



wwPDB EM Validation Summary Report ⓘ

Jun 25, 2025 – 01:56 PM JST

PDB ID : 7DZ8 / pdb_00007dz8
EMDB ID : EMD-30926
Title : State transition supercomplex PSI-LHCI-LHCII from the LhcbM1 lacking mutant of *Chlamydomonas reinhardtii*
Authors : Pan, X.W.; Li, A.J.; Liu, Z.F.; Li, M.
Deposited on : 2021-01-23
Resolution : 3.16 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

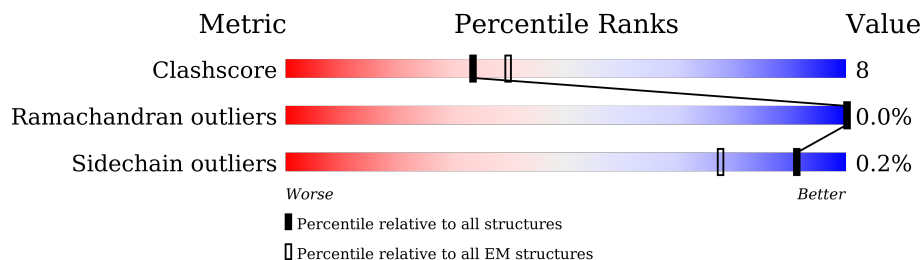
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	751	 84% 15% .
2	B	735	 82% 18%
3	C	81	 78% 19% ...
4	D	196	 62% 10% . 27%
5	E	97	 60% 5% 35%
6	F	227	 65% 7% 27%
7	G	126	 65% 10% 25%
8	H	130	 67% 10% 23%

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Mol	Chain	Length	Quality of chain
9	I	106	
10	J	41	
11	K	113	
12	L	196	
13	O	126	
14	1	228	
14	a	228	
15	2	246	
16	3	298	
17	4	264	
18	5	257	
19	6	257	
20	7	241	
21	8	243	
22	9	213	
23	W	249	
23	X	249	
24	U	257	
24	Y	257	
24	Z	257	
25	V	268	

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
26	CLA	1	602	X	-	-	-
26	CLA	1	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	1	604	X	-	-	-
26	CLA	1	606	X	-	-	-
26	CLA	1	607	X	-	-	-
26	CLA	1	608	X	-	-	-
26	CLA	1	609	X	-	-	-
26	CLA	1	610	X	-	-	-
26	CLA	1	611	X	-	-	-
26	CLA	1	612	X	-	-	-
26	CLA	1	613	X	-	-	-
26	CLA	1	614	X	-	-	-
26	CLA	1	616	X	-	-	-
26	CLA	2	601	X	-	-	-
26	CLA	2	602	X	-	-	-
26	CLA	2	603	X	-	-	-
26	CLA	2	604	X	-	-	-
26	CLA	2	606	X	-	-	-
26	CLA	2	607	X	-	-	-
26	CLA	2	609	X	-	-	-
26	CLA	2	610	X	-	-	-
26	CLA	2	611	X	-	-	-
26	CLA	2	612	X	-	-	-
26	CLA	2	613	X	-	-	-
26	CLA	2	614	X	-	-	-
26	CLA	2	616	X	-	-	-
26	CLA	3	602	X	-	-	-
26	CLA	3	603	X	-	-	-
26	CLA	3	604	X	-	-	-
26	CLA	3	606	X	-	-	-
26	CLA	3	607	X	-	-	-
26	CLA	3	608	X	-	-	-
26	CLA	3	609	X	-	-	-
26	CLA	3	610	X	-	-	-
26	CLA	3	611	X	-	-	-
26	CLA	3	612	X	-	-	-
26	CLA	3	613	X	-	-	-
26	CLA	3	614	X	-	-	-
26	CLA	3	615	X	-	-	-
26	CLA	3	617	X	-	-	-
26	CLA	4	601	X	-	-	-
26	CLA	4	602	X	-	-	-
26	CLA	4	603	X	-	-	-
26	CLA	4	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	4	606	X	-	-	-
26	CLA	4	607	X	-	-	-
26	CLA	4	608	X	-	-	-
26	CLA	4	609	X	-	-	-
26	CLA	4	610	X	-	-	-
26	CLA	4	611	X	-	-	-
26	CLA	4	612	X	-	-	-
26	CLA	4	613	X	-	-	-
26	CLA	4	616	X	-	-	-
26	CLA	4	618	X	-	-	-
26	CLA	5	601	X	-	-	-
26	CLA	5	602	X	-	-	-
26	CLA	5	603	X	-	-	-
26	CLA	5	604	X	-	-	-
26	CLA	5	607	X	-	-	-
26	CLA	5	608	X	-	-	-
26	CLA	5	609	X	-	-	-
26	CLA	5	610	X	-	-	-
26	CLA	5	611	X	-	-	-
26	CLA	5	612	X	-	-	-
26	CLA	5	613	X	-	-	-
26	CLA	5	614	X	-	-	-
26	CLA	5	616	X	-	-	-
26	CLA	5	617	X	-	-	-
26	CLA	5	618	X	-	-	-
26	CLA	5	619	X	-	-	-
26	CLA	6	601	X	-	-	-
26	CLA	6	603	X	-	-	-
26	CLA	6	604	X	-	-	-
26	CLA	6	606	X	-	-	-
26	CLA	6	607	X	-	-	-
26	CLA	6	609	X	-	-	-
26	CLA	6	610	X	-	-	-
26	CLA	6	611	X	-	-	-
26	CLA	6	612	X	-	-	-
26	CLA	6	614	X	-	-	-
26	CLA	6	616	X	-	-	-
26	CLA	6	617	X	-	-	-
26	CLA	6	618	X	-	-	-
26	CLA	6	620	X	-	-	-
26	CLA	7	601	X	-	-	-
26	CLA	7	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	7	603	X	-	-	-
26	CLA	7	604	X	-	-	-
26	CLA	7	606	X	-	-	-
26	CLA	7	607	X	-	-	-
26	CLA	7	609	X	-	-	-
26	CLA	7	610	X	-	-	-
26	CLA	7	611	X	-	-	-
26	CLA	7	612	X	-	-	-
26	CLA	7	613	X	-	-	-
26	CLA	7	614	X	-	-	-
26	CLA	7	615	X	-	-	-
26	CLA	7	616	X	-	-	-
26	CLA	8	601	X	-	-	-
26	CLA	8	603	X	-	-	-
26	CLA	8	604	X	-	-	-
26	CLA	8	606	X	-	-	-
26	CLA	8	607	X	-	-	-
26	CLA	8	609	X	-	-	-
26	CLA	8	610	X	-	-	-
26	CLA	8	611	X	-	-	-
26	CLA	8	612	X	-	-	-
26	CLA	8	613	X	-	-	-
26	CLA	8	614	X	-	-	-
26	CLA	8	616	X	-	-	-
26	CLA	9	601	X	-	-	-
26	CLA	9	602	X	-	-	-
26	CLA	9	603	X	-	-	-
26	CLA	9	604	X	-	-	-
26	CLA	9	606	X	-	-	-
26	CLA	9	609	X	-	-	-
26	CLA	9	610	X	-	-	-
26	CLA	9	611	X	-	-	-
26	CLA	9	612	X	-	-	-
26	CLA	9	613	X	-	-	-
26	CLA	9	614	X	-	-	-
26	CLA	A	801	X	-	-	-
26	CLA	A	802	X	-	-	-
26	CLA	A	803	X	-	-	-
26	CLA	A	804	X	-	-	-
26	CLA	A	806	X	-	-	-
26	CLA	A	807	X	-	-	-
26	CLA	A	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	A	809	X	-	-	-
26	CLA	A	811	X	-	-	-
26	CLA	A	812	X	-	-	-
26	CLA	A	813	X	-	-	-
26	CLA	A	814	X	-	-	-
26	CLA	A	815	X	-	-	-
26	CLA	A	816	X	-	-	-
26	CLA	A	819	X	-	-	-
26	CLA	A	820	X	-	-	-
26	CLA	A	822	X	-	-	-
26	CLA	A	823	X	-	-	-
26	CLA	A	824	X	-	-	-
26	CLA	A	825	X	-	-	-
26	CLA	A	826	X	-	-	-
26	CLA	A	827	X	-	-	-
26	CLA	A	828	X	-	-	-
26	CLA	A	829	X	-	-	-
26	CLA	A	830	X	-	-	-
26	CLA	A	831	X	-	-	-
26	CLA	A	832	X	-	-	-
26	CLA	A	833	X	-	-	-
26	CLA	A	834	X	-	-	-
26	CLA	A	836	X	-	-	-
26	CLA	A	837	X	-	-	-
26	CLA	A	838	X	-	-	-
26	CLA	A	839	X	-	-	-
26	CLA	A	841	X	-	-	-
26	CLA	A	842	X	-	-	-
26	CLA	A	843	X	-	-	-
26	CLA	A	845	X	-	-	-
26	CLA	A	854	X	-	-	-
26	CLA	B	802	X	-	-	-
26	CLA	B	803	X	-	-	-
26	CLA	B	804	X	-	-	-
26	CLA	B	805	X	-	-	-
26	CLA	B	806	X	-	-	-
26	CLA	B	808	X	-	-	-
26	CLA	B	809	X	-	-	-
26	CLA	B	810	X	-	-	-
26	CLA	B	811	X	-	-	-
26	CLA	B	812	X	-	-	-
26	CLA	B	813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	B	814	X	-	-	-
26	CLA	B	815	X	-	-	-
26	CLA	B	816	X	-	-	-
26	CLA	B	817	X	-	-	-
26	CLA	B	819	X	-	-	-
26	CLA	B	820	X	-	-	-
26	CLA	B	821	X	-	-	-
26	CLA	B	823	X	-	-	-
26	CLA	B	824	X	-	-	-
26	CLA	B	826	X	-	-	-
26	CLA	B	827	X	-	-	-
26	CLA	B	828	X	-	-	-
26	CLA	B	829	X	-	-	-
26	CLA	B	830	X	-	-	-
26	CLA	B	831	X	-	-	-
26	CLA	B	832	X	-	-	-
26	CLA	B	833	X	-	-	-
26	CLA	B	834	X	-	-	-
26	CLA	B	835	X	-	-	-
26	CLA	B	836	X	-	-	-
26	CLA	B	838	X	-	-	-
26	CLA	B	839	X	-	-	-
26	CLA	B	840	X	-	-	-
26	CLA	B	841	X	-	-	-
26	CLA	F	301	X	-	-	-
26	CLA	G	203	X	-	-	-
26	CLA	G	204	X	-	-	-
26	CLA	H	202	X	-	-	-
26	CLA	H	203	X	-	-	-
26	CLA	J	101	X	-	-	-
26	CLA	K	201	X	-	-	-
26	CLA	K	204	X	-	-	-
26	CLA	K	206	X	-	-	-
26	CLA	L	302	X	-	-	-
26	CLA	L	304	X	-	-	-
26	CLA	L	306	X	-	-	-
26	CLA	L	307	X	-	-	-
26	CLA	O	2001	X	-	-	-
26	CLA	O	2002	X	-	-	-
26	CLA	O	2003	X	-	-	-
26	CLA	U	602	X	-	-	-
26	CLA	U	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	U	604	X	-	-	-
26	CLA	U	610	X	-	-	-
26	CLA	U	611	X	-	-	-
26	CLA	U	612	X	-	-	-
26	CLA	U	613	X	-	-	-
26	CLA	U	614	X	-	-	-
26	CLA	V	602	X	-	-	-
26	CLA	V	603	X	-	-	-
26	CLA	V	604	X	-	-	-
26	CLA	V	610	X	-	-	-
26	CLA	V	611	X	-	-	-
26	CLA	V	612	X	-	-	-
26	CLA	V	613	X	-	-	-
26	CLA	V	614	X	-	-	-
26	CLA	W	602	X	-	-	-
26	CLA	W	603	X	-	-	-
26	CLA	W	604	X	-	-	-
26	CLA	W	610	X	-	-	-
26	CLA	W	611	X	-	-	-
26	CLA	W	612	X	-	-	-
26	CLA	W	613	X	-	-	-
26	CLA	W	614	X	-	-	-
26	CLA	X	602	X	-	-	-
26	CLA	X	603	X	-	-	-
26	CLA	X	604	X	-	-	-
26	CLA	X	610	X	-	-	-
26	CLA	X	611	X	-	-	-
26	CLA	X	612	X	-	-	-
26	CLA	X	613	X	-	-	-
26	CLA	X	614	X	-	-	-
26	CLA	Y	602	X	-	-	-
26	CLA	Y	603	X	-	-	-
26	CLA	Y	604	X	-	-	-
26	CLA	Y	610	X	-	-	-
26	CLA	Y	611	X	-	-	-
26	CLA	Y	612	X	-	-	-
26	CLA	Y	614	X	-	-	-
26	CLA	Z	602	X	-	-	-
26	CLA	Z	603	X	-	-	-
26	CLA	Z	604	X	-	-	-
26	CLA	Z	610	X	-	-	-
26	CLA	Z	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	Z	612	X	-	-	-
26	CLA	Z	613	X	-	-	-
26	CLA	Z	614	X	-	-	-
26	CLA	a	602	X	-	-	-
26	CLA	a	603	X	-	-	-
26	CLA	a	604	X	-	-	-
26	CLA	a	606	X	-	-	-
26	CLA	a	607	X	-	-	-
26	CLA	a	608	X	-	-	-
26	CLA	a	609	X	-	-	-
26	CLA	a	610	X	-	-	-
26	CLA	a	611	X	-	-	-
26	CLA	a	612	X	-	-	-
26	CLA	a	613	X	-	-	-
26	CLA	a	614	X	-	-	-
26	CLA	a	616	X	-	-	-
37	CHL	U	601	X	-	-	-
37	CHL	U	605	X	-	-	-
37	CHL	U	606	X	-	-	-
37	CHL	U	607	X	-	-	-
37	CHL	U	608	X	-	-	-
37	CHL	U	609	X	-	-	-
37	CHL	V	601	X	-	-	-
37	CHL	V	605	X	-	-	-
37	CHL	V	606	X	-	-	-
37	CHL	V	607	X	-	-	-
37	CHL	V	608	X	-	-	-
37	CHL	V	609	X	-	-	-
37	CHL	W	601	X	-	-	-
37	CHL	W	605	X	-	-	-
37	CHL	W	606	X	-	-	-
37	CHL	W	607	X	-	-	-
37	CHL	W	608	X	-	-	-
37	CHL	W	609	X	-	-	-
37	CHL	X	601	X	-	-	-
37	CHL	X	605	X	-	-	-
37	CHL	X	606	X	-	-	-
37	CHL	X	607	X	-	-	-
37	CHL	X	608	X	-	-	-
37	CHL	X	609	X	-	-	-
37	CHL	Y	601	X	-	-	-
37	CHL	Y	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CHL	Y	606	X	-	-	-
37	CHL	Y	607	X	-	-	-
37	CHL	Y	608	X	-	-	-
37	CHL	Y	609	X	-	-	-
37	CHL	Z	601	X	-	-	-
37	CHL	Z	605	X	-	-	-
37	CHL	Z	606	X	-	-	-
37	CHL	Z	607	X	-	-	-
37	CHL	Z	608	X	-	-	-
37	CHL	Z	609	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 69460 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5819	3805	993	999	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5824	3825	977	1004	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	116	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1124	719	199	199	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	63	Total	C	N	O	0	0
			496	316	87	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1265	817	213	232	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	94	Total	C	N	O	0	0
			699	449	118	132		

- Molecule 8 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	100	Total	C	N	O	S	0	0
			776	482	138	154	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	42	Total	C	N	O	S	0	0
			316	217	45	53	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			337	231	47	58	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	86	Total	C	N	O	S	0	0
			582	370	100	110	2		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	159	Total	C	N	O	S	0	0
			1161	757	189	212	3		

- Molecule 13 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	O	97	Total	C	N	O	0	0
			758	503	123	132		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
14	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2	217	Total	C	N	O	S	0	0
			1682	1094	274	304	10		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	220	Total	C	N	O	S	0	0
			1678	1097	270	303	8		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	4	210	Total	C	N	O	S	0	0
			1631	1071	263	292	5		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	227	Total	C	N	O	S	0	0
			1774	1154	297	315	8		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	230	Total	C	N	O	S	0	0
			1771	1167	293	305	6		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	7	213	Total	C	N	O	S	0	0
			1649	1072	274	297	6		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	8	216	Total	C	N	O	S	0	0
			1641	1067	279	291	4		

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	9	183	Total	C	N	O	S	0	0
			1403	909	235	252	7		

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	221	Total	C	N	O	S	0	0
			1680	1091	274	310	5		
23	W	220	Total	C	N	O	S	0	0
			1671	1085	273	308	5		

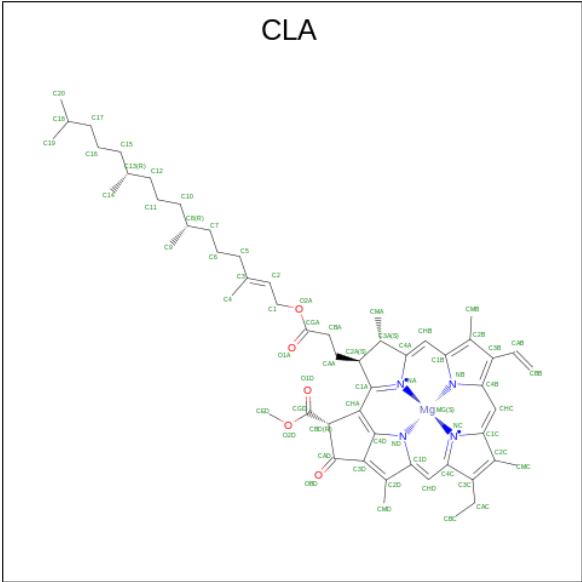
- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	219	Total	C	N	O	S	0	0
			1675	1084	272	314	5		
24	Z	221	Total	C	N	O	S	0	0
			1684	1089	274	316	5		
24	U	219	Total	C	N	O	S	0	0
			1669	1080	272	312	5		

- Molecule 25 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	238	Total	C	N	O	P S	0	0
			1815	1176	300	333	1 5		

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
26	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
26	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 64	C 55	Mg 1	N 4	O 4	0
26	B	1	Total 52	C 43	Mg 1	N 4	O 4	0
26	B	1	Total 43	C 35	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
26	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	B	1	Total 54	C 45	Mg 1	N 4	O 4	0
26	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
26	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	B	1	Total 43	C 33	Mg 1	N 4	O 5	0
26	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	F	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	F	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
26	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	H	1	Total 39	C 31	Mg 1	N 4	O 3	0
26	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	K	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	L	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	L	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	L	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
26	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
26	O	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	1	1	Total 54	C 44	Mg 1	N 4	O 5	0
26	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	1	1	Total 53	C 44	Mg 1	N 4	O 4	0
26	1	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	1	1	Total 39	C 32	Mg 1	N 4	O 2	0
26	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
26	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	1	1	Total 39	C 31	Mg 1	N 4	O 3	0
26	1	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	1	1	Total 37	C 29	Mg 1	N 4	O 3	0
26	1	1	Total 43	C 33	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
26	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
26	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
26	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			63	54	1	3	5	
26	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	2	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
26	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
26	3	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
26	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
26	4	1	Total 54	C 44	Mg 1	N 4	O 5	0
26	4	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	4	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	4	1	Total 61	C 51	Mg 1	N 4	O 5	0
26	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
26	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	4	1	Total 43	C 33	Mg 1	N 4	O 5	0
26	4	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	5	1	Total 54	C 44	Mg 1	N 4	O 5	0
26	5	1	Total 63	C 53	Mg 1	N 4	O 5	0
26	5	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	5	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	5	1	Total 54	C 44	Mg 1	N 4	O 5	0
26	5	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
26	5	1	Total 64	C 55	Mg 1	N 4	O 4	0
26	5	1	Total 44	C 34	Mg 1	N 4	O 5	0
26	5	1	Total 42	C 33	Mg 1	N 4	O 4	0
26	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	5	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	5	1	Total 43	C 33	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	6	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
26	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	6	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
26	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
26	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
26	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
26	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
26	7	1	Total	C	Mg	N	O	0
			43	33	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
26	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	8	1	Total 64	C 54	Mg 1	N 4	O 5	0
26	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
26	8	1	Total 51	C 41	Mg 1	N 4	O 5	0
26	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
26	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	8	1	Total 53	C 43	Mg 1	N 4	O 5	0
26	8	1	Total 43	C 33	Mg 1	N 4	O 5	0
26	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	9	1	Total 44	C 34	Mg 1	N 4	O 5	0
26	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	9	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	9	1	Total 61	C 51	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
26	9	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	9	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
26	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	X	1	Total 62	C 52	Mg 1	N 4	O 5	0
26	X	1	Total 49	C 39	Mg 1	N 4	O 5	0
26	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	X	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	X	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	Y	1	Total 58	C 48	Mg 1	N 4	O 5	0
26	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
26	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	Y	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	Y	1	Total 48	C 38	Mg 1	N 4	O 5	0

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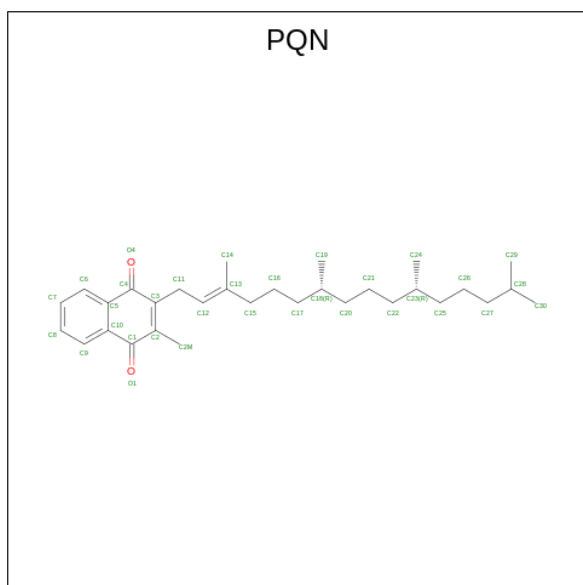
Mol	Chain	Residues	Atoms					AltConf
26	Z	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			49	40	1	4	4	
26	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			48	39	1	4	4	
26	U	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	U	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
26	U	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	V	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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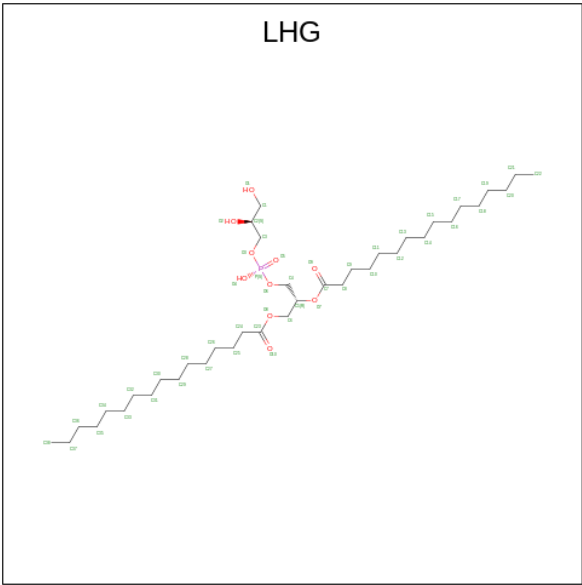
Mol	Chain	Residues	Atoms					AltConf
26	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



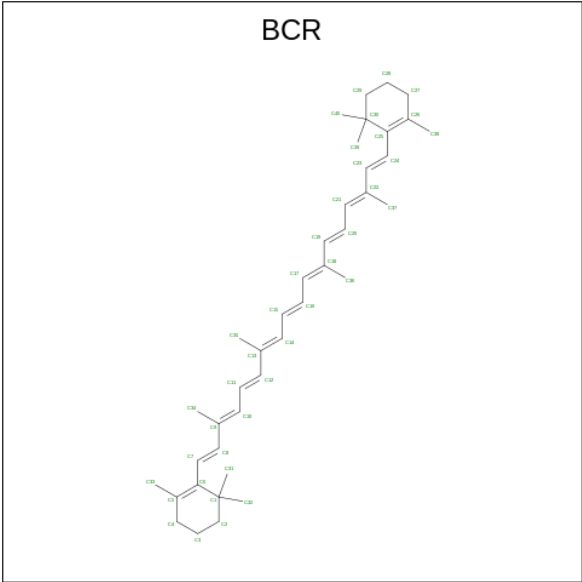
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			49	38	10	1	
28	A	1	Total	C	O	P	0
			30	19	10	1	
28	A	1	Total	C	O	P	0
			49	38	10	1	
28	B	1	Total	C	O	P	0
			38	27	10	1	
28	H	1	Total	C	O	P	0
			49	38	10	1	
28	O	1	Total	C	O	P	0
			36	25	10	1	
28	1	1	Total	C	O	P	0
			49	38	10	1	
28	a	1	Total	C	O	P	0
			43	32	10	1	
28	2	1	Total	C	O	P	0
			36	25	10	1	

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Mol	Chain	Residues	Atoms				AltConf
28	3	1	Total	C	O	P	0
			45	34	10	1	
28	3	1	Total	C	O	P	0
			49	38	10	1	
28	4	1	Total	C	O	P	0
			49	38	10	1	
28	5	1	Total	C	O	P	0
			49	38	10	1	
28	5	1	Total	C	O	P	0
			49	38	10	1	
28	6	1	Total	C	O	P	0
			48	37	10	1	
28	7	1	Total	C	O	P	0
			37	26	10	1	
28	8	1	Total	C	O	P	0
			49	38	10	1	
28	8	1	Total	C	O	P	0
			40	29	10	1	
28	9	1	Total	C	O	P	0
			30	19	10	1	
28	9	1	Total	C	O	P	0
			49	38	10	1	
28	9	1	Total	C	O	P	0
			49	38	10	1	
28	X	1	Total	C	O	P	0
			49	38	10	1	
28	Y	1	Total	C	O	P	0
			49	38	10	1	
28	Z	1	Total	C	O	P	0
			49	38	10	1	
28	U	1	Total	C	O	P	0
			49	38	10	1	
28	V	1	Total	C	O	P	0
			36	25	10	1	
28	W	1	Total	C	O	P	0
			34	23	10	1	

- Molecule 29 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0

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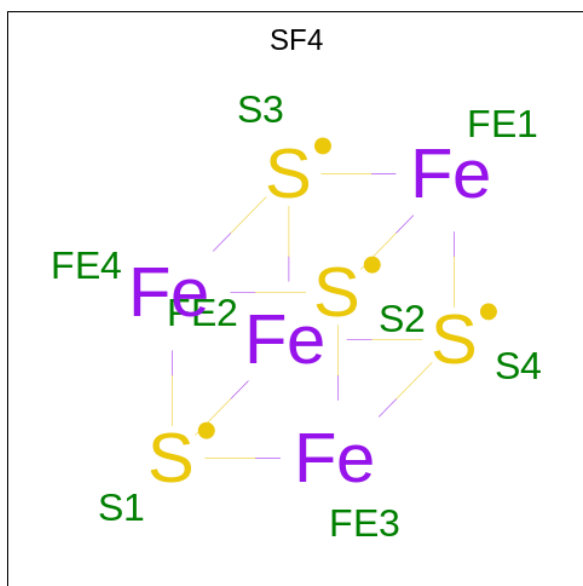
Mol	Chain	Residues	Atoms	AltConf
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	F	1	Total C 40 40	0
29	G	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	1	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	2	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	4	1	Total C 40 40	0
29	5	1	Total C 40 40	0

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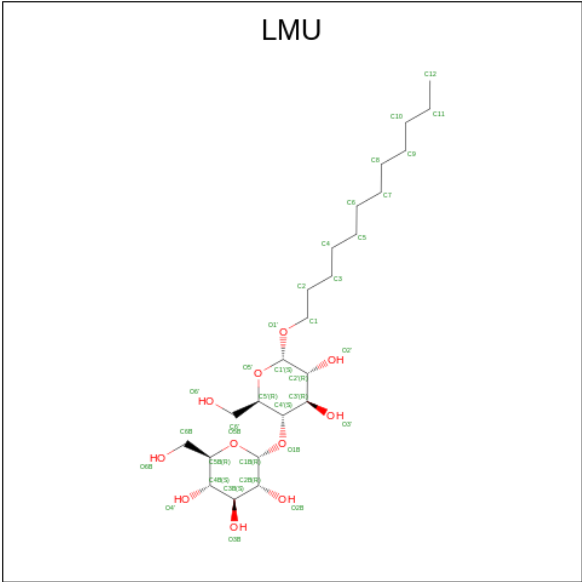
Mol	Chain	Residues	Atoms	AltConf
29	6	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	8	1	Total C 40 40	0
29	9	1	Total C 40 40	0

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



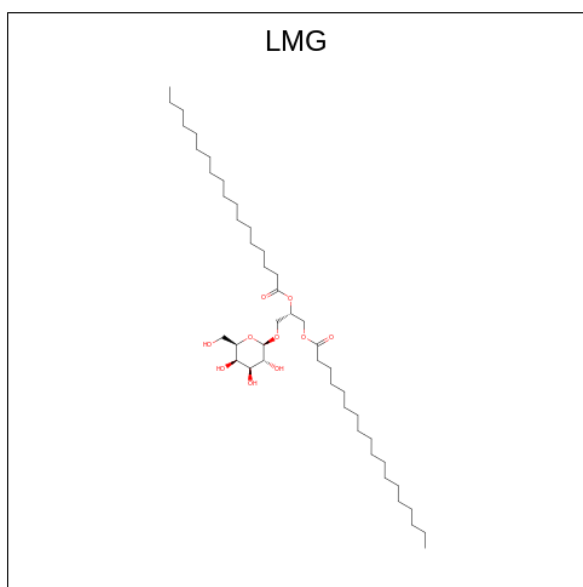
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total Fe S 8 4 4	0
30	C	1	Total Fe S 8 4 4	0
30	C	1	Total Fe S 8 4 4	0

- Molecule 31 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



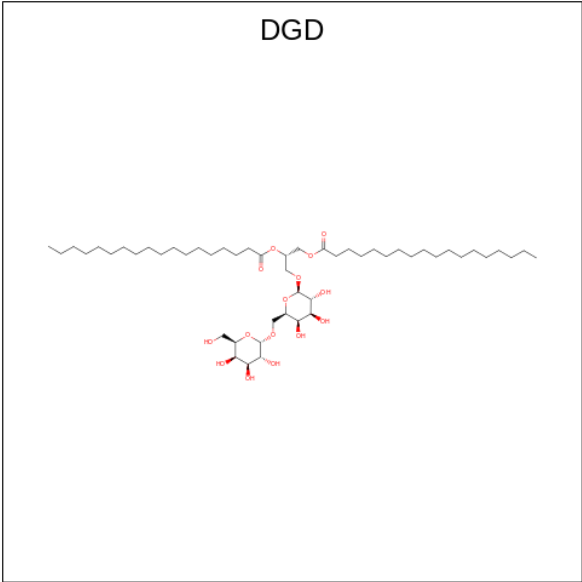
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			35	24	11	
31	A	1	Total	C	O	0
			34	24	10	
31	K	1	Total	C	O	0
			35	24	11	
31	1	1	Total	C	O	0
			35	24	11	
31	5	1	Total	C	O	0
			33	22	11	
31	5	1	Total	C	O	0
			32	21	11	
31	8	1	Total	C	O	0
			35	24	11	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



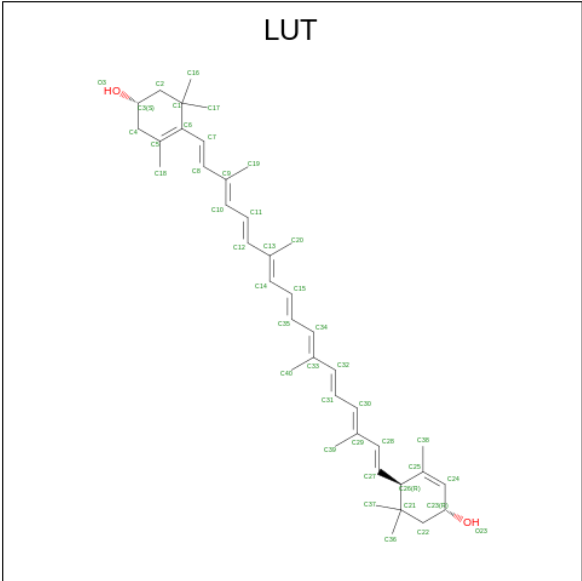
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			40	30	10	
32	H	1	Total	C	O	0
			55	45	10	
32	J	1	Total	C	O	0
			42	32	10	
32	J	1	Total	C	O	0
			40	30	10	
32	L	1	Total	C	O	0
			37	27	10	
32	4	1	Total	C	O	0
			40	30	10	
32	4	1	Total	C	O	0
			40	30	10	
32	5	1	Total	C	O	0
			40	30	10	
32	8	1	Total	C	O	0
			46	36	10	
32	9	1	Total	C	O	0
			55	45	10	
32	V	1	Total	C	O	0
			55	45	10	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			62	47	15	

- Molecule 34 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



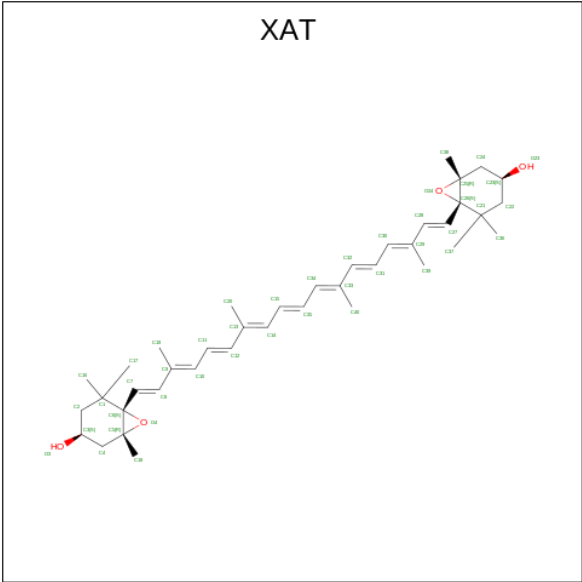
Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total	C	O	0
			42	40	2	
34	a	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
34	2	1	Total	C	O	0
			42	40	2	
34	3	1	Total	C	O	0
			42	40	2	
34	4	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	
34	6	1	Total	C	O	0
			42	40	2	
34	7	1	Total	C	O	0
			42	40	2	
34	8	1	Total	C	O	0
			42	40	2	
34	9	1	Total	C	O	0
			42	40	2	
34	X	1	Total	C	O	0
			42	40	2	
34	X	1	Total	C	O	0
			42	40	2	
34	Y	1	Total	C	O	0
			42	40	2	
34	Y	1	Total	C	O	0
			42	40	2	
34	Z	1	Total	C	O	0
			42	40	2	
34	Z	1	Total	C	O	0
			42	40	2	
34	U	1	Total	C	O	0
			42	40	2	
34	U	1	Total	C	O	0
			42	40	2	
34	V	1	Total	C	O	0
			42	40	2	
34	V	1	Total	C	O	0
			42	40	2	
34	W	1	Total	C	O	0
			42	40	2	
34	W	1	Total	C	O	0
			42	40	2	

- Molecule 35 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



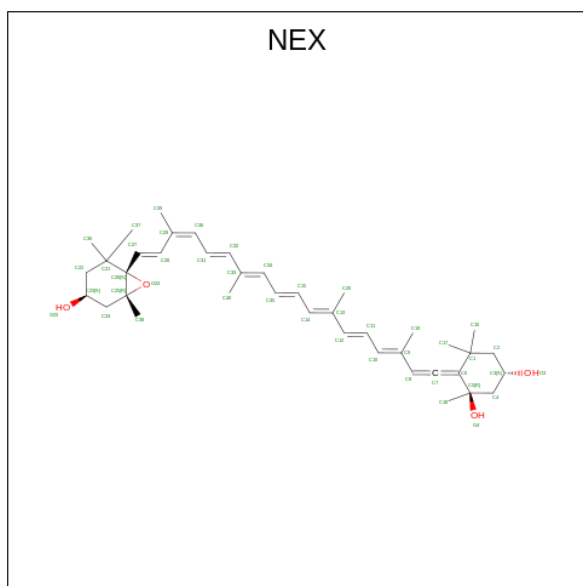
Mol	Chain	Residues	Atoms			AltConf
35	1	1	Total	C	O	0
			44	40	4	
35	a	1	Total	C	O	0
			44	40	4	
35	2	1	Total	C	O	0
			44	40	4	
35	3	1	Total	C	O	0
			44	40	4	
35	4	1	Total	C	O	0
			44	40	4	
35	5	1	Total	C	O	0
			44	40	4	
35	6	1	Total	C	O	0
			44	40	4	
35	7	1	Total	C	O	0
			44	40	4	
35	8	1	Total	C	O	0
			44	40	4	
35	9	1	Total	C	O	0
			44	40	4	
35	X	1	Total	C	O	0
			44	40	4	
35	Y	1	Total	C	O	0
			44	40	4	
35	Z	1	Total	C	O	0
			44	40	4	
35	U	1	Total	C	O	0
			44	40	4	

