



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 07:18 AM UTC

PDB ID : 7Y7B / pdb_00007y7b
EMDB ID : EMD-33659
Title : Cryo-EM structure of cryptophyte photosystem I
Authors : Zhao, L.S.; Li, K.; Zhang, Y.Z.; Liu, L.N.
Deposited on : 2022-06-22
Resolution : 2.66 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:

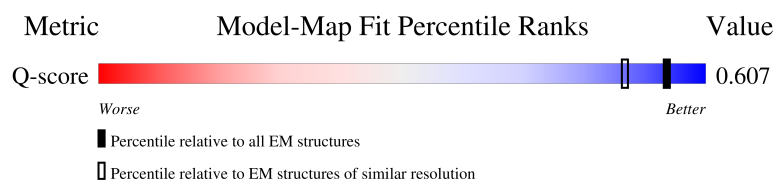
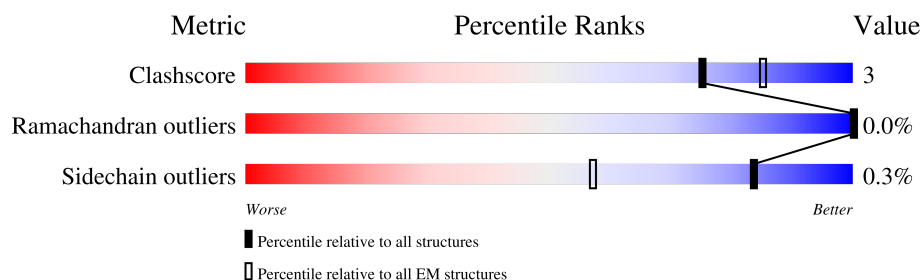
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 2.66 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.



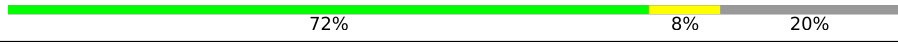
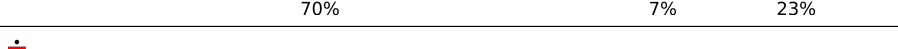
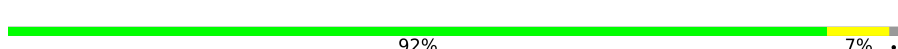
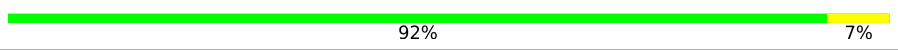
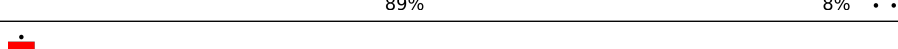
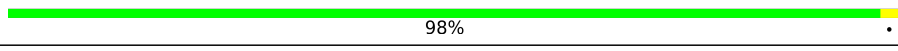
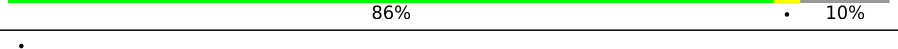
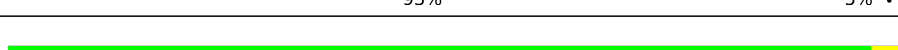
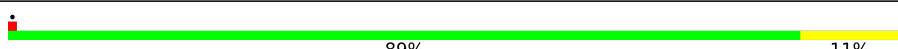
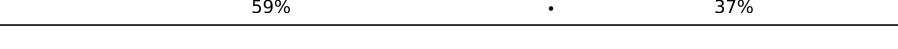
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9119 (2.16 - 3.16)

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	5% 66% 14% 19%
2	2	216	70% 7% 22%
3	3	236	72% 5% 24%
4	4	217	76% 5% 19%

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Mol	Chain	Length	Quality of chain
5	5	229	
6	6	215	
7	7	230	
8	8	227	
9	9	220	
10	A	752	
11	B	734	
12	C	81	
13	D	141	
14	E	64	
15	F	183	
16	I	36	
17	J	42	
18	K	87	
19	L	153	
20	M	30	
21	O	99	
22	R	133	
23	X	164	
24	Z	242	
25	a	215	
25	d	215	
26	b	218	
27	c	257	
28	e	208	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	1	601	X	-	-	-
29	CLA	1	602	X	-	-	-
29	CLA	1	603	X	-	-	-
29	CLA	1	604	X	-	-	-
29	CLA	1	605	X	-	-	-
29	CLA	1	606	X	-	-	-
29	CLA	1	607	X	-	-	-
29	CLA	1	608	X	-	-	-
29	CLA	1	609	X	-	-	-
29	CLA	1	611	X	-	-	-
29	CLA	1	612	X	-	-	-
29	CLA	1	613	X	-	-	-
29	CLA	2	601	X	-	-	-
29	CLA	2	602	X	-	-	-
29	CLA	2	603	X	-	-	-
29	CLA	2	604	X	-	-	-
29	CLA	2	605	X	-	-	-
29	CLA	2	606	X	-	-	-
29	CLA	2	607	X	-	-	-
29	CLA	2	608	X	-	-	-
29	CLA	2	609	X	-	-	-
29	CLA	2	611	X	-	-	-
29	CLA	2	612	X	-	-	-
29	CLA	3	601	X	-	-	-
29	CLA	3	602	X	-	-	-
29	CLA	3	603	X	-	-	-
29	CLA	3	604	X	-	-	-
29	CLA	3	605	X	-	-	-
29	CLA	3	607	X	-	-	-
29	CLA	3	608	X	-	-	-
29	CLA	3	609	X	-	-	-
29	CLA	3	610	X	-	-	-
29	CLA	3	611	X	-	-	-
29	CLA	3	612	X	-	-	-
29	CLA	4	601	X	-	-	-
29	CLA	4	602	X	-	-	-
29	CLA	4	603	X	-	-	-
29	CLA	4	604	X	-	-	-
29	CLA	4	606	X	-	-	-
29	CLA	4	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	4	608	X	-	-	-
29	CLA	4	609	X	-	-	-
29	CLA	4	610	X	-	-	-
29	CLA	4	611	X	-	-	-
29	CLA	5	601	X	-	-	-
29	CLA	5	602	X	-	-	-
29	CLA	5	603	X	-	-	-
29	CLA	5	604	X	-	-	-
29	CLA	5	605	X	-	-	-
29	CLA	5	606	X	-	-	-
29	CLA	5	607	X	-	-	-
29	CLA	5	608	X	-	-	-
29	CLA	5	609	X	-	-	-
29	CLA	5	611	X	-	-	-
29	CLA	5	612	X	-	-	-
29	CLA	5	613	X	-	-	-
29	CLA	6	601	X	-	-	-
29	CLA	6	602	X	-	-	-
29	CLA	6	603	X	-	-	-
29	CLA	6	604	X	-	-	-
29	CLA	6	605	X	-	-	-
29	CLA	6	606	X	-	-	-
29	CLA	6	607	X	-	-	-
29	CLA	6	608	X	-	-	-
29	CLA	6	609	X	-	-	-
29	CLA	6	611	X	-	-	-
29	CLA	6	612	X	-	-	-
29	CLA	7	601	X	-	-	-
29	CLA	7	602	X	-	-	-
29	CLA	7	603	X	-	-	-
29	CLA	7	604	X	-	-	-
29	CLA	7	605	X	-	-	-
29	CLA	7	607	X	-	-	-
29	CLA	7	608	X	-	-	-
29	CLA	7	609	X	-	-	-
29	CLA	7	611	X	-	-	-
29	CLA	7	612	X	-	-	-
29	CLA	8	601	X	-	-	-
29	CLA	8	602	X	-	-	-
29	CLA	8	603	X	-	-	-
29	CLA	8	604	X	-	-	-
29	CLA	8	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	8	606	X	-	-	-
29	CLA	8	607	X	-	-	-
29	CLA	8	608	X	-	-	-
29	CLA	8	615	X	-	-	-
29	CLA	9	601	X	-	-	-
29	CLA	9	602	X	-	-	-
29	CLA	9	603	X	-	-	-
29	CLA	9	604	X	-	-	-
29	CLA	9	605	X	-	-	-
29	CLA	9	606	X	-	-	-
29	CLA	9	607	X	-	-	-
29	CLA	9	608	X	-	-	-
29	CLA	9	609	X	-	-	-
29	CLA	9	611	X	-	-	-
29	CLA	9	612	X	-	-	-
29	CLA	9	613	X	-	-	-
29	CLA	9	614	X	-	-	-
29	CLA	A	801	X	-	-	-
29	CLA	A	802	X	-	-	-
29	CLA	A	803	X	-	-	-
29	CLA	A	804	X	-	-	-
29	CLA	A	805	X	-	-	-
29	CLA	A	806	X	-	-	-
29	CLA	A	807	X	-	-	-
29	CLA	A	808	X	-	-	-
29	CLA	A	809	X	-	-	-
29	CLA	A	810	X	-	-	-
29	CLA	A	811	X	-	-	-
29	CLA	A	812	X	-	-	-
29	CLA	A	813	X	-	-	-
29	CLA	A	814	X	-	-	-
29	CLA	A	815	X	-	-	-
29	CLA	A	816	X	-	-	-
29	CLA	A	817	X	-	-	-
29	CLA	A	818	X	-	-	-
29	CLA	A	819	X	-	-	-
29	CLA	A	820	X	-	-	-
29	CLA	A	821	X	-	-	-
29	CLA	A	822	X	-	-	-
29	CLA	A	823	X	-	-	-
29	CLA	A	824	X	-	-	-
29	CLA	A	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	826	X	-	-	-
29	CLA	A	827	X	-	-	-
29	CLA	A	828	X	-	-	-
29	CLA	A	829	X	-	-	-
29	CLA	A	830	X	-	-	-
29	CLA	A	831	X	-	-	-
29	CLA	A	832	X	-	-	-
29	CLA	A	833	X	-	-	-
29	CLA	A	834	X	-	-	-
29	CLA	A	835	X	-	-	-
29	CLA	A	836	X	-	-	-
29	CLA	A	837	X	-	-	-
29	CLA	A	838	X	-	-	-
29	CLA	A	839	X	-	-	-
29	CLA	A	840	X	-	-	-
29	CLA	A	841	X	-	-	-
29	CLA	A	842	X	-	-	-
29	CLA	A	843	X	-	-	-
29	CLA	A	844	X	-	-	-
29	CLA	B	802	X	-	-	-
29	CLA	B	803	X	-	-	-
29	CLA	B	804	X	-	-	-
29	CLA	B	805	X	-	-	-
29	CLA	B	806	X	-	-	-
29	CLA	B	807	X	-	-	-
29	CLA	B	808	X	-	-	-
29	CLA	B	809	X	-	-	-
29	CLA	B	810	X	-	-	-
29	CLA	B	811	X	-	-	-
29	CLA	B	812	X	-	-	-
29	CLA	B	813	X	-	-	-
29	CLA	B	814	X	-	-	-
29	CLA	B	815	X	-	-	-
29	CLA	B	816	X	-	-	-
29	CLA	B	817	X	-	-	-
29	CLA	B	818	X	-	-	-
29	CLA	B	819	X	-	-	-
29	CLA	B	820	X	-	-	-
29	CLA	B	821	X	-	-	-
29	CLA	B	822	X	-	-	-
29	CLA	B	823	X	-	-	-
29	CLA	B	824	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	B	825	X	-	-	-
29	CLA	B	826	X	-	-	-
29	CLA	B	827	X	-	-	-
29	CLA	B	828	X	-	-	-
29	CLA	B	829	X	-	-	-
29	CLA	B	830	X	-	-	-
29	CLA	B	831	X	-	-	-
29	CLA	B	832	X	-	-	-
29	CLA	B	833	X	-	-	-
29	CLA	B	834	X	-	-	-
29	CLA	B	835	X	-	-	-
29	CLA	B	836	X	-	-	-
29	CLA	B	837	X	-	-	-
29	CLA	B	838	X	-	-	-
29	CLA	B	839	X	-	-	-
29	CLA	B	840	X	-	-	-
29	CLA	B	841	X	-	-	-
29	CLA	F	202	X	-	-	-
29	CLA	F	203	X	-	-	-
29	CLA	F	204	X	-	-	-
29	CLA	J	102	X	-	-	-
29	CLA	K	101	X	-	-	-
29	CLA	K	102	X	-	-	-
29	CLA	L	201	X	-	-	-
29	CLA	L	202	X	-	-	-
29	CLA	L	203	X	-	-	-
29	CLA	L	204	X	-	-	-
29	CLA	L	207	X	-	-	-
29	CLA	O	201	X	-	-	-
29	CLA	O	202	X	-	-	-
29	CLA	O	203	X	-	-	-
29	CLA	R	202	X	-	-	-
29	CLA	Z	301	X	-	-	-
29	CLA	Z	304	X	-	-	-
29	CLA	Z	305	X	-	-	-
29	CLA	Z	306	X	-	-	-
29	CLA	a	601	X	-	-	-
29	CLA	a	602	X	-	-	-
29	CLA	a	603	X	-	-	-
29	CLA	a	604	X	-	-	-
29	CLA	a	605	X	-	-	-
29	CLA	a	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	a	607	X	-	-	-
29	CLA	a	608	X	-	-	-
29	CLA	a	609	X	-	-	-
29	CLA	a	611	X	-	-	-
29	CLA	a	612	X	-	-	-
29	CLA	b	601	X	-	-	-
29	CLA	b	602	X	-	-	-
29	CLA	b	603	X	-	-	-
29	CLA	b	604	X	-	-	-
29	CLA	b	606	X	-	-	-
29	CLA	b	607	X	-	-	-
29	CLA	b	608	X	-	-	-
29	CLA	b	610	X	-	-	-
29	CLA	b	611	X	-	-	-
29	CLA	c	601	X	-	-	-
29	CLA	c	602	X	-	-	-
29	CLA	c	603	X	-	-	-
29	CLA	c	604	X	-	-	-
29	CLA	c	605	X	-	-	-
29	CLA	c	606	X	-	-	-
29	CLA	c	607	X	-	-	-
29	CLA	c	608	X	-	-	-
29	CLA	c	609	X	-	-	-
29	CLA	c	612	X	-	-	-
29	CLA	c	613	X	-	-	-
29	CLA	c	614	X	-	-	-
29	CLA	d	601	X	-	-	-
29	CLA	d	602	X	-	-	-
29	CLA	d	603	X	-	-	-
29	CLA	d	604	X	-	-	-
29	CLA	d	605	X	-	-	-
29	CLA	d	606	X	-	-	-
29	CLA	d	607	X	-	-	-
29	CLA	d	608	X	-	-	-
29	CLA	d	609	X	-	-	-
29	CLA	d	611	X	-	-	-
29	CLA	d	612	X	-	-	-
29	CLA	e	601	X	-	-	-
29	CLA	e	602	X	-	-	-
29	CLA	e	603	X	-	-	-
29	CLA	e	604	X	-	-	-
29	CLA	e	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	e	607	X	-	-	-
29	CLA	e	608	X	-	-	-
29	CLA	e	610	X	-	-	-
29	CLA	e	611	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 60515 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	150	Total	C	N	O	S	0	0
			1143	746	184	211	2		

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

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

- Molecule 21 is a protein called Psao.

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

- Molecule 22 is a protein called PsaR.

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

- Molecule 23 is a protein called 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-13/10.

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

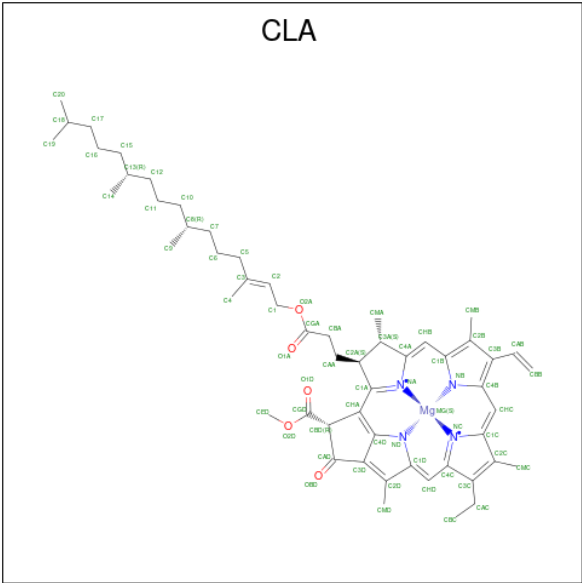
- Molecule 27 is a protein called ACPI-9.

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

- Molecule 28 is a protein called ACPI-11.

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

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



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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
29	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
29	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	9	1	Total 64	C 54	Mg 1	N 4	O 5	0
29	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	9	1	Total 55	C 45	Mg 1	N 4	O 5	0

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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

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

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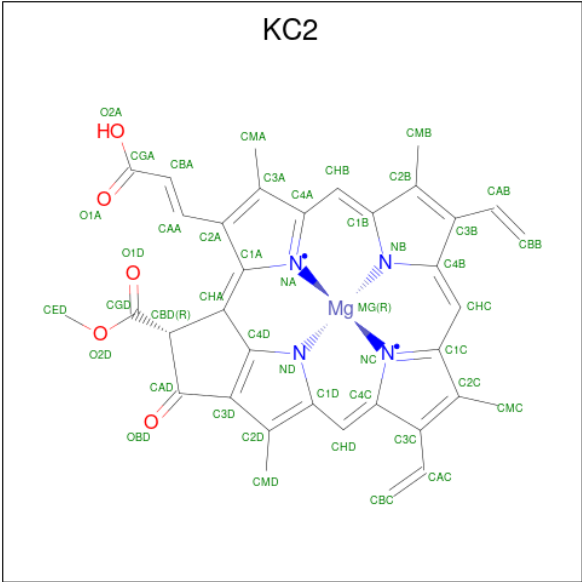
Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
29	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
29	c	1	Total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

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

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



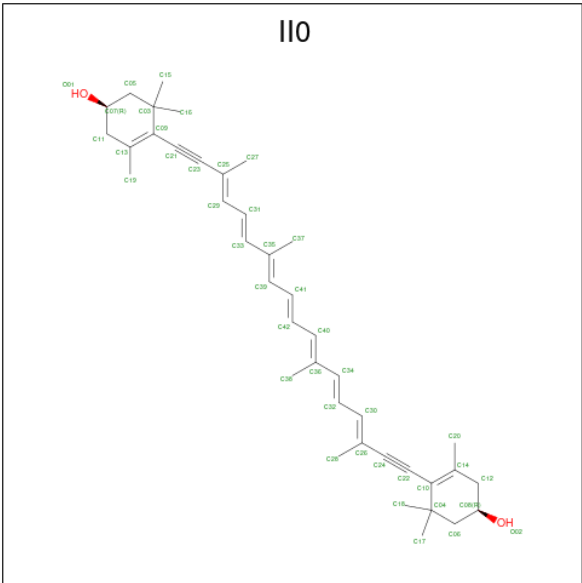
Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	6	1	Total	C	Mg	N	O	0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

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

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



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

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

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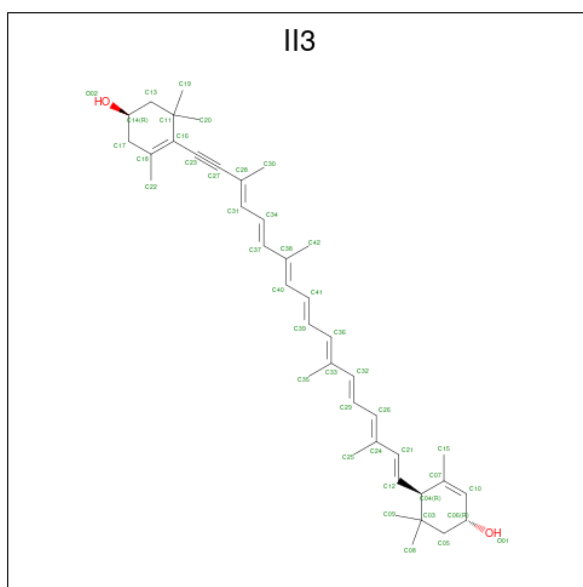
Mol	Chain	Residues	Atoms			AltConf
31	7	1	Total 42	C 40	O 2	0
31	7	1	Total 42	C 40	O 2	0
31	7	1	Total 42	C 40	O 2	0
31	8	1	Total 42	C 40	O 2	0
31	8	1	Total 42	C 40	O 2	0
31	8	1	Total 42	C 40	O 2	0
31	8	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O 2	0
31	9	1	Total 42	C 40	O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

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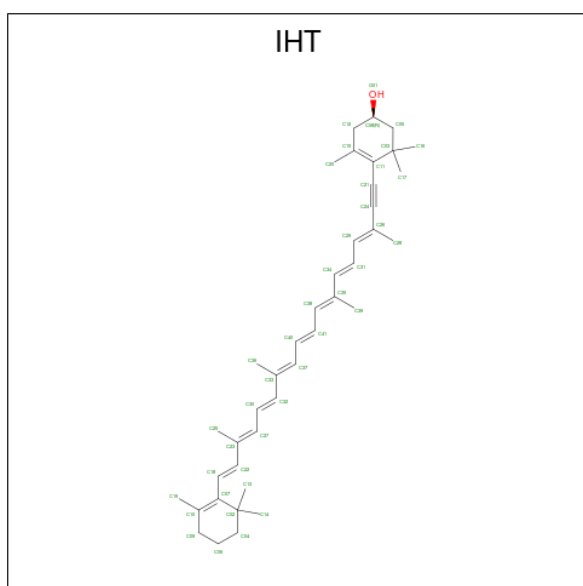
Mol	Chain	Residues	Atoms			AltConf
31	b	1	Total	C	O	0
			42	40	2	
31	b	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	c	1	Total	C	O	0
			42	40	2	
31	d	1	Total	C	O	0
			42	40	2	
31	d	1	Total	C	O	0
			42	40	2	
31	d	1	Total	C	O	0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

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



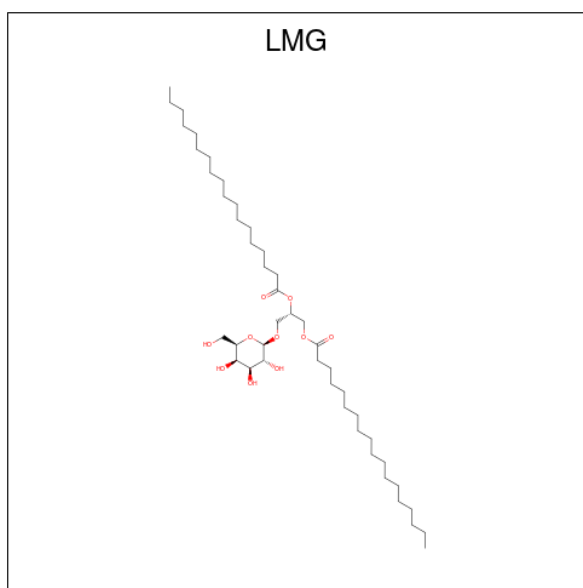
Mol	Chain	Residues	Atoms			AltConf
32	1	1	Total	C	O	0
			42	40	2	
32	b	1	Total	C	O	0
			42	40	2	
32	e	1	Total	C	O	0
			42	40	2	

- Molecule 33 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).



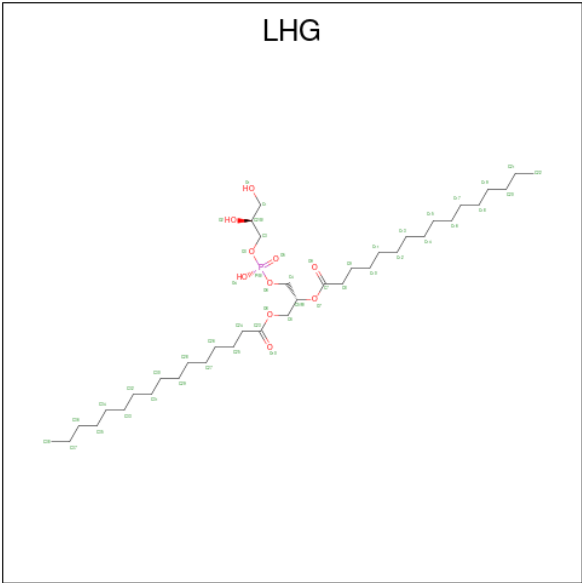
Mol	Chain	Residues	Atoms			AltConf
33	1	1	Total	C	O	0
			41	40	1	
33	2	1	Total	C	O	0
			41	40	1	
33	5	1	Total	C	O	0
			41	40	1	
33	6	1	Total	C	O	0
			41	40	1	
33	8	1	Total	C	O	0
			41	40	1	
33	9	1	Total	C	O	0
			41	40	1	
33	K	1	Total	C	O	0
			41	40	1	
33	L	1	Total	C	O	0
			41	40	1	
33	Z	1	Total	C	O	0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

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
34	2	1	Total	C	O	0
			36	26	10	
34	3	1	Total	C	O	0
			30	20	10	
34	3	1	Total	C	O	0
			32	22	10	
34	6	1	Total	C	O	0
			32	22	10	
34	8	1	Total	C	O	0
			52	42	10	
34	F	1	Total	C	O	0
			32	22	10	
34	I	1	Total	C	O	0
			51	41	10	

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



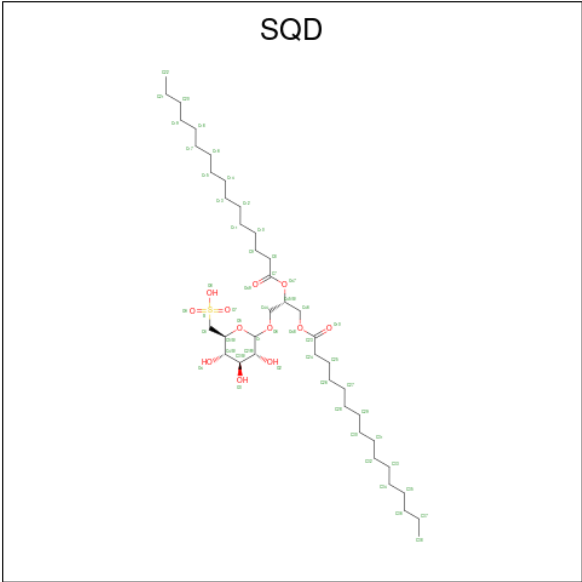
Mol	Chain	Residues	Atoms				AltConf
35	2	1	Total	C	O	P	0
			22	12	9	1	
35	2	1	Total	C	O	P	0
			39	28	10	1	
35	2	1	Total	C	O	P	0
			42	31	10	1	
35	3	1	Total	C	O	P	0
			49	38	10	1	

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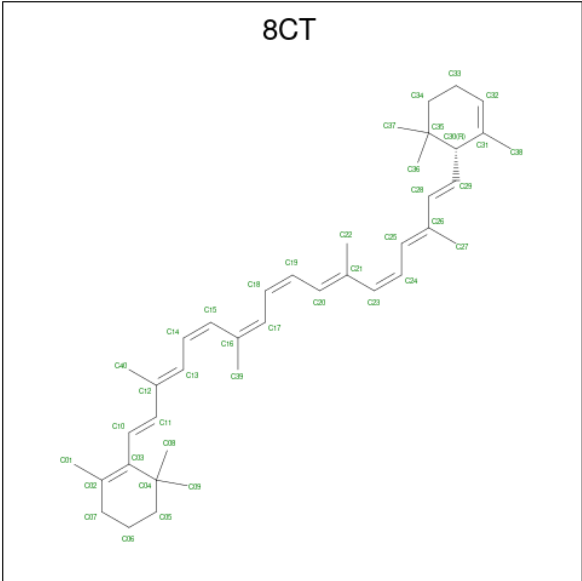
Mol	Chain	Residues	Atoms				AltConf
35	3	1	Total	C	O	P	0
			34	23	10	1	
35	3	1	Total	C	O	P	0
			49	38	10	1	
35	4	1	Total	C	O	P	0
			47	36	10	1	
35	4	1	Total	C	O	P	0
			45	34	10	1	
35	5	1	Total	C	O	P	0
			23	12	10	1	
35	6	1	Total	C	O	P	0
			35	24	10	1	
35	7	1	Total	C	O	P	0
			31	20	10	1	
35	7	1	Total	C	O	P	0
			39	28	10	1	
35	8	1	Total	C	O	P	0
			33	22	10	1	
35	A	1	Total	C	O	P	0
			49	38	10	1	
35	A	1	Total	C	O	P	0
			39	28	10	1	
35	B	1	Total	C	O	P	0
			45	34	10	1	
35	L	1	Total	C	O	P	0
			34	23	10	1	
35	Z	1	Total	C	O	P	0
			46	35	10	1	
35	a	1	Total	C	O	P	0
			29	18	10	1	
35	b	1	Total	C	O	P	0
			49	38	10	1	
35	c	1	Total	C	O	P	0
			29	18	10	1	
35	d	1	Total	C	O	P	0
			23	13	9	1	
35	d	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 36 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
36	3	1	Total	C	O	S	0
			42	29	12	1	
36	O	1	Total	C	O	S	0
			29	16	12	1	

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



Mol	Chain	Residues	Atoms		AltConf
37	4	1	Total	C	0
			40	40	

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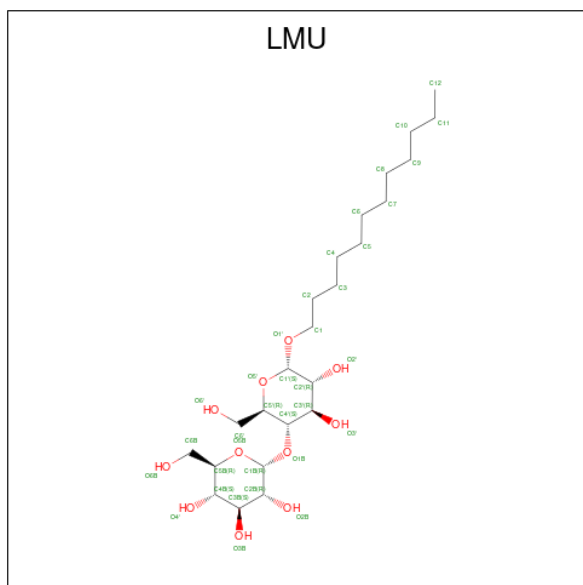
Mol	Chain	Residues	Atoms	AltConf
37	7	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	A	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	B	1	Total C 40 40	0
37	F	1	Total C 40 40	0
37	I	1	Total C 40 40	0
37	J	1	Total C 40 40	0
37	K	1	Total C 40 40	0
37	L	1	Total C 40 40	0
37	M	1	Total C 40 40	0
37	R	1	Total C 40 40	0
37	R	1	Total C 40 40	0
37	Z	1	Total C 40 40	0

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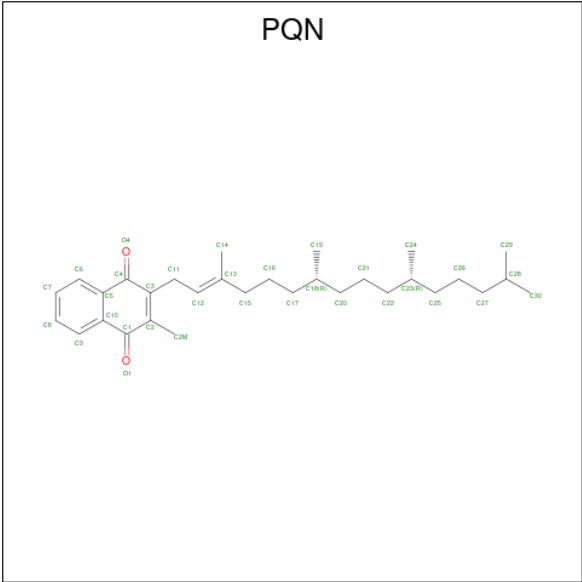
Mol	Chain	Residues	Atoms	AltConf
37	Z	1	Total C 40 40	0
37	b	1	Total C 40 40	0
37	e	1	Total C 40 40	0

- Molecule 38 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



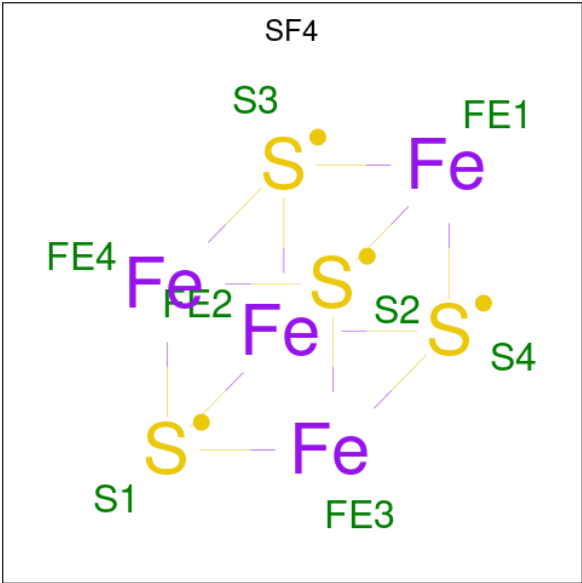
Mol	Chain	Residues	Atoms	AltConf
38	4	1	Total C O 35 24 11	0
38	7	1	Total C O 35 24 11	0
38	J	1	Total C O 31 20 11	0
38	O	1	Total C O 30 19 11	0
38	e	1	Total C O 31 20 11	0

- Molecule 39 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 40 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



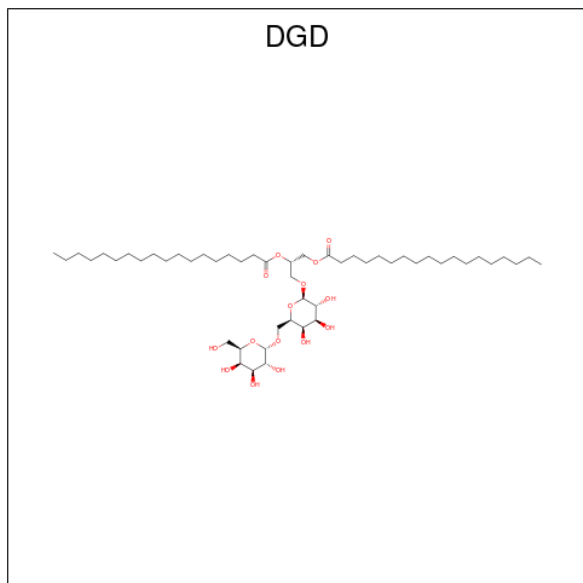
Mol	Chain	Residues	Atoms			AltConf
40	B	1	Total	Fe	S	0
			8	4	4	
40	C	1	Total	Fe	S	0
			8	4	4	

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

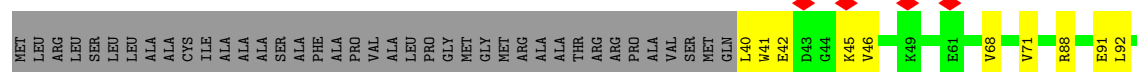
- Molecule 41 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



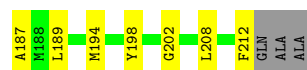
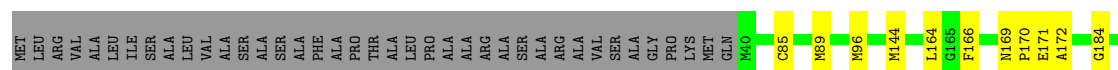
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
41	B	1	59	44	15	0
41	Z	1	60	45	15	0



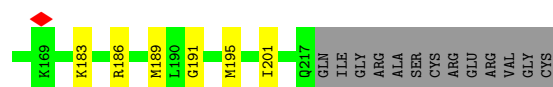
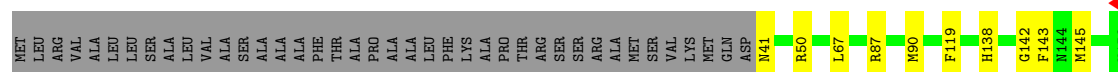
- Molecule 5: ACPI-5



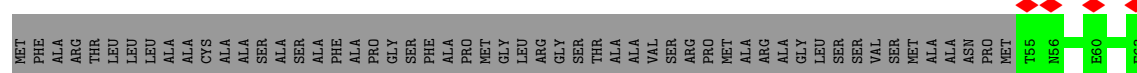
- Molecule 6: ACPI-6



- Molecule 7: ACPI-7

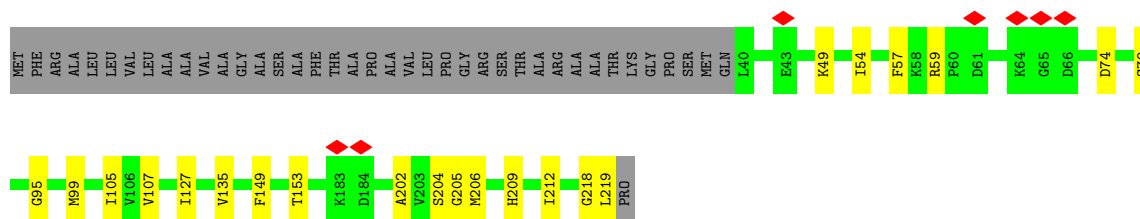


- Molecule 8: ACPI-8



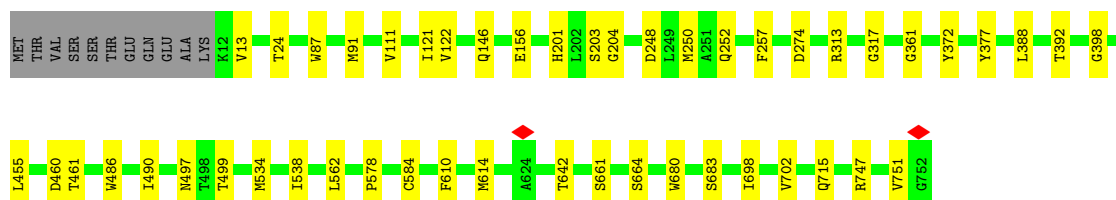
- Molecule 9: ACPI-12





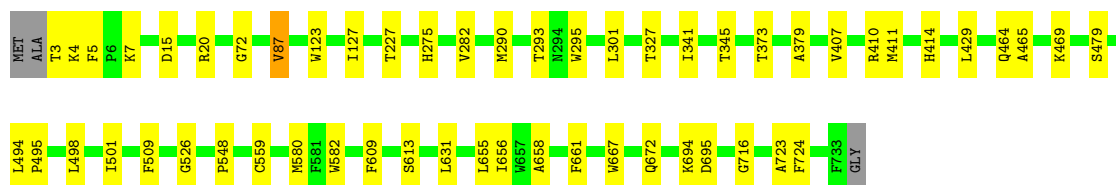
- Molecule 10: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 92% 7%



- Molecule 11: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 92% 7%



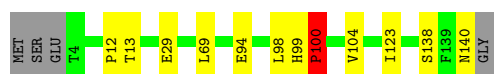
- Molecule 12: Photosystem I iron-sulfur center

Chain C: 81% 15% ...



- Molecule 13: Photosystem I reaction center subunit II

Chain D: 89% 8%



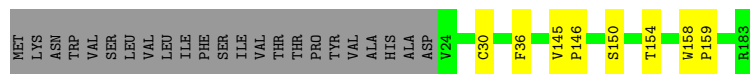
- Molecule 14: Photosystem I reaction center subunit IV

Chain E: 89% 6% 5%



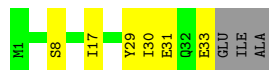
- Molecule 15: Photosystem I reaction center subunit III

Chain F:  83% 13%

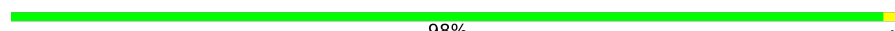


- Molecule 16: Photosystem I reaction center subunit VIII

Chain I:  75% 17% 8%



- Molecule 17: Photosystem I reaction center subunit IX

Chain J:  98%

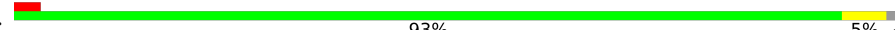


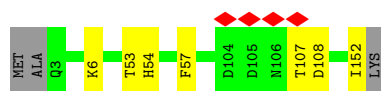
- Molecule 18: Photosystem I reaction center subunit PsaK

Chain K:  86% 10%

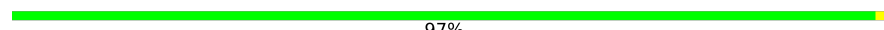


- Molecule 19: Photosystem I reaction center subunit XI

Chain L:  93% 5%



- Molecule 20: Photosystem I reaction center subunit XII

Chain M:  97%

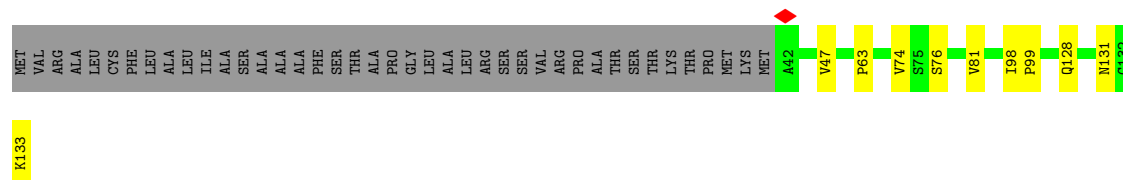


- Molecule 21: PsaO

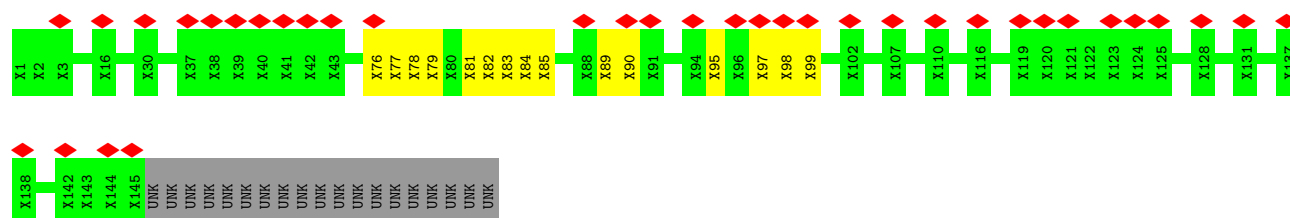
Chain O:  89% 11%



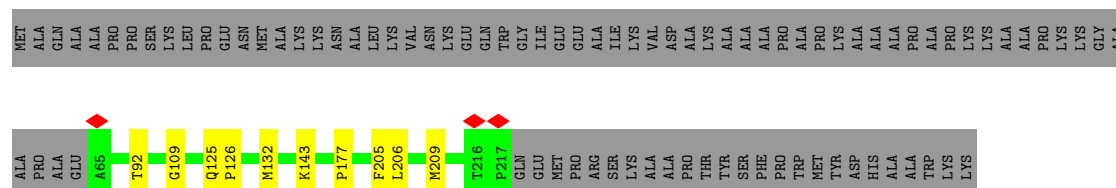
• Molecule 22: PsaR

Chain R:  62% 8% 31%

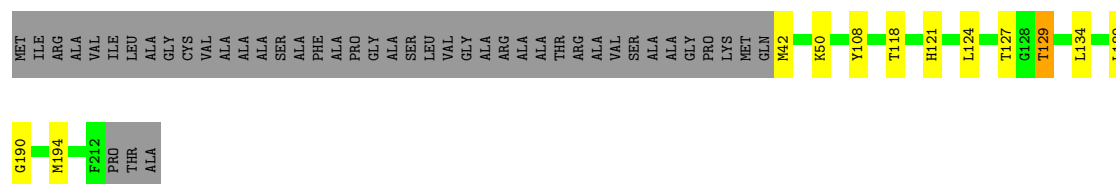
• Molecule 23: Unk1

Chain X:  22% 79% 9% 12%

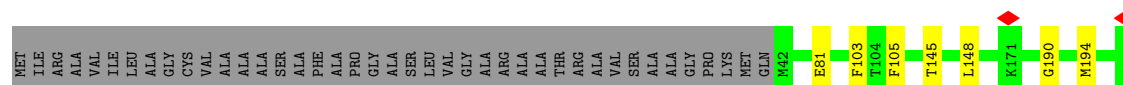
• Molecule 24: ACPI-S

Chain Z:  59% 37%

• Molecule 25: ACPI-13/10

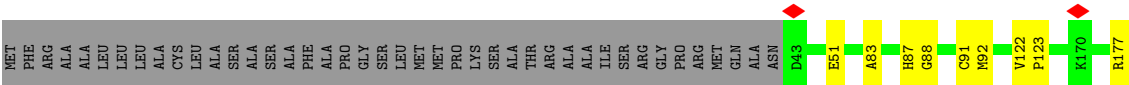
Chain a:  74% 5% 20%

• Molecule 25: ACPI-13/10

Chain d:  76% 20%



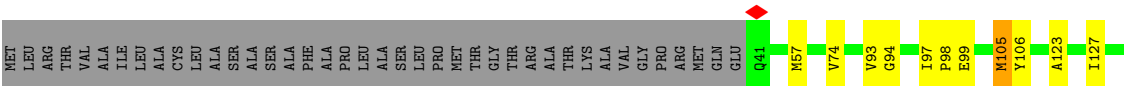
• Molecule 26: ACPI-14



• Molecule 27: ACPI-9



• Molecule 28: ACPI-11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133521	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	2.411	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.032	Depositor
Map value standard deviation	0.064	Depositor
Recommended contour level	0.35	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: LHG, LMU, KC2, 8CT, SQD, IHT, CLA, II3, II0, LMG, PQN, DGD, SF4

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	0.33	0/1371	0.51	1/1854 (0.1%)
2	2	0.23	0/1356	0.31	0/1835
3	3	0.18	0/1392	0.29	0/1883
4	4	0.18	0/1406	0.32	0/1900
5	5	0.32	0/1438	0.45	0/1940
6	6	0.36	0/1334	0.39	0/1796
7	7	0.22	0/1373	0.35	0/1858
8	8	0.22	0/1326	0.35	0/1804
9	9	0.20	0/1376	0.34	0/1846
10	A	0.23	0/6019	0.35	0/8204
11	B	0.26	0/6046	0.37	1/8254 (0.0%)
12	C	0.48	1/600 (0.2%)	0.64	4/812 (0.5%)
13	D	0.22	0/1094	0.41	0/1476
14	E	0.21	0/499	0.33	0/677
15	F	0.22	0/1290	0.33	0/1745
16	I	0.23	0/266	0.34	0/362
17	J	0.26	0/353	0.34	0/481
18	K	0.23	0/563	0.36	0/768
19	L	0.31	0/1171	0.40	0/1594
20	M	0.19	0/228	0.26	0/310
21	O	0.22	0/796	0.36	0/1091
22	R	0.17	0/700	0.31	0/963
24	Z	0.20	0/1163	0.32	0/1572
25	a	0.21	0/1299	0.33	0/1747
25	d	0.24	0/1299	0.33	0/1747
26	b	0.21	0/1404	0.33	0/1902
27	c	0.29	0/1658	0.45	1/2241 (0.0%)
28	e	0.24	0/1325	0.36	0/1793
All	All	0.25	1/40145 (0.0%)	0.37	7/54455 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	61	ASP	CA-C	-5.09	1.46	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	61	ASP	CA-C-N	-6.23	112.87	122.09
12	C	61	ASP	C-N-CA	-6.23	112.87	122.09
1	1	50	VAL	N-CA-C	6.07	117.42	109.58
27	c	229	PRO	N-CA-C	-5.95	103.24	113.70
12	C	62	PHE	N-CA-CB	5.34	118.88	110.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1338	0	1329	26	0
2	2	1320	0	1309	12	0
3	3	1362	0	1389	8	0
4	4	1366	0	1349	7	0
5	5	1403	0	1398	20	0
6	6	1305	0	1324	16	0
7	7	1337	0	1317	11	0
8	8	1298	0	1322	9	0
9	9	1349	0	1358	15	0
10	A	5824	0	5672	36	0
11	B	5828	0	5626	44	0
12	C	591	0	568	11	0
13	D	1070	0	1076	17	0
14	E	491	0	491	2	0
15	F	1258	0	1266	5	0
16	I	258	0	268	6	0
17	J	342	0	344	1	0
18	K	553	0	581	3	0
19	L	1143	0	1145	5	0
20	M	227	0	257	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	O	766	0	752	10	0
22	R	680	0	674	6	0
23	X	725	0	152	11	0
24	Z	1130	0	1088	6	0
25	a	1271	0	1281	13	0
25	d	1271	0	1281	5	0
26	b	1368	0	1346	10	0
27	c	1615	0	1646	27	0
28	e	1288	0	1282	10	0
29	1	584	0	476	7	0
29	2	547	0	456	1	0
29	3	625	0	596	0	0
29	4	598	0	597	2	0
29	5	563	0	442	6	0
29	6	581	0	514	1	0
29	7	509	0	431	4	0
29	8	496	0	471	4	0
29	9	642	0	539	6	0
29	A	2679	0	2767	11	0
29	B	2406	0	2458	13	0
29	F	160	0	141	0	0
29	J	41	0	29	0	0
29	K	120	0	121	0	0
29	L	267	0	240	2	0
29	O	165	0	147	4	0
29	R	55	0	49	0	0
29	Z	225	0	206	2	0
29	a	645	0	632	1	0
29	b	530	0	525	2	0
29	c	666	0	632	7	0
29	d	589	0	538	1	0
29	e	472	0	414	3	0
30	1	45	0	0	0	0
30	2	45	0	0	0	0
30	3	45	0	0	0	0
30	4	45	0	0	0	0
30	5	45	0	0	0	0
30	6	90	0	0	0	0
30	7	90	0	0	0	0
30	9	45	0	0	0	0
30	Z	45	0	0	0	0
30	a	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	b	90	0	0	1	0
30	c	135	0	0	3	0
30	d	45	0	0	0	0
30	e	90	0	0	0	0
31	1	168	0	0	2	0
31	2	126	0	0	1	0
31	3	210	0	0	1	0
31	4	168	0	0	2	0
31	5	210	0	0	3	0
31	6	126	0	0	0	0
31	7	168	0	0	0	0
31	8	168	0	0	1	0
31	9	168	0	0	0	0
31	B	42	0	0	0	0
31	J	42	0	0	0	0
31	O	84	0	0	0	0
31	R	42	0	0	0	0
31	a	210	0	0	2	0
31	b	84	0	0	0	0
31	c	168	0	0	0	0
31	d	168	0	0	0	0
31	e	126	0	0	0	0
32	1	42	0	0	0	0
32	b	42	0	0	1	0
32	e	42	0	0	0	0
33	1	41	0	0	0	0
33	2	41	0	0	1	0
33	5	41	0	0	0	0
33	6	41	0	0	1	0
33	8	41	0	0	0	0
33	9	41	0	0	1	0
33	K	41	0	0	0	0
33	L	41	0	0	0	0
33	Z	41	0	0	0	0
33	a	41	0	0	1	0
33	c	41	0	0	1	0
33	d	41	0	0	1	0
34	2	36	0	42	0	0
34	3	62	0	64	0	0
34	6	32	0	34	0	0
34	8	52	0	77	0	0
34	F	32	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	I	51	0	75	0	0
35	2	103	0	125	0	0
35	3	132	0	186	0	0
35	4	92	0	130	0	0
35	5	23	0	16	0	0
35	6	35	0	40	0	0
35	7	70	0	83	0	0
35	8	33	0	36	0	0
35	A	88	0	122	0	0
35	B	45	0	60	0	0
35	L	34	0	38	1	0
35	Z	46	0	65	0	0
35	a	29	0	28	0	0
35	b	49	0	74	0	0
35	c	29	0	28	0	0
35	d	62	0	73	0	0
36	3	42	0	48	0	0
36	O	29	0	22	0	0
37	4	40	0	0	1	0
37	7	40	0	0	1	0
37	A	200	0	0	0	0
37	B	240	0	0	0	0
37	F	40	0	0	1	0
37	I	40	0	0	0	0
37	J	40	0	0	0	0
37	K	40	0	0	0	0
37	L	40	0	0	0	0
37	M	40	0	0	0	0
37	R	80	0	0	0	0
37	Z	80	0	0	0	0
37	b	40	0	0	0	0
37	e	40	0	0	0	0
38	4	35	0	46	1	0
38	7	35	0	46	1	0
38	J	31	0	35	1	0
38	O	30	0	33	4	0
38	e	31	0	35	0	0
39	A	33	0	46	0	0
39	B	33	0	46	0	0
40	B	8	0	0	0	0
40	C	16	0	0	1	0
41	B	59	0	79	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	Z	60	0	78	1	0
All	All	60515	0	54256	360	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 360 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)
25:a:127:THR:HG23	26:b:218:MET:HE1	1.50	0.93
26:b:177:ARG:NH2	30:b:609:KC2:O1A	2.13	0.81
11:B:609:PHE:O	11:B:613:SER:OG	2.00	0.80
6:6:89:MET:HE3	6:6:184:GLY:HA2	1.64	0.78
38:J:104:LMU:O5B	38:J:104:LMU:O3'	2.03	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	177/222 (80%)	172 (97%)	5 (3%)	0	100	100
2	2	166/216 (77%)	161 (97%)	5 (3%)	0	100	100
3	3	178/236 (75%)	174 (98%)	4 (2%)	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%)	163 (95%)	8 (5%)	0	100	100
7	7	175/230 (76%)	172 (98%)	3 (2%)	0	100	100
8	8	171/227 (75%)	168 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	9	178/220 (81%)	174 (98%)	4 (2%)	0	100	100
10	A	739/752 (98%)	713 (96%)	26 (4%)	0	100	100
11	B	729/734 (99%)	706 (97%)	23 (3%)	0	100	100
12	C	78/81 (96%)	73 (94%)	4 (5%)	1 (1%)	9	16
13	D	135/141 (96%)	124 (92%)	10 (7%)	1 (1%)	18	30
14	E	59/64 (92%)	57 (97%)	2 (3%)	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%)	72 (95%)	4 (5%)	0	100	100
19	L	148/153 (97%)	143 (97%)	5 (3%)	0	100	100
20	M	28/30 (93%)	28 (100%)	0	0	100	100
21	O	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
22	R	90/133 (68%)	88 (98%)	2 (2%)	0	100	100
24	Z	151/242 (62%)	150 (99%)	1 (1%)	0	100	100
25	a	169/215 (79%)	165 (98%)	4 (2%)	0	100	100
25	d	169/215 (79%)	166 (98%)	3 (2%)	0	100	100
26	b	174/218 (80%)	171 (98%)	3 (2%)	0	100	100
27	c	213/257 (83%)	203 (95%)	10 (5%)	0	100	100
28	e	166/208 (80%)	165 (99%)	1 (1%)	0	100	100
All	All	5026/5902 (85%)	4871 (97%)	153 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	D	100	PRO
12	C	61	ASP

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%)	138 (99%)	1 (1%)	76	86
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%)	133 (99%)	1 (1%)	76	86
9	9	138/164 (84%)	138 (100%)	0	100	100
10	A	607/617 (98%)	605 (100%)	2 (0%)	86	94
11	B	592/593 (100%)	591 (100%)	1 (0%)	87	95
12	C	66/67 (98%)	66 (100%)	0	100	100
13	D	114/117 (97%)	112 (98%)	2 (2%)	51	72
14	E	56/59 (95%)	55 (98%)	1 (2%)	51	72
15	F	133/154 (86%)	133 (100%)	0	100	100
16	I	27/29 (93%)	27 (100%)	0	100	100
17	J	38/38 (100%)	38 (100%)	0	100	100
18	K	62/69 (90%)	62 (100%)	0	100	100
19	L	126/128 (98%)	125 (99%)	1 (1%)	73	85
20	M	25/25 (100%)	25 (100%)	0	100	100
21	O	81/81 (100%)	81 (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	85
25	d	128/153 (84%)	128 (100%)	0	100	100
26	b	144/173 (83%)	144 (100%)	0	100	100
27	c	169/195 (87%)	169 (100%)	0	100	100
28	e	133/162 (82%)	132 (99%)	1 (1%)	73	85
All	All	4050/4613 (88%)	4039 (100%)	11 (0%)	84	94

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	E	36	VAL
19	L	6	LYS
28	e	105	MET
25	a	129	THR
11	B	87	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
11	B	10	GLN
27	c	223	GLN
11	B	610	ASN
28	e	48	GLN
26	b	199	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

417 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
33	IHT	L	205	-	40,42,42	2.58	3 (7%)	52,58,58	2.31	16 (30%)
29	CLA	A	818	-	69,73,73	1.71	9 (13%)	82,113,113	1.31	8 (9%)
29	CLA	Z	301	-	64,68,73	1.79	9 (14%)	76,107,113	1.35	8 (10%)
29	CLA	F	202	-	64,68,73	1.79	9 (14%)	76,107,113	1.33	9 (11%)
38	LMU	O	207	-	31,31,36	0.53	1 (3%)	42,42,47	1.08	2 (4%)
29	CLA	c	602	27	69,73,73	1.73	9 (13%)	82,113,113	1.32	7 (8%)
29	CLA	B	802	-	69,73,73	1.66	9 (13%)	82,113,113	1.25	9 (10%)
29	CLA	6	601	6	49,53,73	2.02	9 (18%)	58,89,113	1.52	9 (15%)
31	II0	3	616	-	39,43,43	2.01	2 (5%)	48,60,60	1.29	4 (8%)
38	LMU	e	617	-	32,32,36	0.40	0	43,43,47	1.05	2 (4%)
29	CLA	5	603	-	49,53,73	2.04	9 (18%)	58,89,113	1.52	9 (15%)
37	8CT	4	616	-	40,41,41	0.19	0	51,56,56	0.32	0
37	8CT	A	848	-	40,41,41	0.36	0	51,56,56	0.56	0
29	CLA	A	821	-	59,63,73	1.84	9 (15%)	70,101,113	1.46	8 (11%)
29	CLA	8	604	-	69,73,73	1.72	9 (13%)	82,113,113	1.32	11 (13%)
29	CLA	A	840	-	59,63,73	1.82	9 (15%)	70,101,113	1.43	7 (10%)
31	II0	1	614	-	39,43,43	2.03	2 (5%)	48,60,60	1.29	5 (10%)
31	II0	c	619	-	39,43,43	2.02	2 (5%)	48,60,60	1.35	5 (10%)
29	CLA	a	607	25	69,73,73	1.70	9 (13%)	82,113,113	1.29	8 (9%)
39	PQN	A	849	-	34,34,34	0.38	0	43,45,45	0.77	2 (4%)
29	CLA	A	834	10	59,63,73	1.84	9 (15%)	70,101,113	1.40	10 (14%)
29	CLA	e	603	28	54,58,73	1.96	9 (16%)	64,95,113	1.50	8 (12%)
35	LHG	3	619	-	48,48,48	0.61	1 (2%)	51,54,54	1.24	6 (11%)
29	CLA	b	608	-	69,73,73	1.70	9 (13%)	82,113,113	1.27	9 (10%)
37	8CT	I	101	-	40,41,41	0.27	0	51,56,56	0.42	0
29	CLA	B	832	-	69,73,73	1.70	9 (13%)	82,113,113	1.27	9 (10%)
35	LHG	3	622	30	33,33,48	0.72	1 (3%)	36,39,54	1.29	3 (8%)
29	CLA	6	612	-	49,53,73	2.01	9 (18%)	58,89,113	1.51	8 (13%)
29	CLA	9	604	-	59,63,73	1.86	9 (15%)	70,101,113	1.39	8 (11%)
29	CLA	1	609	-	45,49,73	2.20	10 (22%)	54,84,113	1.63	8 (14%)
30	KC2	3	606	35	49,53,53	1.79	4 (8%)	60,89,89	1.17	8 (13%)
29	CLA	B	818	-	64,68,73	1.78	9 (14%)	76,107,113	1.37	8 (10%)
29	CLA	J	102	17	45,49,73	2.24	10 (22%)	54,84,113	1.65	9 (16%)
31	II0	b	612	-	39,43,43	1.99	2 (5%)	48,60,60	1.30	6 (12%)
30	KC2	4	605	4	49,53,53	1.81	4 (8%)	60,89,89	1.11	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	II0	c	618	-	39,43,43	2.03	2 (5%)	48,60,60	1.37	8 (16%)
31	II0	a	614	-	39,43,43	2.02	2 (5%)	48,60,60	1.34	5 (10%)
35	LHG	A	851	-	38,38,48	0.71	1 (2%)	41,44,54	1.28	3 (7%)
31	II0	O	205	-	39,43,43	2.04	2 (5%)	48,60,60	1.36	7 (14%)
29	CLA	K	102	-	59,63,73	1.87	9 (15%)	70,101,113	1.41	8 (11%)
29	CLA	A	809	29	64,68,73	1.82	9 (14%)	76,107,113	1.45	10 (13%)
29	CLA	c	606	-	69,73,73	1.71	9 (13%)	82,113,113	1.34	9 (10%)
34	LMG	I	102	-	51,51,55	0.71	0	59,59,63	1.30	7 (11%)
29	CLA	8	603	-	69,73,73	1.73	9 (13%)	82,113,113	1.31	8 (9%)
35	LHG	L	208	-	33,33,48	0.74	1 (3%)	36,39,54	1.23	2 (5%)
29	CLA	1	606	-	49,53,73	2.03	9 (18%)	58,89,113	1.55	8 (13%)
29	CLA	F	204	15	59,63,73	1.84	9 (15%)	70,101,113	1.40	9 (12%)
29	CLA	A	804	10	69,73,73	1.71	9 (13%)	82,113,113	1.30	10 (12%)
29	CLA	2	602	2	63,67,73	1.80	9 (14%)	74,105,113	1.50	10 (13%)
29	CLA	A	836	-	59,63,73	1.84	9 (15%)	70,101,113	1.38	9 (12%)
29	CLA	Z	306	24	64,68,73	1.76	9 (14%)	76,107,113	1.37	8 (10%)
33	IHT	1	618	-	40,42,42	2.60	4 (10%)	52,58,58	2.11	13 (25%)
29	CLA	9	611	-	45,49,73	2.18	10 (22%)	54,84,113	1.63	8 (14%)
29	CLA	B	830	-	64,68,73	1.77	9 (14%)	76,107,113	1.37	8 (10%)
29	CLA	B	826	-	69,73,73	1.68	9 (13%)	82,113,113	1.26	8 (9%)
32	II3	b	613	-	40,43,43	1.55	2 (5%)	47,60,60	1.84	14 (29%)
34	LMG	8	614	-	52,52,55	0.83	3 (5%)	60,60,63	1.29	6 (10%)
30	KC2	d	610	25	49,53,53	1.82	4 (8%)	60,89,89	1.16	4 (6%)
29	CLA	2	604	2	59,63,73	1.87	9 (15%)	70,101,113	1.40	7 (10%)
29	CLA	6	605	6	59,63,73	1.83	9 (15%)	70,101,113	1.37	9 (12%)
29	CLA	9	603	-	49,53,73	2.05	9 (18%)	58,89,113	1.53	8 (13%)
29	CLA	7	611	-	59,63,73	1.86	9 (15%)	70,101,113	1.40	8 (11%)
35	LHG	a	618	-	28,28,48	0.82	1 (3%)	31,34,54	1.36	3 (9%)
29	CLA	A	823	-	69,73,73	1.71	9 (13%)	82,113,113	1.26	9 (10%)
29	CLA	A	839	-	69,73,73	1.70	9 (13%)	82,113,113	1.32	9 (10%)
29	CLA	A	806	10	69,73,73	1.70	9 (13%)	82,113,113	1.28	9 (10%)
29	CLA	A	814	-	49,53,73	2.05	9 (18%)	58,89,113	1.53	8 (13%)
29	CLA	7	609	35	45,49,73	2.20	10 (22%)	54,84,113	1.62	8 (14%)
29	CLA	B	821	-	64,68,73	1.76	9 (14%)	76,107,113	1.38	9 (11%)
35	LHG	8	613	-	32,32,48	0.77	2 (6%)	35,38,54	1.22	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	8CT	B	851	-	40,41,41	0.24	0	51,56,56	0.46	0
29	CLA	5	611	-	49,53,73	2.03	9 (18%)	58,89,113	1.50	8 (13%)
31	II0	d	614	-	39,43,43	2.02	2 (5%)	48,60,60	1.33	6 (12%)
34	LMG	F	205	-	32,32,55	0.83	0	40,40,63	1.29	6 (15%)
33	IHT	K	104	-	40,42,42	2.69	4 (10%)	52,58,58	2.04	19 (36%)
29	CLA	4	610	-	69,73,73	1.69	9 (13%)	82,113,113	1.29	8 (9%)
29	CLA	B	811	-	59,63,73	1.85	9 (15%)	70,101,113	1.41	8 (11%)
39	PQN	B	842	-	34,34,34	0.38	0	43,45,45	0.68	1 (2%)
37	8CT	A	845	-	40,41,41	0.25	0	51,56,56	0.40	0
33	IHT	Z	302	-	40,42,42	2.60	3 (7%)	52,58,58	2.17	13 (25%)
29	CLA	A	837	-	69,73,73	1.67	9 (13%)	82,113,113	1.27	8 (9%)
33	IHT	5	618	-	40,42,42	2.59	4 (10%)	52,58,58	2.28	16 (30%)
35	LHG	4	617	29	46,46,48	0.63	1 (2%)	49,52,54	1.21	4 (8%)
29	CLA	B	836	-	51,55,73	1.97	9 (17%)	60,91,113	1.49	8 (13%)
29	CLA	B	823	-	69,73,73	1.72	9 (13%)	82,113,113	1.29	10 (12%)
29	CLA	B	840	-	69,73,73	1.67	9 (13%)	82,113,113	1.26	8 (9%)
31	II0	9	615	-	39,43,43	2.02	2 (5%)	48,60,60	1.40	7 (14%)
29	CLA	8	602	8	49,53,73	2.05	9 (18%)	58,89,113	1.44	6 (10%)
29	CLA	A	817	-	69,73,73	1.72	9 (13%)	82,113,113	1.41	8 (9%)
29	CLA	Z	304	24	59,63,73	1.86	9 (15%)	70,101,113	1.37	8 (11%)
29	CLA	A	816	-	64,68,73	1.74	9 (14%)	76,107,113	1.36	8 (10%)
29	CLA	a	601	25	49,53,73	2.03	9 (18%)	58,89,113	1.52	8 (13%)
31	II0	a	619	-	39,43,43	2.00	2 (5%)	48,60,60	1.34	6 (12%)
29	CLA	2	601	2	46,50,73	2.12	9 (19%)	53,85,113	1.66	9 (16%)
29	CLA	A	841	-	69,73,73	1.71	9 (13%)	82,113,113	1.29	8 (9%)
29	CLA	d	606	-	45,49,73	2.16	10 (22%)	54,84,113	1.64	9 (16%)
31	II0	d	616	-	39,43,43	2.03	2 (5%)	48,60,60	1.44	8 (16%)
35	LHG	7	619	29	38,38,48	0.66	1 (2%)	41,44,54	1.19	3 (7%)
35	LHG	d	619	-	38,38,48	0.71	2 (5%)	41,44,54	1.19	2 (4%)
36	SQD	3	621	-	40,42,54	1.26	3 (7%)	50,53,65	1.09	3 (6%)
29	CLA	B	815	-	69,73,73	1.75	9 (13%)	82,113,113	1.33	8 (9%)
29	CLA	6	607	6	59,63,73	1.84	9 (15%)	70,101,113	1.38	8 (11%)
29	CLA	B	808	-	69,73,73	1.69	9 (13%)	82,113,113	1.25	8 (9%)
29	CLA	B	812	-	69,73,73	1.70	9 (13%)	82,113,113	1.32	8 (9%)
29	CLA	L	203	-	64,68,73	1.80	9 (14%)	76,107,113	1.37	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	II0	d	615	-	39,43,43	2.09	2 (5%)	48,60,60	1.39	6 (12%)
35	LHG	A	850	-	48,48,48	0.60	0	51,54,54	1.17	4 (7%)
29	CLA	b	610	26	55,59,73	1.94	9 (16%)	64,96,113	1.50	9 (14%)
38	LMU	J	104	-	32,32,36	0.41	0	43,43,47	1.04	2 (4%)
29	CLA	A	802	29	59,63,73	1.81	9 (15%)	70,101,113	1.37	8 (11%)
29	CLA	5	602	5	59,63,73	1.87	9 (15%)	70,101,113	1.43	9 (12%)
29	CLA	9	612	-	49,53,73	2.02	9 (18%)	58,89,113	1.50	8 (13%)
29	CLA	A	835	-	64,68,73	1.76	9 (14%)	76,107,113	1.34	8 (10%)
29	CLA	8	605	8	54,58,73	1.95	9 (16%)	64,95,113	1.52	9 (14%)
35	LHG	2	620	-	41,41,48	0.66	1 (2%)	44,47,54	1.23	3 (6%)
29	CLA	d	607	25	69,73,73	1.70	9 (13%)	82,113,113	1.32	9 (10%)
29	CLA	9	614	-	45,49,73	2.24	10 (22%)	54,84,113	1.68	9 (16%)
31	II0	3	614	-	39,43,43	2.02	2 (5%)	48,60,60	1.39	6 (12%)
29	CLA	A	805	-	54,58,73	1.93	9 (16%)	64,95,113	1.49	8 (12%)
29	CLA	B	803	-	69,73,73	1.71	9 (13%)	82,113,113	1.22	9 (10%)
29	CLA	O	202	-	59,63,73	1.81	9 (15%)	70,101,113	1.44	9 (12%)
29	CLA	d	603	-	54,58,73	1.94	9 (16%)	64,95,113	1.47	9 (14%)
31	II0	5	615	-	39,43,43	2.05	2 (5%)	48,60,60	1.39	6 (12%)
29	CLA	L	207	-	45,49,73	2.23	10 (22%)	54,84,113	1.67	7 (12%)
29	CLA	a	605	-	59,63,73	1.82	9 (15%)	70,101,113	1.43	9 (12%)
29	CLA	7	601	7	49,53,73	2.02	9 (18%)	58,89,113	1.50	8 (13%)
29	CLA	8	601	8	49,53,73	2.03	9 (18%)	58,89,113	1.50	8 (13%)
29	CLA	A	830	-	64,68,73	1.78	9 (14%)	76,107,113	1.35	8 (10%)
37	8CT	B	846	-	40,41,41	0.11	0	51,56,56	0.49	0
29	CLA	B	824	-	64,68,73	1.79	9 (14%)	76,107,113	1.40	8 (10%)
29	CLA	a	606	-	69,73,73	1.70	9 (13%)	82,113,113	1.33	8 (9%)
35	LHG	d	618	-	22,22,48	0.81	1 (4%)	24,27,54	1.32	3 (12%)
30	KC2	c	610	27	49,53,53	1.77	4 (8%)	60,89,89	1.19	5 (8%)
29	CLA	4	602	4	63,67,73	1.79	9 (14%)	74,105,113	1.41	10 (13%)
29	CLA	Z	305	24	54,58,73	1.91	9 (16%)	64,95,113	1.45	9 (14%)
29	CLA	b	611	-	59,63,73	1.83	9 (15%)	70,101,113	1.39	8 (11%)
29	CLA	B	805	-	69,73,73	1.70	9 (13%)	82,113,113	1.30	9 (10%)
30	KC2	c	611	-	49,53,53	1.82	4 (8%)	60,89,89	1.15	5 (8%)
31	II0	4	613	-	39,43,43	2.03	2 (5%)	48,60,60	1.31	6 (12%)
29	CLA	b	607	26	64,68,73	1.79	9 (14%)	76,107,113	1.36	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	822	-	69,73,73	1.69	9 (13%)	82,113,113	1.28	9 (10%)
29	CLA	3	608	3	64,68,73	1.79	9 (14%)	76,107,113	1.38	8 (10%)
29	CLA	e	602	28	59,63,73	1.88	9 (15%)	70,101,113	1.52	10 (14%)
29	CLA	O	201	-	59,63,73	1.83	9 (15%)	70,101,113	1.42	9 (12%)
37	8CT	B	847	-	40,41,41	0.15	0	51,56,56	0.48	0
29	CLA	1	602	1	63,67,73	1.79	9 (14%)	74,105,113	1.41	10 (13%)
29	CLA	4	601	4	59,63,73	1.83	9 (15%)	70,101,113	1.38	8 (11%)
29	CLA	7	604	7	57,61,73	1.90	9 (15%)	67,98,113	1.46	9 (13%)
29	CLA	3	612	-	49,53,73	2.01	9 (18%)	58,89,113	1.49	8 (13%)
31	II0	1	619	-	39,43,43	2.10	2 (5%)	48,60,60	1.39	10 (20%)
31	II0	e	614	-	39,43,43	2.09	2 (5%)	48,60,60	1.42	7 (14%)
33	IHT	6	617	-	40,42,42	2.57	3 (7%)	52,58,58	2.20	16 (30%)
35	LHG	Z	310	-	45,45,48	0.64	1 (2%)	48,51,54	1.21	4 (8%)
29	CLA	c	601	27	49,53,73	2.07	9 (18%)	58,89,113	1.57	8 (13%)
29	CLA	9	605	-	49,53,73	2.03	9 (18%)	58,89,113	1.54	8 (13%)
29	CLA	2	606	-	49,53,73	2.04	9 (18%)	58,89,113	1.51	8 (13%)
29	CLA	9	601	9	49,53,73	2.03	9 (18%)	58,89,113	1.55	8 (13%)
29	CLA	8	608	-	69,73,73	1.73	9 (13%)	82,113,113	1.29	8 (9%)
29	CLA	B	833	-	49,53,73	2.03	9 (18%)	58,89,113	1.48	8 (13%)
29	CLA	c	603	-	69,73,73	1.69	9 (13%)	82,113,113	1.31	10 (12%)
38	LMU	4	618	-	36,36,36	0.48	1 (2%)	47,47,47	0.95	3 (6%)
29	CLA	e	604	-	64,68,73	1.79	9 (14%)	76,107,113	1.34	8 (10%)
29	CLA	A	838	-	69,73,73	1.71	9 (13%)	82,113,113	1.28	8 (9%)
29	CLA	1	604	1	49,53,73	2.09	9 (18%)	58,89,113	1.52	8 (13%)
29	CLA	F	203	-	49,53,73	2.03	9 (18%)	58,89,113	1.49	8 (13%)
30	KC2	a	610	-	49,53,53	1.81	4 (8%)	60,89,89	1.12	4 (6%)
29	CLA	3	602	3	59,63,73	1.86	9 (15%)	70,101,113	1.42	7 (10%)
29	CLA	6	602	6	69,73,73	1.76	9 (13%)	82,113,113	1.38	6 (7%)
37	8CT	L	206	-	40,41,41	0.20	0	51,56,56	0.43	0
35	LHG	7	618	-	30,30,48	0.76	1 (3%)	33,36,54	1.22	3 (9%)
29	CLA	5	606	-	49,53,73	2.03	9 (18%)	58,89,113	1.54	9 (15%)
31	II0	8	612	-	39,43,43	2.01	2 (5%)	48,60,60	1.35	5 (10%)
29	CLA	3	607	3	64,68,73	1.77	9 (14%)	76,107,113	1.32	8 (10%)
31	II0	4	612	-	39,43,43	2.01	2 (5%)	48,60,60	1.30	5 (10%)
31	II0	4	615	-	39,43,43	2.00	2 (5%)	48,60,60	1.33	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	II0	a	613	-	39,43,43	2.03	2 (5%)	48,60,60	1.37	6 (12%)
29	CLA	d	605	25	49,53,73	2.06	9 (18%)	58,89,113	1.56	8 (13%)
29	CLA	A	811	-	69,73,73	1.74	9 (13%)	82,113,113	1.35	7 (8%)
30	KC2	9	610	9	49,53,53	1.80	4 (8%)	60,89,89	1.16	5 (8%)
31	II0	2	615	-	39,43,43	2.05	2 (5%)	48,60,60	1.42	9 (18%)
31	II0	6	616	-	39,43,43	2.05	2 (5%)	48,60,60	1.51	10 (20%)
29	CLA	b	603	-	64,68,73	1.78	9 (14%)	76,107,113	1.37	8 (10%)
30	KC2	e	605	28	49,53,53	1.81	4 (8%)	60,89,89	1.12	4 (6%)
31	II0	R	204	-	39,43,43	2.03	2 (5%)	48,60,60	1.32	8 (16%)
29	CLA	3	603	-	64,68,73	1.78	9 (14%)	76,107,113	1.37	7 (9%)
29	CLA	B	820	-	64,68,73	1.78	9 (14%)	76,107,113	1.35	9 (11%)
29	CLA	6	603	-	49,53,73	2.10	9 (18%)	58,89,113	1.55	9 (15%)
29	CLA	e	606	28	64,68,73	1.77	9 (14%)	76,107,113	1.29	9 (11%)
29	CLA	c	604	-	64,68,73	1.82	9 (14%)	76,107,113	1.37	7 (9%)
31	II0	O	204	-	39,43,43	2.05	2 (5%)	48,60,60	1.29	5 (10%)
37	8CT	B	845	-	40,41,41	0.38	1 (2%)	51,56,56	0.61	1 (1%)
29	CLA	a	612	-	69,73,73	1.68	9 (13%)	82,113,113	1.28	7 (8%)
29	CLA	B	835	-	69,73,73	1.75	9 (13%)	82,113,113	1.44	8 (9%)
29	CLA	2	607	2	49,53,73	2.03	9 (18%)	58,89,113	1.54	9 (15%)
34	LMG	2	617	-	36,36,55	0.84	1 (2%)	44,44,63	1.21	4 (9%)
29	CLA	9	613	9	49,53,73	2.05	9 (18%)	58,89,113	1.49	8 (13%)
31	II0	8	610	-	39,43,43	2.08	2 (5%)	48,60,60	1.44	7 (14%)
40	SF4	C	102	12	0,12,12	-	-	-	-	-
34	LMG	6	619	-	32,32,55	0.96	2 (6%)	40,40,63	1.23	5 (12%)
29	CLA	A	813	-	46,50,73	2.10	9 (19%)	53,85,113	1.62	8 (15%)
29	CLA	d	601	25	49,53,73	2.03	9 (18%)	58,89,113	1.52	8 (13%)
29	CLA	A	825	-	69,73,73	1.72	9 (13%)	82,113,113	1.30	9 (10%)
29	CLA	B	804	-	49,53,73	2.02	9 (18%)	58,89,113	1.47	7 (12%)
29	CLA	L	204	-	54,58,73	1.91	9 (16%)	64,95,113	1.54	9 (14%)
30	KC2	c	615	-	49,53,53	1.80	4 (8%)	60,89,89	1.13	4 (6%)
34	LMG	3	618	-	30,30,55	0.95	1 (3%)	38,38,63	1.21	5 (13%)
29	CLA	9	606	-	68,72,73	1.70	9 (13%)	80,111,113	1.33	9 (11%)
31	II0	a	616	-	39,43,43	2.10	2 (5%)	48,60,60	1.46	8 (16%)
29	CLA	8	607	8	45,49,73	2.17	10 (22%)	54,84,113	1.63	9 (16%)
29	CLA	e	607	28	49,53,73	2.06	9 (18%)	58,89,113	1.56	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	8CT	Z	309	-	40,41,41	0.24	0	51,56,56	0.68	1 (1%)
29	CLA	c	607	27	69,73,73	1.70	9 (13%)	82,113,113	1.28	8 (9%)
29	CLA	5	612	-	49,53,73	2.04	9 (18%)	58,89,113	1.57	9 (15%)
29	CLA	B	806	-	69,73,73	1.70	9 (13%)	82,113,113	1.31	11 (13%)
29	CLA	e	611	-	69,73,73	1.73	9 (13%)	82,113,113	1.26	9 (10%)
29	CLA	B	827	-	69,73,73	1.70	9 (13%)	82,113,113	1.30	8 (9%)
29	CLA	B	838	-	69,73,73	1.72	9 (13%)	82,113,113	1.33	9 (10%)
29	CLA	A	812	-	59,63,73	1.84	9 (15%)	70,101,113	1.44	10 (14%)
29	CLA	c	608	27	64,68,73	1.78	9 (14%)	76,107,113	1.38	7 (9%)
29	CLA	a	608	25	64,68,73	1.77	9 (14%)	76,107,113	1.39	7 (9%)
29	CLA	b	602	26	68,72,73	1.75	9 (13%)	80,111,113	1.41	10 (12%)
29	CLA	9	608	9	59,63,73	1.86	9 (15%)	70,101,113	1.47	7 (10%)
31	II0	7	613	-	39,43,43	2.03	2 (5%)	48,60,60	1.32	6 (12%)
37	8CT	M	101	-	40,41,41	0.18	0	51,56,56	0.86	1 (1%)
37	8CT	7	617	-	40,41,41	0.40	1 (2%)	51,56,56	0.59	0
31	II0	6	615	-	39,43,43	2.01	2 (5%)	48,60,60	1.29	6 (12%)
29	CLA	B	837	-	69,73,73	1.73	9 (13%)	82,113,113	1.26	8 (9%)
29	CLA	6	608	6	64,68,73	1.77	9 (14%)	76,107,113	1.39	9 (11%)
37	8CT	R	201	-	40,41,41	0.18	0	51,56,56	0.42	0
37	8CT	B	844	-	40,41,41	0.22	0	51,56,56	0.62	0
31	II0	7	614	-	39,43,43	2.00	2 (5%)	48,60,60	1.36	6 (12%)
37	8CT	e	616	-	40,41,41	0.15	0	51,56,56	0.35	0
29	CLA	5	604	-	59,63,73	1.89	9 (15%)	70,101,113	1.45	8 (11%)
29	CLA	7	607	7	49,53,73	2.06	9 (18%)	58,89,113	1.55	8 (13%)
31	II0	8	611	-	39,43,43	2.06	2 (5%)	48,60,60	1.31	7 (14%)
30	KC2	6	613	6	49,53,53	1.80	4 (8%)	60,89,89	1.11	3 (5%)
29	CLA	A	844	-	69,73,73	1.64	9 (13%)	82,113,113	1.34	8 (9%)
30	KC2	e	609	-	49,53,53	1.81	4 (8%)	60,89,89	1.13	4 (6%)
35	LHG	b	616	-	48,48,48	0.57	1 (2%)	51,54,54	1.16	4 (7%)
31	II0	5	614	-	39,43,43	1.99	2 (5%)	48,60,60	1.28	6 (12%)
29	CLA	6	609	35	45,49,73	2.22	10 (22%)	54,84,113	1.62	8 (14%)
29	CLA	R	202	-	59,63,73	1.88	9 (15%)	70,101,113	1.57	9 (12%)
35	LHG	3	623	-	48,48,48	0.61	2 (4%)	51,54,54	1.22	5 (9%)
37	8CT	A	846	-	40,41,41	0.15	0	51,56,56	0.36	0
29	CLA	4	609	4	64,68,73	1.79	9 (14%)	76,107,113	1.36	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	B	816	-	63,67,73	1.79	9 (14%)	74,105,113	1.36	10 (13%)
29	CLA	4	607	4	64,68,73	1.78	9 (14%)	76,107,113	1.38	9 (11%)
31	II0	a	615	-	39,43,43	2.03	2 (5%)	48,60,60	1.34	8 (16%)
29	CLA	2	611	-	49,53,73	2.04	9 (18%)	58,89,113	1.52	9 (15%)
32	II3	e	613	-	40,43,43	1.54	2 (5%)	47,60,60	1.81	13 (27%)
29	CLA	7	605	7	49,53,73	2.07	9 (18%)	58,89,113	1.53	8 (13%)
29	CLA	B	819	-	64,68,73	1.79	9 (14%)	76,107,113	1.44	10 (13%)
31	II0	9	617	-	39,43,43	2.03	2 (5%)	48,60,60	1.35	7 (14%)
29	CLA	2	609	-	45,49,73	2.24	10 (22%)	54,84,113	1.65	9 (16%)
29	CLA	A	803	-	69,73,73	1.70	9 (13%)	82,113,113	1.35	9 (10%)
29	CLA	1	612	-	64,68,73	1.75	9 (14%)	76,107,113	1.30	9 (11%)
30	KC2	6	610	6	49,53,53	1.81	4 (8%)	60,89,89	1.13	4 (6%)
37	8CT	A	847	-	40,41,41	0.23	0	51,56,56	0.78	1 (1%)
29	CLA	2	603	-	54,58,73	1.95	9 (16%)	64,95,113	1.45	9 (14%)
29	CLA	d	602	25	68,72,73	1.74	9 (13%)	80,111,113	1.37	9 (11%)
29	CLA	5	601	5	45,49,73	2.23	10 (22%)	54,84,113	1.70	8 (14%)
29	CLA	5	609	-	45,49,73	2.20	10 (22%)	54,84,113	1.60	8 (14%)
31	II0	7	616	-	39,43,43	2.01	2 (5%)	48,60,60	1.39	8 (16%)
29	CLA	5	607	5	49,53,73	2.02	9 (18%)	58,89,113	1.50	8 (13%)
31	II0	d	613	-	39,43,43	2.02	2 (5%)	48,60,60	1.35	5 (10%)
29	CLA	K	101	-	69,73,73	1.71	9 (13%)	82,113,113	1.27	8 (9%)
29	CLA	1	613	-	49,53,73	2.08	9 (18%)	58,89,113	1.56	9 (15%)
29	CLA	A	810	-	69,73,73	1.69	9 (13%)	82,113,113	1.29	10 (12%)
29	CLA	O	203	-	59,63,73	1.82	9 (15%)	70,101,113	1.49	9 (12%)
31	II0	5	616	-	39,43,43	2.06	2 (5%)	48,60,60	1.40	8 (16%)
37	8CT	A	852	-	40,41,41	0.24	0	51,56,56	0.68	1 (1%)
31	II0	5	620	-	39,43,43	2.07	2 (5%)	48,60,60	1.43	5 (10%)
35	LHG	c	621	-	28,28,48	0.79	1 (3%)	31,34,54	1.30	3 (9%)
33	IHT	d	617	-	40,42,42	2.52	3 (7%)	52,58,58	2.31	15 (28%)
29	CLA	3	609	-	69,73,73	1.70	9 (13%)	82,113,113	1.25	7 (8%)
29	CLA	c	605	-	49,53,73	2.02	9 (18%)	58,89,113	1.51	8 (13%)
29	CLA	A	824	-	69,73,73	1.73	9 (13%)	82,113,113	1.29	8 (9%)
29	CLA	a	609	-	64,68,73	1.76	9 (14%)	76,107,113	1.41	8 (10%)
30	KC2	2	610	-	49,53,53	1.82	4 (8%)	60,89,89	1.12	3 (5%)
29	CLA	4	604	-	59,63,73	1.86	9 (15%)	70,101,113	1.37	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	DGD	Z	303	-	61,61,67	0.95	3 (4%)	75,75,81	1.35	8 (10%)
29	CLA	a	603	-	64,68,73	1.78	9 (14%)	76,107,113	1.36	9 (11%)
29	CLA	d	612	-	67,71,73	1.73	9 (13%)	79,110,113	1.28	10 (12%)
41	DGD	B	848	-	60,60,67	0.90	2 (3%)	74,74,81	1.30	7 (9%)
29	CLA	B	817	-	64,68,73	1.75	9 (14%)	76,107,113	1.33	8 (10%)
29	CLA	B	831	-	59,63,73	1.89	9 (15%)	70,101,113	1.51	8 (11%)
29	CLA	4	608	35	69,73,73	1.70	9 (13%)	82,113,113	1.28	9 (10%)
29	CLA	L	202	19	55,59,73	1.92	9 (16%)	64,96,113	1.48	9 (14%)
29	CLA	B	814	-	46,50,73	2.12	9 (19%)	53,85,113	1.62	9 (16%)
29	CLA	A	822	-	69,73,73	1.71	9 (13%)	82,113,113	1.30	8 (9%)
29	CLA	7	612	-	54,58,73	1.94	9 (16%)	64,95,113	1.48	9 (14%)
29	CLA	A	827	-	69,73,73	1.68	9 (13%)	82,113,113	1.27	9 (10%)
29	CLA	8	615	-	69,73,73	1.72	9 (13%)	82,113,113	1.30	9 (10%)
29	CLA	5	613	5	45,49,73	2.19	10 (22%)	54,84,113	1.60	9 (16%)
31	II0	9	618	-	39,43,43	2.01	2 (5%)	48,60,60	1.33	4 (8%)
29	CLA	b	604	-	69,73,73	1.72	9 (13%)	82,113,113	1.28	8 (9%)
40	SF4	B	801	10,11	0,12,12	-	-	-	-	-
35	LHG	4	619	-	44,44,48	0.66	2 (4%)	47,50,54	1.22	4 (8%)
29	CLA	4	611	-	69,73,73	1.69	9 (13%)	82,113,113	1.28	9 (10%)
29	CLA	1	605	-	45,50,73	2.09	9 (20%)	52,85,113	1.54	8 (15%)
31	II0	9	616	-	39,43,43	2.02	2 (5%)	48,60,60	1.31	7 (14%)
29	CLA	1	601	1	49,53,73	2.10	9 (18%)	58,89,113	1.62	9 (15%)
38	LMU	7	620	-	36,36,36	0.39	0	47,47,47	1.06	3 (6%)
29	CLA	2	605	2	64,68,73	1.76	9 (14%)	76,107,113	1.31	8 (10%)
29	CLA	c	613	27	49,53,73	2.06	9 (18%)	58,89,113	1.49	8 (13%)
29	CLA	e	601	28	49,53,73	2.04	9 (18%)	58,89,113	1.52	8 (13%)
29	CLA	1	603	-	56,60,73	1.91	9 (16%)	65,97,113	1.42	8 (12%)
29	CLA	9	609	-	45,49,73	2.19	10 (22%)	54,84,113	1.63	9 (16%)
29	CLA	5	605	5	49,53,73	2.03	9 (18%)	58,89,113	1.50	9 (15%)
29	CLA	4	603	-	58,62,73	1.88	9 (15%)	68,99,113	1.45	8 (11%)
29	CLA	A	826	-	69,73,73	1.67	9 (13%)	82,113,113	1.23	8 (9%)
35	LHG	B	849	29	44,44,48	0.68	1 (2%)	47,50,54	1.22	5 (10%)
29	CLA	1	608	1	64,68,73	1.77	9 (14%)	76,107,113	1.39	8 (10%)
29	CLA	A	819	-	69,73,73	1.72	9 (13%)	82,113,113	1.34	9 (10%)
29	CLA	3	601	3	49,53,73	2.05	9 (18%)	58,89,113	1.52	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	2	608	2	64,68,73	1.77	9 (14%)	76,107,113	1.38	8 (10%)
29	CLA	a	611	-	59,63,73	1.86	9 (15%)	70,101,113	1.43	9 (12%)
29	CLA	7	603	-	59,63,73	1.86	9 (15%)	70,101,113	1.42	9 (12%)
29	CLA	B	829	-	49,53,73	2.07	9 (18%)	58,89,113	1.64	9 (15%)
29	CLA	2	612	-	49,53,73	2.02	9 (18%)	58,89,113	1.55	8 (13%)
29	CLA	a	604	25	64,68,73	1.82	9 (14%)	76,107,113	1.38	6 (7%)
29	CLA	b	606	26	69,73,73	1.71	9 (13%)	82,113,113	1.27	9 (10%)
31	II0	b	614	-	39,43,43	2.01	2 (5%)	48,60,60	1.33	5 (10%)
29	CLA	5	608	-	64,68,73	1.79	9 (14%)	76,107,113	1.53	8 (10%)
31	II0	e	612	-	39,43,43	2.00	2 (5%)	48,60,60	1.34	8 (16%)
29	CLA	c	609	-	45,49,73	2.18	10 (22%)	54,84,113	1.62	9 (16%)
29	CLA	A	832	-	69,73,73	1.70	9 (13%)	82,113,113	1.26	9 (10%)
33	IHT	c	620	-	40,42,42	2.53	3 (7%)	52,58,58	2.22	15 (28%)
37	8CT	R	203	-	40,41,41	0.16	0	51,56,56	0.57	1 (1%)
37	8CT	K	103	-	40,41,41	0.15	0	51,56,56	0.35	0
31	II0	J	101	-	39,43,43	2.02	2 (5%)	48,60,60	1.41	9 (18%)
30	KC2	b	605	26	49,53,53	1.81	4 (8%)	60,89,89	1.16	5 (8%)
29	CLA	3	605	3	59,63,73	1.86	9 (15%)	70,101,113	1.43	7 (10%)
37	8CT	Z	308	-	40,41,41	0.15	0	51,56,56	0.32	0
31	II0	2	613	-	39,43,43	2.07	2 (5%)	48,60,60	1.36	8 (16%)
33	IHT	2	616	-	40,42,42	2.61	3 (7%)	52,58,58	2.28	15 (28%)
31	II0	3	615	-	39,43,43	2.03	2 (5%)	48,60,60	1.31	5 (10%)
29	CLA	A	831	-	69,73,73	1.69	9 (13%)	82,113,113	1.25	8 (9%)
30	KC2	Z	307	-	49,53,53	1.79	4 (8%)	60,89,89	1.13	4 (6%)
33	IHT	8	609	-	40,42,42	2.56	3 (7%)	52,58,58	2.40	16 (30%)
29	CLA	A	815	-	66,70,73	1.77	9 (13%)	78,109,113	1.29	8 (10%)
29	CLA	3	610	-	69,73,73	1.72	9 (13%)	82,113,113	1.34	10 (12%)
34	LMG	3	620	-	32,32,55	0.89	1 (3%)	40,40,63	1.27	6 (15%)
30	KC2	5	610	5	49,53,53	1.81	4 (8%)	60,89,89	1.11	3 (5%)
29	CLA	B	834	-	59,63,73	1.85	9 (15%)	70,101,113	1.44	7 (10%)
40	SF4	C	101	12	0,12,12	-	-	-	-	-
29	CLA	B	807	-	69,73,73	1.68	9 (13%)	82,113,113	1.32	9 (10%)
35	LHG	5	619	-	22,22,48	0.90	1 (4%)	25,28,54	1.36	3 (12%)
29	CLA	d	611	-	54,58,73	1.94	9 (16%)	64,95,113	1.52	10 (15%)
31	II0	8	616	-	39,43,43	2.12	3 (7%)	48,60,60	1.49	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LHG	2	618	-	21,21,48	0.76	0	23,26,54	1.29	2 (8%)
29	CLA	d	609	-	45,49,73	2.18	10 (22%)	54,84,113	1.60	9 (16%)
30	KC2	7	606	-	49,53,53	1.82	4 (8%)	60,89,89	1.17	4 (6%)
30	KC2	7	610	7	49,53,53	1.81	4 (8%)	60,89,89	1.15	4 (6%)
29	CLA	B	810	-	64,68,73	1.74	9 (14%)	76,107,113	1.35	8 (10%)
29	CLA	B	809	11	69,73,73	1.68	9 (13%)	82,113,113	1.26	9 (10%)
29	CLA	A	807	10	54,58,73	1.94	9 (16%)	64,95,113	1.49	9 (14%)
29	CLA	7	608	7	59,63,73	1.84	9 (15%)	70,101,113	1.53	8 (11%)
29	CLA	1	611	-	49,53,73	2.09	9 (18%)	58,89,113	1.54	8 (13%)
33	IHT	9	619	-	40,42,42	2.58	4 (10%)	52,58,58	2.47	14 (26%)
29	CLA	1	607	1	49,53,73	2.05	9 (18%)	58,89,113	1.52	8 (13%)
29	CLA	e	608	-	45,49,73	2.20	10 (22%)	54,84,113	1.61	9 (16%)
29	CLA	9	607	9	69,73,73	1.68	9 (13%)	82,113,113	1.28	10 (12%)
29	CLA	A	833	-	69,73,73	1.71	9 (13%)	82,113,113	1.31	8 (9%)
30	KC2	b	609	-	49,53,53	1.83	4 (8%)	60,89,89	1.14	3 (5%)
31	II0	1	616	-	39,43,43	1.99	2 (5%)	48,60,60	1.35	6 (12%)
29	CLA	9	602	9	59,63,73	1.86	9 (15%)	70,101,113	1.46	8 (11%)
29	CLA	8	606	8	59,63,73	1.85	9 (15%)	70,101,113	1.39	8 (11%)
37	8CT	b	615	-	40,41,41	0.19	0	51,56,56	0.35	0
29	CLA	6	604	-	64,68,73	1.80	9 (14%)	76,107,113	1.37	8 (10%)
29	CLA	B	828	-	69,73,73	1.71	9 (13%)	82,113,113	1.26	8 (9%)
29	CLA	A	843	-	69,73,73	1.74	9 (13%)	82,113,113	1.35	7 (8%)
29	CLA	B	839	35	69,73,73	1.74	9 (13%)	82,113,113	1.35	9 (10%)
31	II0	4	614	-	39,43,43	2.02	2 (5%)	48,60,60	1.28	7 (14%)
29	CLA	7	602	7	69,73,73	1.73	9 (13%)	82,113,113	1.34	10 (12%)
30	KC2	1	610	1	49,53,53	1.82	4 (8%)	60,89,89	1.12	4 (6%)
37	8CT	J	103	-	40,41,41	0.18	0	51,56,56	0.42	0
29	CLA	B	813	-	65,69,73	1.72	9 (13%)	77,108,113	1.35	9 (11%)
29	CLA	B	825	-	69,73,73	1.70	9 (13%)	82,113,113	1.28	10 (12%)
29	CLA	c	612	-	59,63,73	1.84	9 (15%)	70,101,113	1.47	9 (12%)
33	IHT	a	617	-	40,42,42	2.57	3 (7%)	52,58,58	2.31	15 (28%)
29	CLA	d	608	25	69,73,73	1.72	9 (13%)	82,113,113	1.34	8 (9%)
29	CLA	c	614	-	59,63,73	1.84	9 (15%)	70,101,113	1.36	7 (10%)
32	II3	1	615	-	40,43,43	1.55	2 (5%)	47,60,60	1.71	12 (25%)
29	CLA	A	820	-	69,73,73	1.73	9 (13%)	82,113,113	1.28	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	8CT	B	850	-	40,41,41	0.37	1 (2%)	51,56,56	0.78	1 (1%)
31	II0	e	615	-	39,43,43	2.02	2 (5%)	48,60,60	1.39	6 (12%)
29	CLA	A	801	-	69,73,73	1.69	8 (11%)	82,113,113	1.23	10 (12%)
31	II0	1	617	-	39,43,43	2.04	2 (5%)	48,60,60	1.35	7 (14%)
29	CLA	B	841	-	56,60,73	1.89	9 (16%)	65,97,113	1.45	8 (12%)
29	CLA	L	201	-	69,73,73	1.73	9 (13%)	82,113,113	1.34	9 (10%)
29	CLA	e	610	-	55,59,73	1.94	9 (16%)	64,96,113	1.50	8 (12%)
29	CLA	a	602	25	59,63,73	1.86	9 (15%)	70,101,113	1.48	9 (12%)
37	8CT	F	201	-	40,41,41	0.46	1 (2%)	51,56,56	0.44	0
35	LHG	6	618	29	34,34,48	0.76	2 (5%)	37,40,54	1.21	3 (8%)
29	CLA	b	601	26	49,53,73	2.03	9 (18%)	58,89,113	1.53	8 (13%)
29	CLA	6	606	-	59,63,73	1.88	9 (15%)	70,101,113	1.47	8 (11%)
29	CLA	3	611	3	54,58,73	1.94	9 (16%)	64,95,113	1.45	8 (12%)
31	II0	6	614	-	39,43,43	2.02	2 (5%)	48,60,60	1.36	6 (12%)
29	CLA	d	604	-	64,68,73	1.82	9 (14%)	76,107,113	1.38	7 (9%)
29	CLA	3	604	-	69,73,73	1.71	9 (13%)	82,113,113	1.29	8 (9%)
29	CLA	6	611	-	59,63,73	1.85	9 (15%)	70,101,113	1.43	9 (12%)
31	II0	5	617	-	39,43,43	2.04	2 (5%)	48,60,60	1.40	7 (14%)
31	II0	3	617	-	39,43,43	2.02	2 (5%)	48,60,60	1.27	5 (10%)
31	II0	c	616	-	39,43,43	1.99	2 (5%)	48,60,60	1.22	4 (8%)
36	SQD	O	206	-	27,29,54	1.56	4 (14%)	37,40,65	1.44	5 (13%)
29	CLA	4	606	4	64,68,73	1.79	9 (14%)	76,107,113	1.35	9 (11%)
31	II0	B	843	-	39,43,43	2.04	2 (5%)	48,60,60	1.32	5 (10%)
29	CLA	A	842	-	69,73,73	1.72	9 (13%)	82,113,113	1.33	9 (10%)
31	II0	7	615	-	39,43,43	2.05	2 (5%)	48,60,60	1.34	8 (16%)
31	II0	c	617	-	39,43,43	2.01	2 (5%)	48,60,60	1.33	5 (10%)
29	CLA	A	808	-	59,63,73	1.84	9 (15%)	70,101,113	1.42	9 (12%)
31	II0	3	613	-	39,43,43	2.00	2 (5%)	48,60,60	1.28	6 (12%)
29	CLA	A	828	-	69,73,73	1.71	9 (13%)	82,113,113	1.25	9 (10%)
31	II0	2	614	-	39,43,43	2.00	2 (5%)	48,60,60	1.34	6 (12%)
35	LHG	2	619	-	38,38,48	0.69	0	41,44,54	1.26	4 (9%)
29	CLA	A	829	-	54,58,73	1.93	9 (16%)	64,95,113	1.50	8 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	IHT	L	205	-	-	2/25/65/65	0/2/2/2
29	CLA	A	818	-	1/1/15/20	7/39/115/115	-
29	CLA	Z	301	-	1/1/14/20	13/33/109/115	-
29	CLA	F	202	-	1/1/14/20	10/33/109/115	-
38	LMU	O	207	-	-	9/16/56/61	0/2/2/2
29	CLA	c	602	27	1/1/15/20	10/39/115/115	-
29	CLA	B	802	-	1/1/15/20	6/39/115/115	-
29	CLA	6	601	6	1/1/11/20	4/15/91/115	-
31	II0	3	616	-	-	2/21/67/67	0/2/2/2
38	LMU	e	617	-	-	7/17/57/61	0/2/2/2
29	CLA	5	603	-	1/1/11/20	3/15/91/115	-
37	8CT	4	616	-	-	5/29/63/63	0/2/2/2
37	8CT	A	848	-	-	0/29/63/63	0/2/2/2
29	CLA	A	821	-	1/1/13/20	3/27/103/115	-
29	CLA	8	604	-	1/1/15/20	6/39/115/115	-
29	CLA	A	840	-	1/1/13/20	4/27/103/115	-
31	II0	1	614	-	-	1/21/67/67	0/2/2/2
31	II0	c	619	-	-	2/21/67/67	0/2/2/2
29	CLA	a	607	25	1/1/15/20	4/39/115/115	-
39	PQN	A	849	-	-	11/23/43/43	0/2/2/2
29	CLA	A	834	10	1/1/13/20	5/27/103/115	-
29	CLA	e	603	28	1/1/12/20	6/21/97/115	-
35	LHG	3	619	-	-	23/53/53/53	-
29	CLA	b	608	-	1/1/15/20	12/39/115/115	-
37	8CT	I	101	-	-	4/29/63/63	0/2/2/2
29	CLA	B	832	-	1/1/15/20	15/39/115/115	-
35	LHG	3	622	30	-	13/38/38/53	-
29	CLA	6	612	-	1/1/11/20	6/15/91/115	-
29	CLA	9	604	-	1/1/13/20	3/27/103/115	-
29	CLA	1	609	-	1/1/10/20	2/10/86/115	-
30	KC2	3	606	35	-	8/15/71/71	-
29	CLA	B	818	-	1/1/14/20	5/33/109/115	-
29	CLA	J	102	17	1/1/10/20	1/10/86/115	-
31	II0	b	612	-	-	1/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	KC2	4	605	4	-	6/15/71/71	-
31	II0	c	618	-	-	2/21/67/67	0/2/2/2
31	II0	a	614	-	-	1/21/67/67	0/2/2/2
35	LHG	A	851	-	-	21/43/43/53	-
31	II0	O	205	-	-	1/21/67/67	0/2/2/2
29	CLA	K	102	-	1/1/13/20	3/27/103/115	-
29	CLA	A	809	29	1/1/14/20	6/33/109/115	-
29	CLA	c	606	-	1/1/15/20	13/39/115/115	-
34	LMG	I	102	-	-	22/46/66/70	0/1/1/1
29	CLA	8	603	-	1/1/15/20	11/39/115/115	-
35	LHG	L	208	-	-	15/38/38/53	-
29	CLA	1	606	-	1/1/11/20	0/15/91/115	-
29	CLA	F	204	15	1/1/13/20	6/27/103/115	-
29	CLA	A	804	10	1/1/15/20	13/39/115/115	-
29	CLA	2	602	2	1/1/13/20	12/32/108/115	-
29	CLA	A	836	-	1/1/13/20	2/27/103/115	-
29	CLA	Z	306	24	1/1/14/20	12/33/109/115	-
33	IHT	1	618	-	-	2/25/65/65	0/2/2/2
29	CLA	9	611	-	1/1/10/20	2/10/86/115	-
29	CLA	B	830	-	1/1/14/20	1/33/109/115	-
29	CLA	B	826	-	1/1/15/20	12/39/115/115	-
32	II3	b	613	-	-	1/25/67/67	0/2/2/2
34	LMG	8	614	-	-	23/47/67/70	0/1/1/1
30	KC2	d	610	25	-	8/15/71/71	-
29	CLA	2	604	2	1/1/13/20	2/27/103/115	-
29	CLA	6	605	6	1/1/13/20	7/27/103/115	-
29	CLA	9	603	-	1/1/11/20	3/15/91/115	-
29	CLA	7	611	-	1/1/13/20	3/27/103/115	-
35	LHG	a	618	-	-	15/33/33/53	-
29	CLA	A	823	-	1/1/15/20	12/39/115/115	-
29	CLA	A	839	-	1/1/15/20	12/39/115/115	-
29	CLA	A	806	10	1/1/15/20	8/39/115/115	-
29	CLA	A	814	-	1/1/11/20	3/15/91/115	-
29	CLA	7	609	35	1/1/10/20	2/10/86/115	-
29	CLA	B	821	-	1/1/14/20	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LHG	8	613	-	-	23/37/37/53	-
37	8CT	B	851	-	-	9/29/63/63	0/2/2/2
29	CLA	5	611	-	1/1/11/20	5/15/91/115	-
31	II0	d	614	-	-	2/21/67/67	0/2/2/2
34	LMG	F	205	-	-	13/27/47/70	0/1/1/1
33	IHT	K	104	-	-	1/25/65/65	0/2/2/2
29	CLA	4	610	-	1/1/15/20	5/39/115/115	-
29	CLA	B	811	-	1/1/13/20	8/27/103/115	-
39	PQN	B	842	-	-	5/23/43/43	0/2/2/2
37	8CT	A	845	-	-	1/29/63/63	0/2/2/2
33	IHT	Z	302	-	-	2/25/65/65	0/2/2/2
29	CLA	A	837	-	1/1/15/20	10/39/115/115	-
33	IHT	5	618	-	-	1/25/65/65	0/2/2/2
35	LHG	4	617	29	-	18/51/51/53	-
29	CLA	B	836	-	1/1/11/20	2/18/94/115	-
29	CLA	B	823	-	1/1/15/20	11/39/115/115	-
29	CLA	B	840	-	1/1/15/20	2/39/115/115	-
31	II0	9	615	-	-	2/21/67/67	0/2/2/2
29	CLA	8	602	8	1/1/11/20	4/15/91/115	-
29	CLA	A	817	-	1/1/15/20	11/39/115/115	-
29	CLA	Z	304	24	1/1/13/20	3/27/103/115	-
29	CLA	A	816	-	1/1/14/20	9/33/109/115	-
29	CLA	a	601	25	1/1/11/20	3/15/91/115	-
31	II0	a	619	-	-	1/21/67/67	0/2/2/2
29	CLA	2	601	2	1/1/10/20	3/12/88/115	-
29	CLA	A	841	-	1/1/15/20	5/39/115/115	-
29	CLA	d	606	-	1/1/10/20	0/10/86/115	-
31	II0	d	616	-	-	4/21/67/67	0/2/2/2
35	LHG	7	619	29	-	20/43/43/53	-
35	LHG	d	619	-	-	20/43/43/53	-
36	SQD	3	621	-	-	16/37/57/69	0/1/1/1
29	CLA	B	815	-	1/1/15/20	10/39/115/115	-
29	CLA	6	607	6	1/1/13/20	4/27/103/115	-
29	CLA	B	808	-	1/1/15/20	12/39/115/115	-
29	CLA	B	812	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	L	203	-	1/1/14/20	7/33/109/115	-
31	II0	d	615	-	-	2/21/67/67	0/2/2/2
35	LHG	A	850	-	-	21/53/53/53	-
29	CLA	b	610	26	1/1/12/20	7/23/99/115	-
38	LMU	J	104	-	-	10/17/57/61	0/2/2/2
29	CLA	A	802	29	1/1/13/20	4/27/103/115	-
29	CLA	5	602	5	1/1/13/20	5/27/103/115	-
29	CLA	9	612	-	1/1/11/20	4/15/91/115	-
29	CLA	A	835	-	1/1/14/20	5/33/109/115	-
29	CLA	8	605	8	1/1/12/20	2/21/97/115	-
35	LHG	2	620	-	-	16/46/46/53	-
29	CLA	d	607	25	1/1/15/20	6/39/115/115	-
29	CLA	9	614	-	1/1/10/20	2/10/86/115	-
31	II0	3	614	-	-	0/21/67/67	0/2/2/2
29	CLA	A	805	-	1/1/12/20	3/21/97/115	-
29	CLA	B	803	-	1/1/15/20	11/39/115/115	-
29	CLA	O	202	-	1/1/13/20	9/27/103/115	-
29	CLA	d	603	-	1/1/12/20	2/21/97/115	-
31	II0	5	615	-	-	2/21/67/67	0/2/2/2
29	CLA	L	207	-	1/1/10/20	4/10/86/115	-
29	CLA	a	605	-	1/1/13/20	12/27/103/115	-
29	CLA	7	601	7	1/1/11/20	2/15/91/115	-
29	CLA	8	601	8	1/1/11/20	2/15/91/115	-
29	CLA	A	830	-	1/1/14/20	5/33/109/115	-
37	8CT	B	846	-	-	8/29/63/63	0/2/2/2
29	CLA	B	824	-	1/1/14/20	3/33/109/115	-
29	CLA	a	606	-	1/1/15/20	8/39/115/115	-
35	LHG	d	618	-	-	7/26/26/53	-
30	KC2	c	610	27	-	4/15/71/71	-
29	CLA	4	602	4	1/1/13/20	4/32/108/115	-
29	CLA	Z	305	24	1/1/12/20	2/21/97/115	-
29	CLA	b	611	-	1/1/13/20	3/27/103/115	-
29	CLA	B	805	-	1/1/15/20	8/39/115/115	-
30	KC2	c	611	-	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	II0	4	613	-	-	0/21/67/67	0/2/2/2
29	CLA	b	607	26	1/1/14/20	3/33/109/115	-
29	CLA	B	822	-	1/1/15/20	9/39/115/115	-
29	CLA	3	608	3	1/1/14/20	5/33/109/115	-
29	CLA	e	602	28	1/1/13/20	11/27/103/115	-
29	CLA	O	201	-	1/1/13/20	1/27/103/115	-
37	8CT	B	847	-	-	4/29/63/63	0/2/2/2
29	CLA	1	602	1	1/1/13/20	4/32/108/115	-
29	CLA	4	601	4	1/1/13/20	7/27/103/115	-
29	CLA	7	604	7	1/1/12/20	7/25/101/115	-
29	CLA	3	612	-	1/1/11/20	4/15/91/115	-
31	II0	1	619	-	-	0/21/67/67	0/2/2/2
31	II0	e	614	-	-	1/21/67/67	0/2/2/2
33	IHT	6	617	-	-	3/25/65/65	0/2/2/2
35	LHG	Z	310	-	-	23/50/50/53	-
29	CLA	c	601	27	1/1/11/20	2/15/91/115	-
29	CLA	9	605	-	1/1/11/20	0/15/91/115	-
29	CLA	2	606	-	1/1/11/20	2/15/91/115	-
29	CLA	9	601	9	1/1/11/20	5/15/91/115	-
29	CLA	8	608	-	1/1/15/20	7/39/115/115	-
29	CLA	B	833	-	1/1/11/20	2/15/91/115	-
29	CLA	c	603	-	1/1/15/20	13/39/115/115	-
38	LMU	4	618	-	-	12/21/61/61	0/2/2/2
29	CLA	e	604	-	1/1/14/20	2/33/109/115	-
29	CLA	A	838	-	1/1/15/20	7/39/115/115	-
29	CLA	1	604	1	1/1/11/20	3/15/91/115	-
29	CLA	F	203	-	1/1/11/20	3/15/91/115	-
30	KC2	a	610	-	-	2/15/71/71	-
29	CLA	3	602	3	1/1/13/20	2/27/103/115	-
29	CLA	6	602	6	1/1/15/20	5/39/115/115	-
37	8CT	L	206	-	-	3/29/63/63	0/2/2/2
35	LHG	7	618	-	-	9/35/35/53	-
29	CLA	5	606	-	1/1/11/20	4/15/91/115	-
31	II0	8	612	-	-	1/21/67/67	0/2/2/2
29	CLA	3	607	3	1/1/14/20	5/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	II0	4	612	-	-	2/21/67/67	0/2/2/2
31	II0	4	615	-	-	0/21/67/67	0/2/2/2
31	II0	a	613	-	-	1/21/67/67	0/2/2/2
29	CLA	d	605	25	1/1/11/20	4/15/91/115	-
29	CLA	A	811	-	1/1/15/20	11/39/115/115	-
30	KC2	9	610	9	-	6/15/71/71	-
31	II0	2	615	-	-	2/21/67/67	0/2/2/2
31	II0	6	616	-	-	2/21/67/67	0/2/2/2
29	CLA	b	603	-	1/1/14/20	8/33/109/115	-
30	KC2	e	605	28	-	7/15/71/71	-
31	II0	R	204	-	-	1/21/67/67	0/2/2/2
29	CLA	3	603	-	1/1/14/20	4/33/109/115	-
29	CLA	B	820	-	1/1/14/20	10/33/109/115	-
29	CLA	6	603	-	1/1/11/20	7/15/91/115	-
29	CLA	e	606	28	1/1/14/20	9/33/109/115	-
29	CLA	c	604	-	1/1/14/20	5/33/109/115	-
31	II0	O	204	-	-	2/21/67/67	0/2/2/2
37	8CT	B	845	-	-	8/29/63/63	0/2/2/2
29	CLA	a	612	-	1/1/15/20	7/39/115/115	-
29	CLA	B	835	-	1/1/15/20	8/39/115/115	-
29	CLA	2	607	2	1/1/11/20	2/15/91/115	-
34	LMG	2	617	-	-	7/31/51/70	0/1/1/1
29	CLA	9	613	9	1/1/11/20	5/15/91/115	-
31	II0	8	610	-	-	2/21/67/67	0/2/2/2
40	SF4	C	102	12	-	-	0/6/5/5
34	LMG	6	619	-	-	5/27/47/70	0/1/1/1
29	CLA	A	813	-	1/1/10/20	0/12/88/115	-
29	CLA	d	601	25	1/1/11/20	4/15/91/115	-
29	CLA	A	825	-	1/1/15/20	6/39/115/115	-
29	CLA	B	804	-	1/1/11/20	5/15/91/115	-
29	CLA	L	204	-	1/1/12/20	6/21/97/115	-
30	KC2	c	615	-	-	6/15/71/71	-
34	LMG	3	618	-	-	10/25/45/70	0/1/1/1
29	CLA	9	606	-	1/1/14/20	12/38/114/115	-
31	II0	a	616	-	-	0/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	8	607	8	1/1/10/20	4/10/86/115	-
29	CLA	e	607	28	1/1/11/20	2/15/91/115	-
37	8CT	Z	309	-	-	6/29/63/63	0/2/2/2
29	CLA	c	607	27	1/1/15/20	11/39/115/115	-
29	CLA	5	612	-	1/1/11/20	3/15/91/115	-
29	CLA	B	806	-	1/1/15/20	12/39/115/115	-
29	CLA	e	611	-	1/1/15/20	10/39/115/115	-
29	CLA	B	827	-	1/1/15/20	5/39/115/115	-
29	CLA	B	838	-	1/1/15/20	5/39/115/115	-
29	CLA	A	812	-	1/1/13/20	3/27/103/115	-
29	CLA	c	608	27	1/1/14/20	10/33/109/115	-
29	CLA	a	608	25	1/1/14/20	2/33/109/115	-
29	CLA	b	602	26	1/1/14/20	14/38/114/115	-
29	CLA	9	608	9	1/1/13/20	11/27/103/115	-
31	II0	7	613	-	-	1/21/67/67	0/2/2/2
37	8CT	M	101	-	-	6/29/63/63	0/2/2/2
37	8CT	7	617	-	-	9/29/63/63	0/2/2/2
31	II0	6	615	-	-	2/21/67/67	0/2/2/2
29	CLA	B	837	-	1/1/15/20	6/39/115/115	-
29	CLA	6	608	6	1/1/14/20	6/33/109/115	-
37	8CT	R	201	-	-	7/29/63/63	0/2/2/2
37	8CT	B	844	-	-	4/29/63/63	0/2/2/2
31	II0	7	614	-	-	1/21/67/67	0/2/2/2
37	8CT	e	616	-	-	1/29/63/63	0/2/2/2
29	CLA	5	604	-	1/1/13/20	7/27/103/115	-
29	CLA	7	607	7	1/1/11/20	2/15/91/115	-
31	II0	8	611	-	-	2/21/67/67	0/2/2/2
30	KC2	6	613	6	-	8/15/71/71	-
29	CLA	A	844	-	1/1/15/20	8/39/115/115	-
30	KC2	e	609	-	-	6/15/71/71	-
35	LHG	b	616	-	-	26/53/53/53	-
31	II0	5	614	-	-	2/21/67/67	0/2/2/2
29	CLA	6	609	35	1/1/10/20	2/10/86/115	-
29	CLA	R	202	-	1/1/13/20	7/27/103/115	-
35	LHG	3	623	-	-	24/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	8CT	A	846	-	-	4/29/63/63	0/2/2/2
29	CLA	4	609	4	1/1/14/20	5/33/109/115	-
29	CLA	B	816	-	1/1/13/20	14/32/108/115	-
29	CLA	4	607	4	1/1/14/20	9/33/109/115	-
31	II0	a	615	-	-	1/21/67/67	0/2/2/2
29	CLA	2	611	-	1/1/11/20	0/15/91/115	-
32	II3	e	613	-	-	3/25/67/67	0/2/2/2
29	CLA	7	605	7	1/1/11/20	6/15/91/115	-
29	CLA	B	819	-	1/1/14/20	8/33/109/115	-
31	II0	9	617	-	-	2/21/67/67	0/2/2/2
29	CLA	2	609	-	1/1/10/20	1/10/86/115	-
29	CLA	A	803	-	1/1/15/20	6/39/115/115	-
29	CLA	1	612	-	1/1/14/20	9/33/109/115	-
30	KC2	6	610	6	-	6/15/71/71	-
37	8CT	A	847	-	-	8/29/63/63	0/2/2/2
29	CLA	2	603	-	1/1/12/20	4/21/97/115	-
29	CLA	d	602	25	1/1/14/20	10/38/114/115	-
29	CLA	5	601	5	1/1/10/20	2/10/86/115	-
29	CLA	5	609	-	1/1/10/20	2/10/86/115	-
31	II0	7	616	-	-	1/21/67/67	0/2/2/2
29	CLA	5	607	5	1/1/11/20	2/15/91/115	-
31	II0	d	613	-	-	2/21/67/67	0/2/2/2
29	CLA	K	101	-	1/1/15/20	8/39/115/115	-
29	CLA	1	613	-	1/1/11/20	3/15/91/115	-
29	CLA	A	810	-	1/1/15/20	17/39/115/115	-
29	CLA	O	203	-	1/1/13/20	10/27/103/115	-
31	II0	5	616	-	-	0/21/67/67	0/2/2/2
37	8CT	A	852	-	-	6/29/63/63	0/2/2/2
31	II0	5	620	-	-	1/21/67/67	0/2/2/2
35	LHG	c	621	-	-	15/33/33/53	-
33	IHT	d	617	-	-	1/25/65/65	0/2/2/2
29	CLA	3	609	-	1/1/15/20	3/39/115/115	-
29	CLA	c	605	-	1/1/11/20	5/15/91/115	-
29	CLA	A	824	-	1/1/15/20	5/39/115/115	-
29	CLA	a	609	-	1/1/14/20	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	KC2	2	610	-	-	9/15/71/71	-
29	CLA	4	604	-	1/1/13/20	9/27/103/115	-
41	DGD	Z	303	-	-	27/49/89/95	0/2/2/2
29	CLA	a	603	-	1/1/14/20	7/33/109/115	-
29	CLA	d	612	-	1/1/14/20	4/37/113/115	-
41	DGD	B	848	-	-	17/48/88/95	0/2/2/2
29	CLA	B	817	-	1/1/14/20	1/33/109/115	-
29	CLA	B	831	-	1/1/13/20	9/27/103/115	-
29	CLA	4	608	35	1/1/15/20	4/39/115/115	-
29	CLA	L	202	19	1/1/12/20	0/23/99/115	-
29	CLA	B	814	-	1/1/10/20	4/12/88/115	-
29	CLA	A	822	-	1/1/15/20	8/39/115/115	-
29	CLA	7	612	-	1/1/12/20	6/21/97/115	-
29	CLA	A	827	-	1/1/15/20	5/39/115/115	-
29	CLA	8	615	-	1/1/15/20	7/39/115/115	-
29	CLA	5	613	5	1/1/10/20	4/10/86/115	-
31	II0	9	618	-	-	2/21/67/67	0/2/2/2
29	CLA	b	604	-	1/1/15/20	12/39/115/115	-
40	SF4	B	801	10,11	-	-	0/6/5/5
35	LHG	4	619	-	-	18/49/49/53	-
29	CLA	4	611	-	1/1/15/20	12/39/115/115	-
29	CLA	1	605	-	1/1/10/20	3/11/87/115	-
31	II0	9	616	-	-	2/21/67/67	0/2/2/2
29	CLA	1	601	1	1/1/11/20	4/15/91/115	-
38	LMU	7	620	-	-	8/21/61/61	0/2/2/2
29	CLA	2	605	2	1/1/14/20	5/33/109/115	-
29	CLA	c	613	27	1/1/11/20	7/15/91/115	-
29	CLA	e	601	28	1/1/11/20	5/15/91/115	-
29	CLA	1	603	-	1/1/12/20	4/24/100/115	-
29	CLA	9	609	-	1/1/10/20	1/10/86/115	-
29	CLA	5	605	5	1/1/11/20	2/15/91/115	-
29	CLA	4	603	-	1/1/12/20	5/26/102/115	-
29	CLA	A	826	-	1/1/15/20	5/39/115/115	-
35	LHG	B	849	29	-	18/49/49/53	-
29	CLA	1	608	1	1/1/14/20	5/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	819	-	1/1/15/20	5/39/115/115	-
29	CLA	3	601	3	1/1/11/20	6/15/91/115	-
29	CLA	2	608	2	1/1/14/20	4/33/109/115	-
29	CLA	a	611	-	1/1/13/20	6/27/103/115	-
29	CLA	7	603	-	1/1/13/20	3/27/103/115	-
29	CLA	B	829	-	1/1/11/20	0/15/91/115	-
29	CLA	2	612	-	1/1/11/20	5/15/91/115	-
29	CLA	a	604	25	1/1/14/20	12/33/109/115	-
29	CLA	b	606	26	1/1/15/20	5/39/115/115	-
31	II0	b	614	-	-	1/21/67/67	0/2/2/2
29	CLA	5	608	-	1/1/14/20	12/33/109/115	-
31	II0	e	612	-	-	0/21/67/67	0/2/2/2
29	CLA	c	609	-	1/1/10/20	2/10/86/115	-
29	CLA	A	832	-	1/1/15/20	8/39/115/115	-
33	IHT	c	620	-	-	1/25/65/65	0/2/2/2
37	8CT	R	203	-	-	4/29/63/63	0/2/2/2
37	8CT	K	103	-	-	2/29/63/63	0/2/2/2
31	II0	J	101	-	-	1/21/67/67	0/2/2/2
30	KC2	b	605	26	-	6/15/71/71	-
29	CLA	3	605	3	1/1/13/20	4/27/103/115	-
37	8CT	Z	308	-	-	3/29/63/63	0/2/2/2
31	II0	2	613	-	-	2/21/67/67	0/2/2/2
33	IHT	2	616	-	-	2/25/65/65	0/2/2/2
31	II0	3	615	-	-	1/21/67/67	0/2/2/2
29	CLA	A	831	-	1/1/15/20	10/39/115/115	-
30	KC2	Z	307	-	-	8/15/71/71	-
33	IHT	8	609	-	-	1/25/65/65	0/2/2/2
29	CLA	A	815	-	1/1/14/20	2/36/112/115	-
29	CLA	3	610	-	1/1/15/20	7/39/115/115	-
34	LMG	3	620	-	-	12/27/47/70	0/1/1/1
30	KC2	5	610	5	-	4/15/71/71	-
29	CLA	B	834	-	1/1/13/20	3/27/103/115	-
40	SF4	C	101	12	-	-	0/6/5/5
29	CLA	B	807	-	1/1/15/20	6/39/115/115	-
35	LHG	5	619	-	-	13/26/26/53	-
29	CLA	d	611	-	1/1/12/20	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	II0	8	616	-	-	0/21/67/67	0/2/2/2
35	LHG	2	618	-	-	9/24/24/53	-
29	CLA	d	609	-	1/1/10/20	0/10/86/115	-
30	KC2	7	606	-	-	7/15/71/71	-
30	KC2	7	610	7	-	6/15/71/71	-
29	CLA	B	810	-	1/1/14/20	5/33/109/115	-
29	CLA	B	809	11	1/1/15/20	10/39/115/115	-
29	CLA	A	807	10	1/1/12/20	2/21/97/115	-
29	CLA	7	608	7	1/1/13/20	12/27/103/115	-
29	CLA	1	611	-	1/1/11/20	2/15/91/115	-
33	IHT	9	619	-	-	4/25/65/65	0/2/2/2
29	CLA	1	607	1	1/1/11/20	0/15/91/115	-
29	CLA	e	608	-	1/1/10/20	2/10/86/115	-
29	CLA	9	607	9	1/1/15/20	10/39/115/115	-
29	CLA	A	833	-	1/1/15/20	7/39/115/115	-
30	KC2	b	609	-	-	2/15/71/71	-
31	II0	1	616	-	-	1/21/67/67	0/2/2/2
29	CLA	9	602	9	1/1/13/20	10/27/103/115	-
29	CLA	8	606	8	1/1/13/20	4/27/103/115	-
37	8CT	b	615	-	-	5/29/63/63	0/2/2/2
29	CLA	6	604	-	1/1/14/20	5/33/109/115	-
29	CLA	B	828	-	1/1/15/20	7/39/115/115	-
29	CLA	A	843	-	1/1/15/20	8/39/115/115	-
29	CLA	B	839	35	1/1/15/20	4/39/115/115	-
31	II0	4	614	-	-	1/21/67/67	0/2/2/2
29	CLA	7	602	7	1/1/15/20	5/39/115/115	-
30	KC2	1	610	1	-	8/15/71/71	-
37	8CT	J	103	-	-	7/29/63/63	0/2/2/2
29	CLA	B	813	-	1/1/14/20	9/35/111/115	-
29	CLA	B	825	-	1/1/15/20	4/39/115/115	-
29	CLA	c	612	-	1/1/13/20	4/27/103/115	-
33	IHT	a	617	-	-	4/25/65/65	0/2/2/2
29	CLA	d	608	25	1/1/15/20	5/39/115/115	-
29	CLA	c	614	-	1/1/13/20	8/27/103/115	-
32	II3	1	615	-	-	1/25/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	820	-	1/1/15/20	7/39/115/115	-
37	8CT	B	850	-	-	4/29/63/63	0/2/2/2
31	II0	e	615	-	-	0/21/67/67	0/2/2/2
29	CLA	A	801	-	1/1/15/20	8/39/115/115	-
31	II0	1	617	-	-	1/21/67/67	0/2/2/2
29	CLA	B	841	-	1/1/12/20	8/24/100/115	-
29	CLA	L	201	-	1/1/15/20	12/39/115/115	-
29	CLA	e	610	-	1/1/12/20	5/23/99/115	-
29	CLA	a	602	25	1/1/13/20	9/27/103/115	-
37	8CT	F	201	-	-	3/29/63/63	0/2/2/2
35	LHG	6	618	29	-	16/39/39/53	-
29	CLA	b	601	26	1/1/11/20	3/15/91/115	-
29	CLA	6	606	-	1/1/13/20	8/27/103/115	-
29	CLA	3	611	3	1/1/12/20	3/21/97/115	-
31	II0	6	614	-	-	1/21/67/67	0/2/2/2
29	CLA	d	604	-	1/1/14/20	5/33/109/115	-
29	CLA	3	604	-	1/1/15/20	3/39/115/115	-
29	CLA	6	611	-	1/1/13/20	2/27/103/115	-
31	II0	5	617	-	-	2/21/67/67	0/2/2/2
31	II0	3	617	-	-	1/21/67/67	0/2/2/2
31	II0	c	616	-	-	2/21/67/67	0/2/2/2
36	SQD	O	206	-	-	11/24/44/69	0/1/1/1
29	CLA	4	606	4	1/1/14/20	6/33/109/115	-
31	II0	B	843	-	-	2/21/67/67	0/2/2/2
29	CLA	A	842	-	1/1/15/20	6/39/115/115	-
31	II0	7	615	-	-	2/21/67/67	0/2/2/2
31	II0	c	617	-	-	0/21/67/67	0/2/2/2
29	CLA	A	808	-	1/1/13/20	1/27/103/115	-
31	II0	3	613	-	-	2/21/67/67	0/2/2/2
29	CLA	A	828	-	1/1/15/20	7/39/115/115	-
31	II0	2	614	-	-	0/21/67/67	0/2/2/2
35	LHG	2	619	-	-	17/43/43/53	-
29	CLA	A	829	-	1/1/12/20	5/21/97/115	-

The worst 5 of 2598 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	K	104	IHT	C10-C07	10.52	1.52	1.34
30	b	609	KC2	MG-ND	-10.26	1.85	2.05
33	1	618	IHT	C10-C07	10.23	1.51	1.34
30	3	606	KC2	MG-ND	-10.16	1.85	2.05
30	2	610	KC2	MG-ND	-10.14	1.85	2.05

The worst 5 of 2993 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	8	609	IHT	C02-C07-C10	-10.58	108.18	122.64
33	9	619	IHT	C02-C07-C10	-10.52	108.27	122.64
33	d	617	IHT	C02-C07-C10	-9.69	109.40	122.64
33	5	618	IHT	C02-C07-C10	-9.26	109.98	122.64
33	L	205	IHT	C02-C07-C10	-9.16	110.12	122.64

5 of 254 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	1	601	CLA	ND
29	1	602	CLA	ND
29	1	603	CLA	ND
29	1	604	CLA	ND
29	1	605	CLA	ND

5 of 2451 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	1	603	CLA	C1A-C2A-CAA-CBA
29	1	605	CLA	C2B-C3B-CAB-CBB
29	1	605	CLA	C4B-C3B-CAB-CBB
29	2	601	CLA	C3A-C2A-CAA-CBA
29	2	602	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

90 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	O	207	LMU	4	0
29	c	602	CLA	1	0
37	4	616	8CT	1	0
29	A	821	CLA	1	0
31	1	614	II0	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	A	834	CLA	1	0
29	B	832	CLA	1	0
29	6	612	CLA	1	0
29	9	604	CLA	2	0
29	1	609	CLA	1	0
29	B	818	CLA	3	0
29	8	603	CLA	1	0
35	L	208	LHG	1	0
29	A	836	CLA	2	0
29	Z	306	CLA	1	0
29	9	611	CLA	2	0
29	B	826	CLA	1	0
32	b	613	II3	1	0
29	7	611	CLA	2	0
29	A	823	CLA	1	0
29	7	609	CLA	1	0
29	B	823	CLA	1	0
29	Z	304	CLA	1	0
29	B	815	CLA	1	0
29	B	808	CLA	1	0
29	b	610	CLA	1	0
38	J	104	LMU	1	0
29	8	605	CLA	1	0
31	3	614	II0	1	0
29	B	803	CLA	1	0
30	c	611	KC2	3	0
31	4	613	II0	1	0
29	O	201	CLA	2	0
33	6	617	IHT	1	0
29	c	601	CLA	2	0
29	8	608	CLA	1	0
38	4	618	LMU	1	0
29	1	604	CLA	1	0
29	B	835	CLA	1	0
31	8	610	II0	1	0
40	C	102	SF4	1	0
29	9	606	CLA	1	0
31	a	616	II0	1	0
29	5	612	CLA	1	0
29	e	611	CLA	2	0
29	9	608	CLA	1	0
37	7	617	8CT	1	0

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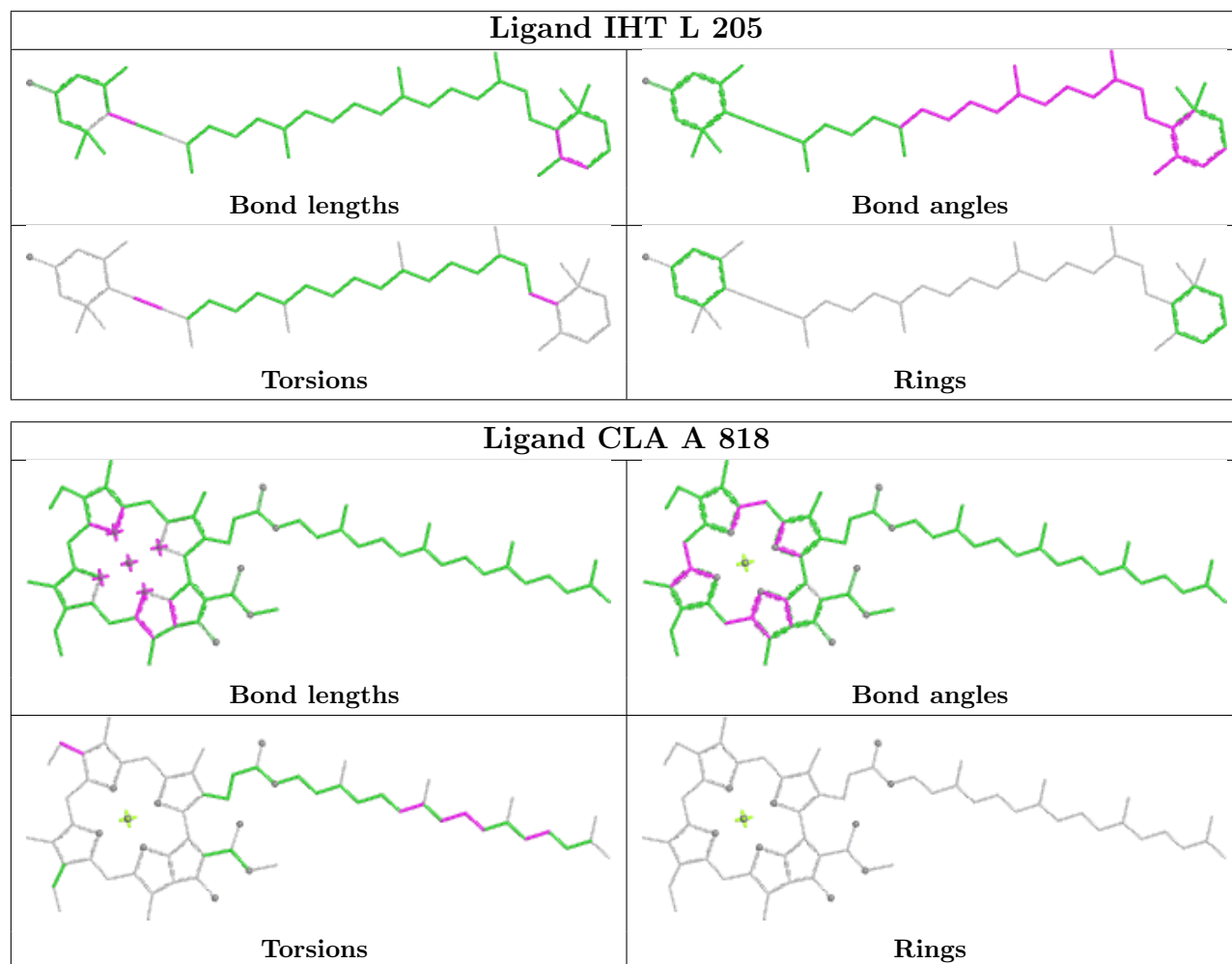
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	5	604	CLA	2	0
29	A	844	CLA	1	0
31	5	614	II0	2	0
29	B	816	CLA	2	0
31	a	615	II0	1	0
29	5	609	CLA	2	0
29	1	613	CLA	1	0
29	A	810	CLA	2	0
29	O	203	CLA	2	0
31	5	620	II0	1	0
33	d	617	IHT	1	0
29	A	824	CLA	1	0
41	Z	303	DGD	1	0
29	a	603	CLA	1	0
29	d	612	CLA	1	0
29	L	202	CLA	1	0
29	7	612	CLA	1	0
29	8	615	CLA	1	0
29	b	604	CLA	1	0
29	4	611	CLA	2	0
29	1	605	CLA	1	0
29	1	601	CLA	1	0
38	7	620	LMU	1	0
29	A	826	CLA	2	0
29	2	612	CLA	1	0
29	5	608	CLA	1	0
29	c	609	CLA	1	0
33	c	620	IHT	1	0
33	2	616	IHT	1	0
29	B	834	CLA	1	0
29	B	809	CLA	1	0
29	1	611	CLA	2	0
33	9	619	IHT	1	0
30	b	609	KC2	1	0
31	4	614	II0	1	0
29	c	612	CLA	1	0
33	a	617	IHT	1	0
29	c	614	CLA	2	0
29	L	201	CLA	1	0
29	e	610	CLA	1	0
37	F	201	8CT	1	0
29	A	842	CLA	1	0

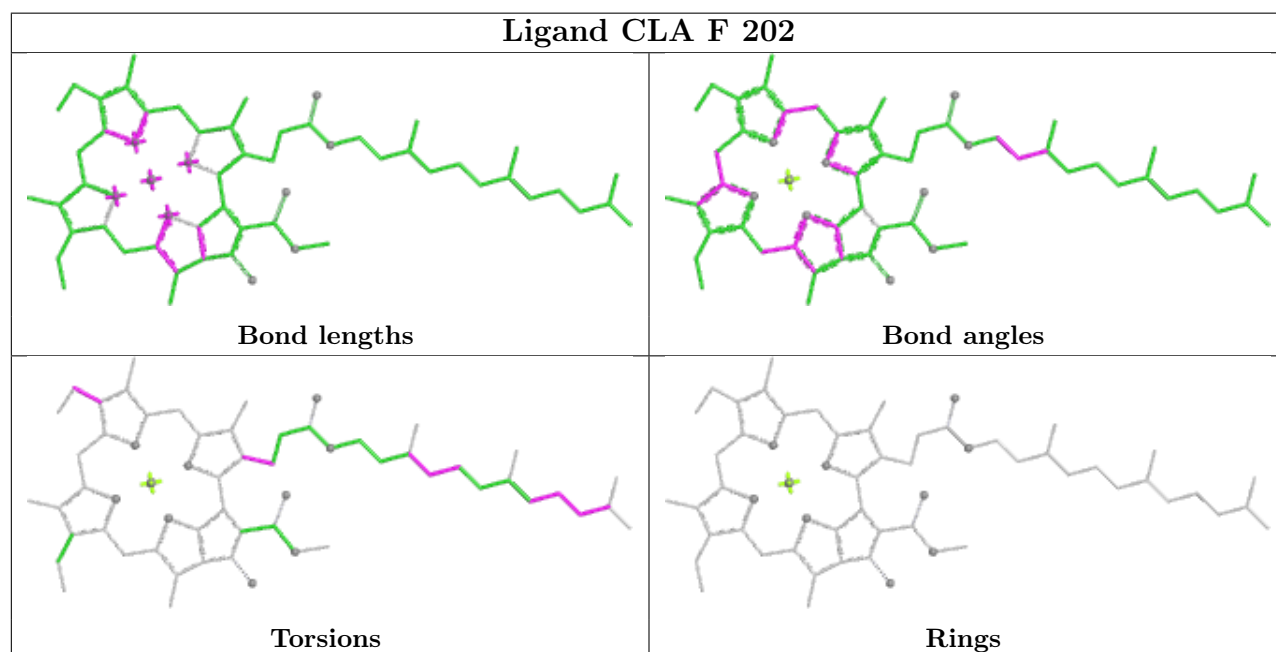
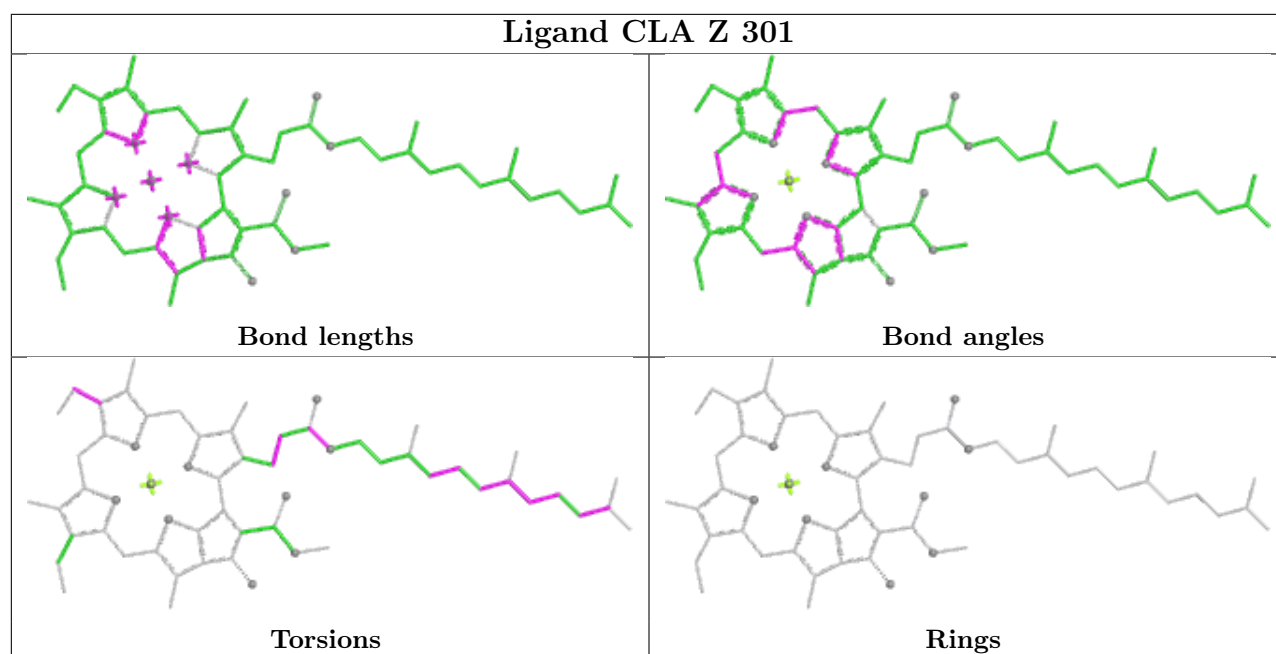
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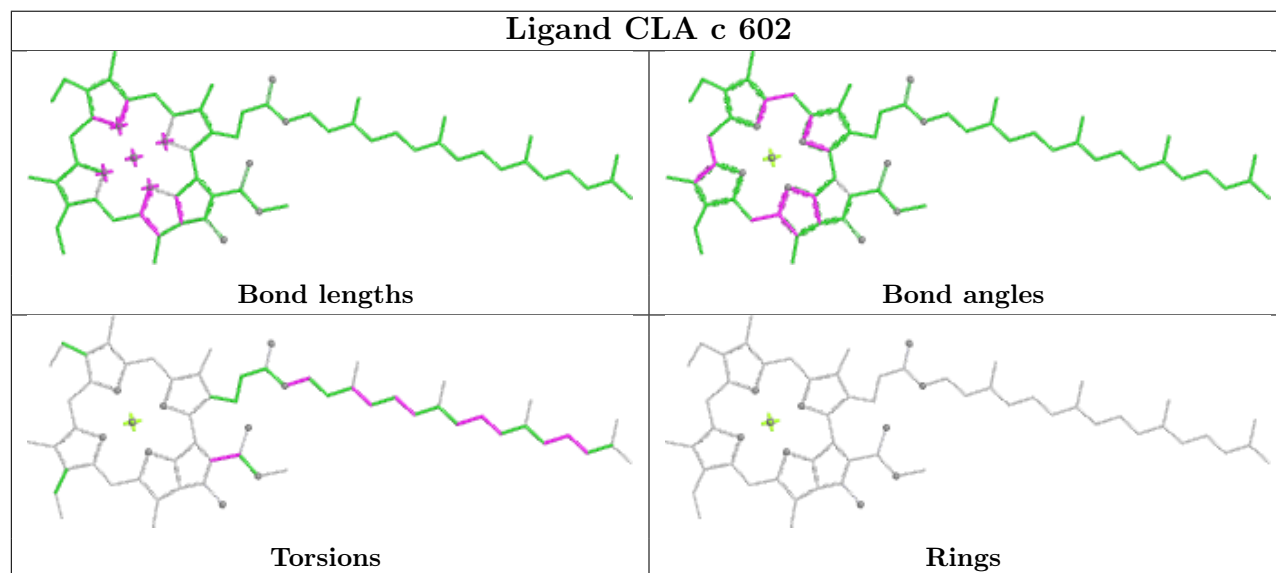
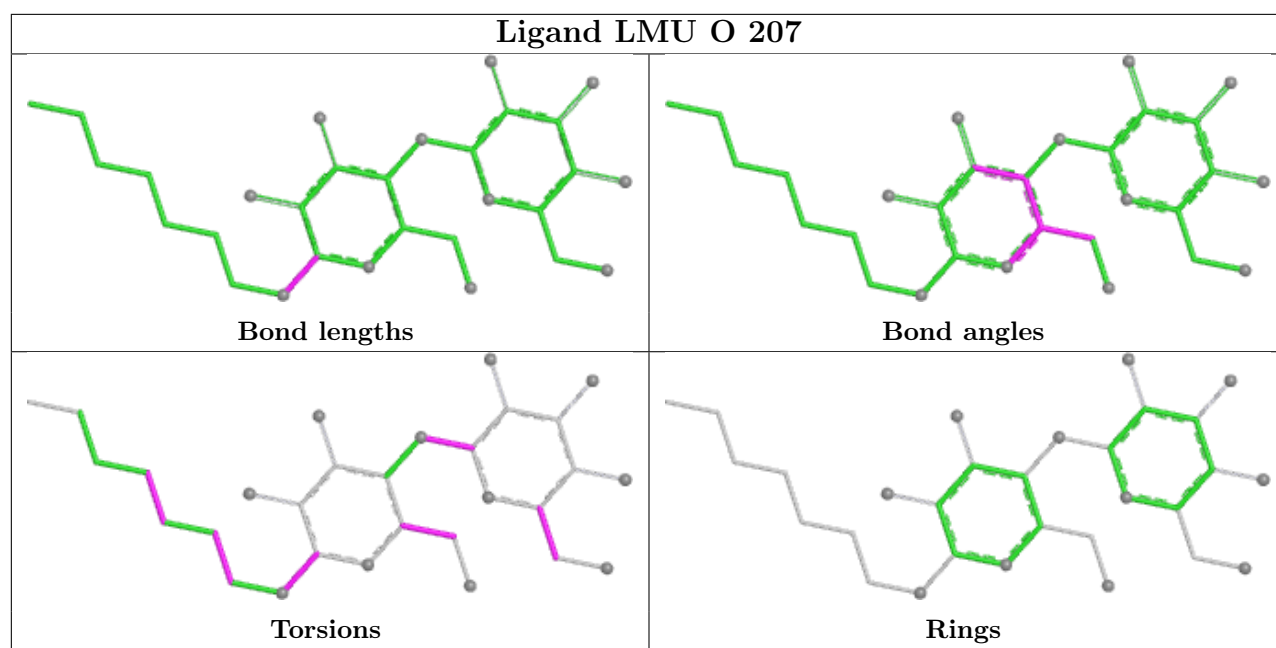
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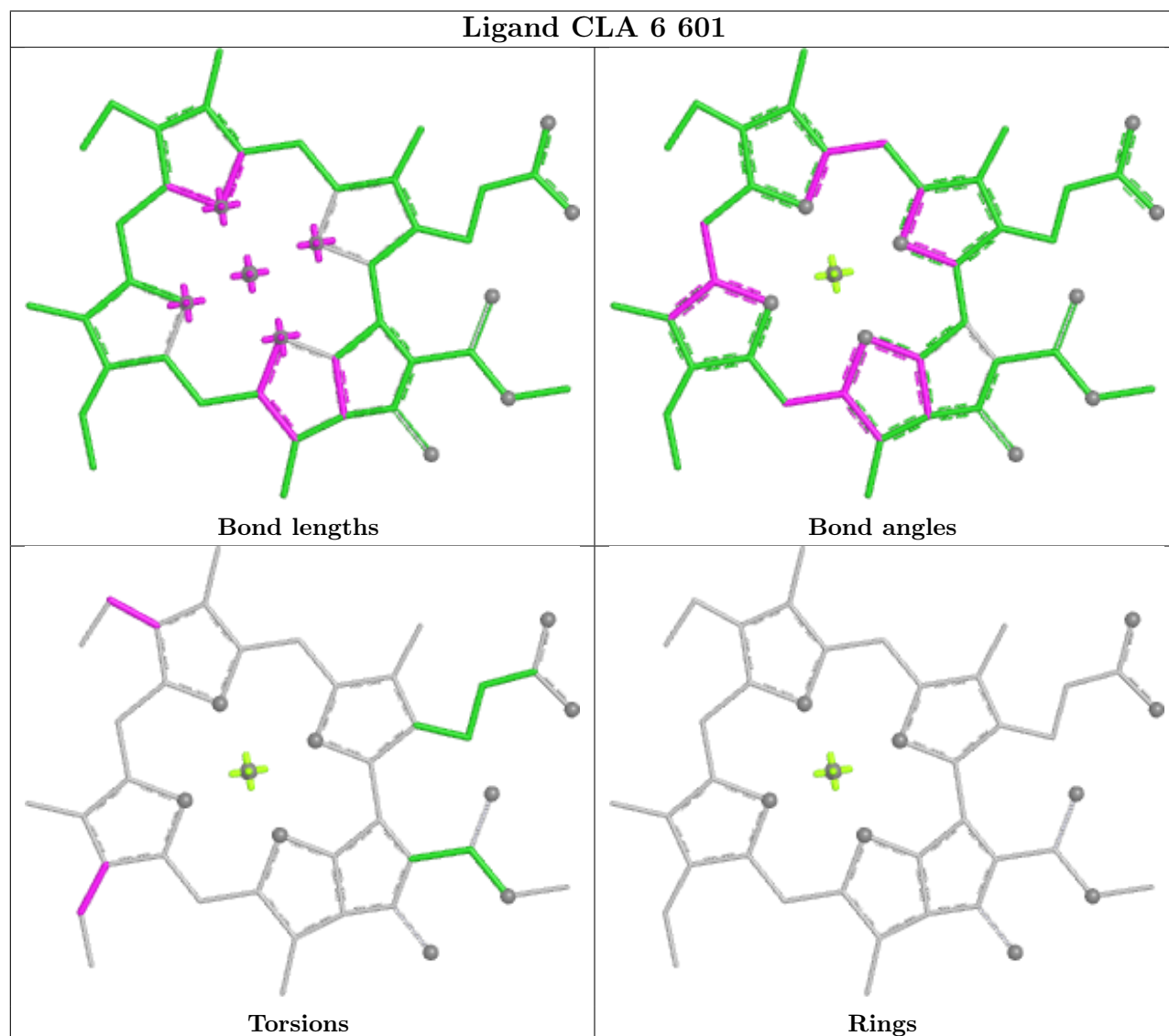
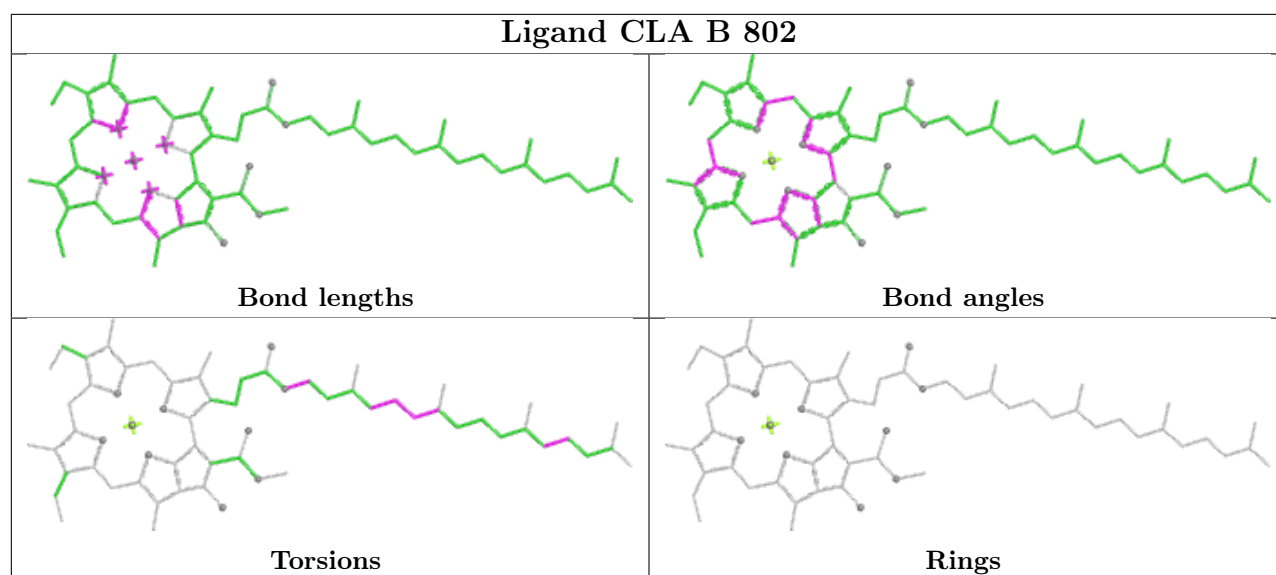
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	2	614	II0	1	0

