



wwPDB EM Validation Summary Report ⓘ

Sep 9, 2026 – 06:33 PM JST

PDB ID : 7Y8A / pdb_00007y8a
EMDB ID : EMD-33683
Title : Cryo-EM structure of cryptophyte photosystem I
Authors : Zhao, L.S.; Zhang, Y.Z.; Liu, L.N.; Li, K.
Deposited on : 2022-06-23
Resolution : 2.71 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

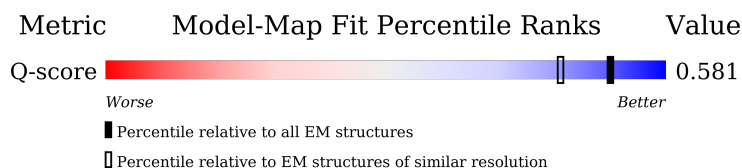
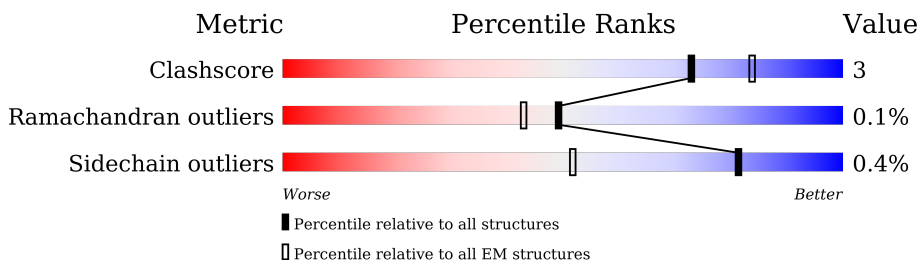
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.71 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	10297 (2.21 - 3.21)

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	
2	2	216	
3	3	236	
4	4	217	

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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	154	
22	R	133	
23	X	164	
24	Z	242	
25	a	215	
26	b	218	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 53404 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	179	Total	C	N	O	S	0	0
			1338	861	227	242	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	180	Total	C	N	O	S	0	0
			1362	875	231	246	10		

- 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	177	Total	C	N	O	S	0	0
			1337	861	230	238	8		

- Molecule 8 is a protein called ACPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	173	Total	C	N	O	S	0	0
			1298	842	217	235	4		

- 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	147	Total	C	N	O	S	0	0
			1119	730	180	207	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	92	Total	C	N	O	S	0	0
			709	481	104	123	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 Unk1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	145	Total	C	N	O	0	0
			725	435	145	145		

- Molecule 24 is a protein called ACPI-S.

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

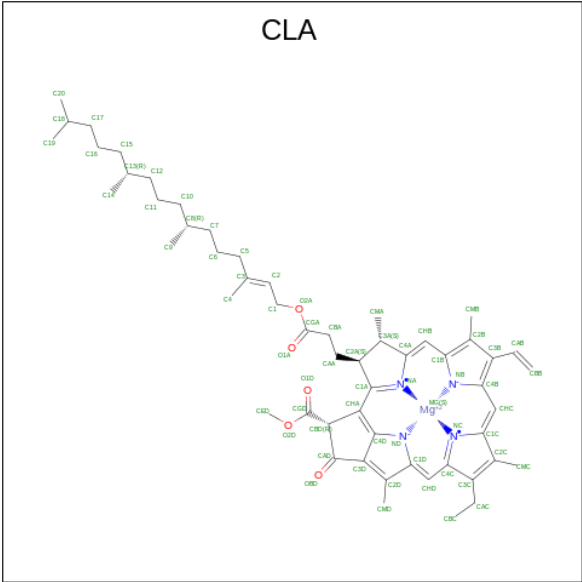
- Molecule 25 is a protein called ACPI-13.

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

- Molecule 26 is a protein called ACPI-14.

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

- Molecule 27 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	2	1	Total	C	Mg	N	O	0
			59	49	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	4	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	4	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
27	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	7	1	Total 53	C 43	Mg 1	N 4	O 5	0
27	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	7	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	9	1	Total 64	C 54	Mg 1	N 4	O 5	0
27	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	9	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
27	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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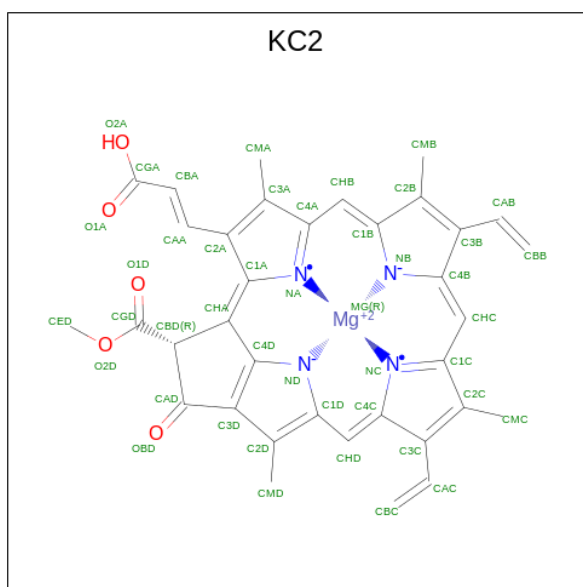
Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	J	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	L	1	Total 51	C 41	Mg 1	N 4	O 5	0
27	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0

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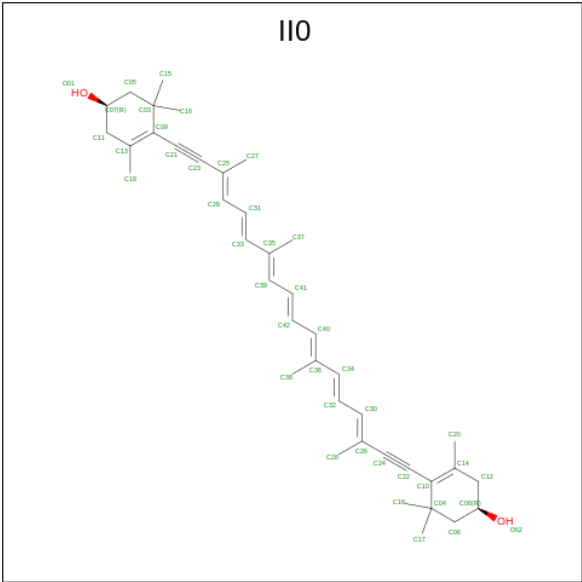
Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 28 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
28	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	b	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 29 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
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	

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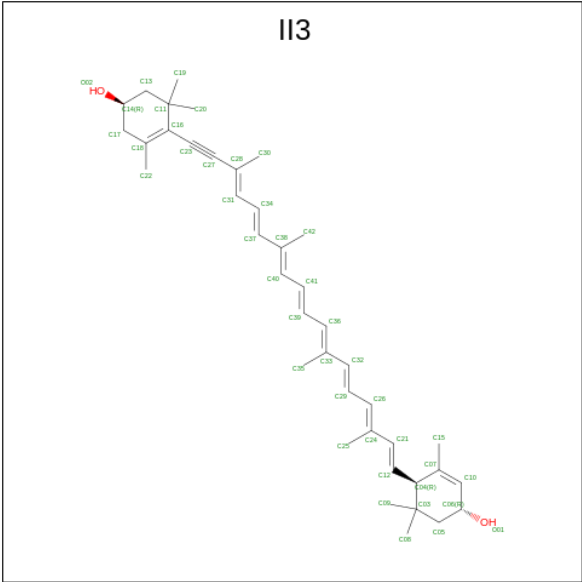
Mol	Chain	Residues	Atoms			AltConf
29	3	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	9	1	Total	C	O	0
			42	40	2	

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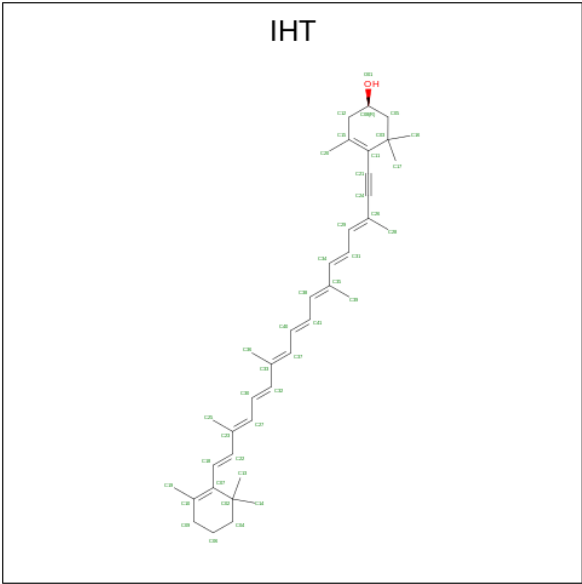
Mol	Chain	Residues	Atoms			AltConf
29	9	1	Total	C	O	0
			42	40	2	
29	9	1	Total	C	O	0
			42	40	2	
29	9	1	Total	C	O	0
			42	40	2	
29	B	1	Total	C	O	0
			42	40	2	
29	J	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	
29	Z	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	b	1	Total	C	O	0
			42	40	2	
29	b	1	Total	C	O	0
			42	40	2	

- Molecule 30 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).



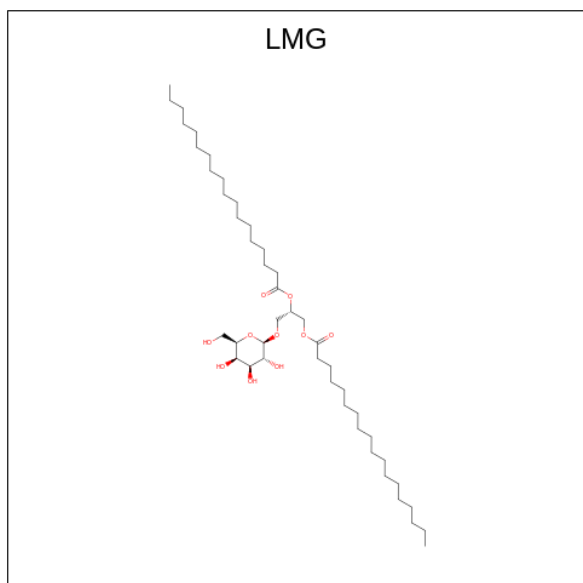
Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			42	40	2	
30	b	1	Total	C	O	0
			42	40	2	

- Molecule 31 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-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: C₄₀H₅₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			41	40	1	
31	2	1	Total	C	O	0
			41	40	1	
31	5	1	Total	C	O	0
			41	40	1	
31	6	1	Total	C	O	0
			41	40	1	
31	8	1	Total	C	O	0
			41	40	1	
31	9	1	Total	C	O	0
			41	40	1	
31	A	1	Total	C	O	0
			41	40	1	
31	L	1	Total	C	O	0
			41	40	1	
31	Z	1	Total	C	O	0
			41	40	1	
31	a	1	Total	C	O	0
			41	40	1	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



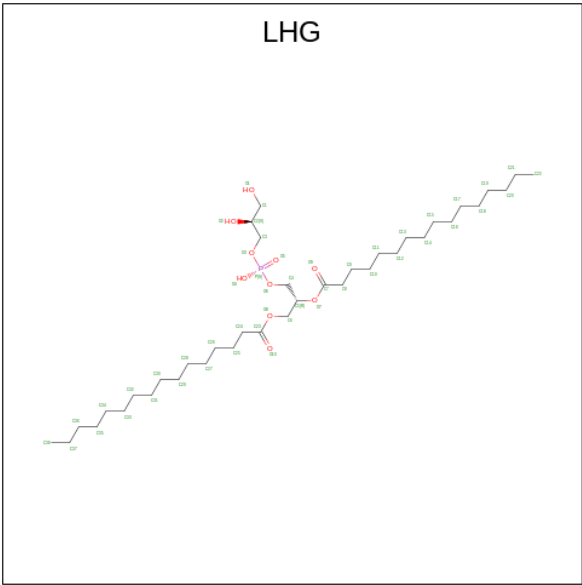
Mol	Chain	Residues	Atoms			AltConf
32	2	1	Total	C	O	0
			36	26	10	

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Mol	Chain	Residues	Atoms			AltConf
32	3	1	Total	C	O	0
			30	20	10	
32	3	1	Total	C	O	0
			32	22	10	
32	6	1	Total	C	O	0
			32	22	10	
32	8	1	Total	C	O	0
			52	42	10	
32	8	1	Total	C	O	0
			51	41	10	
32	F	1	Total	C	O	0
			32	22	10	

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



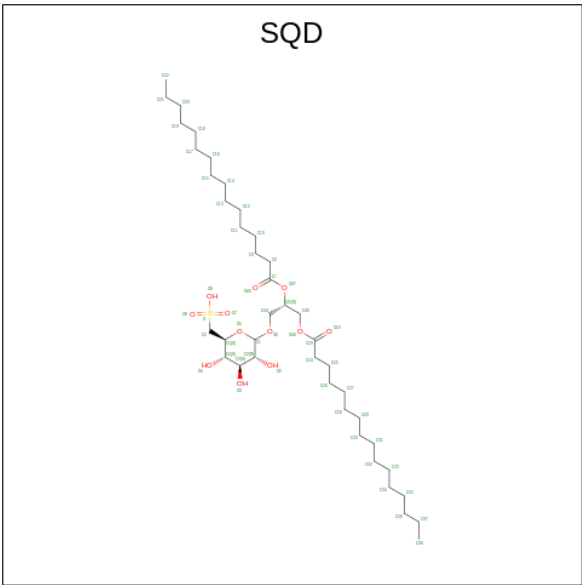
Mol	Chain	Residues	Atoms				AltConf
33	2	1	Total	C	O	P	0
			22	12	9	1	
33	2	1	Total	C	O	P	0
			39	28	10	1	
33	2	1	Total	C	O	P	0
			42	31	10	1	
33	3	1	Total	C	O	P	0
			49	38	10	1	
33	3	1	Total	C	O	P	0
			34	23	10	1	

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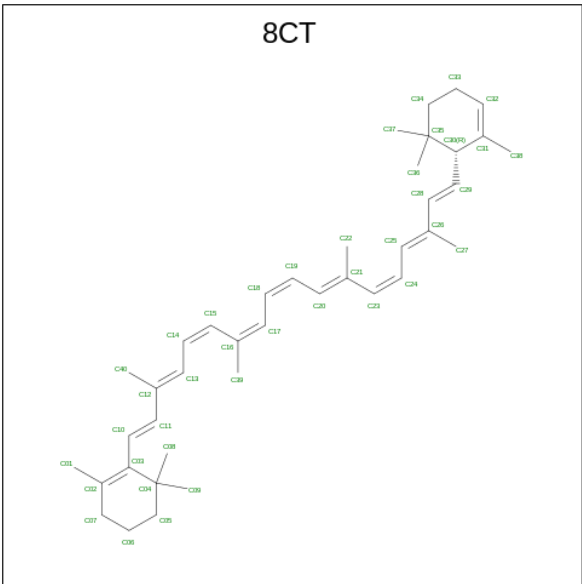
Mol	Chain	Residues	Atoms				AltConf
33	4	1	Total	C	O	P	0
			47	36	10	1	
33	4	1	Total	C	O	P	0
			45	34	10	1	
33	4	1	Total	C	O	P	0
			45	34	10	1	
33	5	1	Total	C	O	P	0
			23	12	10	1	
33	6	1	Total	C	O	P	0
			35	24	10	1	
33	7	1	Total	C	O	P	0
			31	20	10	1	
33	7	1	Total	C	O	P	0
			39	28	10	1	
33	8	1	Total	C	O	P	0
			33	22	10	1	
33	A	1	Total	C	O	P	0
			49	38	10	1	
33	A	1	Total	C	O	P	0
			39	28	10	1	
33	Z	1	Total	C	O	P	0
			46	35	10	1	
33	a	1	Total	C	O	P	0
			49	38	10	1	
33	a	1	Total	C	O	P	0
			29	18	10	1	
33	b	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
34	3	1	Total	C	O	S	0
			42	29	12	1	
34	O	1	Total	C	O	S	0
			24	12	11	1	

- Molecule 35 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).



Mol	Chain	Residues	Atoms		AltConf
35	4	1	Total	C	0
			40	40	

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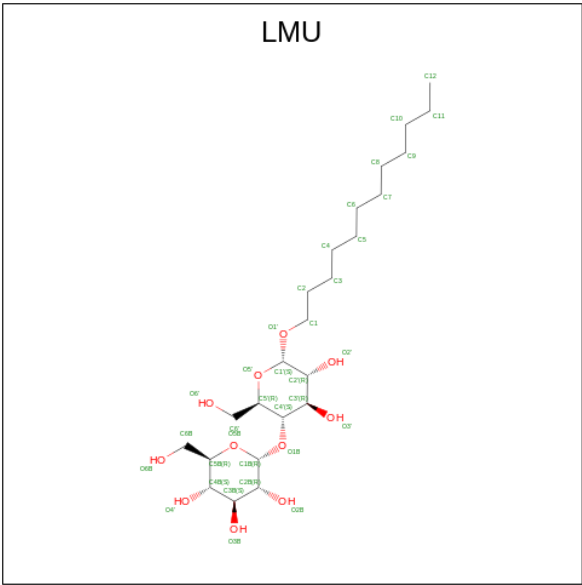
Mol	Chain	Residues	Atoms	AltConf
35	7	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	F	1	Total C 40 40	0
35	I	1	Total C 40 40	0
35	J	1	Total C 40 40	0
35	K	1	Total C 40 40	0
35	L	1	Total C 40 40	0
35	M	1	Total C 40 40	0
35	R	1	Total C 40 40	0
35	R	1	Total C 40 40	0
35	Z	1	Total C 40 40	0

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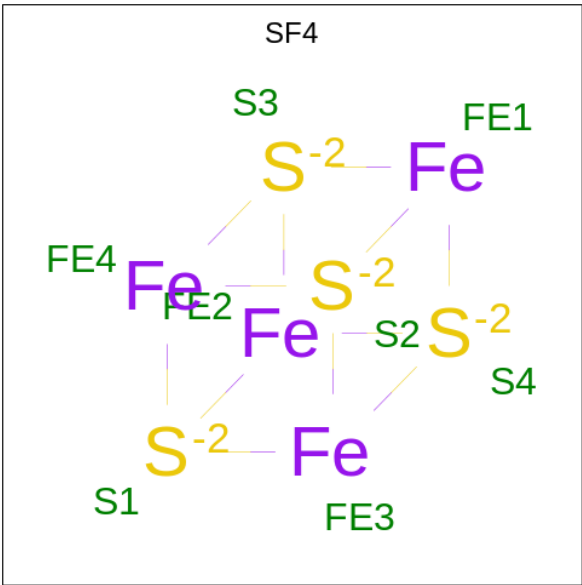
Mol	Chain	Residues	Atoms		AltConf
35	Z	1	Total	C	0
			40	40	
35	b	1	Total	C	0
			40	40	

- Molecule 36 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



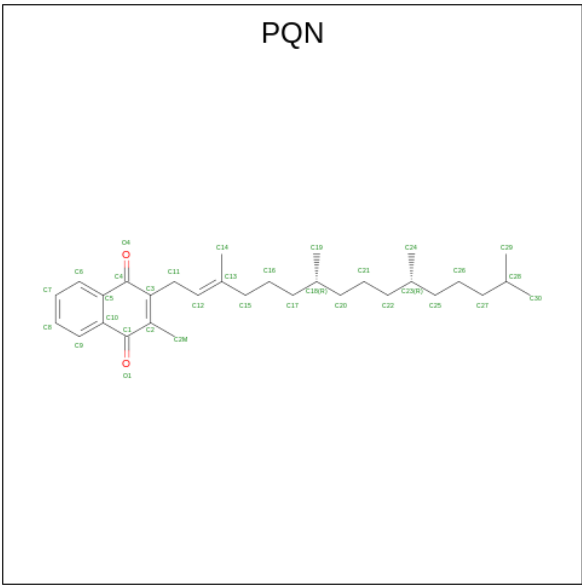
Mol	Chain	Residues	Atoms			AltConf
36	4	1	Total	C	O	0
			35	24	11	
36	7	1	Total	C	O	0
			35	24	11	
36	J	1	Total	C	O	0
			31	20	11	

- Molecule 37 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 38 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



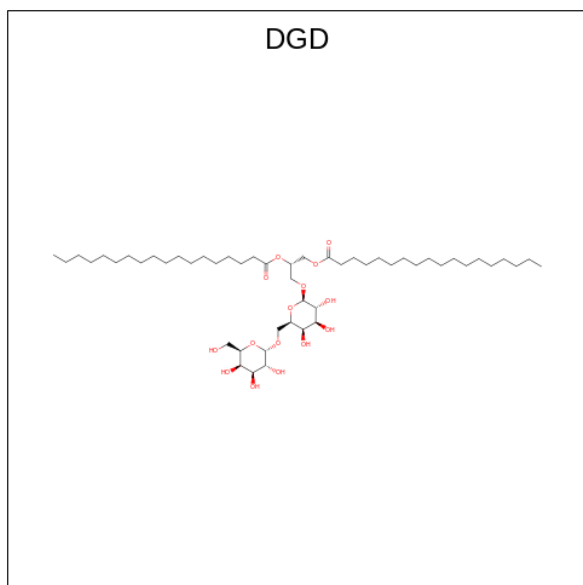
Mol	Chain	Residues	Atoms			AltConf
38	A	1	Total	C	O	0
			33	31	2	

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

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

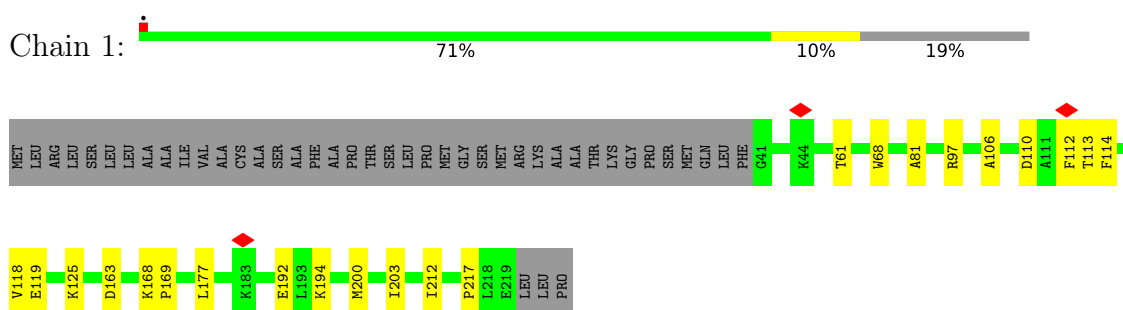


Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			59	44	15	
39	Z	1	Total	C	O	0
			60	45	15	

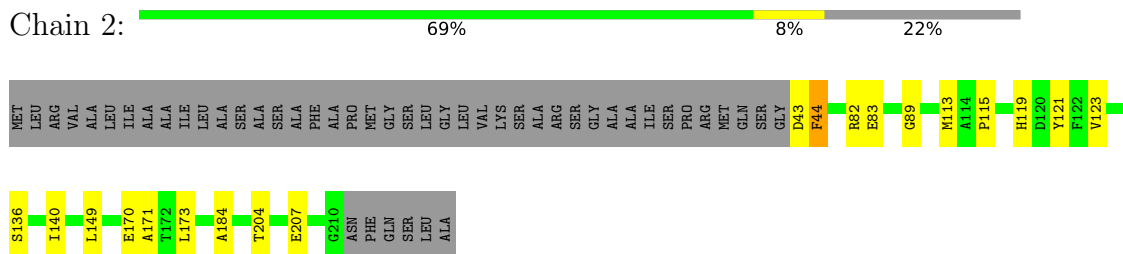
3 Residue-property plots

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.

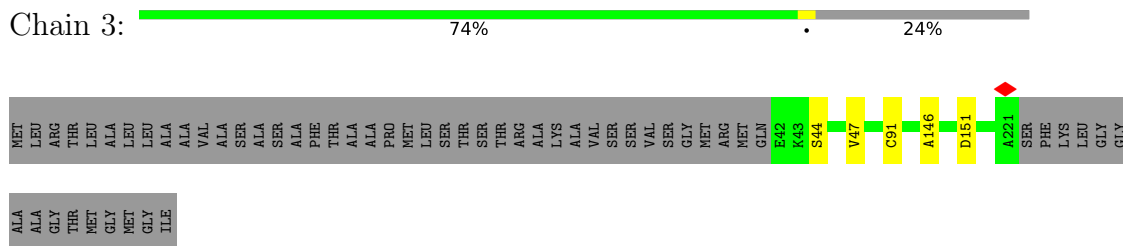
• Molecule 1: ACPI-1



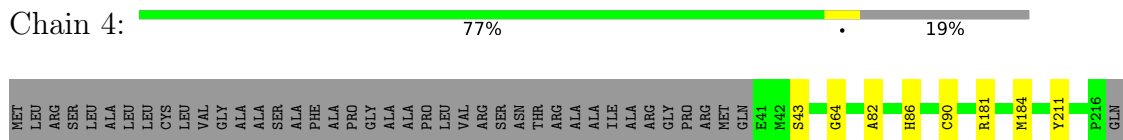
• Molecule 2: ACPI-2



• Molecule 3: ACPI-3

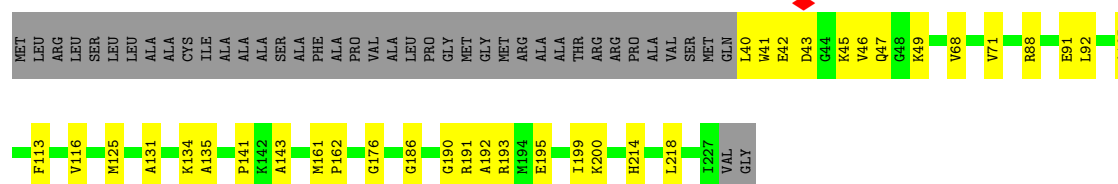


• Molecule 4: ACPI-4



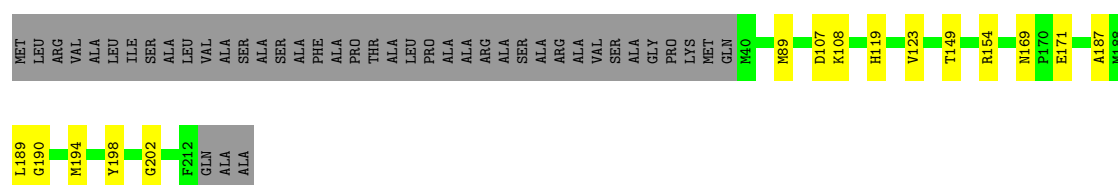
- Molecule 5: ACPI-5

Chain 5:  67% 15% 18%



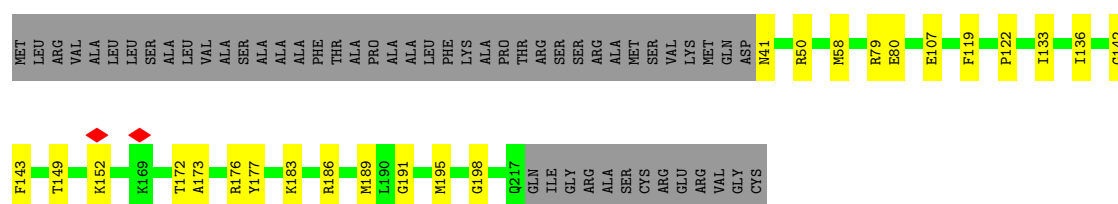
- Molecule 6: ACPI-6

Chain 6:  73% 7% 20%



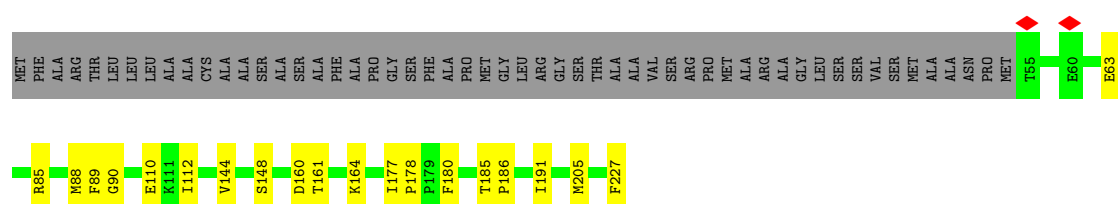
- Molecule 7: ACPI-7

Chain 7:  67% 10% 23%



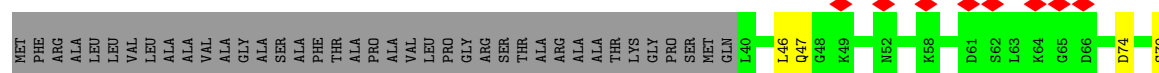
- Molecule 8: ACPI-8

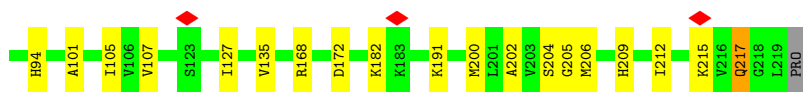
Chain 8:  67% 9% 24%



- Molecule 9: ACPI-12

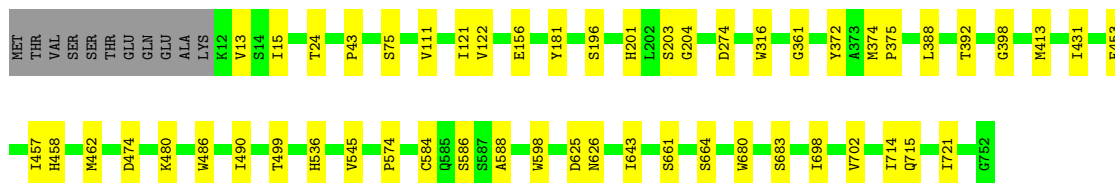
Chain 9:  5% 71% 10% 18%





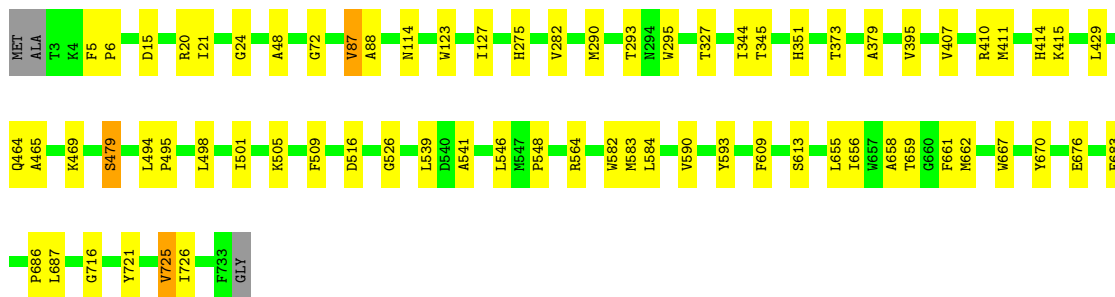
- Molecule 10: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 91% 7%



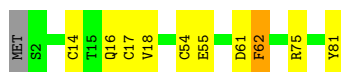
- Molecule 11: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 90% 9%



- Molecule 12: Photosystem I iron-sulfur center

Chain C: 86% 11%



- Molecule 13: Photosystem I reaction center subunit II

Chain D: 87% 9%



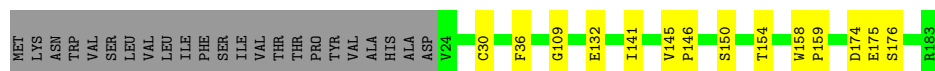
- Molecule 14: Photosystem I reaction center subunit IV

Chain E: 89% 6% 5%



- Molecule 15: Photosystem I reaction center subunit III

Chain F:  80% 8% 13%

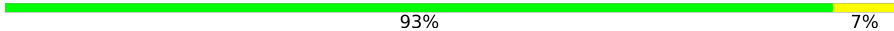


- Molecule 16: Photosystem I reaction center subunit VIII

Chain I:  86% 6% 8%



- Molecule 17: Photosystem I reaction center subunit IX

Chain J:  93% 7%



- Molecule 18: Photosystem I reaction center subunit PsaK

Chain K:  82% 8% 10%



- Molecule 19: Photosystem I reaction center subunit XI

Chain L:  7% 88% 8%



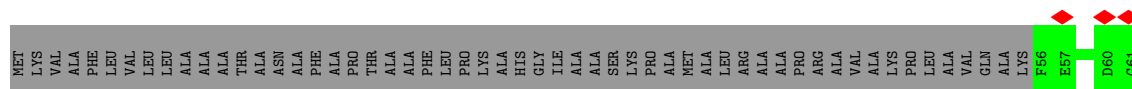
- Molecule 20: Photosystem I reaction center subunit XII

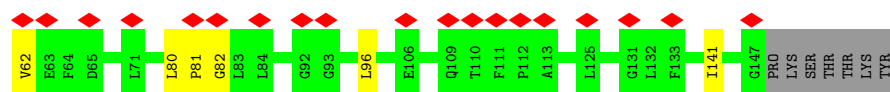
Chain M:  90% 10%



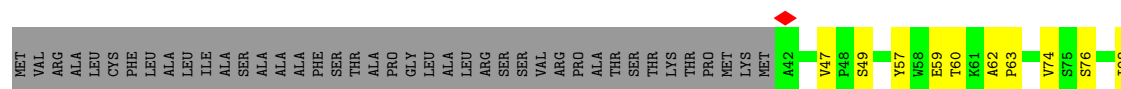
- Molecule 21: PsaO

Chain O:  14% 56% 40%

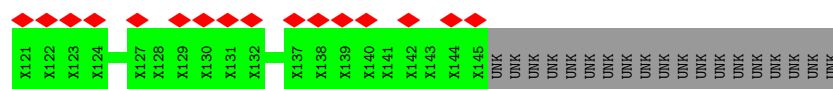
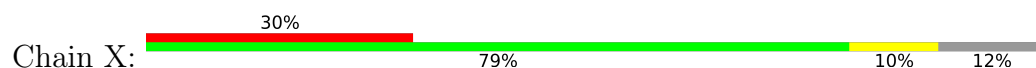




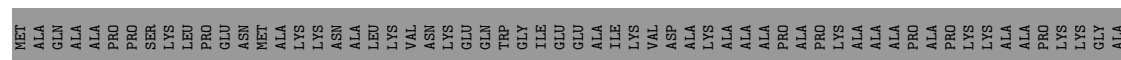
• Molecule 22: PsaR



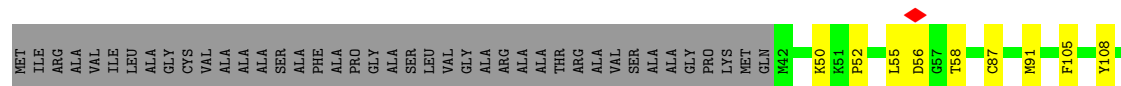
• Molecule 23: Unk1



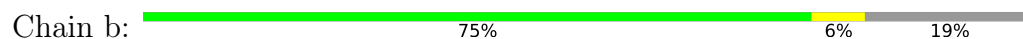
• Molecule 24: ACPI-S

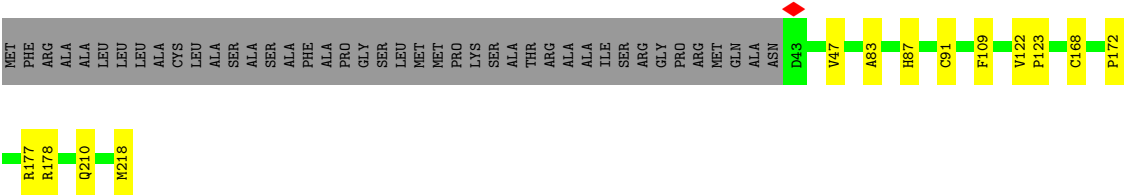


• Molecule 25: ACPI-13



• Molecule 26: ACPI-14





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118810	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.988	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.033	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: SF4, KC2, LMU, SQD, II3, PQN, CLA, IHT, LMG, LHG, II0, 8CT, DGD

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	0.37	0/1371	0.63	0/1854
2	2	0.18	0/1356	0.33	0/1835
3	3	0.19	0/1392	0.32	0/1883
4	4	0.18	0/1406	0.29	0/1900
5	5	0.37	0/1438	0.57	1/1940 (0.1%)
6	6	0.18	0/1334	0.32	0/1796
7	7	0.33	1/1373 (0.1%)	0.47	0/1858
8	8	0.23	0/1326	0.35	0/1804
9	9	0.20	0/1376	0.34	0/1846
10	A	0.24	3/6019 (0.0%)	0.35	0/8204
11	B	0.30	3/6046 (0.0%)	0.45	3/8254 (0.0%)
12	C	0.27	0/600	0.42	0/812
13	D	0.24	0/1094	0.43	0/1476
14	E	0.33	0/499	0.54	0/677
15	F	0.21	0/1290	0.35	0/1745
16	I	0.17	0/266	0.30	0/362
17	J	0.21	0/353	0.32	0/481
18	K	0.41	0/563	0.40	0/768
19	L	0.41	0/1147	0.55	4/1561 (0.3%)
20	M	0.17	0/228	0.22	0/310
21	O	0.27	0/737	0.50	0/1011
22	R	0.35	0/700	0.46	2/963 (0.2%)
24	Z	0.20	0/1163	0.35	0/1572
25	a	0.40	2/1299 (0.2%)	0.52	2/1747 (0.1%)
26	b	0.24	0/1404	0.41	3/1902 (0.2%)
All	All	0.28	9/35780 (0.0%)	0.42	15/48561 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	172	ASN	C-N	-7.75	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	171	LYS	C-N	-7.27	1.23	1.33
11	B	683	GLU	C-N	-6.88	1.23	1.33
10	A	196	SER	C-N	6.42	1.42	1.34
11	B	583	MET	C-O	-6.42	1.16	1.24

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	80	PHE	CA-C-O	-6.55	113.48	120.42
5	5	141	PRO	N-CA-C	-6.41	99.26	112.47
11	B	546	LEU	CA-C-O	-5.99	114.53	120.70
25	a	172	ASN	CA-C-N	5.87	128.62	120.29
25	a	172	ASN	C-N-CA	5.87	128.62	120.29

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	1338	0	1329	18	0
2	2	1320	0	1309	12	0
3	3	1362	0	1389	4	0
4	4	1366	0	1349	5	0
5	5	1403	0	1398	33	0
6	6	1305	0	1324	8	0
7	7	1337	0	1317	16	0
8	8	1298	0	1322	16	0
9	9	1349	0	1358	20	0
10	A	5824	0	5672	38	0
11	B	5828	0	5626	44	0
12	C	591	0	568	9	0
13	D	1070	0	1076	10	0
14	E	491	0	491	3	0
15	F	1258	0	1266	11	0
16	I	258	0	268	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	J	342	0	344	2	0
18	K	553	0	581	8	0
19	L	1119	0	1117	7	0
20	M	227	0	257	3	0
21	O	709	0	691	4	0
22	R	680	0	674	7	0
23	X	725	0	151	12	0
24	Z	1130	0	1088	6	0
25	a	1271	0	1281	15	0
26	b	1368	0	1346	6	0
27	1	584	0	476	5	0
27	2	547	0	456	1	0
27	3	625	0	596	0	0
27	4	598	0	597	1	0
27	5	563	0	442	7	0
27	6	581	0	514	2	0
27	7	509	0	431	4	0
27	8	496	0	471	4	0
27	9	642	0	539	6	0
27	A	2679	0	2767	18	0
27	B	2471	0	2530	20	0
27	F	160	0	141	0	0
27	J	41	0	29	0	0
27	K	120	0	121	1	0
27	L	161	0	139	2	0
27	O	206	0	176	1	0
27	R	55	0	49	1	0
27	Z	290	0	278	1	0
27	a	580	0	560	5	0
27	b	530	0	525	1	0
28	1	45	0	0	0	0
28	2	45	0	0	0	0
28	3	45	0	0	0	0
28	4	45	0	0	0	0
28	5	45	0	0	0	0
28	6	90	0	0	0	0
28	7	90	0	0	2	0
28	9	45	0	0	1	0
28	Z	45	0	0	0	0
28	a	45	0	0	0	0
28	b	90	0	0	1	0
29	1	168	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	2	126	0	0	1	0
29	3	210	0	0	1	0
29	4	168	0	0	1	0
29	5	210	0	0	1	0
29	6	84	0	0	0	0
29	7	210	0	0	0	0
29	8	126	0	0	1	0
29	9	168	0	0	0	0
29	B	42	0	0	0	0
29	J	42	0	0	0	0
29	O	84	0	0	0	0
29	R	42	0	0	0	0
29	Z	42	0	0	0	0
29	a	168	0	0	1	0
29	b	84	0	0	0	0
30	1	42	0	0	0	0
30	b	42	0	0	1	0
31	1	41	0	0	0	0
31	2	41	0	0	1	0
31	5	41	0	0	0	0
31	6	41	0	0	1	0
31	8	41	0	0	0	0
31	9	41	0	0	1	0
31	A	41	0	0	1	0
31	L	41	0	0	0	0
31	Z	41	0	0	0	0
31	a	41	0	0	1	0
32	2	36	0	42	0	0
32	3	62	0	64	0	0
32	6	32	0	34	0	0
32	8	103	0	152	0	0
32	F	32	0	34	0	0
33	2	103	0	125	1	0
33	3	83	0	112	0	0
33	4	137	0	190	0	0
33	5	23	0	16	0	0
33	6	35	0	40	1	0
33	7	70	0	83	0	0
33	8	33	0	36	0	0
33	A	88	0	122	0	0
33	Z	46	0	65	0	0
33	a	78	0	102	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	b	49	0	74	0	0
34	3	42	0	48	0	0
34	O	24	0	18	0	0
35	4	40	0	0	1	0
35	7	40	0	0	1	0
35	A	200	0	0	0	0
35	B	240	0	0	0	0
35	F	40	0	0	0	0
35	I	40	0	0	0	0
35	J	40	0	0	0	0
35	K	40	0	0	0	0
35	L	40	0	0	0	0
35	M	40	0	0	1	0
35	R	80	0	0	0	0
35	Z	80	0	0	0	0
35	b	40	0	0	0	0
36	4	35	0	46	2	0
36	7	35	0	46	1	0
36	J	31	0	35	1	0
37	A	8	0	0	0	0
37	C	16	0	0	1	0
38	A	33	0	46	0	0
38	B	33	0	46	0	0
39	B	59	0	79	0	0
39	Z	60	0	78	1	0
All	All	53404	0	48162	332	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 3.

The worst 5 of 332 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)
5:5:41:TRP:HB2	5:5:192:ALA:HB1	1.44	0.99
13:D:99:HIS:HB3	13:D:100:PRO:HD3	1.55	0.88
5:5:42:GLU:HB3	5:5:45:LYS:HB2	1.58	0.84
22:R:74:VAL:O	22:R:128:GLN:NE2	2.13	0.81
26:b:177:ARG:NH2	28:b:609:KC2:O1A	2.14	0.80

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	177/222 (80%)	167 (94%)	10 (6%)	0	100	100
2	2	166/216 (77%)	162 (98%)	3 (2%)	1 (1%)	21	42
3	3	178/236 (75%)	176 (99%)	2 (1%)	0	100	100
4	4	174/217 (80%)	173 (99%)	1 (1%)	0	100	100
5	5	186/229 (81%)	176 (95%)	10 (5%)	0	100	100
6	6	171/215 (80%)	168 (98%)	3 (2%)	0	100	100
7	7	175/230 (76%)	171 (98%)	4 (2%)	0	100	100
8	8	171/227 (75%)	168 (98%)	3 (2%)	0	100	100
9	9	178/220 (81%)	175 (98%)	3 (2%)	0	100	100
10	A	739/752 (98%)	714 (97%)	25 (3%)	0	100	100
11	B	729/734 (99%)	708 (97%)	21 (3%)	0	100	100
12	C	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	9	23
13	D	135/141 (96%)	127 (94%)	7 (5%)	1 (1%)	18	39
14	E	59/64 (92%)	59 (100%)	0	0	100	100
15	F	158/183 (86%)	152 (96%)	6 (4%)	0	100	100
16	I	31/36 (86%)	29 (94%)	2 (6%)	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	145/153 (95%)	139 (96%)	6 (4%)	0	100	100
20	M	28/30 (93%)	28 (100%)	0	0	100	100
21	O	90/154 (58%)	88 (98%)	2 (2%)	0	100	100
22	R	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
24	Z	151/242 (62%)	147 (97%)	4 (3%)	0	100	100
25	a	169/215 (79%)	165 (98%)	4 (2%)	0	100	100
26	b	174/218 (80%)	171 (98%)	2 (1%)	1 (1%)	21	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4468/5277 (85%)	4338 (97%)	126 (3%)	4 (0%)	49 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	C	62	PHE
2	2	44	PHE
13	D	99	HIS
26	b	172	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	130/163 (80%)	130 (100%)	0	100 100
2	2	134/167 (80%)	134 (100%)	0	100 100
3	3	145/183 (79%)	145 (100%)	0	100 100
4	4	139/167 (83%)	139 (100%)	0	100 100
5	5	139/166 (84%)	139 (100%)	0	100 100
6	6	134/160 (84%)	134 (100%)	0	100 100
7	7	137/176 (78%)	137 (100%)	0	100 100
8	8	134/169 (79%)	134 (100%)	0	100 100
9	9	138/164 (84%)	136 (99%)	2 (1%)	59 80
10	A	607/617 (98%)	606 (100%)	1 (0%)	87 95
11	B	592/593 (100%)	587 (99%)	5 (1%)	73 87
12	C	66/67 (98%)	66 (100%)	0	100 100
13	D	114/117 (97%)	112 (98%)	2 (2%)	51 76
14	E	56/59 (95%)	55 (98%)	1 (2%)	51 76
15	F	133/154 (86%)	133 (100%)	0	100 100
16	I	27/29 (93%)	27 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	J	38/38 (100%)	38 (100%)	0	100	100
18	K	62/69 (90%)	62 (100%)	0	100	100
19	L	123/128 (96%)	123 (100%)	0	100	100
20	M	25/25 (100%)	25 (100%)	0	100	100
21	O	74/115 (64%)	74 (100%)	0	100	100
22	R	74/105 (70%)	74 (100%)	0	100	100
24	Z	117/180 (65%)	117 (100%)	0	100	100
25	a	128/153 (84%)	127 (99%)	1 (1%)	73	87
26	b	144/173 (83%)	142 (99%)	2 (1%)	59	80
All	All	3610/4137 (87%)	3596 (100%)	14 (0%)	81	92

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	B	725	VAL
13	D	107	GLU
26	b	218	MET
25	a	129	THR
26	b	47	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
18	K	28	ASN
19	L	33	ASN
25	a	183	ASN
9	9	217	GLN
9	9	213	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

357 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
27	CLA	A	803	10	69,73,73	1.76	9 (13%)	83,113,113	1.46	10 (12%)
27	CLA	8	605	8	54,58,73	2.01	9 (16%)	65,95,113	1.62	11 (16%)
27	CLA	6	608	6	64,68,73	1.83	9 (14%)	77,107,113	1.46	11 (14%)
27	CLA	9	602	9	59,63,73	1.94	9 (15%)	71,101,113	1.56	10 (14%)
27	CLA	A	816	10	64,68,73	1.80	9 (14%)	77,107,113	1.47	8 (10%)
27	CLA	9	613	9	49,53,73	2.12	9 (18%)	59,89,113	1.61	8 (13%)
35	8CT	B	849	-	40,41,41	0.33	0	50,56,56	0.72	1 (2%)
29	II0	2	615	-	39,43,43	2.72	4 (10%)	50,60,60	1.50	10 (20%)
27	CLA	8	602	8	49,53,73	2.12	9 (18%)	59,89,113	1.56	7 (11%)
27	CLA	b	610	26	55,59,73	2.00	9 (16%)	66,96,113	1.59	10 (15%)
27	CLA	K	101	-	69,73,73	1.78	9 (13%)	83,113,113	1.35	8 (9%)
31	IHT	6	616	-	40,42,42	2.81	4 (10%)	53,58,58	2.16	16 (30%)
31	IHT	A	854	-	40,42,42	2.93	5 (12%)	53,58,58	1.95	17 (32%)
27	CLA	7	312	-	59,63,73	1.92	9 (15%)	71,101,113	1.50	8 (11%)
33	LHG	A	851	-	48,48,48	0.59	0	51,54,54	1.17	4 (7%)
27	CLA	2	611	-	49,53,73	2.11	9 (18%)	59,89,113	1.62	10 (16%)
32	LMG	6	618	-	32,32,55	0.98	1 (3%)	40,40,63	1.23	5 (12%)
27	CLA	4	603	4	58,62,73	1.94	9 (15%)	69,99,113	1.56	9 (13%)
27	CLA	B	828	11	69,73,73	1.77	9 (13%)	83,113,113	1.37	8 (9%)
29	II0	9	616	-	39,43,43	2.68	4 (10%)	50,60,60	1.37	9 (18%)
27	CLA	B	820	11	64,68,73	1.86	9 (14%)	77,107,113	1.45	8 (10%)
27	CLA	b	611	26	59,63,73	1.89	9 (15%)	71,101,113	1.48	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	IHT	L	204	-	40,42,42	2.83	4 (10%)	53,58,58	2.23	16 (30%)
27	CLA	a	604	-	64,68,73	1.87	9 (14%)	77,107,113	1.47	8 (10%)
27	CLA	A	813	10	46,50,73	2.18	9 (19%)	55,85,113	1.73	9 (16%)
27	CLA	a	602	25	59,63,73	1.92	9 (15%)	71,101,113	1.59	12 (16%)
27	CLA	A	830	10	64,68,73	1.85	9 (14%)	77,107,113	1.47	9 (11%)
29	II0	b	612	-	39,43,43	2.65	4 (10%)	50,60,60	1.48	7 (14%)
33	LHG	Z	311	-	45,45,48	0.63	0	48,51,54	1.20	4 (8%)
37	SF4	A	849	10,11	0,12,12	-	-	-	-	-
27	CLA	8	608	-	69,73,73	1.78	9 (13%)	83,113,113	1.38	8 (9%)
27	CLA	A	826	10	69,73,73	1.73	9 (13%)	83,113,113	1.35	10 (12%)
27	CLA	9	603	9	49,53,73	2.14	9 (18%)	59,89,113	1.65	9 (15%)
29	II0	4	613	-	39,43,43	2.67	4 (10%)	50,60,60	1.35	7 (14%)
27	CLA	B	814	-	46,50,73	2.19	9 (19%)	55,85,113	1.73	8 (14%)
29	II0	7	301	-	39,43,43	2.72	4 (10%)	50,60,60	1.63	13 (26%)
28	KC2	6	610	6	49,53,53	1.86	4 (8%)	62,89,89	1.37	7 (11%)
35	8CT	4	616	-	40,41,41	0.18	0	50,56,56	0.31	0
27	CLA	b	608	-	69,73,73	1.77	9 (13%)	83,113,113	1.38	9 (10%)
27	CLA	a	607	25	64,68,73	1.84	9 (14%)	77,107,113	1.47	9 (11%)
27	CLA	7	303	7	69,73,73	1.78	9 (13%)	83,113,113	1.43	10 (12%)
27	CLA	7	302	7	49,53,73	2.10	9 (18%)	59,89,113	1.61	8 (13%)
27	CLA	A	805	10	54,58,73	2.00	9 (16%)	65,95,113	1.60	9 (13%)
27	CLA	7	304	7	59,63,73	1.94	9 (15%)	71,101,113	1.53	10 (14%)
27	CLA	L	203	-	54,58,73	1.97	9 (16%)	65,95,113	1.63	10 (15%)
27	CLA	B	841	-	56,60,73	1.95	9 (16%)	67,97,113	1.55	9 (13%)
28	KC2	b	605	26	49,53,53	1.85	4 (8%)	62,89,89	1.41	8 (12%)
37	SF4	C	101	12	0,12,12	-	-	-	-	-
27	CLA	4	607	4	64,68,73	1.84	9 (14%)	77,107,113	1.47	9 (11%)
27	CLA	B	806	11	69,73,73	1.72	9 (13%)	83,113,113	1.42	10 (12%)
34	SQD	O	207	-	23,24,54	1.57	4 (17%)	31,34,65	1.39	4 (12%)
35	8CT	b	615	-	40,41,41	0.22	0	50,56,56	0.30	0
27	CLA	8	601	8	49,53,73	2.11	9 (18%)	59,89,113	1.62	8 (13%)
36	LMU	J	104	-	32,32,36	0.46	0	43,43,47	1.03	2 (4%)
33	LHG	2	619	-	38,38,48	0.69	1 (2%)	41,44,54	1.25	4 (9%)
27	CLA	J	102	-	45,49,73	2.27	10 (22%)	54,84,113	1.75	10 (18%)
38	PQN	B	842	-	34,34,34	0.35	0	42,45,45	0.59	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	B	819	11	64,68,73	1.85	9 (14%)	77,107,113	1.53	12 (15%)
27	CLA	5	602	5	59,63,73	1.93	9 (15%)	71,101,113	1.52	8 (11%)
27	CLA	9	609	-	45,49,73	2.25	10 (22%)	54,84,113	1.73	10 (18%)
27	CLA	A	839	-	69,73,73	1.76	9 (13%)	83,113,113	1.45	10 (12%)
27	CLA	A	821	10	59,63,73	1.90	9 (15%)	71,101,113	1.57	9 (12%)
27	CLA	A	841	-	69,73,73	1.77	9 (13%)	83,113,113	1.39	10 (12%)
27	CLA	A	823	-	69,73,73	1.78	9 (13%)	83,113,113	1.36	9 (10%)
27	CLA	8	603	-	69,73,73	1.79	9 (13%)	83,113,113	1.40	9 (10%)
27	CLA	3	612	3	49,53,73	2.09	9 (18%)	59,89,113	1.63	8 (13%)
35	8CT	B	845	-	40,41,41	0.35	0	50,56,56	0.60	1 (2%)
27	CLA	9	611	9	45,49,73	2.23	10 (22%)	54,84,113	1.74	10 (18%)
27	CLA	B	822	11	69,73,73	1.74	9 (13%)	83,113,113	1.41	9 (10%)
28	KC2	3	606	33	49,53,53	1.85	4 (8%)	62,89,89	1.41	8 (12%)
36	LMU	7	321	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
27	CLA	1	603	1	56,60,73	1.96	9 (16%)	67,97,113	1.54	8 (11%)
27	CLA	L	202	-	64,68,73	1.86	9 (14%)	77,107,113	1.46	9 (11%)
27	CLA	A	815	-	66,70,73	1.84	9 (13%)	79,109,113	1.42	8 (10%)
27	CLA	2	603	2	54,58,73	2.02	9 (16%)	65,95,113	1.56	8 (12%)
27	CLA	F	204	15	59,63,73	1.89	9 (15%)	71,101,113	1.47	9 (12%)
33	LHG	b	616	-	48,48,48	0.57	1 (2%)	51,54,54	1.16	4 (7%)
27	CLA	2	602	2	63,67,73	1.86	9 (14%)	75,105,113	1.60	12 (16%)
31	IHT	5	618	-	40,42,42	2.80	5 (12%)	53,58,58	2.24	15 (28%)
27	CLA	3	611	3	54,58,73	2.04	9 (16%)	65,95,113	1.55	9 (13%)
33	LHG	8	613	-	32,32,48	0.76	1 (3%)	35,38,54	1.20	2 (5%)
27	CLA	A	832	-	69,73,73	1.77	9 (13%)	83,113,113	1.37	8 (9%)
27	CLA	B	838	-	69,73,73	1.78	9 (13%)	83,113,113	1.41	10 (12%)
27	CLA	8	615	-	69,73,73	1.79	9 (13%)	83,113,113	1.41	10 (12%)
27	CLA	5	605	5	49,53,73	2.10	9 (18%)	59,89,113	1.63	8 (13%)
27	CLA	R	202	22	59,63,73	1.93	9 (15%)	71,101,113	1.66	10 (14%)
27	CLA	B	817	11	64,68,73	1.80	9 (14%)	77,107,113	1.45	8 (10%)
29	II0	7	315	-	39,43,43	2.67	4 (10%)	50,60,60	1.51	9 (18%)
35	8CT	B	846	-	40,41,41	0.10	0	50,56,56	0.48	0
29	II0	6	614	-	39,43,43	2.67	4 (10%)	50,60,60	1.38	7 (14%)
27	CLA	a	601	25	49,53,73	2.10	9 (18%)	59,89,113	1.62	8 (13%)
27	CLA	5	601	5	45,49,73	2.31	10 (22%)	54,84,113	1.83	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	b	607	26	64,68,73	1.86	9 (14%)	77,107,113	1.45	9 (11%)
27	CLA	F	203	-	49,53,73	2.09	9 (18%)	59,89,113	1.61	8 (13%)
38	PQN	A	850	-	34,34,34	0.35	0	42,45,45	0.72	1 (2%)
27	CLA	4	604	-	59,63,73	1.92	9 (15%)	71,101,113	1.49	8 (11%)
27	CLA	A	809	27	64,68,73	1.88	9 (14%)	77,107,113	1.56	10 (12%)
27	CLA	7	308	7	49,53,73	2.12	9 (18%)	59,89,113	1.69	9 (15%)
27	CLA	9	614	-	45,49,73	2.29	10 (22%)	54,84,113	1.80	10 (18%)
27	CLA	2	609	-	45,49,73	2.28	10 (22%)	54,84,113	1.77	9 (16%)
27	CLA	Z	301	-	64,68,73	1.86	9 (14%)	77,107,113	1.46	9 (11%)
33	LHG	2	620	-	41,41,48	0.65	1 (2%)	44,47,54	1.21	4 (9%)
27	CLA	b	604	-	69,73,73	1.78	9 (13%)	83,113,113	1.37	8 (9%)
27	CLA	3	610	3	69,73,73	1.78	9 (13%)	83,113,113	1.41	9 (10%)
35	8CT	B	844	-	40,41,41	0.18	0	50,56,56	0.58	0
35	8CT	Z	309	-	40,41,41	0.23	0	50,56,56	0.63	1 (2%)
33	LHG	7	320	27	38,38,48	0.65	0	41,44,54	1.17	3 (7%)
27	CLA	2	606	-	49,53,73	2.09	9 (18%)	59,89,113	1.62	9 (15%)
27	CLA	O	203	21	59,63,73	1.92	9 (15%)	71,101,113	1.49	8 (11%)
32	LMG	8	614	-	52,52,55	0.81	2 (3%)	60,60,63	1.30	6 (10%)
39	DGD	Z	303	-	61,61,67	0.94	3 (4%)	75,75,81	1.37	7 (9%)
27	CLA	B	801	-	69,73,73	1.71	9 (13%)	83,113,113	1.36	10 (12%)
29	II0	3	613	-	39,43,43	2.68	4 (10%)	50,60,60	1.45	8 (16%)
27	CLA	5	608	5	64,68,73	1.85	9 (14%)	77,107,113	1.60	10 (12%)
27	CLA	1	611	1	49,53,73	2.15	9 (18%)	59,89,113	1.65	8 (13%)
27	CLA	B	829	11	49,53,73	2.13	9 (18%)	59,89,113	1.72	10 (16%)
27	CLA	O	201	-	59,63,73	1.90	9 (15%)	71,101,113	1.55	12 (16%)
29	II0	4	614	-	39,43,43	2.67	4 (10%)	50,60,60	1.37	6 (12%)
29	II0	2	614	-	39,43,43	2.66	4 (10%)	50,60,60	1.43	8 (16%)
29	II0	9	618	-	39,43,43	2.67	4 (10%)	50,60,60	1.40	8 (16%)
31	IHT	2	616	-	40,42,42	2.85	4 (10%)	53,58,58	2.20	16 (30%)
33	LHG	4	617	27	46,46,48	0.61	0	49,52,54	1.21	6 (12%)
33	LHG	2	618	-	21,21,48	0.75	0	23,26,54	1.25	2 (8%)
27	CLA	A	844	-	69,73,73	1.69	9 (13%)	83,113,113	1.43	11 (13%)
29	II0	a	612	-	39,43,43	2.72	4 (10%)	50,60,60	1.43	7 (14%)
37	SF4	C	102	12	0,12,12	-	-	-	-	-
27	CLA	2	605	-	64,68,73	1.82	9 (14%)	77,107,113	1.44	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	II3	1	615	-	40,43,43	2.03	3 (7%)	47,60,60	1.57	9 (19%)
27	CLA	a	605	-	59,63,73	1.89	9 (15%)	71,101,113	1.53	9 (12%)
27	CLA	B	803	11	49,53,73	2.08	9 (18%)	59,89,113	1.58	8 (13%)
35	8CT	A	846	-	40,41,41	0.19	0	50,56,56	0.35	0
35	8CT	A	845	-	40,41,41	0.25	0	50,56,56	0.32	0
27	CLA	4	609	4	64,68,73	1.84	9 (14%)	77,107,113	1.43	8 (10%)
33	LHG	a	617	-	48,48,48	0.60	1 (2%)	51,54,54	1.20	5 (9%)
27	CLA	1	613	-	49,53,73	2.16	9 (18%)	59,89,113	1.68	10 (16%)
27	CLA	6	609	33	45,49,73	2.27	10 (22%)	54,84,113	1.74	8 (14%)
27	CLA	a	611	25	69,73,73	1.73	9 (13%)	83,113,113	1.37	10 (12%)
27	CLA	B	836	11	51,55,73	2.03	9 (17%)	61,91,113	1.59	8 (13%)
27	CLA	O	204	-	59,63,73	1.96	9 (15%)	71,101,113	1.59	9 (12%)
27	CLA	2	604	2	59,63,73	1.93	9 (15%)	71,101,113	1.52	9 (12%)
27	CLA	1	606	-	49,53,73	2.10	9 (18%)	59,89,113	1.66	10 (16%)
27	CLA	B	807	11	69,73,73	1.74	9 (13%)	83,113,113	1.37	9 (10%)
28	KC2	b	609	-	49,53,53	1.87	4 (8%)	62,89,89	1.39	8 (12%)
35	8CT	F	201	-	40,41,41	0.43	1 (2%)	50,56,56	0.45	0
27	CLA	3	608	3	64,68,73	1.85	9 (14%)	77,107,113	1.45	10 (12%)
27	CLA	b	602	26	68,72,73	1.81	9 (13%)	81,111,113	1.48	11 (13%)
29	II0	O	205	-	39,43,43	2.73	4 (10%)	50,60,60	1.40	6 (12%)
27	CLA	A	835	10	64,68,73	1.82	9 (14%)	77,107,113	1.42	8 (10%)
29	II0	7	317	-	39,43,43	2.71	4 (10%)	50,60,60	1.53	9 (18%)
27	CLA	6	601	6	49,53,73	2.09	9 (18%)	59,89,113	1.66	9 (15%)
27	CLA	4	606	4	64,68,73	1.86	9 (14%)	77,107,113	1.43	9 (11%)
29	II0	b	614	-	39,43,43	2.70	4 (10%)	50,60,60	1.45	8 (16%)
29	II0	1	614	-	39,43,43	2.70	4 (10%)	50,60,60	1.40	6 (12%)
27	CLA	4	608	33	69,73,73	1.76	9 (13%)	83,113,113	1.39	9 (10%)
29	II0	7	314	-	39,43,43	2.68	4 (10%)	50,60,60	1.43	8 (16%)
27	CLA	A	831	10	69,73,73	1.75	9 (13%)	83,113,113	1.35	8 (9%)
27	CLA	B	818	-	64,68,73	1.83	9 (14%)	77,107,113	1.47	9 (11%)
27	CLA	7	305	7	57,61,73	1.95	9 (15%)	68,98,113	1.54	9 (13%)
30	II3	b	613	-	40,43,43	2.00	3 (7%)	47,60,60	1.66	12 (25%)
27	CLA	6	611	-	59,63,73	1.91	9 (15%)	71,101,113	1.56	10 (14%)
32	LMG	F	205	-	32,32,55	0.85	0	40,40,63	1.29	6 (15%)
27	CLA	a	608	-	64,68,73	1.83	9 (14%)	77,107,113	1.47	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	II0	5	617	-	39,43,43	2.69	4 (10%)	50,60,60	1.53	9 (18%)
27	CLA	1	602	1	63,67,73	1.85	9 (14%)	75,105,113	1.48	9 (12%)
27	CLA	B	809	11	69,73,73	1.79	9 (13%)	83,113,113	1.43	9 (10%)
35	8CT	B	850	-	40,41,41	0.21	0	50,56,56	0.40	0
27	CLA	7	313	-	54,58,73	2.01	9 (16%)	65,95,113	1.60	9 (13%)
32	LMG	3	618	-	30,30,55	0.96	1 (3%)	38,38,63	1.21	6 (15%)
27	CLA	L	201	19	55,59,73	1.99	9 (16%)	66,96,113	1.56	9 (13%)
27	CLA	A	814	-	49,53,73	2.13	9 (18%)	59,89,113	1.65	8 (13%)
27	CLA	8	607	8	45,49,73	2.26	10 (22%)	54,84,113	1.74	9 (16%)
27	CLA	Z	304	24	59,63,73	1.91	9 (15%)	71,101,113	1.47	8 (11%)
27	CLA	A	806	10	69,73,73	1.76	9 (13%)	83,113,113	1.36	9 (10%)
27	CLA	5	611	5	49,53,73	2.11	9 (18%)	59,89,113	1.60	8 (13%)
27	CLA	B	827	-	69,73,73	1.76	9 (13%)	83,113,113	1.39	8 (9%)
27	CLA	A	834	10	59,63,73	1.90	9 (15%)	71,101,113	1.52	10 (14%)
33	LHG	6	617	27	34,34,48	0.74	1 (2%)	37,40,54	1.19	3 (8%)
27	CLA	A	836	10	59,63,73	1.92	9 (15%)	71,101,113	1.51	8 (11%)
27	CLA	B	816	11	63,67,73	1.85	9 (14%)	75,105,113	1.47	9 (12%)
35	8CT	M	101	-	40,41,41	0.15	0	50,56,56	0.80	1 (2%)
29	II0	5	616	-	39,43,43	2.71	4 (10%)	50,60,60	1.48	9 (18%)
29	II0	7	316	-	39,43,43	2.73	4 (10%)	50,60,60	1.45	8 (16%)
35	8CT	B	847	-	40,41,41	0.16	0	50,56,56	0.46	0
29	II0	O	206	-	39,43,43	2.72	4 (10%)	50,60,60	1.40	10 (20%)
29	II0	2	613	-	39,43,43	2.75	4 (10%)	50,60,60	1.47	8 (16%)
27	CLA	A	824	-	69,73,73	1.80	9 (13%)	83,113,113	1.41	8 (9%)
27	CLA	4	602	4	63,67,73	1.84	9 (14%)	75,105,113	1.50	9 (12%)
33	LHG	3	619	-	48,48,48	0.61	0	51,54,54	1.22	6 (11%)
31	IHT	8	609	-	40,42,42	2.80	4 (10%)	53,58,58	2.33	16 (30%)
28	KC2	9	610	-	49,53,53	1.86	4 (8%)	62,89,89	1.38	8 (12%)
27	CLA	6	603	6	49,53,73	2.15	9 (18%)	59,89,113	1.66	8 (13%)
27	CLA	8	606	8	59,63,73	1.93	9 (15%)	71,101,113	1.50	9 (12%)
35	8CT	I	101	-	40,41,41	0.25	0	50,56,56	0.44	0
27	CLA	2	607	2	49,53,73	2.09	9 (18%)	59,89,113	1.67	9 (15%)
27	CLA	B	815	11	69,73,73	1.81	9 (13%)	83,113,113	1.43	10 (12%)
31	IHT	1	618	-	40,42,42	2.83	5 (12%)	53,58,58	2.05	14 (26%)
27	CLA	6	606	-	59,63,73	1.95	9 (15%)	71,101,113	1.56	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	II0	1	619	-	39,43,43	2.79	4 (10%)	50,60,60	1.54	11 (22%)
27	CLA	1	605	-	45,50,73	2.16	9 (20%)	53,85,113	1.67	7 (13%)
27	CLA	A	804	10	69,73,73	1.77	9 (13%)	83,113,113	1.39	9 (10%)
27	CLA	B	821	-	64,68,73	1.82	9 (14%)	77,107,113	1.49	10 (12%)
27	CLA	B	826	11	69,73,73	1.75	9 (13%)	83,113,113	1.38	8 (9%)
28	KC2	4	605	4	49,53,53	1.85	4 (8%)	62,89,89	1.37	7 (11%)
27	CLA	B	837	-	69,73,73	1.79	9 (13%)	83,113,113	1.38	8 (9%)
27	CLA	1	604	1	49,53,73	2.16	9 (18%)	59,89,113	1.63	9 (15%)
27	CLA	A	840	-	59,63,73	1.87	9 (15%)	71,101,113	1.52	7 (9%)
27	CLA	3	602	3	59,63,73	1.91	9 (15%)	71,101,113	1.53	9 (12%)
27	CLA	A	838	-	69,73,73	1.76	9 (13%)	83,113,113	1.37	8 (9%)
29	II0	9	617	-	39,43,43	2.71	4 (10%)	50,60,60	1.46	8 (16%)
27	CLA	9	607	9	69,73,73	1.73	9 (13%)	83,113,113	1.37	10 (12%)
29	II0	a	613	-	39,43,43	2.68	4 (10%)	50,60,60	1.43	8 (16%)
27	CLA	A	825	10	69,73,73	1.77	9 (13%)	83,113,113	1.39	10 (12%)
28	KC2	5	610	5	49,53,53	1.87	4 (8%)	62,89,89	1.36	8 (12%)
27	CLA	1	612	1	64,68,73	1.81	9 (14%)	77,107,113	1.40	9 (11%)
27	CLA	4	611	4	69,73,73	1.76	9 (13%)	83,113,113	1.38	9 (10%)
27	CLA	B	808	11	69,73,73	1.74	9 (13%)	83,113,113	1.35	9 (10%)
28	KC2	7	307	-	49,53,53	1.88	4 (8%)	62,89,89	1.42	8 (12%)
27	CLA	1	608	1	64,68,73	1.83	9 (14%)	77,107,113	1.47	11 (14%)
27	CLA	2	612	2	49,53,73	2.09	9 (18%)	59,89,113	1.65	8 (13%)
29	II0	Z	312	-	39,43,43	2.67	4 (10%)	50,60,60	1.39	8 (16%)
27	CLA	b	603	26	64,68,73	1.84	9 (14%)	77,107,113	1.47	9 (11%)
28	KC2	a	609	-	49,53,53	1.86	4 (8%)	62,89,89	1.36	7 (11%)
29	II0	3	615	-	39,43,43	2.70	4 (10%)	50,60,60	1.37	8 (16%)
27	CLA	B	813	11	65,69,73	1.78	9 (13%)	78,108,113	1.43	9 (11%)
27	CLA	A	833	10	69,73,73	1.78	9 (13%)	83,113,113	1.43	10 (12%)
35	8CT	A	853	-	40,41,41	0.24	0	50,56,56	0.60	1 (2%)
27	CLA	B	804	11	69,73,73	1.75	9 (13%)	83,113,113	1.39	9 (10%)
27	CLA	a	603	25	64,68,73	1.84	9 (14%)	77,107,113	1.43	8 (10%)
27	CLA	5	603	5	49,53,73	2.12	9 (18%)	59,89,113	1.65	9 (15%)
29	II0	8	610	-	39,43,43	2.75	4 (10%)	50,60,60	1.41	8 (16%)
27	CLA	3	604	-	69,73,73	1.76	9 (13%)	83,113,113	1.39	8 (9%)
27	CLA	5	609	-	45,49,73	2.26	10 (22%)	54,84,113	1.73	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	A	817	10	69,73,73	1.77	9 (13%)	83,113,113	1.52	10 (12%)
27	CLA	B	832	-	69,73,73	1.77	9 (13%)	83,113,113	1.40	9 (10%)
29	II0	9	615	-	39,43,43	2.66	4 (10%)	50,60,60	1.46	9 (18%)
29	II0	3	617	-	39,43,43	2.72	4 (10%)	50,60,60	1.39	7 (14%)
27	CLA	3	601	3	49,53,73	2.12	9 (18%)	59,89,113	1.59	8 (13%)
27	CLA	B	831	11	59,63,73	1.94	9 (15%)	71,101,113	1.57	10 (14%)
27	CLA	1	607	1	49,53,73	2.12	9 (18%)	59,89,113	1.65	9 (15%)
27	CLA	9	601	9	49,53,73	2.10	9 (18%)	59,89,113	1.65	9 (15%)
27	CLA	B	825	11	69,73,73	1.75	9 (13%)	83,113,113	1.36	10 (12%)
33	LHG	4	619	27	44,44,48	0.64	1 (2%)	47,50,54	1.21	5 (10%)
27	CLA	B	802	-	69,73,73	1.79	9 (13%)	83,113,113	1.35	11 (13%)
34	SQD	3	621	-	41,42,54	1.33	4 (9%)	50,53,65	1.09	3 (6%)
33	LHG	3	622	28	33,33,48	0.72	0	36,39,54	1.27	3 (8%)
27	CLA	A	811	10	69,73,73	1.78	9 (13%)	83,113,113	1.46	7 (8%)
27	CLA	3	609	-	69,73,73	1.78	9 (13%)	83,113,113	1.37	8 (9%)
27	CLA	A	842	10	69,73,73	1.78	9 (13%)	83,113,113	1.42	9 (10%)
27	CLA	9	604	-	59,63,73	1.93	9 (15%)	71,101,113	1.51	9 (12%)
27	CLA	7	306	7	49,53,73	2.14	9 (18%)	59,89,113	1.63	8 (13%)
27	CLA	B	834	11	59,63,73	1.89	9 (15%)	71,101,113	1.52	10 (14%)
27	CLA	B	835	11	69,73,73	1.80	9 (13%)	83,113,113	1.51	9 (10%)
27	CLA	4	610	4	69,73,73	1.75	9 (13%)	83,113,113	1.39	8 (9%)
27	CLA	B	811	11	59,63,73	1.92	9 (15%)	71,101,113	1.53	8 (11%)
27	CLA	A	807	10	54,58,73	2.01	9 (16%)	65,95,113	1.60	9 (13%)
31	IHT	9	619	-	40,42,42	2.81	5 (12%)	53,58,58	2.40	14 (26%)
31	IHT	Z	302	-	40,42,42	2.84	4 (10%)	53,58,58	2.12	14 (26%)
29	II0	1	617	-	39,43,43	2.70	4 (10%)	50,60,60	1.47	10 (20%)
29	II0	3	616	-	39,43,43	2.69	4 (10%)	50,60,60	1.43	6 (12%)
27	CLA	A	837	-	69,73,73	1.74	9 (13%)	83,113,113	1.36	8 (9%)
35	8CT	7	318	-	40,41,41	0.41	1 (2%)	50,56,56	0.59	0
27	CLA	A	802	10,27	59,63,73	1.88	9 (15%)	71,101,113	1.49	9 (12%)
35	8CT	A	847	-	40,41,41	0.23	0	50,56,56	0.77	1 (2%)
35	8CT	R	203	-	40,41,41	0.16	0	50,56,56	0.46	1 (2%)
27	CLA	A	801	-	69,73,73	1.73	8 (11%)	83,113,113	1.37	10 (12%)
27	CLA	a	606	25	69,73,73	1.77	9 (13%)	83,113,113	1.36	8 (9%)
36	LMU	4	618	-	36,36,36	0.47	0	47,47,47	0.92	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	A	828	10	69,73,73	1.79	9 (13%)	83,113,113	1.38	9 (10%)
27	CLA	B	810	-	64,68,73	1.82	9 (14%)	77,107,113	1.46	8 (10%)
27	CLA	5	613	5	45,49,73	2.28	10 (22%)	54,84,113	1.71	10 (18%)
27	CLA	A	829	10	54,58,73	2.00	9 (16%)	65,95,113	1.63	9 (13%)
29	II0	5	615	-	39,43,43	2.71	4 (10%)	50,60,60	1.48	8 (16%)
27	CLA	5	604	5	59,63,73	1.97	9 (15%)	71,101,113	1.54	9 (12%)
27	CLA	5	612	5	49,53,73	2.09	9 (18%)	59,89,113	1.65	9 (15%)
27	CLA	Z	310	-	69,73,73	1.74	9 (13%)	83,113,113	1.39	9 (10%)
33	LHG	4	620	-	44,44,48	0.65	2 (4%)	47,50,54	1.19	4 (8%)
27	CLA	5	606	-	49,53,73	2.11	9 (18%)	59,89,113	1.66	10 (16%)
27	CLA	Z	306	24	64,68,73	1.82	9 (14%)	77,107,113	1.46	8 (10%)
27	CLA	b	601	26	49,53,73	2.11	9 (18%)	59,89,113	1.65	8 (13%)
27	CLA	1	601	1	49,53,73	2.16	9 (18%)	59,89,113	1.71	10 (16%)
35	8CT	K	103	-	40,41,41	0.16	0	50,56,56	0.33	0
32	LMG	3	620	-	32,32,55	0.91	0	40,40,63	1.28	6 (15%)
27	CLA	6	612	-	49,53,73	2.08	9 (18%)	59,89,113	1.65	9 (15%)
27	CLA	A	822	10	69,73,73	1.77	9 (13%)	83,113,113	1.40	9 (10%)
27	CLA	Z	305	-	54,58,73	1.98	9 (16%)	65,95,113	1.59	9 (13%)
27	CLA	A	812	10	59,63,73	1.93	9 (15%)	71,101,113	1.56	11 (15%)
27	CLA	1	609	-	45,49,73	2.27	10 (22%)	54,84,113	1.75	8 (14%)
27	CLA	9	605	-	49,53,73	2.10	9 (18%)	59,89,113	1.67	9 (15%)
27	CLA	6	602	6	69,73,73	1.82	9 (13%)	83,113,113	1.47	8 (9%)
32	LMG	2	617	-	36,36,55	0.85	0	44,44,63	1.23	5 (11%)
31	IHT	a	616	-	40,42,42	2.81	4 (10%)	53,58,58	2.33	17 (32%)
29	II0	a	615	-	39,43,43	2.70	4 (10%)	50,60,60	1.44	11 (22%)
27	CLA	B	830	11	64,68,73	1.85	9 (14%)	77,107,113	1.47	8 (10%)
27	CLA	A	819	-	69,73,73	1.79	9 (13%)	83,113,113	1.41	9 (10%)
27	CLA	3	603	3	64,68,73	1.83	9 (14%)	77,107,113	1.44	9 (11%)
27	CLA	2	608	2	64,68,73	1.84	9 (14%)	77,107,113	1.47	11 (14%)
29	II0	4	615	-	39,43,43	2.68	4 (10%)	50,60,60	1.46	9 (18%)
28	KC2	1	610	-	49,53,53	1.87	4 (8%)	62,89,89	1.34	7 (11%)
27	CLA	A	810	10	69,73,73	1.75	9 (13%)	83,113,113	1.39	11 (13%)
27	CLA	6	607	6	59,63,73	1.90	9 (15%)	71,101,113	1.50	9 (12%)
29	II0	8	612	-	39,43,43	2.70	4 (10%)	50,60,60	1.42	7 (14%)
28	KC2	2	610	2	49,53,53	1.88	4 (8%)	62,89,89	1.36	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	O	202	-	45,49,73	2.28	10 (22%)	54,84,113	1.79	9 (16%)
28	KC2	7	311	7	49,53,53	1.85	4 (8%)	62,89,89	1.40	7 (11%)
27	CLA	A	827	-	69,73,73	1.73	9 (13%)	83,113,113	1.38	9 (10%)
27	CLA	7	309	7	59,63,73	1.90	9 (15%)	71,101,113	1.56	11 (15%)
27	CLA	B	833	-	49,53,73	2.09	9 (18%)	59,89,113	1.61	8 (13%)
27	CLA	b	606	26	69,73,73	1.77	9 (13%)	83,113,113	1.36	8 (9%)
27	CLA	9	612	-	49,53,73	2.09	9 (18%)	59,89,113	1.61	9 (15%)
29	II0	1	616	-	39,43,43	2.66	4 (10%)	50,60,60	1.48	8 (16%)
27	CLA	K	102	18	59,63,73	1.94	9 (15%)	71,101,113	1.51	10 (14%)
29	II0	B	843	-	39,43,43	2.73	4 (10%)	50,60,60	1.40	6 (12%)
27	CLA	3	607	3	64,68,73	1.83	9 (14%)	77,107,113	1.43	9 (11%)
29	II0	a	614	-	39,43,43	2.74	4 (10%)	50,60,60	1.39	7 (14%)
29	II0	5	614	-	39,43,43	2.66	4 (10%)	50,60,60	1.46	9 (18%)
33	LHG	a	618	-	28,28,48	0.82	1 (3%)	31,34,54	1.32	3 (9%)
27	CLA	F	202	-	64,68,73	1.85	9 (14%)	77,107,113	1.44	10 (12%)
27	CLA	9	608	9	59,63,73	1.90	9 (15%)	71,101,113	1.53	10 (14%)
27	CLA	7	310	33	45,49,73	2.26	10 (22%)	54,84,113	1.74	8 (14%)
29	II0	5	620	-	39,43,43	2.72	4 (10%)	50,60,60	1.51	7 (14%)
29	II0	4	612	-	39,43,43	2.69	4 (10%)	50,60,60	1.39	6 (12%)
32	LMG	8	616	-	51,51,55	0.73	0	59,59,63	1.29	7 (11%)
35	8CT	R	201	-	40,41,41	0.20	0	50,56,56	0.41	0
27	CLA	8	604	8	69,73,73	1.78	9 (13%)	83,113,113	1.41	11 (13%)
39	DGD	B	848	-	60,60,67	0.88	2 (3%)	74,74,81	1.34	8 (10%)
27	CLA	B	839	33	69,73,73	1.81	9 (13%)	83,113,113	1.41	9 (10%)
29	II0	6	615	-	39,43,43	2.68	4 (10%)	50,60,60	1.41	7 (14%)
28	KC2	6	613	6	49,53,53	1.86	4 (8%)	62,89,89	1.39	8 (12%)
29	II0	J	101	-	39,43,43	2.71	4 (10%)	50,60,60	1.47	8 (16%)
27	CLA	9	606	-	68,72,73	1.76	9 (13%)	81,111,113	1.41	10 (12%)
27	CLA	B	805	11	69,73,73	1.78	9 (13%)	83,113,113	1.40	9 (10%)
33	LHG	7	319	-	30,30,48	0.75	1 (3%)	33,36,54	1.20	3 (9%)
35	8CT	A	848	-	40,41,41	0.37	0	50,56,56	0.56	0
35	8CT	L	205	-	40,41,41	0.16	0	50,56,56	0.38	0
28	KC2	Z	307	24	49,53,53	1.83	4 (8%)	62,89,89	1.39	8 (12%)
33	LHG	5	619	-	22,22,48	0.87	1 (4%)	25,28,54	1.30	3 (12%)
27	CLA	6	605	6	59,63,73	1.89	9 (15%)	71,101,113	1.49	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	B	840	11	69,73,73	1.73	9 (13%)	83,113,113	1.38	8 (9%)
33	LHG	A	852	-	38,38,48	0.70	0	41,44,54	1.26	3 (7%)
27	CLA	B	824	-	64,68,73	1.85	9 (14%)	77,107,113	1.51	9 (11%)
27	CLA	A	820	10	69,73,73	1.79	9 (13%)	83,113,113	1.40	8 (9%)
27	CLA	A	818	10	69,73,73	1.77	9 (13%)	83,113,113	1.43	8 (9%)
35	8CT	Z	308	-	40,41,41	0.16	0	50,56,56	0.30	0
27	CLA	6	604	6	64,68,73	1.85	9 (14%)	77,107,113	1.45	9 (11%)
27	CLA	B	812	11	69,73,73	1.76	9 (13%)	83,113,113	1.42	9 (10%)
27	CLA	5	607	5	49,53,73	2.08	9 (18%)	59,89,113	1.64	9 (15%)
27	CLA	3	605	3	59,63,73	1.91	9 (15%)	71,101,113	1.54	10 (14%)
29	II0	3	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.43	7 (14%)
27	CLA	a	610	-	59,63,73	1.93	9 (15%)	71,101,113	1.48	8 (11%)
29	II0	8	611	-	39,43,43	2.73	4 (10%)	50,60,60	1.32	6 (12%)
35	8CT	J	103	-	40,41,41	0.17	0	50,56,56	0.38	0
27	CLA	B	823	-	69,73,73	1.77	9 (13%)	83,113,113	1.36	10 (12%)
29	II0	R	204	-	39,43,43	2.70	4 (10%)	50,60,60	1.42	10 (20%)
27	CLA	A	843	10	69,73,73	1.80	9 (13%)	83,113,113	1.48	8 (9%)
27	CLA	4	601	4	59,63,73	1.89	9 (15%)	71,101,113	1.47	8 (11%)
27	CLA	A	808	10	59,63,73	1.92	9 (15%)	71,101,113	1.51	9 (12%)
27	CLA	2	601	2	46,50,73	2.20	9 (19%)	55,85,113	1.76	8 (14%)

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
27	CLA	A	803	10	-	8/39/115/115	-
27	CLA	8	605	8	-	3/21/97/115	-
27	CLA	6	608	6	-	7/33/109/115	-
27	CLA	9	602	9	-	9/27/103/115	-
27	CLA	A	816	10	-	9/33/109/115	-
27	CLA	9	613	9	-	3/15/91/115	-
35	8CT	B	849	-	-	4/29/63/63	0/2/2/2
29	II0	2	615	-	-	2/21/67/67	0/2/2/2
27	CLA	8	602	8	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	b	610	26	-	9/23/99/115	-
27	CLA	K	101	-	-	6/39/115/115	-
31	IHT	6	616	-	-	3/25/65/65	0/2/2/2
31	IHT	A	854	-	-	2/25/65/65	0/2/2/2
27	CLA	7	312	-	-	5/27/103/115	-
33	LHG	A	851	-	-	22/53/53/53	-
27	CLA	2	611	-	-	2/15/91/115	-
32	LMG	6	618	-	-	5/27/47/70	0/1/1/1
27	CLA	4	603	4	-	5/26/102/115	-
27	CLA	B	828	11	-	9/39/115/115	-
29	II0	9	616	-	-	2/21/67/67	0/2/2/2
27	CLA	B	820	11	-	8/33/109/115	-
27	CLA	b	611	26	-	4/27/103/115	-
31	IHT	L	204	-	-	2/25/65/65	0/2/2/2
27	CLA	a	604	-	-	11/33/109/115	-
27	CLA	A	813	10	-	1/12/88/115	-
27	CLA	a	602	25	-	9/27/103/115	-
27	CLA	A	830	10	-	4/33/109/115	-
29	II0	b	612	-	-	1/21/67/67	0/2/2/2
33	LHG	Z	311	-	-	23/50/50/53	-
37	SF4	A	849	10,11	-	-	0/6/5/5
27	CLA	8	608	-	-	6/39/115/115	-
27	CLA	A	826	10	-	5/39/115/115	-
27	CLA	9	603	9	-	6/15/91/115	-
29	II0	4	613	-	-	1/21/67/67	0/2/2/2
27	CLA	B	814	-	-	4/12/88/115	-
29	II0	7	301	-	-	2/21/67/67	0/2/2/2
28	KC2	6	610	6	-	6/15/71/71	-
35	8CT	4	616	-	-	5/29/63/63	0/2/2/2
27	CLA	b	608	-	-	9/39/115/115	-
27	CLA	a	607	25	-	3/33/109/115	-
27	CLA	7	303	7	-	7/39/115/115	-
27	CLA	7	302	7	-	2/15/91/115	-
27	CLA	A	805	10	-	3/21/97/115	-
27	CLA	7	304	7	-	1/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	L	203	-	-	5/21/97/115	-
27	CLA	B	841	-	-	7/24/100/115	-
28	KC2	b	605	26	-	7/15/71/71	-
37	SF4	C	101	12	-	-	0/6/5/5
27	CLA	4	607	4	-	7/33/109/115	-
27	CLA	B	806	11	-	6/39/115/115	-
34	SQD	O	207	-	-	7/18/38/69	0/1/1/1
35	8CT	b	615	-	-	6/29/63/63	0/2/2/2
27	CLA	8	601	8	-	3/15/91/115	-
36	LMU	J	104	-	-	9/17/57/61	0/2/2/2
33	LHG	2	619	-	-	17/43/43/53	-
27	CLA	J	102	-	-	3/10/86/115	-
38	PQN	B	842	-	-	5/23/43/43	0/2/2/2
27	CLA	B	819	11	-	8/33/109/115	-
27	CLA	5	602	5	-	6/27/103/115	-
27	CLA	9	609	-	-	3/10/86/115	-
27	CLA	A	839	-	-	13/39/115/115	-
27	CLA	A	821	10	-	2/27/103/115	-
27	CLA	A	841	-	-	5/39/115/115	-
27	CLA	A	823	-	-	10/39/115/115	-
27	CLA	8	603	-	-	10/39/115/115	-
27	CLA	3	612	3	-	4/15/91/115	-
35	8CT	B	845	-	-	8/29/63/63	0/2/2/2
27	CLA	9	611	9	-	3/10/86/115	-
27	CLA	B	822	11	-	7/39/115/115	-
28	KC2	3	606	33	-	8/15/71/71	-
36	LMU	7	321	-	-	8/21/61/61	0/2/2/2
27	CLA	1	603	1	-	4/24/100/115	-
27	CLA	L	202	-	-	11/33/109/115	-
27	CLA	A	815	-	-	1/36/112/115	-
27	CLA	2	603	2	-	4/21/97/115	-
27	CLA	F	204	15	-	6/27/103/115	-
33	LHG	b	616	-	-	25/53/53/53	-
27	CLA	2	602	2	-	14/32/108/115	-
31	IHT	5	618	-	-	1/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	3	611	3	-	3/21/97/115	-
33	LHG	8	613	-	-	21/37/37/53	-
27	CLA	A	832	-	-	8/39/115/115	-
27	CLA	B	838	-	-	5/39/115/115	-
27	CLA	8	615	-	-	7/39/115/115	-
27	CLA	5	605	5	-	4/15/91/115	-
27	CLA	R	202	22	-	10/27/103/115	-
27	CLA	B	817	11	-	1/33/109/115	-
29	II0	7	315	-	-	1/21/67/67	0/2/2/2
35	8CT	B	846	-	-	8/29/63/63	0/2/2/2
29	II0	6	614	-	-	1/21/67/67	0/2/2/2
27	CLA	a	601	25	-	6/15/91/115	-
27	CLA	5	601	5	-	2/10/86/115	-
27	CLA	b	607	26	-	5/33/109/115	-
27	CLA	F	203	-	-	5/15/91/115	-
38	PQN	A	850	-	-	10/23/43/43	0/2/2/2
27	CLA	4	604	-	-	11/27/103/115	-
27	CLA	A	809	27	-	5/33/109/115	-
27	CLA	7	308	7	-	1/15/91/115	-
27	CLA	9	614	-	-	3/10/86/115	-
27	CLA	2	609	-	-	2/10/86/115	-
27	CLA	Z	301	-	-	13/33/109/115	-
33	LHG	2	620	-	-	17/46/46/53	-
27	CLA	b	604	-	-	16/39/115/115	-
27	CLA	3	610	3	-	8/39/115/115	-
35	8CT	B	844	-	-	3/29/63/63	0/2/2/2
35	8CT	Z	309	-	-	6/29/63/63	0/2/2/2
33	LHG	7	320	27	-	20/43/43/53	-
27	CLA	2	606	-	-	2/15/91/115	-
27	CLA	O	203	21	-	6/27/103/115	-
32	LMG	8	614	-	-	23/47/67/70	0/1/1/1
39	DGD	Z	303	-	-	27/49/89/95	0/2/2/2
27	CLA	B	801	-	-	5/39/115/115	-
29	II0	3	613	-	-	2/21/67/67	0/2/2/2
27	CLA	5	608	5	-	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	1	611	1	-	3/15/91/115	-
27	CLA	B	829	11	-	2/15/91/115	-
27	CLA	O	201	-	-	3/27/103/115	-
29	II0	4	614	-	-	2/21/67/67	0/2/2/2
29	II0	2	614	-	-	0/21/67/67	0/2/2/2
29	II0	9	618	-	-	2/21/67/67	0/2/2/2
31	IHT	2	616	-	-	2/25/65/65	0/2/2/2
33	LHG	4	617	27	-	18/51/51/53	-
33	LHG	2	618	-	-	9/24/24/53	-
27	CLA	A	844	-	-	6/39/115/115	-
29	II0	a	612	-	-	2/21/67/67	0/2/2/2
37	SF4	C	102	12	-	-	0/6/5/5
27	CLA	2	605	-	-	6/33/109/115	-
30	II3	1	615	-	-	1/25/67/67	0/2/2/2
27	CLA	a	605	-	-	12/27/103/115	-
27	CLA	B	803	11	-	3/15/91/115	-
35	8CT	A	846	-	-	3/29/63/63	0/2/2/2
35	8CT	A	845	-	-	1/29/63/63	0/2/2/2
27	CLA	4	609	4	-	4/33/109/115	-
33	LHG	a	617	-	-	25/53/53/53	-
27	CLA	1	613	-	-	3/15/91/115	-
27	CLA	6	609	33	-	2/10/86/115	-
27	CLA	a	611	25	-	7/39/115/115	-
27	CLA	B	836	11	-	3/18/94/115	-
27	CLA	O	204	-	-	8/27/103/115	-
27	CLA	2	604	2	-	1/27/103/115	-
27	CLA	1	606	-	-	0/15/91/115	-
27	CLA	B	807	11	-	11/39/115/115	-
28	KC2	b	609	-	-	2/15/71/71	-
35	8CT	F	201	-	-	4/29/63/63	0/2/2/2
27	CLA	3	608	3	-	4/33/109/115	-
27	CLA	b	602	26	-	16/38/114/115	-
29	II0	O	205	-	-	2/21/67/67	0/2/2/2
27	CLA	A	835	10	-	6/33/109/115	-
29	II0	7	317	-	-	1/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	6	601	6	-	4/15/91/115	-
27	CLA	4	606	4	-	4/33/109/115	-
29	II0	b	614	-	-	0/21/67/67	0/2/2/2
29	II0	1	614	-	-	2/21/67/67	0/2/2/2
27	CLA	4	608	33	-	4/39/115/115	-
29	II0	7	314	-	-	0/21/67/67	0/2/2/2
27	CLA	A	831	10	-	13/39/115/115	-
27	CLA	B	818	-	-	3/33/109/115	-
27	CLA	7	305	7	-	8/25/101/115	-
30	II3	b	613	-	-	1/25/67/67	0/2/2/2
27	CLA	6	611	-	-	4/27/103/115	-
32	LMG	F	205	-	-	11/27/47/70	0/1/1/1
27	CLA	a	608	-	-	9/33/109/115	-
29	II0	5	617	-	-	2/21/67/67	0/2/2/2
27	CLA	1	602	1	-	8/32/108/115	-
27	CLA	B	809	11	-	10/39/115/115	-
35	8CT	B	850	-	-	9/29/63/63	0/2/2/2
27	CLA	7	313	-	-	8/21/97/115	-
32	LMG	3	618	-	-	9/25/45/70	0/1/1/1
27	CLA	L	201	19	-	1/23/99/115	-
27	CLA	A	814	-	-	6/15/91/115	-
27	CLA	8	607	8	-	3/10/86/115	-
27	CLA	Z	304	24	-	4/27/103/115	-
27	CLA	A	806	10	-	7/39/115/115	-
27	CLA	5	611	5	-	8/15/91/115	-
27	CLA	B	827	-	-	6/39/115/115	-
27	CLA	A	834	10	-	7/27/103/115	-
33	LHG	6	617	27	-	16/39/39/53	-
27	CLA	A	836	10	-	2/27/103/115	-
27	CLA	B	816	11	-	14/32/108/115	-
35	8CT	M	101	-	-	5/29/63/63	0/2/2/2
29	II0	5	616	-	-	1/21/67/67	0/2/2/2
29	II0	7	316	-	-	2/21/67/67	0/2/2/2
35	8CT	B	847	-	-	4/29/63/63	0/2/2/2
29	II0	O	206	-	-	1/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	II0	2	613	-	-	1/21/67/67	0/2/2/2
27	CLA	A	824	-	-	5/39/115/115	-
27	CLA	4	602	4	-	4/32/108/115	-
33	LHG	3	619	-	-	23/53/53/53	-
31	IHT	8	609	-	-	1/25/65/65	0/2/2/2
28	KC2	9	610	-	-	6/15/71/71	-
27	CLA	6	603	6	-	7/15/91/115	-
27	CLA	8	606	8	-	3/27/103/115	-
35	8CT	I	101	-	-	3/29/63/63	0/2/2/2
27	CLA	2	607	2	-	2/15/91/115	-
27	CLA	B	815	11	-	10/39/115/115	-
31	IHT	1	618	-	-	2/25/65/65	0/2/2/2
27	CLA	6	606	-	-	8/27/103/115	-
29	II0	1	619	-	-	1/21/67/67	0/2/2/2
27	CLA	1	605	-	-	3/11/87/115	-
27	CLA	A	804	10	-	18/39/115/115	-
27	CLA	B	821	-	-	11/33/109/115	-
27	CLA	B	826	11	-	13/39/115/115	-
28	KC2	4	605	4	-	7/15/71/71	-
27	CLA	B	837	-	-	5/39/115/115	-
27	CLA	1	604	1	-	3/15/91/115	-
27	CLA	A	840	-	-	5/27/103/115	-
27	CLA	3	602	3	-	4/27/103/115	-
27	CLA	A	838	-	-	5/39/115/115	-
29	II0	9	617	-	-	2/21/67/67	0/2/2/2
27	CLA	9	607	9	-	10/39/115/115	-
29	II0	a	613	-	-	2/21/67/67	0/2/2/2
27	CLA	A	825	10	-	7/39/115/115	-
28	KC2	5	610	5	-	4/15/71/71	-
27	CLA	1	612	1	-	8/33/109/115	-
27	CLA	4	611	4	-	11/39/115/115	-
27	CLA	B	808	11	-	8/39/115/115	-
28	KC2	7	307	-	-	6/15/71/71	-
27	CLA	1	608	1	-	5/33/109/115	-
27	CLA	2	612	2	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	II0	Z	312	-	-	1/21/67/67	0/2/2/2
27	CLA	b	603	26	-	7/33/109/115	-
28	KC2	a	609	-	-	3/15/71/71	-
29	II0	3	615	-	-	1/21/67/67	0/2/2/2
27	CLA	B	813	11	-	11/35/111/115	-
27	CLA	A	833	10	-	5/39/115/115	-
35	8CT	A	853	-	-	6/29/63/63	0/2/2/2
27	CLA	B	804	11	-	10/39/115/115	-
27	CLA	a	603	25	-	7/33/109/115	-
27	CLA	5	603	5	-	4/15/91/115	-
29	II0	8	610	-	-	2/21/67/67	0/2/2/2
27	CLA	3	604	-	-	3/39/115/115	-
27	CLA	5	609	-	-	2/10/86/115	-
27	CLA	A	817	10	-	13/39/115/115	-
27	CLA	B	832	-	-	15/39/115/115	-
29	II0	9	615	-	-	1/21/67/67	0/2/2/2
29	II0	3	617	-	-	2/21/67/67	0/2/2/2
27	CLA	3	601	3	-	6/15/91/115	-
27	CLA	B	831	11	-	10/27/103/115	-
27	CLA	1	607	1	-	0/15/91/115	-
27	CLA	9	601	9	-	7/15/91/115	-
27	CLA	B	825	11	-	4/39/115/115	-
33	LHG	4	619	27	-	20/49/49/53	-
27	CLA	B	802	-	-	8/39/115/115	-
34	SQD	3	621	-	-	14/37/57/69	0/1/1/1
33	LHG	3	622	28	-	13/38/38/53	-
27	CLA	A	811	10	-	12/39/115/115	-
27	CLA	3	609	-	-	2/39/115/115	-
27	CLA	A	842	10	-	6/39/115/115	-
27	CLA	9	604	-	-	1/27/103/115	-
27	CLA	7	306	7	-	6/15/91/115	-
27	CLA	B	834	11	-	2/27/103/115	-
27	CLA	B	835	11	-	10/39/115/115	-
27	CLA	4	610	4	-	7/39/115/115	-
27	CLA	B	811	11	-	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	807	10	-	2/21/97/115	-
31	IHT	9	619	-	-	3/25/65/65	0/2/2/2
31	IHT	Z	302	-	-	2/25/65/65	0/2/2/2
29	II0	1	617	-	-	2/21/67/67	0/2/2/2
29	II0	3	616	-	-	2/21/67/67	0/2/2/2
27	CLA	A	837	-	-	9/39/115/115	-
35	8CT	7	318	-	-	9/29/63/63	0/2/2/2
27	CLA	A	802	10,27	-	3/27/103/115	-
35	8CT	A	847	-	-	9/29/63/63	0/2/2/2
35	8CT	R	203	-	-	4/29/63/63	0/2/2/2
27	CLA	A	801	-	-	10/39/115/115	-
27	CLA	a	606	25	-	4/39/115/115	-
36	LMU	4	618	-	-	11/21/61/61	0/2/2/2
27	CLA	A	828	10	-	7/39/115/115	-
27	CLA	B	810	-	-	4/33/109/115	-
27	CLA	5	613	5	-	3/10/86/115	-
27	CLA	A	829	10	-	6/21/97/115	-
29	II0	5	615	-	-	1/21/67/67	0/2/2/2
27	CLA	5	604	5	-	9/27/103/115	-
27	CLA	5	612	5	-	5/15/91/115	-
27	CLA	Z	310	-	-	7/39/115/115	-
33	LHG	4	620	-	-	17/49/49/53	-
27	CLA	5	606	-	-	5/15/91/115	-
27	CLA	Z	306	24	-	13/33/109/115	-
27	CLA	b	601	26	-	5/15/91/115	-
27	CLA	1	601	1	-	5/15/91/115	-
35	8CT	K	103	-	-	3/29/63/63	0/2/2/2
32	LMG	3	620	-	-	11/27/47/70	0/1/1/1
27	CLA	6	612	-	-	4/15/91/115	-
27	CLA	A	822	10	-	10/39/115/115	-
27	CLA	Z	305	-	-	3/21/97/115	-
27	CLA	A	812	10	-	3/27/103/115	-
27	CLA	1	609	-	-	3/10/86/115	-
27	CLA	9	605	-	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	6	602	6	-	7/39/115/115	-
32	LMG	2	617	-	-	8/31/51/70	0/1/1/1
31	IHT	a	616	-	-	6/25/65/65	0/2/2/2
29	II0	a	615	-	-	1/21/67/67	0/2/2/2
27	CLA	B	830	11	-	2/33/109/115	-
27	CLA	A	819	-	-	7/39/115/115	-
27	CLA	3	603	3	-	3/33/109/115	-
27	CLA	2	608	2	-	8/33/109/115	-
29	II0	4	615	-	-	0/21/67/67	0/2/2/2
28	KC2	1	610	-	-	7/15/71/71	-
27	CLA	A	810	10	-	17/39/115/115	-
27	CLA	6	607	6	-	2/27/103/115	-
29	II0	8	612	-	-	1/21/67/67	0/2/2/2
28	KC2	2	610	2	-	6/15/71/71	-
27	CLA	O	202	-	-	4/10/86/115	-
28	KC2	7	311	7	-	7/15/71/71	-
27	CLA	A	827	-	-	5/39/115/115	-
27	CLA	7	309	7	-	9/27/103/115	-
27	CLA	B	833	-	-	2/15/91/115	-
27	CLA	b	606	26	-	5/39/115/115	-
27	CLA	9	612	-	-	2/15/91/115	-
29	II0	1	616	-	-	2/21/67/67	0/2/2/2
27	CLA	K	102	18	-	3/27/103/115	-
29	II0	B	843	-	-	2/21/67/67	0/2/2/2
27	CLA	3	607	3	-	4/33/109/115	-
29	II0	a	614	-	-	2/21/67/67	0/2/2/2
29	II0	5	614	-	-	2/21/67/67	0/2/2/2
33	LHG	a	618	-	-	16/33/33/53	-
27	CLA	F	202	-	-	12/33/109/115	-
27	CLA	9	608	9	-	11/27/103/115	-
27	CLA	7	310	33	-	2/10/86/115	-
29	II0	5	620	-	-	1/21/67/67	0/2/2/2
29	II0	4	612	-	-	2/21/67/67	0/2/2/2
32	LMG	8	616	-	-	24/46/66/70	0/1/1/1
35	8CT	R	201	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	8	604	8	-	6/39/115/115	-
39	DGD	B	848	-	-	15/48/88/95	0/2/2/2
27	CLA	B	839	33	-	5/39/115/115	-
29	II0	6	615	-	-	1/21/67/67	0/2/2/2
28	KC2	6	613	6	-	9/15/71/71	-
29	II0	J	101	-	-	1/21/67/67	0/2/2/2
27	CLA	9	606	-	-	10/38/114/115	-
27	CLA	B	805	11	-	12/39/115/115	-
33	LHG	7	319	-	-	9/35/35/53	-
35	8CT	A	848	-	-	1/29/63/63	0/2/2/2
35	8CT	L	205	-	-	2/29/63/63	0/2/2/2
28	KC2	Z	307	24	-	7/15/71/71	-
33	LHG	5	619	-	-	14/26/26/53	-
27	CLA	6	605	6	-	7/27/103/115	-
27	CLA	B	840	11	-	1/39/115/115	-
33	LHG	A	852	-	-	20/43/43/53	-
27	CLA	B	824	-	-	5/33/109/115	-
27	CLA	A	820	10	-	8/39/115/115	-
27	CLA	A	818	10	-	9/39/115/115	-
35	8CT	Z	308	-	-	6/29/63/63	0/2/2/2
27	CLA	6	604	6	-	6/33/109/115	-
27	CLA	B	812	11	-	13/39/115/115	-
27	CLA	5	607	5	-	2/15/91/115	-
27	CLA	3	605	3	-	4/27/103/115	-
29	II0	3	614	-	-	0/21/67/67	0/2/2/2
27	CLA	a	610	-	-	6/27/103/115	-
29	II0	8	611	-	-	2/21/67/67	0/2/2/2
35	8CT	J	103	-	-	7/29/63/63	0/2/2/2
27	CLA	B	823	-	-	12/39/115/115	-
29	II0	R	204	-	-	2/21/67/67	0/2/2/2
27	CLA	A	843	10	-	10/39/115/115	-
27	CLA	4	601	4	-	5/27/103/115	-
27	CLA	A	808	10	-	2/27/103/115	-
27	CLA	2	601	2	-	5/12/88/115	-

The worst 5 of 2335 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	854	IHT	C10-C07	10.21	1.52	1.34
28	2	610	KC2	MG-ND	-10.00	1.86	2.05
28	7	307	KC2	MG-ND	-9.99	1.86	2.05
28	b	609	KC2	MG-ND	-9.99	1.86	2.05
28	3	606	KC2	MG-ND	-9.96	1.86	2.05

The worst 5 of 2816 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	8	609	IHT	C02-C07-C10	-10.15	108.32	122.61
31	9	619	IHT	C02-C07-C10	-10.12	108.35	122.61
31	L	204	IHT	C02-C07-C10	-9.21	109.64	122.61
31	5	618	IHT	C02-C07-C10	-8.96	110.00	122.61
31	6	616	IHT	C02-C07-C10	-8.07	111.24	122.61

There are no chirality outliers.

5 of 2201 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	1	603	CLA	C1A-C2A-CAA-CBA
27	1	605	CLA	C2B-C3B-CAB-CBB
27	1	605	CLA	C4B-C3B-CAB-CBB
27	2	601	CLA	C3A-C2A-CAA-CBA
27	2	601	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

82 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	8	605	CLA	2	0
27	b	610	CLA	1	0
31	6	616	IHT	1	0
31	A	854	IHT	1	0
27	8	608	CLA	1	0
27	A	826	CLA	2	0
29	4	613	II0	1	0
35	4	616	8CT	1	0
27	L	203	CLA	1	0
36	J	104	LMU	1	0
33	2	619	LHG	1	0
27	9	609	CLA	1	0
27	A	823	CLA	2	0

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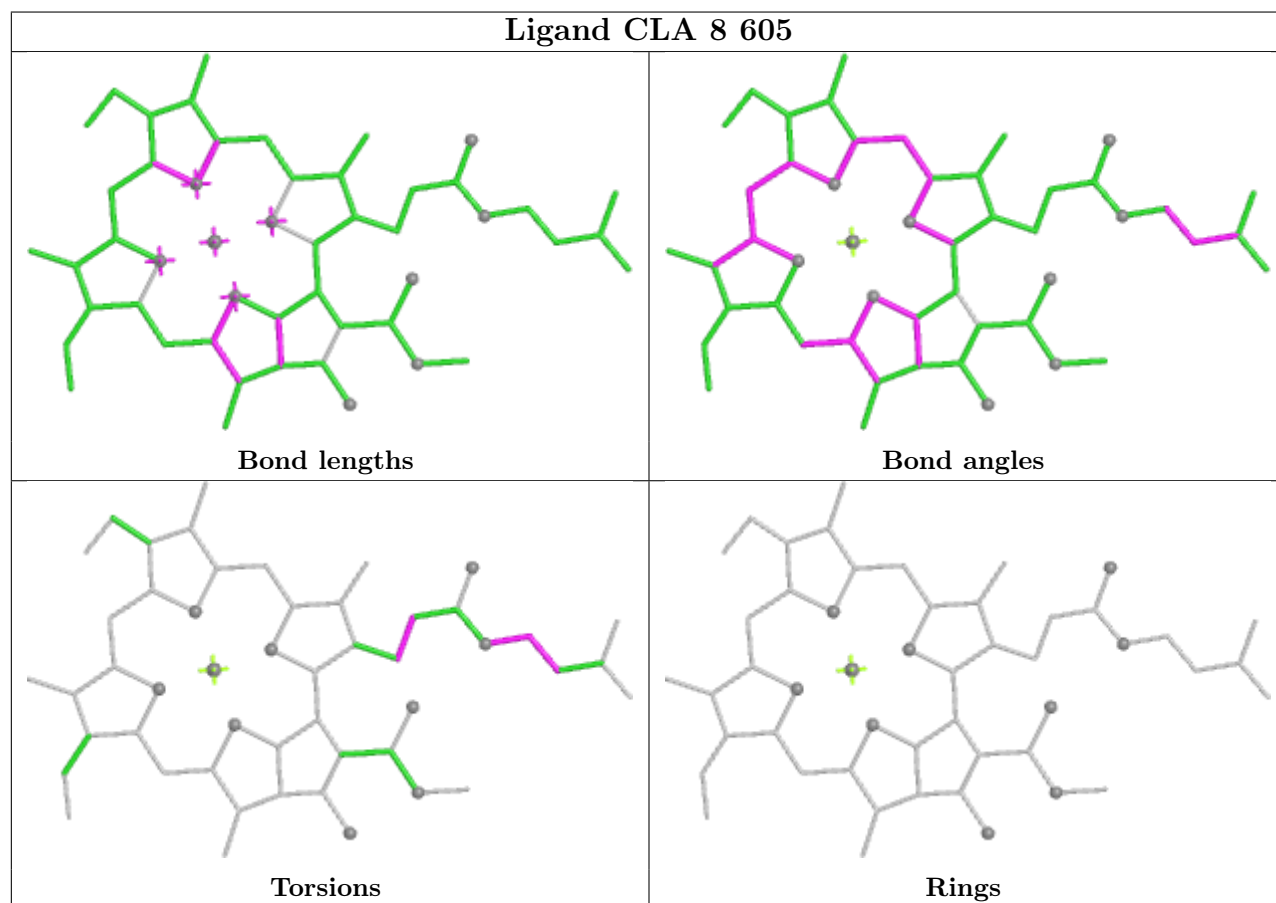
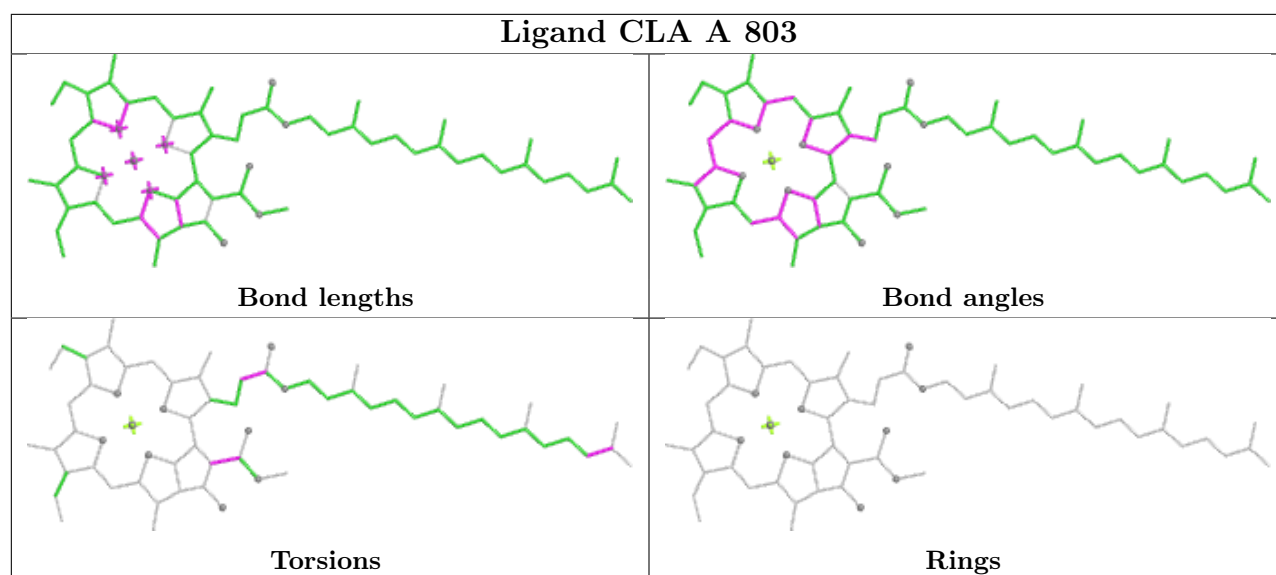
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	8	603	CLA	1	0
27	9	611	CLA	2	0
36	7	321	LMU	1	0
27	R	202	CLA	1	0
27	7	308	CLA	1	0
39	Z	303	DGD	1	0
27	B	801	CLA	2	0
27	5	608	CLA	2	0
27	1	611	CLA	2	0
27	O	201	CLA	1	0
29	2	614	II0	1	0
31	2	616	IHT	1	0
27	A	844	CLA	3	0
37	C	102	SF4	1	0
27	6	609	CLA	1	0
27	a	611	CLA	3	0
27	B	807	CLA	1	0
28	b	609	KC2	1	0
27	B	818	CLA	2	0
30	b	613	II3	1	0
27	B	809	CLA	1	0
27	7	313	CLA	2	0
27	L	201	CLA	1	0
27	Z	304	CLA	1	0
27	5	611	CLA	1	0
27	A	834	CLA	1	0
33	6	617	LHG	1	0
27	A	836	CLA	2	0
27	B	816	CLA	2	0
35	M	101	8CT	1	0
28	9	610	KC2	1	0
27	B	815	CLA	1	0
27	B	826	CLA	1	0
27	1	604	CLA	2	0
27	4	611	CLA	1	0
27	2	612	CLA	1	0
27	a	603	CLA	2	0
29	8	610	II0	1	0
27	5	609	CLA	2	0
27	B	832	CLA	1	0
27	B	831	CLA	1	0
27	B	825	CLA	1	0

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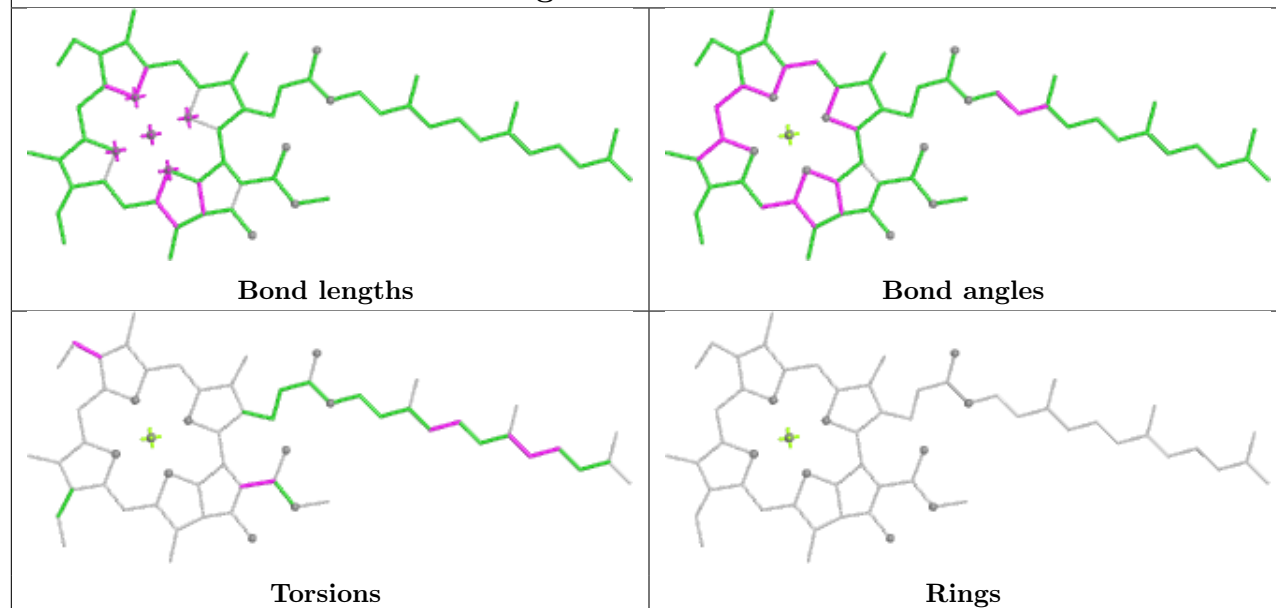
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	802	CLA	2	0
27	A	842	CLA	1	0
27	9	604	CLA	2	0
27	B	834	CLA	2	0
27	B	835	CLA	1	0
31	9	619	IHT	1	0
35	7	318	8CT	1	0
36	4	618	LMU	2	0
27	5	604	CLA	1	0
27	5	612	CLA	1	0
27	6	612	CLA	1	0
27	1	609	CLA	1	0
31	a	616	IHT	1	0
27	A	819	CLA	1	0
27	A	810	CLA	3	0
28	7	311	KC2	2	0
27	K	102	CLA	1	0
29	a	614	II0	1	0
27	7	310	CLA	1	0
29	5	620	II0	1	0
27	B	839	CLA	1	0
27	9	606	CLA	1	0
27	B	840	CLA	2	0
27	A	818	CLA	3	0
29	3	614	II0	1	0
27	B	823	CLA	1	0
27	A	808	CLA	1	0

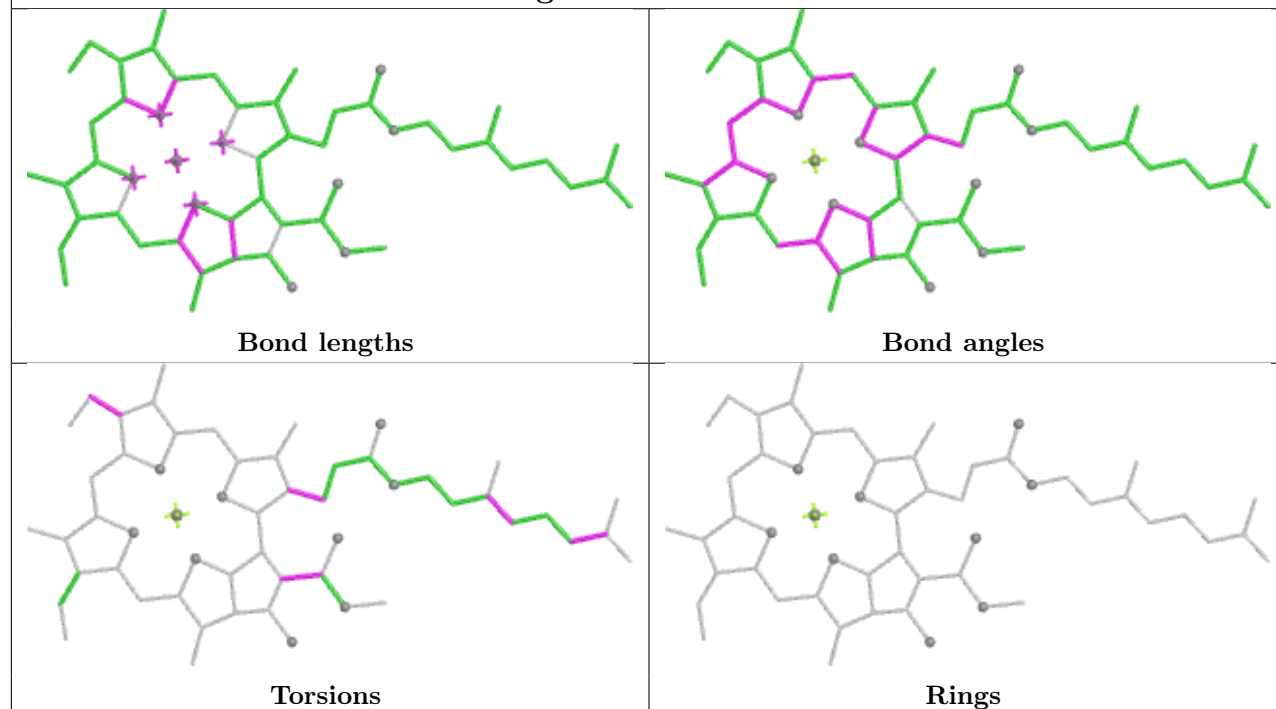
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