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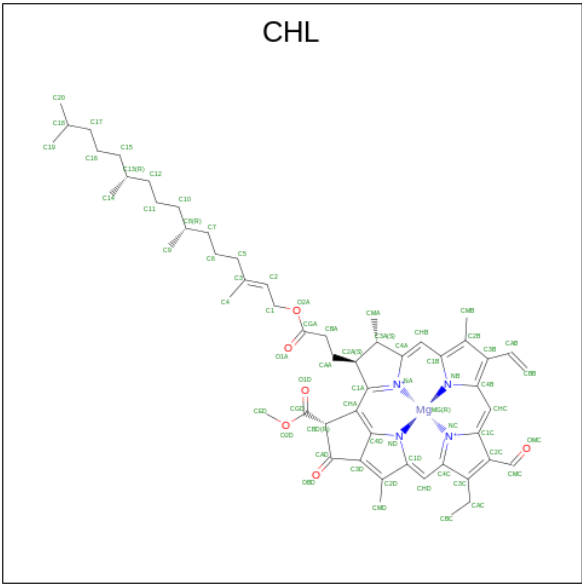
Mol	Chain	Residues	Atoms			AltConf
35	V	1	Total	C	O	0
			44	40	4	
35	W	1	Total	C	O	0
			44	40	4	

- Molecule 36 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
36	5	1	Total	C	O	0
			44	40	4	
36	6	1	Total	C	O	0
			44	40	4	
36	X	1	Total	C	O	0
			44	40	4	
36	Y	1	Total	C	O	0
			44	40	4	
36	Z	1	Total	C	O	0
			44	40	4	
36	U	1	Total	C	O	0
			44	40	4	
36	V	1	Total	C	O	0
			44	40	4	
36	W	1	Total	C	O	0
			44	40	4	

- Molecule 37 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
37	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	X	1	Total 46	C 35	Mg 1	N 4	O 6	0
37	X	1	Total 44	C 35	Mg 1	N 4	O 4	0
37	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
37	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	Y	1	Total 42	C 33	Mg 1	N 4	O 4	0
37	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
37	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	Y	1	Total 49	C 38	Mg 1	N 4	O 6	0
37	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
37	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	Z	1	Total 42	C 33	Mg 1	N 4	O 4	0
37	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
37	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	Z	1	Total 49	C 38	Mg 1	N 4	O 6	0
37	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	U	1	Total 43	C 34	Mg 1	N 4	O 4	0
37	U	1	Total 44	C 35	Mg 1	N 4	O 4	0
37	U	1	Total 46	C 35	Mg 1	N 4	O 6	0
37	U	1	Total 44	C 35	Mg 1	N 4	O 4	0
37	U	1	Total 60	C 49	Mg 1	N 4	O 6	0
37	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	V	1	Total 44	C 35	Mg 1	N 4	O 4	0
37	V	1	Total 44	C 35	Mg 1	N 4	O 4	0
37	V	1	Total 46	C 35	Mg 1	N 4	O 6	0
37	V	1	Total 48	C 37	Mg 1	N 4	O 6	0
37	V	1	Total 61	C 50	Mg 1	N 4	O 6	0
37	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	W	1	Total 46	C 35	Mg 1	N 4	O 6	0
37	W	1	Total 46	C 35	Mg 1	N 4	O 6	0

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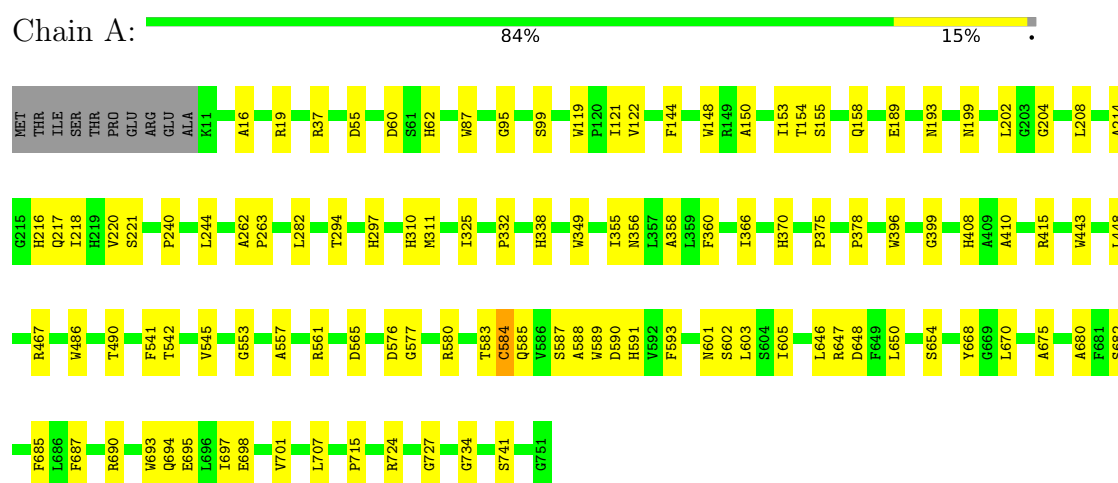
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Mol	Chain	Residues	Atoms					AltConf
37	W	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

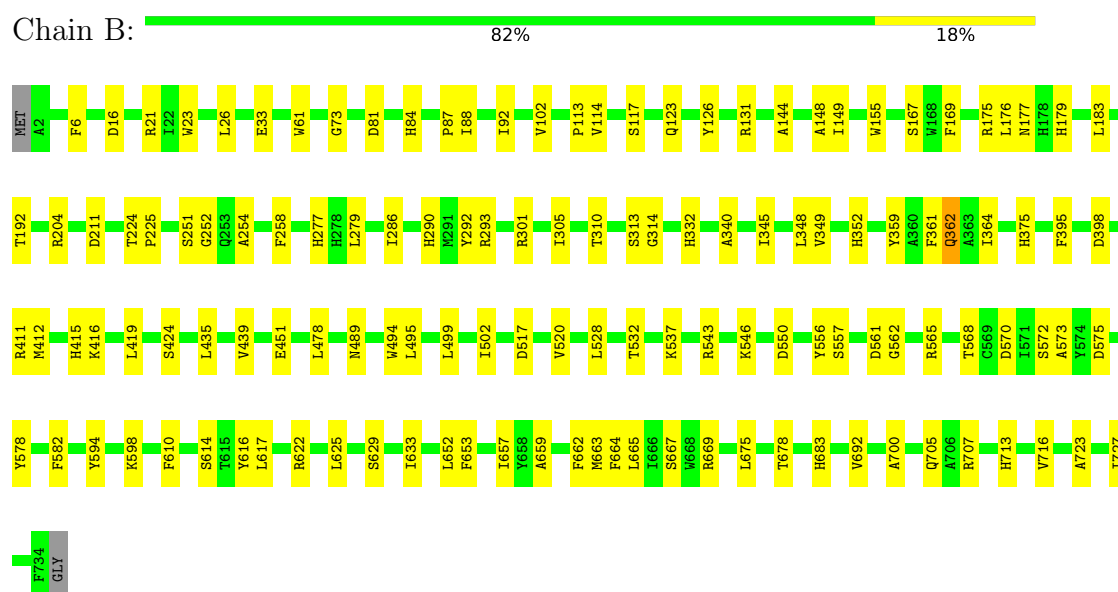
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

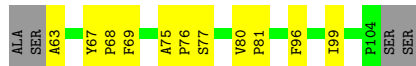
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



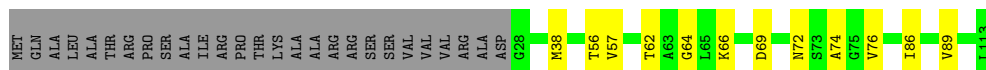
- Molecule 3: Photosystem I iron-sulfur center



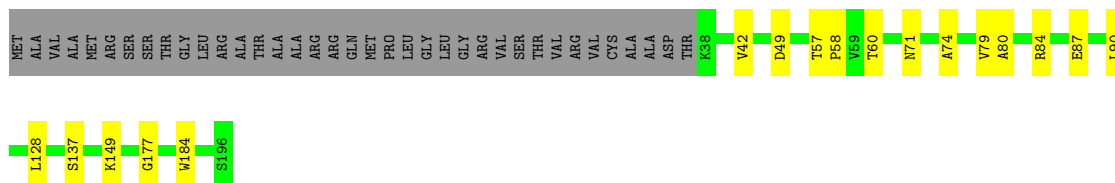
- Chain J:  93% 7%



- Chain K:  65% 11% 24%



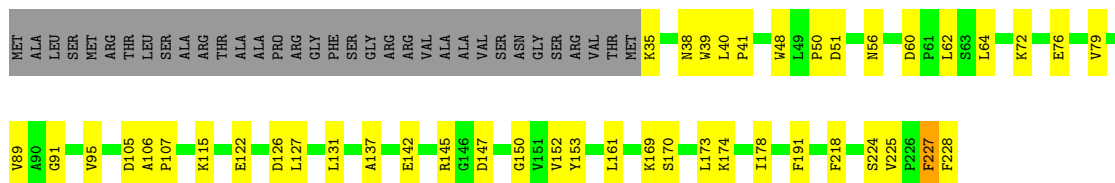
- Chain L: 72% 9% 19%



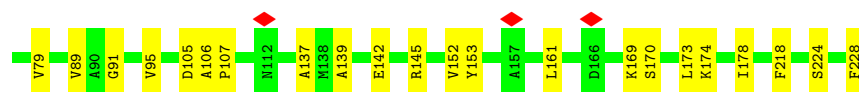
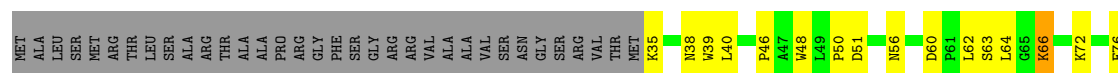
- Chain O:  64% 13% 23%



- Chain 1: 65% 19% 15%

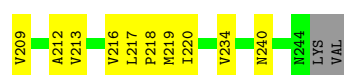
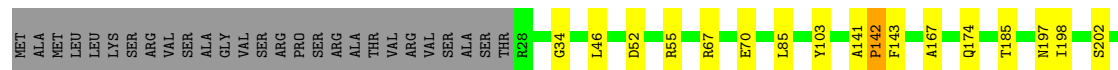


- Chain a:  68% 16% 15%



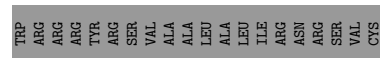
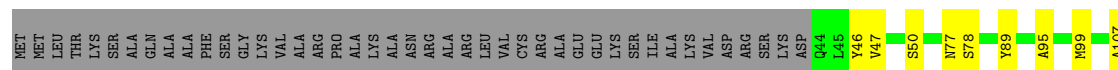
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 2: 77% 11% 12%



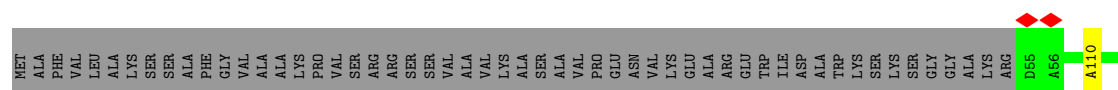
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 63% 11% 26%



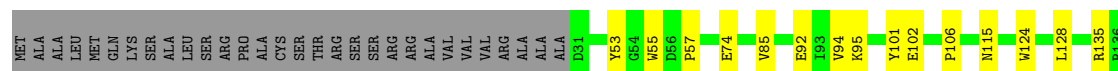
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 70% 9% 20%




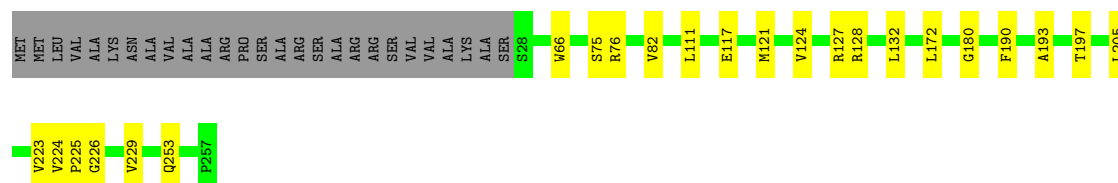
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 5: 74% 14% 12%




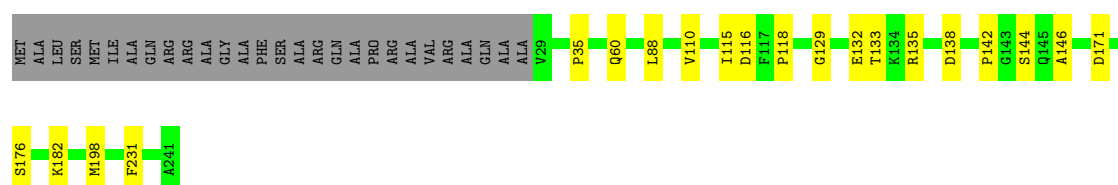
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 6:  81% 9% 11%




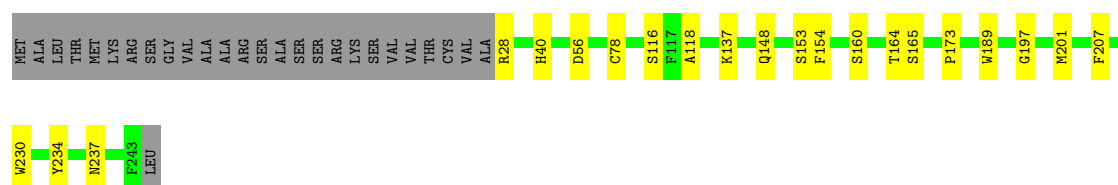
- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 7:  80% 8% 12%



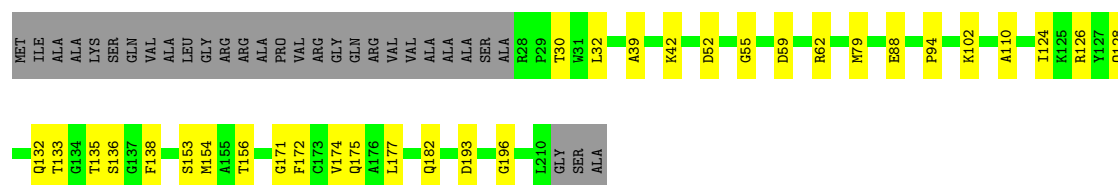
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 8:  80% 9% 11%



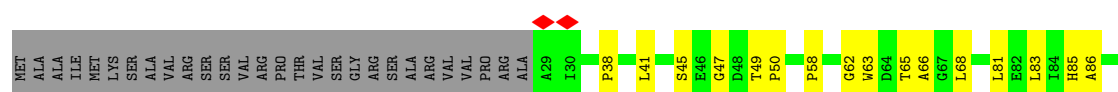
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

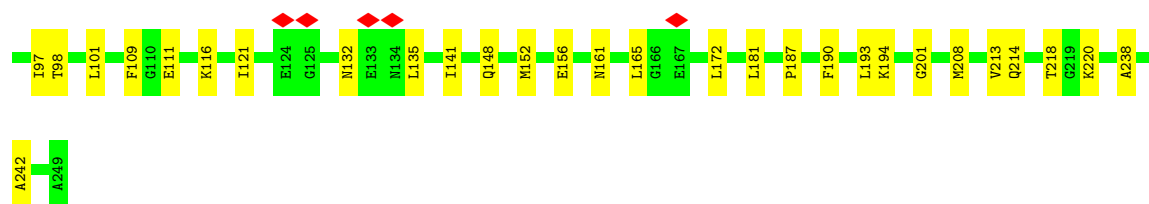
Chain 9:  71% 15% 14%



- Molecule 23: Chlorophyll a-b binding protein, chloroplastic

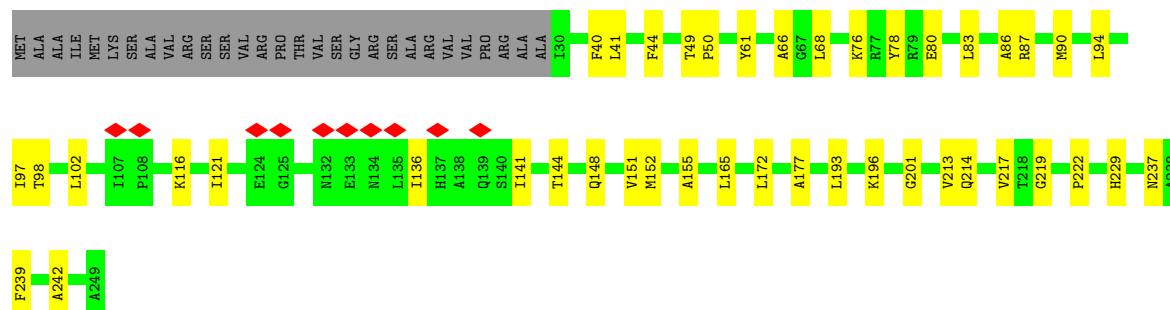
Chain X:  70% 18% 11%





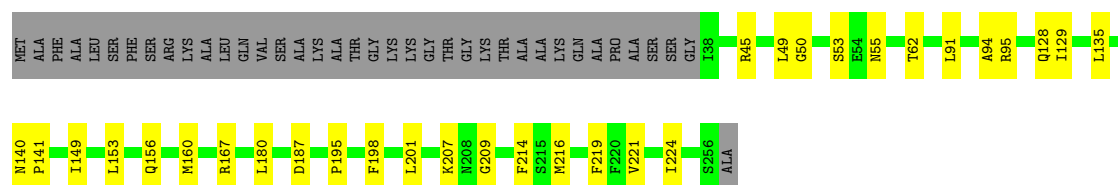
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic

Chain W: 71% 17% 12%



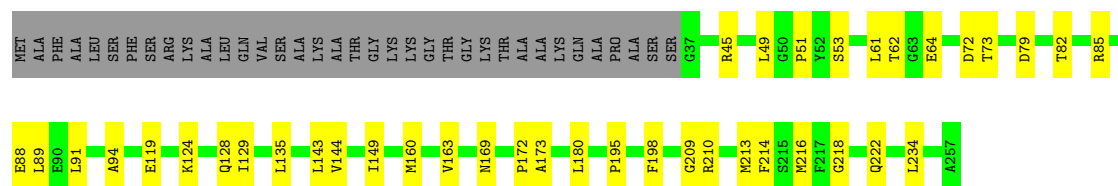
- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain Y: 73% 12% 15%



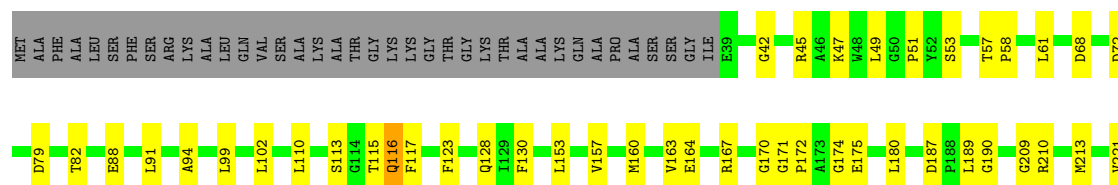
- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

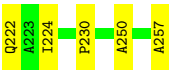
Chain Z: 70% 16% 14%



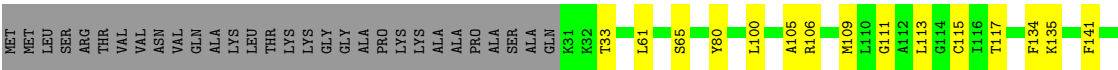
- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain U: 66% 19% 15%





● Molecule 25: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123997	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5625	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	360.0, 360.0, 360.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, LMG, XAT, TPO, BCR, LUT, DGD, CLA, LMU, NEX, PQN, CHL, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.53	0/6015	0.39	0/8201
2	B	0.52	0/6036	0.45	5/8242 (0.1%)
3	C	0.51	0/610	0.62	1/826 (0.1%)
4	D	0.44	0/1152	0.46	1/1556 (0.1%)
5	E	0.41	0/506	0.34	0/689
6	F	0.39	0/1291	0.37	0/1747
7	G	0.27	0/714	0.34	0/972
8	H	0.39	0/788	0.37	0/1059
9	I	0.52	0/329	0.46	0/456
10	J	0.45	0/349	0.33	0/478
11	K	0.38	0/587	0.42	0/795
12	L	0.47	0/1190	0.41	0/1628
13	O	0.40	0/784	0.39	0/1069
14	1	0.37	0/1490	0.46	0/2028
14	a	0.37	0/1490	0.46	0/2028
15	2	0.38	0/1730	0.43	0/2353
16	3	0.43	0/1726	0.38	0/2342
17	4	0.29	0/1686	0.34	0/2300
18	5	0.37	0/1829	0.40	0/2492
19	6	0.34	0/1833	0.38	0/2505
20	7	0.44	0/1701	0.38	0/2310
21	8	0.40	0/1692	0.37	0/2304
22	9	0.36	0/1444	0.43	0/1964
23	W	0.22	0/1721	0.54	0/2341
23	X	0.24	0/1730	0.54	0/2355
24	U	0.23	0/1717	0.55	1/2336 (0.0%)
24	Y	0.25	0/1723	0.53	0/2345
24	Z	0.23	0/1732	0.53	0/2357
25	V	0.22	0/1856	0.46	0/2518
All	All	0.41	0/47451	0.44	8/64596 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	150	LEU	N-CA-C	7.75	122.50	112.12
24	U	116	GLN	N-CA-C	6.74	118.62	111.28
2	B	495	LEU	N-CA-C	5.71	121.31	113.77
2	B	362	GLN	N-CA-C	-5.51	101.81	110.36
2	B	310	THR	CA-C-N	-5.44	114.78	120.38

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	A	5819	0	5670	87	0
2	B	5824	0	5579	104	0
3	C	600	0	581	15	0
4	D	1124	0	1139	16	0
5	E	496	0	491	5	0
6	F	1265	0	1301	19	0
7	G	699	0	681	11	0
8	H	776	0	765	10	0
9	I	316	0	321	9	0
10	J	337	0	336	2	0
11	K	582	0	620	10	0
12	L	1161	0	1184	15	0
13	O	758	0	740	13	0
14	1	1444	0	1396	34	0
14	a	1444	0	1396	27	0
15	2	1682	0	1665	22	0
16	3	1678	0	1637	25	0
17	4	1631	0	1587	18	0
18	5	1774	0	1746	42	0
19	6	1771	0	1770	21	0
20	7	1649	0	1589	15	0
21	8	1641	0	1618	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	9	1403	0	1381	21	0
23	W	1671	0	1604	30	0
23	X	1680	0	1622	32	0
24	U	1669	0	1603	40	0
24	Y	1675	0	1617	26	0
24	Z	1684	0	1625	29	0
25	V	1815	0	1766	50	0
26	1	666	0	522	6	0
26	2	637	0	530	4	0
26	3	724	0	628	5	0
26	4	778	0	678	7	0
26	5	878	0	758	17	0
26	6	903	0	831	11	0
26	7	756	0	635	13	0
26	8	724	0	629	8	0
26	9	595	0	491	4	0
26	A	2669	0	2693	56	0
26	B	2284	0	2237	33	0
26	F	140	0	113	6	0
26	G	87	0	64	0	0
26	H	104	0	93	0	0
26	J	42	0	31	0	0
26	K	191	0	150	3	0
26	L	235	0	184	7	0
26	O	116	0	61	0	0
26	U	400	0	342	11	0
26	V	415	0	365	11	0
26	W	426	0	377	12	0
26	X	436	0	415	16	0
26	Y	429	0	389	10	0
26	Z	427	0	386	17	0
26	a	710	0	591	8	0
27	A	33	0	46	2	0
27	B	33	0	46	3	0
28	1	49	0	74	0	0
28	2	36	0	42	0	0
28	3	94	0	137	3	0
28	4	49	0	74	0	0
28	5	98	0	148	6	0
28	6	48	0	69	0	0
28	7	37	0	44	0	0
28	8	89	0	124	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	9	128	0	178	1	0
28	A	128	0	178	0	0
28	B	38	0	46	0	0
28	H	49	0	74	0	0
28	O	36	0	42	1	0
28	U	49	0	74	1	0
28	V	36	0	42	3	0
28	W	34	0	38	1	0
28	X	49	0	74	6	0
28	Y	49	0	74	6	0
28	Z	49	0	74	9	0
28	a	43	0	59	1	0
29	1	40	0	56	2	0
29	2	40	0	56	5	0
29	3	120	0	168	19	0
29	4	40	0	56	5	0
29	5	40	0	56	2	0
29	6	40	0	56	1	0
29	7	80	0	112	8	0
29	8	40	0	56	3	0
29	9	40	0	56	7	0
29	A	240	0	336	42	0
29	B	400	0	560	44	0
29	F	40	0	56	7	0
29	G	40	0	56	4	0
29	J	40	0	56	8	0
29	K	80	0	112	8	0
29	L	160	0	224	29	0
29	O	80	0	112	9	0
29	a	40	0	56	3	0
30	A	8	0	0	0	0
30	C	16	0	0	1	0
31	1	35	0	46	0	0
31	5	65	0	76	0	0
31	8	35	0	46	0	0
31	A	69	0	90	1	0
31	K	35	0	46	0	0
32	4	80	0	100	0	0
32	5	40	0	50	1	0
32	8	46	0	65	3	0
32	9	55	0	86	2	0
32	A	40	0	50	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	H	55	0	86	0	0
32	J	82	0	107	0	0
32	L	37	0	44	0	0
32	V	55	0	86	2	0
33	B	62	0	85	1	0
34	1	42	0	56	6	0
34	2	42	0	56	7	0
34	3	42	0	56	7	0
34	4	42	0	56	3	0
34	5	42	0	56	4	0
34	6	42	0	56	5	0
34	7	42	0	56	3	0
34	8	42	0	56	6	0
34	9	42	0	56	5	0
34	U	84	0	112	8	0
34	V	84	0	112	10	0
34	W	84	0	112	8	0
34	X	84	0	112	12	0
34	Y	84	0	112	9	0
34	Z	84	0	112	10	0
34	a	42	0	56	5	0
35	1	44	0	56	3	0
35	2	44	0	56	1	0
35	3	44	0	56	2	0
35	4	44	0	56	3	0
35	5	44	0	56	2	0
35	6	44	0	56	1	0
35	7	44	0	56	1	0
35	8	44	0	56	1	0
35	9	44	0	56	0	0
35	U	44	0	56	5	0
35	V	44	0	56	6	0
35	W	44	0	56	3	0
35	X	44	0	56	3	0
35	Y	44	0	56	3	0
35	Z	44	0	56	5	0
35	a	44	0	56	3	0
36	5	44	0	56	1	0
36	6	44	0	56	6	0
36	U	44	0	56	0	0
36	V	44	0	56	11	0
36	W	44	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	X	44	0	56	2	0
36	Y	44	0	56	2	0
36	Z	44	0	56	3	0
37	U	303	0	248	14	0
37	V	309	0	253	15	0
37	W	336	0	298	9	0
37	X	353	0	342	15	0
37	Y	335	0	302	16	0
37	Z	335	0	302	14	0
All	All	69460	0	68604	1115	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 8.

The worst 5 of 1115 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)
21:8:78:CYS:SG	21:8:201:MET:HE2	1.64	1.34
25:V:174:ILE:CG2	36:V:1623:NEX:H15	1.78	1.14
21:8:78:CYS:SG	21:8:201:MET:CE	2.44	1.06
18:5:192:LEU:CD1	26:5:611:CLA:HMD1	1.87	1.04
25:V:174:ILE:HG22	36:V:1623:NEX:H201	1.42	1.00

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	713 (96%)	26 (4%)	0	100	100
2	B	731/735 (100%)	701 (96%)	30 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	78/81 (96%)	67 (86%)	11 (14%)	0	100	100
4	D	141/196 (72%)	135 (96%)	6 (4%)	0	100	100
5	E	61/97 (63%)	57 (93%)	4 (7%)	0	100	100
6	F	163/227 (72%)	156 (96%)	7 (4%)	0	100	100
7	G	92/126 (73%)	86 (94%)	6 (6%)	0	100	100
8	H	98/130 (75%)	94 (96%)	4 (4%)	0	100	100
9	I	40/106 (38%)	35 (88%)	5 (12%)	0	100	100
10	J	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
11	K	84/113 (74%)	78 (93%)	6 (7%)	0	100	100
12	L	157/196 (80%)	146 (93%)	11 (7%)	0	100	100
13	O	95/126 (75%)	87 (92%)	8 (8%)	0	100	100
14	1	192/228 (84%)	186 (97%)	6 (3%)	0	100	100
14	a	192/228 (84%)	186 (97%)	6 (3%)	0	100	100
15	2	215/246 (87%)	203 (94%)	10 (5%)	2 (1%)	14	45
16	3	218/298 (73%)	211 (97%)	7 (3%)	0	100	100
17	4	208/264 (79%)	202 (97%)	6 (3%)	0	100	100
18	5	225/257 (88%)	211 (94%)	14 (6%)	0	100	100
19	6	228/257 (89%)	210 (92%)	18 (8%)	0	100	100
20	7	211/241 (88%)	197 (93%)	14 (7%)	0	100	100
21	8	214/243 (88%)	210 (98%)	4 (2%)	0	100	100
22	9	181/213 (85%)	165 (91%)	16 (9%)	0	100	100
23	W	218/249 (88%)	202 (93%)	16 (7%)	0	100	100
23	X	219/249 (88%)	194 (89%)	25 (11%)	0	100	100
24	U	217/257 (84%)	196 (90%)	21 (10%)	0	100	100
24	Y	217/257 (84%)	198 (91%)	19 (9%)	0	100	100
24	Z	219/257 (85%)	204 (93%)	15 (7%)	0	100	100
25	V	235/268 (88%)	222 (94%)	13 (6%)	0	100	100
All	All	5927/6937 (85%)	5590 (94%)	335 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	2	142	PRO

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Mol	Chain	Res	Type
15	2	143	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/610 (98%)	600 (100%)	1 (0%)	92	96
2	B	596/597 (100%)	596 (100%)	0	100	100
3	C	69/70 (99%)	67 (97%)	2 (3%)	37	63
4	D	120/152 (79%)	120 (100%)	0	100	100
5	E	54/81 (67%)	54 (100%)	0	100	100
6	F	127/169 (75%)	127 (100%)	0	100	100
7	G	70/94 (74%)	70 (100%)	0	100	100
8	H	81/102 (79%)	81 (100%)	0	100	100
9	I	33/76 (43%)	33 (100%)	0	100	100
10	J	37/37 (100%)	37 (100%)	0	100	100
11	K	59/80 (74%)	59 (100%)	0	100	100
12	L	121/148 (82%)	121 (100%)	0	100	100
13	O	78/101 (77%)	78 (100%)	0	100	100
14	1	137/162 (85%)	135 (98%)	2 (2%)	60	78
14	a	137/162 (85%)	135 (98%)	2 (2%)	60	78
15	2	173/198 (87%)	173 (100%)	0	100	100
16	3	167/230 (73%)	167 (100%)	0	100	100
17	4	165/205 (80%)	164 (99%)	1 (1%)	84	91
18	5	184/206 (89%)	184 (100%)	0	100	100
19	6	184/203 (91%)	184 (100%)	0	100	100
20	7	164/181 (91%)	164 (100%)	0	100	100
21	8	162/183 (88%)	162 (100%)	0	100	100
22	9	140/159 (88%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	164/187 (88%)	164 (100%)	0	100	100
23	X	165/187 (88%)	164 (99%)	1 (1%)	84	91
24	U	168/194 (87%)	168 (100%)	0	100	100
24	Y	170/194 (88%)	170 (100%)	0	100	100
24	Z	170/194 (88%)	170 (100%)	0	100	100
25	V	178/201 (89%)	178 (100%)	0	100	100
All	All	4674/5363 (87%)	4665 (100%)	9 (0%)	91	96

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	4	177	ASP
23	X	165	LEU
14	1	72	LYS
14	1	227	PHE
14	a	66	LYS

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

Mol	Chain	Res	Type
13	O	82	ASN
24	U	147	GLN
15	2	196	ASN
23	W	161	ASN
23	X	161	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
25	TPO	V	33	25	8,10,11	1.56	1 (12%)	10,14,16	1.95	2 (20%)

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
25	TPO	V	33	25	-	3/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	33	TPO	P-O1P	3.28	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	V	33	TPO	P-OG1-CB	-5.21	107.48	123.21
25	V	33	TPO	CG2-CB-CA	-2.55	108.14	113.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	V	33	TPO	N-CA-CB-CG2
25	V	33	TPO	N-CA-CB-OG1
25	V	33	TPO	C-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

