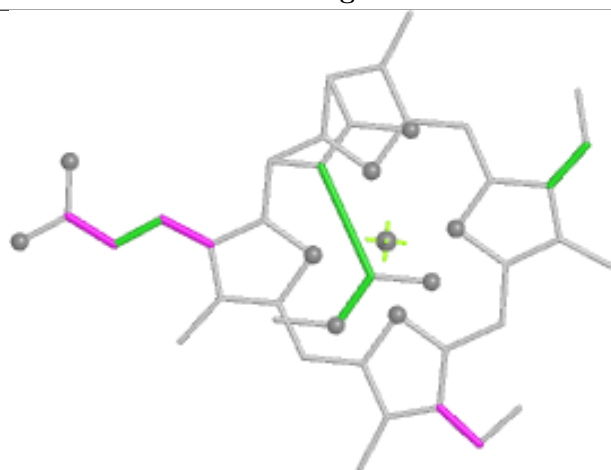
Ligand KC2 1 610



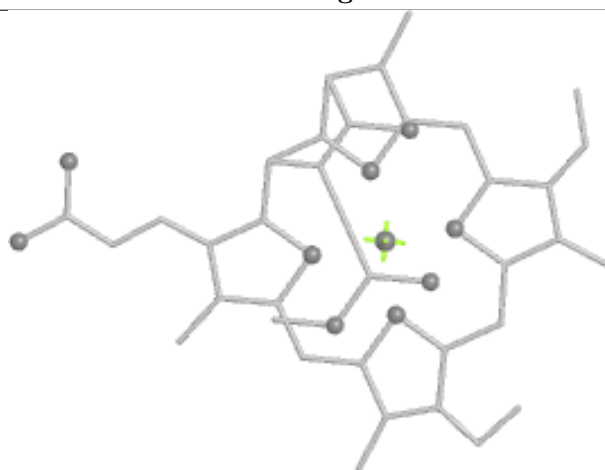
Bond lengths



Bond angles

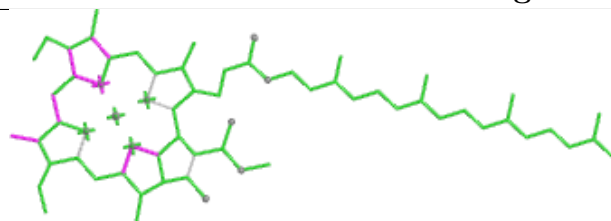


Torsions

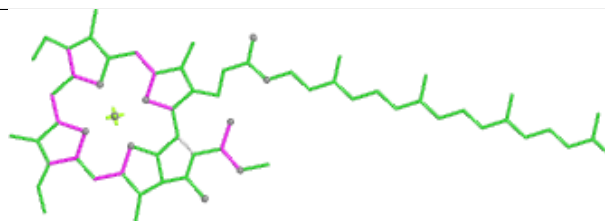


Rings

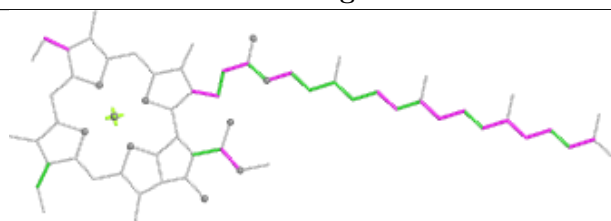
Ligand CLA A 854



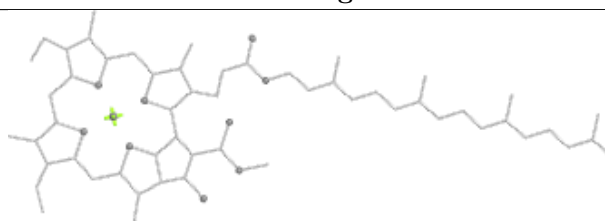
Bond lengths



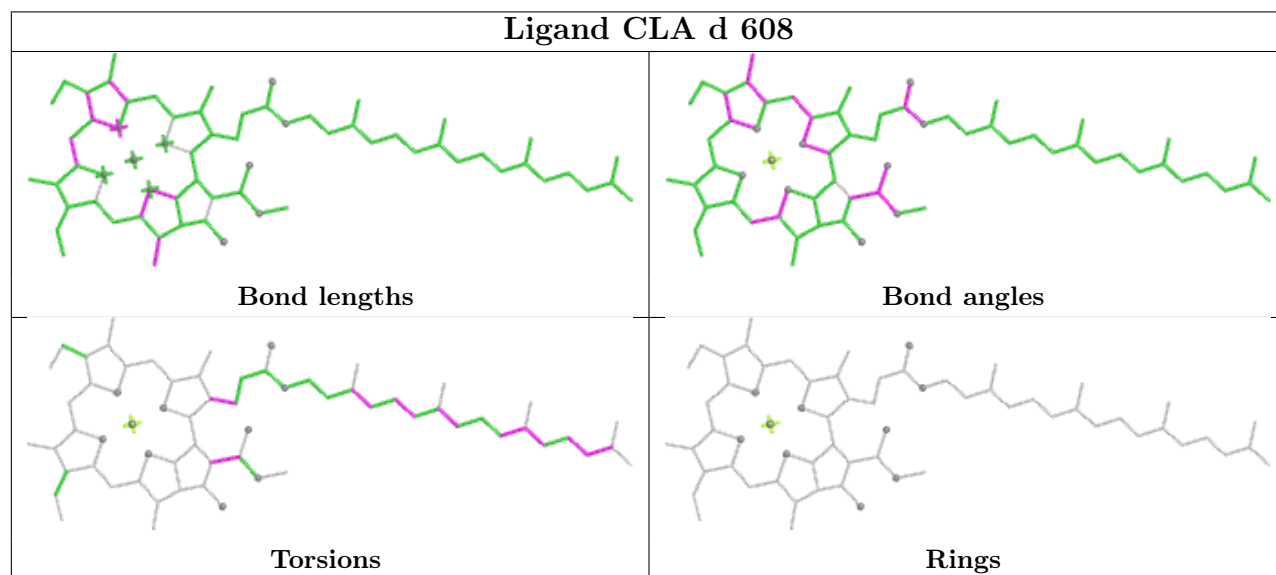
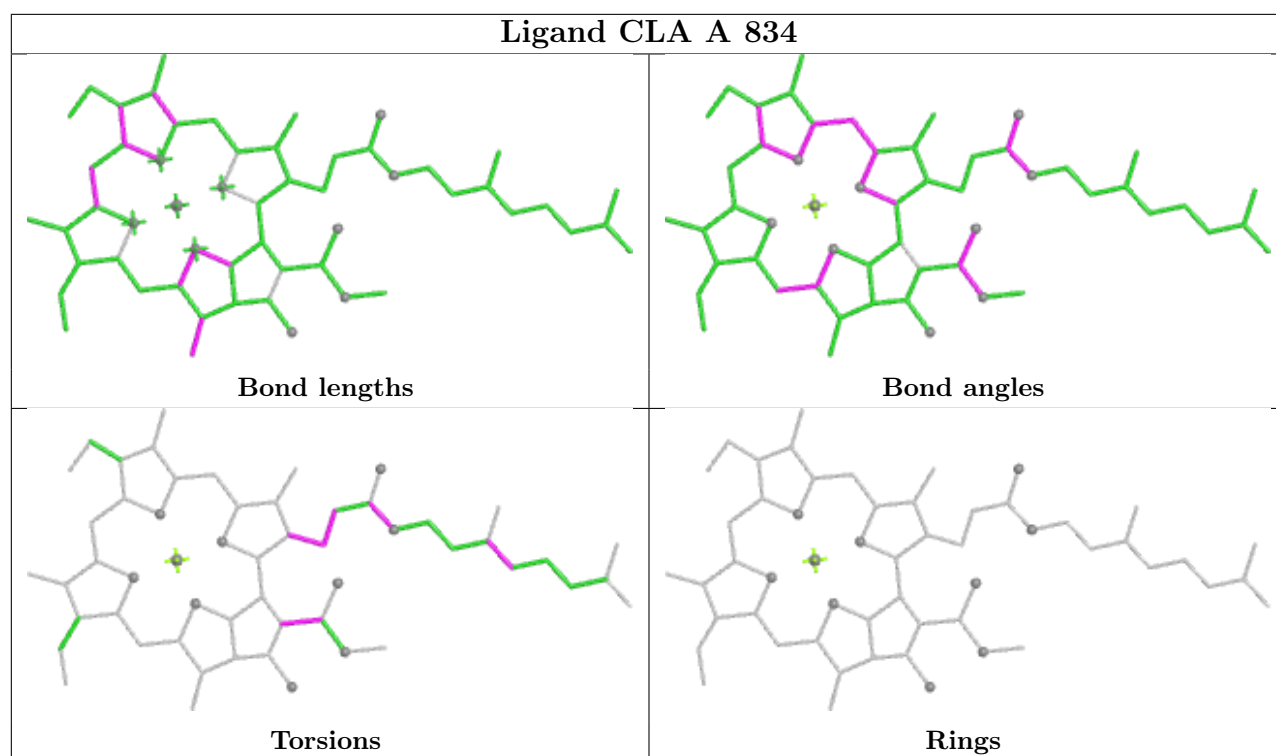
Bond angles

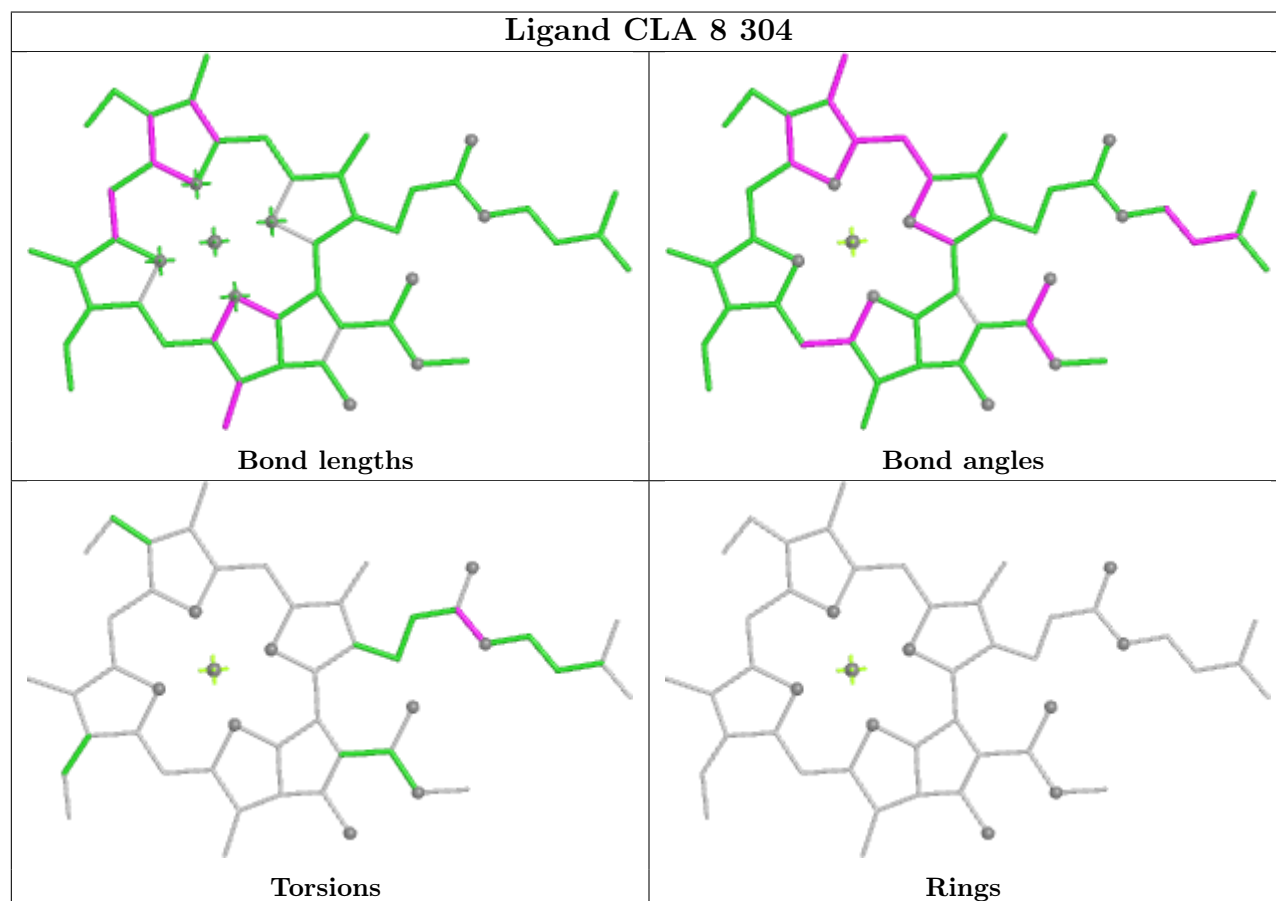
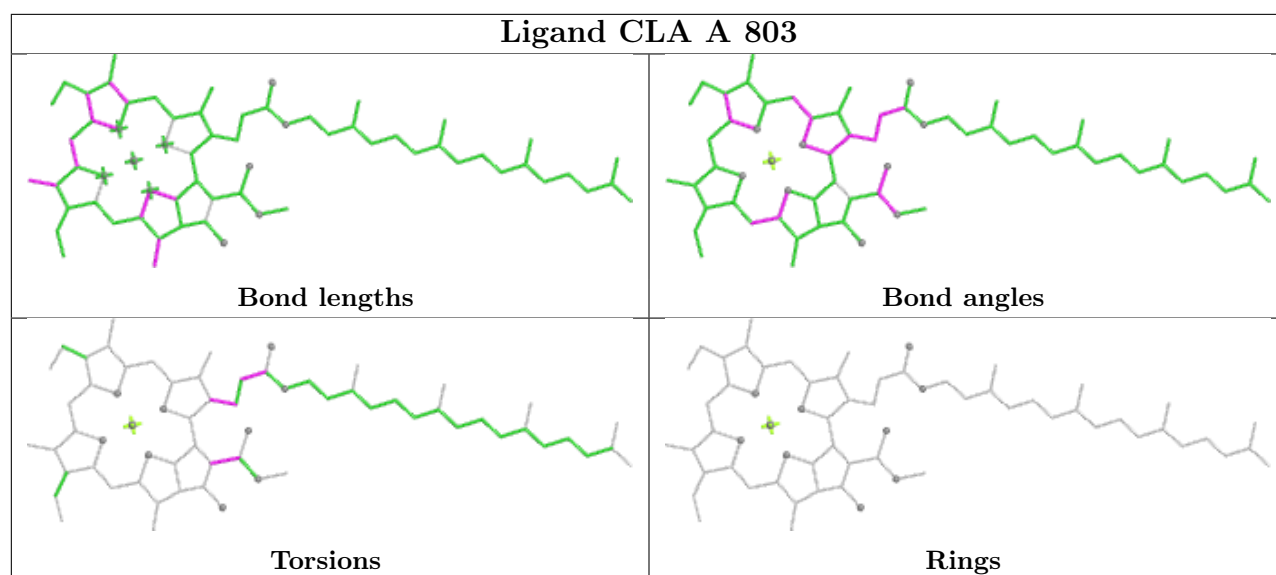


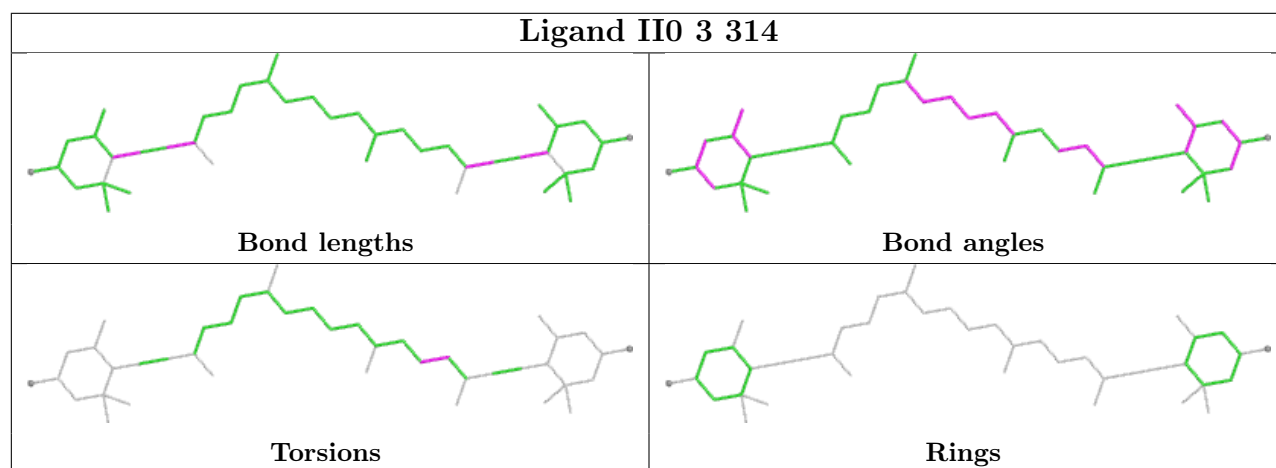
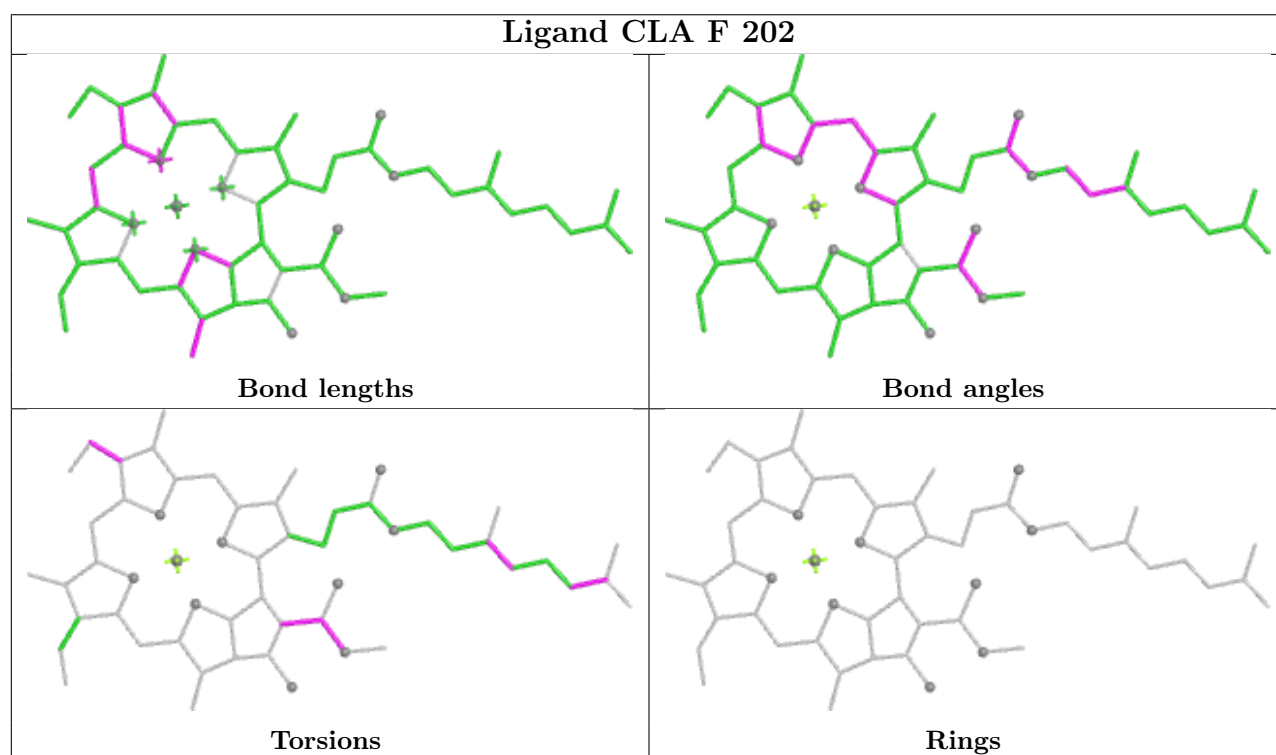
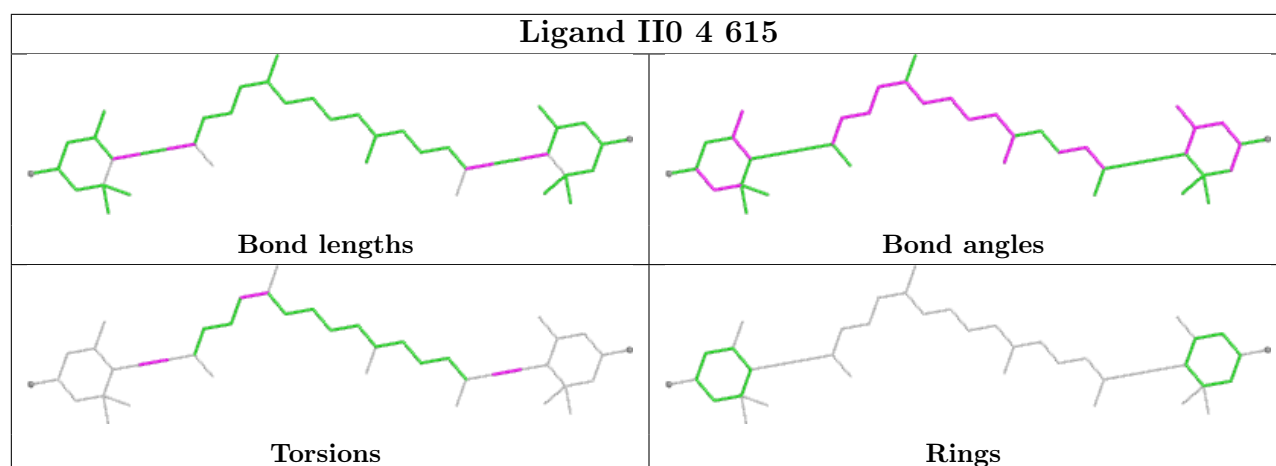
Torsions

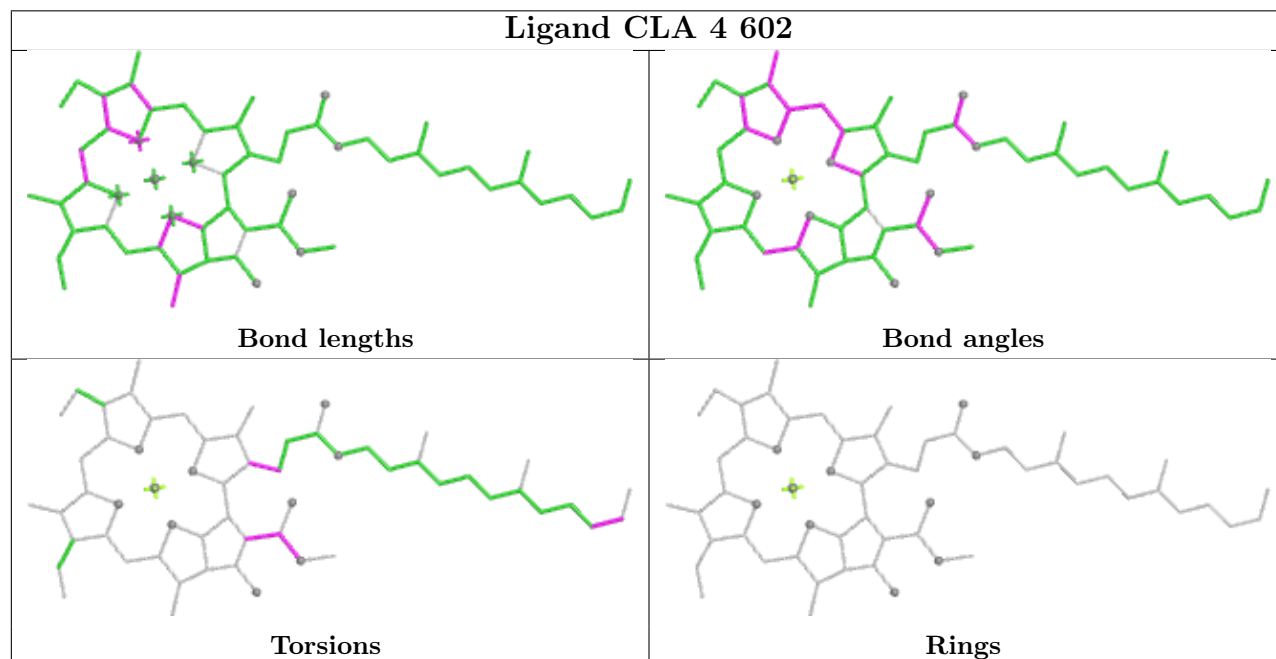
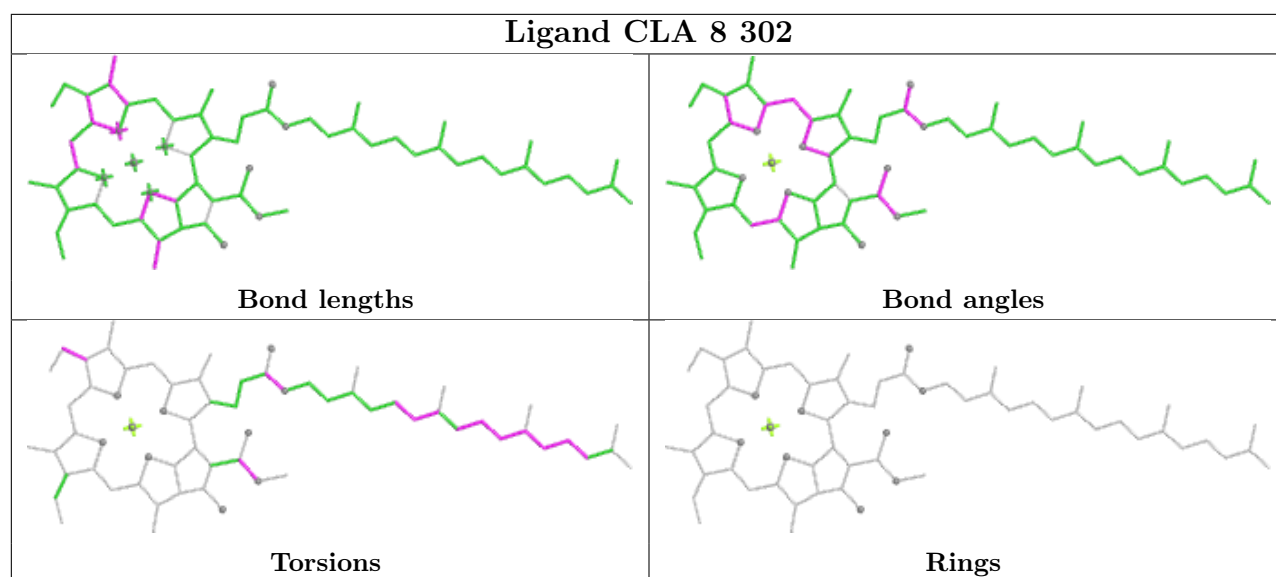


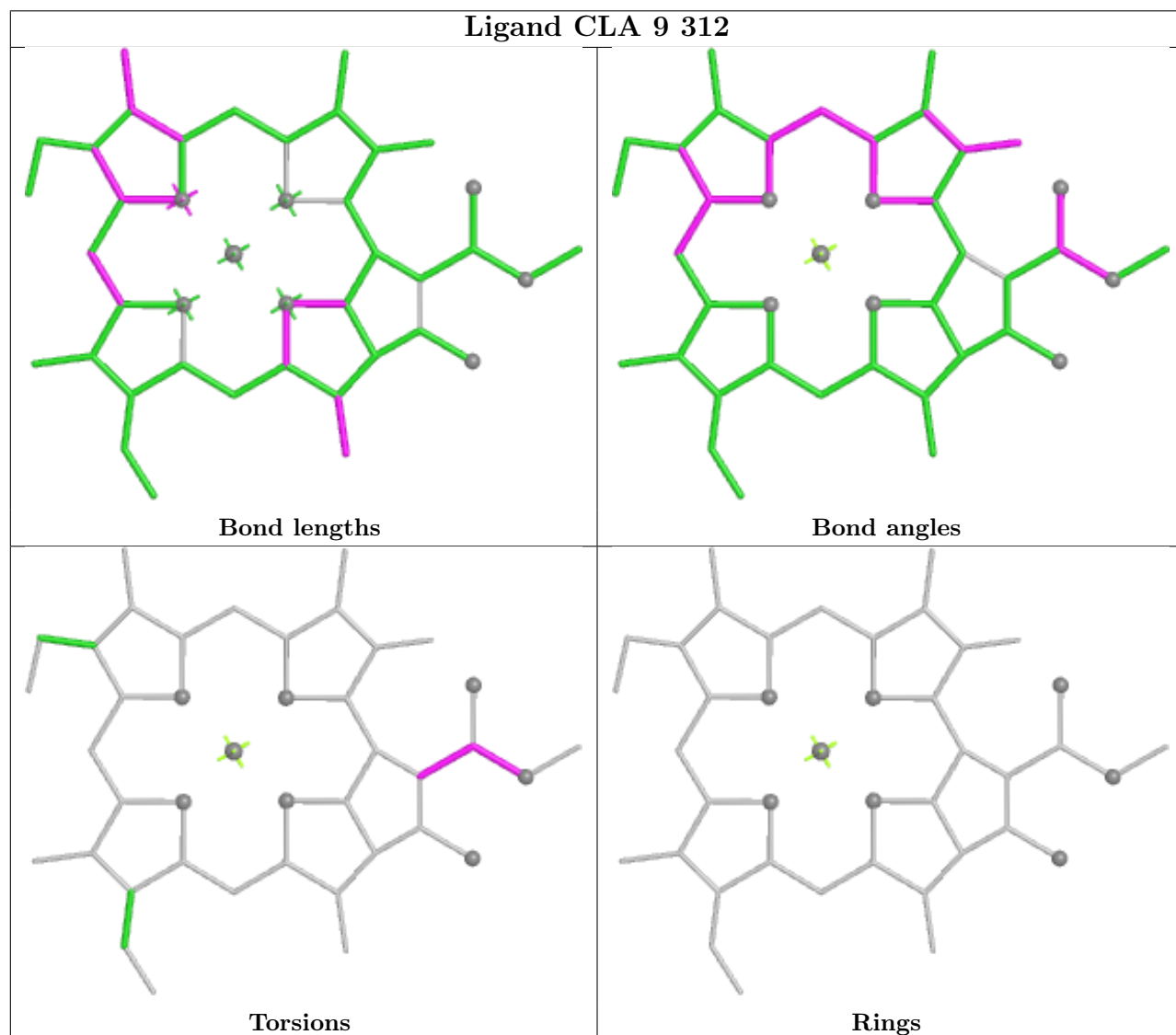
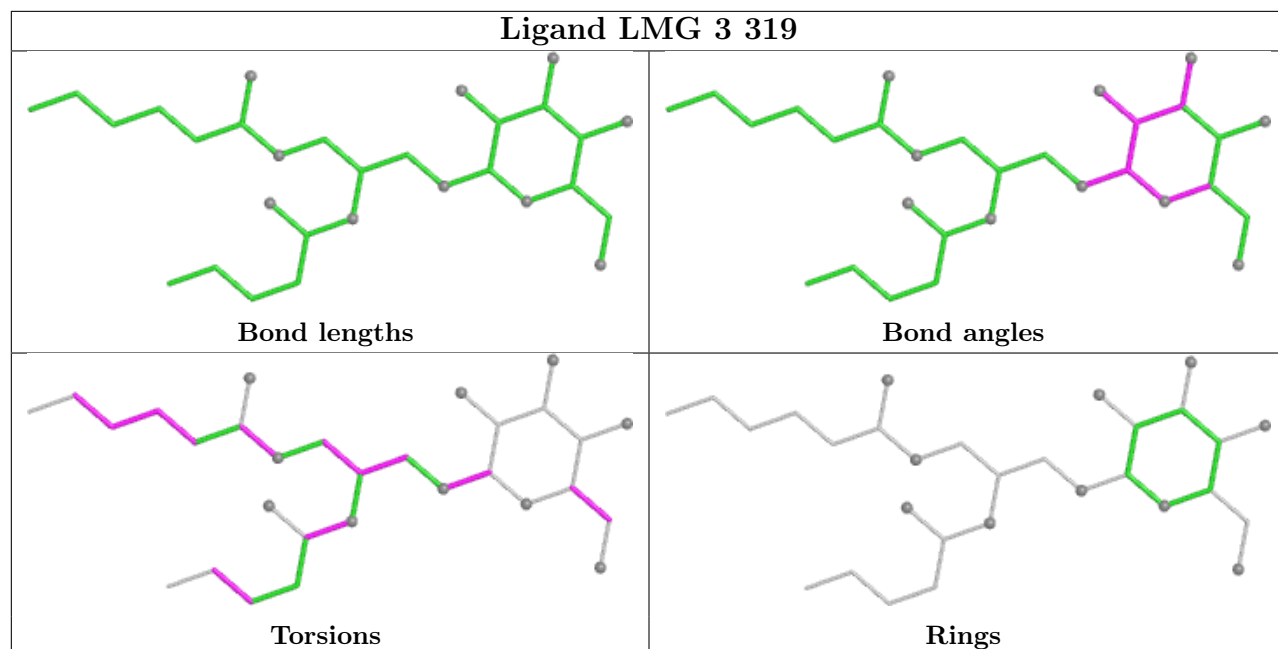
Rings

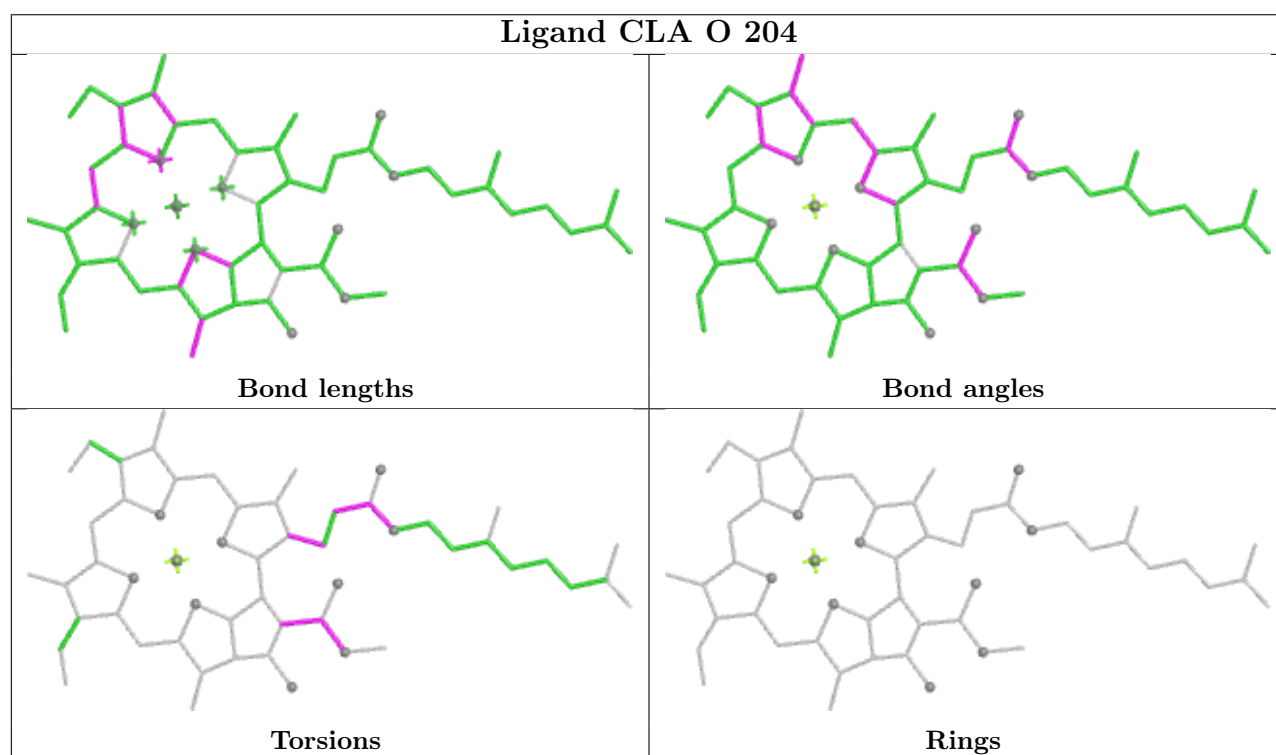
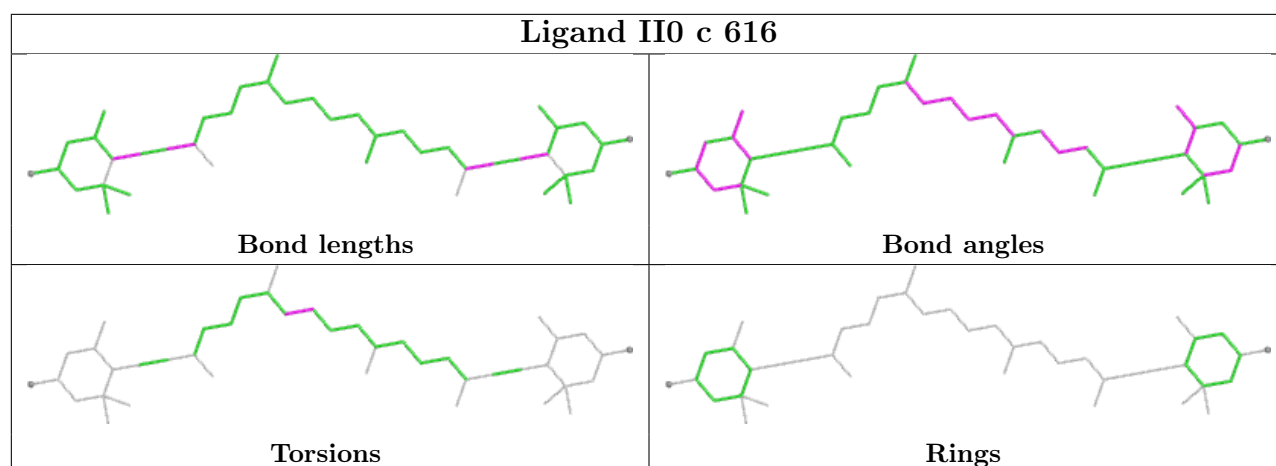




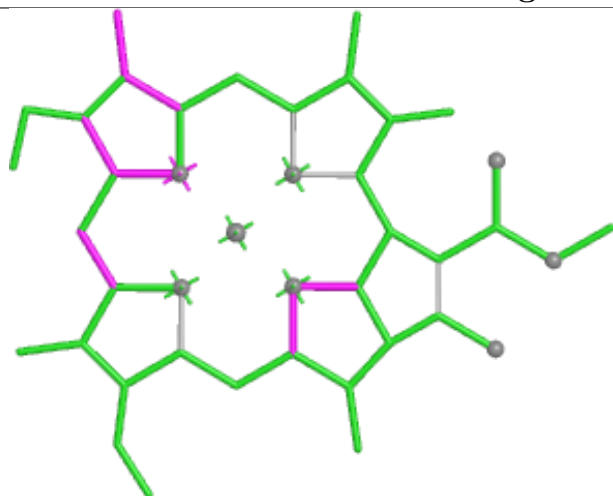




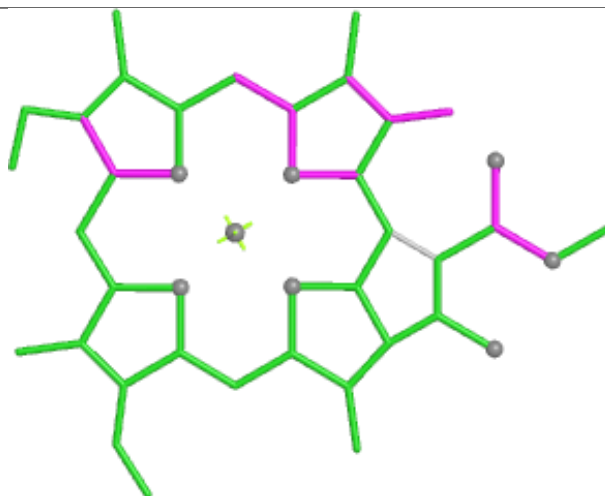




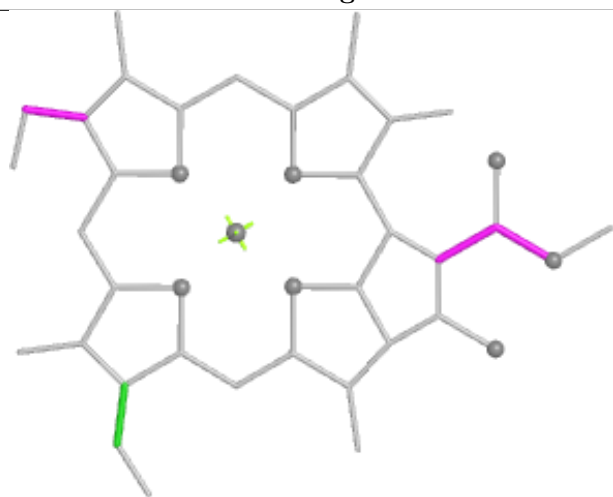
Ligand CLA 1 609



Bond lengths



Bond angles

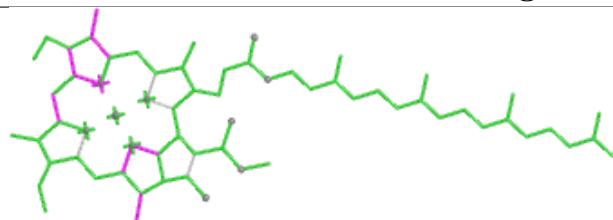


Torsions

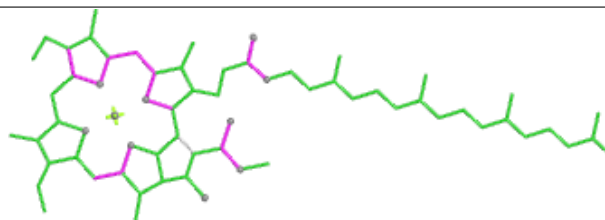


Rings

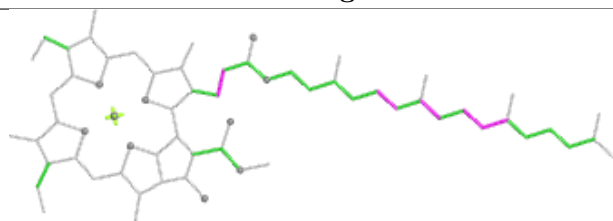
Ligand CLA 8 308



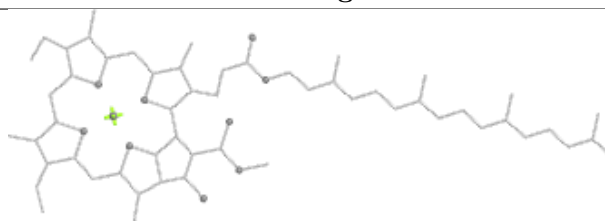
Bond lengths



Bond angles

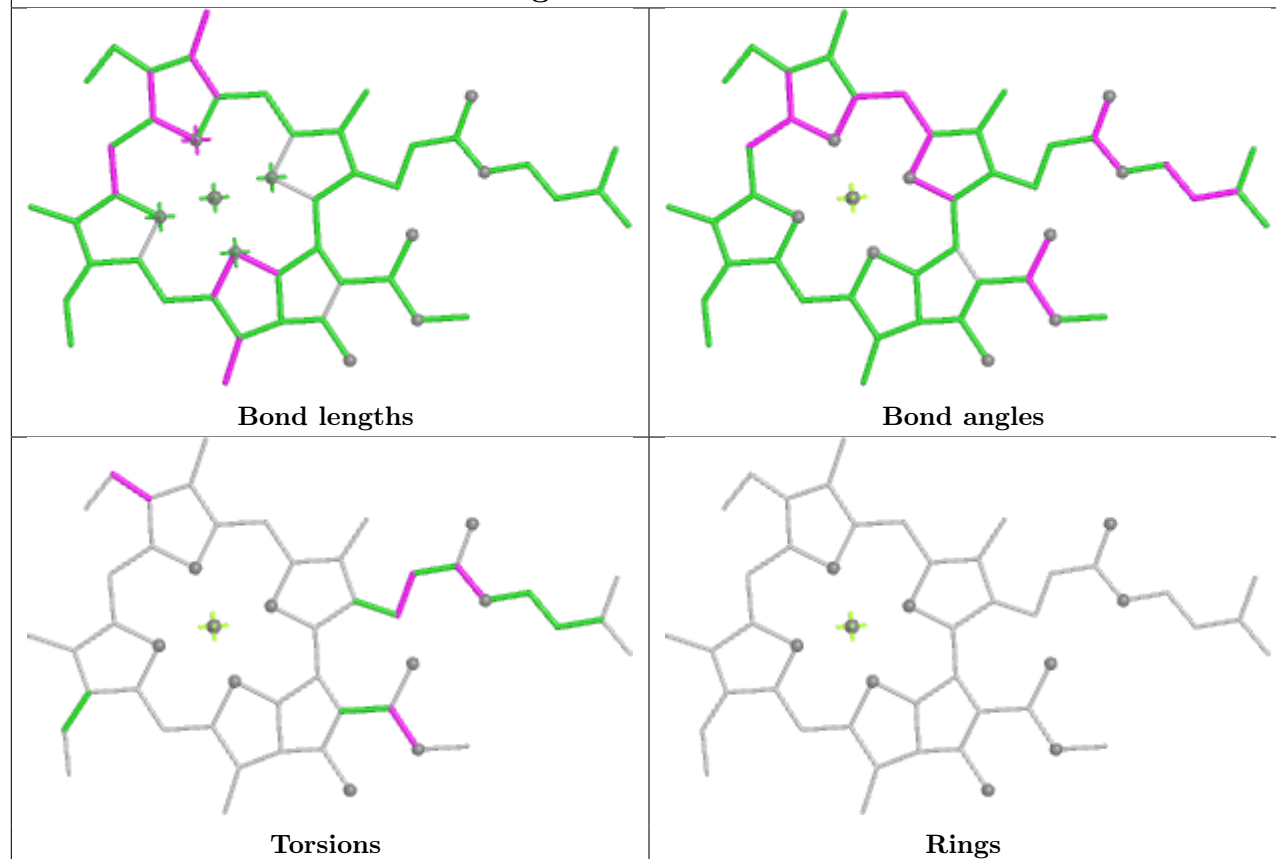


Torsions

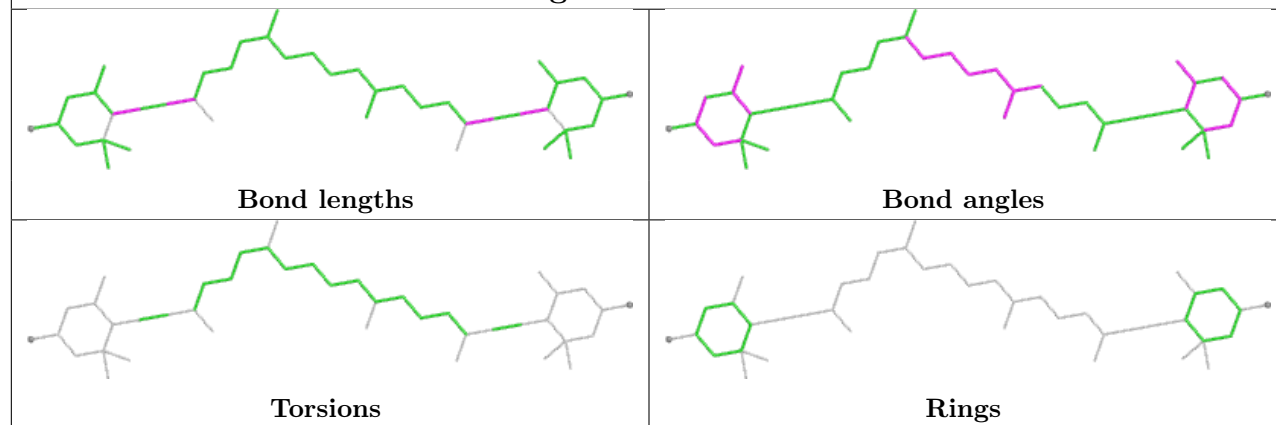


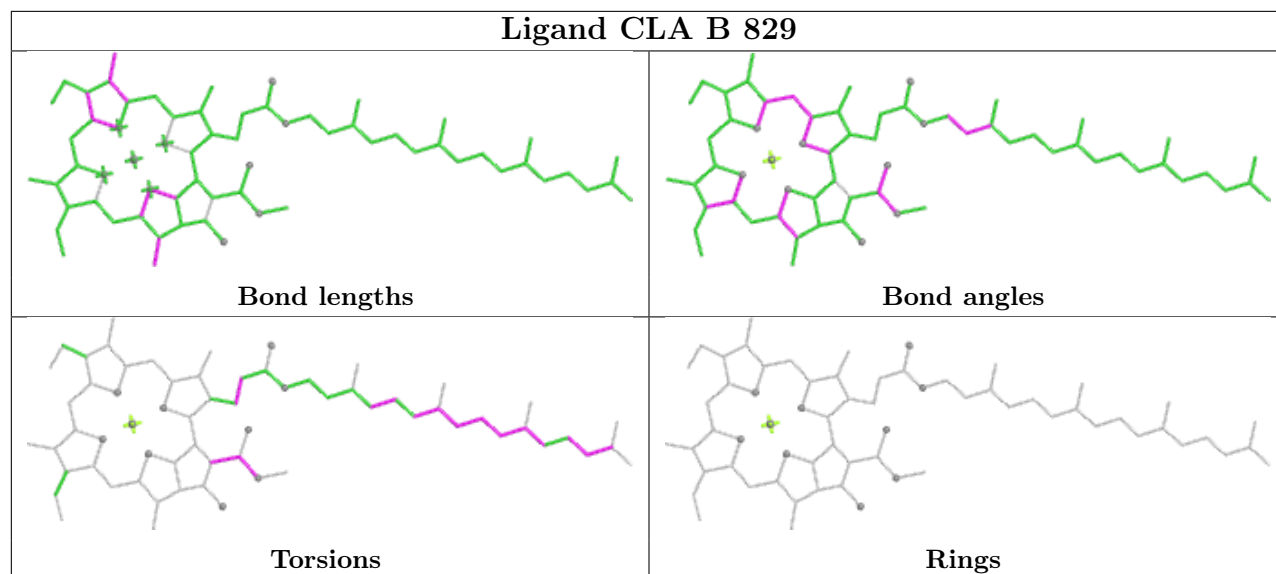
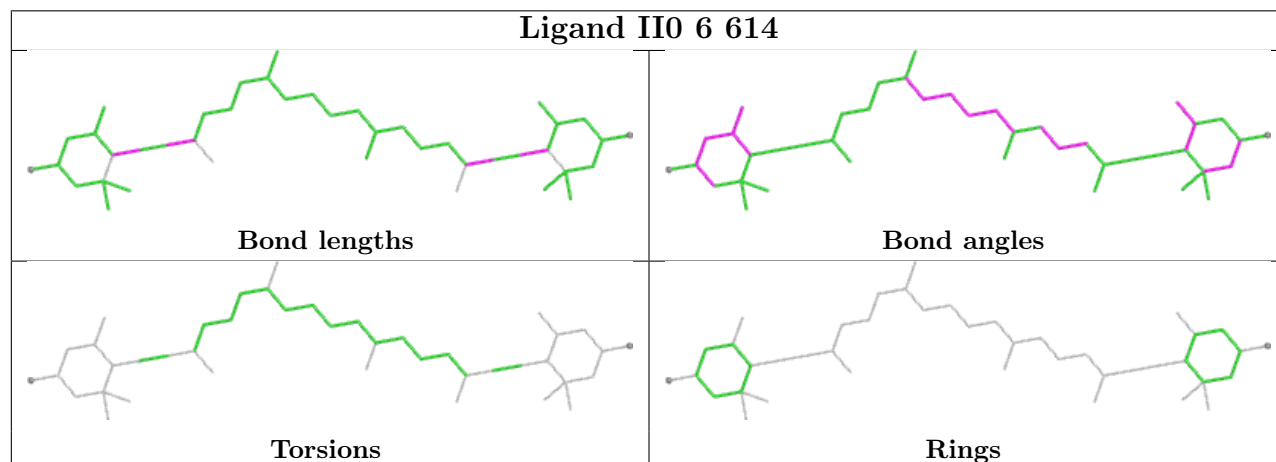
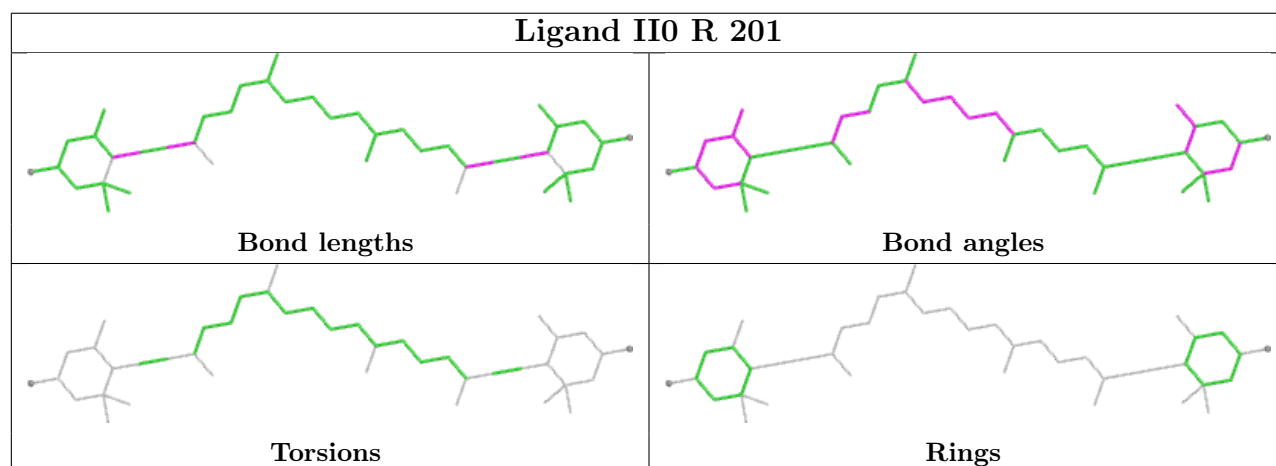
Rings

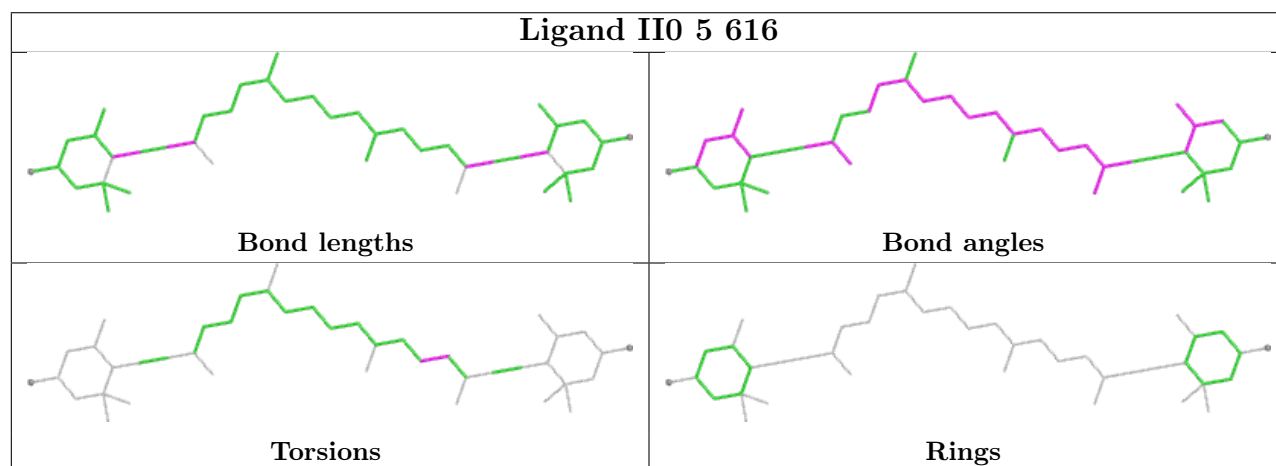
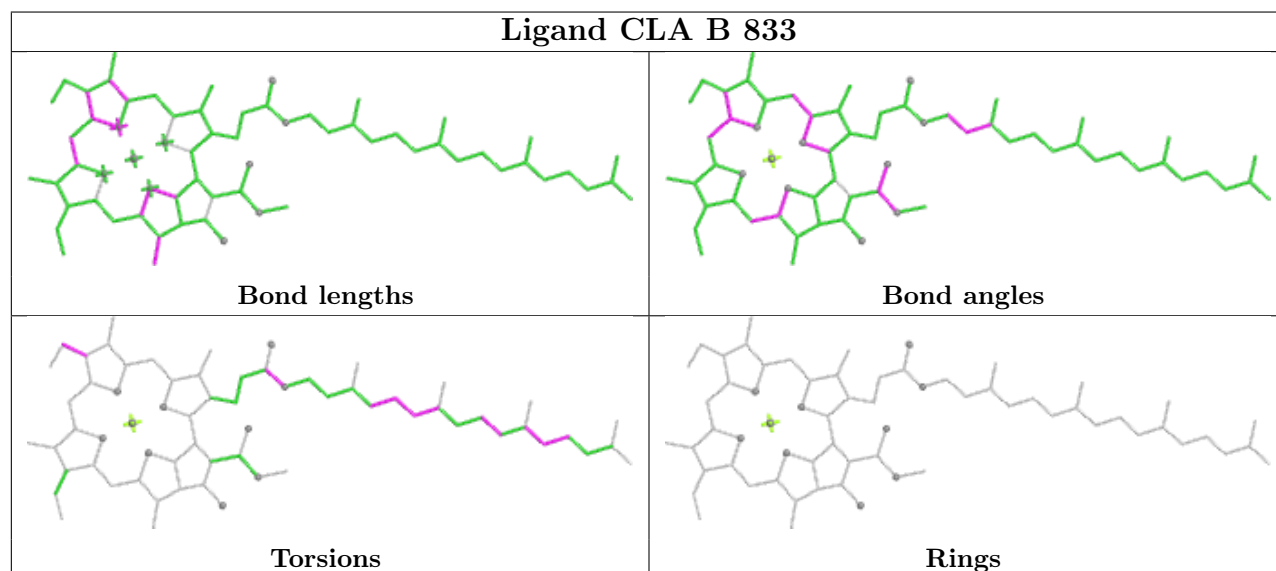
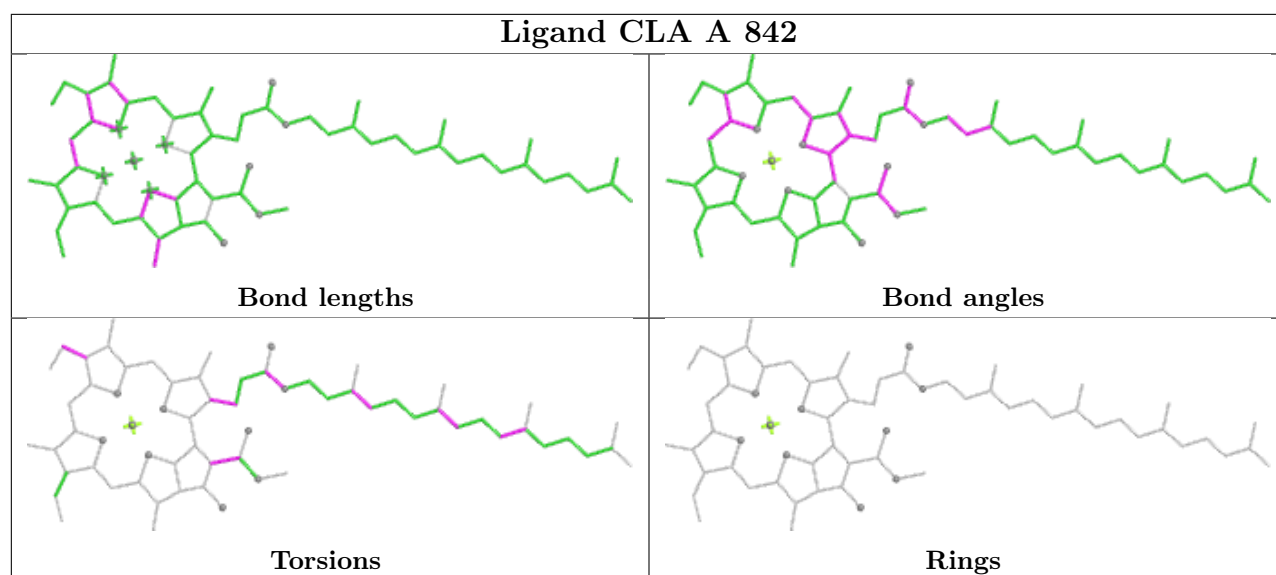
Ligand CLA A 829

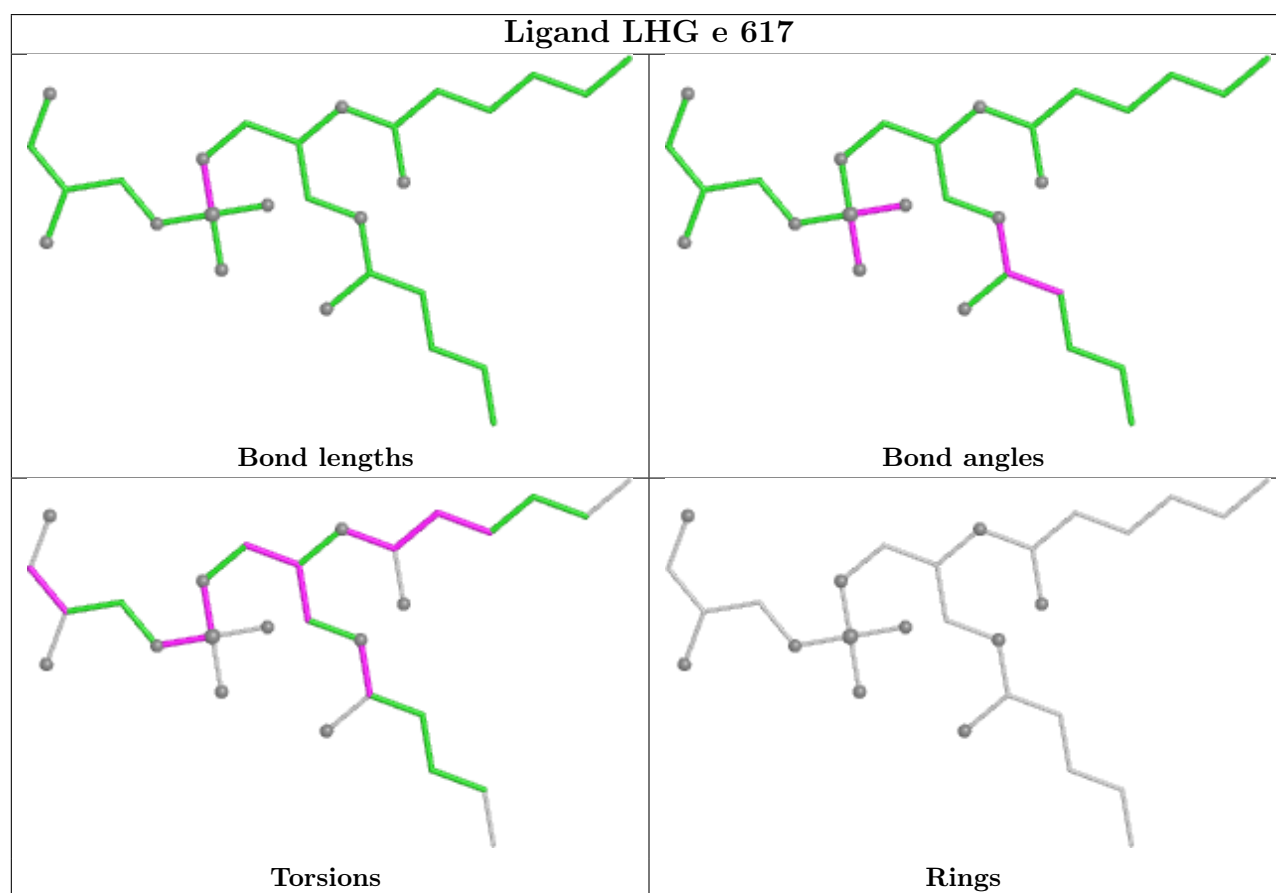
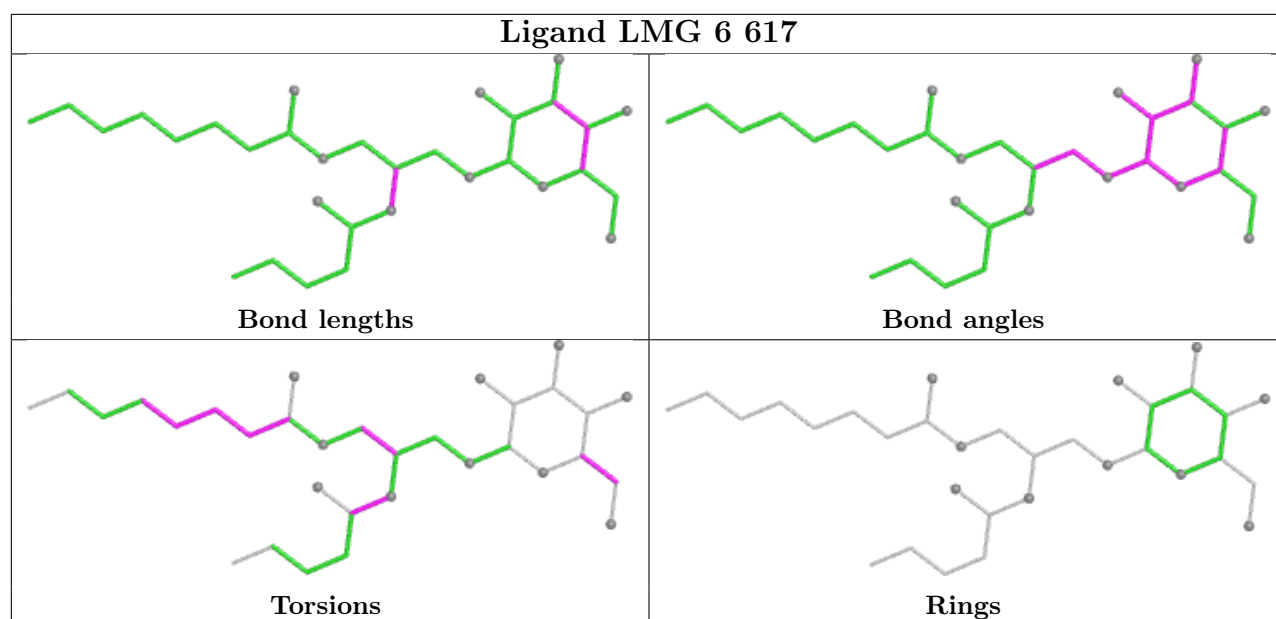


Ligand II0 d 614

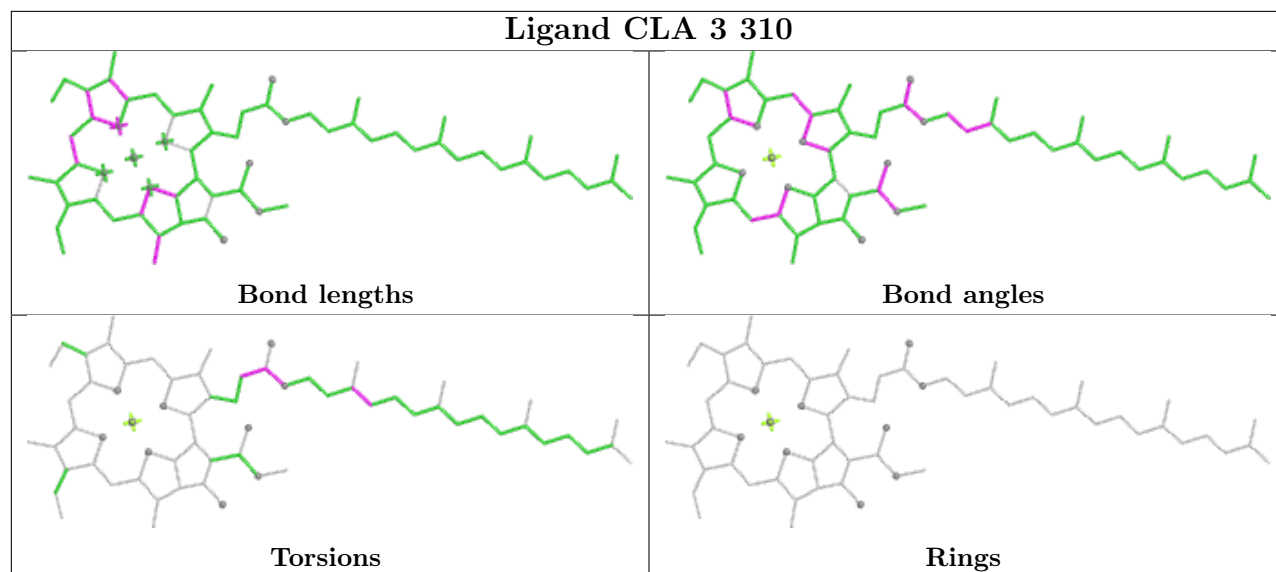


Ligand CLA B 829**Ligand II0 6 614****Ligand II0 R 201**

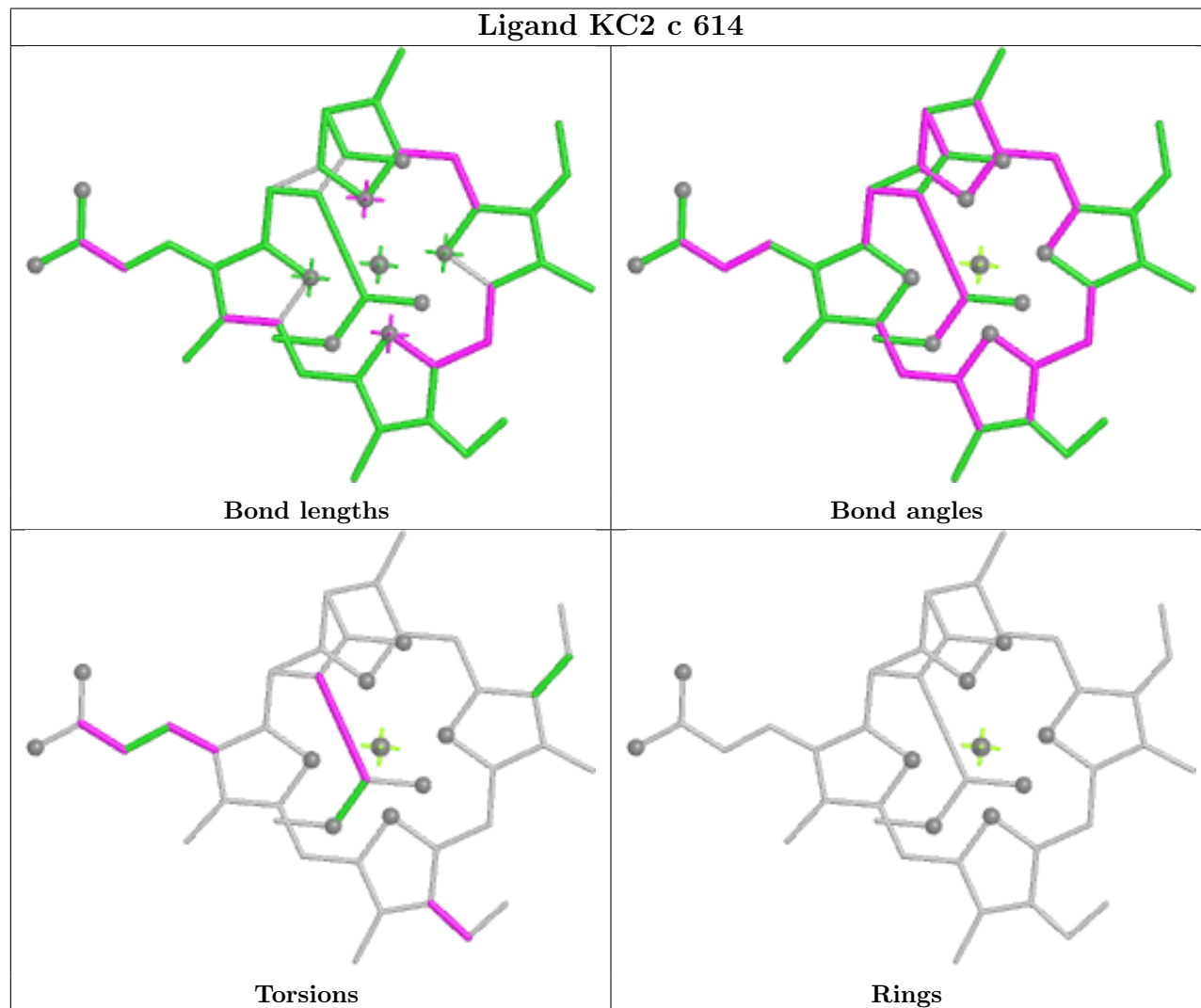


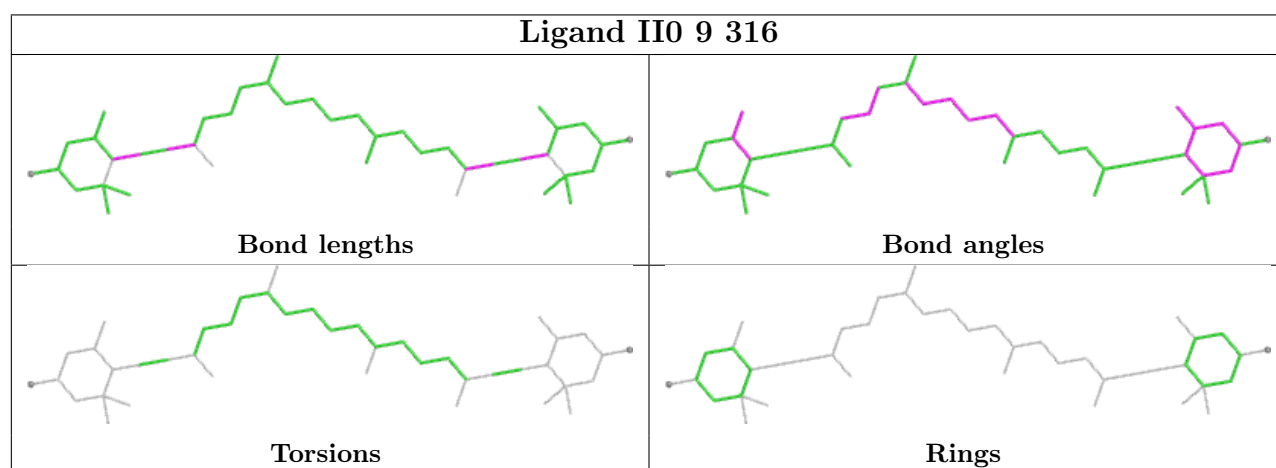
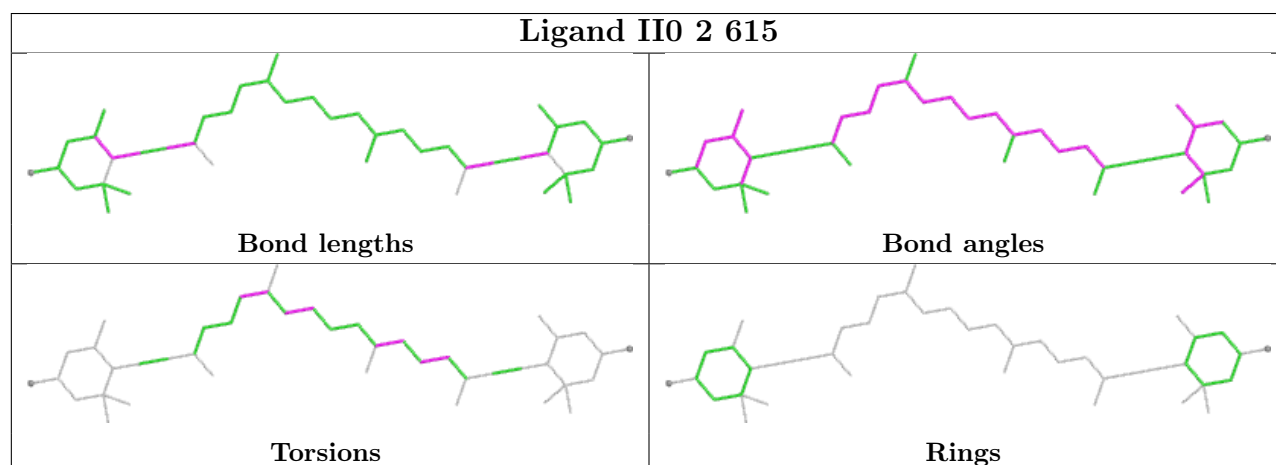
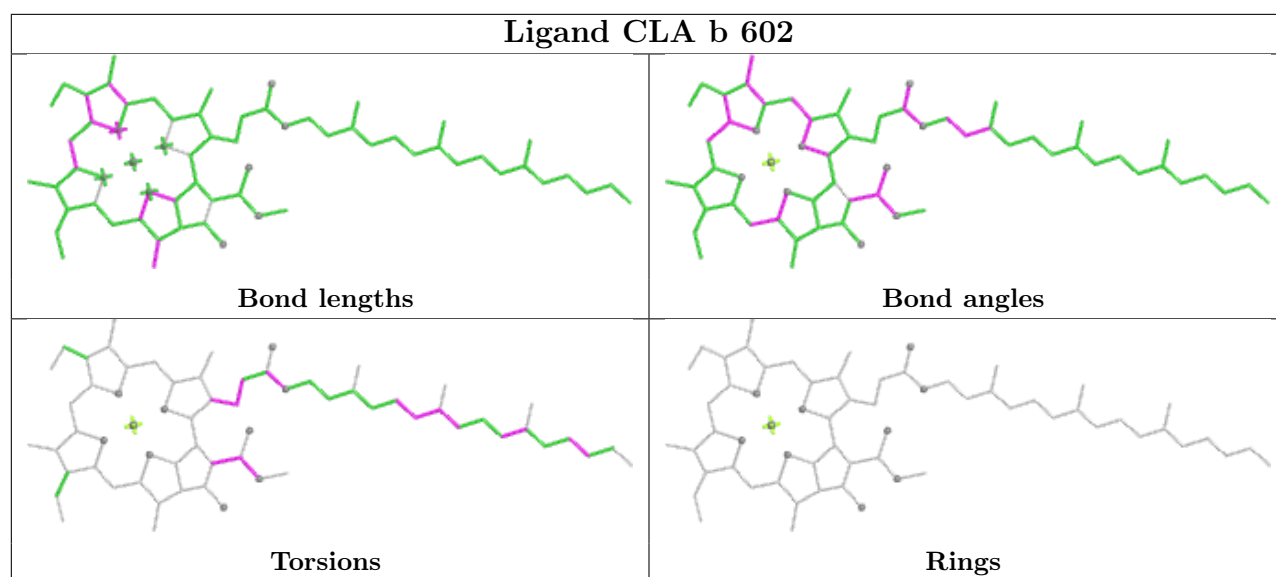


Ligand CLA 3 310

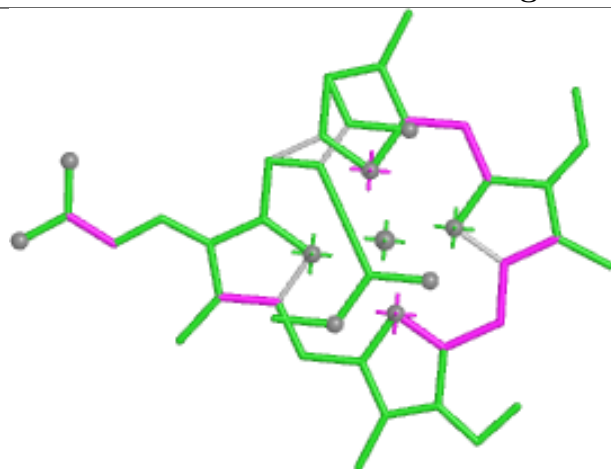


Ligand KC2 c 614

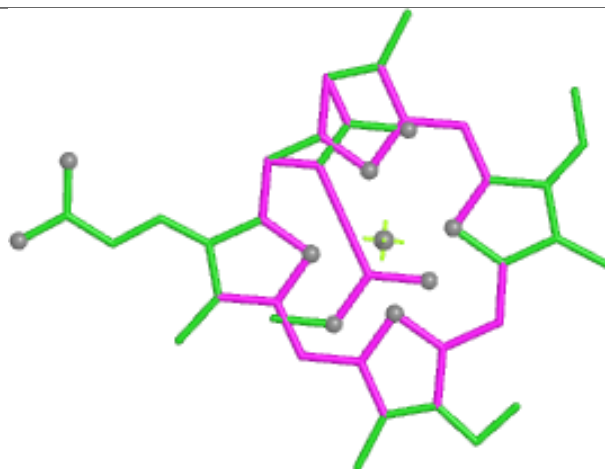




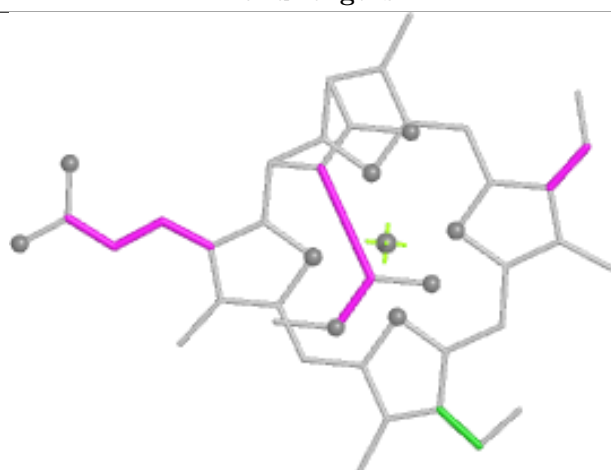
Ligand KC2 7 310



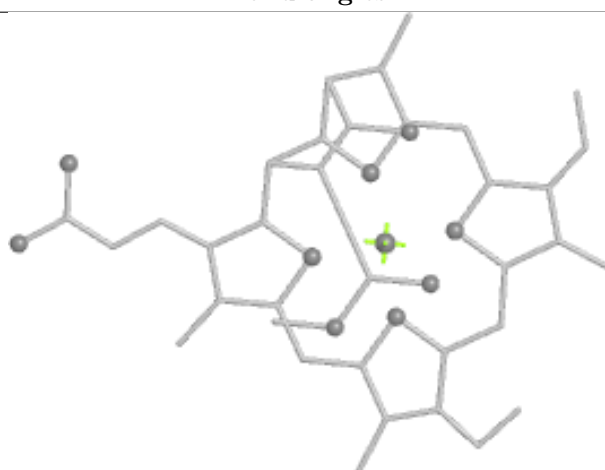
Bond lengths



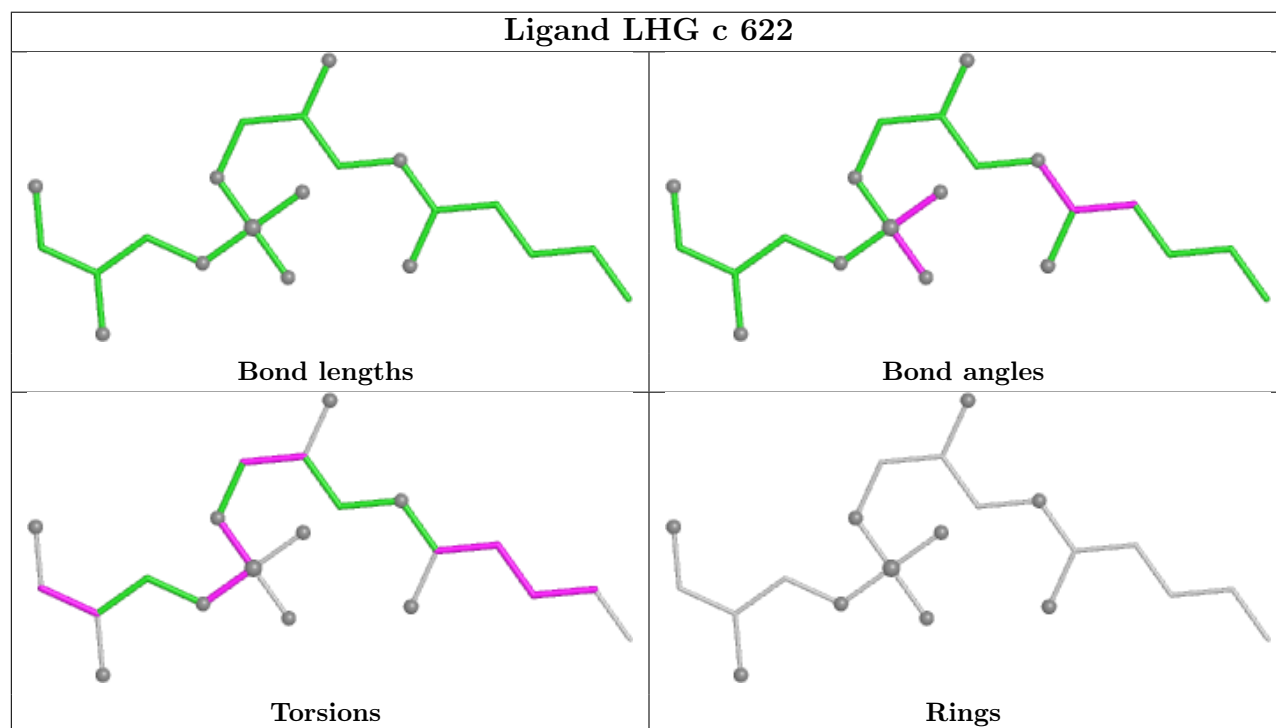
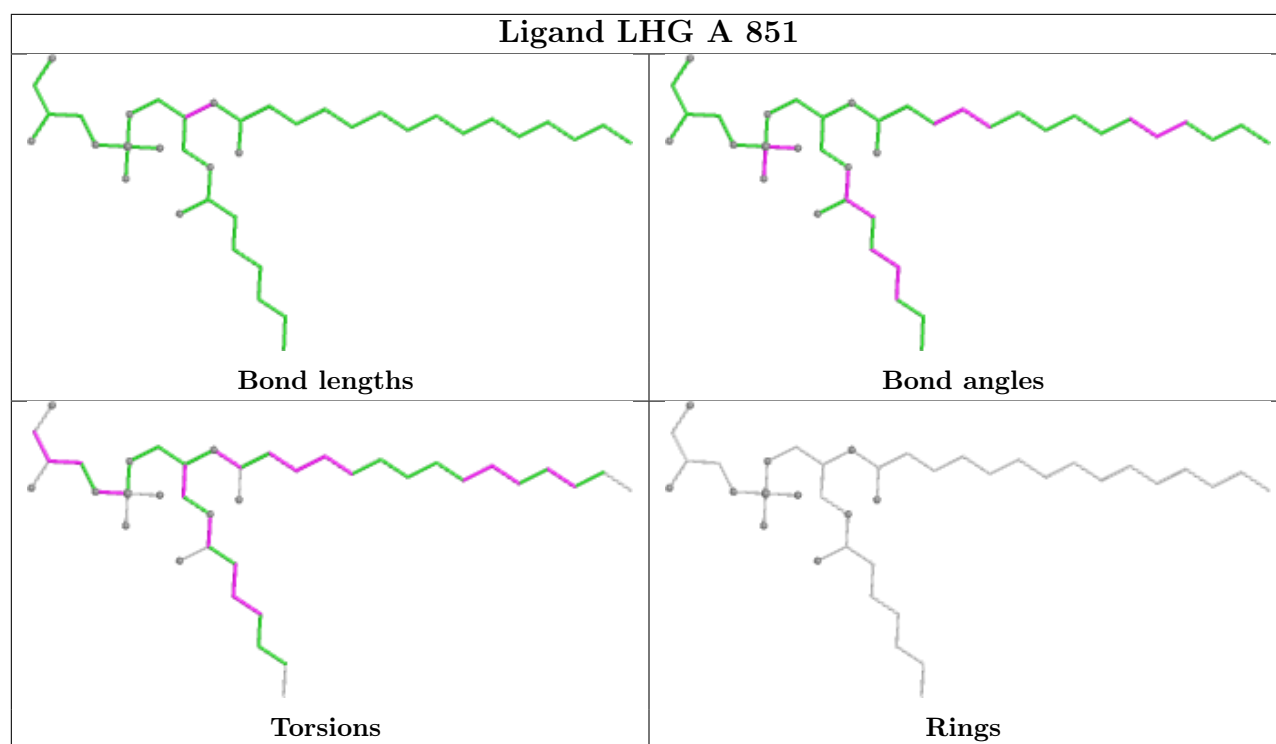
Bond angles

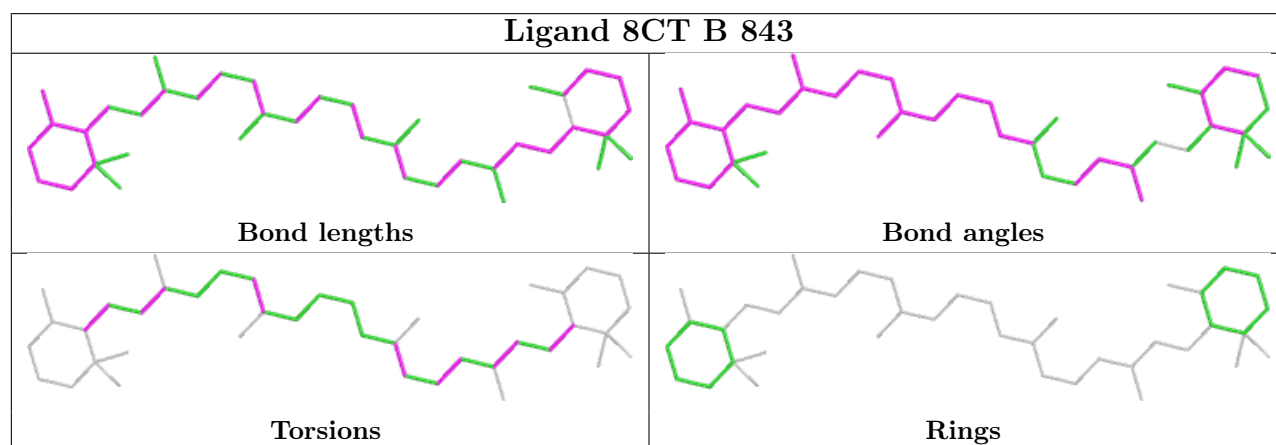
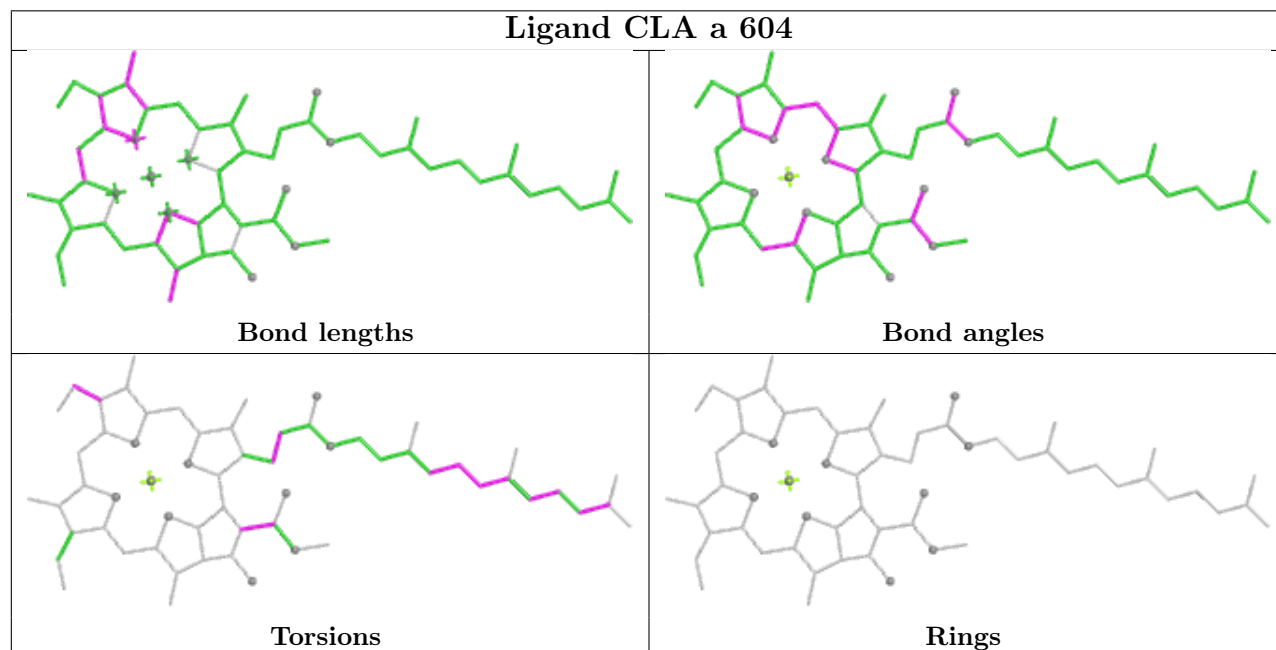
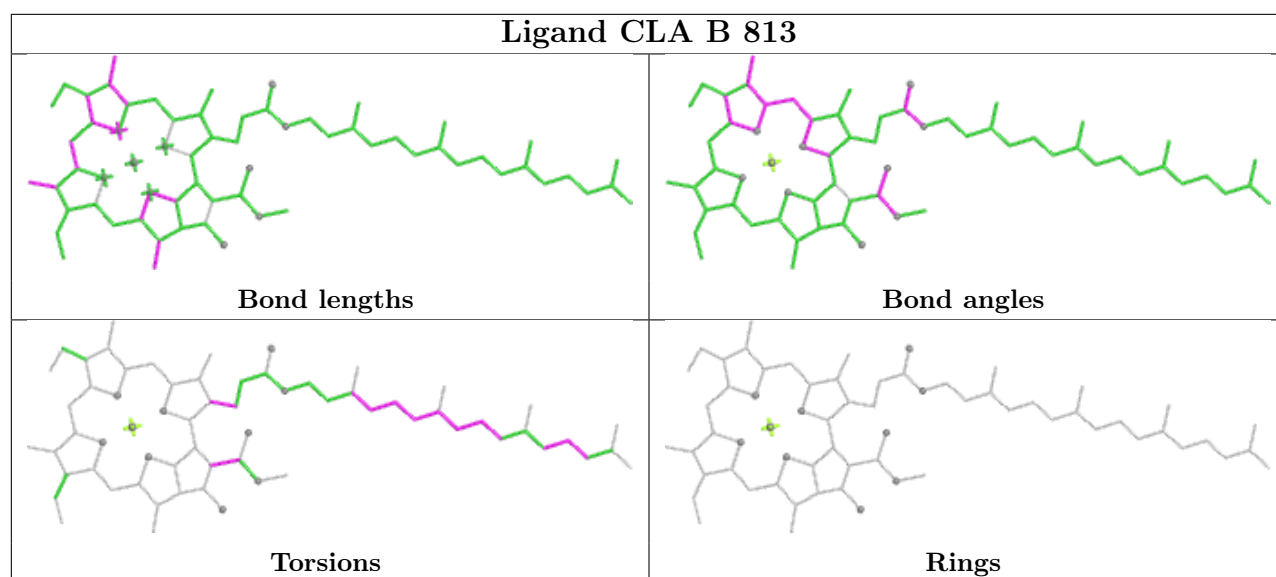


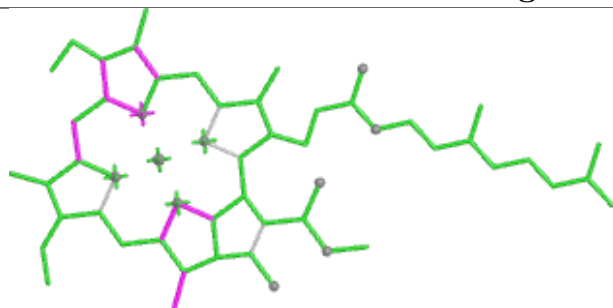
Torsions



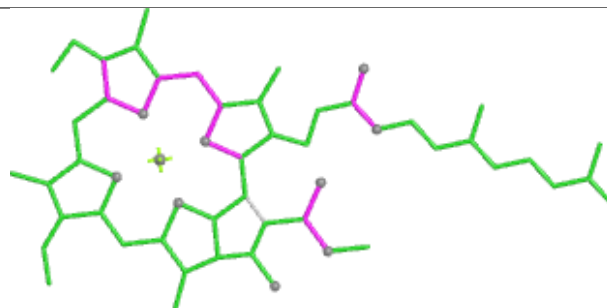
Rings



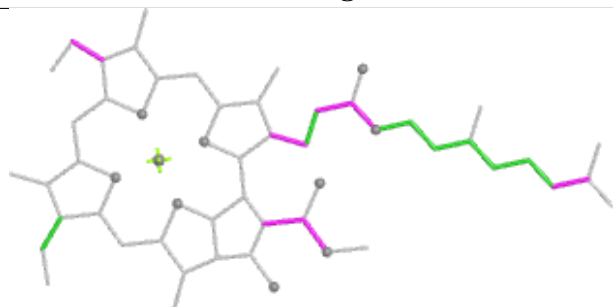


Ligand CLA a 605

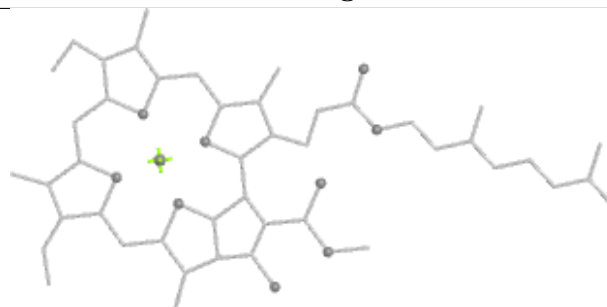
Bond lengths



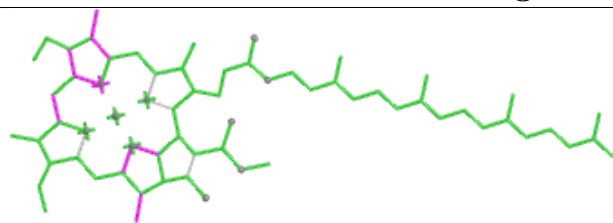
Bond angles



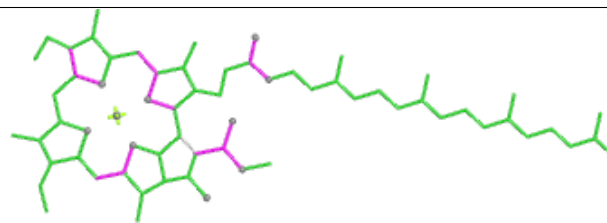
Torsions



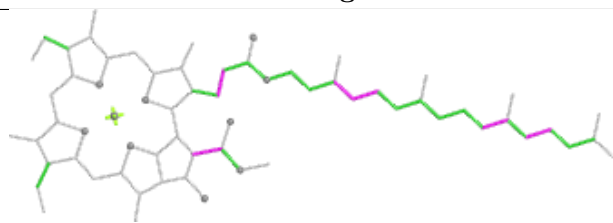
Rings

Ligand CLA B 807

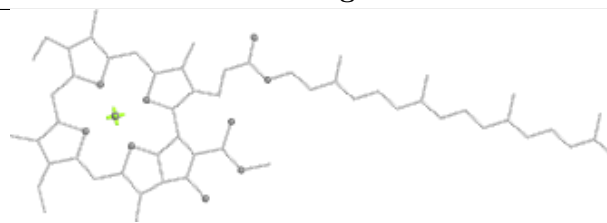
Bond lengths



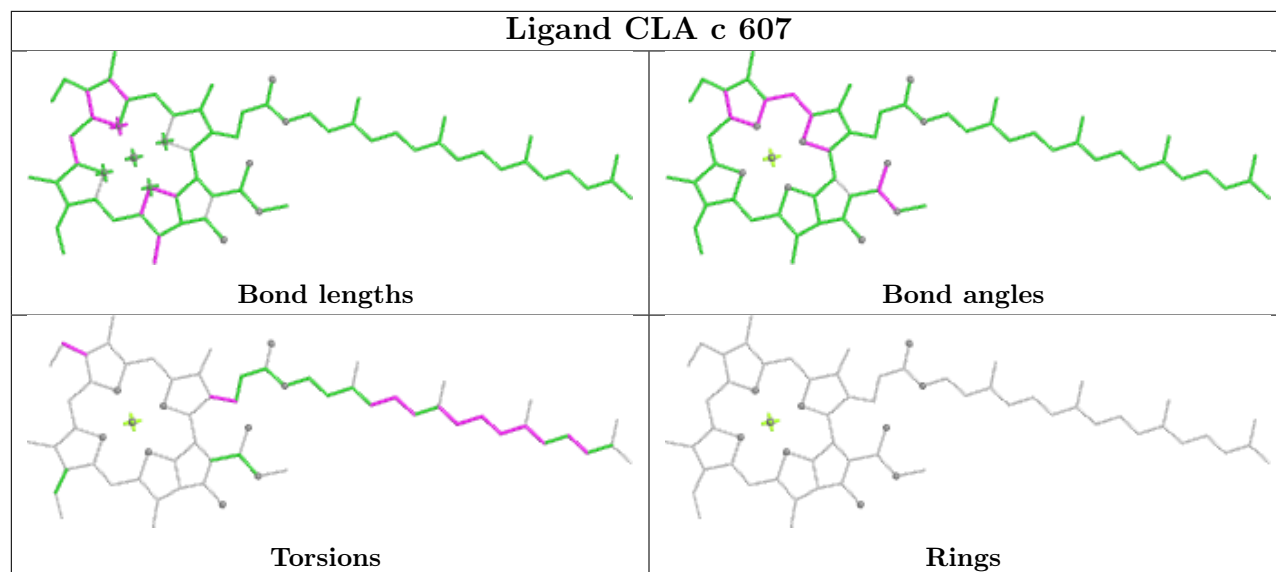
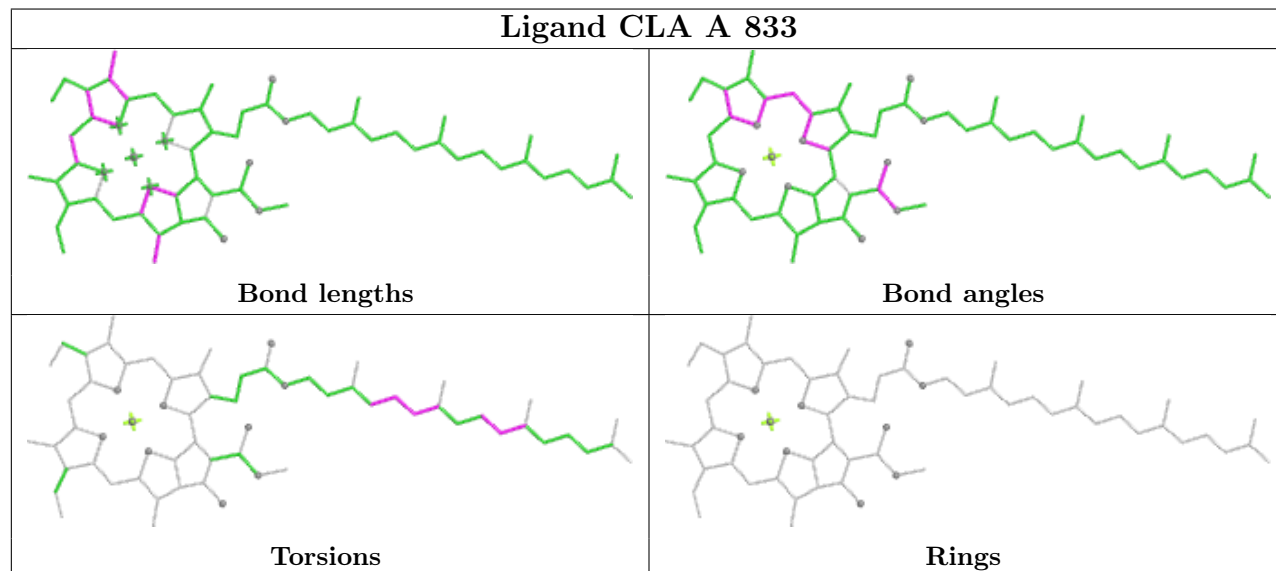
Bond angles



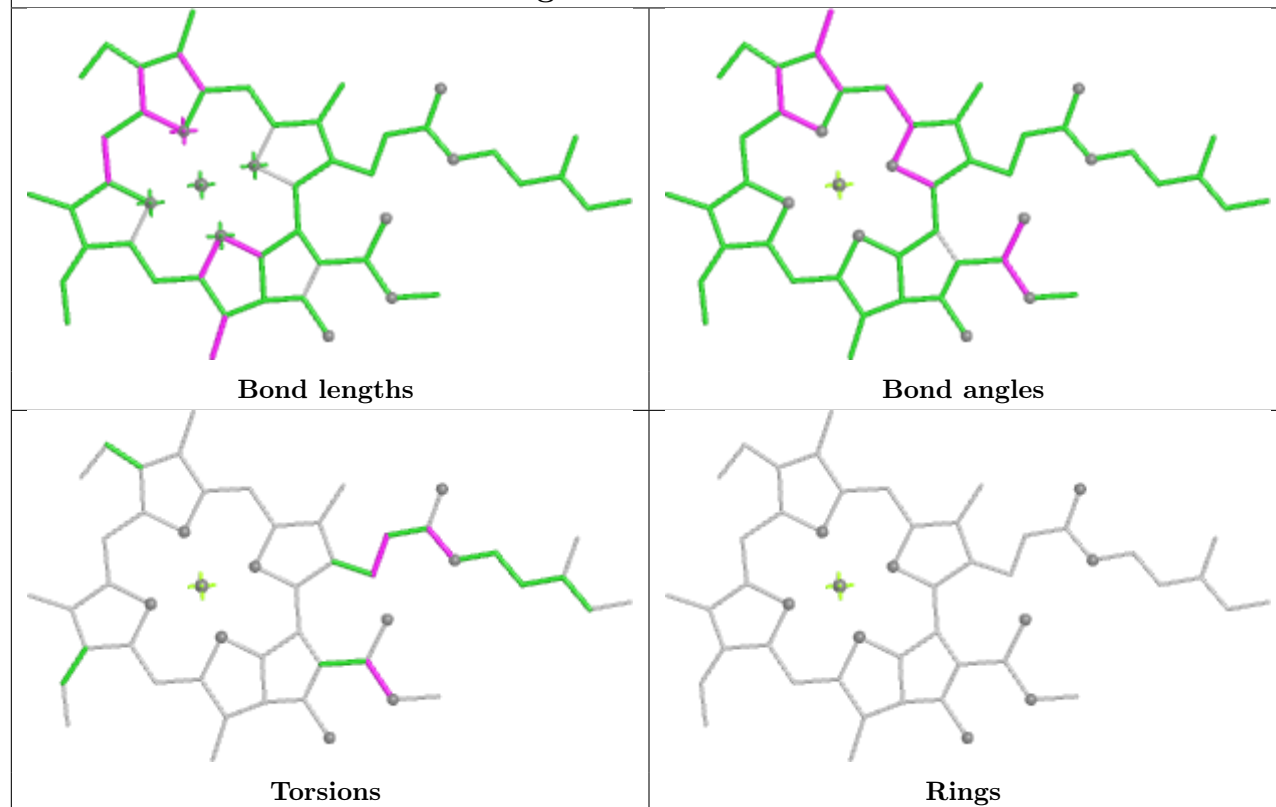
Torsions



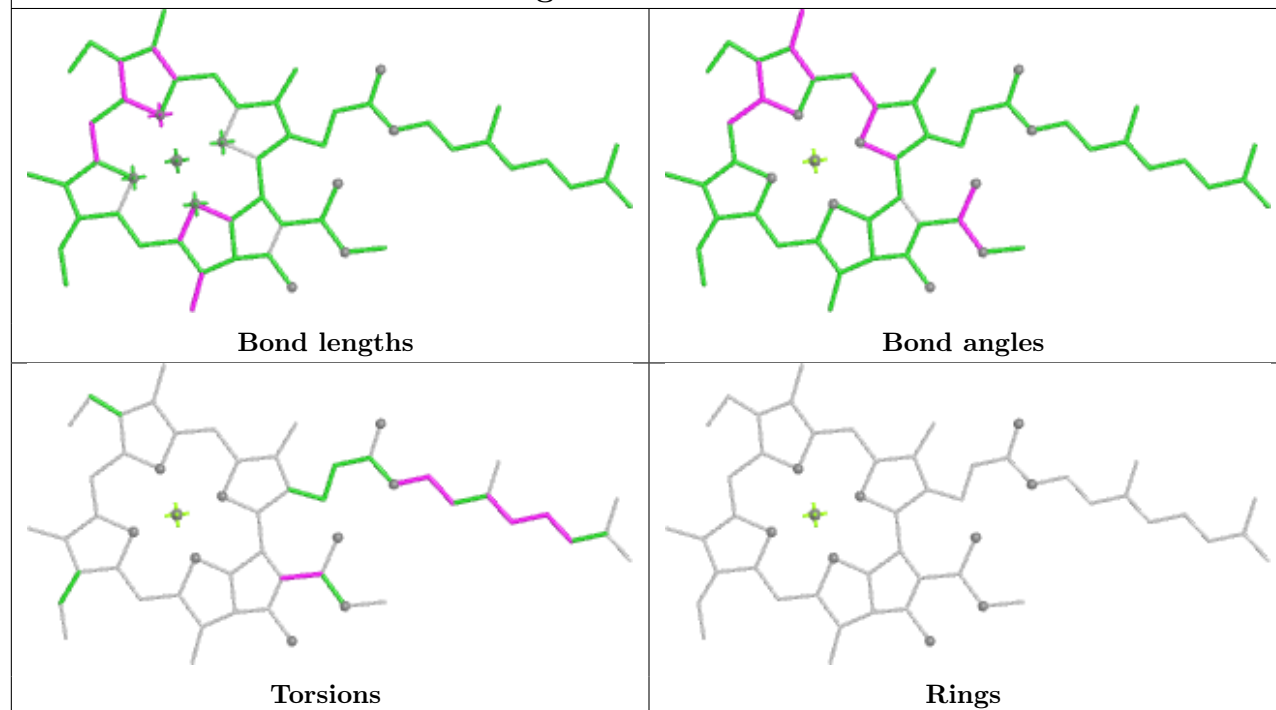
Rings

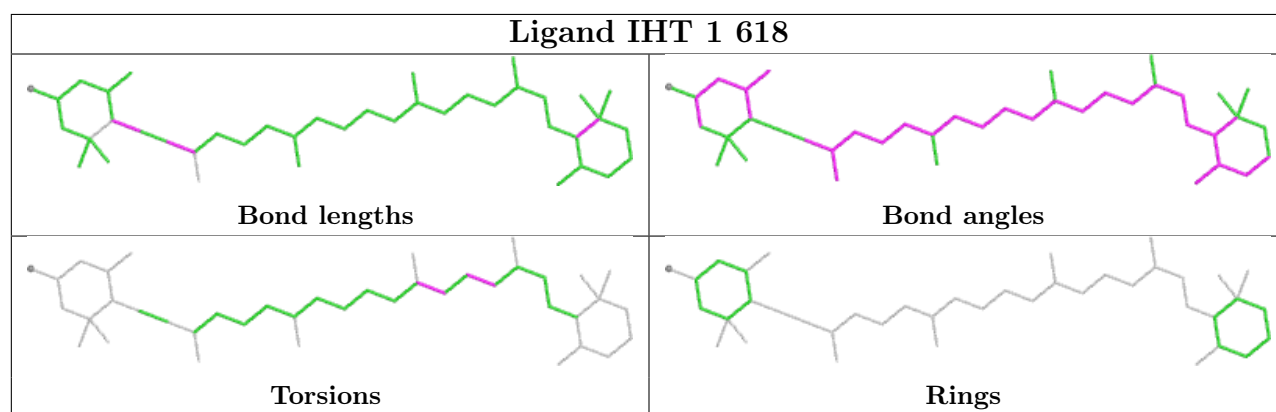
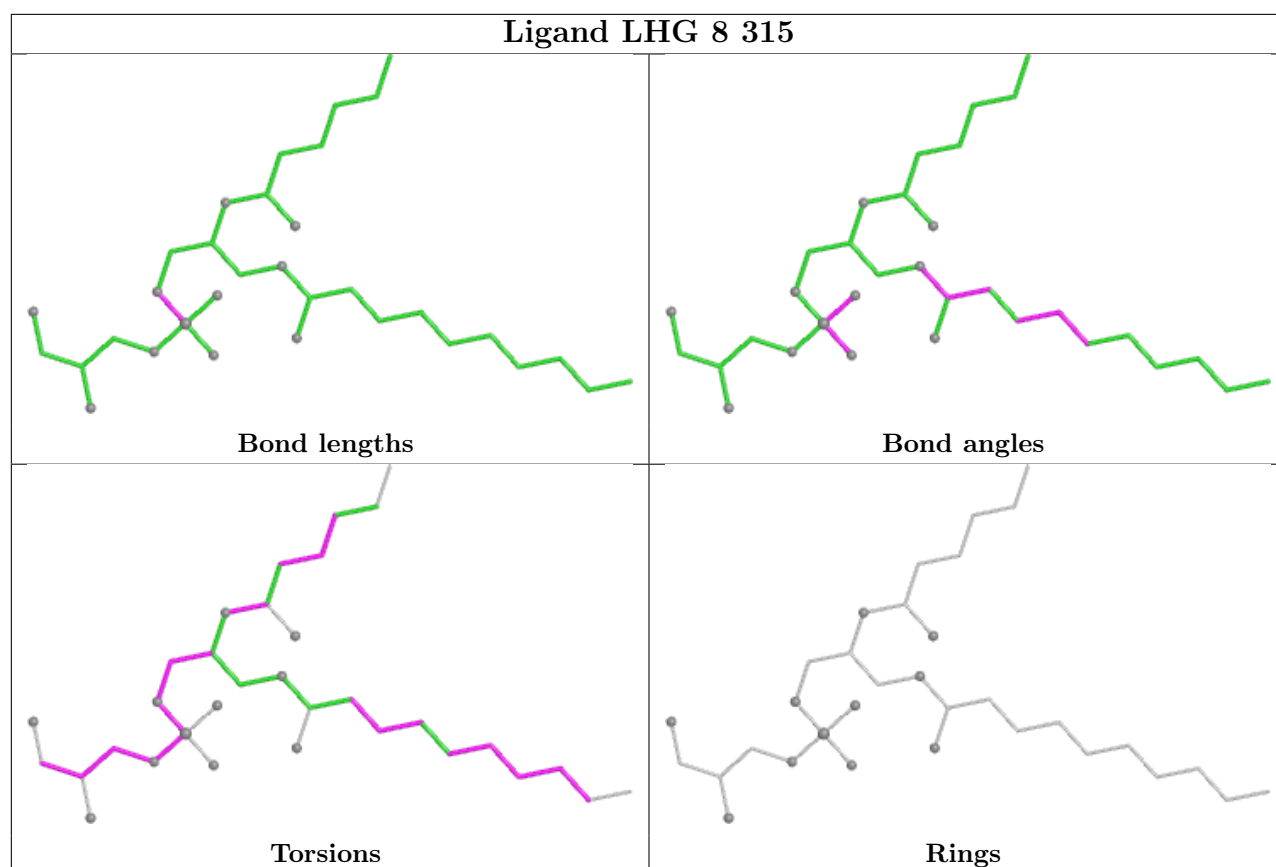
Ligand CLA c 607**Ligand CLA A 833**

Ligand CLA e 610

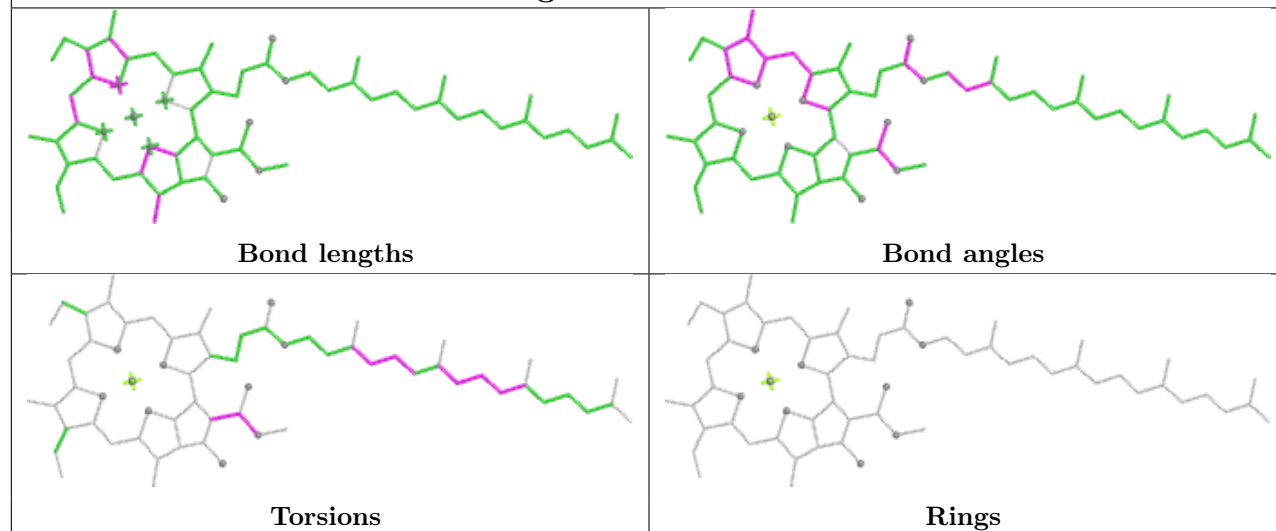


Ligand CLA 7 311

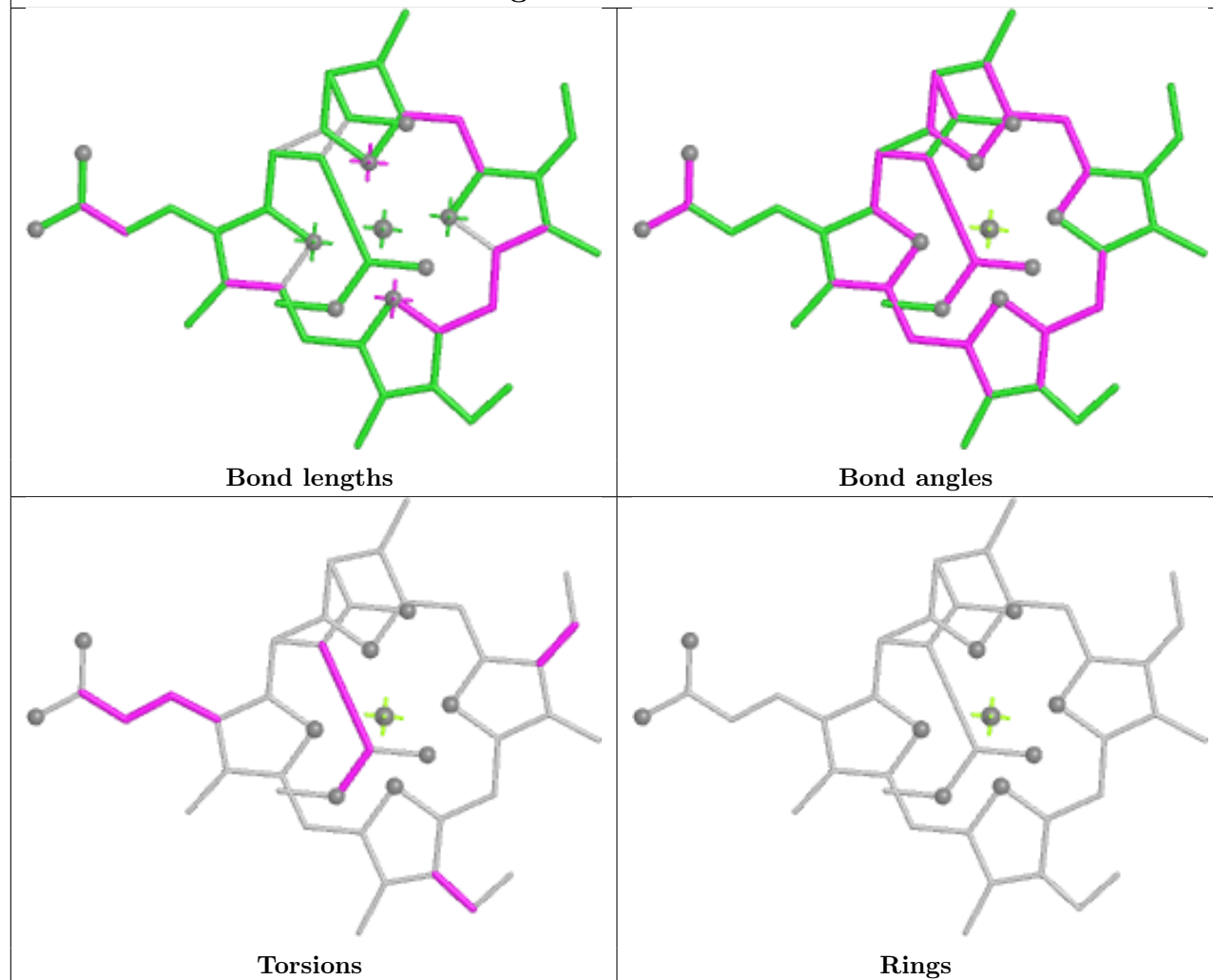


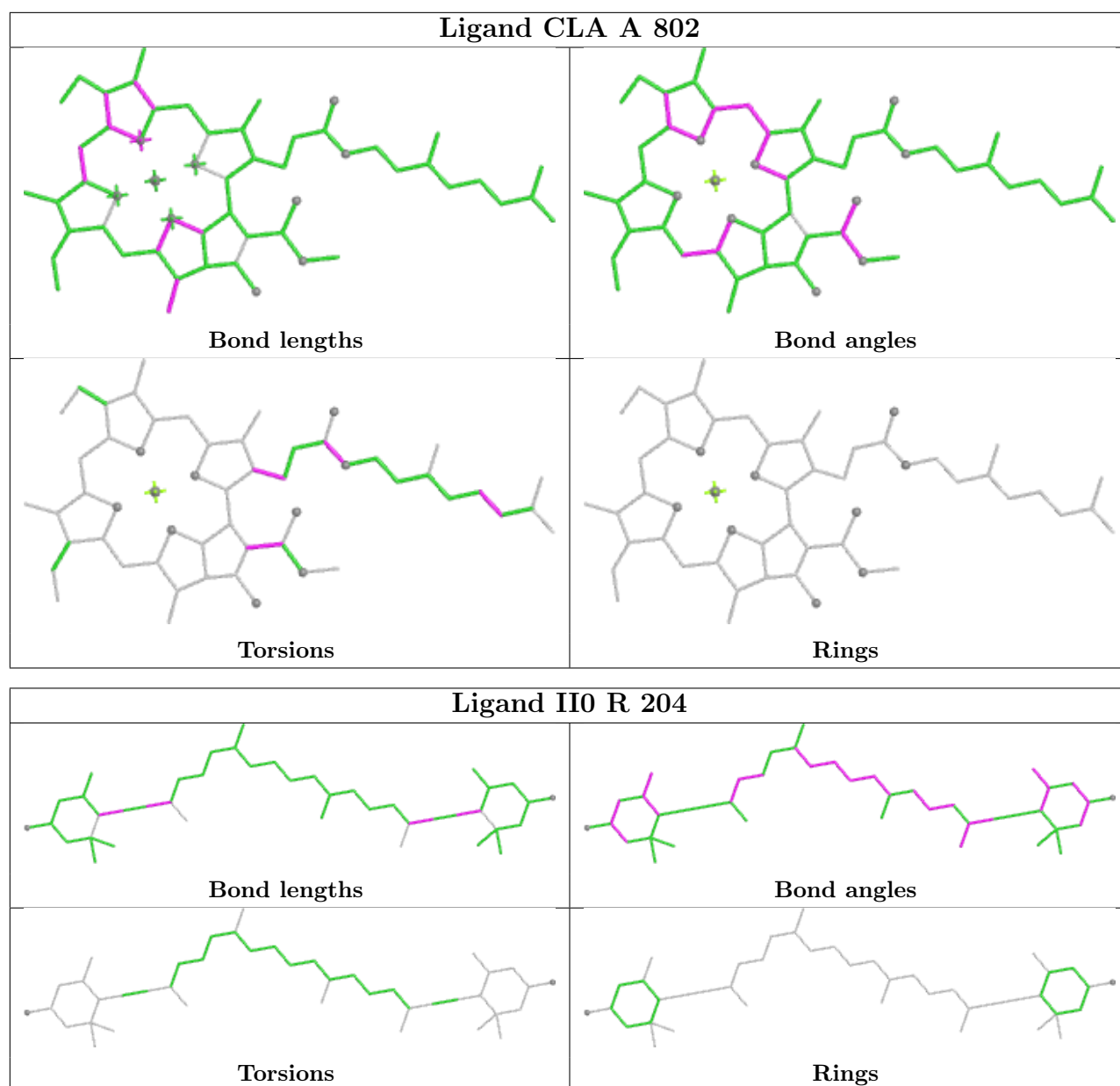


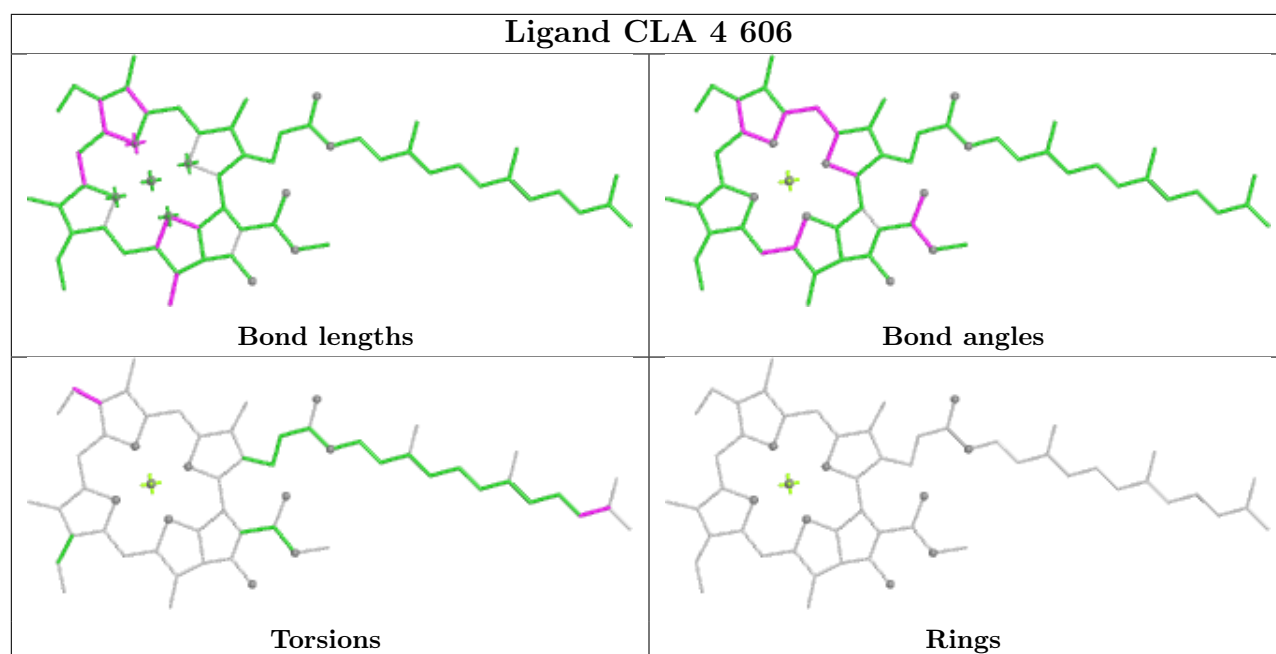
Ligand CLA c 603

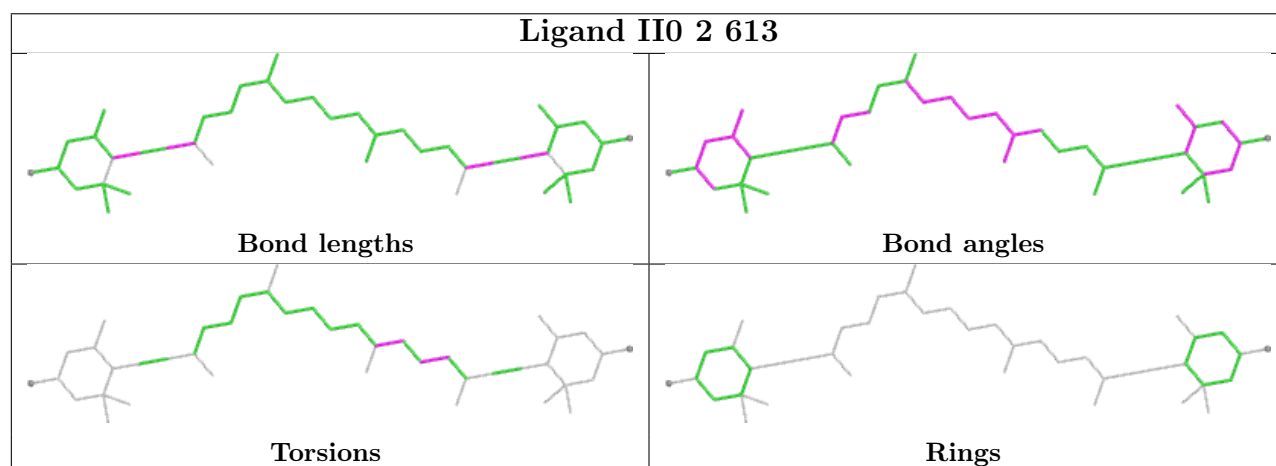
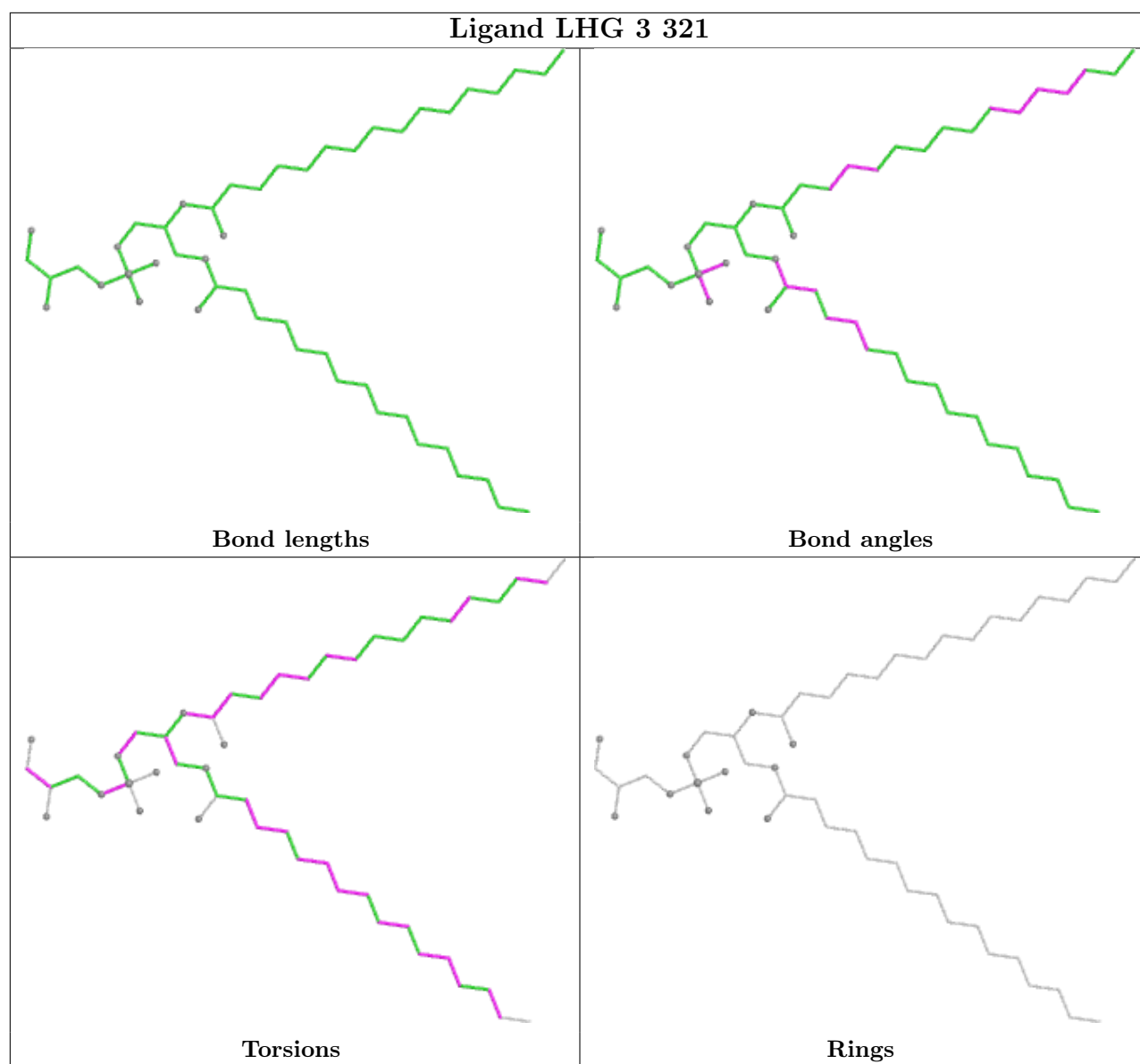