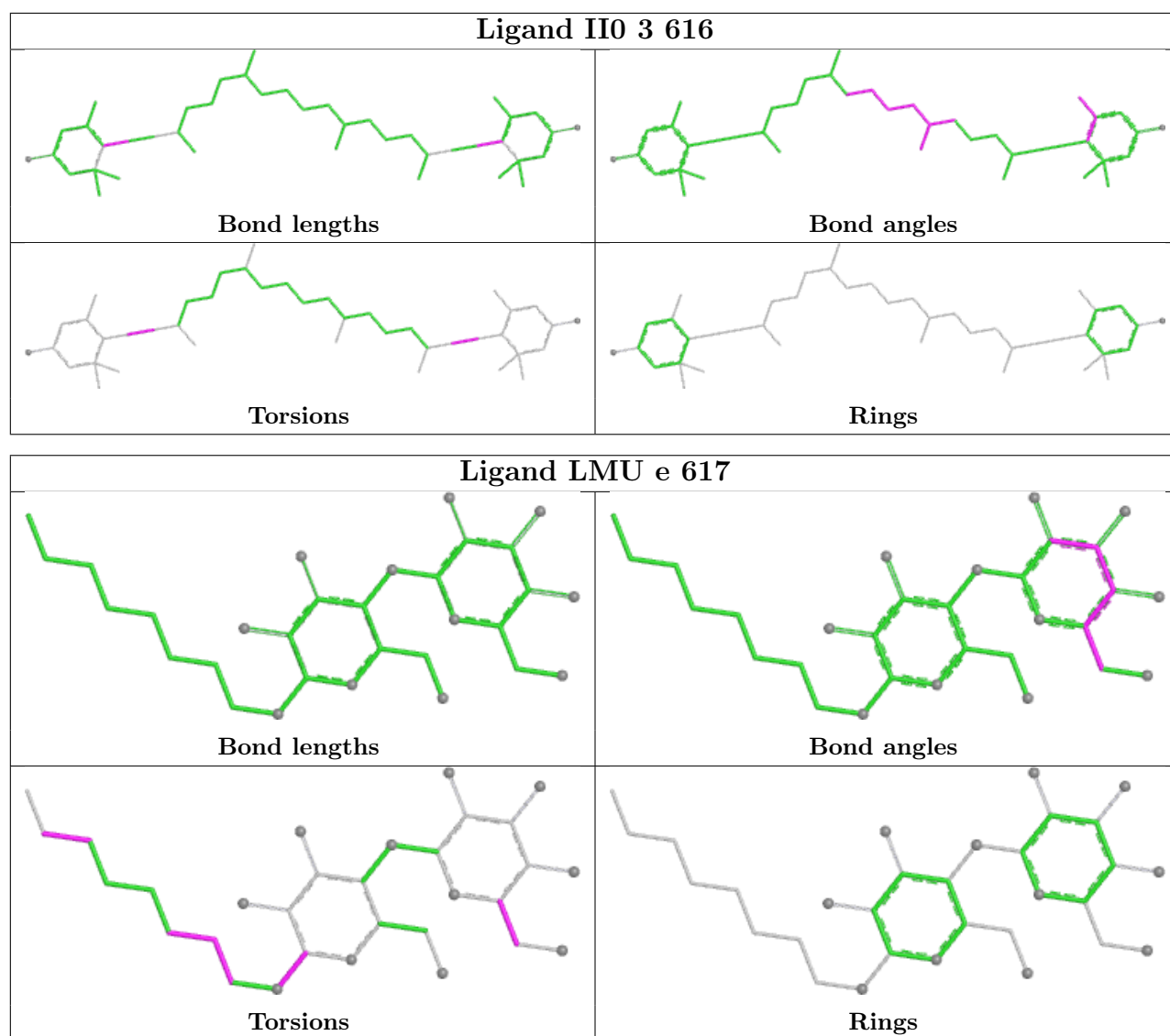
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



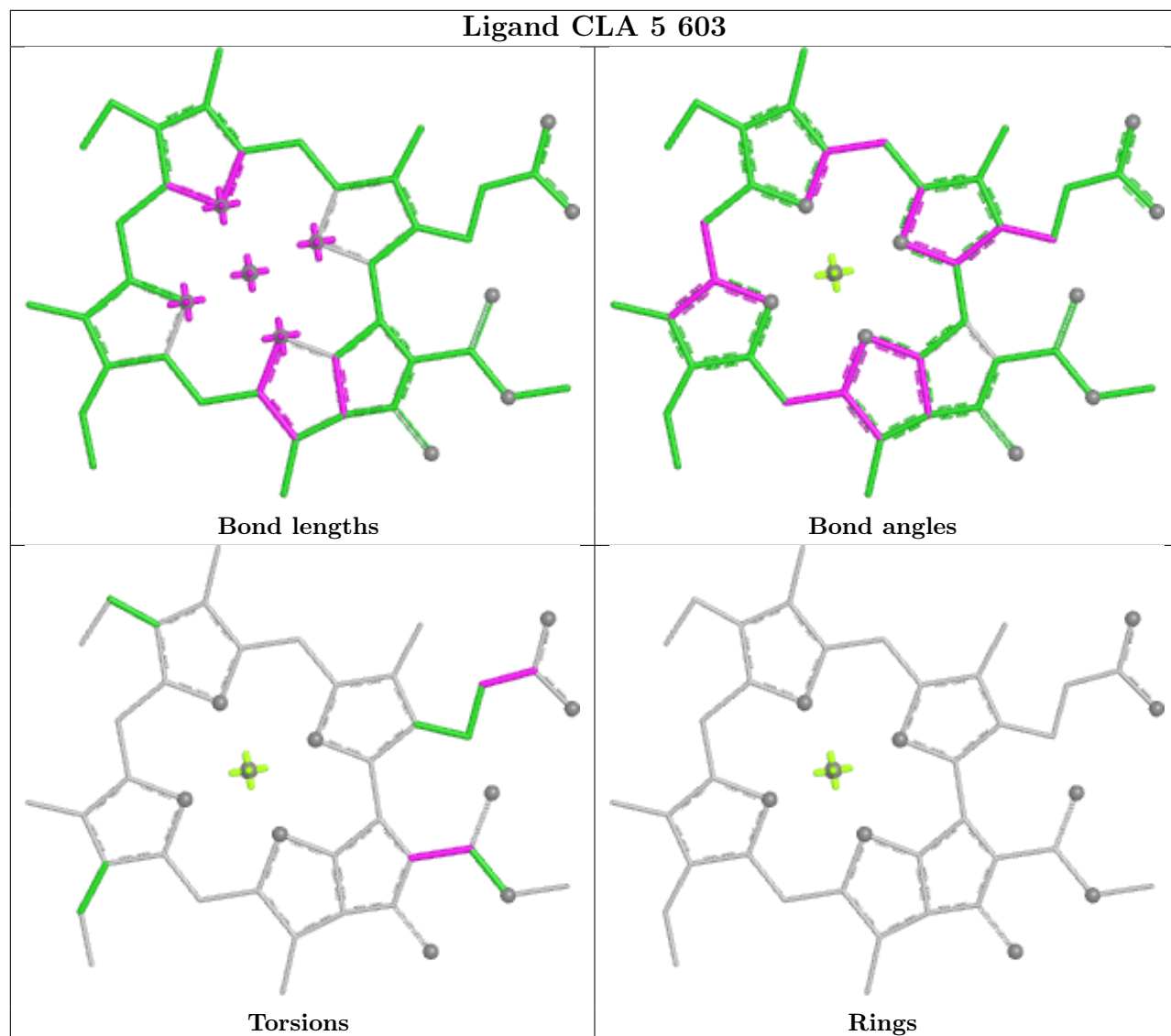




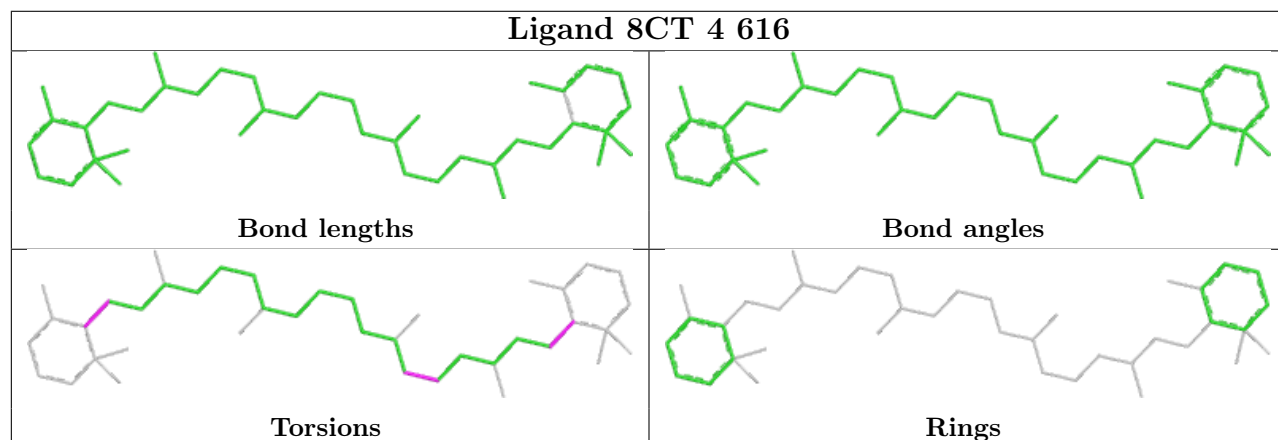


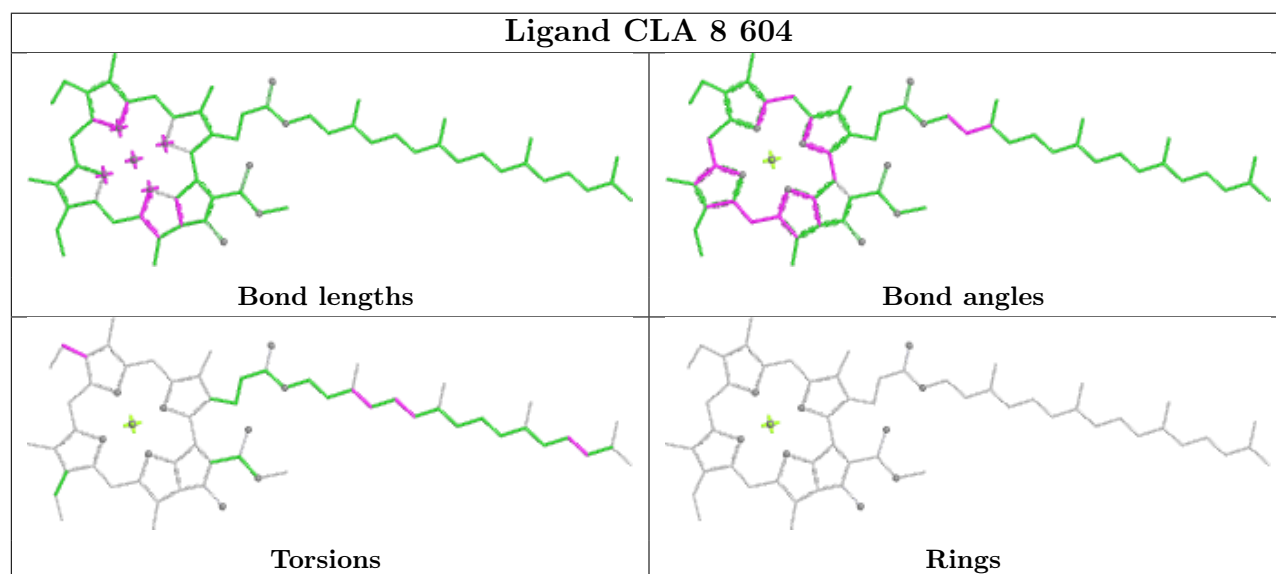
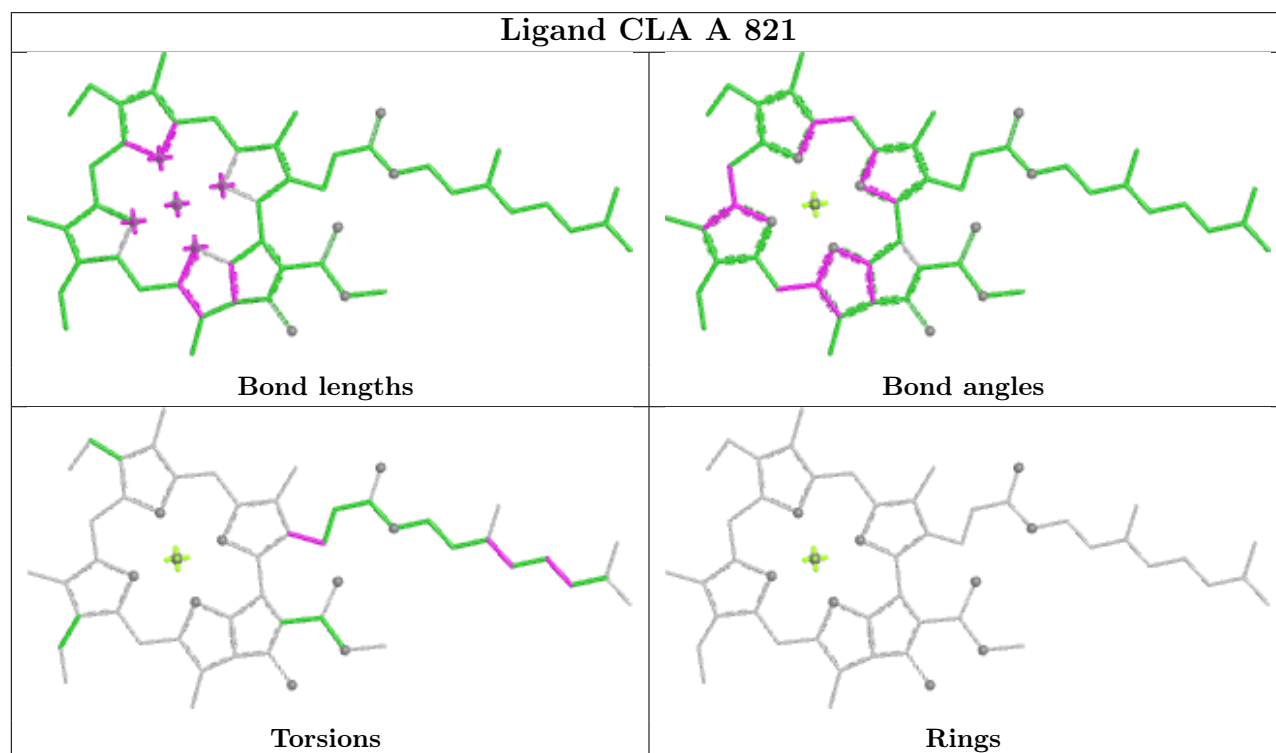
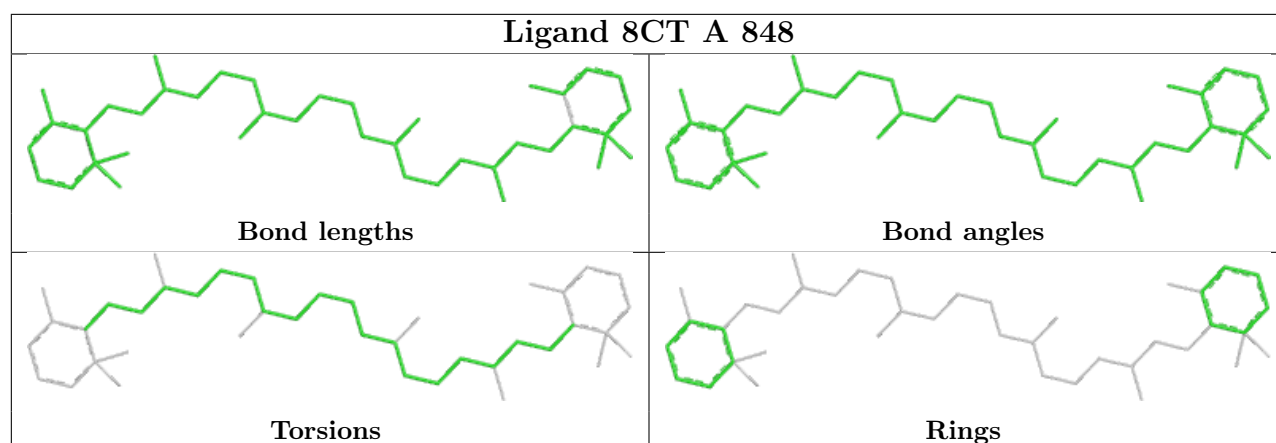


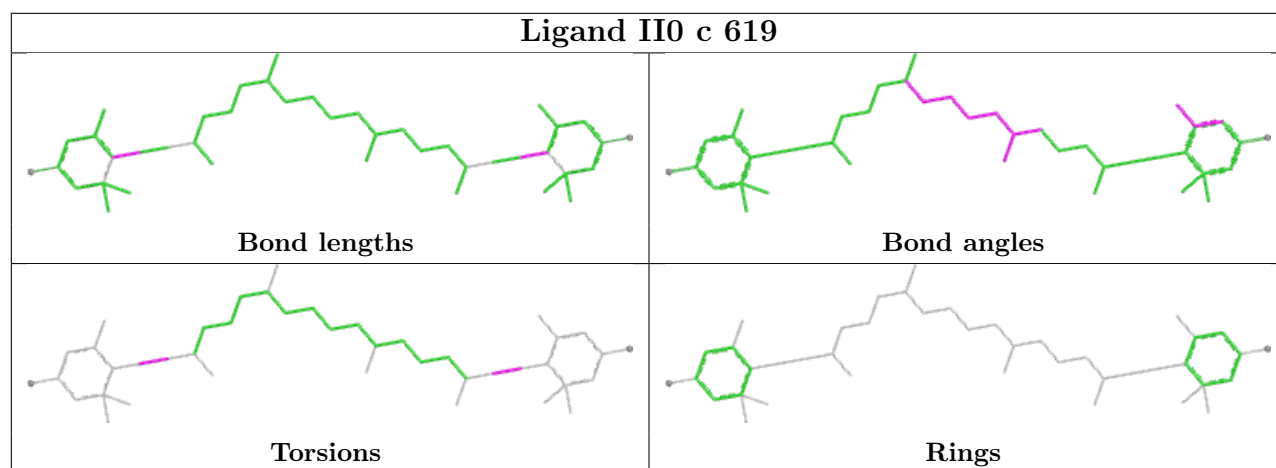
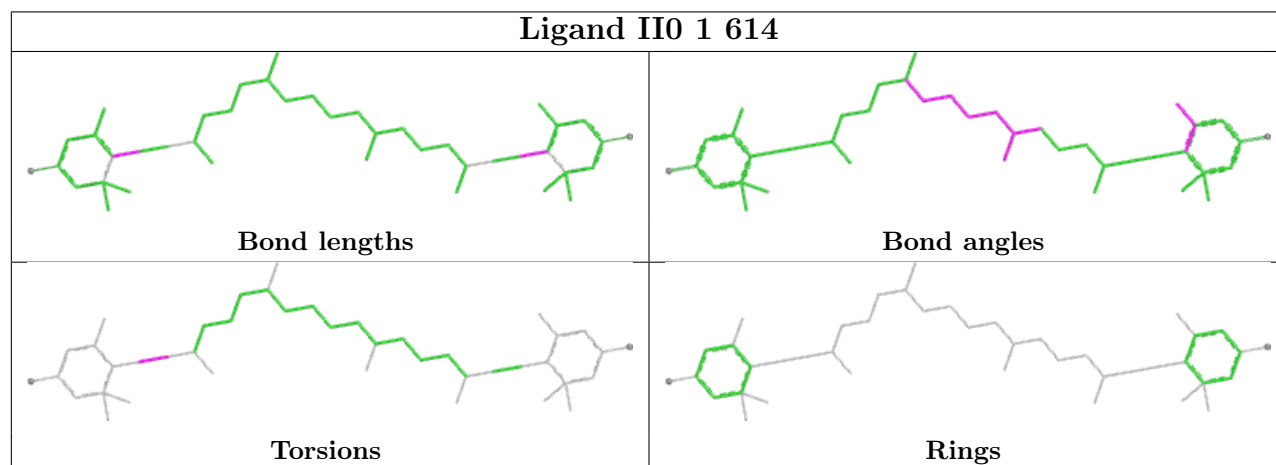
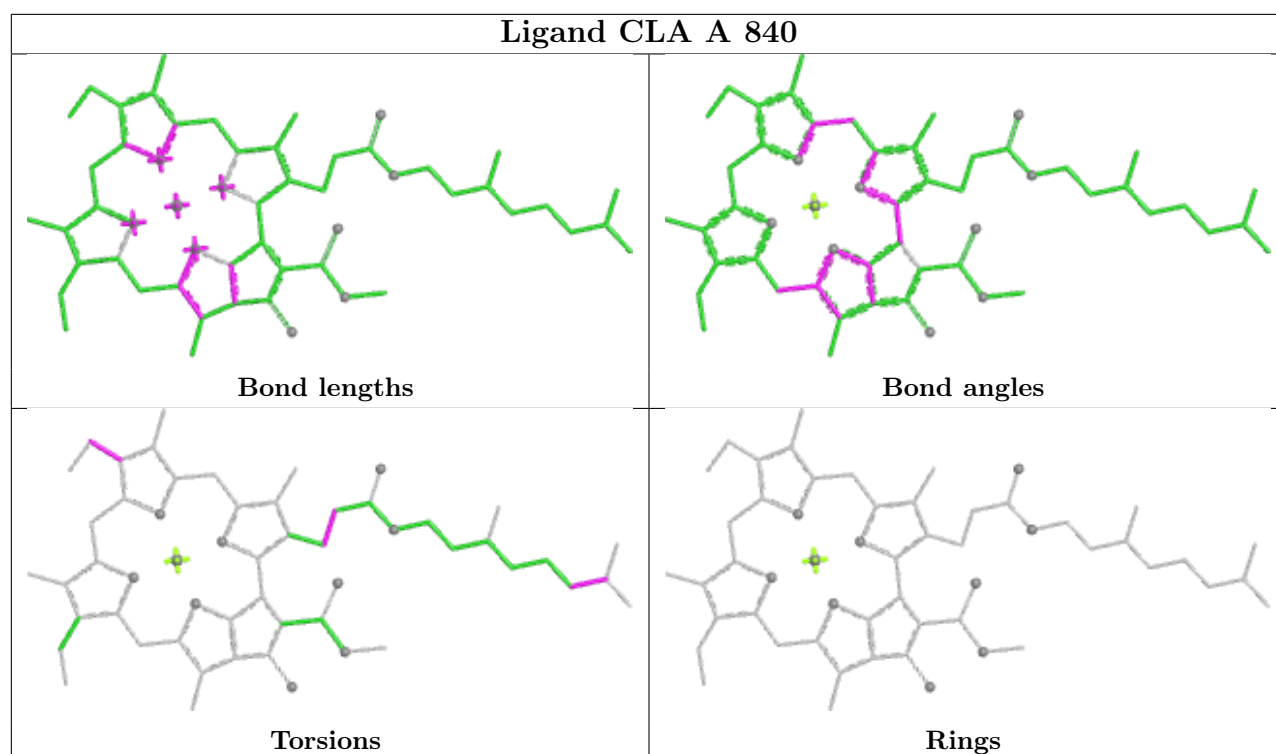
Ligand CLA 5 603

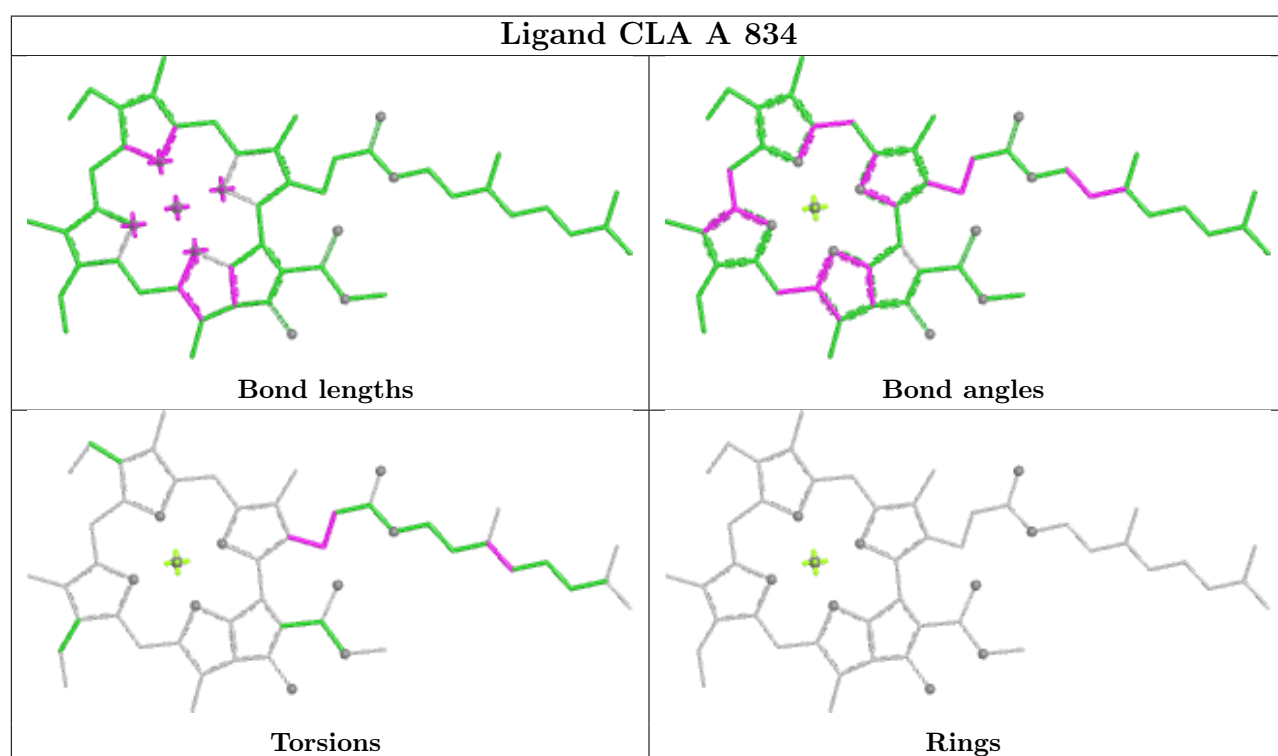
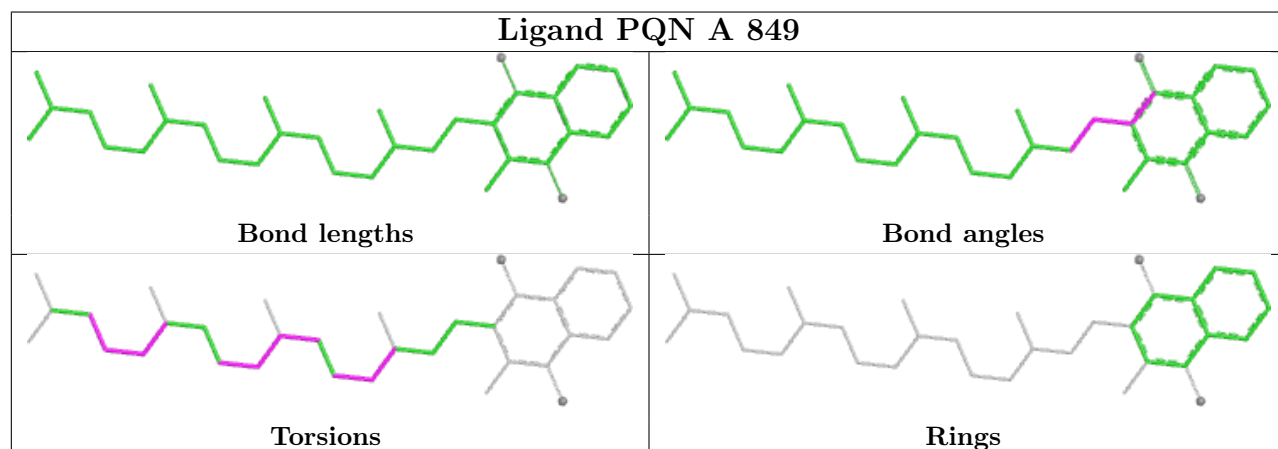
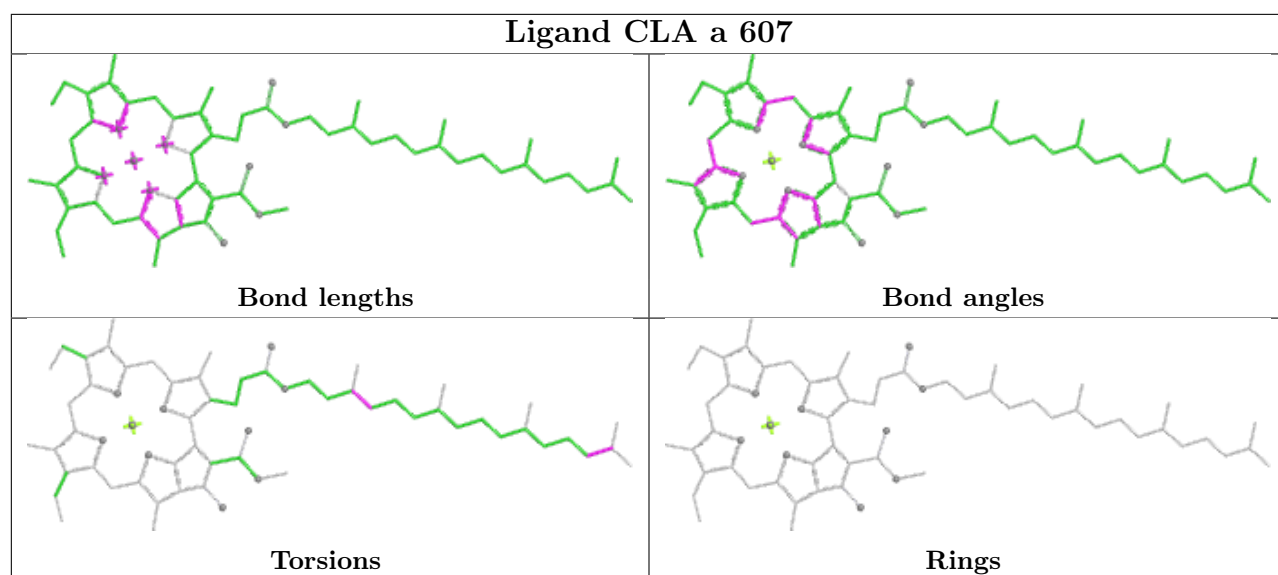


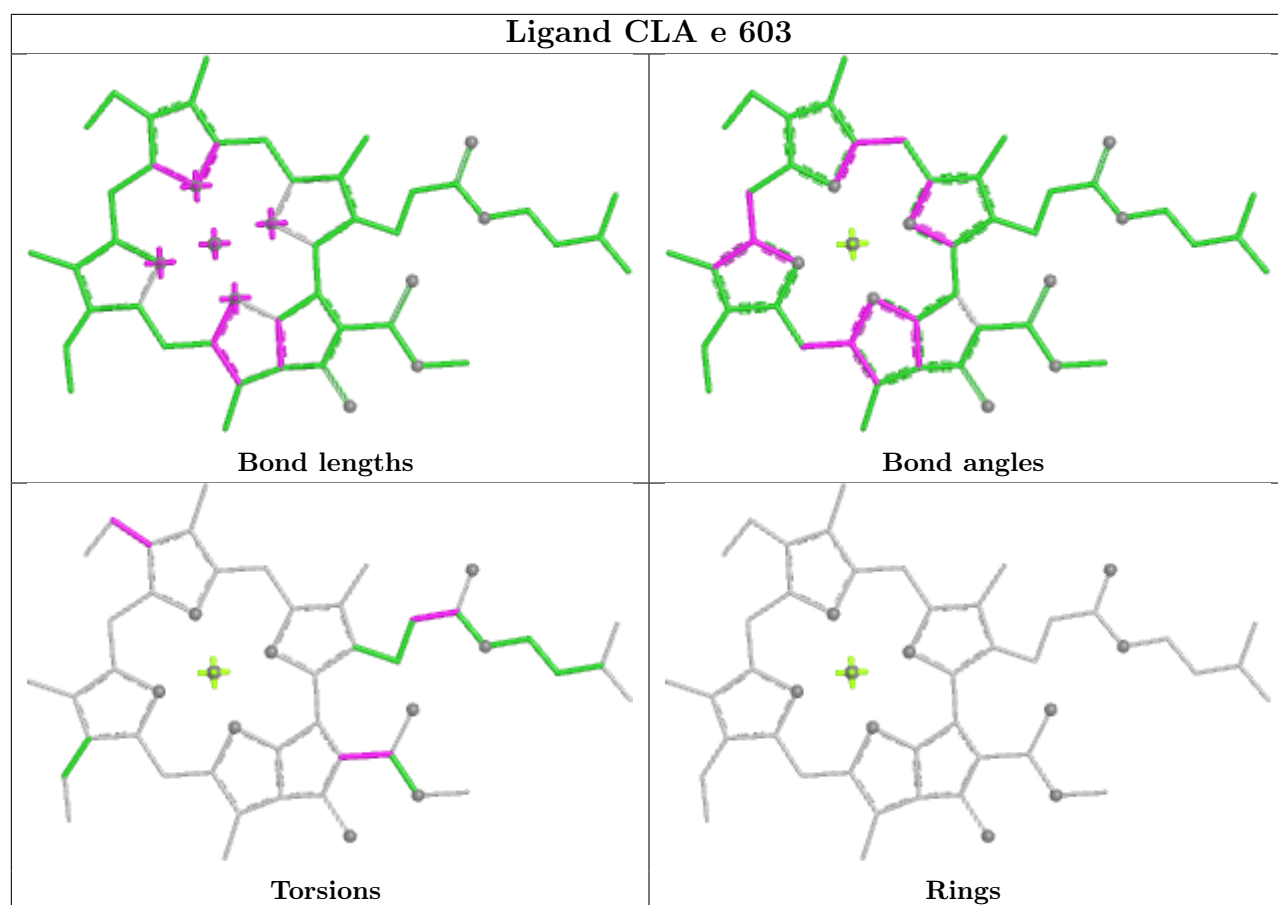
Ligand 8CT 4 616

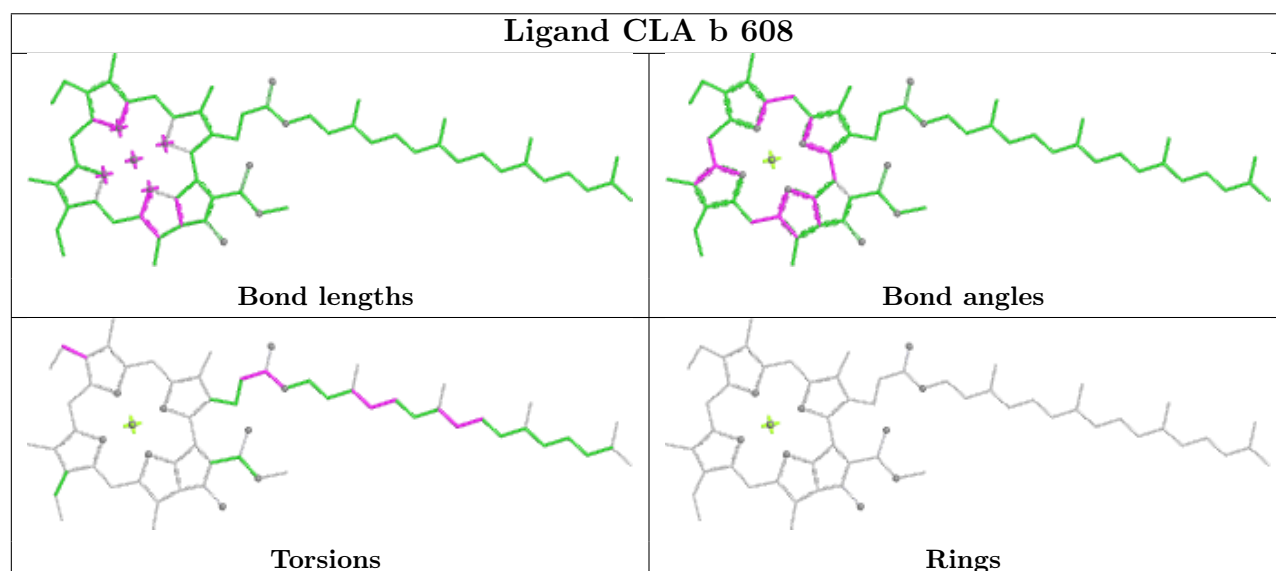
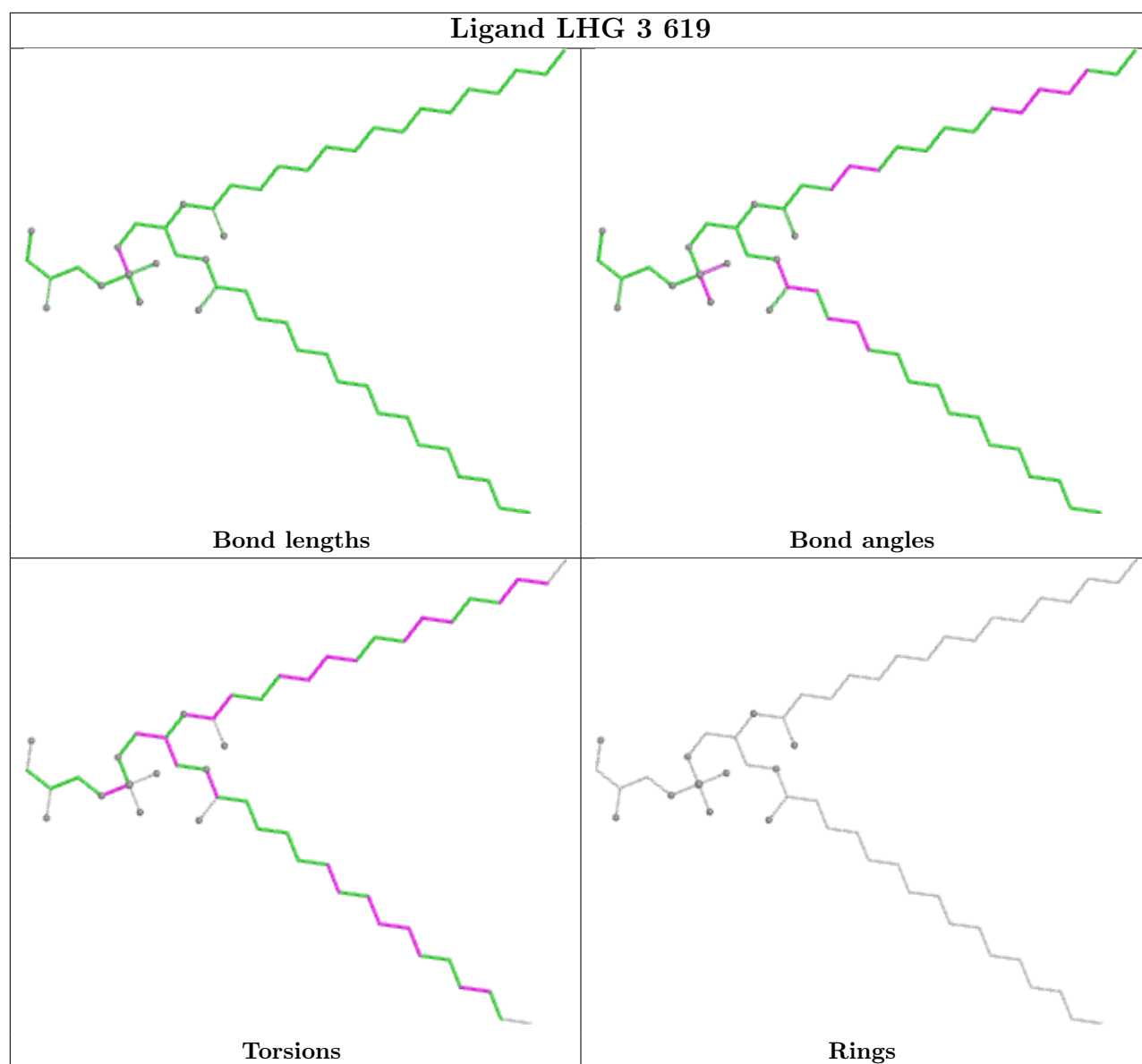


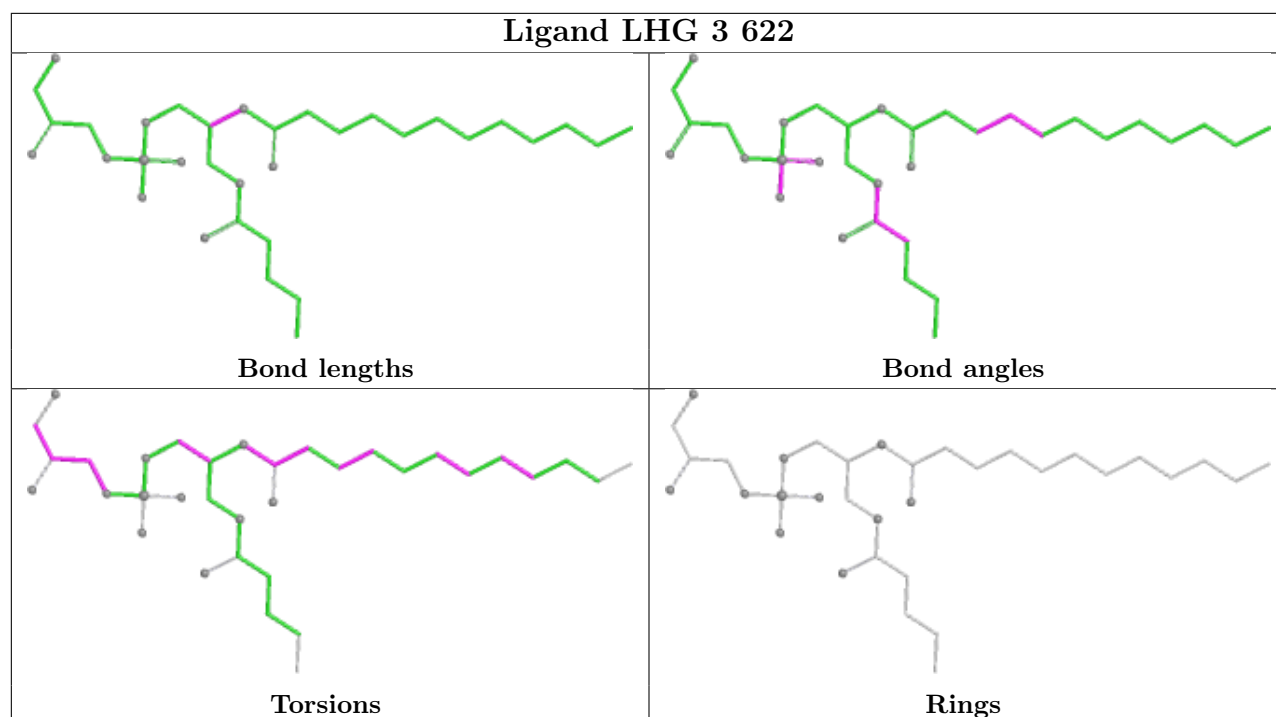
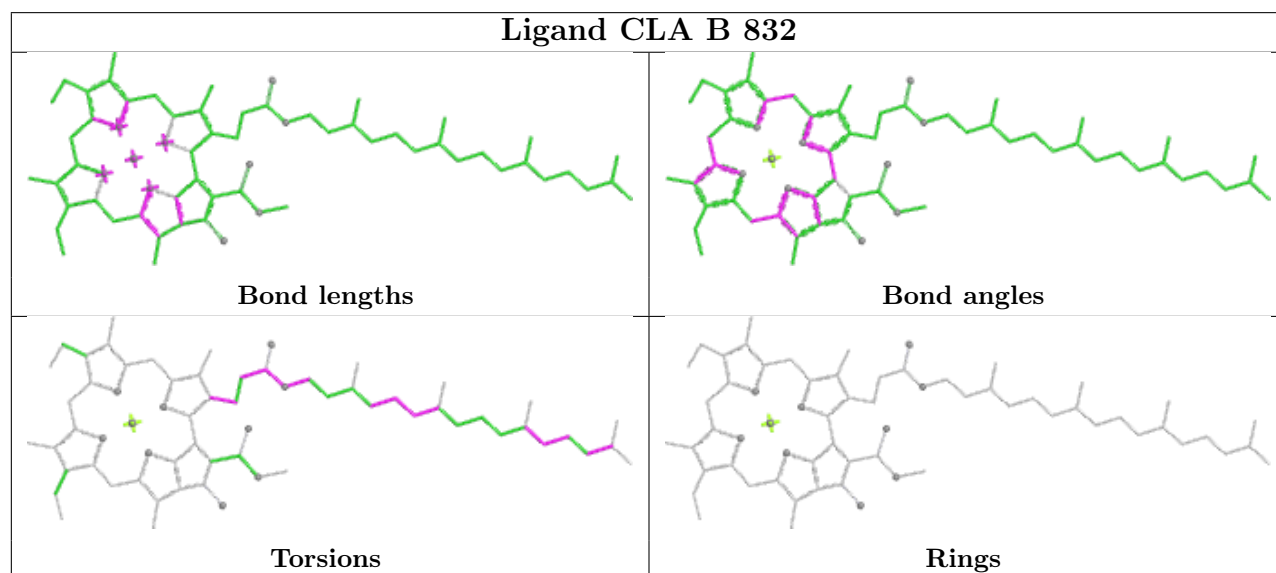
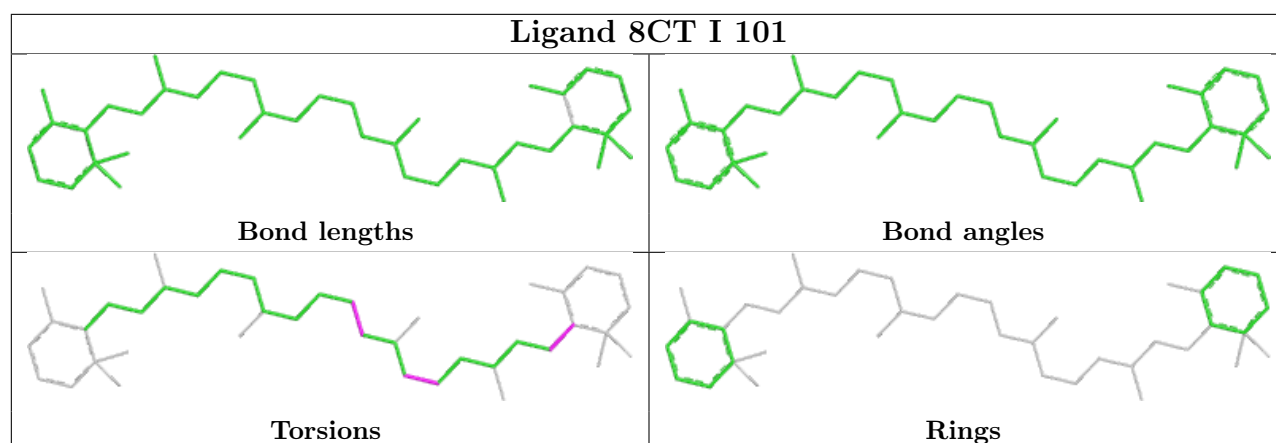




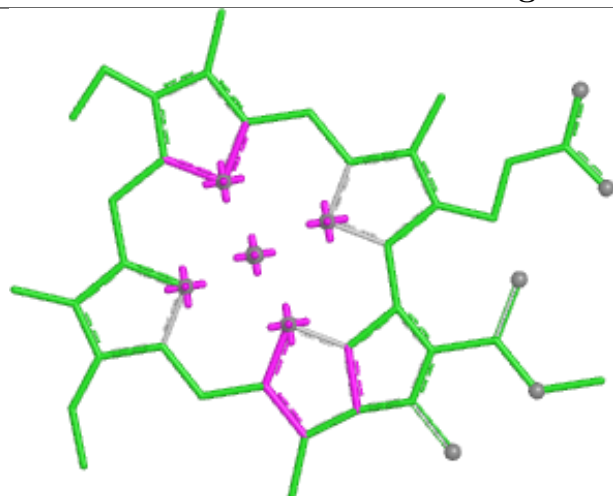




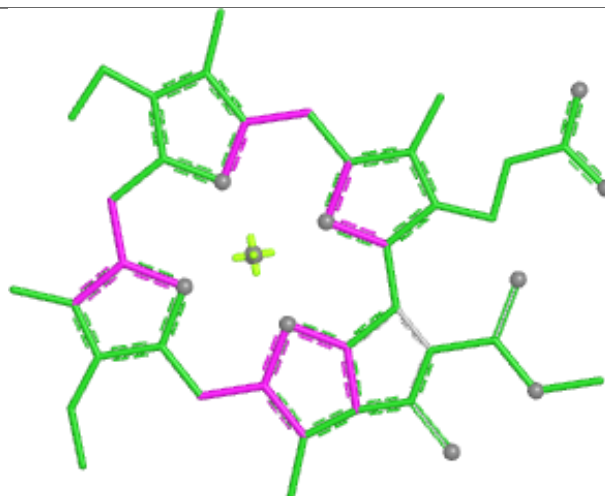




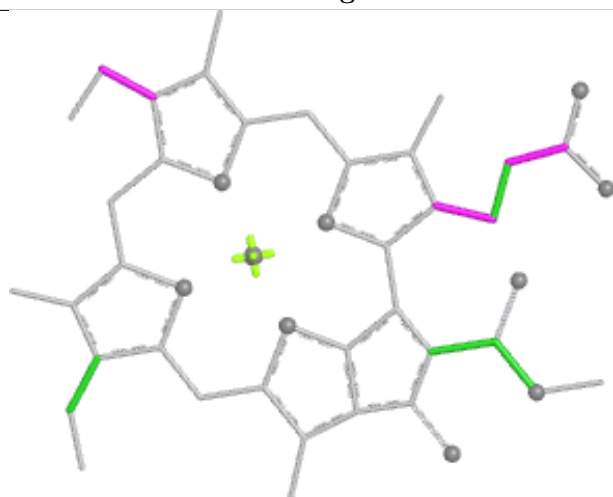
Ligand CLA 6 612



Bond lengths



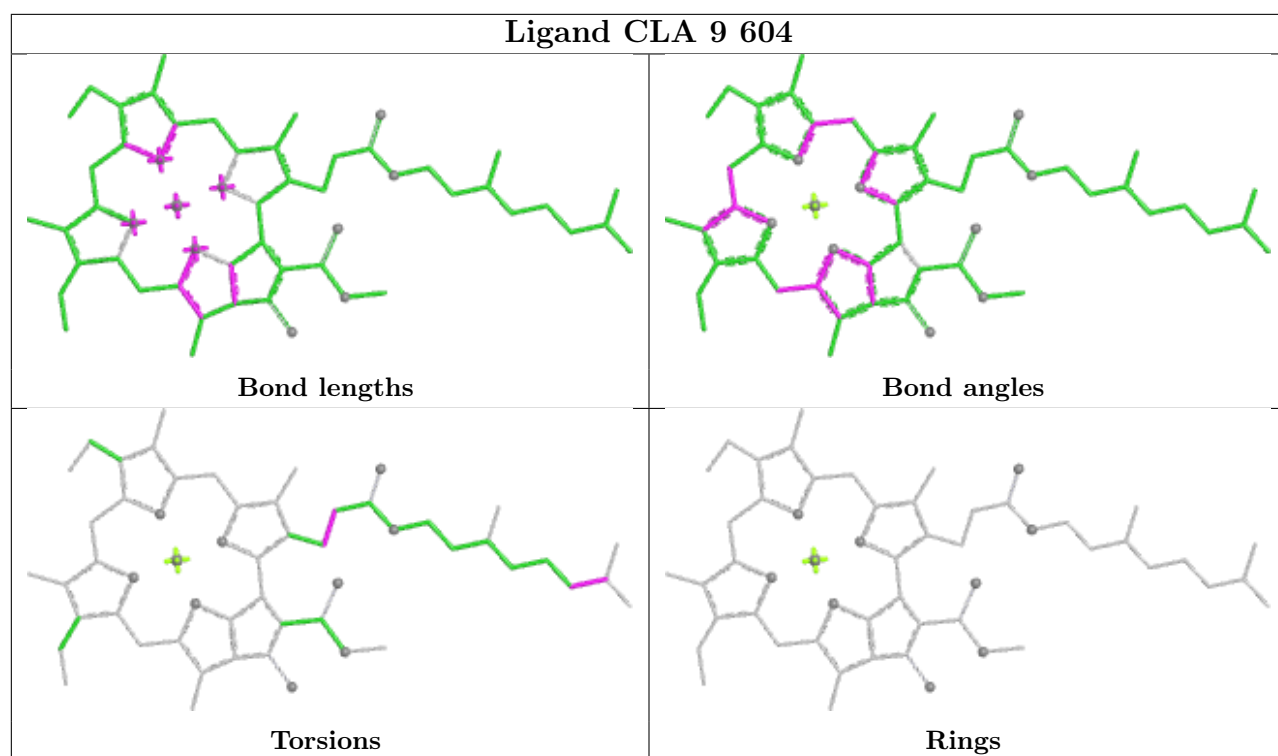
Bond angles



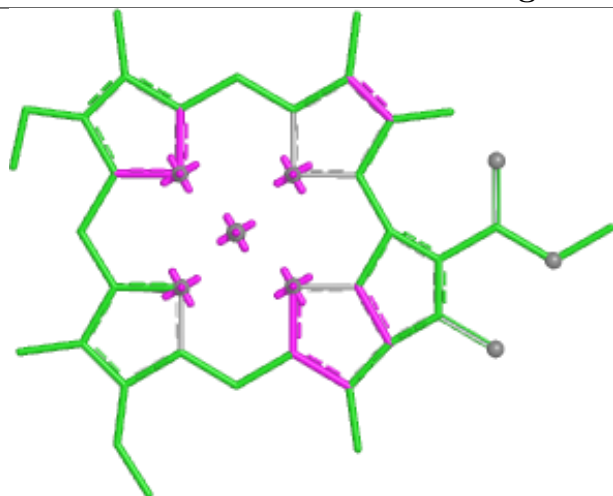
Torsions



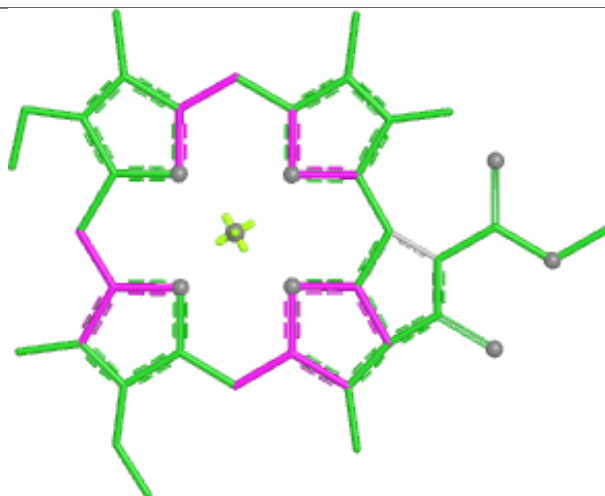
Rings



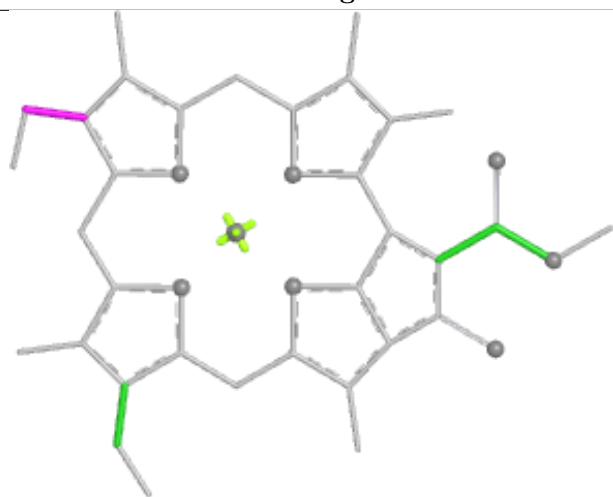
Ligand CLA 1 609



Bond lengths



Bond angles

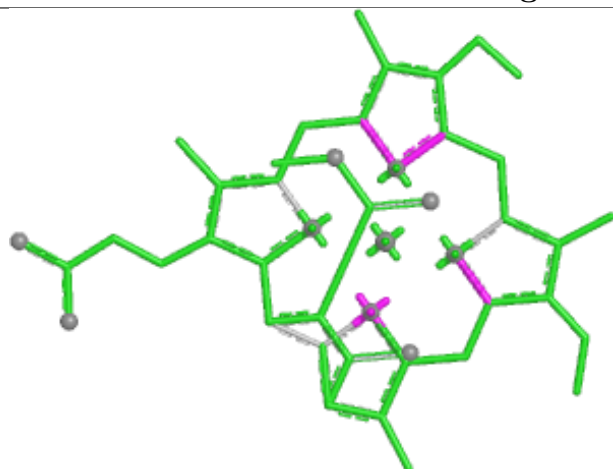


Torsions

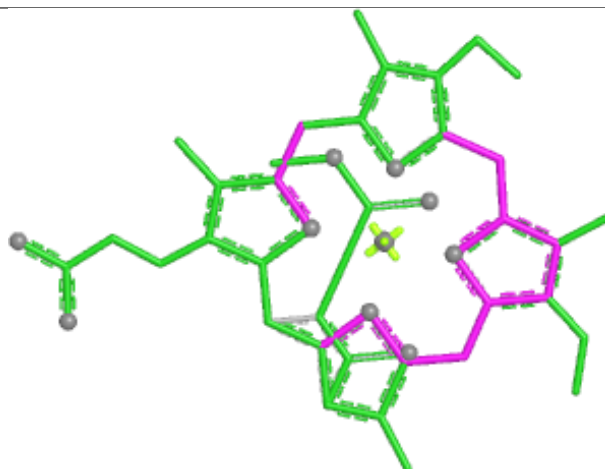


Rings

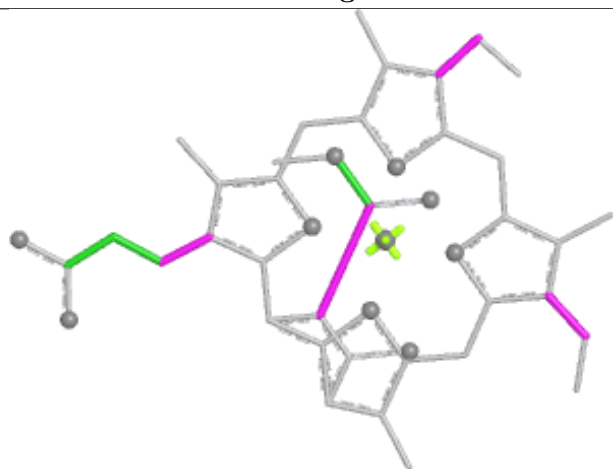
Ligand KC2 3 606



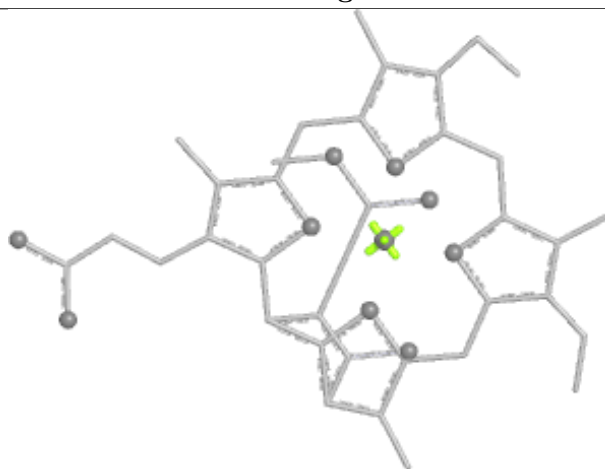
Bond lengths



Bond angles

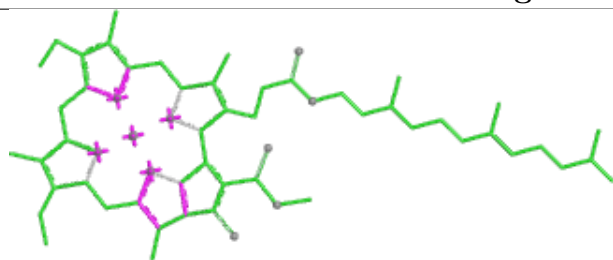


Torsions

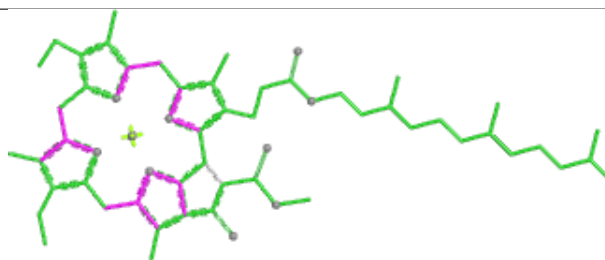


Rings

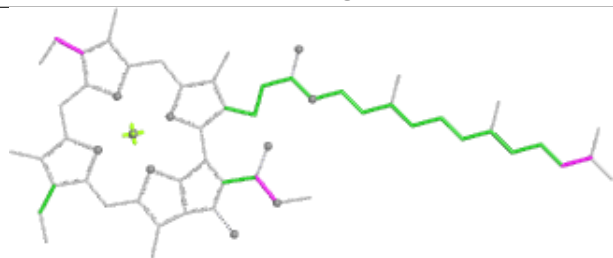
Ligand CLA B 818



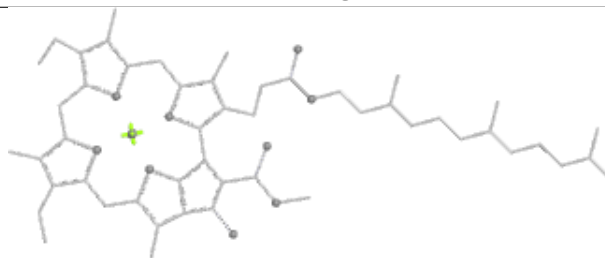
Bond lengths



Bond angles

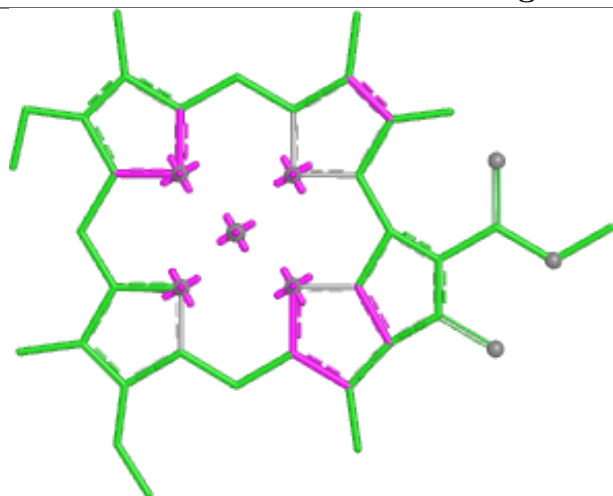


Torsions

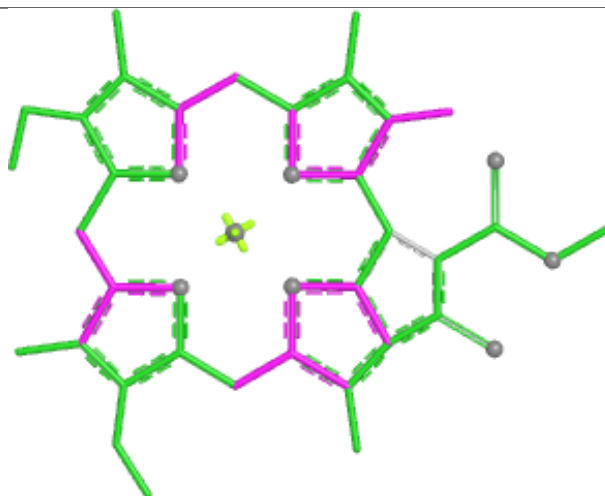


Rings

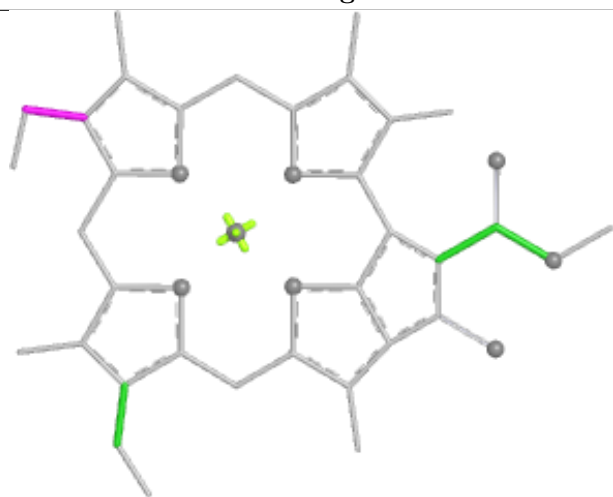
Ligand CLA J 102



Bond lengths



Bond angles

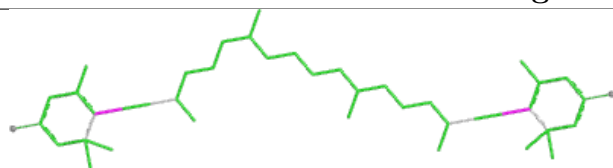


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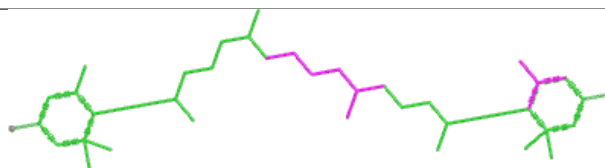


Rings

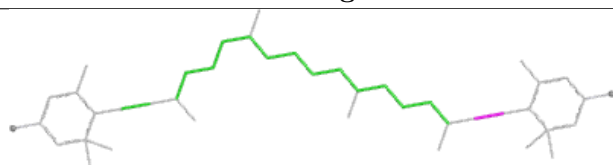
Ligand II0 b 612



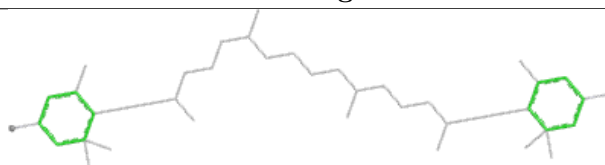
Bond lengths



Bond angles

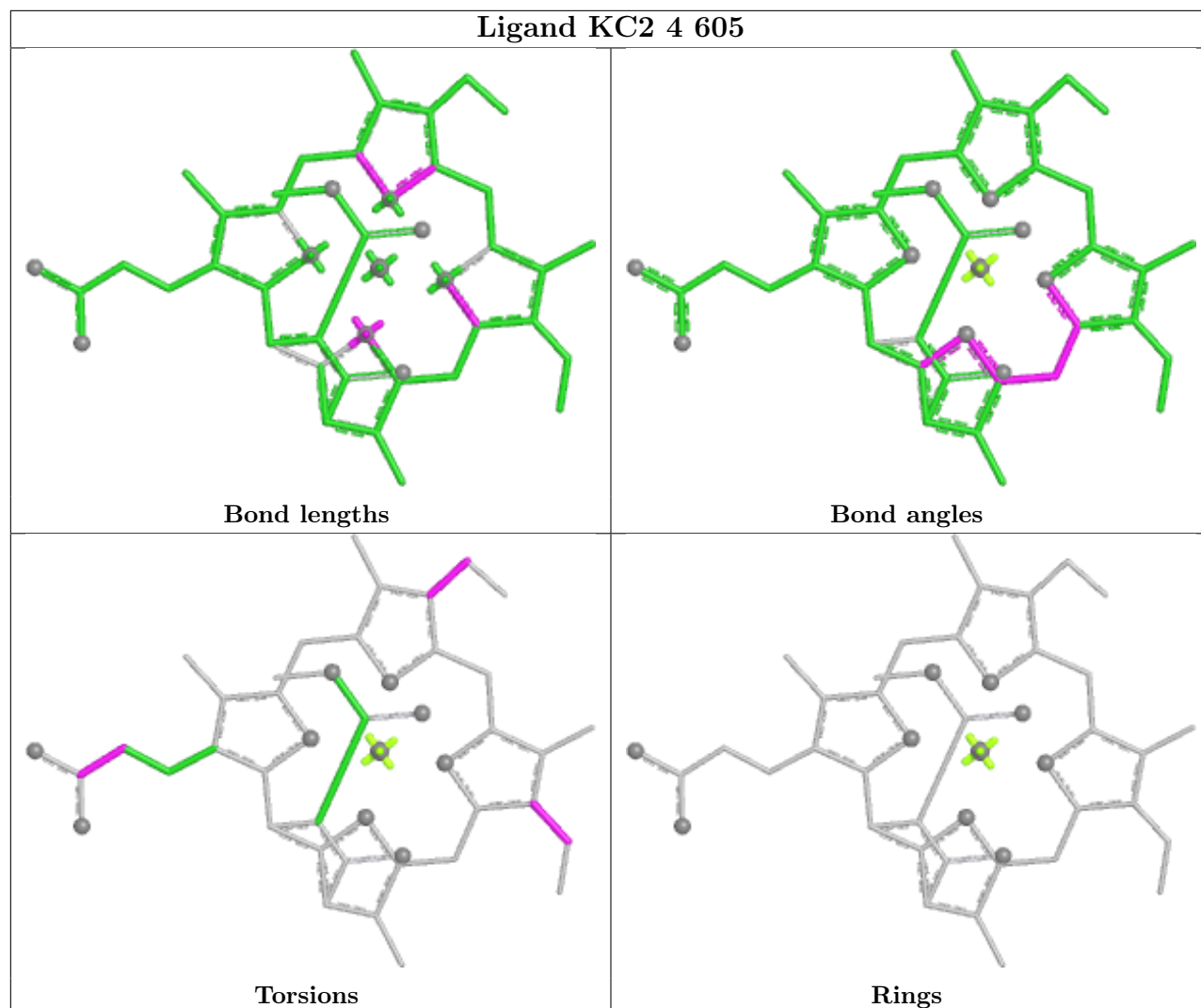


Torsions

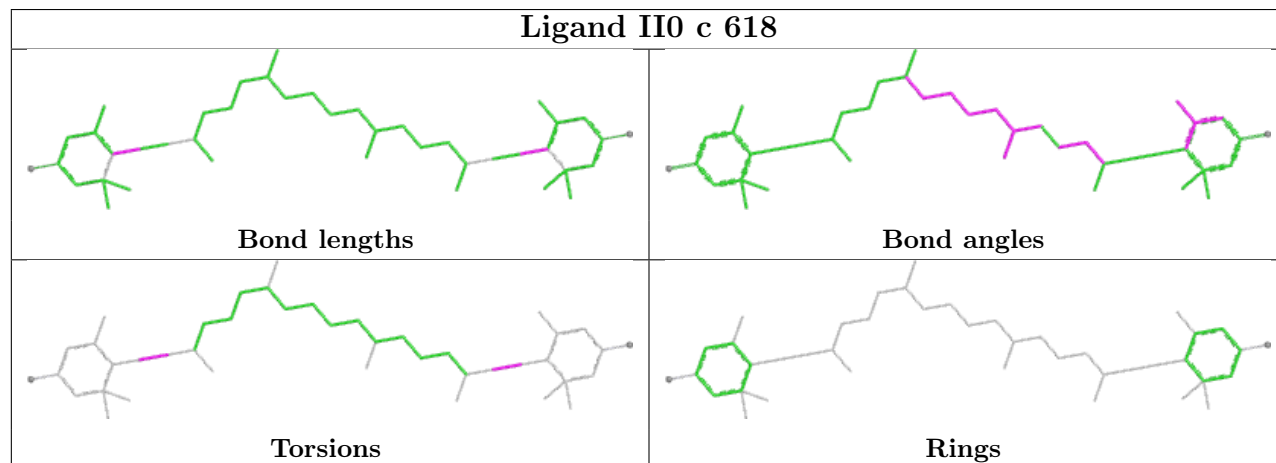


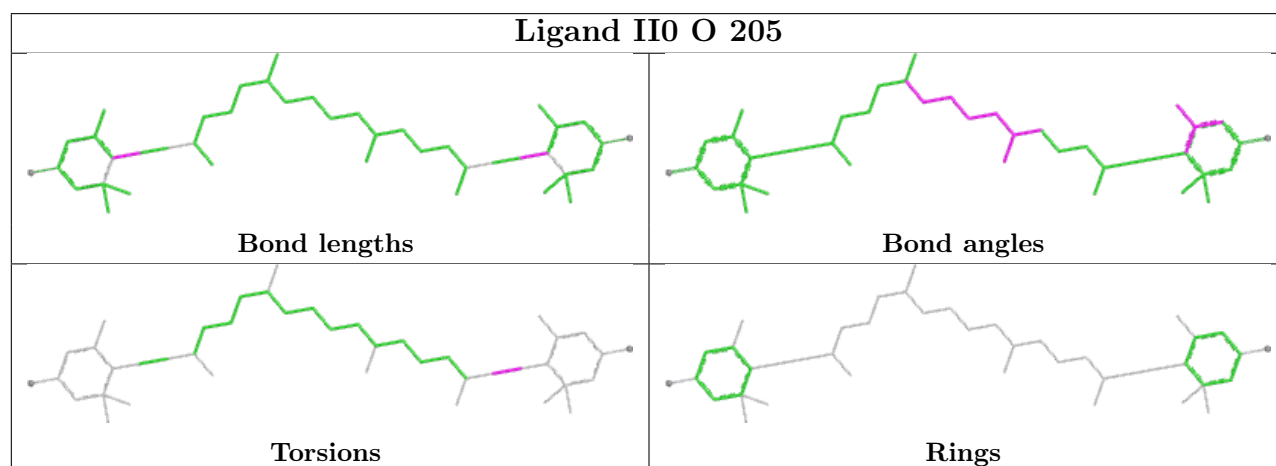
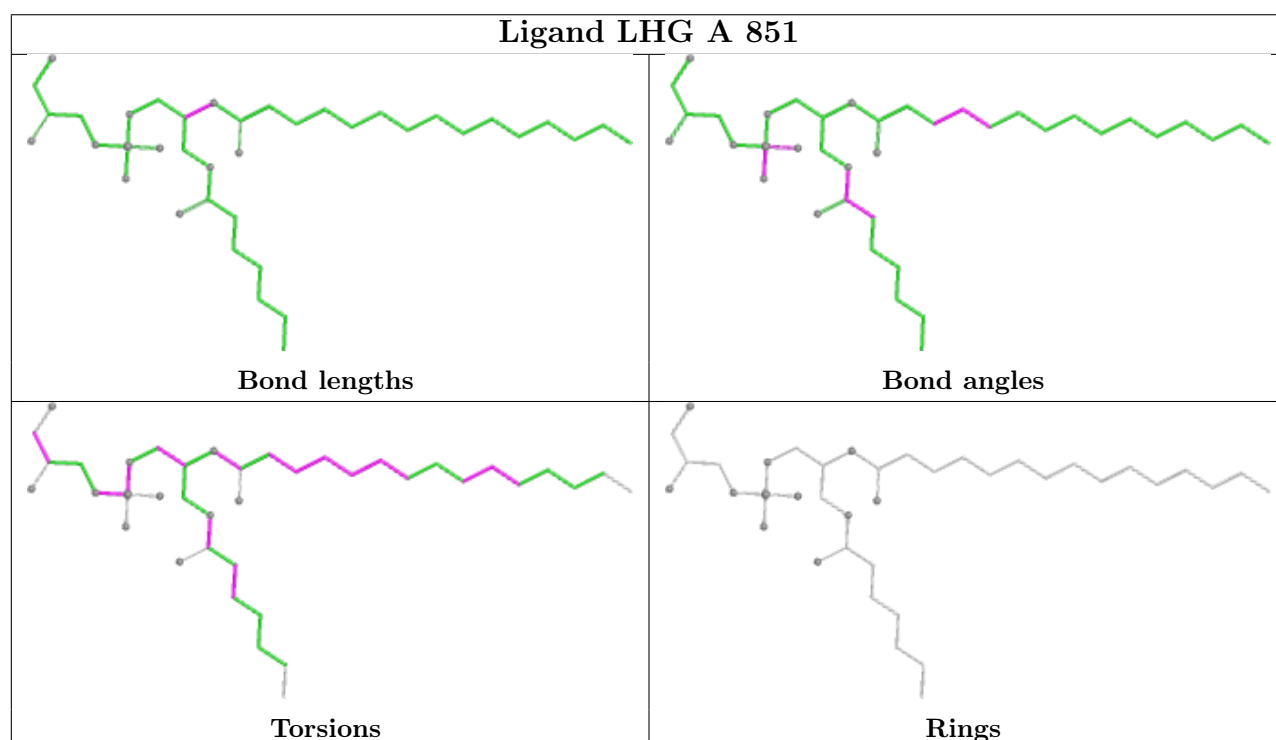
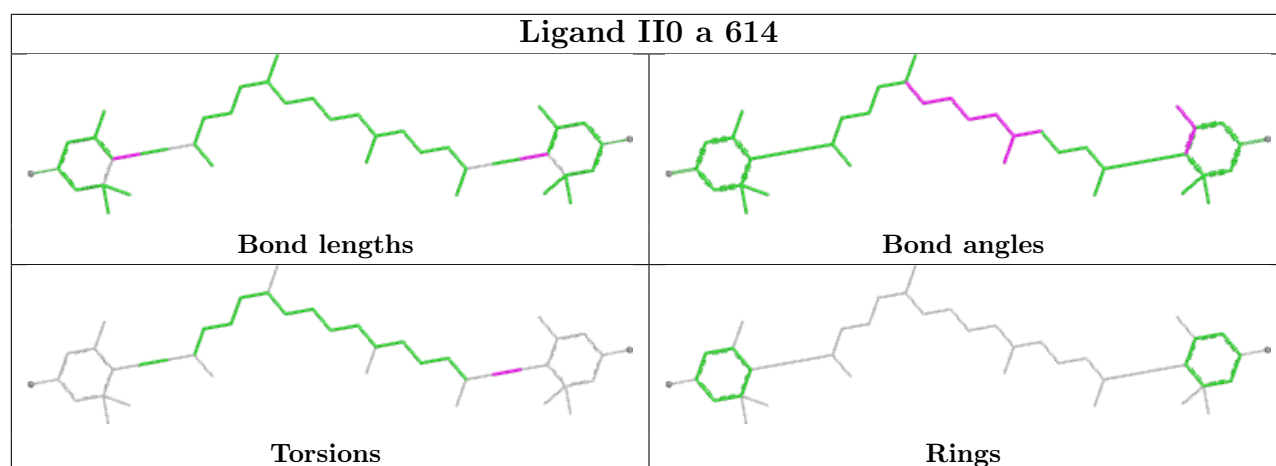
Rings

Ligand KC2 4 605

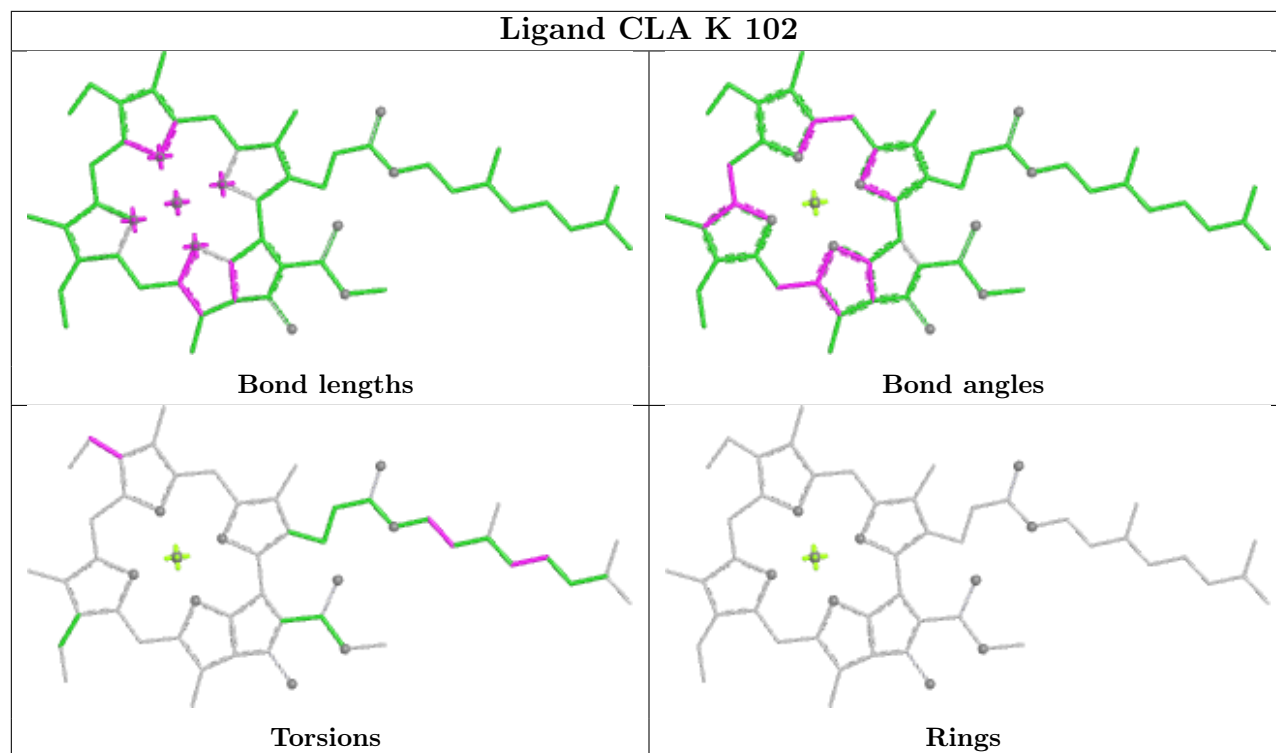


Ligand II0 c 618

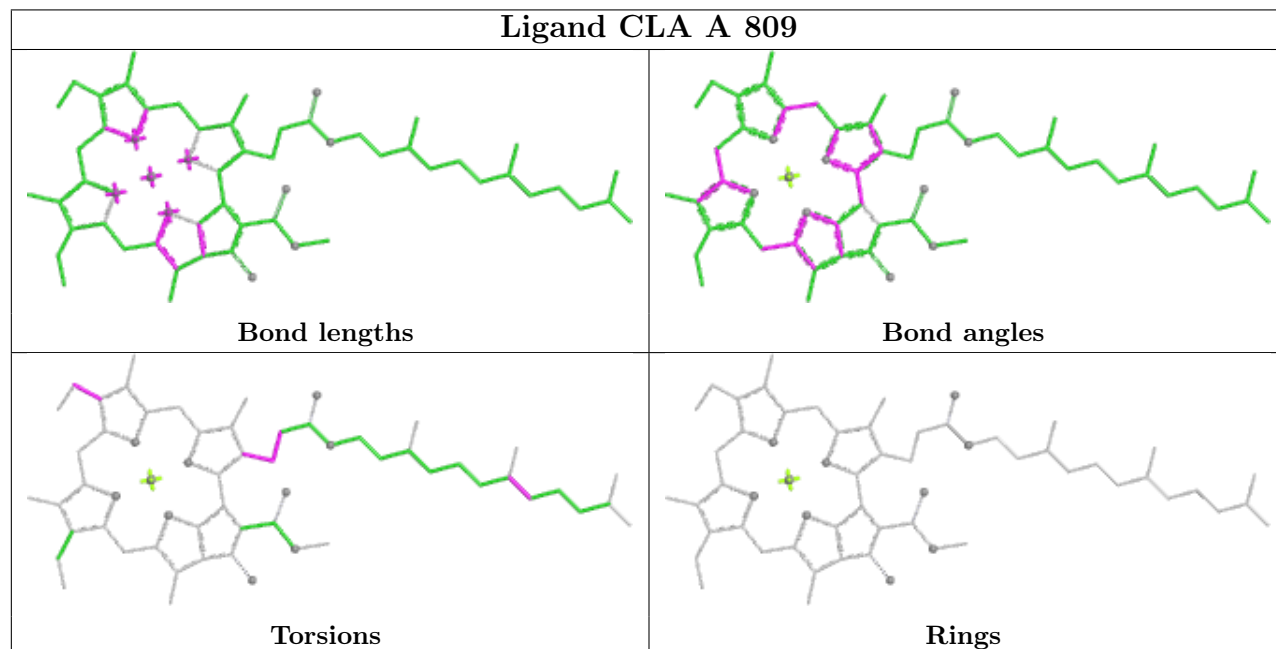


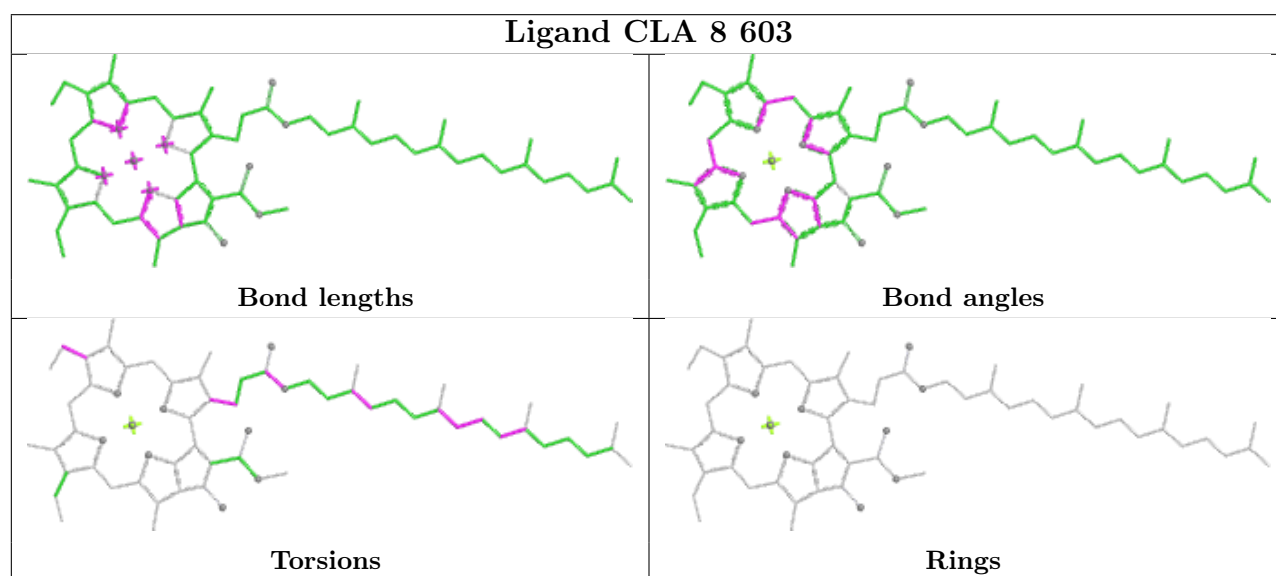
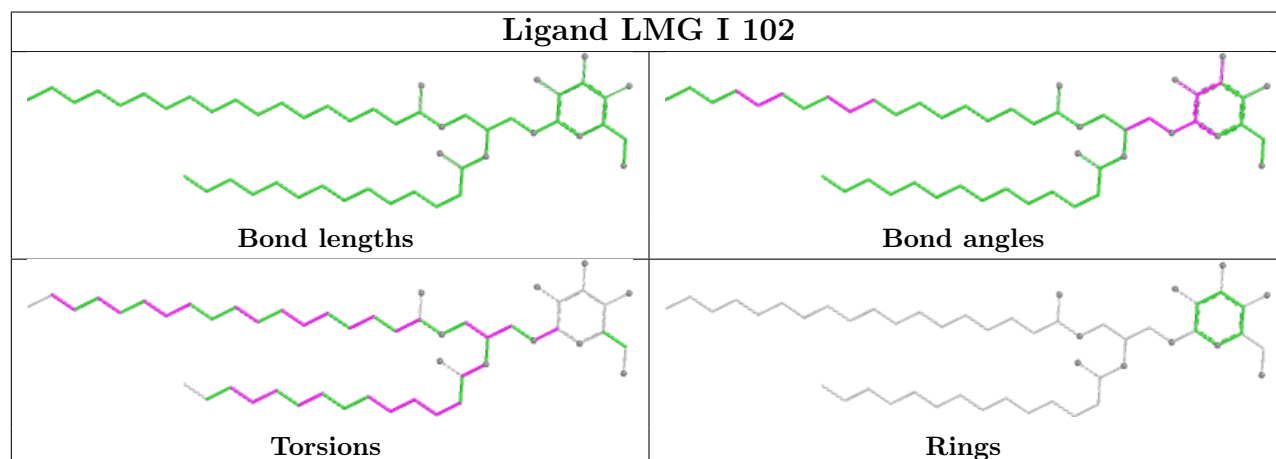
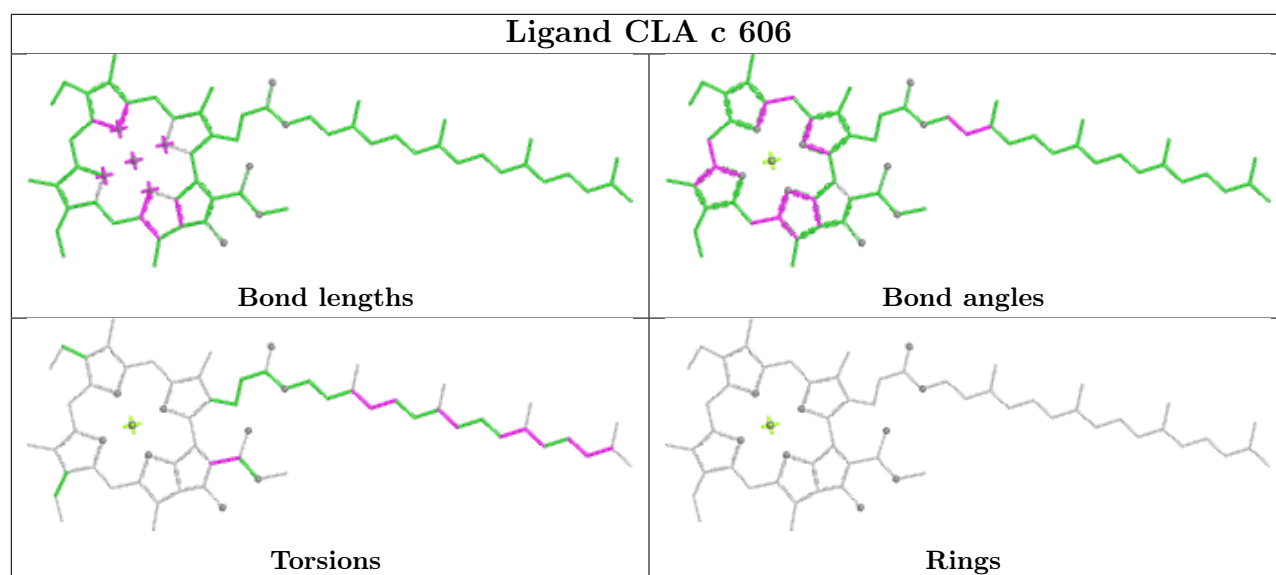


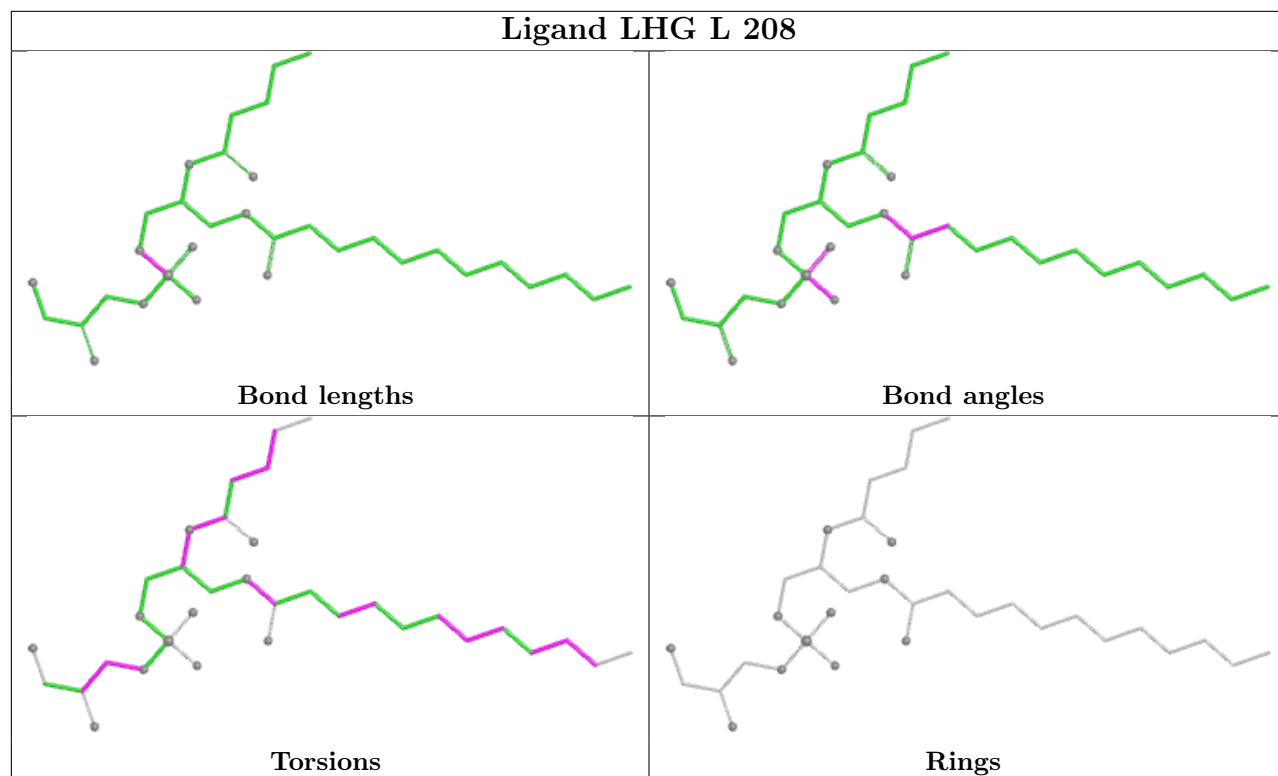
Ligand CLA K 102



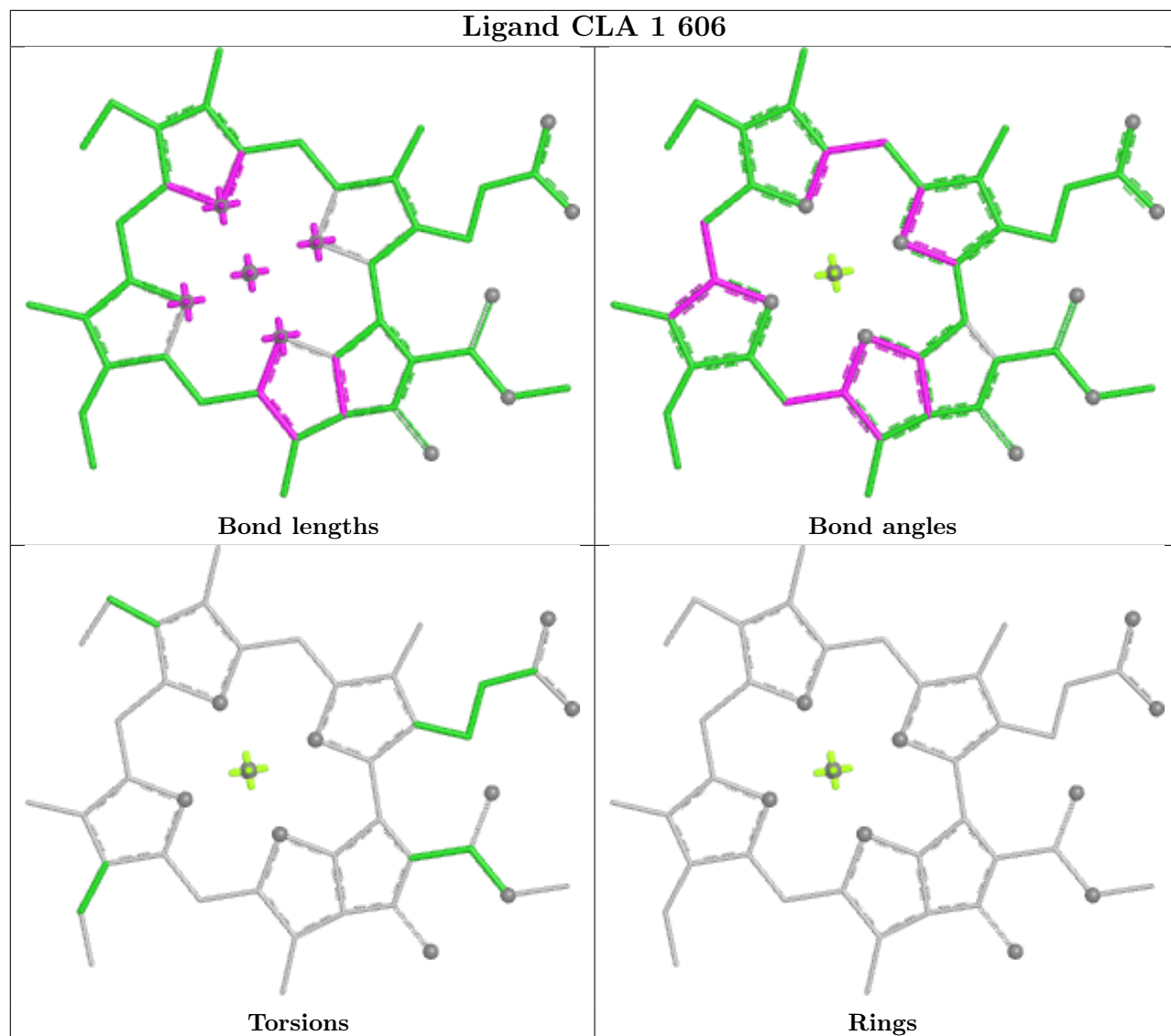
Ligand CLA A 809

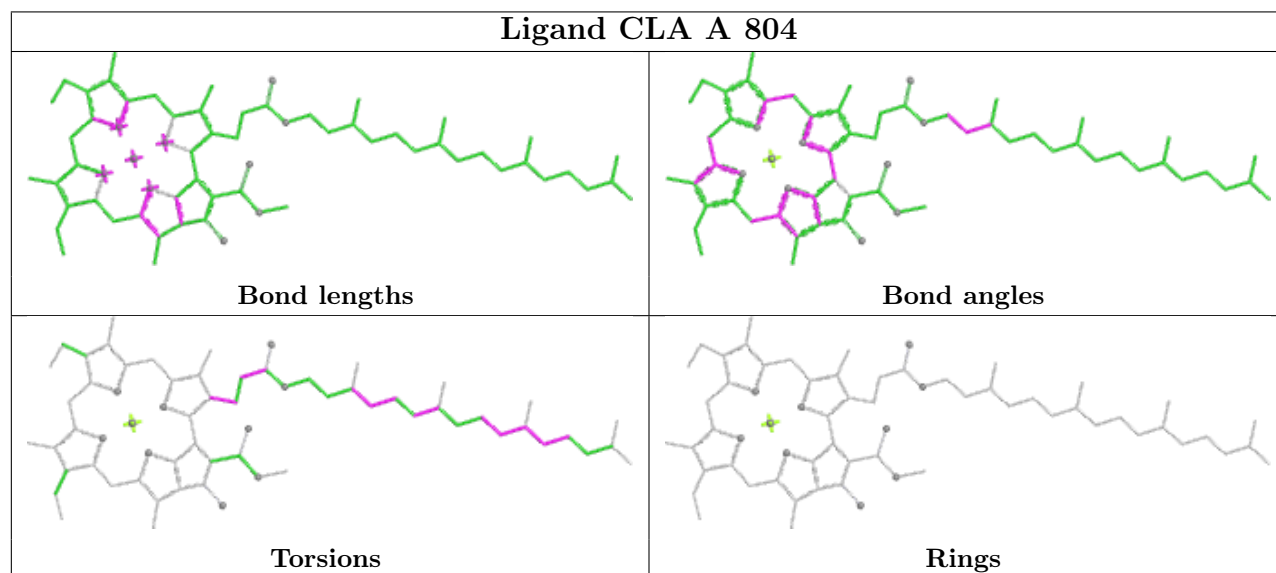
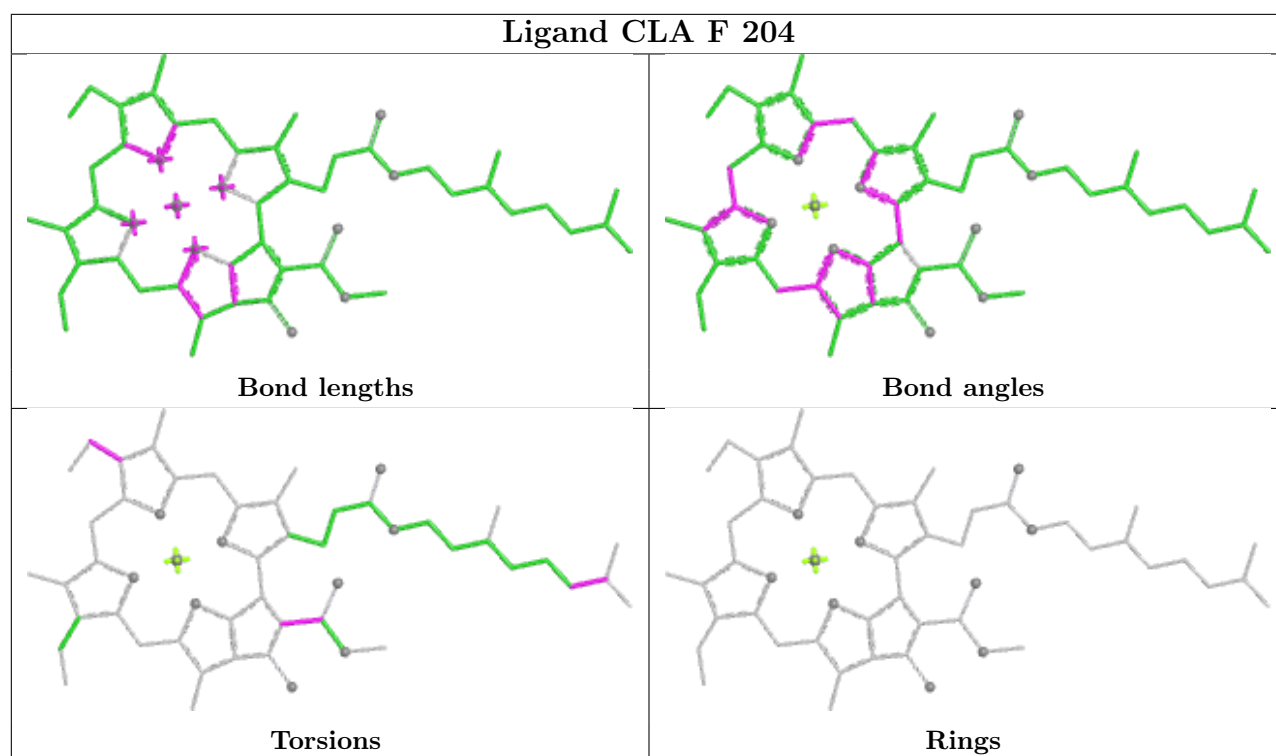


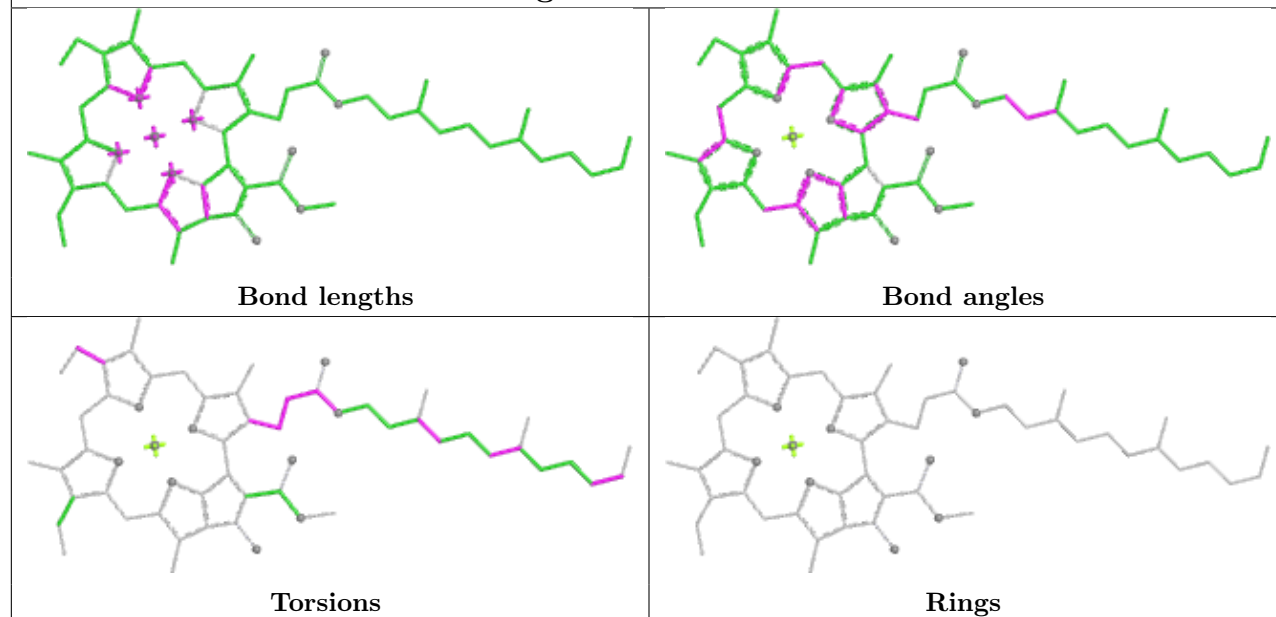
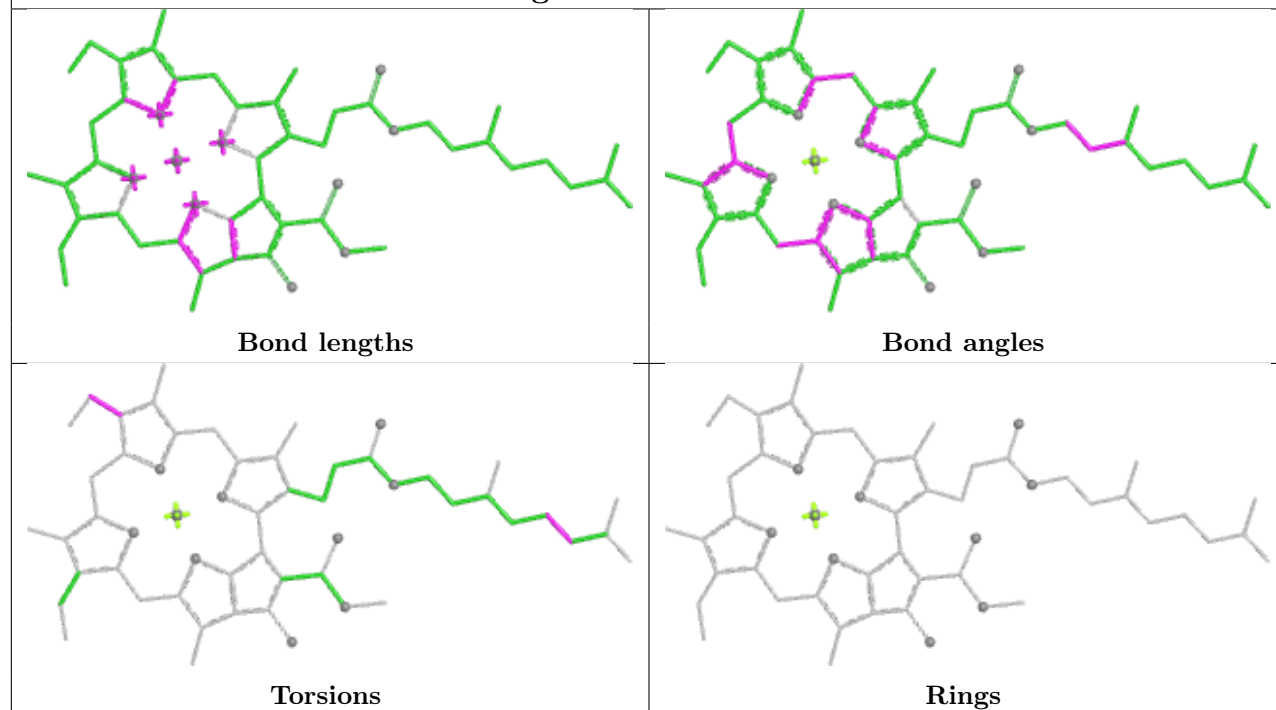


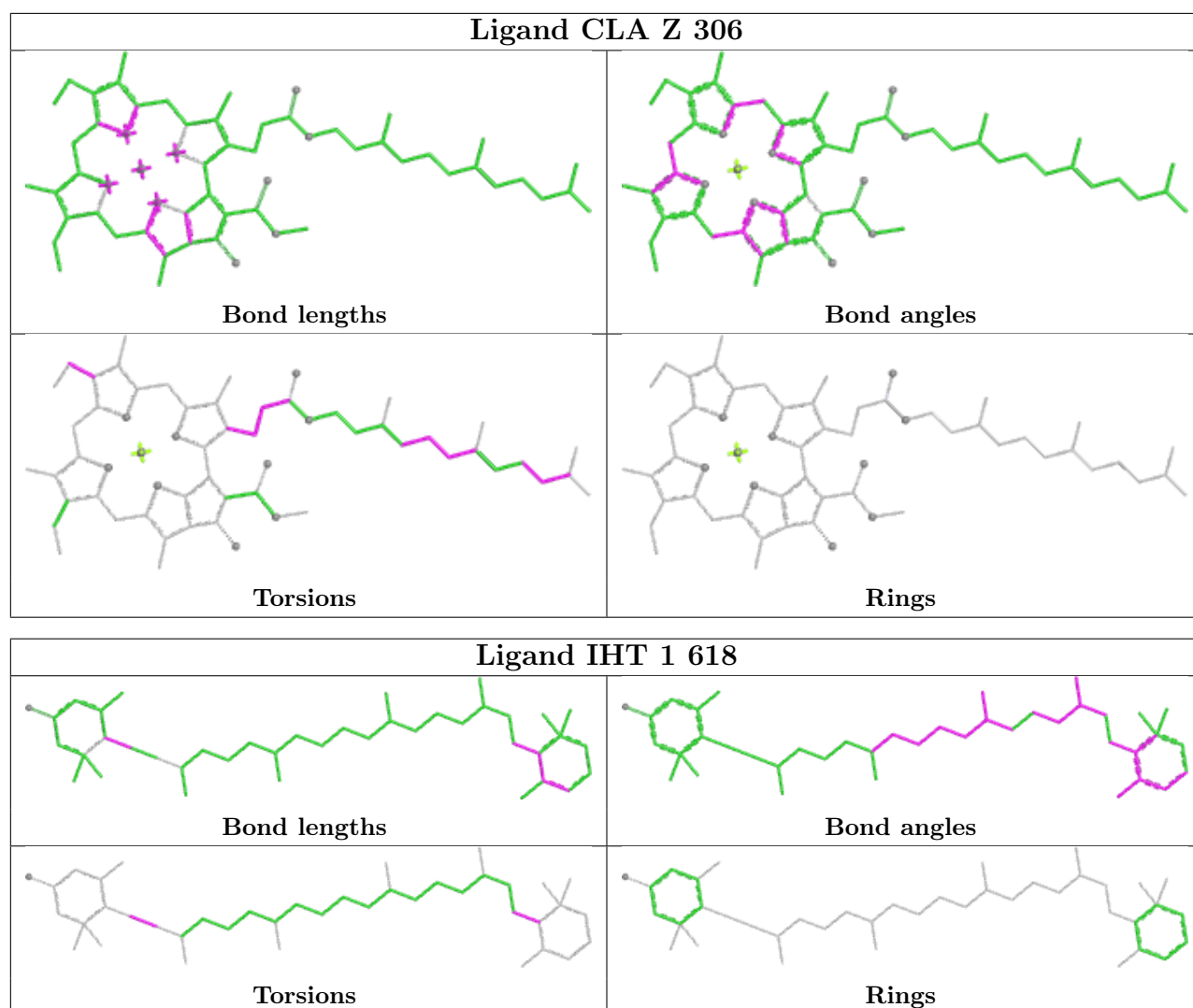


Ligand CLA 1 606

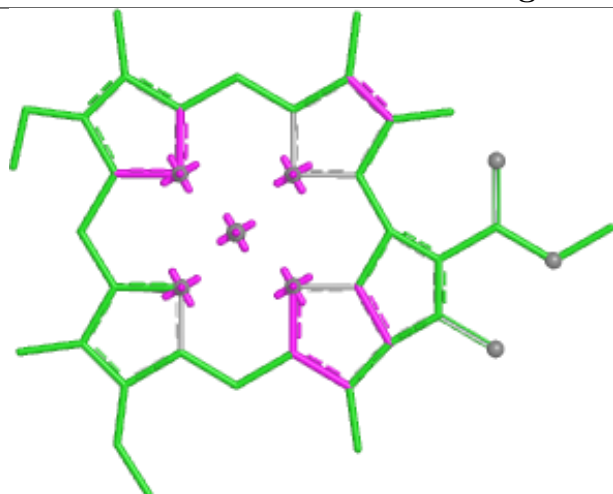




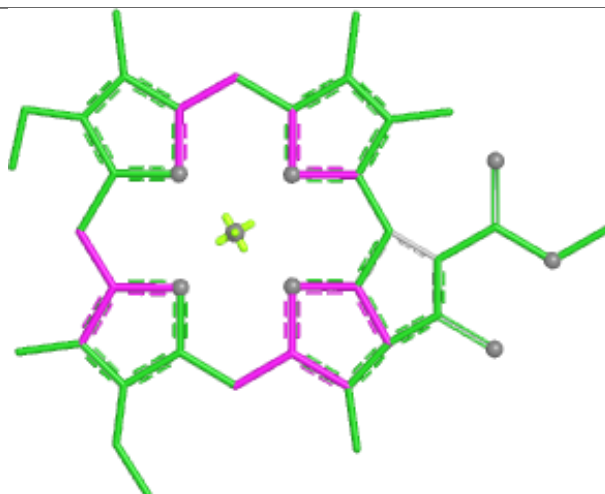
Ligand CLA 2 602**Ligand CLA A 836**



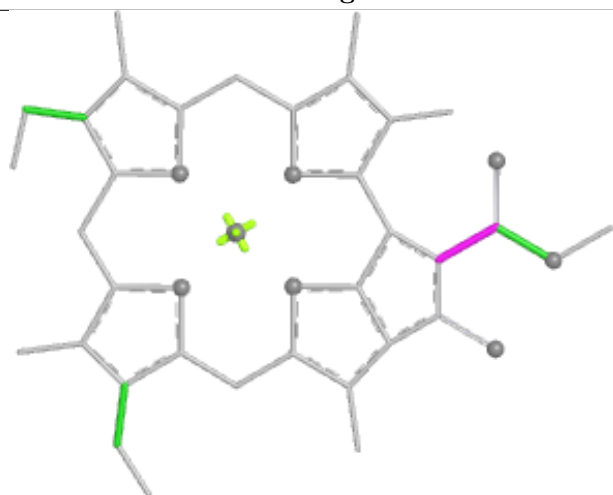
Ligand CLA 9 611



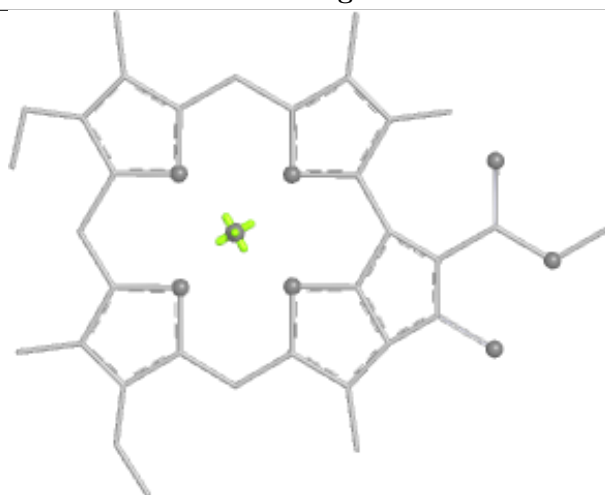
Bond lengths



Bond angles

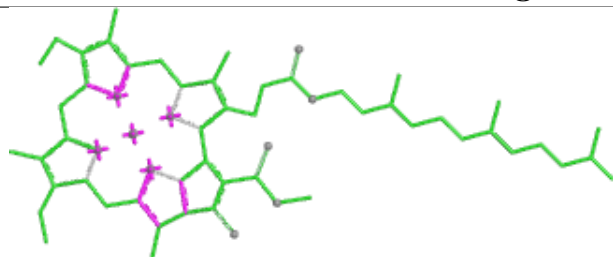


Torsions

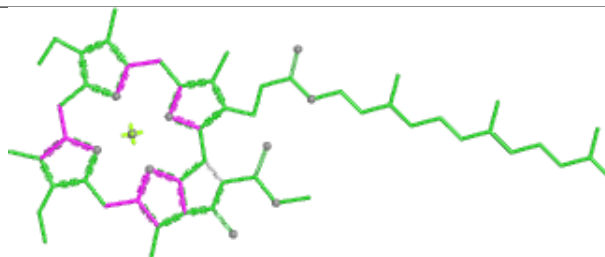


Rings

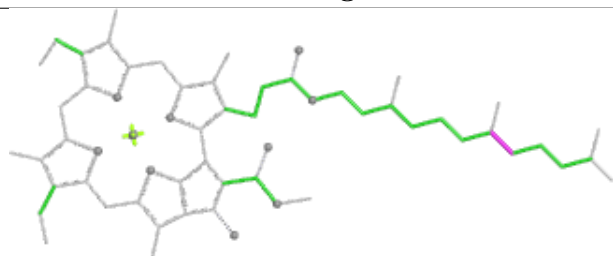
Ligand CLA B 830



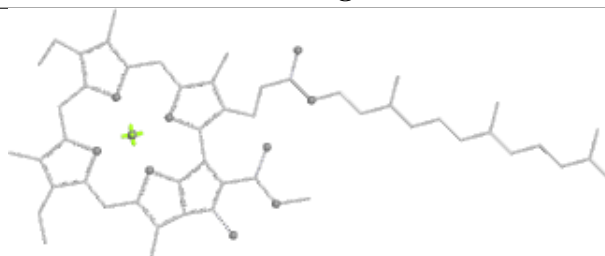
Bond lengths



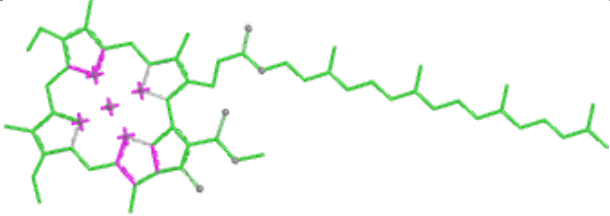
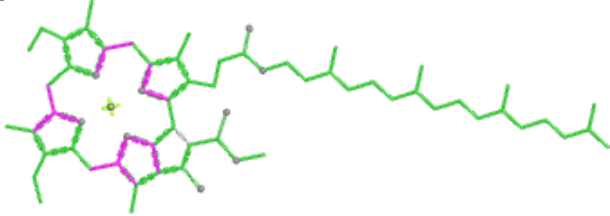
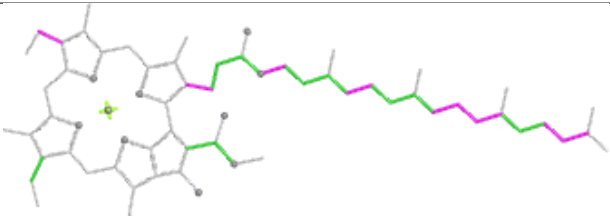
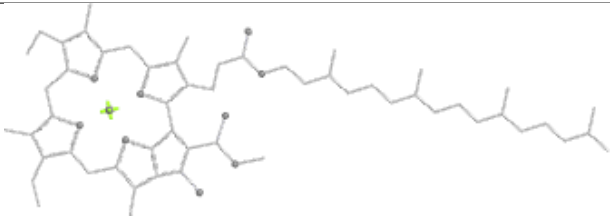
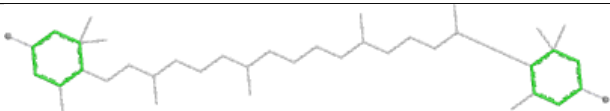
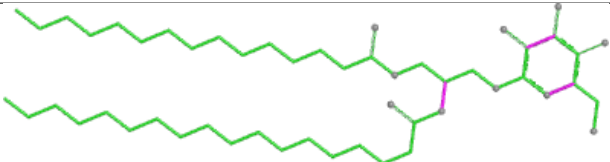
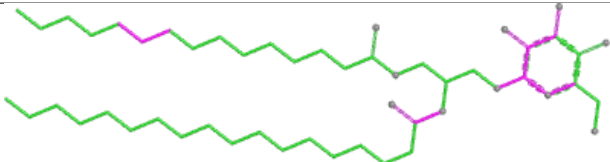
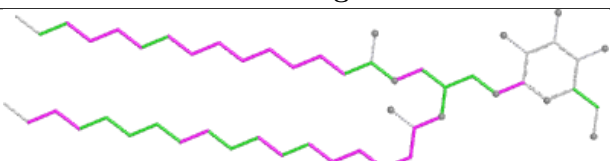
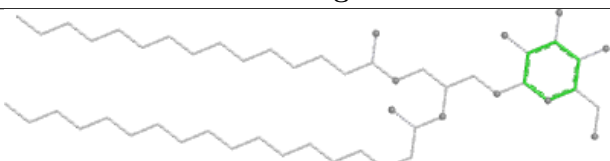
Bond angles



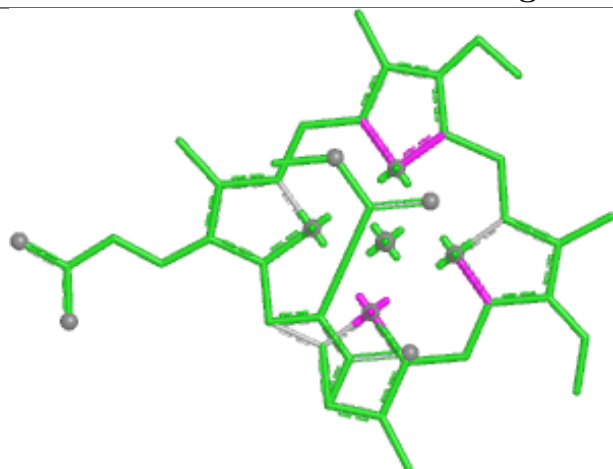
Torsions



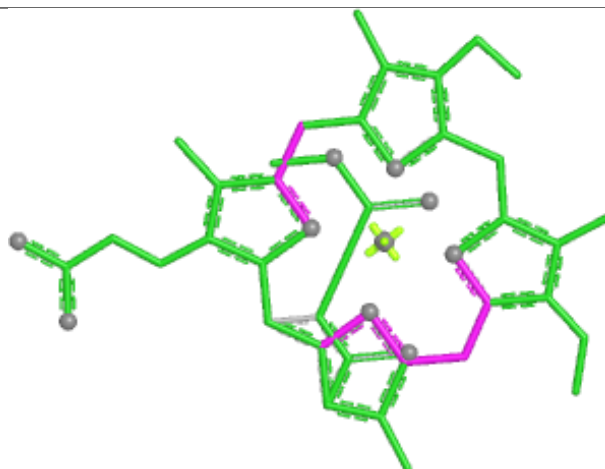
Rings

Ligand CLA B 826	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand II3 b 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG 8 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

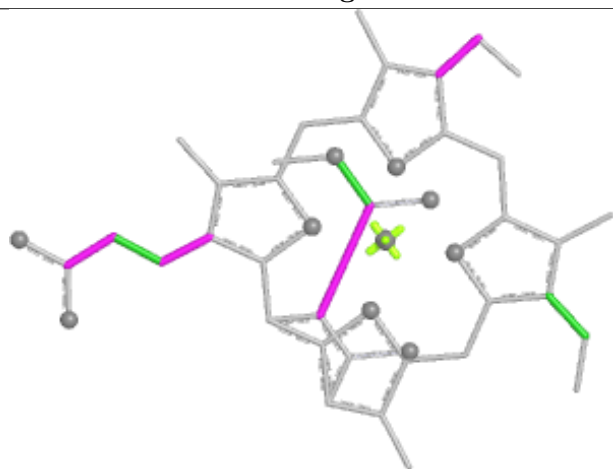
Ligand KC2 d 610



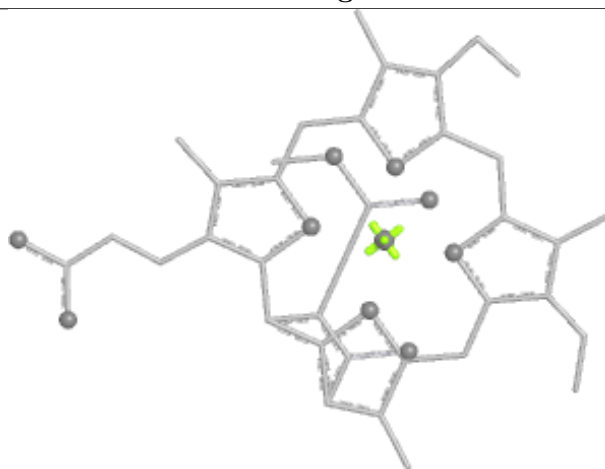
Bond lengths



Bond angles

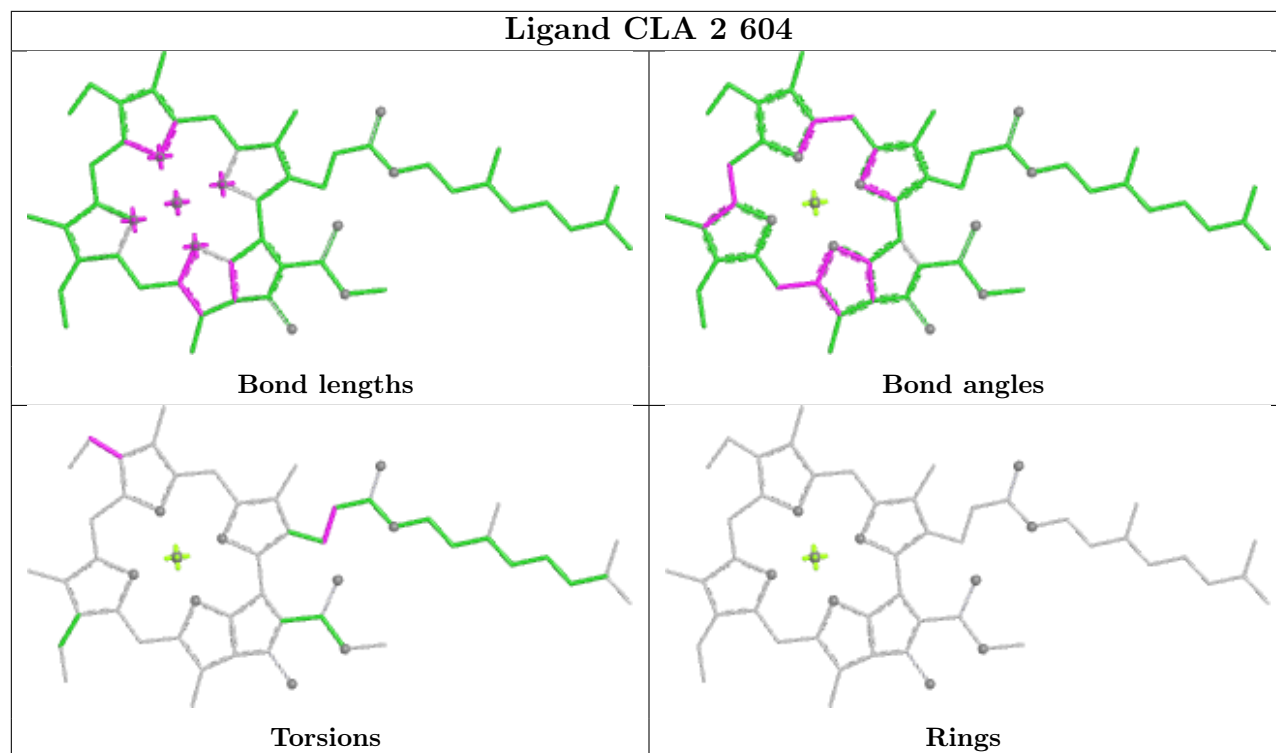


Torsions

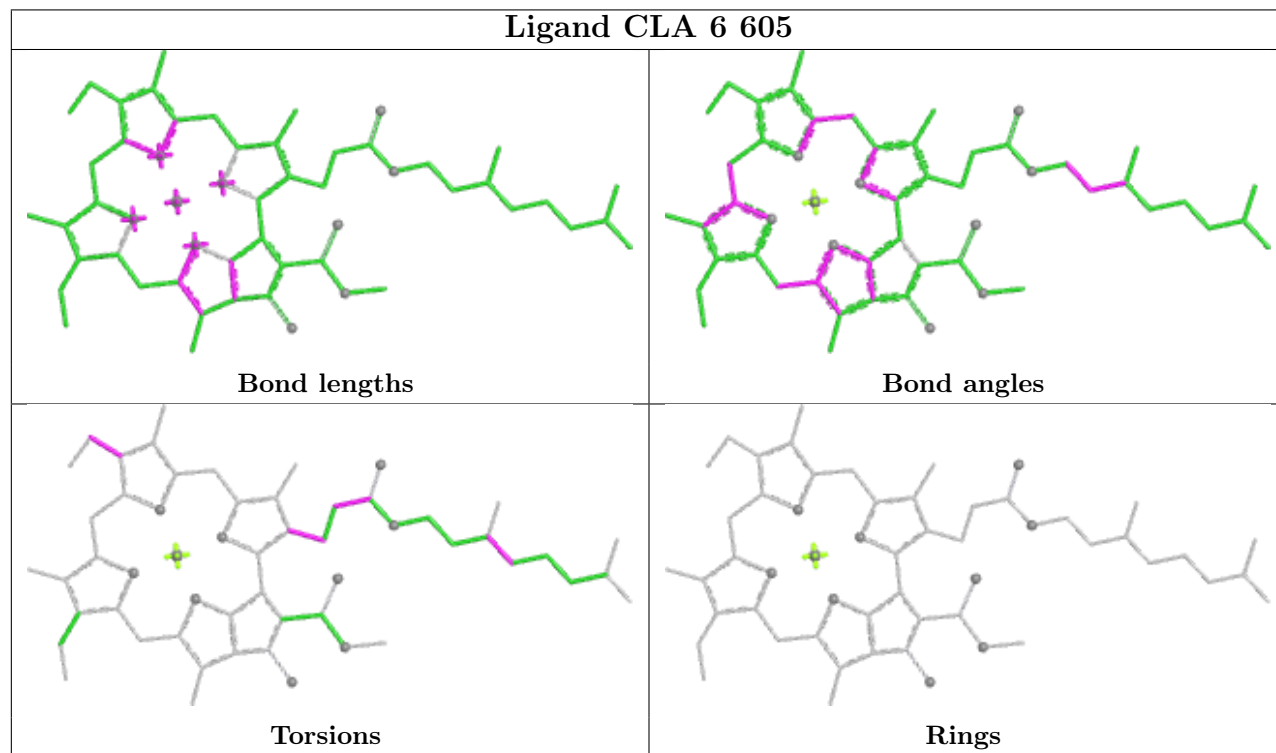


Rings

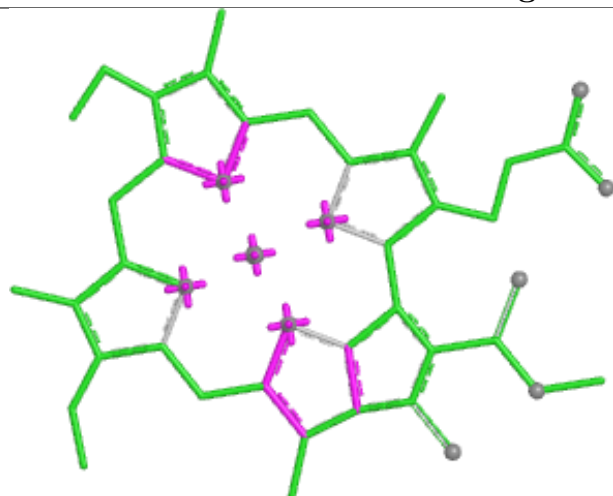
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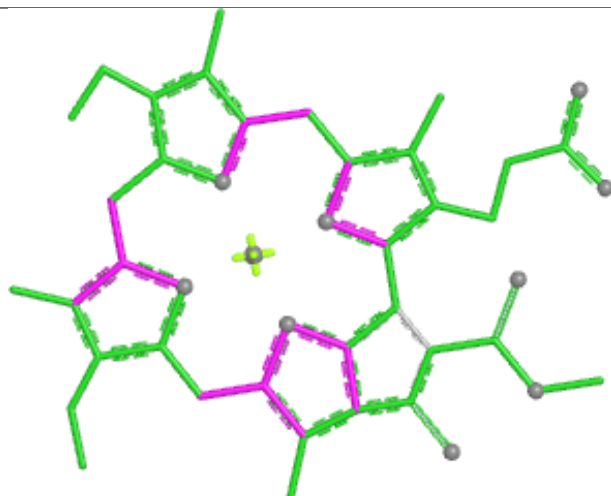
Ligand CLA 6 605



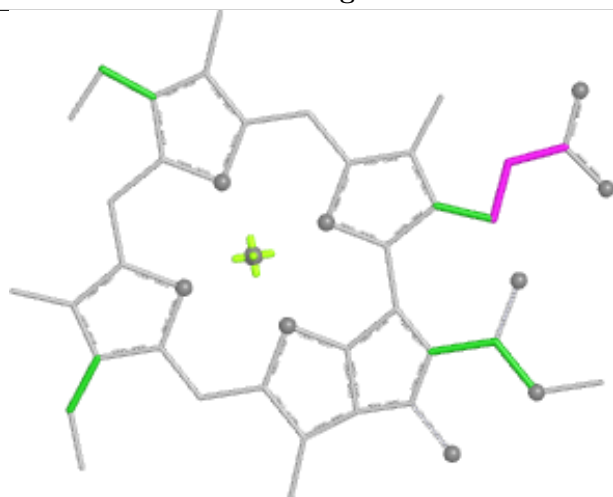
Ligand CLA 9 603



Bond lengths



Bond angles

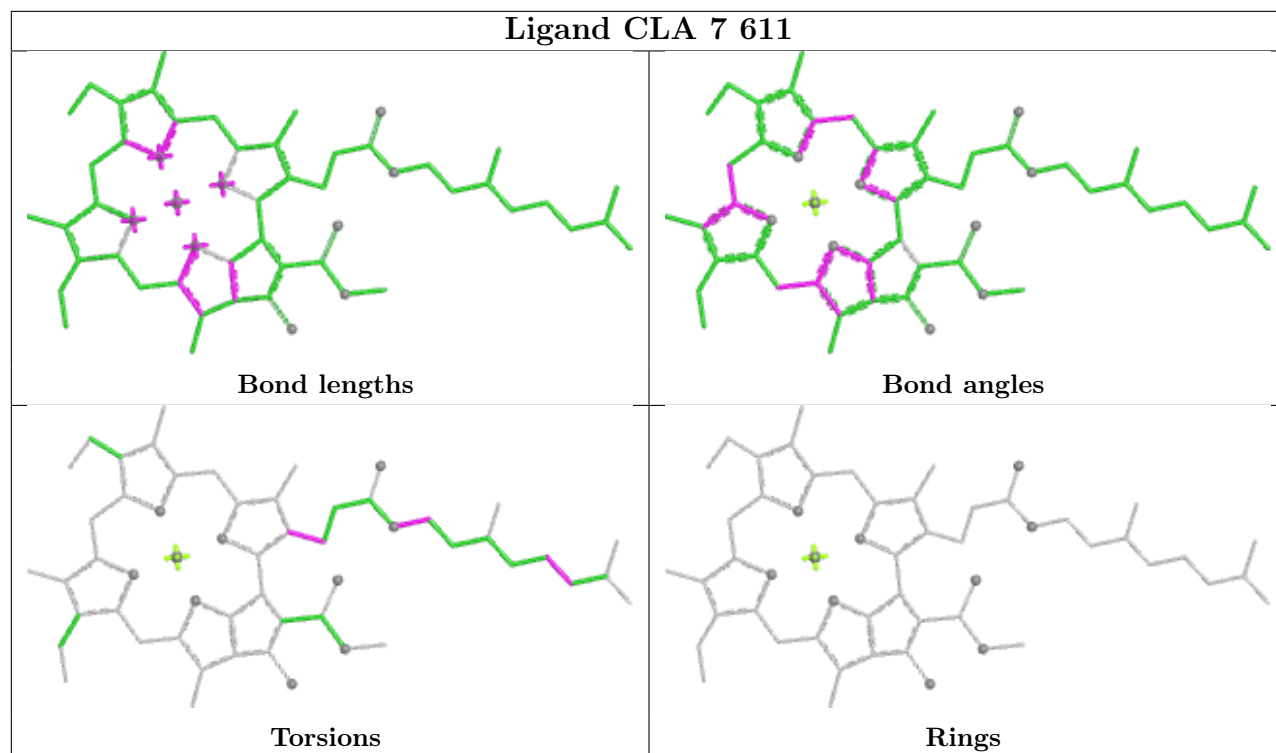


Torsions

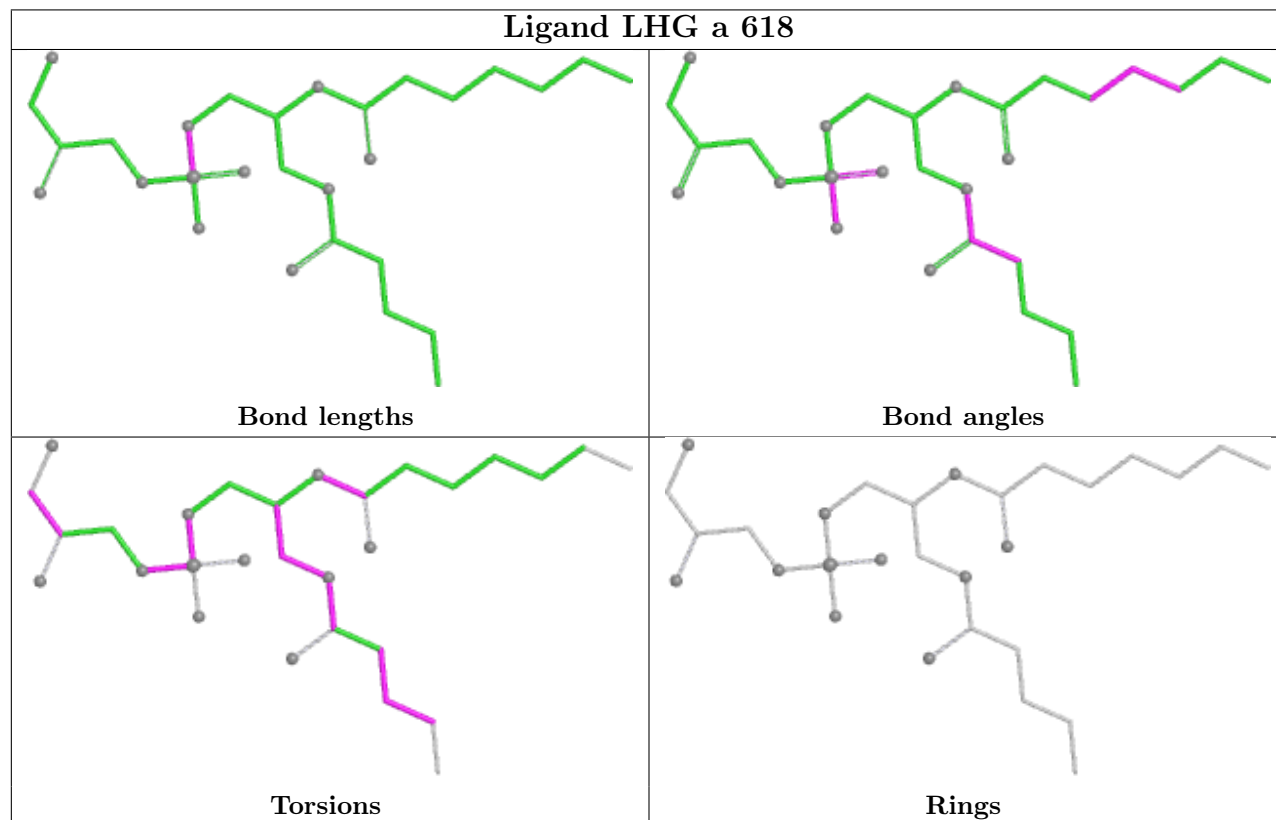


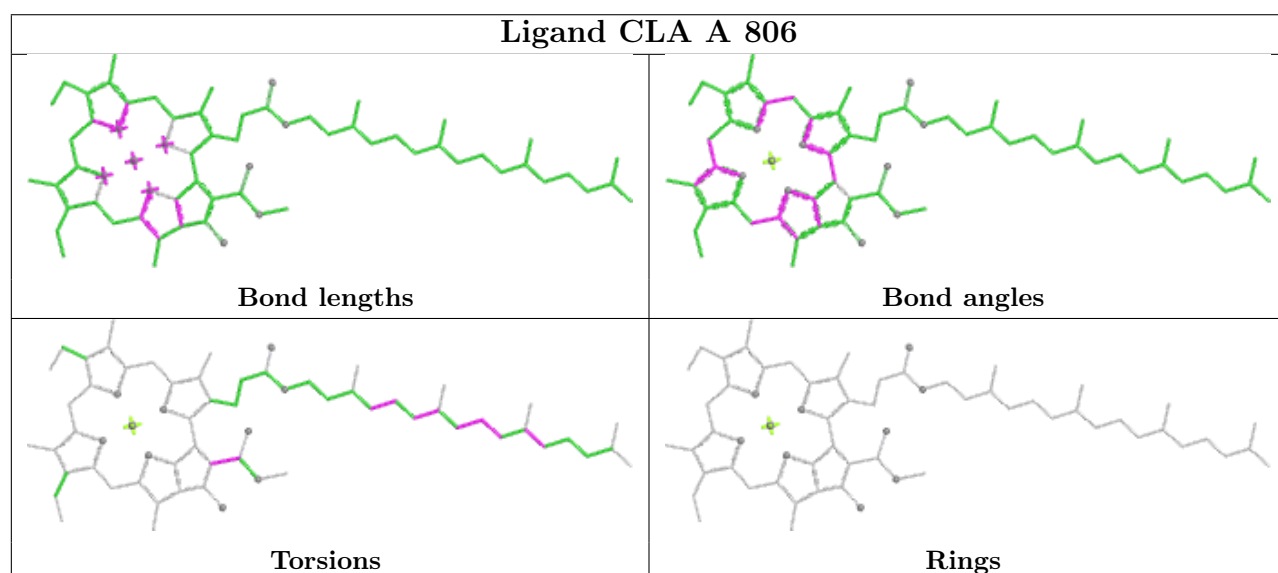
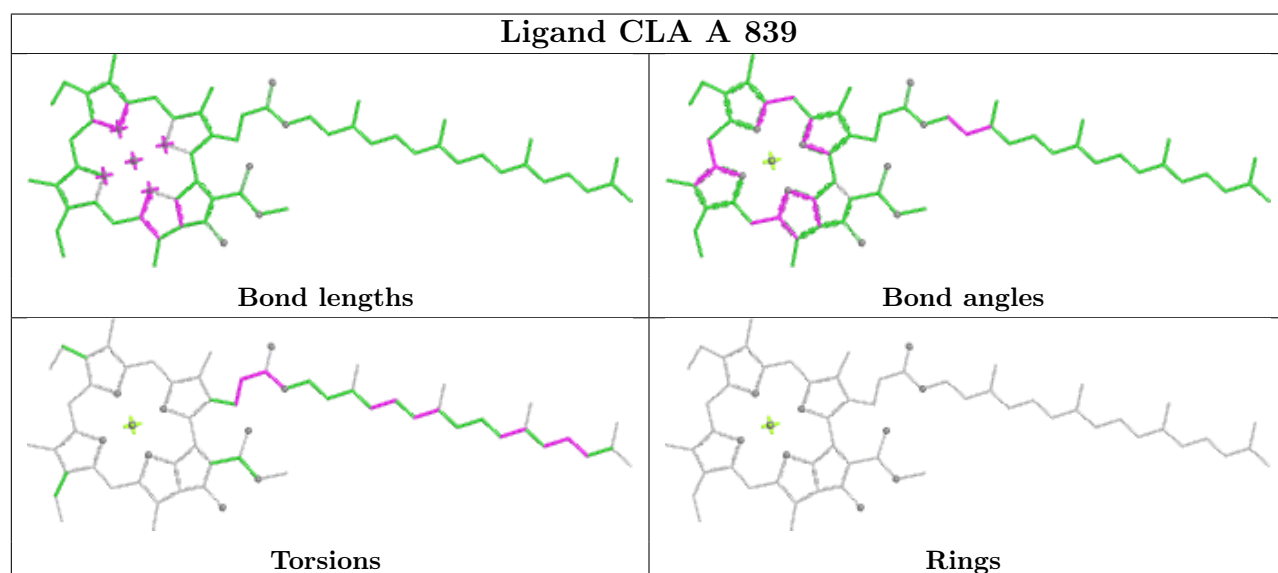
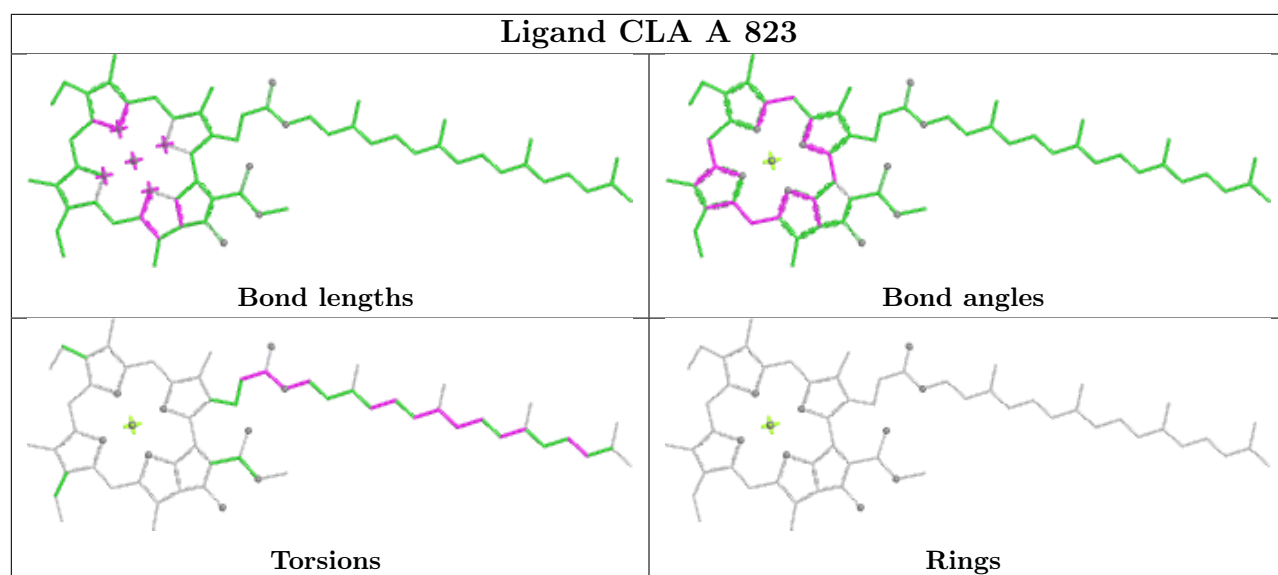
Rings