471 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
31	LMU	A	857	-	36,36,36	1.09	2 (5%)	47,47,47	1.37	8 (17%)
30	SF4	C	101	3	0,12,12	-	-	-		
28	LHG	9	623	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
26	CLA	5	607	-	65,73,73	1.50	10 (15%)	76,113,113	1.28	8 (10%)
26	CLA	A	801	-	65,73,73	1.48	11 (16%)	76,113,113	1.36	9 (11%)
29	BCR	3	622	-	41,41,41	0.89	1 (2%)	56,56,56	2.23	18 (32%)
37	CHL	W	606	-	46,54,74	2.21	15 (32%)	49,90,114	3.12	20 (40%)
34	LUT	Y	1620	-	42,43,43	0.80	0	51,60,60	3.18	18 (35%)
37	CHL	Z	607	-	66,74,74	1.90	15 (22%)	73,114,114	2.67	18 (24%)
26	CLA	Z	611	28	42,50,73	1.87	8 (19%)	52,85,113	1.59	9 (17%)
26	CLA	A	841	-	65,73,73	1.48	10 (15%)	76,113,113	1.28	7 (9%)
26	CLA	W	613	23	65,73,73	1.53	8 (12%)	76,113,113	1.27	6 (7%)
37	CHL	W	607	-	65,73,74	2.00	16 (24%)	73,113,114	2.54	21 (28%)
28	LHG	1	620	26	48,48,48	0.92	2 (4%)	51,54,54	0.79	2 (3%)
28	LHG	A	861	-	48,48,48	0.94	2 (4%)	51,54,54	1.00	2 (3%)
36	NEX	V	1623	-	38,46,46	0.94	2 (5%)	50,70,70	2.30	18 (36%)
36	NEX	5	624	-	38,46,46	1.08	1 (2%)	50,70,70	2.27	18 (36%)
26	CLA	3	612	16	43,51,73	1.86	7 (16%)	49,86,113	1.41	6 (12%)
26	CLA	B	810	-	64,72,73	1.48	10 (15%)	74,111,113	1.52	11 (14%)
29	BCR	A	849	-	41,41,41	0.85	0	56,56,56	2.22	21 (37%)
26	CLA	B	815	-	43,51,73	1.80	10 (23%)	49,86,113	1.42	6 (12%)
26	CLA	3	609	16	60,68,73	1.59	10 (16%)	70,107,113	1.38	8 (11%)
26	CLA	6	610	19	65,73,73	1.55	9 (13%)	76,113,113	1.24	8 (10%)
29	BCR	4	621	-	41,41,41	0.83	1 (2%)	56,56,56	2.03	18 (32%)
26	CLA	1	616	14	43,51,73	1.86	7 (16%)	54,87,113	1.63	9 (16%)
26	CLA	A	817	-	45,53,73	1.81	10 (22%)	52,89,113	1.54	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	9	603	22	44,52,73	1.88	9 (20%)	55,88,113	1.52	7 (12%)
26	CLA	A	805	-	52,60,73	1.67	12 (23%)	60,97,113	1.66	9 (15%)
26	CLA	A	845	28	50,58,73	1.68	7 (14%)	58,95,113	1.62	7 (12%)
35	XAT	8	620	-	39,47,47	1.02	2 (5%)	54,74,74	2.45	24 (44%)
29	BCR	7	621	-	41,41,41	0.80	1 (2%)	56,56,56	2.28	22 (39%)
26	CLA	B	839	-	65,73,73	1.48	11 (16%)	76,113,113	1.32	8 (10%)
31	LMU	K	208	-	36,36,36	1.14	2 (5%)	47,47,47	1.00	3 (6%)
26	CLA	2	613	15	65,73,73	1.47	8 (12%)	76,113,113	1.25	7 (9%)
34	LUT	U	1621	-	42,43,43	0.75	0	51,60,60	1.55	9 (17%)
28	LHG	2	622	26	35,35,48	1.05	2 (5%)	38,41,54	1.16	3 (7%)
32	LMG	H	205	-	55,55,55	0.86	2 (3%)	63,63,63	1.11	6 (9%)
26	CLA	6	617	-	45,53,73	1.76	9 (20%)	52,89,113	1.48	8 (15%)
26	CLA	1	603	-	52,61,73	1.64	8 (15%)	59,98,113	1.49	7 (11%)
28	LHG	O	2631	-	35,35,48	1.07	2 (5%)	38,41,54	1.12	3 (7%)
34	LUT	Z	1620	-	42,43,43	0.78	0	51,60,60	1.80	12 (23%)
37	CHL	Y	601	24	66,74,74	1.94	16 (24%)	73,114,114	2.63	21 (28%)
29	BCR	F	305	-	41,41,41	0.89	1 (2%)	56,56,56	2.34	20 (35%)
26	CLA	B	816	-	54,62,73	1.62	9 (16%)	62,99,113	1.42	8 (12%)
32	LMG	L	2631	-	37,37,55	1.08	2 (5%)	45,45,63	1.18	4 (8%)
26	CLA	1	609	14	40,48,73	1.88	8 (20%)	50,83,113	1.69	10 (20%)
26	CLA	K	203	-	56,64,73	1.60	10 (17%)	65,102,113	1.48	10 (15%)
26	CLA	5	617	-	50,58,73	1.69	11 (22%)	58,95,113	1.38	8 (13%)
26	CLA	a	608	-	43,52,73	1.83	8 (18%)	49,88,113	1.46	8 (16%)
26	CLA	V	612	25	45,53,73	1.81	8 (17%)	52,89,113	1.50	8 (15%)
26	CLA	9	601	22	45,53,73	1.81	8 (17%)	52,89,113	1.46	8 (15%)
26	CLA	B	830	-	43,51,73	1.87	9 (20%)	49,86,113	1.54	11 (22%)
28	LHG	9	624	-	48,48,48	0.93	2 (4%)	51,54,54	0.87	2 (3%)
26	CLA	4	608	-	65,73,73	1.50	9 (13%)	76,113,113	1.27	9 (11%)
26	CLA	4	612	17	40,49,73	1.88	8 (20%)	45,84,113	1.45	6 (13%)
34	LUT	4	619	-	42,43,43	0.80	1 (2%)	51,60,60	2.02	18 (35%)
26	CLA	W	611	28	57,65,73	1.62	5 (8%)	66,103,113	1.27	7 (10%)
28	LHG	3	623	-	44,44,48	0.93	2 (4%)	47,50,54	1.00	3 (6%)
26	CLA	B	812	-	43,51,73	1.80	8 (18%)	49,86,113	1.40	6 (12%)
26	CLA	2	614	-	41,50,73	1.86	8 (19%)	46,85,113	1.54	7 (15%)
26	CLA	V	610	25	62,70,73	1.52	8 (12%)	72,109,113	1.33	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	B	822	-	42,50,73	1.81	10 (23%)	48,85,113	1.44	7 (14%)
26	CLA	U	604	-	49,56,73	1.82	7 (14%)	50,91,113	1.58	7 (14%)
28	LHG	X	2630	26	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
29	BCR	K	202	-	41,41,41	0.94	2 (4%)	56,56,56	2.28	21 (37%)
26	CLA	8	610	21	60,68,73	1.52	7 (11%)	70,107,113	1.51	9 (12%)
26	CLA	L	302	12	45,53,73	1.86	10 (22%)	52,89,113	1.53	7 (13%)
26	CLA	B	809	2	65,73,73	1.53	11 (16%)	76,113,113	1.37	8 (10%)
37	CHL	Y	608	-	49,57,74	2.19	15 (30%)	52,93,114	3.13	20 (38%)
26	CLA	2	606	-	43,51,73	1.81	10 (23%)	49,86,113	1.49	8 (16%)
27	PQN	A	844	-	34,34,34	3.31	9 (26%)	42,45,45	2.07	4 (9%)
26	CLA	A	815	-	50,58,73	1.70	9 (18%)	58,95,113	1.49	7 (12%)
26	CLA	Z	603	-	55,63,73	1.62	7 (12%)	64,101,113	1.51	10 (15%)
26	CLA	1	604	-	49,57,73	1.74	9 (18%)	55,93,113	1.47	8 (14%)
34	LUT	1	617	-	42,43,43	0.80	1 (2%)	51,60,60	1.89	16 (31%)
35	XAT	Z	1622	-	39,47,47	0.93	0	54,74,74	2.87	21 (38%)
34	LUT	X	1620	-	42,43,43	0.73	0	51,60,60	1.54	9 (17%)
26	CLA	6	607	-	41,49,73	1.91	8 (19%)	51,84,113	1.52	8 (15%)
26	CLA	5	608	-	50,58,73	1.71	10 (20%)	58,95,113	1.32	7 (12%)
26	CLA	Z	602	24	58,66,73	1.58	7 (12%)	67,104,113	1.37	6 (8%)
26	CLA	A	812	-	65,73,73	1.51	10 (15%)	76,113,113	1.30	8 (10%)
26	CLA	U	602	24	59,67,73	1.57	7 (11%)	68,105,113	1.36	8 (11%)
29	BCR	O	2005	-	41,41,41	0.88	1 (2%)	56,56,56	3.05	23 (41%)
26	CLA	5	602	18	65,73,73	1.52	9 (13%)	76,113,113	1.26	8 (10%)
26	CLA	7	616	20	43,51,73	1.87	8 (18%)	54,87,113	1.53	8 (14%)
34	LUT	X	1621	-	42,43,43	0.81	0	51,60,60	1.74	15 (29%)
29	BCR	G	205	-	41,41,41	0.80	1 (2%)	56,56,56	1.97	15 (26%)
26	CLA	7	613	20	65,73,73	1.49	10 (15%)	76,113,113	1.35	8 (10%)
26	CLA	A	830	-	65,73,73	1.49	10 (15%)	76,113,113	1.29	8 (10%)
37	CHL	U	601	24	66,74,74	1.96	17 (25%)	73,114,114	2.52	20 (27%)
26	CLA	U	611	28	42,50,73	1.86	5 (11%)	48,85,113	1.51	7 (14%)
26	CLA	6	616	19	65,73,73	1.49	10 (15%)	76,113,113	1.38	10 (13%)
26	CLA	B	814	-	64,72,73	1.48	10 (15%)	74,111,113	1.43	9 (12%)
26	CLA	B	821	-	43,51,73	1.93	9 (20%)	48,86,113	1.54	9 (18%)
26	CLA	A	837	1	45,53,73	1.81	10 (22%)	52,89,113	1.62	8 (15%)
36	NEX	Z	1623	-	38,46,46	1.02	1 (2%)	50,70,70	2.64	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	B	823	-	45,53,73	1.79	10 (22%)	52,89,113	1.46	8 (15%)
26	CLA	7	603	-	43,52,73	1.82	11 (25%)	49,88,113	1.63	8 (16%)
26	CLA	7	604	-	50,58,73	1.69	9 (18%)	58,95,113	1.37	7 (12%)
29	BCR	a	619	-	41,41,41	0.84	0	56,56,56	2.38	22 (39%)
26	CLA	4	606	-	39,48,73	1.90	9 (23%)	44,83,113	1.39	6 (13%)
26	CLA	a	602	14	61,69,73	1.54	8 (13%)	71,108,113	1.43	8 (11%)
26	CLA	J	101	10	42,50,73	1.86	9 (21%)	48,85,113	1.41	7 (14%)
26	CLA	Z	610	24	65,73,73	1.53	9 (13%)	76,113,113	1.28	8 (10%)
26	CLA	B	834	-	60,68,73	1.52	11 (18%)	70,107,113	1.39	9 (12%)
28	LHG	V	2630	26	35,35,48	1.07	2 (5%)	38,41,54	1.08	2 (5%)
29	BCR	8	621	-	41,41,41	0.75	0	56,56,56	2.77	21 (37%)
33	DGD	B	850	-	63,63,67	0.83	2 (3%)	77,77,81	1.24	7 (9%)
36	NEX	W	1623	-	38,46,46	0.90	2 (5%)	50,70,70	2.54	12 (24%)
26	CLA	A	813	-	54,62,73	1.66	10 (18%)	62,99,113	1.42	8 (12%)
26	CLA	B	811	-	53,60,73	1.74	10 (18%)	62,97,113	1.48	11 (17%)
29	BCR	A	850	-	41,41,41	0.93	1 (2%)	56,56,56	2.02	14 (25%)
26	CLA	6	620	-	64,72,73	1.51	10 (15%)	74,111,113	1.28	8 (10%)
37	CHL	Z	609	24	66,74,74	1.94	14 (21%)	73,114,114	2.64	22 (30%)
26	CLA	X	602	23	65,73,73	1.50	7 (10%)	76,113,113	1.36	6 (7%)
32	LMG	J	103	-	42,42,55	0.98	2 (4%)	50,50,63	1.22	6 (12%)
26	CLA	6	609	19	45,53,73	1.83	10 (22%)	52,89,113	1.45	7 (13%)
29	BCR	B	846	-	41,41,41	0.81	1 (2%)	56,56,56	2.34	21 (37%)
26	CLA	Z	614	-	48,56,73	1.76	7 (14%)	55,92,113	1.42	7 (12%)
30	SF4	C	102	3	0,12,12	-	-	-	-	-
26	CLA	Y	611	28	43,51,73	1.85	7 (16%)	49,86,113	1.44	6 (12%)
26	CLA	B	828	-	65,73,73	1.51	10 (15%)	76,113,113	1.29	7 (9%)
26	CLA	B	832	-	60,68,73	1.58	9 (15%)	70,107,113	1.44	10 (14%)
34	LUT	9	619	-	42,43,43	0.87	1 (2%)	51,60,60	1.90	14 (27%)
26	CLA	2	604	-	42,50,73	1.82	7 (16%)	48,85,113	1.58	7 (14%)
26	CLA	a	606	-	43,52,73	1.86	8 (18%)	48,87,113	1.39	5 (10%)
26	CLA	H	202	-	38,47,73	1.96	8 (21%)	43,82,113	1.42	6 (13%)
26	CLA	5	614	-	45,52,73	1.90	10 (22%)	48,87,113	1.47	6 (12%)
36	NEX	X	1623	-	38,46,46	0.90	1 (2%)	50,70,70	4.33	20 (40%)
26	CLA	B	841	28	65,73,73	1.49	9 (13%)	76,113,113	1.32	8 (10%)
29	BCR	A	856	-	41,41,41	0.91	2 (4%)	56,56,56	1.97	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	B	818	-	60,68,73	1.57	11 (18%)	70,107,113	1.47	9 (12%)
26	CLA	Y	610	24	65,73,73	1.55	8 (12%)	76,113,113	1.24	8 (10%)
29	BCR	O	2004	-	41,41,41	0.82	0	56,56,56	1.96	14 (25%)
26	CLA	1	614	-	37,45,73	2.10	8 (21%)	44,79,113	1.72	9 (20%)
26	CLA	A	803	-	65,73,73	1.53	12 (18%)	76,113,113	1.41	5 (6%)
31	LMU	5	628	-	34,34,36	1.19	2 (5%)	45,45,47	1.14	5 (11%)
27	PQN	B	842	-	34,34,34	3.33	8 (23%)	42,45,45	2.02	7 (16%)
26	CLA	6	606	-	39,48,73	1.90	8 (20%)	44,83,113	1.35	5 (11%)
31	LMU	8	625	-	36,36,36	1.10	2 (5%)	47,47,47	1.24	3 (6%)
26	CLA	6	604	-	65,73,73	1.48	10 (15%)	76,113,113	1.21	8 (10%)
26	CLA	A	843	-	64,72,73	1.53	10 (15%)	74,111,113	1.35	9 (12%)
26	CLA	B	819	-	55,63,73	1.65	9 (16%)	64,101,113	1.36	8 (12%)
32	LMG	V	2631	-	55,55,55	0.87	2 (3%)	63,63,63	1.11	5 (7%)
35	XAT	5	621	-	39,47,47	0.95	2 (5%)	54,74,74	2.52	18 (33%)
37	CHL	V	608	-	48,56,74	2.18	14 (29%)	51,92,114	3.21	20 (39%)
26	CLA	L	307	8	39,48,73	1.81	8 (20%)	44,83,113	1.66	6 (13%)
26	CLA	3	606	-	53,62,73	1.61	10 (18%)	61,100,113	1.46	9 (14%)
26	CLA	A	836	-	65,73,73	1.47	11 (16%)	76,113,113	1.38	9 (11%)
26	CLA	A	821	-	53,61,73	1.64	9 (16%)	61,98,113	1.43	9 (14%)
35	XAT	6	621	-	39,47,47	0.98	3 (7%)	54,74,74	2.42	23 (42%)
26	CLA	A	828	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	8 (10%)
37	CHL	U	607	-	46,54,74	2.28	14 (30%)	49,90,114	3.11	18 (36%)
34	LUT	7	619	-	42,43,43	0.91	2 (4%)	51,60,60	1.99	14 (27%)
26	CLA	9	602	22	60,68,73	1.55	7 (11%)	70,107,113	1.44	8 (11%)
34	LUT	W	1621	-	42,43,43	0.69	0	51,60,60	1.78	13 (25%)
26	CLA	a	604	-	49,57,73	1.73	9 (18%)	55,93,113	1.46	7 (12%)
29	BCR	A	851	-	41,41,41	0.91	1 (2%)	56,56,56	2.29	24 (42%)
26	CLA	7	608	-	50,58,73	1.71	11 (22%)	58,95,113	1.45	9 (15%)
26	CLA	5	619	-	43,51,73	1.91	9 (20%)	54,87,113	1.60	10 (18%)
29	BCR	B	845	-	41,41,41	0.93	1 (2%)	56,56,56	2.50	23 (41%)
26	CLA	B	813	-	65,73,73	1.52	10 (15%)	76,113,113	1.31	8 (10%)
28	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	0.87	2 (3%)
26	CLA	1	608	-	43,52,73	1.83	8 (18%)	49,88,113	1.45	8 (16%)
37	CHL	W	601	23	66,74,74	1.97	16 (24%)	73,114,114	2.57	21 (28%)
35	XAT	W	1622	-	39,47,47	0.92	1 (2%)	54,74,74	4.26	25 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CHL	Z	608	-	49,57,74	2.23	16 (32%)	52,93,114	3.07	19 (36%)
26	CLA	A	819	-	59,67,73	1.53	11 (18%)	68,105,113	1.50	6 (8%)
26	CLA	8	616	21	43,51,73	1.88	6 (13%)	54,87,113	1.53	11 (20%)
26	CLA	Y	612	24	45,53,73	1.85	7 (15%)	52,89,113	1.48	7 (13%)
32	LMG	J	104	-	40,40,55	1.02	2 (5%)	48,48,63	1.30	6 (12%)
26	CLA	B	838	-	46,54,73	1.74	7 (15%)	53,90,113	1.58	7 (13%)
26	CLA	L	304	-	45,53,73	1.76	9 (20%)	52,89,113	1.45	8 (15%)
35	XAT	2	620	-	39,47,47	1.05	2 (5%)	54,74,74	2.48	26 (48%)
26	CLA	B	837	-	65,73,73	1.54	10 (15%)	76,113,113	1.39	10 (13%)
26	CLA	W	602	23	60,68,73	1.58	7 (11%)	70,107,113	1.33	9 (12%)
26	CLA	A	802	-	65,73,73	1.48	10 (15%)	76,113,113	1.55	10 (13%)
26	CLA	9	613	22	65,73,73	1.51	9 (13%)	76,113,113	1.35	8 (10%)
26	CLA	8	613	21	65,73,73	1.53	9 (13%)	76,113,113	1.25	7 (9%)
37	CHL	U	605	24	43,51,74	2.41	15 (34%)	45,86,114	3.09	18 (40%)
28	LHG	W	2630	26	33,33,48	1.13	2 (6%)	36,39,54	1.17	3 (8%)
26	CLA	1	610	14	38,47,73	1.89	7 (18%)	44,81,113	1.62	8 (18%)
26	CLA	8	603	-	44,52,73	1.86	8 (18%)	55,88,113	1.65	8 (14%)
26	CLA	4	613	17	65,73,73	1.56	9 (13%)	76,113,113	1.34	10 (13%)
32	LMG	A	860	-	40,40,55	1.00	2 (5%)	48,48,63	1.09	4 (8%)
26	CLA	W	604	-	47,55,73	1.80	6 (12%)	54,91,113	1.48	7 (12%)
34	LUT	U	1620	-	42,43,43	0.74	0	51,60,60	1.60	10 (19%)
37	CHL	X	609	23	66,74,74	1.95	16 (24%)	73,114,114	2.72	23 (31%)
28	LHG	8	623	-	39,39,48	1.03	2 (5%)	42,45,54	1.07	2 (4%)
26	CLA	B	840	-	65,73,73	1.58	11 (16%)	76,113,113	1.39	8 (10%)
31	LMU	A	858	-	34,35,36	1.26	4 (11%)	42,45,47	0.99	2 (4%)
26	CLA	3	602	16	60,68,73	1.55	9 (15%)	70,107,113	1.33	10 (14%)
26	CLA	B	836	-	50,58,73	1.63	9 (18%)	58,95,113	1.72	8 (13%)
26	CLA	X	614	-	42,50,73	1.87	7 (16%)	48,85,113	1.46	7 (14%)
26	CLA	4	611	28	42,50,73	1.78	8 (19%)	48,85,113	1.54	7 (14%)
26	CLA	A	808	-	50,58,73	1.67	10 (20%)	58,95,113	1.53	8 (13%)
26	CLA	4	618	17	39,48,73	1.95	7 (17%)	48,83,113	1.54	8 (16%)
26	CLA	A	811	-	65,73,73	1.52	10 (15%)	76,113,113	1.36	8 (10%)
26	CLA	B	829	-	65,73,73	1.55	10 (15%)	76,113,113	1.50	10 (13%)
26	CLA	1	612	14	45,53,73	1.79	8 (17%)	52,89,113	1.51	6 (11%)
26	CLA	5	611	28	42,50,73	1.81	6 (14%)	48,85,113	1.44	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	A	809	1	65,73,73	1.48	11 (16%)	76,113,113	1.43	8 (10%)
26	CLA	7	614	-	42,50,73	1.80	9 (21%)	48,85,113	1.45	6 (12%)
26	CLA	a	616	14	45,53,73	1.78	6 (13%)	52,89,113	1.59	7 (13%)
26	CLA	Z	612	24	45,53,73	1.82	7 (15%)	52,89,113	1.45	7 (13%)
26	CLA	A	840	-	52,60,73	1.64	11 (21%)	60,97,113	1.56	8 (13%)
35	XAT	a	618	-	39,47,47	0.90	0	54,74,74	2.47	21 (38%)
26	CLA	5	613	18	64,72,73	1.48	9 (14%)	74,111,113	1.37	9 (12%)
26	CLA	B	831	-	65,73,73	1.49	9 (13%)	76,113,113	1.30	8 (10%)
26	CLA	V	604	-	50,58,73	1.70	7 (14%)	58,95,113	1.52	7 (12%)
26	CLA	6	612	19	40,49,73	1.85	8 (20%)	45,84,113	1.44	7 (15%)
26	CLA	6	614	-	60,68,73	1.56	8 (13%)	70,107,113	1.32	9 (12%)
34	LUT	V	1621	-	42,43,43	0.79	0	51,60,60	1.99	16 (31%)
29	BCR	K	207	-	41,41,41	0.85	1 (2%)	56,56,56	2.72	21 (37%)
26	CLA	L	306	-	39,48,73	1.88	9 (23%)	44,83,113	1.53	6 (13%)
26	CLA	Z	613	24	65,73,73	1.51	7 (10%)	76,113,113	1.28	6 (7%)
26	CLA	X	613	23	65,73,73	1.51	7 (10%)	76,113,113	1.25	8 (10%)
26	CLA	4	601	17	65,73,73	1.49	10 (15%)	76,113,113	1.36	8 (10%)
26	CLA	a	611	28	37,46,73	1.99	8 (21%)	46,81,113	1.58	11 (23%)
29	BCR	B	852	-	41,41,41	0.82	0	56,56,56	4.21	30 (53%)
37	CHL	X	605	-	46,54,74	2.45	16 (34%)	49,90,114	2.96	18 (36%)
26	CLA	A	839	-	55,63,73	1.66	11 (20%)	64,101,113	1.41	9 (14%)
26	CLA	7	611	28	59,67,73	1.55	10 (16%)	68,105,113	1.32	8 (11%)
35	XAT	V	1622	-	39,47,47	0.87	0	54,74,74	2.68	20 (37%)
26	CLA	A	824	-	65,73,73	1.47	10 (15%)	76,113,113	1.41	8 (10%)
26	CLA	1	606	-	37,47,73	1.96	9 (24%)	41,80,113	1.54	7 (17%)
37	CHL	V	606	-	44,52,74	2.17	14 (31%)	46,87,114	3.18	21 (45%)
26	CLA	A	810	1	50,58,73	1.73	9 (18%)	58,95,113	1.52	10 (17%)
26	CLA	U	603	-	52,60,73	1.67	7 (13%)	60,97,113	1.48	9 (15%)
26	CLA	7	609	20	43,52,73	1.84	10 (23%)	48,87,113	1.41	6 (12%)
29	BCR	6	622	-	41,41,41	0.75	0	56,56,56	2.46	25 (44%)
35	XAT	U	1622	-	39,47,47	0.92	1 (2%)	54,74,74	4.40	22 (40%)
37	CHL	Y	607	-	66,74,74	1.86	14 (21%)	73,114,114	2.67	19 (26%)
26	CLA	a	601	14	53,62,73	1.65	9 (16%)	61,100,113	1.31	8 (13%)
30	SF4	A	853	2,1	0,12,12	-	-	-	-	-
37	CHL	X	607	-	66,74,74	1.85	14 (21%)	73,114,114	2.75	20 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	2	611	28	42,50,73	1.81	7 (16%)	48,85,113	1.50	7 (14%)
34	LUT	W	1620	-	42,43,43	0.72	0	51,60,60	1.59	11 (21%)
32	LMG	4	624	-	40,40,55	1.03	2 (5%)	48,48,63	1.15	5 (10%)
29	BCR	L	301	-	41,41,41	0.80	0	56,56,56	2.26	24 (42%)
26	CLA	A	829	-	65,73,73	1.48	8 (12%)	76,113,113	1.55	8 (10%)
34	LUT	8	619	-	42,43,43	0.86	1 (2%)	51,60,60	1.87	11 (21%)
26	CLA	5	616	18	41,50,73	1.90	10 (24%)	50,85,113	1.47	8 (16%)
26	CLA	X	610	23	65,73,73	1.55	7 (10%)	76,113,113	1.26	7 (9%)
26	CLA	8	601	21	65,73,73	1.57	9 (13%)	76,113,113	1.26	7 (9%)
37	CHL	V	607	-	46,54,74	2.29	16 (34%)	49,90,114	3.02	20 (40%)
32	LMG	8	626	-	46,46,55	0.97	2 (4%)	54,54,63	1.10	4 (7%)
36	NEX	6	624	-	38,46,46	1.13	3 (7%)	50,70,70	2.40	18 (36%)
37	CHL	Y	609	24	66,74,74	1.92	14 (21%)	73,114,114	2.67	22 (30%)
26	CLA	A	842	-	65,73,73	1.54	11 (16%)	76,113,113	1.48	10 (13%)
26	CLA	2	616	-	43,51,73	1.88	8 (18%)	54,87,113	1.52	8 (14%)
26	CLA	Y	613	24	65,73,73	1.51	7 (10%)	76,113,113	1.30	7 (9%)
37	CHL	U	608	-	44,52,74	2.22	13 (29%)	46,87,114	3.32	19 (41%)
29	BCR	L	308	-	41,41,41	0.81	0	56,56,56	2.33	23 (41%)
26	CLA	A	822	-	65,73,73	1.51	10 (15%)	76,113,113	1.45	10 (13%)
26	CLA	3	610	16	65,73,73	1.55	9 (13%)	76,113,113	1.22	7 (9%)
26	CLA	B	827	-	62,70,73	1.51	10 (16%)	72,109,113	1.49	9 (12%)
28	LHG	7	622	26	36,36,48	1.05	2 (5%)	39,42,54	1.02	3 (7%)
26	CLA	B	826	-	62,70,73	1.52	9 (14%)	72,109,113	1.56	8 (11%)
26	CLA	7	612	20	44,52,73	1.78	7 (15%)	51,88,113	1.46	6 (11%)
26	CLA	2	607	-	43,52,73	1.81	9 (20%)	49,88,113	1.48	8 (16%)
26	CLA	U	610	24	56,64,73	1.57	7 (12%)	65,102,113	1.44	8 (12%)
28	LHG	H	204	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)
34	LUT	a	617	-	42,43,43	0.80	1 (2%)	51,60,60	1.90	16 (31%)
29	BCR	7	623	-	41,41,41	0.87	0	56,56,56	2.01	17 (30%)
37	CHL	U	609	24	60,68,74	2.01	14 (23%)	65,106,114	2.79	22 (33%)
26	CLA	9	611	28	42,50,73	1.88	7 (16%)	48,85,113	1.43	5 (10%)
26	CLA	A	831	-	65,73,73	1.52	10 (15%)	76,113,113	1.37	9 (11%)
26	CLA	9	607	-	45,53,73	1.78	9 (20%)	52,89,113	1.38	7 (13%)
37	CHL	Y	606	-	46,54,74	2.24	15 (32%)	49,90,114	3.12	18 (36%)
26	CLA	8	607	-	41,49,73	1.91	8 (19%)	51,84,113	1.53	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	4	602	17	60,68,73	1.63	8 (13%)	70,107,113	1.32	8 (11%)
29	BCR	3	621	-	41,41,41	0.83	1 (2%)	56,56,56	1.84	15 (26%)
34	LUT	6	619	-	42,43,43	0.77	1 (2%)	51,60,60	2.07	18 (35%)
37	CHL	Z	606	-	46,54,74	2.29	16 (34%)	49,90,114	3.16	21 (42%)
37	CHL	W	605	23	46,54,74	2.31	17 (36%)	49,90,114	3.20	19 (38%)
28	LHG	9	622	26	29,29,48	1.18	2 (6%)	32,35,54	1.02	1 (3%)
26	CLA	5	601	18	56,64,73	1.59	8 (14%)	65,102,113	1.44	8 (12%)
35	XAT	Y	1622	-	39,47,47	0.92	0	54,74,74	2.75	22 (40%)
26	CLA	A	823	-	42,50,73	1.79	8 (19%)	48,85,113	1.56	7 (14%)
26	CLA	8	611	28	42,50,73	1.83	10 (23%)	48,85,113	1.44	7 (14%)
26	CLA	a	607	-	45,53,73	1.87	9 (20%)	52,89,113	1.35	7 (13%)
29	BCR	B	843	-	41,41,41	1.04	4 (9%)	56,56,56	1.94	18 (32%)
26	CLA	2	609	15	45,53,73	1.86	9 (20%)	52,89,113	1.39	8 (15%)
31	LMU	5	629	-	33,33,36	1.21	2 (6%)	44,44,47	1.27	6 (13%)
26	CLA	U	614	-	42,50,73	1.83	6 (14%)	48,85,113	1.55	7 (14%)
26	CLA	A	814	-	65,73,73	1.47	11 (16%)	76,113,113	1.54	10 (13%)
26	CLA	9	609	22	61,69,73	1.54	10 (16%)	71,108,113	1.35	7 (9%)
26	CLA	8	609	21	45,53,73	1.78	8 (17%)	52,89,113	1.53	7 (13%)
26	CLA	O	2002	-	37,46,73	1.99	8 (21%)	46,81,113	1.62	9 (19%)
36	NEX	Y	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.52	16 (32%)
37	CHL	W	608	-	47,55,74	2.26	15 (31%)	50,91,114	3.07	17 (34%)
28	LHG	Y	2630	26	48,48,48	0.92	2 (4%)	51,54,54	1.01	2 (3%)
26	CLA	A	818	-	60,68,73	1.52	9 (15%)	70,107,113	1.44	8 (11%)
28	LHG	3	624	26	48,48,48	0.91	2 (4%)	51,54,54	0.97	3 (5%)
26	CLA	a	609	14	63,72,73	1.51	9 (14%)	73,112,113	1.29	8 (10%)
26	CLA	1	607	-	39,48,73	1.99	9 (23%)	44,83,113	1.40	7 (15%)
26	CLA	O	2001	-	36,46,73	1.99	9 (25%)	41,80,113	1.49	6 (14%)
26	CLA	8	608	-	51,59,73	1.68	11 (21%)	59,96,113	1.53	8 (13%)
26	CLA	X	611	28	45,53,73	1.81	6 (13%)	52,89,113	1.43	6 (11%)
26	CLA	O	2003	-	39,48,73	1.87	9 (23%)	44,83,113	1.46	6 (13%)
26	CLA	A	833	-	45,53,73	1.77	9 (20%)	52,89,113	1.72	11 (21%)
37	CHL	X	608	-	66,73,74	1.98	14 (21%)	68,112,114	2.63	18 (26%)
26	CLA	3	607	16	56,64,73	1.64	8 (14%)	69,102,113	1.39	10 (14%)
26	CLA	A	825	-	65,73,73	1.49	10 (15%)	76,113,113	1.31	8 (10%)
35	XAT	9	620	-	39,47,47	0.99	2 (5%)	54,74,74	2.51	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	V	614	-	45,53,73	1.81	7 (15%)	52,89,113	1.49	7 (13%)
26	CLA	3	611	28	37,46,73	1.98	7 (18%)	46,81,113	1.54	7 (15%)
26	CLA	6	603	-	51,59,73	1.71	8 (15%)	63,96,113	1.53	9 (14%)
26	CLA	B	820	-	50,58,73	1.69	9 (18%)	58,95,113	1.51	7 (12%)
26	CLA	L	303	-	65,73,73	1.49	10 (15%)	76,113,113	1.37	10 (13%)
29	BCR	J	102	-	41,41,41	0.93	2 (4%)	56,56,56	2.40	22 (39%)
26	CLA	4	614	-	56,64,73	1.61	7 (12%)	65,102,113	1.37	8 (12%)
26	CLA	6	602	19	65,73,73	1.53	9 (13%)	76,113,113	1.24	9 (11%)
37	CHL	U	606	-	44,52,74	2.18	15 (34%)	46,87,114	3.21	18 (39%)
34	LUT	5	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.91	15 (29%)
26	CLA	A	804	-	65,73,73	1.45	11 (16%)	76,113,113	1.38	9 (11%)
26	CLA	a	603	-	54,62,73	1.61	8 (14%)	62,99,113	1.48	7 (11%)
34	LUT	3	618	-	42,43,43	0.83	1 (2%)	51,60,60	2.01	12 (23%)
29	BCR	B	847	-	41,41,41	0.92	2 (4%)	56,56,56	2.20	16 (28%)
26	CLA	A	816	-	65,73,73	1.48	10 (15%)	76,113,113	1.40	9 (11%)
34	LUT	Y	1621	-	42,43,43	0.87	1 (2%)	51,60,60	1.87	14 (27%)
32	LMG	4	623	-	40,40,55	1.07	2 (5%)	48,48,63	1.15	5 (10%)
26	CLA	3	613	16	52,61,73	1.70	9 (17%)	59,98,113	1.30	6 (10%)
28	LHG	5	625	-	48,48,48	0.91	2 (4%)	51,54,54	1.02	3 (5%)
26	CLA	B	804	-	41,49,73	1.80	9 (21%)	47,84,113	1.56	6 (12%)
26	CLA	5	618	18	39,48,73	1.94	8 (20%)	48,83,113	1.57	9 (18%)
29	BCR	A	852	-	41,41,41	0.97	1 (2%)	56,56,56	2.56	26 (46%)
26	CLA	7	601	20	60,68,73	1.54	10 (16%)	70,107,113	1.48	8 (11%)
26	CLA	5	603	-	54,62,73	1.69	10 (18%)	67,100,113	1.48	9 (13%)
26	CLA	K	204	-	45,53,73	1.75	10 (22%)	52,89,113	1.61	7 (13%)
26	CLA	7	607	-	42,50,73	1.82	10 (23%)	48,85,113	1.39	7 (14%)
26	CLA	3	603	-	55,63,73	1.60	11 (20%)	64,101,113	1.52	8 (12%)
26	CLA	B	808	-	65,73,73	1.54	10 (15%)	76,113,113	1.32	11 (14%)
26	CLA	B	824	-	65,73,73	1.49	10 (15%)	76,113,113	1.29	7 (9%)
26	CLA	F	303	-	42,50,73	1.86	10 (23%)	48,85,113	1.55	7 (14%)
37	CHL	V	601	25	66,74,74	1.94	16 (24%)	73,114,114	2.60	20 (27%)
26	CLA	9	604	-	50,58,73	1.76	8 (16%)	62,95,113	1.45	9 (14%)
26	CLA	B	825	-	49,57,73	1.69	9 (18%)	55,93,113	1.56	9 (16%)
26	CLA	7	615	-	41,50,73	1.91	8 (19%)	50,85,113	1.60	7 (14%)
35	XAT	1	618	-	39,47,47	0.91	0	54,74,74	2.46	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	B	848	-	41,41,41	0.84	1 (2%)	56,56,56	2.53	14 (25%)
26	CLA	9	610	22	57,65,73	1.67	8 (14%)	66,103,113	1.35	9 (13%)
26	CLA	5	609	18	65,73,73	1.55	10 (15%)	76,113,113	1.32	8 (10%)
26	CLA	V	602	25	60,68,73	1.53	7 (11%)	70,107,113	1.42	8 (11%)
26	CLA	W	603	-	52,60,73	1.64	6 (11%)	60,97,113	1.57	8 (13%)
26	CLA	A	854	-	65,73,73	1.52	10 (15%)	76,113,113	1.52	8 (10%)
26	CLA	B	817	-	59,67,73	1.59	11 (18%)	68,105,113	1.41	7 (10%)
28	LHG	A	847	26	29,29,48	1.16	2 (6%)	32,35,54	1.04	3 (9%)
26	CLA	U	612	24	42,50,73	1.84	5 (11%)	48,85,113	1.60	7 (14%)
26	CLA	F	301	-	57,65,73	1.62	9 (15%)	66,103,113	1.30	7 (10%)
26	CLA	W	610	23	55,63,73	1.62	5 (9%)	64,101,113	1.43	10 (15%)
26	CLA	8	602	21	60,68,73	1.57	7 (11%)	70,107,113	1.50	9 (12%)
26	CLA	B	806	2	65,73,73	1.48	12 (18%)	76,113,113	1.50	11 (14%)
26	CLA	1	601	14	53,62,73	1.64	9 (16%)	61,100,113	1.30	8 (13%)
26	CLA	4	610	17	61,69,73	1.53	7 (11%)	71,108,113	1.39	8 (11%)
26	CLA	B	803	-	65,73,73	1.45	11 (16%)	76,113,113	1.41	6 (7%)
26	CLA	K	201	11	45,53,73	1.76	8 (17%)	52,89,113	1.37	7 (13%)
29	BCR	1	619	-	41,41,41	0.83	0	56,56,56	2.38	22 (39%)
34	LUT	Z	1621	-	42,43,43	0.79	0	51,60,60	1.41	8 (15%)
37	CHL	W	609	23	66,74,74	1.98	15 (22%)	73,114,114	2.64	20 (27%)
35	XAT	3	619	-	39,47,47	0.98	2 (5%)	54,74,74	2.60	19 (35%)
29	BCR	3	620	-	41,41,41	0.80	0	56,56,56	2.38	23 (41%)
26	CLA	4	616	17	43,51,73	1.90	8 (18%)	54,87,113	1.48	7 (12%)
26	CLA	V	613	25	65,73,73	1.49	7 (10%)	76,113,113	1.28	6 (7%)
26	CLA	B	807	-	52,60,73	1.71	11 (21%)	60,97,113	1.48	9 (15%)
26	CLA	5	606	-	39,48,73	1.95	9 (23%)	44,83,113	1.38	5 (11%)
37	CHL	Z	601	24	66,74,74	1.89	16 (24%)	73,114,114	2.67	19 (26%)
29	BCR	B	853	-	41,41,41	0.87	3 (7%)	56,56,56	1.81	14 (25%)
26	CLA	2	603	15	43,52,73	1.88	10 (23%)	49,88,113	1.39	7 (14%)
37	CHL	X	606	-	44,52,74	2.29	14 (31%)	46,87,114	3.19	18 (39%)
26	CLA	U	613	24	59,67,73	1.61	7 (11%)	68,105,113	1.33	9 (13%)
26	CLA	3	617	16	39,48,73	1.86	9 (23%)	44,83,113	1.58	7 (15%)
26	CLA	A	827	-	58,66,73	1.58	10 (17%)	67,104,113	1.32	7 (10%)
26	CLA	3	604	-	65,73,73	1.50	10 (15%)	76,113,113	1.32	9 (11%)
26	CLA	V	603	-	45,53,73	1.79	6 (13%)	52,89,113	1.63	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	A	848	-	41,41,41	1.01	3 (7%)	56,56,56	2.24	14 (25%)
26	CLA	1	602	14	61,69,73	1.54	7 (11%)	71,108,113	1.44	8 (11%)
28	LHG	6	623	26	47,47,48	0.91	2 (4%)	50,53,54	0.96	3 (6%)
29	BCR	5	622	-	41,41,41	0.87	2 (4%)	56,56,56	2.31	19 (33%)
29	BCR	B	801	-	41,41,41	0.94	1 (2%)	56,56,56	2.10	18 (32%)
29	BCR	B	844	-	41,41,41	1.08	4 (9%)	56,56,56	2.60	26 (46%)
36	NEX	U	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.60	20 (40%)
26	CLA	1	611	28	57,65,73	1.60	7 (12%)	66,103,113	1.31	9 (13%)
28	LHG	4	622	26	48,48,48	0.91	2 (4%)	51,54,54	0.82	2 (3%)
29	BCR	L	309	-	41,41,41	0.78	0	56,56,56	2.40	25 (44%)
26	CLA	a	610	14	59,67,73	1.55	7 (11%)	69,106,113	1.31	7 (10%)
26	CLA	Z	604	-	50,57,73	1.80	8 (16%)	53,93,113	1.57	8 (15%)
26	CLA	7	606	-	41,49,73	1.84	9 (21%)	47,84,113	1.44	6 (12%)
29	BCR	9	621	-	41,41,41	0.76	1 (2%)	56,56,56	2.90	18 (32%)
26	CLA	A	807	1	65,73,73	1.52	11 (16%)	76,113,113	1.36	7 (9%)
26	CLA	Y	603	-	55,63,73	1.64	8 (14%)	64,101,113	1.51	9 (14%)
26	CLA	6	613	-	63,72,73	1.59	10 (15%)	73,112,113	1.31	9 (12%)
37	CHL	V	605	25	44,52,74	2.32	15 (34%)	46,87,114	3.17	17 (36%)
26	CLA	6	611	28	42,50,73	1.82	7 (16%)	48,85,113	1.44	6 (12%)
26	CLA	F	304	6	41,49,73	1.91	10 (24%)	47,84,113	1.52	8 (17%)
26	CLA	G	204	7	45,53,73	1.82	8 (17%)	52,89,113	1.45	7 (13%)
26	CLA	3	608	-	55,63,73	1.67	11 (20%)	64,101,113	1.27	6 (9%)
26	CLA	9	614	-	45,53,73	1.84	8 (17%)	52,89,113	1.35	7 (13%)
26	CLA	Y	602	24	58,66,73	1.58	7 (12%)	67,104,113	1.40	9 (13%)
26	CLA	8	612	21	40,49,73	1.85	9 (22%)	45,84,113	1.51	6 (13%)
26	CLA	3	615	-	39,48,73	1.87	9 (23%)	44,83,113	1.47	6 (13%)
26	CLA	8	614	-	53,61,73	1.64	9 (16%)	61,98,113	1.43	8 (13%)
26	CLA	W	612	23	45,53,73	1.80	9 (20%)	52,89,113	1.55	8 (15%)
26	CLA	W	614	-	45,53,73	1.80	6 (13%)	52,89,113	1.56	6 (11%)
26	CLA	G	203	-	42,50,73	1.82	9 (21%)	48,85,113	1.53	8 (16%)
26	CLA	a	612	14	45,53,73	1.80	8 (17%)	52,89,113	1.51	6 (11%)
26	CLA	a	614	-	55,62,73	1.72	8 (14%)	60,99,113	1.46	7 (11%)
26	CLA	6	618	19	39,48,73	1.92	9 (23%)	48,83,113	1.60	8 (16%)
26	CLA	5	610	18	54,62,73	1.69	9 (16%)	62,99,113	1.30	7 (11%)
26	CLA	4	603	17	44,52,73	1.84	9 (20%)	55,88,113	1.54	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	5	612	18	40,49,73	1.85	7 (17%)	45,84,113	1.49	6 (13%)
37	CHL	V	609	25	61,69,74	2.00	15 (24%)	67,108,114	2.83	21 (31%)
29	BCR	L	305	-	41,41,41	0.89	0	56,56,56	2.52	25 (44%)
26	CLA	Y	604	-	50,58,73	1.77	8 (16%)	58,95,113	1.41	6 (10%)
35	XAT	4	620	-	39,47,47	0.94	2 (5%)	54,74,74	2.49	24 (44%)
26	CLA	Y	614	-	48,56,73	1.75	6 (12%)	55,92,113	1.42	8 (14%)
26	CLA	2	612	15	44,52,73	1.80	8 (18%)	51,88,113	1.42	6 (11%)
26	CLA	X	612	23	43,51,73	1.83	7 (16%)	49,86,113	1.50	8 (16%)
26	CLA	4	604	-	54,62,73	1.67	8 (14%)	67,100,113	1.46	10 (14%)
28	LHG	a	620	26	42,42,48	0.98	2 (4%)	45,48,54	0.82	2 (4%)
26	CLA	4	609	17	57,65,73	1.61	9 (15%)	66,103,113	1.24	6 (9%)
26	CLA	9	612	22	40,49,73	1.90	6 (15%)	45,84,113	1.41	6 (13%)
26	CLA	B	805	-	65,73,73	1.47	11 (16%)	76,113,113	1.40	9 (11%)
35	XAT	7	620	-	39,47,47	0.99	2 (5%)	54,74,74	2.50	18 (33%)
26	CLA	H	203	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	8 (10%)
26	CLA	6	601	19	65,73,73	1.48	10 (15%)	76,113,113	1.24	8 (10%)
26	CLA	X	603	-	62,70,73	1.56	6 (9%)	72,109,113	1.40	8 (11%)
26	CLA	X	604	-	49,57,73	1.78	5 (10%)	55,93,113	1.43	7 (12%)
26	CLA	6	608	-	45,53,73	1.83	9 (20%)	52,89,113	1.46	8 (15%)
26	CLA	5	604	-	63,71,73	1.59	8 (12%)	78,111,113	1.33	10 (12%)
26	CLA	7	602	20	65,73,73	1.57	10 (15%)	76,113,113	1.26	8 (10%)
26	CLA	2	610	15	55,63,73	1.66	9 (16%)	64,101,113	1.30	8 (12%)
34	LUT	V	1620	-	42,43,43	0.75	0	51,60,60	1.65	10 (19%)
26	CLA	A	820	-	65,73,73	1.48	11 (16%)	76,113,113	1.42	9 (11%)
26	CLA	3	614	-	39,48,73	1.93	9 (23%)	44,83,113	1.52	6 (13%)
26	CLA	4	607	-	45,53,73	1.84	9 (20%)	52,89,113	1.43	7 (13%)
37	CHL	Y	605	24	42,50,74	2.50	17 (40%)	44,85,114	3.27	20 (45%)
32	LMG	5	627	-	40,40,55	1.03	2 (5%)	48,48,63	1.02	3 (6%)
29	BCR	2	623	-	41,41,41	0.86	1 (2%)	56,56,56	2.36	20 (35%)
26	CLA	A	834	-	65,73,73	1.50	10 (15%)	76,113,113	1.47	8 (10%)
26	CLA	B	833	-	65,73,73	1.49	10 (15%)	76,113,113	1.28	8 (10%)
26	CLA	A	838	-	50,58,73	1.65	11 (22%)	58,95,113	1.54	9 (15%)
26	CLA	B	835	-	45,53,73	1.77	10 (22%)	52,89,113	1.50	7 (13%)
29	BCR	B	849	-	41,41,41	0.93	2 (4%)	56,56,56	2.53	19 (33%)
26	CLA	K	206	11	45,53,73	1.84	8 (17%)	52,89,113	1.39	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LUT	2	619	-	42,43,43	0.91	2 (4%)	51,60,60	1.95	14 (27%)
28	LHG	8	622	26	48,48,48	0.91	2 (4%)	51,54,54	0.86	2 (3%)
26	CLA	2	601	15	65,73,73	1.43	9 (13%)	76,113,113	1.48	7 (9%)
37	CHL	X	601	23	66,74,74	1.89	16 (24%)	73,114,114	2.64	25 (34%)
28	LHG	B	851	26	37,37,48	1.04	2 (5%)	40,43,54	1.14	4 (10%)
31	LMU	1	621	-	36,36,36	1.15	2 (5%)	47,47,47	1.00	1 (2%)
26	CLA	2	602	15	58,69,73	1.14	6 (10%)	69,102,113	1.04	4 (5%)
26	CLA	B	802	-	65,73,73	1.47	11 (16%)	76,113,113	1.33	8 (10%)
26	CLA	a	613	-	54,62,73	1.62	9 (16%)	62,99,113	1.43	6 (9%)
26	CLA	A	826	-	64,72,73	1.47	8 (12%)	74,111,113	1.45	7 (9%)
26	CLA	9	606	-	39,48,73	1.90	9 (23%)	44,83,113	1.50	6 (13%)
26	CLA	A	832	-	50,58,73	1.75	11 (22%)	58,95,113	1.59	10 (17%)
26	CLA	7	610	20	65,73,73	1.56	9 (13%)	76,113,113	1.19	7 (9%)
28	LHG	U	2630	26	48,48,48	0.94	2 (4%)	51,54,54	1.08	4 (7%)
26	CLA	8	604	-	50,58,73	1.68	7 (14%)	58,95,113	1.59	9 (15%)
26	CLA	8	606	-	64,72,73	1.53	9 (14%)	75,112,113	1.18	8 (10%)
26	CLA	V	611	28	43,51,73	1.86	7 (16%)	49,86,113	1.43	6 (12%)
35	XAT	X	1622	-	39,47,47	0.87	0	54,74,74	2.63	20 (37%)
26	CLA	1	613	-	65,73,73	1.48	9 (13%)	76,113,113	1.31	6 (7%)
28	LHG	Z	2630	26	48,48,48	0.92	2 (4%)	51,54,54	0.97	2 (3%)
26	CLA	A	806	-	65,73,73	1.50	12 (18%)	76,113,113	1.54	11 (14%)
26	CLA	A	835	-	61,69,73	1.55	11 (18%)	71,108,113	1.35	9 (12%)
28	LHG	5	623	26	48,48,48	0.93	2 (4%)	51,54,54	0.87	2 (3%)
37	CHL	Z	605	24	42,50,74	2.37	15 (35%)	44,85,114	3.42	20 (45%)
32	LMG	9	625	-	55,55,55	0.88	2 (3%)	63,63,63	1.03	6 (9%)