Ligand KC2 d 610

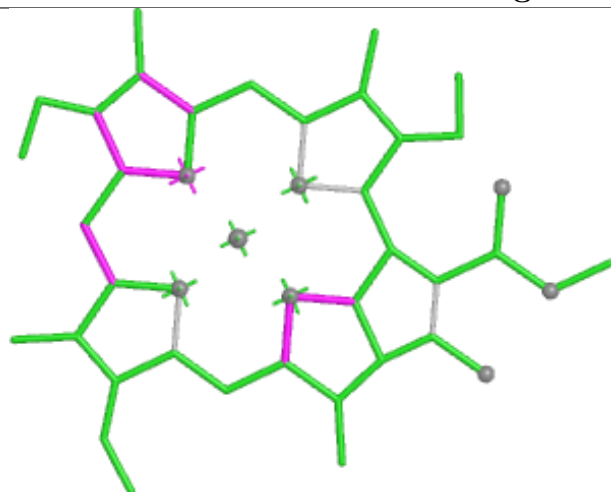




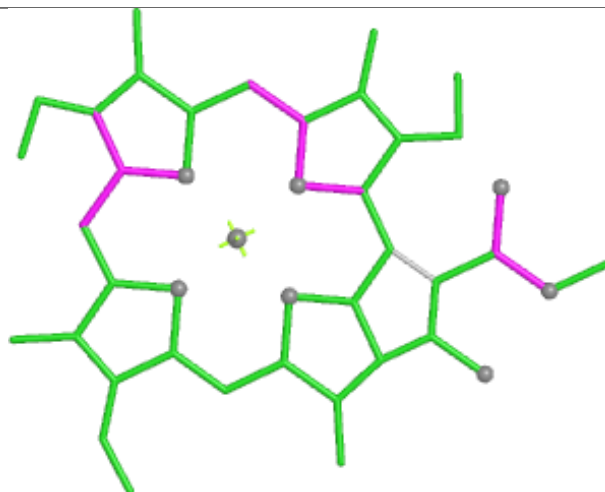




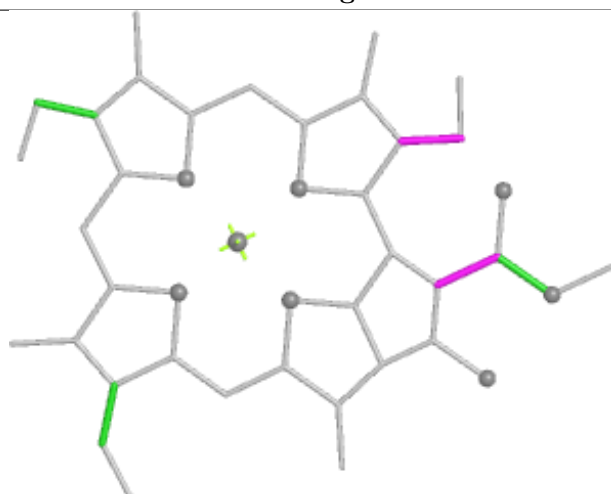
Ligand CLA A 813



Bond lengths



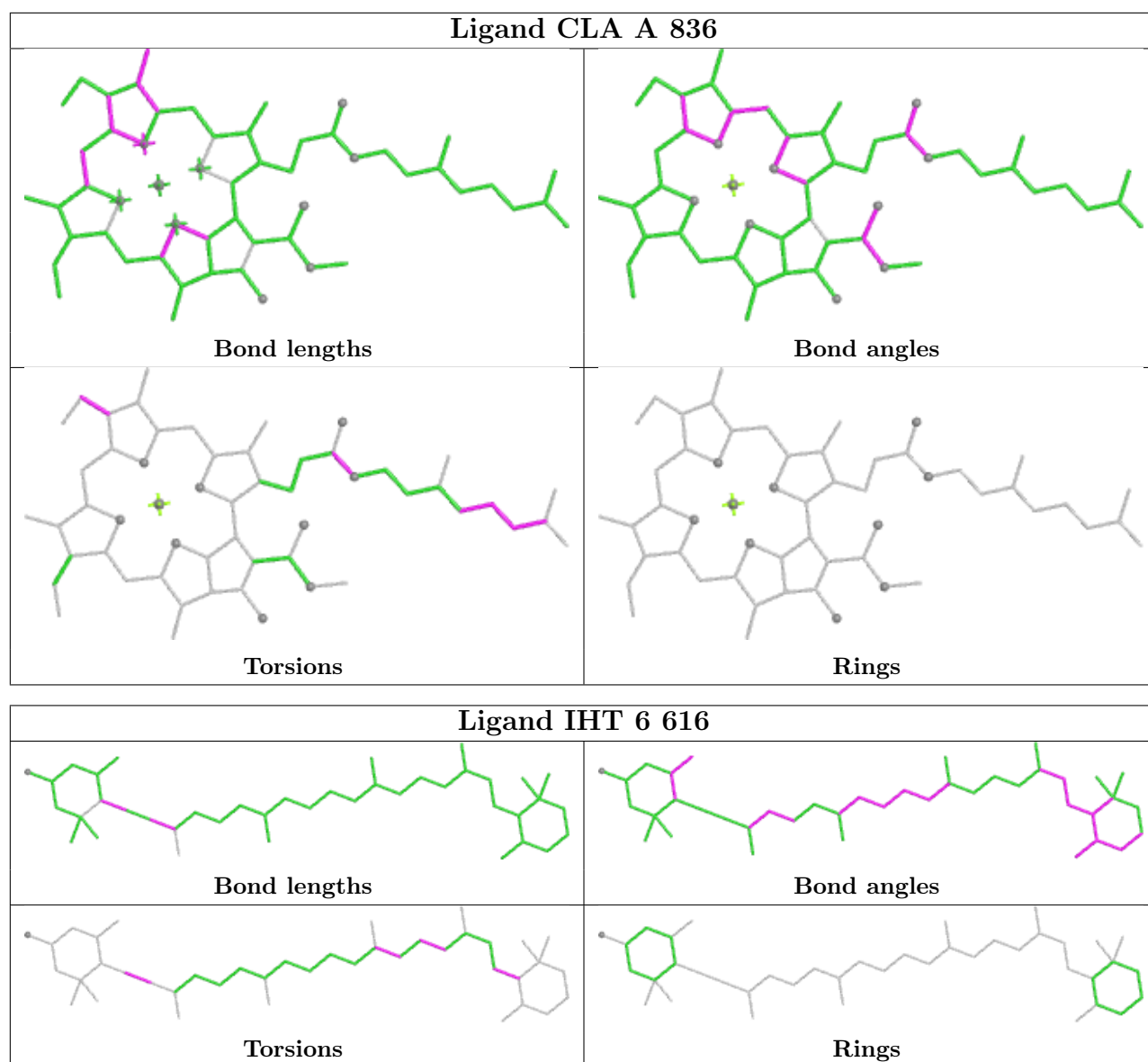
Bond angles



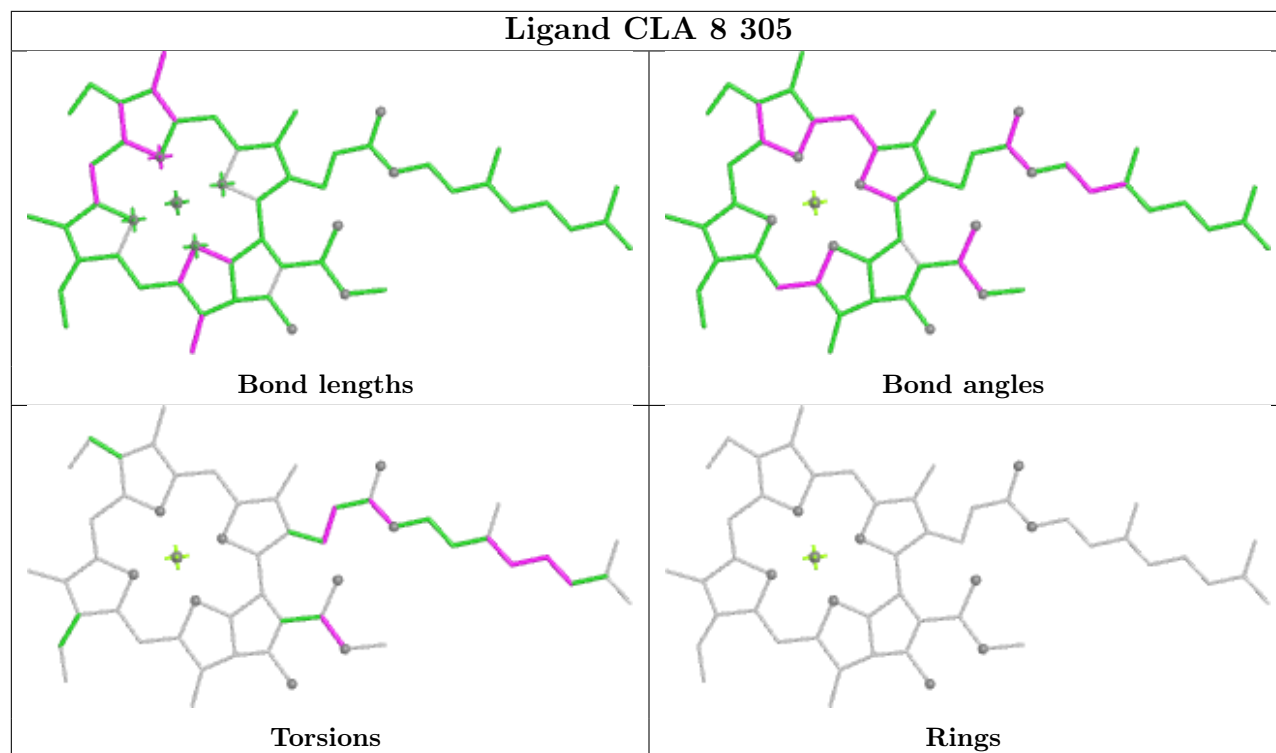
Torsions



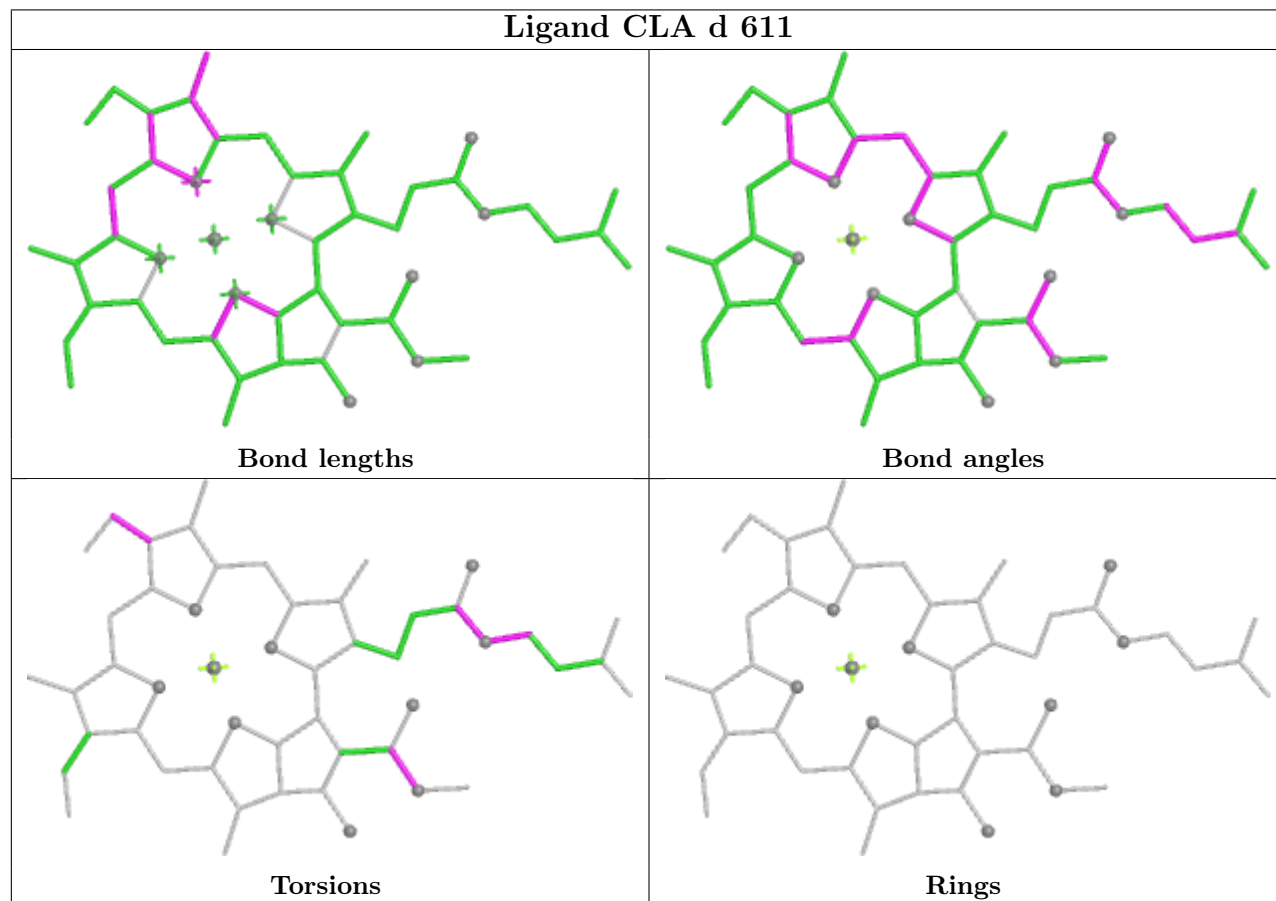
Rings

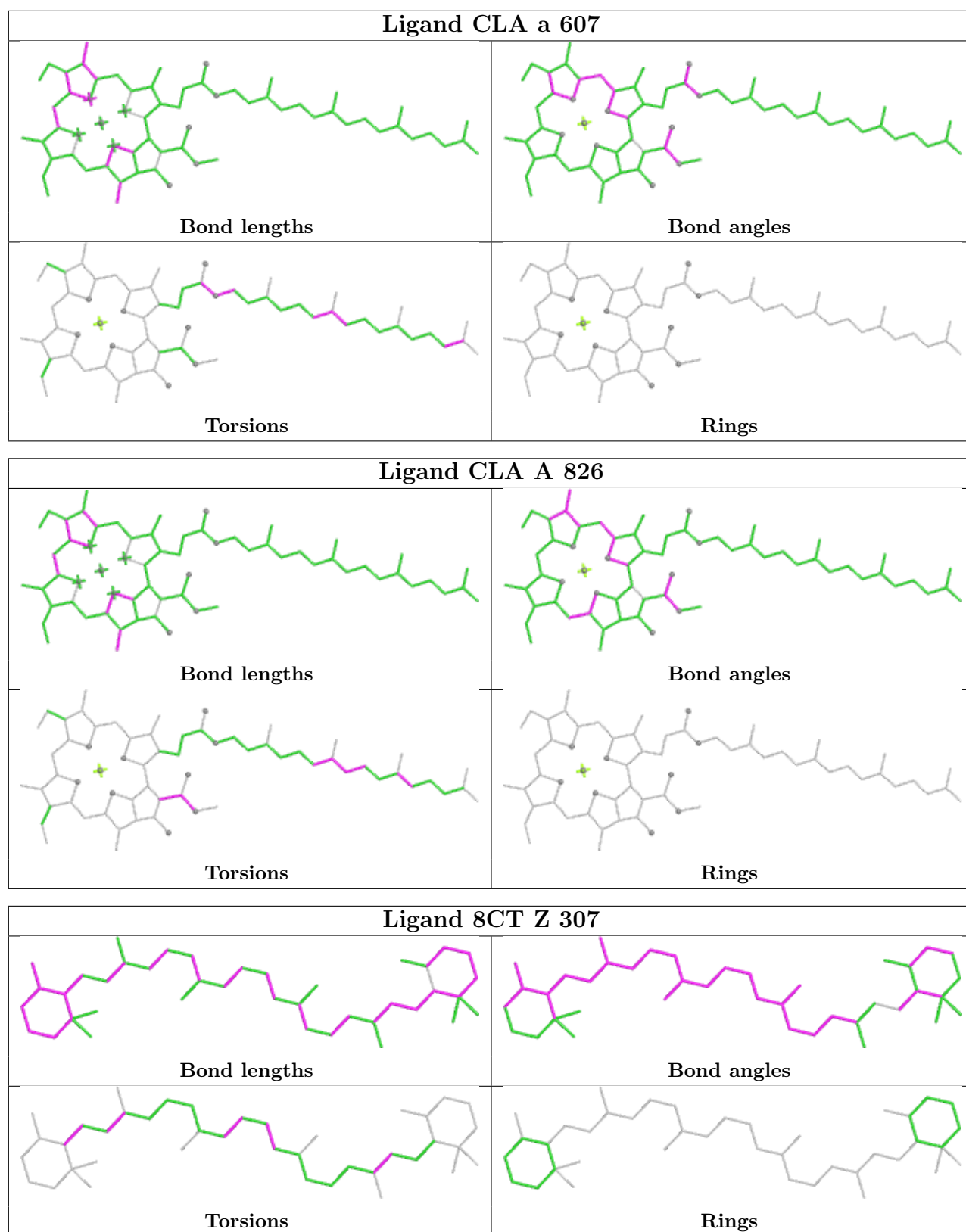


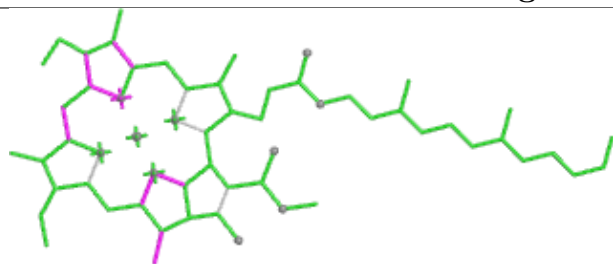
Ligand CLA 8 305



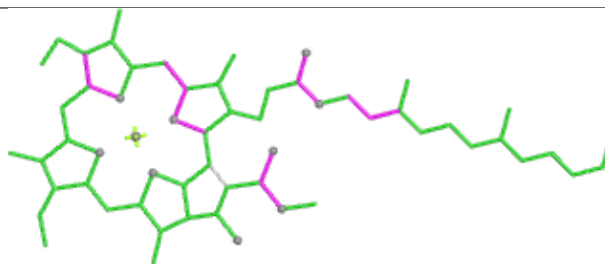
Ligand CLA d 611



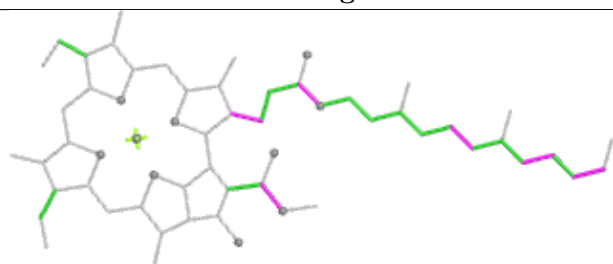


Ligand CLA 2 602

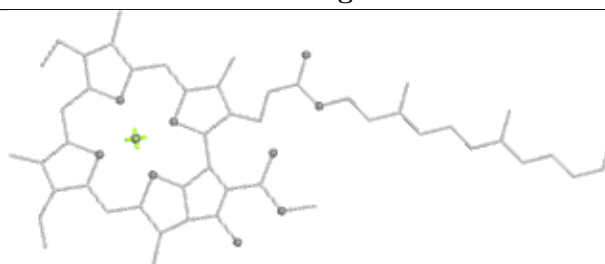
Bond lengths



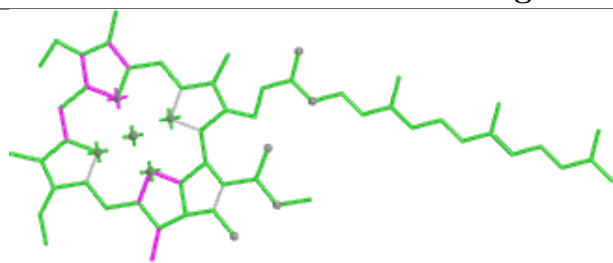
Bond angles



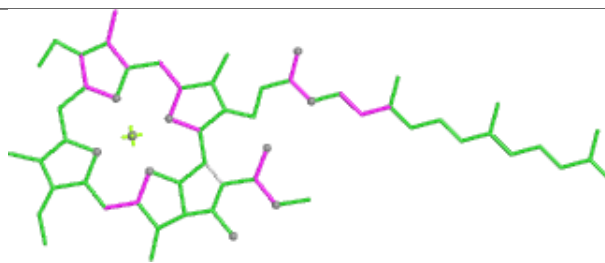
Torsions



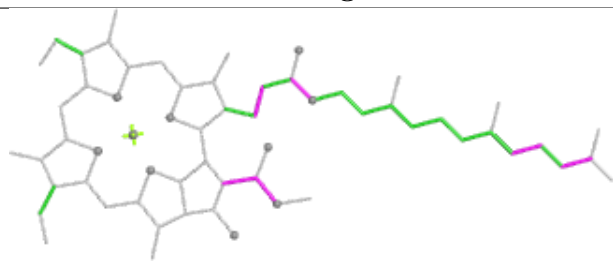
Rings

Ligand CLA B 821

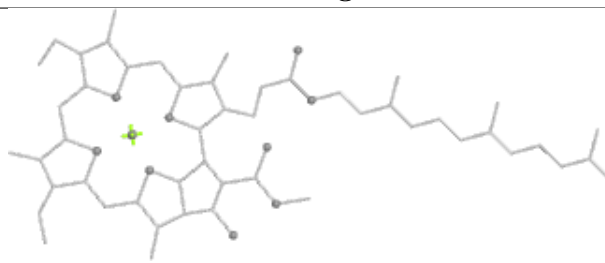
Bond lengths



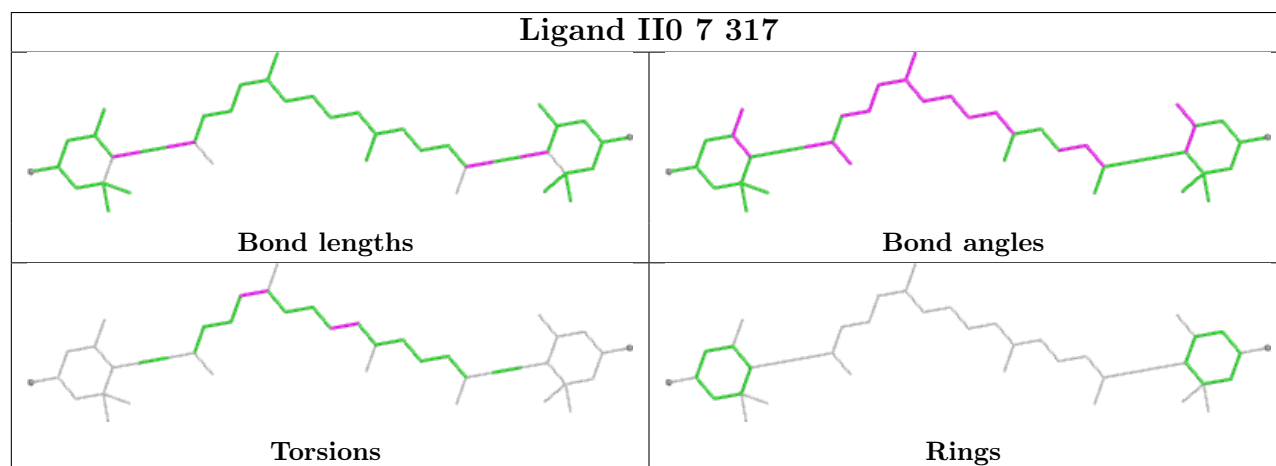
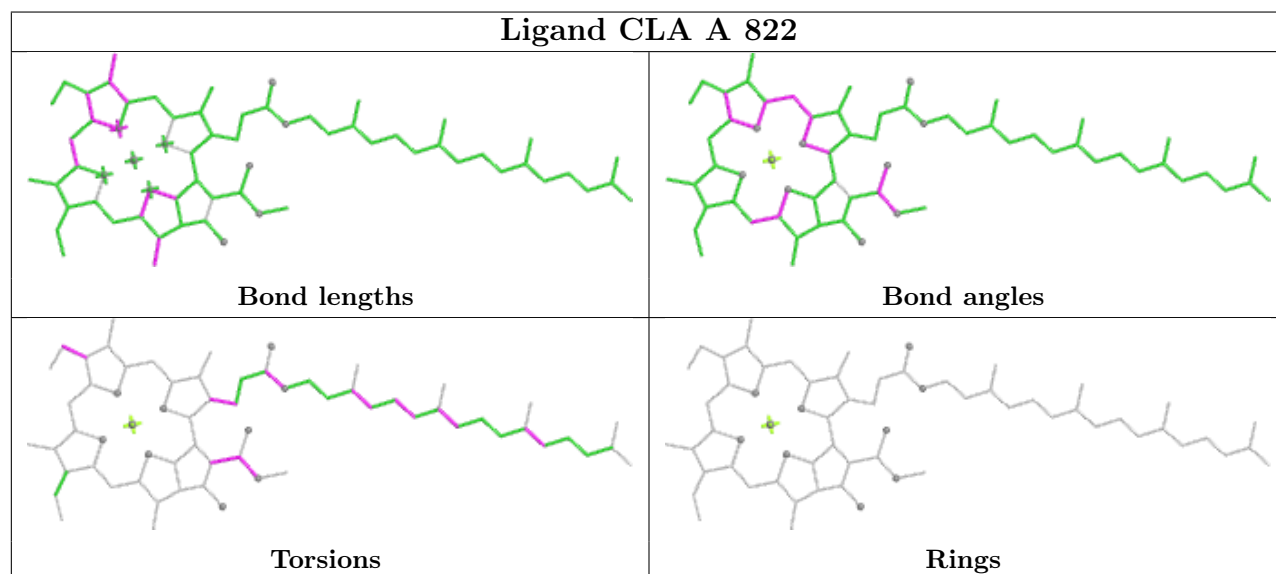
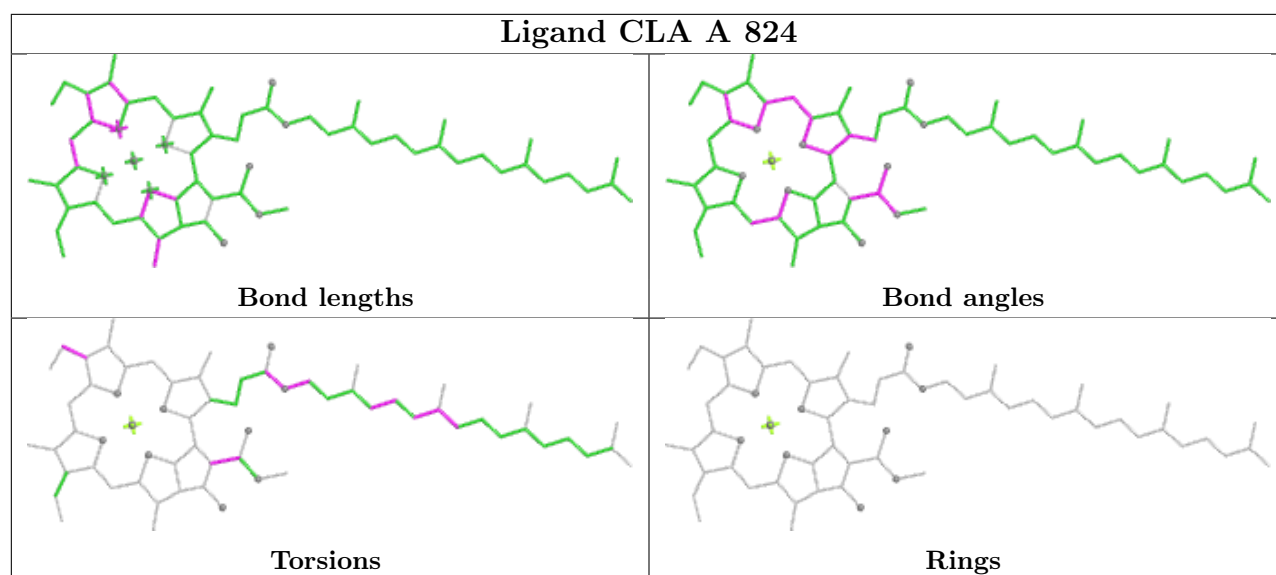
Bond angles

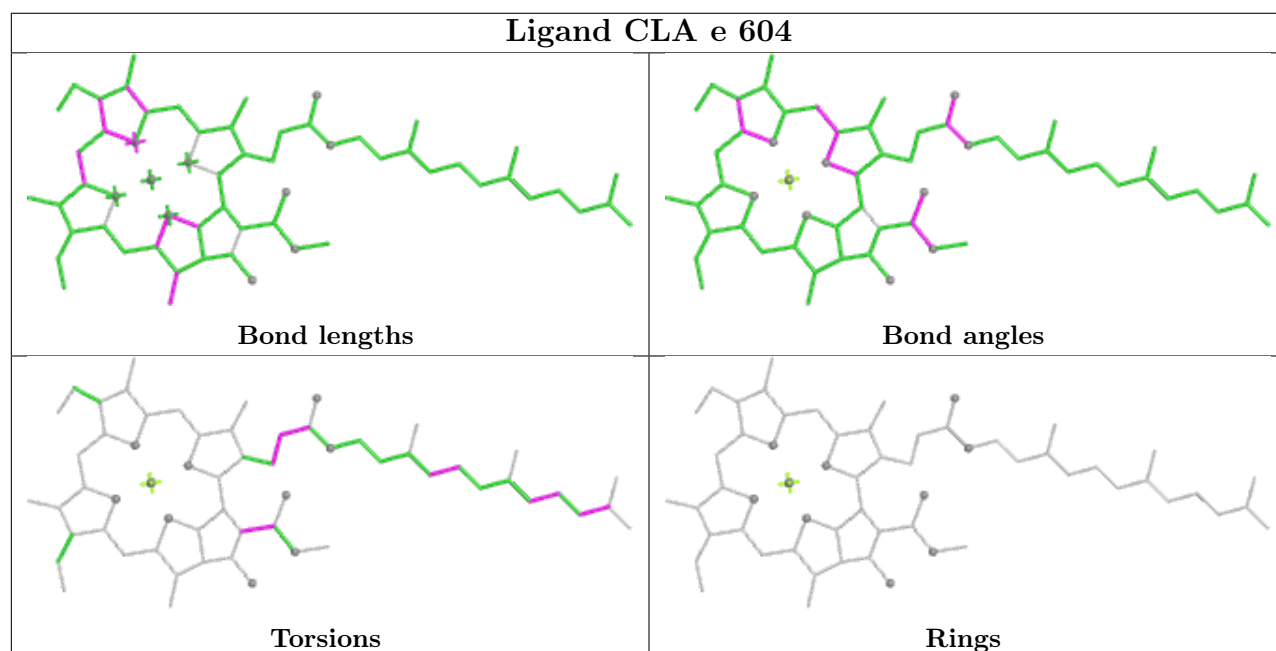
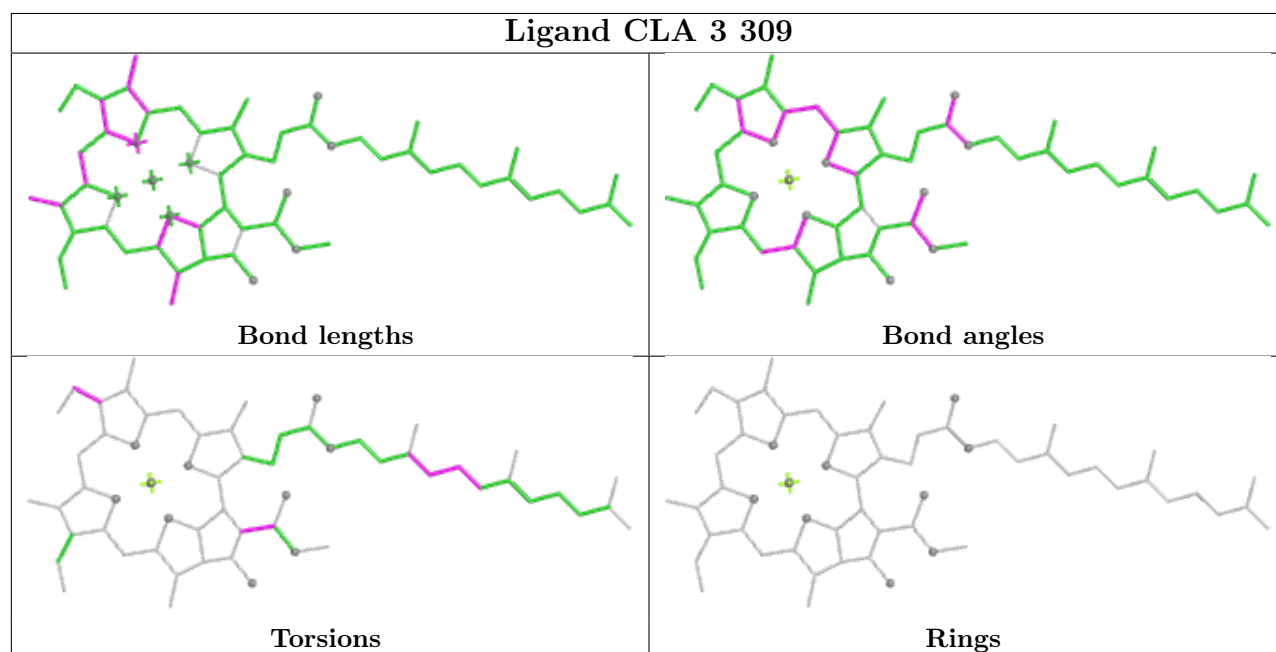
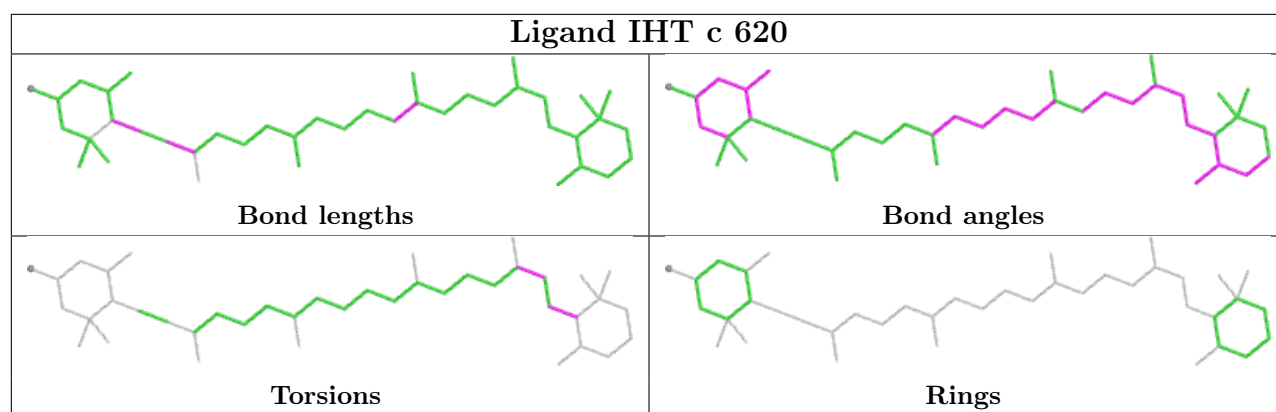


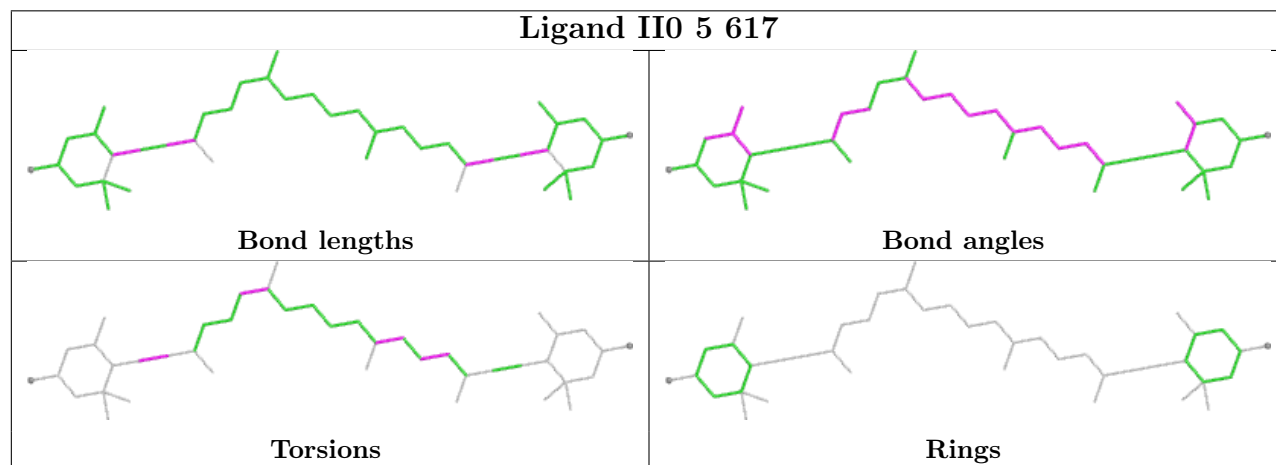
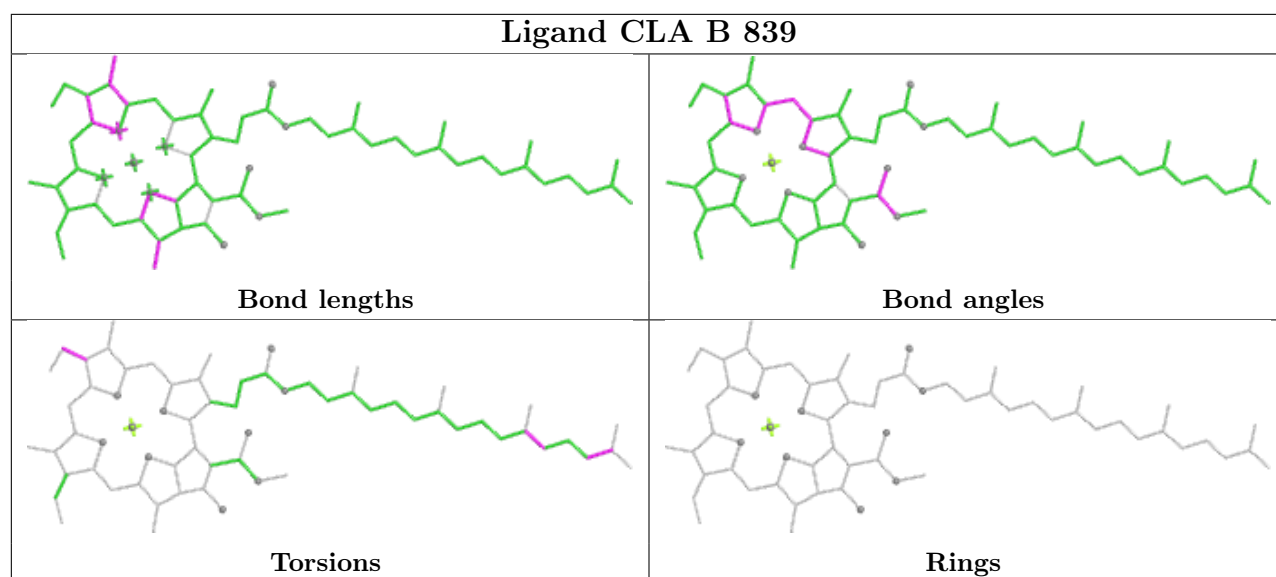
Torsions



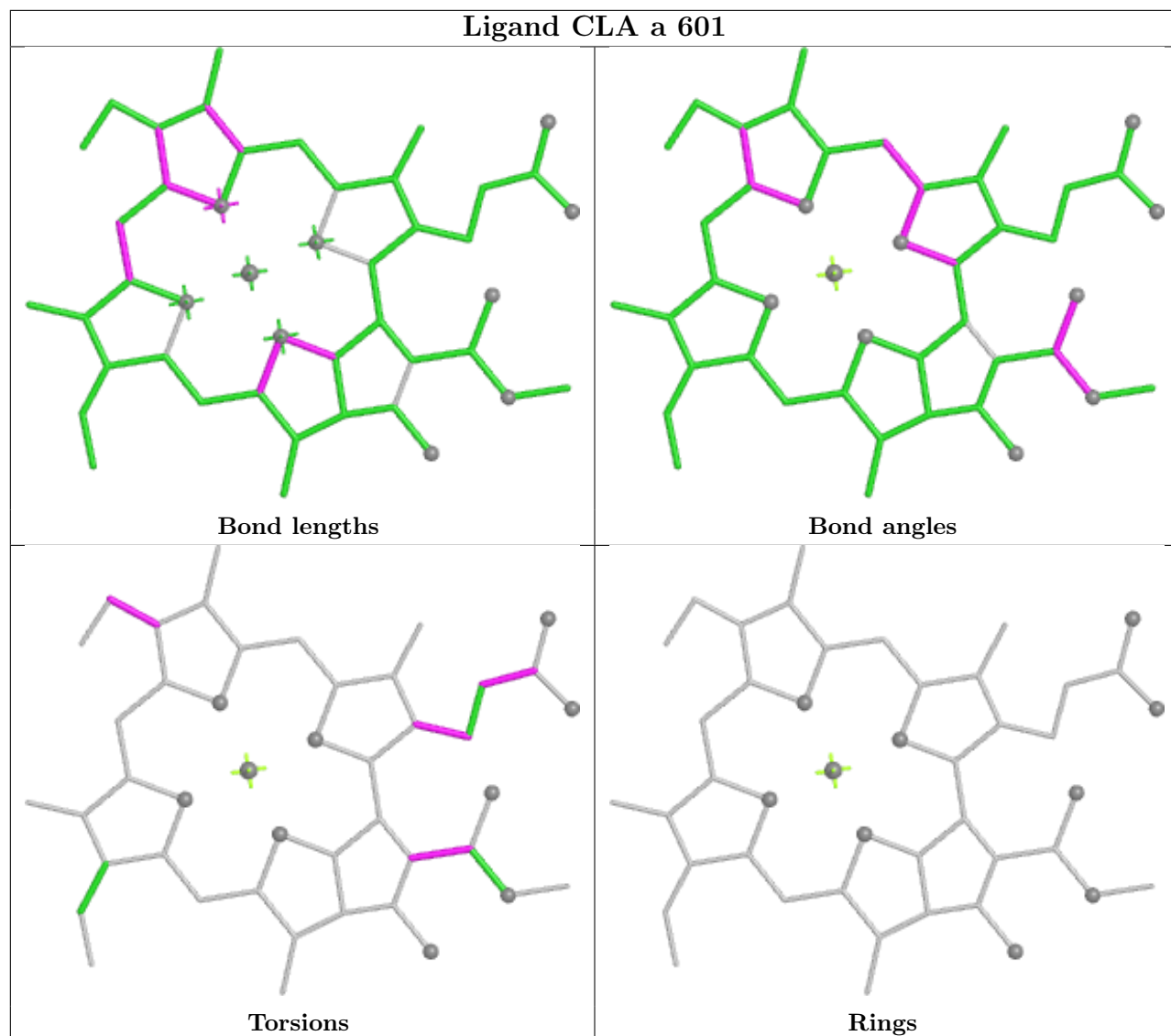
Rings



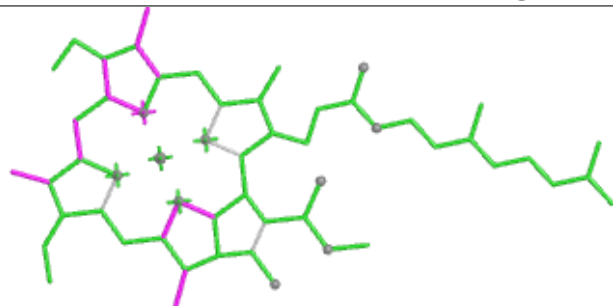




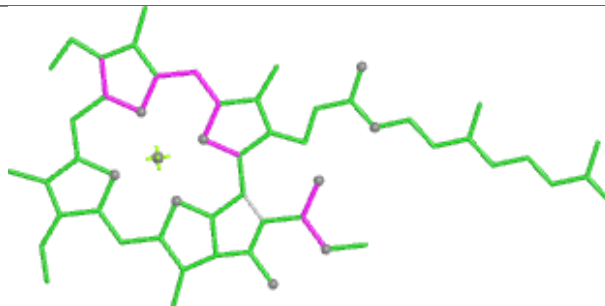
Ligand CLA a 601



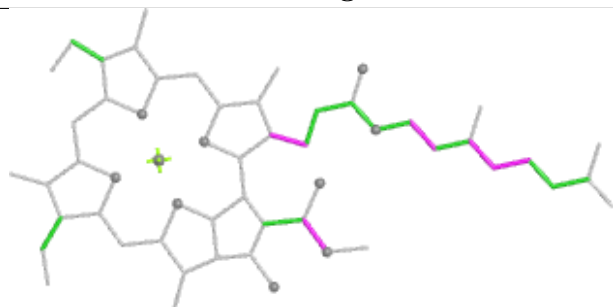
Ligand CLA K 102



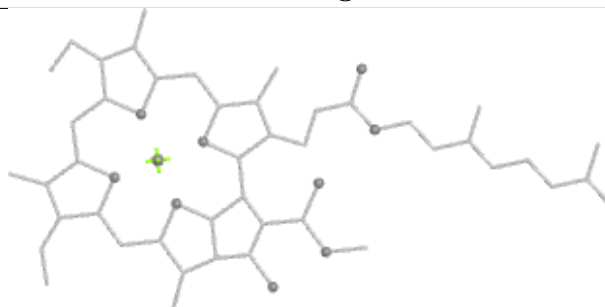
Bond lengths



Bond angles

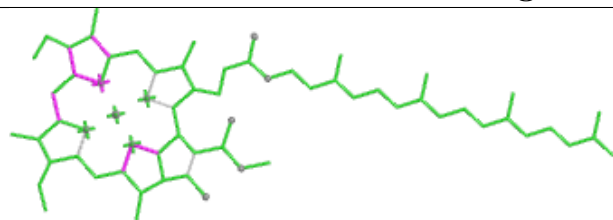


Torsions

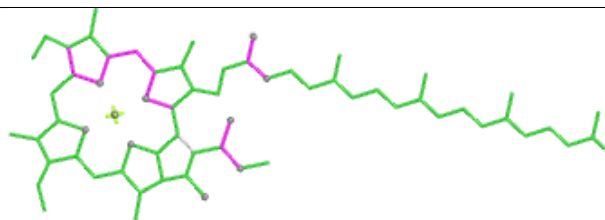


Rings

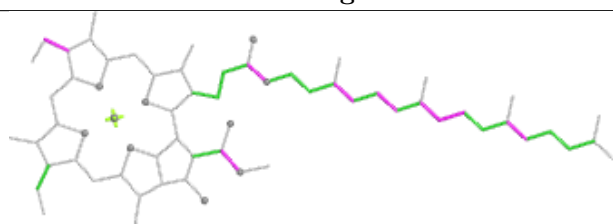
Ligand CLA b 608



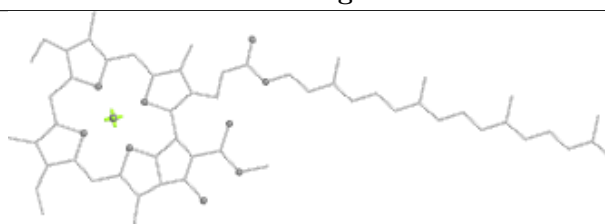
Bond lengths



Bond angles

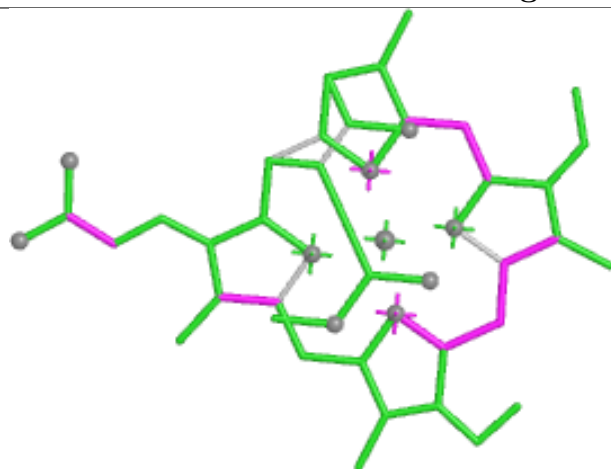


Torsions

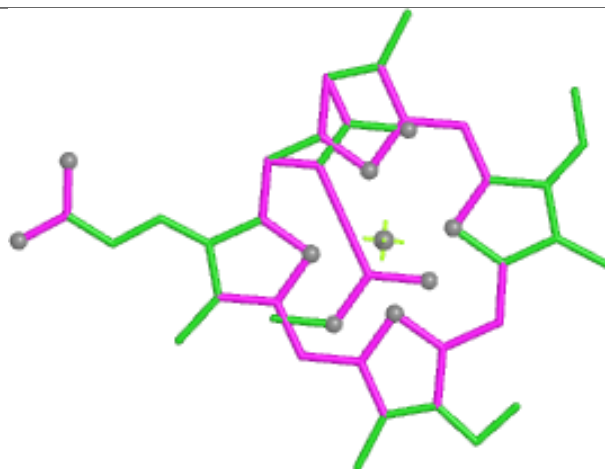


Rings

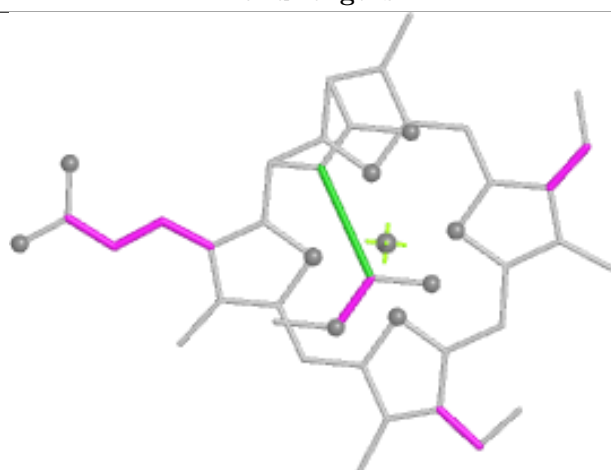
Ligand KC2 6 610



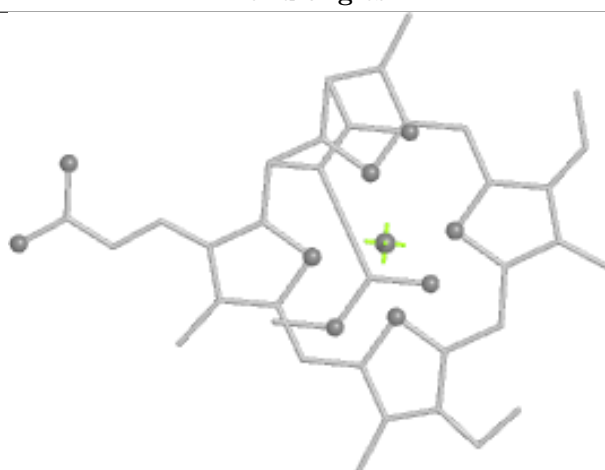
Bond lengths



Bond angles

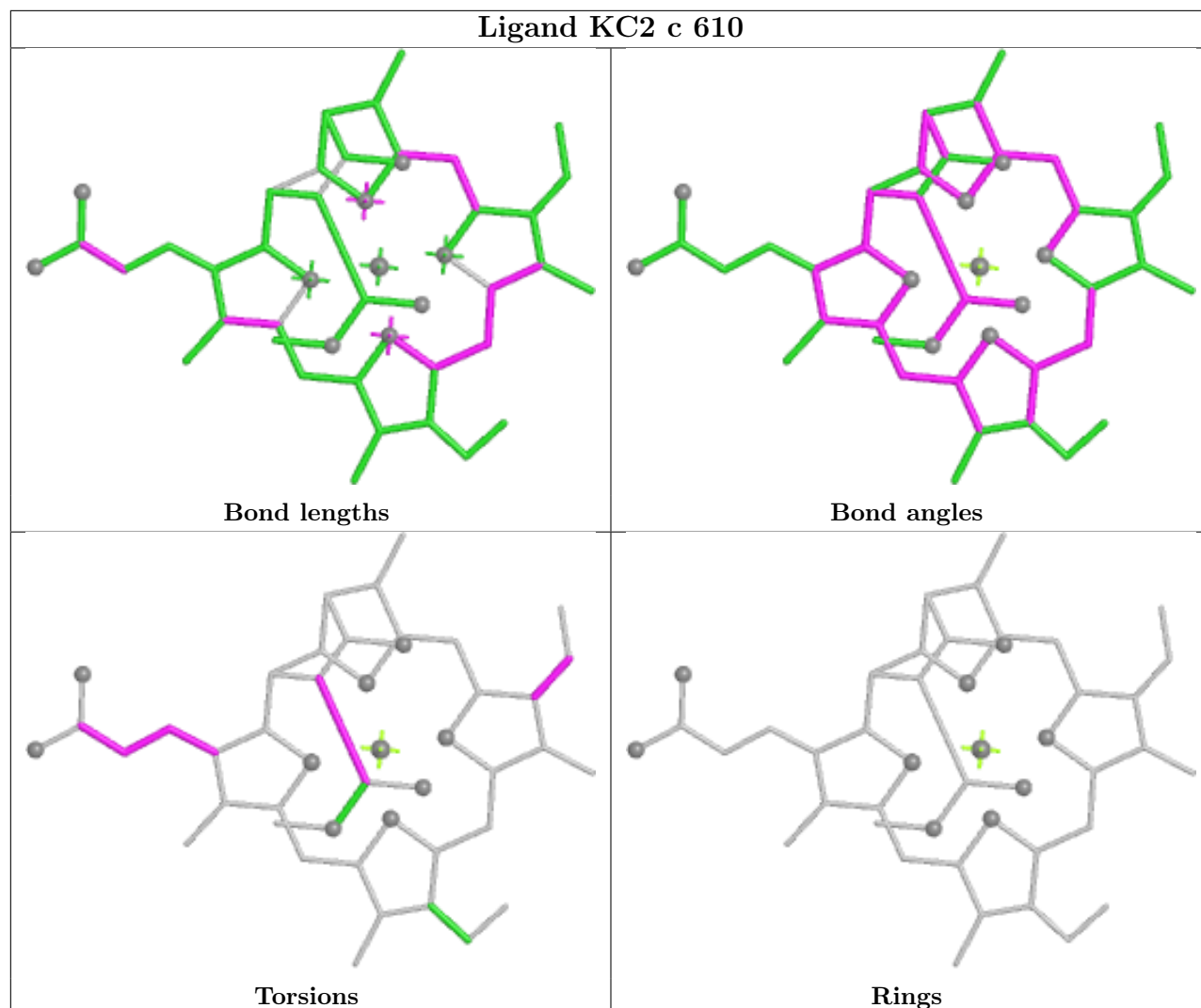


Torsions

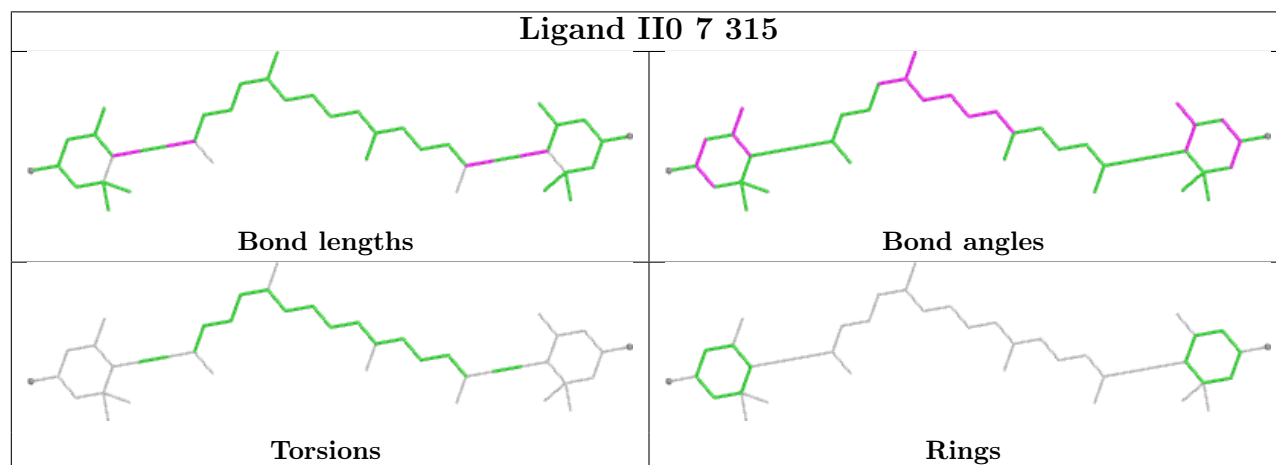


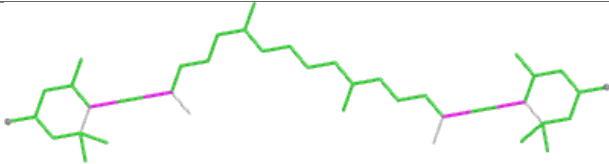
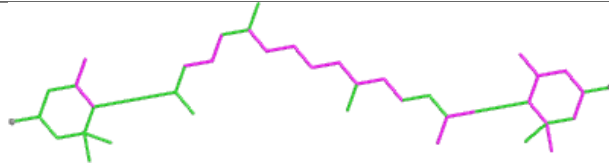
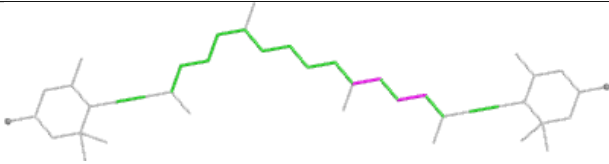
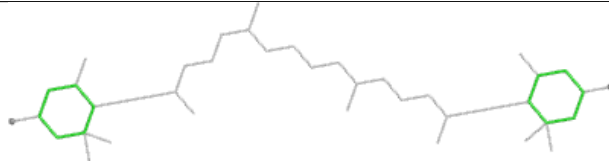
Rings

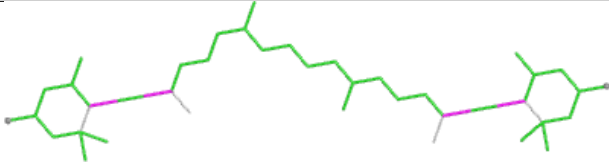
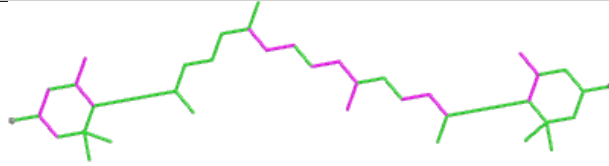
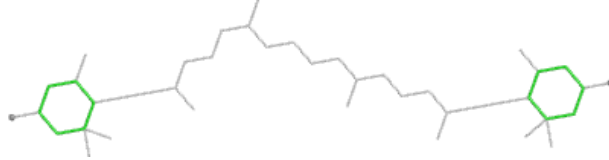
Ligand KC2 c 610

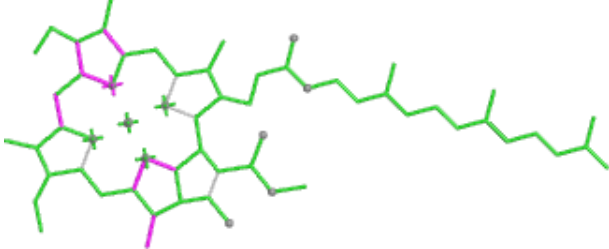
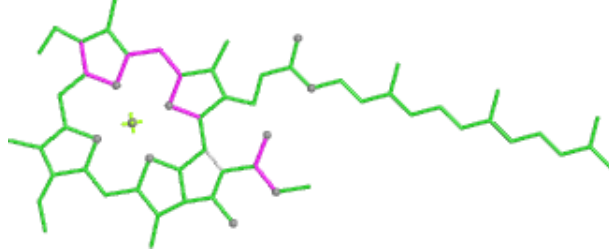
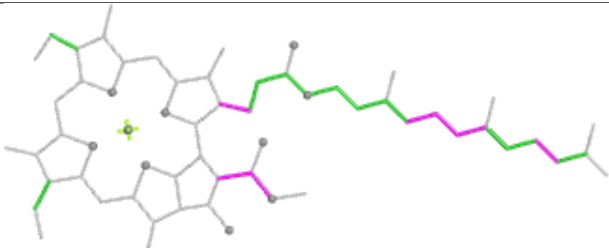
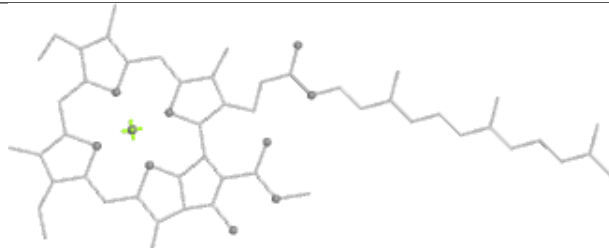


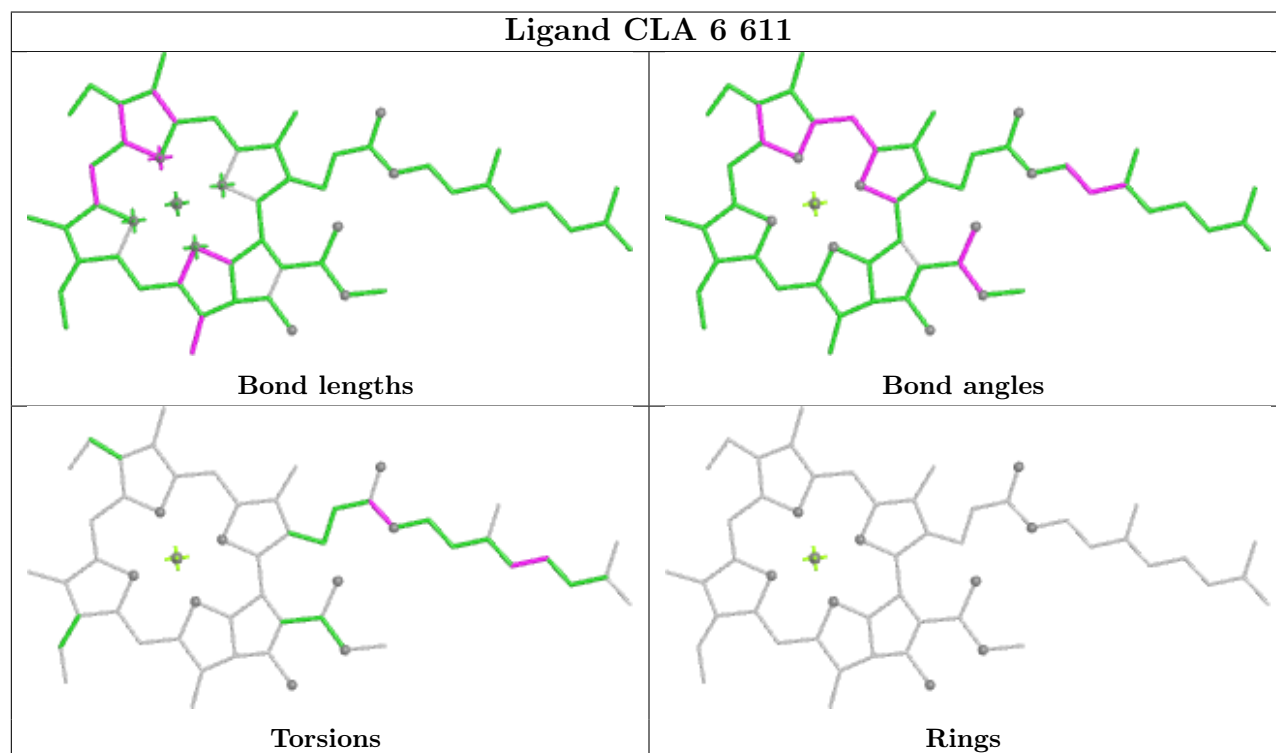
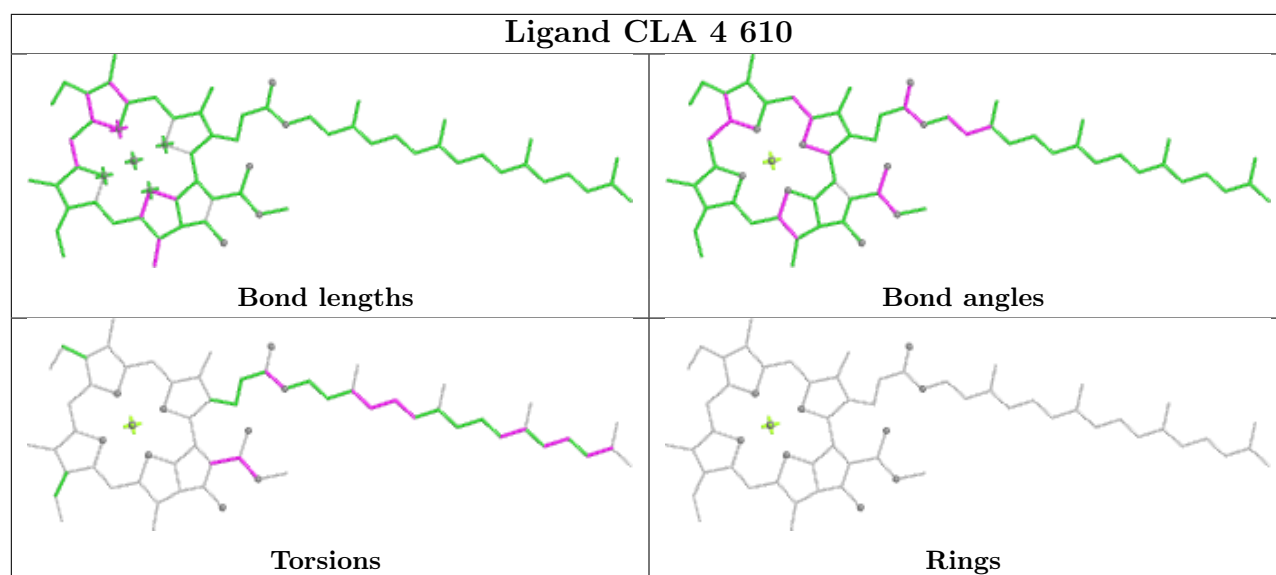
Ligand II0 7 315



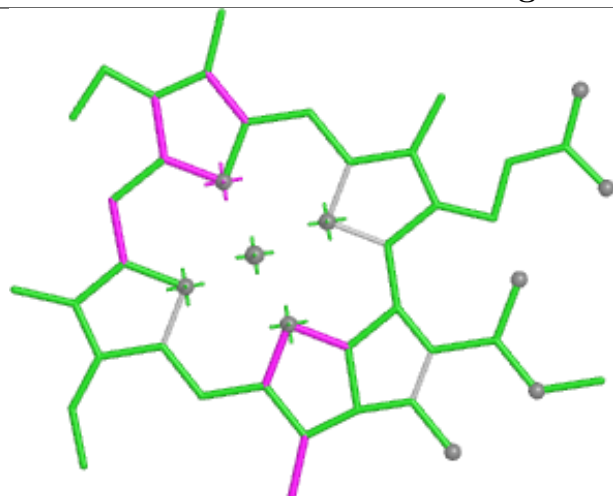
Ligand II0 3 318	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 c 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

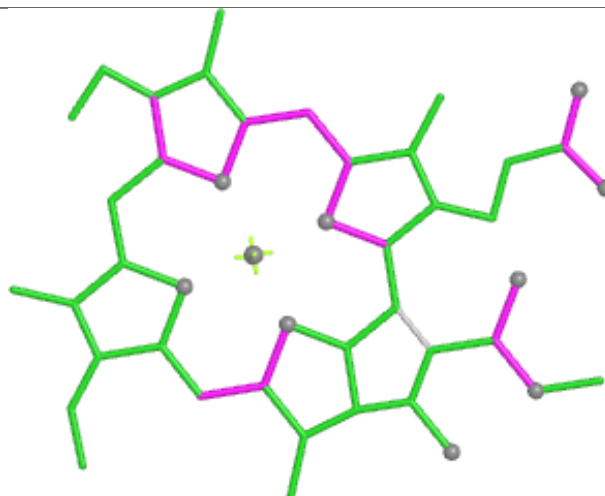
Ligand CLA a 603	
	
Bond lengths	Bond angles
	
Torsions	Rings



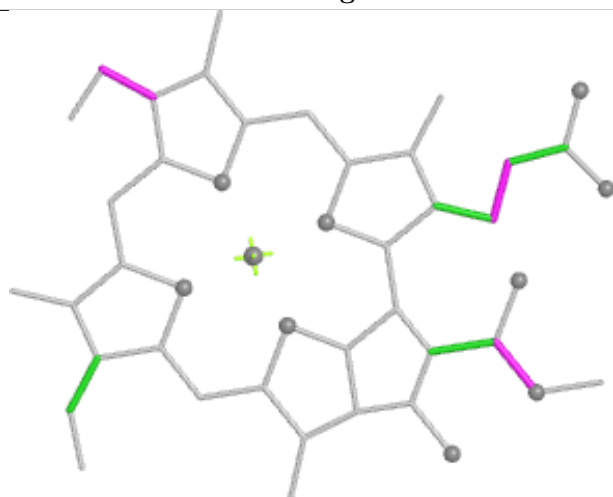
Ligand CLA 1 606



Bond lengths



Bond angles

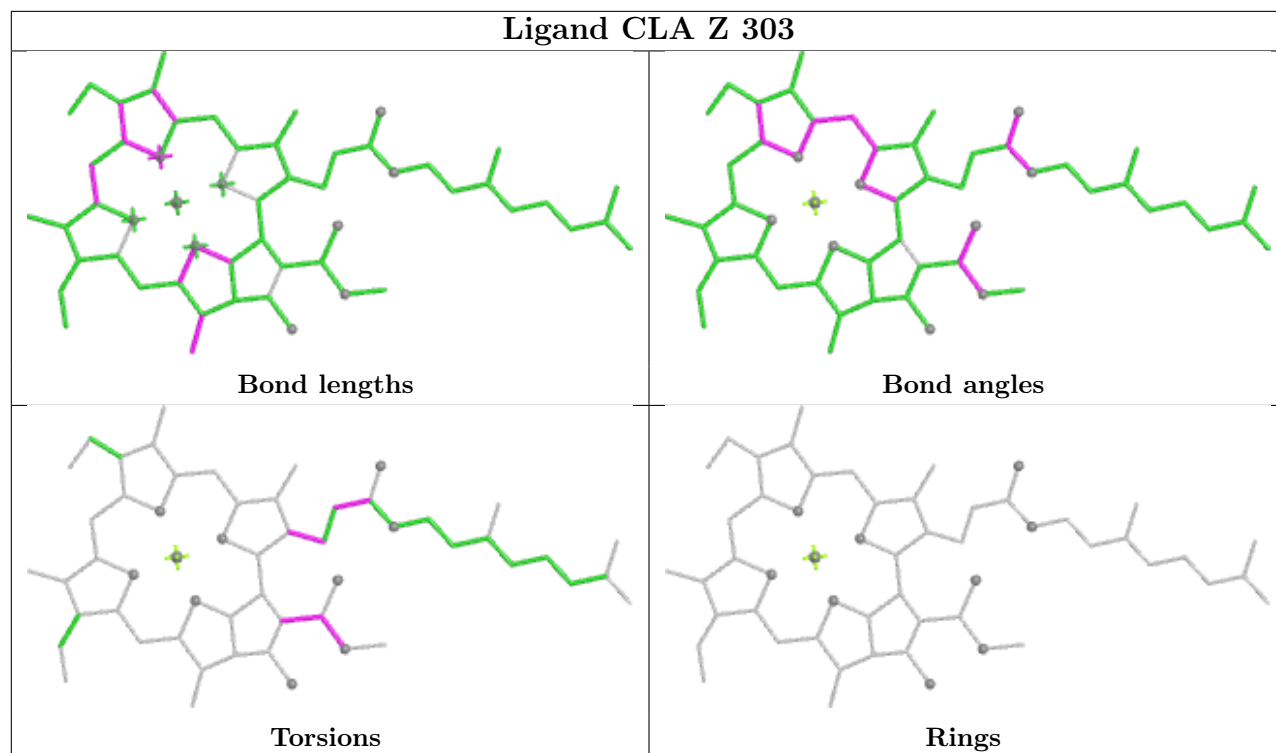


Torsions

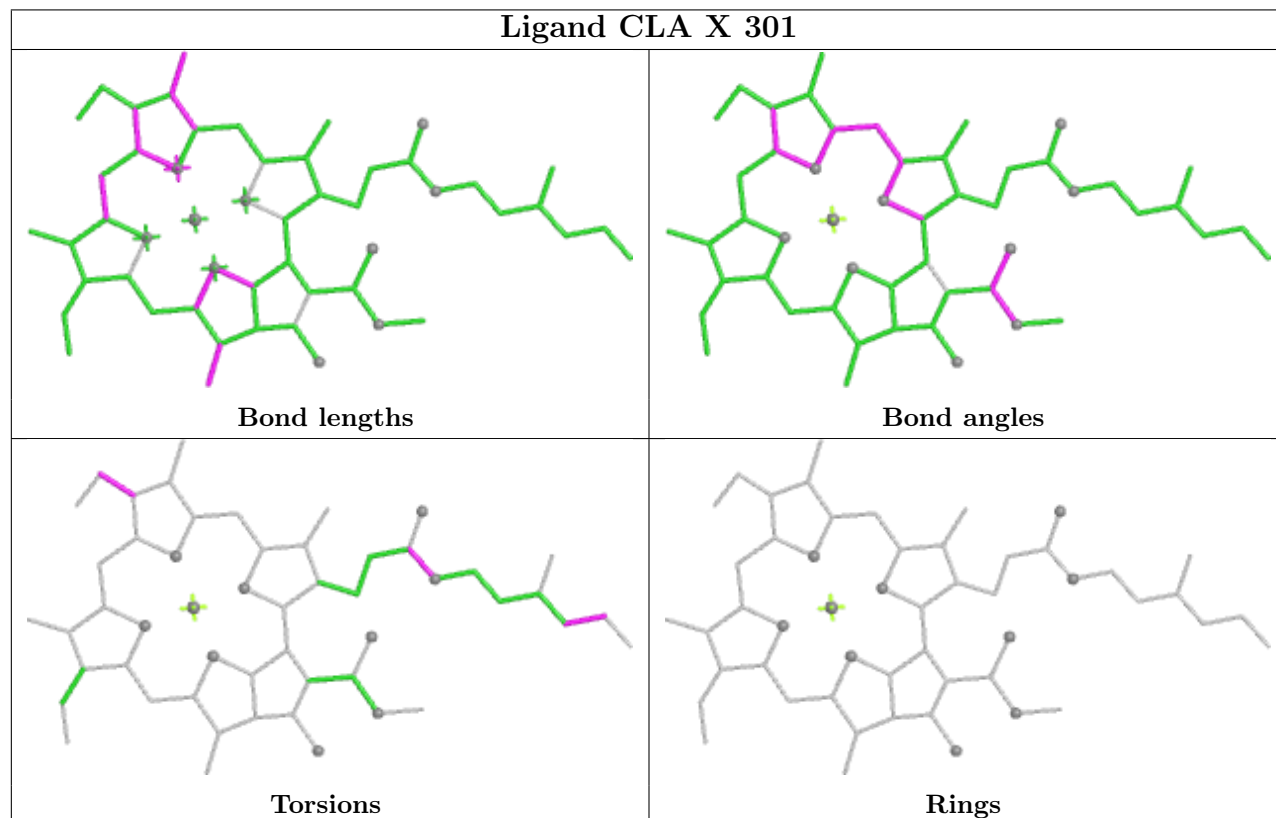


Rings

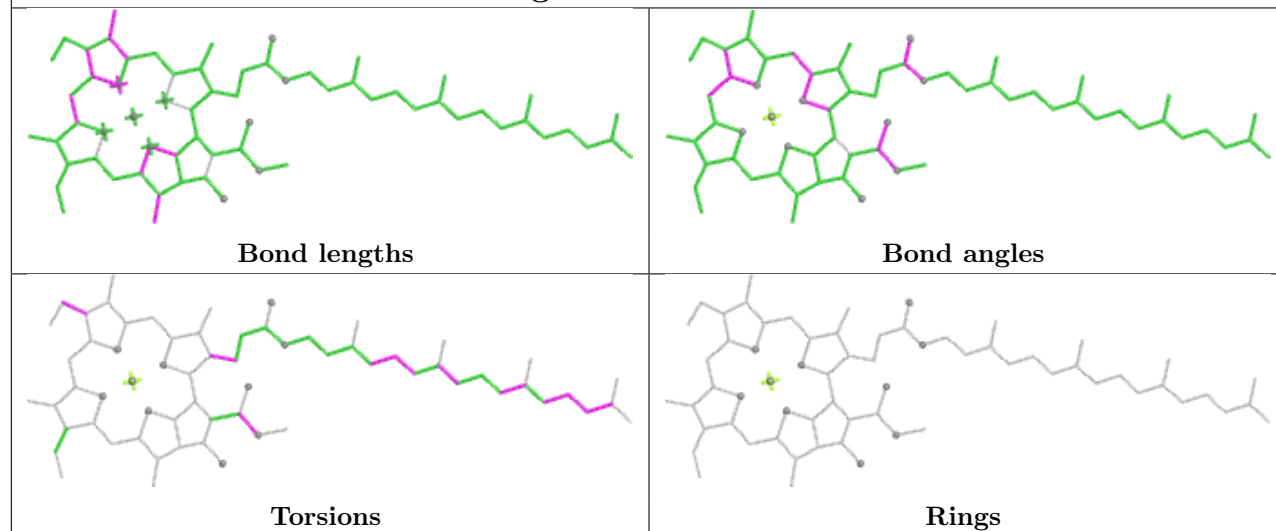
Ligand CLA Z 303



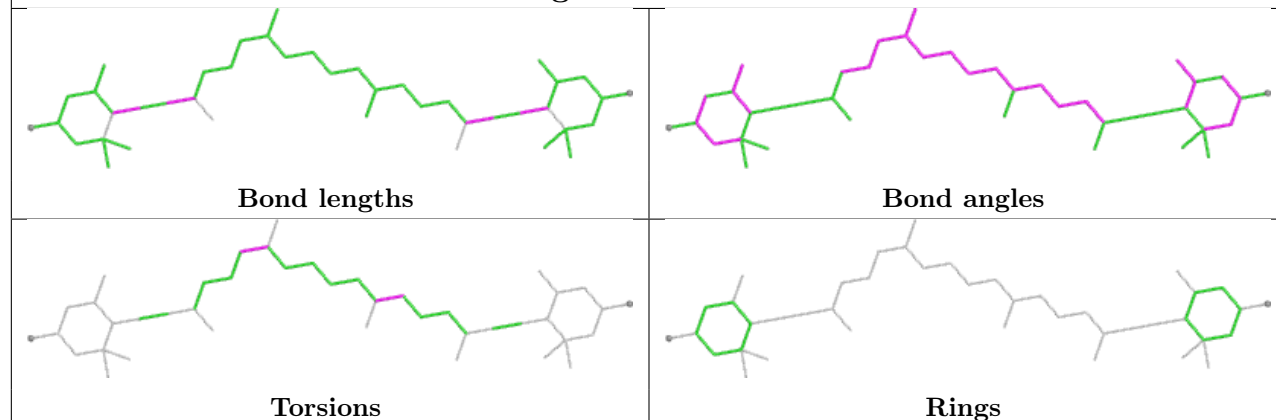
Ligand CLA X 301



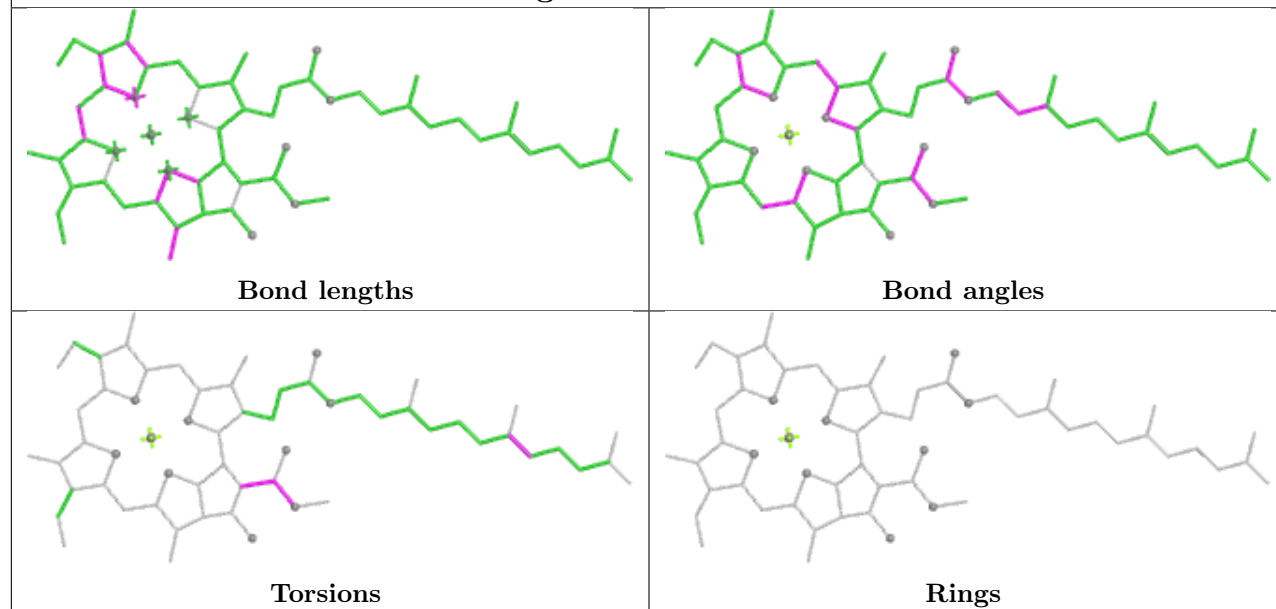
Ligand CLA A 831

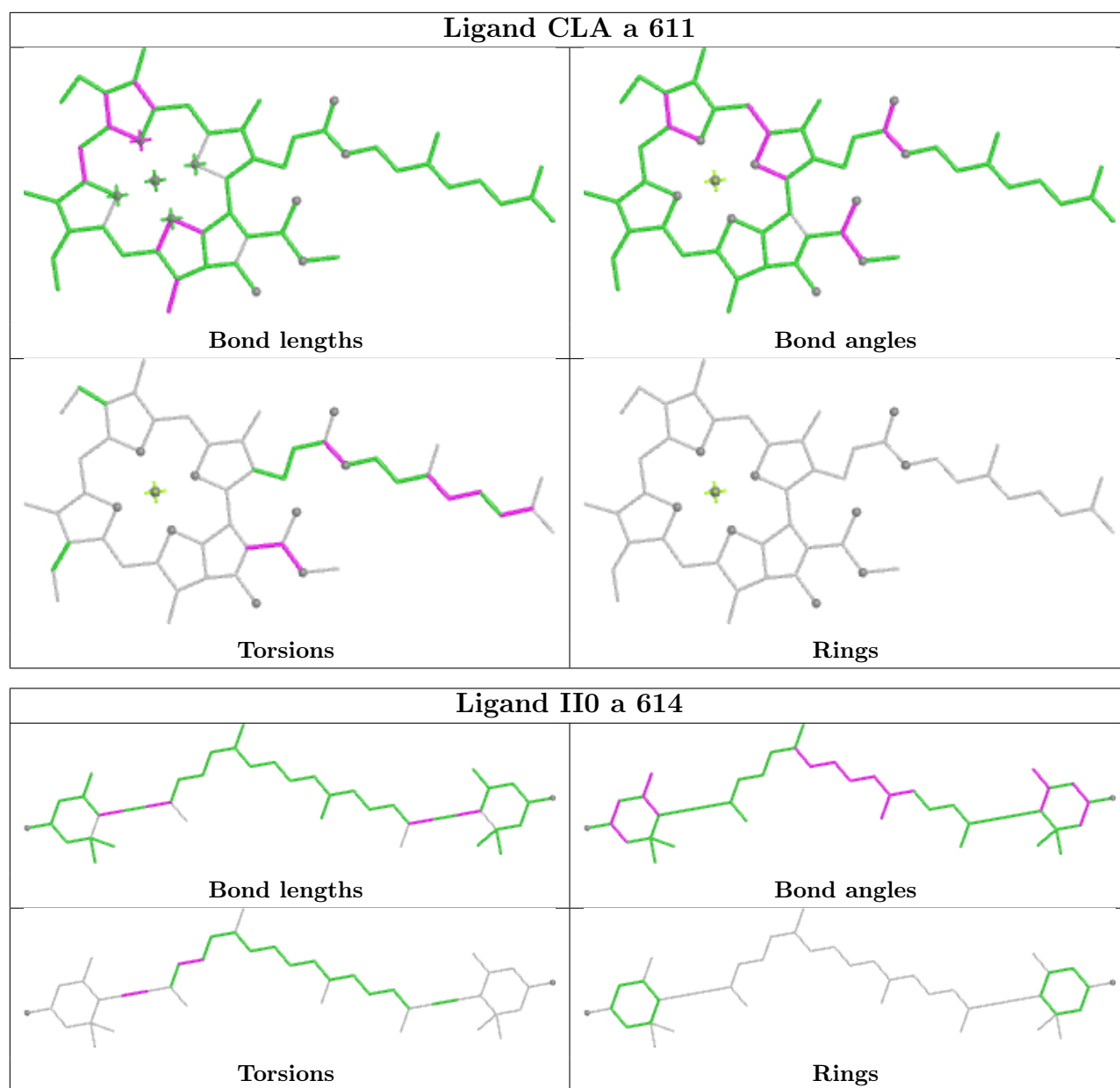


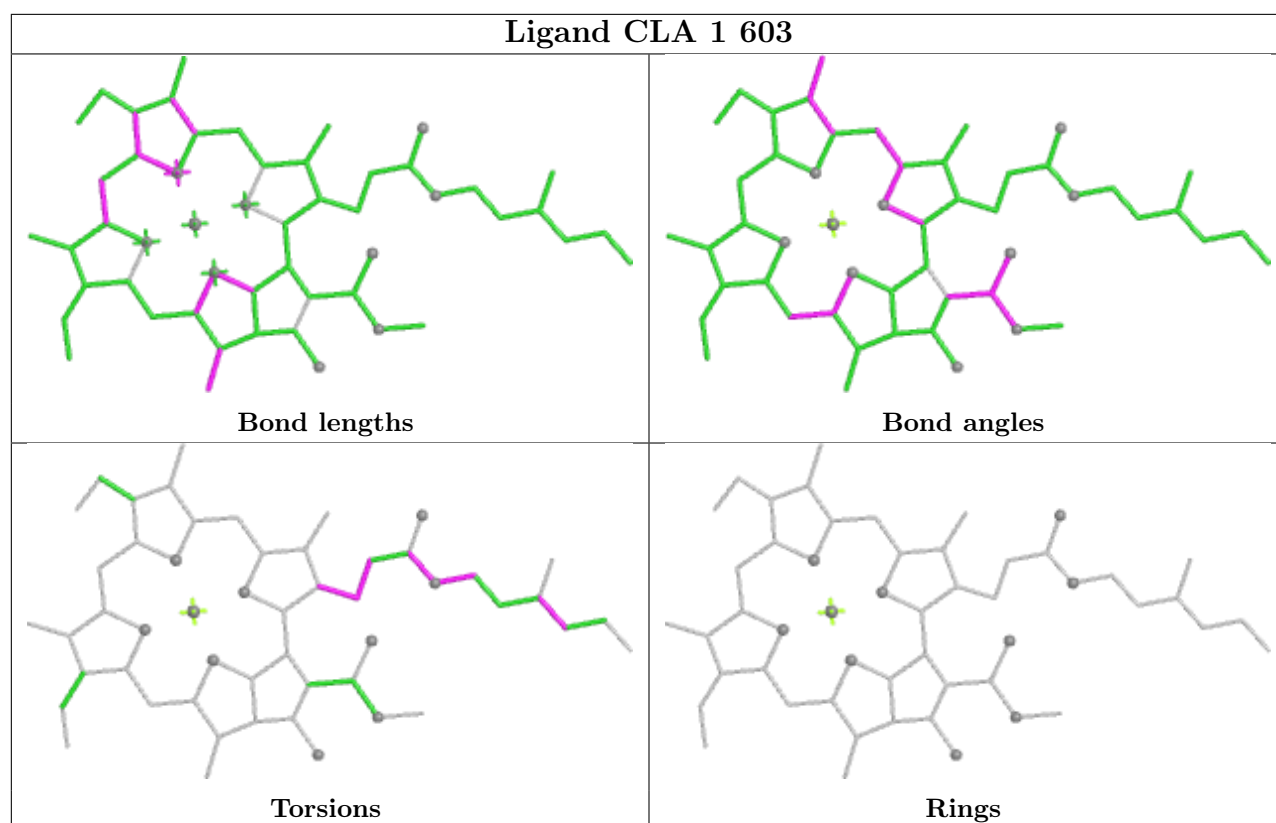
Ligand II0 c 619



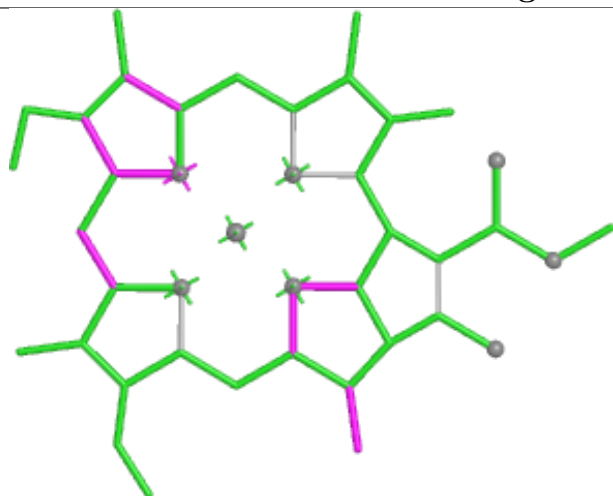
Ligand CLA 6 608



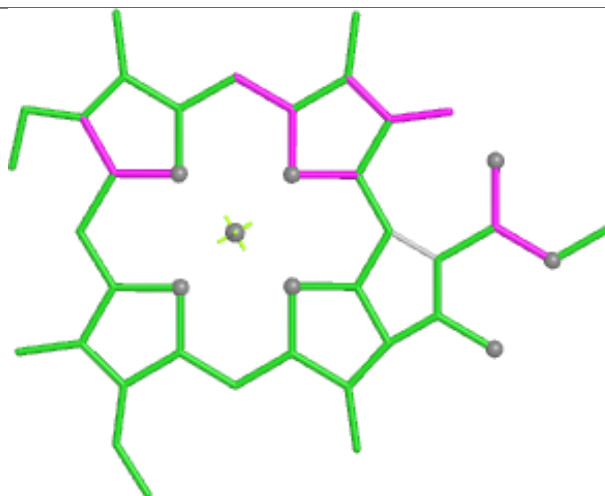




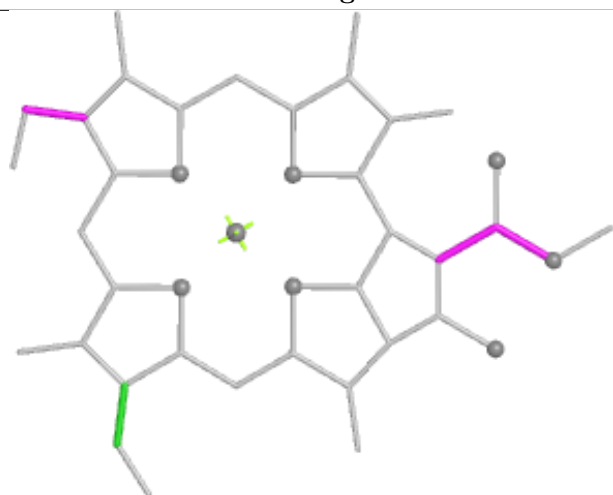
Ligand CLA 8 307



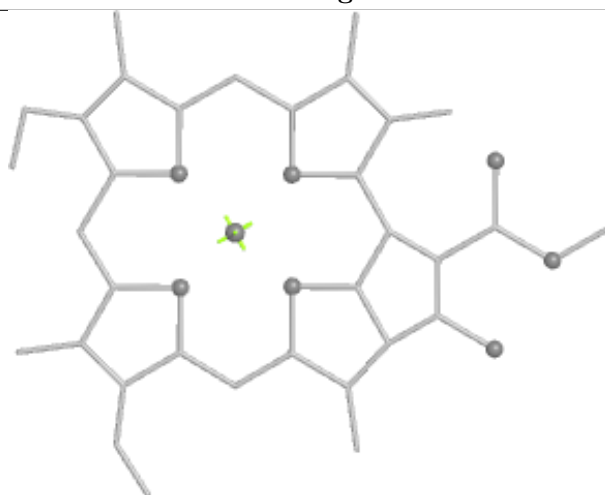
Bond lengths



Bond angles

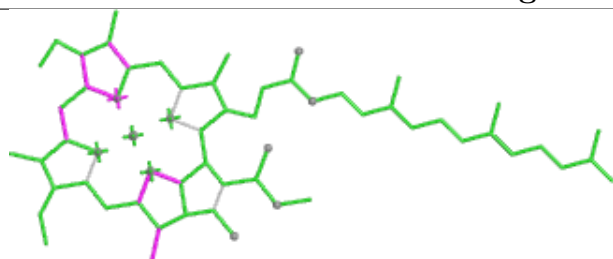


Torsions

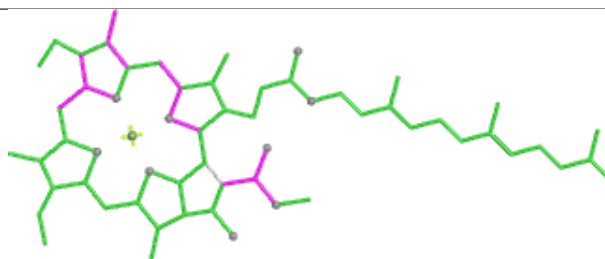


Rings

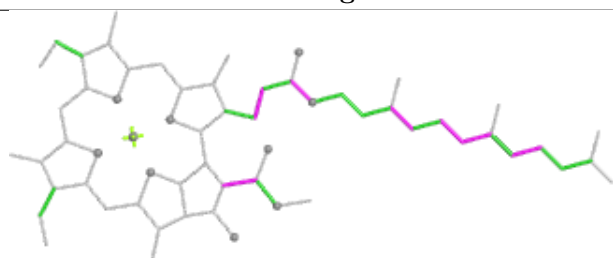
Ligand CLA e 606



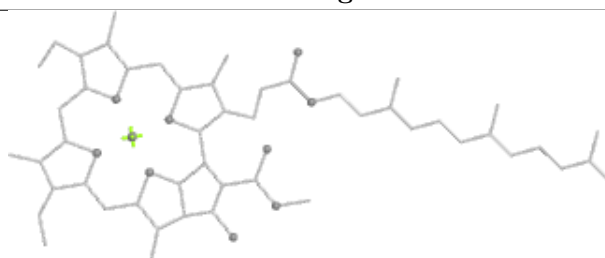
Bond lengths



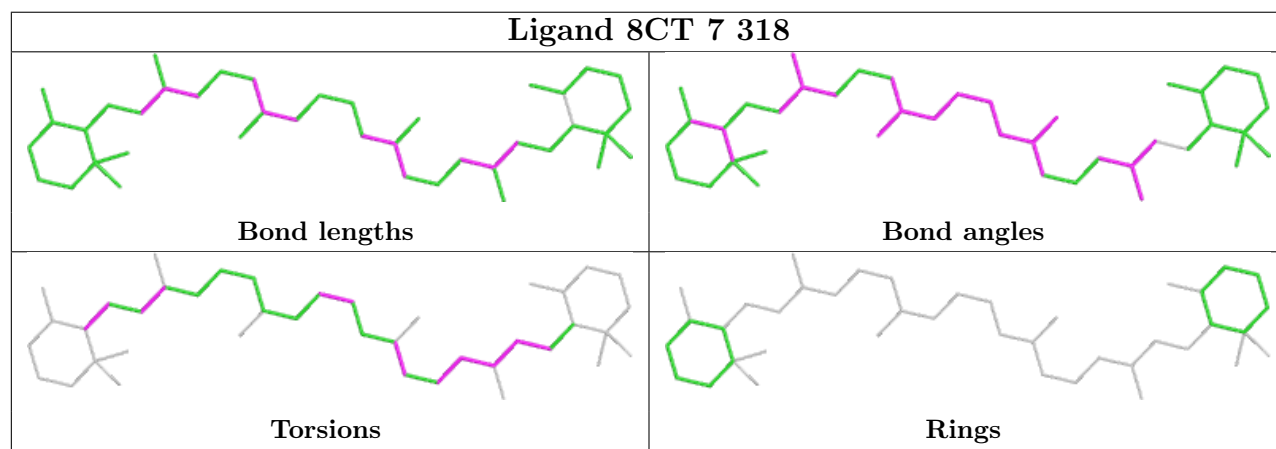
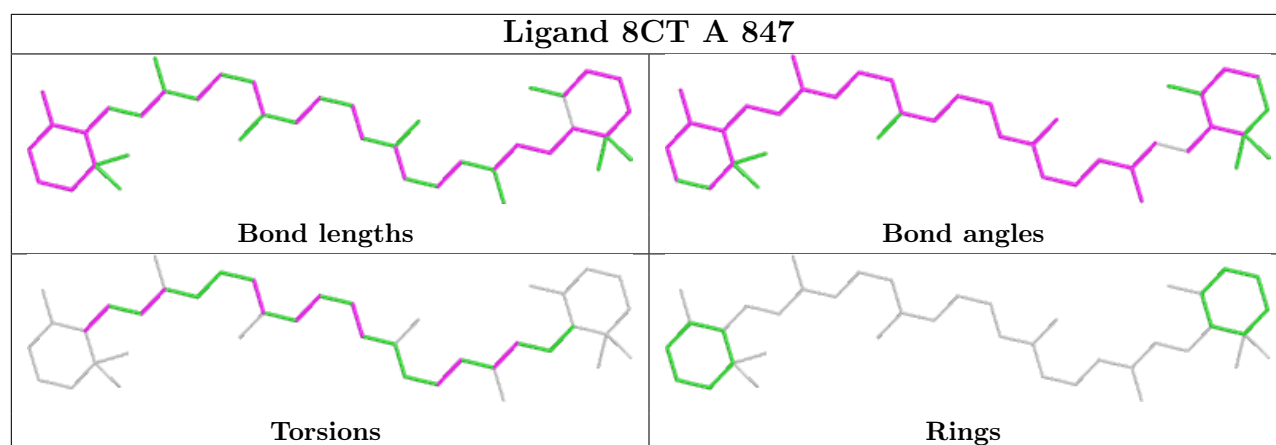
Bond angles



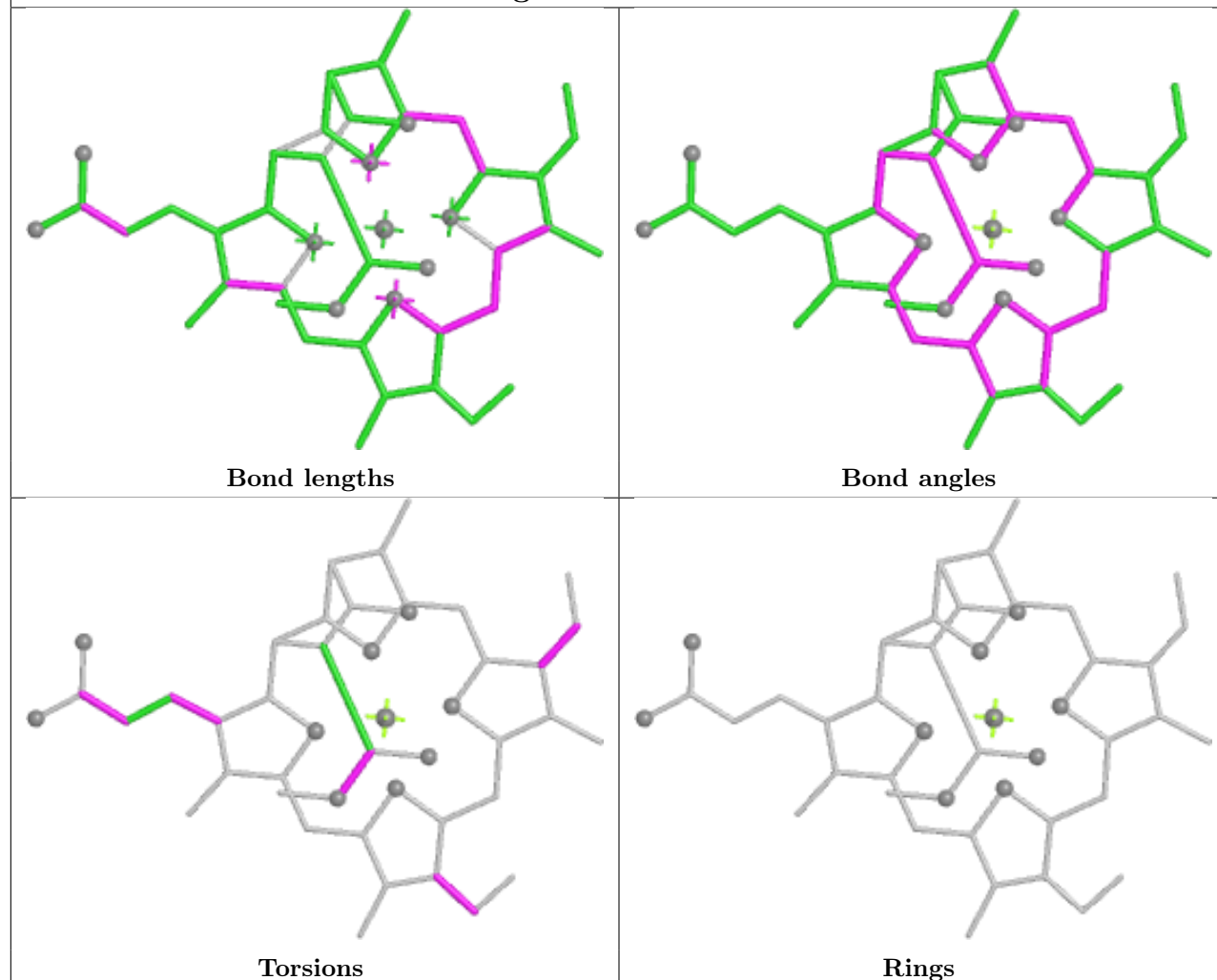
Torsions



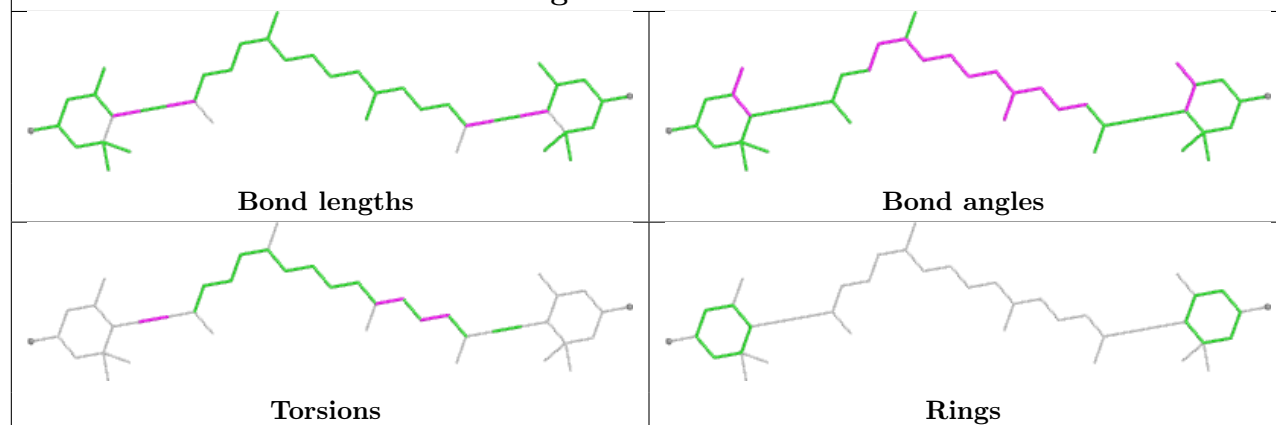
Rings

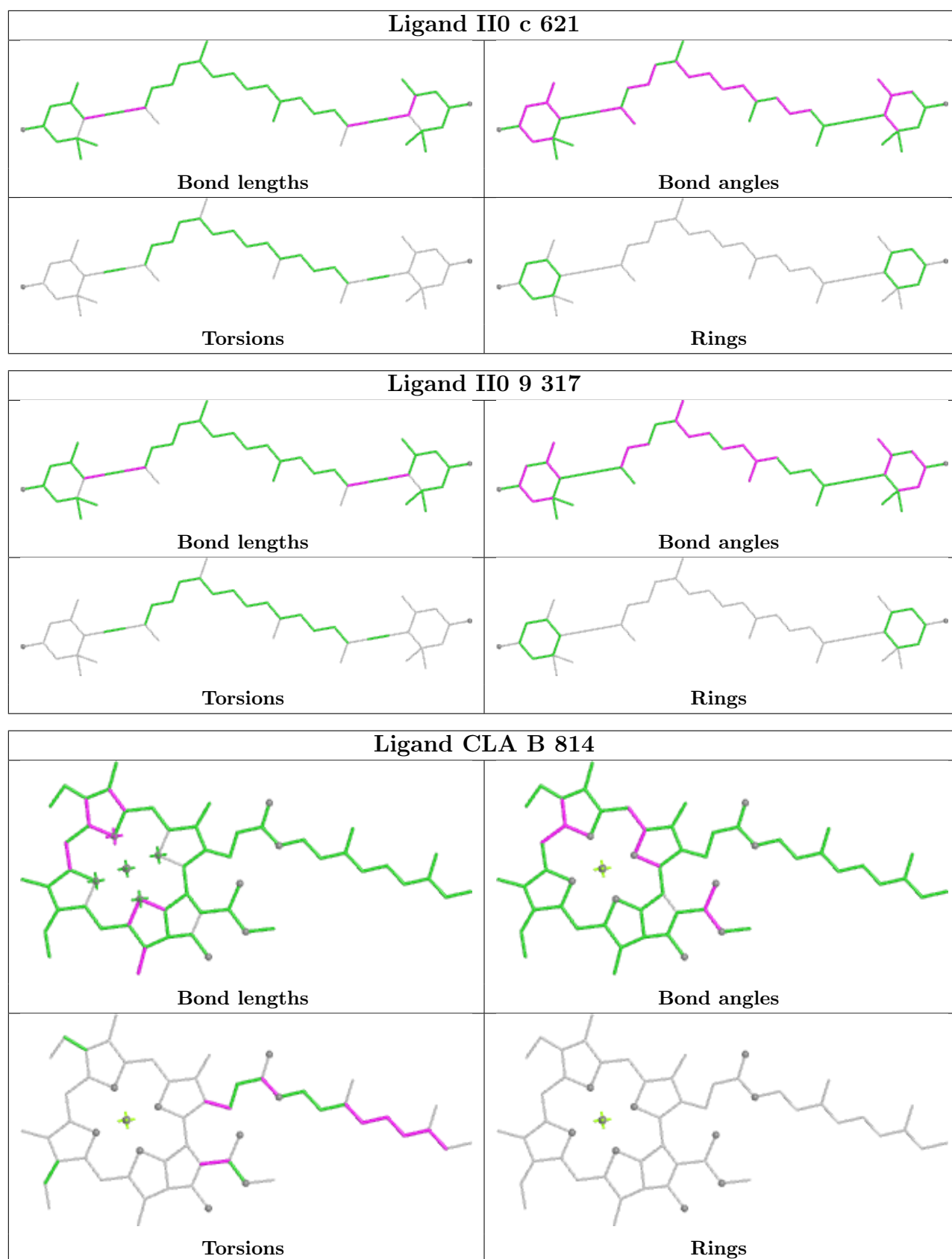


Ligand KC2 6 613

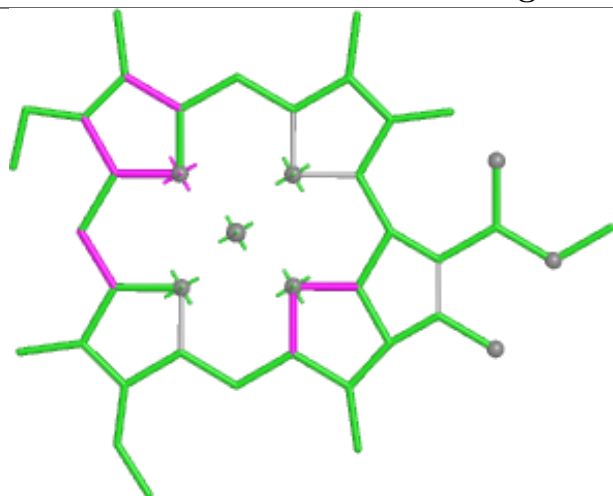


Ligand II0 9 323

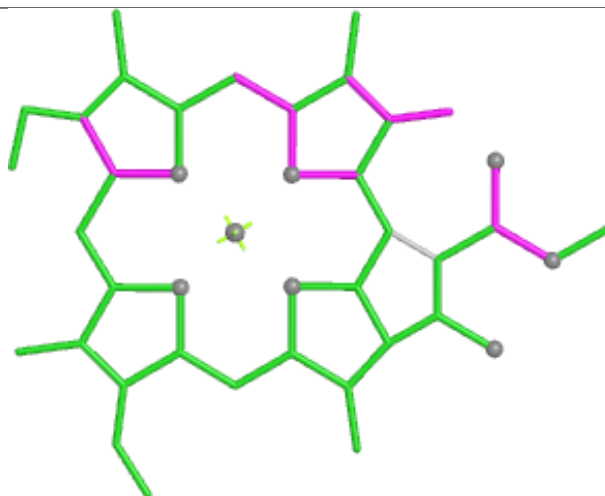




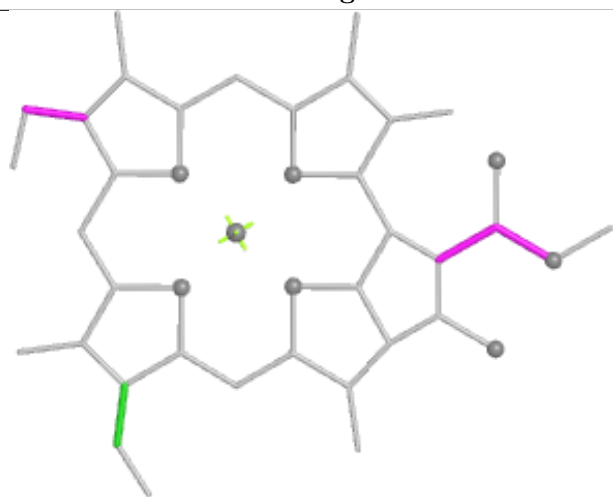
Ligand CLA 5 613



Bond lengths



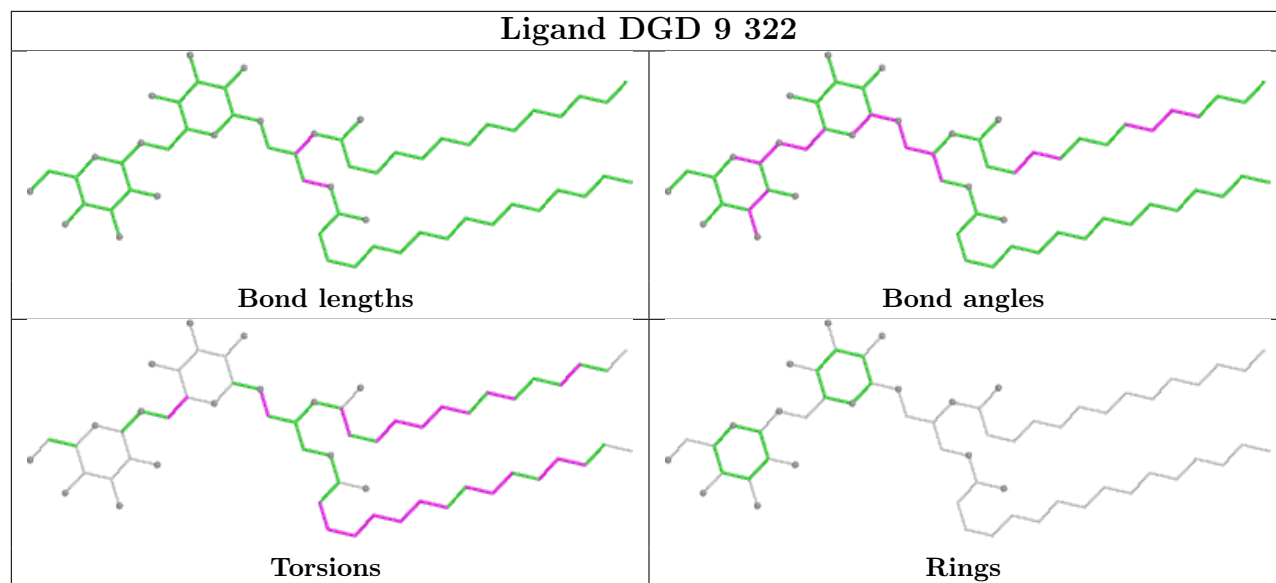
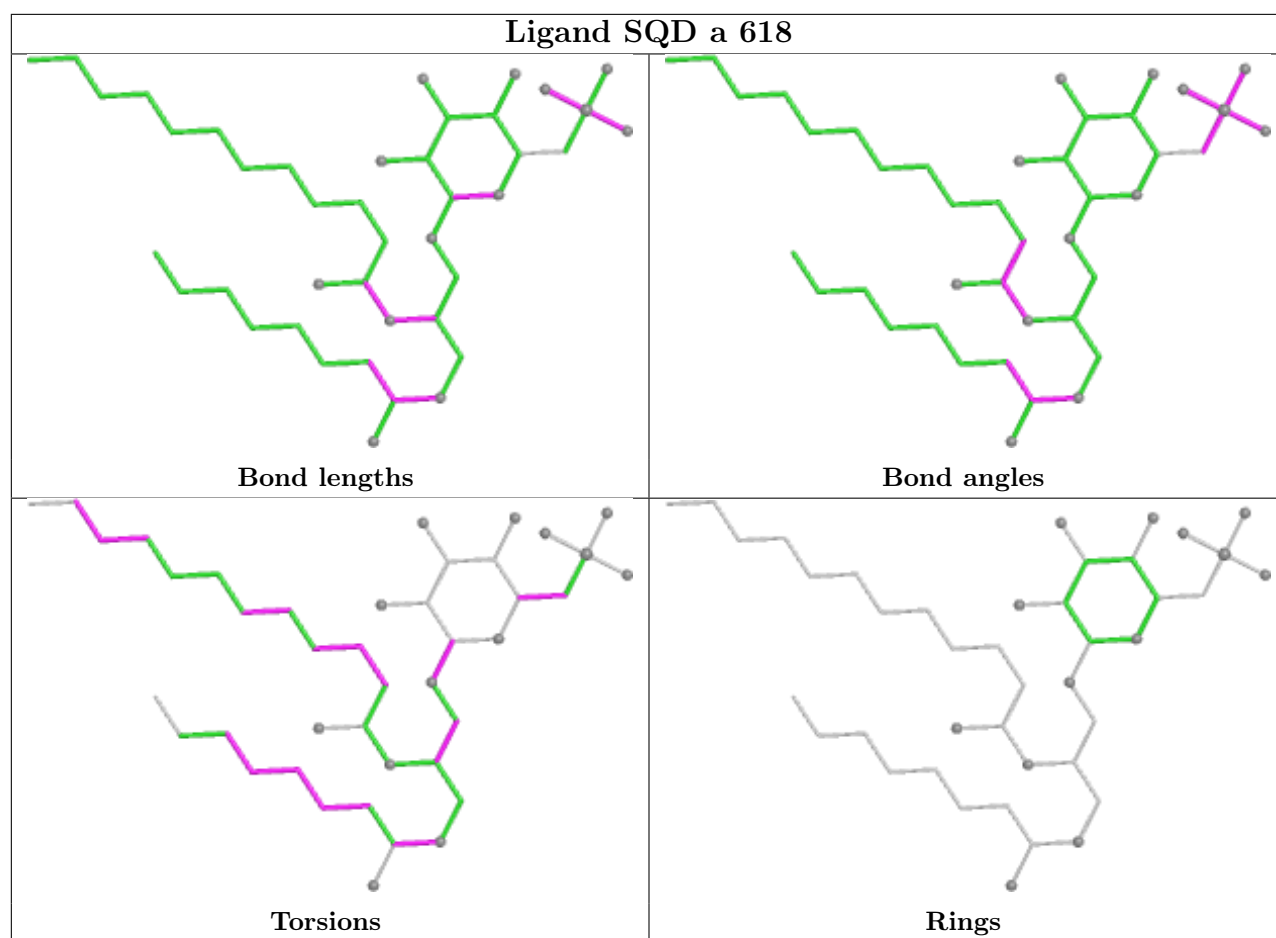
Bond angles



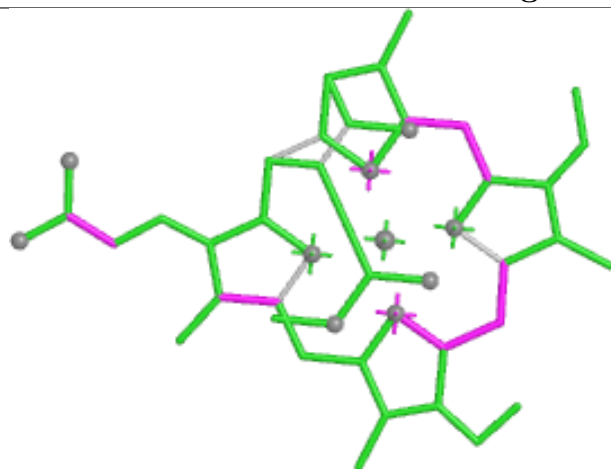
Torsions



Rings



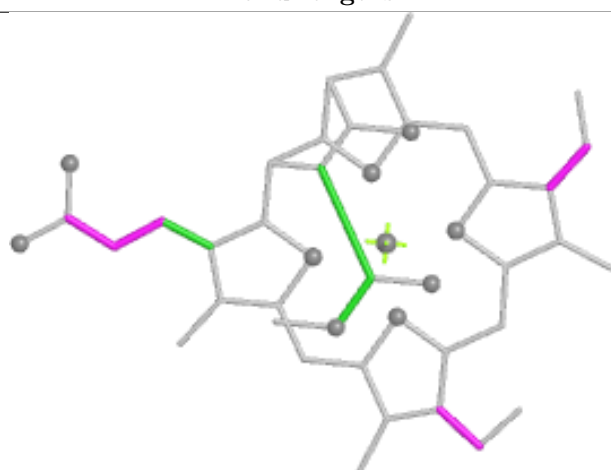
Ligand KC2 e 605



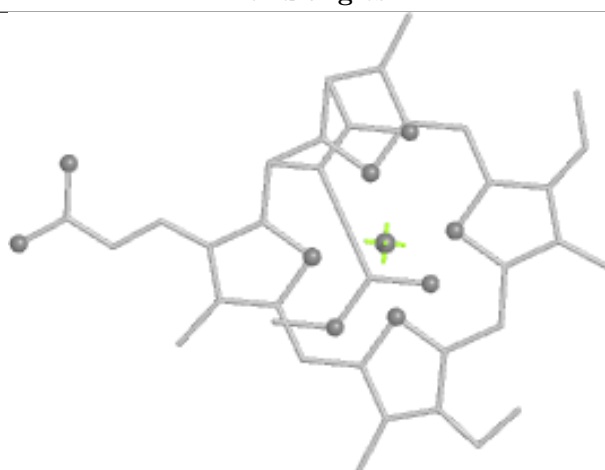
Bond lengths



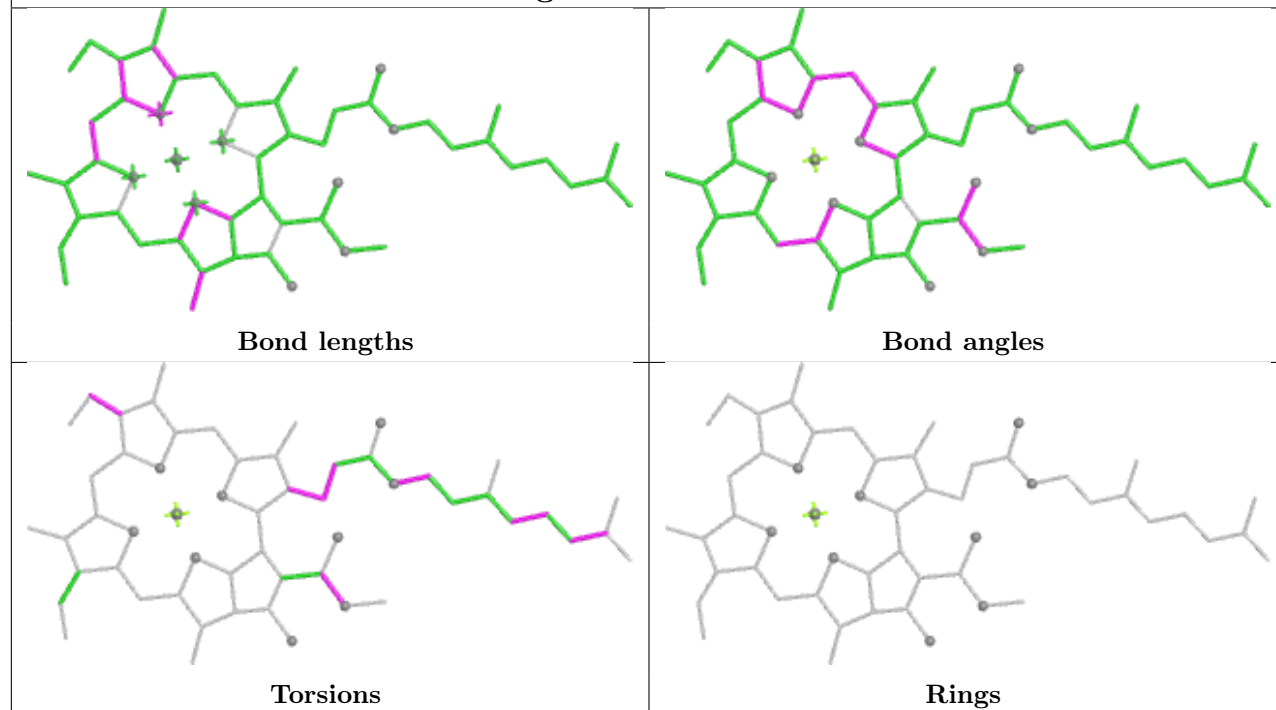
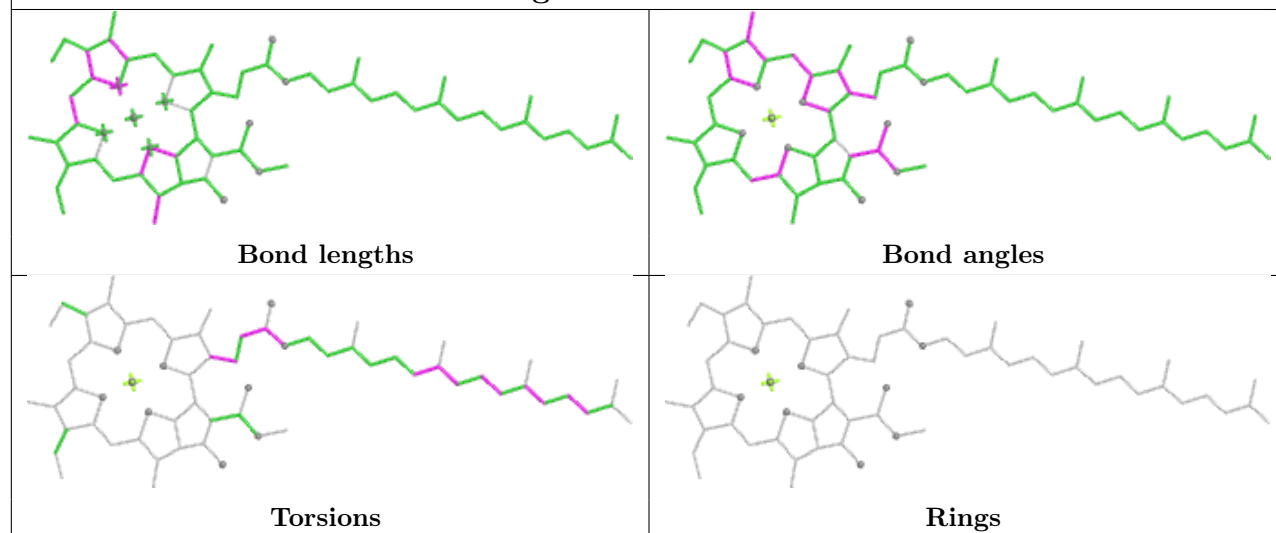
Bond angles

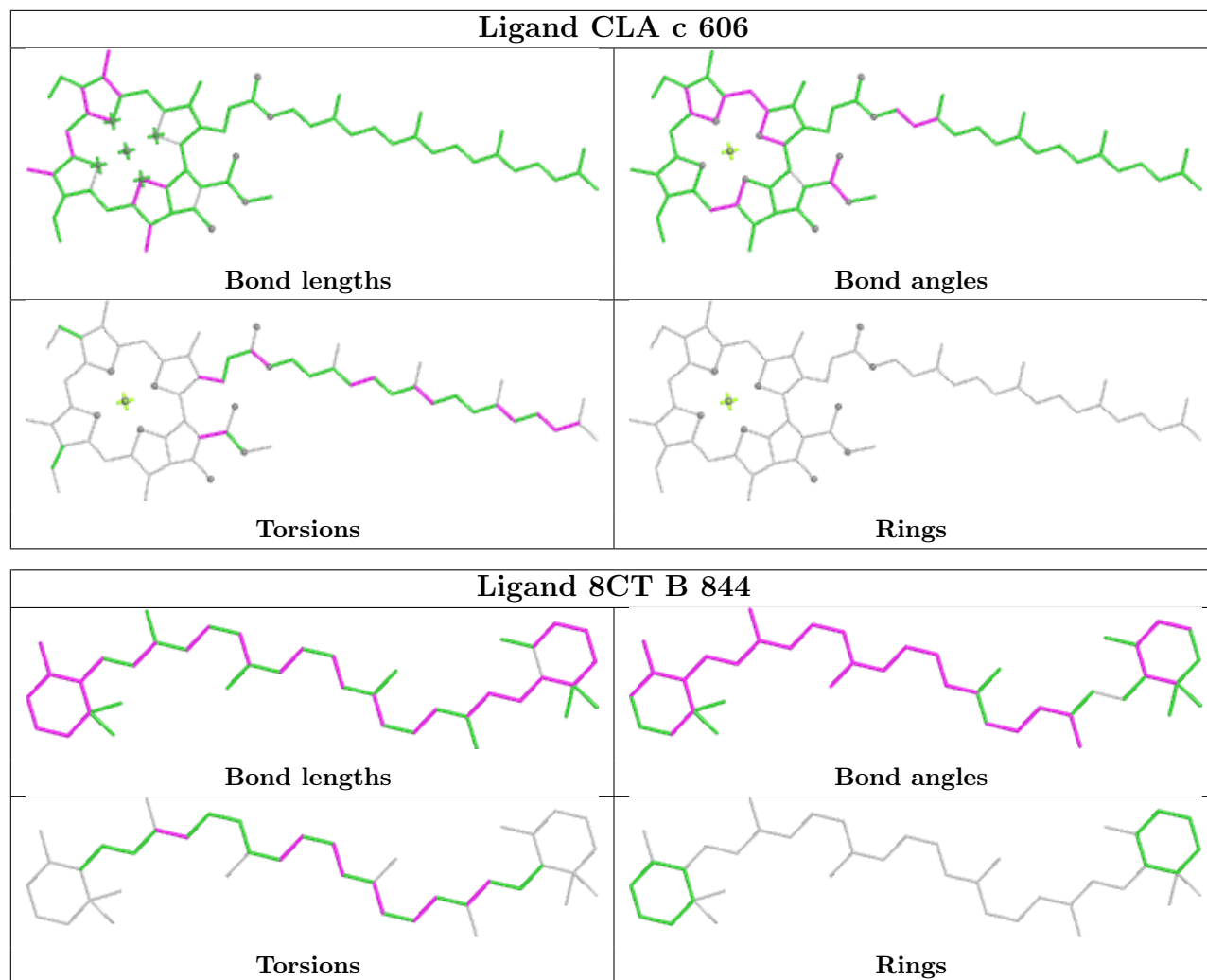


Torsions

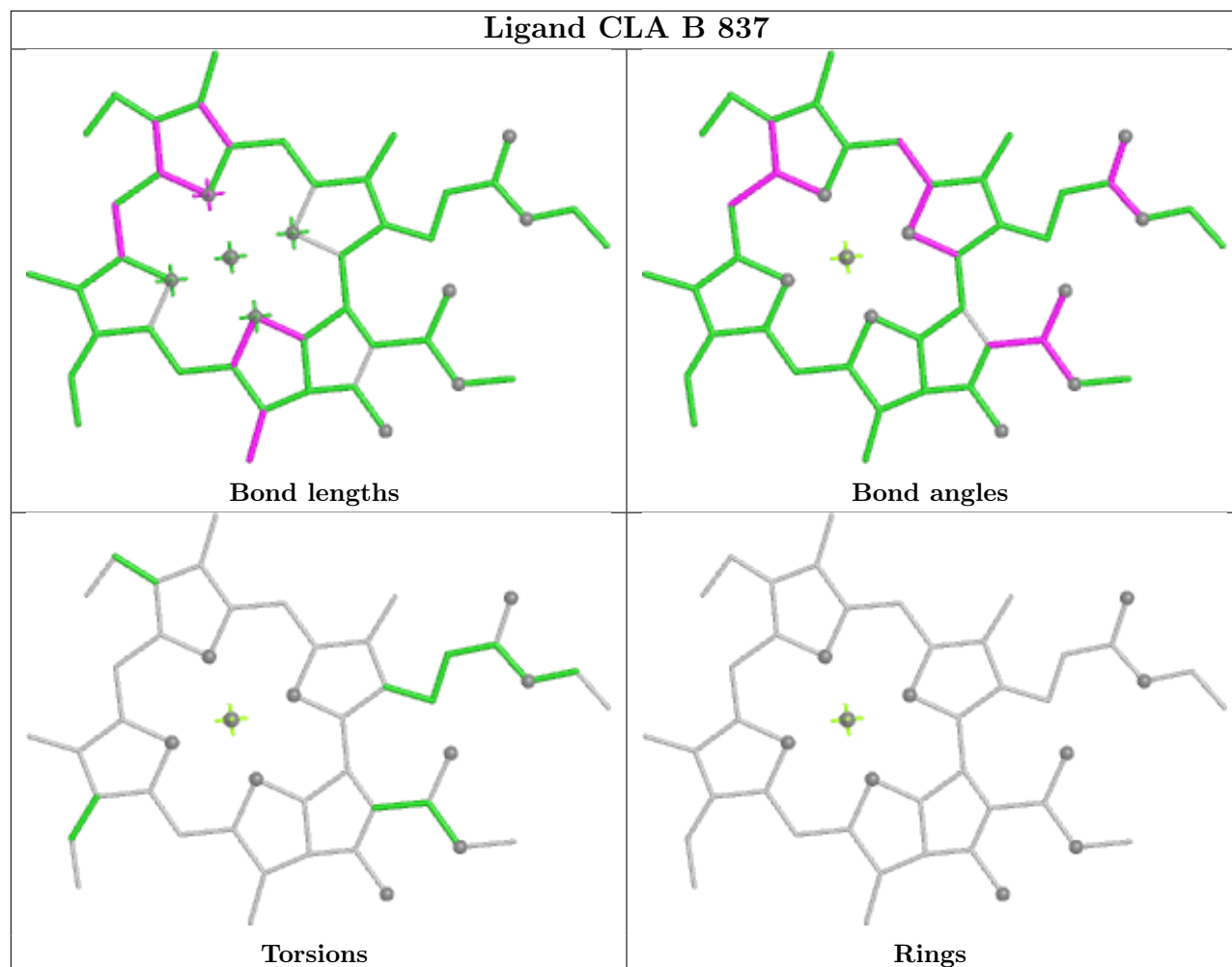


Rings

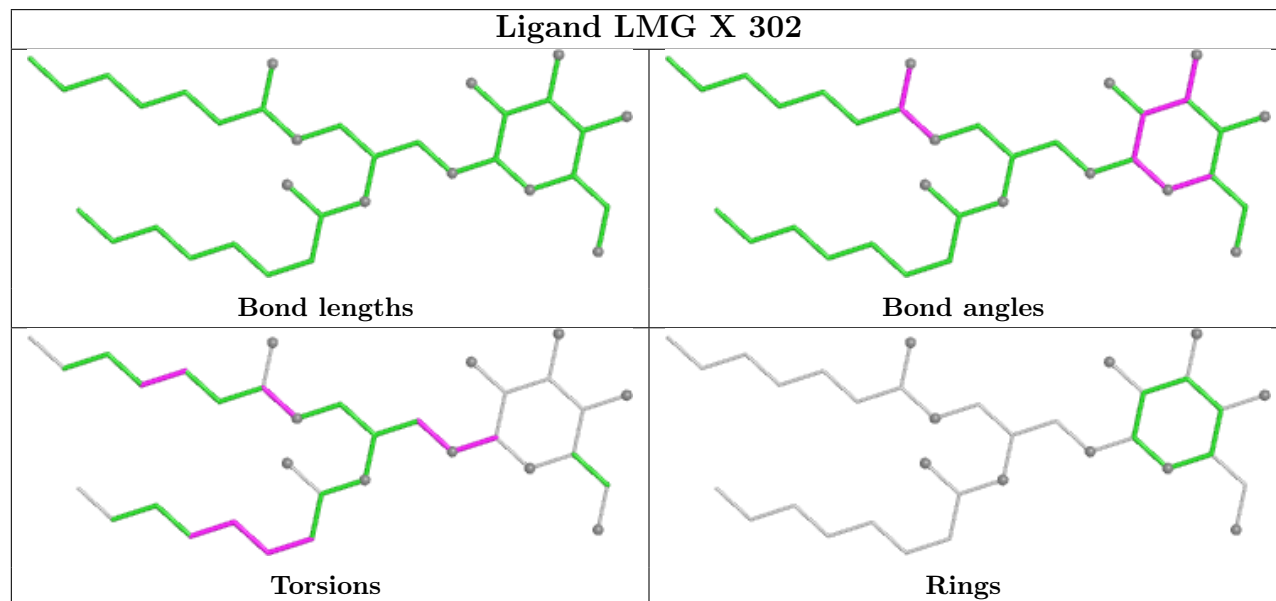
Ligand CLA a 602**Ligand CLA B 836**

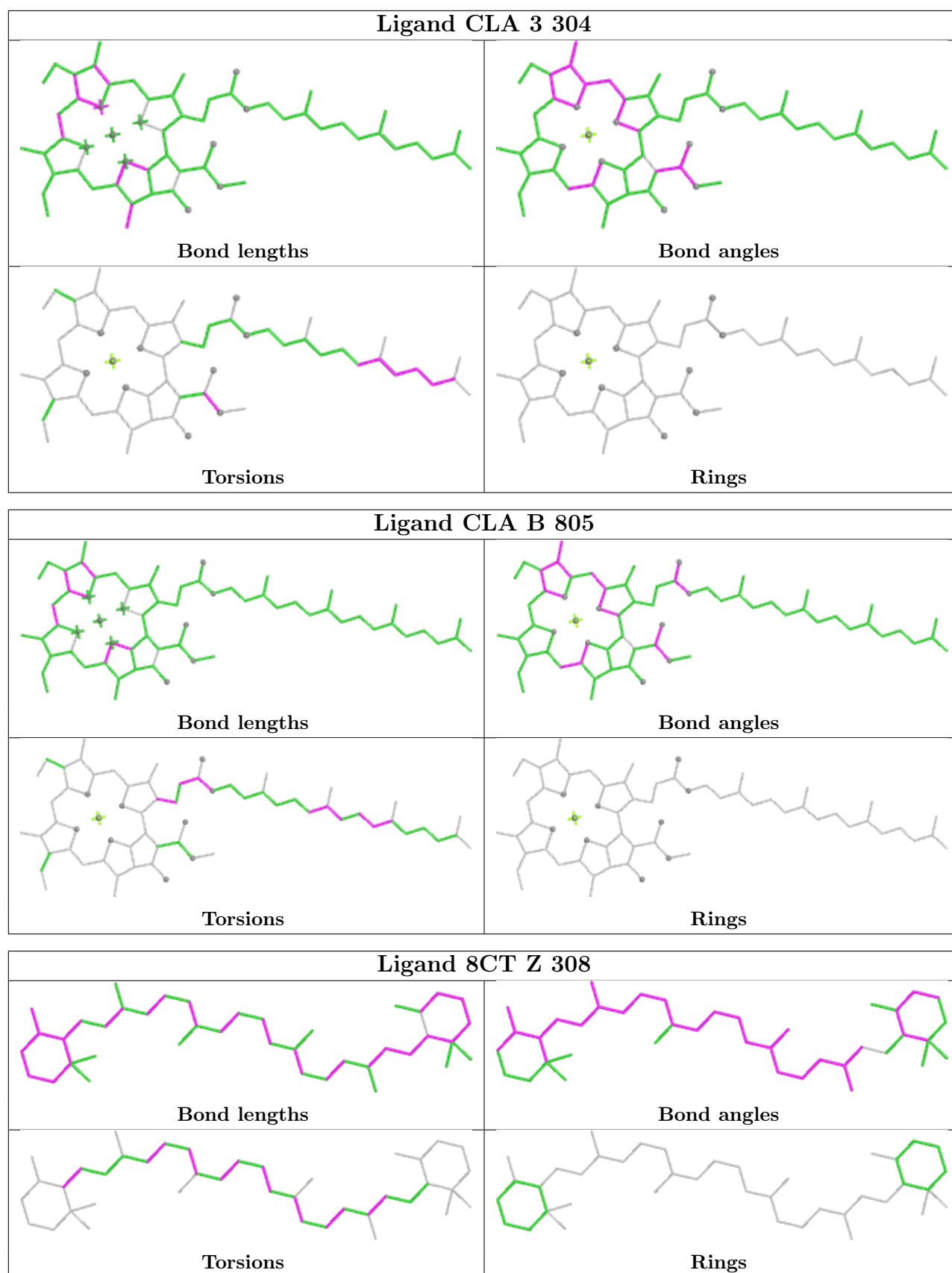


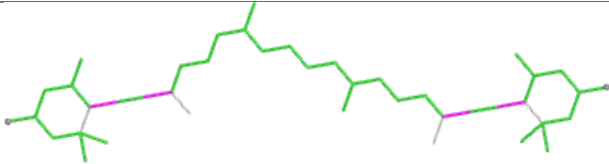
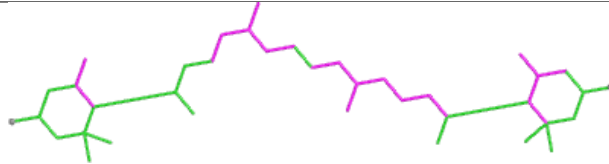
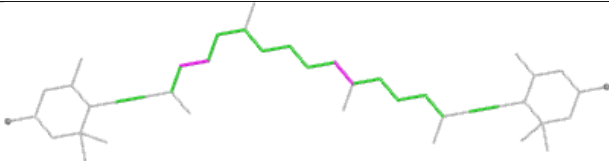
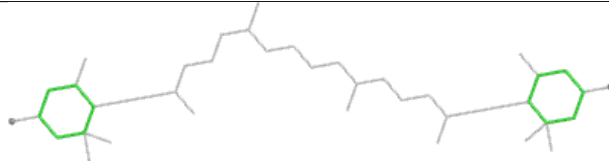
Ligand CLA B 837