Ligand CLA 7 611

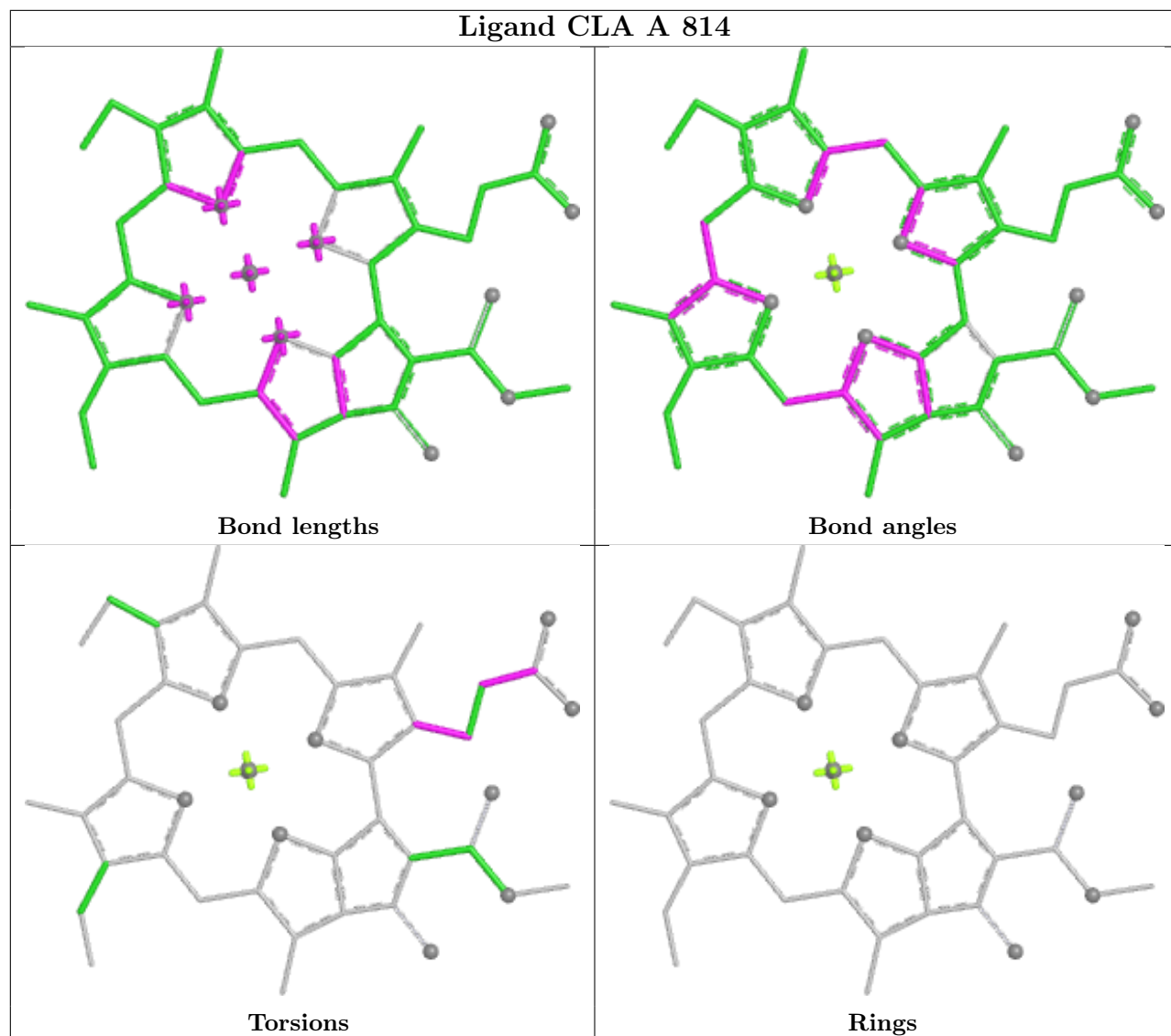


Ligand LHG a 618

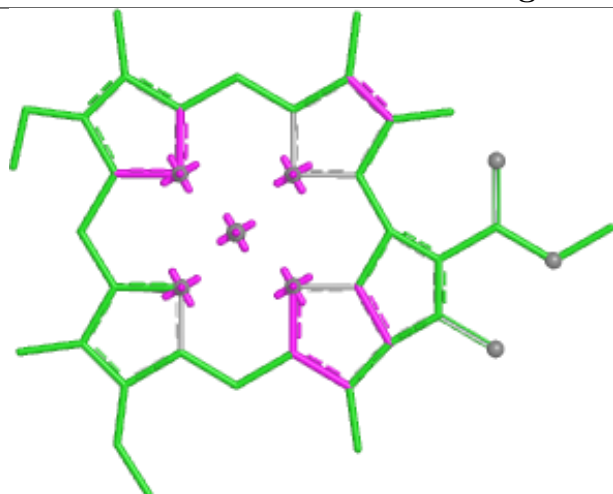




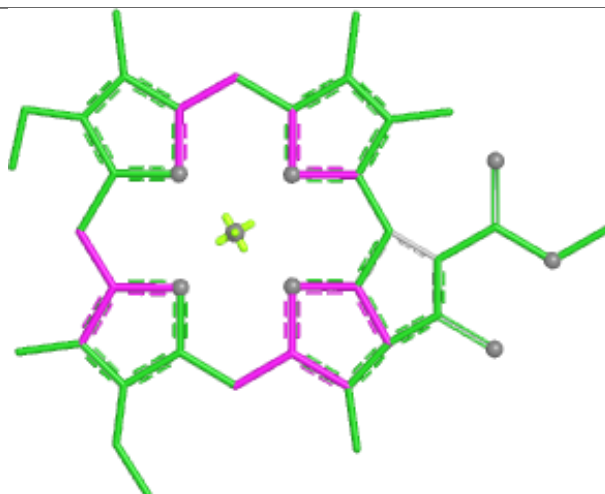
Ligand CLA A 814



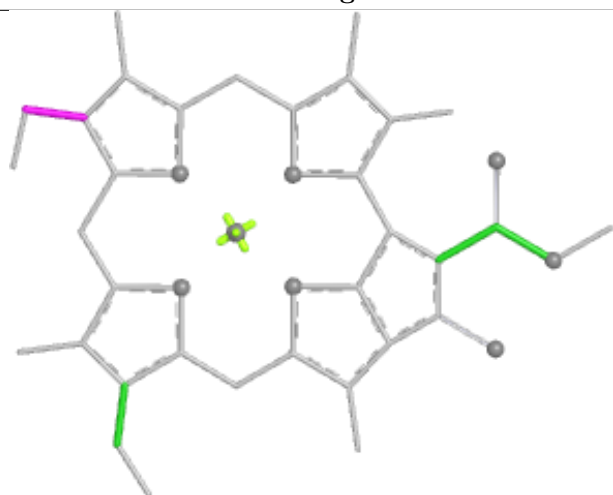
Ligand CLA 7 609



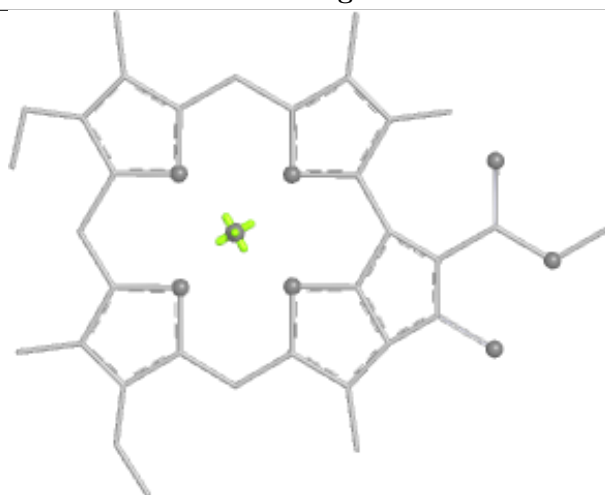
Bond lengths



Bond angles

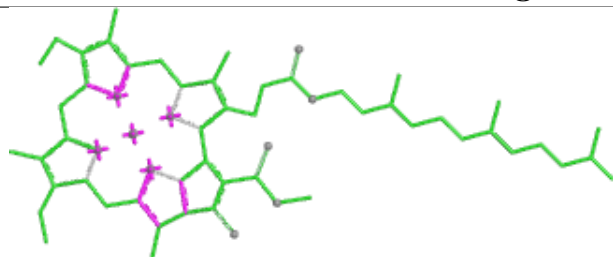


Torsions

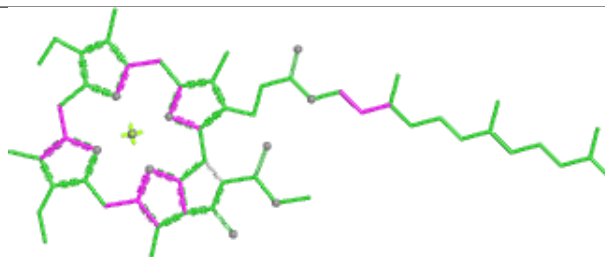


Rings

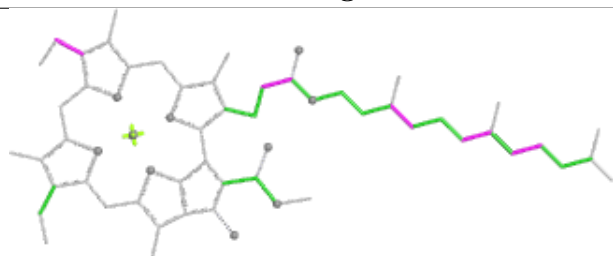
Ligand CLA B 821



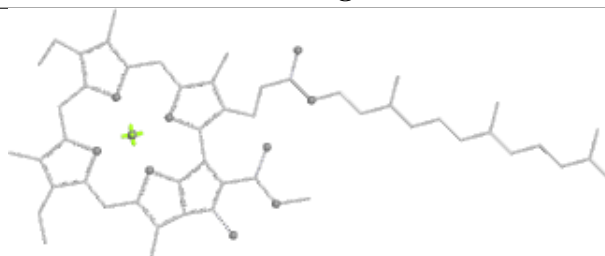
Bond lengths



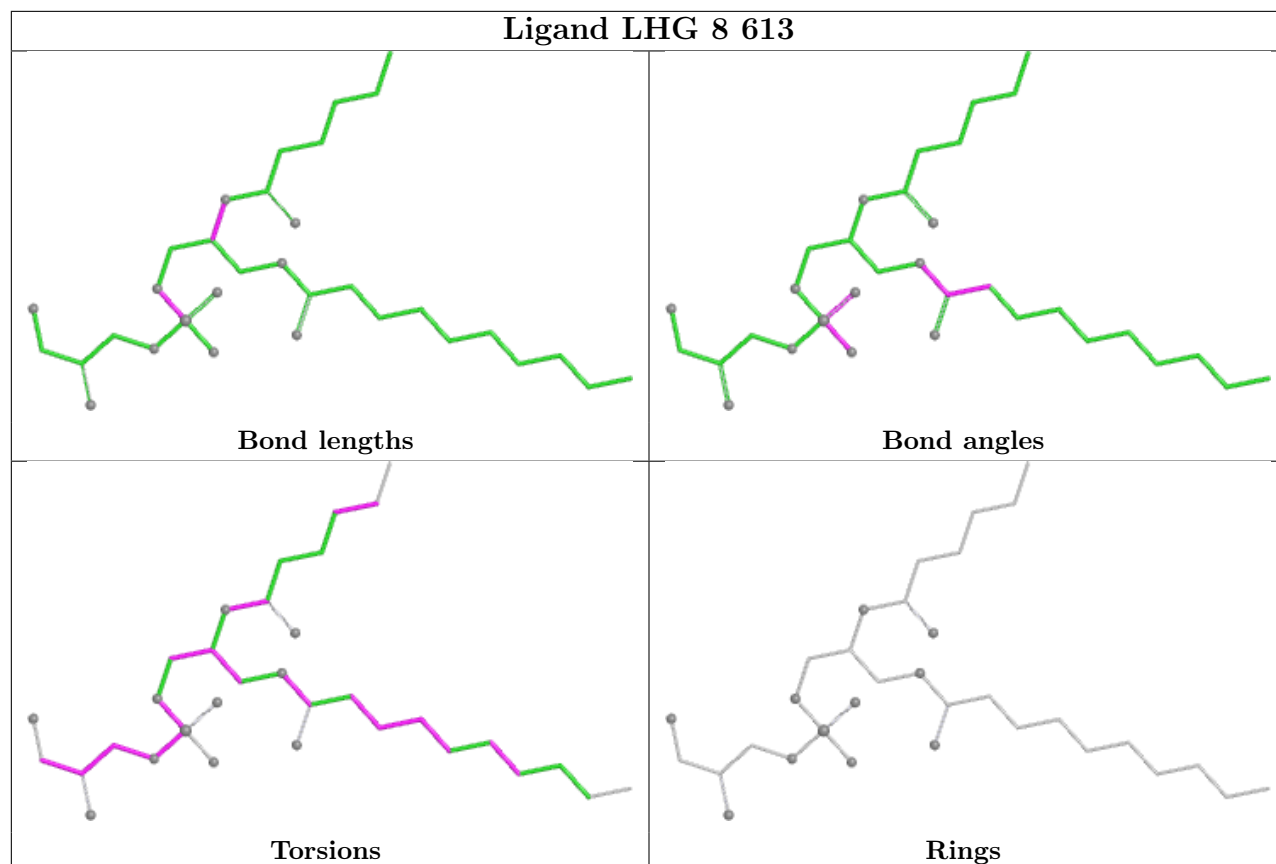
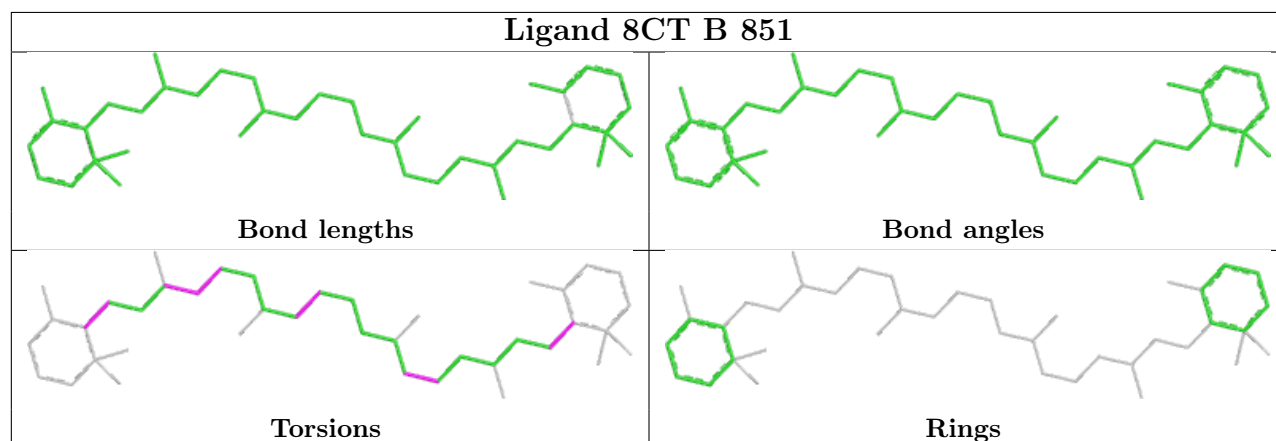
Bond angles



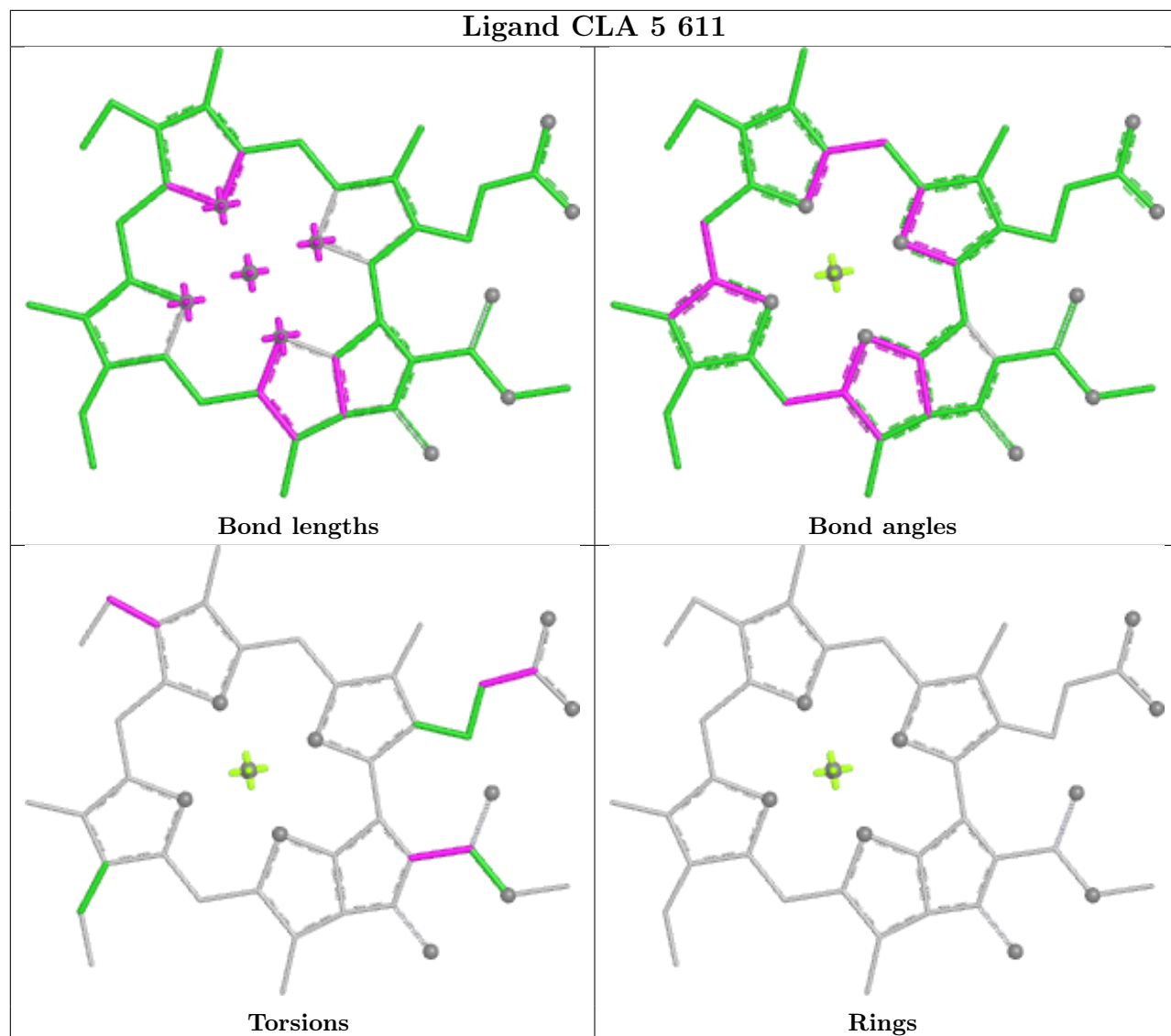
Torsions



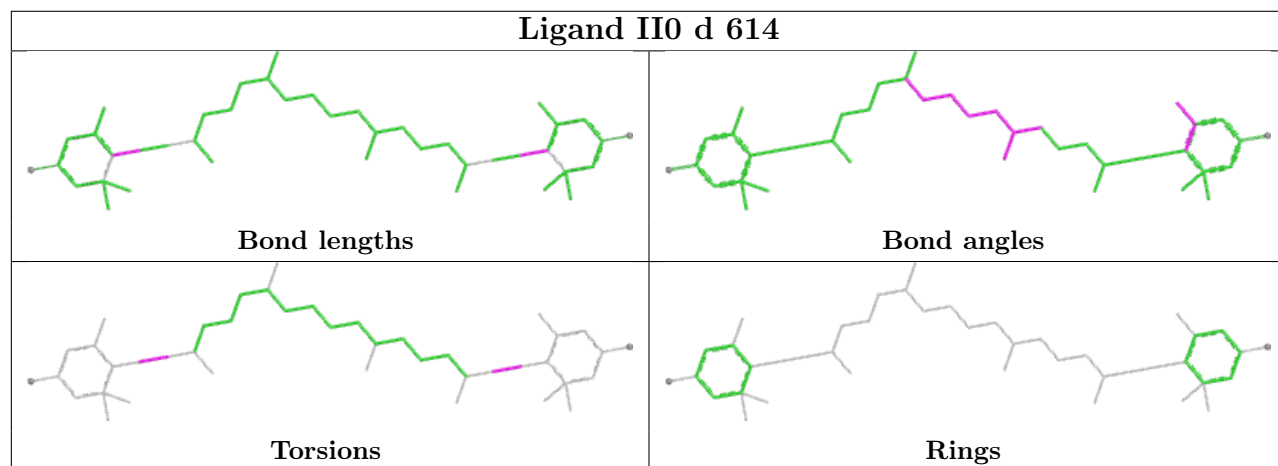
Rings

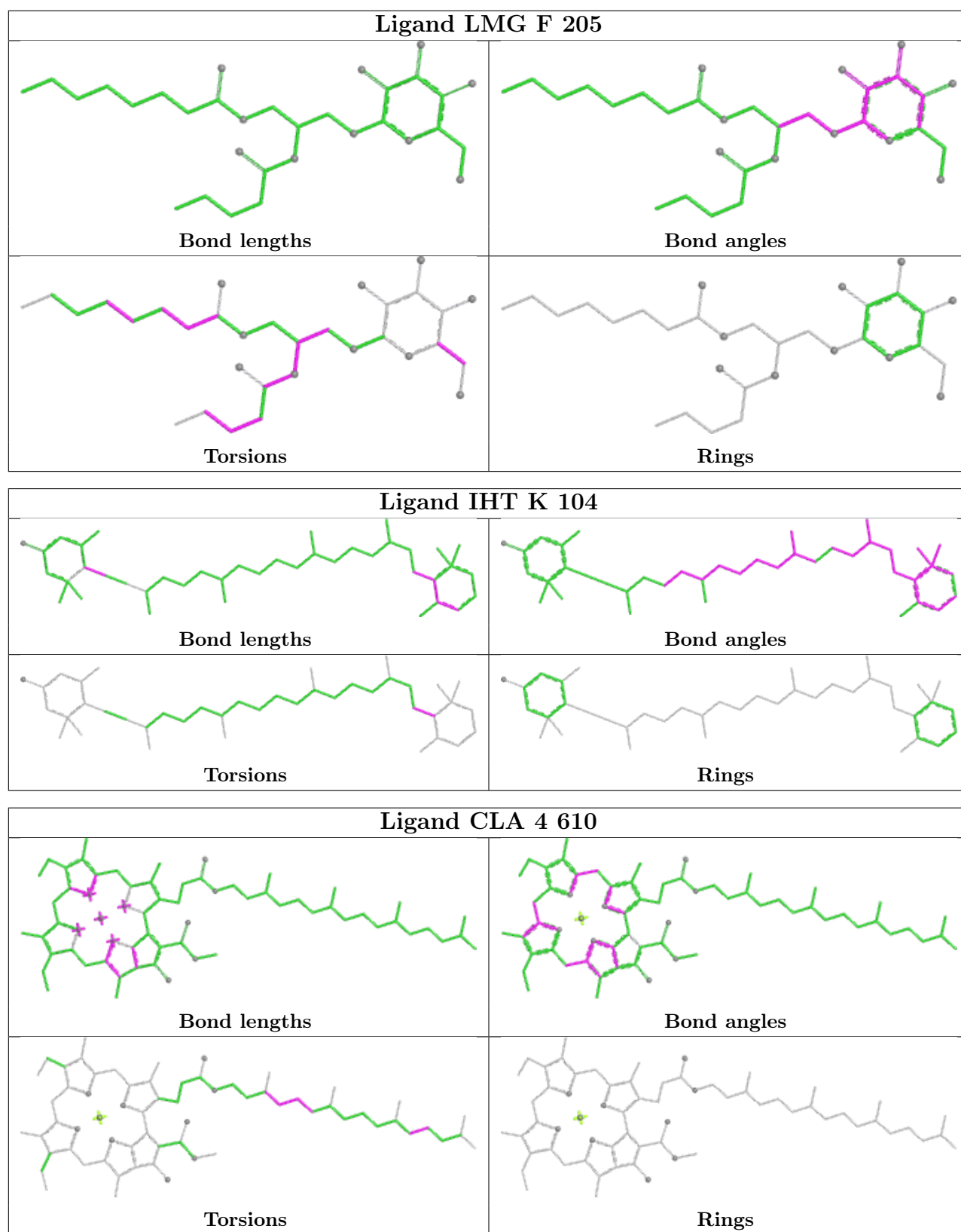
Ligand LHG 8 613**Ligand 8CT B 851**

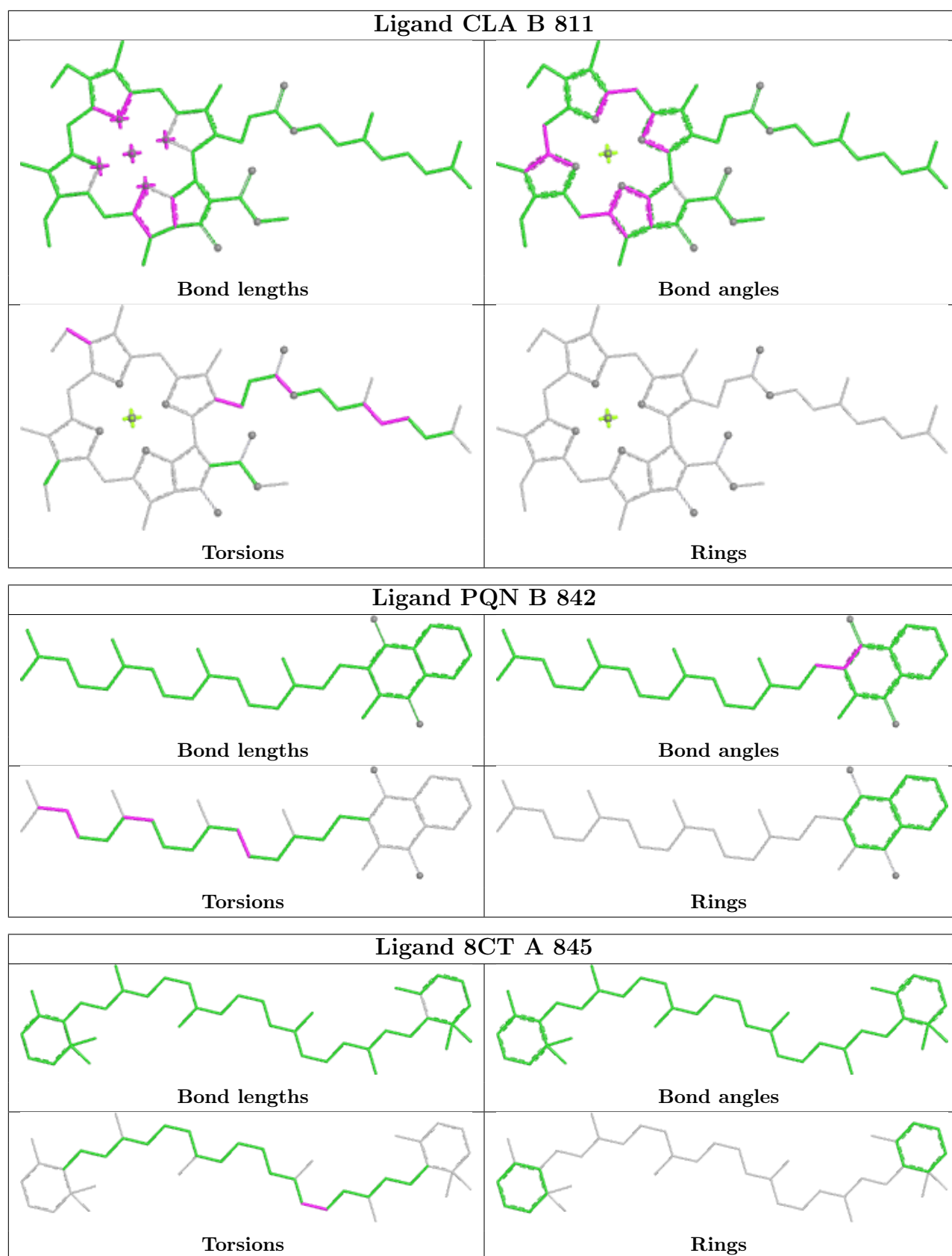
Ligand CLA 5 611

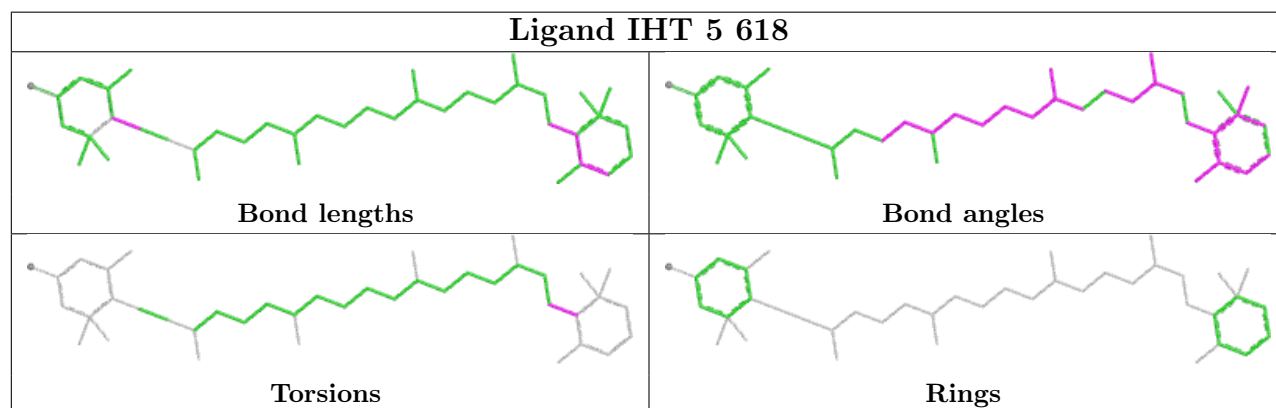
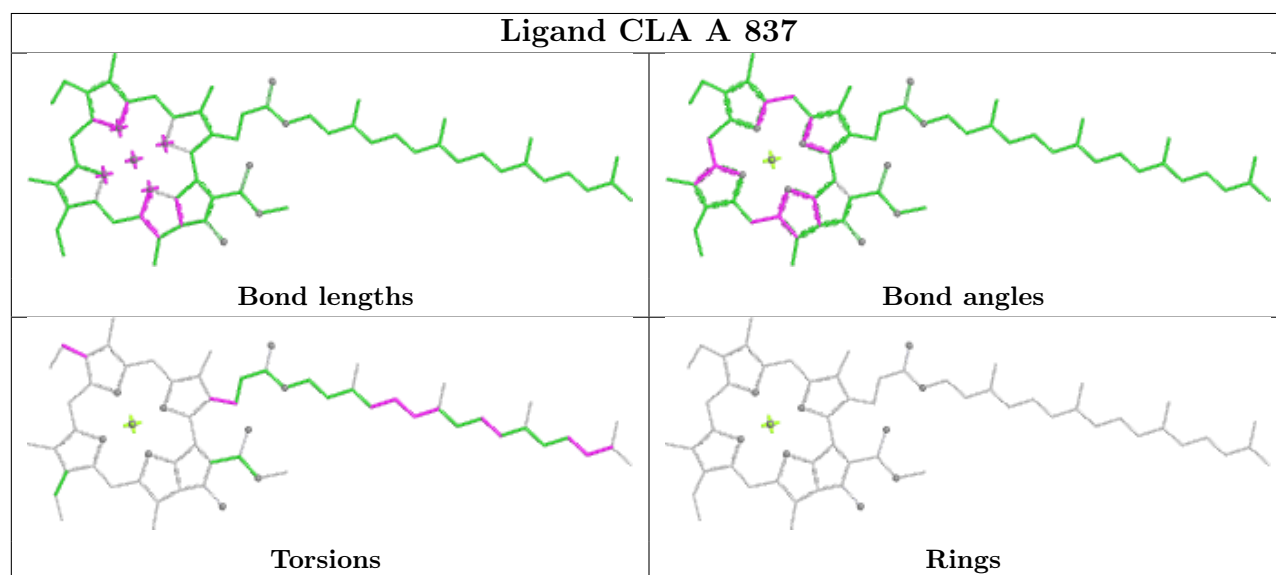
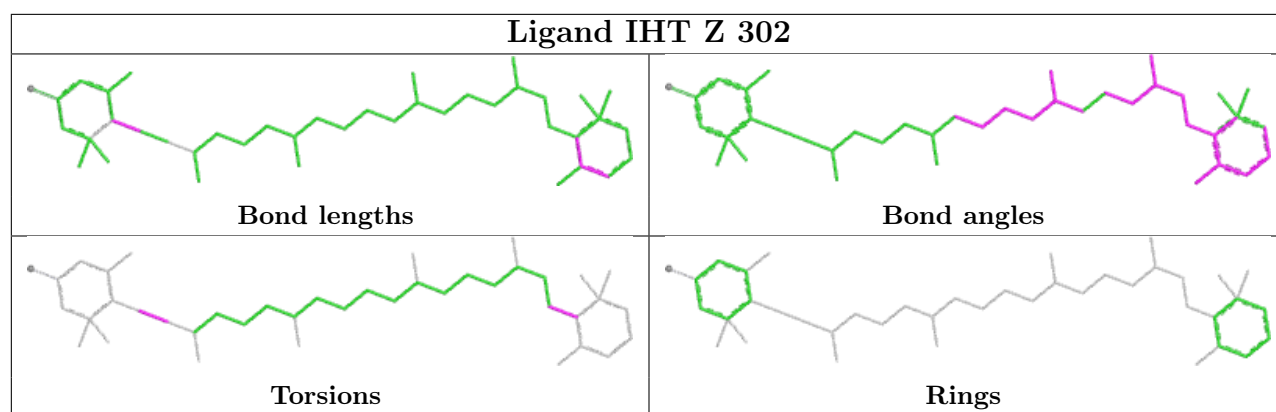


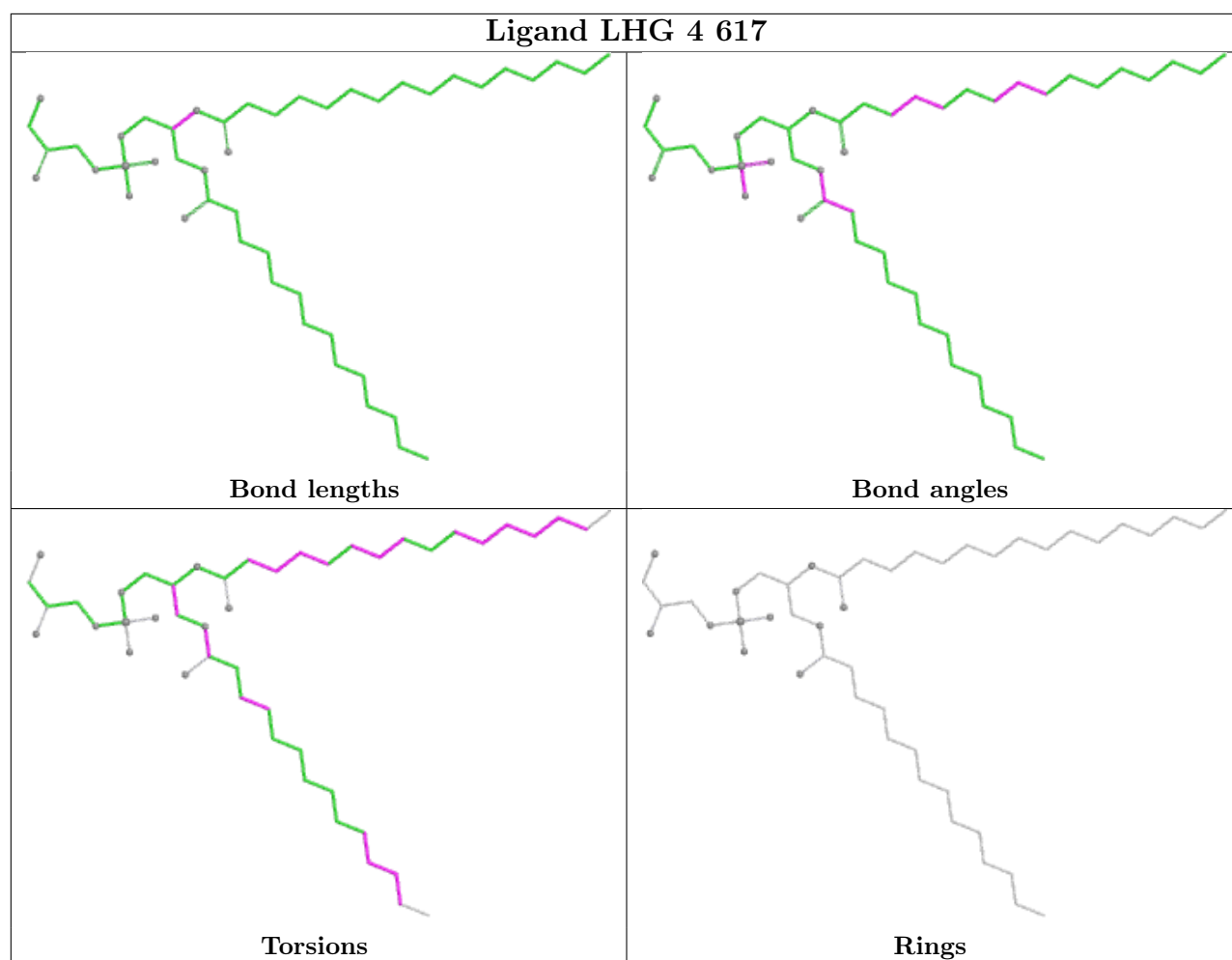
Ligand II0 d 614



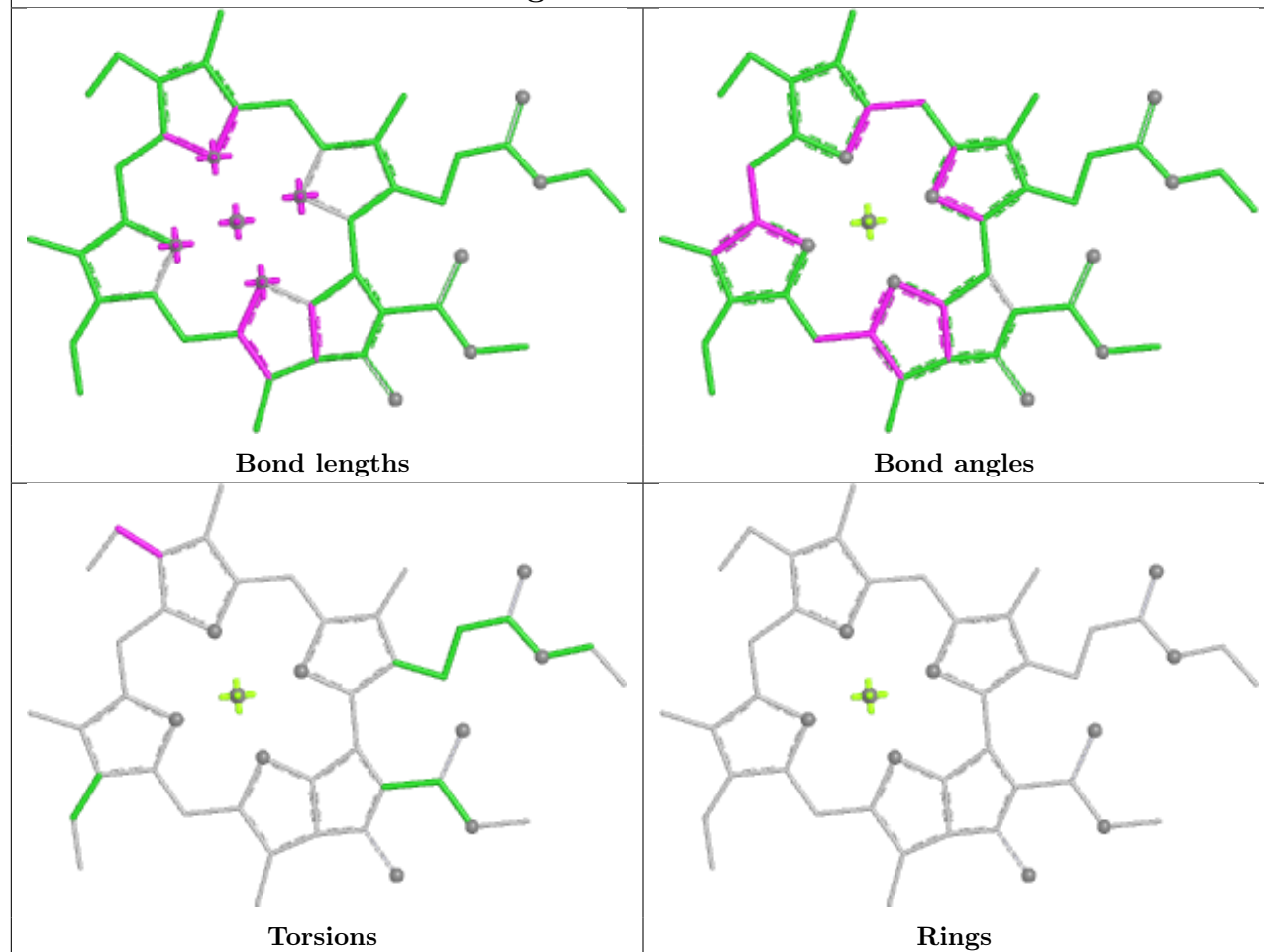




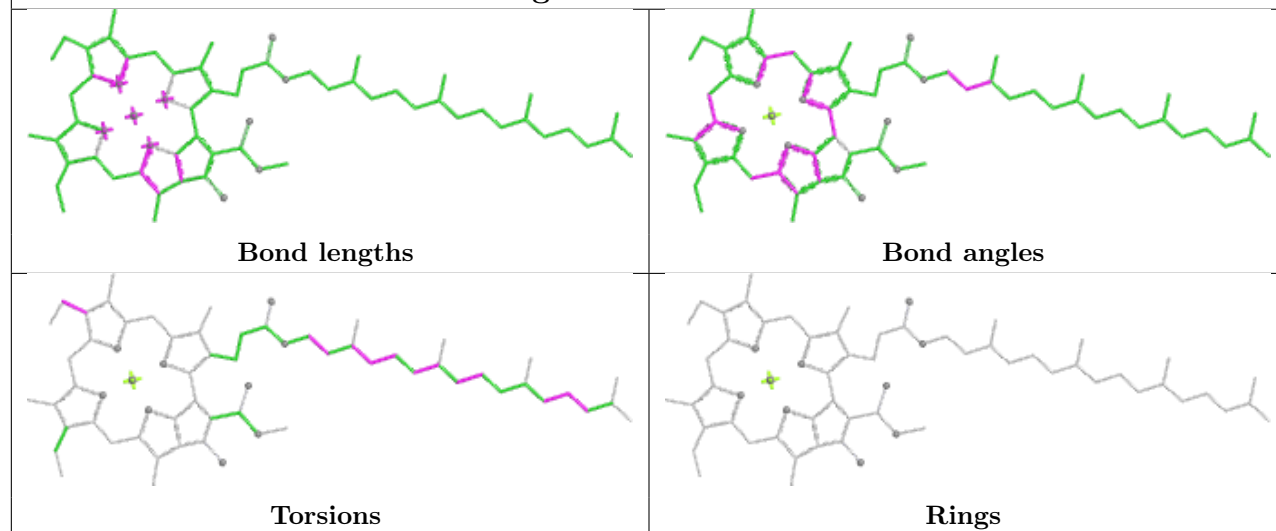


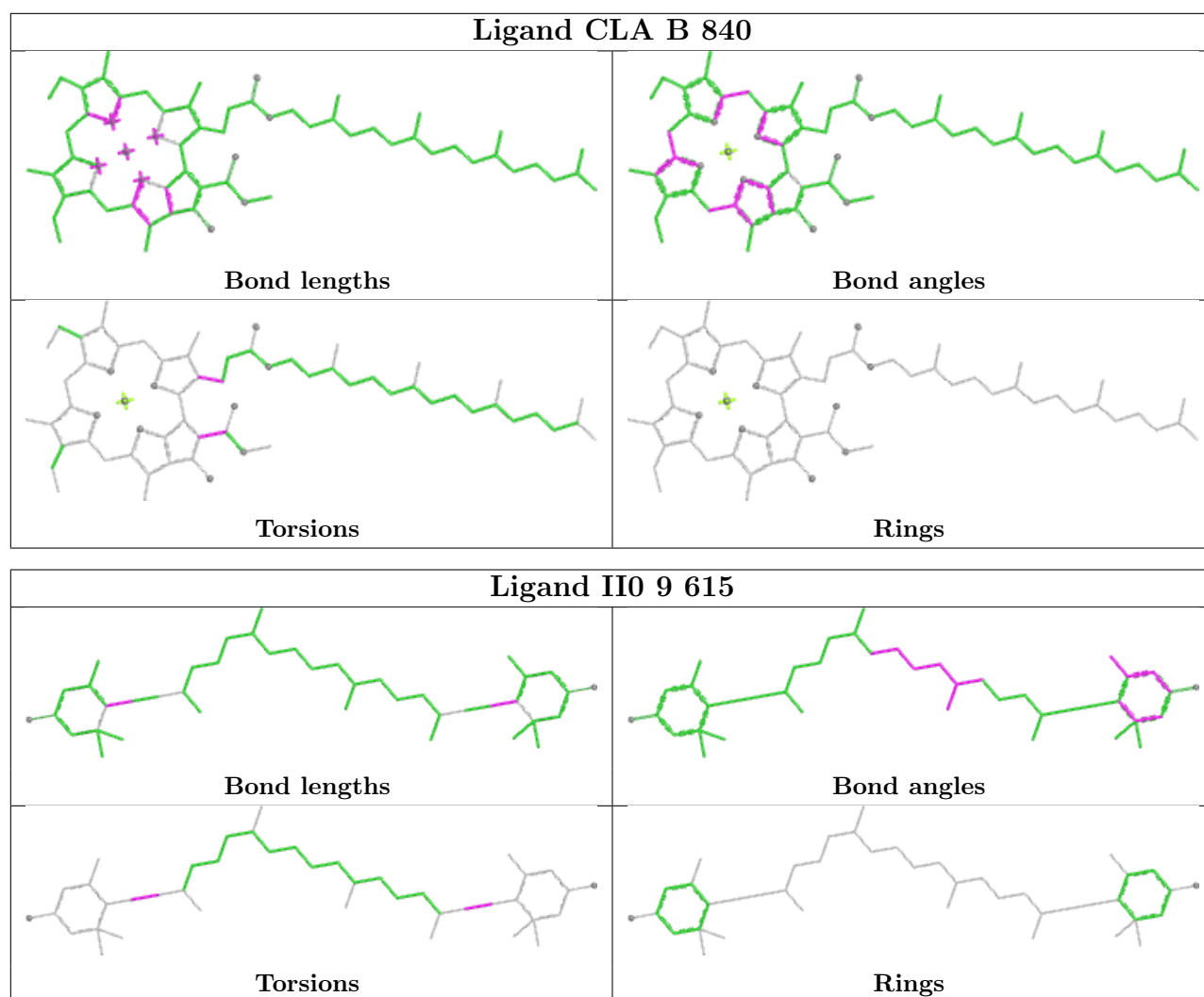


Ligand CLA B 836

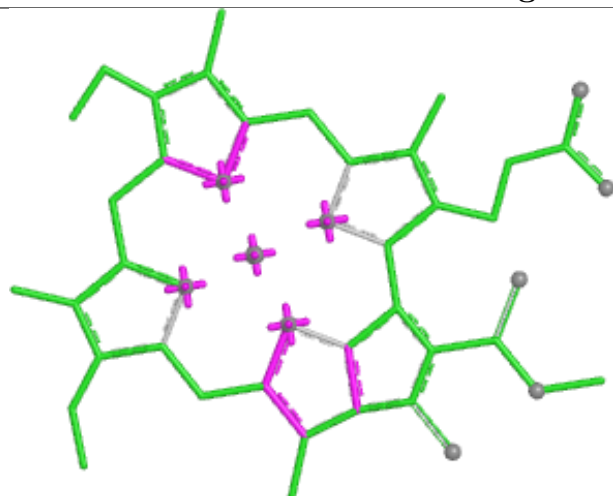


Ligand CLA B 823

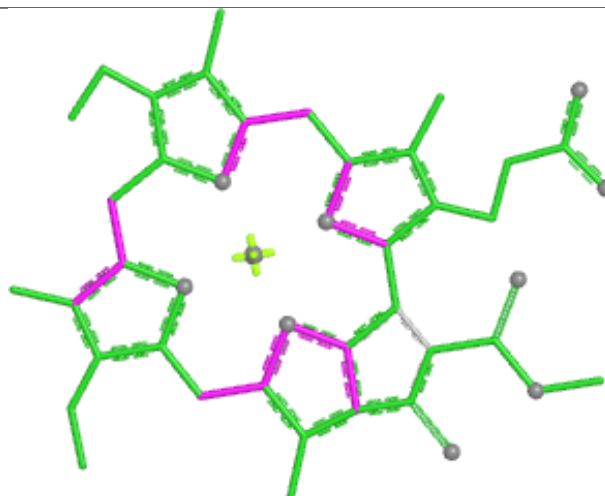




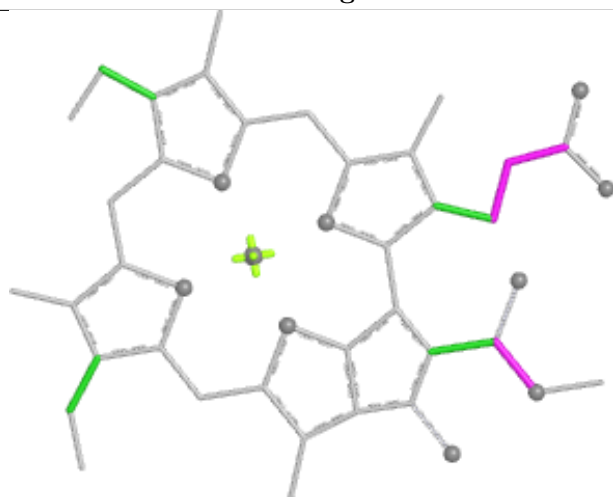
Ligand CLA 8 602



Bond lengths



Bond angles

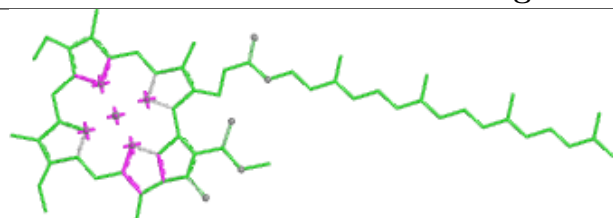


Torsions

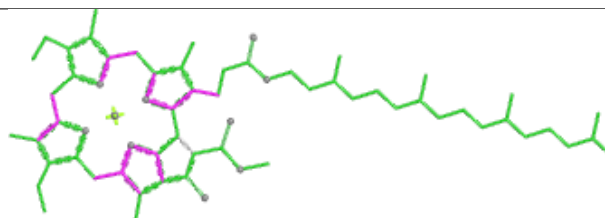


Rings

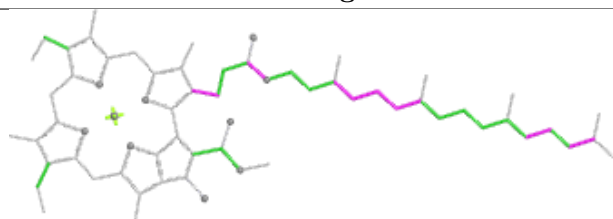
Ligand CLA A 817



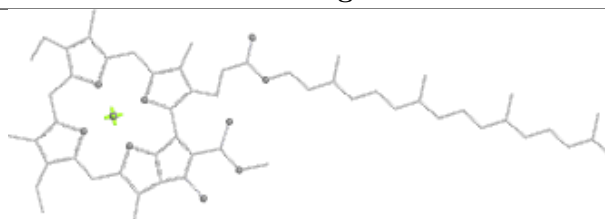
Bond lengths



Bond angles

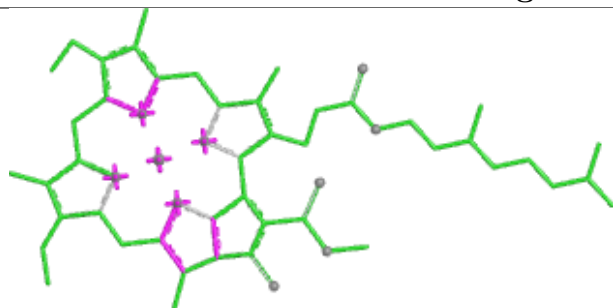


Torsions

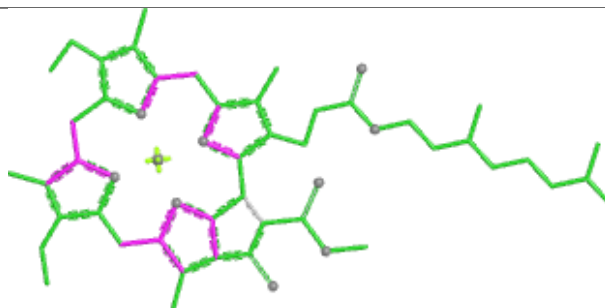


Rings

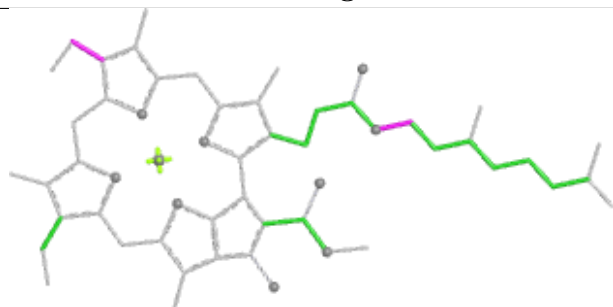
Ligand CLA Z 304



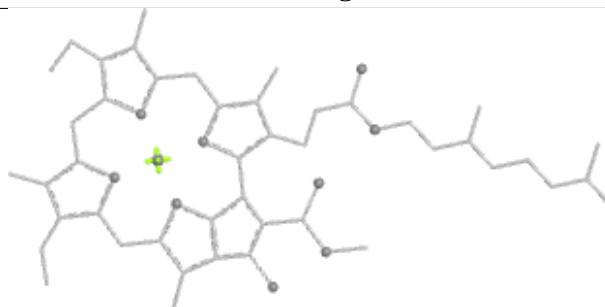
Bond lengths



Bond angles

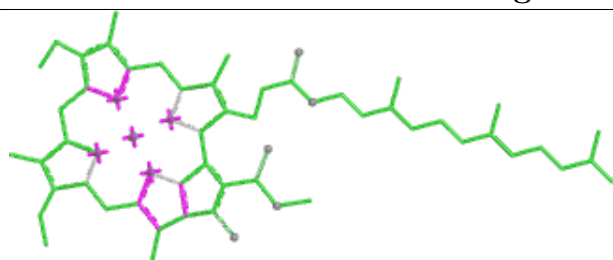


Torsions

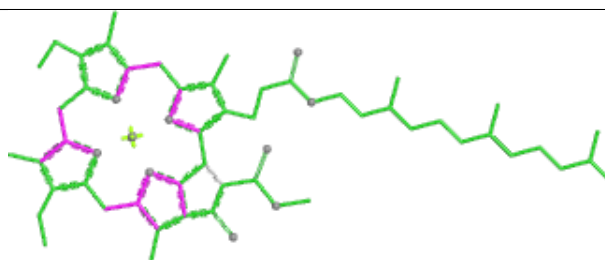


Rings

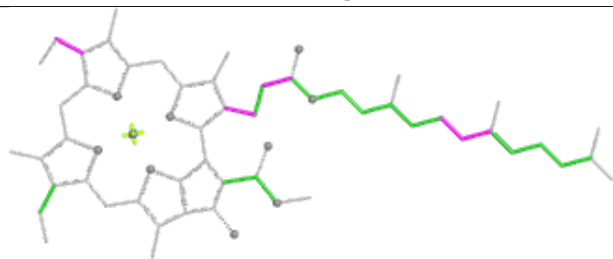
Ligand CLA A 816



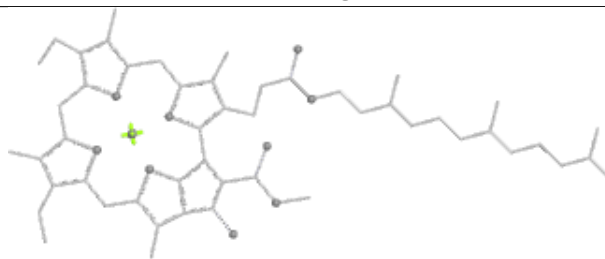
Bond lengths



Bond angles

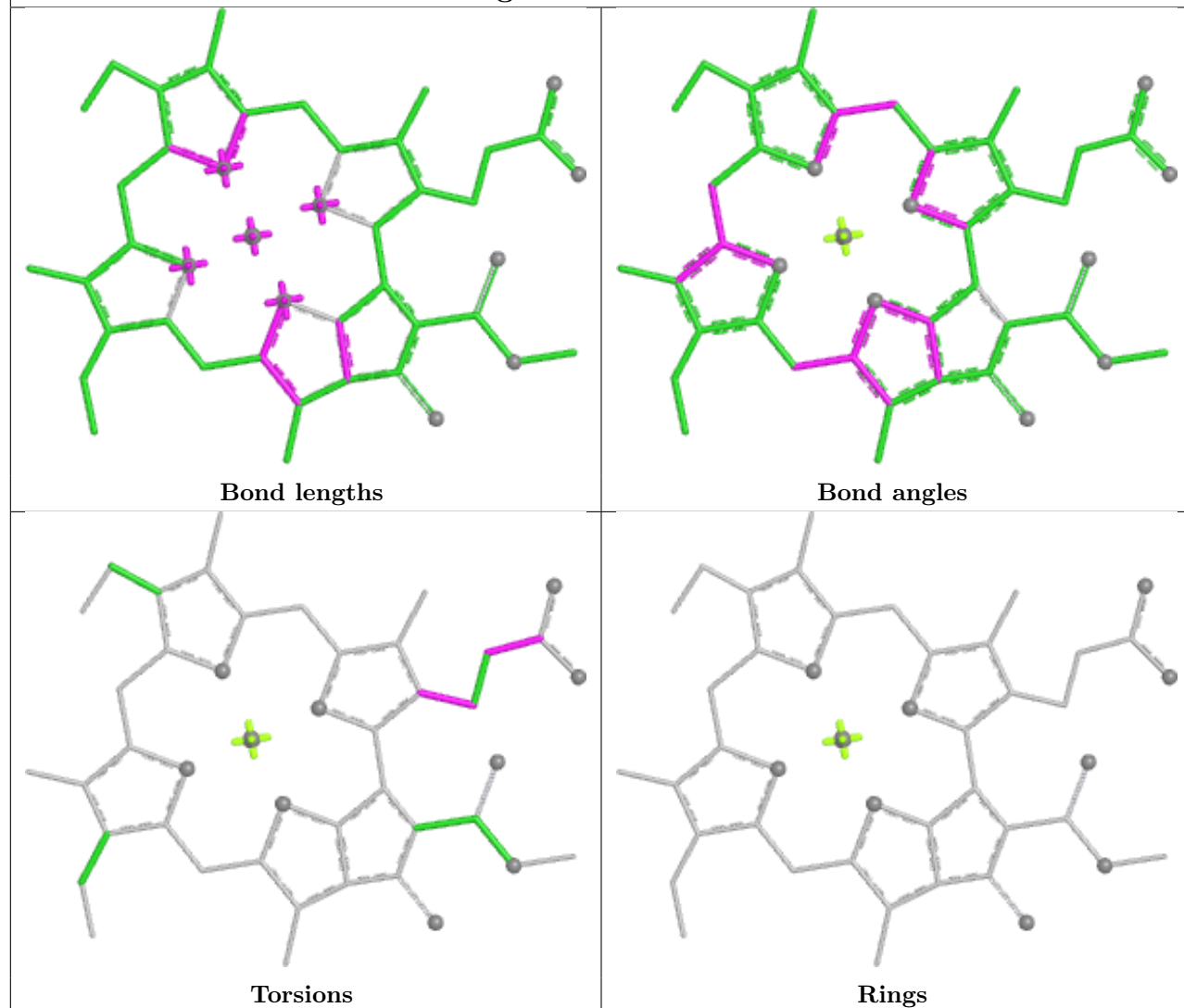


Torsions

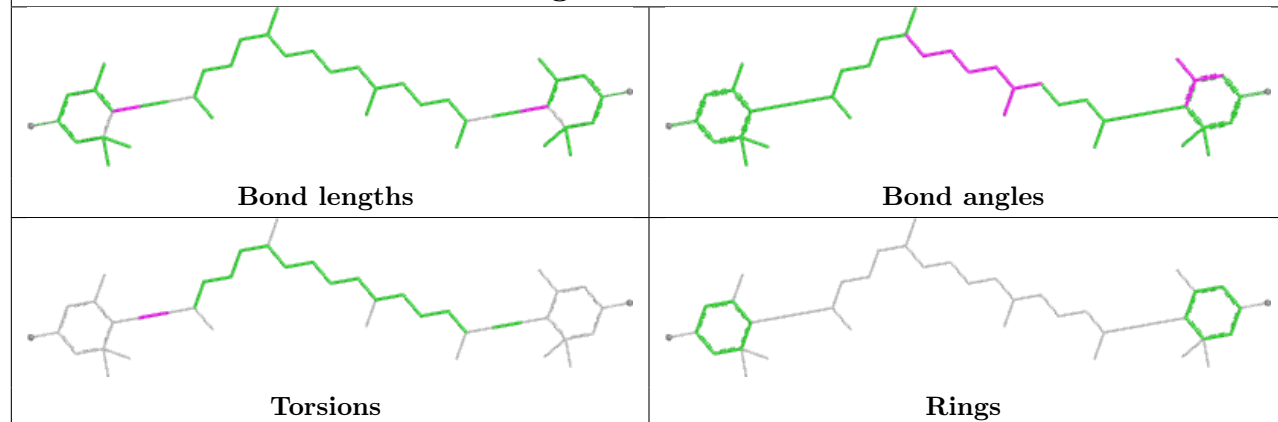


Rings

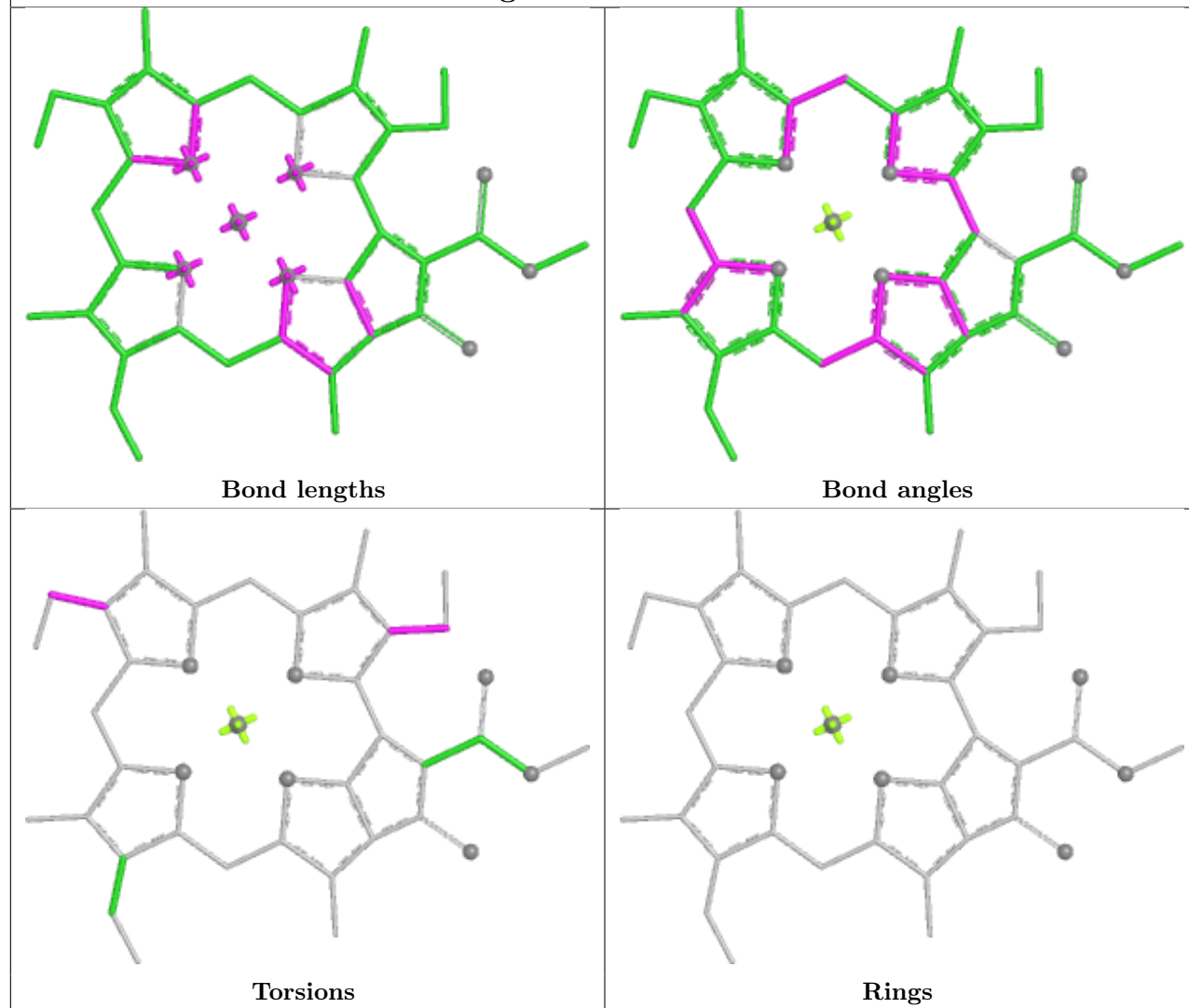
Ligand CLA a 601



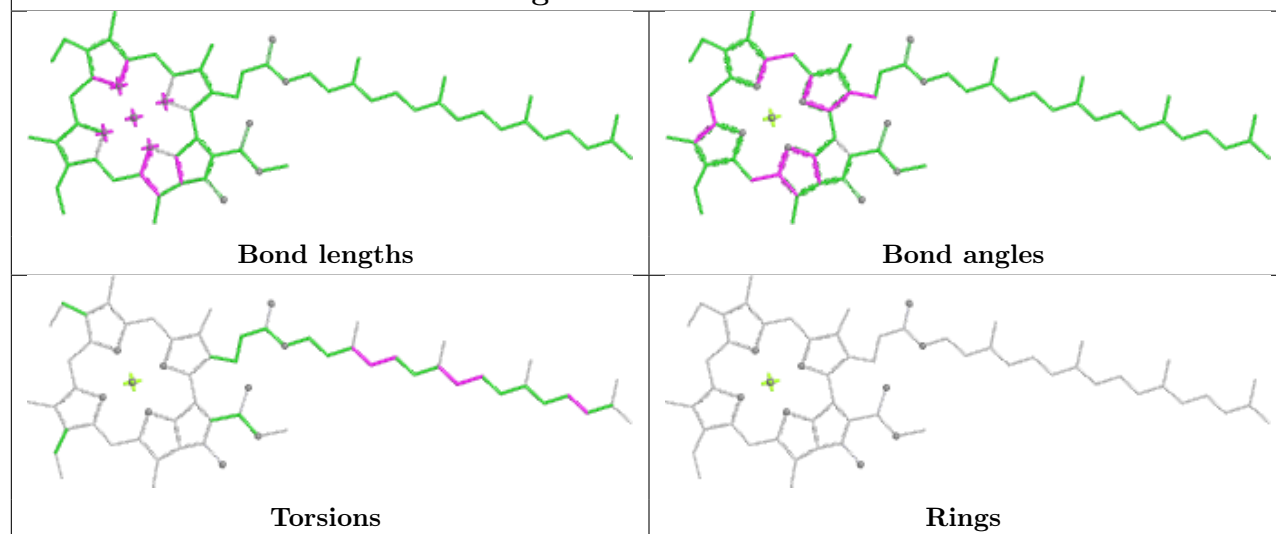
Ligand II0 a 619



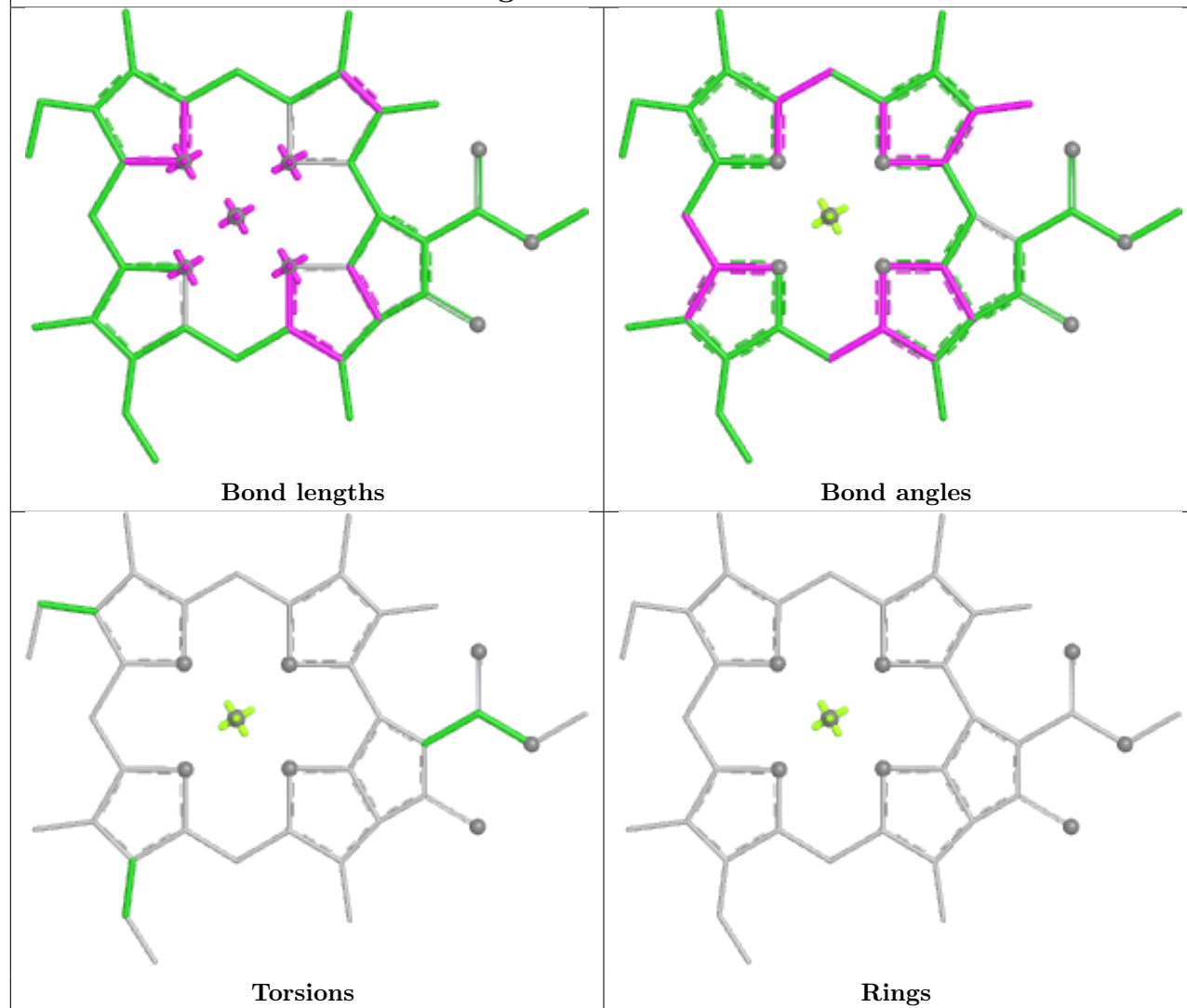
Ligand CLA 2 601



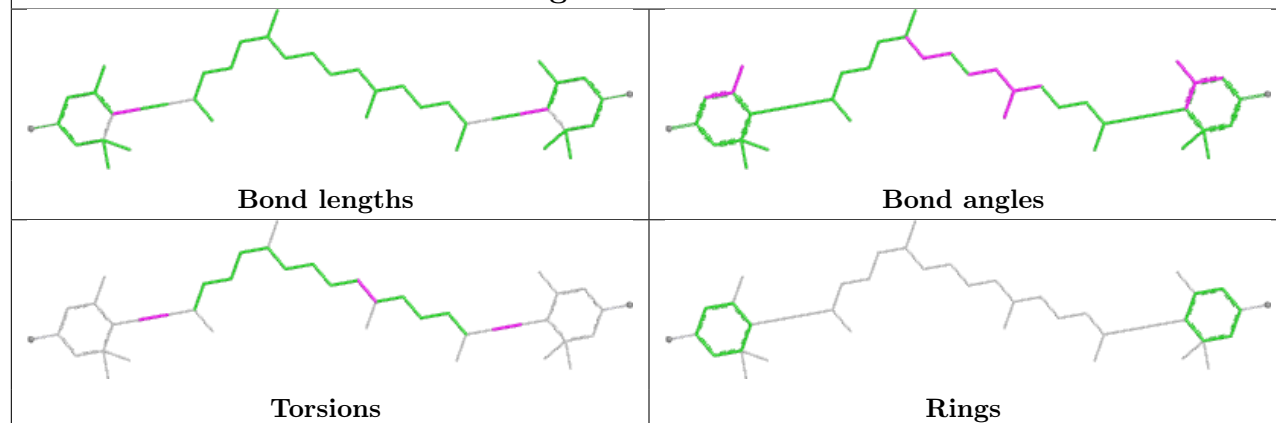
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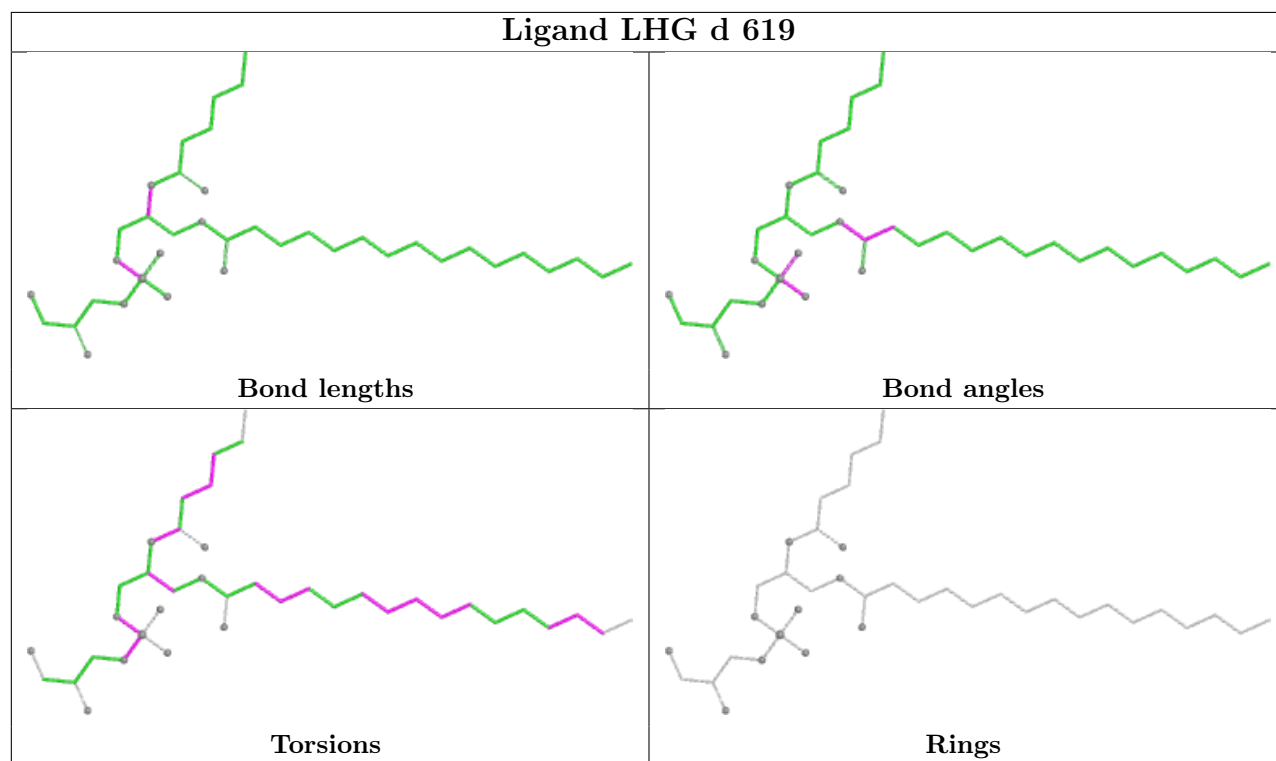
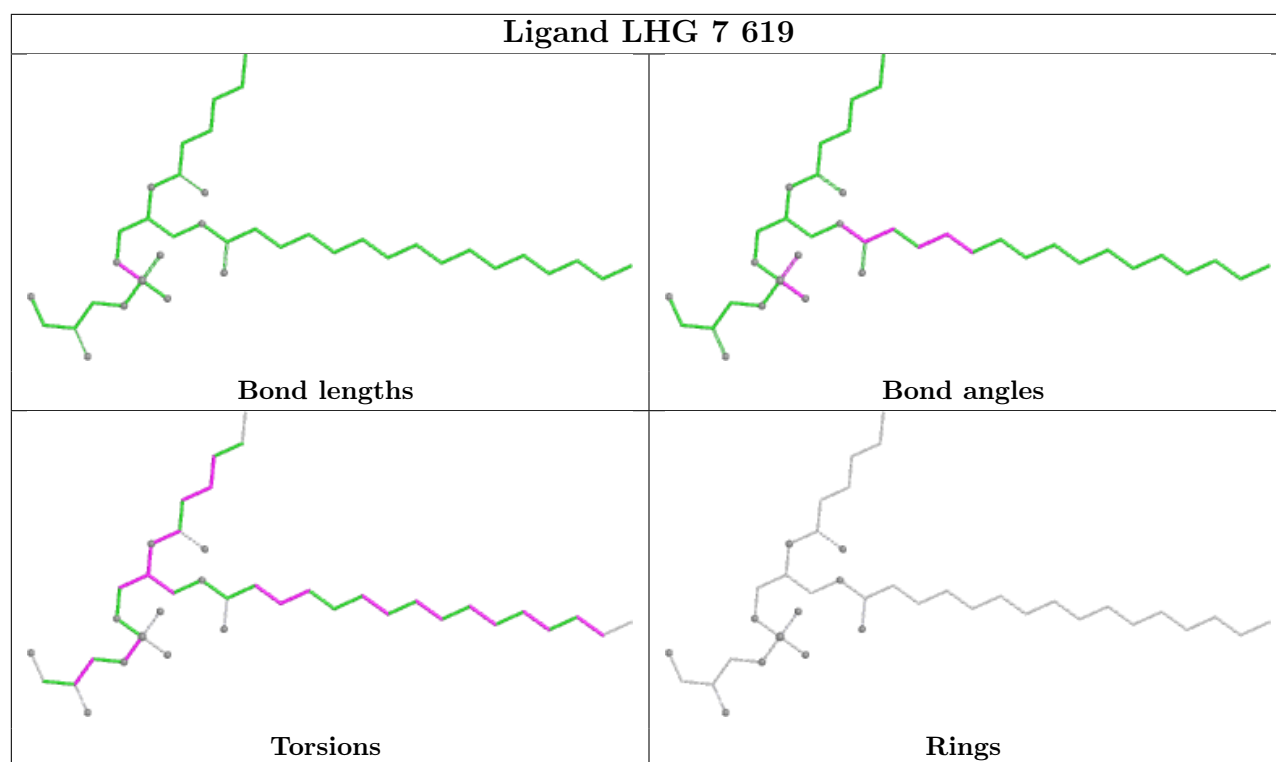


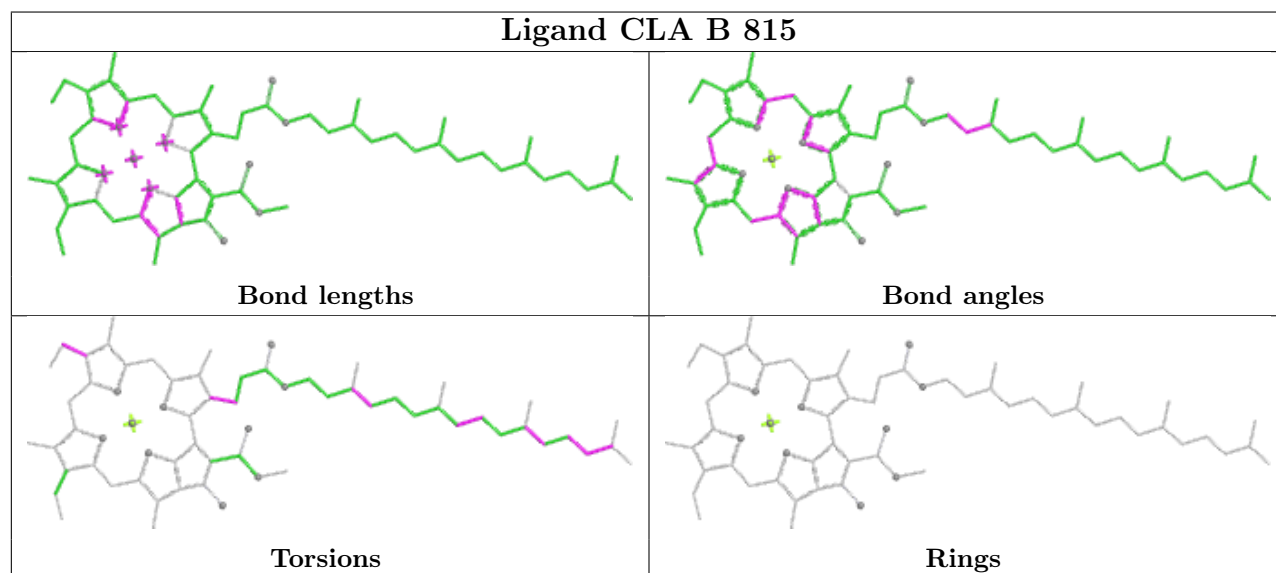
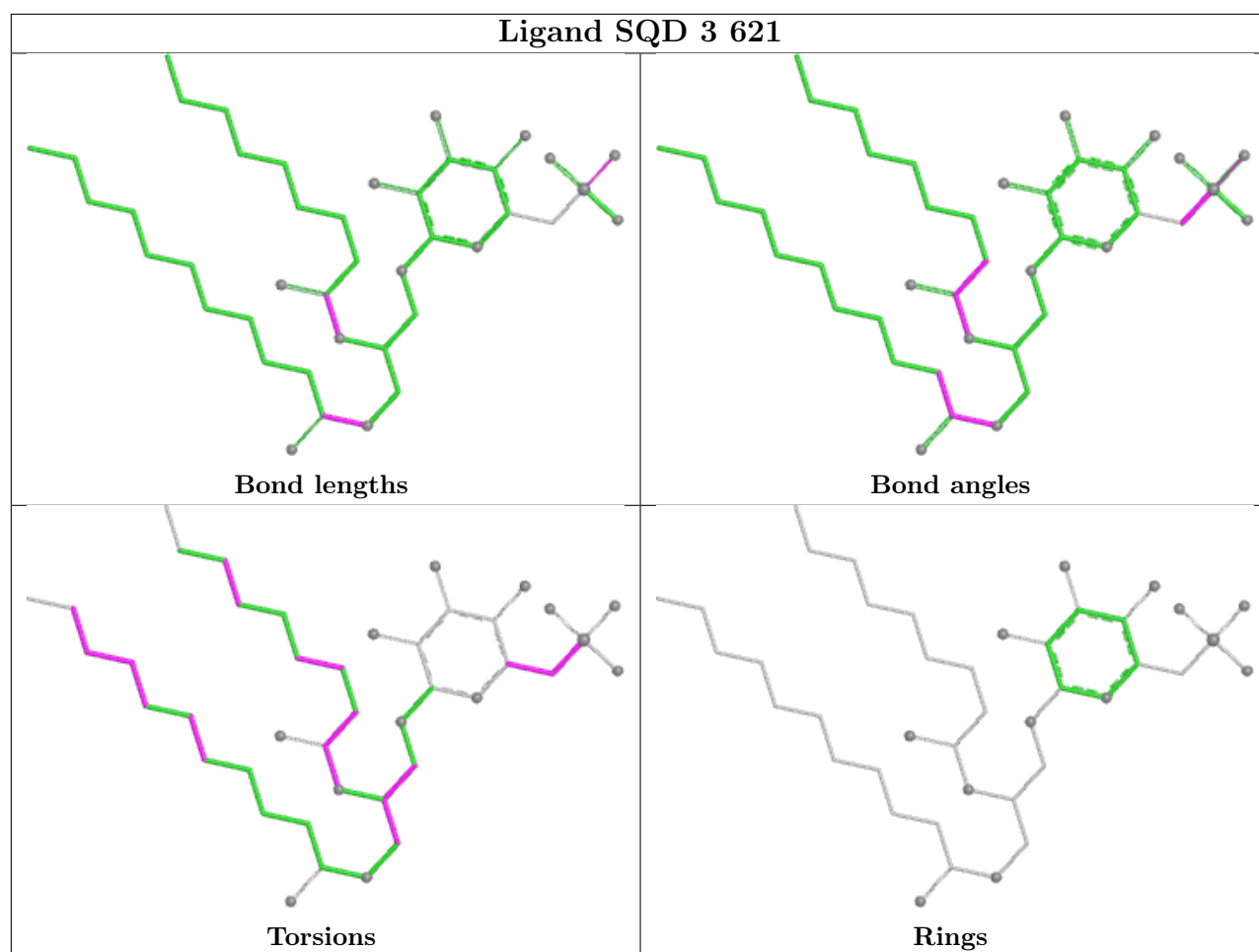
Ligand CLA d 606

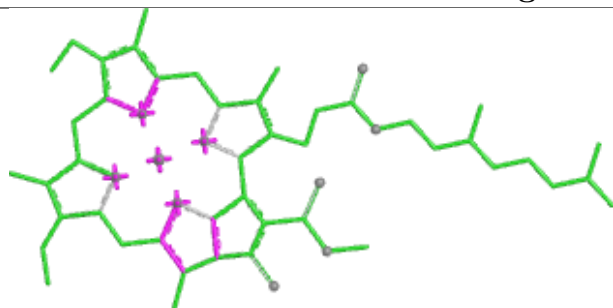


Ligand II0 d 616

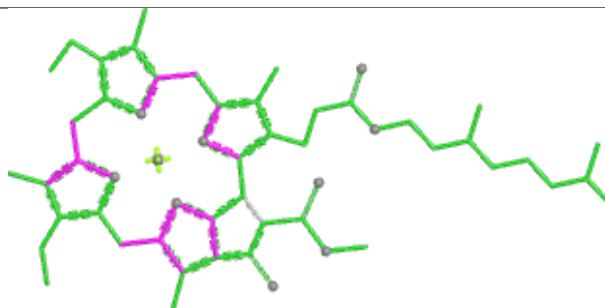




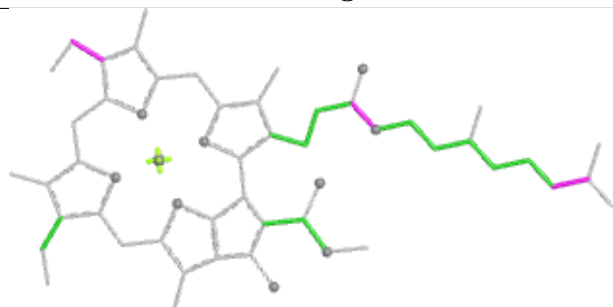


Ligand CLA 6 607

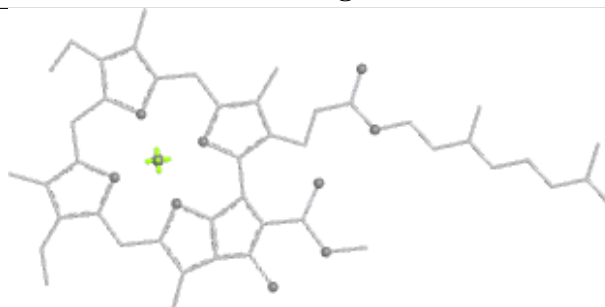
Bond lengths



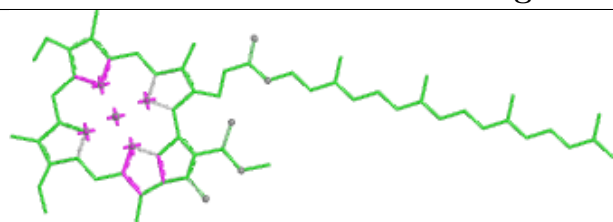
Bond angles



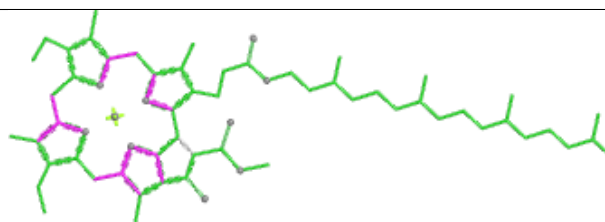
Torsions



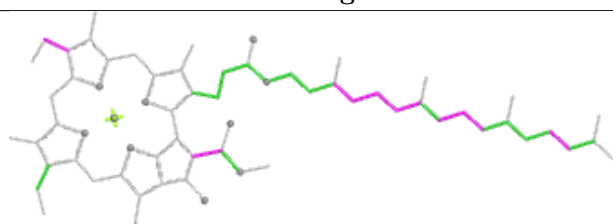
Rings

Ligand CLA B 808

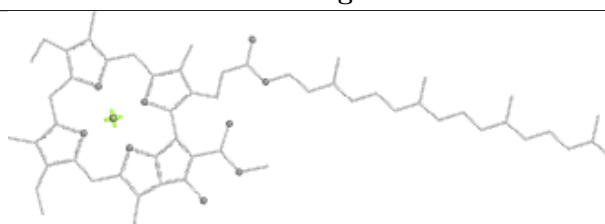
Bond lengths



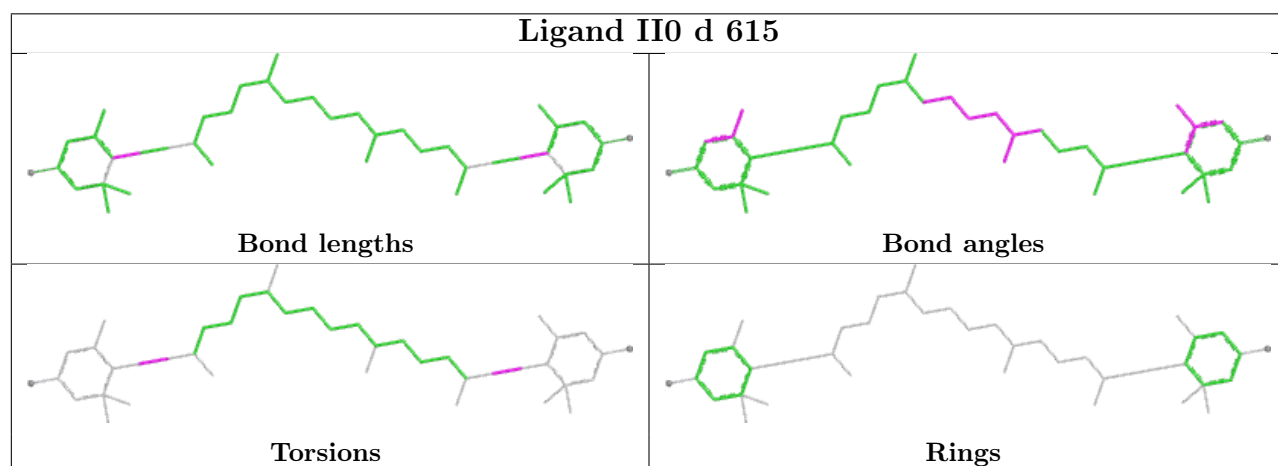
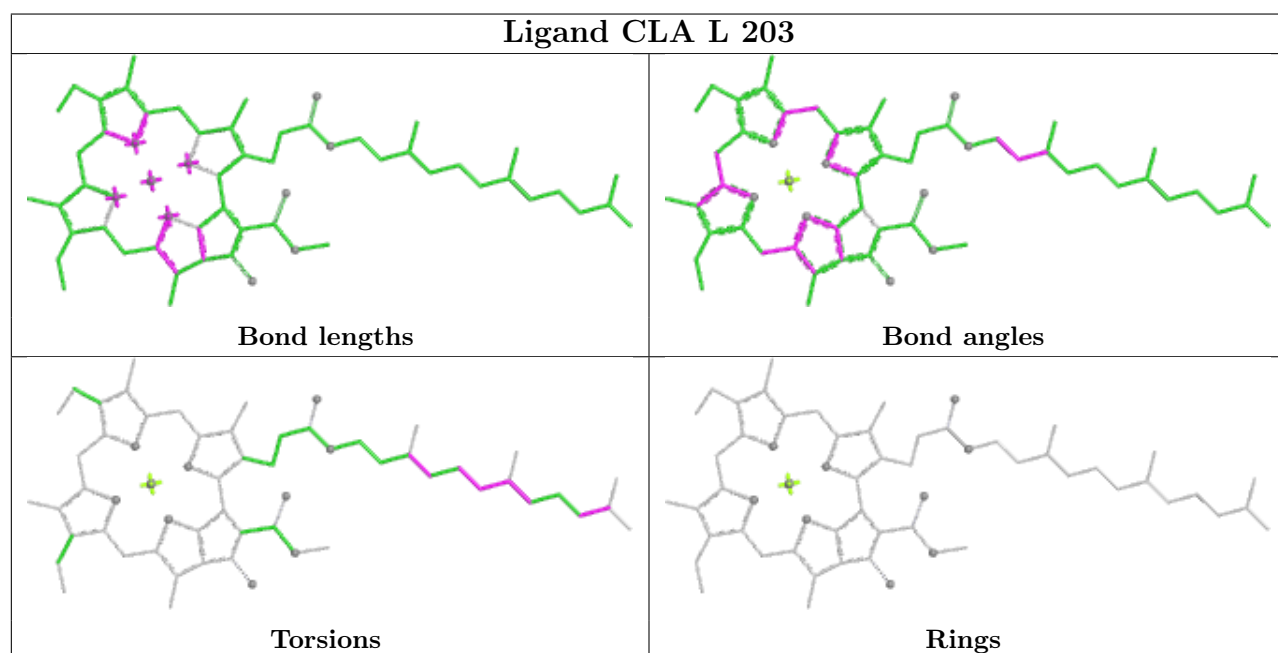
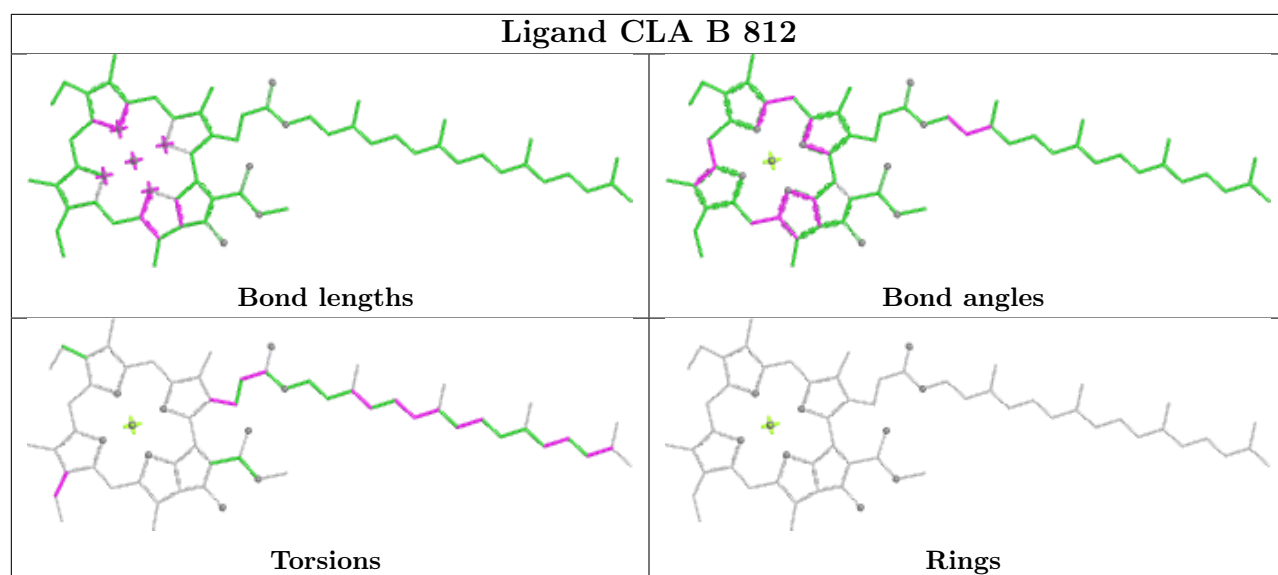
Bond angles

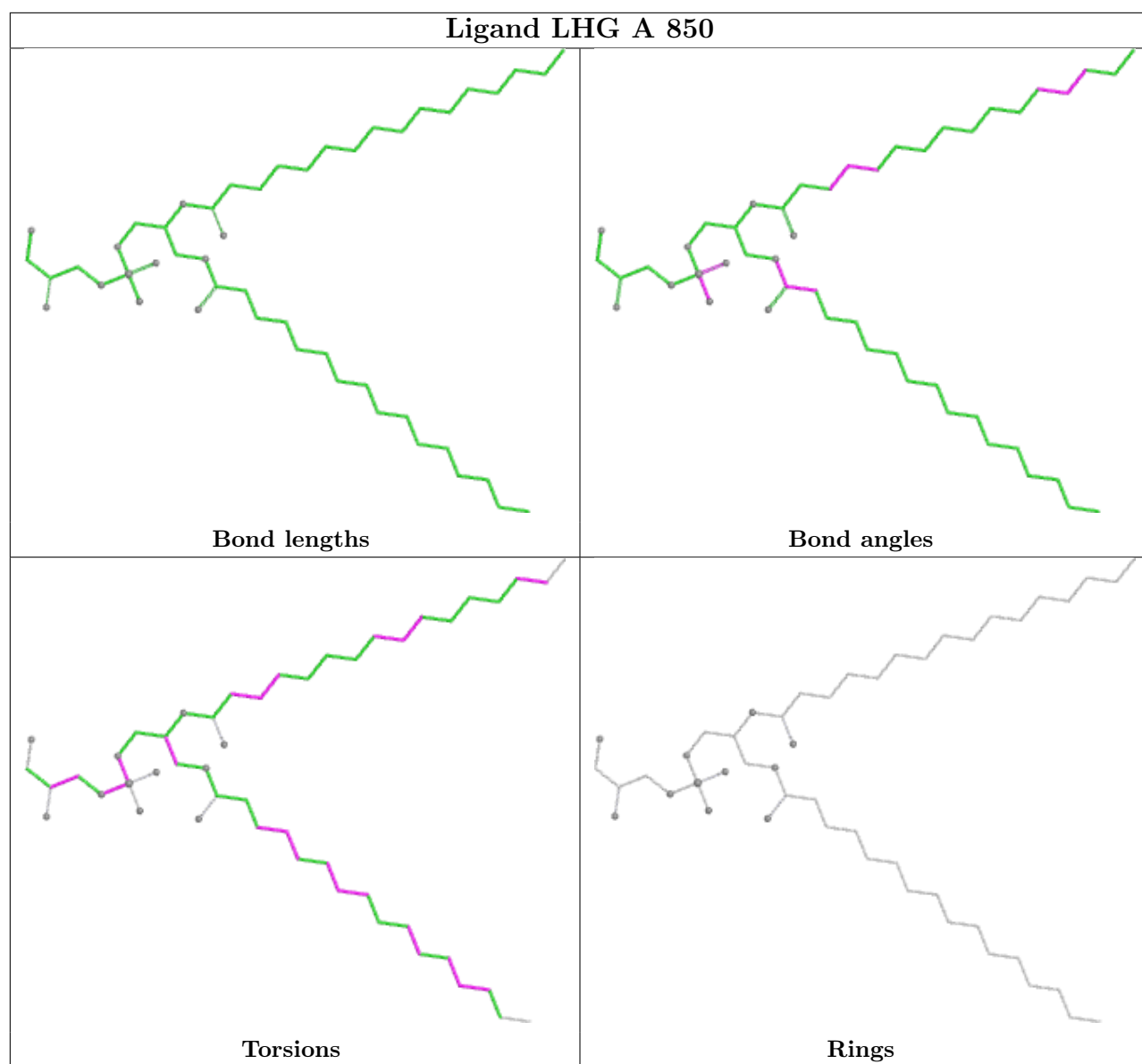


Torsions

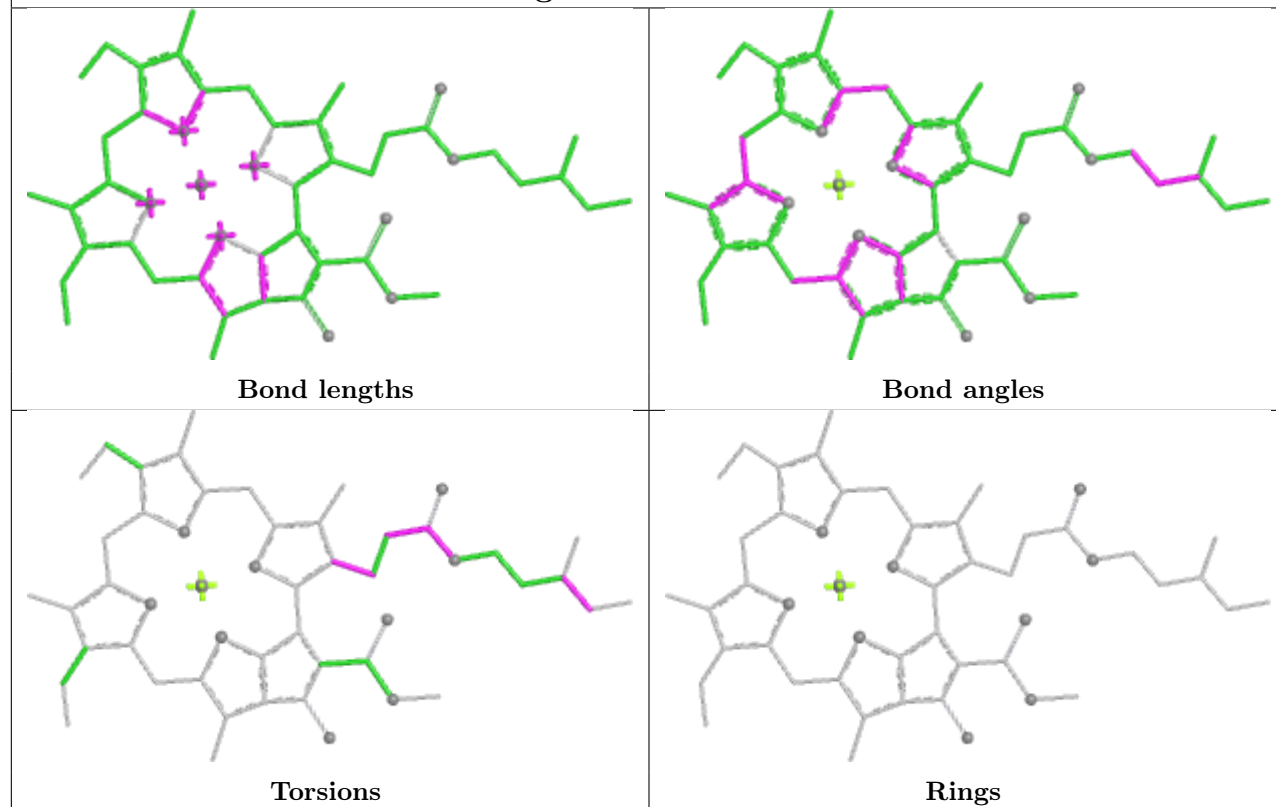


Rings

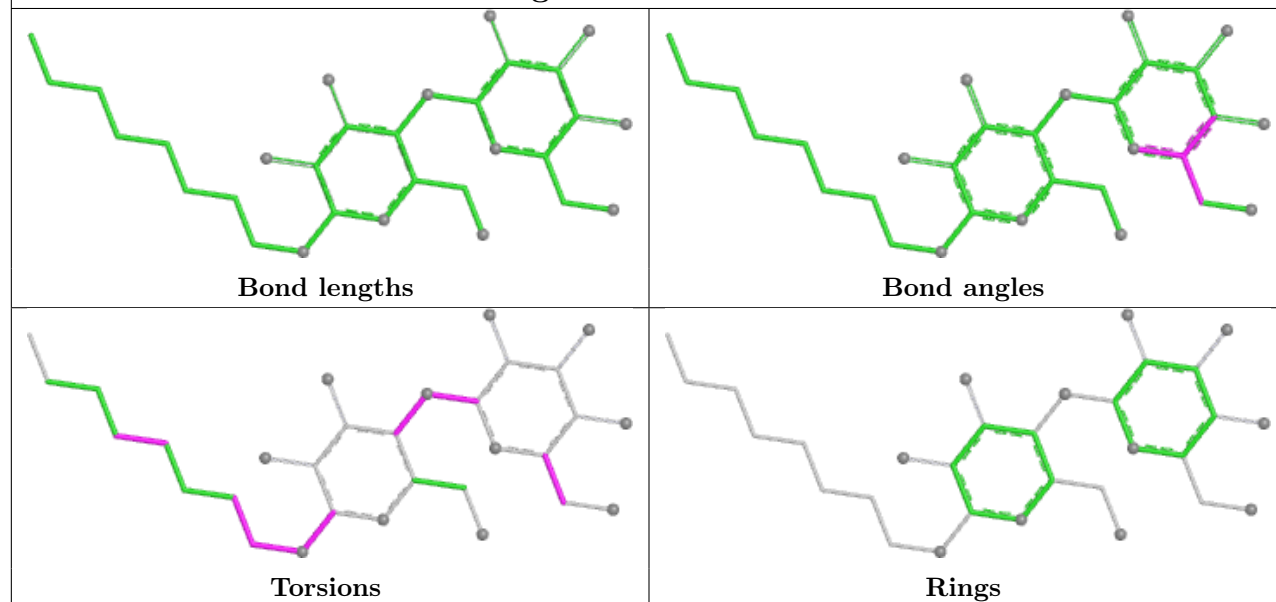


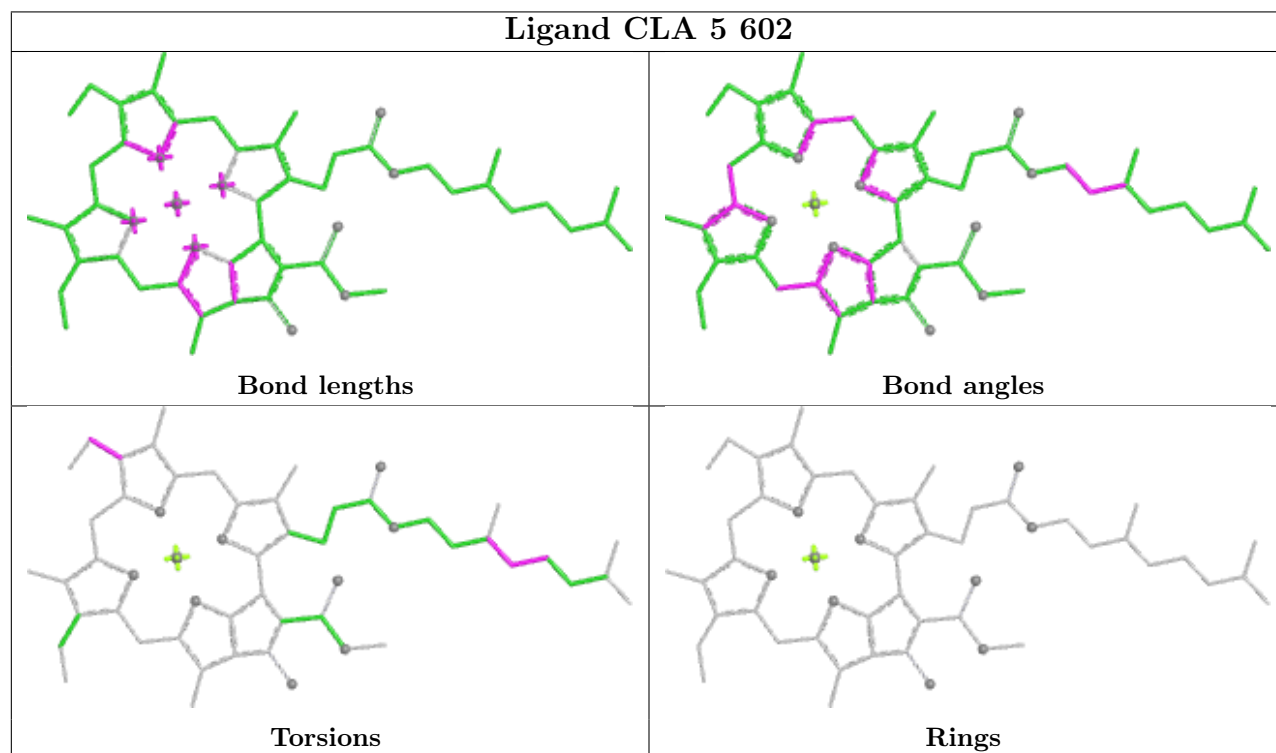
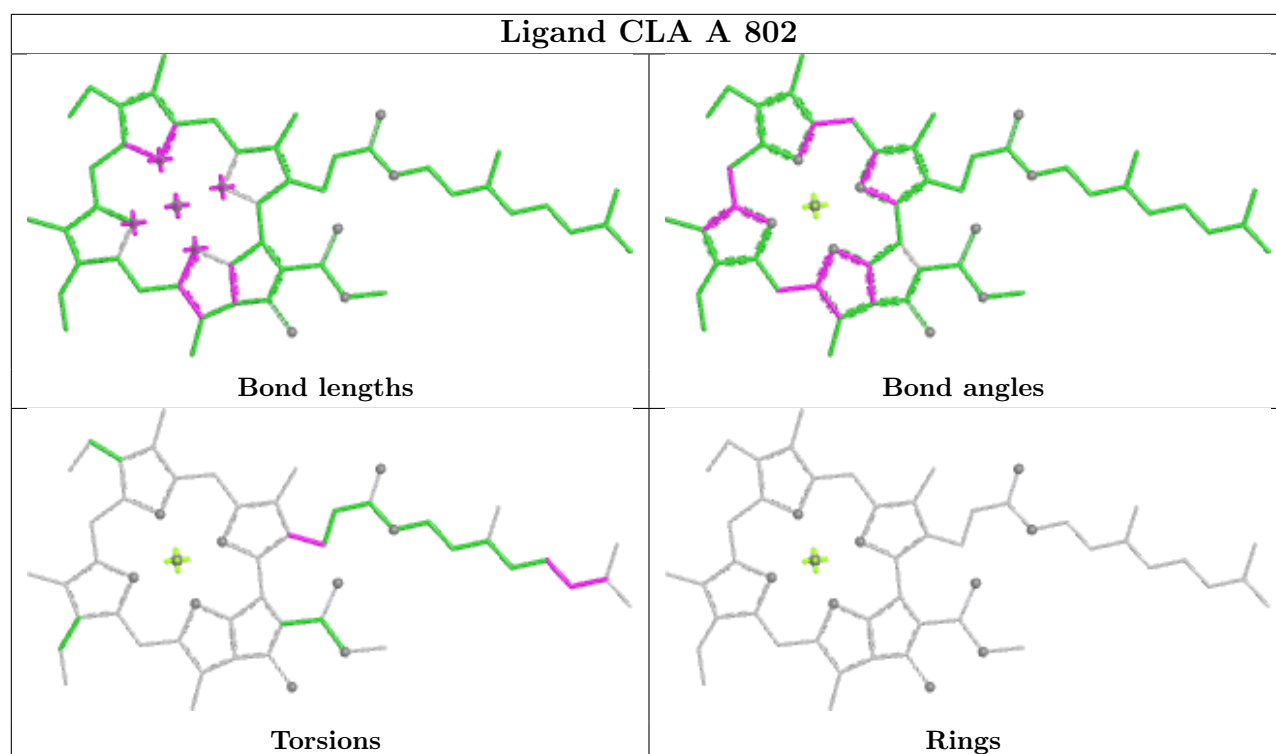


Ligand CLA b 610

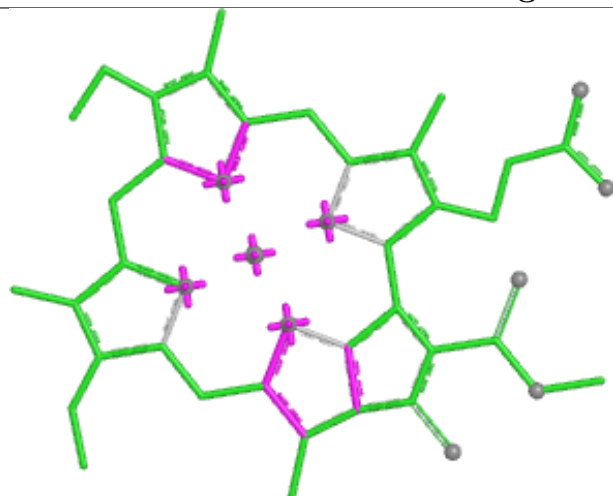


Ligand LMU J 104

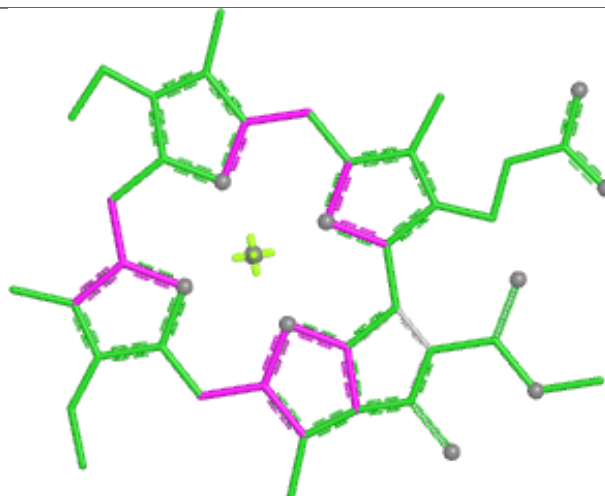




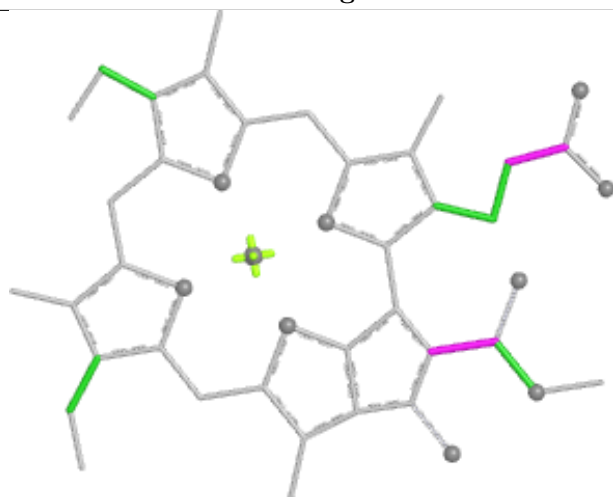
Ligand CLA 9 612



Bond lengths



Bond angles

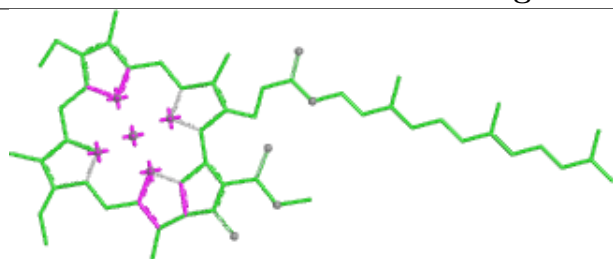


Torsions

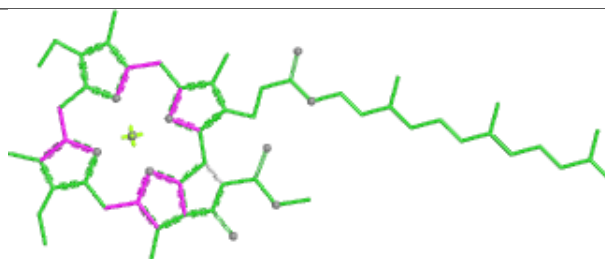


Rings

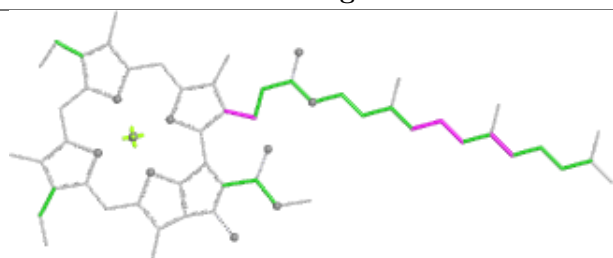
Ligand CLA A 835



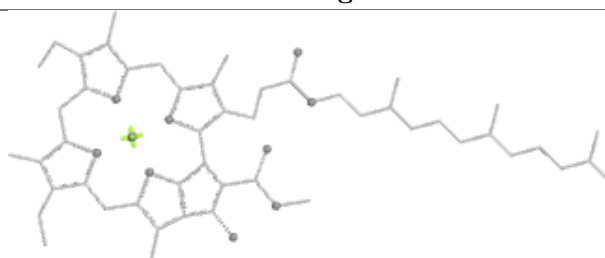
Bond lengths



Bond angles

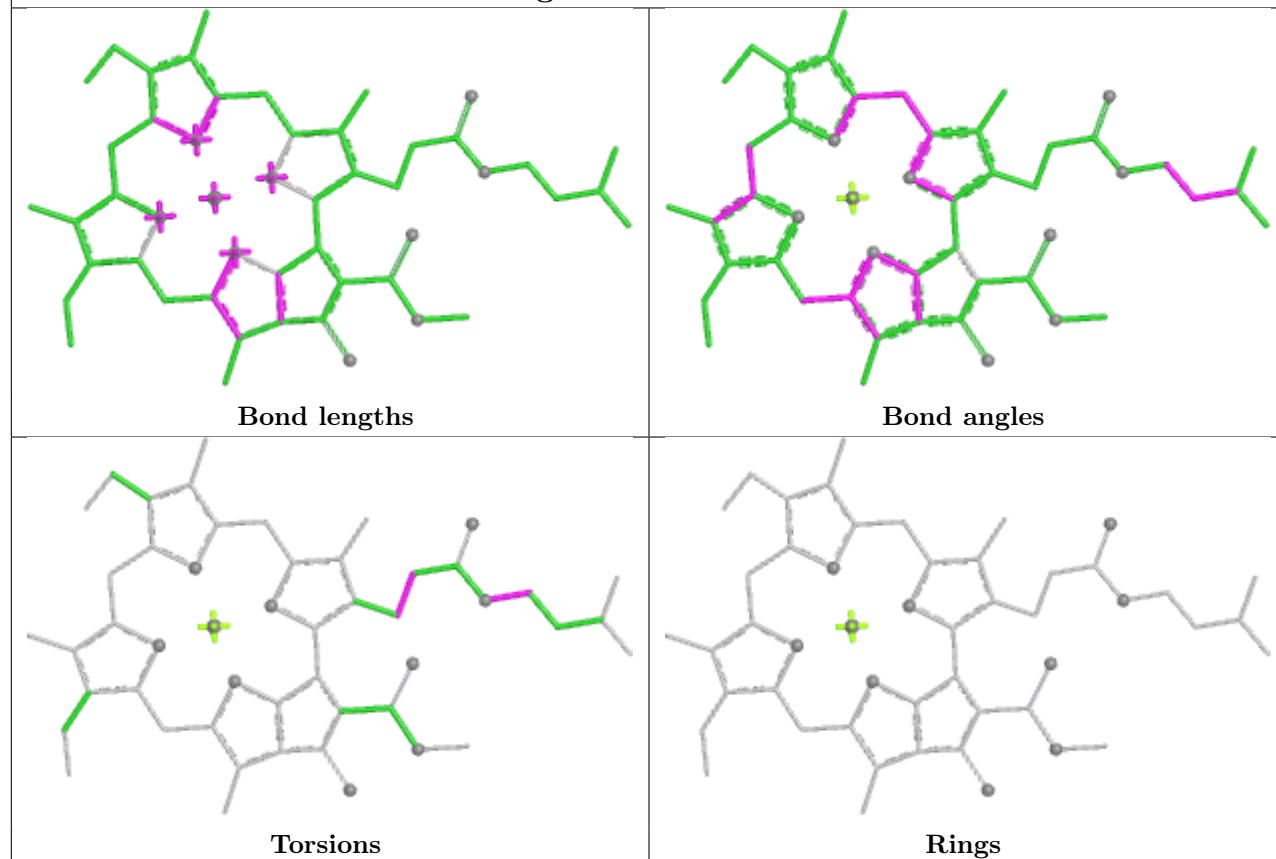


Torsions

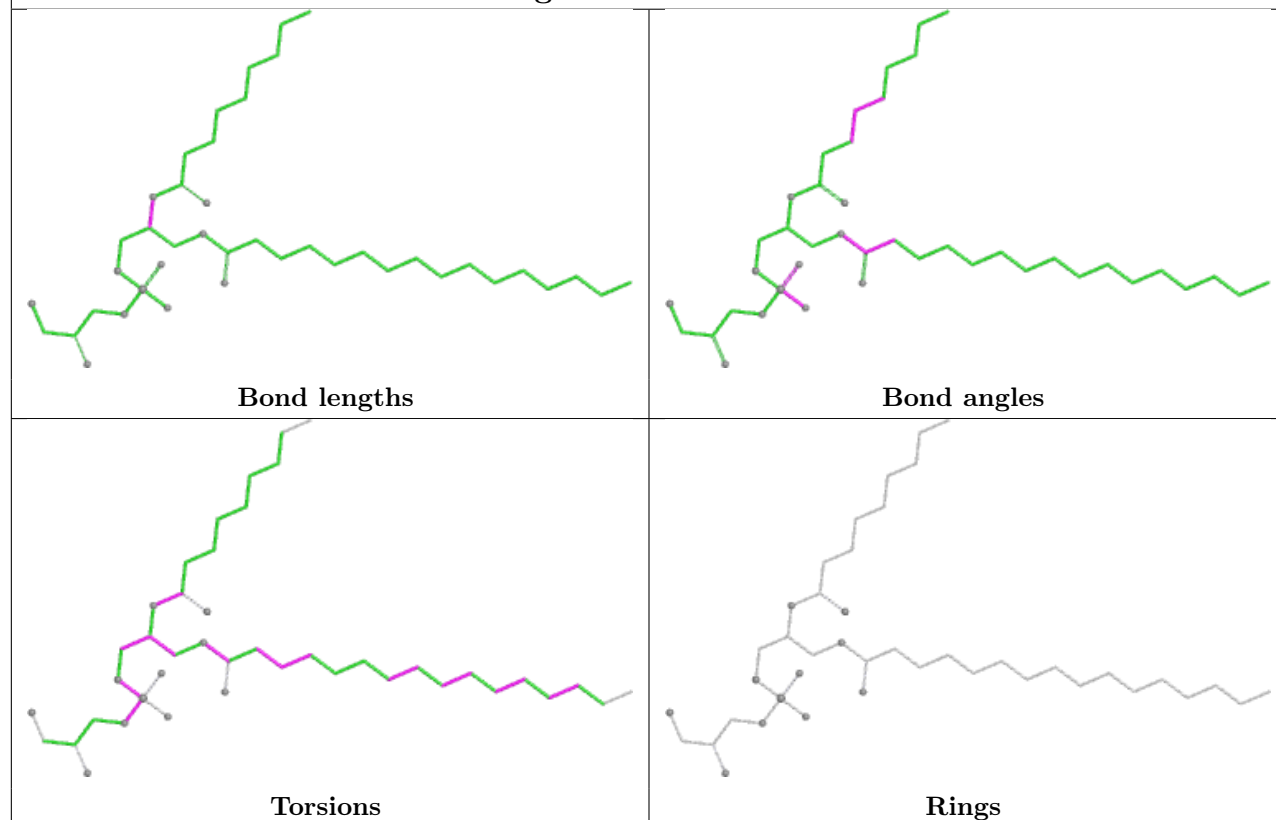


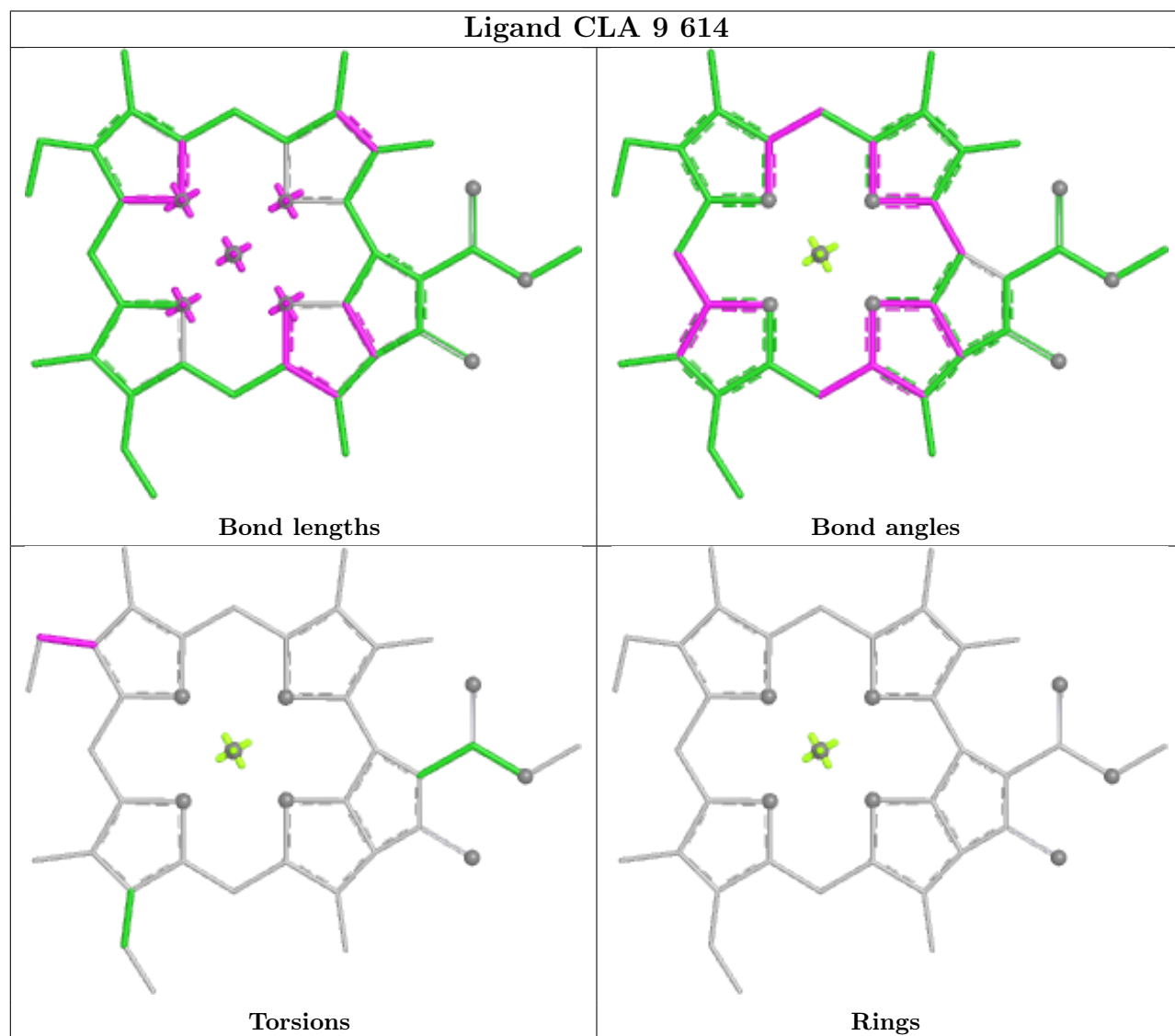
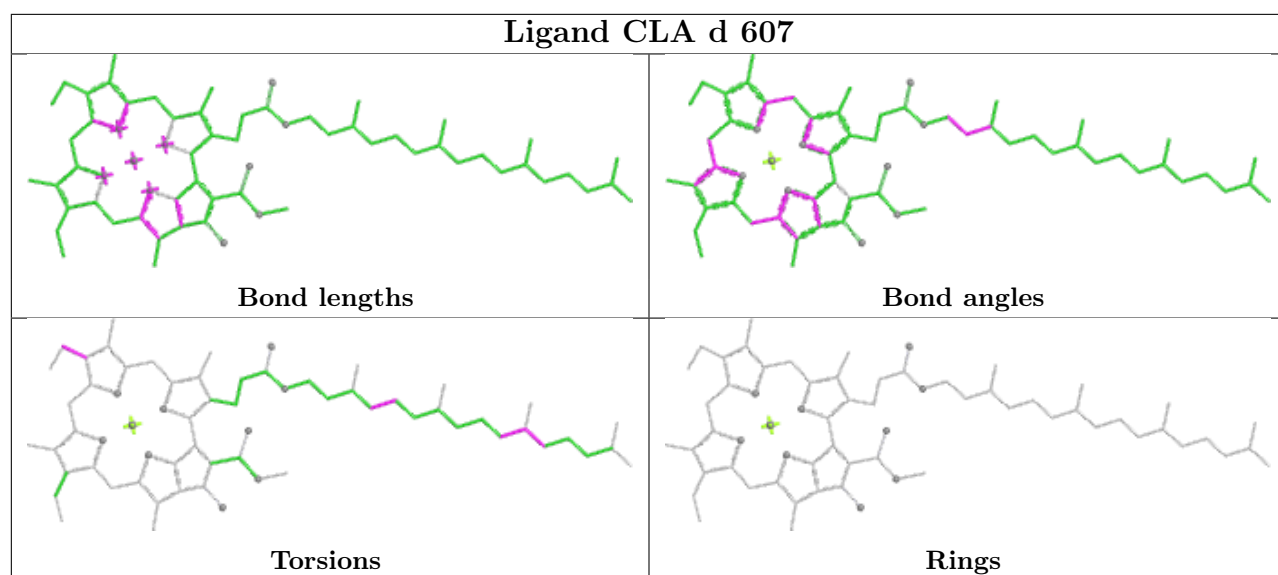
Rings

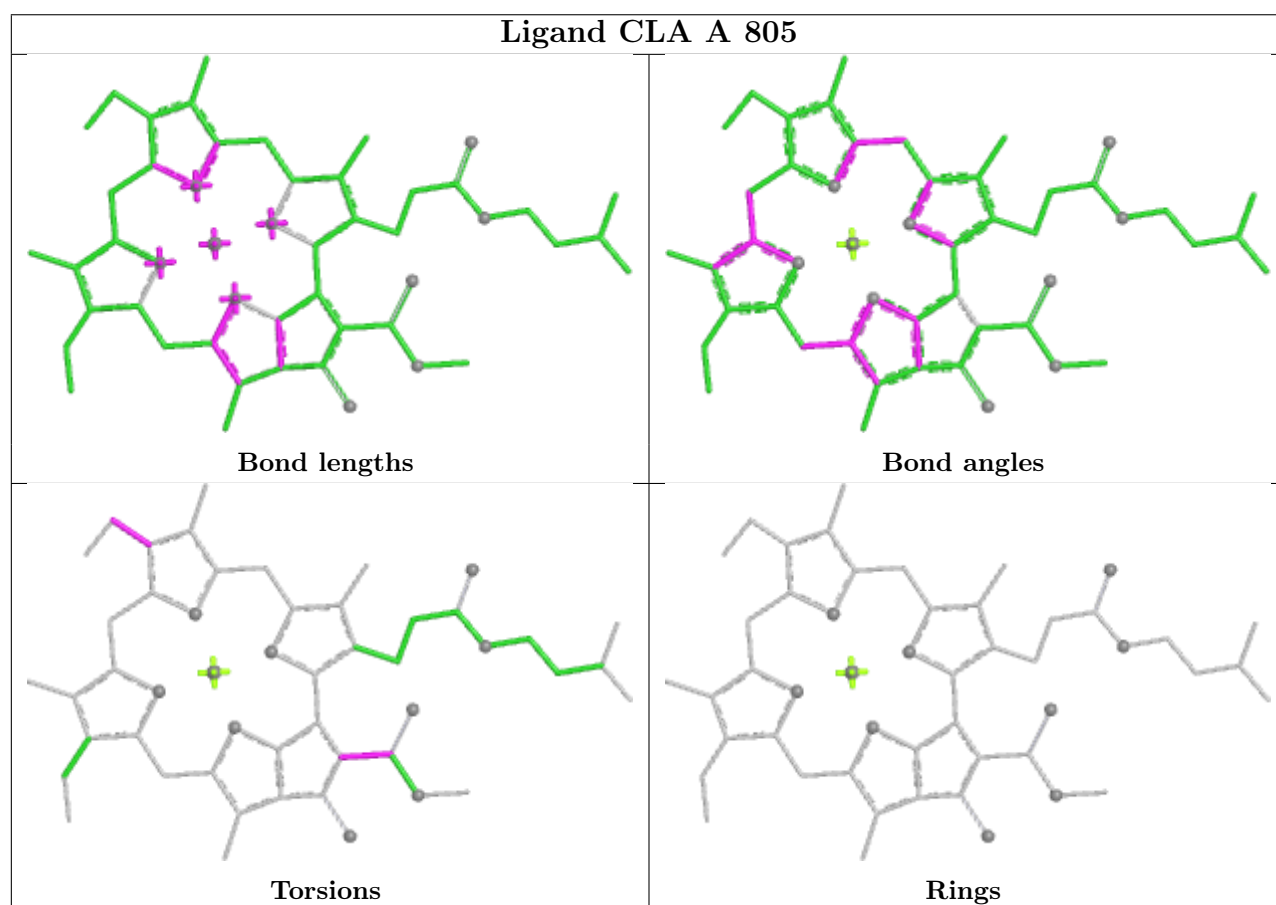
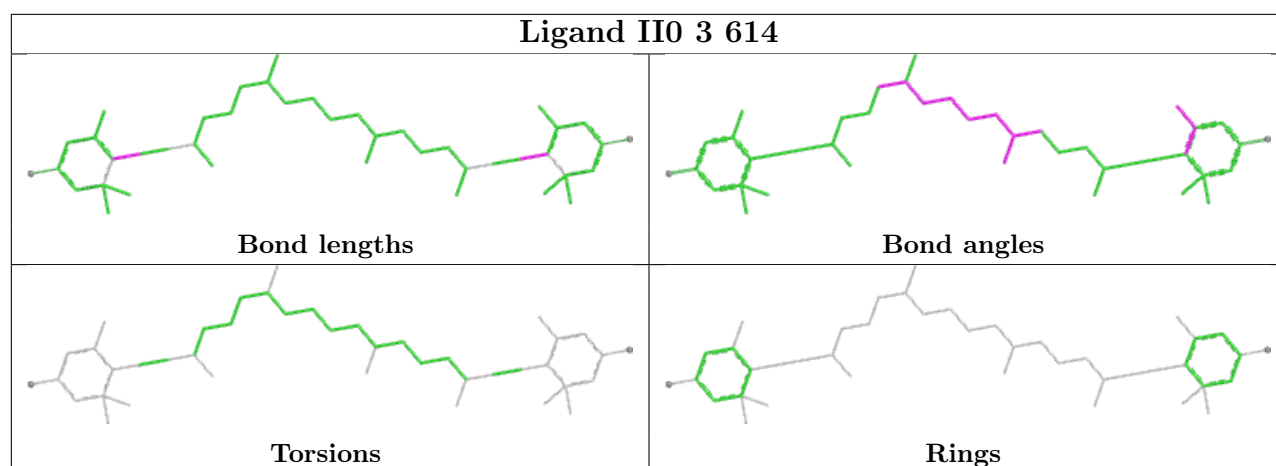
Ligand CLA 8 605

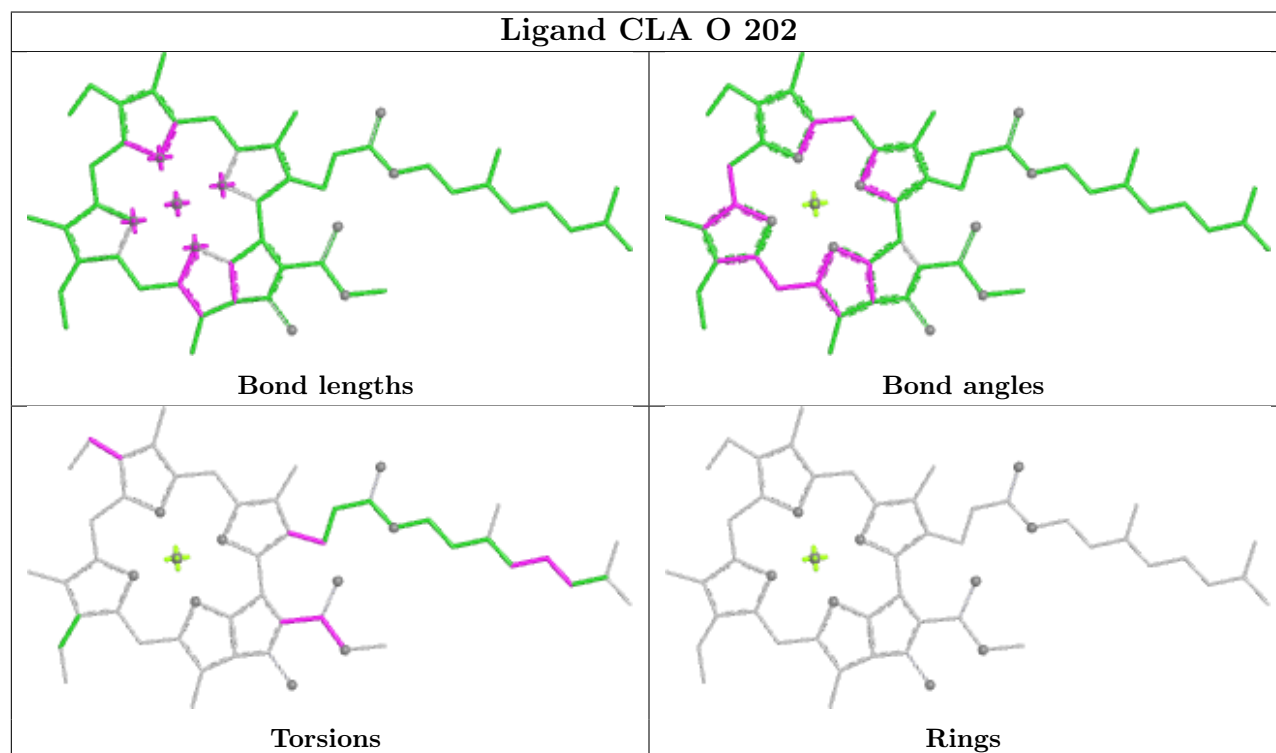
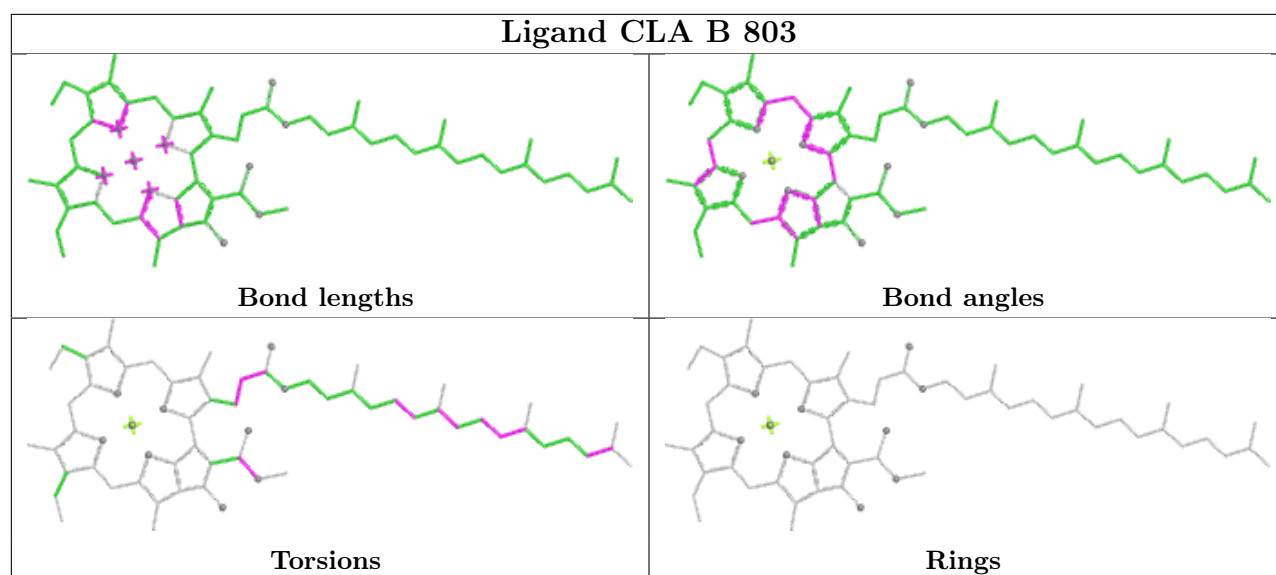