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
31	LMU	A	857	-	-	9/21/61/61	0/2/2/2
30	SF4	C	101	3	-	-	0/6/5/5
28	LHG	9	623	-	-	20/53/53/53	-
26	CLA	5	607	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	801	-	1/1/15/20	10/37/115/115	-
37	CHL	W	606	-	3/3/16/26	2/15/113/137	-
29	BCR	3	622	-	-	3/29/63/63	0/2/2/2
34	LUT	Y	1620	-	-	5/29/67/67	0/2/2/2
37	CHL	Z	607	-	3/3/20/26	21/39/137/137	-
26	CLA	Z	611	28	1/1/10/20	5/11/87/115	-
26	CLA	A	841	-	1/1/15/20	16/37/115/115	-
26	CLA	W	613	23	1/1/15/20	20/37/115/115	-
37	CHL	W	607	-	3/3/20/26	21/37/135/137	-
28	LHG	1	620	26	-	9/53/53/53	-
28	LHG	A	861	-	-	18/53/53/53	-
36	NEX	V	1623	-	-	7/27/83/83	0/3/3/3
36	NEX	5	624	-	-	2/27/83/83	0/3/3/3
26	CLA	3	612	16	1/1/10/20	5/11/89/115	-
26	CLA	B	810	-	1/1/14/20	20/35/113/115	-
29	BCR	A	849	-	-	5/29/63/63	0/2/2/2
26	CLA	B	815	-	1/1/10/20	2/11/89/115	-
26	CLA	3	609	16	1/1/14/20	12/31/109/115	-
26	CLA	6	610	19	1/1/15/20	10/37/115/115	-
29	BCR	4	621	-	-	2/29/63/63	0/2/2/2
26	CLA	1	616	14	1/1/11/20	7/11/87/115	-
26	CLA	A	817	-	-	0/13/91/115	-
26	CLA	9	603	22	1/1/11/20	5/13/89/115	-
26	CLA	A	805	-	-	7/22/100/115	-
26	CLA	A	845	28	1/1/12/20	7/19/97/115	-
35	XAT	8	620	-	-	0/31/93/93	0/4/4/4
29	BCR	7	621	-	-	2/29/63/63	0/2/2/2
26	CLA	B	839	-	1/1/15/20	14/37/115/115	-
31	LMU	K	208	-	-	10/21/61/61	0/2/2/2
26	CLA	2	613	15	1/1/15/20	8/37/115/115	-
34	LUT	U	1621	-	-	5/29/67/67	0/2/2/2
28	LHG	2	622	26	-	9/40/40/53	-
32	LMG	H	205	-	-	14/50/70/70	0/1/1/1
26	CLA	6	617	-	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	1	603	-	1/1/12/20	5/21/99/115	-
28	LHG	O	2631	-	-	13/40/40/53	-
34	LUT	Z	1620	-	-	5/29/67/67	0/2/2/2
37	CHL	Y	601	24	3/3/20/26	19/39/137/137	-
29	BCR	F	305	-	-	6/29/63/63	0/2/2/2
26	CLA	B	816	-	1/1/12/20	10/23/101/115	-
32	LMG	L	2631	-	-	4/32/52/70	0/1/1/1
26	CLA	1	609	14	1/1/10/20	3/8/84/115	-
26	CLA	K	203	-	-	10/27/105/115	-
26	CLA	5	617	-	1/1/12/20	10/19/97/115	-
26	CLA	a	608	-	1/1/11/20	2/11/89/115	-
26	CLA	V	612	25	1/1/11/20	5/13/91/115	-
26	CLA	9	601	22	1/1/11/20	6/13/91/115	-
26	CLA	B	830	-	1/1/10/20	2/11/89/115	-
28	LHG	9	624	-	-	17/53/53/53	-
26	CLA	4	608	-	1/1/15/20	9/37/115/115	-
26	CLA	4	612	17	1/1/10/20	4/8/86/115	-
34	LUT	4	619	-	-	4/29/67/67	0/2/2/2
26	CLA	W	611	28	1/1/13/20	7/28/106/115	-
28	LHG	3	623	-	-	15/49/49/53	-
26	CLA	B	812	-	1/1/10/20	3/11/89/115	-
26	CLA	2	614	-	1/1/10/20	0/9/87/115	-
26	CLA	V	610	25	1/1/14/20	7/34/112/115	-
26	CLA	U	604	-	1/1/10/20	7/18/92/115	-
26	CLA	B	822	-	-	7/10/88/115	-
28	LHG	X	2630	26	-	13/53/53/53	-
29	BCR	K	202	-	-	4/29/63/63	0/2/2/2
26	CLA	8	610	21	1/1/14/20	9/31/109/115	-
26	CLA	L	302	12	1/1/11/20	8/13/91/115	-
26	CLA	B	809	2	1/1/15/20	11/37/115/115	-
37	CHL	Y	608	-	3/3/16/26	6/19/117/137	-
26	CLA	2	606	-	1/1/10/20	3/11/89/115	-
27	PQN	A	844	-	-	6/23/43/43	0/2/2/2
26	CLA	A	815	-	1/1/12/20	10/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	Z	603	-	1/1/13/20	9/25/103/115	-
26	CLA	1	604	-	1/1/11/20	7/18/96/115	-
34	LUT	1	617	-	-	4/29/67/67	0/2/2/2
35	XAT	Z	1622	-	-	4/31/93/93	0/4/4/4
34	LUT	X	1620	-	-	4/29/67/67	0/2/2/2
26	CLA	6	607	-	1/1/10/20	2/10/86/115	-
26	CLA	5	608	-	1/1/12/20	4/19/97/115	-
26	CLA	Z	602	24	1/1/13/20	5/29/107/115	-
26	CLA	A	812	-	1/1/15/20	7/37/115/115	-
26	CLA	U	602	24	1/1/13/20	16/30/108/115	-
29	BCR	O	2005	-	-	2/29/63/63	0/2/2/2
26	CLA	5	602	18	1/1/15/20	10/37/115/115	-
26	CLA	7	616	20	1/1/11/20	8/11/87/115	-
34	LUT	X	1621	-	-	3/29/67/67	0/2/2/2
29	BCR	G	205	-	-	2/29/63/63	0/2/2/2
26	CLA	7	613	20	1/1/15/20	16/37/115/115	-
26	CLA	A	830	-	1/1/15/20	13/37/115/115	-
37	CHL	U	601	24	3/3/20/26	19/39/137/137	-
26	CLA	U	611	28	1/1/10/20	2/10/88/115	-
26	CLA	6	616	19	1/1/15/20	18/37/115/115	-
26	CLA	B	814	-	1/1/14/20	15/36/114/115	-
26	CLA	B	821	-	1/1/11/20	3/11/89/115	-
26	CLA	A	837	1	1/1/11/20	7/13/91/115	-
36	NEX	Z	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	B	823	-	1/1/11/20	6/13/91/115	-
26	CLA	7	603	-	1/1/11/20	5/11/89/115	-
26	CLA	7	604	-	1/1/12/20	7/19/97/115	-
29	BCR	a	619	-	-	3/29/63/63	0/2/2/2
26	CLA	4	606	-	1/1/10/20	2/6/84/115	-
26	CLA	a	602	14	1/1/14/20	5/33/111/115	-
26	CLA	J	101	10	1/1/10/20	5/10/88/115	-
26	CLA	Z	610	24	1/1/15/20	7/37/115/115	-
26	CLA	B	834	-	1/1/14/20	5/31/109/115	-
28	LHG	V	2630	26	-	6/40/40/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	8	621	-	-	2/29/63/63	0/2/2/2
33	DGD	B	850	-	-	15/51/91/95	0/2/2/2
36	NEX	W	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	A	813	-	1/1/12/20	5/24/102/115	-
26	CLA	B	811	-	1/1/12/20	11/23/95/115	-
29	BCR	A	850	-	-	2/29/63/63	0/2/2/2
26	CLA	6	620	-	1/1/14/20	10/35/113/115	-
37	CHL	Z	609	24	3/3/20/26	16/39/137/137	-
26	CLA	X	602	23	1/1/15/20	13/37/115/115	-
32	LMG	J	103	-	-	10/37/57/70	0/1/1/1
26	CLA	6	609	19	1/1/11/20	5/13/91/115	-
29	BCR	B	846	-	-	0/29/63/63	0/2/2/2
26	CLA	Z	614	-	1/1/11/20	7/17/95/115	-
30	SF4	C	102	3	-	-	0/6/5/5
26	CLA	Y	611	28	1/1/10/20	7/11/89/115	-
26	CLA	B	828	-	1/1/15/20	17/37/115/115	-
26	CLA	B	832	-	1/1/14/20	12/31/109/115	-
34	LUT	9	619	-	-	4/29/67/67	0/2/2/2
26	CLA	2	604	-	1/1/10/20	3/9/87/115	-
26	CLA	a	606	-	1/1/10/20	7/10/88/115	-
26	CLA	H	202	-	1/1/10/20	2/4/82/115	-
26	CLA	5	614	-	1/1/10/20	7/13/87/115	-
36	NEX	X	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	B	841	28	1/1/15/20	15/37/115/115	-
29	BCR	A	856	-	-	2/29/63/63	0/2/2/2
26	CLA	B	818	-	-	11/31/109/115	-
26	CLA	Y	610	24	1/1/15/20	8/37/115/115	-
29	BCR	O	2004	-	-	2/29/63/63	0/2/2/2
26	CLA	1	614	-	1/1/9/20	0/4/76/115	-
26	CLA	A	803	-	1/1/15/20	9/37/115/115	-
31	LMU	5	628	-	-	10/19/59/61	0/2/2/2
27	PQN	B	842	-	-	7/23/43/43	0/2/2/2
26	CLA	6	606	-	1/1/10/20	0/6/84/115	-
31	LMU	8	625	-	-	12/21/61/61	0/2/2/2
26	CLA	6	604	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	843	-	1/1/14/20	14/35/113/115	-
26	CLA	B	819	-	1/1/13/20	6/25/103/115	-
32	LMG	V	2631	-	-	12/50/70/70	0/1/1/1
37	CHL	V	608	-	3/3/16/26	5/18/116/137	-
35	XAT	5	621	-	-	0/31/93/93	0/4/4/4
26	CLA	L	307	8	1/1/10/20	2/6/84/115	-
26	CLA	3	606	-	1/1/13/20	2/23/101/115	-
26	CLA	A	836	-	1/1/15/20	9/37/115/115	-
26	CLA	A	821	-	-	12/23/101/115	-
35	XAT	6	621	-	-	0/31/93/93	0/4/4/4
26	CLA	A	828	-	1/1/15/20	16/37/115/115	-
37	CHL	U	607	-	3/3/16/26	9/15/113/137	-
34	LUT	7	619	-	-	2/29/67/67	0/2/2/2
26	CLA	9	602	22	1/1/14/20	7/31/109/115	-
34	LUT	W	1621	-	-	5/29/67/67	0/2/2/2
26	CLA	a	604	-	1/1/11/20	7/18/96/115	-
29	BCR	A	851	-	-	2/29/63/63	0/2/2/2
26	CLA	7	608	-	-	2/19/97/115	-
26	CLA	5	619	-	1/1/11/20	10/11/87/115	-
29	BCR	B	845	-	-	9/29/63/63	0/2/2/2
26	CLA	B	813	-	1/1/15/20	20/37/115/115	-
28	LHG	A	846	-	-	15/53/53/53	-
26	CLA	1	608	-	1/1/11/20	2/11/89/115	-
37	CHL	W	601	23	3/3/20/26	19/39/137/137	-
35	XAT	W	1622	-	-	2/31/93/93	0/4/4/4
37	CHL	Z	608	-	3/3/16/26	6/19/117/137	-
26	CLA	A	819	-	1/1/13/20	5/30/108/115	-
26	CLA	8	616	21	1/1/11/20	5/11/87/115	-
26	CLA	Y	612	24	1/1/11/20	5/13/91/115	-
32	LMG	J	104	-	-	12/35/55/70	0/1/1/1
26	CLA	B	838	-	1/1/11/20	3/15/93/115	-
26	CLA	L	304	-	1/1/11/20	3/13/91/115	-
35	XAT	2	620	-	-	0/31/93/93	0/4/4/4
26	CLA	B	837	-	-	8/37/115/115	-
26	CLA	W	602	23	1/1/14/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	802	-	1/1/15/20	12/37/115/115	-
26	CLA	9	613	22	1/1/15/20	12/37/115/115	-
26	CLA	8	613	21	1/1/15/20	16/37/115/115	-
37	CHL	U	605	24	3/3/15/26	4/12/110/137	-
28	LHG	W	2630	26	-	13/38/38/53	-
26	CLA	1	610	14	1/1/9/20	2/6/80/115	-
26	CLA	8	603	-	1/1/11/20	4/13/89/115	-
26	CLA	4	613	17	1/1/15/20	11/37/115/115	-
32	LMG	A	860	-	-	9/35/55/70	0/1/1/1
26	CLA	W	604	-	1/1/11/20	6/16/94/115	-
34	LUT	U	1620	-	-	7/29/67/67	0/2/2/2
37	CHL	X	609	23	3/3/20/26	24/39/137/137	-
28	LHG	8	623	-	-	12/44/44/53	-
26	CLA	B	840	-	1/1/15/20	7/37/115/115	-
31	LMU	A	858	-	-	10/21/57/61	0/2/2/2
26	CLA	3	602	16	1/1/14/20	3/31/109/115	-
26	CLA	B	836	-	1/1/12/20	4/19/97/115	-
26	CLA	X	614	-	1/1/10/20	1/10/88/115	-
26	CLA	4	611	28	1/1/10/20	7/10/88/115	-
26	CLA	A	808	-	1/1/12/20	3/19/97/115	-
26	CLA	4	618	17	1/1/10/20	2/8/84/115	-
26	CLA	A	811	-	1/1/15/20	15/37/115/115	-
26	CLA	B	829	-	1/1/15/20	8/37/115/115	-
26	CLA	1	612	14	1/1/11/20	6/13/91/115	-
26	CLA	5	611	28	1/1/10/20	0/10/88/115	-
26	CLA	A	809	1	1/1/15/20	9/37/115/115	-
26	CLA	7	614	-	1/1/10/20	1/10/88/115	-
26	CLA	a	616	14	1/1/11/20	7/13/91/115	-
26	CLA	Z	612	24	1/1/11/20	6/13/91/115	-
26	CLA	A	840	-	-	5/22/100/115	-
35	XAT	a	618	-	-	0/31/93/93	0/4/4/4
26	CLA	5	613	18	1/1/14/20	14/35/113/115	-
26	CLA	B	831	-	1/1/15/20	12/37/115/115	-
26	CLA	V	604	-	1/1/12/20	8/19/97/115	-
26	CLA	6	612	19	1/1/10/20	3/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	6	614	-	1/1/14/20	7/31/109/115	-
34	LUT	V	1621	-	-	3/29/67/67	0/2/2/2
29	BCR	K	207	-	-	2/29/63/63	0/2/2/2
26	CLA	L	306	-	1/1/10/20	1/6/84/115	-
26	CLA	Z	613	24	1/1/15/20	6/37/115/115	-
26	CLA	X	613	23	1/1/15/20	12/37/115/115	-
26	CLA	4	601	17	1/1/15/20	14/37/115/115	-
37	CHL	X	605	-	3/3/16/26	7/15/113/137	-
26	CLA	a	611	28	1/1/10/20	0/4/80/115	-
29	BCR	B	852	-	-	6/29/63/63	0/2/2/2
26	CLA	A	839	-	1/1/13/20	8/25/103/115	-
26	CLA	7	611	28	1/1/13/20	6/29/107/115	-
35	XAT	V	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	A	824	-	1/1/15/20	9/37/115/115	-
26	CLA	1	606	-	1/1/8/20	2/5/79/115	-
37	CHL	V	606	-	3/3/15/26	4/13/111/137	-
26	CLA	U	603	-	1/1/12/20	8/22/100/115	-
26	CLA	A	810	1	-	5/19/97/115	-
26	CLA	7	609	20	1/1/10/20	6/10/88/115	-
29	BCR	6	622	-	-	2/29/63/63	0/2/2/2
35	XAT	U	1622	-	-	4/31/93/93	0/4/4/4
37	CHL	Y	607	-	3/3/20/26	19/39/137/137	-
26	CLA	a	601	14	-	2/23/101/115	-
30	SF4	A	853	2,1	-	-	0/6/5/5
37	CHL	X	607	-	3/3/20/26	25/39/137/137	-
26	CLA	2	611	28	1/1/10/20	2/10/88/115	-
34	LUT	W	1620	-	-	6/29/67/67	0/2/2/2
32	LMG	4	624	-	-	5/35/55/70	0/1/1/1
29	BCR	L	301	-	-	4/29/63/63	0/2/2/2
26	CLA	A	829	-	1/1/15/20	10/37/115/115	-
34	LUT	8	619	-	-	4/29/67/67	0/2/2/2
26	CLA	5	616	18	1/1/10/20	4/8/84/115	-
26	CLA	X	610	23	1/1/15/20	11/37/115/115	-
26	CLA	8	601	21	1/1/15/20	14/37/115/115	-
37	CHL	V	607	-	3/3/16/26	10/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	8	626	-	-	16/41/61/70	0/1/1/1
37	CHL	Y	609	24	3/3/20/26	15/39/137/137	-
36	NEX	6	624	-	-	3/27/83/83	0/3/3/3
26	CLA	A	842	-	1/1/15/20	16/37/115/115	-
26	CLA	2	616	-	1/1/11/20	3/11/87/115	-
26	CLA	Y	613	24	-	14/37/115/115	-
37	CHL	U	608	-	3/3/15/26	5/13/111/137	-
29	BCR	L	308	-	-	6/29/63/63	0/2/2/2
26	CLA	A	822	-	1/1/15/20	6/37/115/115	-
26	CLA	3	610	16	1/1/15/20	12/37/115/115	-
26	CLA	B	827	-	1/1/14/20	12/34/112/115	-
28	LHG	7	622	26	-	19/41/41/53	-
26	CLA	B	826	-	1/1/14/20	14/34/112/115	-
26	CLA	7	612	20	1/1/11/20	4/11/89/115	-
26	CLA	2	607	-	1/1/11/20	0/11/89/115	-
26	CLA	U	610	24	1/1/13/20	4/27/105/115	-
28	LHG	H	204	-	-	15/53/53/53	-
34	LUT	a	617	-	-	4/29/67/67	0/2/2/2
29	BCR	7	623	-	-	3/29/63/63	0/2/2/2
37	CHL	U	609	24	3/3/18/26	12/32/130/137	-
26	CLA	9	611	28	1/1/10/20	3/10/88/115	-
26	CLA	A	831	-	1/1/15/20	16/37/115/115	-
26	CLA	9	607	-	-	9/13/91/115	-
37	CHL	Y	606	-	3/3/16/26	8/15/113/137	-
26	CLA	8	607	-	1/1/10/20	2/10/86/115	-
26	CLA	4	602	17	1/1/14/20	6/31/109/115	-
37	CHL	Z	606	-	3/3/16/26	8/15/113/137	-
29	BCR	3	621	-	-	0/29/63/63	0/2/2/2
34	LUT	6	619	-	-	4/29/67/67	0/2/2/2
37	CHL	W	605	23	3/3/16/26	10/15/113/137	-
28	LHG	9	622	26	-	10/34/34/53	-
26	CLA	5	601	18	1/1/13/20	1/27/105/115	-
35	XAT	Y	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	A	823	-	1/1/10/20	1/10/88/115	-
26	CLA	8	611	28	1/1/10/20	4/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	a	607	-	1/1/11/20	4/13/91/115	-
29	BCR	B	843	-	-	4/29/63/63	0/2/2/2
26	CLA	2	609	15	1/1/11/20	3/13/91/115	-
31	LMU	5	629	-	-	11/18/58/61	0/2/2/2
26	CLA	U	614	-	1/1/10/20	3/10/88/115	-
26	CLA	A	814	-	1/1/15/20	18/37/115/115	-
26	CLA	9	609	22	1/1/14/20	4/33/111/115	-
26	CLA	8	609	21	1/1/11/20	2/13/91/115	-
26	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
36	NEX	Y	1623	-	-	6/27/83/83	0/3/3/3
37	CHL	W	608	-	3/3/16/26	9/17/115/137	-
28	LHG	Y	2630	26	-	13/53/53/53	-
26	CLA	A	818	-	-	15/31/109/115	-
28	LHG	3	624	26	-	14/53/53/53	-
26	CLA	a	609	14	1/1/15/20	13/35/113/115	-
26	CLA	1	607	-	1/1/10/20	0/6/84/115	-
26	CLA	O	2001	-	1/1/9/20	2/4/78/115	-
26	CLA	8	608	-	-	5/21/99/115	-
26	CLA	X	611	28	1/1/11/20	4/13/91/115	-
26	CLA	O	2003	-	1/1/10/20	4/6/84/115	-
26	CLA	A	833	-	1/1/11/20	5/13/91/115	-
37	CHL	X	608	-	3/3/19/26	21/39/133/137	-
26	CLA	3	607	16	1/1/13/20	6/28/104/115	-
26	CLA	A	825	-	1/1/15/20	15/37/115/115	-
35	XAT	9	620	-	-	0/31/93/93	0/4/4/4
26	CLA	V	614	-	1/1/11/20	4/13/91/115	-
26	CLA	3	611	28	1/1/10/20	3/4/80/115	-
26	CLA	6	603	-	1/1/12/20	5/22/98/115	-
26	CLA	B	820	-	1/1/12/20	1/19/97/115	-
26	CLA	L	303	-	-	12/37/115/115	-
29	BCR	J	102	-	-	2/29/63/63	0/2/2/2
26	CLA	4	614	-	-	7/27/105/115	-
26	CLA	6	602	19	-	8/37/115/115	-
37	CHL	U	606	-	3/3/15/26	6/13/111/137	-
34	LUT	5	620	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	804	-	1/1/15/20	16/37/115/115	-
26	CLA	a	603	-	1/1/12/20	8/23/101/115	-
34	LUT	3	618	-	-	4/29/67/67	0/2/2/2
29	BCR	B	847	-	-	2/29/63/63	0/2/2/2
26	CLA	A	816	-	1/1/15/20	15/37/115/115	-
34	LUT	Y	1621	-	-	3/29/67/67	0/2/2/2
32	LMG	4	623	-	-	6/35/55/70	0/1/1/1
26	CLA	3	613	16	1/1/12/20	5/21/99/115	-
28	LHG	5	625	-	-	14/53/53/53	-
26	CLA	B	804	-	1/1/10/20	3/8/86/115	-
26	CLA	5	618	18	1/1/10/20	3/8/84/115	-
29	BCR	A	852	-	-	8/29/63/63	0/2/2/2
26	CLA	7	601	20	1/1/14/20	8/31/109/115	-
26	CLA	5	603	-	1/1/13/20	5/25/101/115	-
26	CLA	K	204	-	1/1/11/20	3/13/91/115	-
26	CLA	7	607	-	1/1/10/20	1/10/88/115	-
26	CLA	3	603	-	1/1/13/20	10/25/103/115	-
26	CLA	B	808	-	1/1/15/20	13/37/115/115	-
26	CLA	B	824	-	1/1/15/20	10/37/115/115	-
26	CLA	F	303	-	-	5/10/88/115	-
37	CHL	V	601	25	3/3/20/26	13/39/137/137	-
26	CLA	9	604	-	1/1/12/20	8/20/96/115	-
26	CLA	B	825	-	-	4/18/96/115	-
26	CLA	7	615	-	1/1/10/20	6/8/84/115	-
35	XAT	1	618	-	-	0/31/93/93	0/4/4/4
29	BCR	B	848	-	-	4/29/63/63	0/2/2/2
26	CLA	9	610	22	1/1/13/20	3/28/106/115	-
26	CLA	5	609	18	1/1/15/20	11/37/115/115	-
26	CLA	V	602	25	1/1/14/20	8/31/109/115	-
26	CLA	W	603	-	1/1/12/20	9/22/100/115	-
26	CLA	A	854	-	1/1/15/20	9/37/115/115	-
26	CLA	B	817	-	1/1/13/20	8/30/108/115	-
28	LHG	A	847	26	-	6/34/34/53	-
26	CLA	U	612	24	1/1/10/20	3/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	F	301	-	1/1/13/20	12/28/106/115	-
26	CLA	W	610	23	1/1/13/20	5/25/103/115	-
26	CLA	8	602	21	-	14/31/109/115	-
26	CLA	B	806	2	1/1/15/20	19/37/115/115	-
26	CLA	1	601	14	-	2/23/101/115	-
26	CLA	4	610	17	1/1/14/20	8/33/111/115	-
26	CLA	B	803	-	1/1/15/20	12/37/115/115	-
26	CLA	K	201	11	1/1/11/20	5/13/91/115	-
29	BCR	1	619	-	-	3/29/63/63	0/2/2/2
34	LUT	Z	1621	-	-	3/29/67/67	0/2/2/2
37	CHL	W	609	23	3/3/20/26	11/39/137/137	-
35	XAT	3	619	-	-	0/31/93/93	0/4/4/4
29	BCR	3	620	-	-	4/29/63/63	0/2/2/2
26	CLA	4	616	17	1/1/11/20	7/11/87/115	-
26	CLA	V	613	25	1/1/15/20	18/37/115/115	-
26	CLA	B	807	-	-	2/22/100/115	-
26	CLA	5	606	-	-	1/6/84/115	-
37	CHL	Z	601	24	3/3/20/26	16/39/137/137	-
29	BCR	B	853	-	-	4/29/63/63	0/2/2/2
26	CLA	2	603	15	1/1/11/20	5/11/89/115	-
37	CHL	X	606	-	3/3/15/26	6/13/111/137	-
26	CLA	U	613	24	1/1/13/20	11/30/108/115	-
26	CLA	3	617	16	1/1/10/20	0/6/84/115	-
26	CLA	A	827	-	1/1/13/20	5/29/107/115	-
26	CLA	3	604	-	1/1/15/20	7/37/115/115	-
26	CLA	V	603	-	1/1/11/20	4/13/91/115	-
29	BCR	A	848	-	-	3/29/63/63	0/2/2/2
26	CLA	1	602	14	1/1/14/20	5/33/111/115	-
28	LHG	6	623	26	-	19/52/52/53	-
29	BCR	5	622	-	-	1/29/63/63	0/2/2/2
29	BCR	B	801	-	-	4/29/63/63	0/2/2/2
29	BCR	B	844	-	-	2/29/63/63	0/2/2/2
36	NEX	U	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	1	611	28	1/1/13/20	5/28/106/115	-
28	LHG	4	622	26	-	8/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	L	309	-	-	3/29/63/63	0/2/2/2
26	CLA	a	610	14	1/1/14/20	7/29/107/115	-
26	CLA	Z	604	-	1/1/11/20	5/19/93/115	-
26	CLA	7	606	-	1/1/10/20	2/8/86/115	-
29	BCR	9	621	-	-	4/29/63/63	0/2/2/2
26	CLA	A	807	1	1/1/15/20	20/37/115/115	-
26	CLA	Y	603	-	1/1/13/20	10/25/103/115	-
26	CLA	6	613	-	-	13/35/113/115	-
37	CHL	V	605	25	3/3/15/26	5/13/111/137	-
26	CLA	6	611	28	1/1/10/20	3/10/88/115	-
26	CLA	F	304	6	-	3/8/86/115	-
26	CLA	G	204	7	1/1/11/20	5/13/91/115	-
26	CLA	3	608	-	1/1/13/20	8/25/103/115	-
26	CLA	9	614	-	1/1/11/20	3/13/91/115	-
26	CLA	Y	602	24	1/1/13/20	12/29/107/115	-
26	CLA	8	612	21	1/1/10/20	2/8/86/115	-
26	CLA	3	615	-	1/1/10/20	3/6/84/115	-
26	CLA	8	614	-	1/1/12/20	8/23/101/115	-
26	CLA	W	612	23	1/1/11/20	5/13/91/115	-
26	CLA	W	614	-	1/1/11/20	6/13/91/115	-
26	CLA	G	203	-	1/1/10/20	3/10/88/115	-
26	CLA	a	612	14	1/1/11/20	6/13/91/115	-
26	CLA	a	614	-	1/1/12/20	7/25/99/115	-
26	CLA	6	618	19	1/1/10/20	1/8/84/115	-
26	CLA	5	610	18	1/1/12/20	4/24/102/115	-
26	CLA	4	603	17	1/1/11/20	5/13/89/115	-
26	CLA	5	612	18	1/1/10/20	2/8/86/115	-
37	CHL	V	609	25	3/3/19/26	11/33/131/137	-
29	BCR	L	305	-	-	2/29/63/63	0/2/2/2
26	CLA	Y	604	-	1/1/12/20	6/19/97/115	-
35	XAT	4	620	-	-	2/31/93/93	0/4/4/4
26	CLA	Y	614	-	1/1/11/20	8/17/95/115	-
26	CLA	2	612	15	1/1/11/20	5/11/89/115	-
26	CLA	X	612	23	1/1/10/20	6/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	4	604	-	1/1/13/20	9/25/101/115	-
28	LHG	a	620	26	-	7/47/47/53	-
26	CLA	4	609	17	1/1/13/20	3/28/106/115	-
26	CLA	9	612	22	1/1/10/20	2/8/86/115	-
26	CLA	B	805	-	1/1/15/20	11/37/115/115	-
35	XAT	7	620	-	-	0/31/93/93	0/4/4/4
26	CLA	H	203	-	1/1/15/20	15/37/115/115	-
26	CLA	6	601	19	1/1/15/20	17/37/115/115	-
26	CLA	X	603	-	1/1/14/20	13/34/112/115	-
26	CLA	X	604	-	1/1/11/20	9/18/96/115	-
26	CLA	6	608	-	-	6/13/91/115	-
26	CLA	5	604	-	1/1/15/20	12/35/111/115	-
26	CLA	7	602	20	1/1/15/20	10/37/115/115	-
26	CLA	2	610	15	1/1/13/20	3/25/103/115	-
34	LUT	V	1620	-	-	4/29/67/67	0/2/2/2
26	CLA	A	820	-	1/1/15/20	8/37/115/115	-
26	CLA	3	614	-	1/1/10/20	0/6/84/115	-
26	CLA	4	607	-	1/1/11/20	5/13/91/115	-
37	CHL	Y	605	24	3/3/15/26	4/10/108/137	-
32	LMG	5	627	-	-	7/35/55/70	0/1/1/1
29	BCR	2	623	-	-	4/29/63/63	0/2/2/2
26	CLA	A	834	-	1/1/15/20	10/37/115/115	-
26	CLA	B	833	-	1/1/15/20	11/37/115/115	-
26	CLA	A	838	-	1/1/12/20	8/19/97/115	-
26	CLA	B	835	-	1/1/11/20	2/13/91/115	-
29	BCR	B	849	-	-	5/29/63/63	0/2/2/2
26	CLA	K	206	11	1/1/11/20	4/13/91/115	-
34	LUT	2	619	-	-	2/29/67/67	0/2/2/2
28	LHG	8	622	26	-	13/53/53/53	-
26	CLA	2	601	15	1/1/15/20	8/37/115/115	-
37	CHL	X	601	23	3/3/20/26	19/39/137/137	-
28	LHG	B	851	26	-	14/42/42/53	-
31	LMU	1	621	-	-	7/21/61/61	0/2/2/2
26	CLA	2	602	15	1/1/15/20	14/39/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	802	-	1/1/15/20	16/37/115/115	-
26	CLA	a	613	-	1/1/12/20	9/24/102/115	-
26	CLA	A	826	-	1/1/14/20	8/35/113/115	-
26	CLA	9	606	-	1/1/10/20	2/6/84/115	-
26	CLA	A	832	-	1/1/12/20	9/19/97/115	-
26	CLA	7	610	20	1/1/15/20	5/37/115/115	-
28	LHG	U	2630	26	-	21/53/53/53	-
26	CLA	8	604	-	1/1/12/20	6/19/97/115	-
26	CLA	8	606	-	1/1/15/20	7/35/113/115	-
26	CLA	V	611	28	1/1/10/20	5/11/89/115	-
35	XAT	X	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	1	613	-	1/1/15/20	17/37/115/115	-
28	LHG	Z	2630	26	-	19/53/53/53	-
26	CLA	A	806	-	1/1/15/20	13/37/115/115	-
37	CHL	Z	605	24	3/3/15/26	4/10/108/137	-
26	CLA	A	835	-	-	12/33/111/115	-
28	LHG	5	623	26	-	15/53/53/53	-
32	LMG	9	625	-	-	11/50/70/70	0/1/1/1