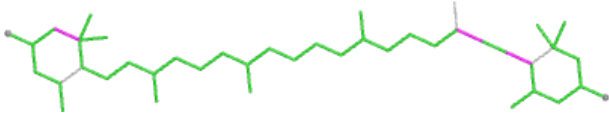
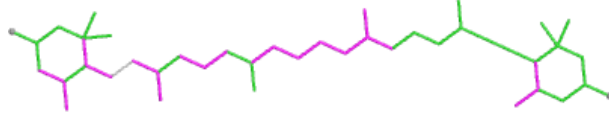
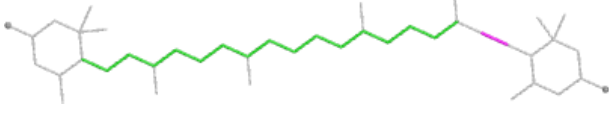
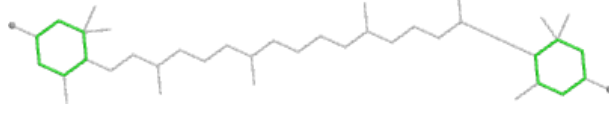


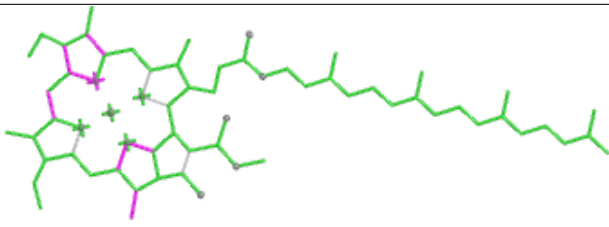
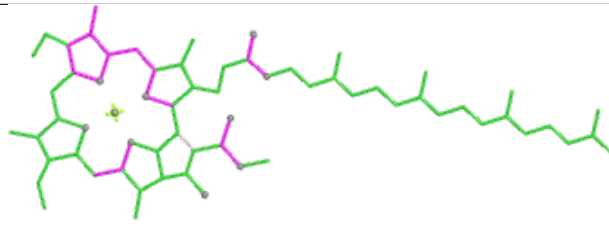
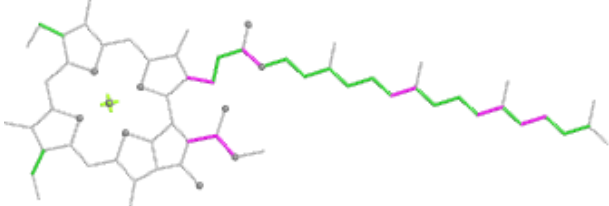
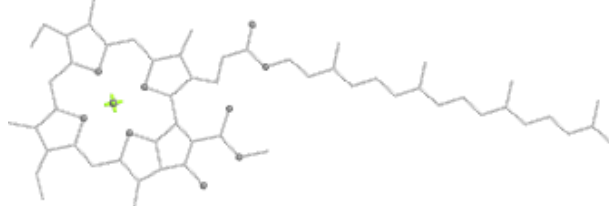
Ligand LMG X 302

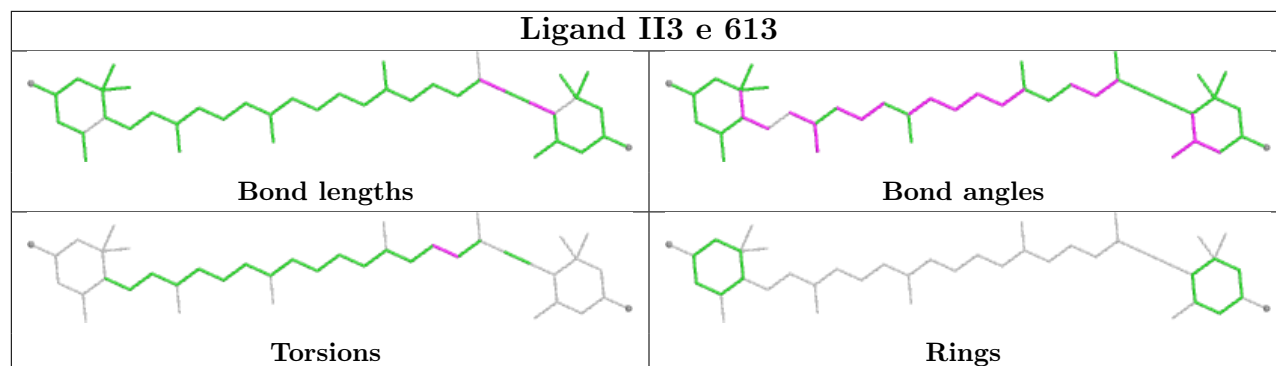
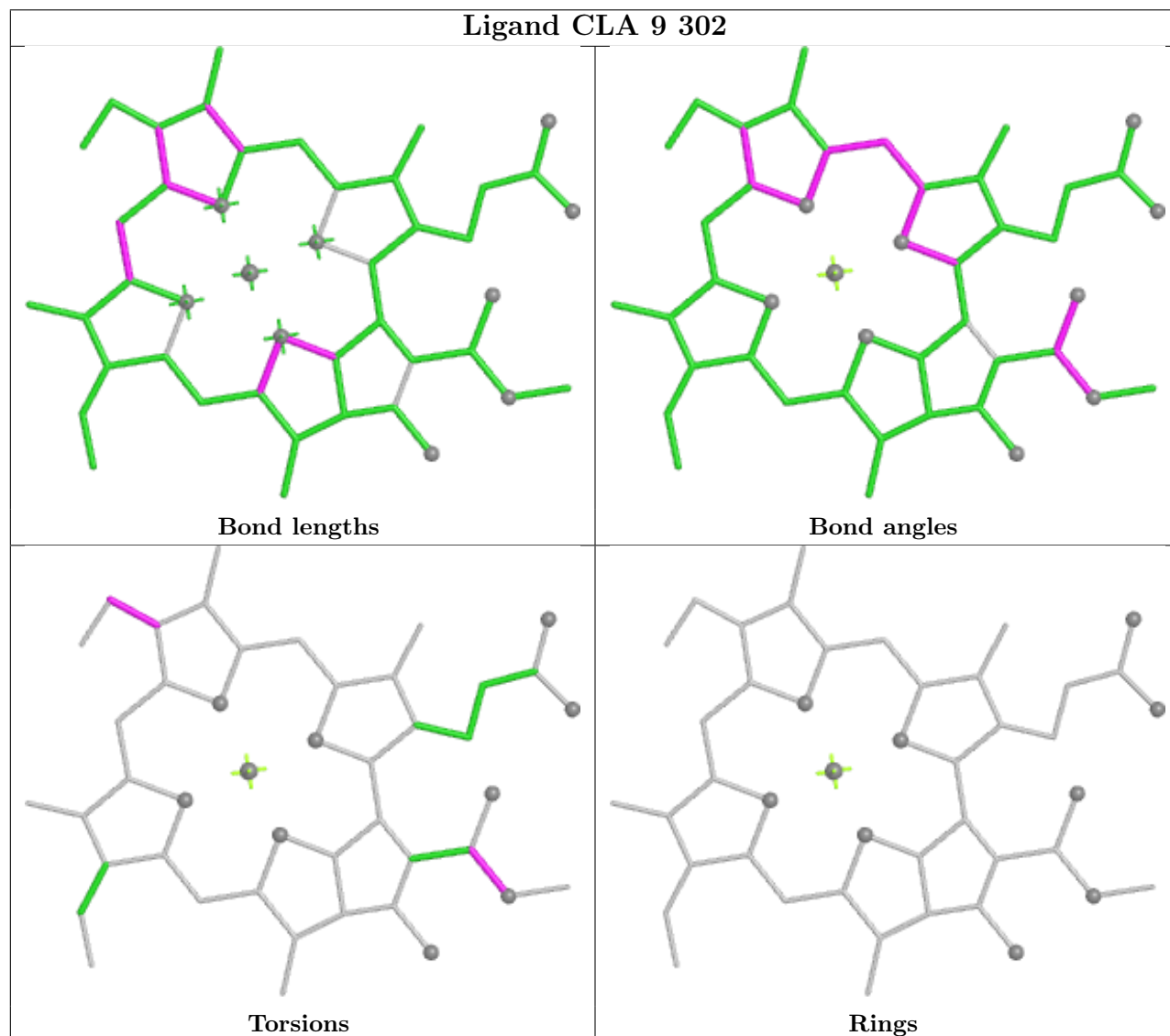


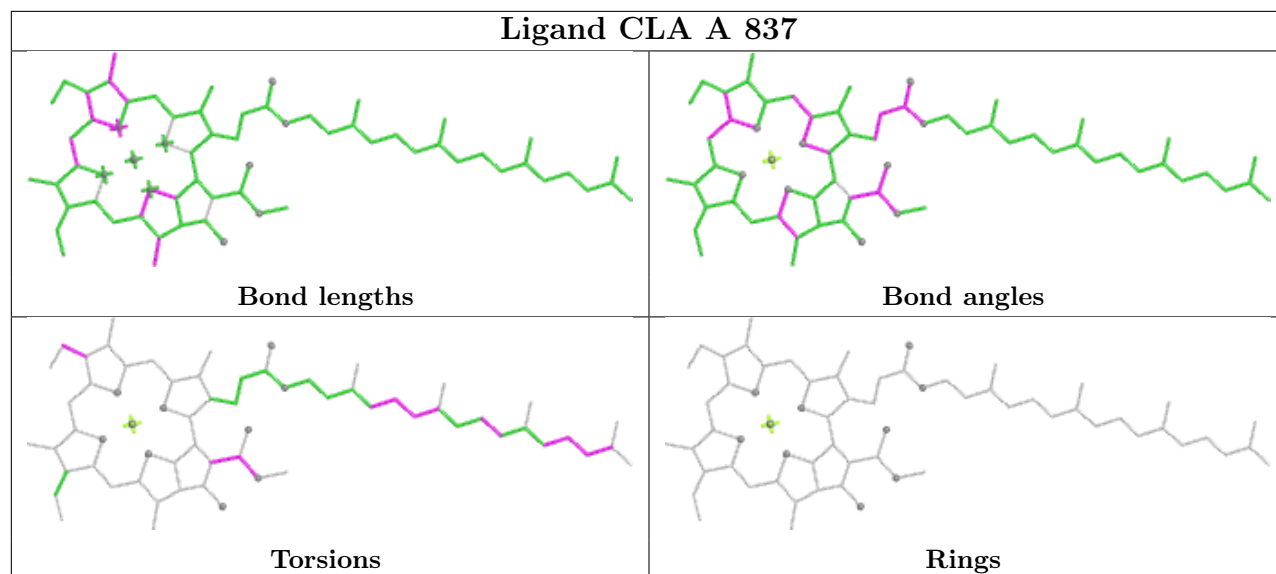
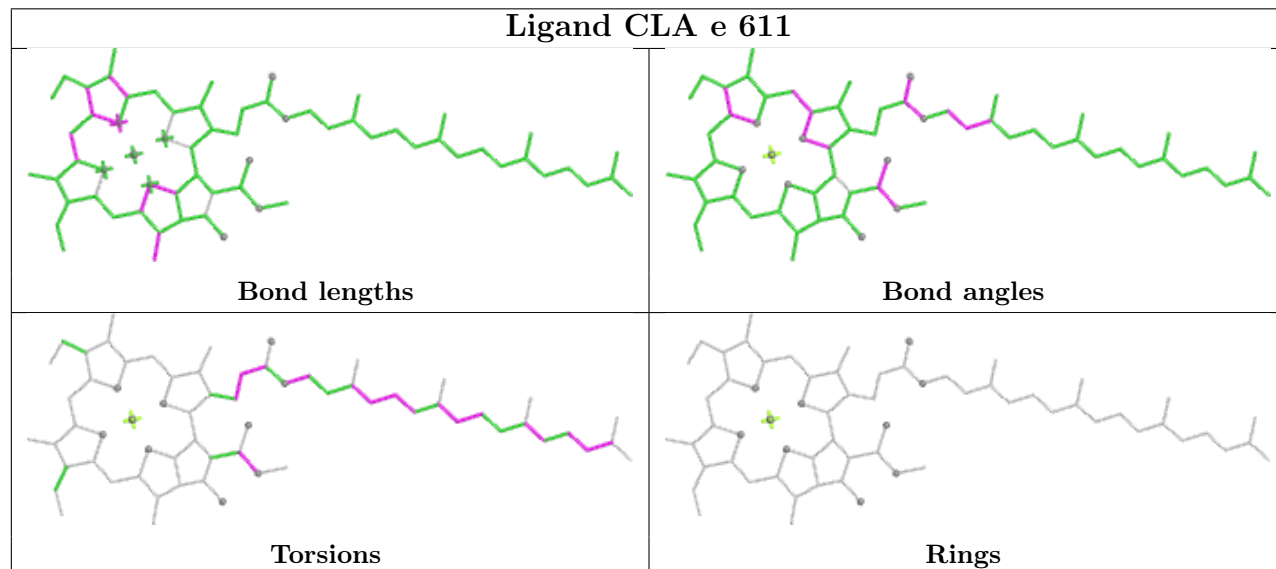


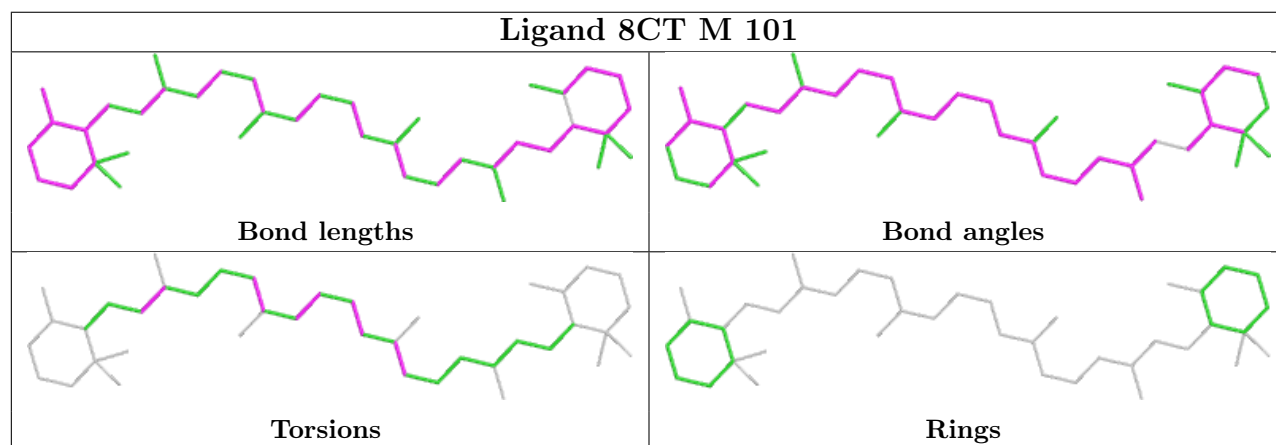
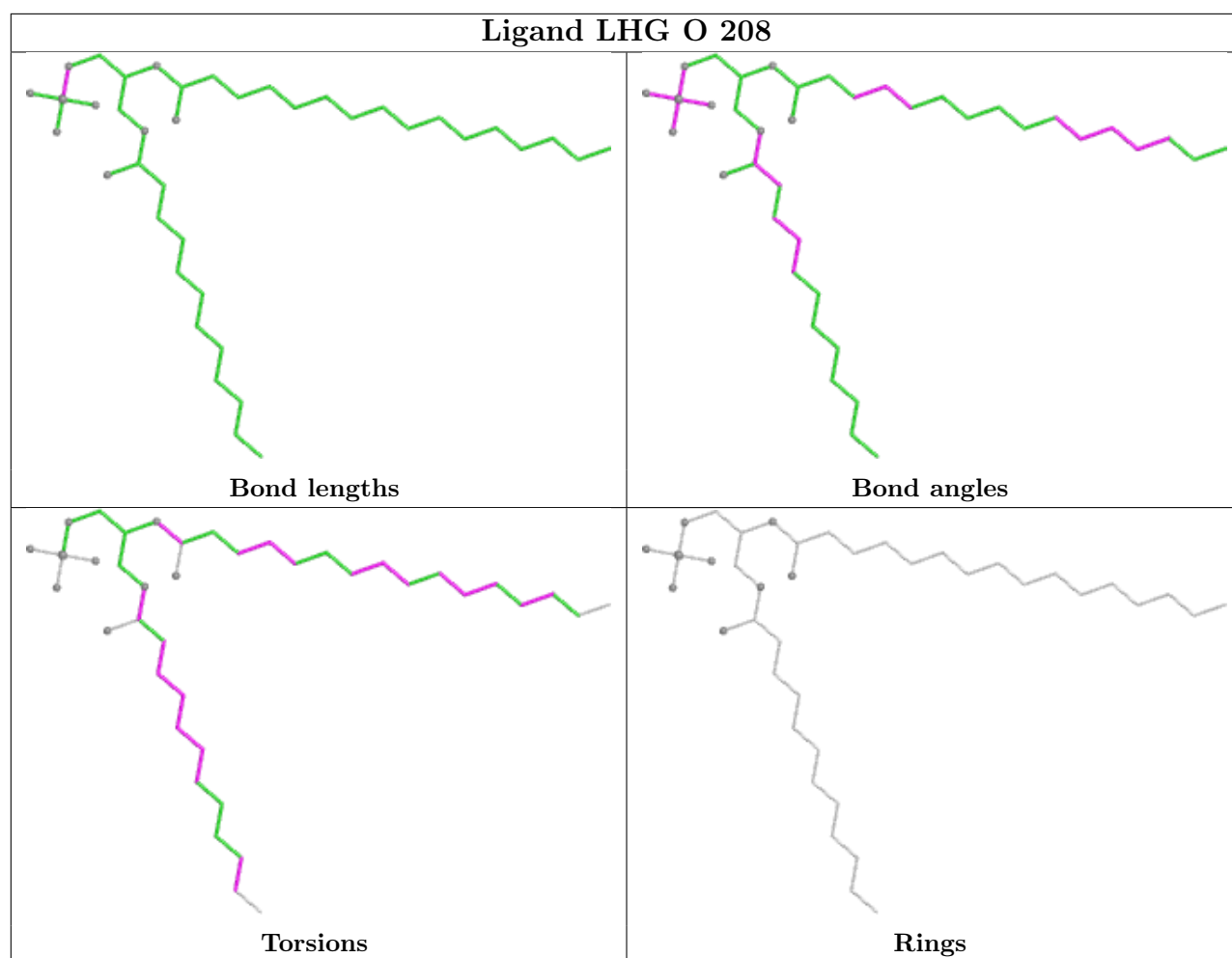
Ligand II0 d 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

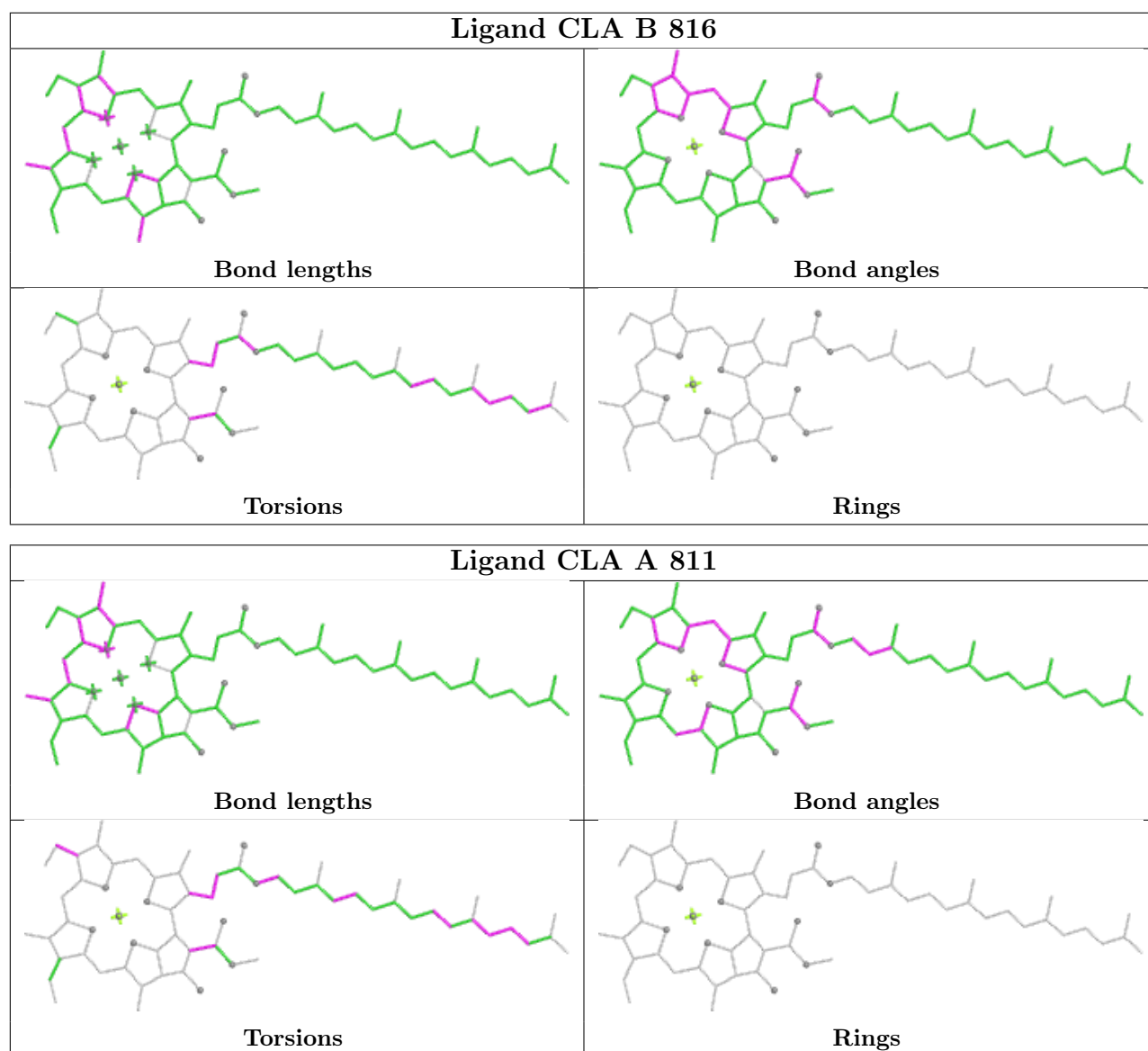
Ligand II3 1 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

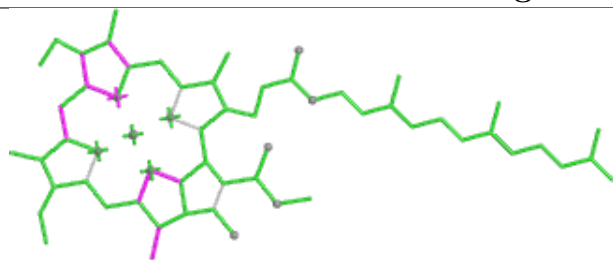
Ligand II3 e 613**Ligand CLA 9 302**

Ligand CLA A 837**Ligand CLA e 611**

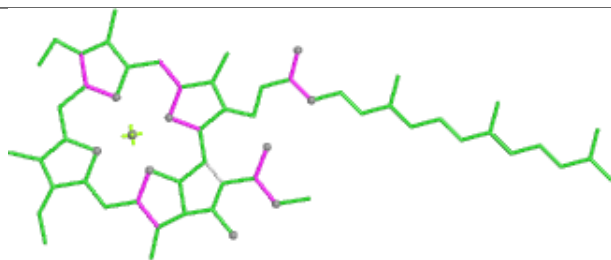




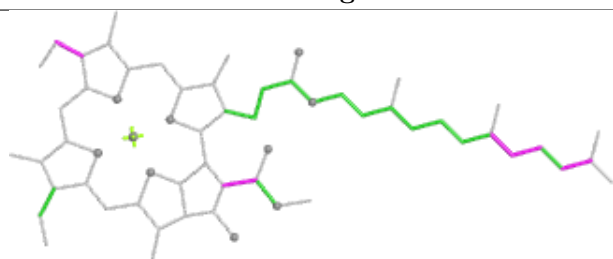
Ligand CLA B 811



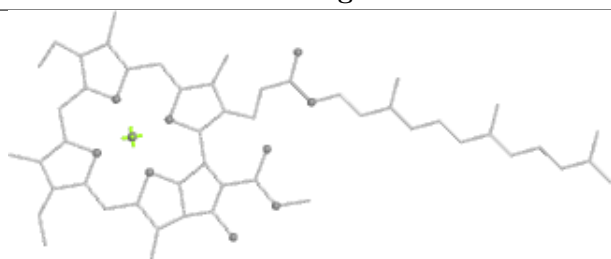
Bond lengths



Bond angles

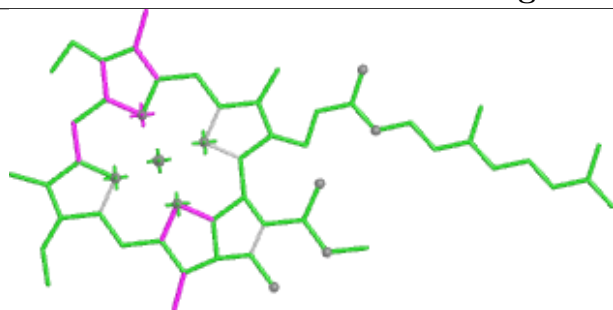


Torsions

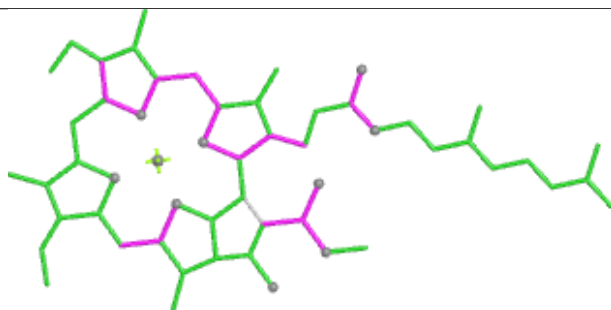


Rings

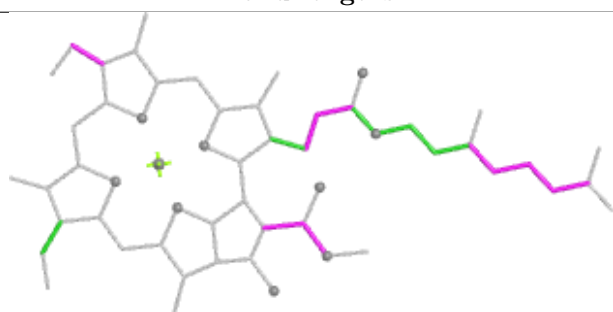
Ligand CLA 5 604



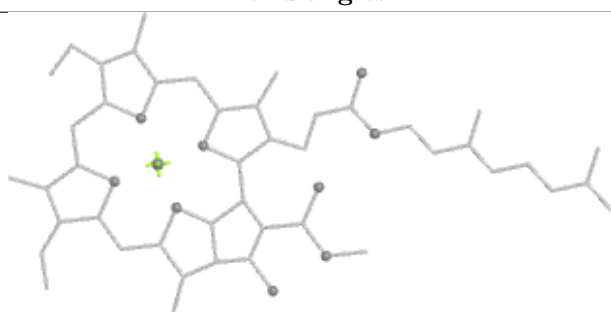
Bond lengths



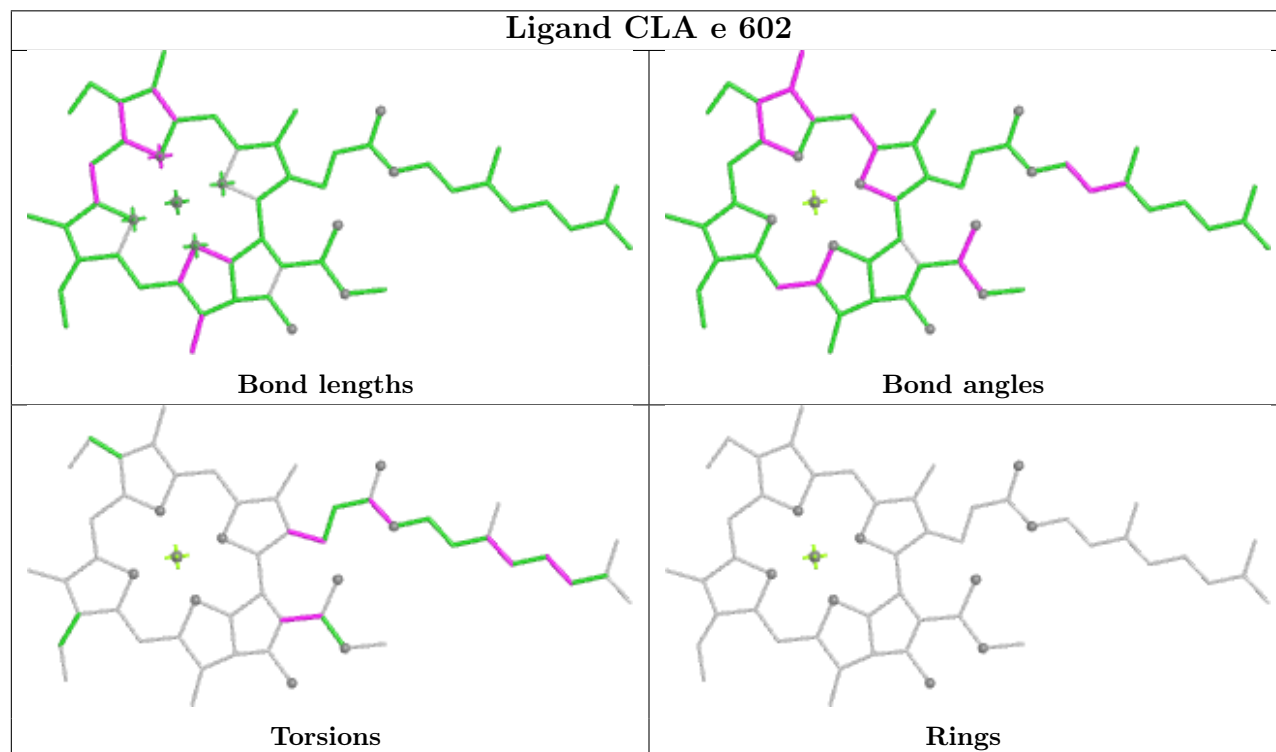
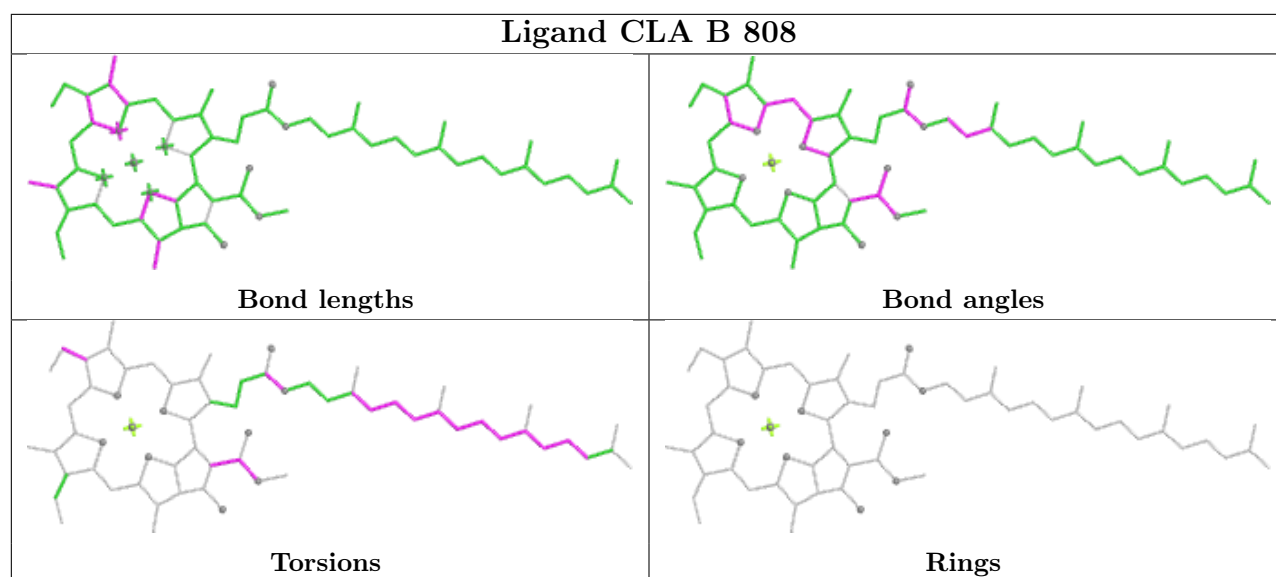
Bond angles

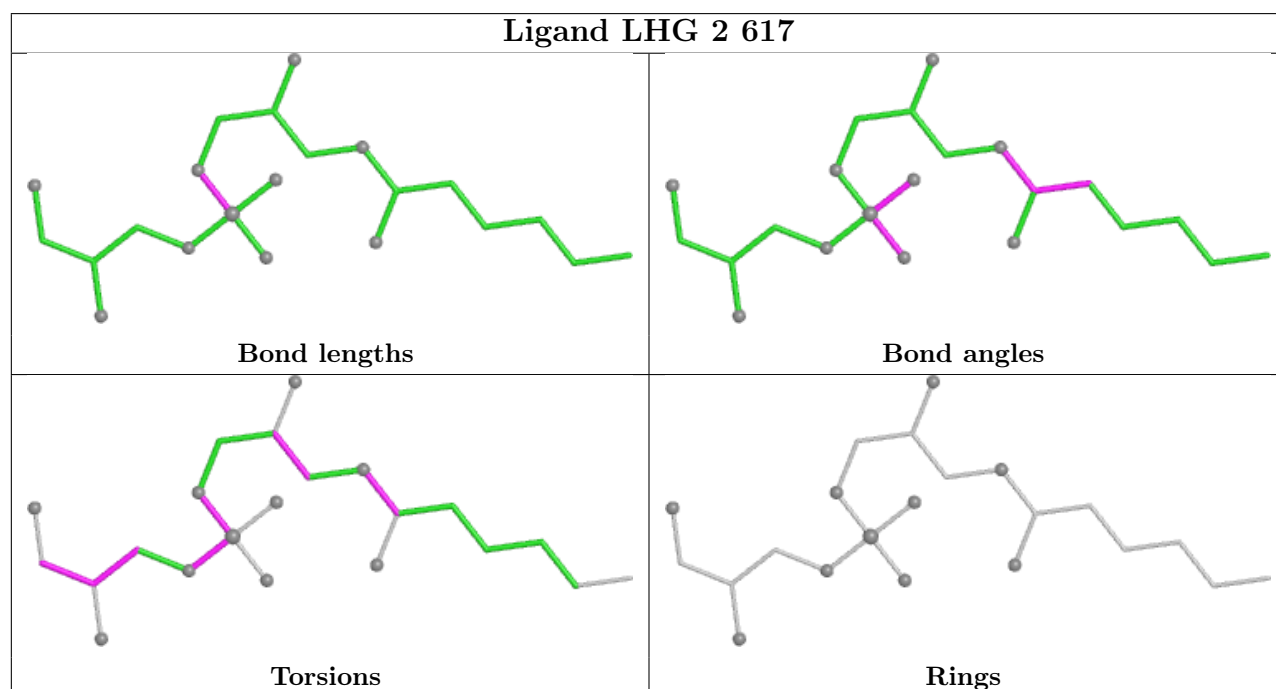
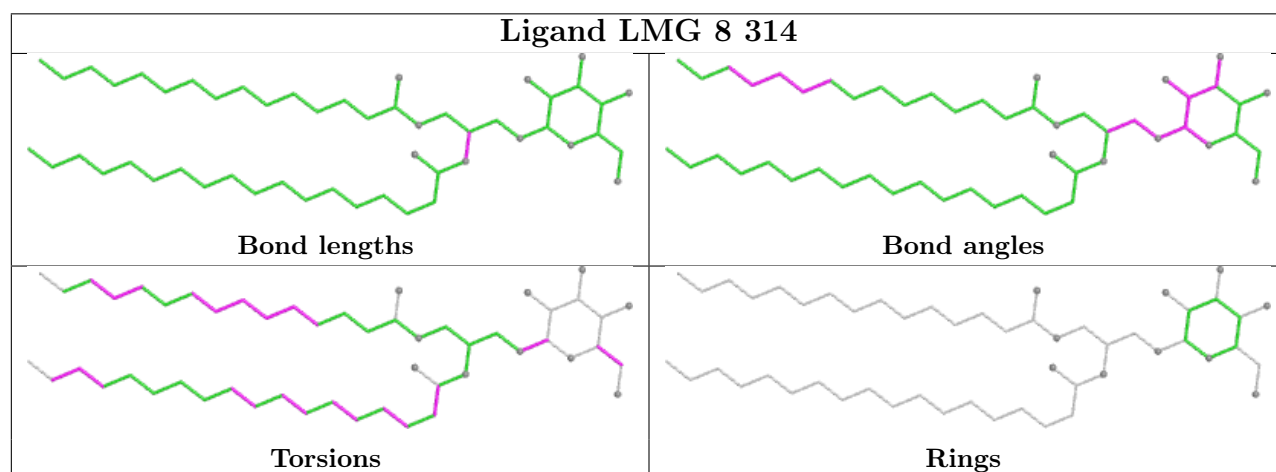
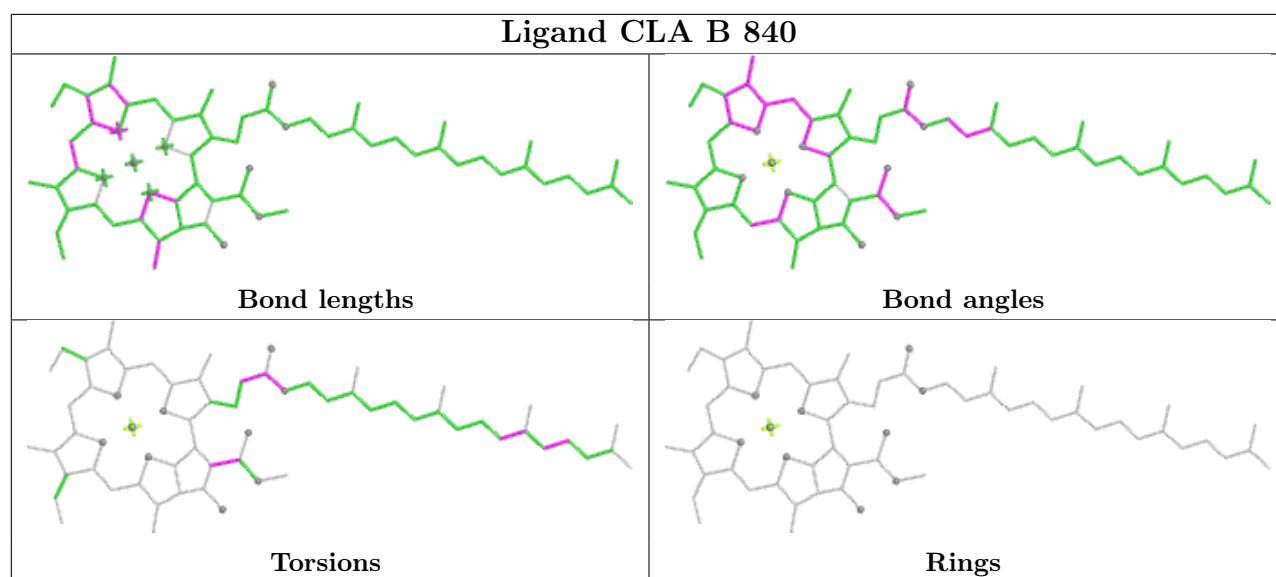


Torsions

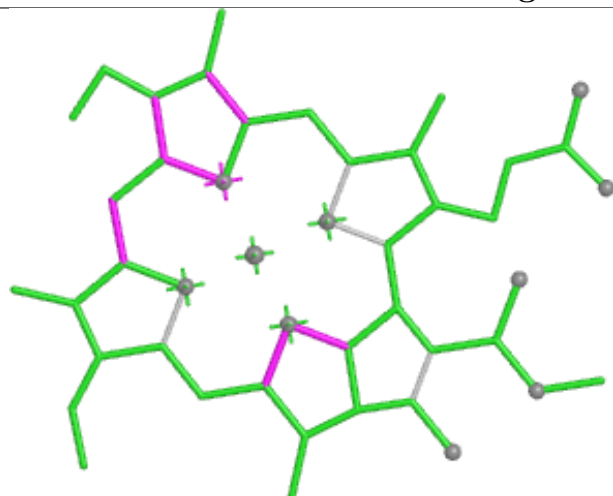


Rings

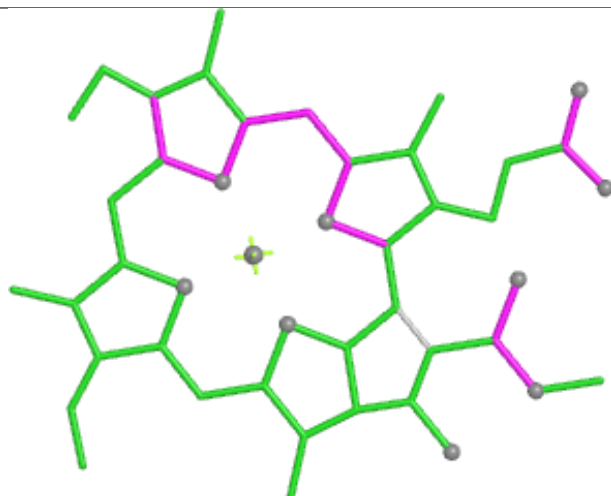




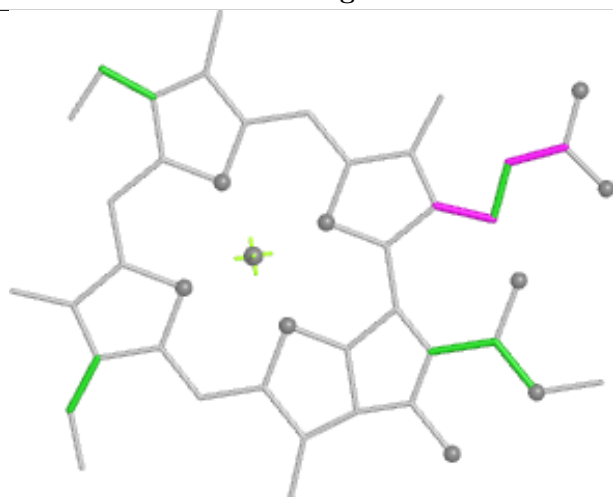
Ligand CLA 5 603



Bond lengths



Bond angles

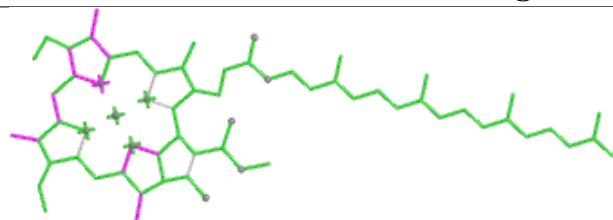


Torsions

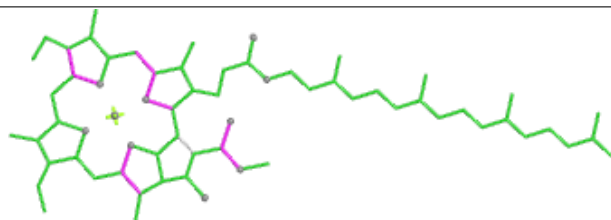


Rings

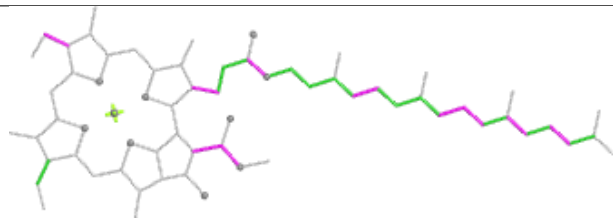
Ligand CLA B 823



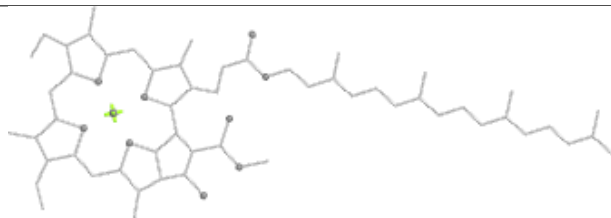
Bond lengths



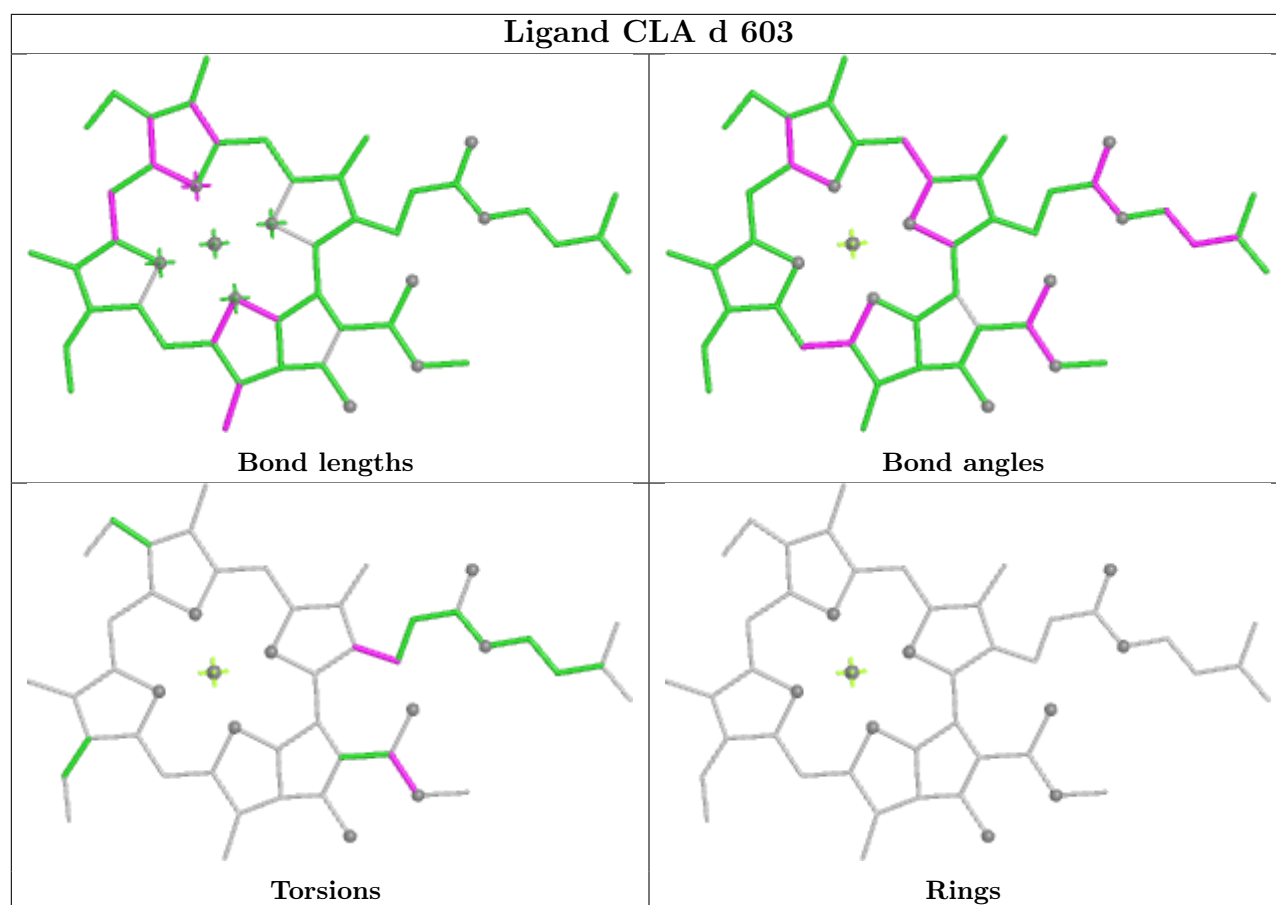
Bond angles



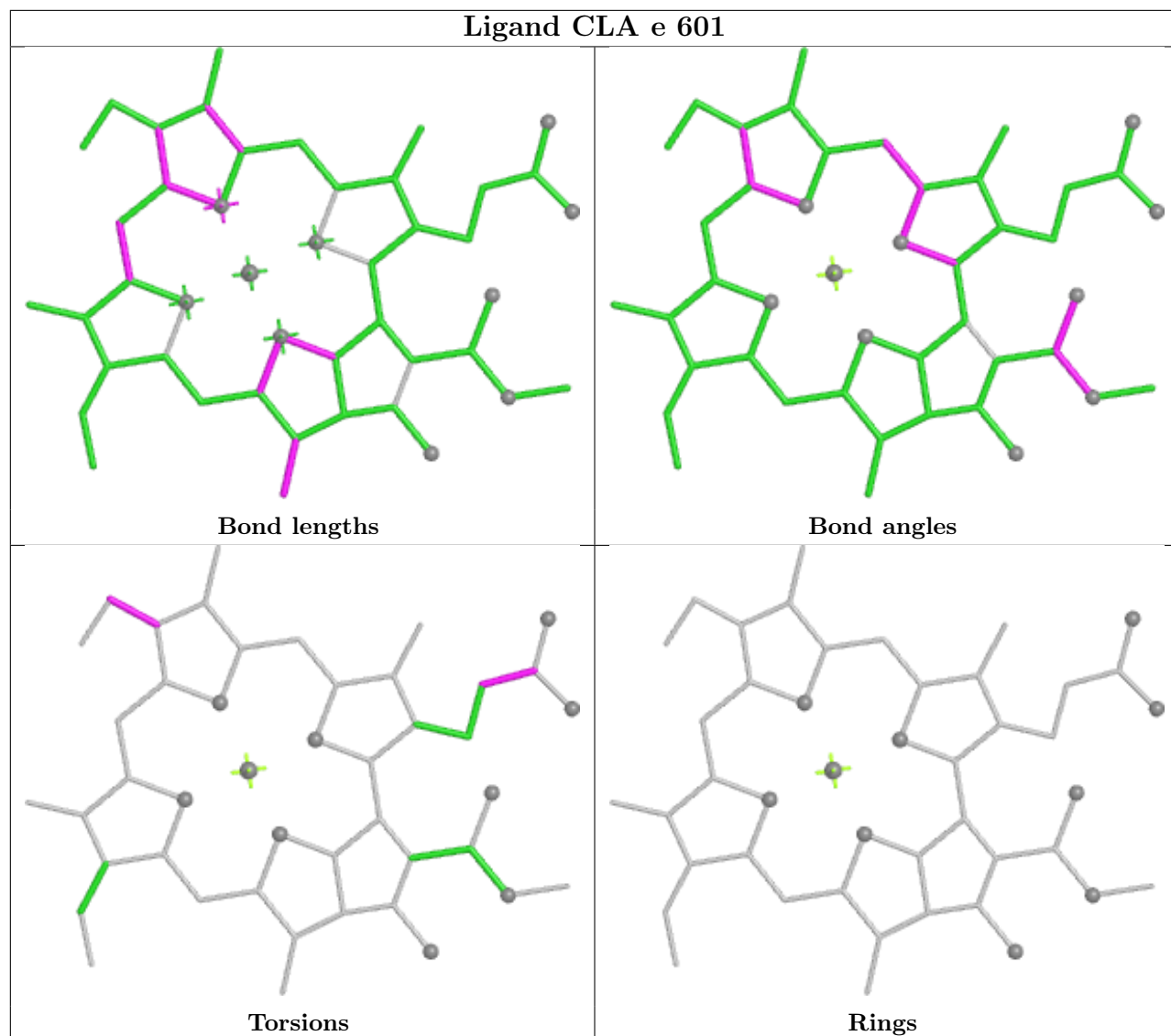
Torsions

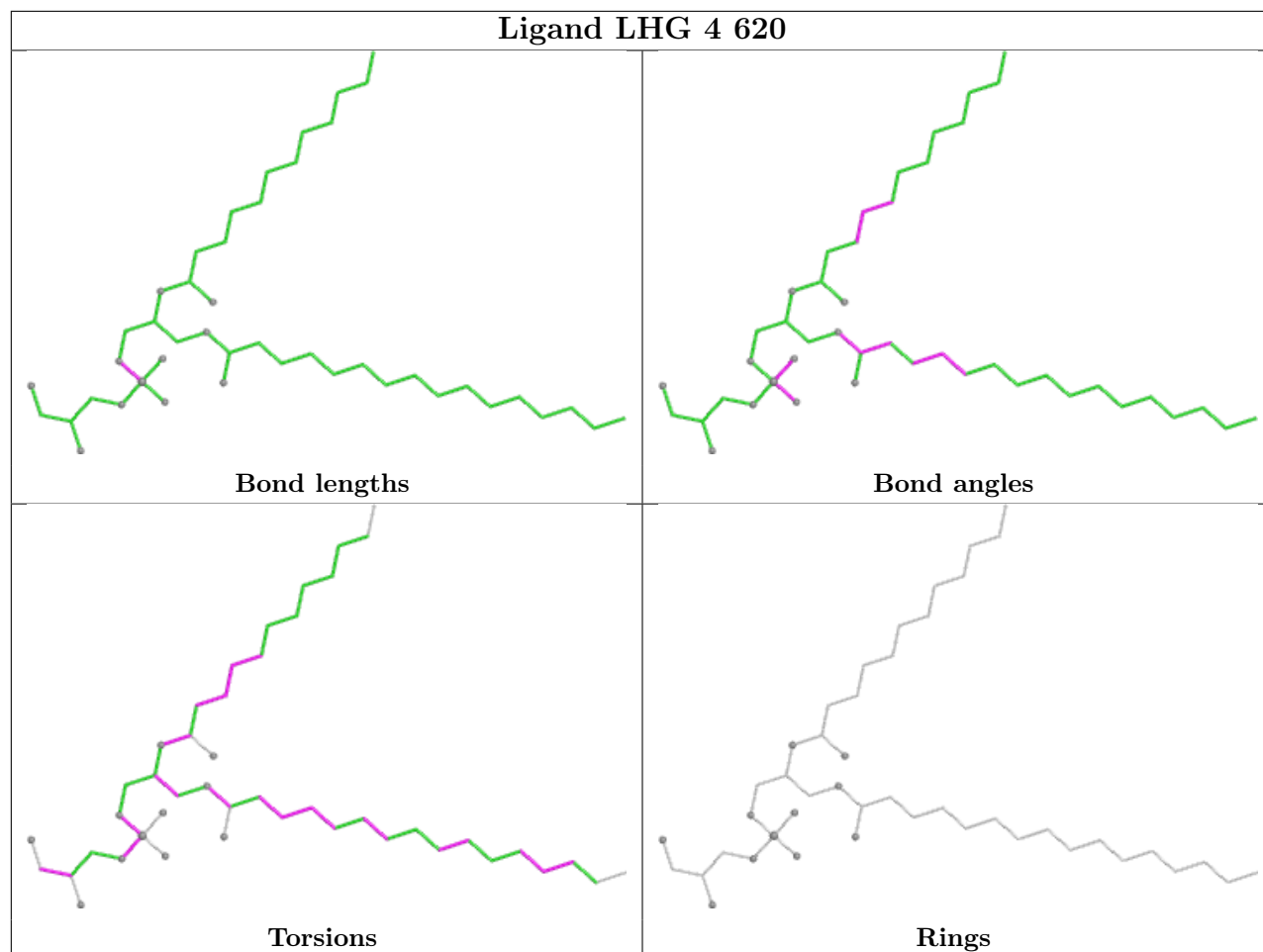
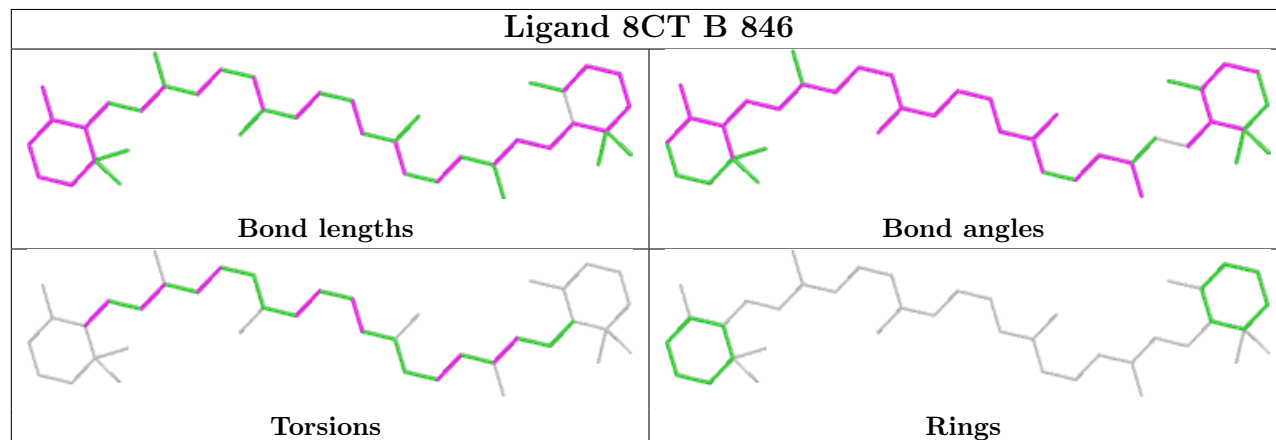


Rings

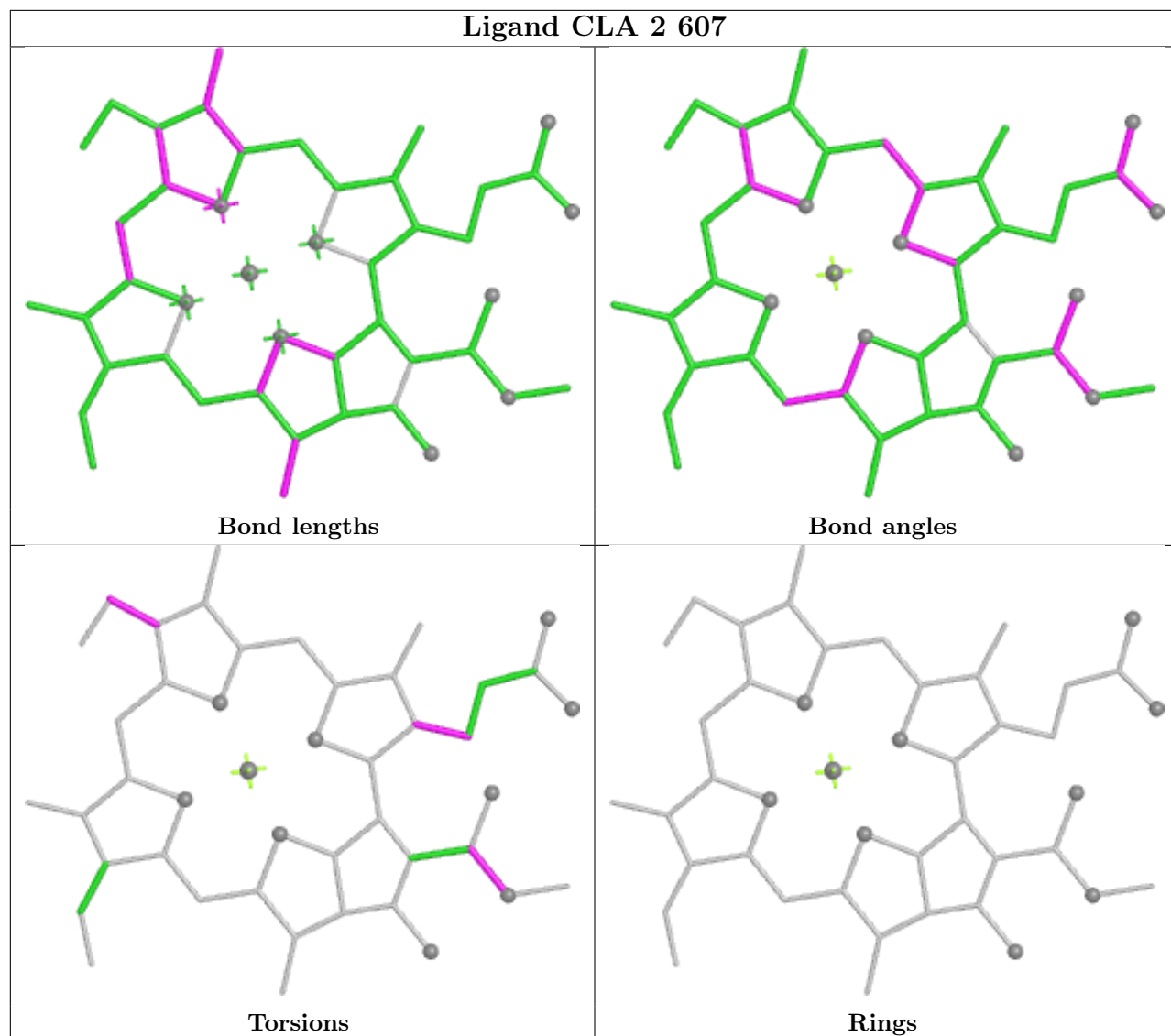


Ligand CLA e 601

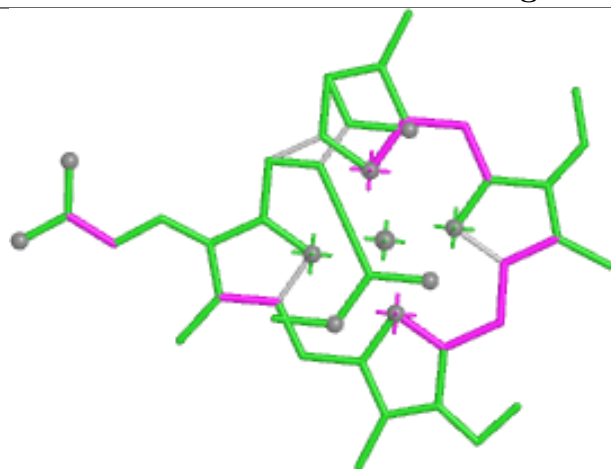


Ligand LHG 4 620**Ligand 8CT B 846**

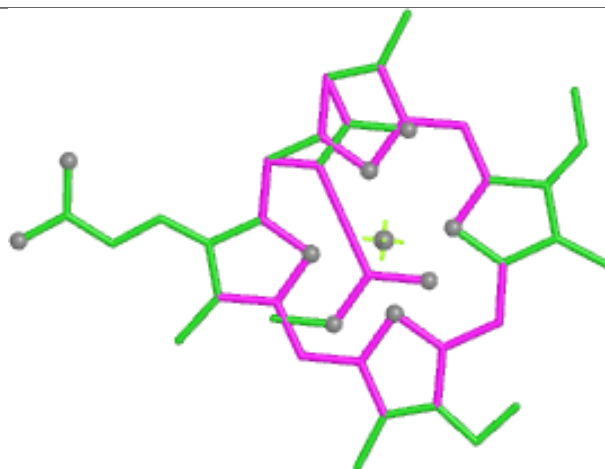
Ligand CLA 2 607



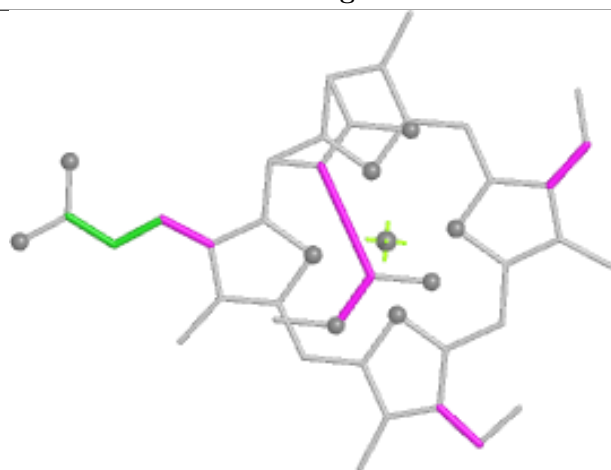
Ligand KC2 5 610



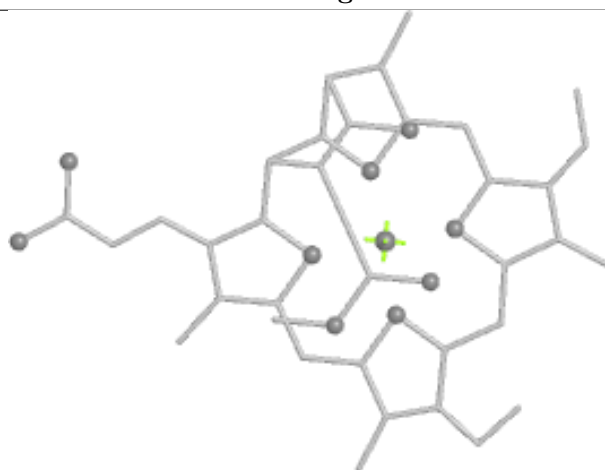
Bond lengths



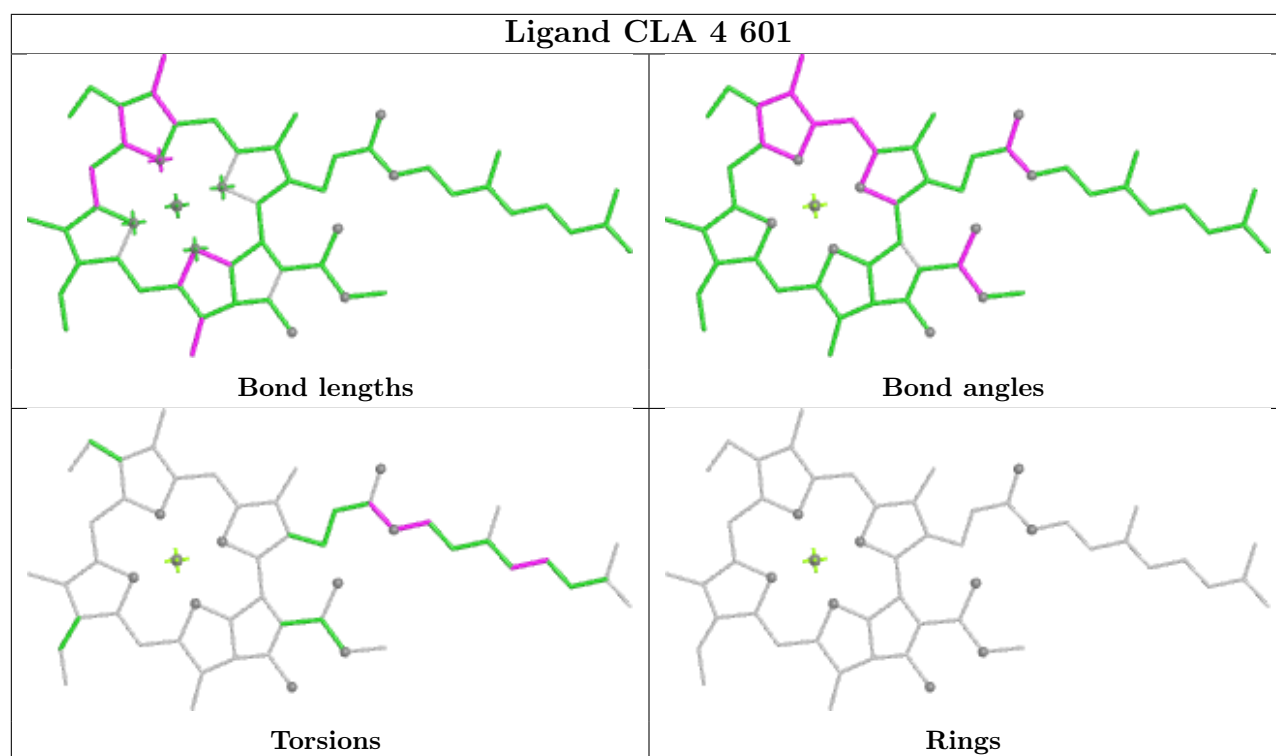
Bond angles



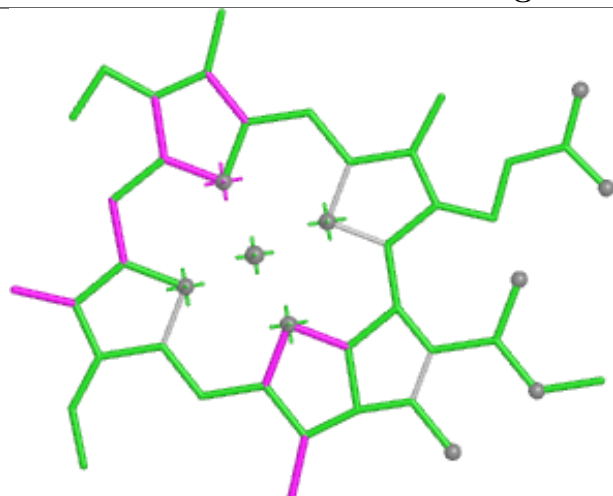
Torsions



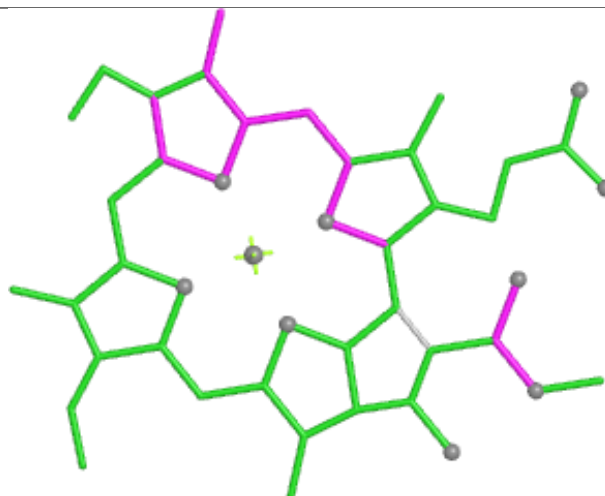
Rings



Ligand CLA B 804



Bond lengths



Bond angles

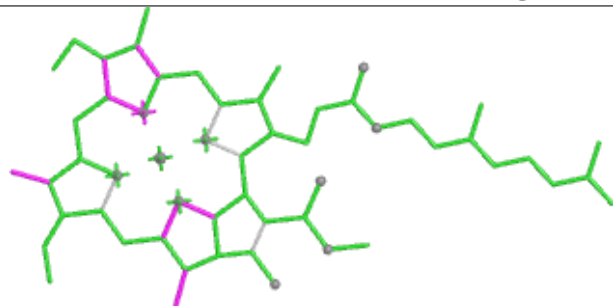


Torsions

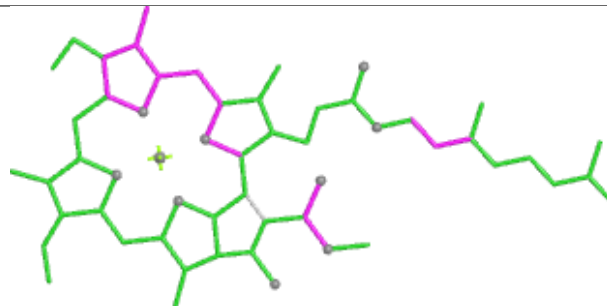


Rings

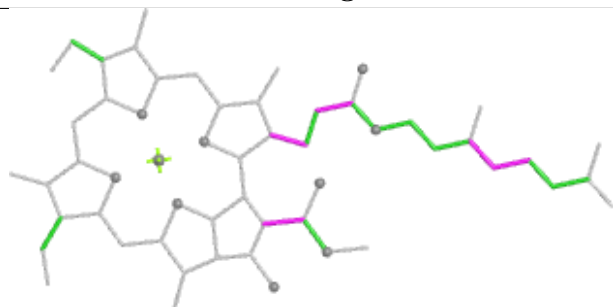
Ligand CLA O 201



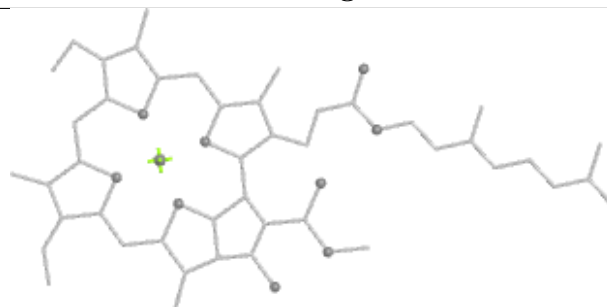
Bond lengths



Bond angles

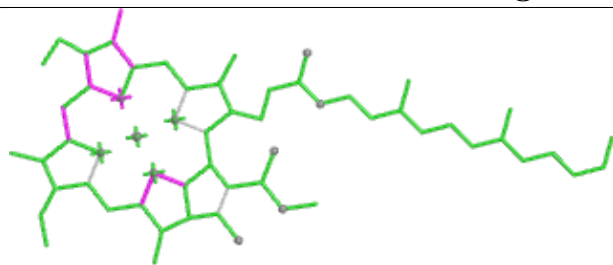


Torsions

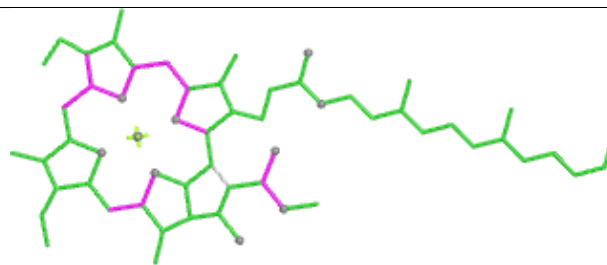


Rings

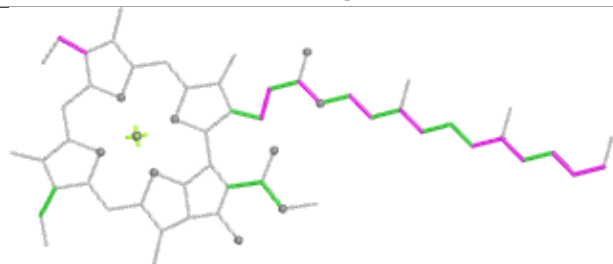
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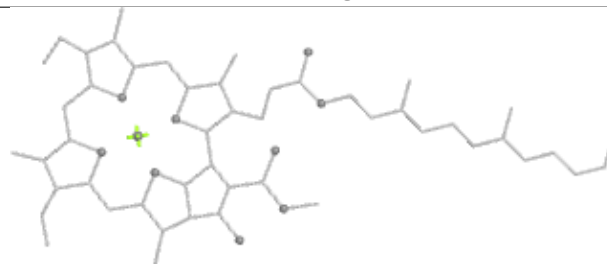
Bond lengths



Bond angles

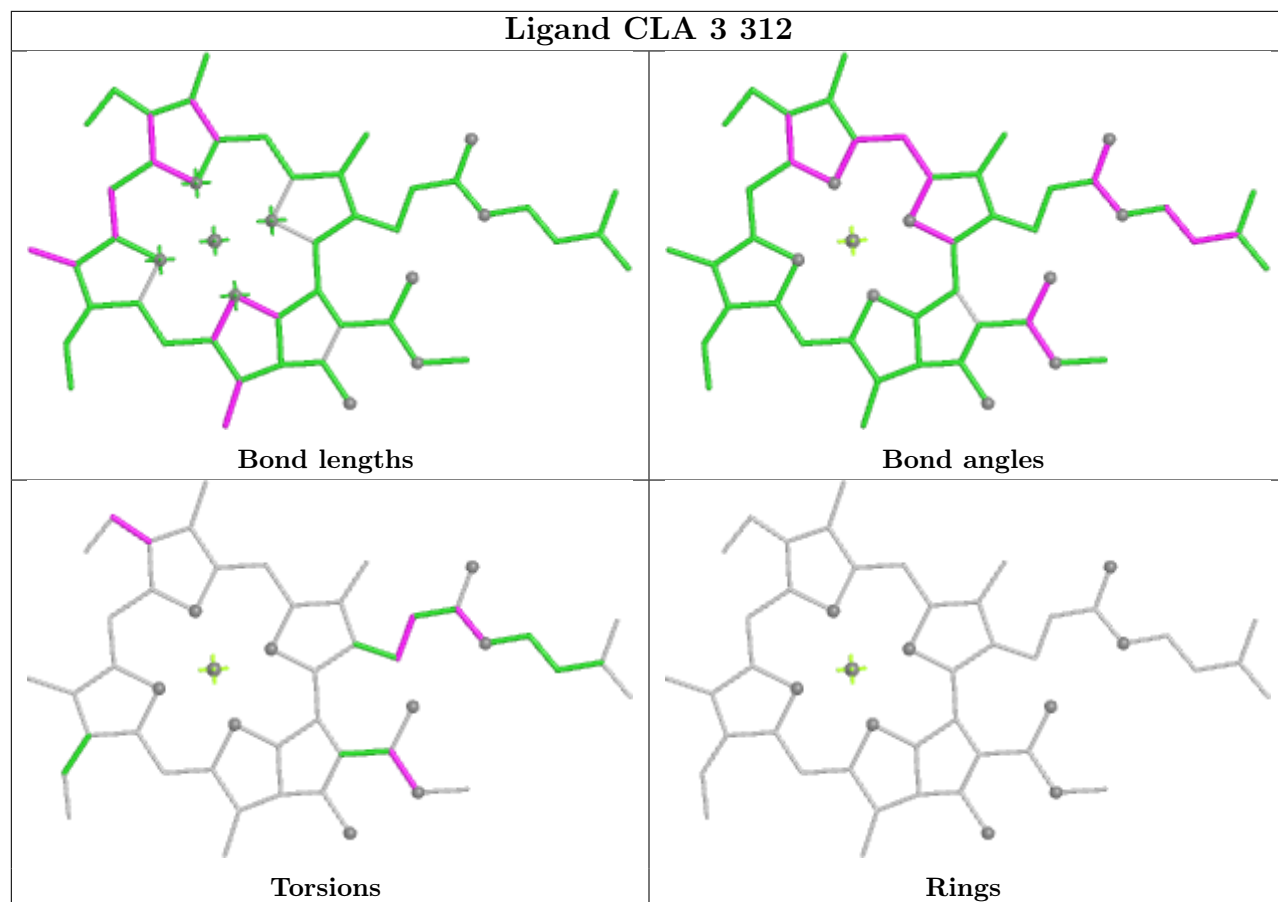


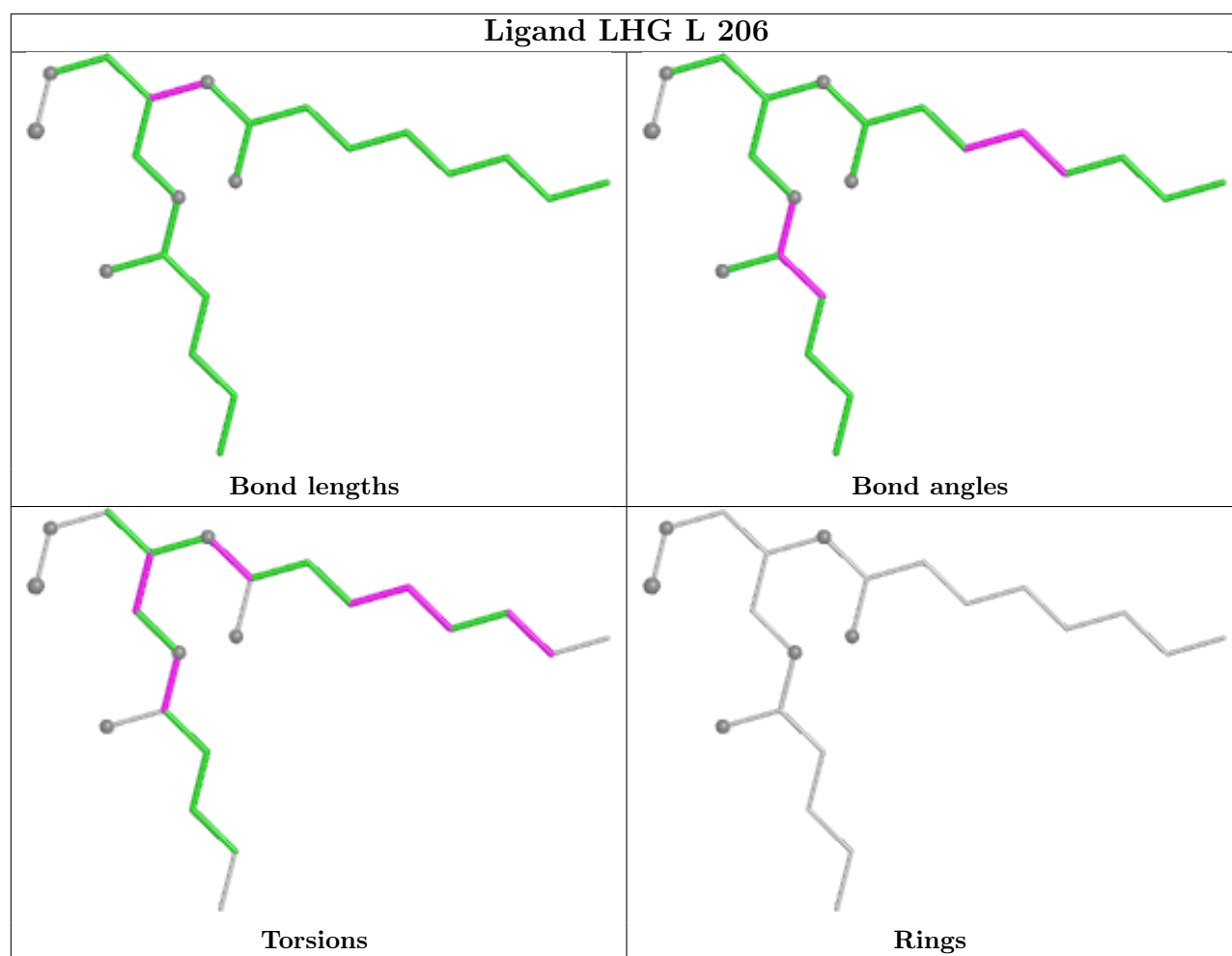
Torsions



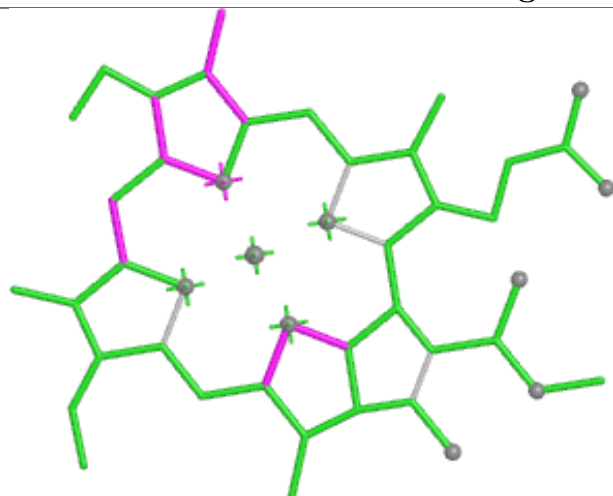
Rings

Ligand CLA 3 312

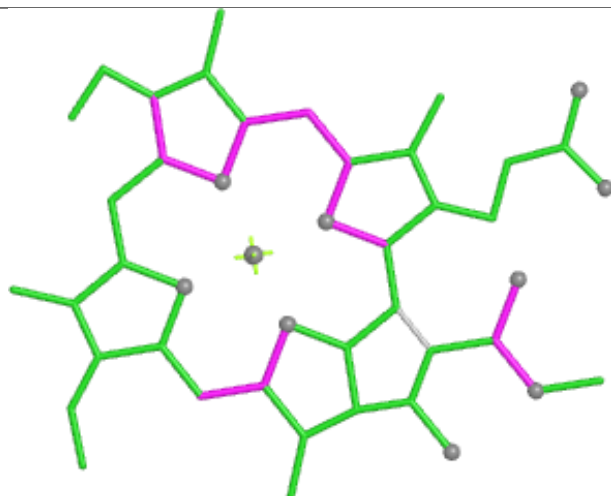




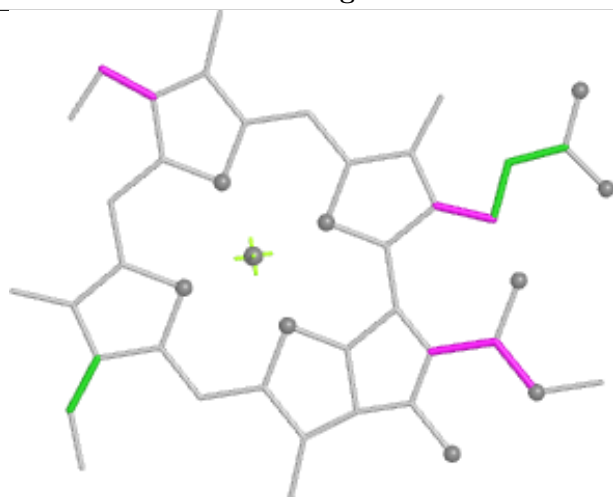
Ligand CLA 9 314



Bond lengths



Bond angles

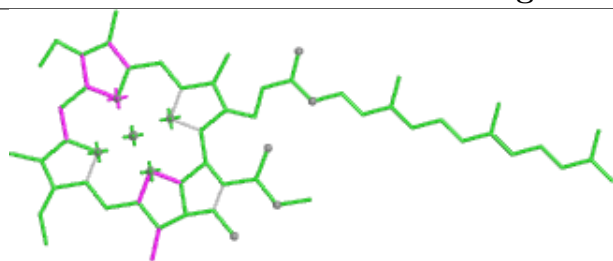


Torsions

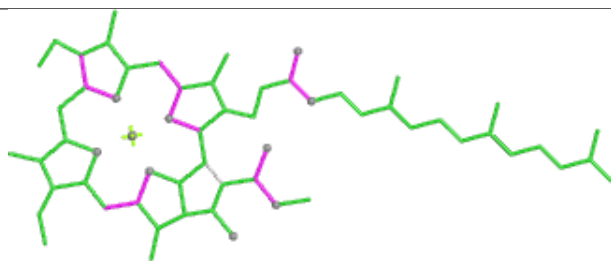


Rings

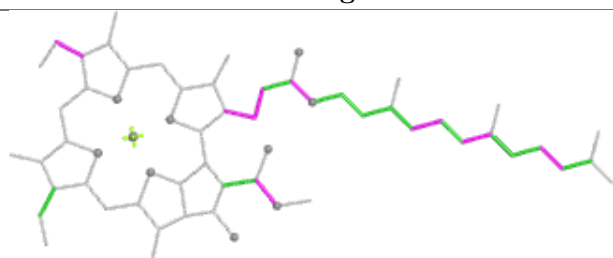
Ligand CLA Z 302



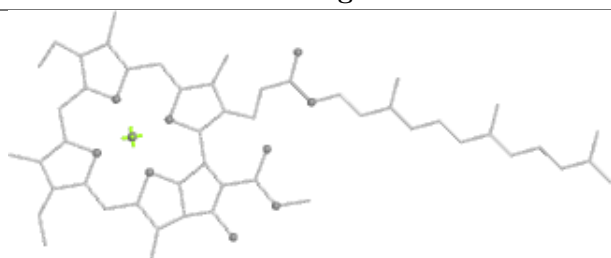
Bond lengths



Bond angles

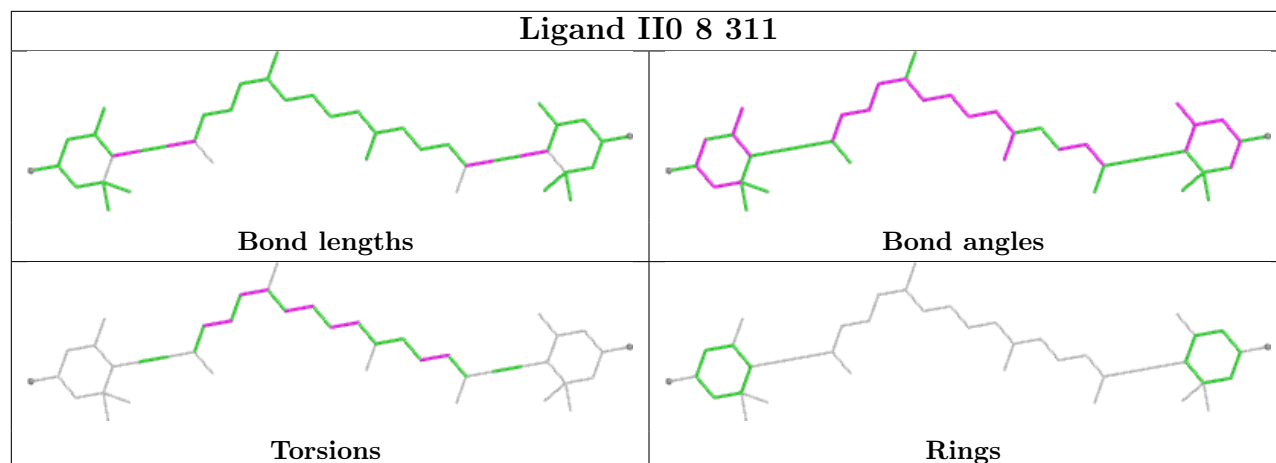


Torsions

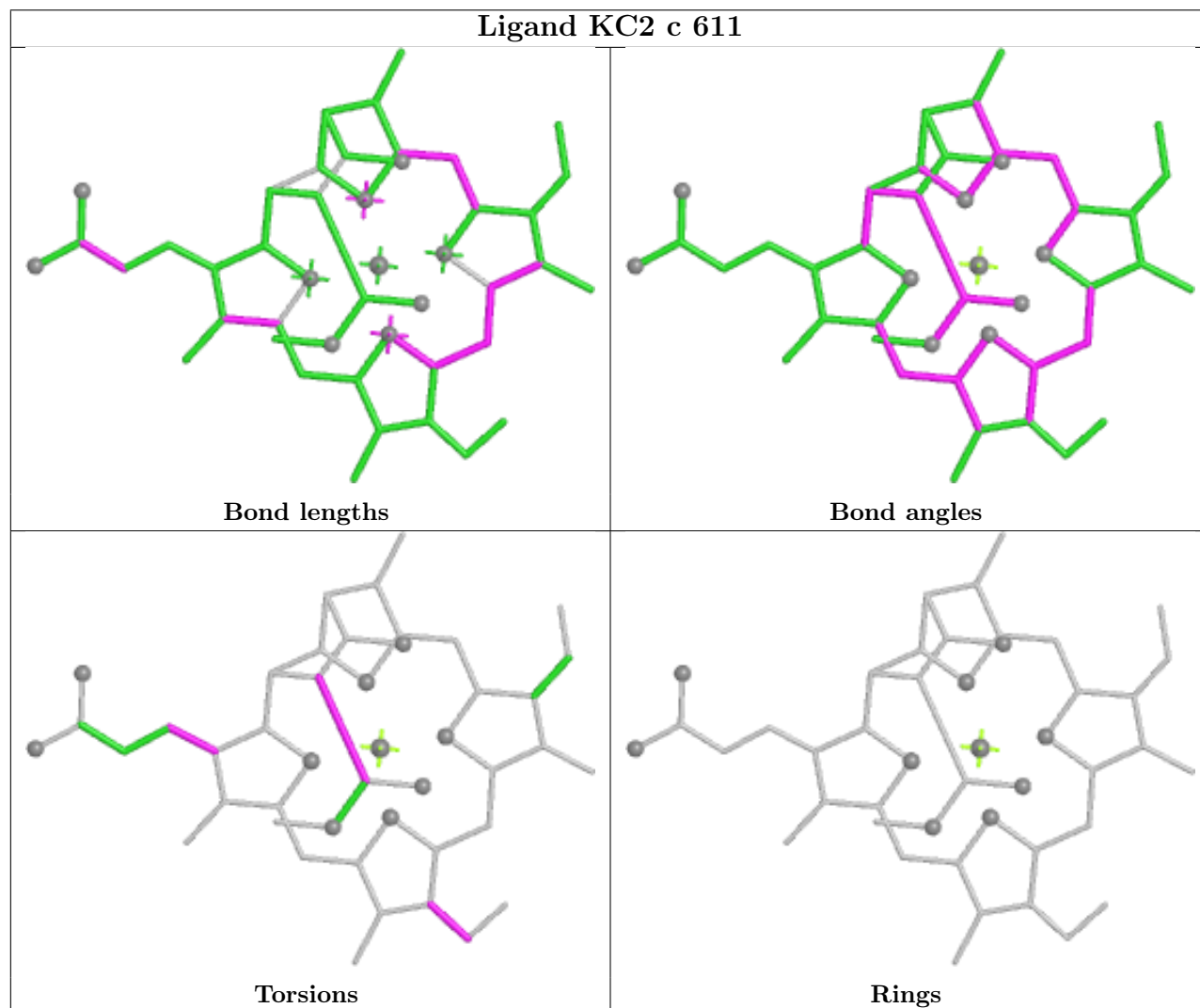


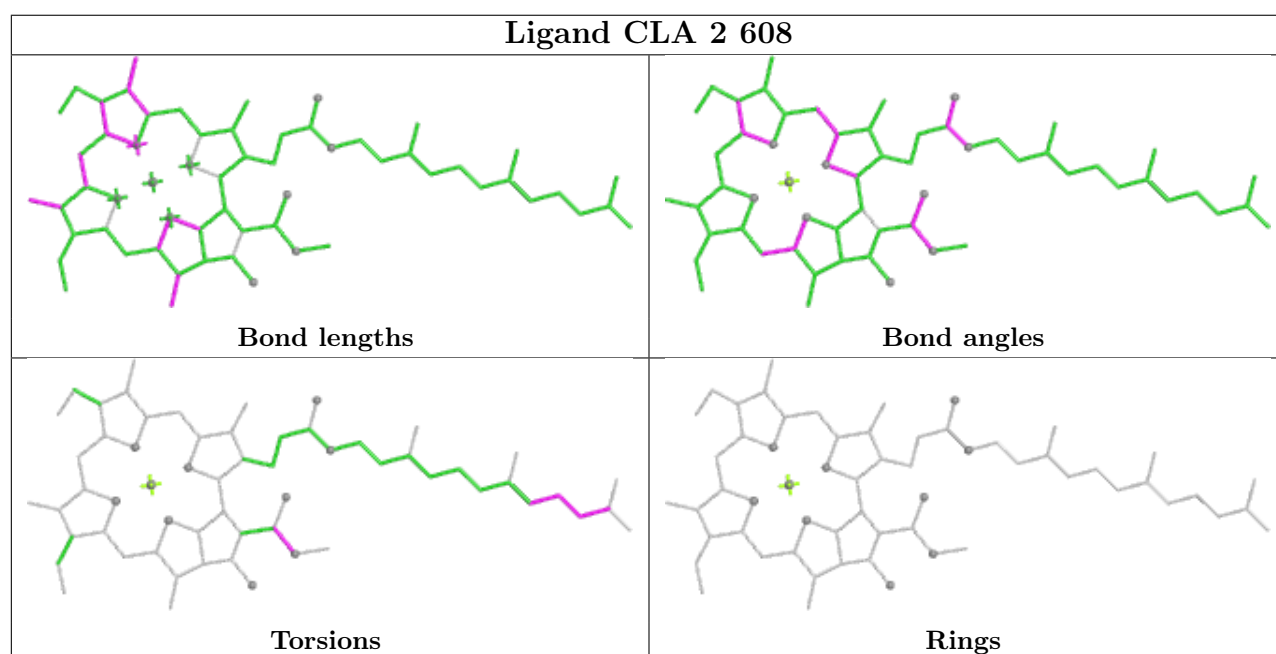
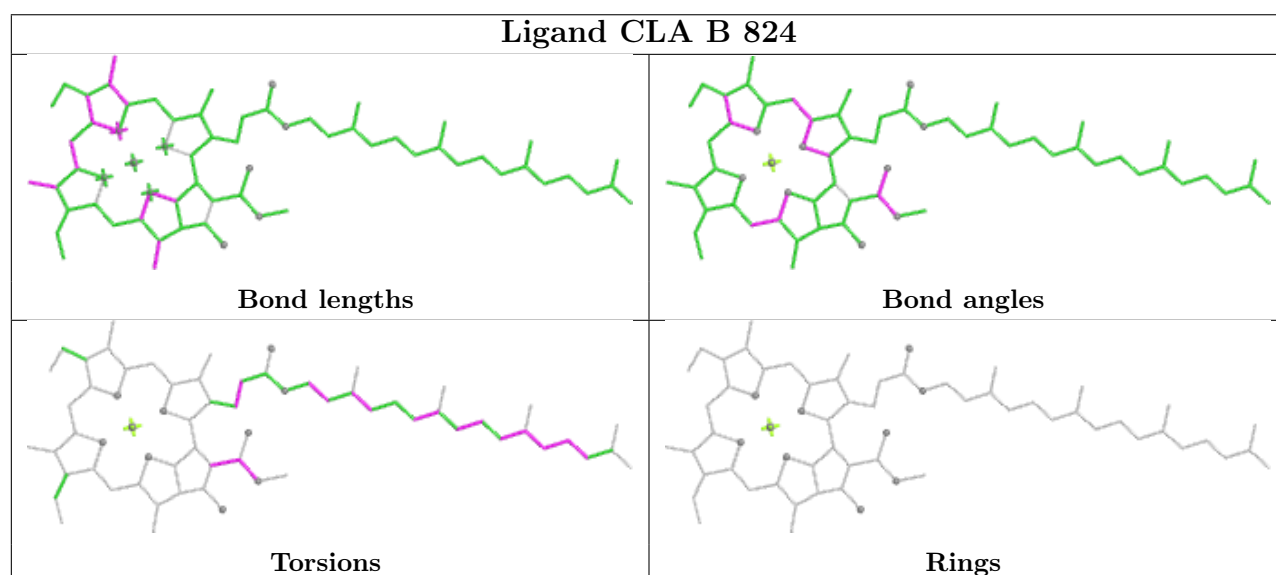
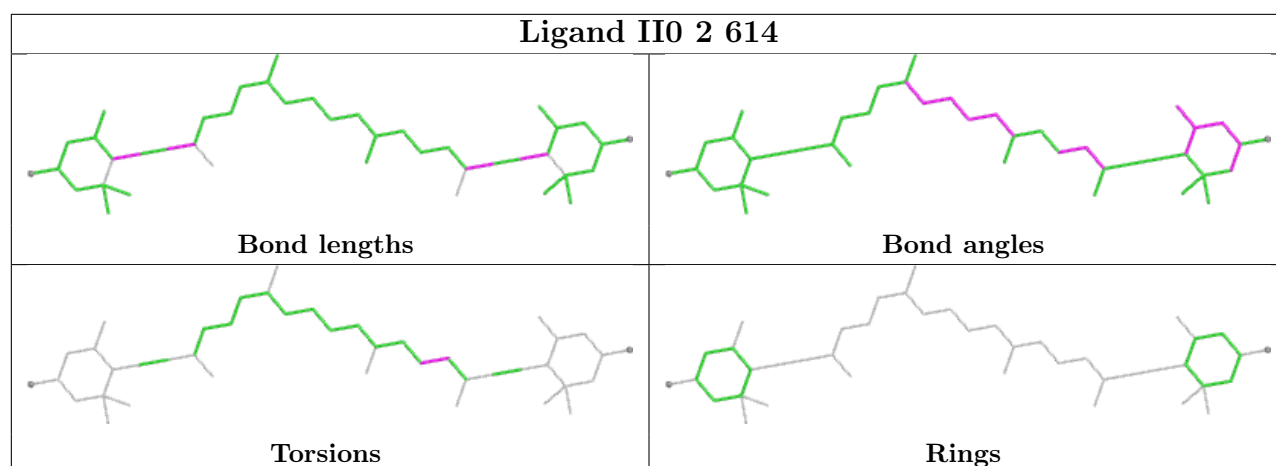
Rings

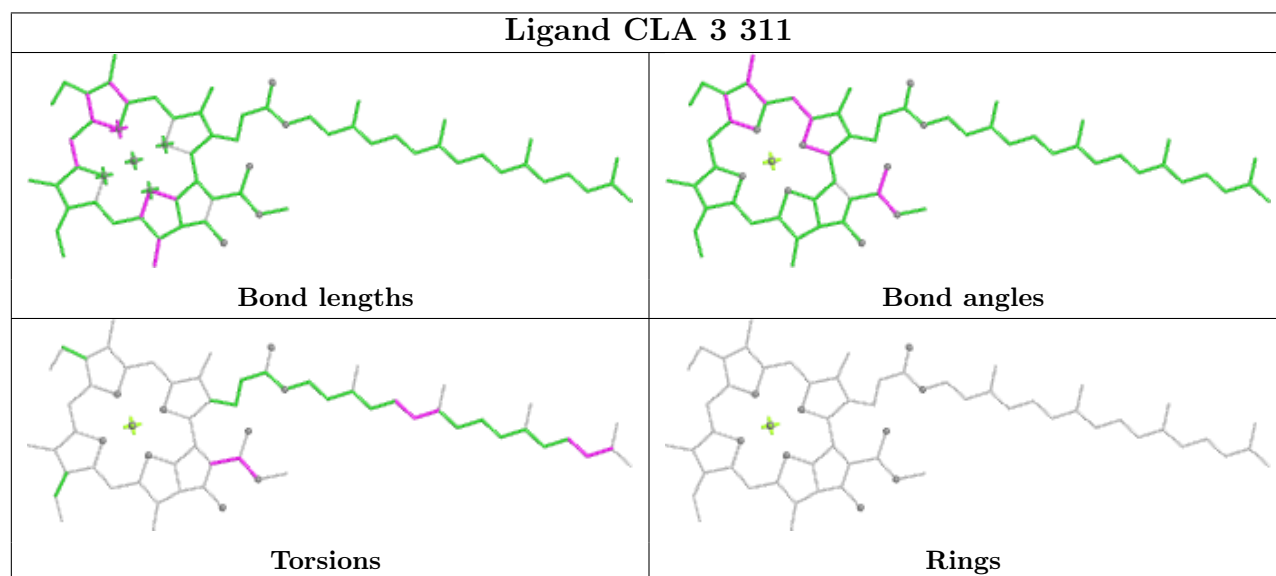
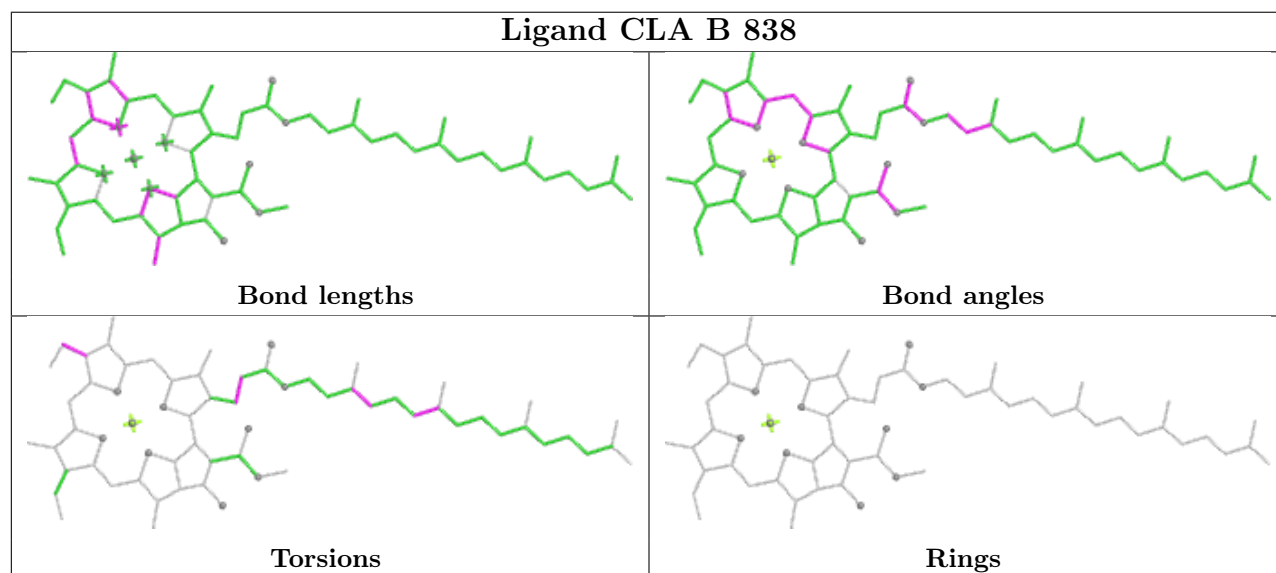
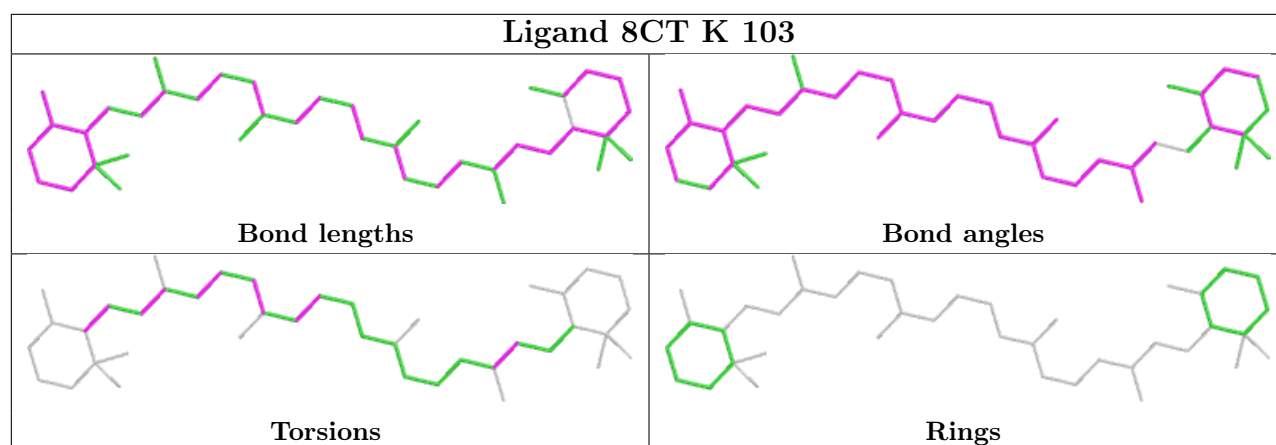
Ligand II0 8 311

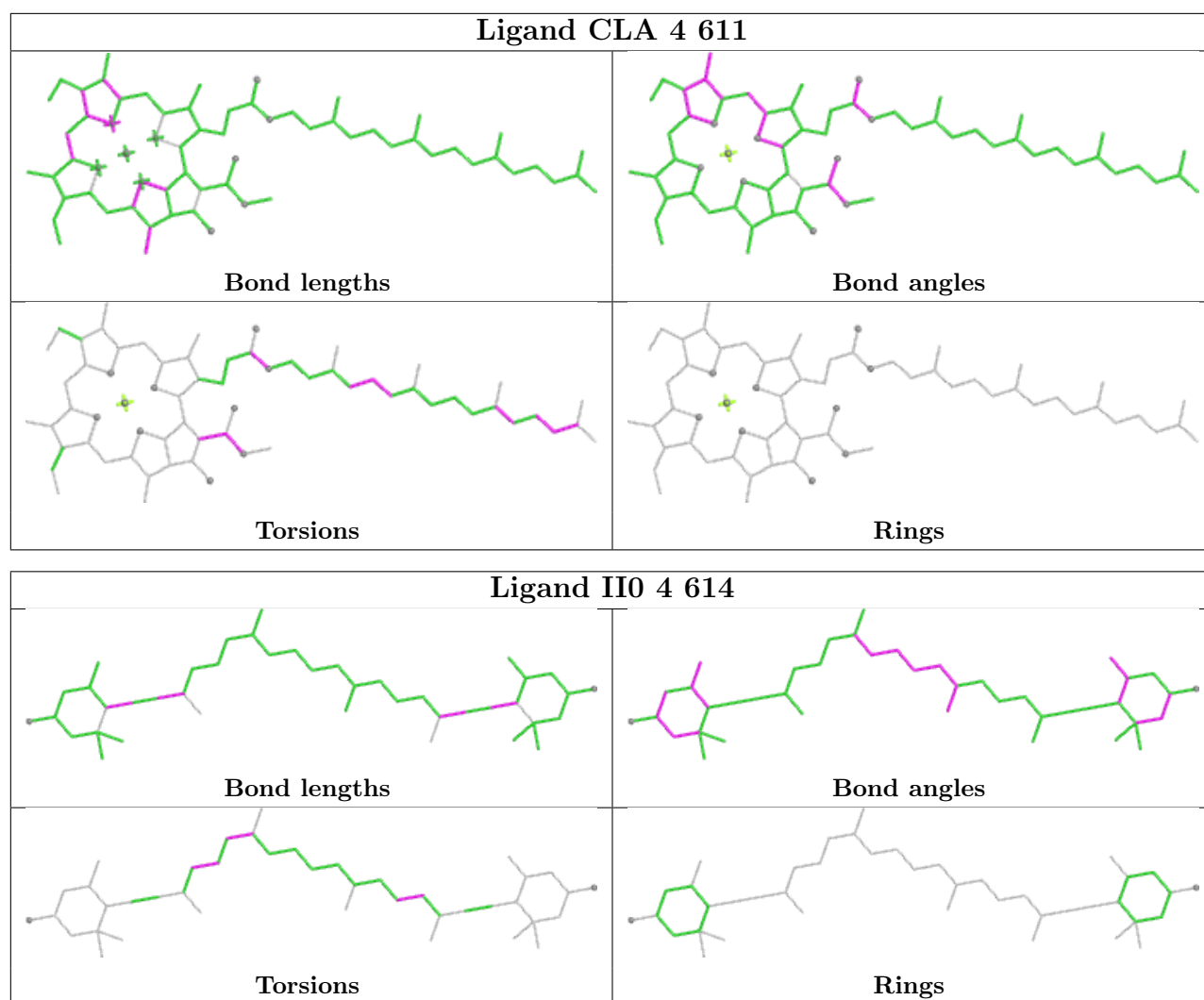


Ligand KC2 c 611

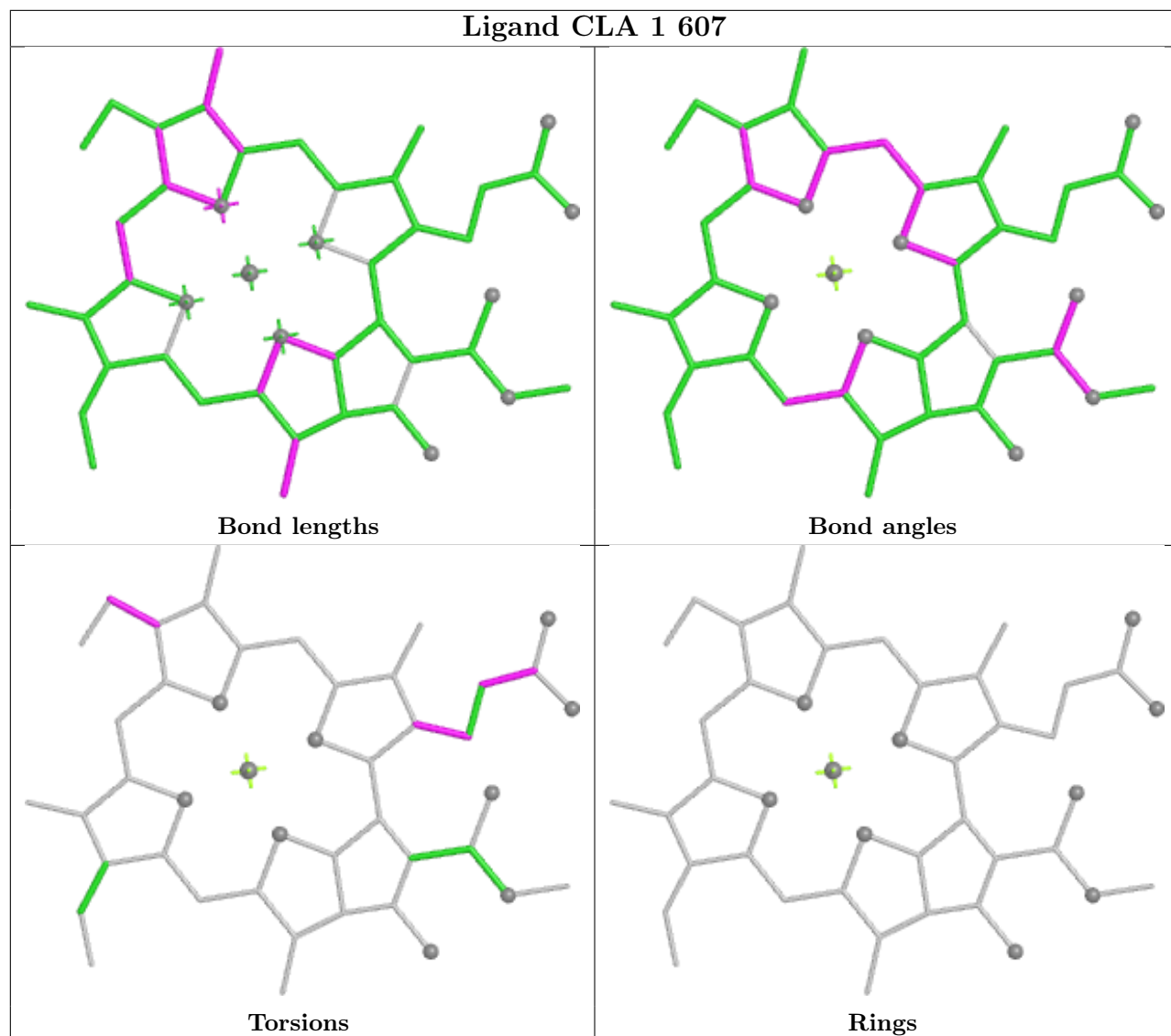


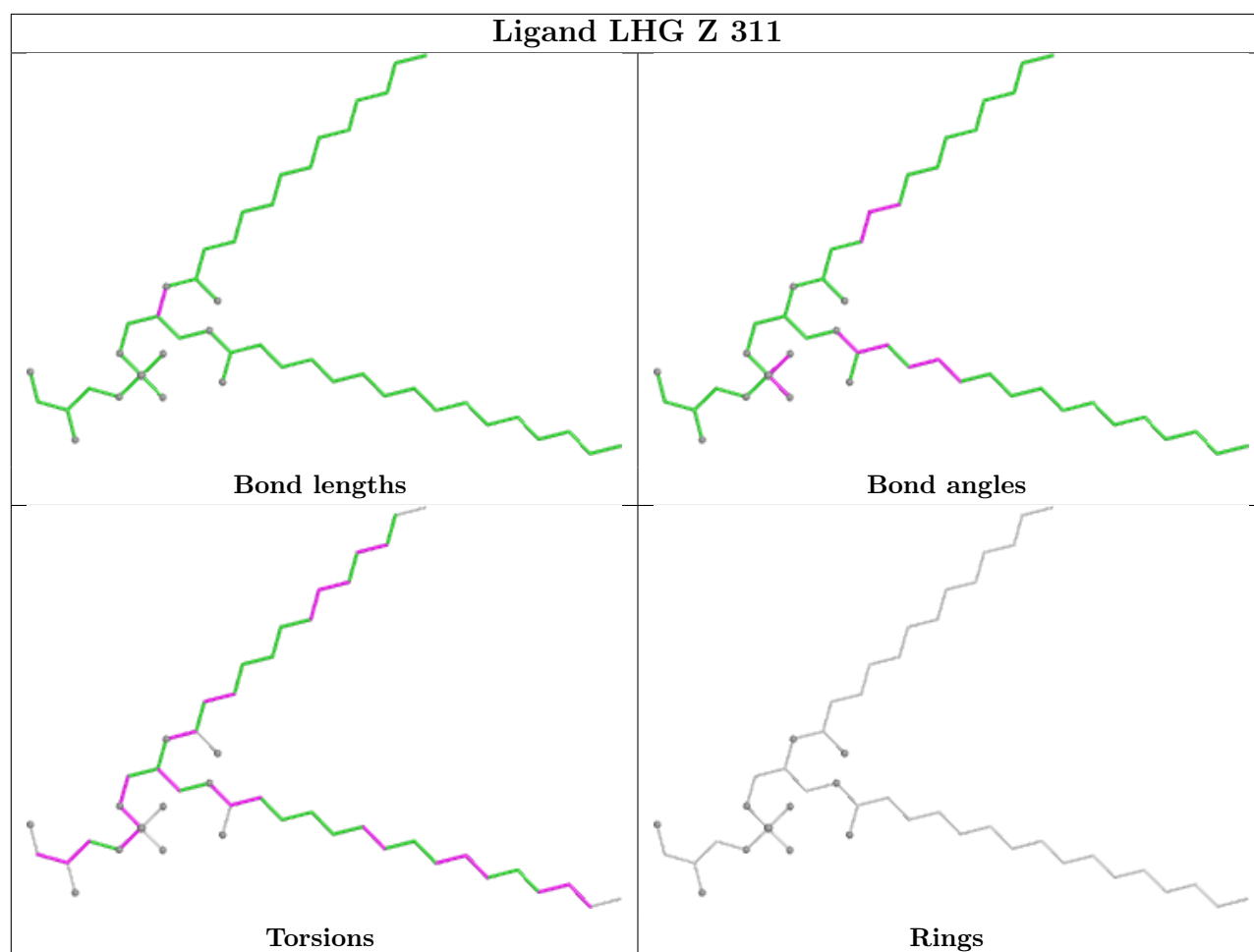


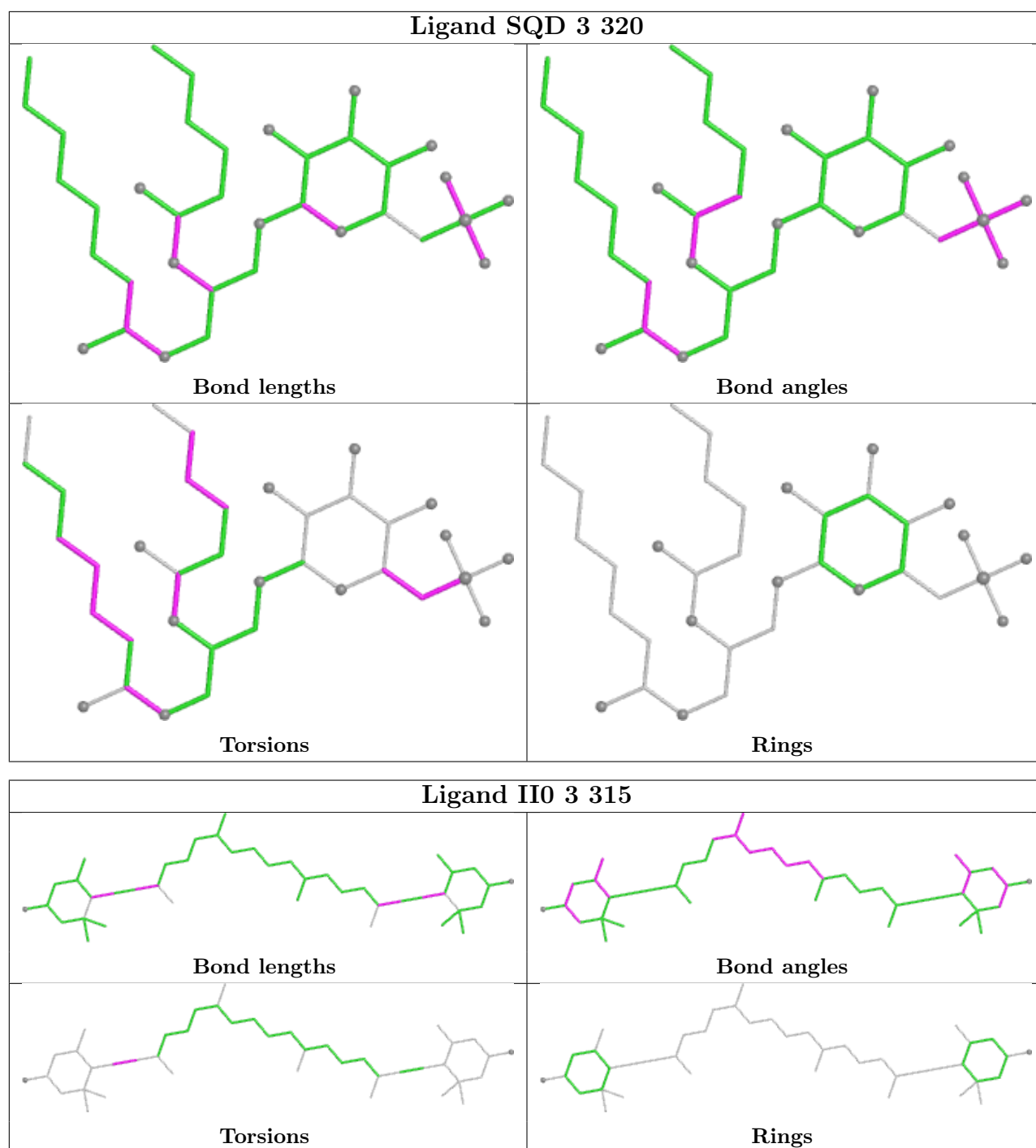


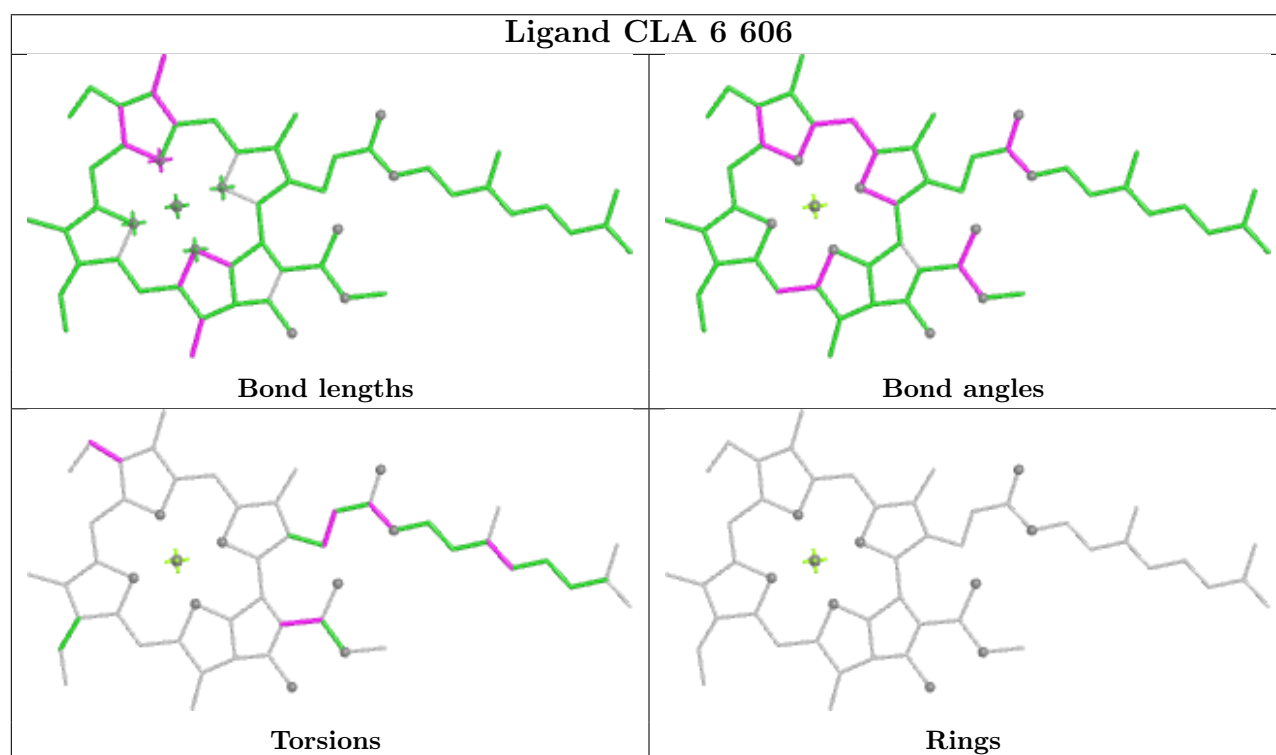
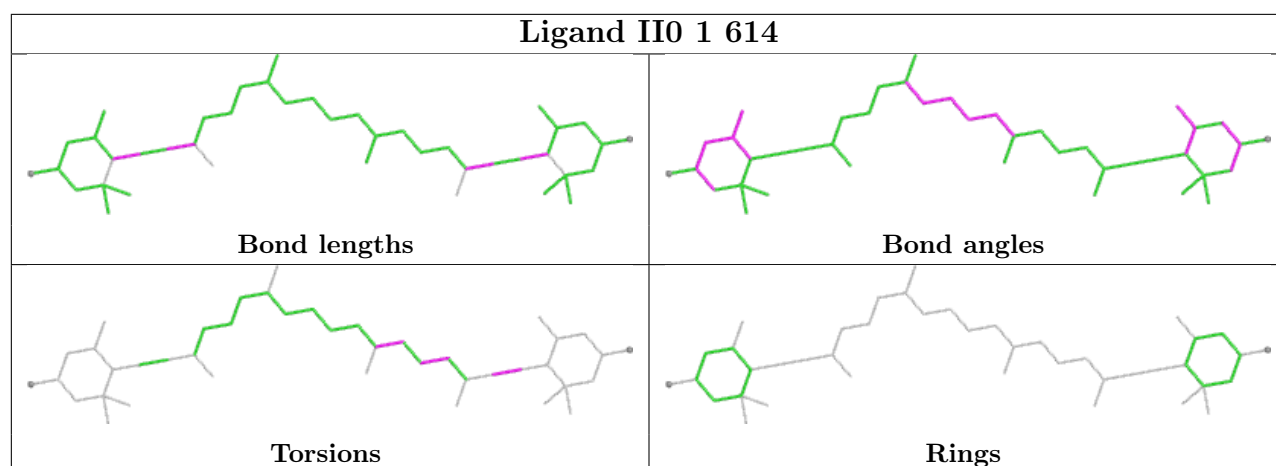