Ligand LHG 2 620

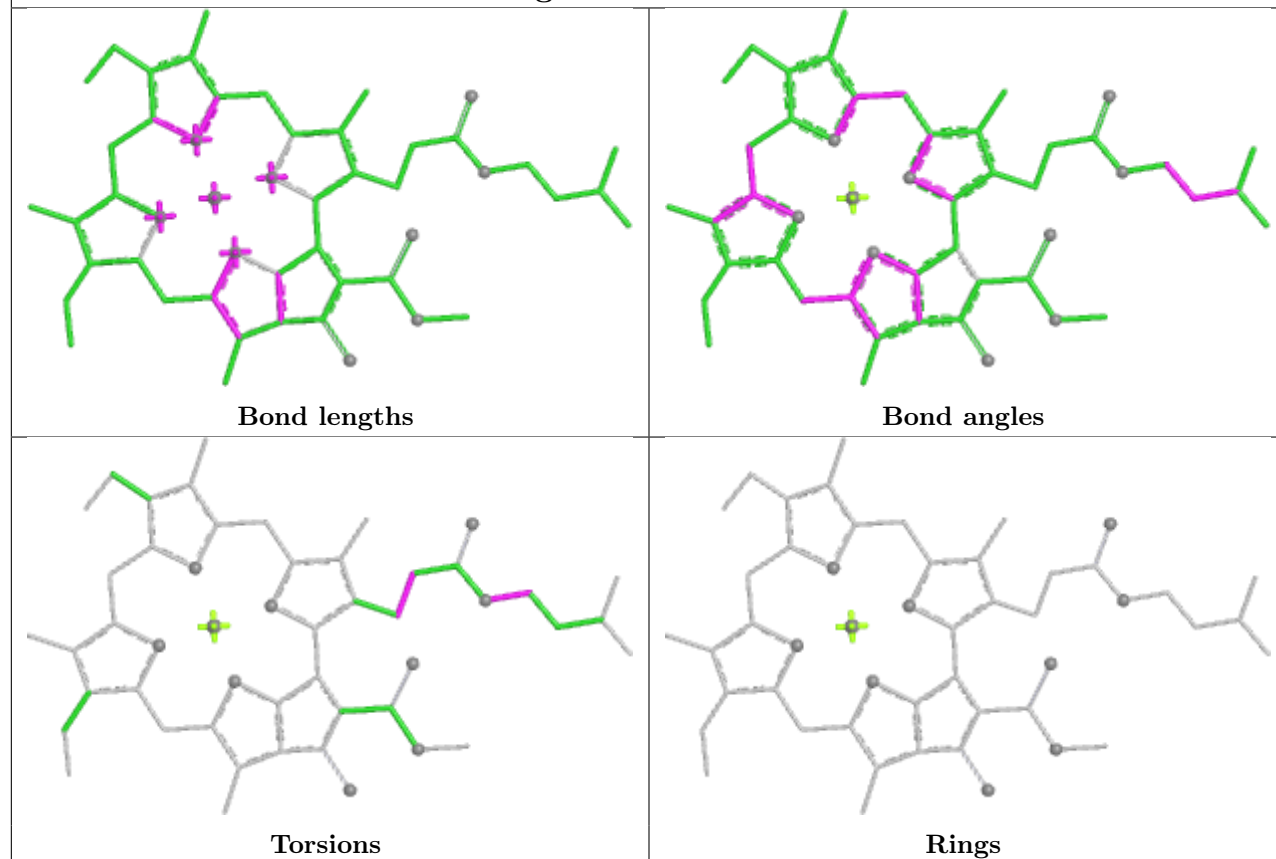




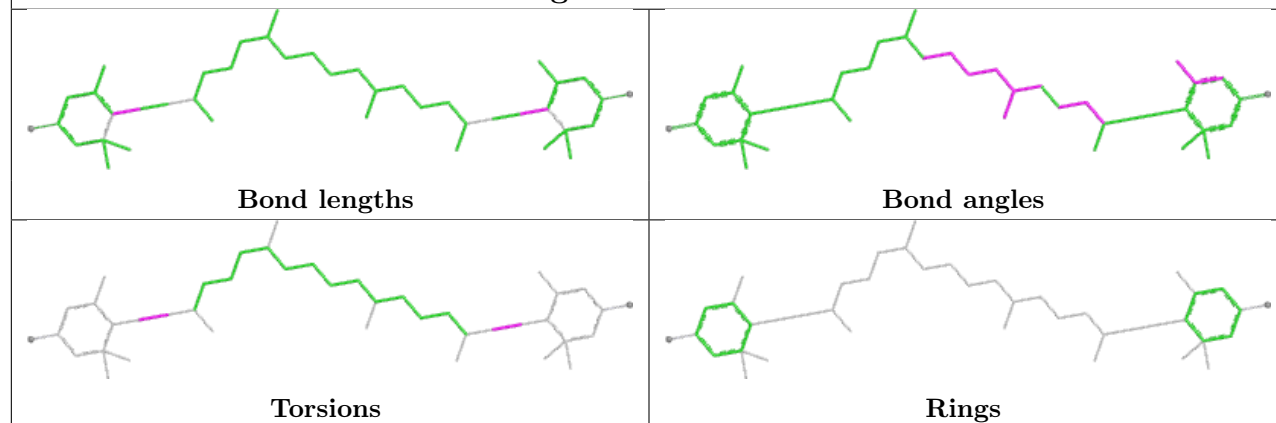




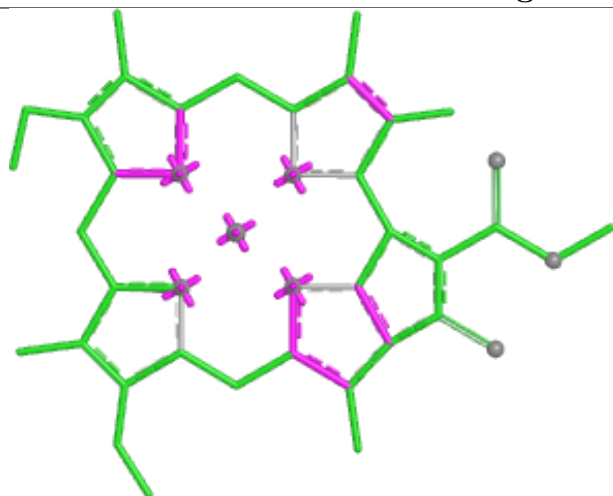
Ligand CLA d 603



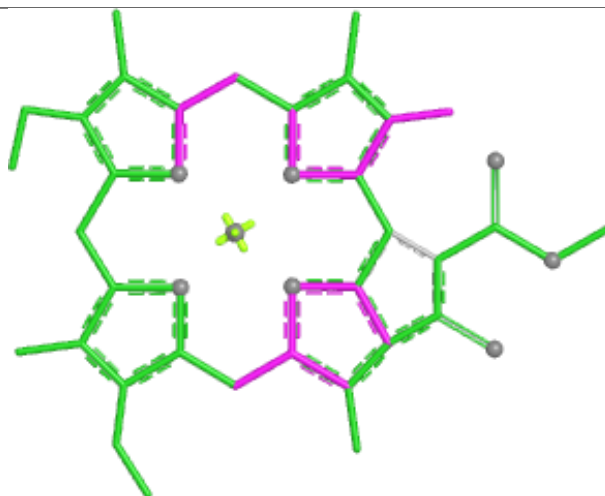
Ligand II0 5 615



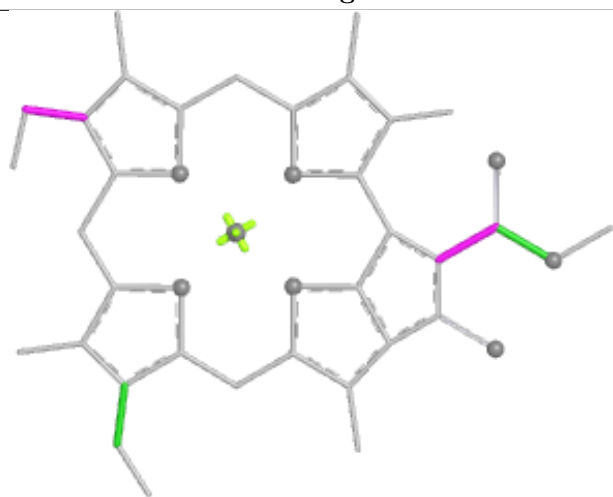
Ligand CLA L 207



Bond lengths



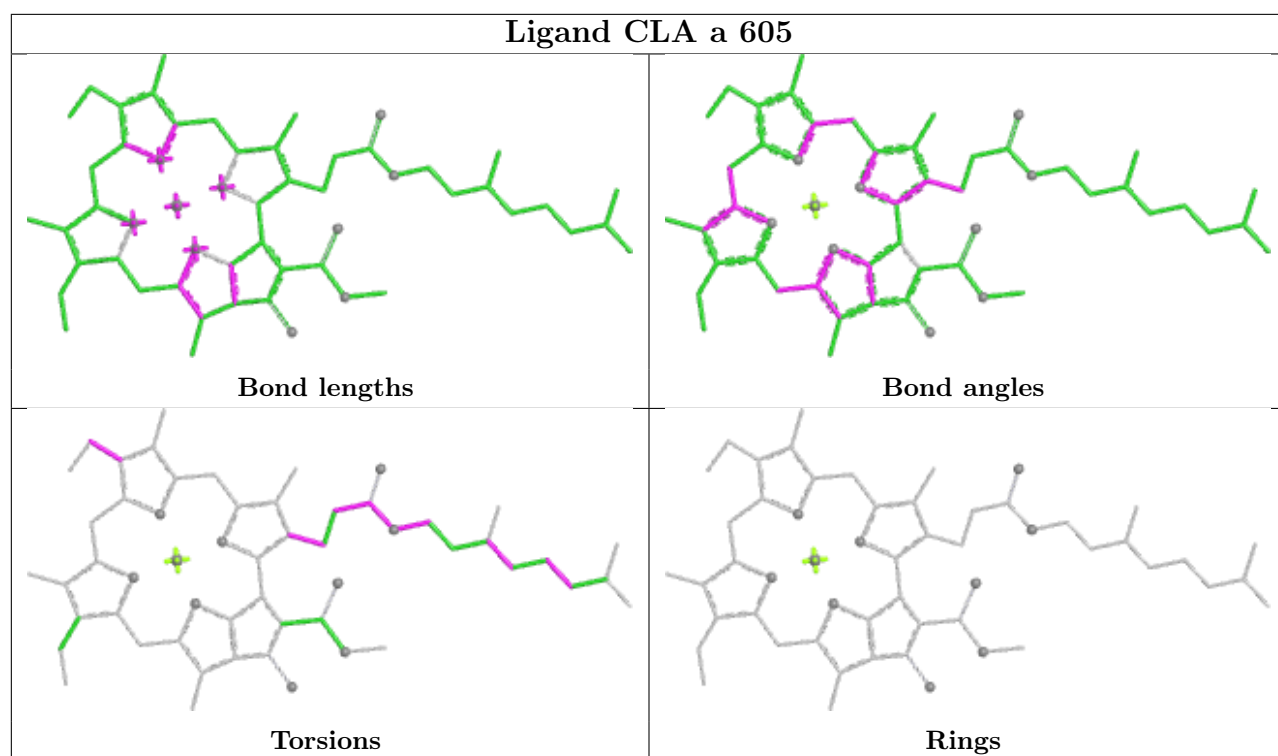
Bond angles



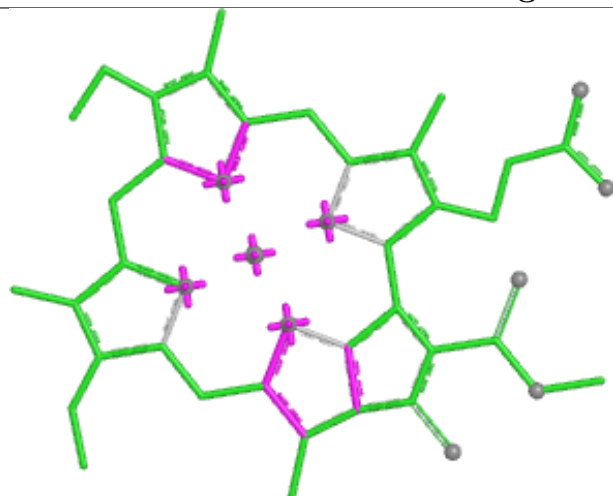
Torsions



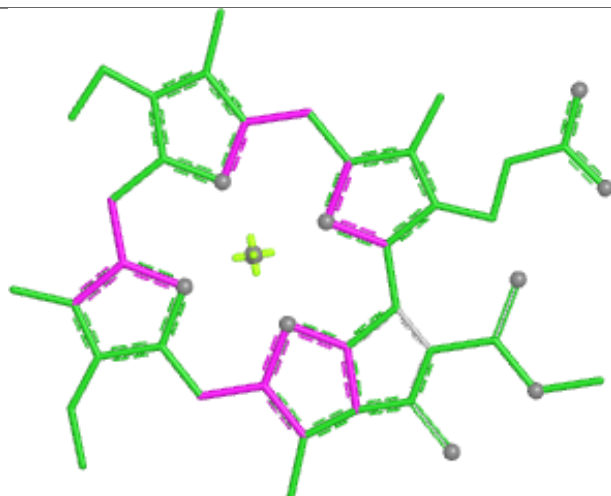
Rings



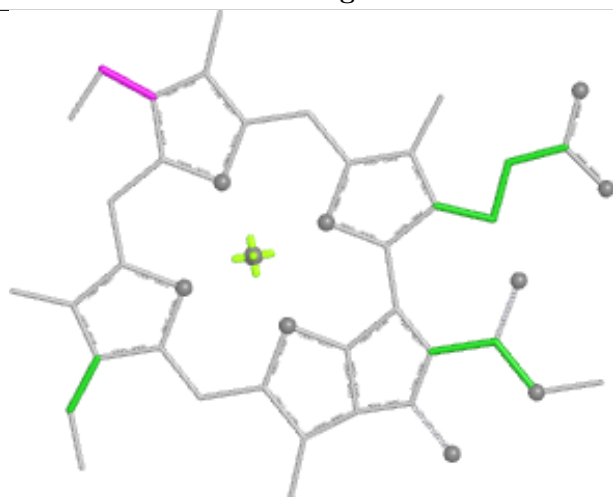
Ligand CLA 7 601



Bond lengths



Bond angles

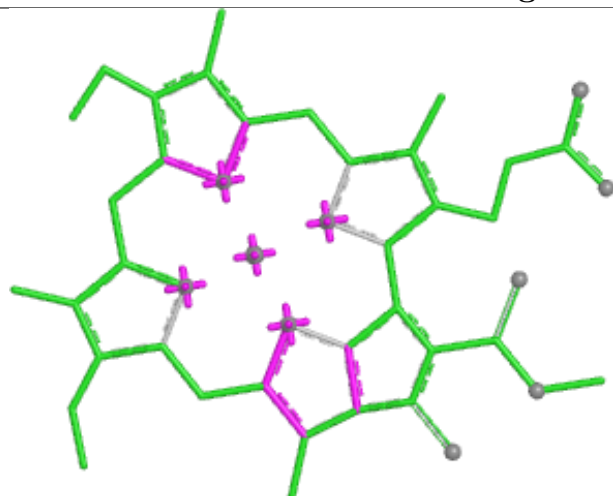


Torsions

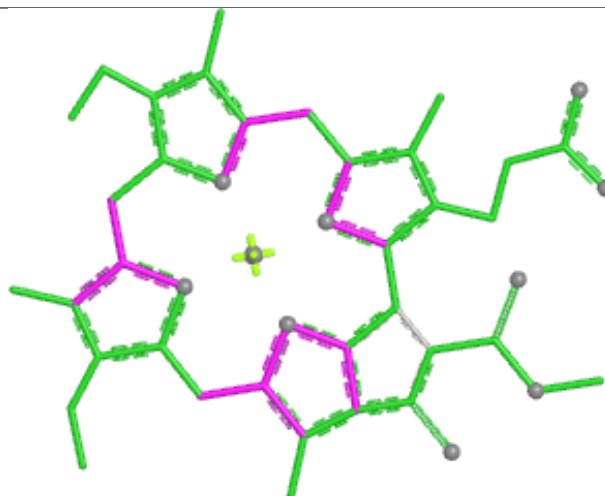


Rings

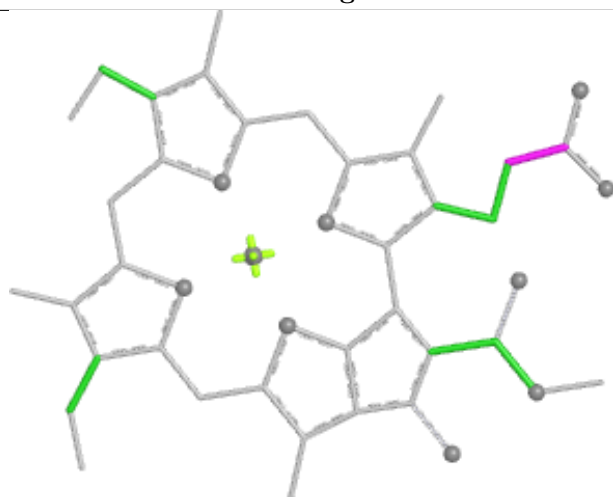
Ligand CLA 8 601



Bond lengths



Bond angles

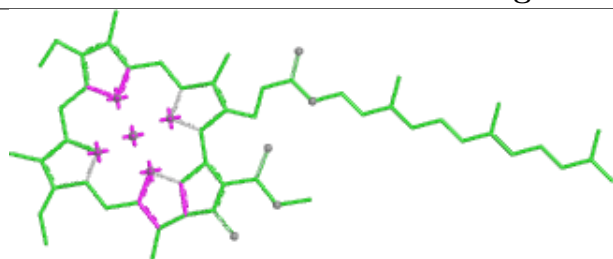


Torsions

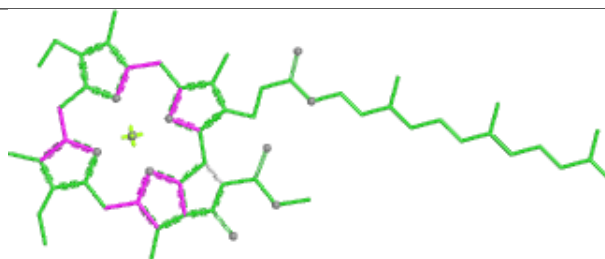


Rings

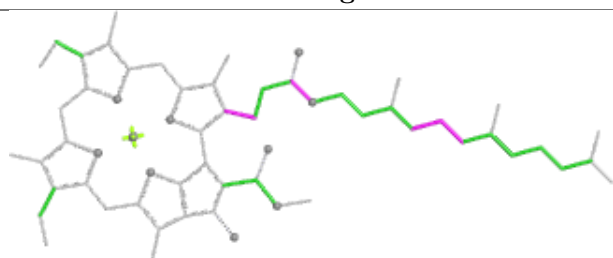
Ligand CLA A 830



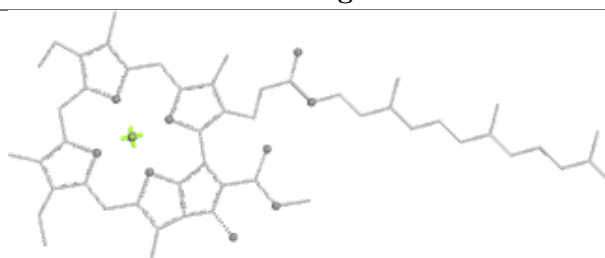
Bond lengths



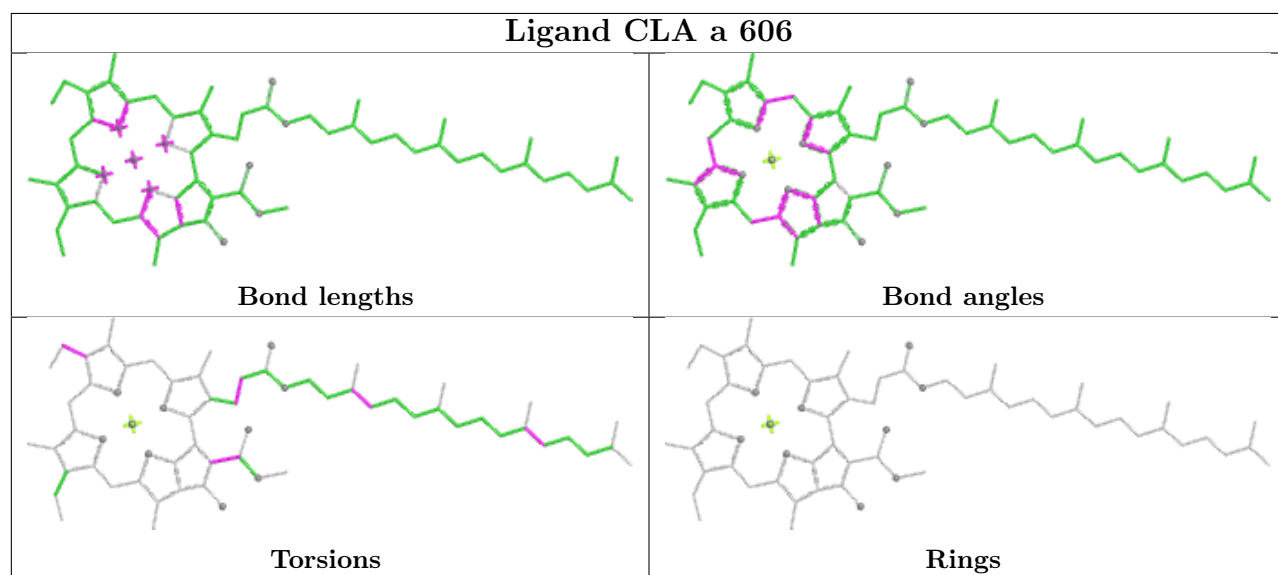
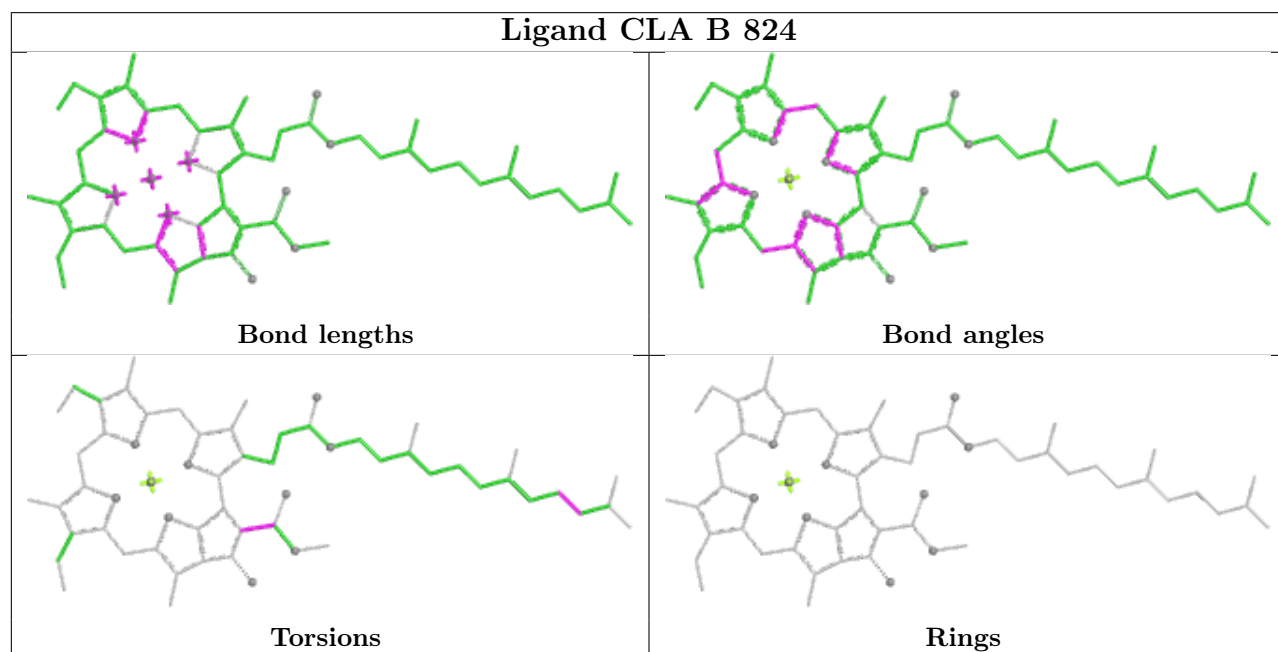
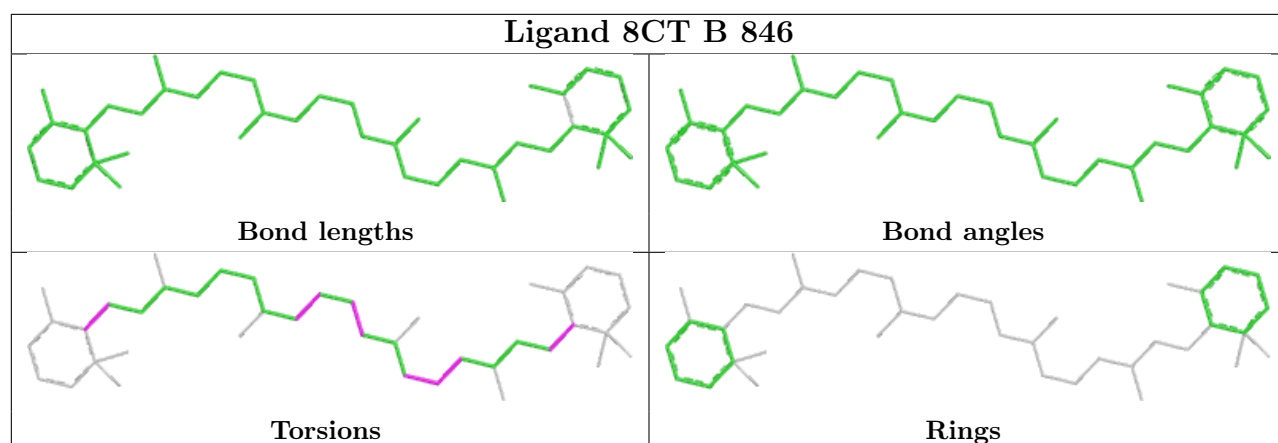
Bond angles

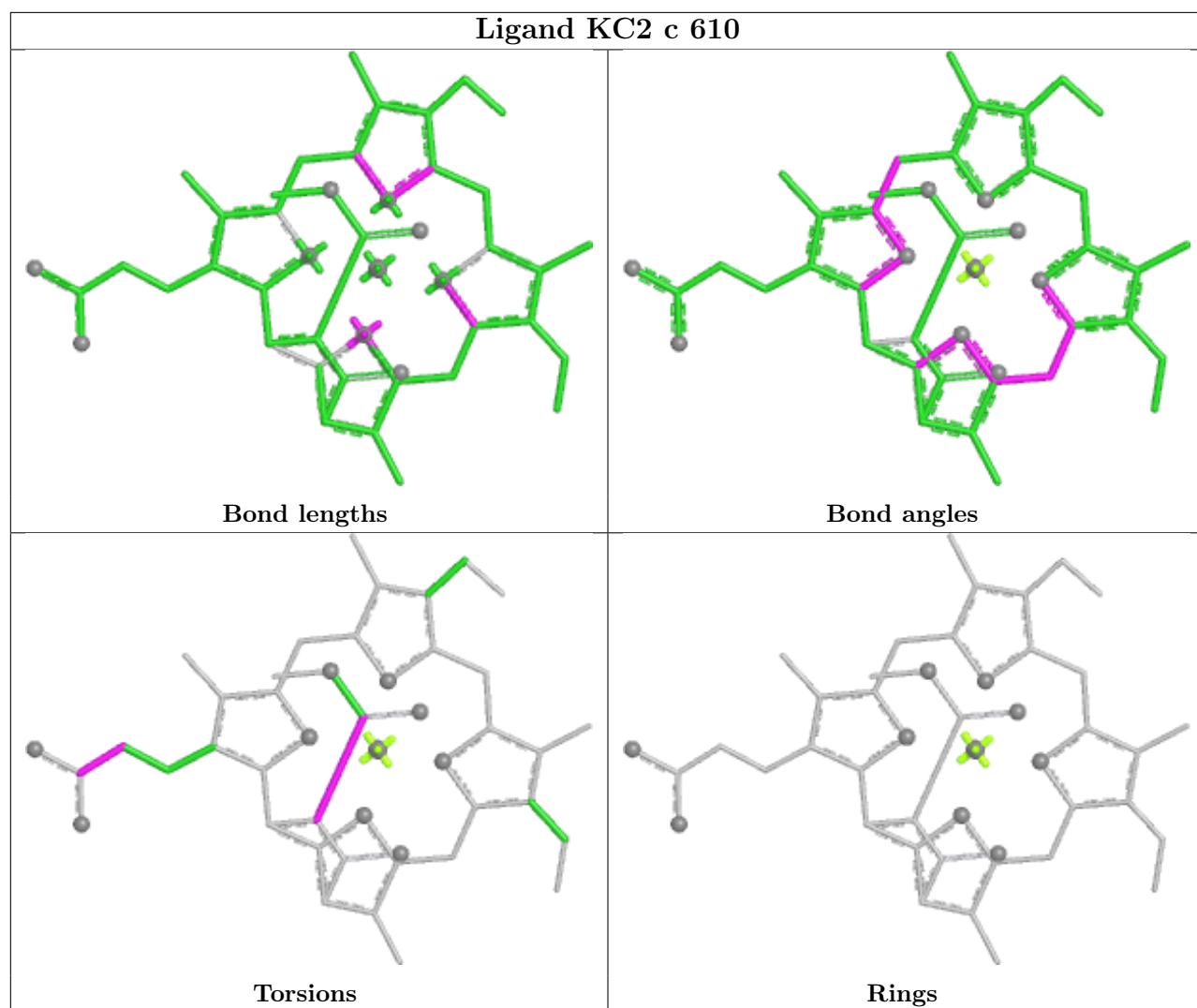
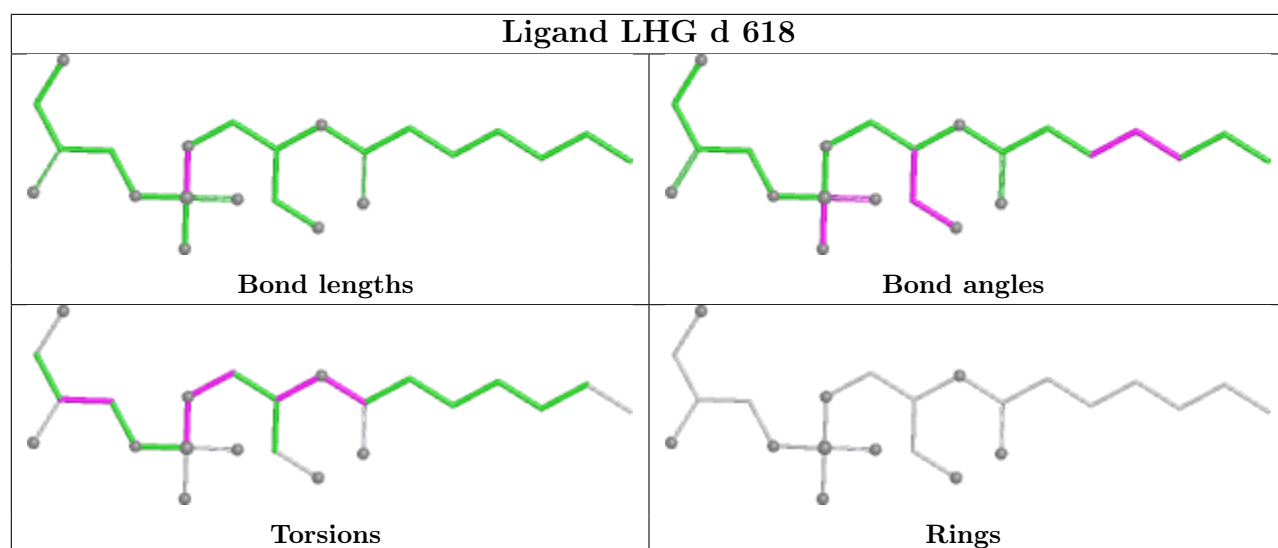


Torsions

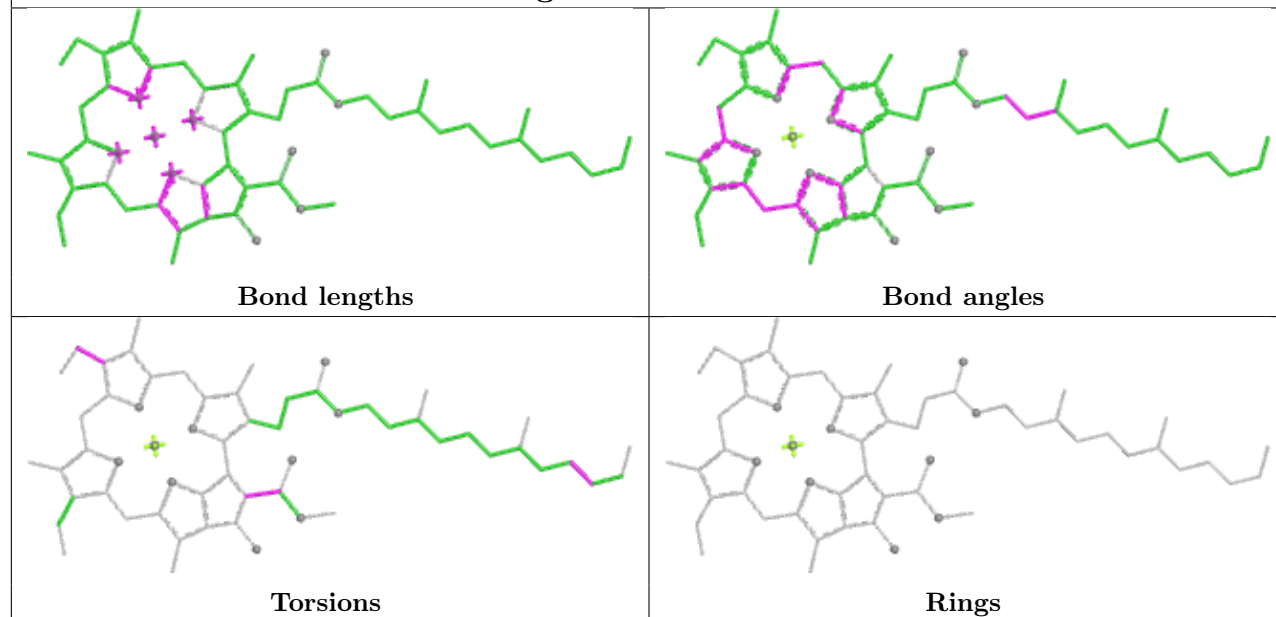


Rings

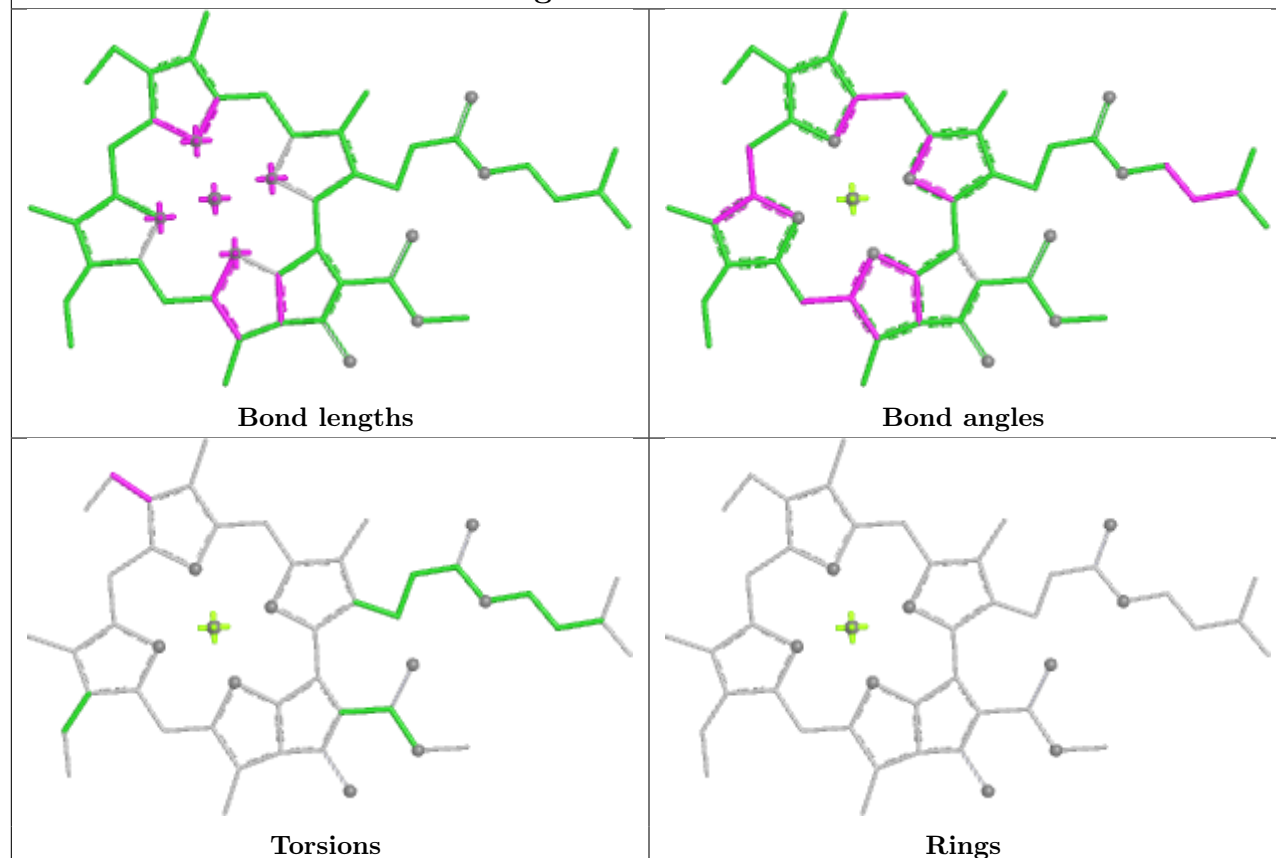


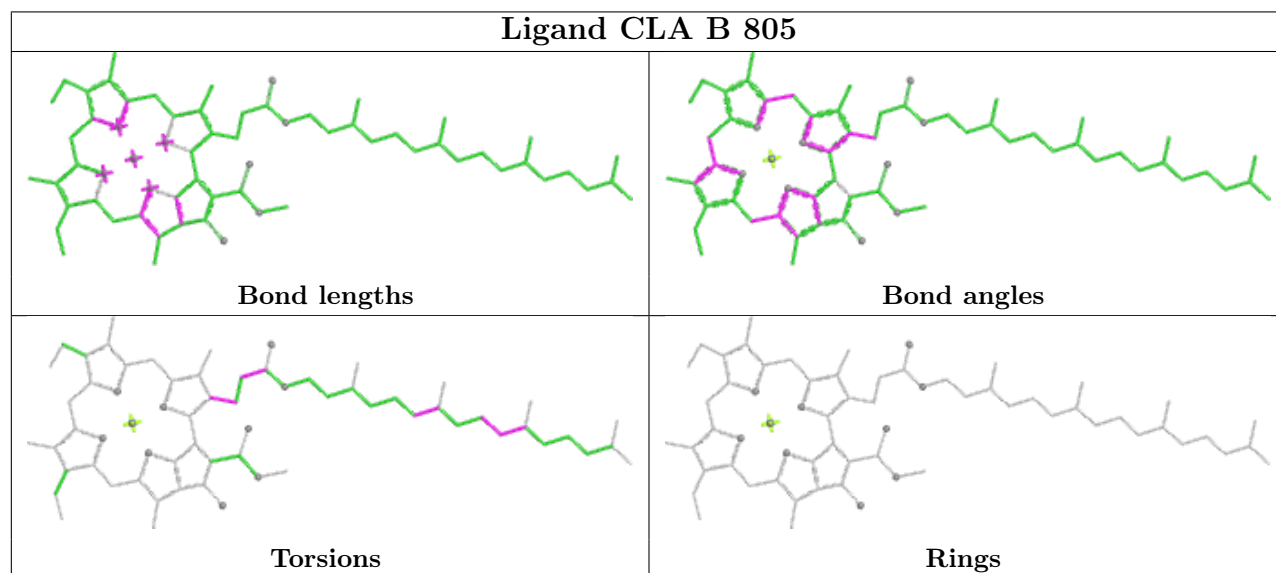
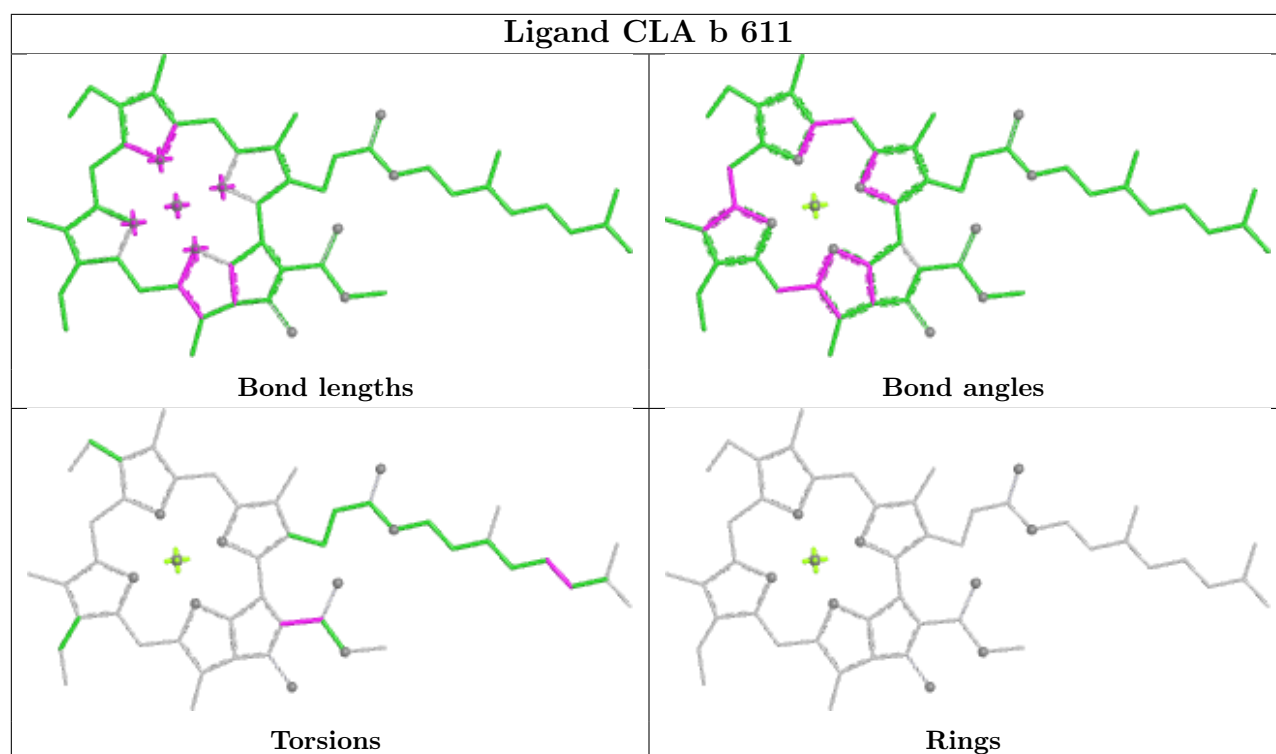


Ligand CLA 4 602

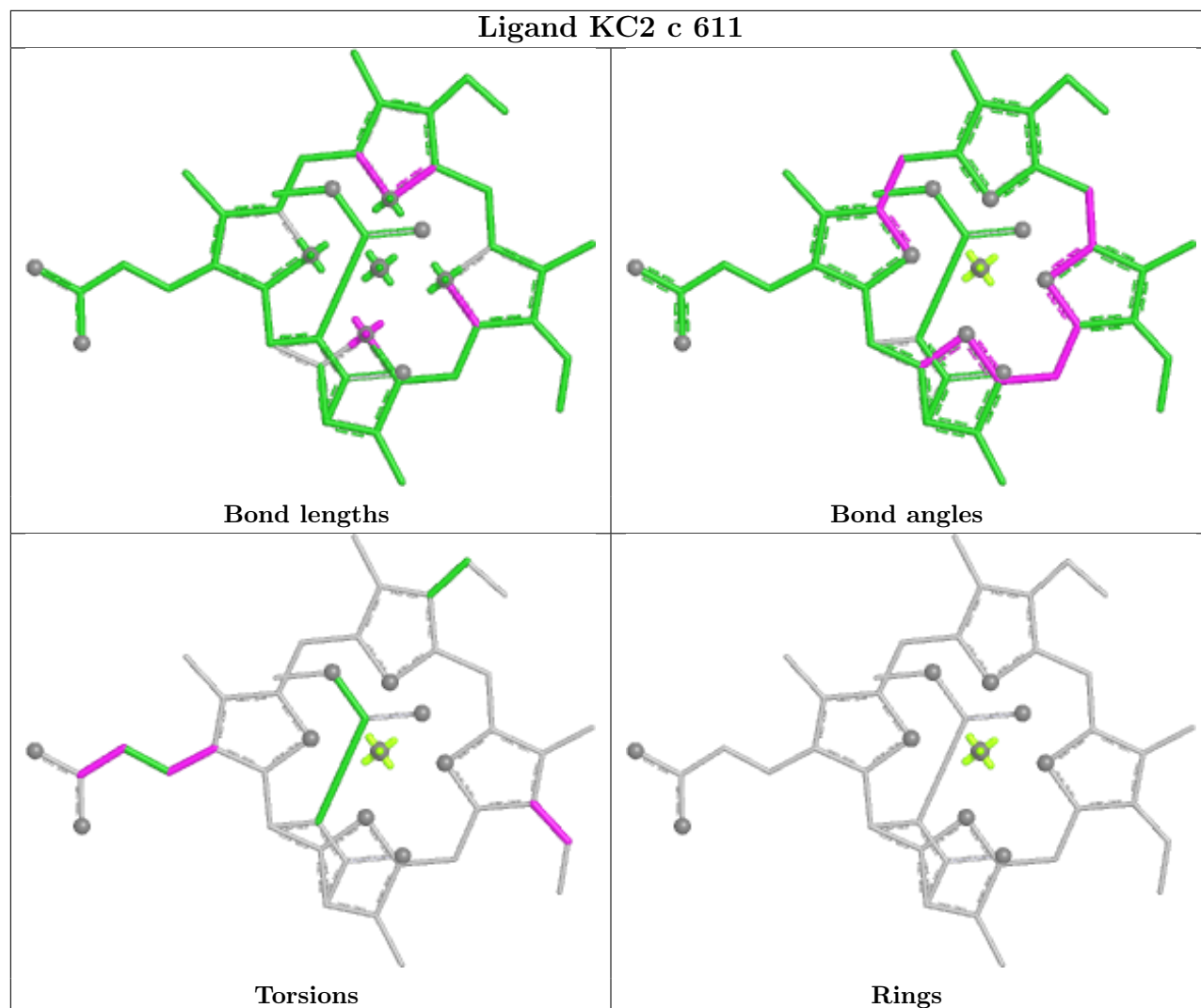


Ligand CLA Z 305

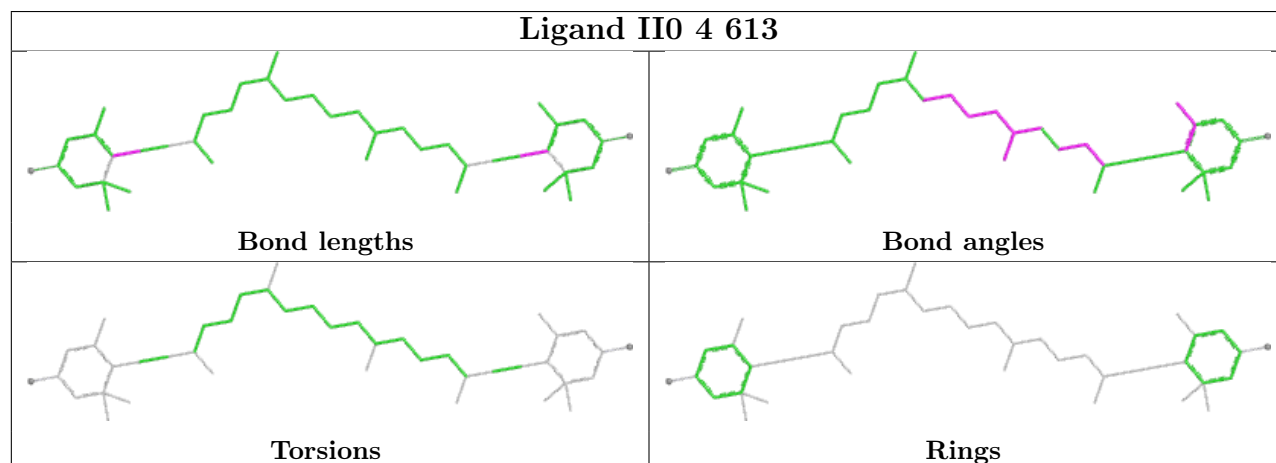


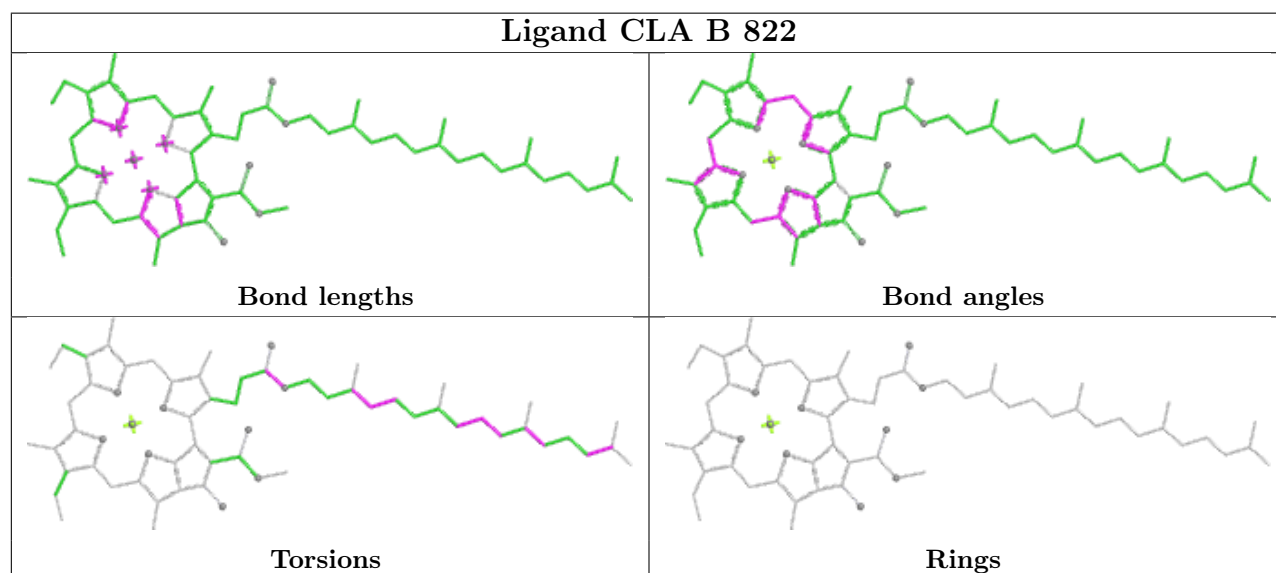
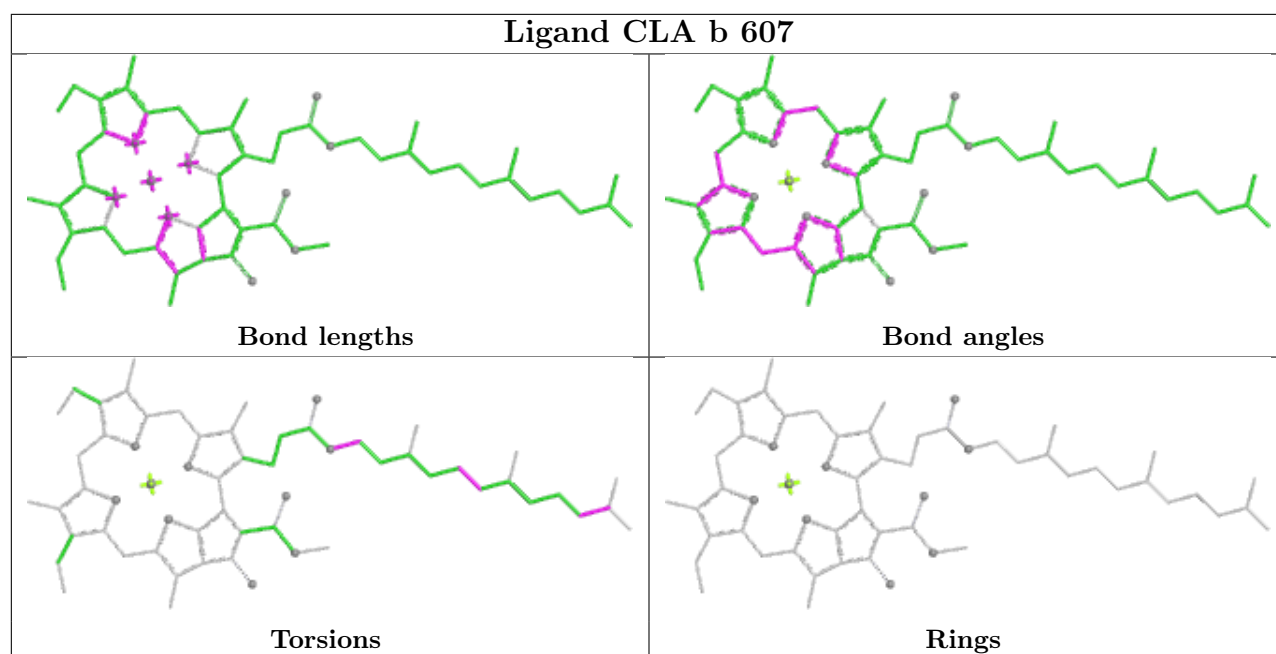


Ligand KC2 c 611

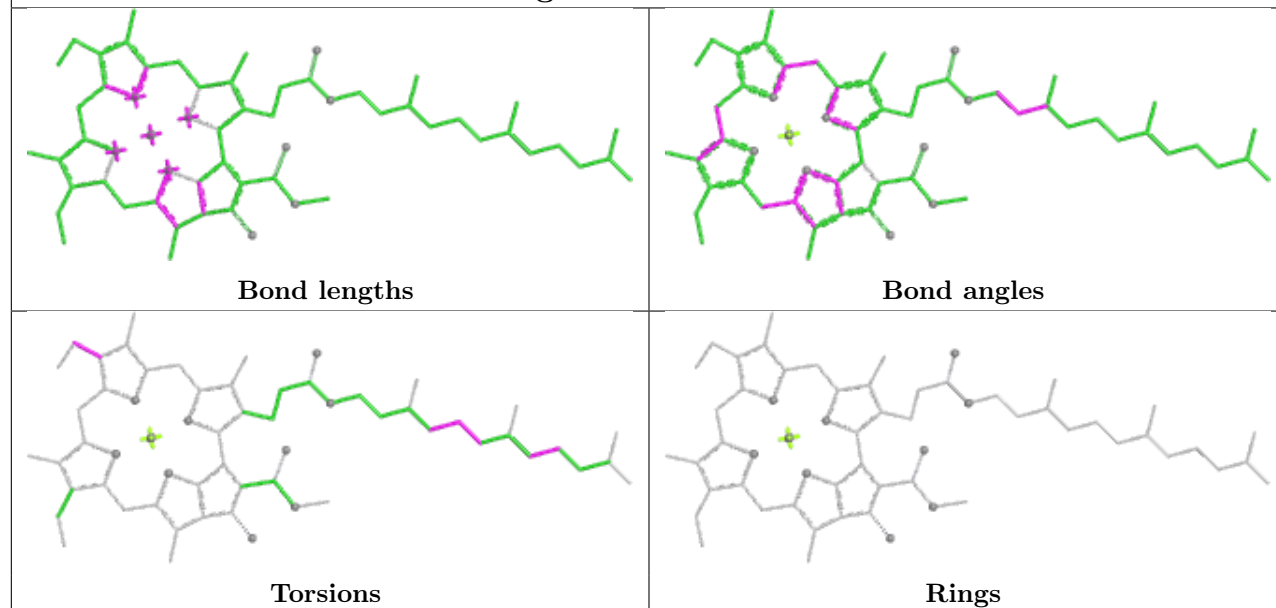


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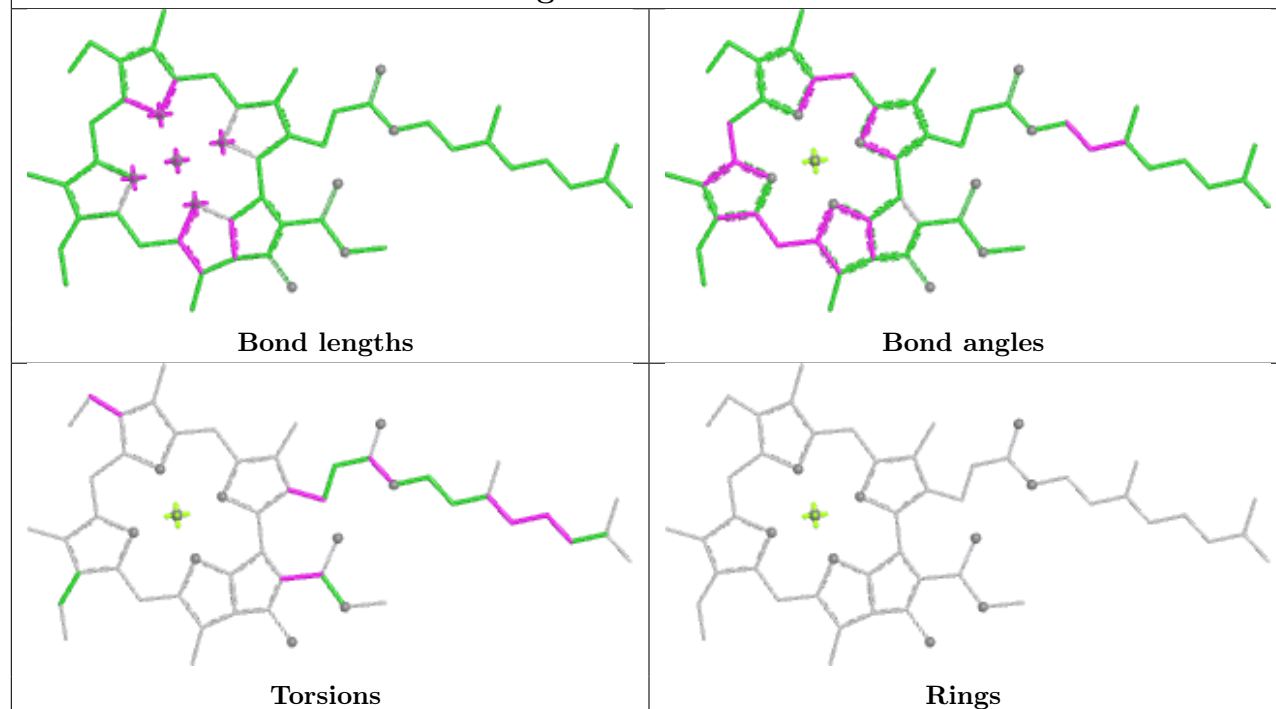


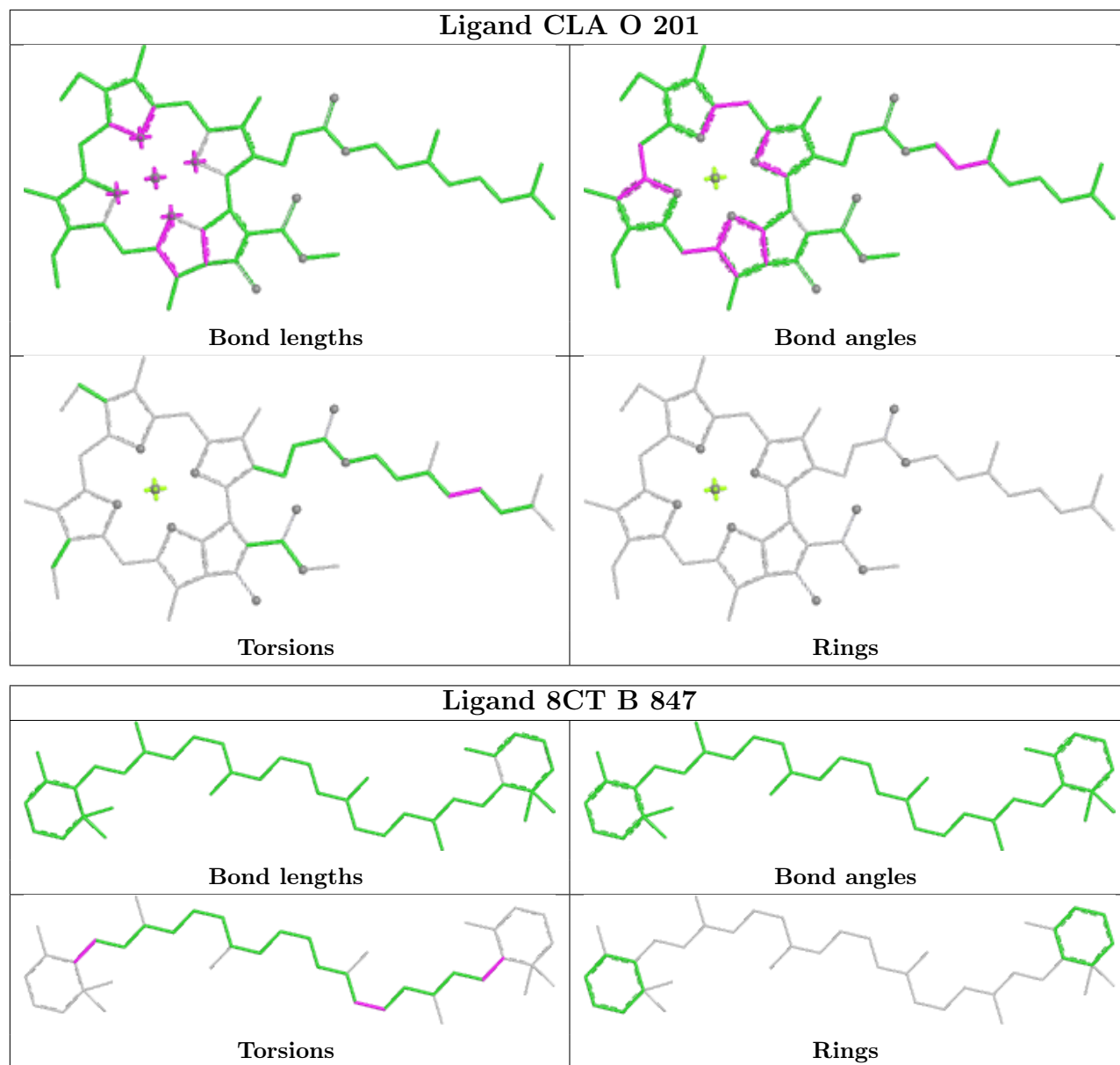


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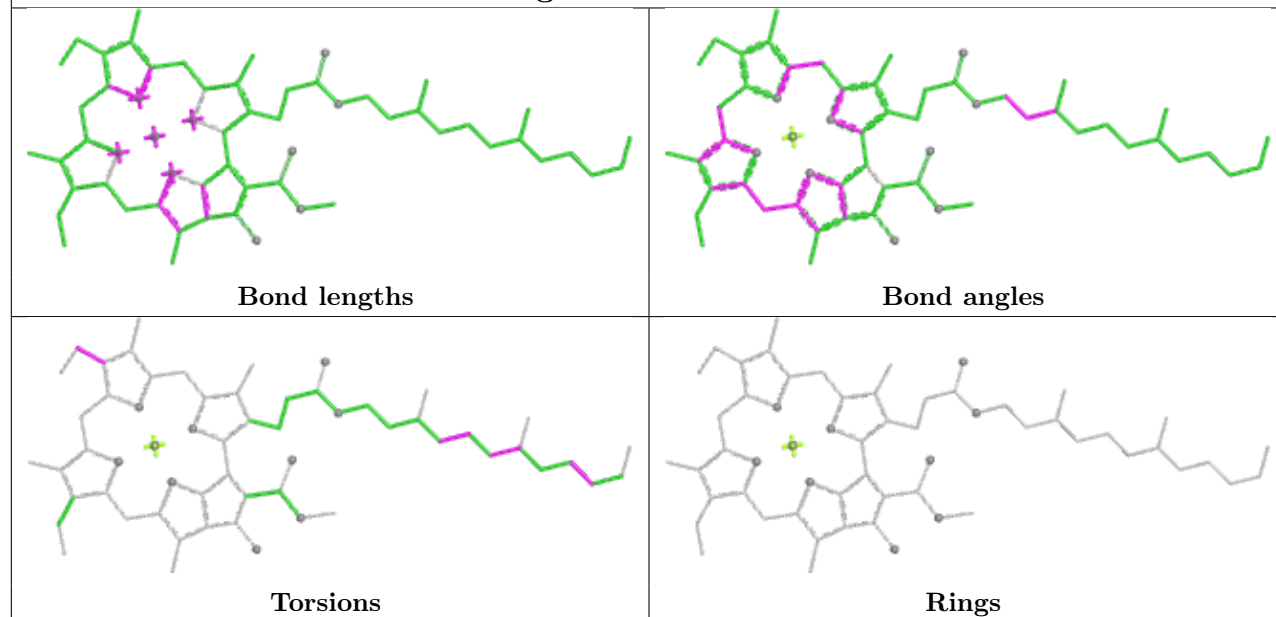


Ligand CLA e 602

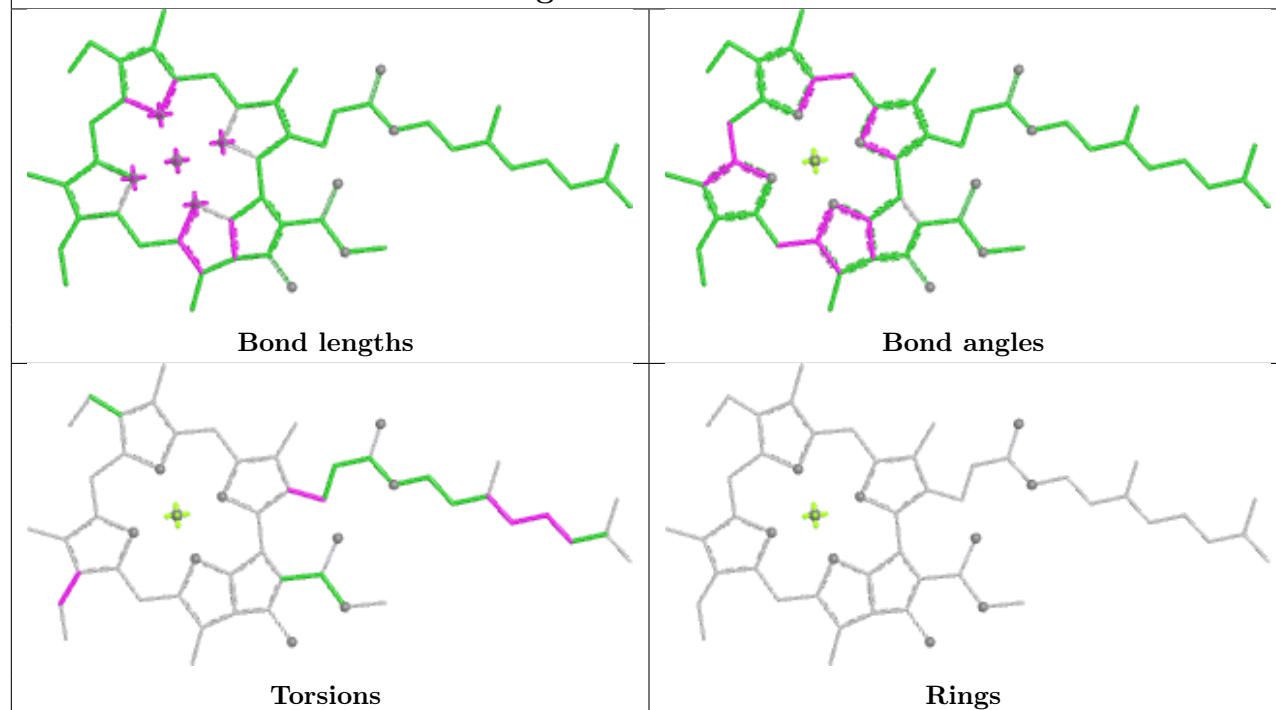


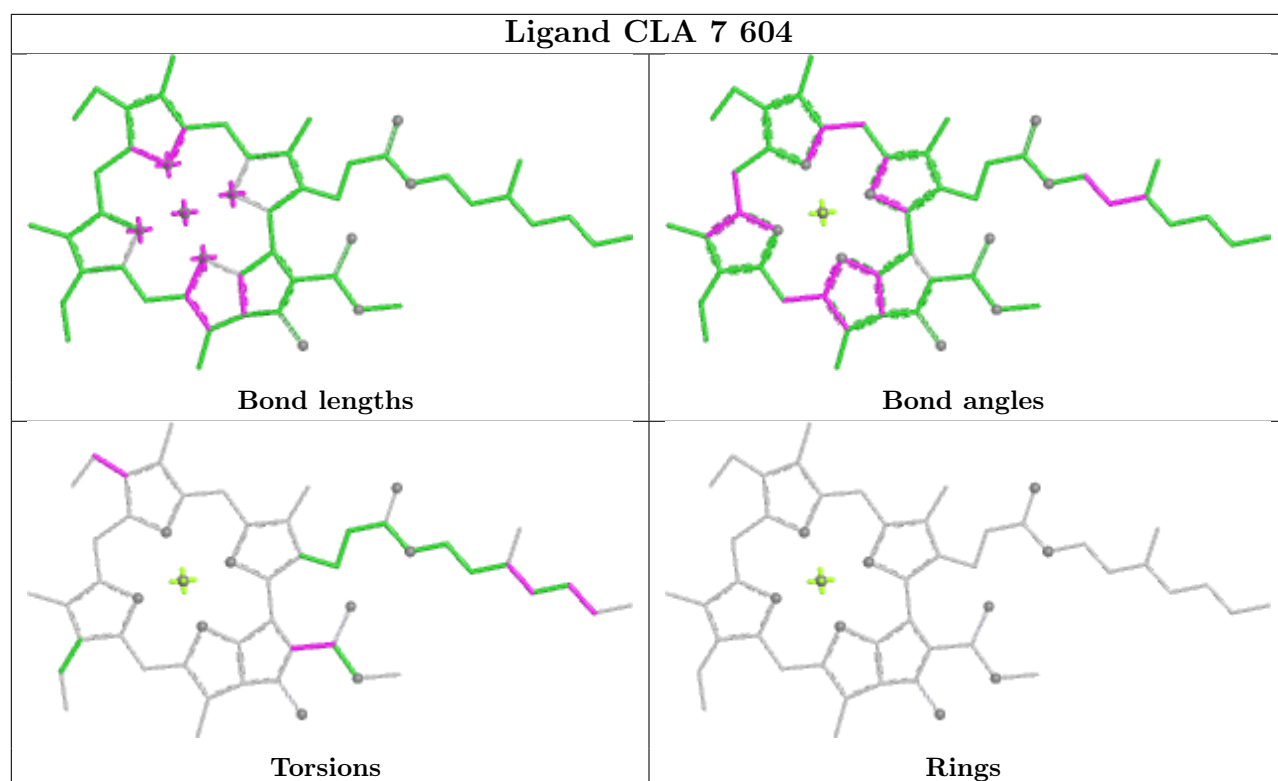


Ligand CLA 1 602

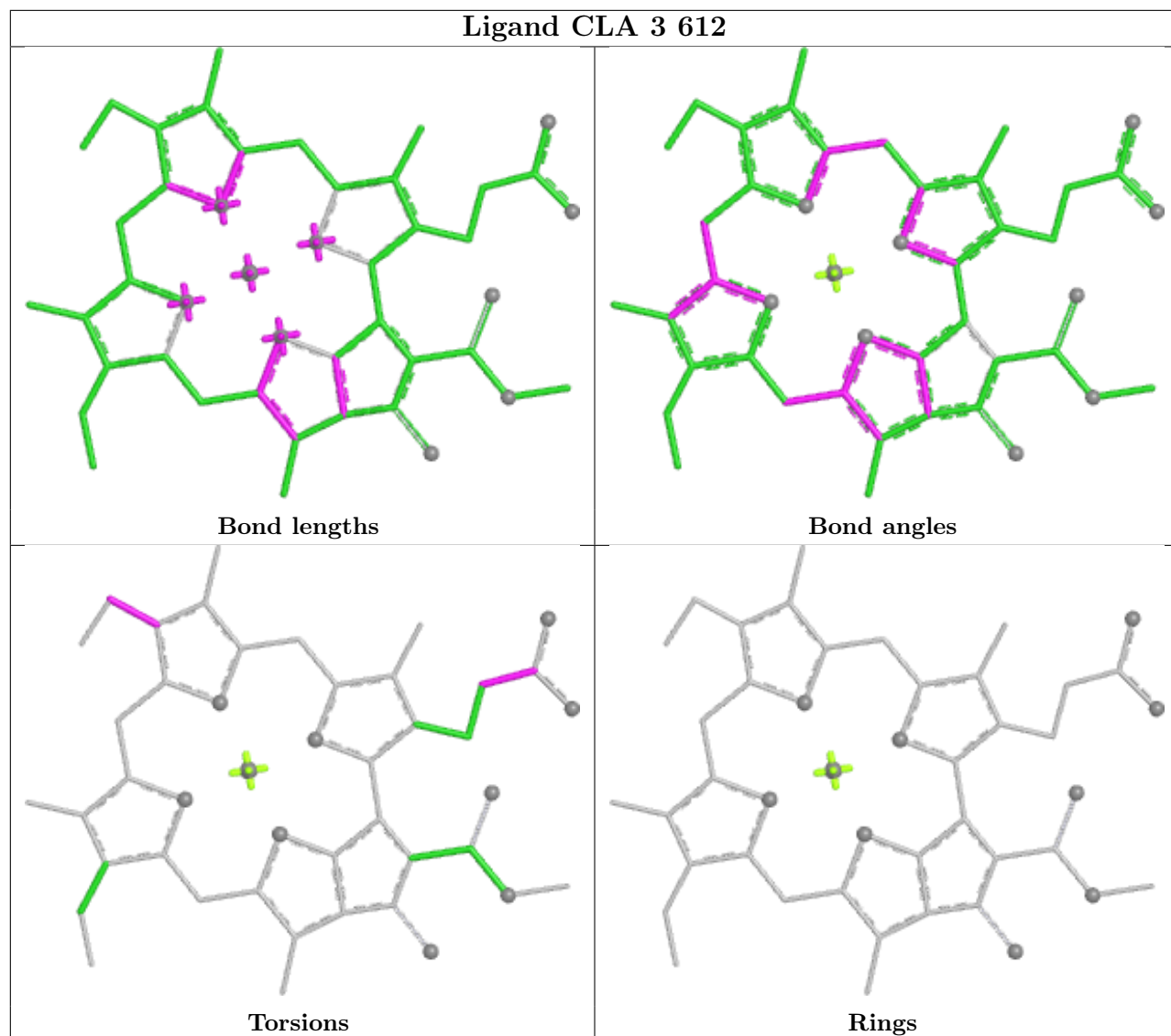


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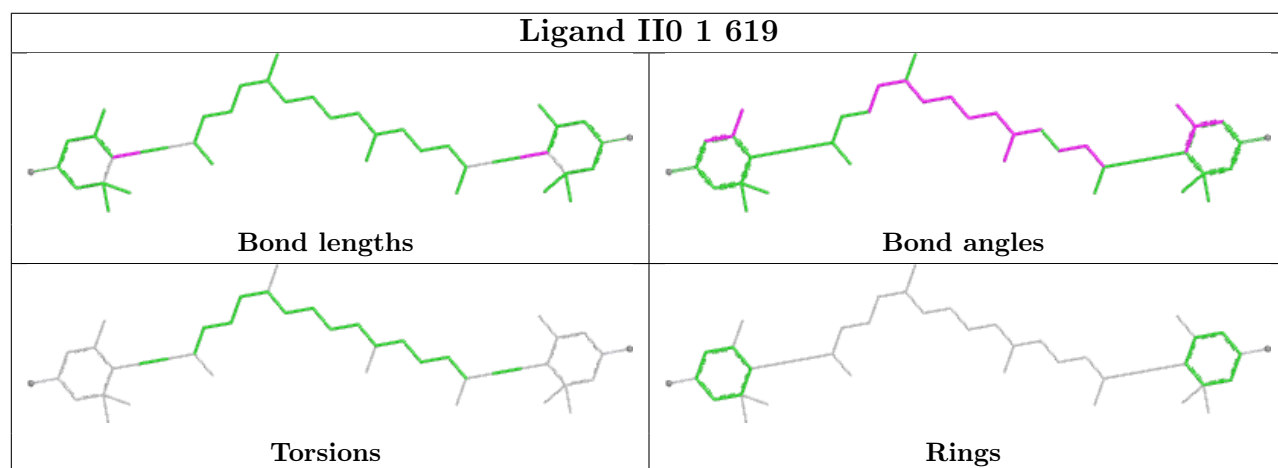


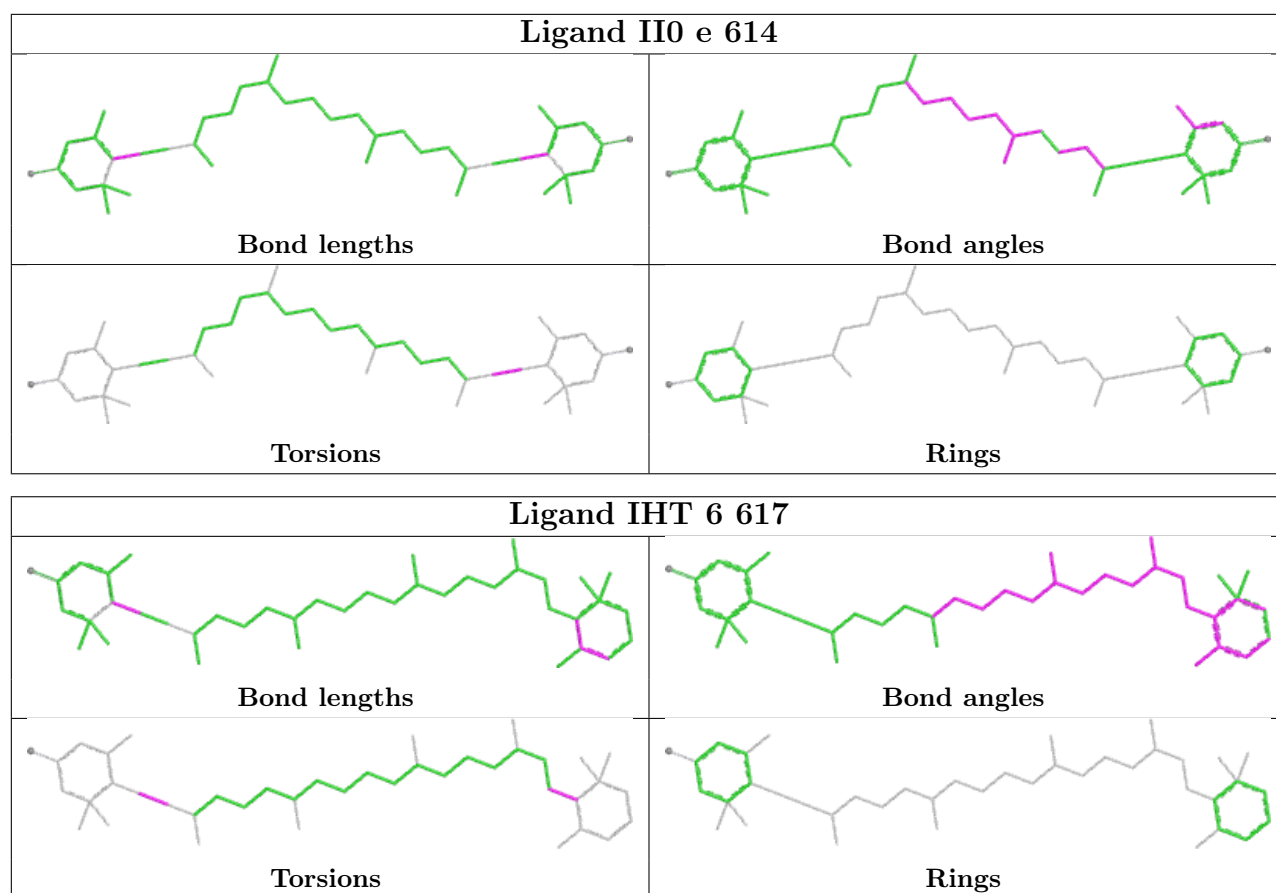


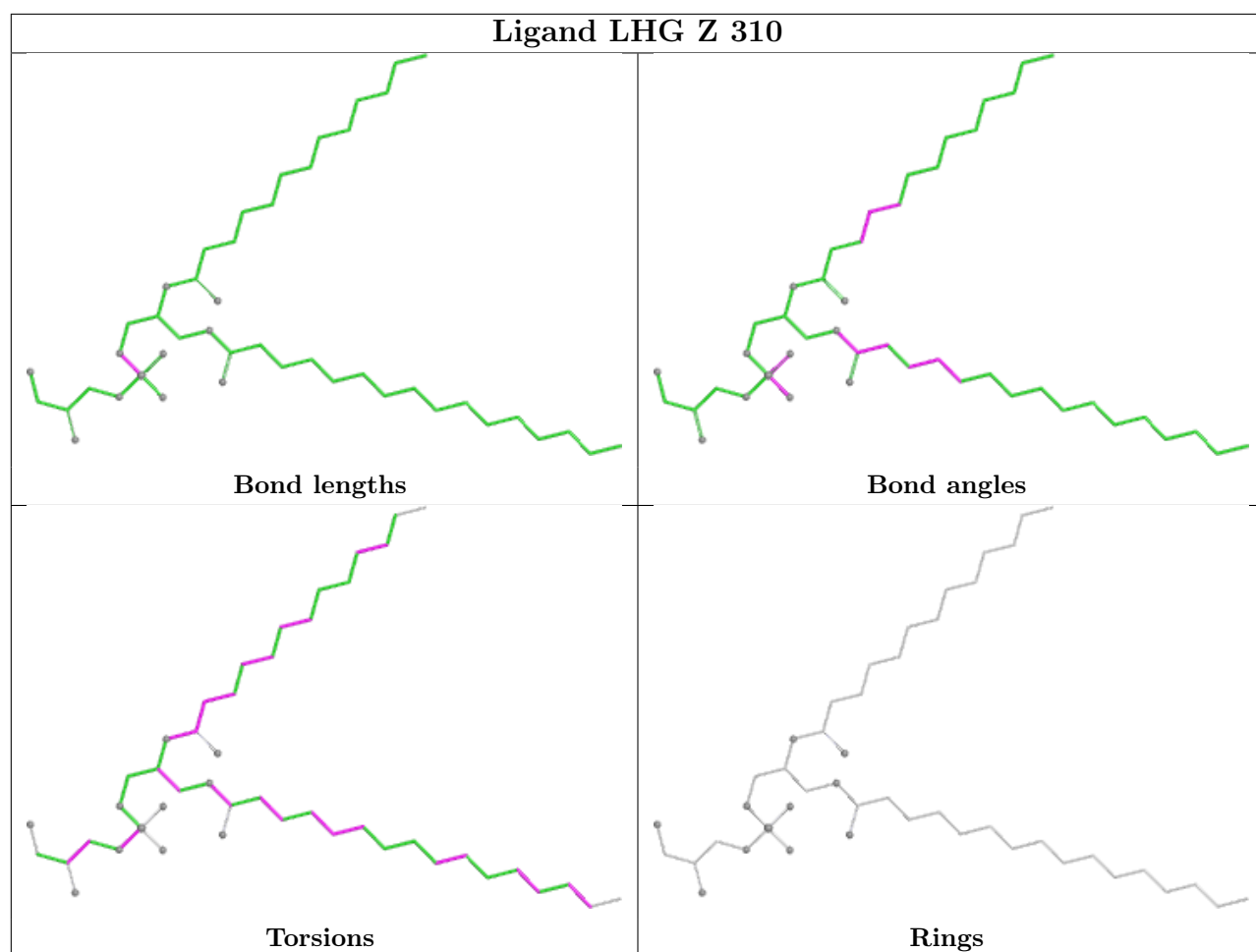
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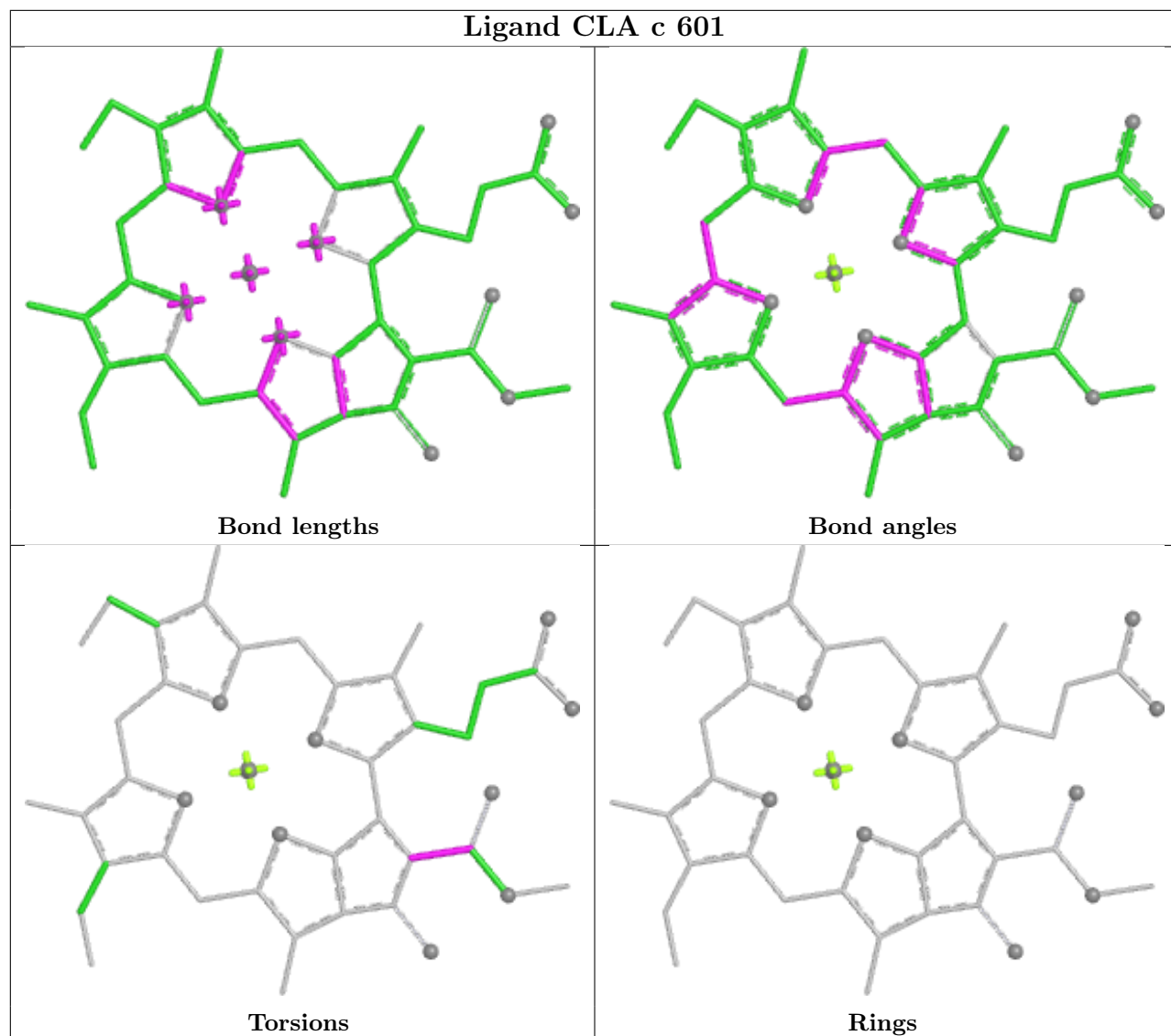
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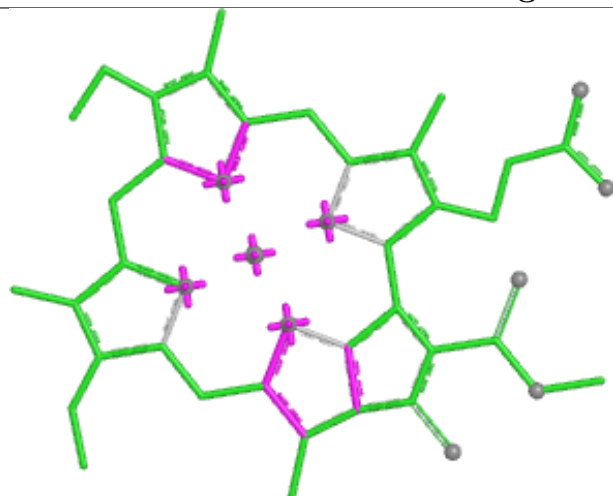




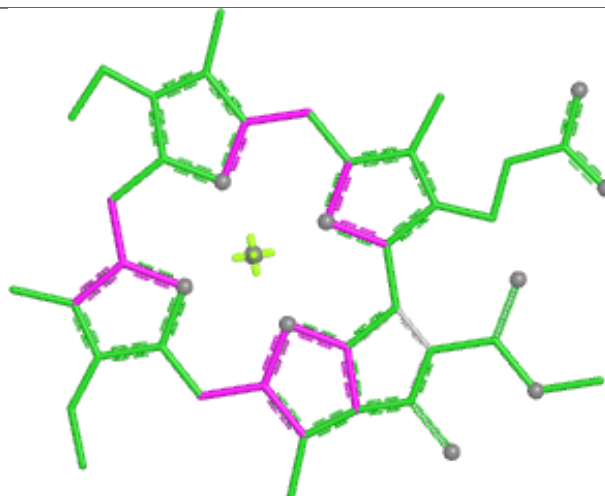
Ligand CLA c 601



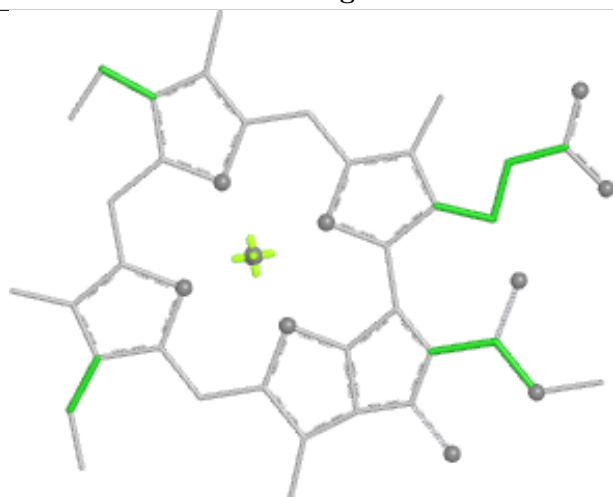
Ligand CLA 9 605



Bond lengths



Bond angles

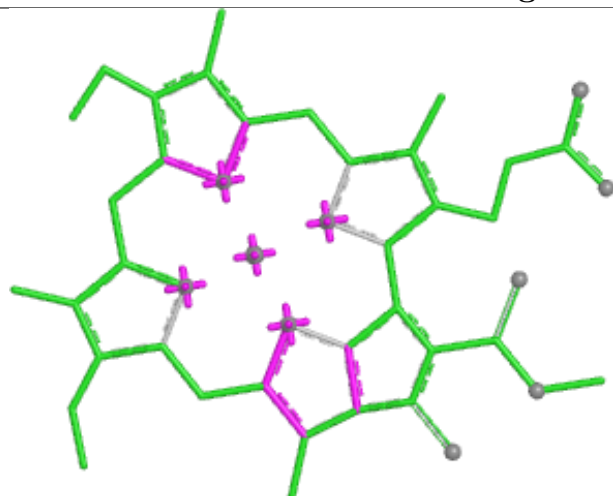


Torsions

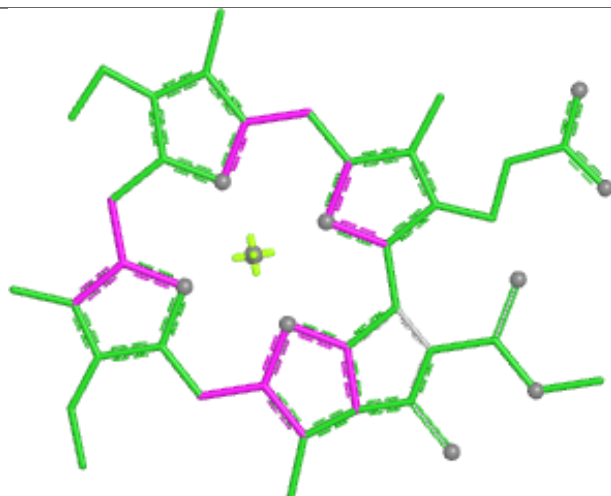


Rings

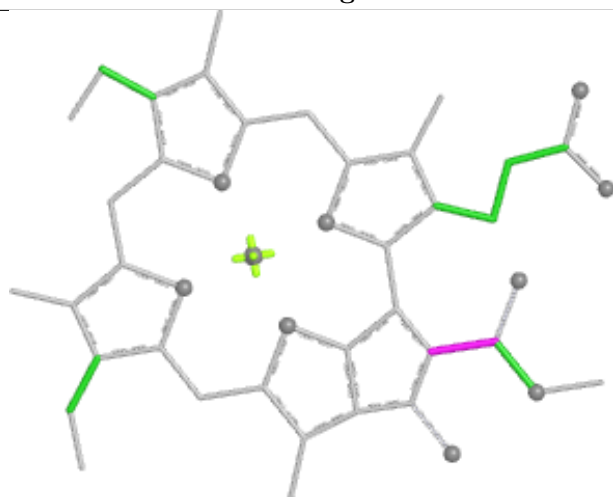
Ligand CLA 2 606



Bond lengths



Bond angles

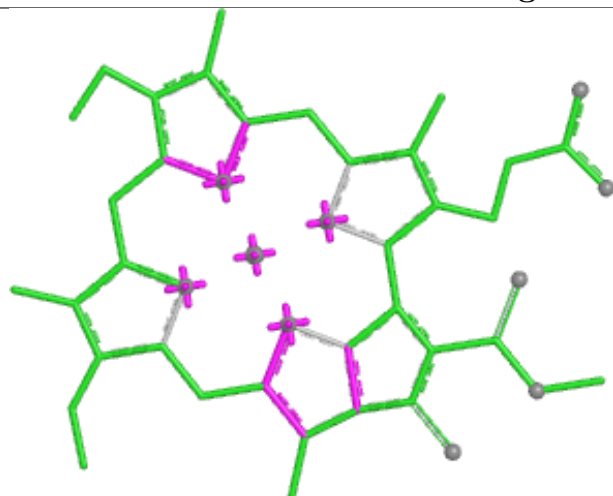


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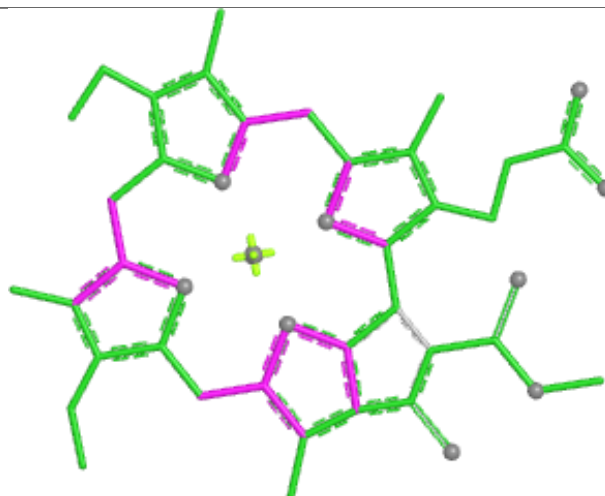


Rings

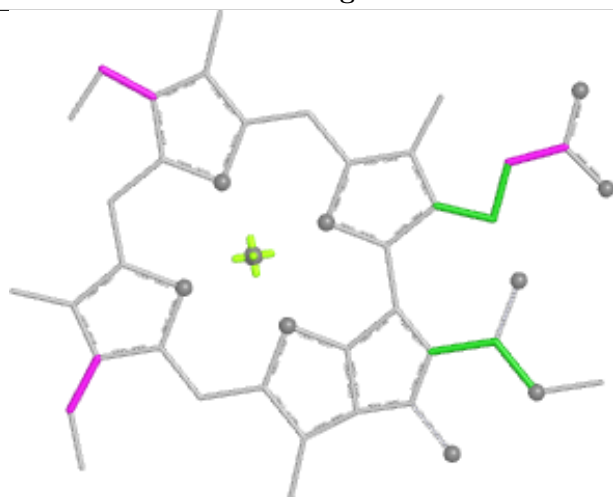
Ligand CLA 9 601



Bond lengths



Bond angles

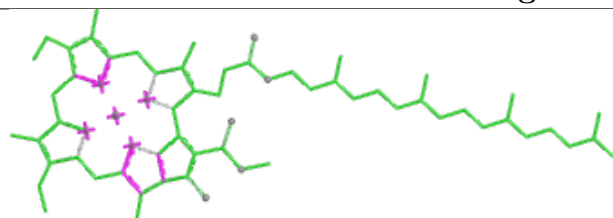


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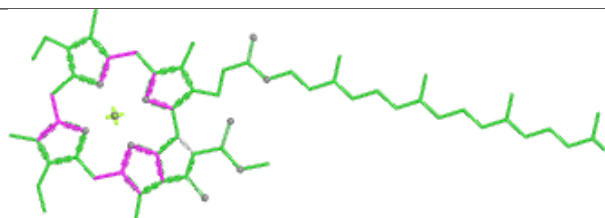


Rings

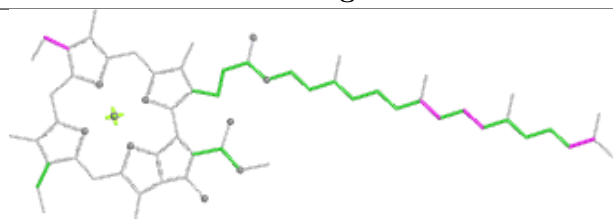
Ligand CLA 8 608



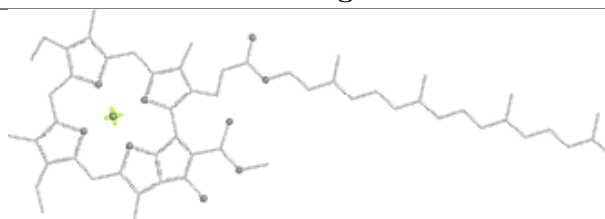
Bond lengths



Bond angles

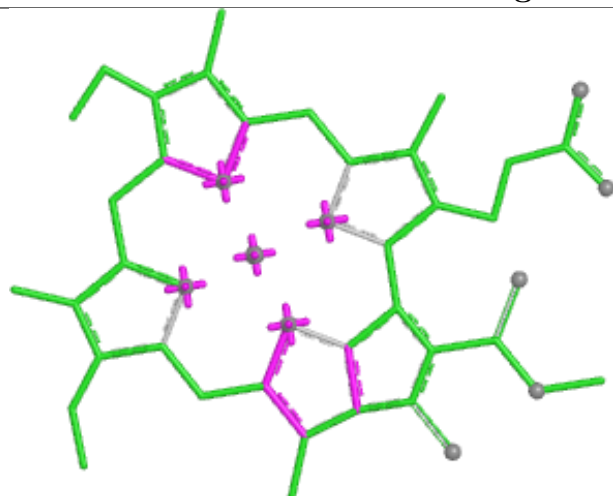


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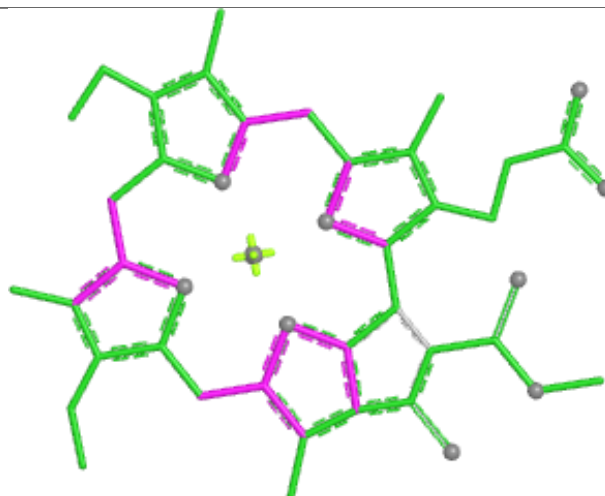


Rings

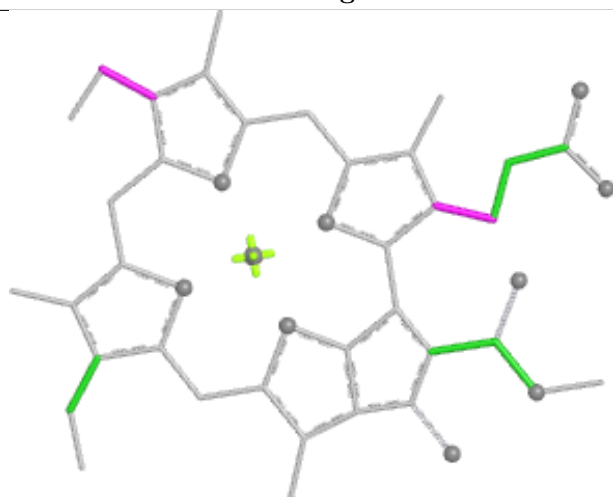
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Bond lengths



Bond angles

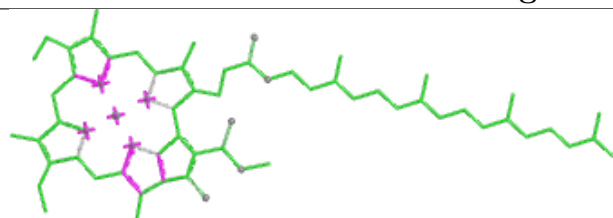


Torsions

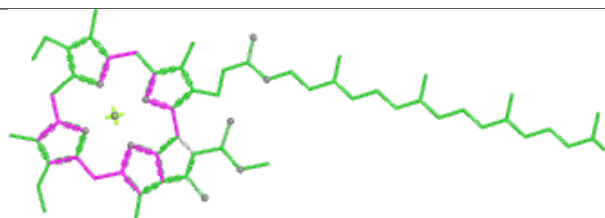


Rings

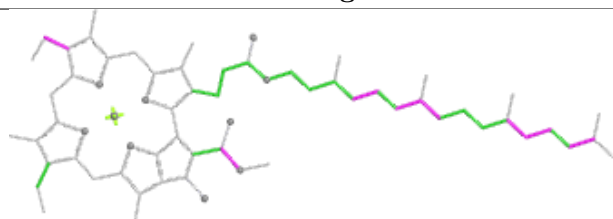
Ligand CLA c 603



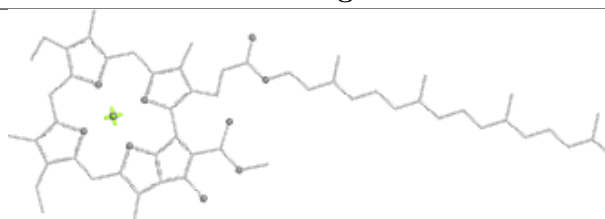
Bond lengths



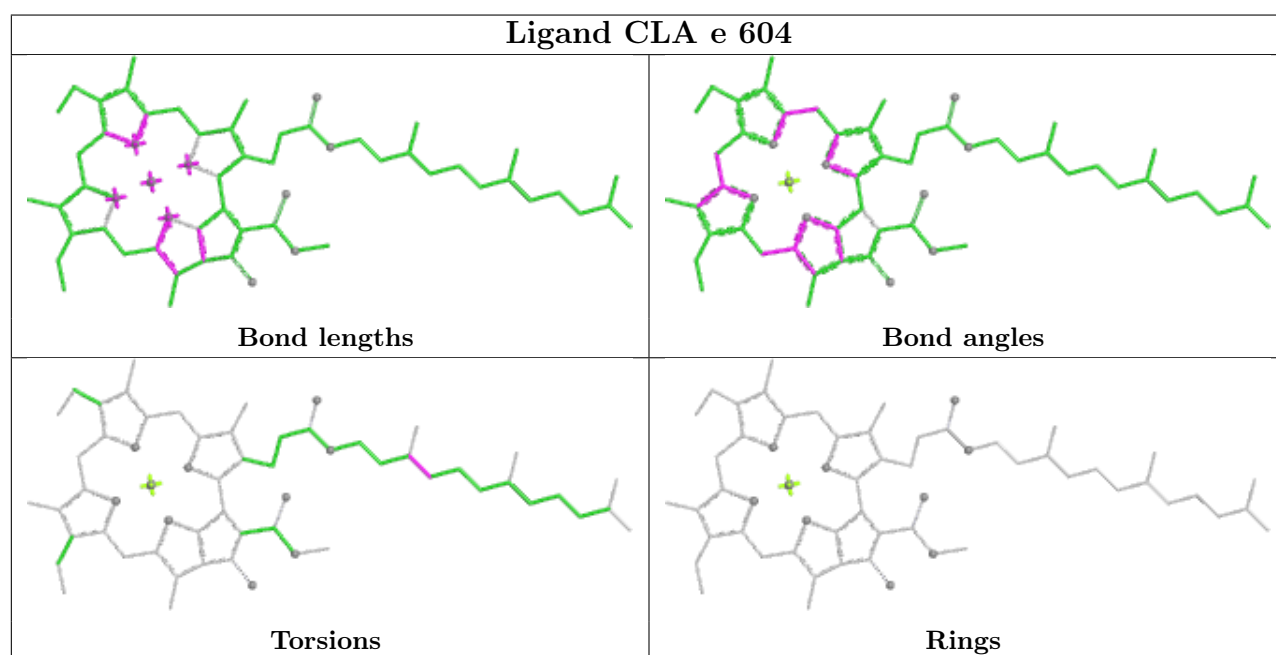
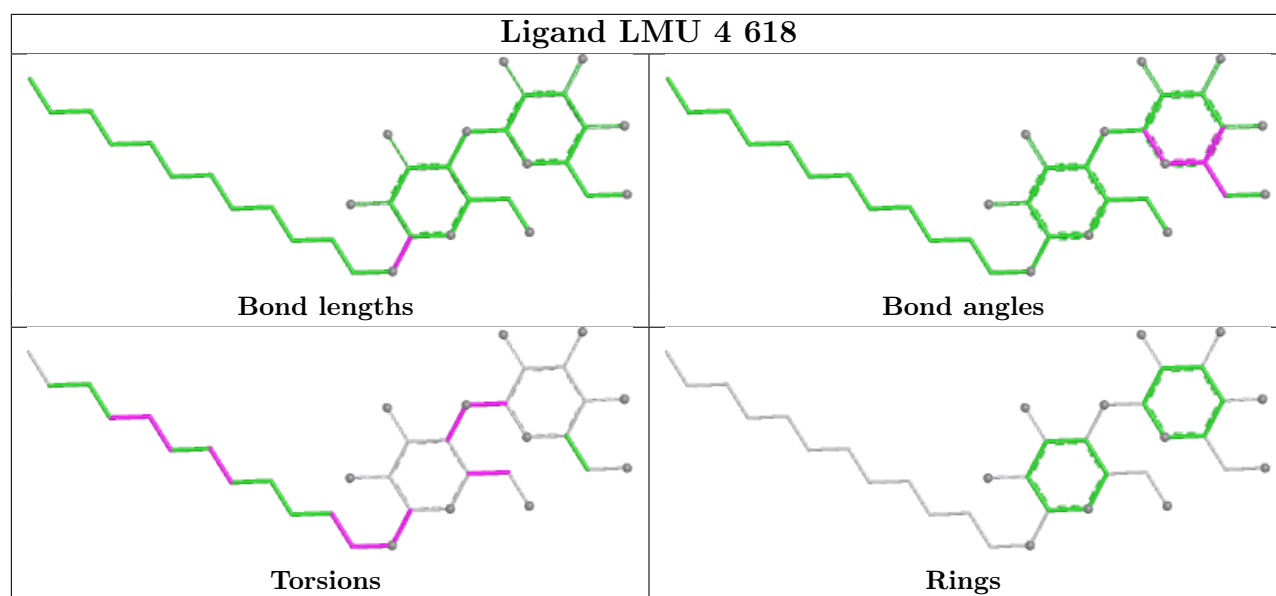
Bond angles

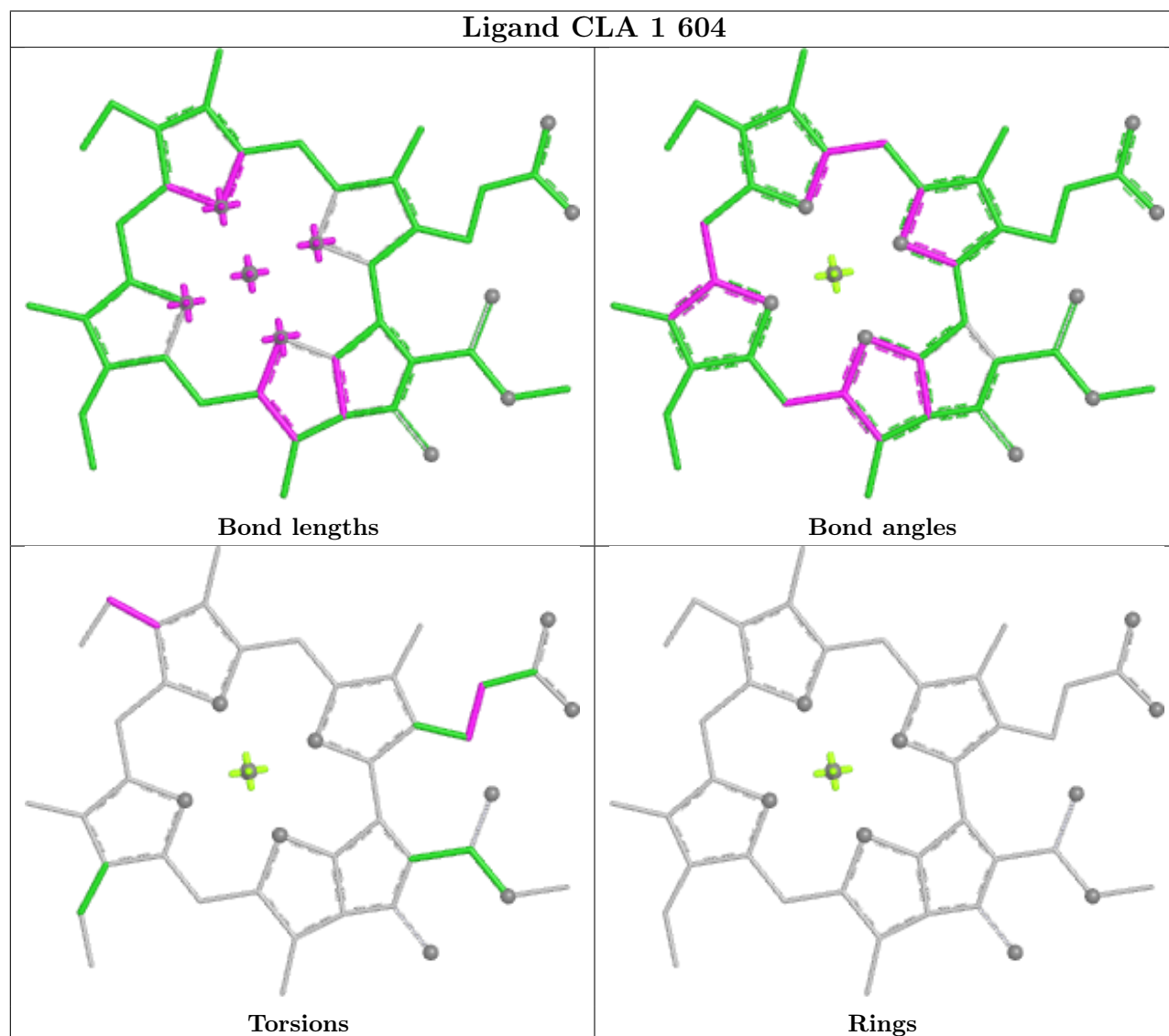
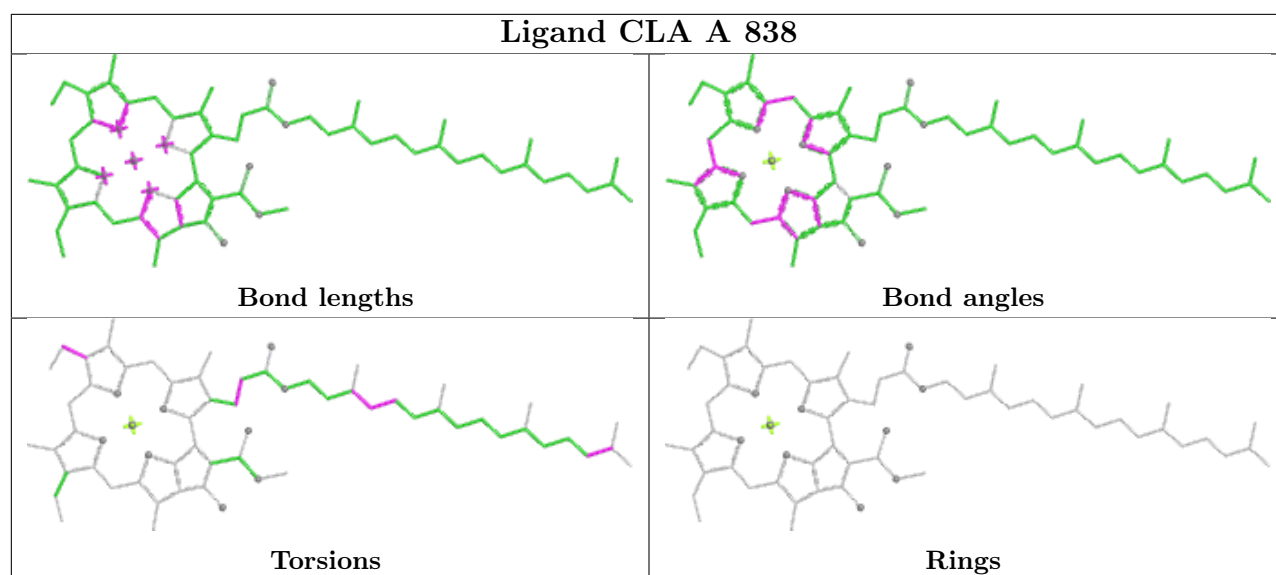


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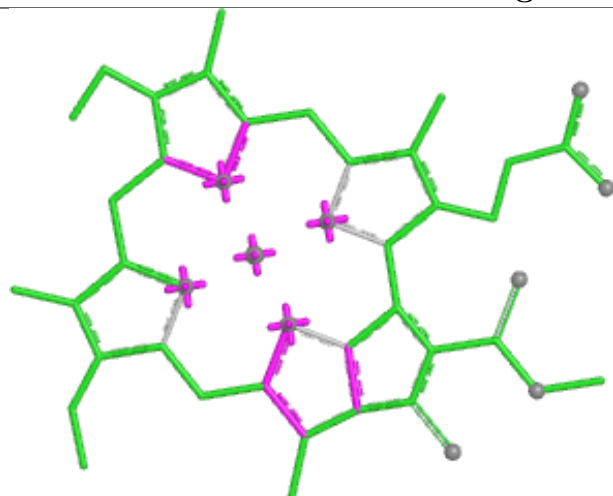


Rings

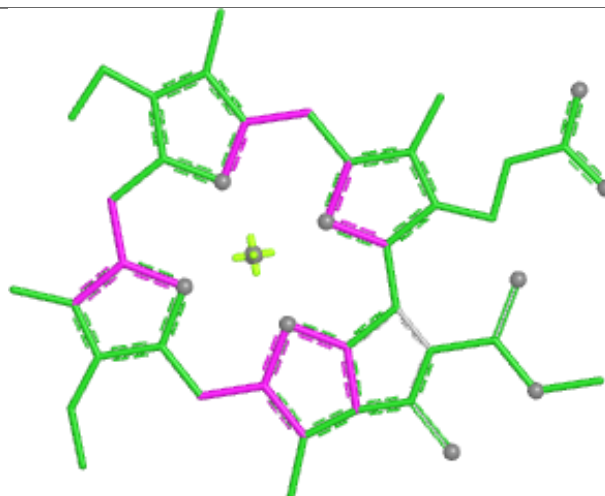




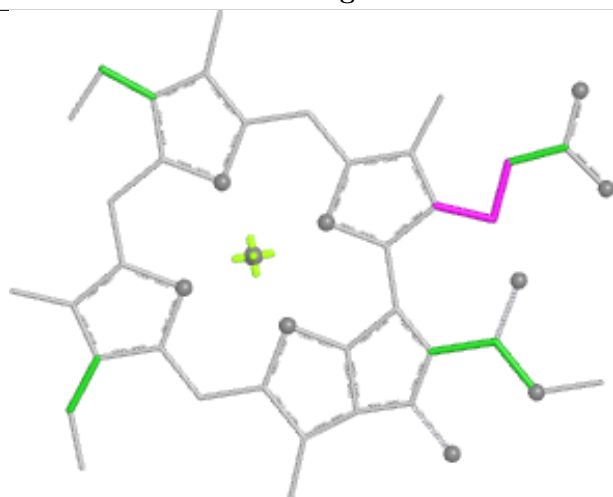
Ligand CLA F 203



Bond lengths



Bond angles

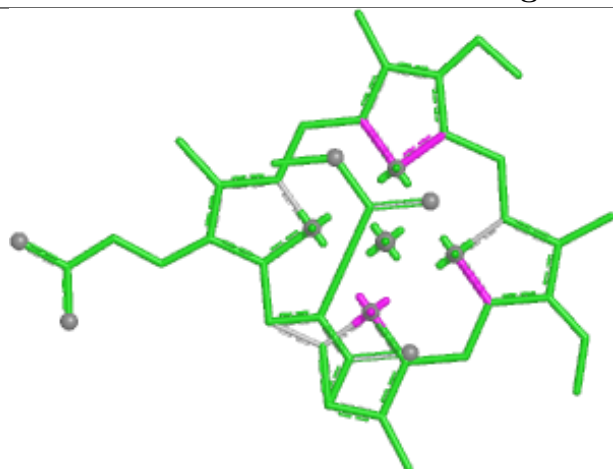


Torsions

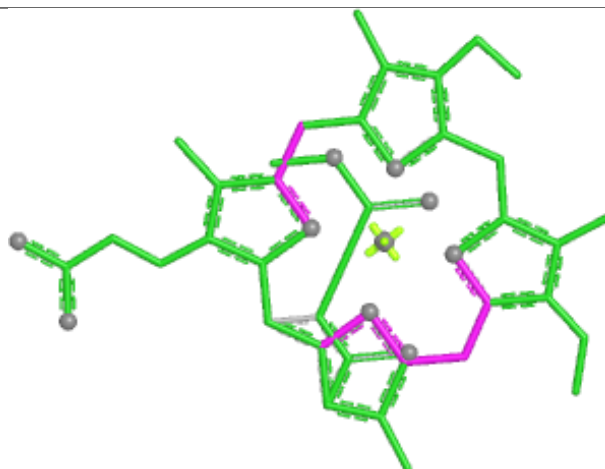


Rings

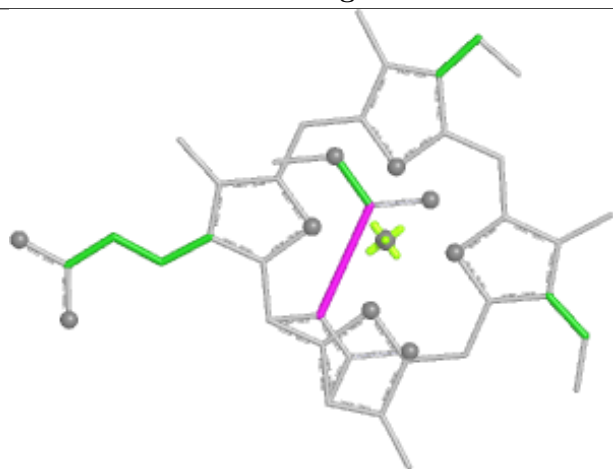
Ligand KC2 a 610



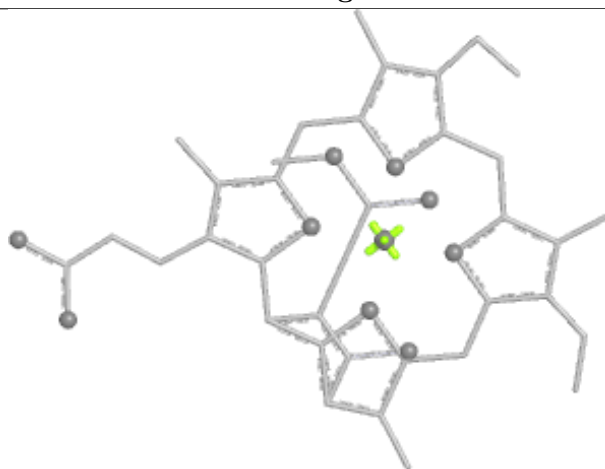
Bond lengths



Bond angles

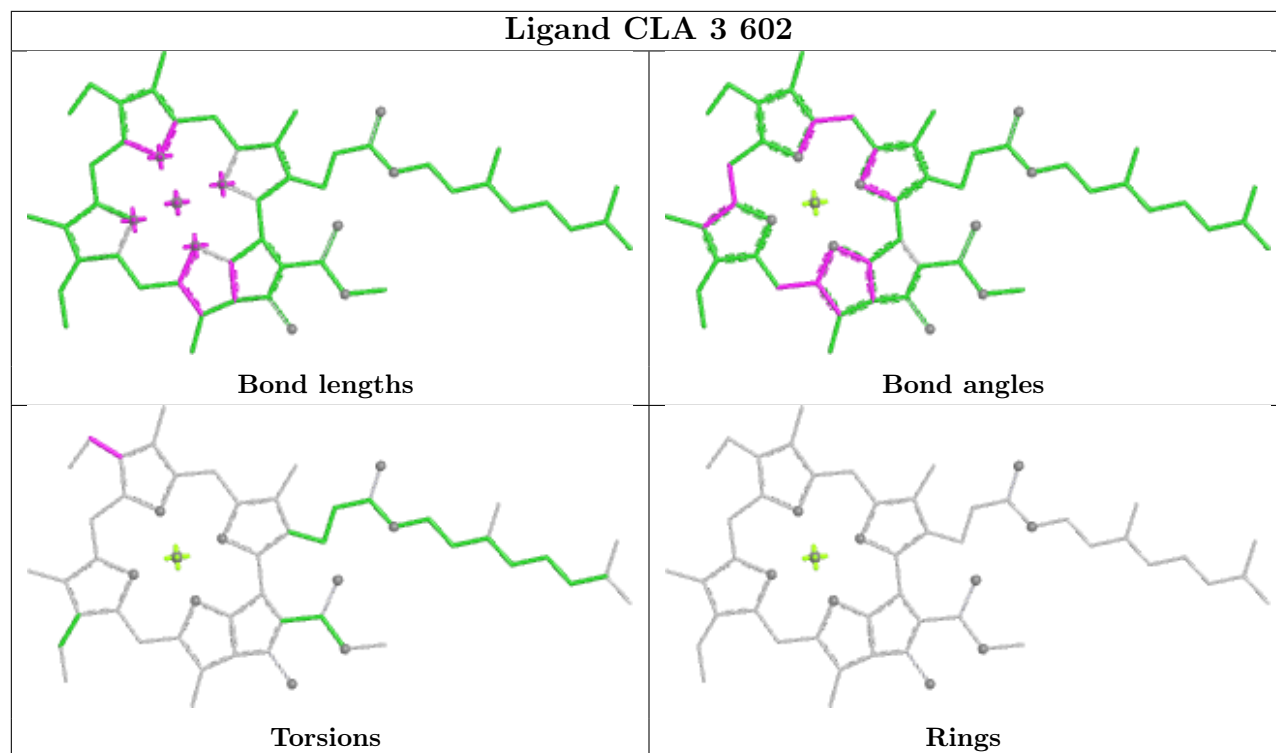


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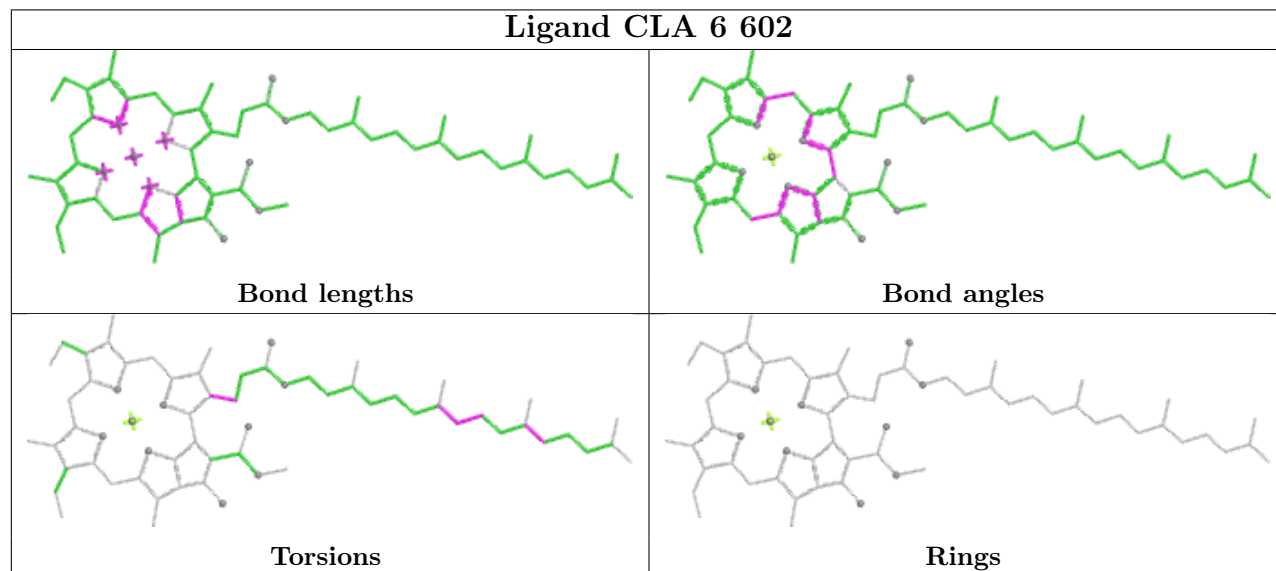


Rings

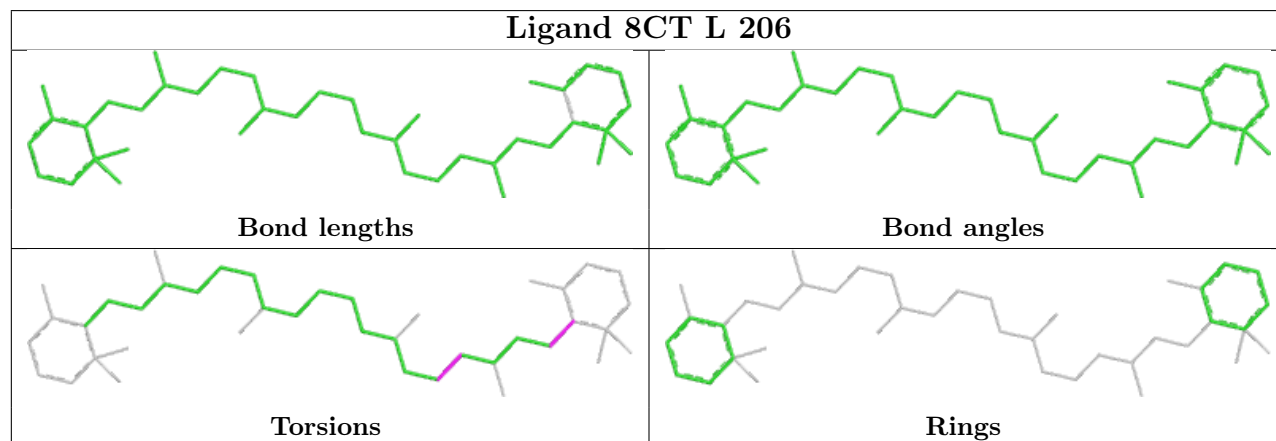
Ligand CLA 3 602

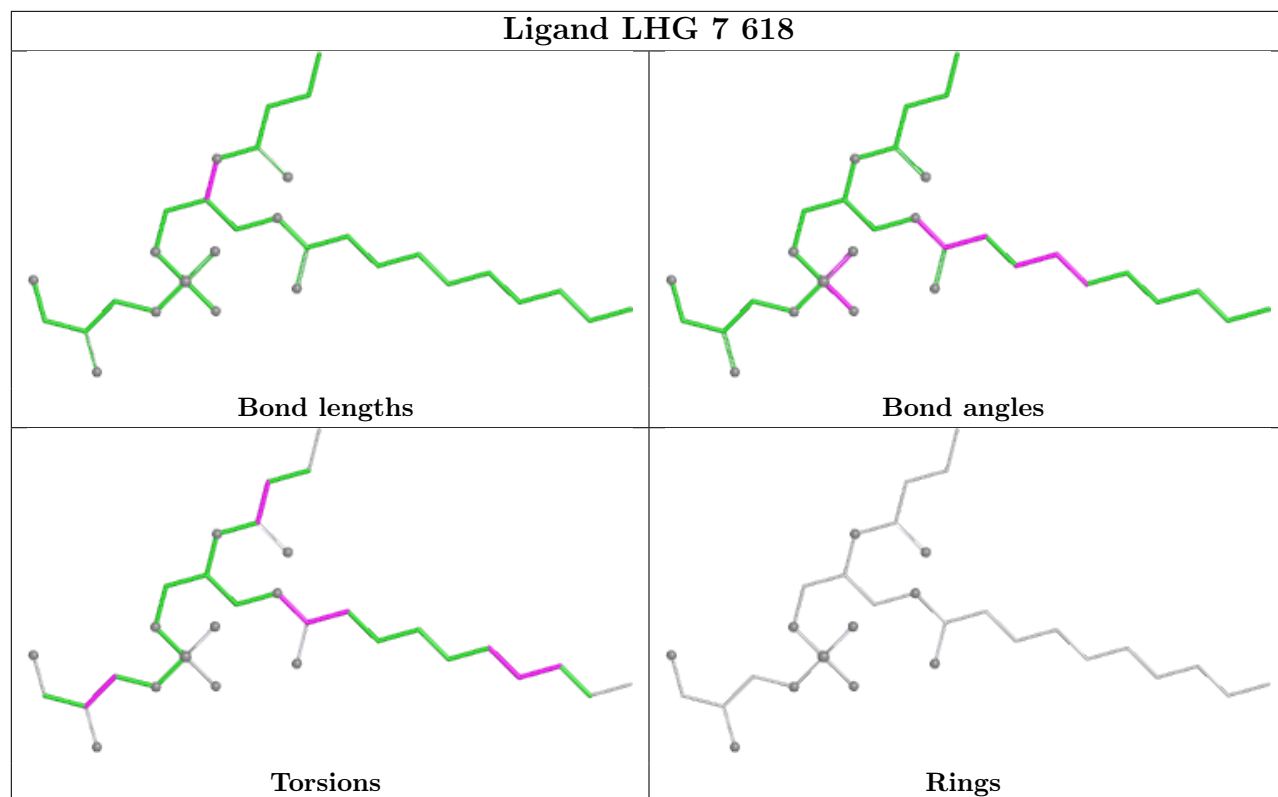


Ligand CLA 6 602

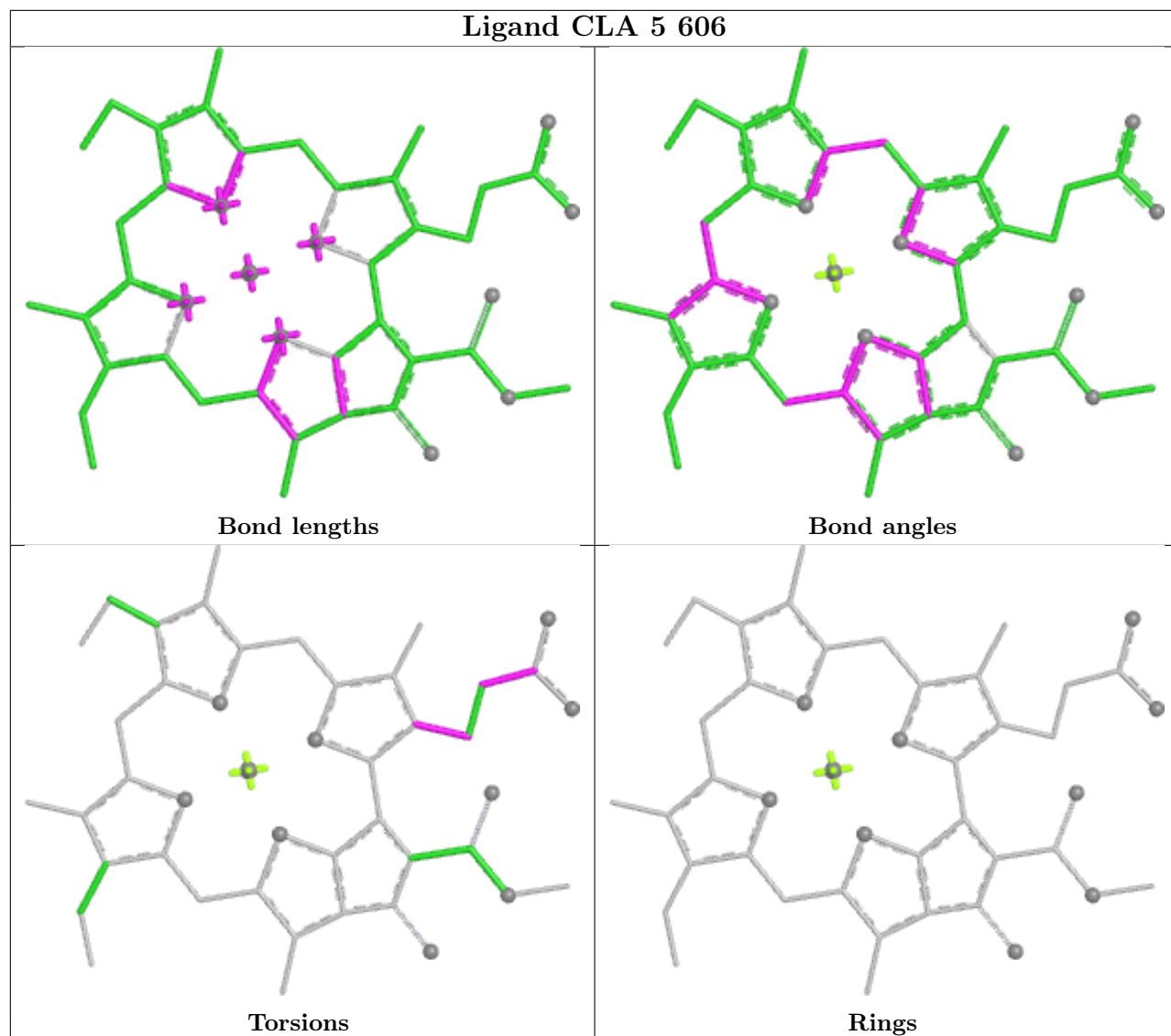


Ligand 8CT L 206

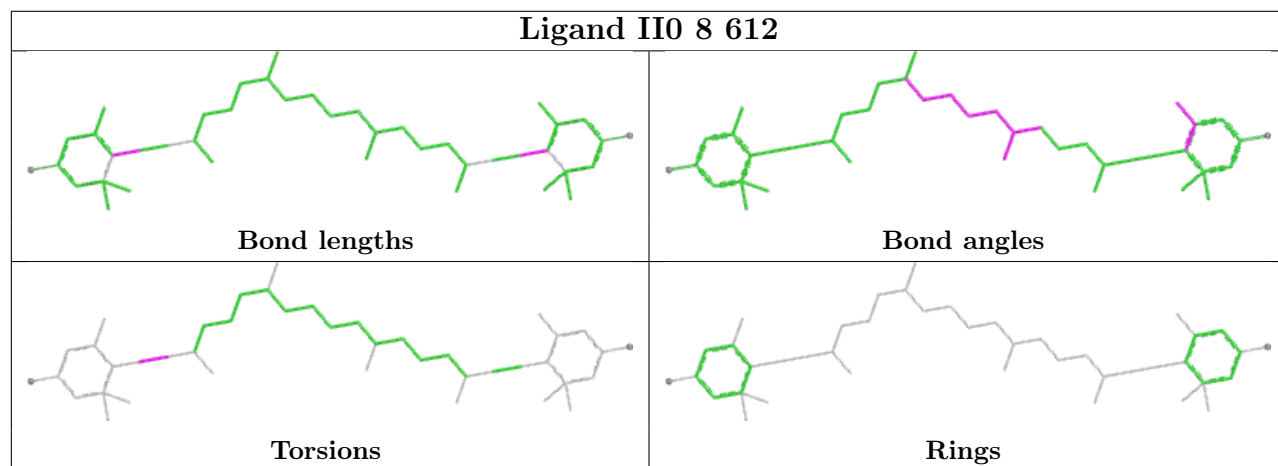


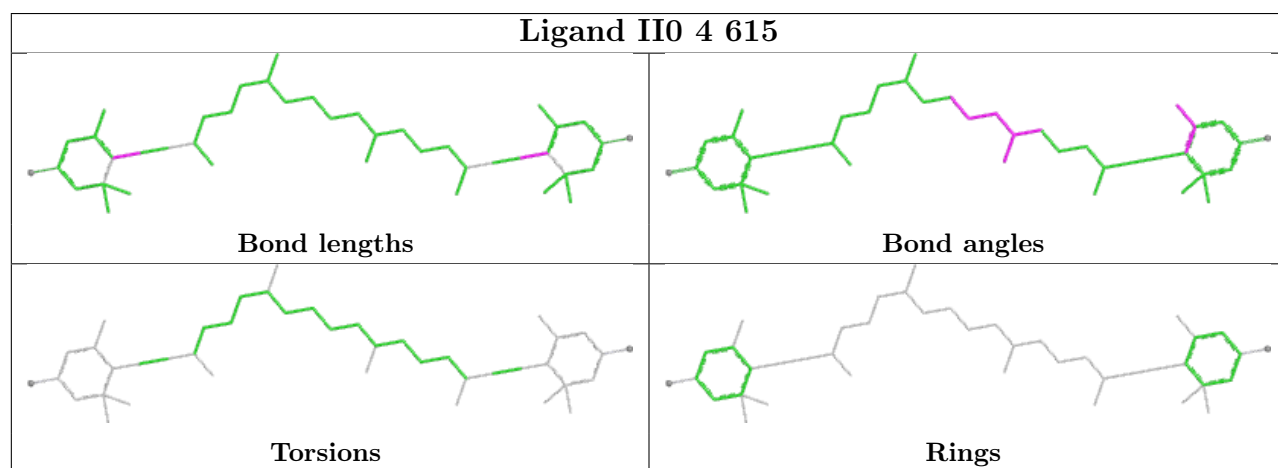
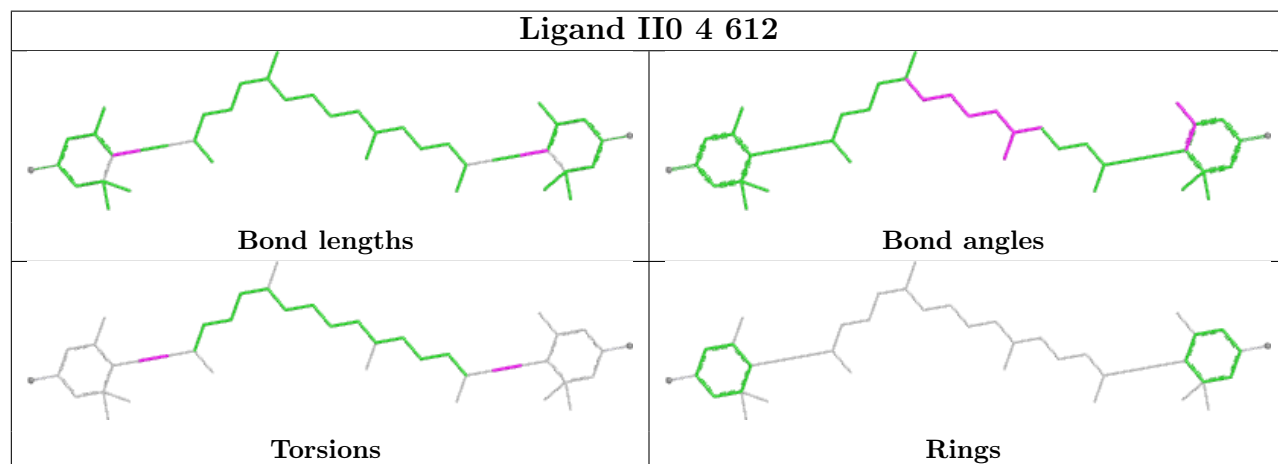
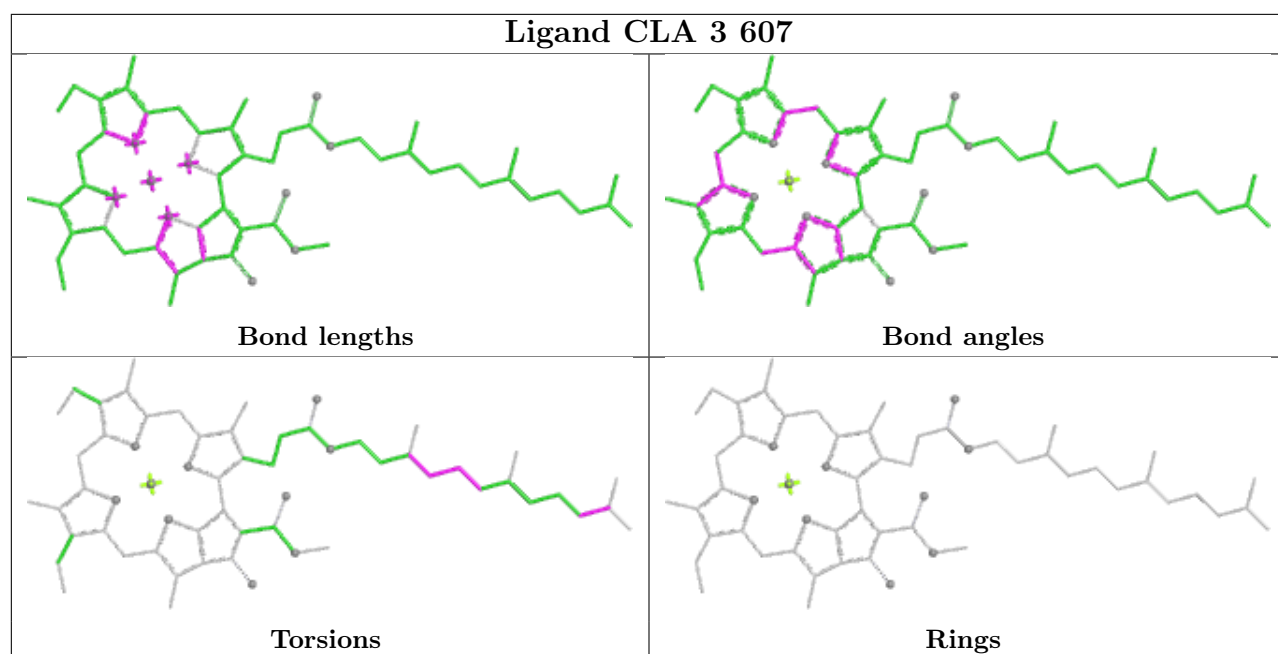


Ligand CLA 5 606

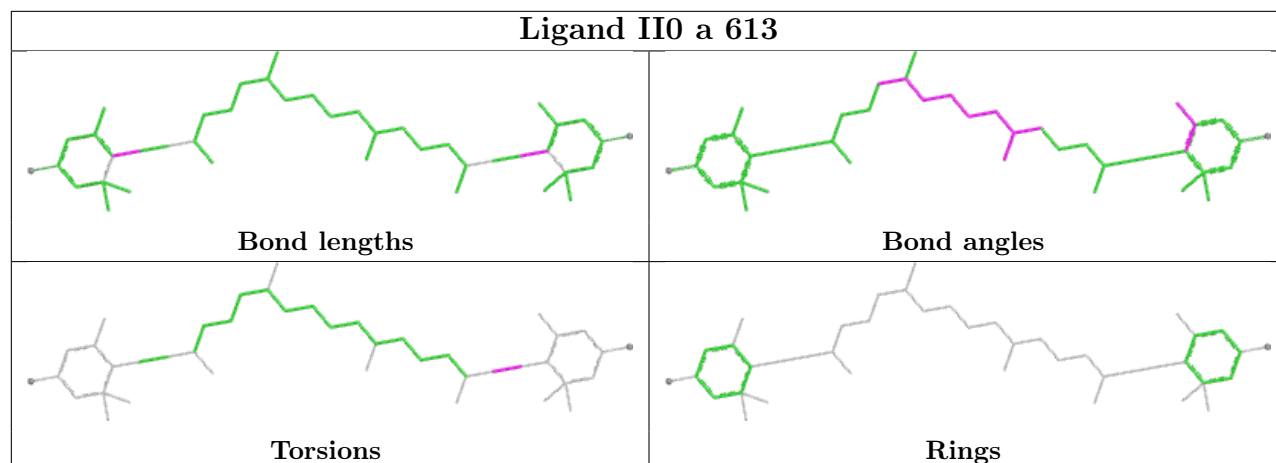


Ligand II0 8 612

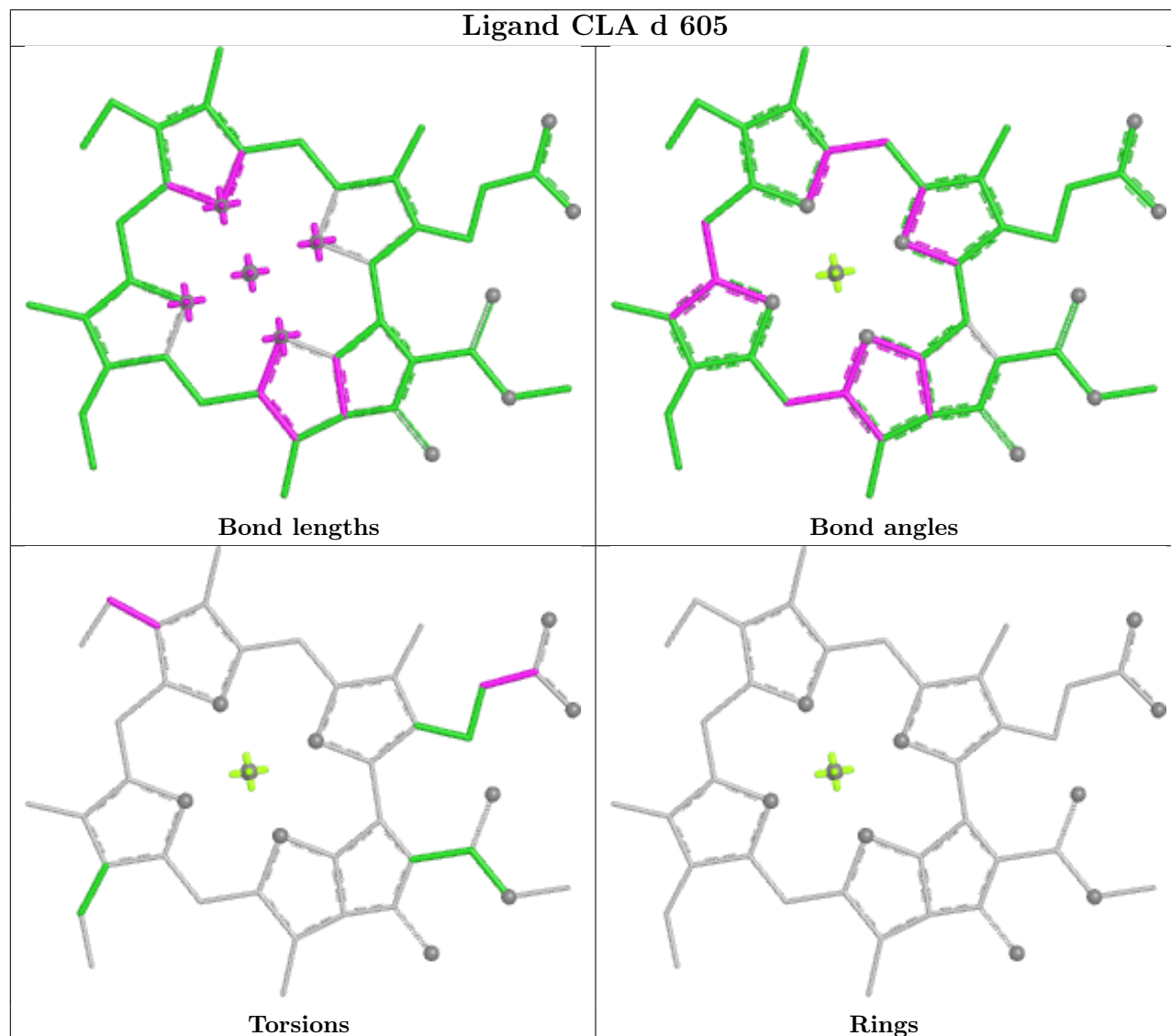


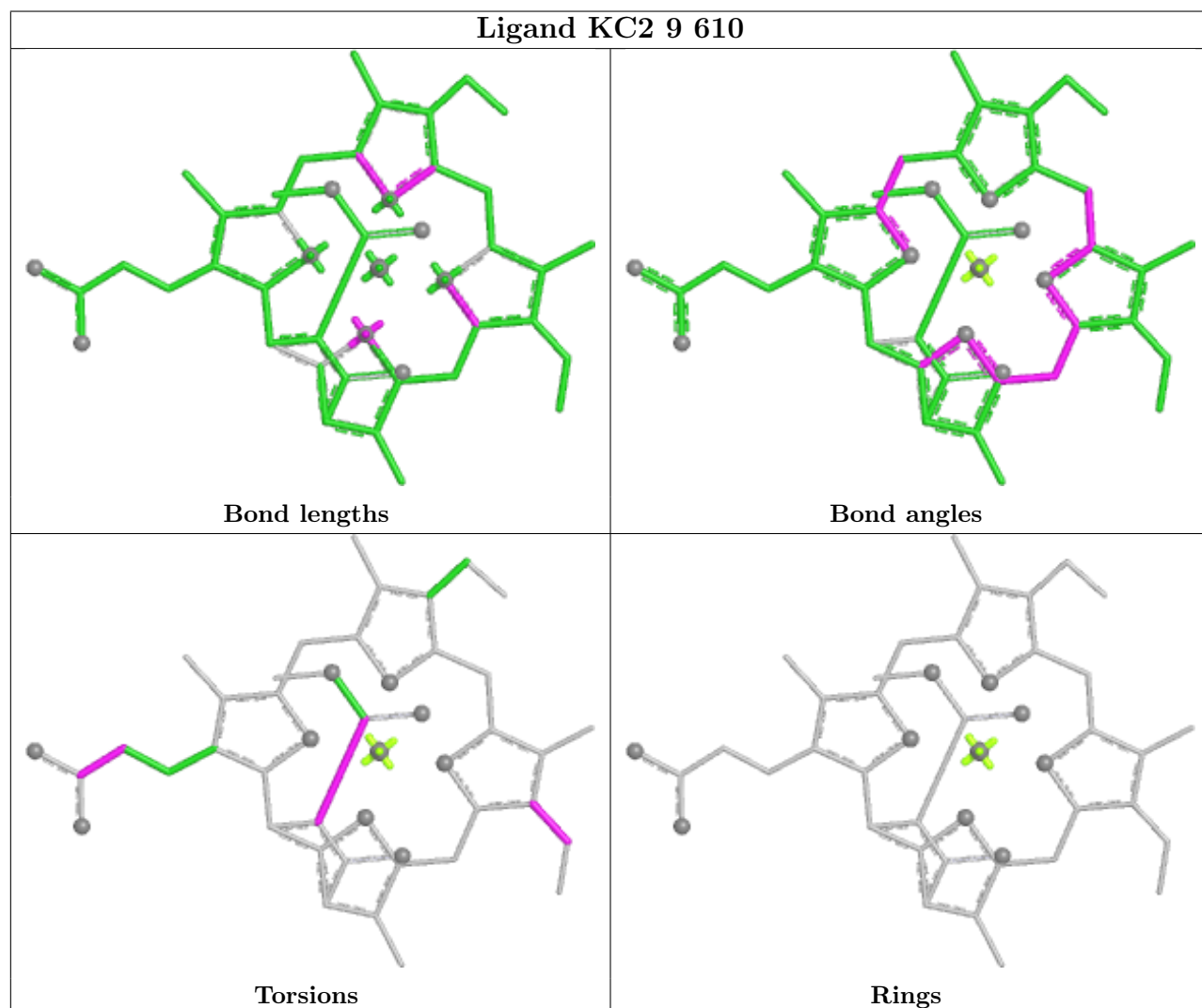
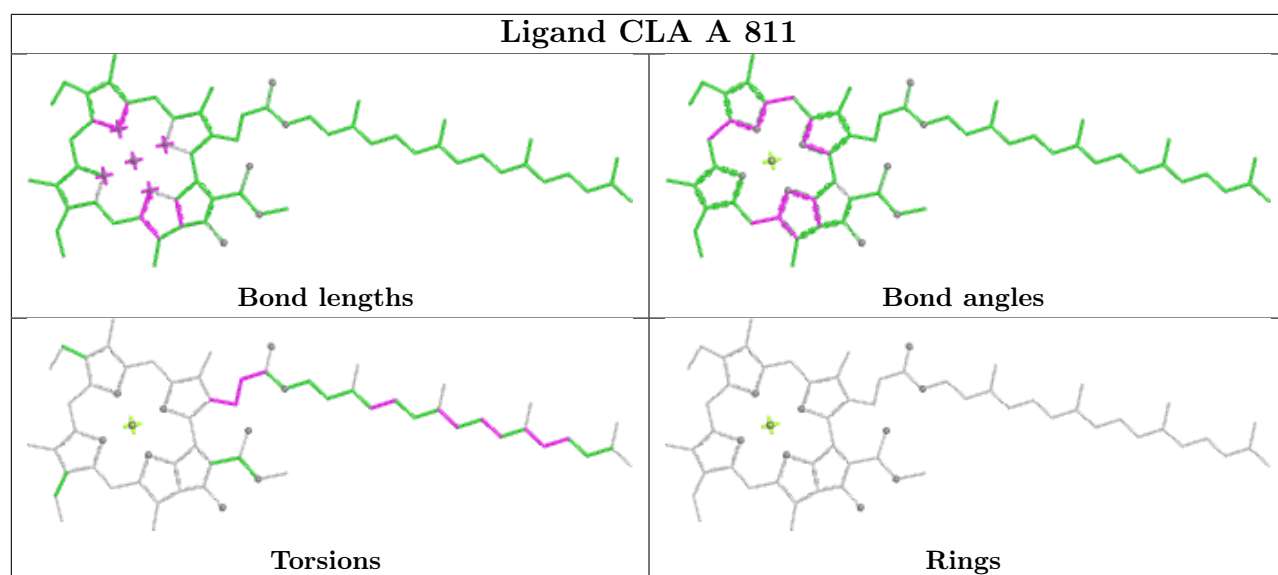


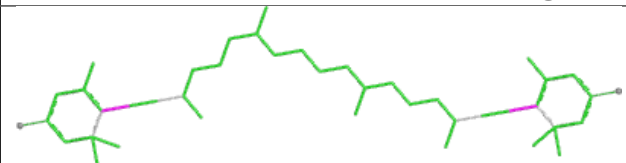
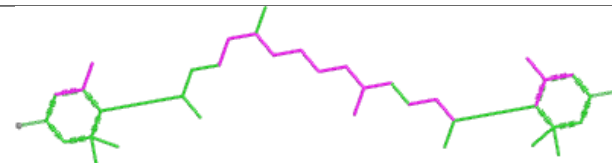
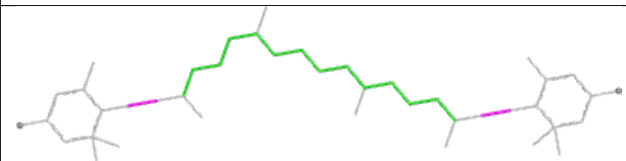
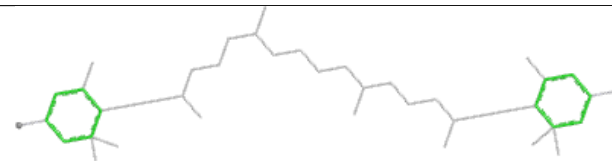
Ligand II0 a 613

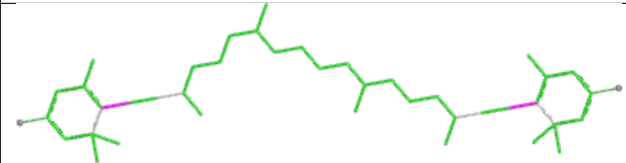
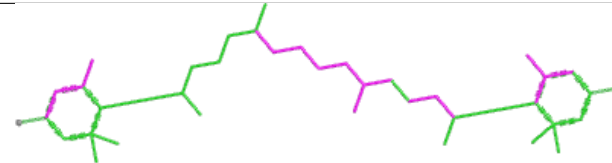
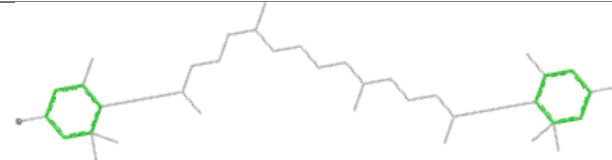


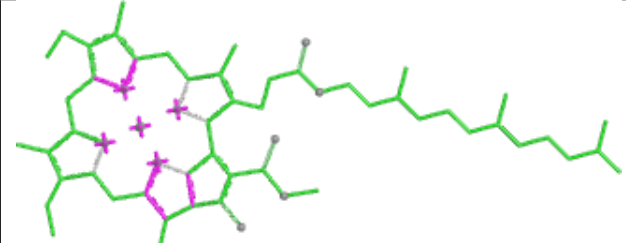
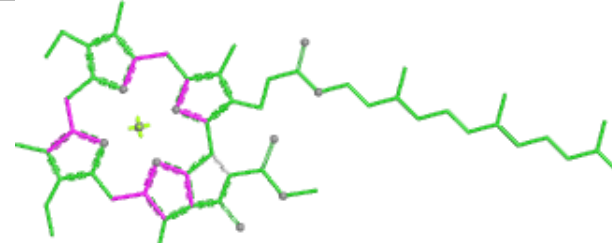
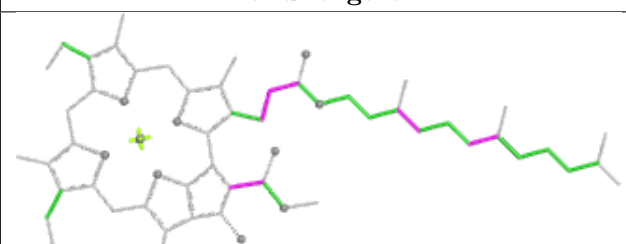
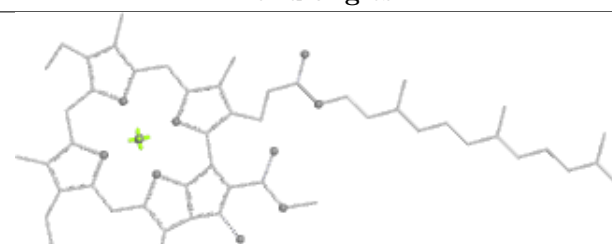
Ligand CLA d 605



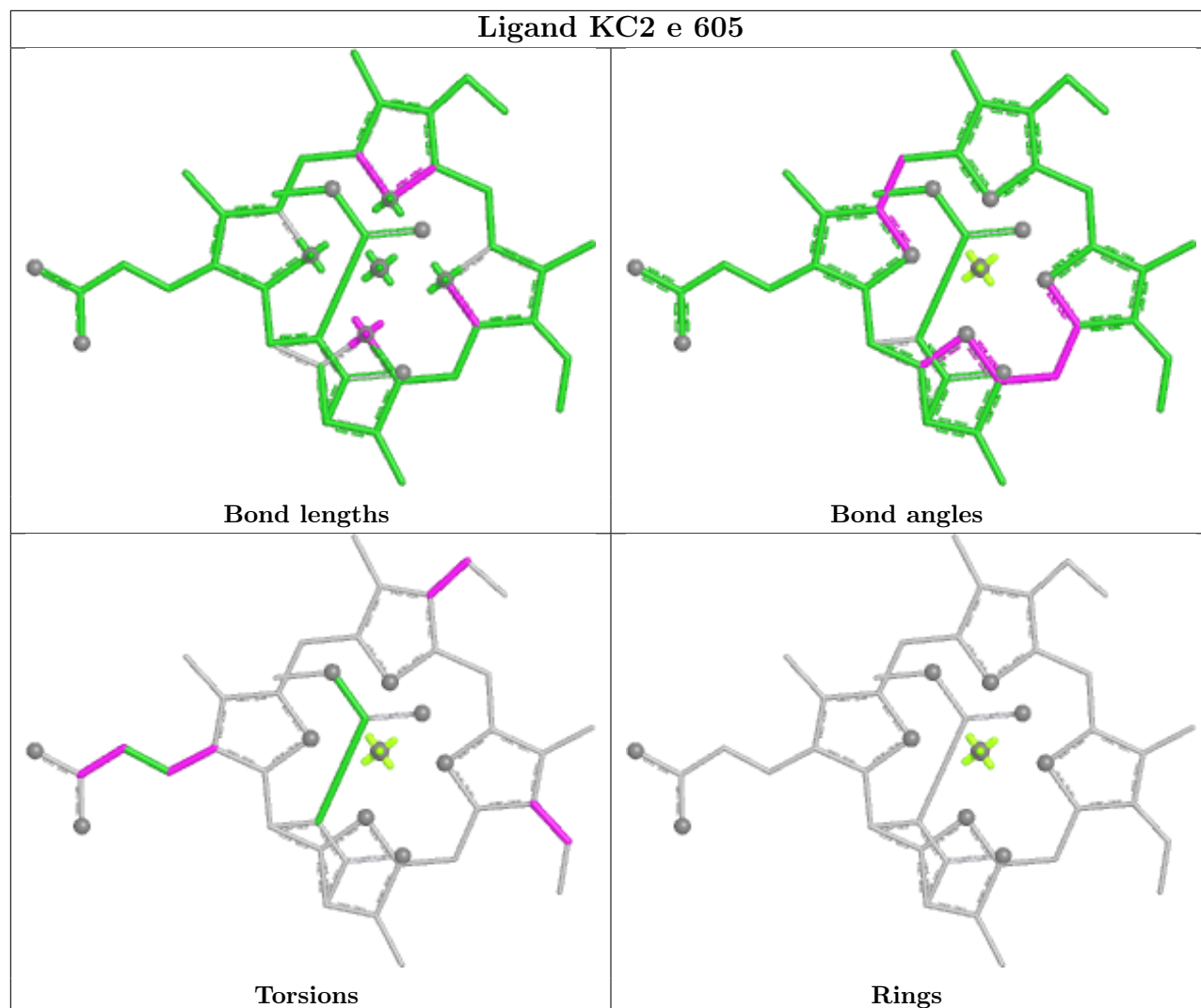


Ligand II0 2 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

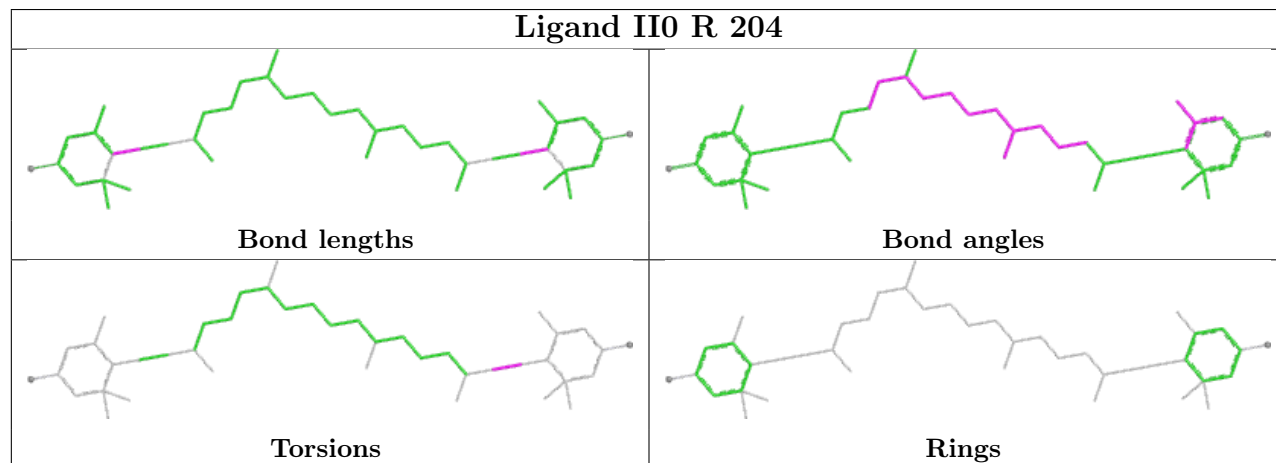
Ligand II0 6 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