The worst 5 of 3353 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	842	PQN	C12-C13	9.58	1.56	1.33
27	A	844	PQN	C12-C13	9.30	1.55	1.33
26	X	604	CLA	C4B-NB	8.04	1.42	1.35
26	3	612	CLA	C4B-NB	8.03	1.42	1.35
26	Y	604	CLA	C4B-NB	8.01	1.42	1.35

The worst 5 of 4786 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	X	1623	NEX	C17-C1-C6	-20.23	92.37	110.47
35	U	1622	XAT	C37-C21-C36	-17.41	81.69	107.37
35	W	1622	XAT	C37-C21-C36	-17.39	81.72	107.37
29	B	852	BCR	C32-C1-C6	-16.31	83.85	110.30
35	U	1622	XAT	C37-C21-C22	-15.46	82.13	108.98

5 of 378 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	A	801	CLA	ND
26	A	802	CLA	ND
26	A	803	CLA	ND
26	A	804	CLA	ND
26	A	806	CLA	ND

5 of 3427 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	801	CLA	CBD-CGD-O2D-CED
26	A	801	CLA	O1D-CGD-O2D-CED
26	A	804	CLA	C1A-C2A-CAA-CBA
26	A	804	CLA	C3A-C2A-CAA-CBA
26	A	804	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

290 monomers are involved in 664 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	857	LMU	1	0
26	5	607	CLA	2	0
29	3	622	BCR	7	0
37	W	606	CHL	1	0
34	Y	1620	LUT	5	0
37	Z	607	CHL	3	0
26	Z	611	CLA	3	0
26	A	841	CLA	4	0
26	W	613	CLA	4	0
37	W	607	CHL	3	0
36	V	1623	NEX	11	0
36	5	624	NEX	1	0
26	3	612	CLA	1	0
29	A	849	BCR	5	0
26	6	610	CLA	3	0
29	4	621	BCR	5	0
26	A	805	CLA	1	0
35	8	620	XAT	1	0
29	7	621	BCR	3	0
26	B	839	CLA	1	0
26	2	613	CLA	3	0
34	U	1621	LUT	2	0
28	O	2631	LHG	1	0
34	Z	1620	LUT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	Y	601	CHL	6	0
29	F	305	BCR	7	0
26	B	816	CLA	1	0
26	K	203	CLA	1	0
26	V	612	CLA	2	0
26	B	830	CLA	1	0
34	4	619	LUT	3	0
28	3	623	LHG	1	0
26	V	610	CLA	3	0
26	B	822	CLA	1	0
26	U	604	CLA	3	0
28	X	2630	LHG	6	0
29	K	202	BCR	5	0
26	8	610	CLA	1	0
26	L	302	CLA	3	0
37	Y	608	CHL	2	0
26	2	606	CLA	1	0
27	A	844	PQN	2	0
26	A	815	CLA	2	0
26	Z	603	CLA	1	0
26	1	604	CLA	1	0
34	1	617	LUT	6	0
35	Z	1622	XAT	5	0
34	X	1620	LUT	6	0
26	6	607	CLA	1	0
26	Z	602	CLA	4	0
26	A	812	CLA	1	0
26	U	602	CLA	1	0
29	O	2005	BCR	6	0
26	5	602	CLA	2	0
26	7	616	CLA	1	0
34	X	1621	LUT	6	0
29	G	205	BCR	4	0
26	7	613	CLA	2	0
26	A	830	CLA	1	0
37	U	601	CHL	4	0
26	6	616	CLA	1	0
26	B	821	CLA	3	0
26	A	837	CLA	1	0
36	Z	1623	NEX	3	0
26	7	604	CLA	1	0
29	a	619	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	4	606	CLA	1	0
26	Z	610	CLA	5	0
26	B	834	CLA	3	0
28	V	2630	LHG	3	0
29	8	621	BCR	3	0
33	B	850	DGD	1	0
36	W	1623	NEX	2	0
29	A	850	BCR	8	0
37	Z	609	CHL	3	0
26	X	602	CLA	4	0
26	6	609	CLA	1	0
29	B	846	BCR	3	0
26	Z	614	CLA	1	0
30	C	102	SF4	1	0
26	B	828	CLA	2	0
34	9	619	LUT	5	0
26	a	606	CLA	1	0
36	X	1623	NEX	2	0
29	A	856	BCR	10	0
26	B	818	CLA	1	0
26	Y	610	CLA	2	0
29	O	2004	BCR	3	0
26	A	803	CLA	3	0
27	B	842	PQN	3	0
26	6	606	CLA	1	0
26	A	843	CLA	2	0
26	B	819	CLA	1	0
32	V	2631	LMG	2	0
35	5	621	XAT	2	0
37	V	608	CHL	2	0
26	L	307	CLA	2	0
26	3	606	CLA	1	0
26	A	821	CLA	1	0
35	6	621	XAT	1	0
37	U	607	CHL	2	0
34	7	619	LUT	3	0
34	W	1621	LUT	4	0
26	a	604	CLA	1	0
29	A	851	BCR	6	0
26	5	619	CLA	3	0
29	B	845	BCR	3	0
26	B	813	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	W	601	CHL	3	0
35	W	1622	XAT	3	0
37	Z	608	CHL	2	0
26	A	819	CLA	2	0
35	2	620	XAT	1	0
26	B	837	CLA	2	0
26	W	602	CLA	2	0
26	A	802	CLA	3	0
26	9	613	CLA	2	0
26	8	613	CLA	2	0
37	U	605	CHL	1	0
28	W	2630	LHG	1	0
32	A	860	LMG	1	0
34	U	1620	LUT	6	0
37	X	609	CHL	4	0
26	B	840	CLA	1	0
26	X	614	CLA	1	0
26	4	611	CLA	1	0
26	A	808	CLA	2	0
26	4	618	CLA	1	0
26	5	611	CLA	7	0
26	A	809	CLA	1	0
26	7	614	CLA	2	0
26	Z	612	CLA	1	0
26	A	840	CLA	1	0
35	a	618	XAT	3	0
26	5	613	CLA	1	0
26	6	614	CLA	2	0
34	V	1621	LUT	5	0
29	K	207	BCR	3	0
26	Z	613	CLA	4	0
26	X	613	CLA	4	0
26	4	601	CLA	1	0
26	a	611	CLA	1	0
29	B	852	BCR	6	0
26	7	611	CLA	4	0
35	V	1622	XAT	6	0
26	A	824	CLA	2	0
26	1	606	CLA	1	0
37	V	606	CHL	2	0
26	7	609	CLA	1	0
29	6	622	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	U	1622	XAT	5	0
37	Y	607	CHL	3	0
26	a	601	CLA	3	0
37	X	607	CHL	2	0
34	W	1620	LUT	4	0
29	L	301	BCR	10	0
26	A	829	CLA	5	0
34	8	619	LUT	6	0
26	X	610	CLA	3	0
37	V	607	CHL	4	0
32	8	626	LMG	3	0
36	6	624	NEX	6	0
37	Y	609	CHL	3	0
26	Y	613	CLA	4	0
37	U	608	CHL	3	0
29	L	308	BCR	7	0
26	A	822	CLA	4	0
26	3	610	CLA	1	0
26	B	827	CLA	1	0
26	U	610	CLA	4	0
34	a	617	LUT	5	0
29	7	623	BCR	5	0
37	U	609	CHL	3	0
26	A	831	CLA	1	0
37	Y	606	CHL	2	0
29	3	621	BCR	4	0
34	6	619	LUT	5	0
37	Z	606	CHL	3	0
37	W	605	CHL	2	0
28	9	622	LHG	1	0
35	Y	1622	XAT	3	0
26	8	611	CLA	2	0
26	a	607	CLA	1	0
29	B	843	BCR	9	0
26	9	609	CLA	1	0
36	Y	1623	NEX	2	0
28	Y	2630	LHG	6	0
26	A	818	CLA	1	0
28	3	624	LHG	2	0
26	1	607	CLA	1	0
26	X	611	CLA	2	0
37	X	608	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	825	CLA	3	0
26	V	614	CLA	1	0
26	L	303	CLA	2	0
29	J	102	BCR	8	0
26	6	602	CLA	1	0
37	U	606	CHL	2	0
34	5	620	LUT	4	0
26	a	603	CLA	1	0
34	3	618	LUT	7	0
29	B	847	BCR	4	0
26	A	816	CLA	1	0
34	Y	1621	LUT	4	0
26	3	613	CLA	1	0
29	A	852	BCR	10	0
26	7	601	CLA	1	0
26	5	603	CLA	1	0
26	K	204	CLA	2	0
26	B	808	CLA	3	0
26	B	824	CLA	1	0
26	F	303	CLA	4	0
37	V	601	CHL	4	0
26	B	825	CLA	2	0
26	7	615	CLA	1	0
35	1	618	XAT	3	0
29	B	848	BCR	2	0
26	9	610	CLA	1	0
26	V	602	CLA	3	0
26	W	603	CLA	2	0
26	A	854	CLA	5	0
26	B	817	CLA	1	0
26	F	301	CLA	1	0
26	W	610	CLA	1	0
26	1	601	CLA	2	0
26	B	803	CLA	2	0
29	1	619	BCR	2	0
34	Z	1621	LUT	4	0
37	W	609	CHL	1	0
35	3	619	XAT	2	0
29	3	620	BCR	8	0
26	4	616	CLA	1	0
26	V	613	CLA	4	0
37	Z	601	CHL	4	0

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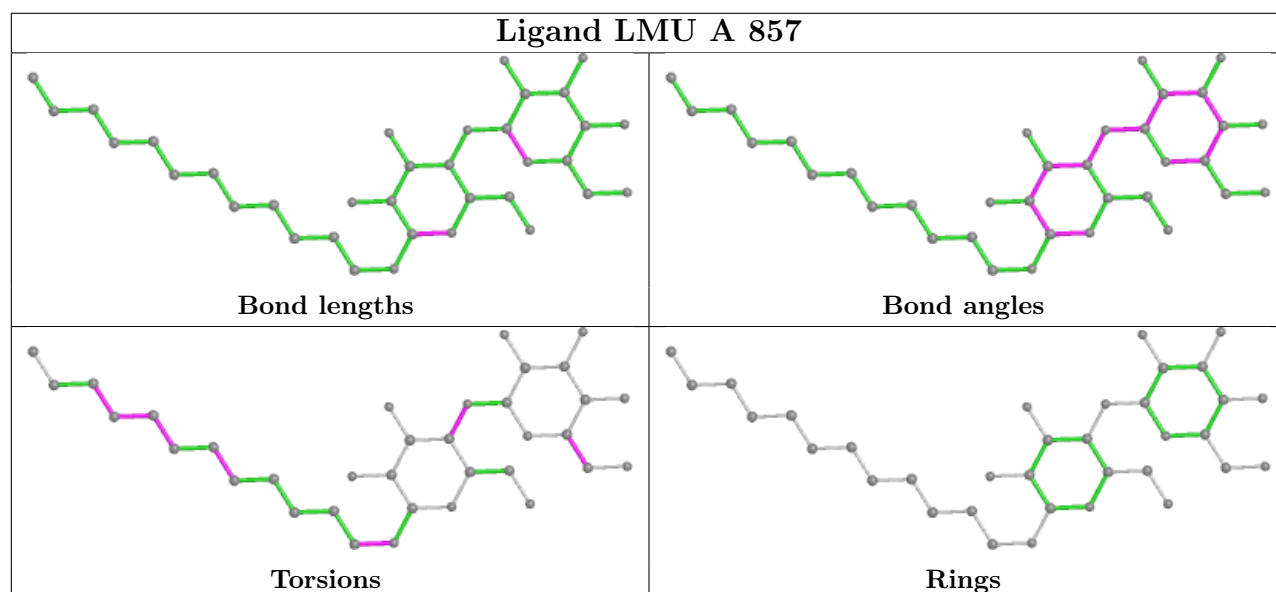
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	B	853	BCR	3	0
26	U	613	CLA	3	0
26	A	827	CLA	1	0
29	A	848	BCR	3	0
29	5	622	BCR	2	0
29	B	801	BCR	7	0
29	B	844	BCR	6	0
26	1	611	CLA	1	0
29	L	309	BCR	4	0
29	9	621	BCR	7	0
26	A	807	CLA	3	0
26	Y	603	CLA	3	0
37	V	605	CHL	1	0
26	F	304	CLA	1	0
26	3	608	CLA	1	0
26	Y	602	CLA	2	0
26	8	612	CLA	2	0
26	W	612	CLA	1	0
26	W	614	CLA	4	0
26	5	610	CLA	1	0
37	V	609	CHL	3	0
29	L	305	BCR	8	0
35	4	620	XAT	3	0
26	X	612	CLA	1	0
28	a	620	LHG	1	0
26	4	609	CLA	1	0
35	7	620	XAT	1	0
26	6	601	CLA	1	0
26	X	603	CLA	1	0
26	X	604	CLA	1	0
26	6	608	CLA	1	0
26	7	602	CLA	1	0
34	V	1620	LUT	5	0
26	A	820	CLA	2	0
26	4	607	CLA	1	0
37	Y	605	CHL	1	0
32	5	627	LMG	1	0
29	2	623	BCR	5	0
26	A	834	CLA	2	0
26	B	833	CLA	2	0
26	B	835	CLA	1	0
29	B	849	BCR	2	0

Continued on next page...

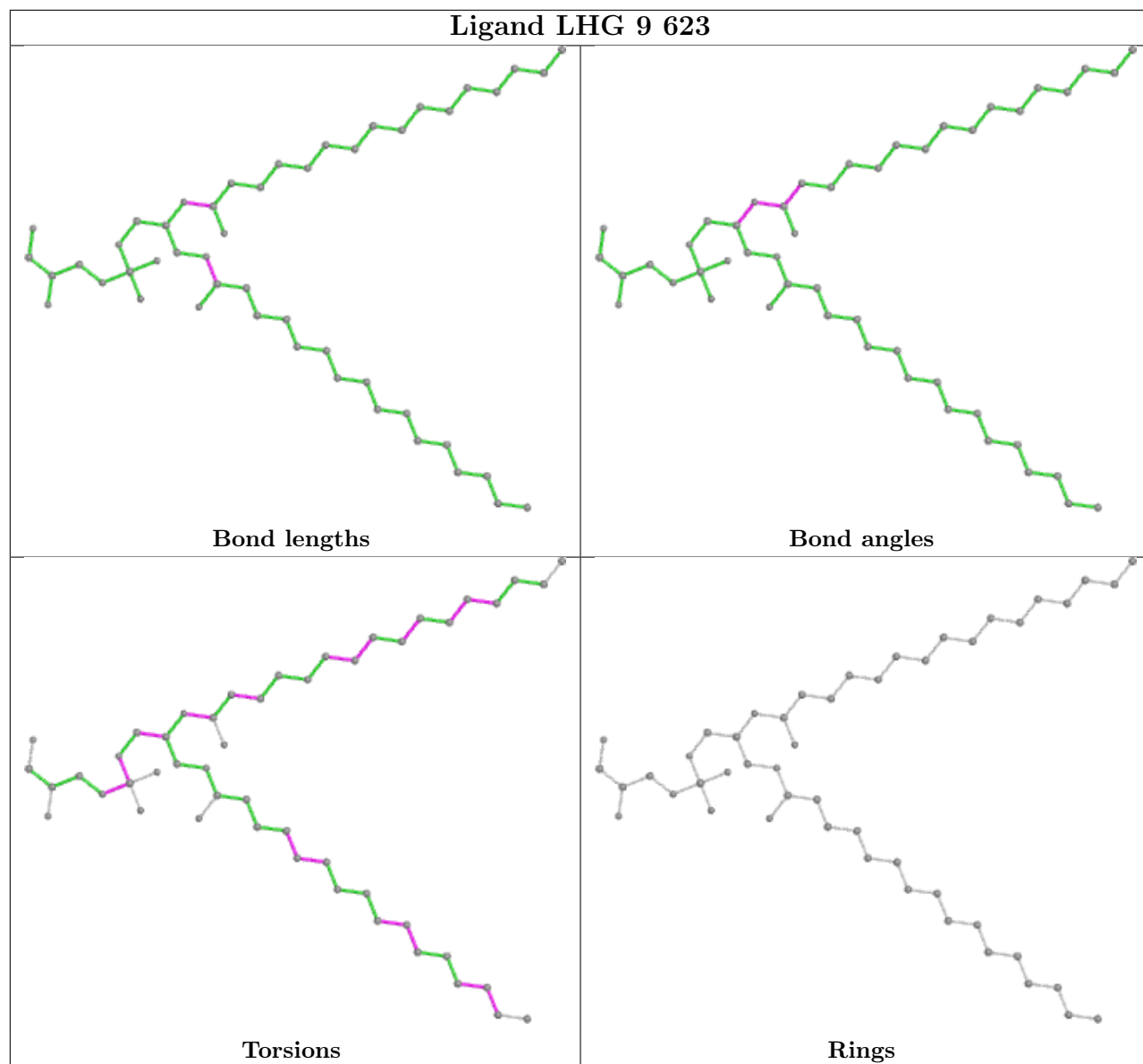
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	2	619	LUT	7	0
37	X	601	CHL	7	0
26	B	802	CLA	1	0
26	a	613	CLA	1	0
28	U	2630	LHG	1	0
26	8	604	CLA	1	0
26	8	606	CLA	1	0
35	X	1622	XAT	3	0
26	1	613	CLA	1	0
28	Z	2630	LHG	9	0
26	A	806	CLA	2	0
26	A	835	CLA	2	0
28	5	623	LHG	6	0
32	9	625	LMG	2	0

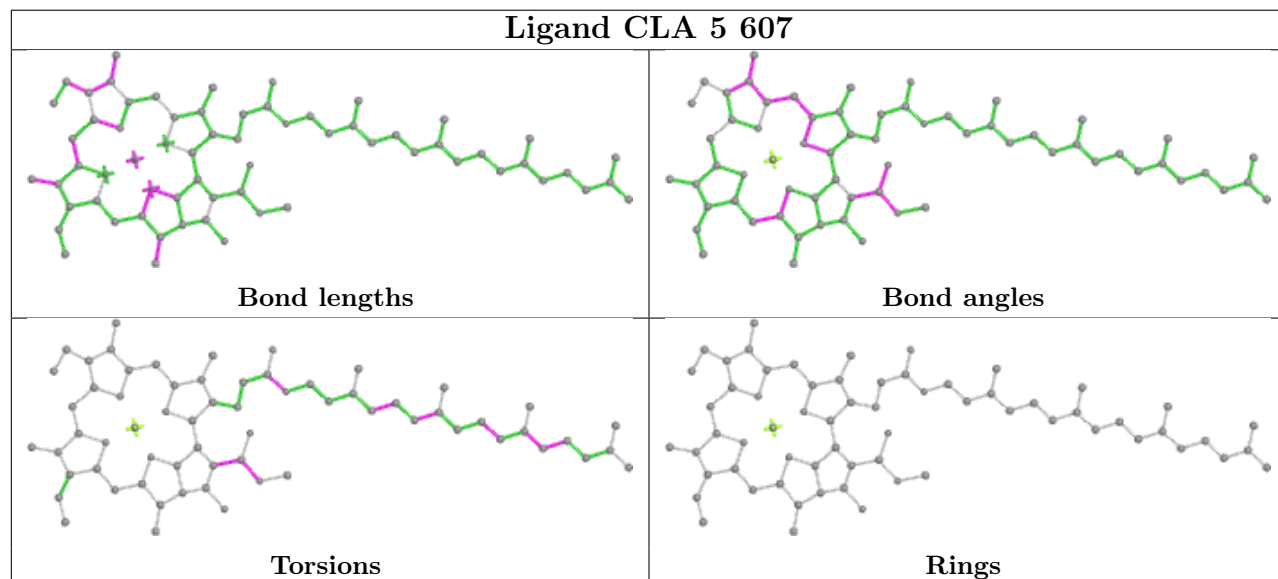
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