Ligand CLA 1 607

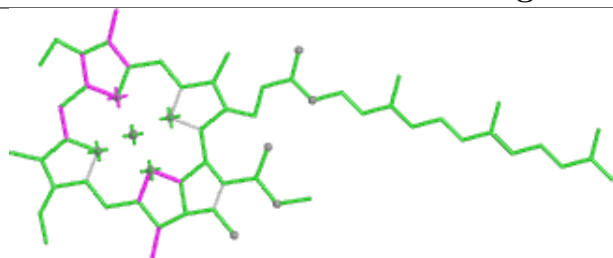




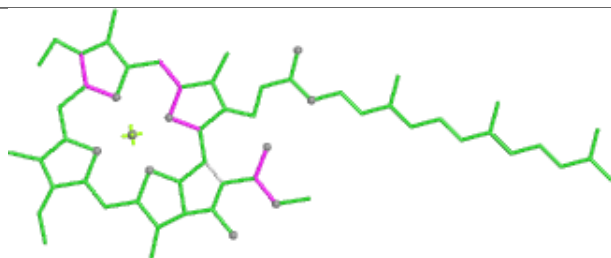




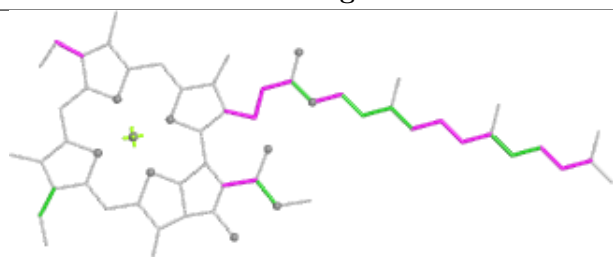
Ligand CLA Z 305



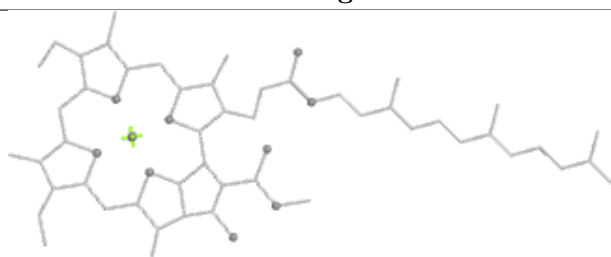
Bond lengths



Bond angles

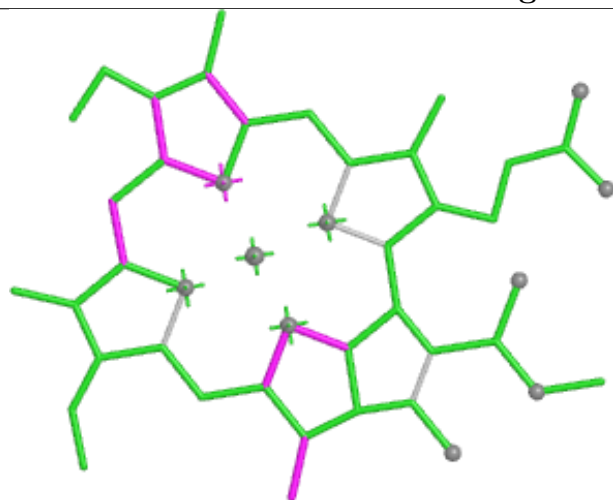


Torsions

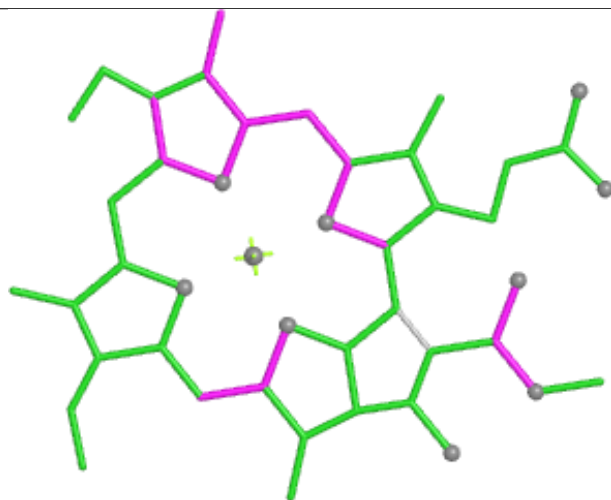


Rings

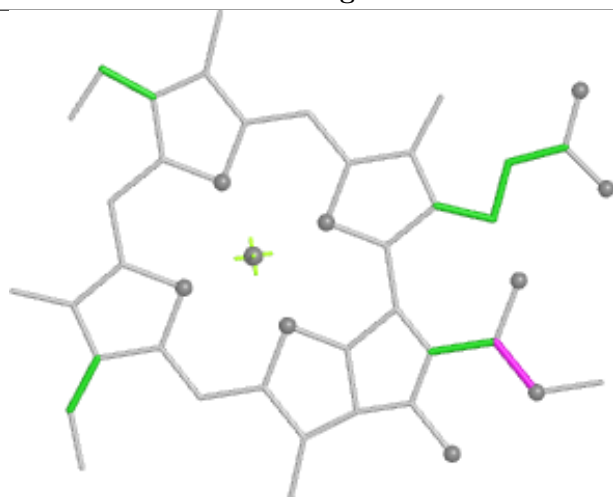
Ligand CLA e 607



Bond lengths



Bond angles

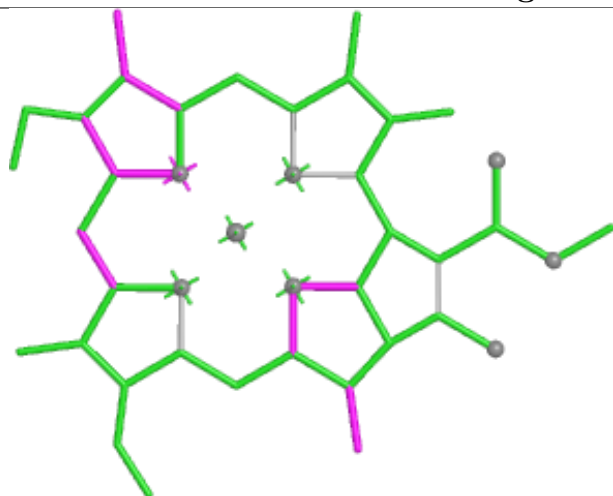


Torsions

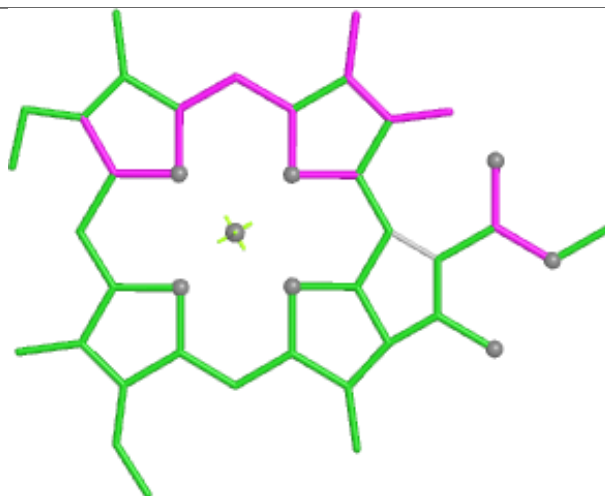


Rings

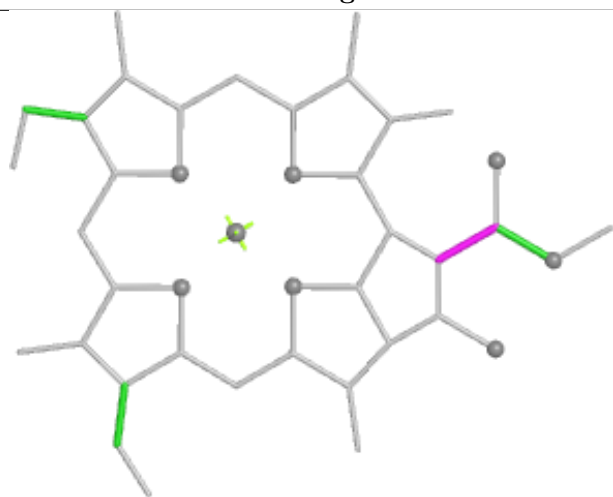
Ligand CLA d 606



Bond lengths



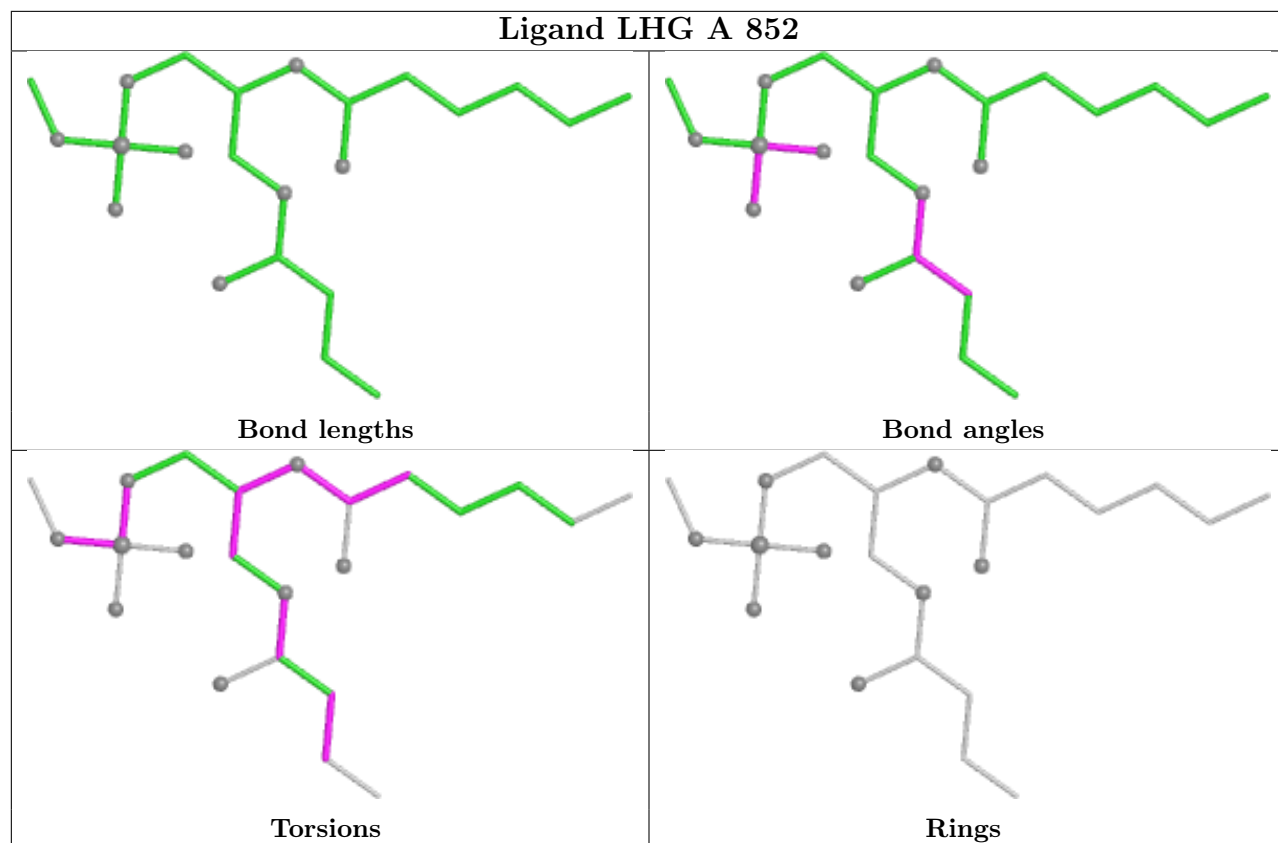
Bond angles



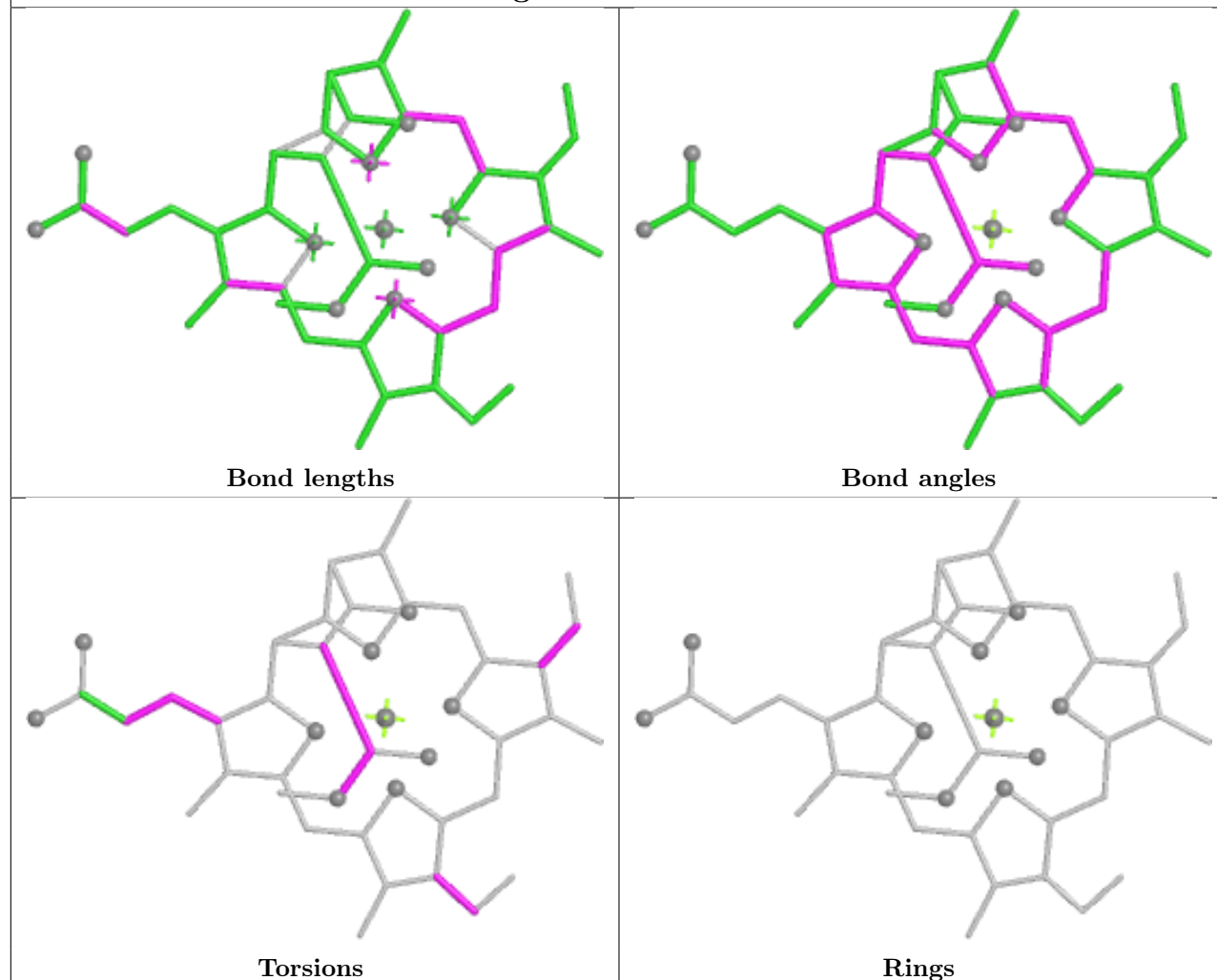
Torsions



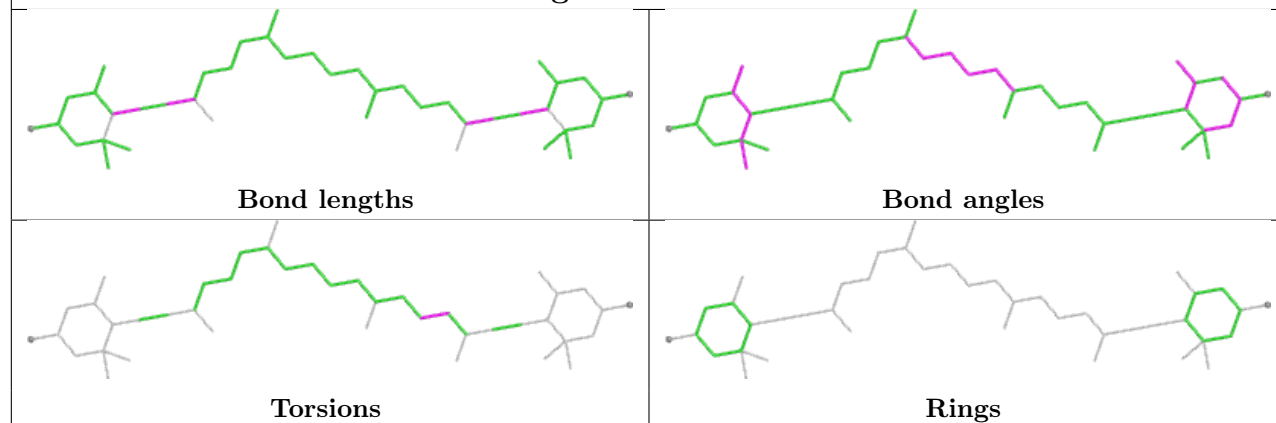
Rings



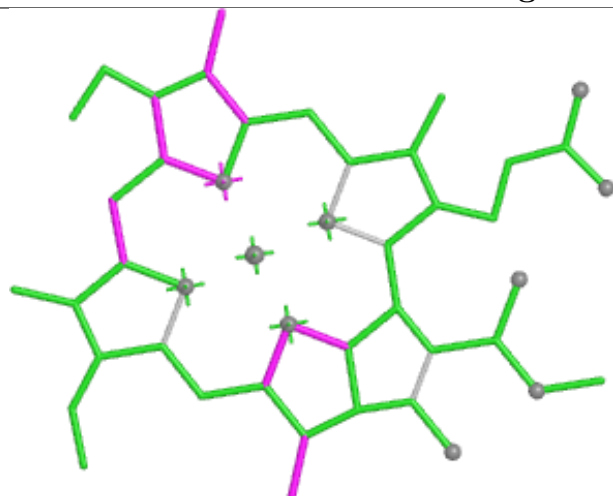
Ligand KC2 2 610



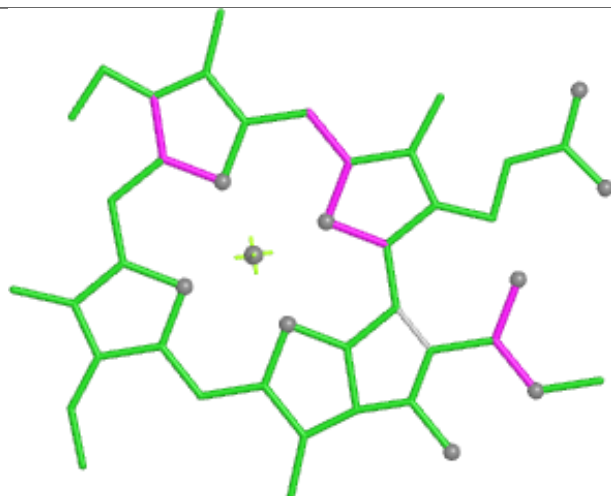
Ligand II0 e 614



Ligand CLA 9 313



Bond lengths



Bond angles

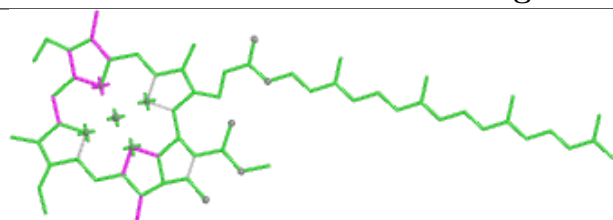


Torsions

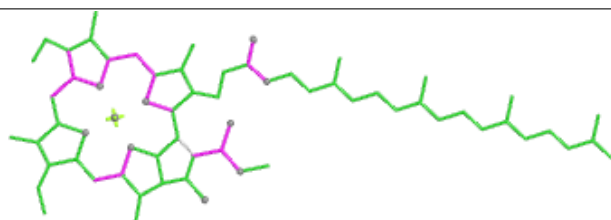


Rings

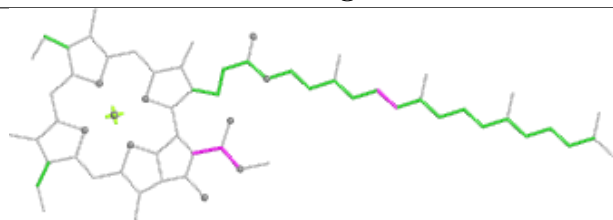
Ligand CLA A 832



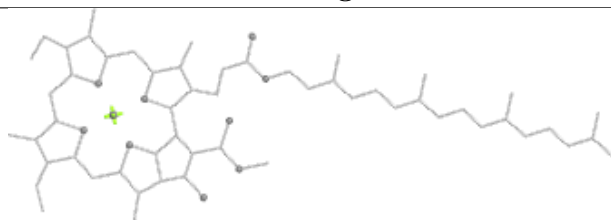
Bond lengths



Bond angles

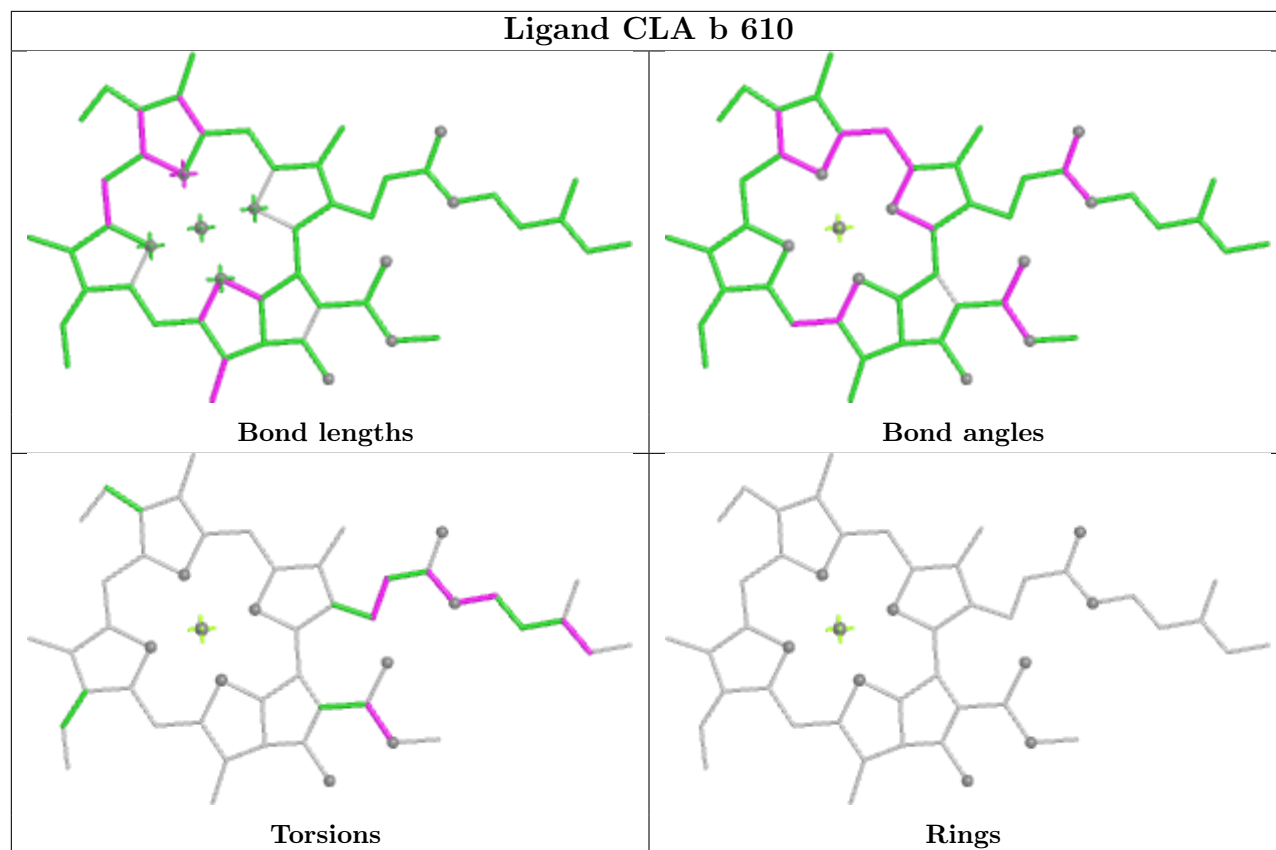


Torsions

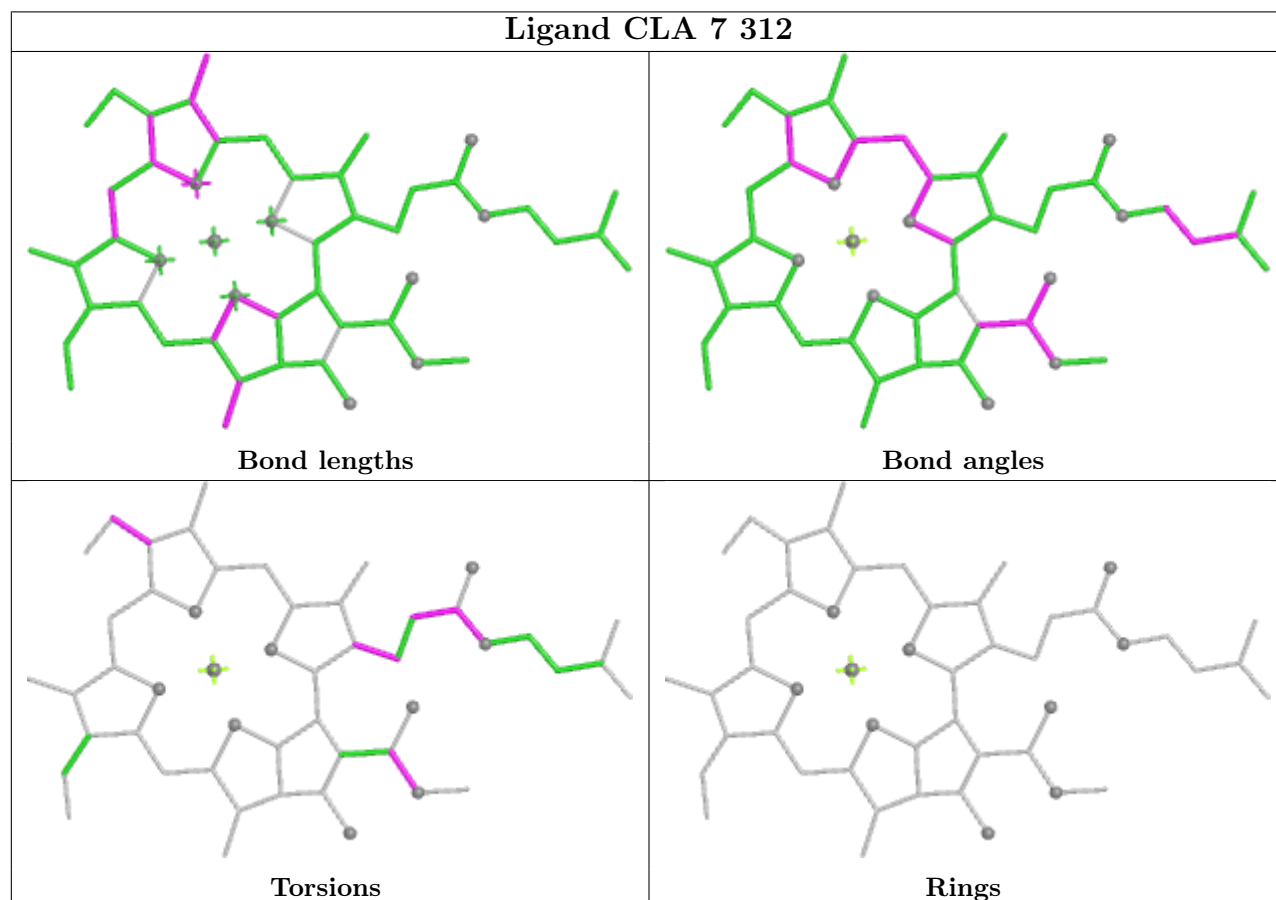


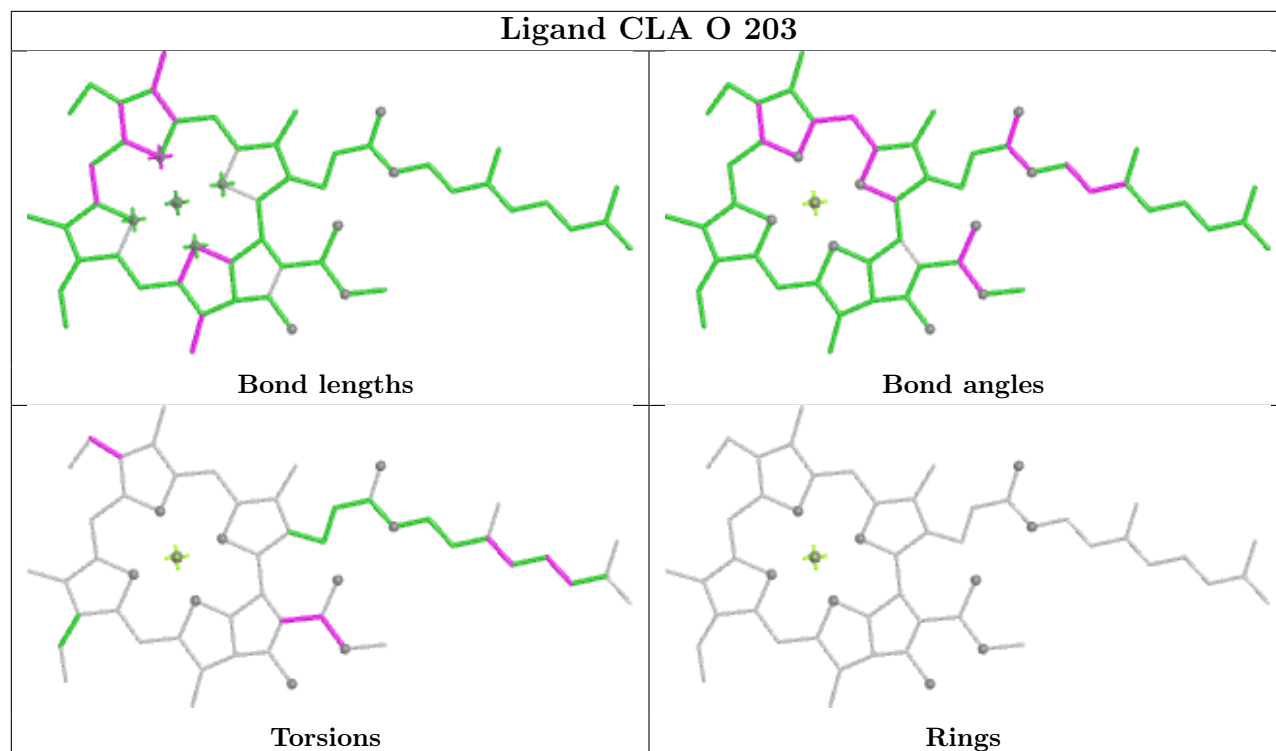
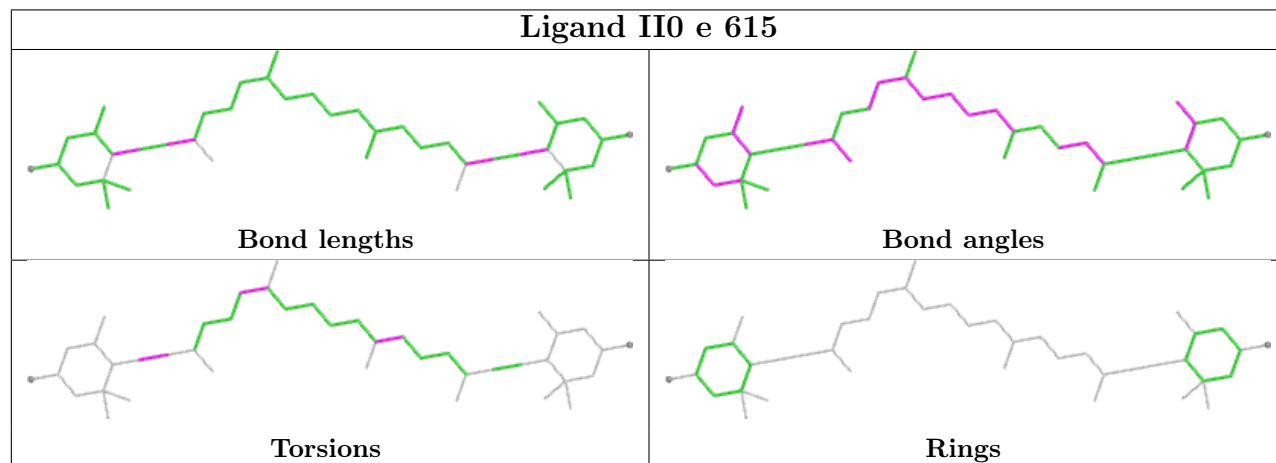
Rings

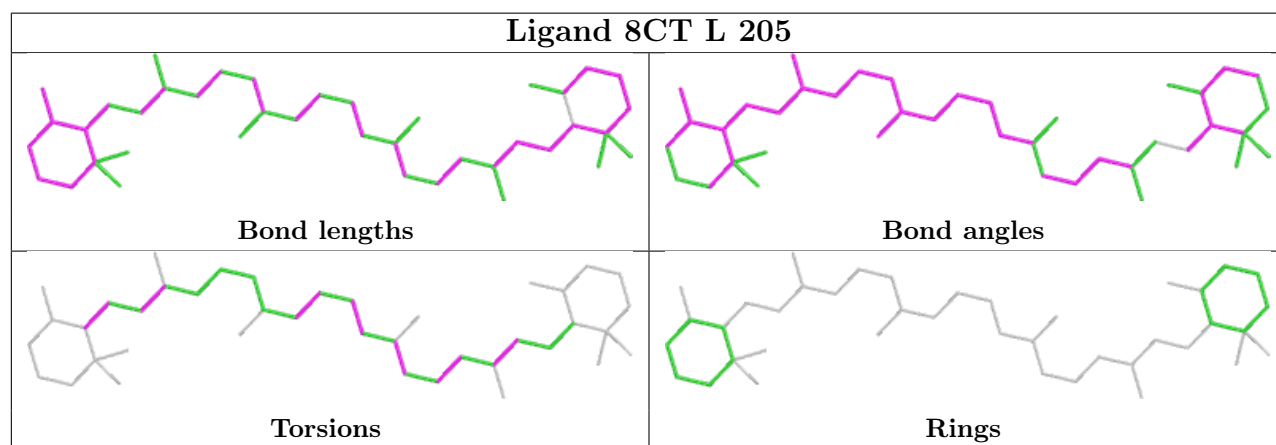
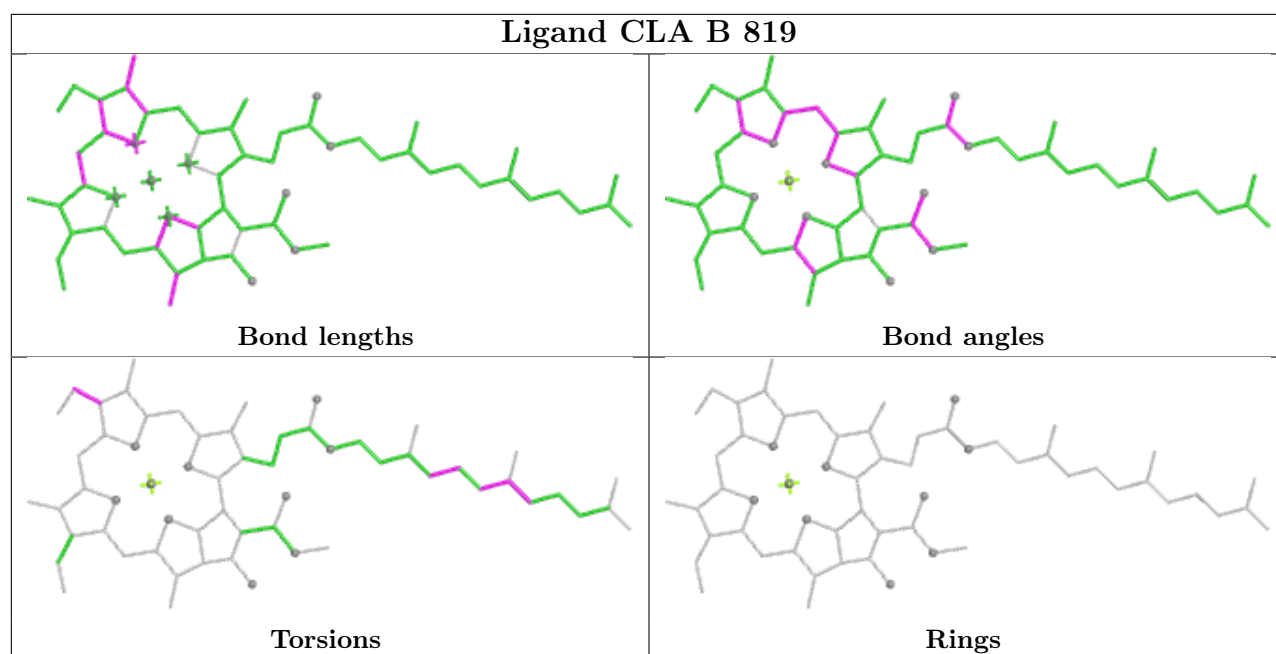
Ligand CLA b 610



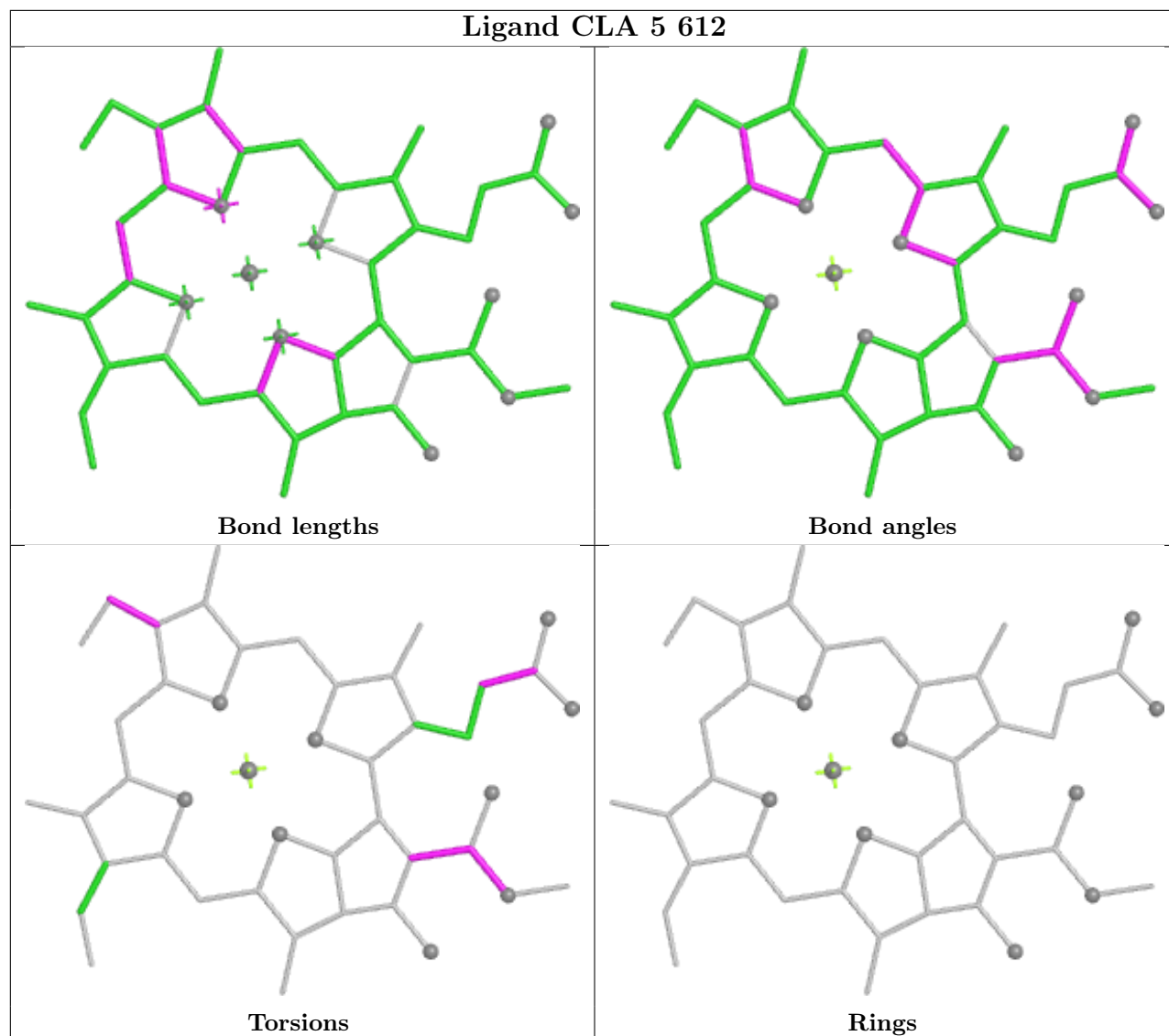
Ligand CLA 7 312



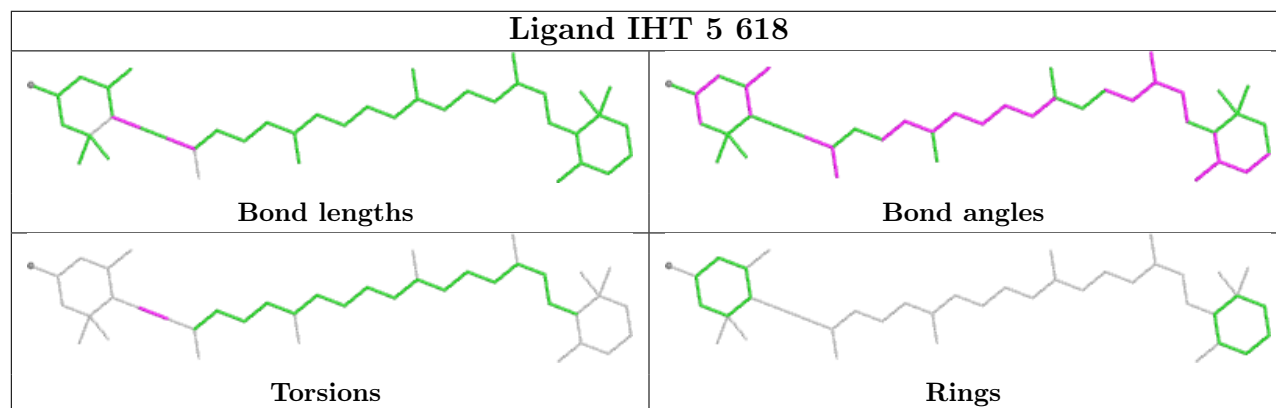
Ligand CLA O 203**Ligand II0 e 615**

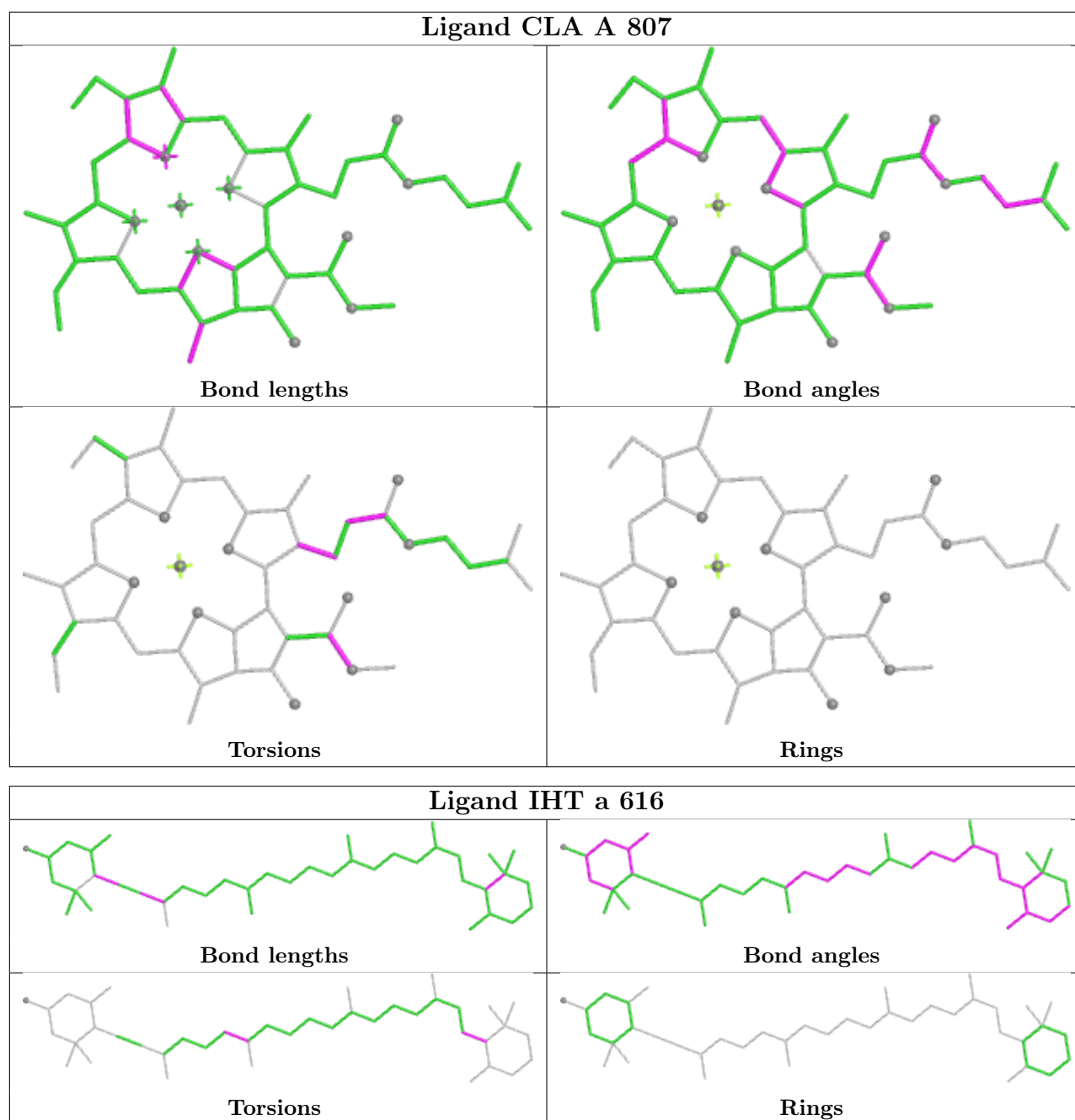


Ligand CLA 5 612

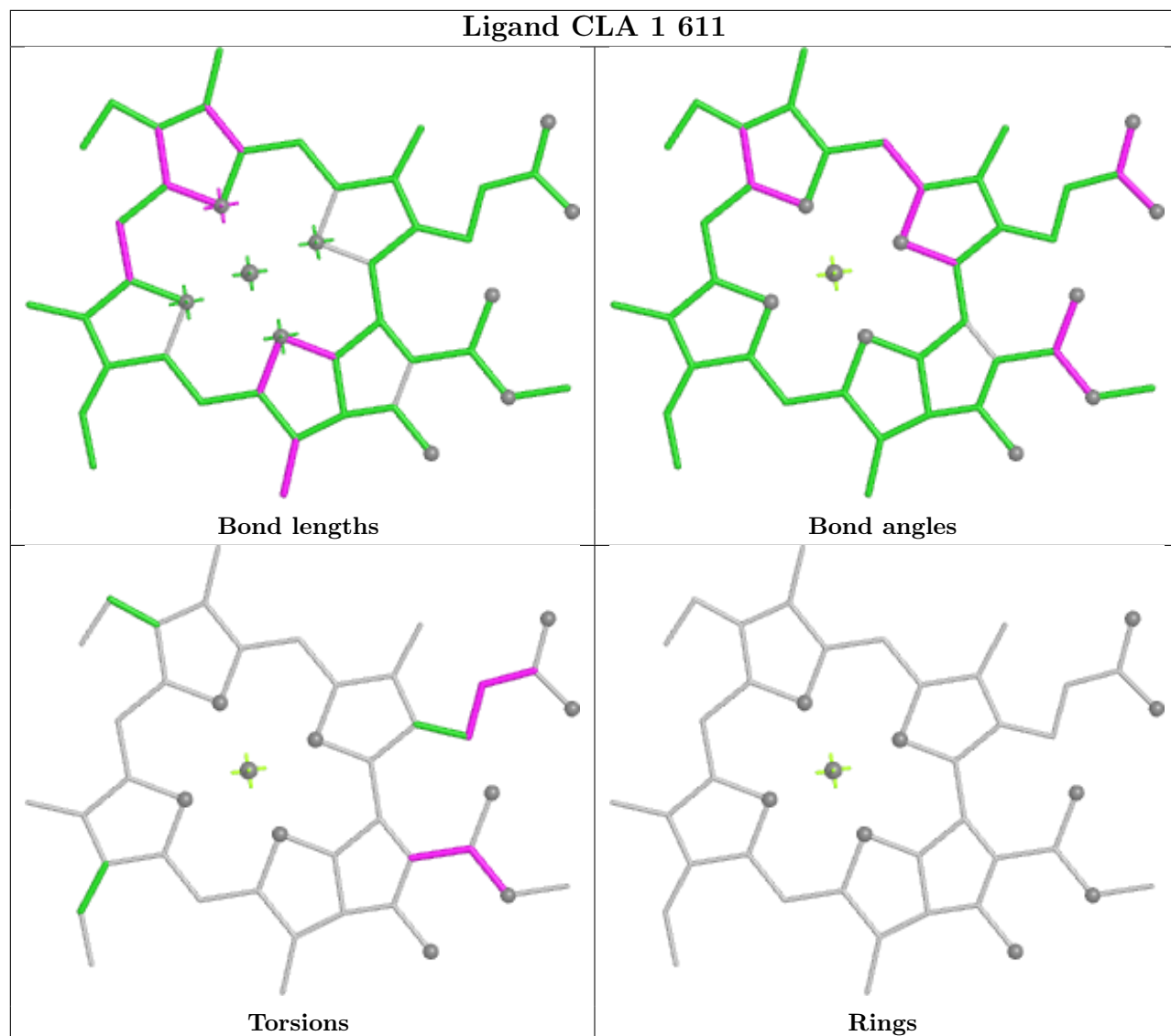


Ligand IHT 5 618

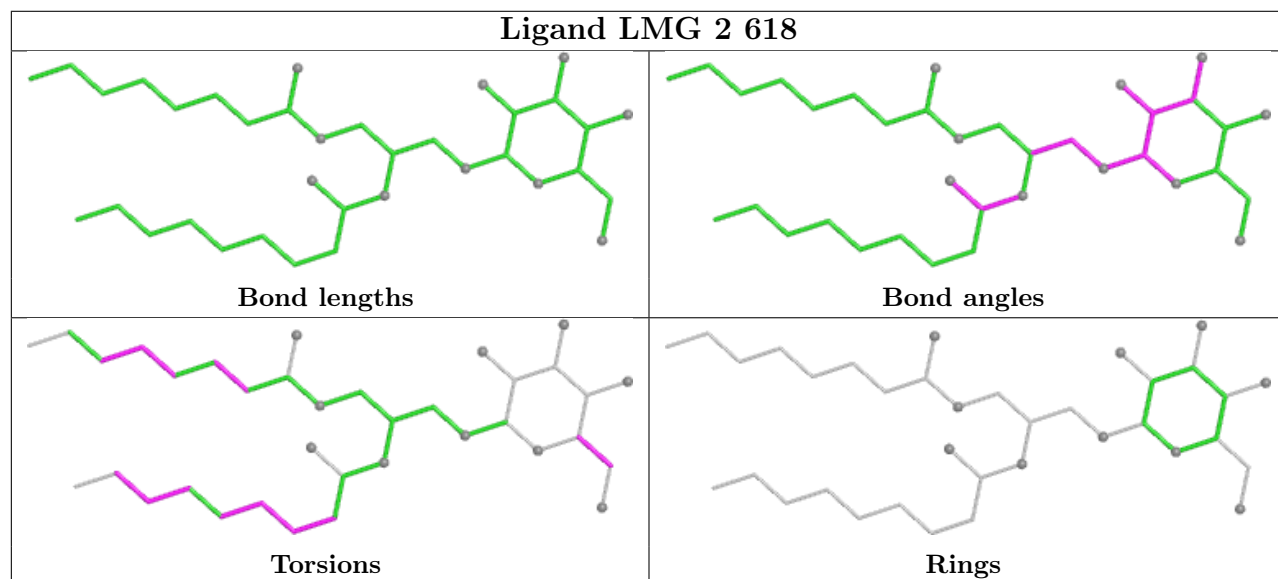




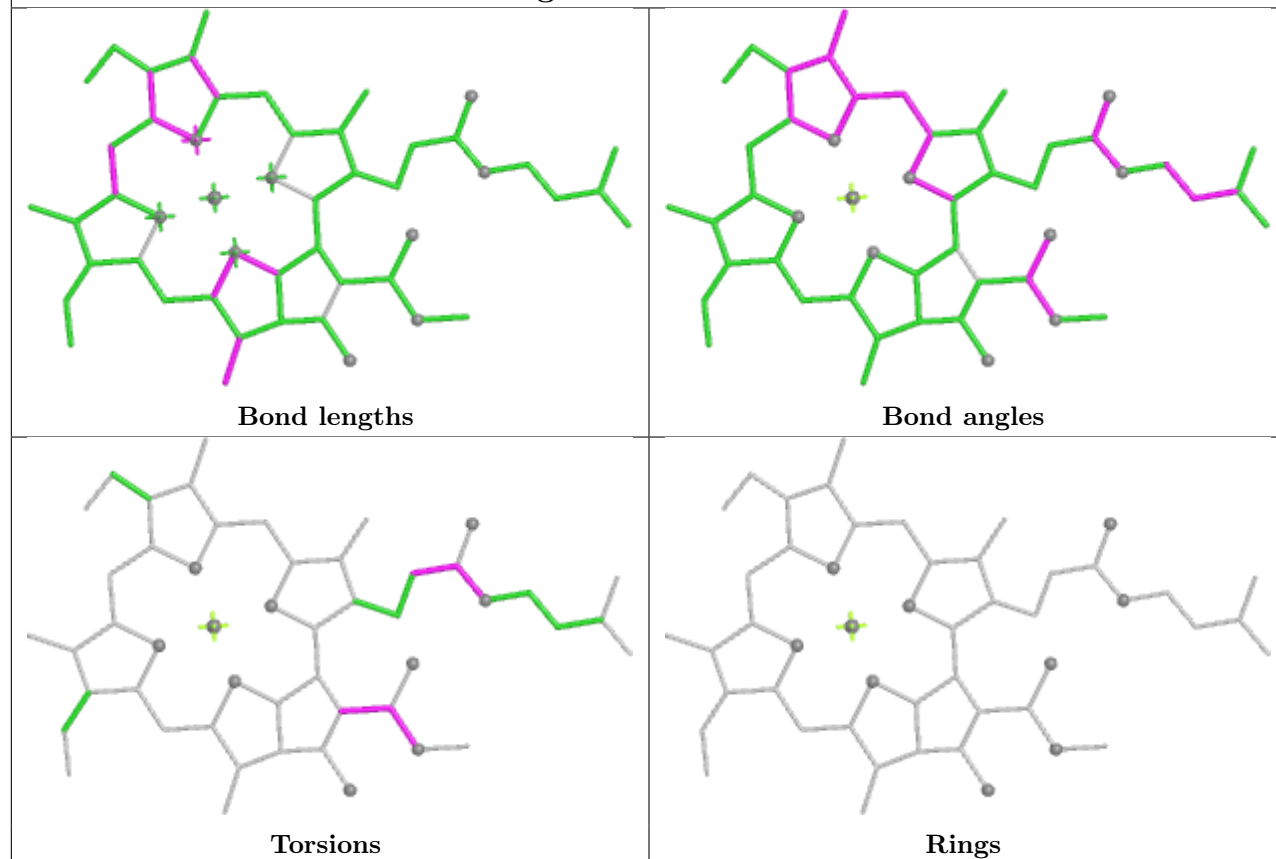
Ligand CLA 1 611



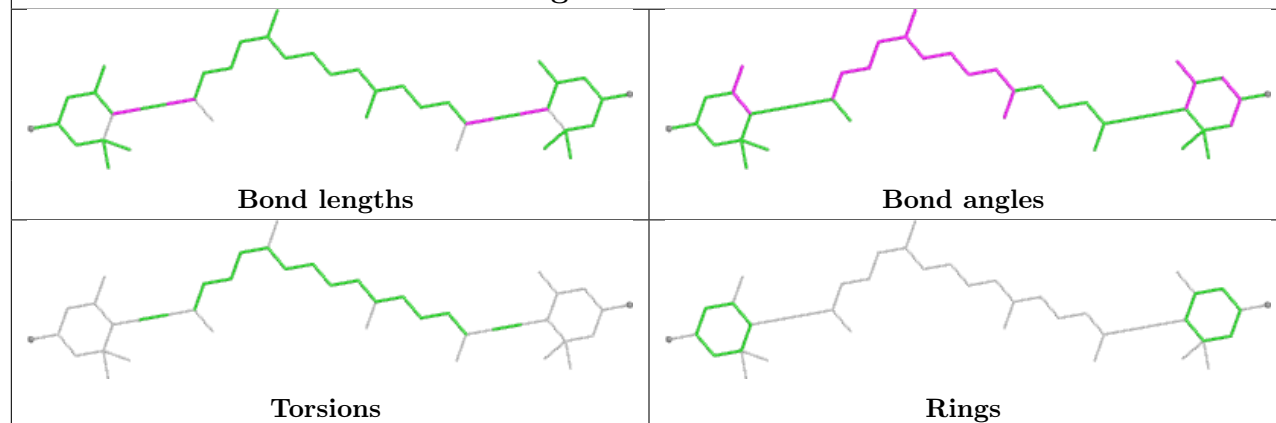
Ligand LMG 2 618



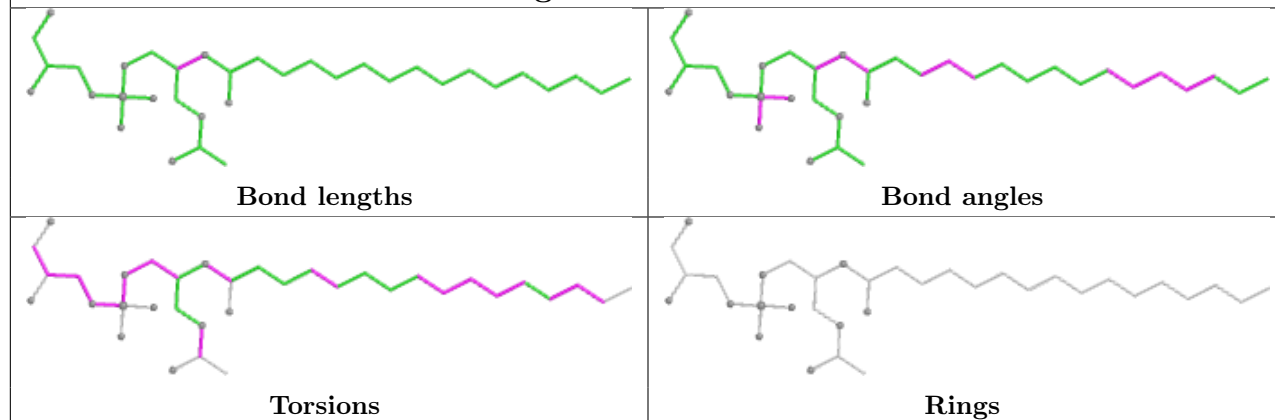
Ligand CLA e 603



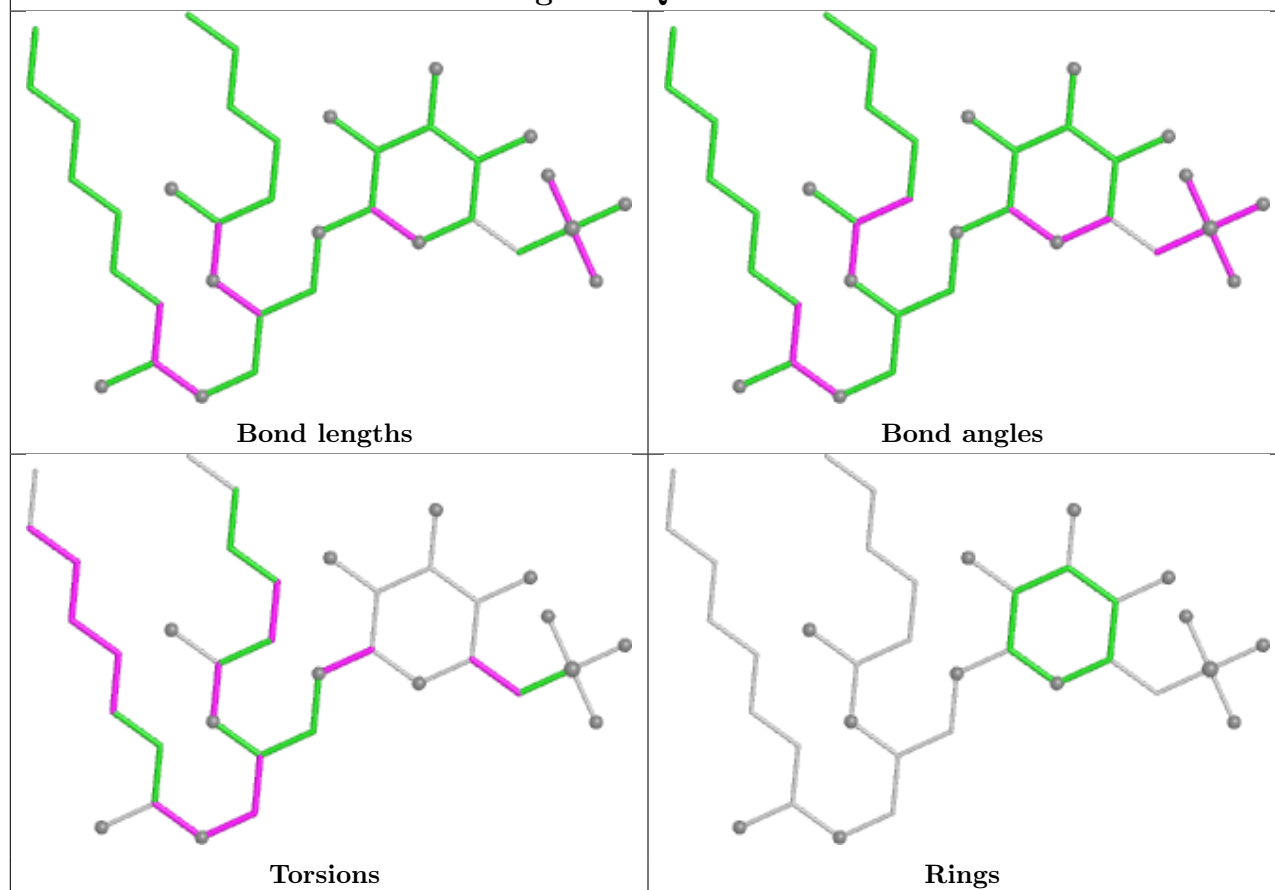
Ligand II0 a 619

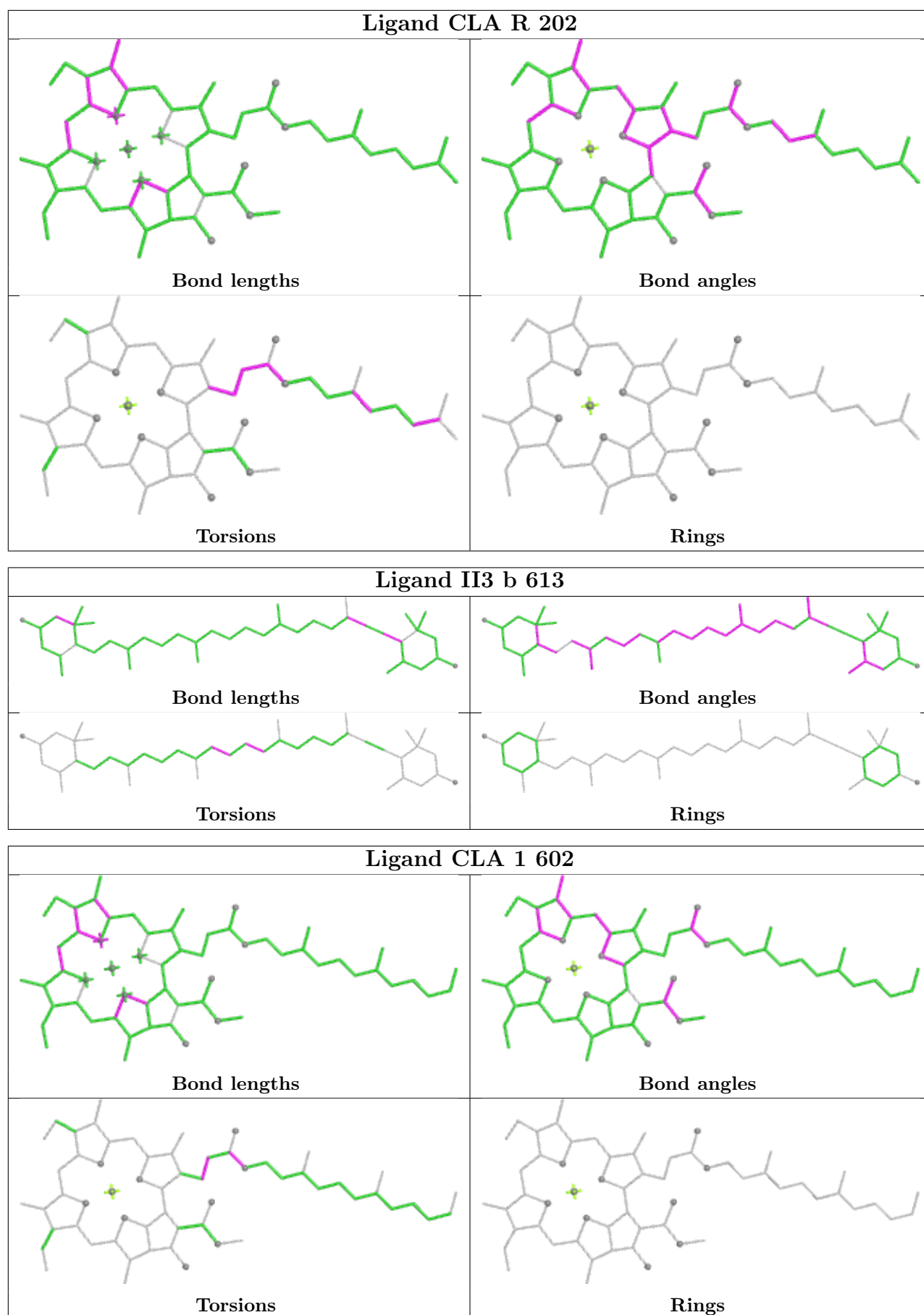


Ligand LHG c 623

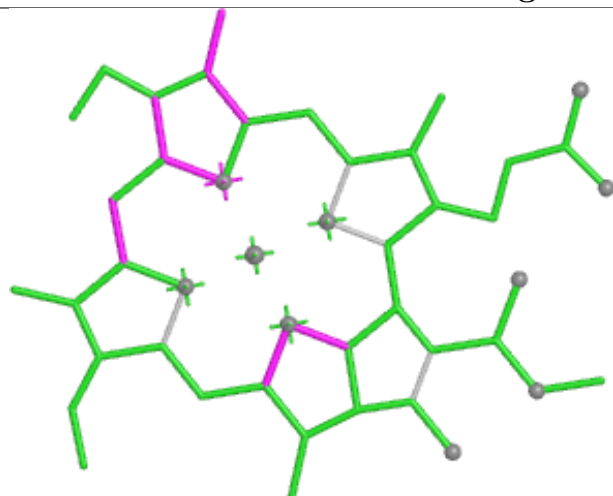


Ligand SQD 3 322

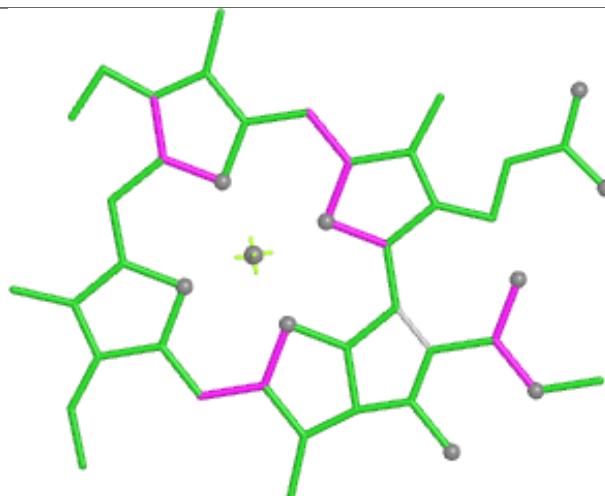




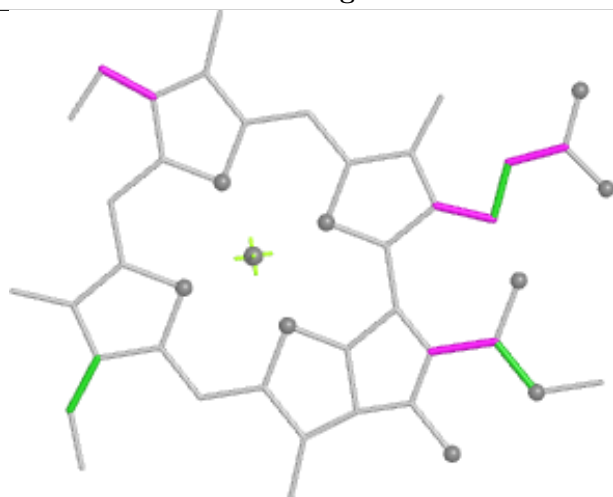
Ligand CLA 7 306



Bond lengths



Bond angles

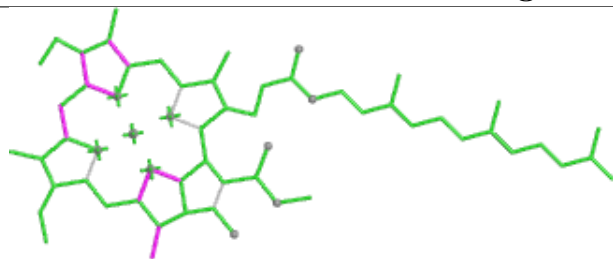


Torsions

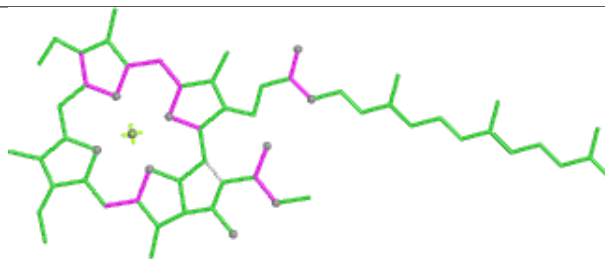


Rings

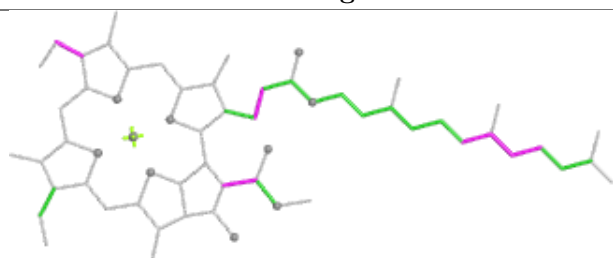
Ligand CLA d 604



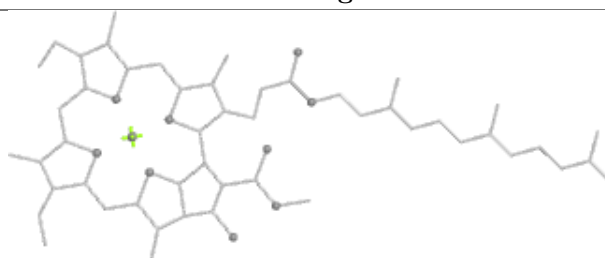
Bond lengths



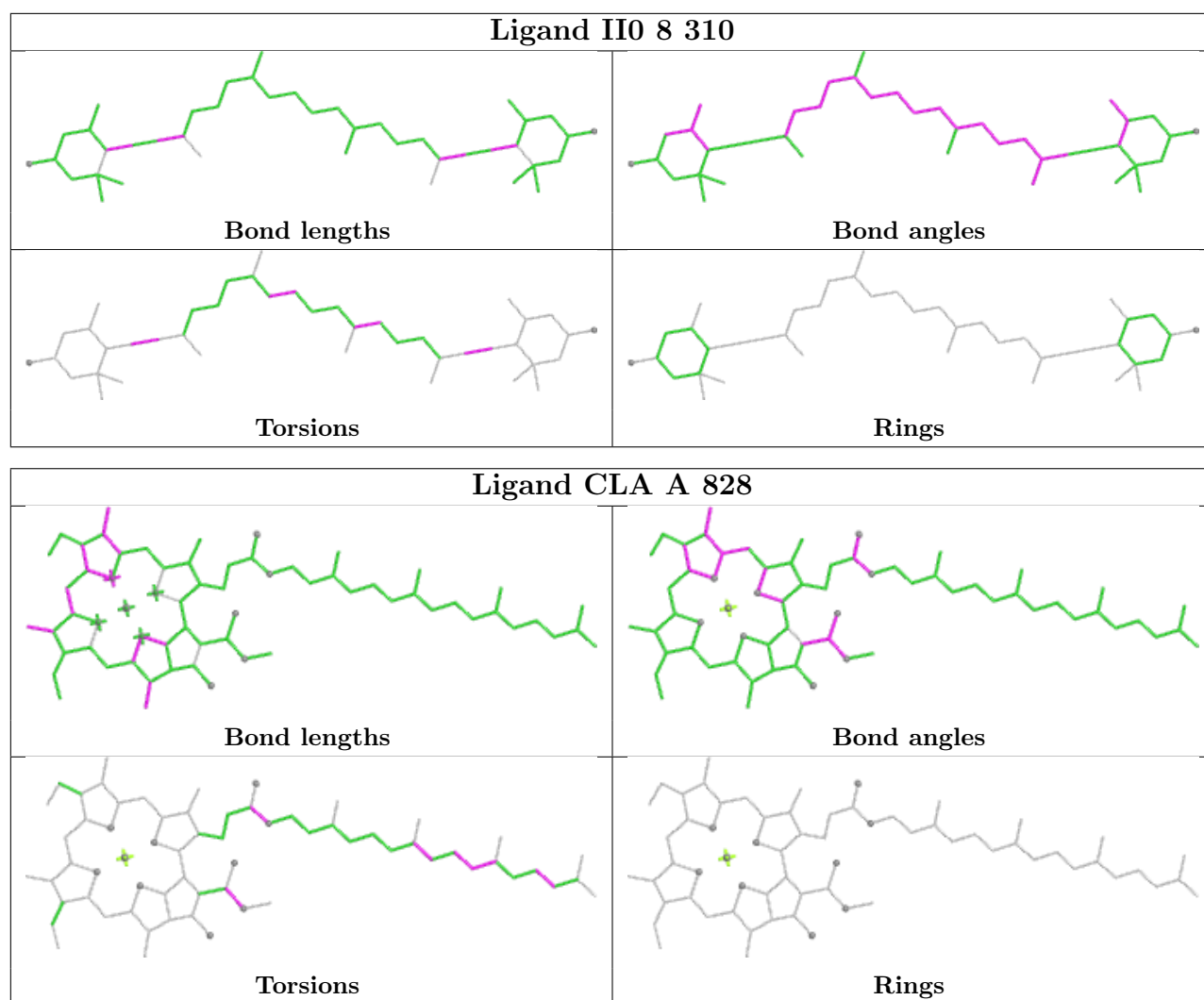
Bond angles

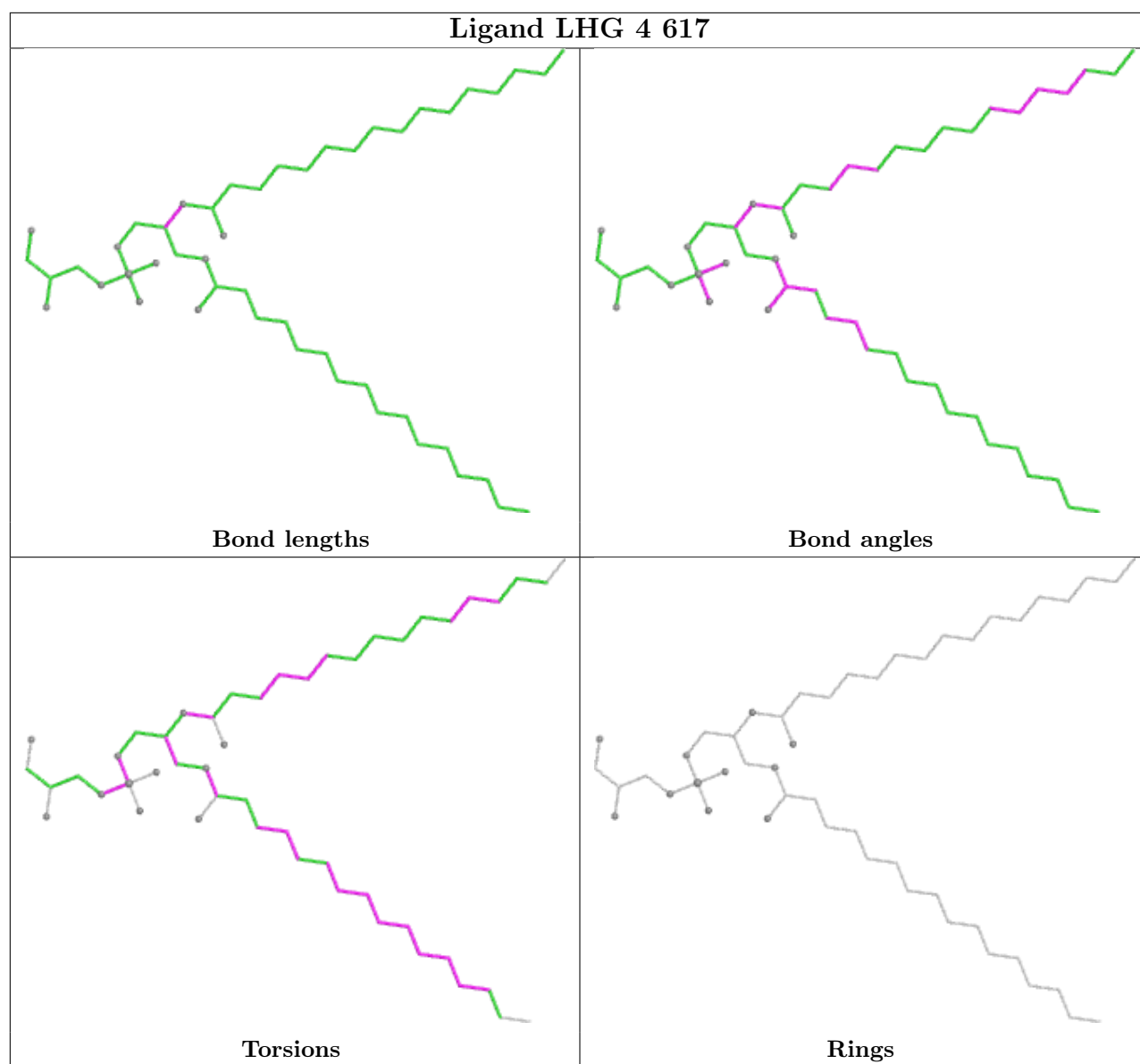


Torsions

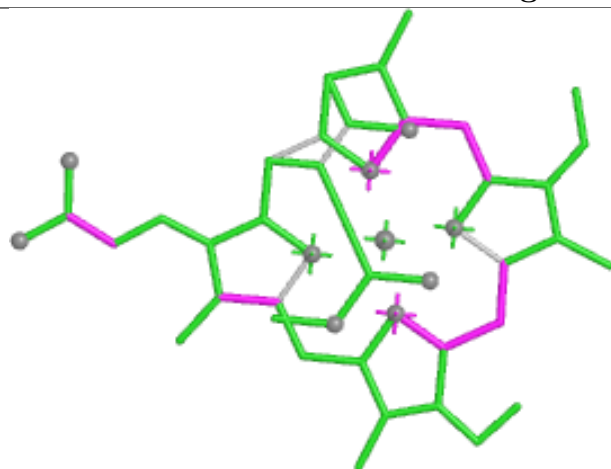


Rings

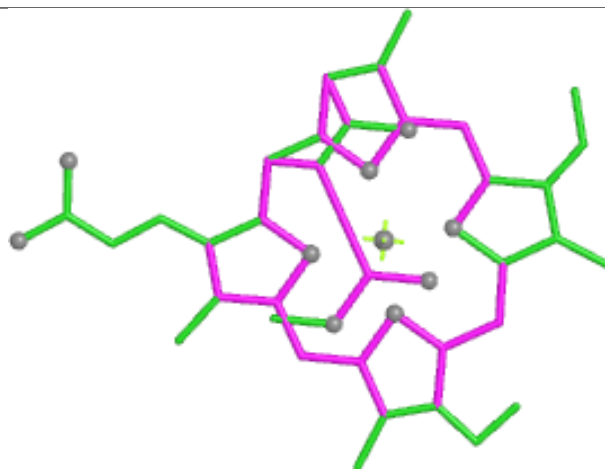




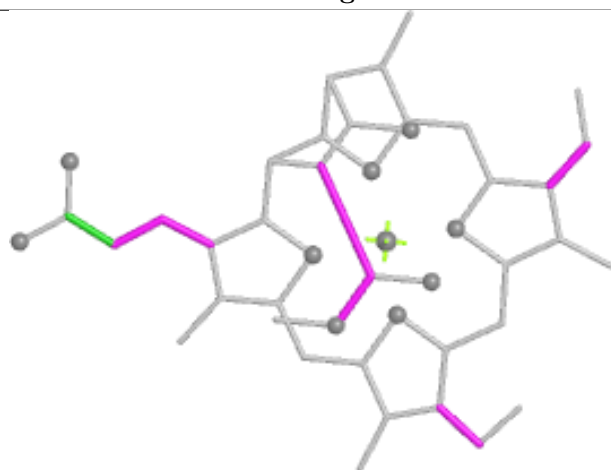
Ligand KC2 7 313



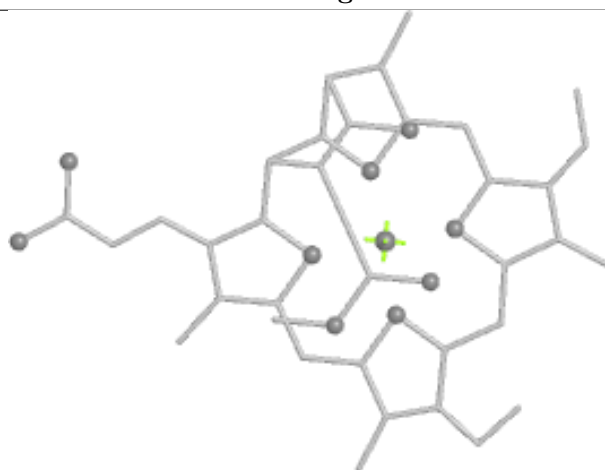
Bond lengths



Bond angles

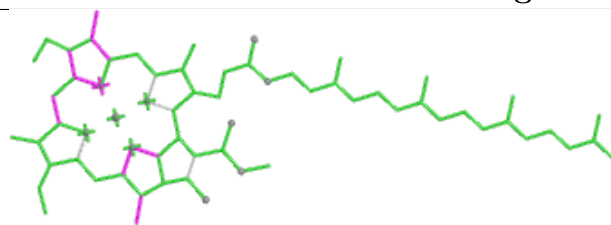


Torsions

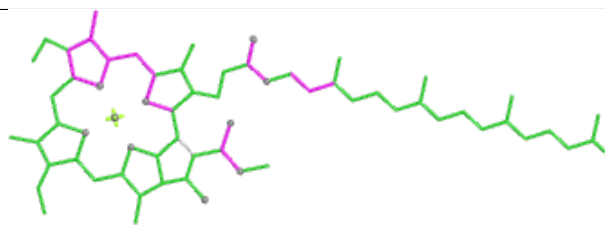


Rings

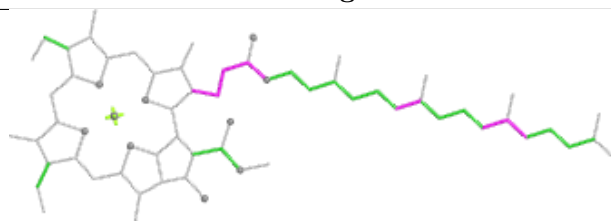
Ligand CLA B 809



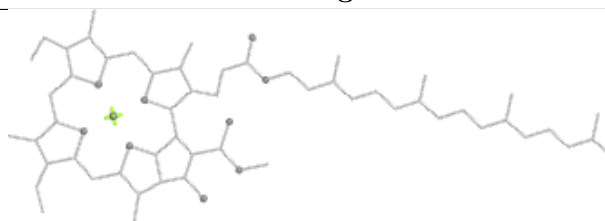
Bond lengths



Bond angles

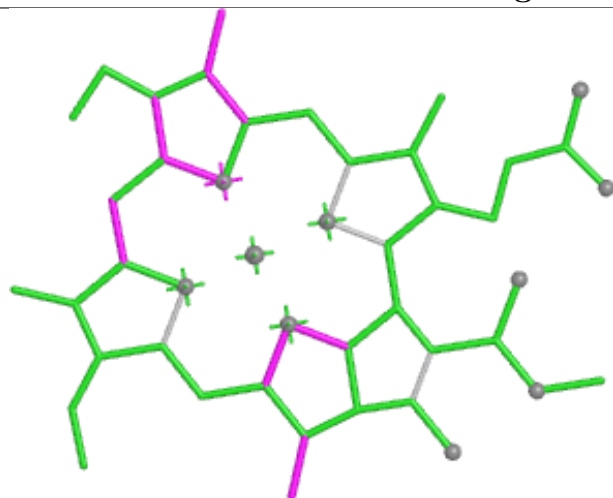


Torsions

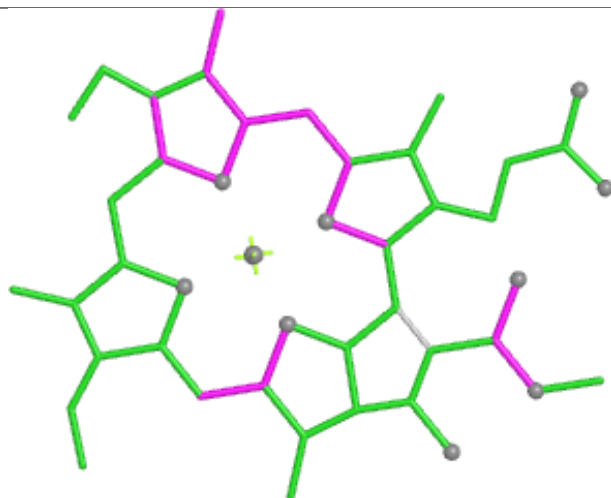


Rings

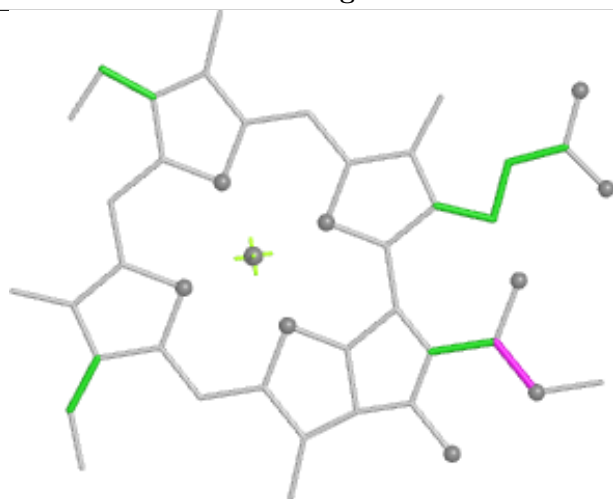
Ligand CLA B 834



Bond lengths



Bond angles

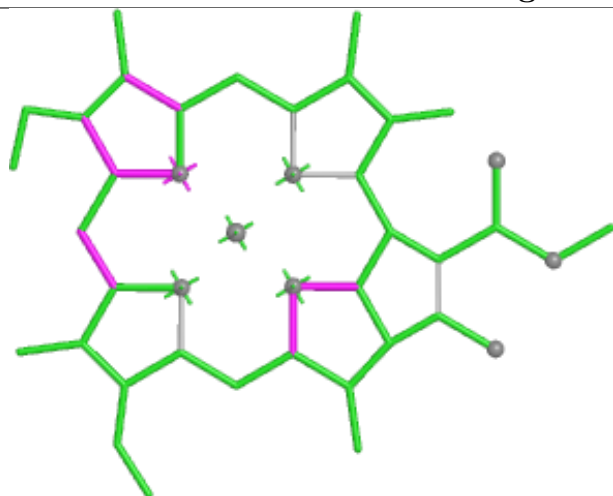


Torsions

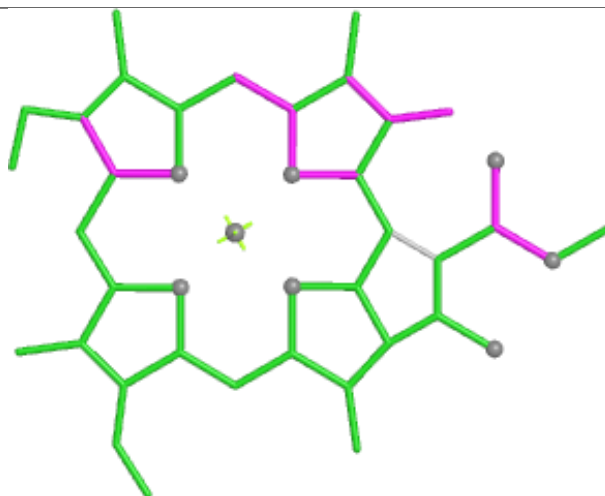


Rings

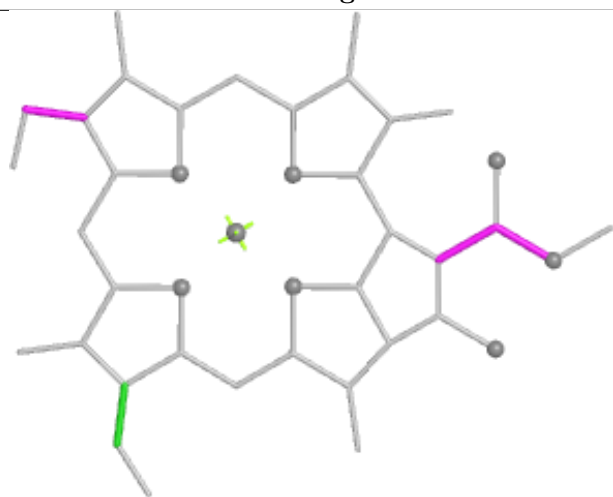
Ligand CLA 7 309



Bond lengths



Bond angles

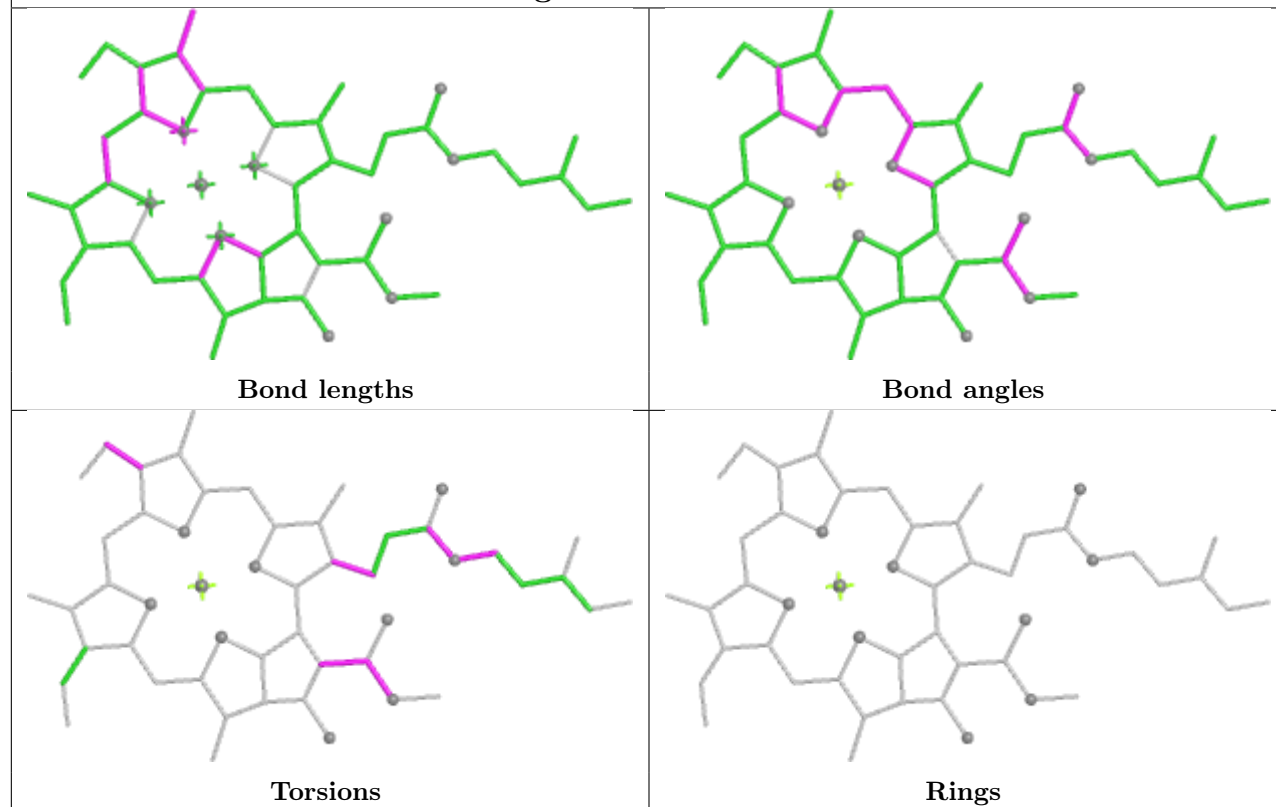


Torsions

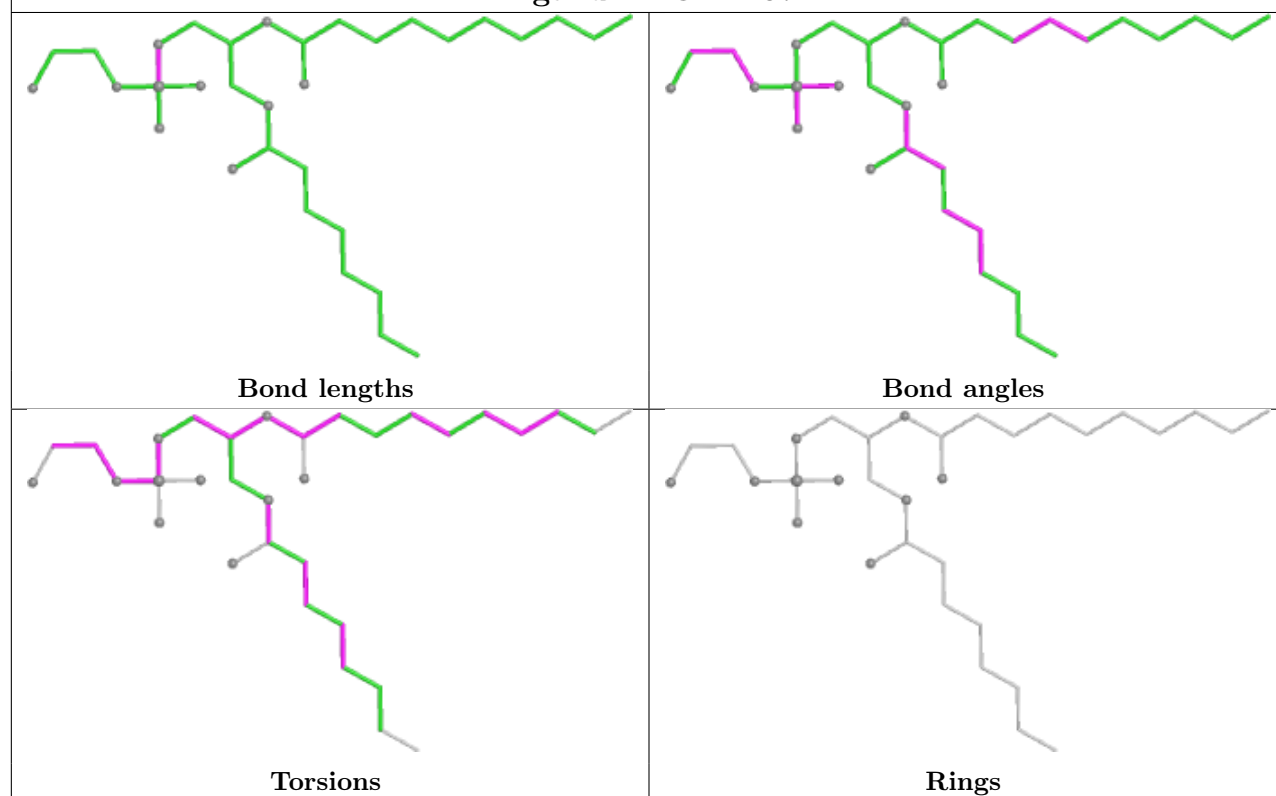


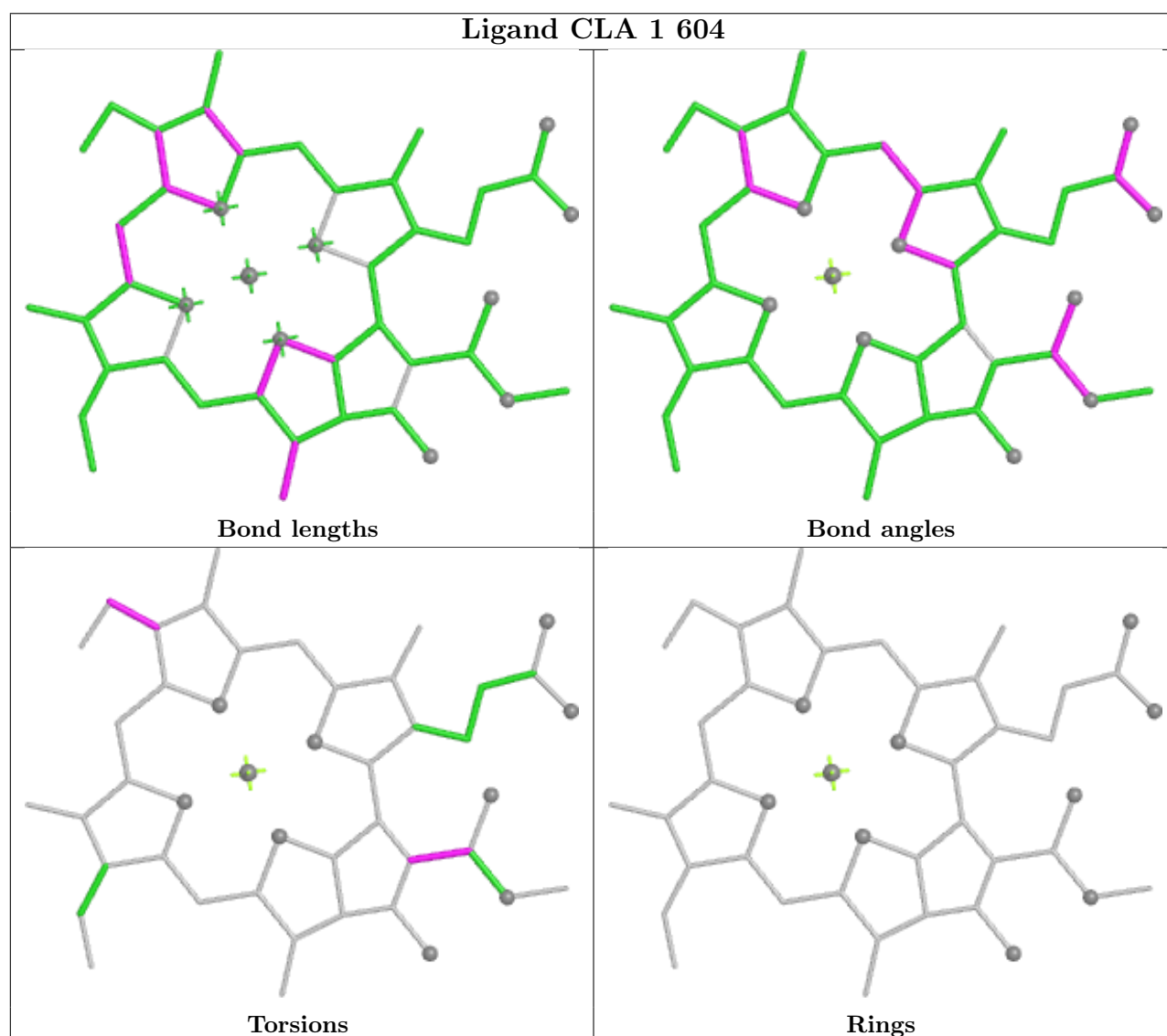
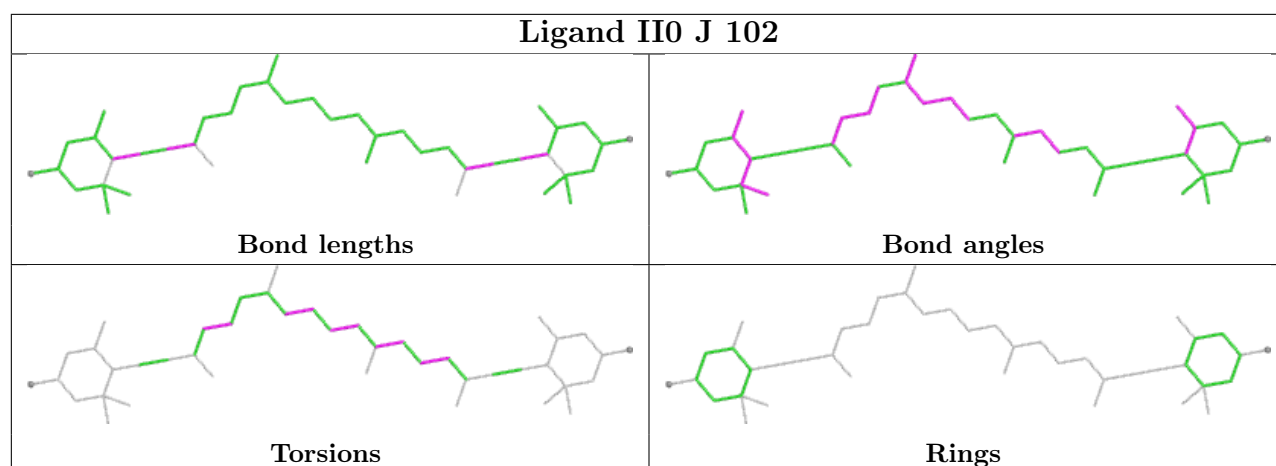
Rings

Ligand CLA L 201

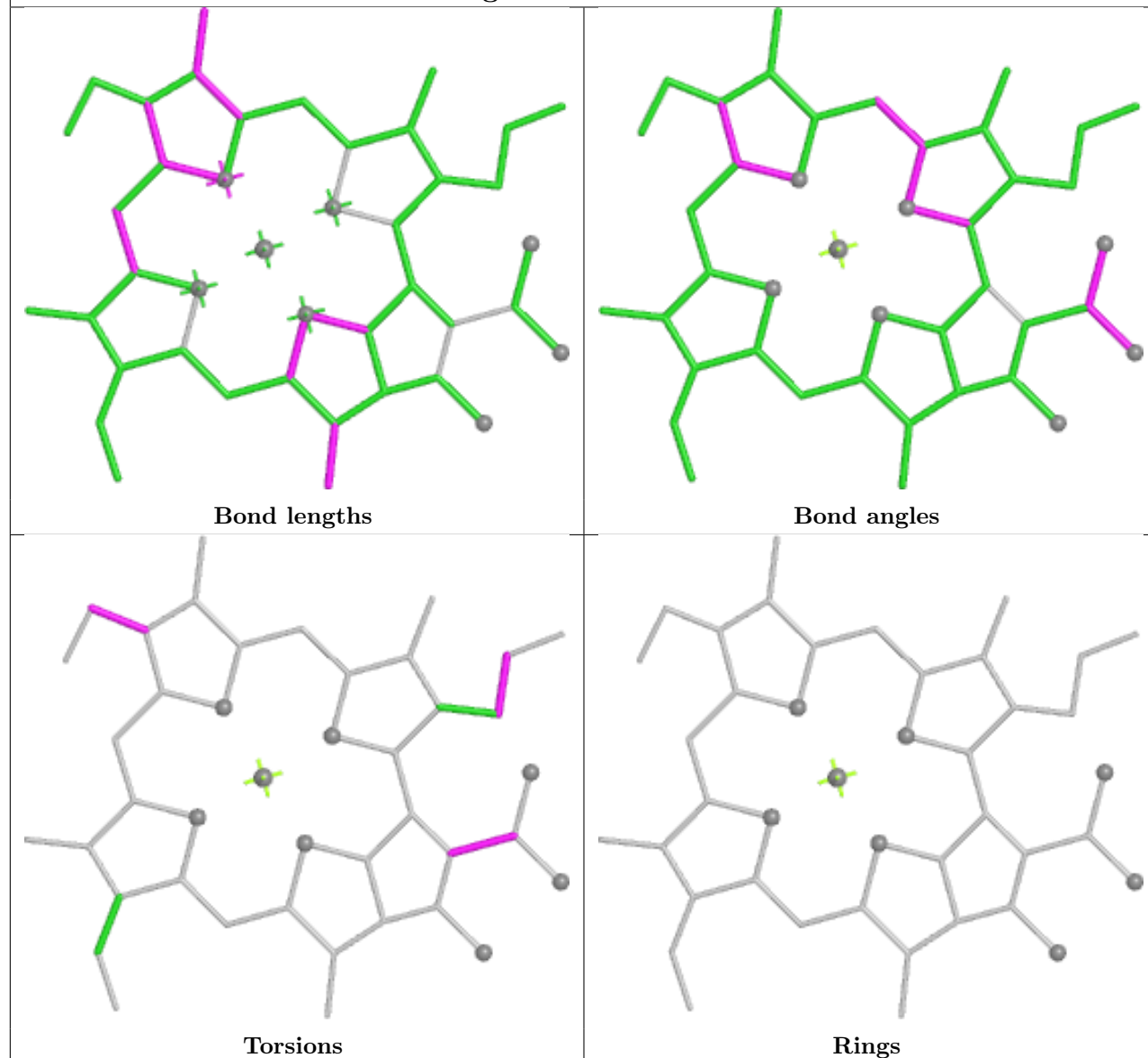


Ligand LHG L 207

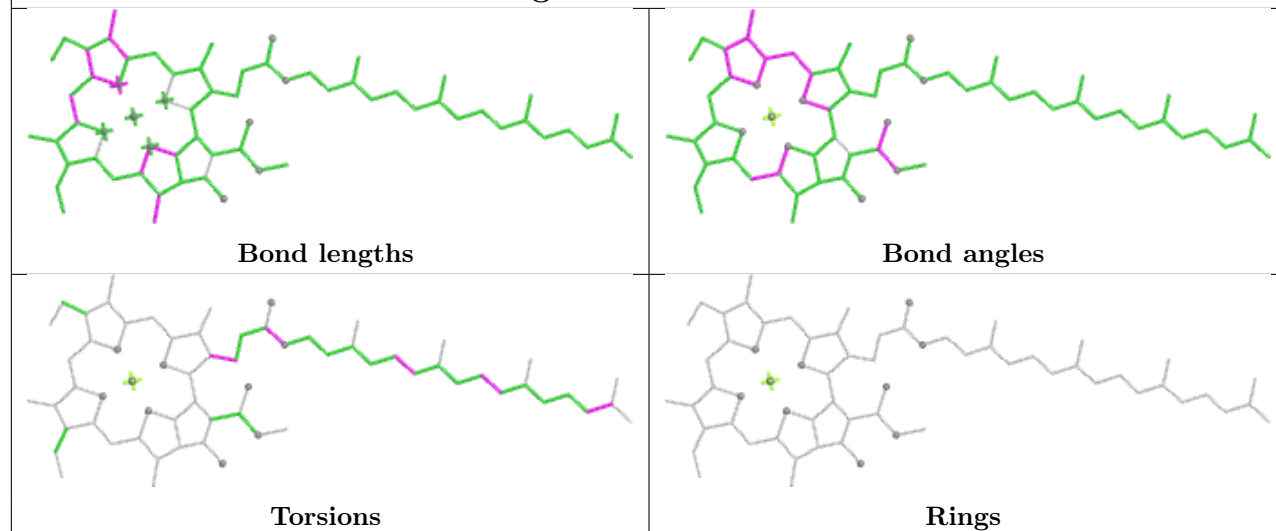




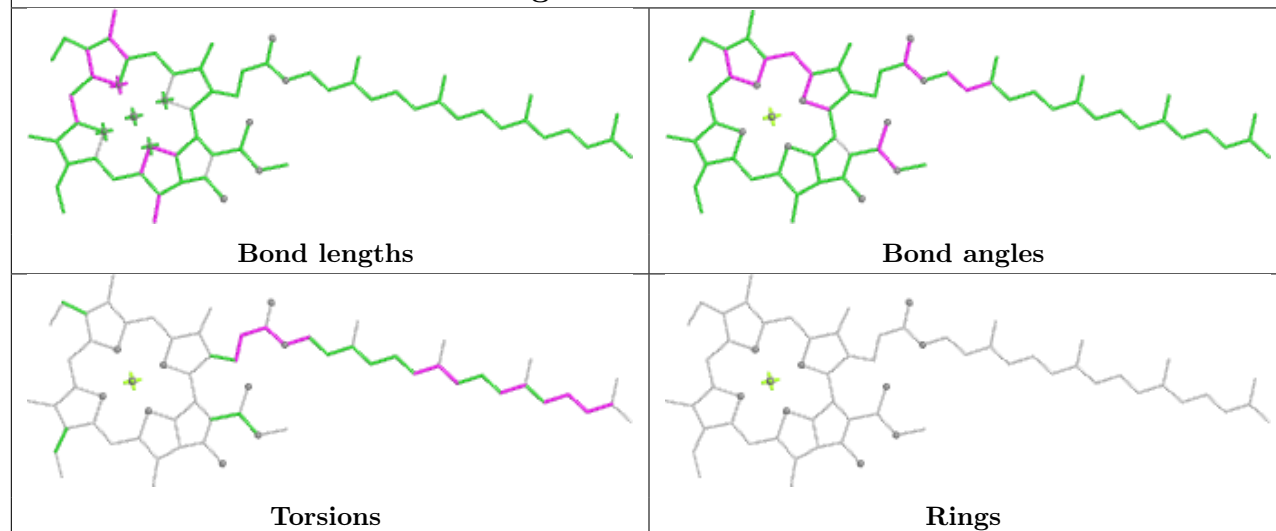
Ligand CLA 1 605



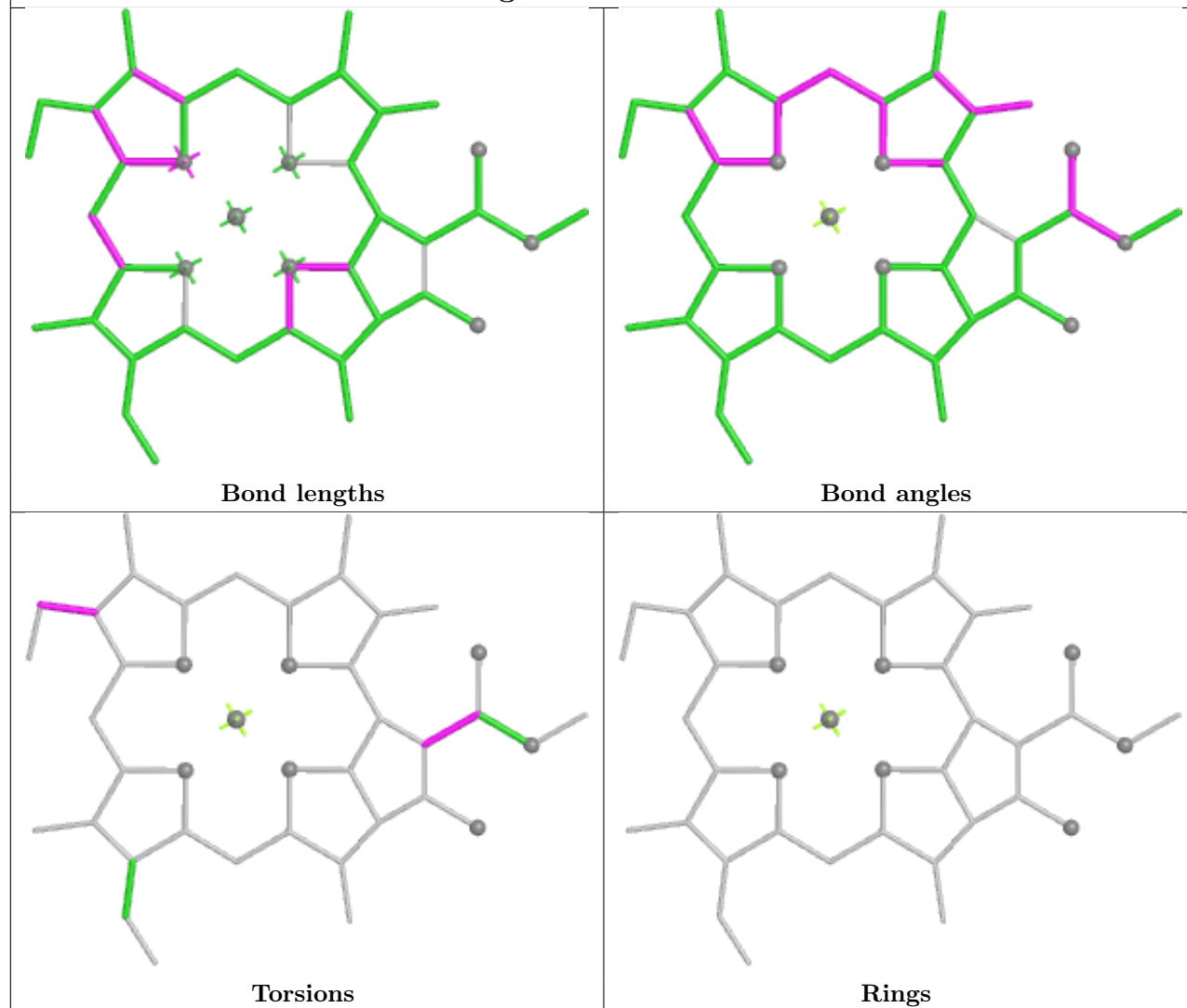
Ligand CLA B 828



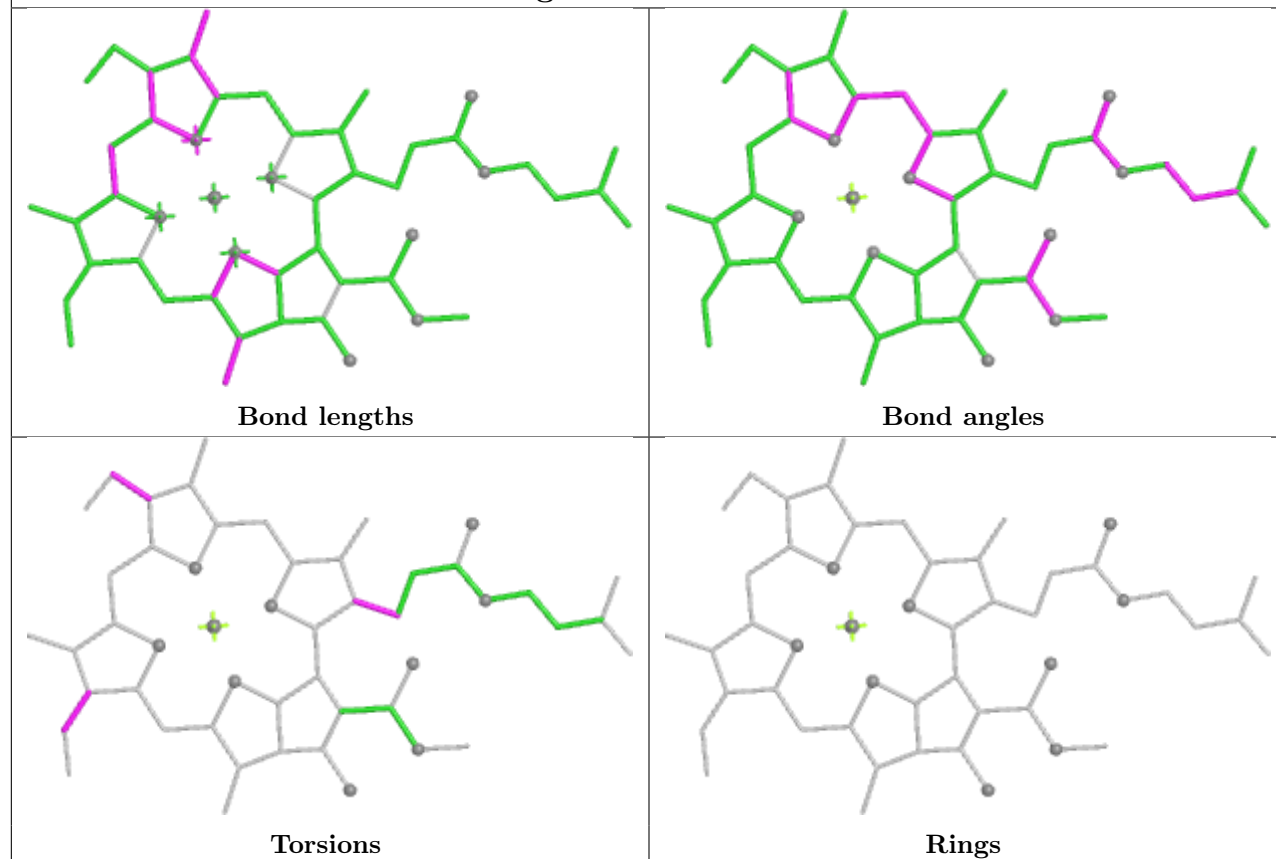
Ligand CLA A 839



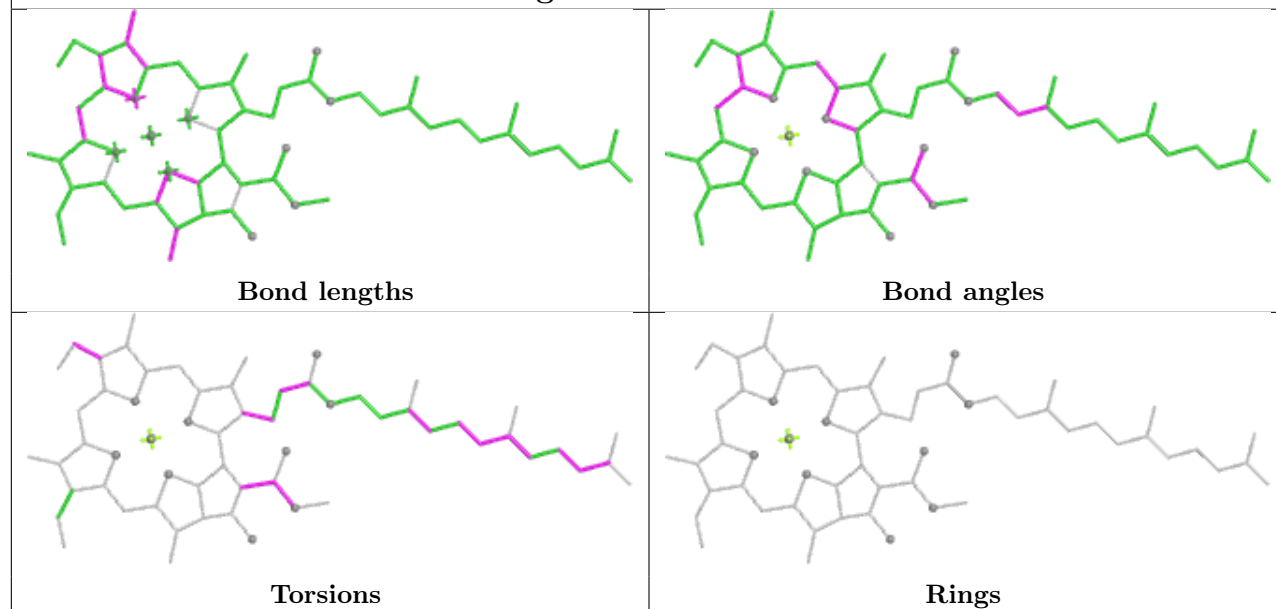
Ligand CLA 9 315

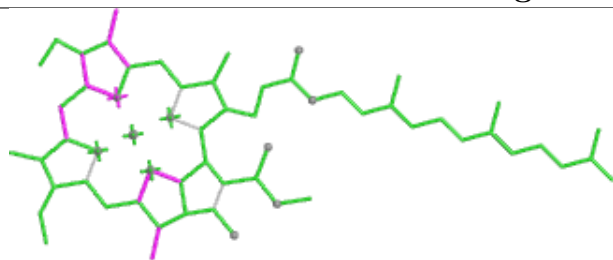
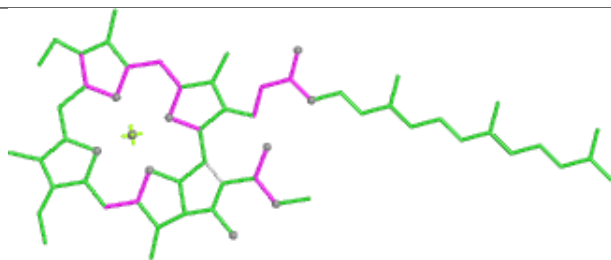
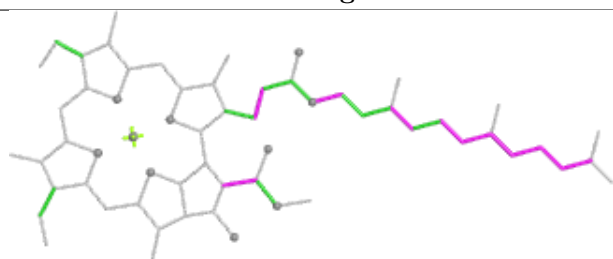
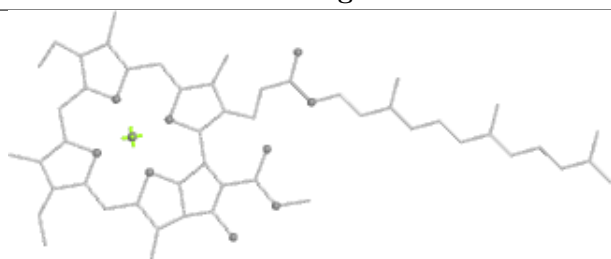
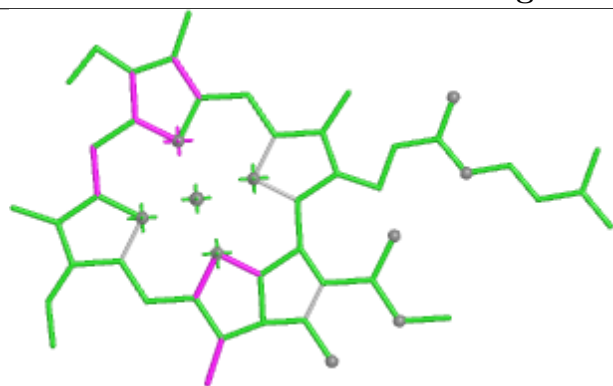
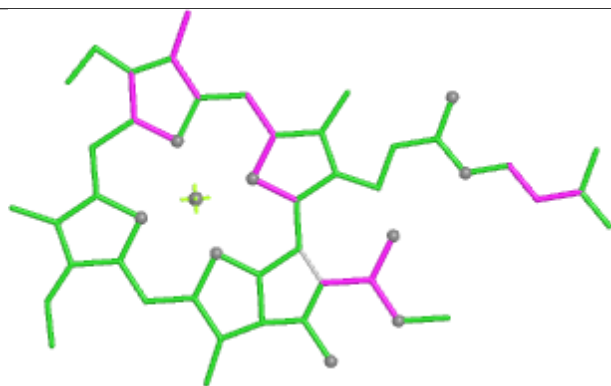
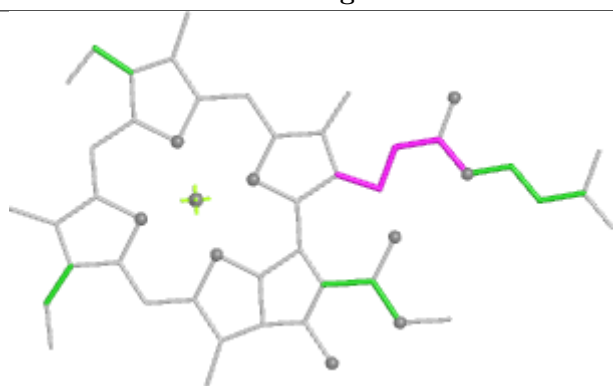
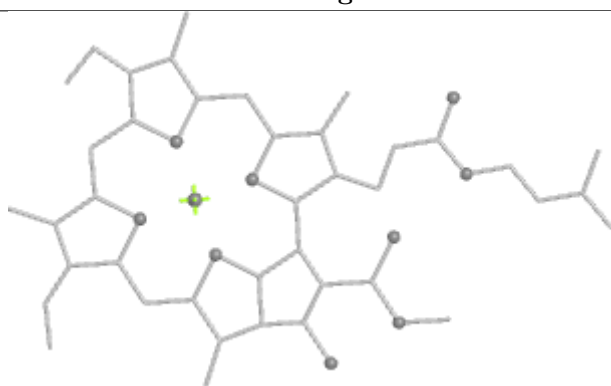


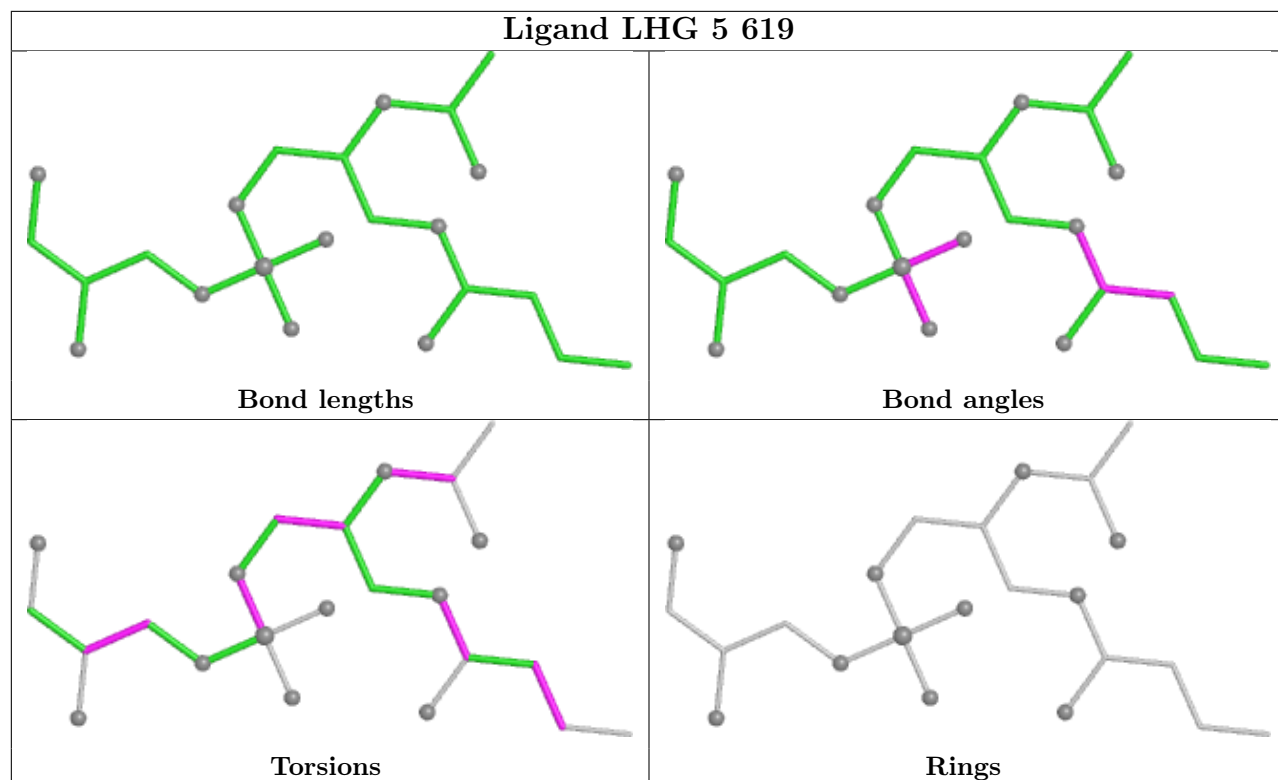
Ligand CLA 2 611



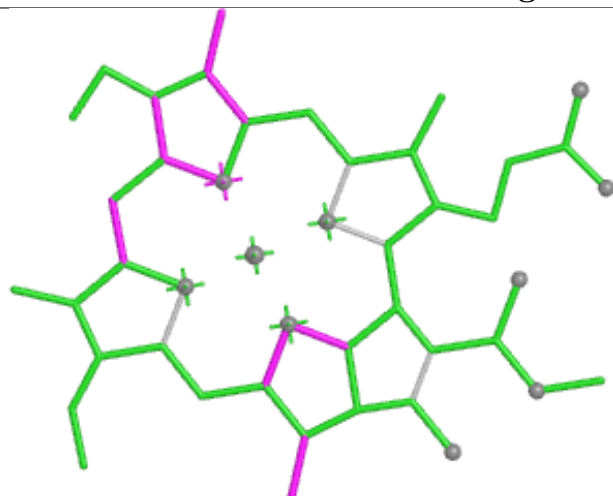
Ligand CLA 3 308



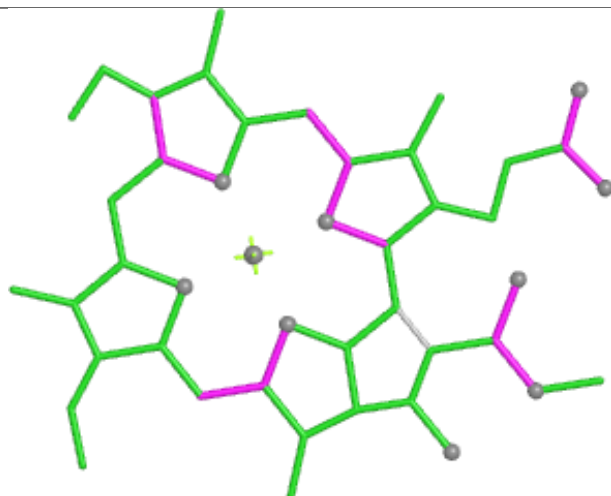
Ligand CLA B 820**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA L 203****Bond lengths****Bond angles****Torsions****Rings**



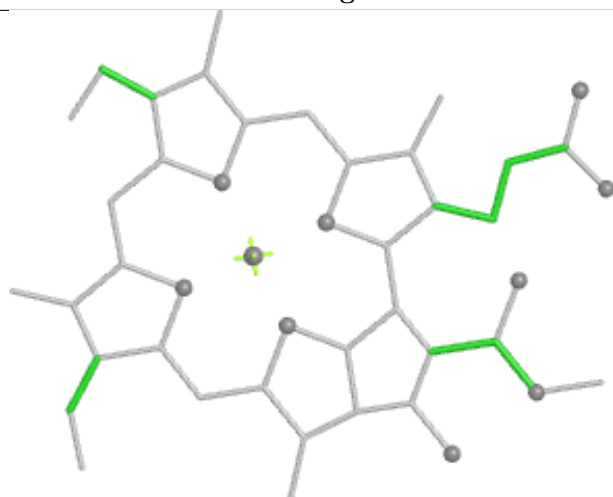
Ligand CLA 9 306



Bond lengths



Bond angles

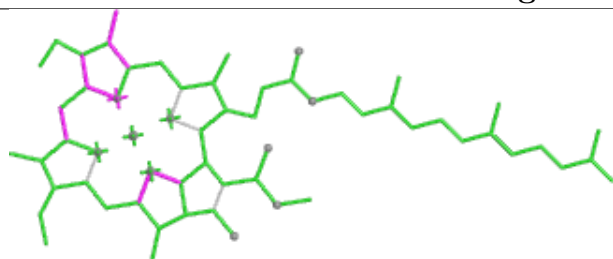


Torsions

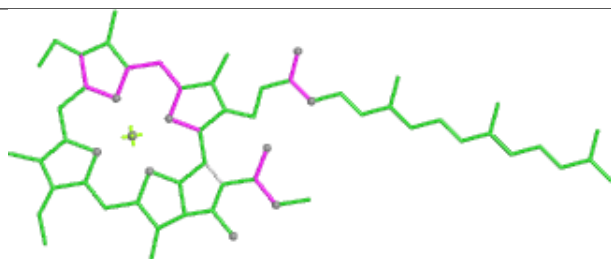


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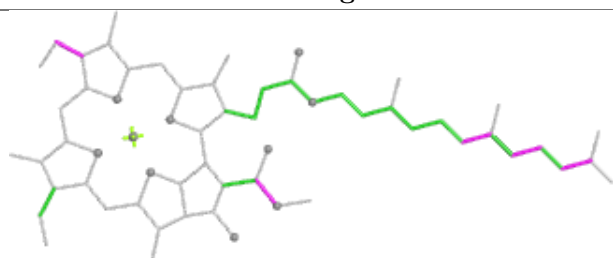
Ligand CLA 1 612