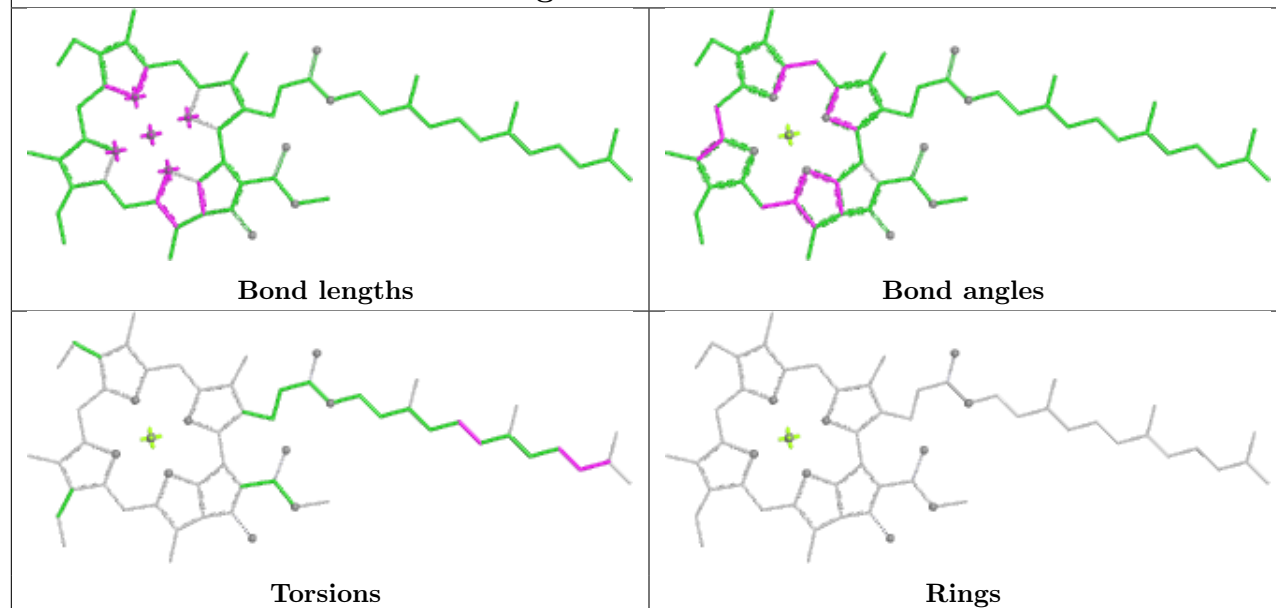
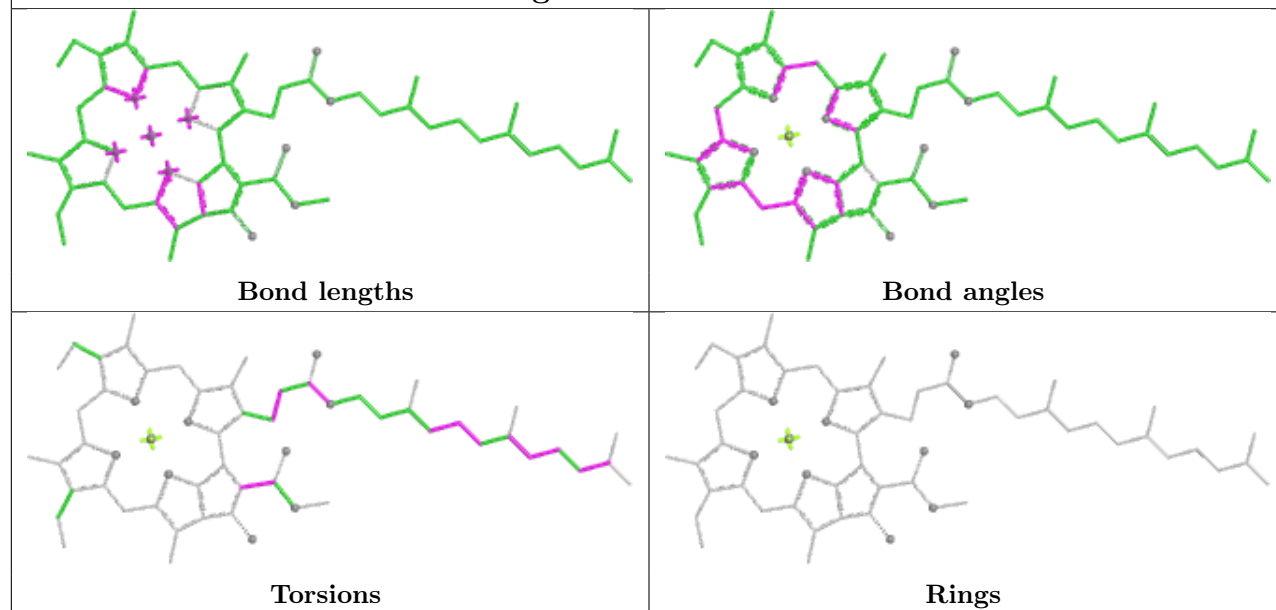
Ligand CLA b 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand KC2 e 605

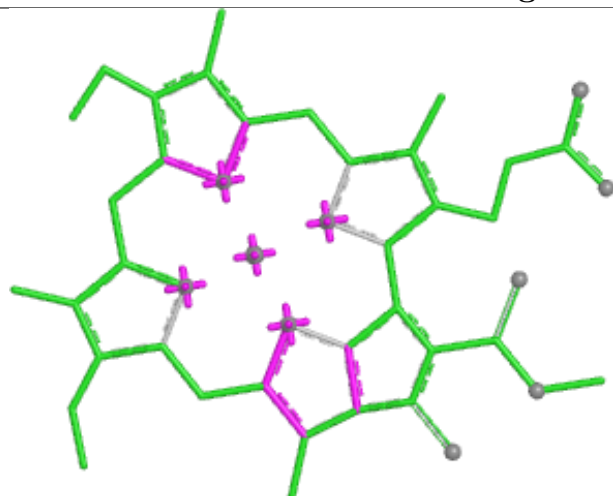


Ligand II0 R 204

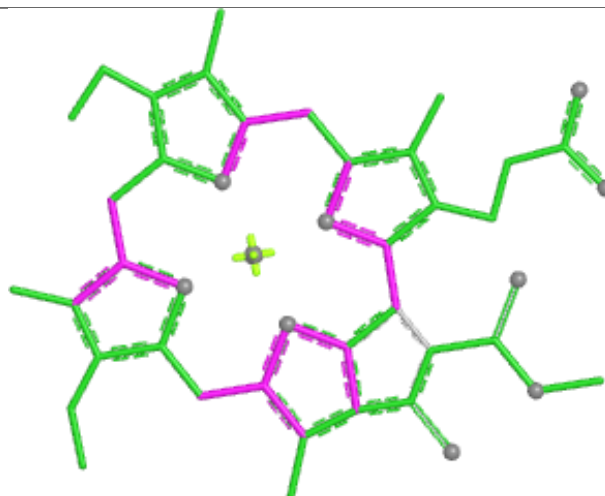


Ligand CLA 3 603**Ligand CLA B 820**

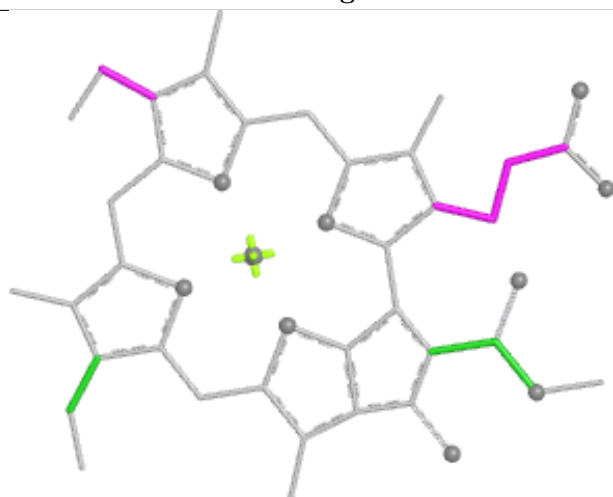
Ligand CLA 6 603



Bond lengths



Bond angles

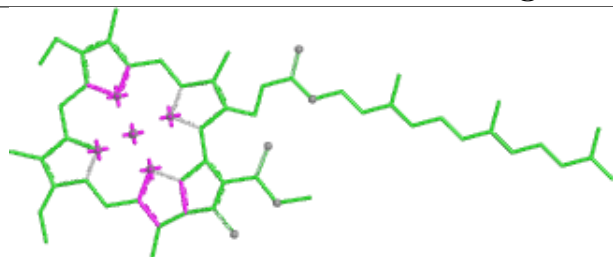


Torsions

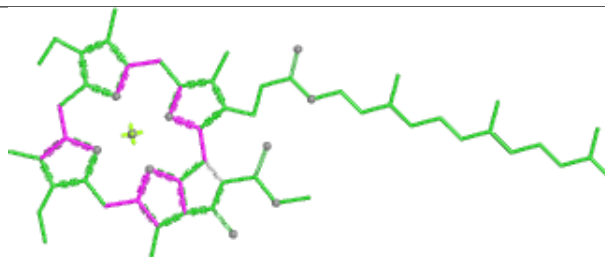


Rings

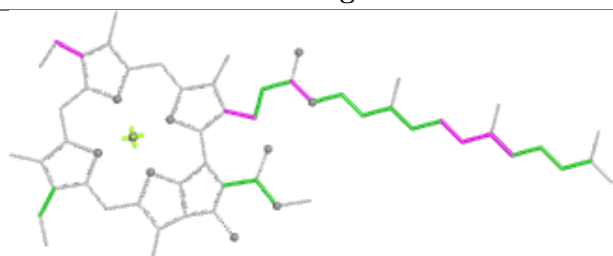
Ligand CLA e 606



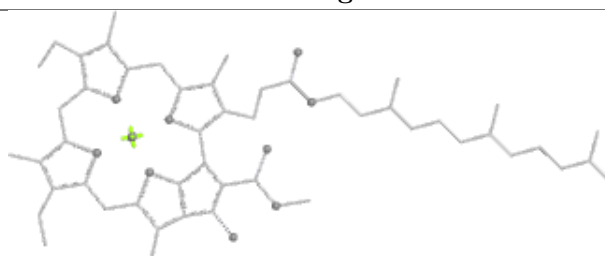
Bond lengths



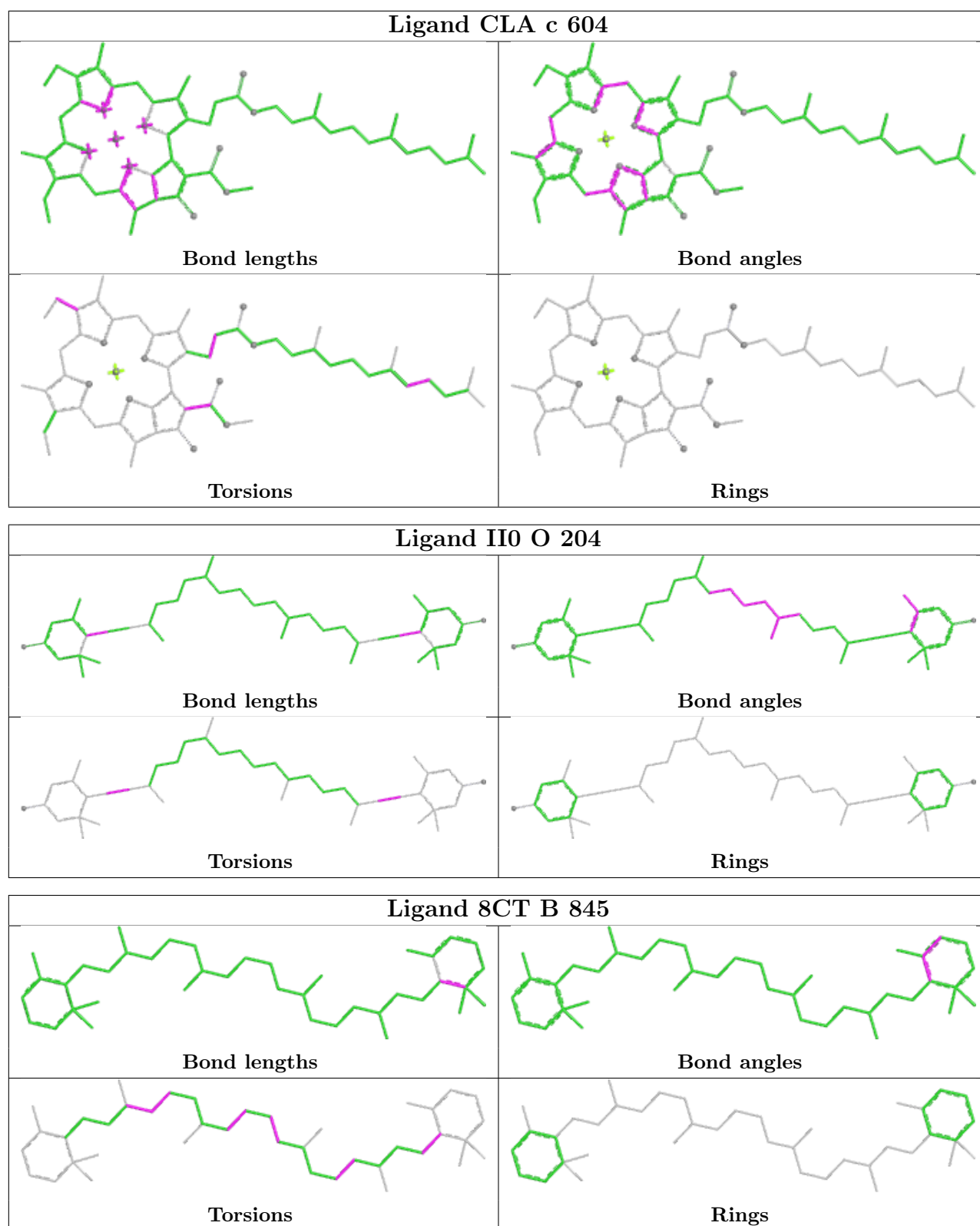
Bond angles

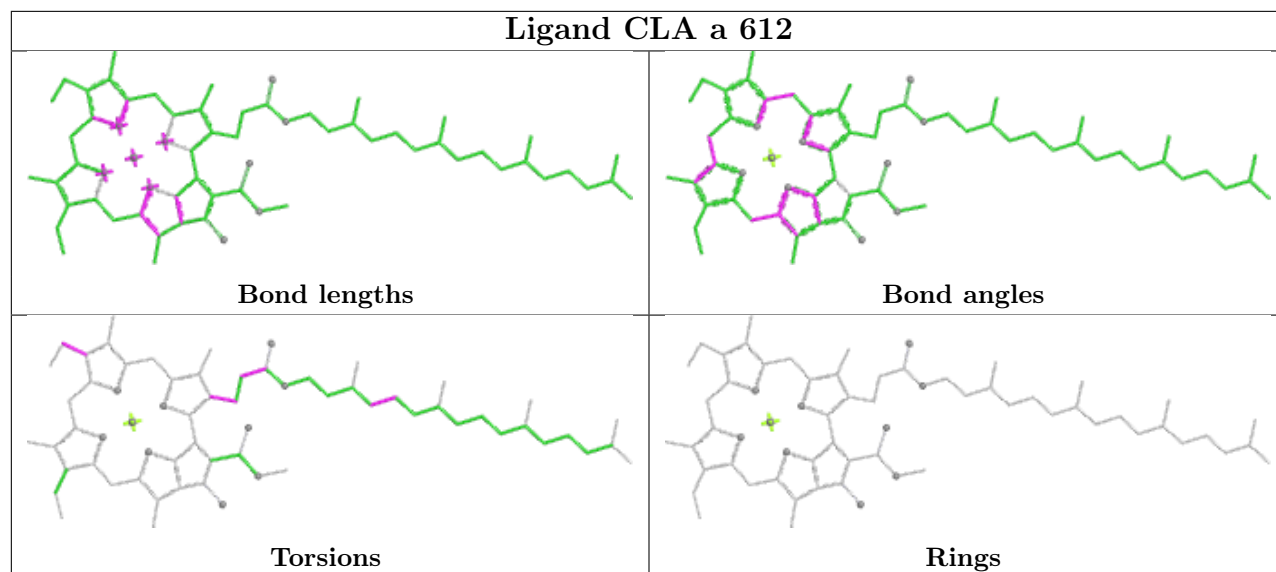
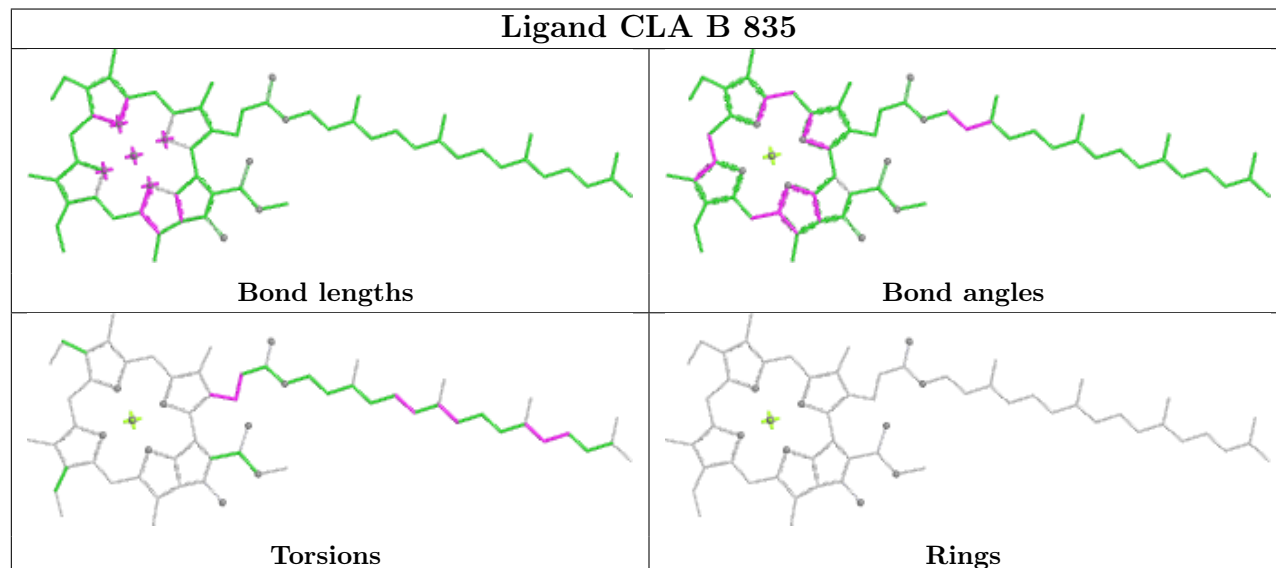


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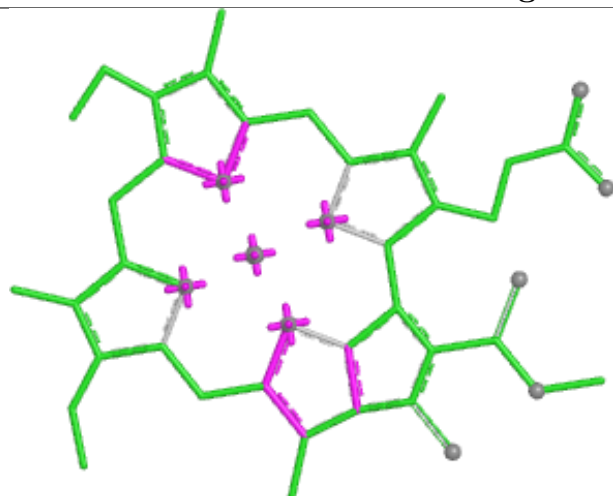


Rings

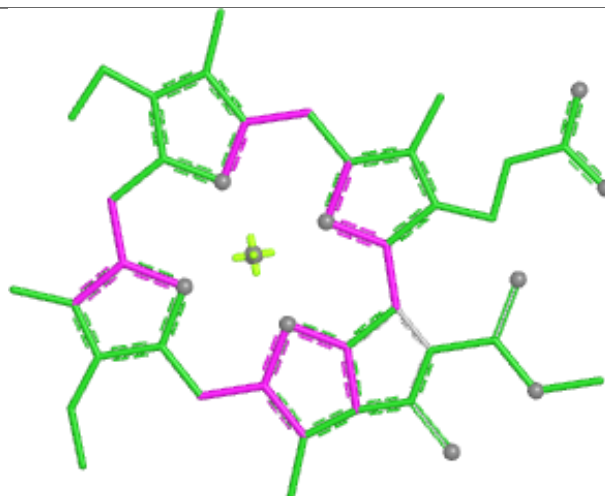


Ligand CLA a 612**Ligand CLA B 835**

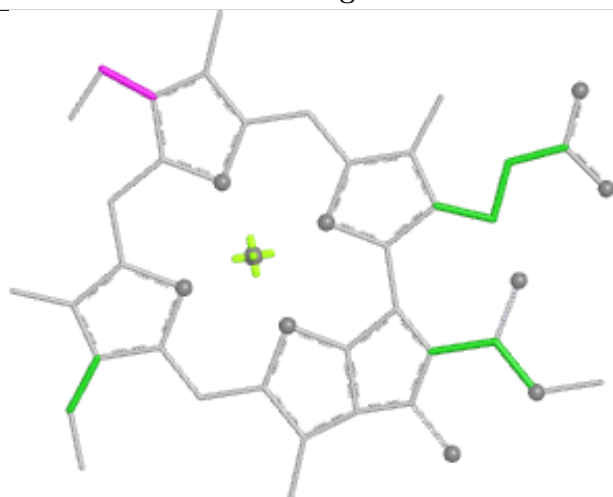
Ligand CLA 2 607



Bond lengths



Bond angles

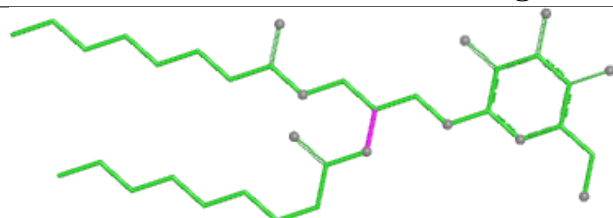


Torsions

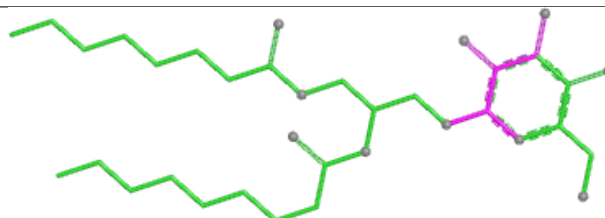


Rings

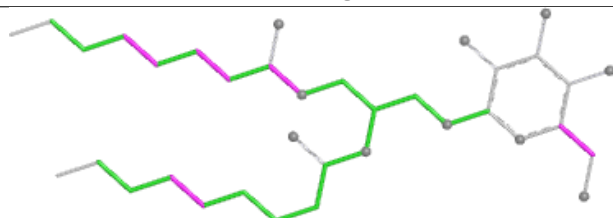
Ligand LMG 2 617



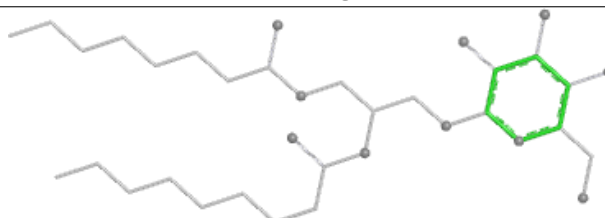
Bond lengths



Bond angles

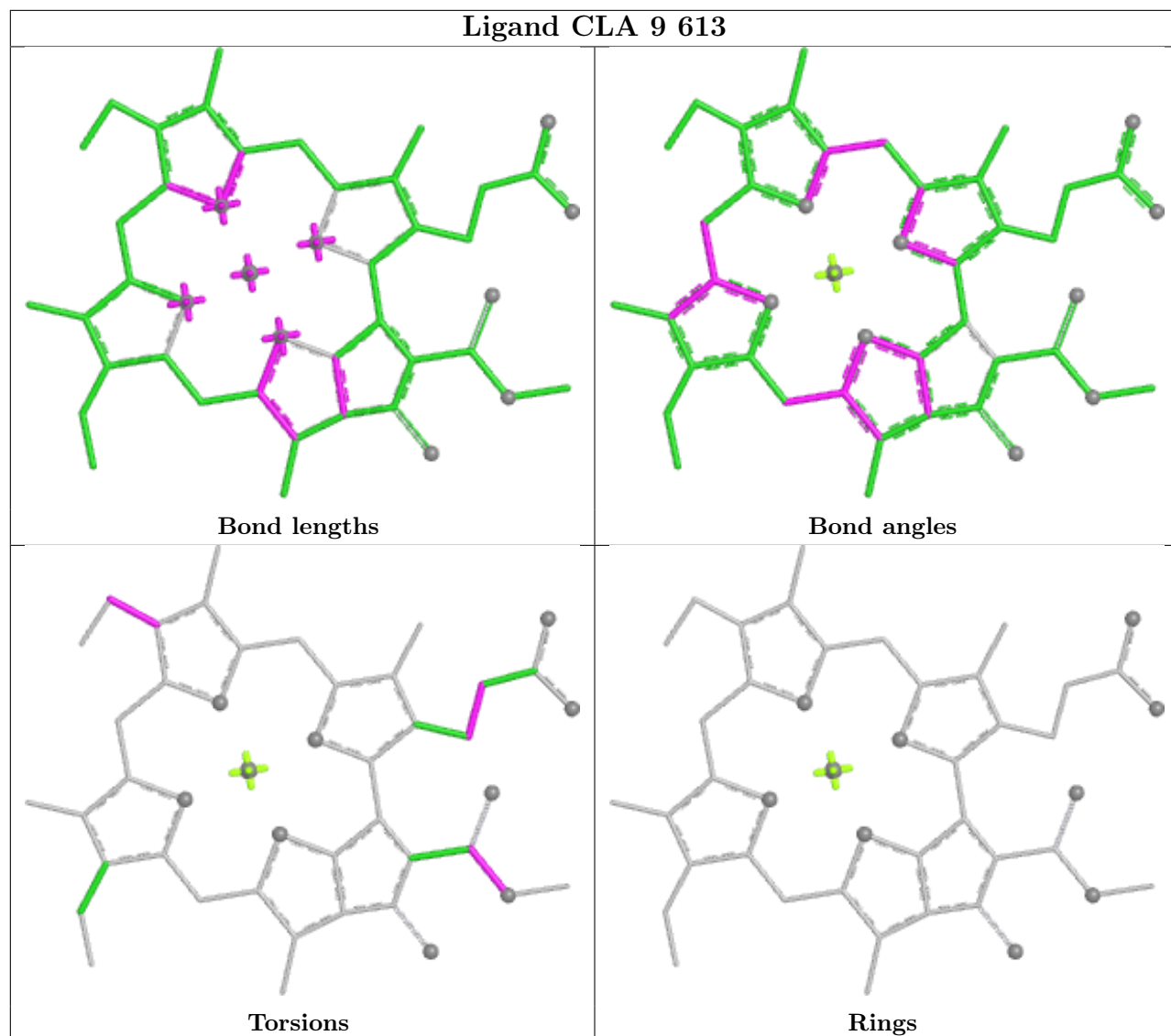


Torsions

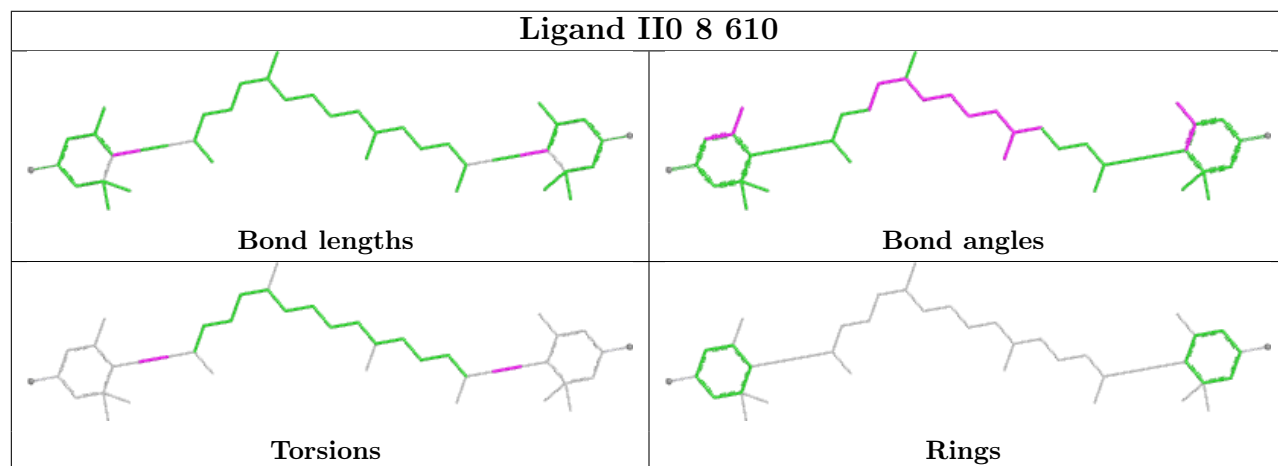


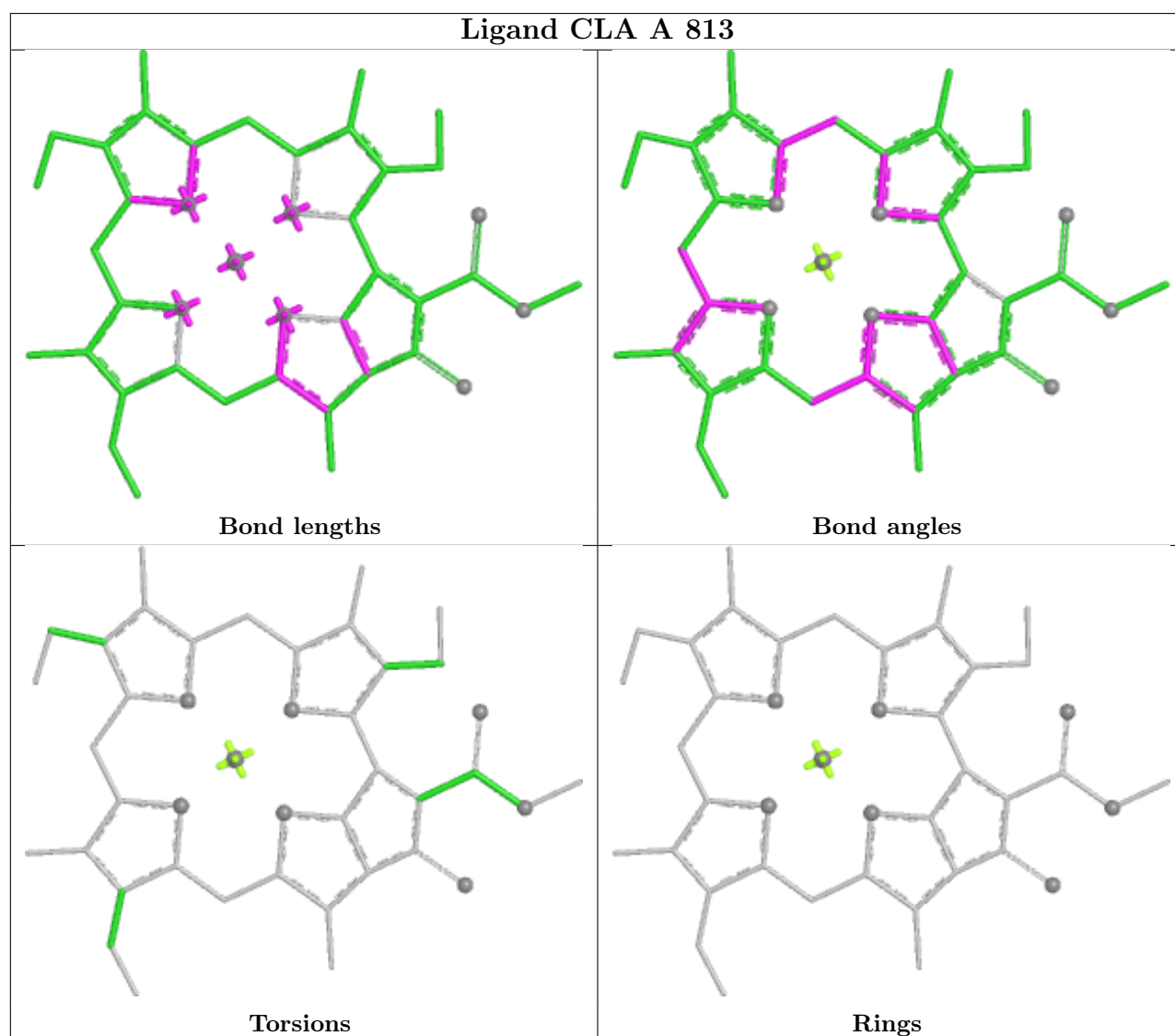
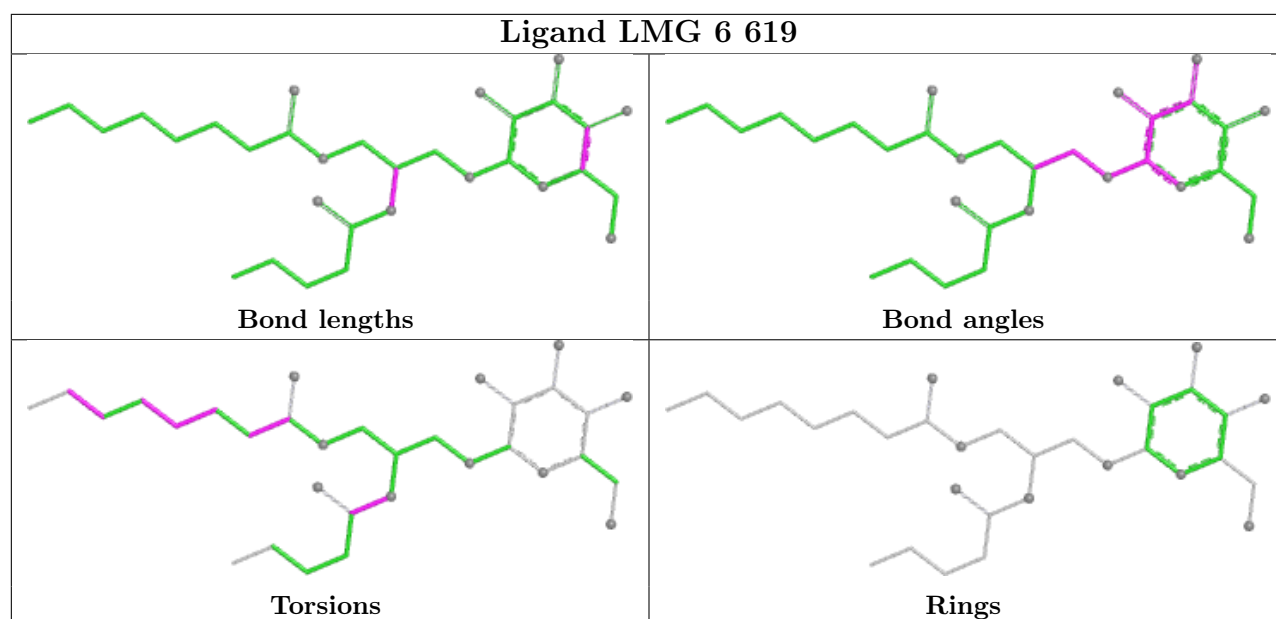
Rings

Ligand CLA 9 613

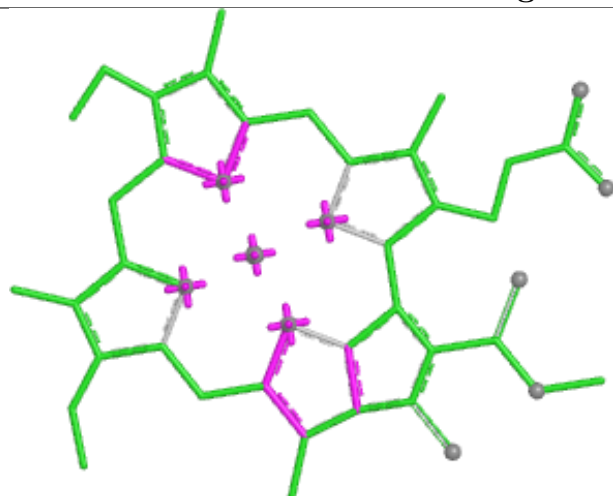


Ligand II0 8 610

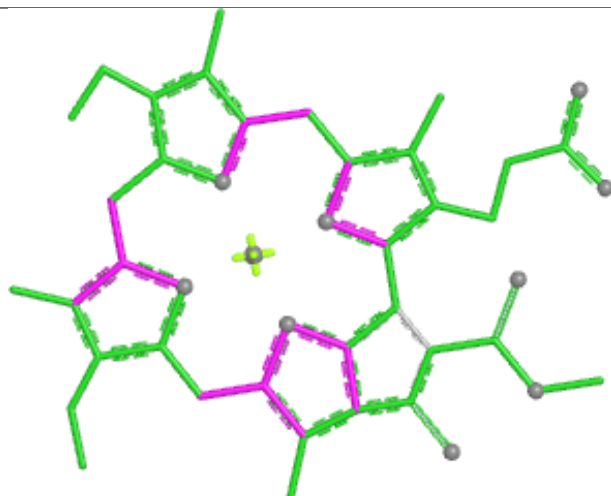




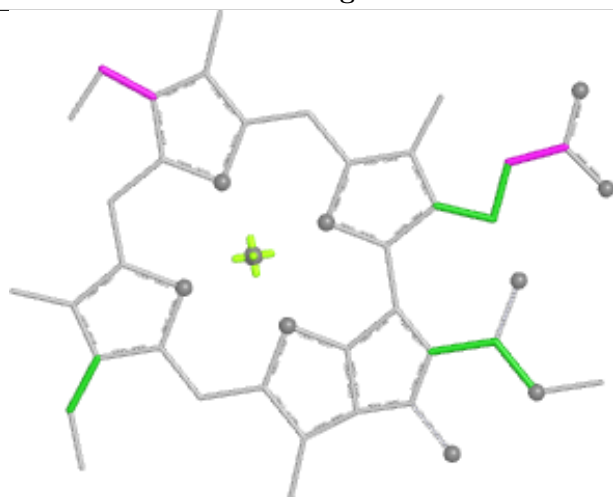
Ligand CLA d 601



Bond lengths



Bond angles

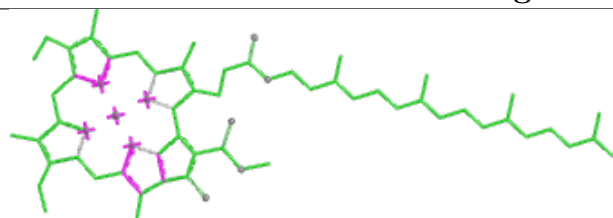


Torsions

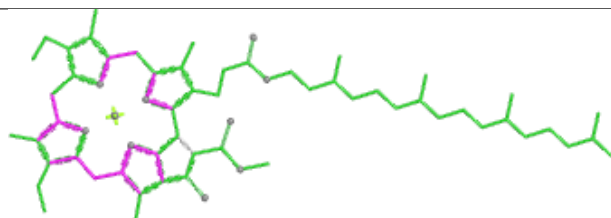


Rings

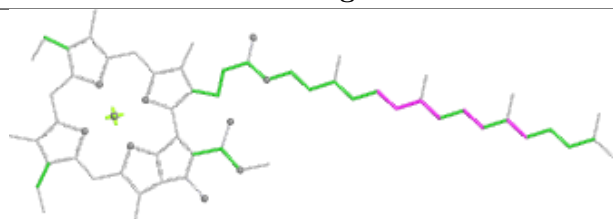
Ligand CLA A 825



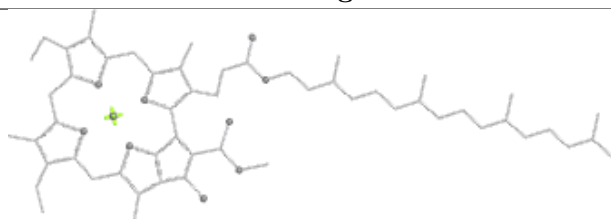
Bond lengths



Bond angles

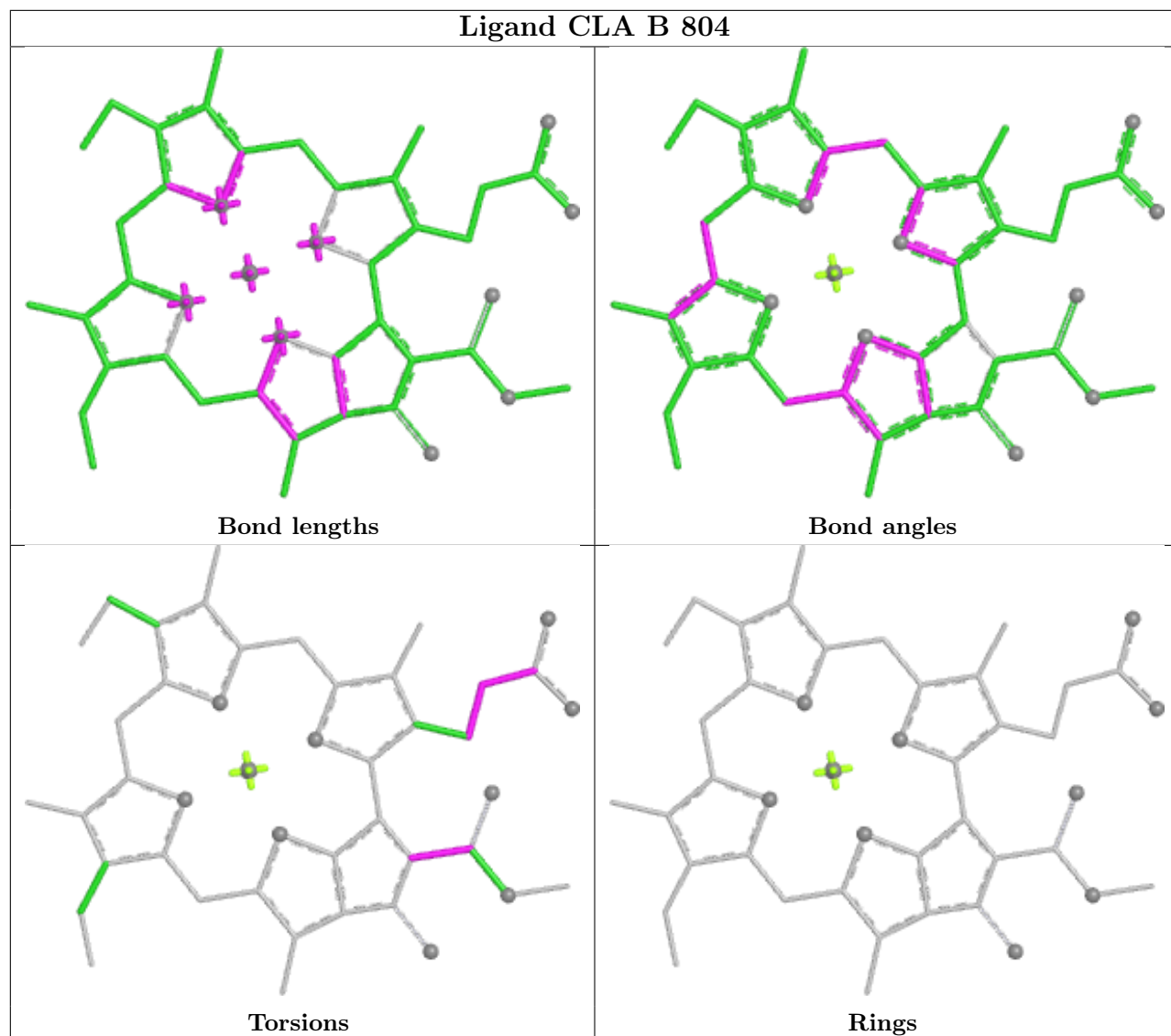


Torsions

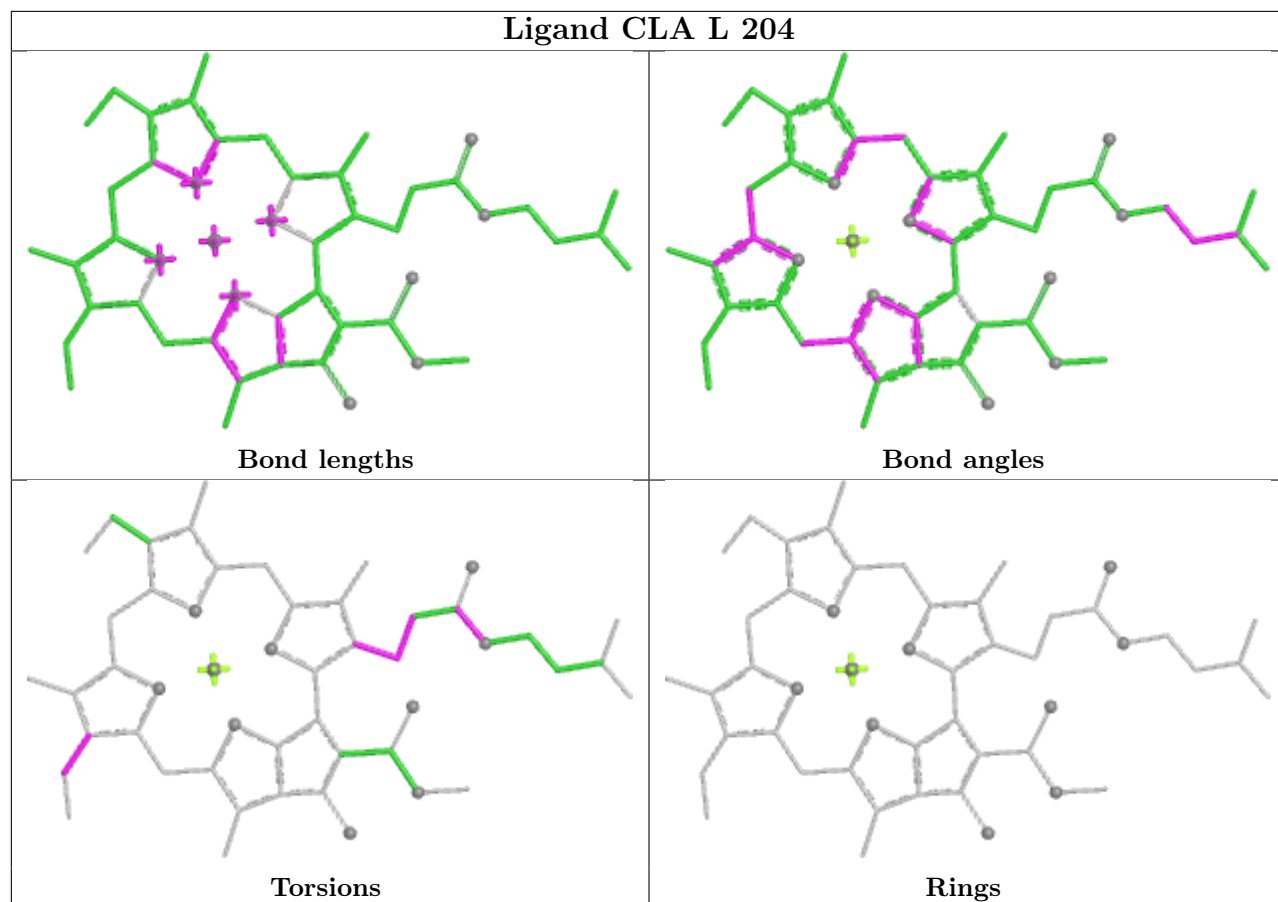


Rings

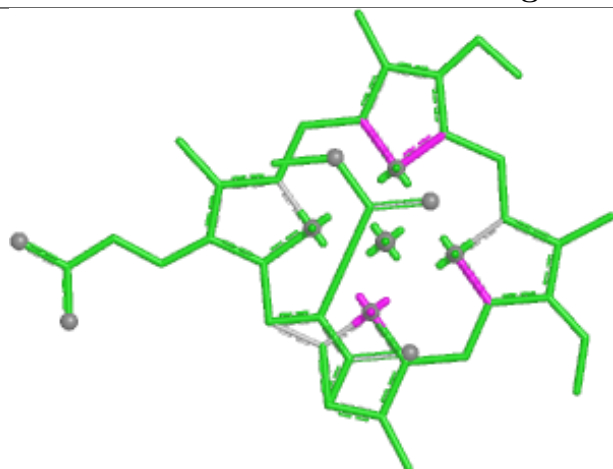
Ligand CLA B 804



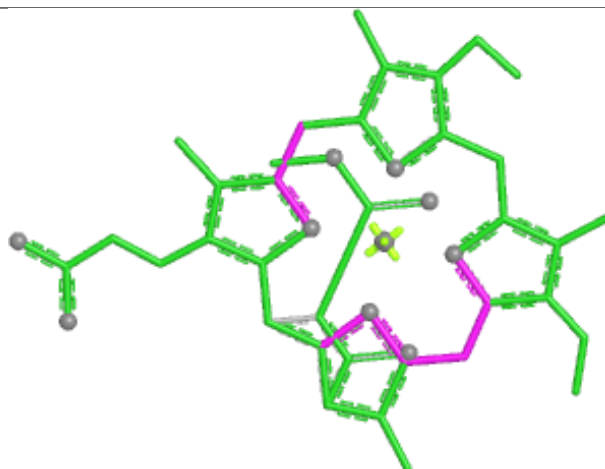
Ligand CLA L 204



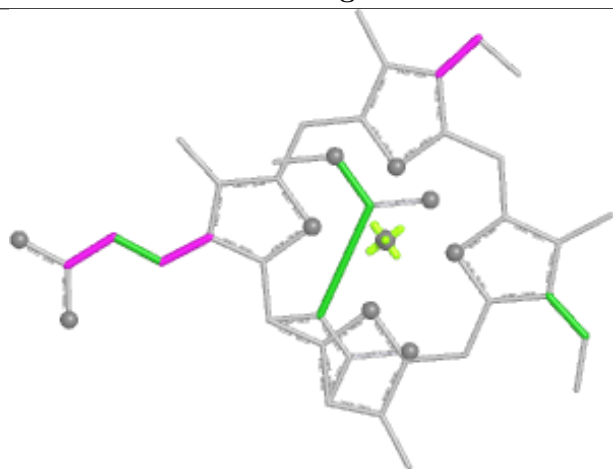
Ligand KC2 c 615



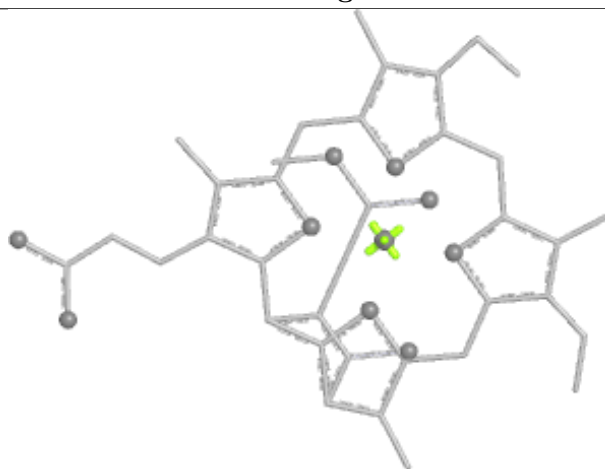
Bond lengths



Bond angles

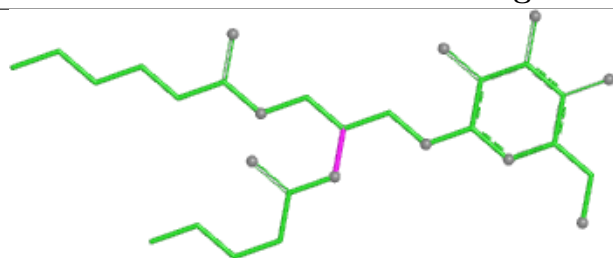


Torsions

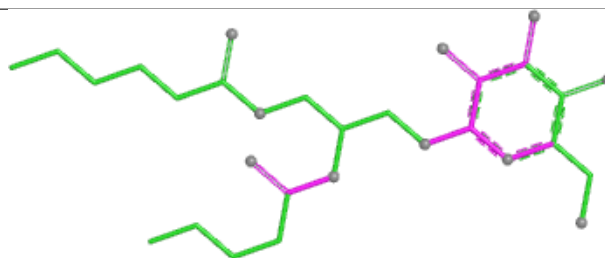


Rings

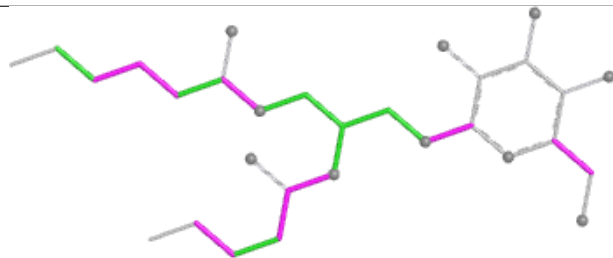
Ligand LMG 3 618



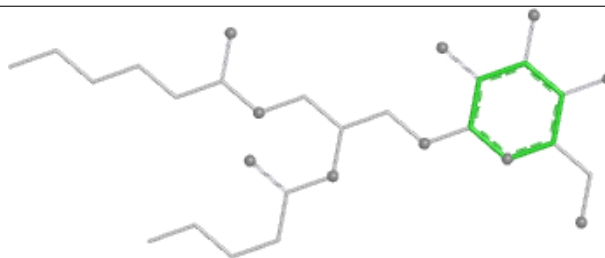
Bond lengths



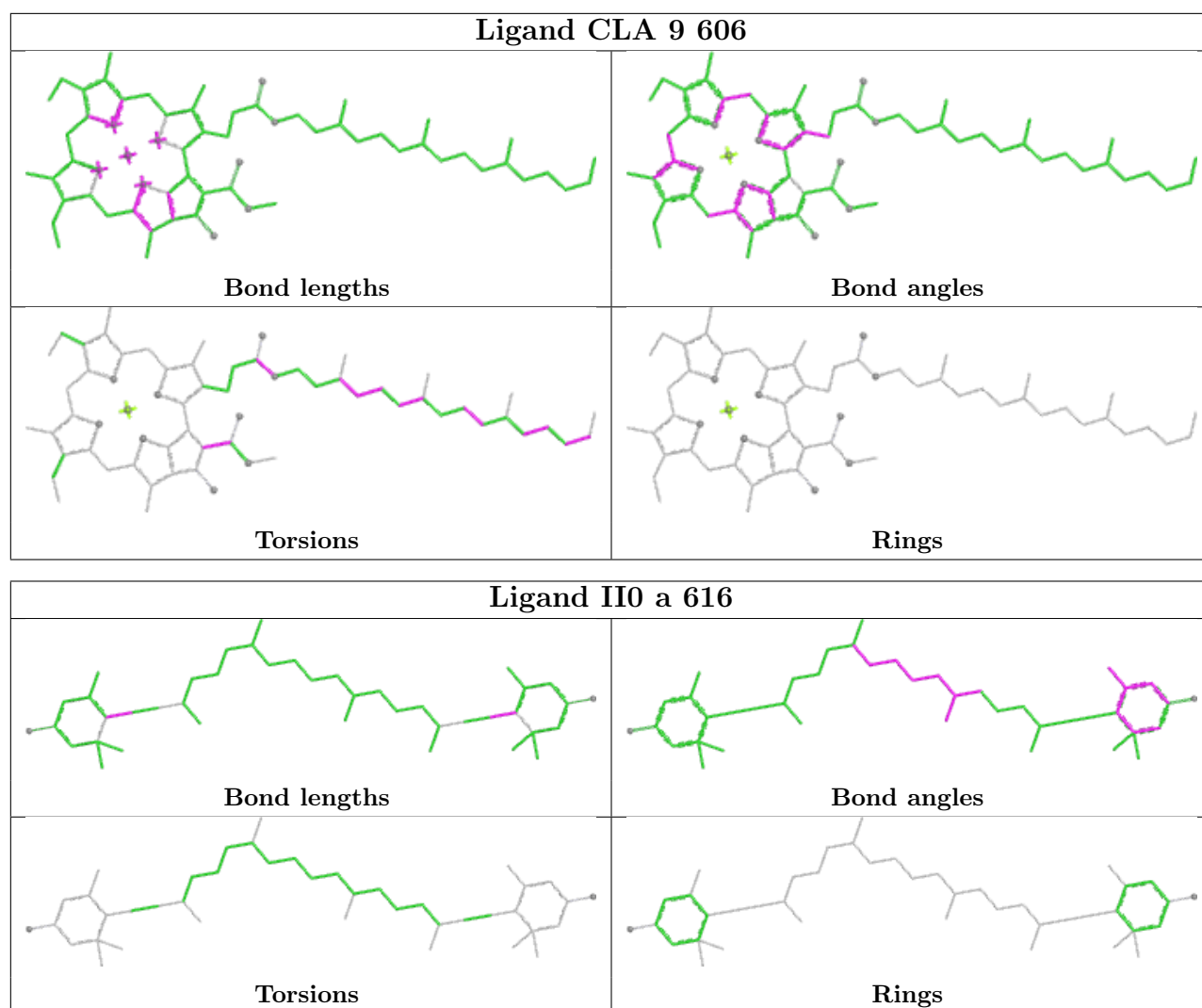
Bond angles



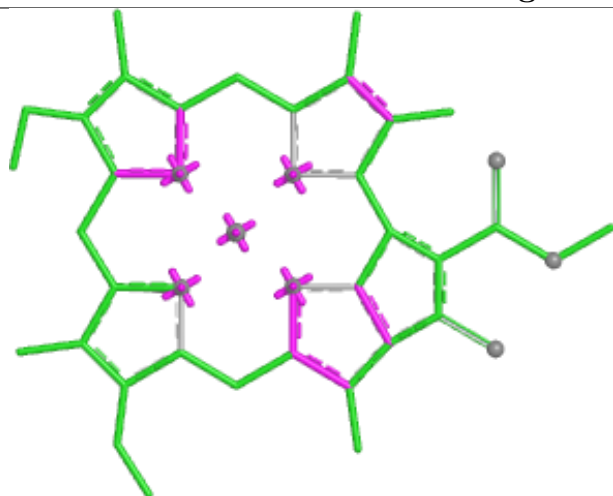
Torsions



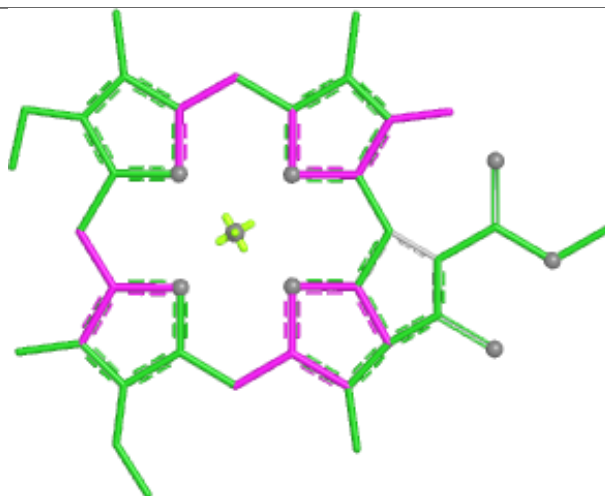
Rings



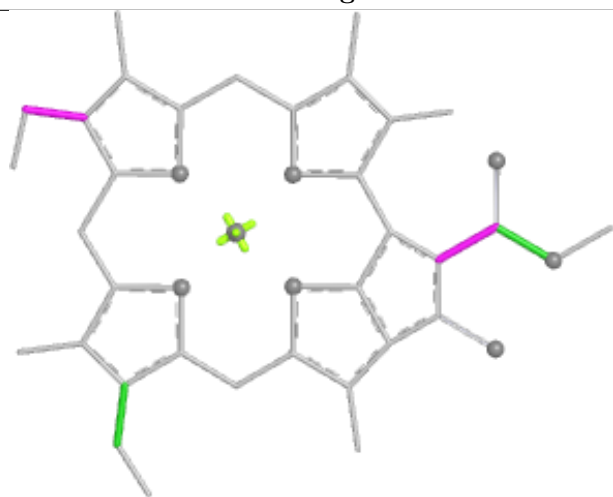
Ligand CLA 8 607



Bond lengths



Bond angles

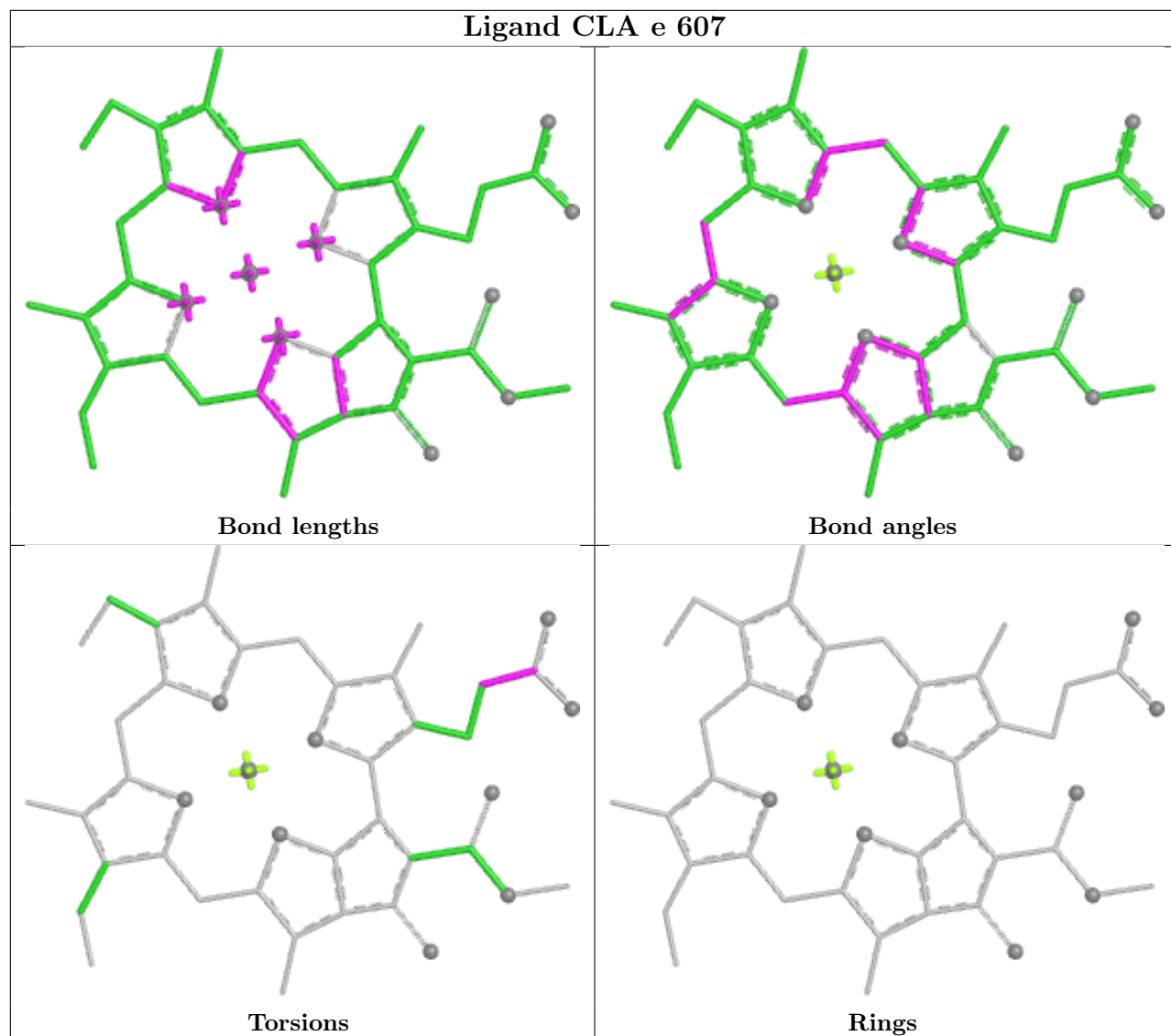


Torsions

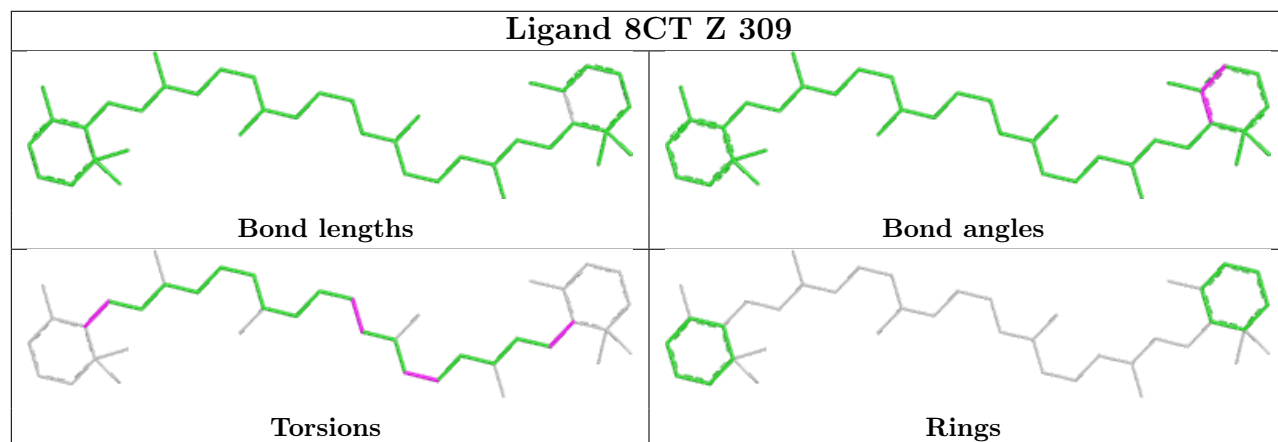


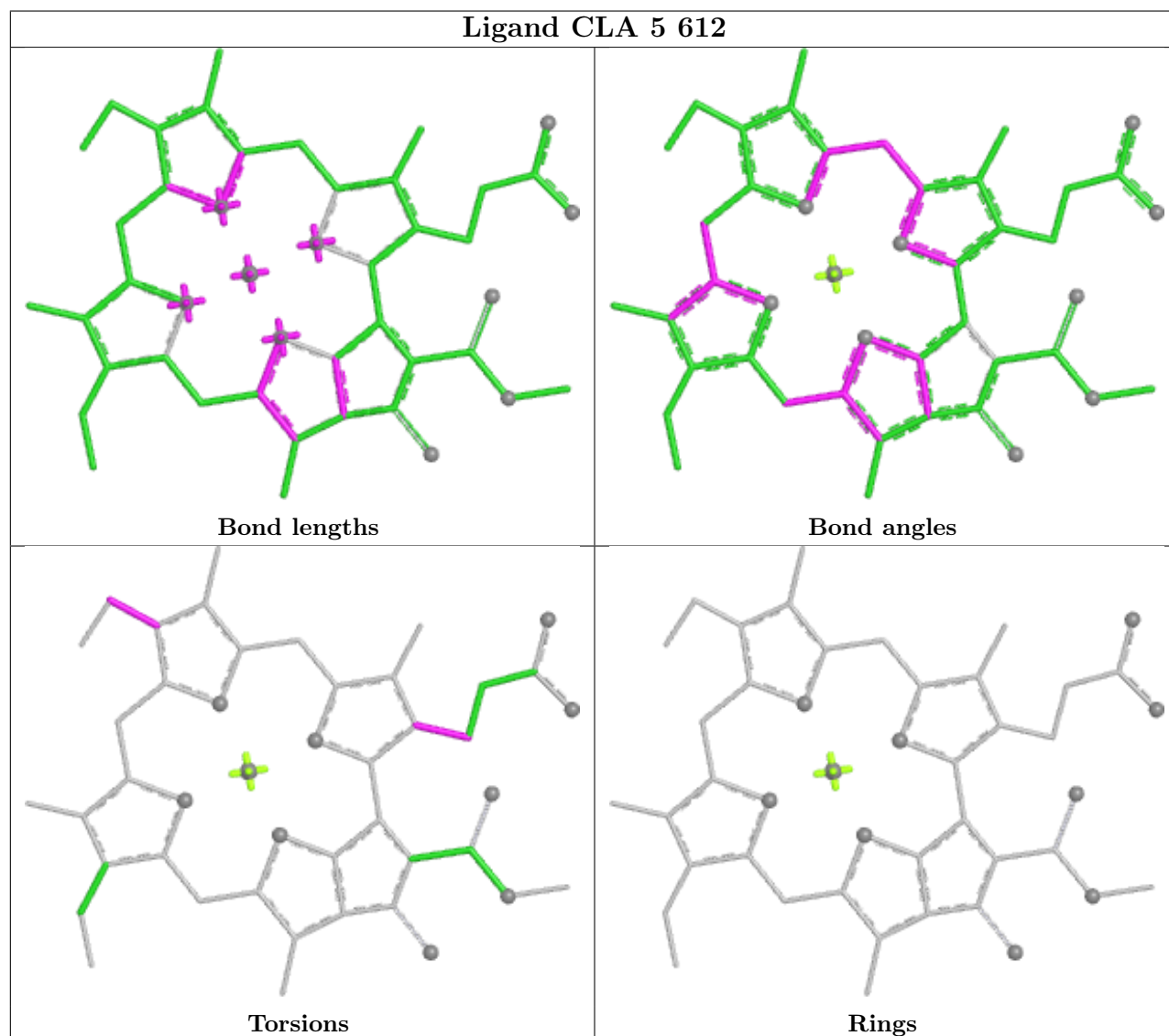
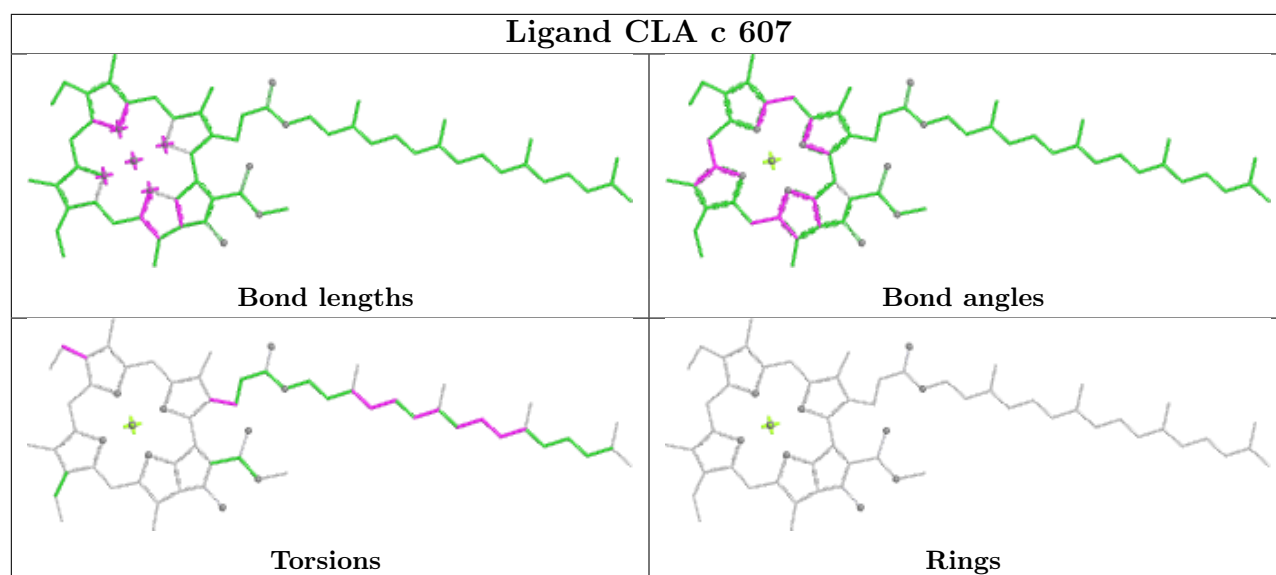
Rings

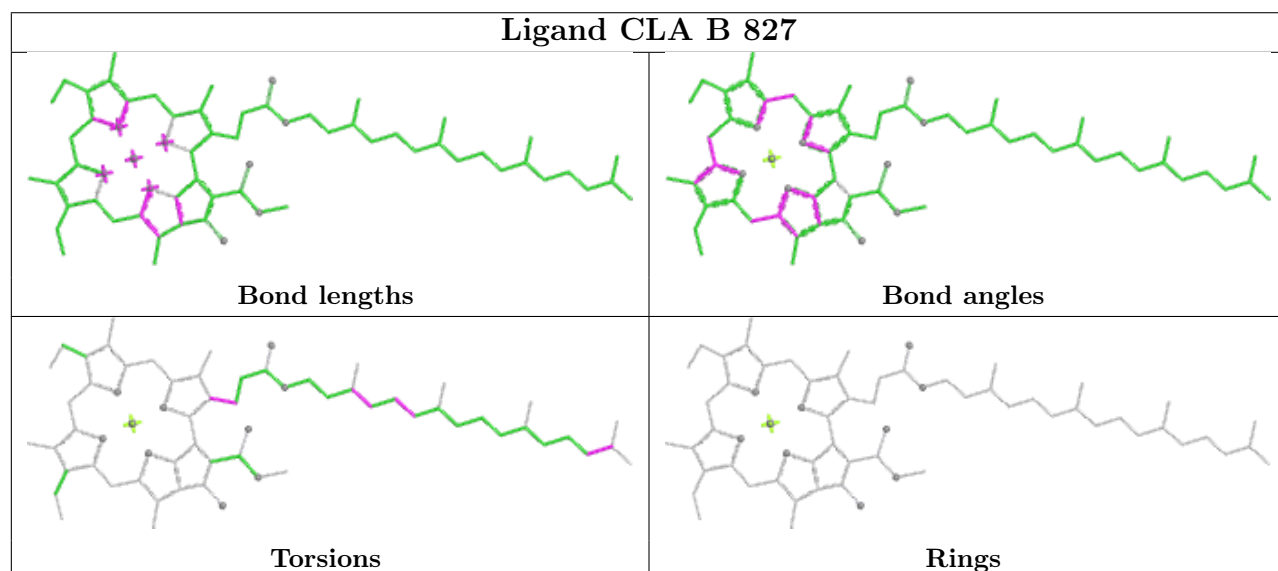
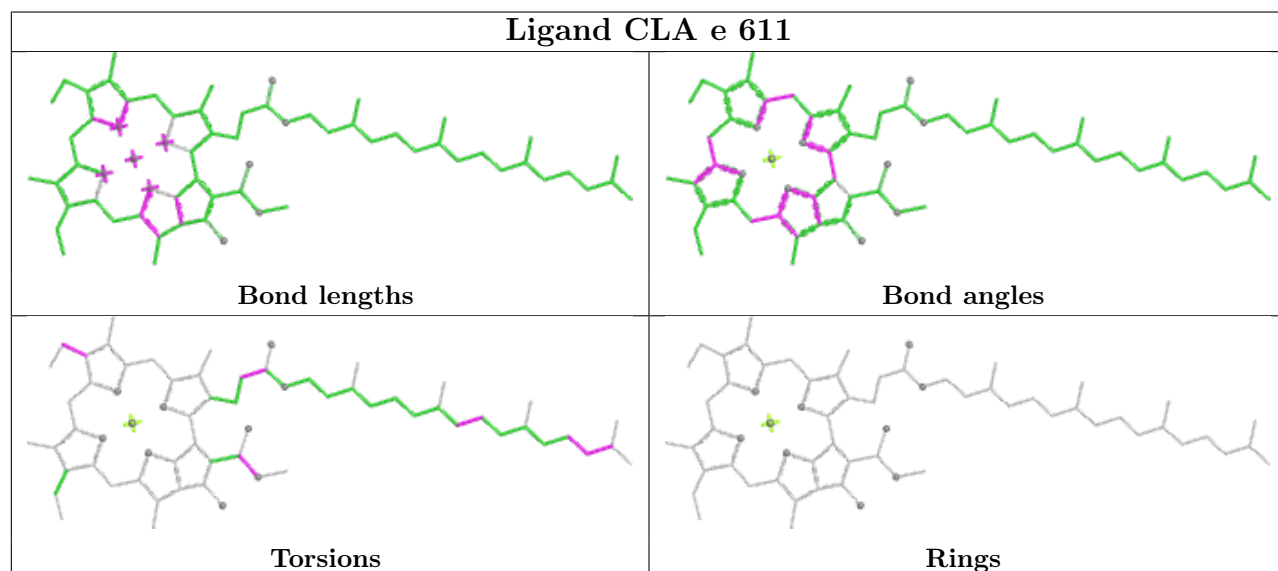
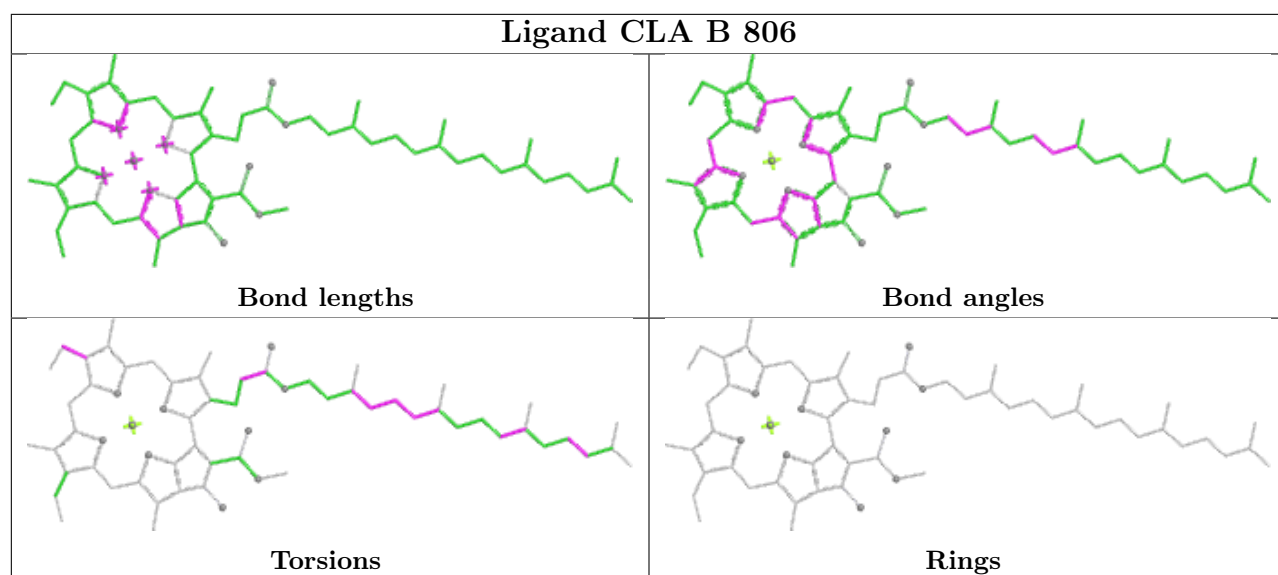
Ligand CLA e 607

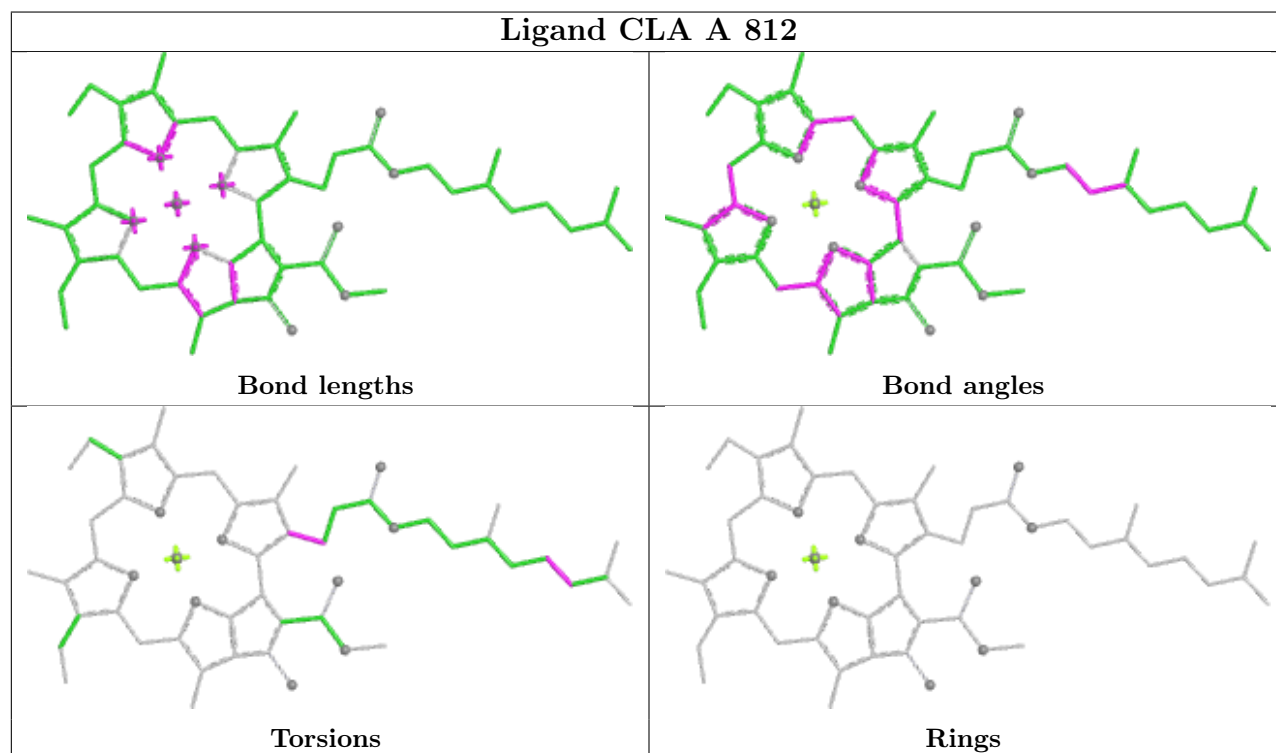
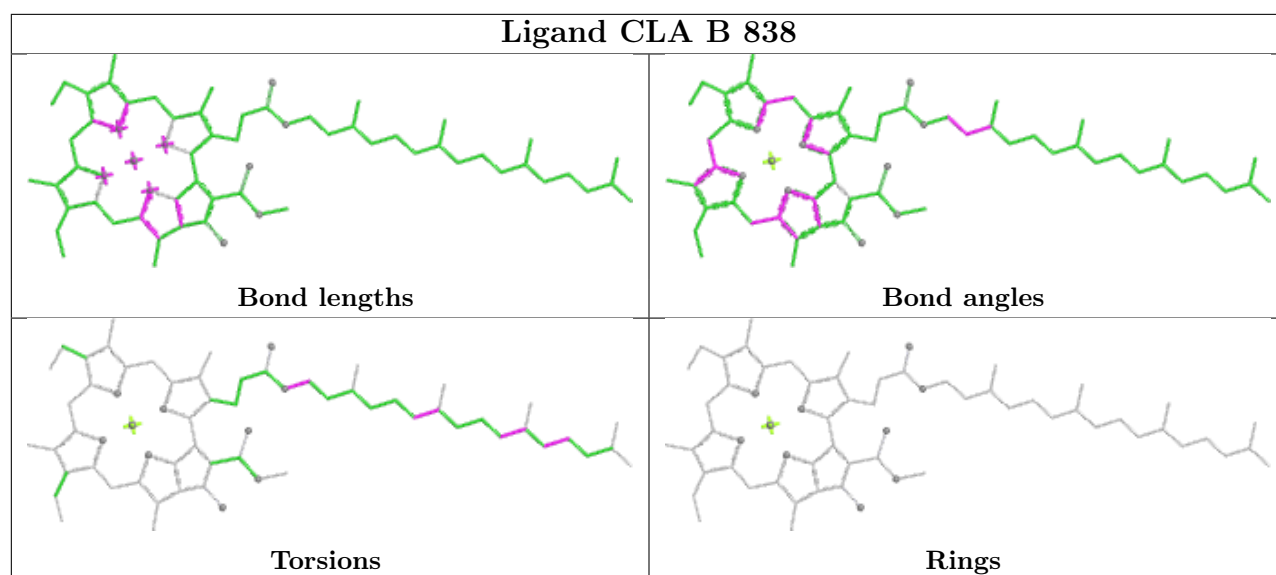


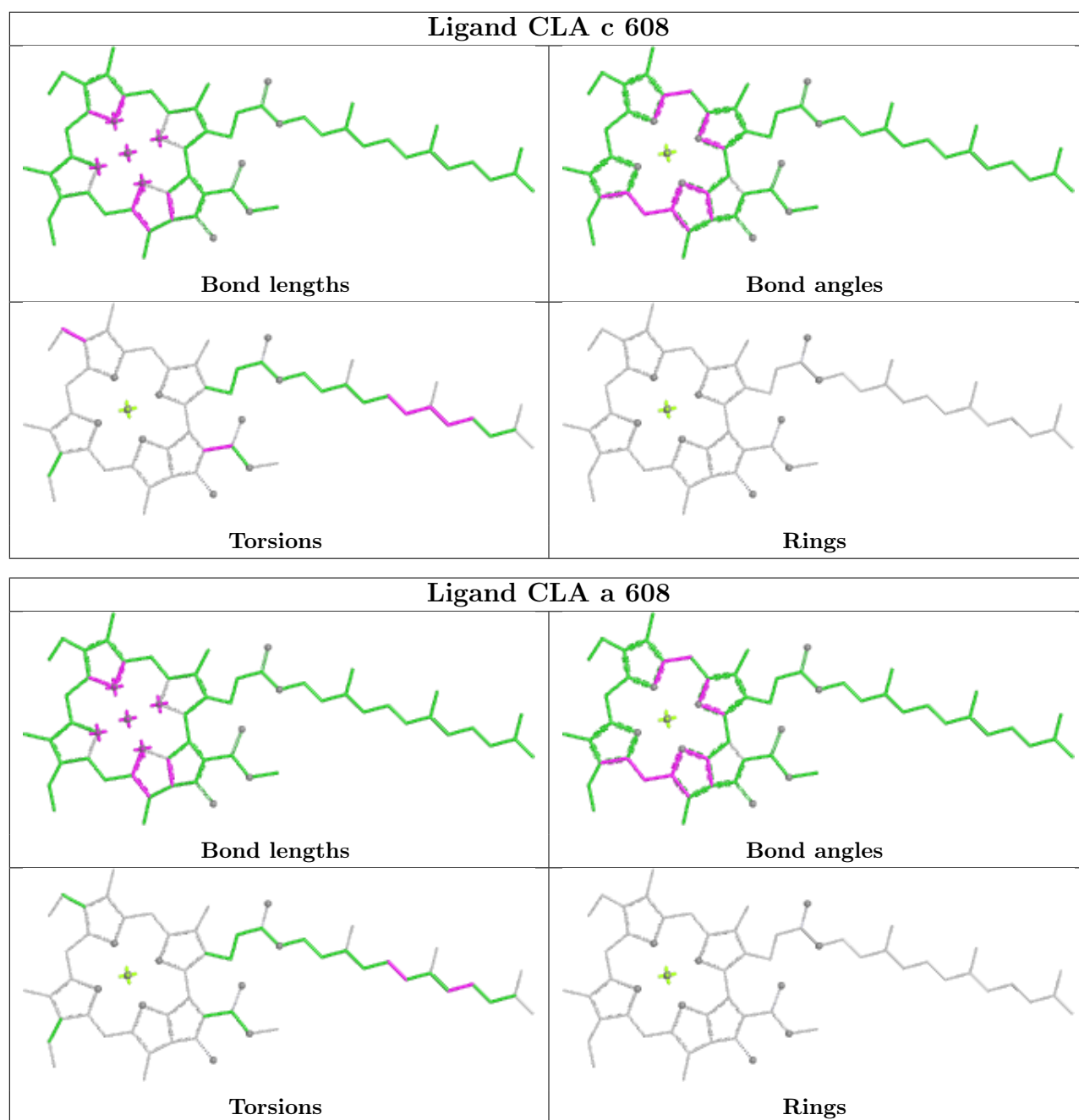
Ligand 8CT Z 309

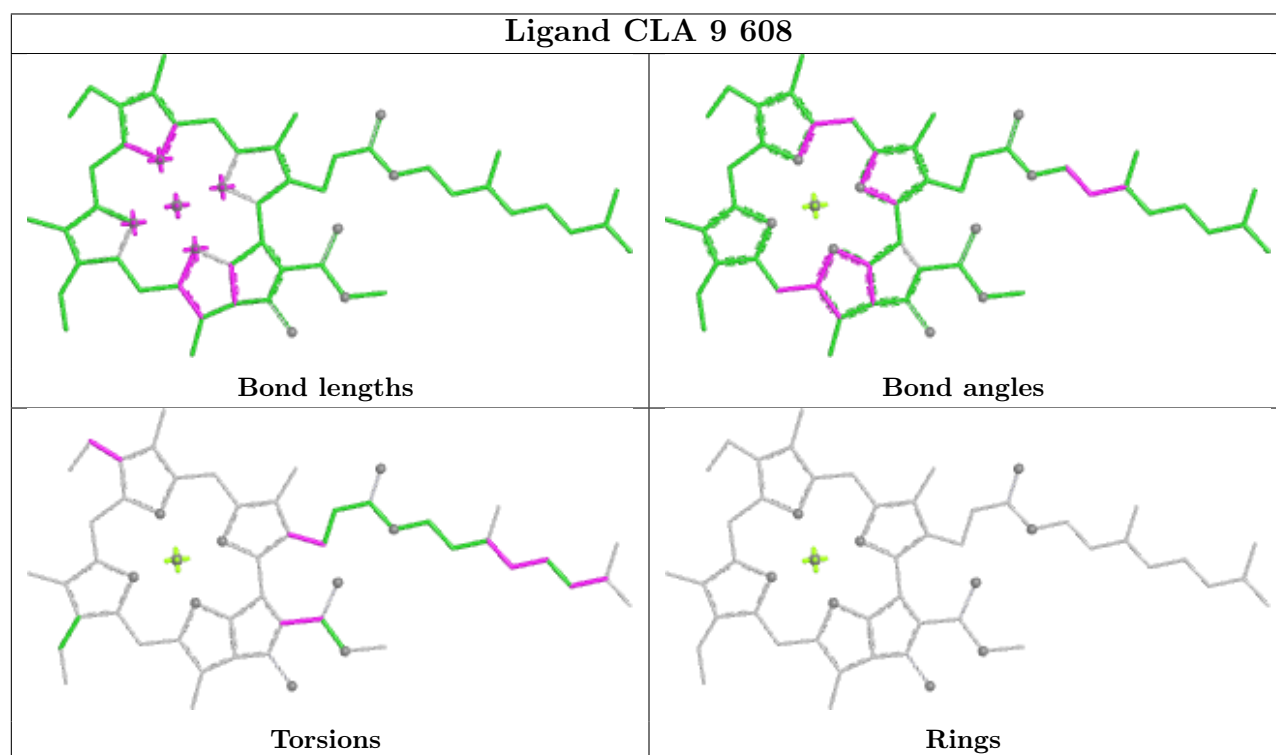
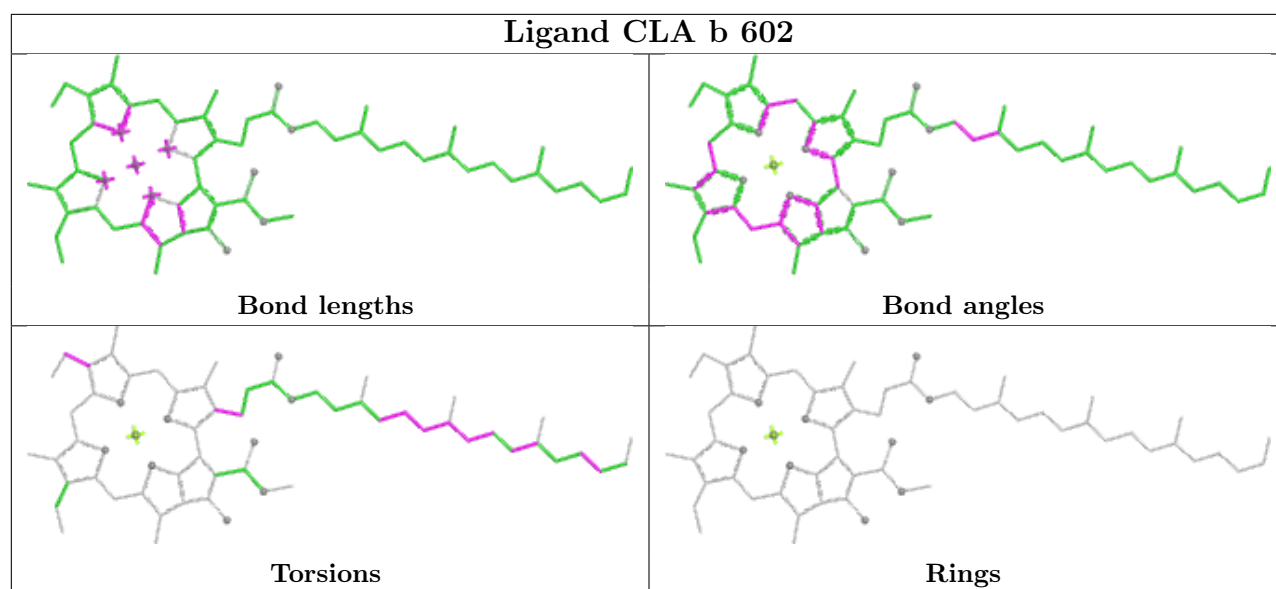


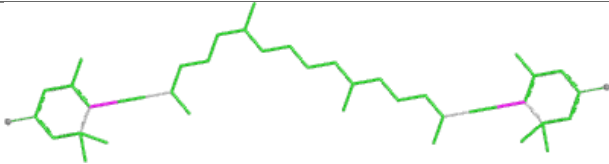
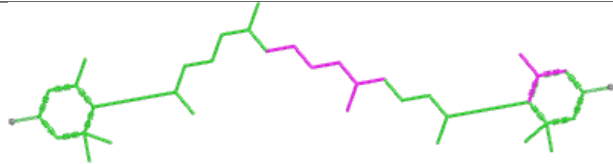
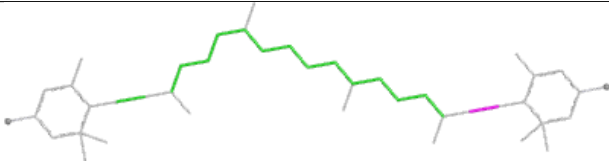
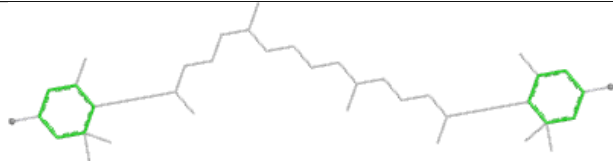


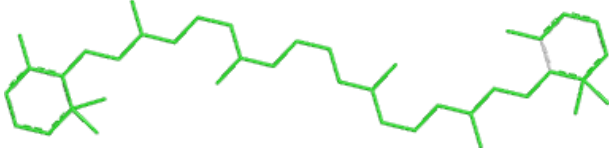
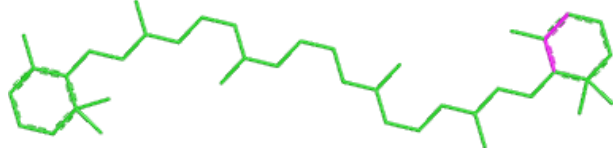
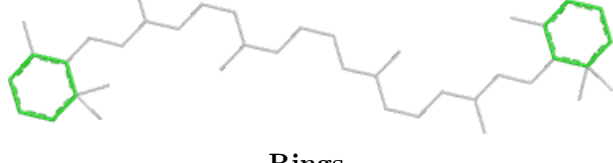


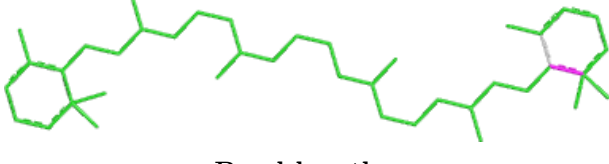
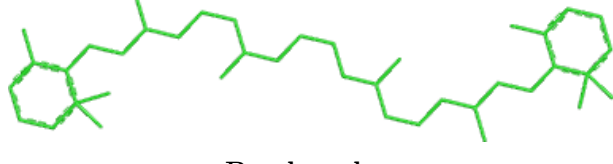
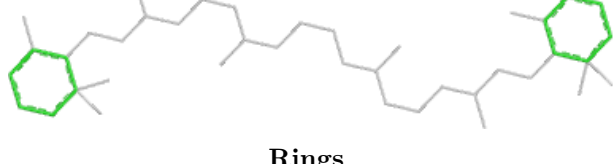




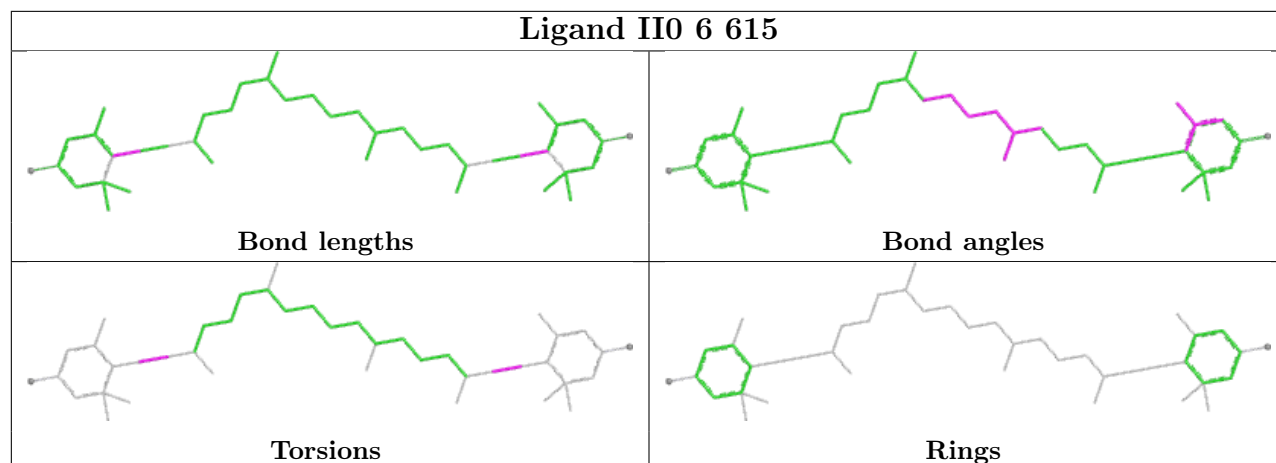


Ligand II0 7 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

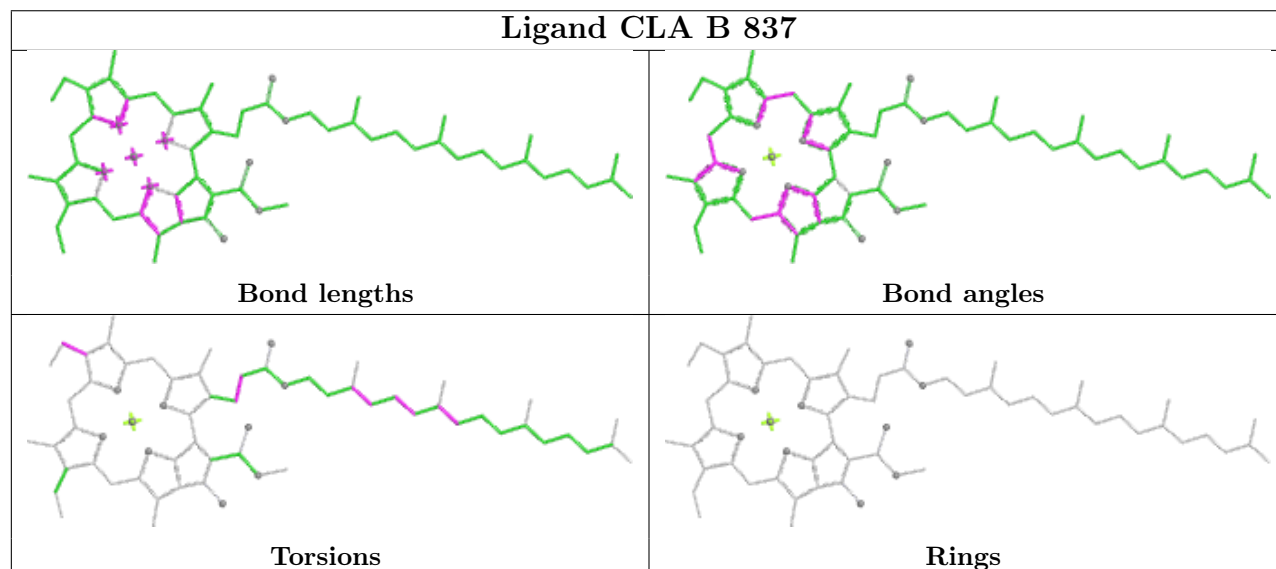
Ligand 8CT M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT 7 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

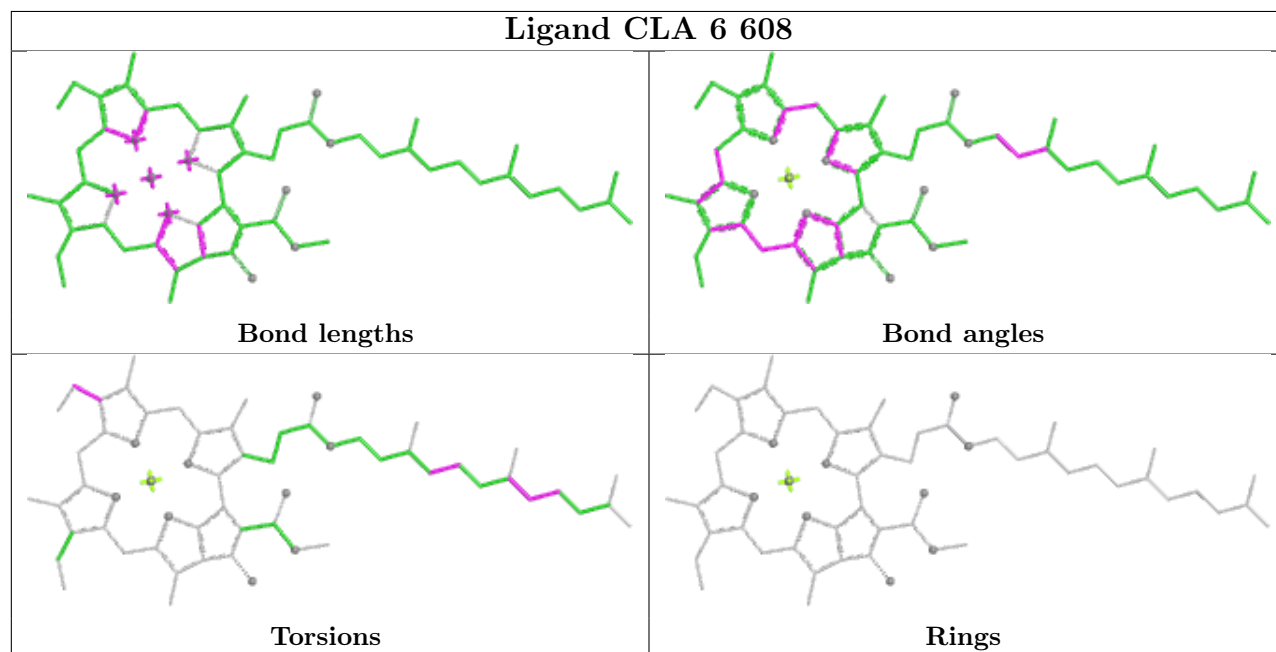
Ligand II0 6 615

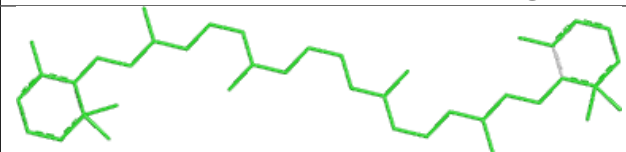
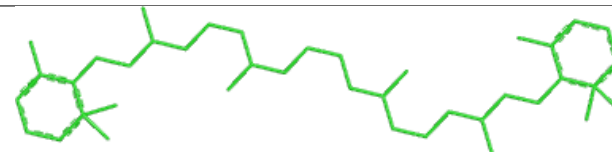
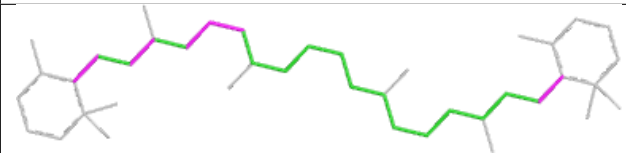
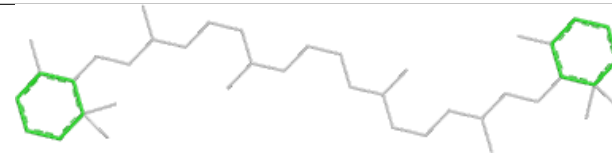


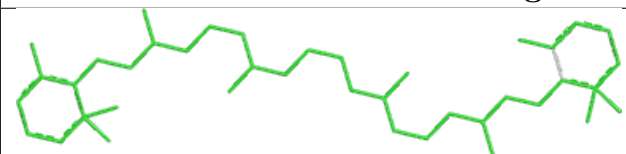
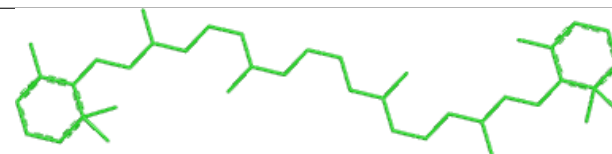
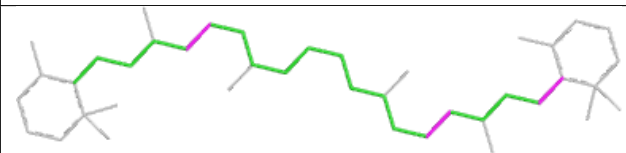
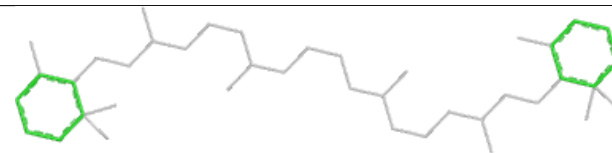
Ligand CLA B 837

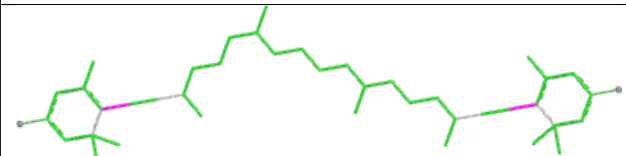
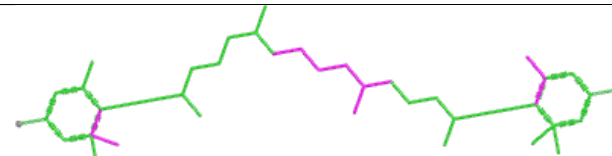
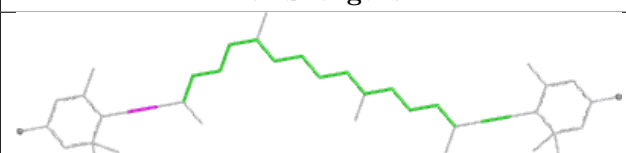
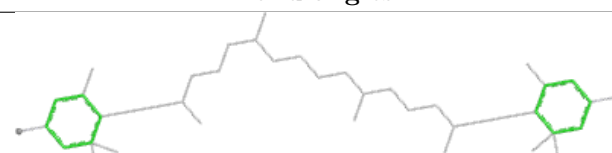


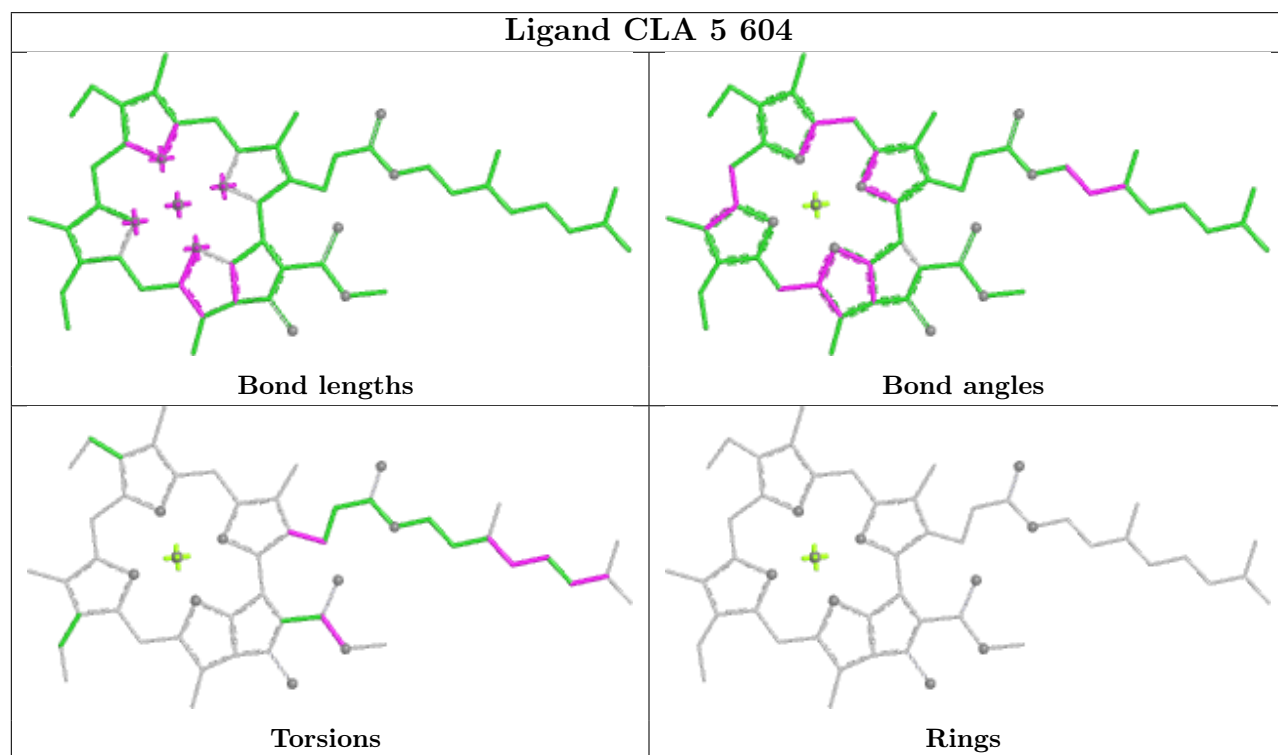
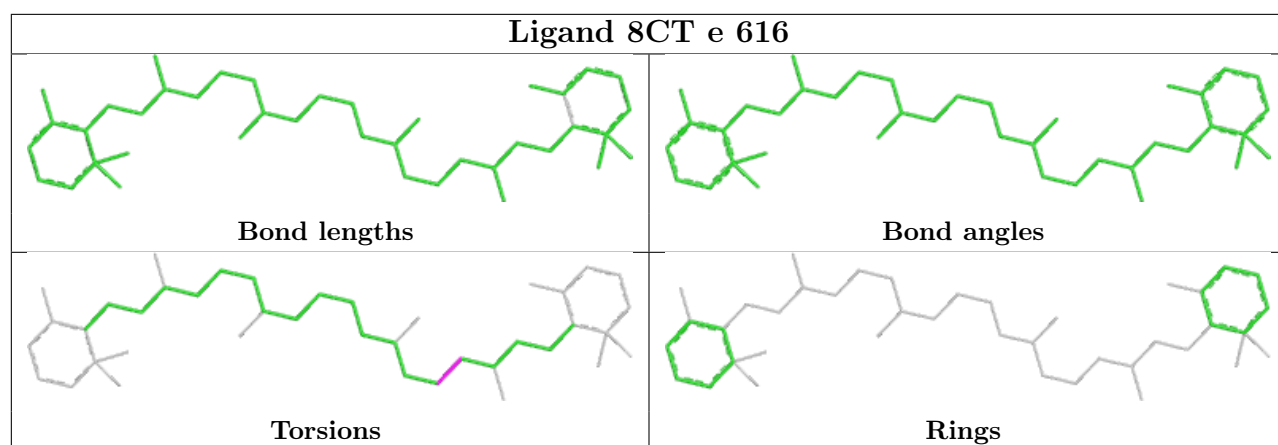
Ligand CLA 6 608



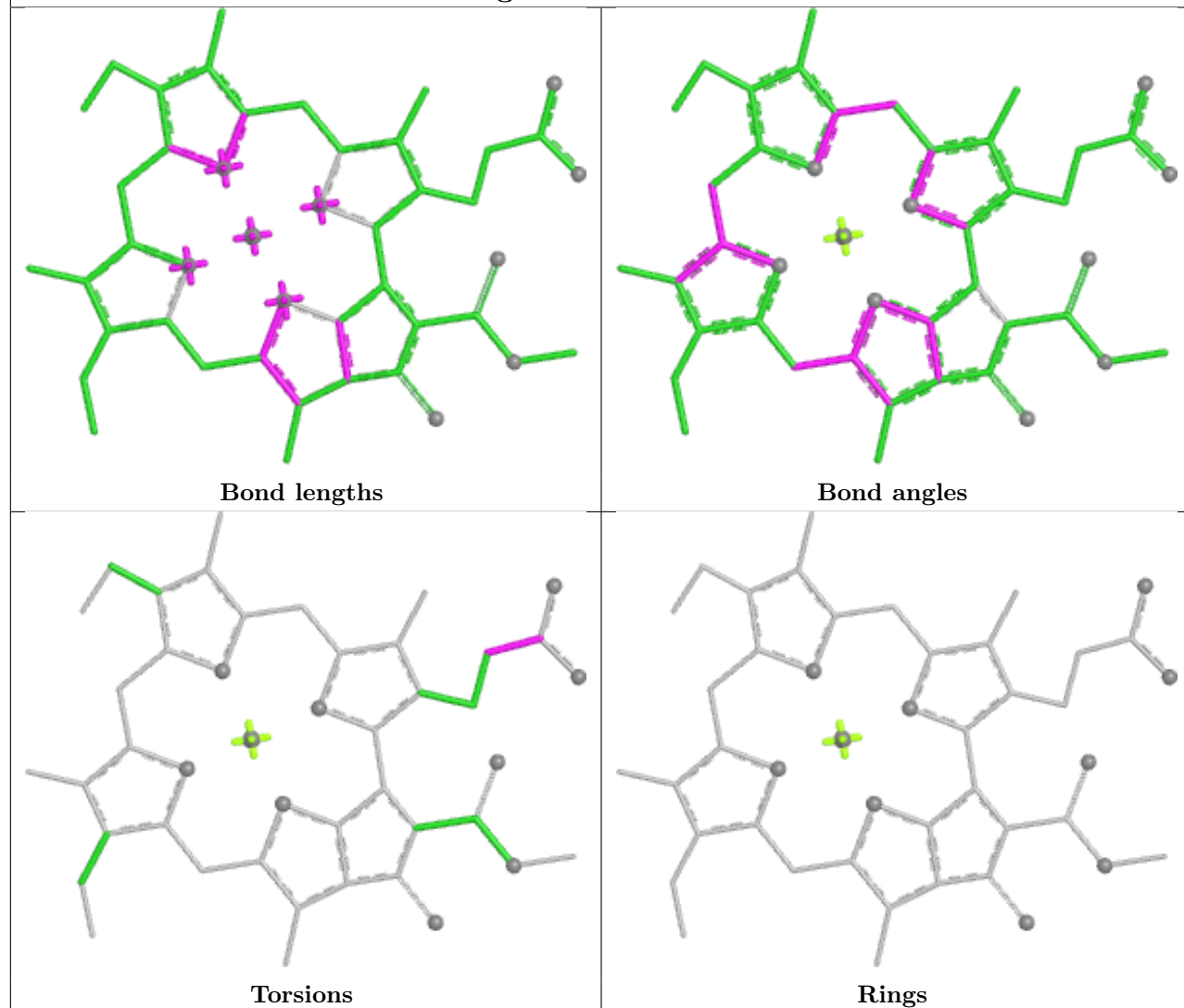
Ligand 8CT R 201	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand 8CT B 844	
	Bond lengths
	Bond angles
	Torsions
	Rings

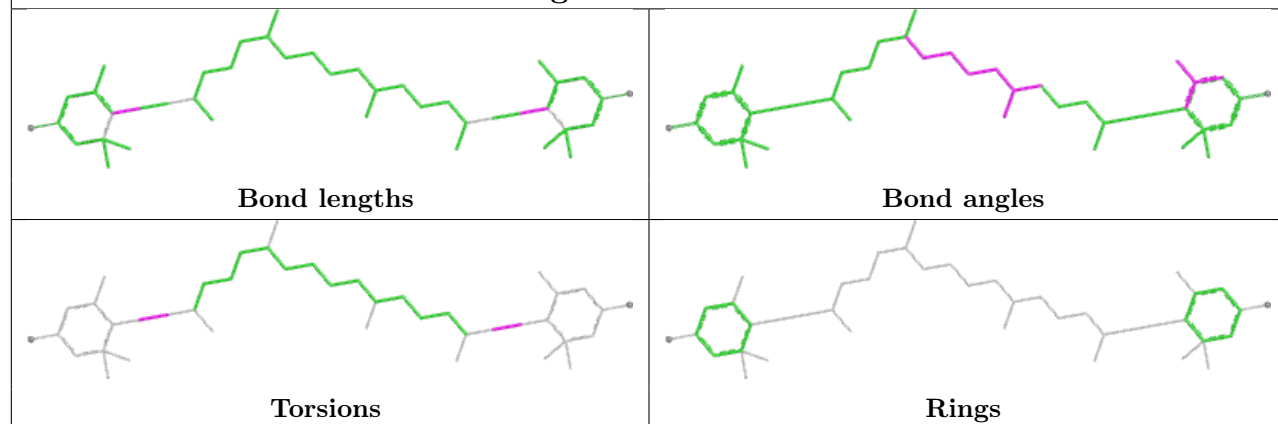
Ligand II0 7 614	
	Bond lengths
	Bond angles
	Torsions
	Rings



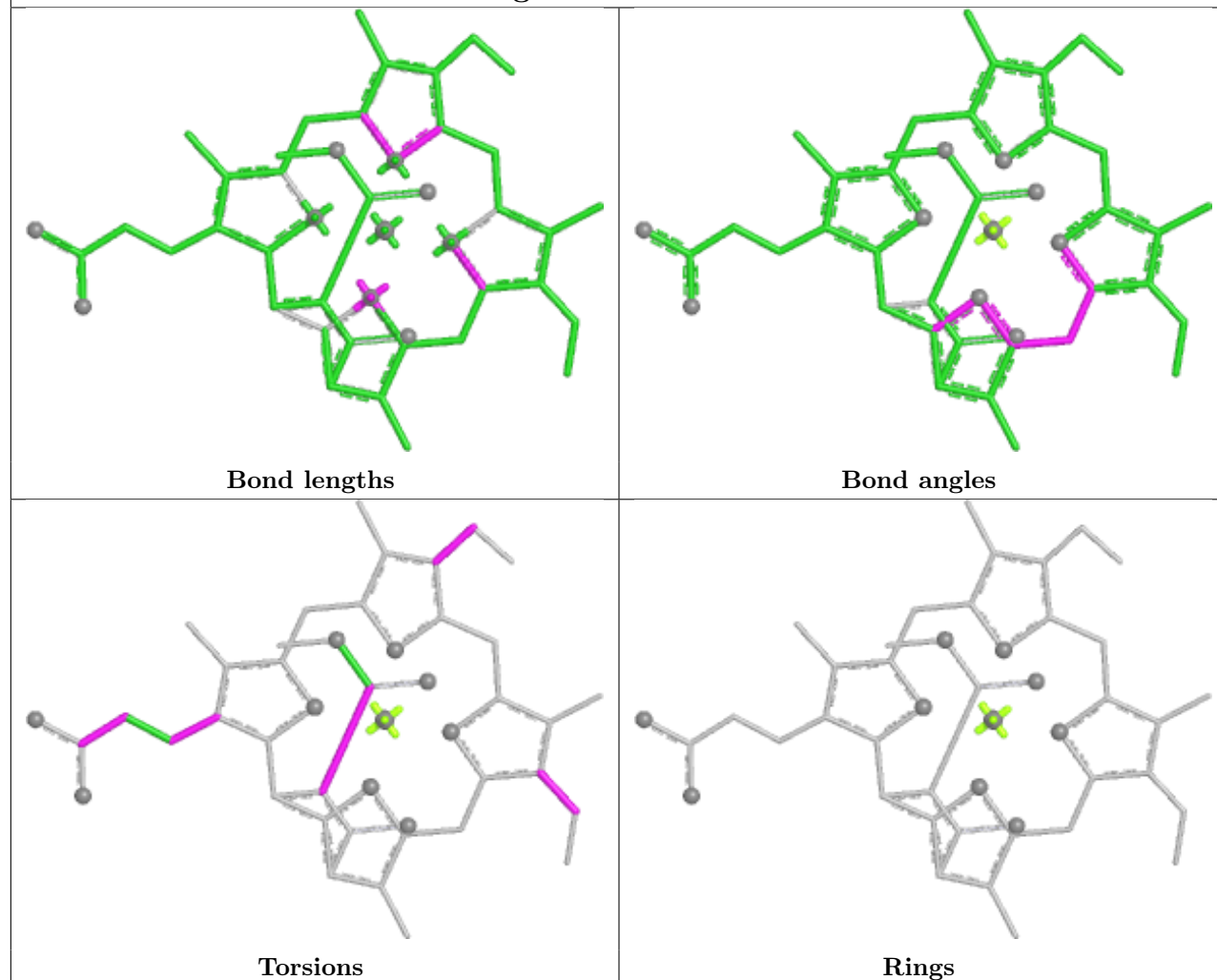
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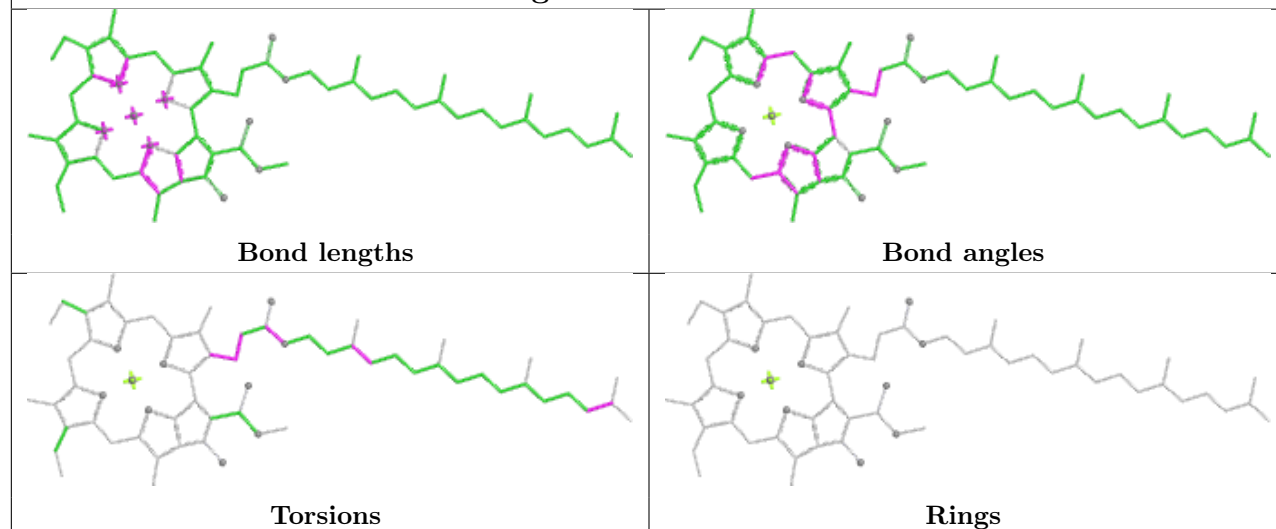
Ligand II0 8 611



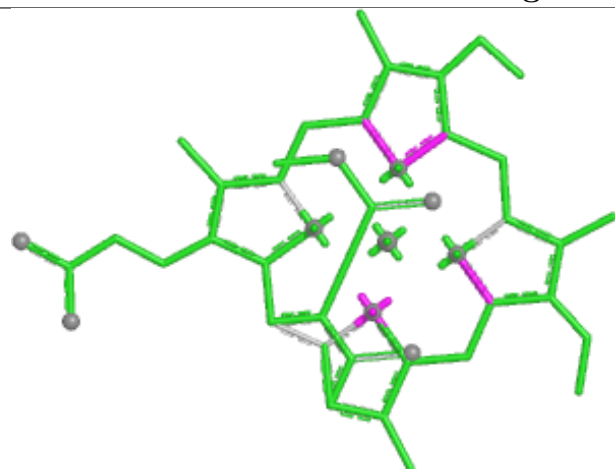
Ligand KC2 6 613



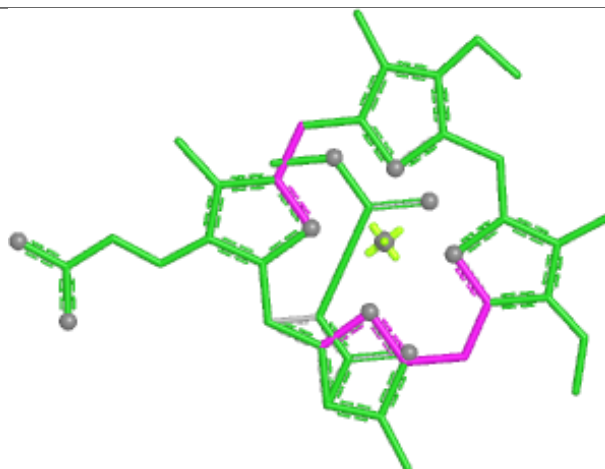
Ligand CLA A 844



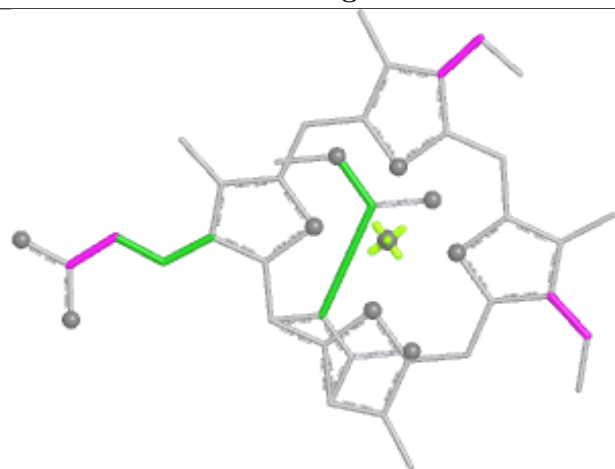
Ligand KC2 e 609



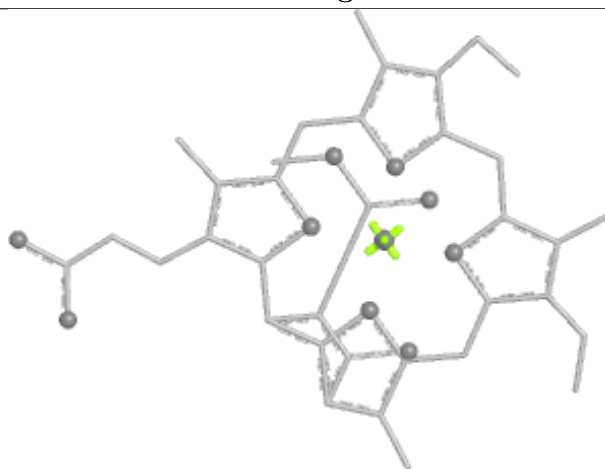
Bond lengths



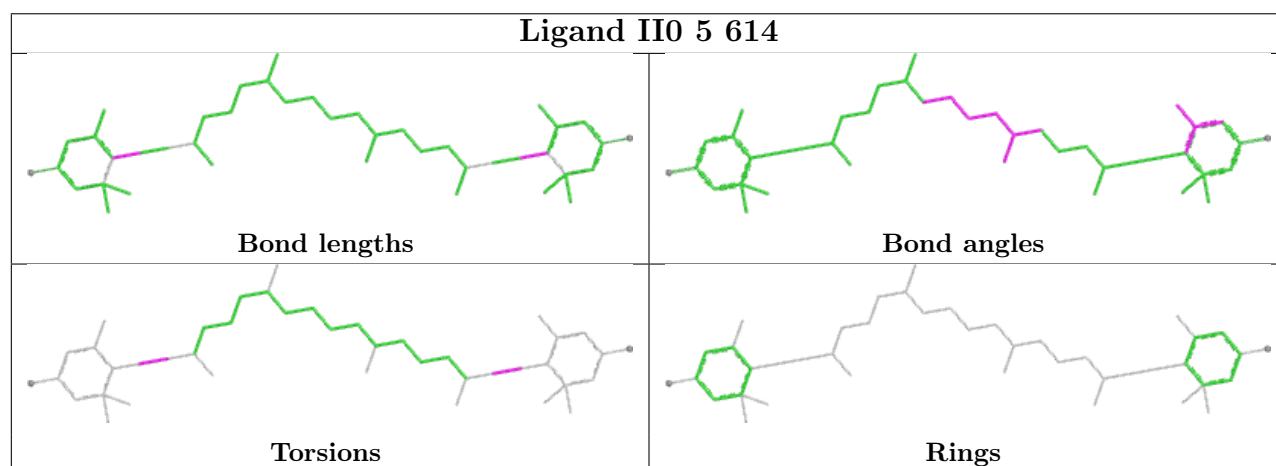
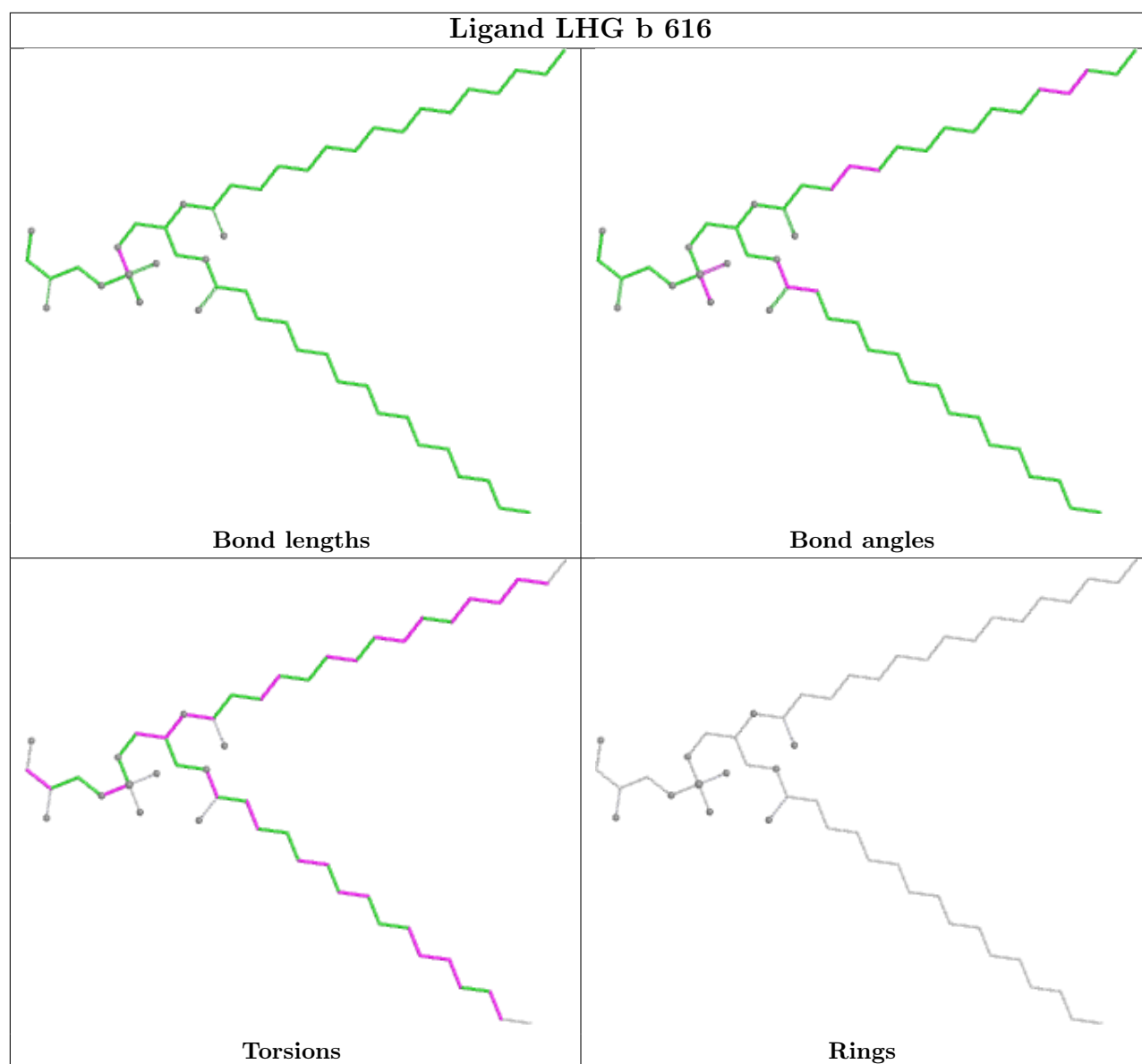
Bond angles



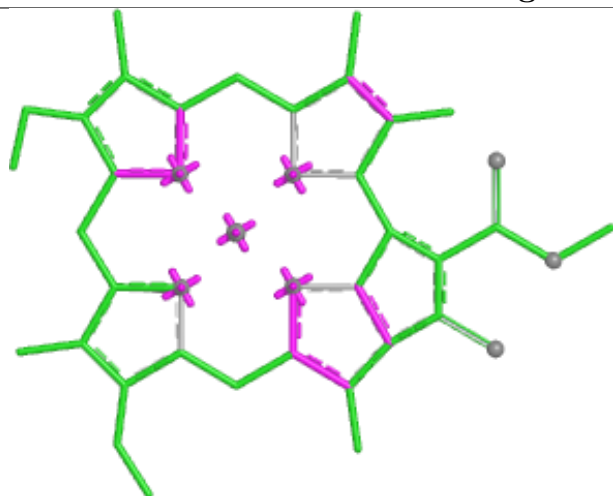
Torsions



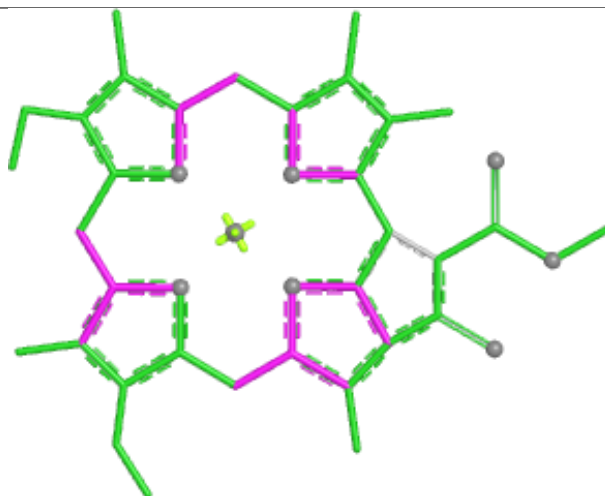
Rings



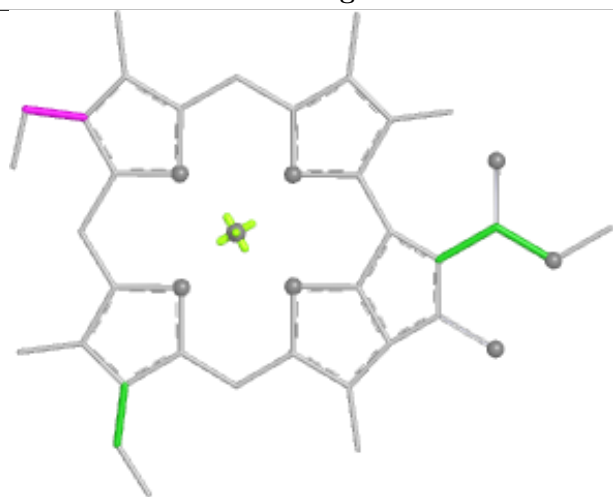
Ligand CLA 6 609



Bond lengths



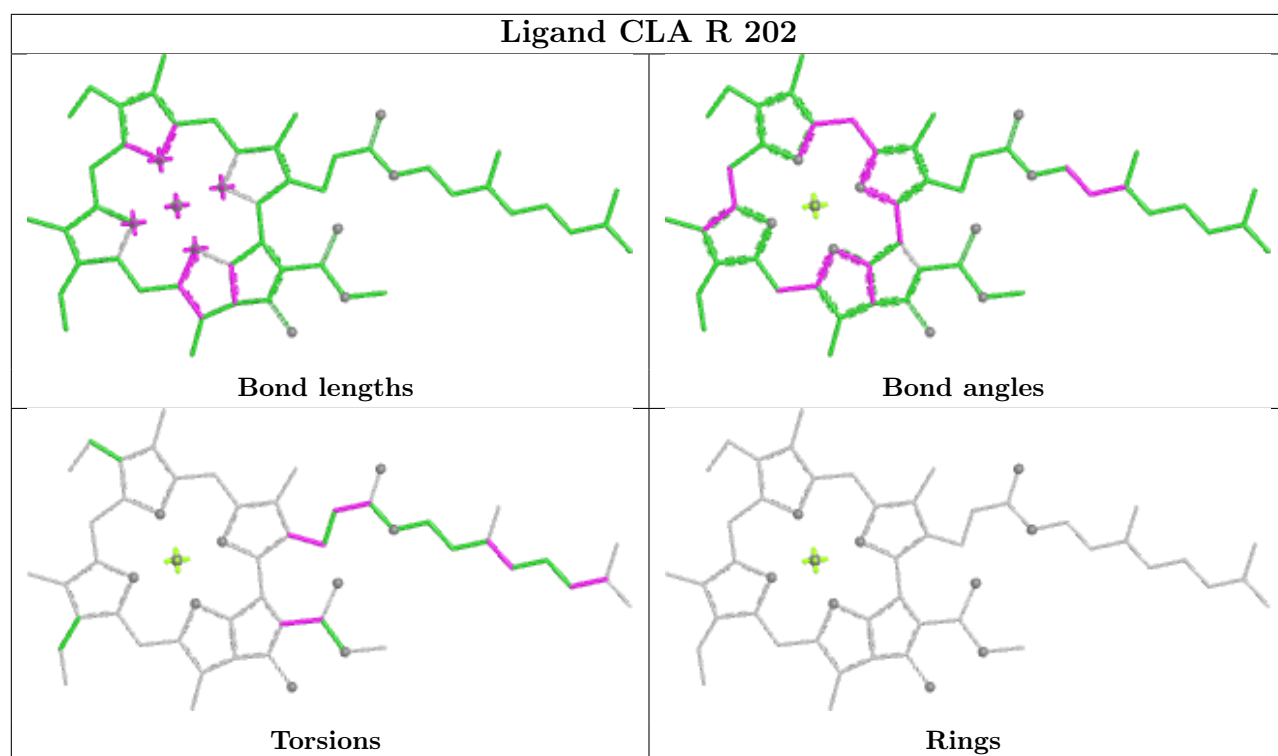
Bond angles

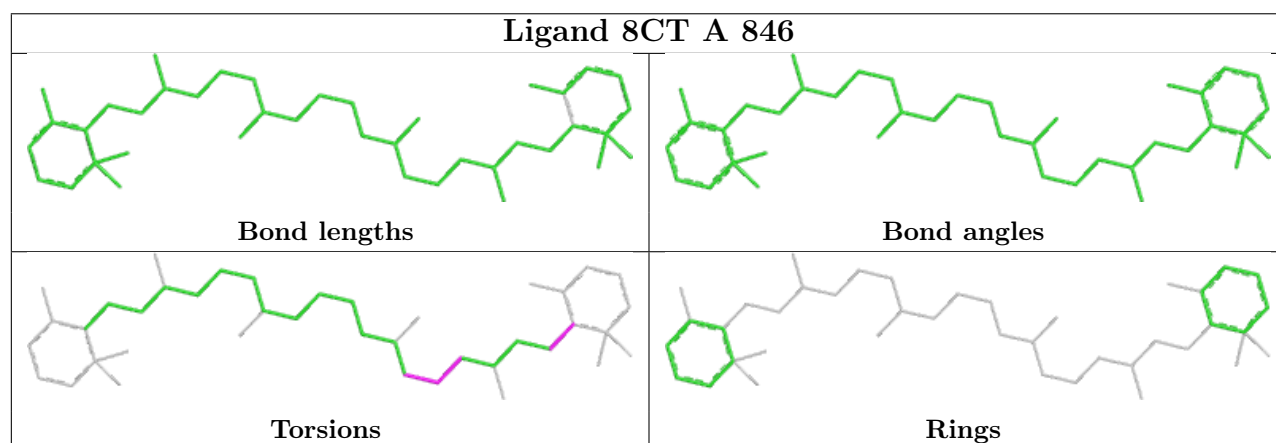
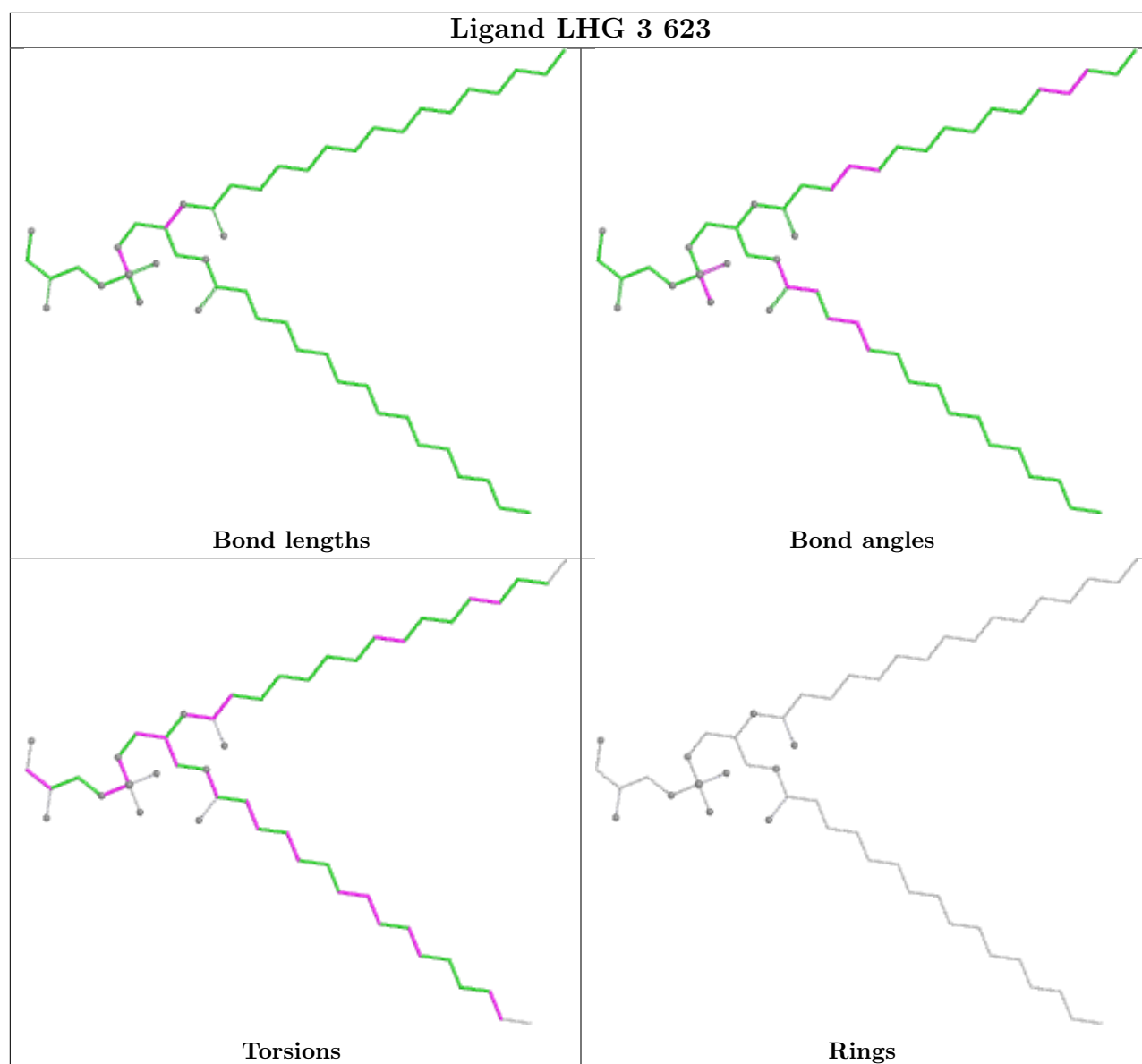


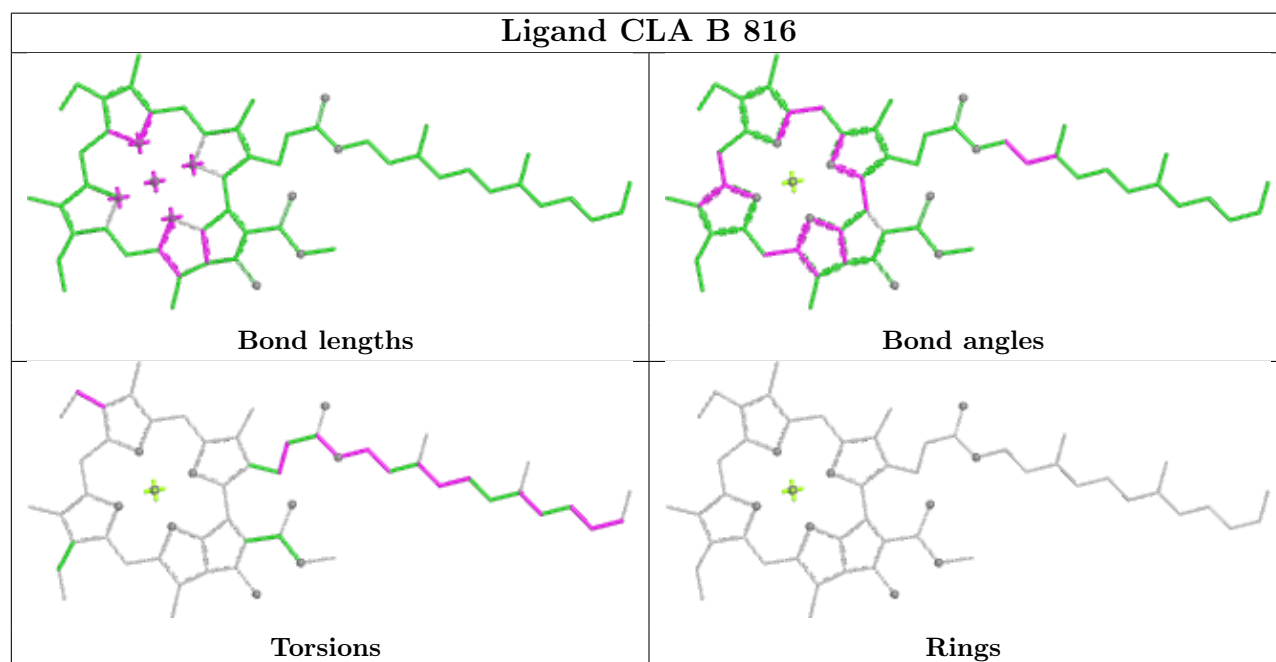
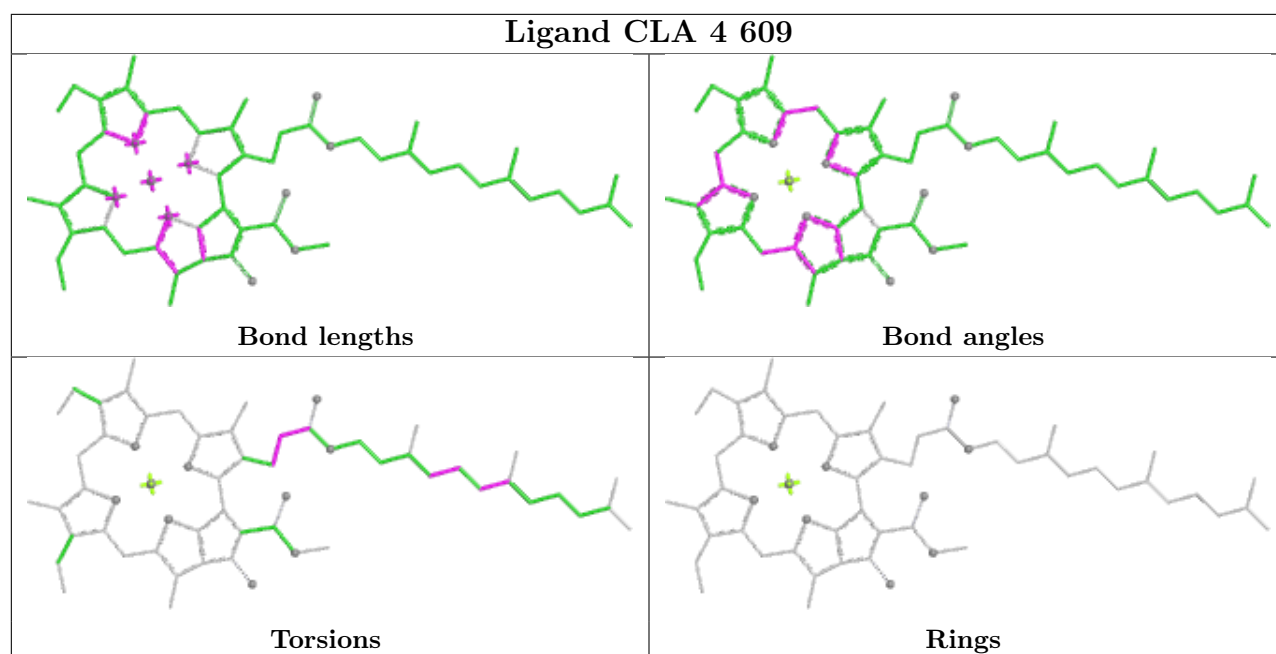
Torsions