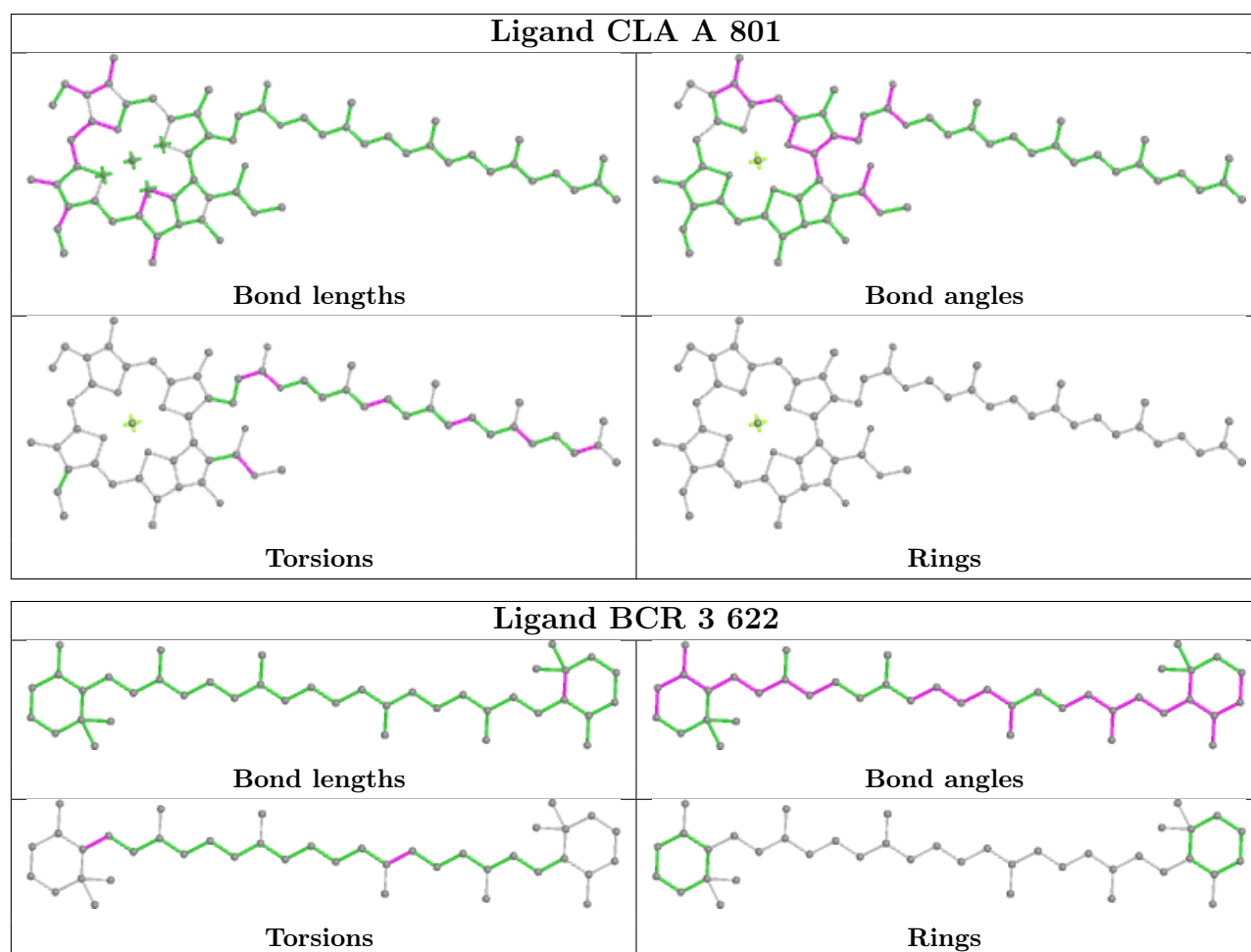


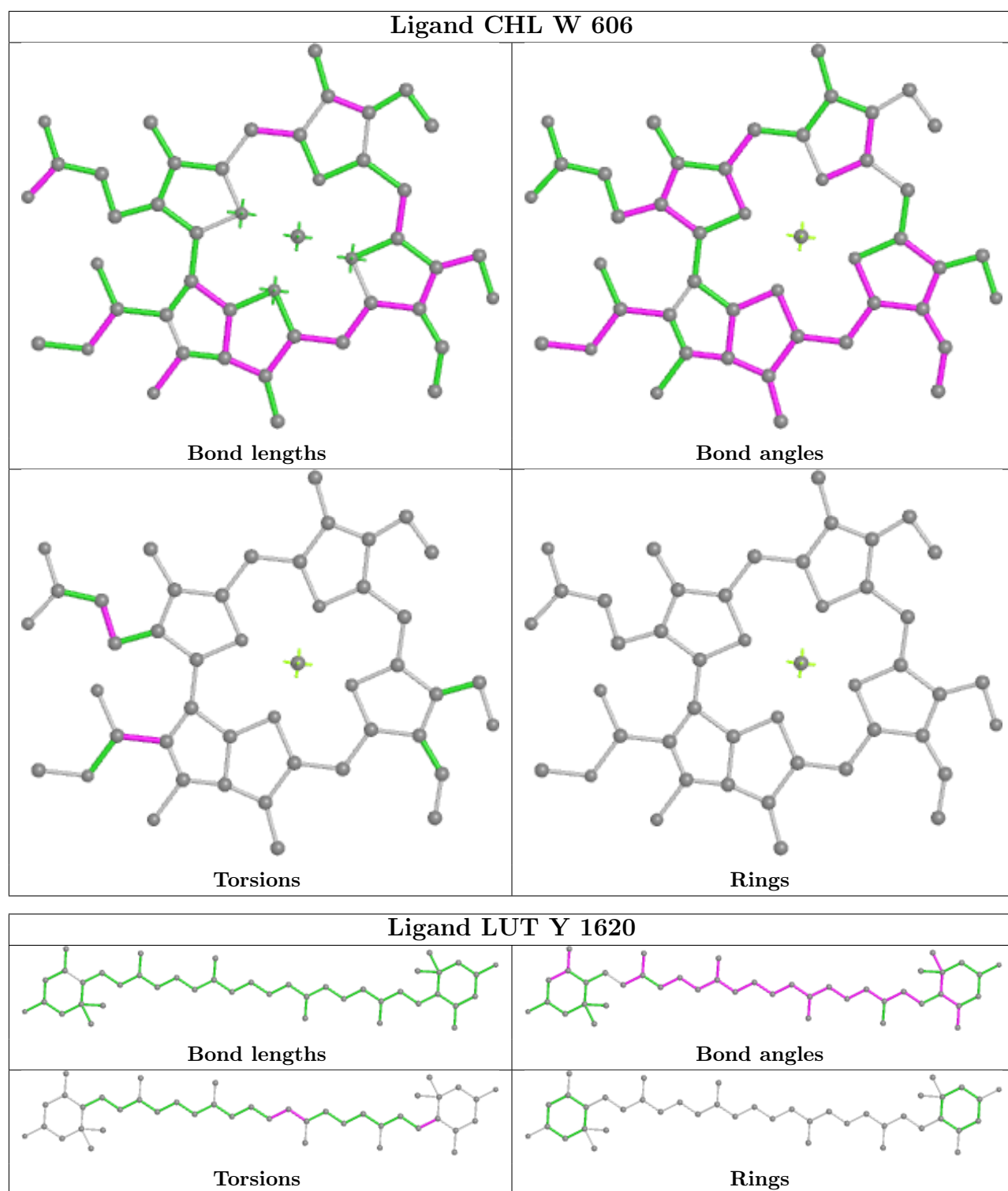
Ligand LHG 9 623



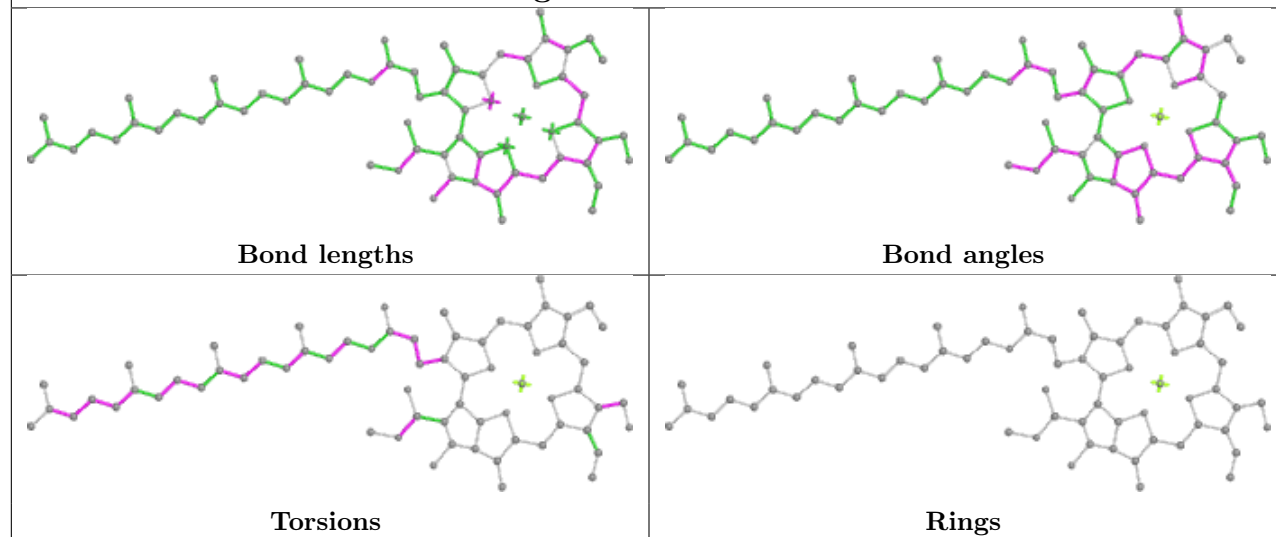
Ligand CLA 5 607



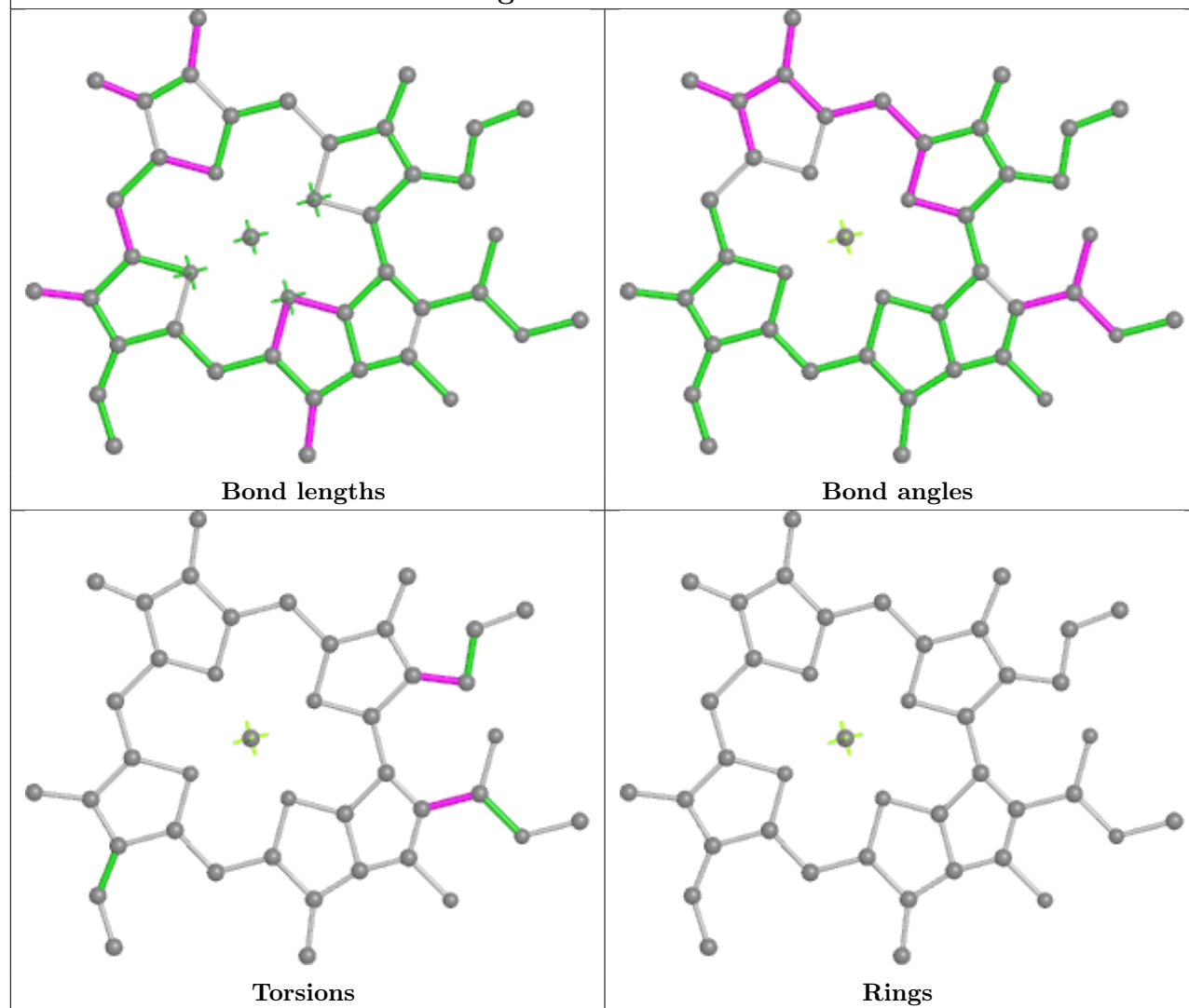




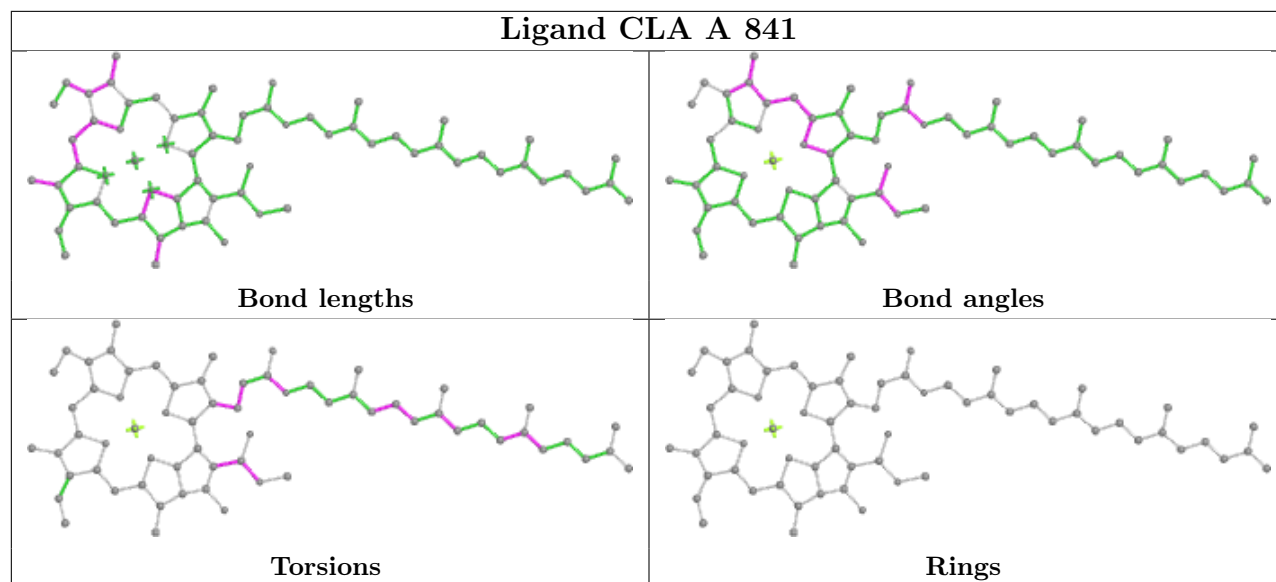
Ligand CHL Z 607



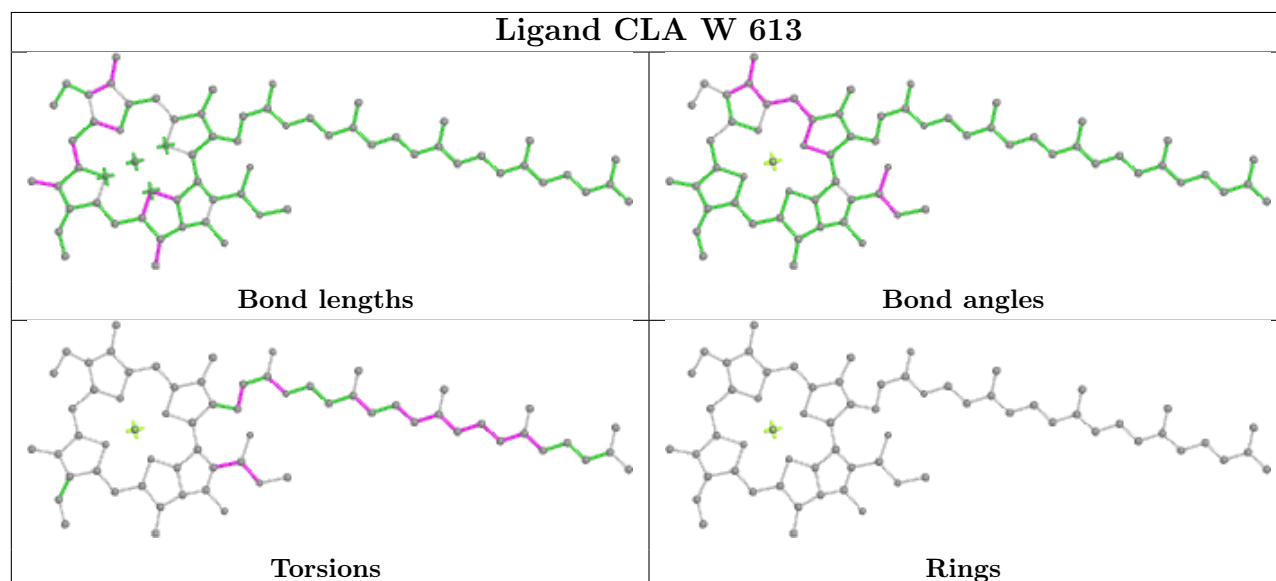
Ligand CLA Z 611



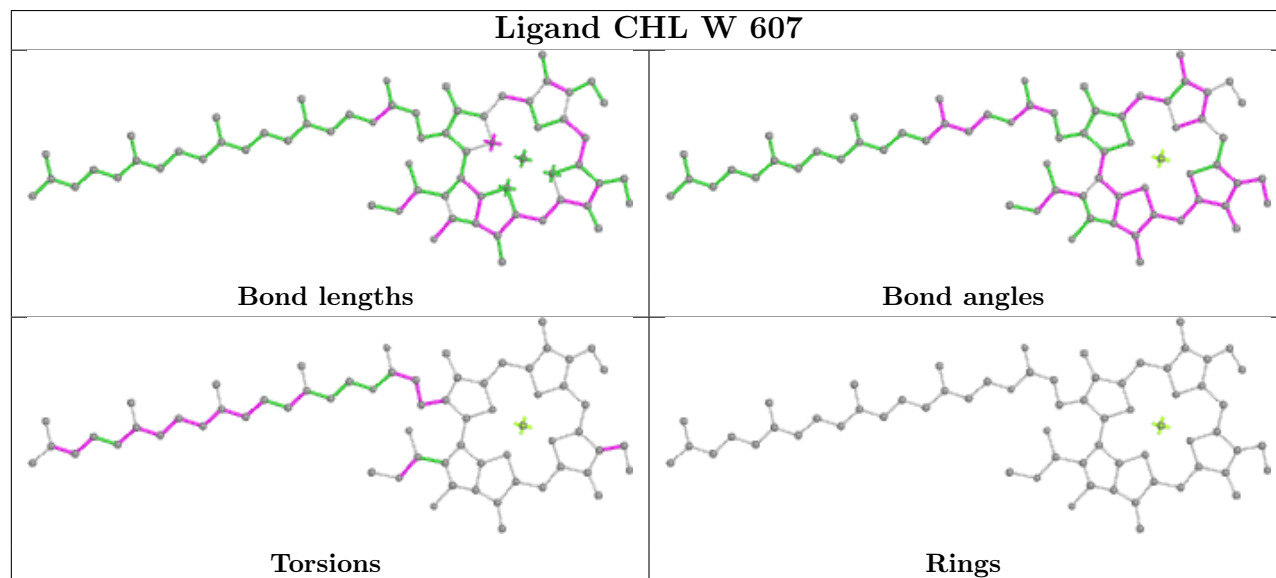
Ligand CLA A 841

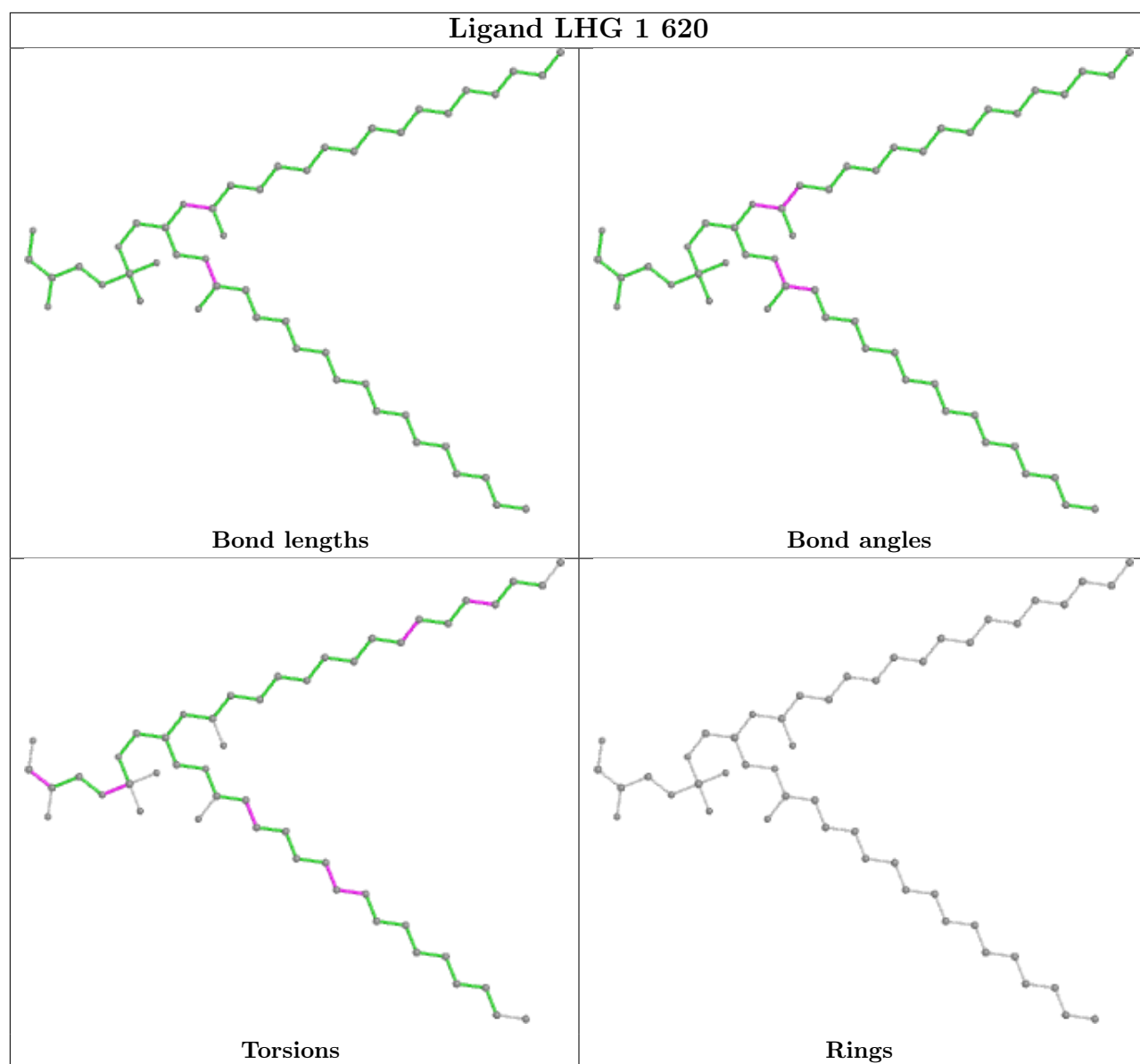


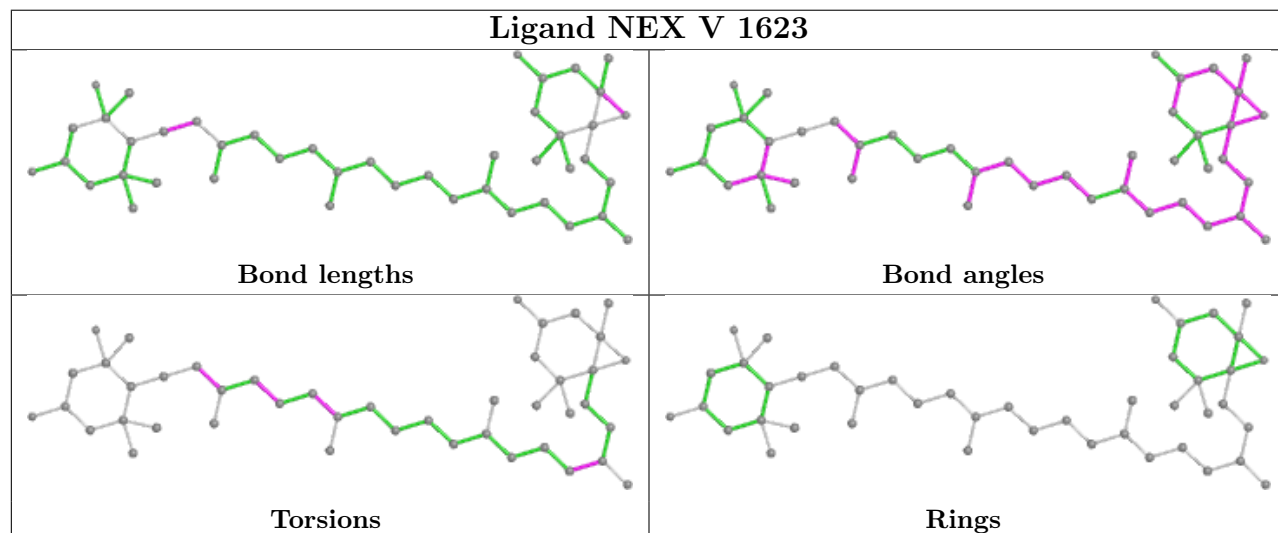
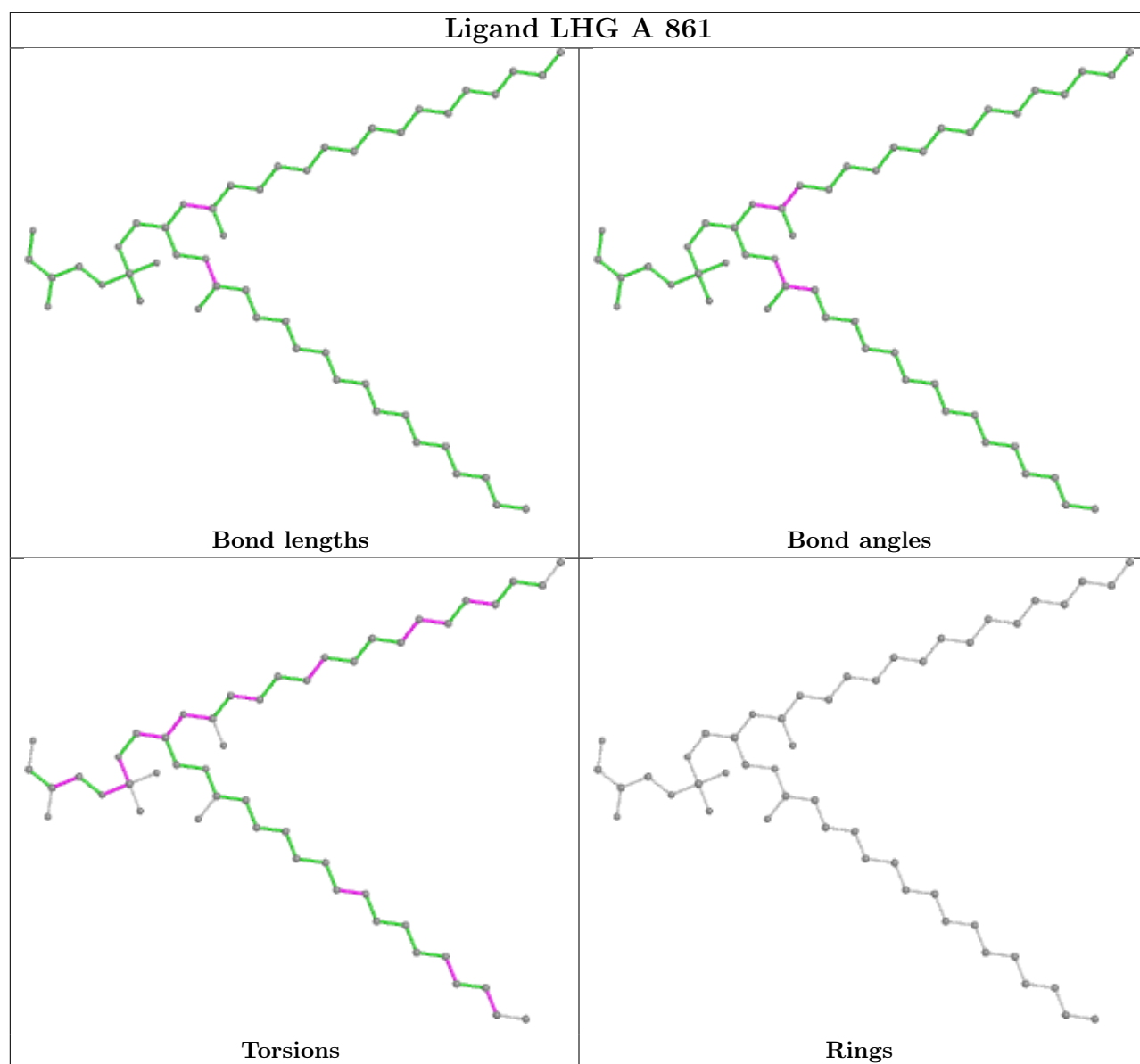
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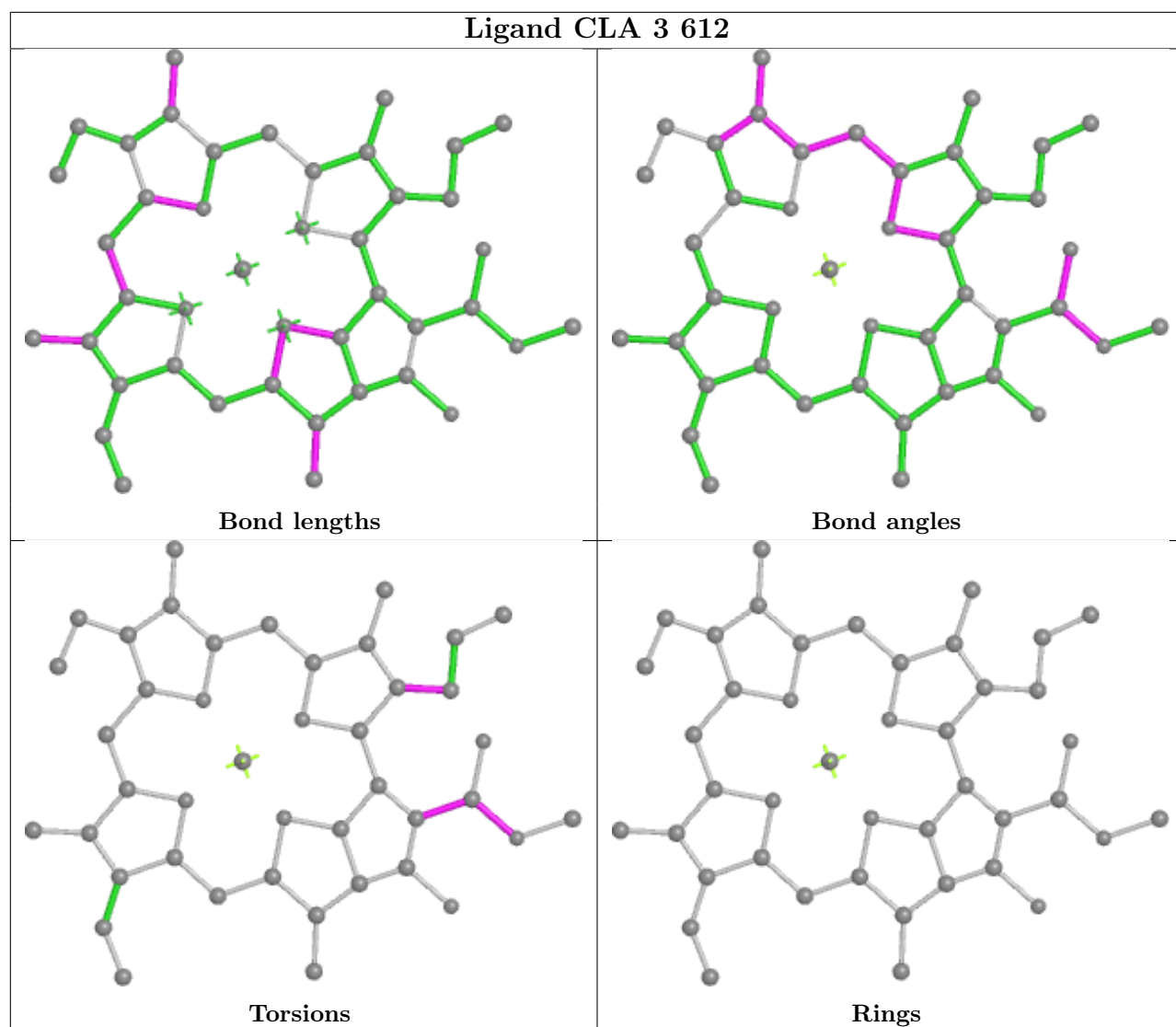
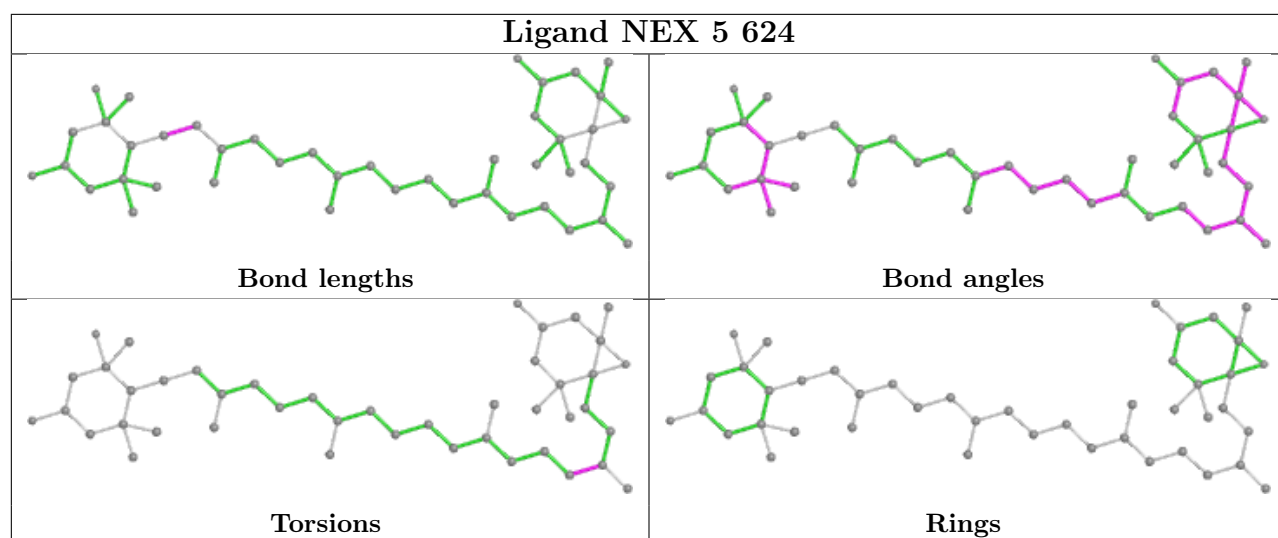


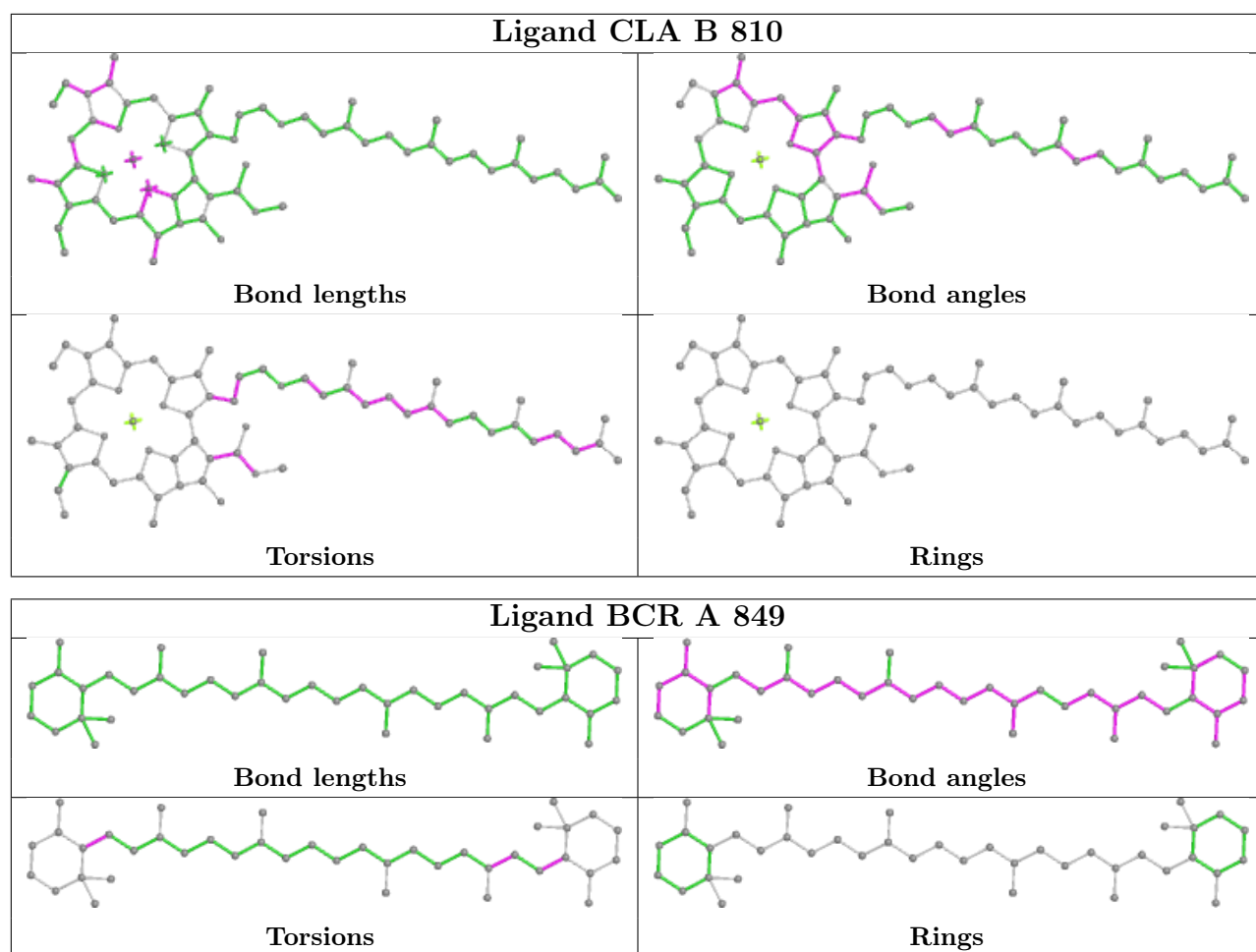
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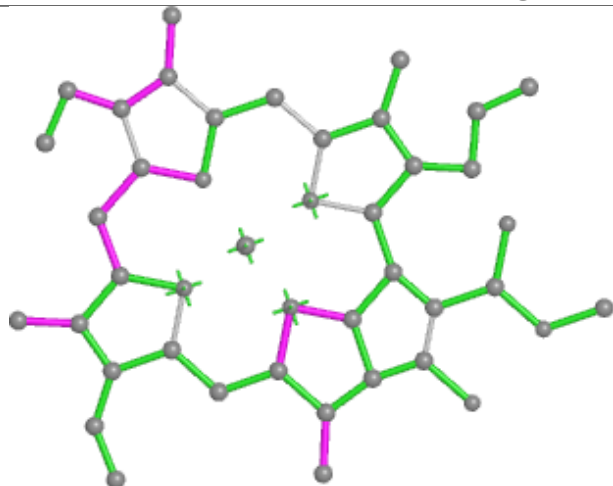




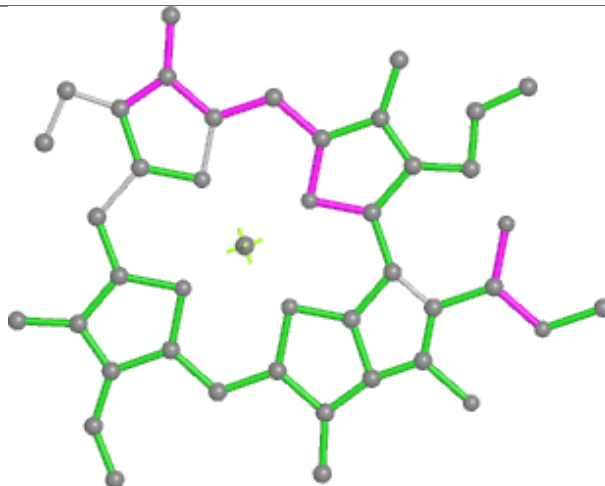




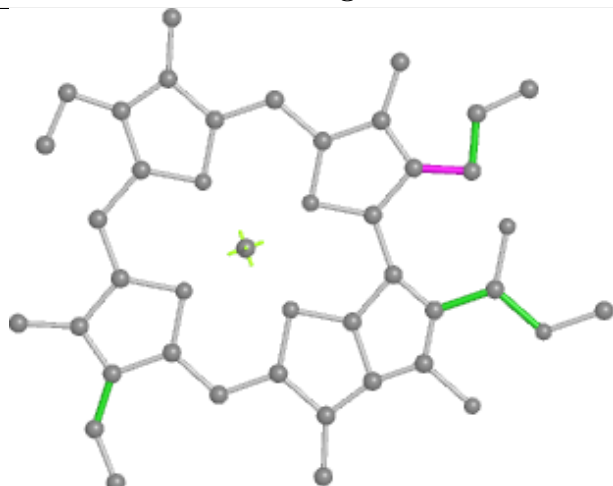
Ligand CLA B 815



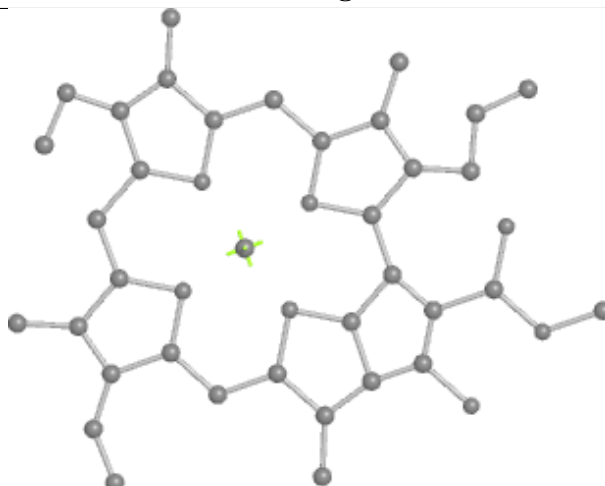
Bond lengths



Bond angles

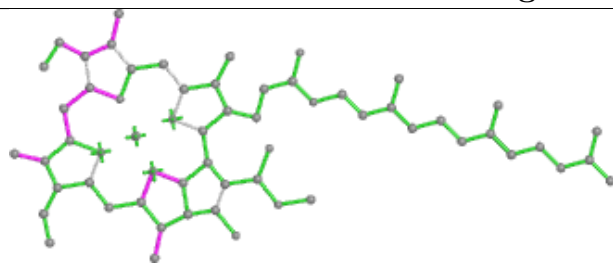


Torsions

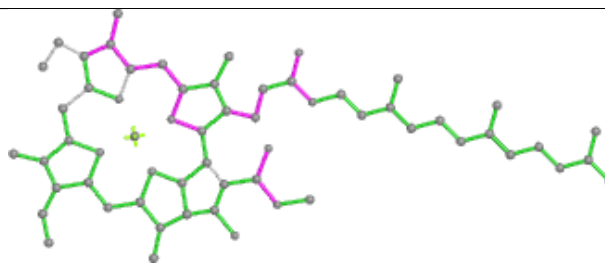


Rings

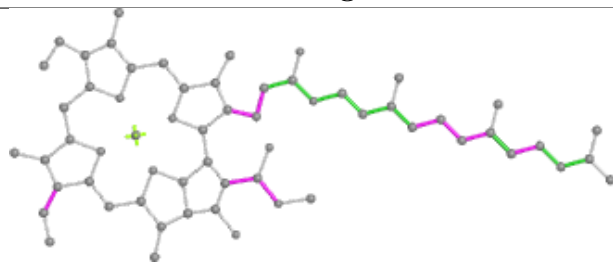
Ligand CLA 3 609



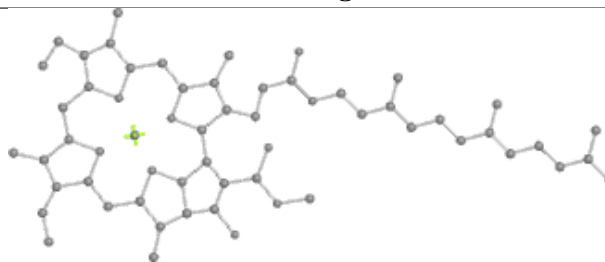
Bond lengths



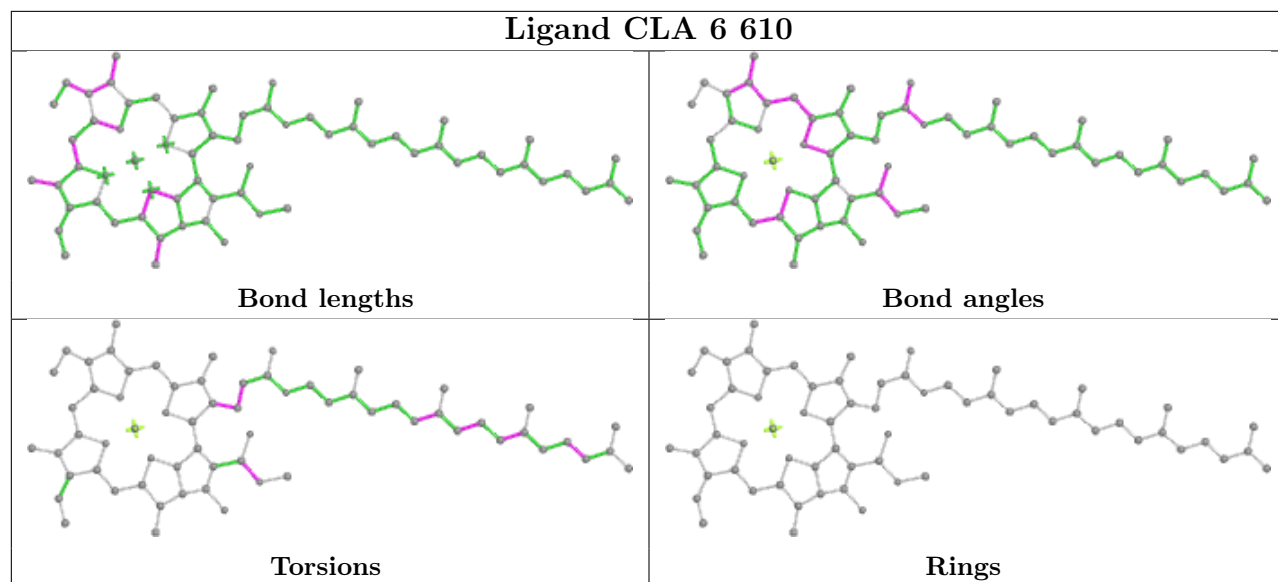
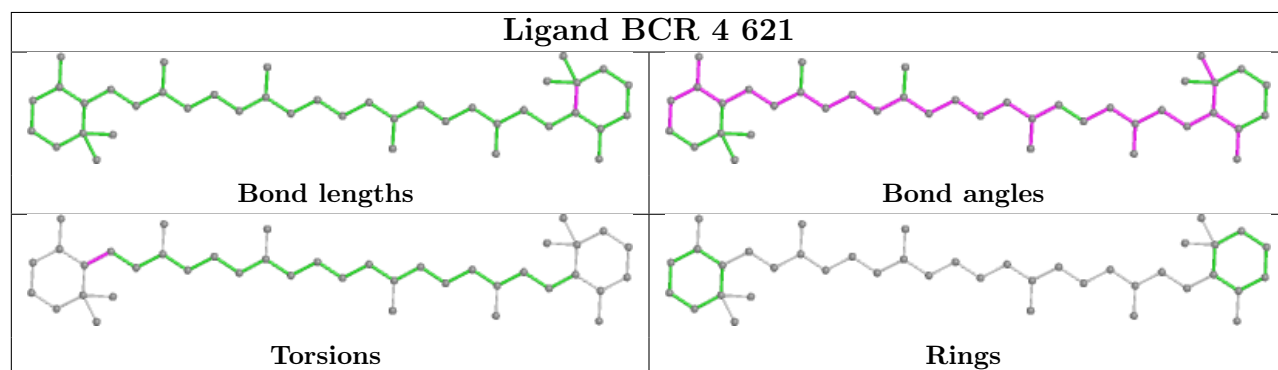
Bond angles