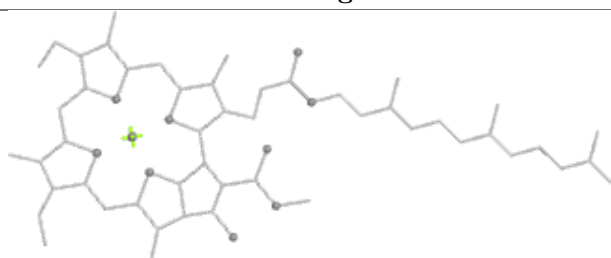
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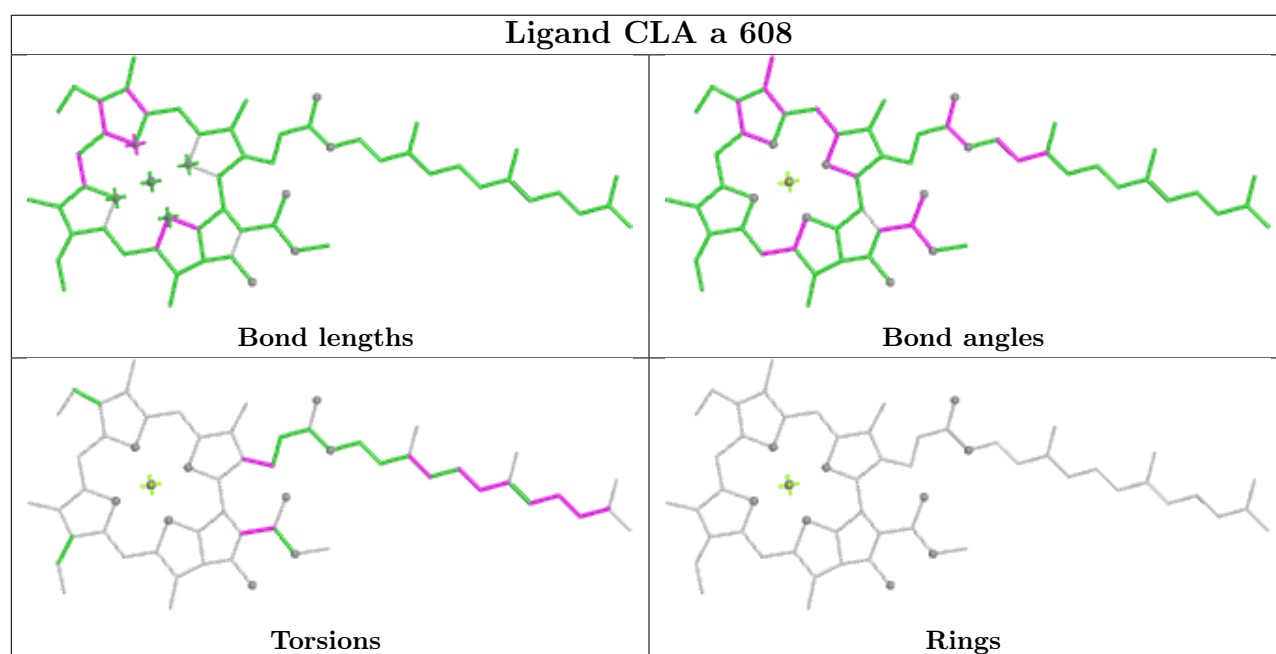
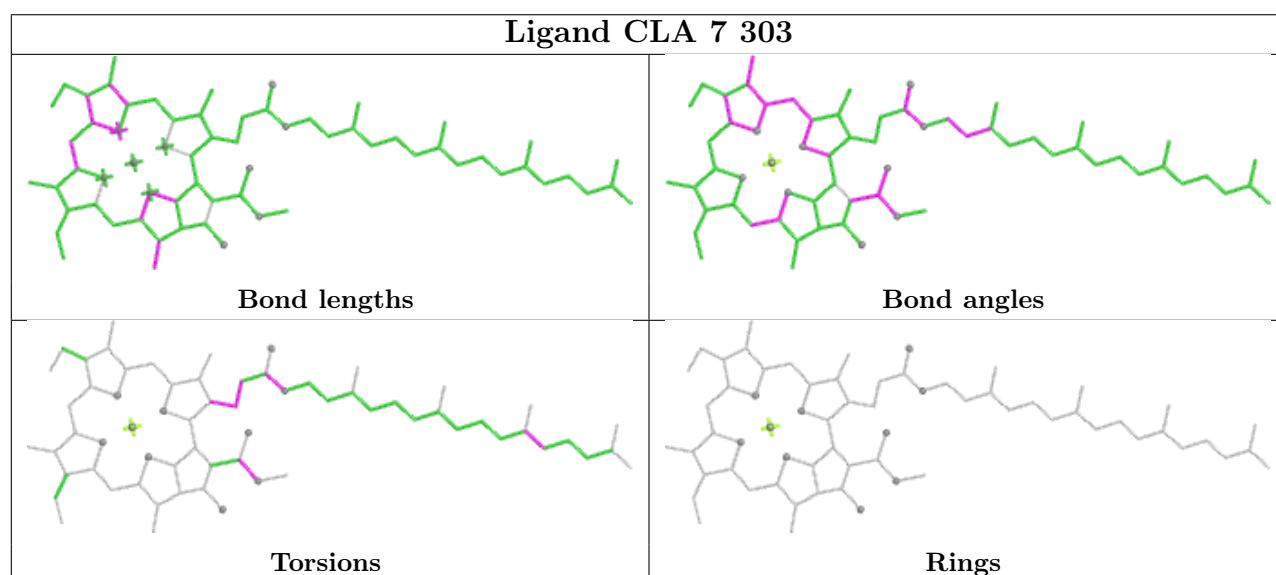
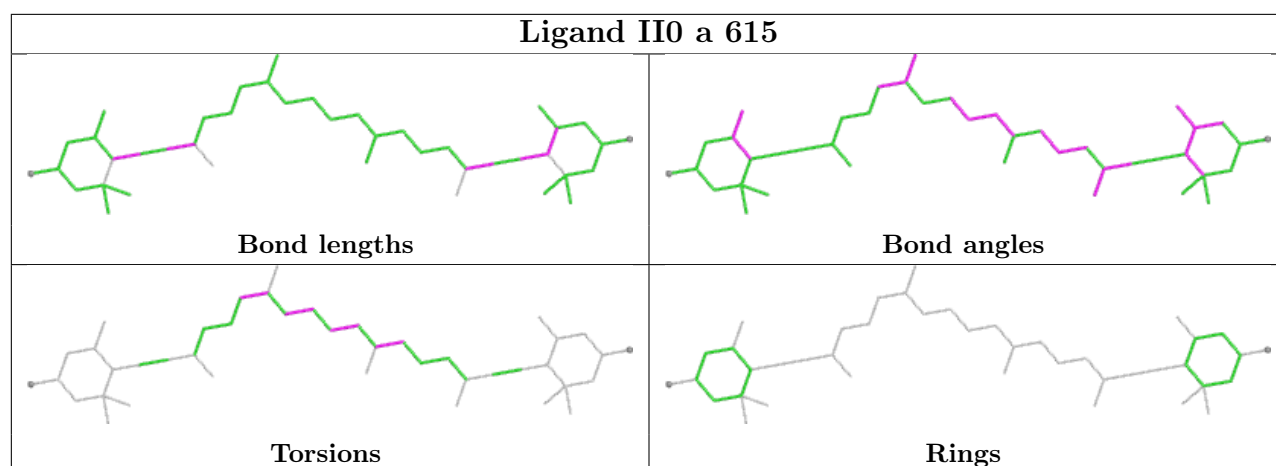
Bond angles

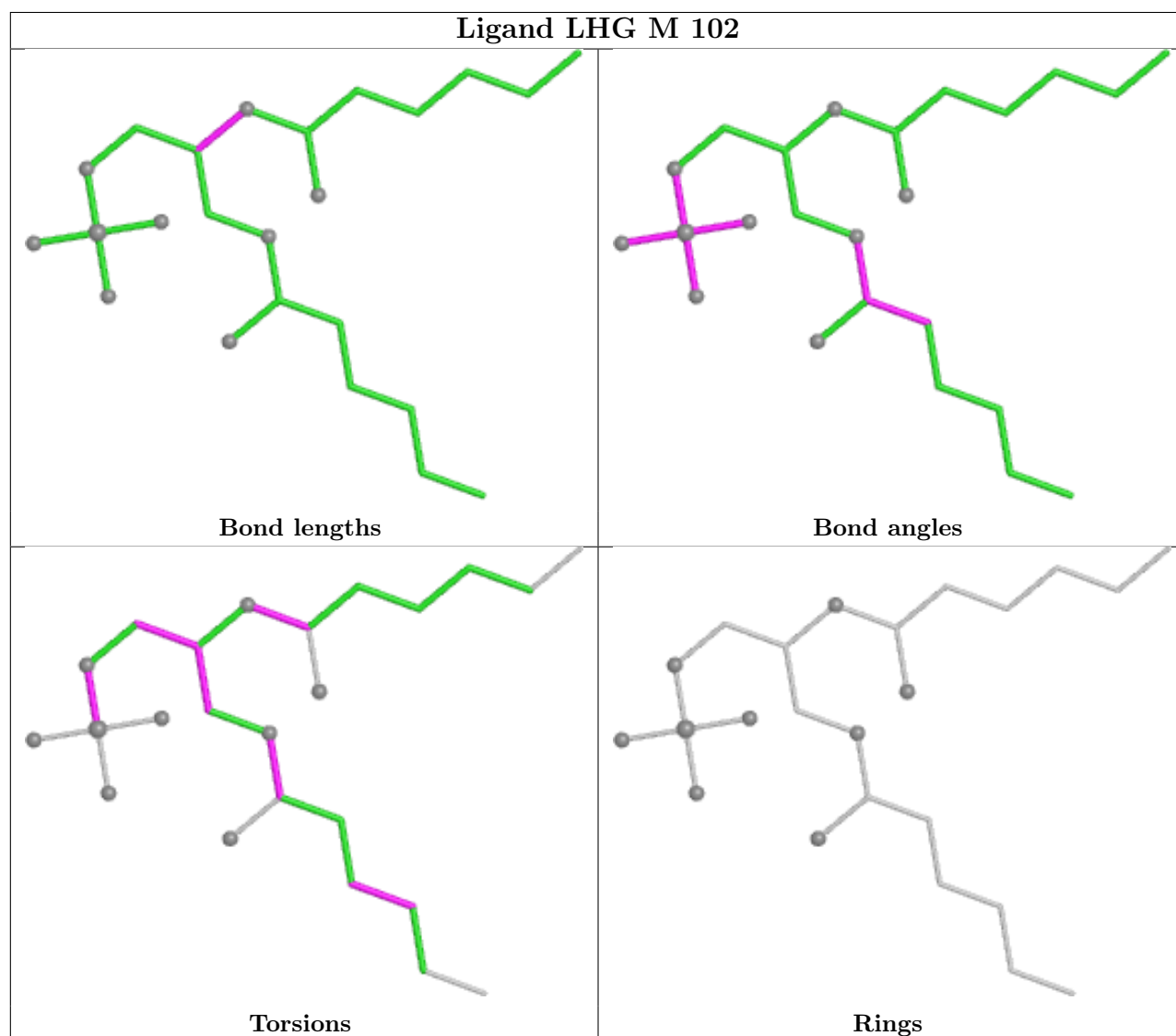
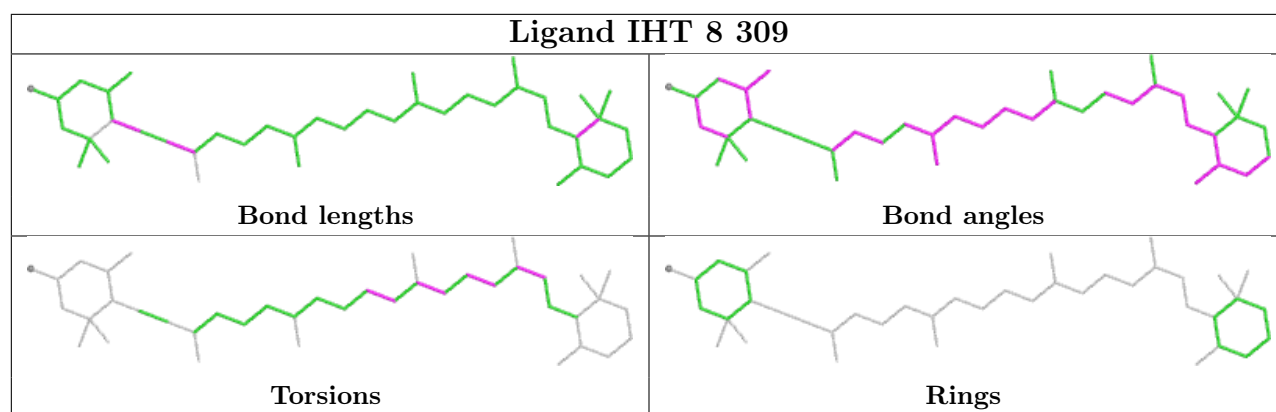


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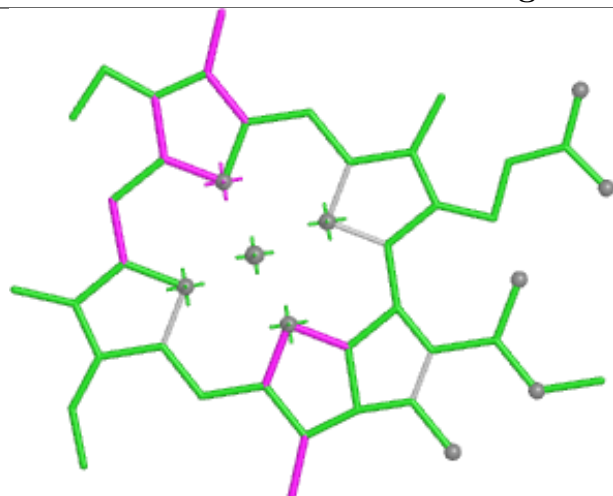


Rings

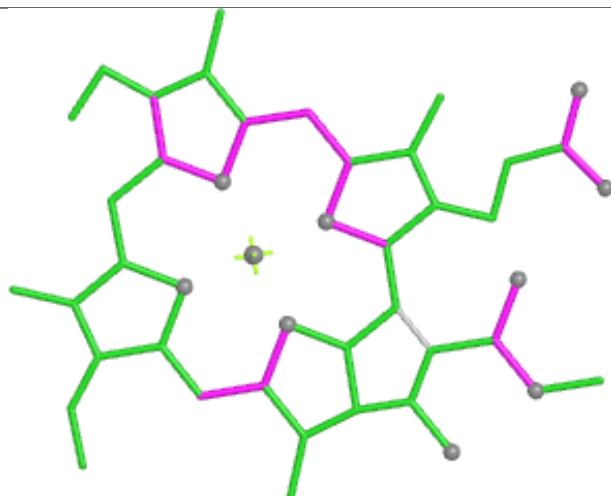




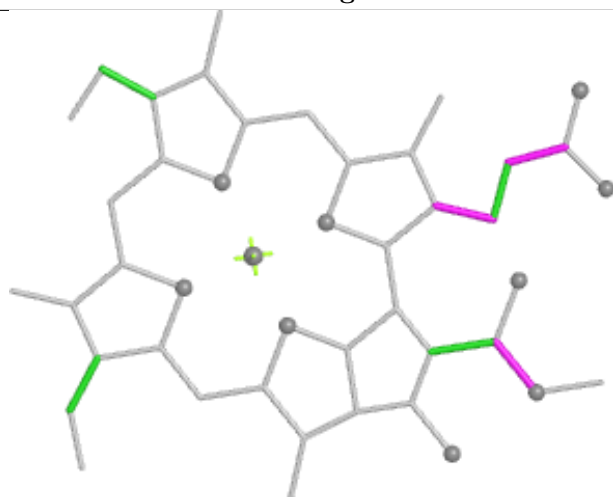
Ligand CLA 9 304



Bond lengths



Bond angles

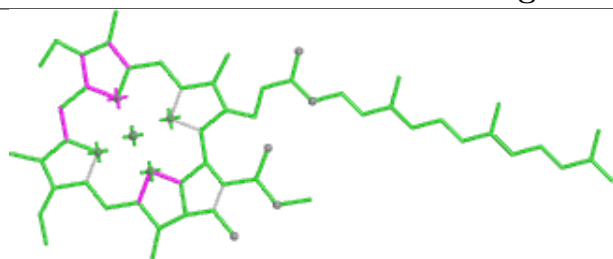


Torsions

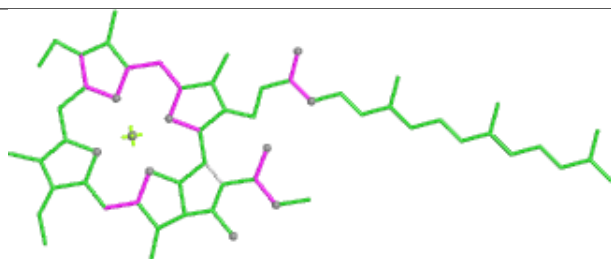


Rings

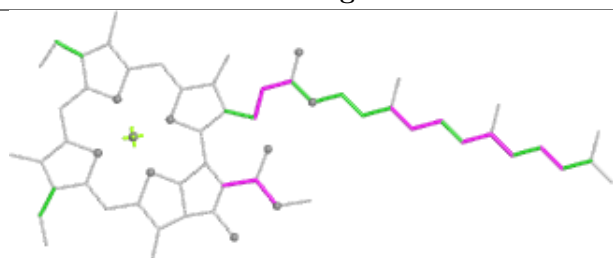
Ligand CLA 6 604



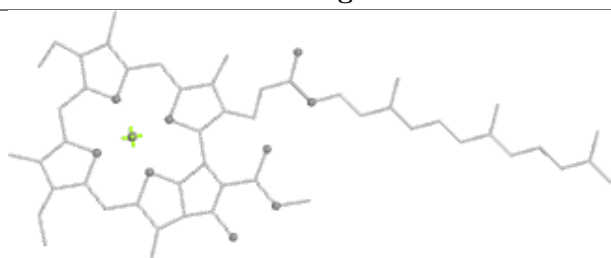
Bond lengths



Bond angles

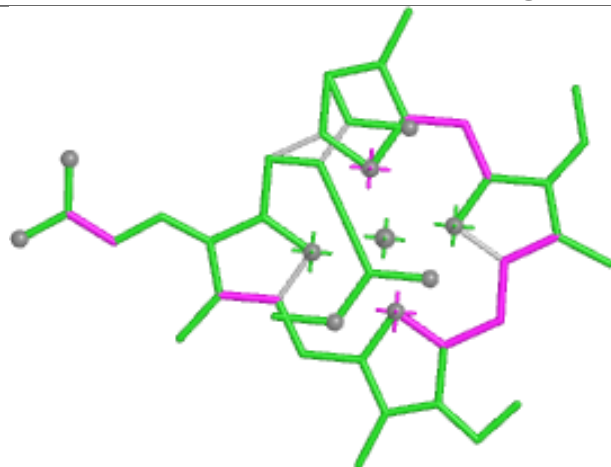


Torsions



Rings

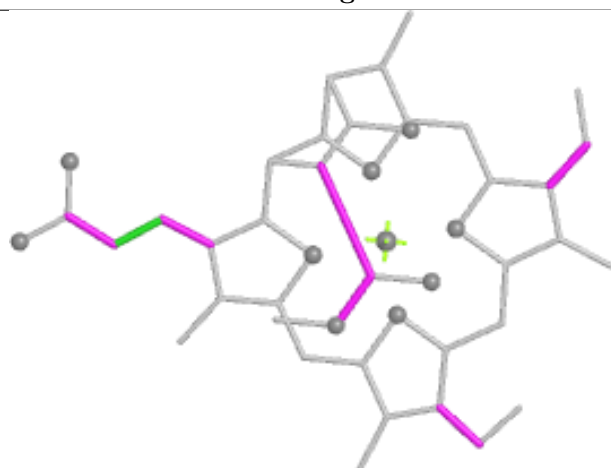
Ligand KC2 9 311



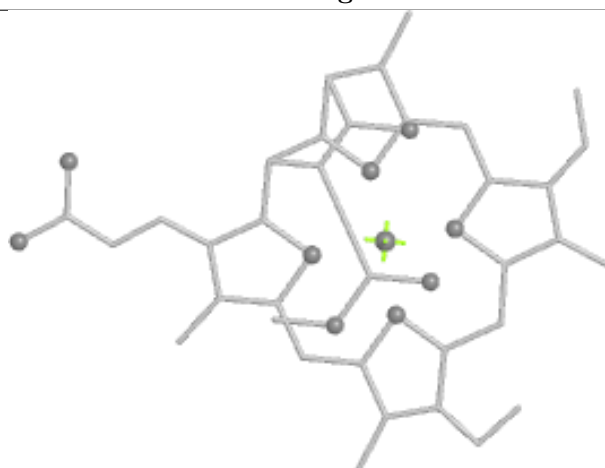
Bond lengths



Bond angles

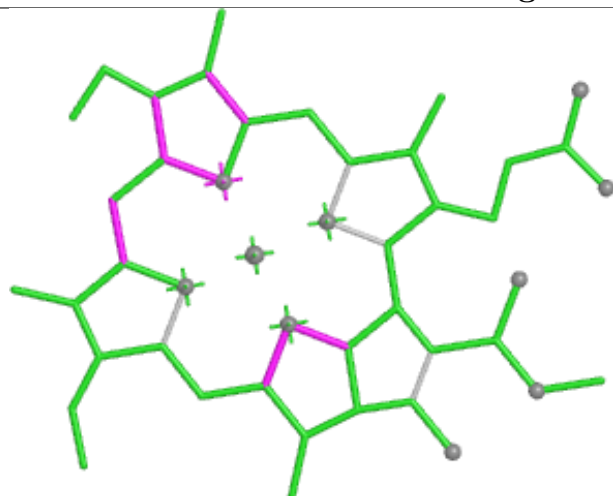


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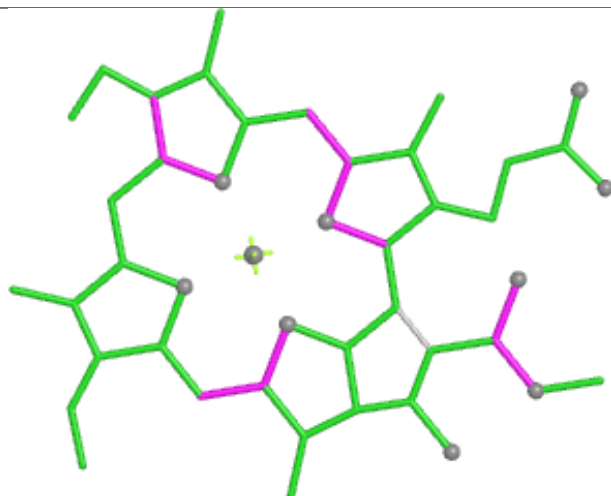


Rings

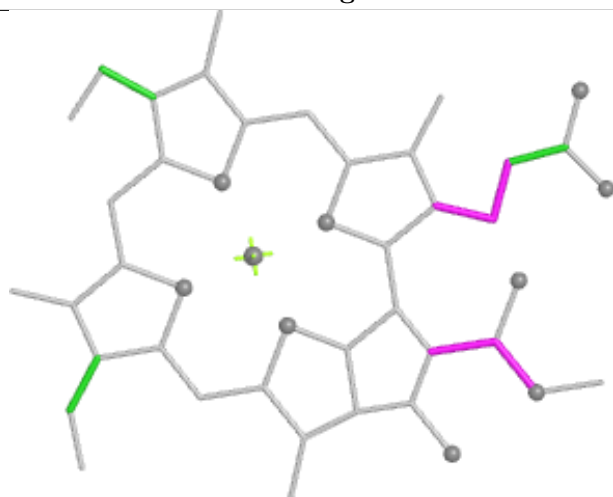
Ligand CLA 5 611



Bond lengths



Bond angles

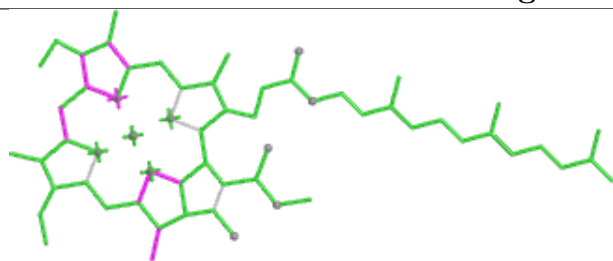


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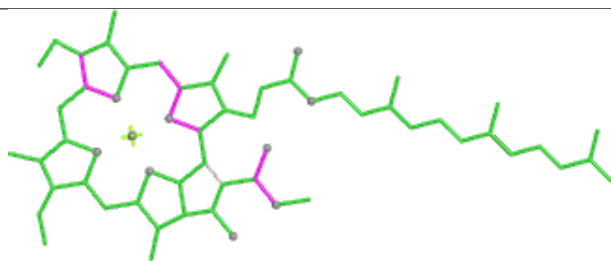


Rings

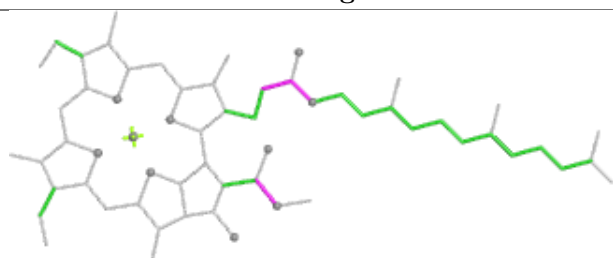
Ligand CLA 4 609



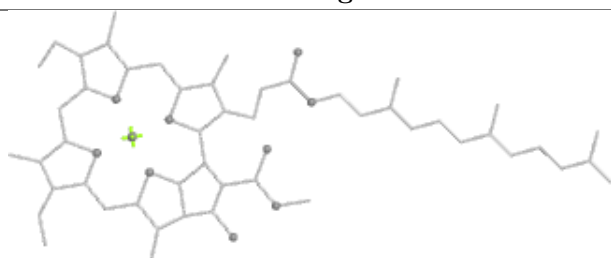
Bond lengths



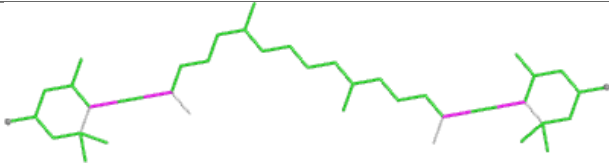
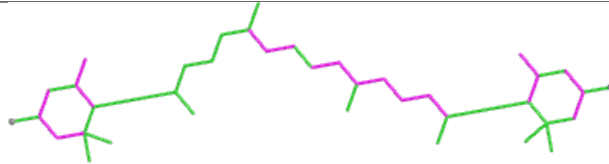
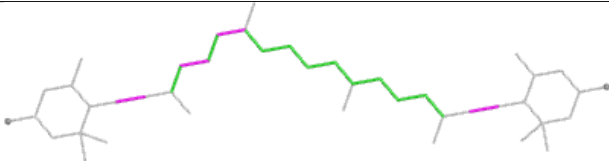
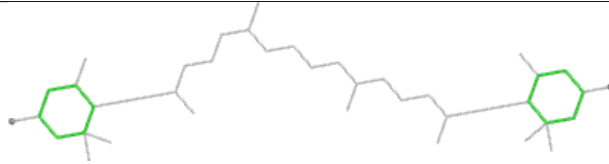
Bond angles

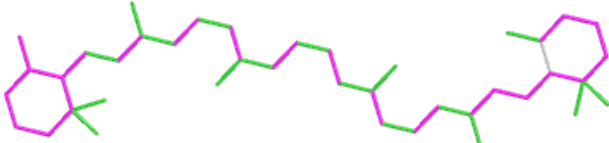
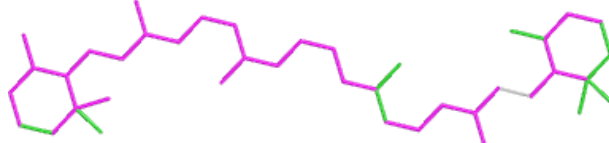
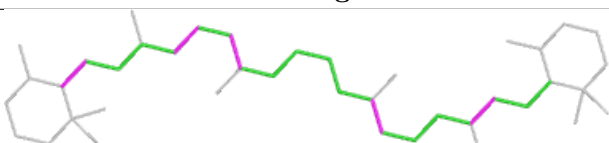
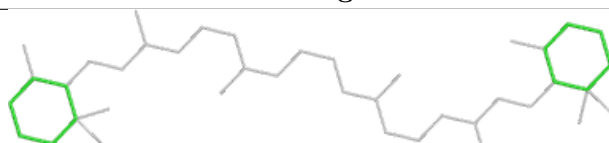


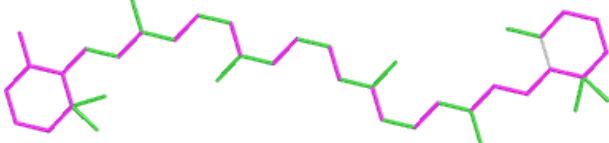
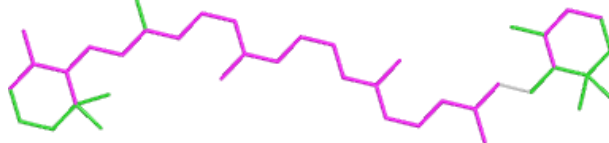
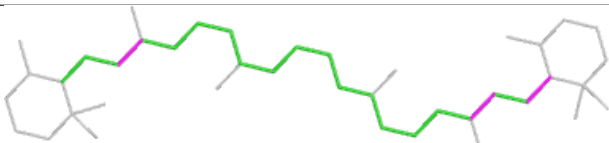
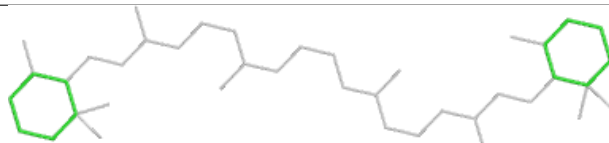
Torsions

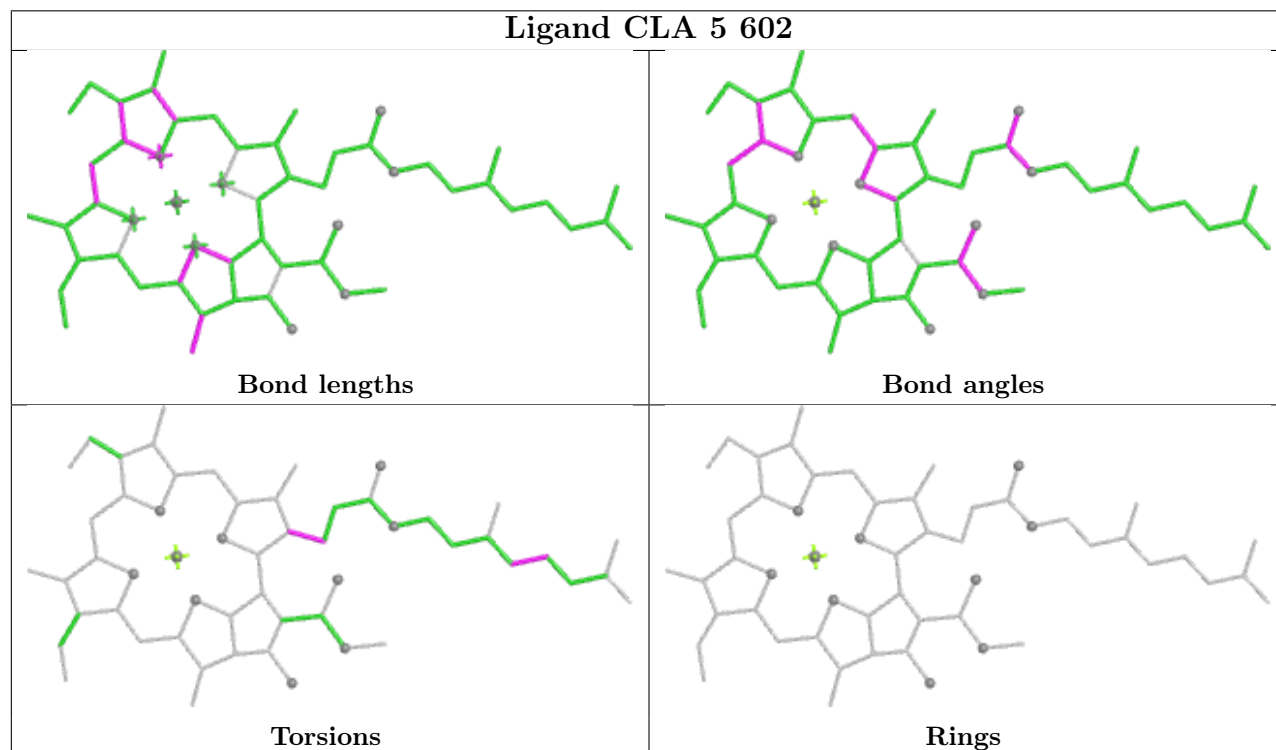
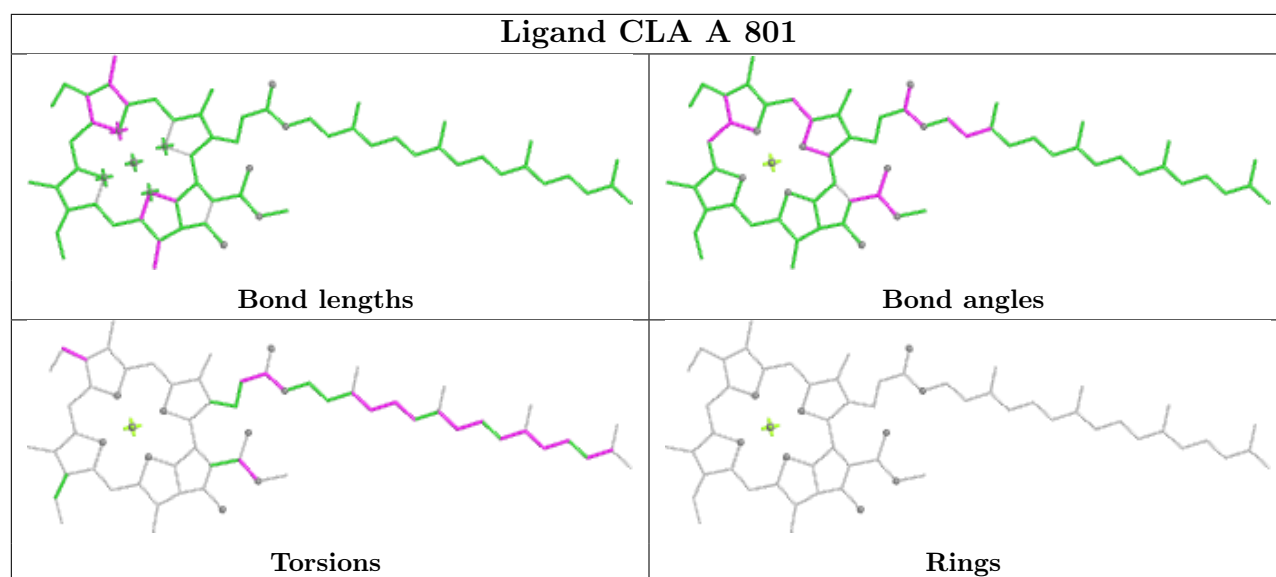


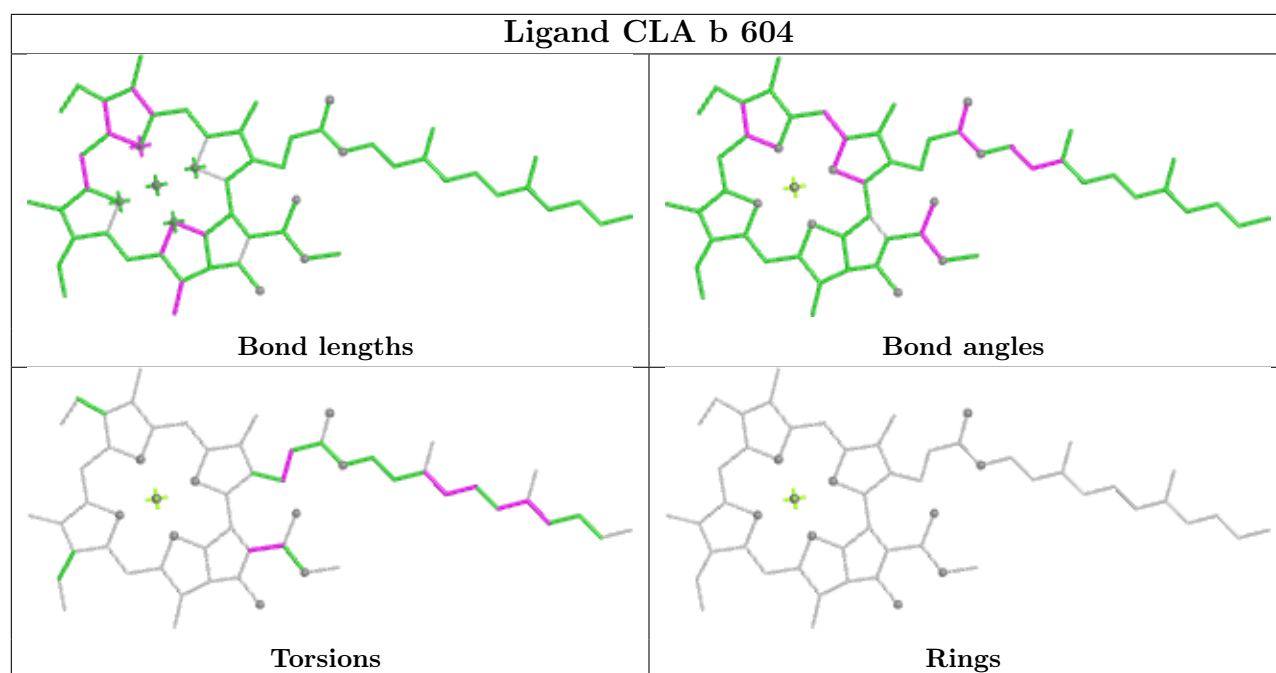
Rings

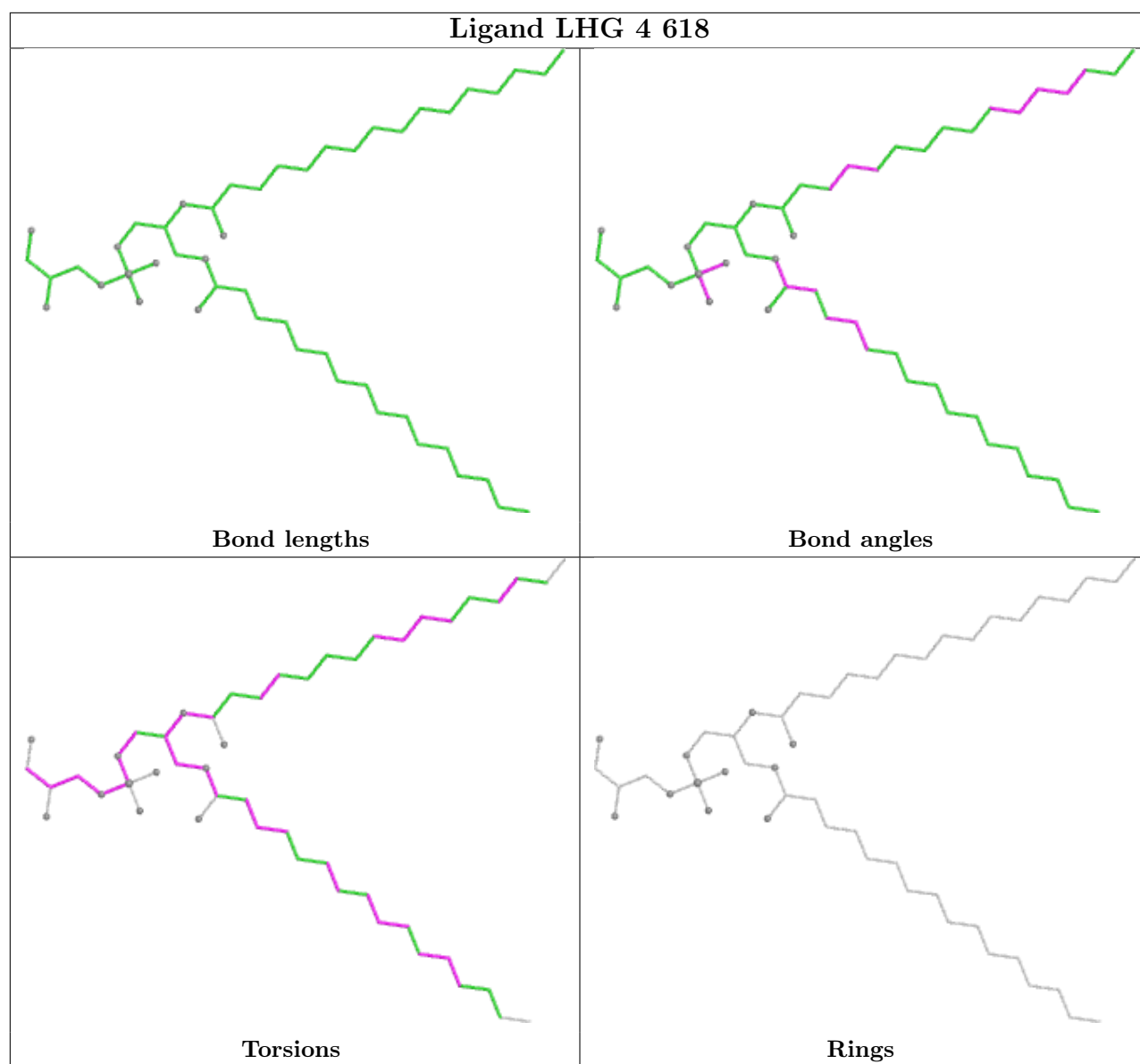
Ligand II0 b 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

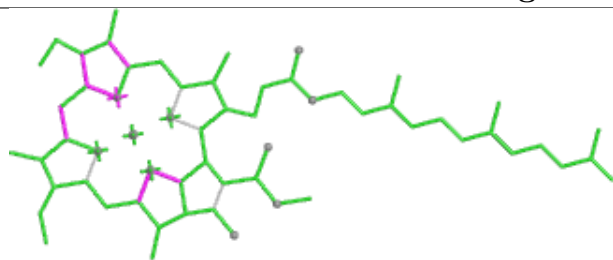
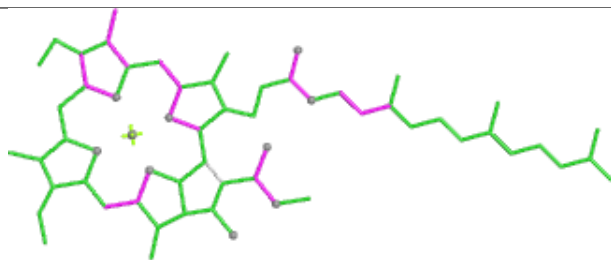
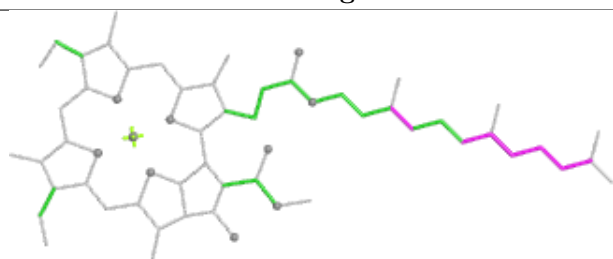
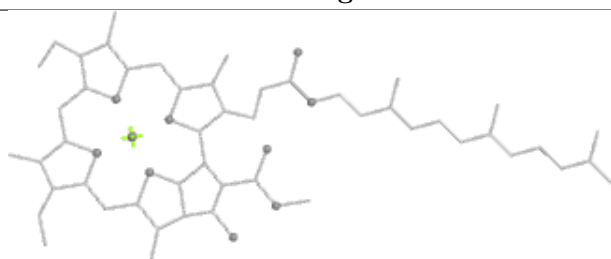
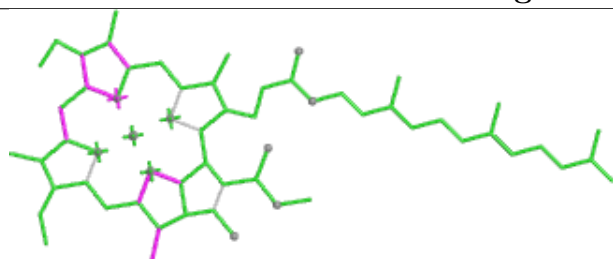
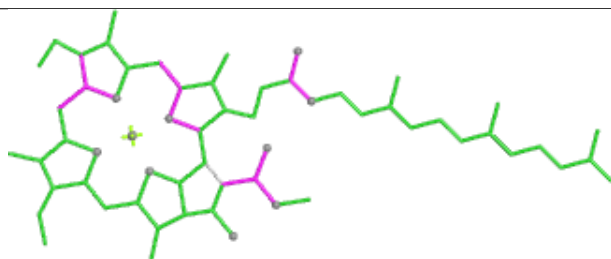
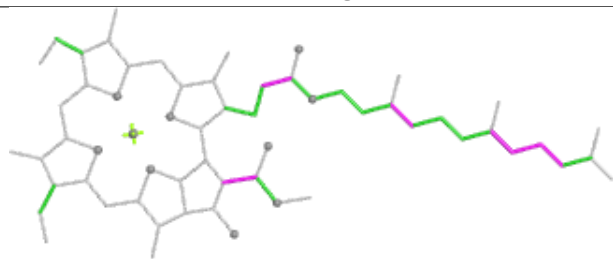
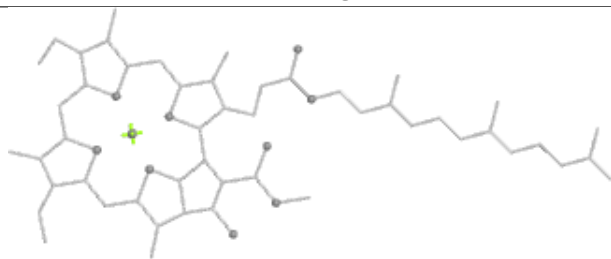
Ligand 8CT J 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

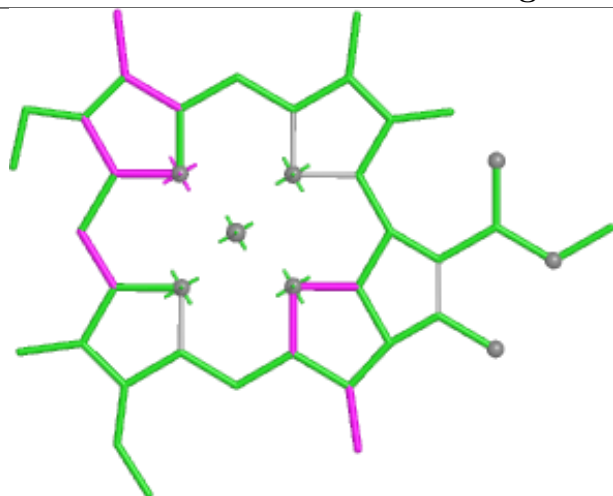




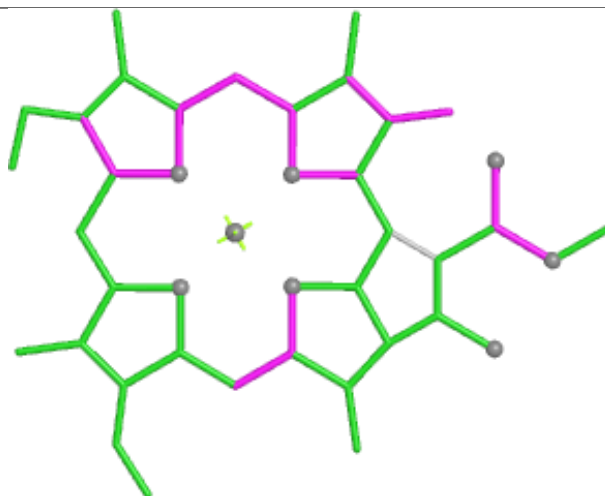


Ligand CLA 1 608**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 822****Bond lengths****Bond angles****Torsions****Rings**

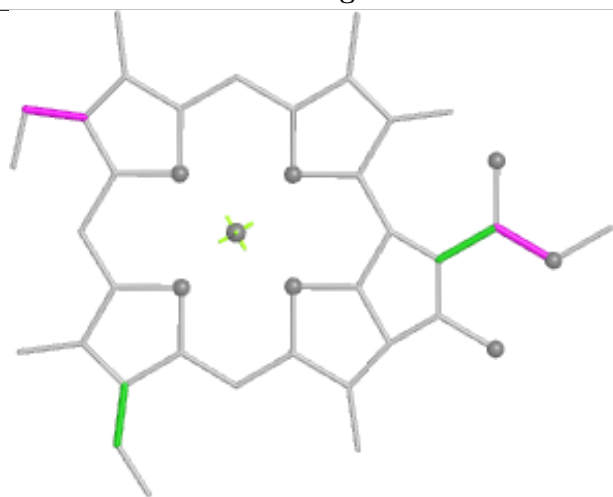
Ligand CLA e 608



Bond lengths



Bond angles

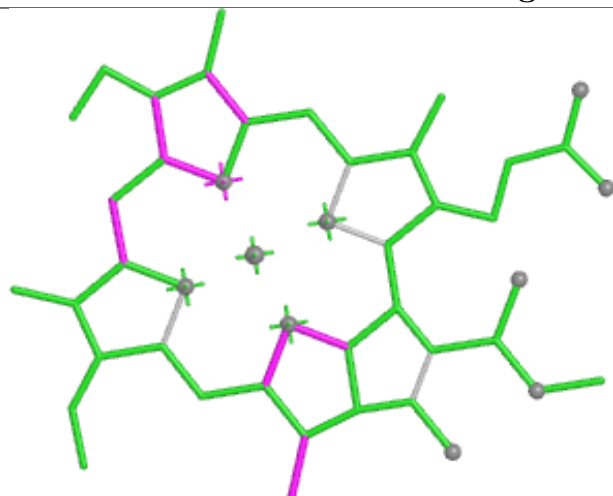


Torsions

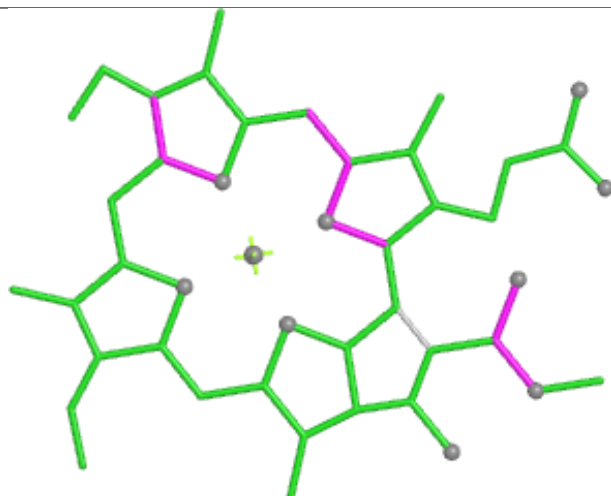


Rings

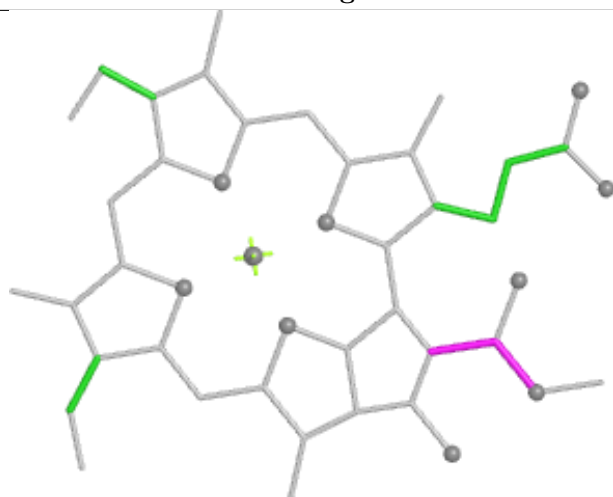
Ligand CLA 7 302



Bond lengths



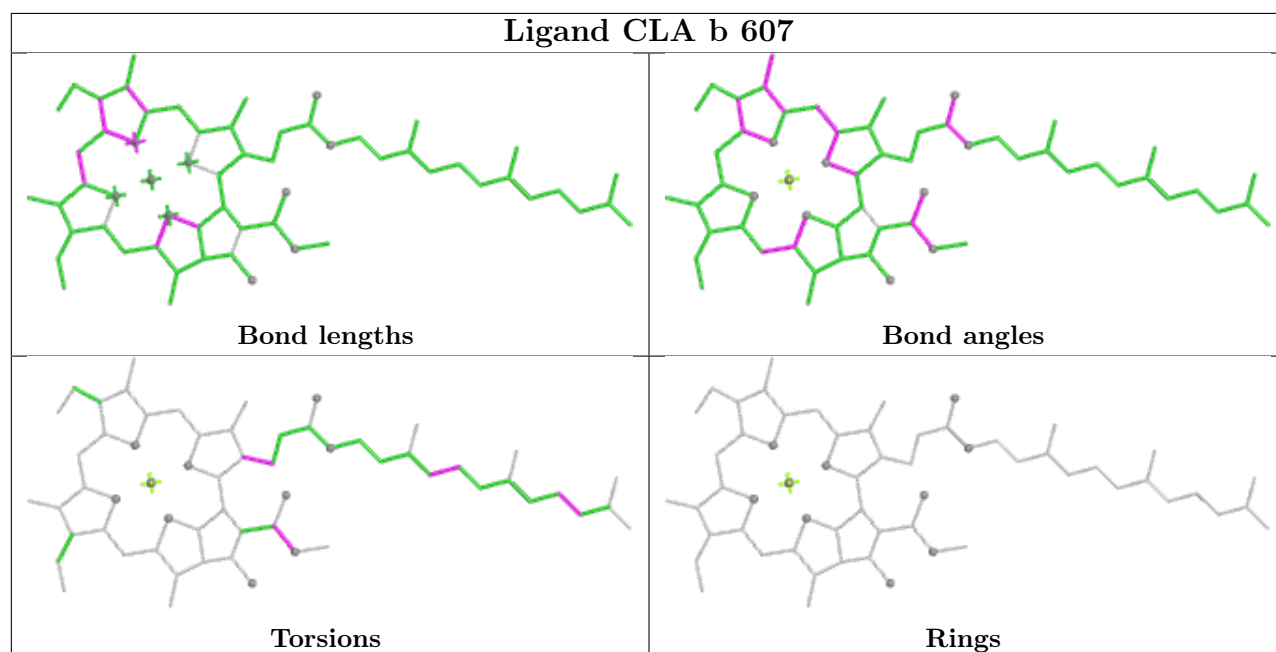
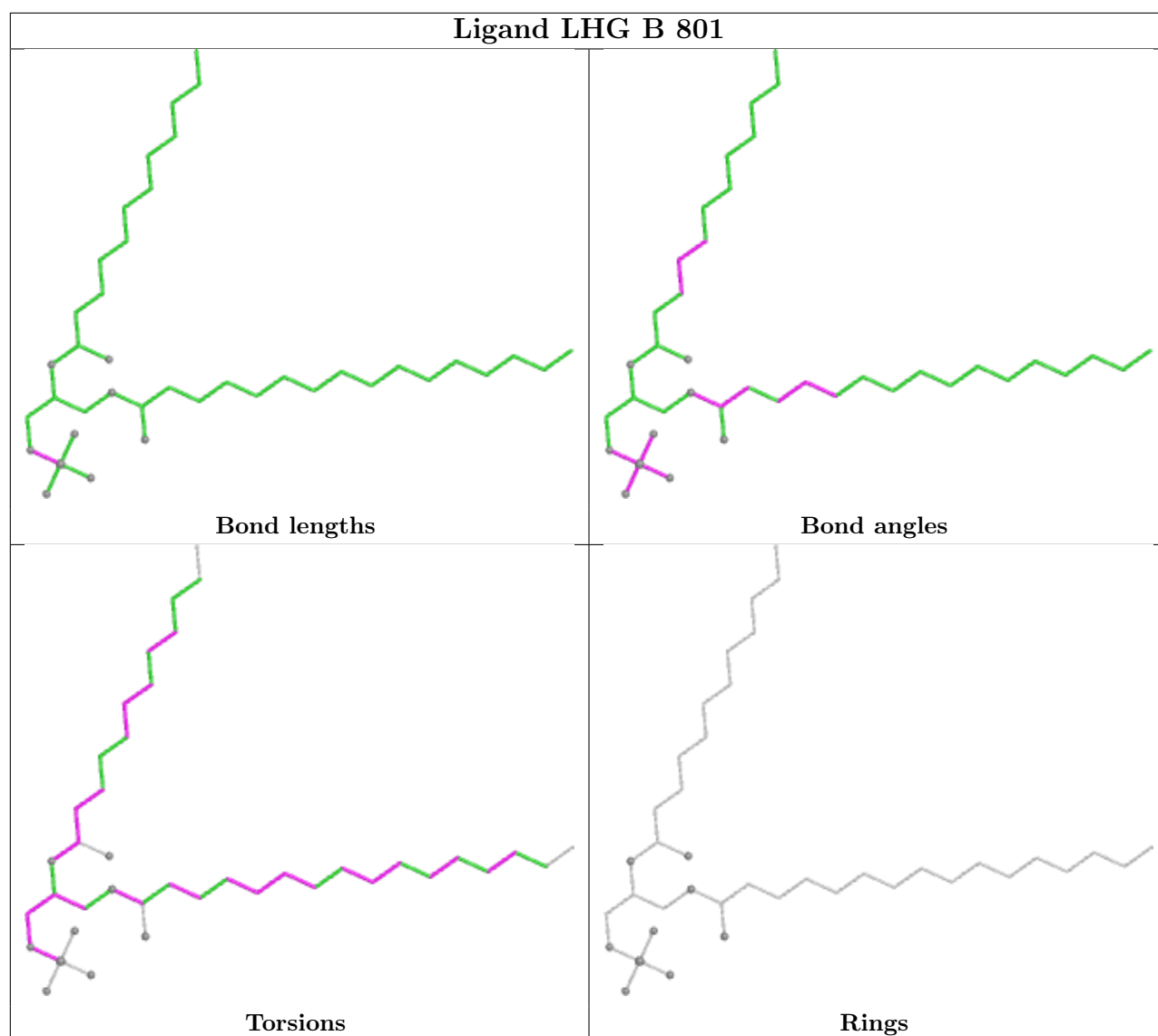
Bond angles



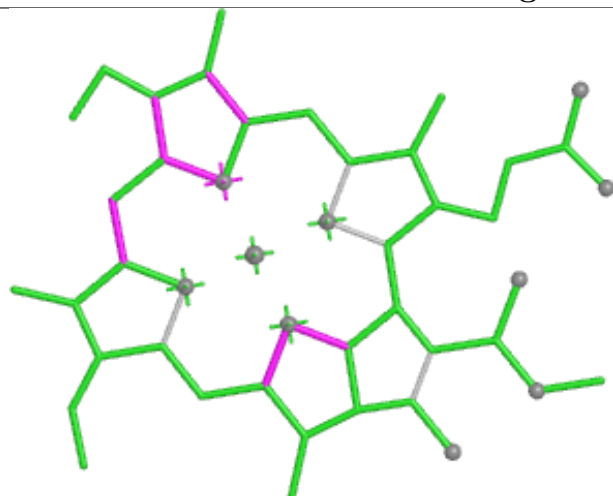
Torsions



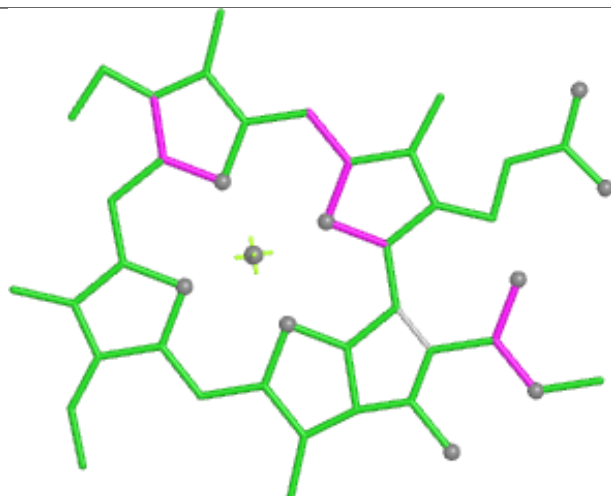
Rings



Ligand CLA c 613



Bond lengths



Bond angles

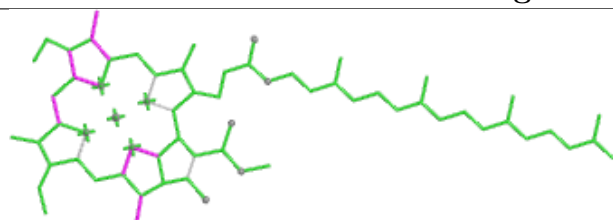


Torsions

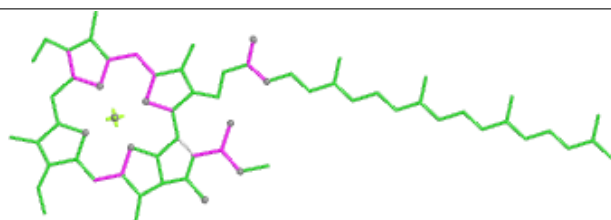


Rings

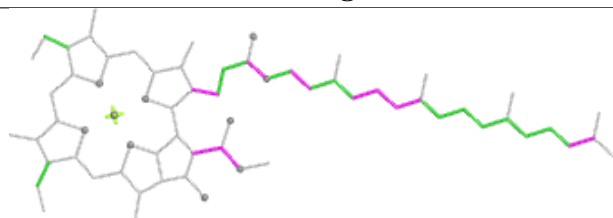
Ligand CLA A 810



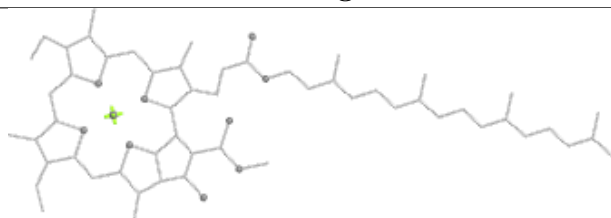
Bond lengths



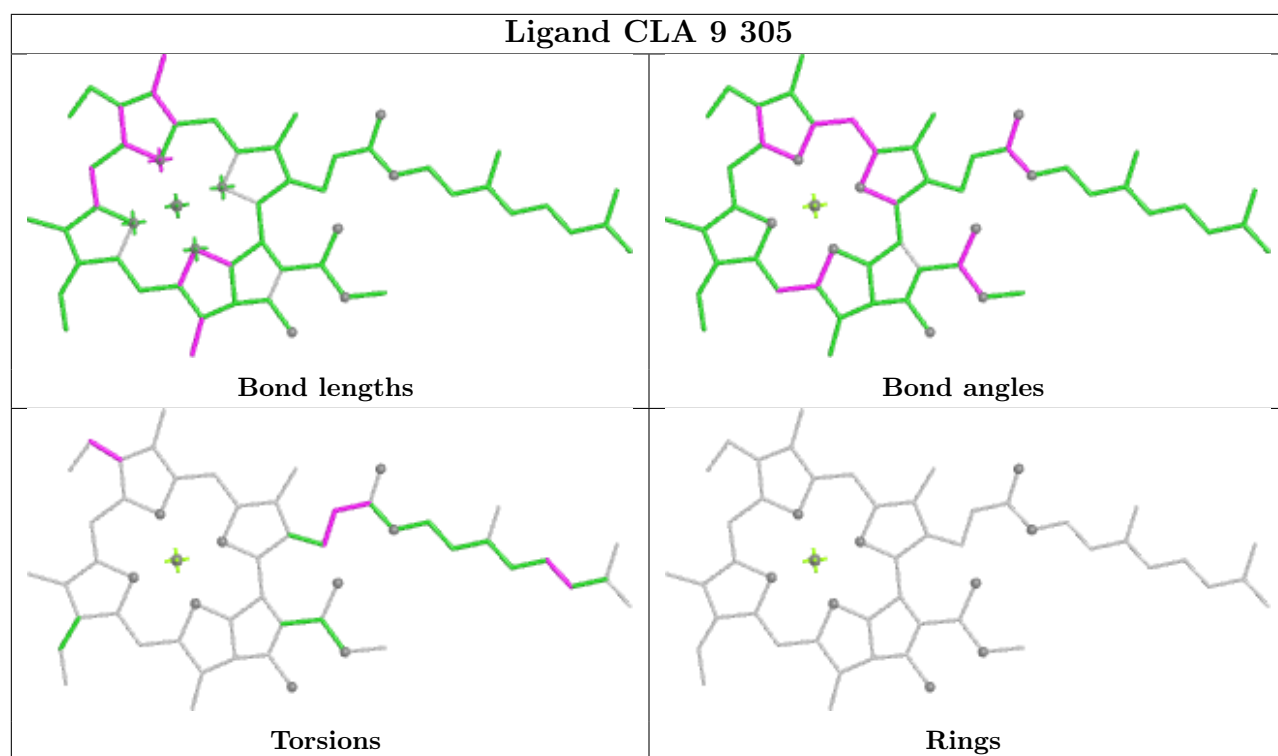
Bond angles



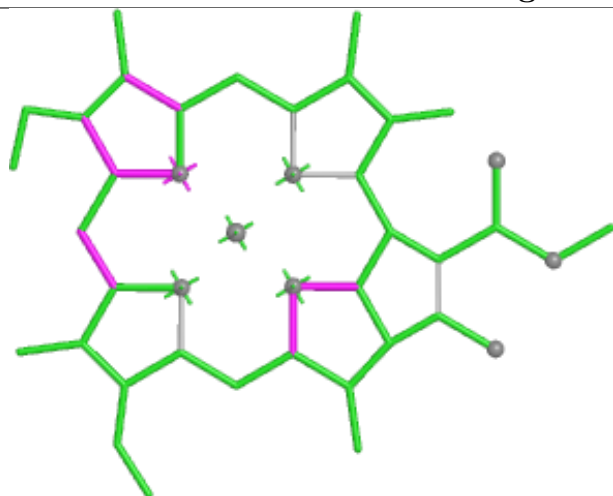
Torsions



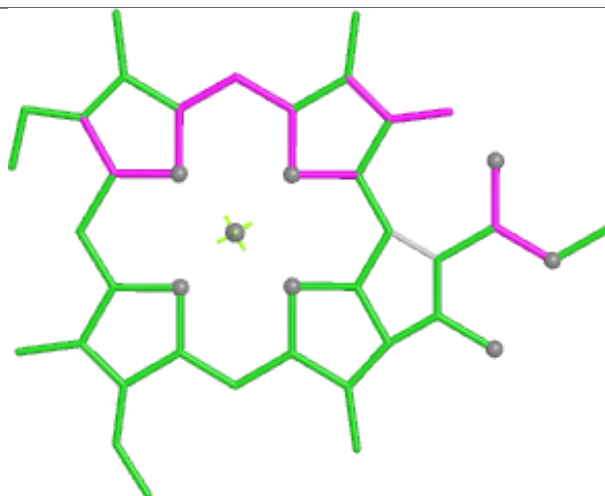
Rings



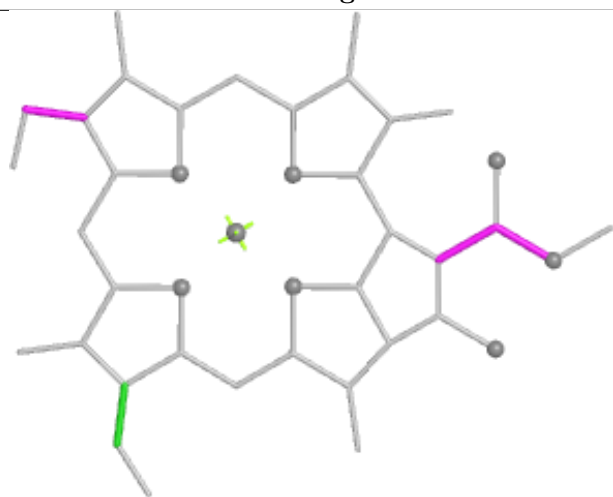
Ligand CLA 9 310



Bond lengths



Bond angles

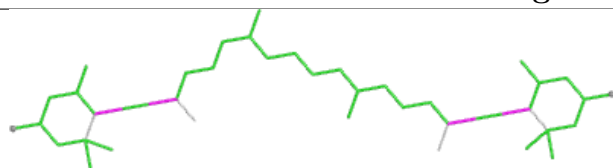


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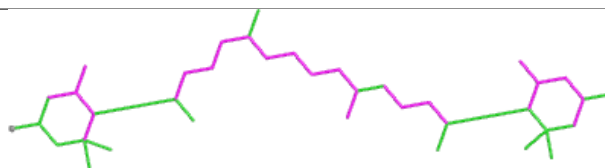


Rings

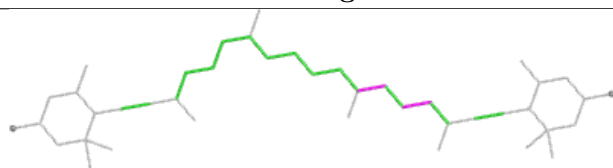
Ligand II0 5 620



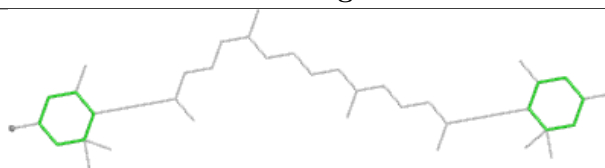
Bond lengths



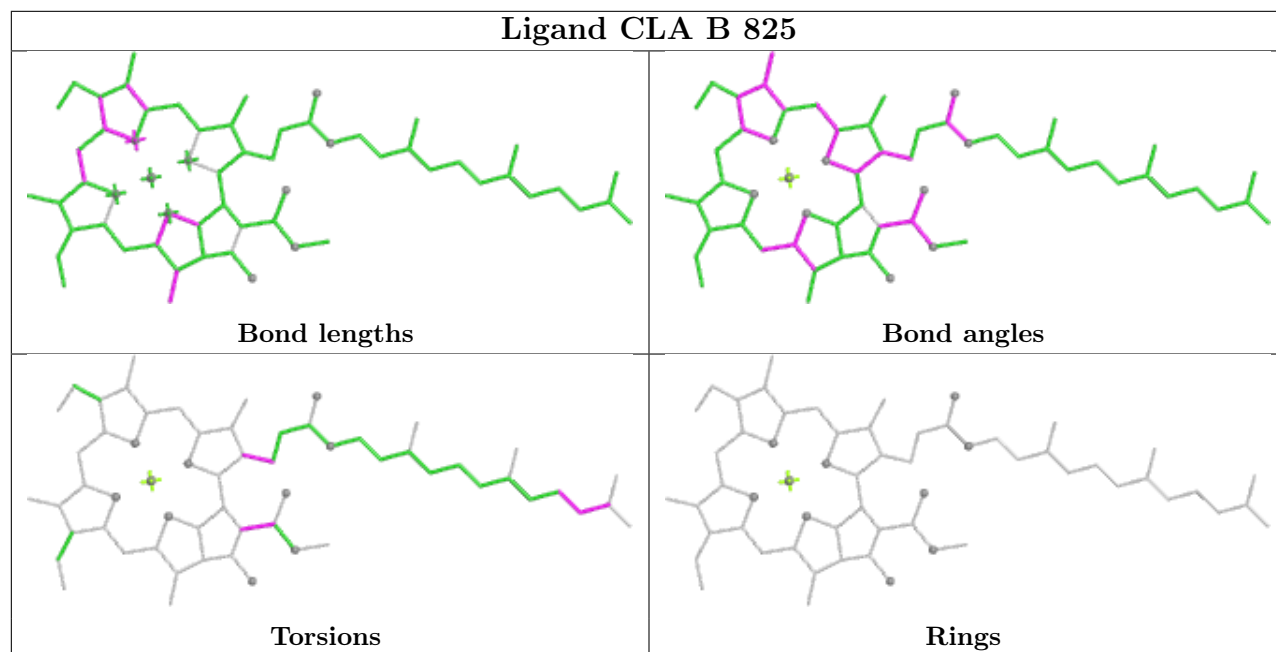
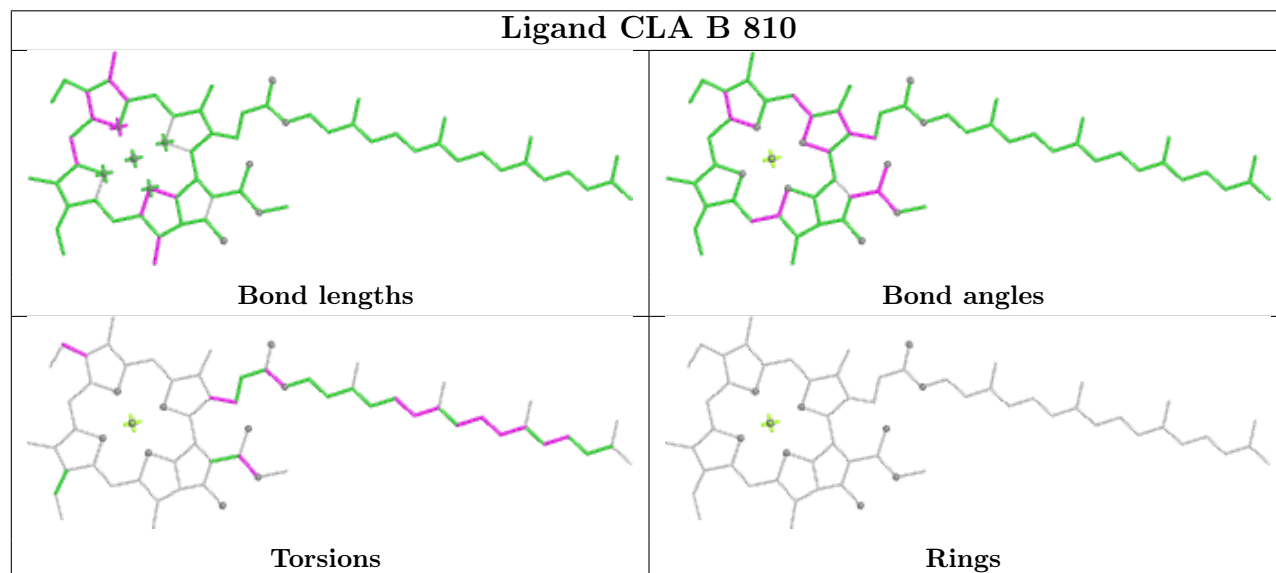
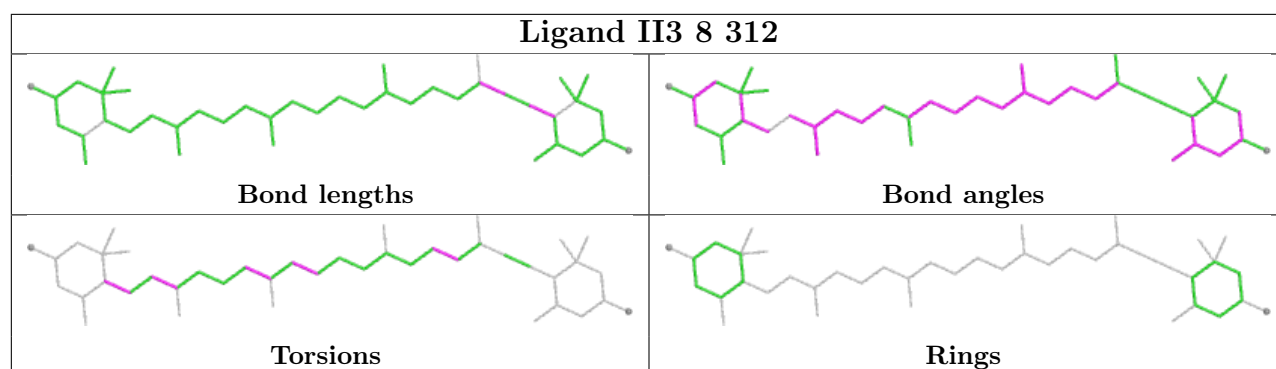
Bond angles



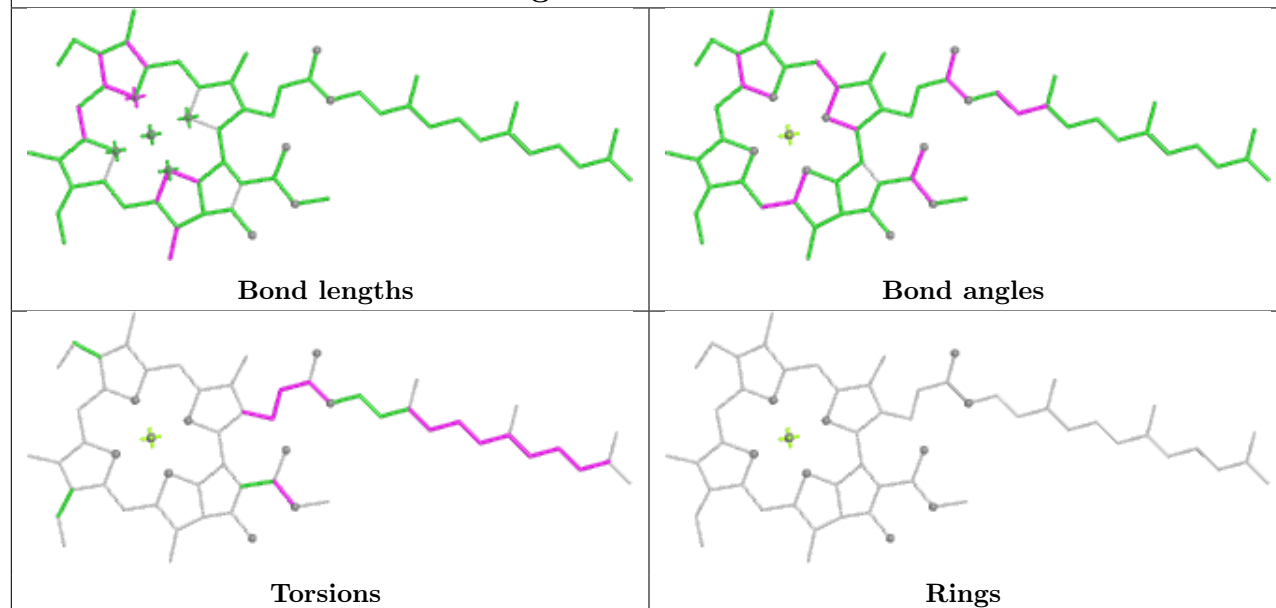
Torsions



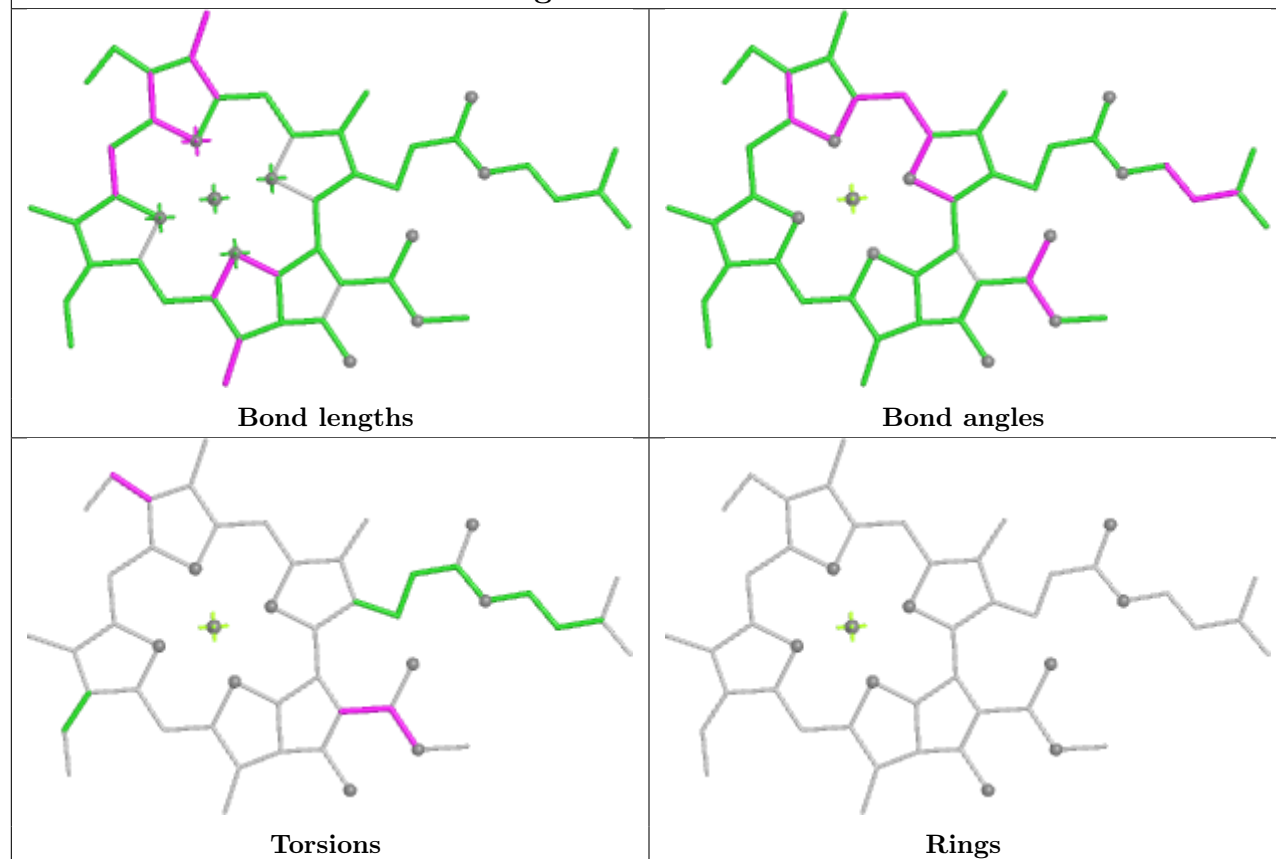
Rings

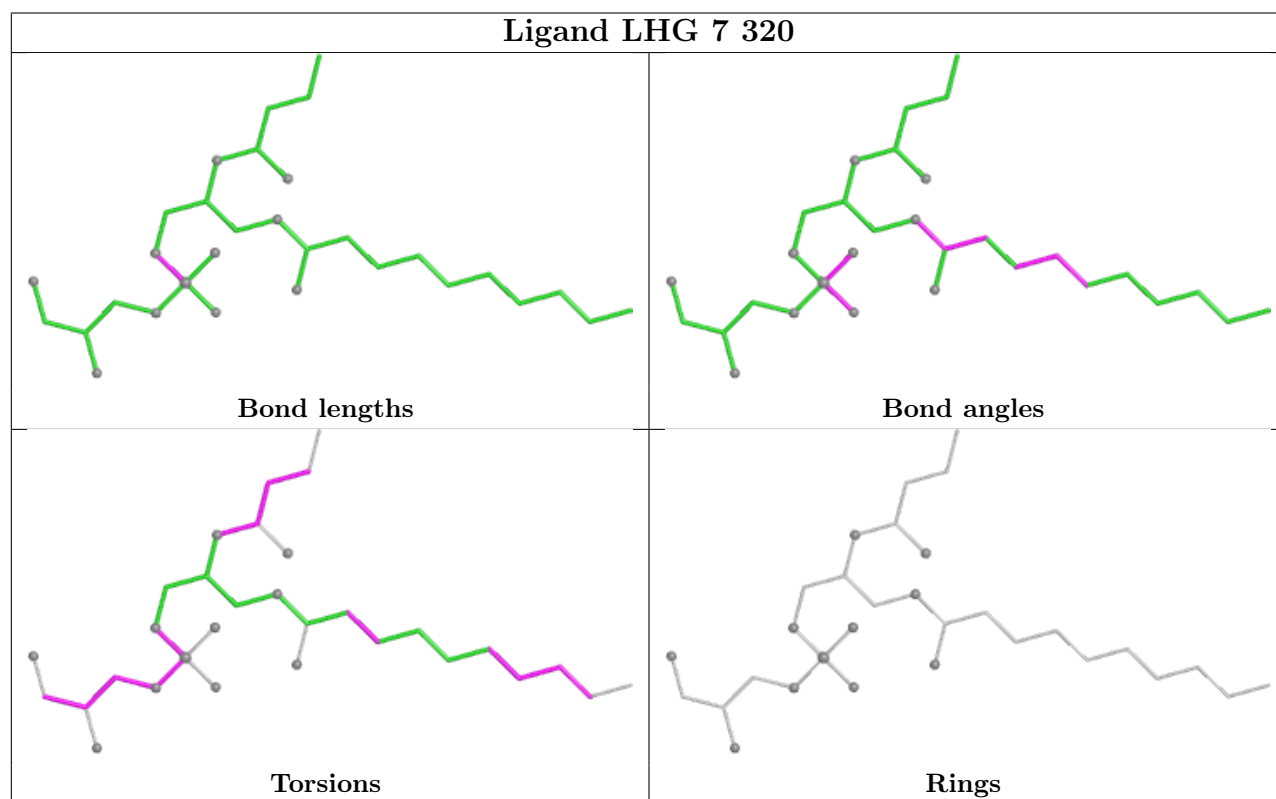
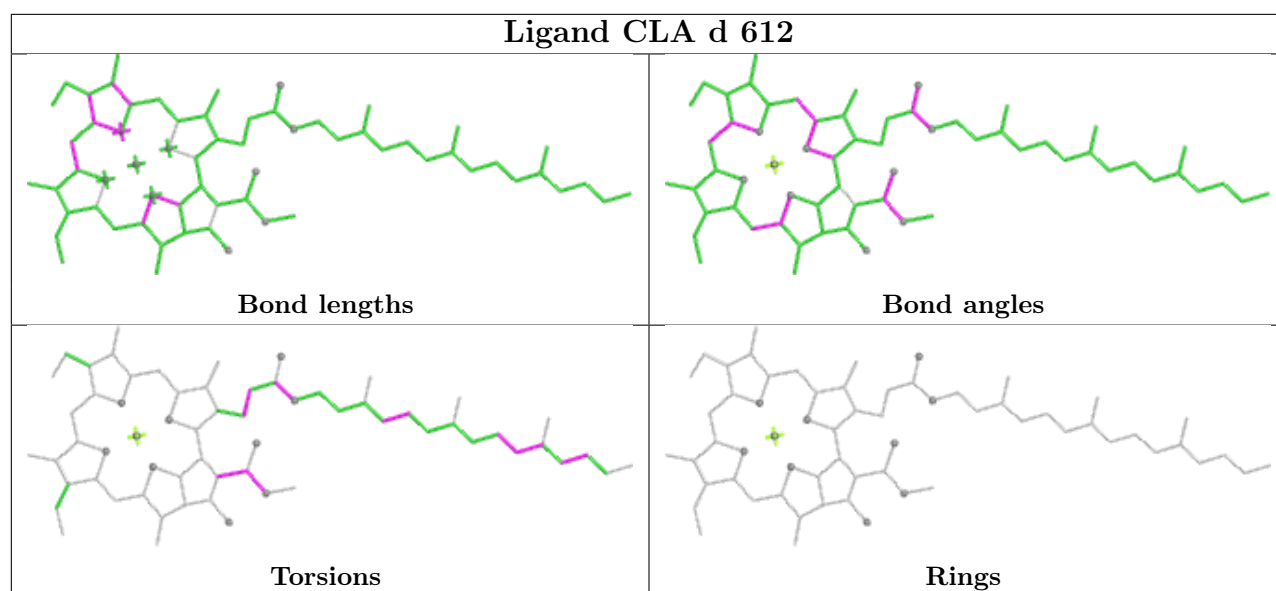


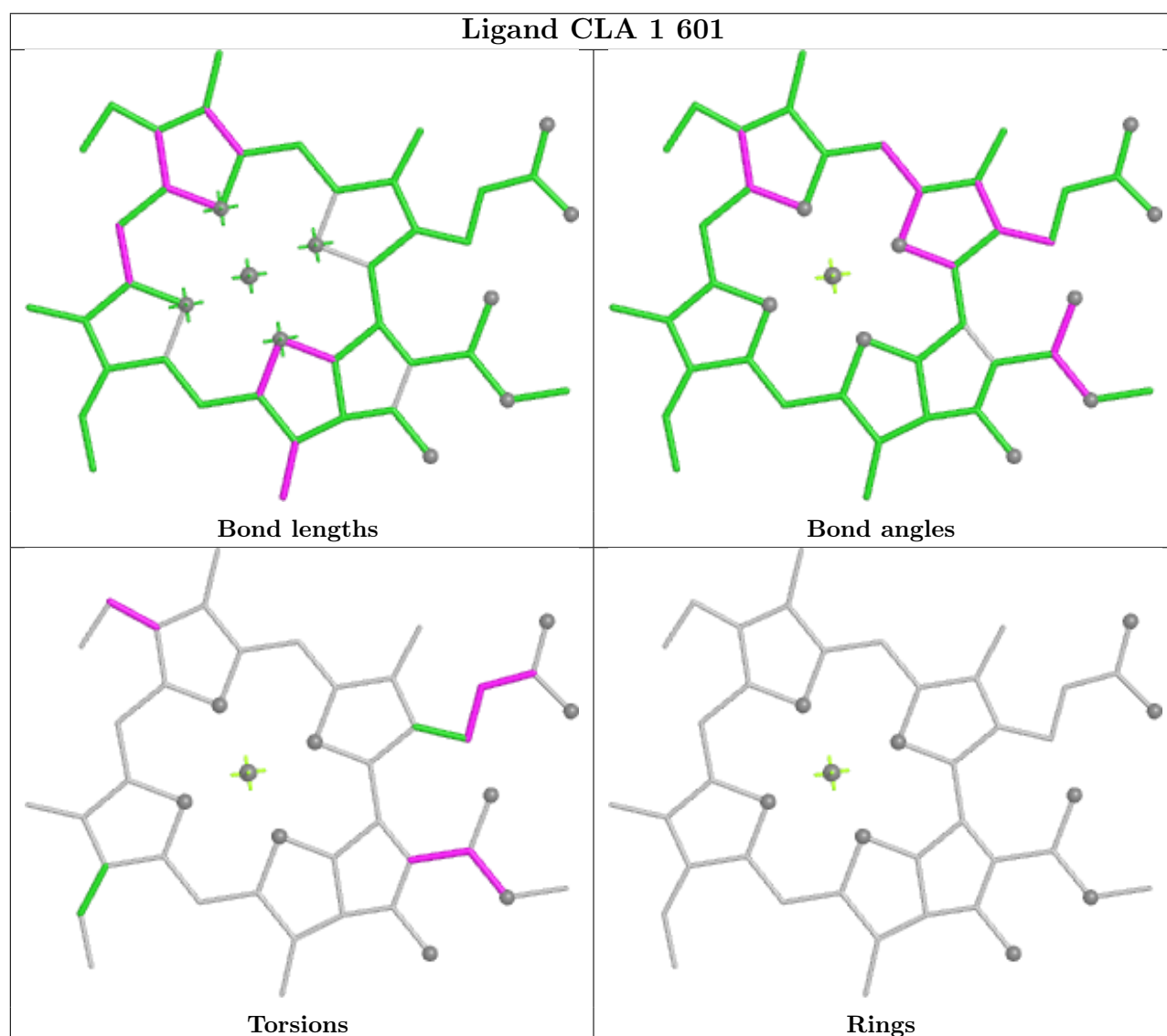
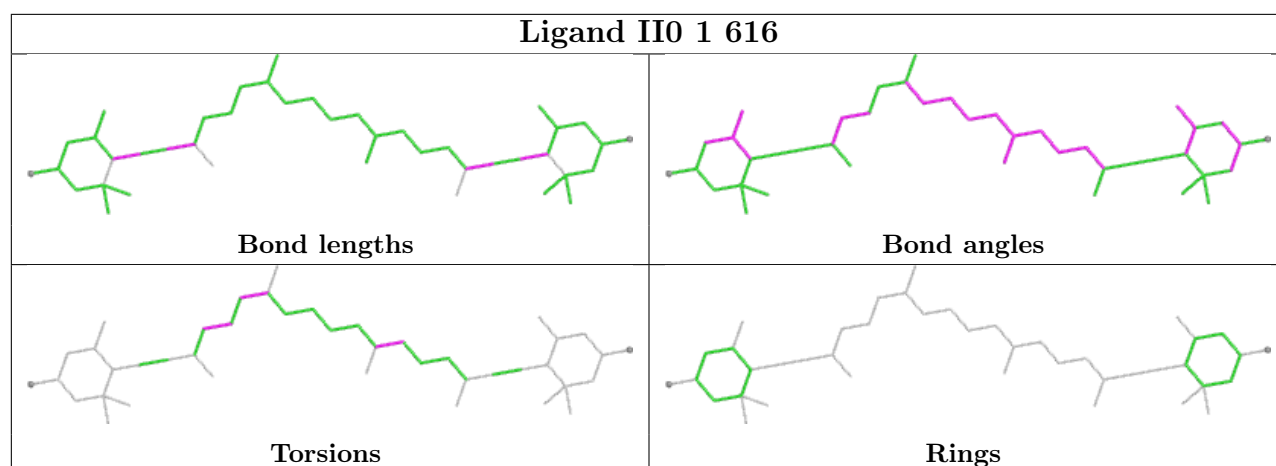
Ligand CLA A 816



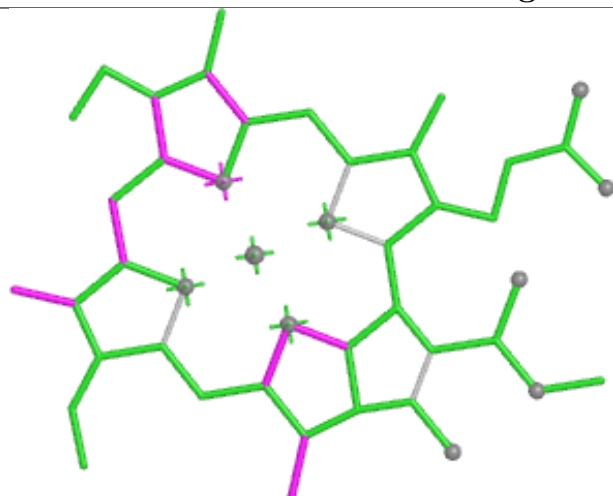
Ligand CLA Z 304



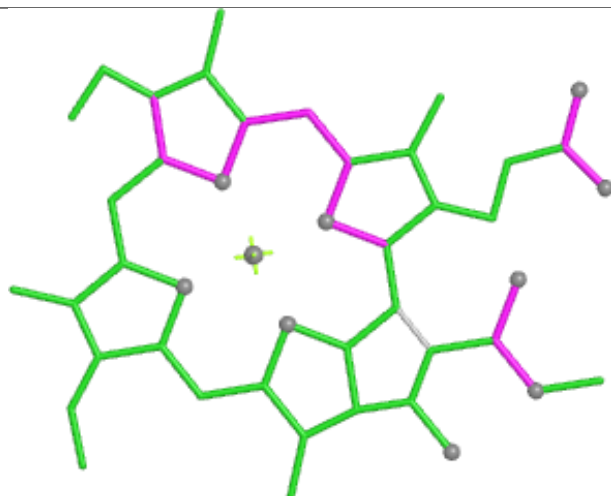




Ligand CLA 8 301



Bond lengths



Bond angles

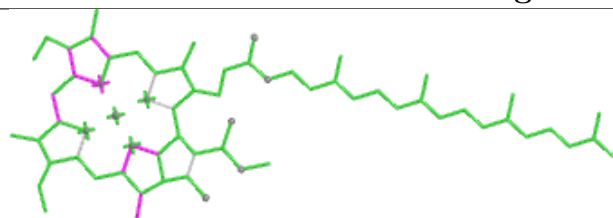


Torsions

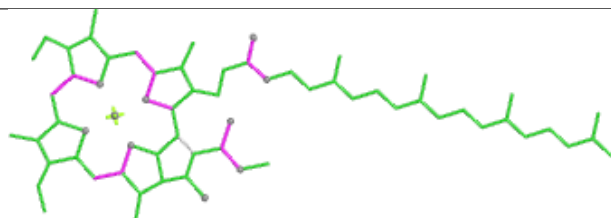


Rings

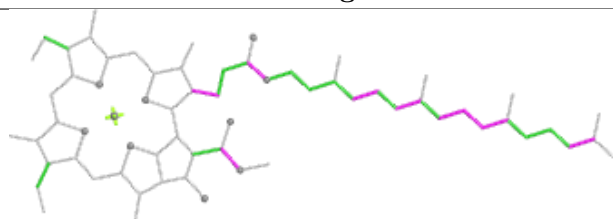
Ligand CLA B 827



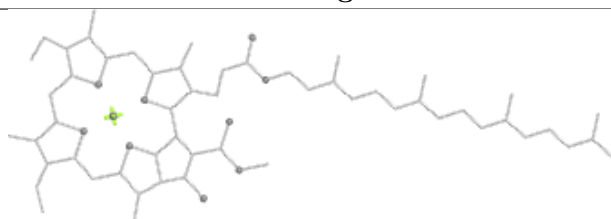
Bond lengths



Bond angles

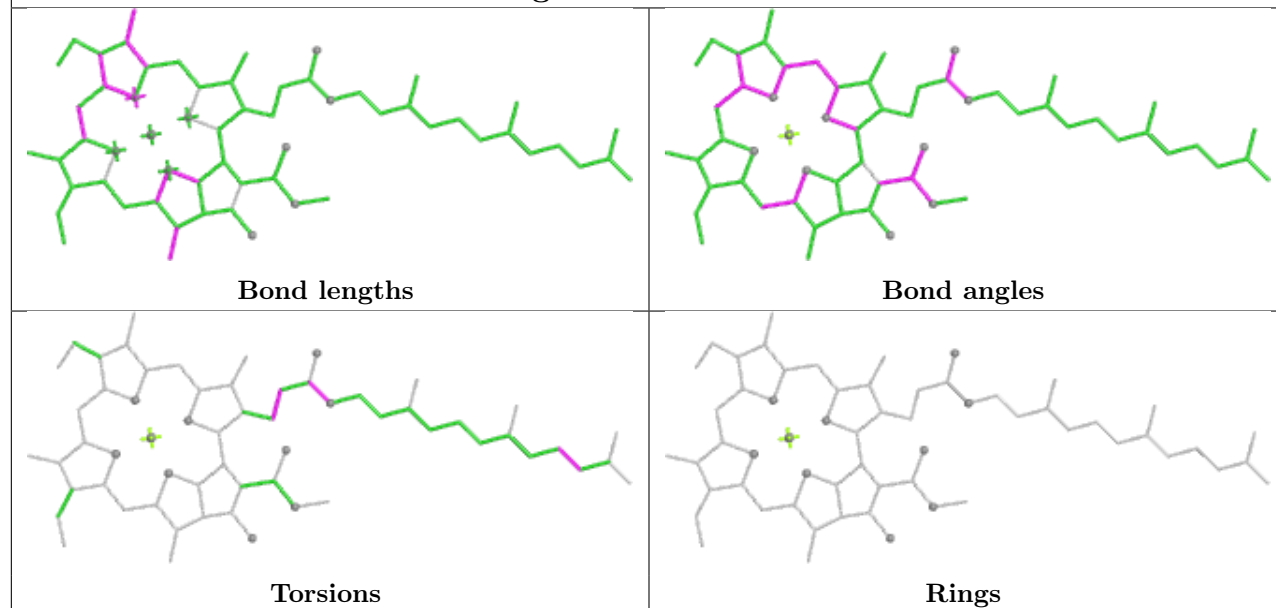


Torsions

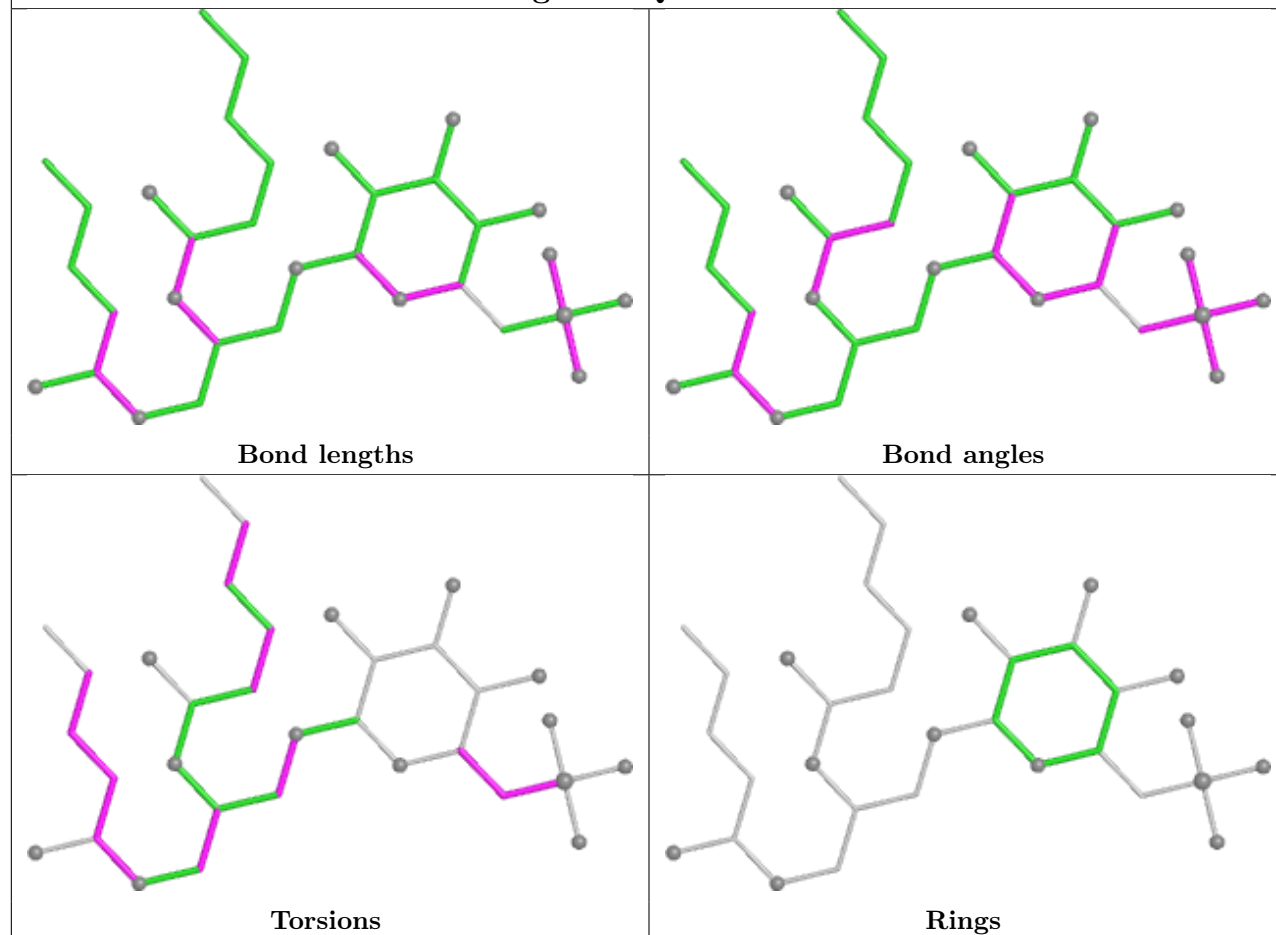


Rings

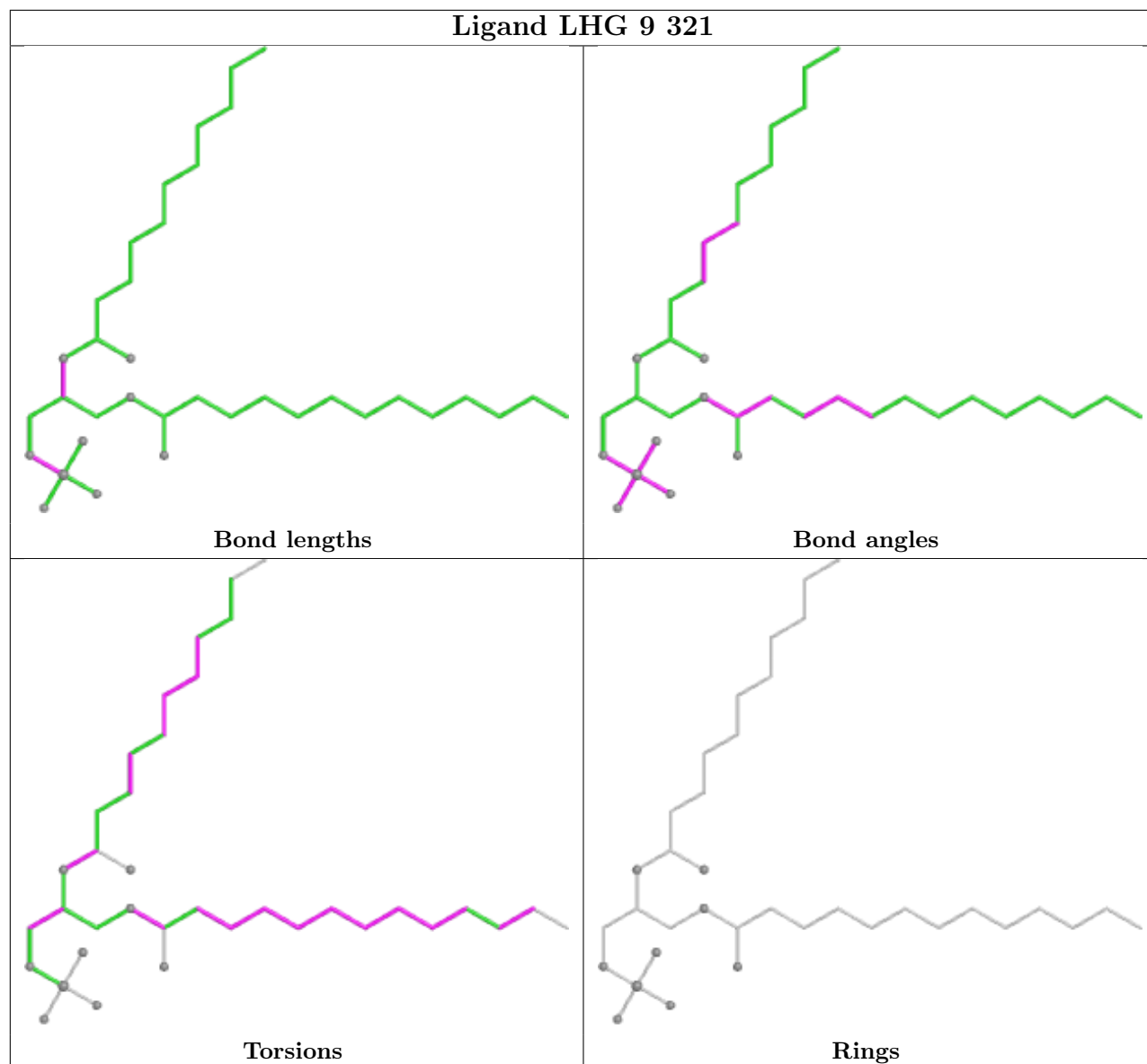
Ligand CLA B 818



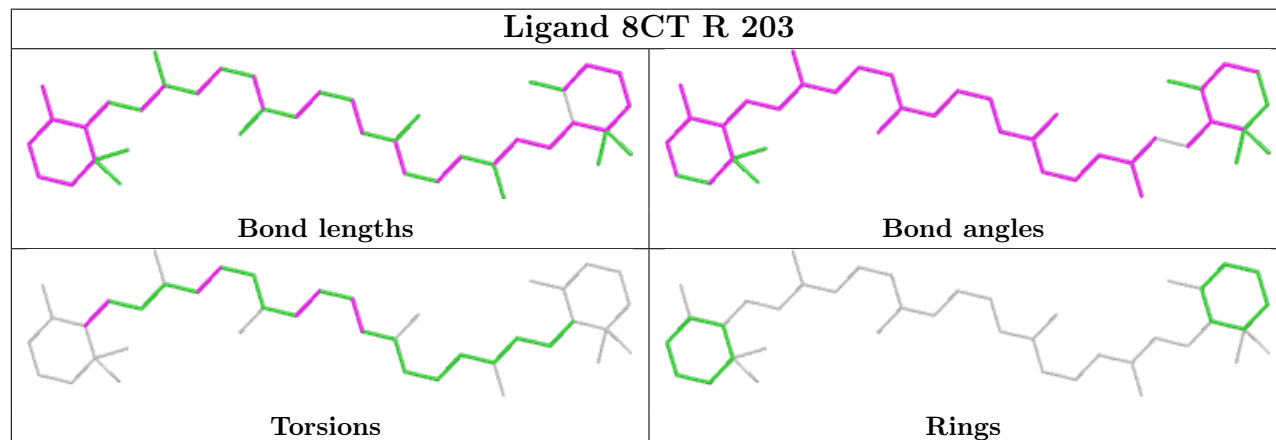
Ligand SQD B 850

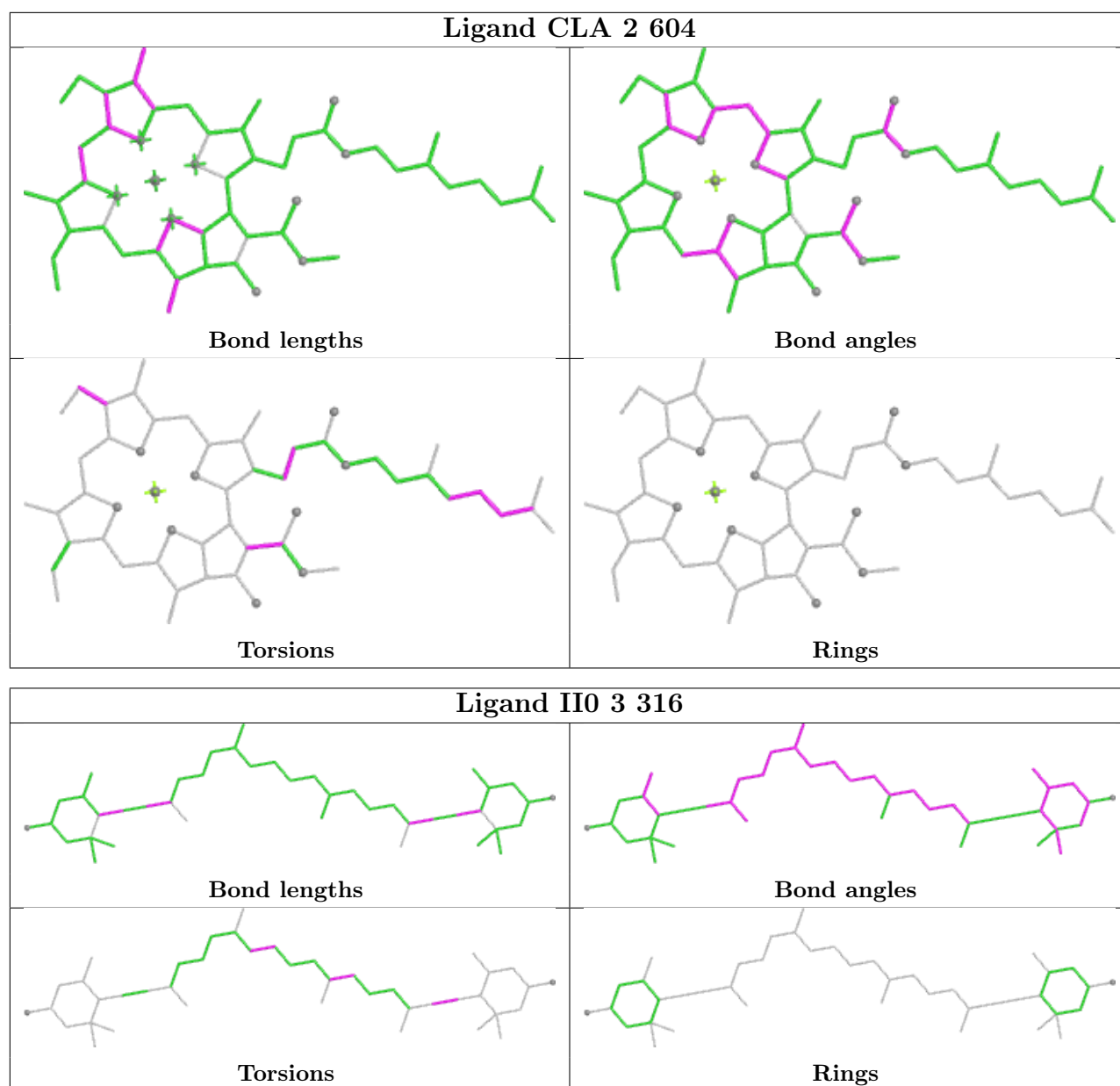


Ligand LHG 9 321

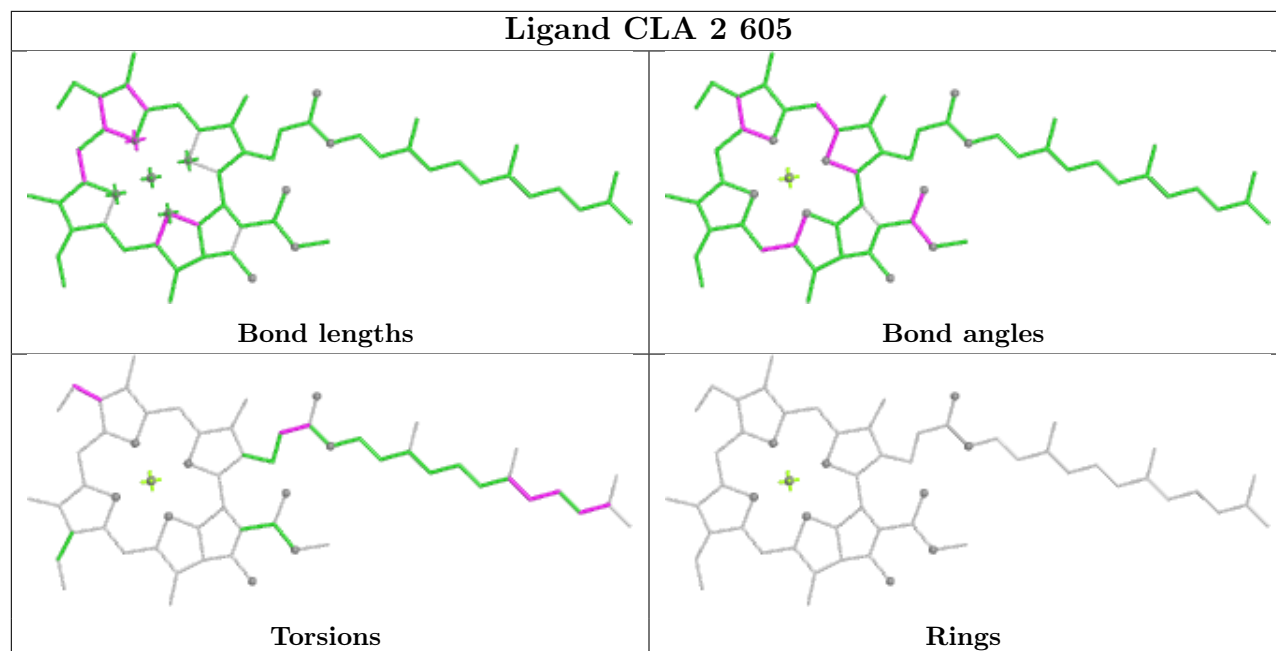


Ligand 8CT R 203

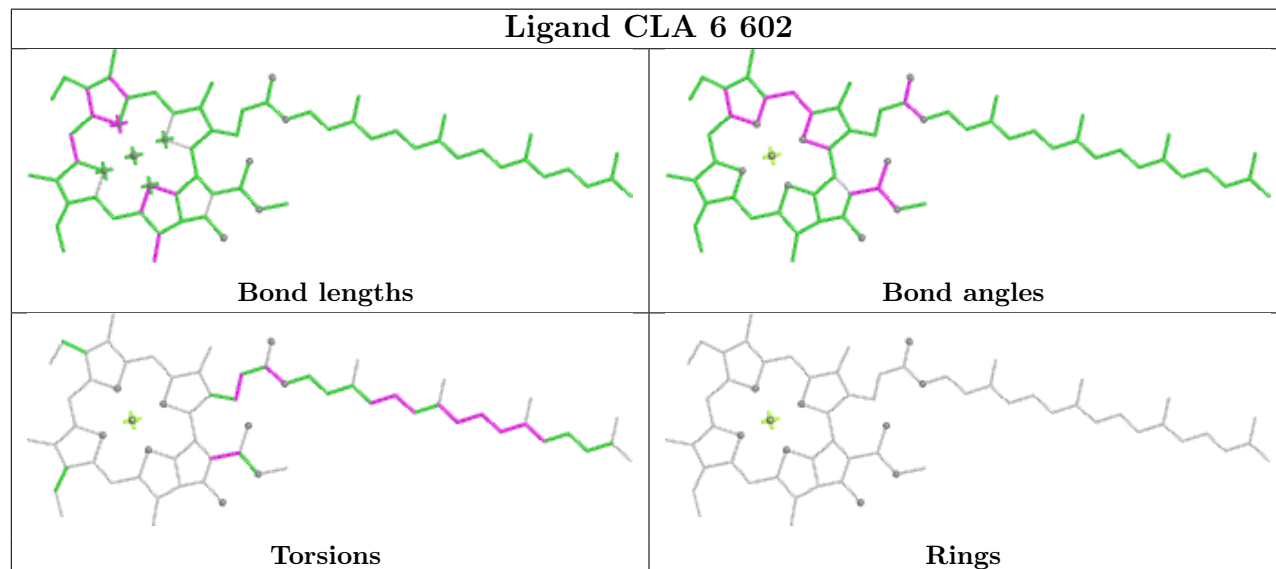




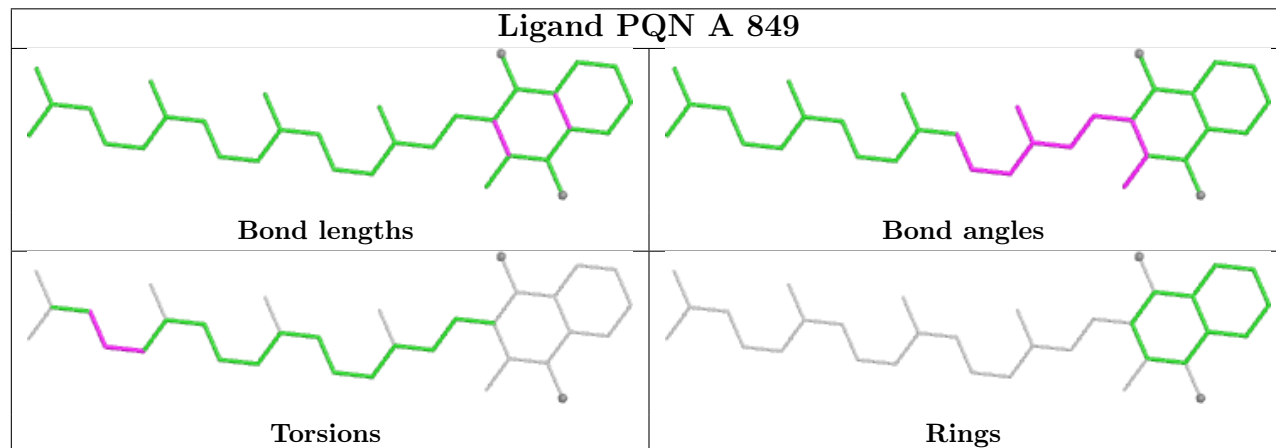
Ligand CLA 2 605

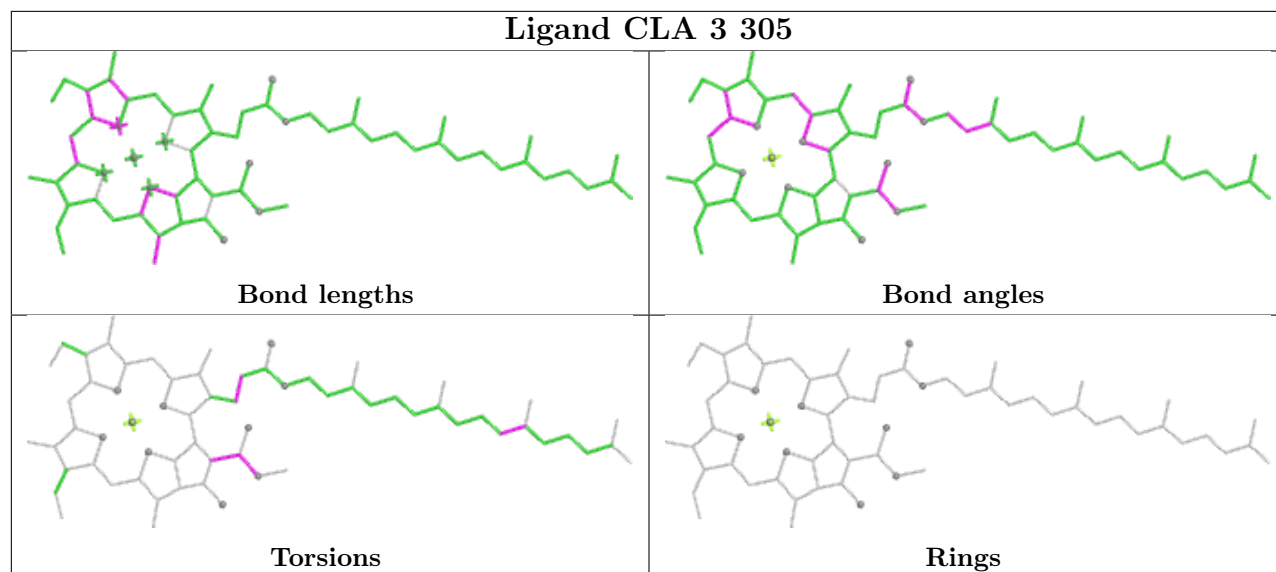
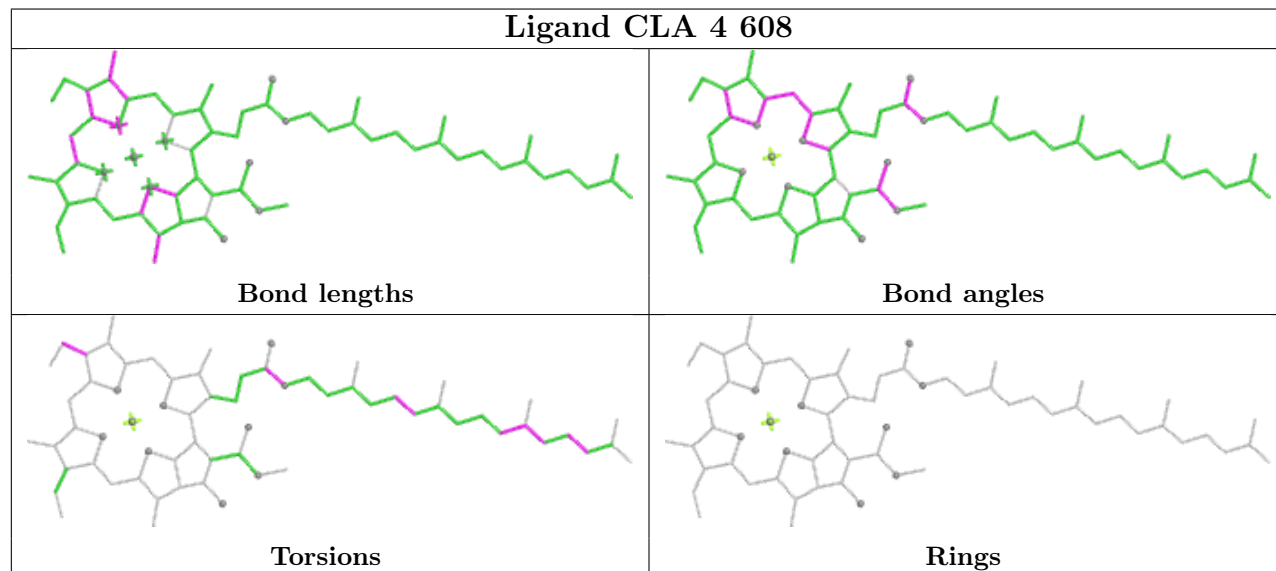


Ligand CLA 6 602

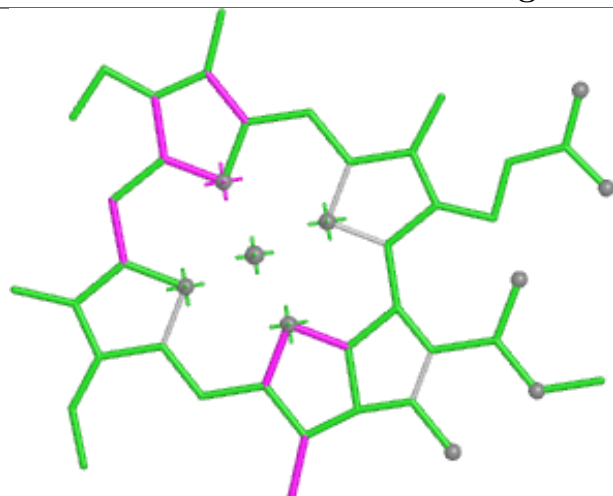


Ligand PQN A 849

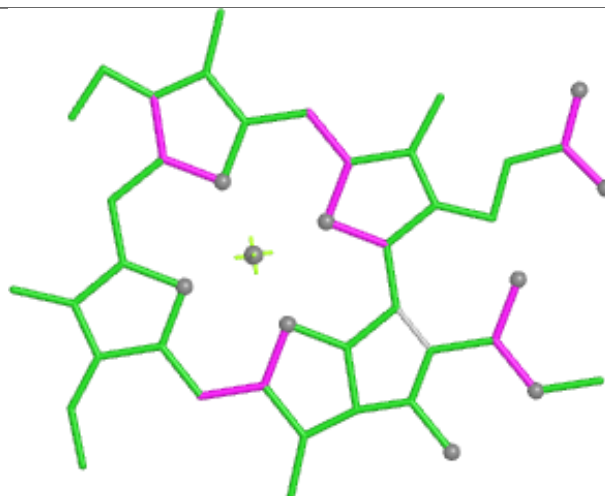


Ligand CLA 3 305**Ligand CLA 4 608**

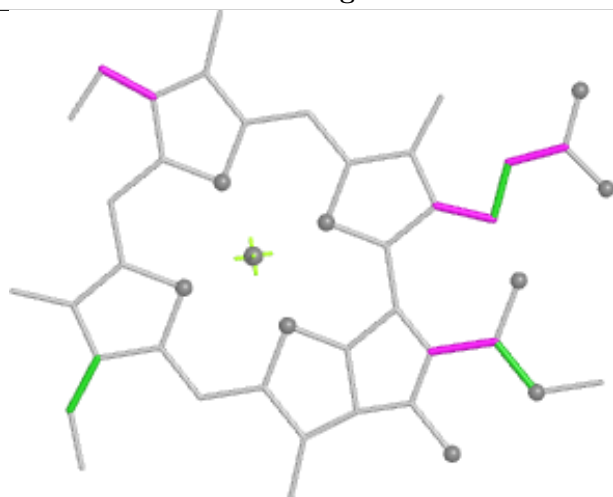
Ligand CLA 6 612



Bond lengths



Bond angles

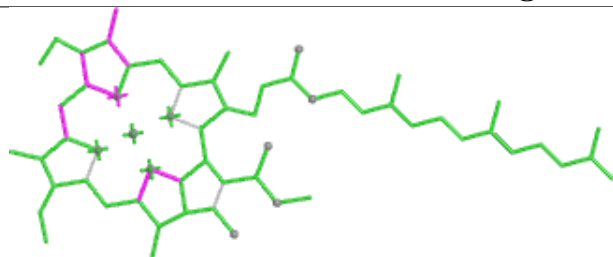


Torsions

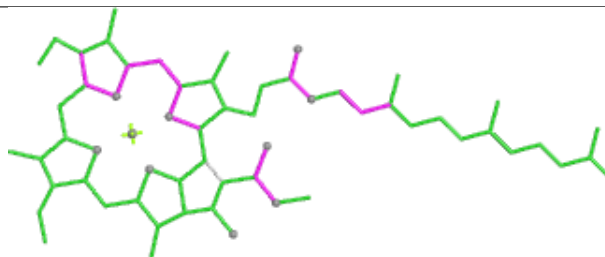


Rings

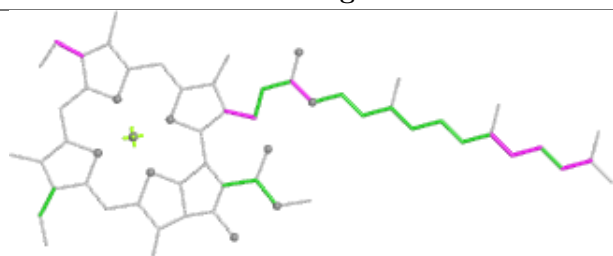
Ligand CLA a 609



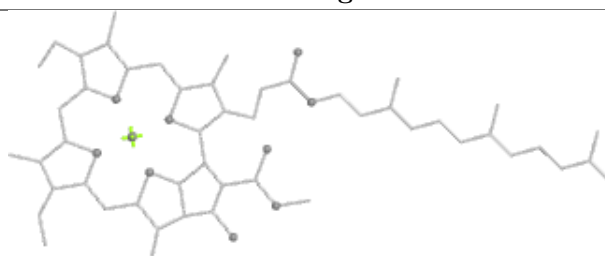
Bond lengths



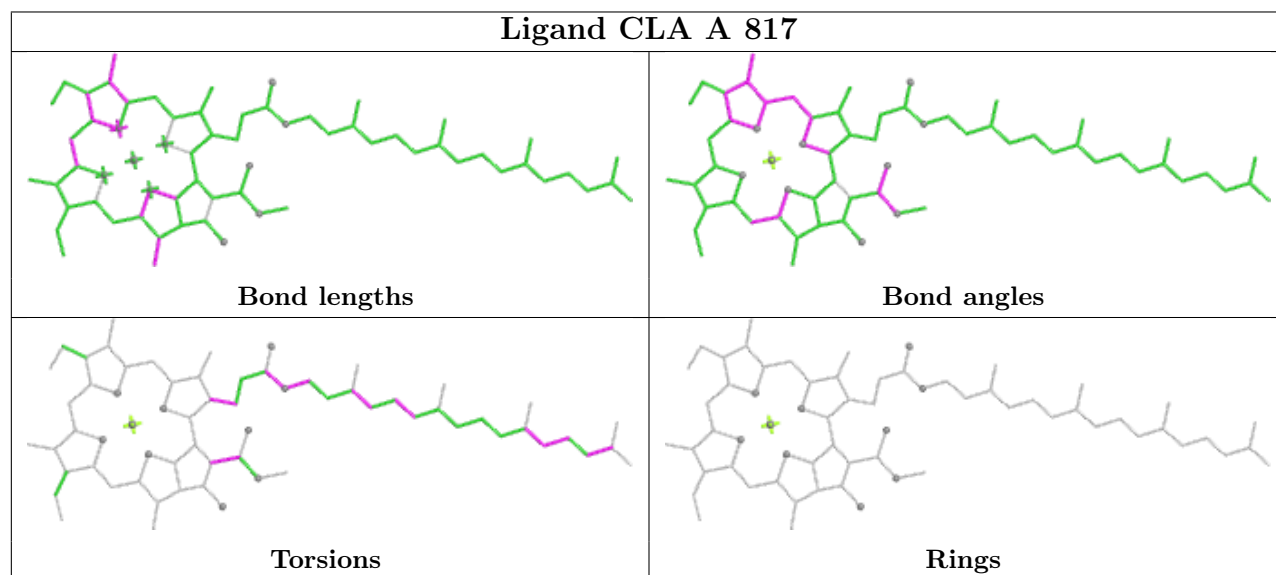
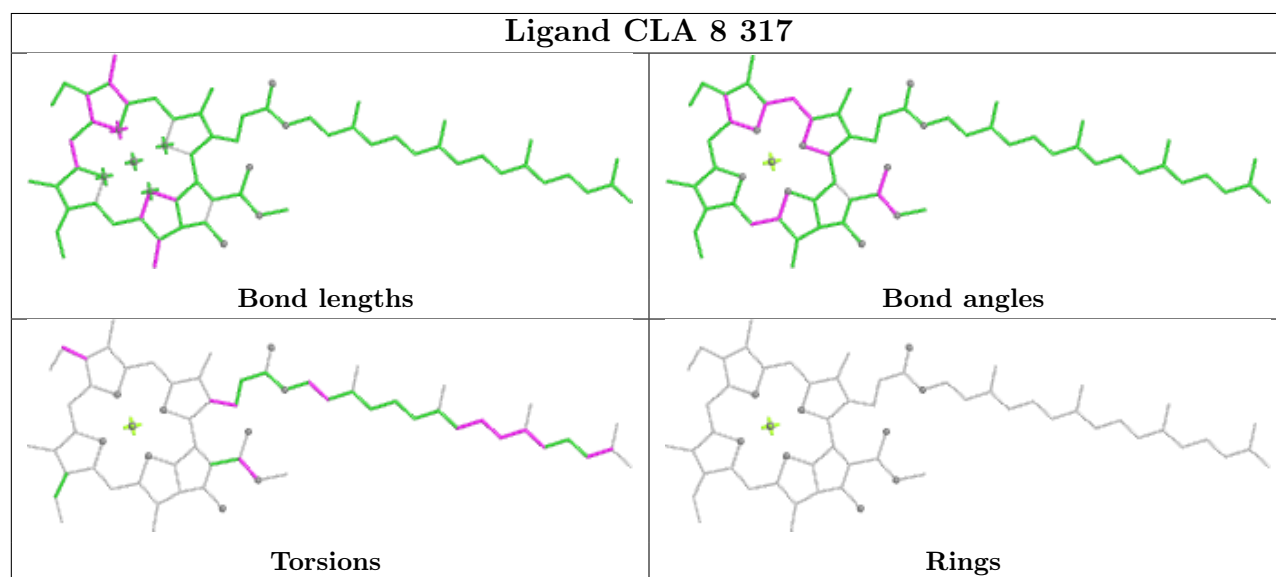
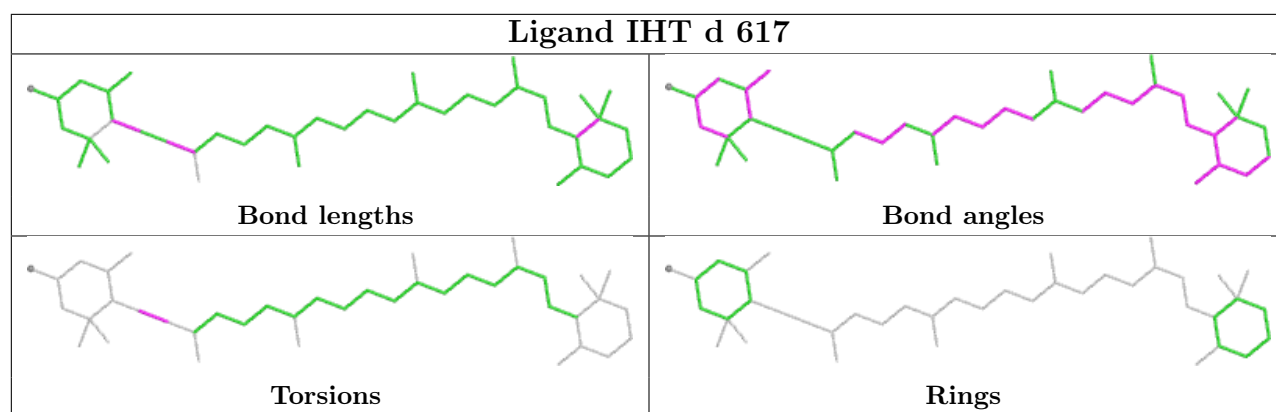
Bond angles