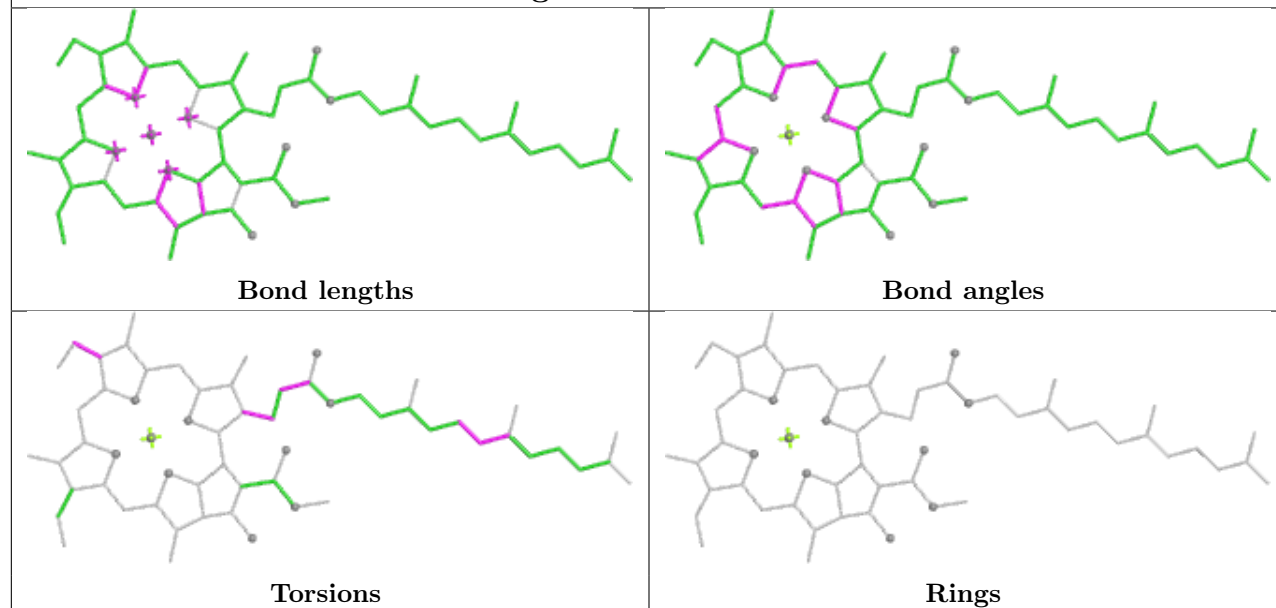
Ligand CLA 6 608



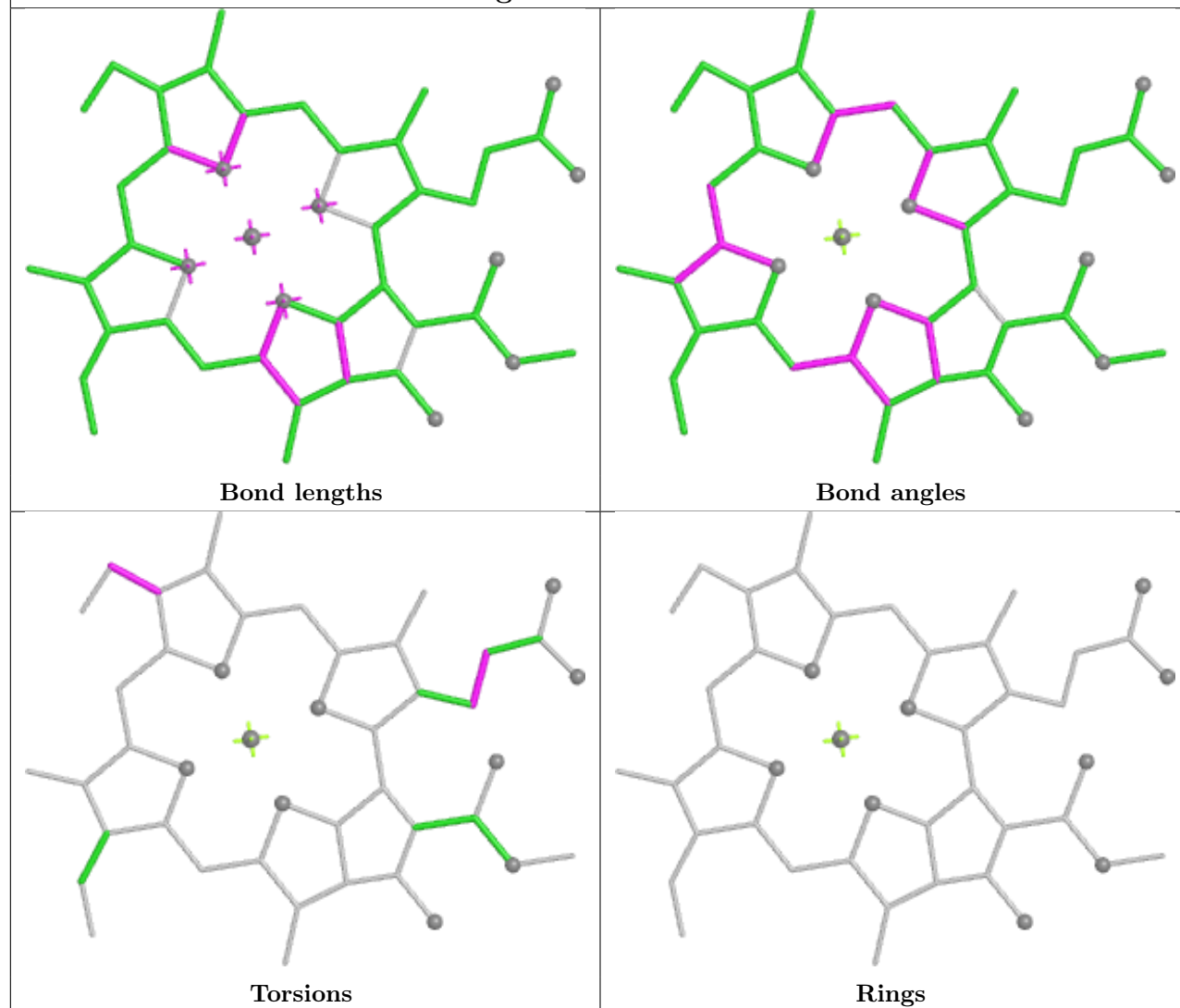
Ligand CLA 9 602

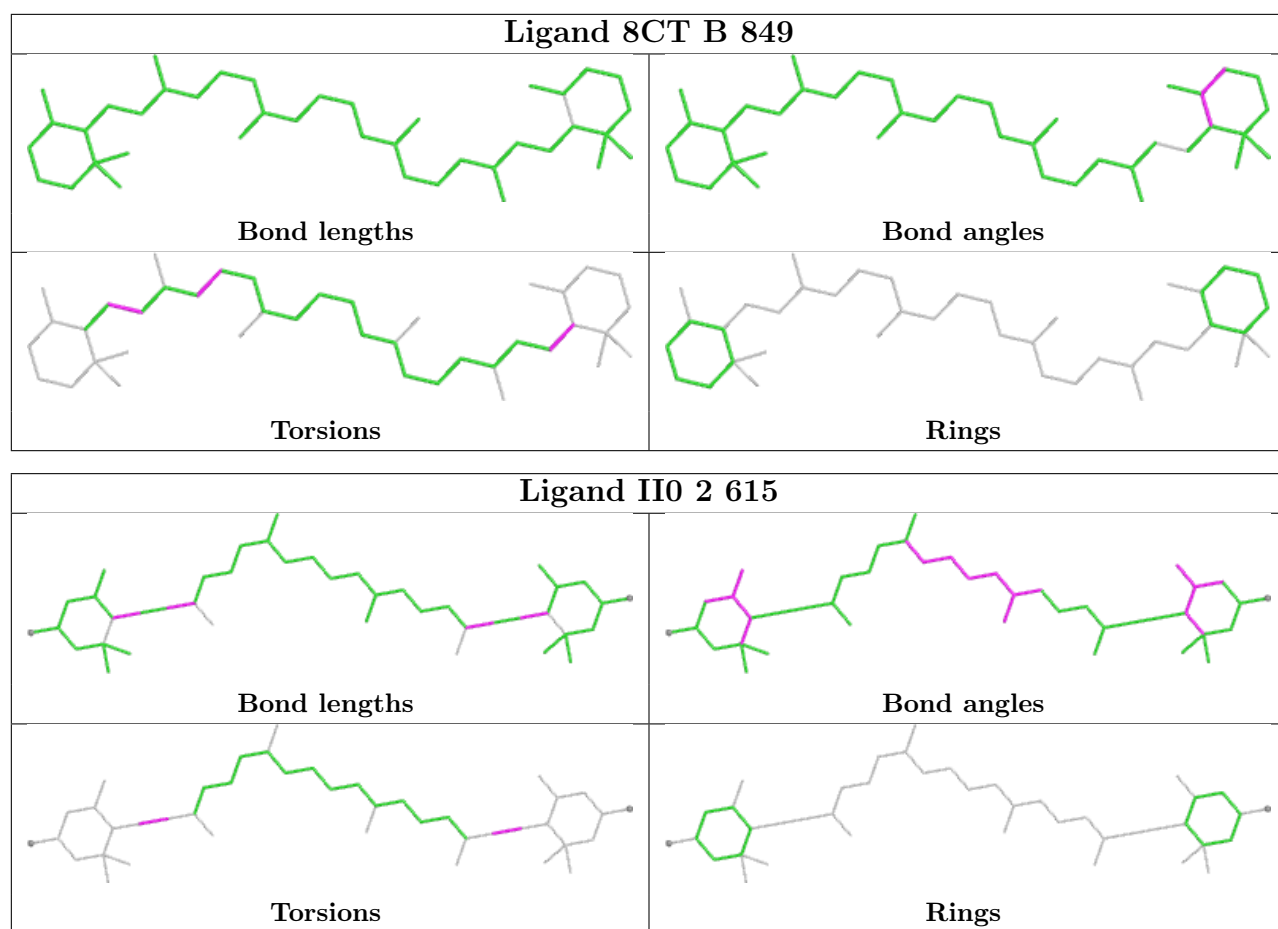


Ligand CLA A 816

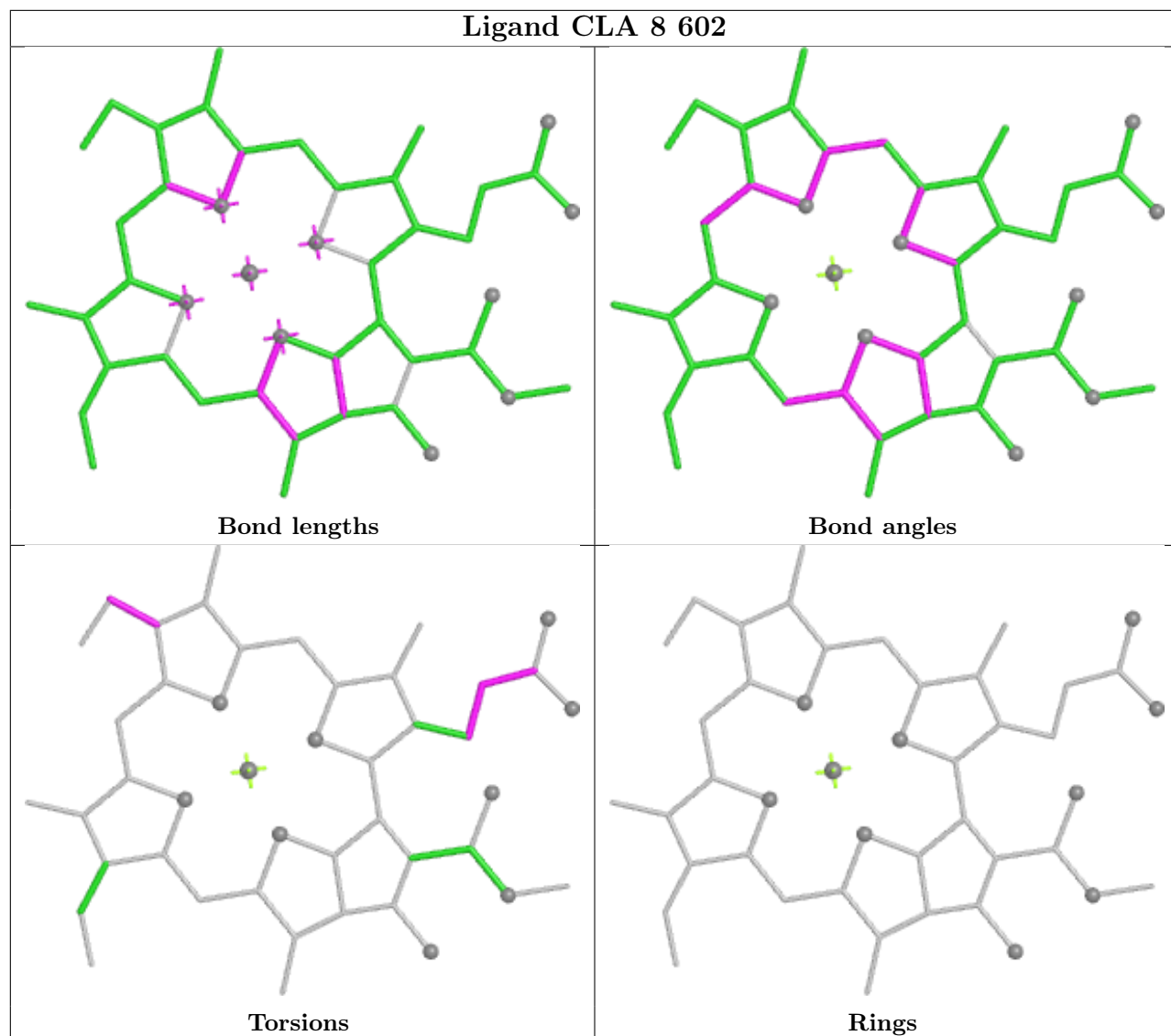


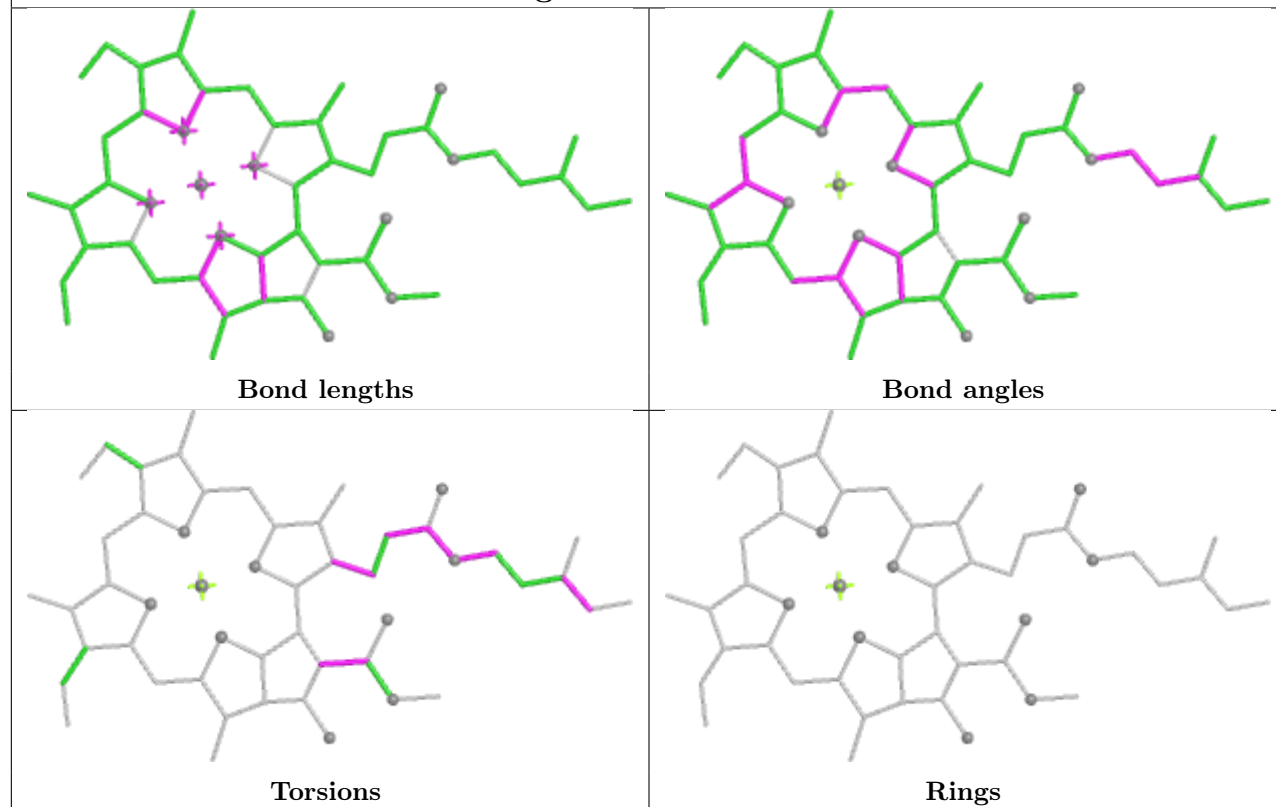
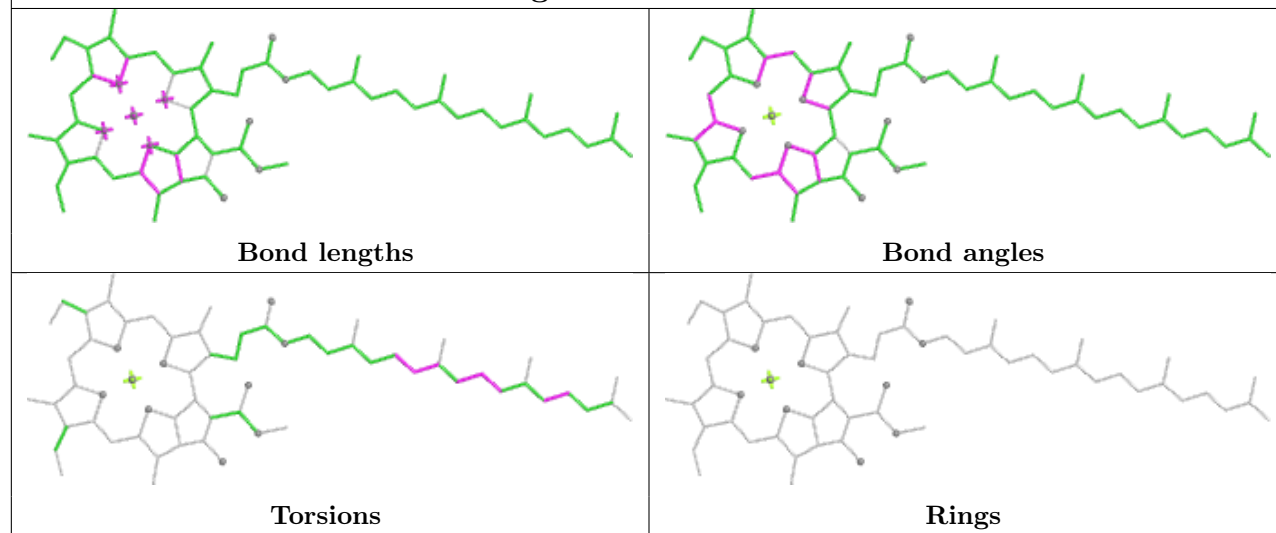
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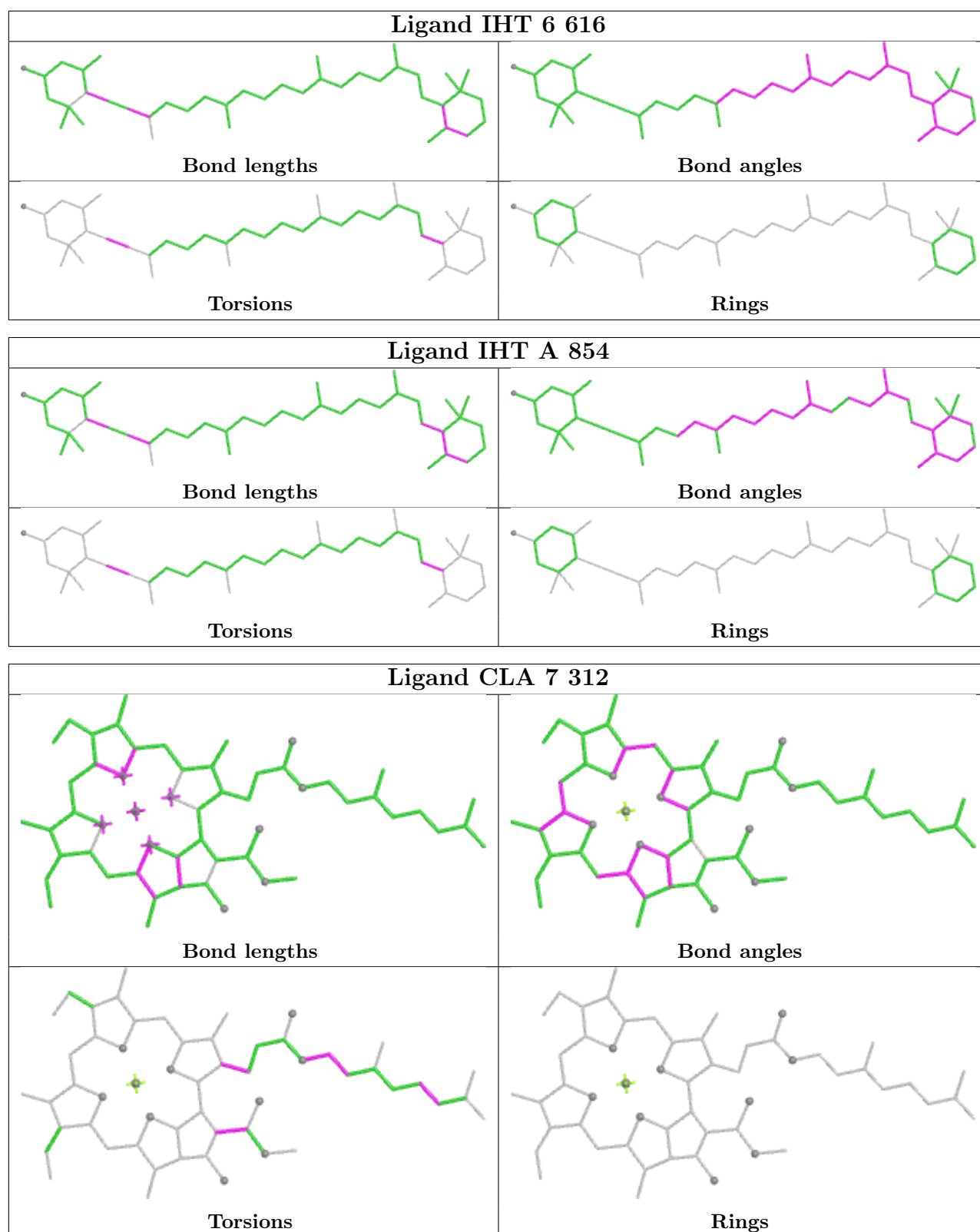


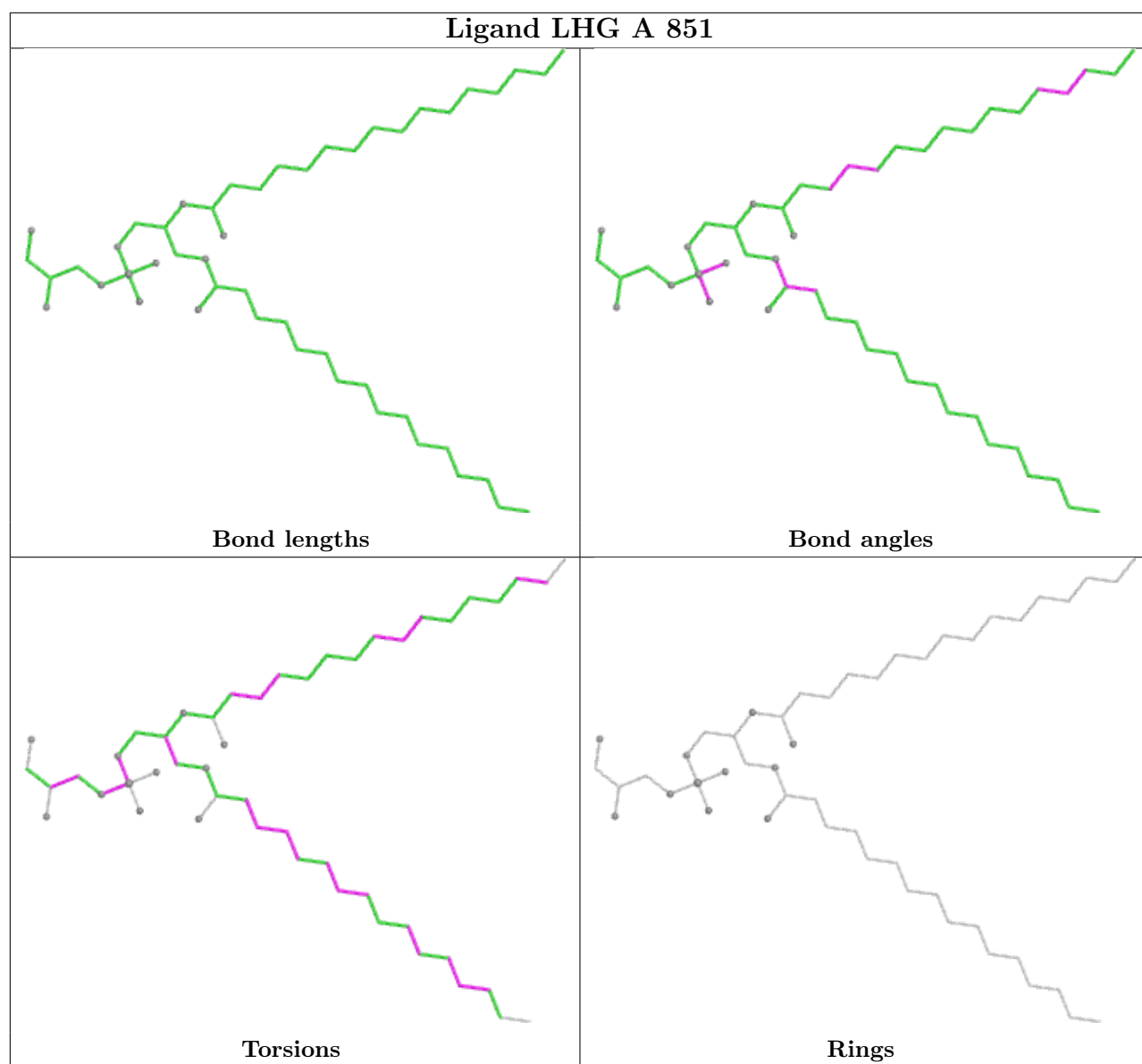


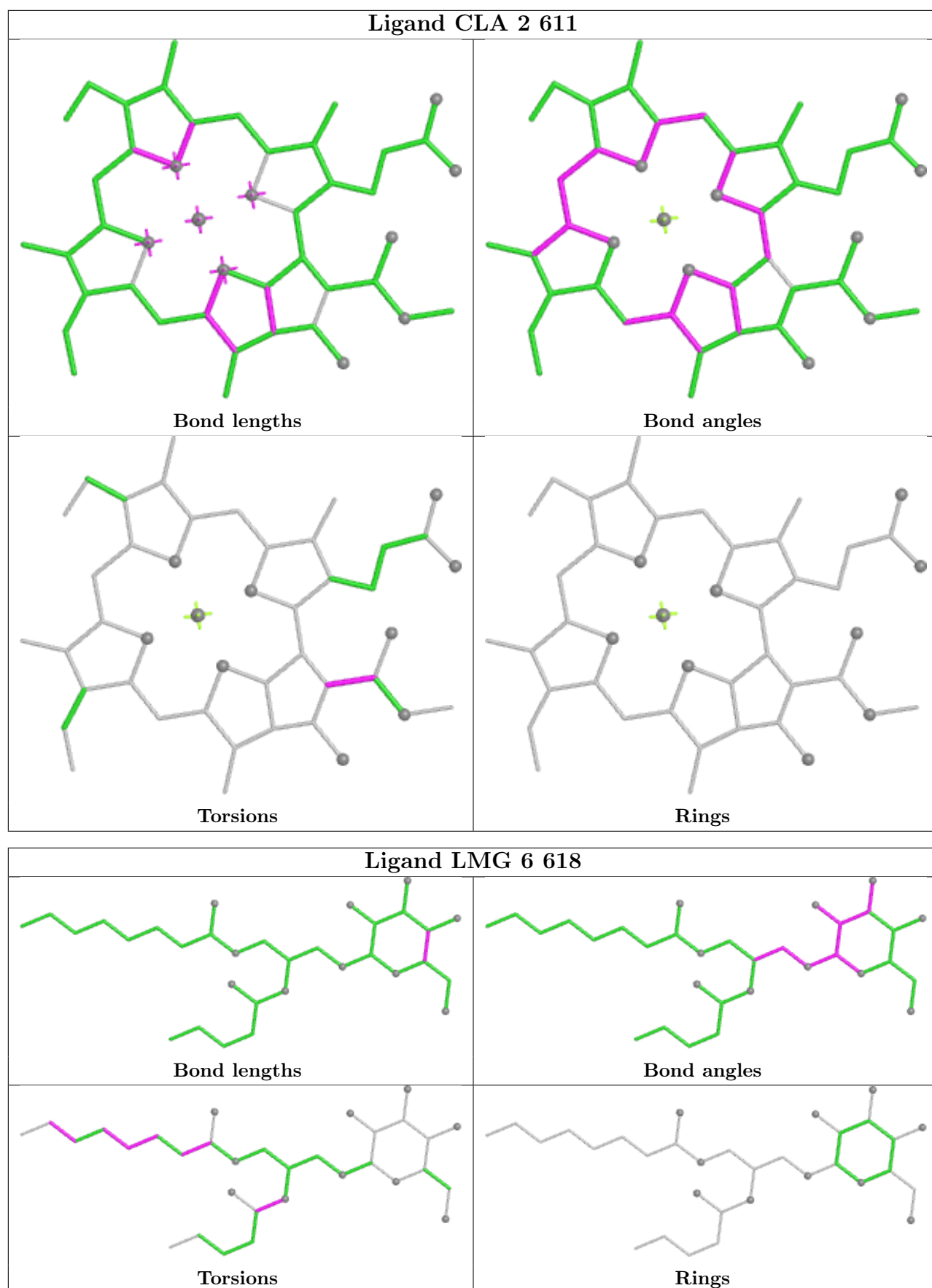
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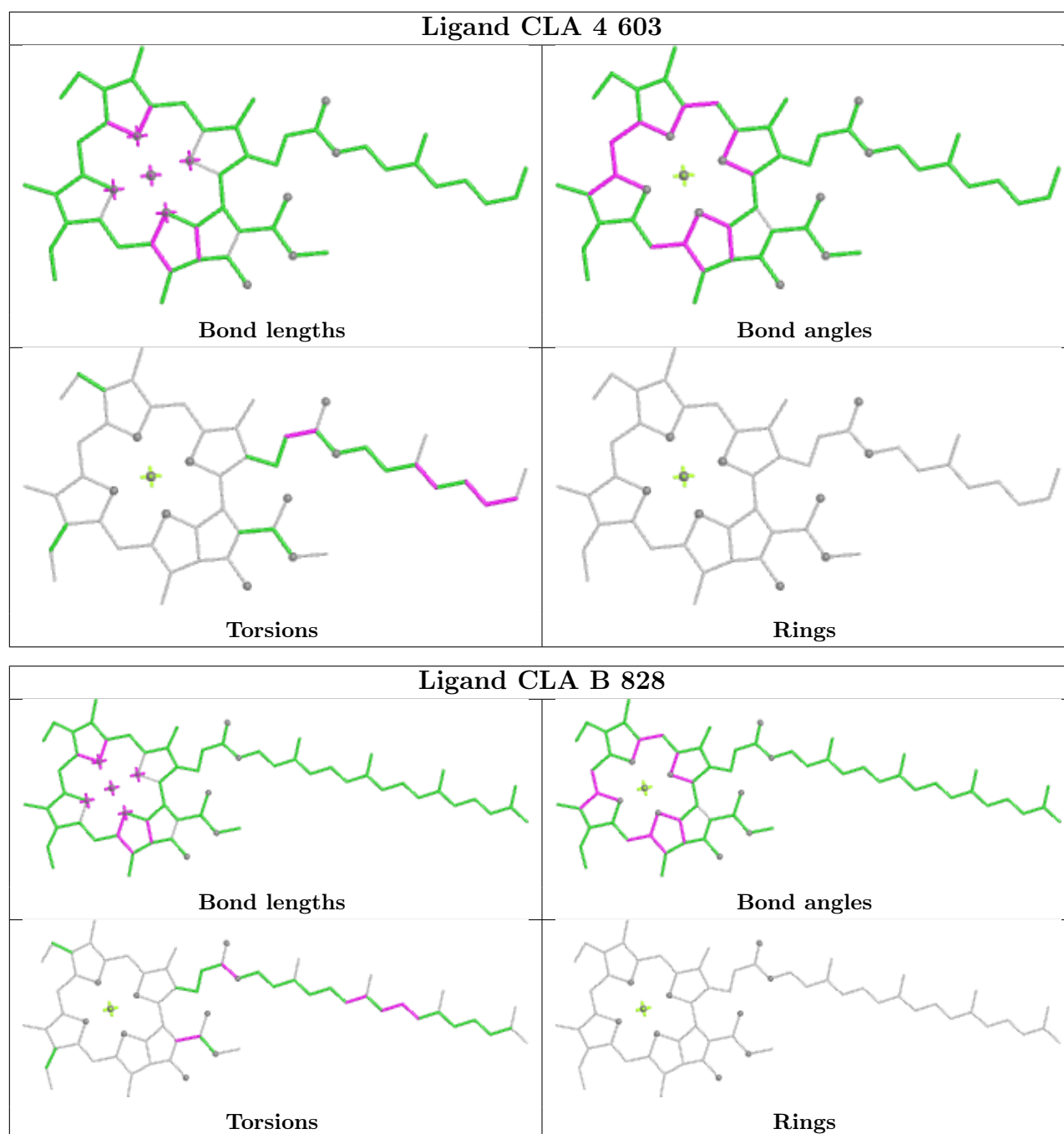


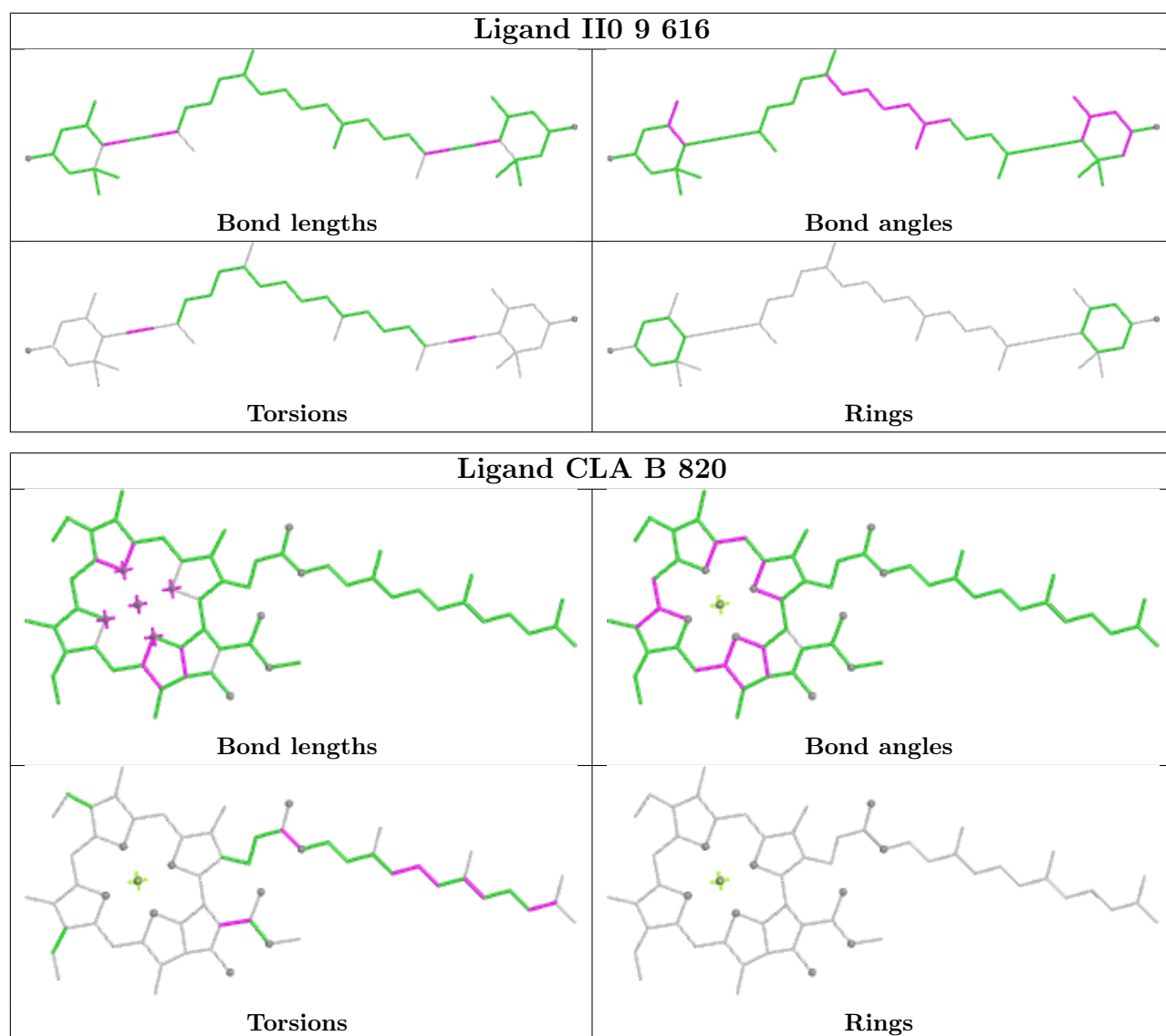
Ligand CLA b 610**Ligand CLA K 101**

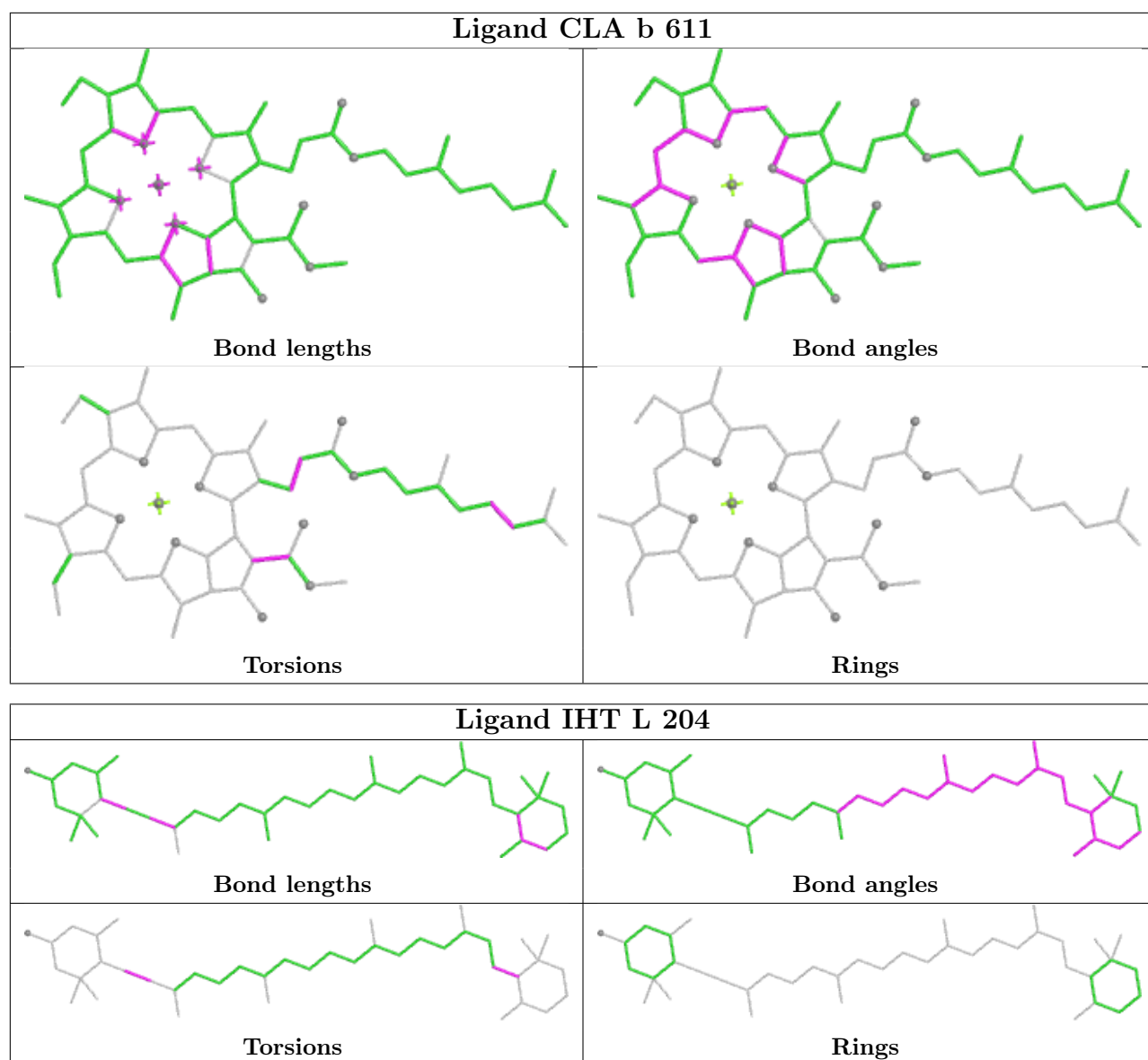




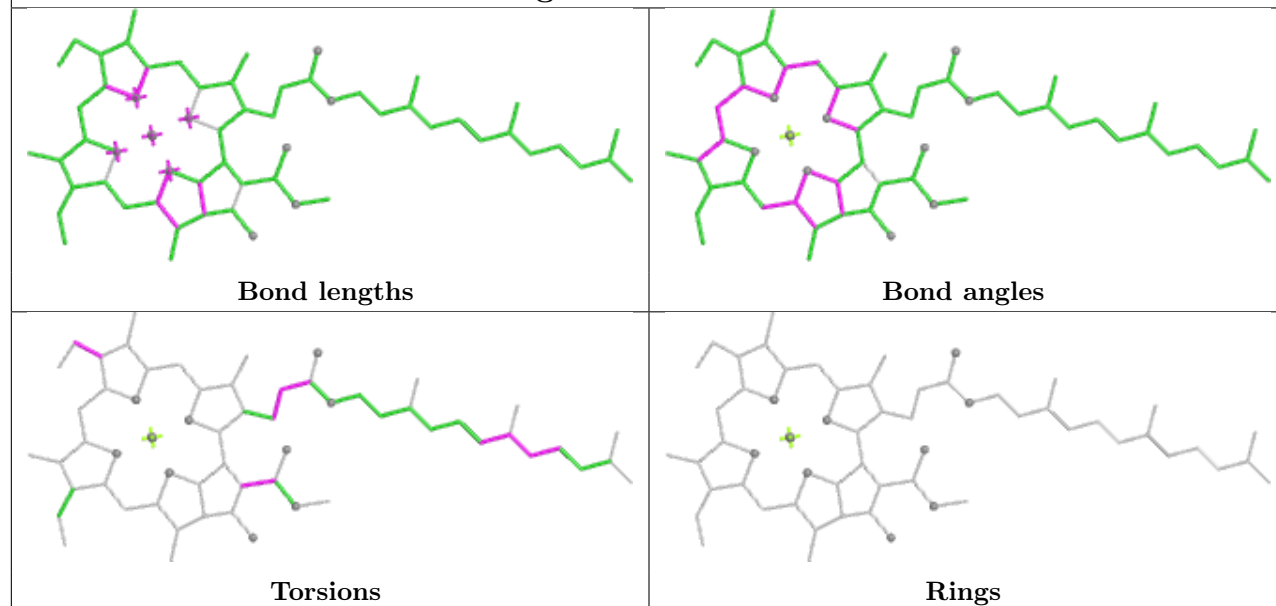




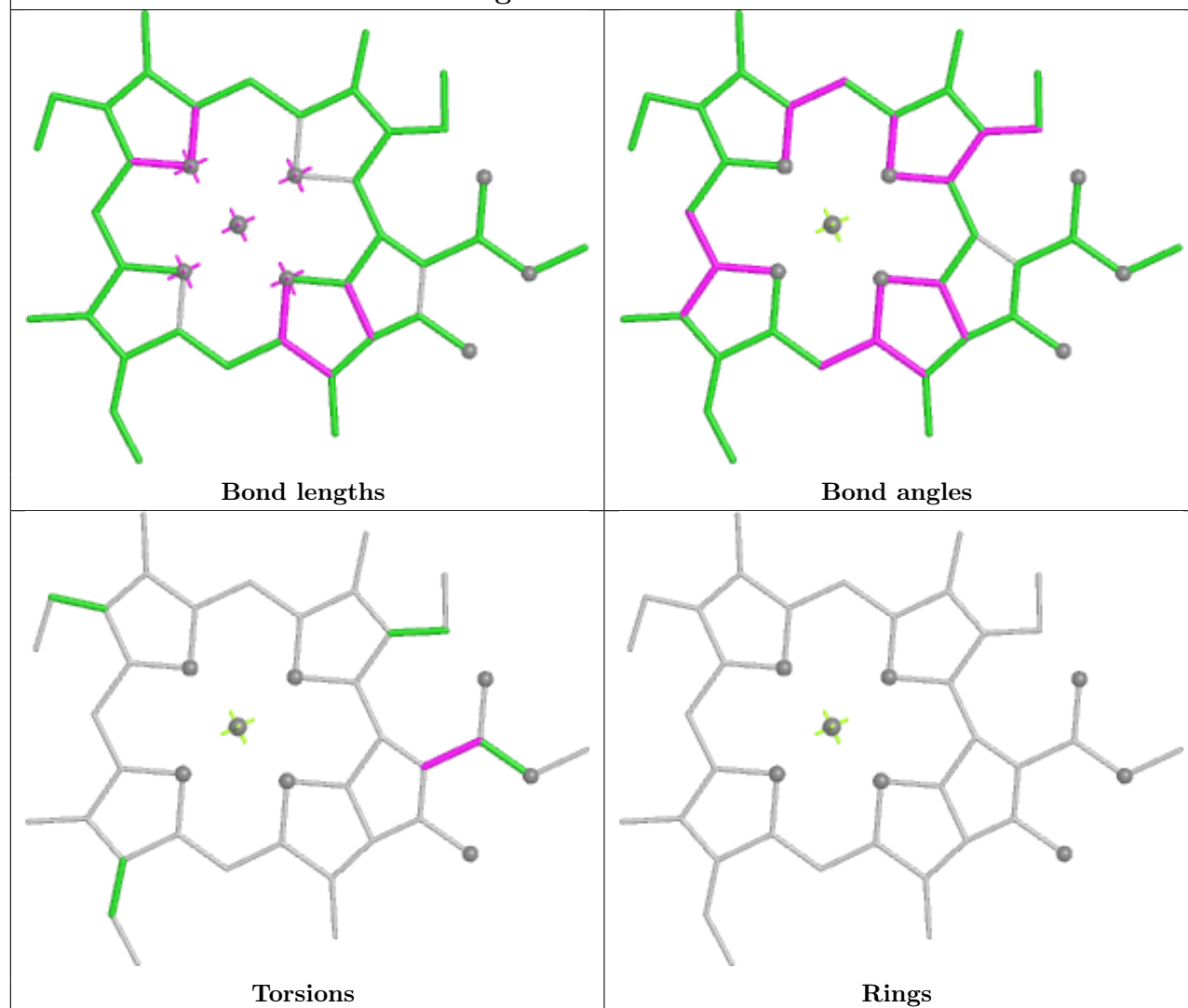


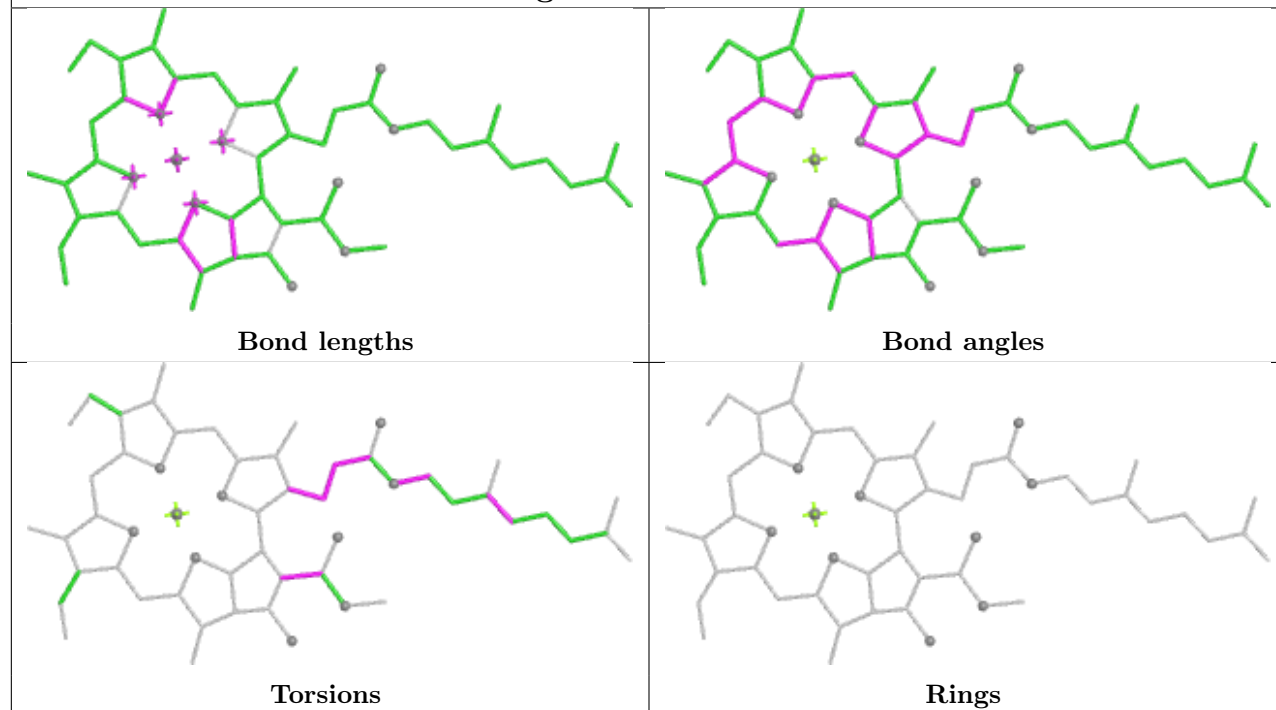
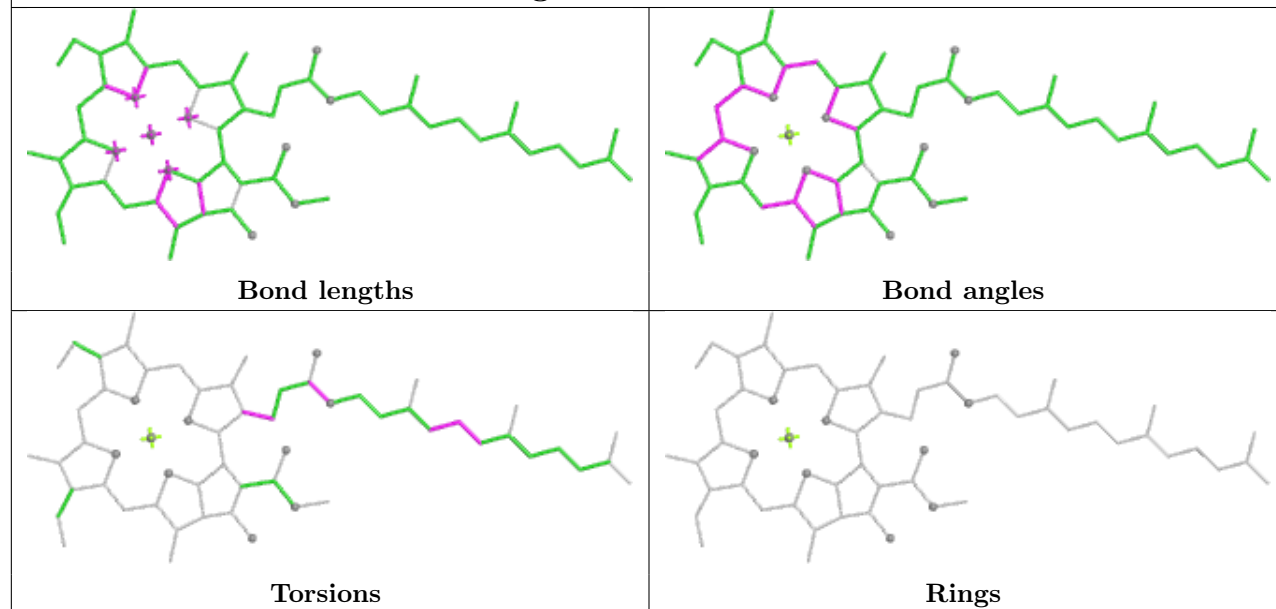


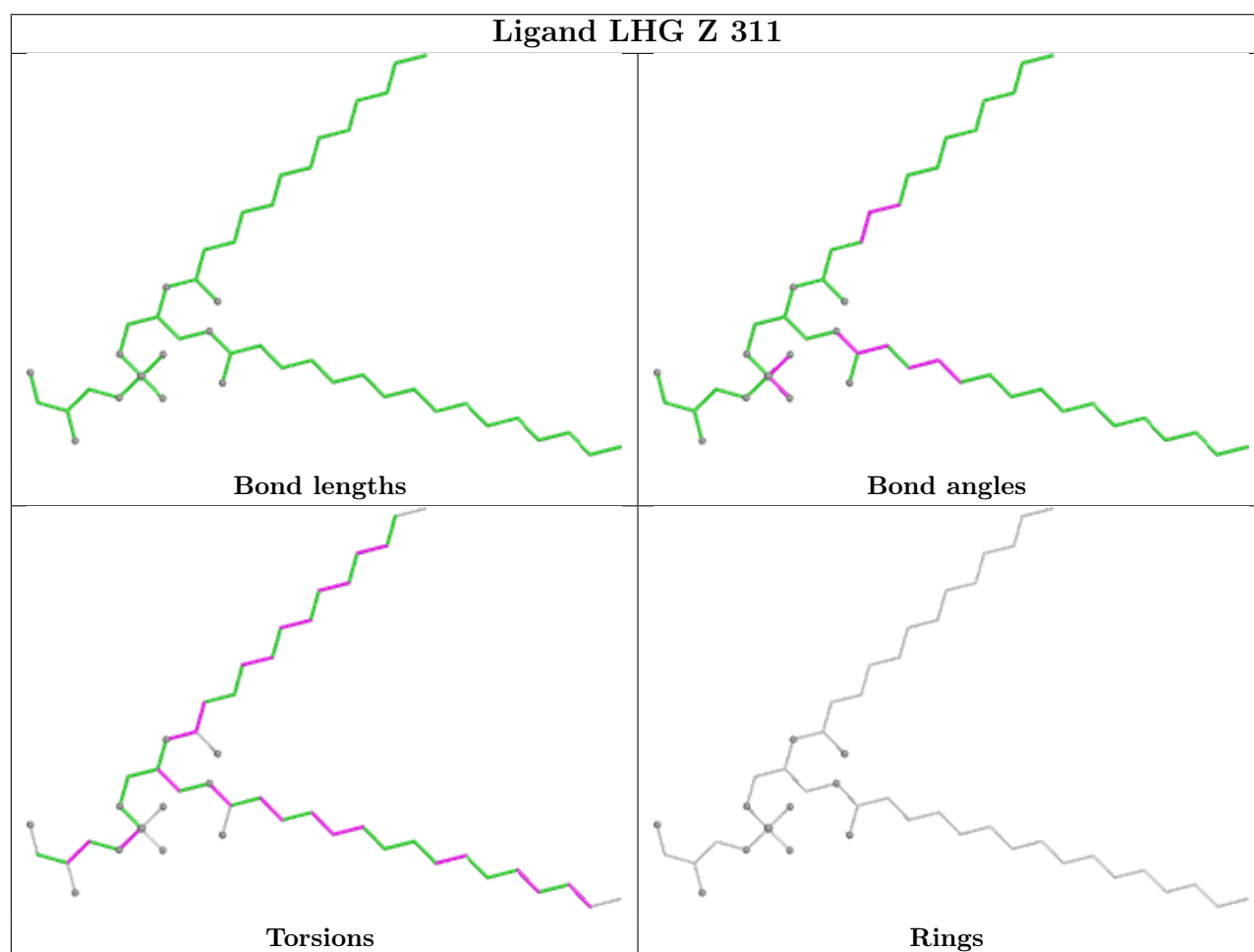
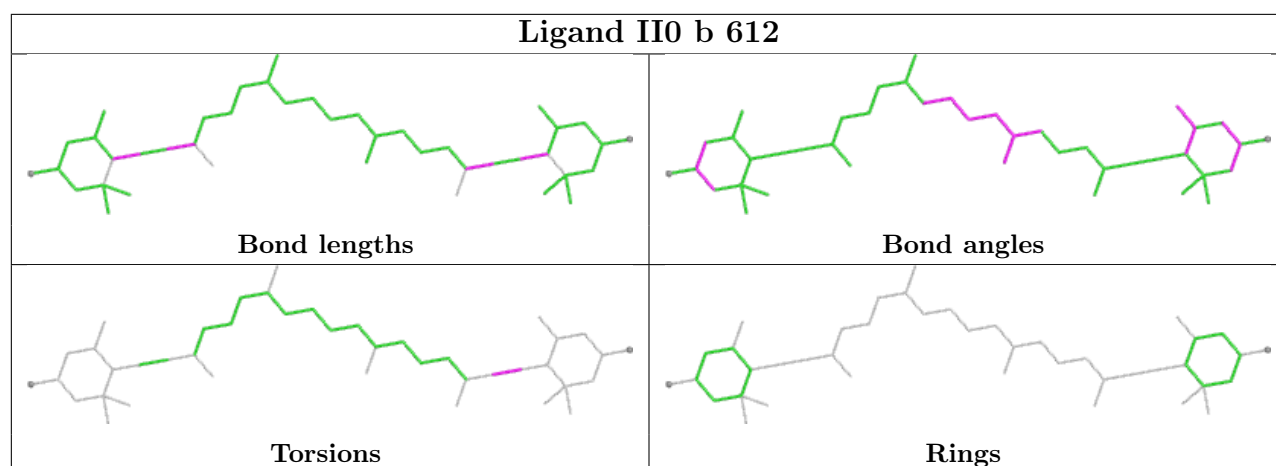
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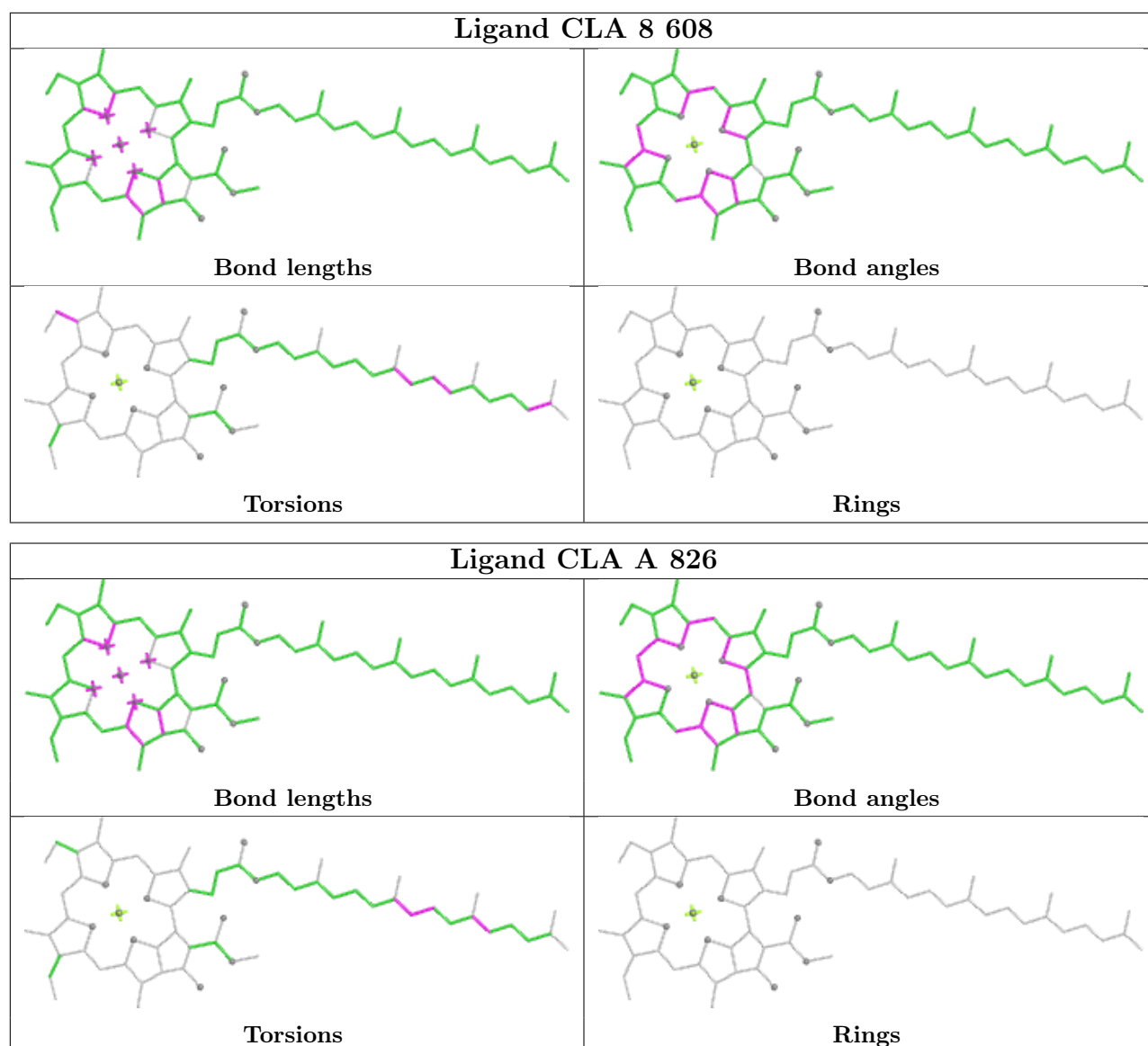


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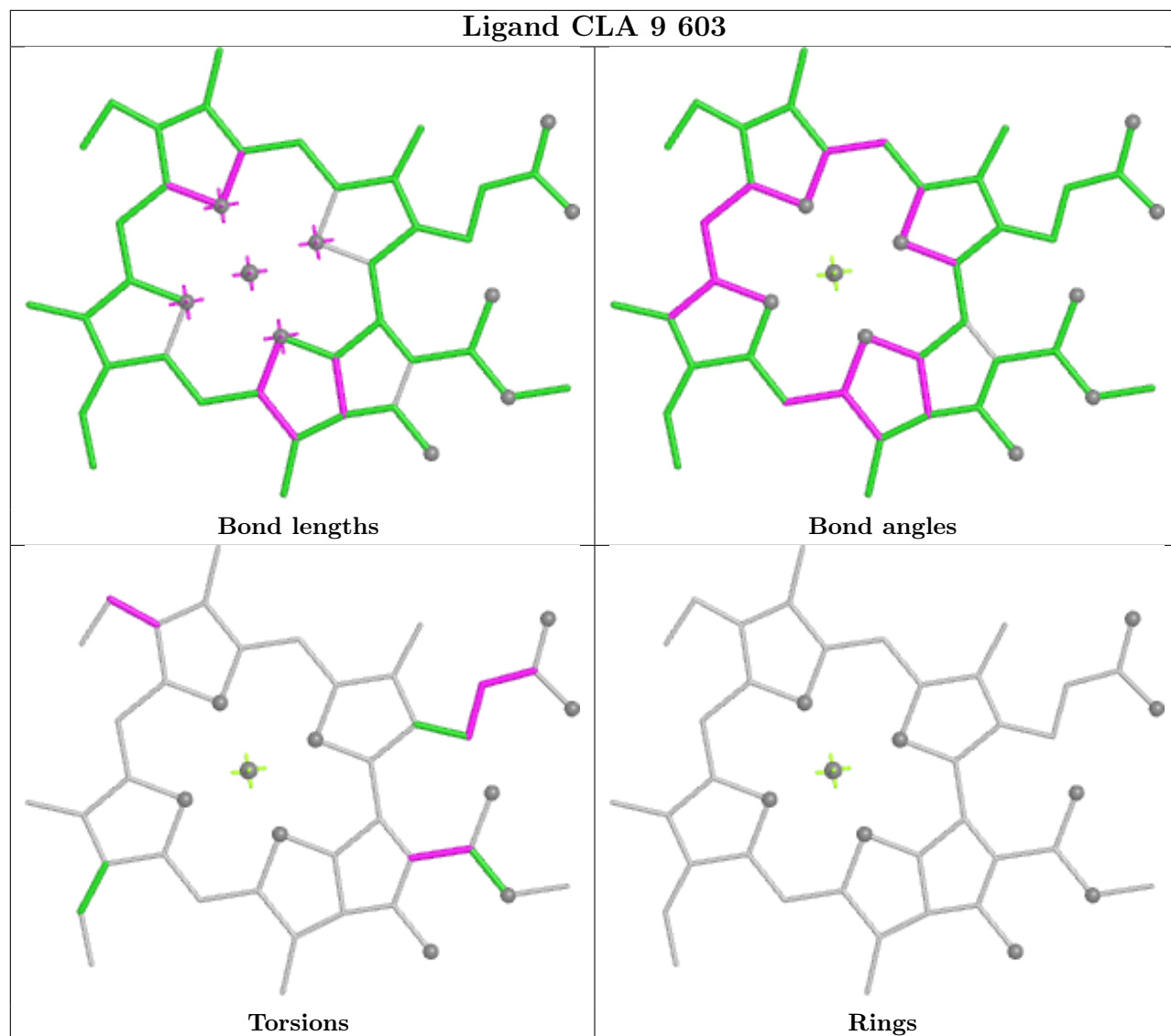


Ligand CLA a 602**Ligand CLA A 830**

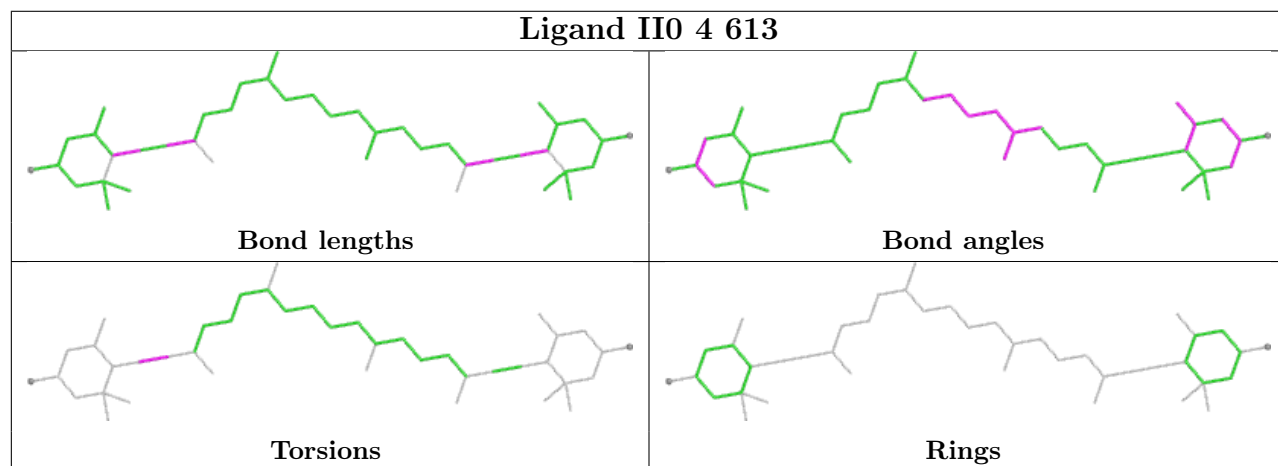




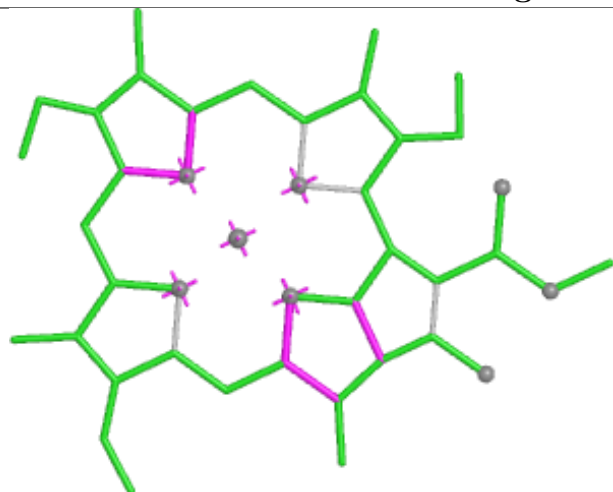
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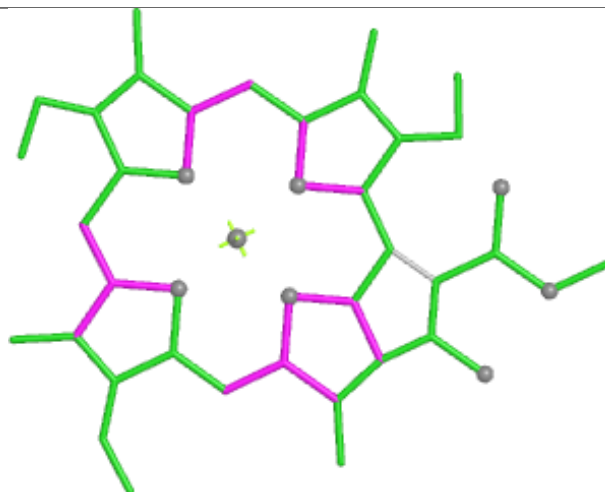
Ligand II0 4 613



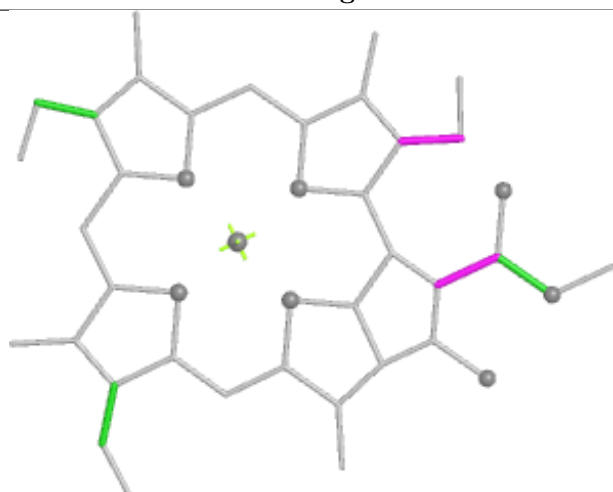
Ligand CLA B 814



Bond lengths



Bond angles

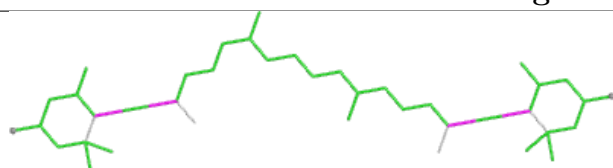


Torsions

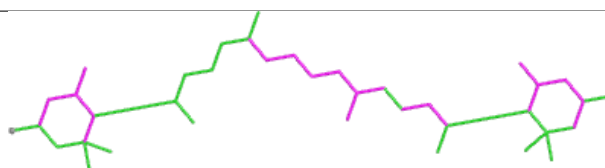


Rings

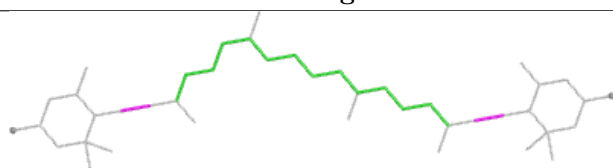
Ligand II0 7 301



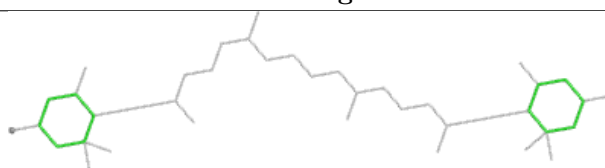
Bond lengths



Bond angles

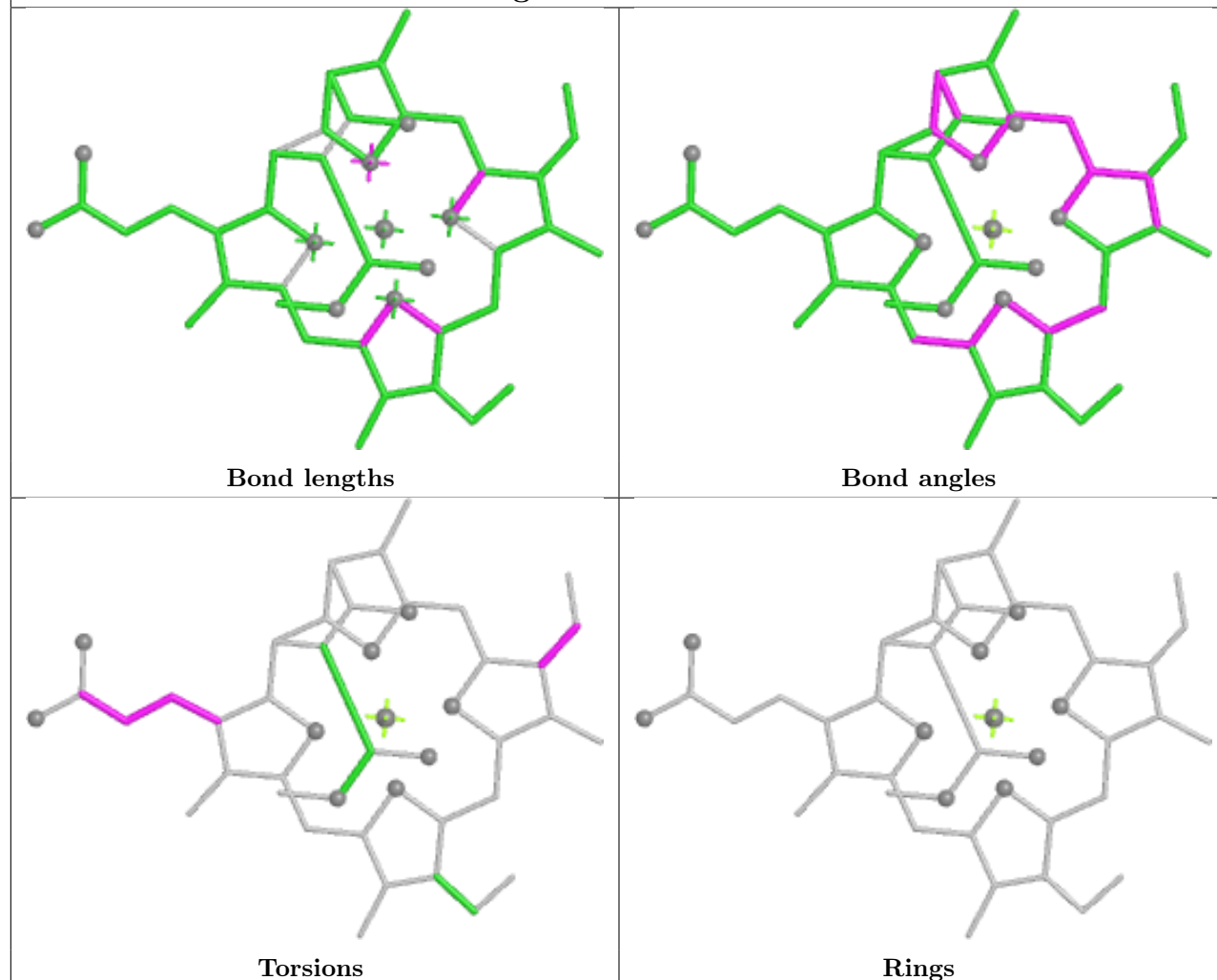


Torsions

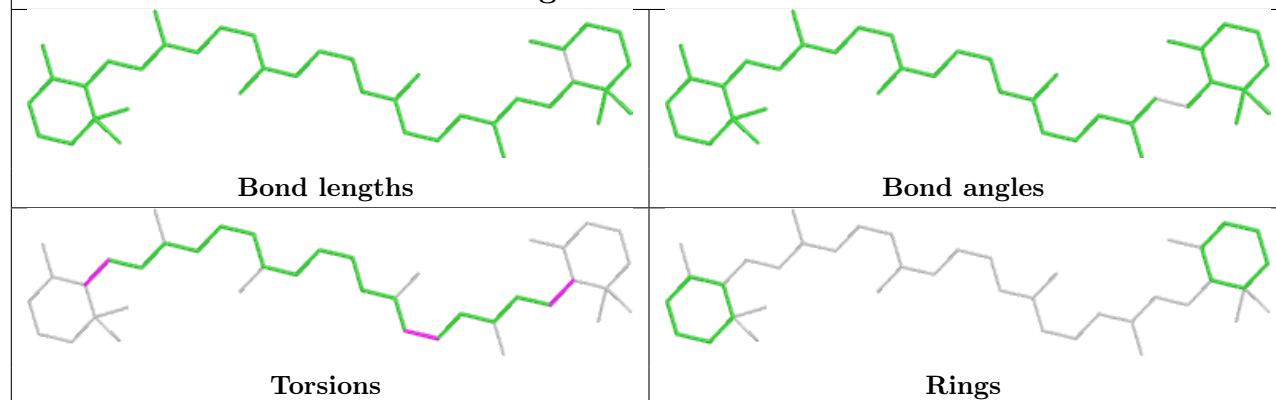


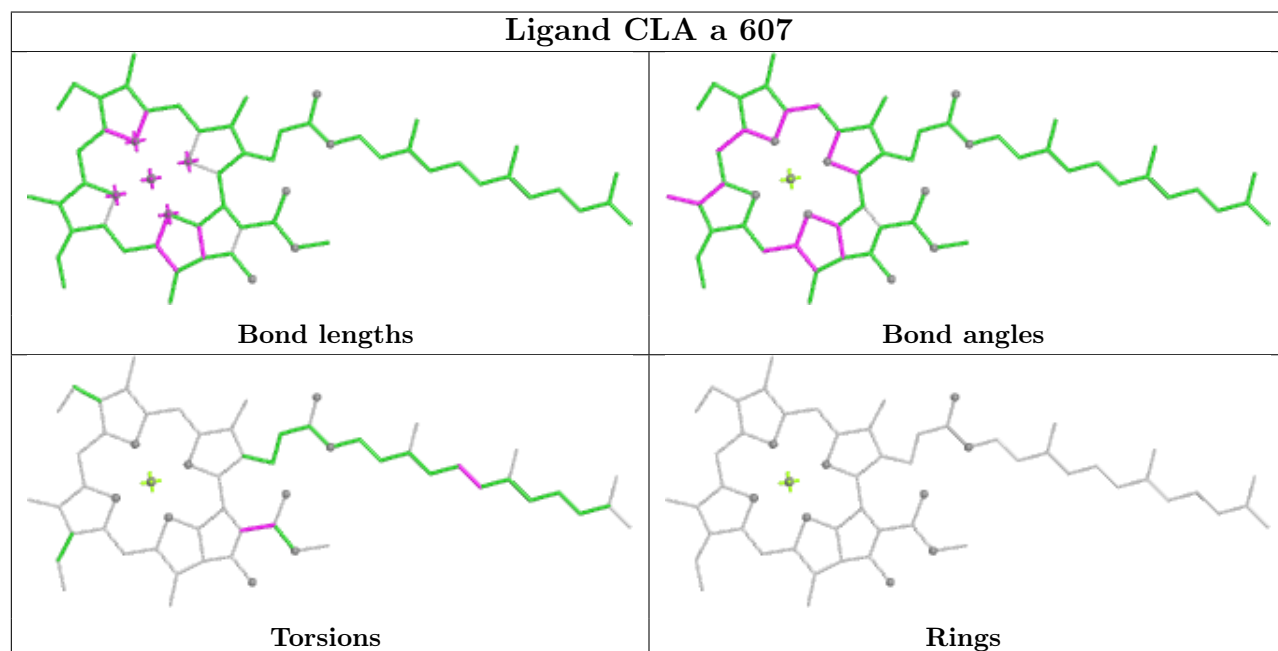
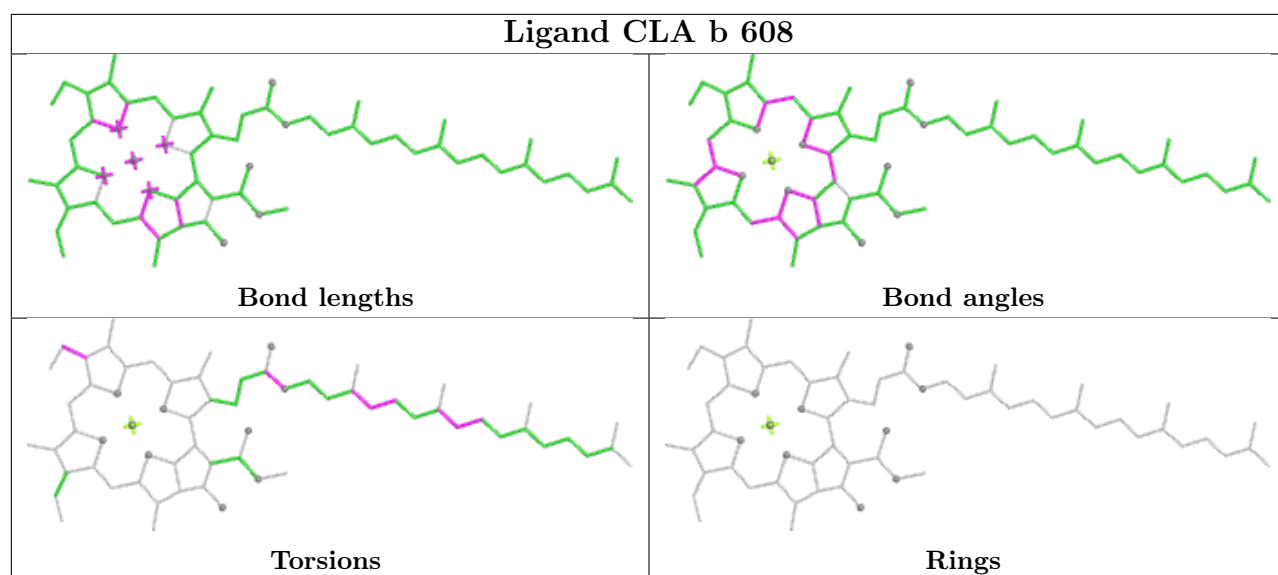
Rings

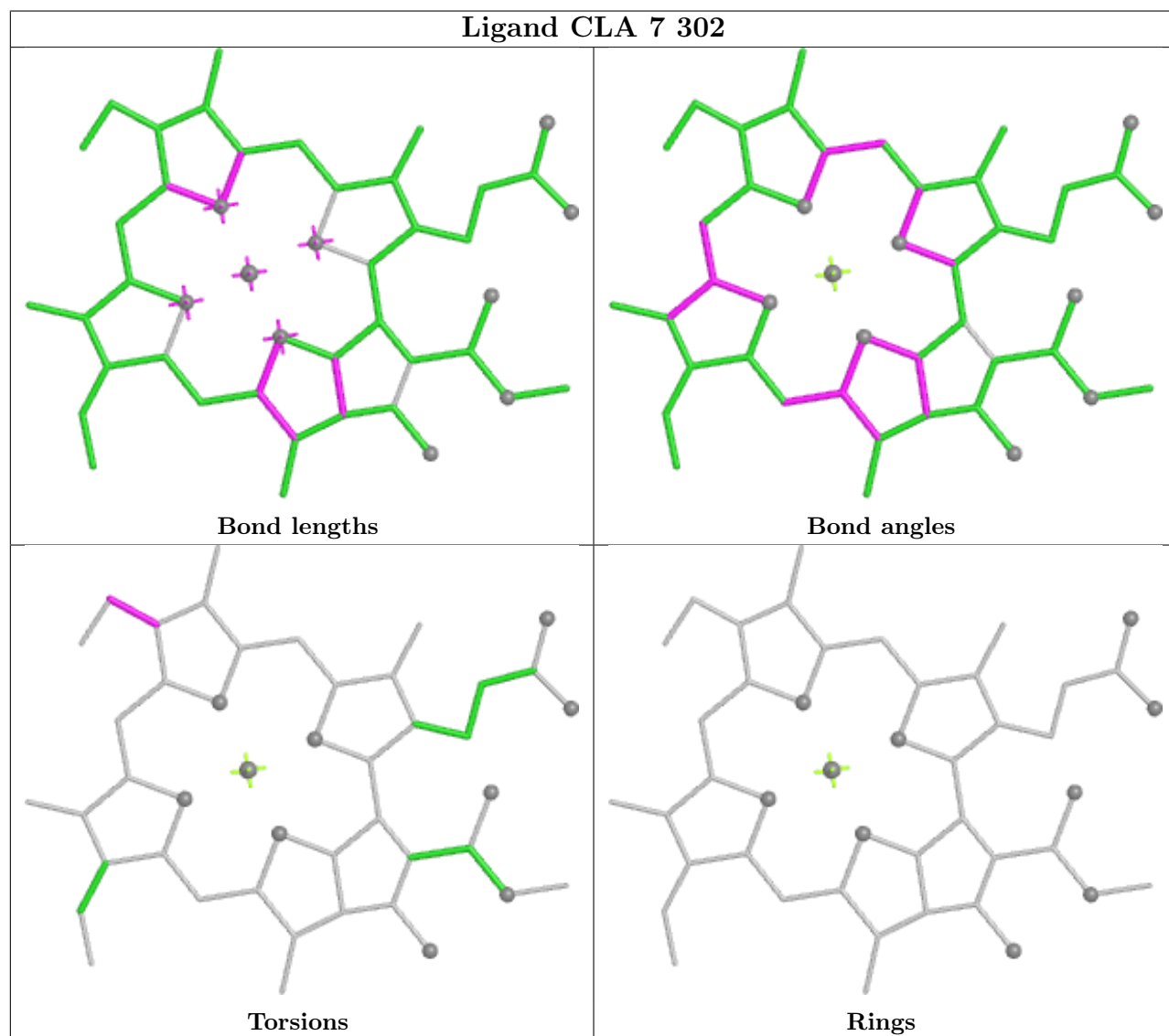
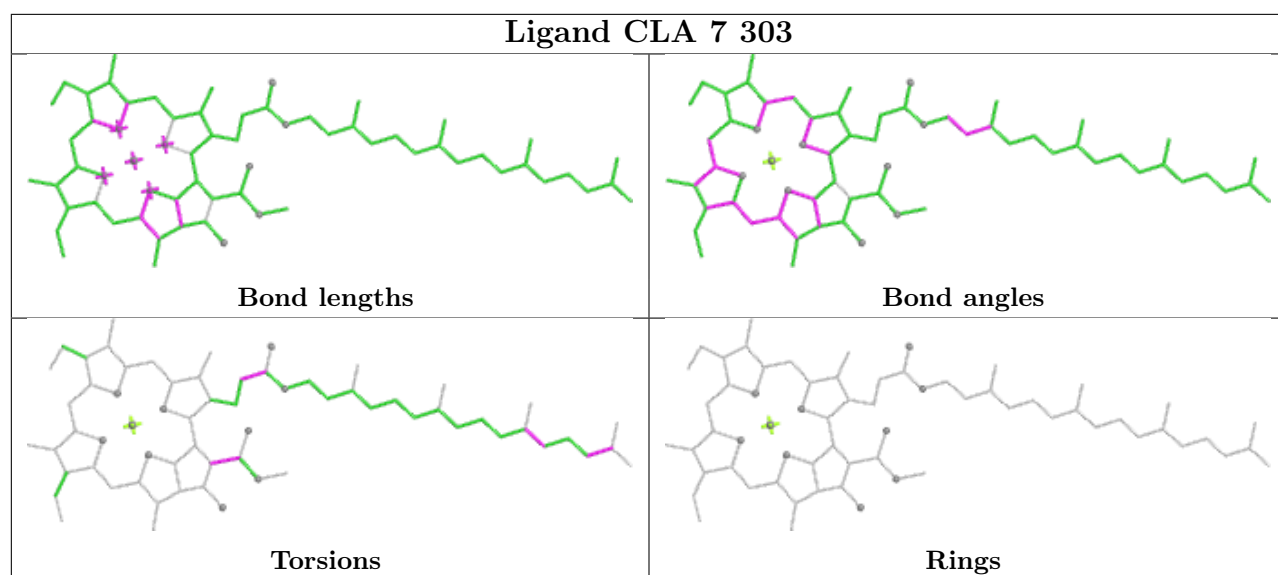
Ligand KC2 6 610



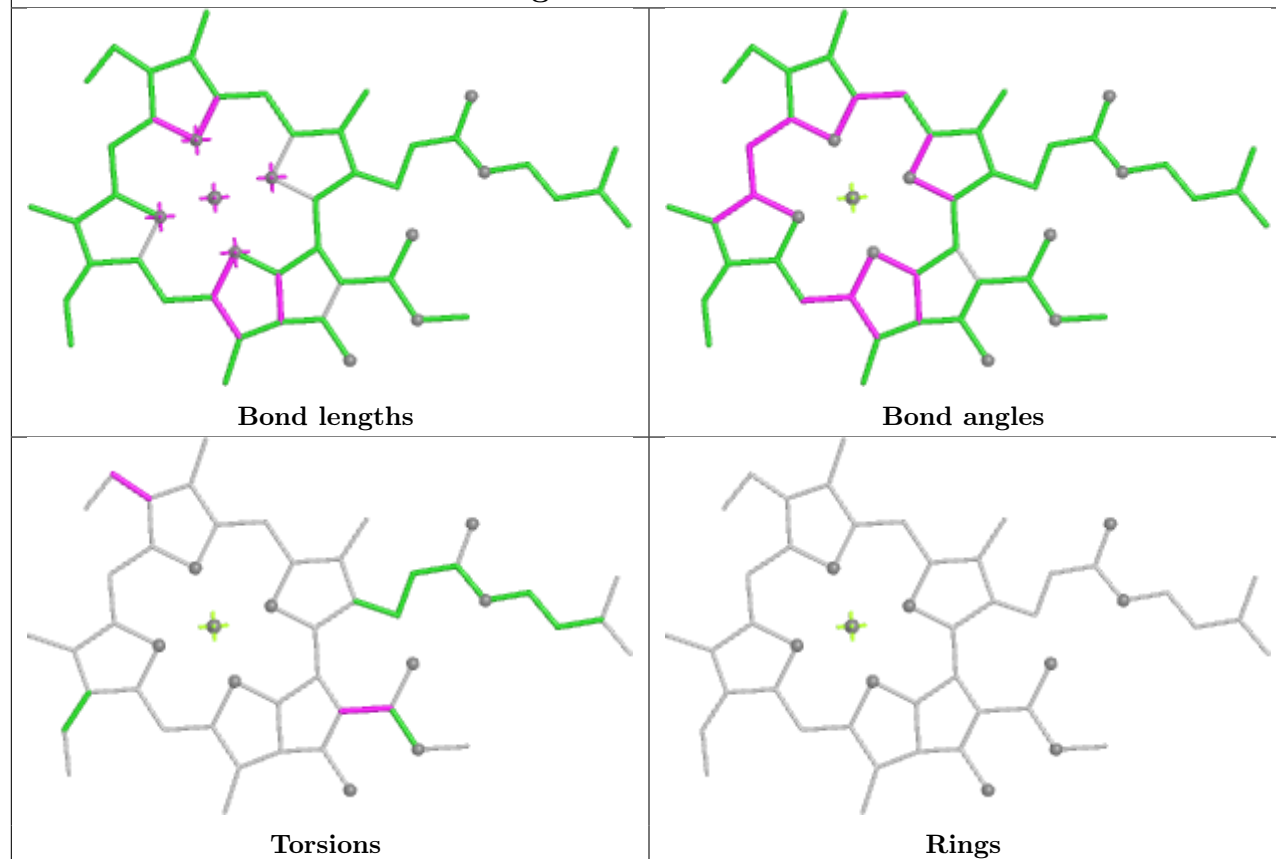
Ligand 8CT 4 616



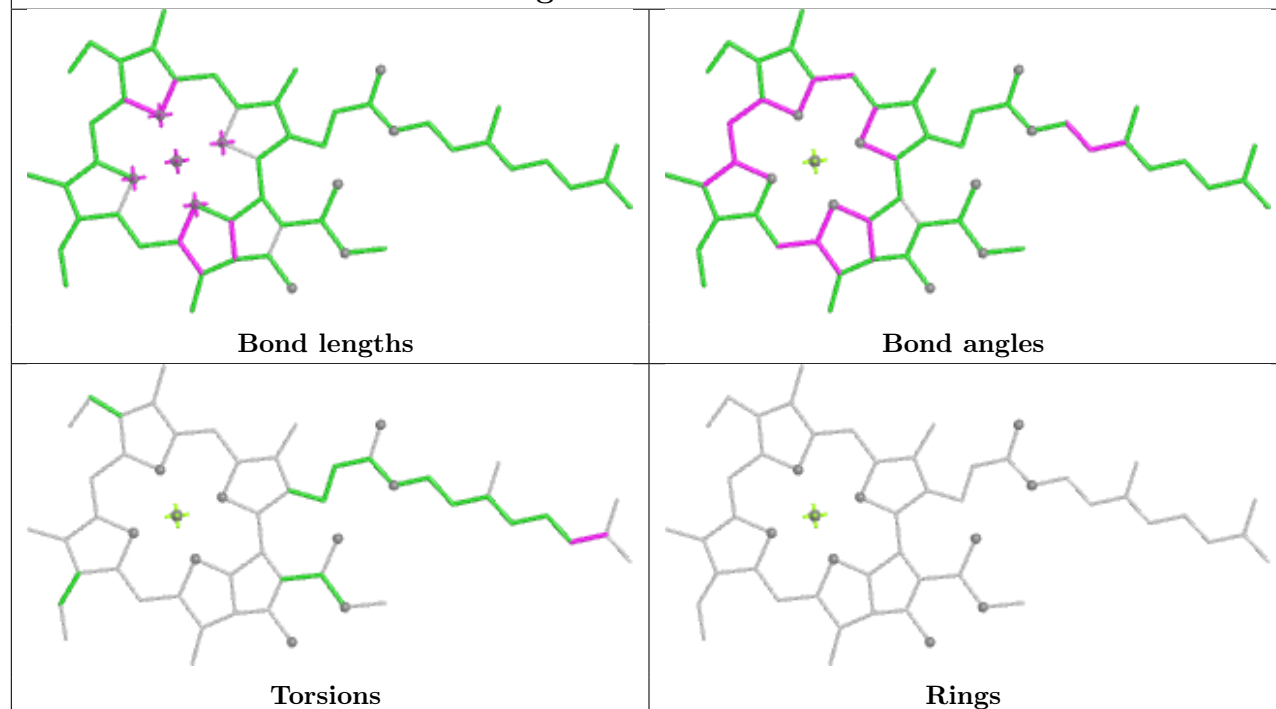




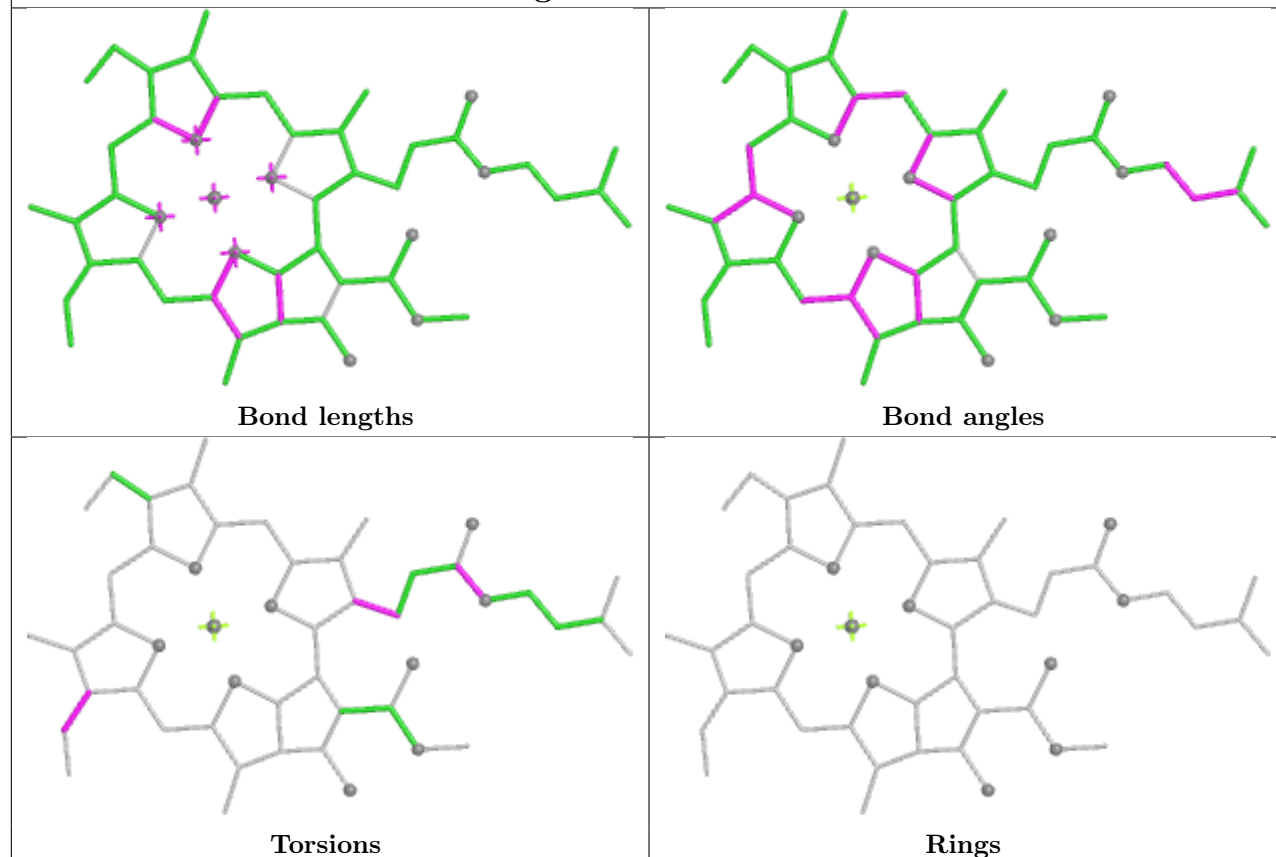
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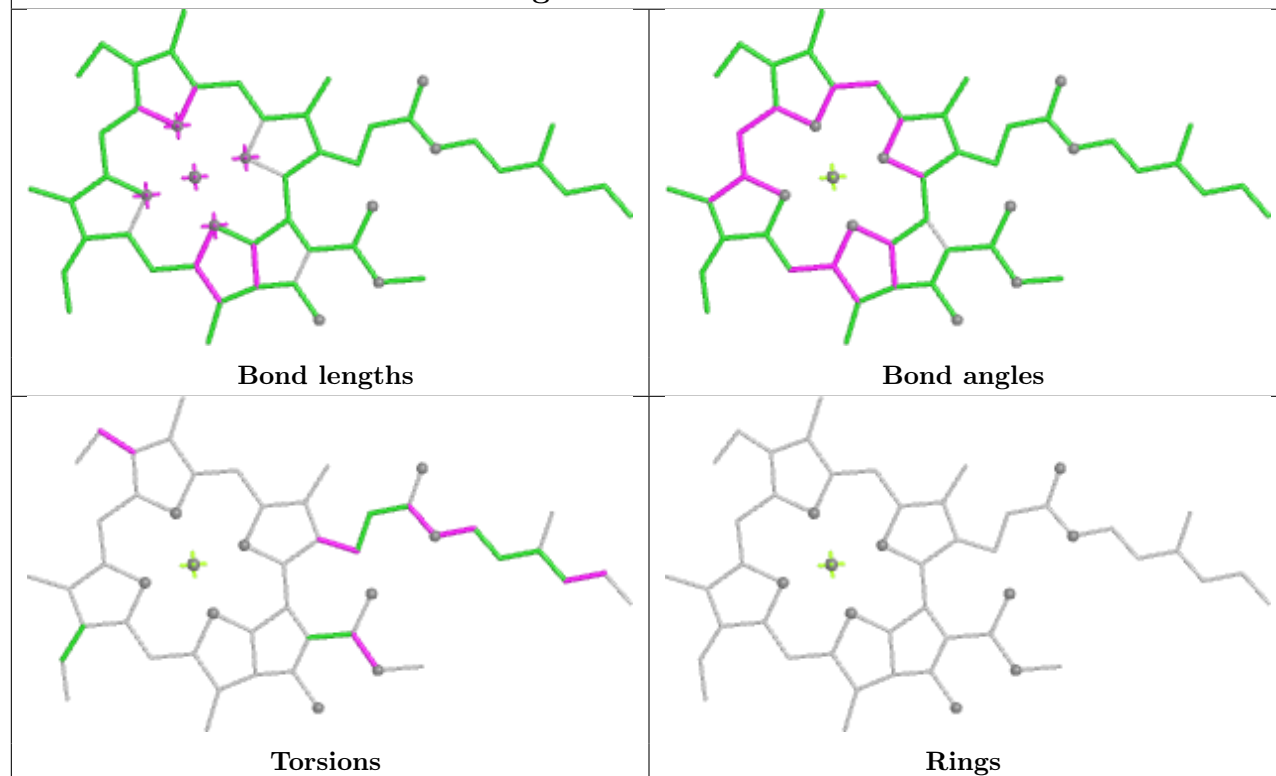
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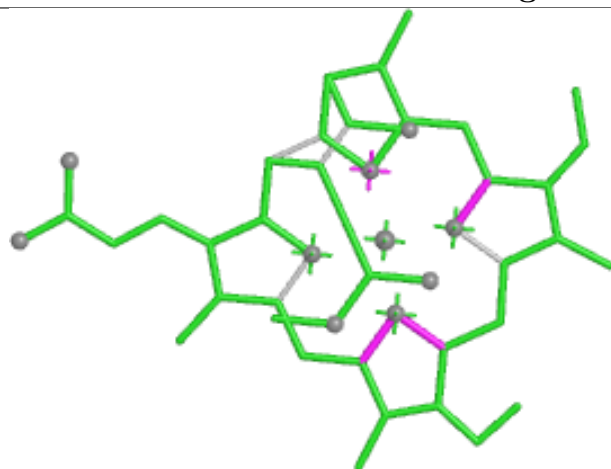
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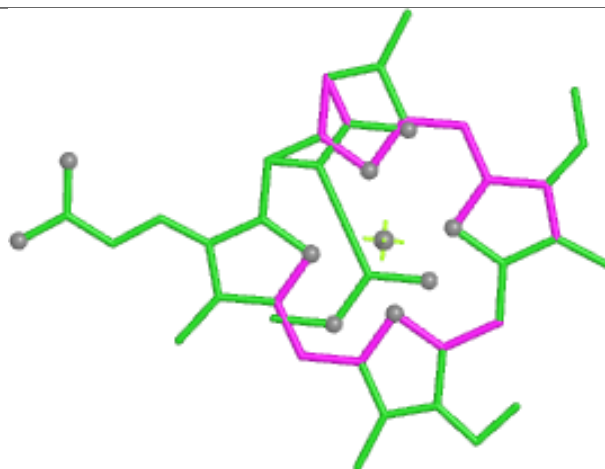
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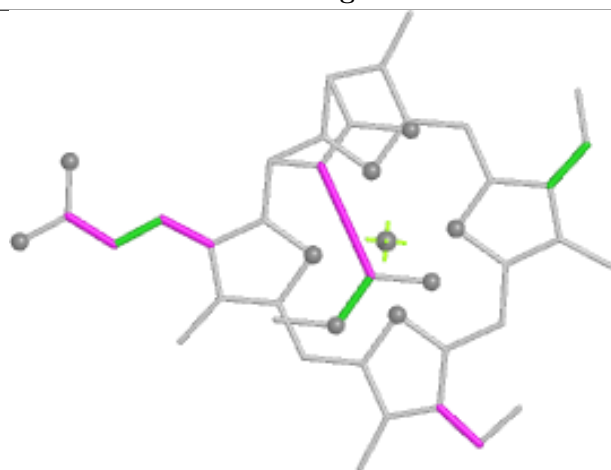
Ligand KC2 b 605



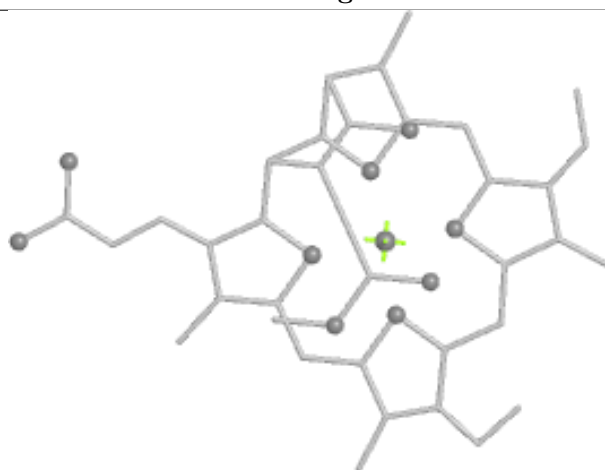
Bond lengths



Bond angles

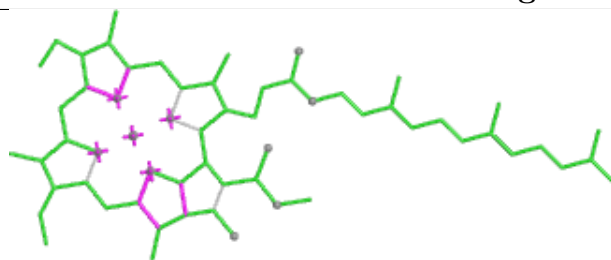


Torsions

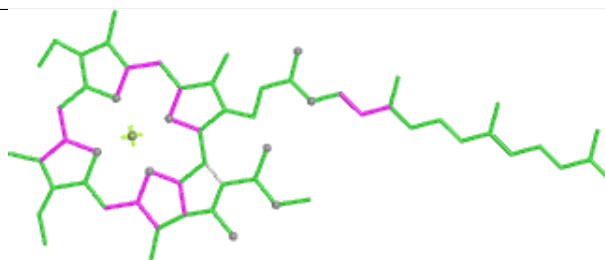


Rings

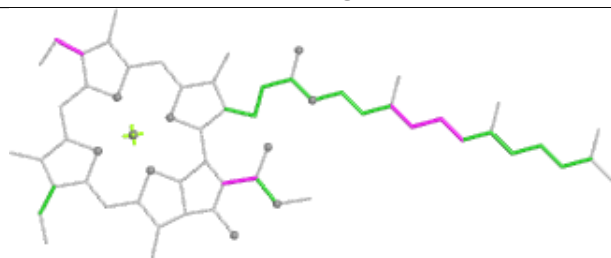
Ligand CLA 4 607



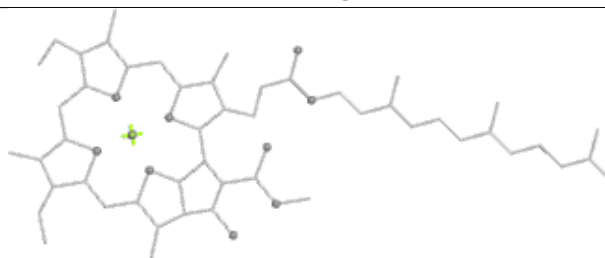
Bond lengths



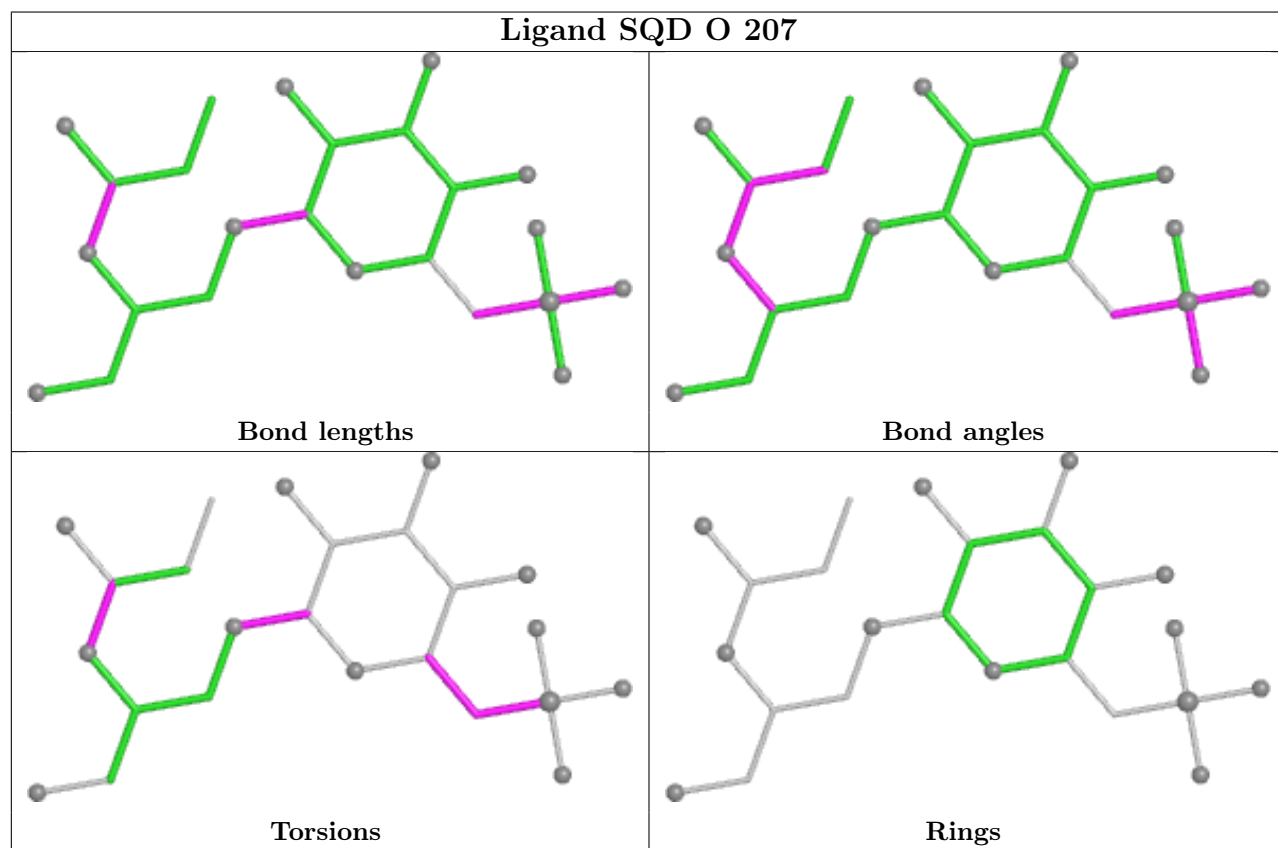
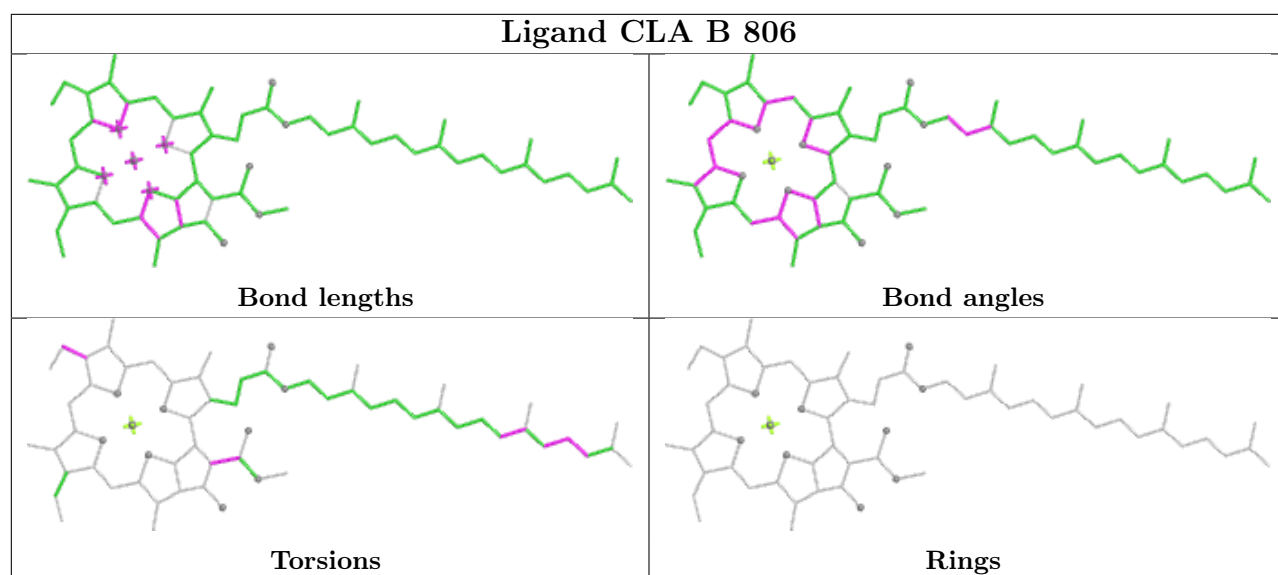
Bond angles

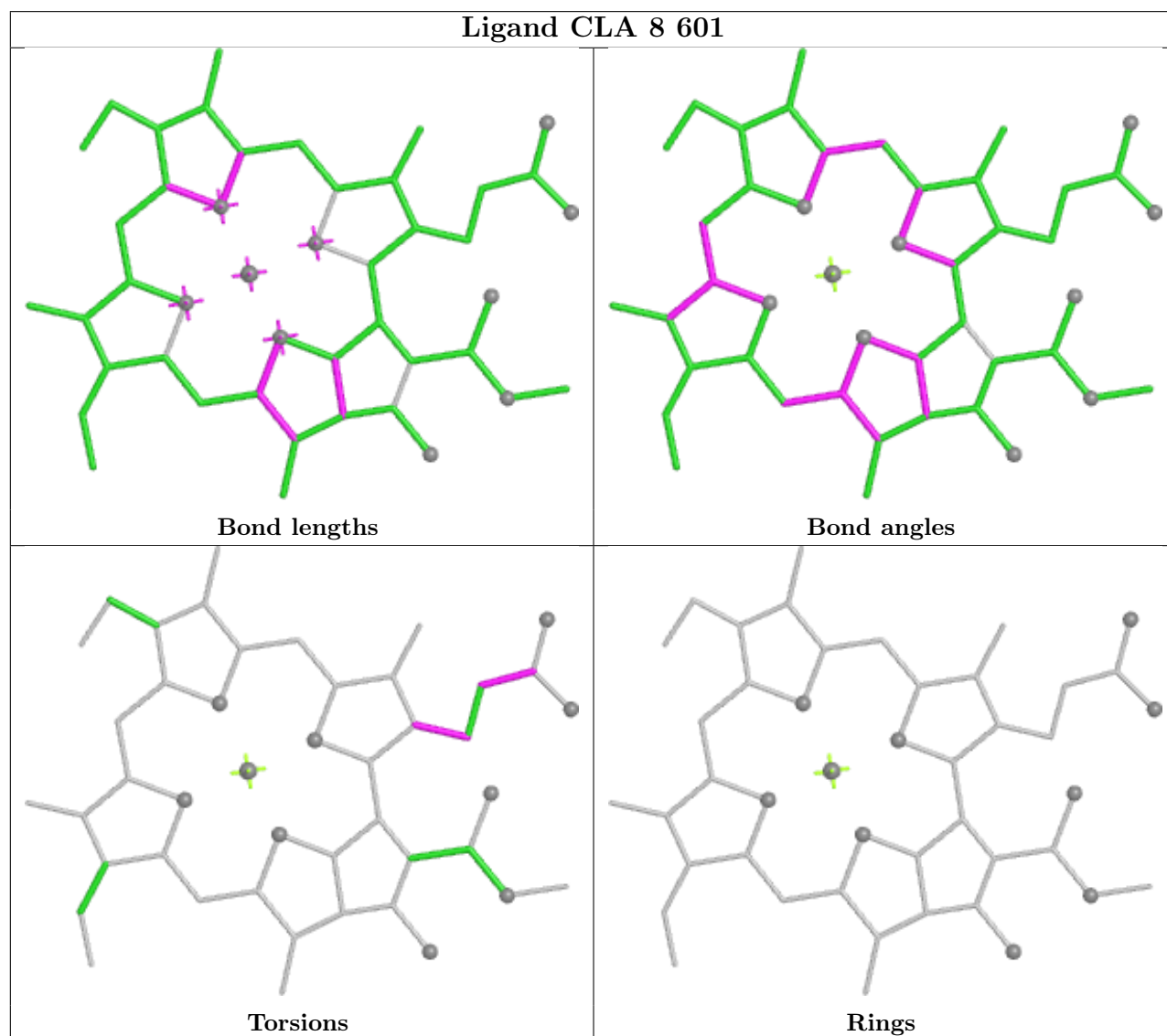
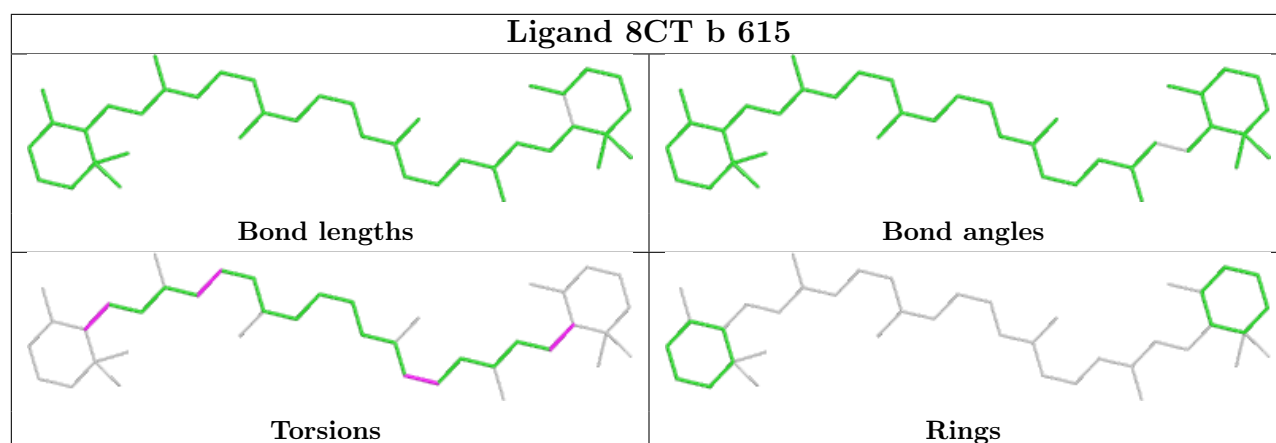


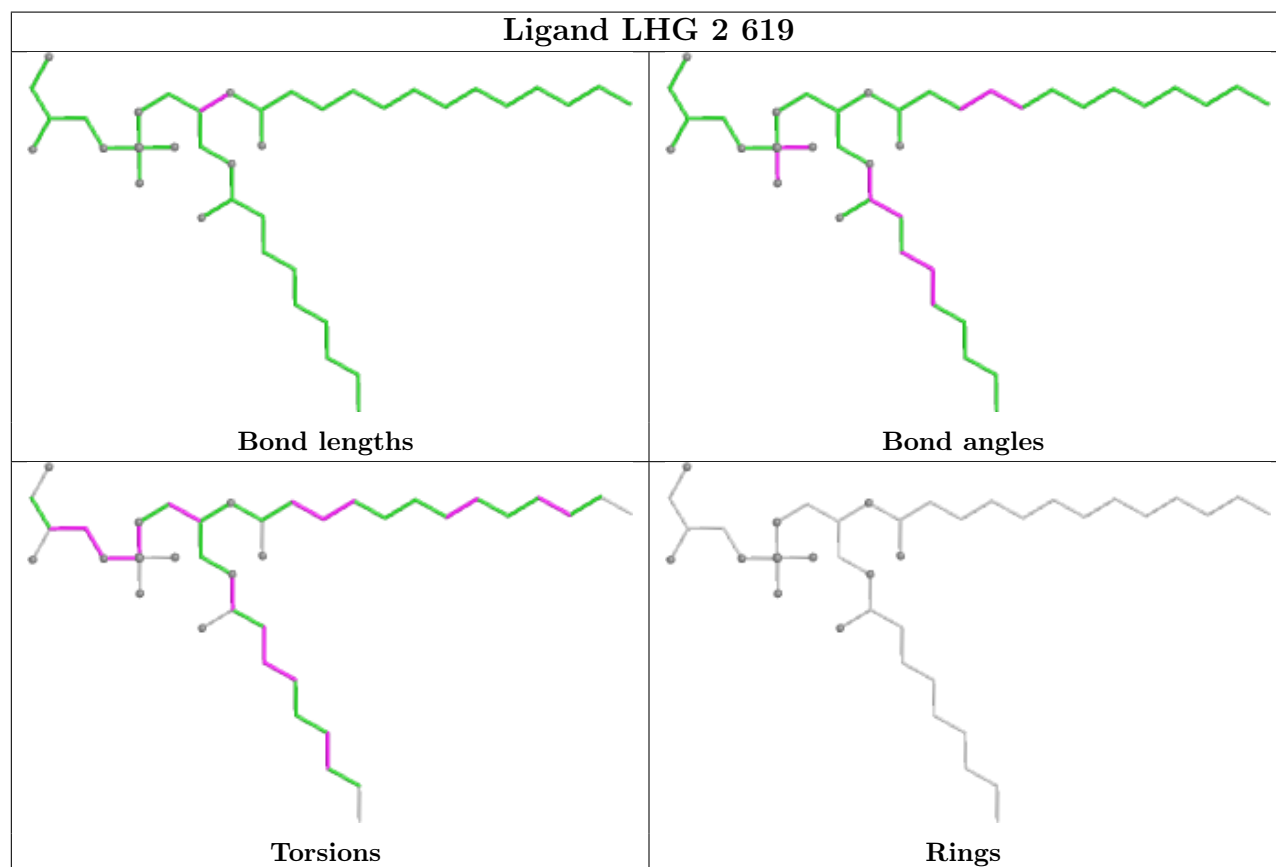
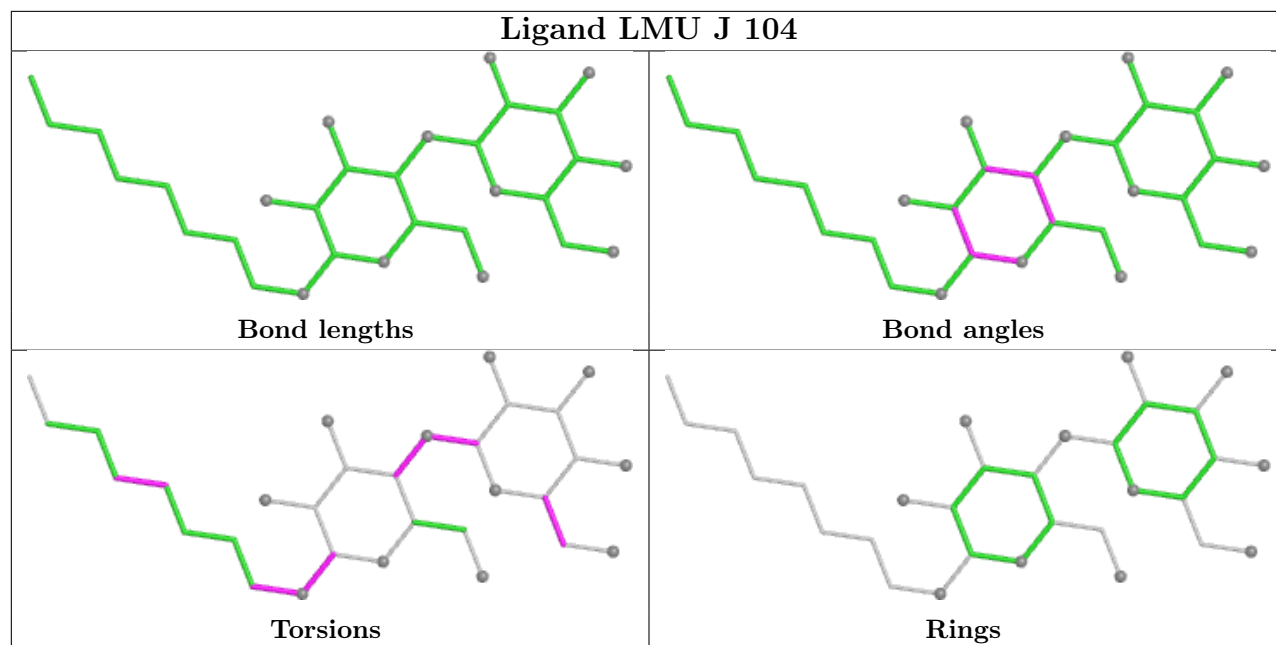
Torsions



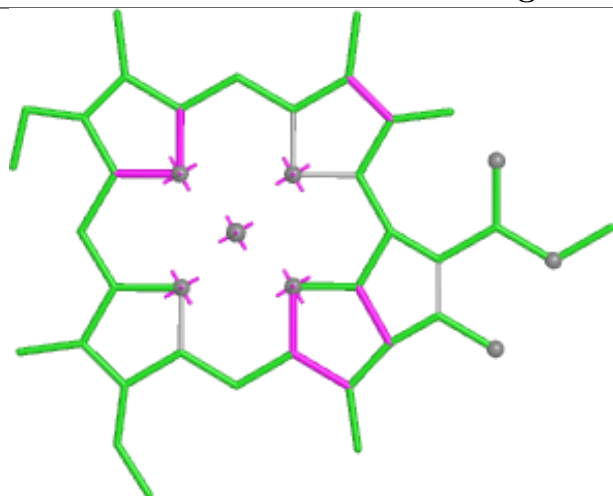
Rings



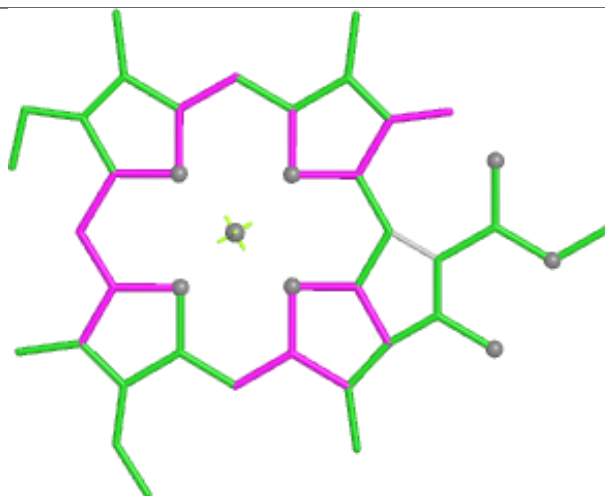




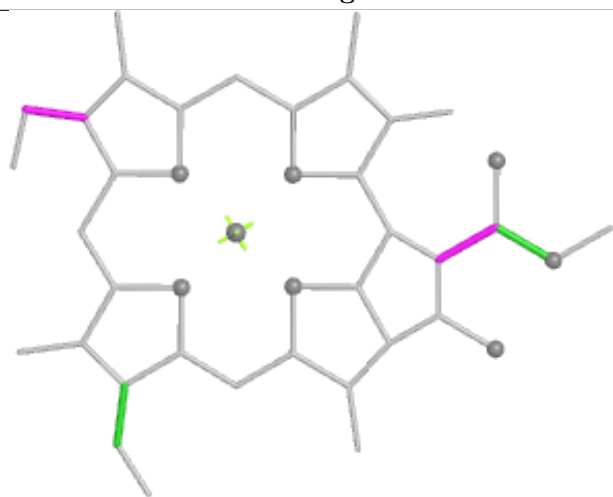
Ligand CLA J 102



Bond lengths



Bond angles

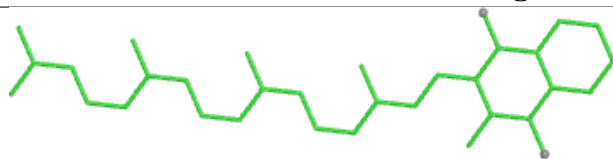


Torsions

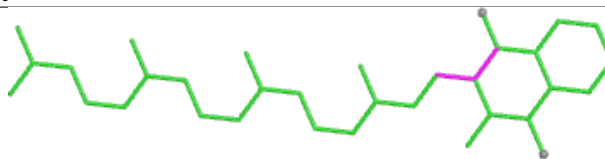


Rings

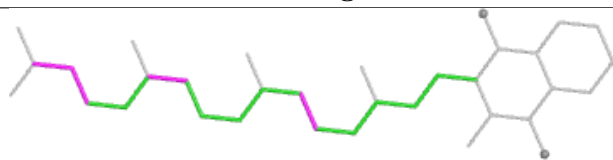
Ligand PQN B 842



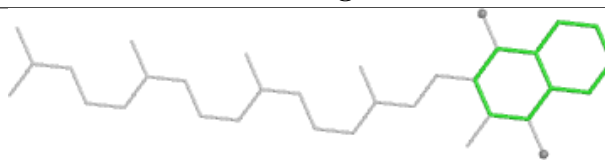
Bond lengths



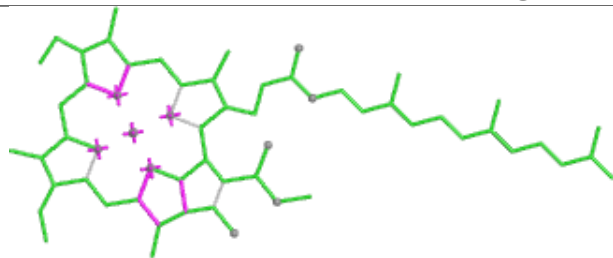
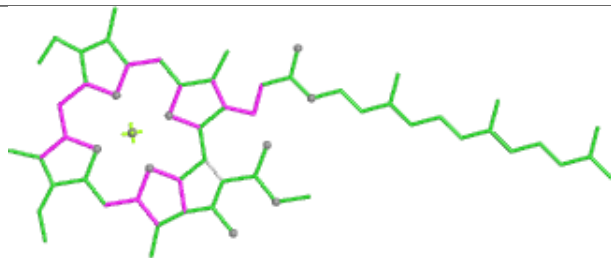
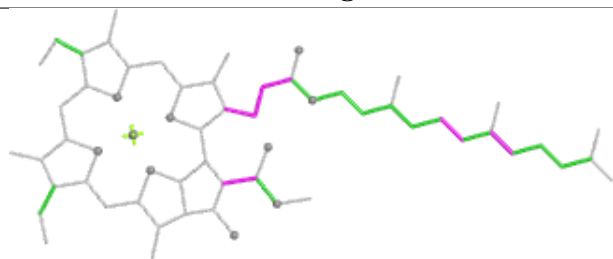
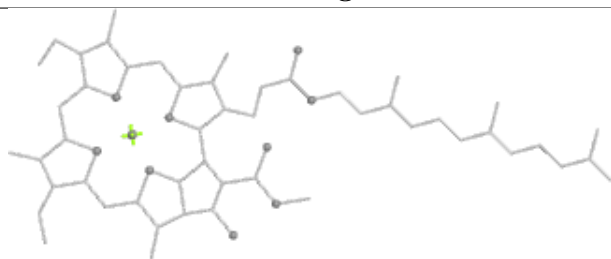
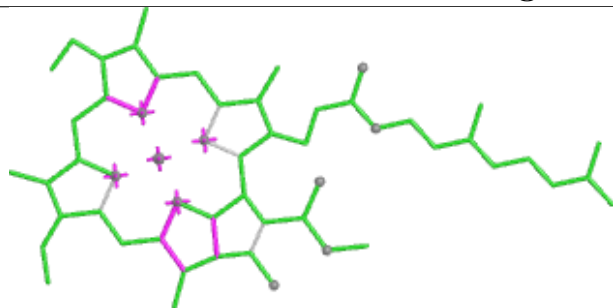
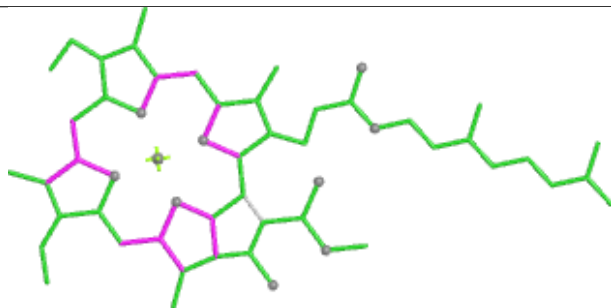
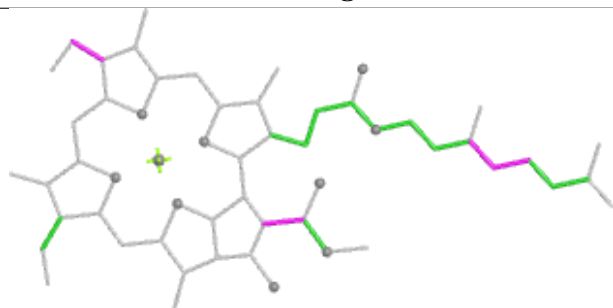
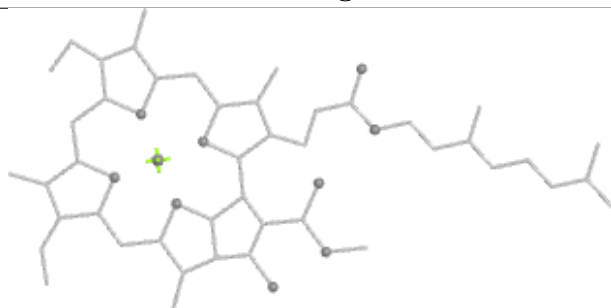
Bond angles