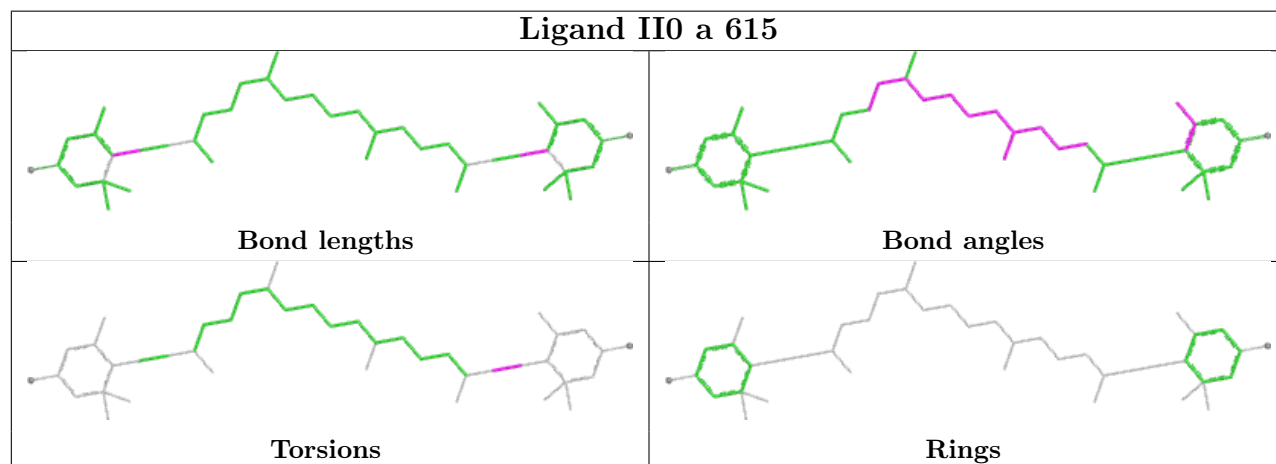
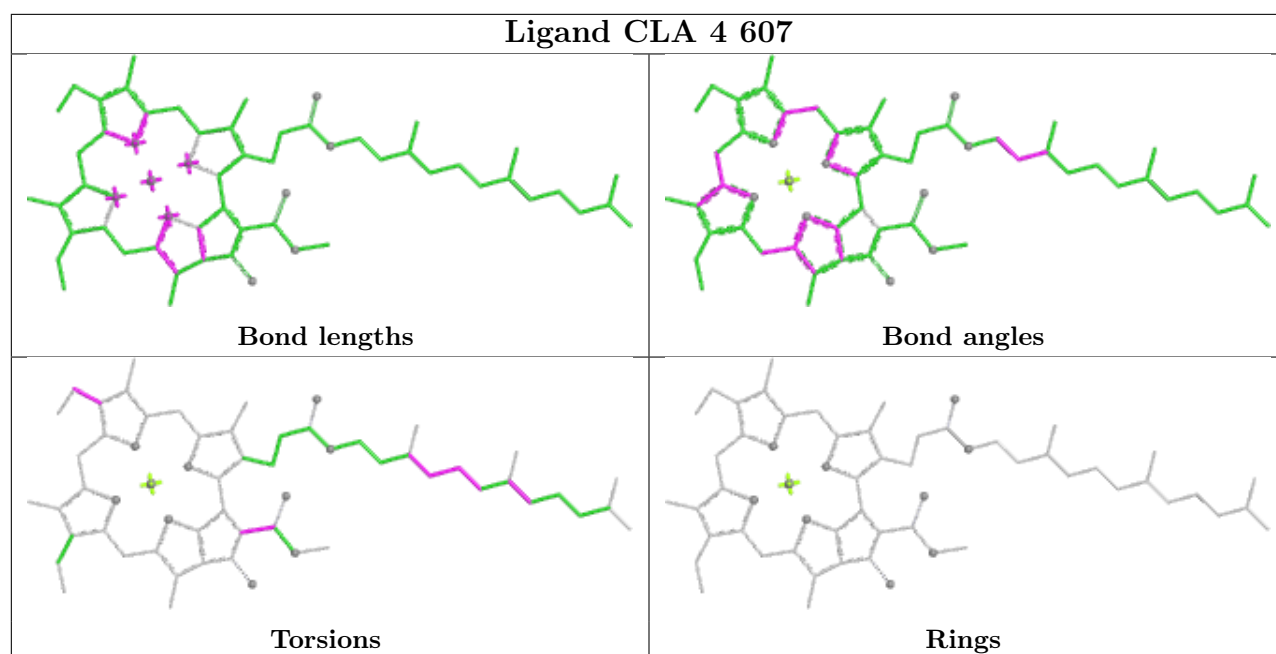


Rings

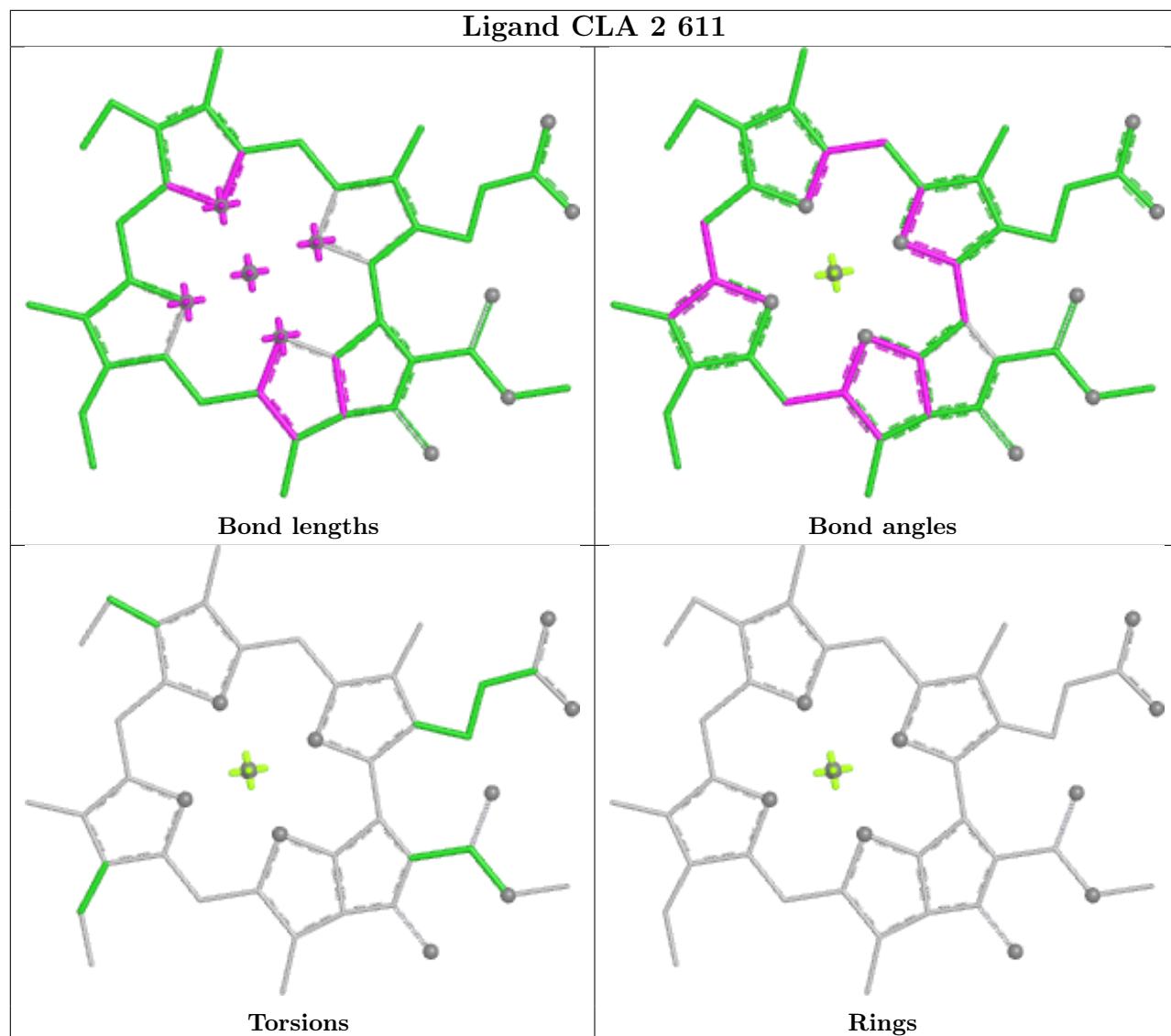




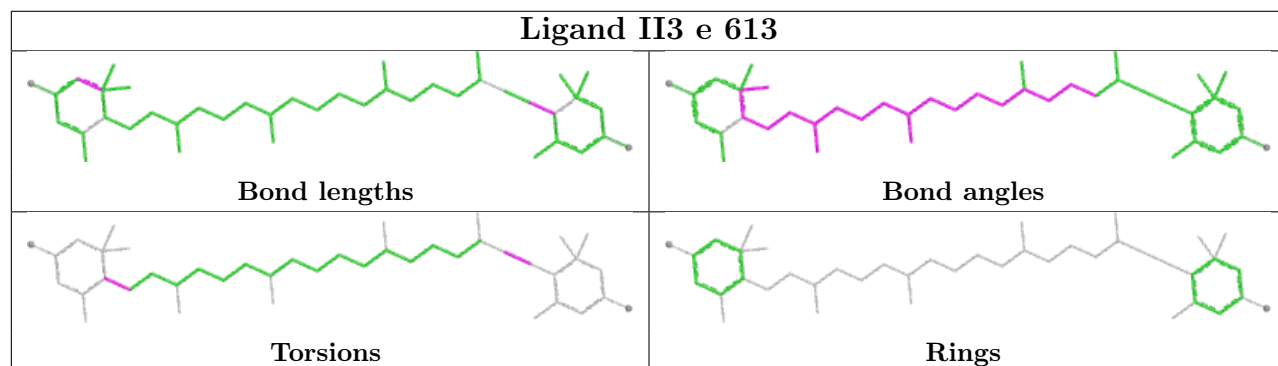




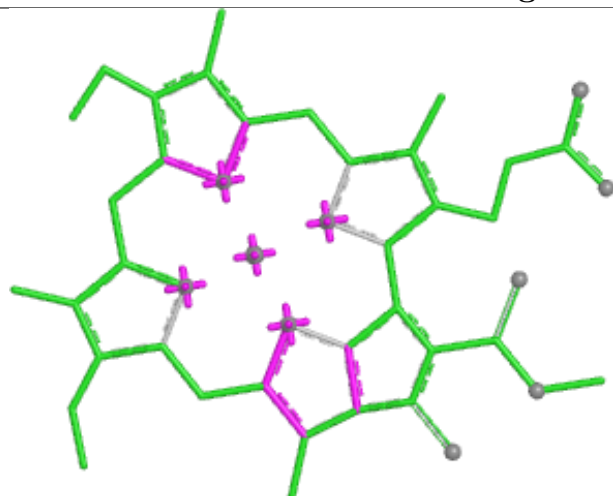
Ligand CLA 2 611



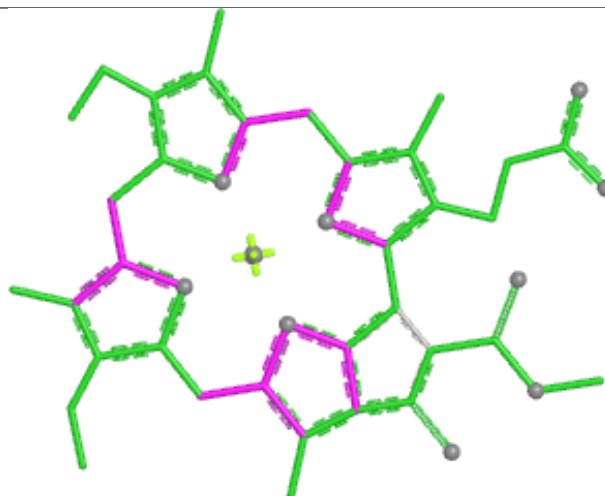
Ligand II3 e 613



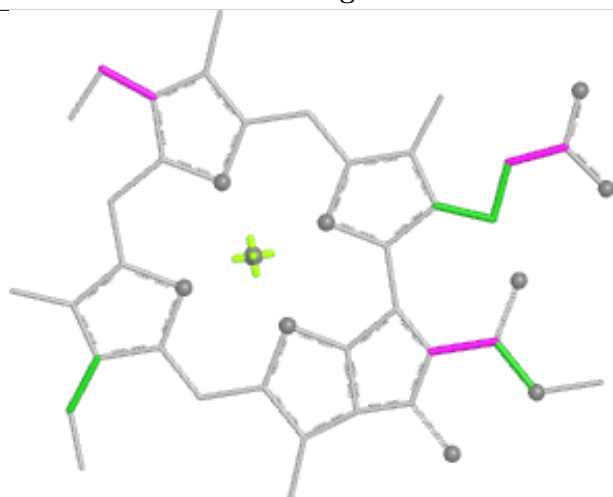
Ligand CLA 7 605



Bond lengths



Bond angles

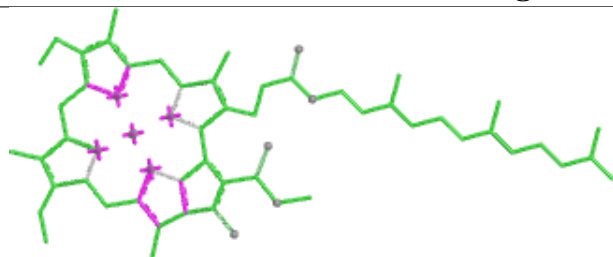


Torsions

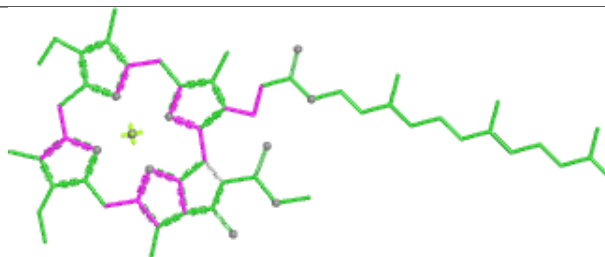


Rings

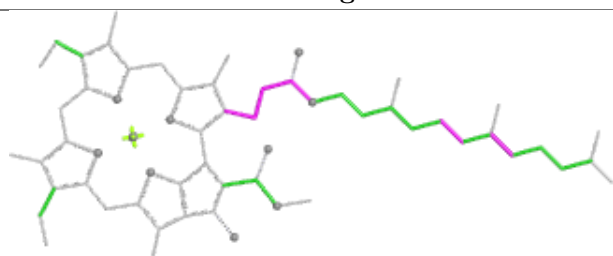
Ligand CLA B 819



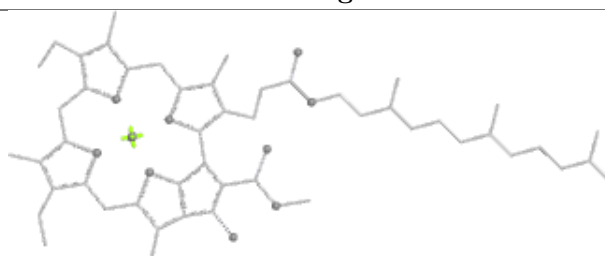
Bond lengths



Bond angles

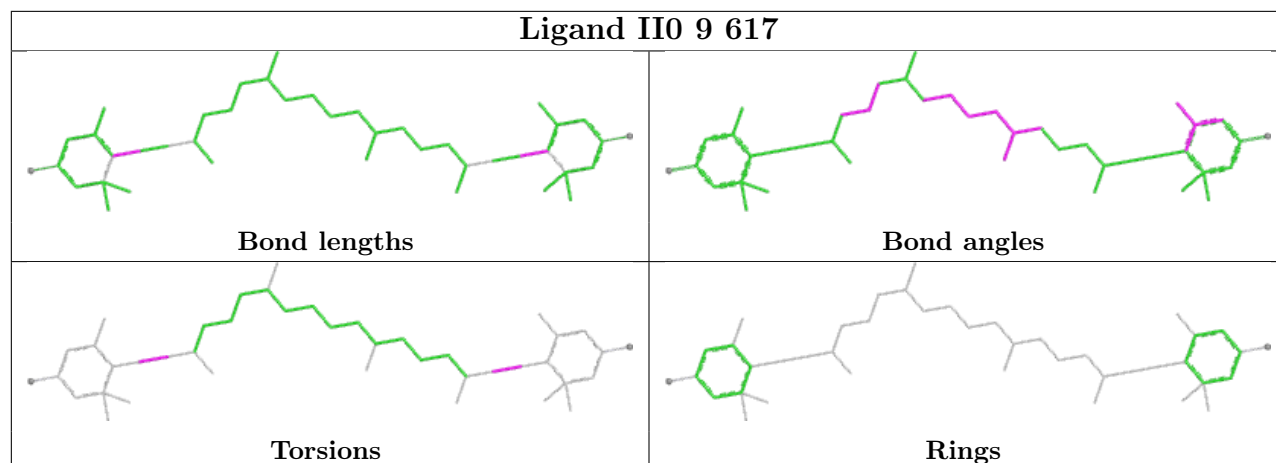


Torsions

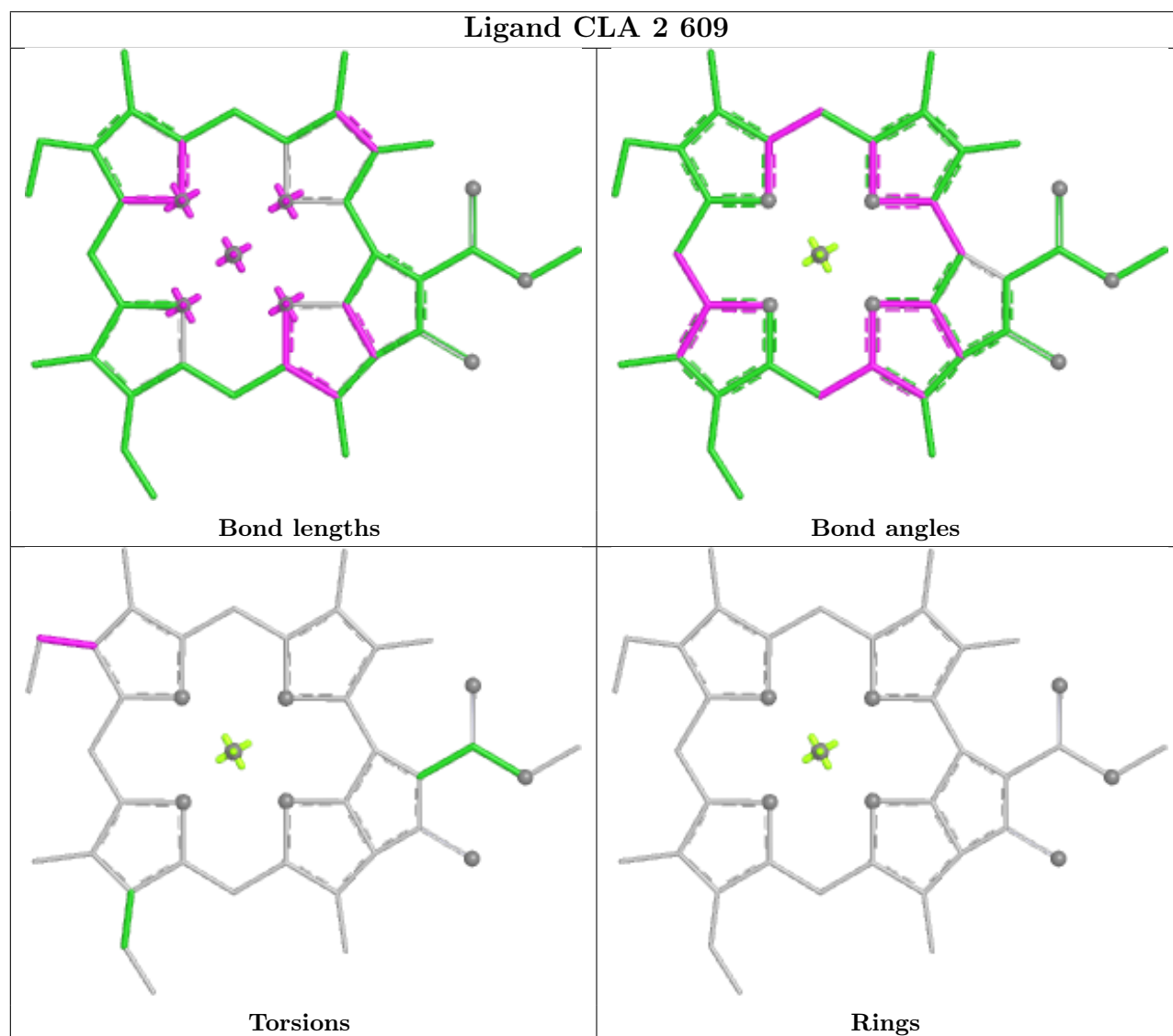


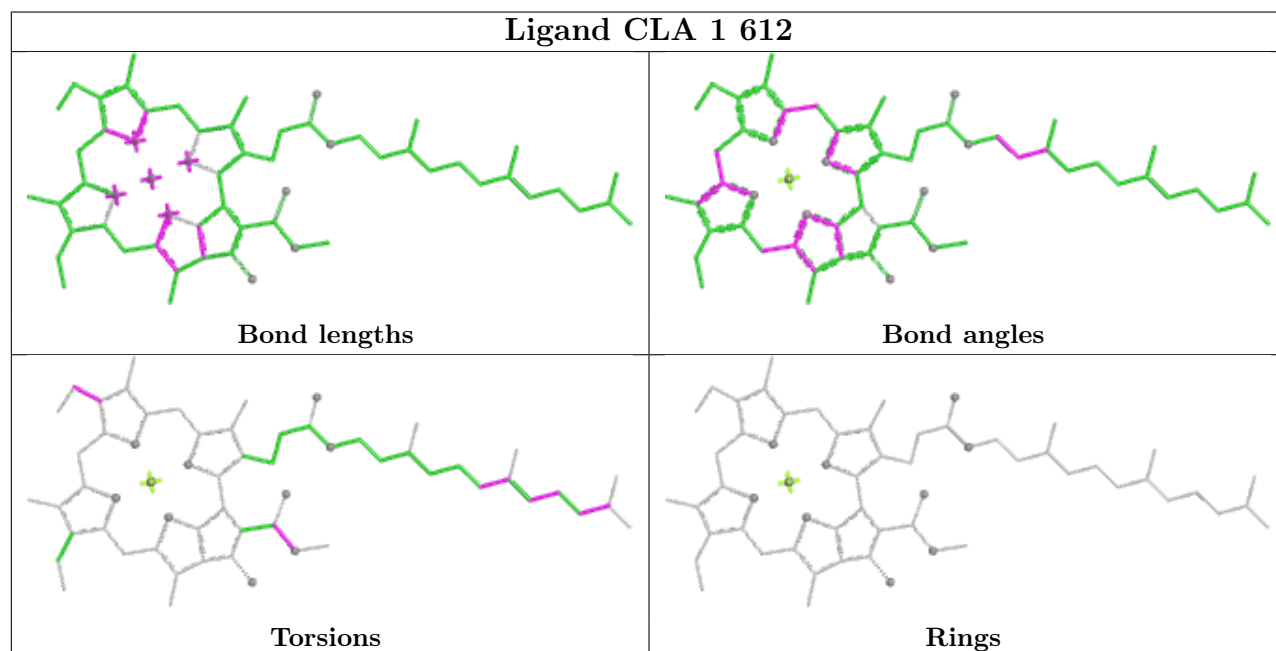
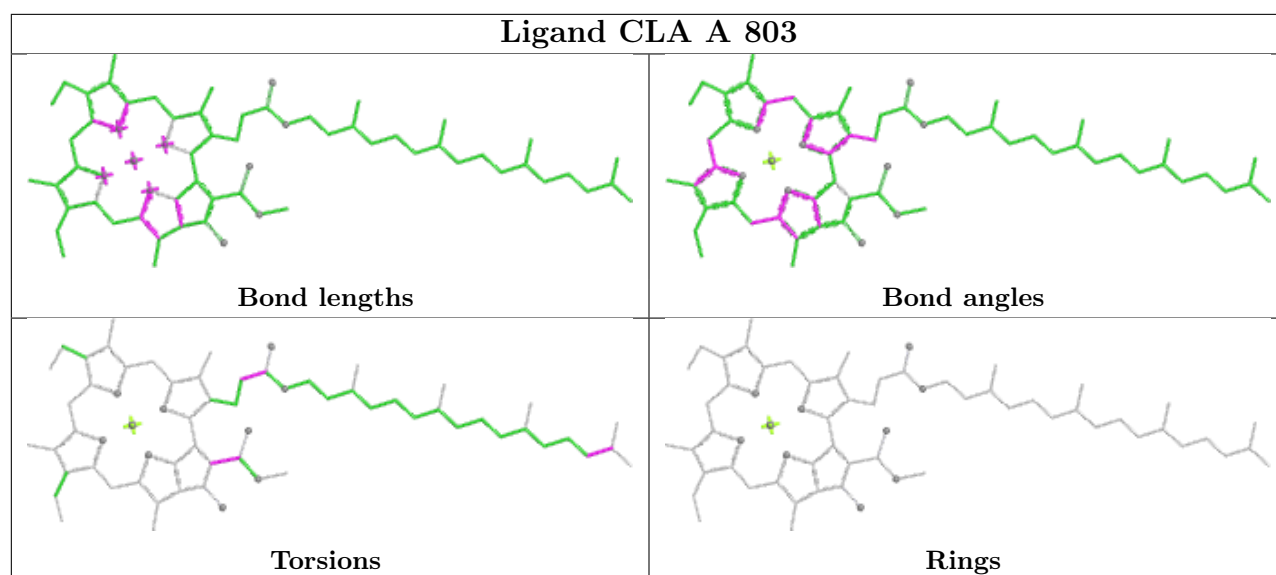
Rings

Ligand II0 9 617

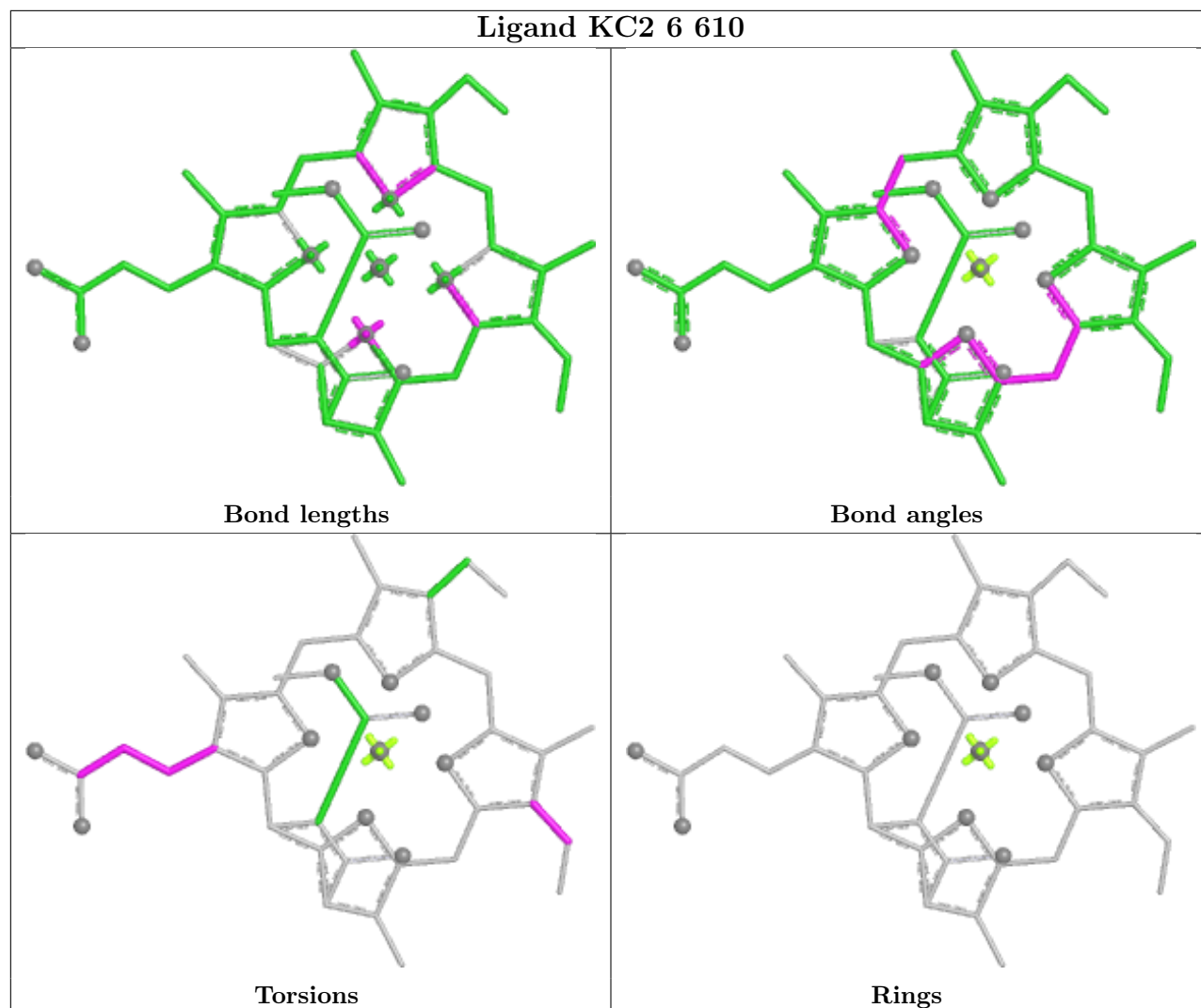


Ligand CLA 2 609

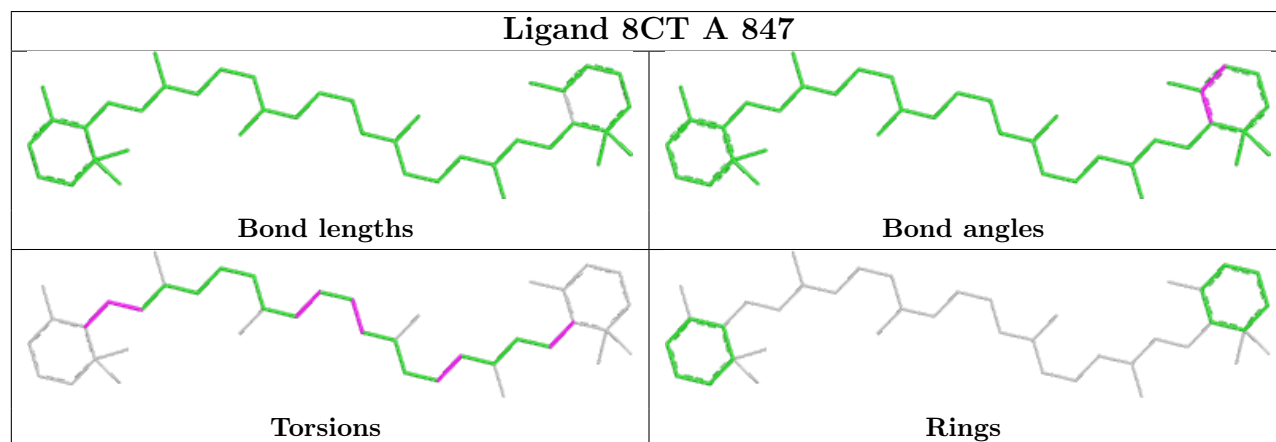




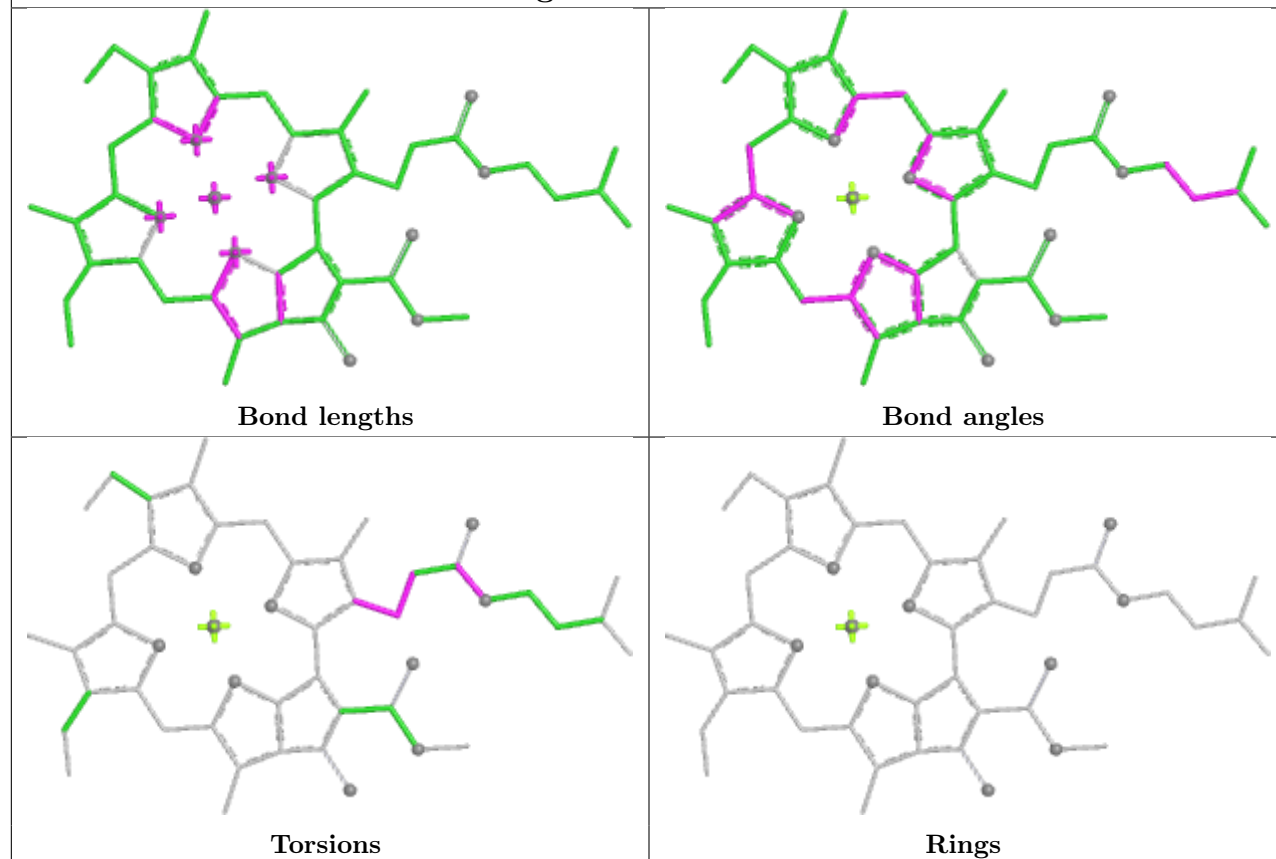
Ligand KC2 6 610



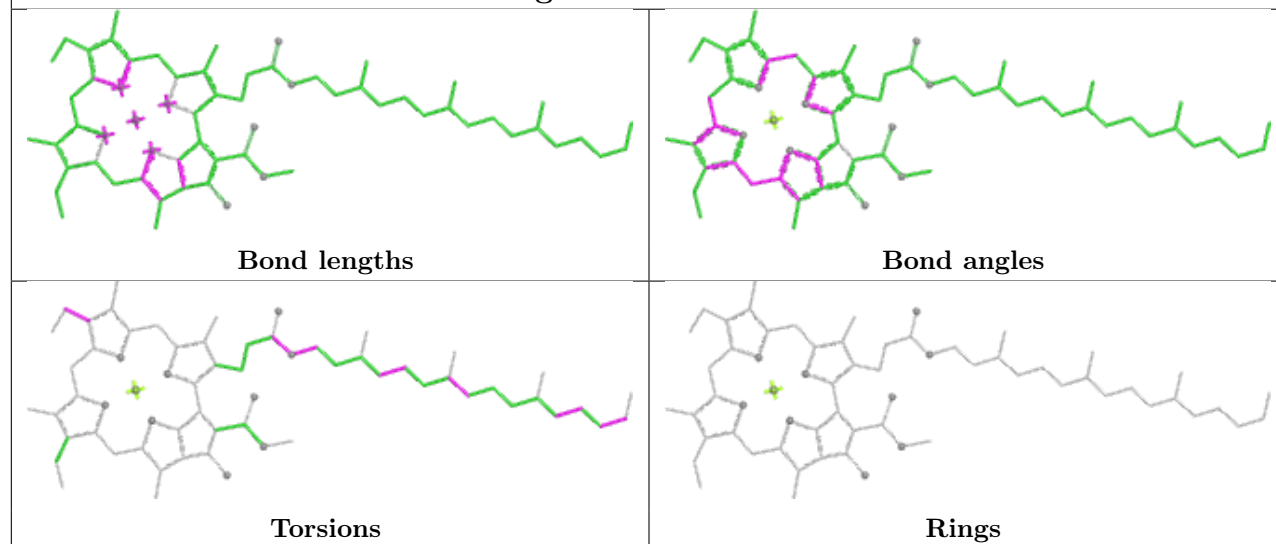
Ligand 8CT A 847



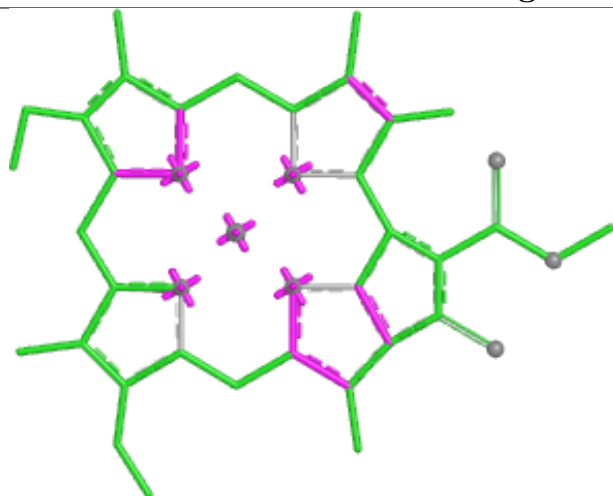
Ligand CLA 2 603



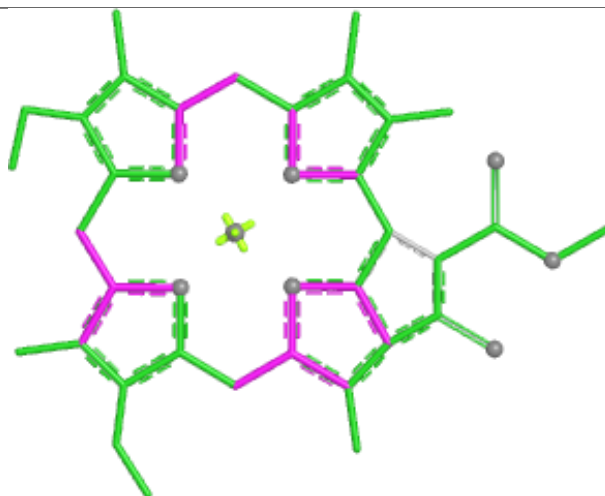
Ligand CLA d 602



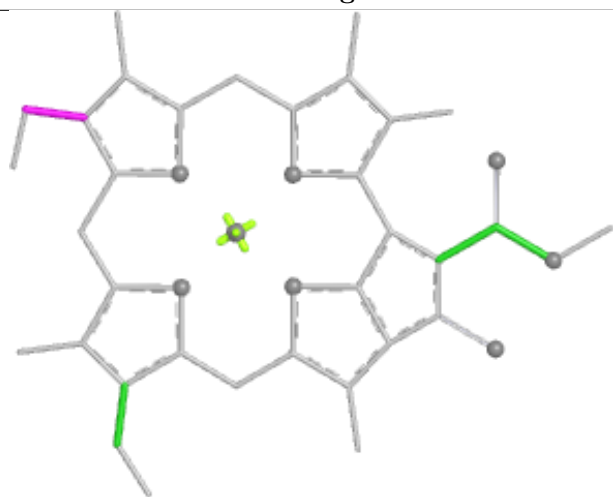
Ligand CLA 5 601



Bond lengths



Bond angles

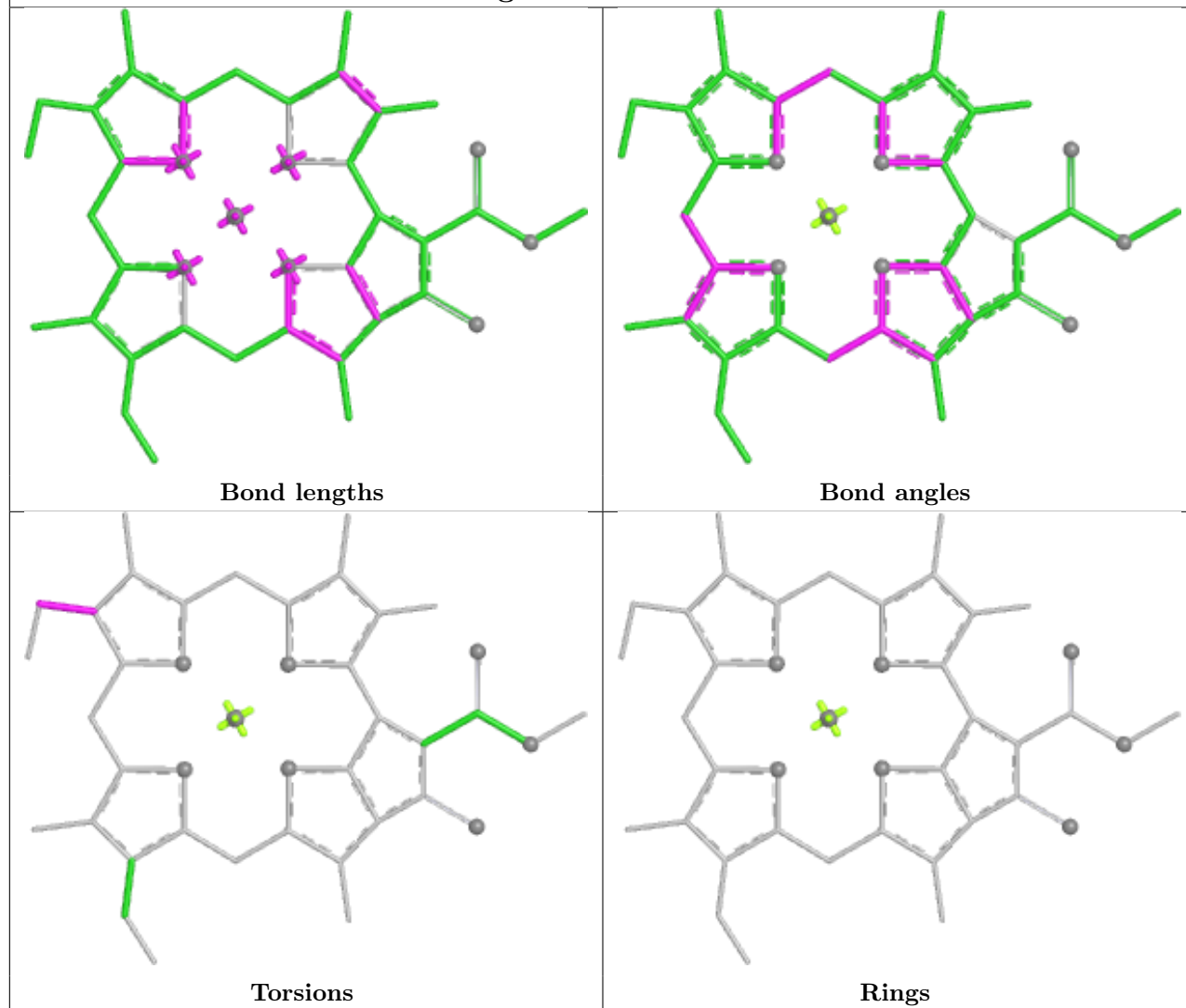


Torsions

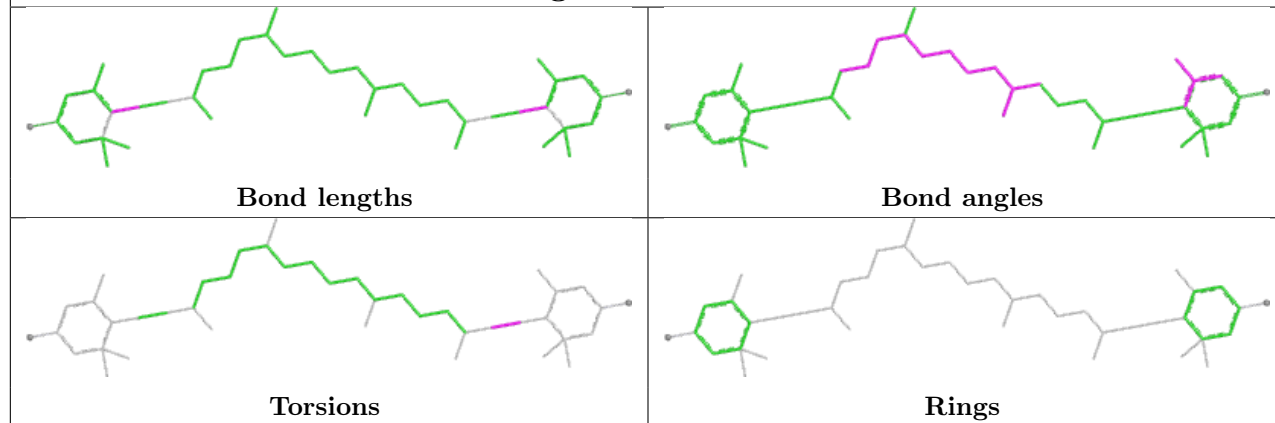


Rings

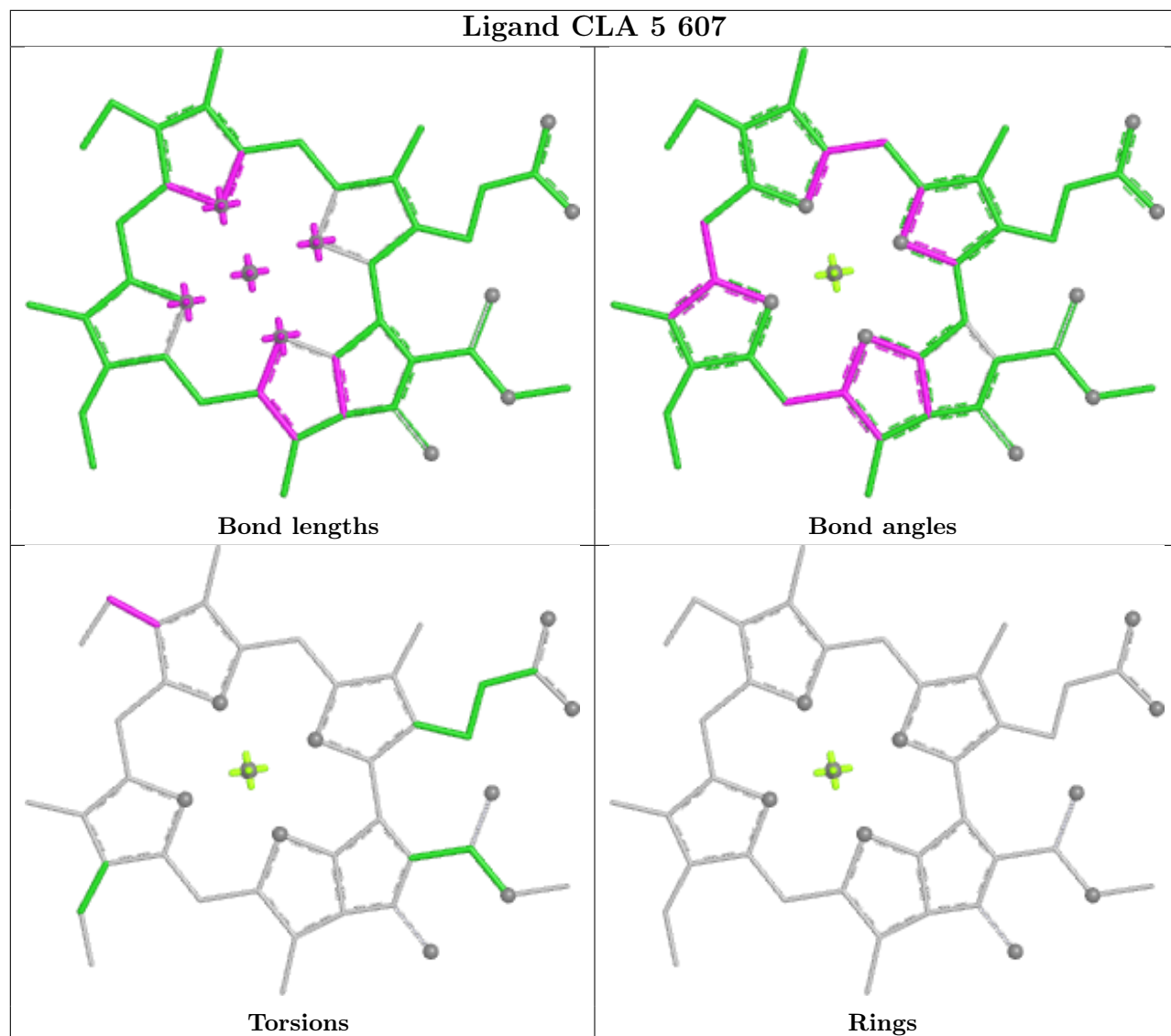
Ligand CLA 5 609



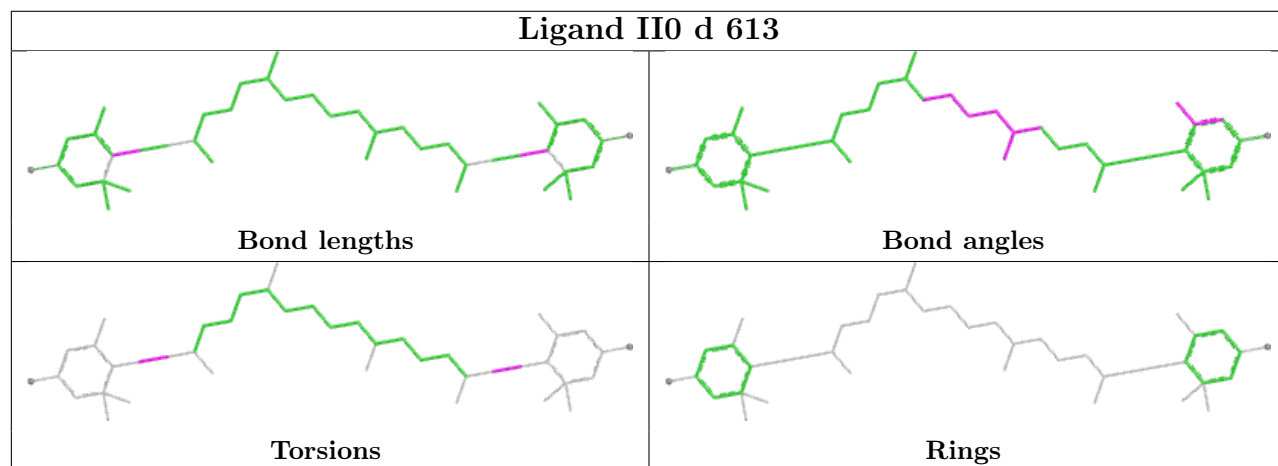
Ligand II0 7 616

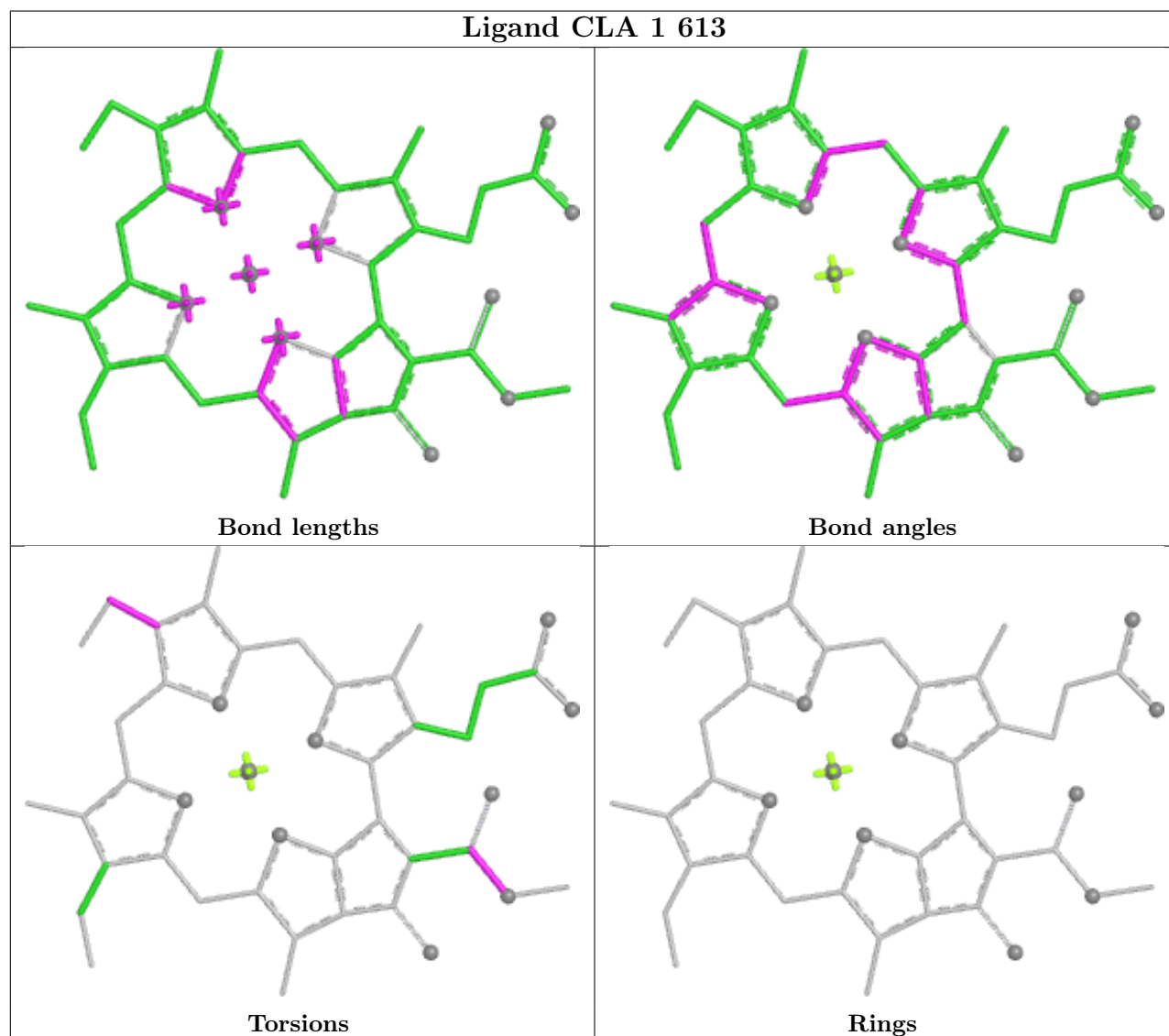
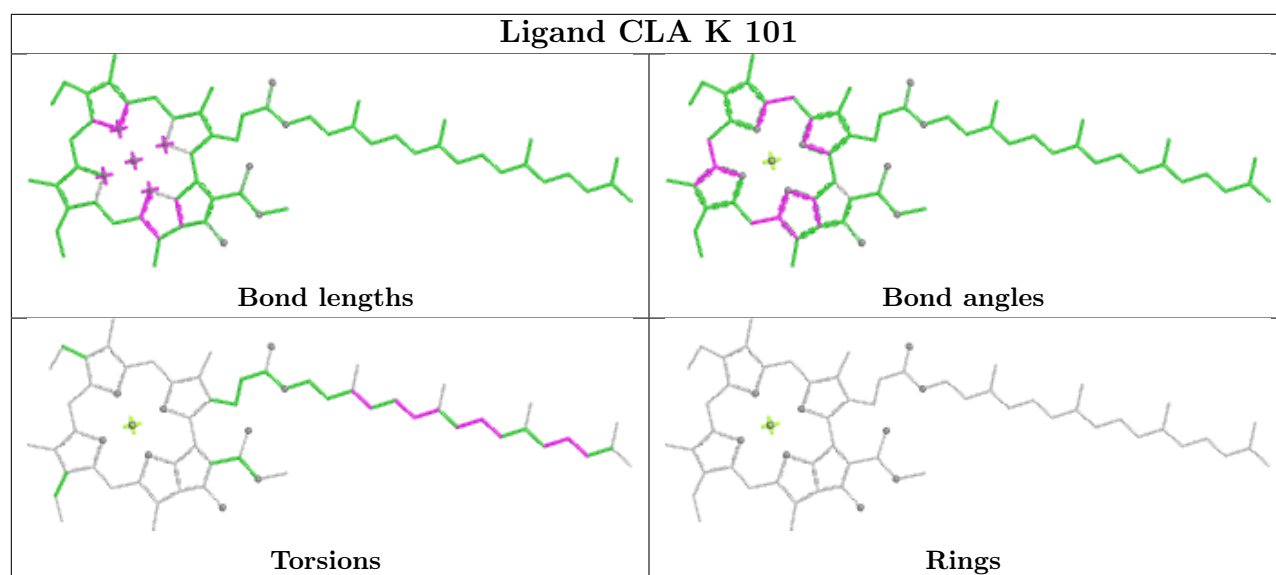


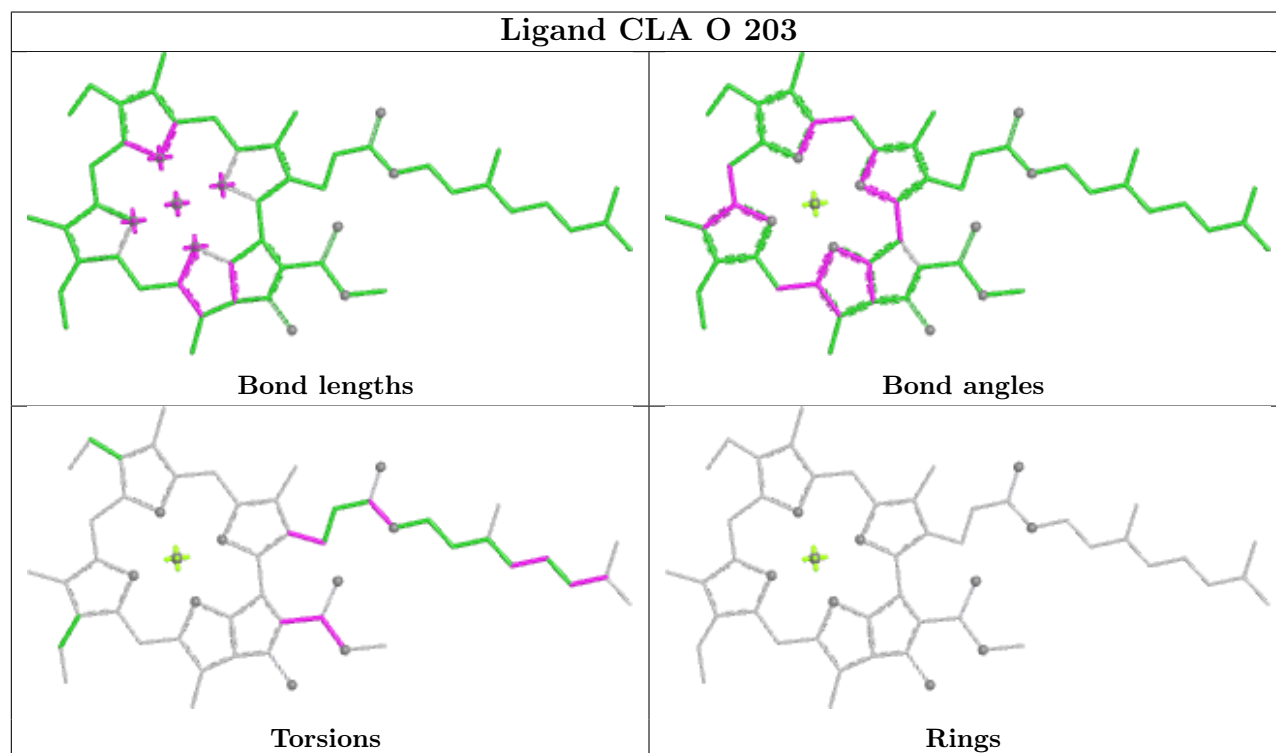
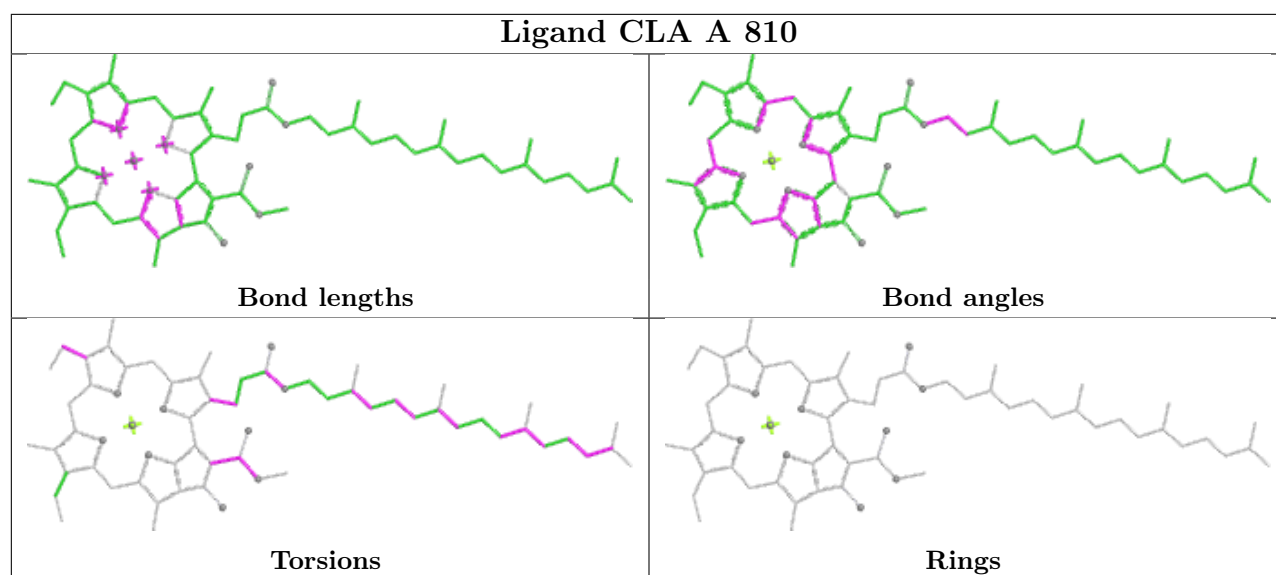
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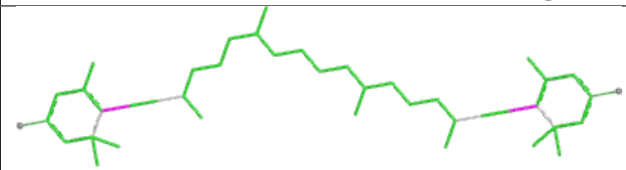
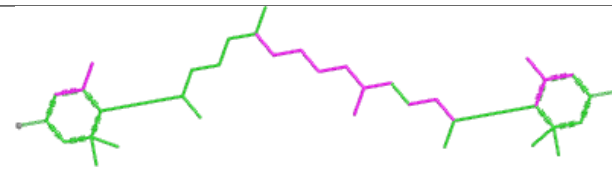
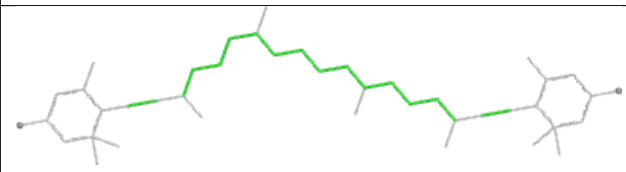
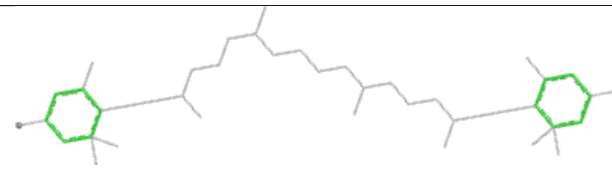


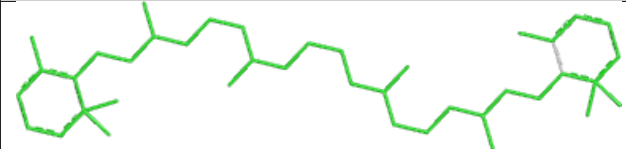
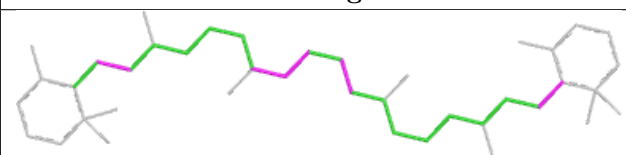
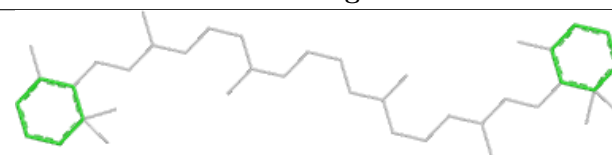
Ligand II0 d 613

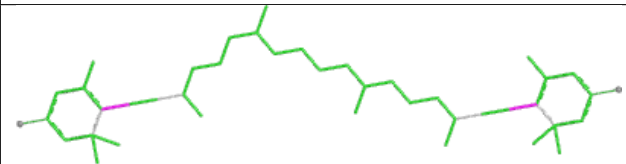
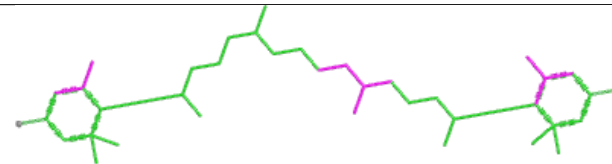
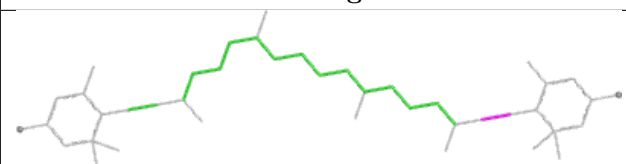
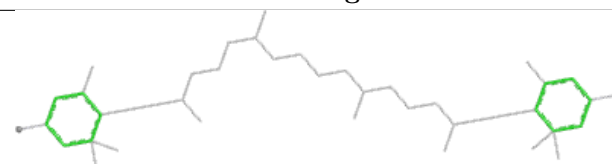


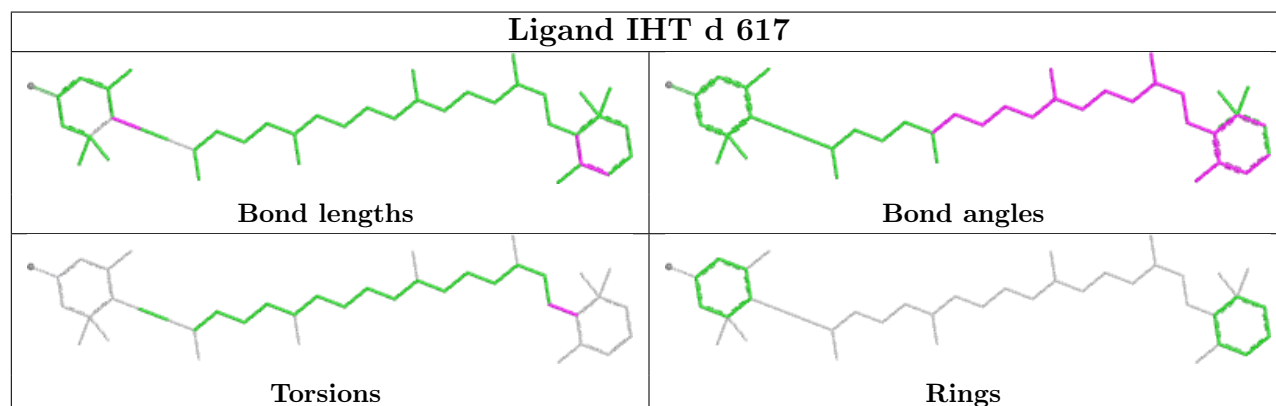
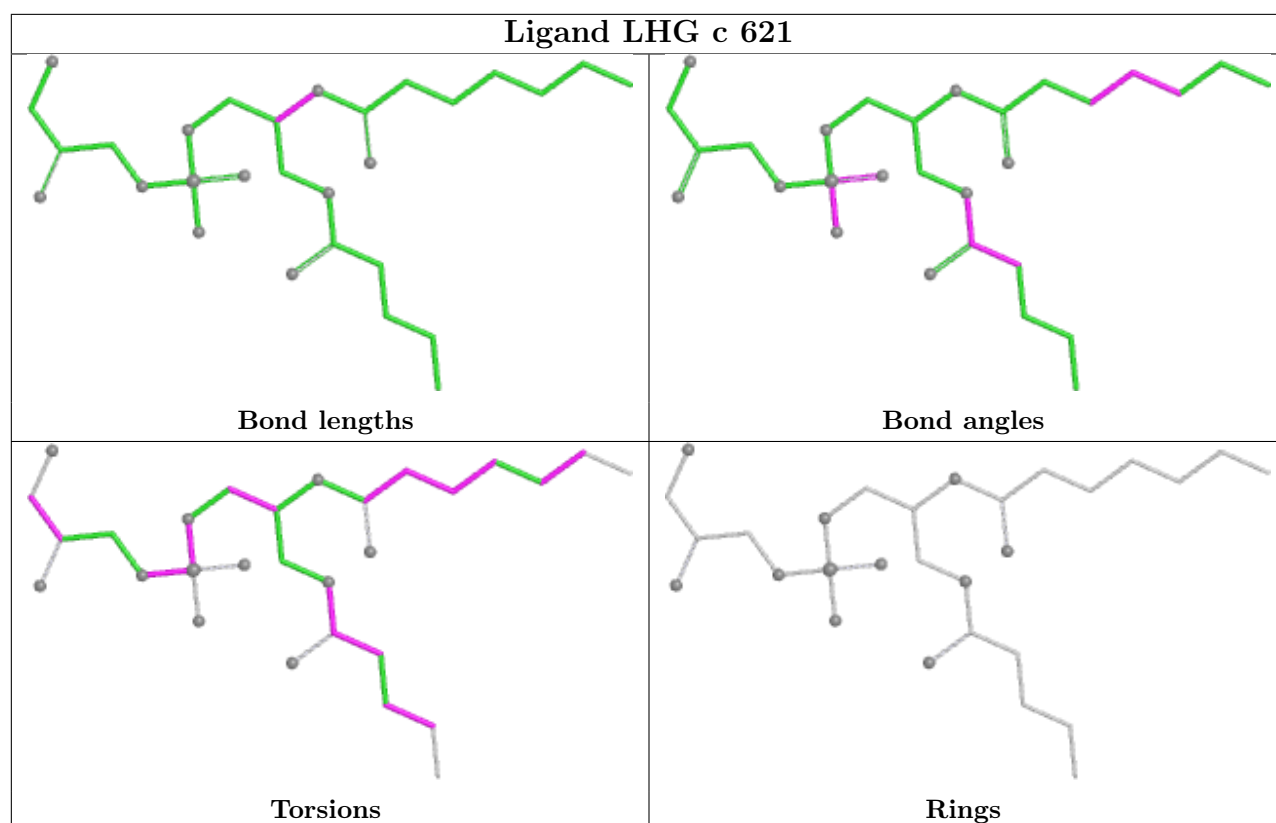


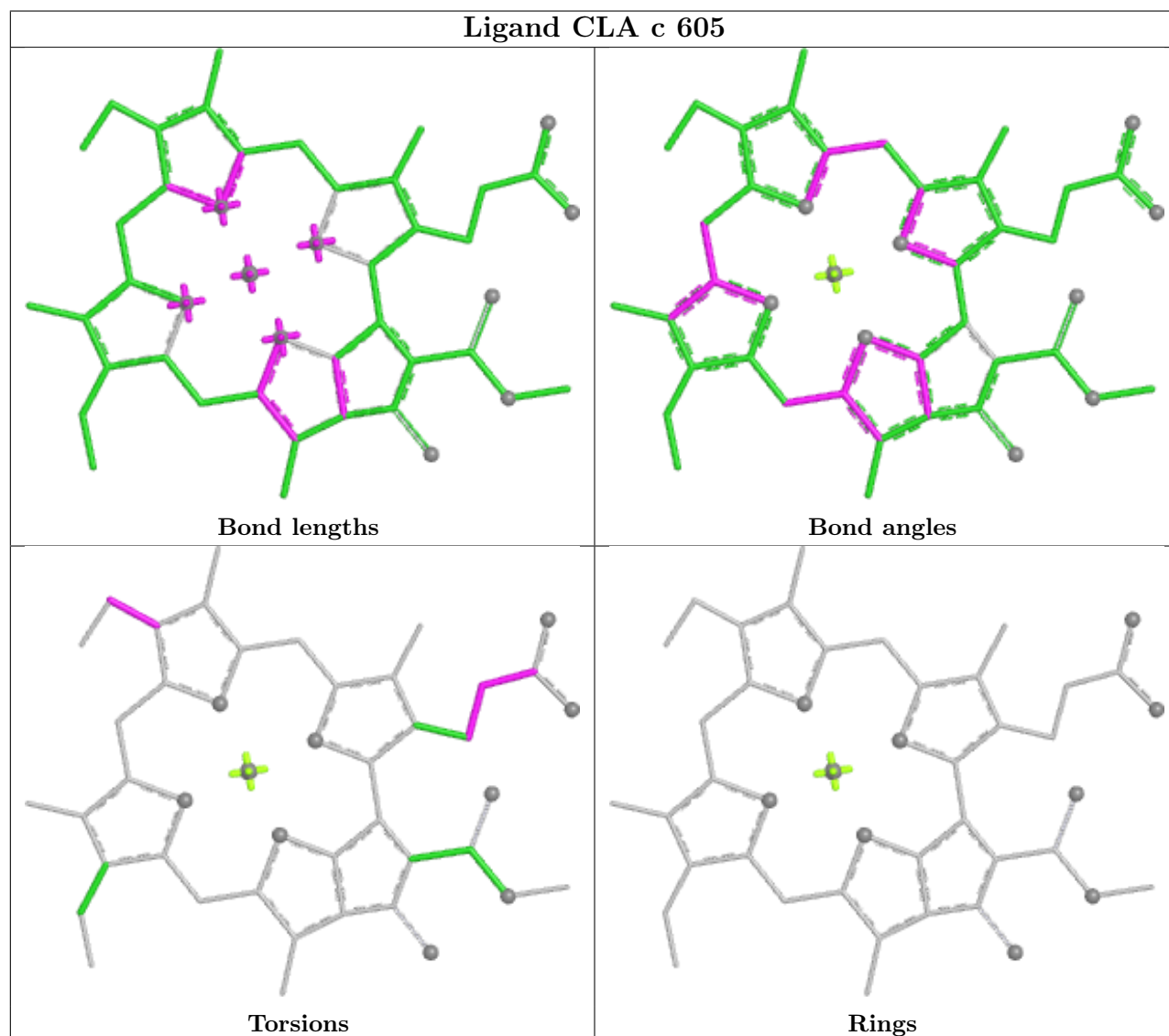
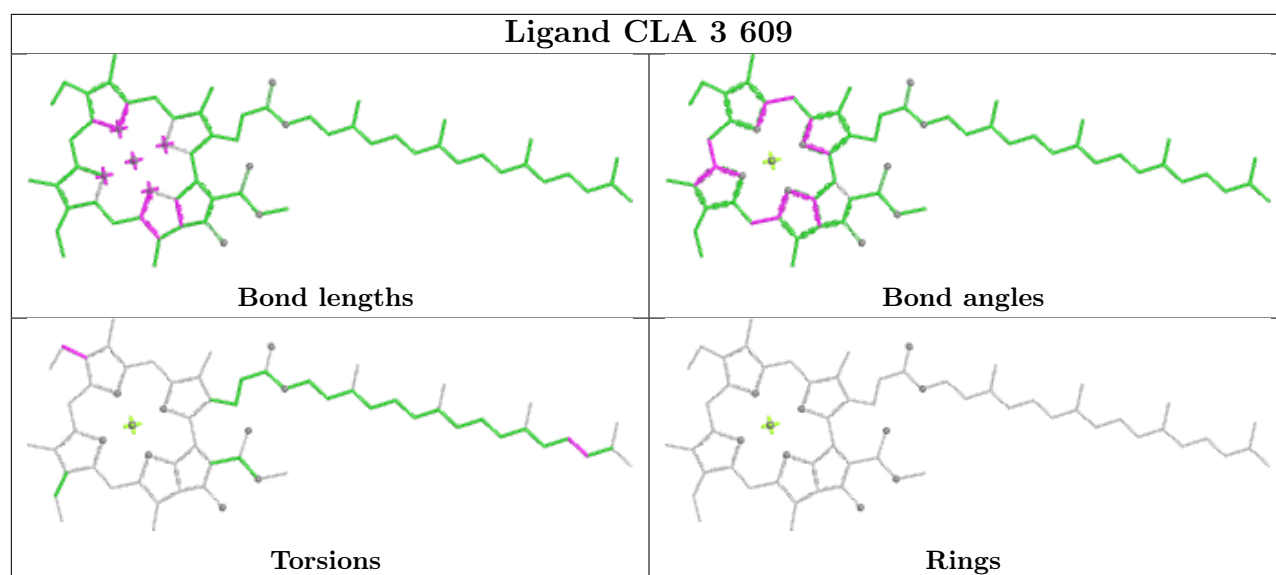


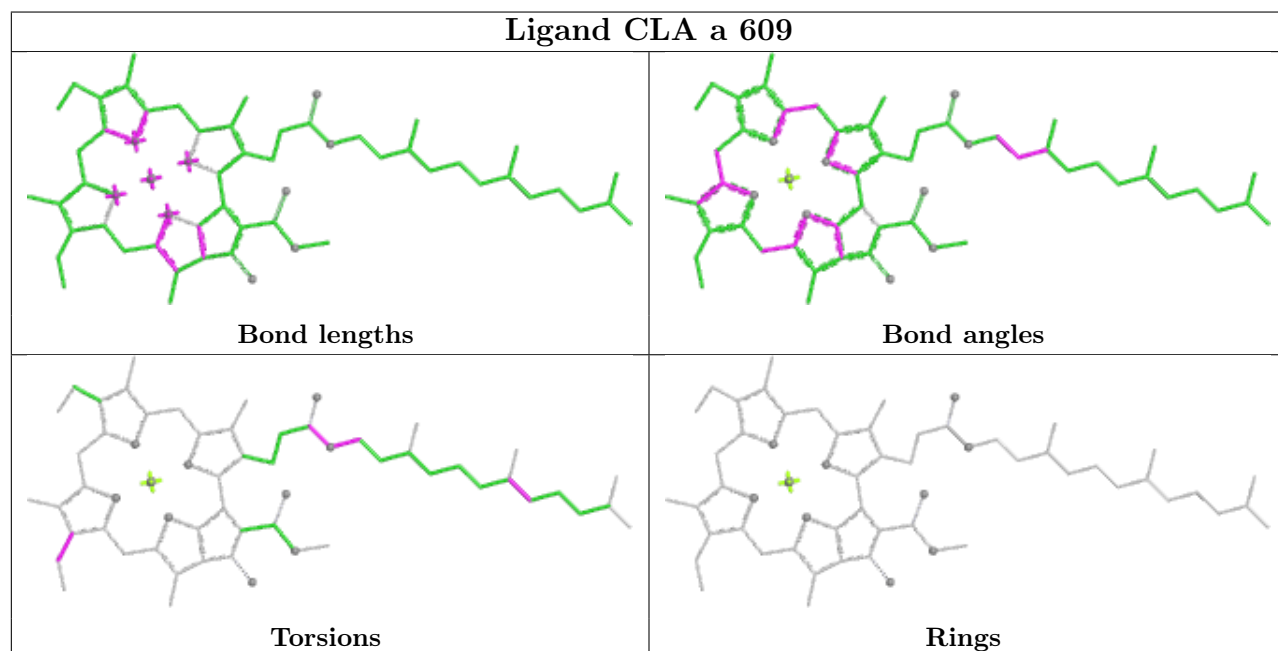
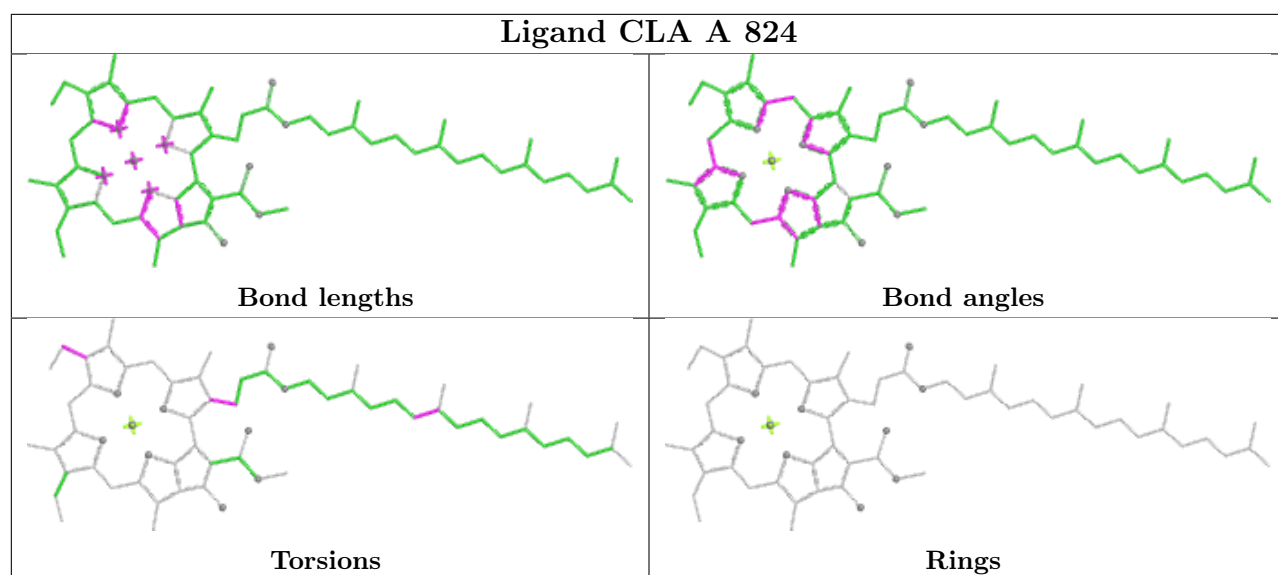
Ligand II0 5 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT A 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

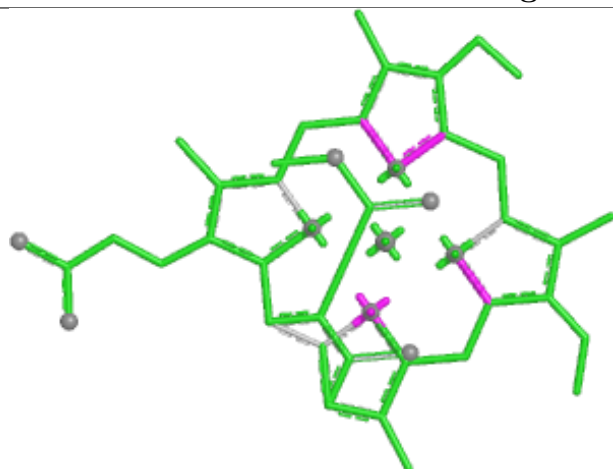
Ligand II0 5 620	
	
Bond lengths	Bond angles
	
Torsions	Rings



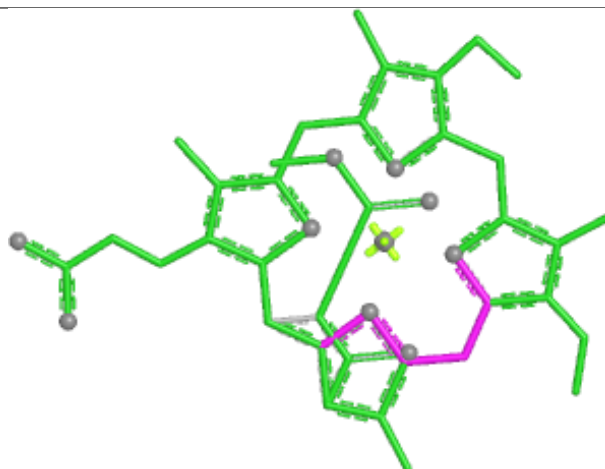




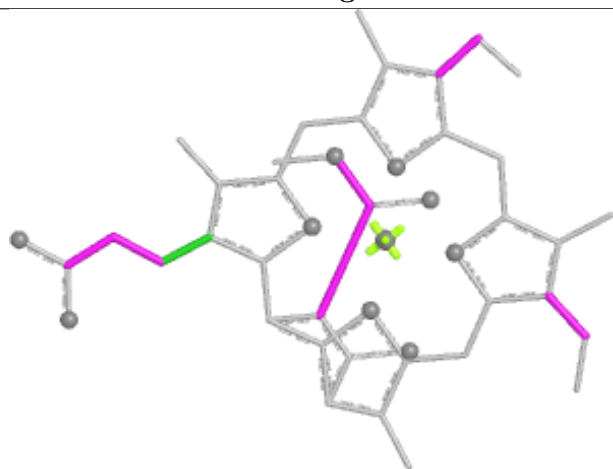
Ligand KC2 2 610



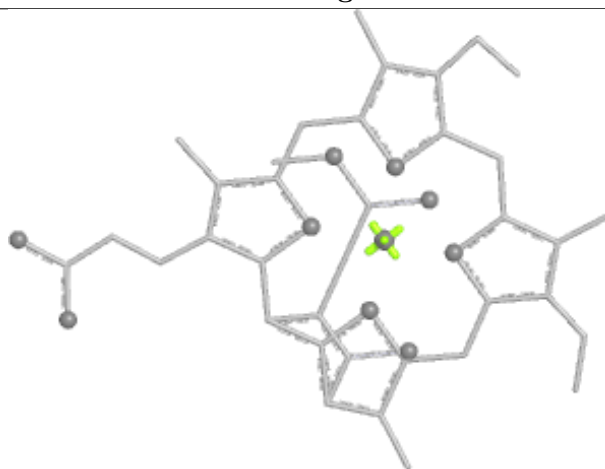
Bond lengths



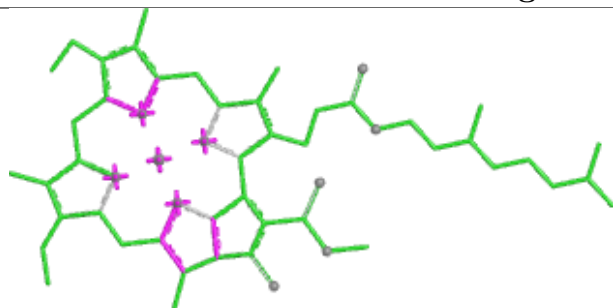
Bond angles



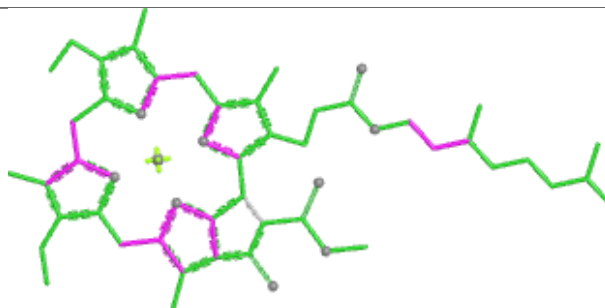
Torsions



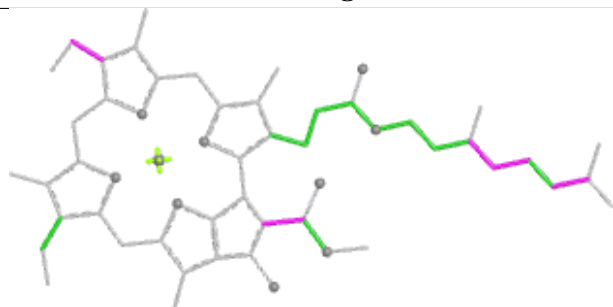
Rings

Ligand CLA 4 604

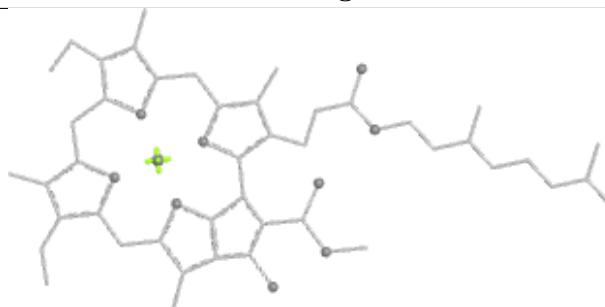
Bond lengths



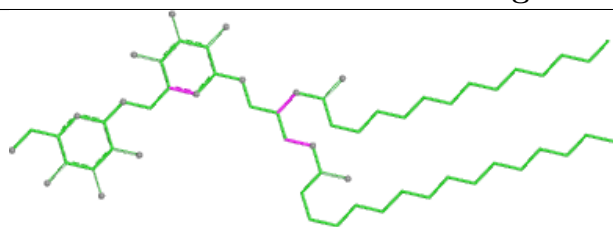
Bond angles



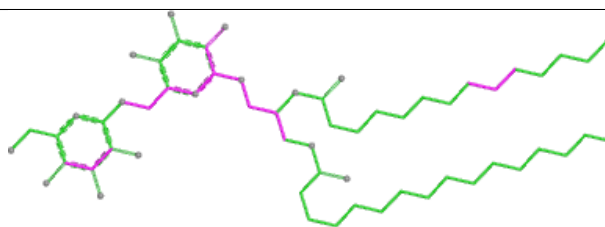
Torsions



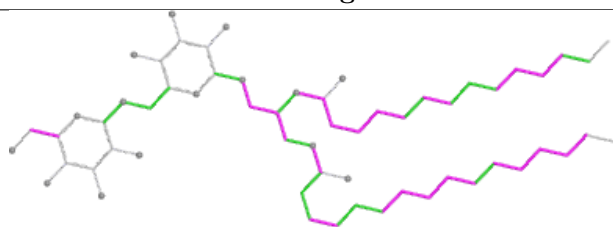
Rings

Ligand DGD Z 303

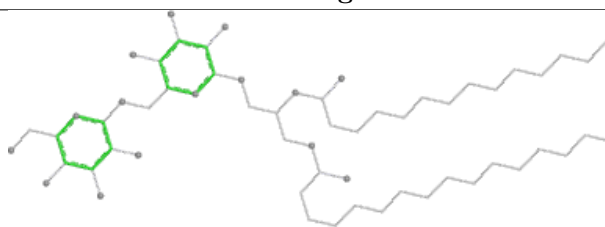
Bond lengths



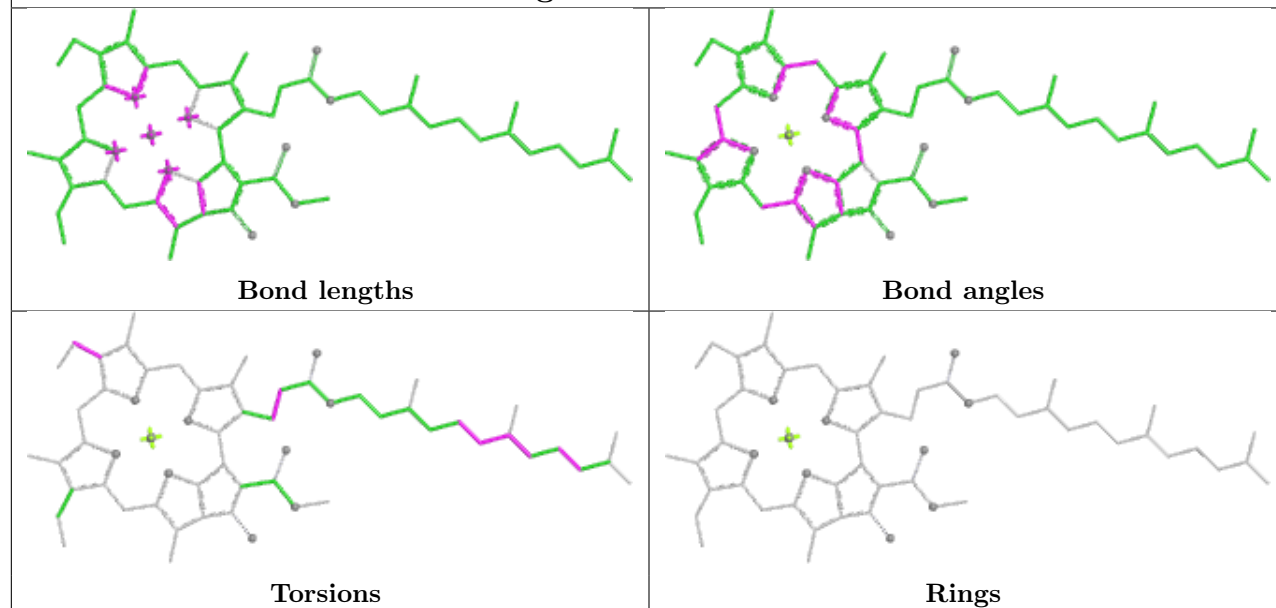
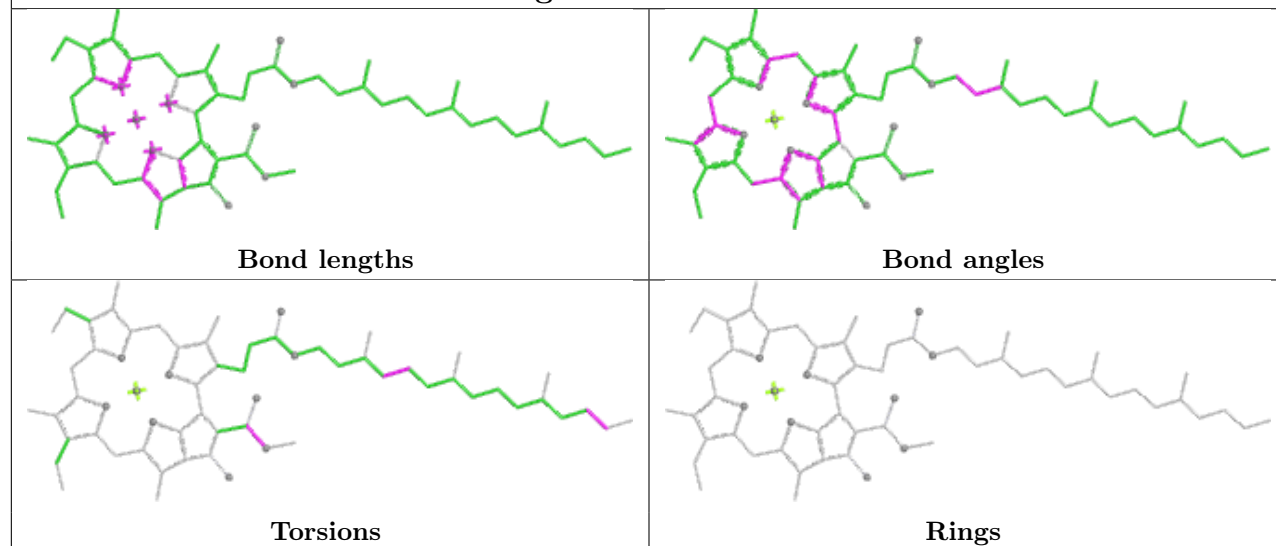
Bond angles

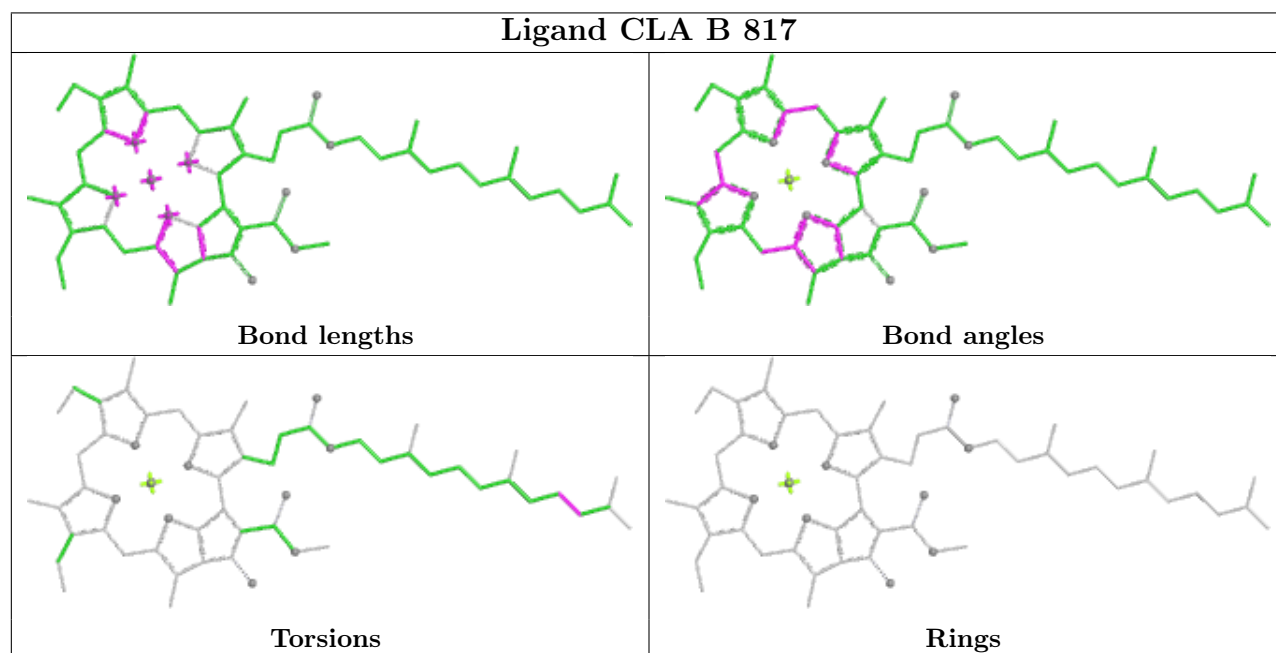
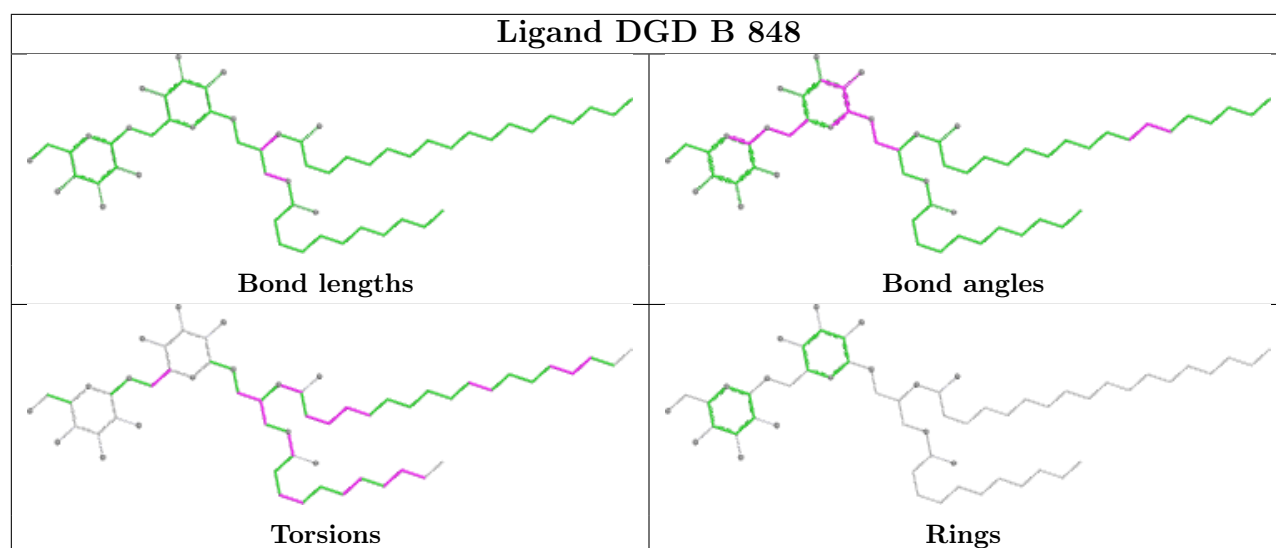


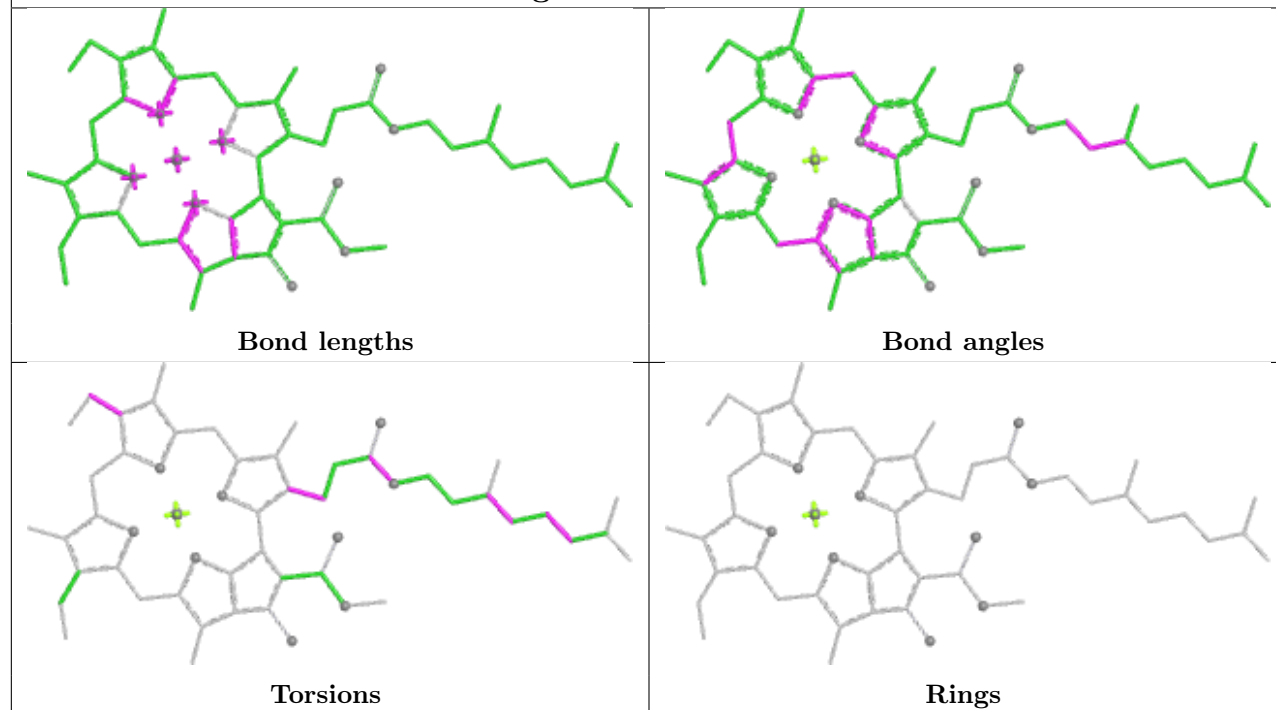
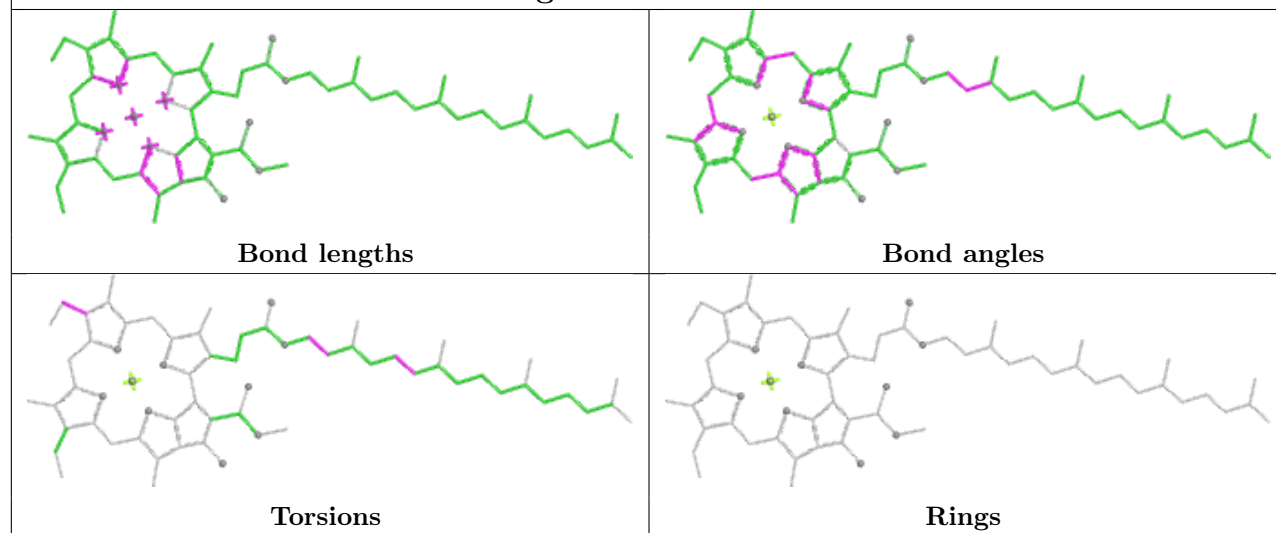
Torsions

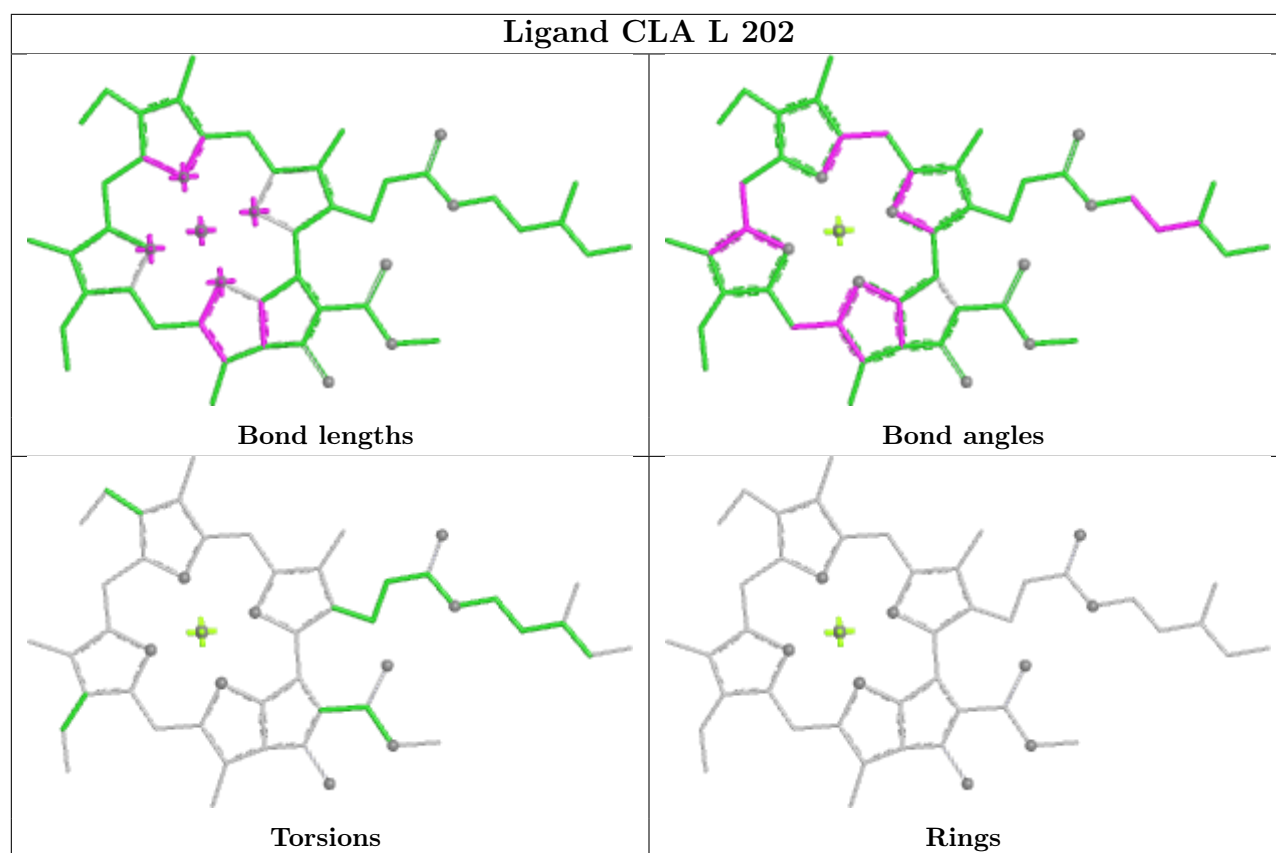


Rings

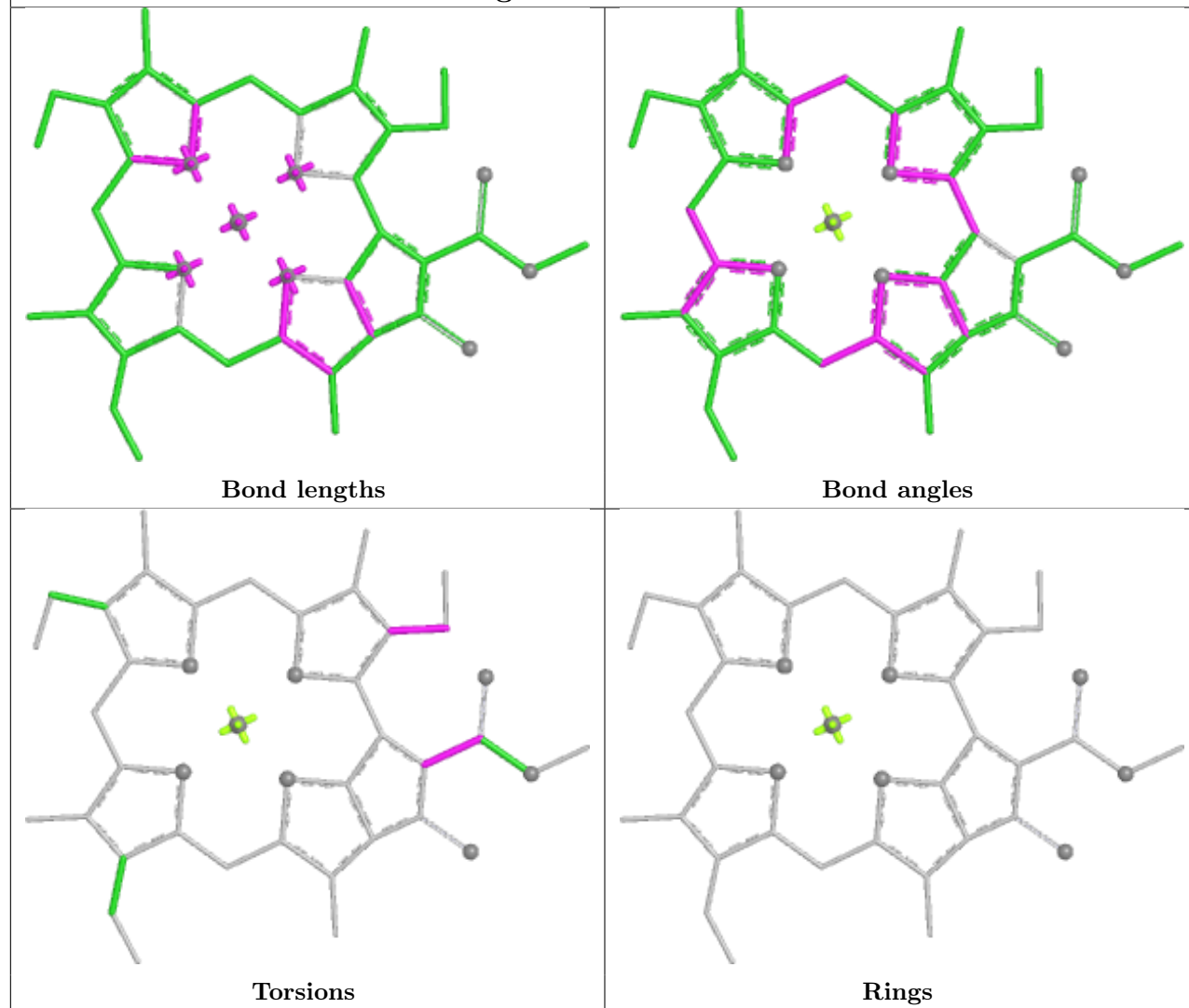
Ligand CLA a 603**Ligand CLA d 612**



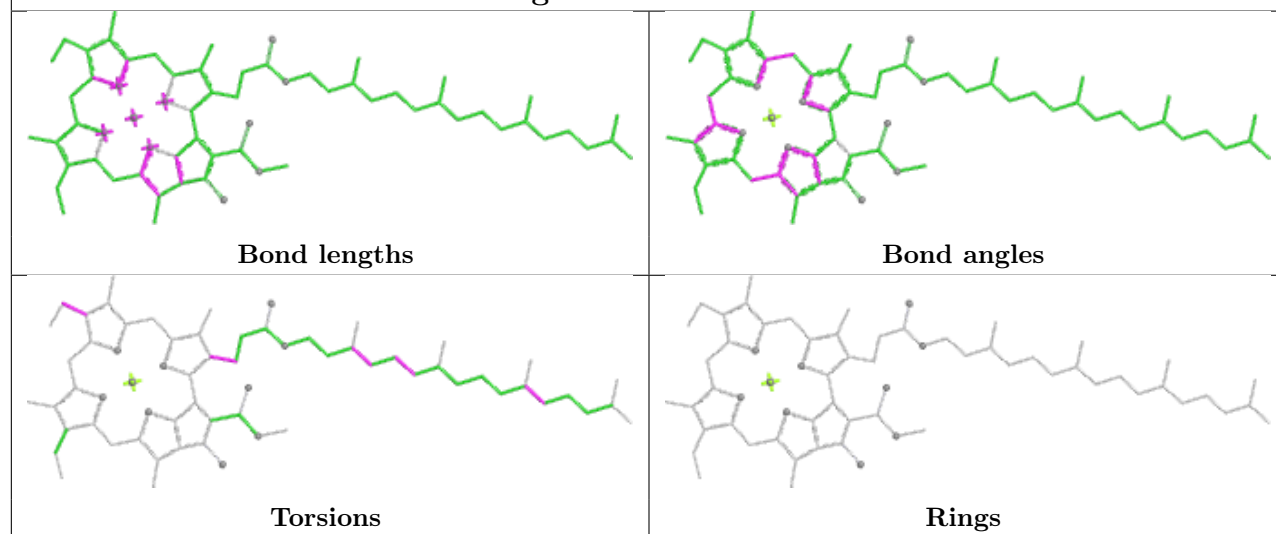
Ligand CLA B 831**Ligand CLA 4 608**



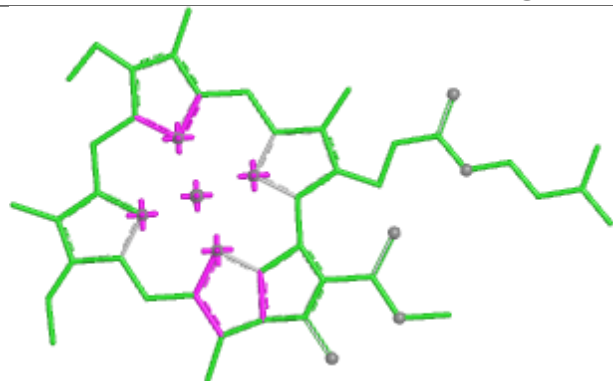
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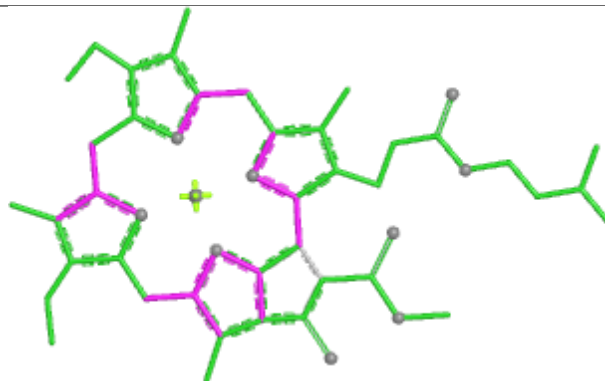
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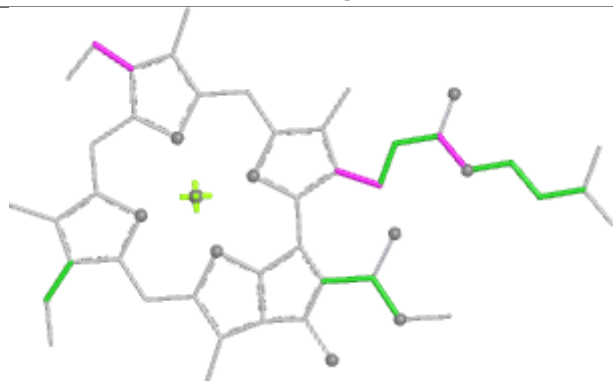
Ligand CLA 7 612



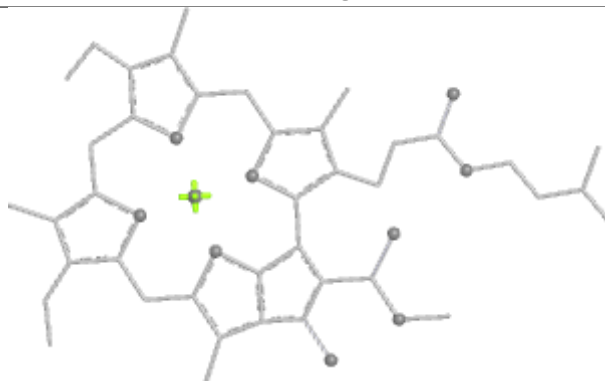
Bond lengths



Bond angles

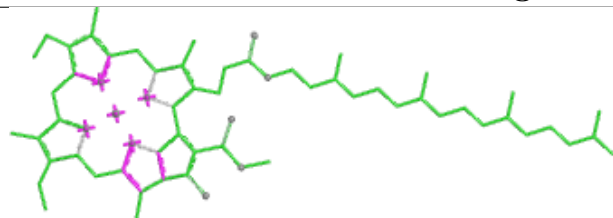


Torsions

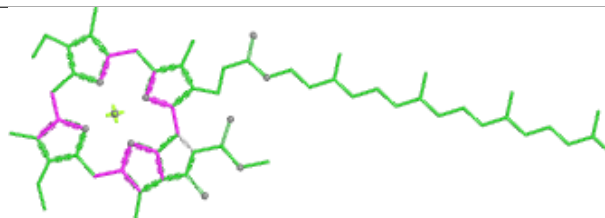


Rings

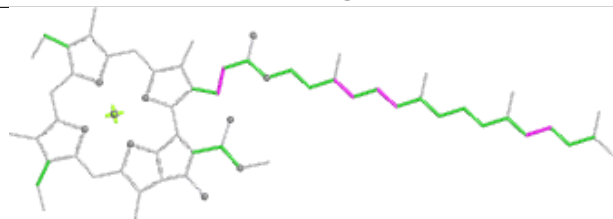
Ligand CLA A 827



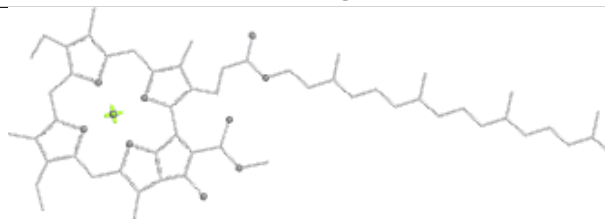
Bond lengths



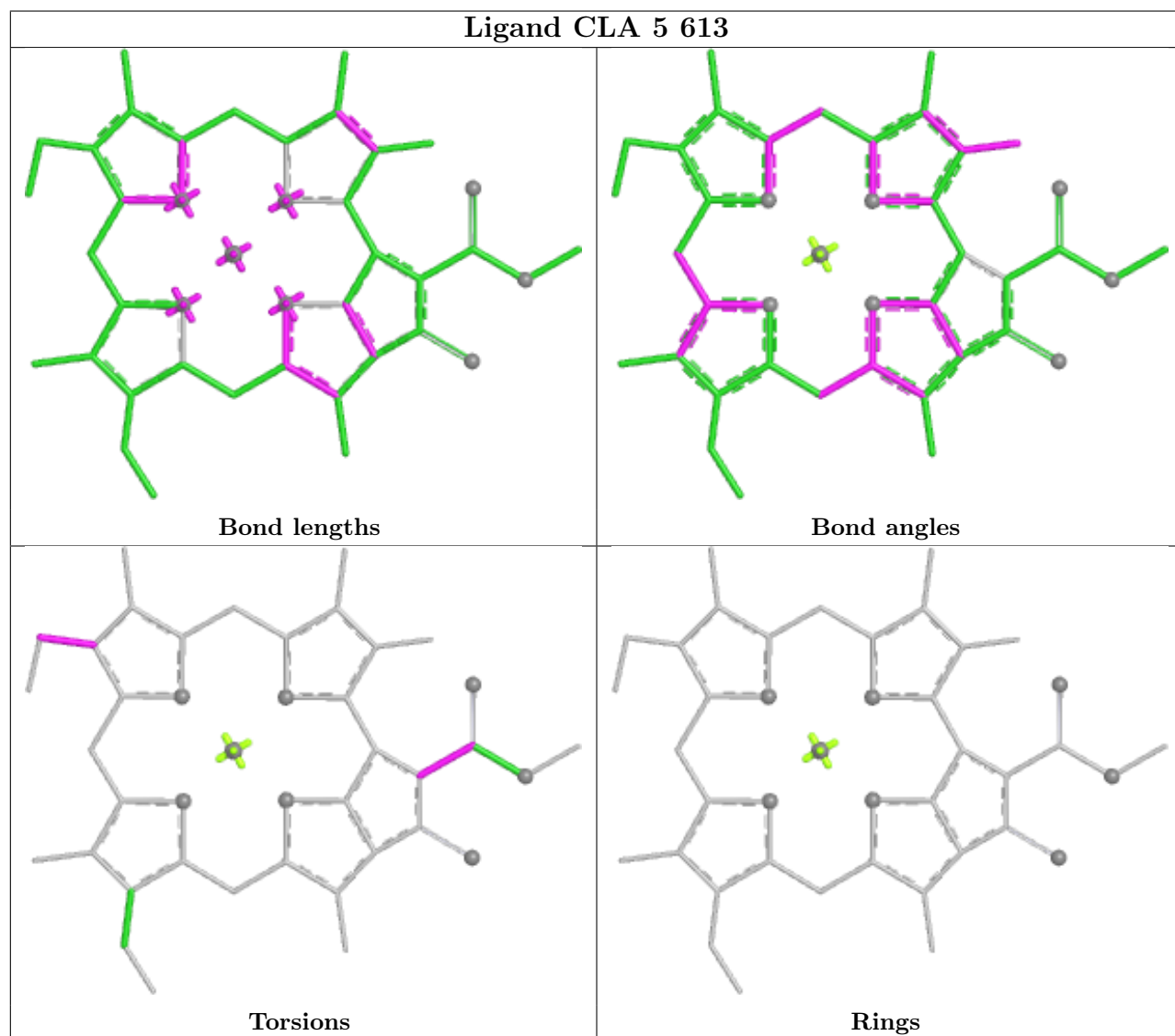
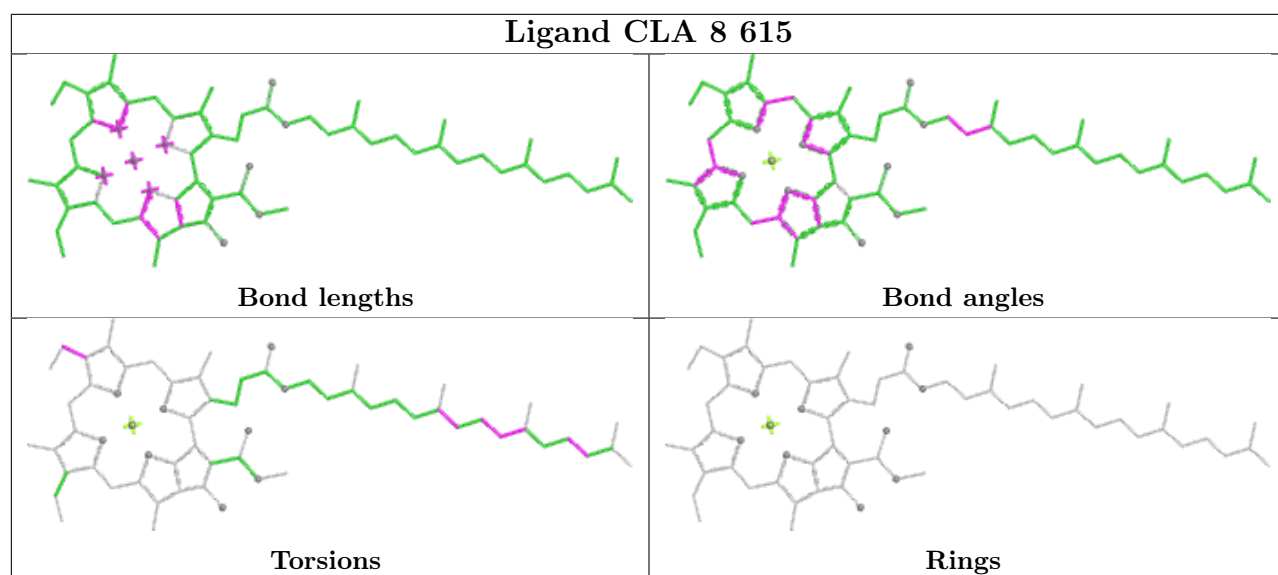
Bond angles

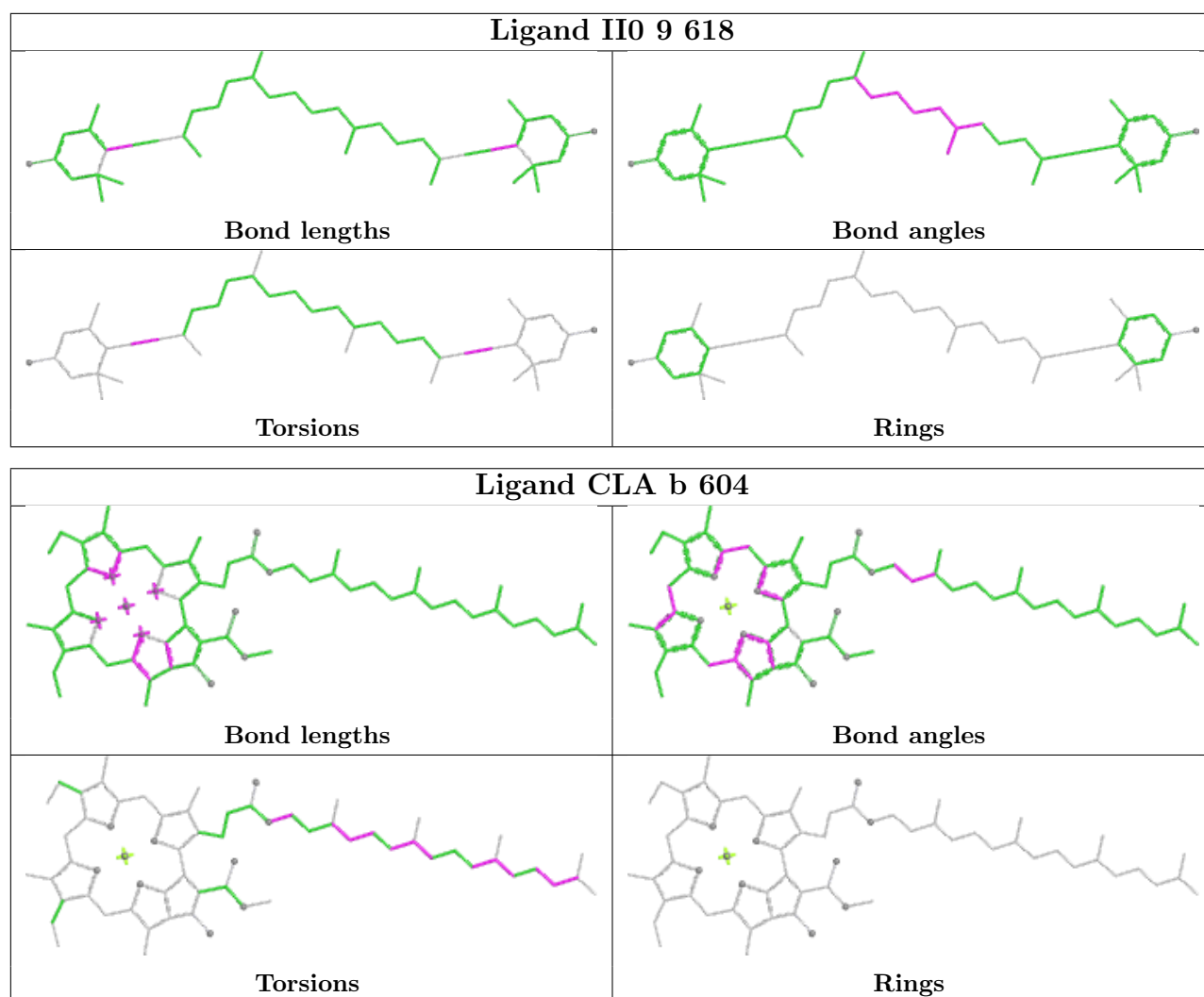


Torsions

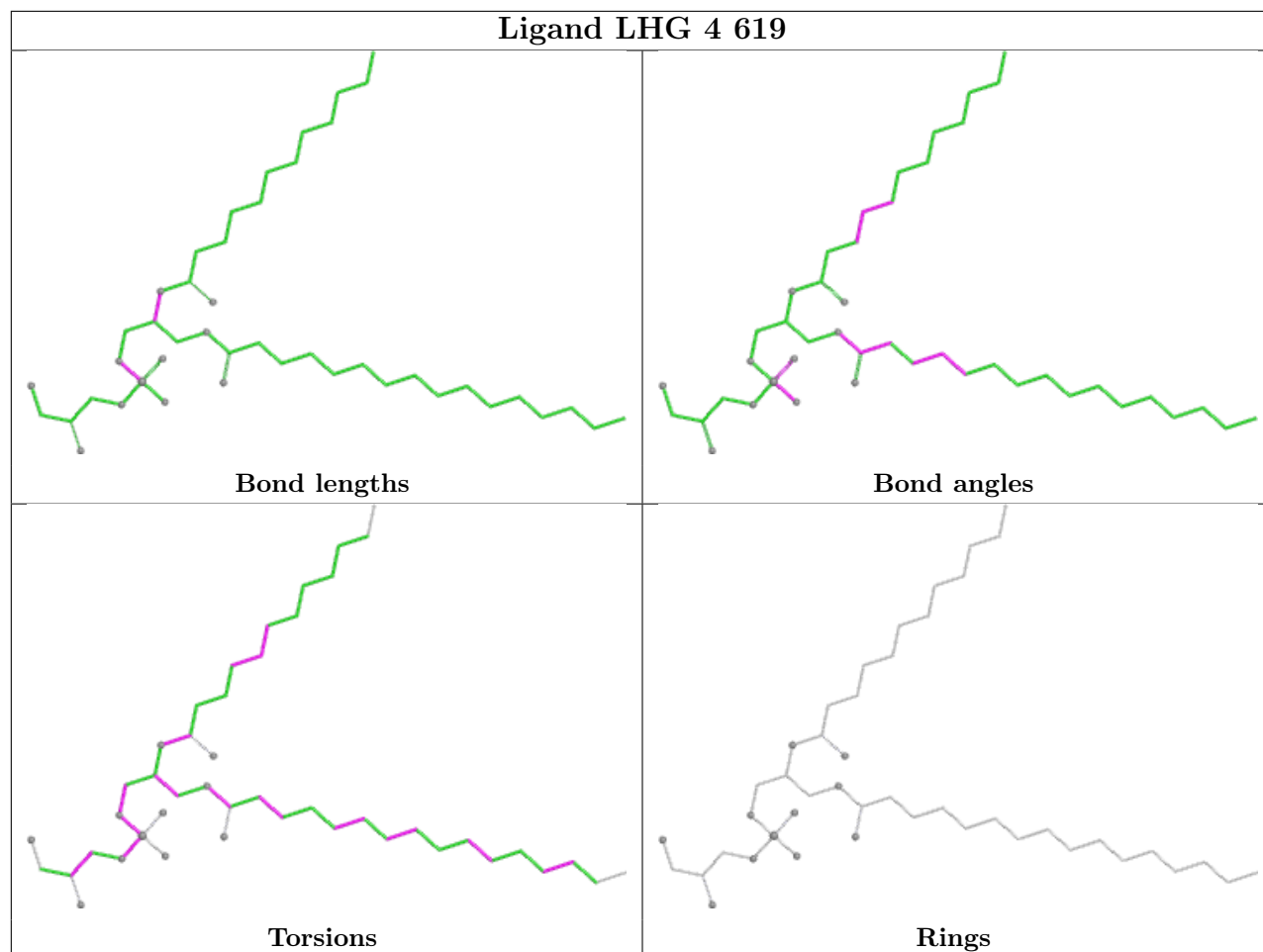


Rings

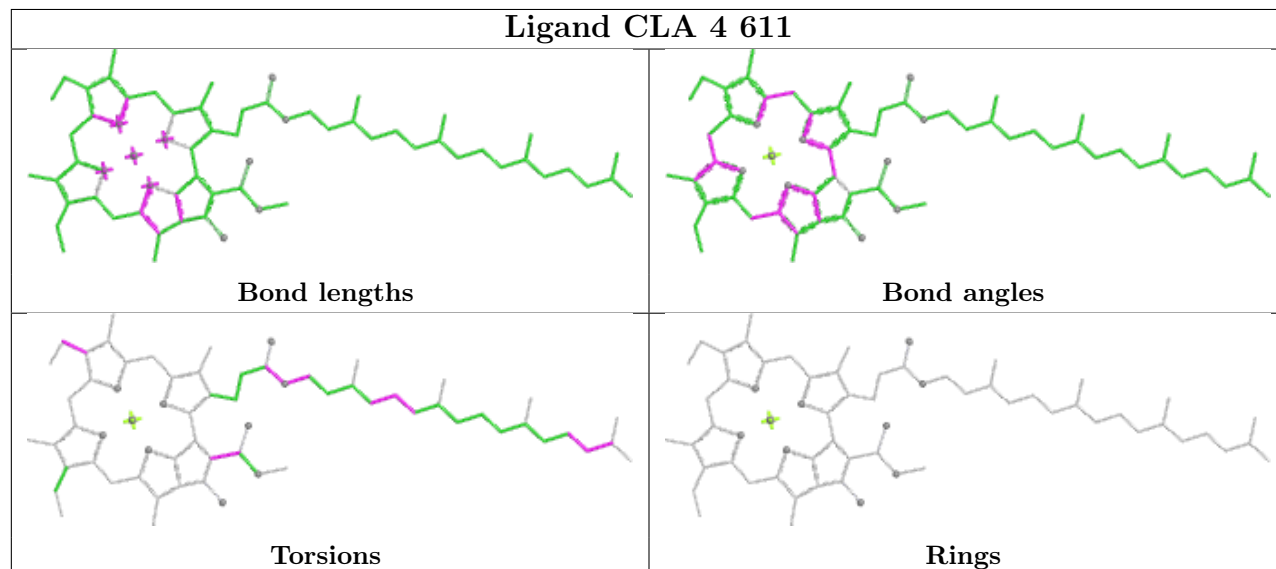




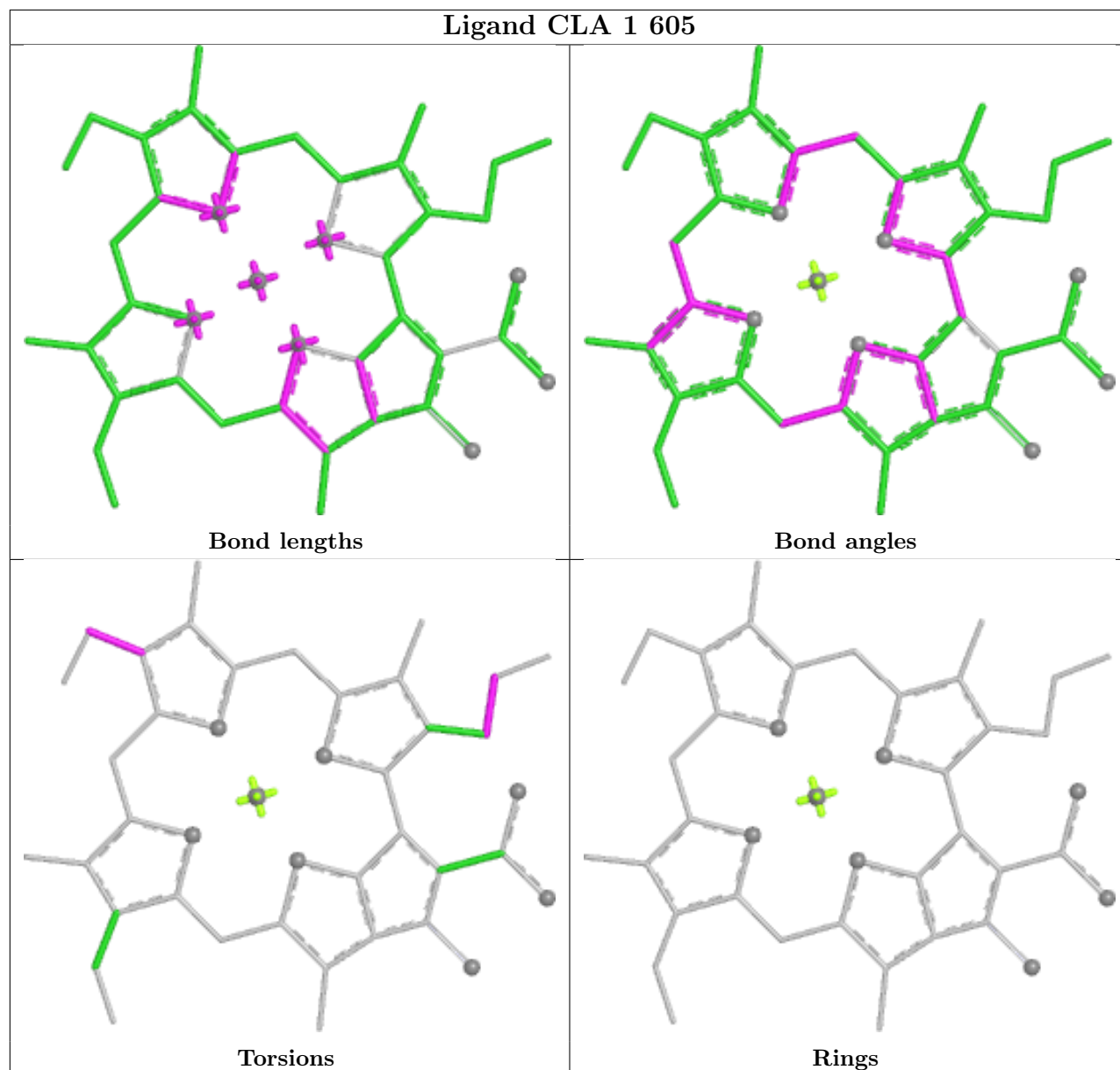
Ligand LHG 4 619



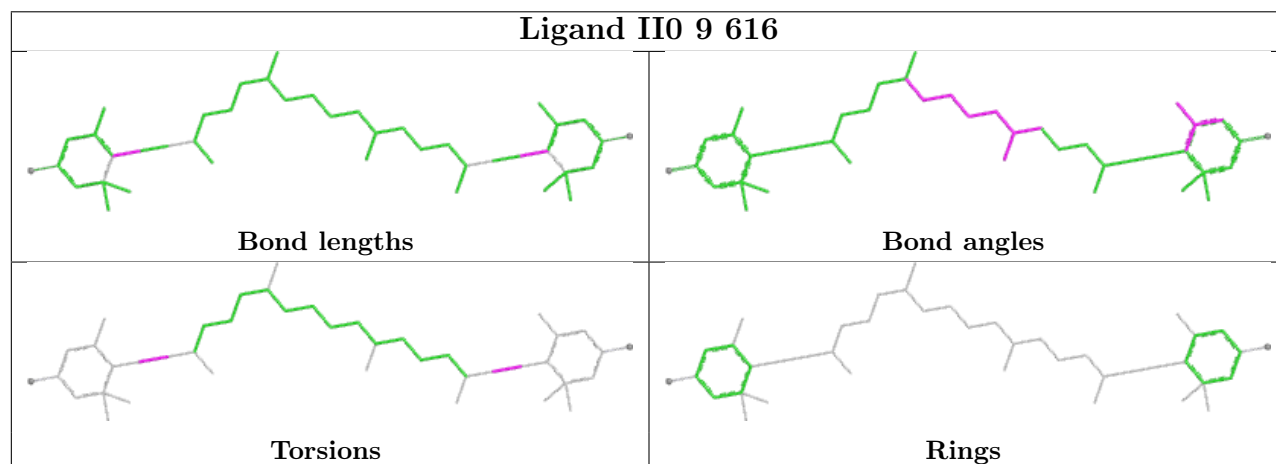
Ligand CLA 4 611



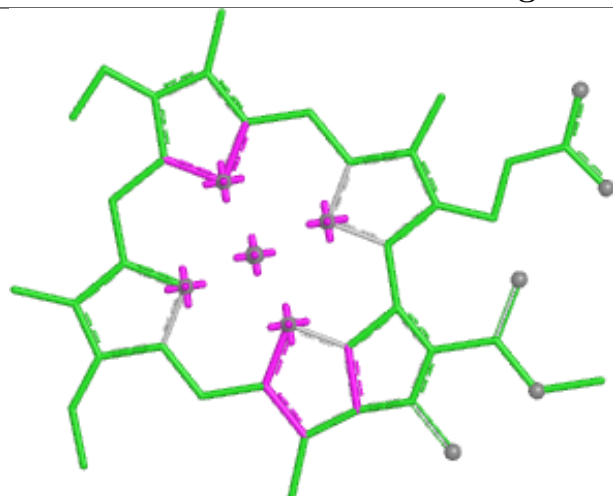
Ligand CLA 1 605



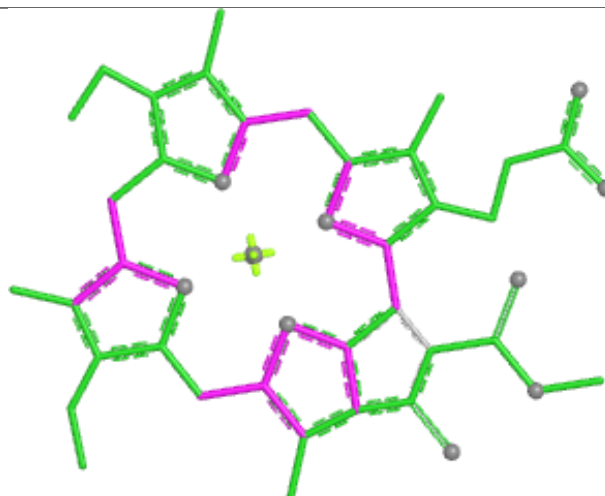
Ligand II0 9 616



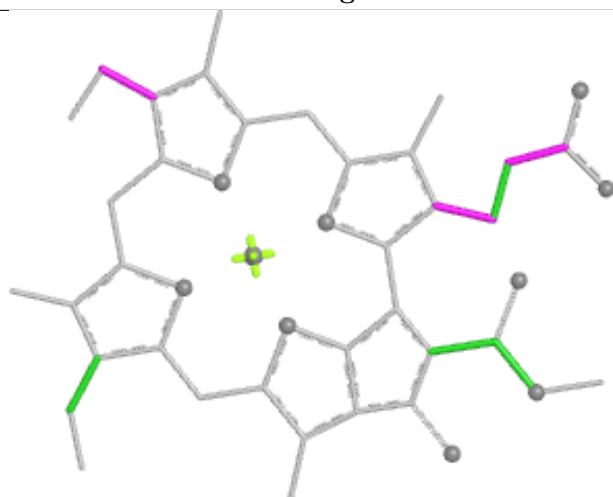
Ligand CLA 1 601



Bond lengths



Bond angles

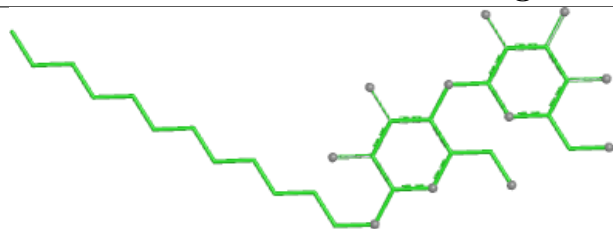


Torsions

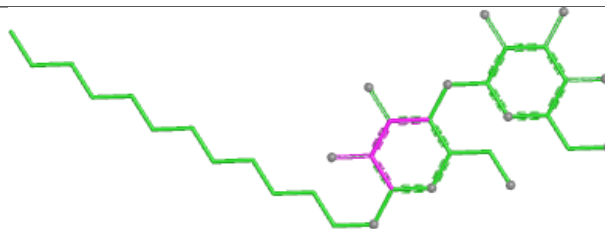


Rings

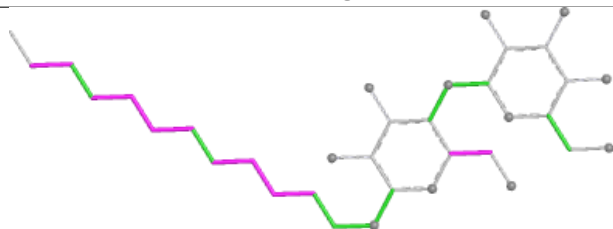
Ligand LMU 7 620



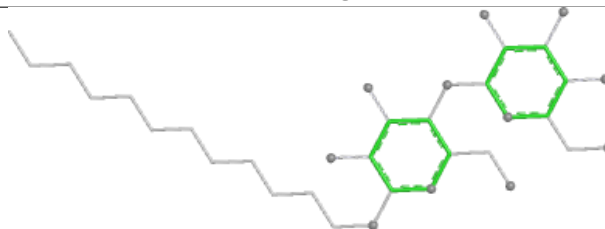
Bond lengths



Bond angles

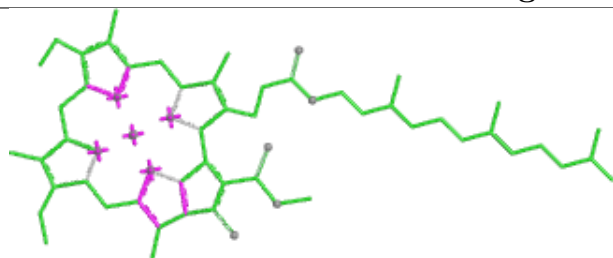


Torsions

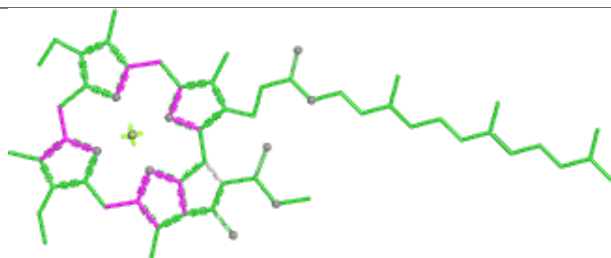


Rings

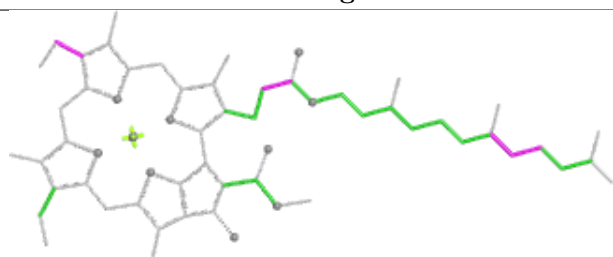
Ligand CLA 2 605



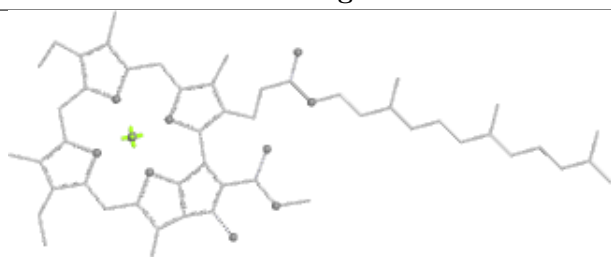
Bond lengths



Bond angles

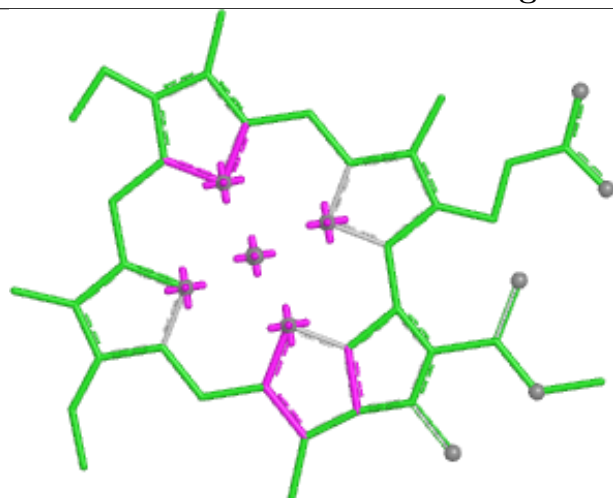


Torsions

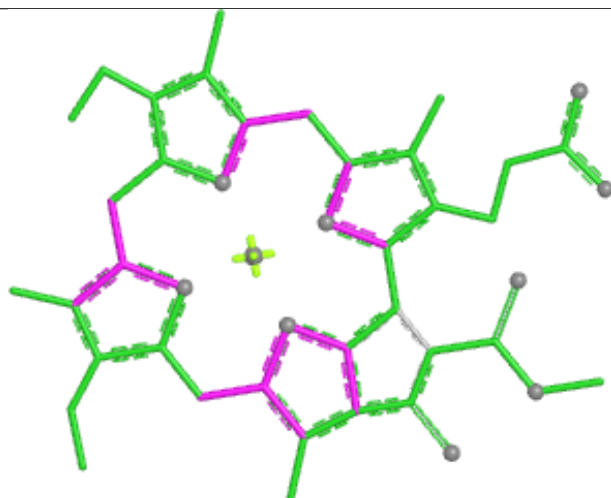


Rings

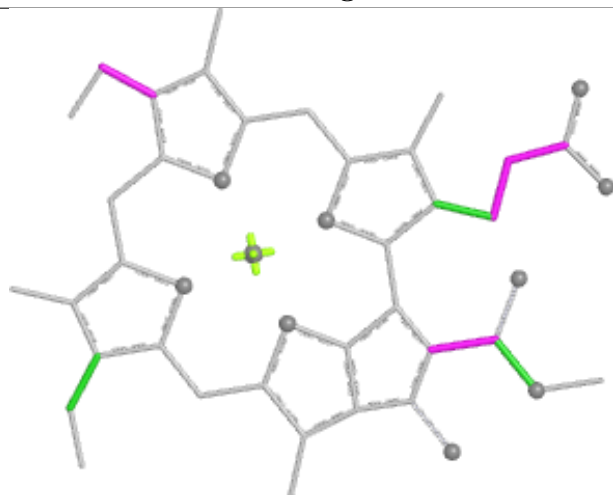
Ligand CLA c 613



Bond lengths



Bond angles

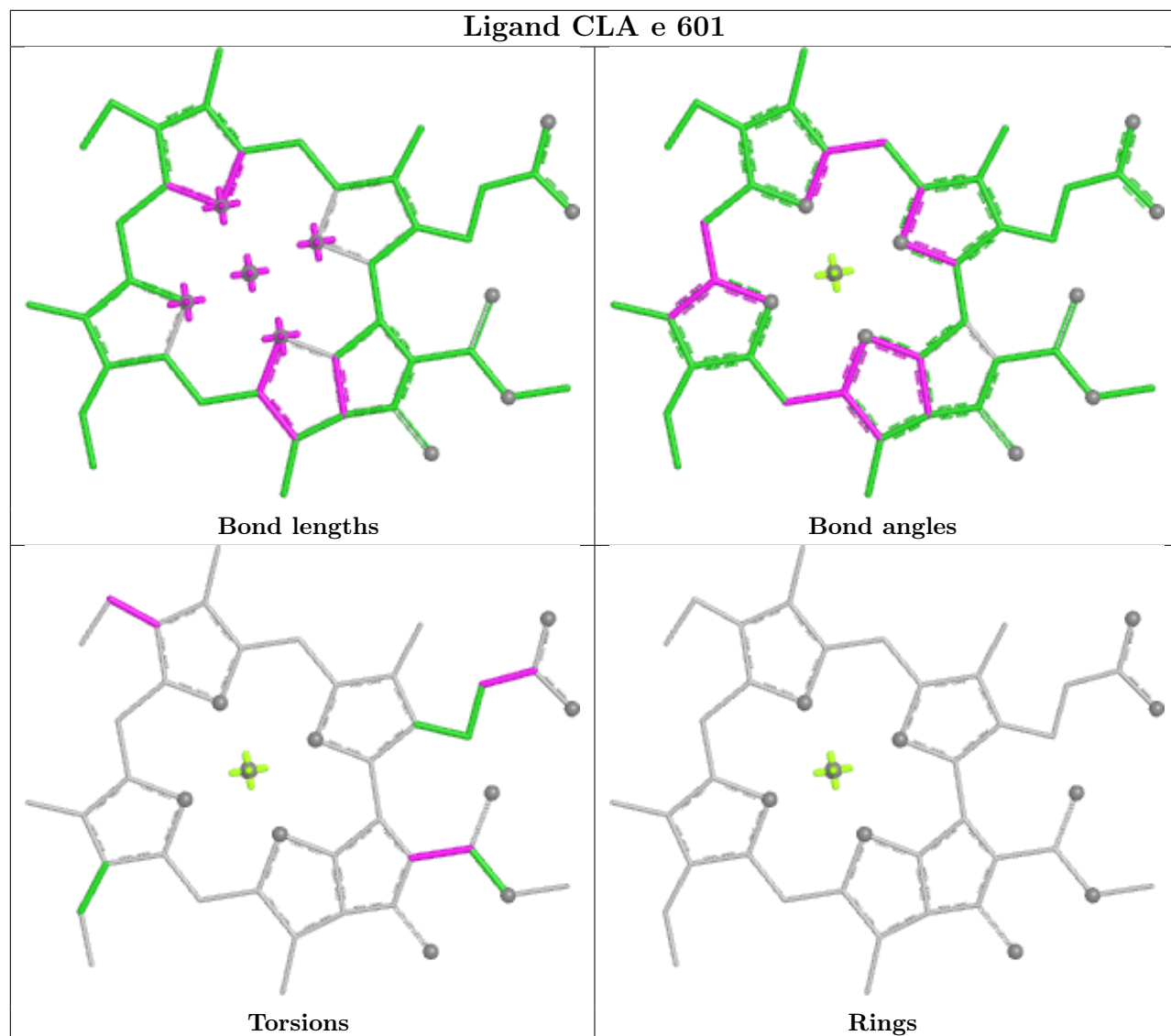


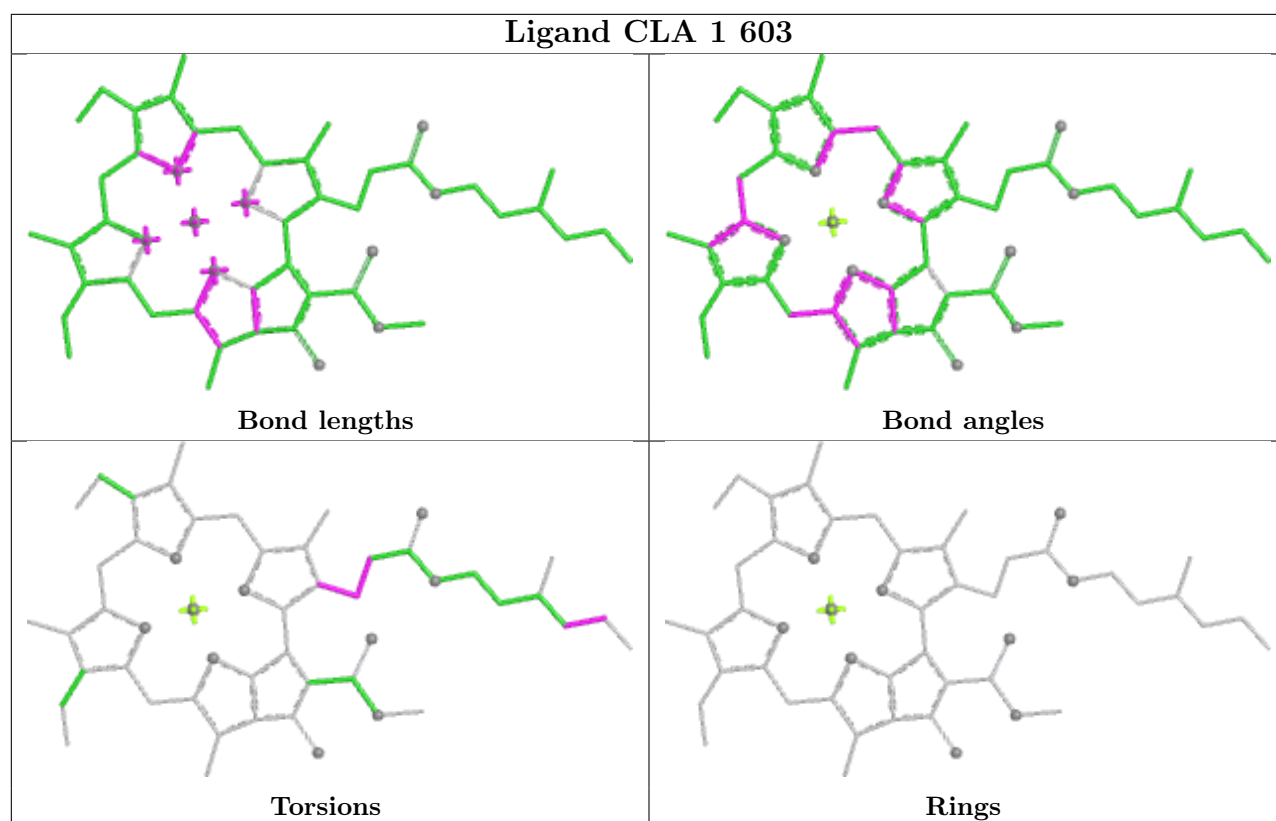
Torsions



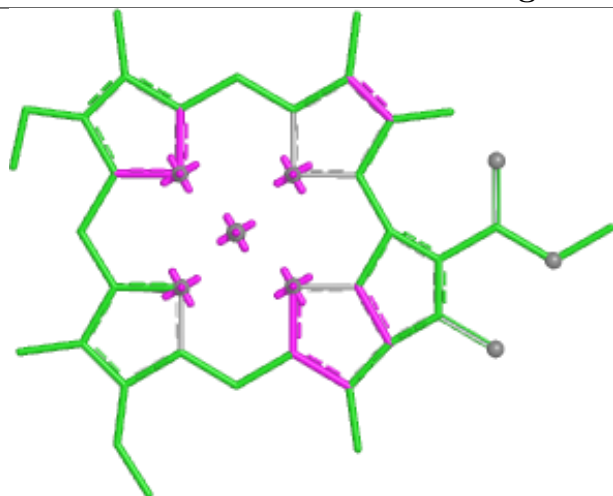
Rings

Ligand CLA e 601

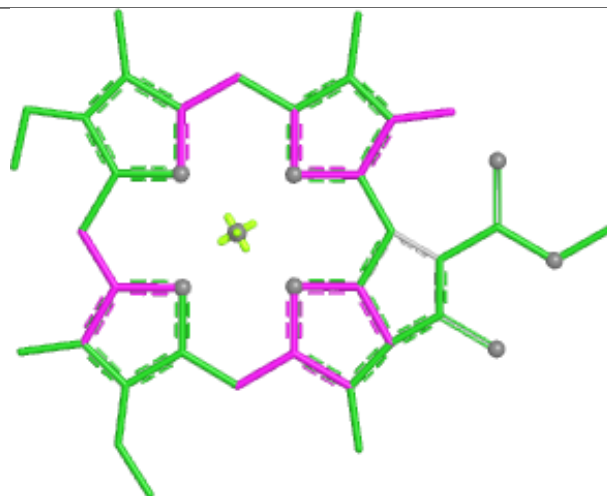




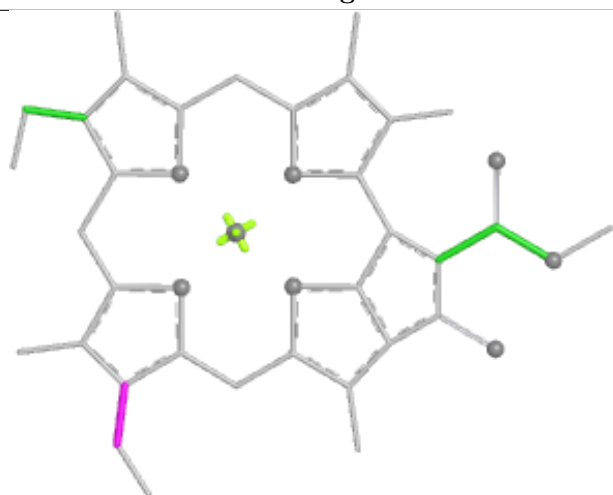
Ligand CLA 9 609



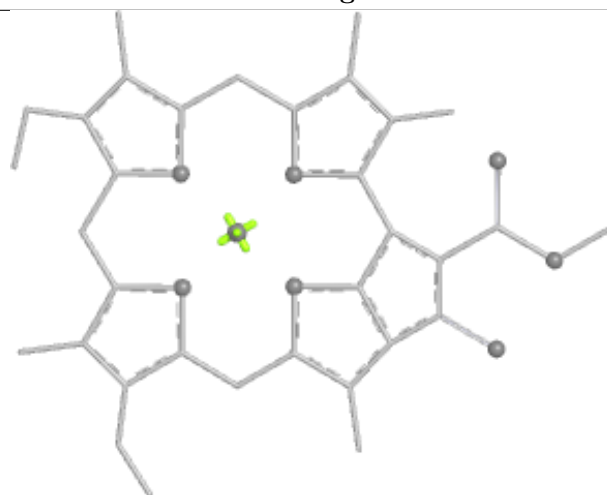
Bond lengths



Bond angles

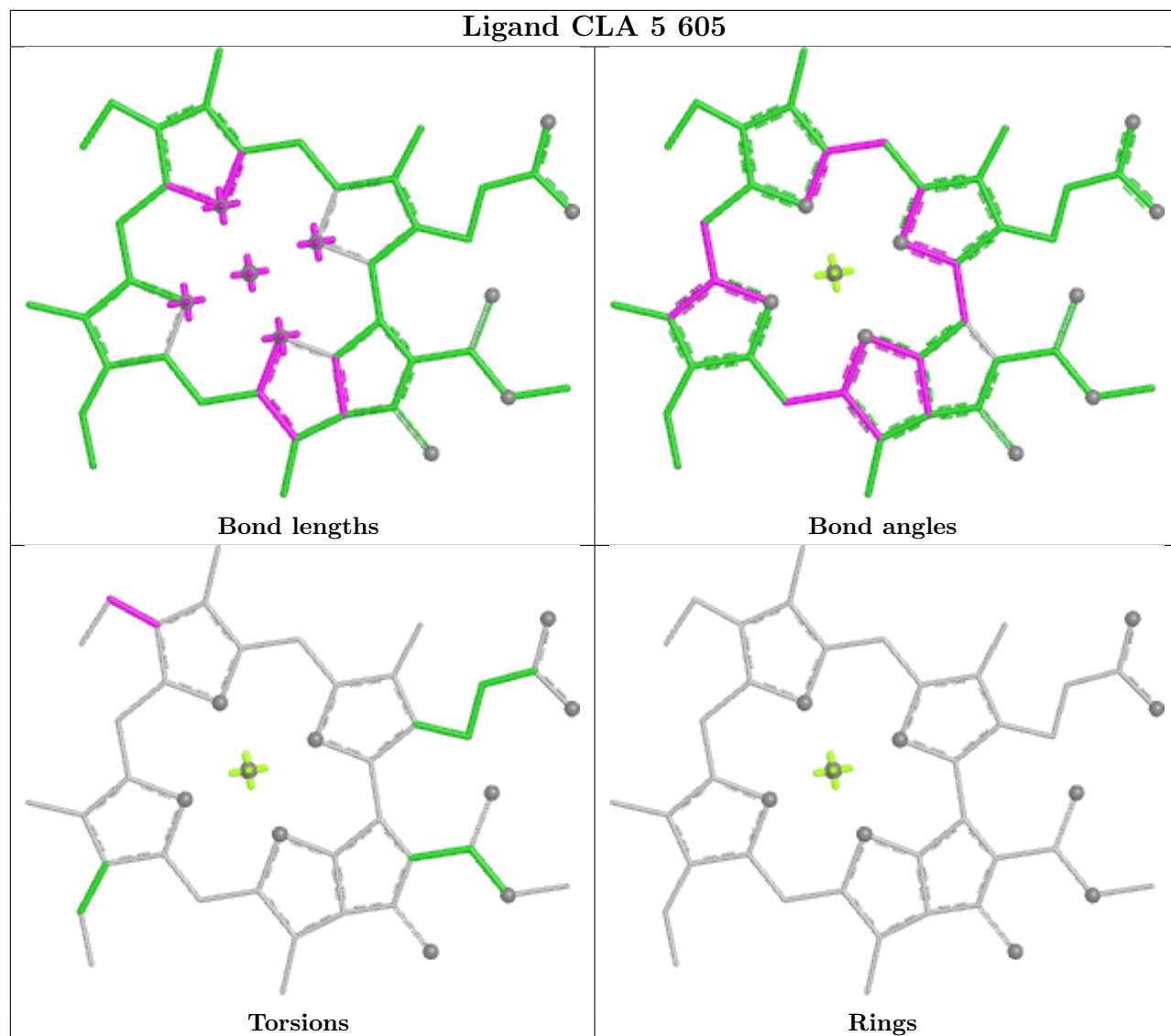


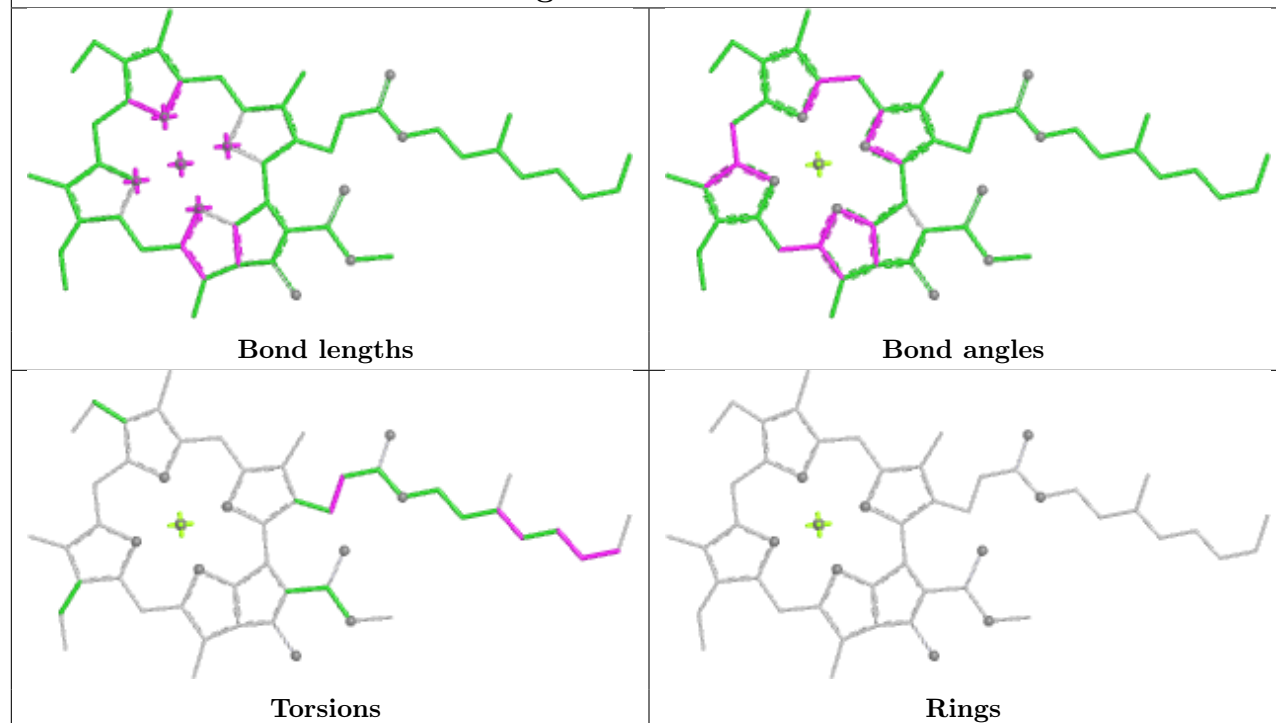
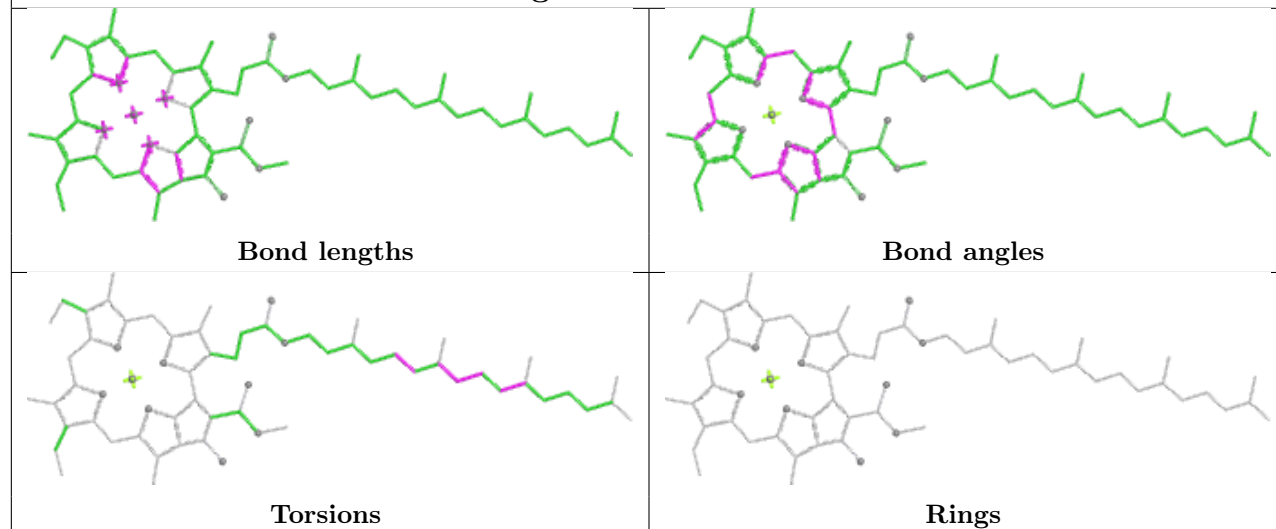
Torsions