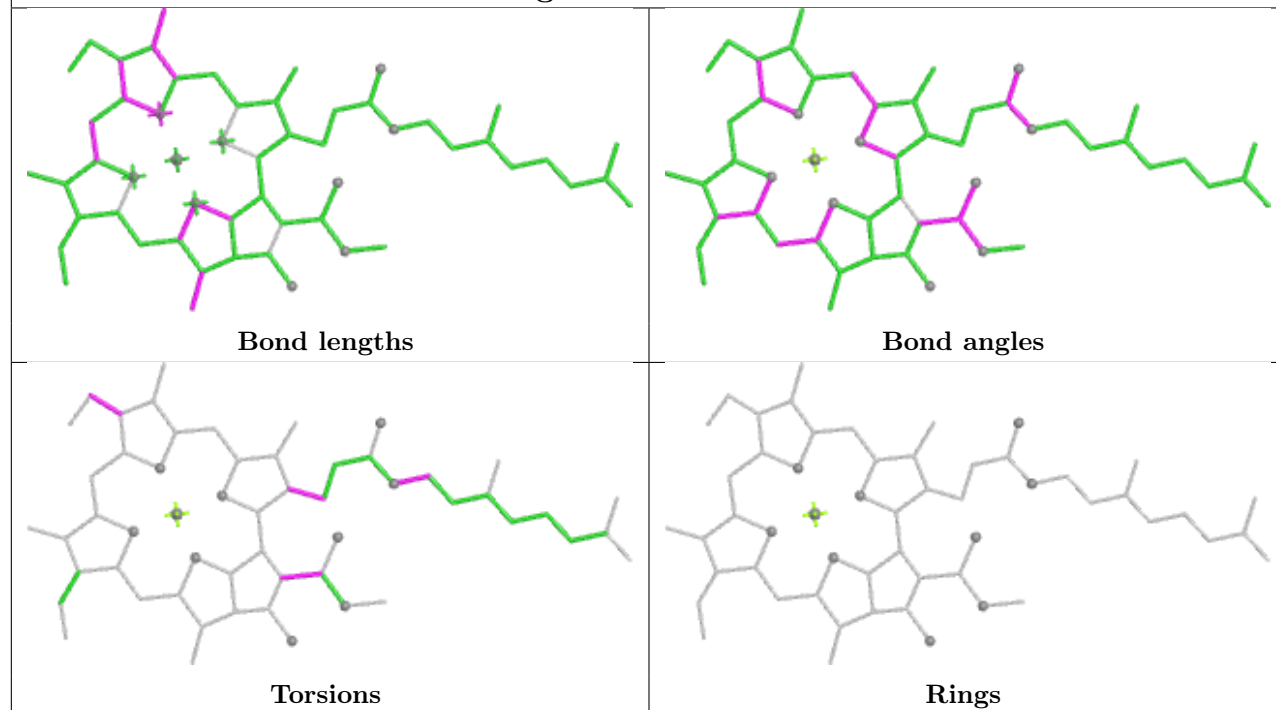
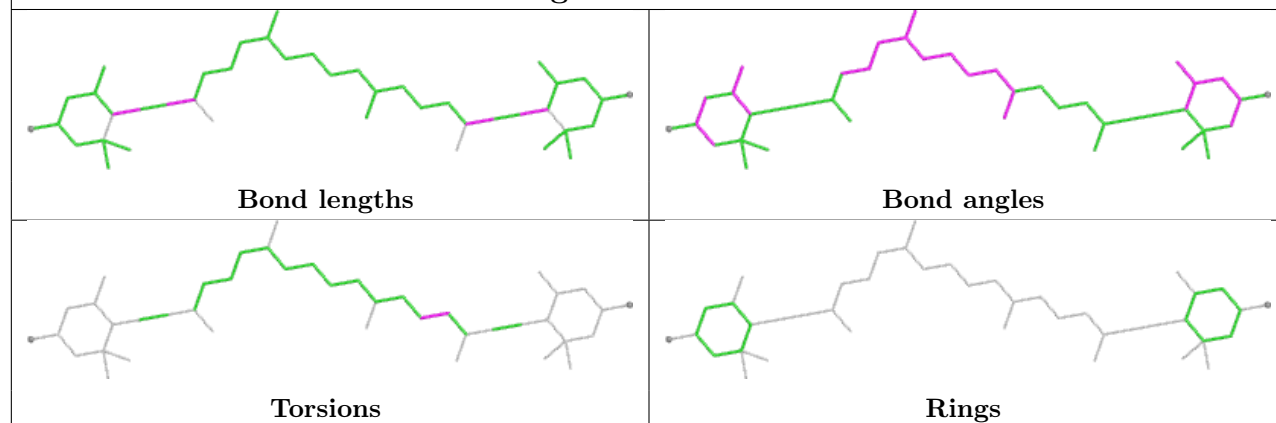


Torsions

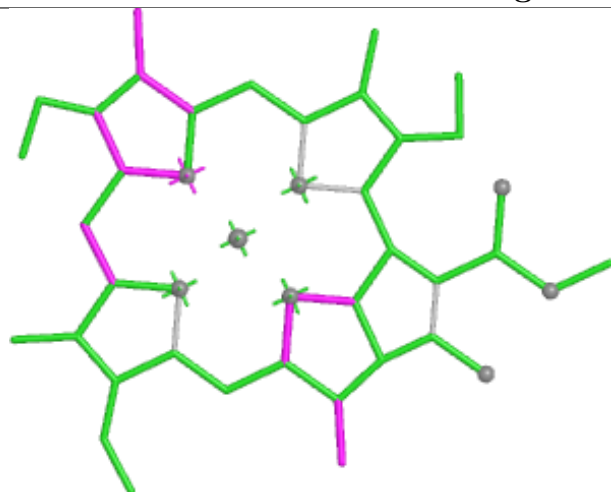


Rings

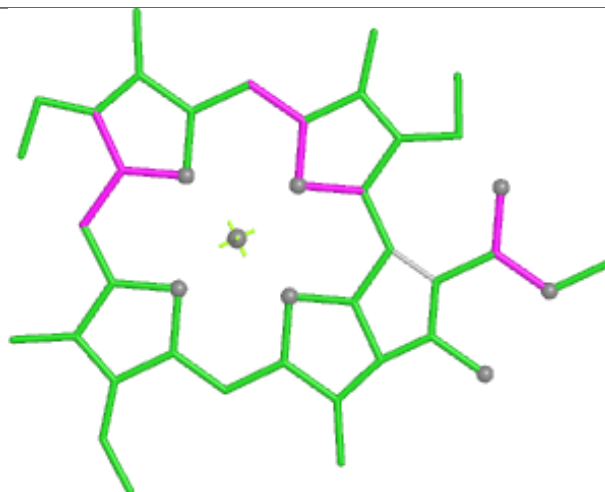


Ligand CLA 3 303**Ligand II0 7 314**

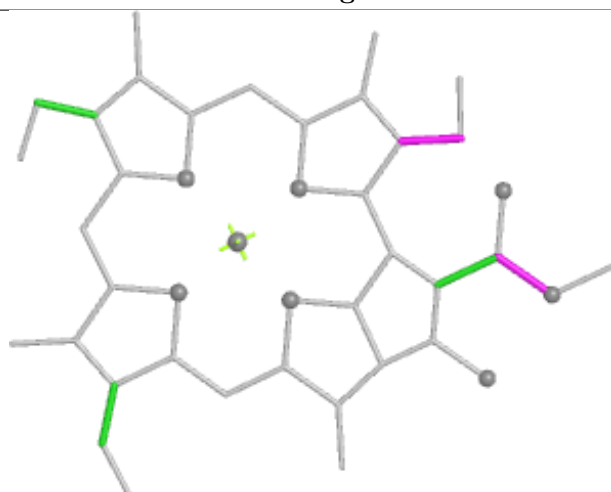
Ligand CLA B 815



Bond lengths



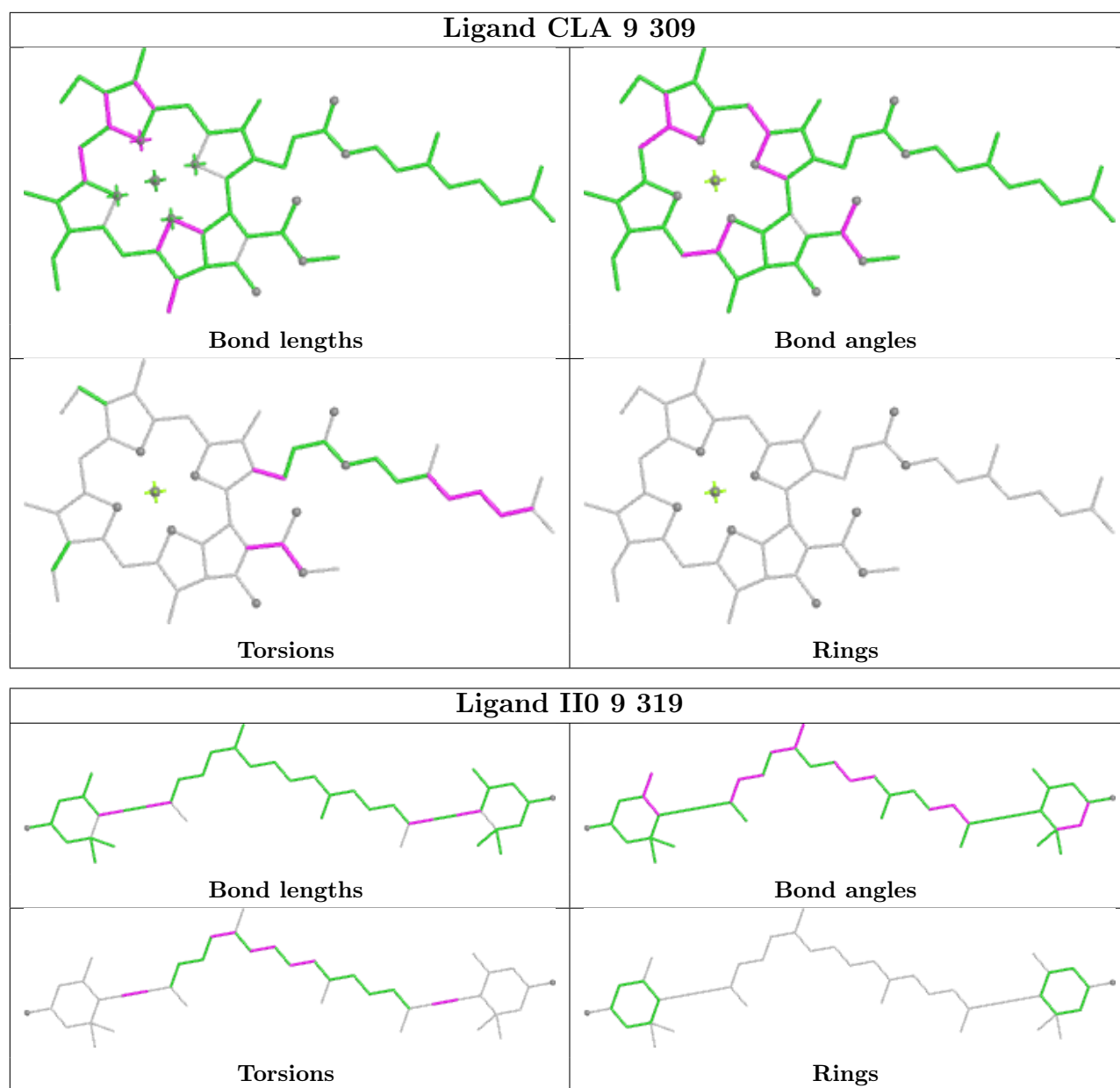
Bond angles

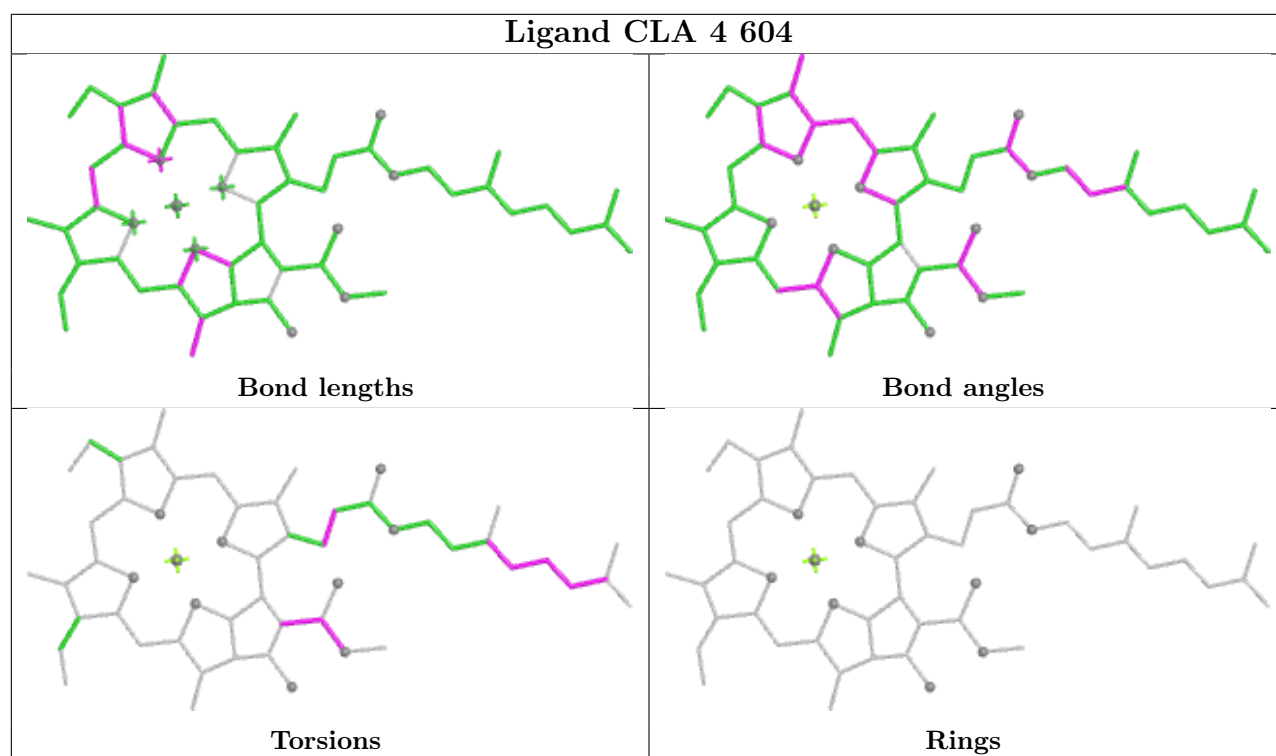


Torsions

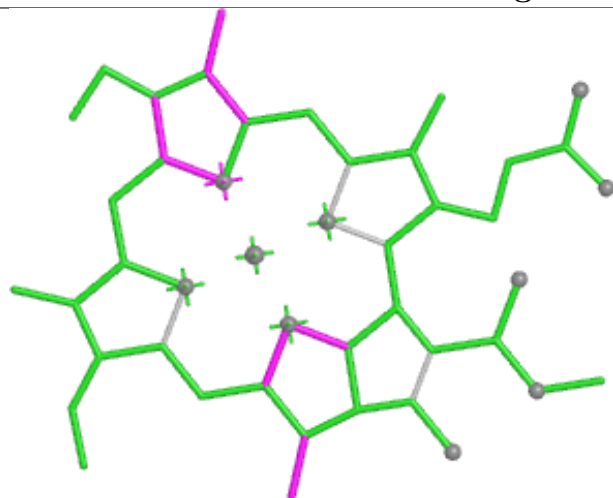


Rings

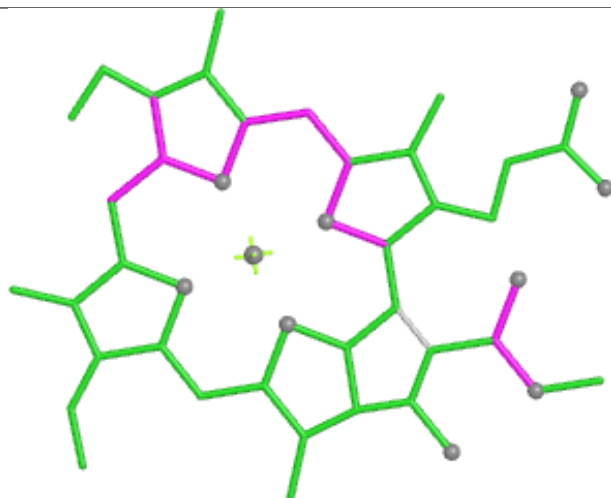




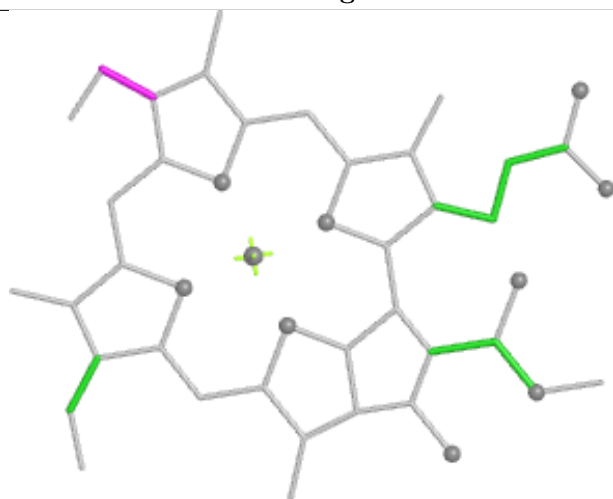
Ligand CLA B 830



Bond lengths



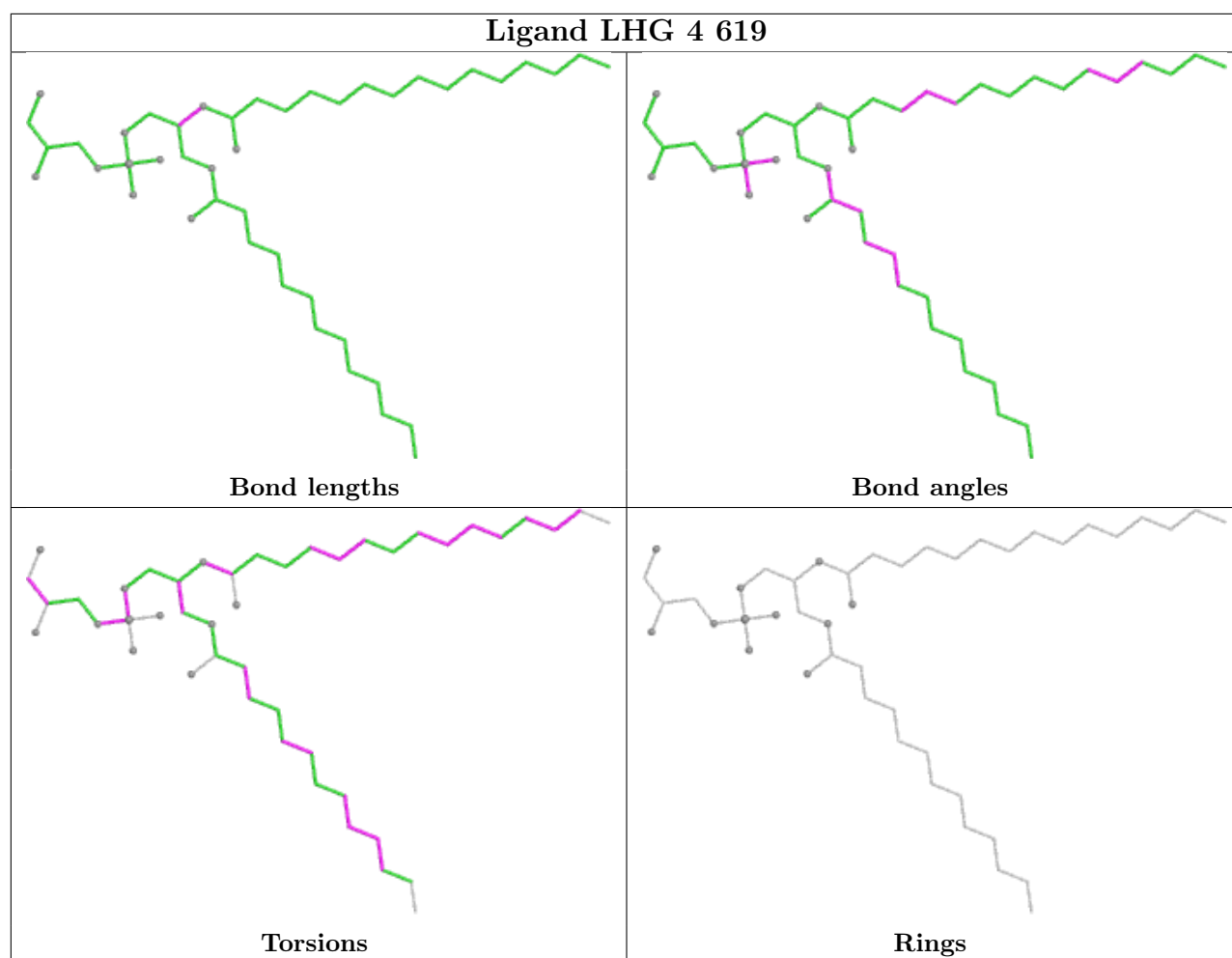
Bond angles



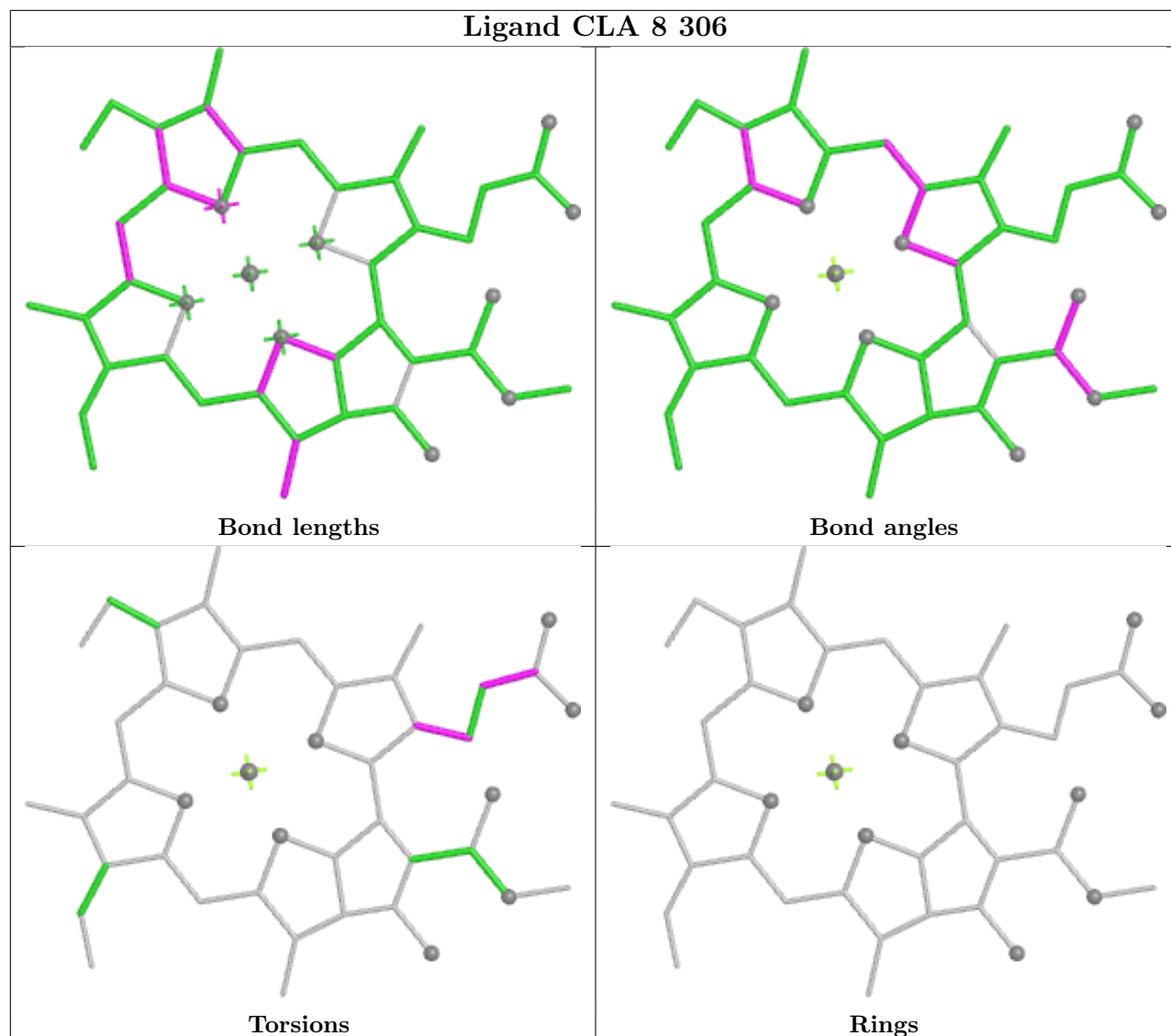
Torsions



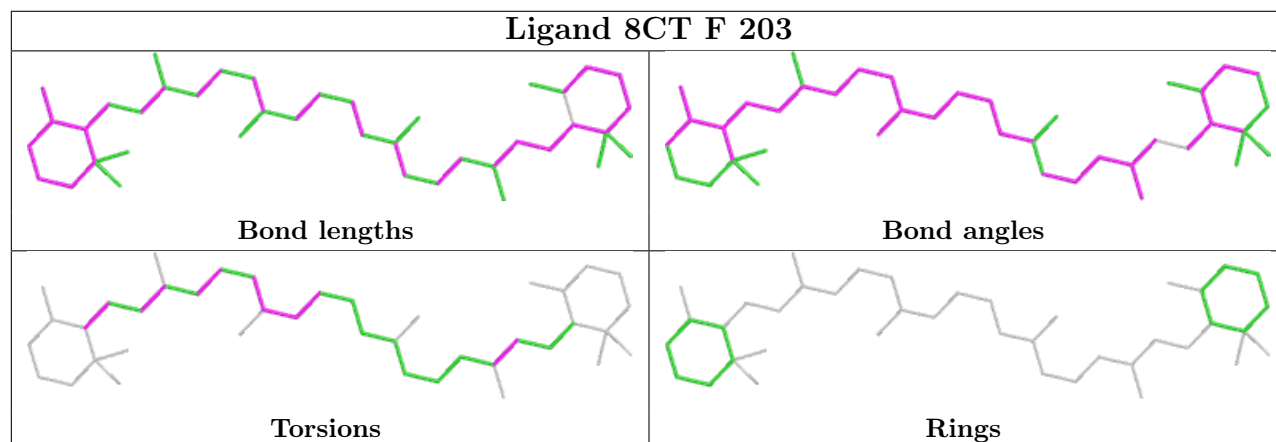
Rings



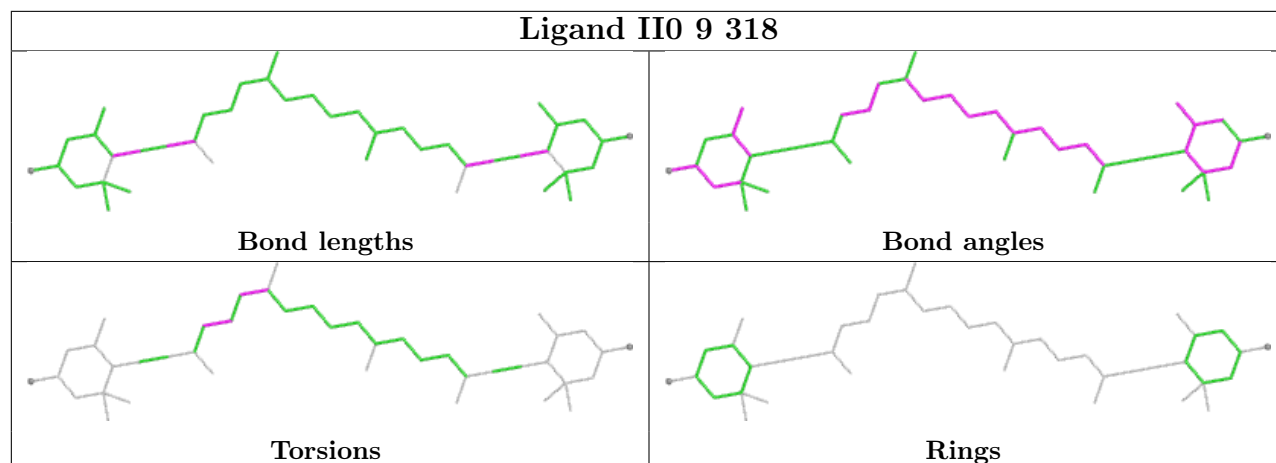
Ligand CLA 8 306



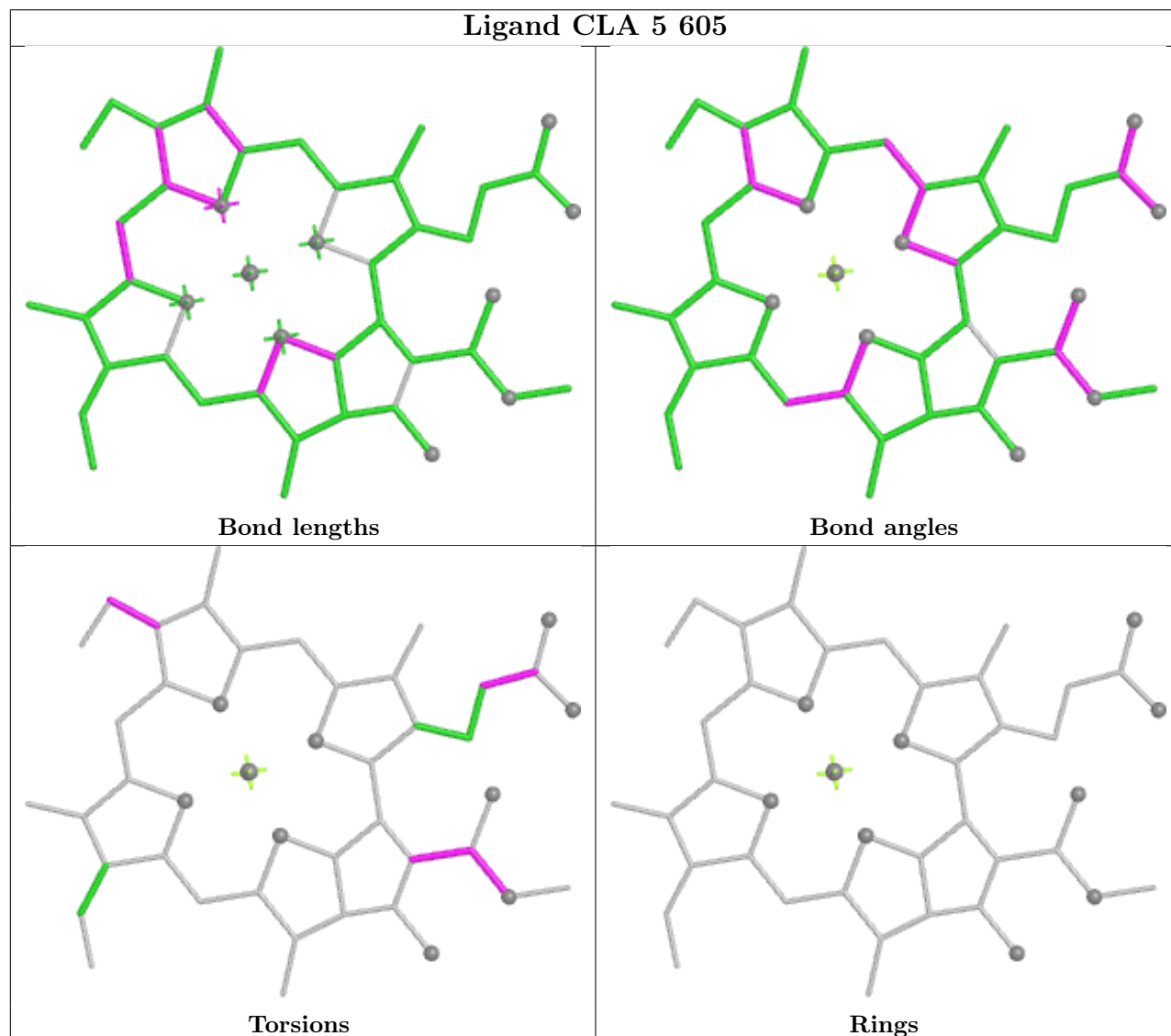
Ligand 8CT F 203



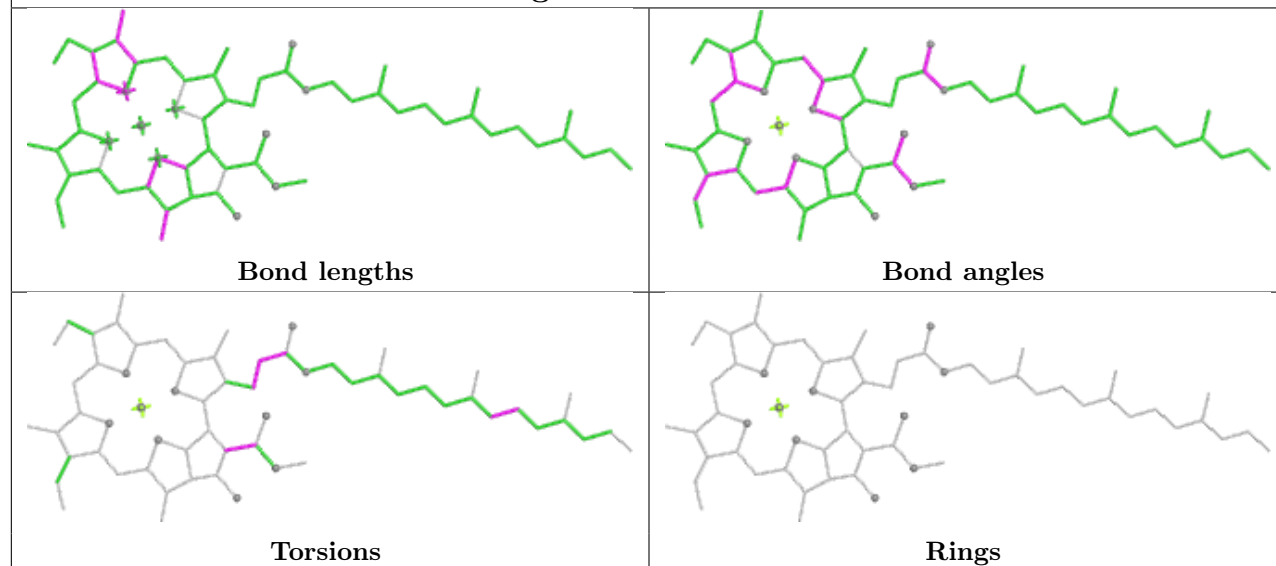
Ligand II0 9 318



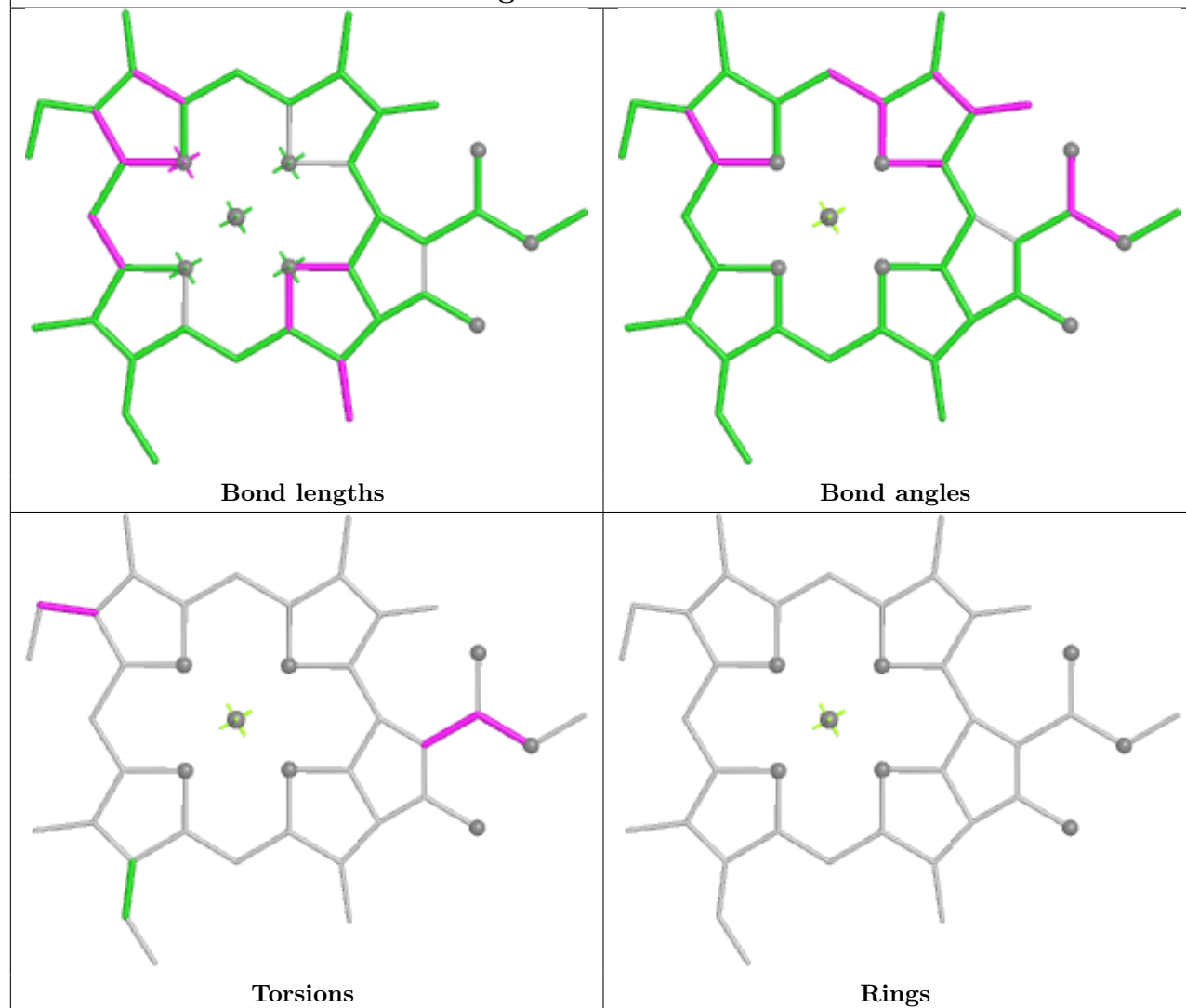
Ligand CLA 5 605

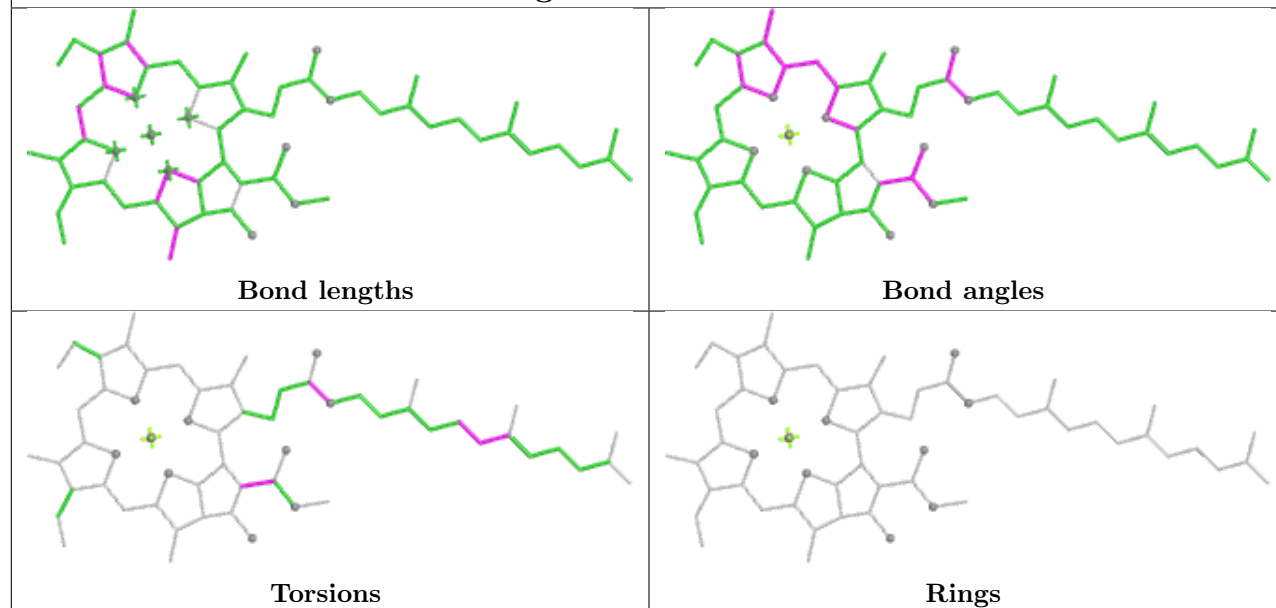
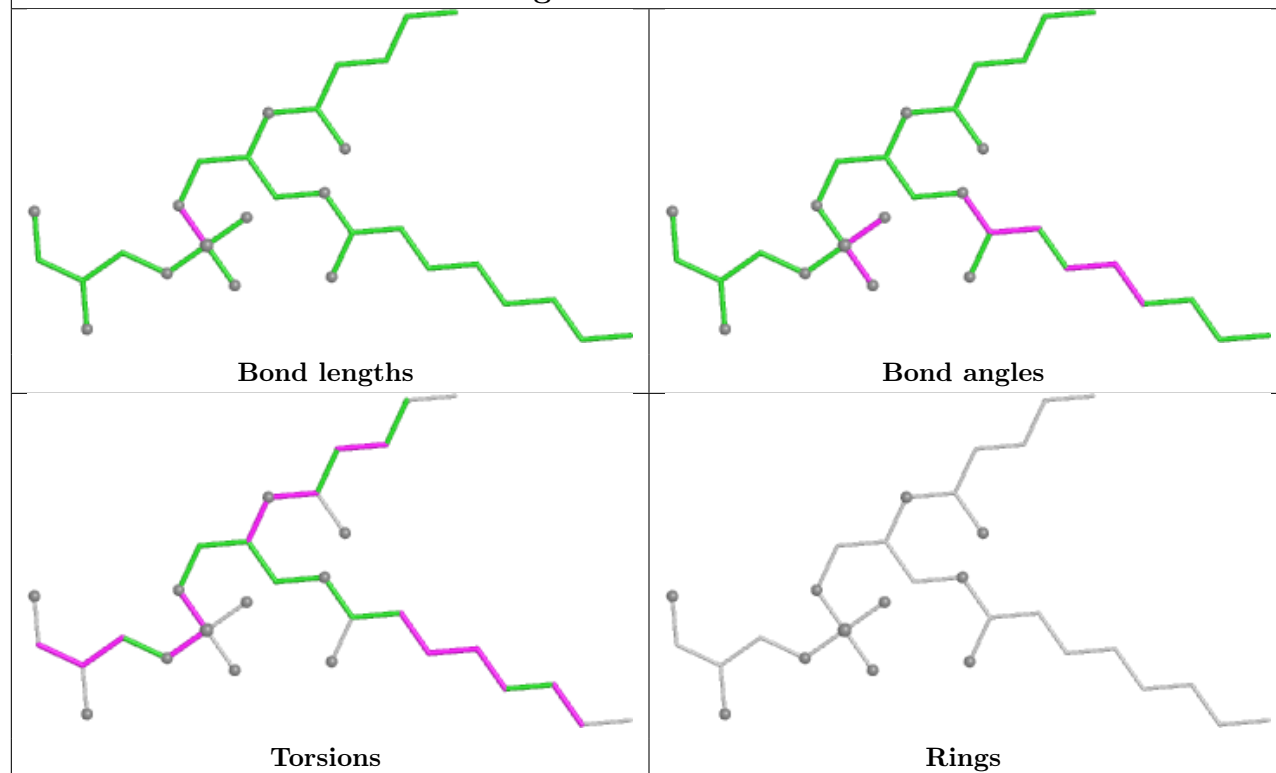


Ligand CLA A 815

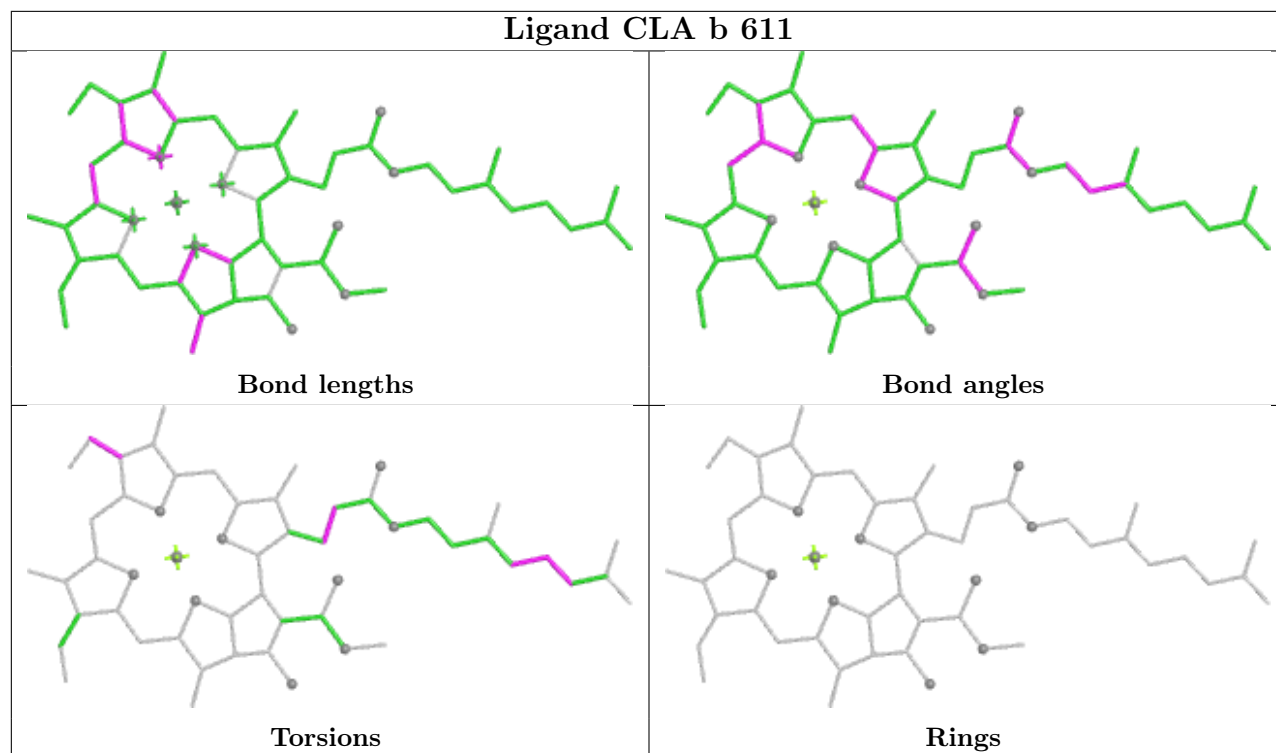


Ligand CLA 5 601

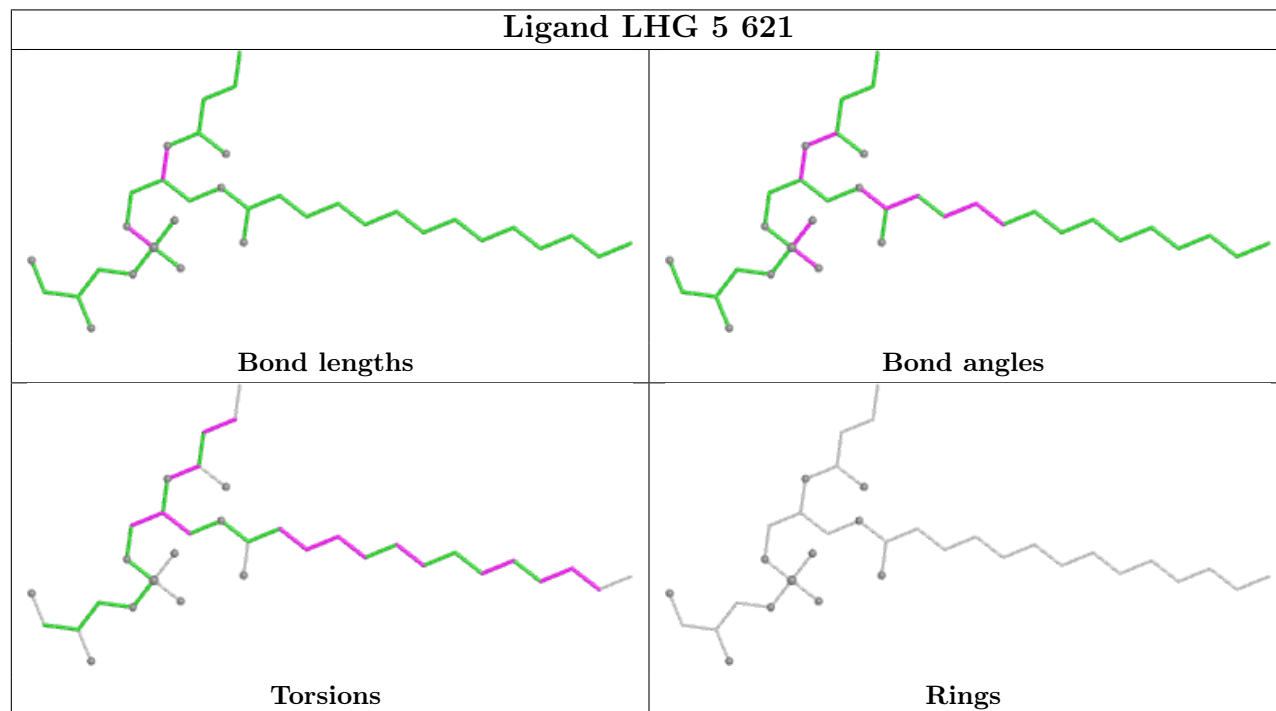


Ligand CLA b 603**Ligand LHG b 616**

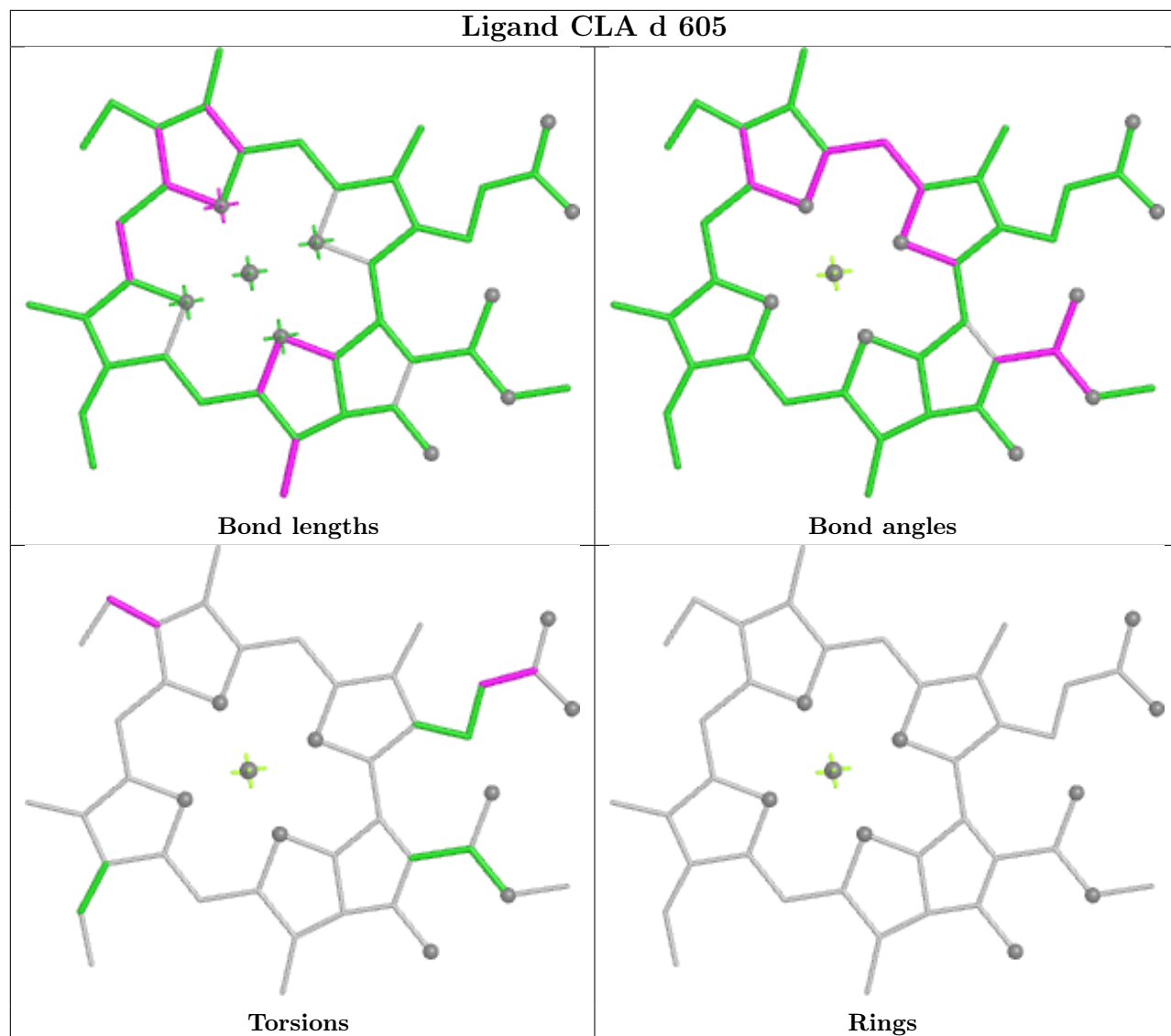
Ligand CLA b 611



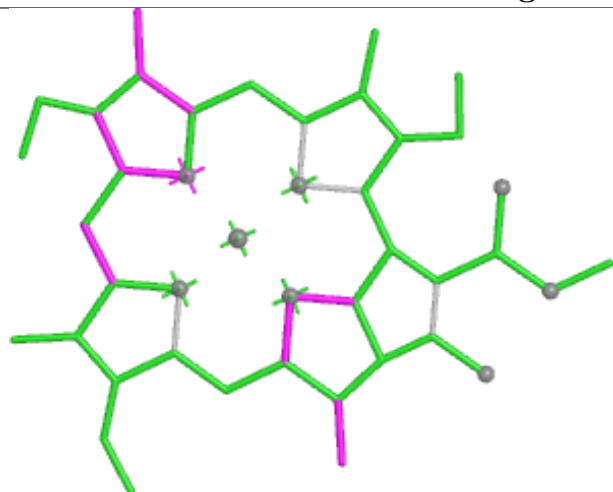
Ligand LHG 5 621



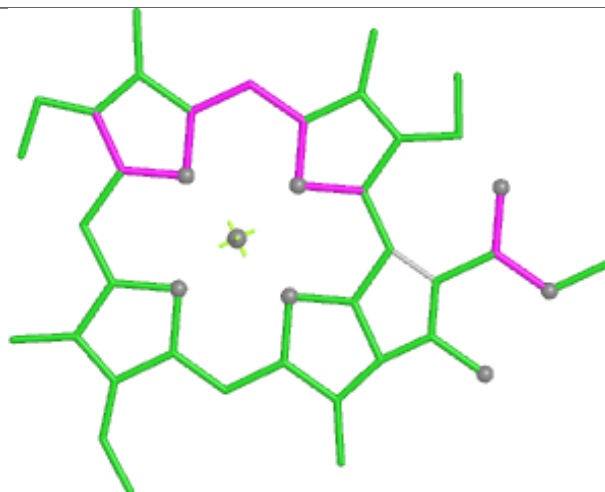
Ligand CLA d 605



Ligand CLA 2 601



Bond lengths



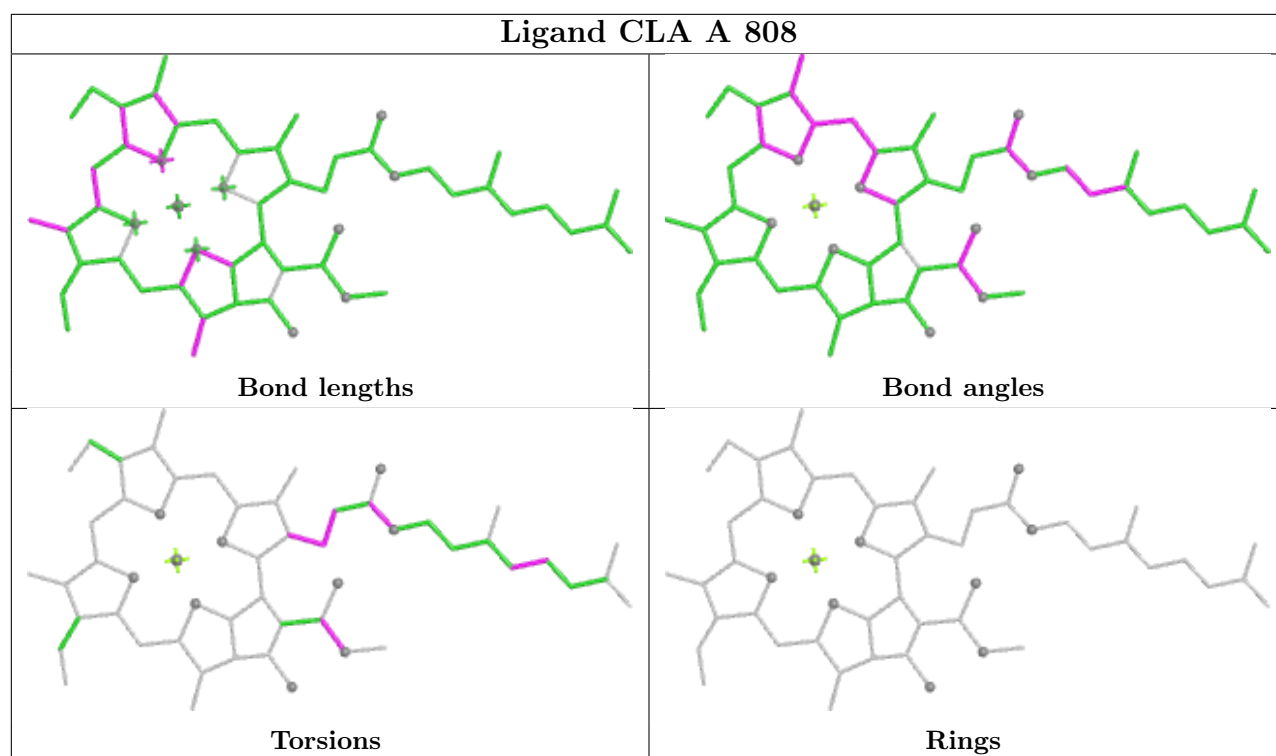
Bond angles



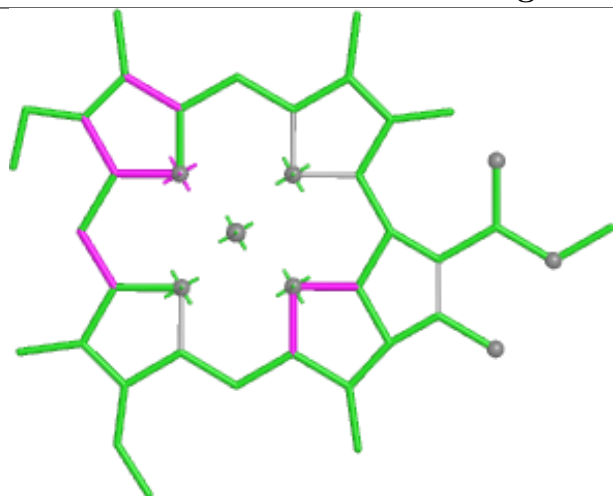
Torsions



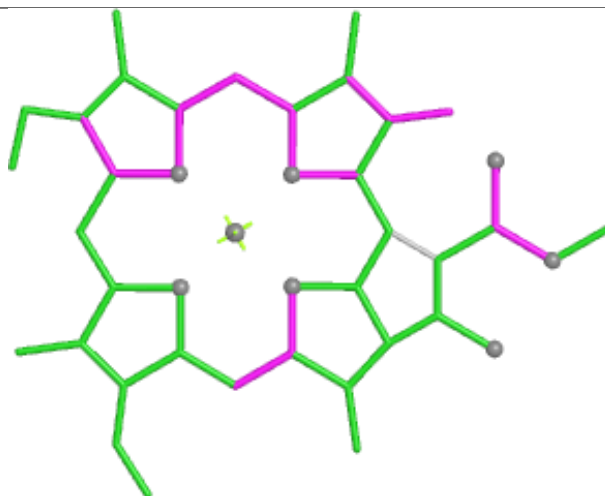
Rings



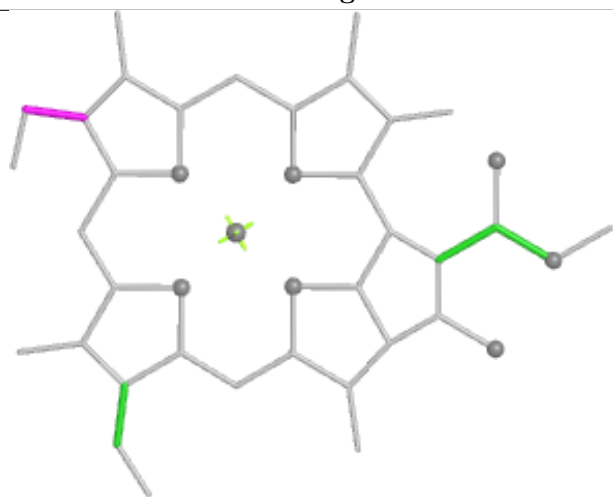
Ligand CLA d 609



Bond lengths



Bond angles

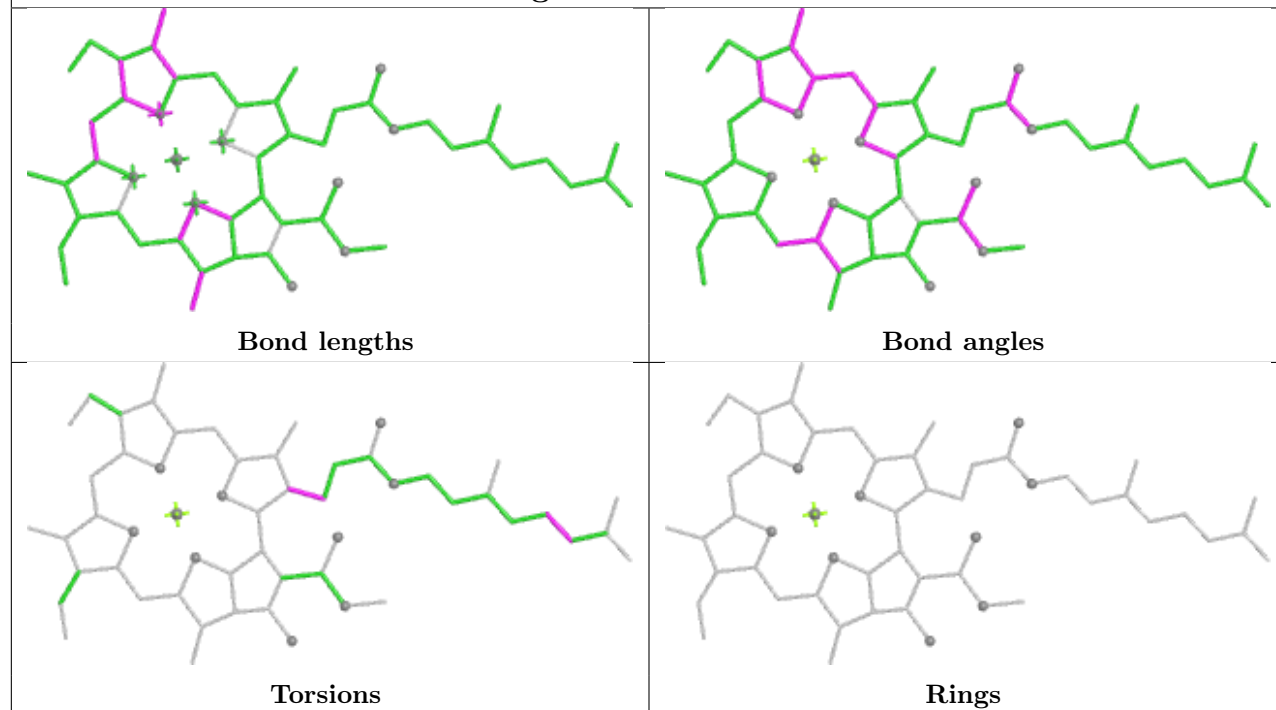


Torsions

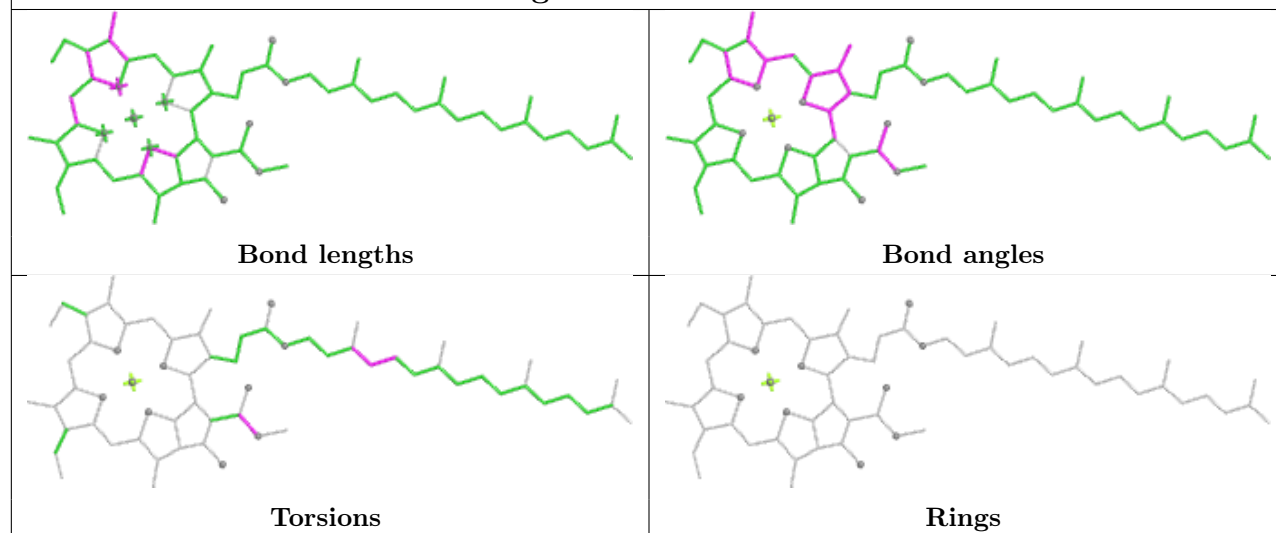


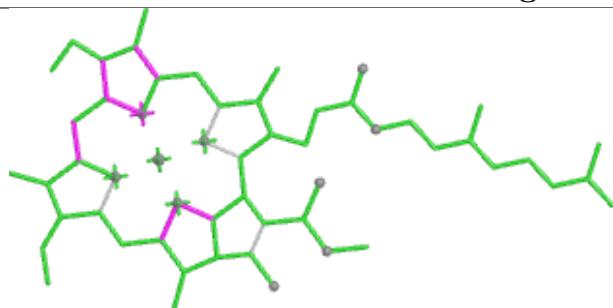
Rings

Ligand CLA A 812

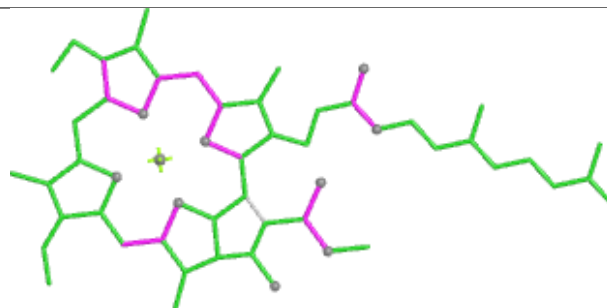


Ligand CLA A 819

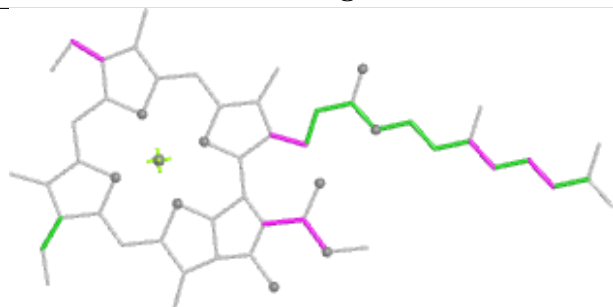


Ligand CLA c 612

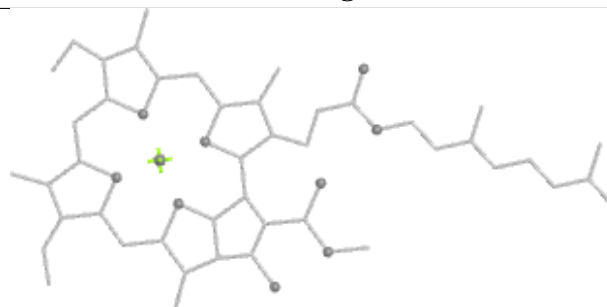
Bond lengths



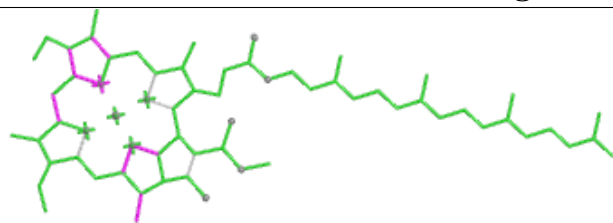
Bond angles



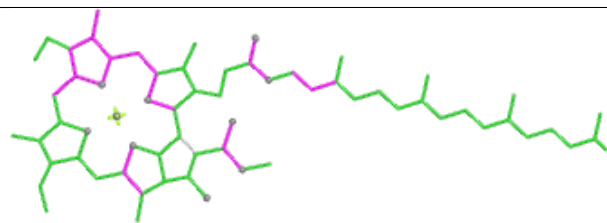
Torsions



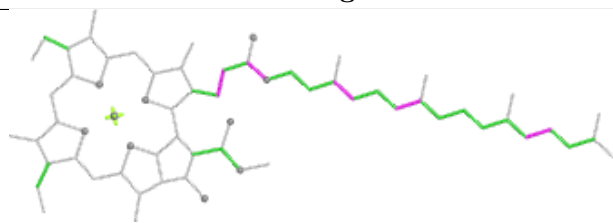
Rings

Ligand CLA A 827

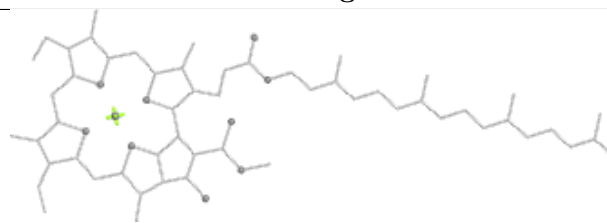
Bond lengths



Bond angles

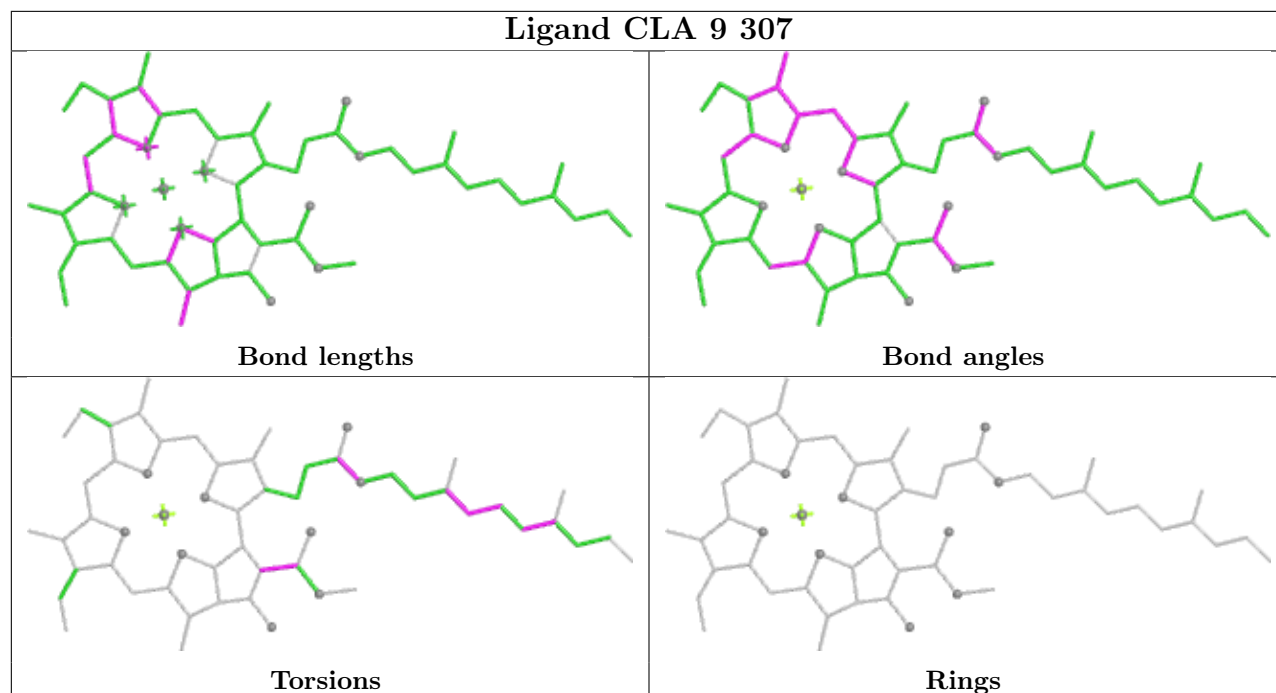


Torsions

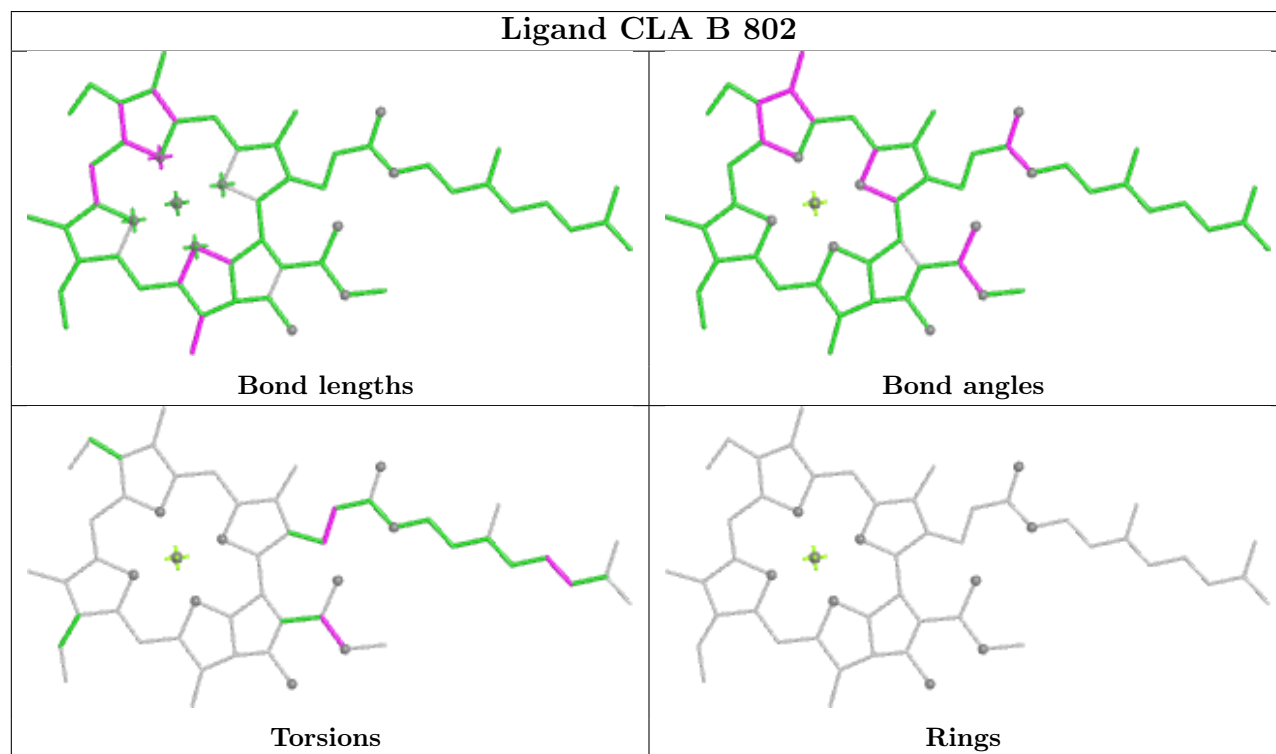


Rings

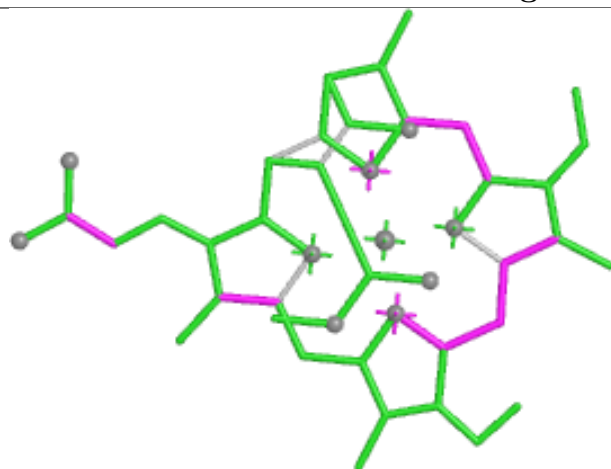
Ligand CLA 9 307



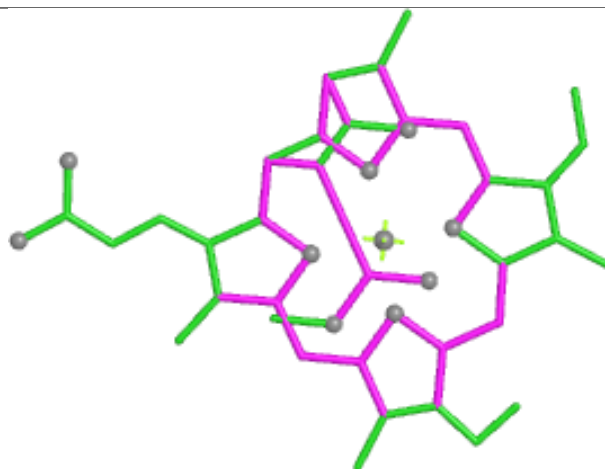
Ligand CLA B 802



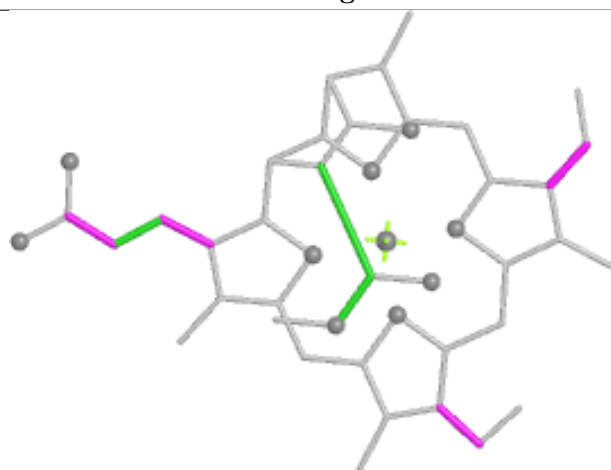
Ligand KC2 4 605



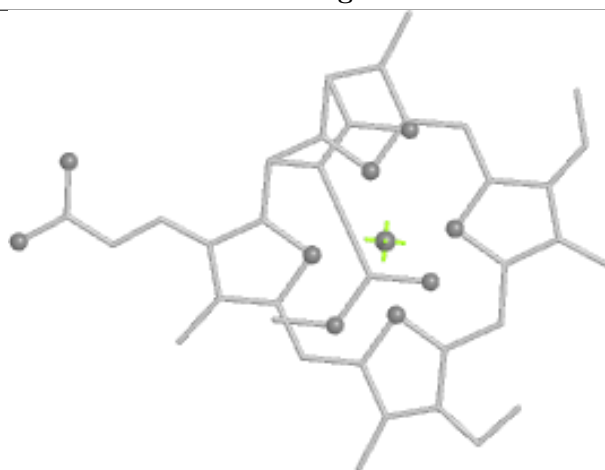
Bond lengths



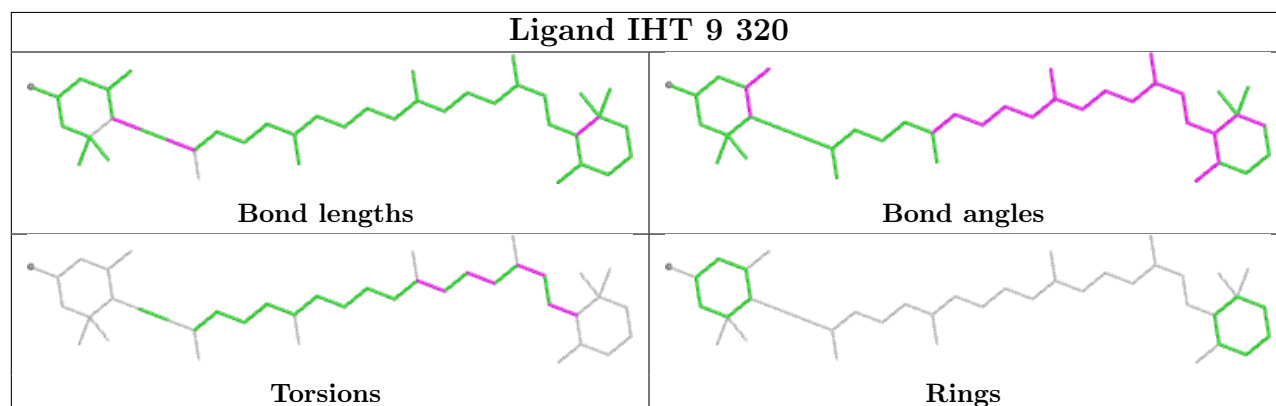
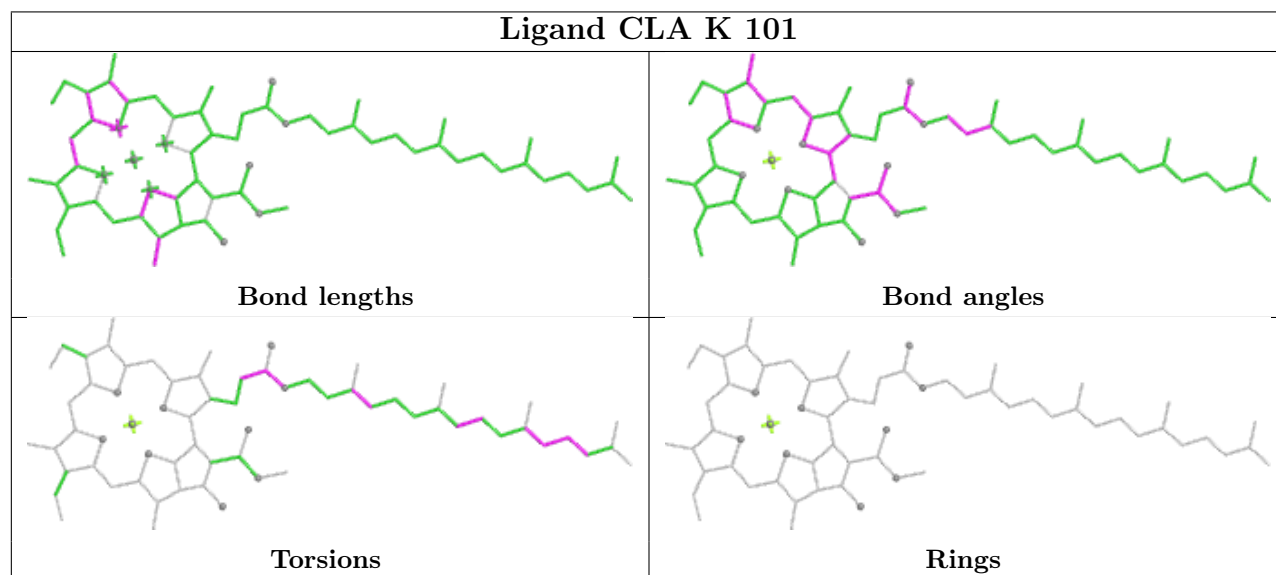
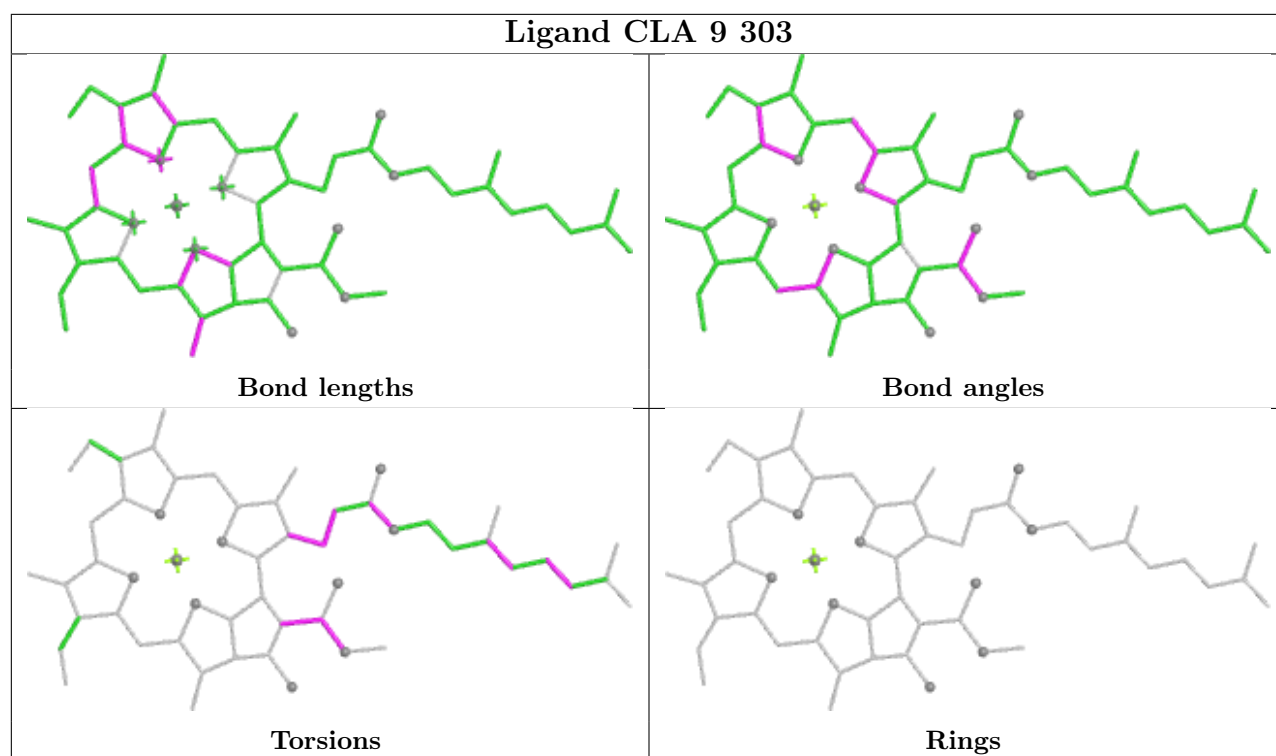
Bond angles

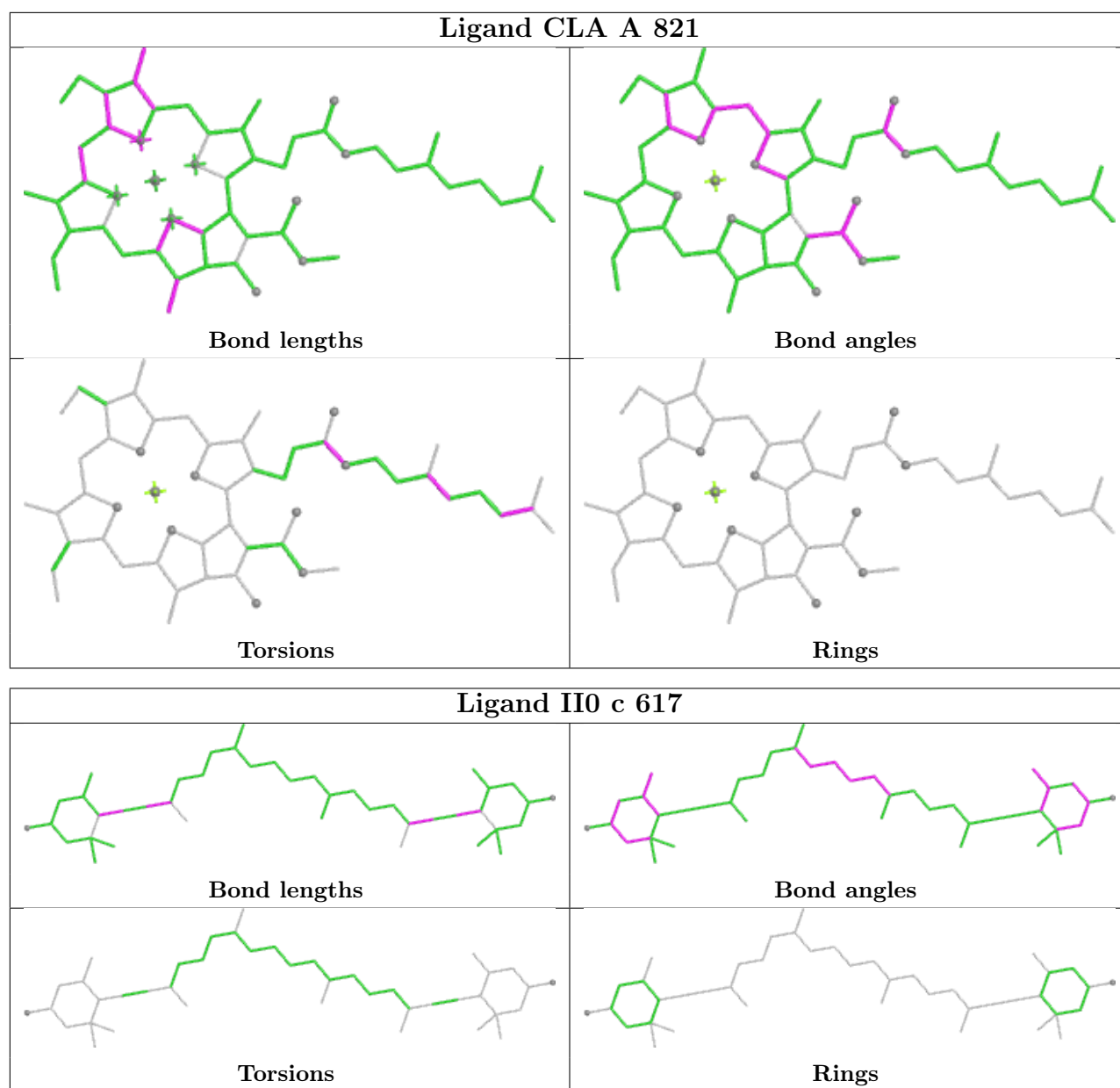


Torsions

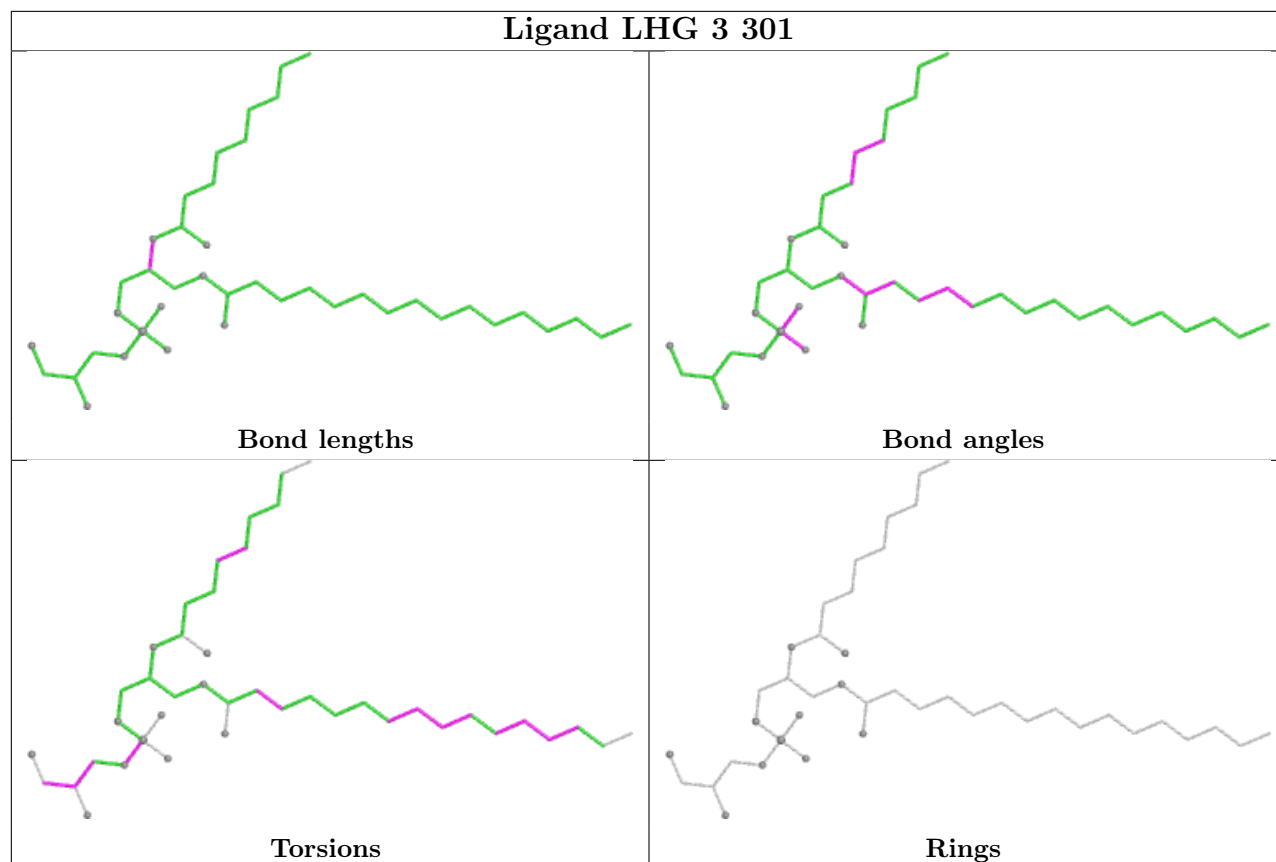


Rings

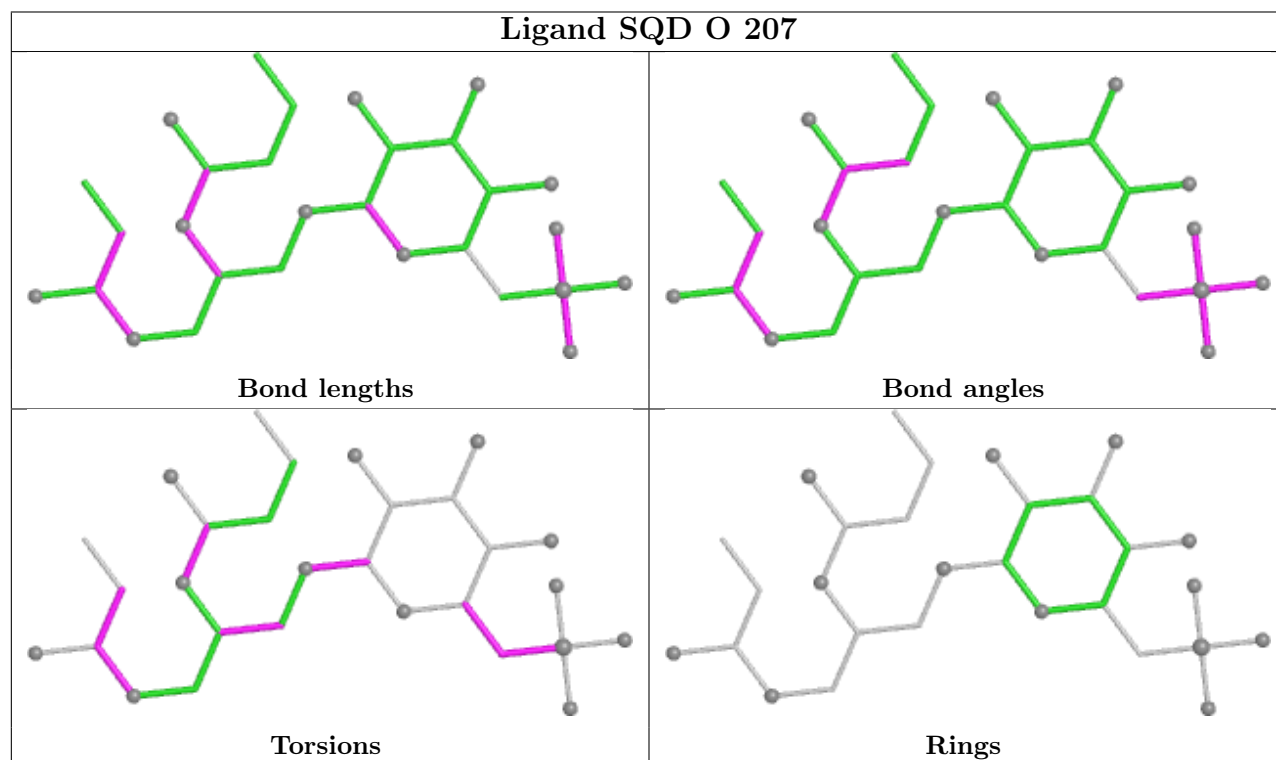


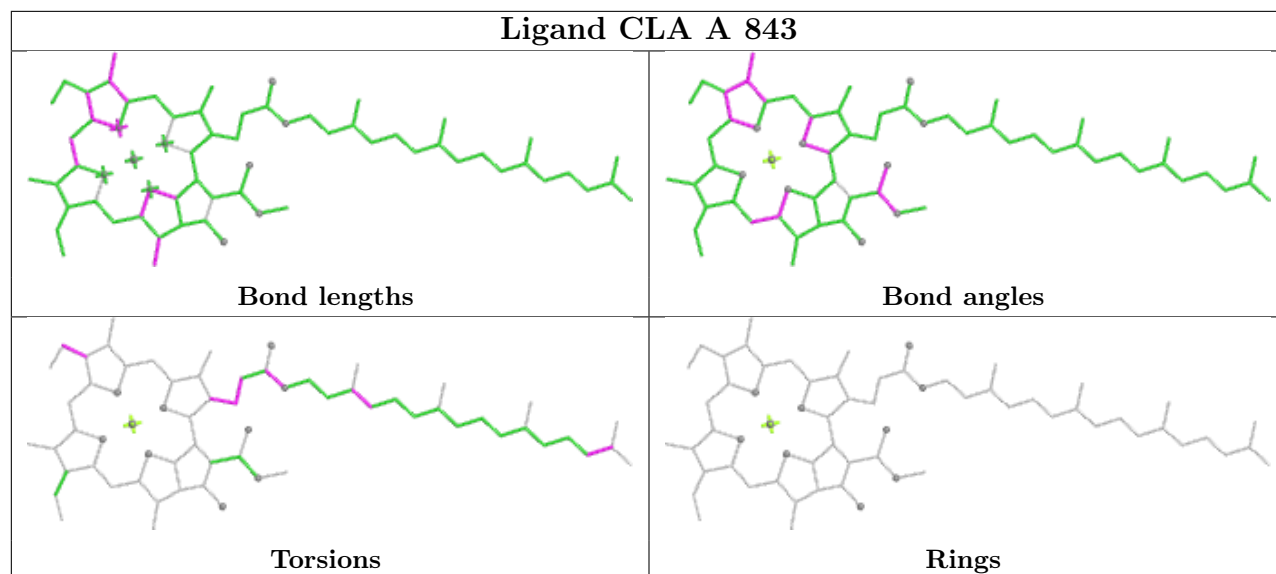
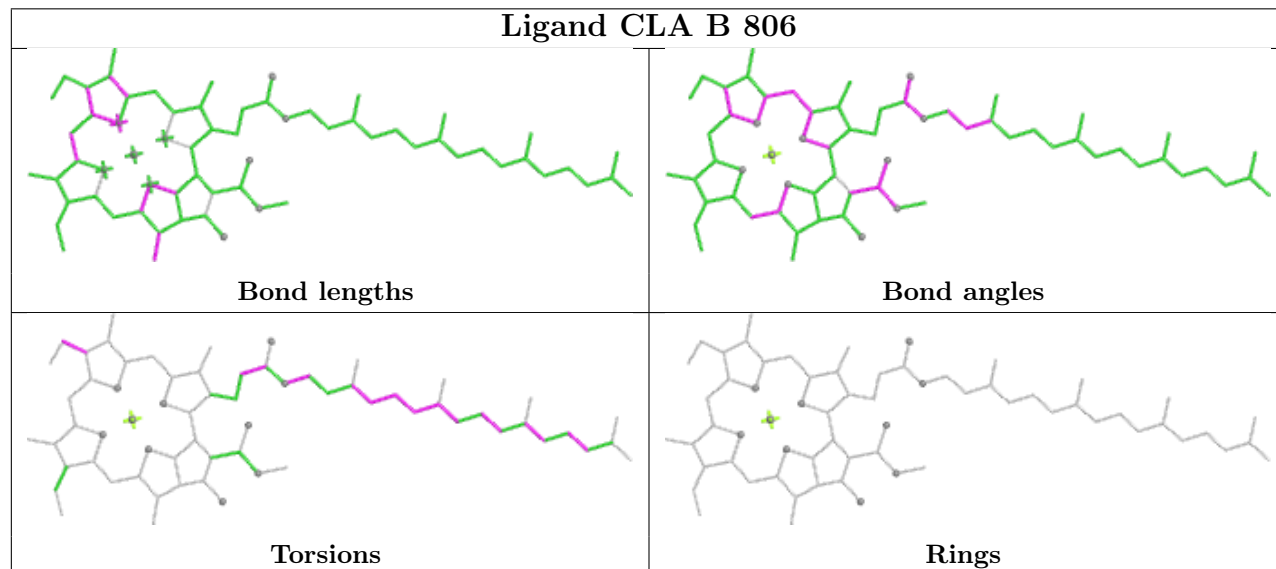


Ligand LHG 3 301

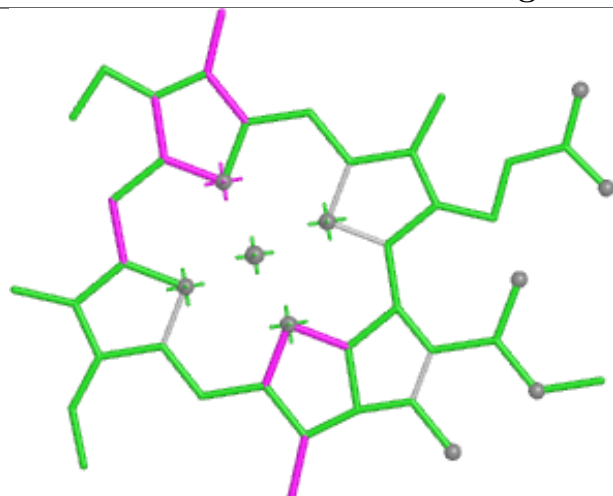


Ligand SQD O 207

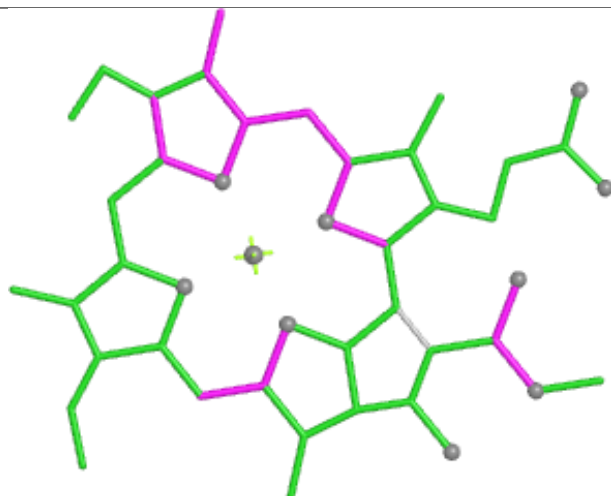


Ligand CLA A 843**Ligand CLA B 806**

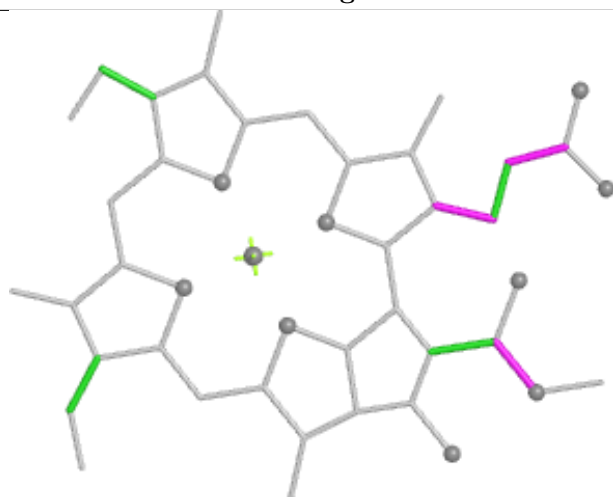
Ligand CLA 6 603



Bond lengths



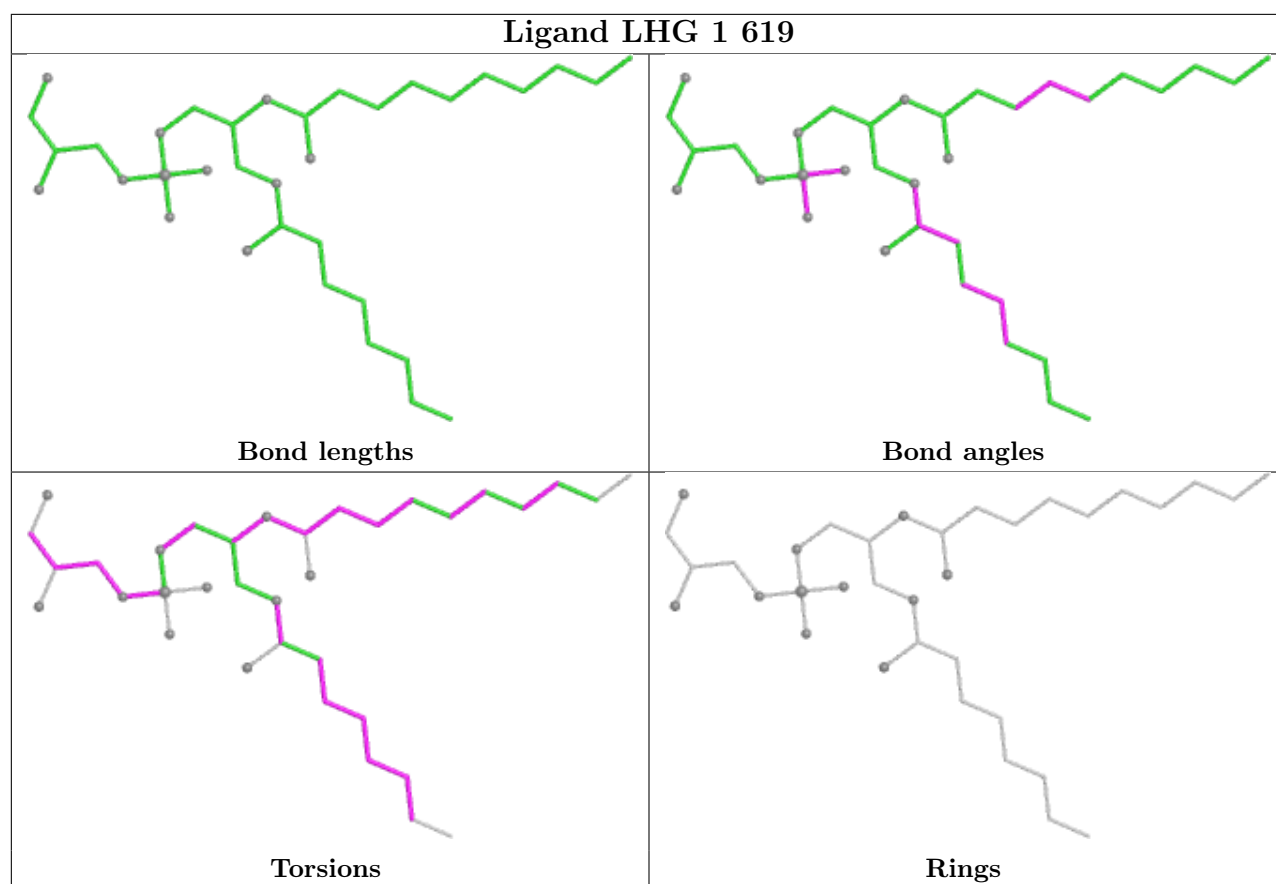
Bond angles



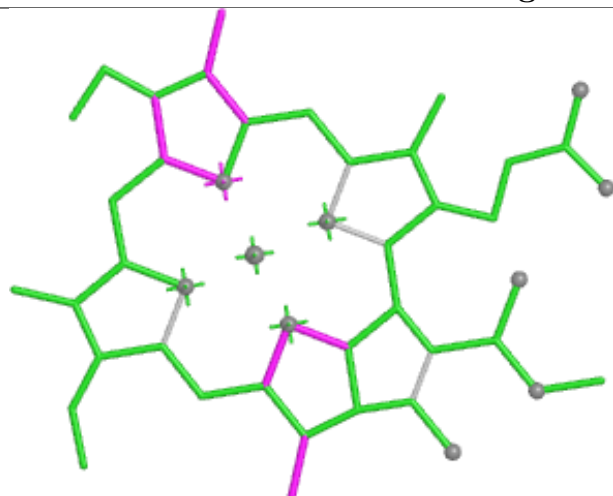
Torsions



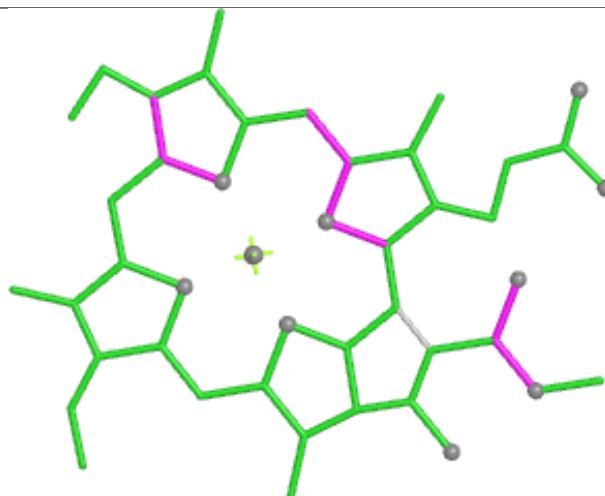
Rings



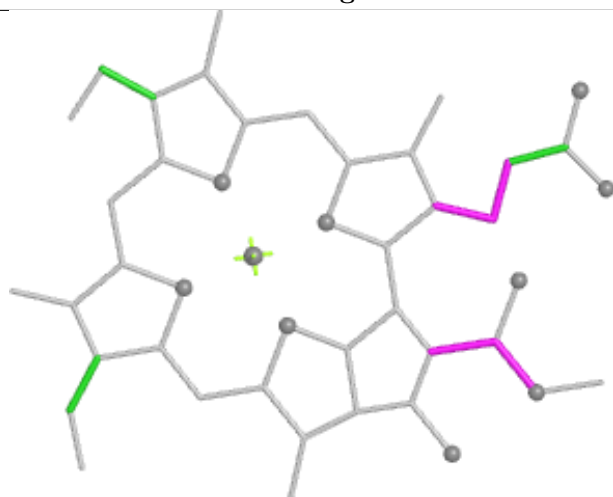
Ligand CLA 7 307



Bond lengths



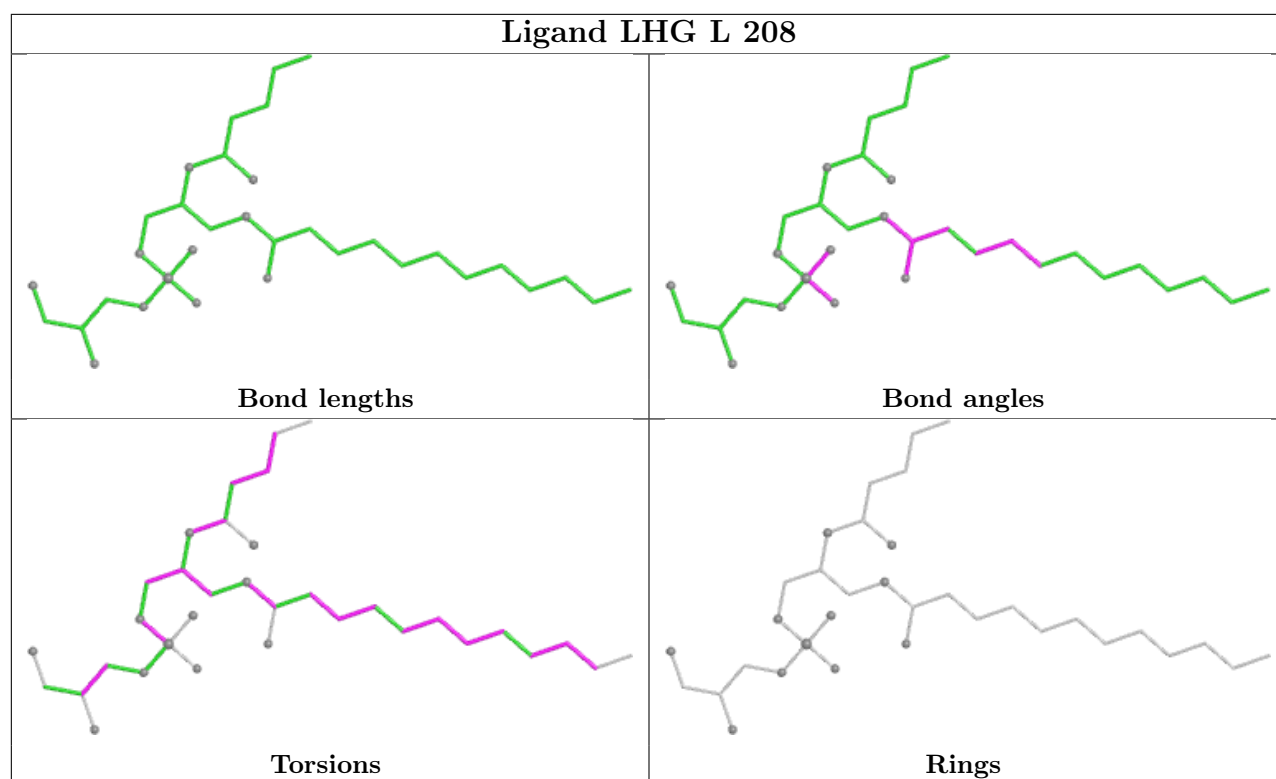
Bond angles



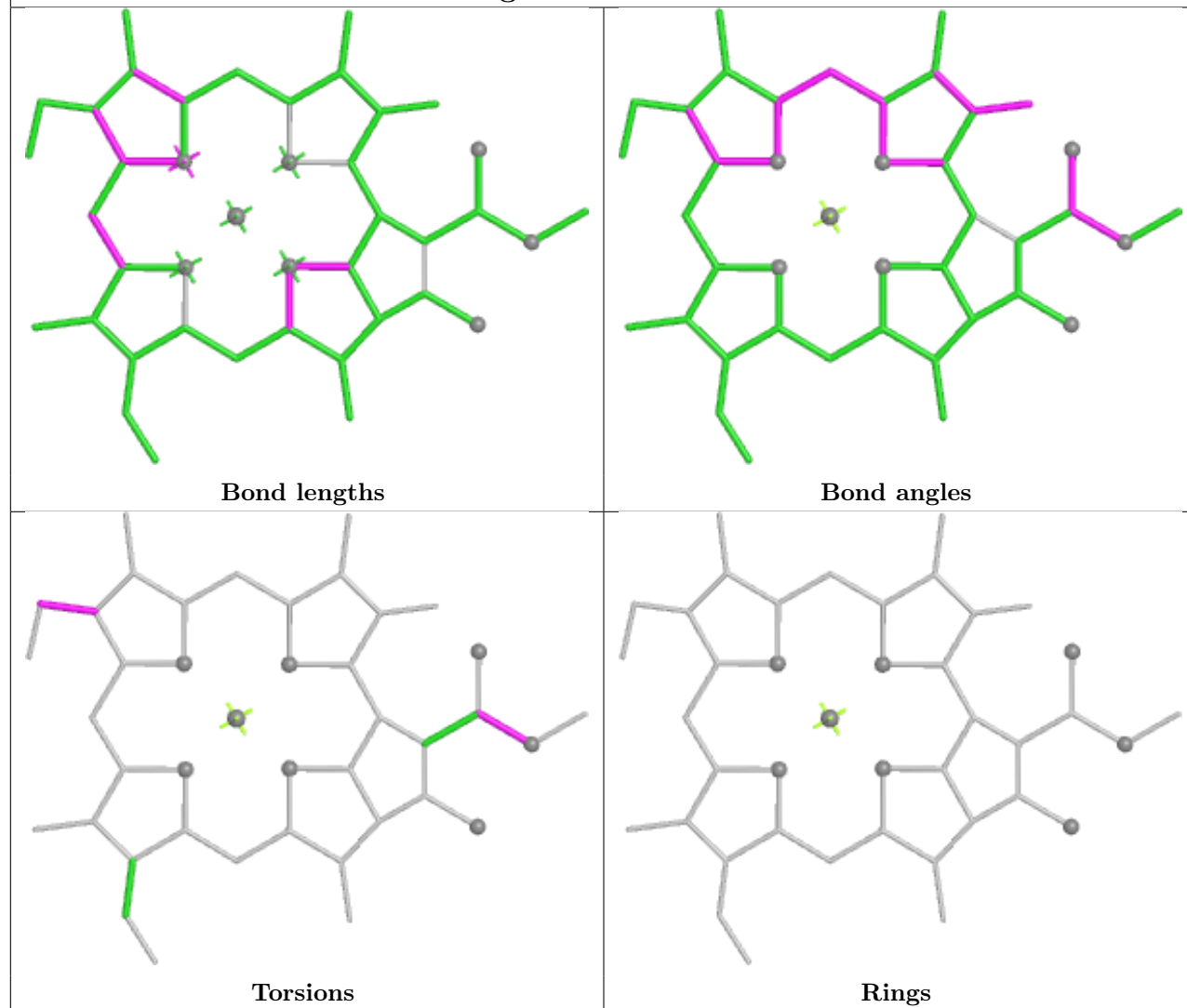
Torsions



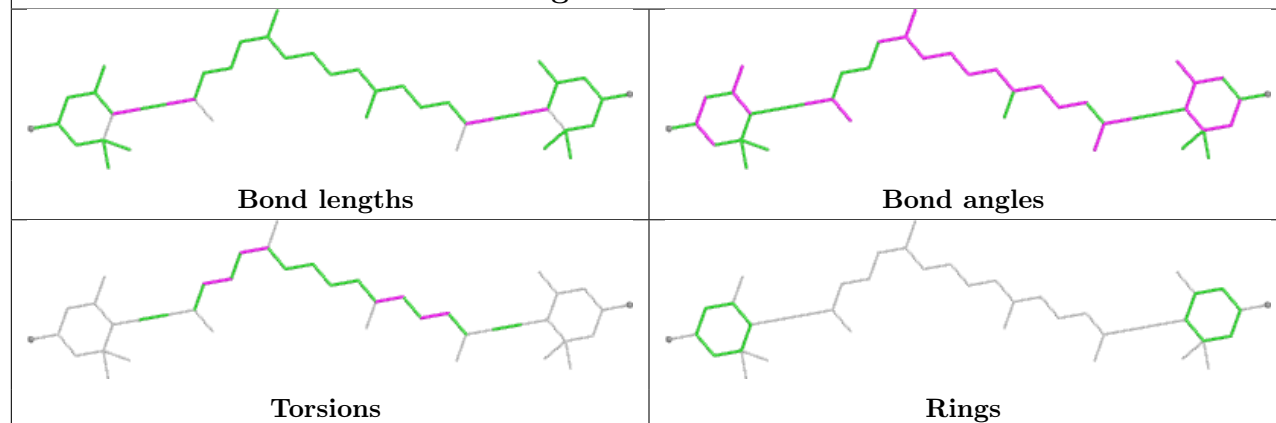
Rings



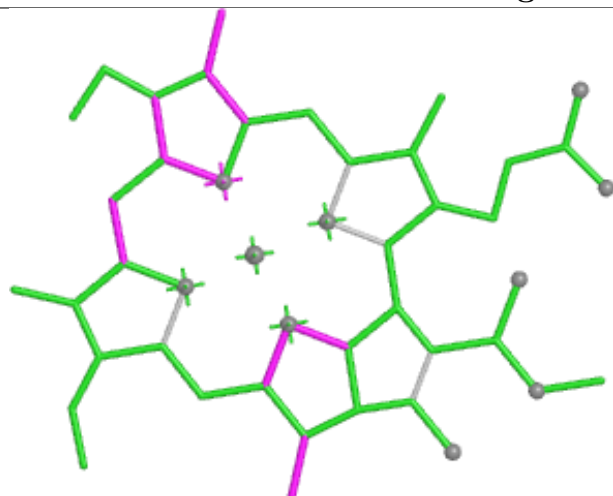
Ligand CLA c 609



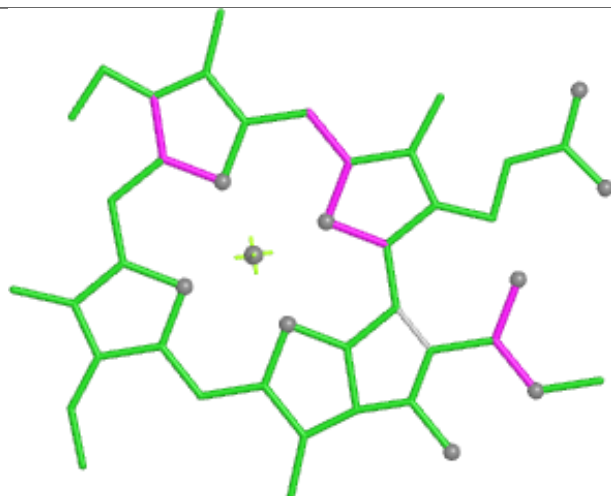
Ligand II0 e 612



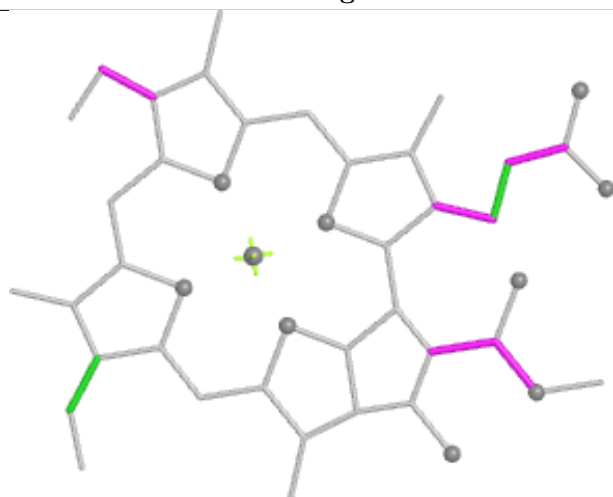
Ligand CLA d 601



Bond lengths



Bond angles

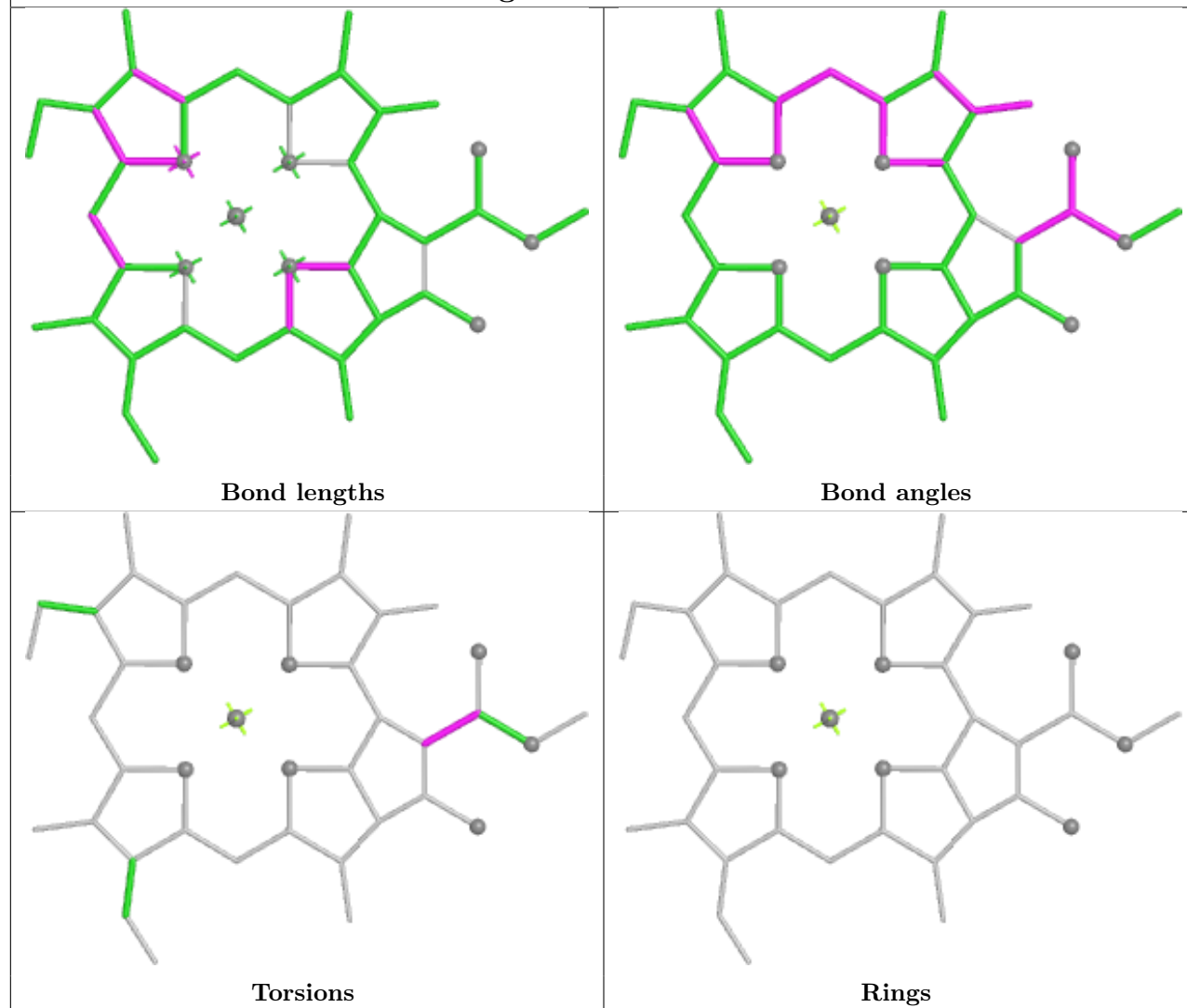


Torsions

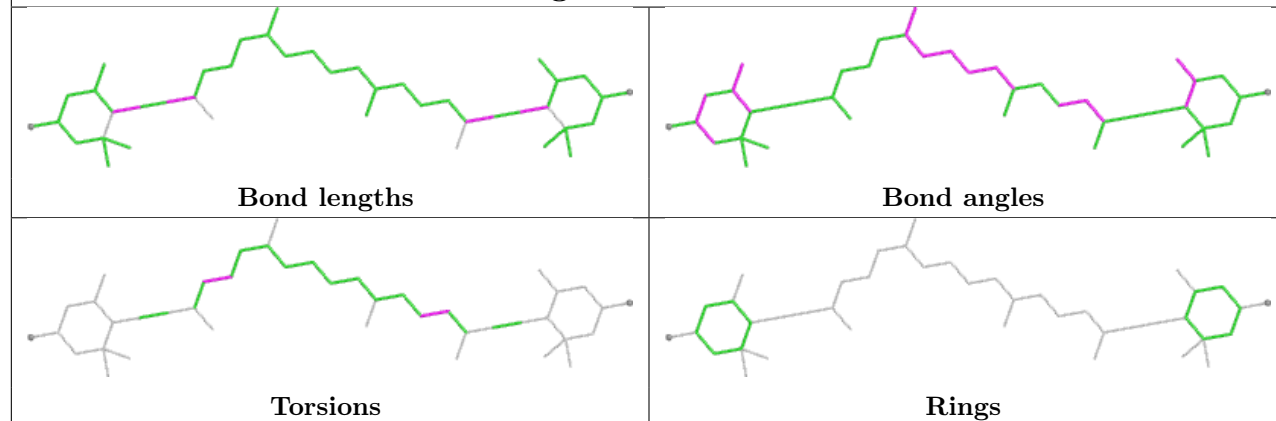


Rings

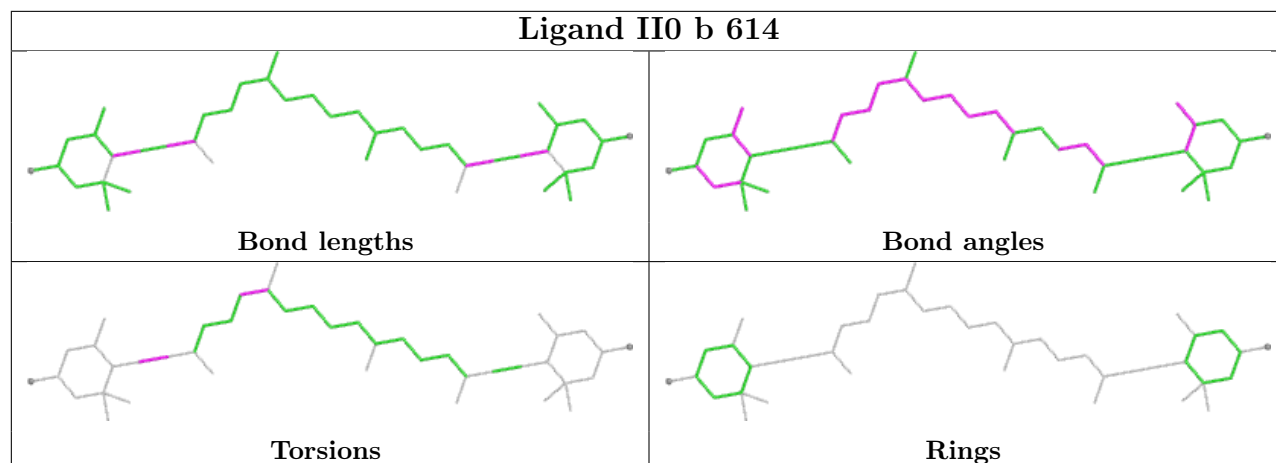
Ligand CLA 6 609



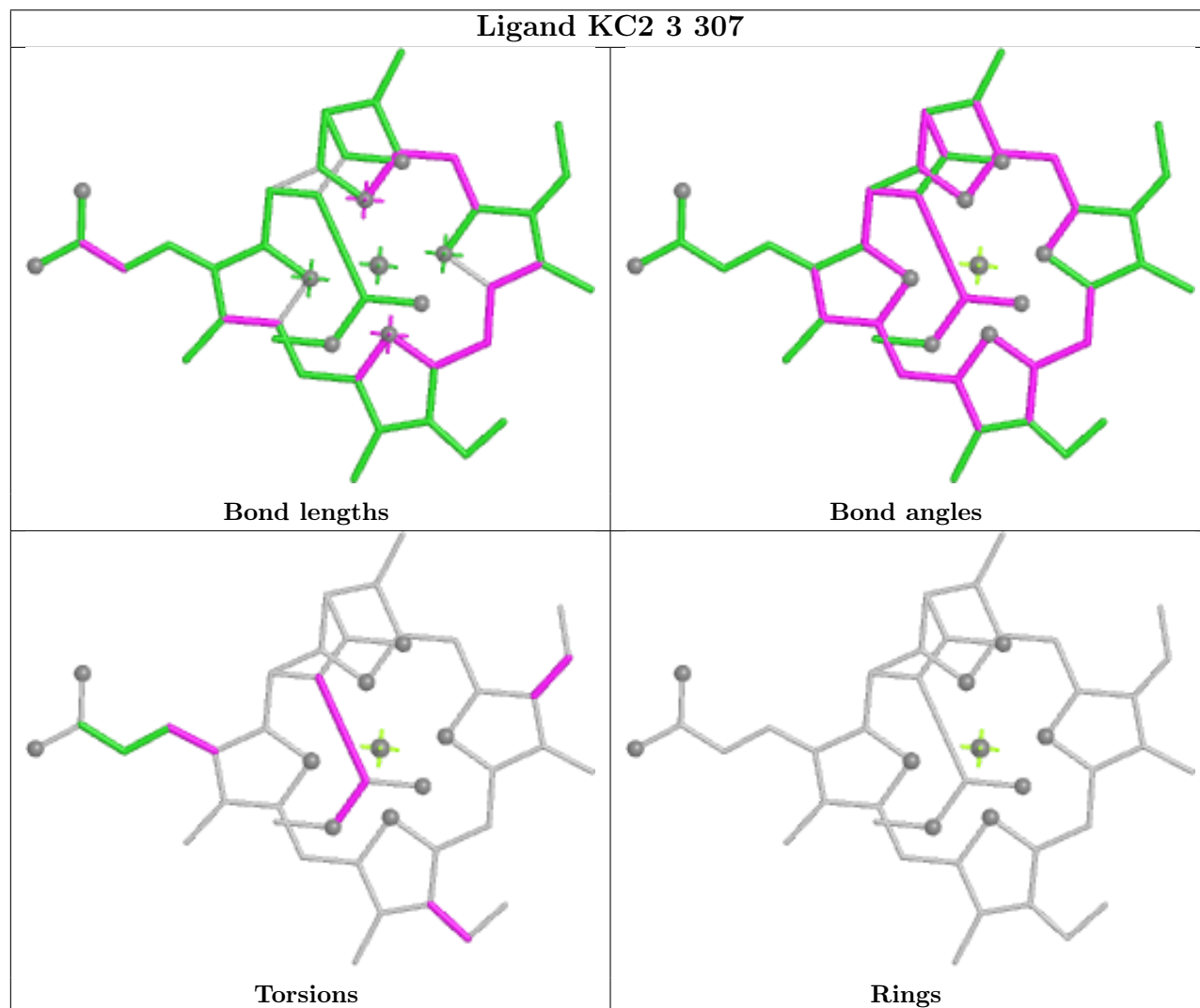
Ligand II0 4 612

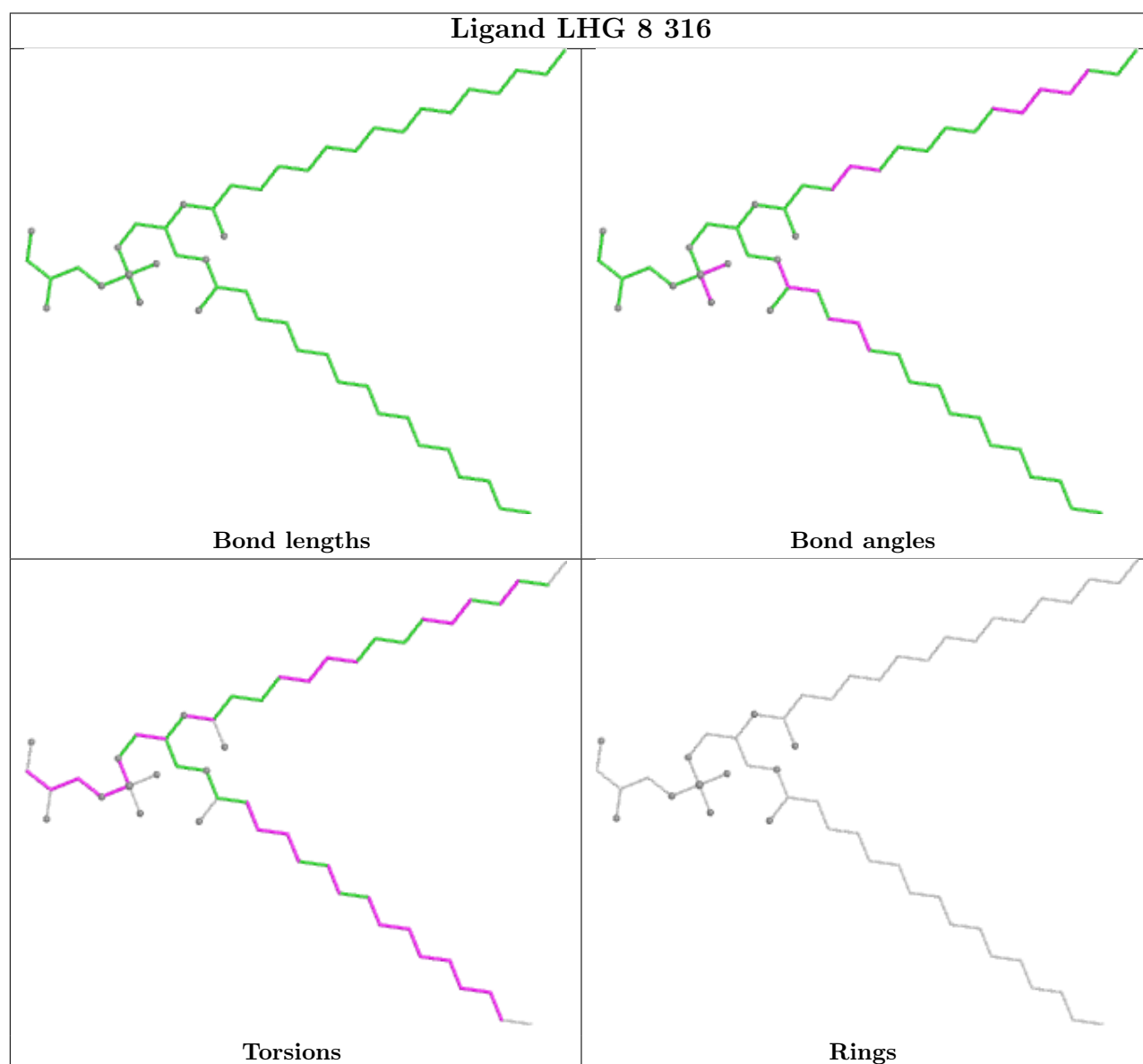
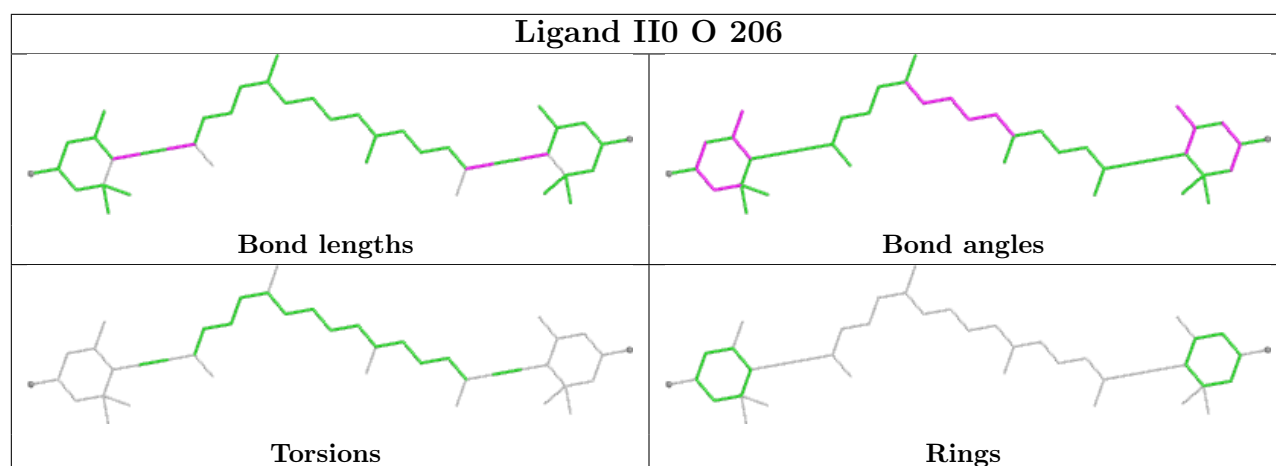