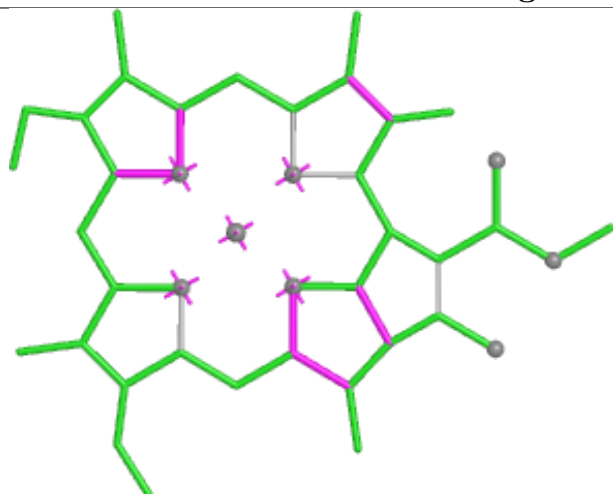
Torsions



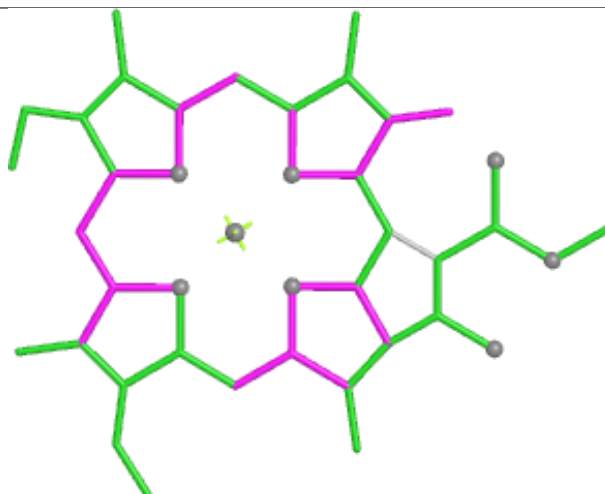
Rings

Ligand CLA B 819**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 5 602****Bond lengths****Bond angles****Torsions****Rings**

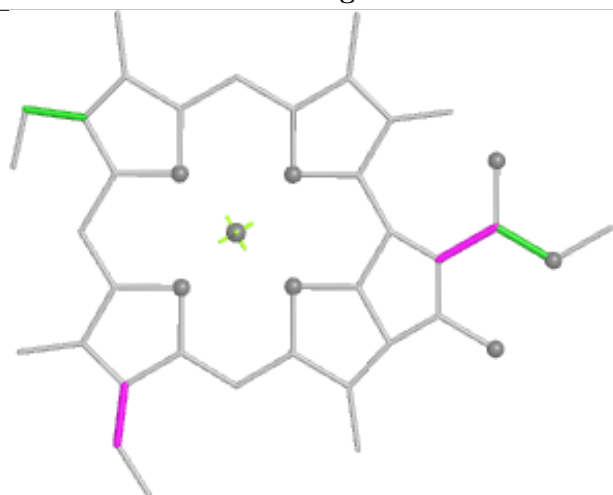
Ligand CLA 9 609



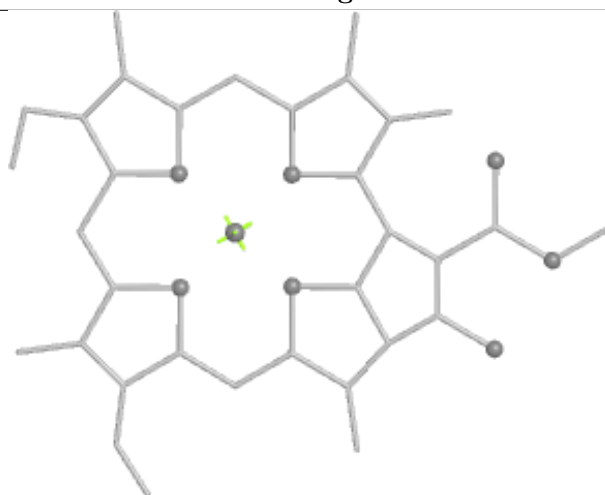
Bond lengths



Bond angles

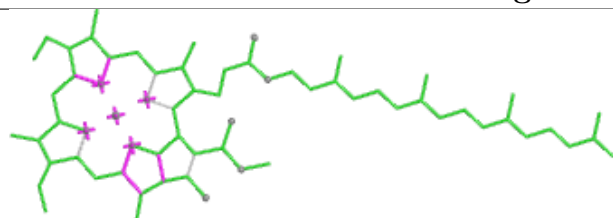


Torsions

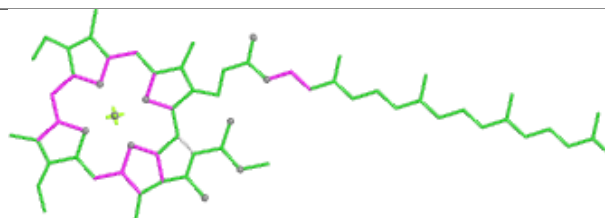


Rings

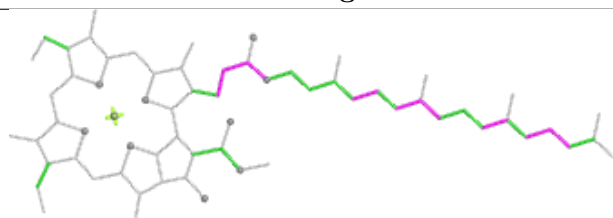
Ligand CLA A 839



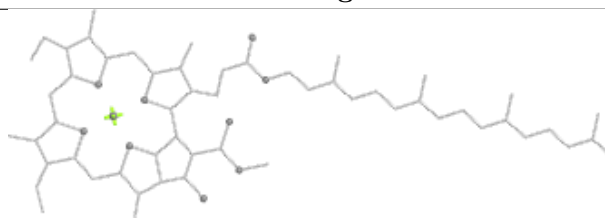
Bond lengths



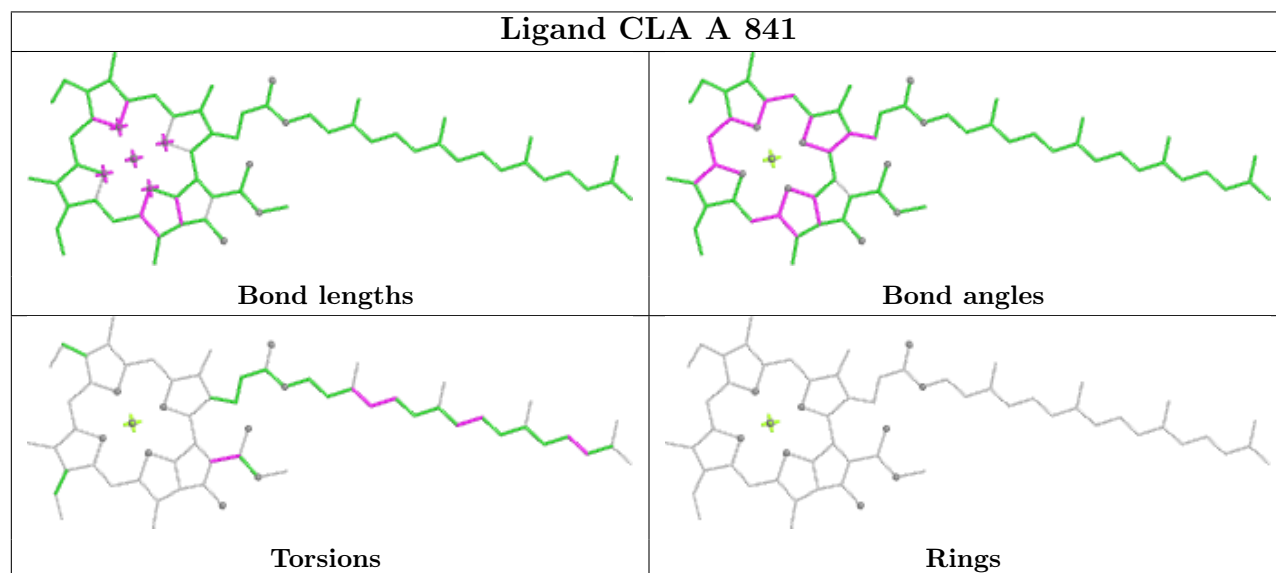
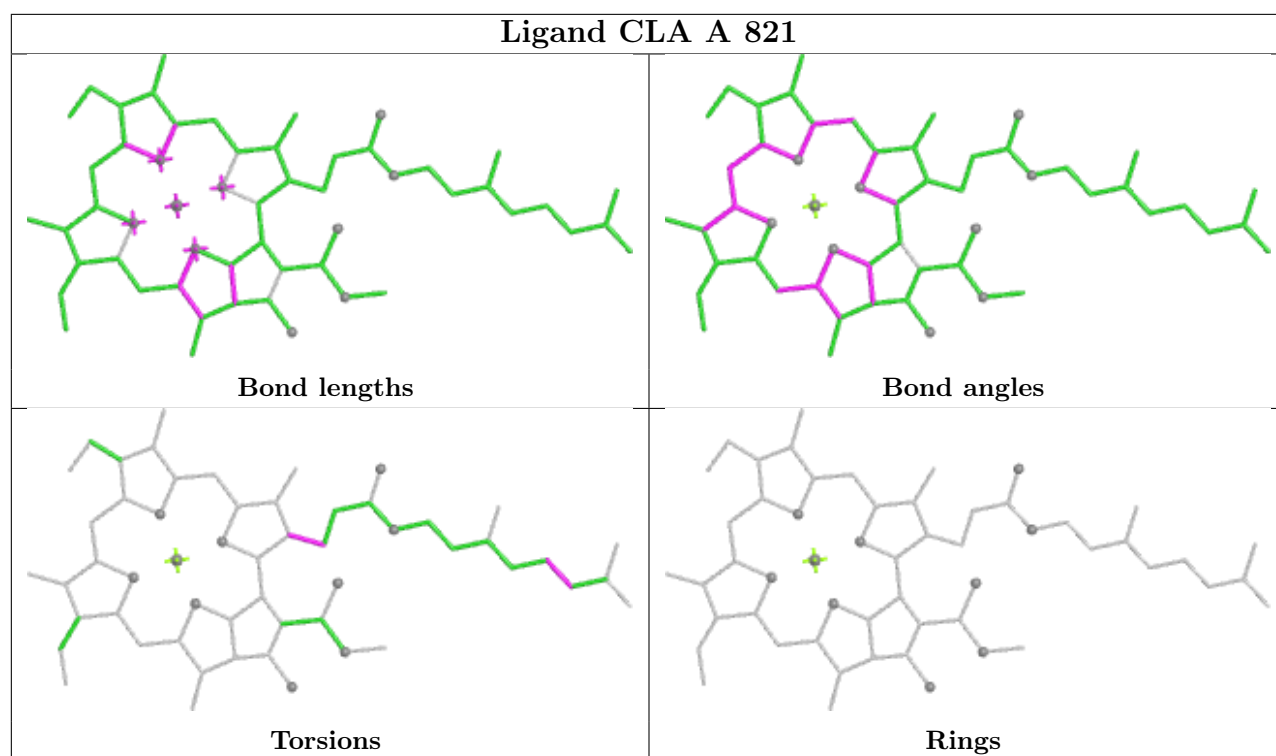
Bond angles

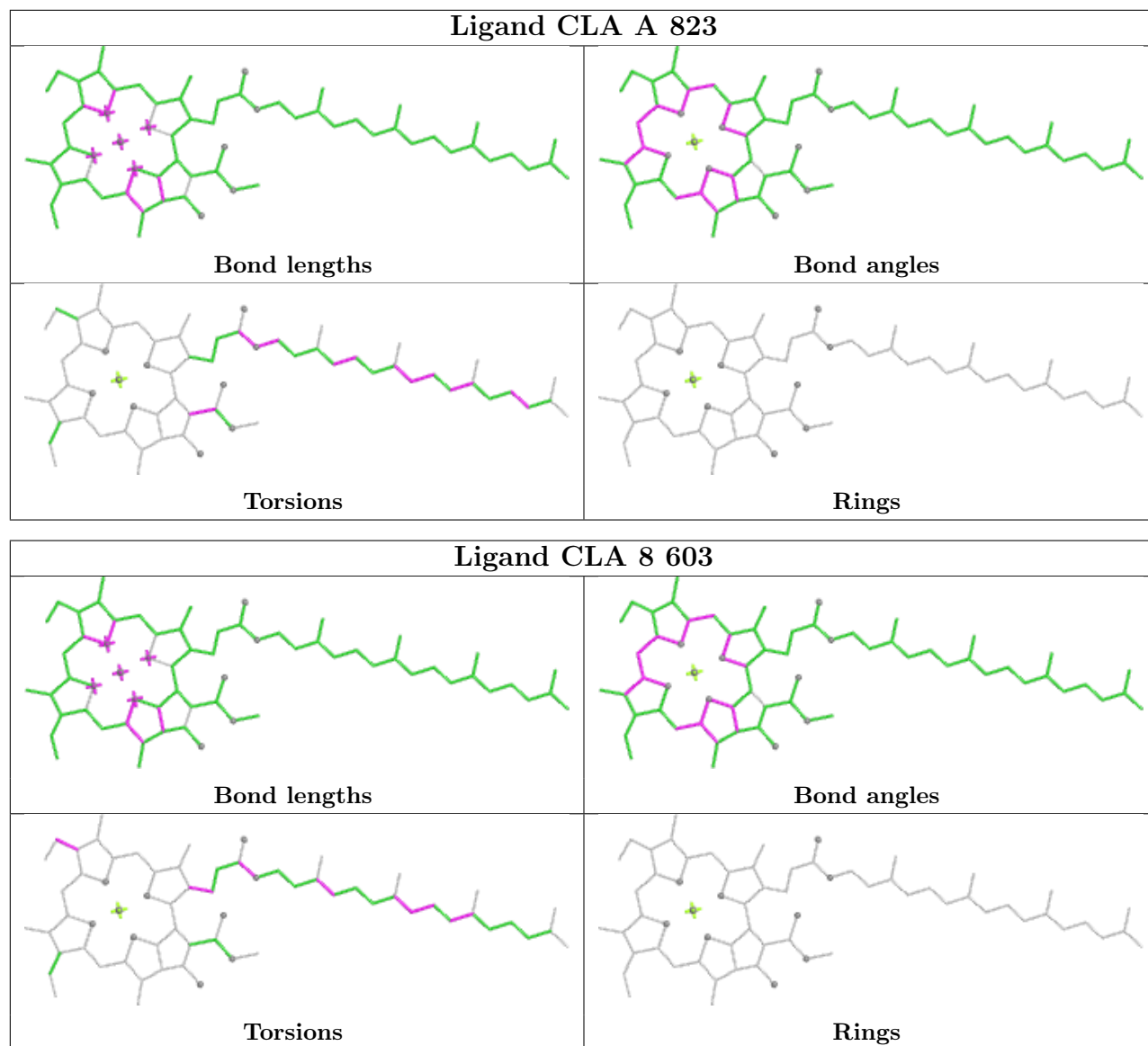


Torsions

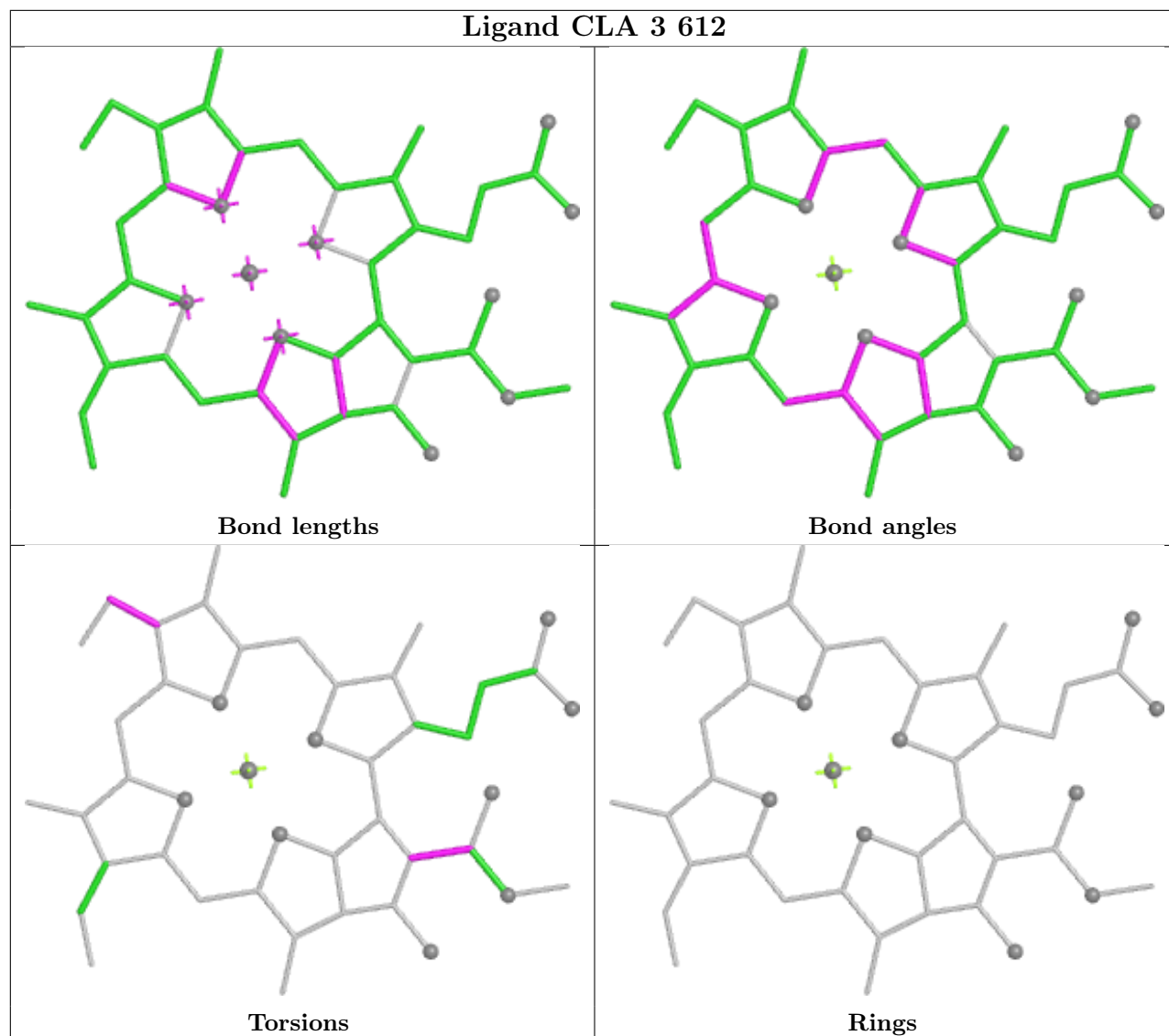


Rings

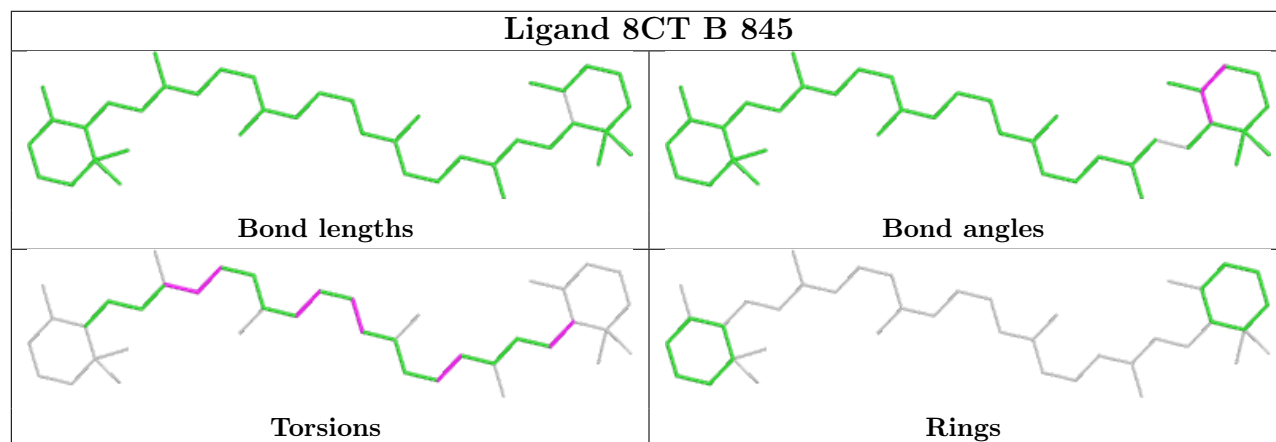




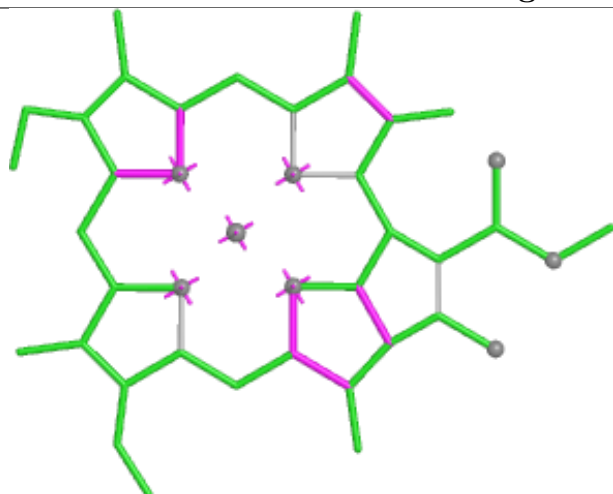
Ligand CLA 3 612



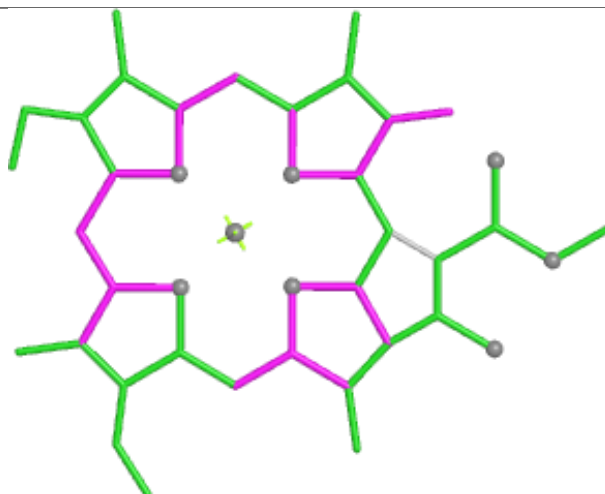
Ligand 8CT B 845



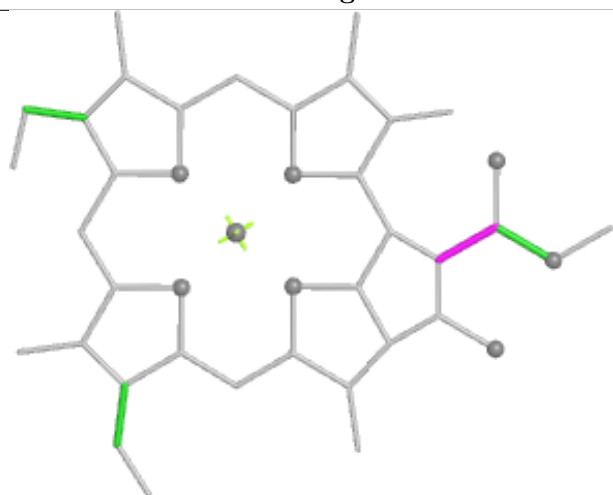
Ligand CLA 9 611



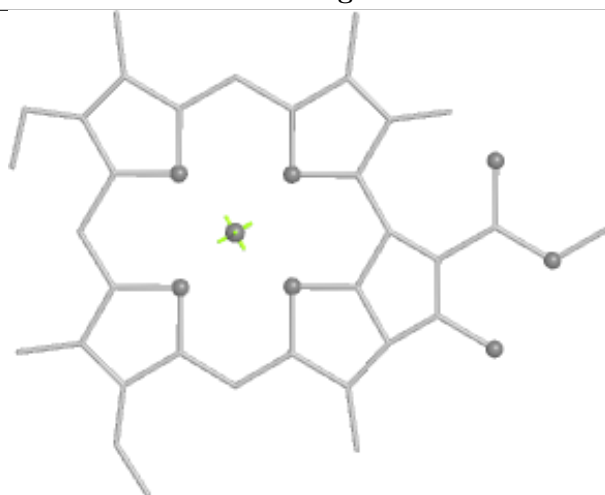
Bond lengths



Bond angles

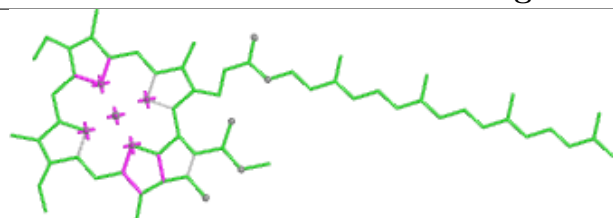


Torsions

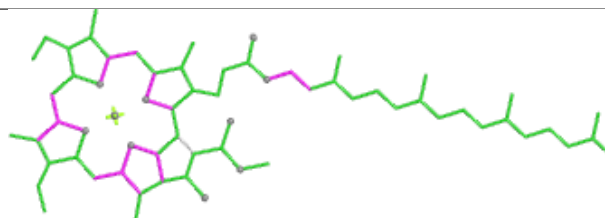


Rings

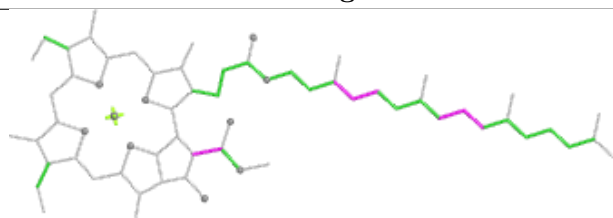
Ligand CLA B 822



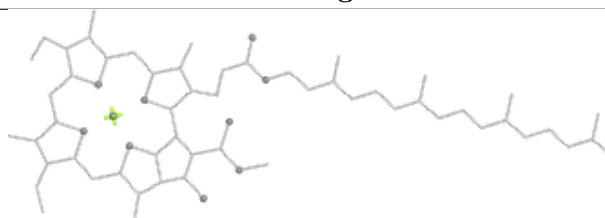
Bond lengths



Bond angles

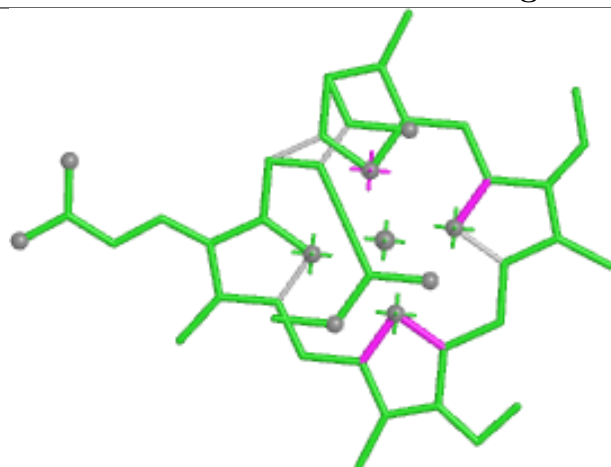


Torsions

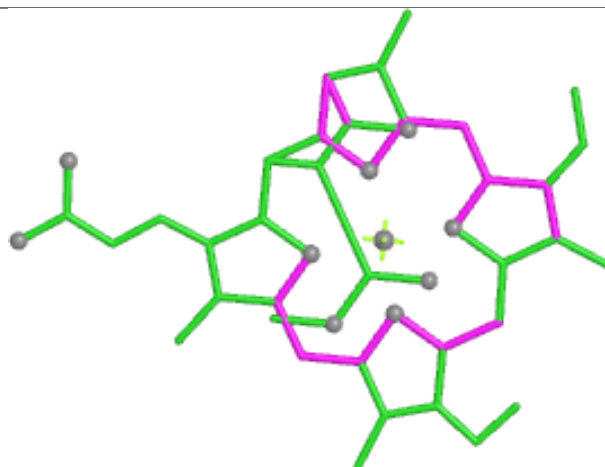


Rings

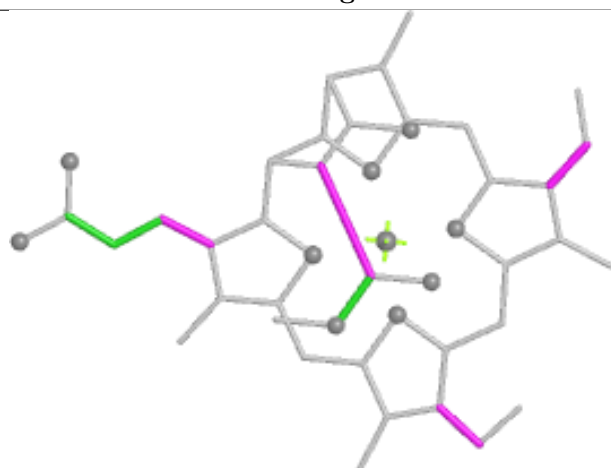
Ligand KC2 3 606



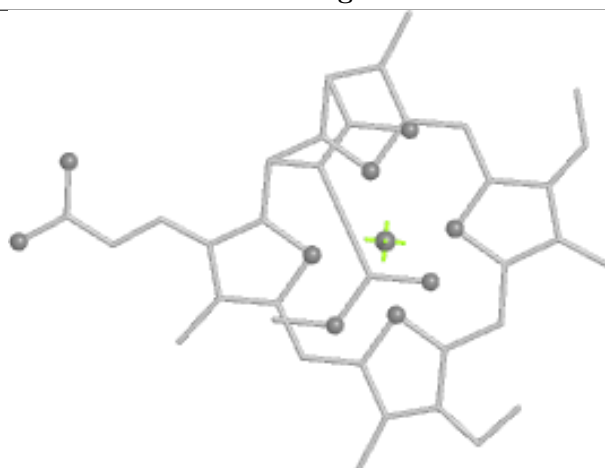
Bond lengths



Bond angles

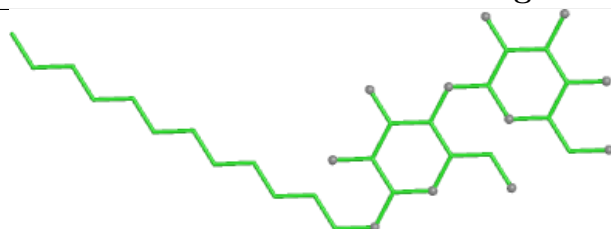


Torsions

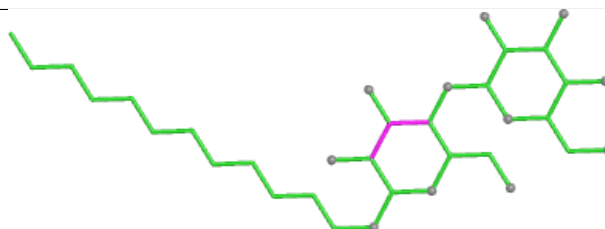


Rings

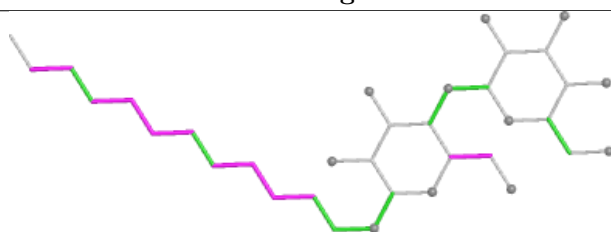
Ligand LMU 7 321



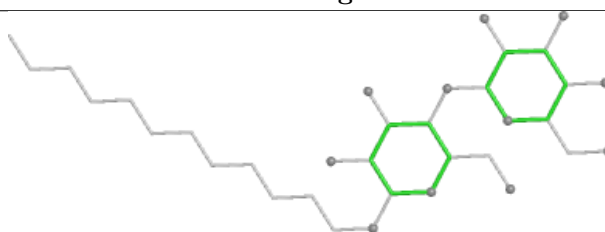
Bond lengths



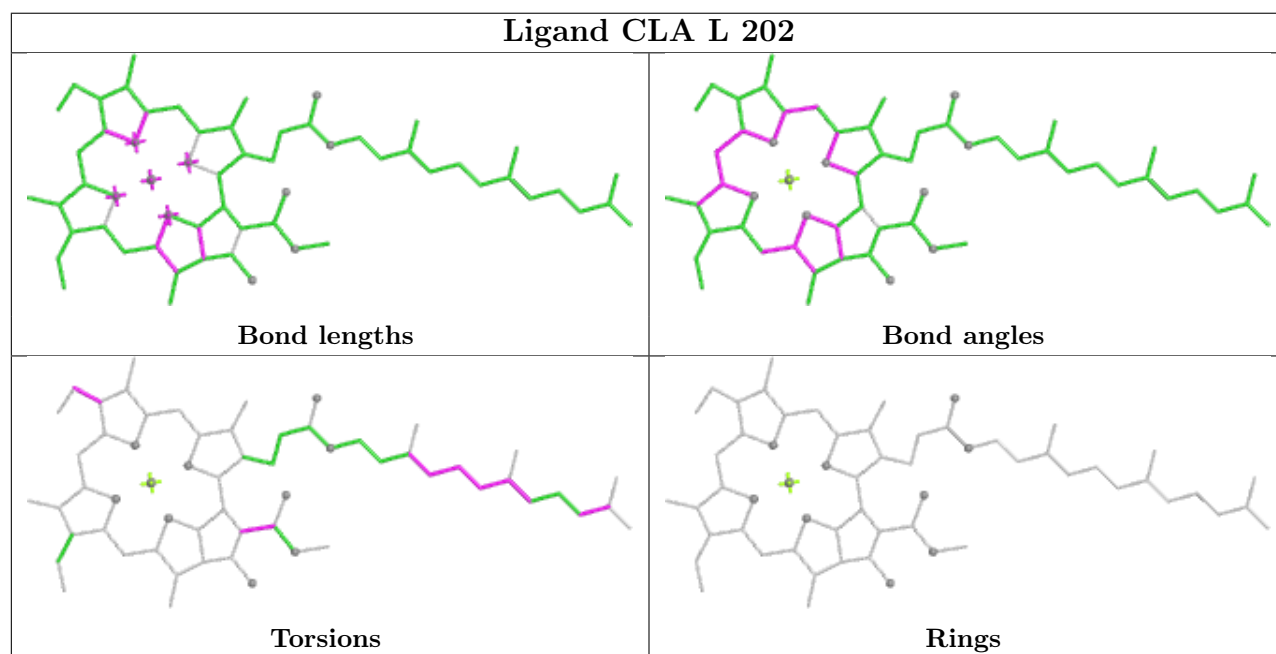
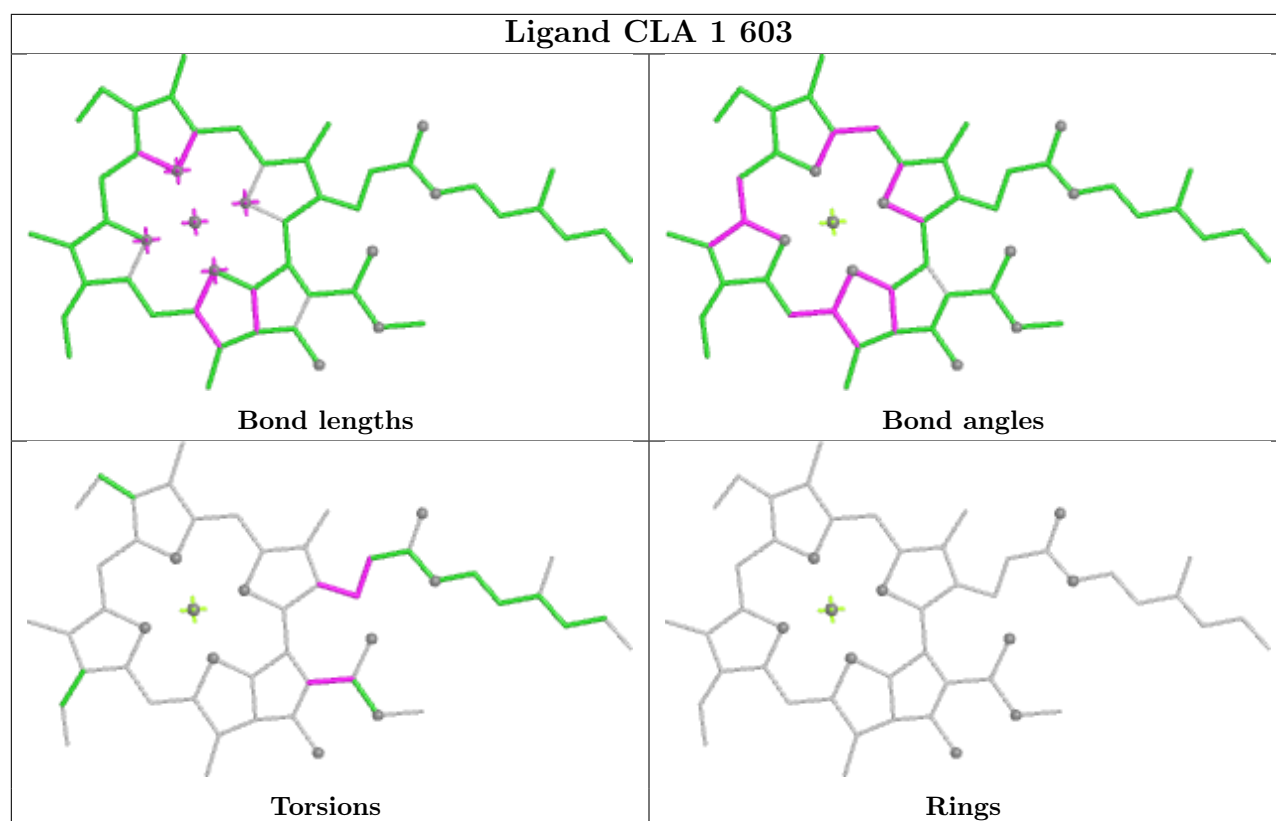
Bond angles



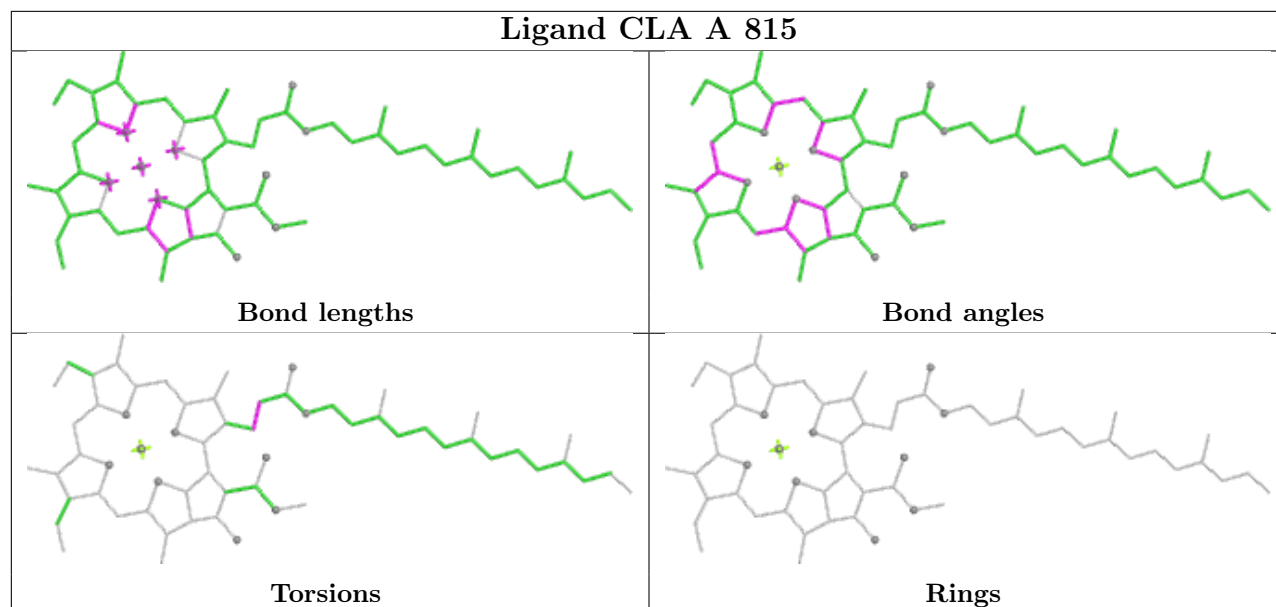
Torsions



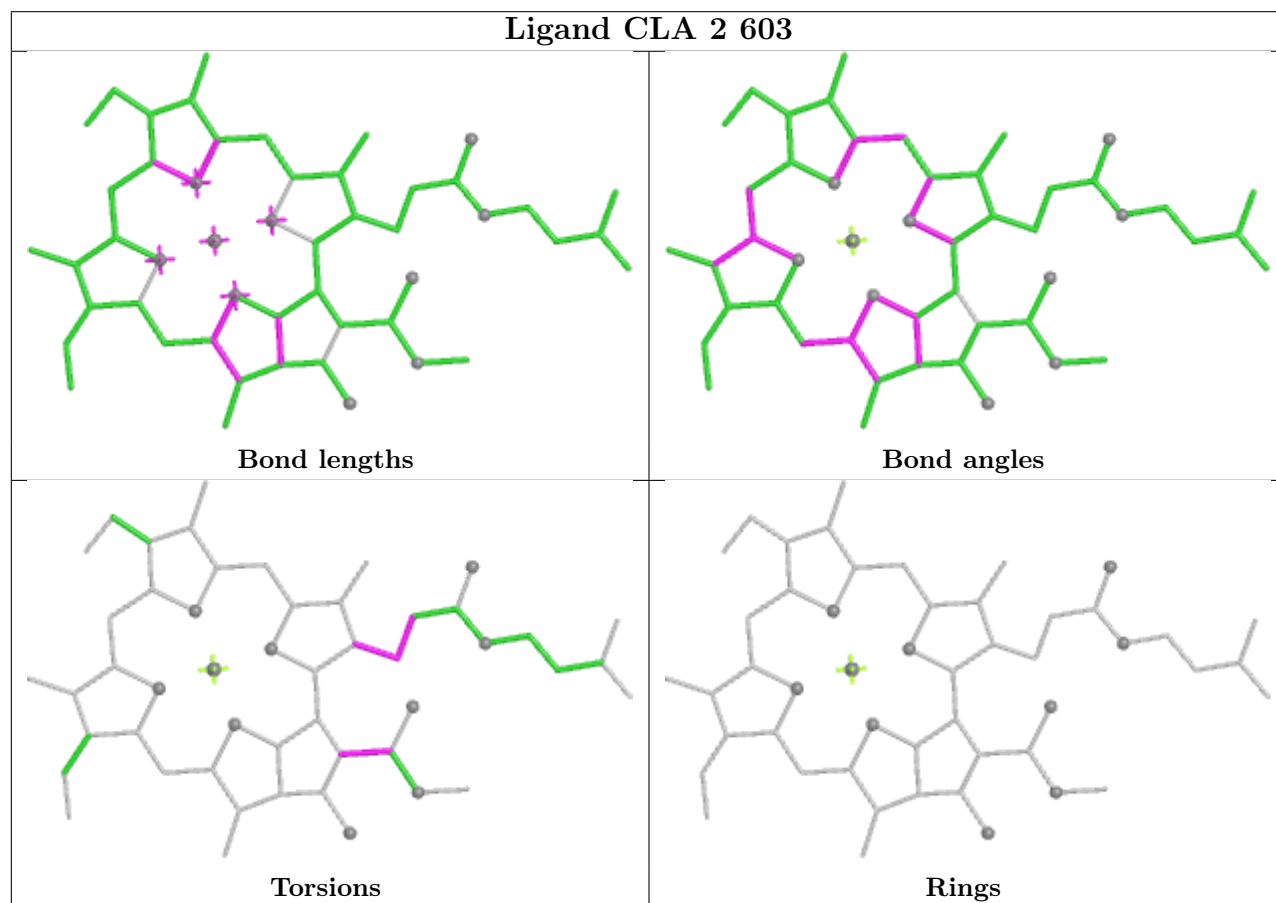
Rings

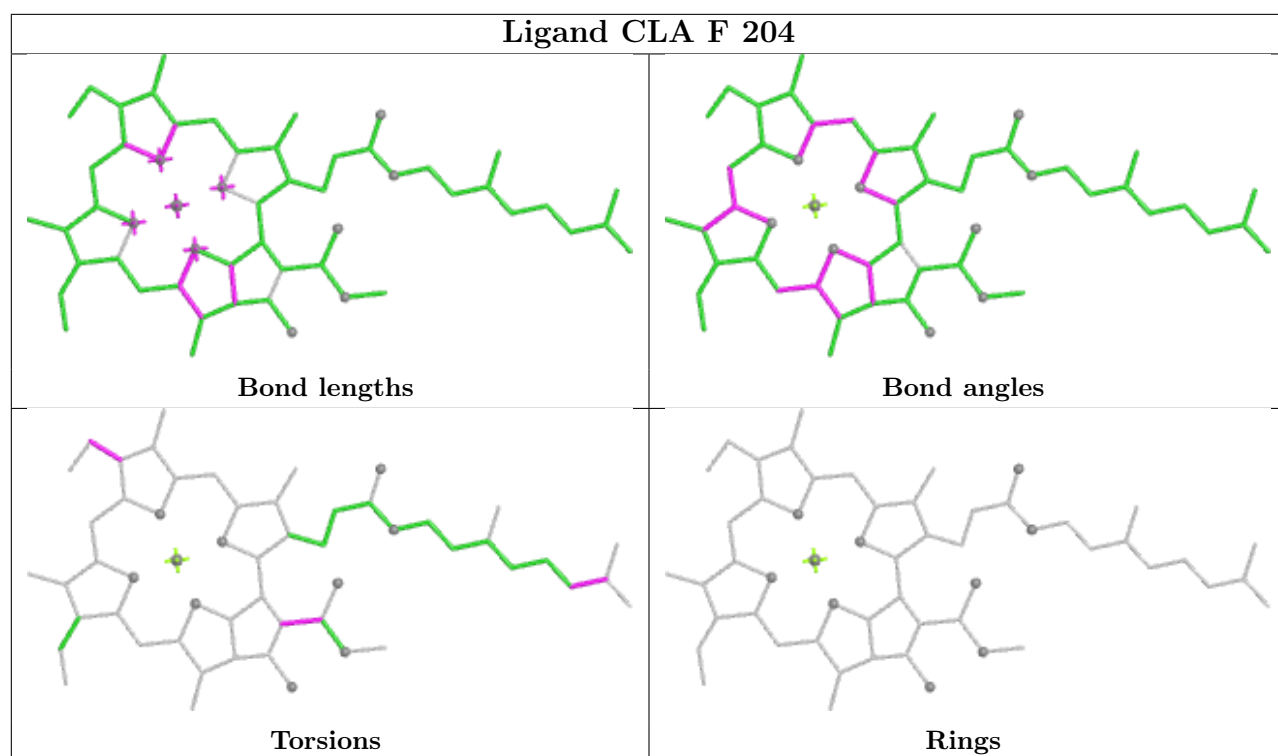


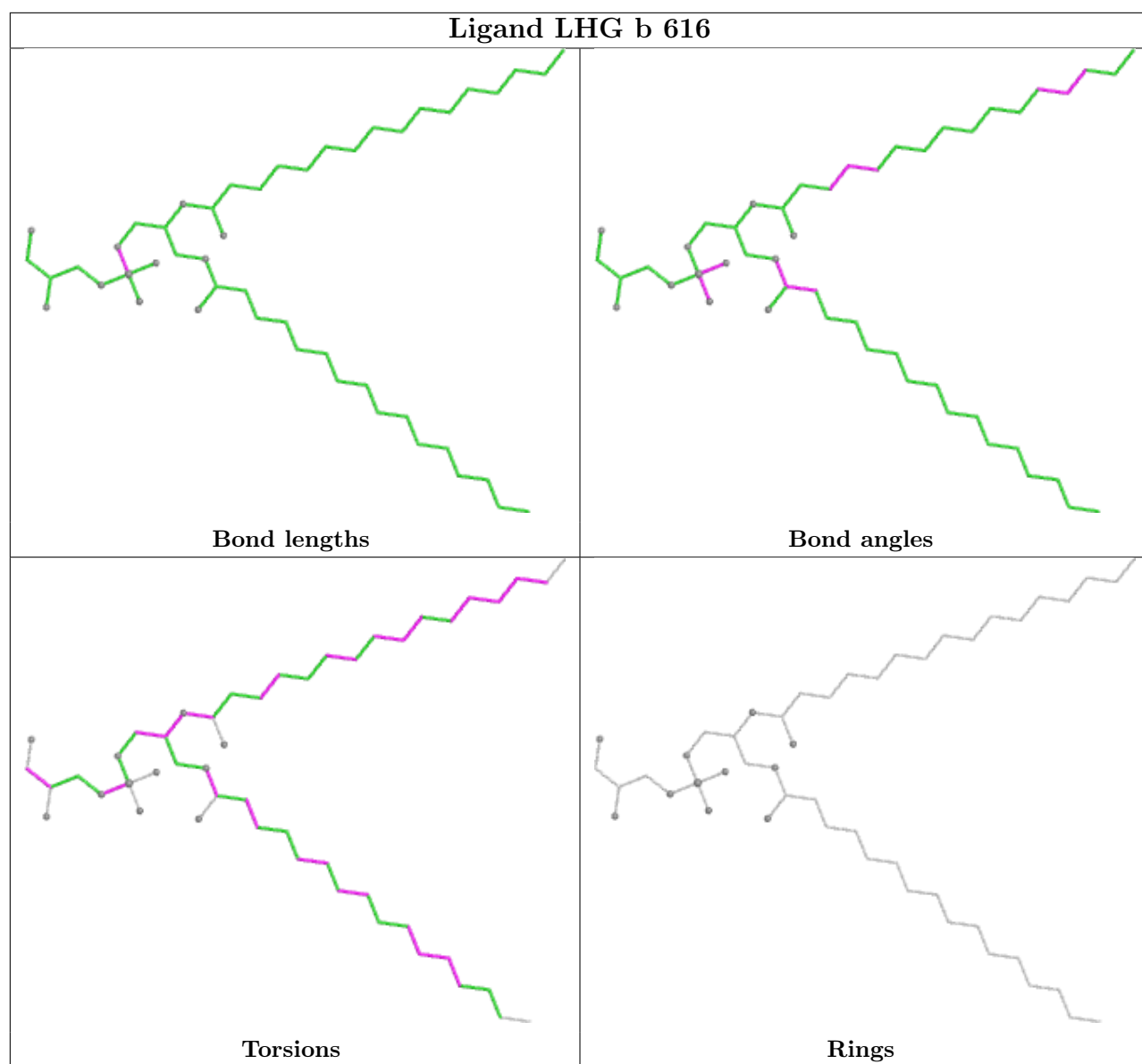
Ligand CLA A 815

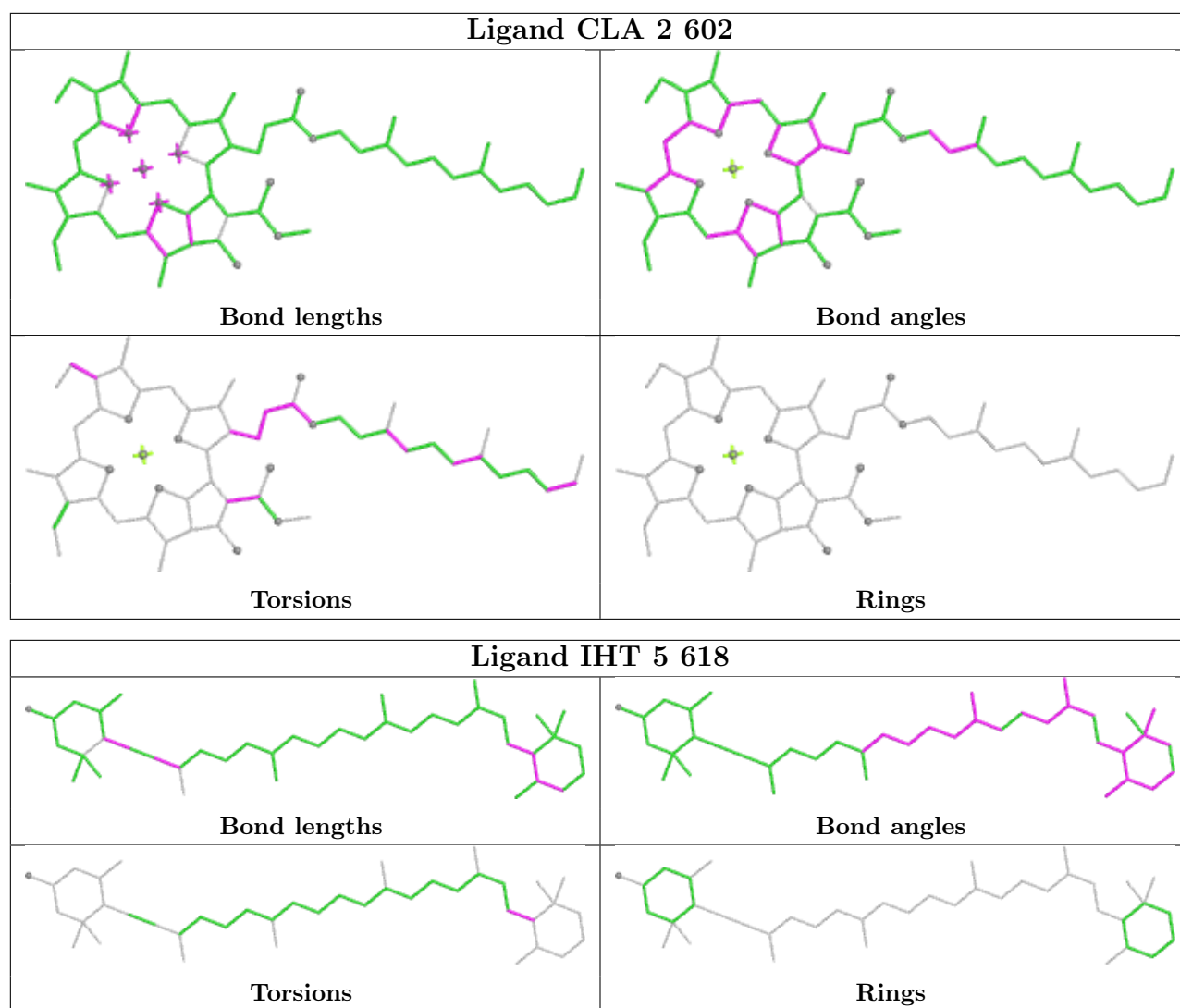


Ligand CLA 2 603

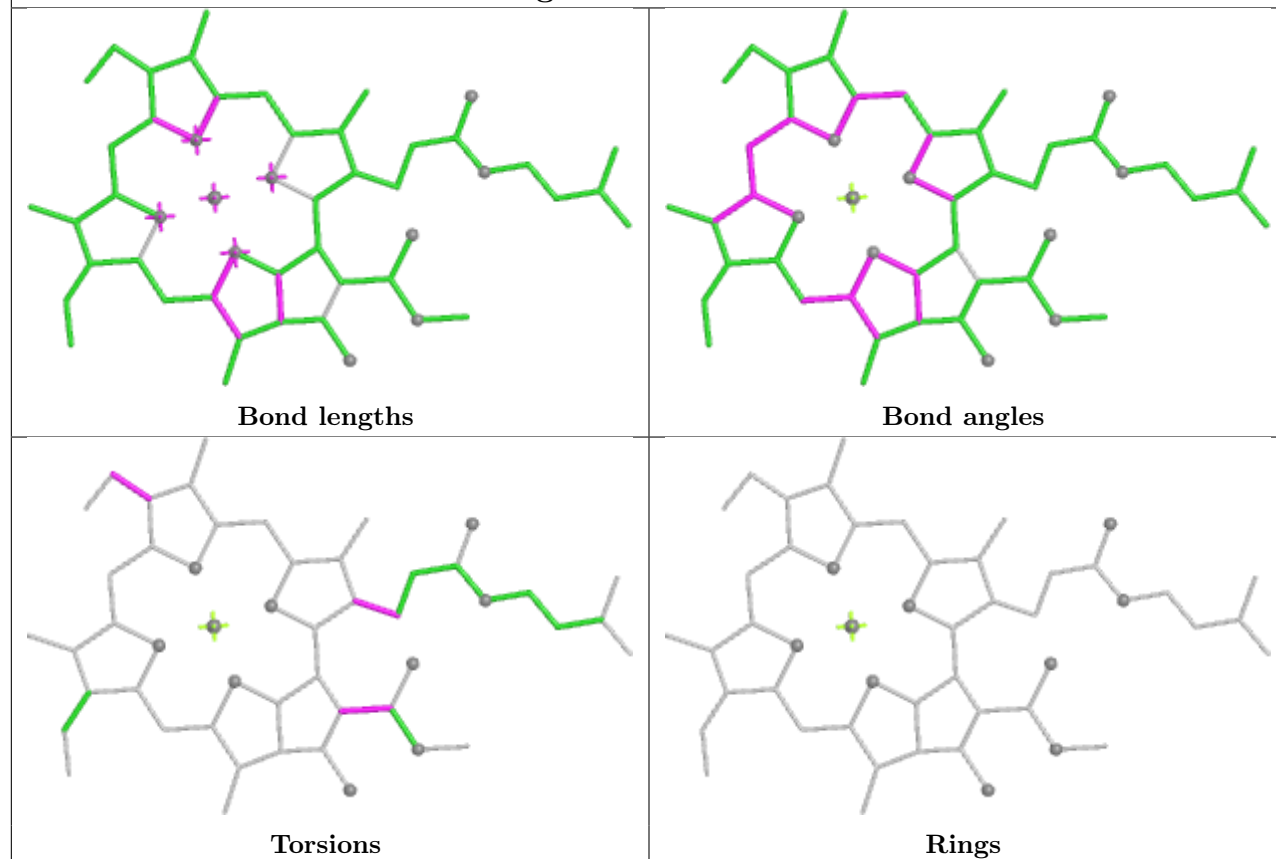




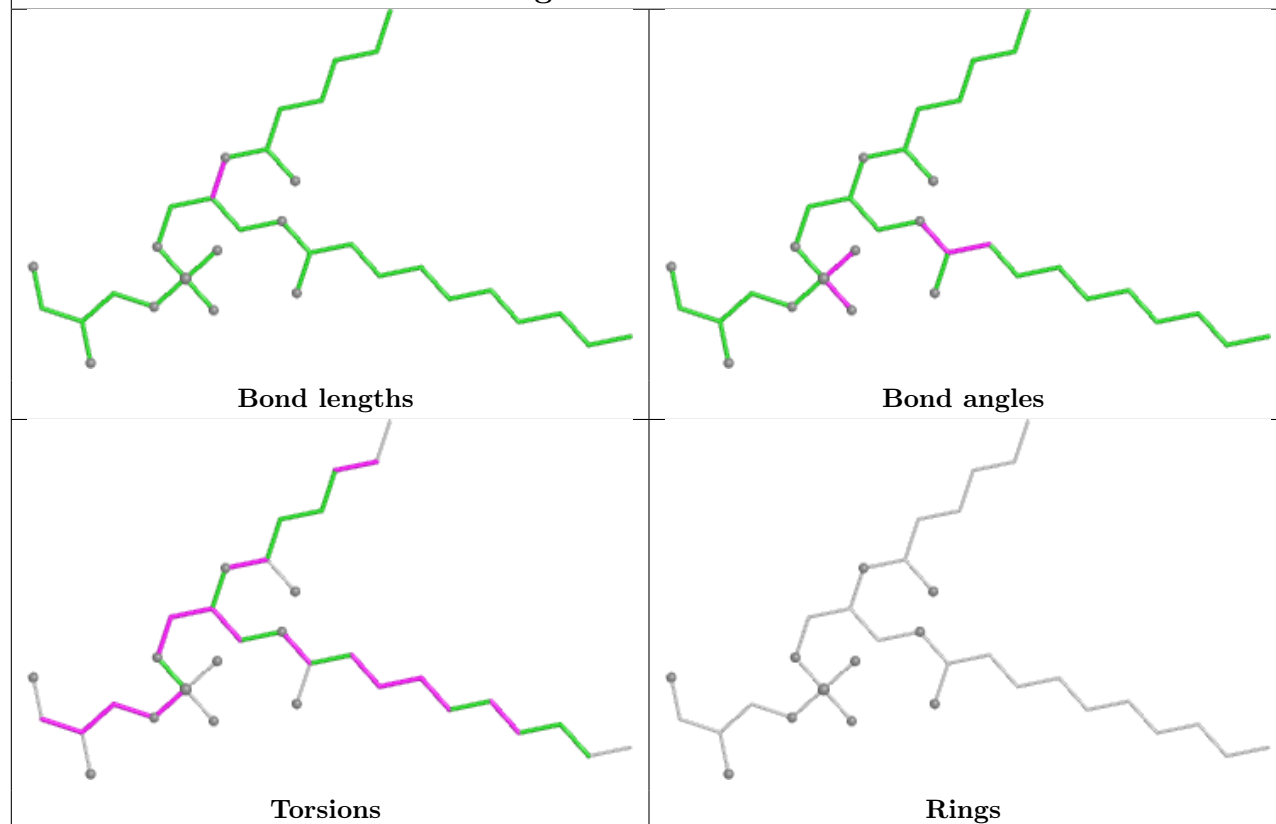


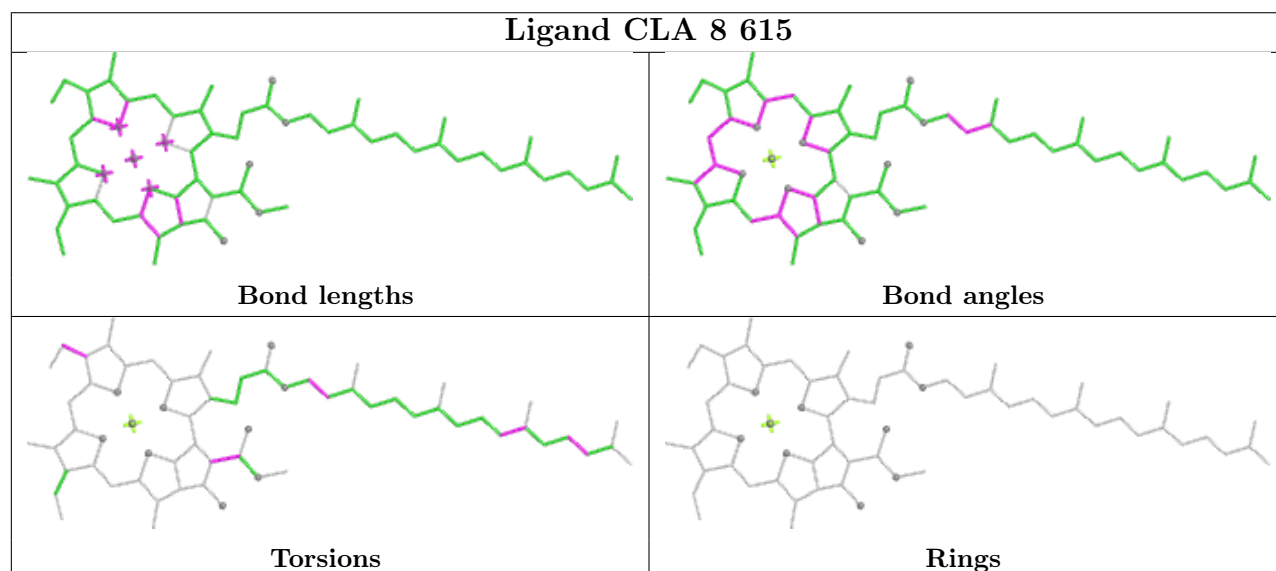
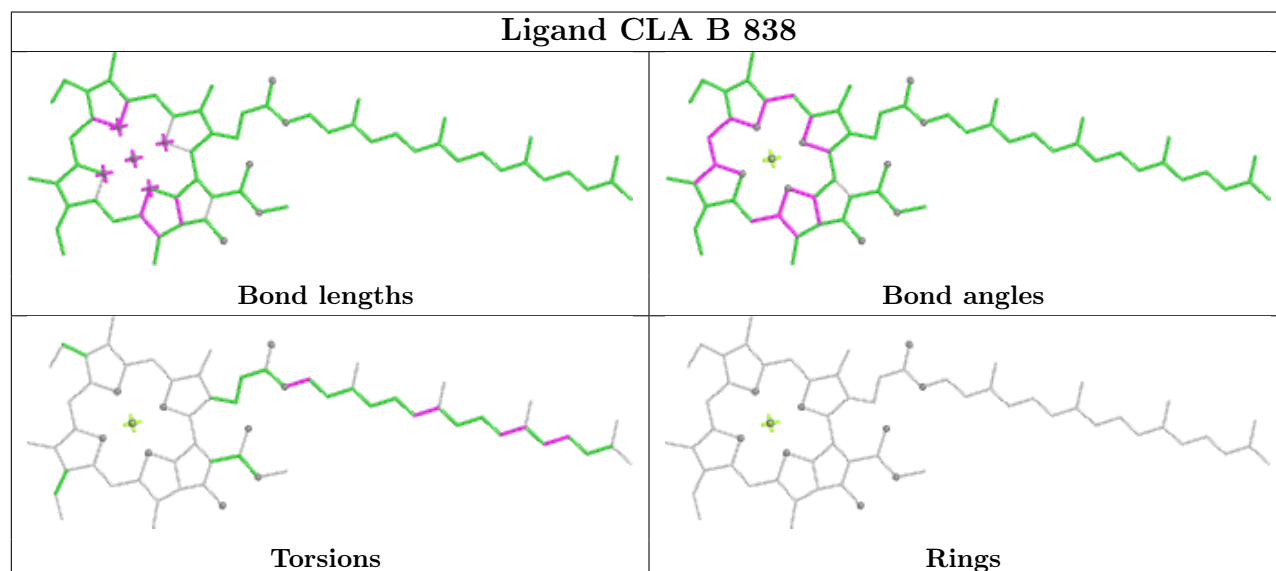
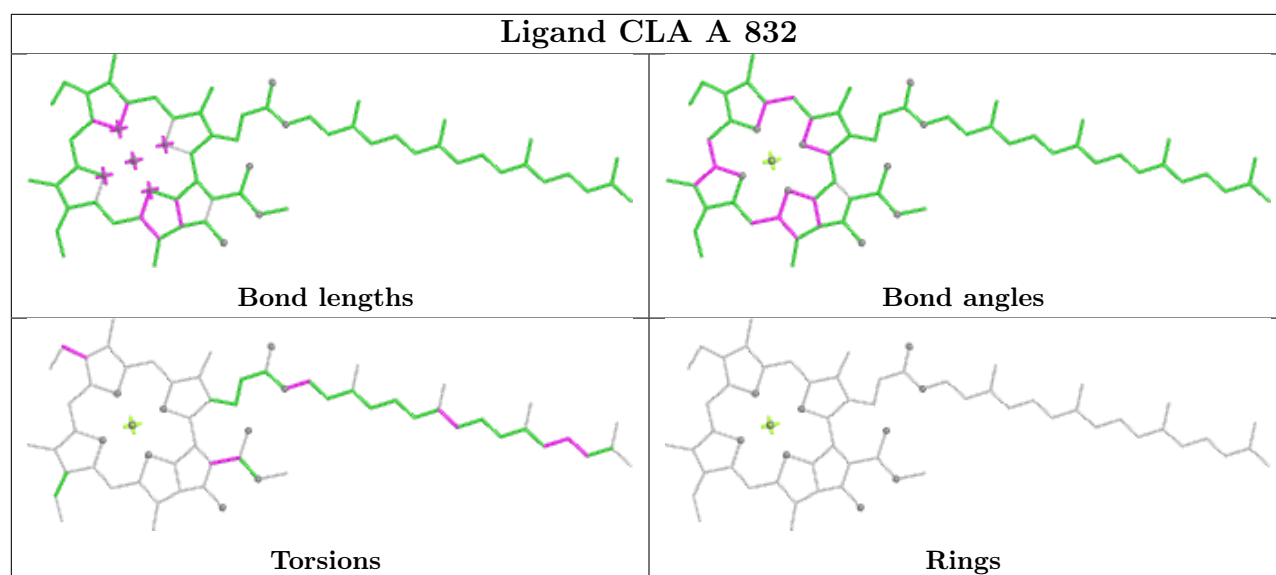


Ligand CLA 3 611

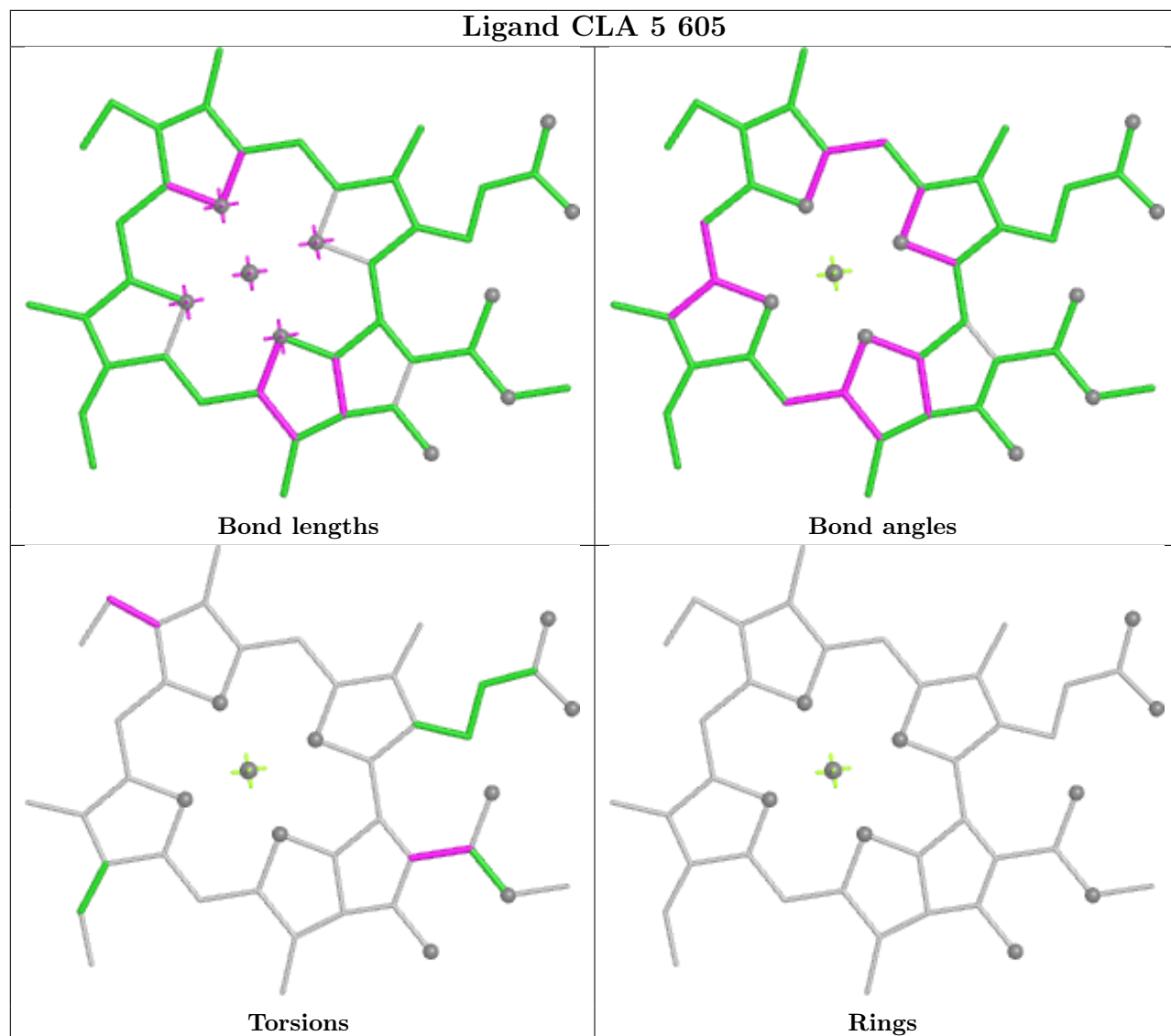


Ligand LHG 8 613

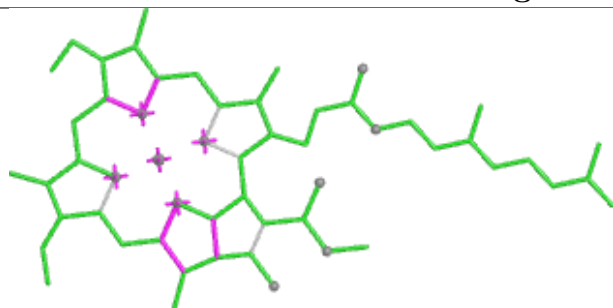




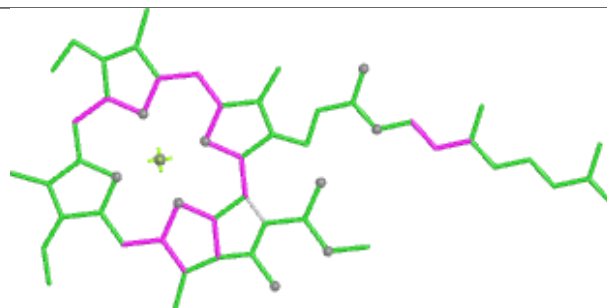
Ligand CLA 5 605



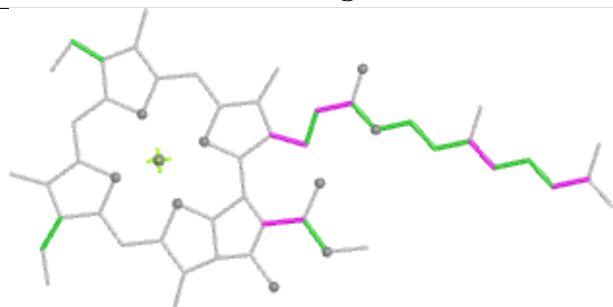
Ligand CLA R 202



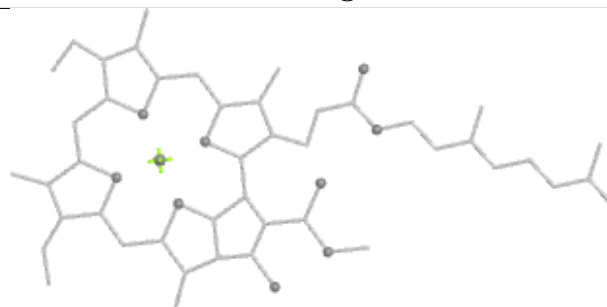
Bond lengths



Bond angles

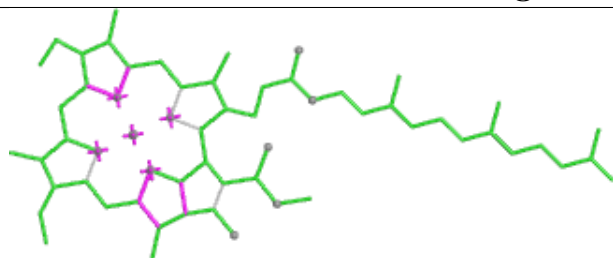


Torsions

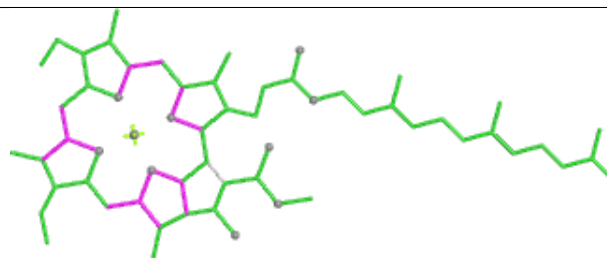


Rings

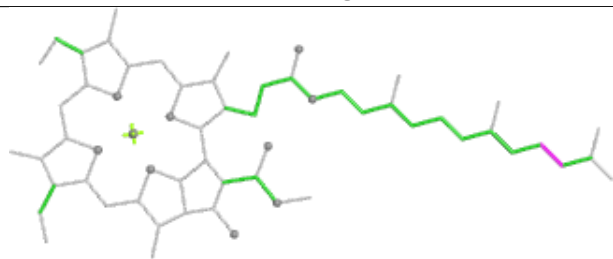
Ligand CLA B 817



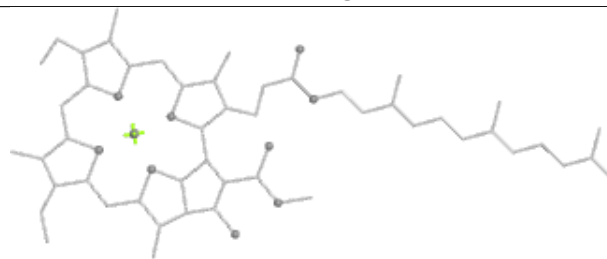
Bond lengths



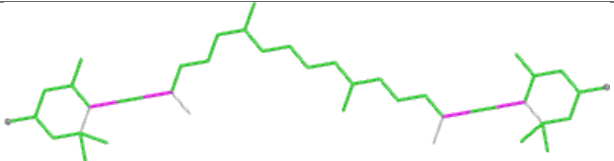
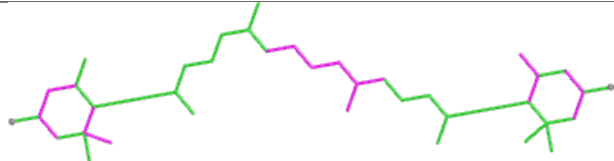
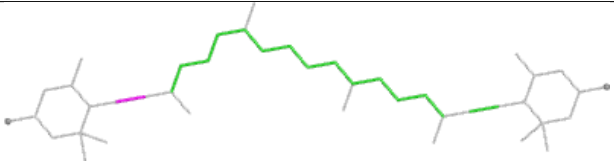
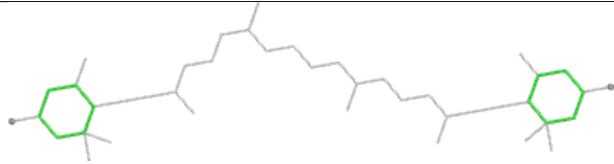
Bond angles

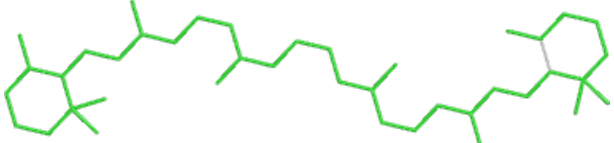
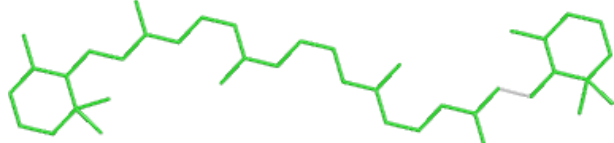
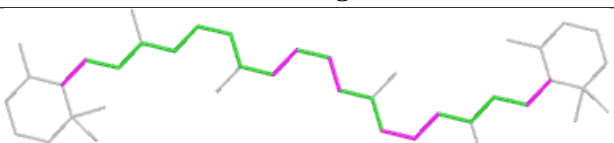
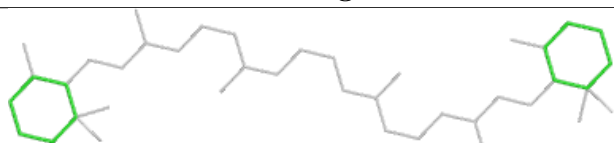


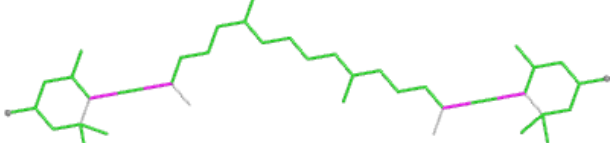
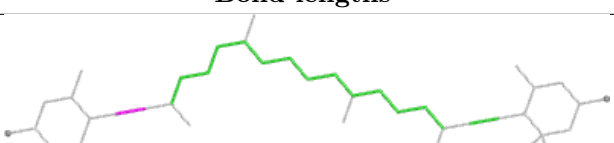
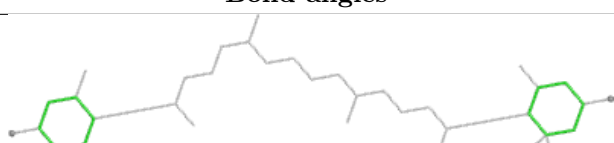
Torsions



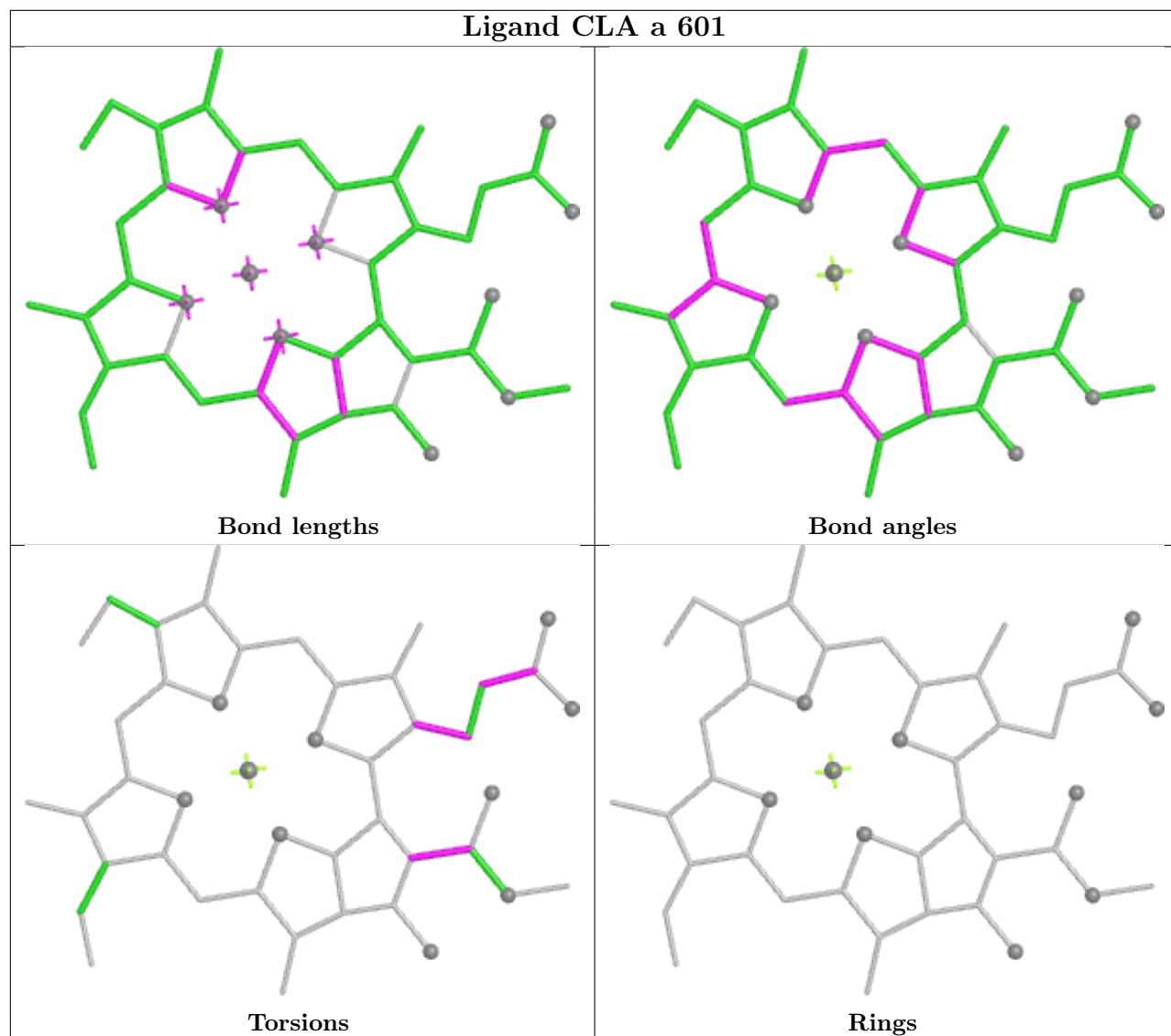
Rings

Ligand II0 7 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

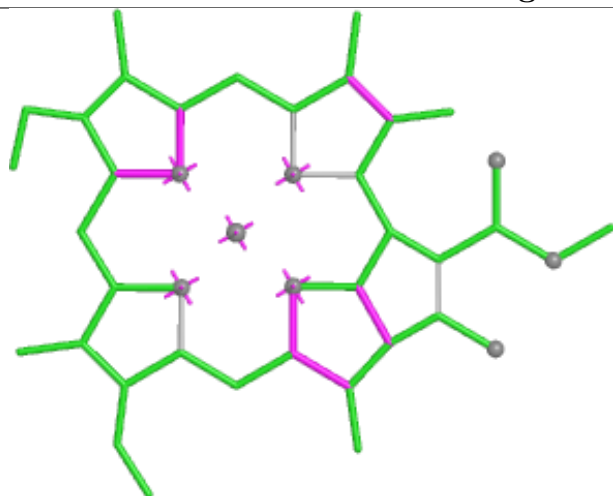
Ligand 8CT B 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 6 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 601



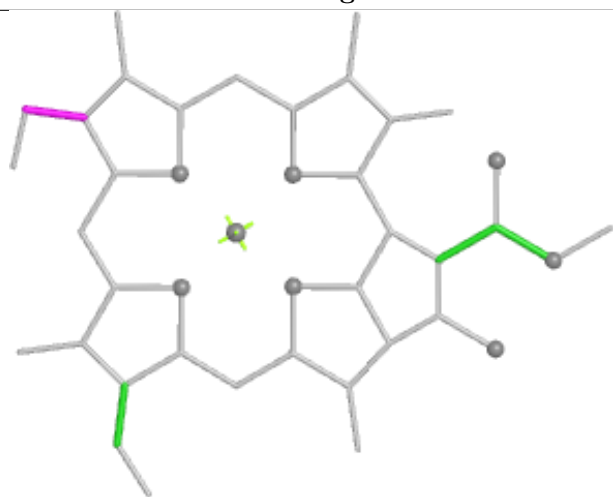
Ligand CLA 5 601



Bond lengths



Bond angles

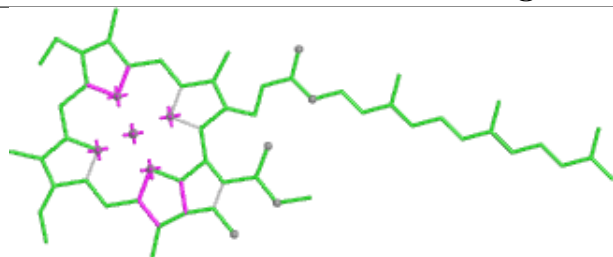


Torsions

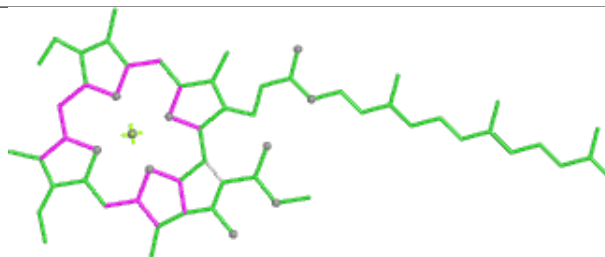


Rings

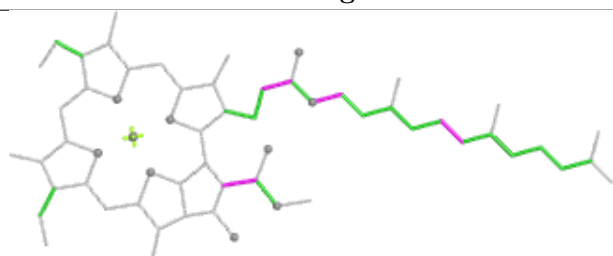
Ligand CLA b 607



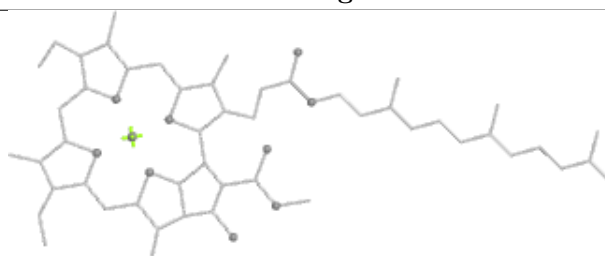
Bond lengths



Bond angles

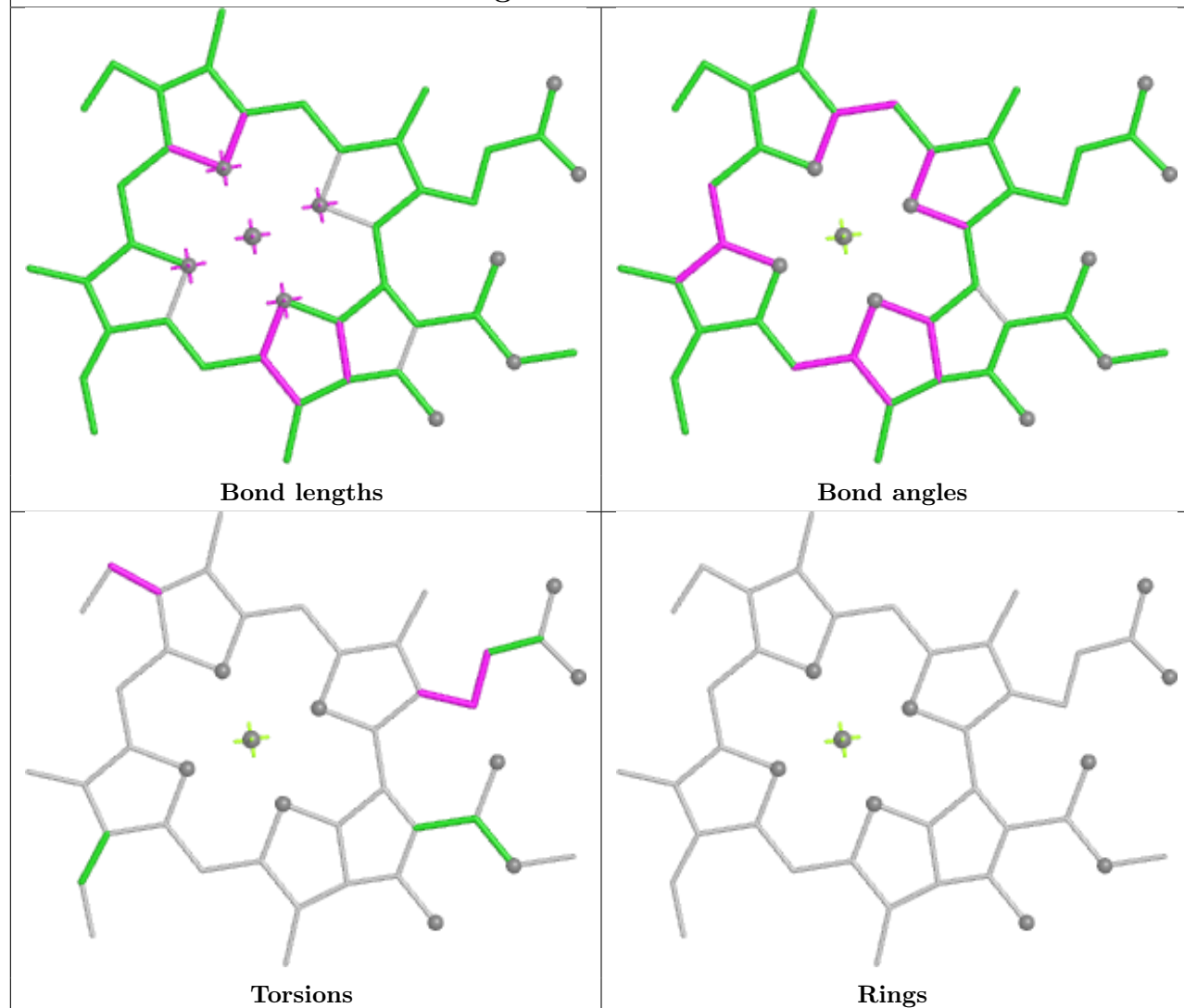


Torsions

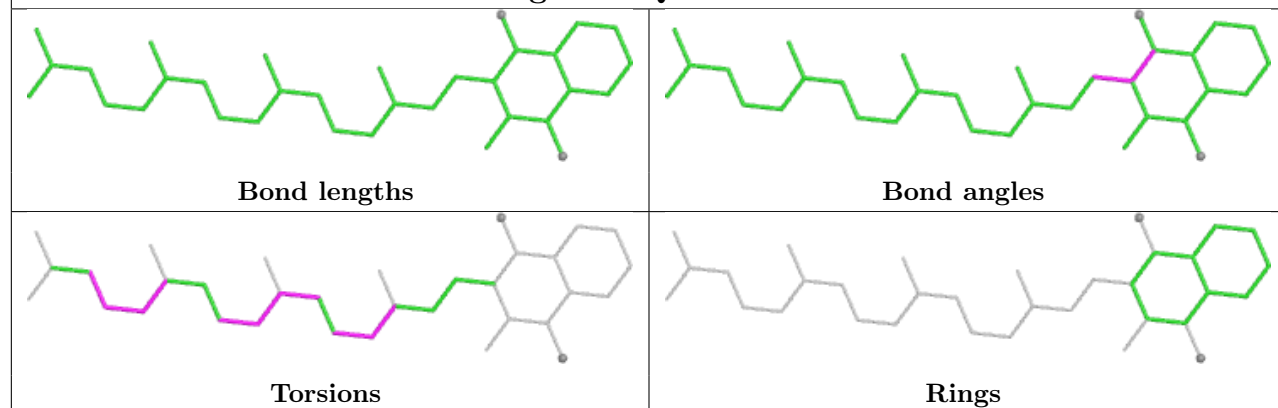


Rings

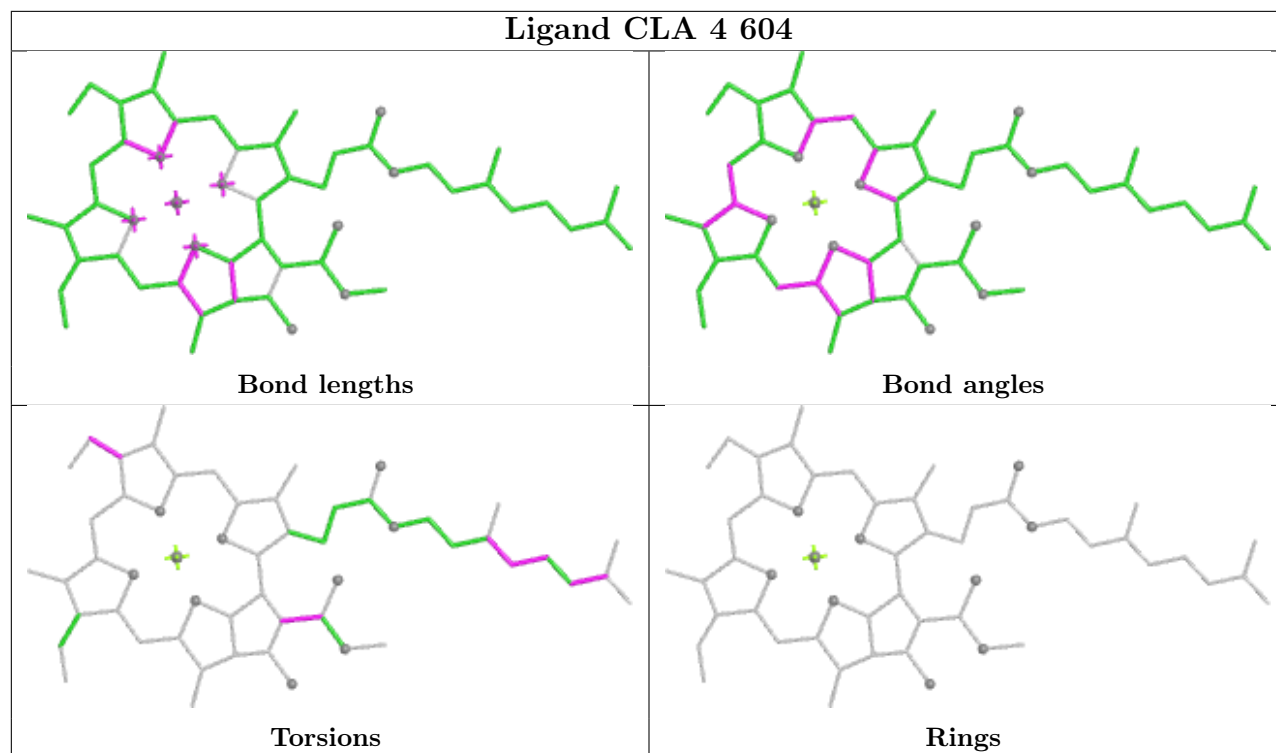
Ligand CLA F 203



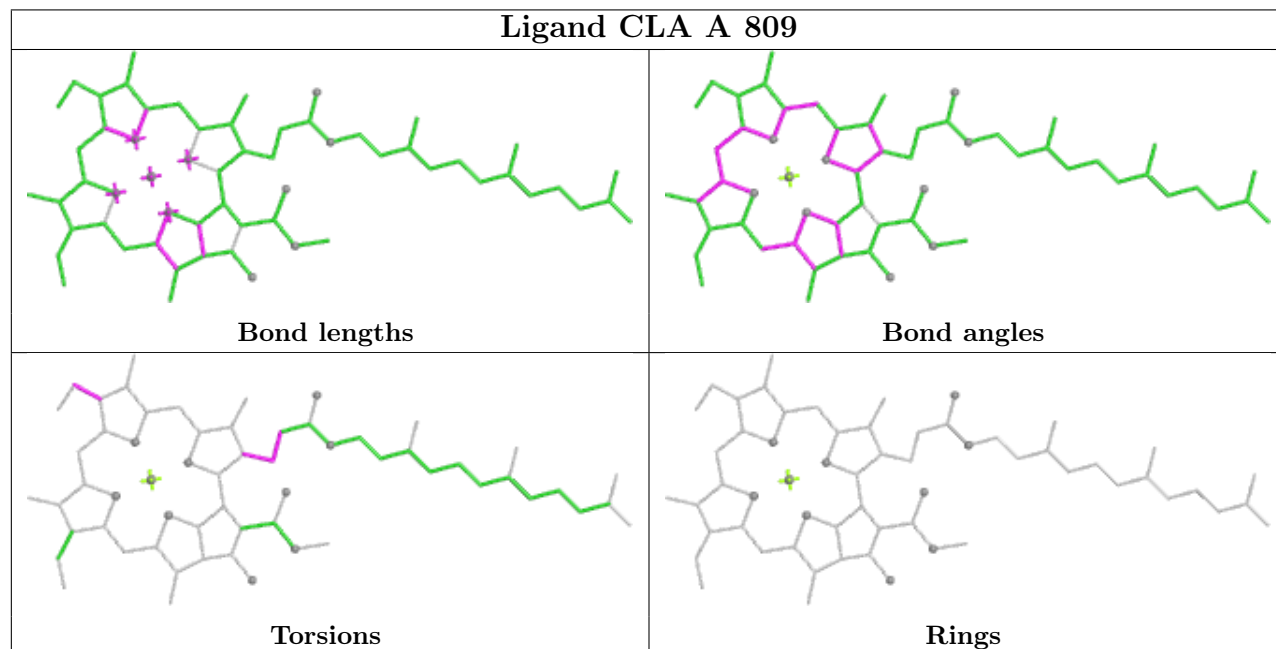
Ligand PQN A 850



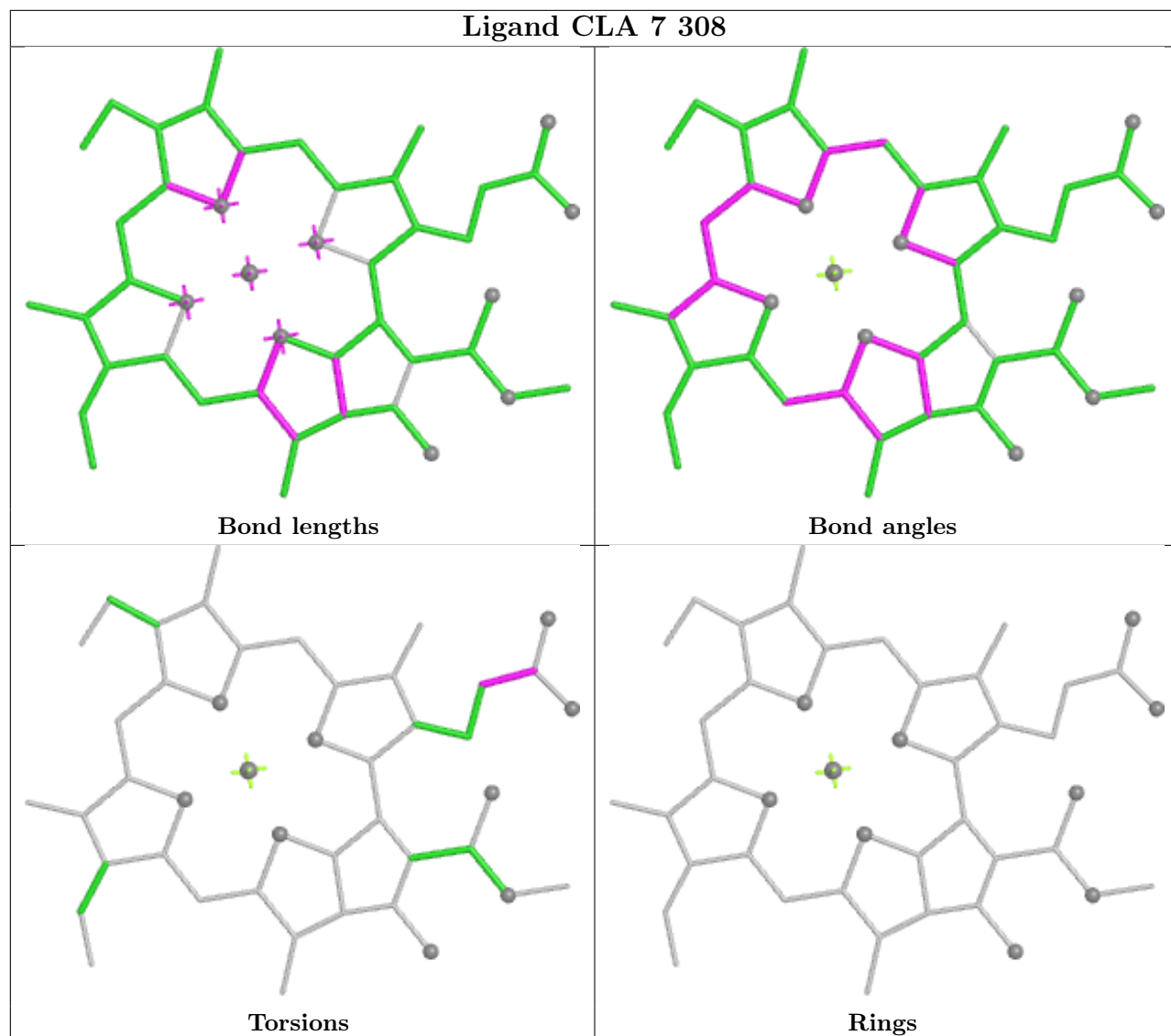
Ligand CLA 4 604



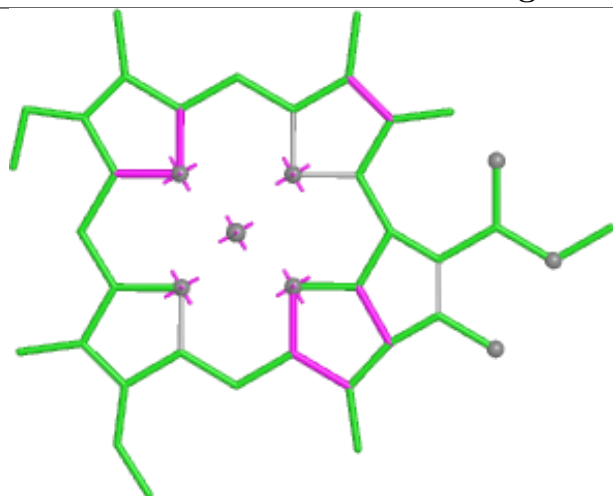
Ligand CLA A 809



Ligand CLA 7 308



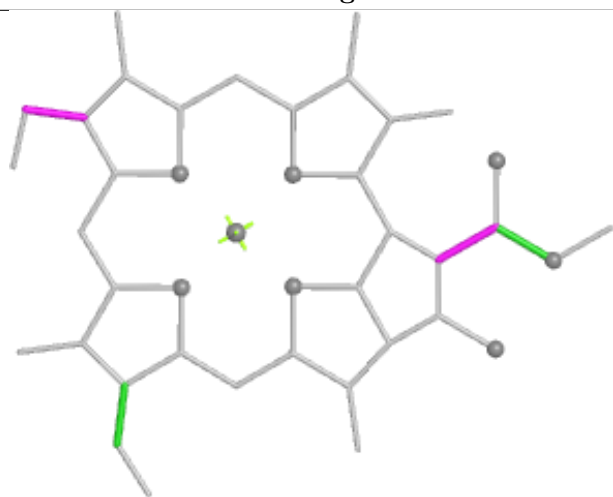
Ligand CLA 9 614



Bond lengths



Bond angles

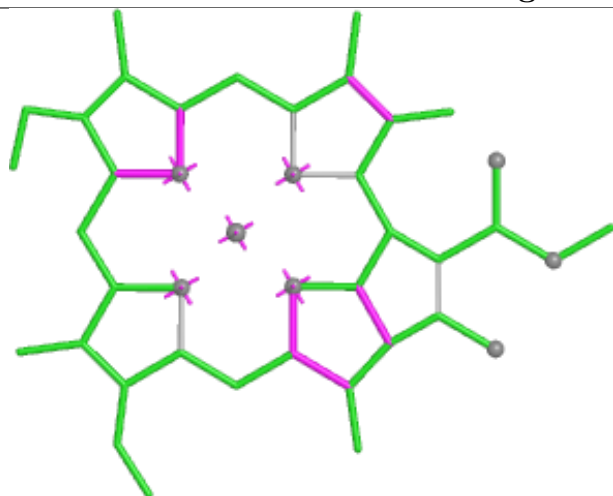


Torsions



Rings

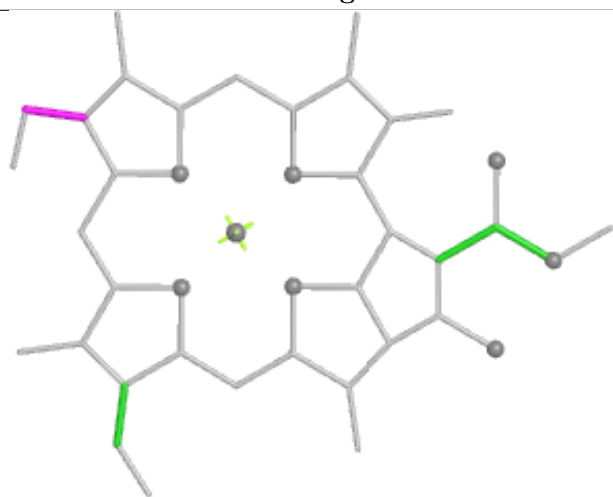
Ligand CLA 2 609



Bond lengths



Bond angles

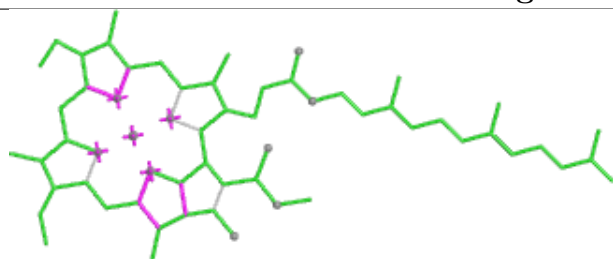


Torsions

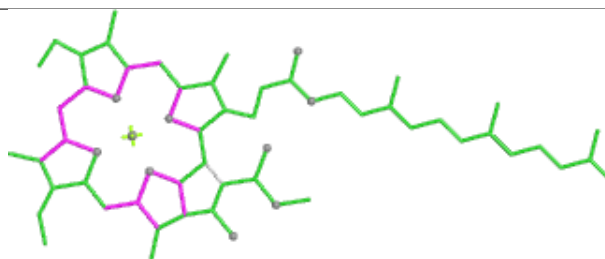


Rings

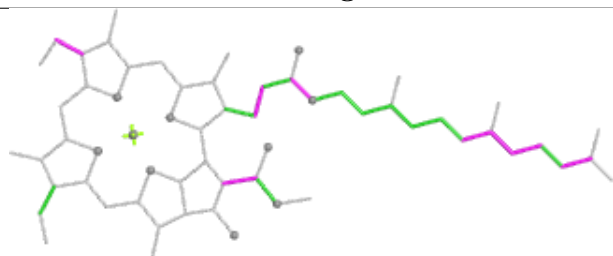
Ligand CLA Z 301



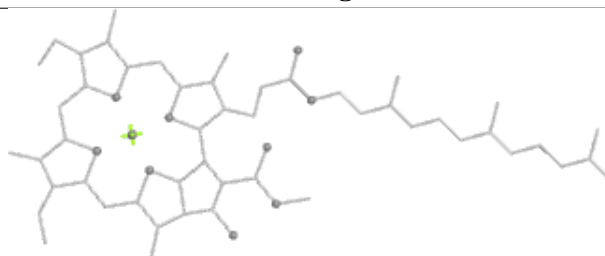
Bond lengths



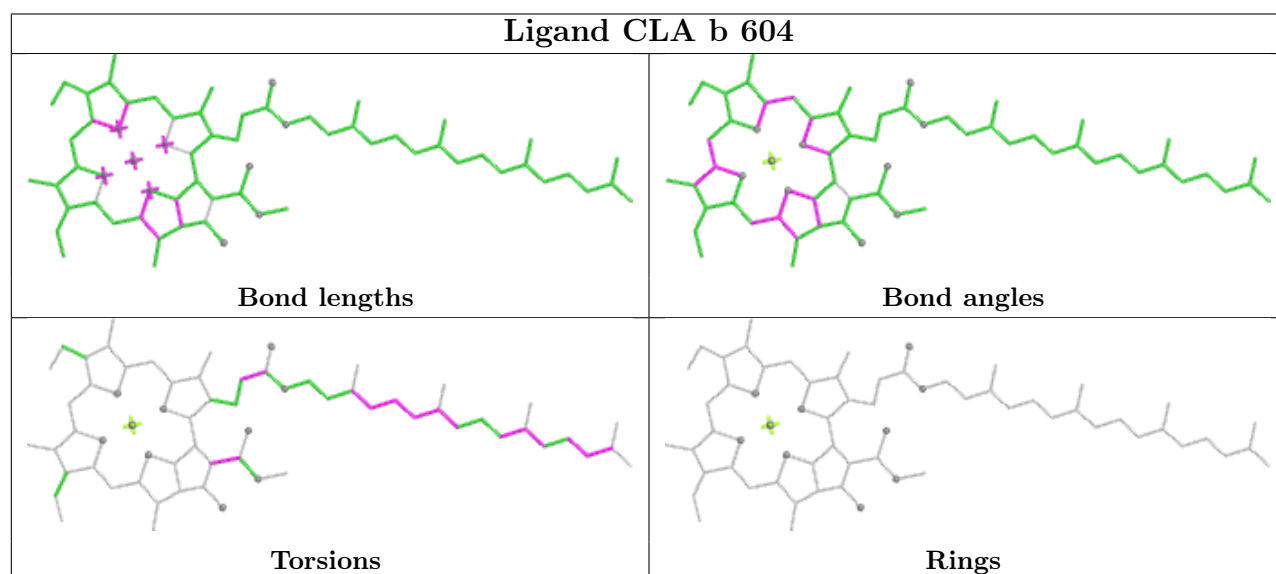
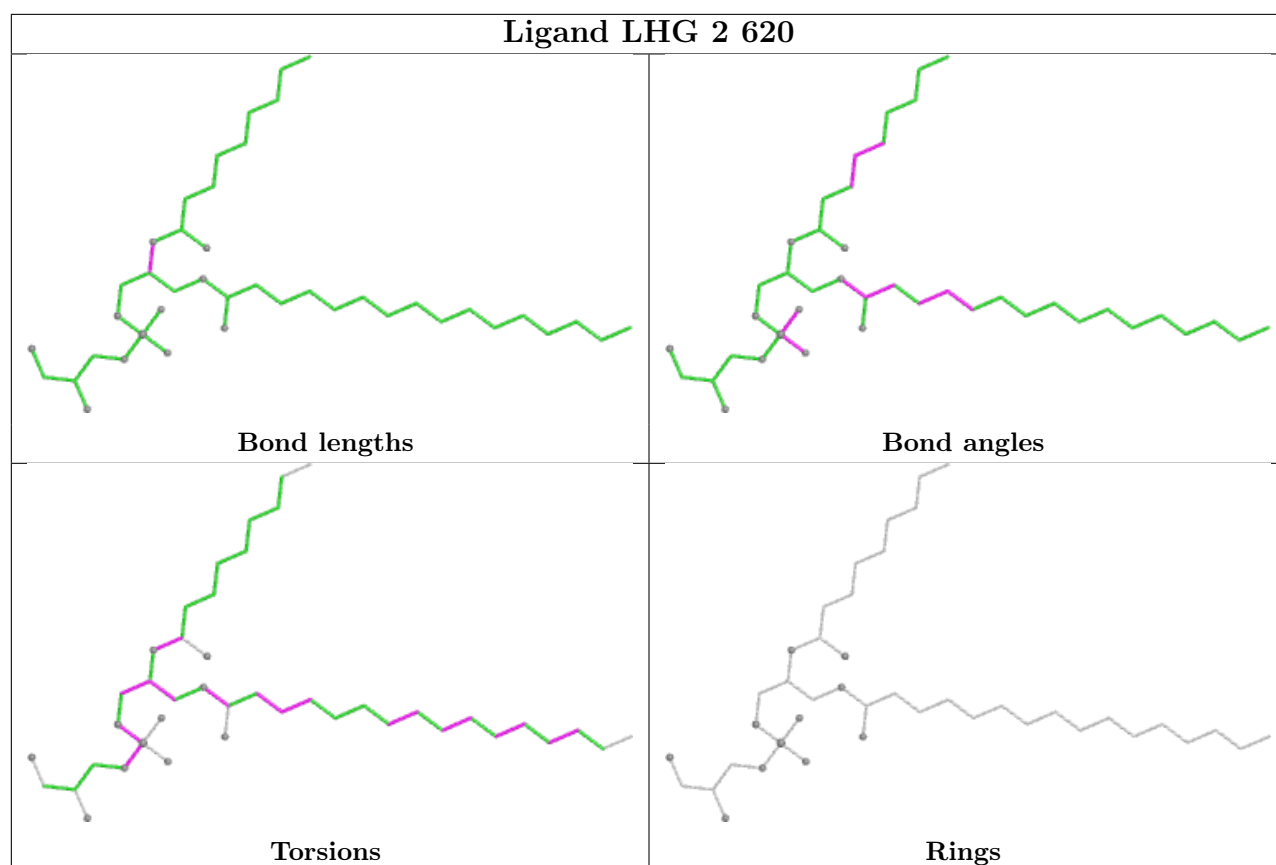
Bond angles