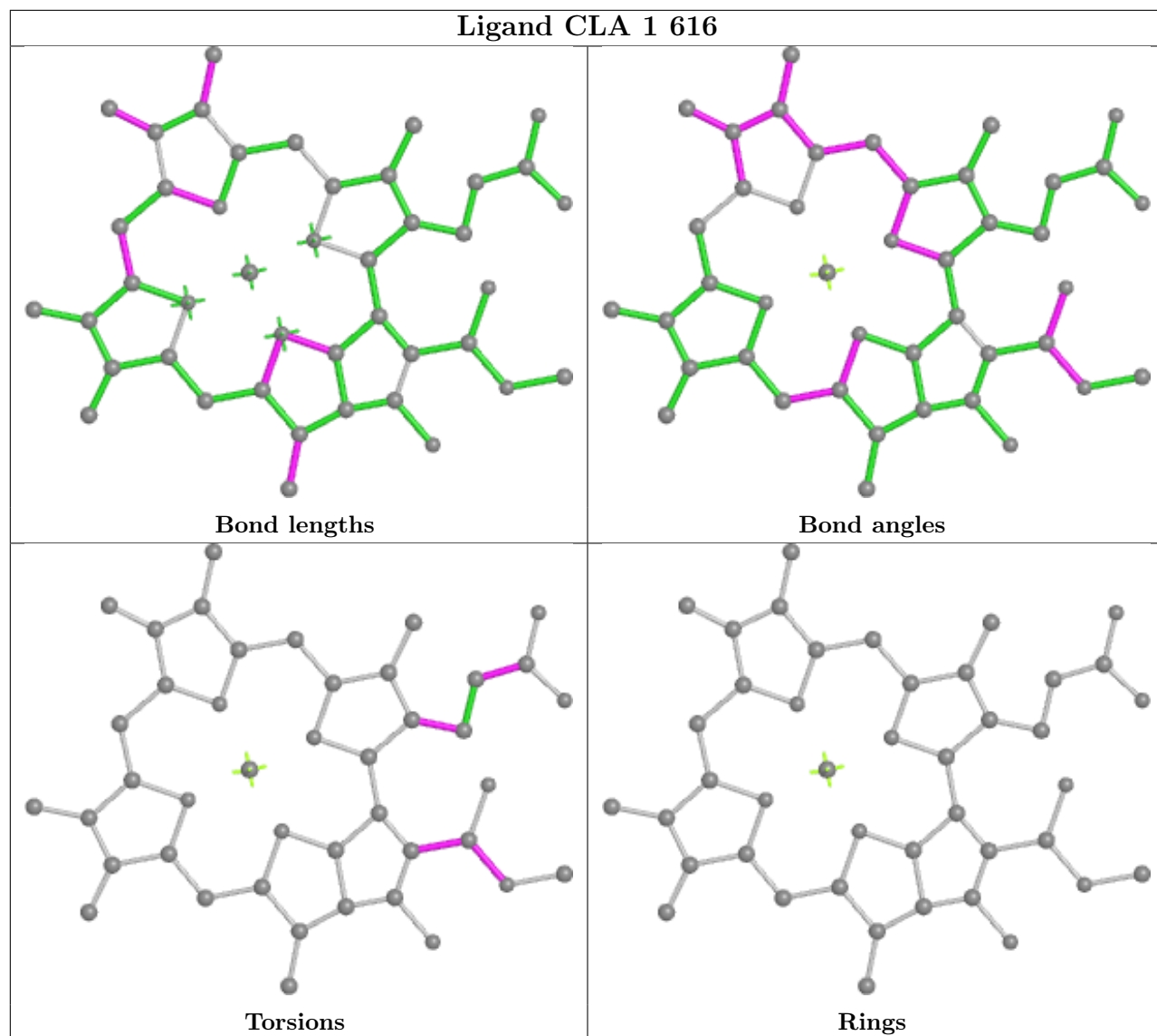
Torsions



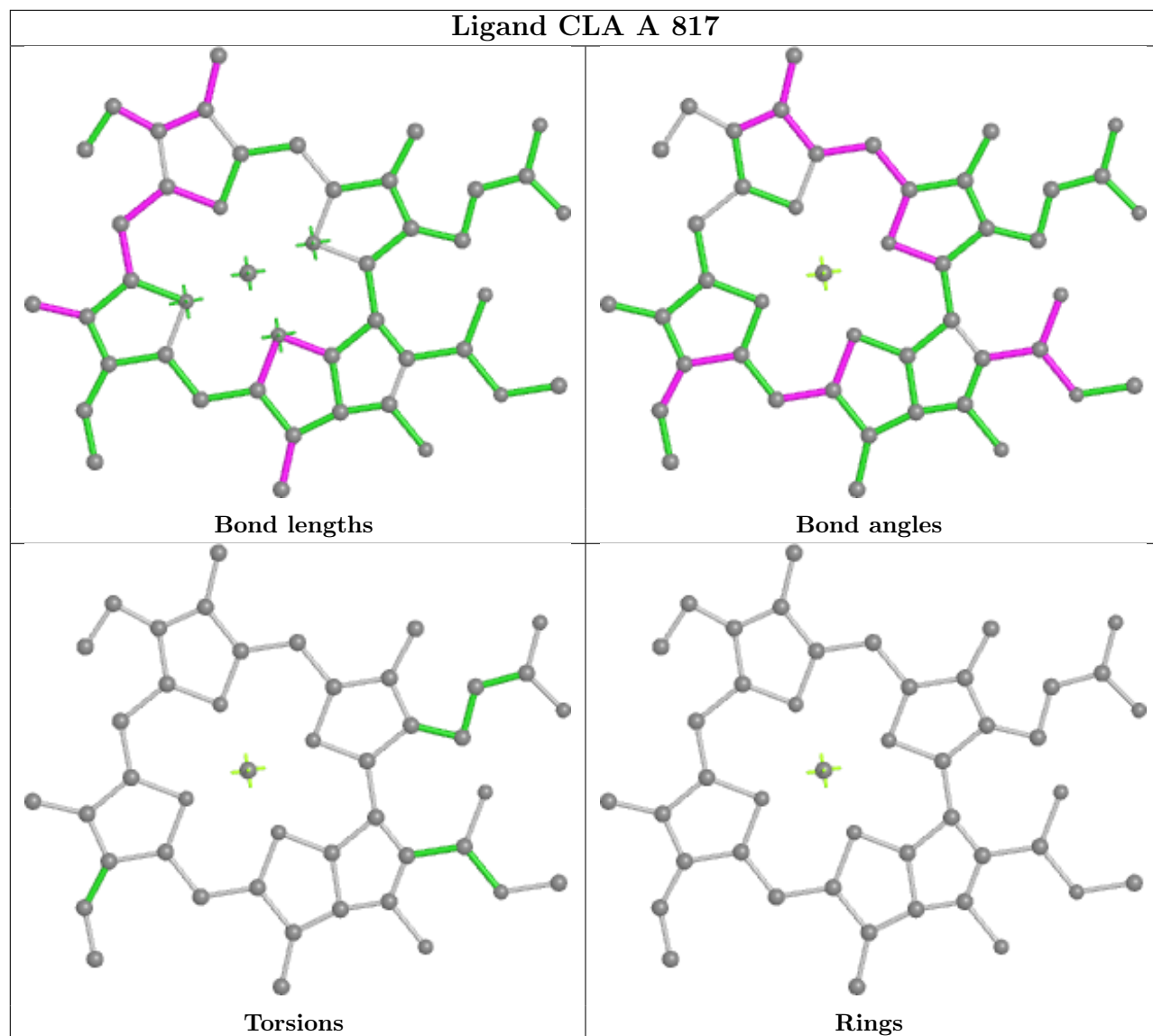
Rings

Ligand CLA 6 610**Ligand BCR 4 621**

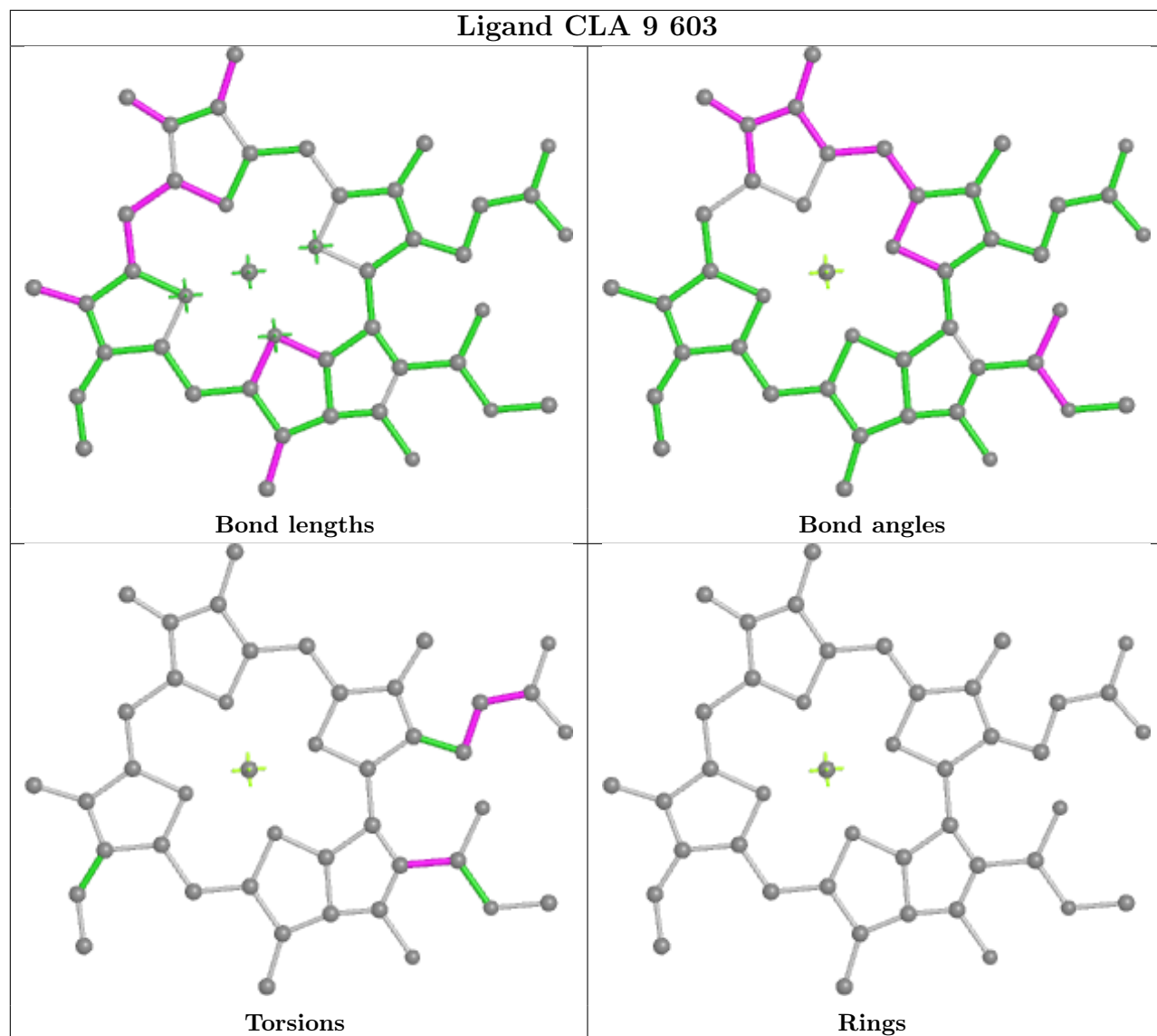
Ligand CLA 1 616

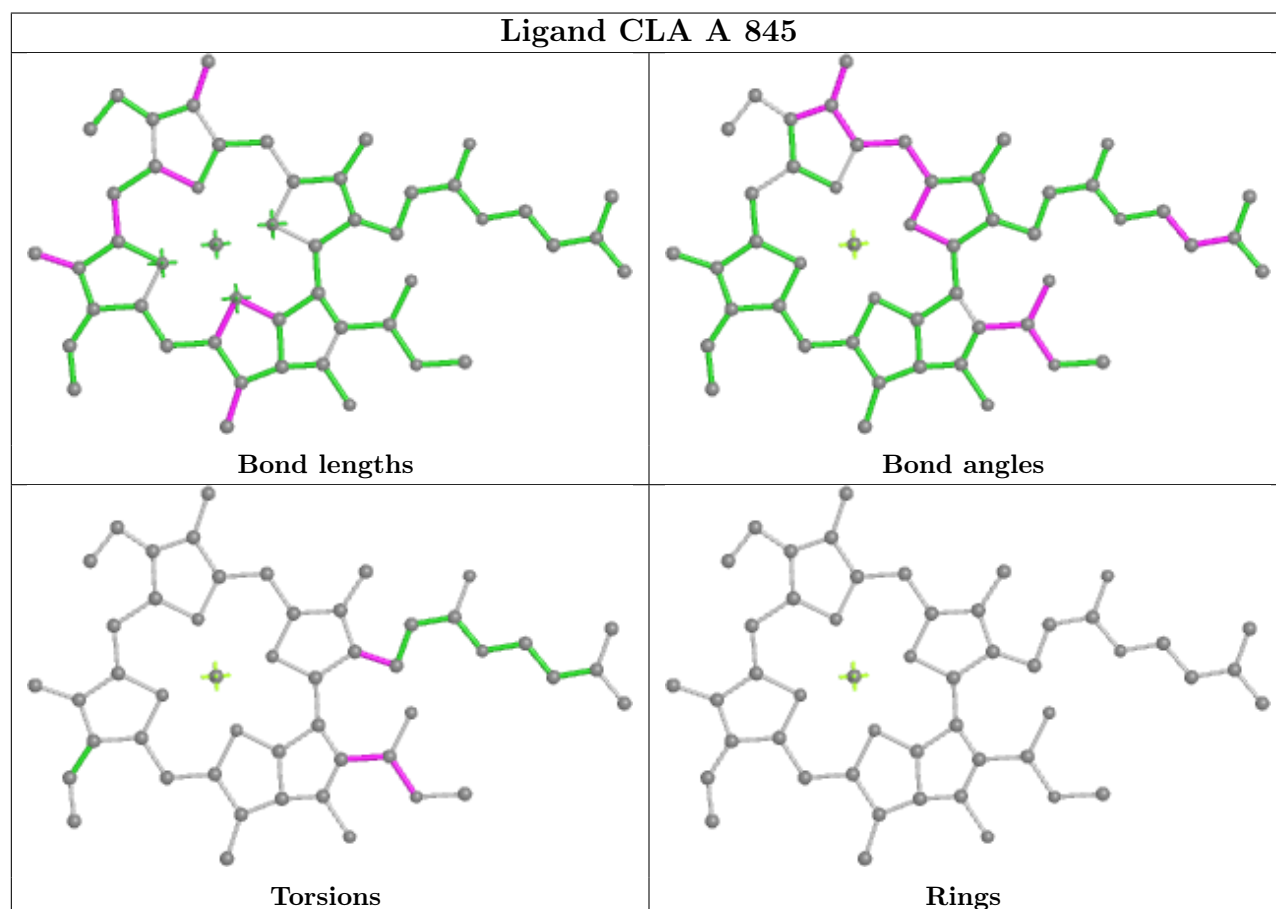
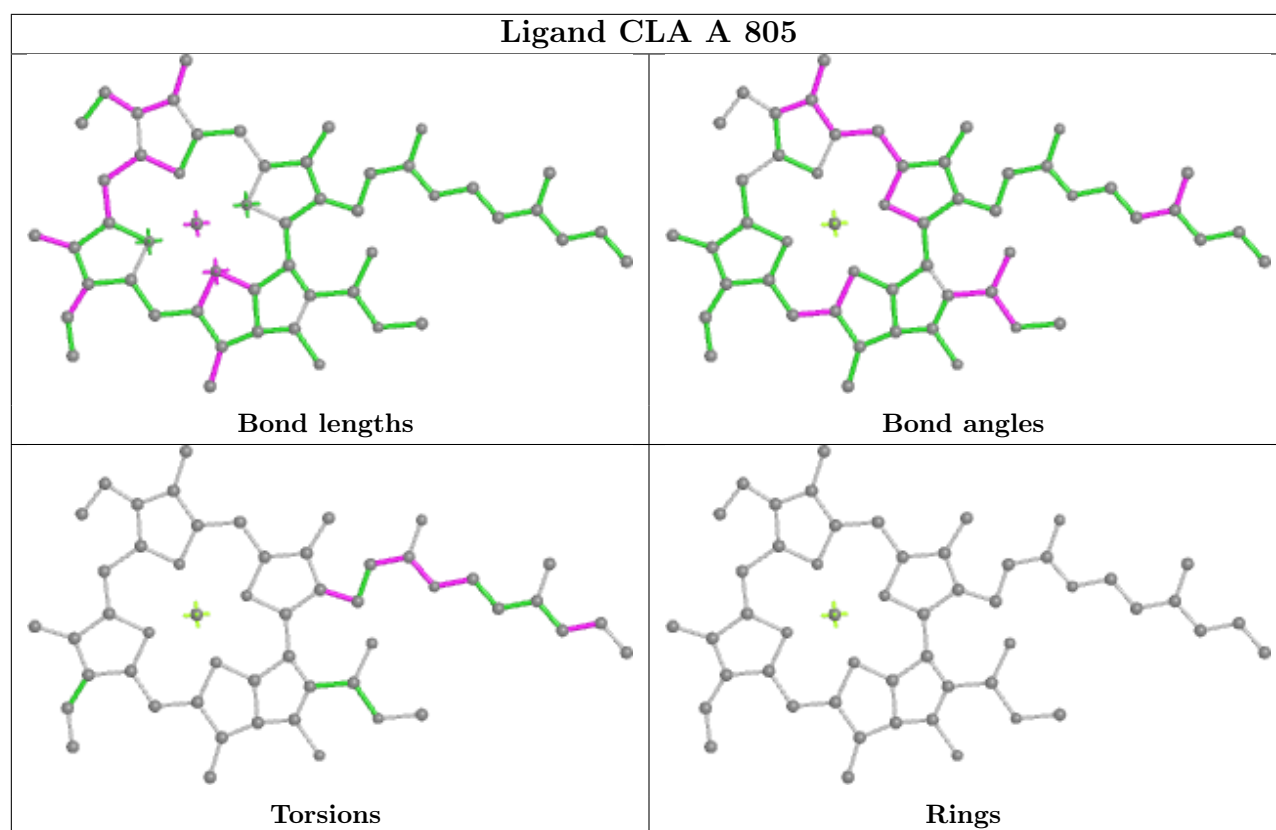


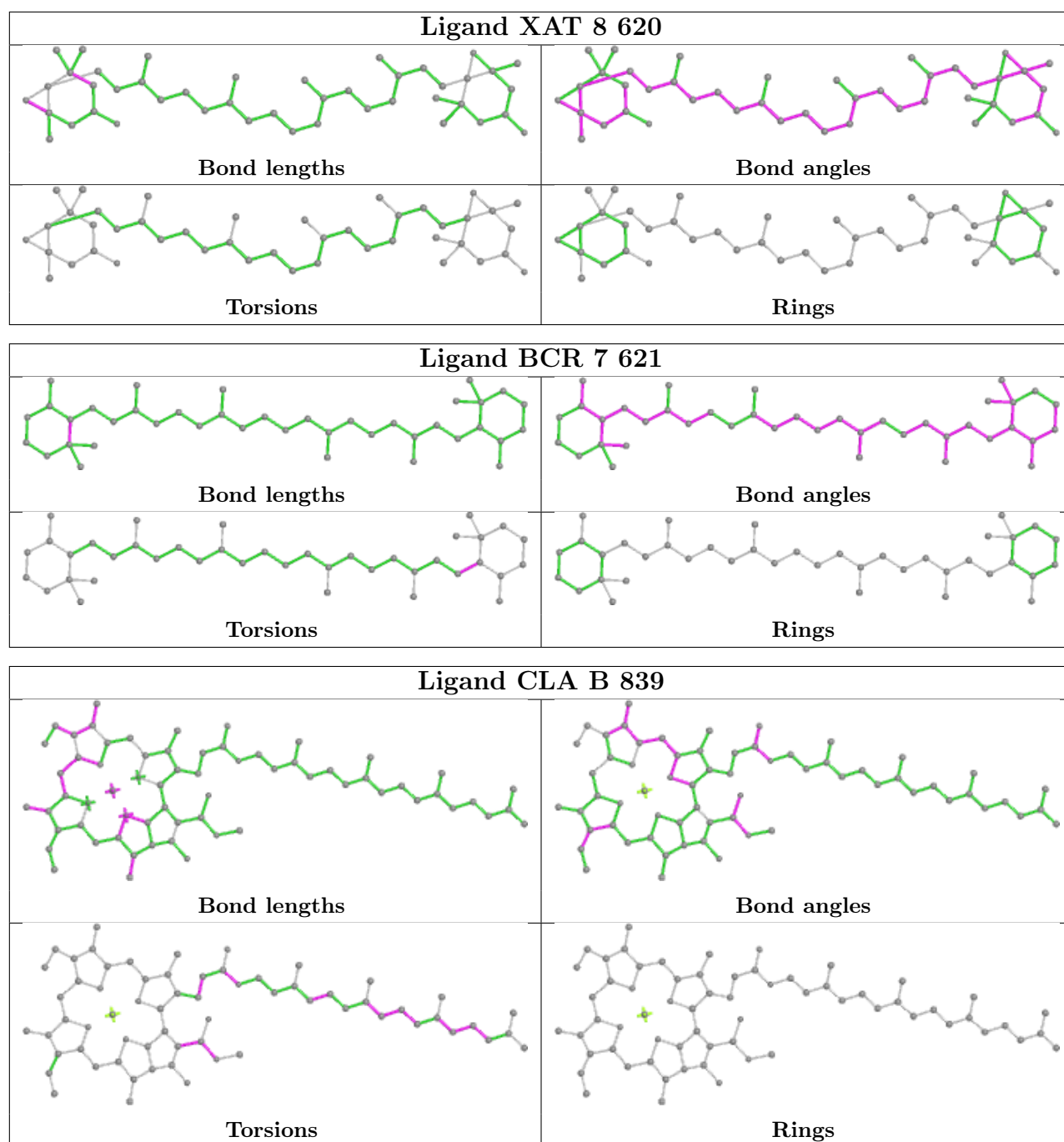
Ligand CLA A 817

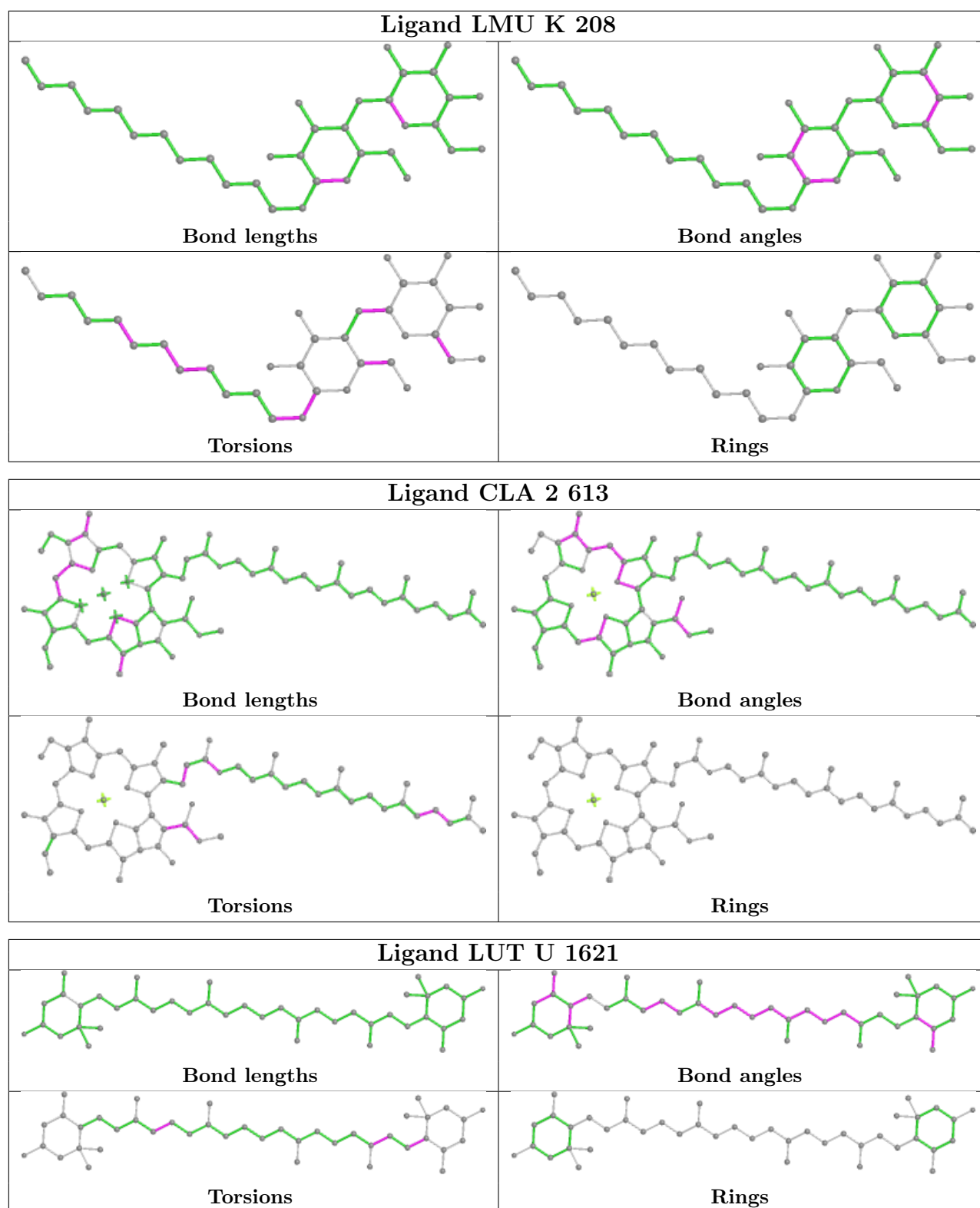


Ligand CLA 9 603

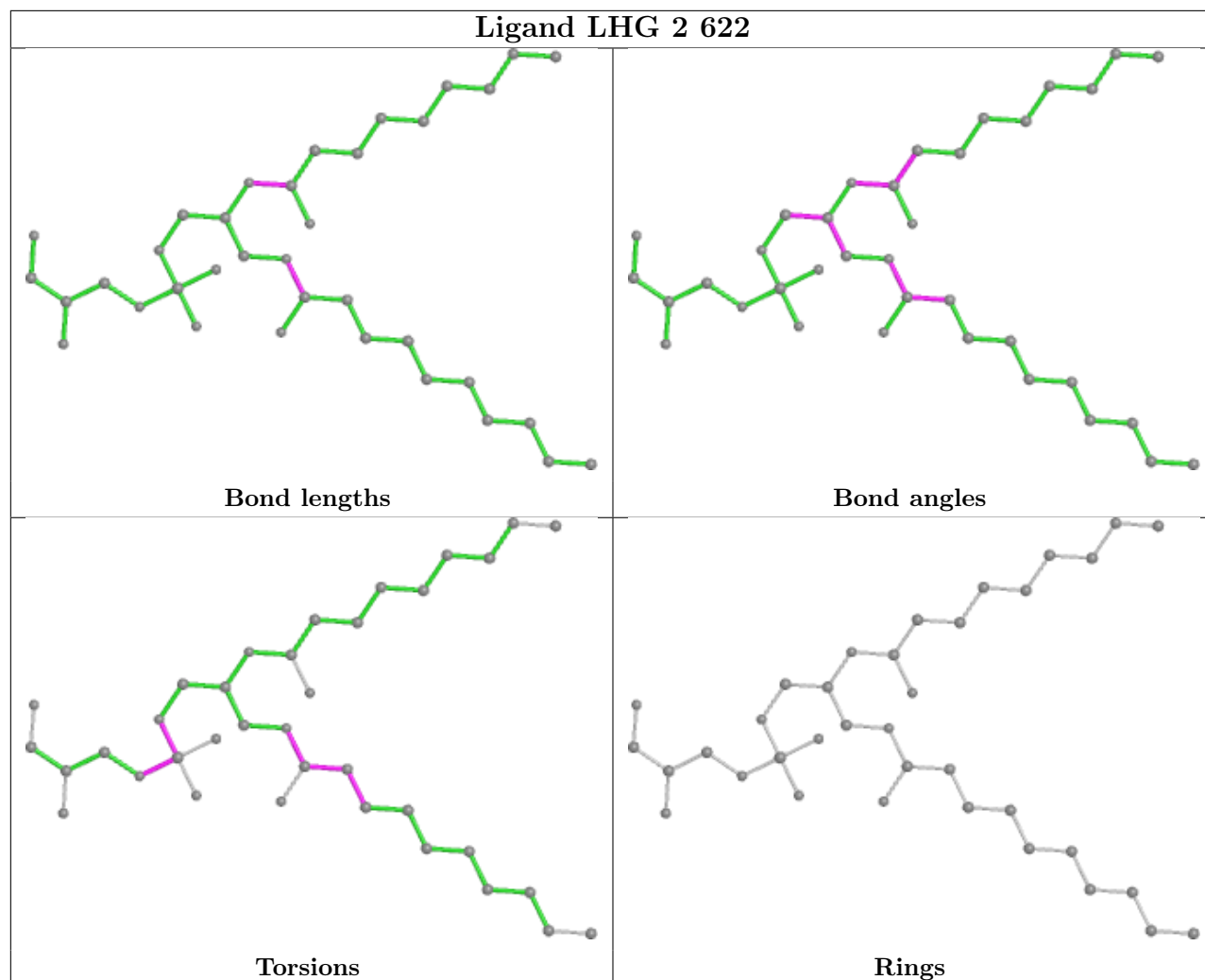




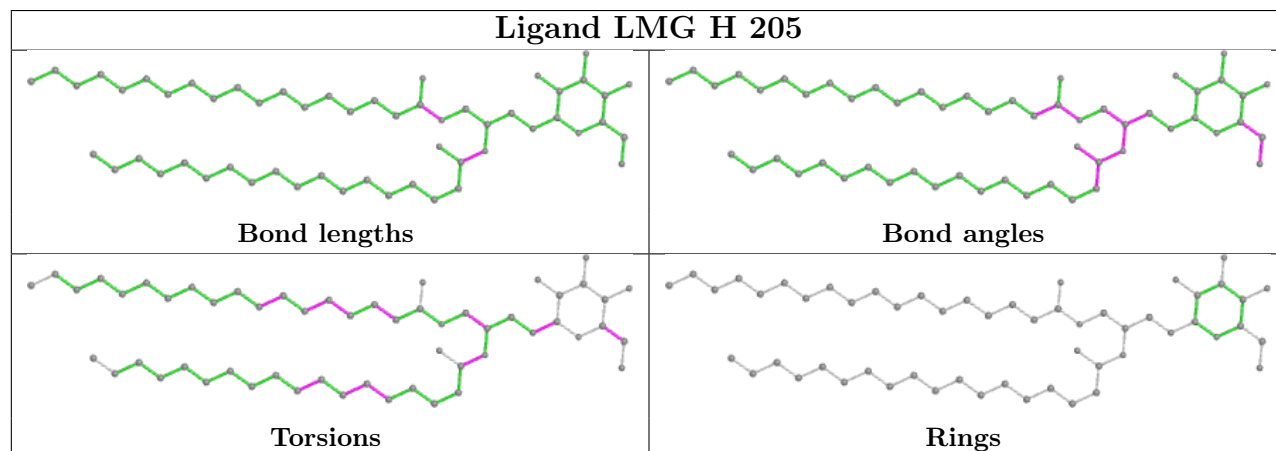




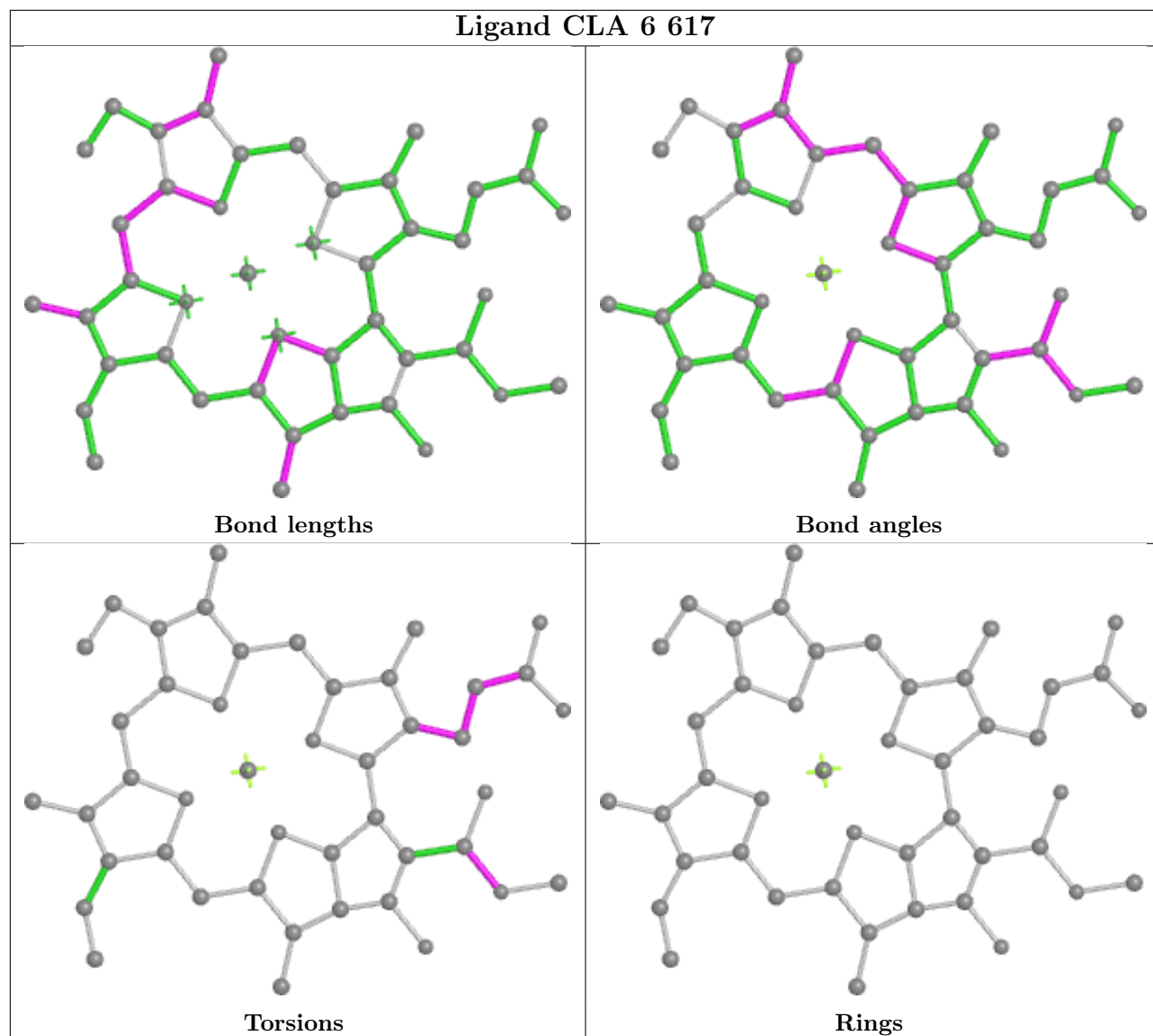
Ligand LHG 2 622

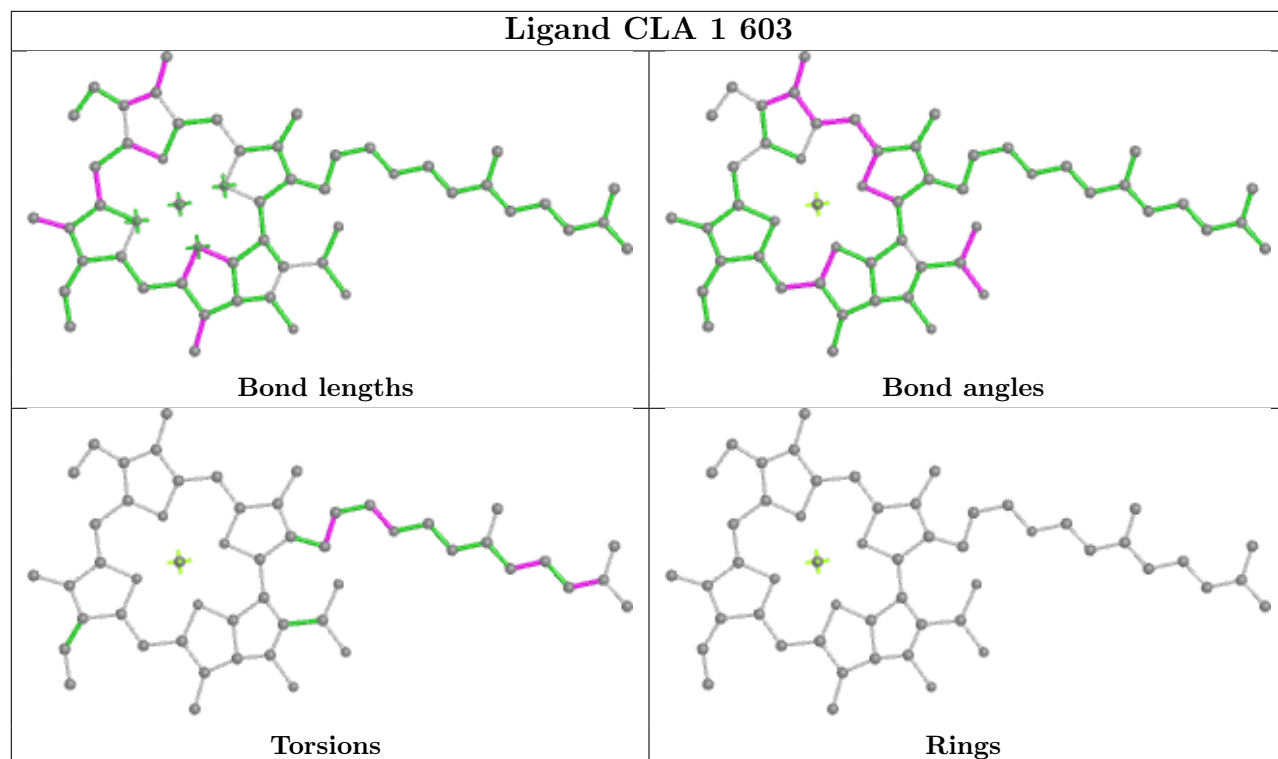
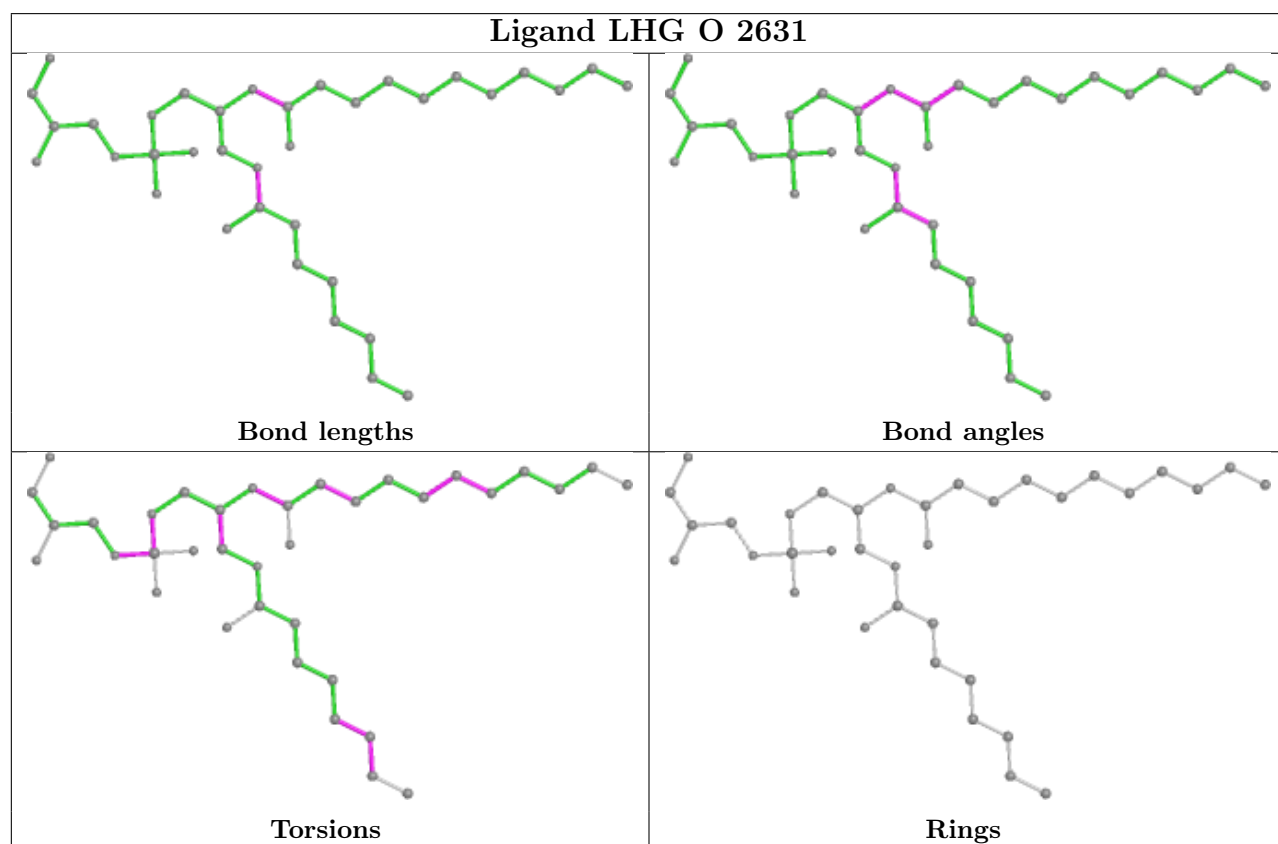