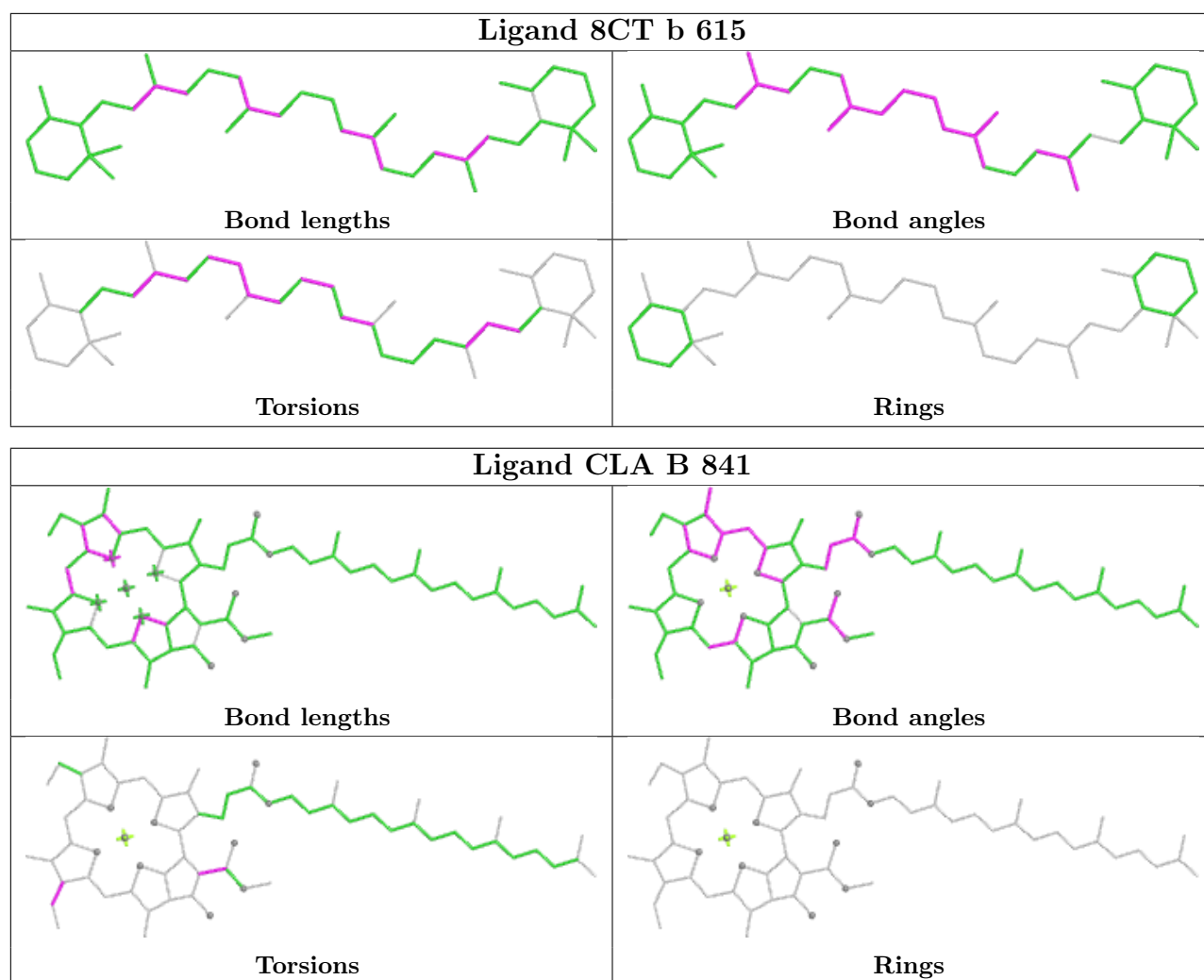
Ligand II0 b 614



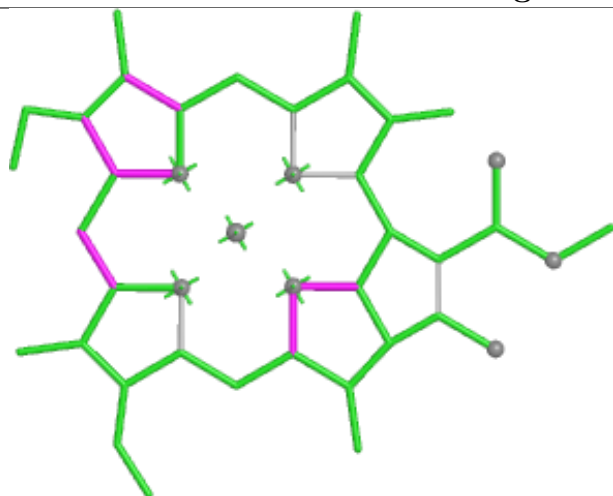
Ligand KC2 3 307







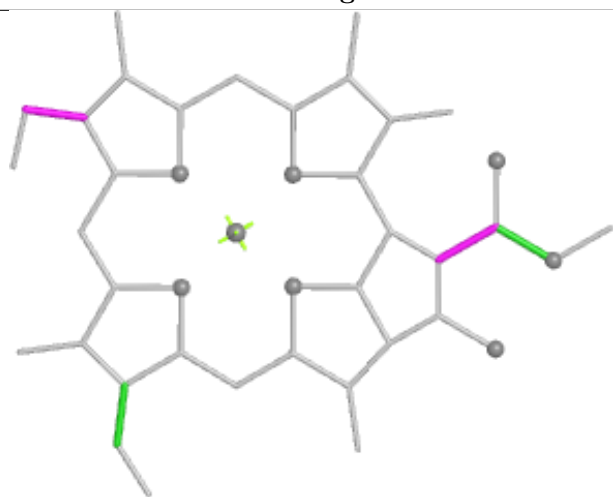
Ligand CLA O 202



Bond lengths



Bond angles

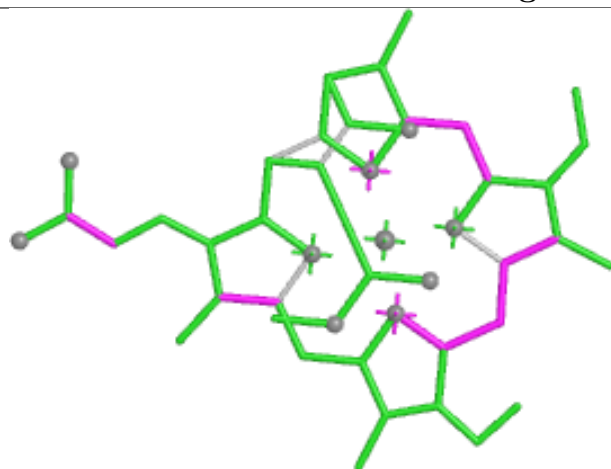


Torsions

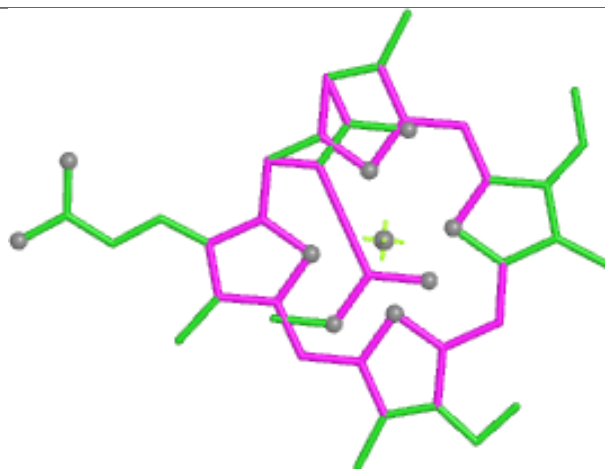


Rings

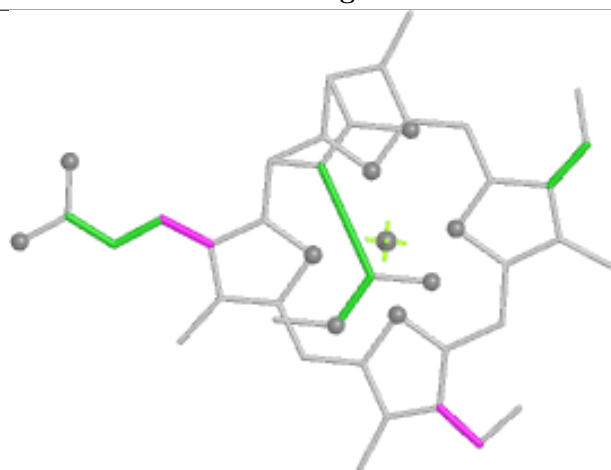
Ligand KC2 b 609



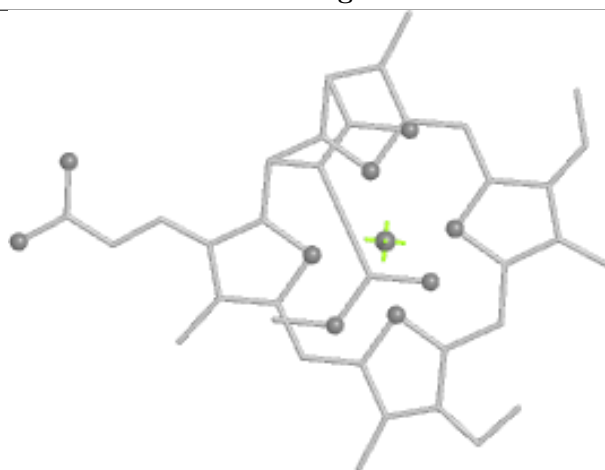
Bond lengths



Bond angles

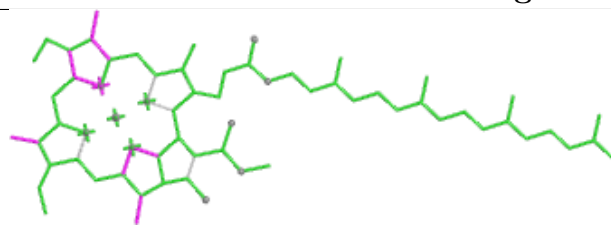


Torsions

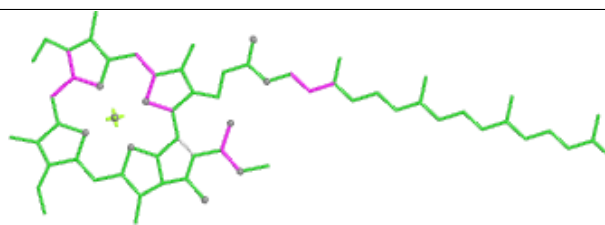


Rings

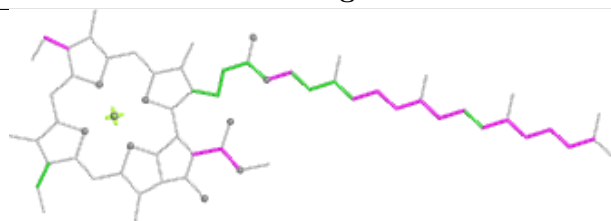
Ligand CLA B 803



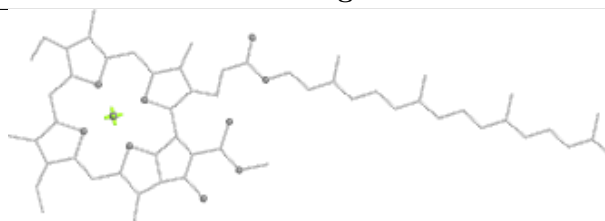
Bond lengths



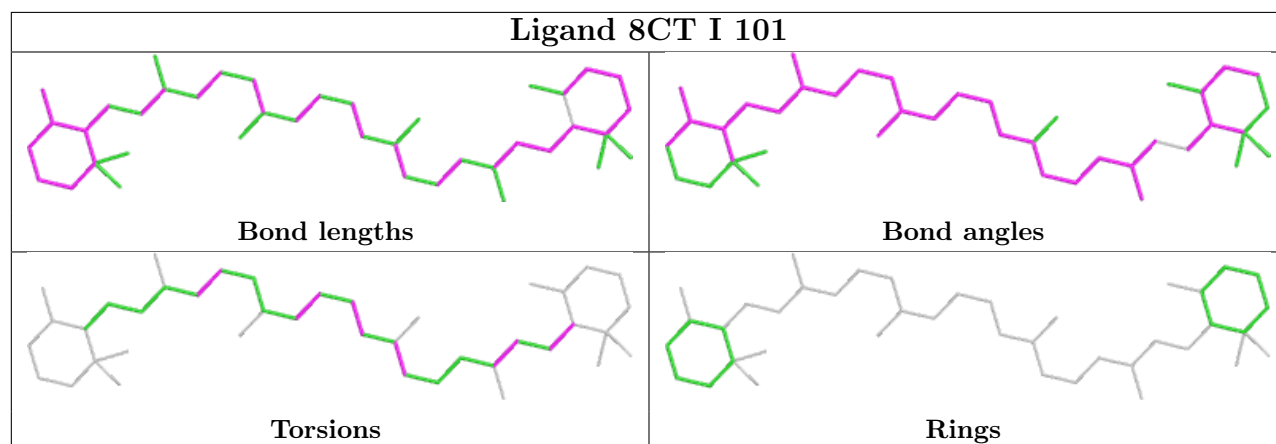
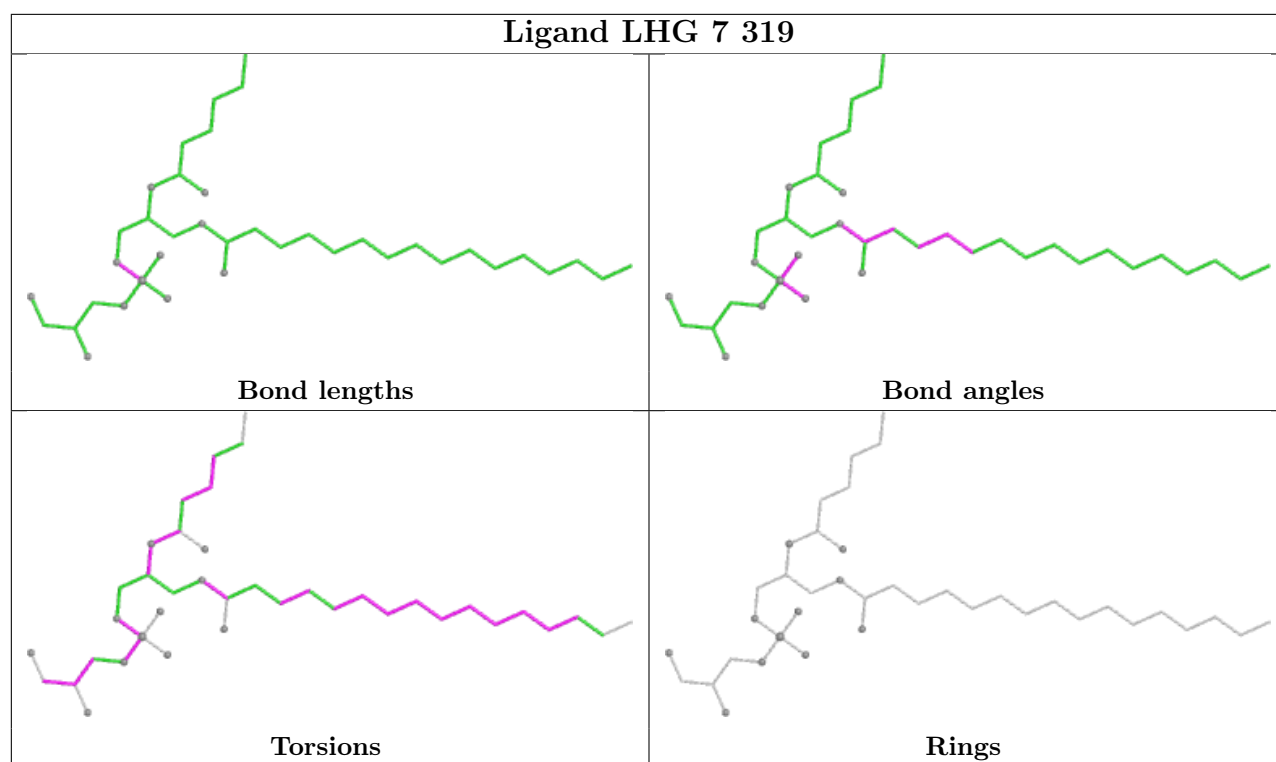
Bond angles



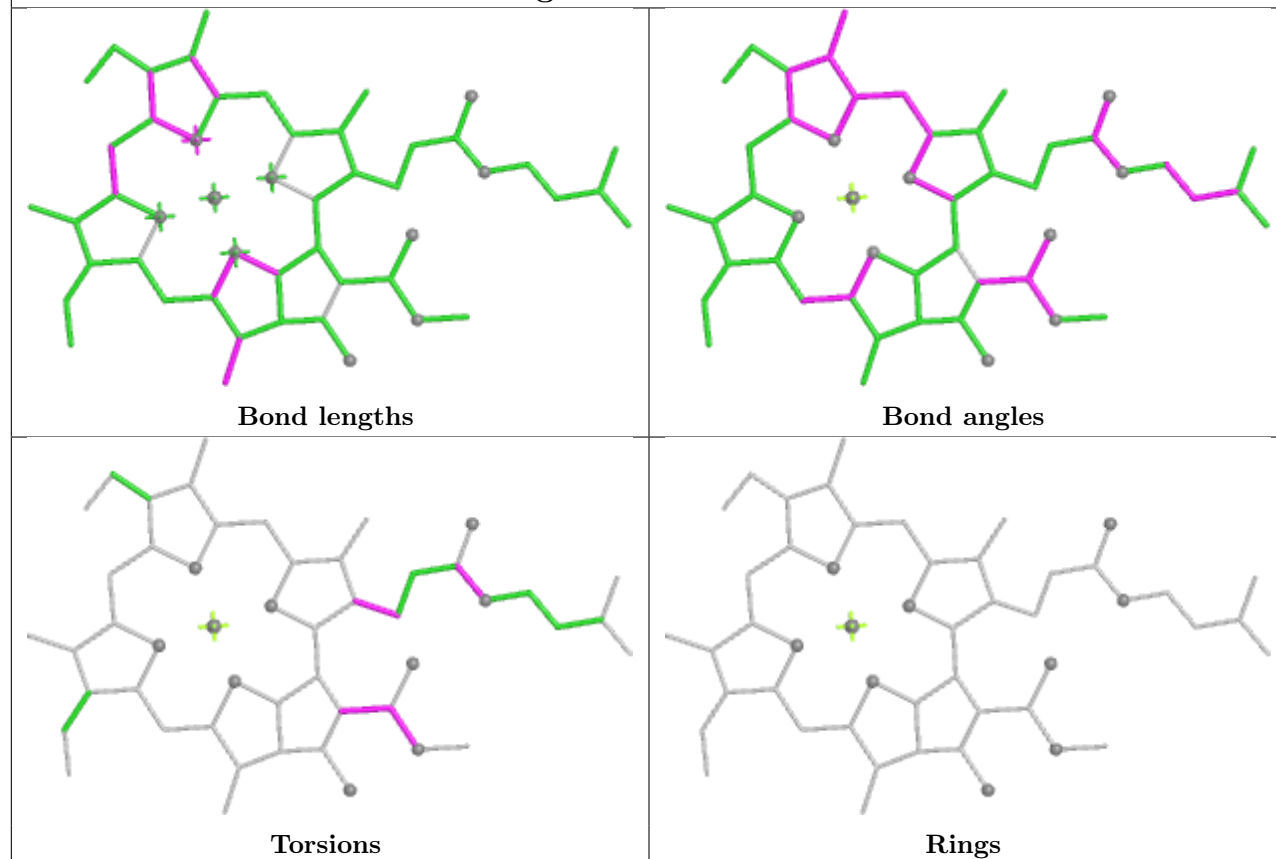
Torsions



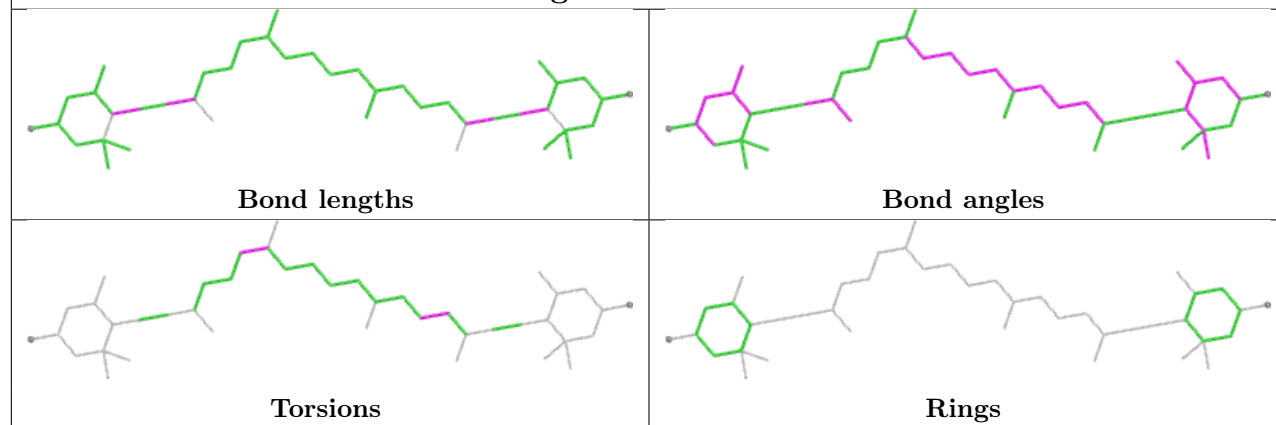
Rings



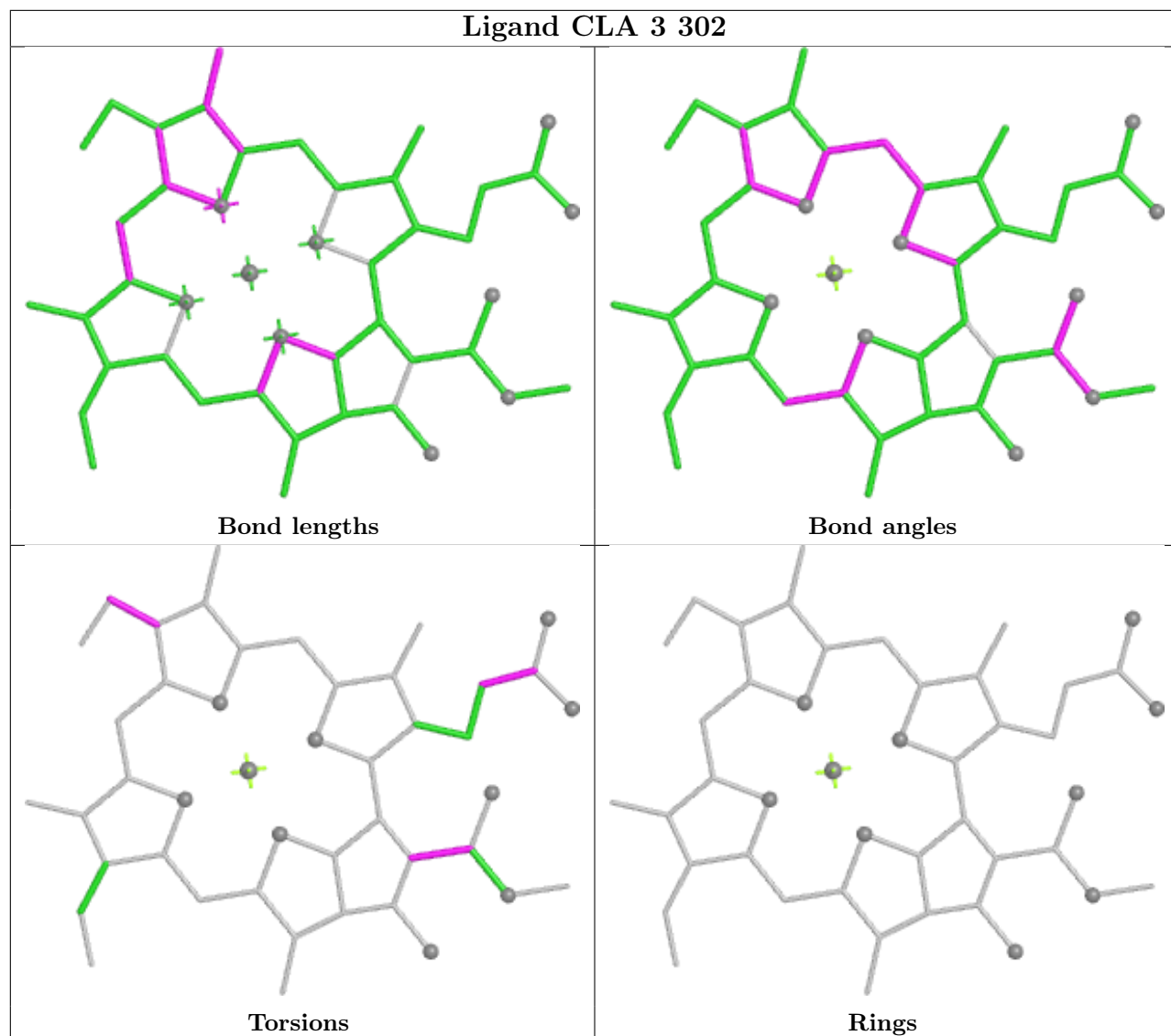
Ligand CLA 2 603



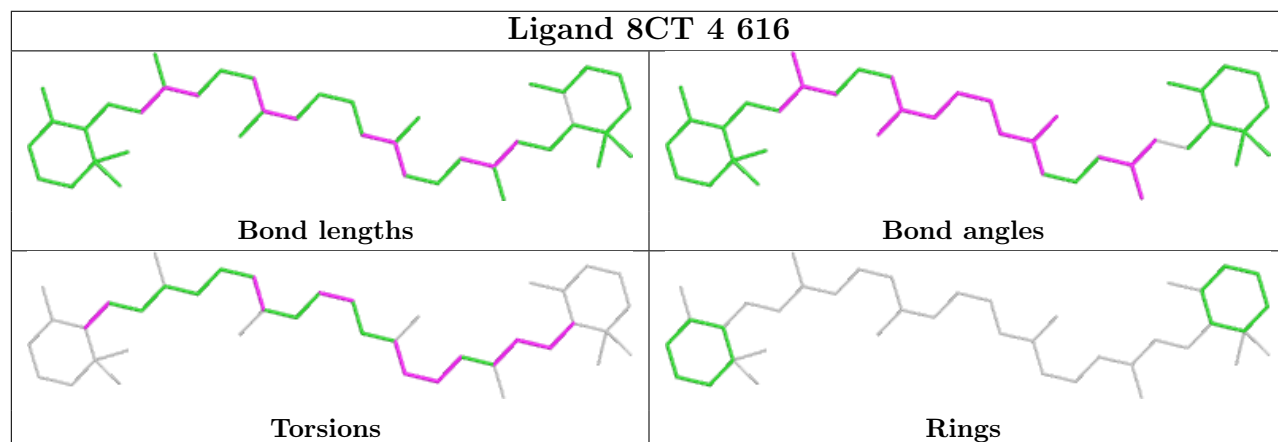
Ligand II0 5 615



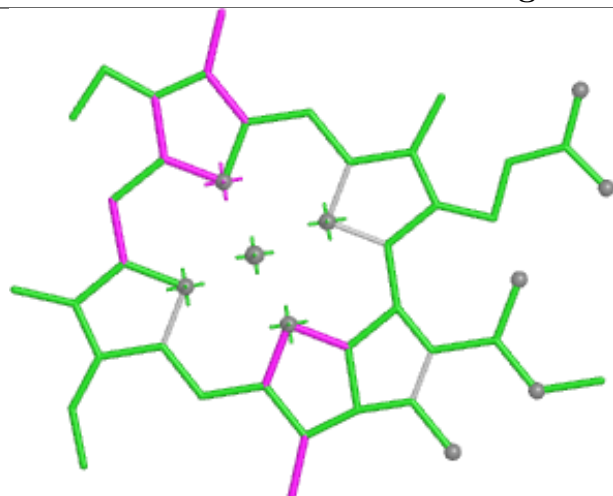
Ligand CLA 3 302



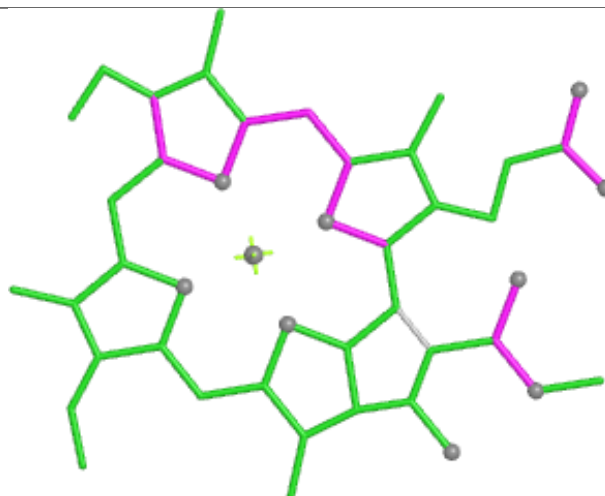
Ligand 8CT 4 616



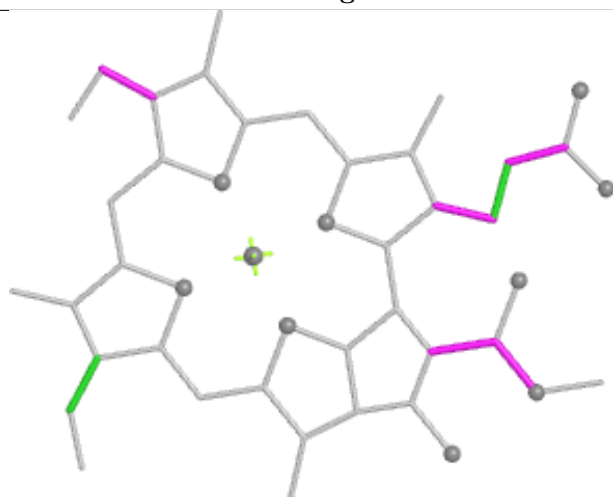
Ligand CLA 1 613



Bond lengths



Bond angles

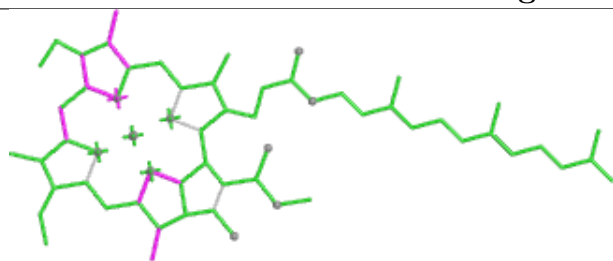


Torsions

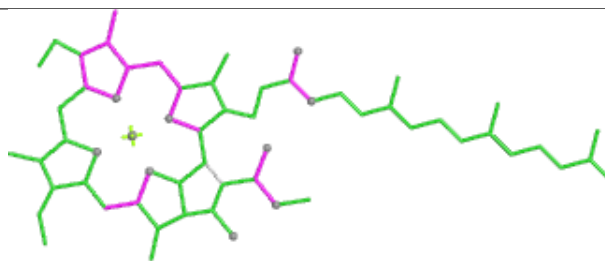


Rings

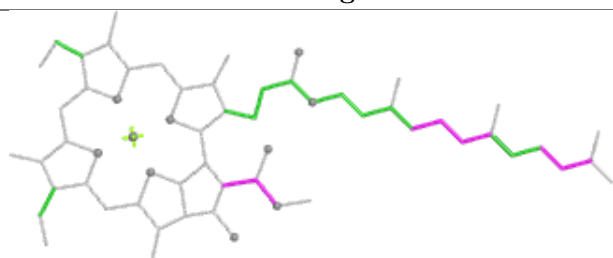
Ligand CLA 4 607



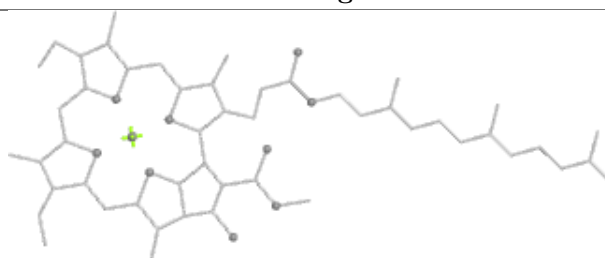
Bond lengths



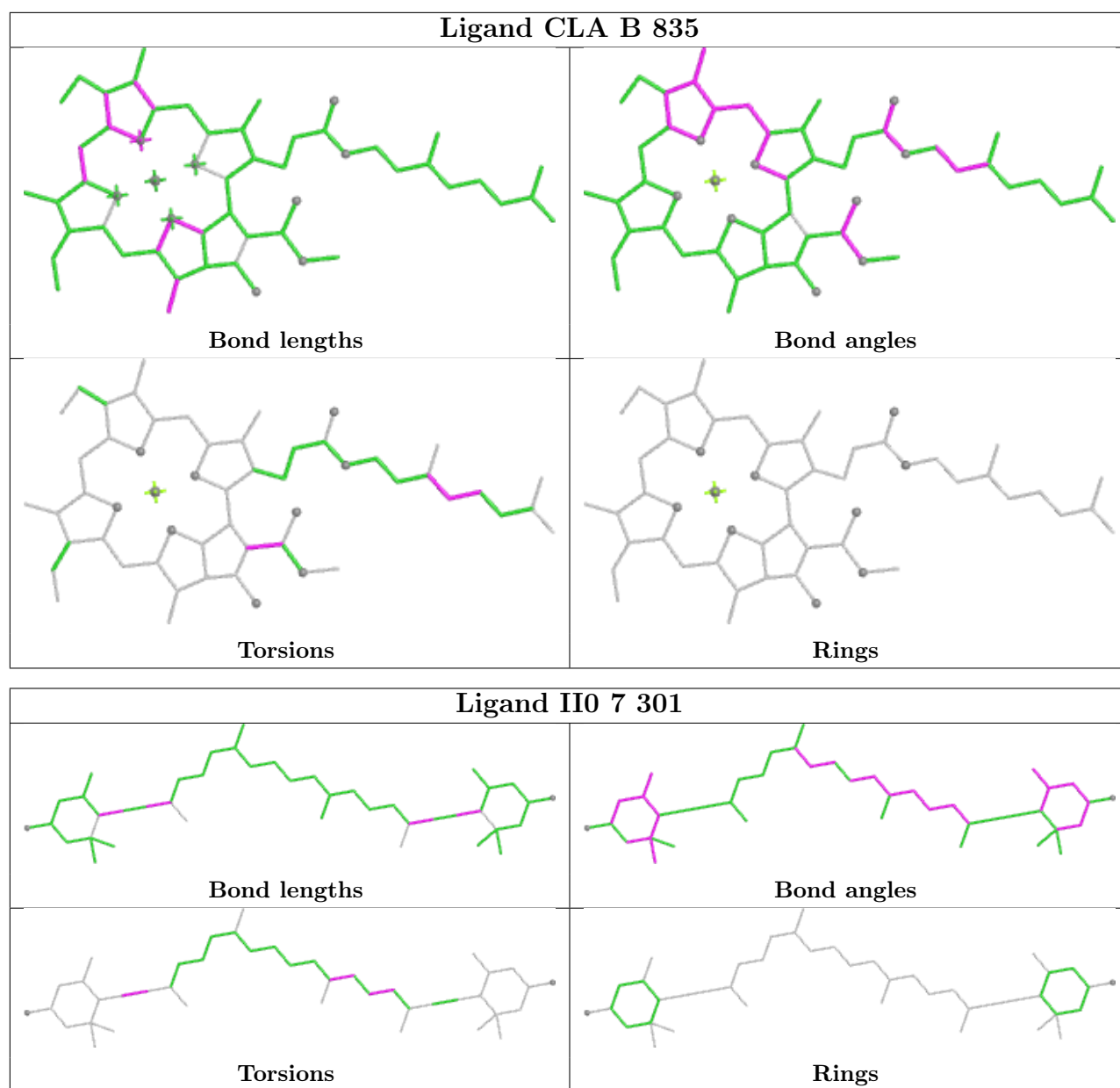
Bond angles

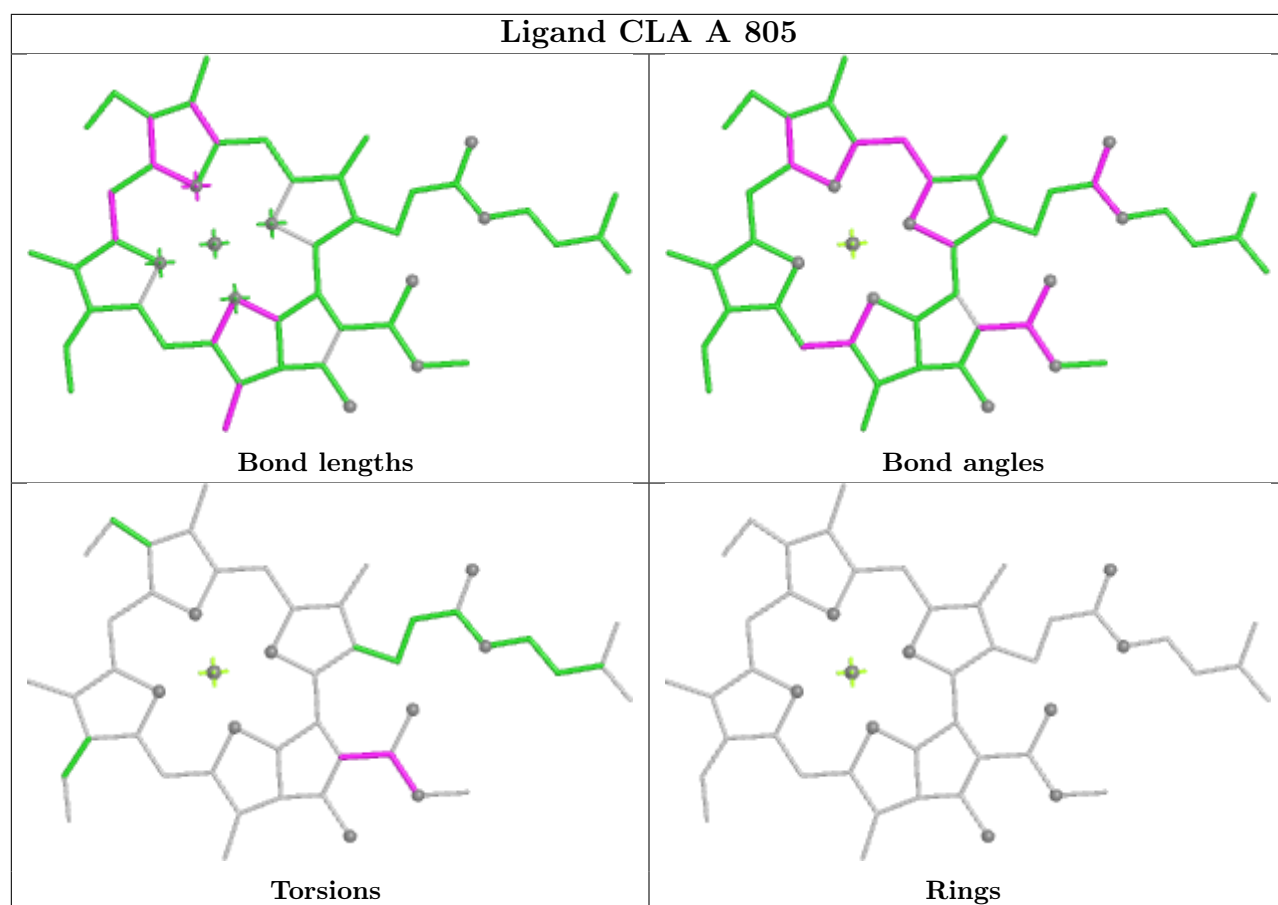


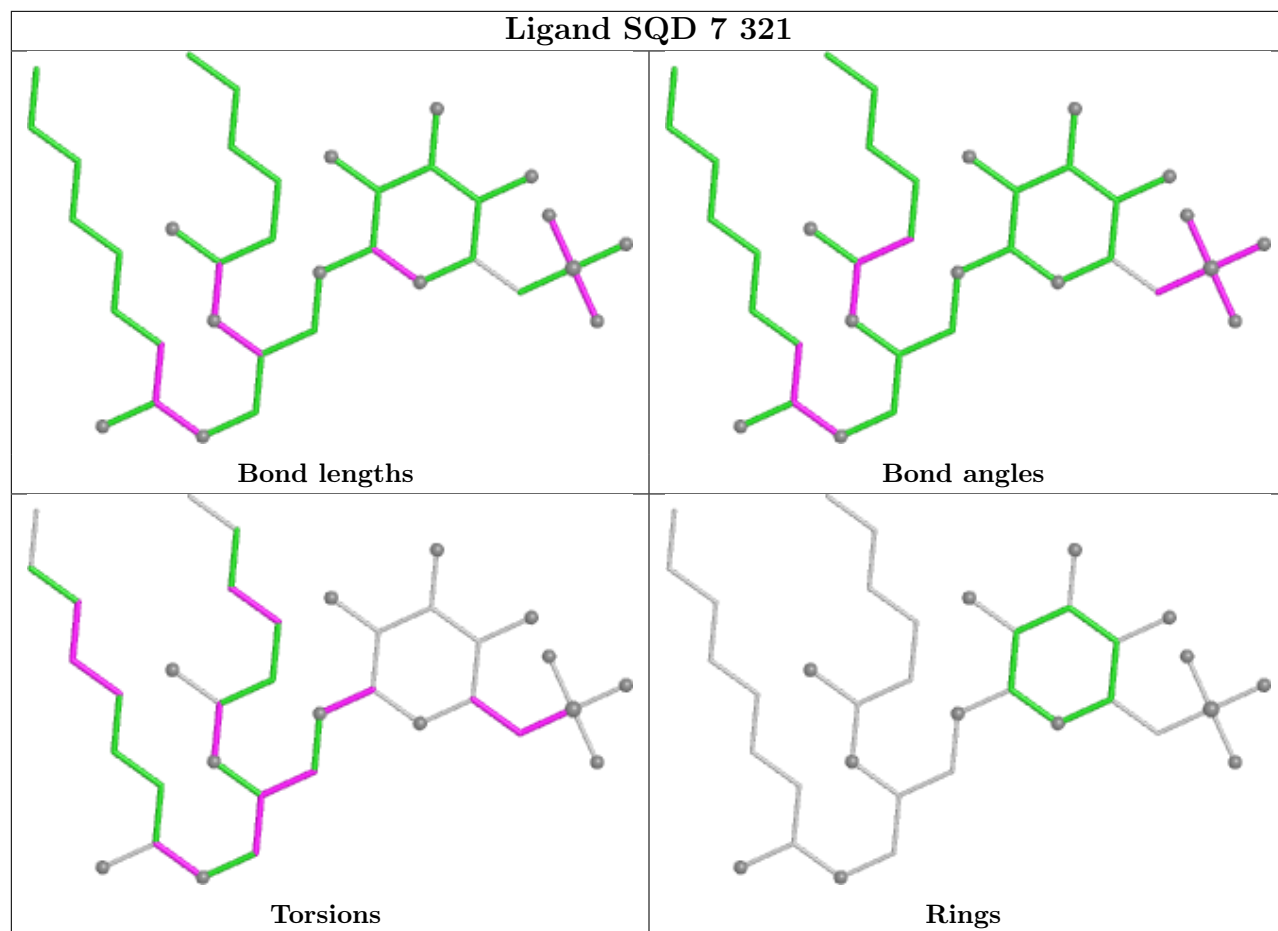
Torsions



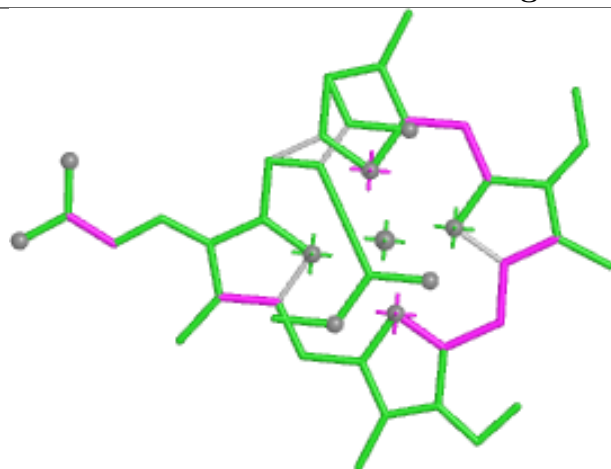
Rings



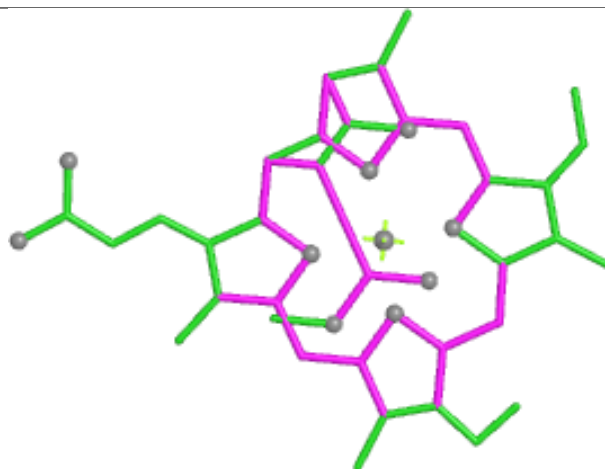




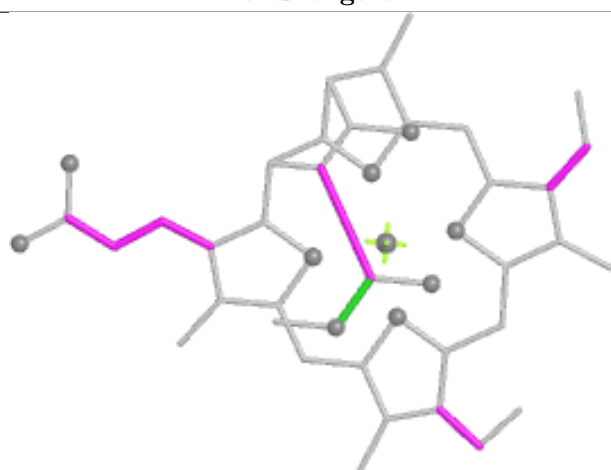
Ligand KC2 a 610



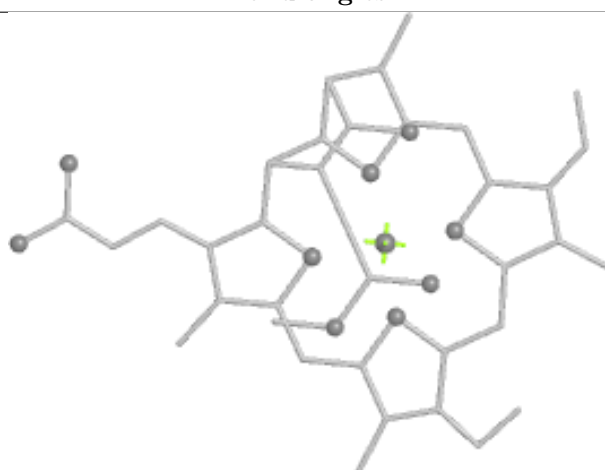
Bond lengths



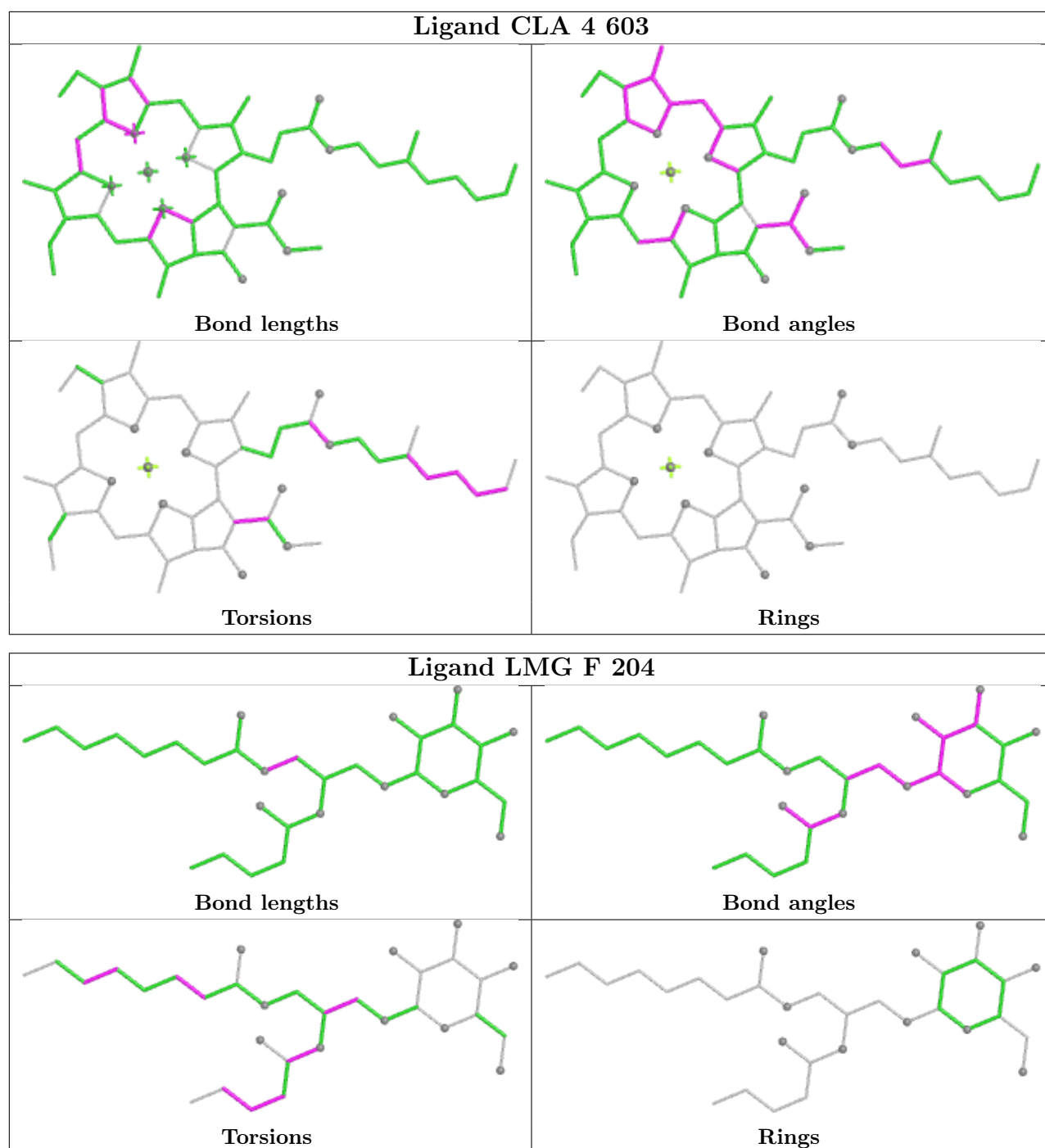
Bond angles

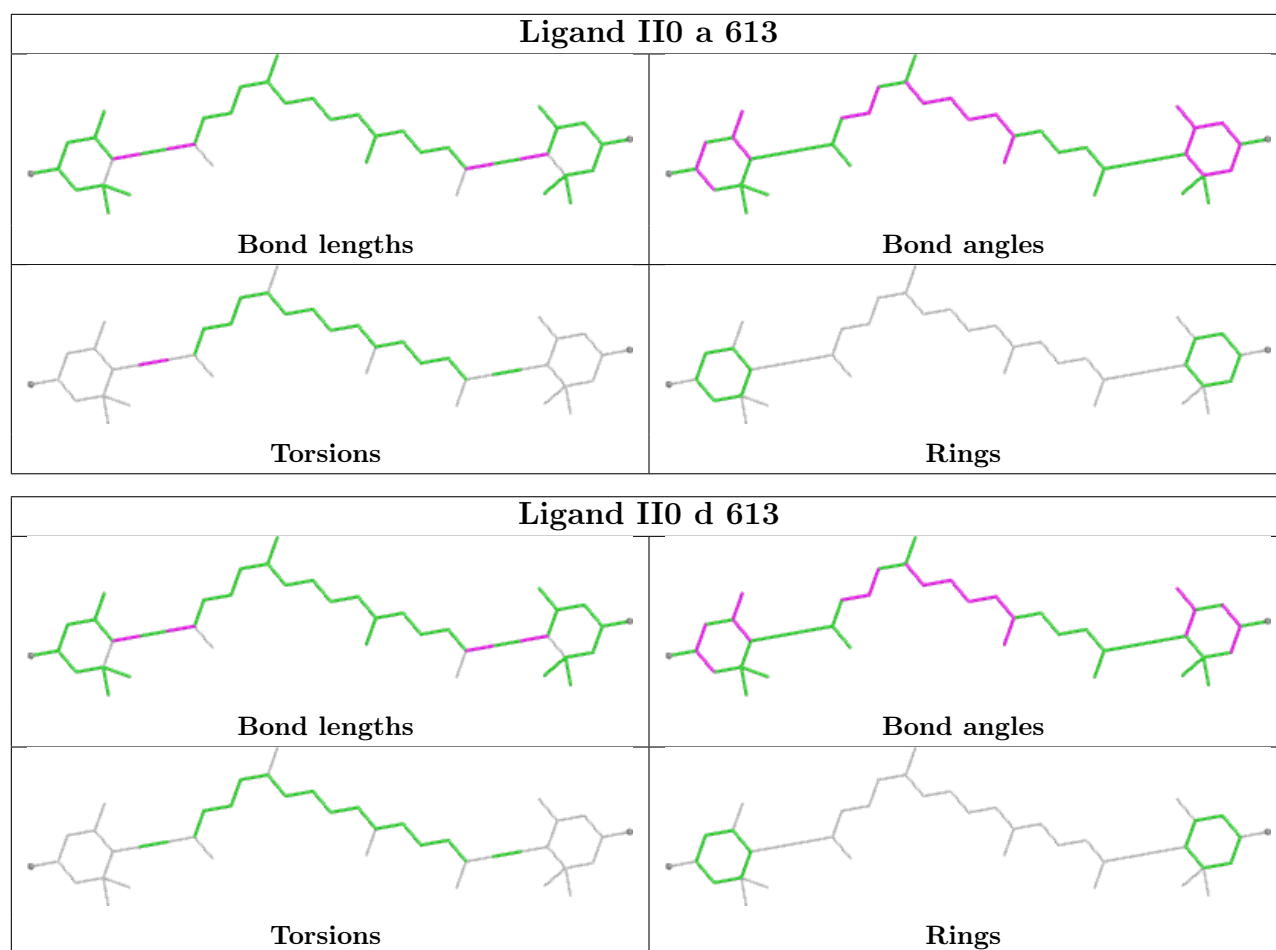


Torsions

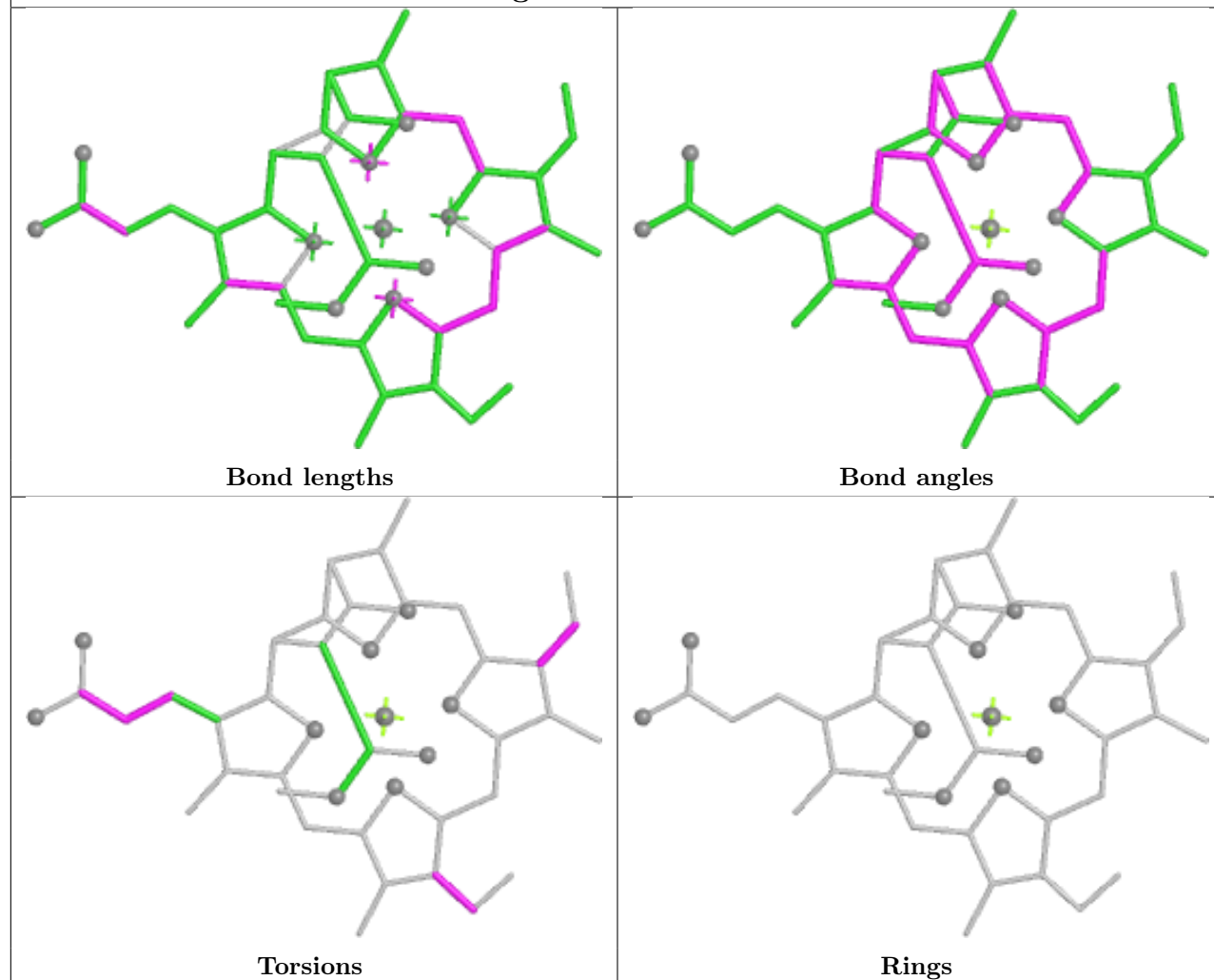


Rings

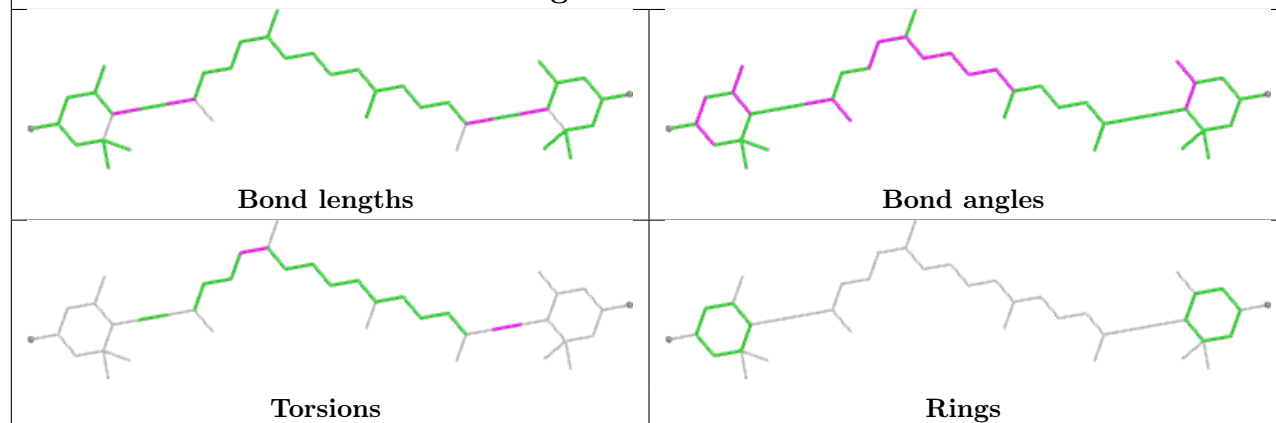




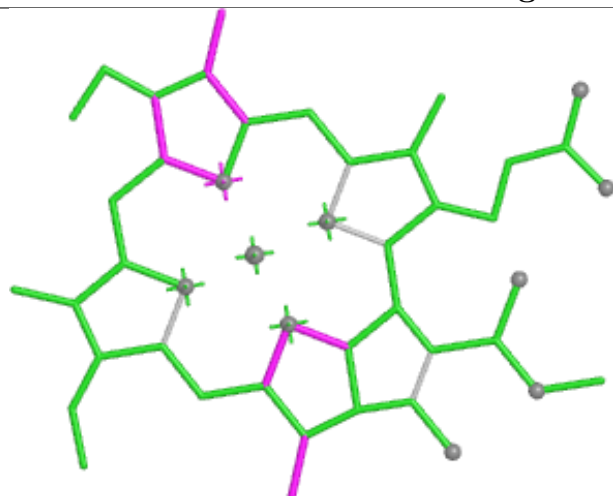
Ligand KC2 e 609



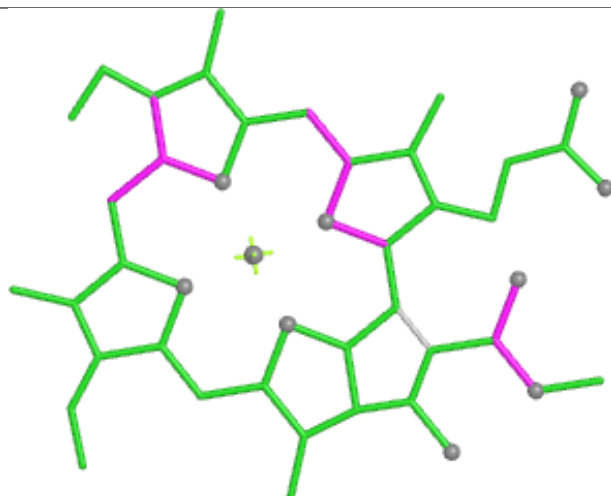
Ligand II0 3 317



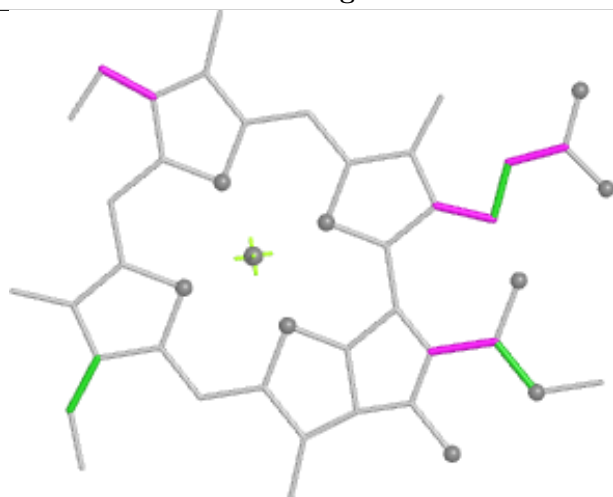
Ligand CLA 5 607



Bond lengths



Bond angles

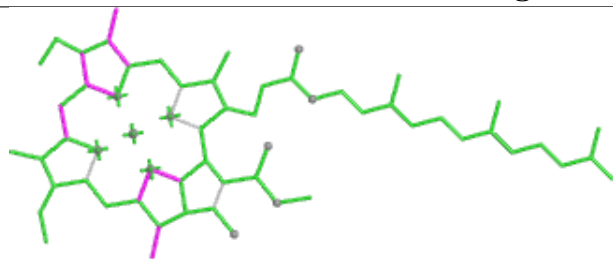


Torsions

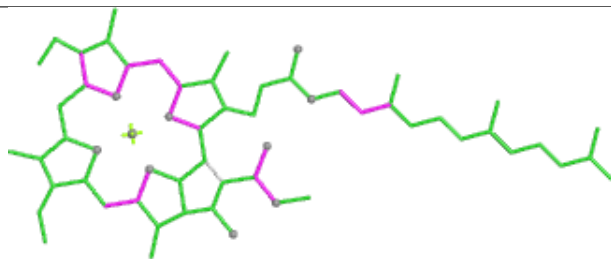


Rings

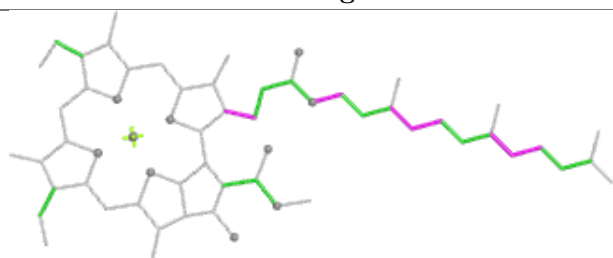
Ligand CLA A 855



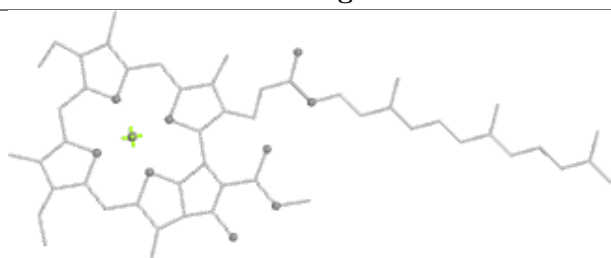
Bond lengths



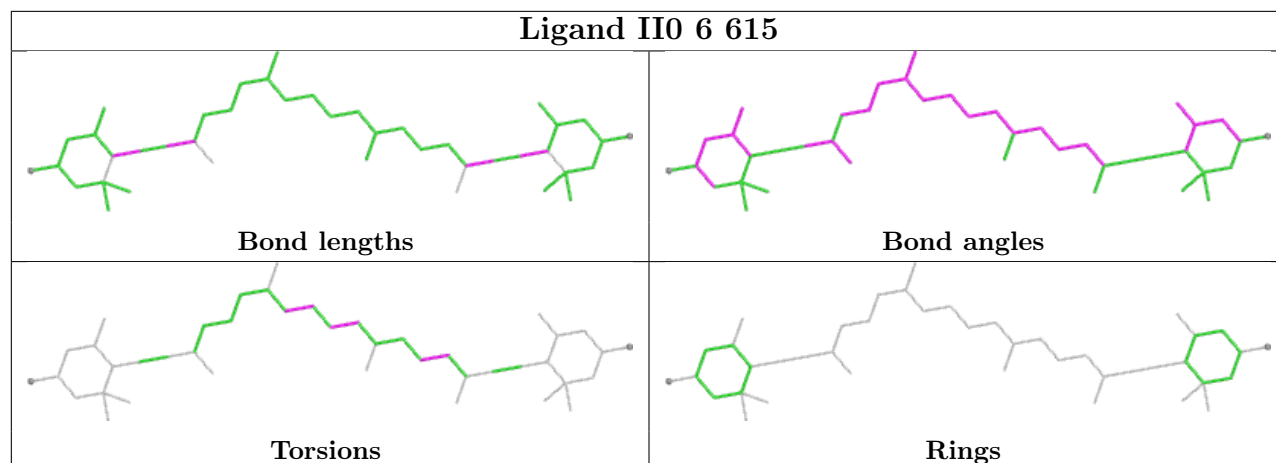
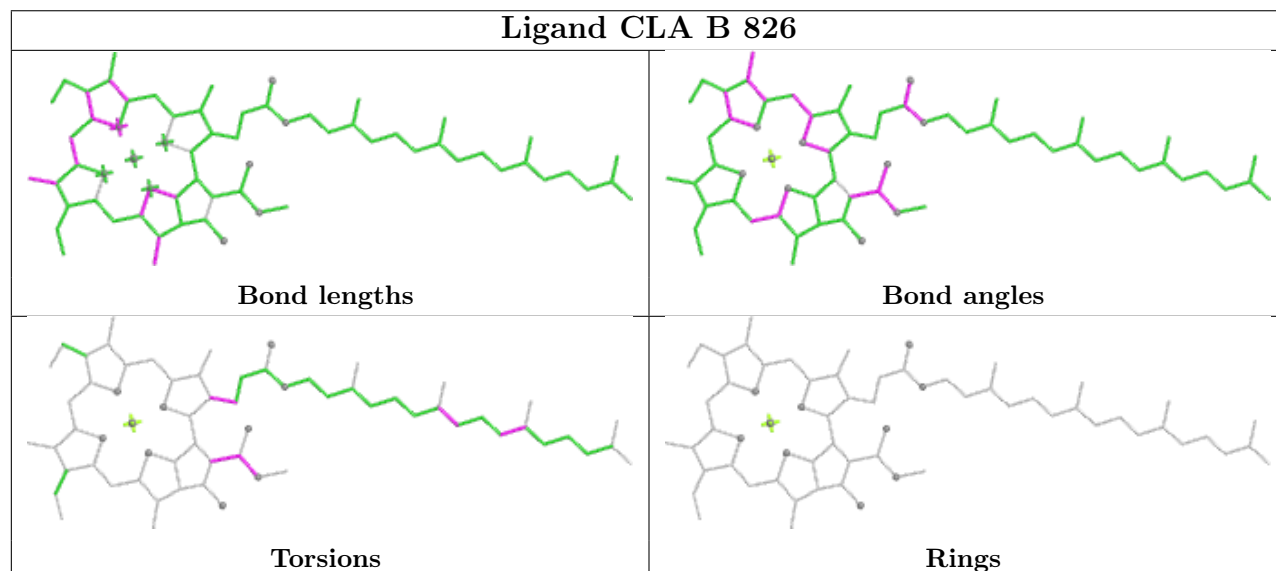
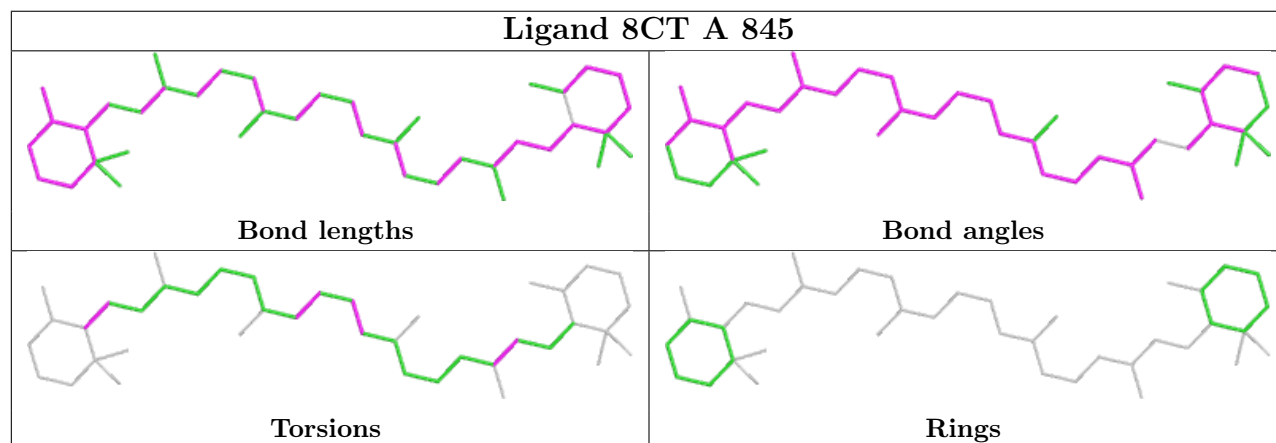
Bond angles



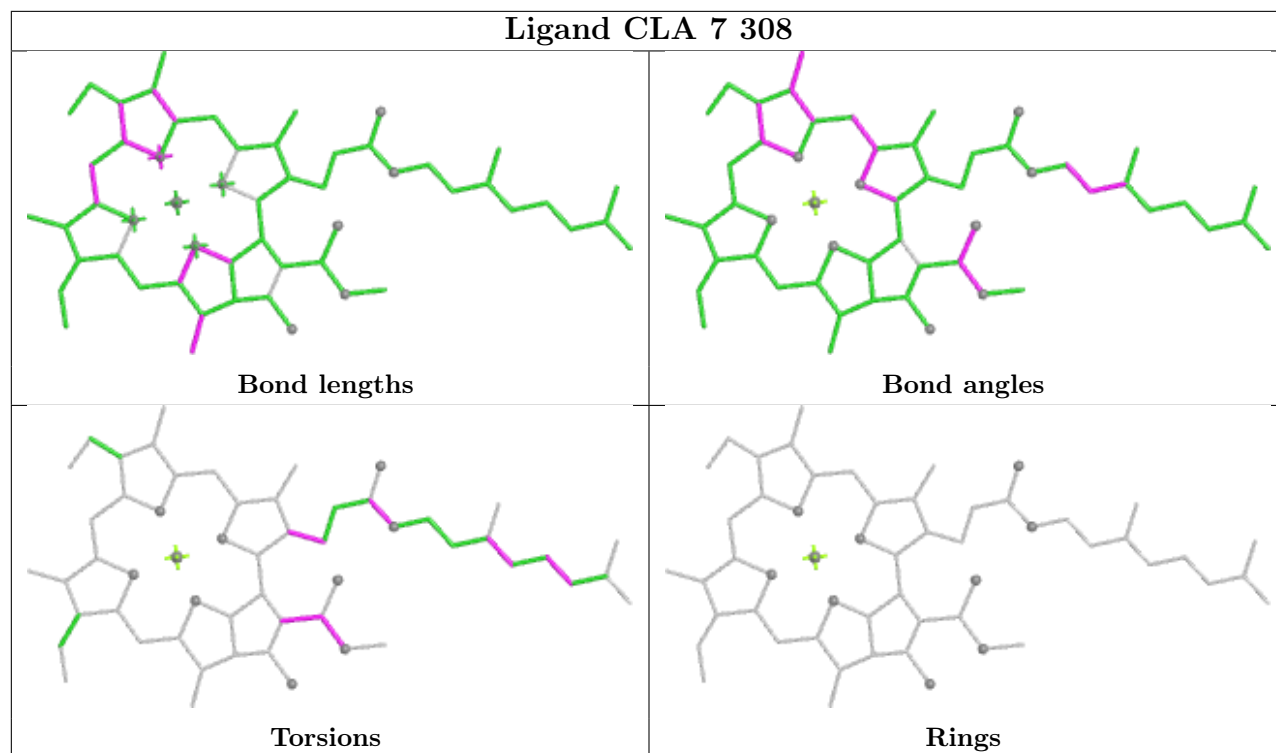
Torsions



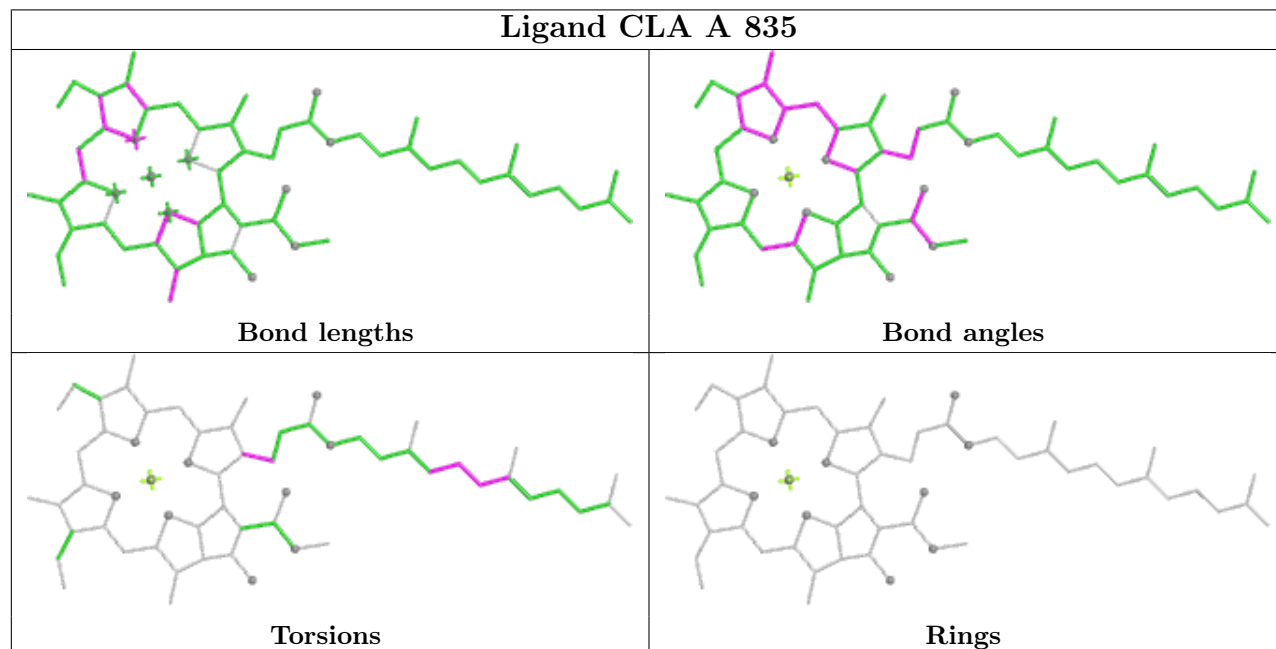
Rings

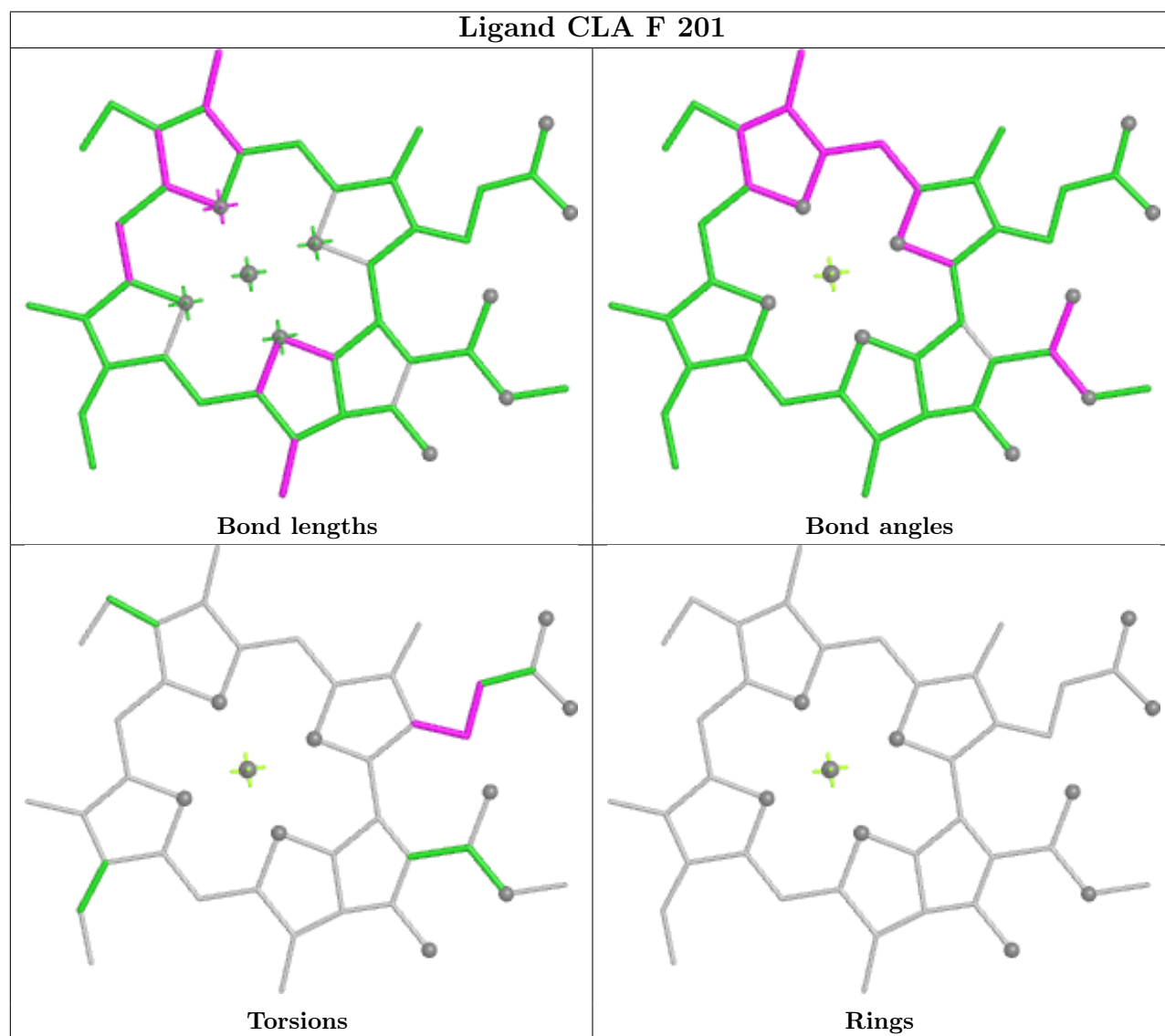
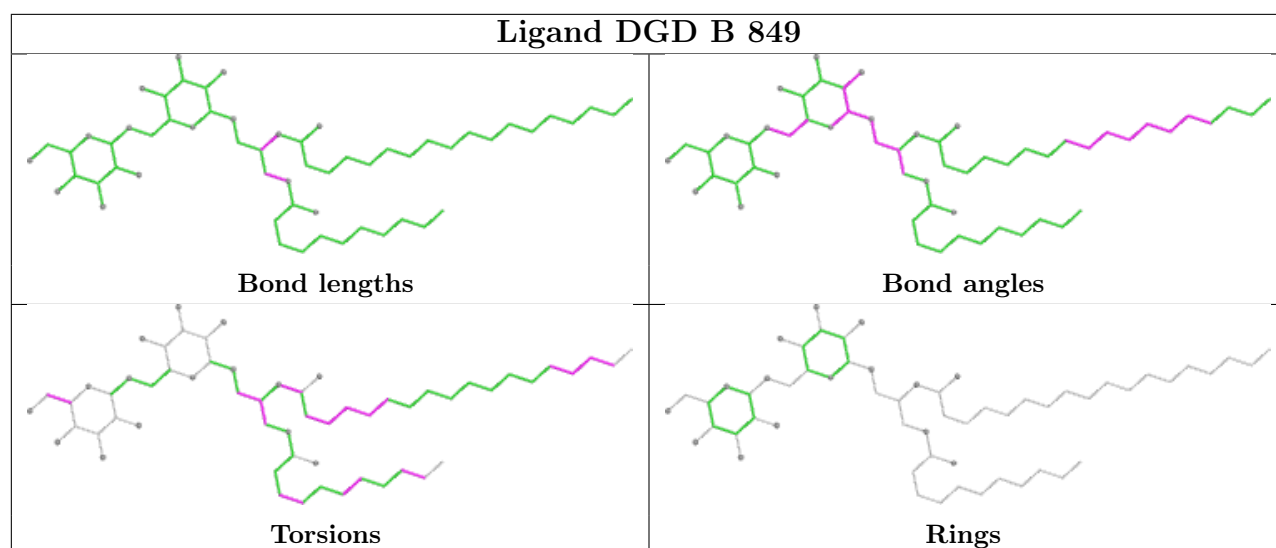
Ligand II0 6 615**Ligand CLA B 826****Ligand 8CT A 845**

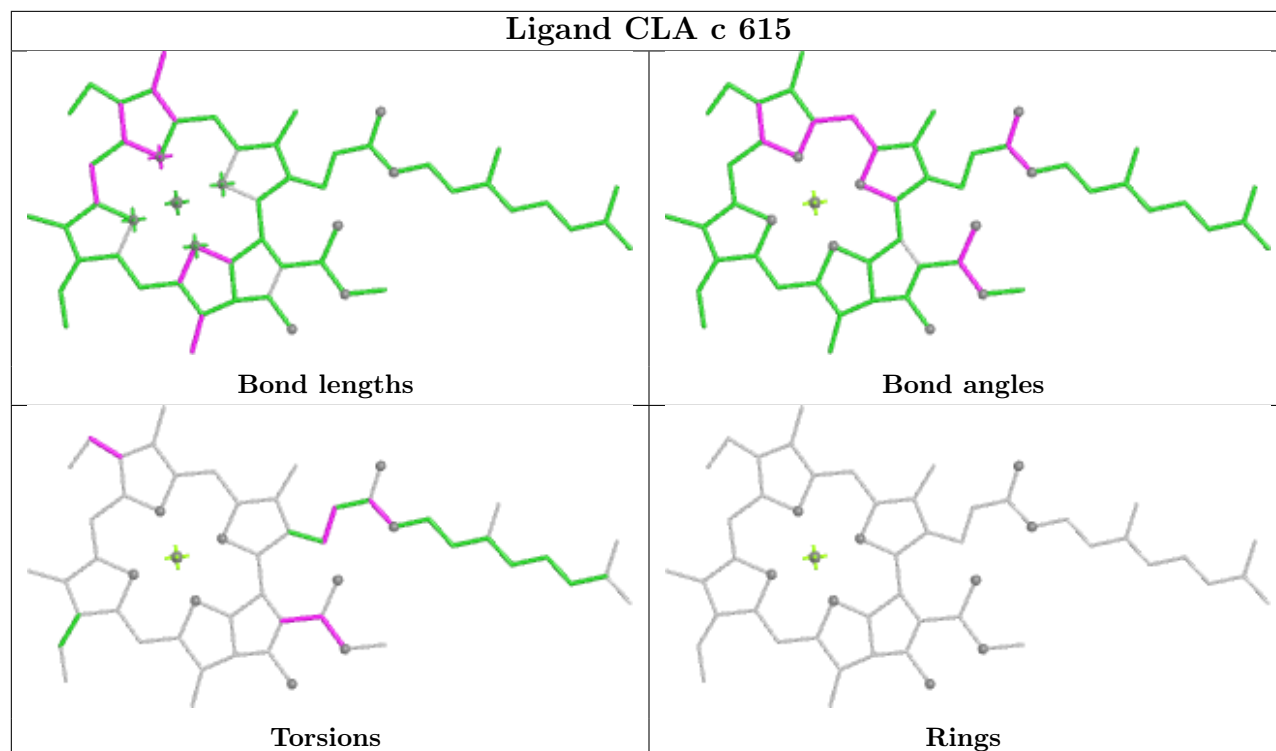
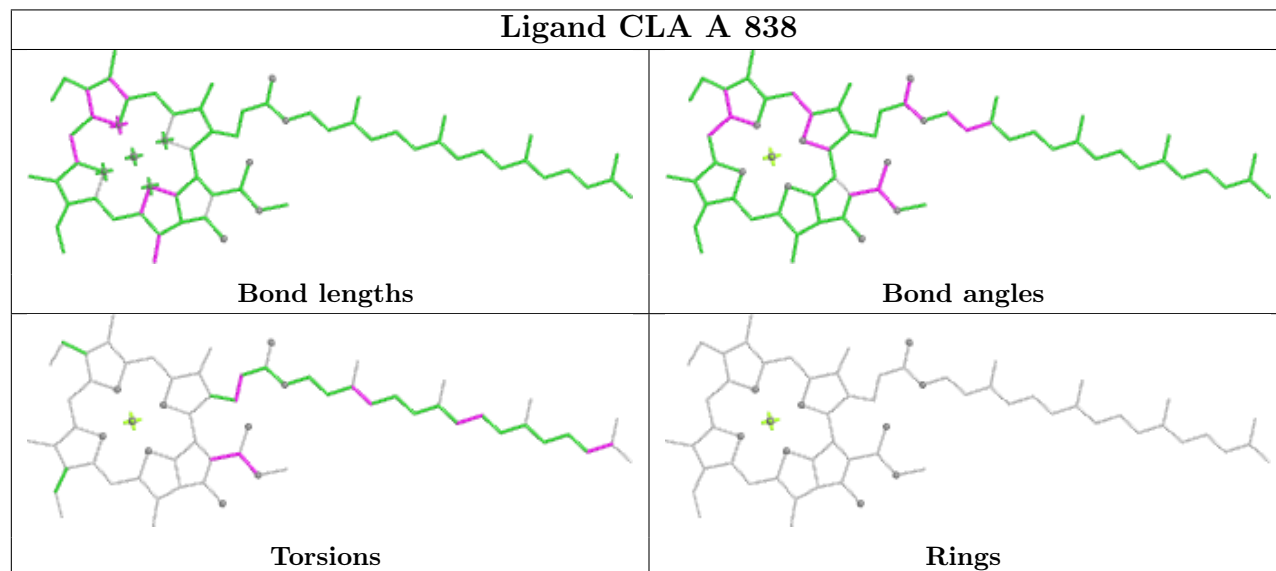
Ligand CLA 7 308

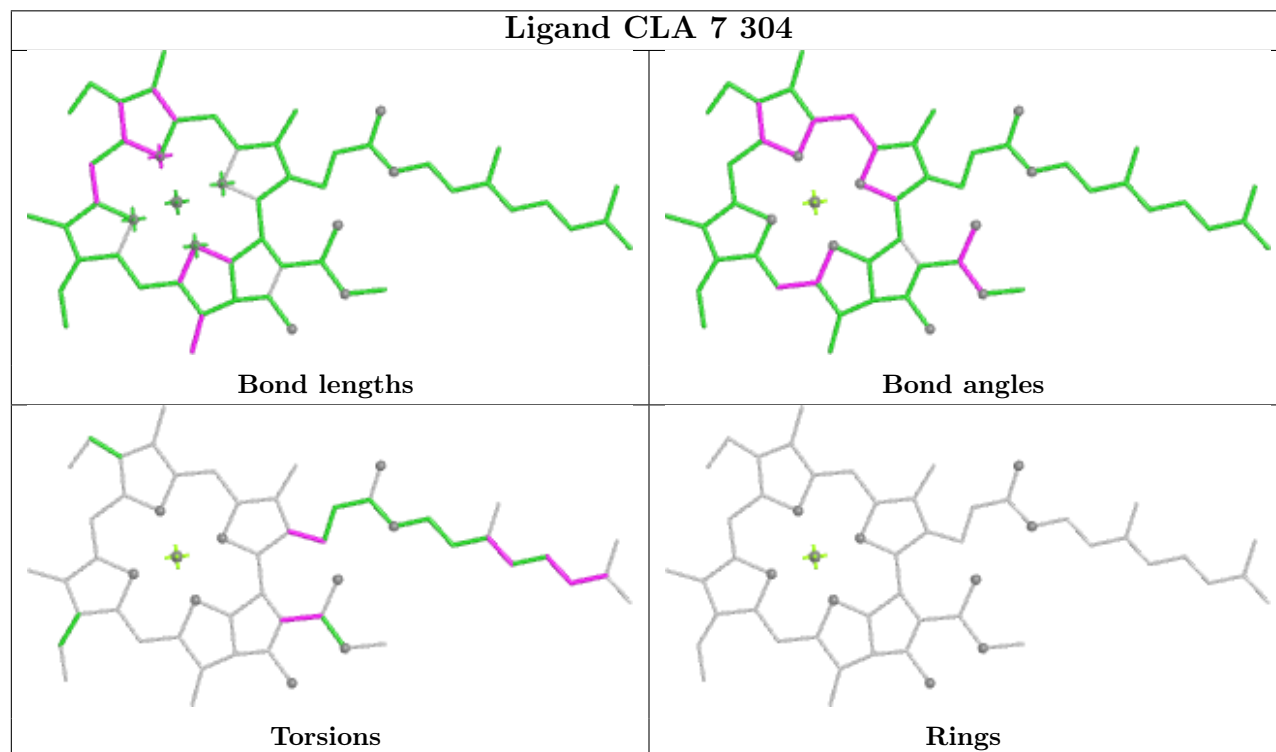
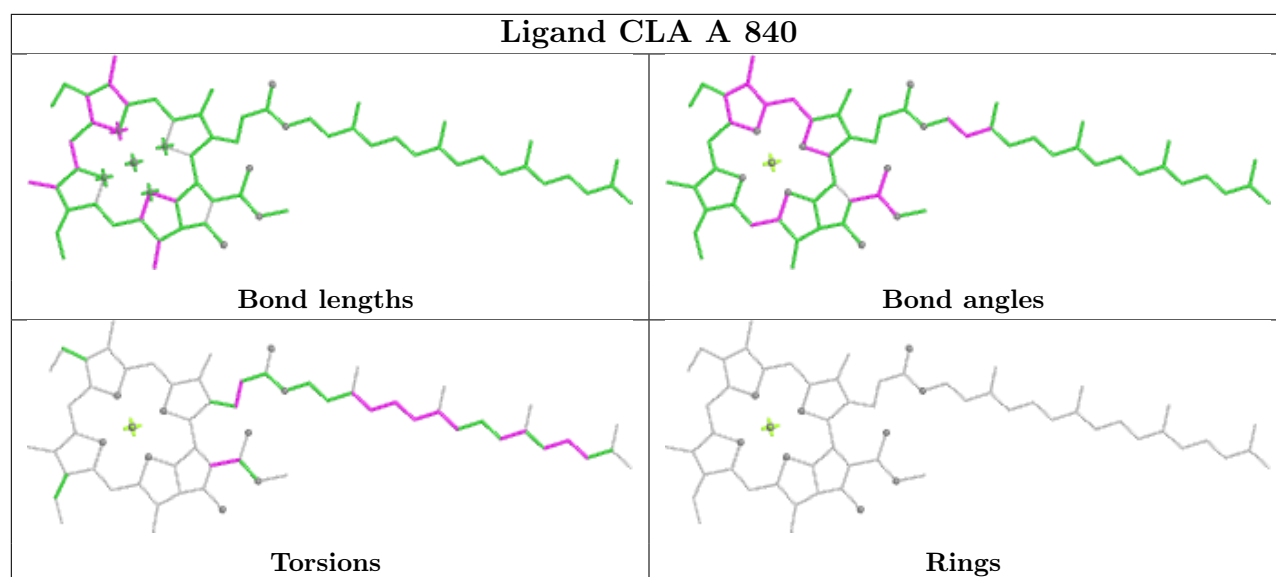


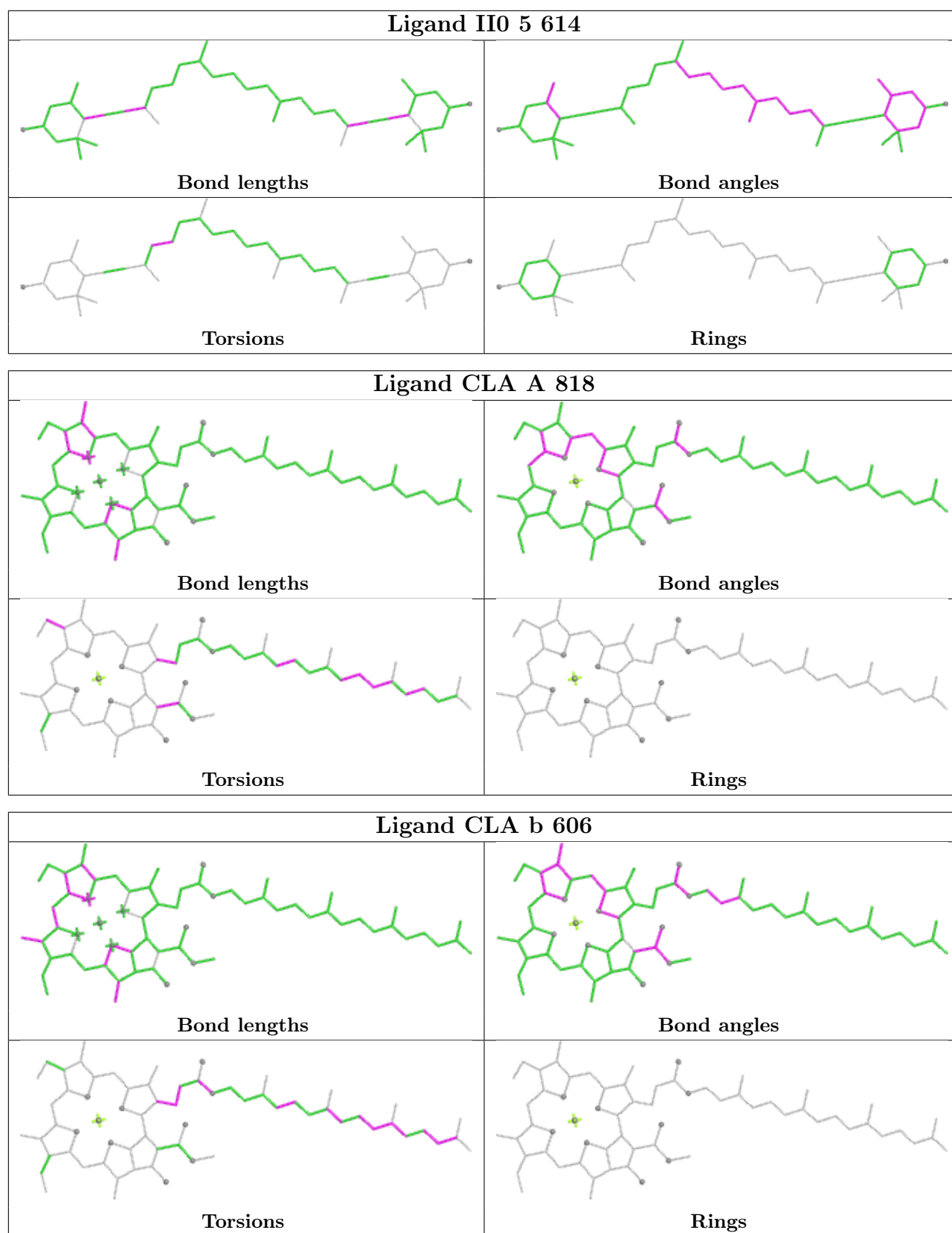
Ligand CLA A 835



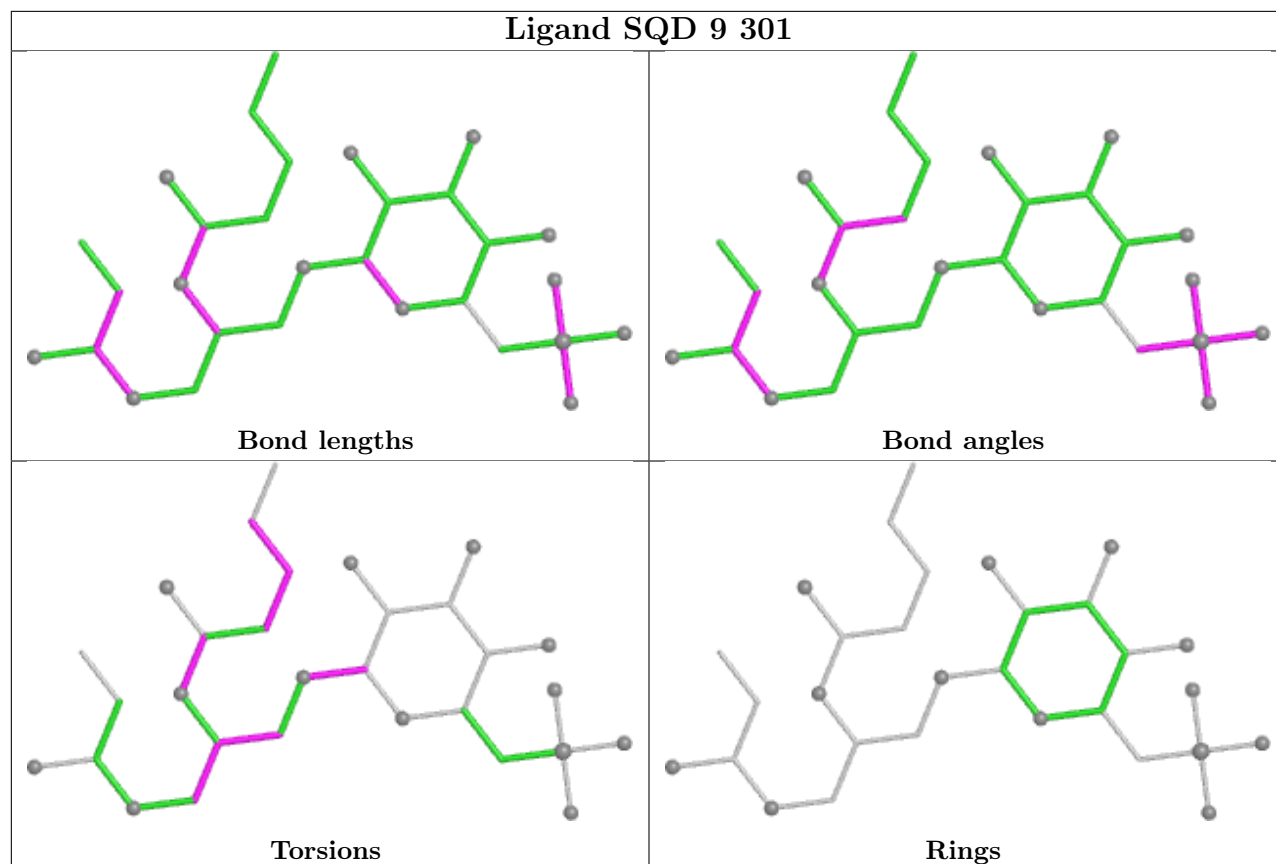


Ligand CLA c 615**Ligand CLA A 838**

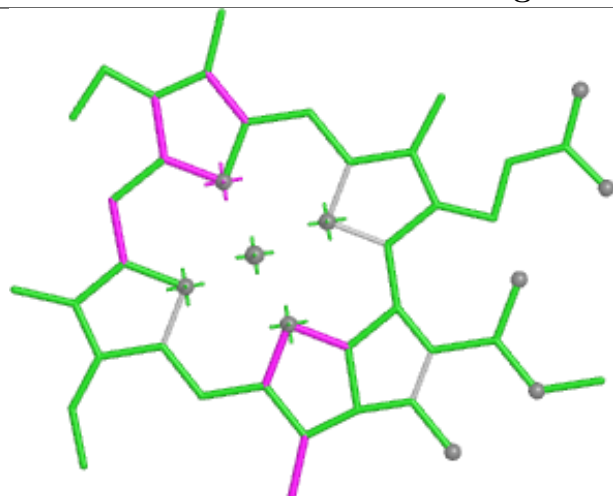




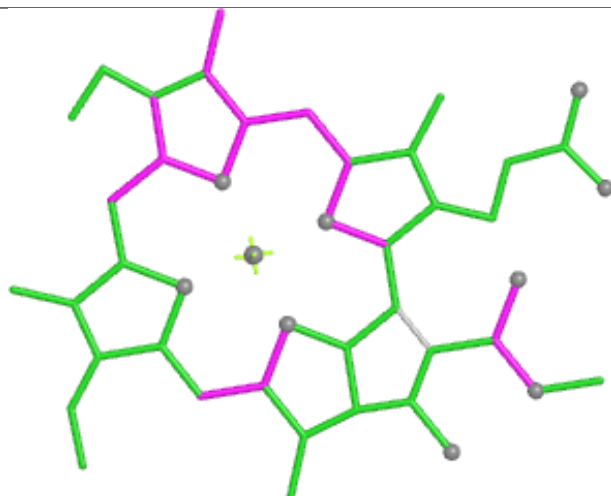
Ligand SQD 9 301



Ligand CLA A 814



Bond lengths



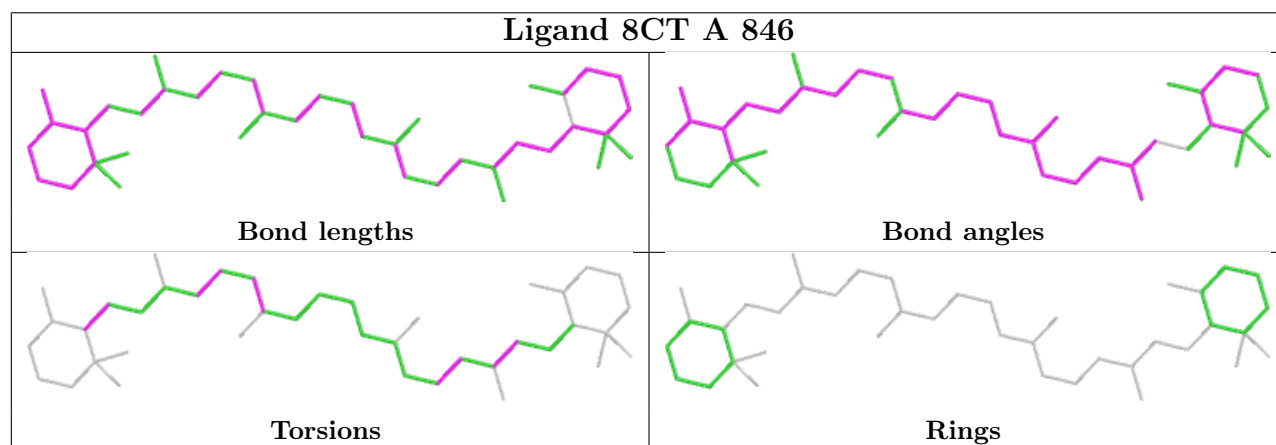
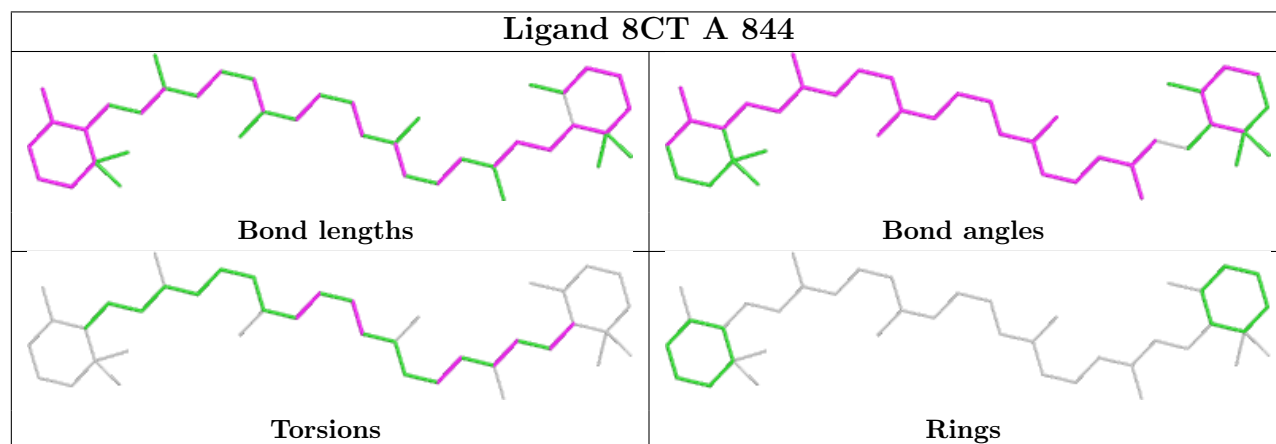
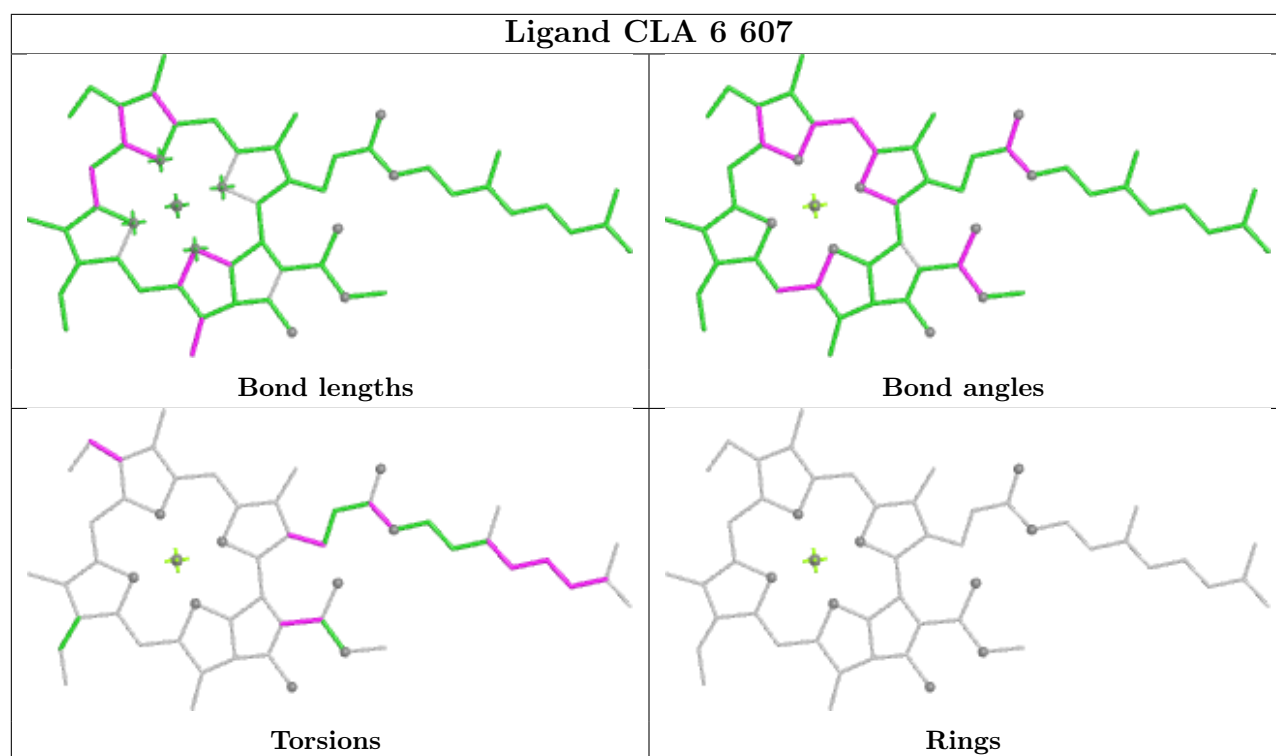
Bond angles

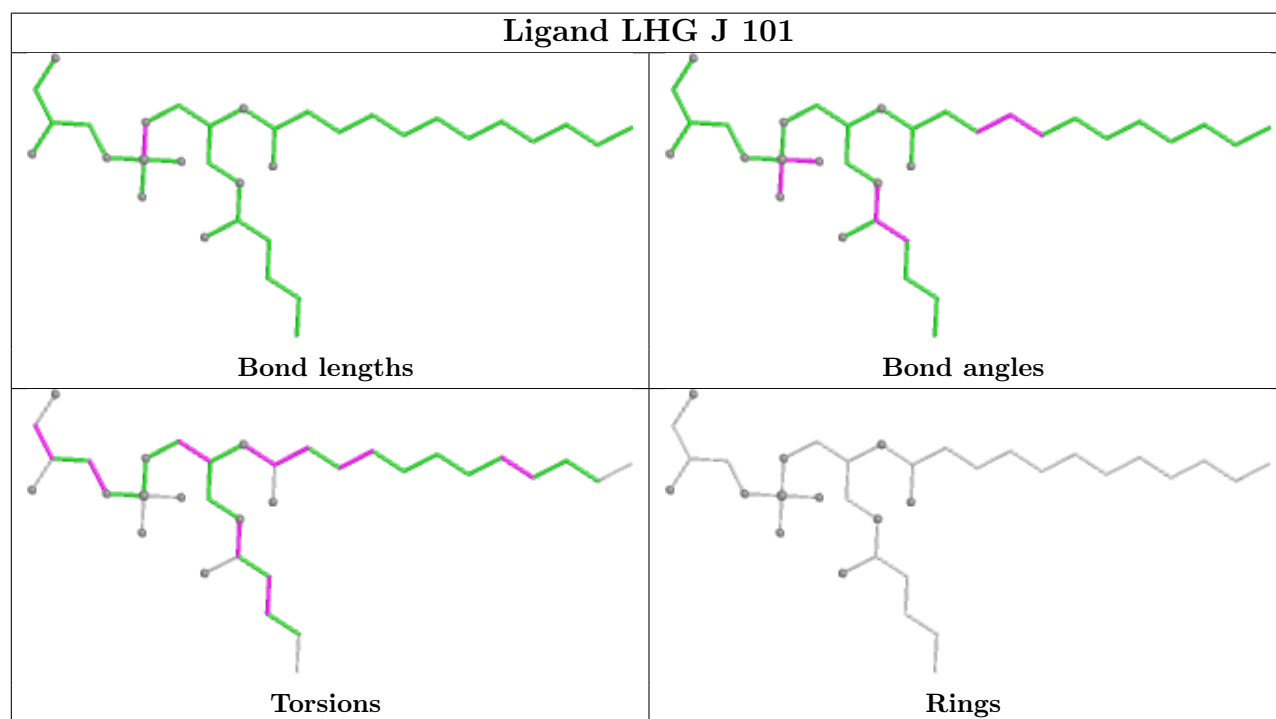
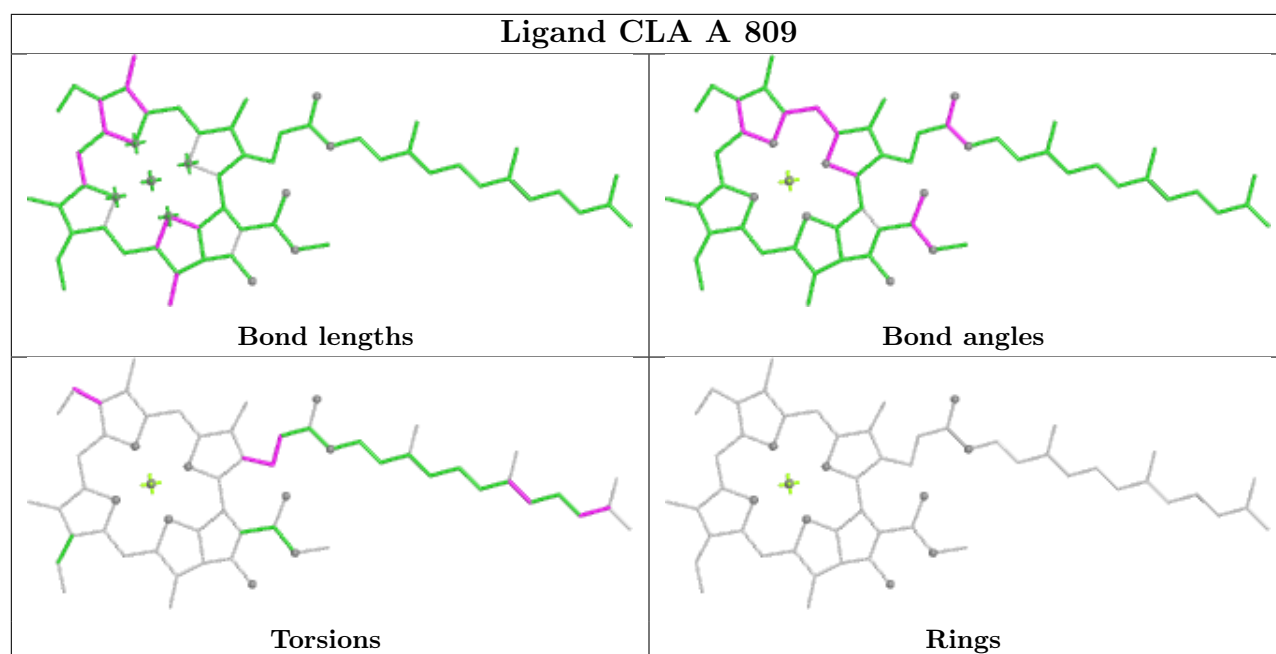


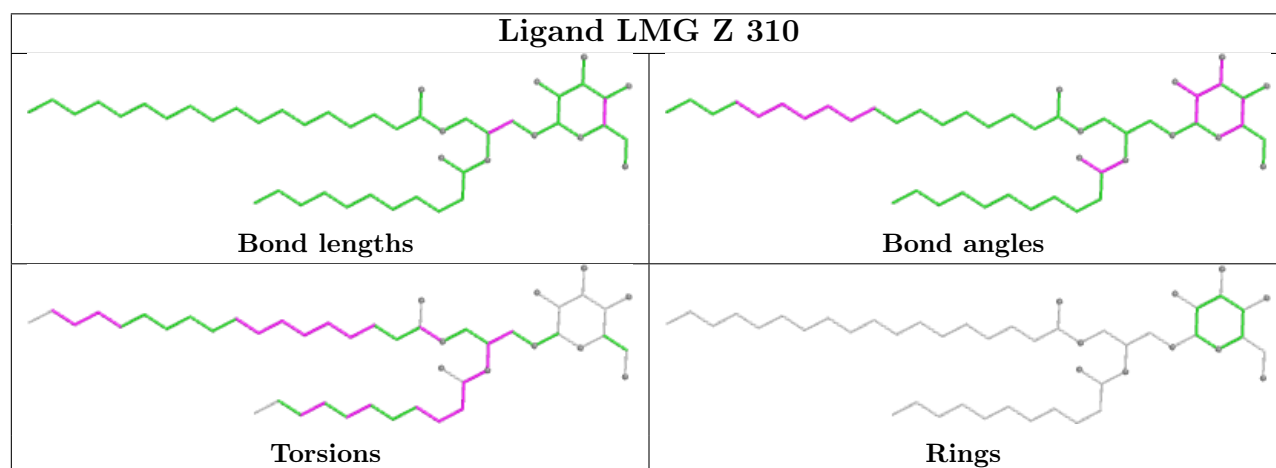
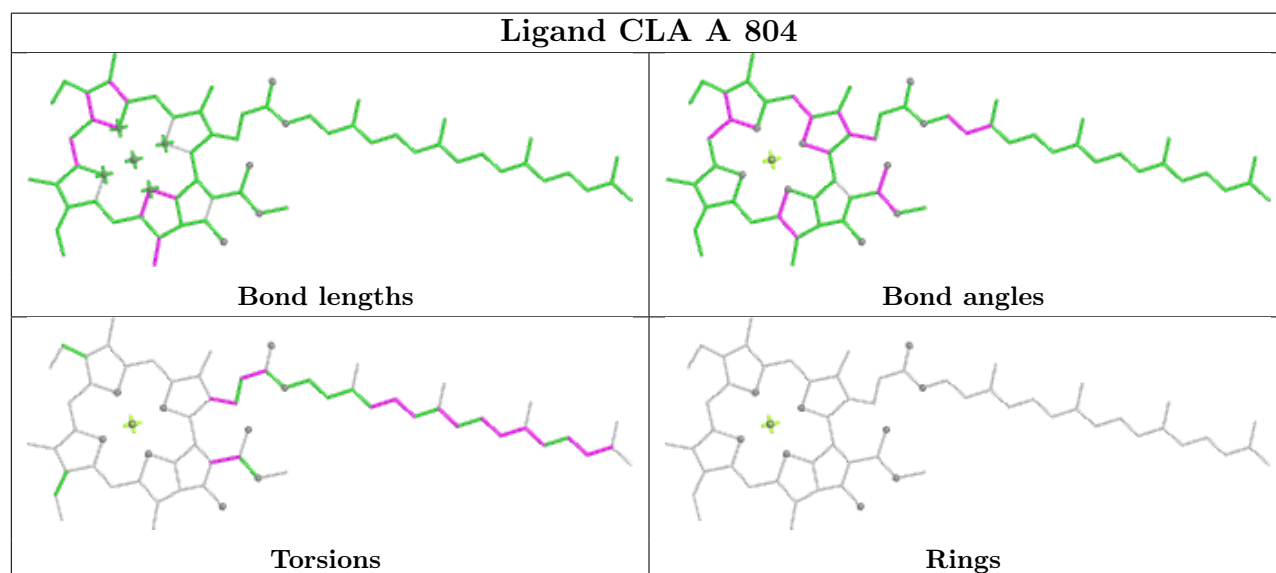
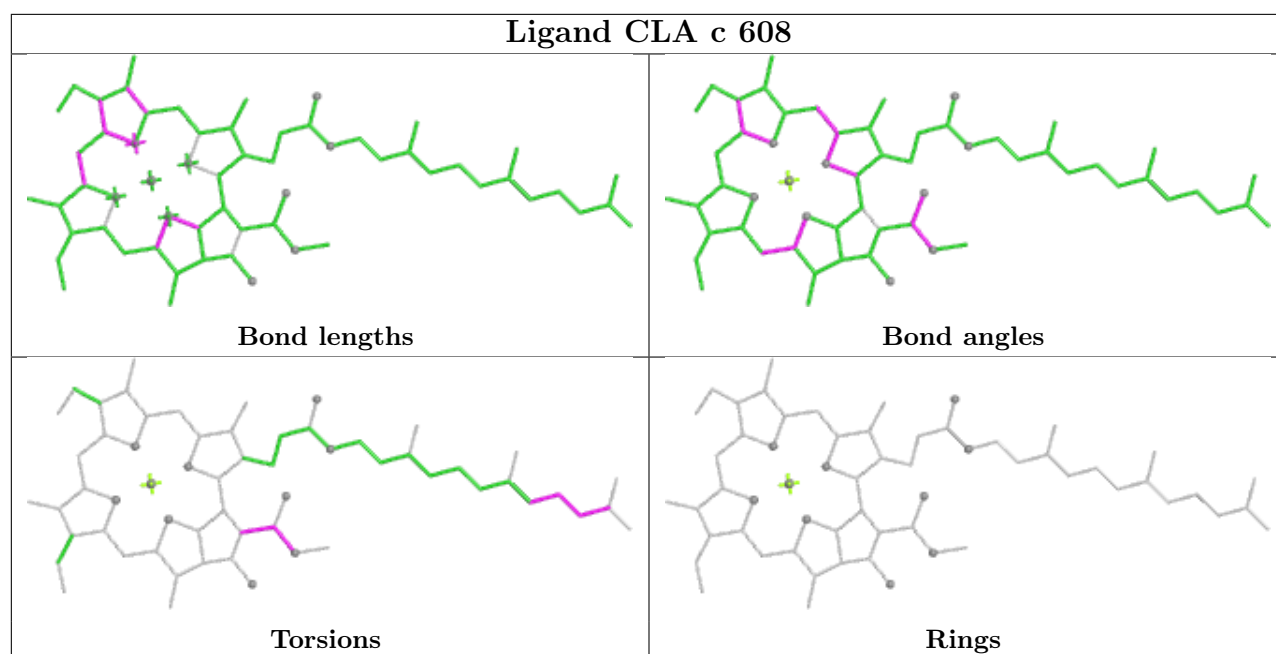
Torsions

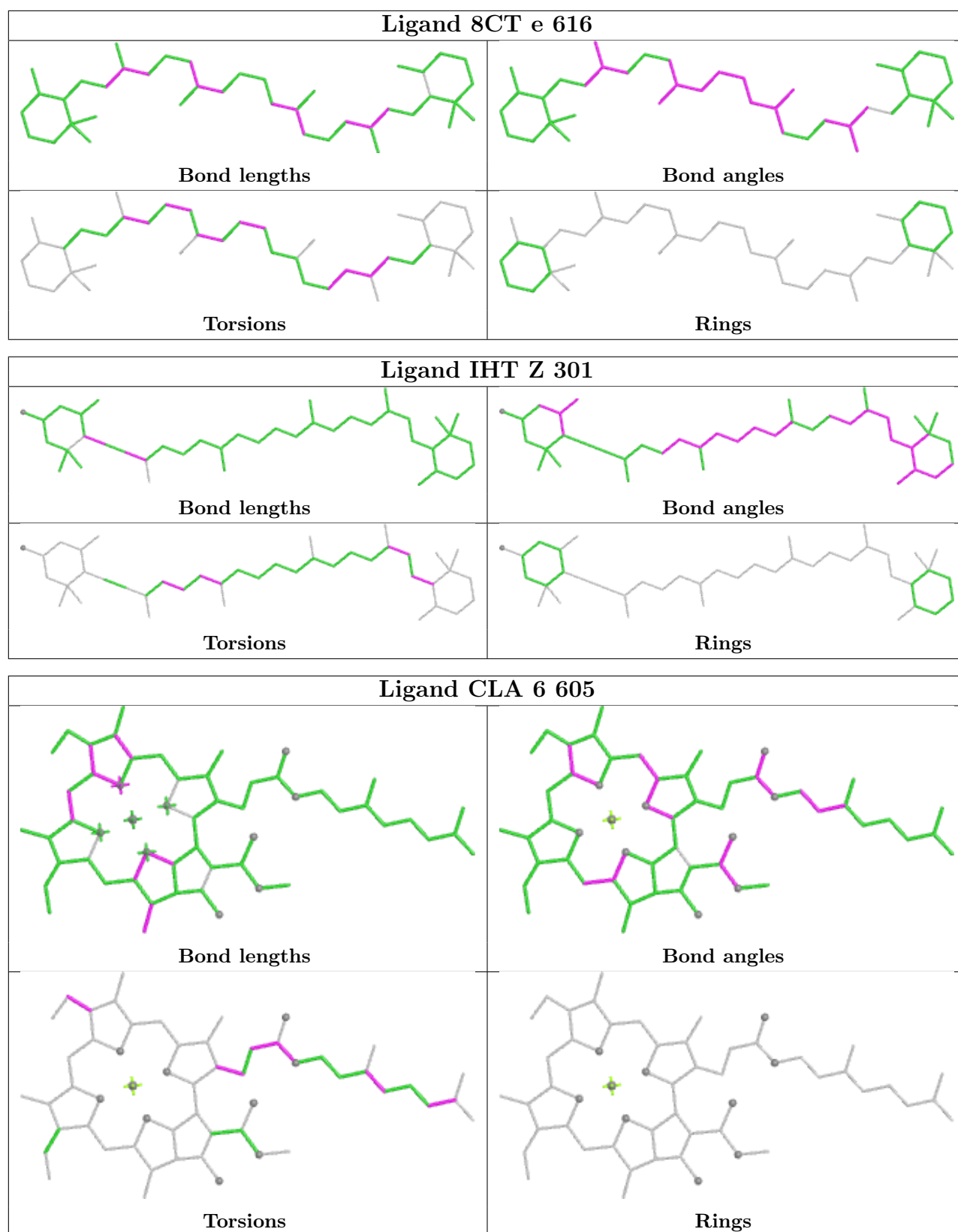


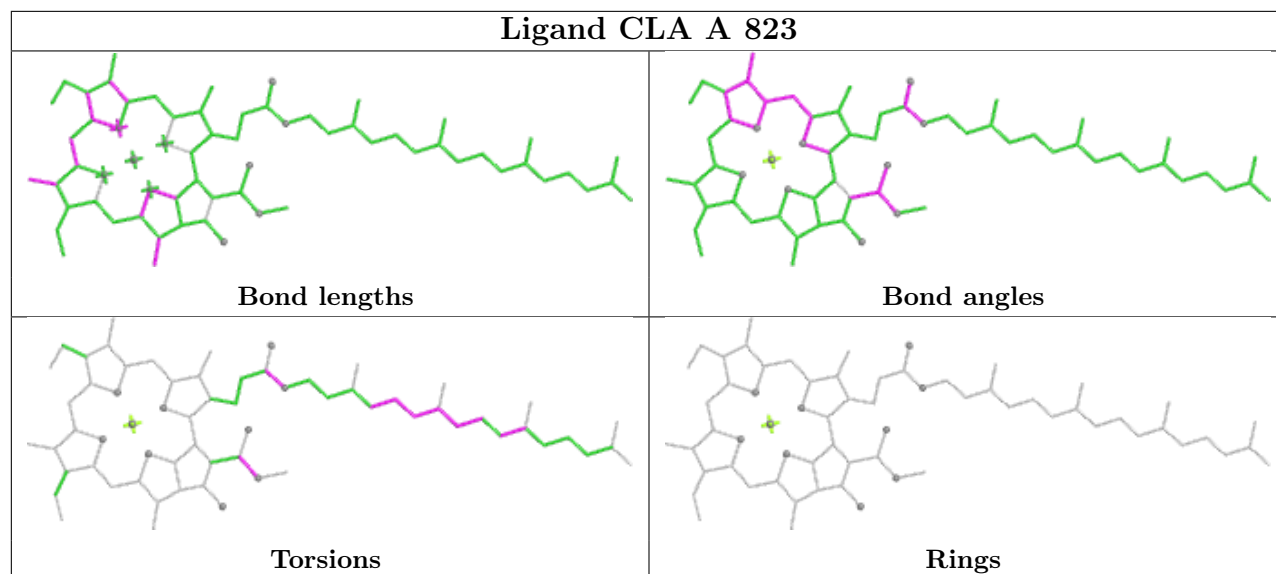
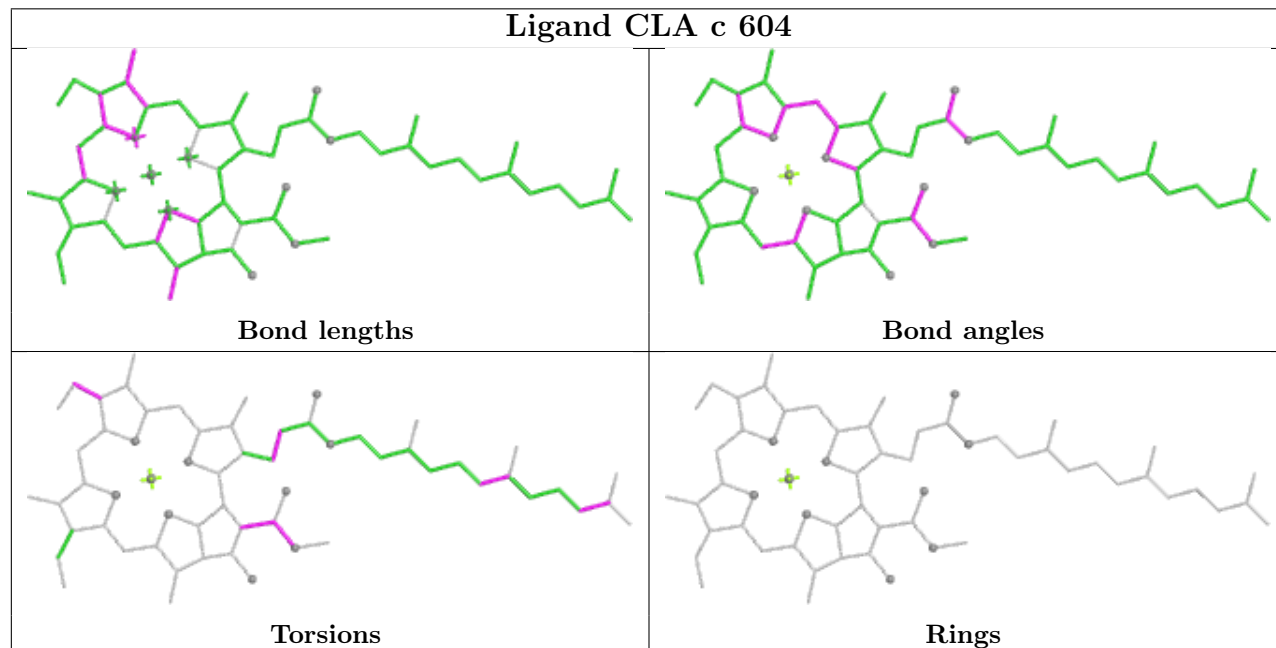
Rings