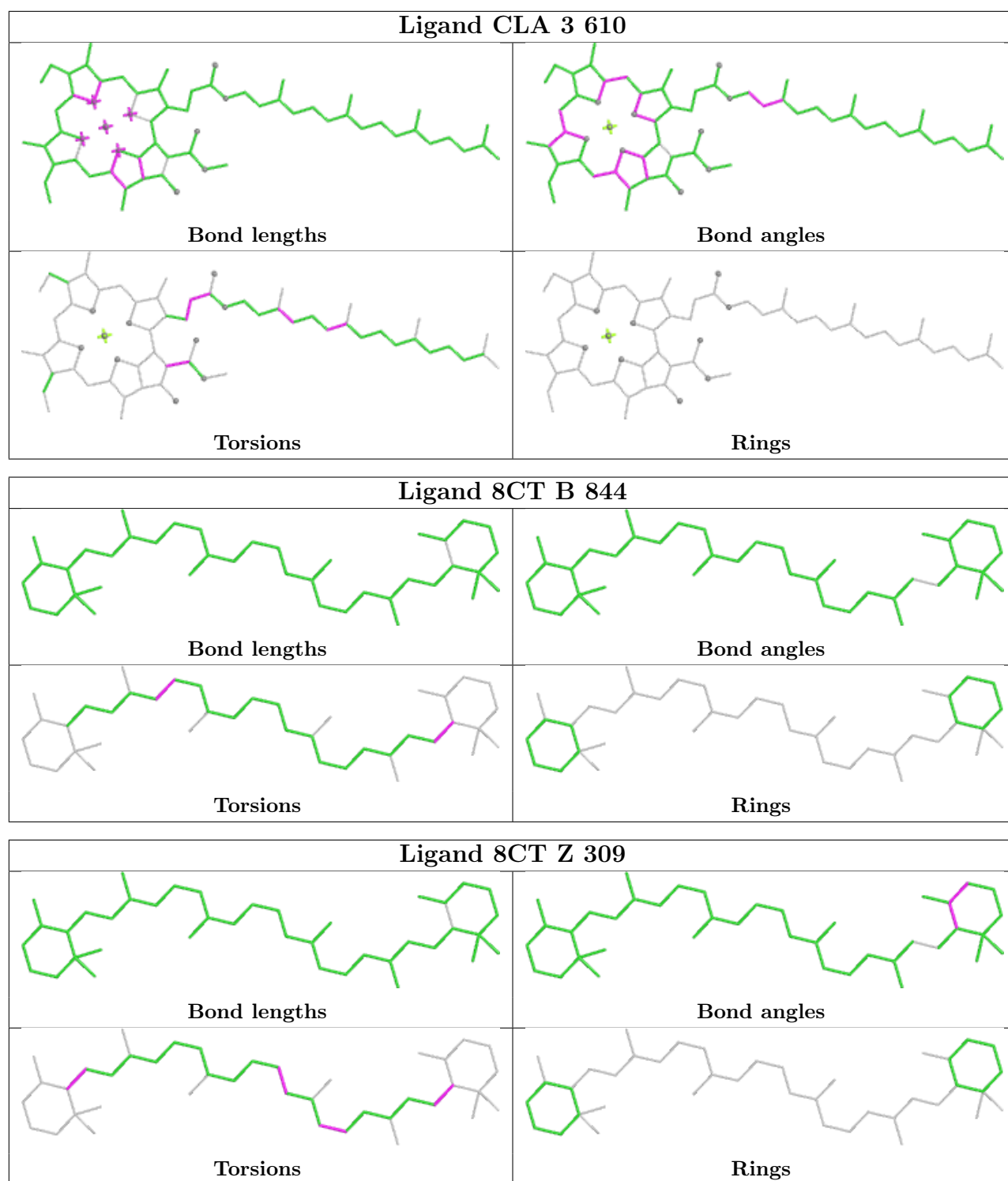


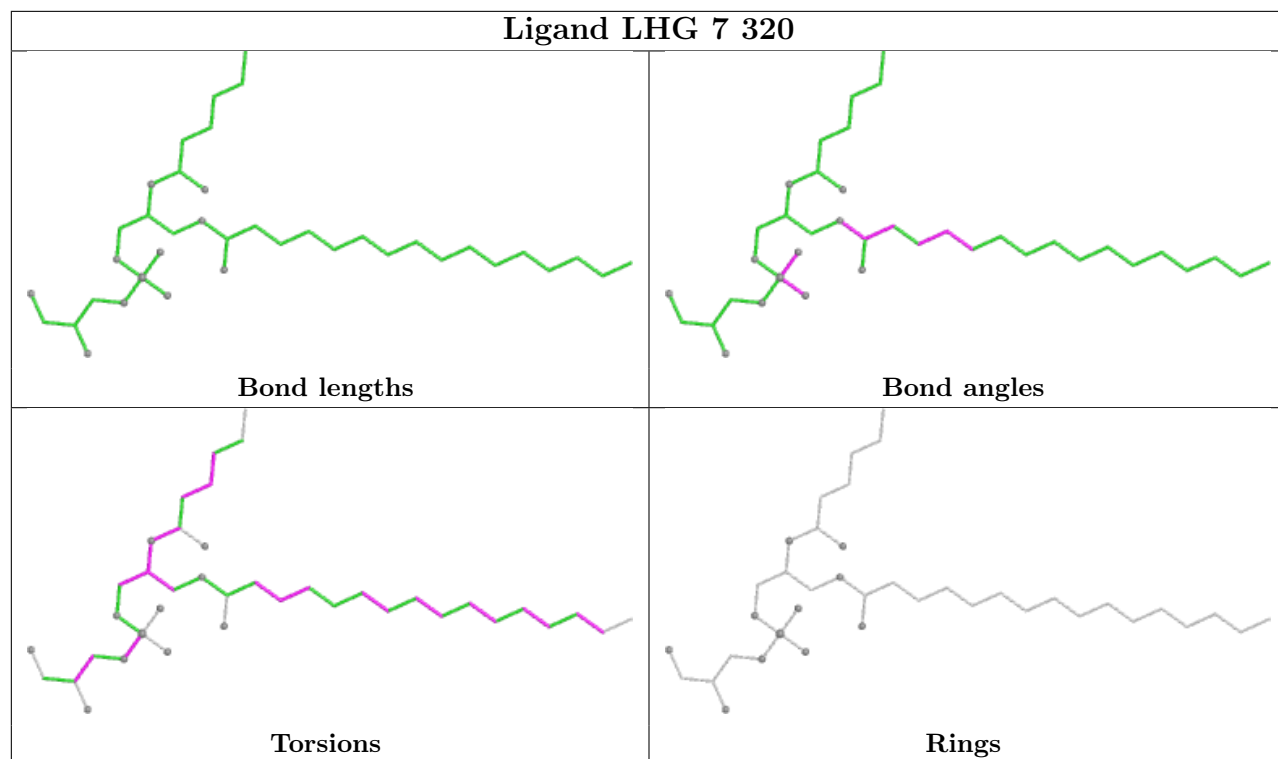
Torsions



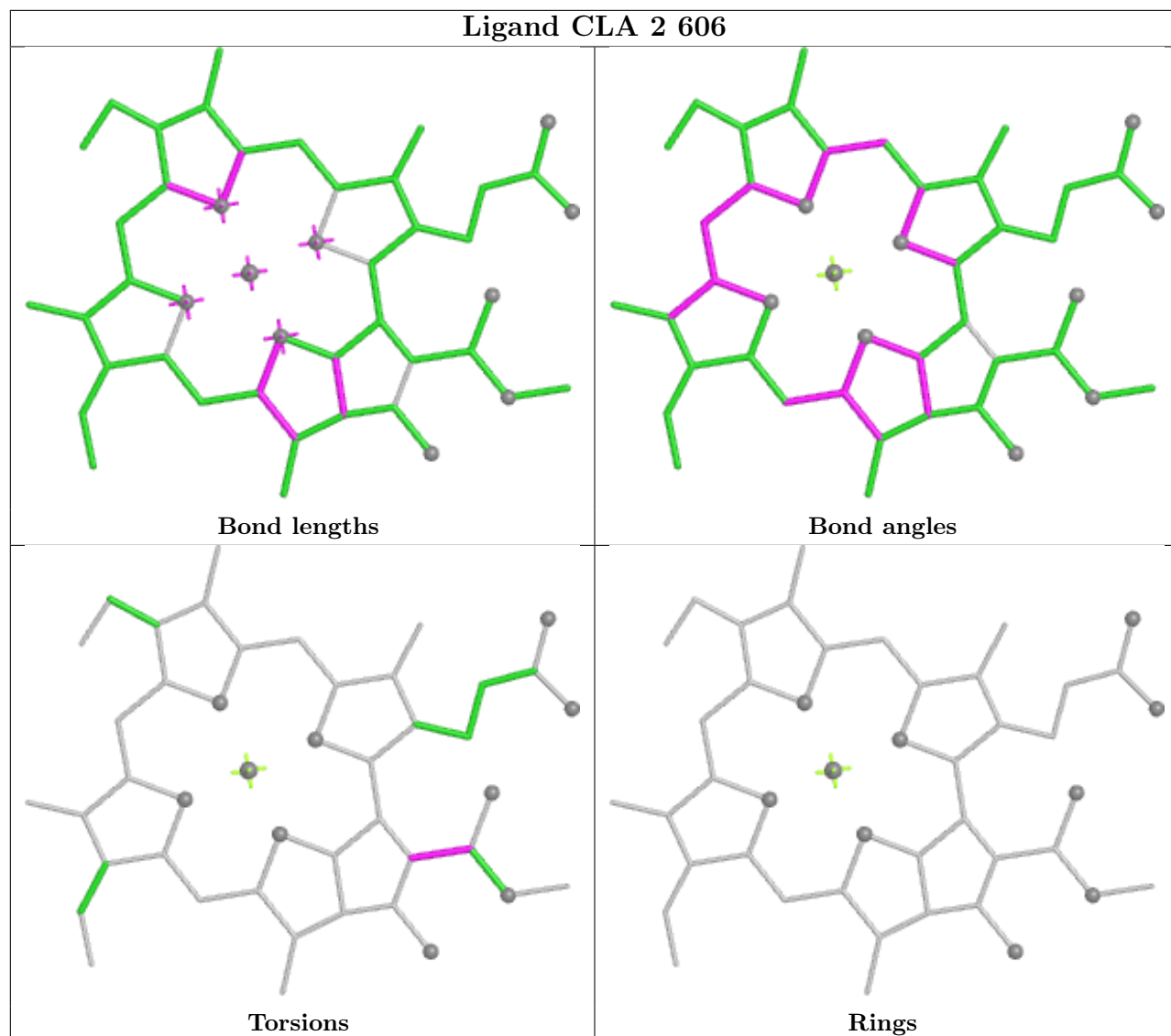
Rings

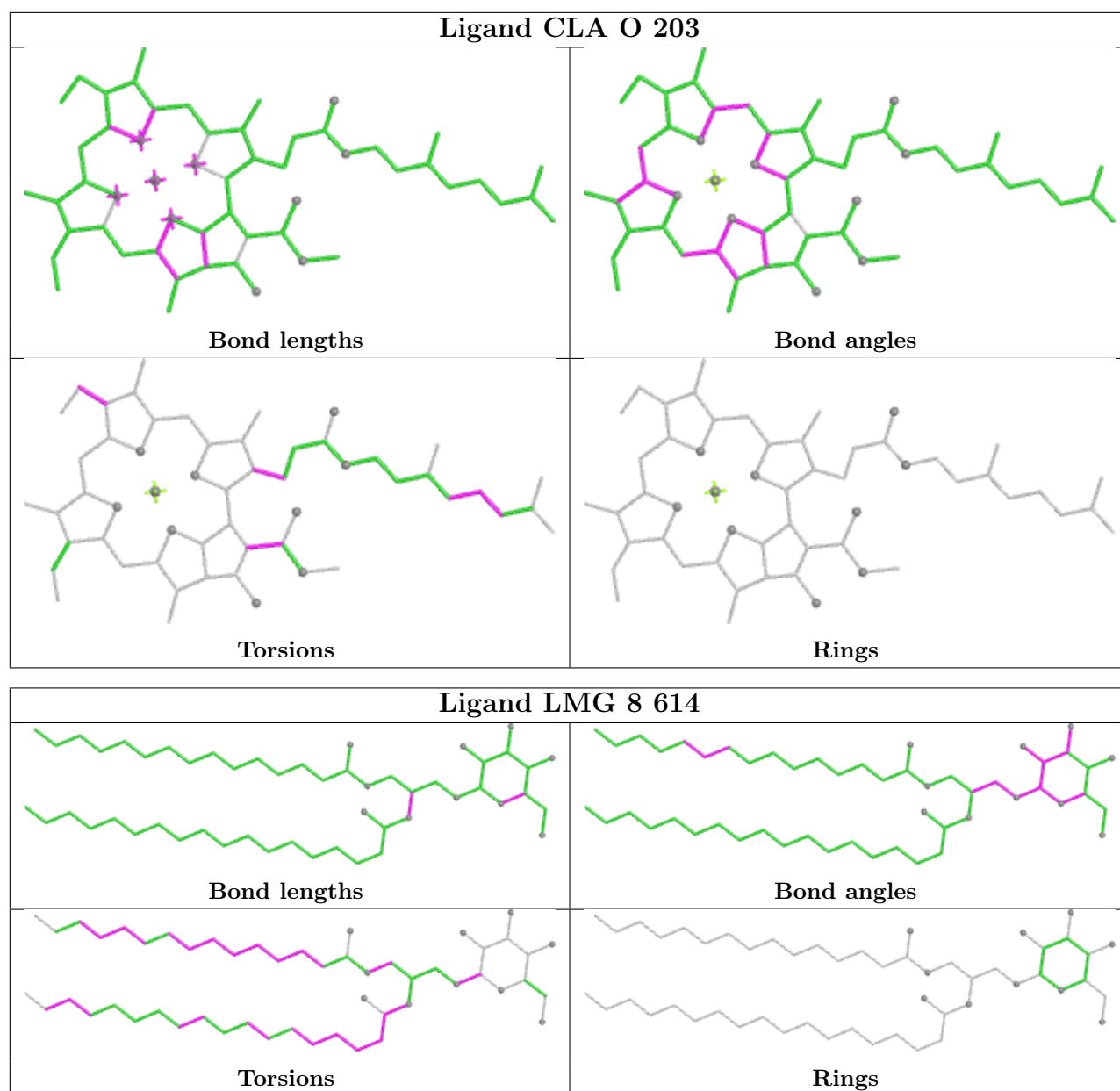


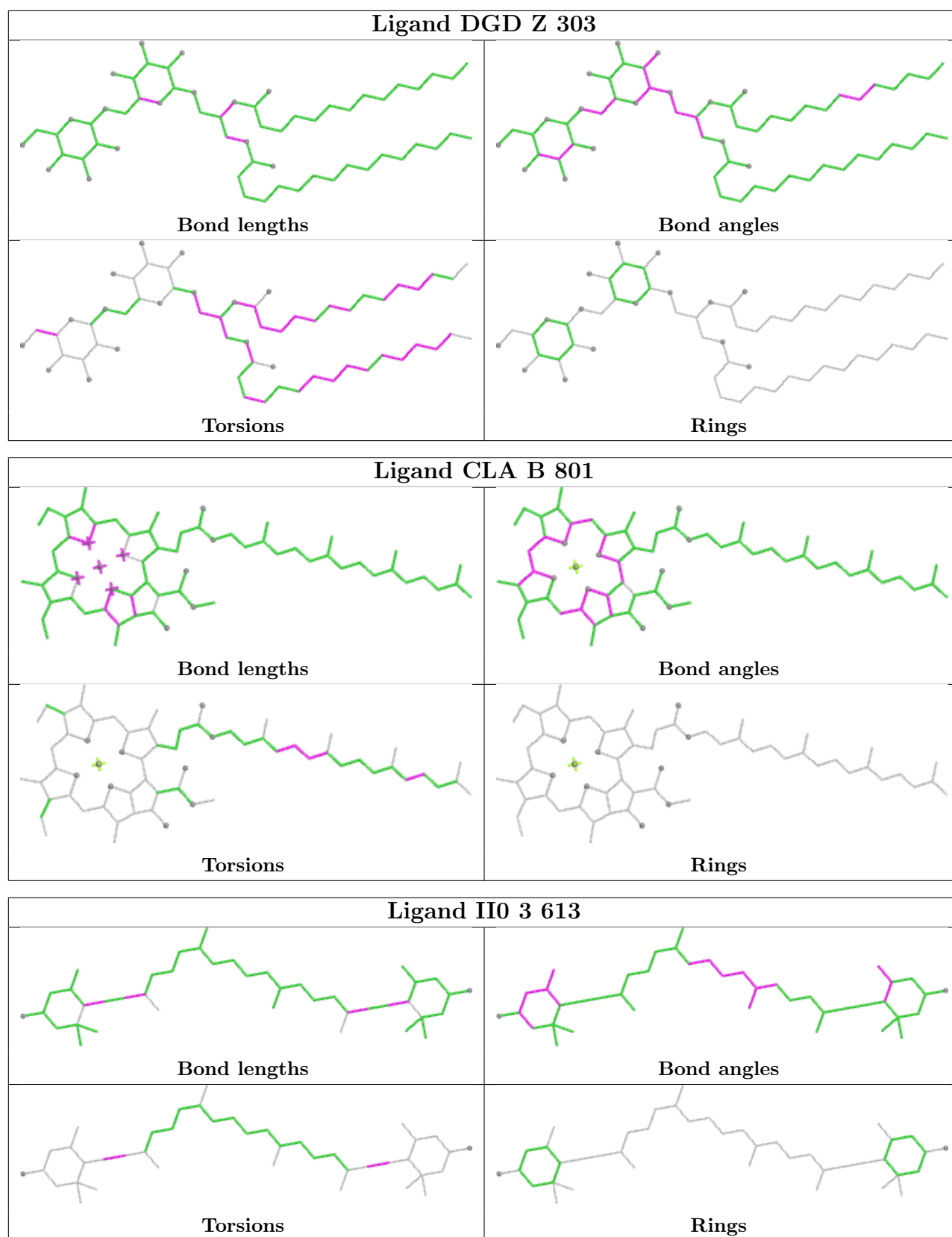




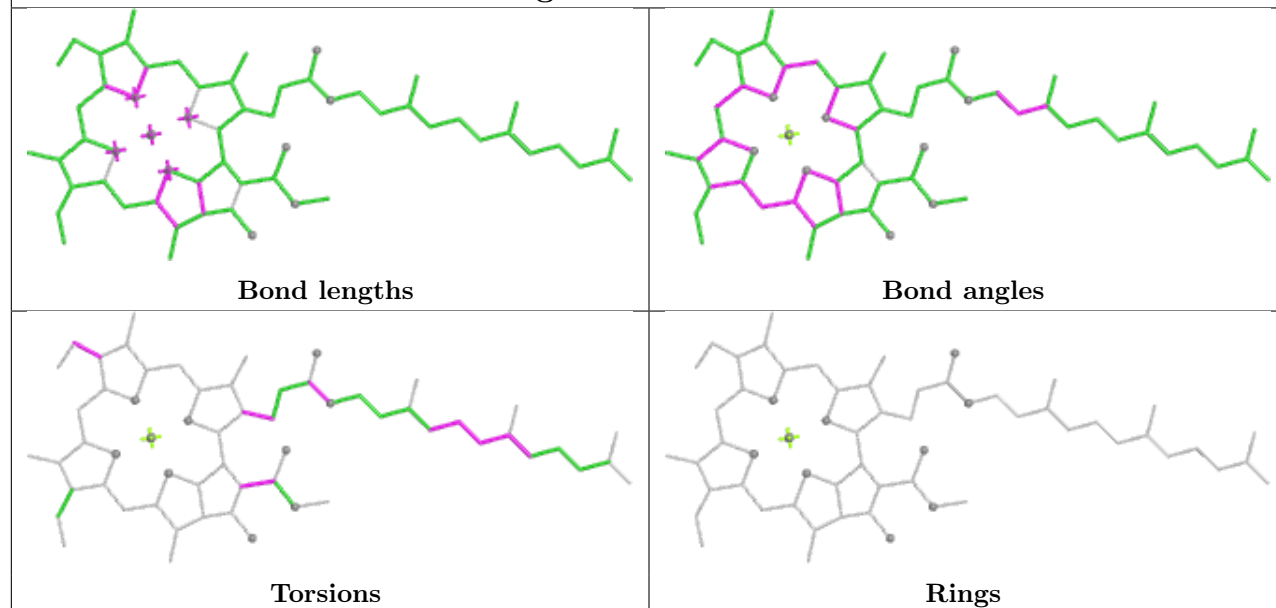
Ligand CLA 2 606



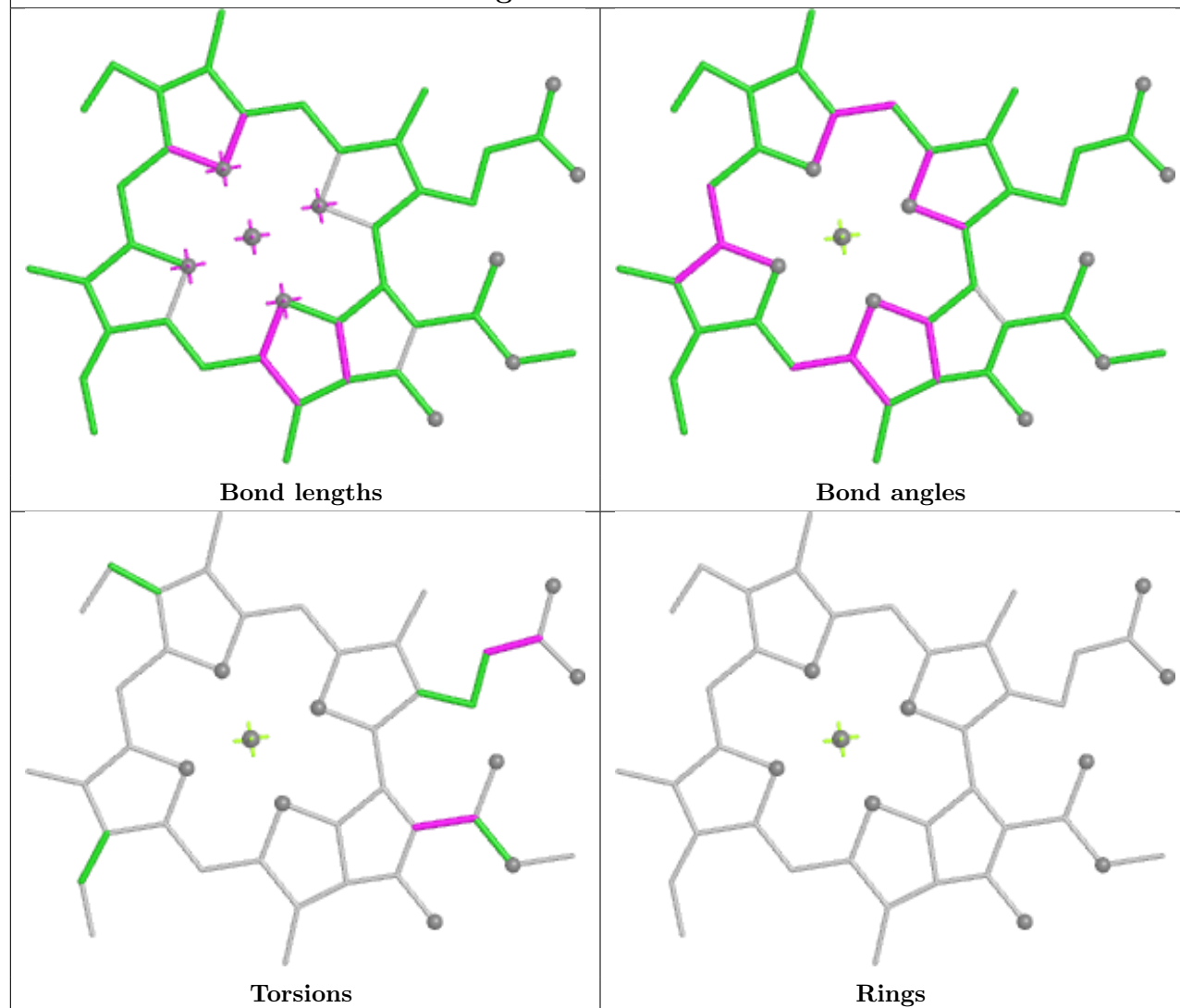


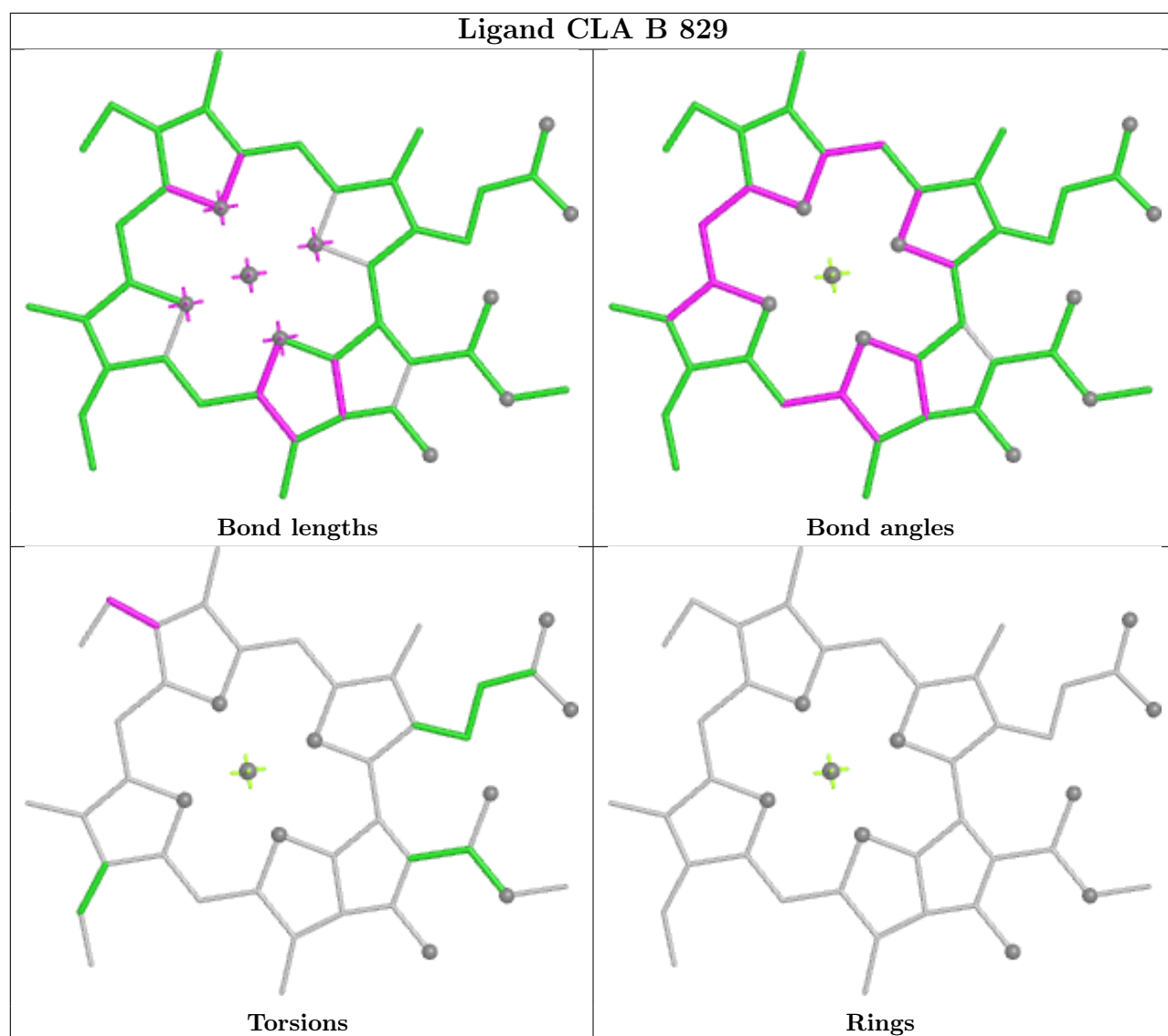


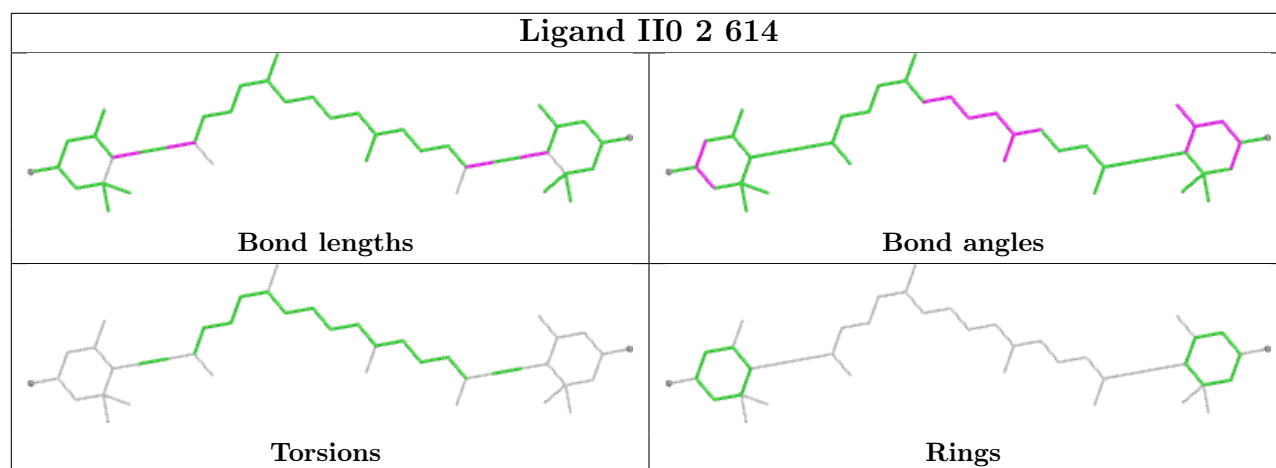
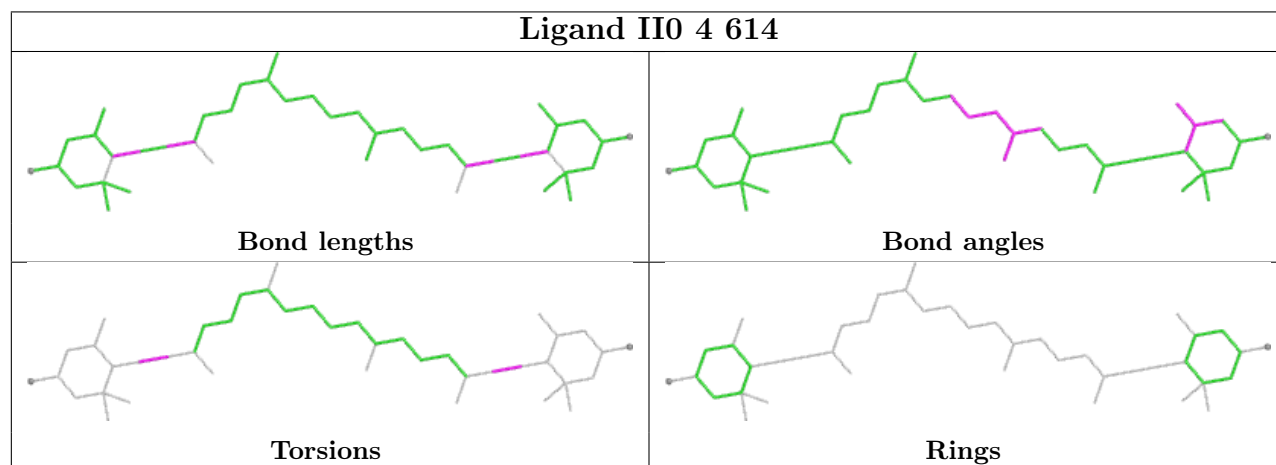
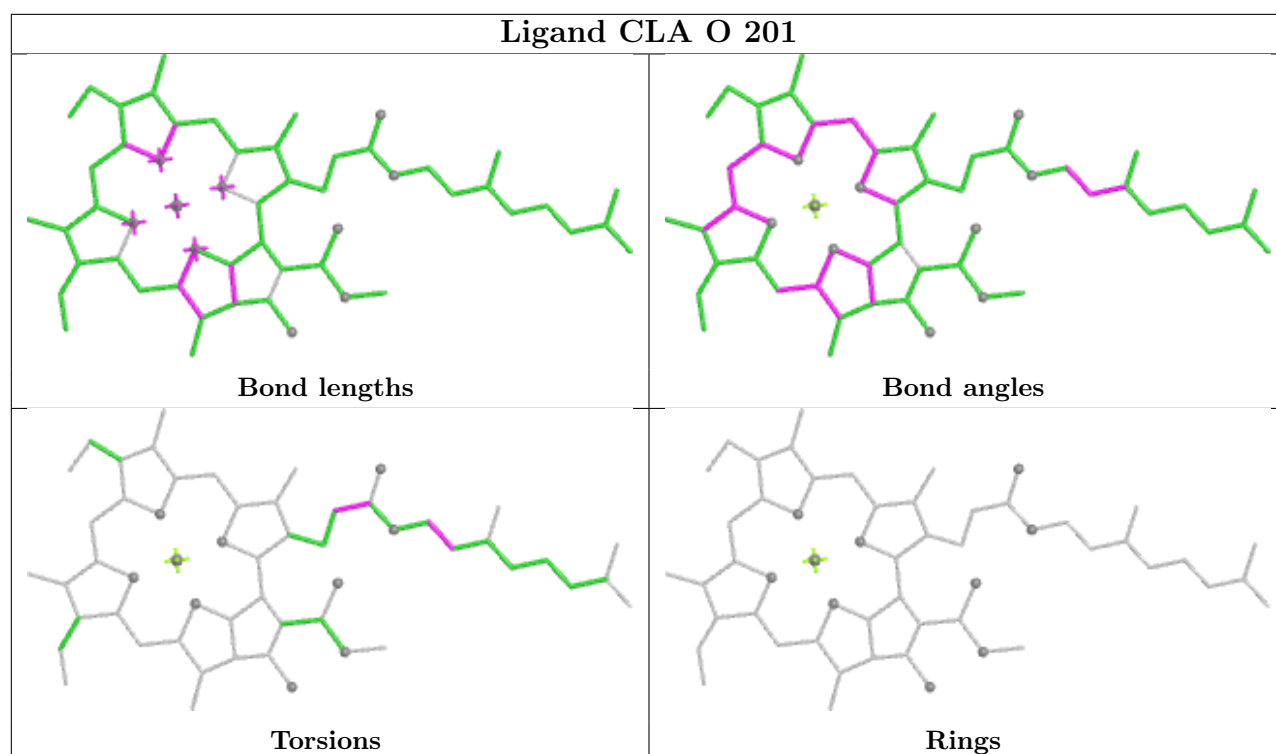
Ligand CLA 5 608

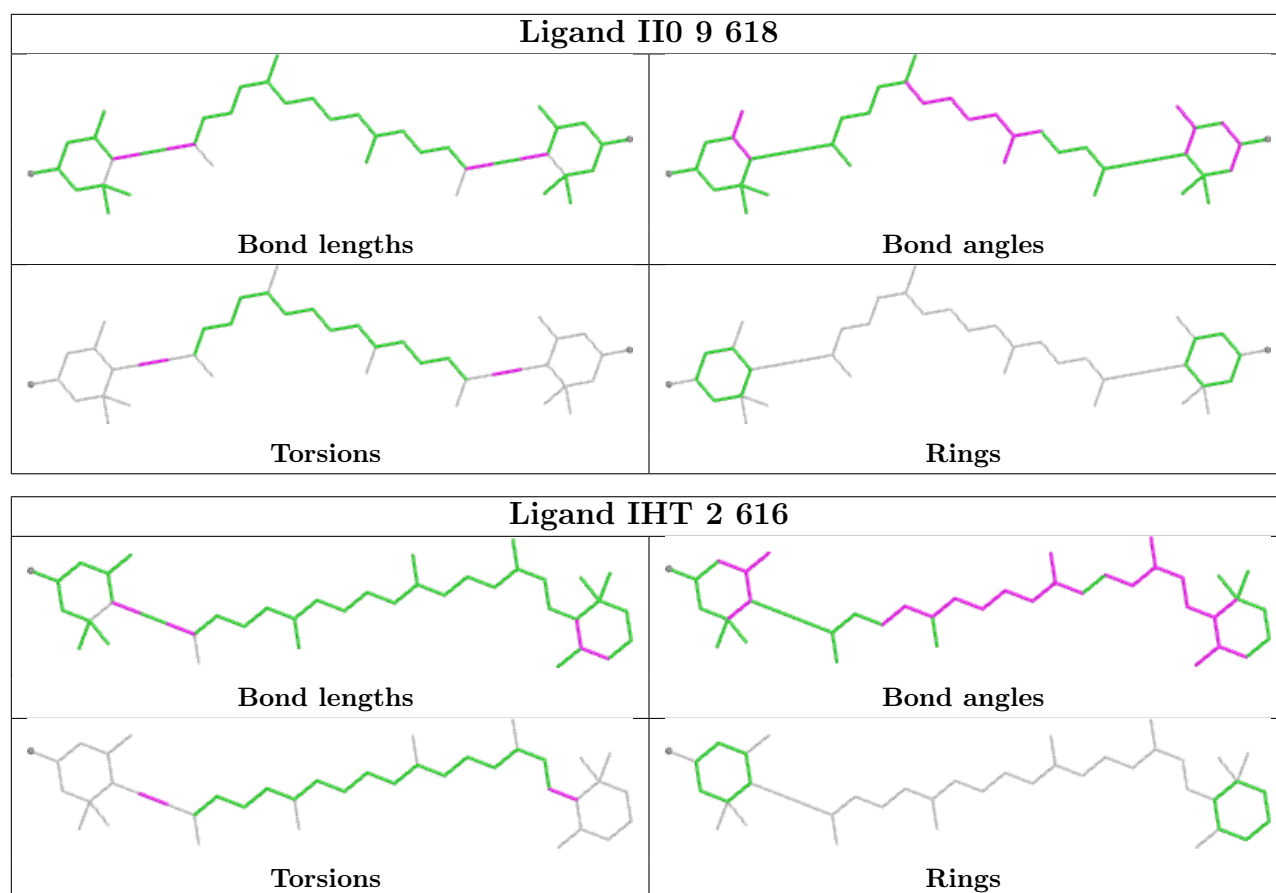


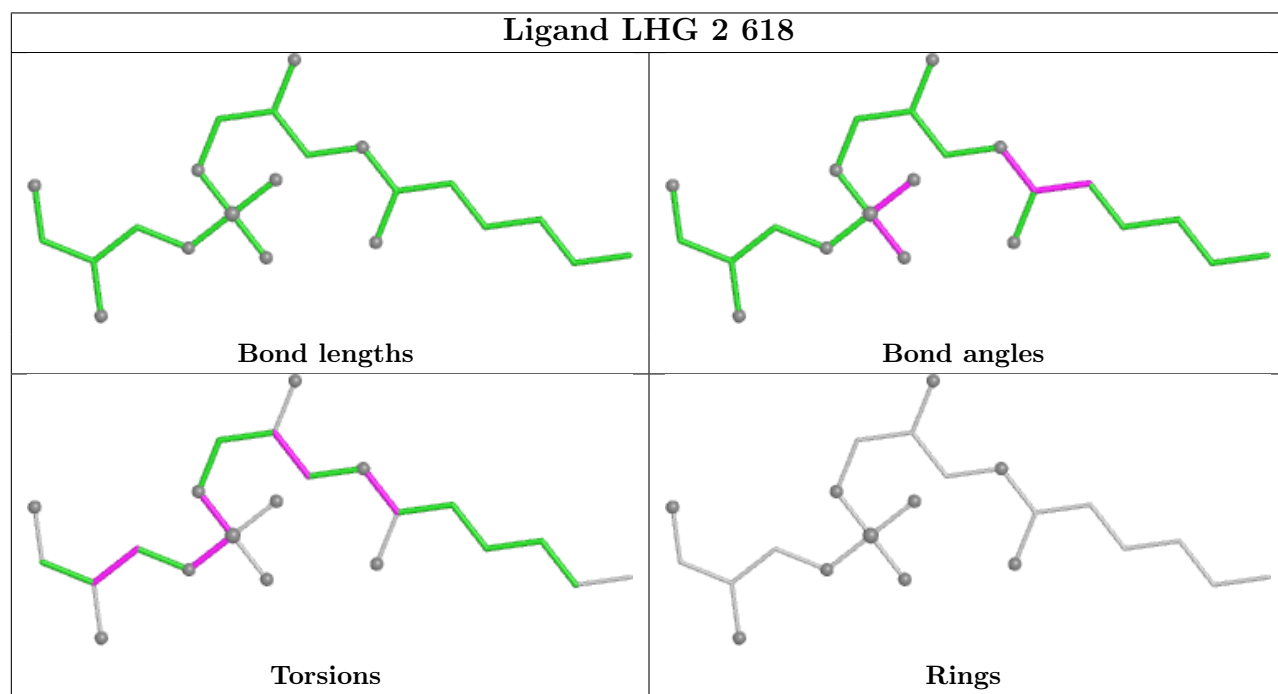
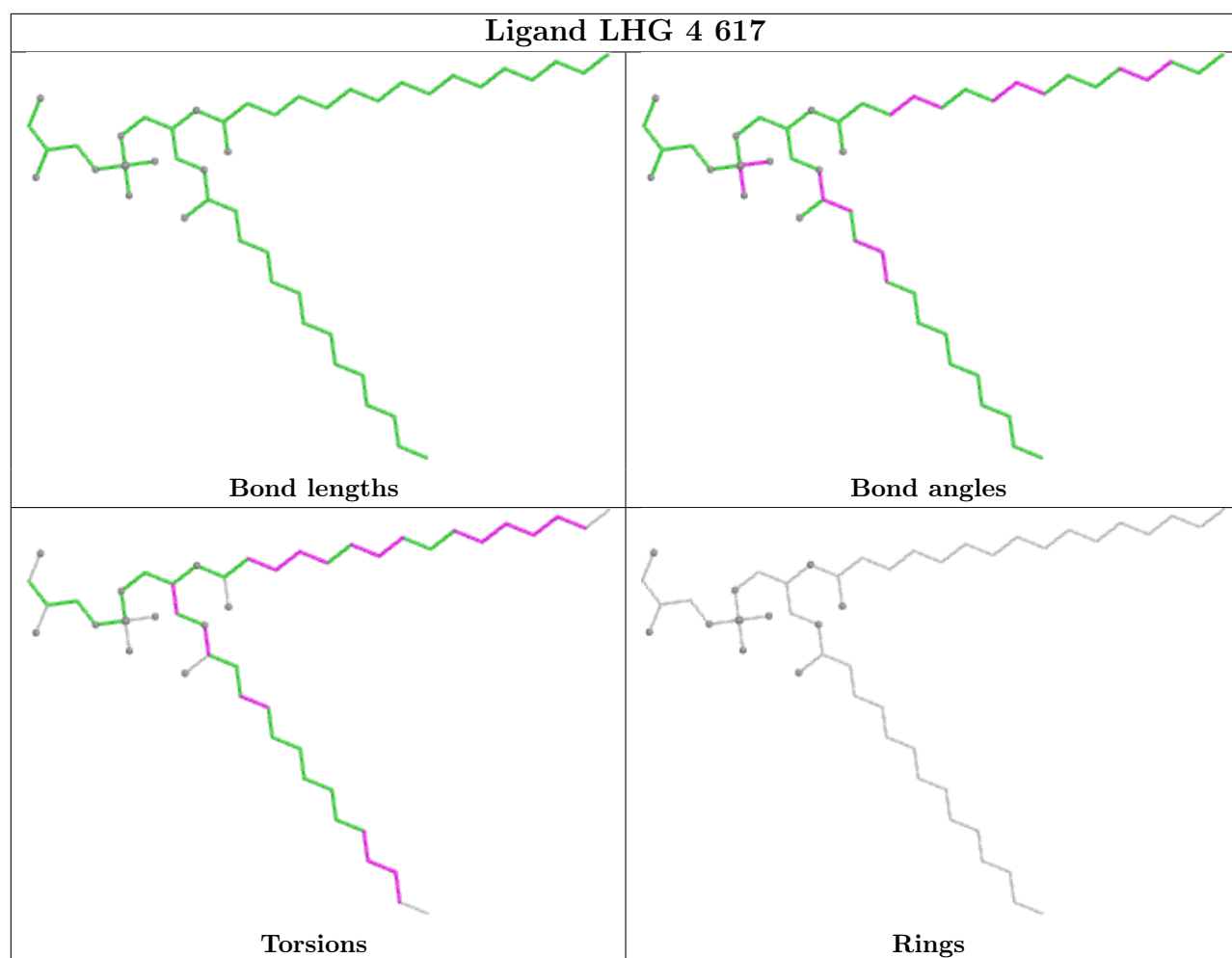
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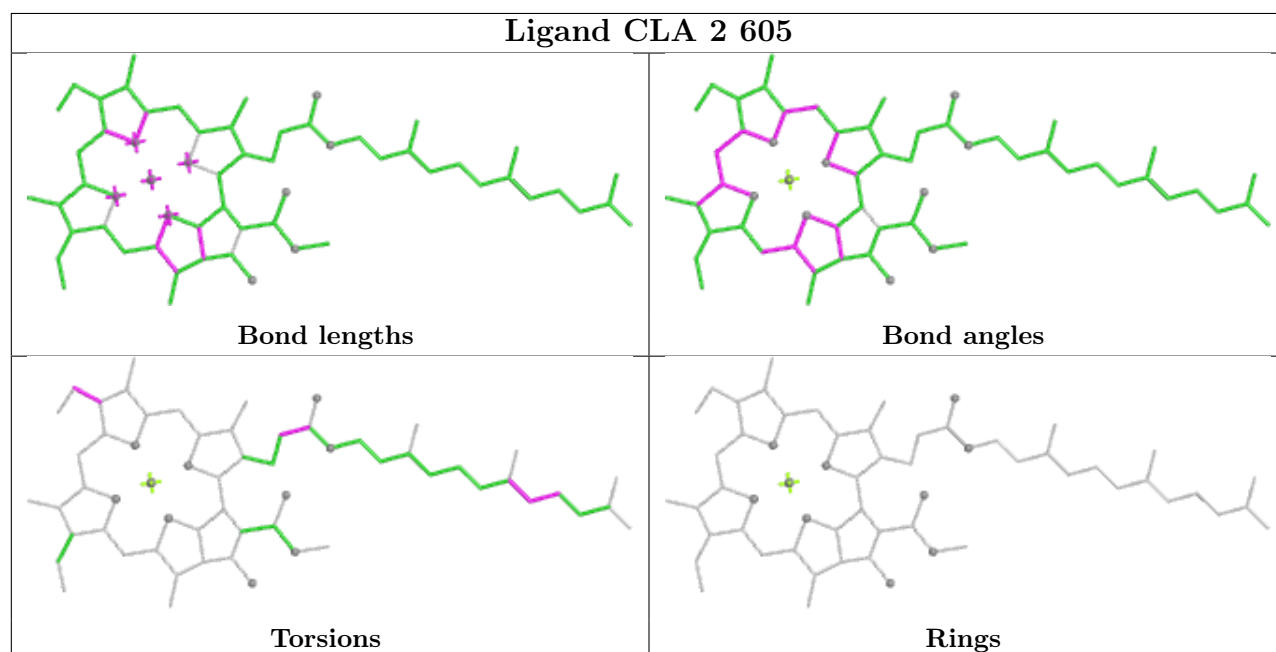
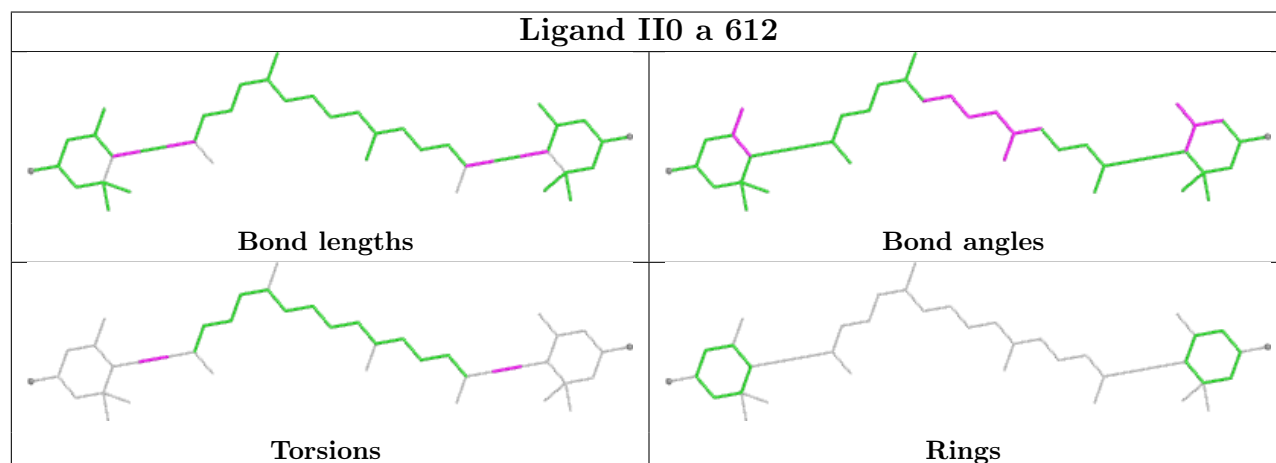
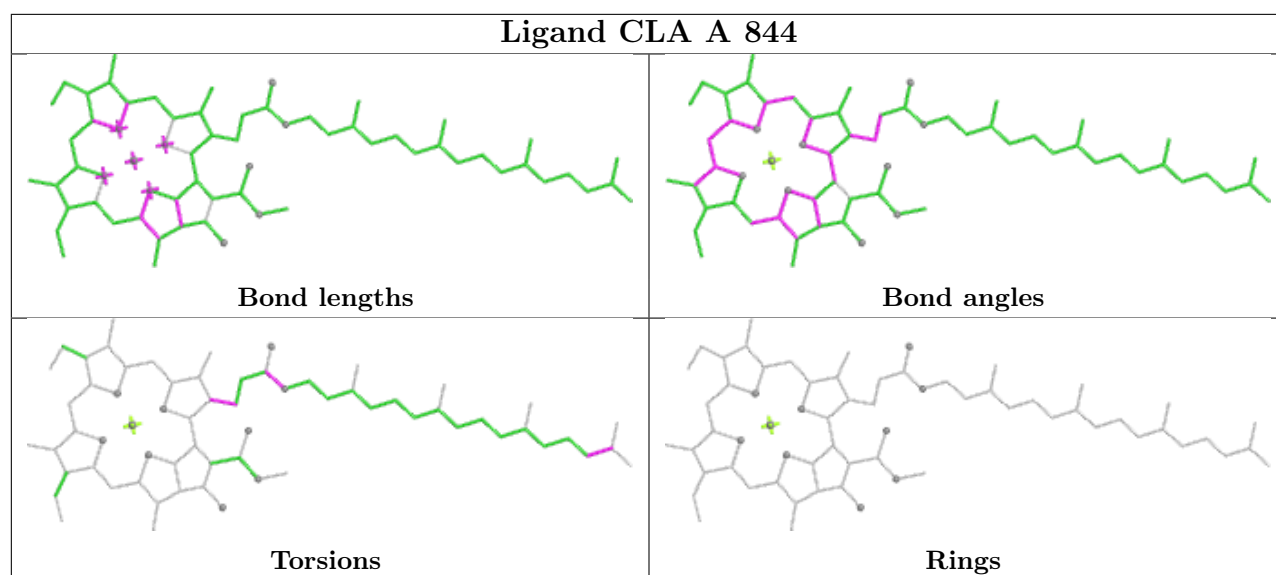


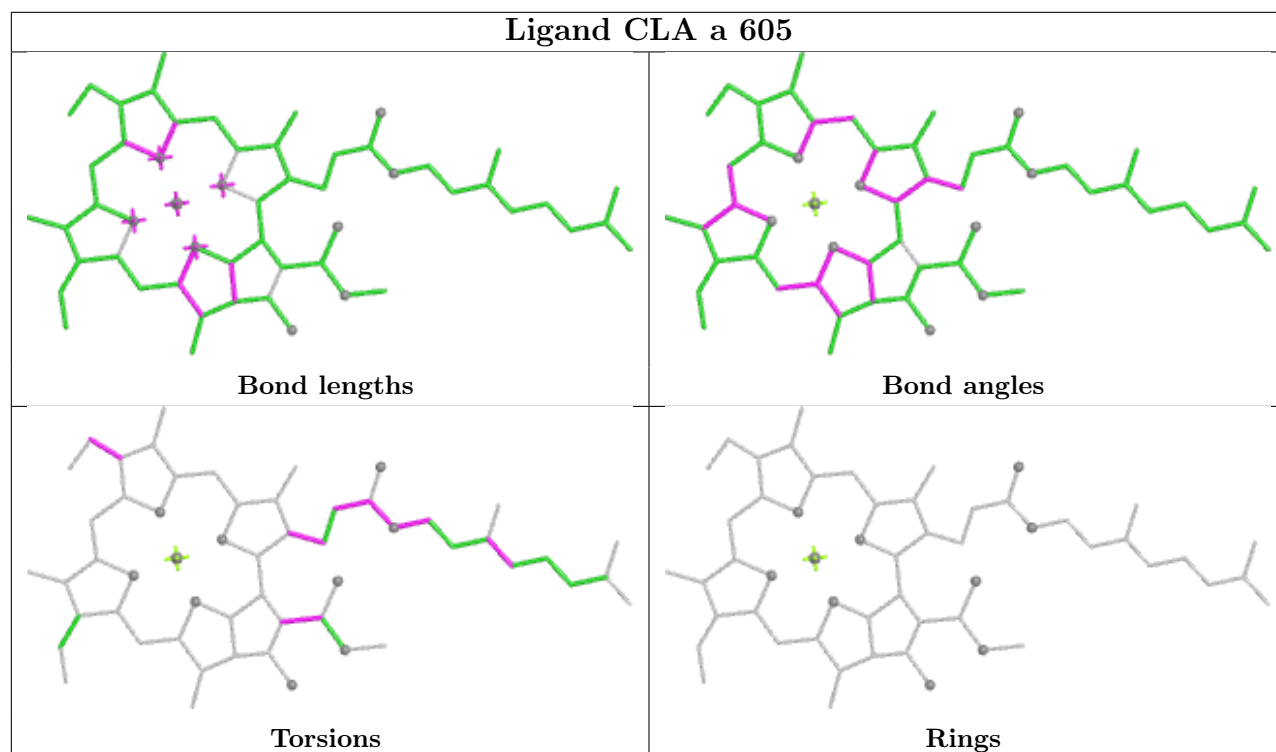
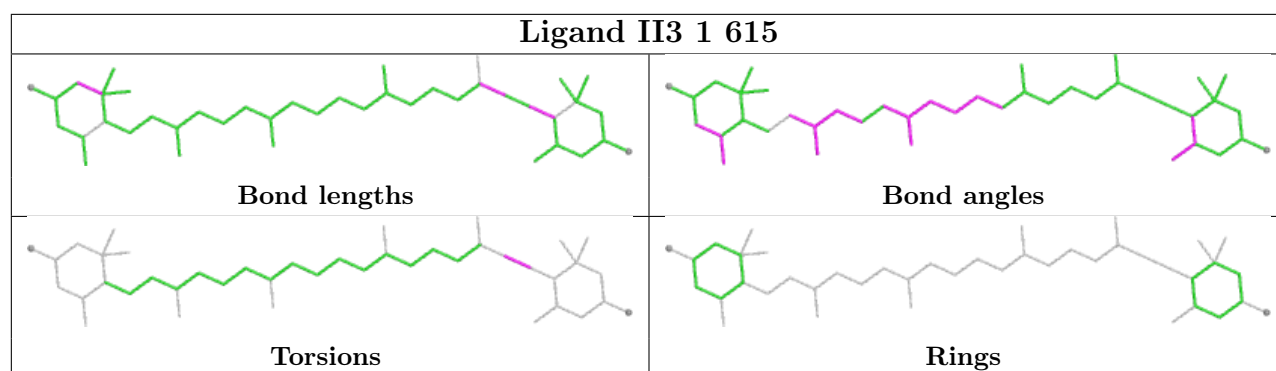




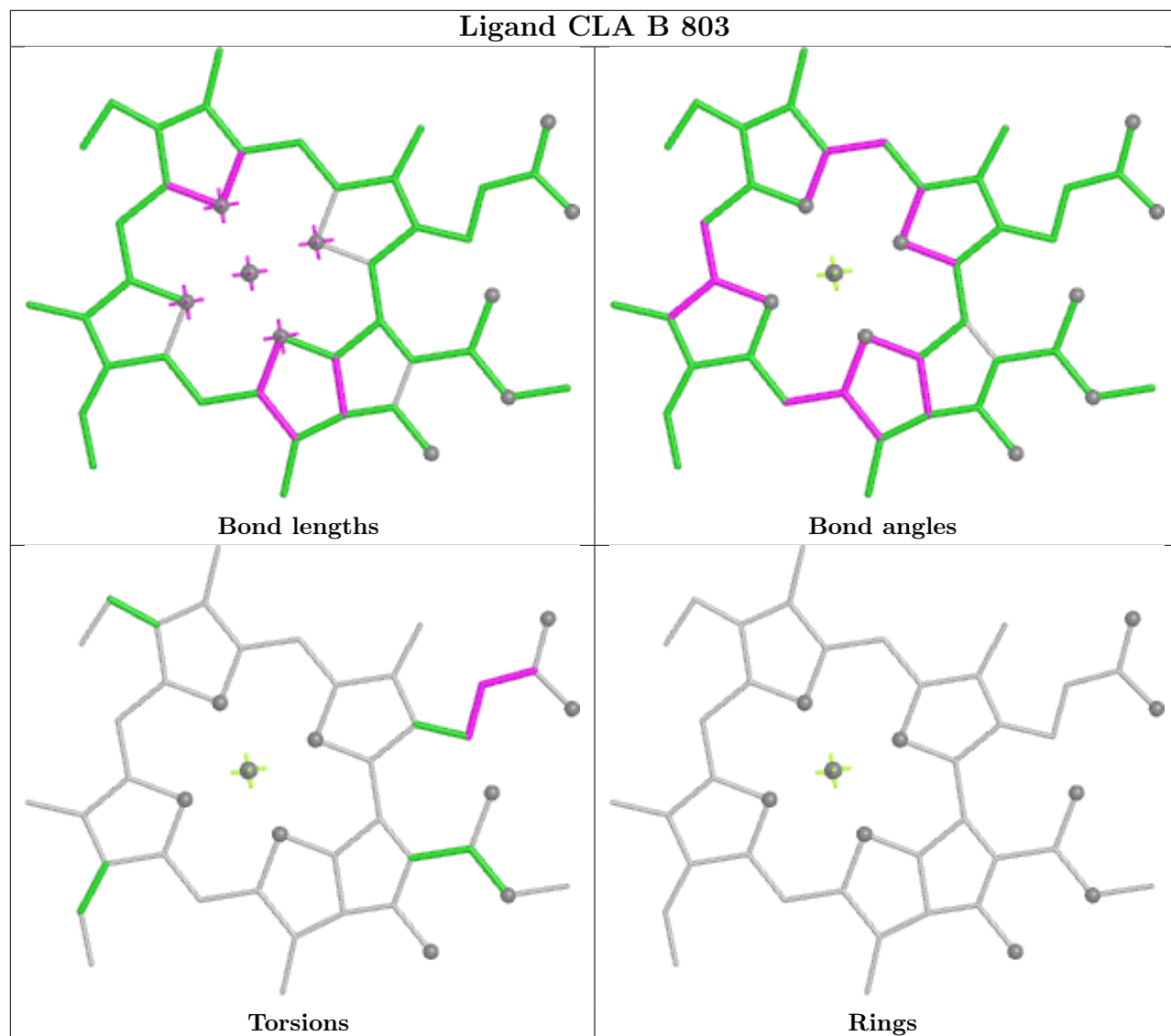




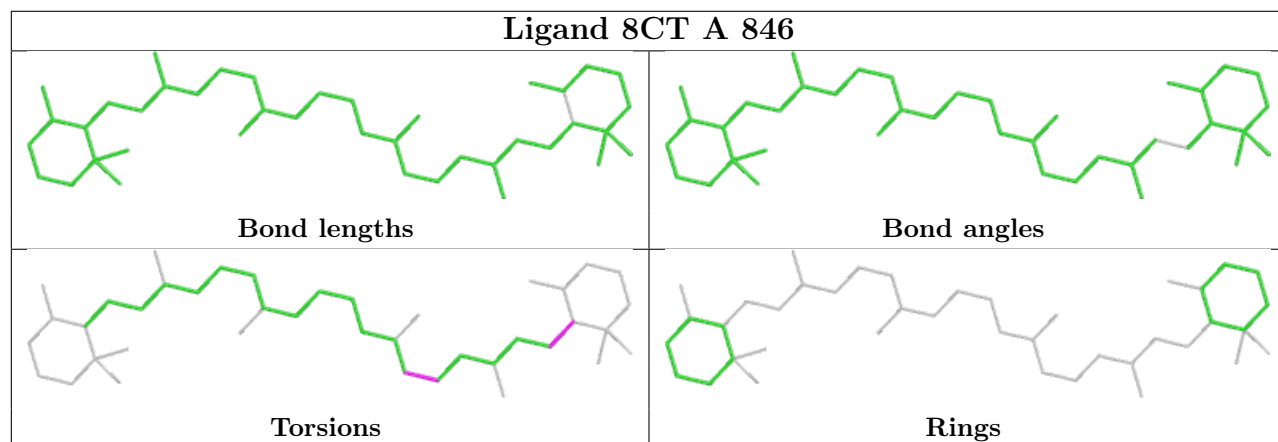


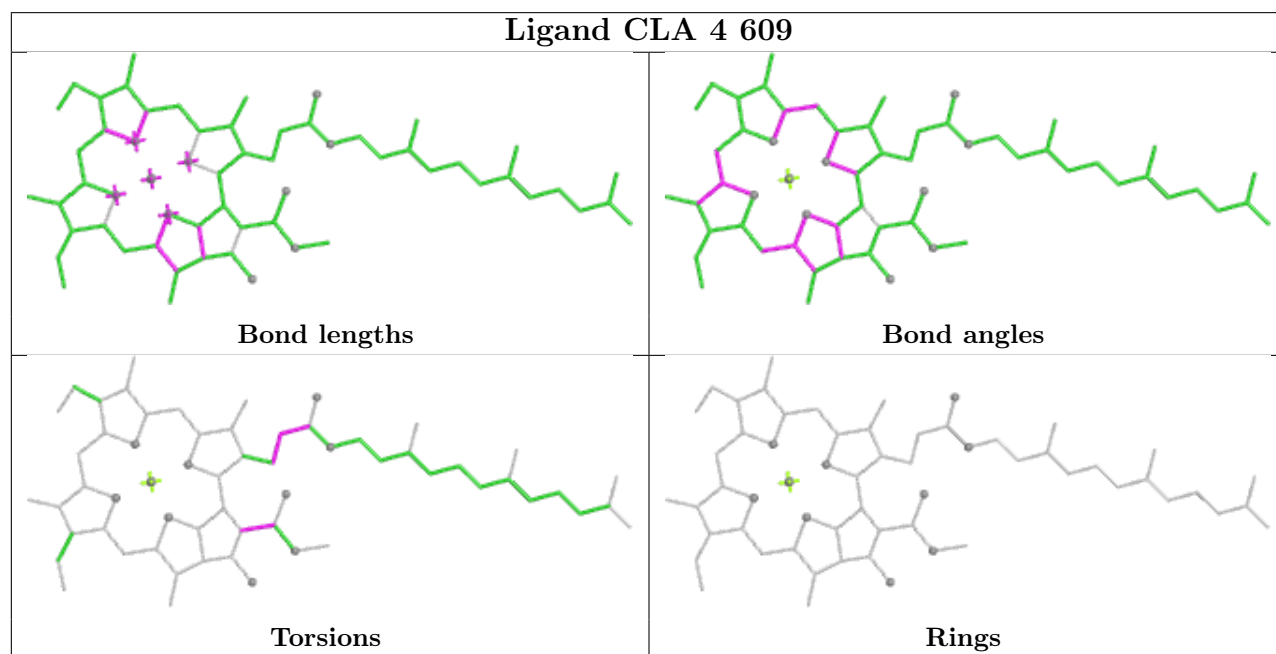
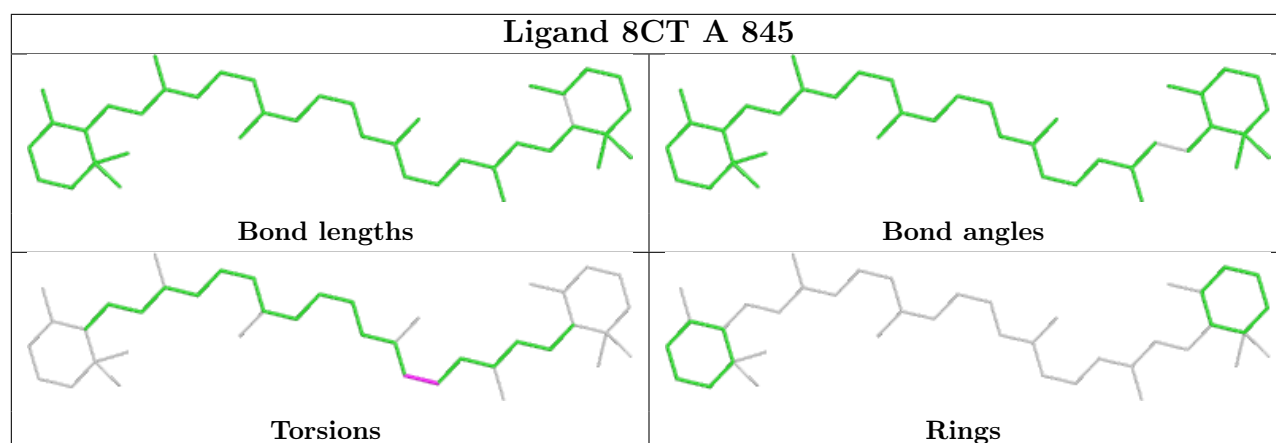


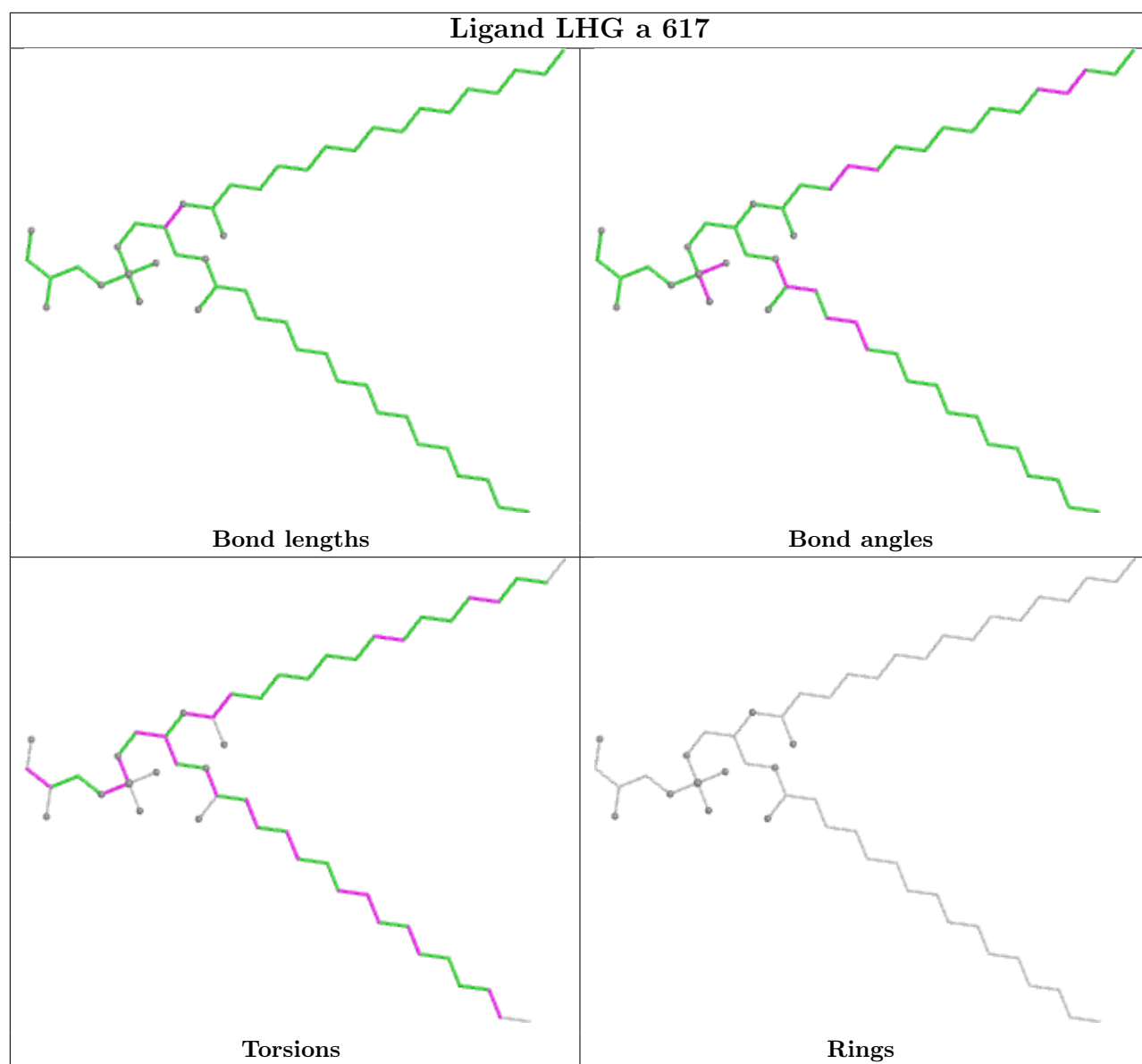
Ligand CLA B 803



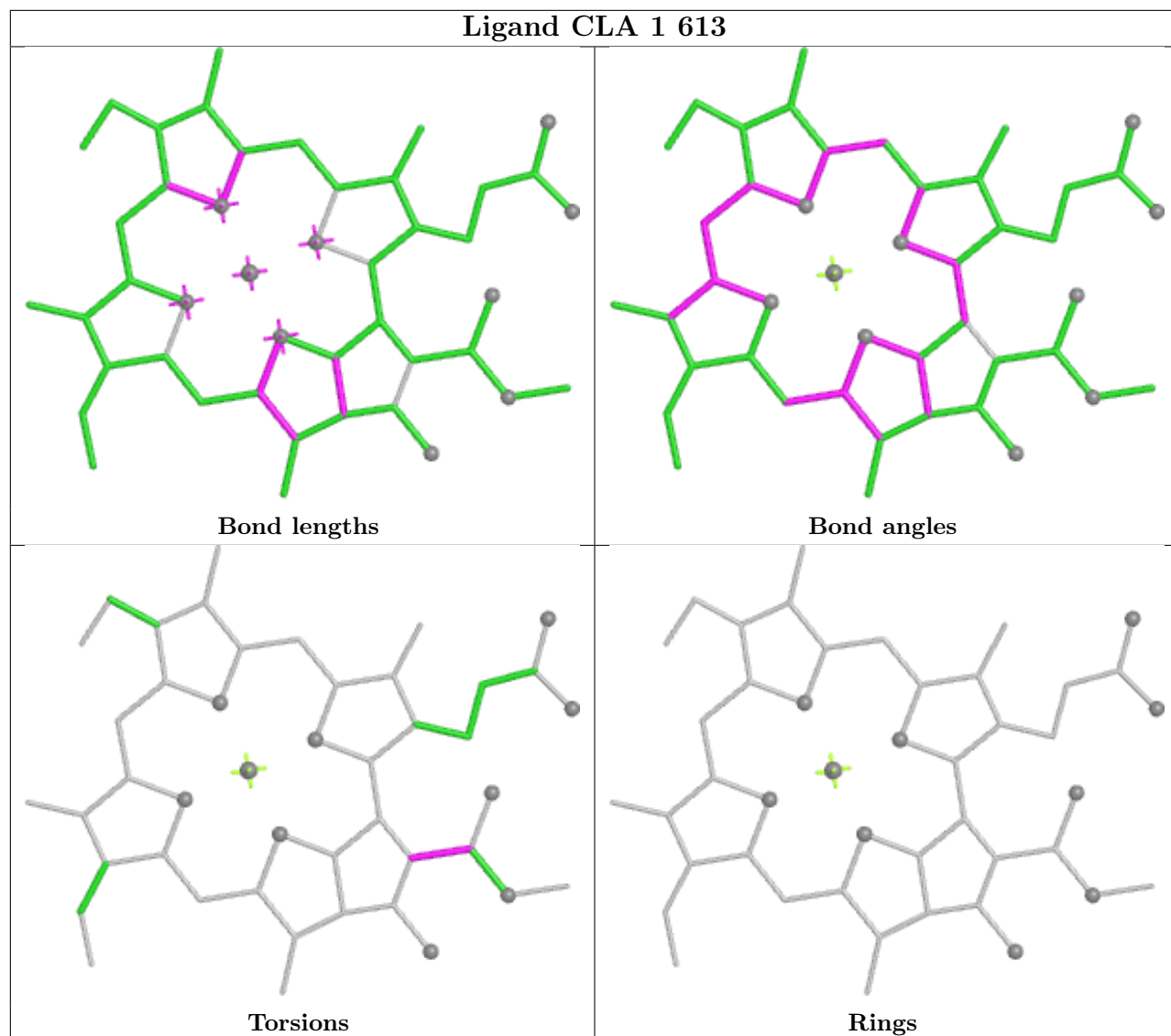
Ligand 8CT A 846



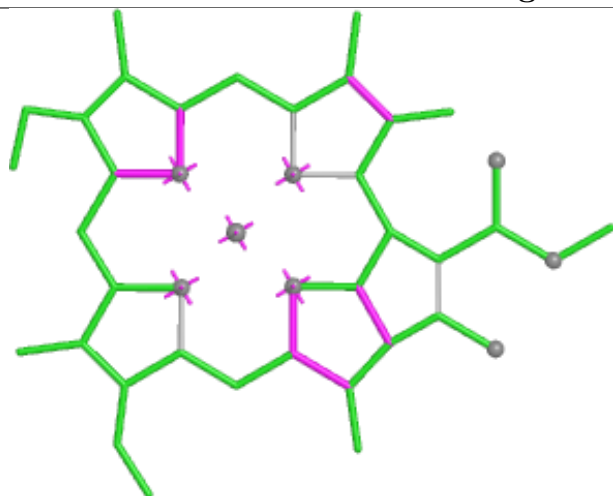




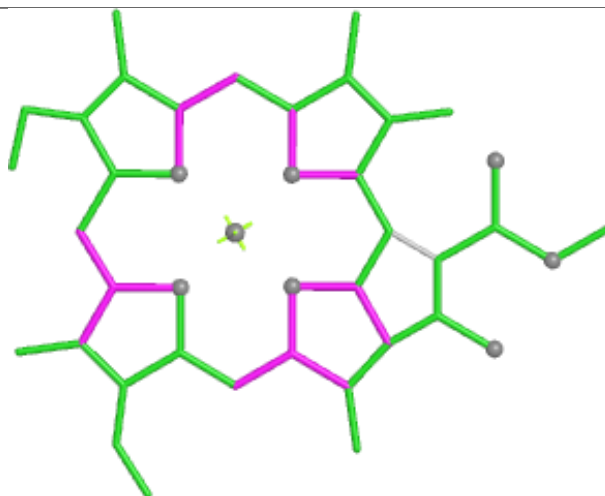
Ligand CLA 1 613



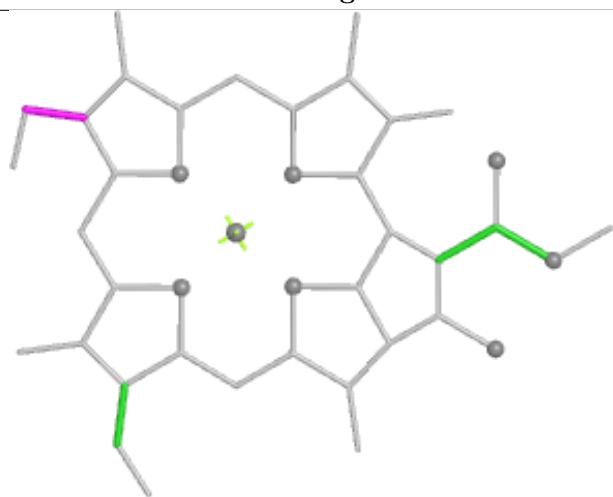
Ligand CLA 6 609



Bond lengths



Bond angles

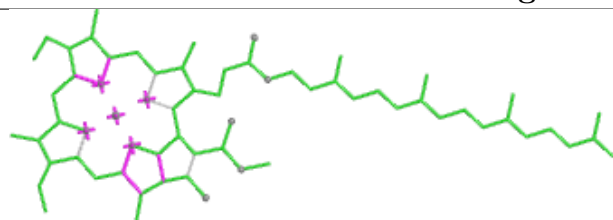


Torsions

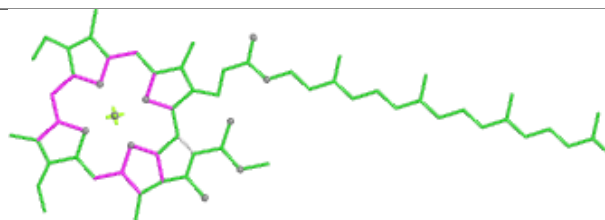


Rings

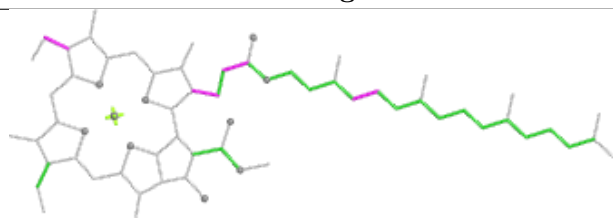
Ligand CLA a 611



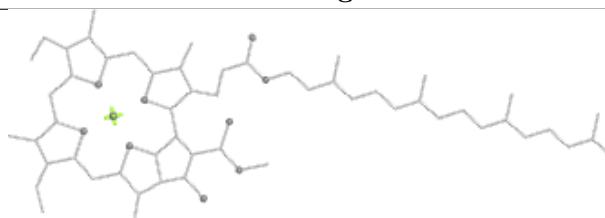
Bond lengths



Bond angles

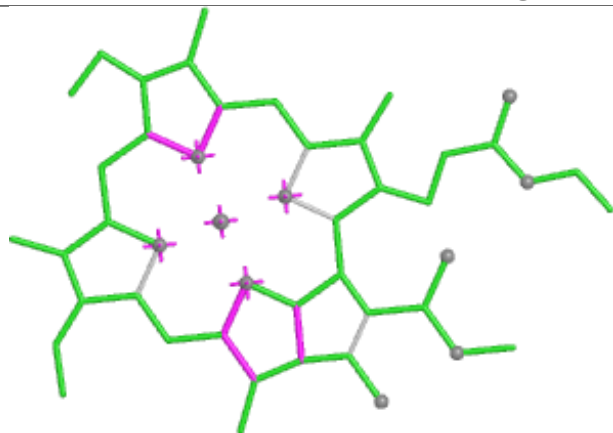


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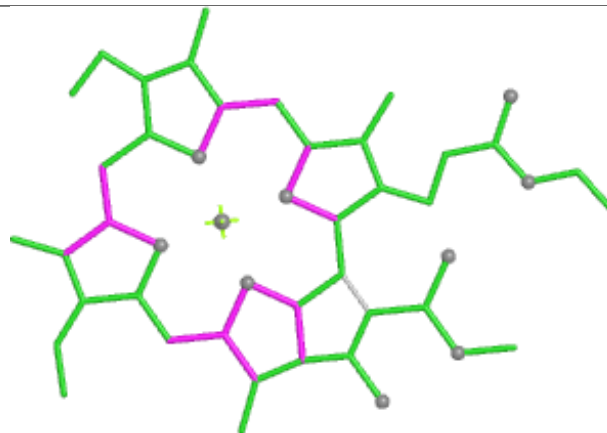


Rings

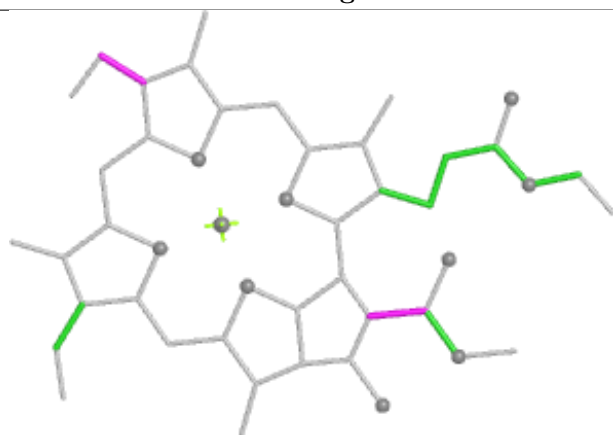
Ligand CLA B 836



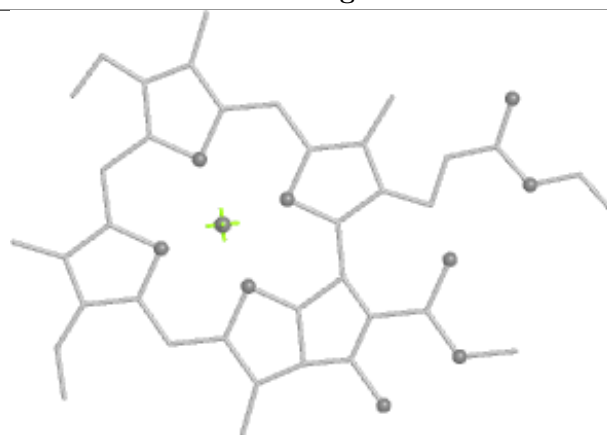
Bond lengths



Bond angles

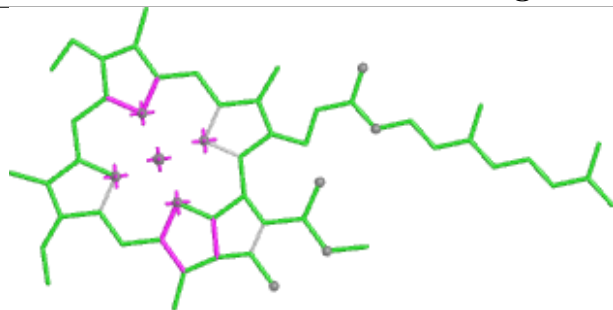


Torsions

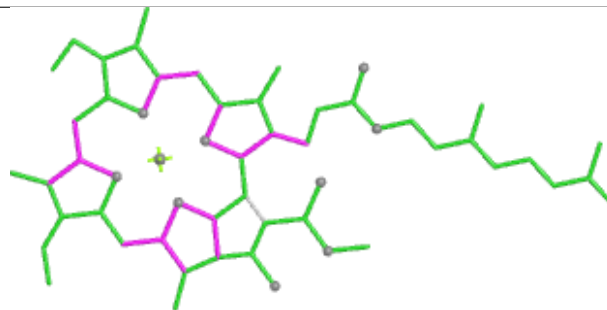


Rings

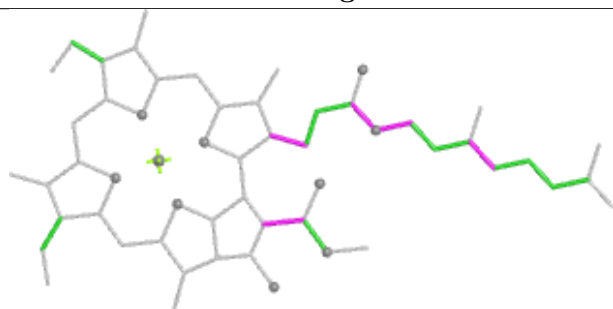
Ligand CLA O 204



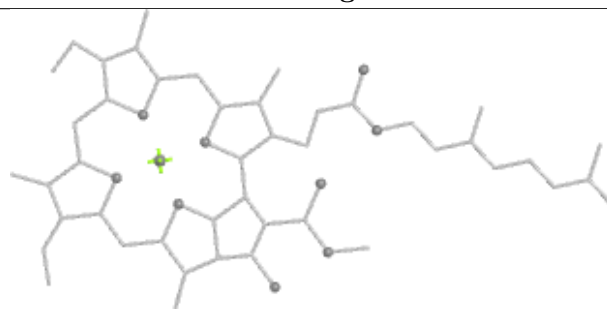
Bond lengths



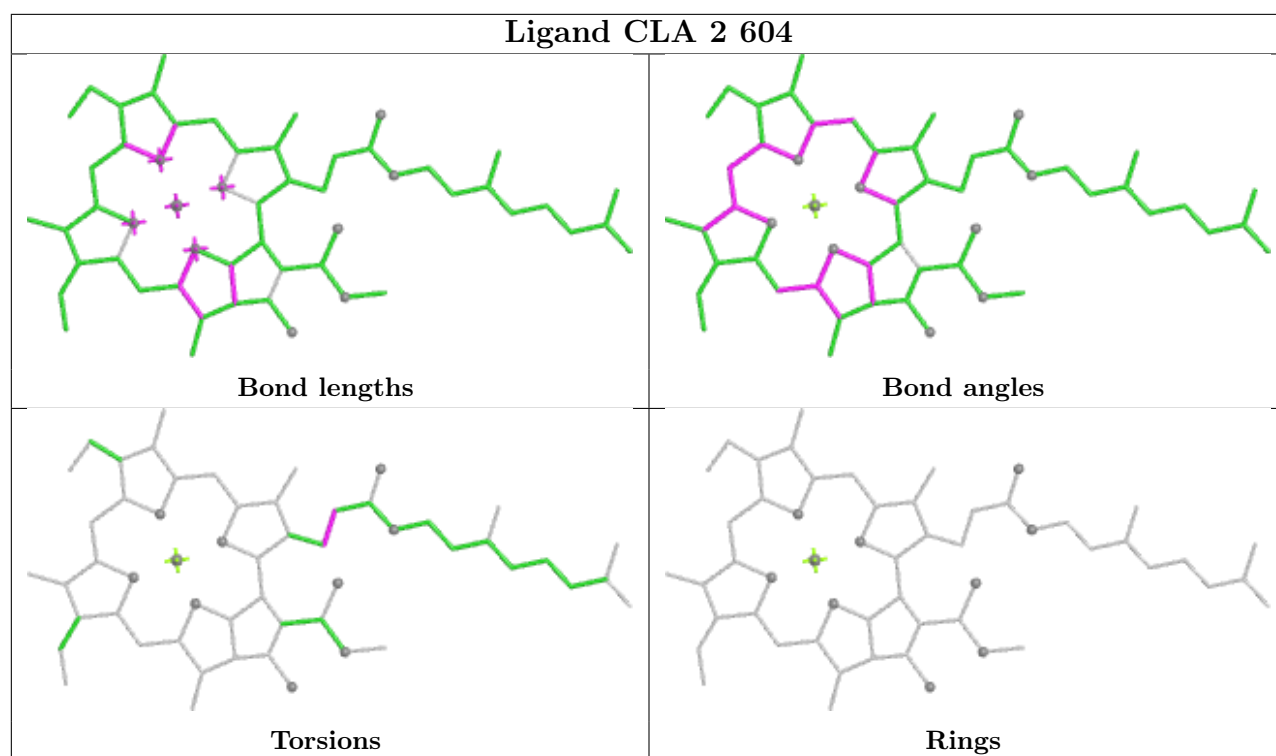
Bond angles



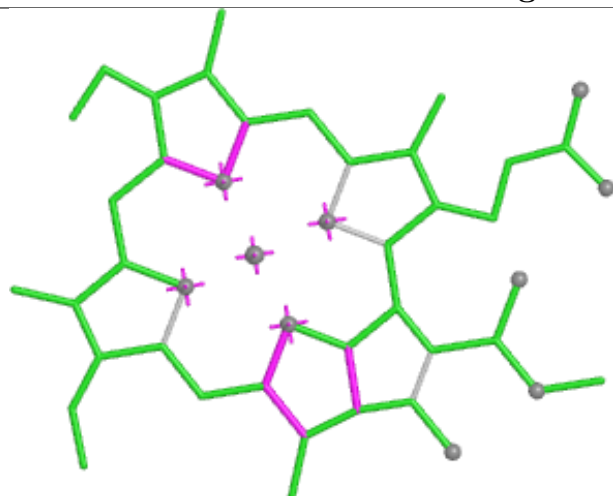
Torsions



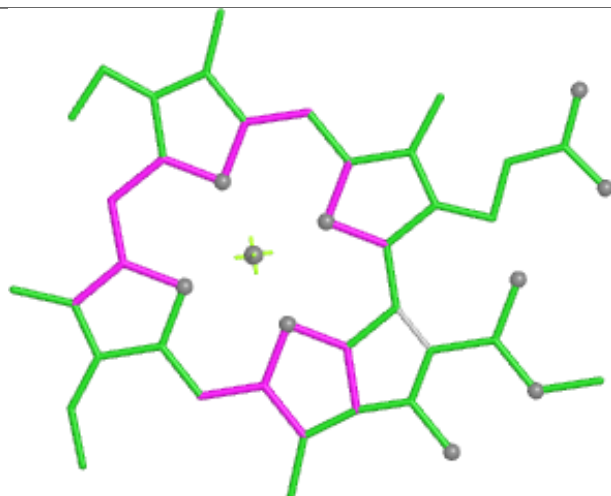
Rings



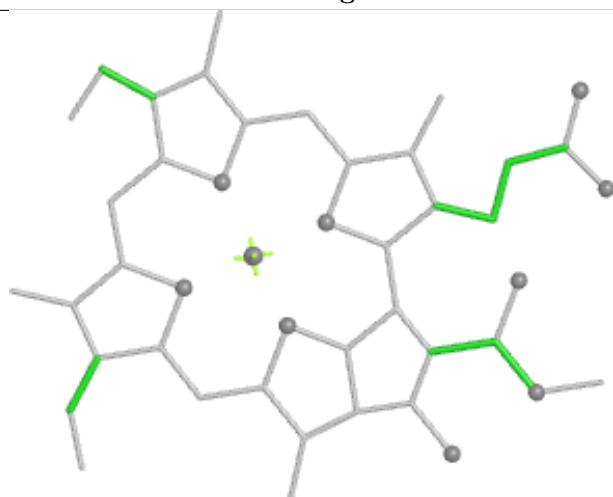
Ligand CLA 1 606



Bond lengths



Bond angles

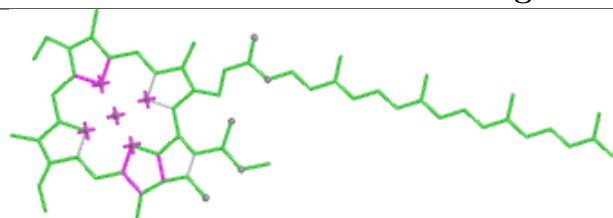


Torsions

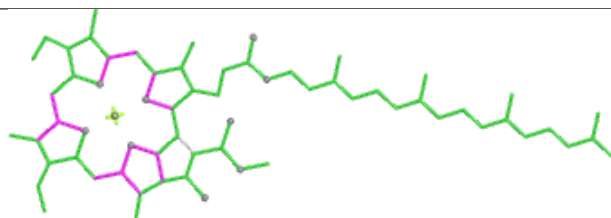


Rings

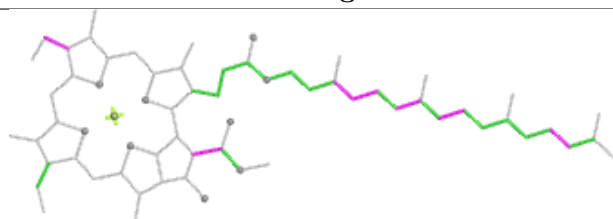
Ligand CLA B 807



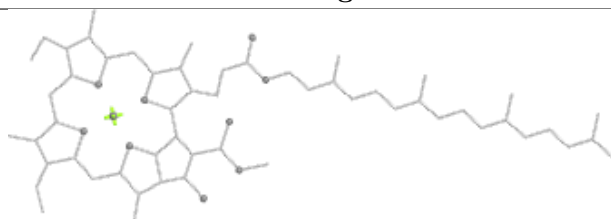
Bond lengths



Bond angles

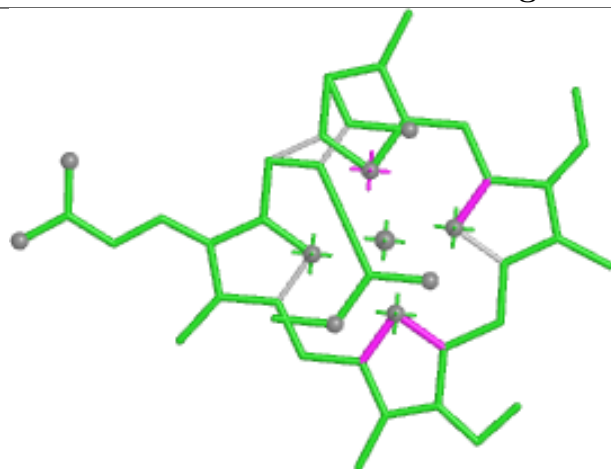


Torsions

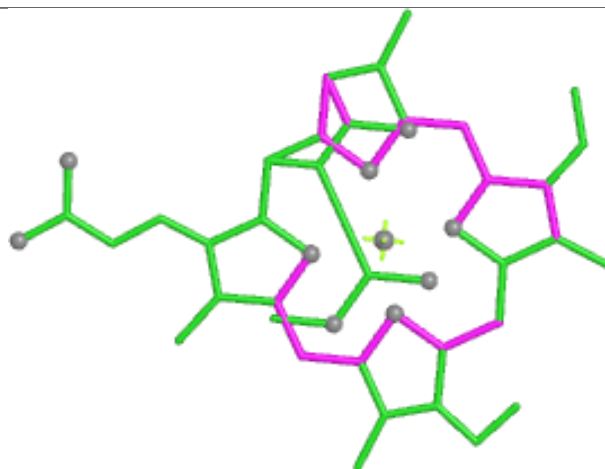


Rings

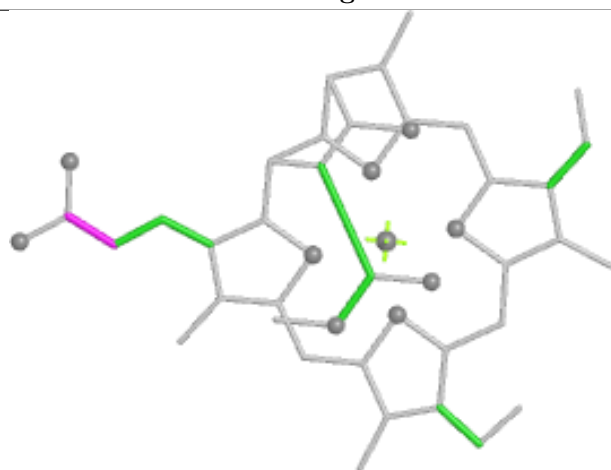
Ligand KC2 b 609



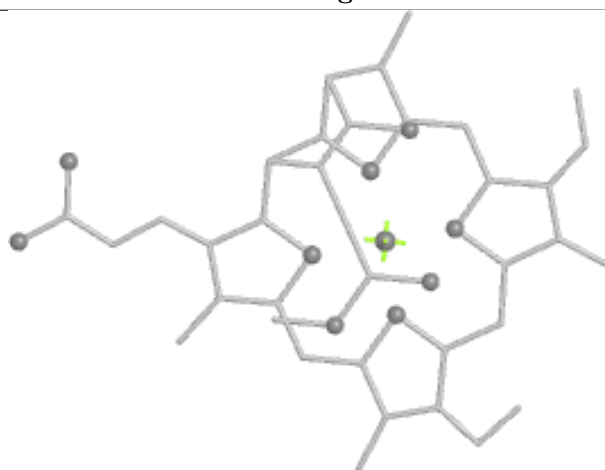
Bond lengths



Bond angles



Torsions



Rings

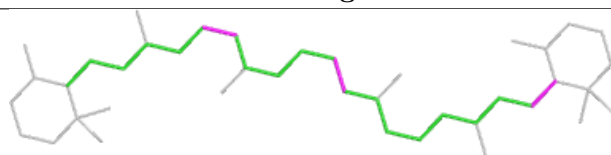
Ligand 8CT F 201



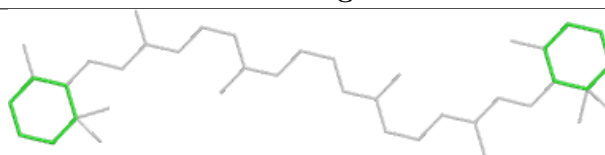
Bond lengths



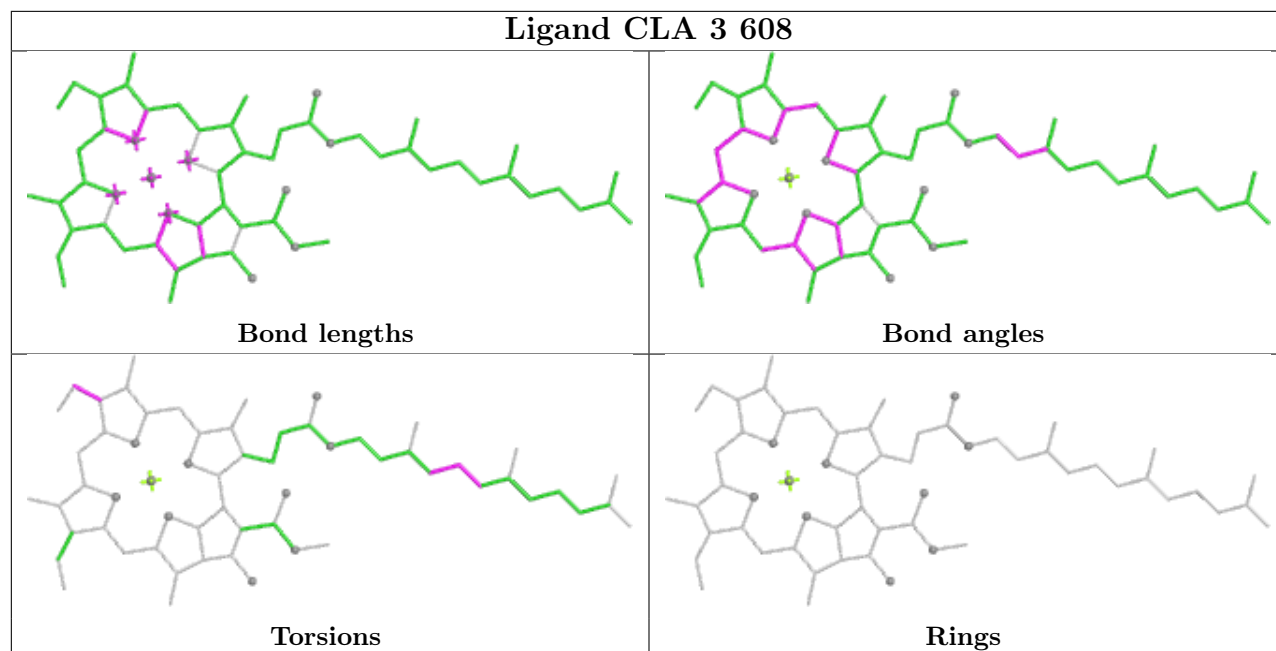
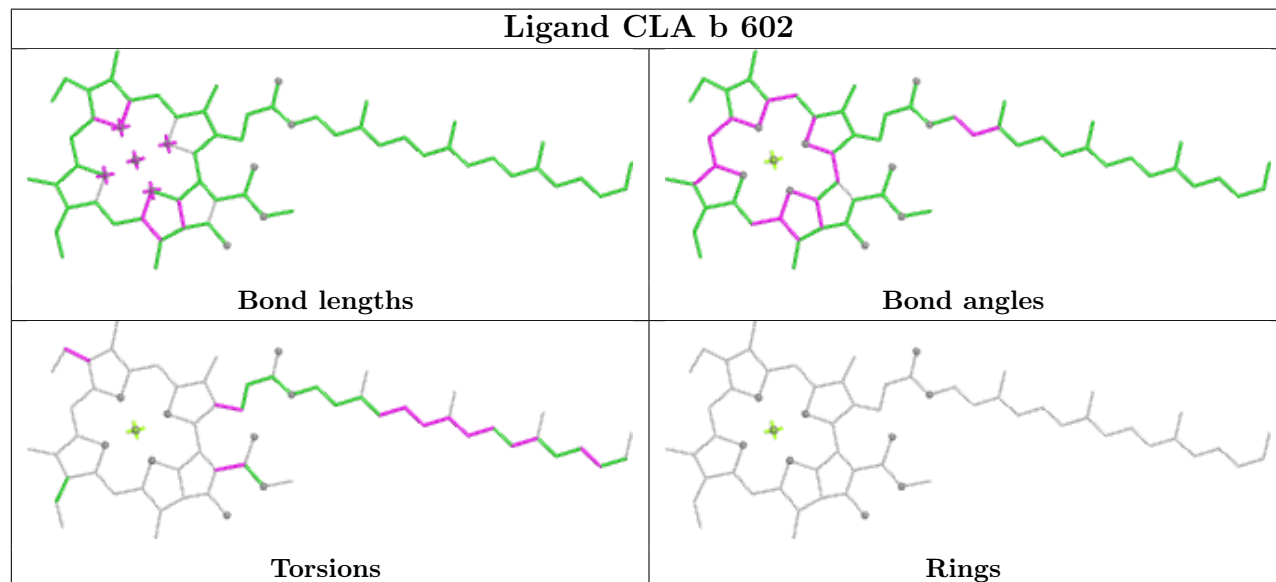
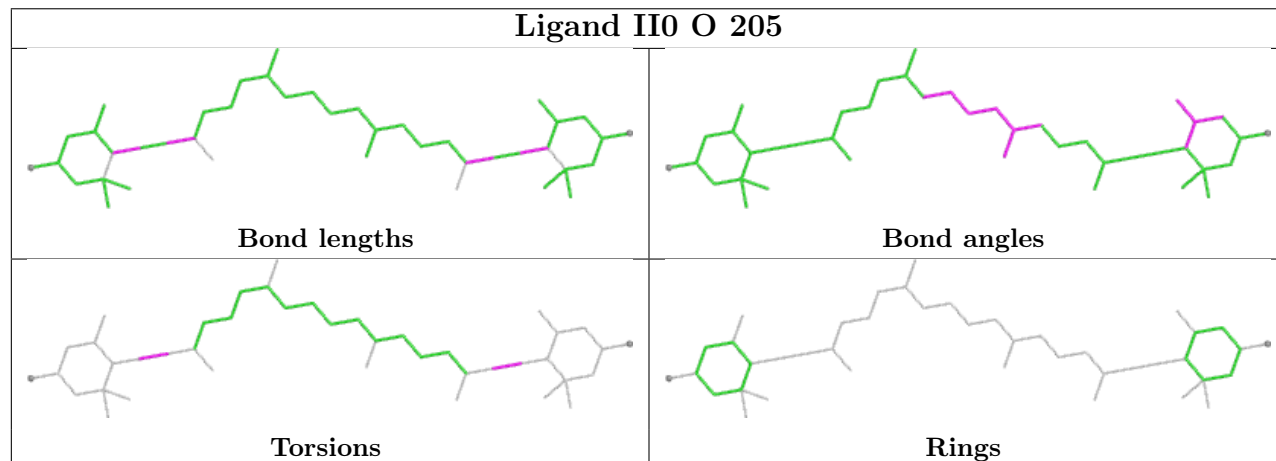
Bond angles

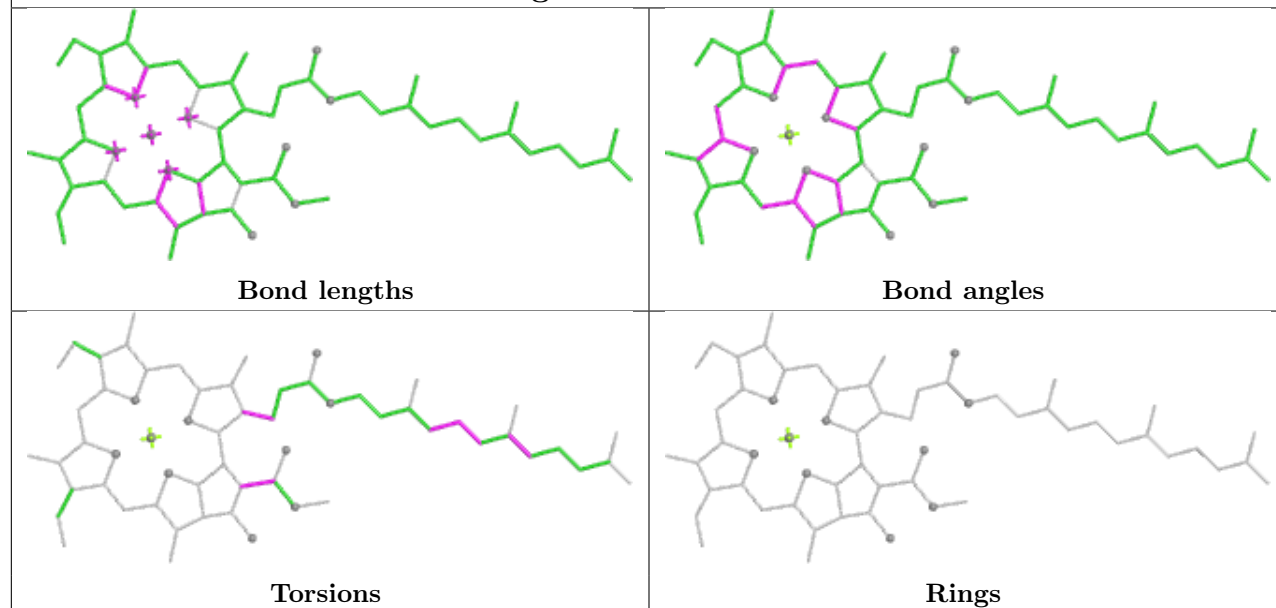
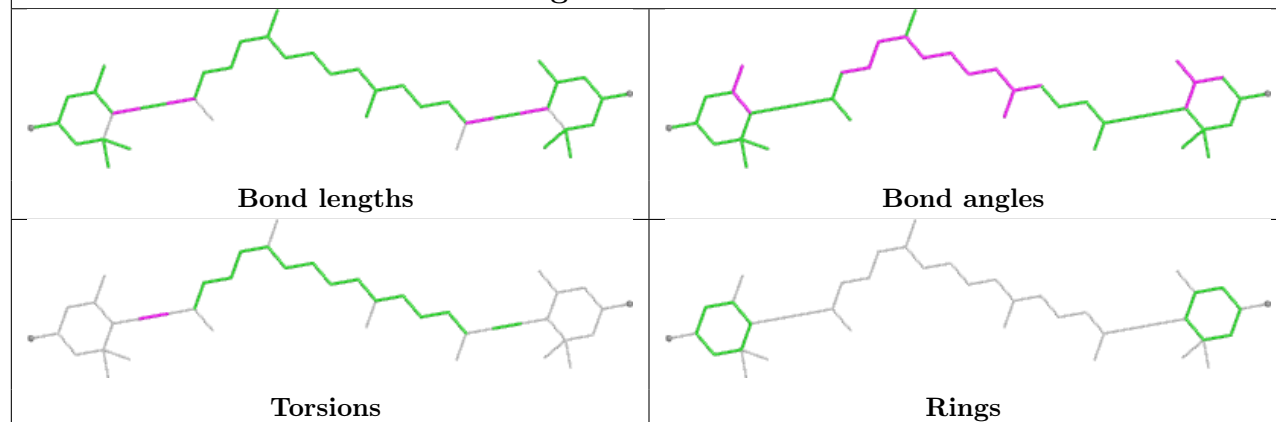


Torsions

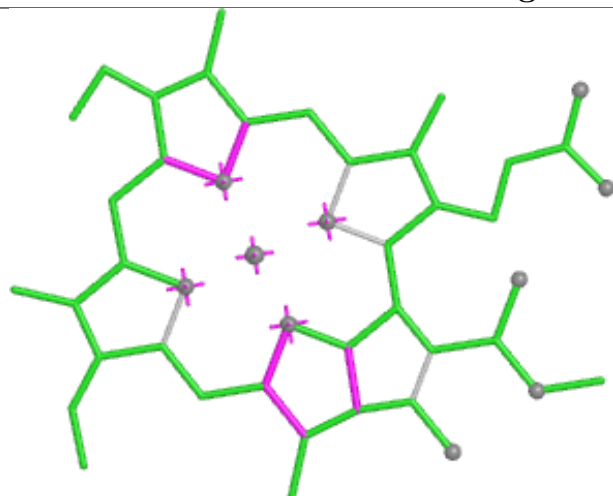


Rings

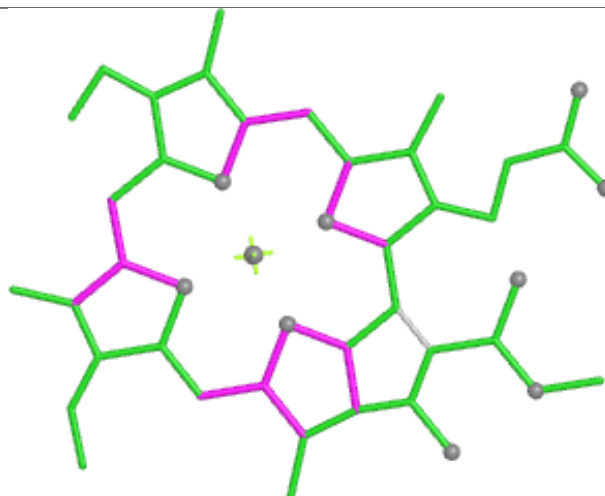
Ligand CLA 3 608**Ligand CLA b 602****Ligand II0 O 205**

Ligand CLA A 835**Ligand II0 7 317**

Ligand CLA 6 601



Bond lengths



Bond angles

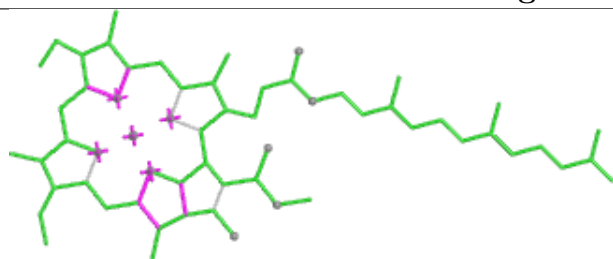


Torsions

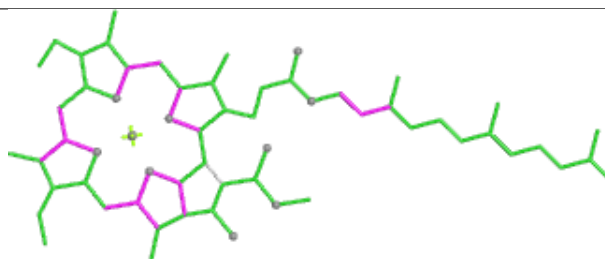


Rings

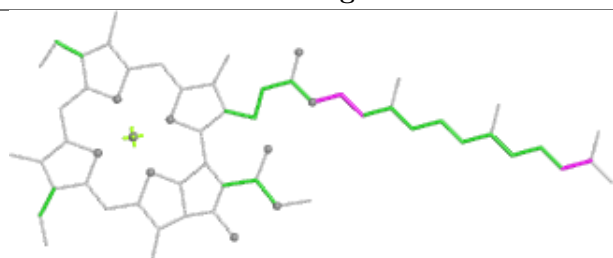
Ligand CLA 4 606



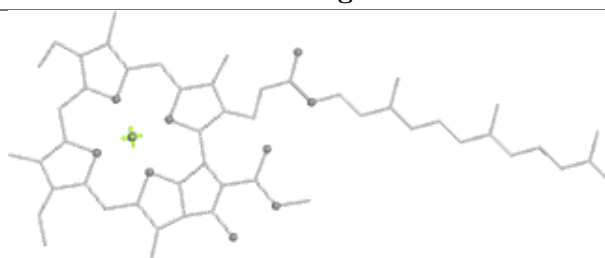
Bond lengths



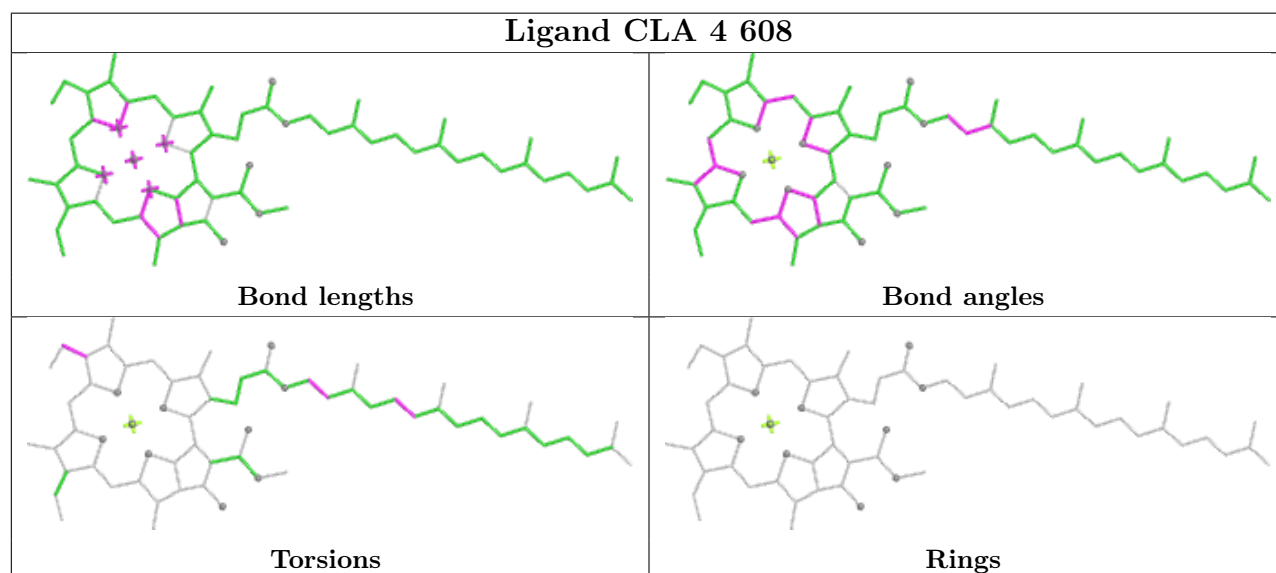
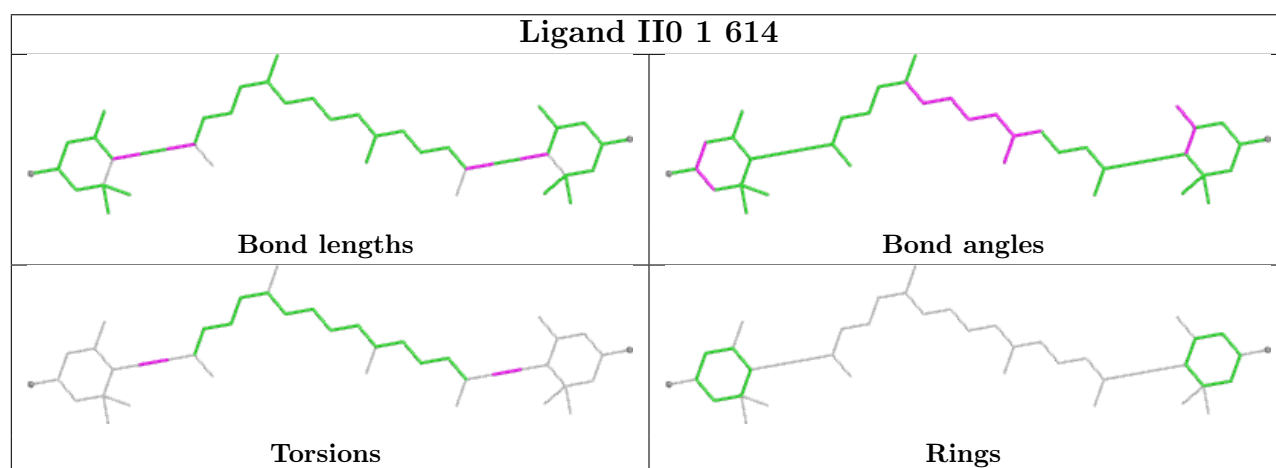
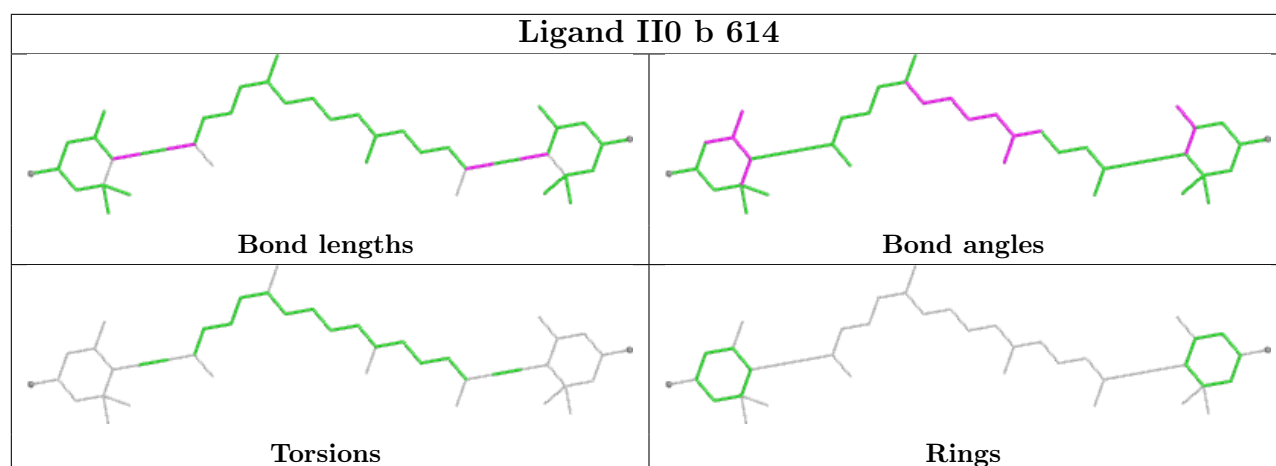
Bond angles

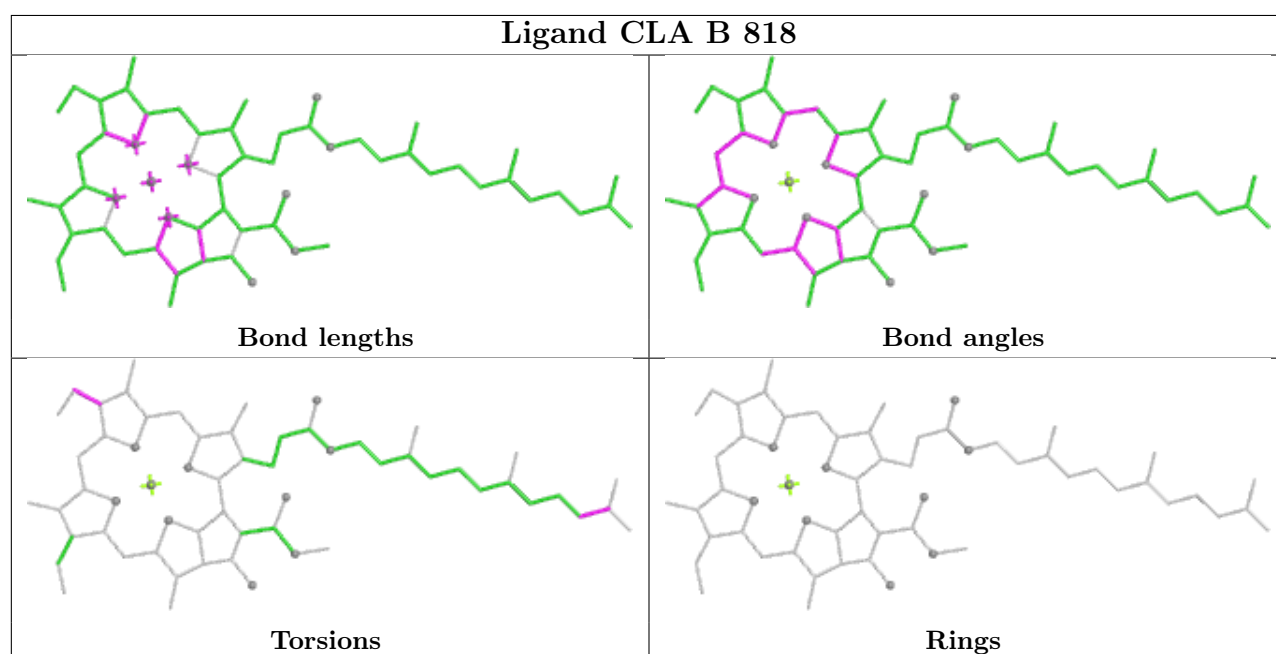
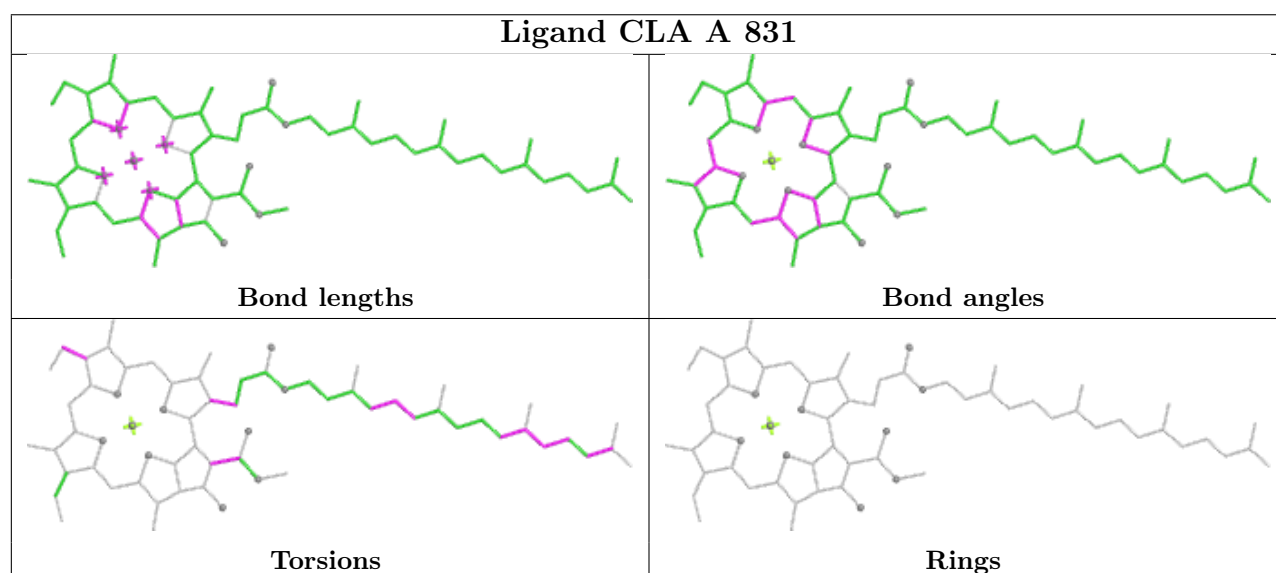
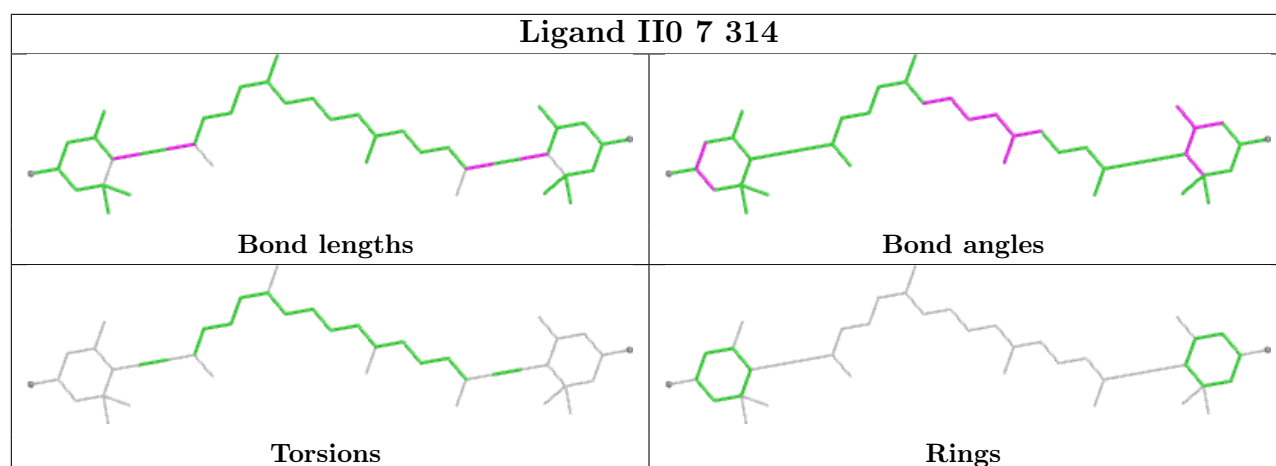


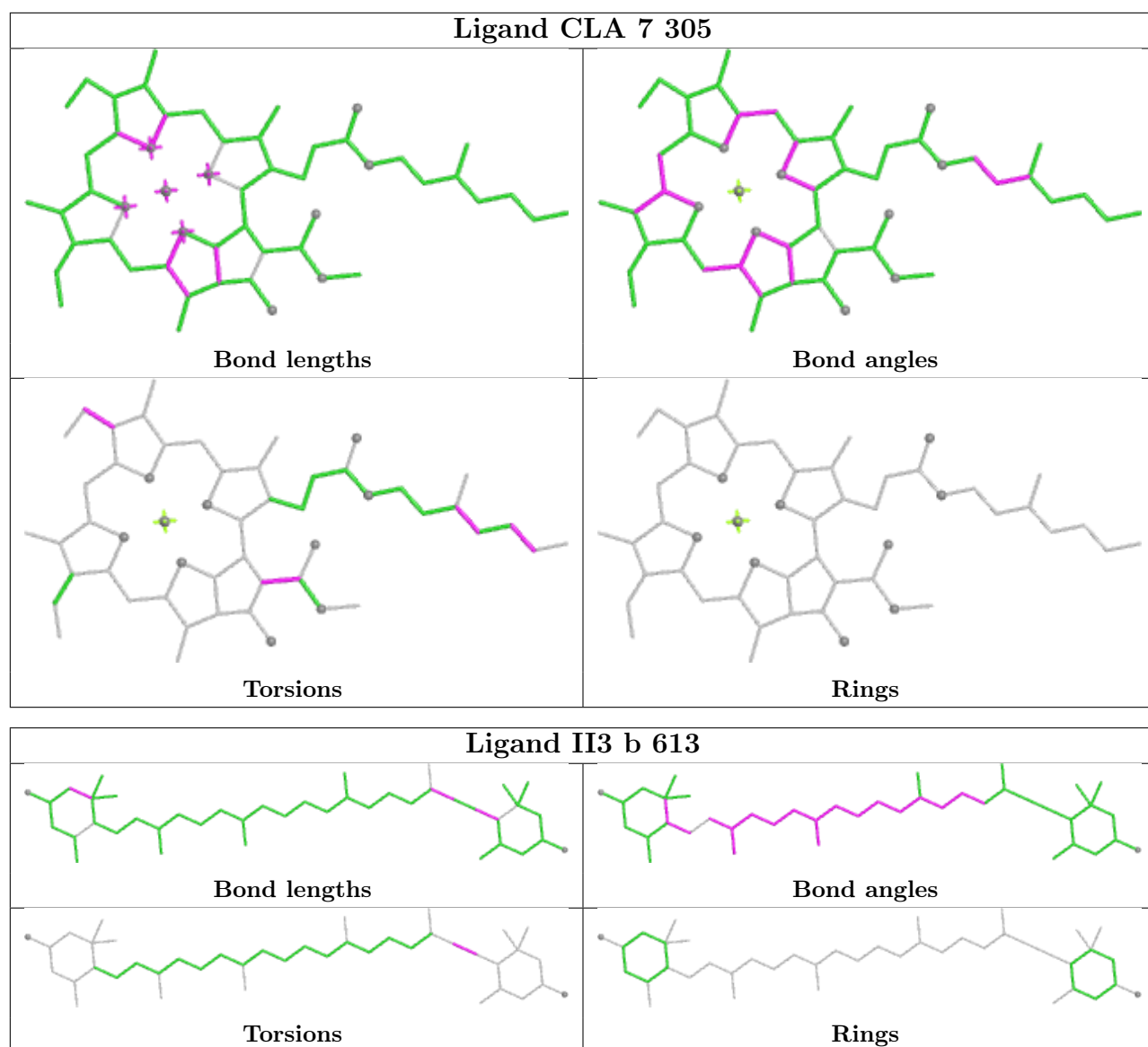
Torsions

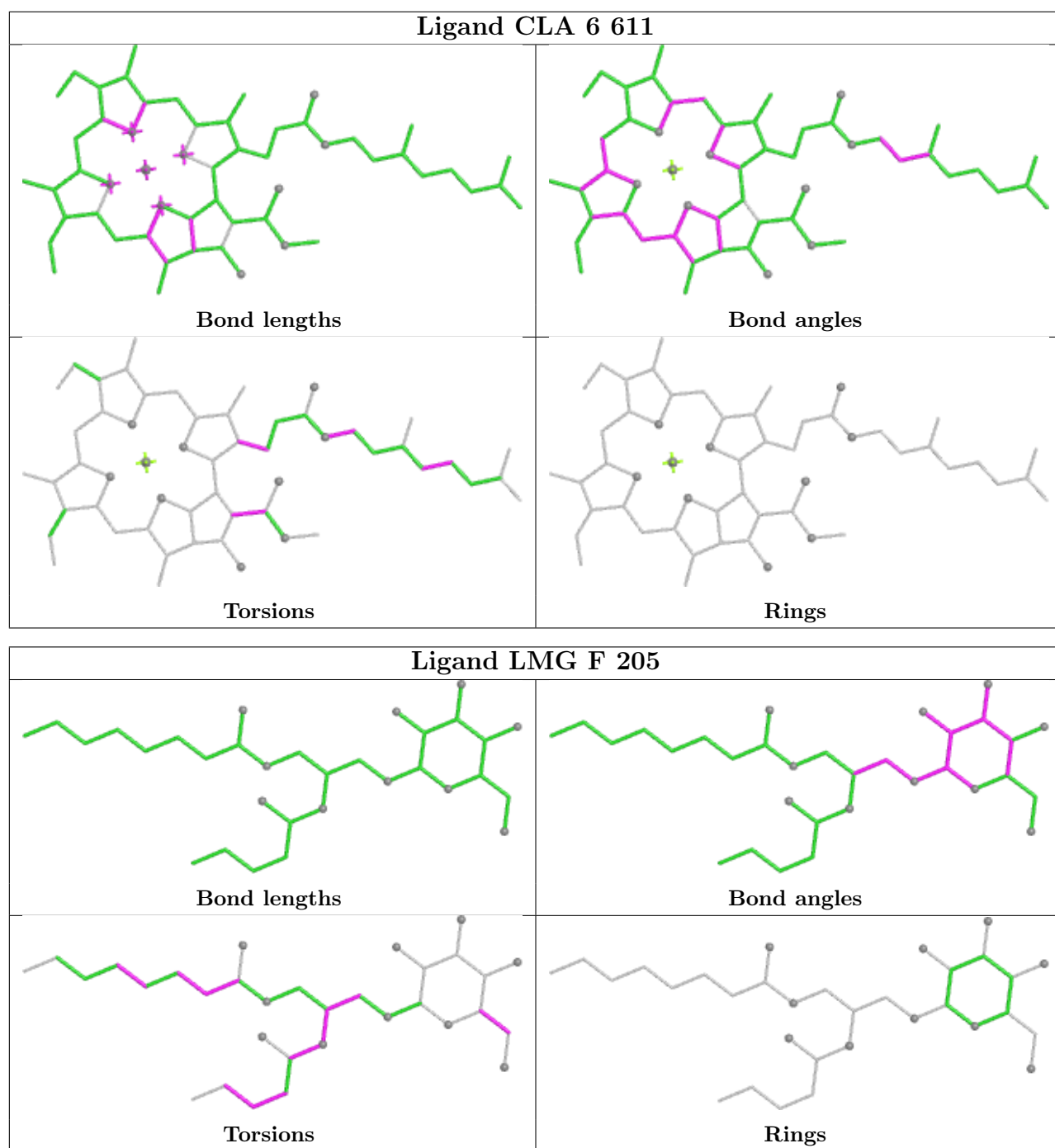


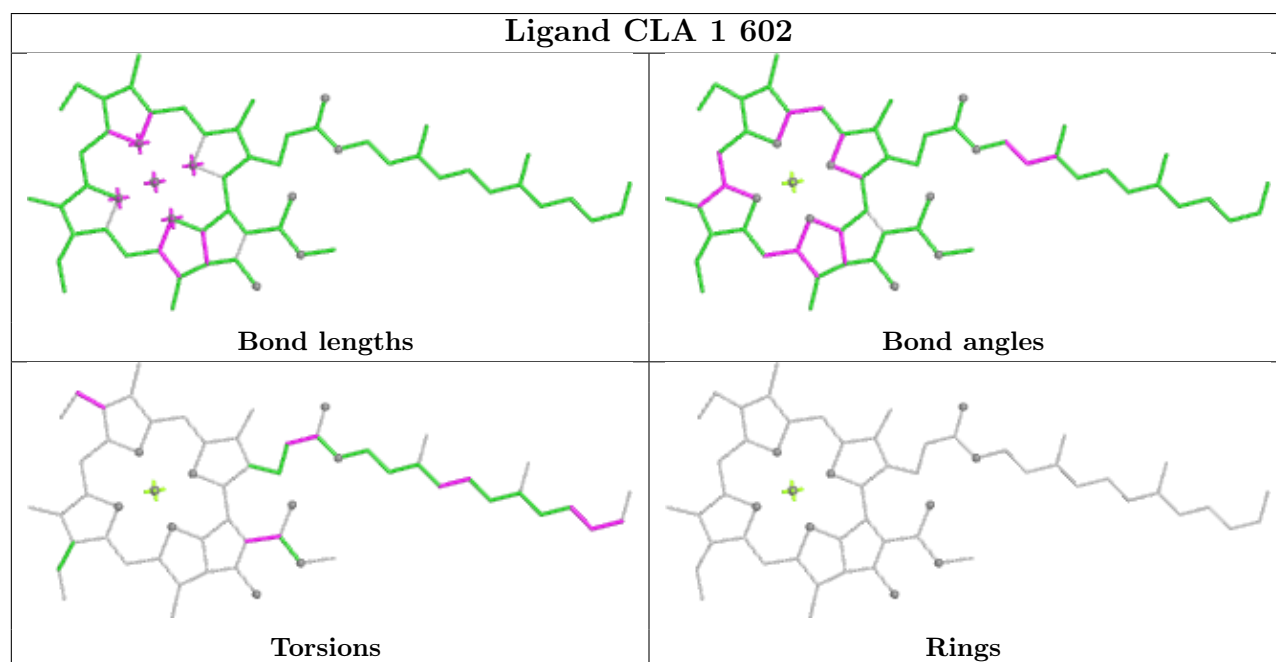
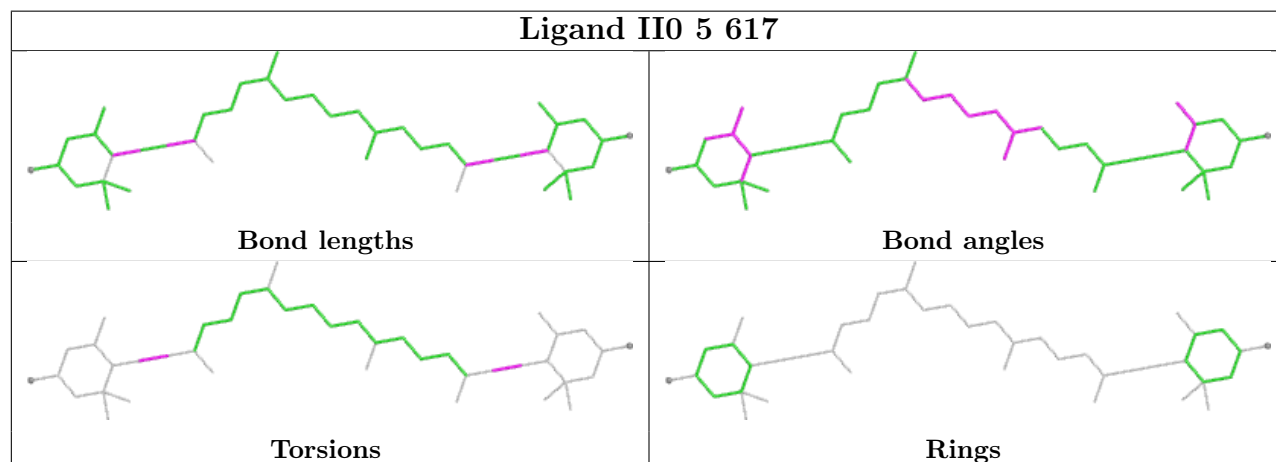
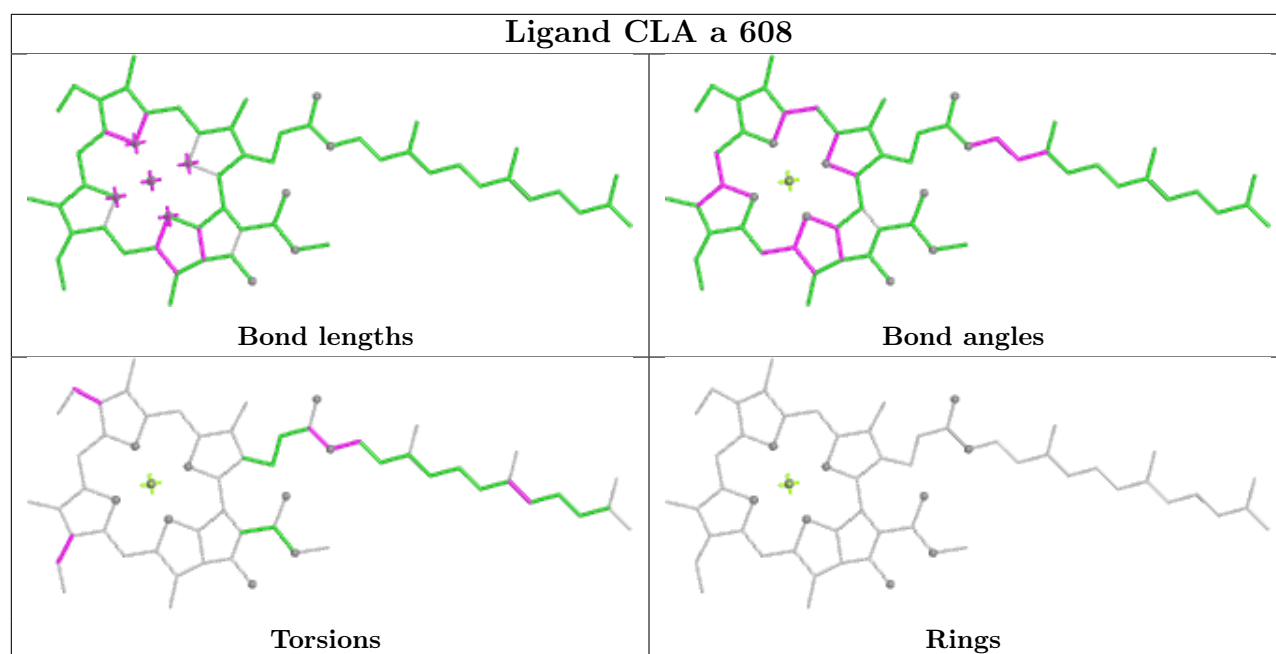
Rings