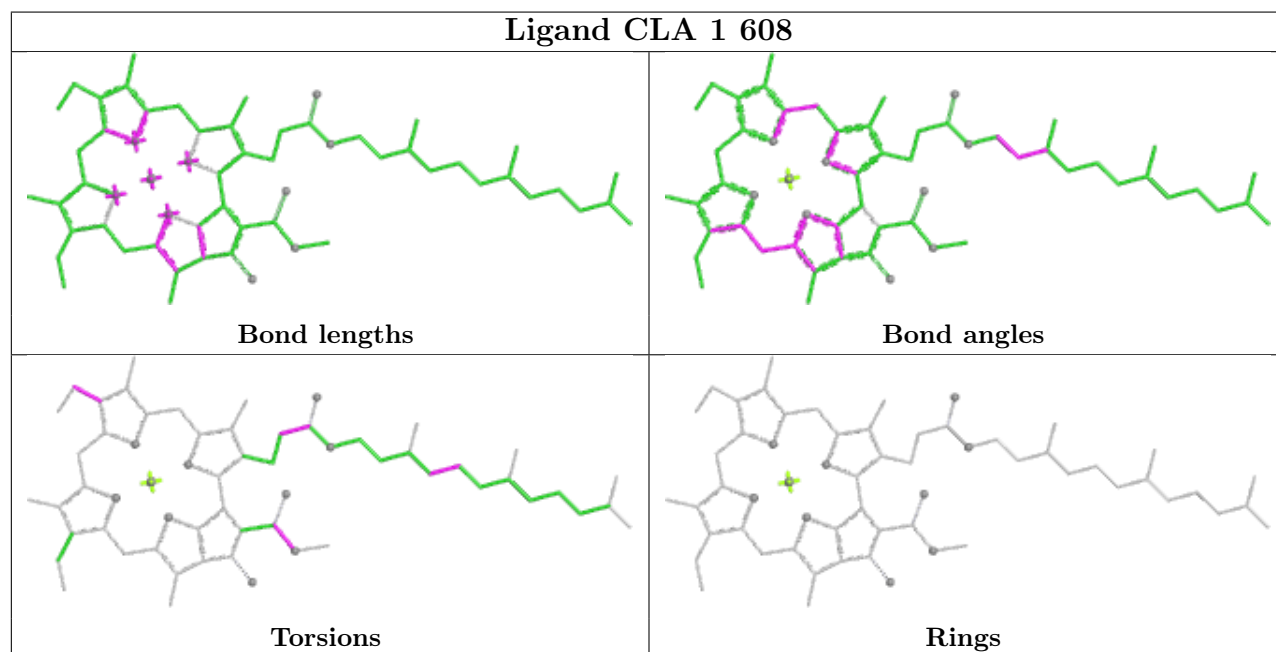
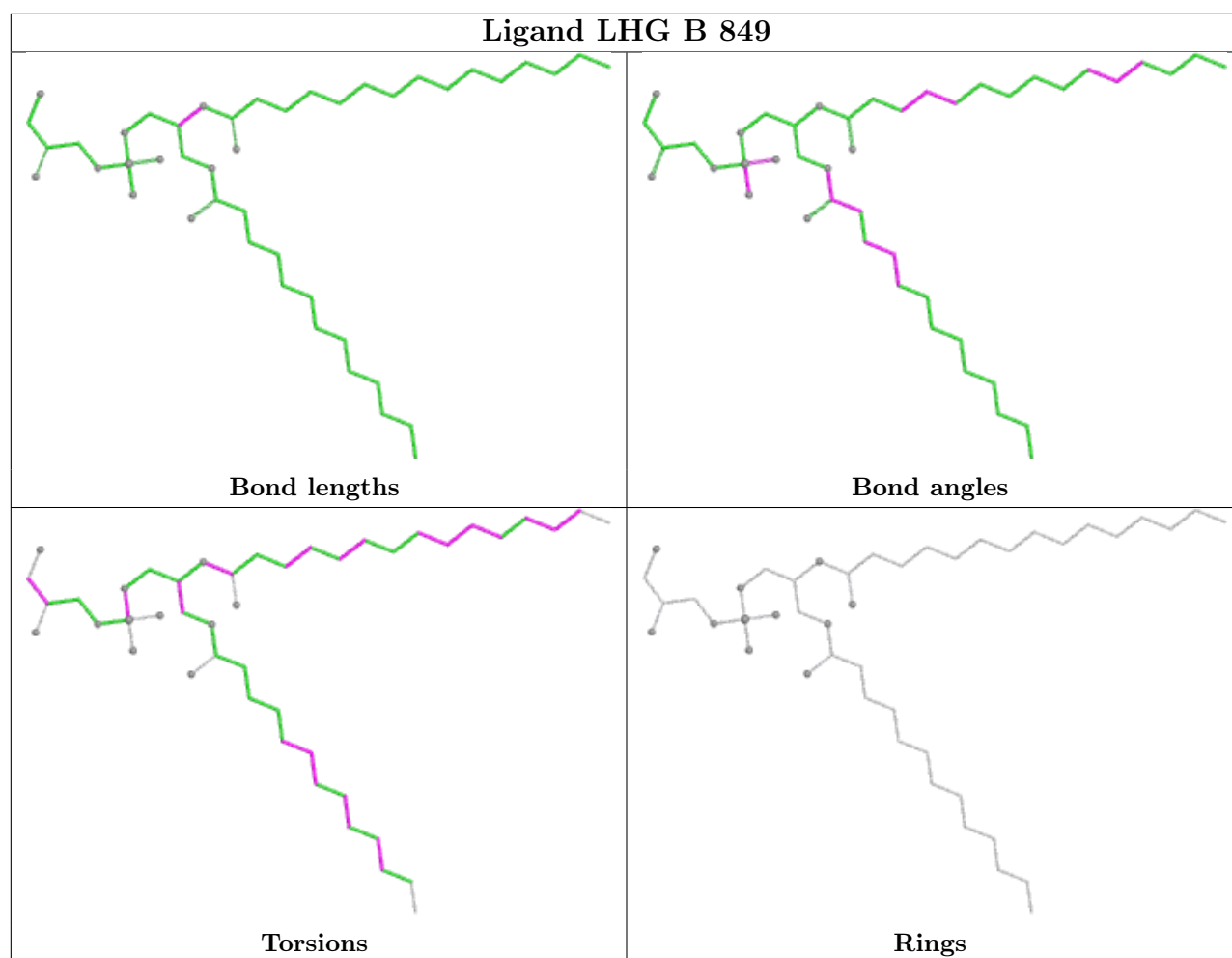


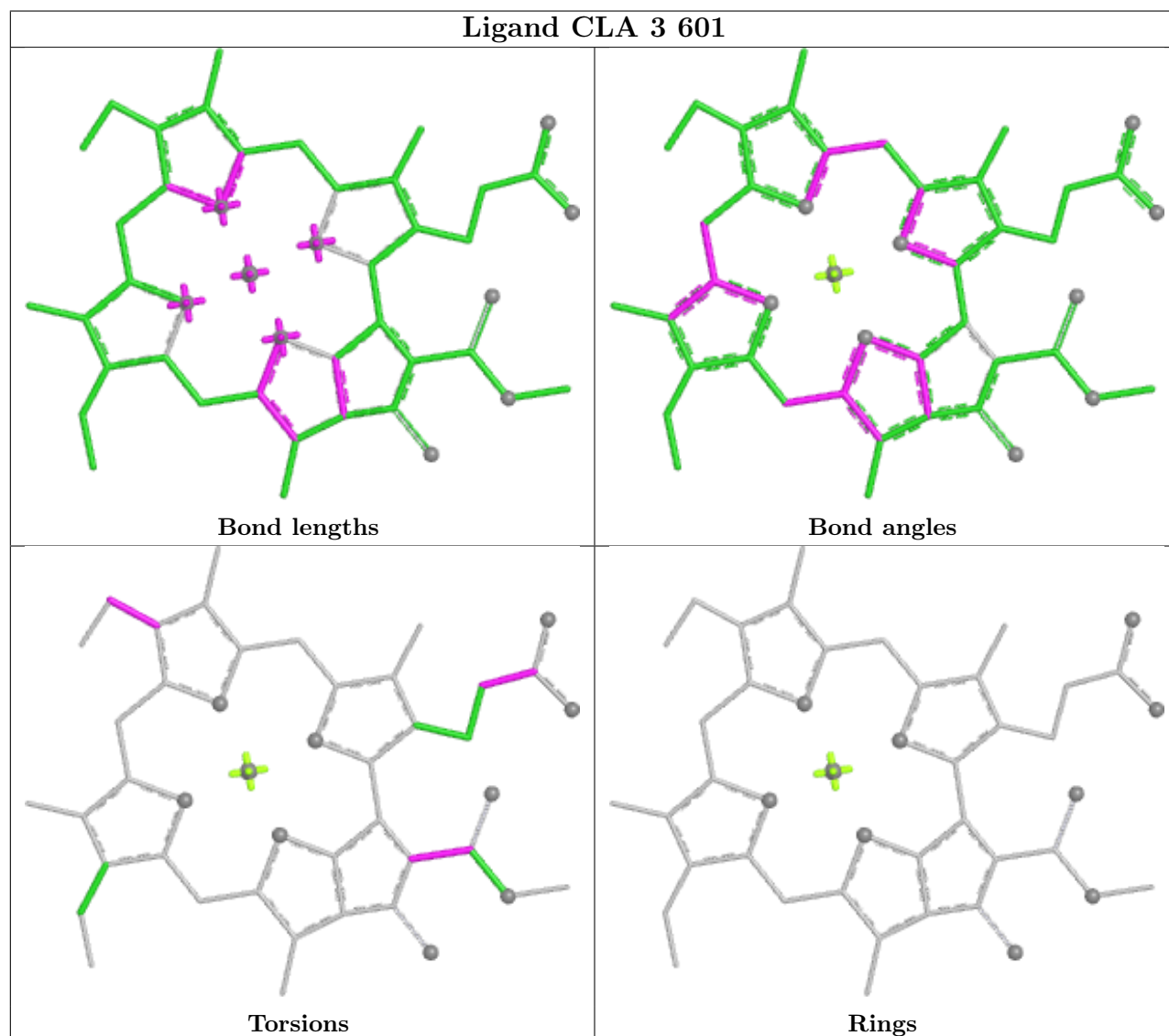
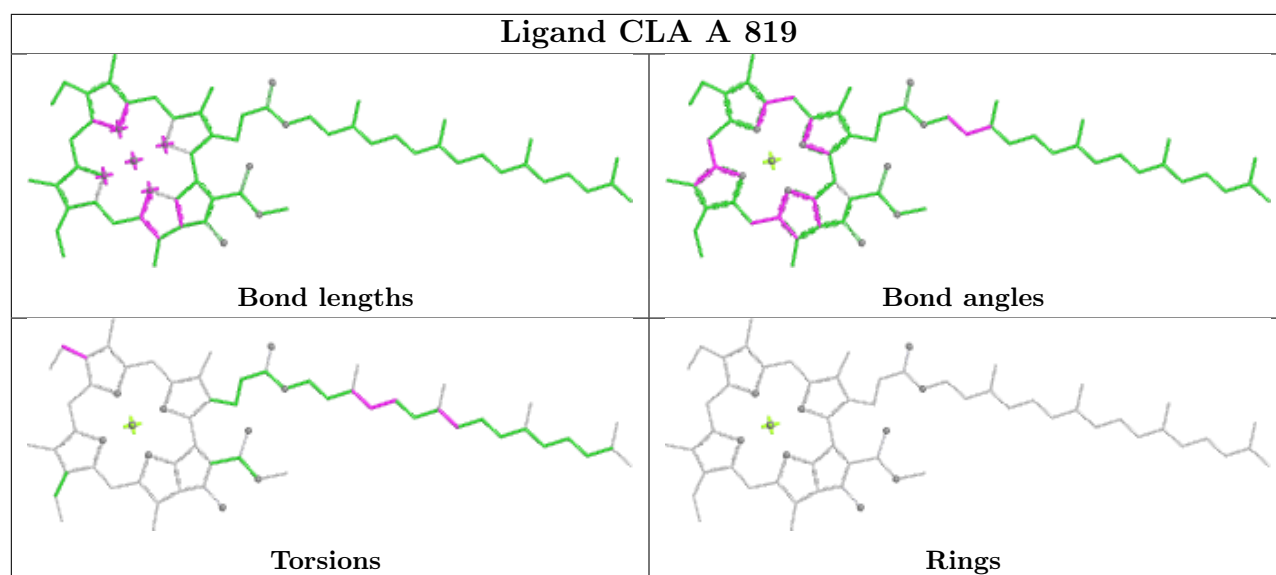
Rings

Ligand CLA 5 605

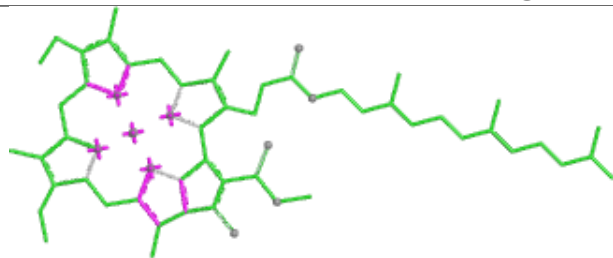


Ligand CLA 4 603**Ligand CLA A 826**

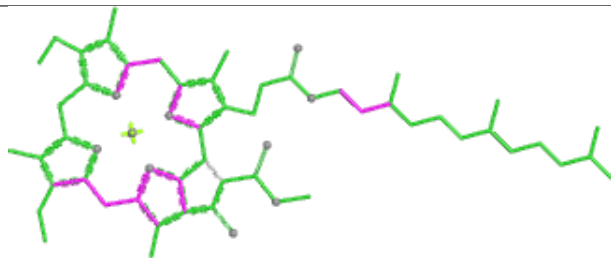




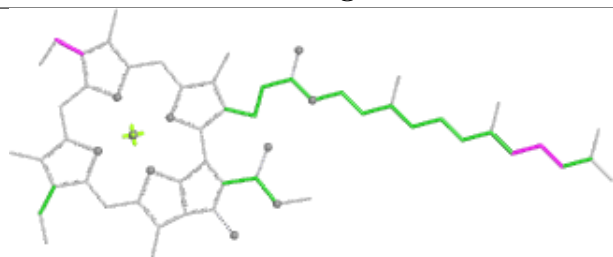
Ligand CLA 2 608



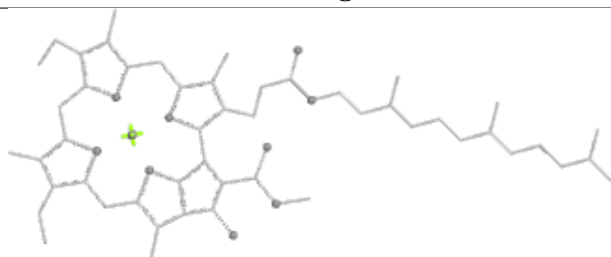
Bond lengths



Bond angles

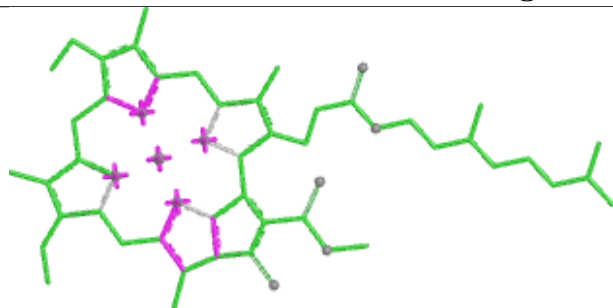


Torsions

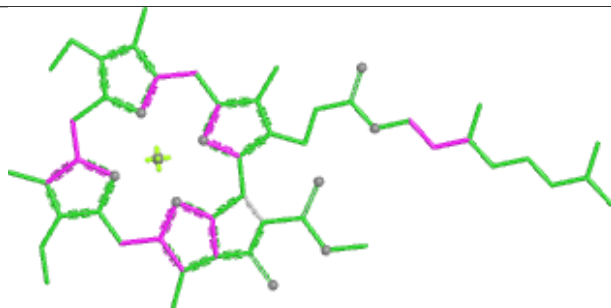


Rings

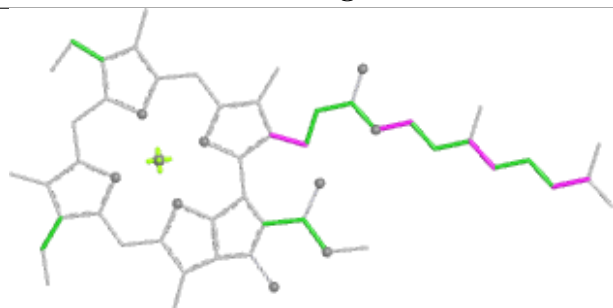
Ligand CLA a 611



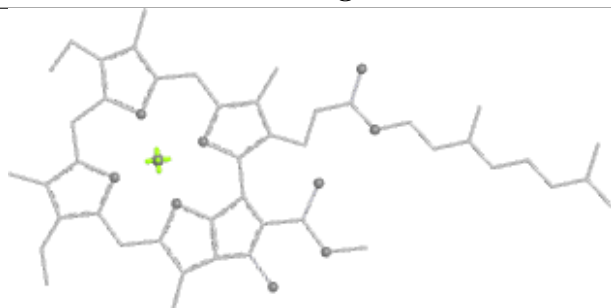
Bond lengths



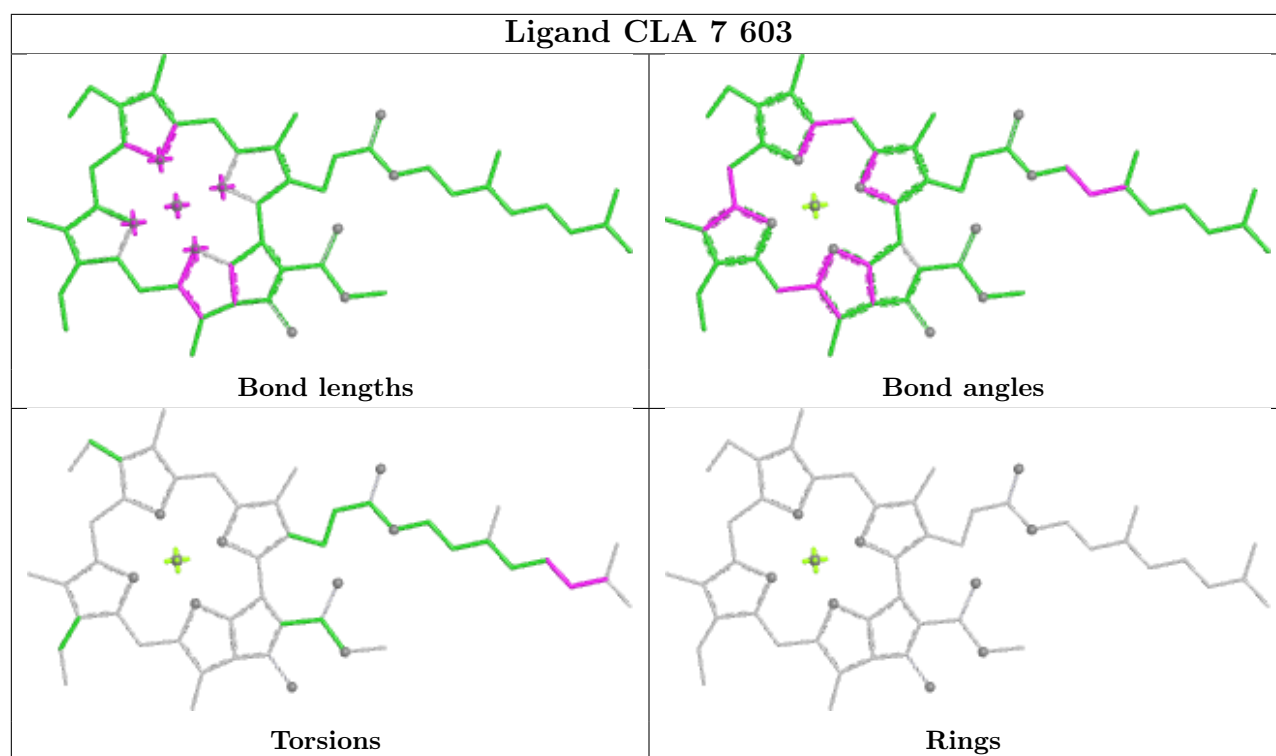
Bond angles



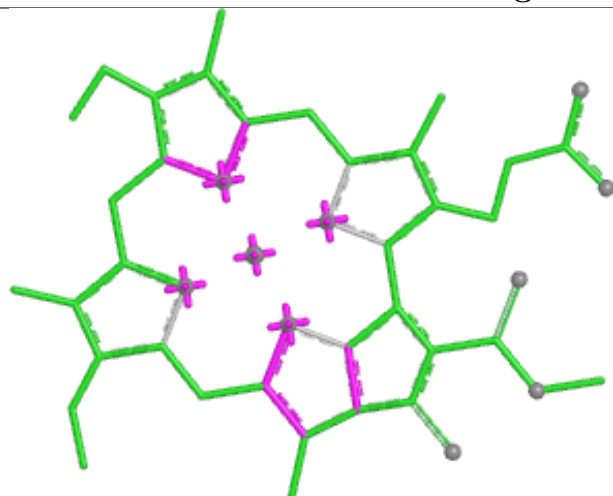
Torsions



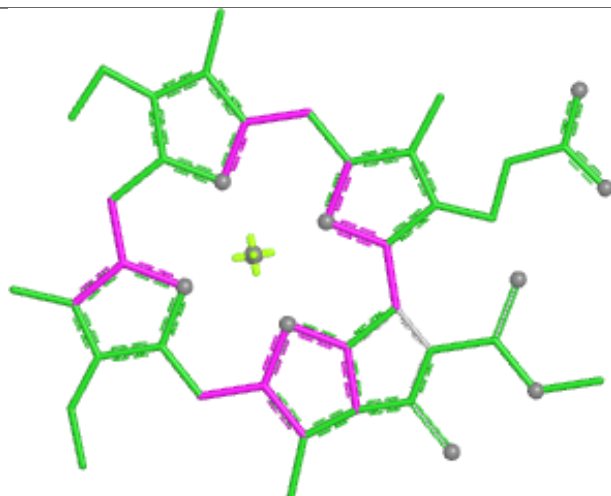
Rings



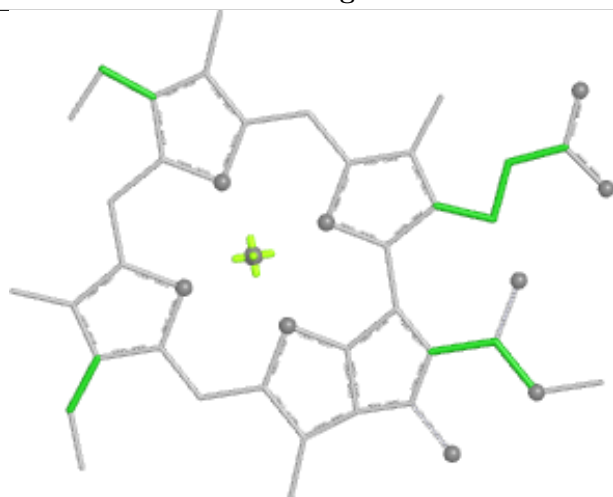
Ligand CLA B 829



Bond lengths



Bond angles

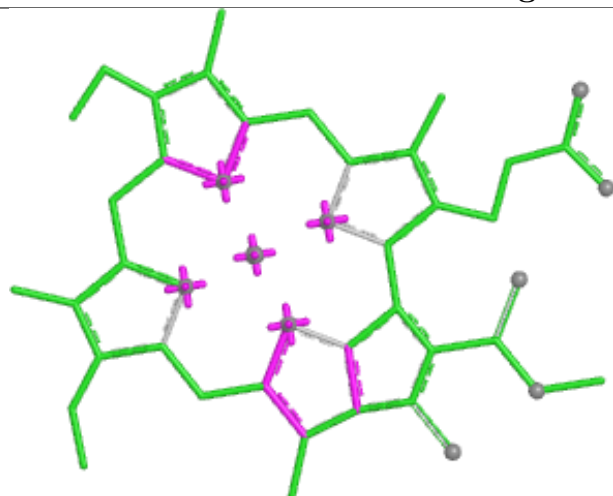


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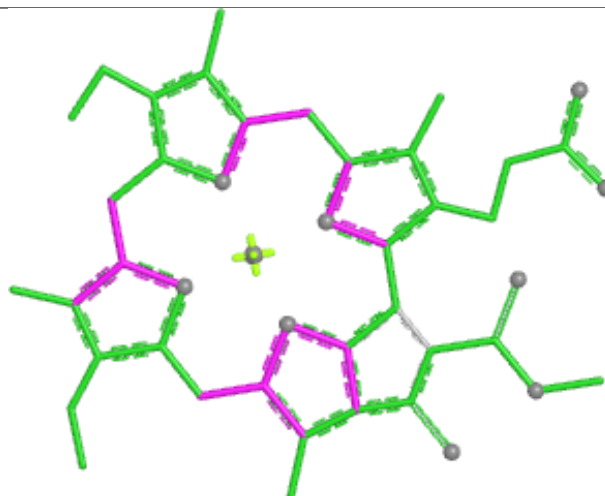


Rings

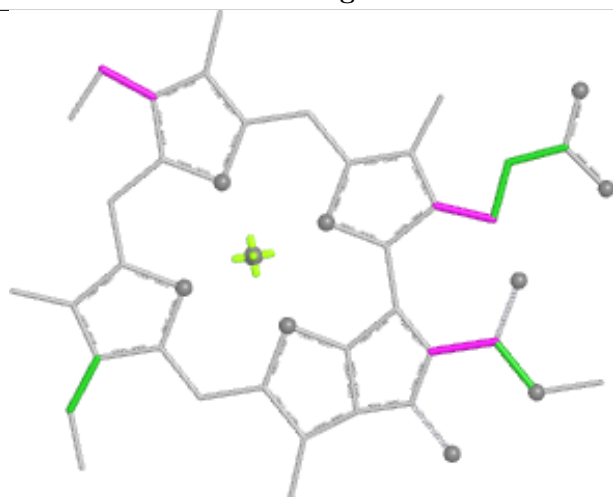
Ligand CLA 2 612



Bond lengths



Bond angles

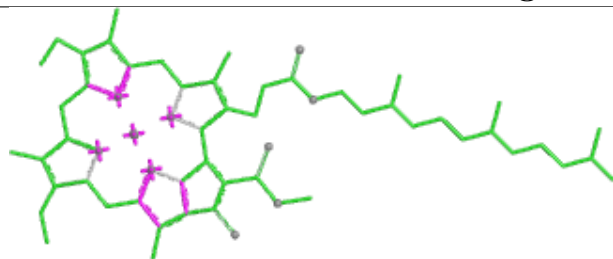


Torsions

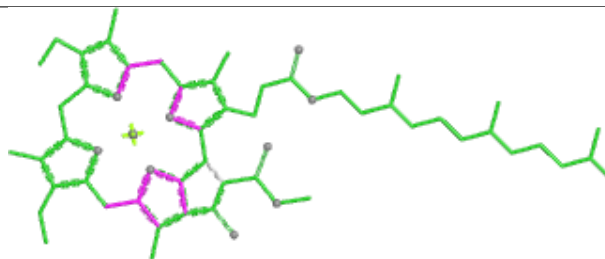


Rings

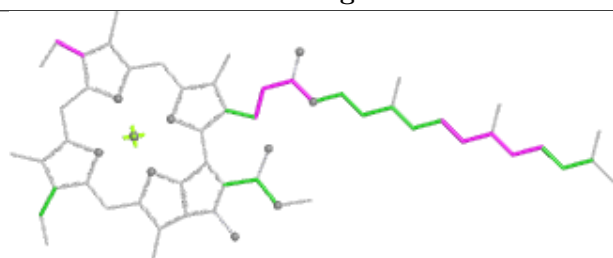
Ligand CLA a 604



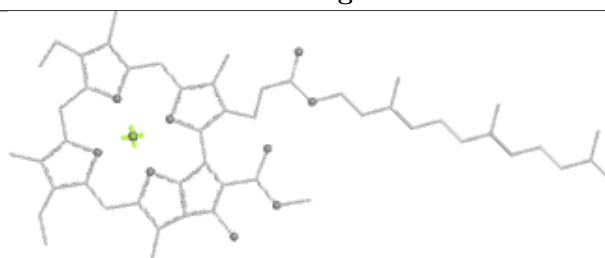
Bond lengths



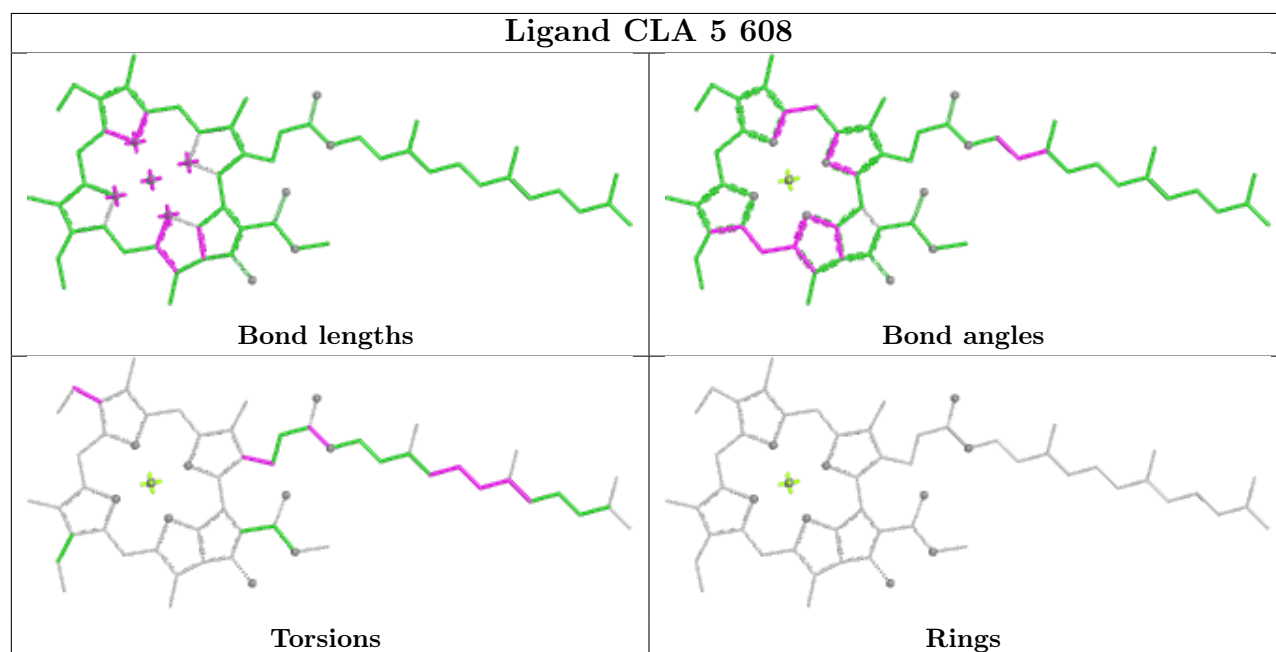
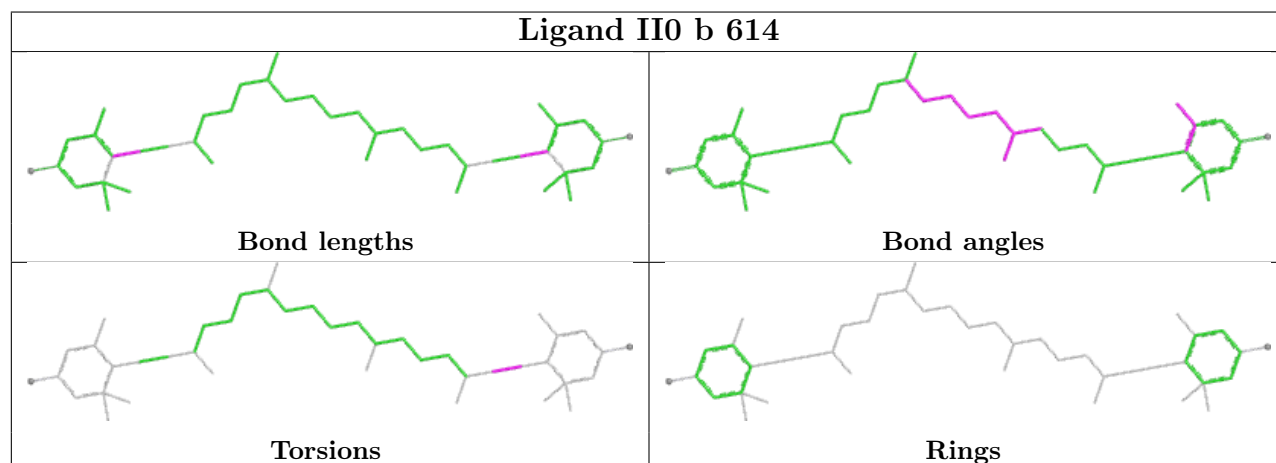
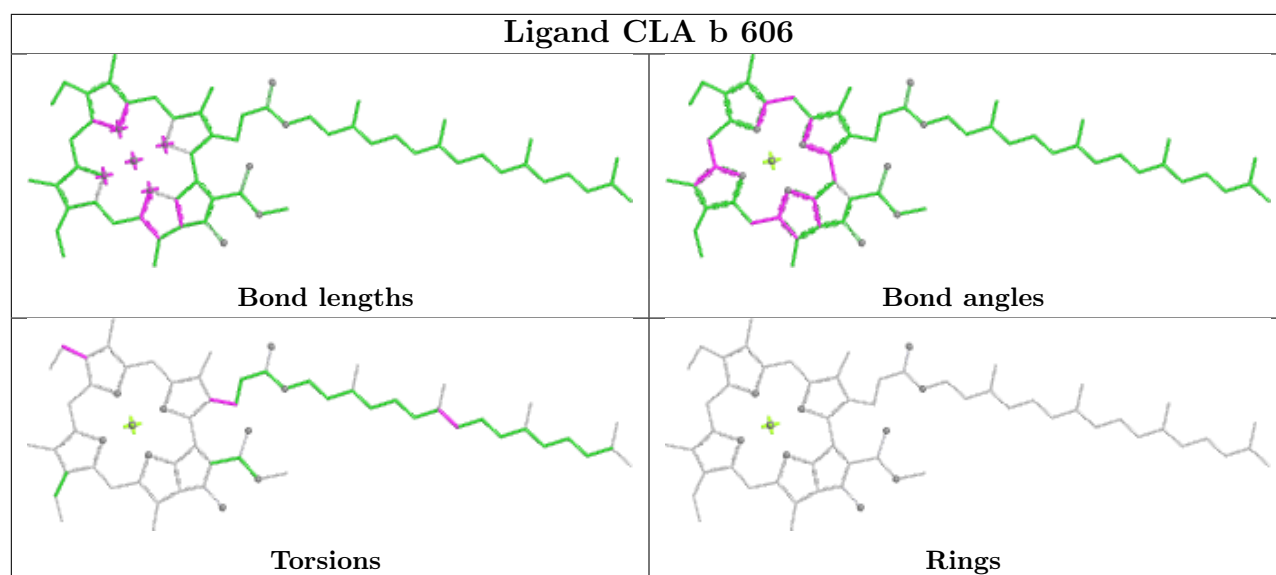
Bond angles



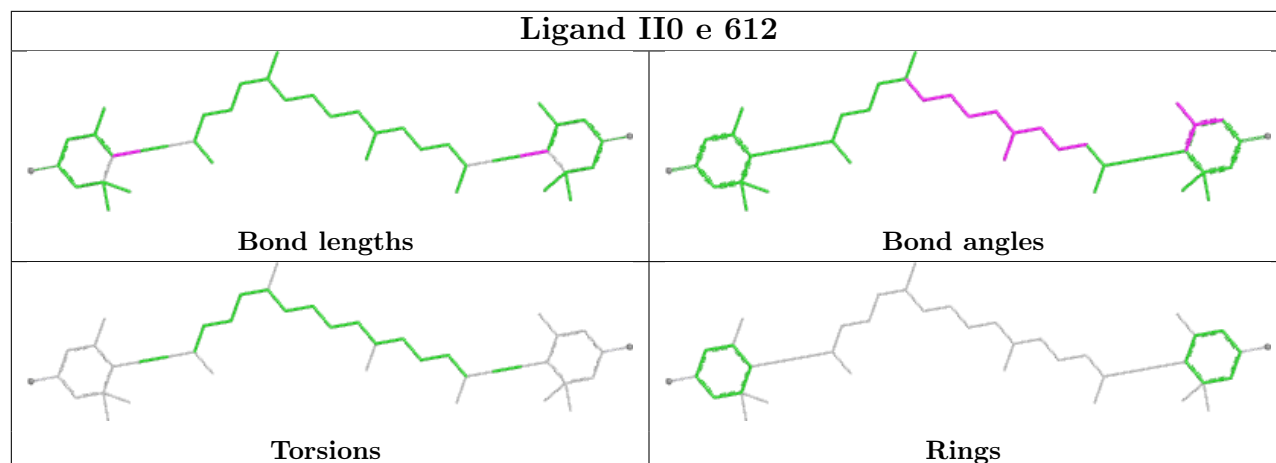
Torsions



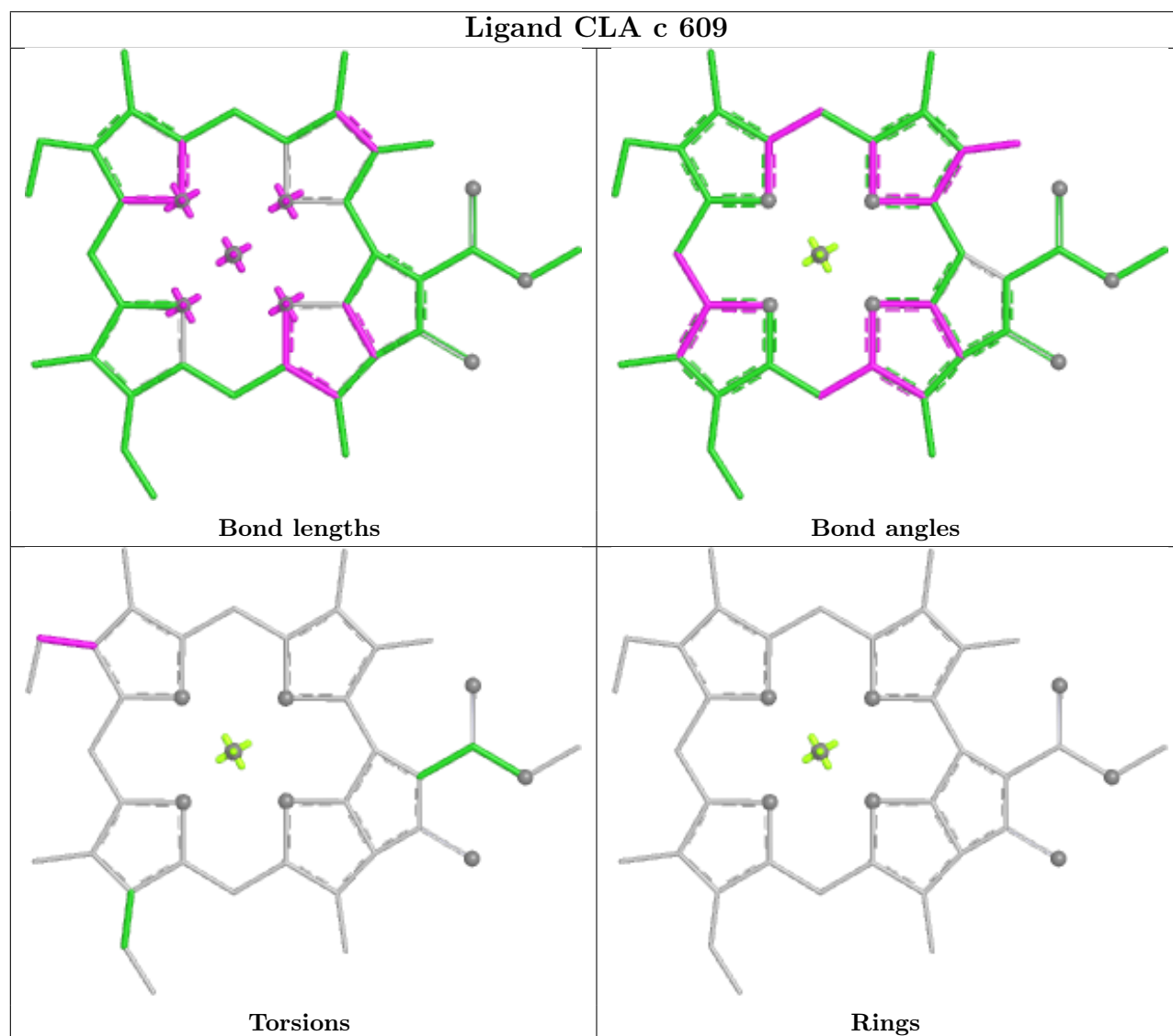
Rings

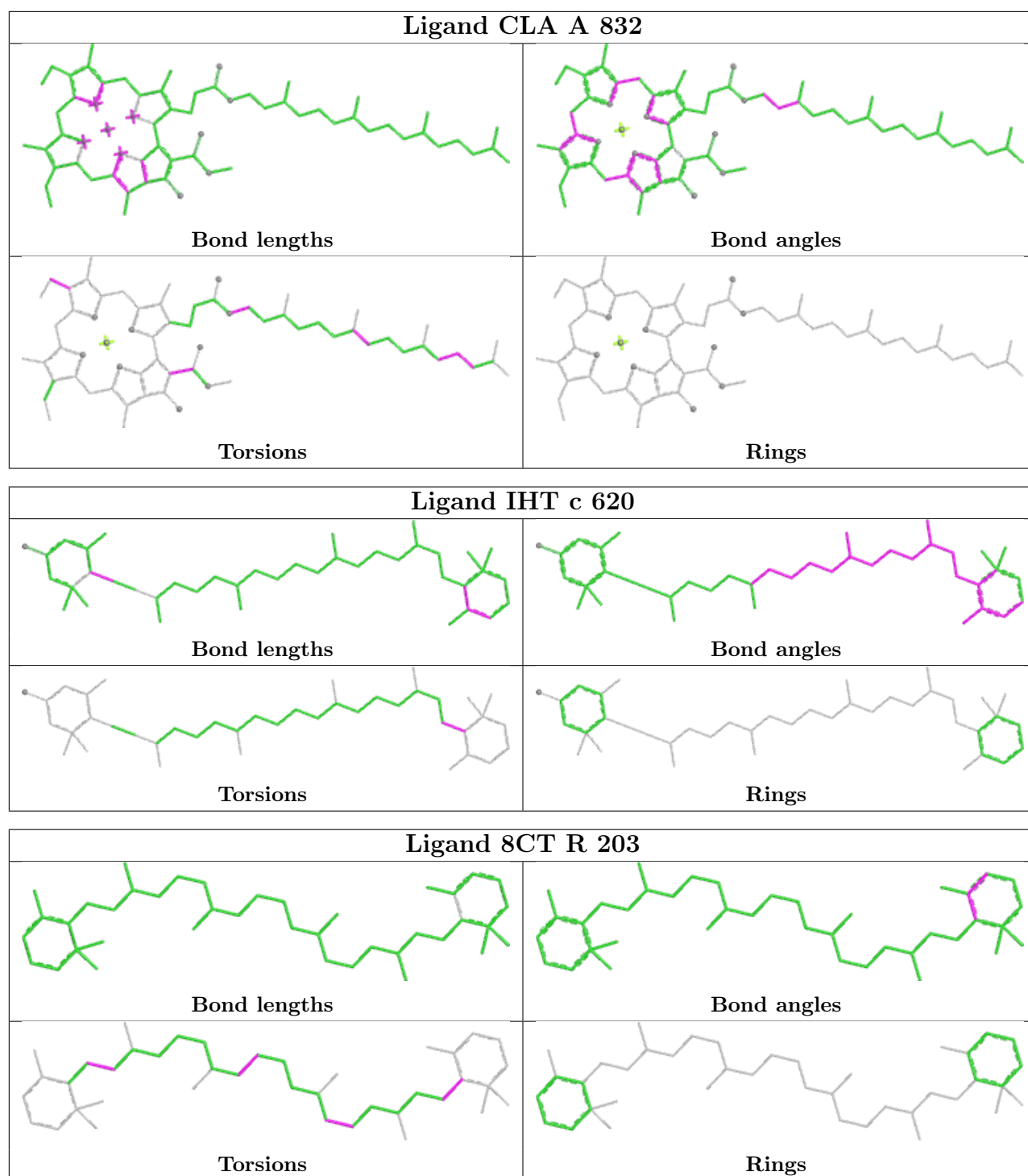


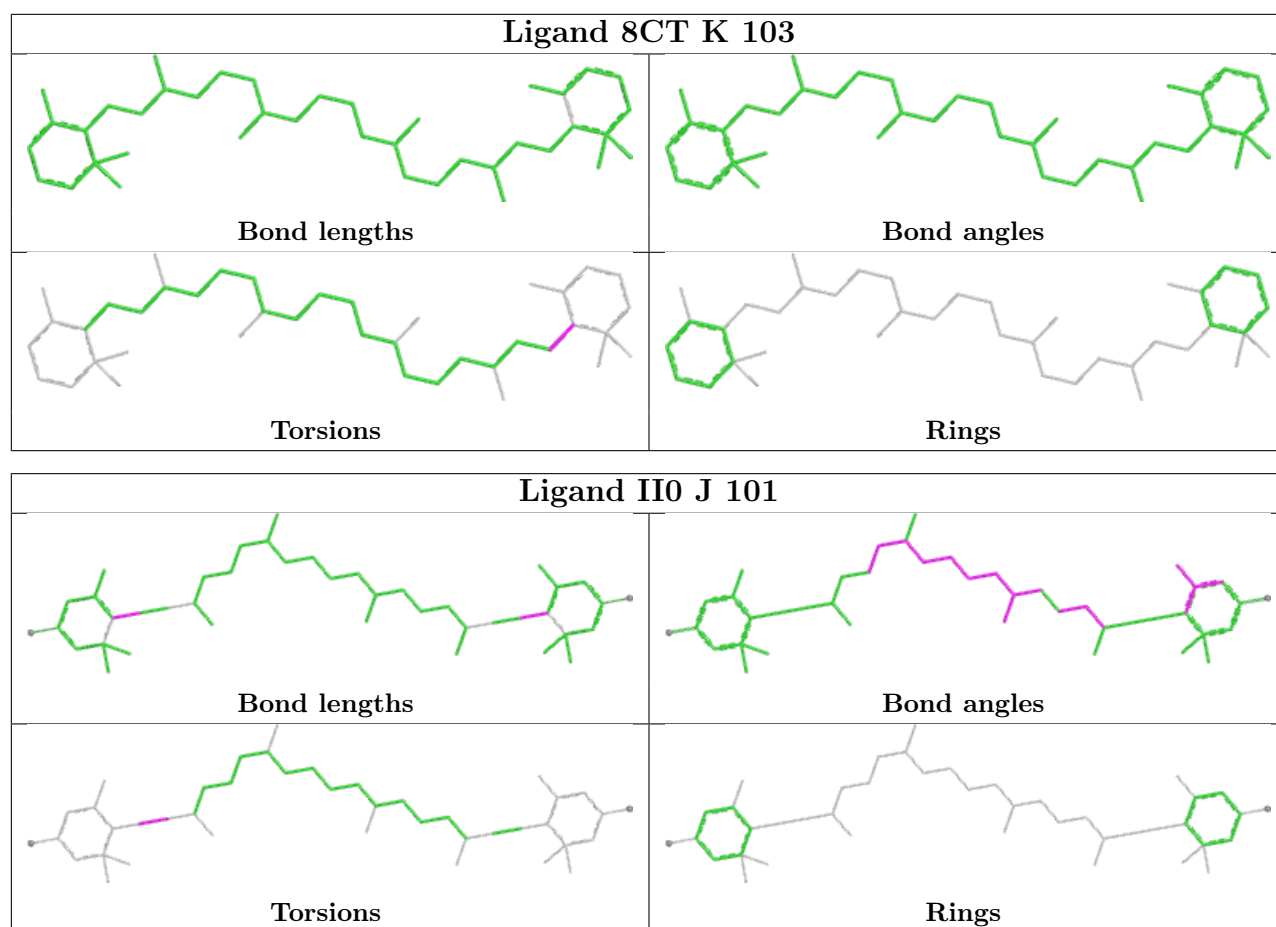
Ligand II0 e 612



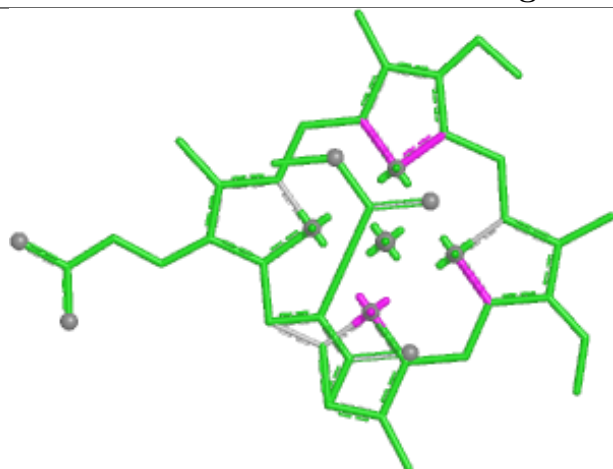
Ligand CLA c 609



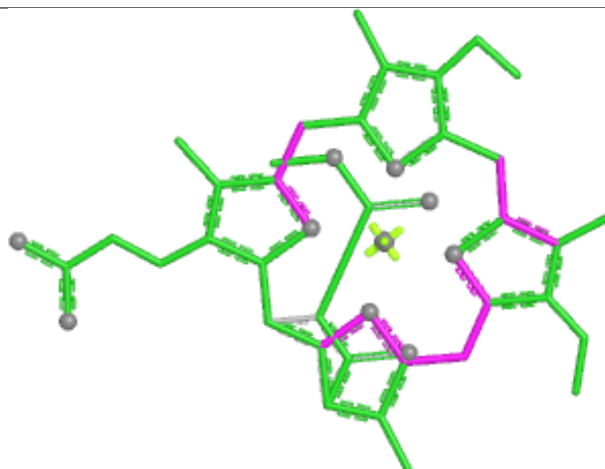




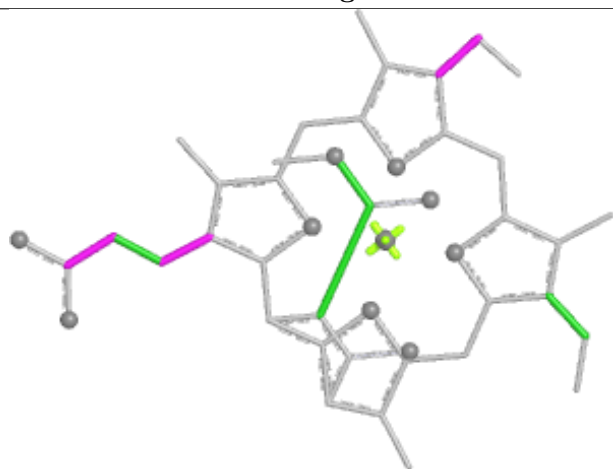
Ligand KC2 b 605



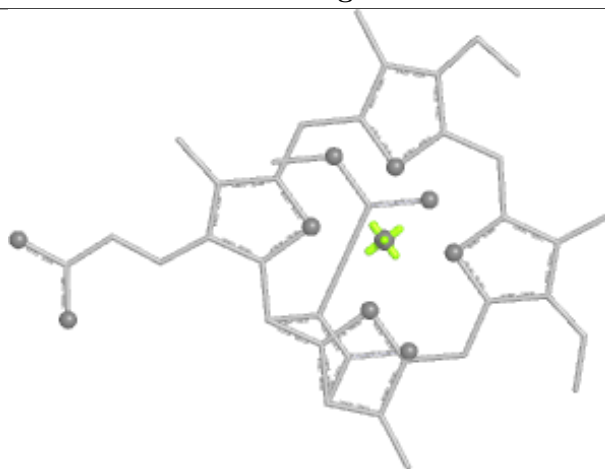
Bond lengths



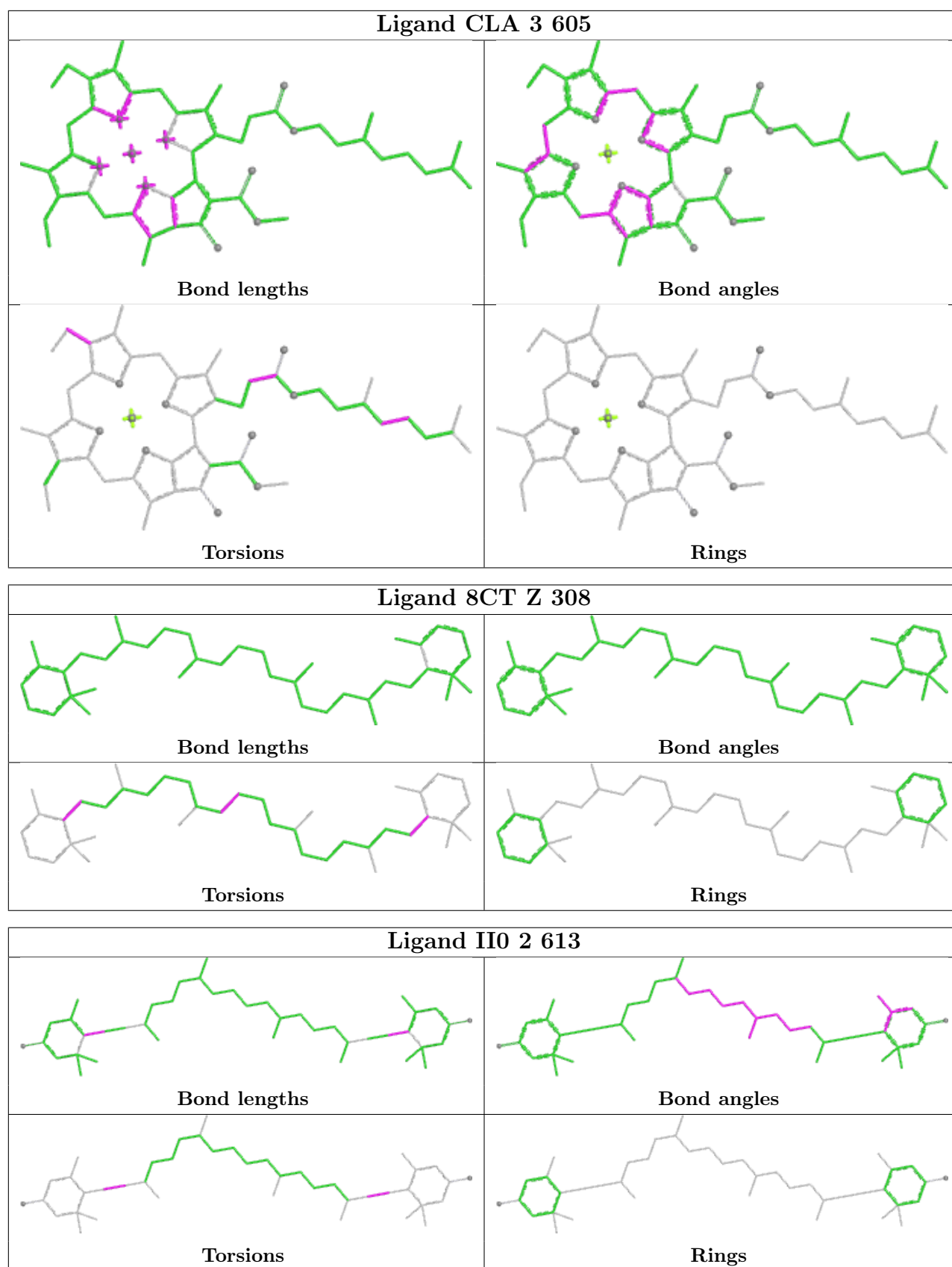
Bond angles

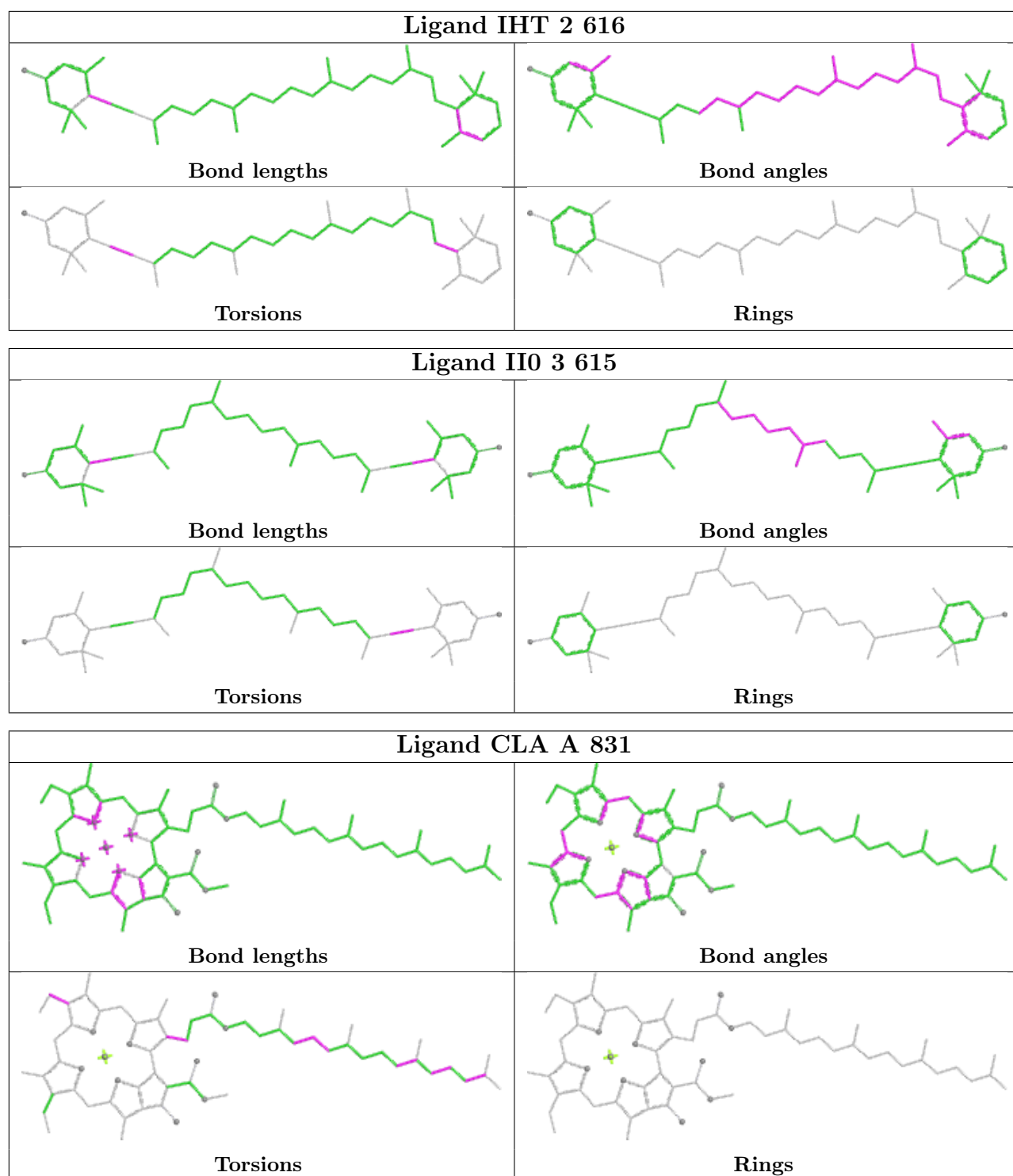


Torsions

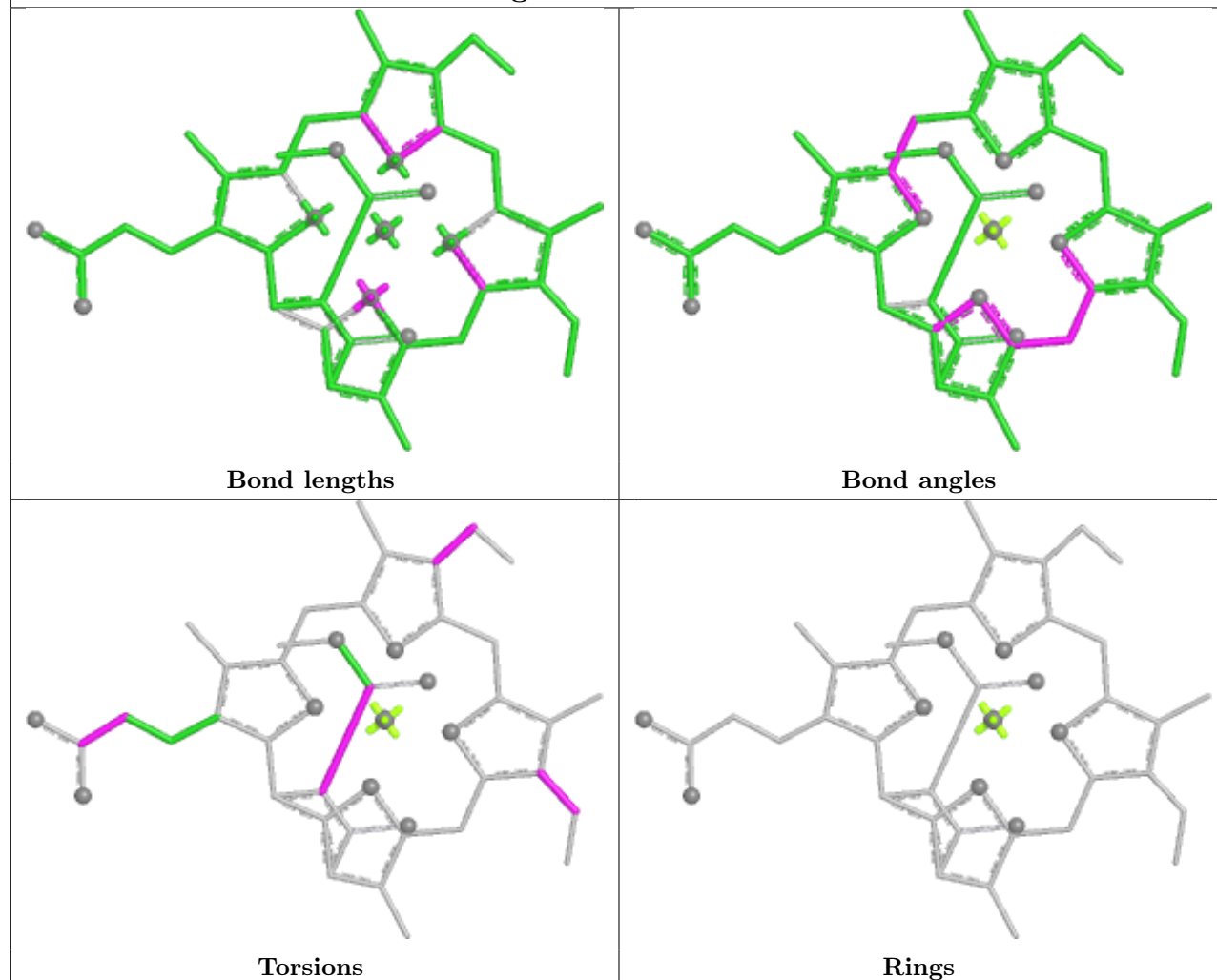


Rings

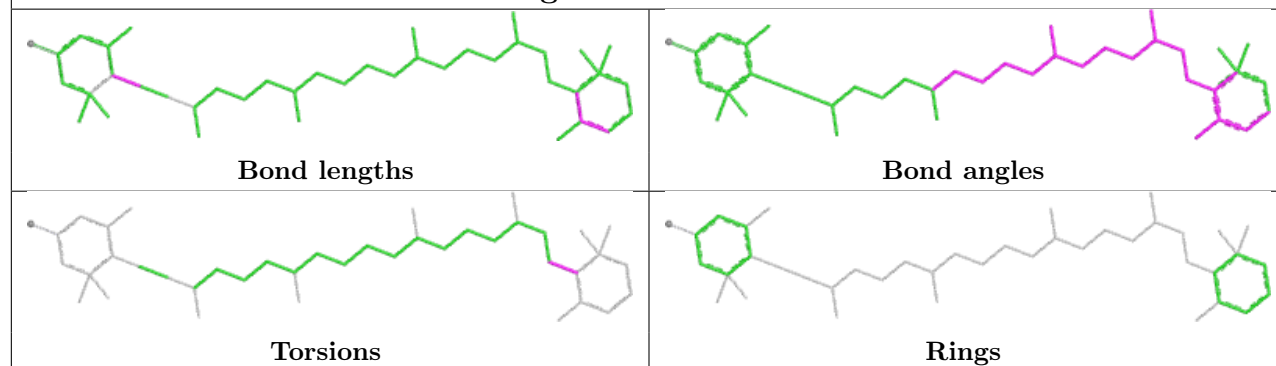


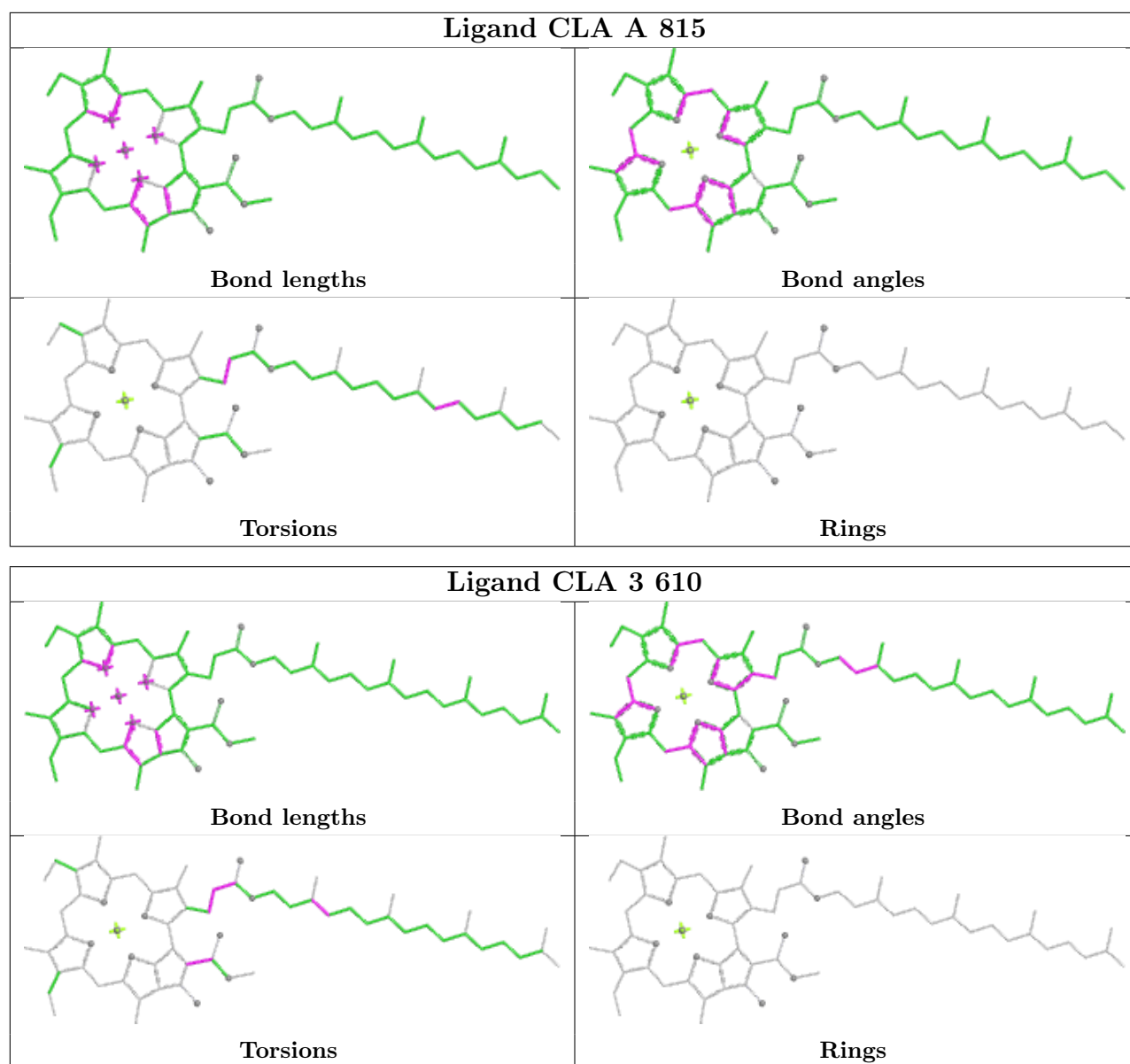


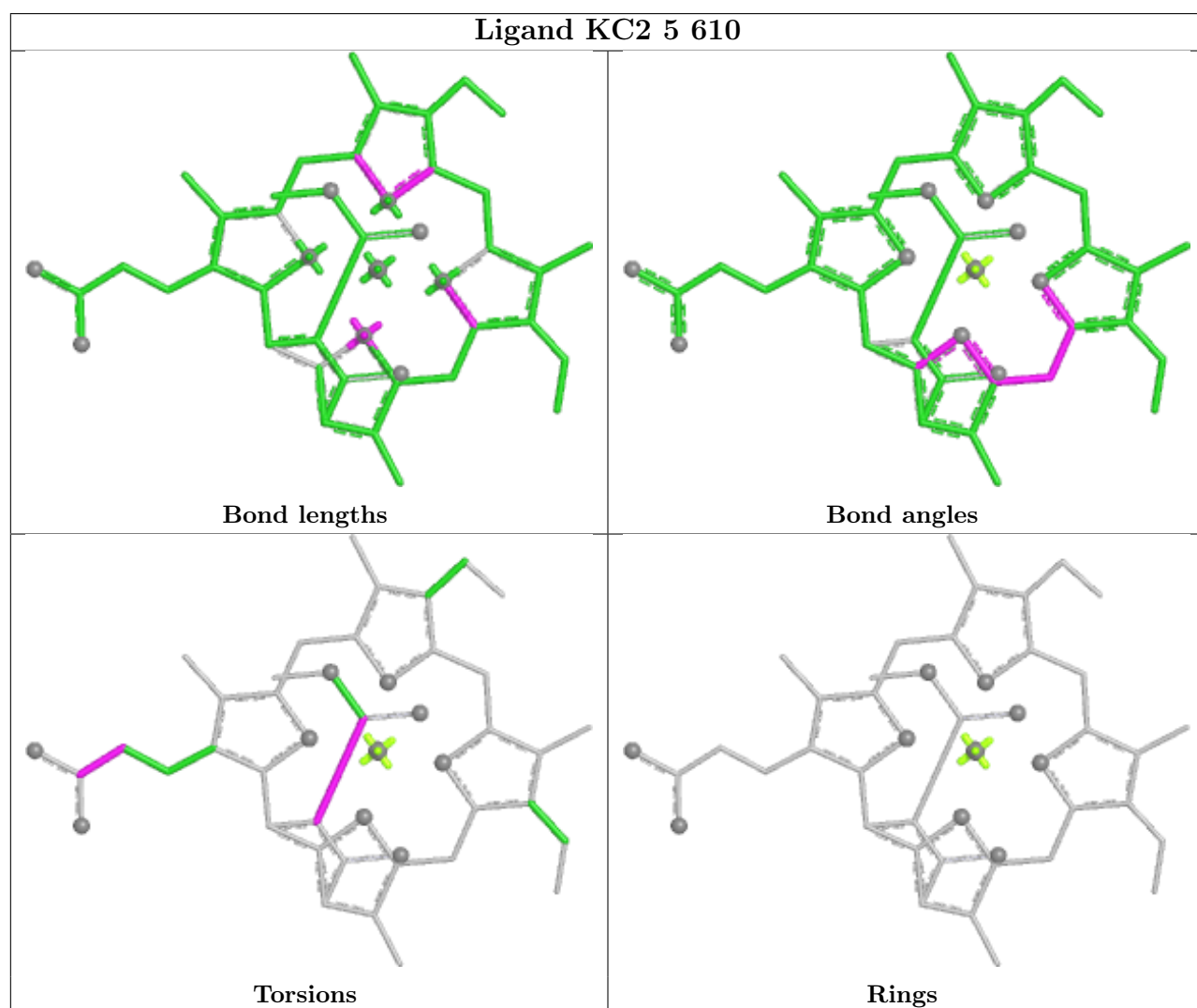
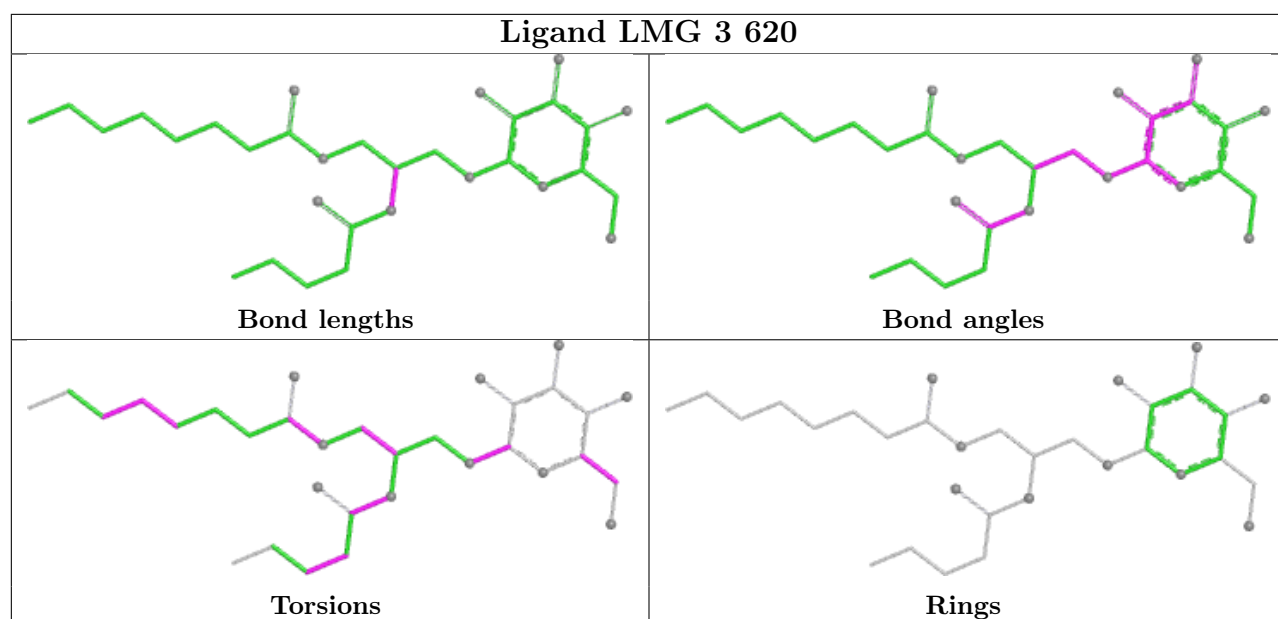
Ligand KC2 Z 307

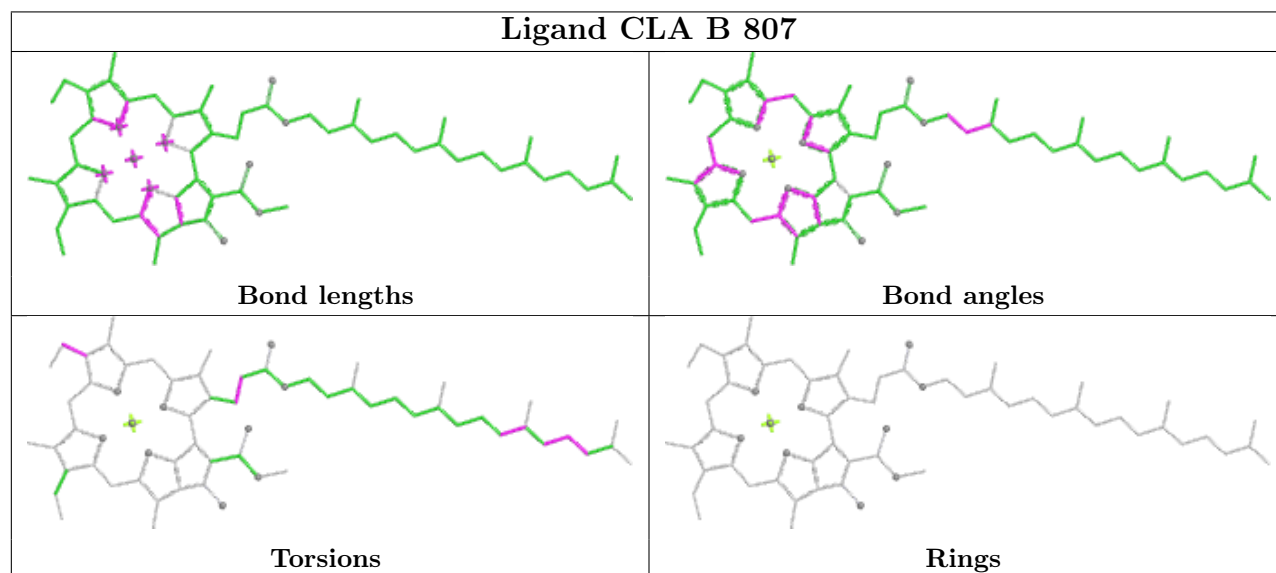
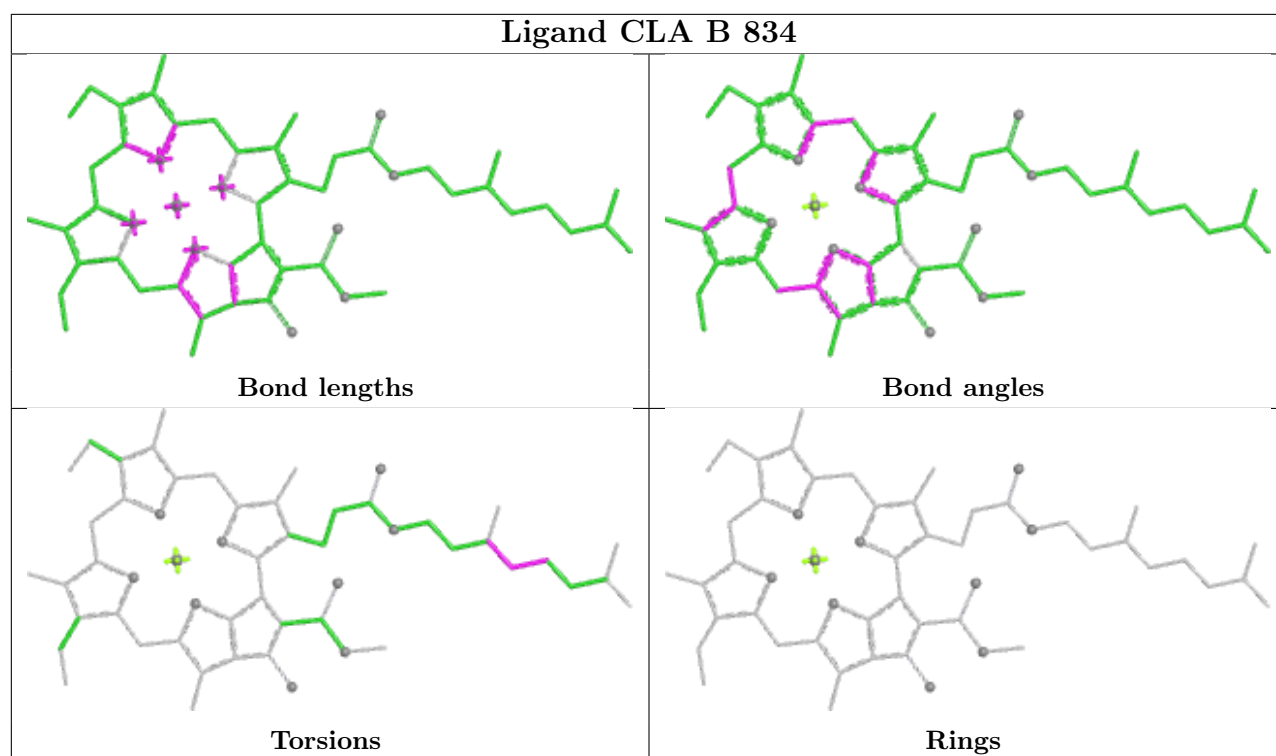


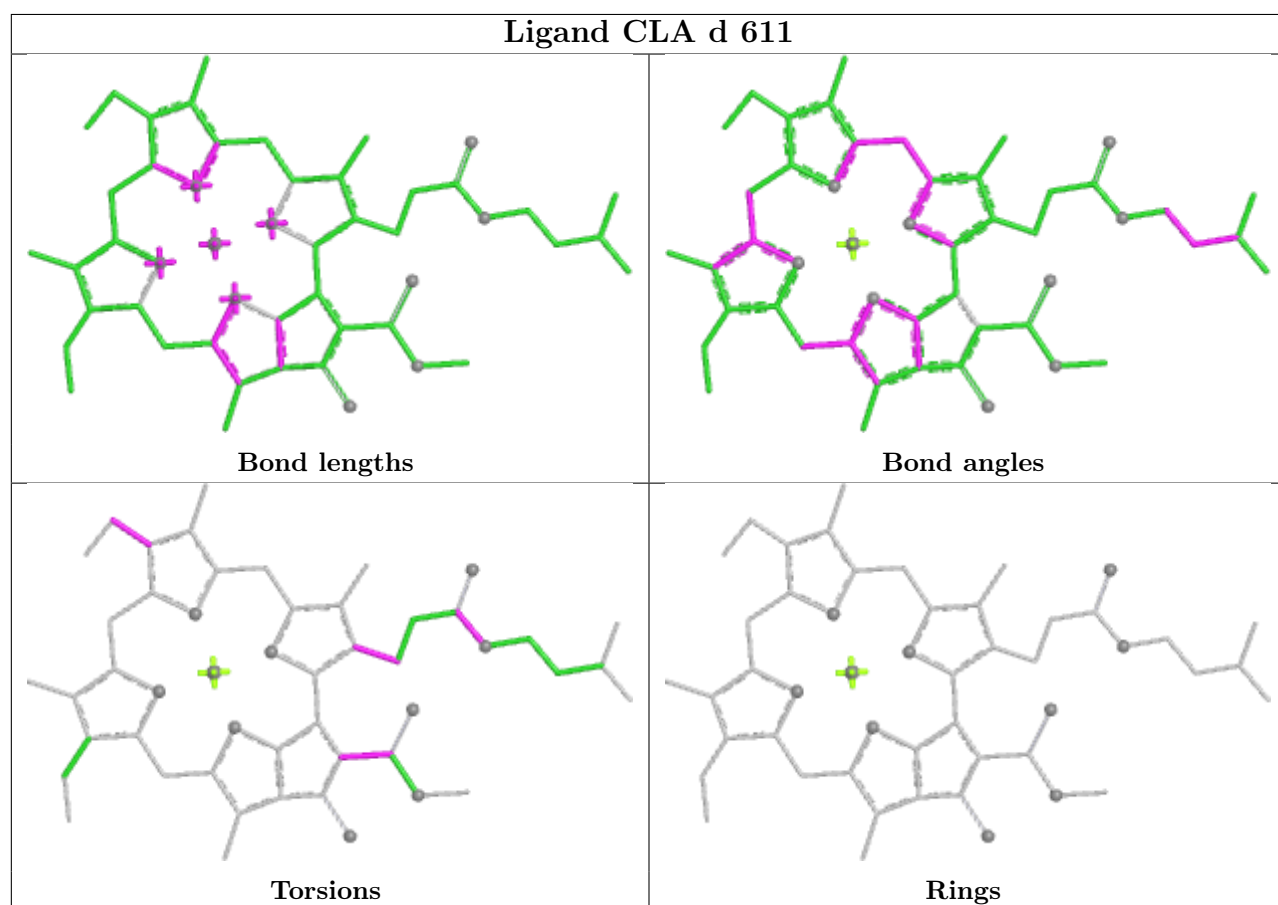
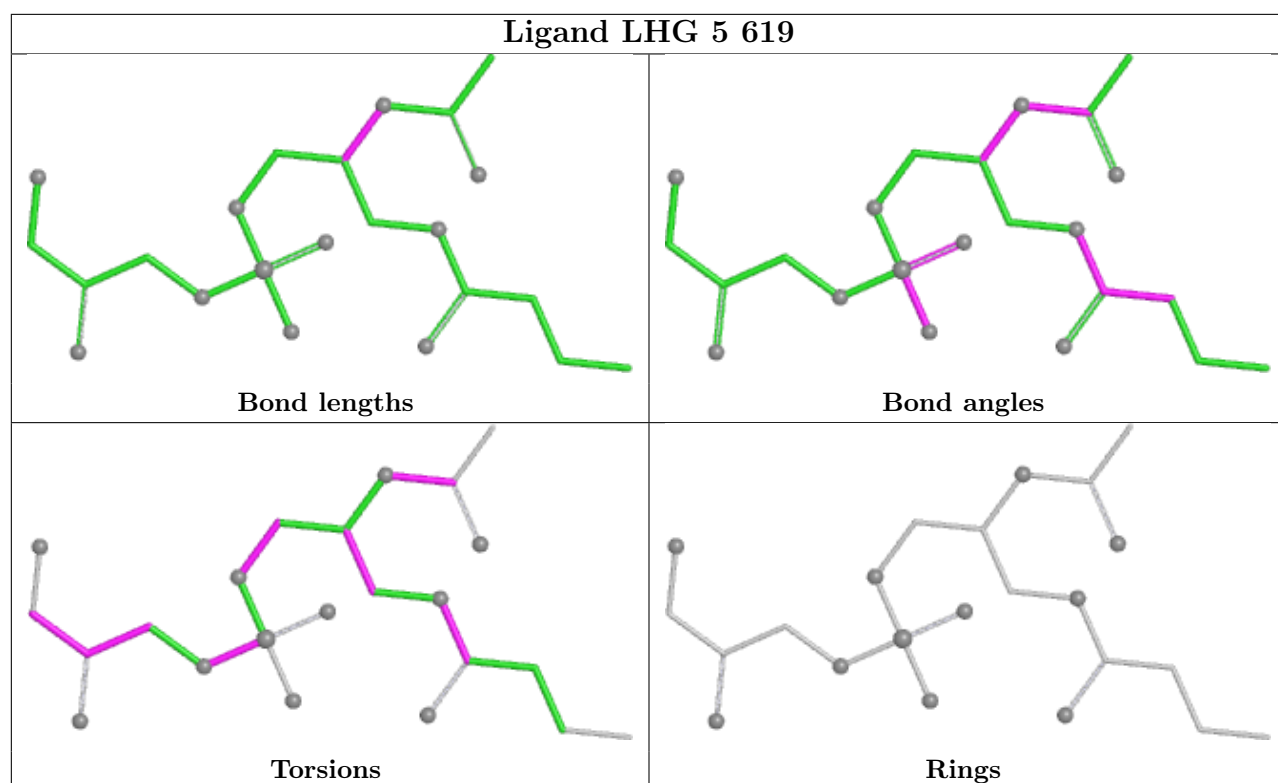
Ligand IHT 8 609

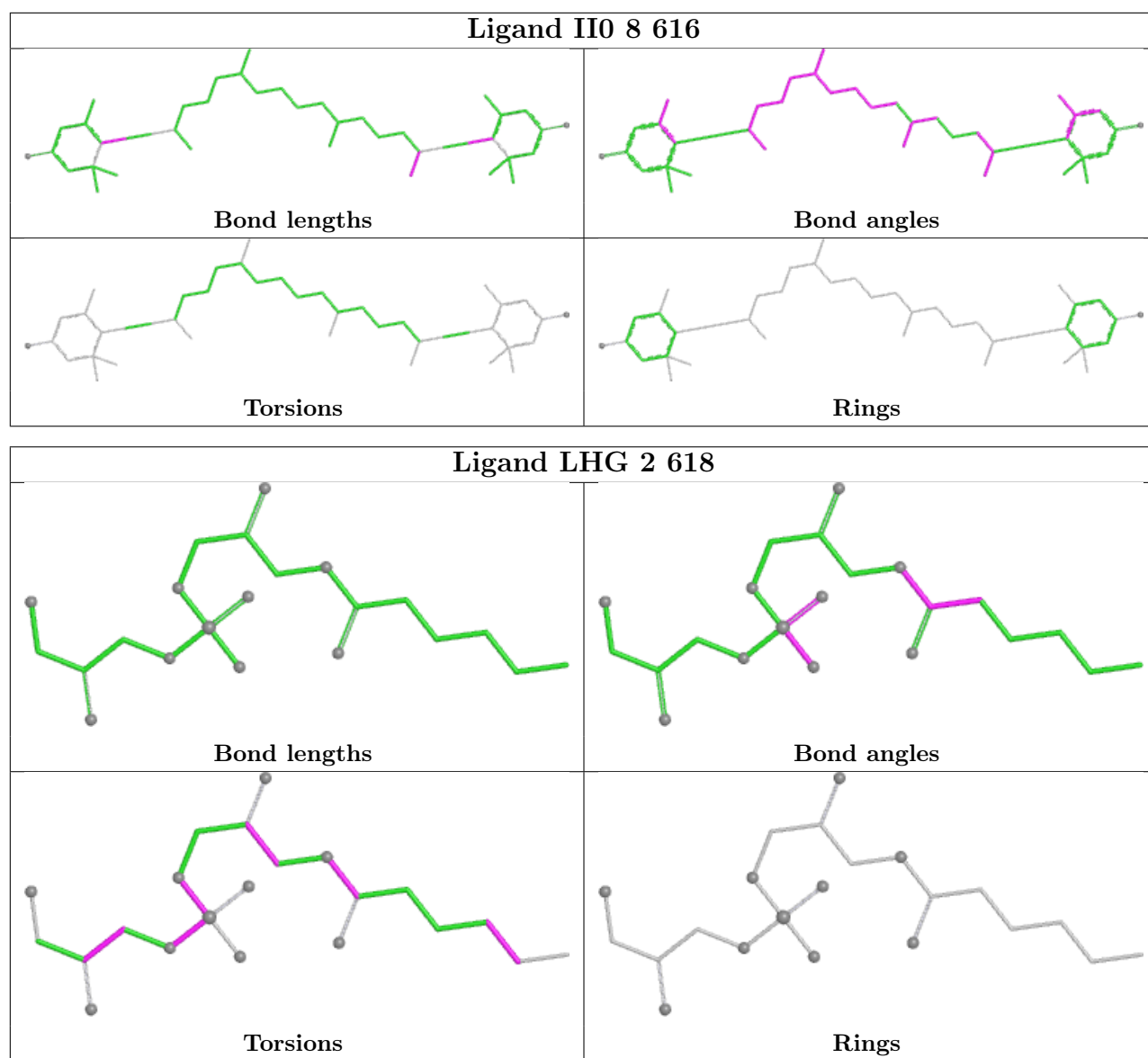




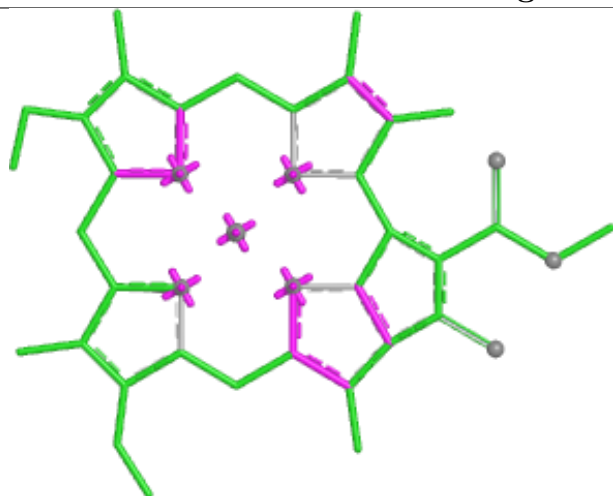




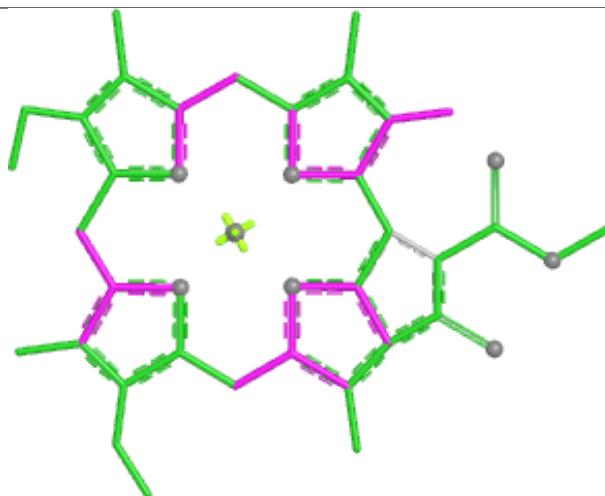




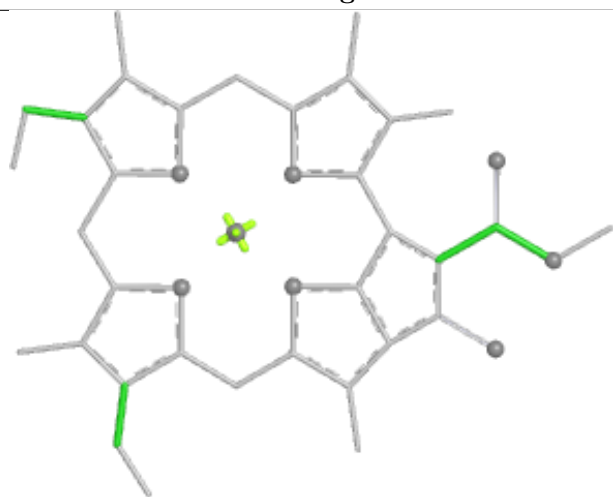
Ligand CLA d 609



Bond lengths



Bond angles

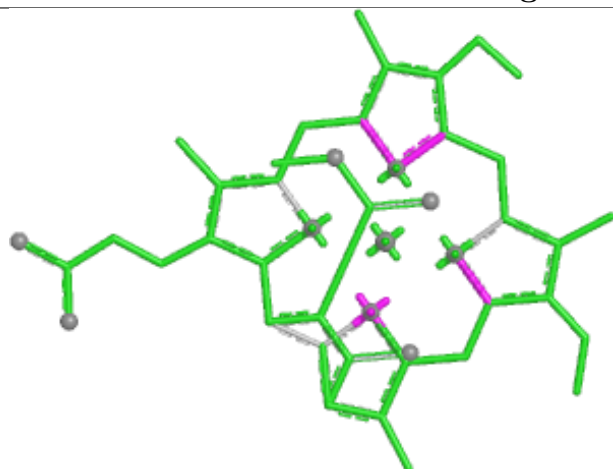


Torsions

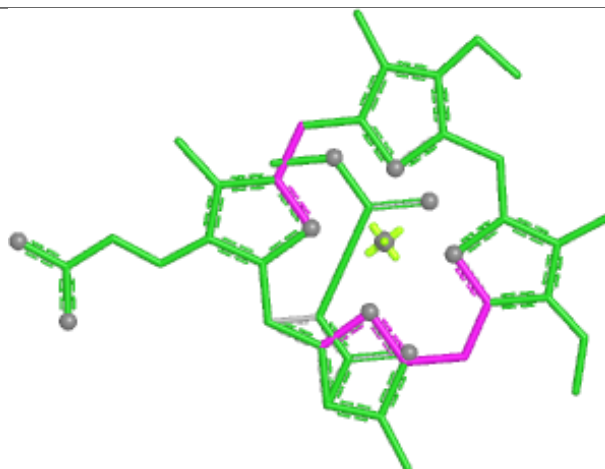


Rings

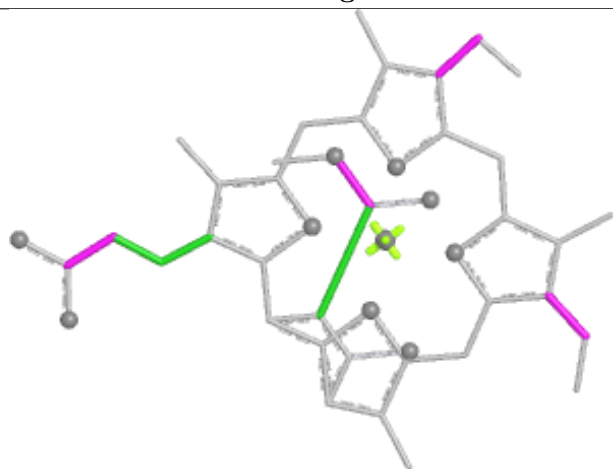
Ligand KC2 7 606



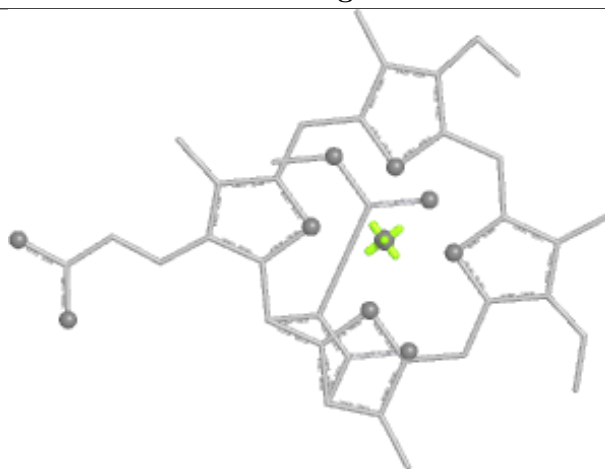
Bond lengths



Bond angles

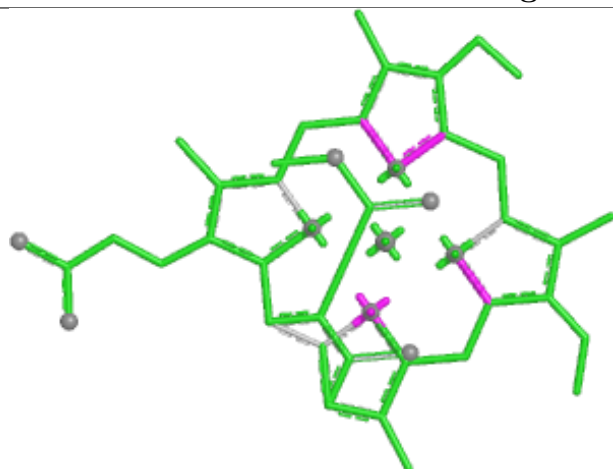


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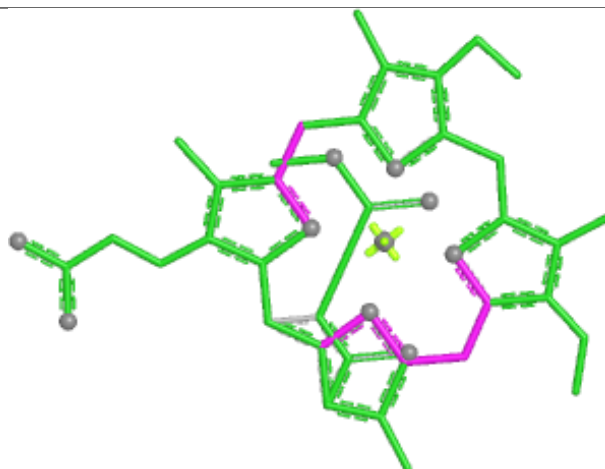


Rings

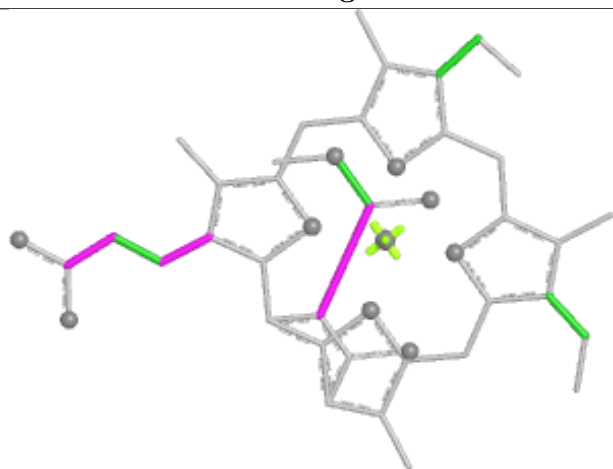
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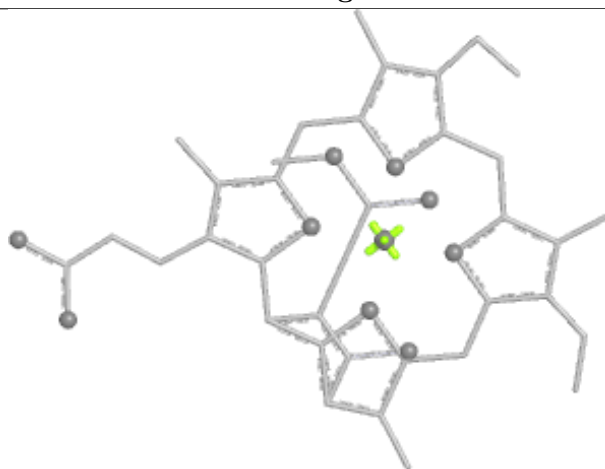
Bond lengths



Bond angles

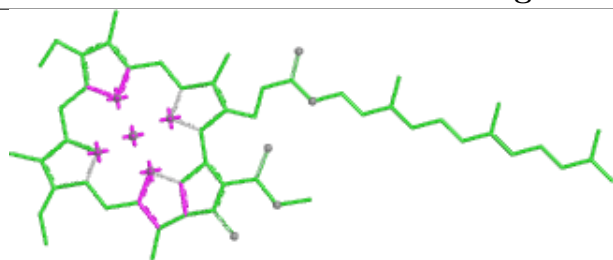


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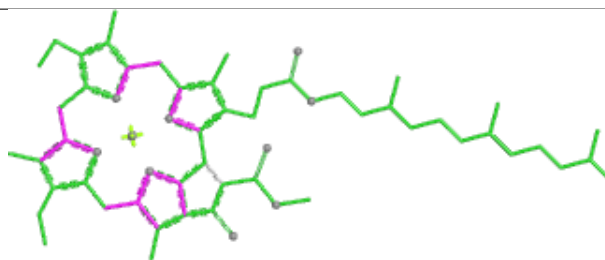


Rings

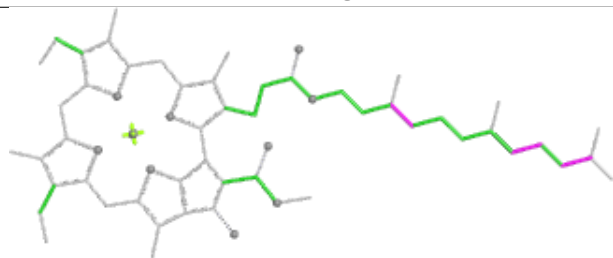
Ligand CLA B 810



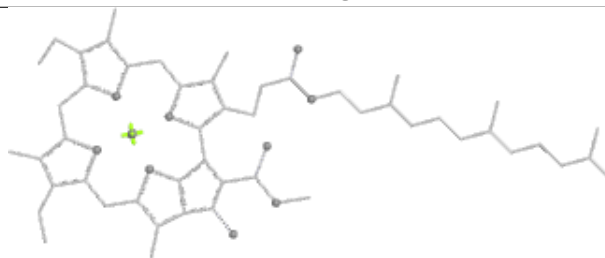
Bond lengths



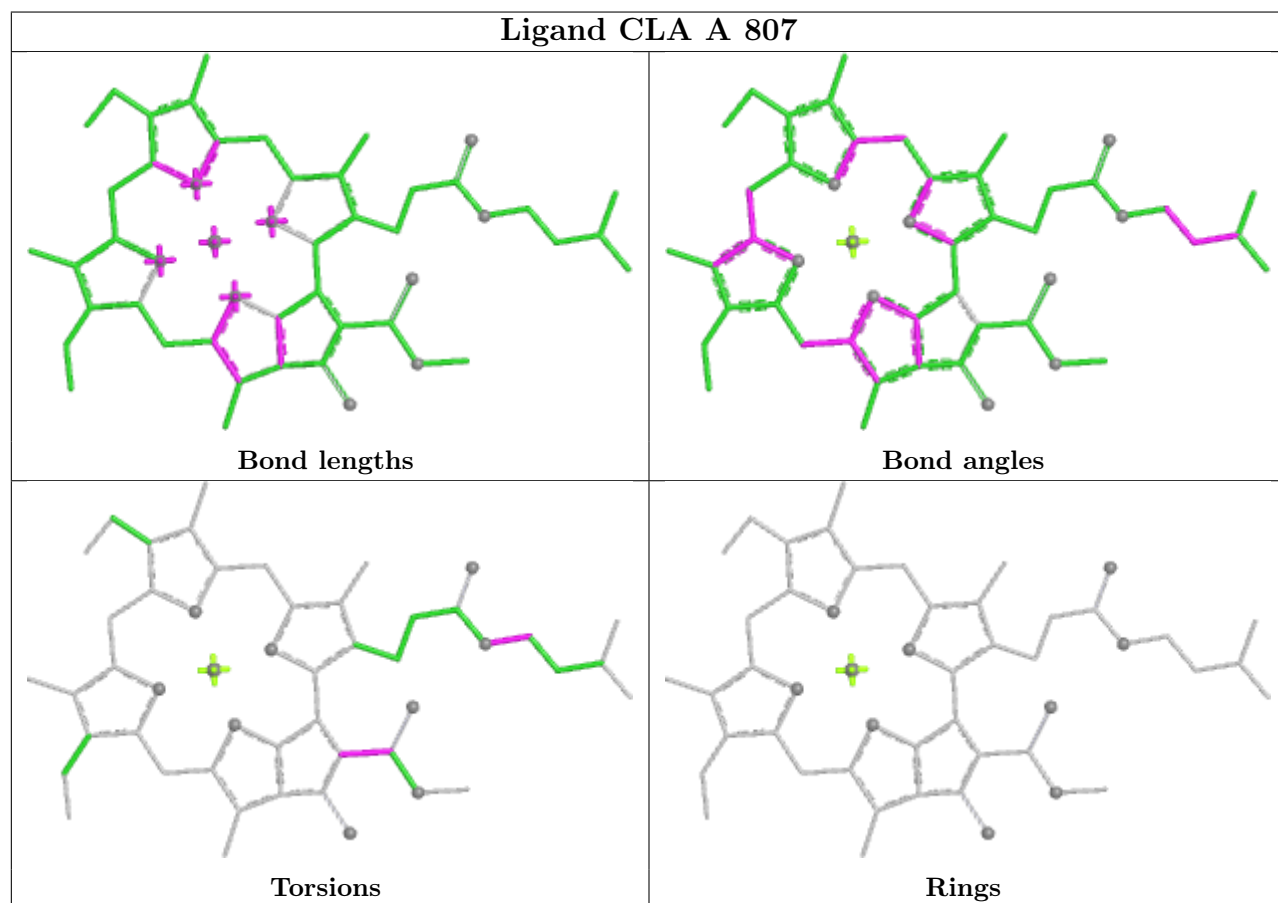
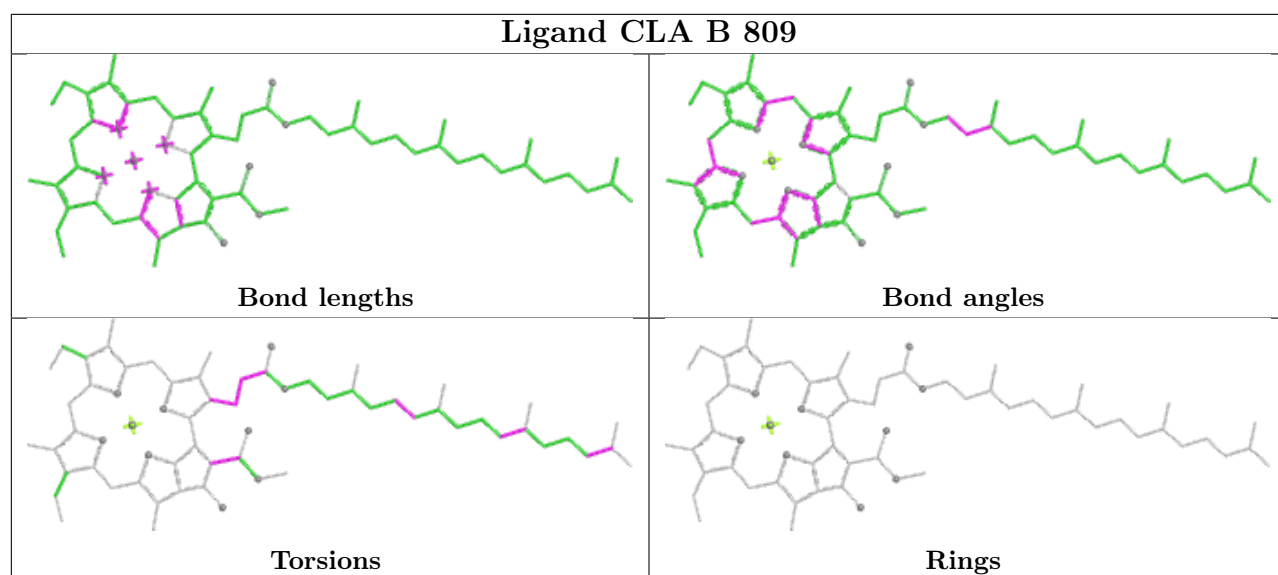
Bond angles

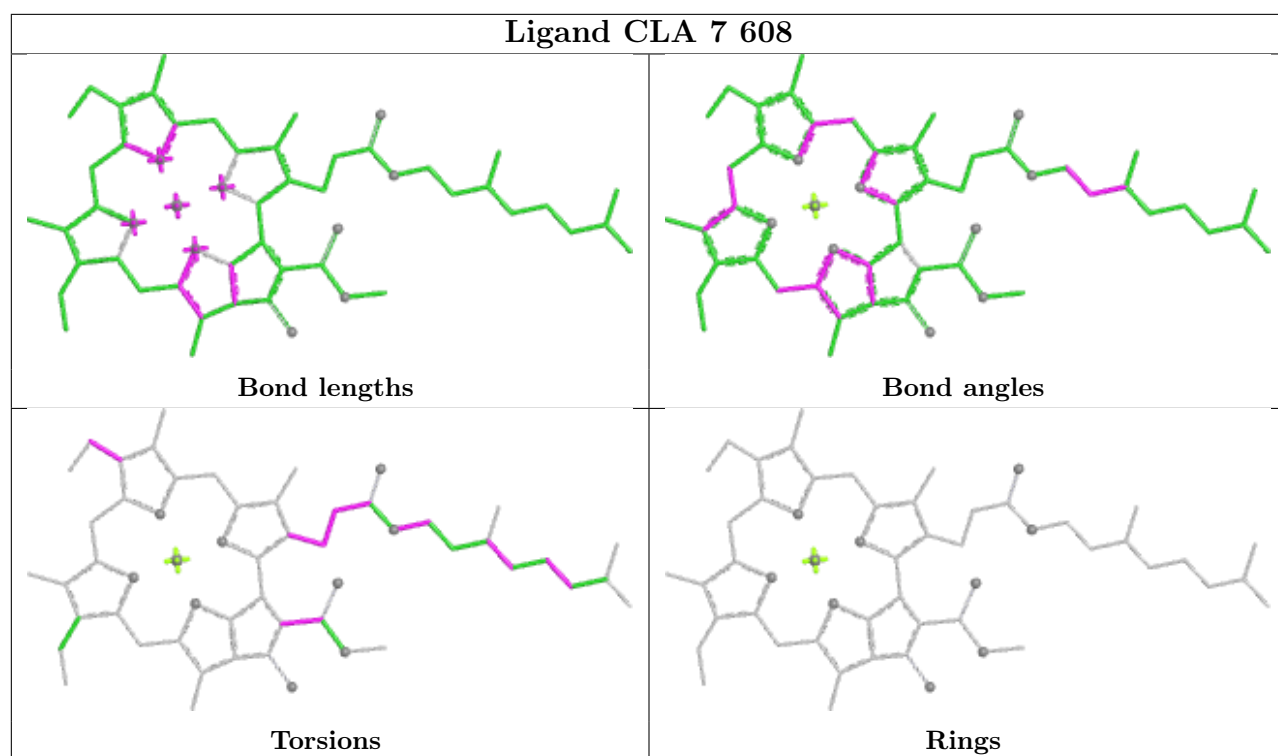


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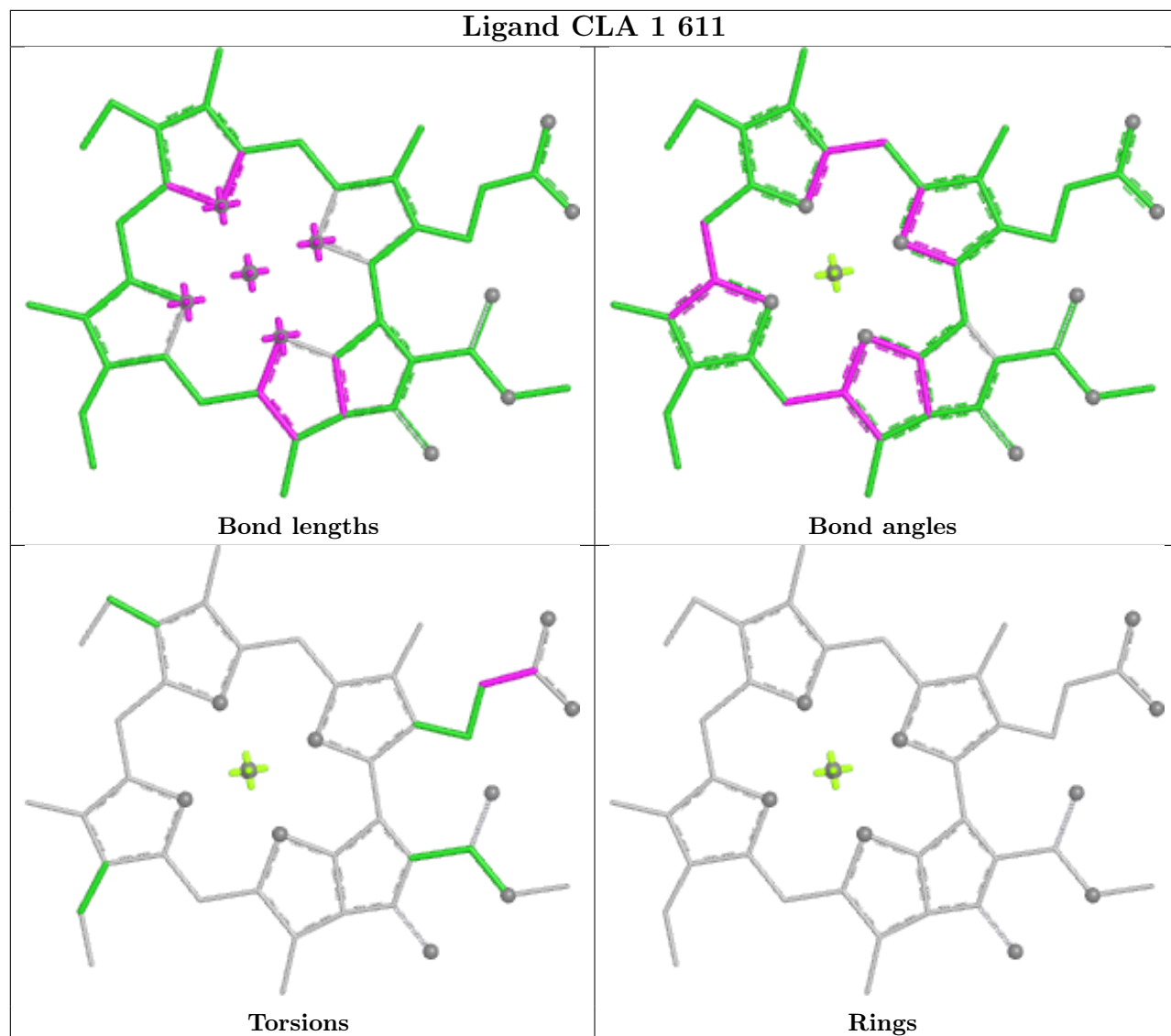


Rings

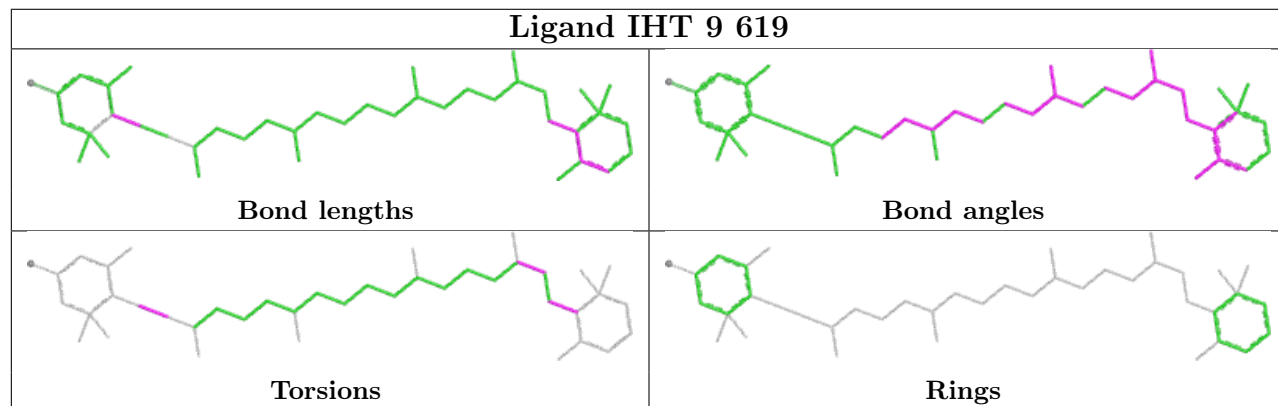




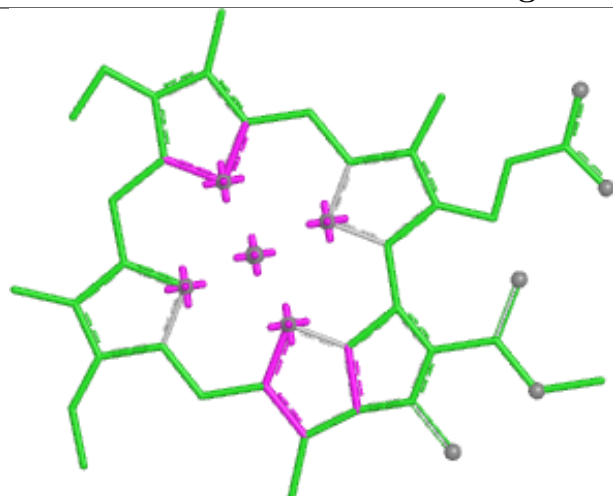
Ligand CLA 1 611



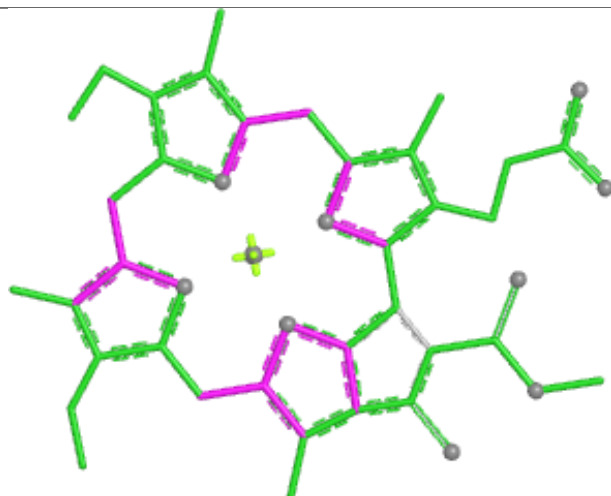
Ligand IHT 9 619



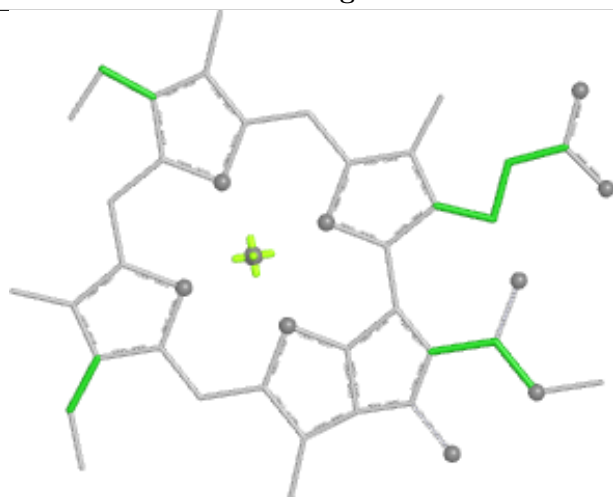
Ligand CLA 1 607



Bond lengths



Bond angles

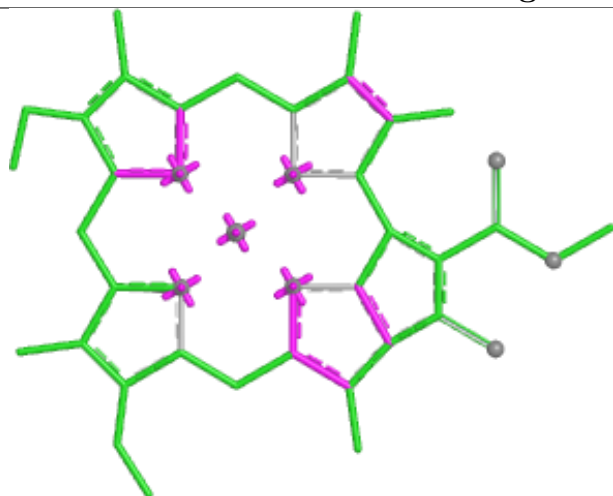


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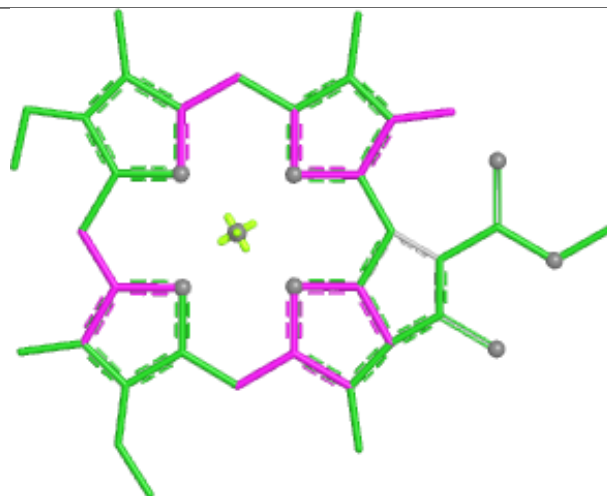


Rings

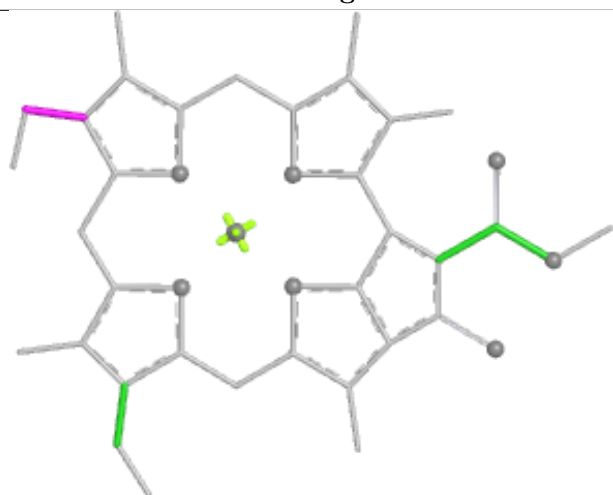
Ligand CLA e 608



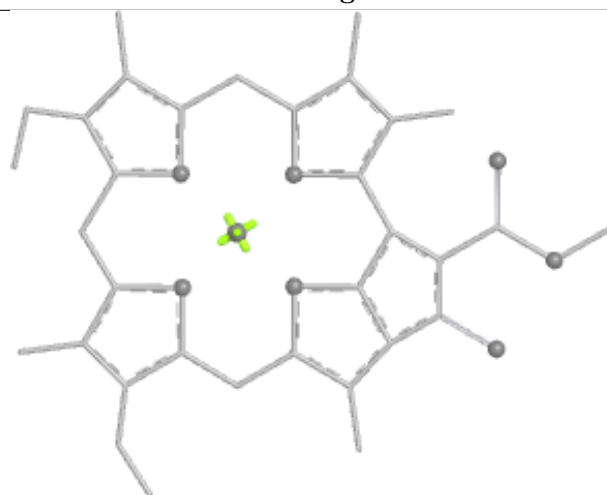
Bond lengths



Bond angles

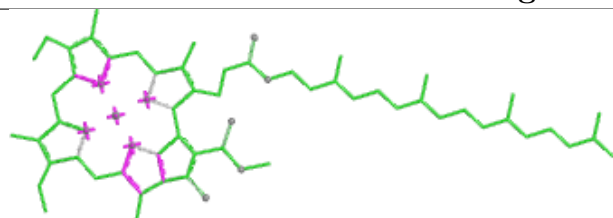


Torsions

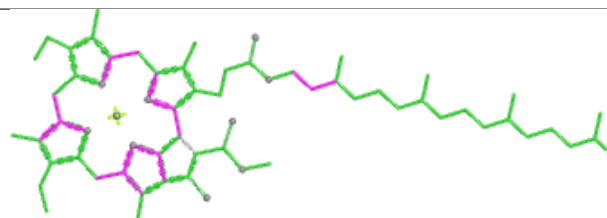


Rings

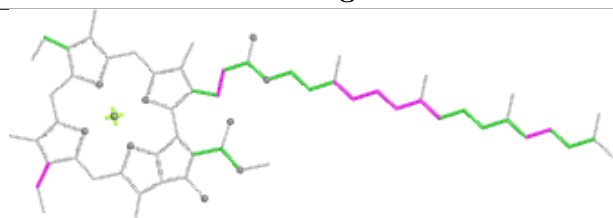
Ligand CLA 9 607



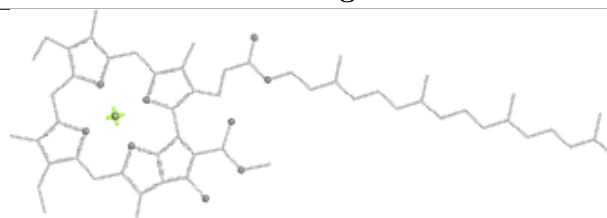
Bond lengths



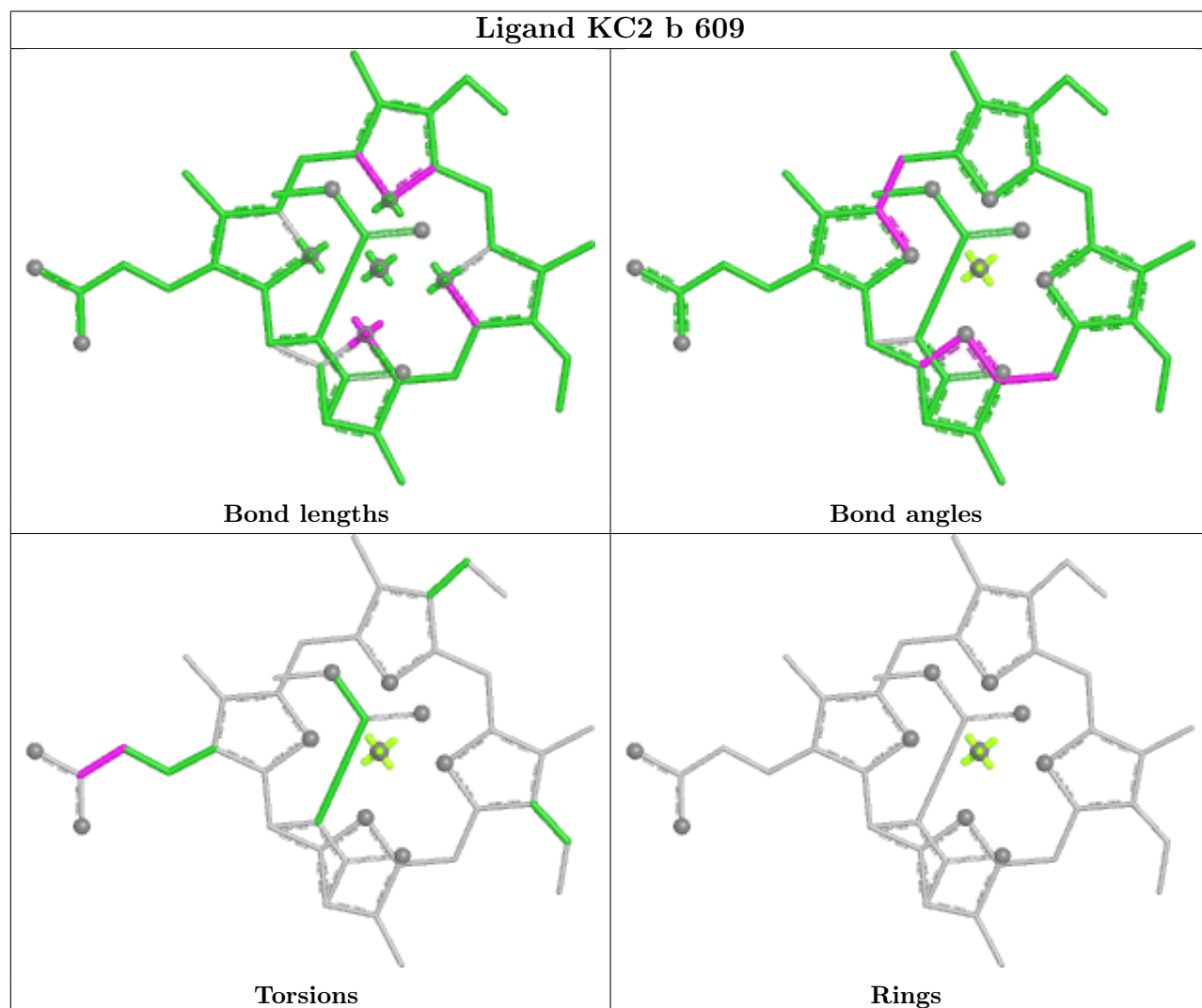
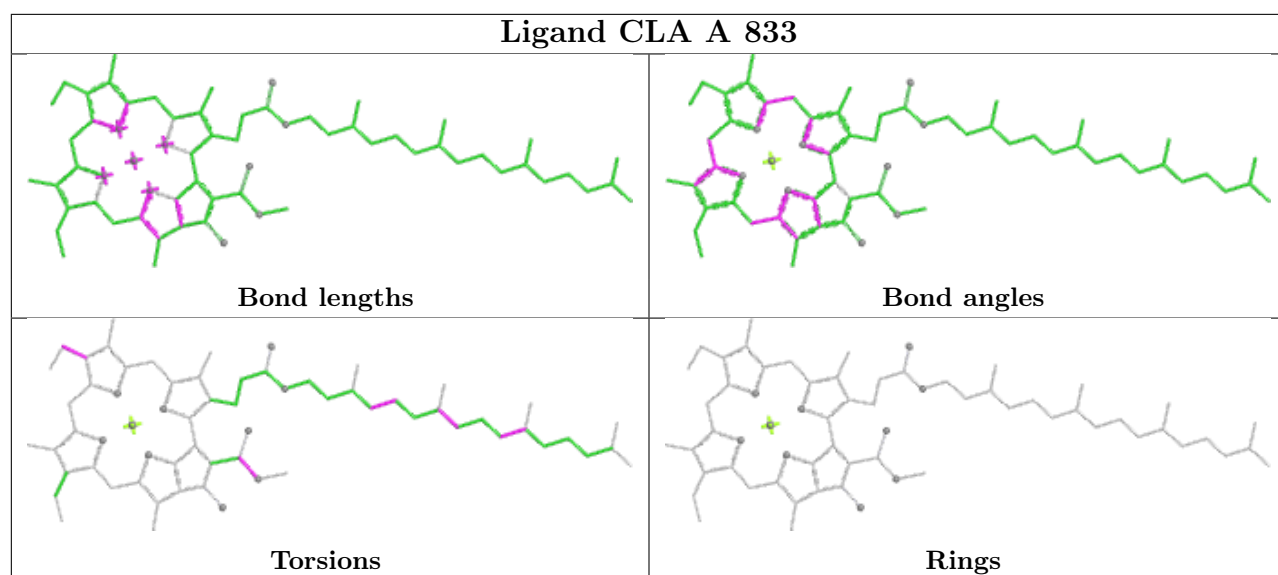
Bond angles