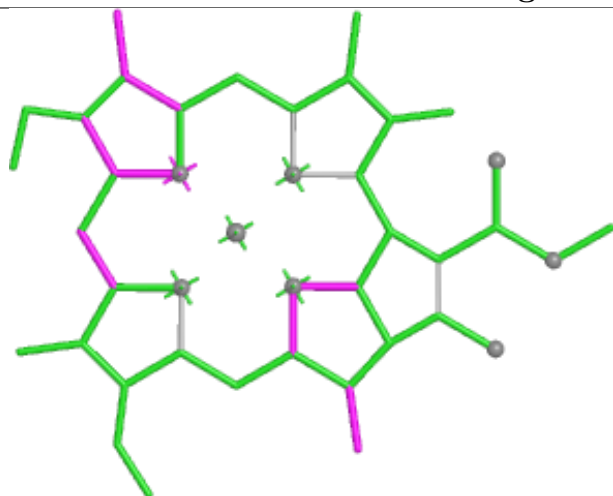




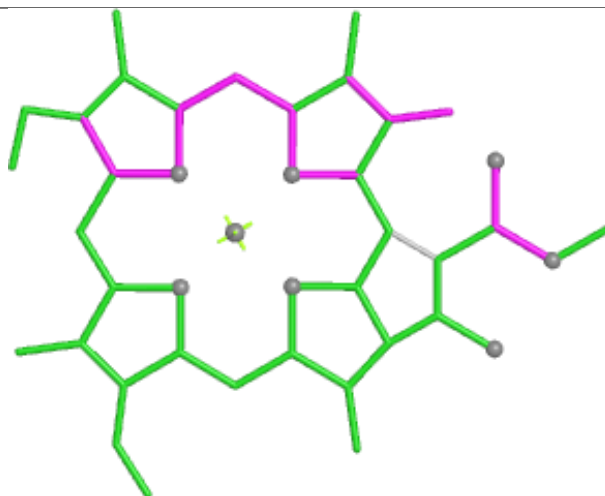


Ligand CLA A 823**Ligand CLA c 604**

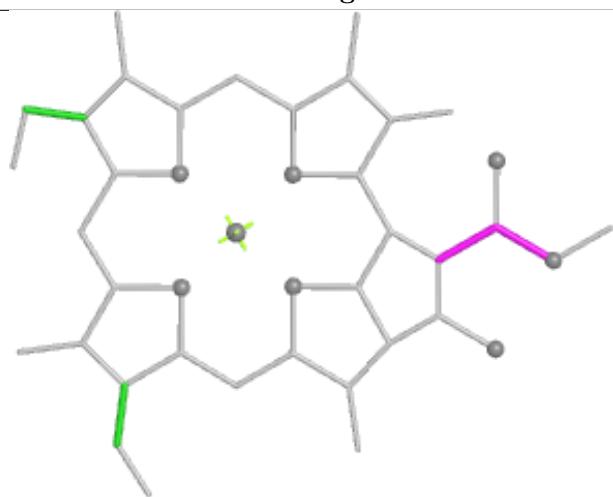
Ligand CLA J 103



Bond lengths



Bond angles

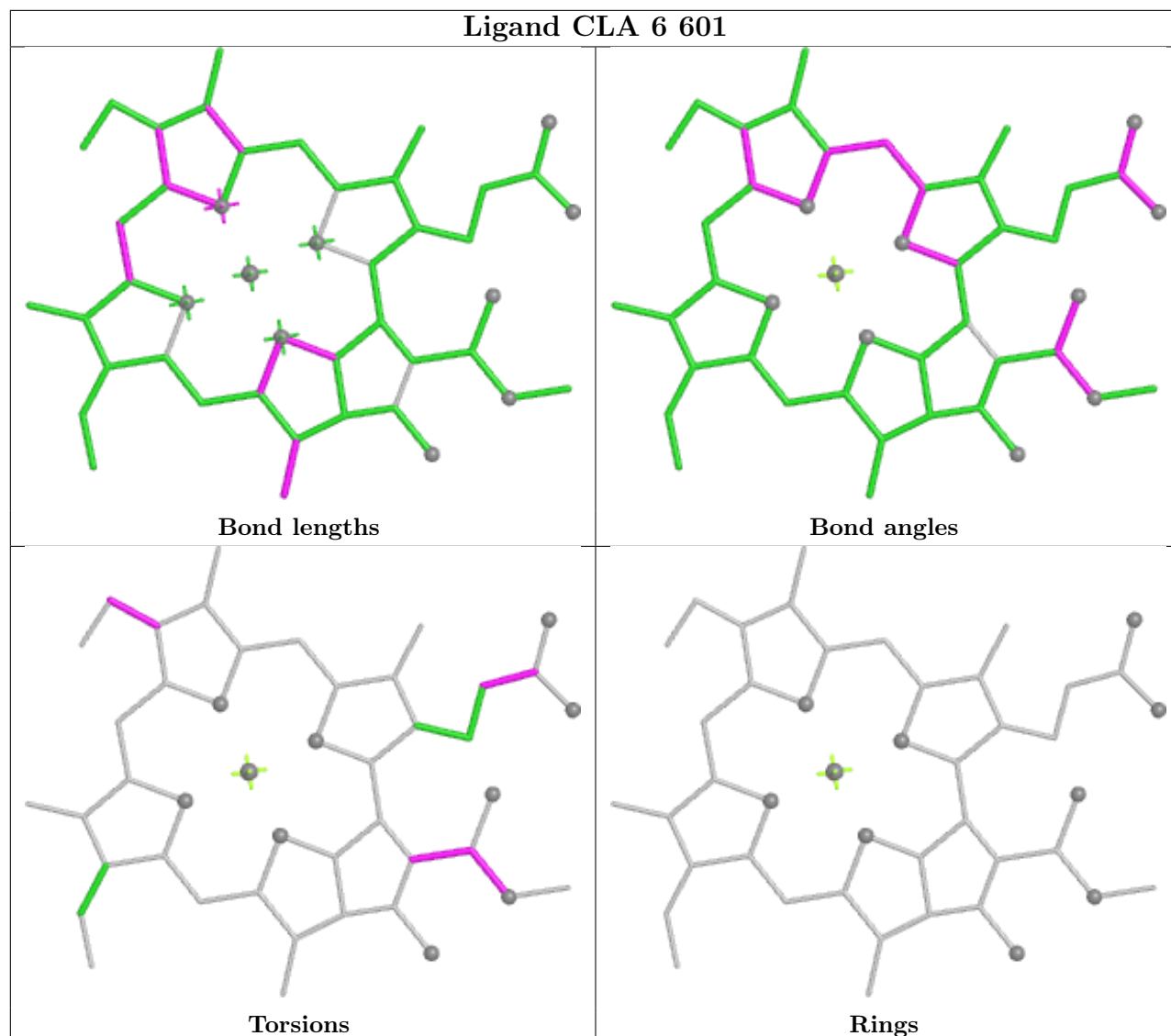


Torsions

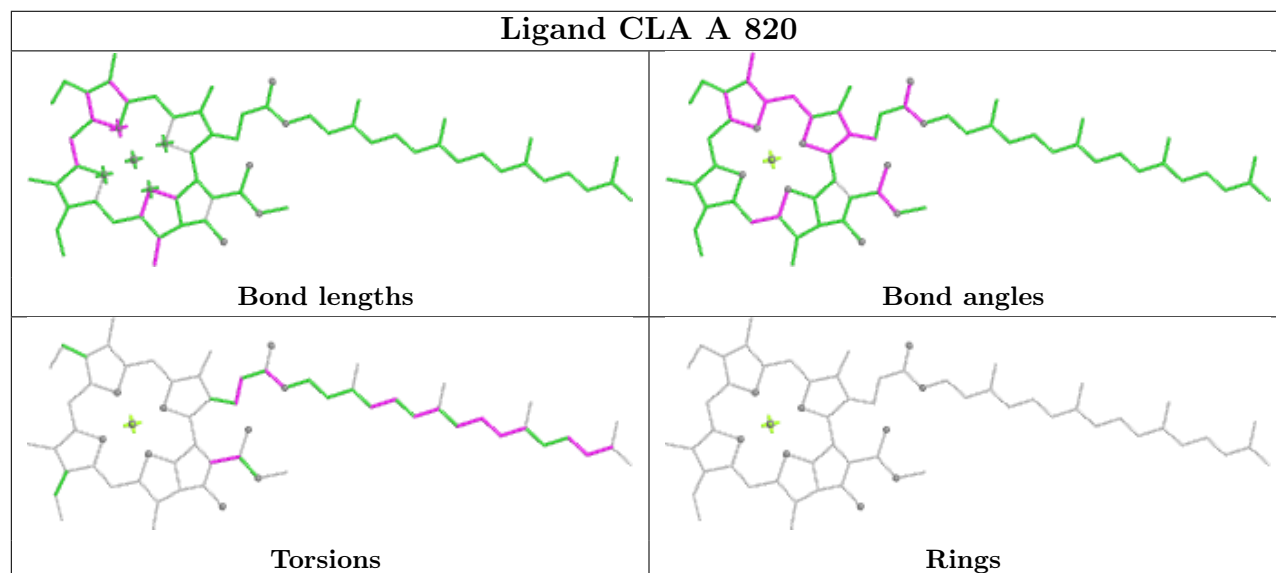


Rings

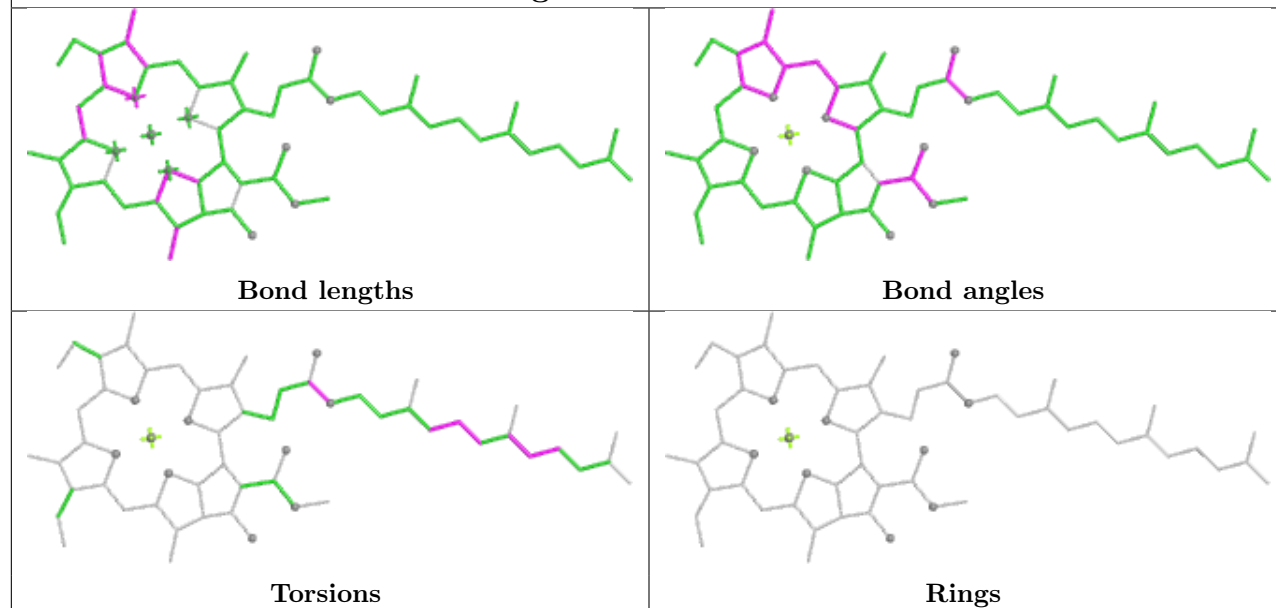
Ligand CLA 6 601



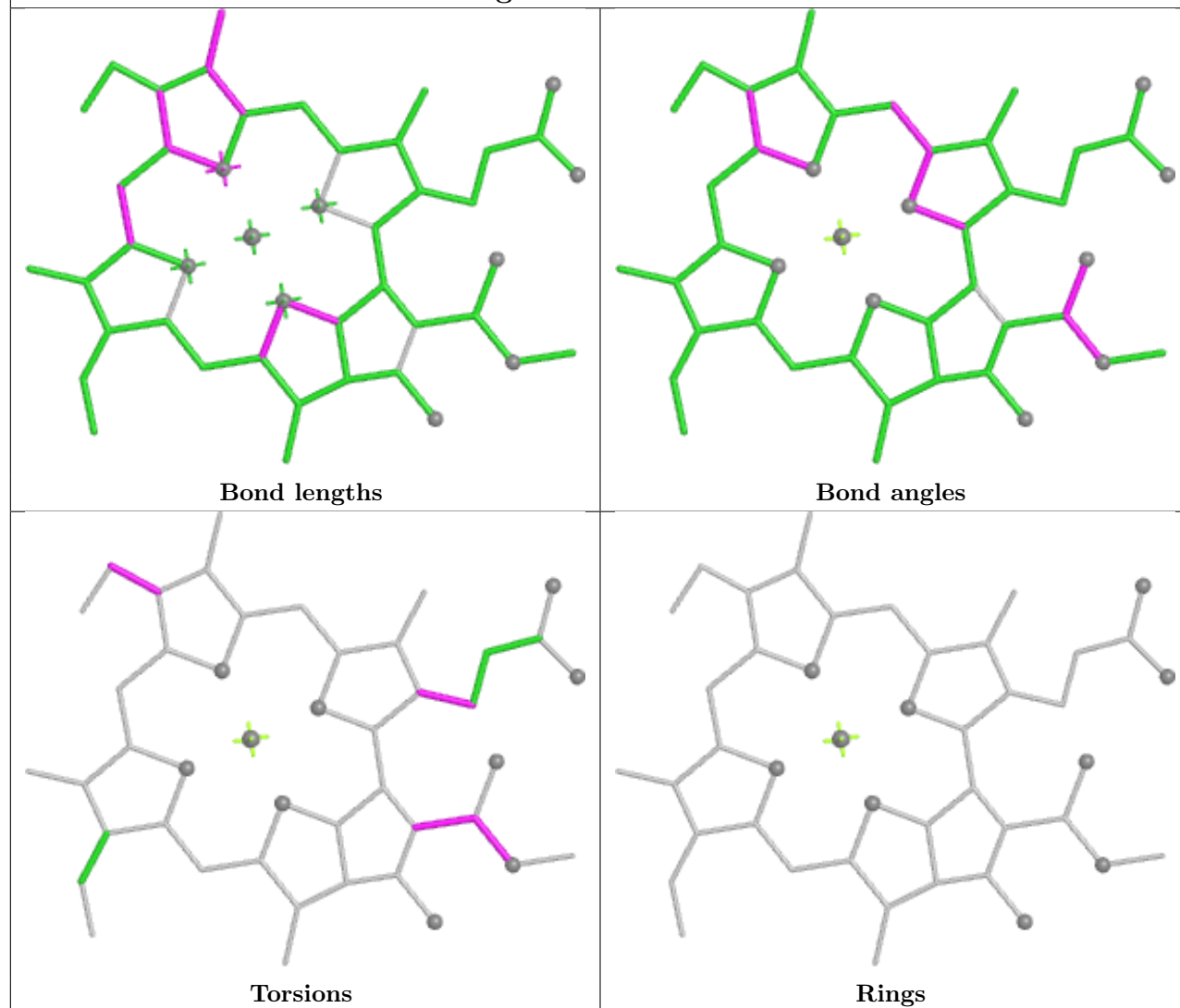
Ligand CLA A 820



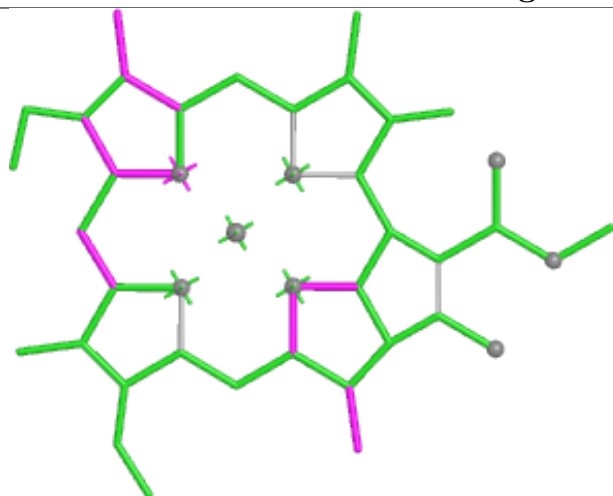
Ligand CLA A 830



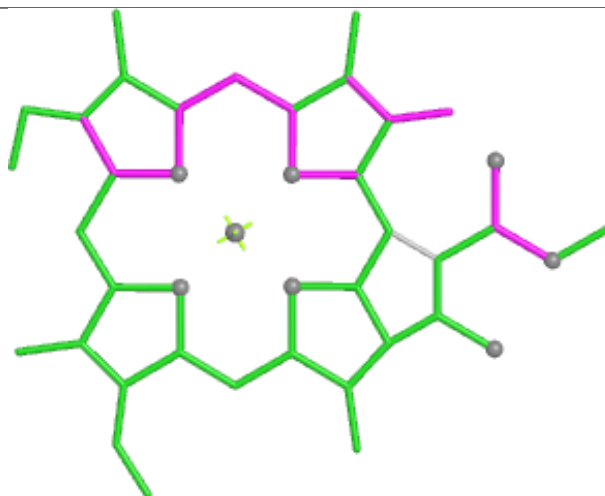
Ligand CLA 2 612



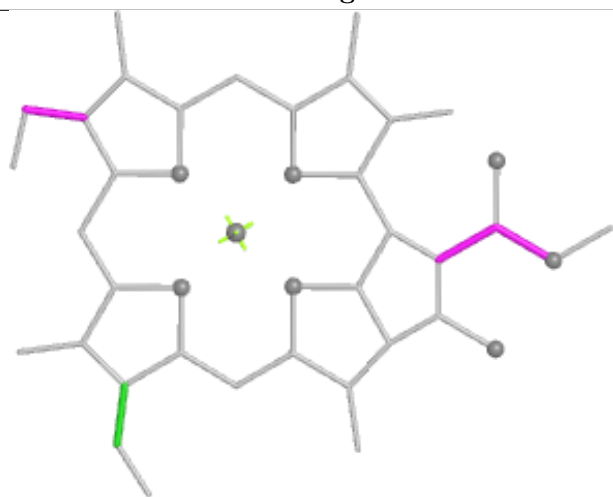
Ligand CLA 2 609



Bond lengths



Bond angles

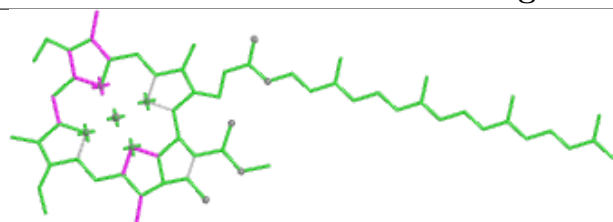


Torsions

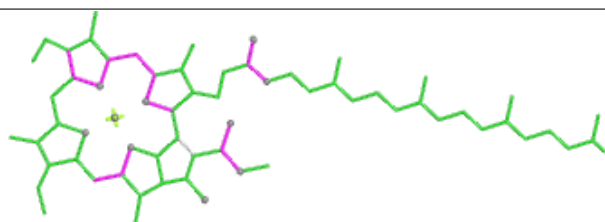


Rings

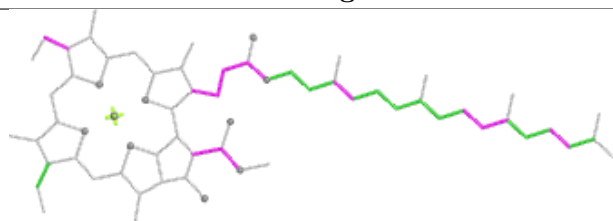
Ligand CLA 8 303



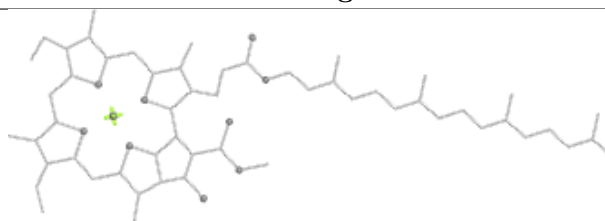
Bond lengths



Bond angles

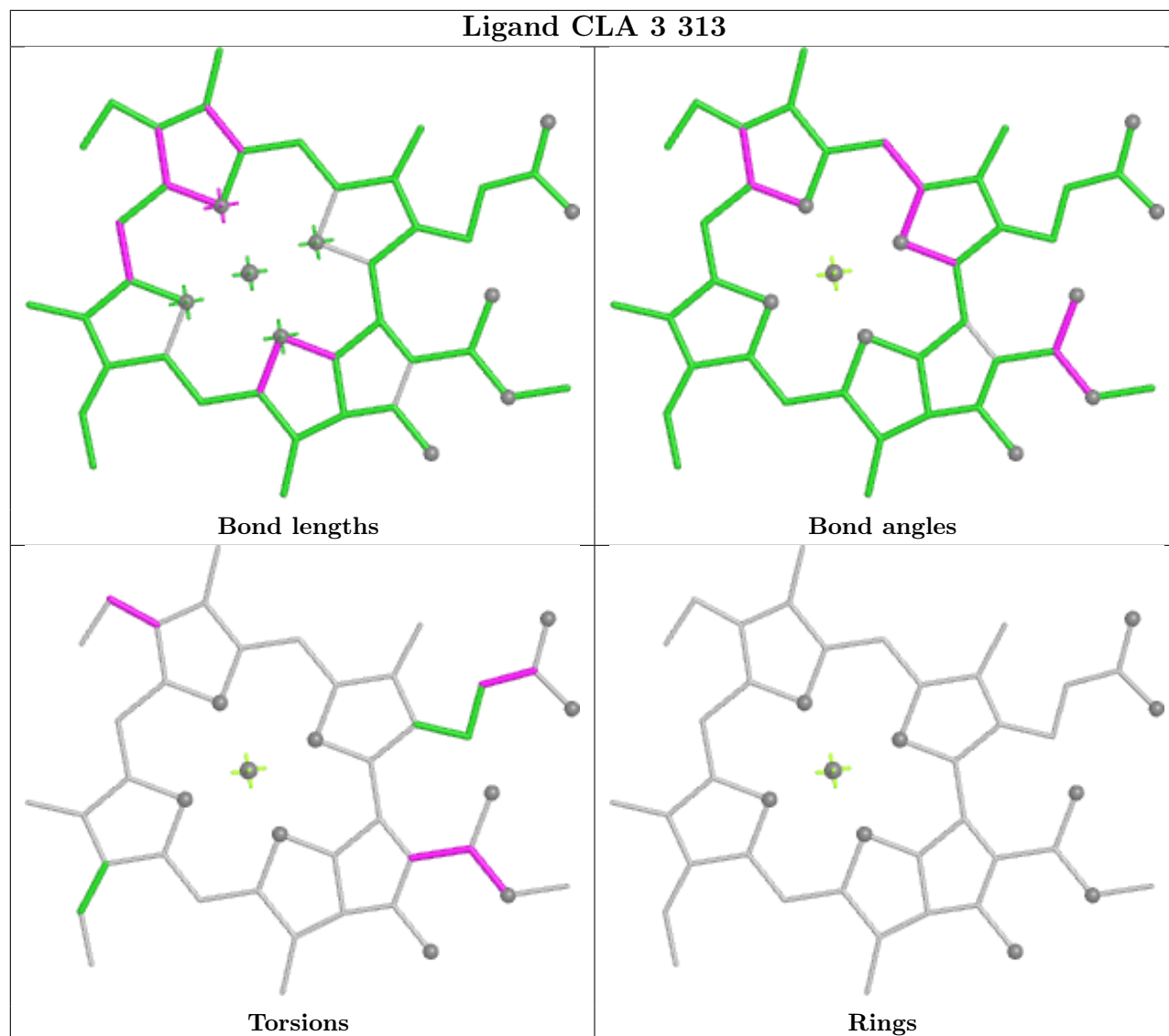


Torsions

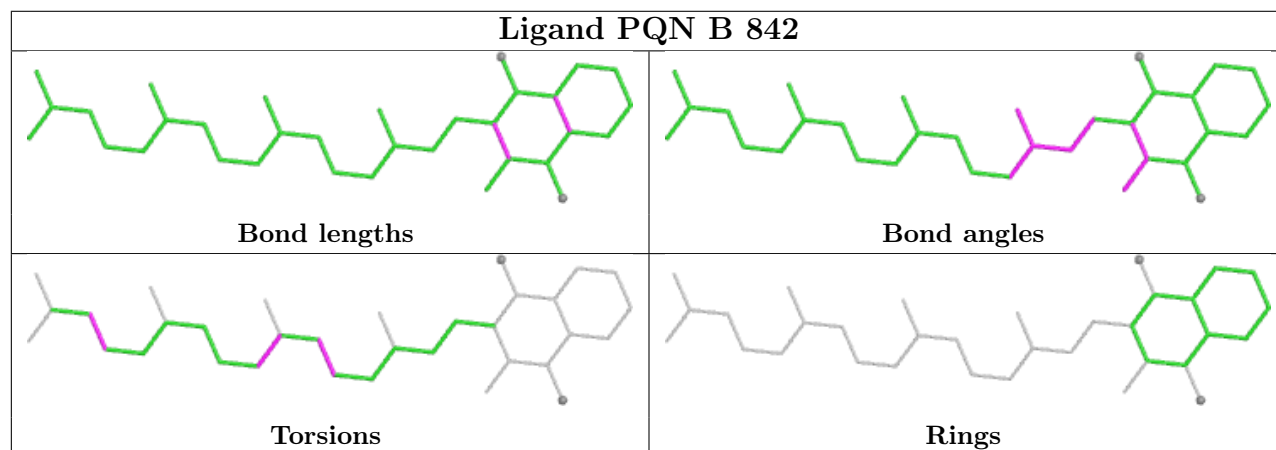


Rings

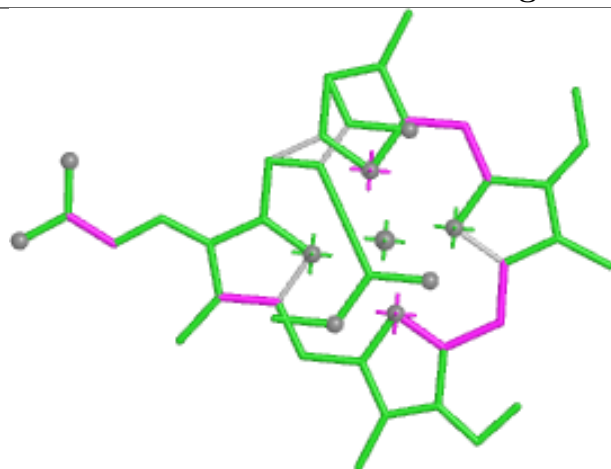
Ligand CLA 3 313



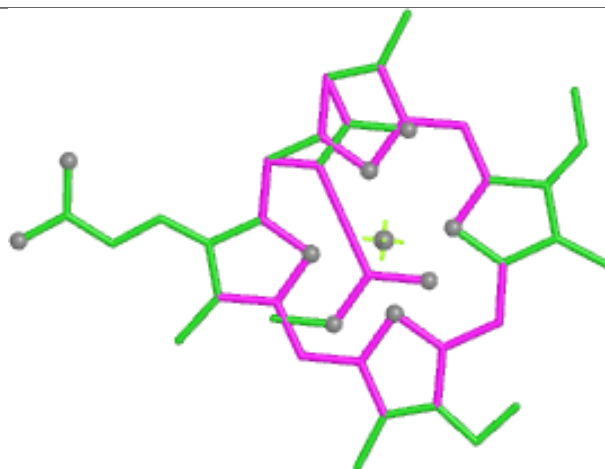
Ligand PQN B 842



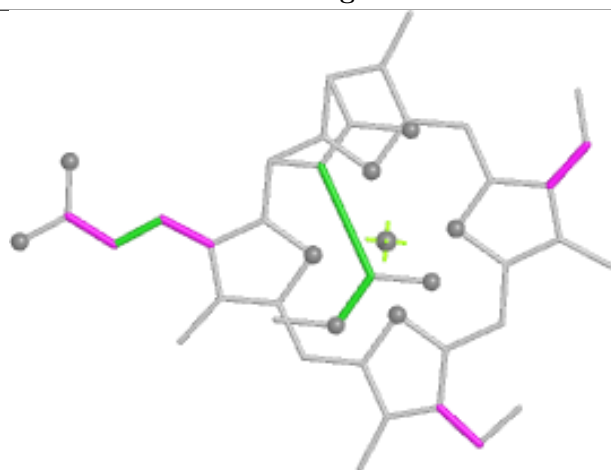
Ligand KC2 b 605



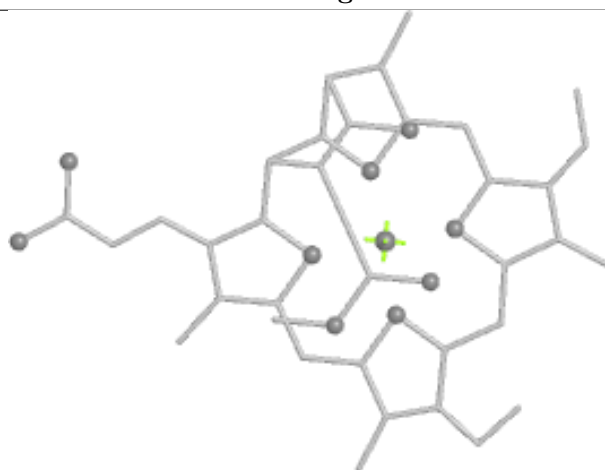
Bond lengths



Bond angles

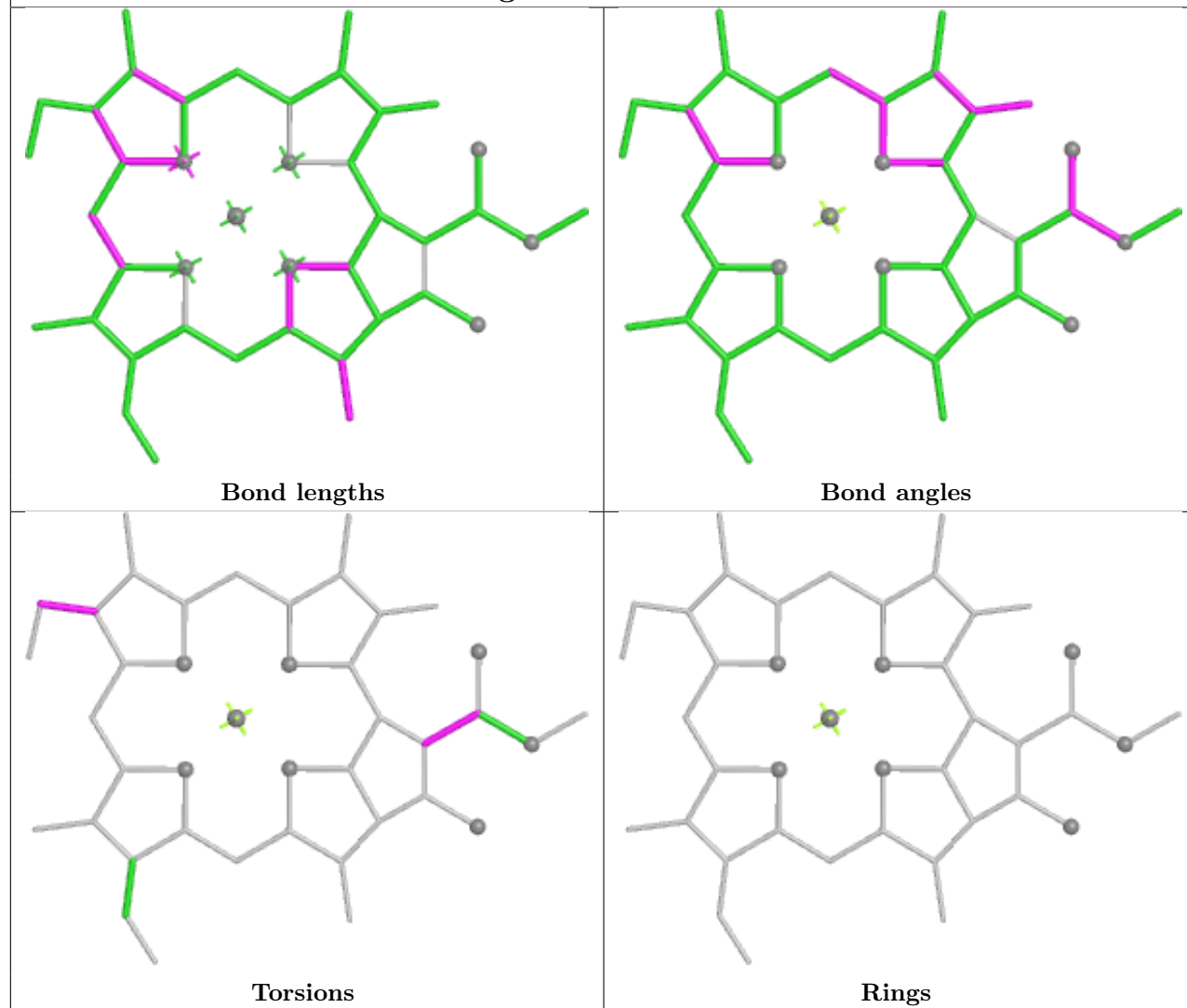


Torsions

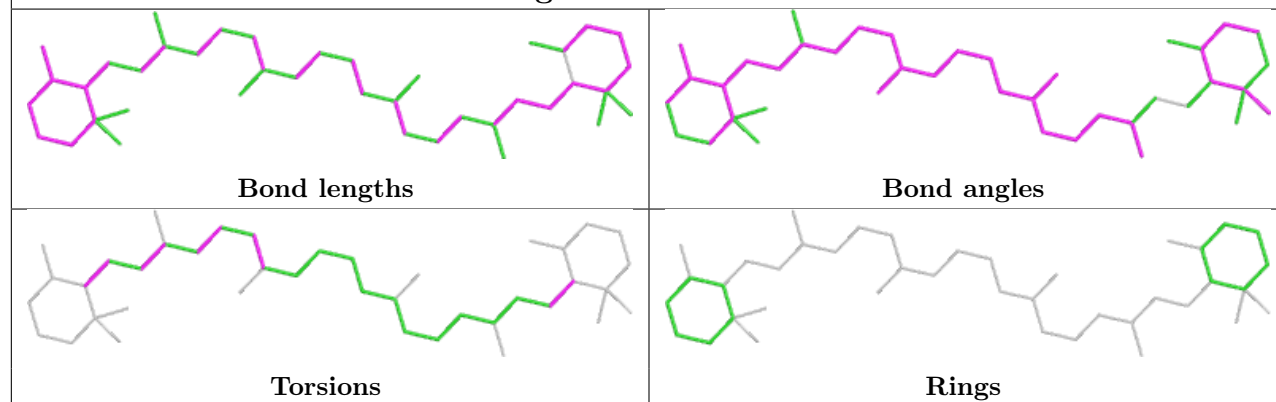


Rings

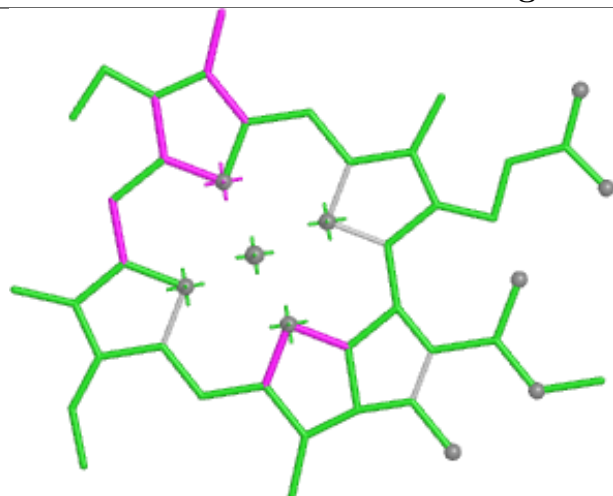
Ligand CLA 5 609



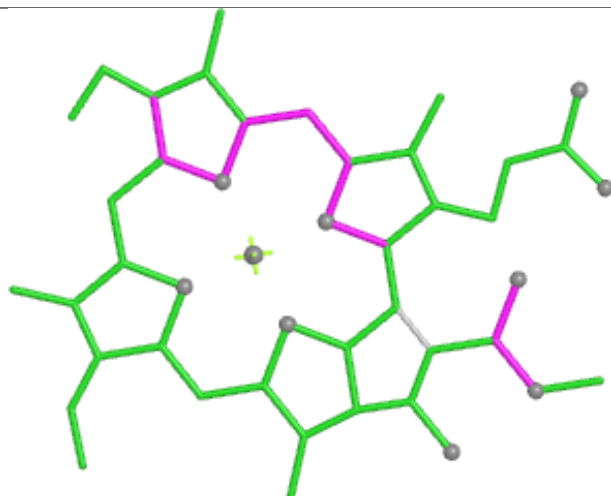
Ligand 8CT B 848



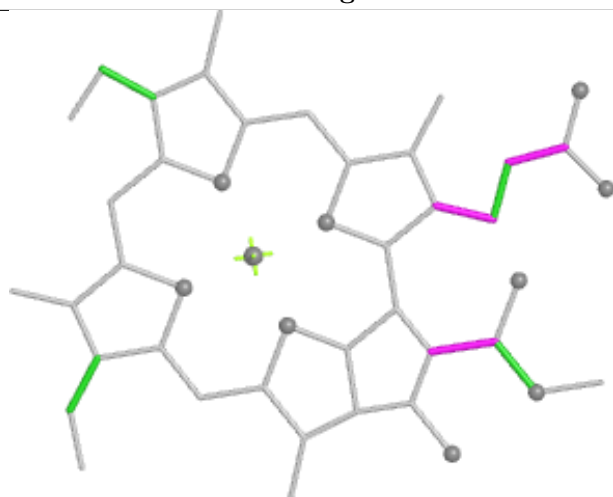
Ligand CLA 5 606



Bond lengths



Bond angles

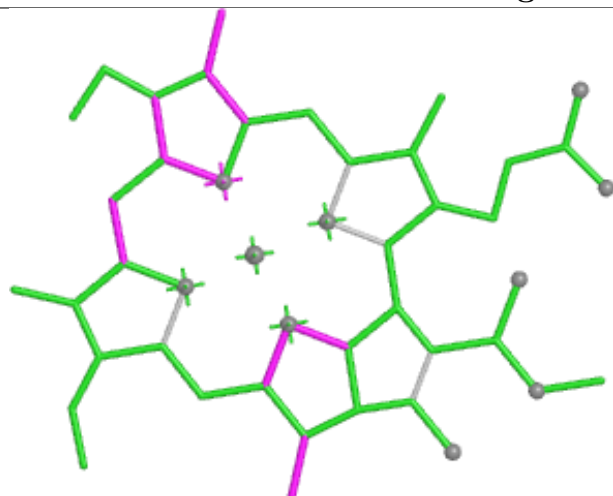


Torsions

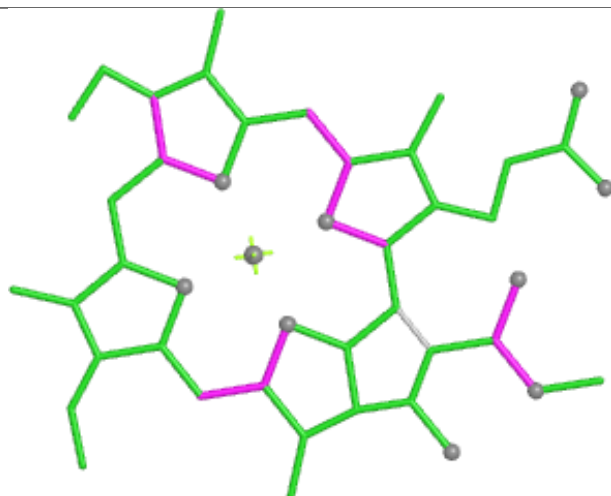


Rings

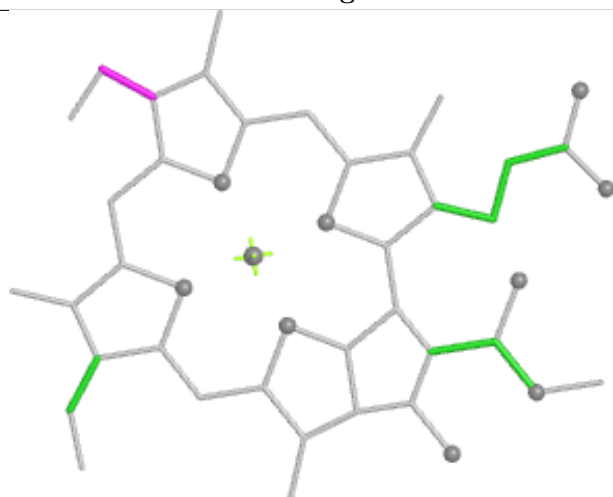
Ligand CLA b 601



Bond lengths



Bond angles

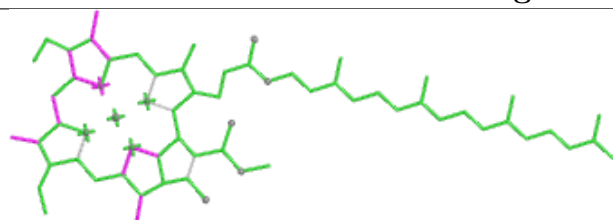


Torsions

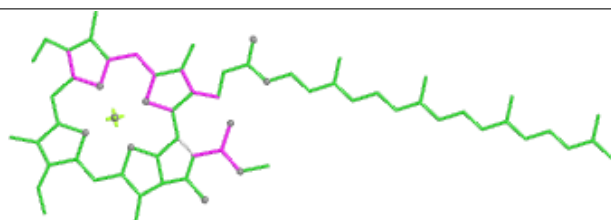


Rings

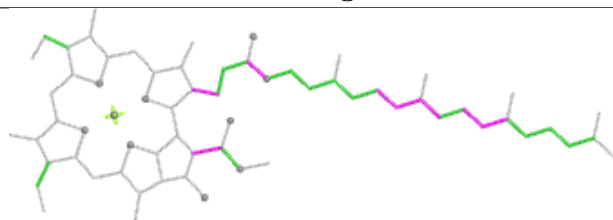
Ligand CLA A 841



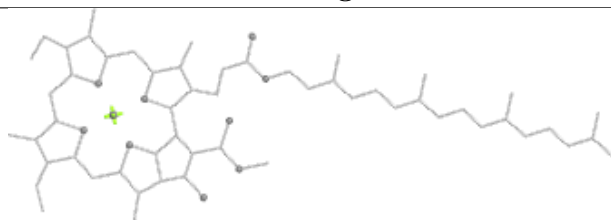
Bond lengths



Bond angles

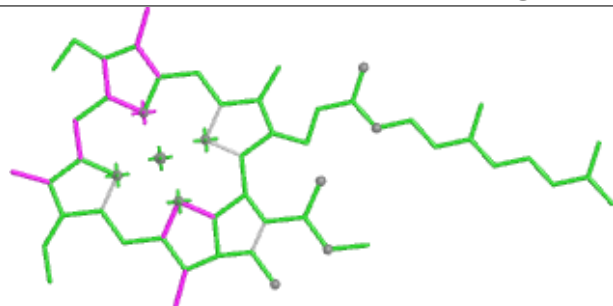


Torsions

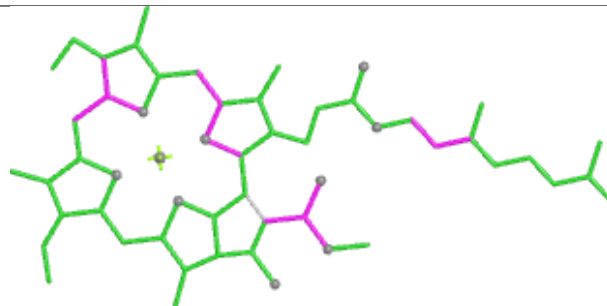


Rings

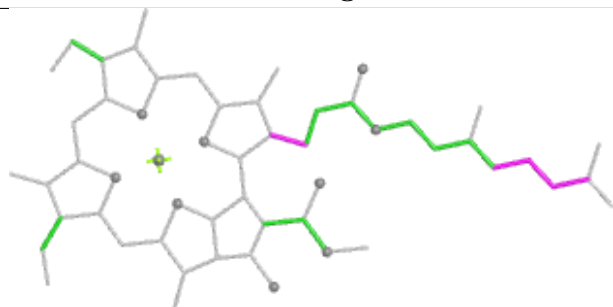
Ligand CLA B 812



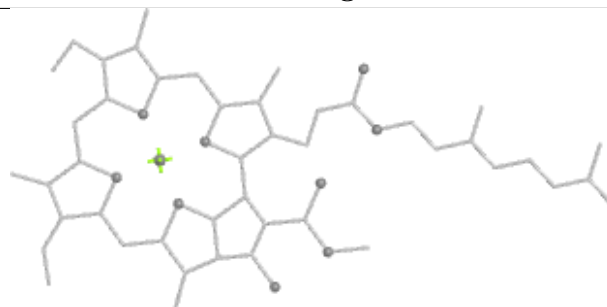
Bond lengths



Bond angles

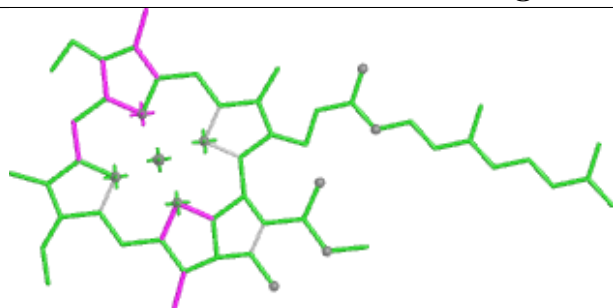


Torsions

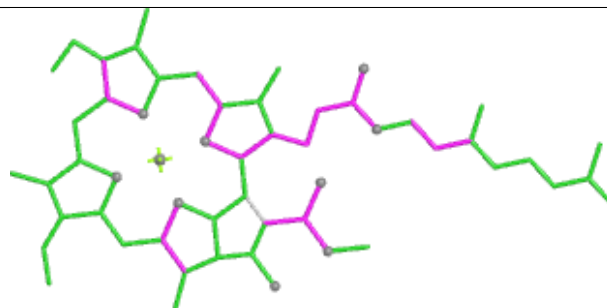


Rings

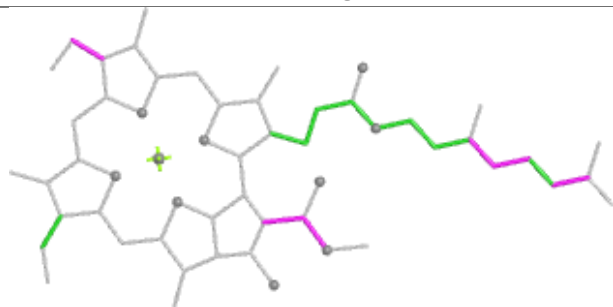
Ligand CLA B 832



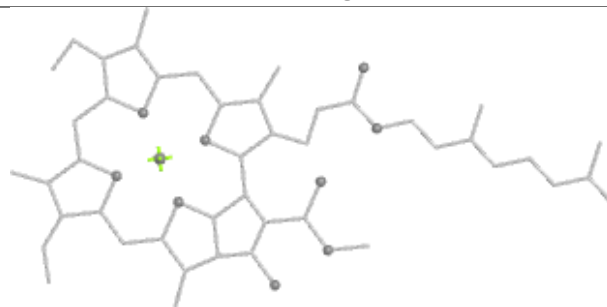
Bond lengths



Bond angles

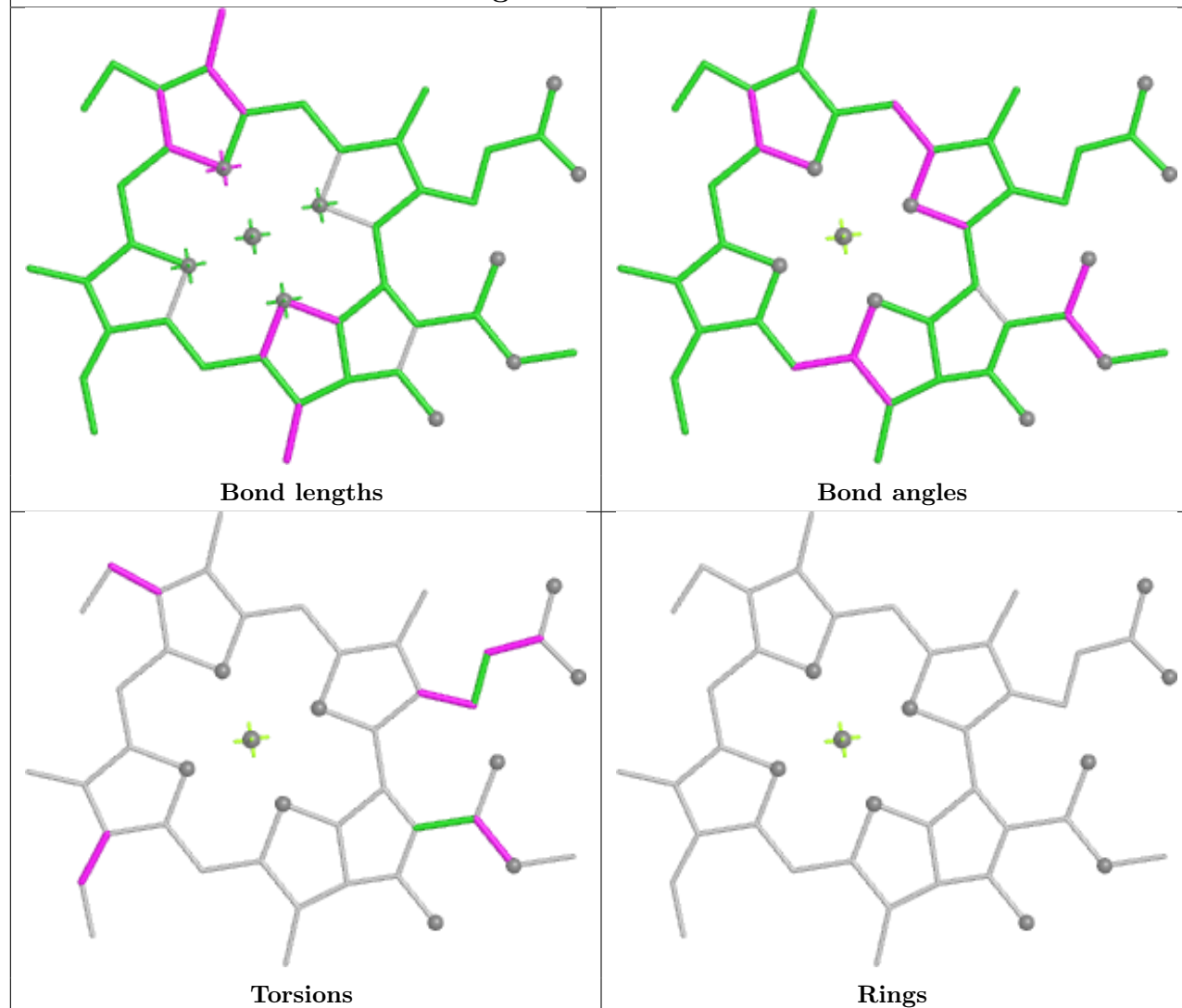


Torsions

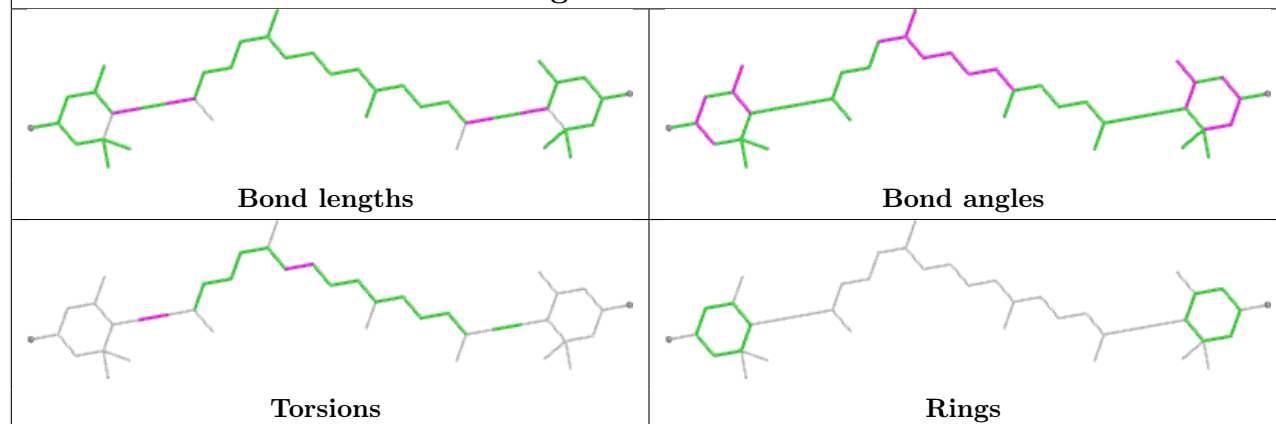


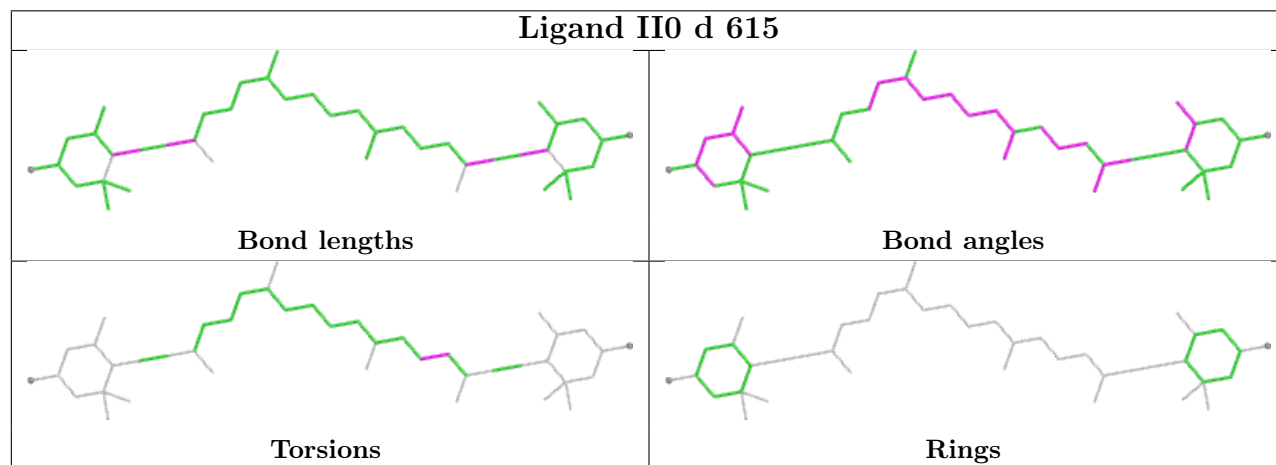
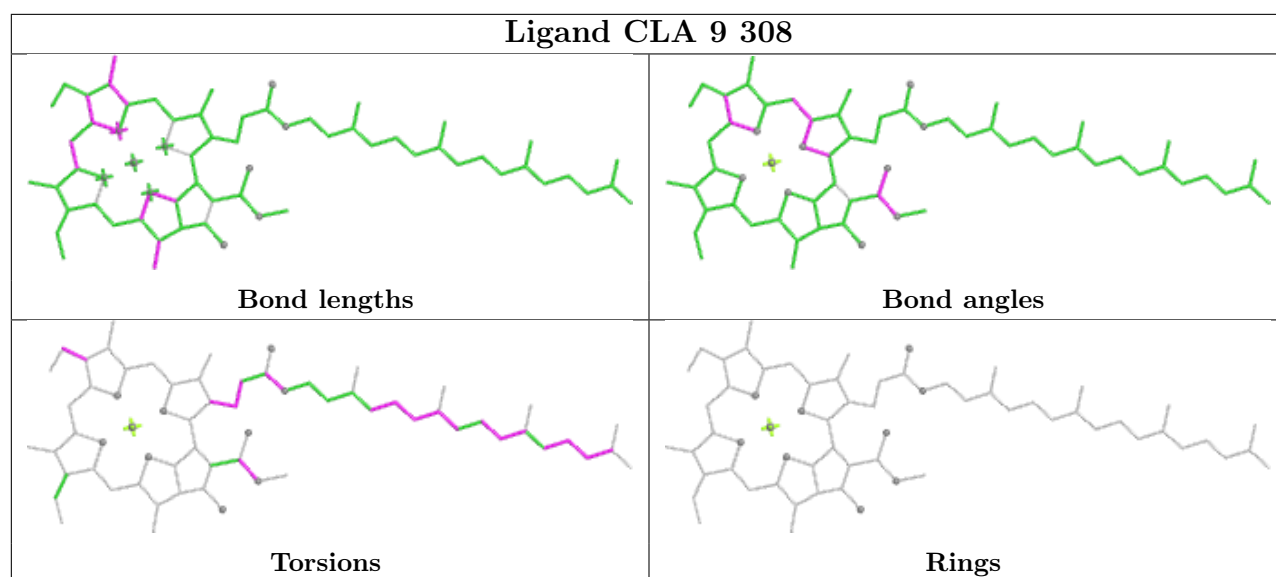
Rings

Ligand CLA A 853

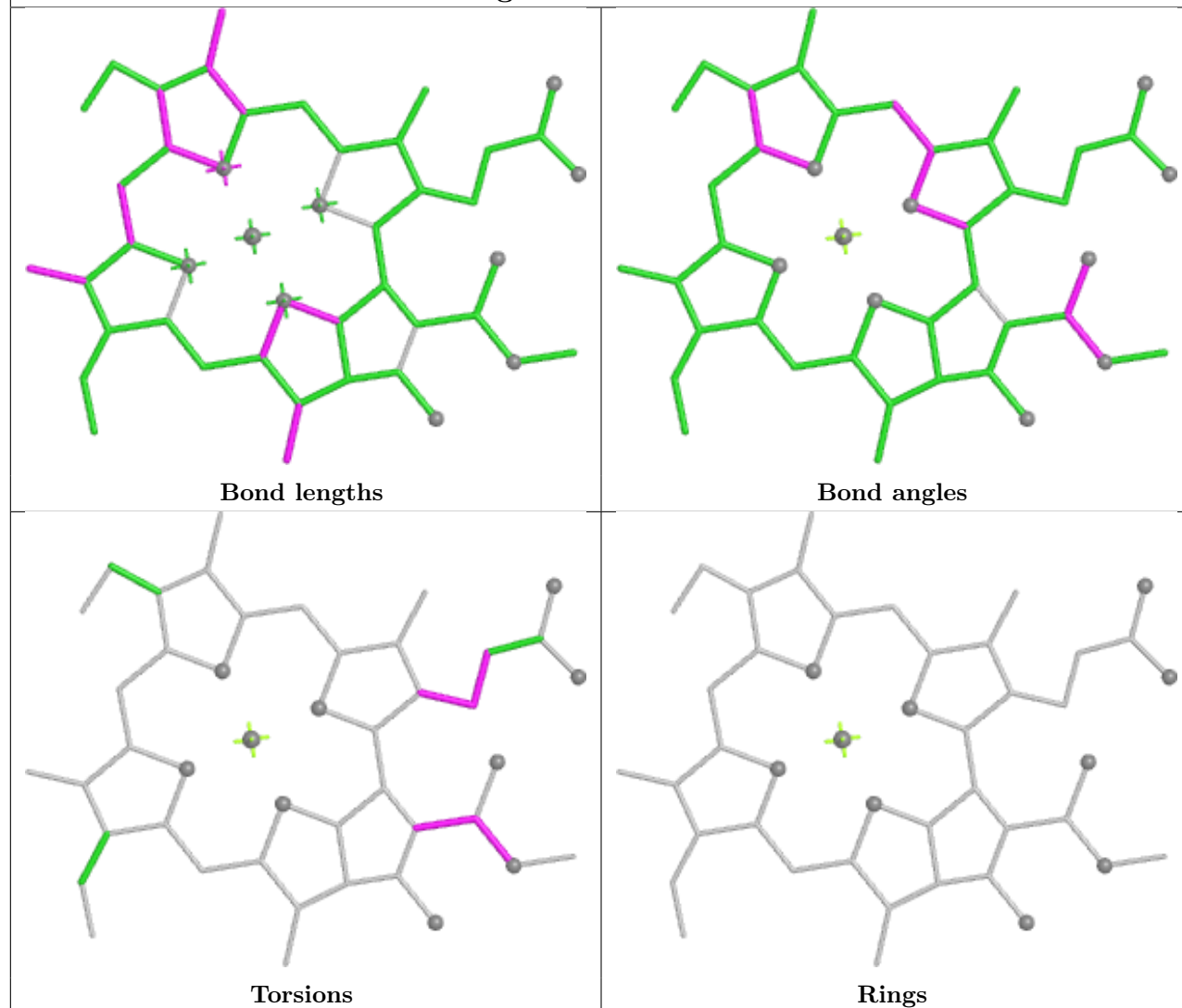


Ligand II0 4 613

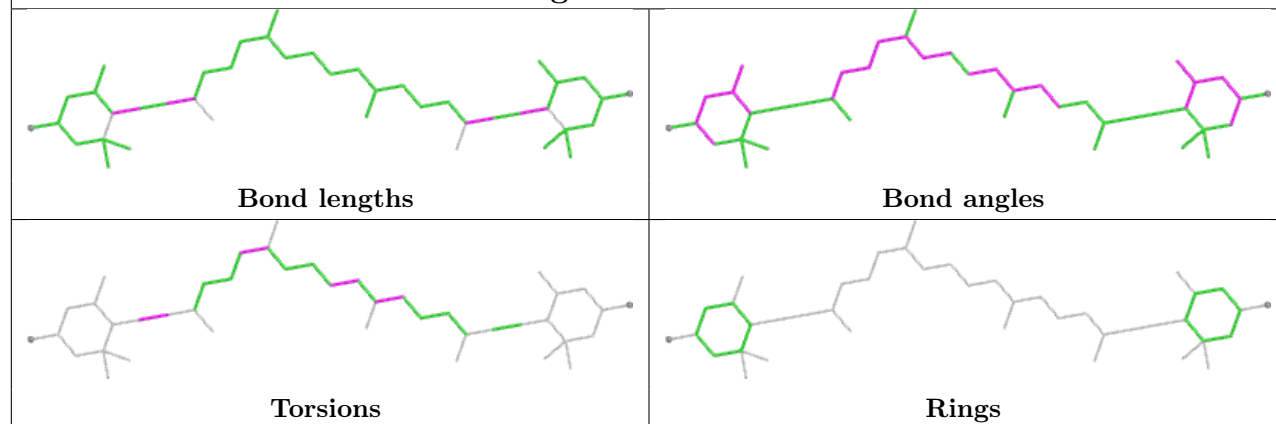




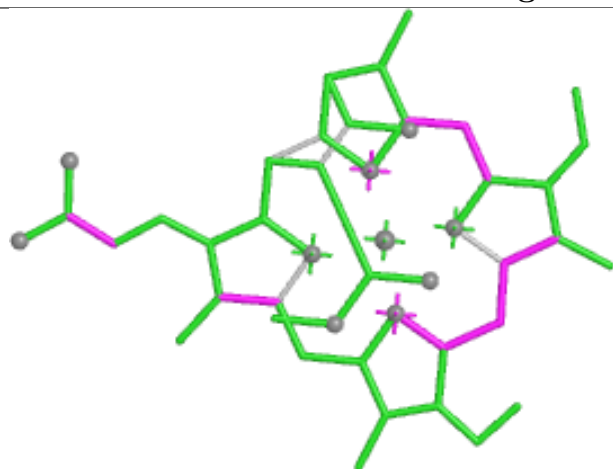
Ligand CLA 2 606



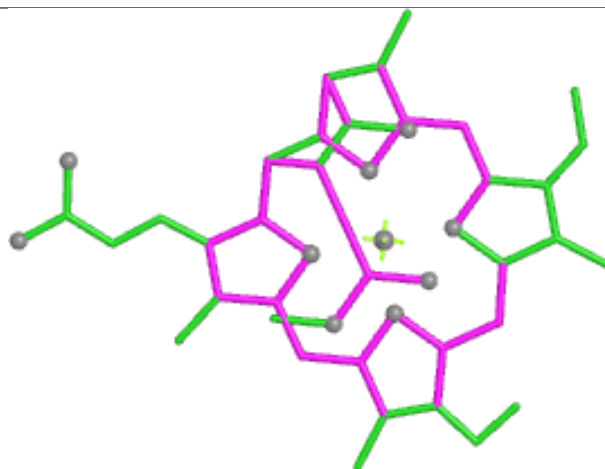
Ligand II0 1 617



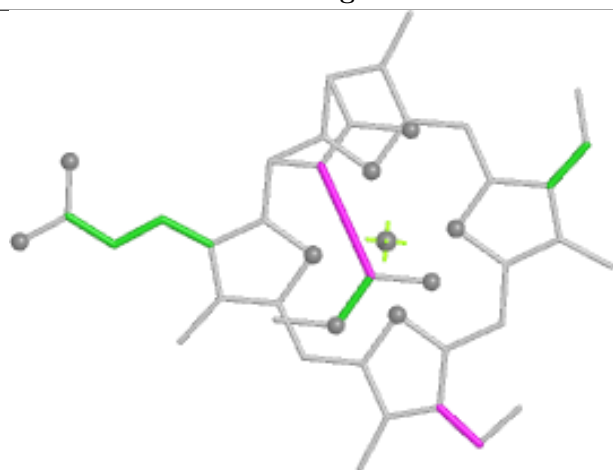
Ligand KC2 Z 306



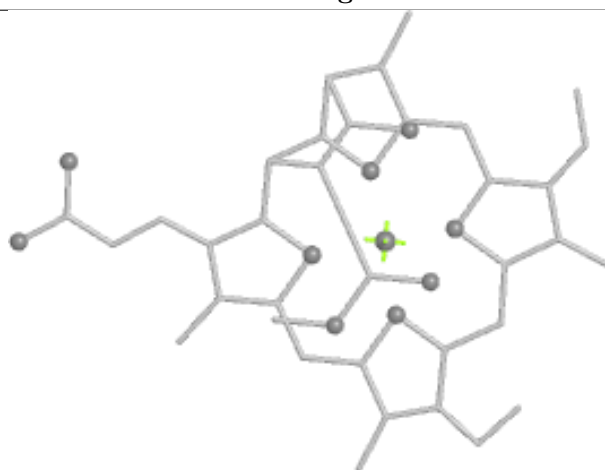
Bond lengths



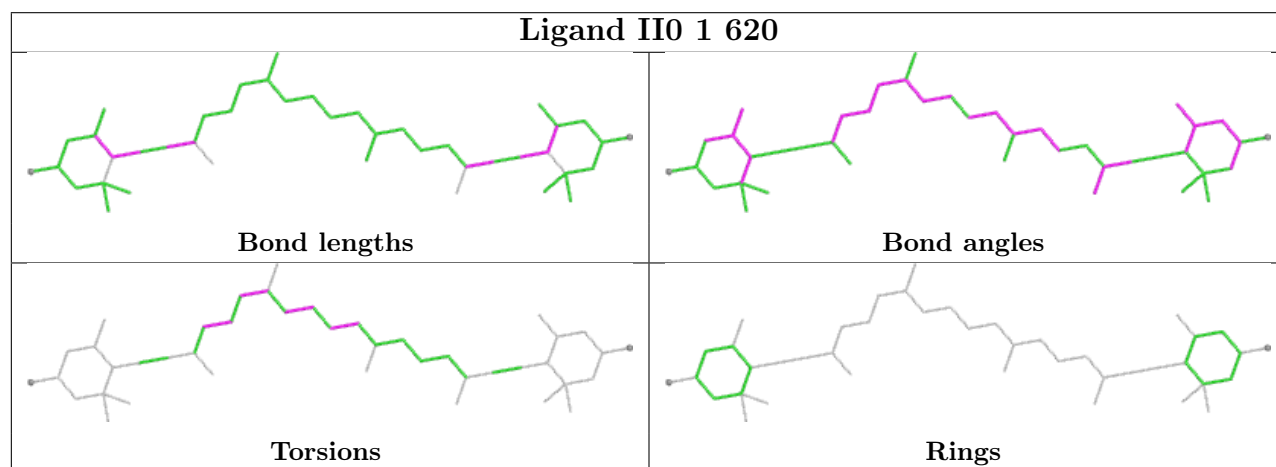
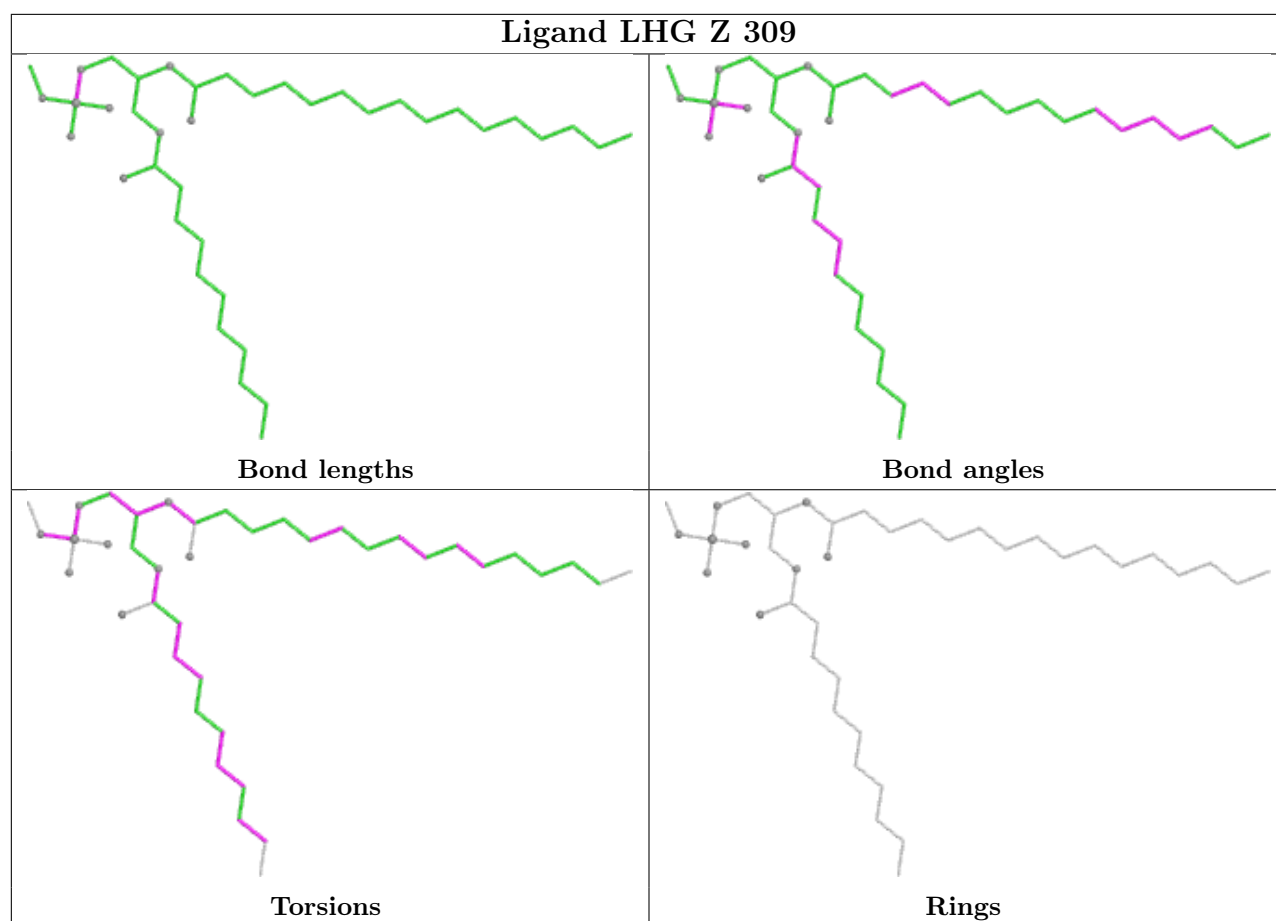
Bond angles

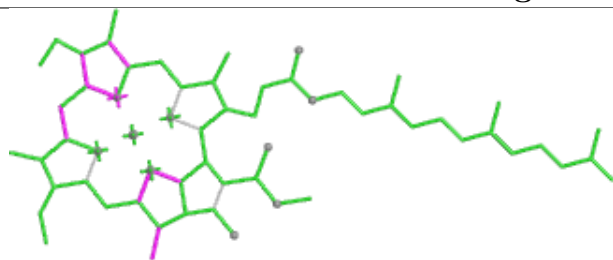
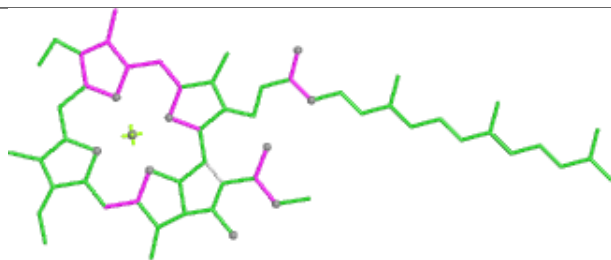
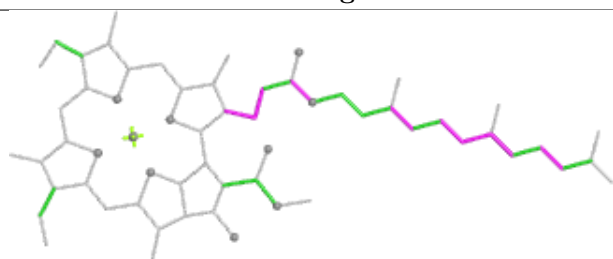
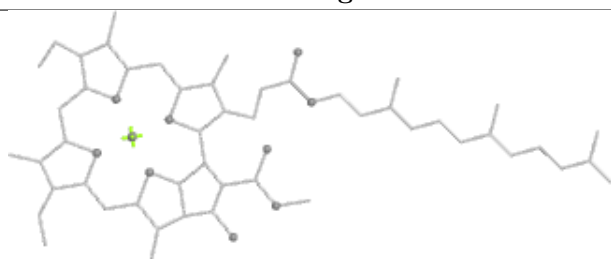
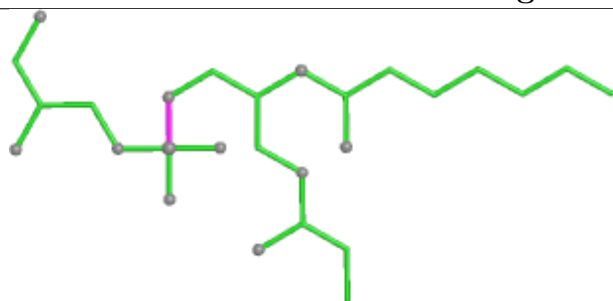
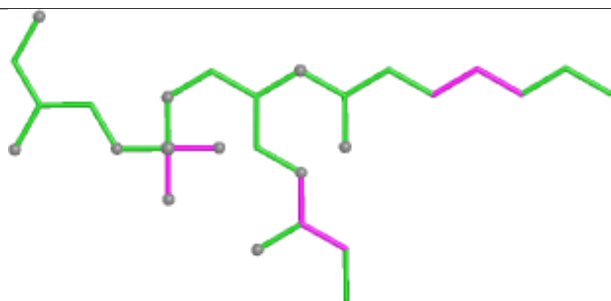
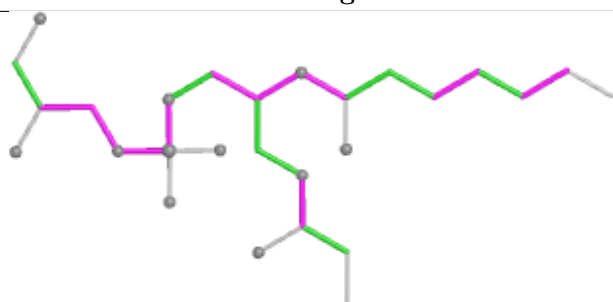
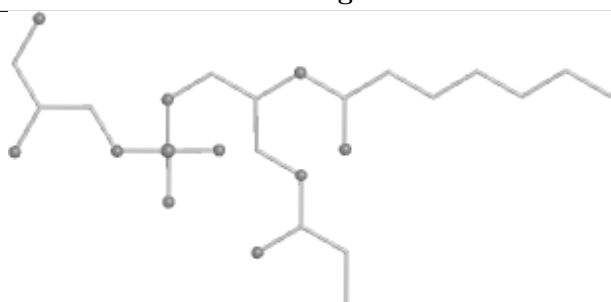


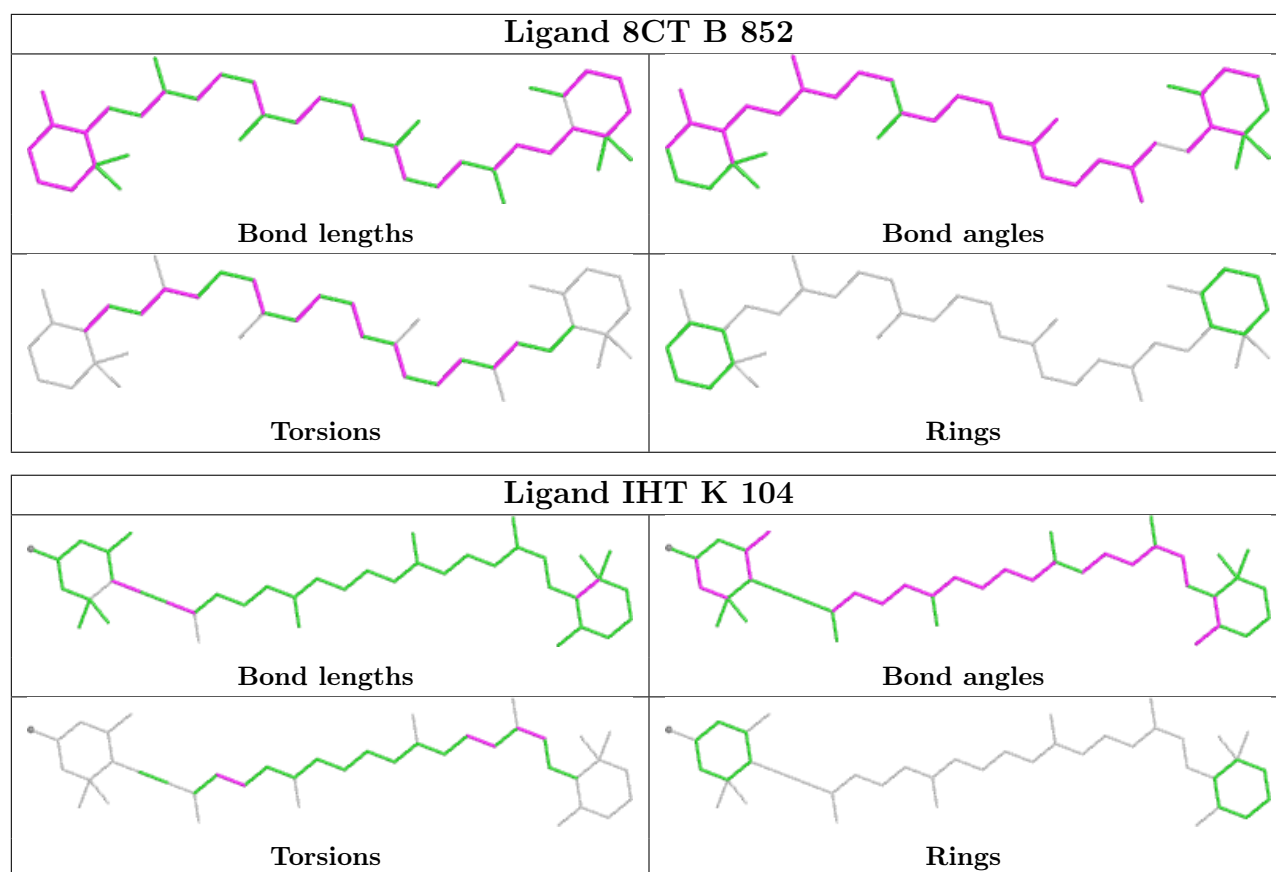
Torsions



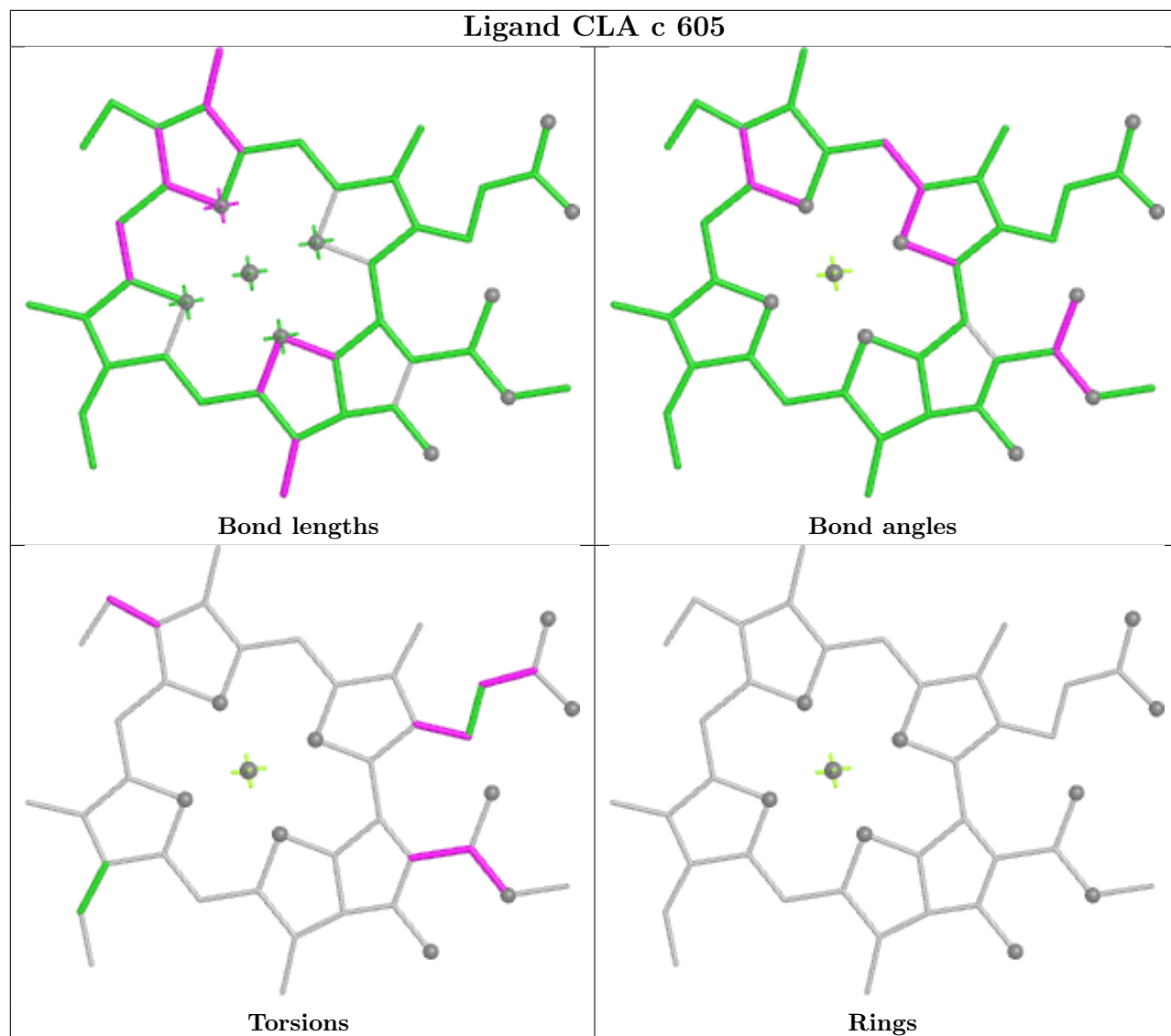
Rings

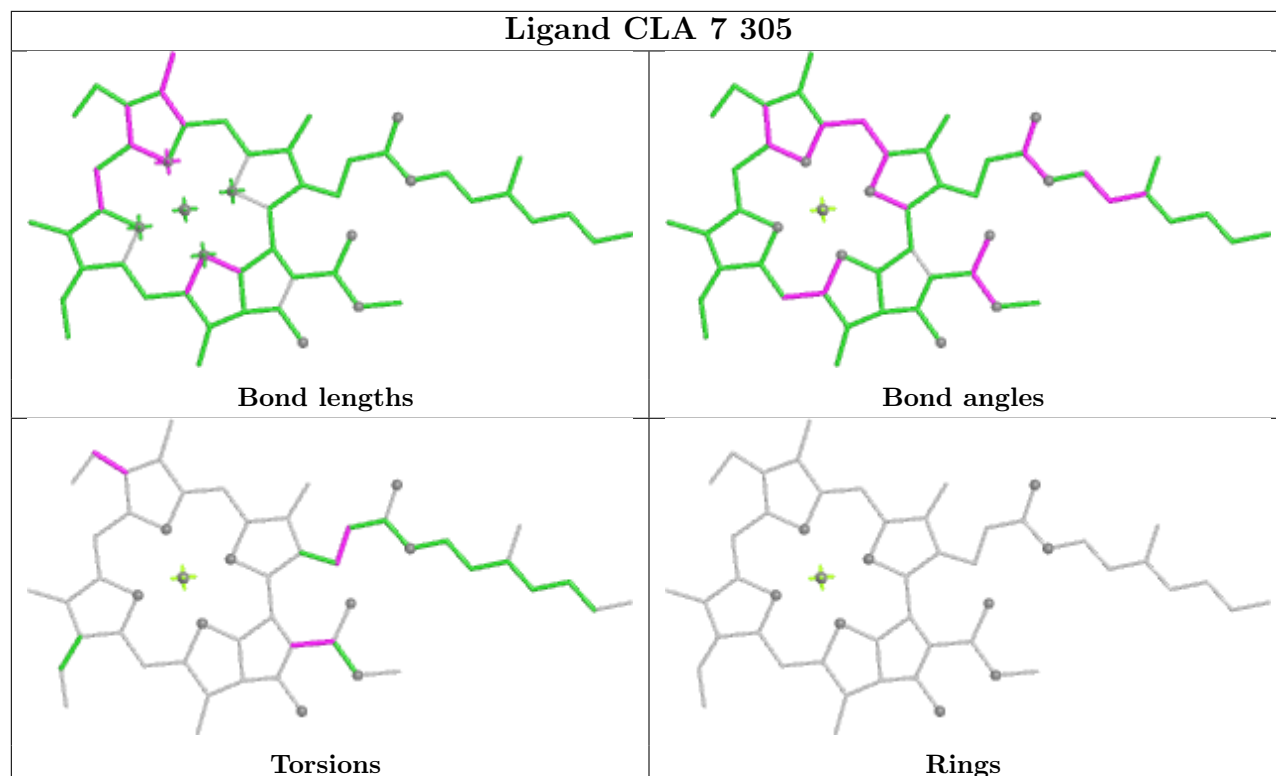
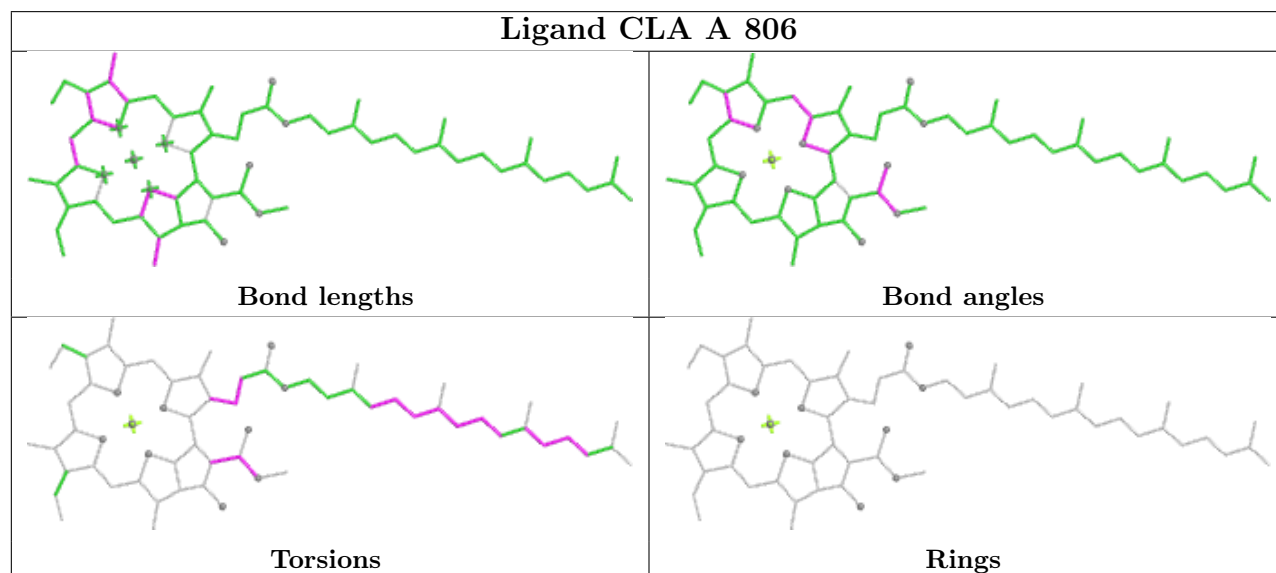


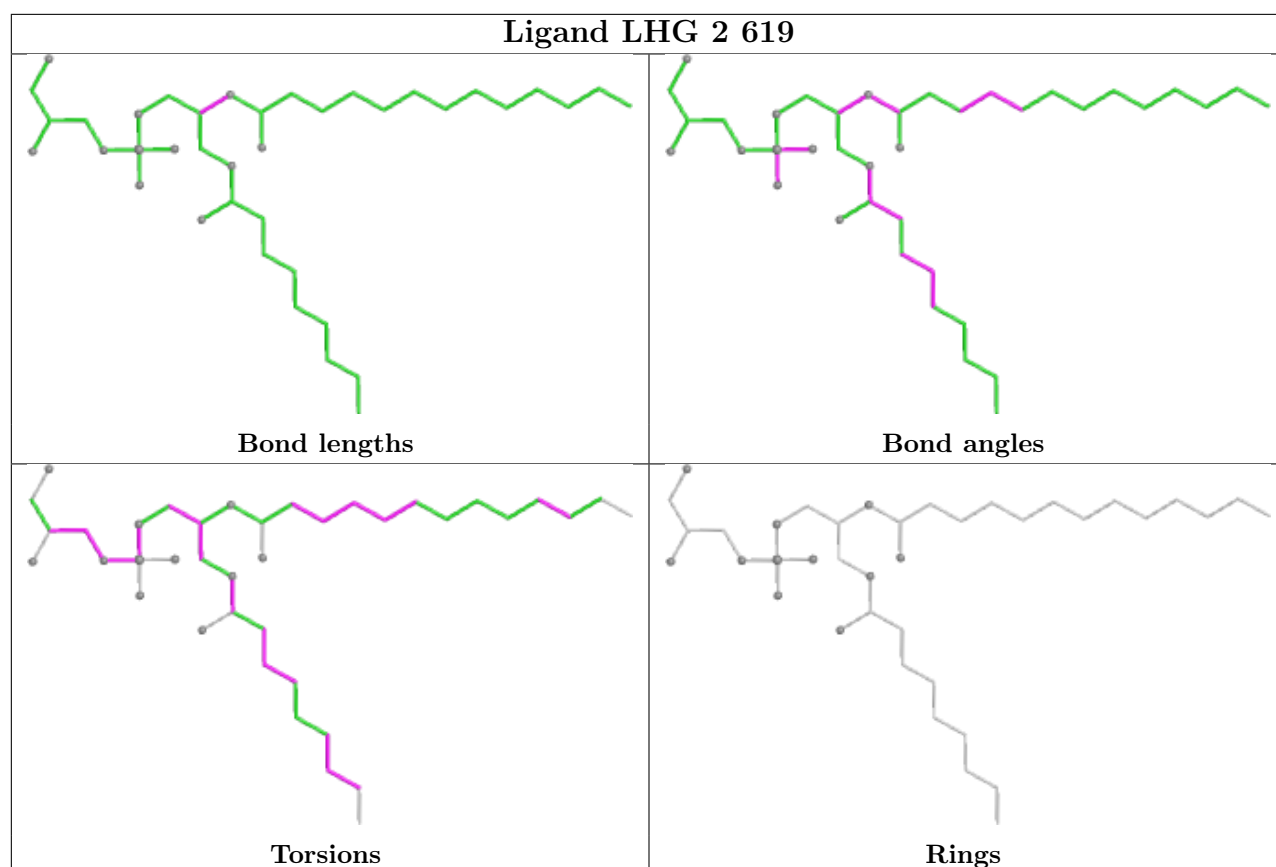
Ligand CLA B 831**Bond lengths****Bond angles****Torsions****Rings****Ligand LHG a 617****Bond lengths****Bond angles****Torsions****Rings**



Ligand CLA c 605



Ligand CLA 7 305**Ligand CLA A 806**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

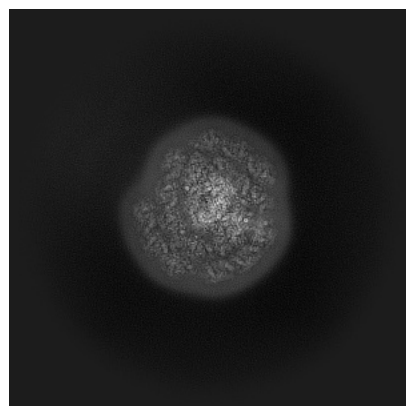
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66373. These allow visual inspection of the internal detail of the map and identification of artifacts.

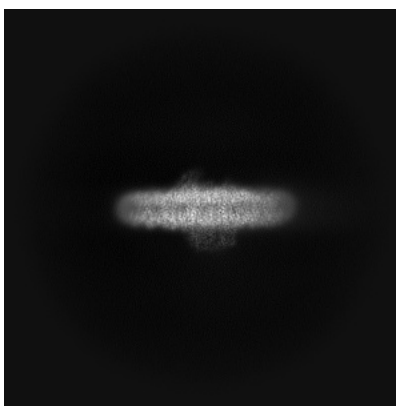
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

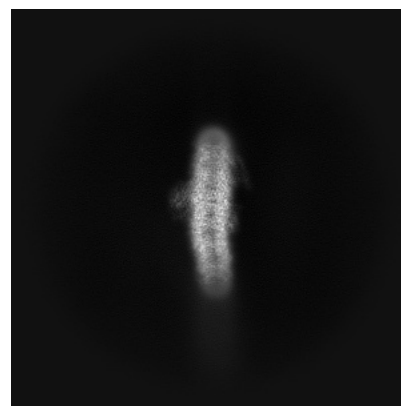
6.1.1 Primary map



X

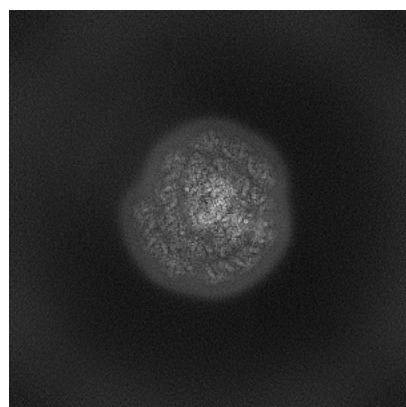


Y

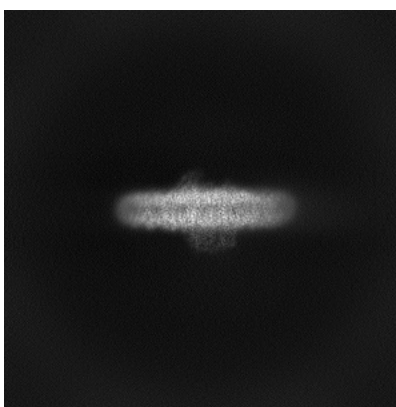


Z

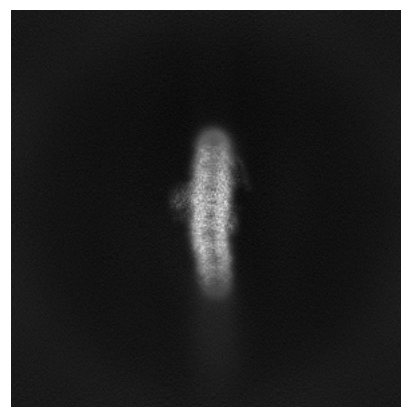
6.1.2 Raw map



X



Y

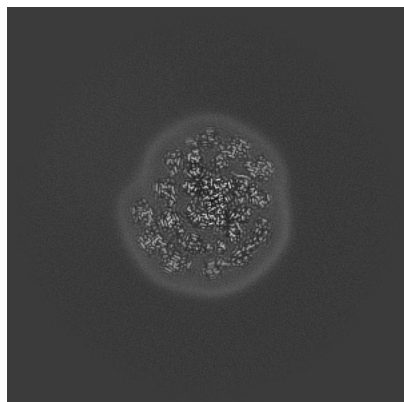


Z

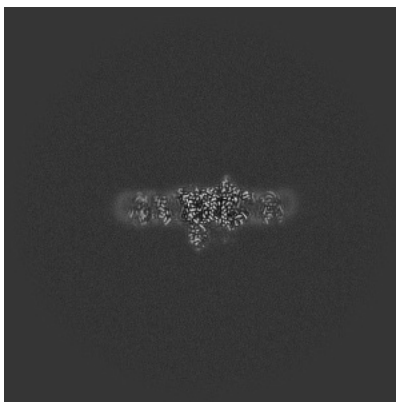
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

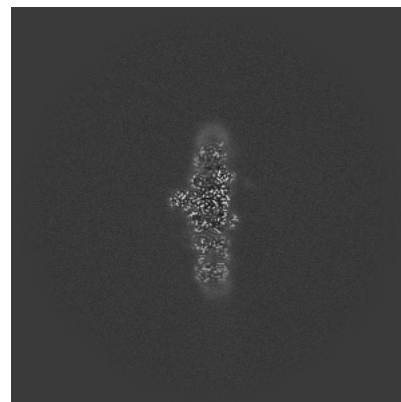
6.2.1 Primary map



X Index: 256

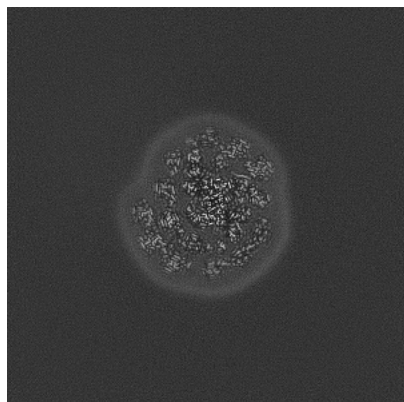


Y Index: 256

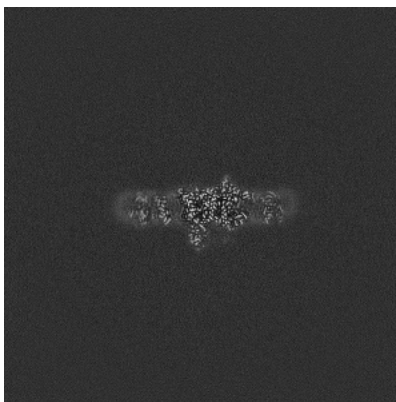


Z Index: 256

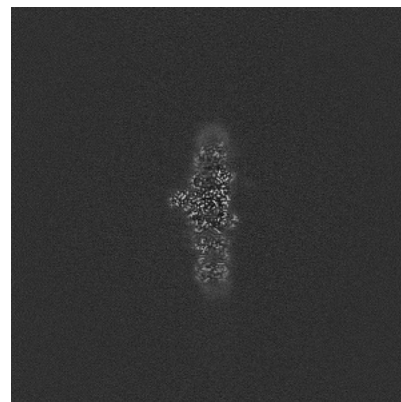
6.2.2 Raw map



X Index: 256



Y Index: 256

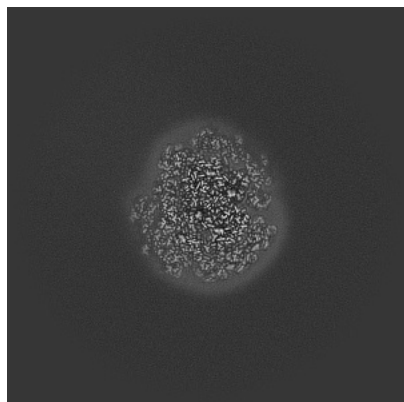


Z Index: 256

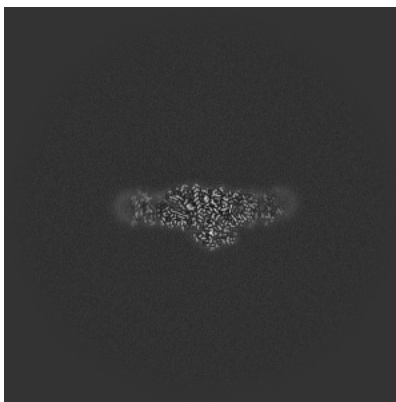
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

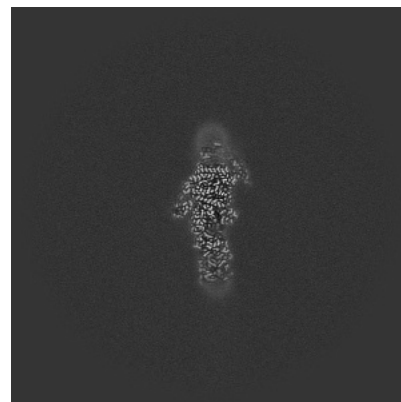
6.3.1 Primary map



X Index: 243

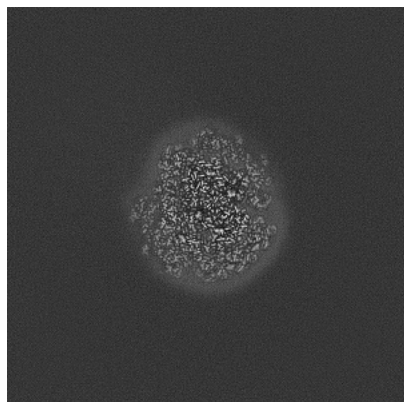


Y Index: 269

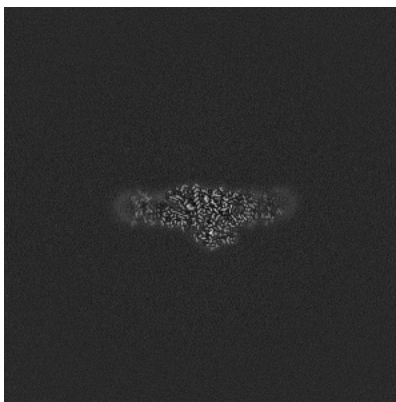


Z Index: 242

6.3.2 Raw map



X Index: 243



Y Index: 269

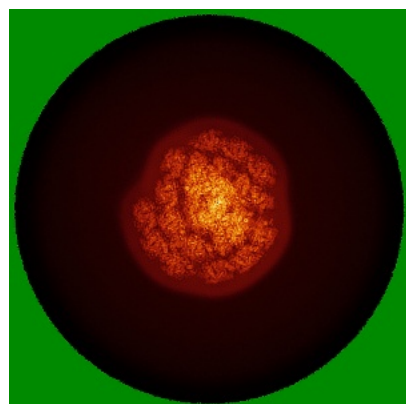


Z Index: 242

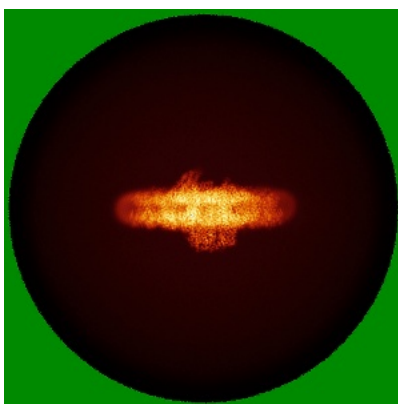
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

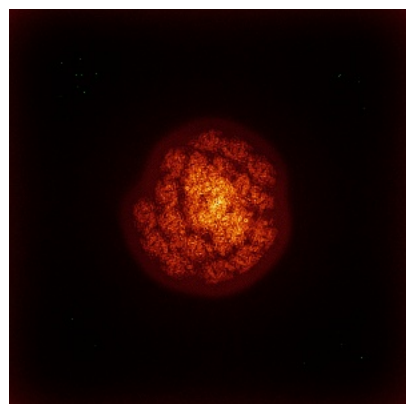


Y

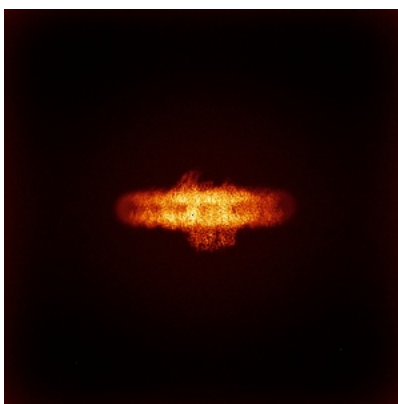


Z

6.4.2 Raw map



X



Y

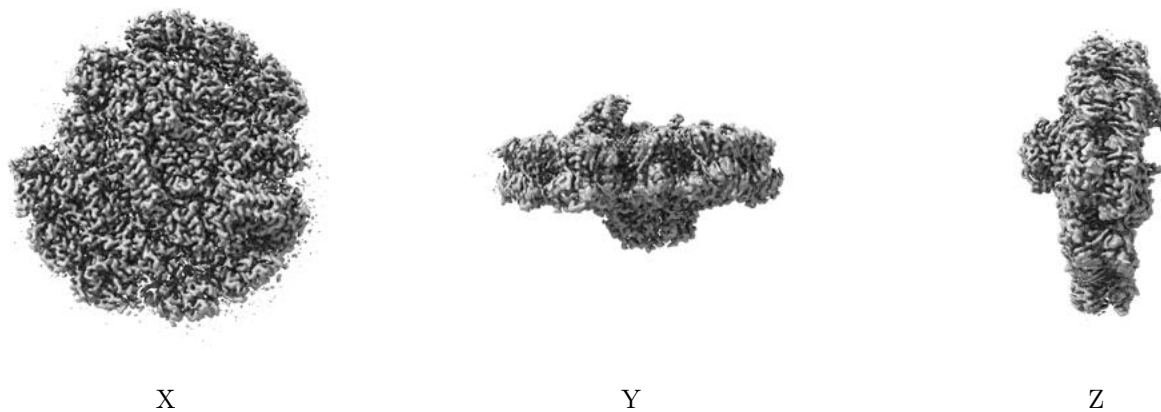


Z

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

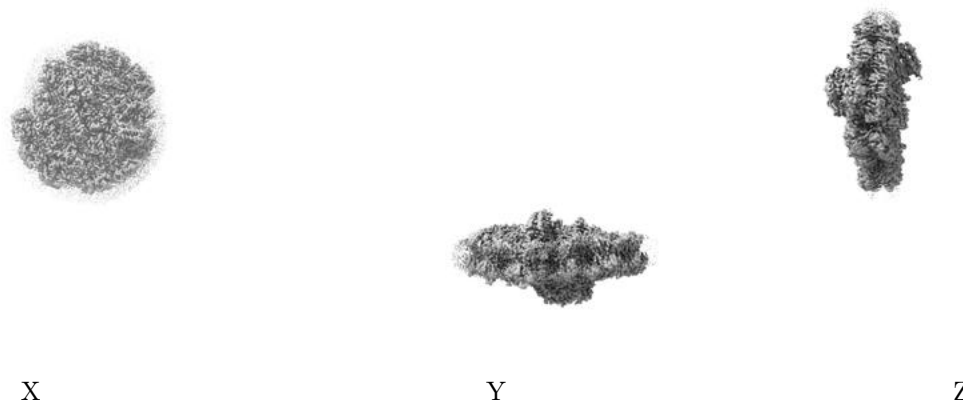
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

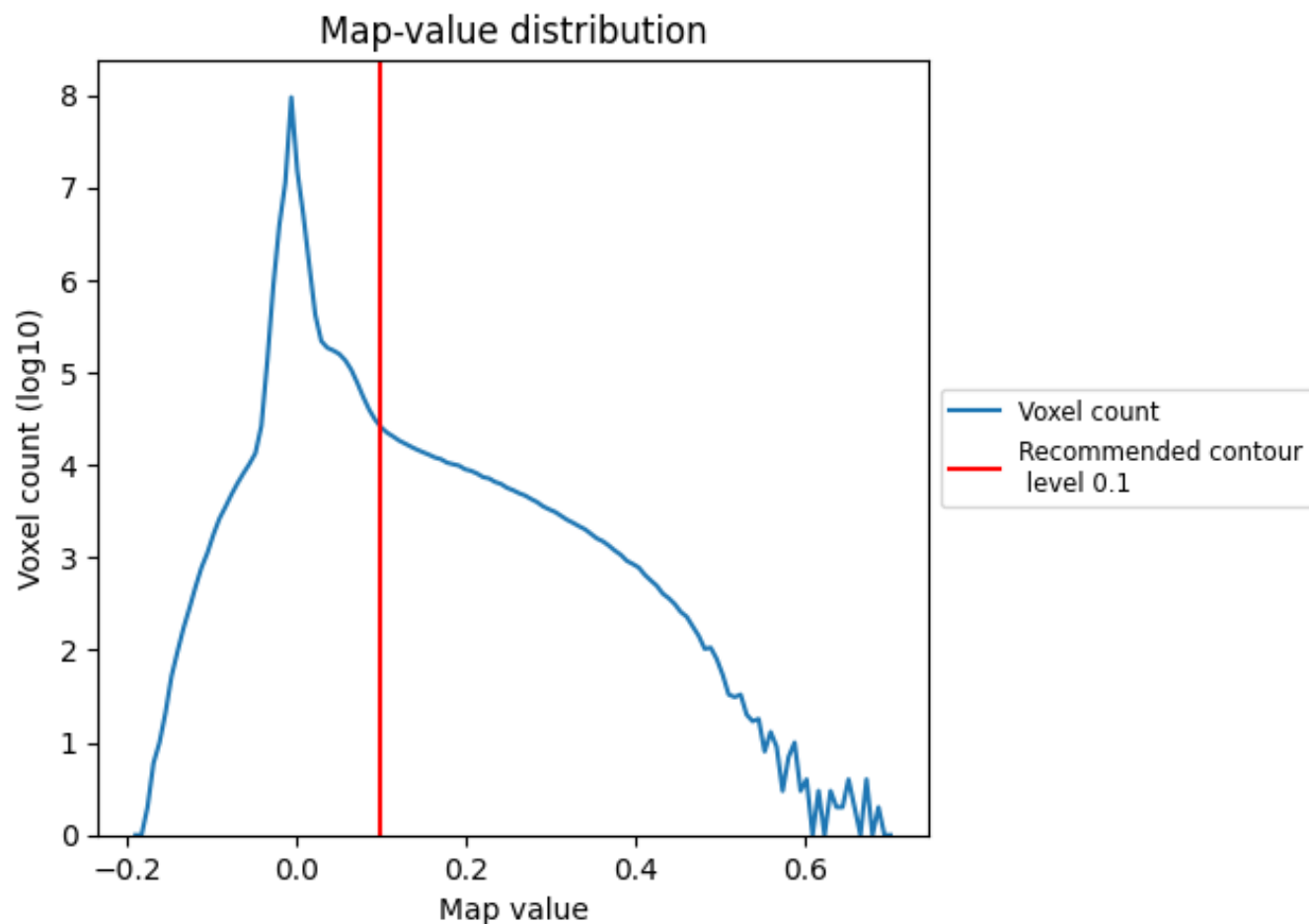
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

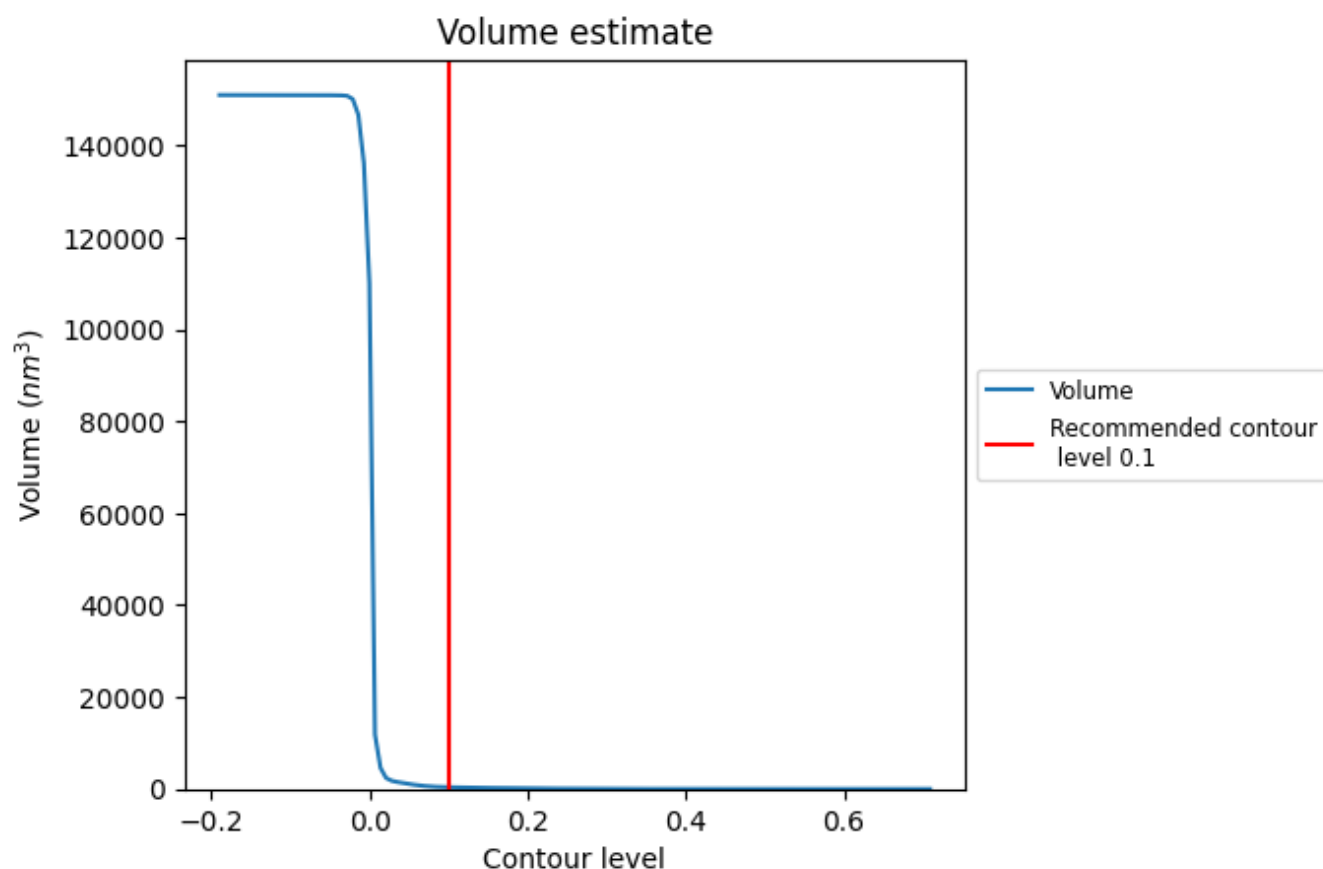
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

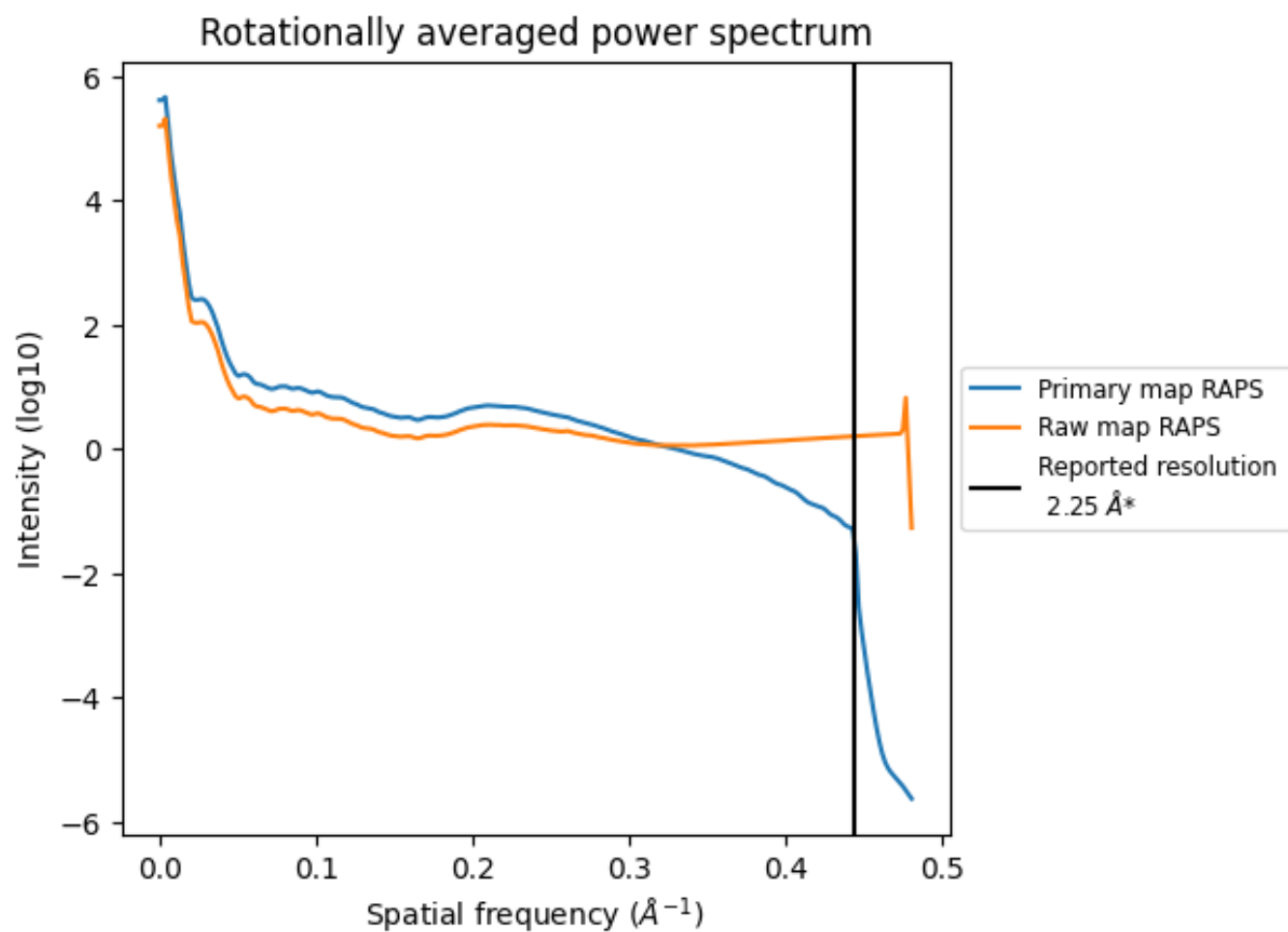
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm^3 ; this corresponds to an approximate mass of 341 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

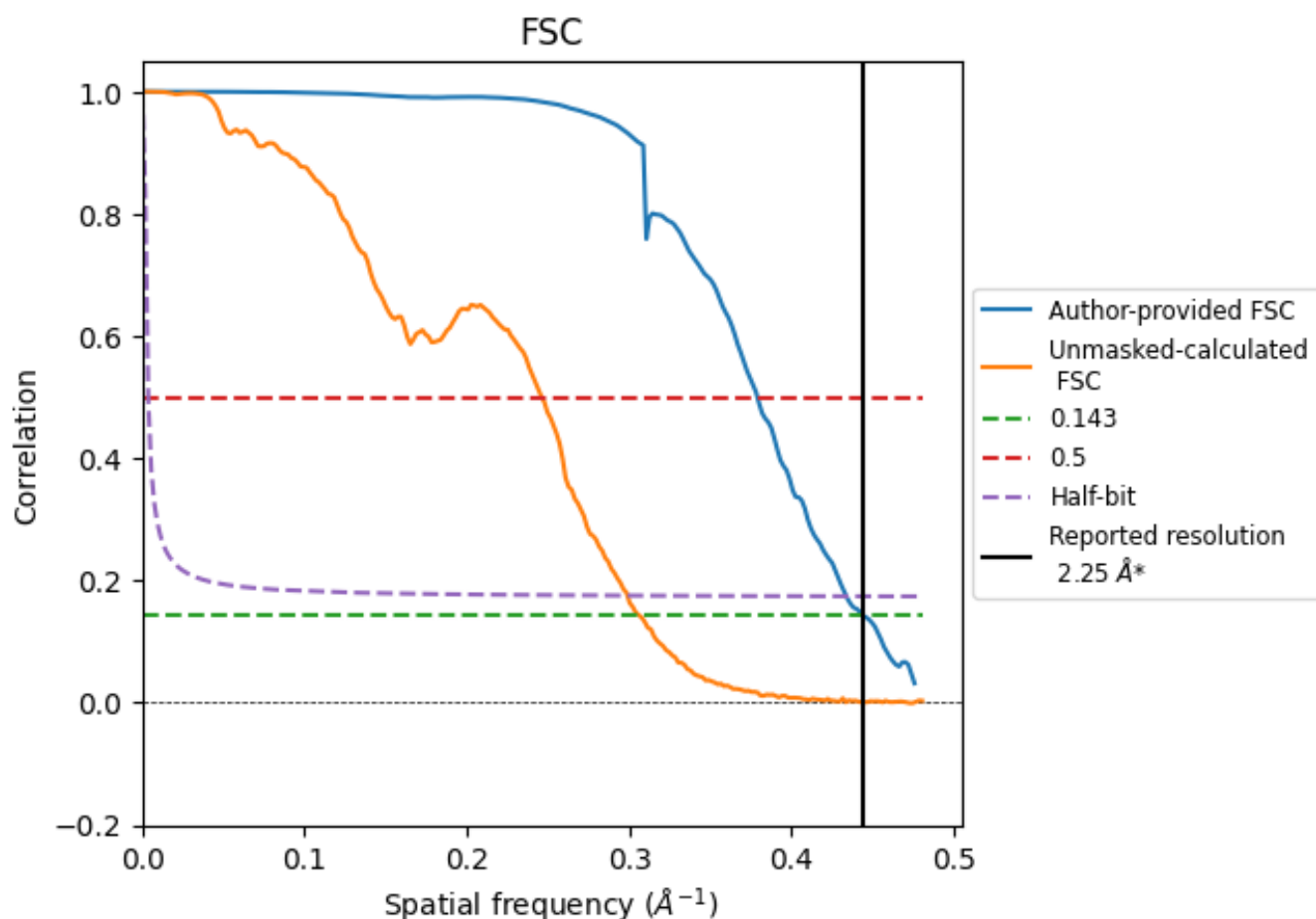


*Reported resolution corresponds to spatial frequency of 0.444 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.444 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

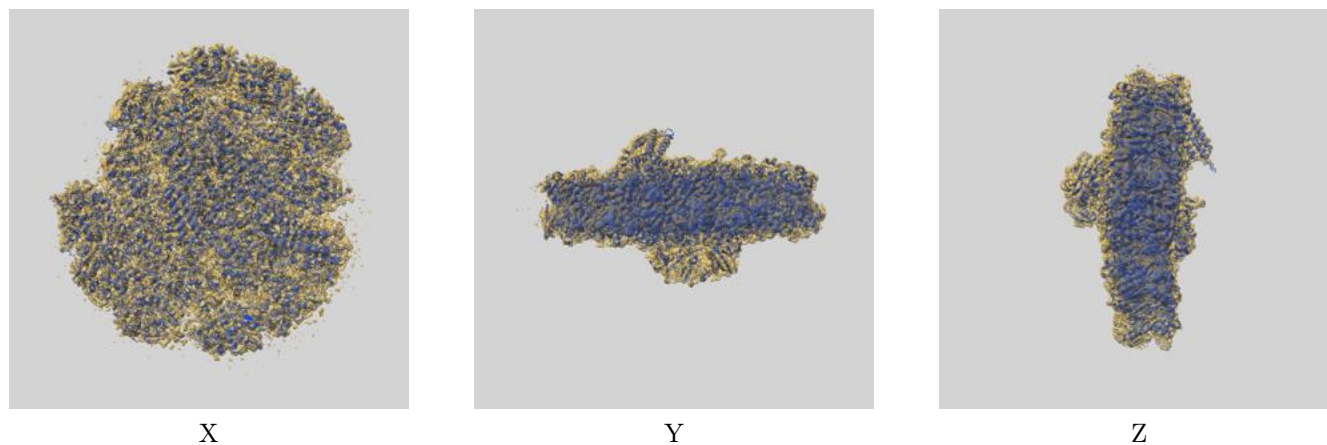
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.25	2.64	2.30
Unmasked-calculated*	3.27	4.06	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.27 differs from the reported value 2.25 by more than 10 %

9 Map-model fit [i](#)

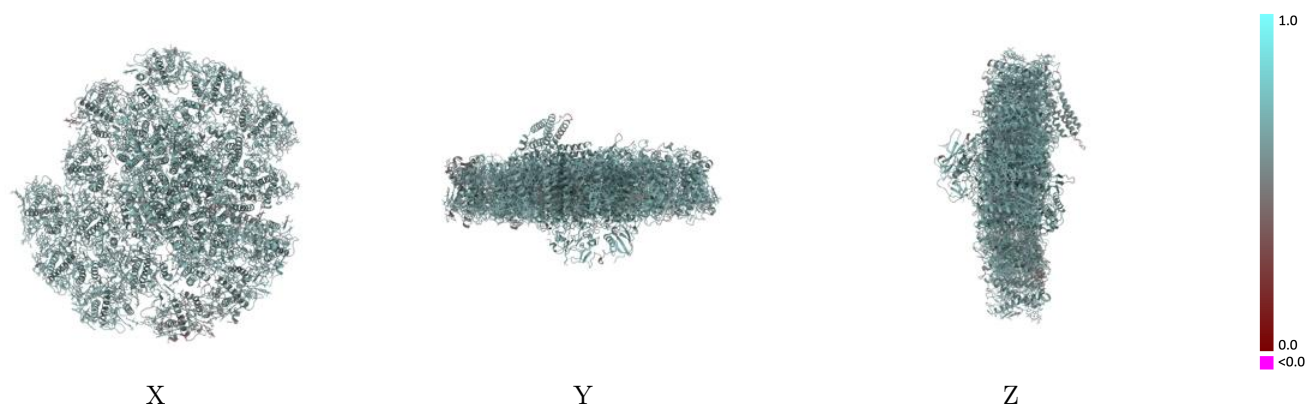
This section contains information regarding the fit between EMDB map EMD-66373 and PDB model 9WYP. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



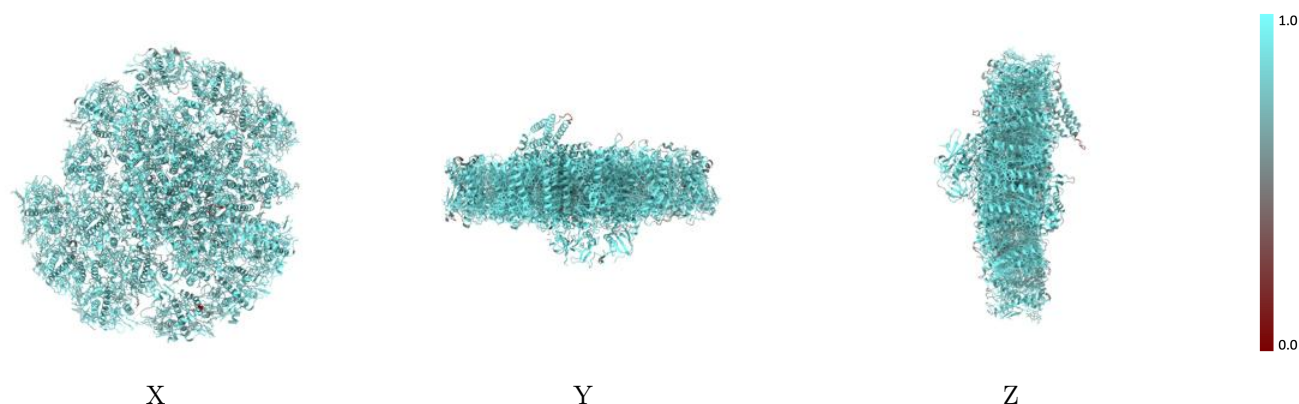
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



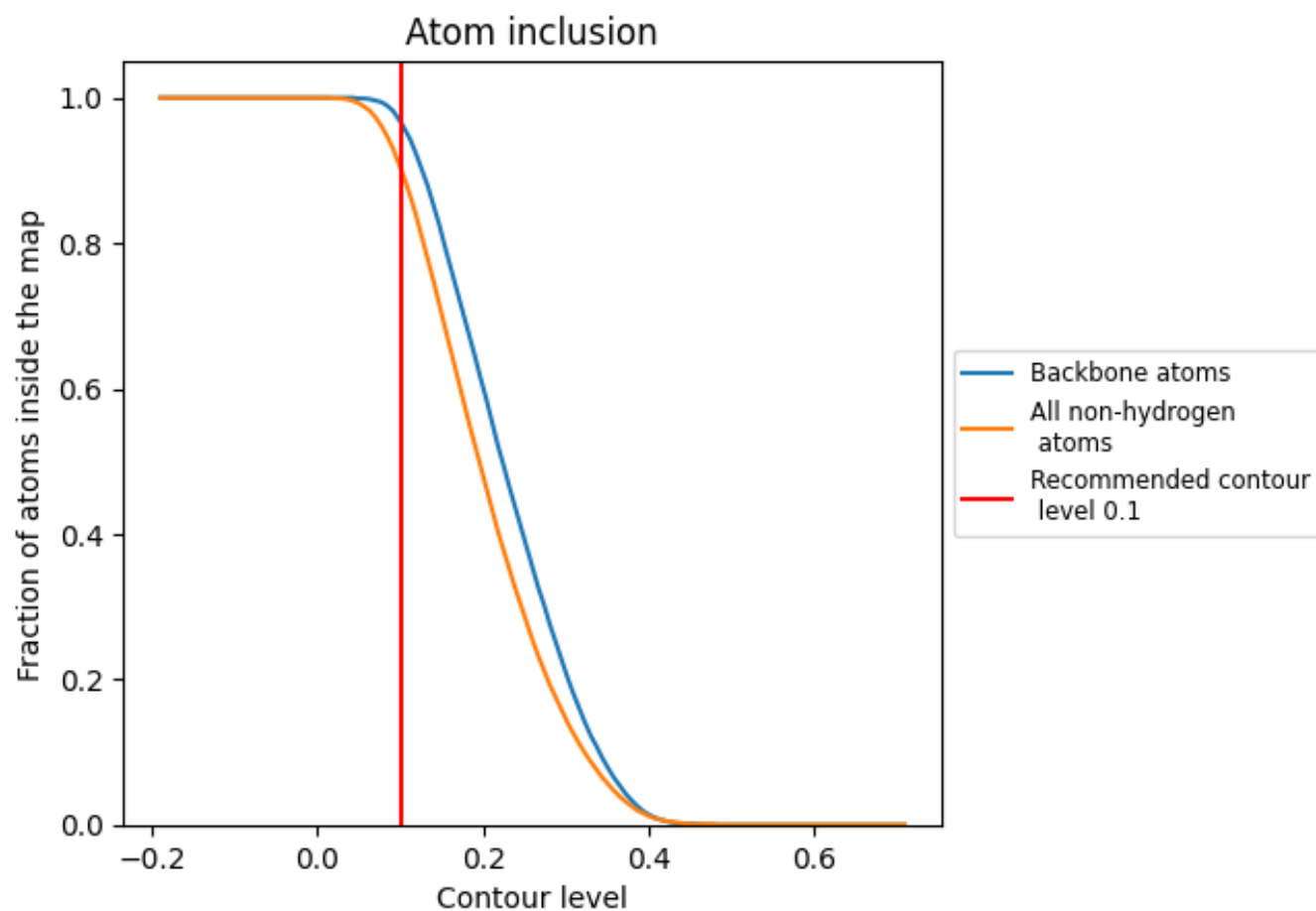
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9040	 0.6200
1	 0.8350	 0.5750
2	 0.9170	 0.6150
3	 0.9330	 0.6340
4	 0.9310	 0.6320
5	 0.7930	 0.5440
6	 0.8870	 0.5920
7	 0.9110	 0.5960
8	 0.8910	 0.6070
9	 0.8420	 0.6060
A	 0.9590	 0.6500
B	 0.9660	 0.6510
C	 0.9760	 0.6440
D	 0.9180	 0.6230
E	 0.9100	 0.6200
F	 0.9150	 0.6210
I	 0.9430	 0.6220
J	 0.9630	 0.6390
K	 0.9160	 0.6140
L	 0.9240	 0.6290
M	 0.9270	 0.6310
O	 0.9150	 0.6270
R	 0.9430	 0.6290
X	 0.8100	 0.5710
Z	 0.8620	 0.6150
a	 0.8790	 0.6160
b	 0.8800	 0.6070
c	 0.8240	 0.6010
d	 0.8440	 0.6140
e	 0.8300	 0.5990