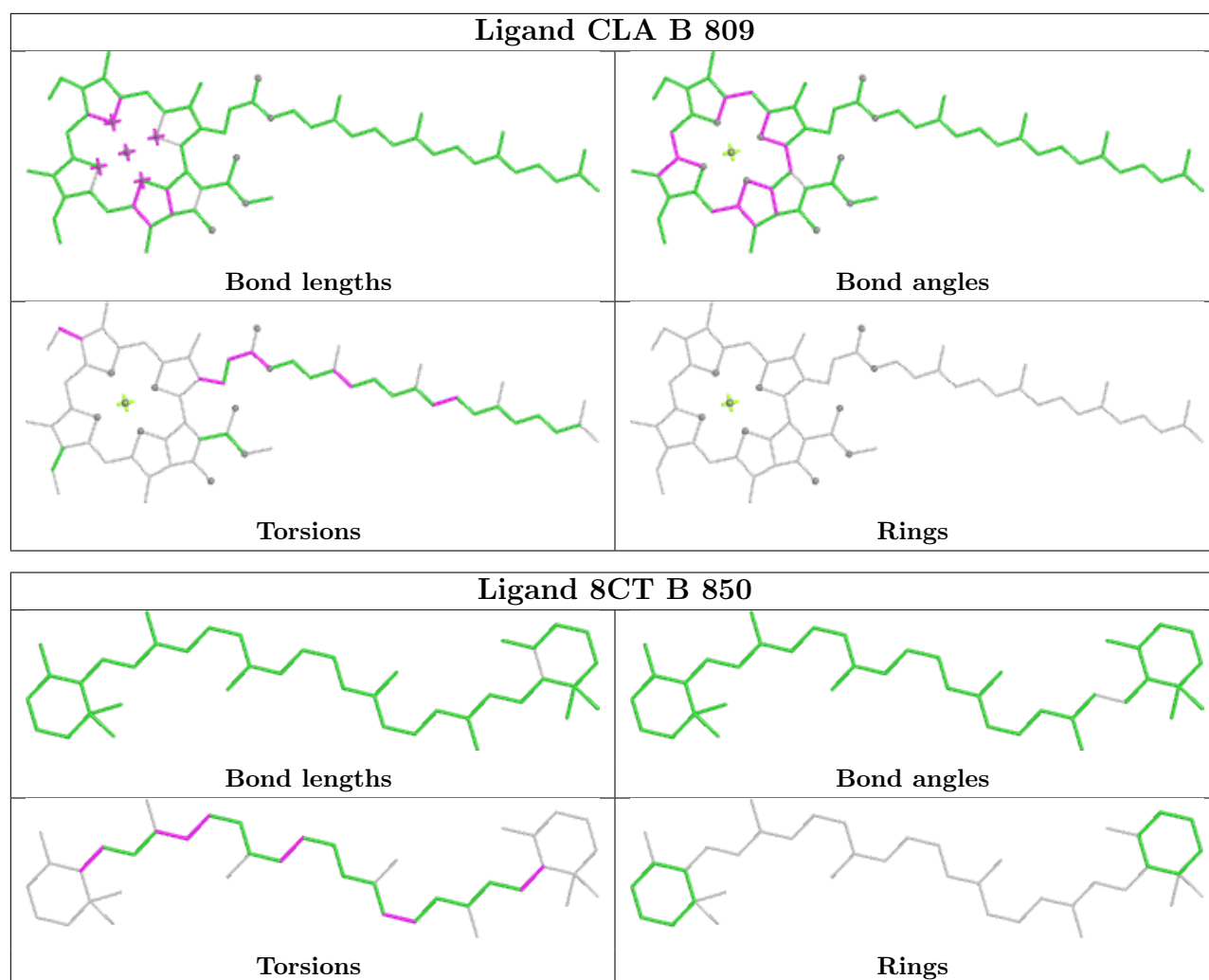




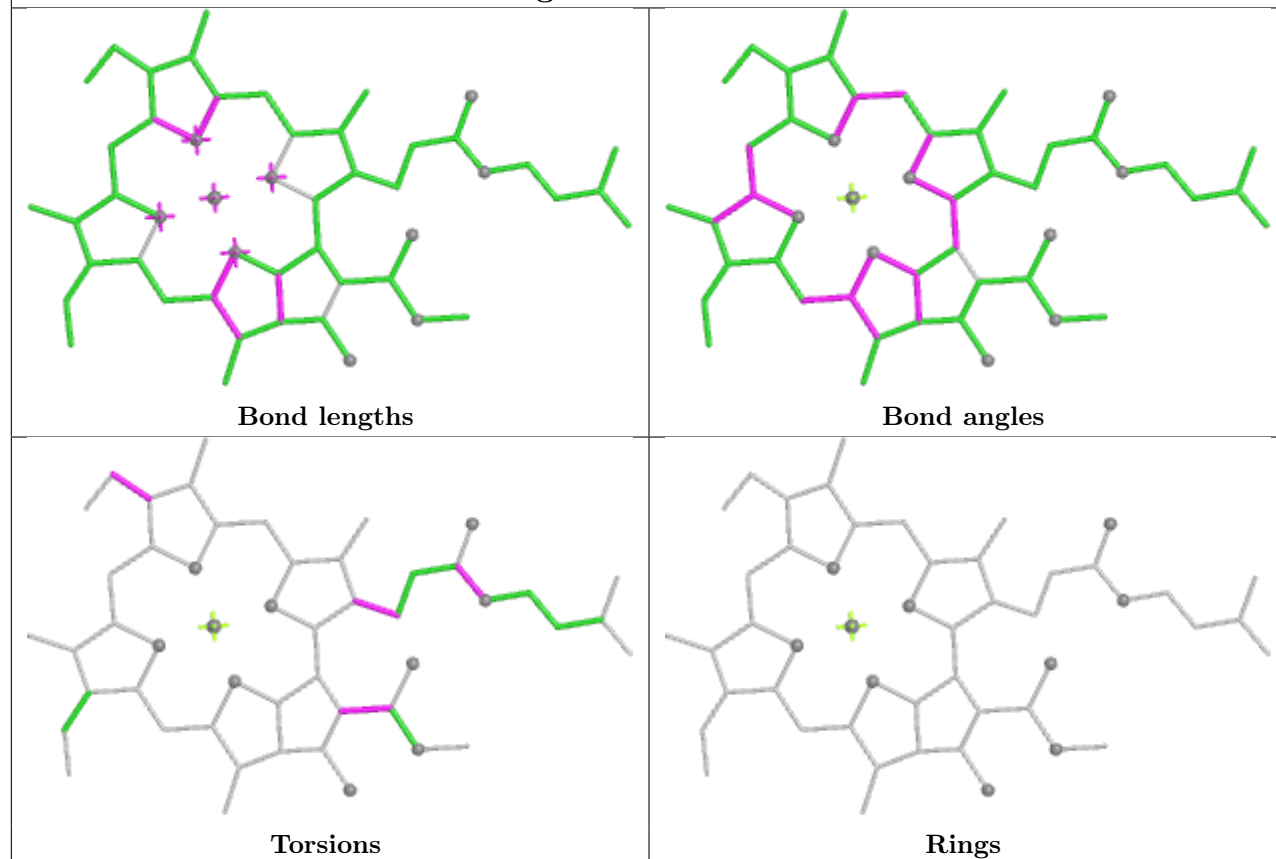




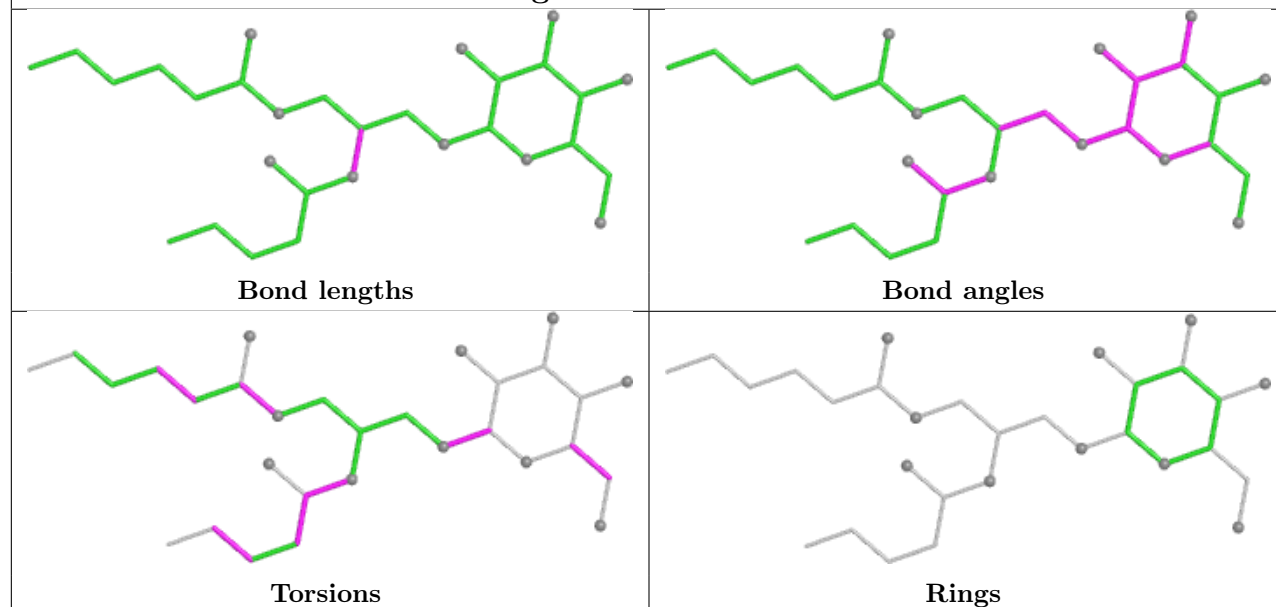


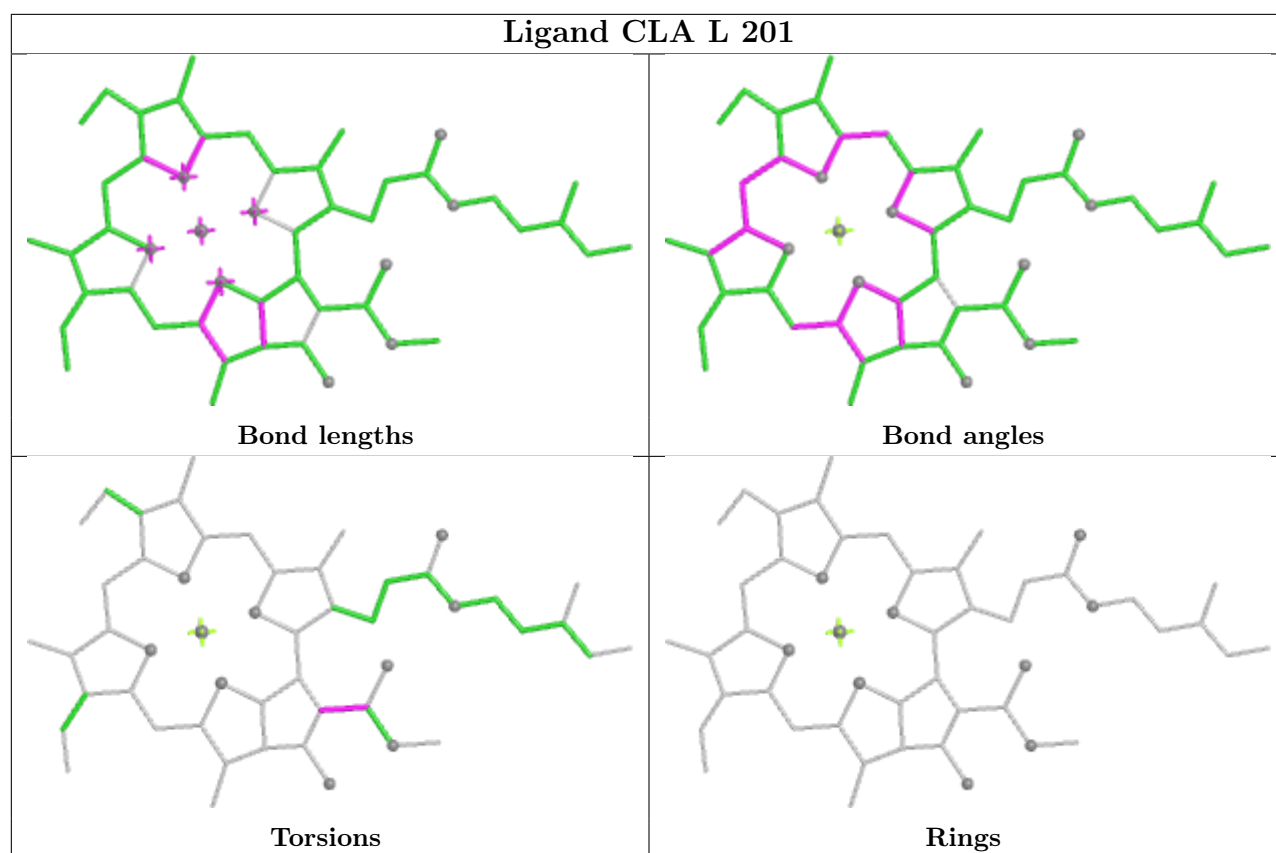


Ligand CLA 7 313

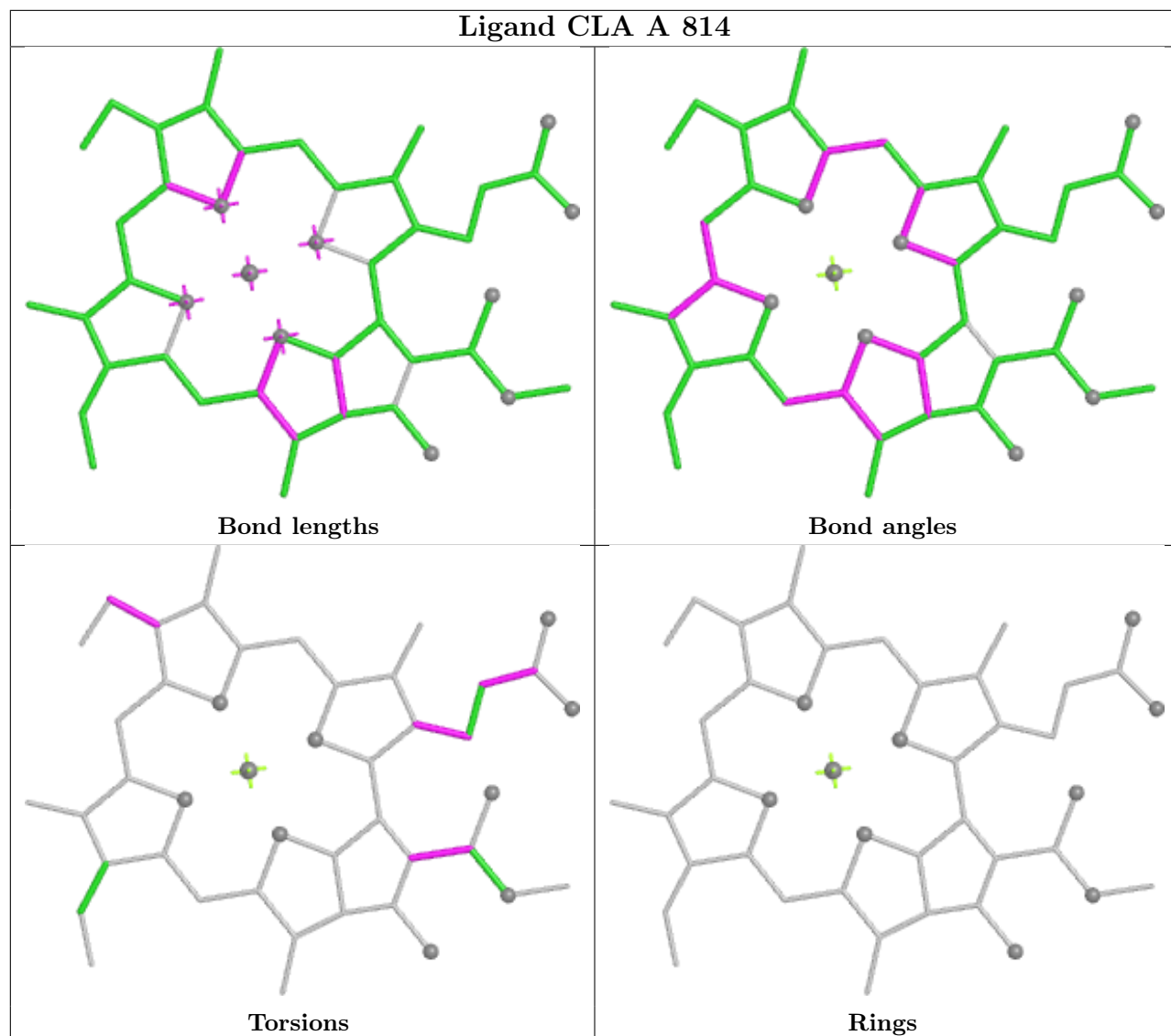


Ligand LMG 3 618

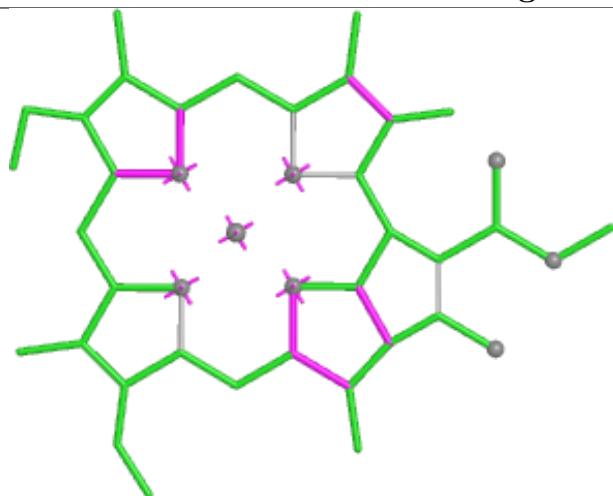




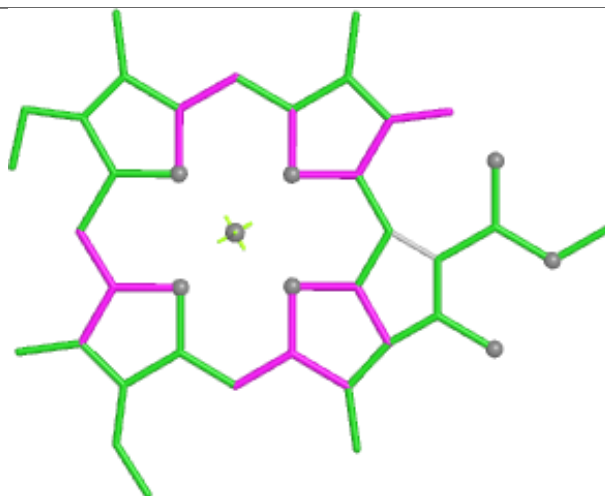
Ligand CLA A 814



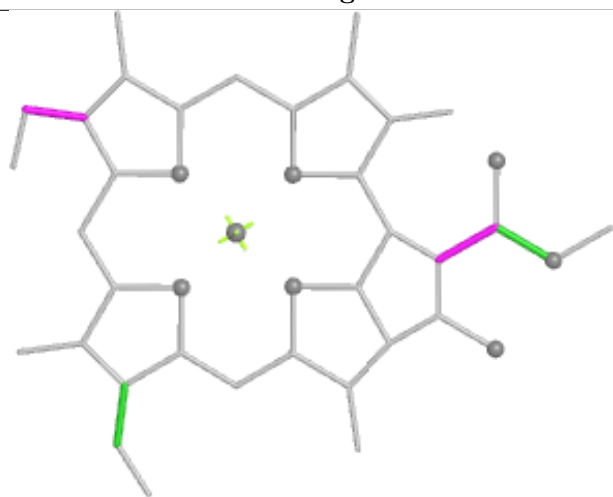
Ligand CLA 8 607



Bond lengths



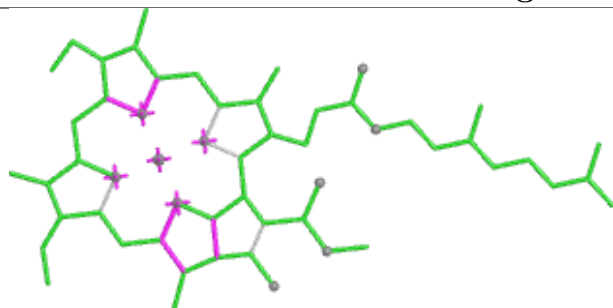
Bond angles



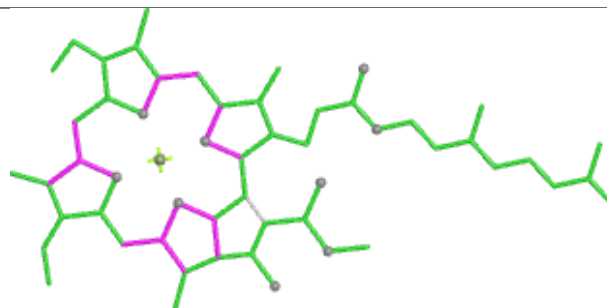
Torsions



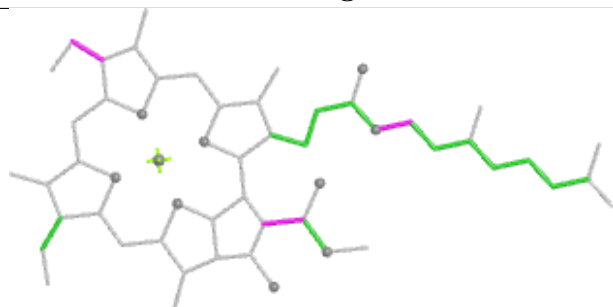
Rings

Ligand CLA Z 304

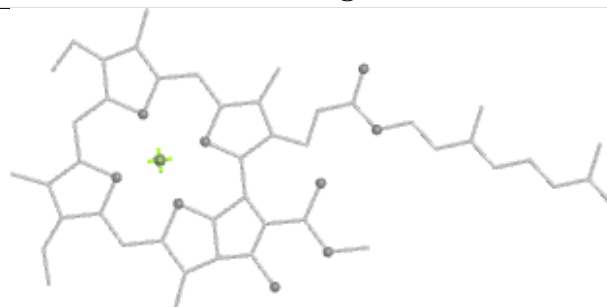
Bond lengths



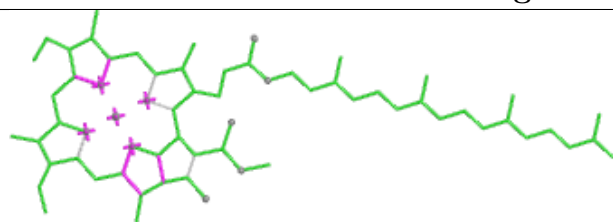
Bond angles



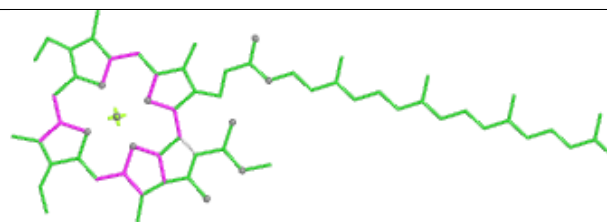
Torsions



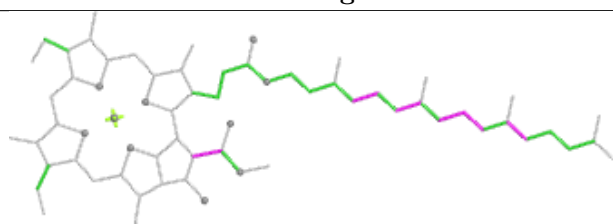
Rings

Ligand CLA A 806

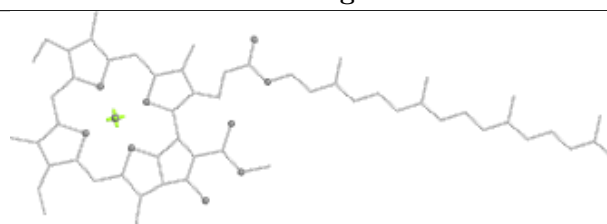
Bond lengths



Bond angles

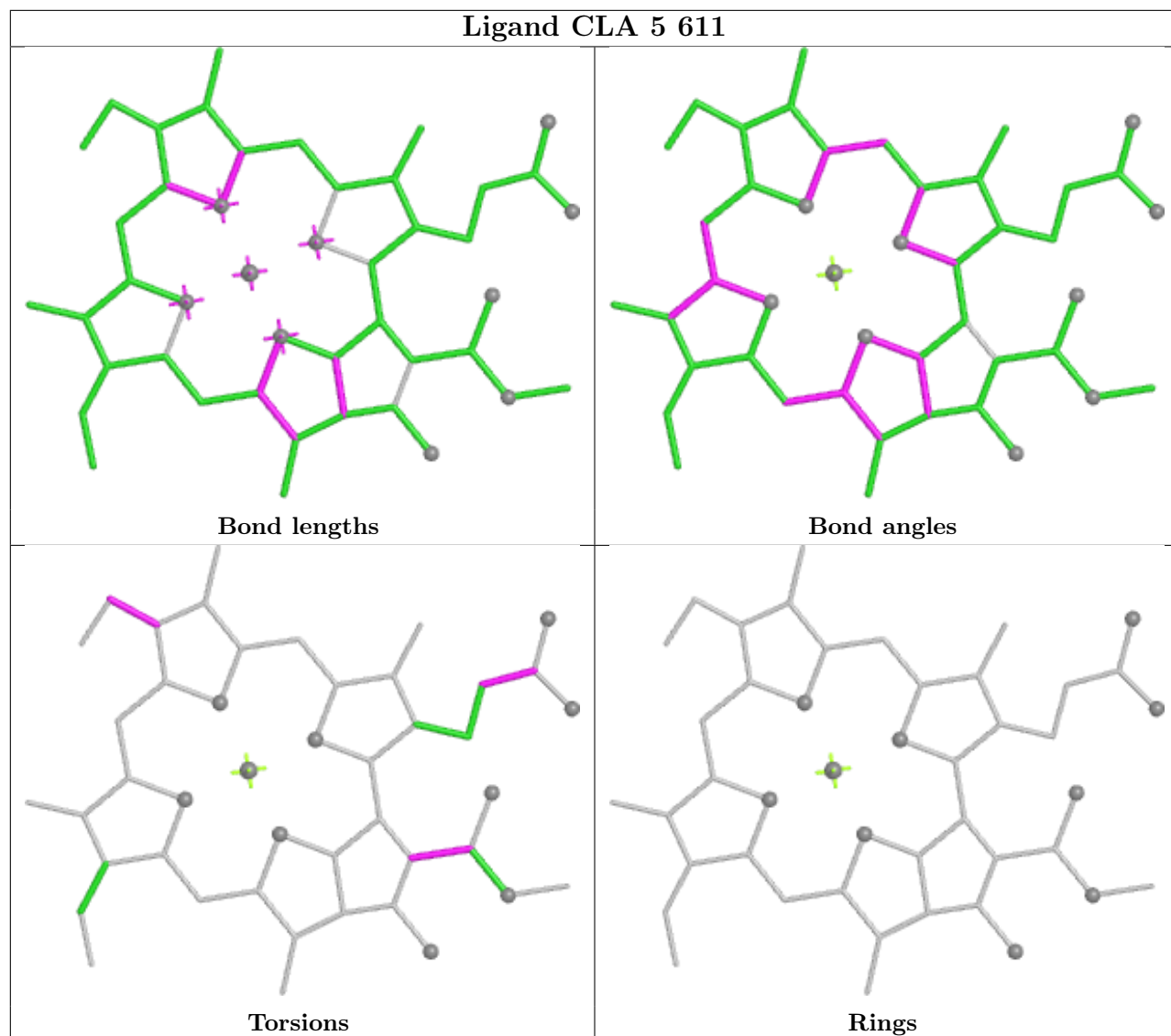


Torsions

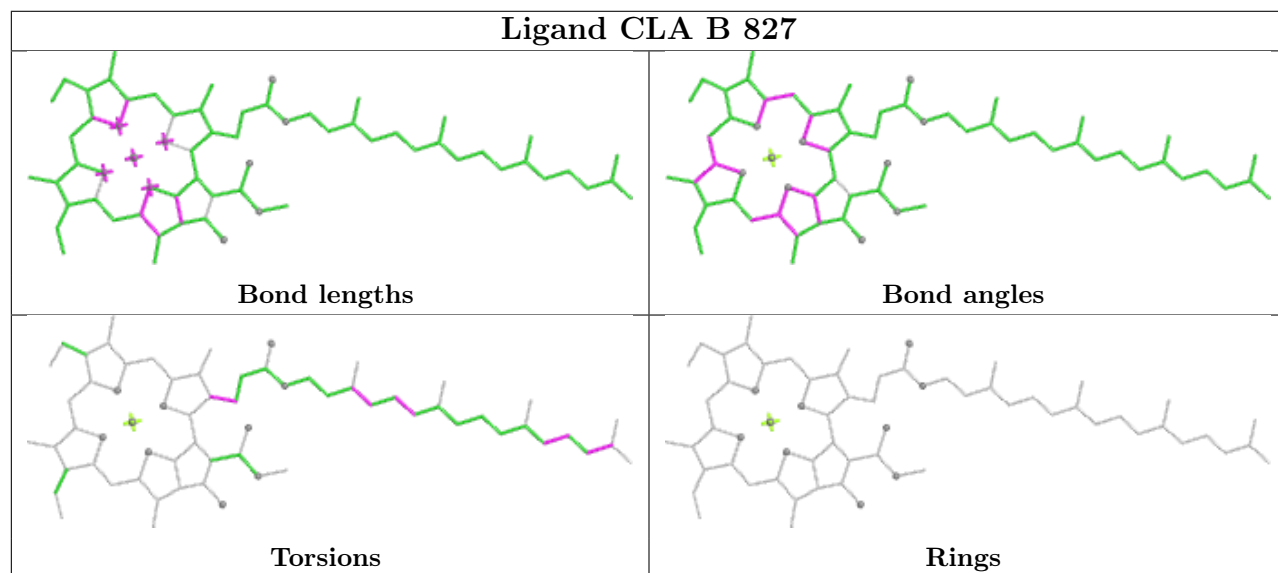


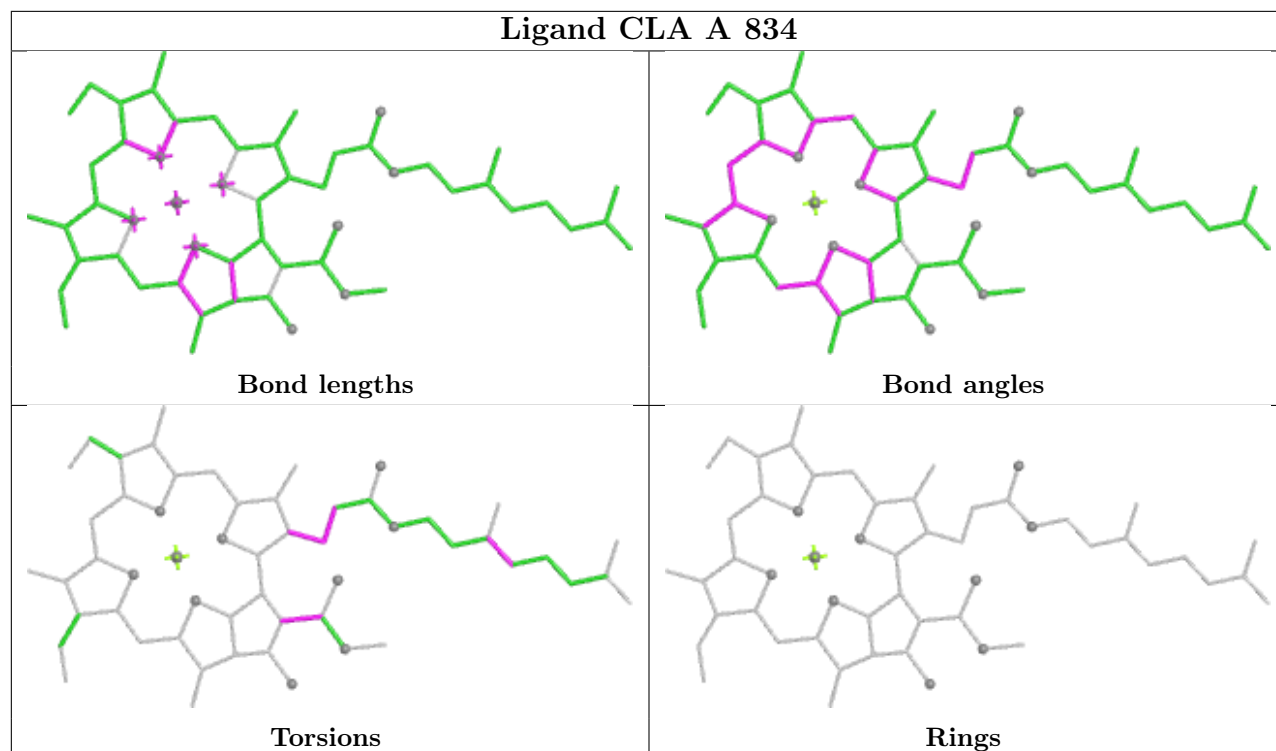
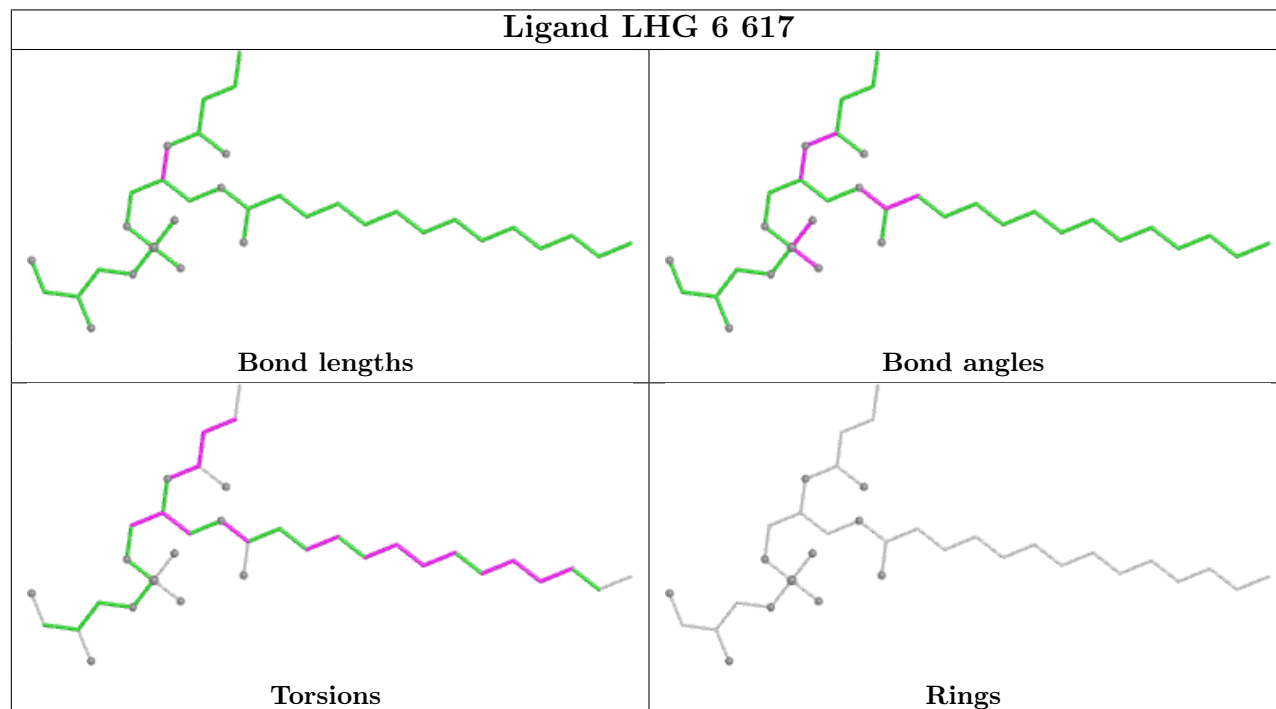
Rings

Ligand CLA 5 611

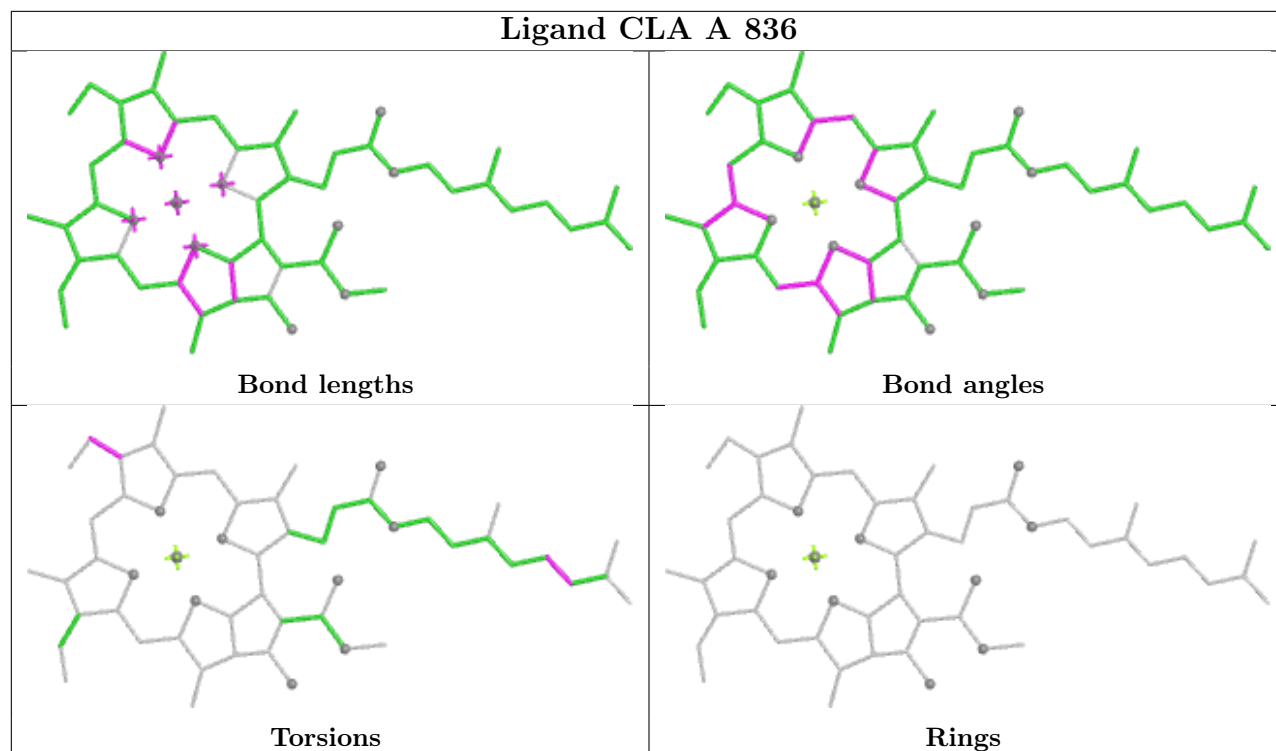


Ligand CLA B 827

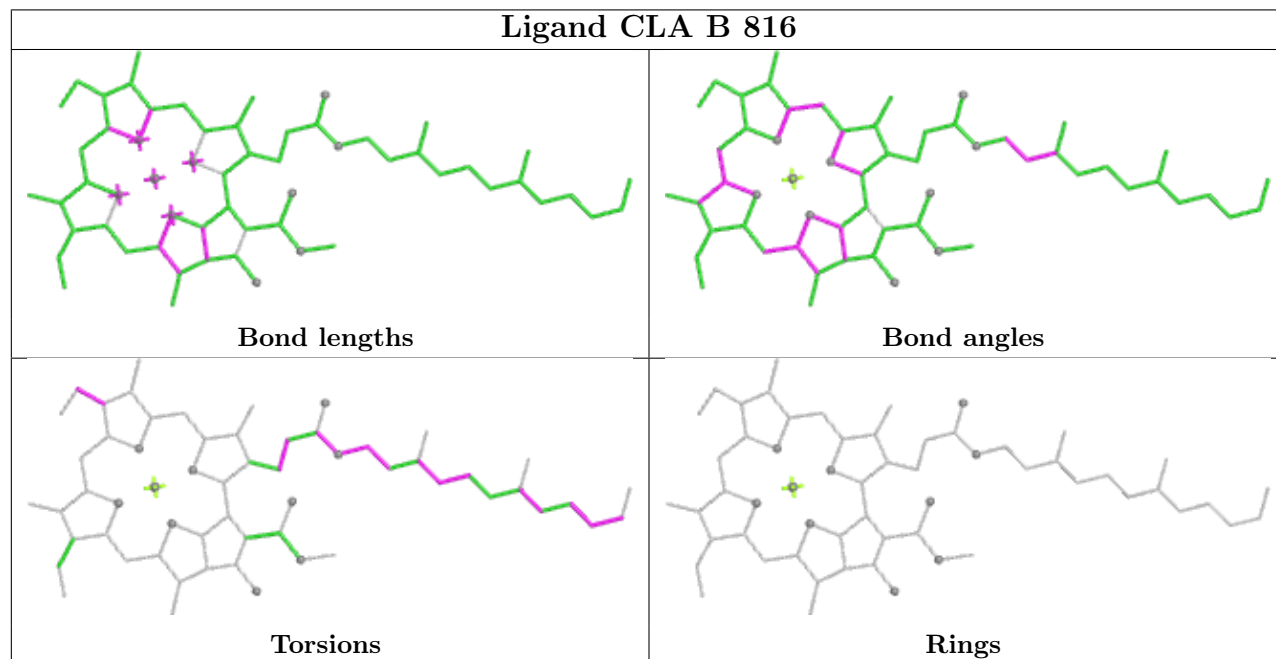


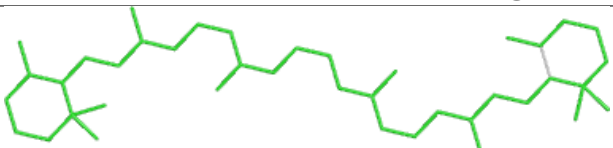
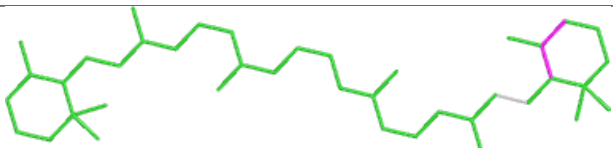
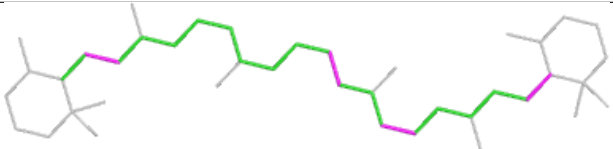
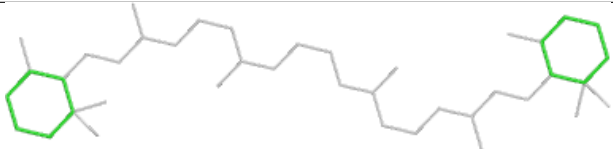
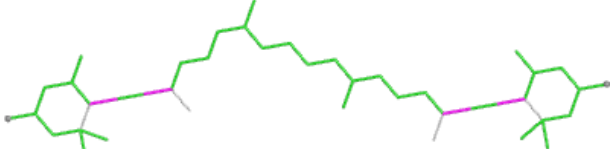
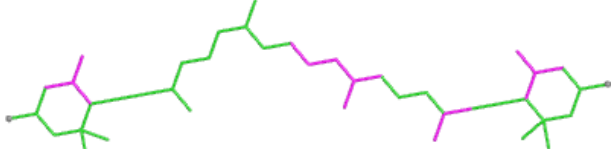
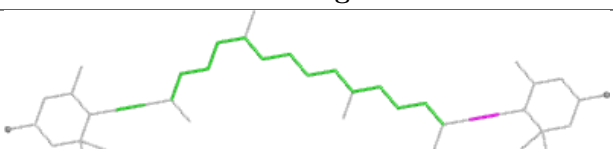
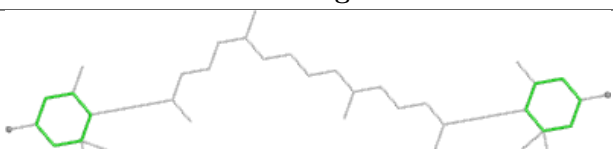
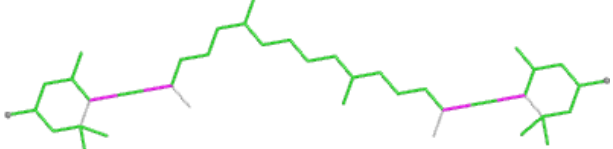
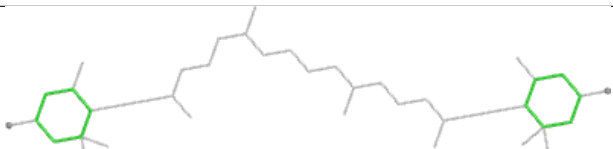
Ligand CLA A 834**Ligand LHG 6 617**

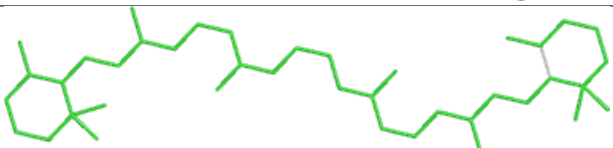
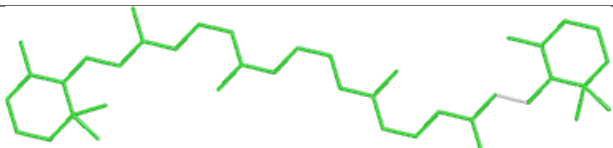
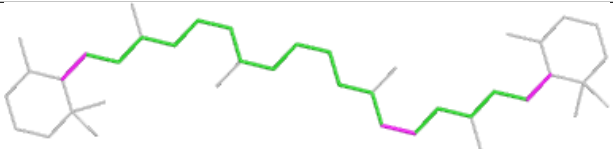
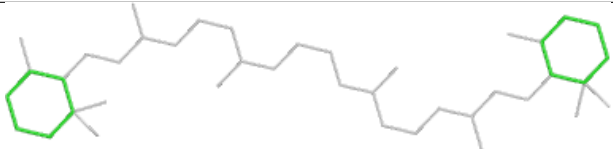
Ligand CLA A 836

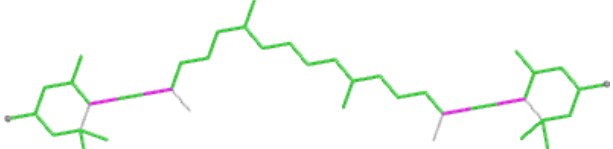
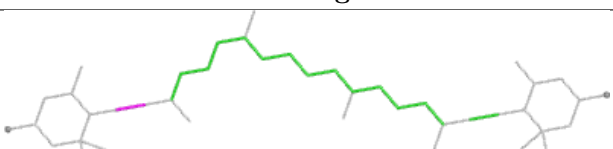
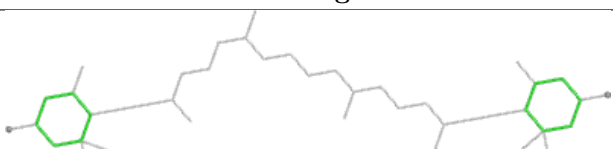


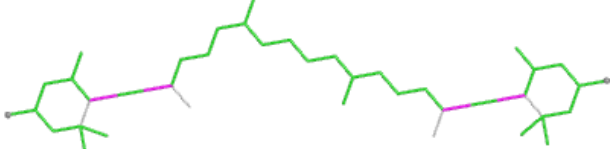
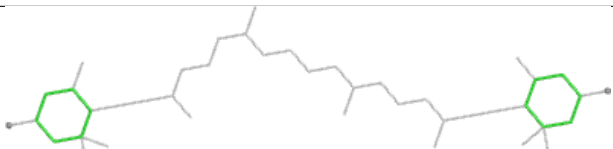
Ligand CLA B 816

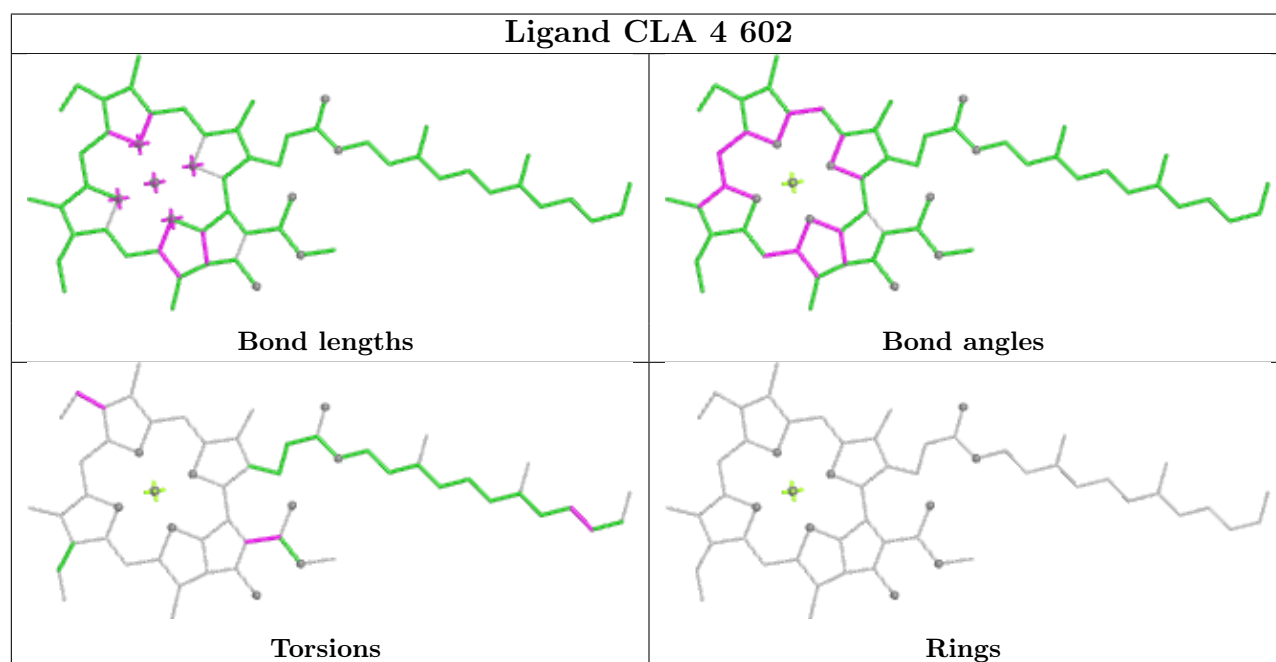
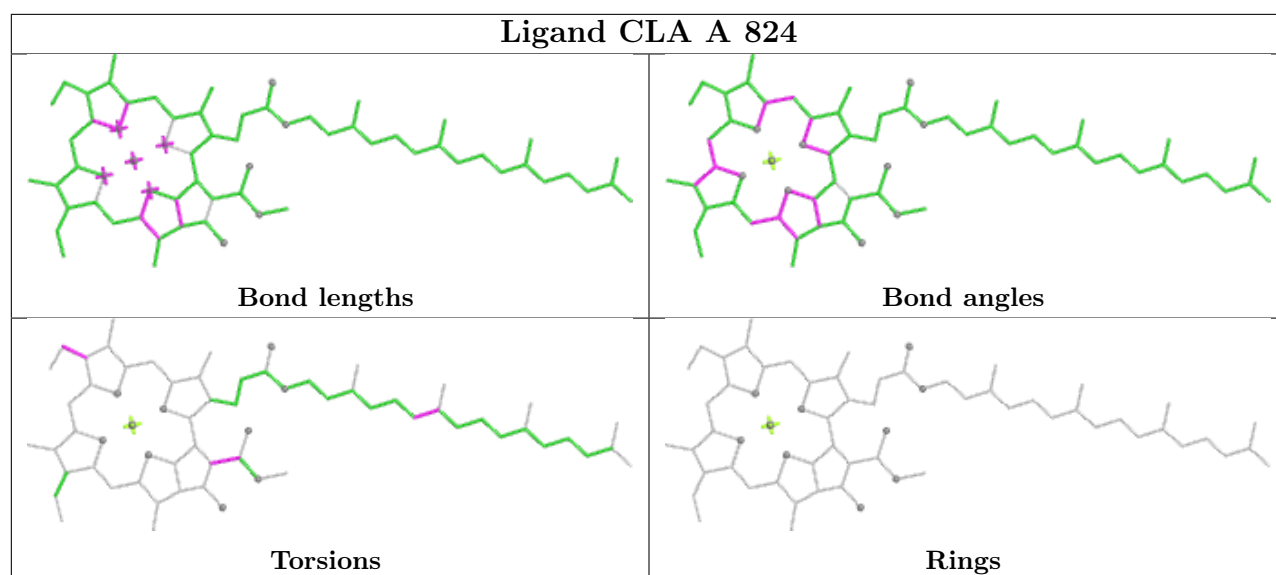


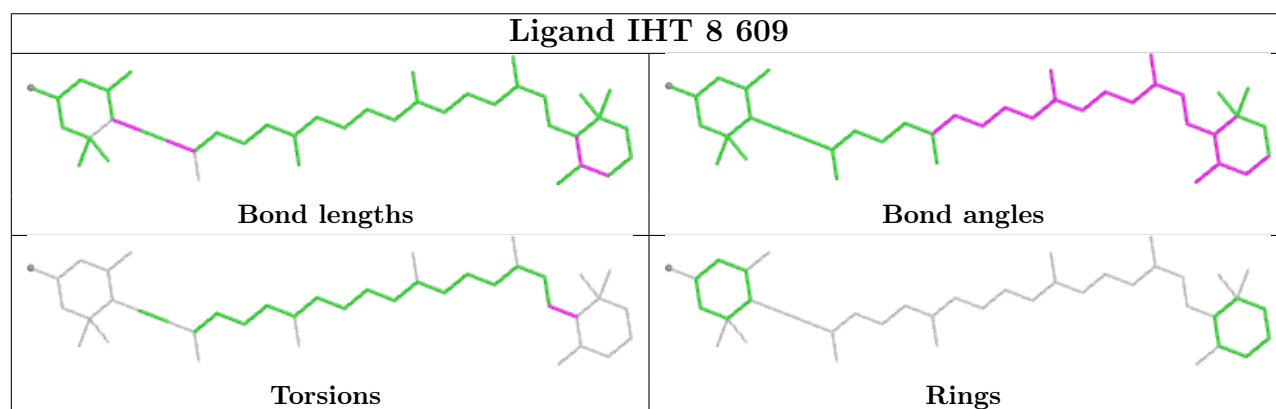
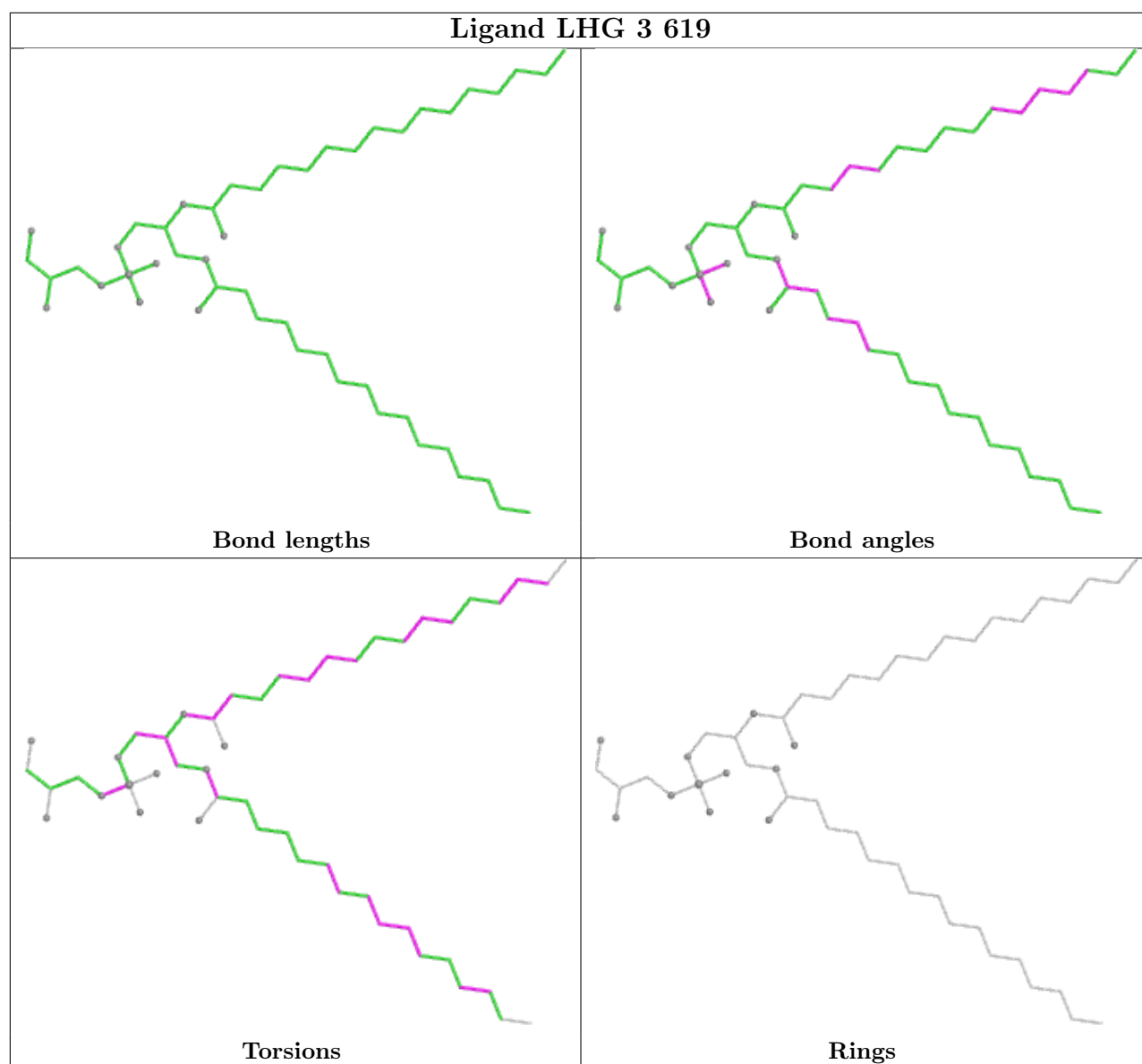
Ligand 8CT M 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand II0 5 616	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand II0 7 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 8CT B 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

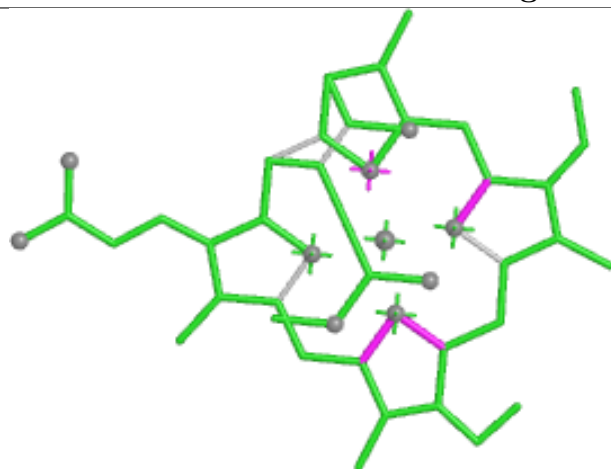
Ligand II0 O 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 2 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

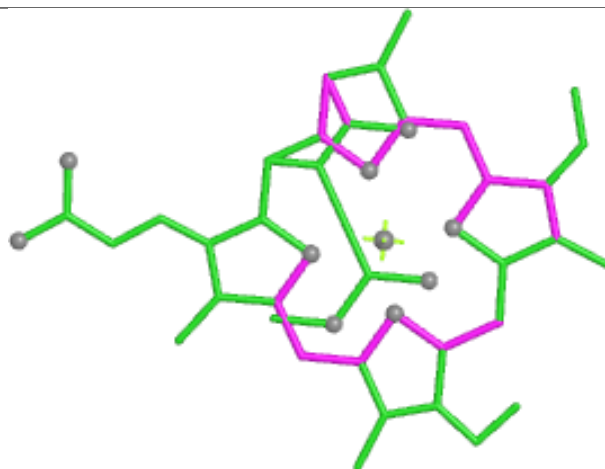




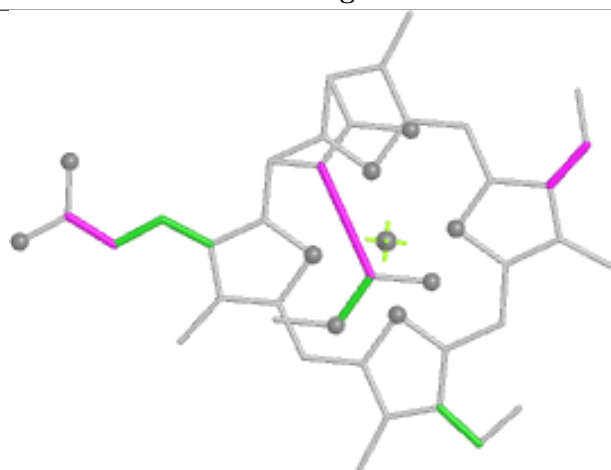
Ligand KC2 9 610



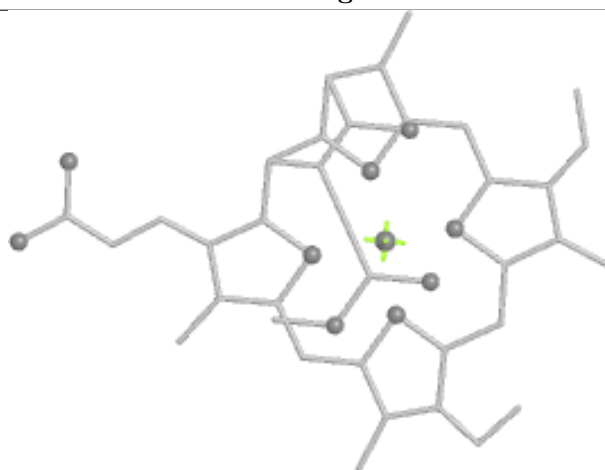
Bond lengths



Bond angles

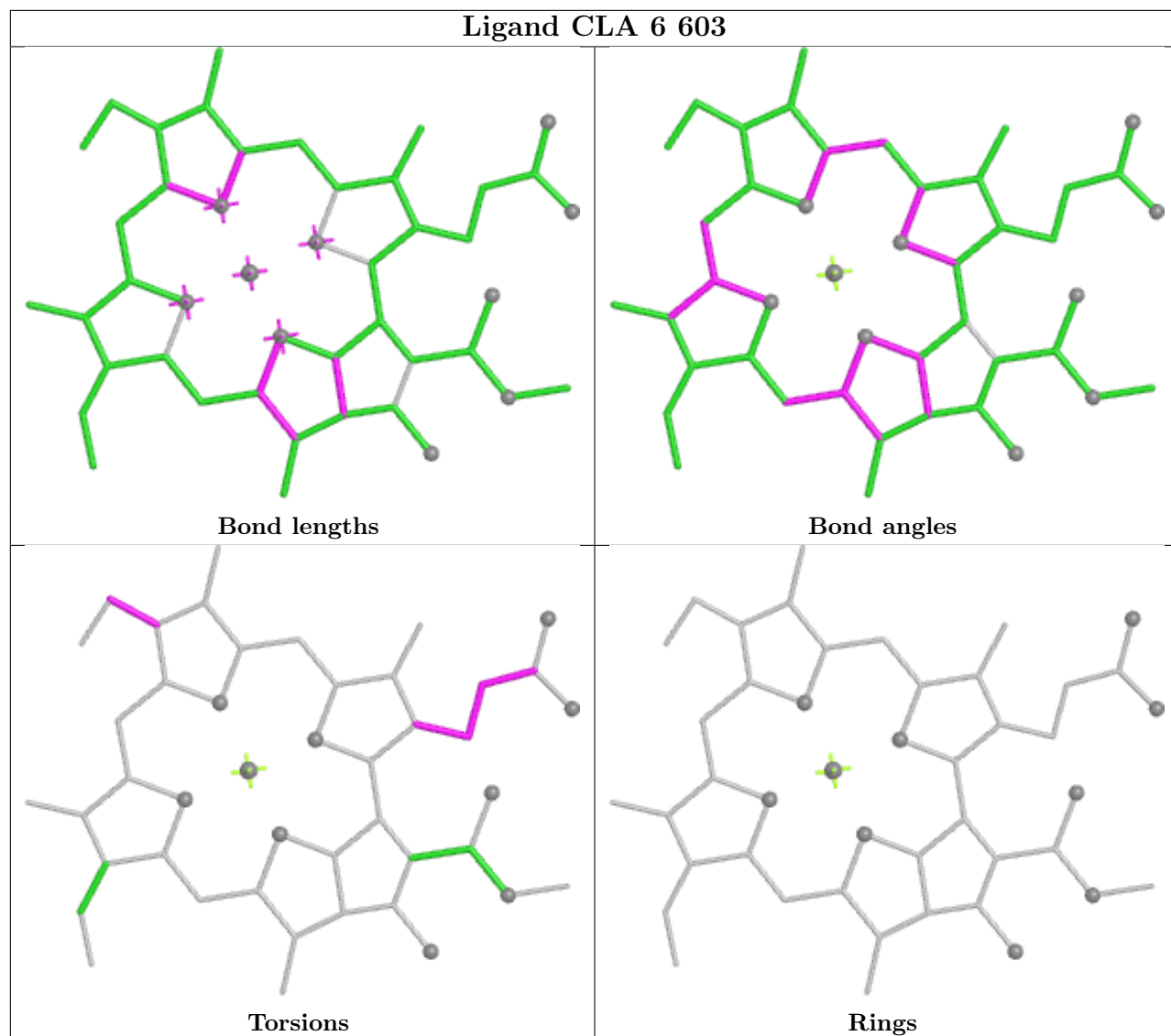


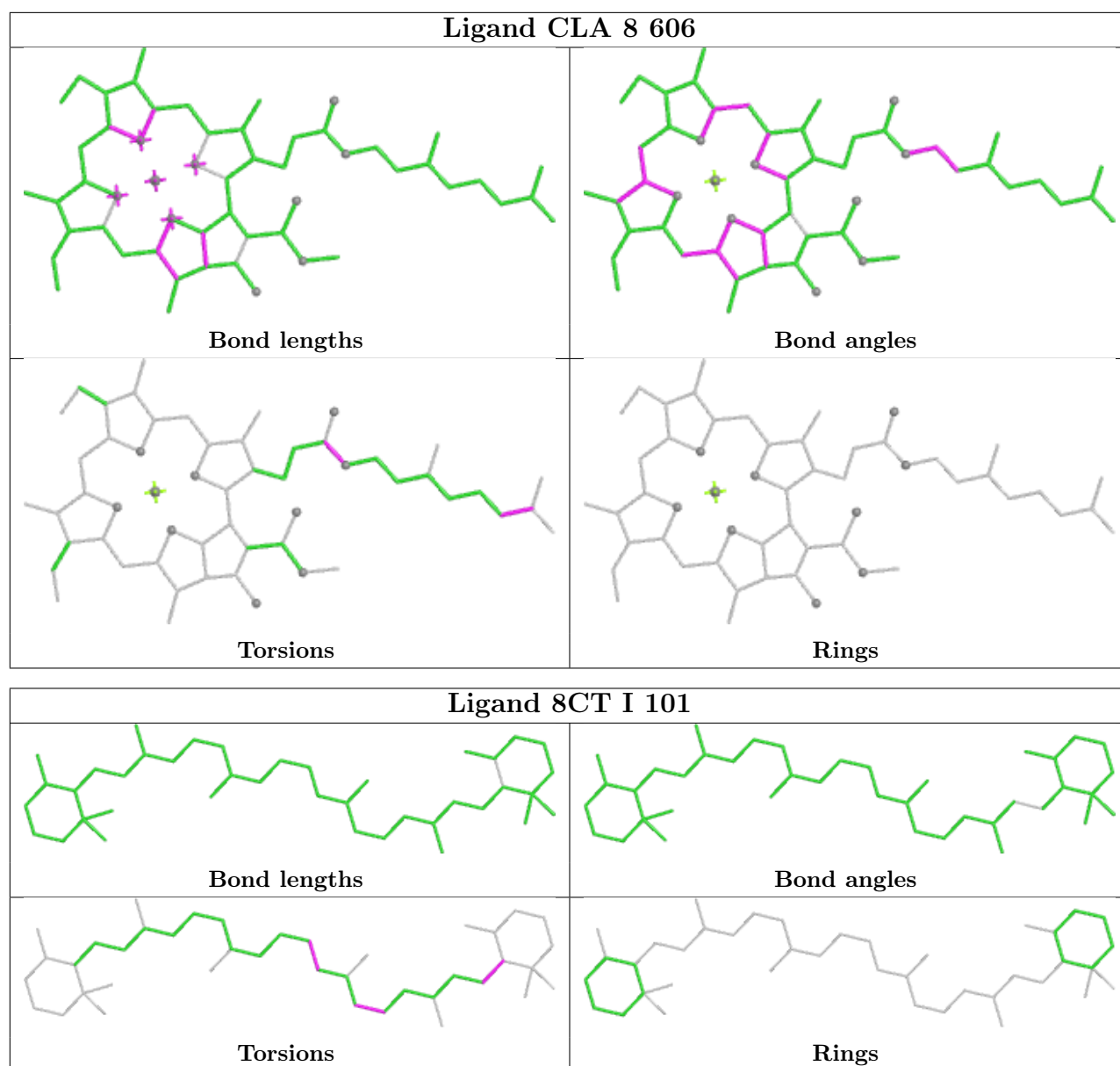
Torsions



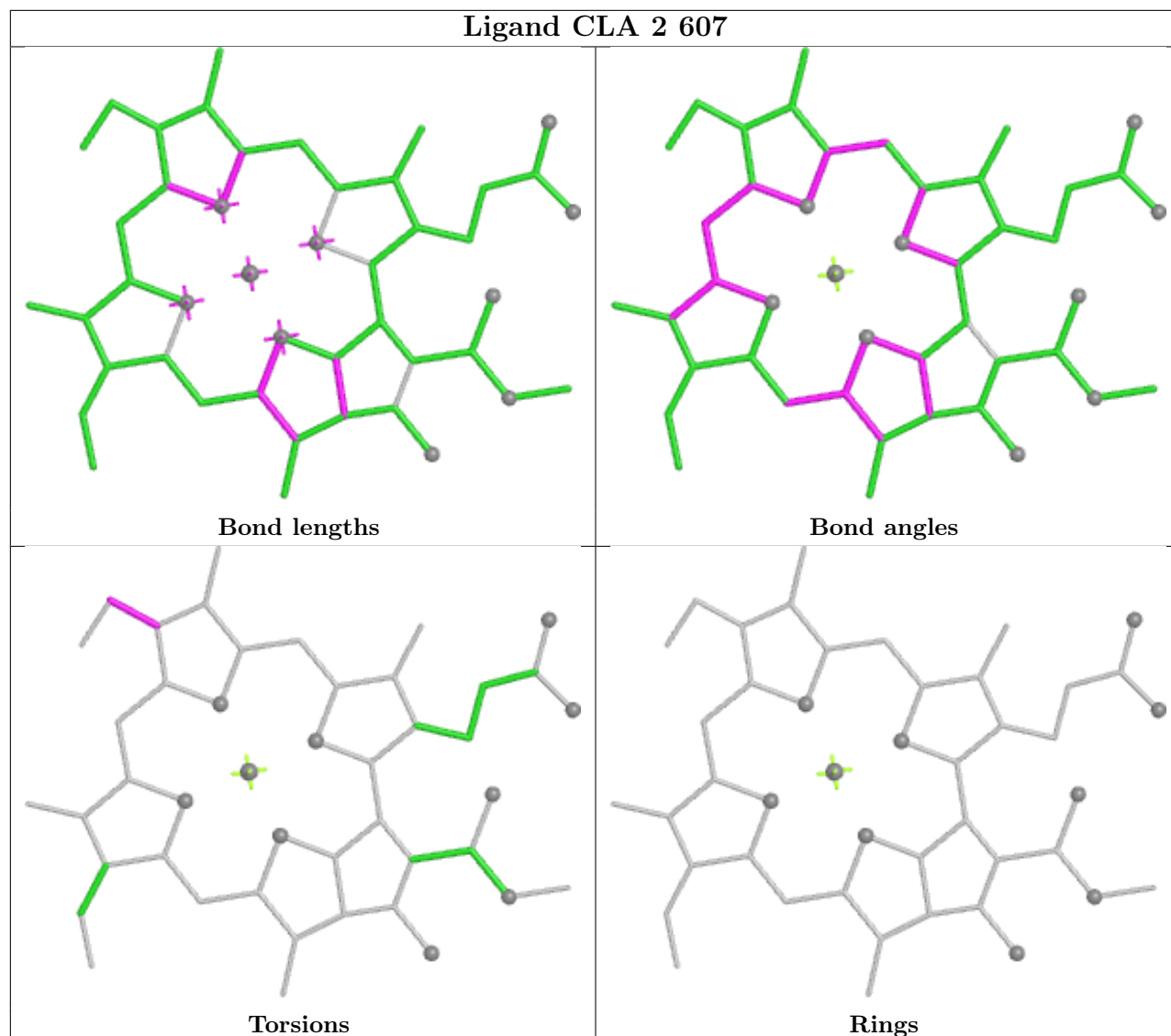
Rings

Ligand CLA 6 603

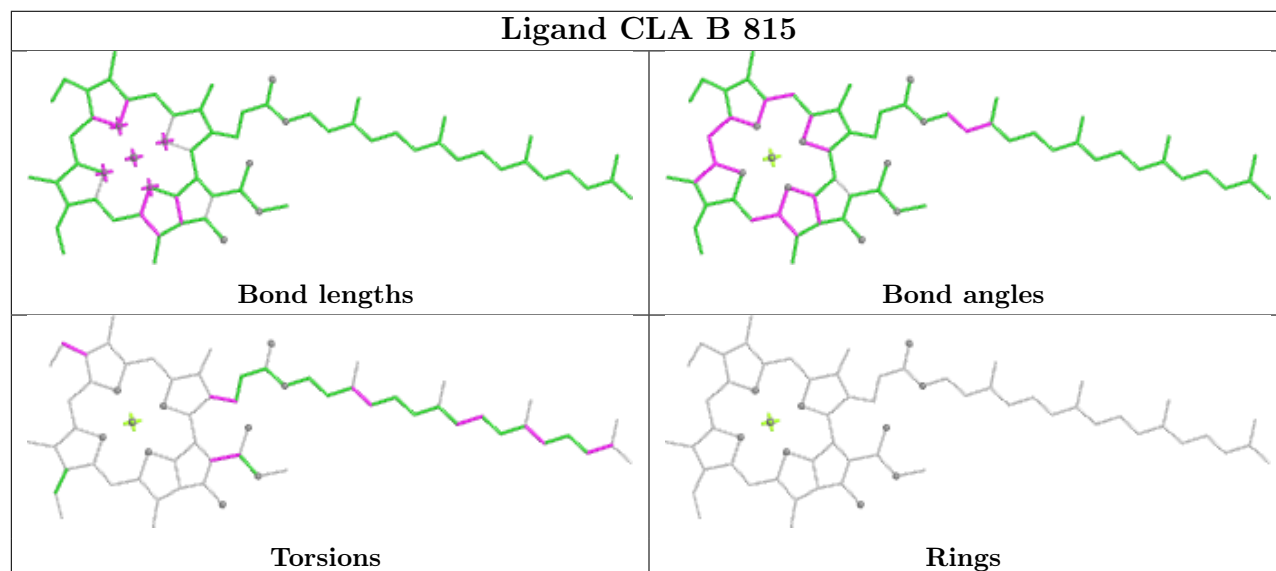


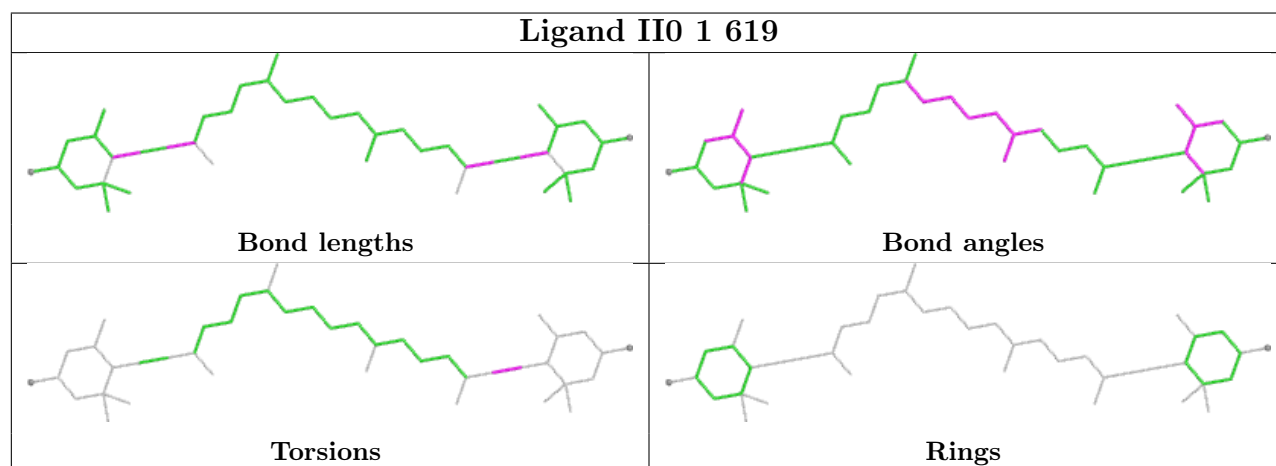
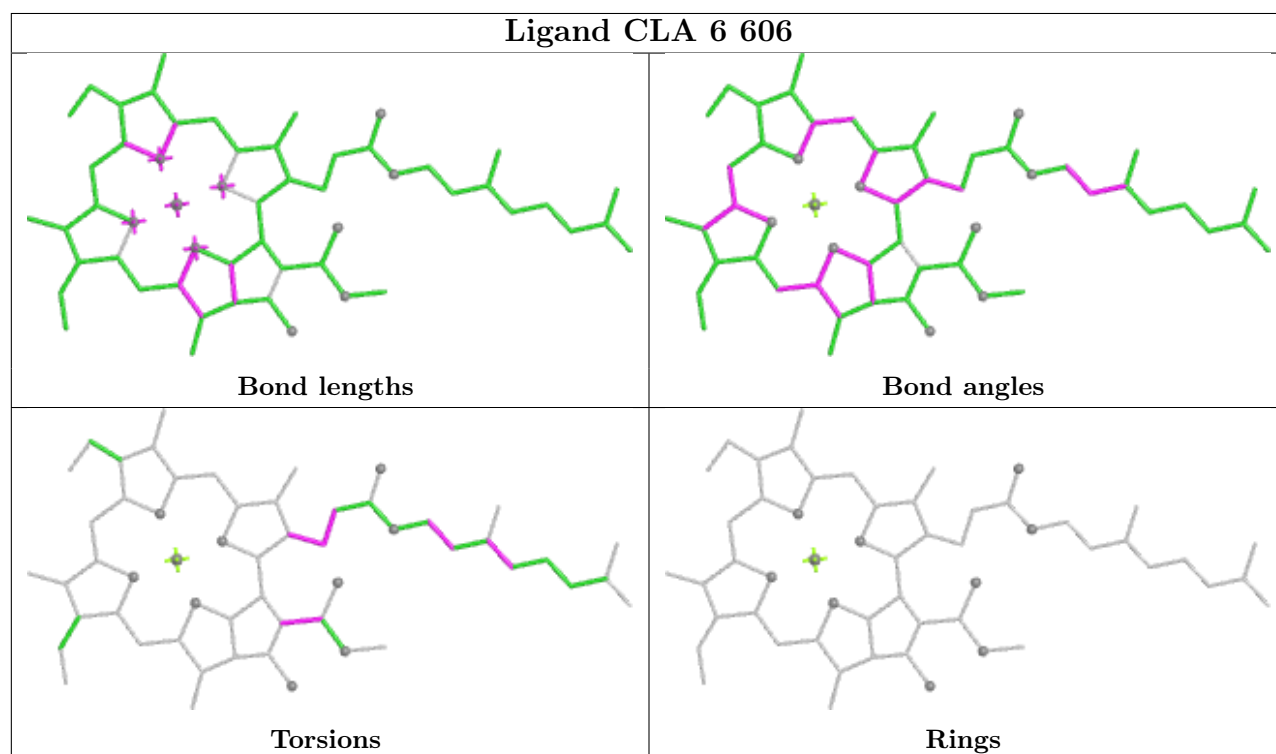
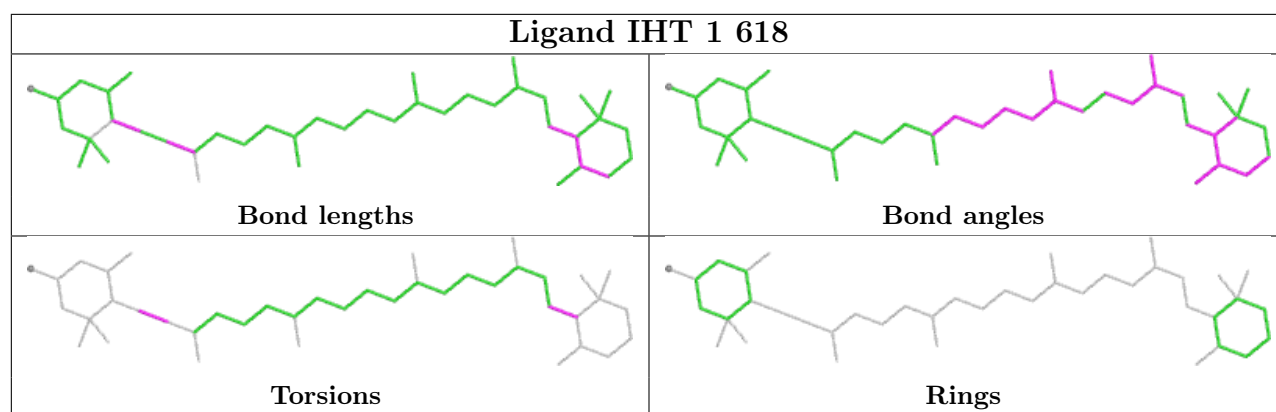


Ligand CLA 2 607

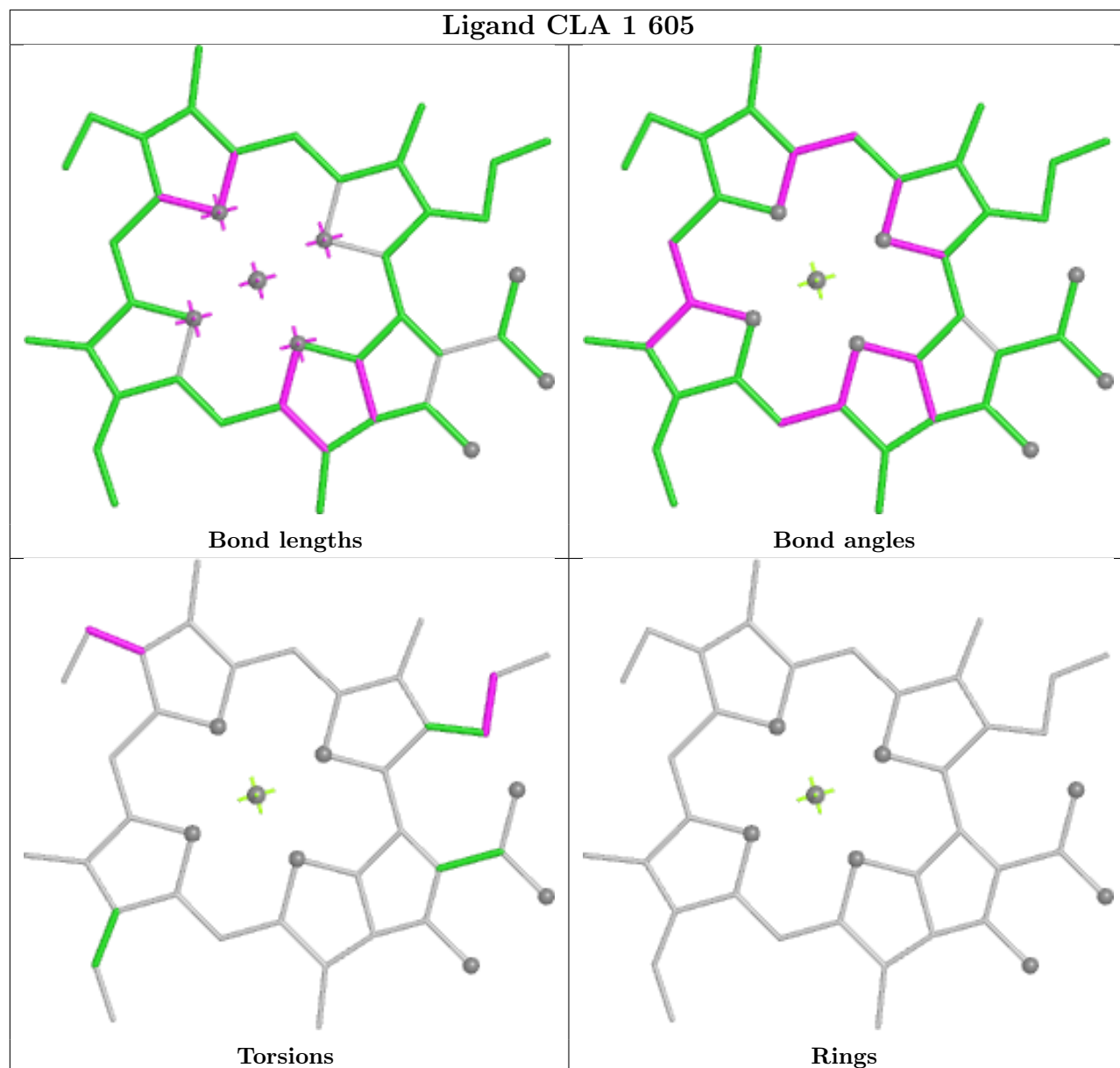


Ligand CLA B 815

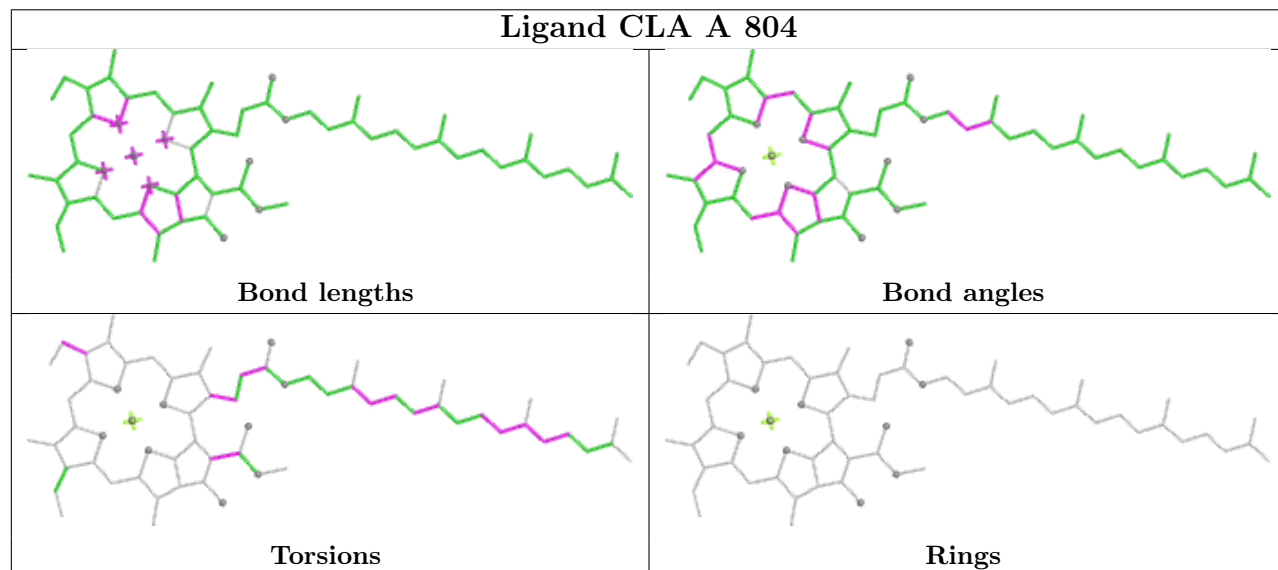


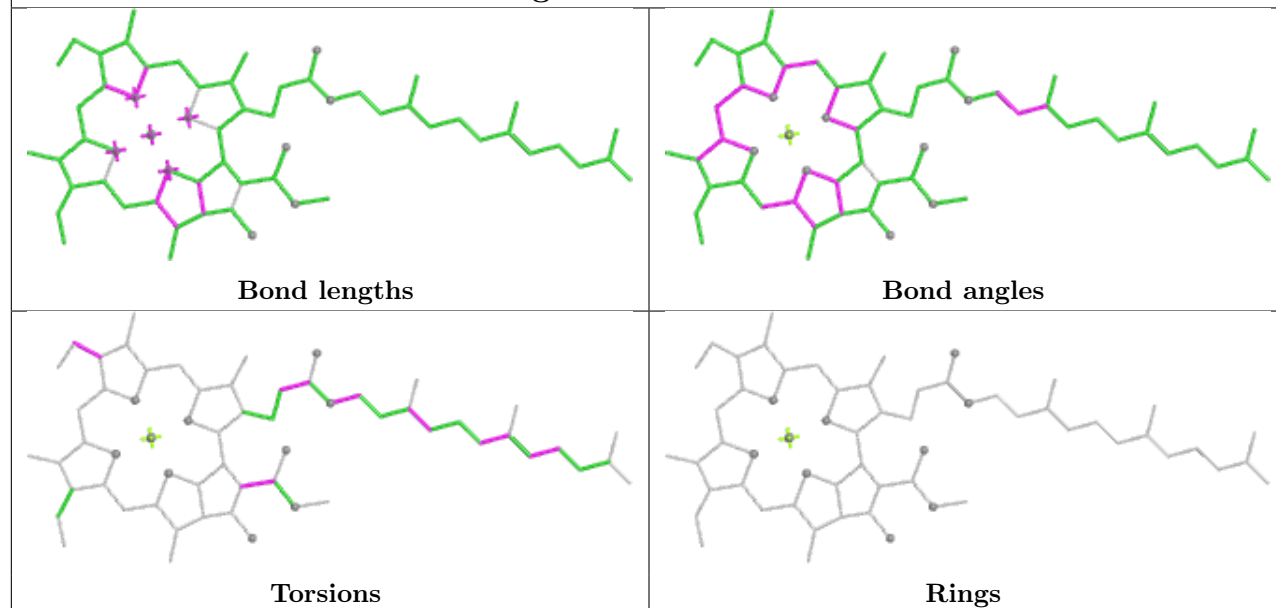
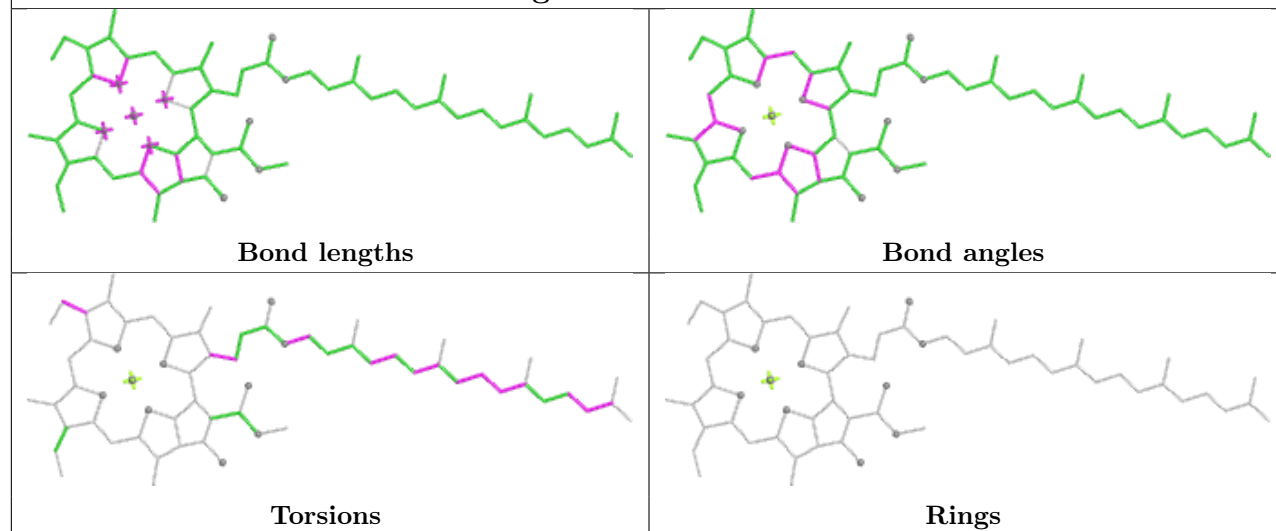


Ligand CLA 1 605

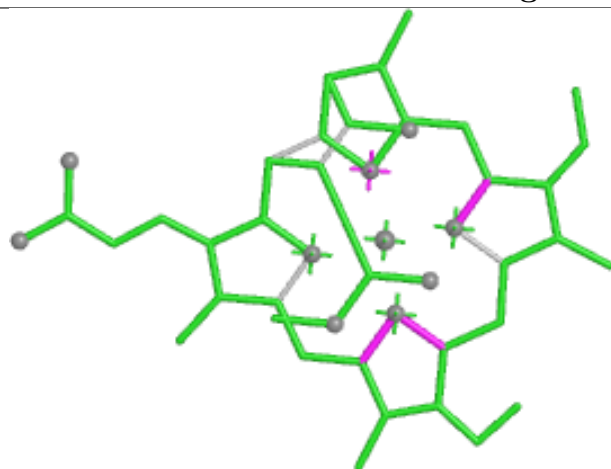


Ligand CLA A 804

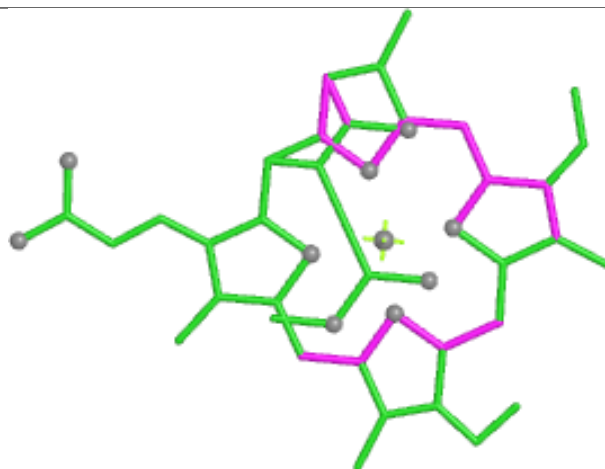


Ligand CLA B 821**Ligand CLA B 826**

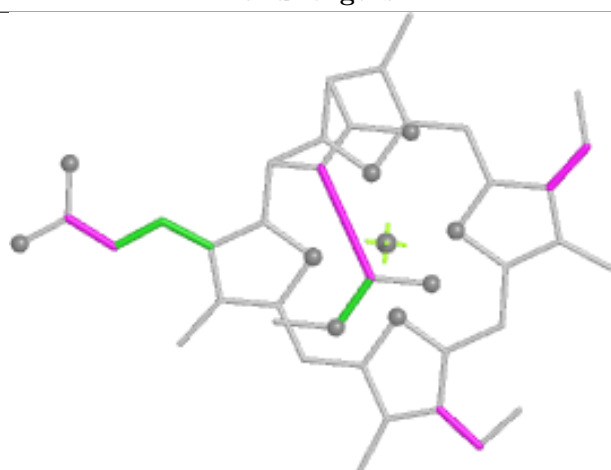
Ligand KC2 4 605



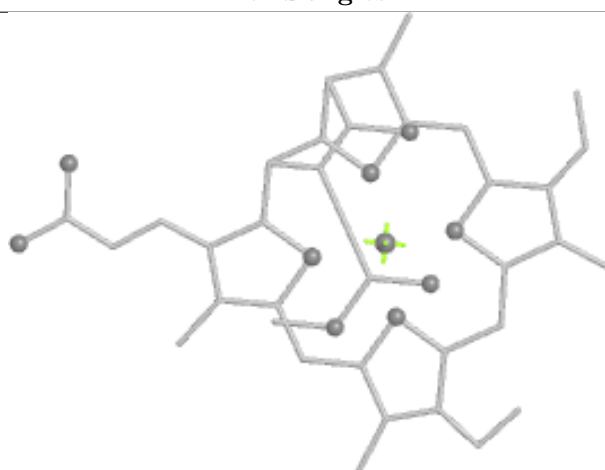
Bond lengths



Bond angles

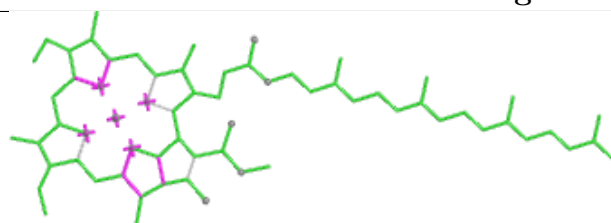


Torsions

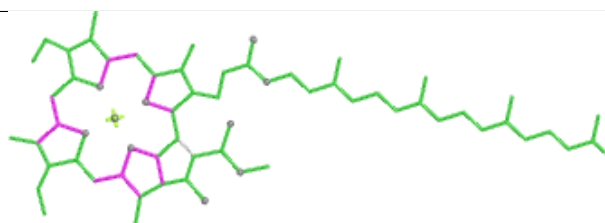


Rings

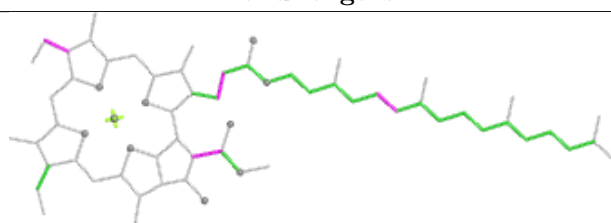
Ligand CLA B 837



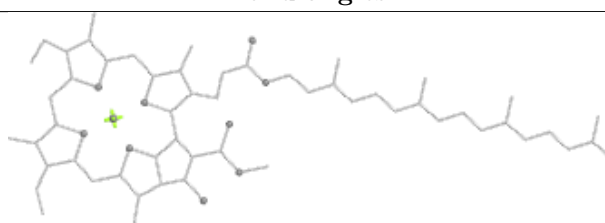
Bond lengths



Bond angles

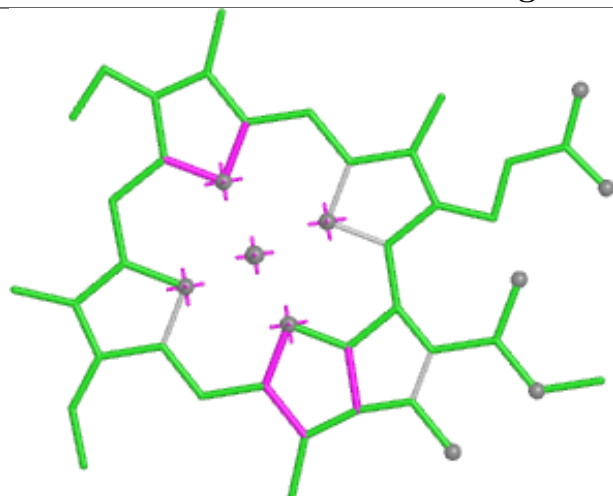


Torsions

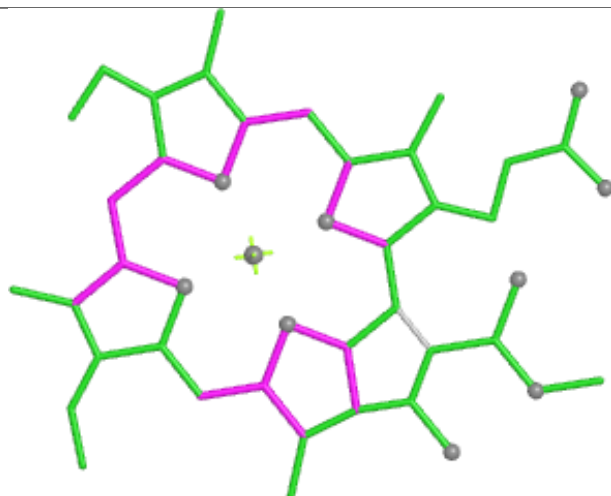


Rings

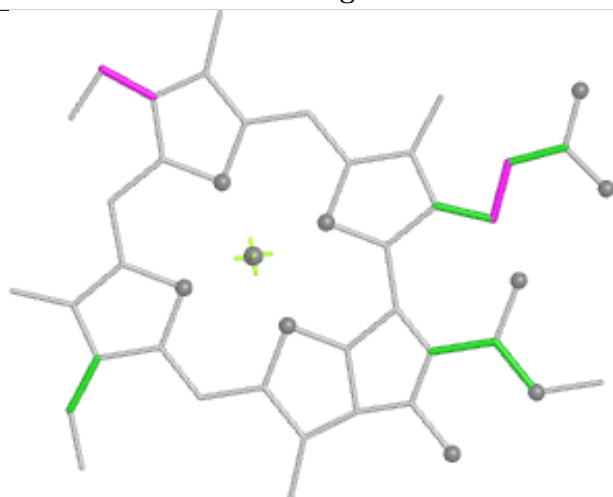
Ligand CLA 1 604



Bond lengths



Bond angles

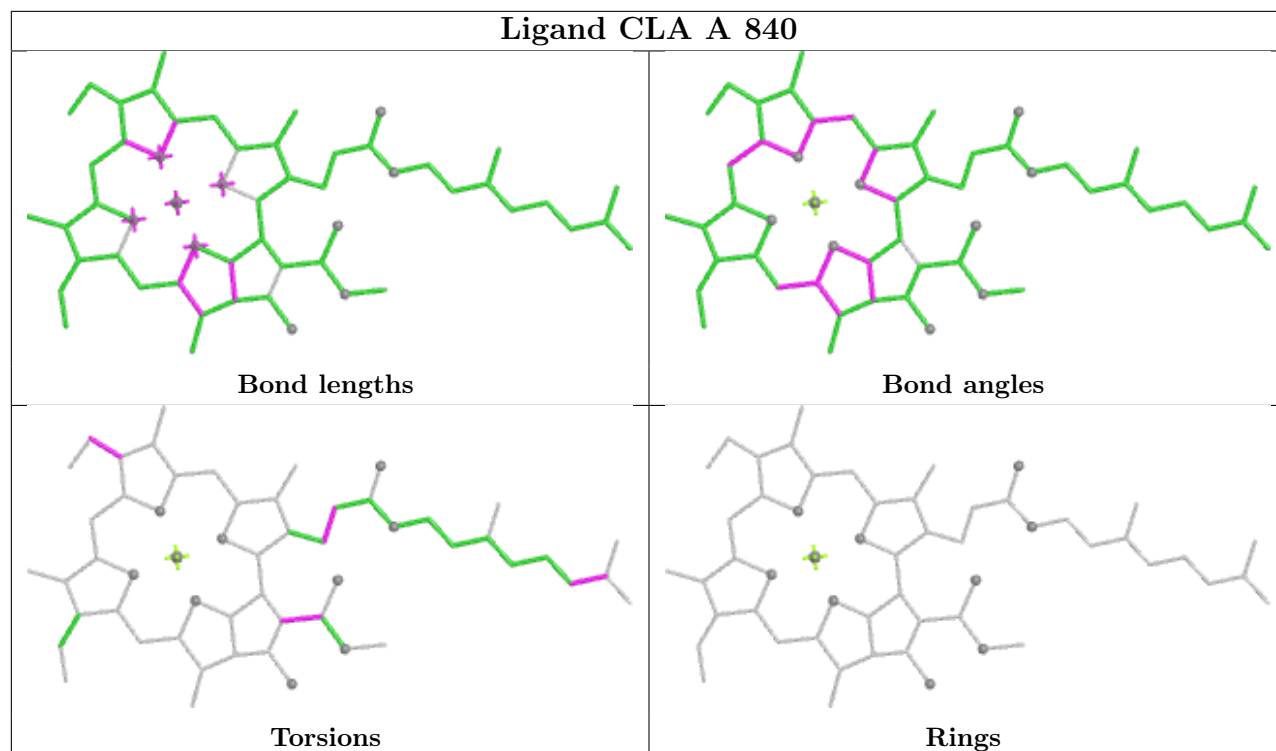


Torsions

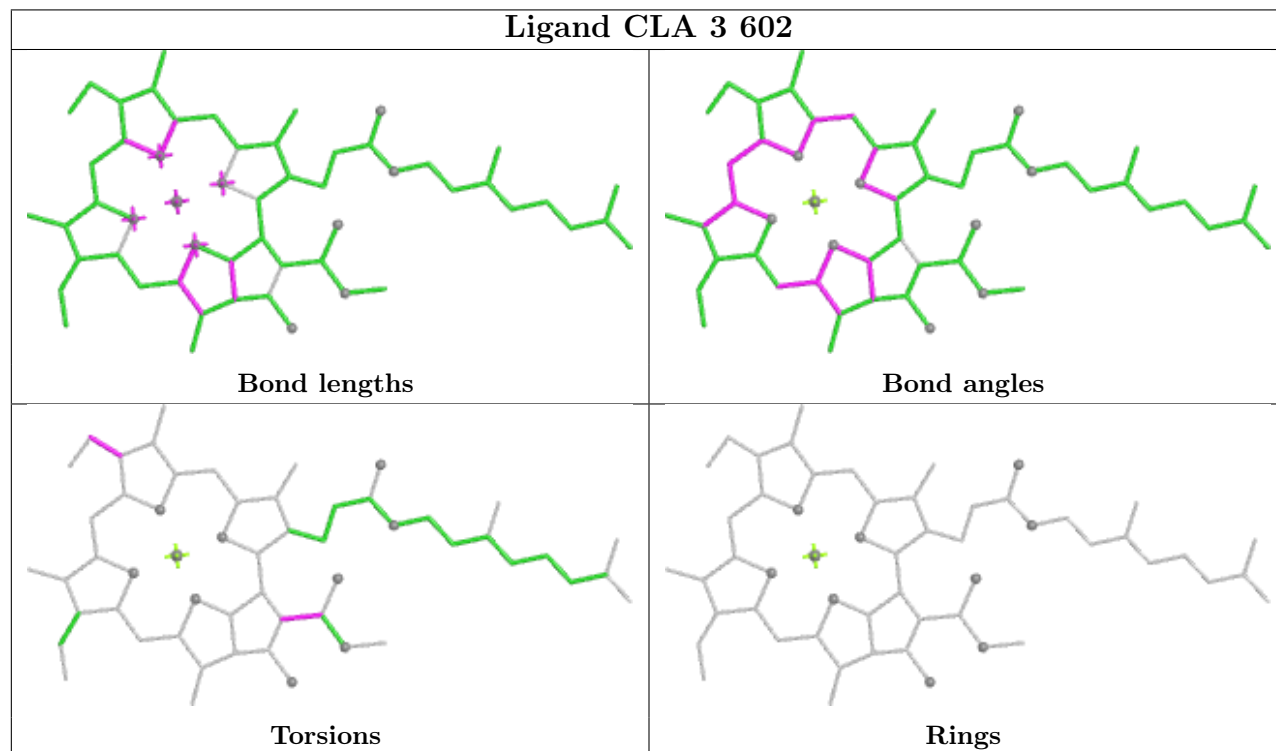


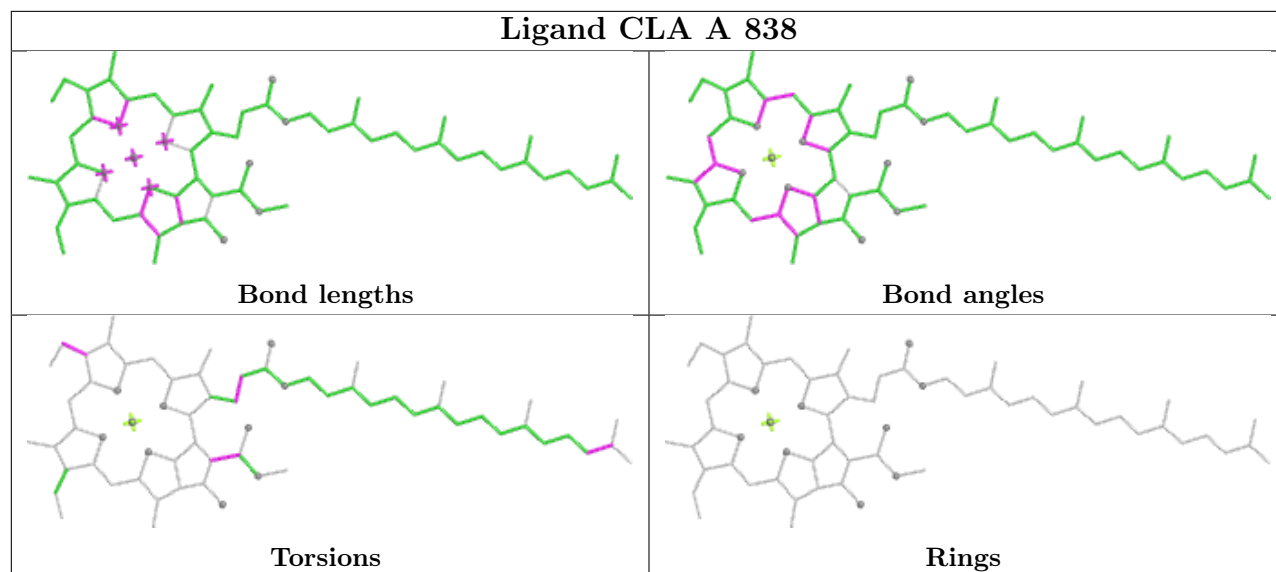
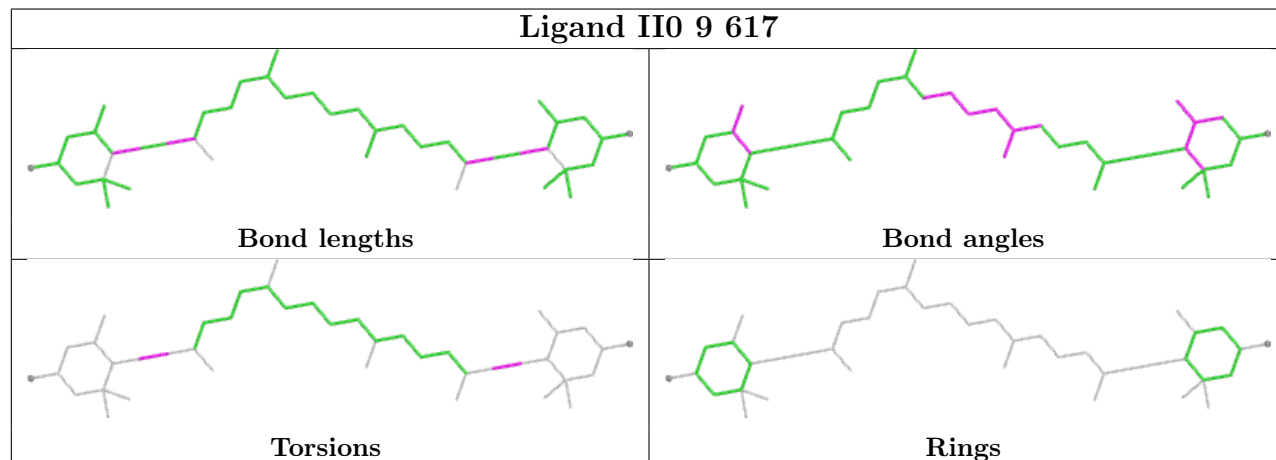
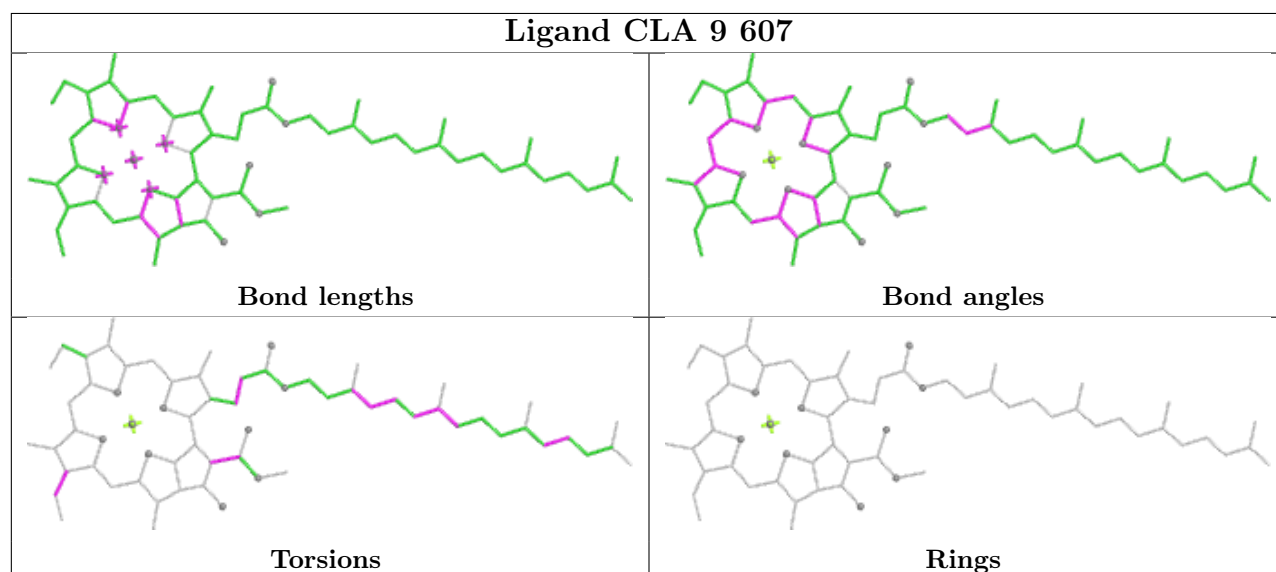
Rings

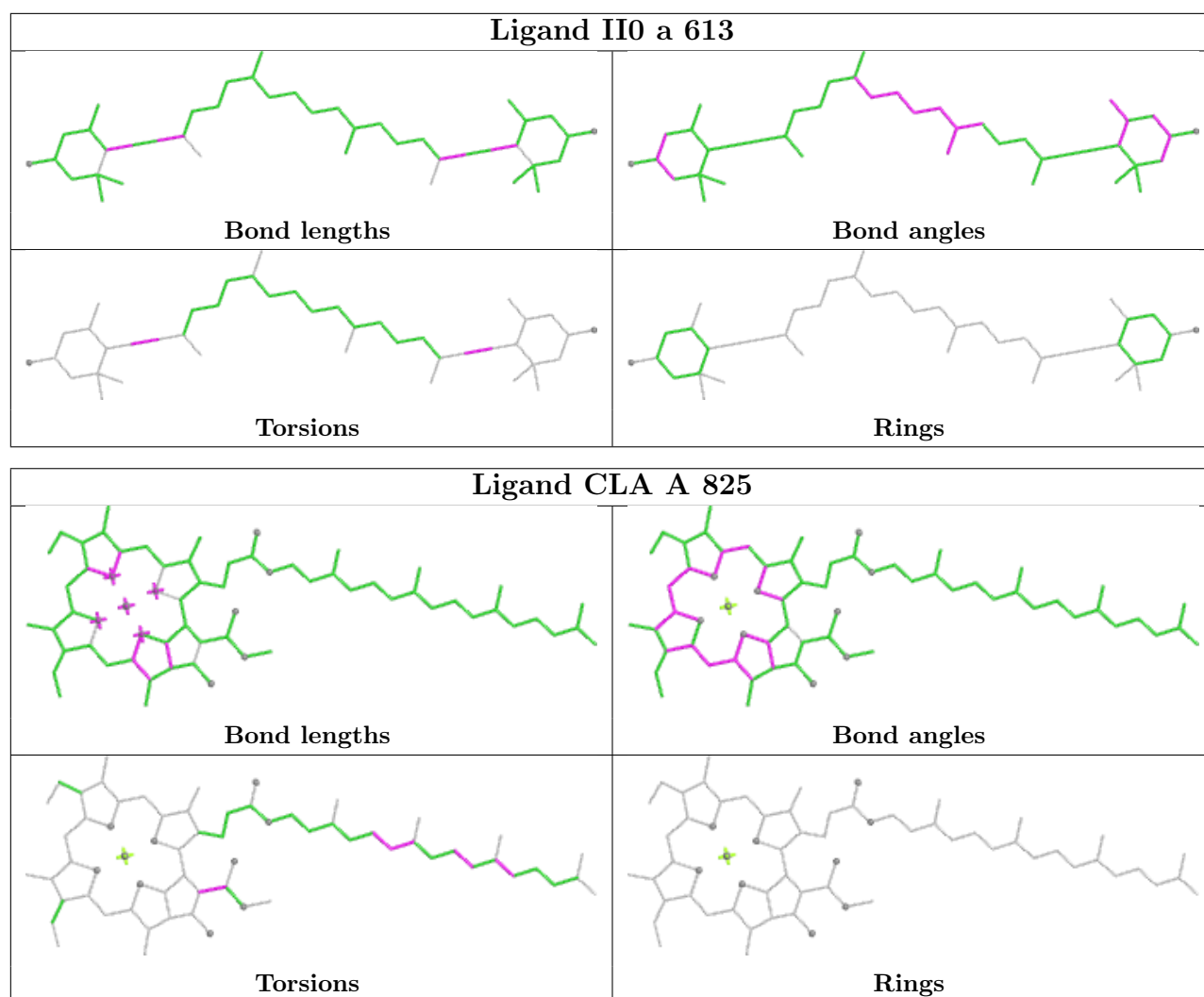
Ligand CLA A 840



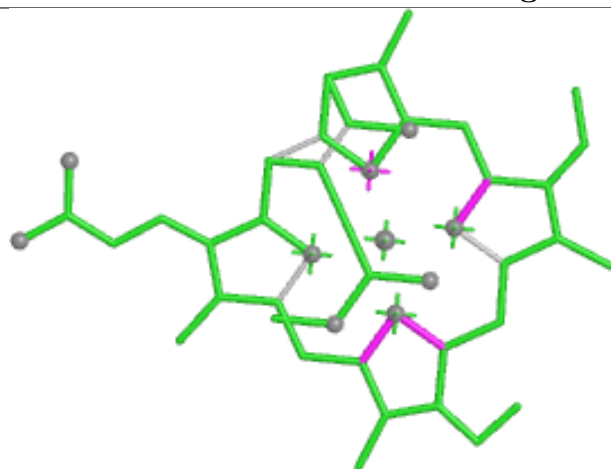
Ligand CLA 3 602



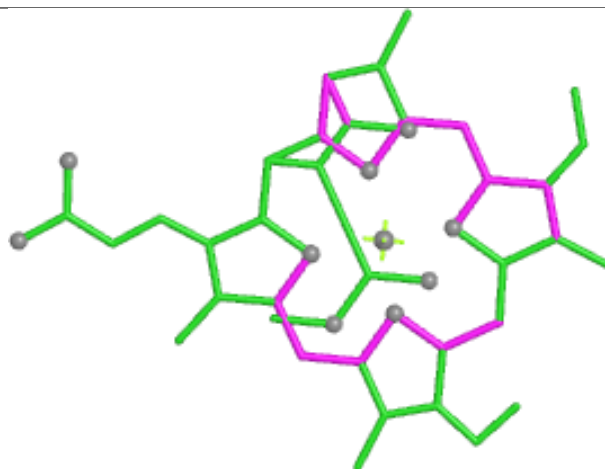
Ligand CLA A 838**Ligand II0 9 617****Ligand CLA 9 607**



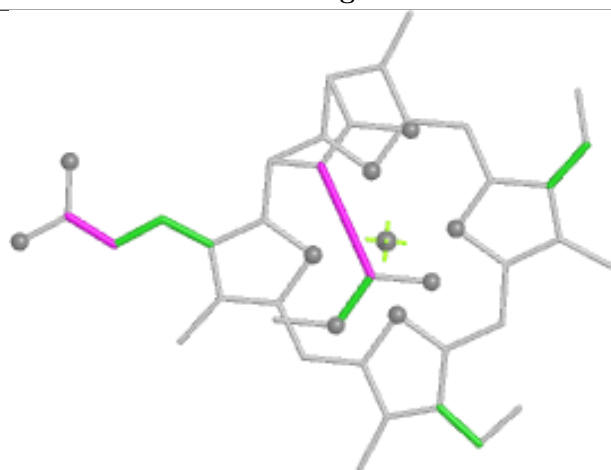
Ligand KC2 5 610



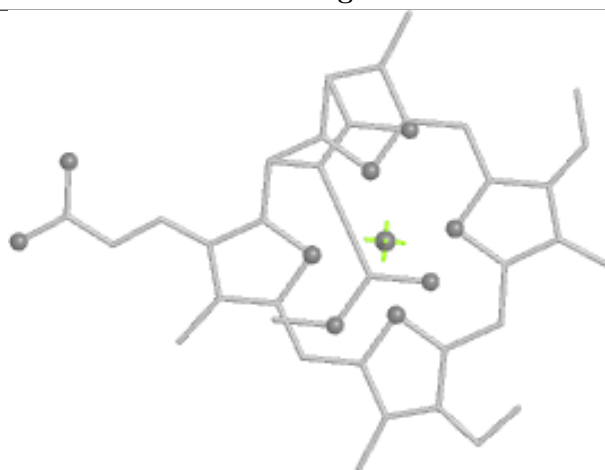
Bond lengths



Bond angles

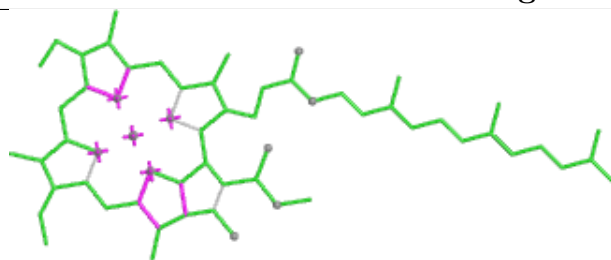


Torsions

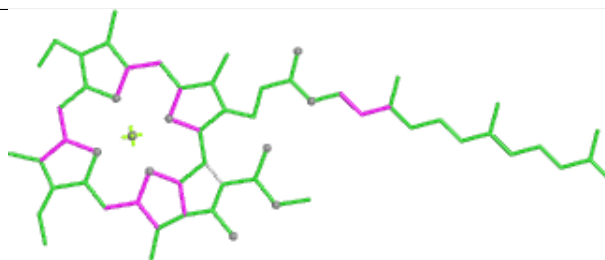


Rings

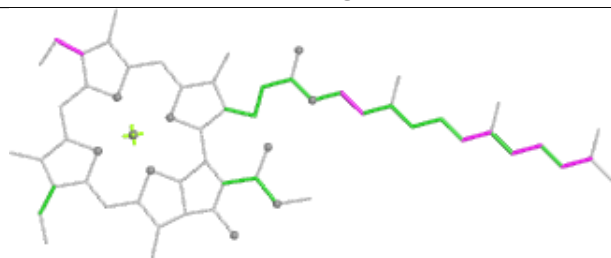
Ligand CLA 1 612



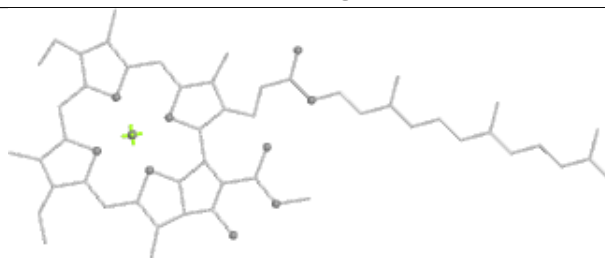
Bond lengths



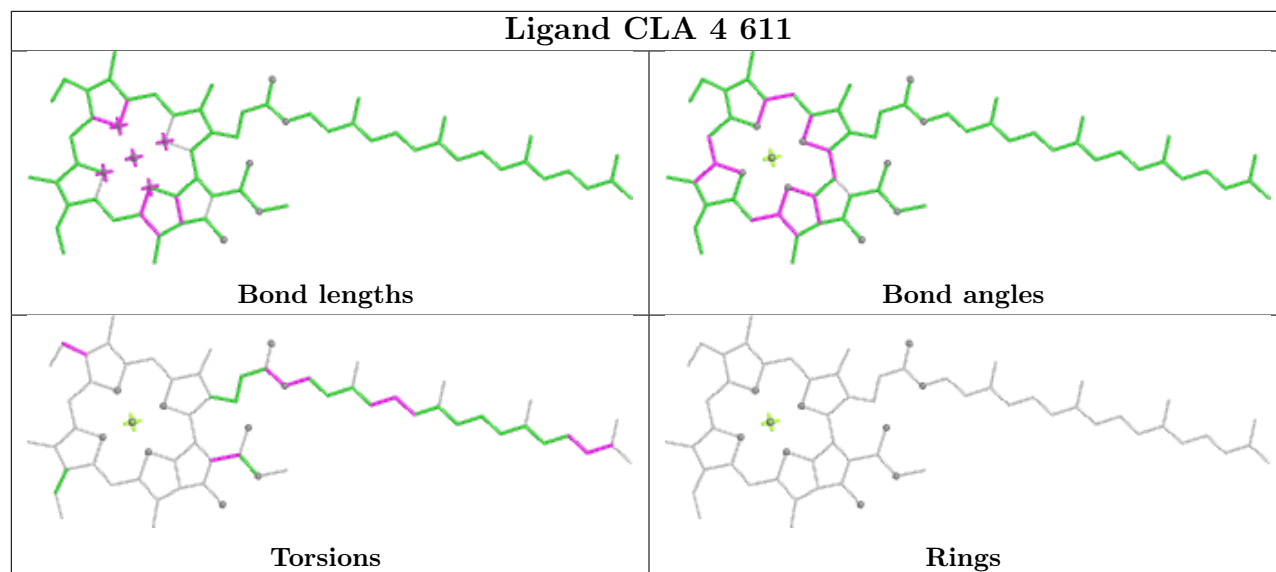
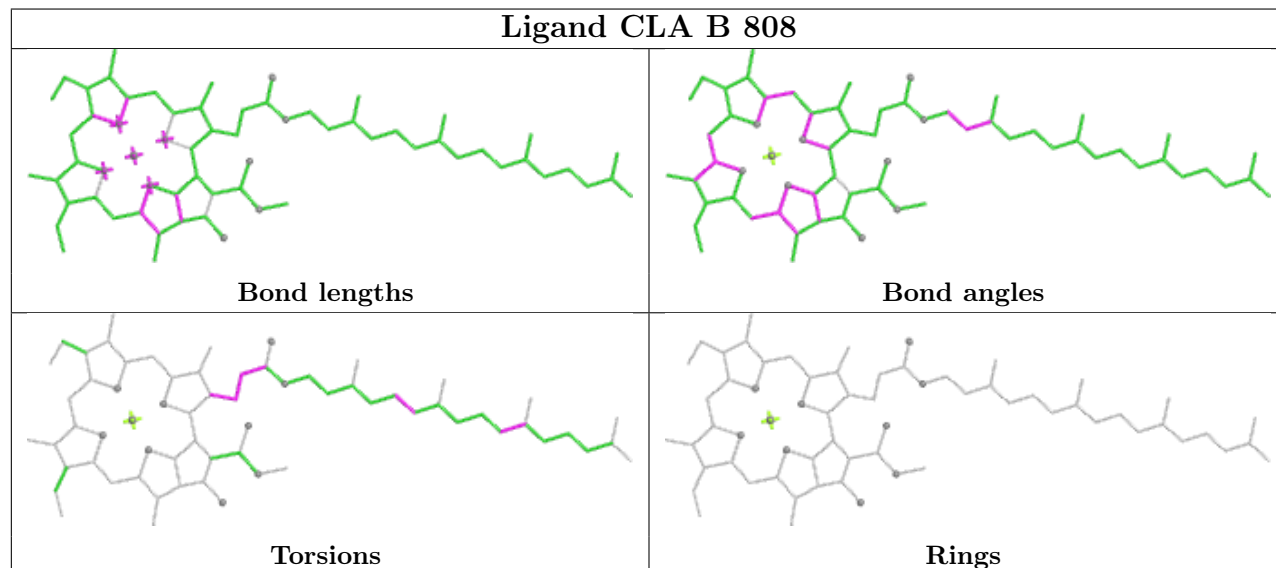
Bond angles