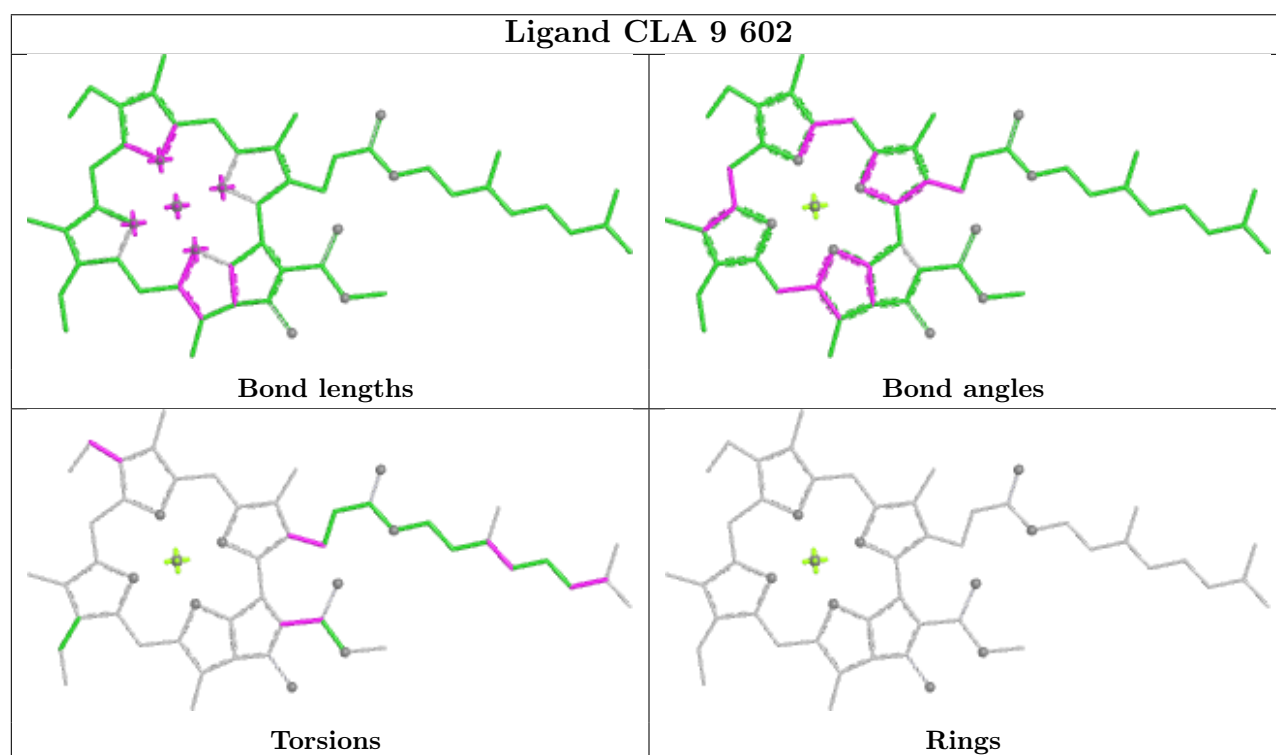
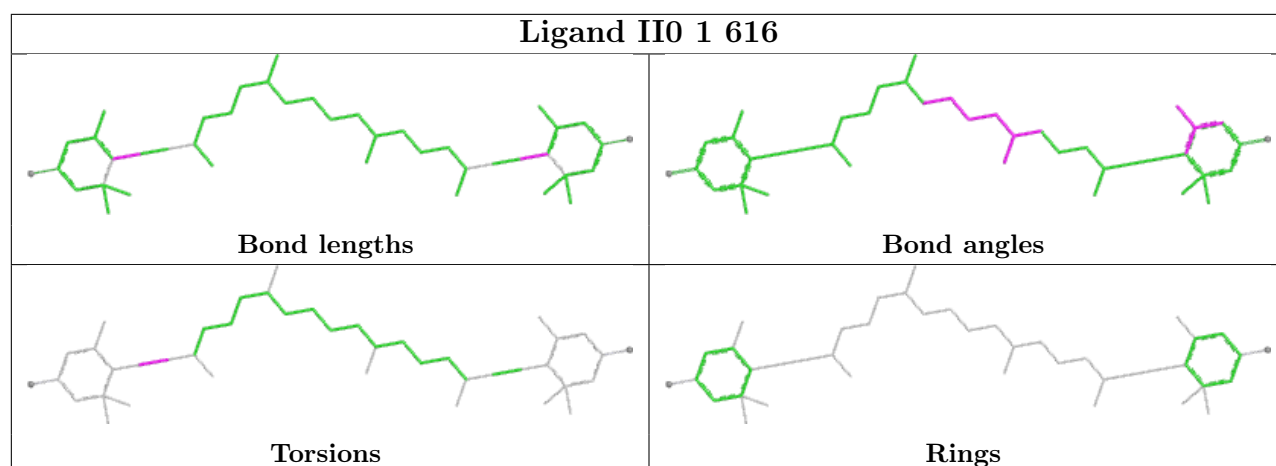


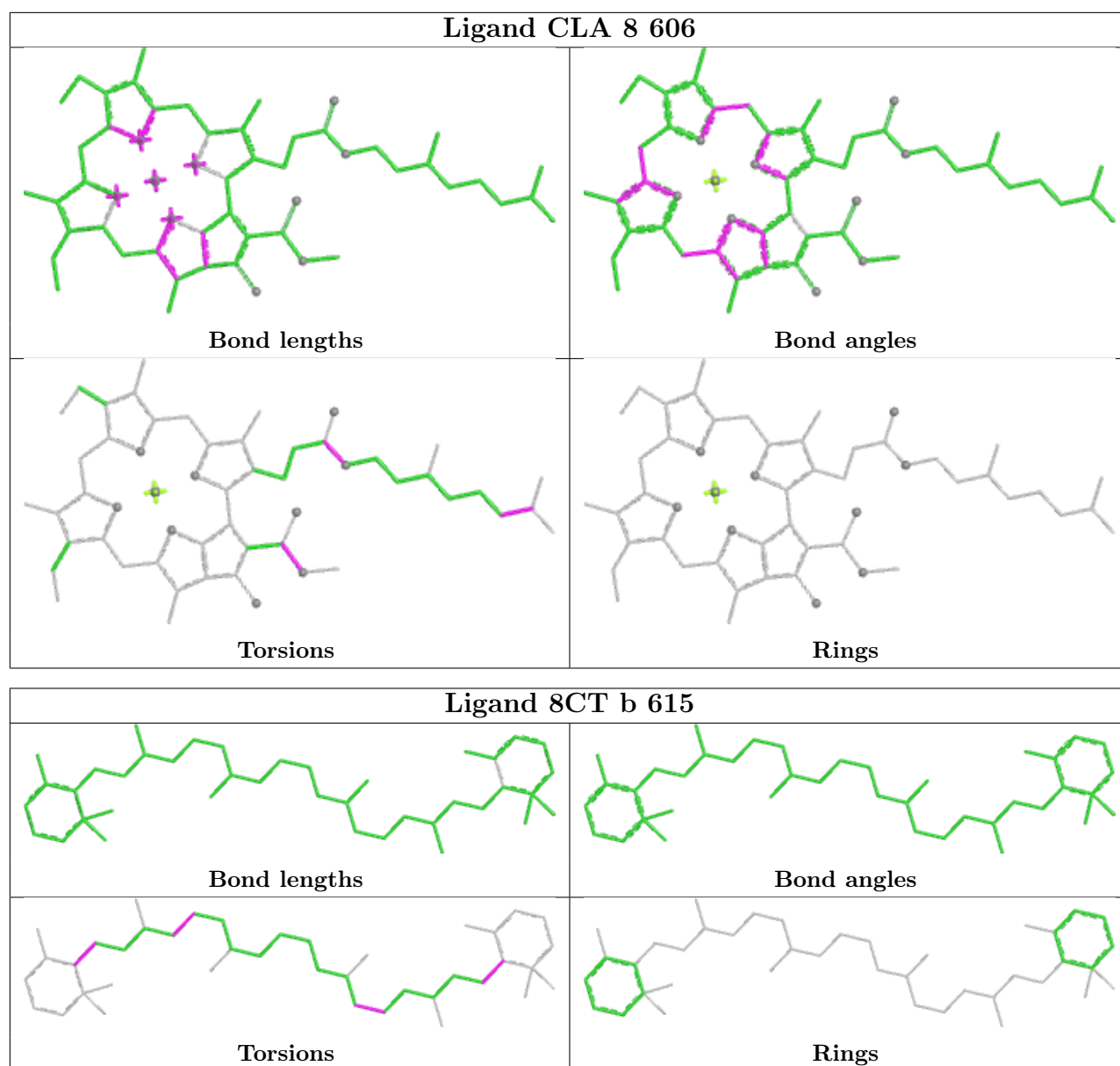
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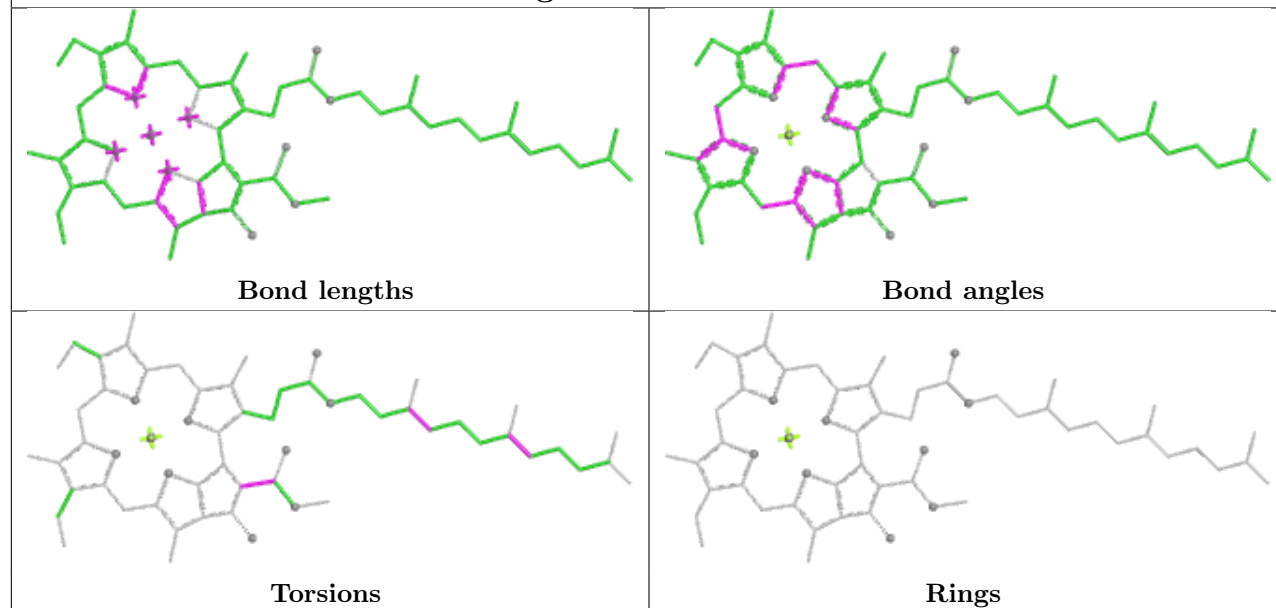
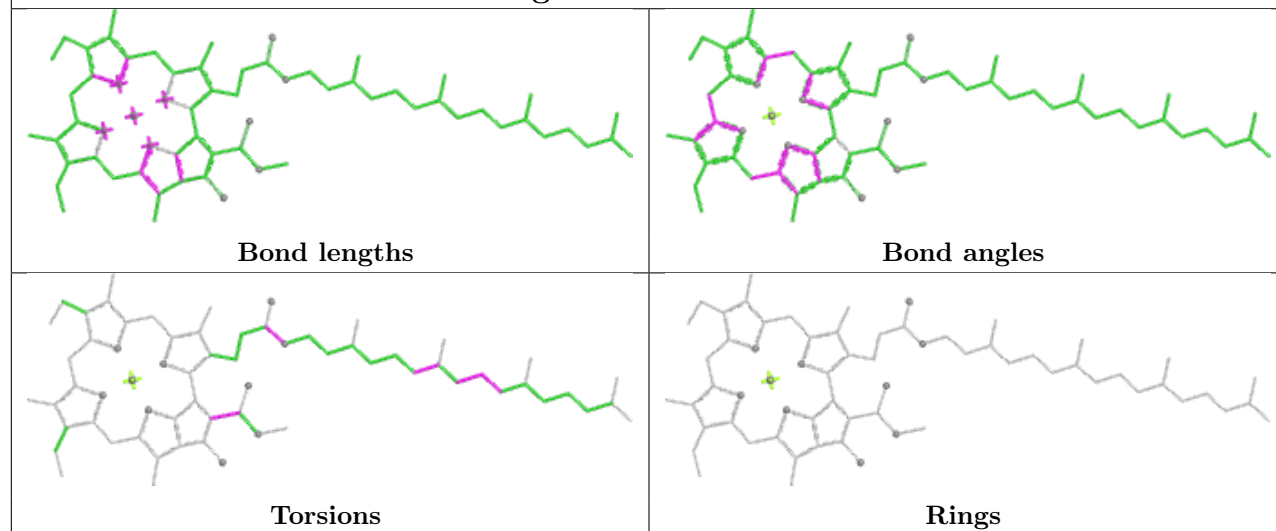


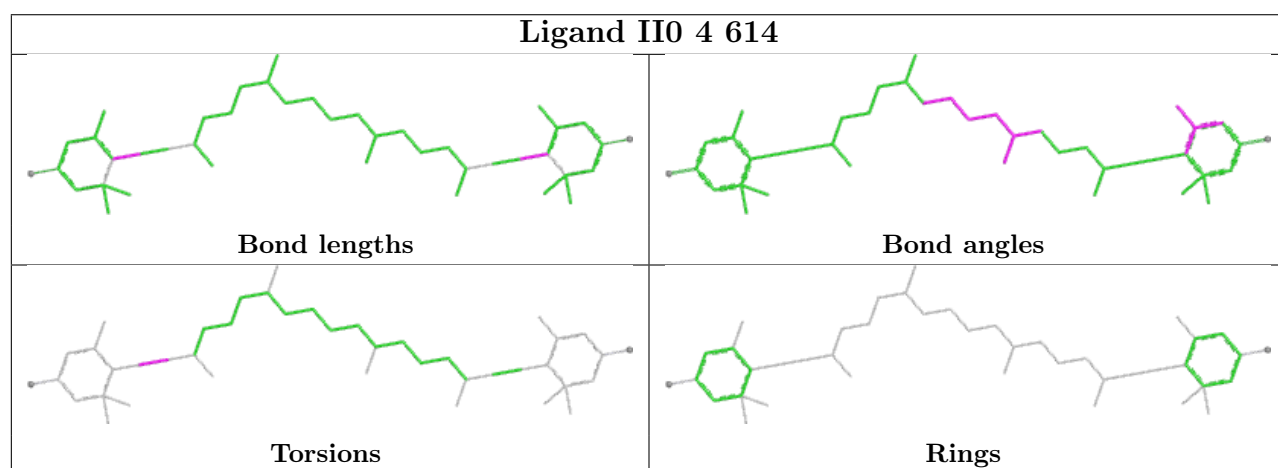
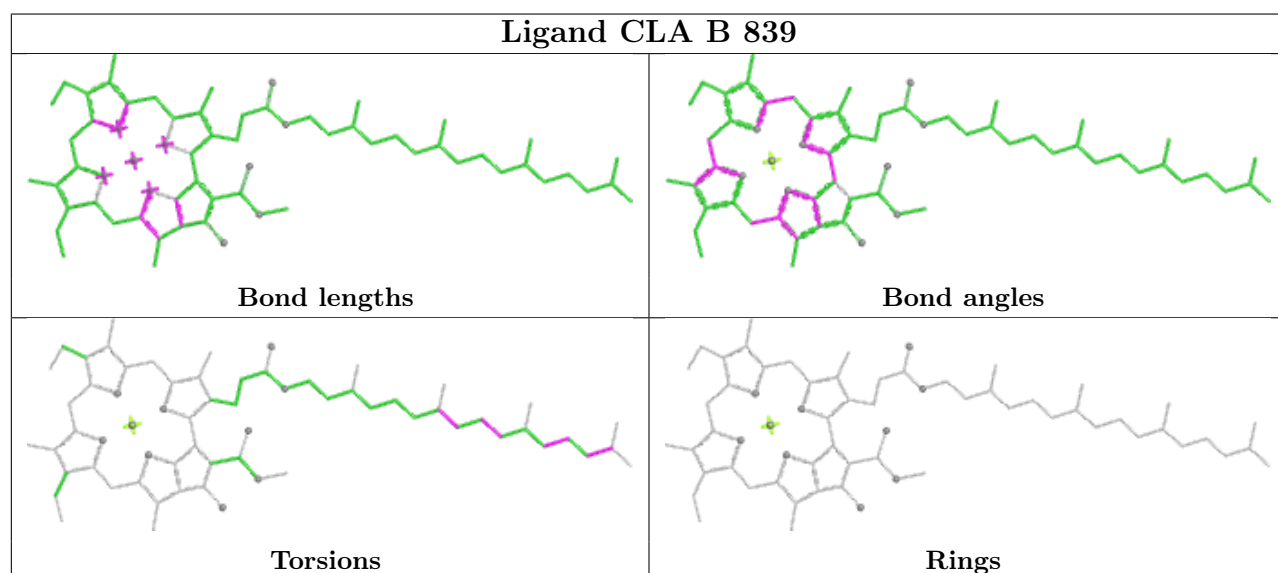
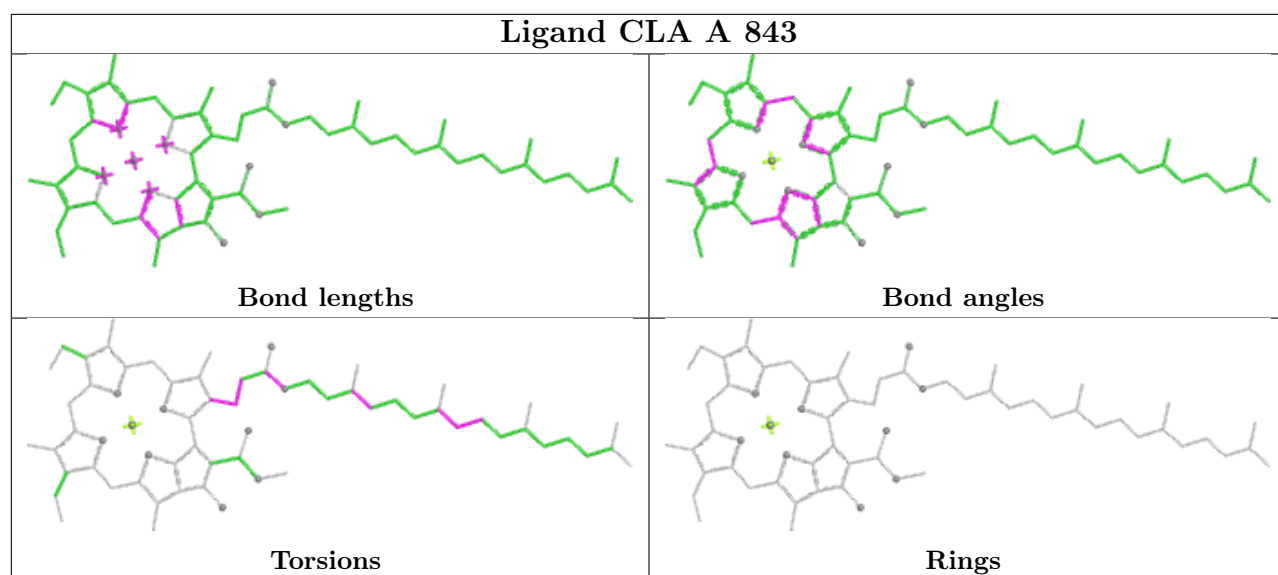
Rings



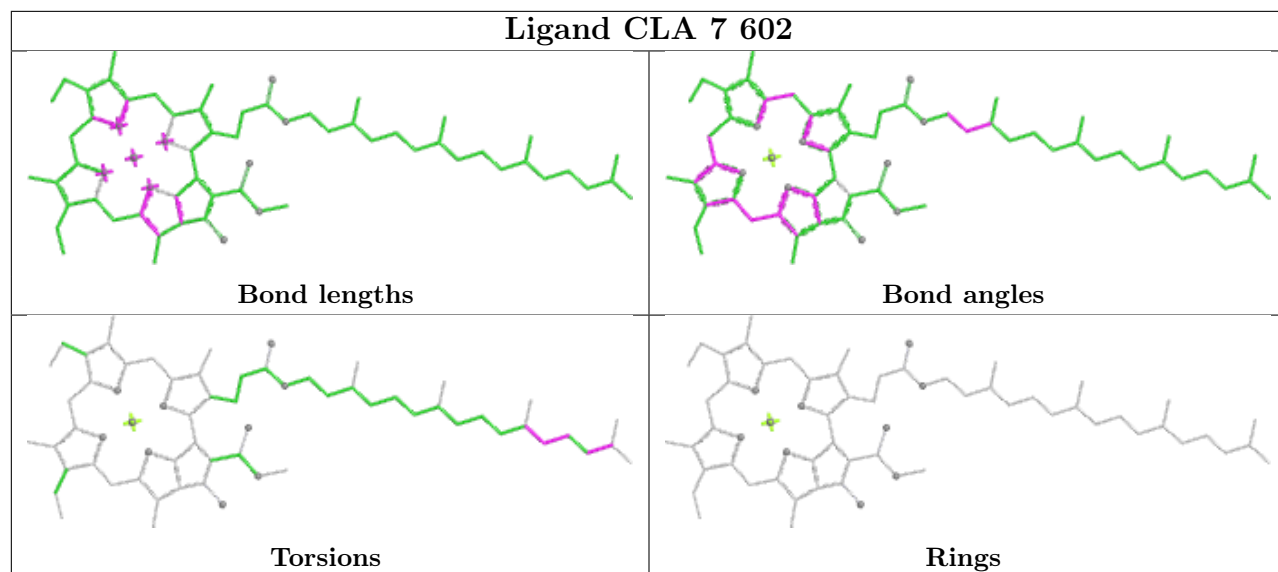




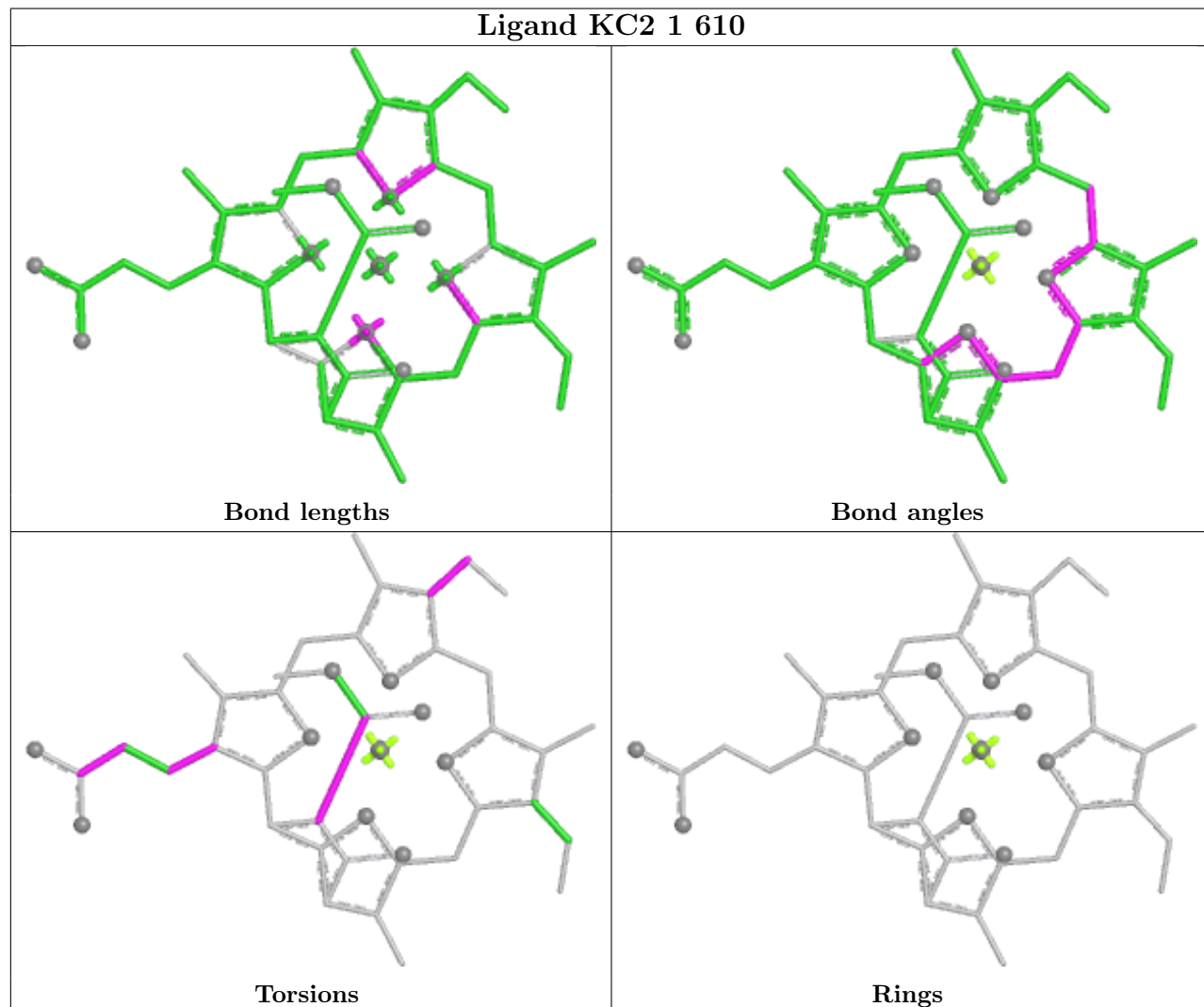
Ligand CLA 6 604**Ligand CLA B 828**

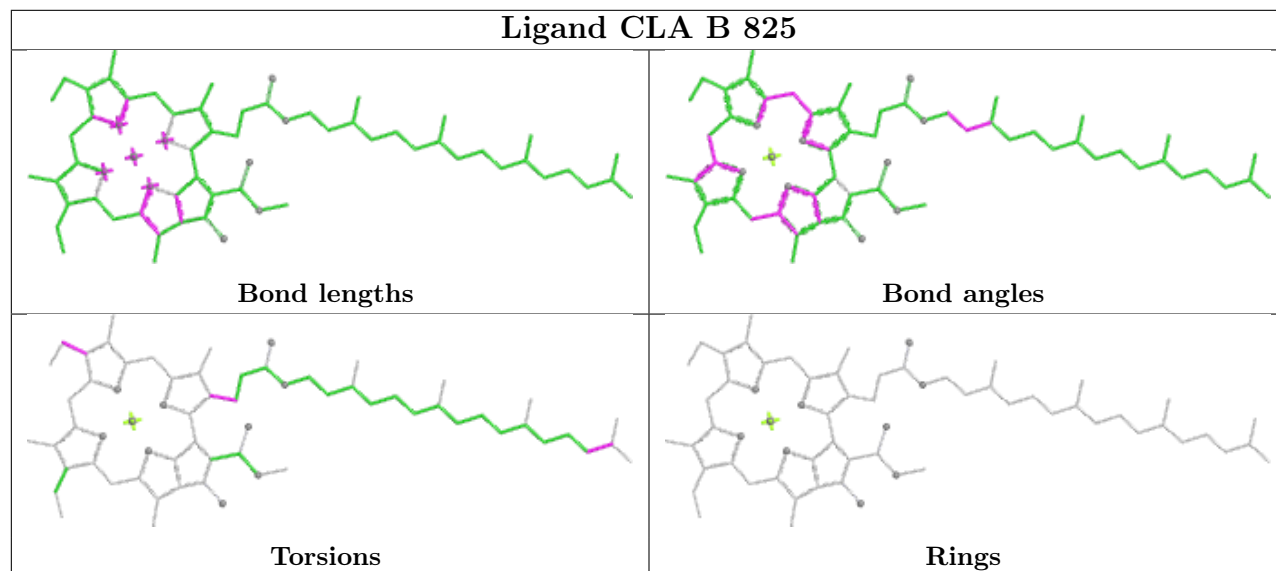
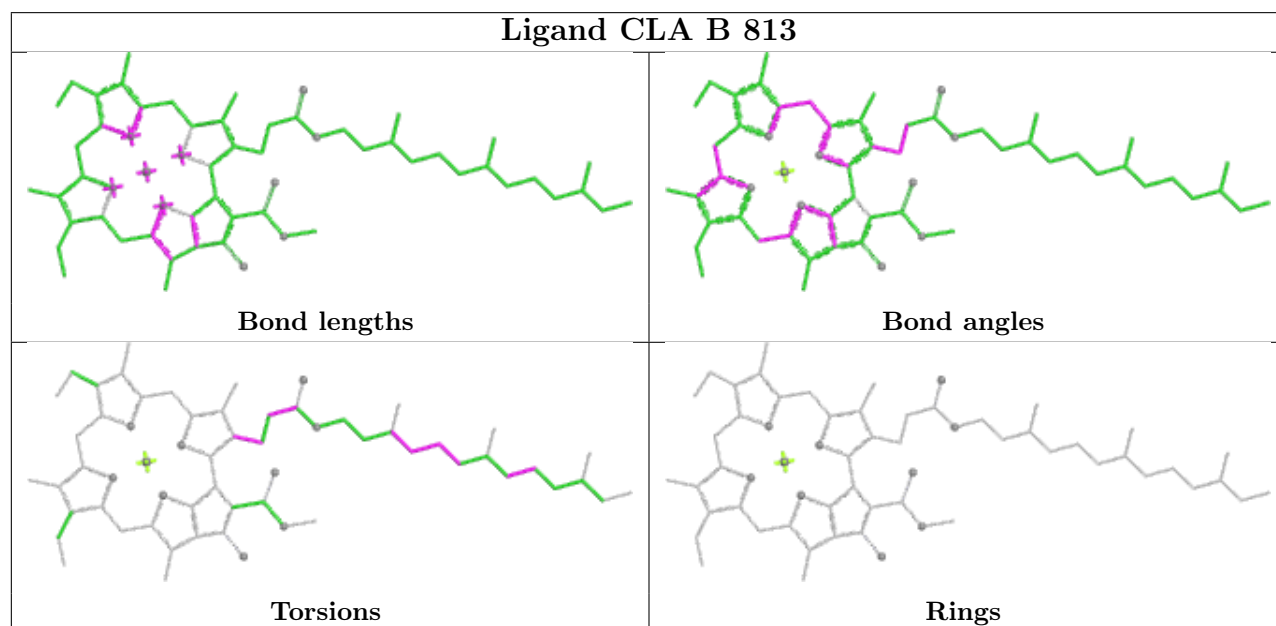
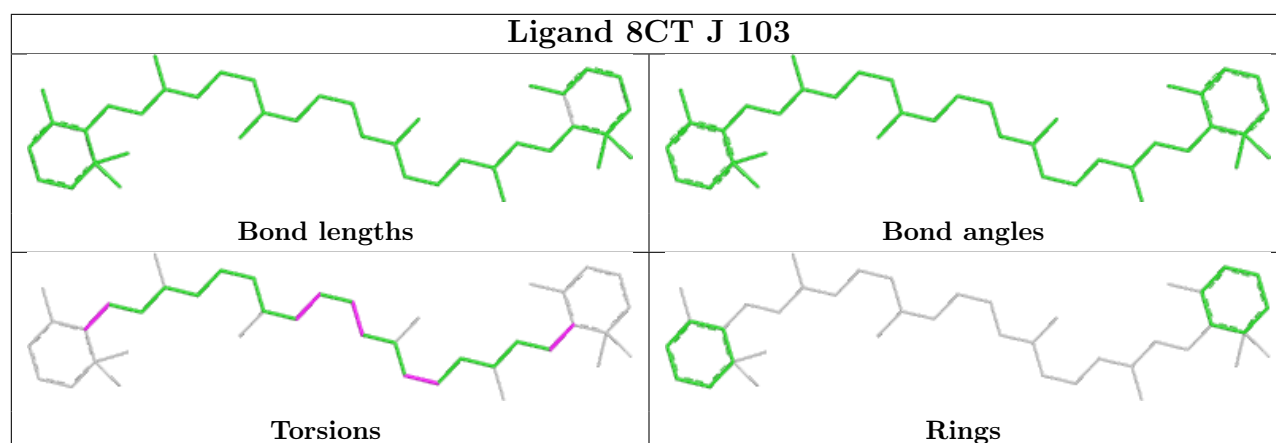


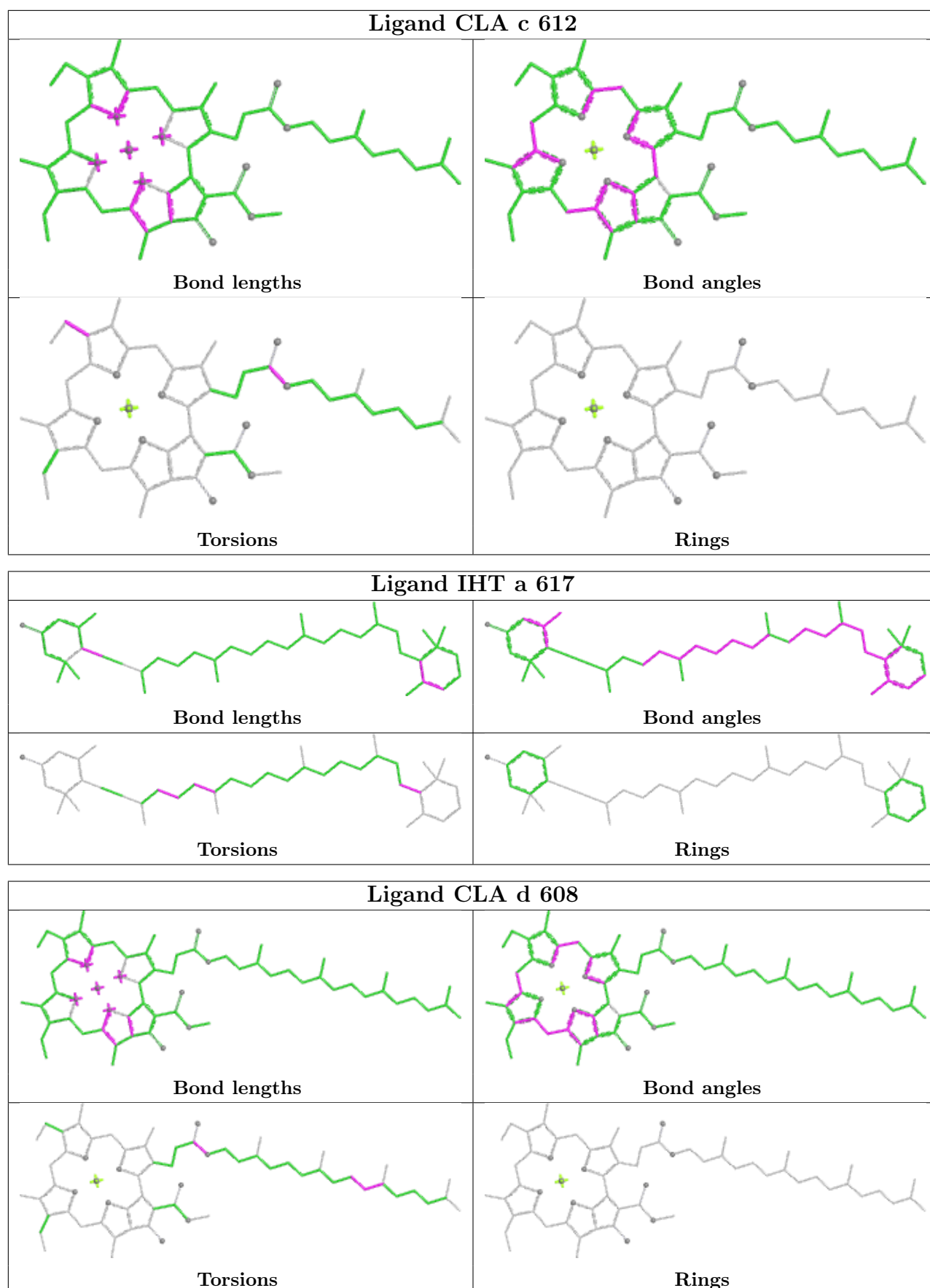
Ligand CLA 7 602

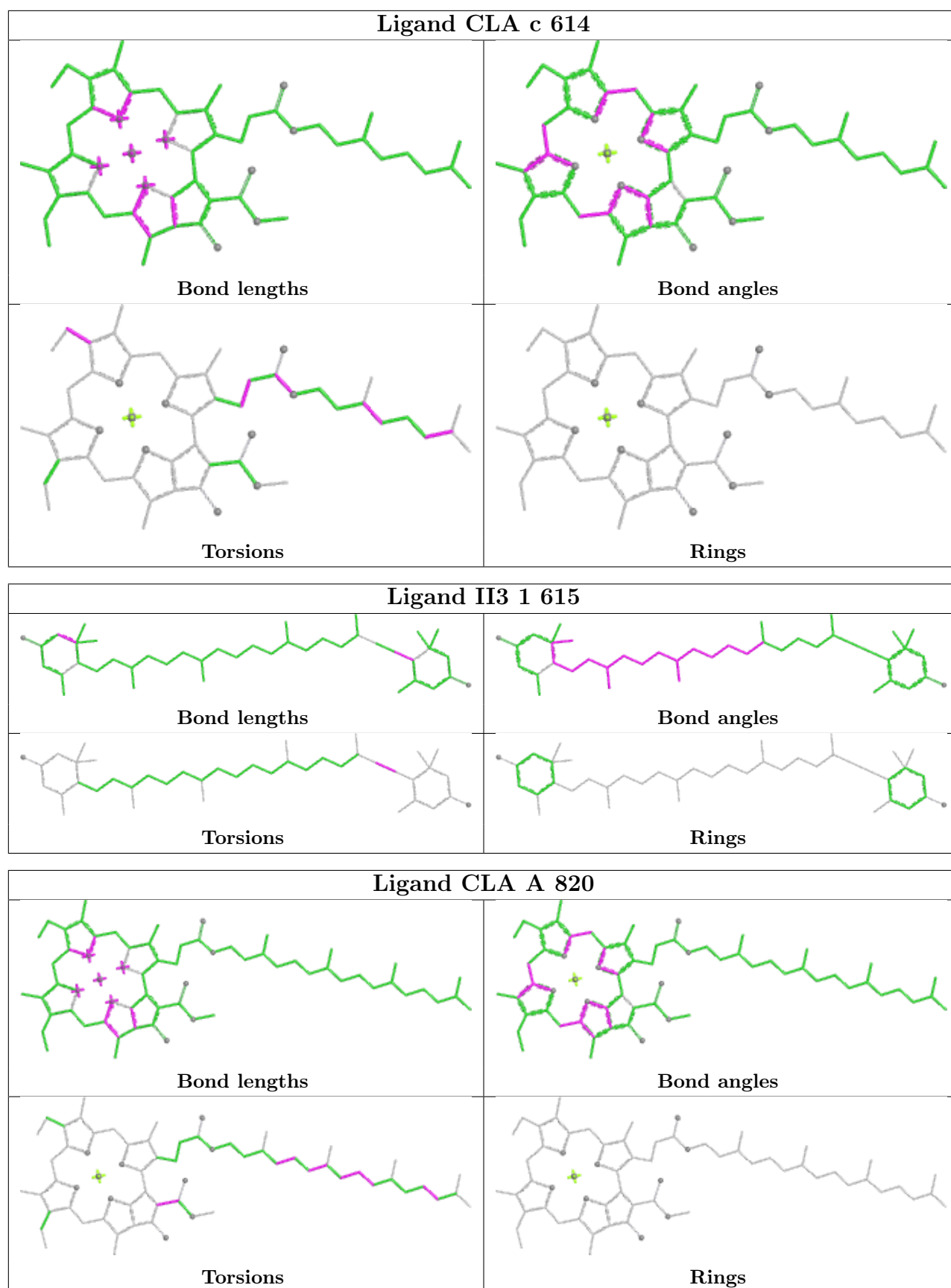


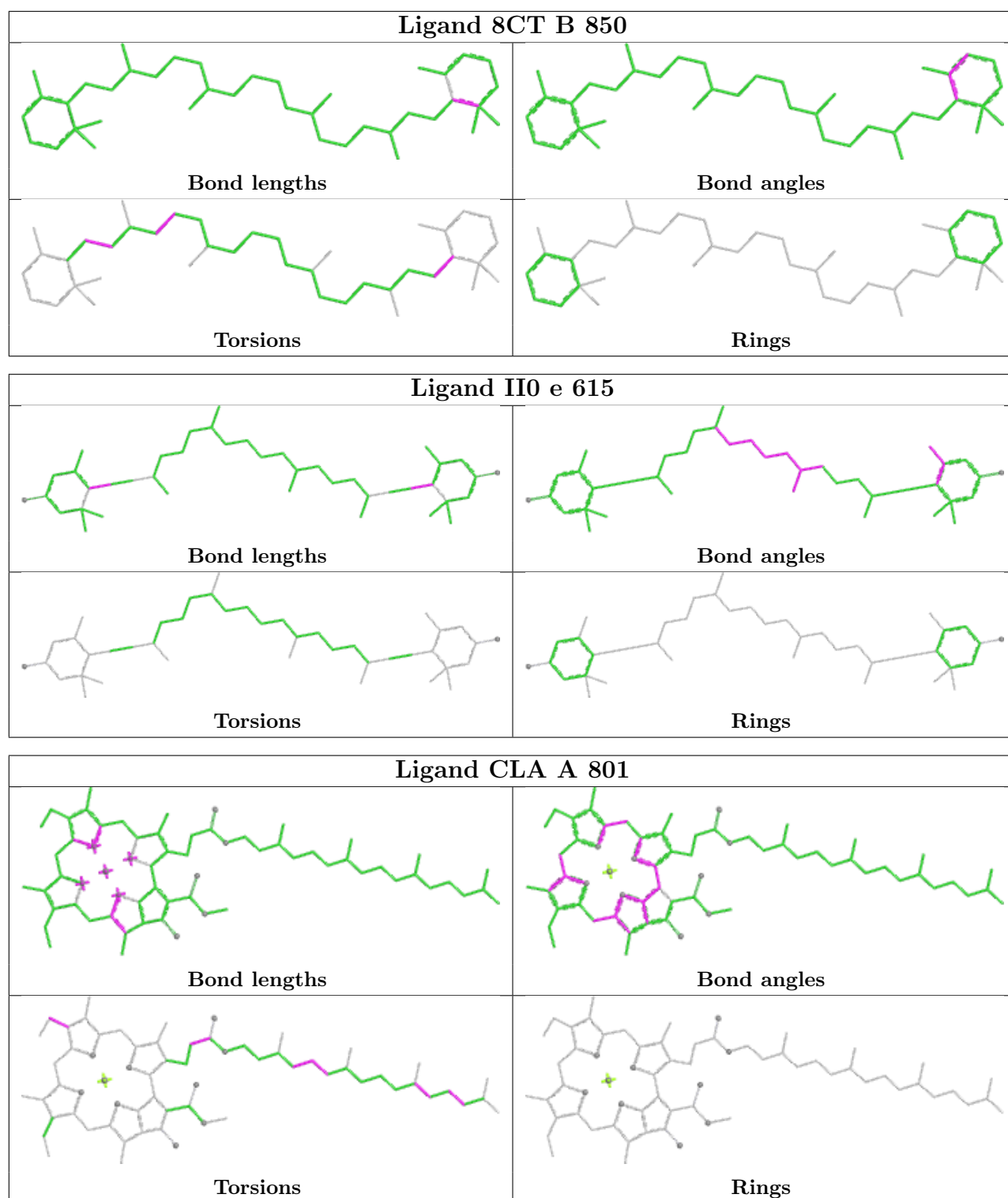
Ligand KC2 1 610

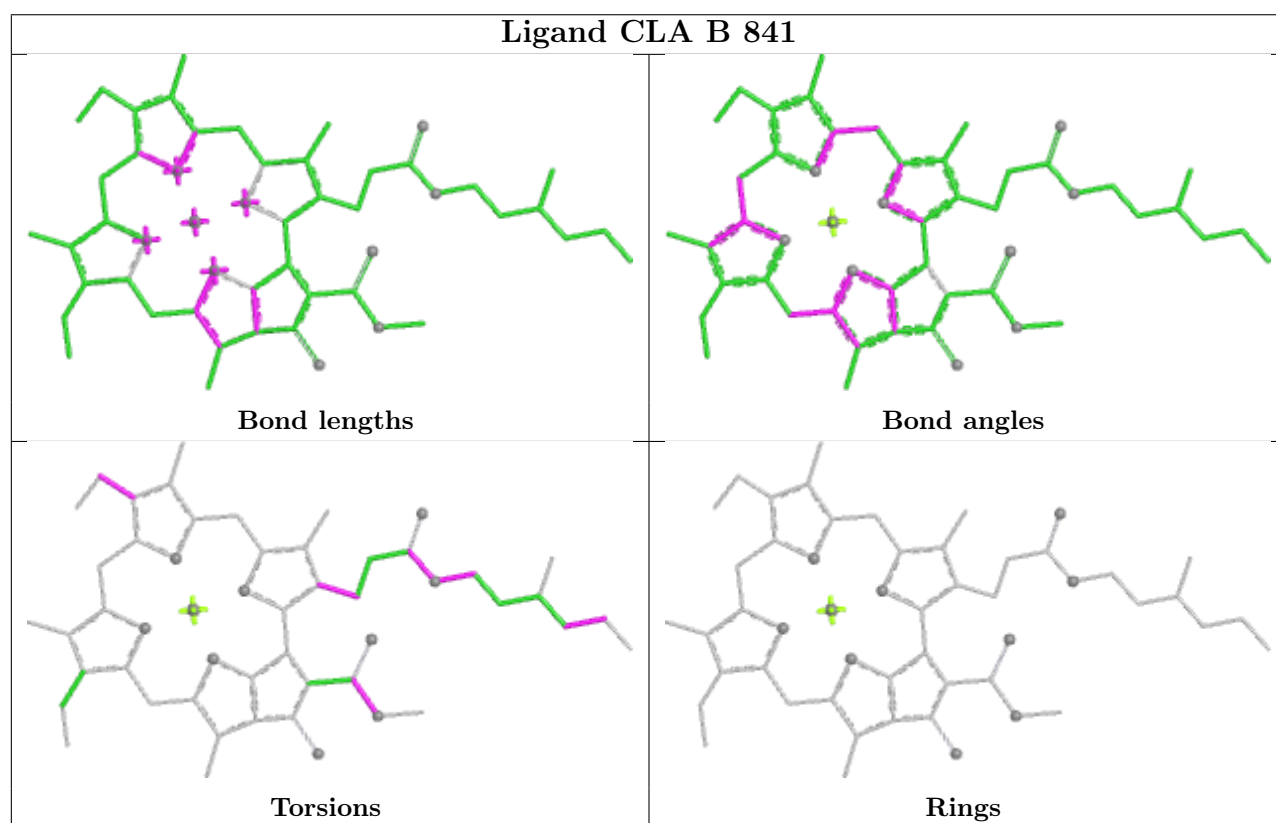
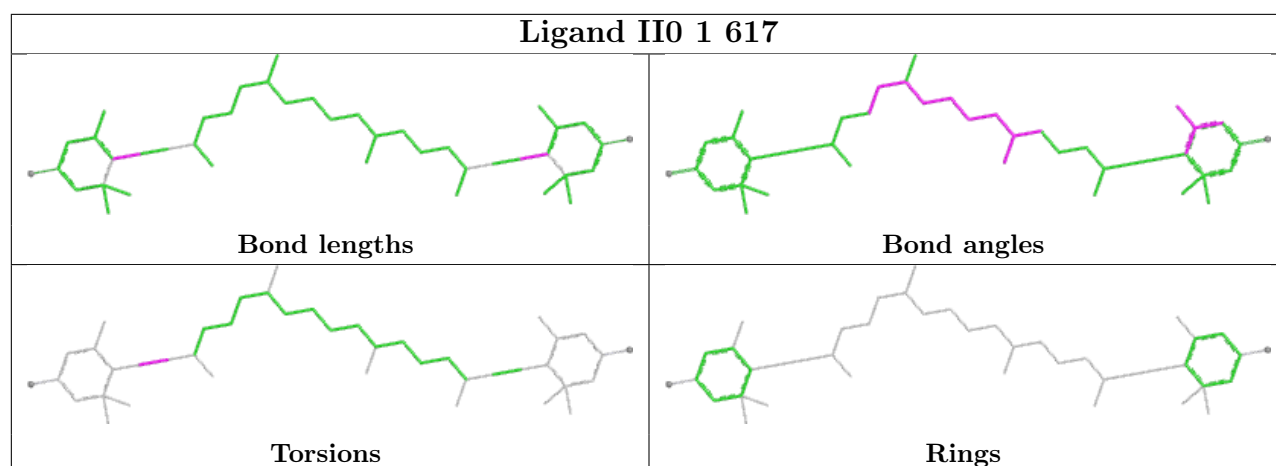


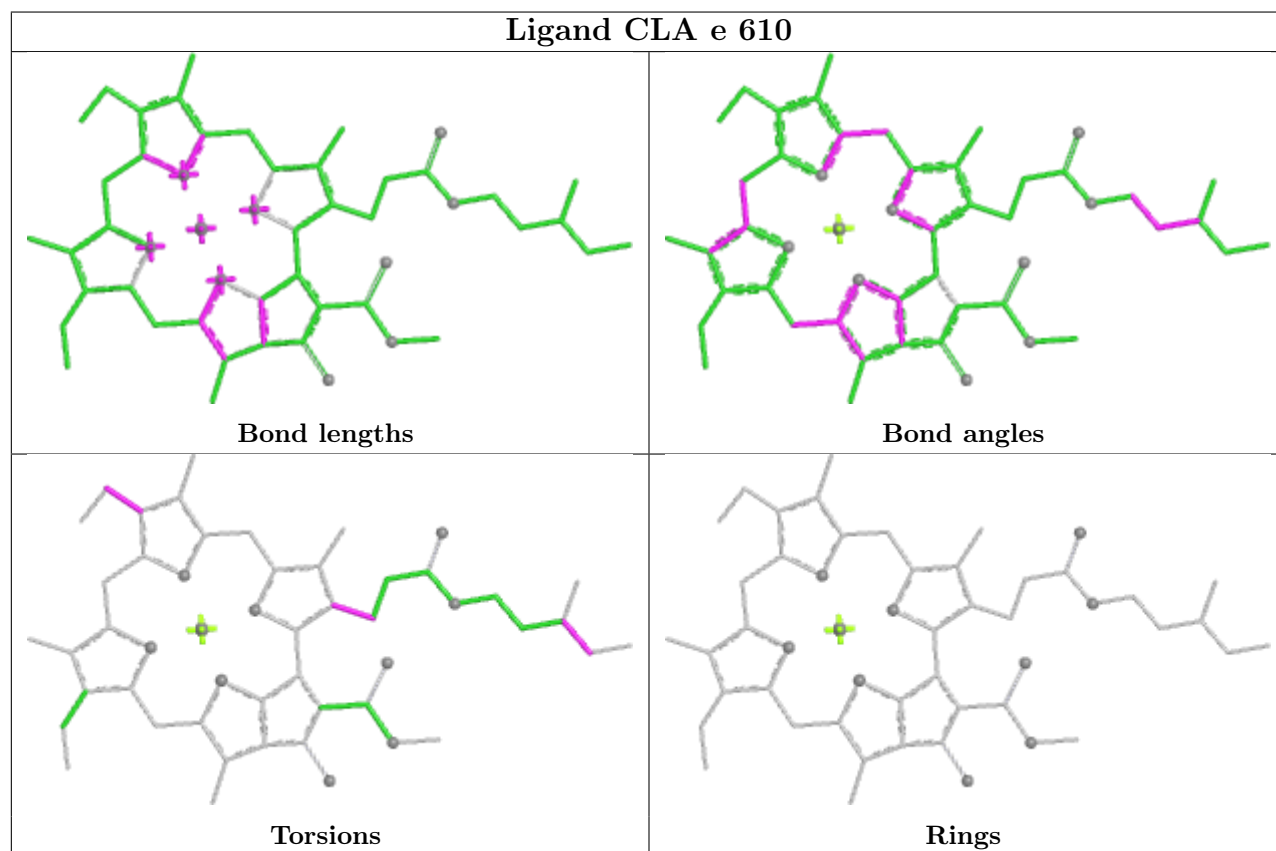
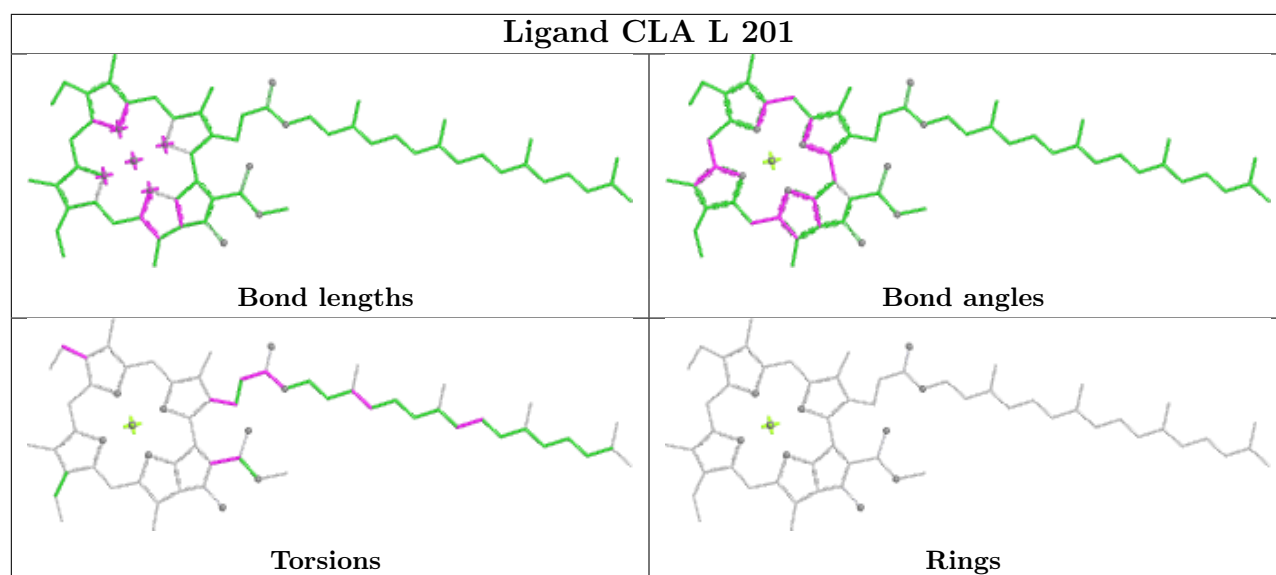


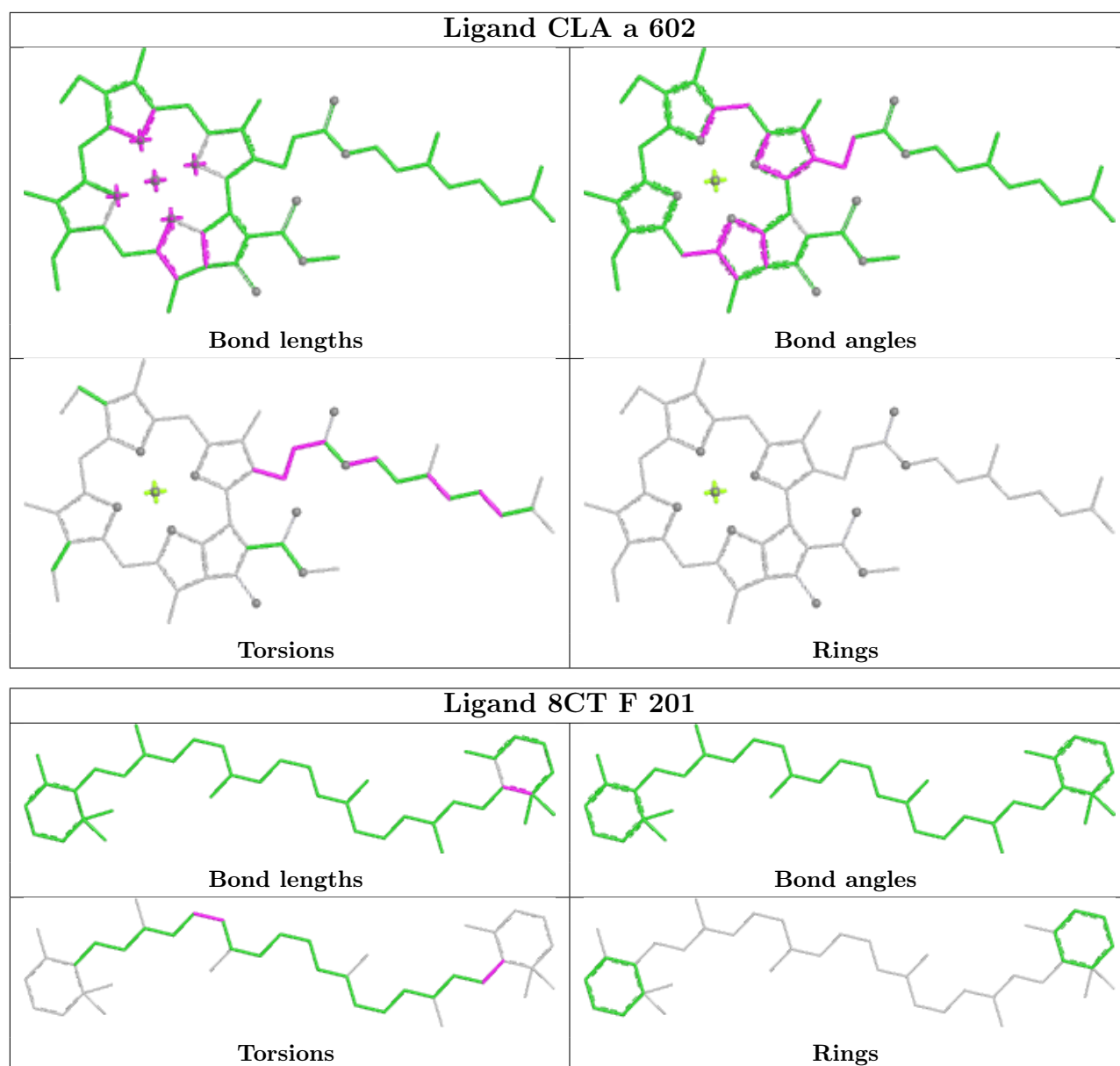


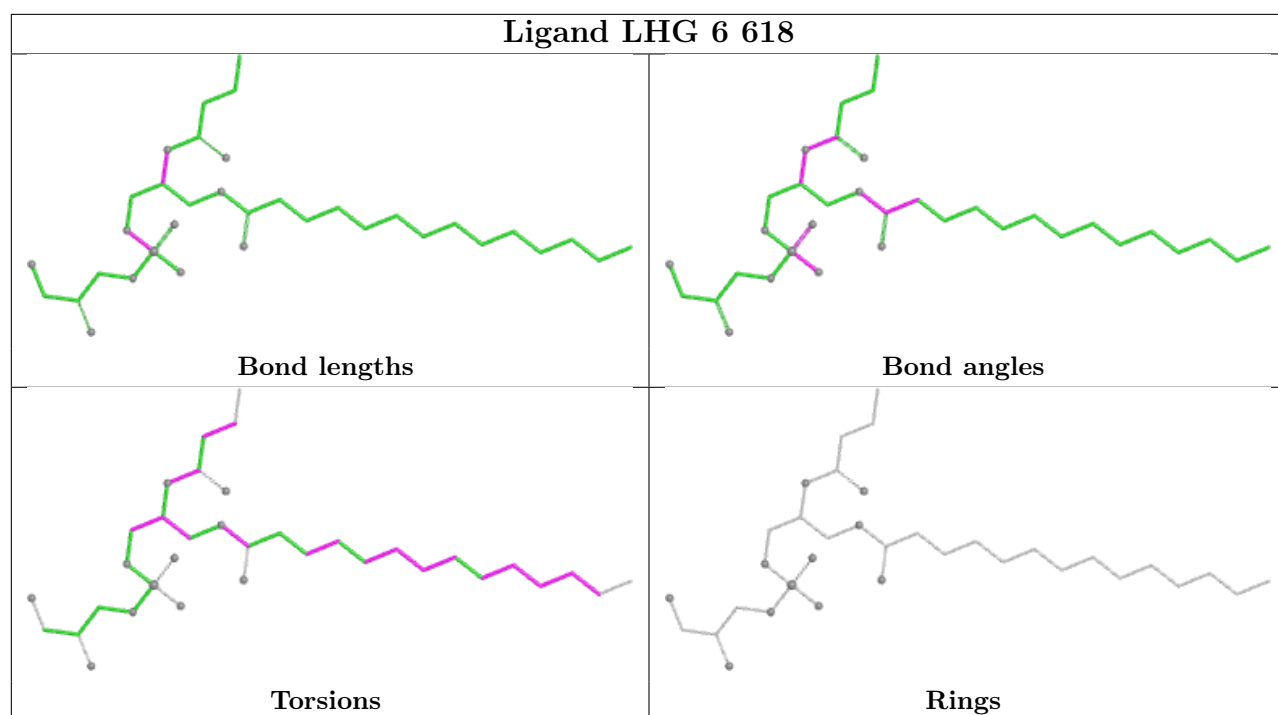




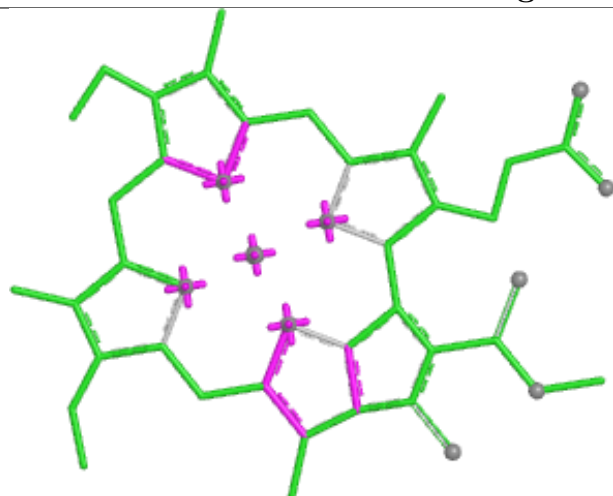




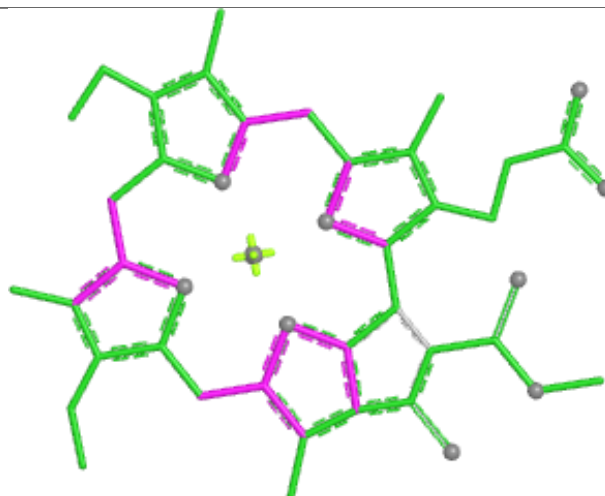




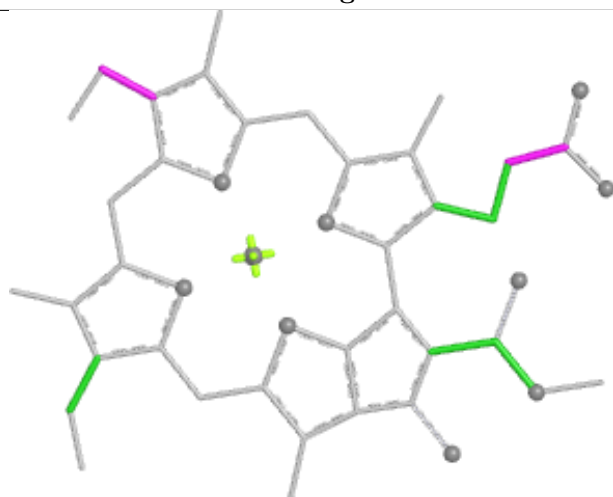
Ligand CLA b 601



Bond lengths



Bond angles

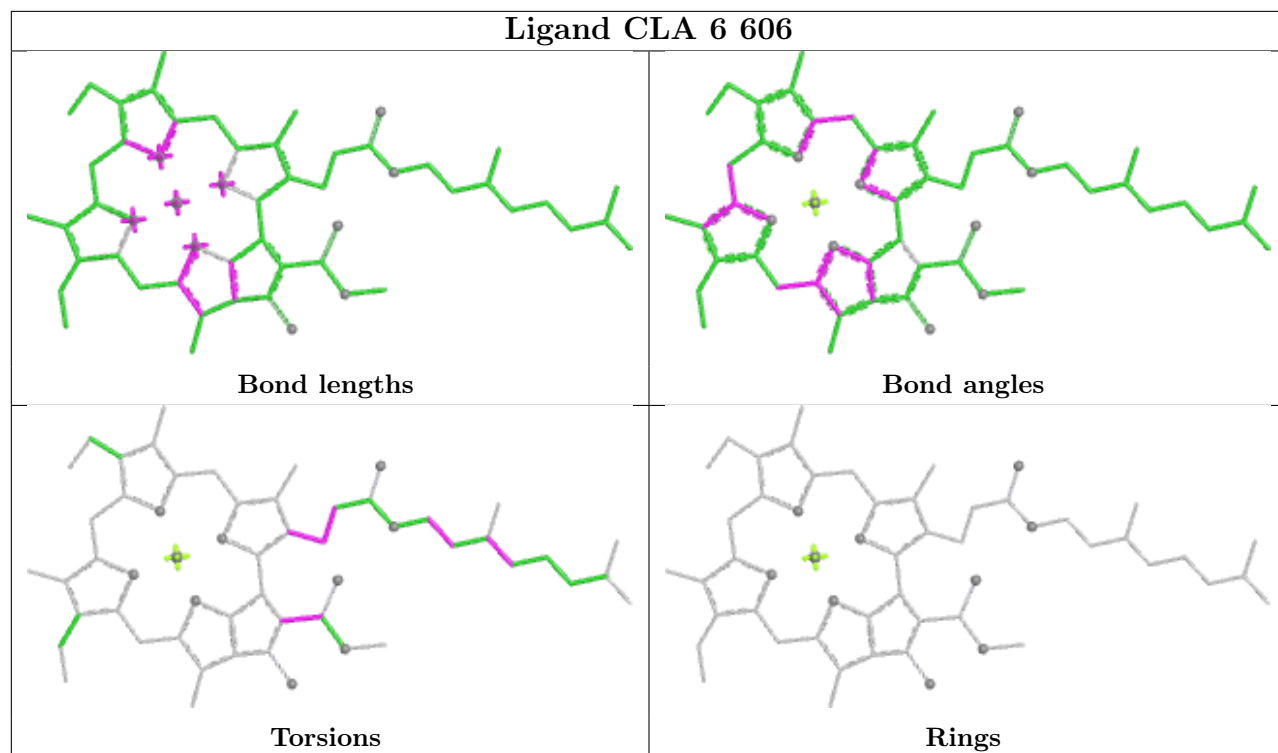


Torsions

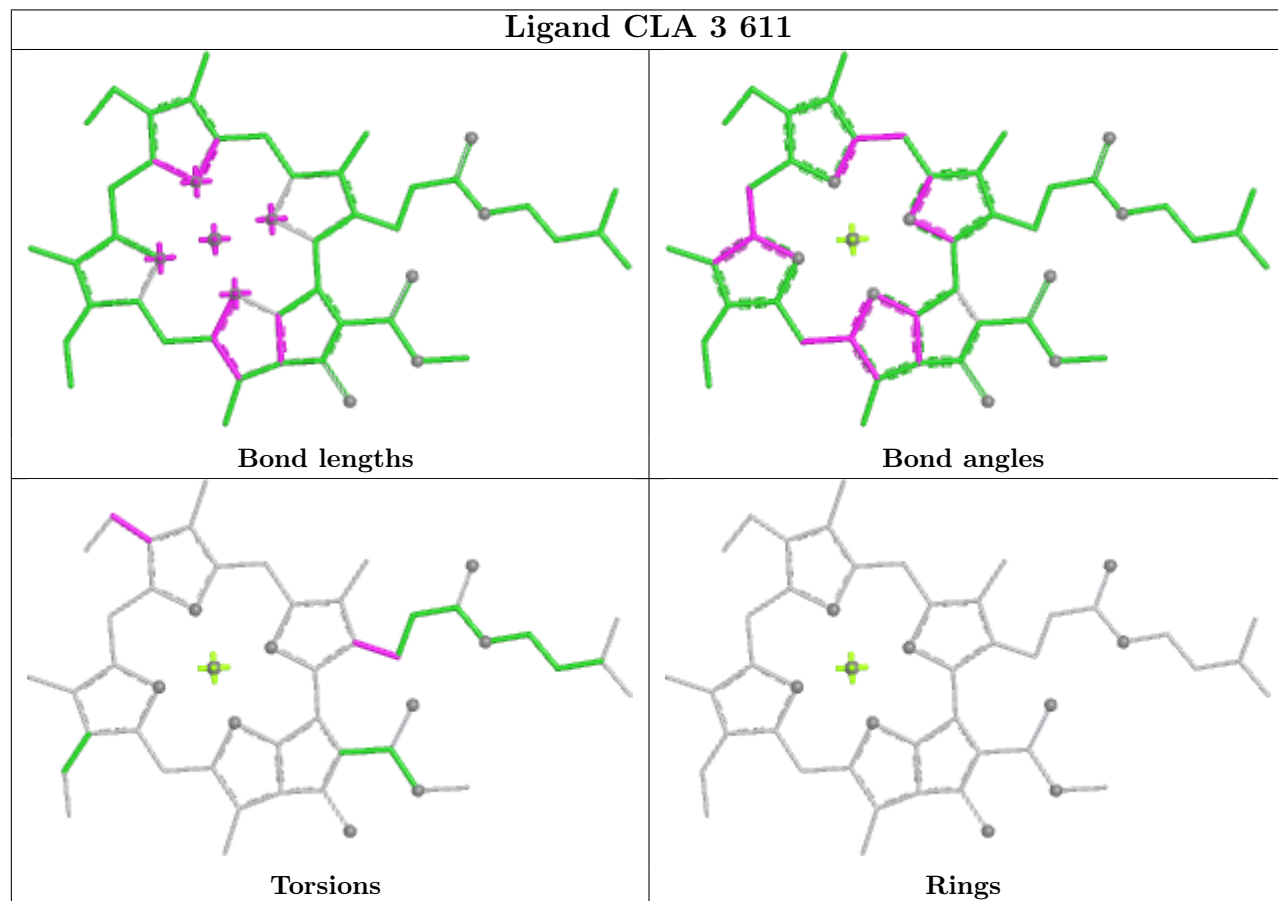


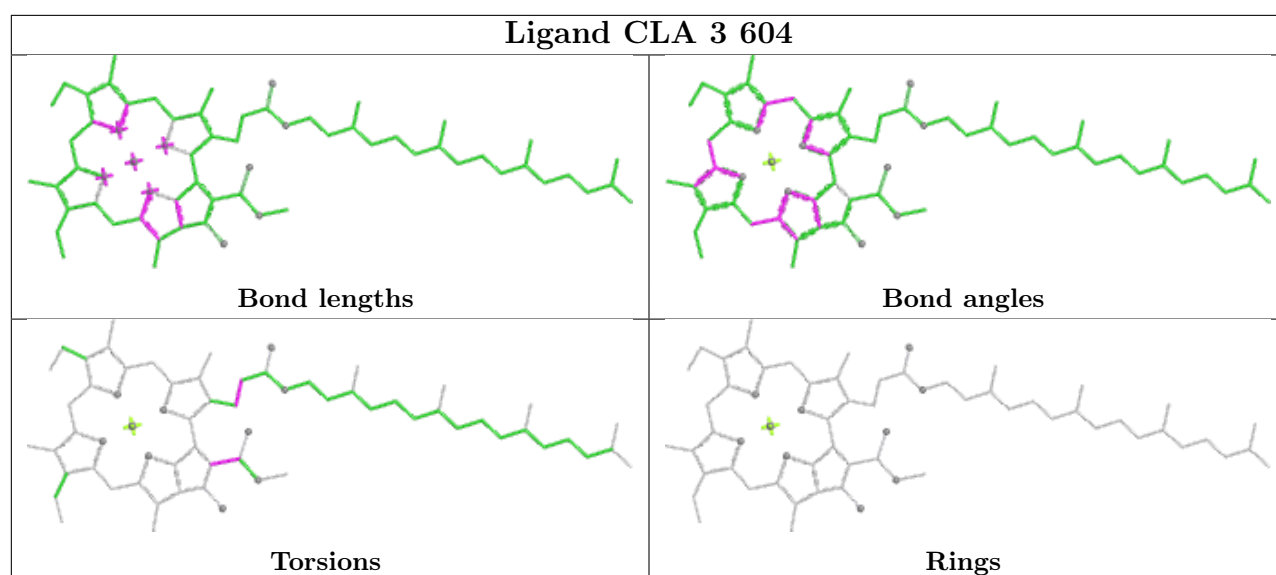
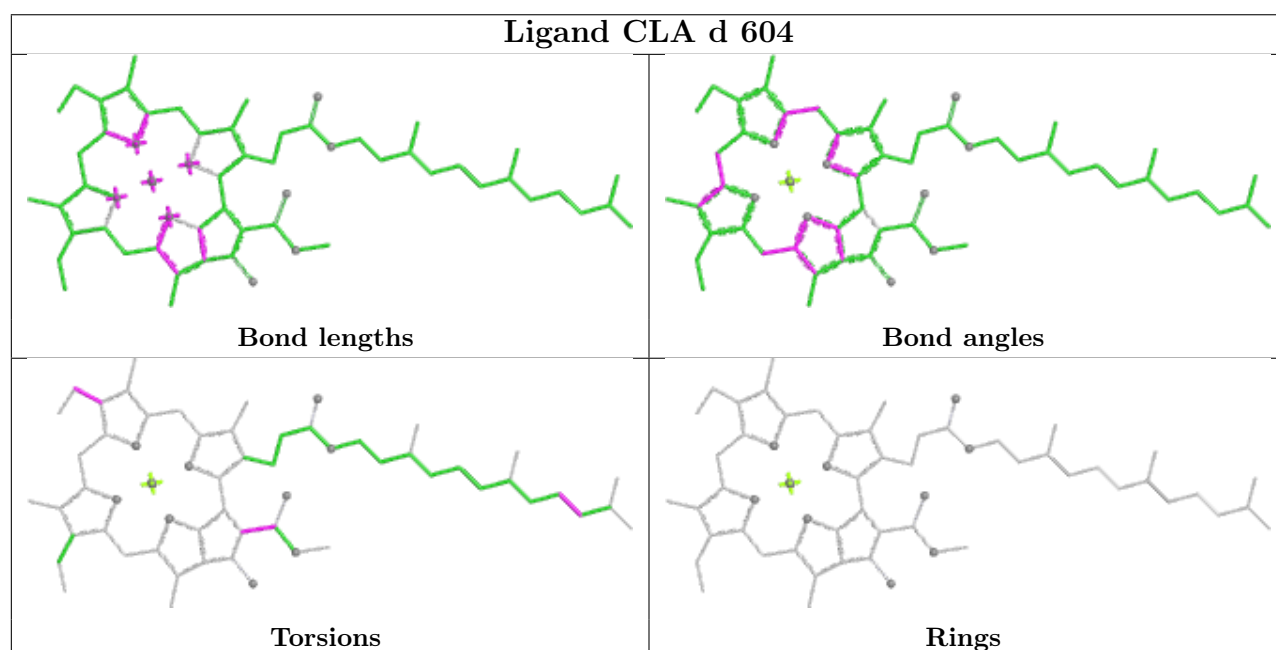
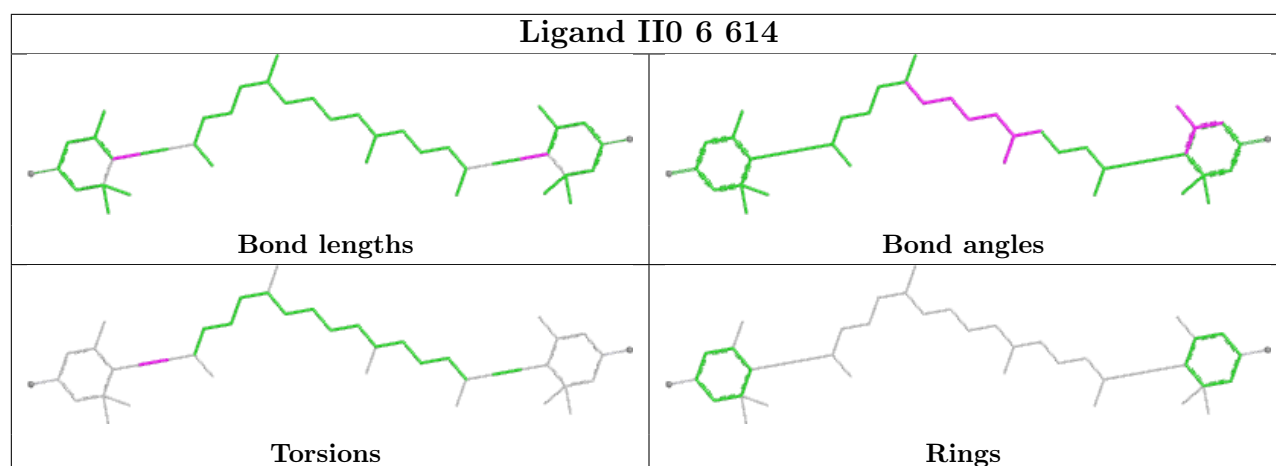
Rings

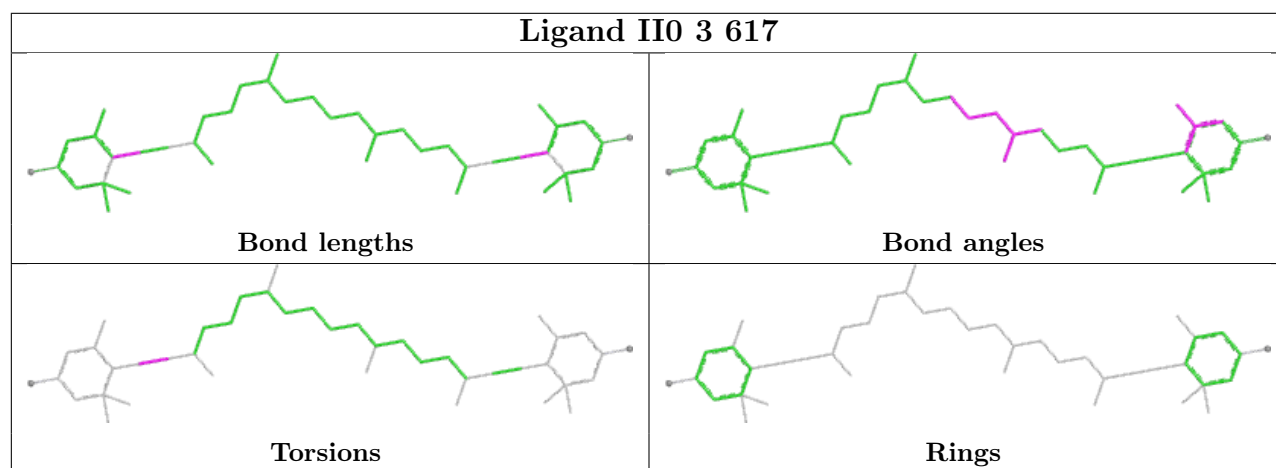
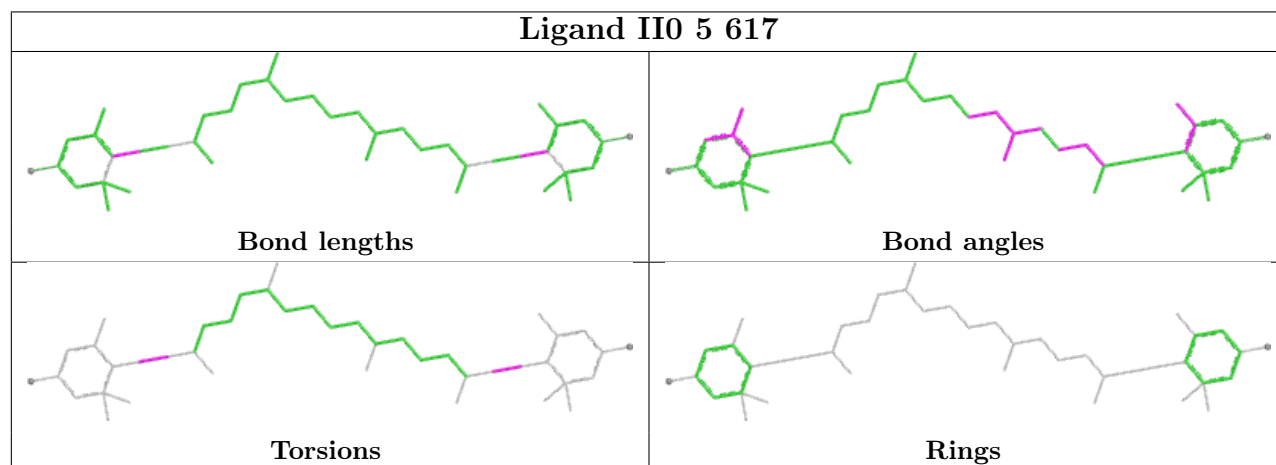
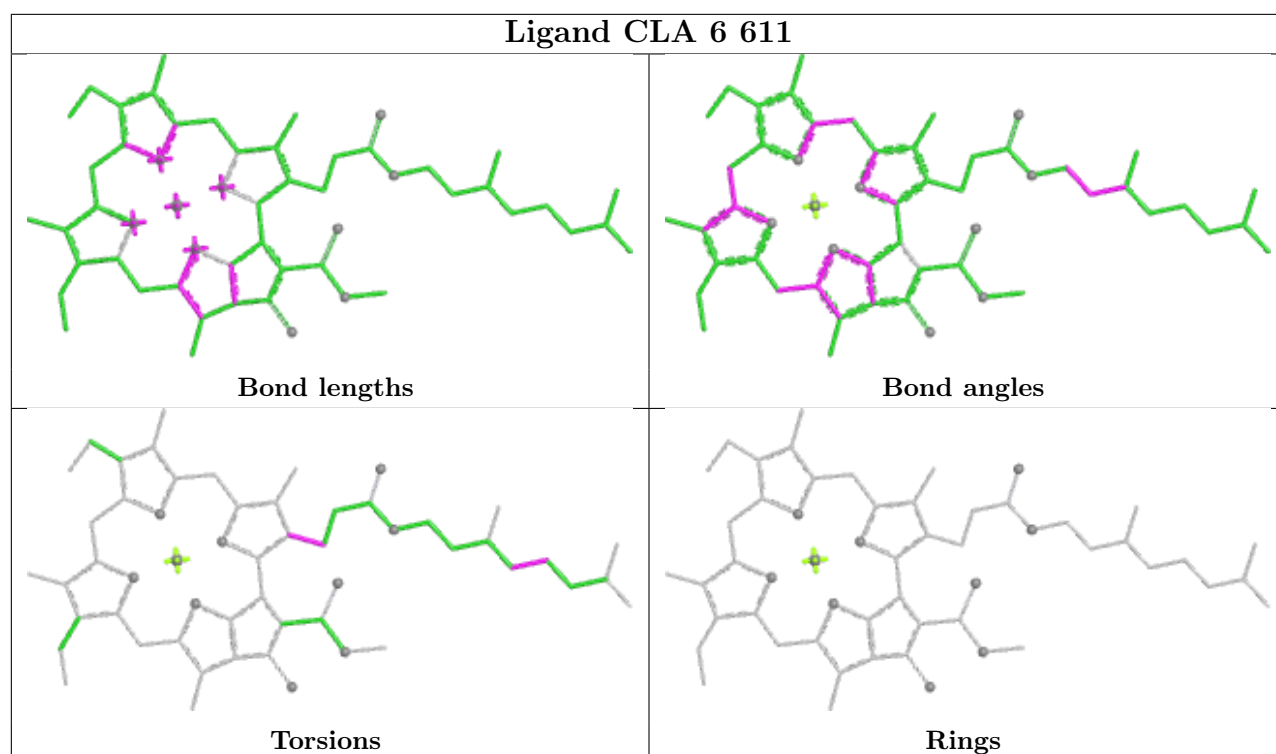
Ligand CLA 6 606

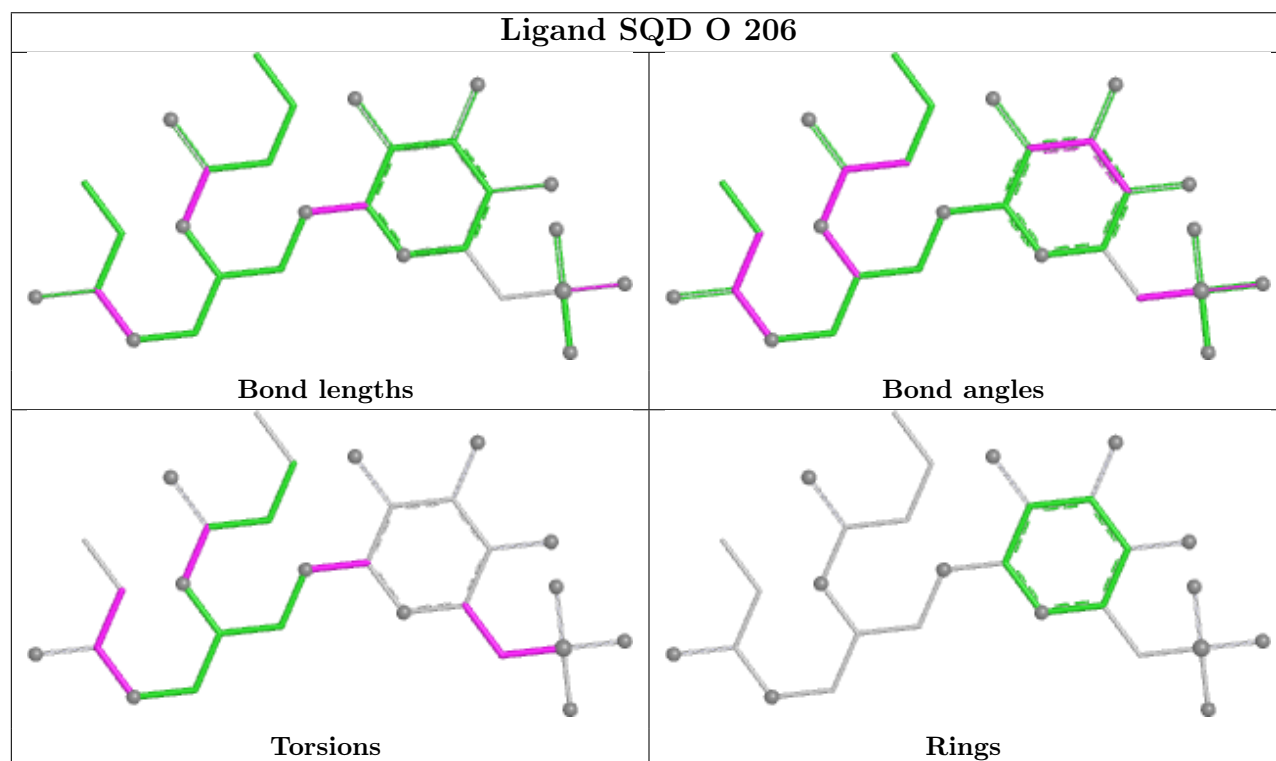
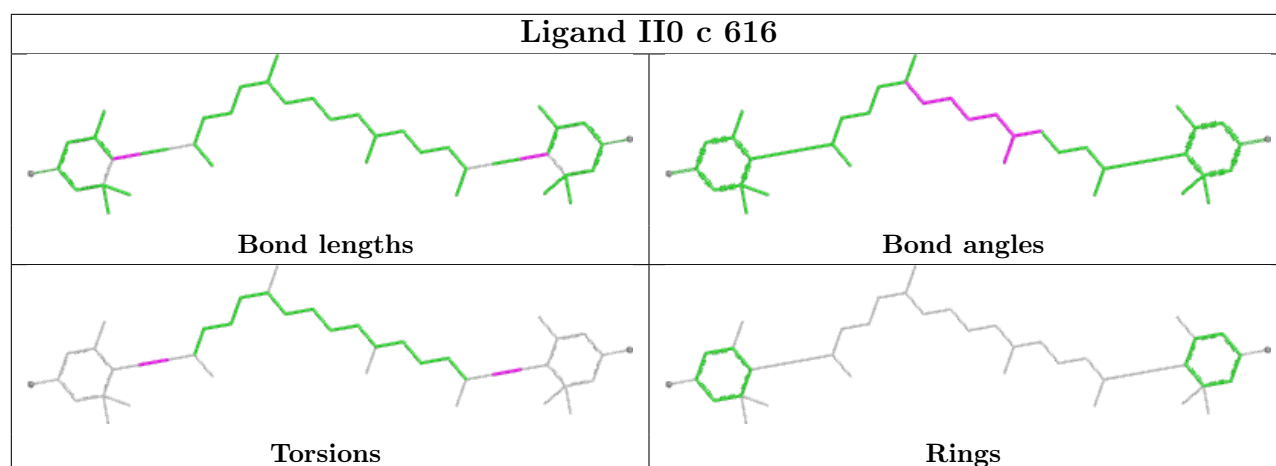


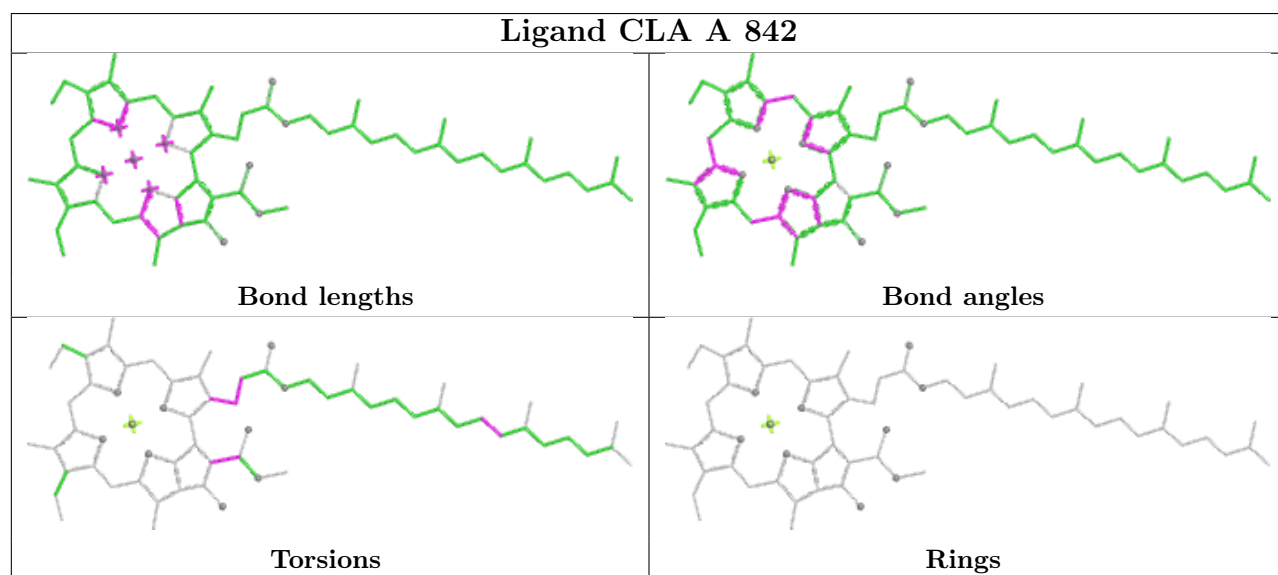
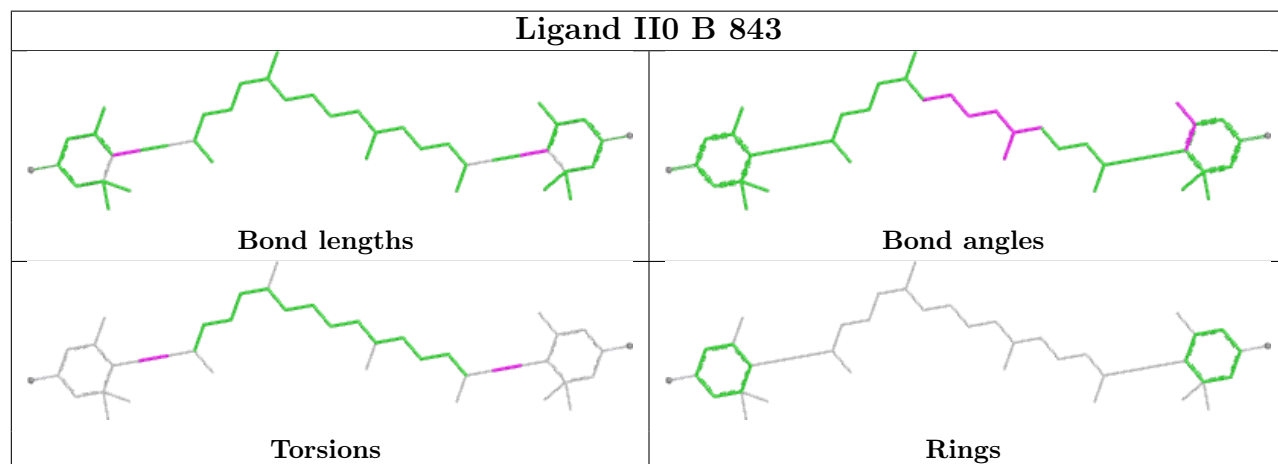
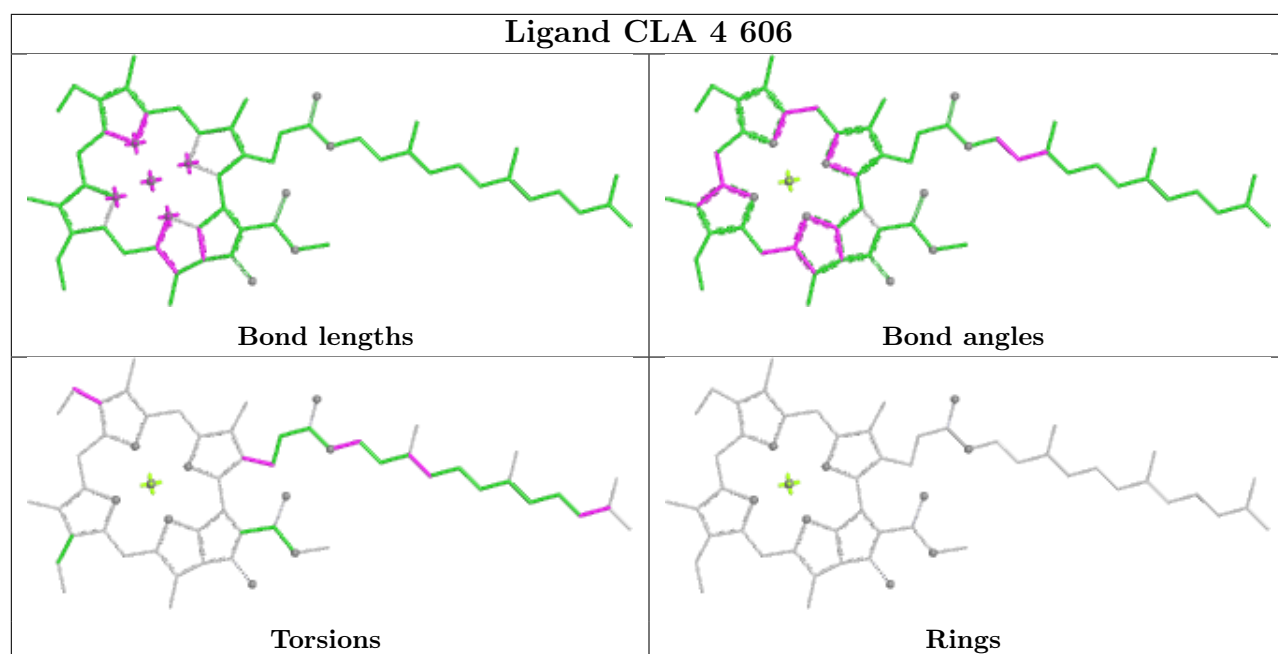
Ligand CLA 3 611

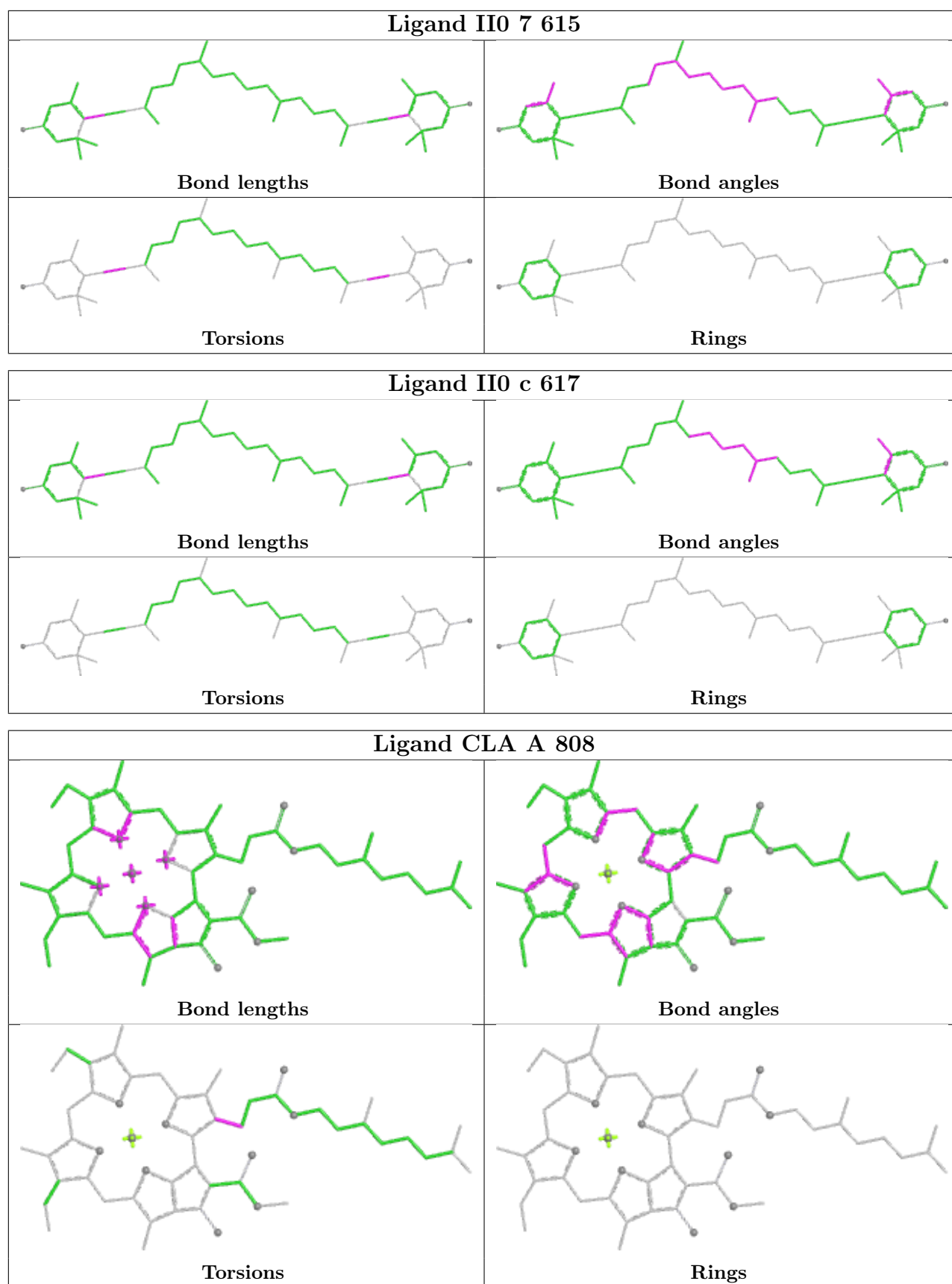


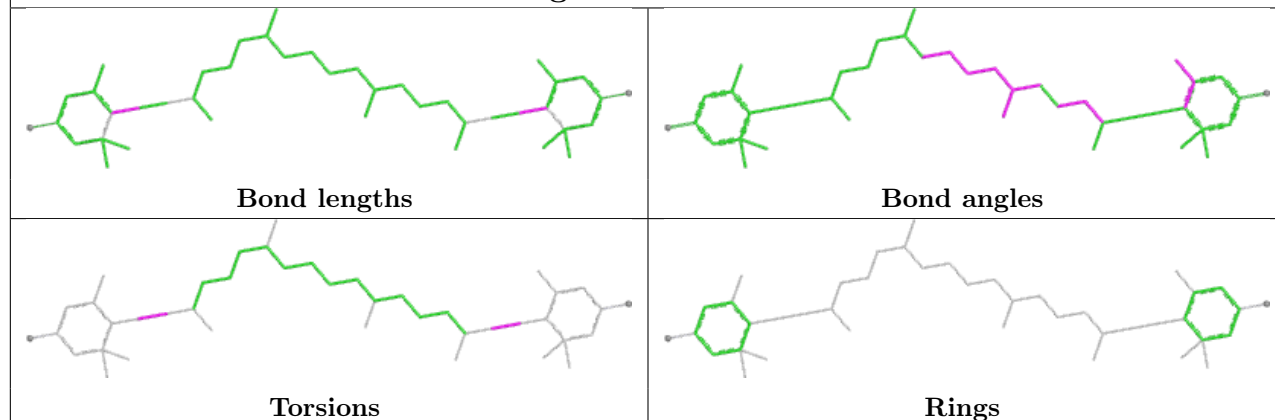
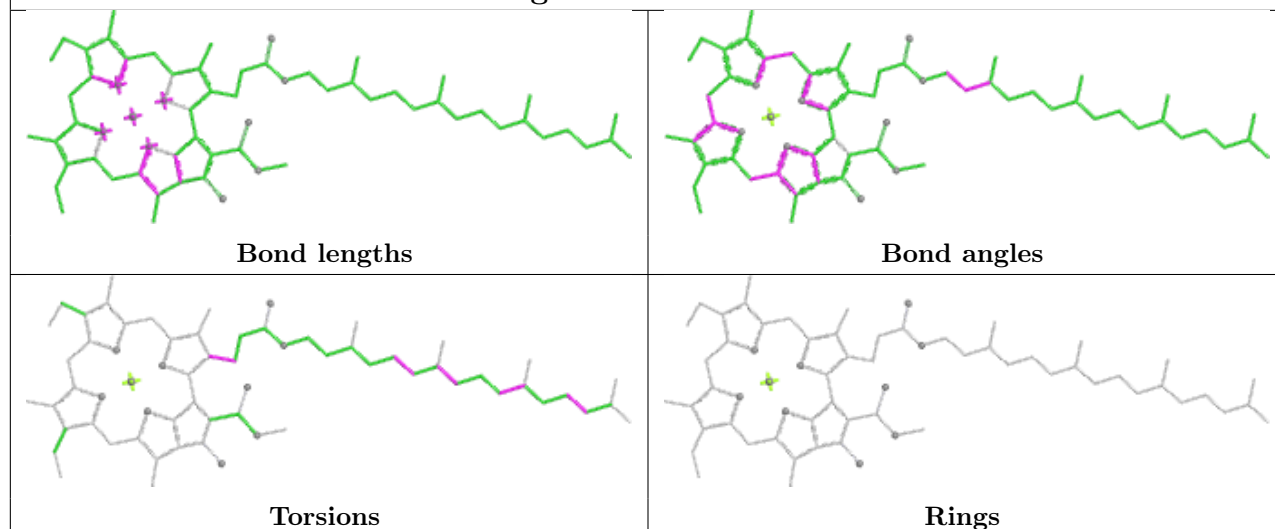
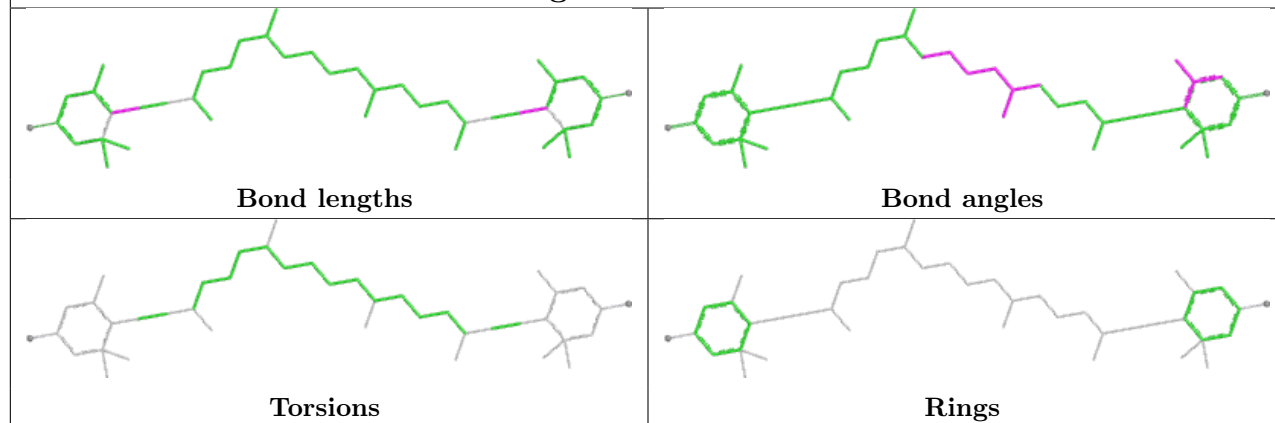


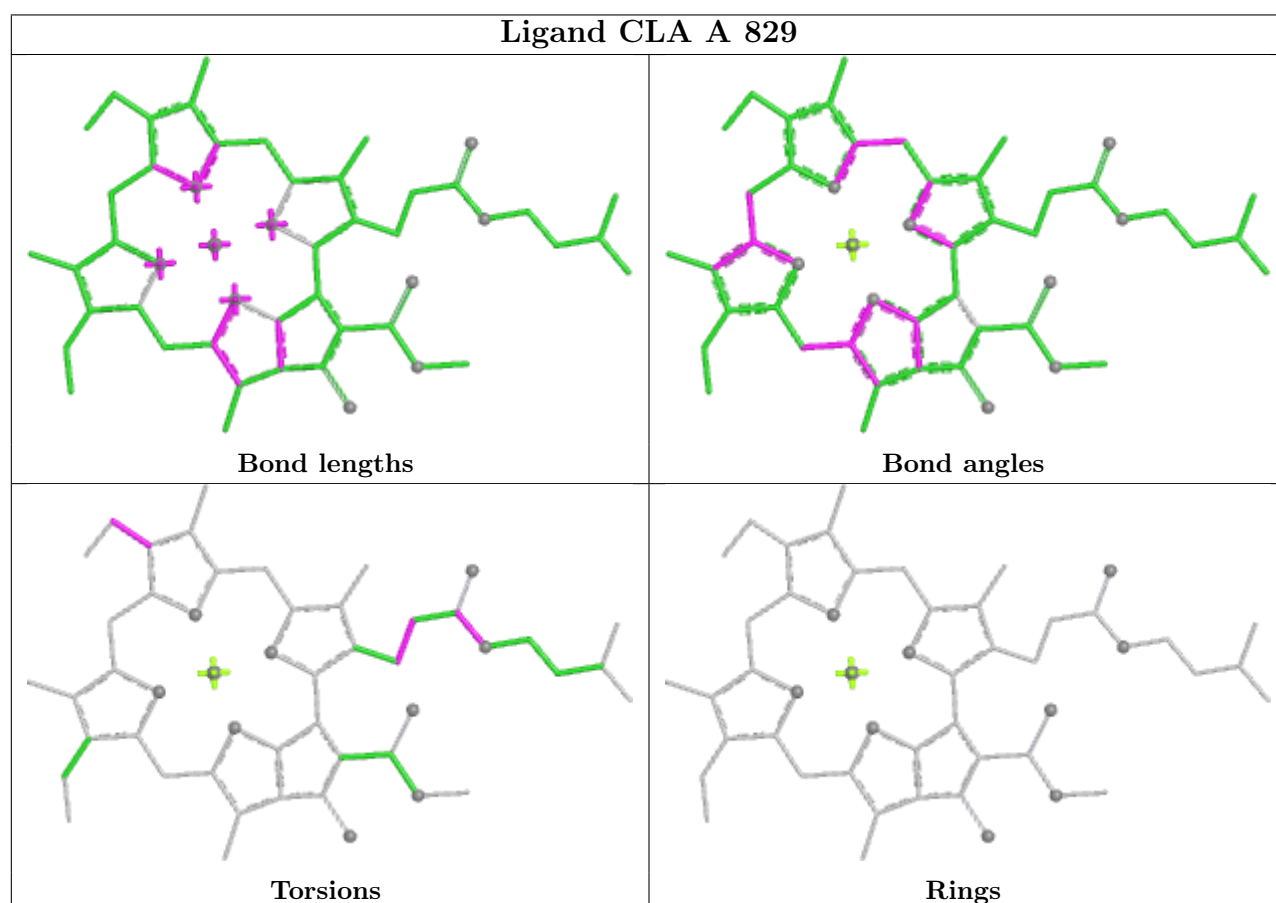
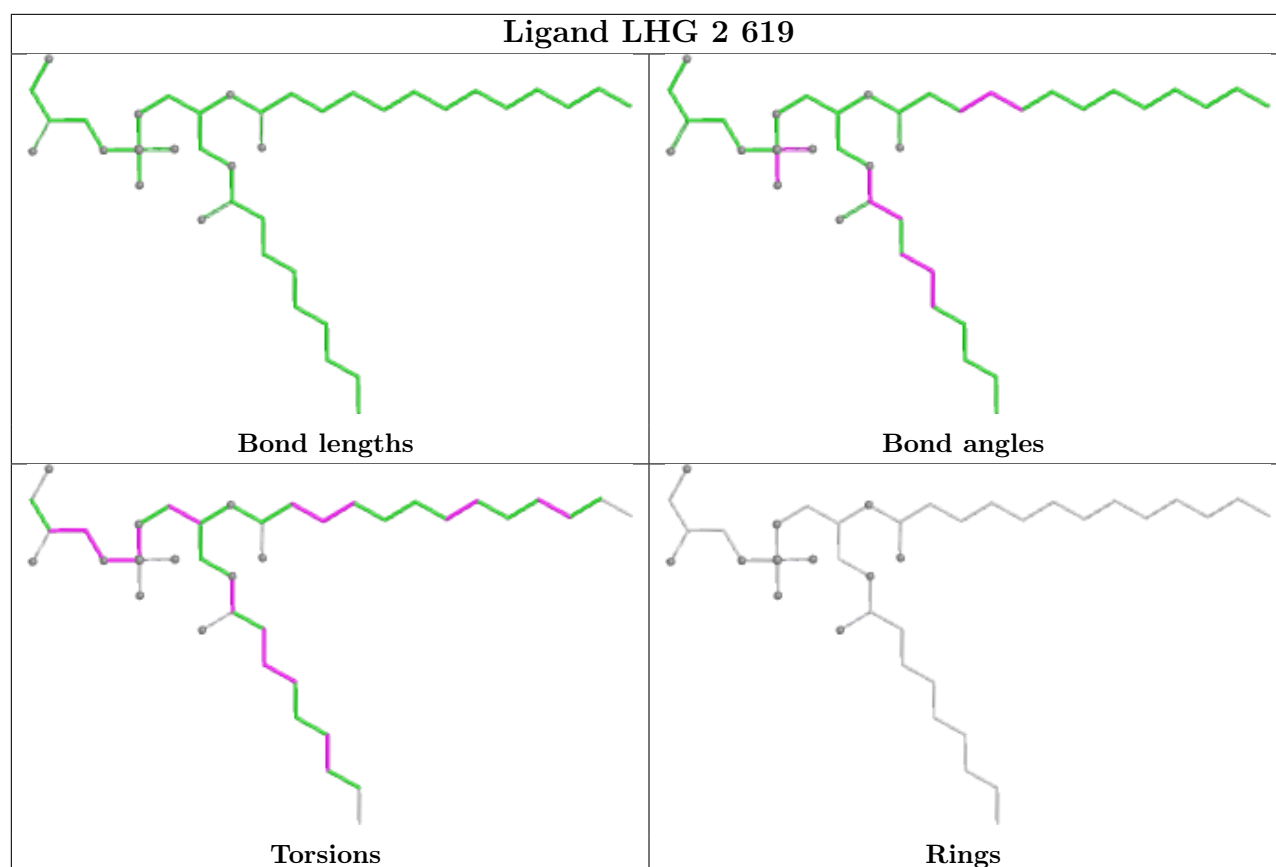








Ligand II0 3 613**Ligand CLA A 828****Ligand II0 2 614**



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.

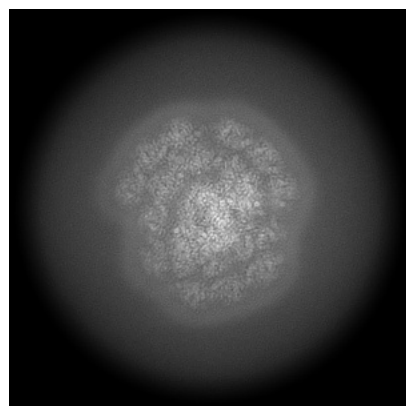
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33659. These allow visual inspection of the internal detail of the map and identification of artifacts.

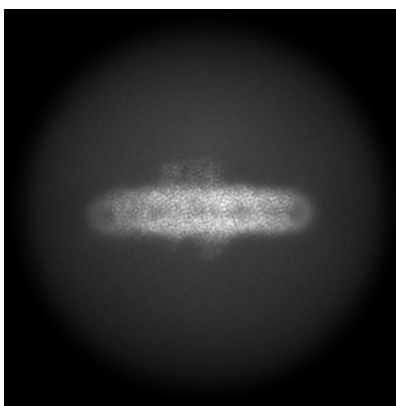
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

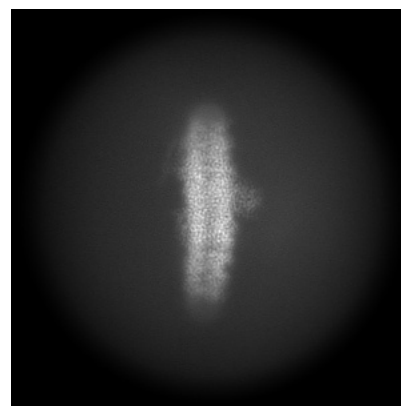
6.1.1 Primary map



X

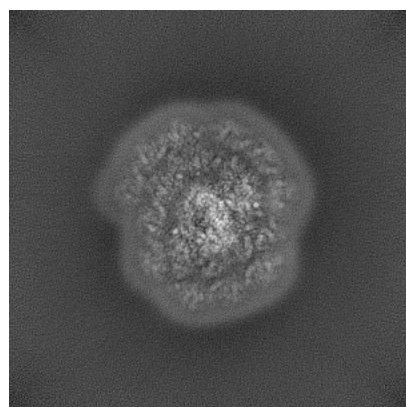


Y

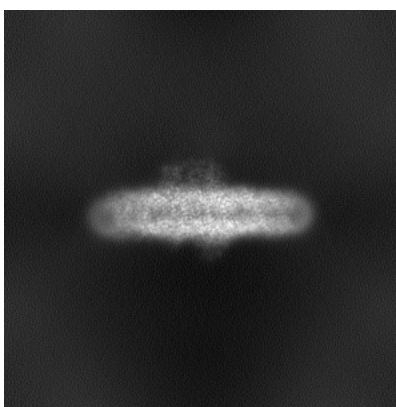


Z

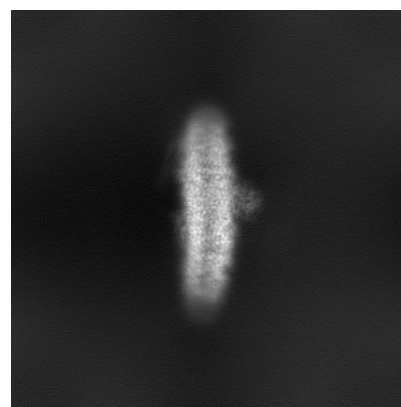
6.1.2 Raw map



X



Y

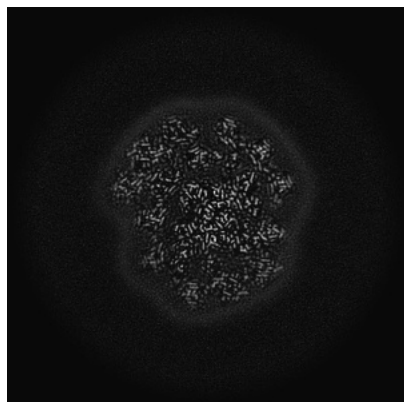


Z

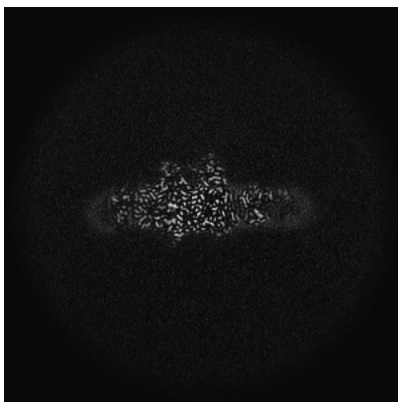
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

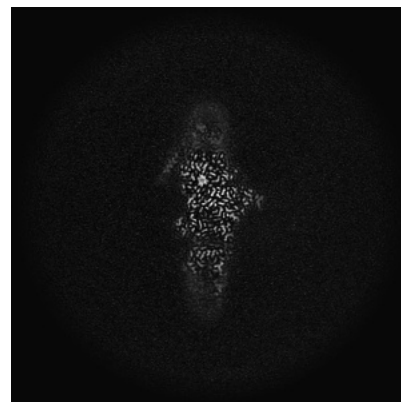
6.2.1 Primary map



X Index: 200

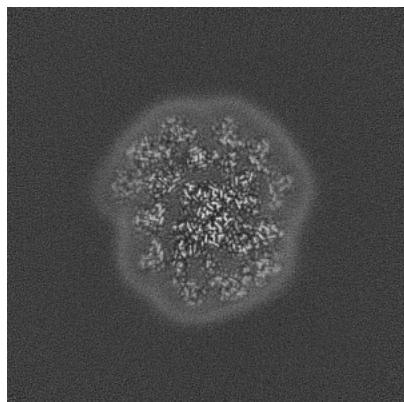


Y Index: 200

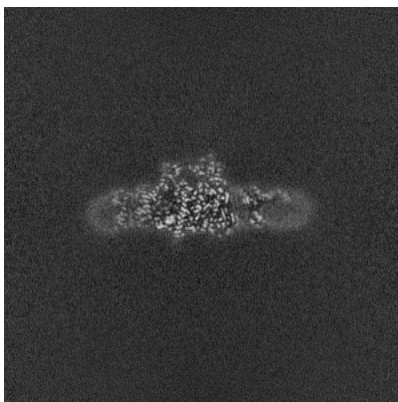


Z Index: 200

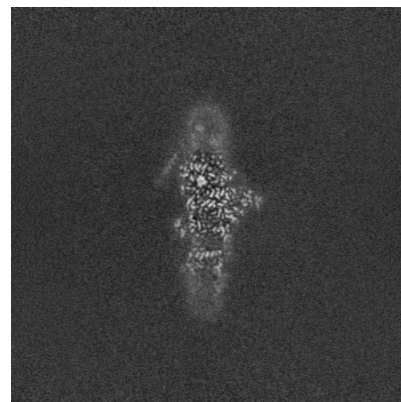
6.2.2 Raw map



X Index: 200



Y Index: 200

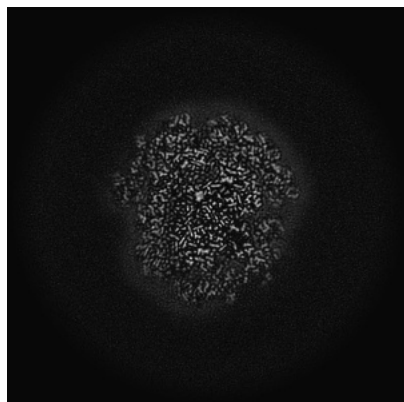


Z Index: 200

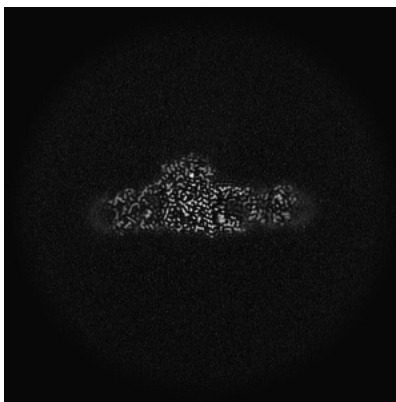
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

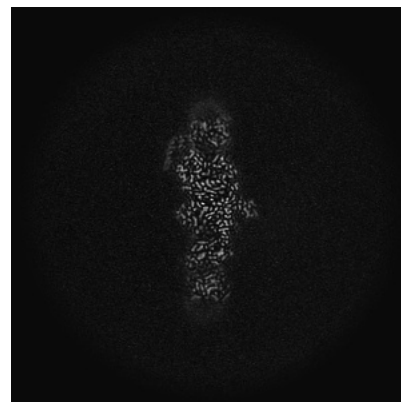
6.3.1 Primary map



X Index: 210

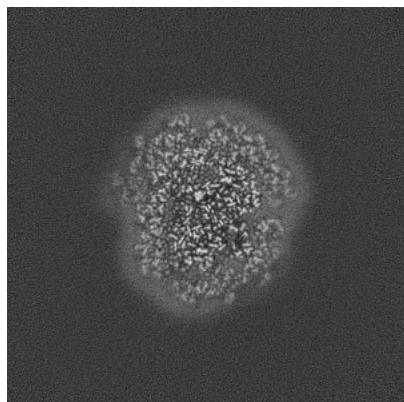


Y Index: 212

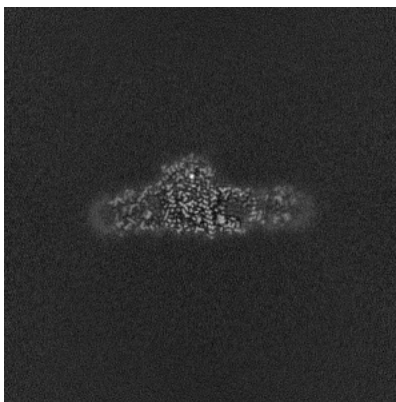


Z Index: 215

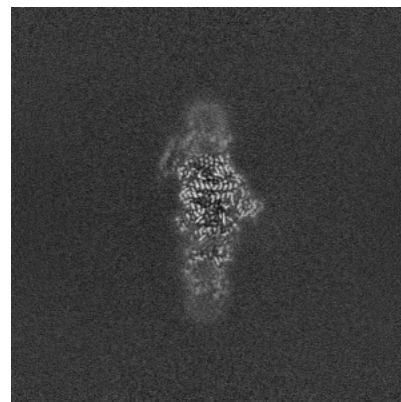
6.3.2 Raw map



X Index: 209



Y Index: 211

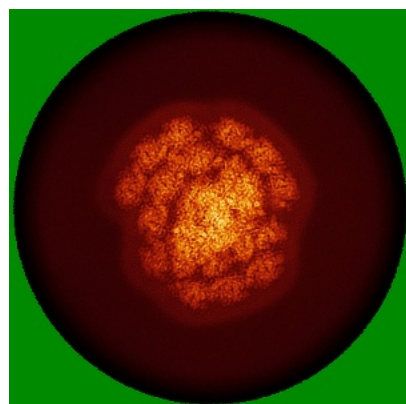


Z Index: 207

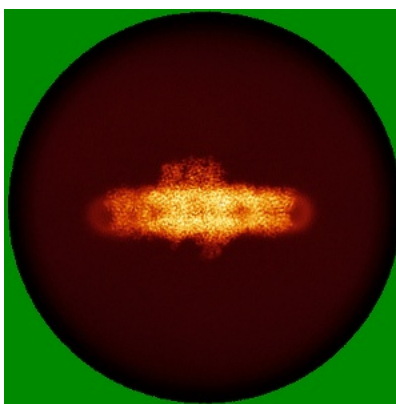
The images above show the largest variance slices of the map in three orthogonal directions.

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

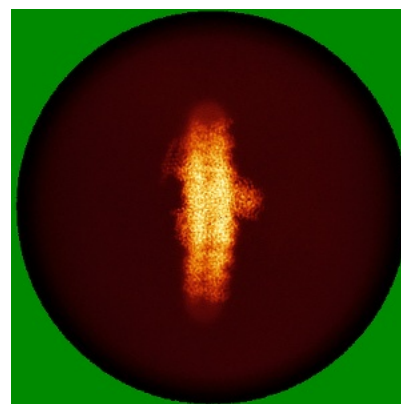
6.4.1 Primary map



X

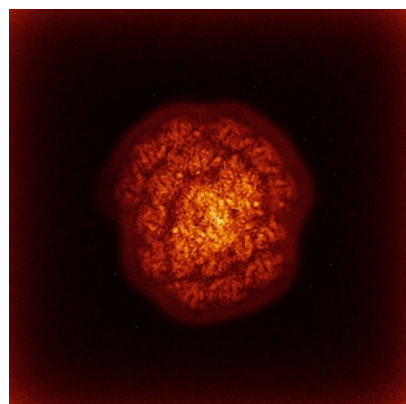


Y

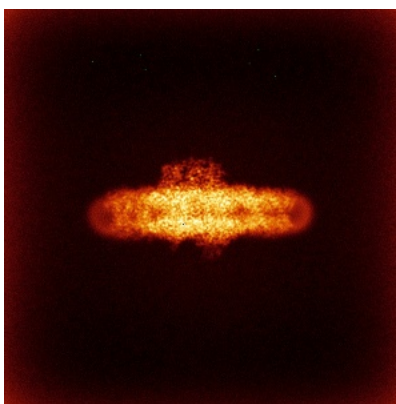


Z

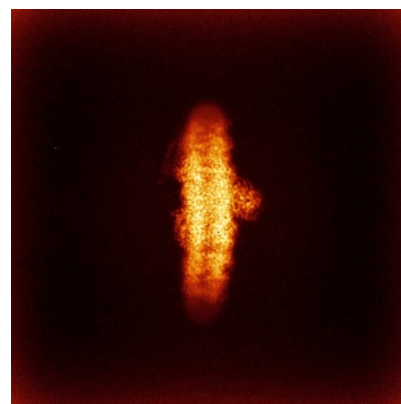
6.4.2 Raw map



X



Y

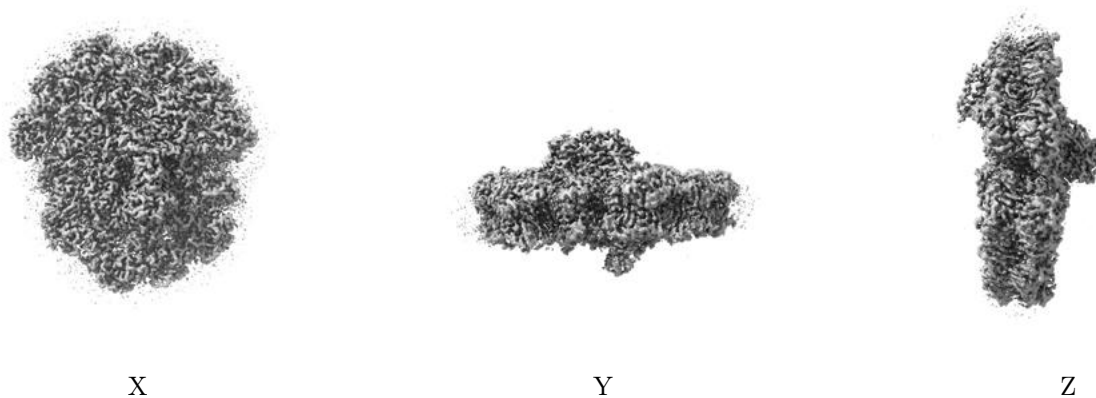


Z

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.

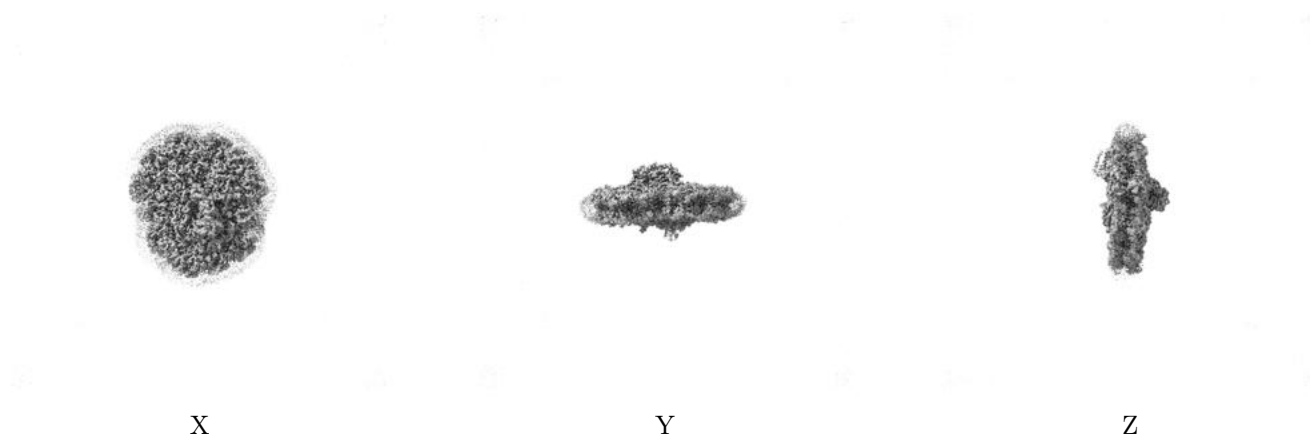
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

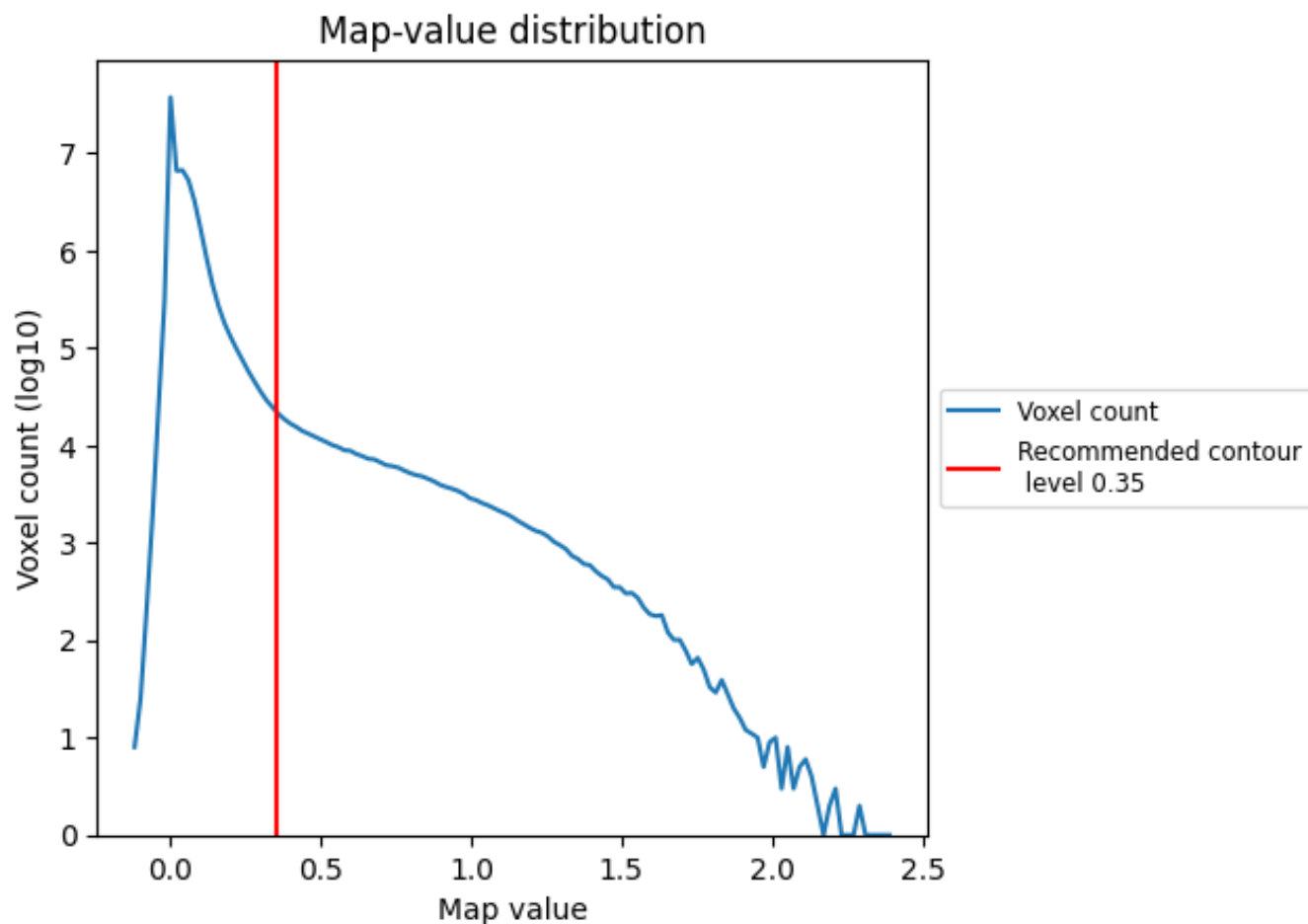
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

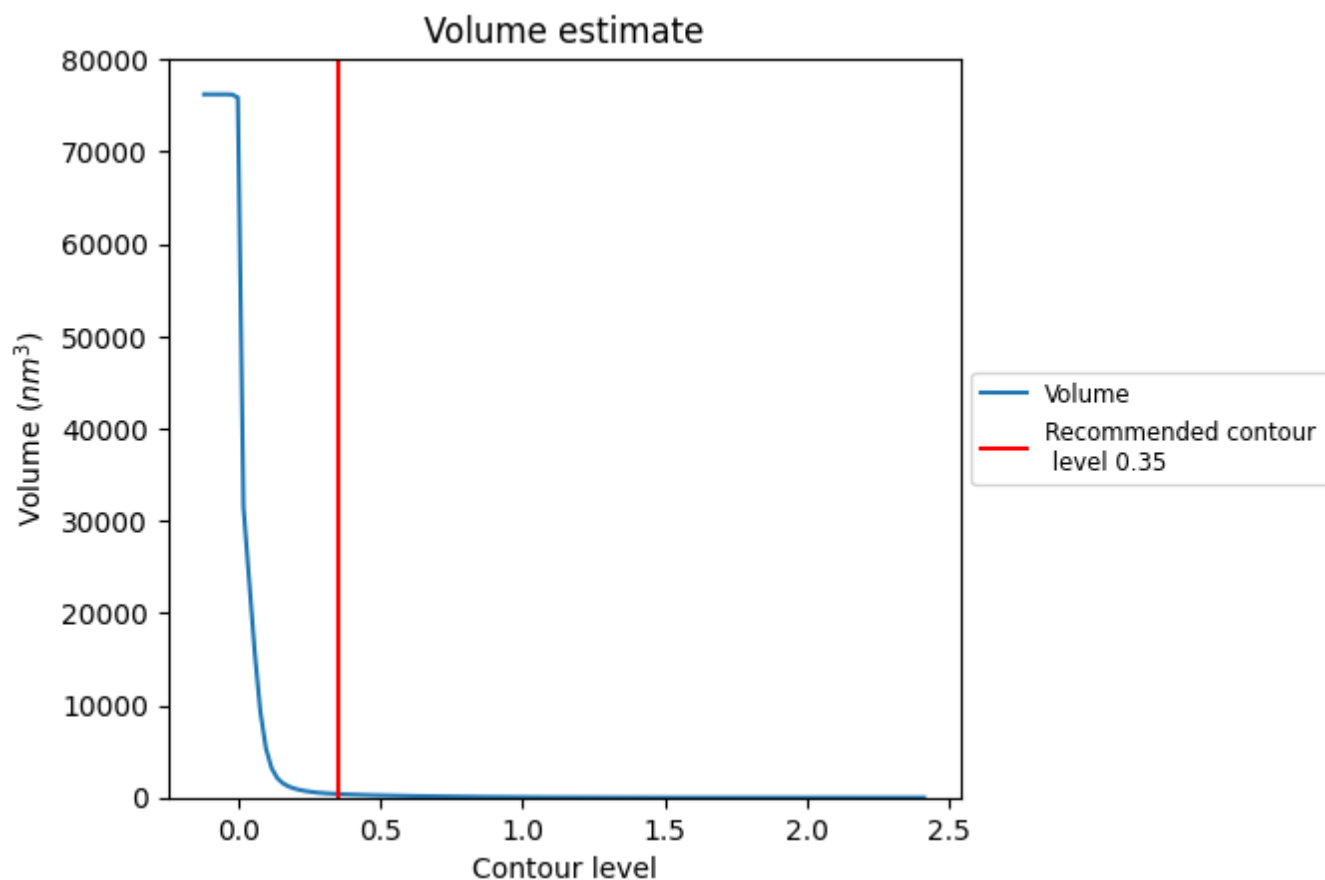
This section contains the results of statistical analysis of the map.

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.

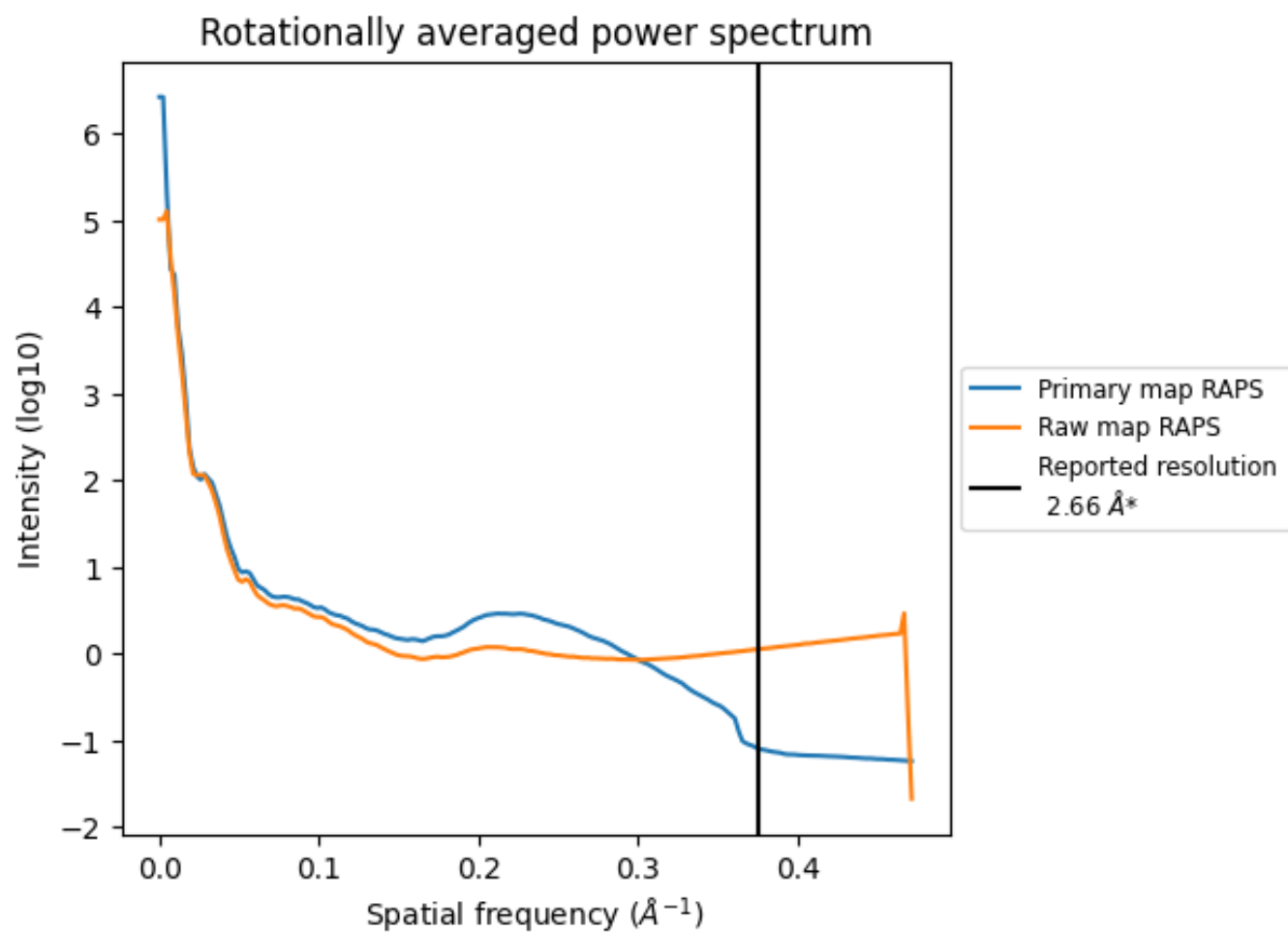
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 384 nm³; this corresponds to an approximate mass of 347 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 ⓘ

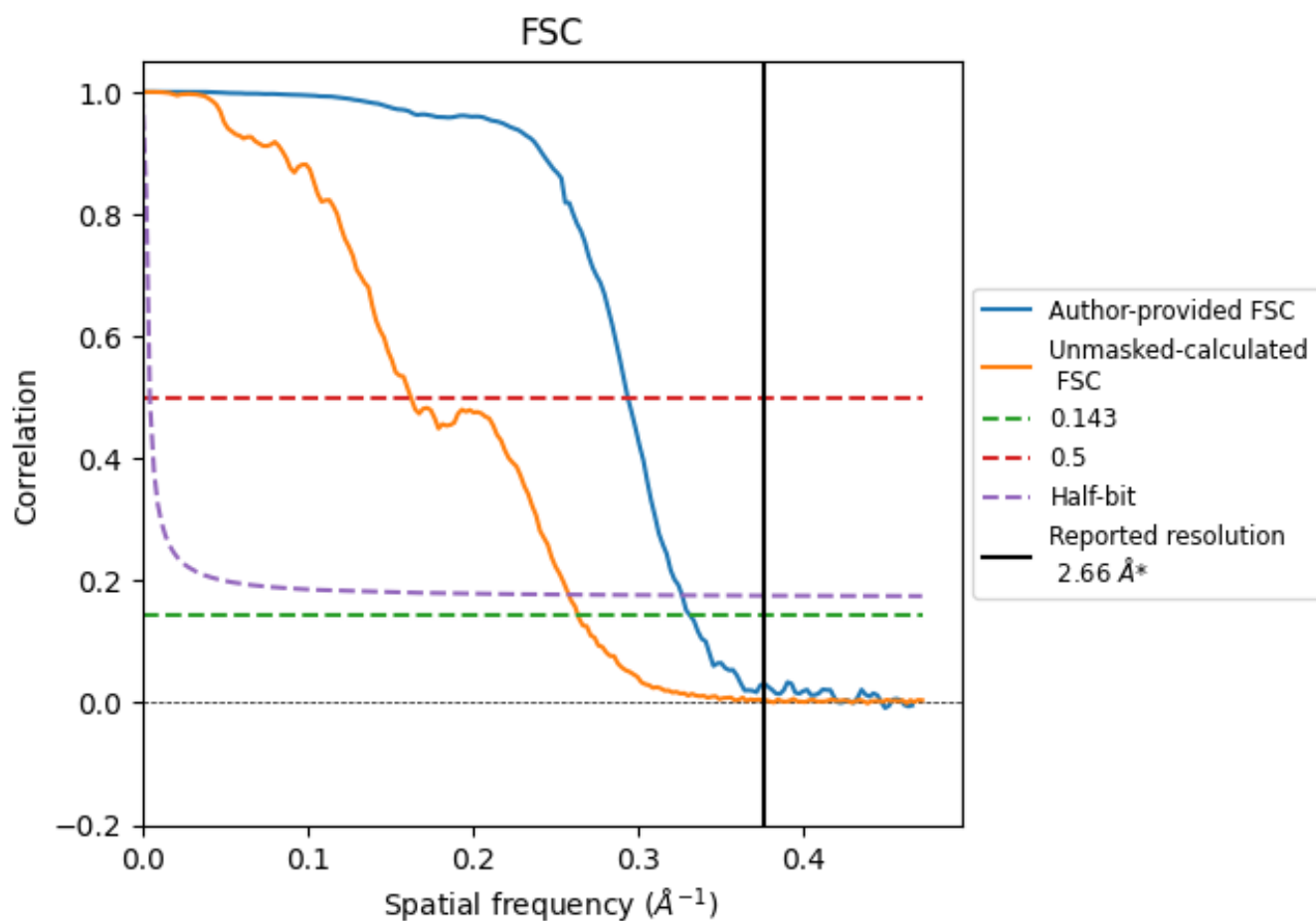


*Reported resolution corresponds to spatial frequency of 0.376 Å⁻¹

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 0.376 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	3.02	3.41	3.06
Unmasked-calculated*	3.80	6.16	3.88

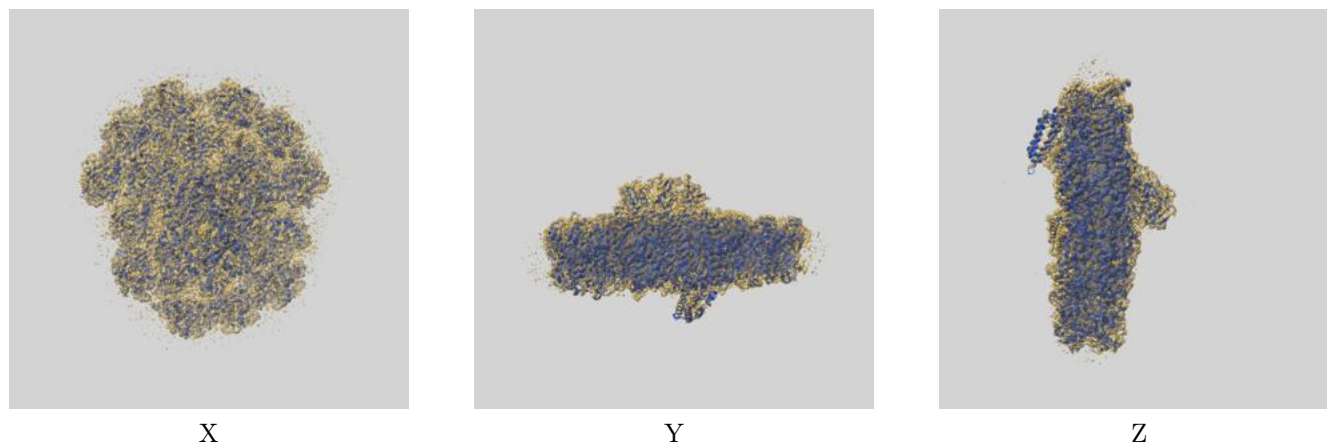
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.02 differs from the reported value 2.66 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 2.66 by more than 10 %

9 Map-model fit [i](#)

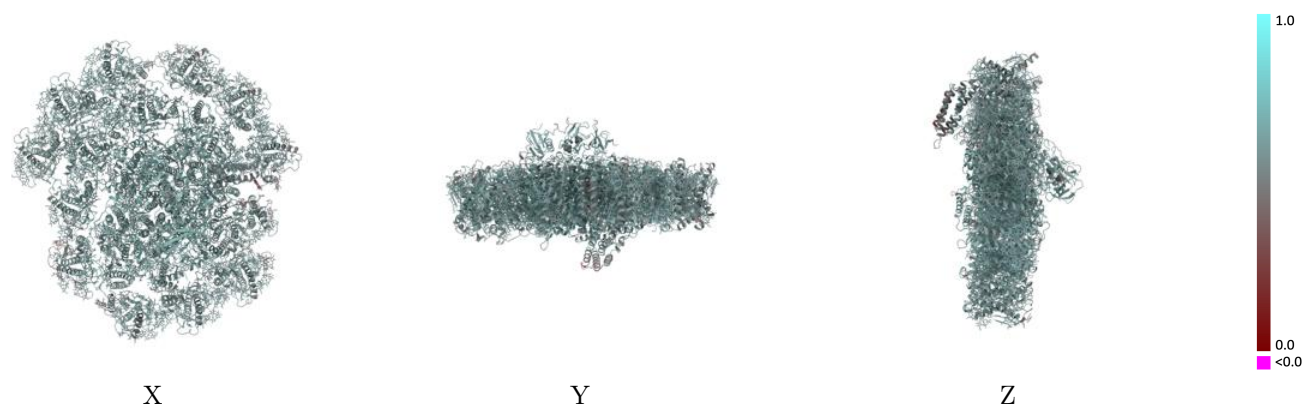
This section contains information regarding the fit between EMDB map EMD-33659 and PDB model 7Y7B. Per-residue inclusion information can be found in [section 3](#) on [page 42](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

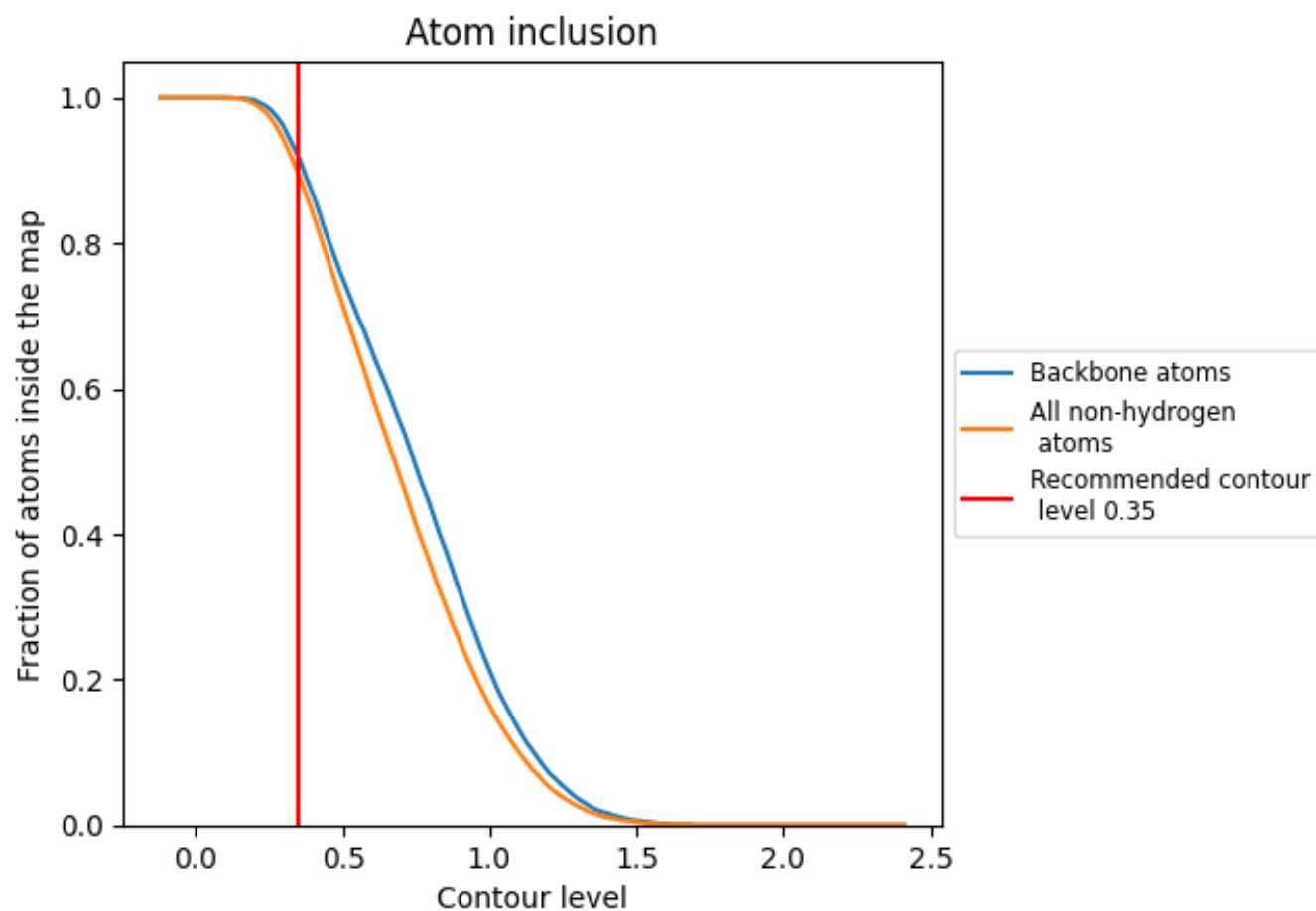


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8950	 0.6070
1	 0.7250	 0.5490
2	 0.9010	 0.6030
3	 0.9390	 0.6270
4	 0.9380	 0.6130
5	 0.8570	 0.5600
6	 0.8970	 0.5810
7	 0.8520	 0.5580
8	 0.8610	 0.5920
9	 0.7980	 0.5750
A	 0.9650	 0.6450
B	 0.9720	 0.6440
C	 0.9490	 0.6110
D	 0.8930	 0.6030
E	 0.8550	 0.6070
F	 0.9160	 0.6230
I	 0.9370	 0.6280
J	 0.9430	 0.6340
K	 0.8640	 0.6050
L	 0.9120	 0.6160
M	 0.9510	 0.6260
O	 0.8750	 0.6090
R	 0.9350	 0.6080
X	 0.6110	 0.5150
Z	 0.8810	 0.6030
a	 0.8970	 0.5970
b	 0.9060	 0.5930
c	 0.8000	 0.5840
d	 0.8270	 0.5950
e	 0.8160	 0.5770