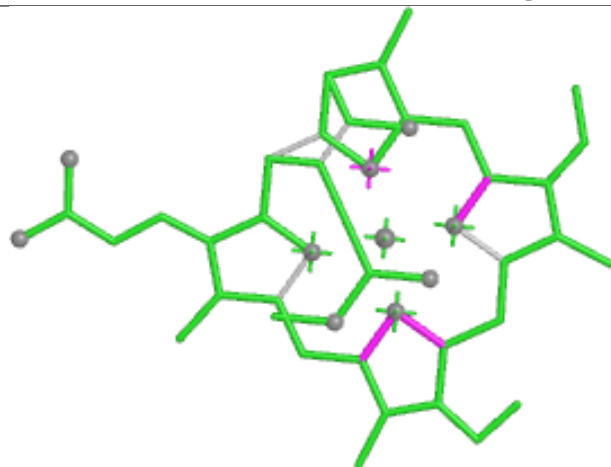
Torsions



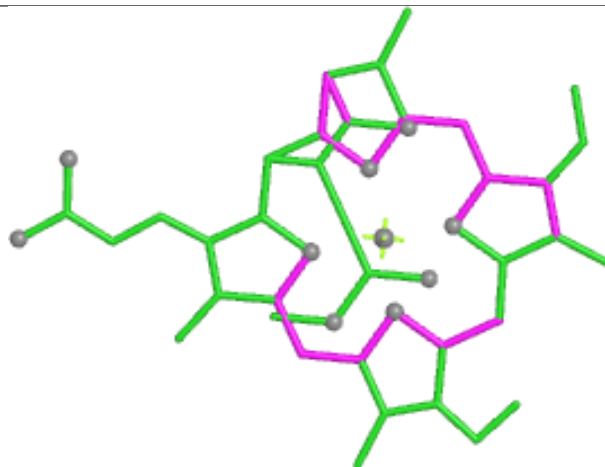
Rings

Ligand CLA 4 611**Ligand CLA B 808**

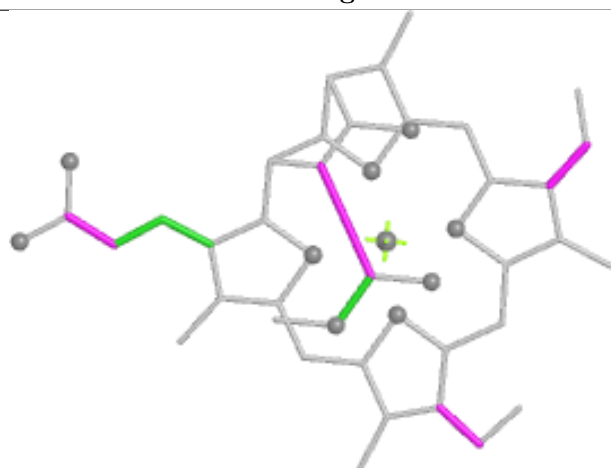
Ligand KC2 7 307



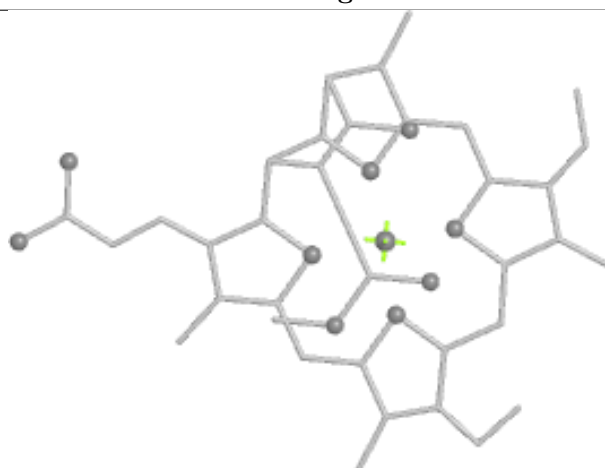
Bond lengths



Bond angles

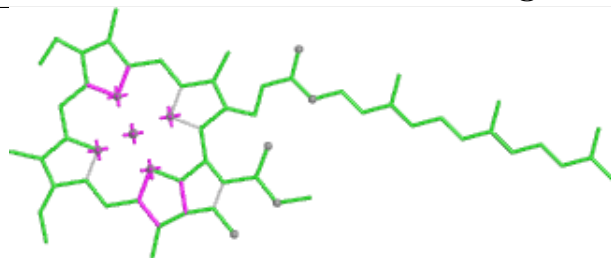


Torsions

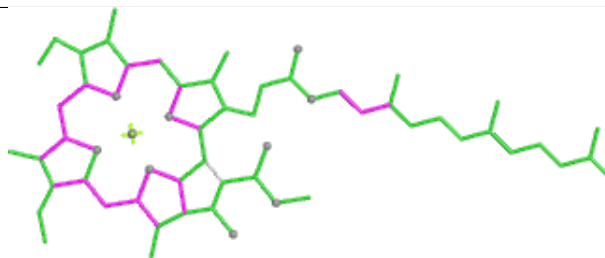


Rings

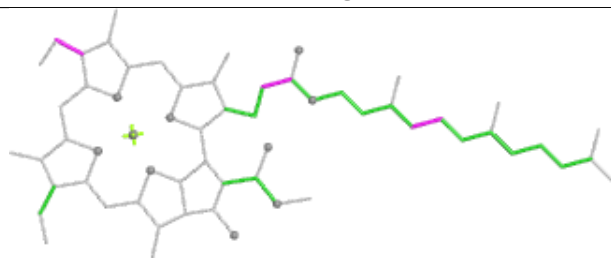
Ligand CLA 1 608



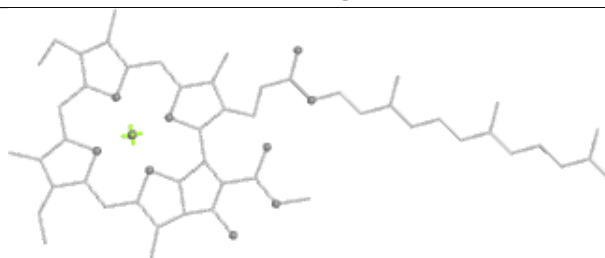
Bond lengths



Bond angles

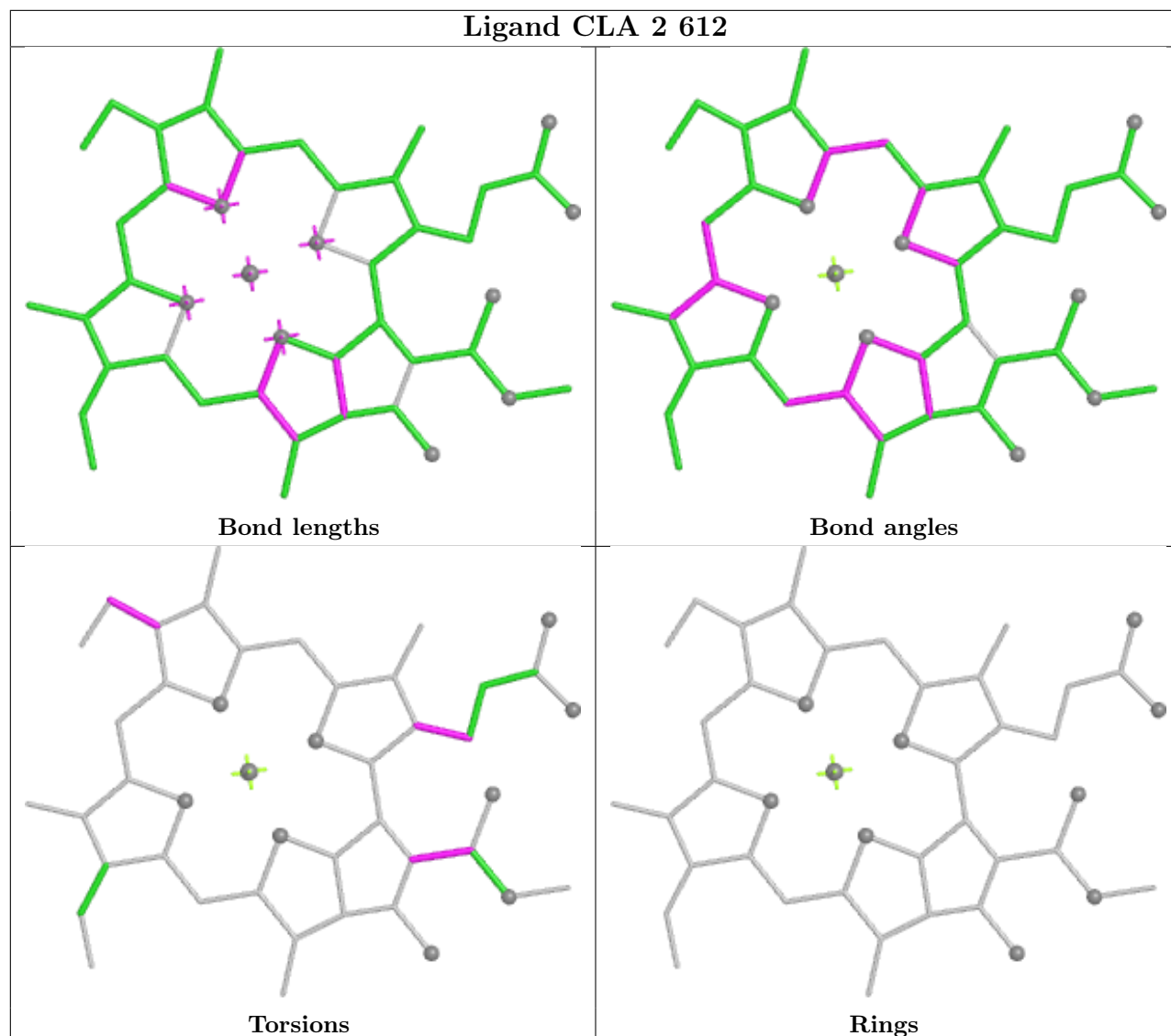


Torsions

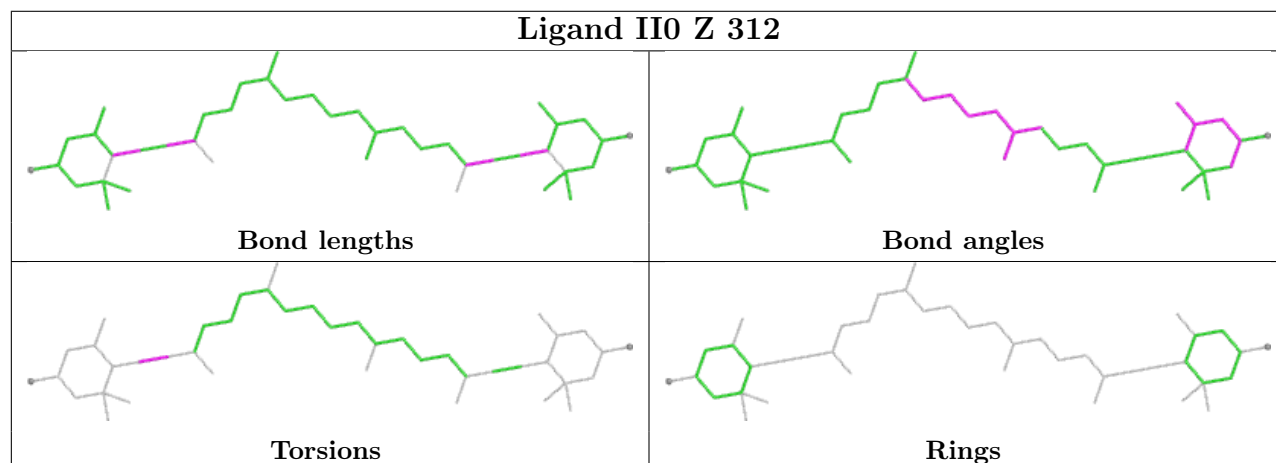


Rings

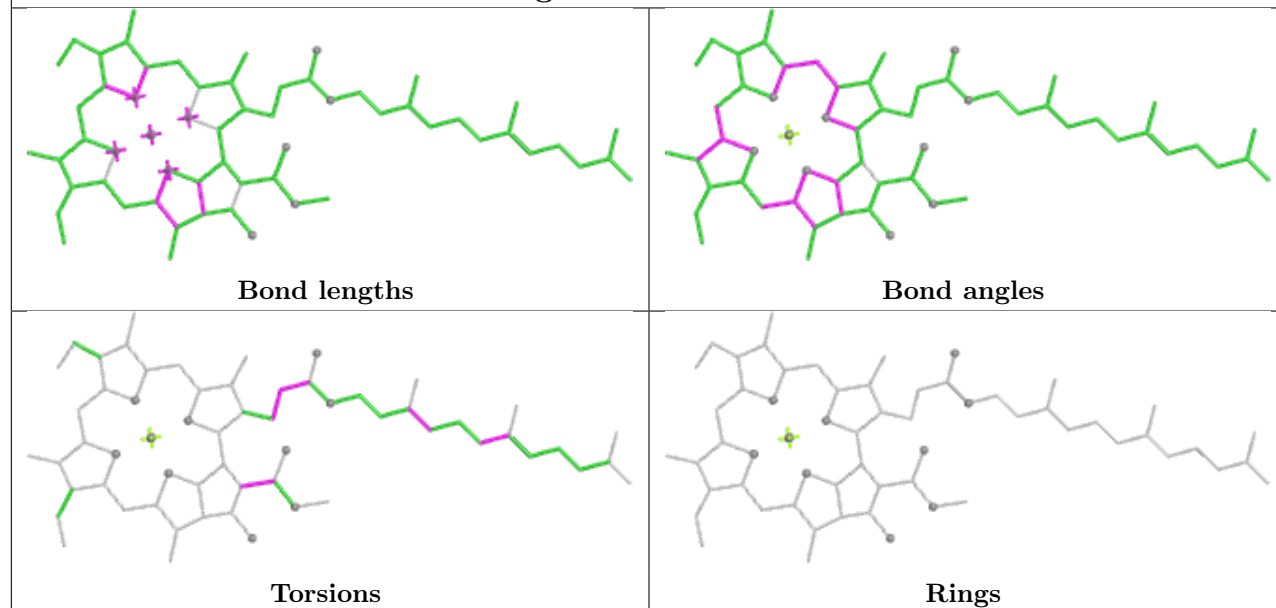
Ligand CLA 2 612



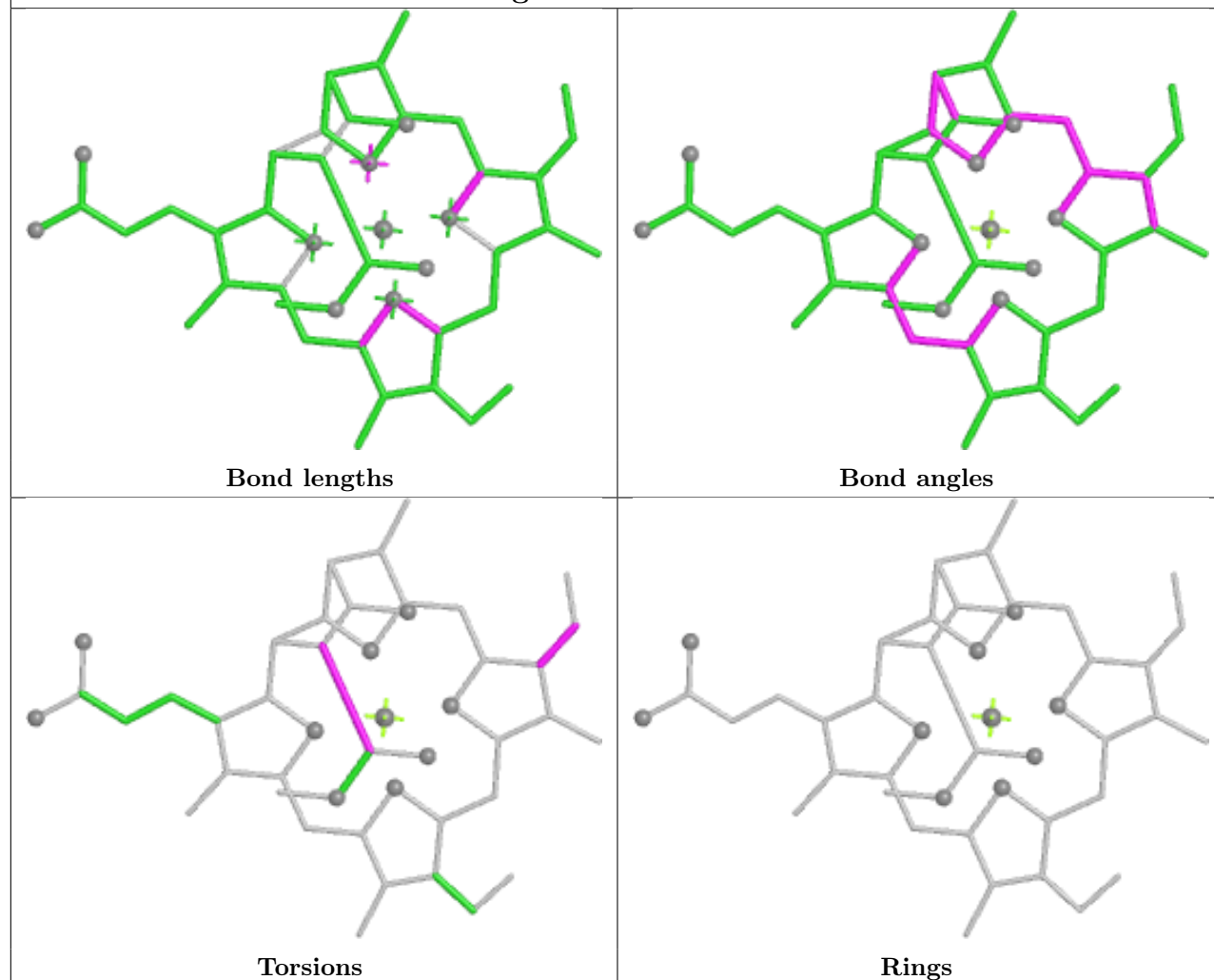
Ligand II0 Z 312

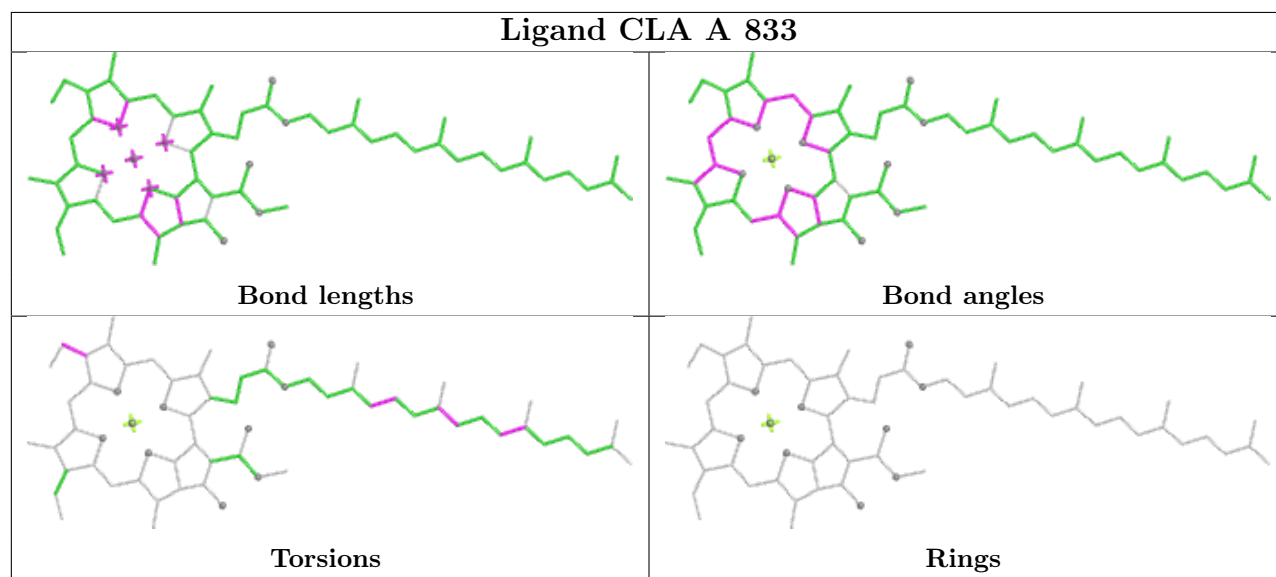
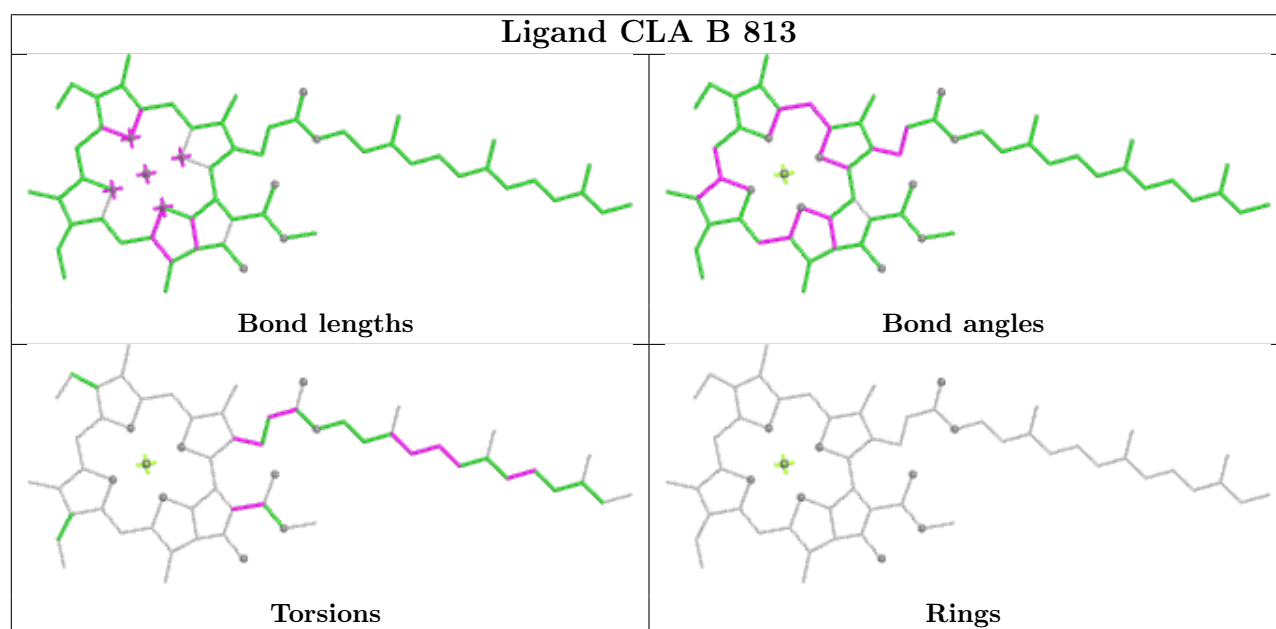
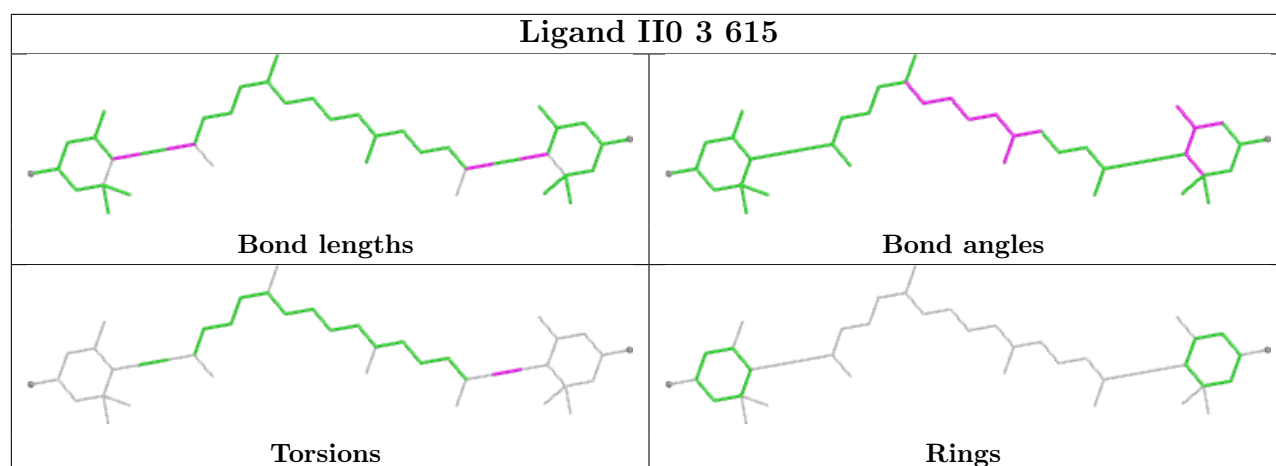


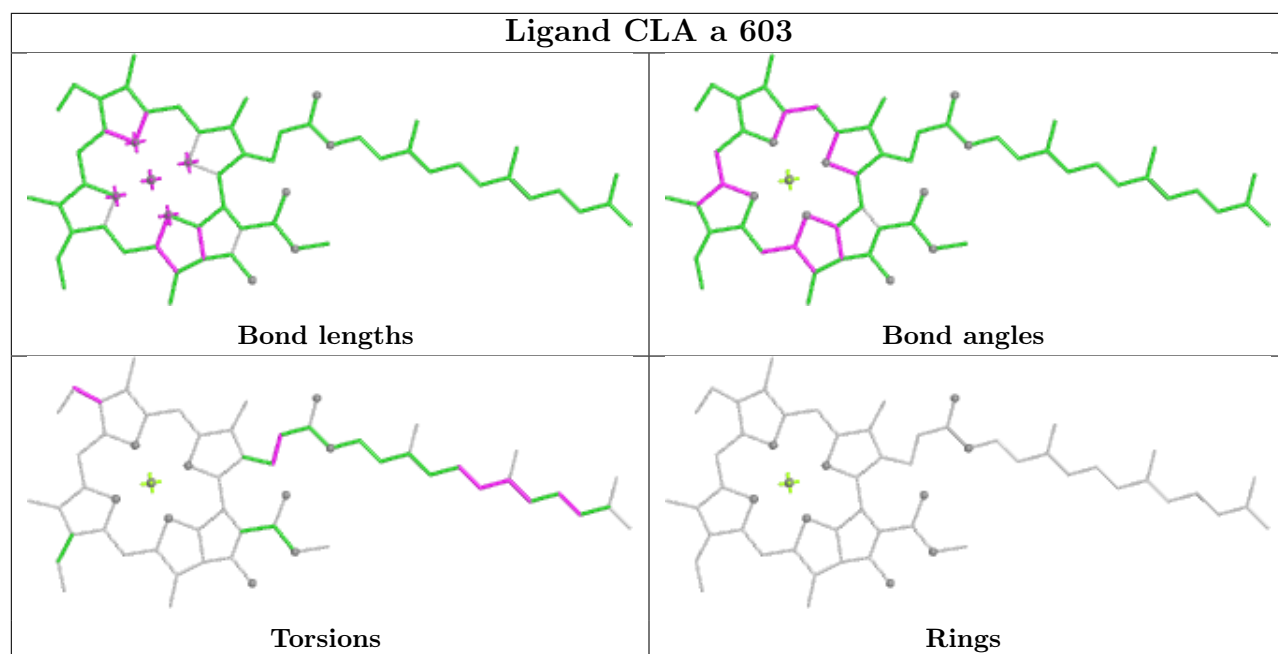
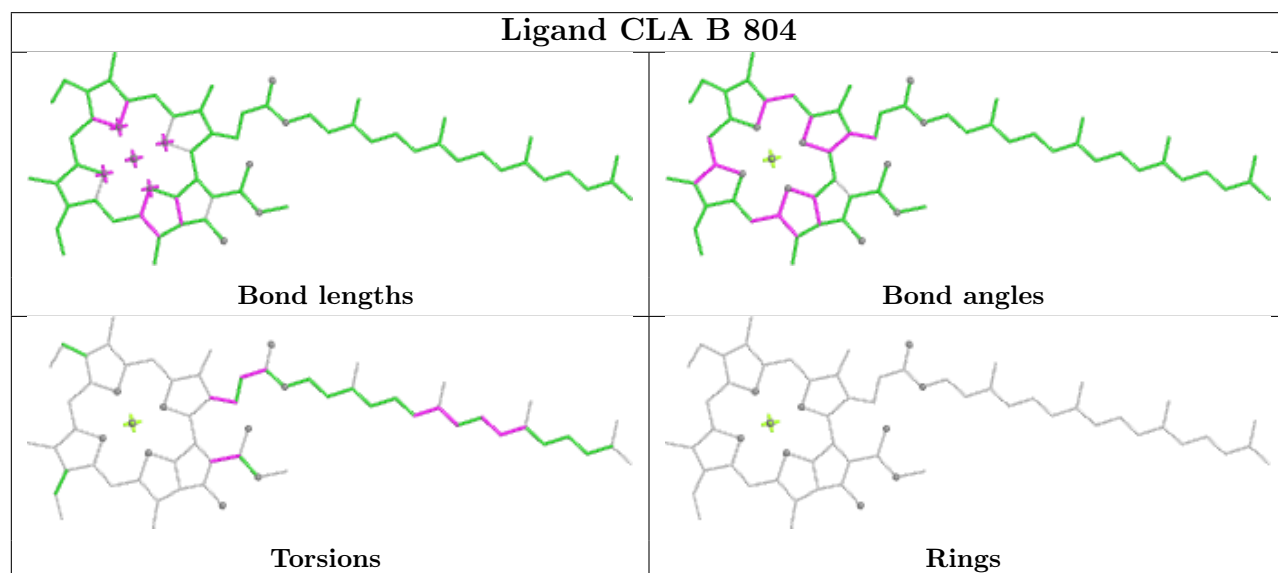
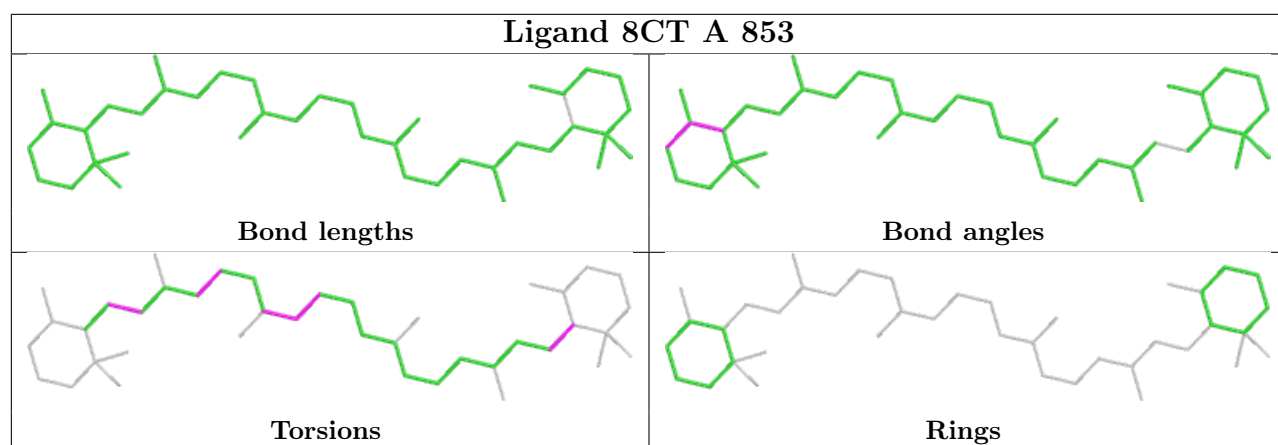
Ligand CLA b 603



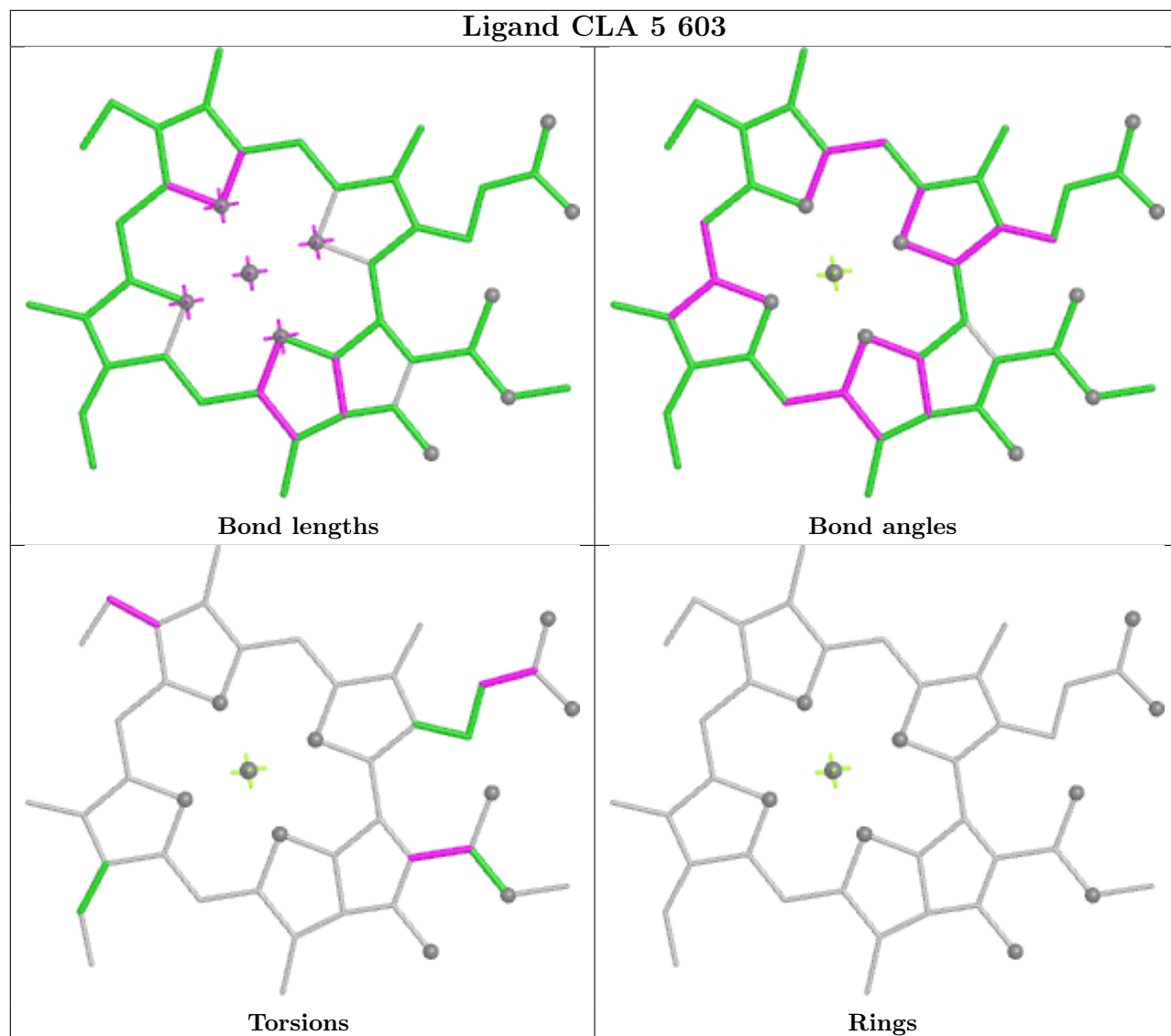
Ligand KC2 a 609



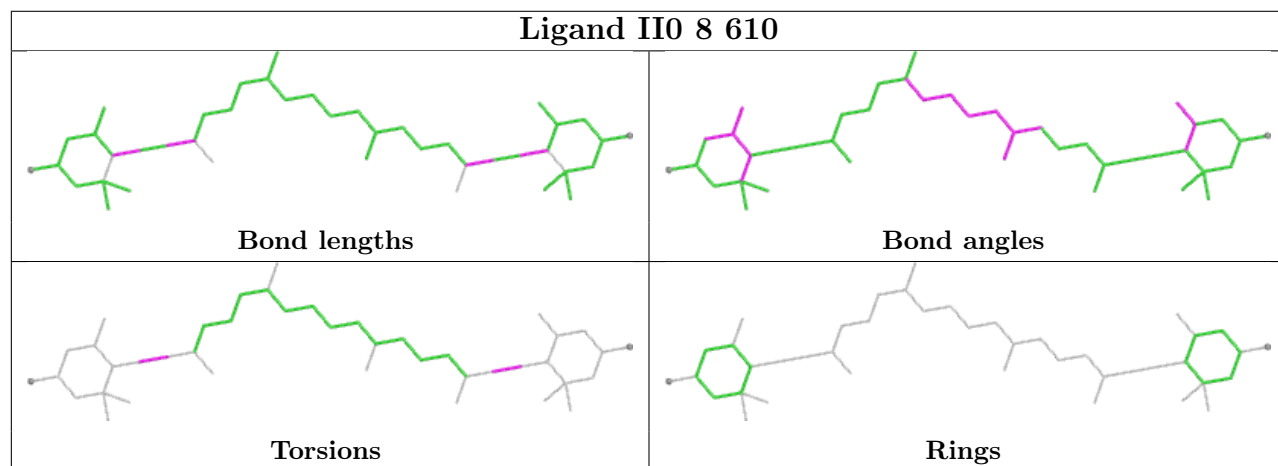


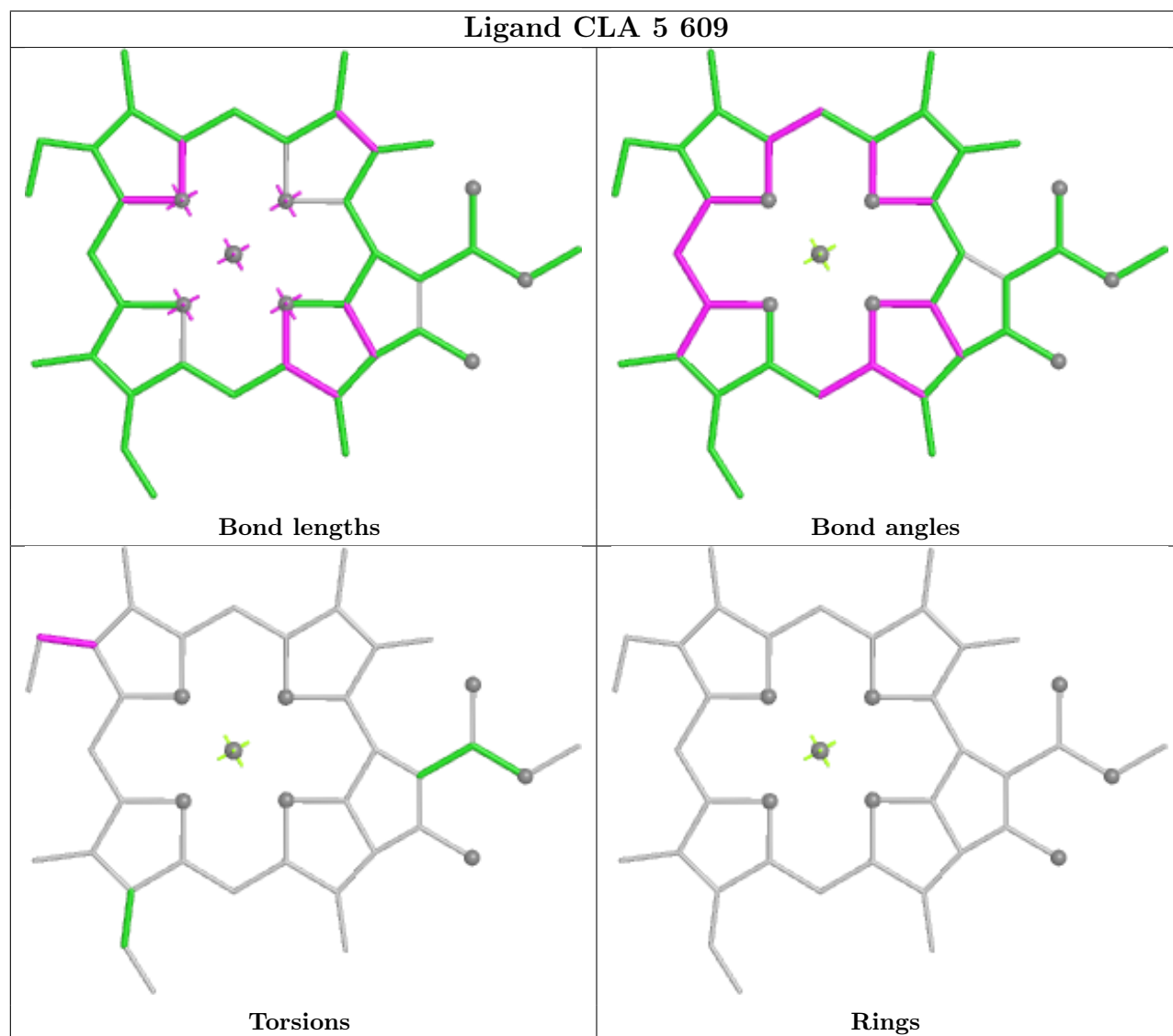
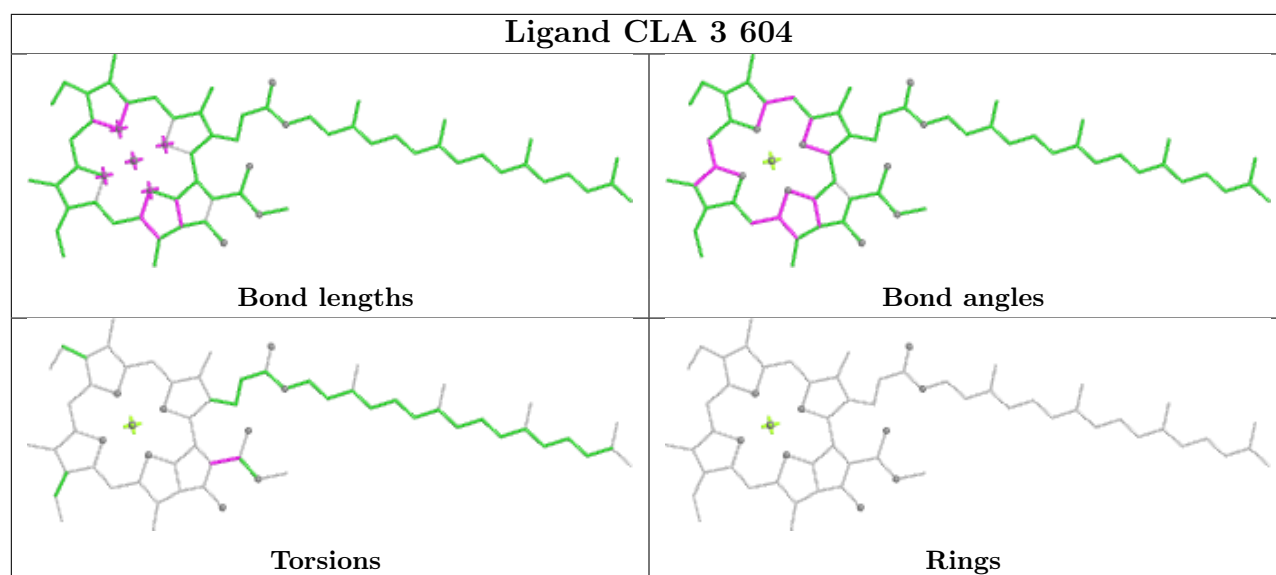


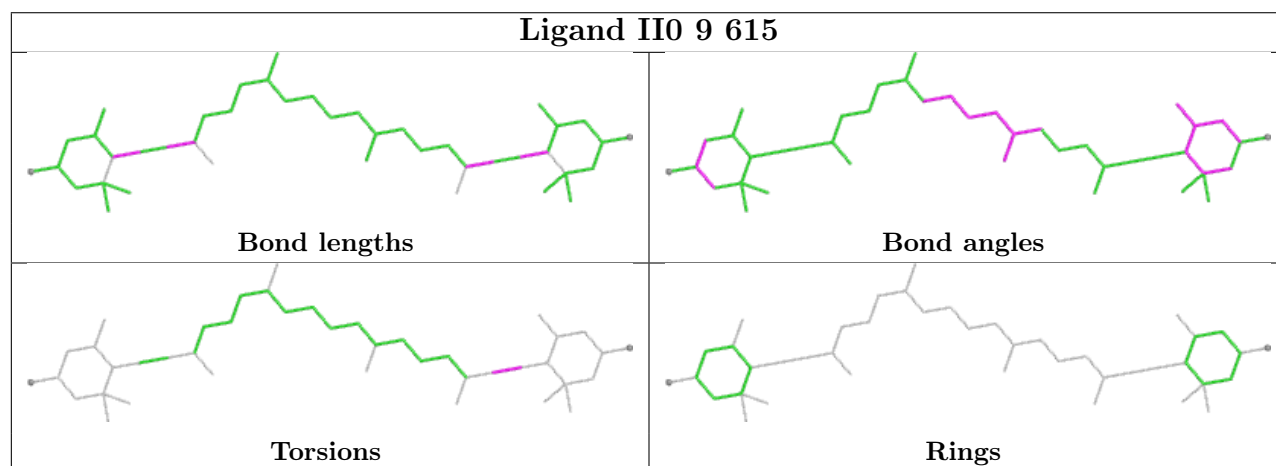
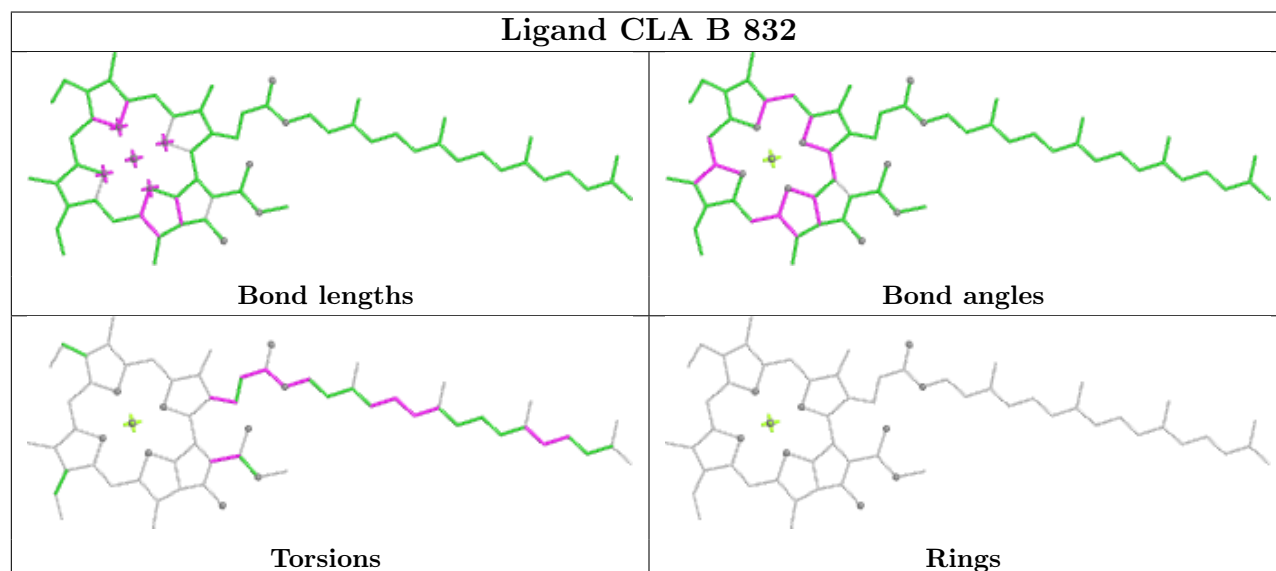
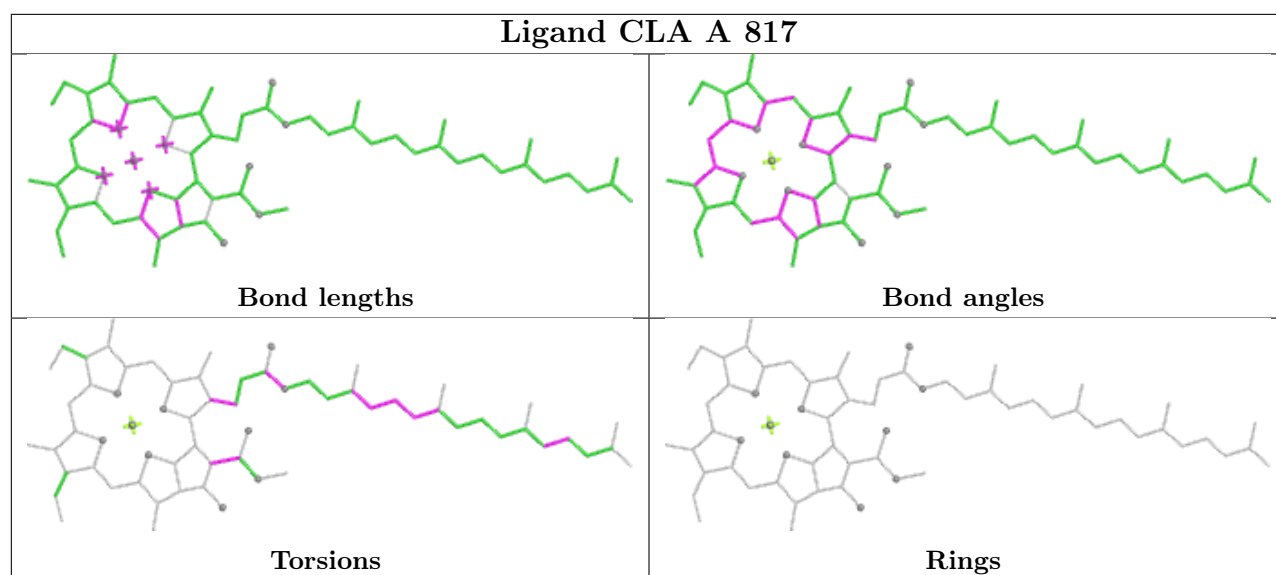
Ligand CLA 5 603



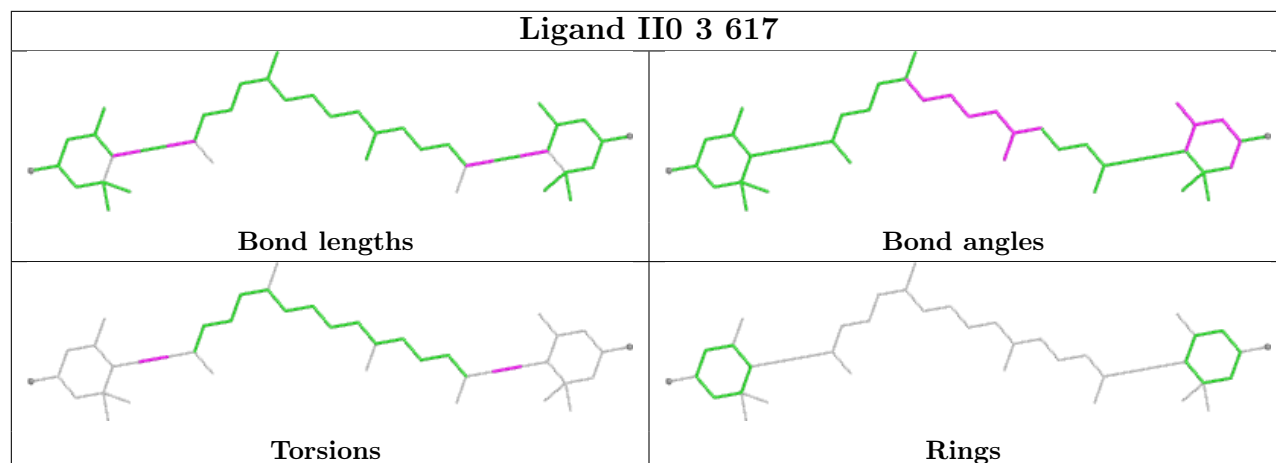
Ligand II0 8 610



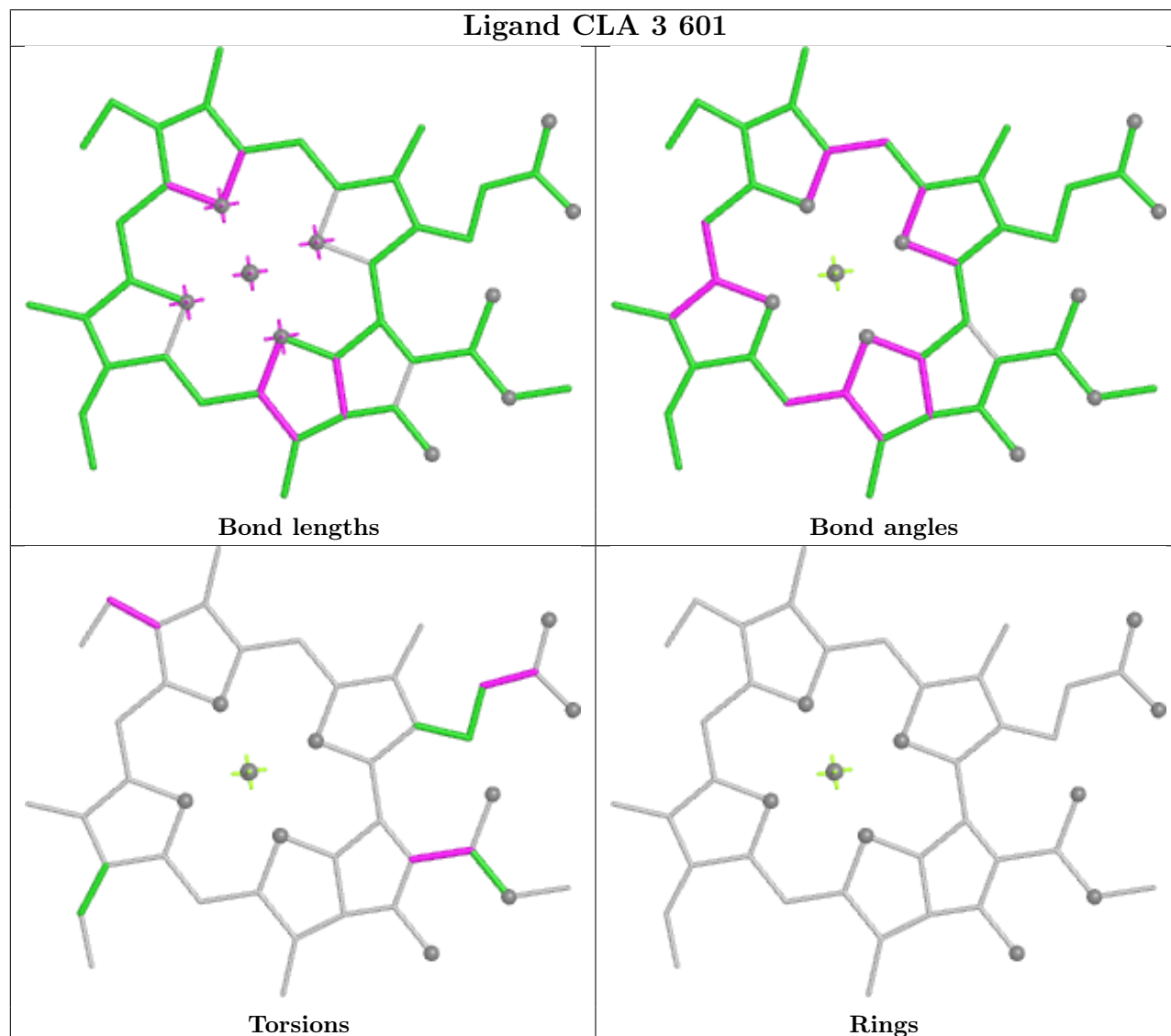


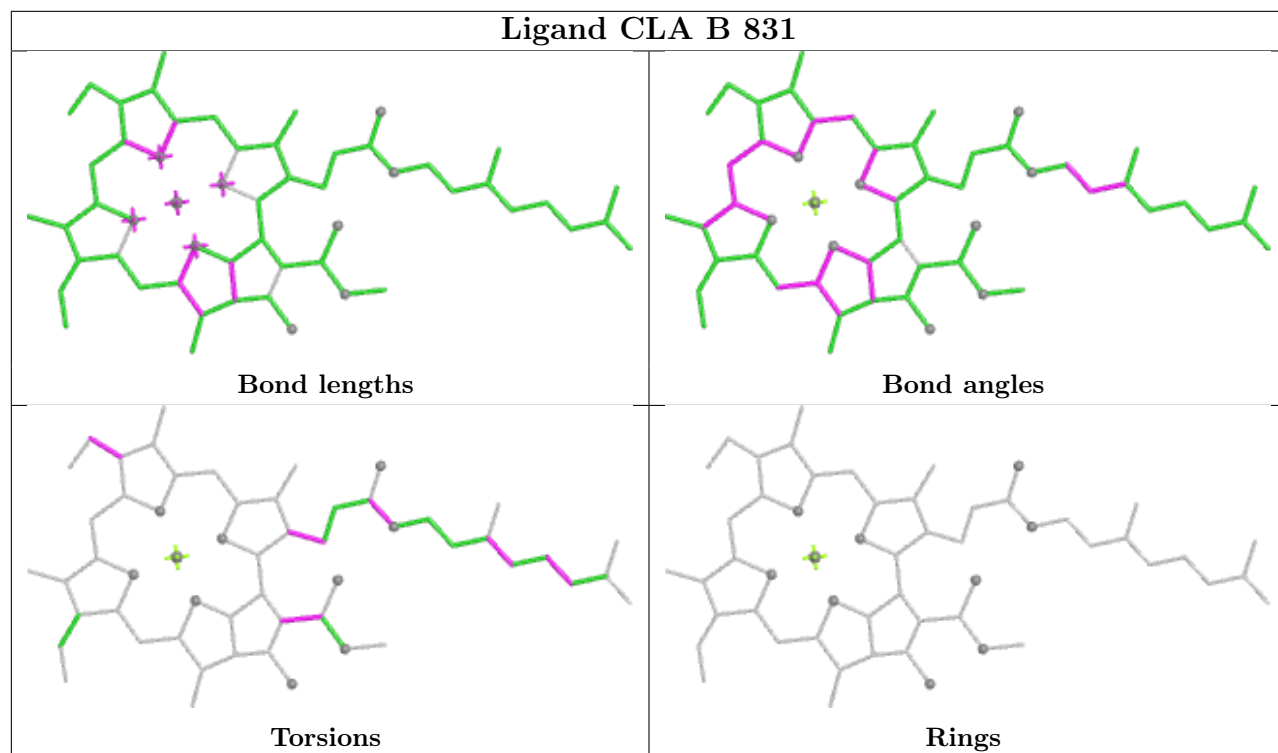


Ligand II0 3 617

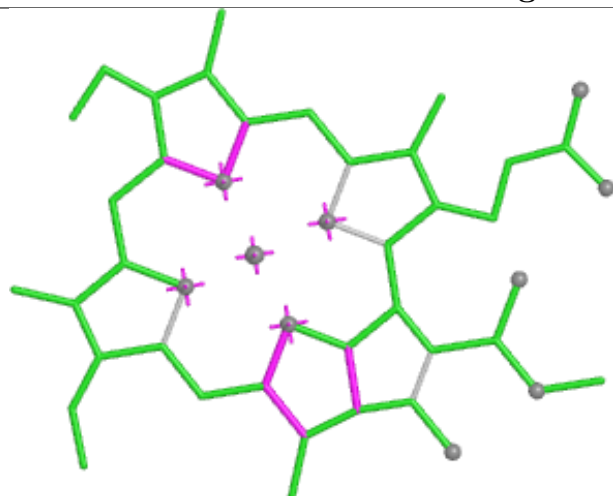


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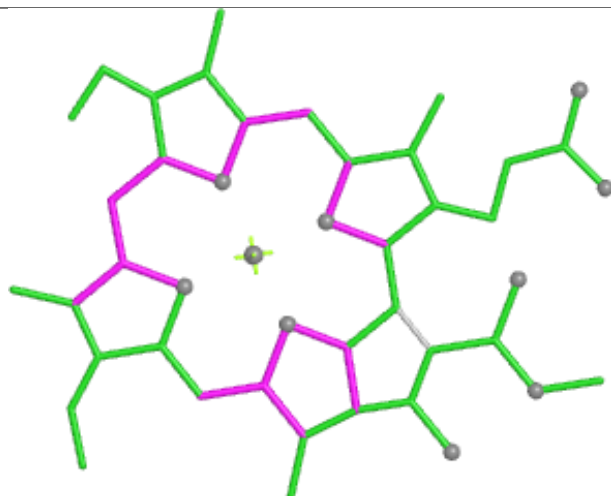




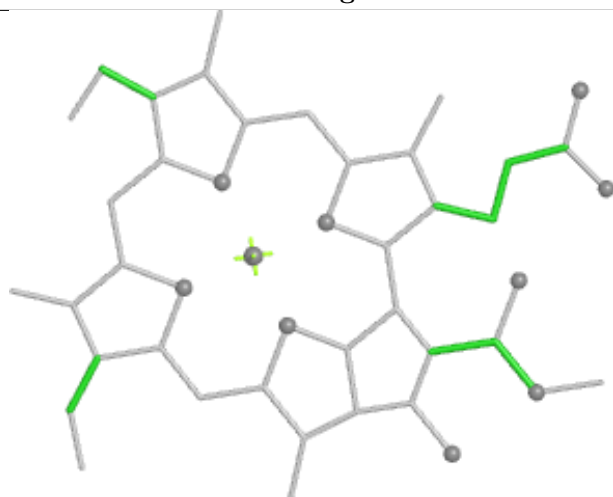
Ligand CLA 1 607



Bond lengths



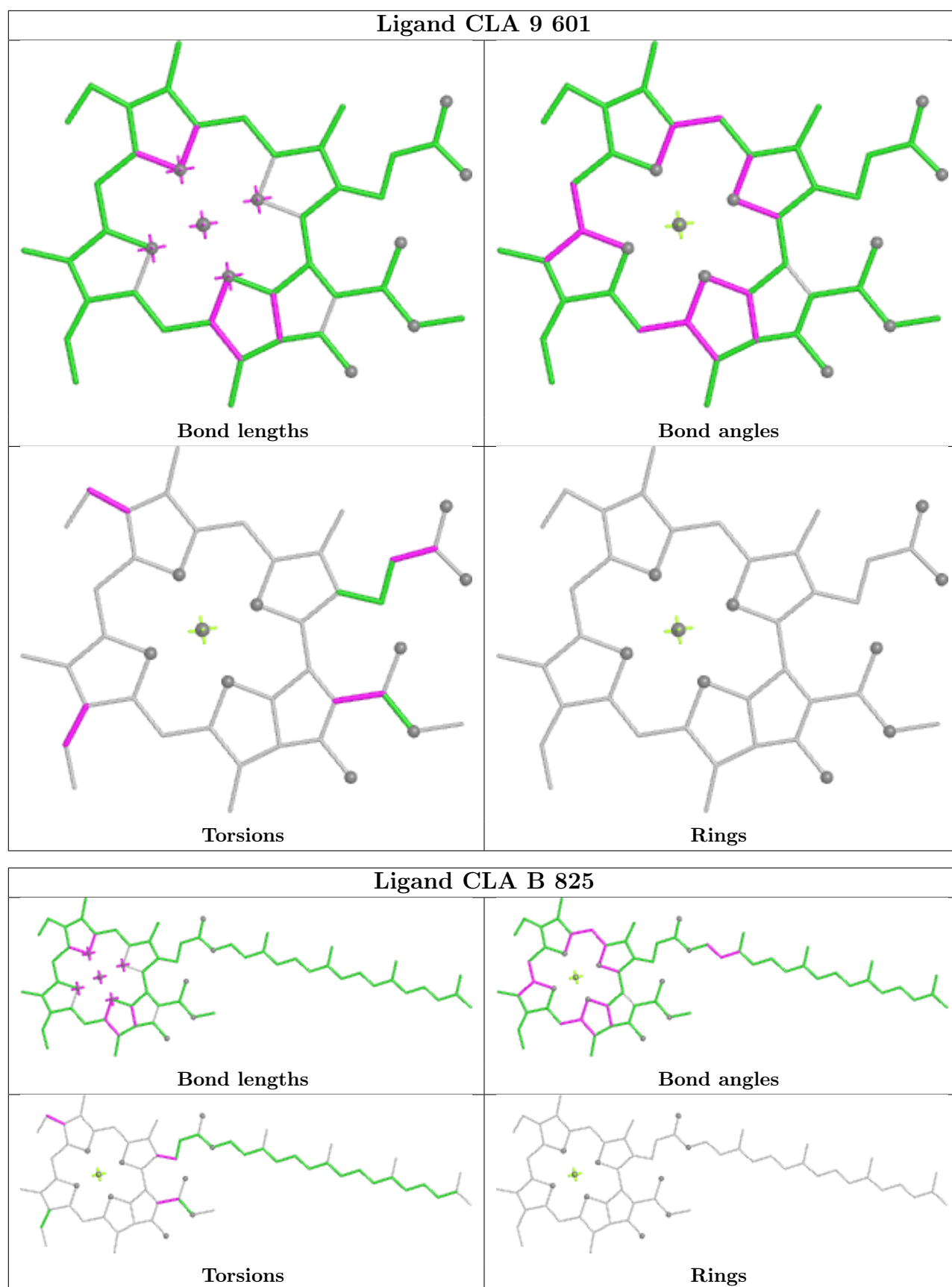
Bond angles

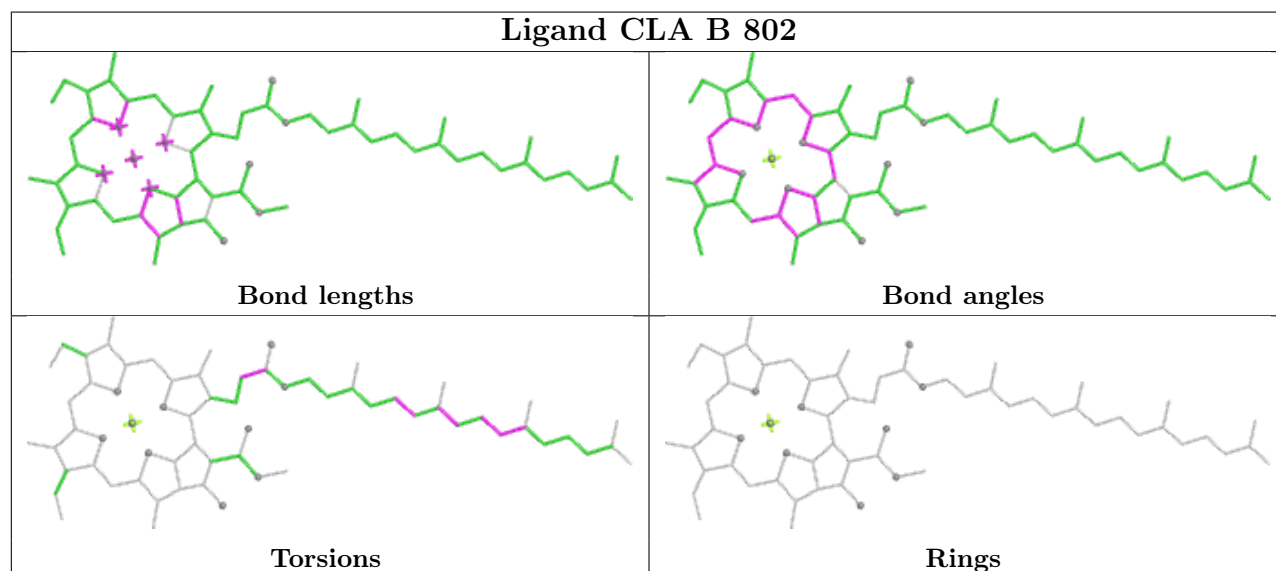
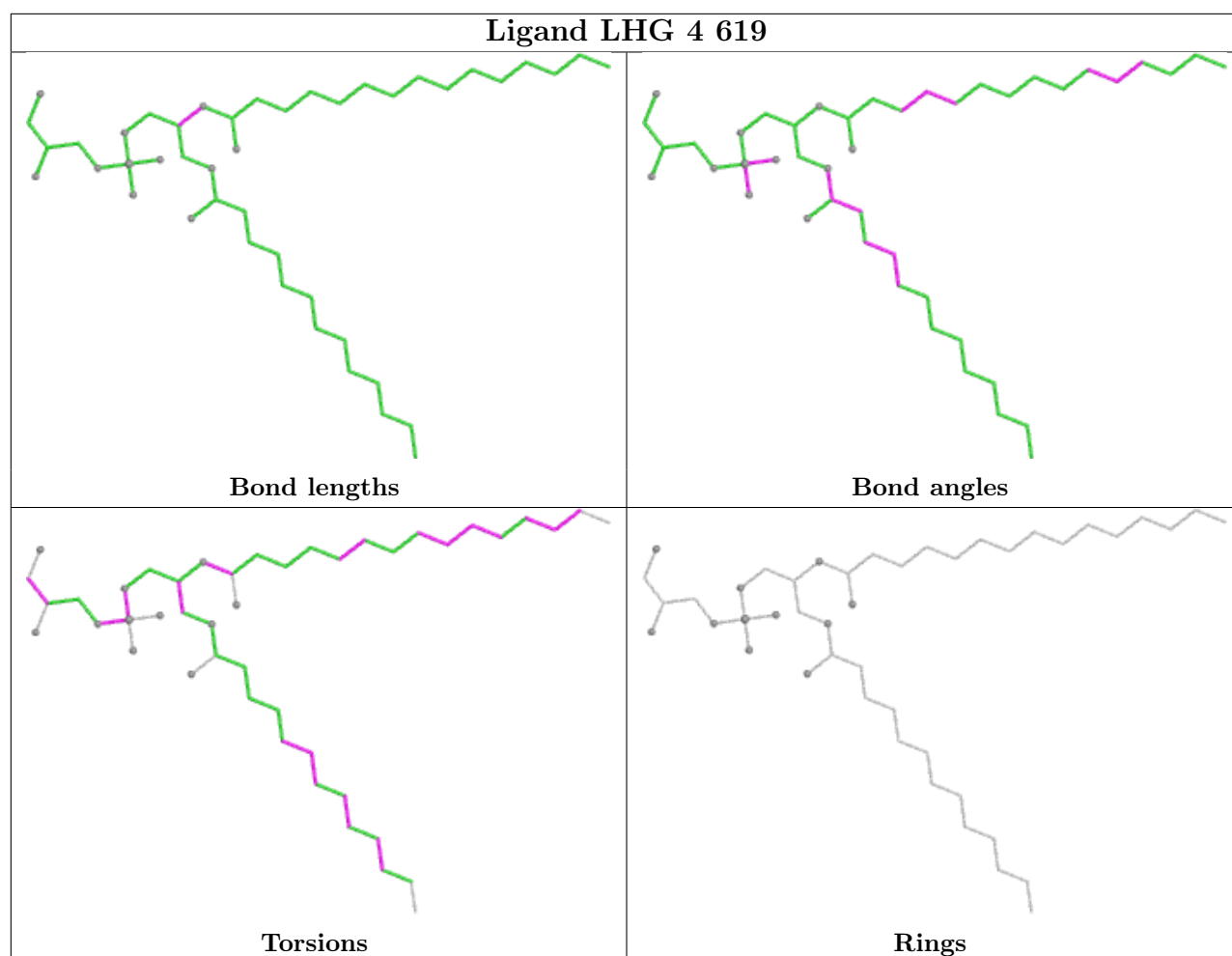


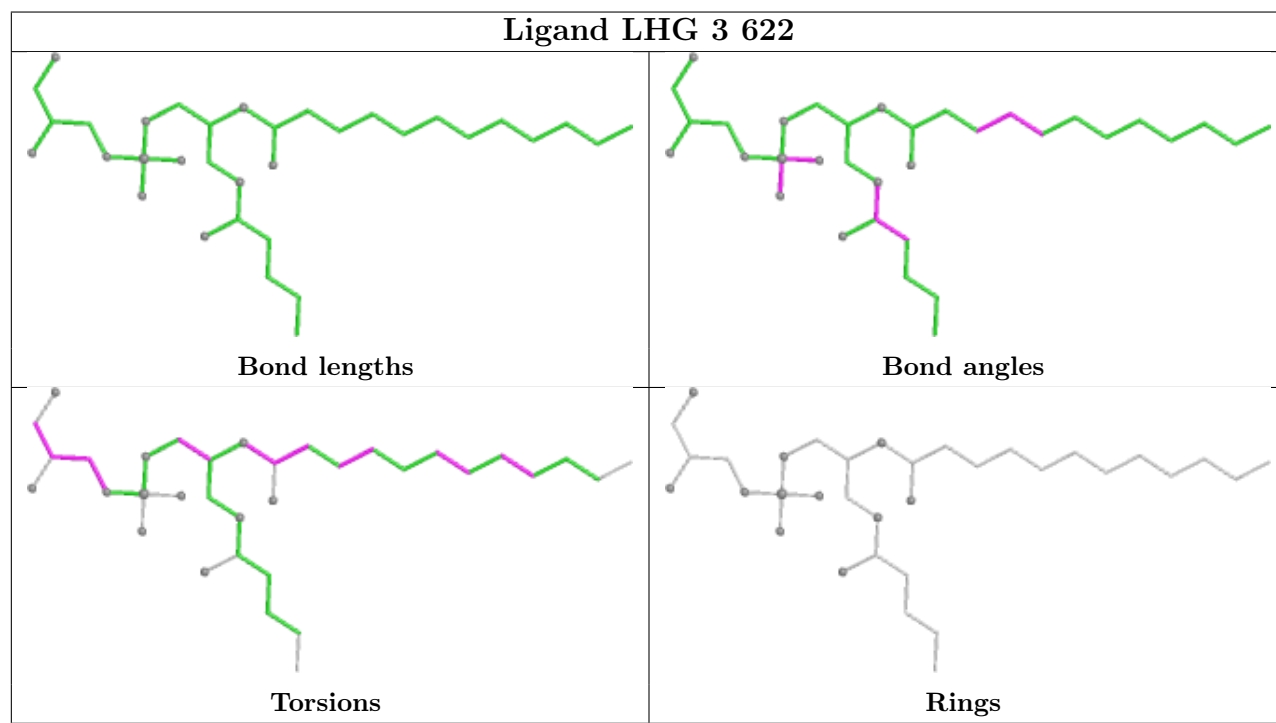
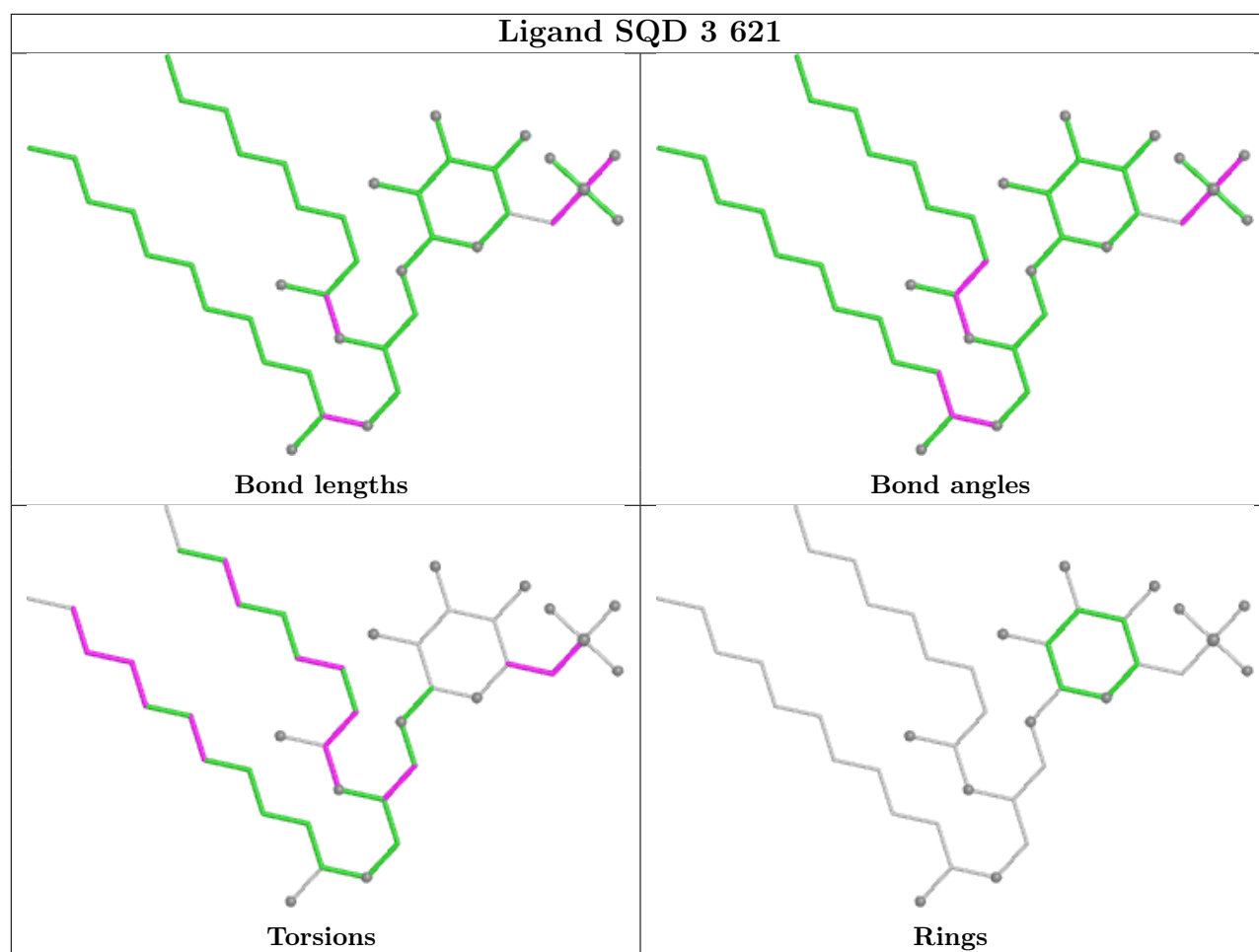
Torsions

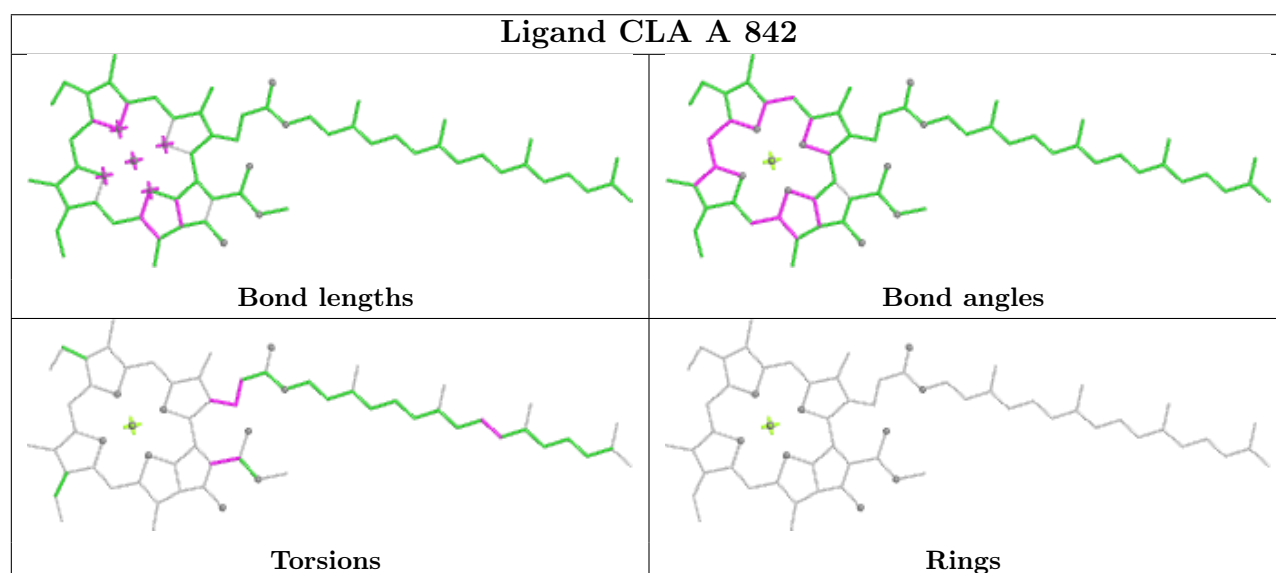
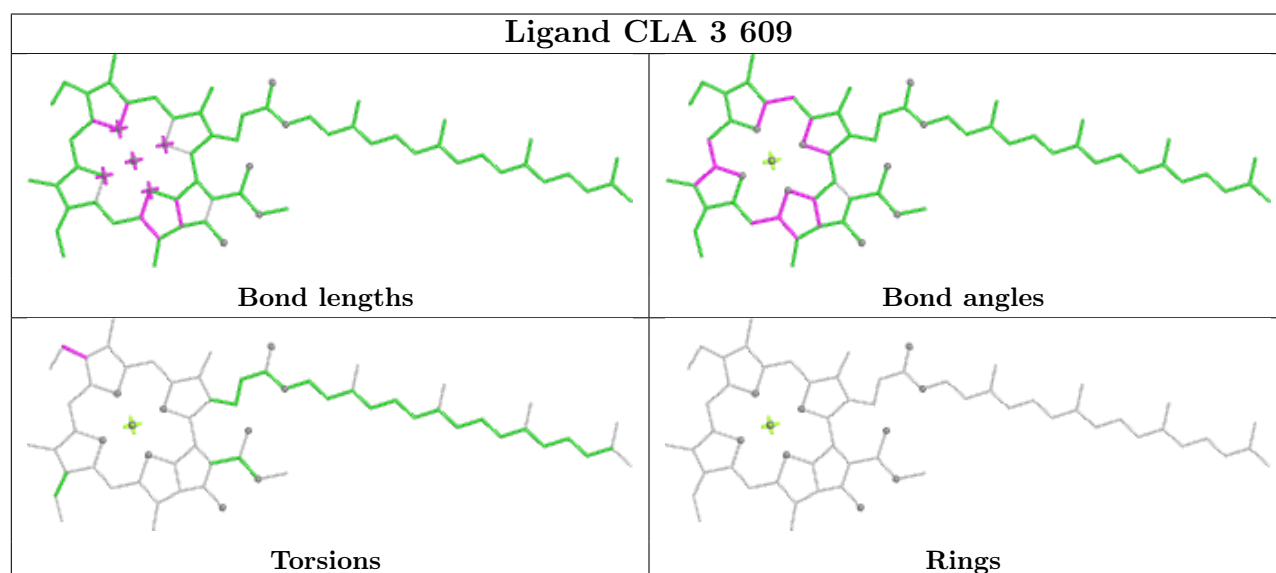
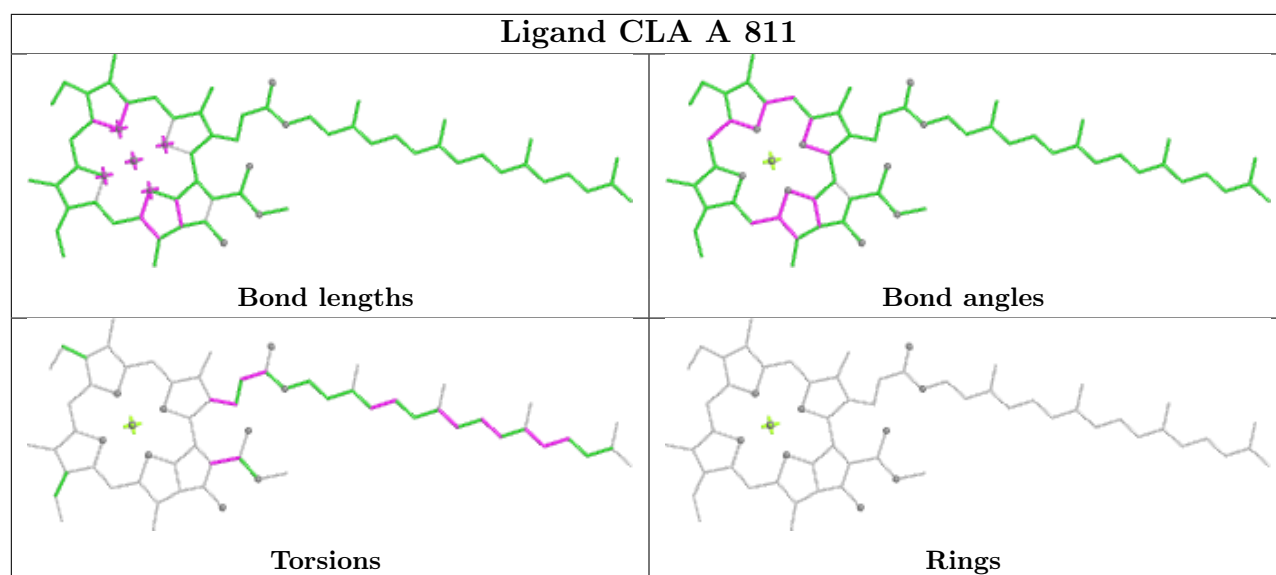


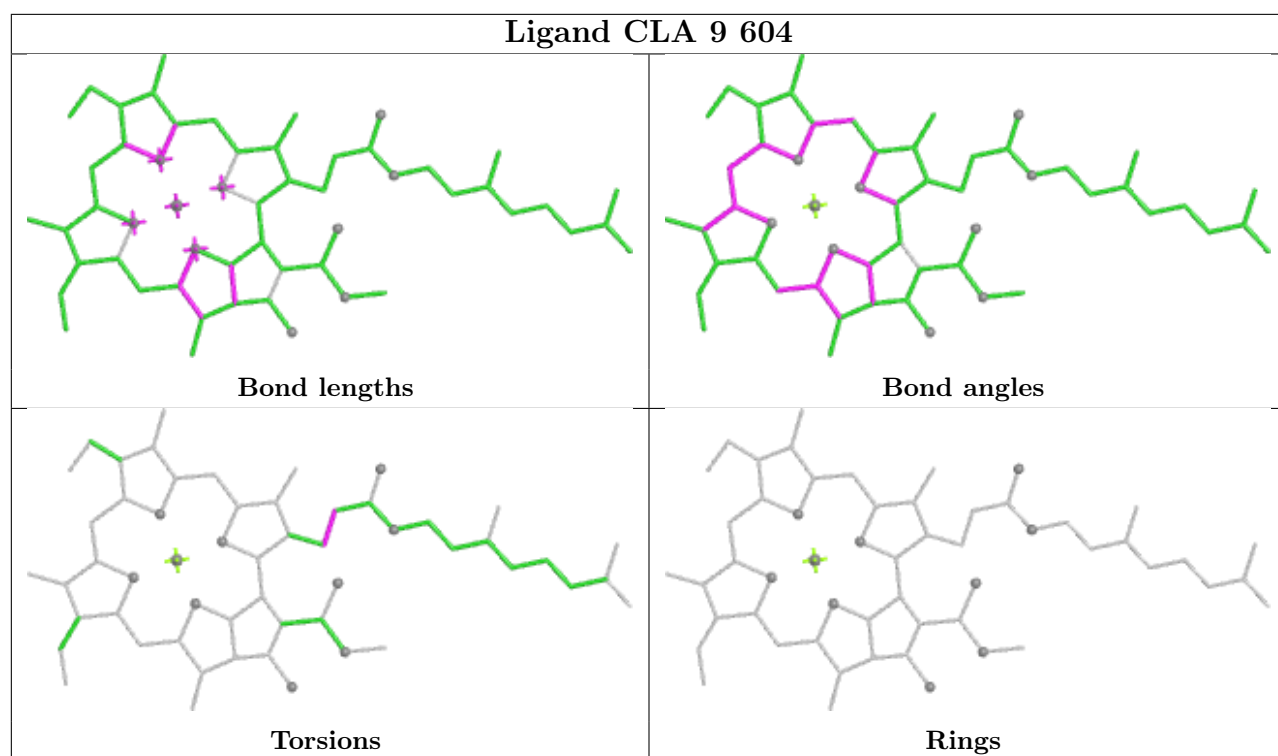
Rings



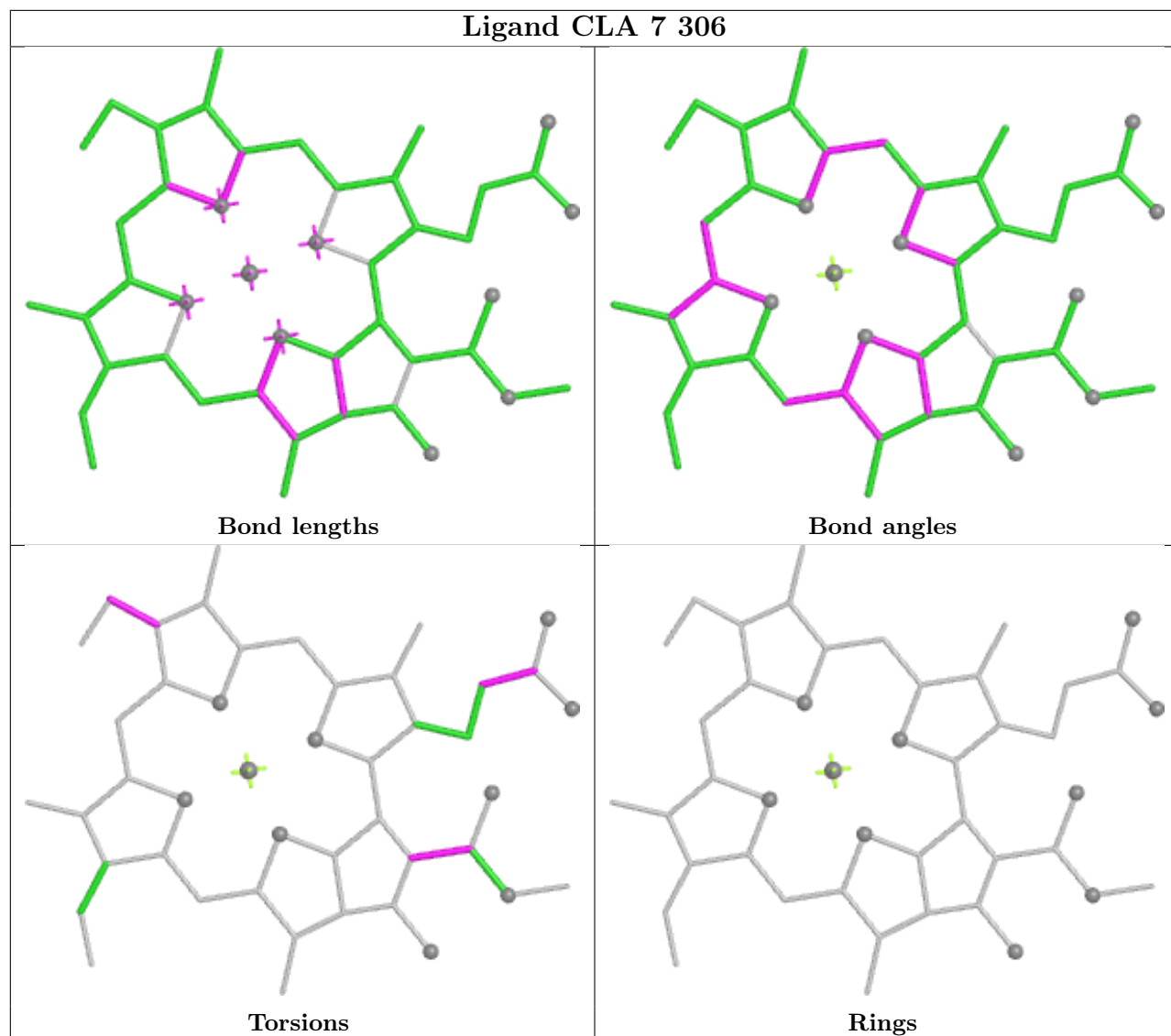


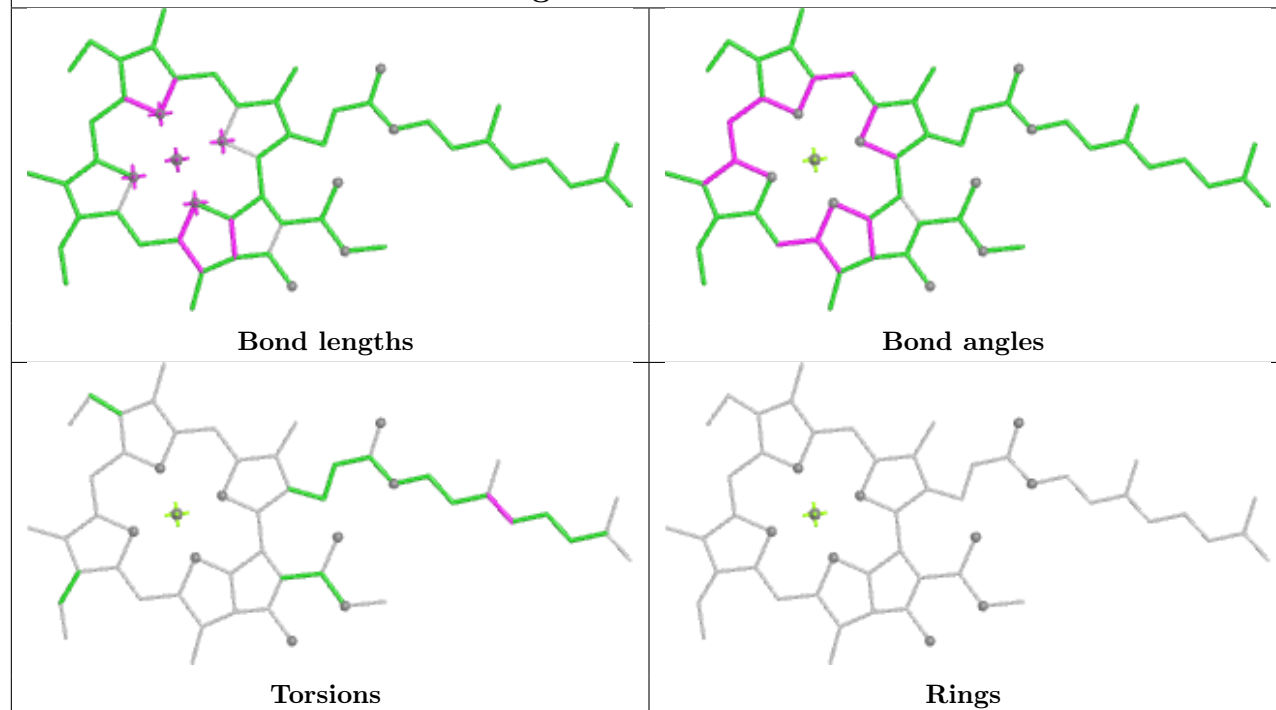
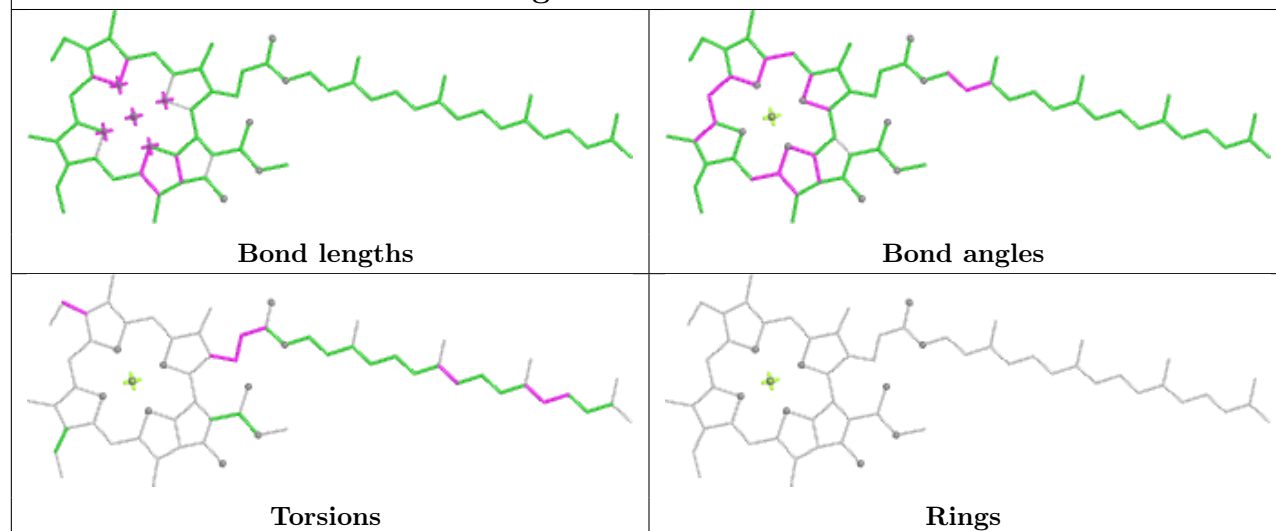


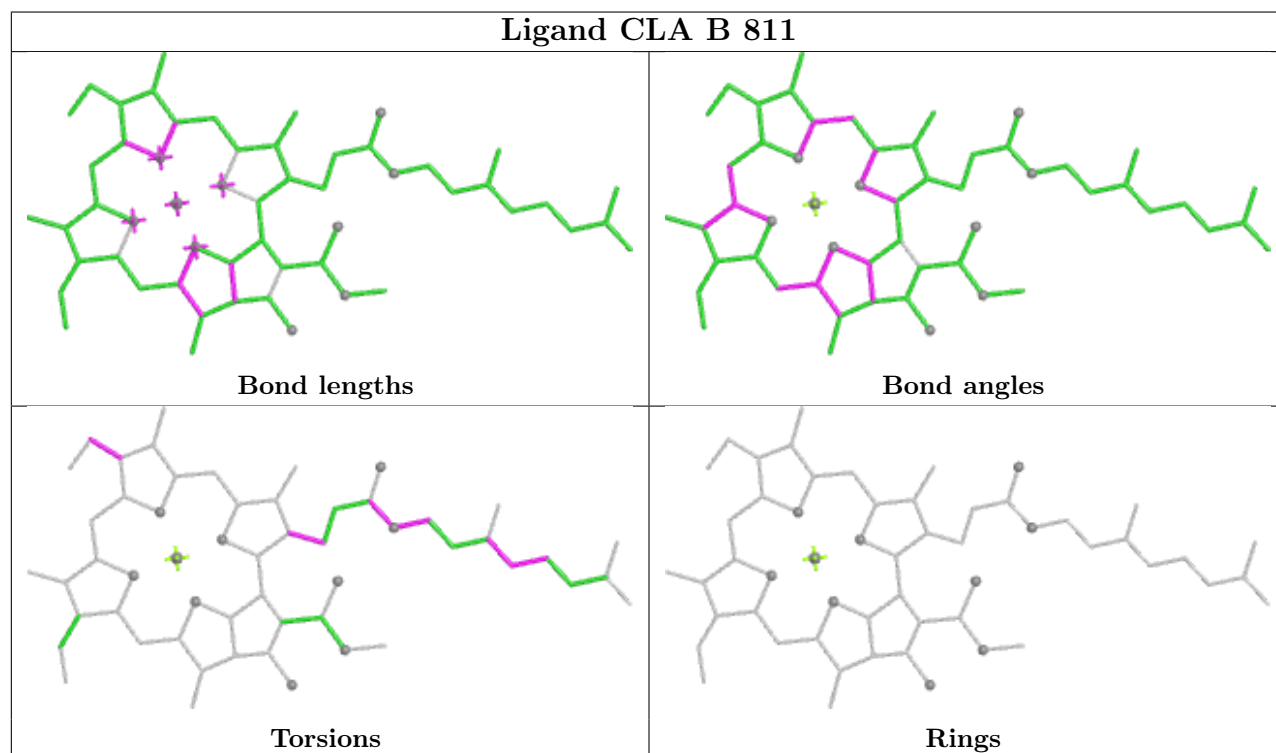
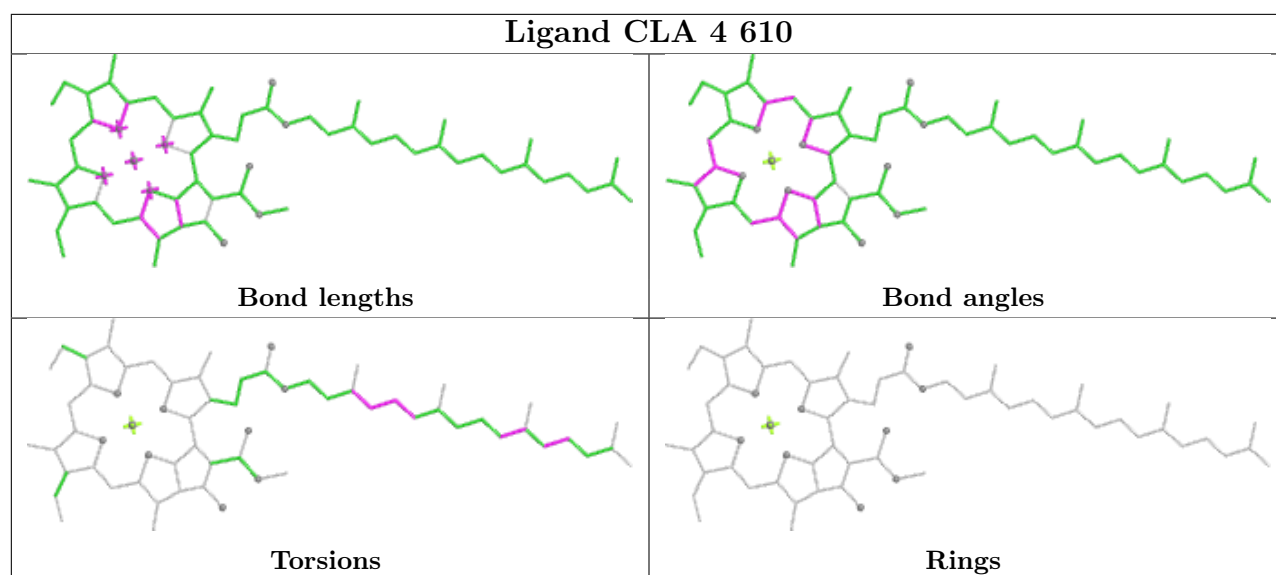


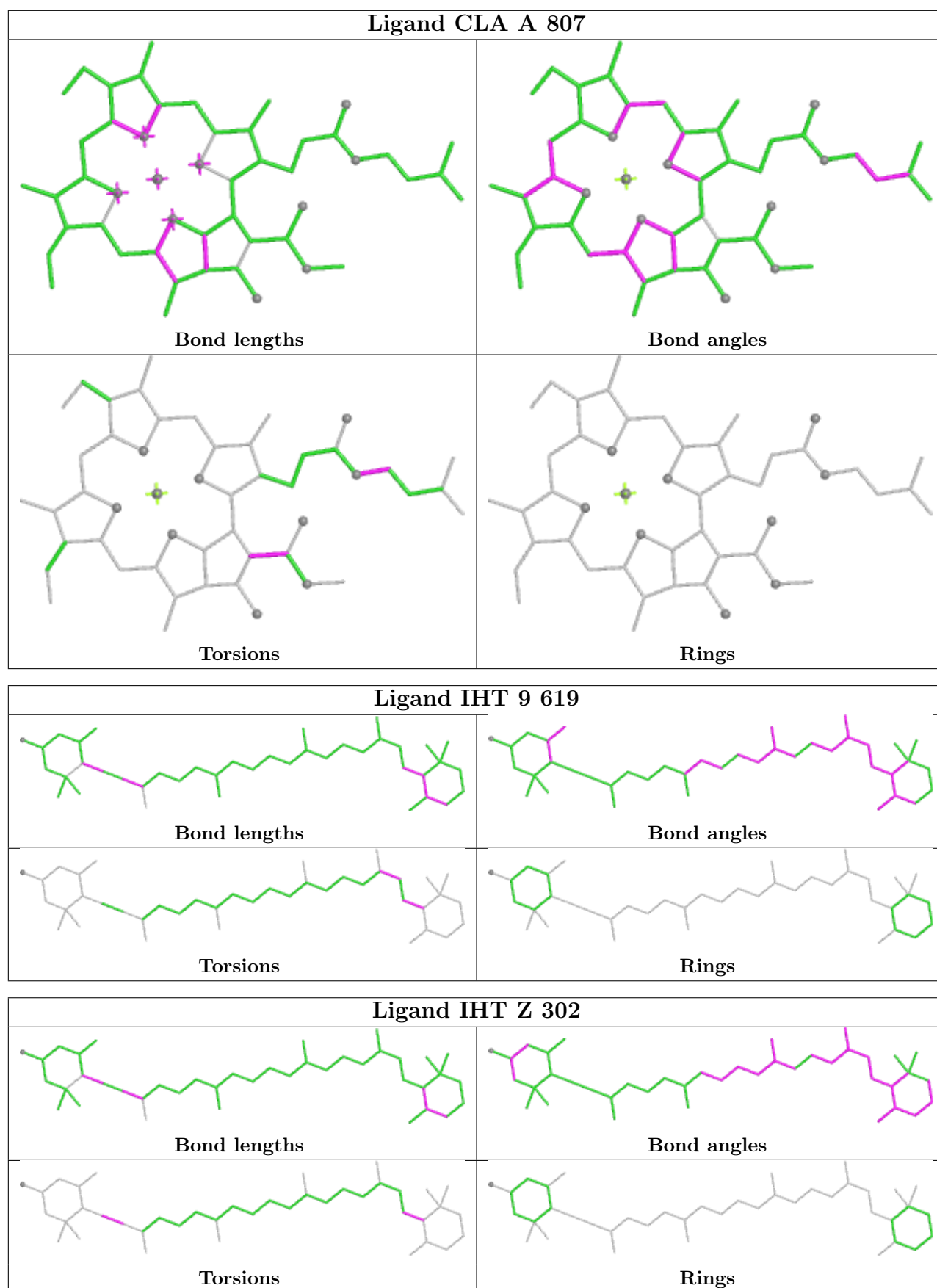


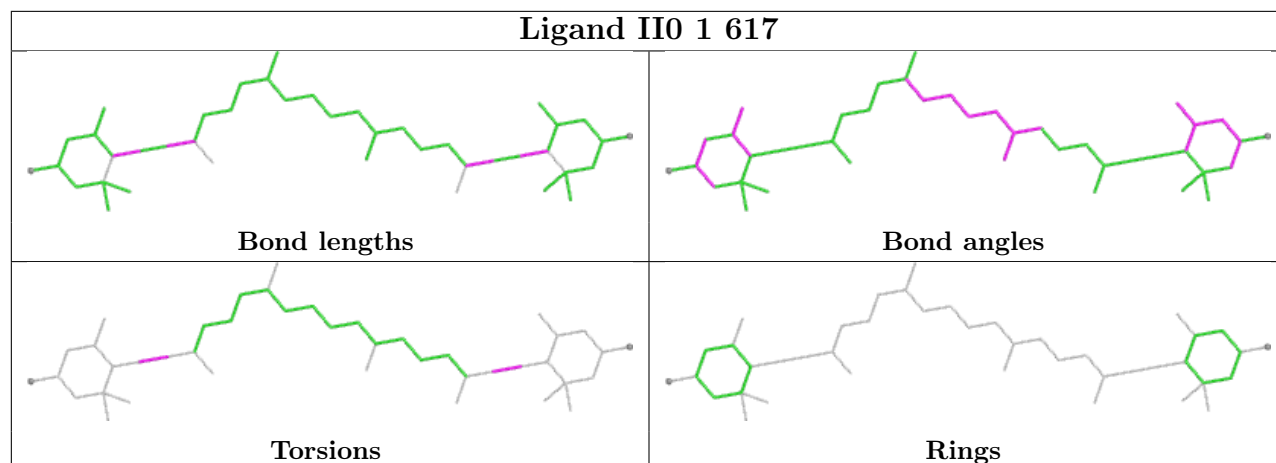
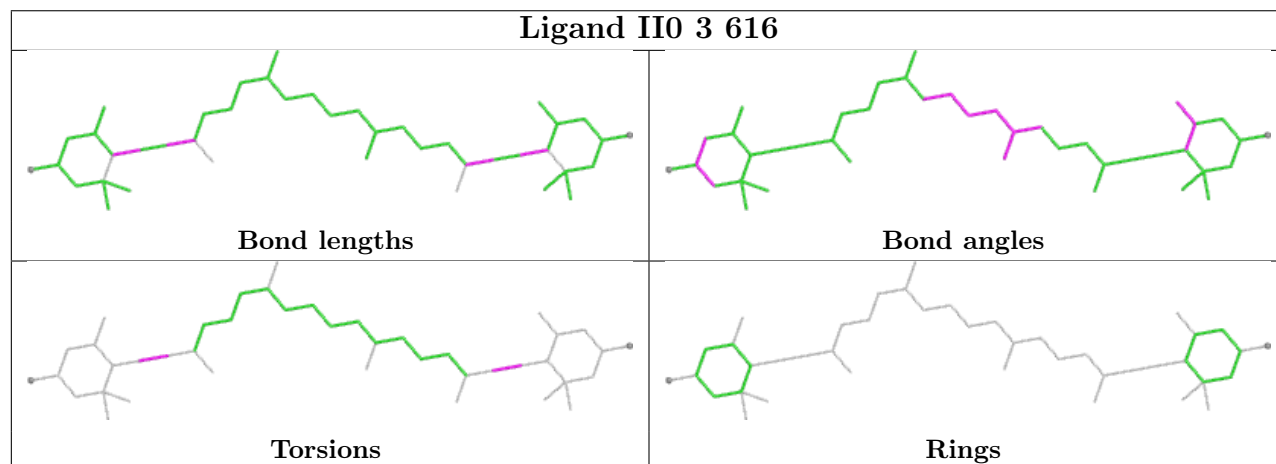
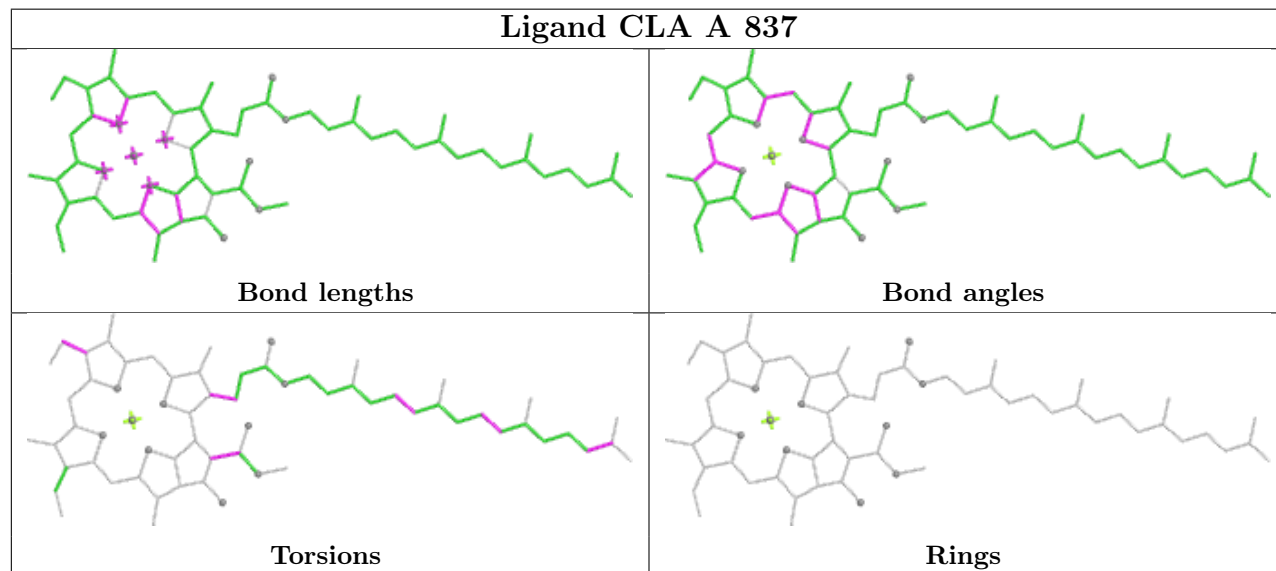
Ligand CLA 7 306

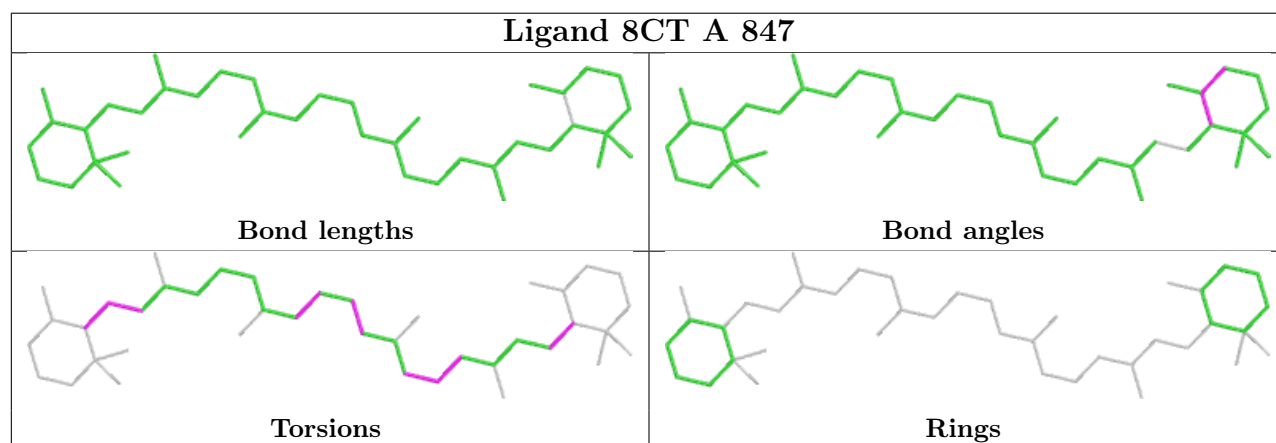
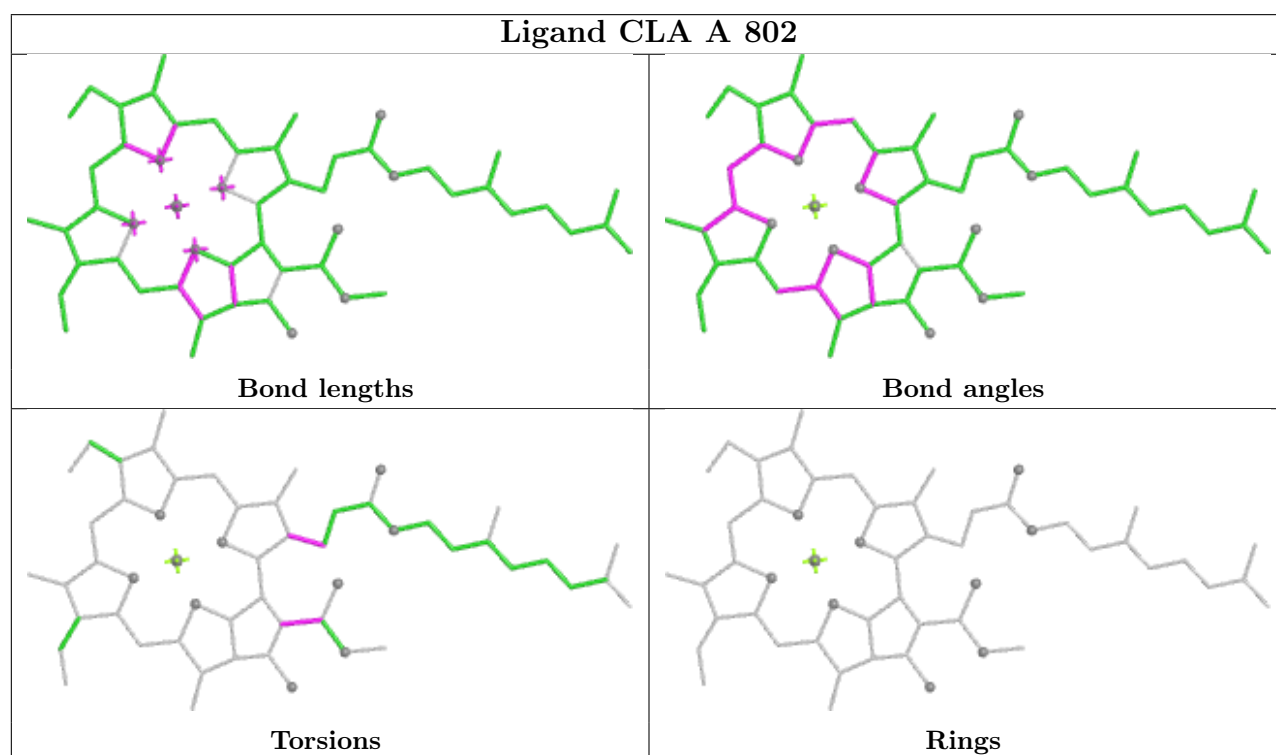
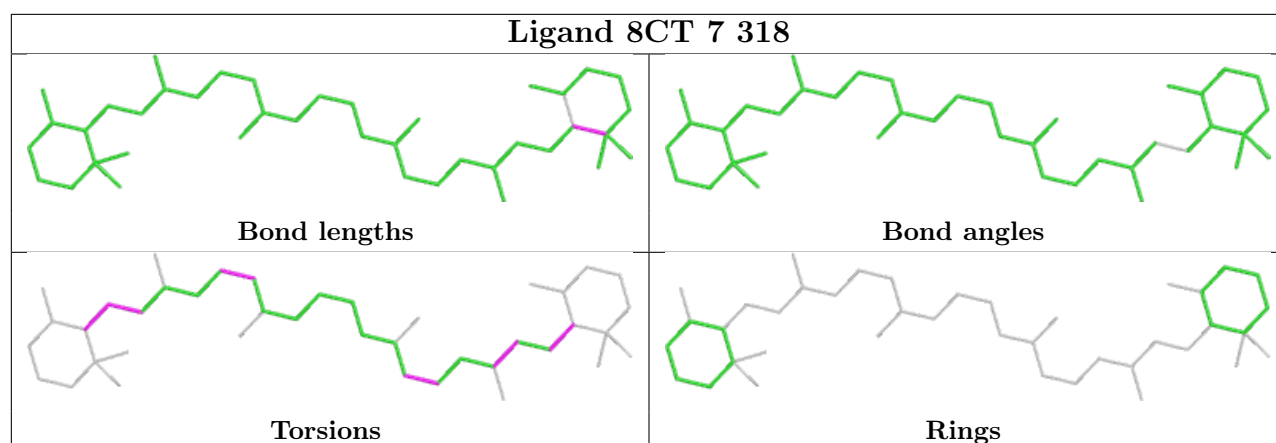


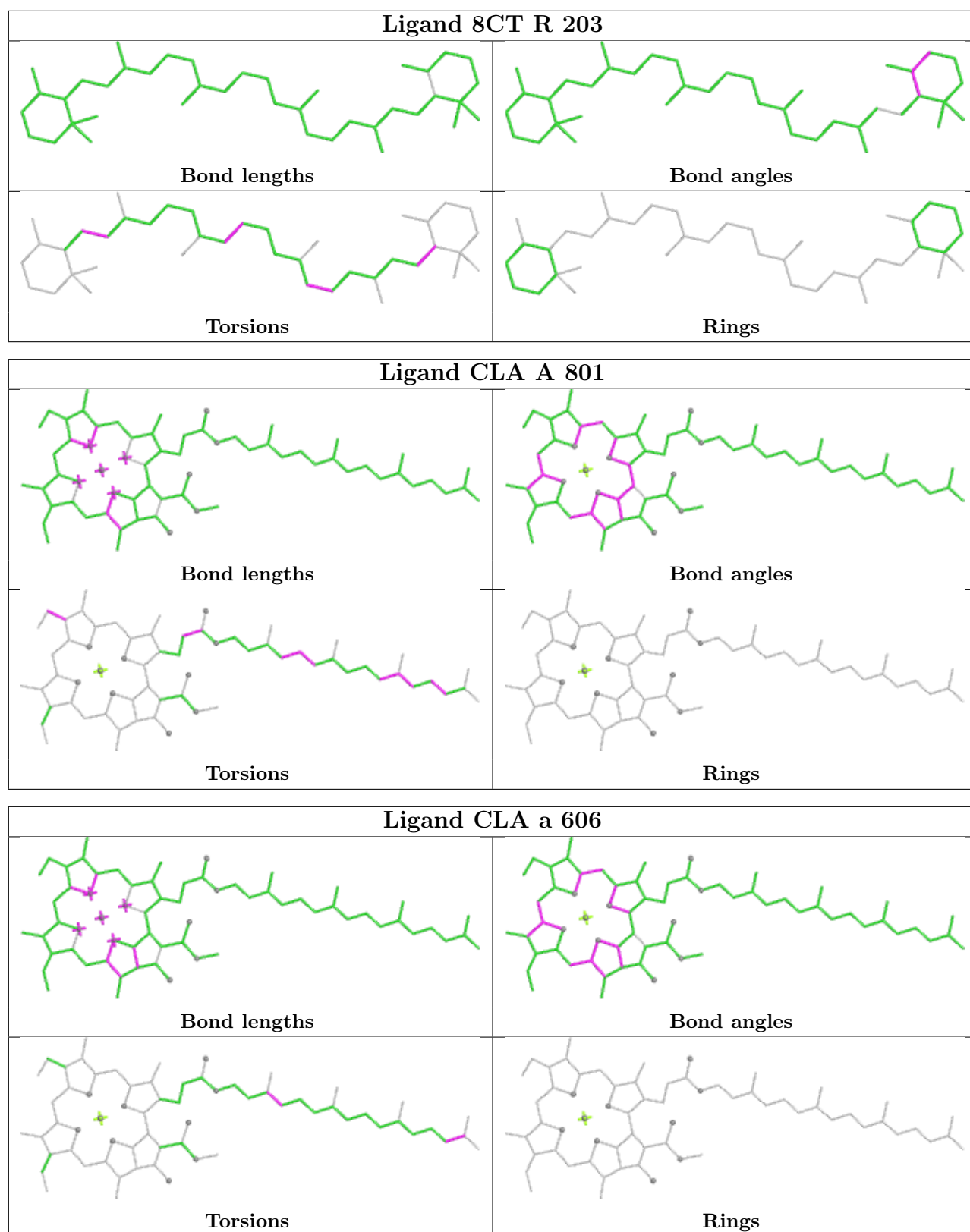
Ligand CLA B 834**Ligand CLA B 835**

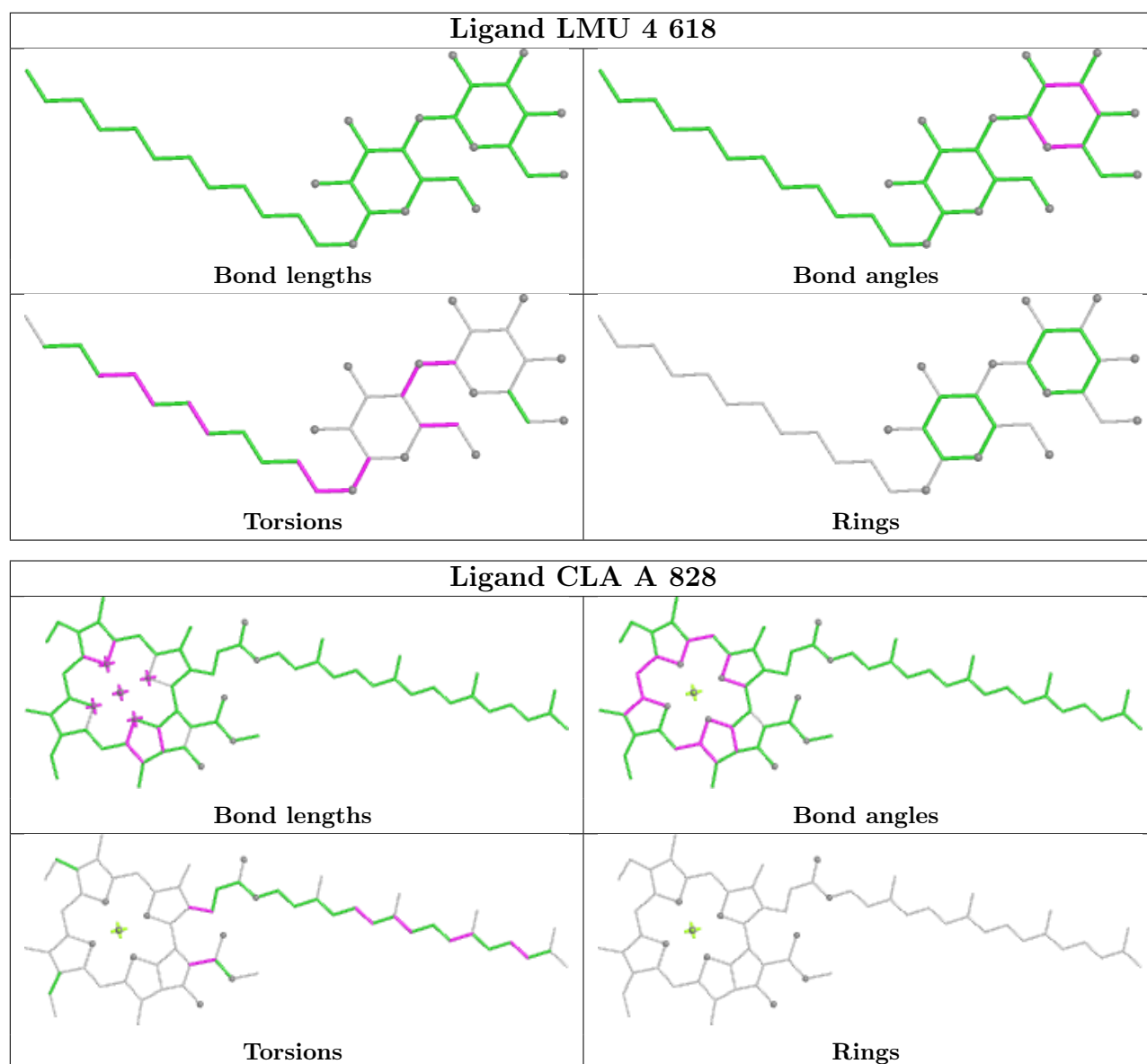




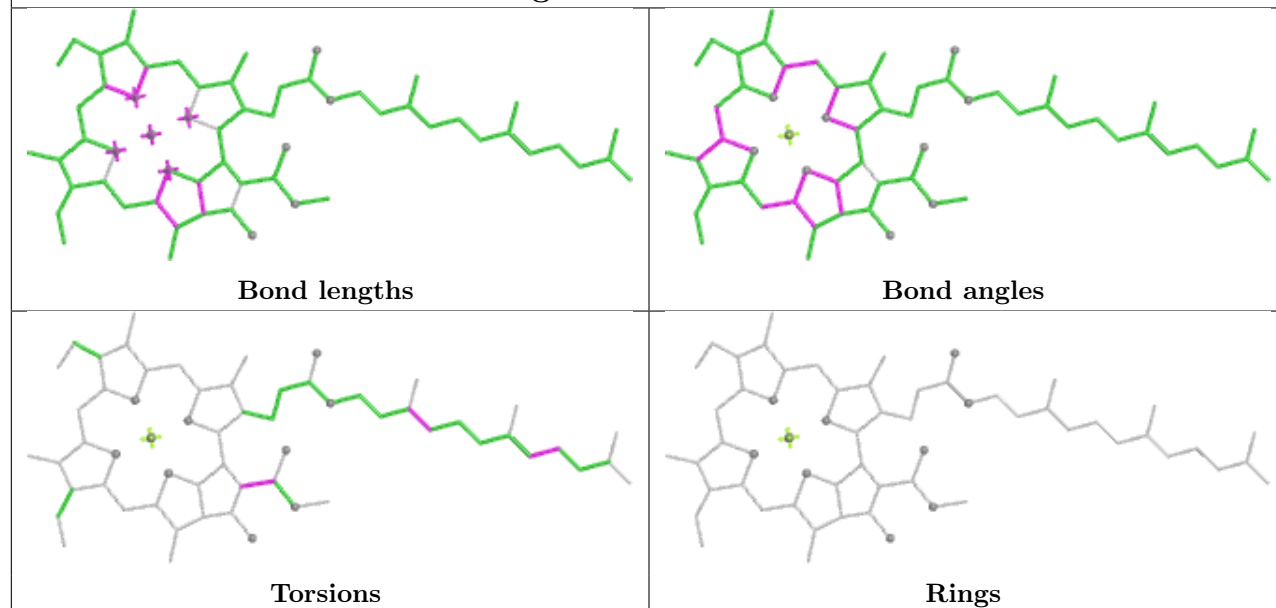
Ligand II0 1 617**Ligand II0 3 616****Ligand CLA A 837**



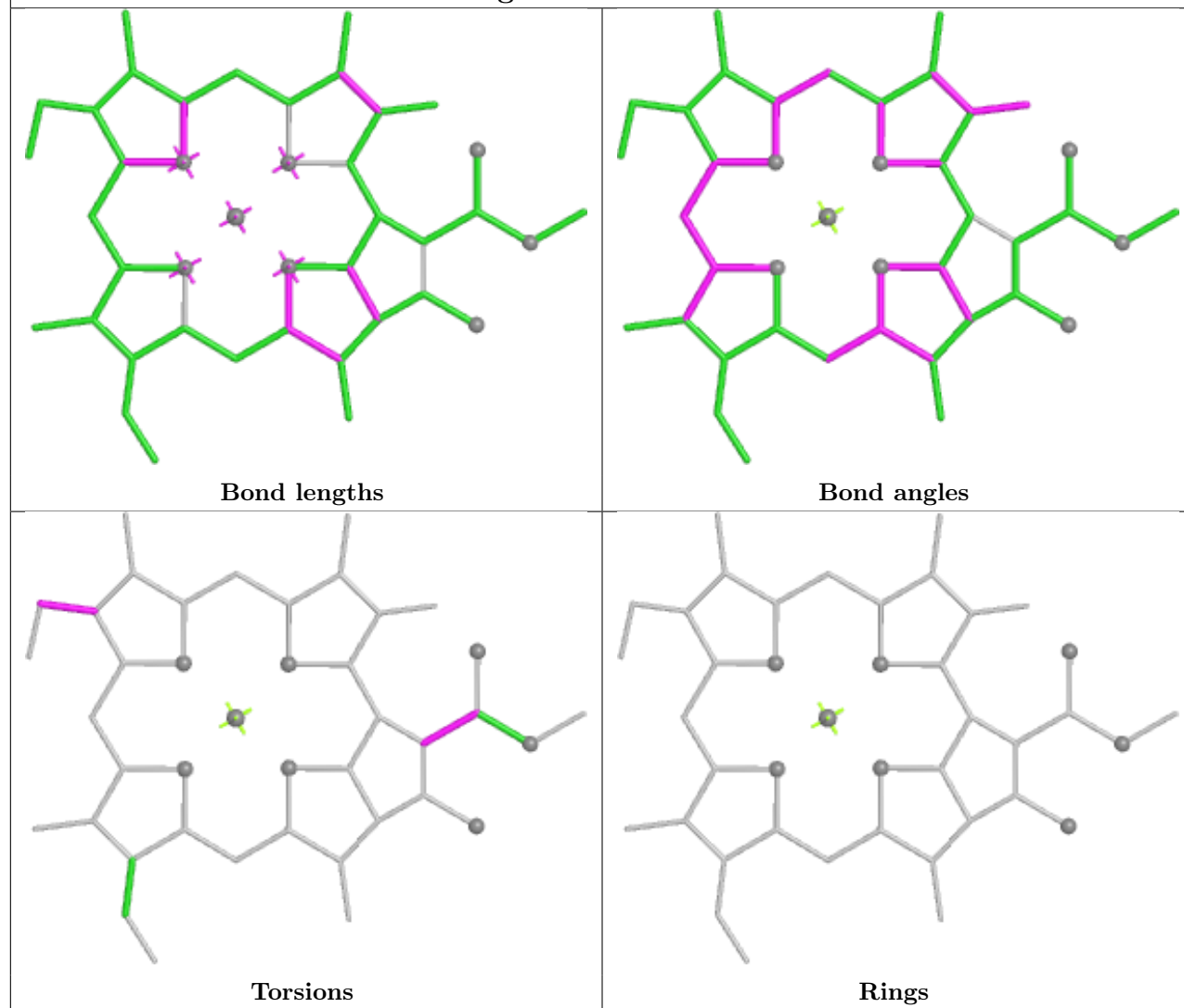


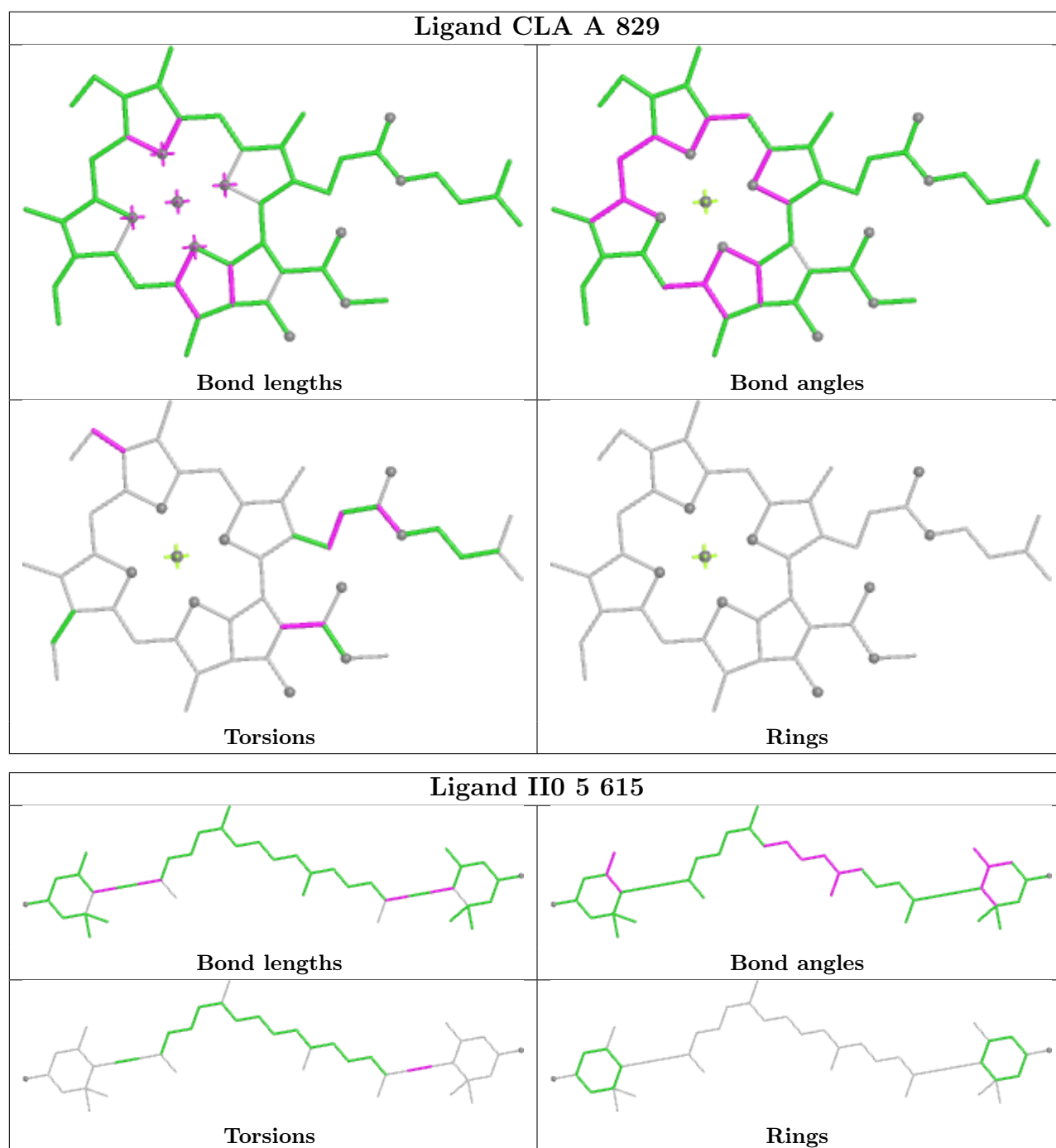


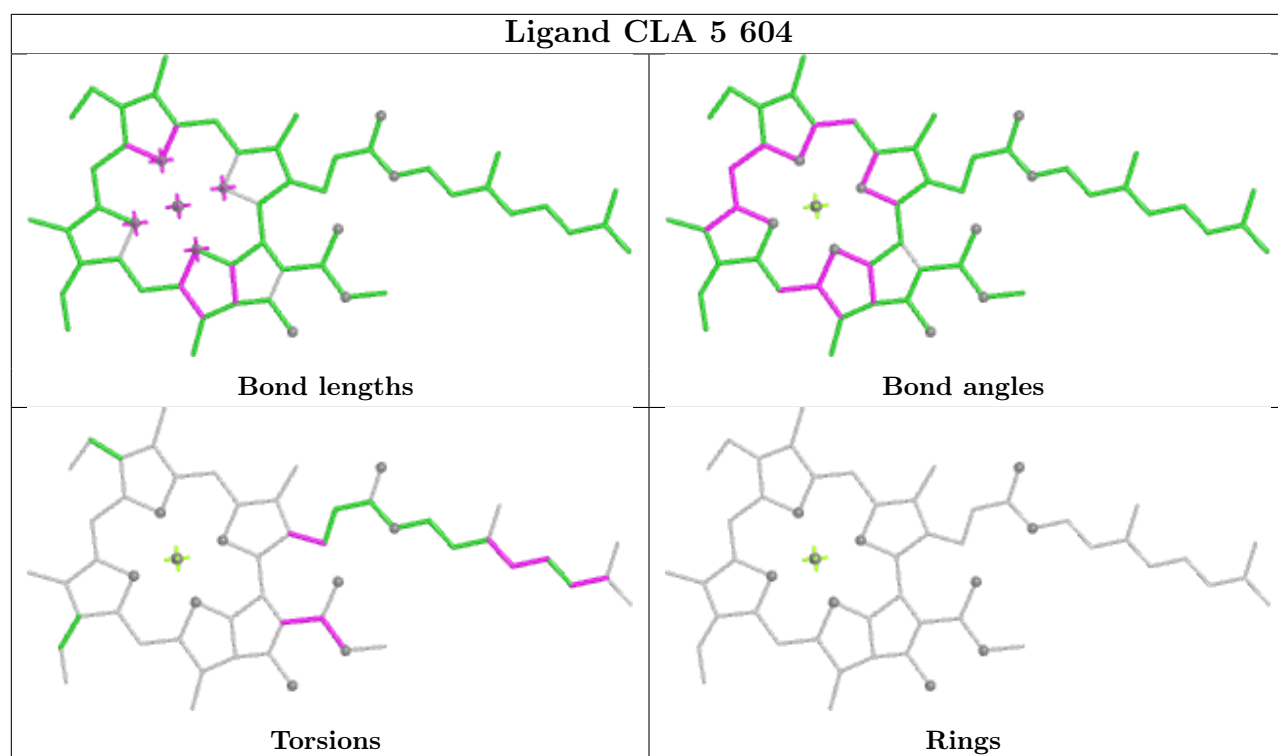
Ligand CLA B 810



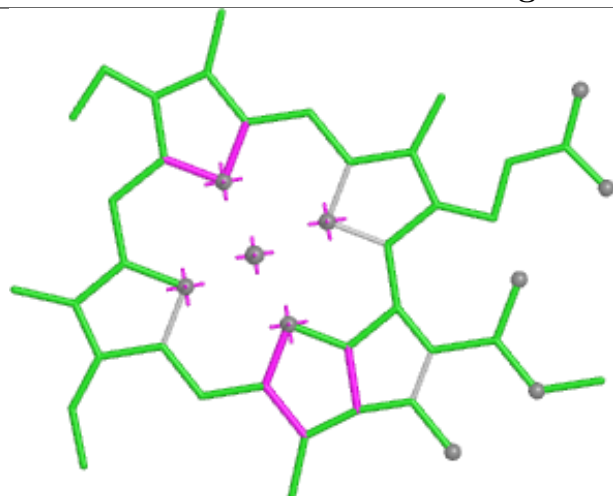
Ligand CLA 5 613



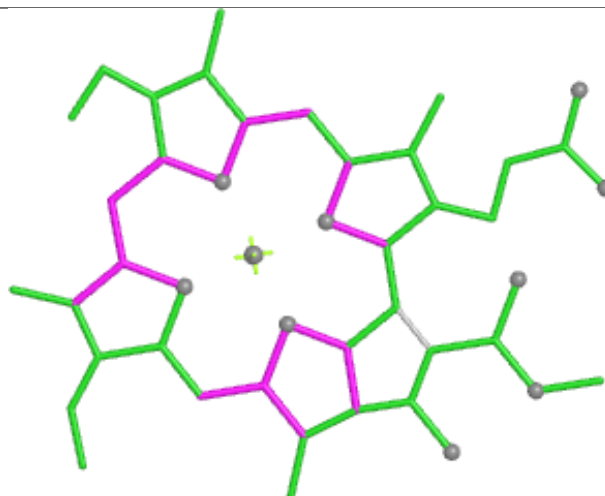




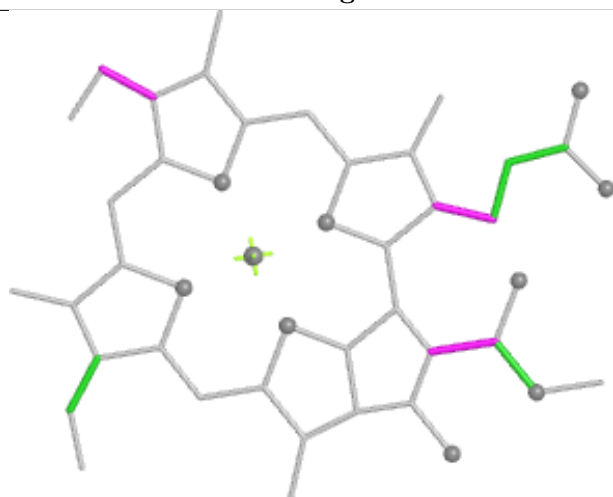
Ligand CLA 5 612



Bond lengths



Bond angles

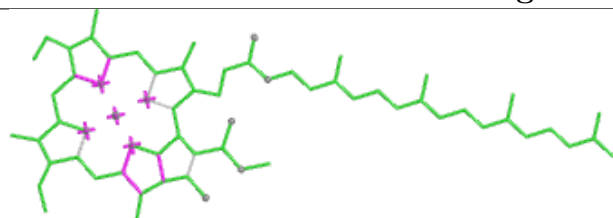


Torsions

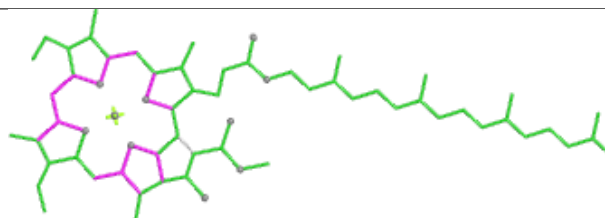


Rings

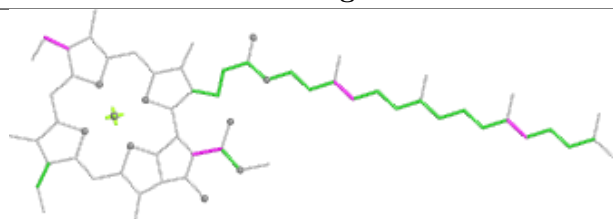
Ligand CLA Z 310



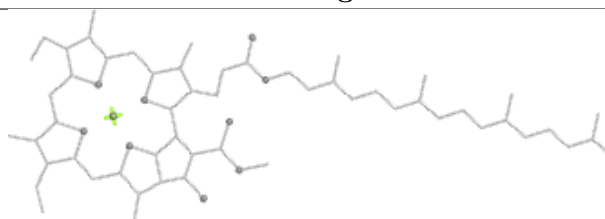
Bond lengths



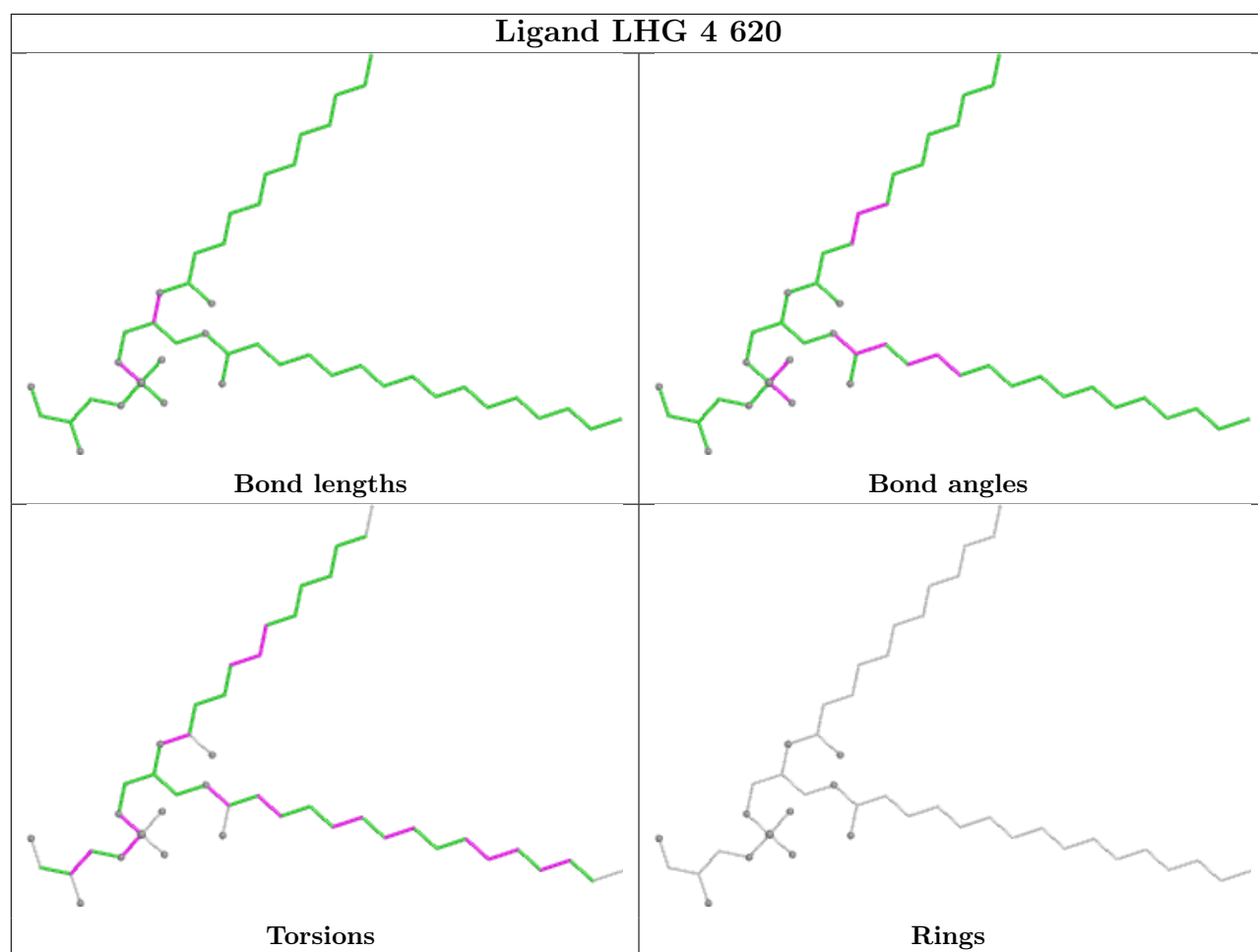
Bond angles



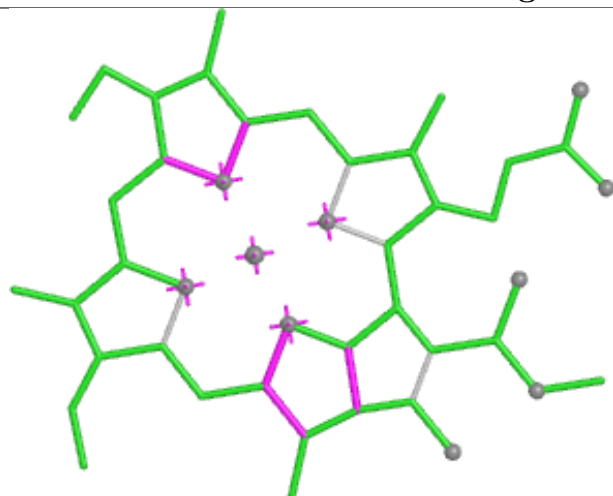
Torsions



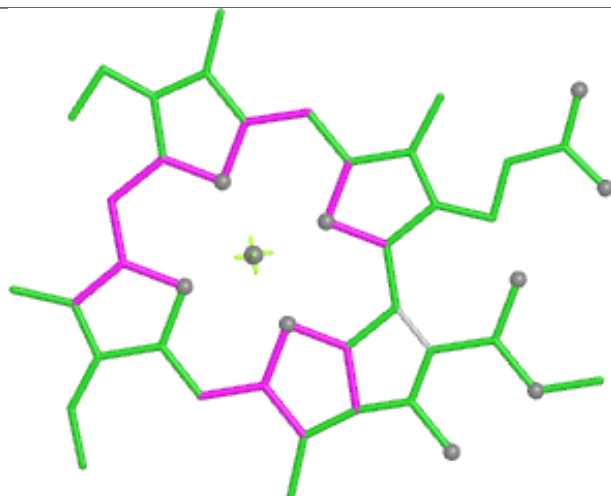
Rings



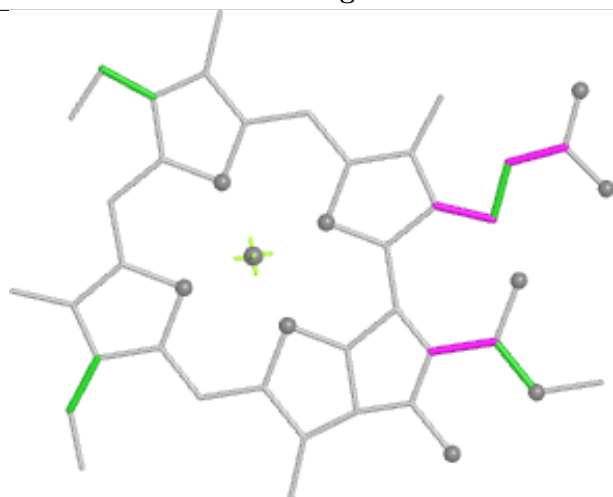
Ligand CLA 5 606



Bond lengths



Bond angles

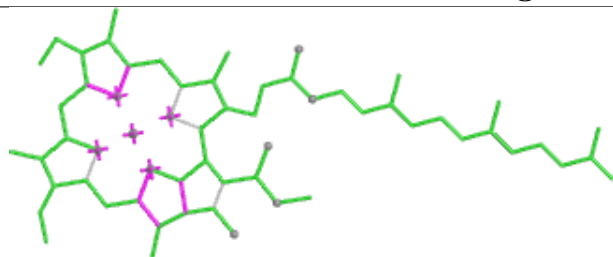


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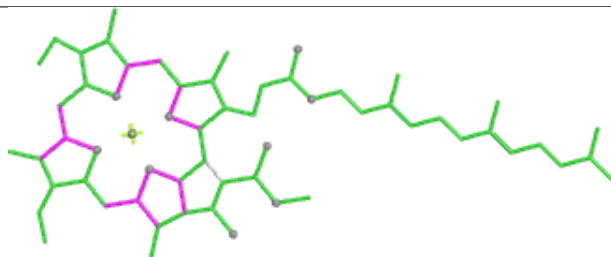


Rings

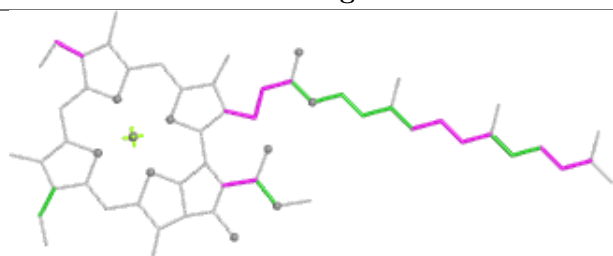
Ligand CLA Z 306



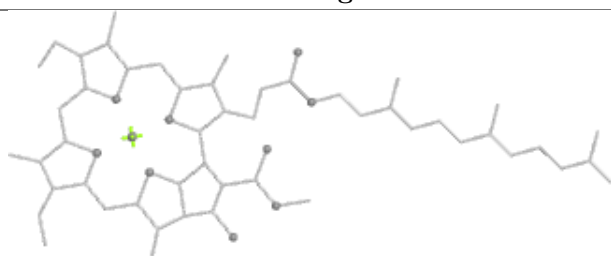
Bond lengths



Bond angles

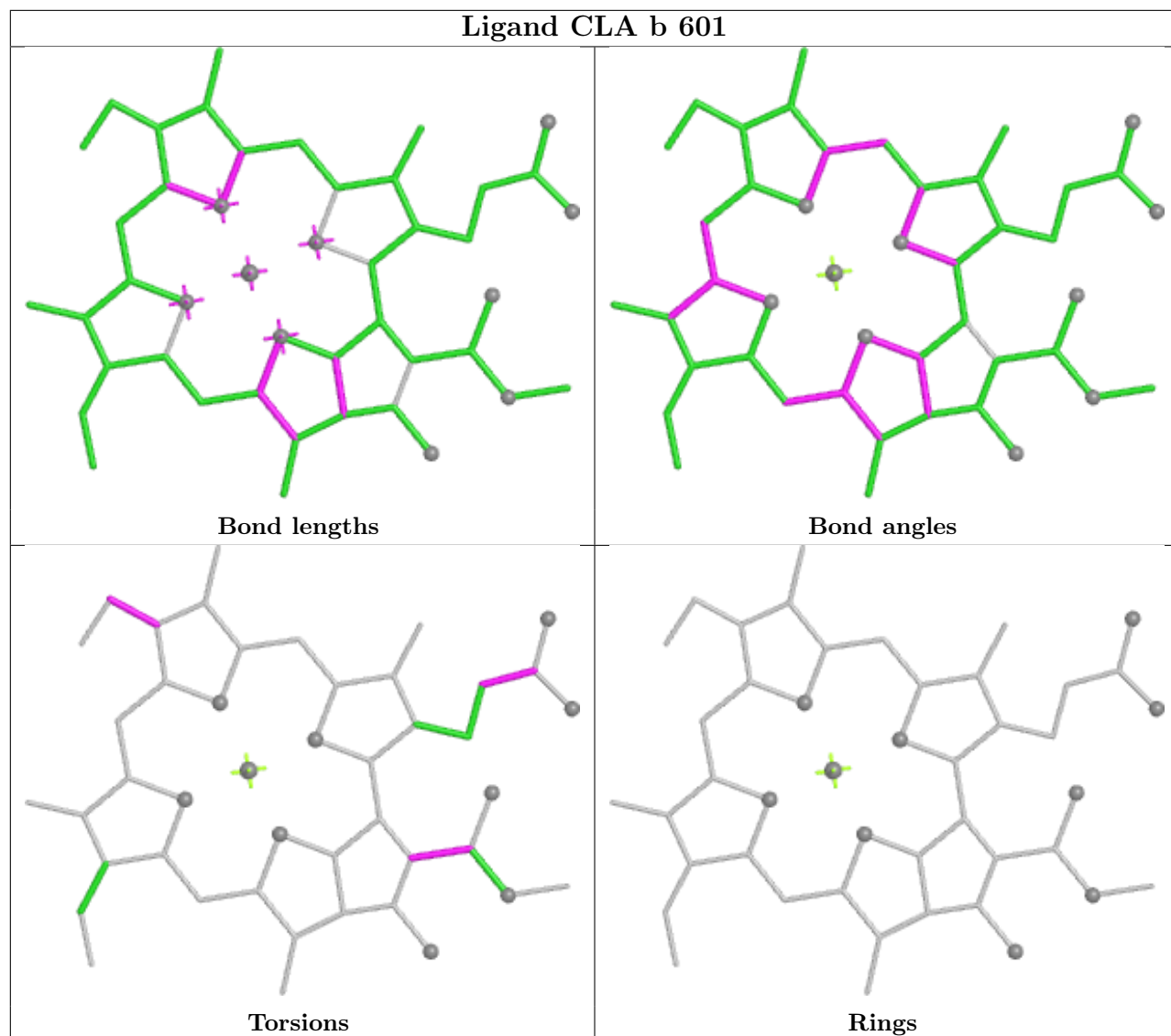


Torsions

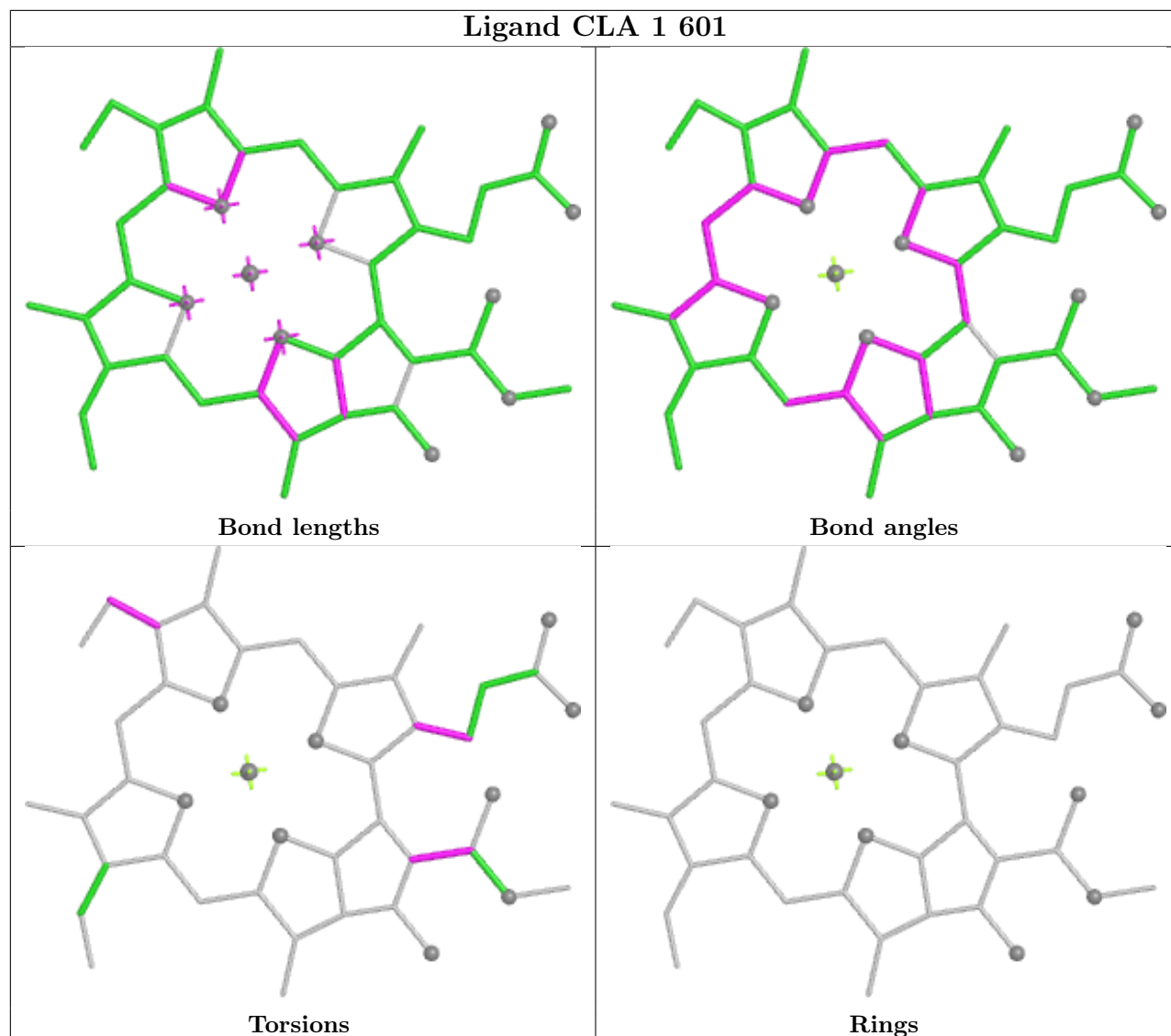


Rings

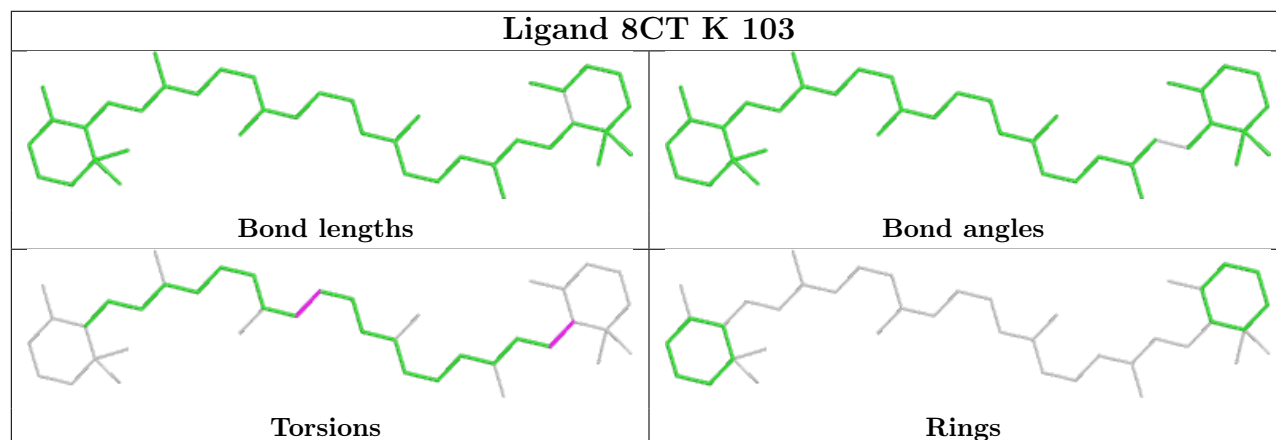
Ligand CLA b 601

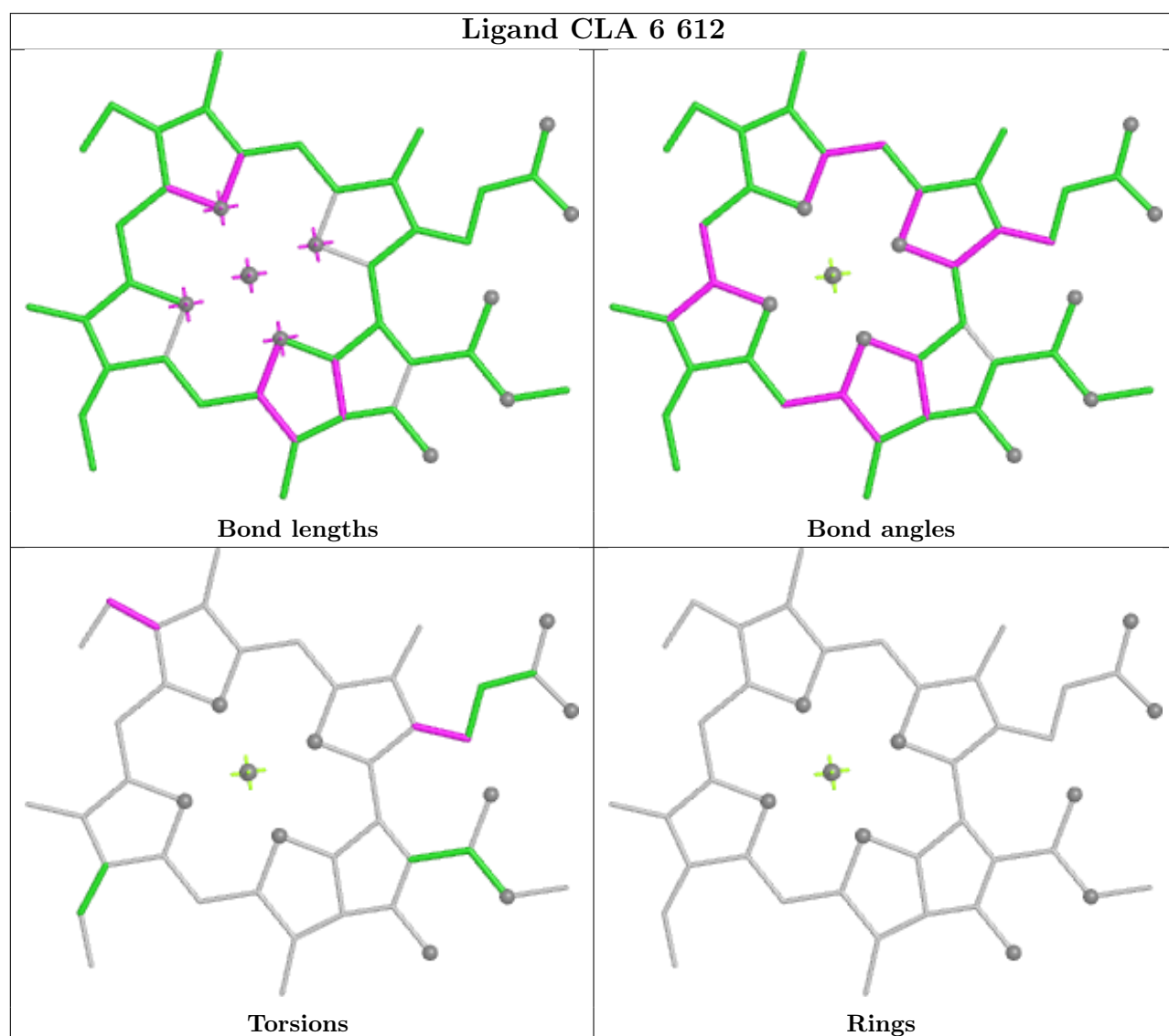
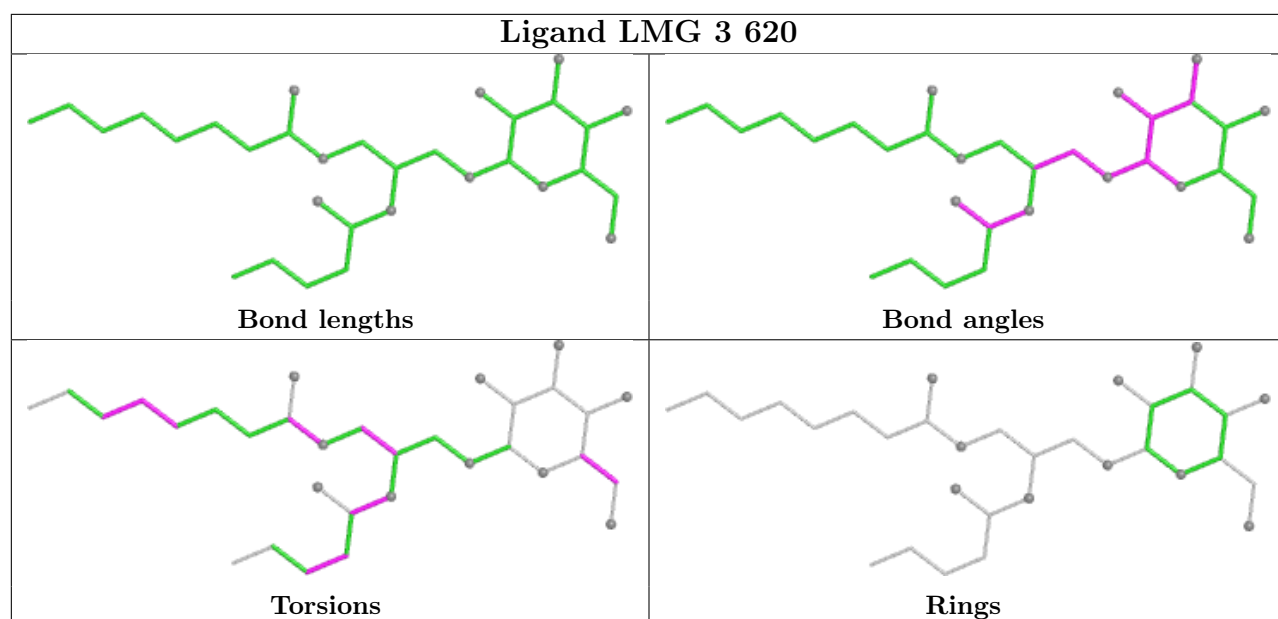


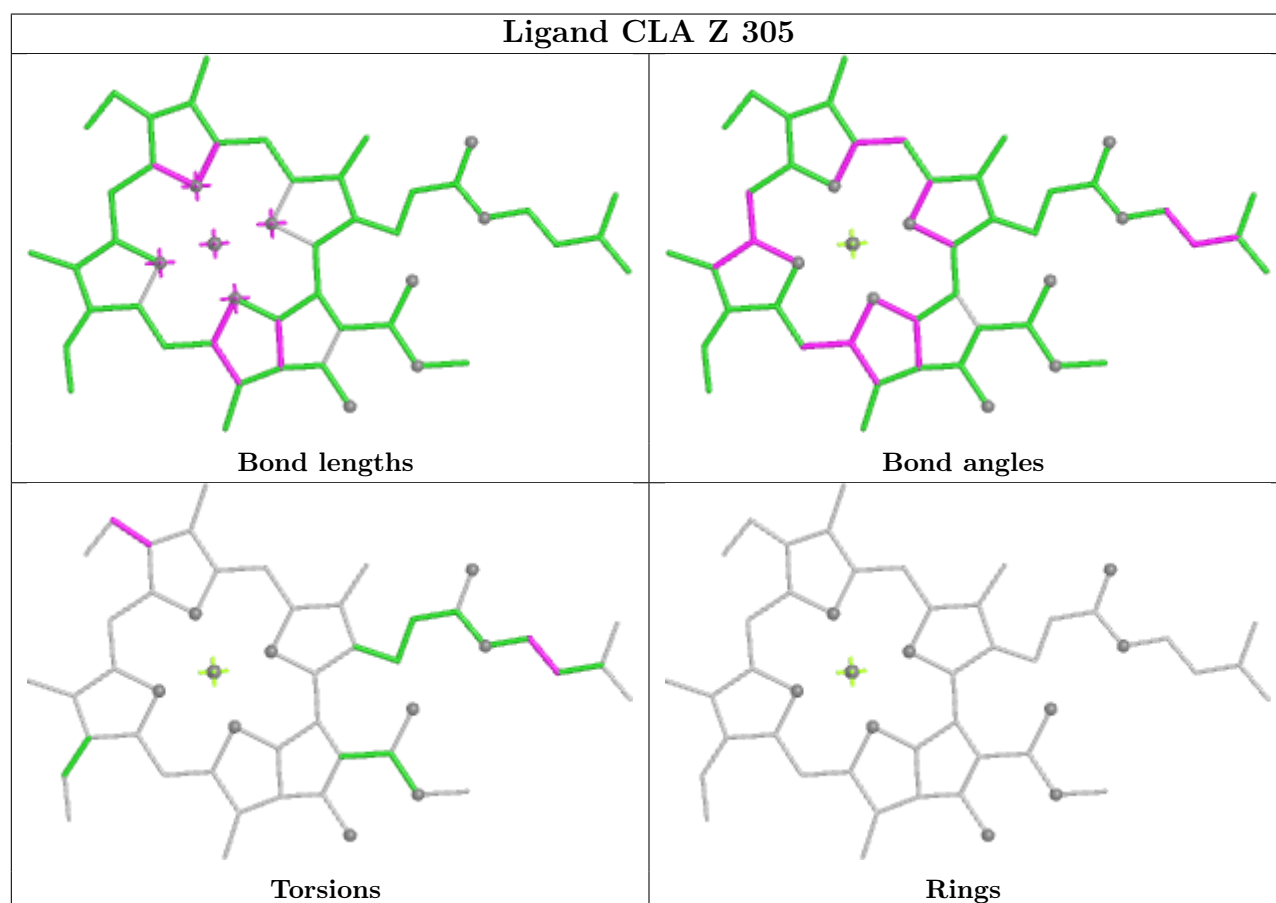
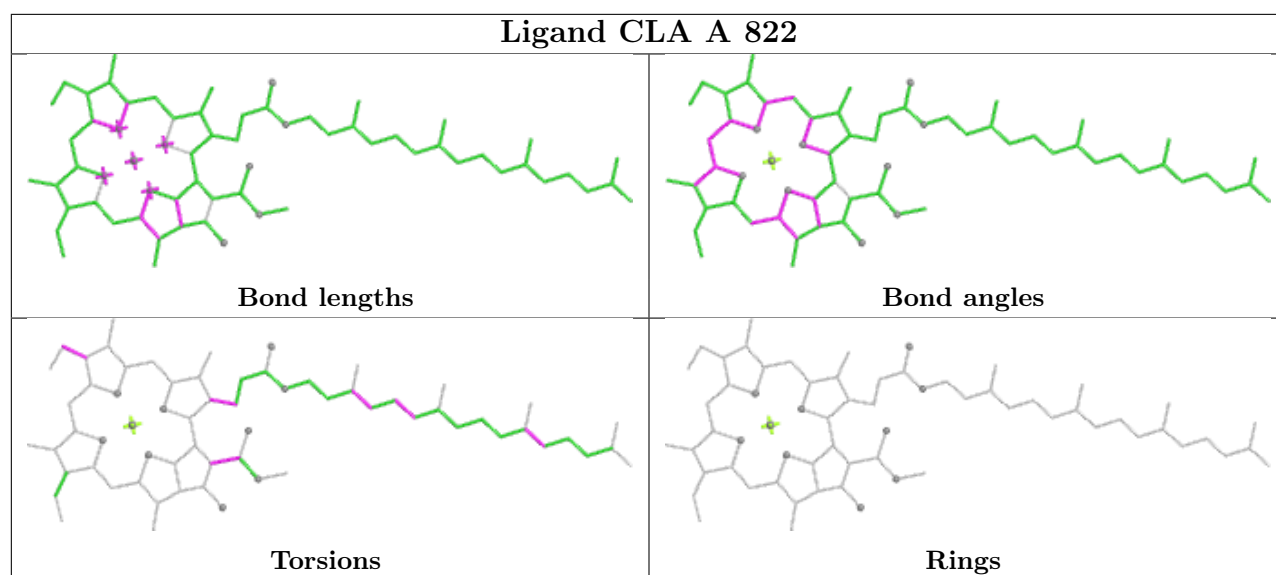
Ligand CLA 1 601

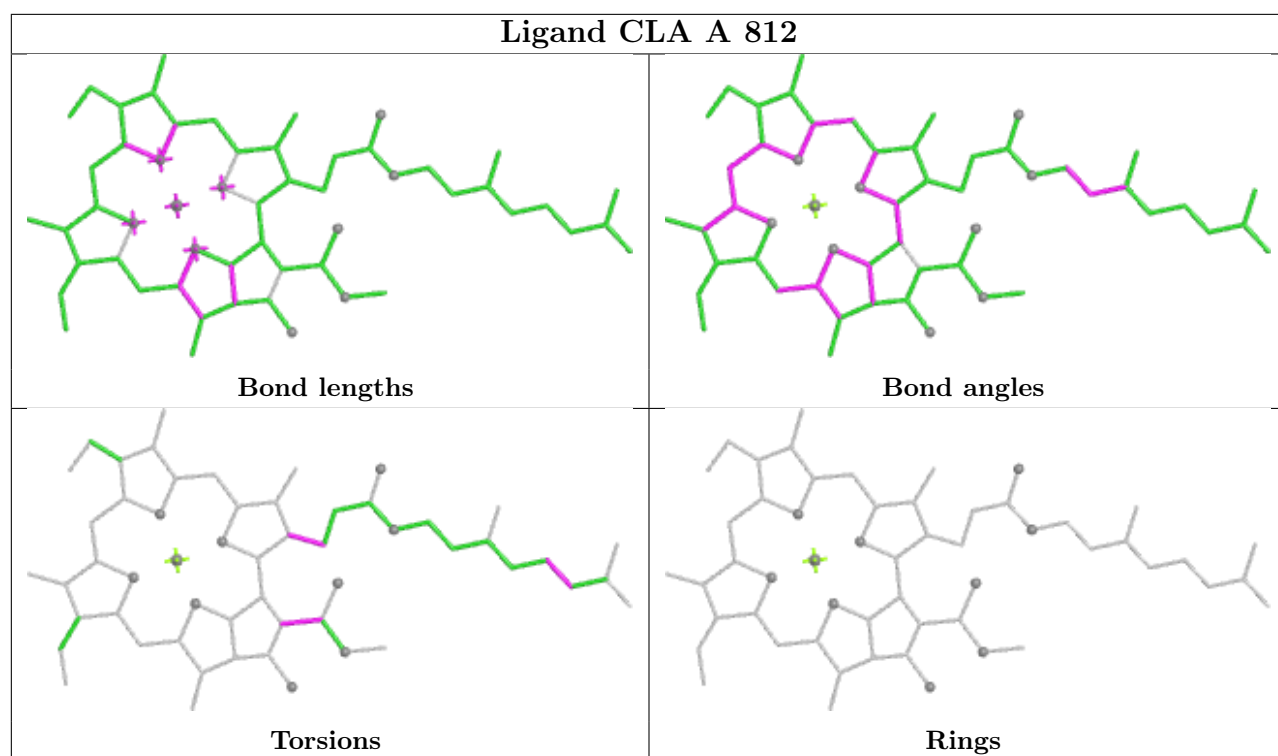


Ligand 8CT K 103

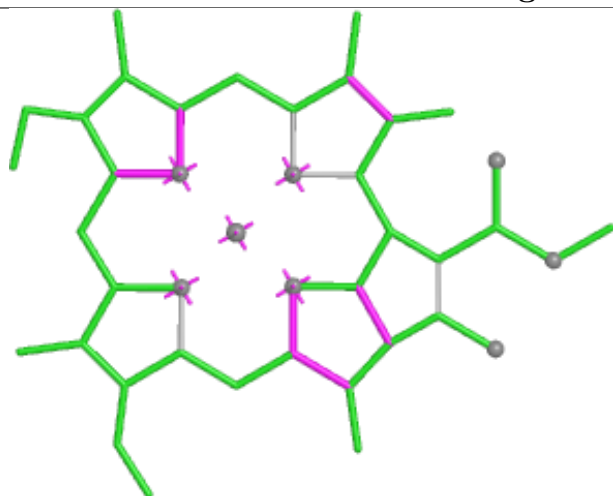




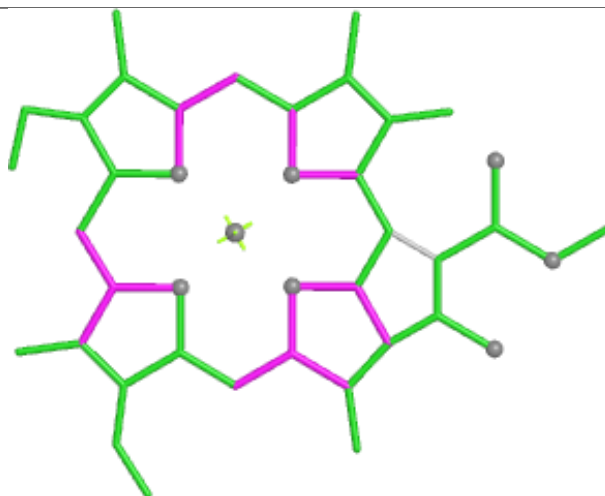




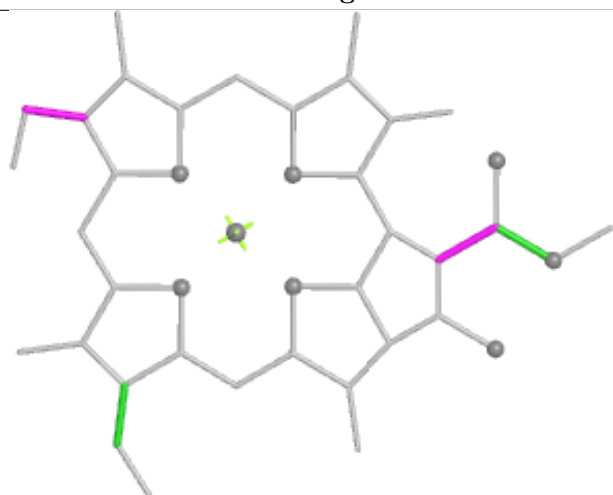
Ligand CLA 1 609



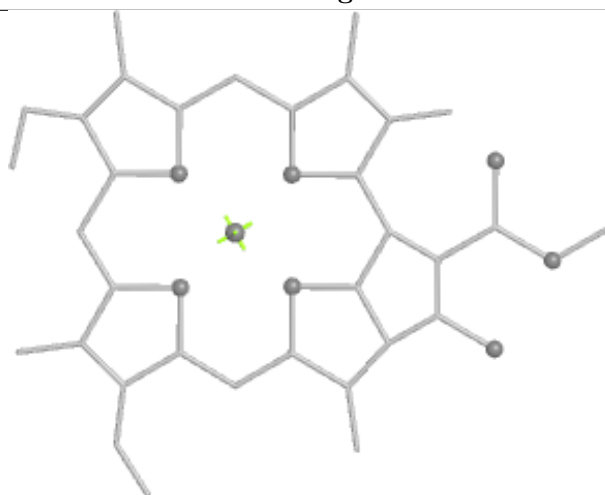
Bond lengths



Bond angles

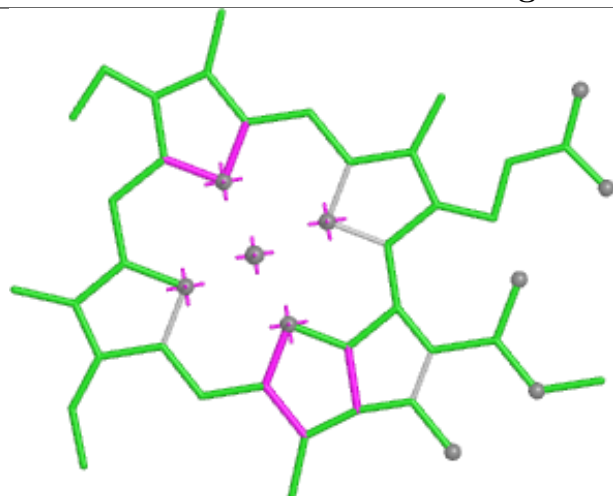


Torsions

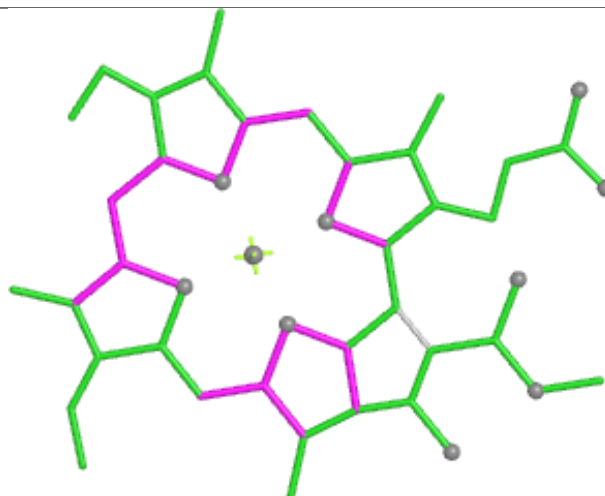


Rings

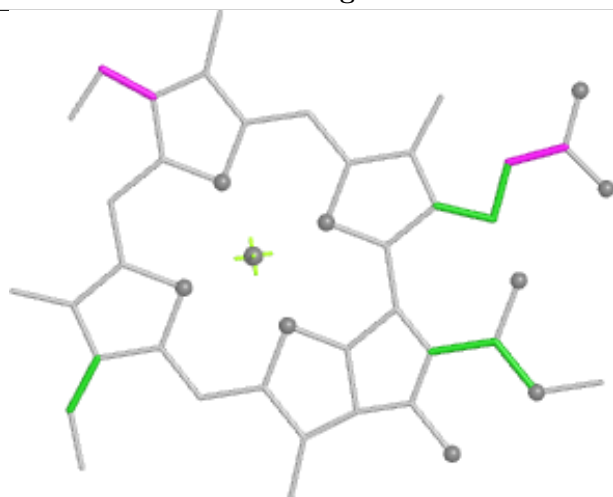
Ligand CLA 9 605



Bond lengths



Bond angles

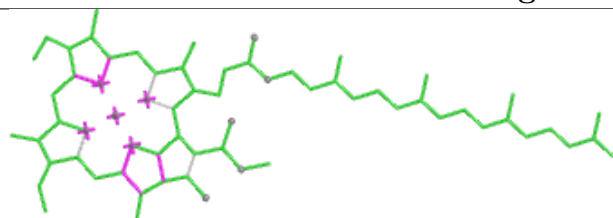


Torsions

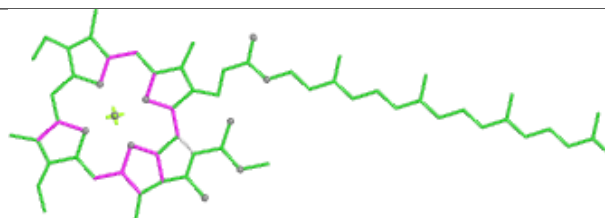


Rings

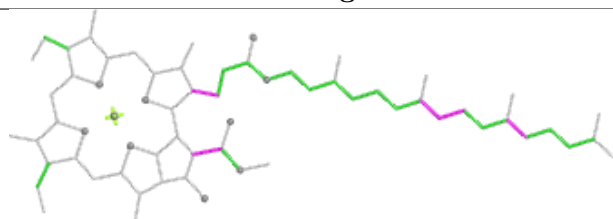
Ligand CLA 6 602



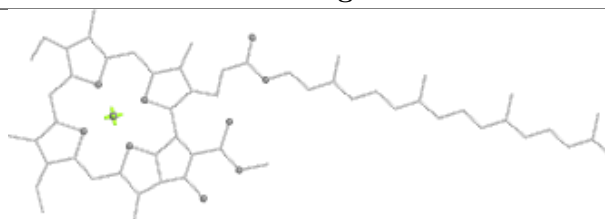
Bond lengths



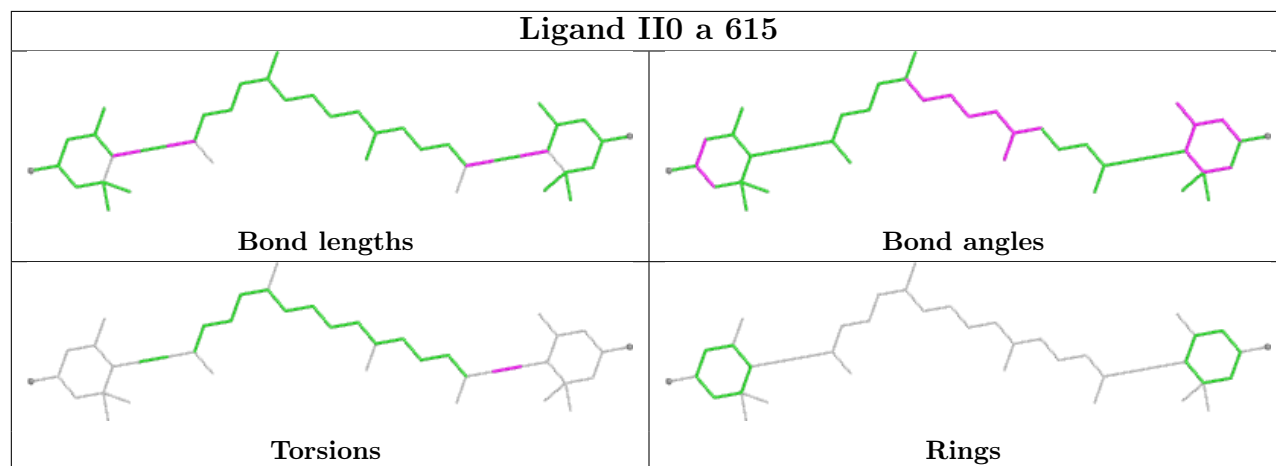
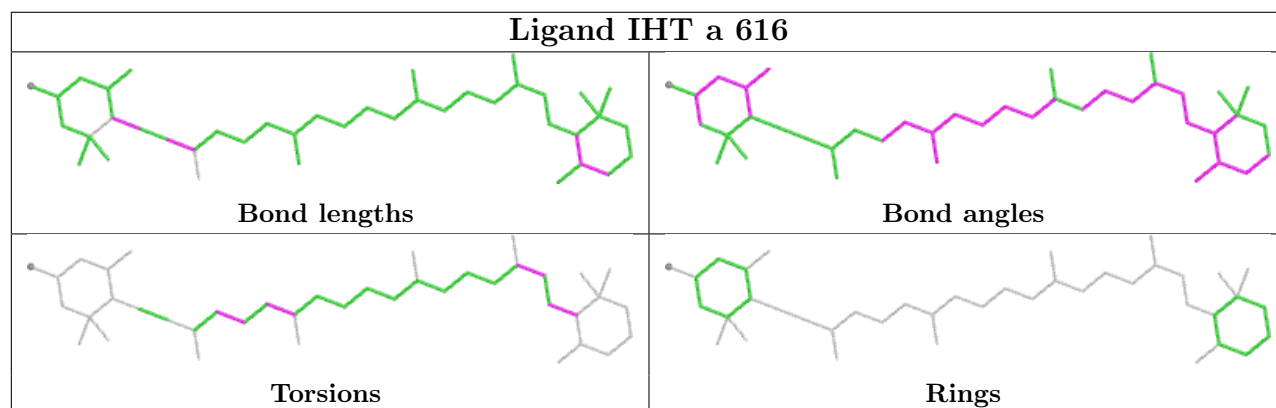
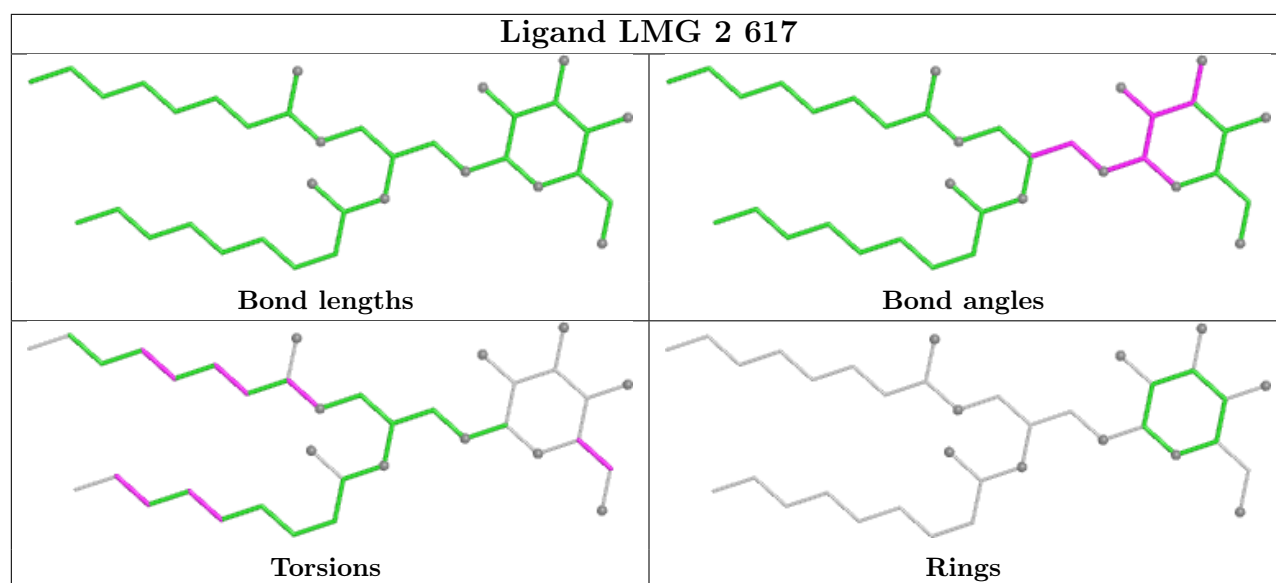
Bond angles

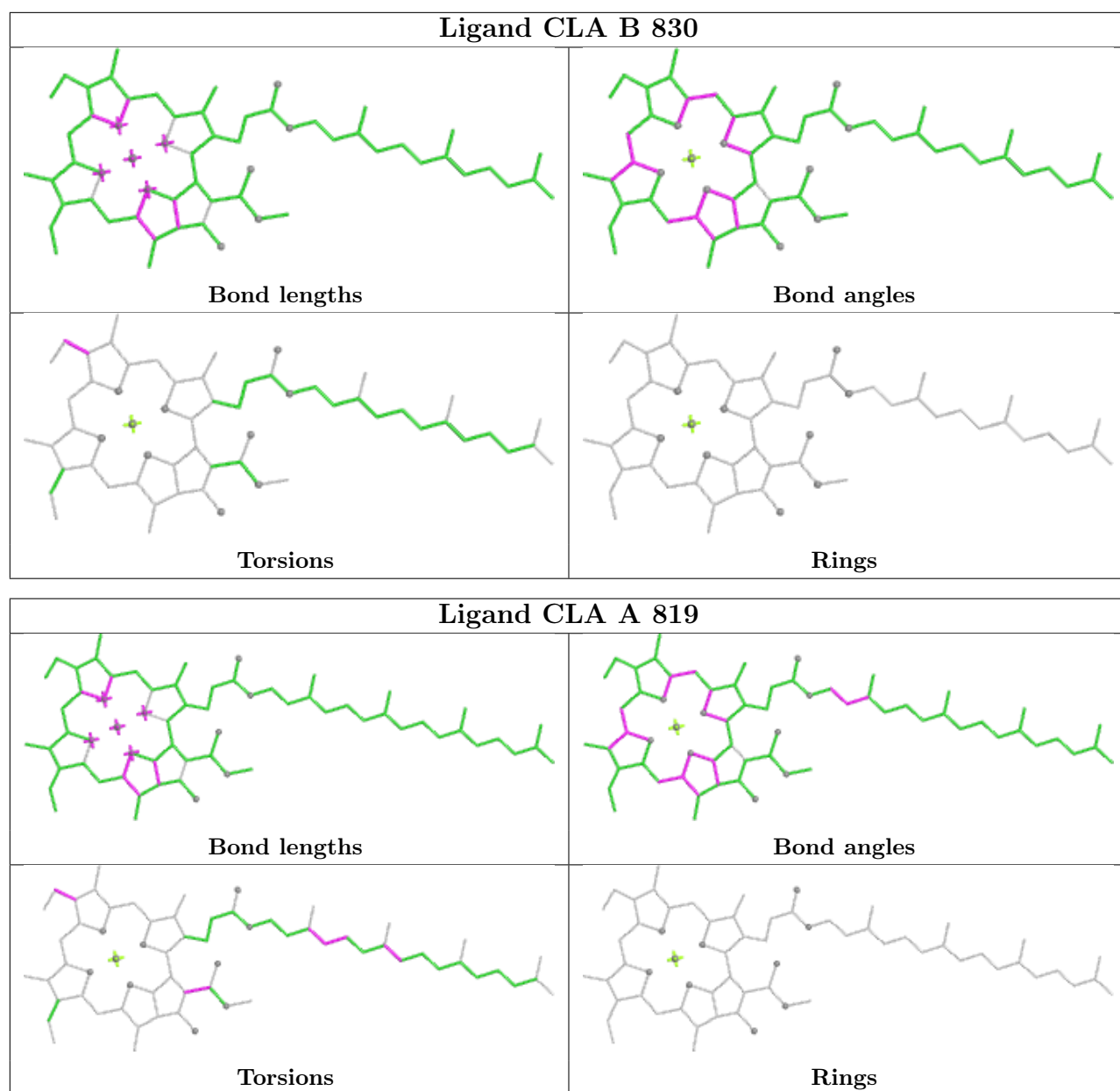


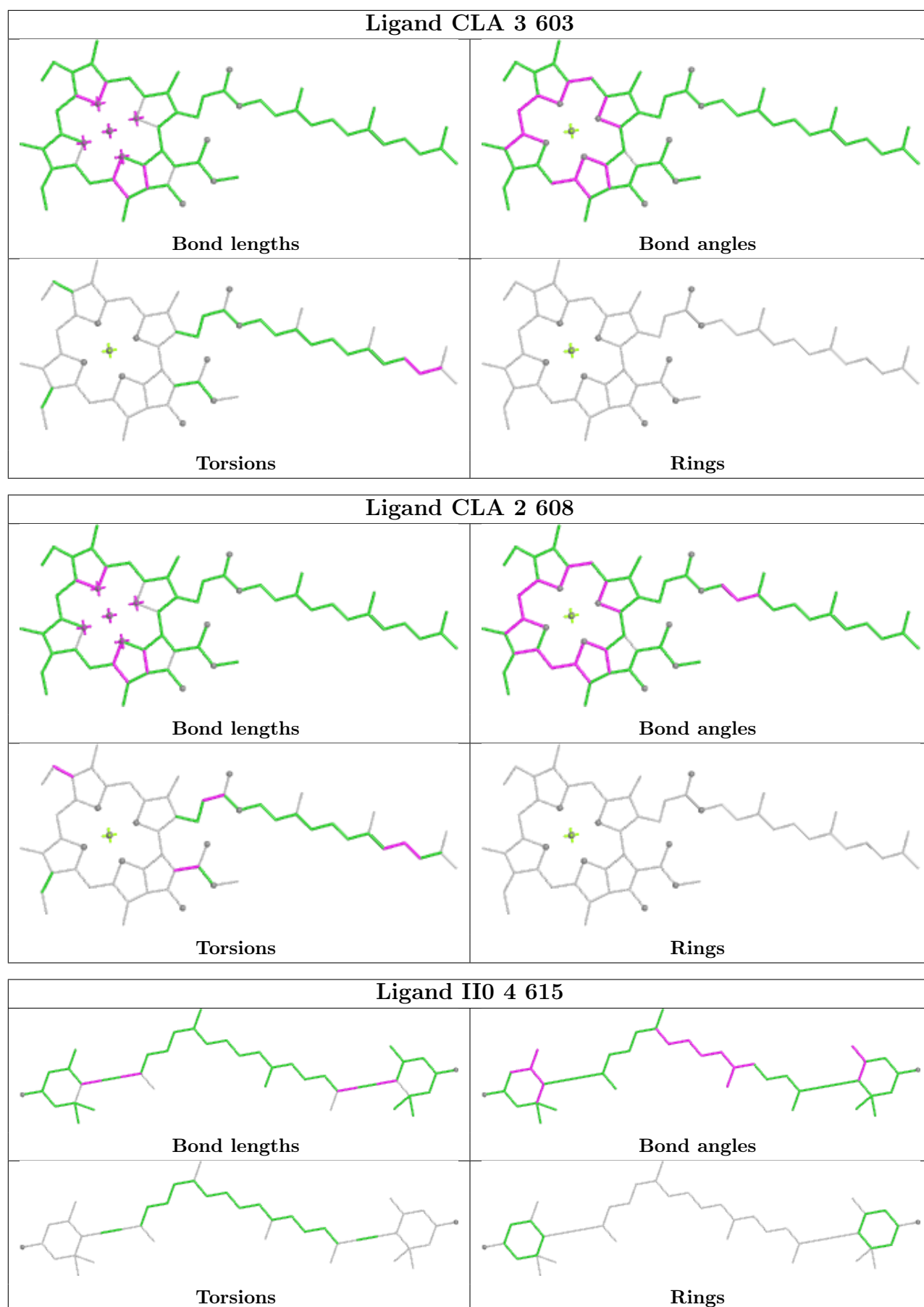
Torsions



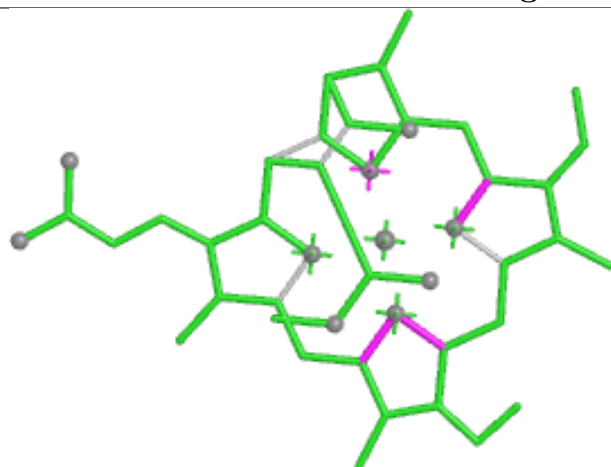
Rings



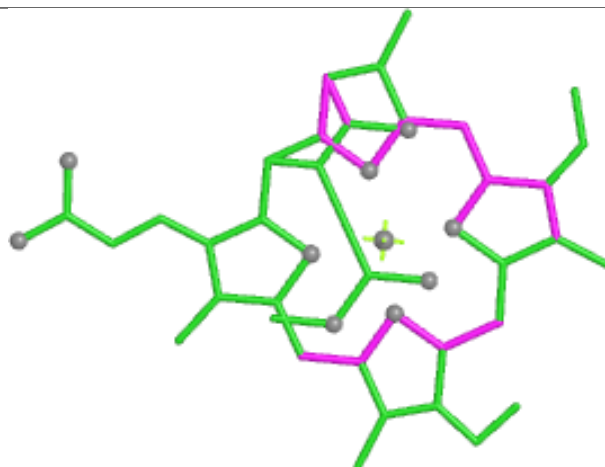




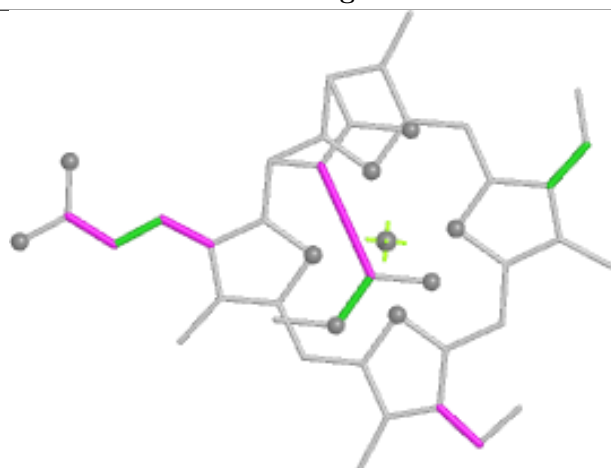
Ligand KC2 1 610



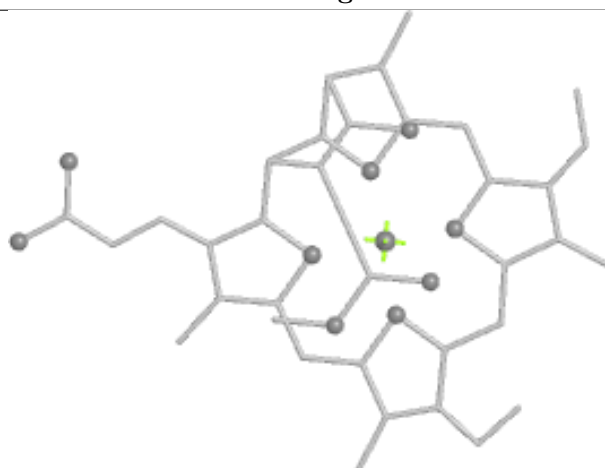
Bond lengths



Bond angles

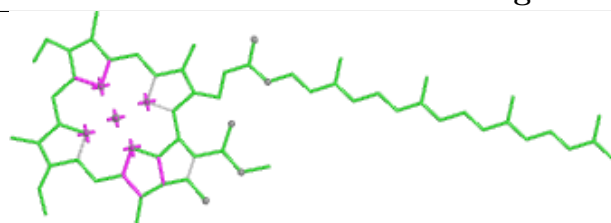


Torsions

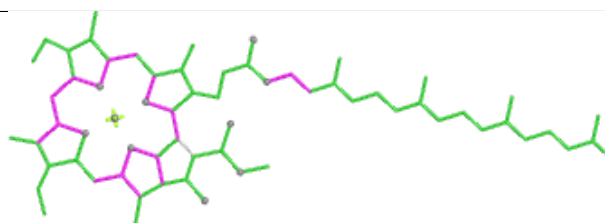


Rings

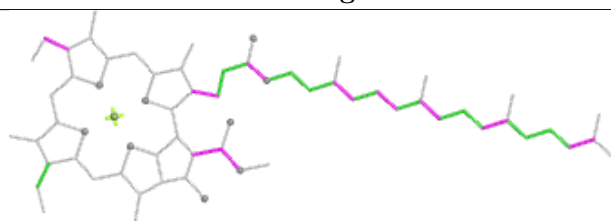
Ligand CLA A 810



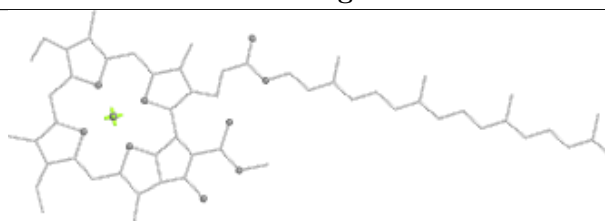
Bond lengths



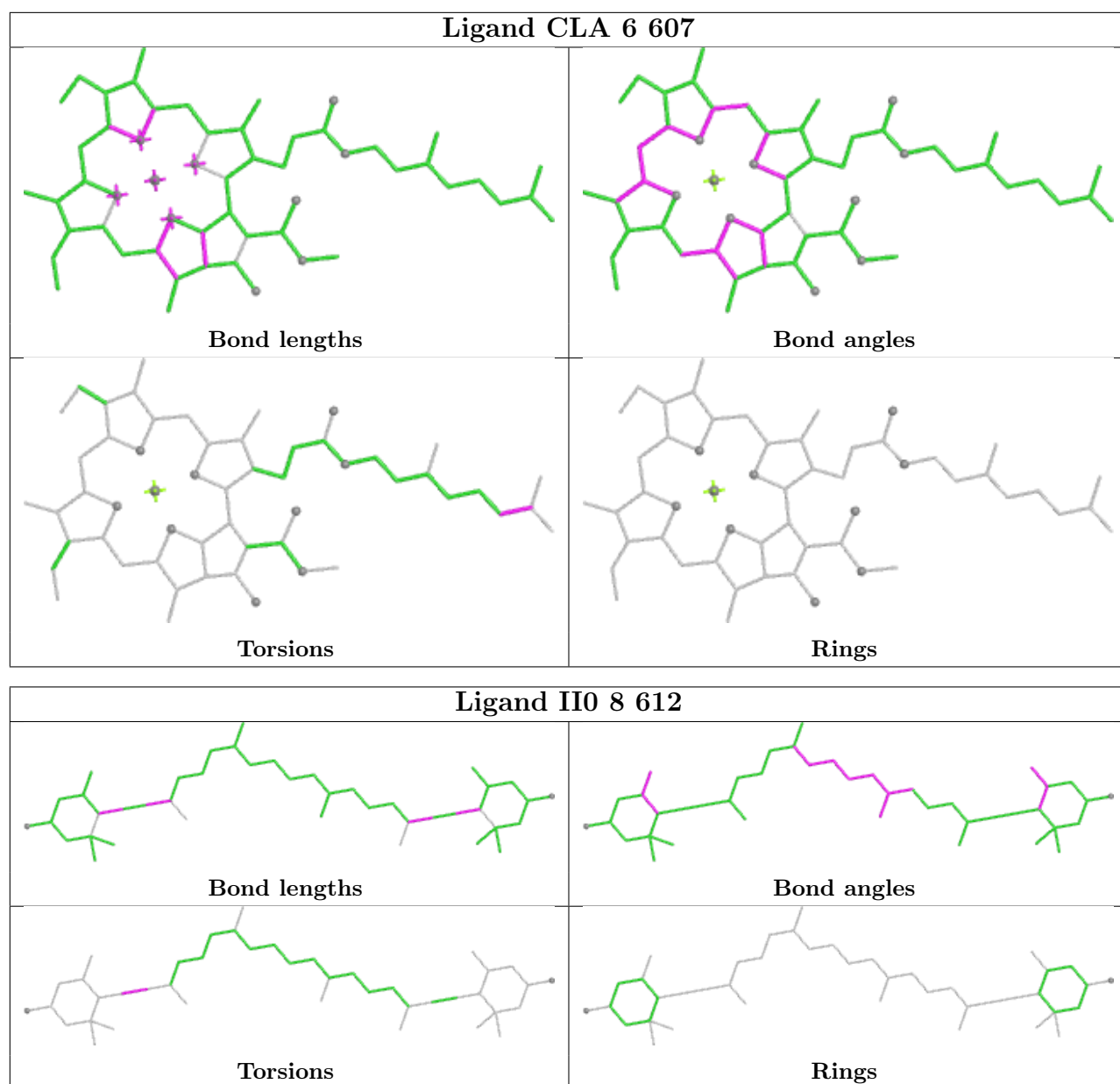
Bond angles



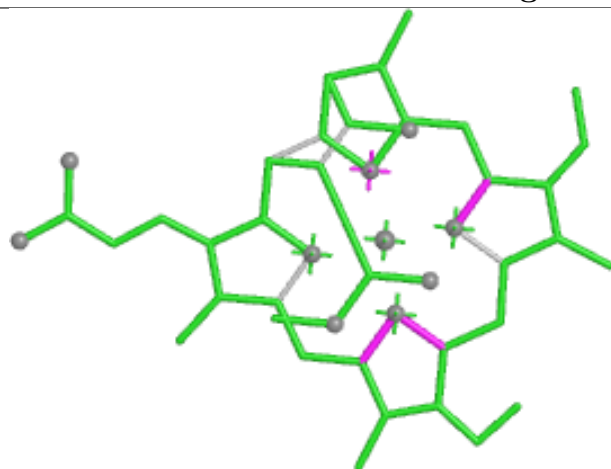
Torsions



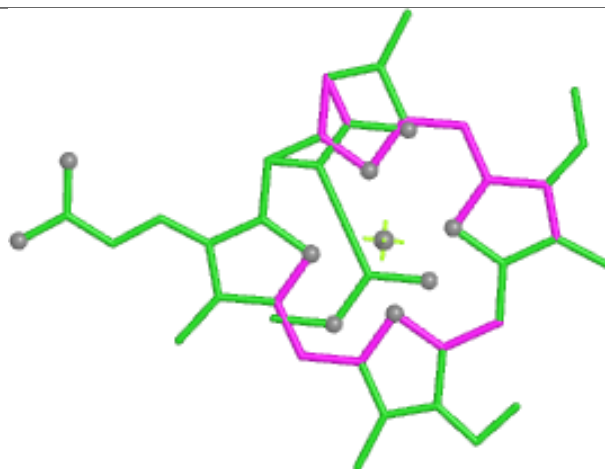
Rings



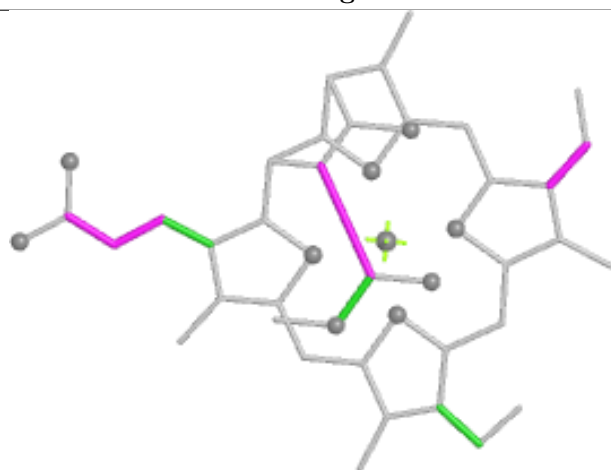
Ligand KC2 2 610



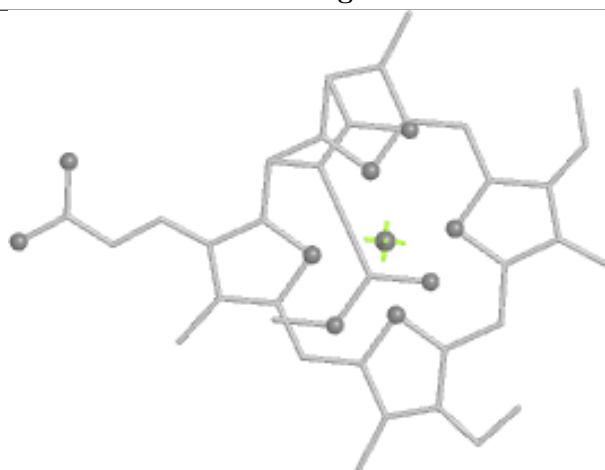
Bond lengths



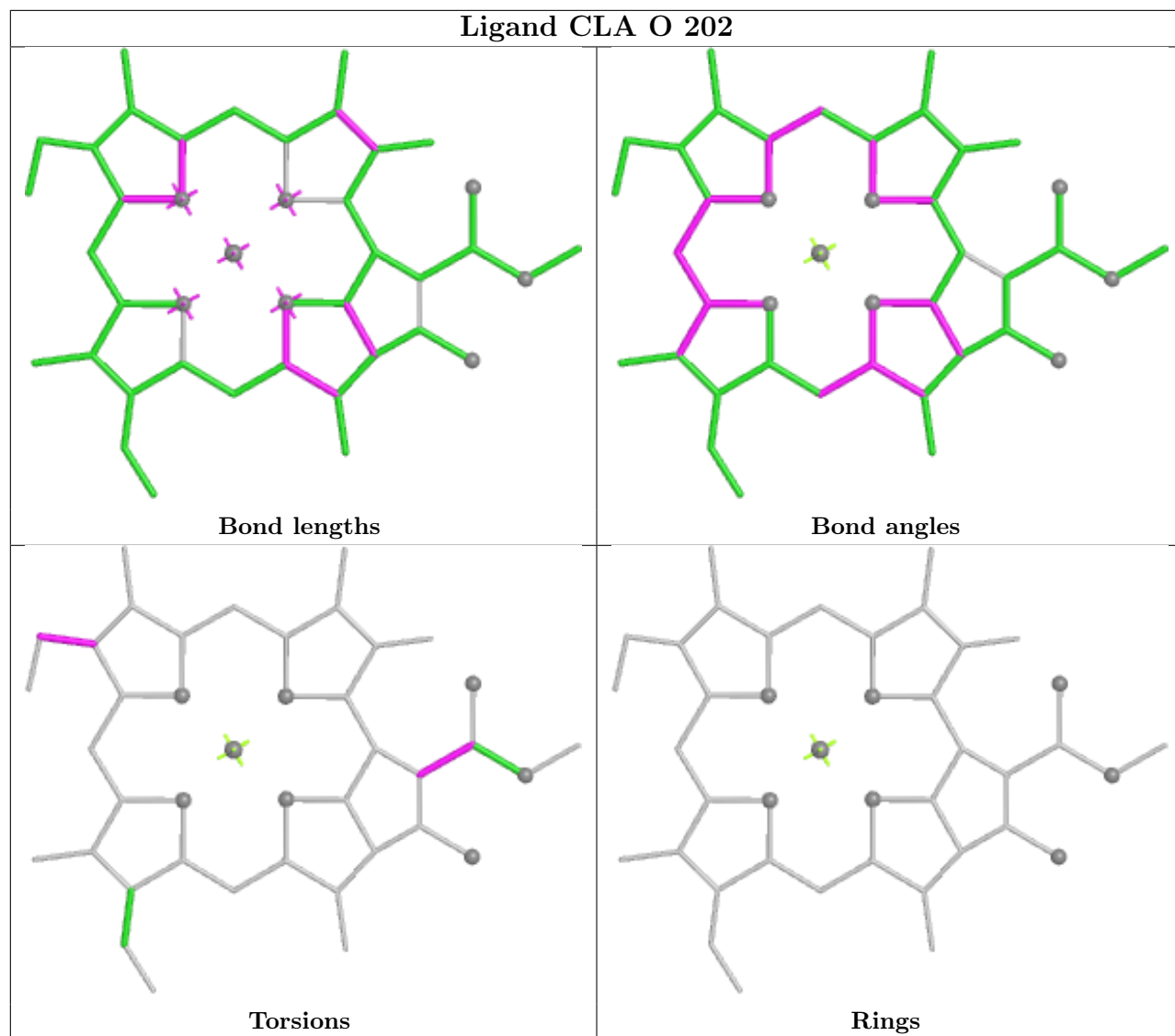
Bond angles



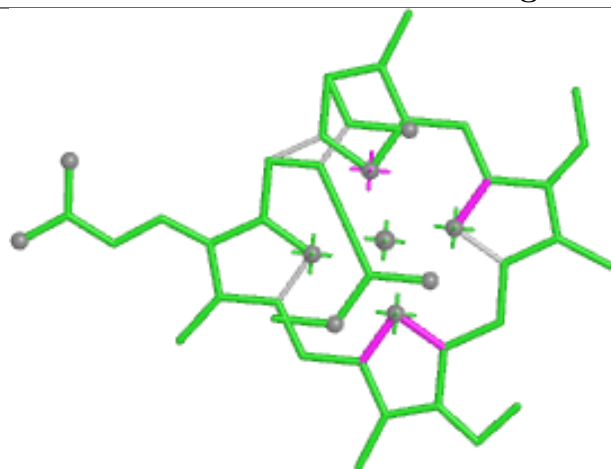
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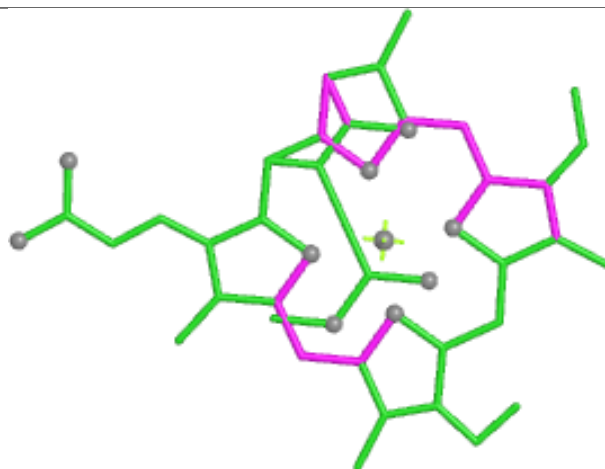
Rings



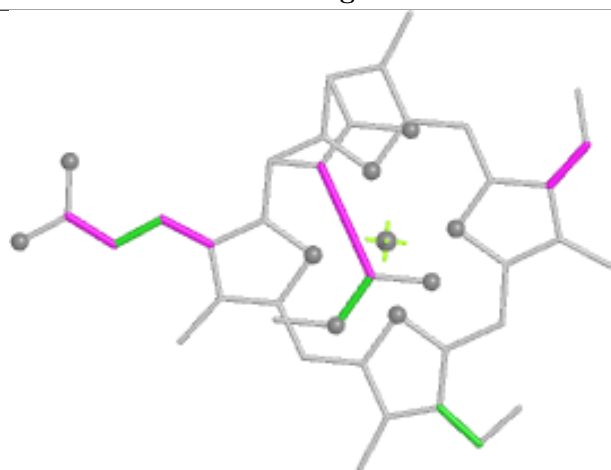
Ligand KC2 7 311



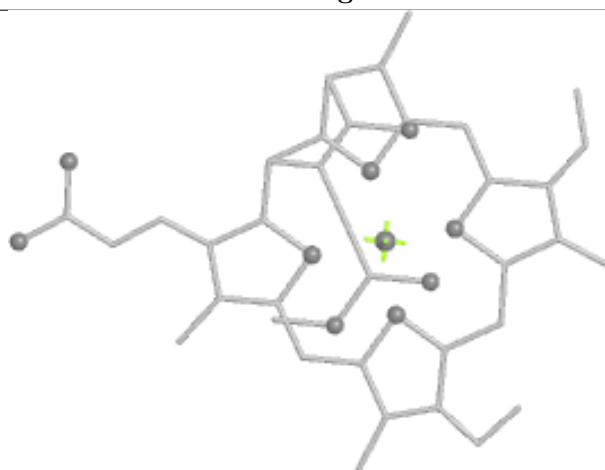
Bond lengths



Bond angles

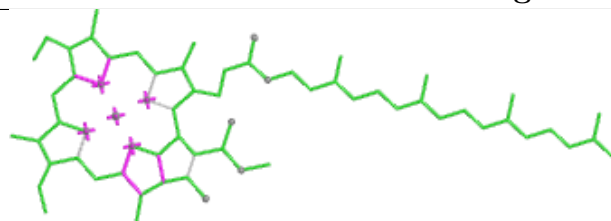


Torsions

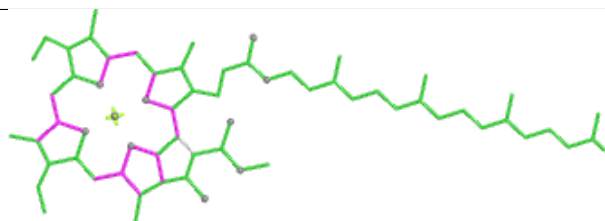


Rings

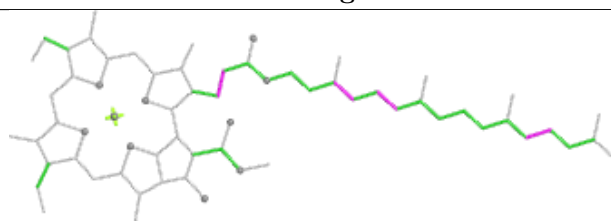
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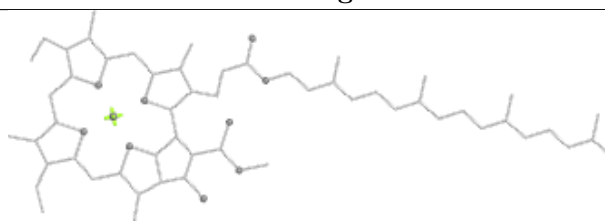
Bond lengths



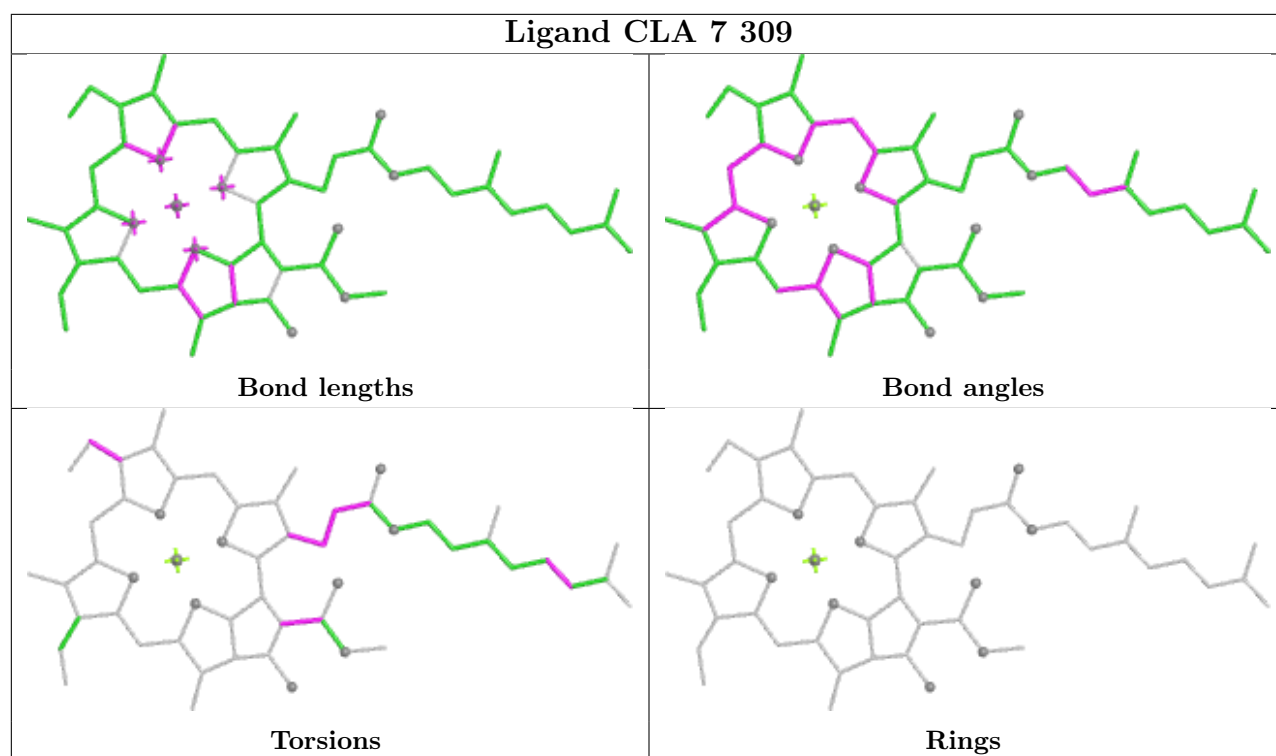
Bond angles

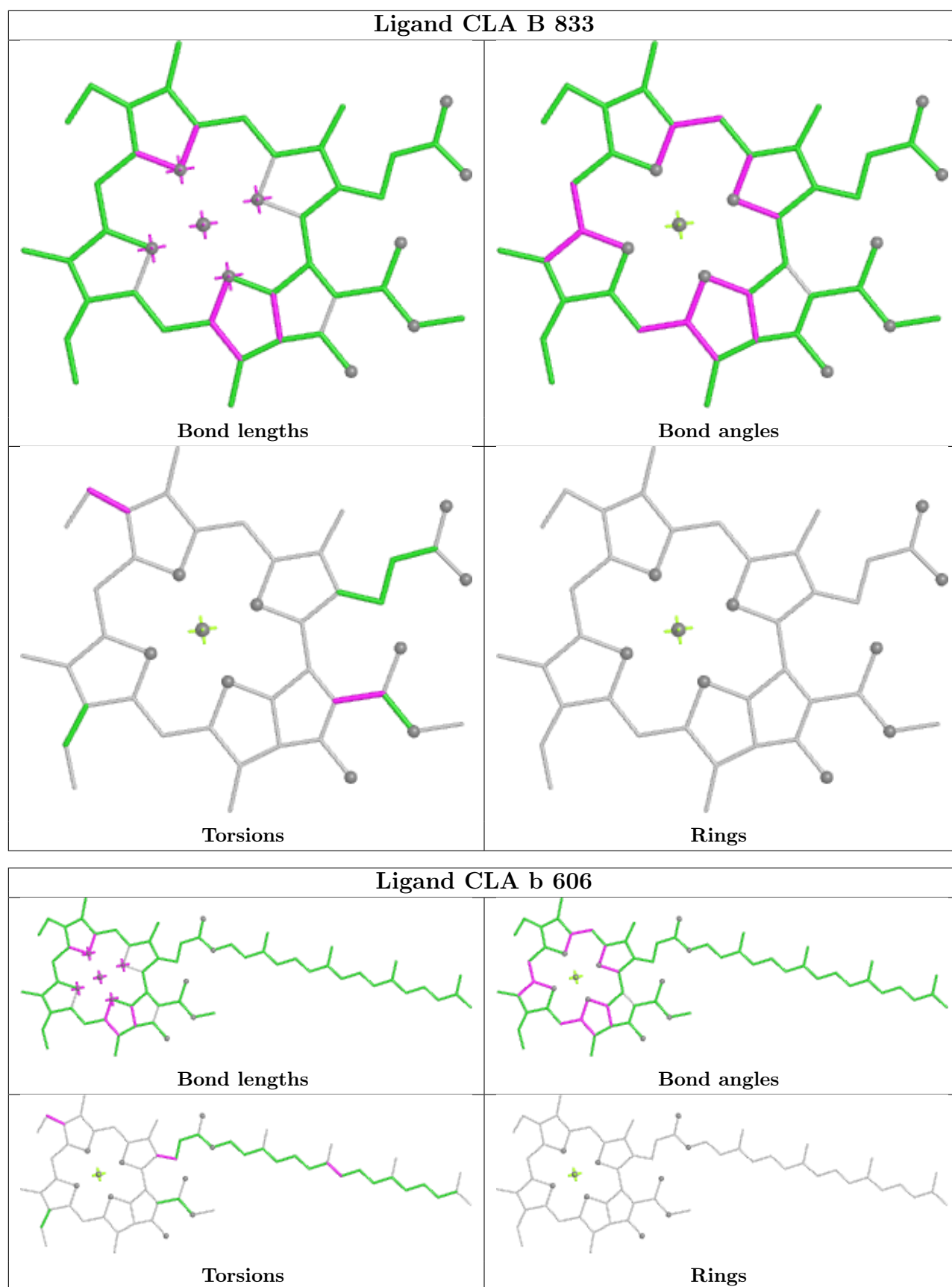


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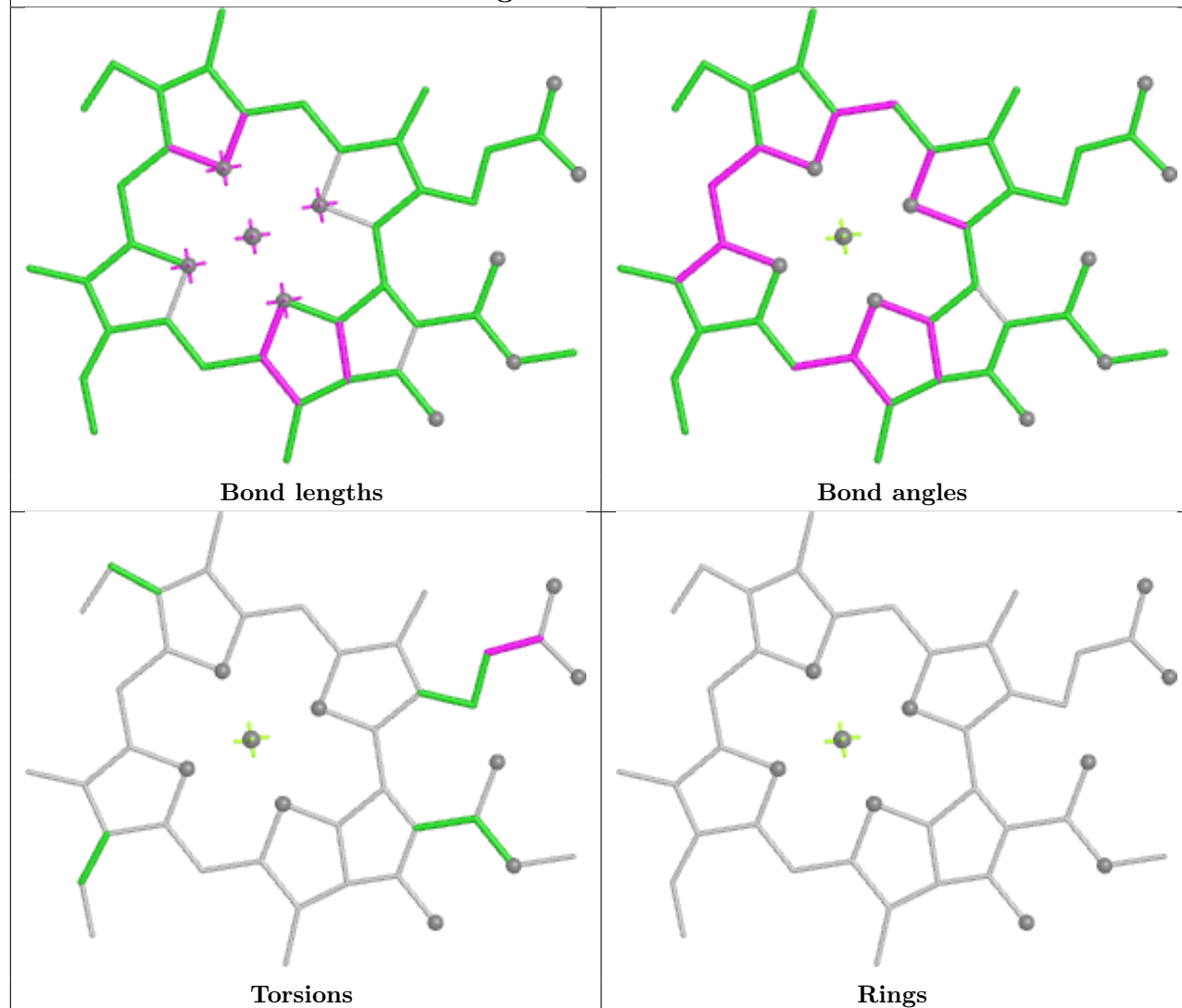


Rings

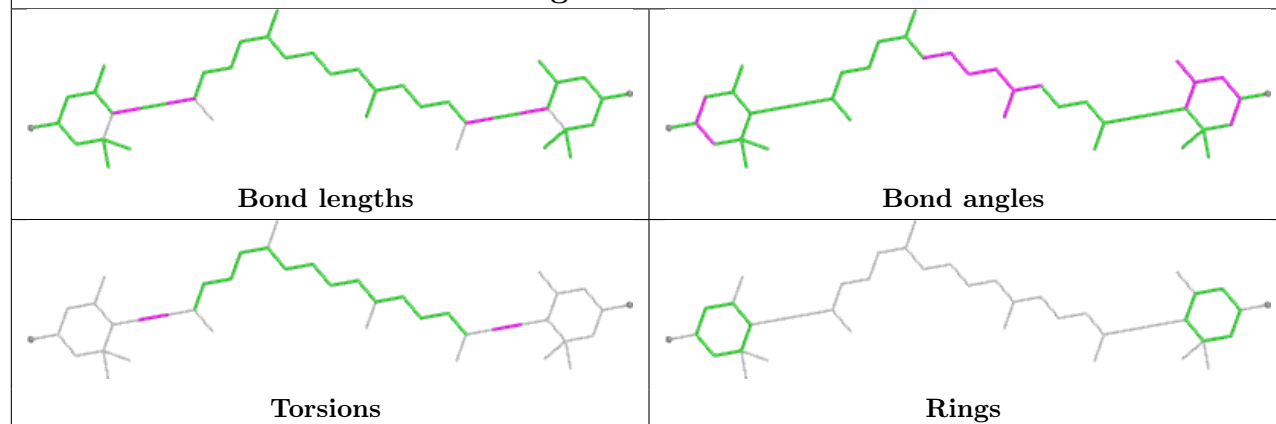


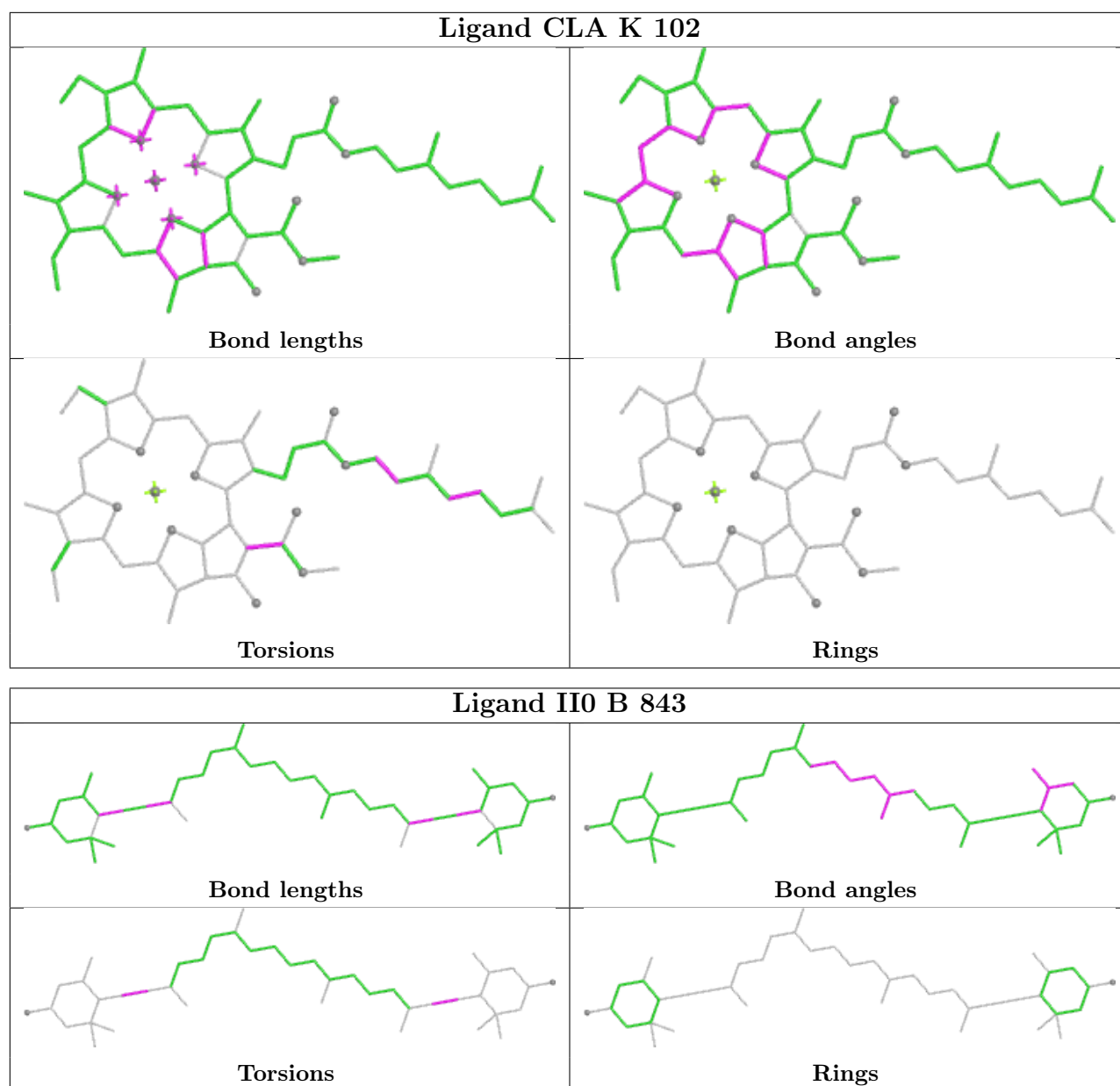


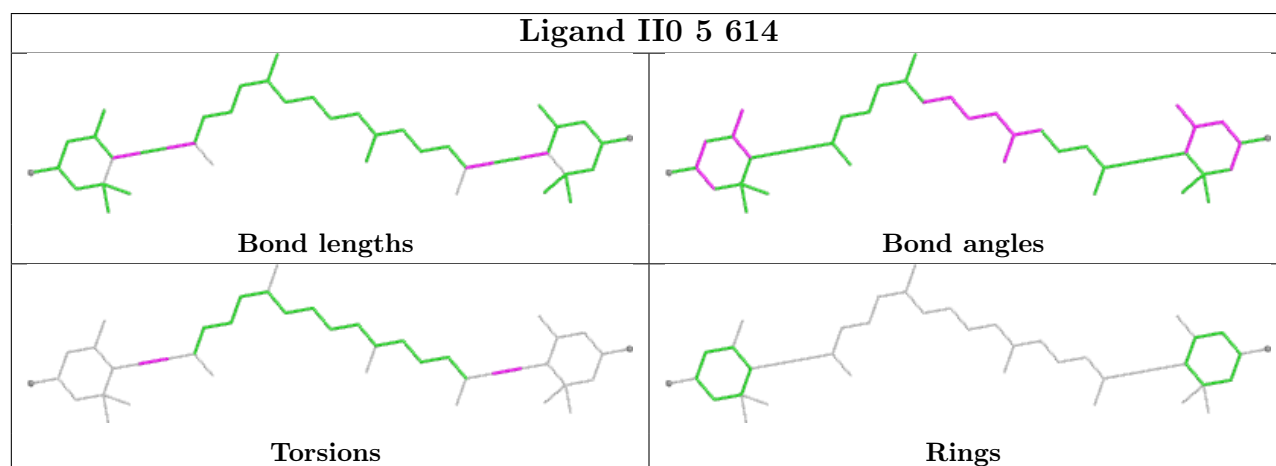
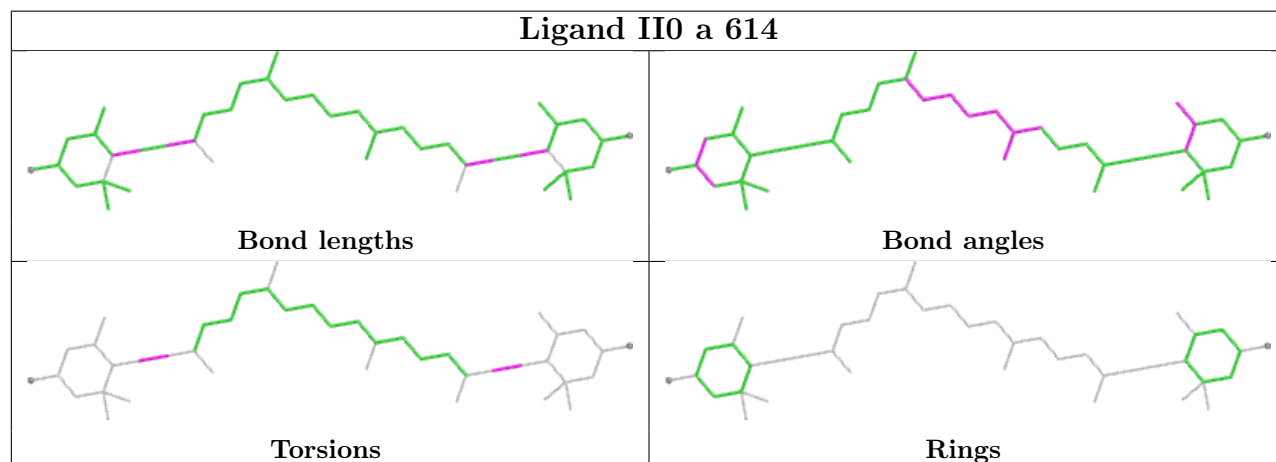
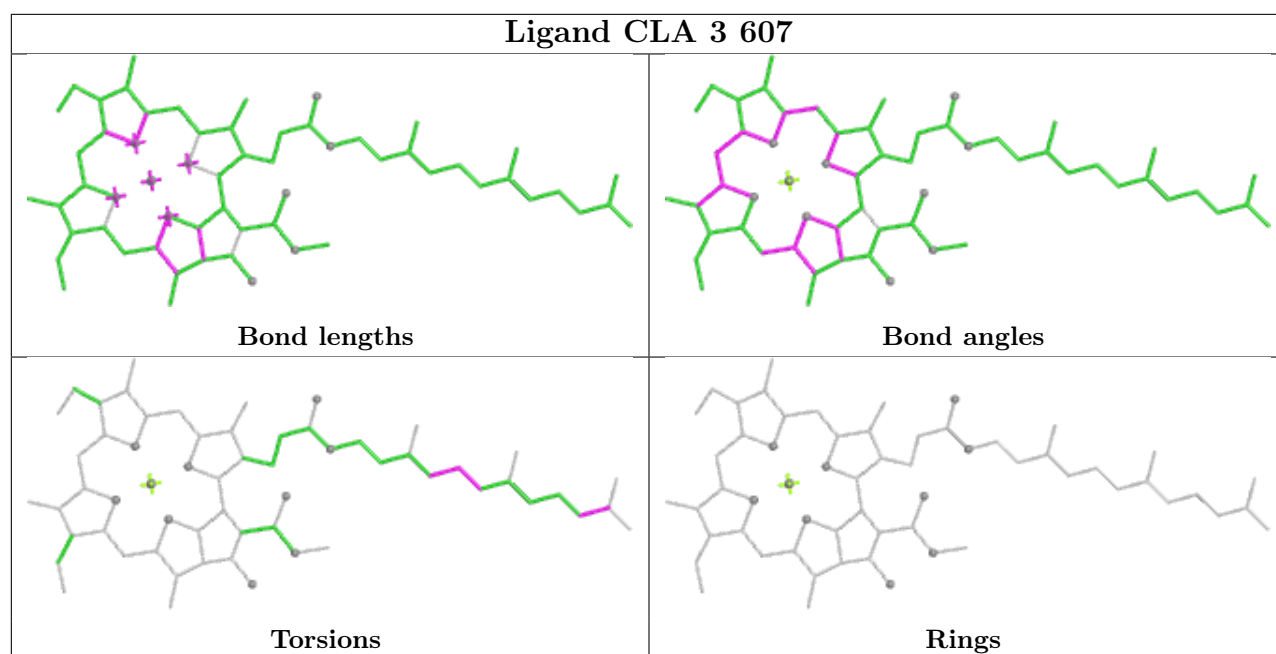
Ligand CLA 9 612

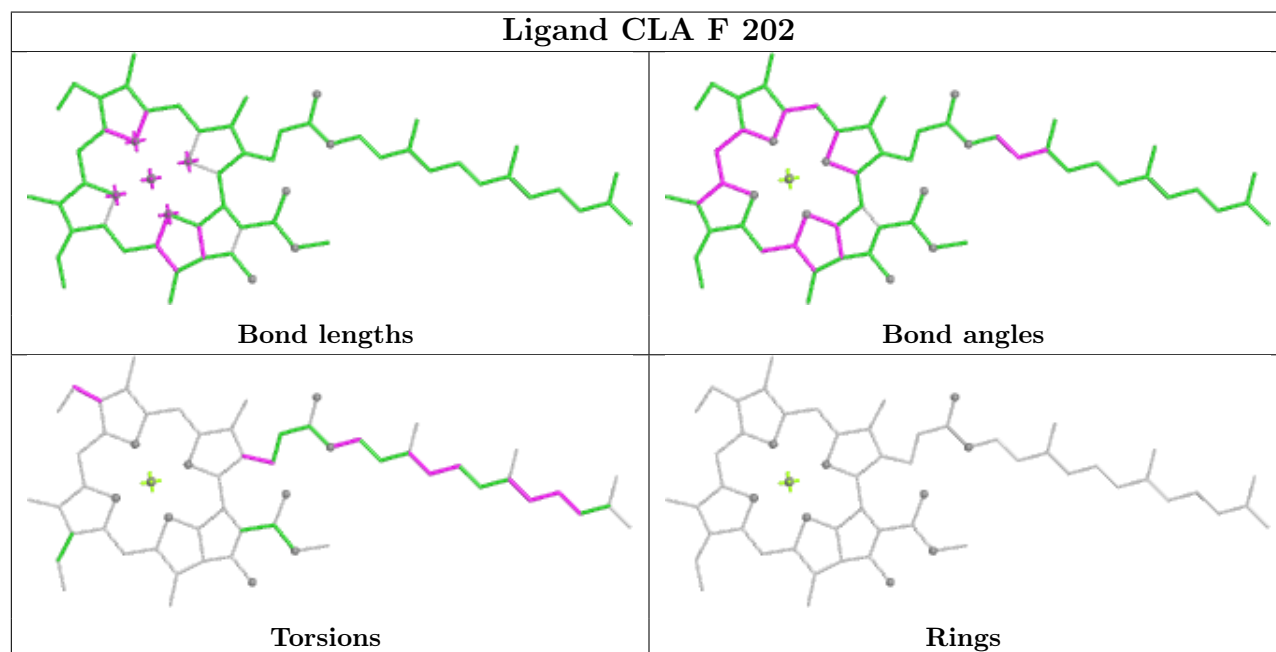
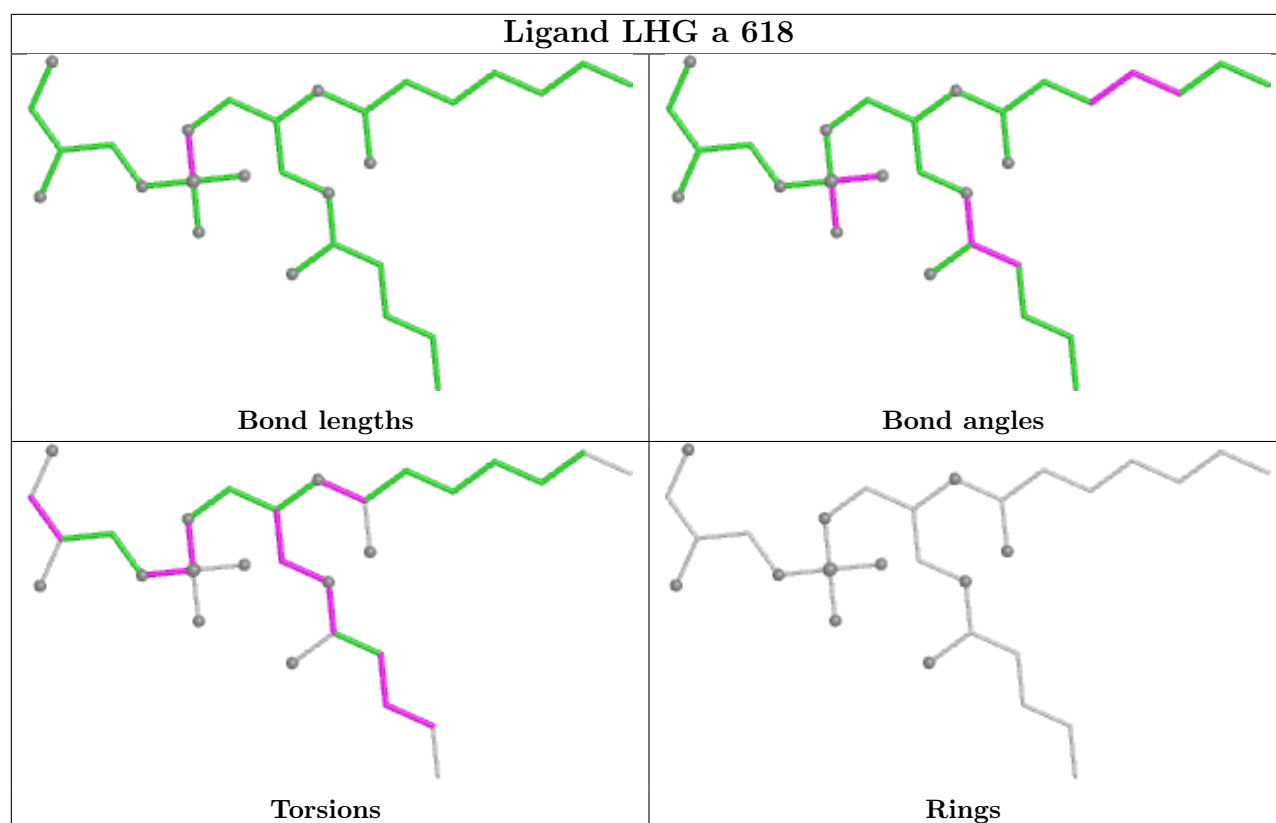


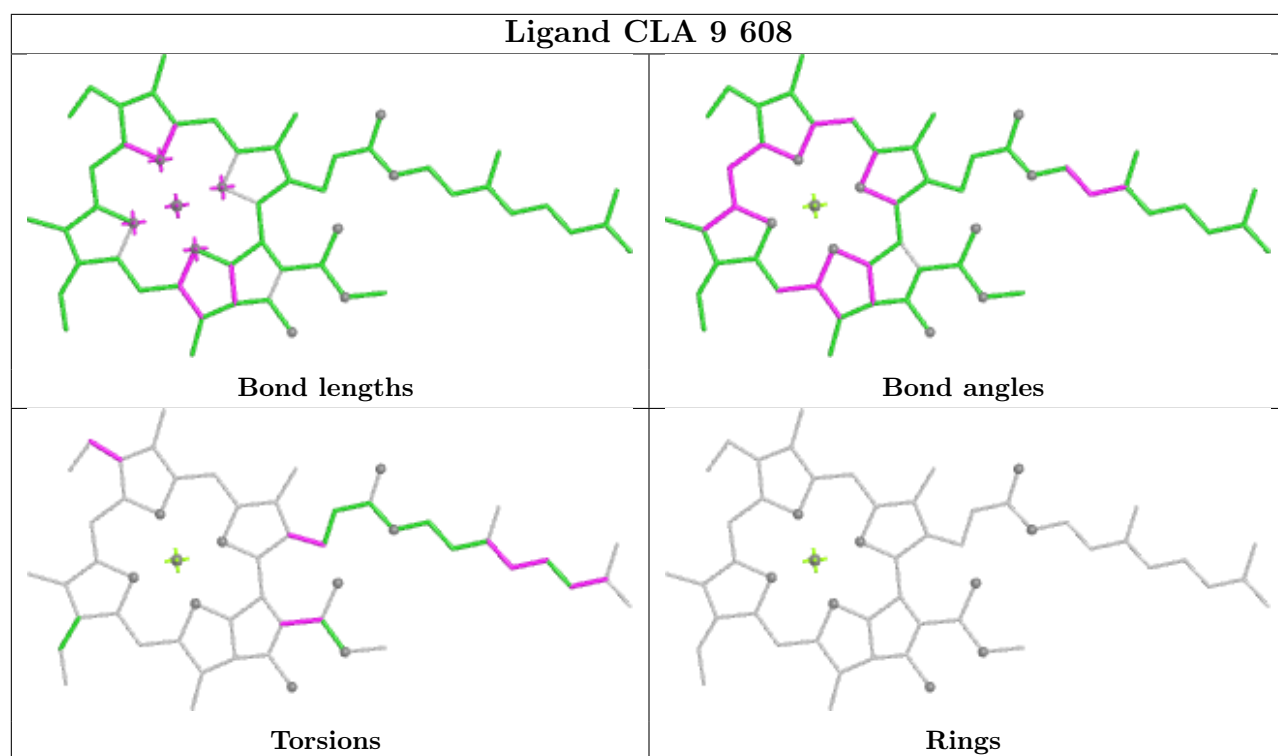
Ligand II0 1 616



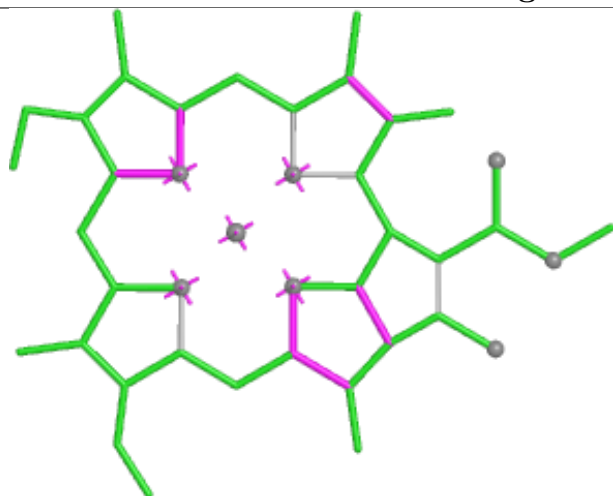




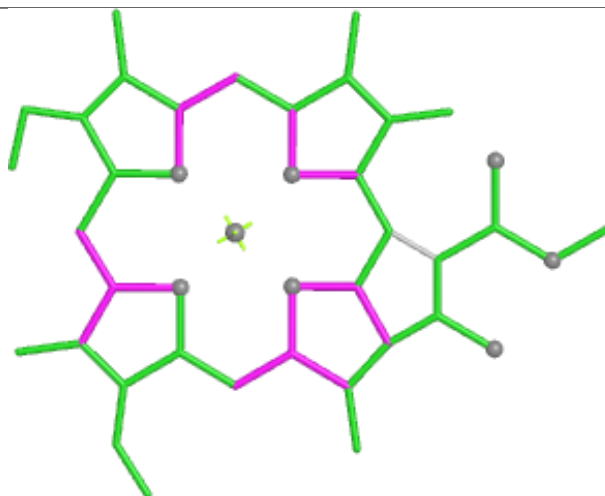




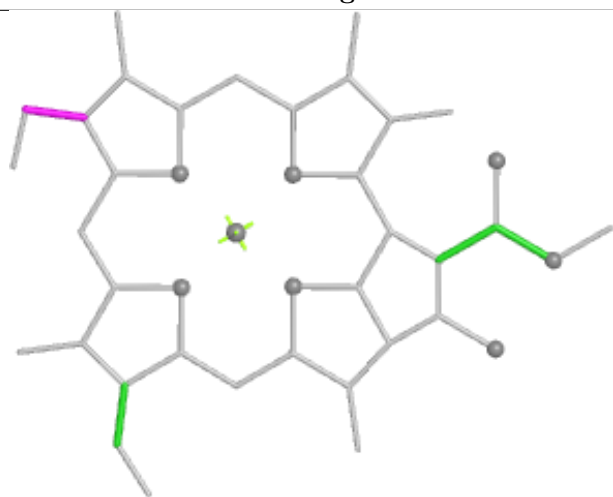
Ligand CLA 7 310



Bond lengths



Bond angles

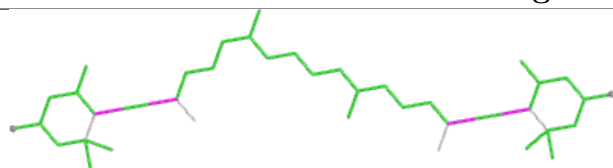


Torsions

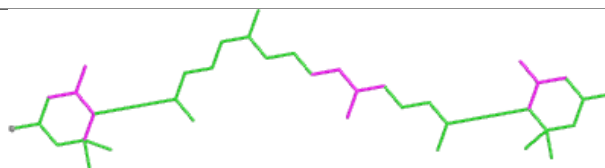


Rings

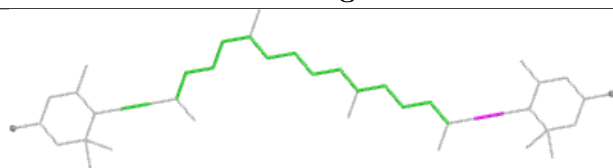
Ligand II0 5 620



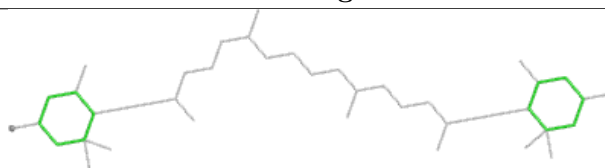
Bond lengths



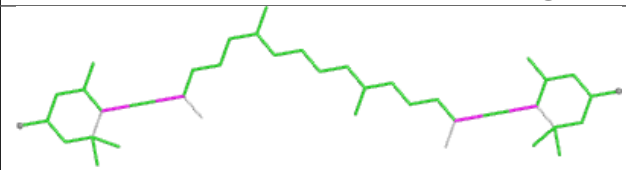
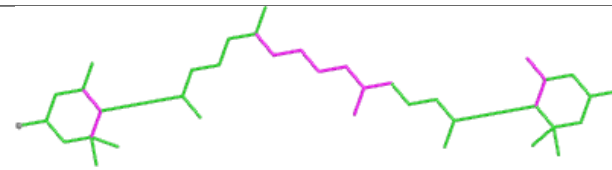
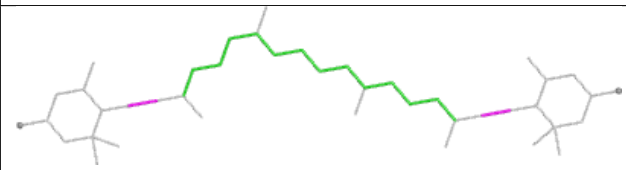
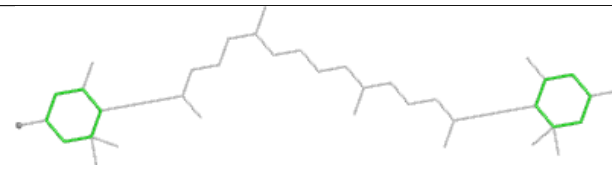
Bond angles

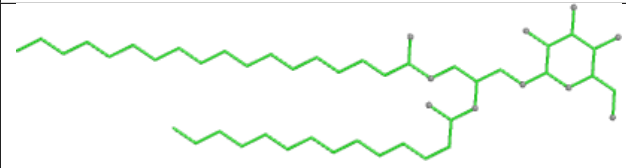
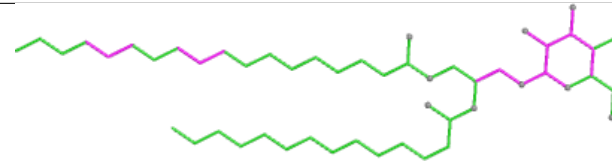
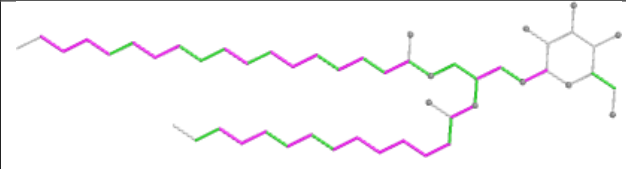
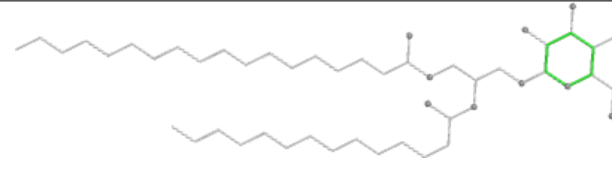


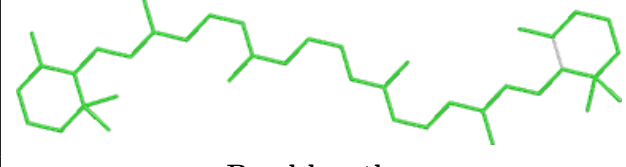
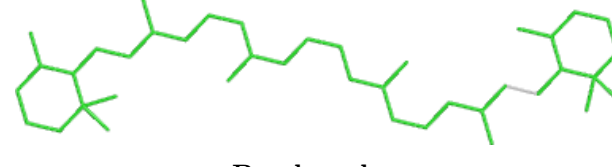
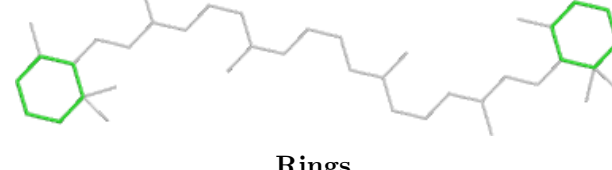
Torsions

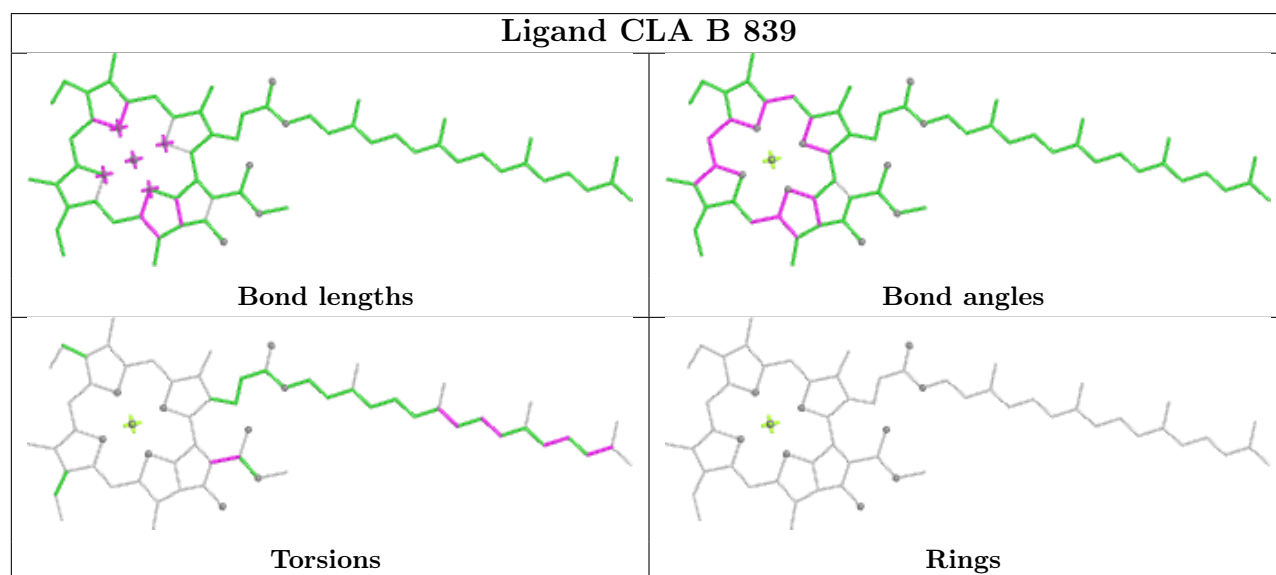
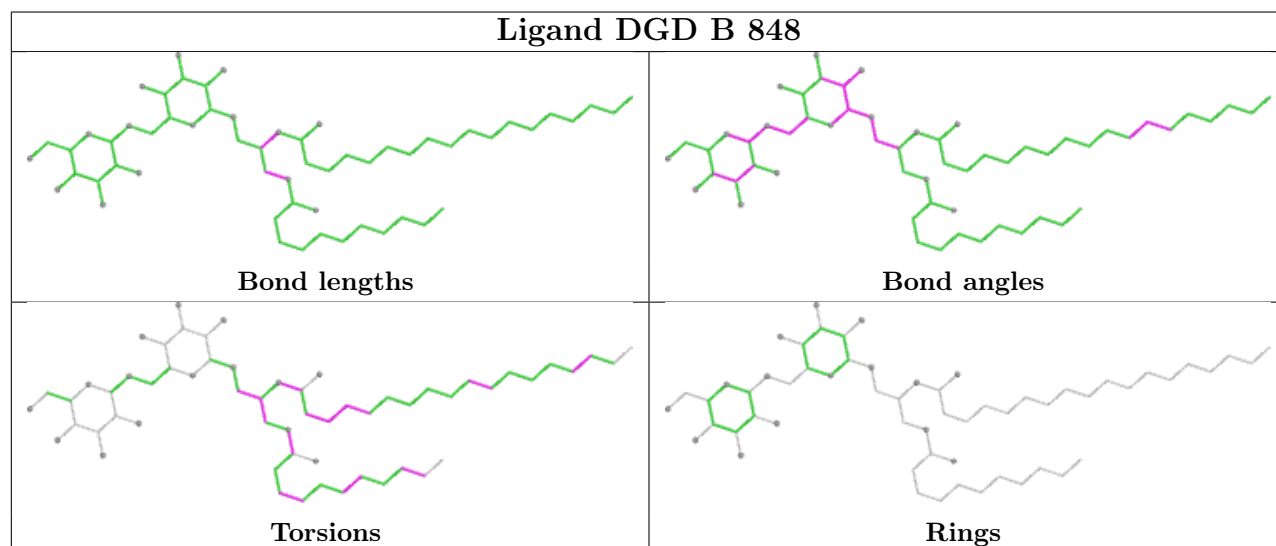
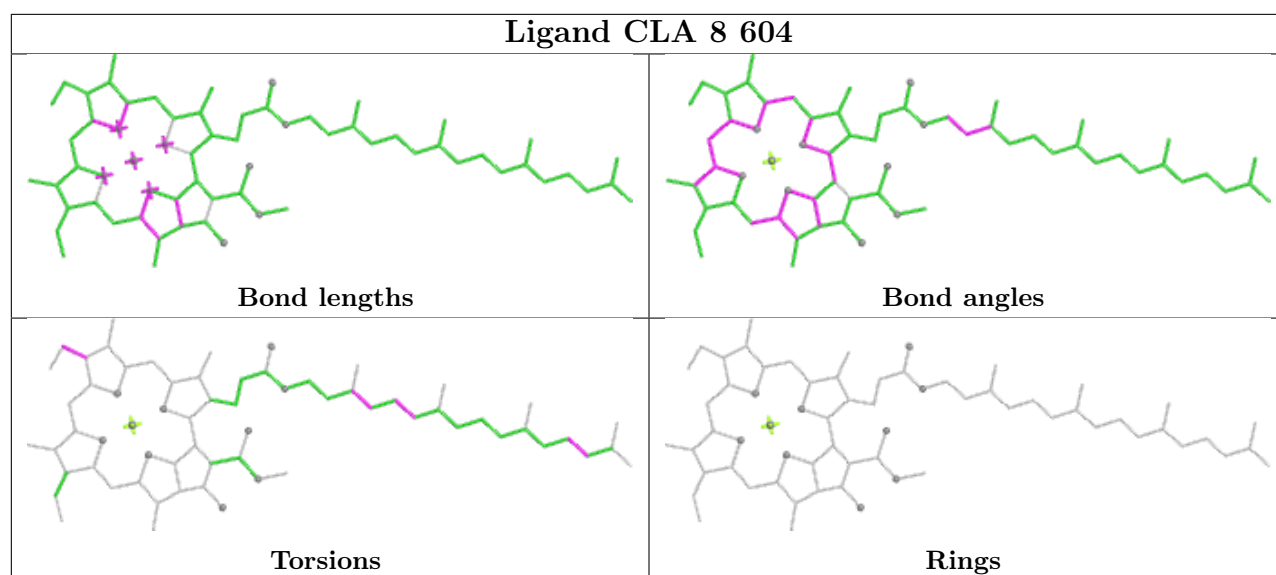


Rings

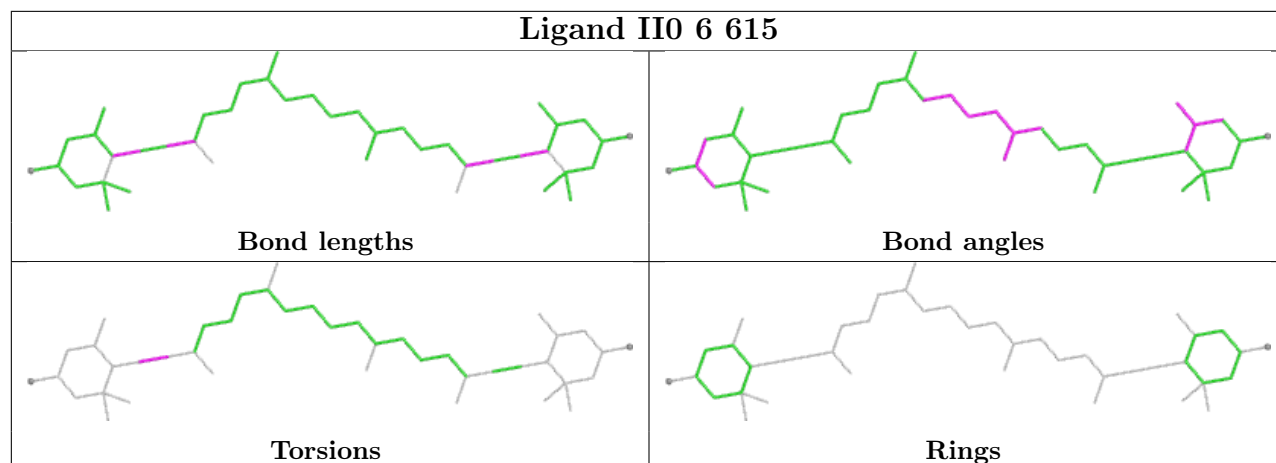
Ligand II0 4 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG 8 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

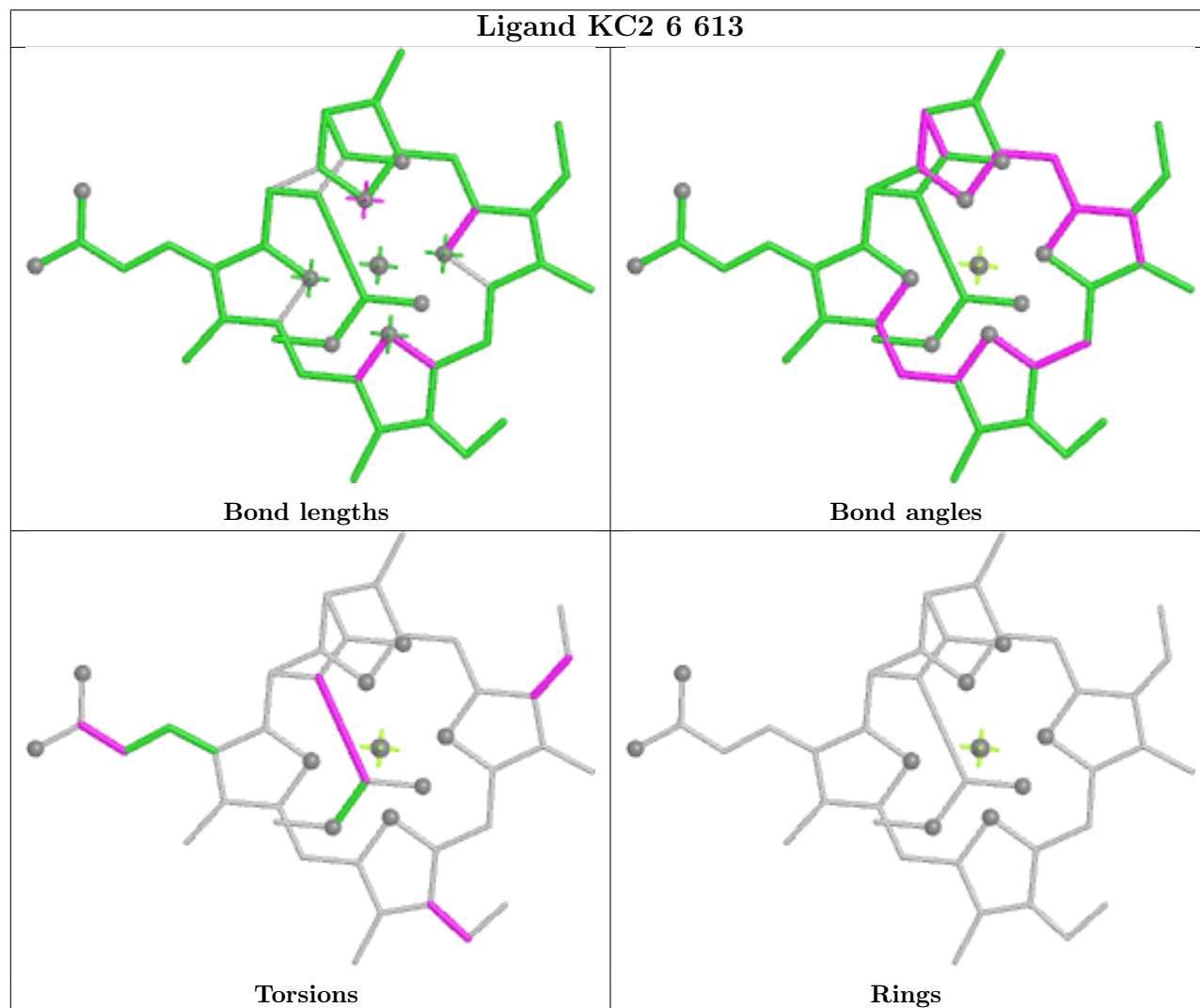
Ligand 8CT R 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

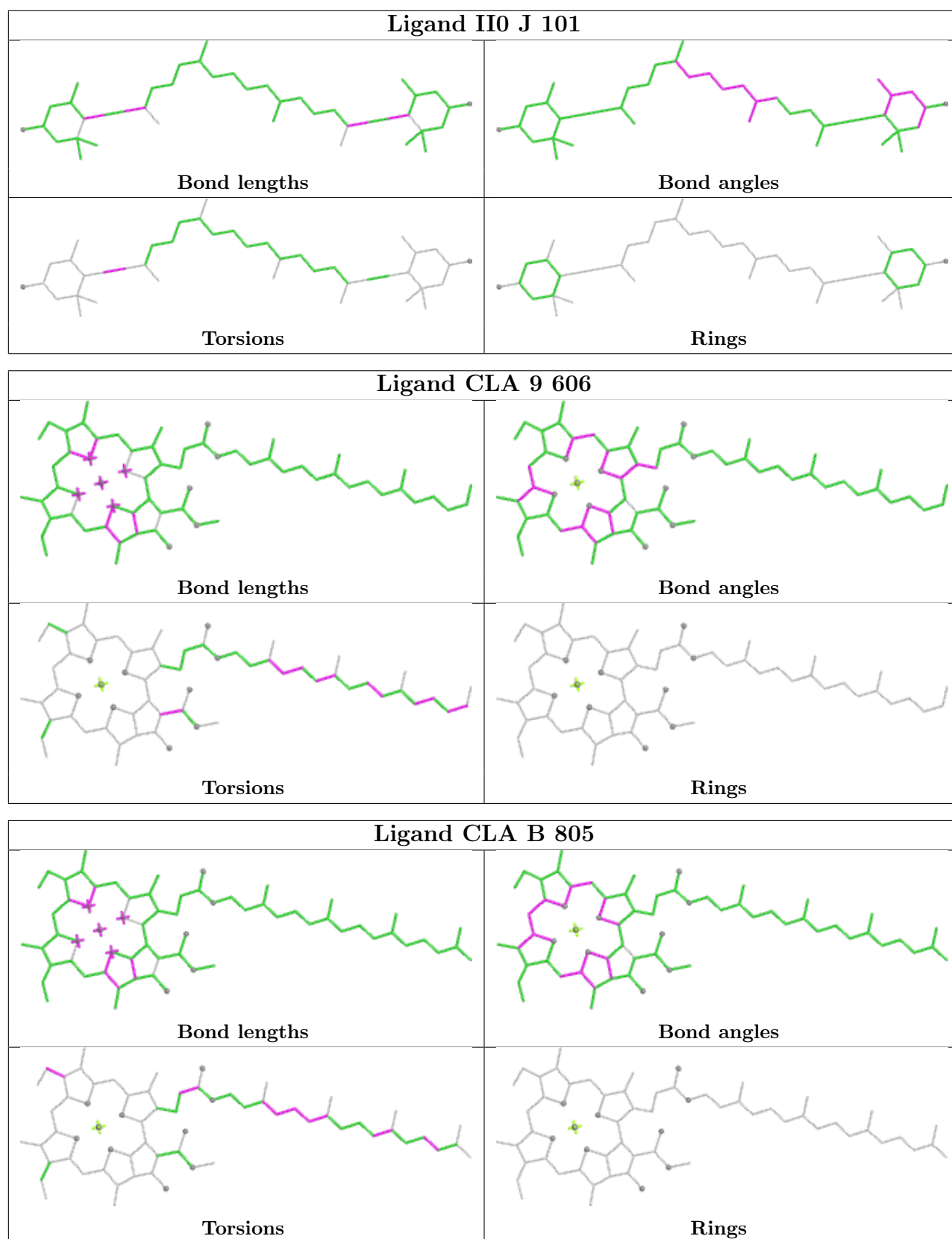


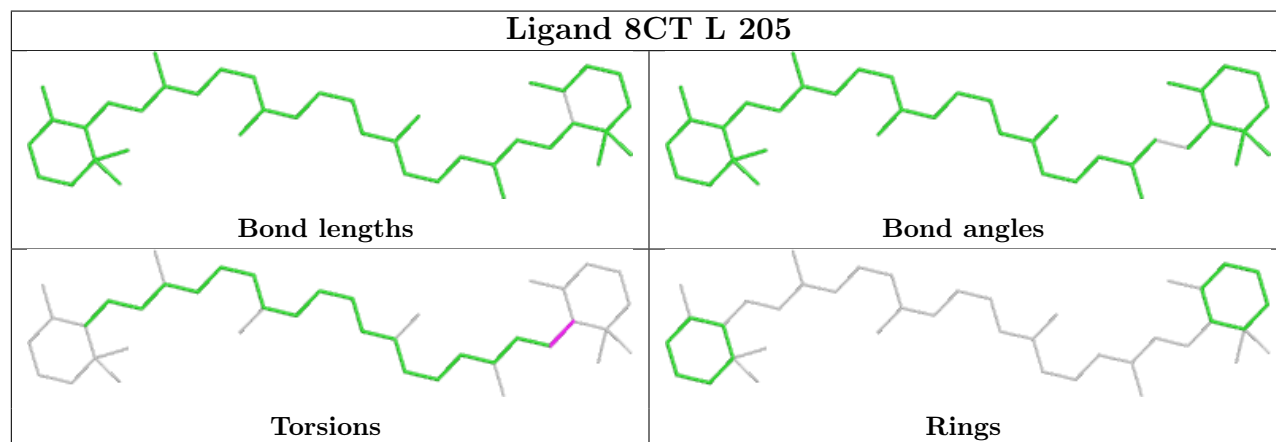
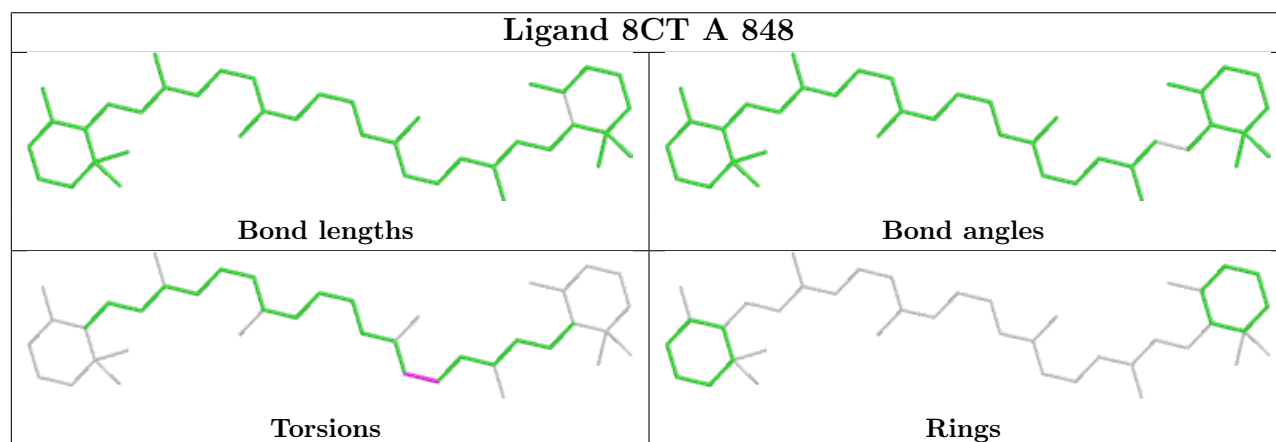
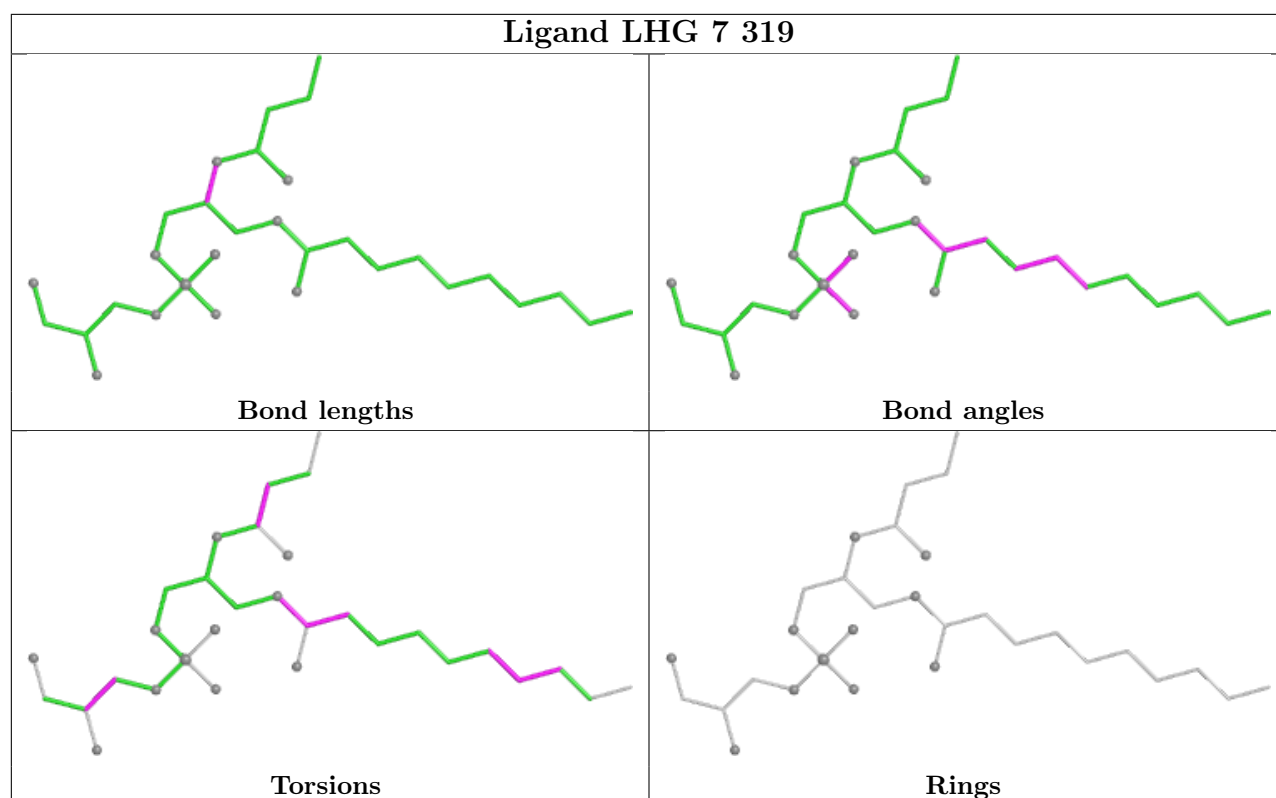
Ligand II0 6 615



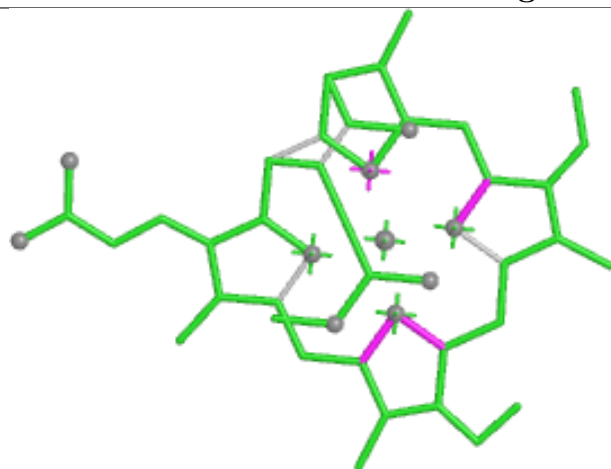
Ligand KC2 6 613



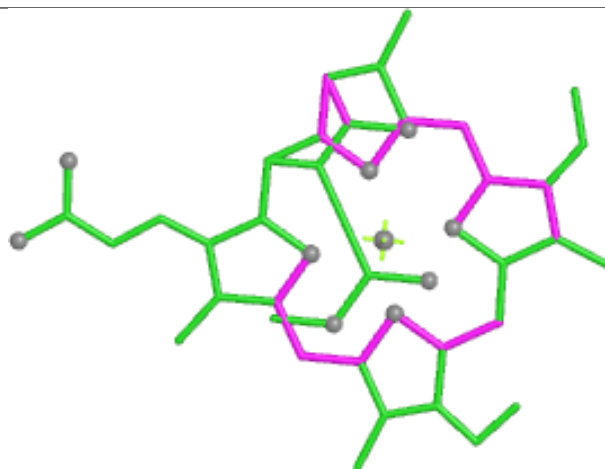




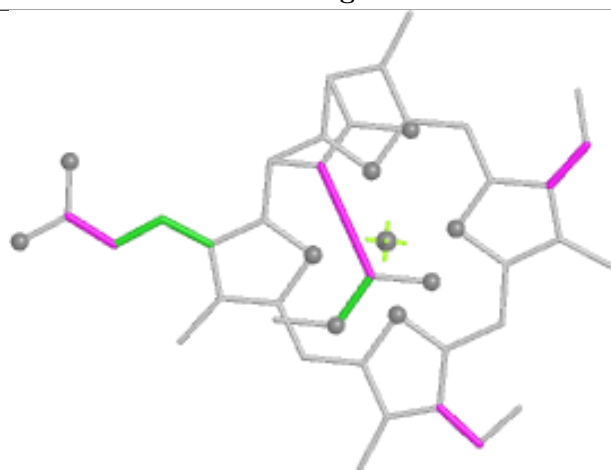
Ligand KC2 Z 307



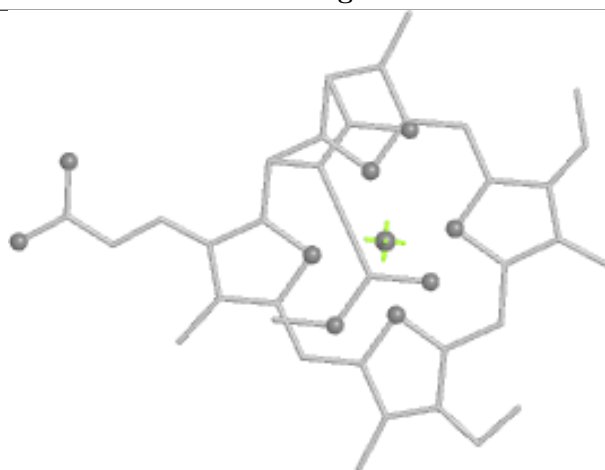
Bond lengths



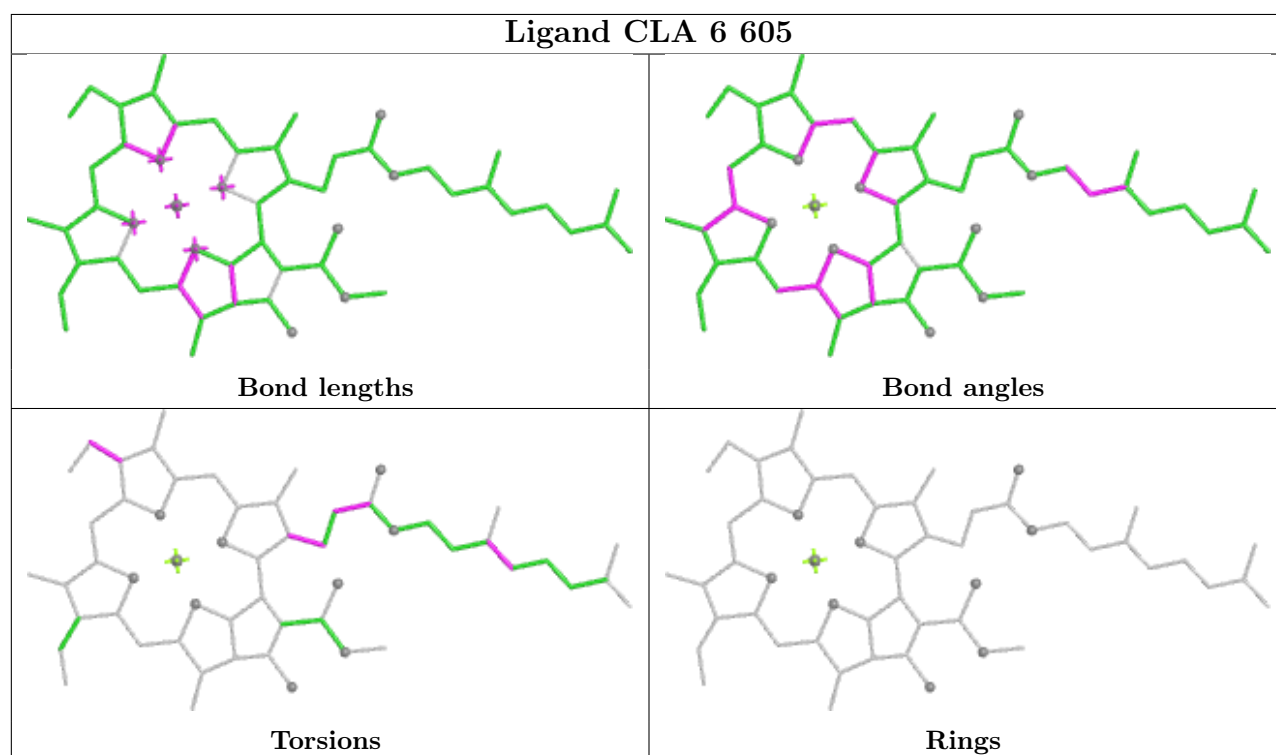
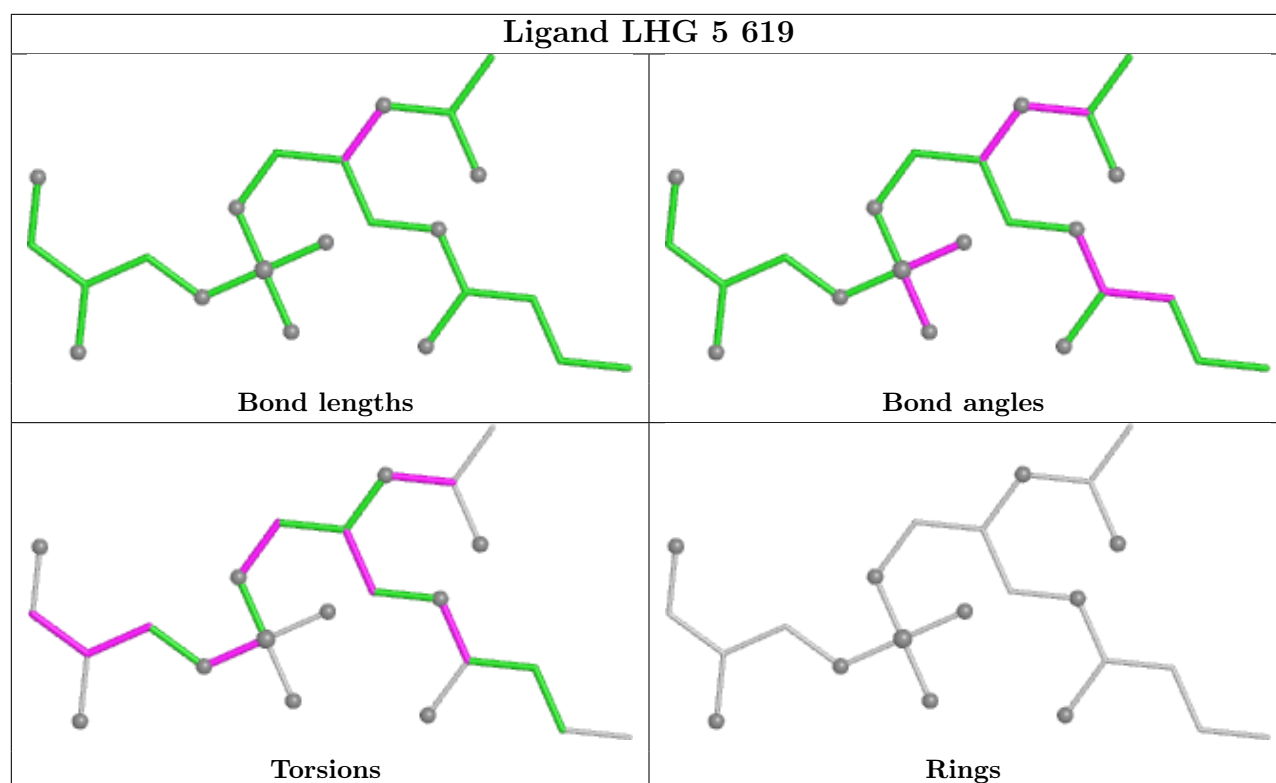
Bond angles

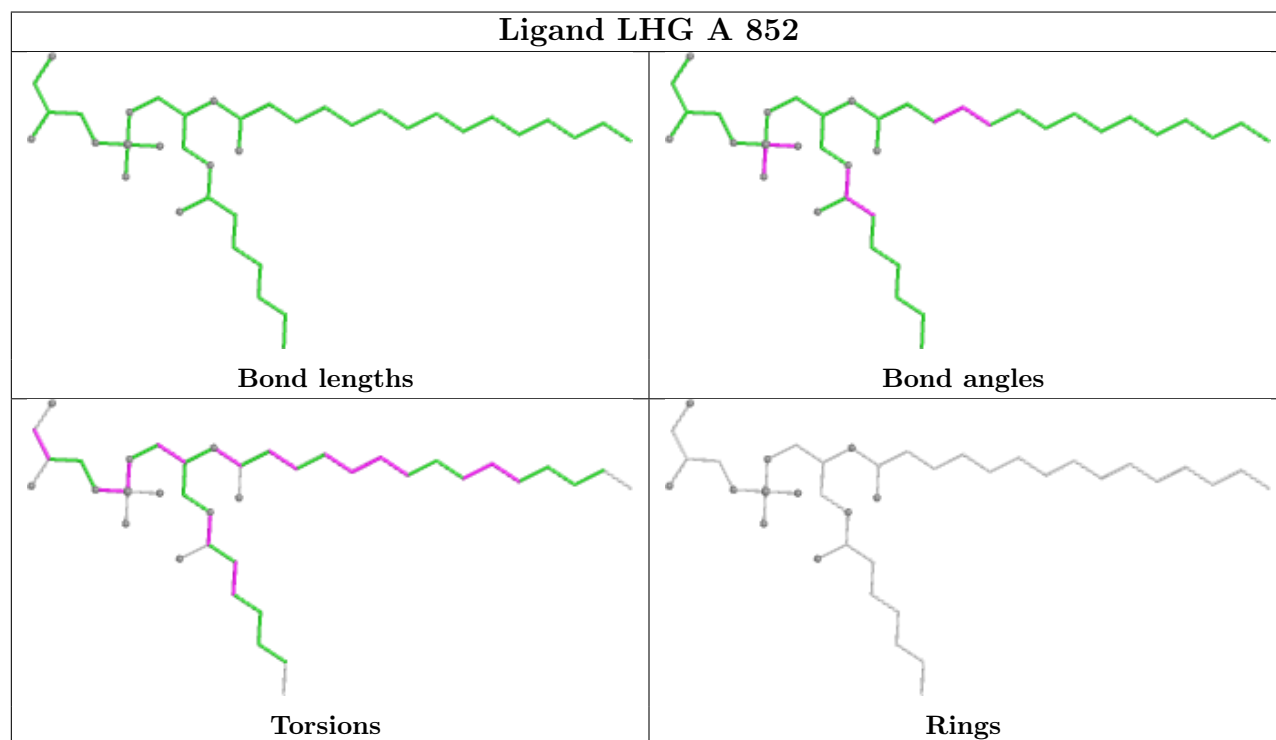
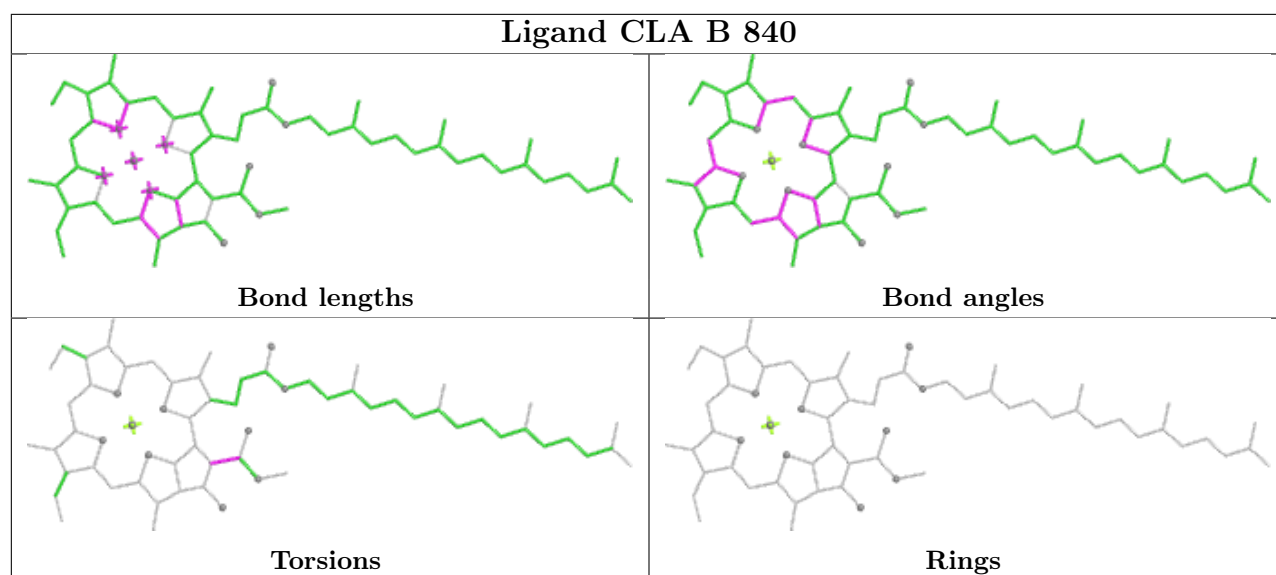


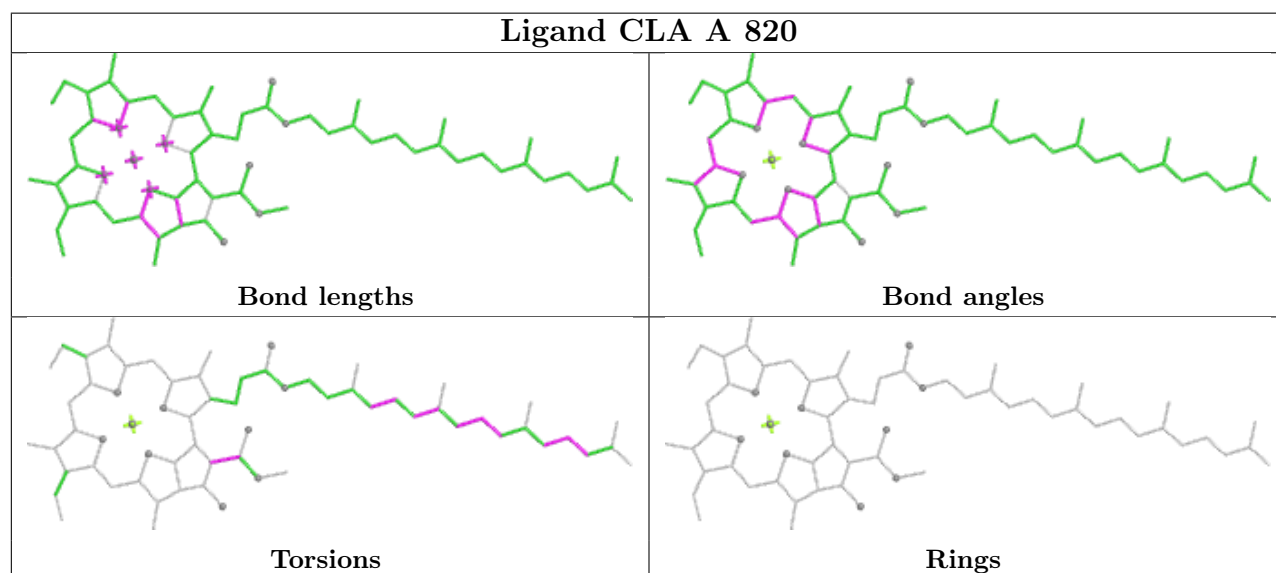
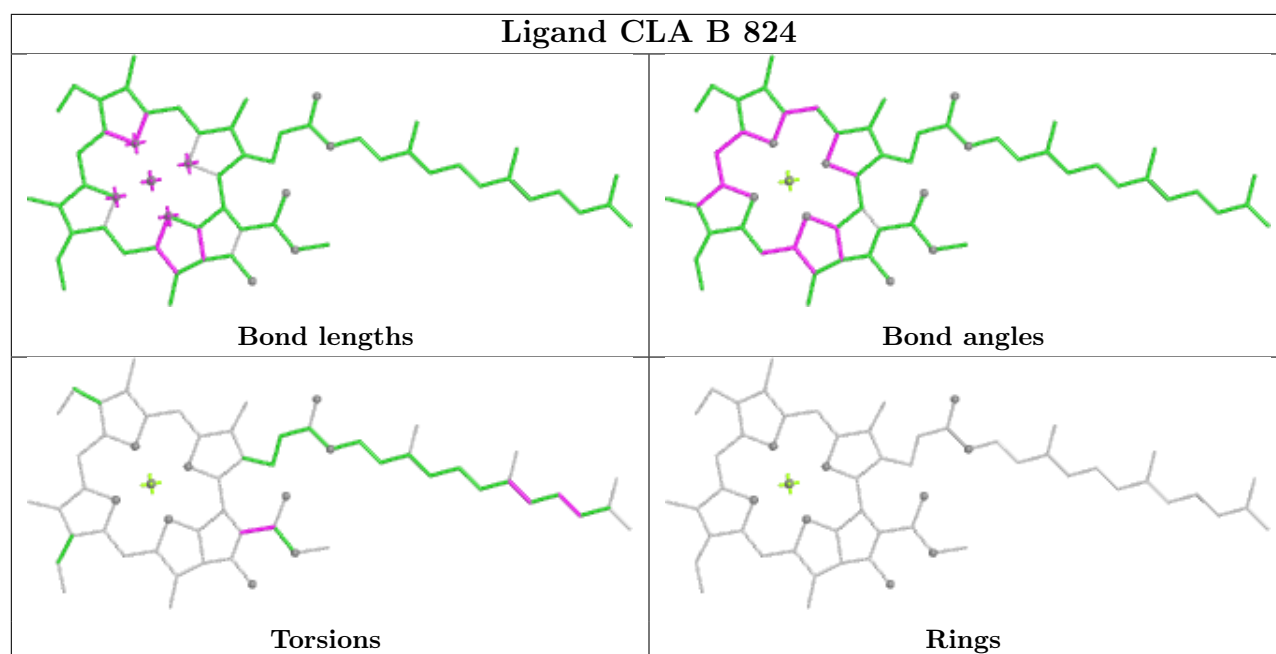
Torsions

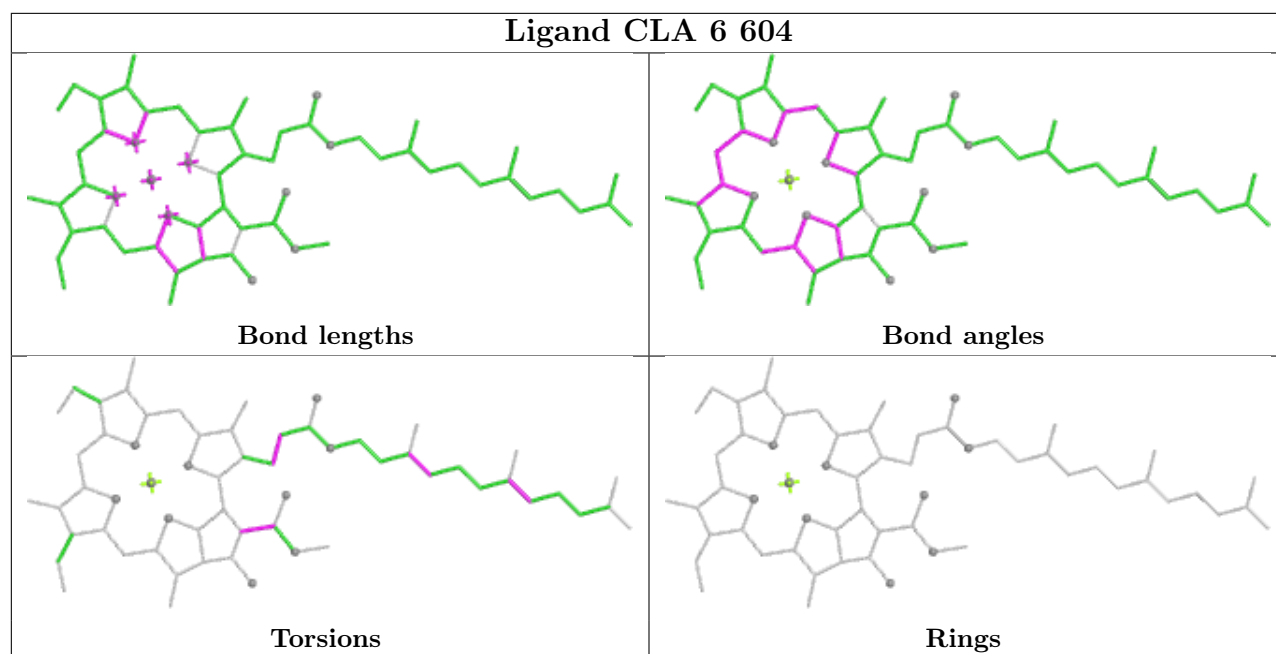
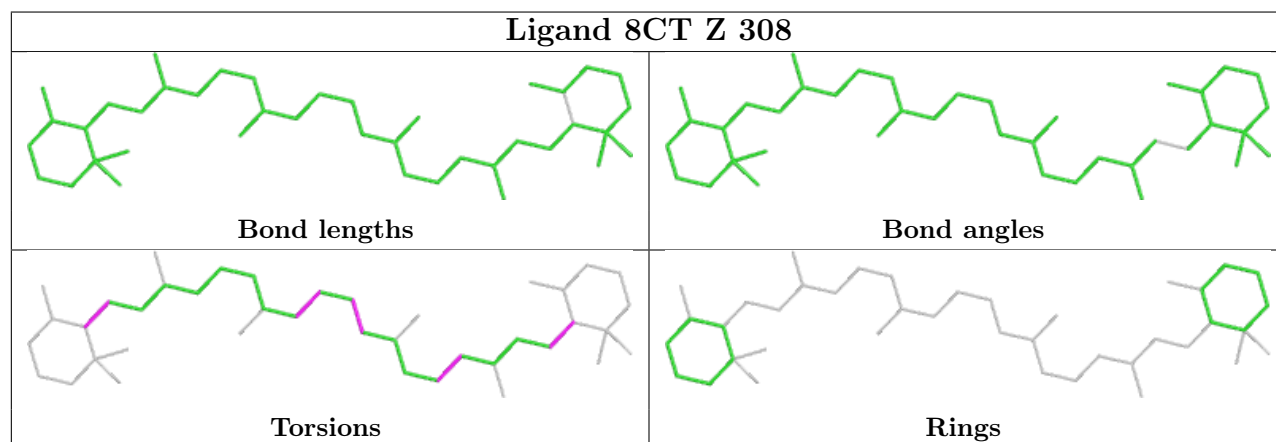
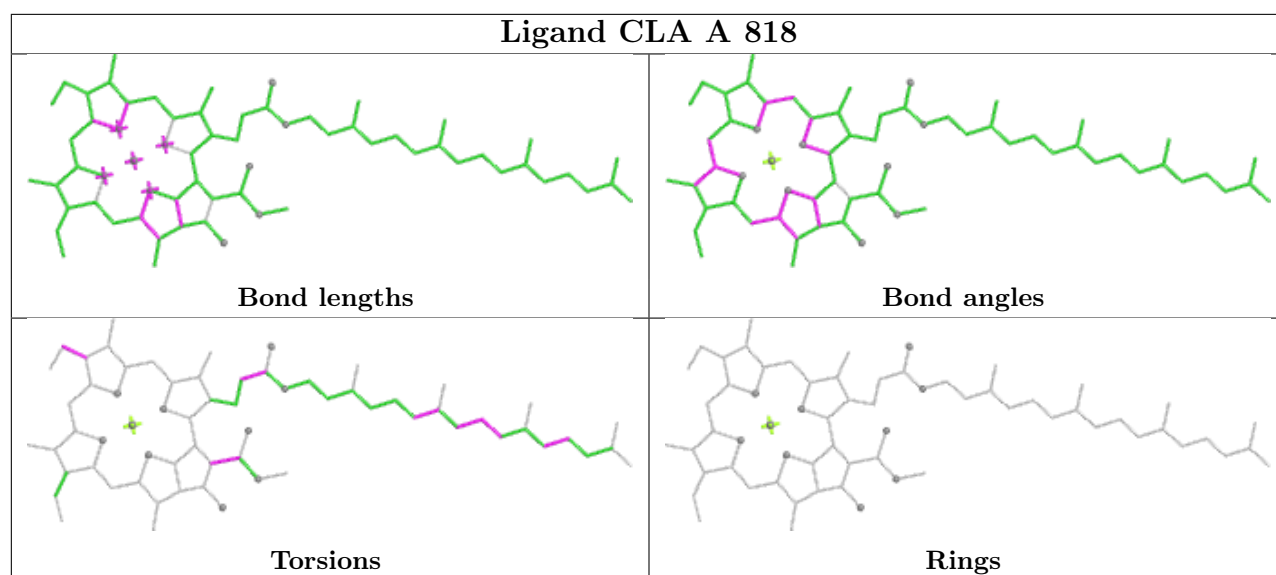


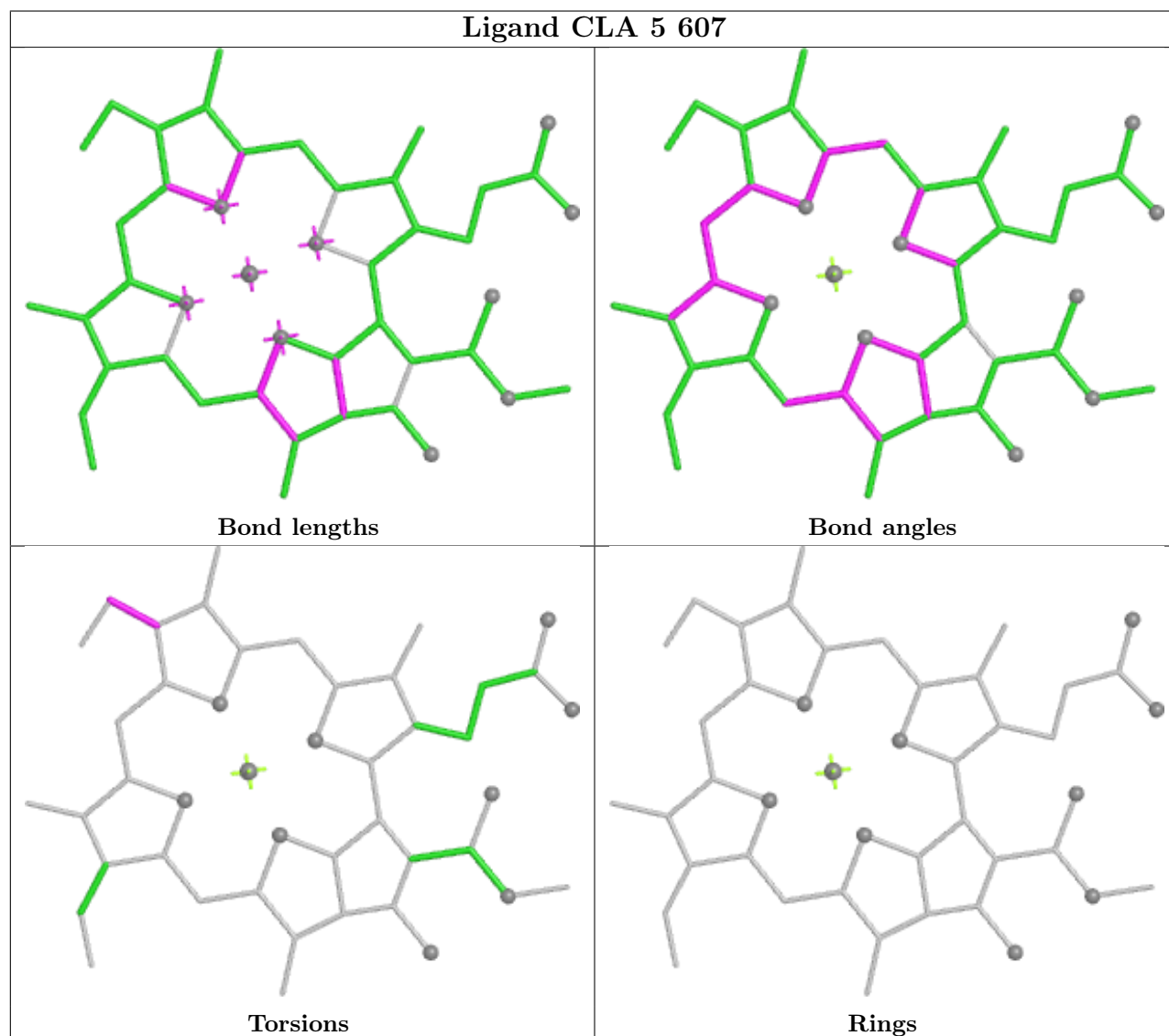
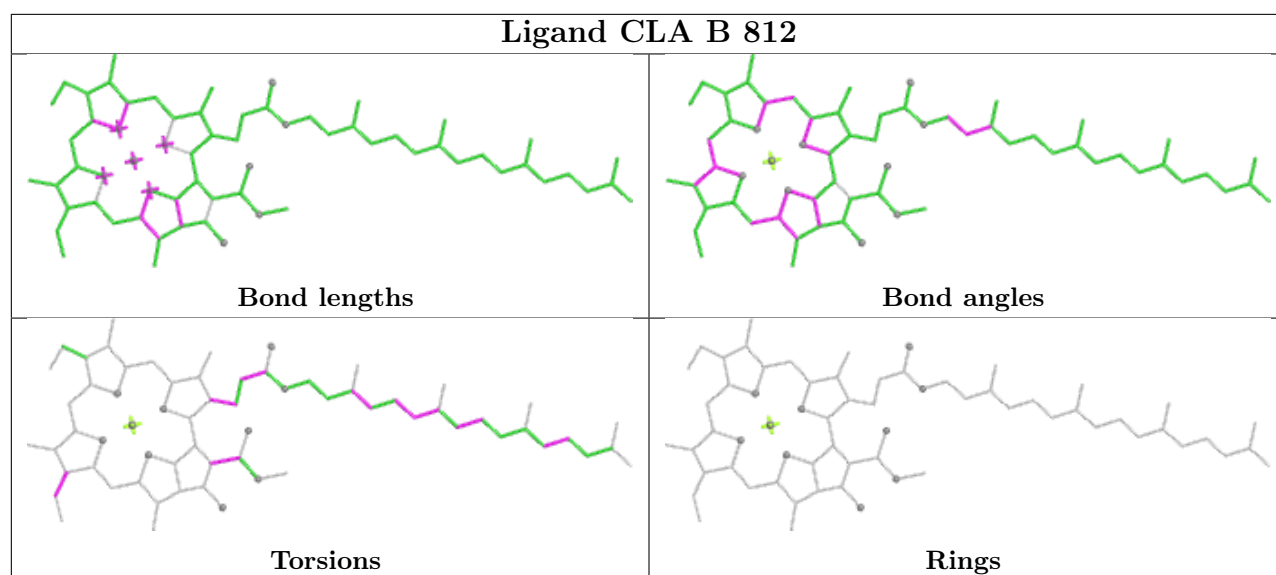
Rings

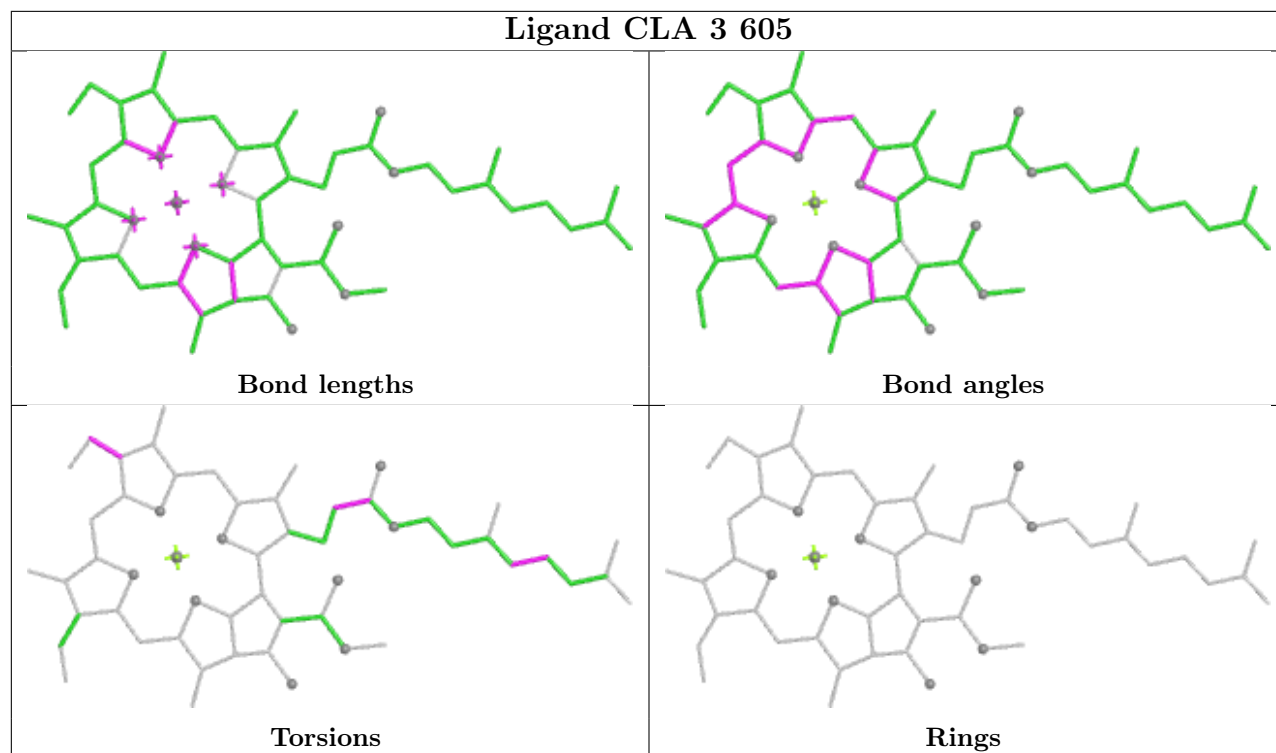
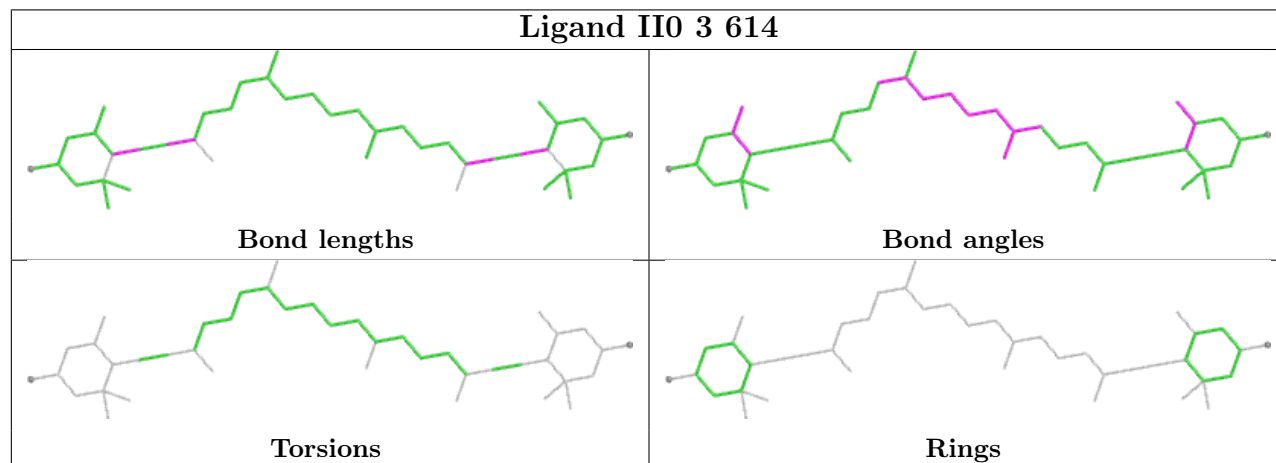


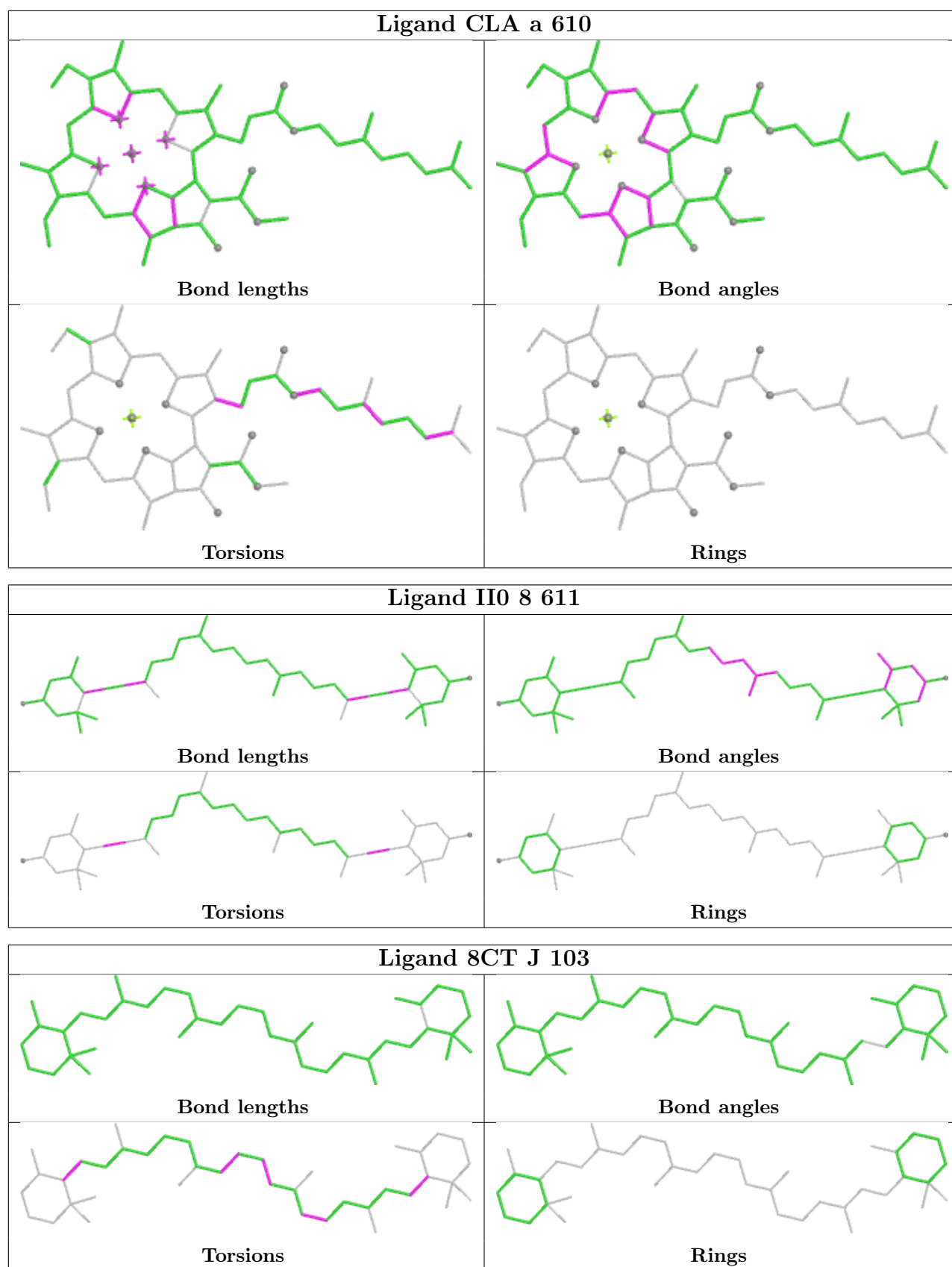


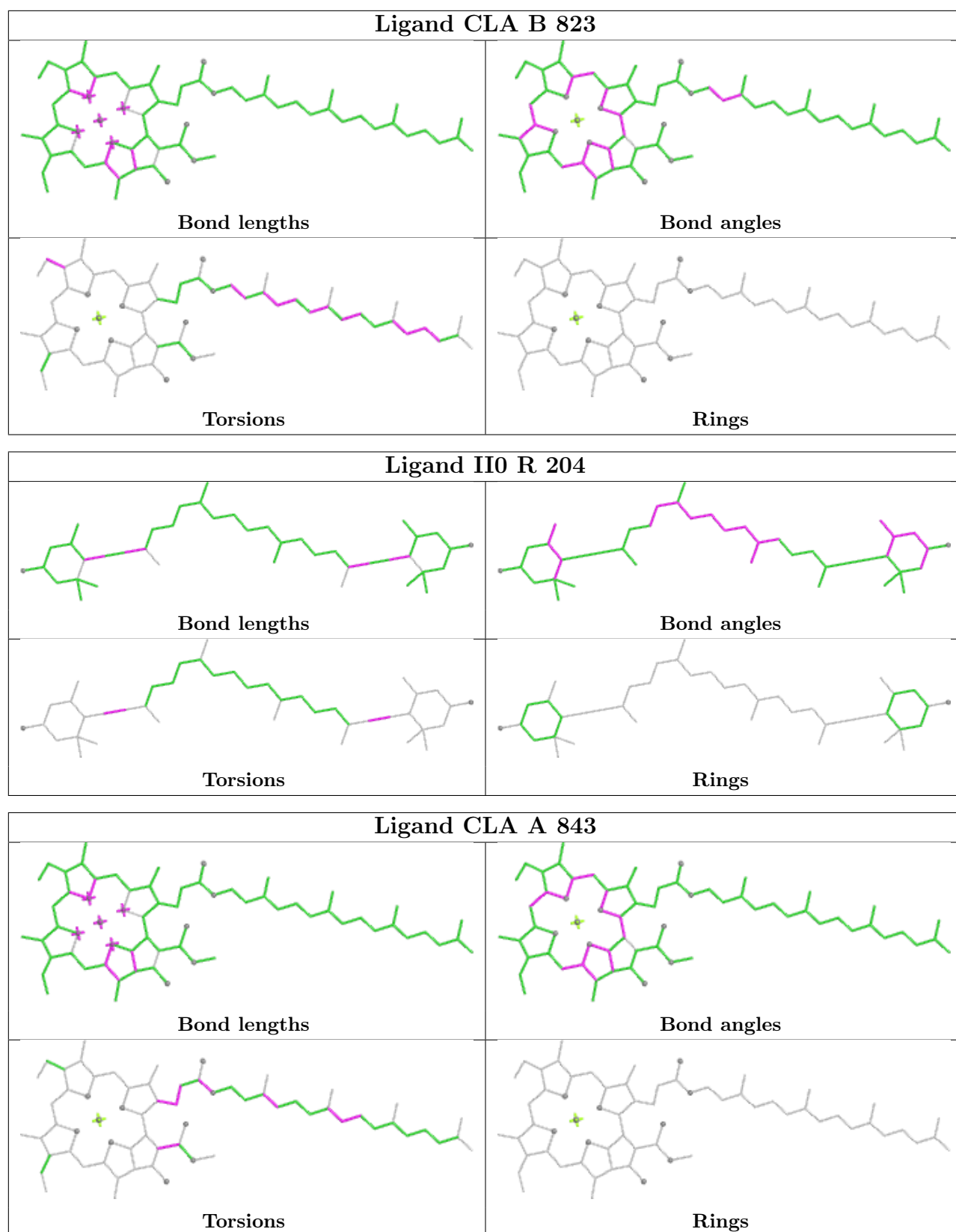




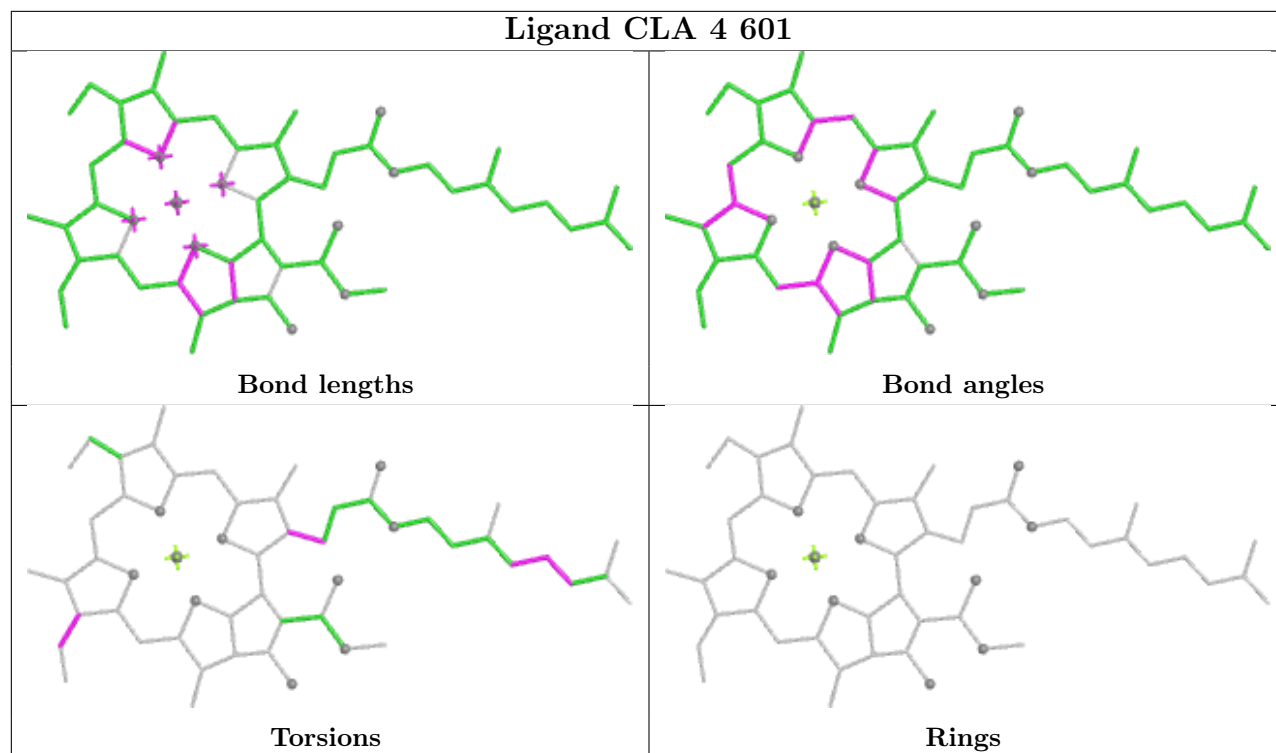


Ligand CLA 3 605**Ligand II0 3 614**

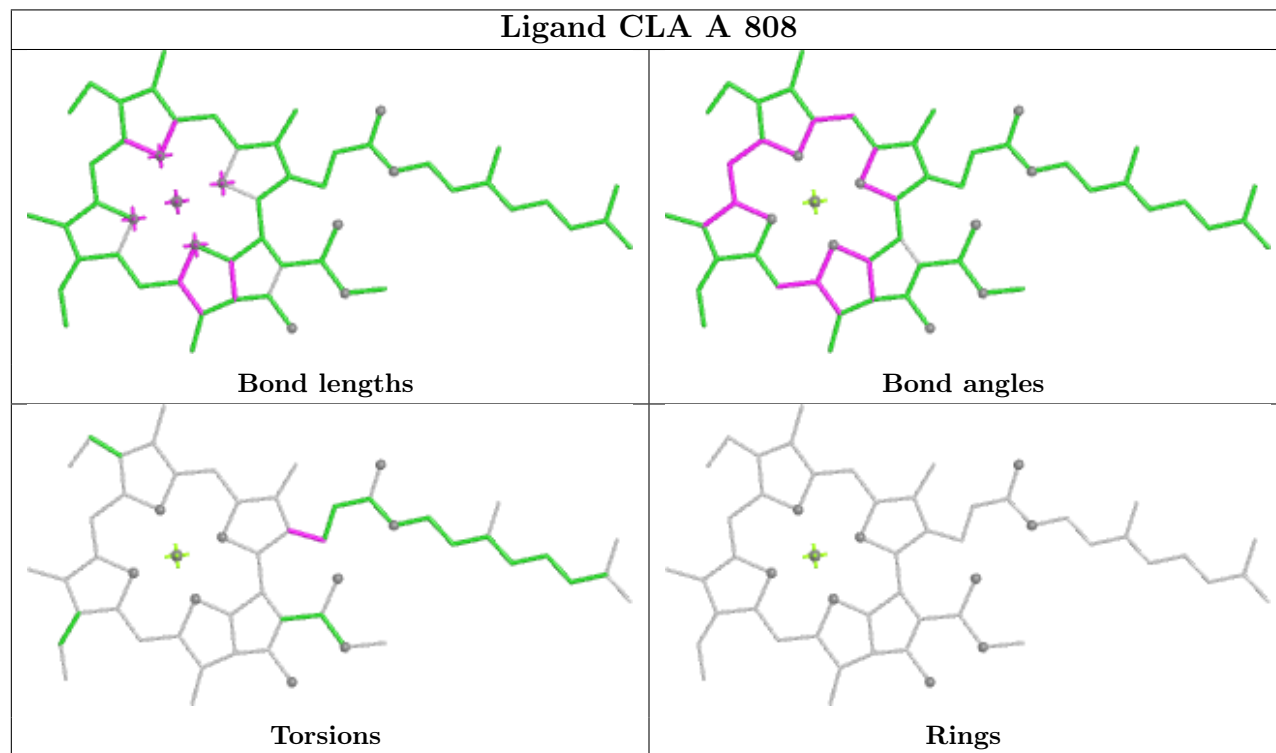


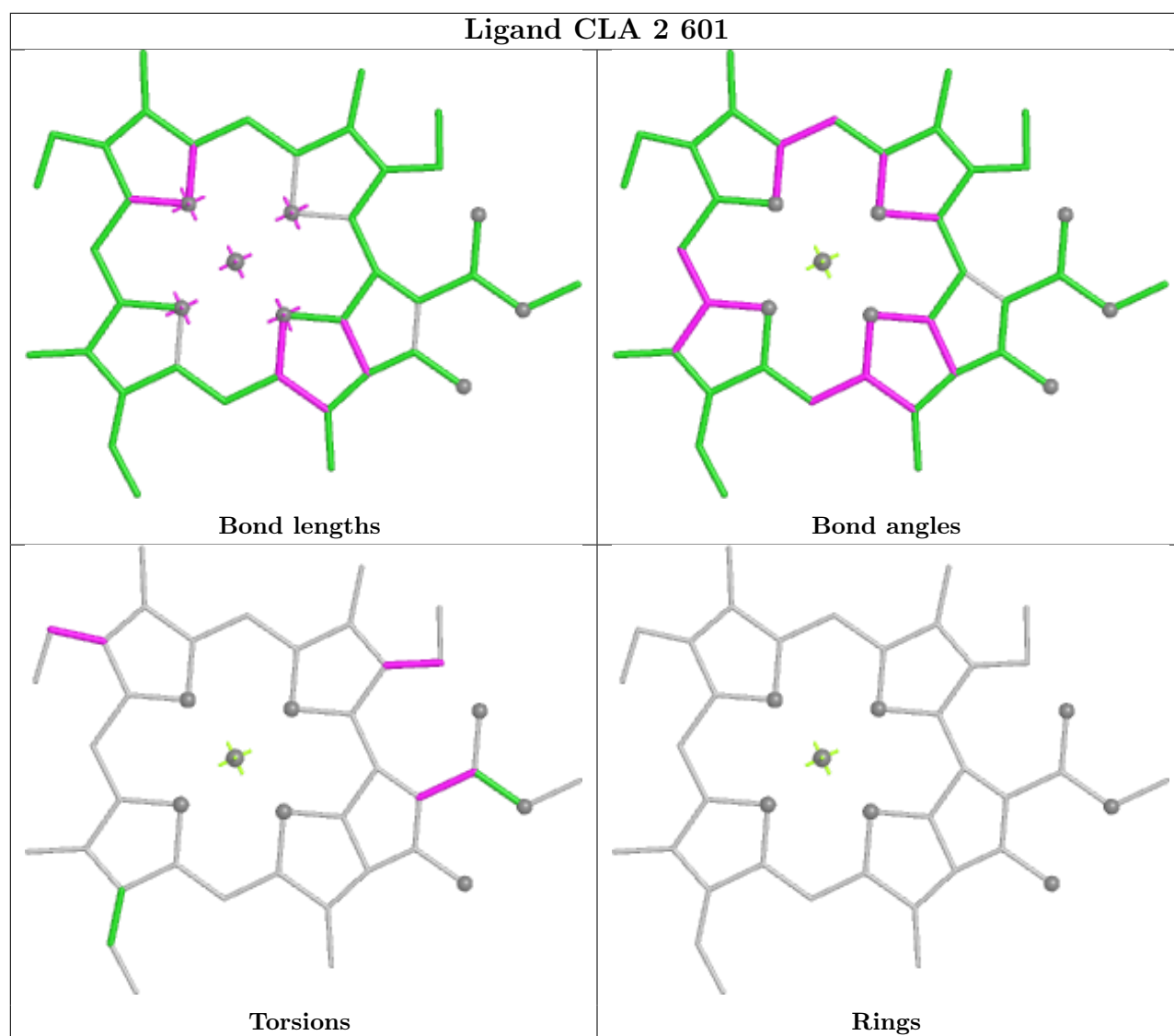


Ligand CLA 4 601



Ligand CLA A 808





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.

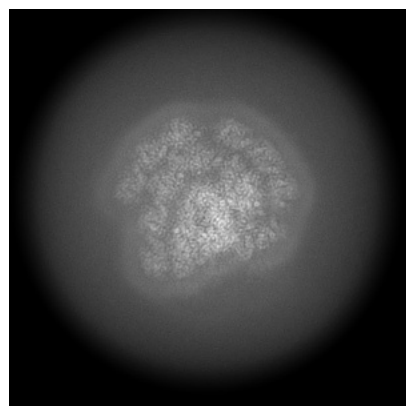
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33683. These allow visual inspection of the internal detail of the map and identification of artifacts.

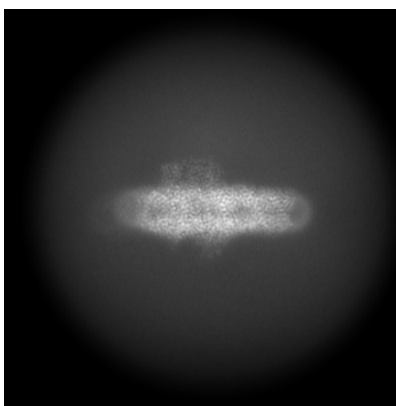
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

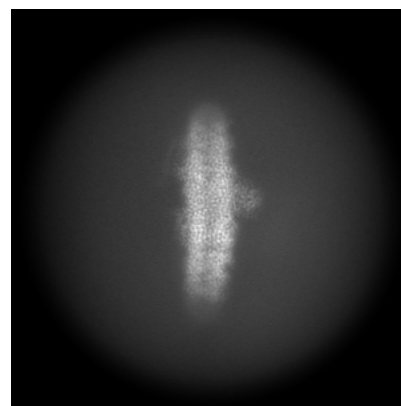
6.1.1 Primary map



X

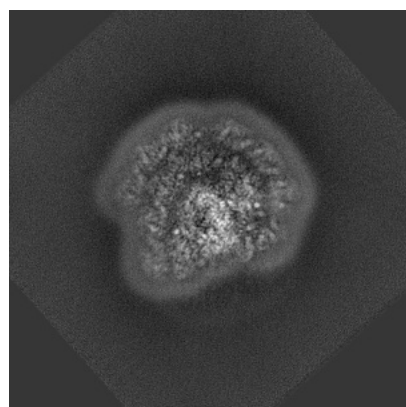


Y

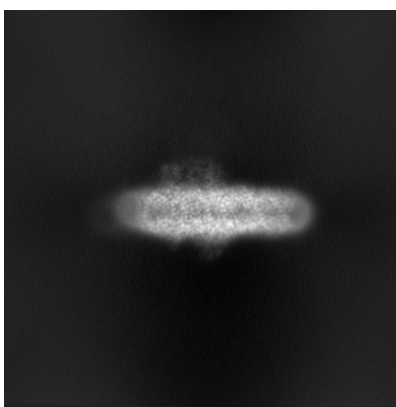


Z

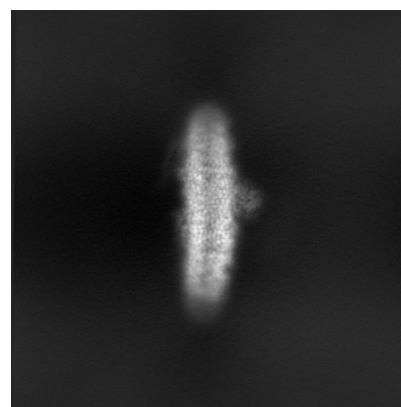
6.1.2 Raw map



X



Y

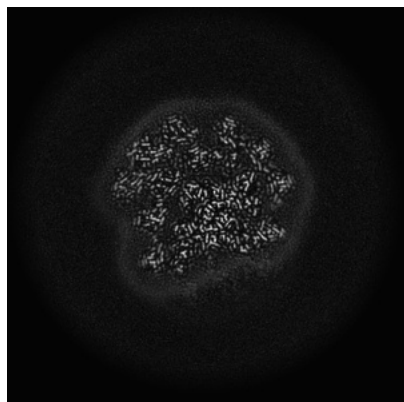


Z

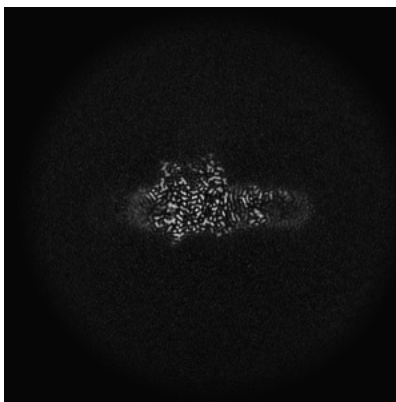
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

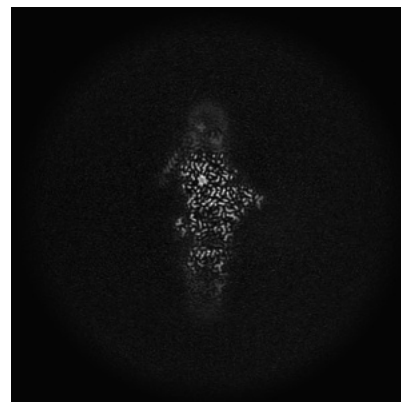
6.2.1 Primary map



X Index: 200

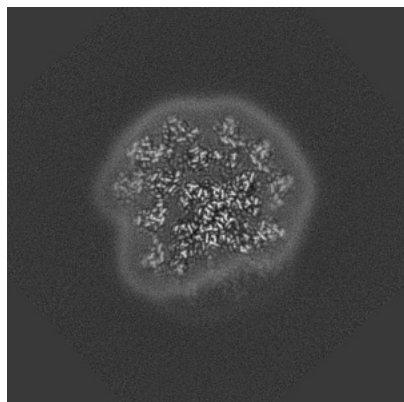


Y Index: 200

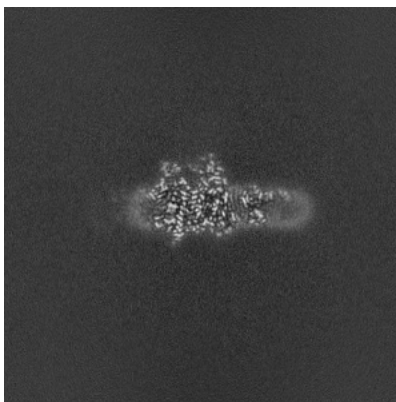


Z Index: 200

6.2.2 Raw map



X Index: 200



Y Index: 200

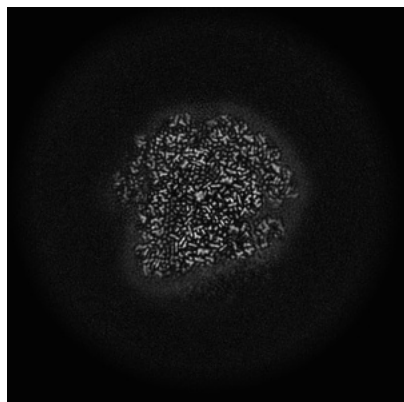


Z Index: 200

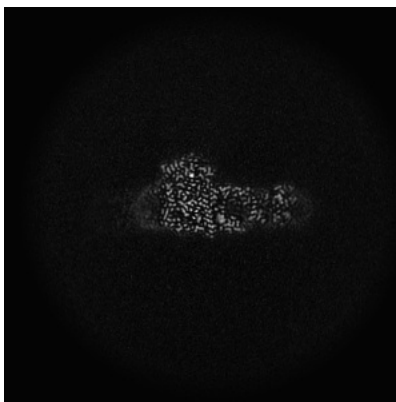
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

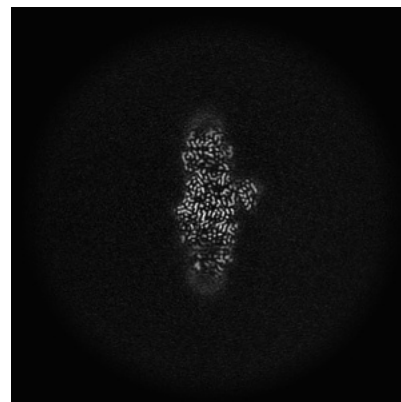
6.3.1 Primary map



X Index: 210

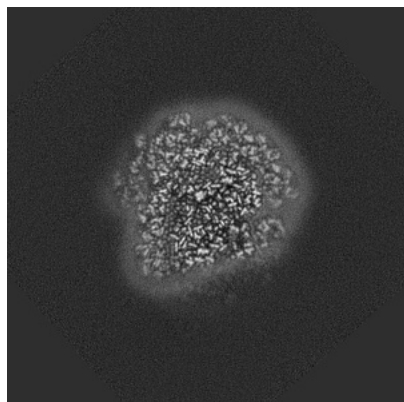


Y Index: 212

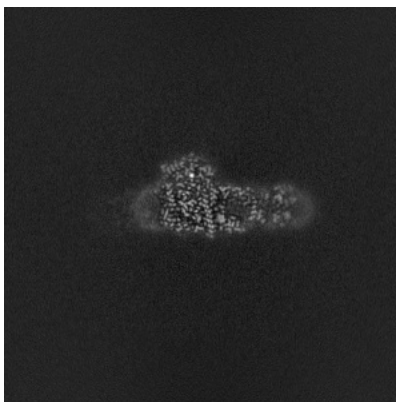


Z Index: 174

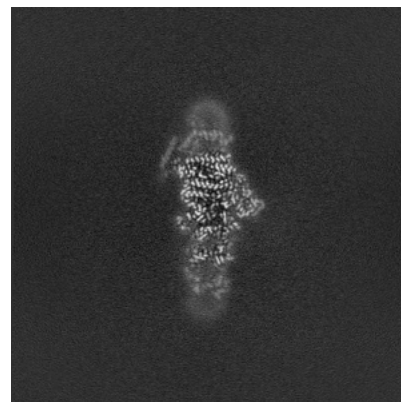
6.3.2 Raw map



X Index: 210



Y Index: 212

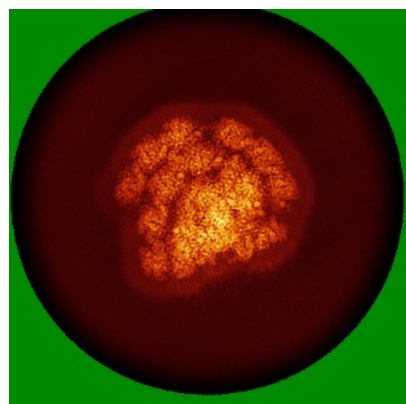


Z Index: 206

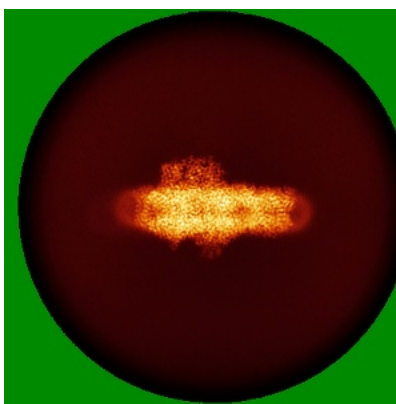
The images above show the largest variance slices of the map in three orthogonal directions.

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

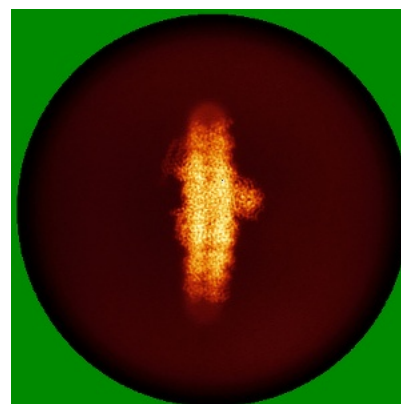
6.4.1 Primary map



X

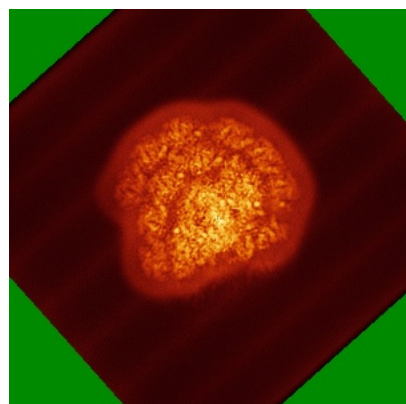


Y

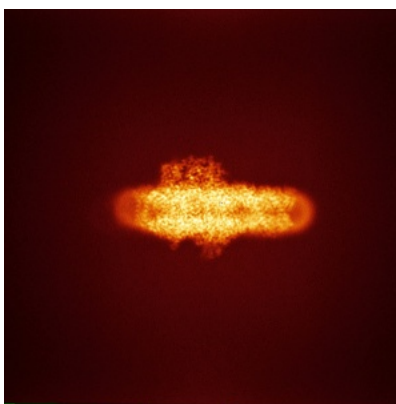


Z

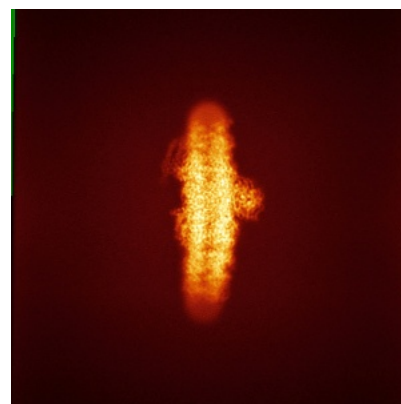
6.4.2 Raw map



X



Y

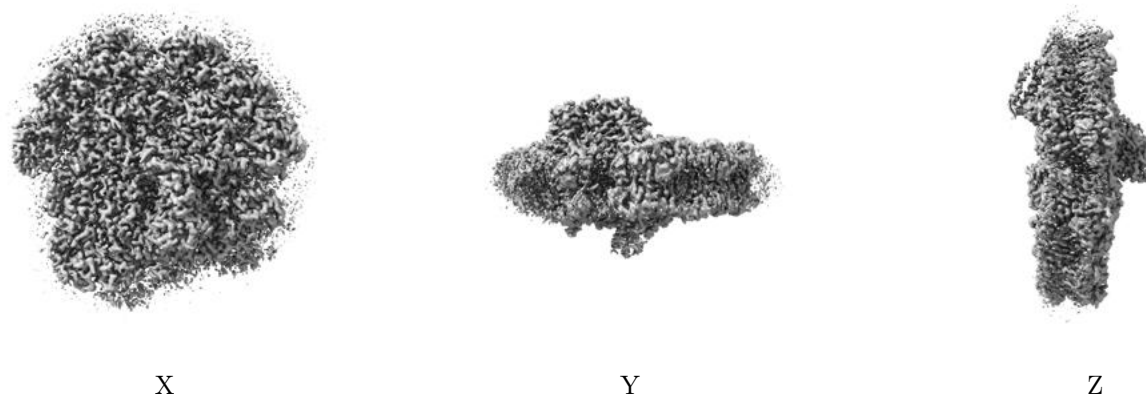


Z

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.

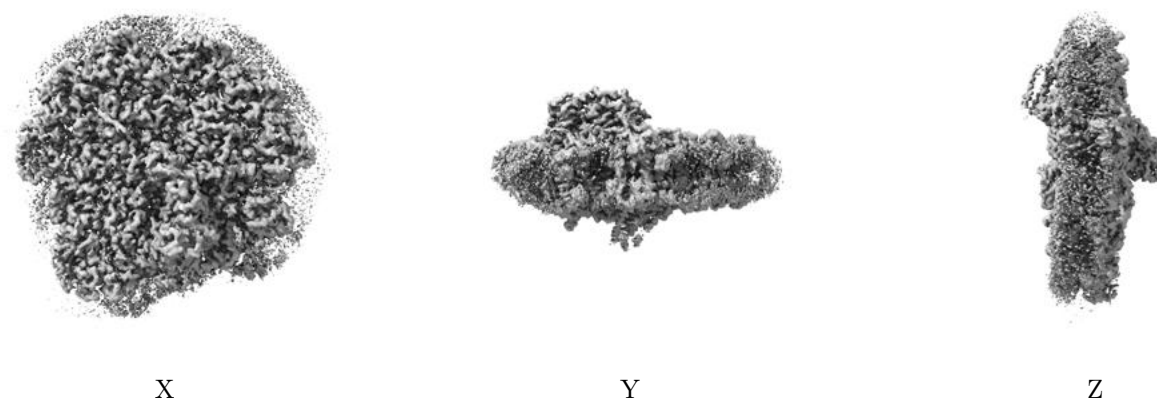
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

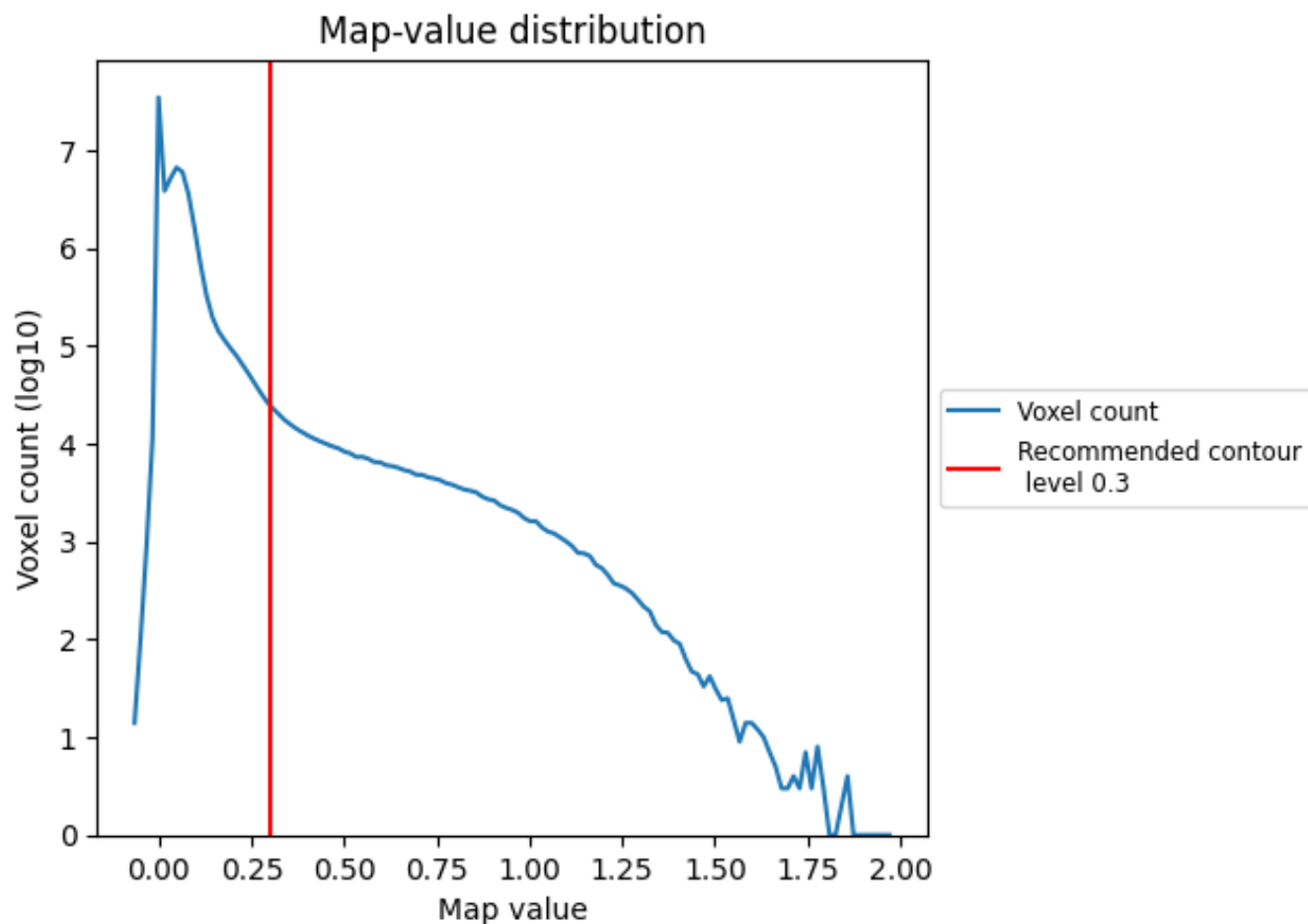
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

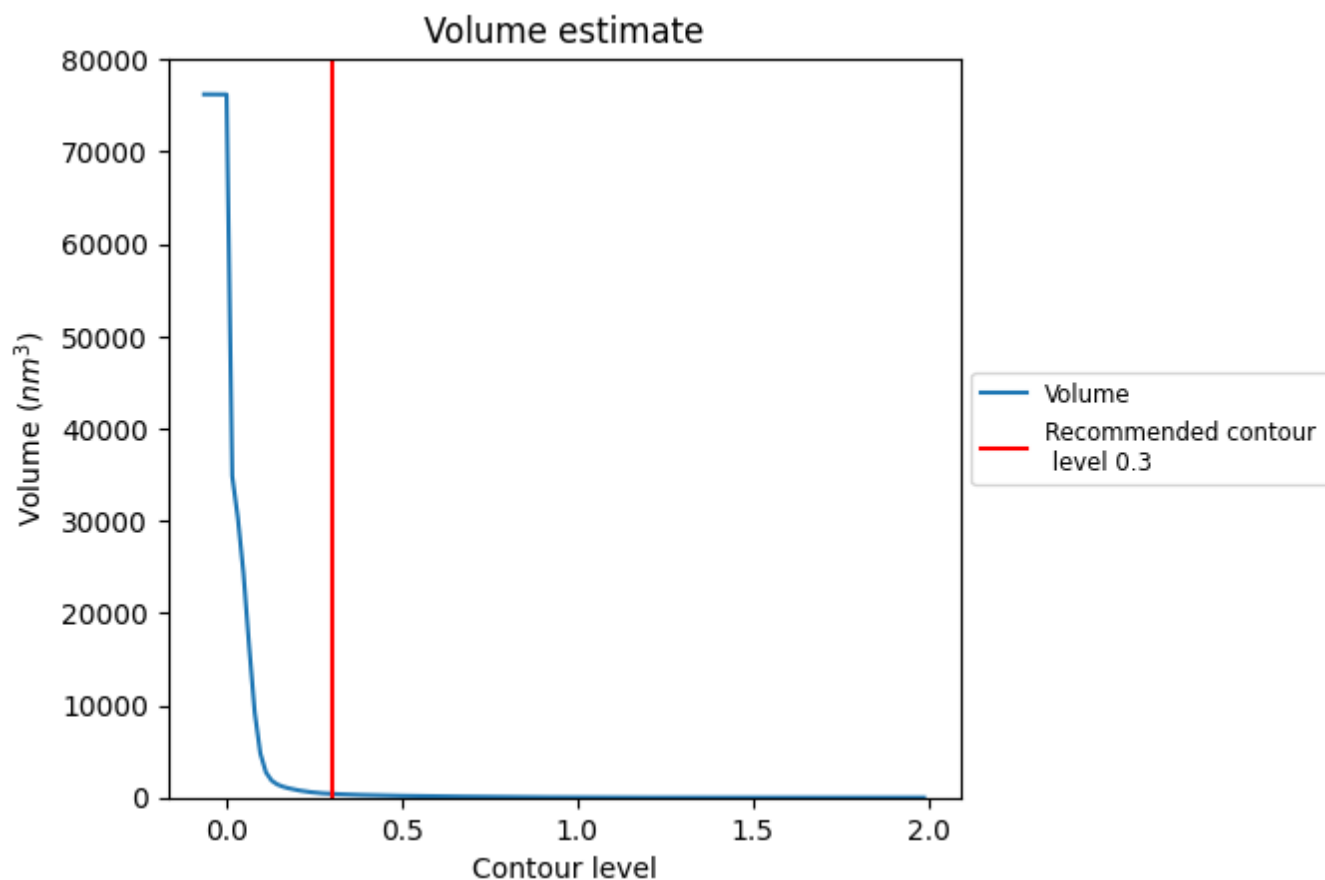
This section contains the results of statistical analysis of the map.

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.

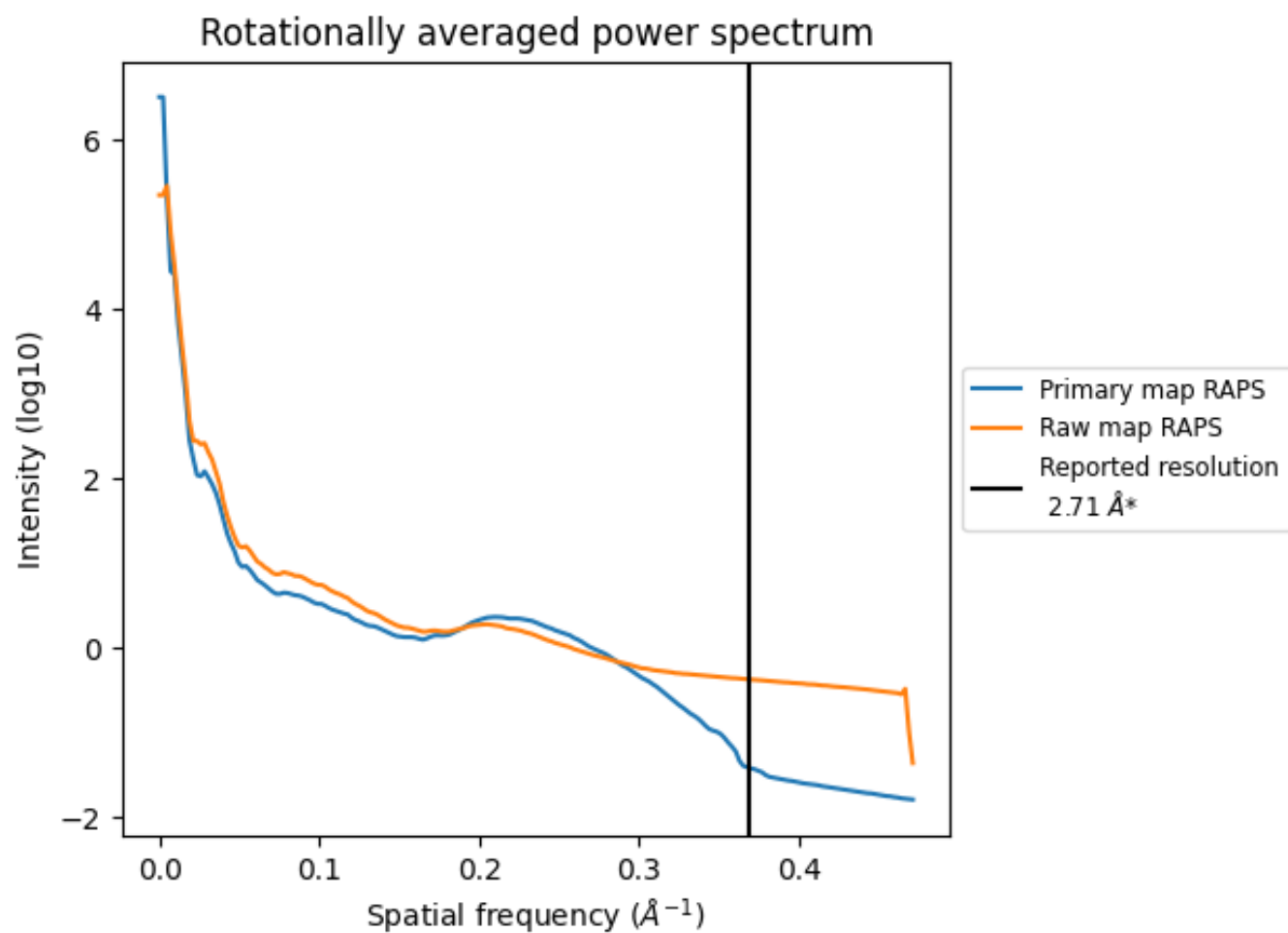
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 402 nm³; this corresponds to an approximate mass of 363 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 ⓘ

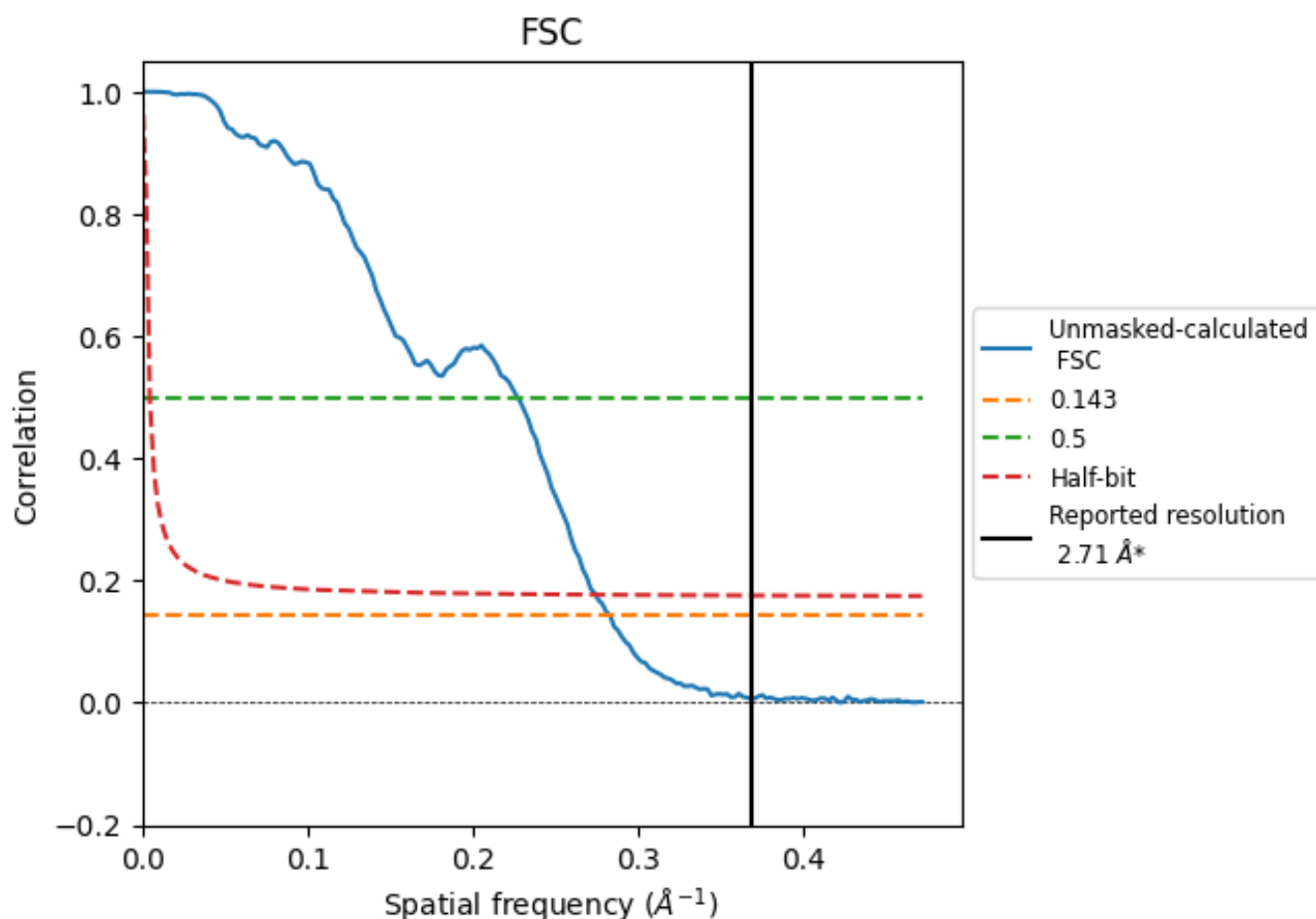


*Reported resolution corresponds to spatial frequency of 0.369 Å⁻¹

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 0.369 Å⁻¹

8.2 Resolution estimates [i](#)

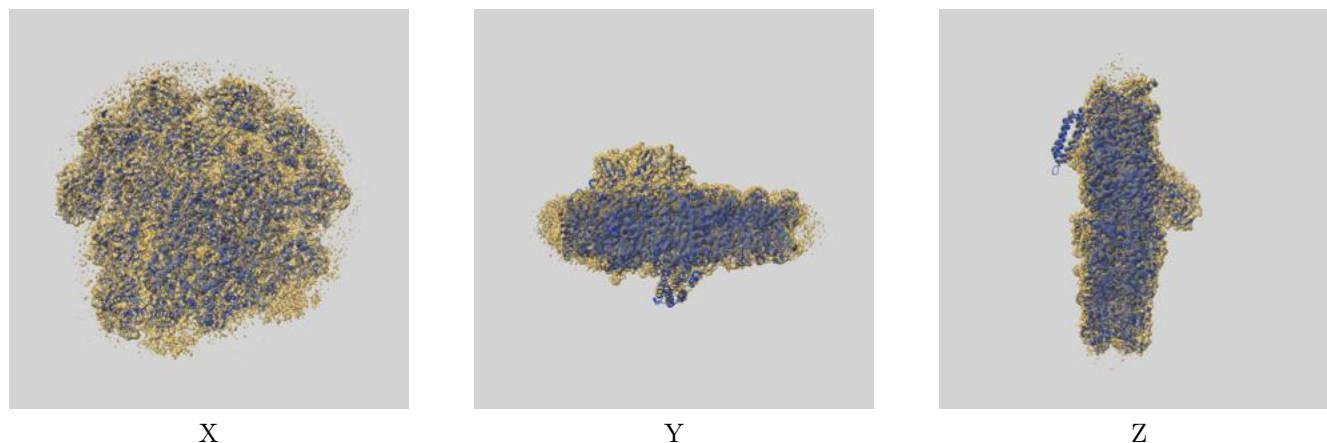
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.41	3.65

*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 3.54 differs from the reported value 2.71 by more than 10 %

9 Map-model fit [i](#)

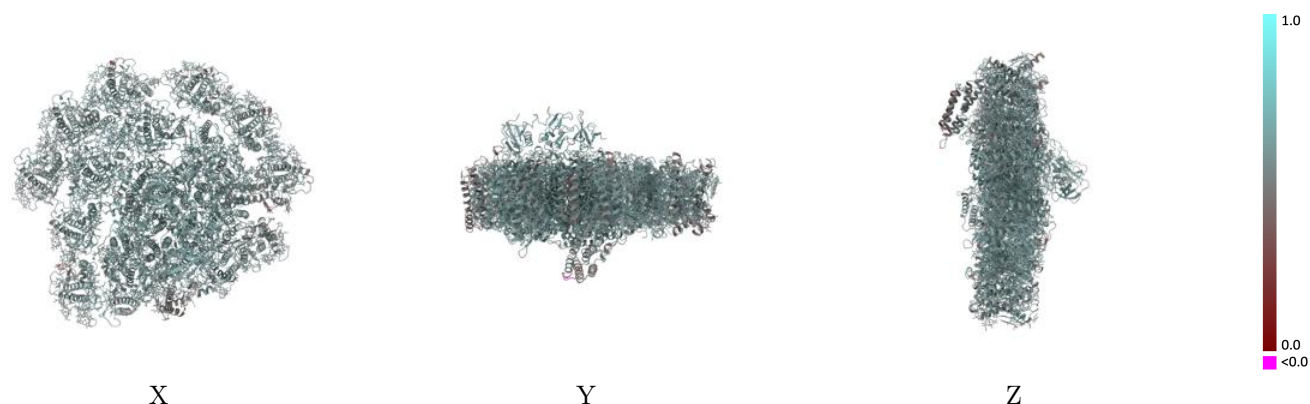
This section contains information regarding the fit between EMDB map EMD-33683 and PDB model 7Y8A. Per-residue inclusion information can be found in [section 3](#) on [page 32](#).

9.1 Map-model overlay [i](#)



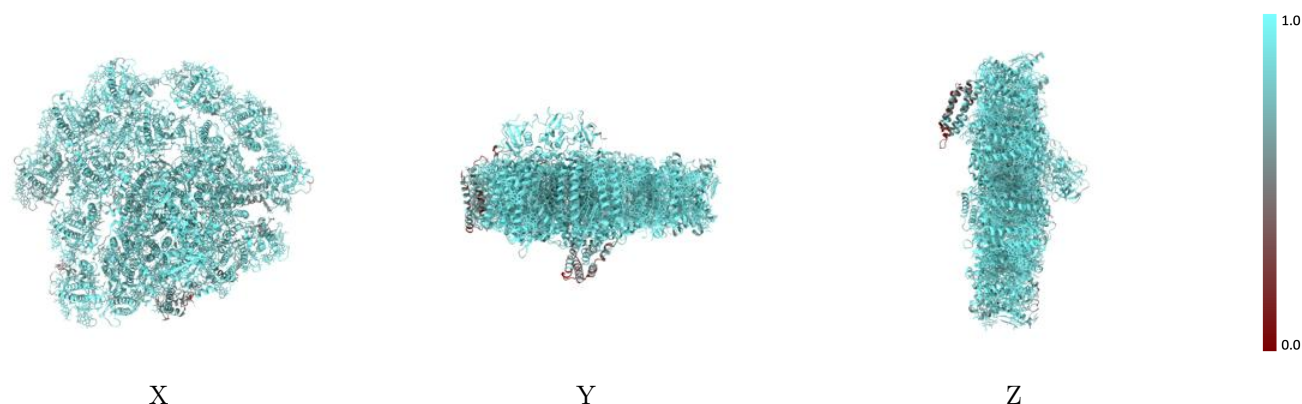
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



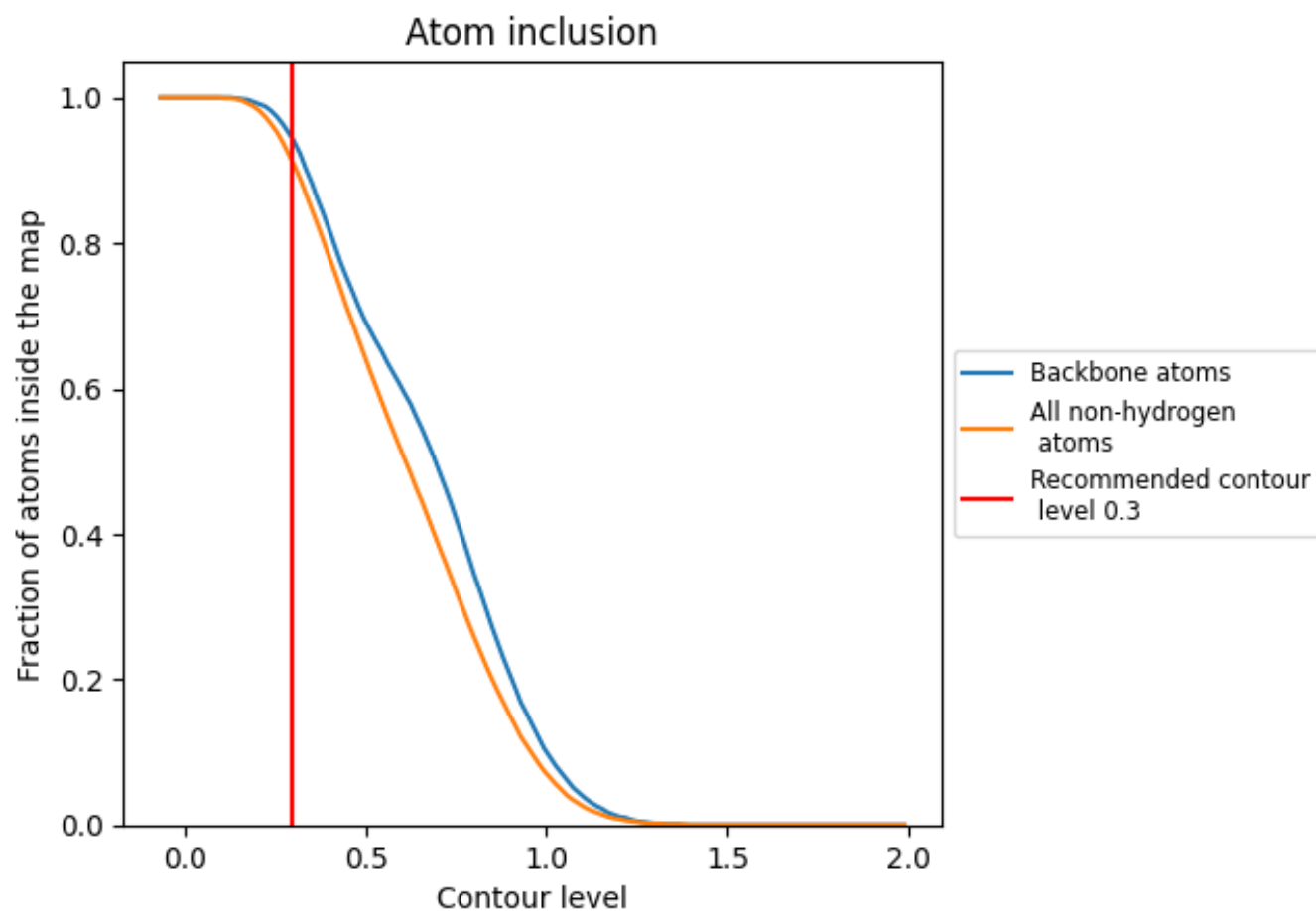
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9110	 0.5810
1	 0.8440	 0.5270
2	 0.9210	 0.5810
3	 0.9450	 0.6080
4	 0.9400	 0.5980
5	 0.8730	 0.5370
6	 0.9080	 0.5580
7	 0.8780	 0.5340
8	 0.8870	 0.5560
9	 0.7800	 0.5420
A	 0.9690	 0.6140
B	 0.9730	 0.6220
C	 0.9680	 0.6020
D	 0.9470	 0.5840
E	 0.8740	 0.5850
F	 0.9230	 0.5960
I	 0.9760	 0.6120
J	 0.9610	 0.6110
K	 0.8740	 0.5370
L	 0.8760	 0.5640
M	 0.9430	 0.5940
O	 0.5870	 0.4700
R	 0.9360	 0.5890
X	 0.5590	 0.4670
Z	 0.8960	 0.5790
a	 0.9040	 0.5640
b	 0.9200	 0.5640