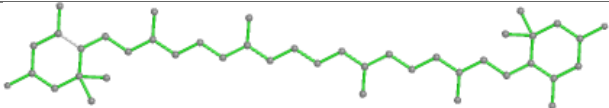
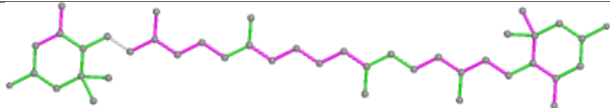
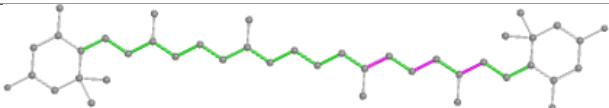
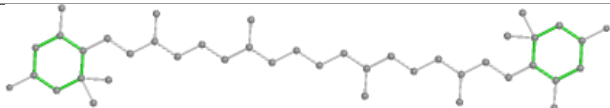
Ligand LMG H 205

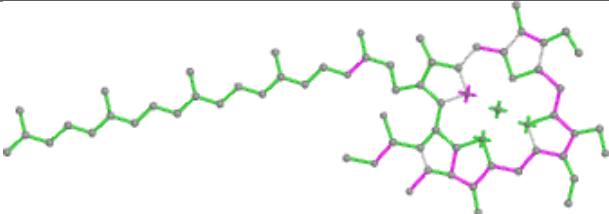
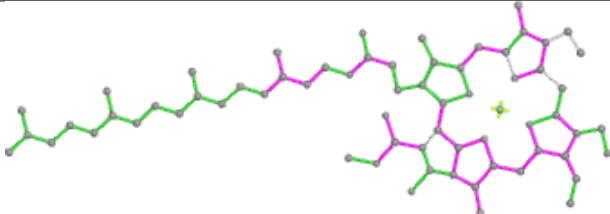
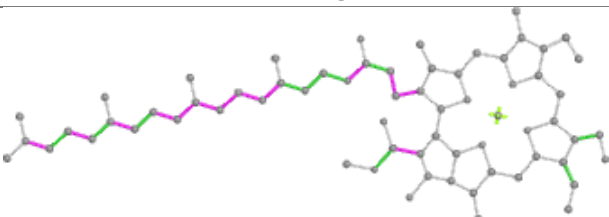
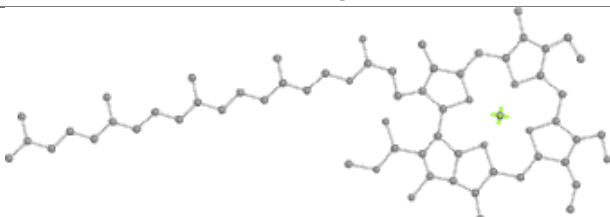


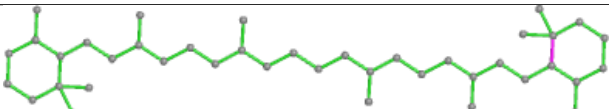
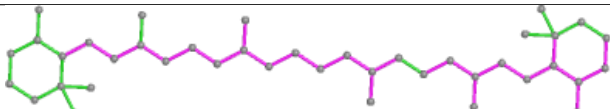
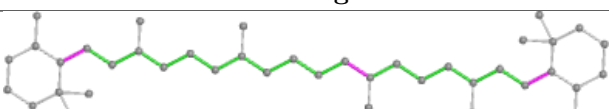

Ligand CLA 6 617



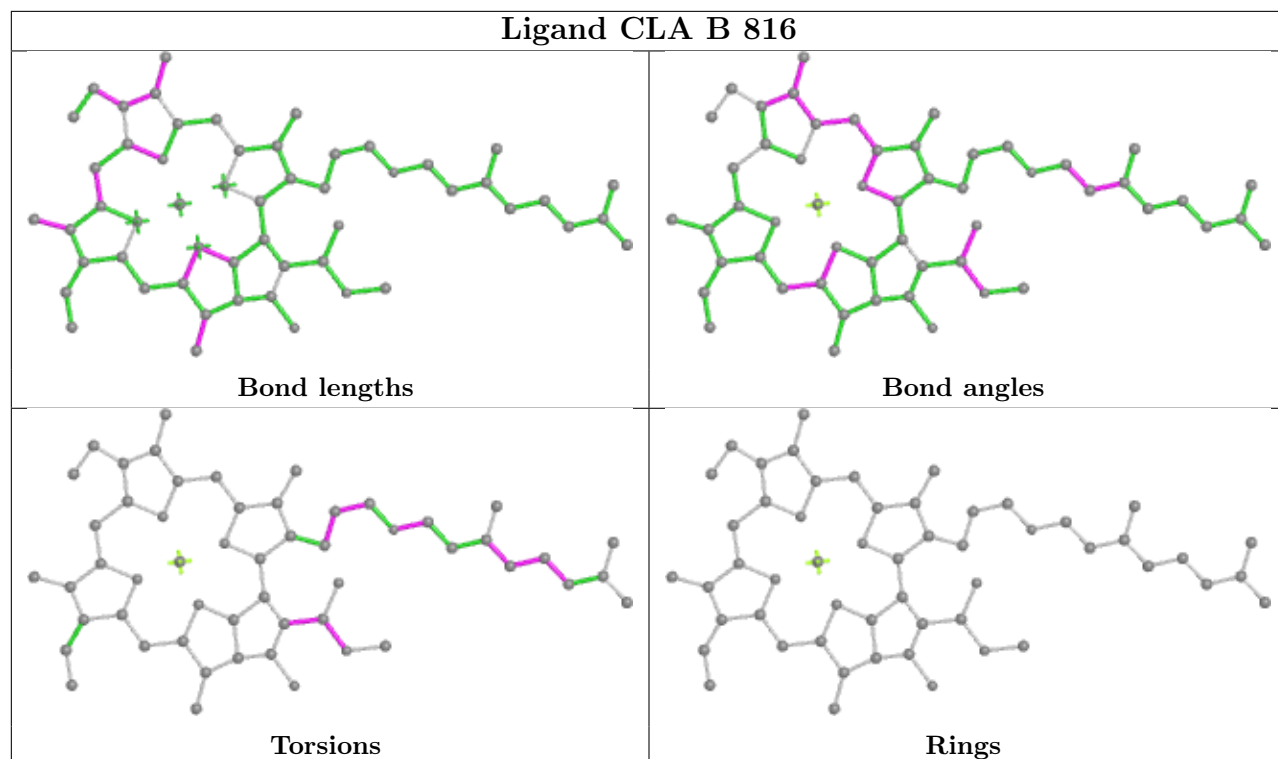
Ligand CLA 1 603**Ligand LHG O 2631**

Ligand LUT Z 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

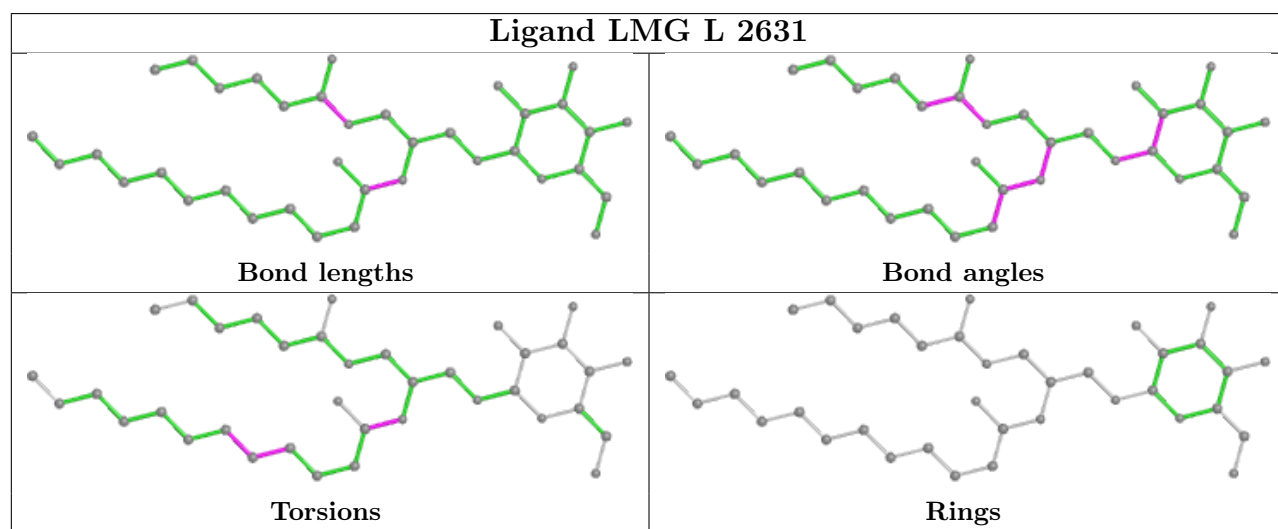
Ligand CHL Y 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

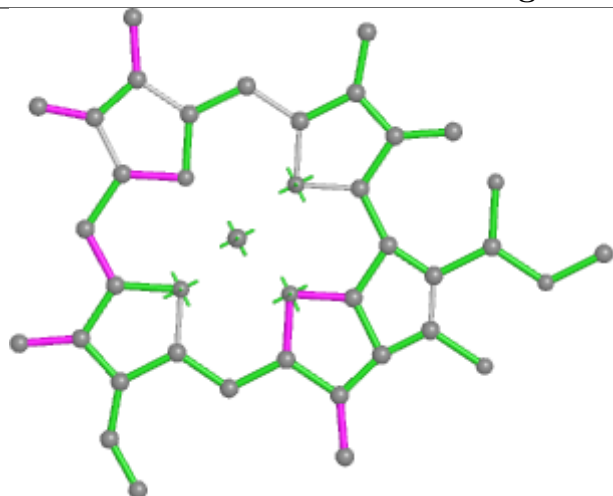
Ligand CLA B 816



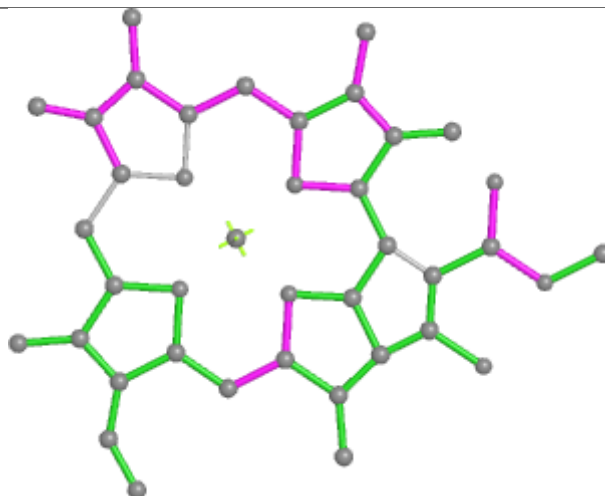
Ligand LMG L 2631



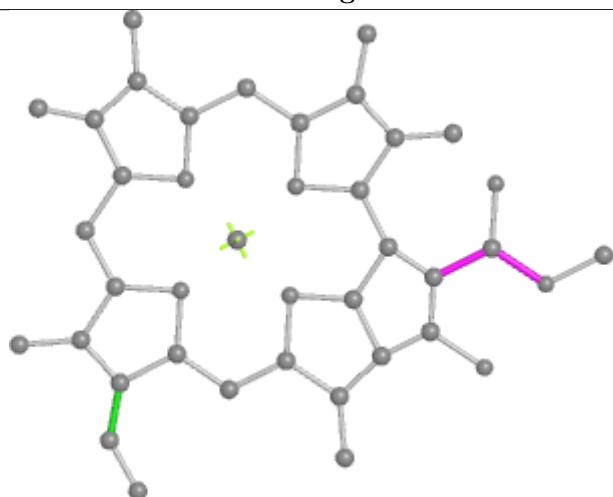
Ligand CLA 1 609



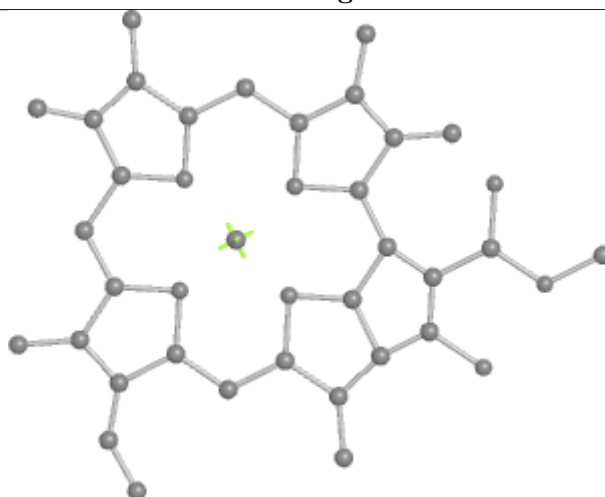
Bond lengths



Bond angles

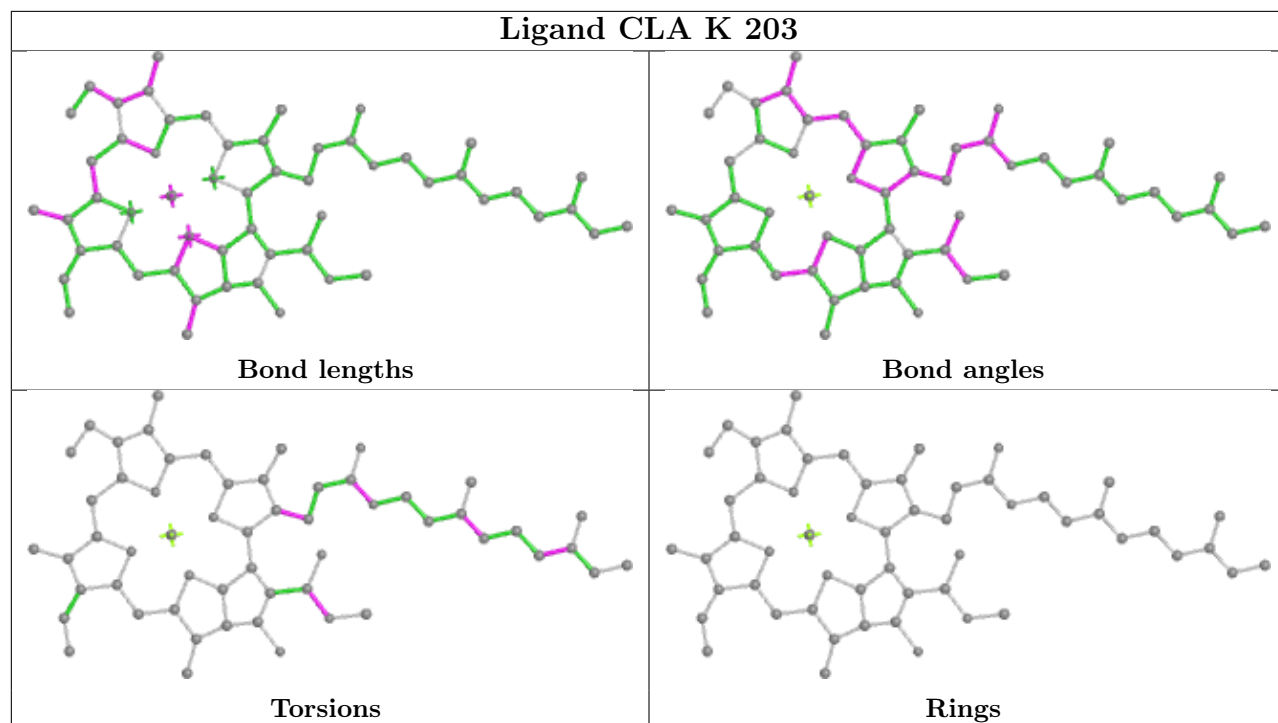


Torsions

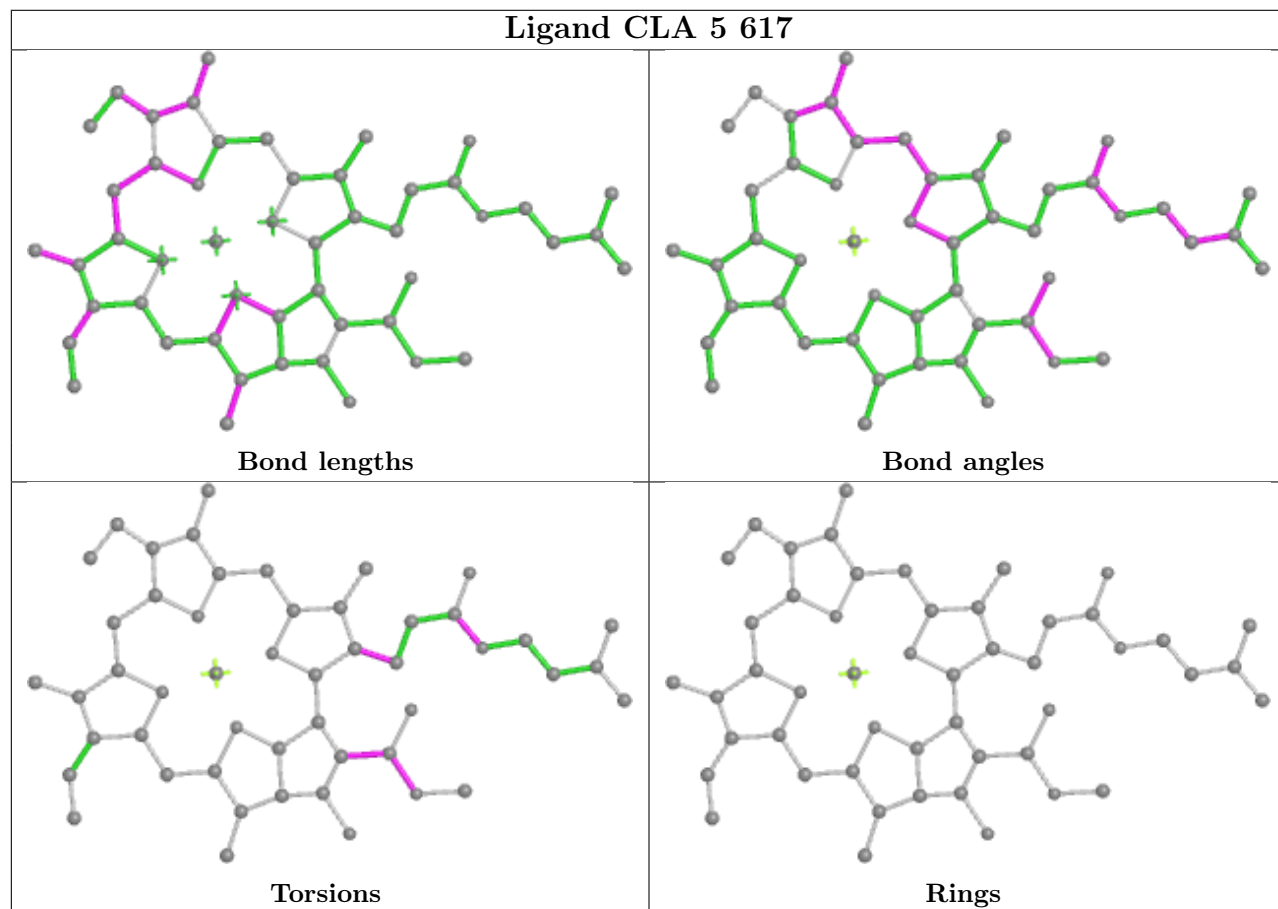


Rings

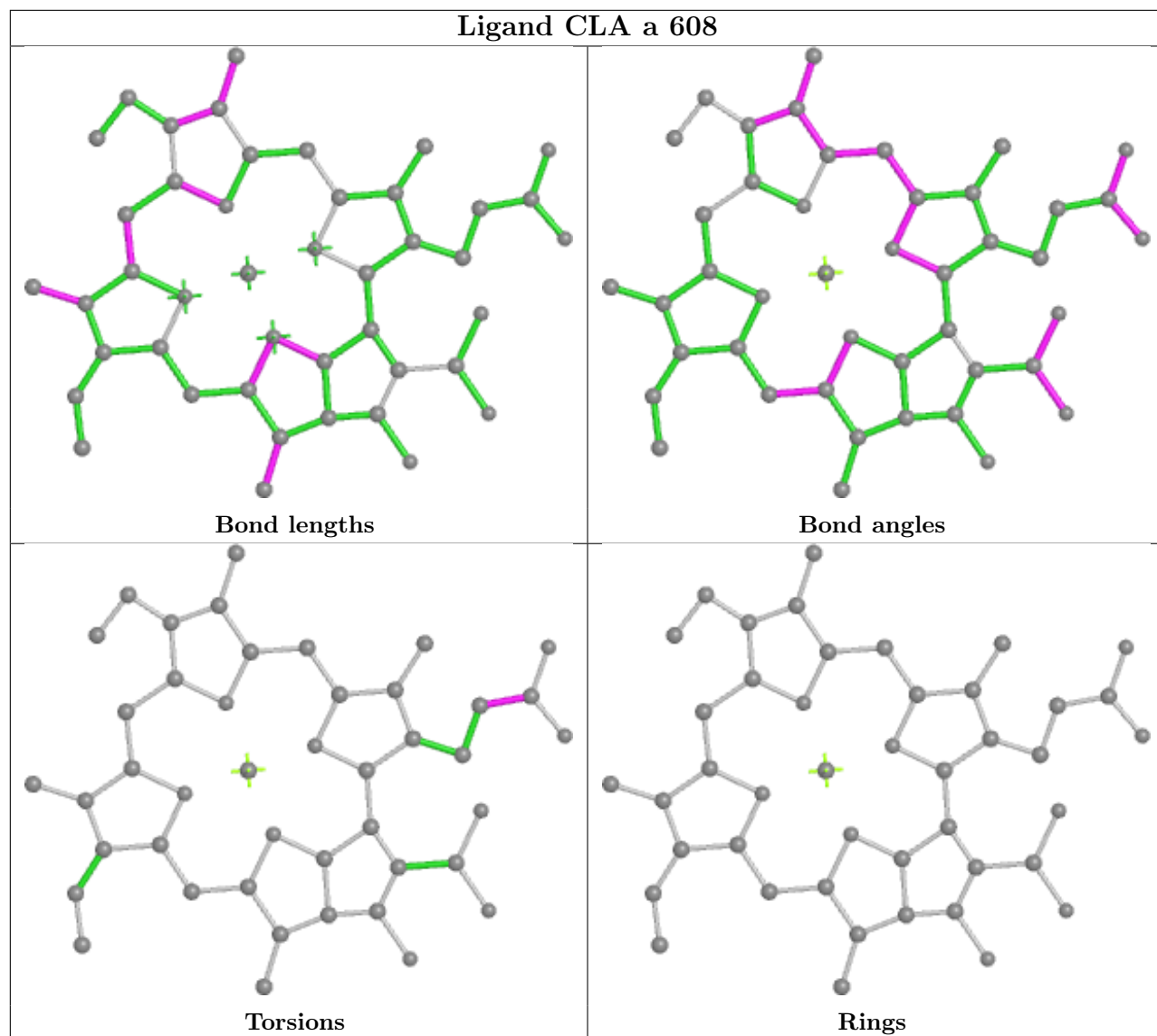
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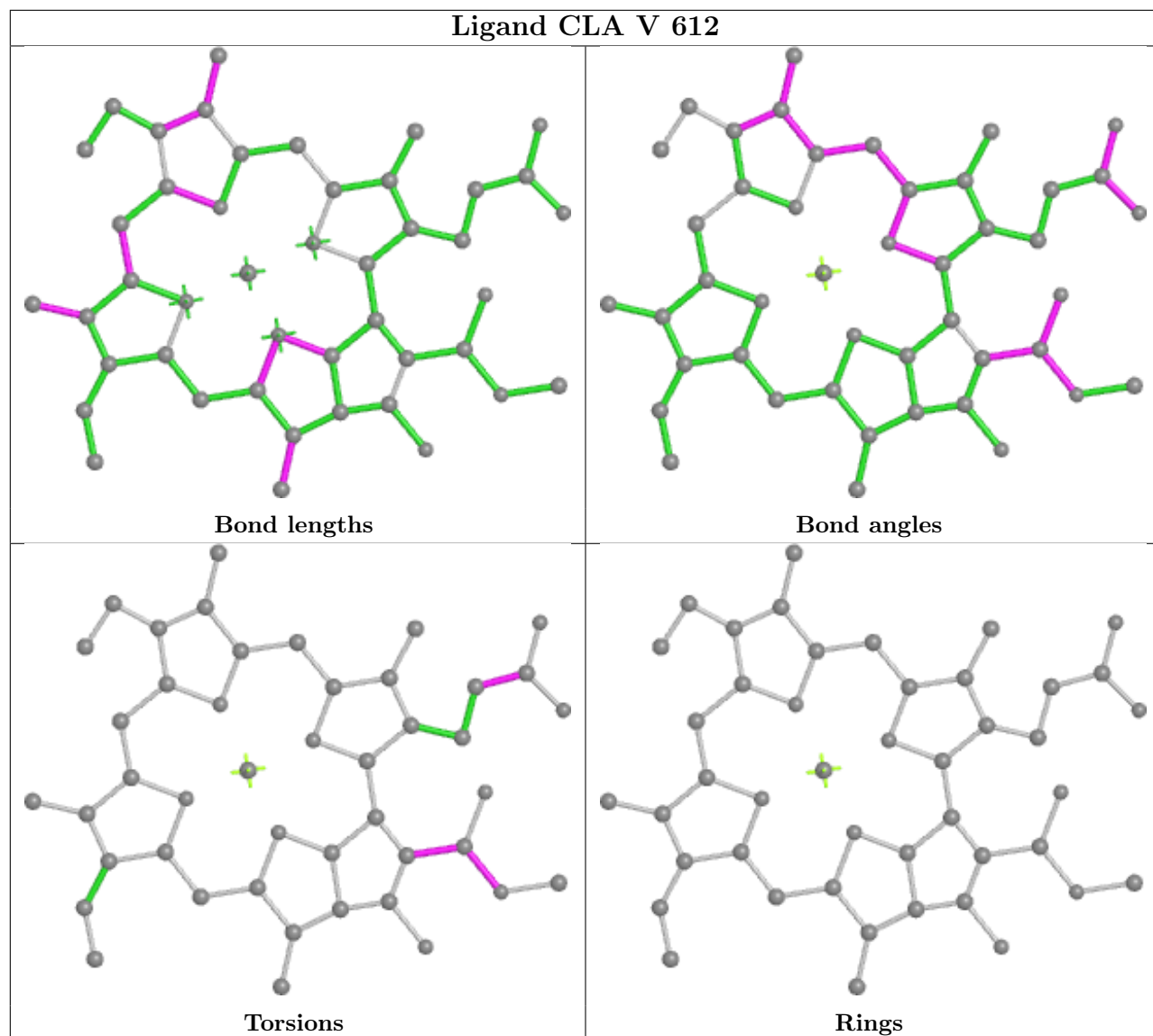
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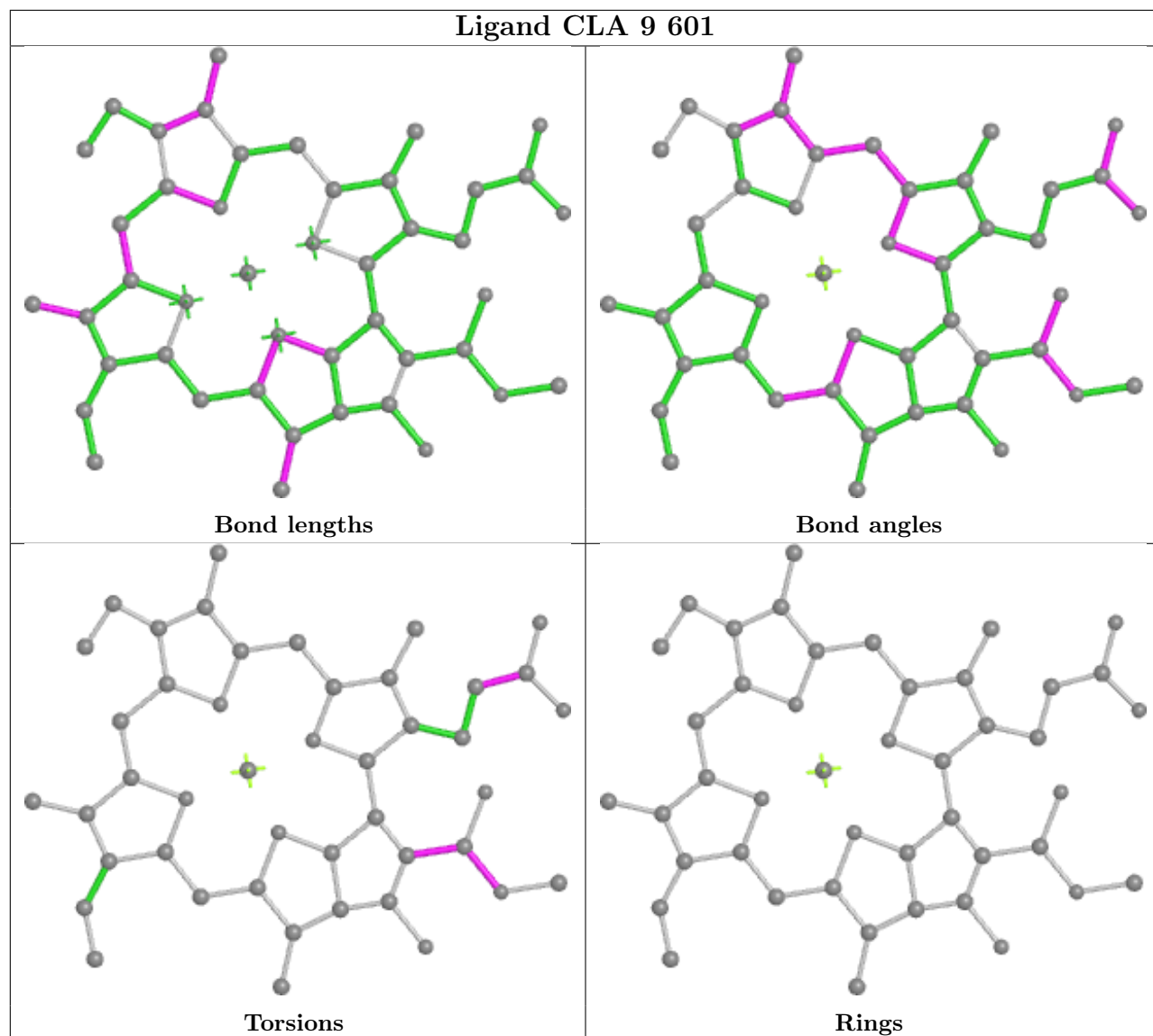
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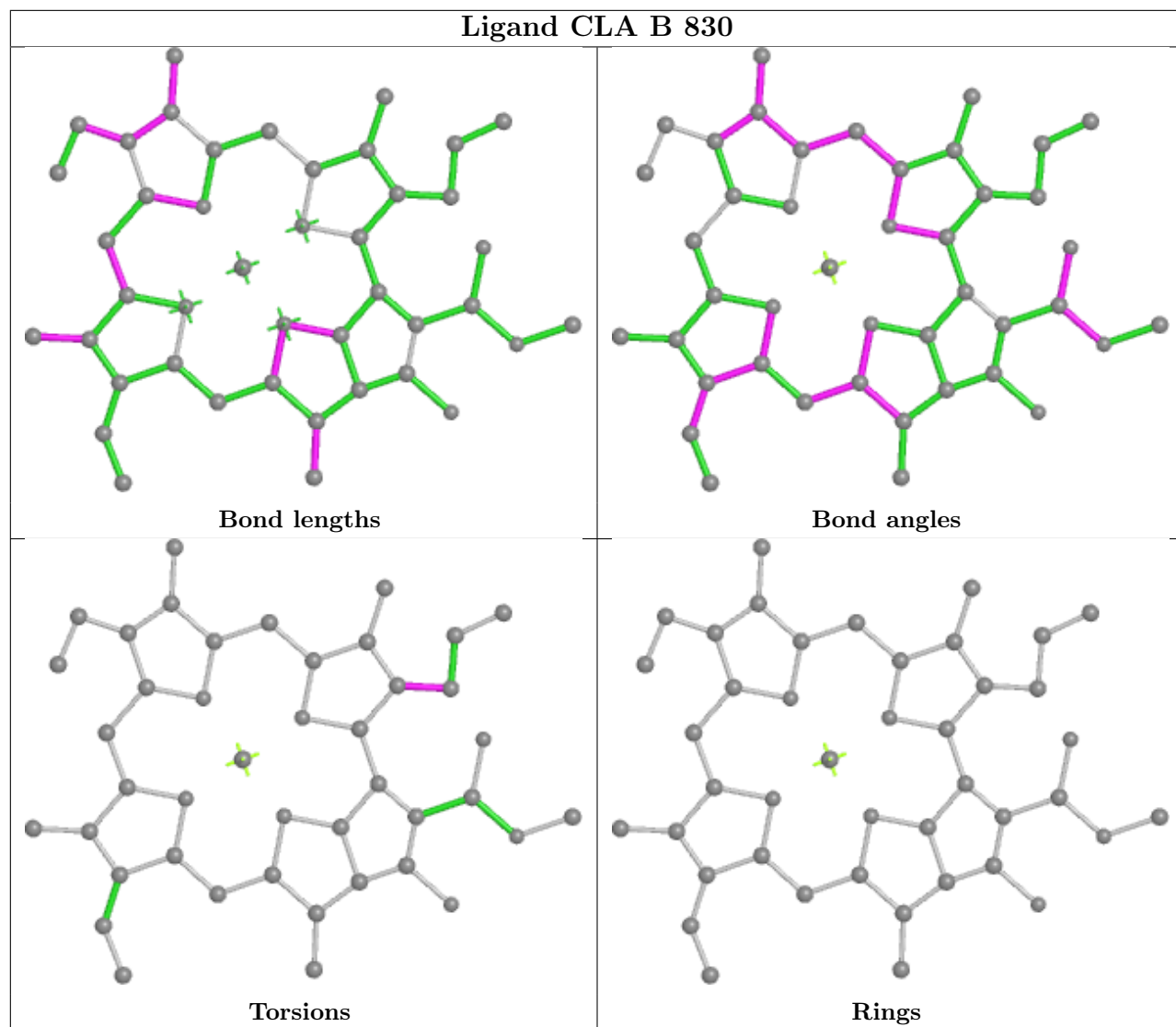
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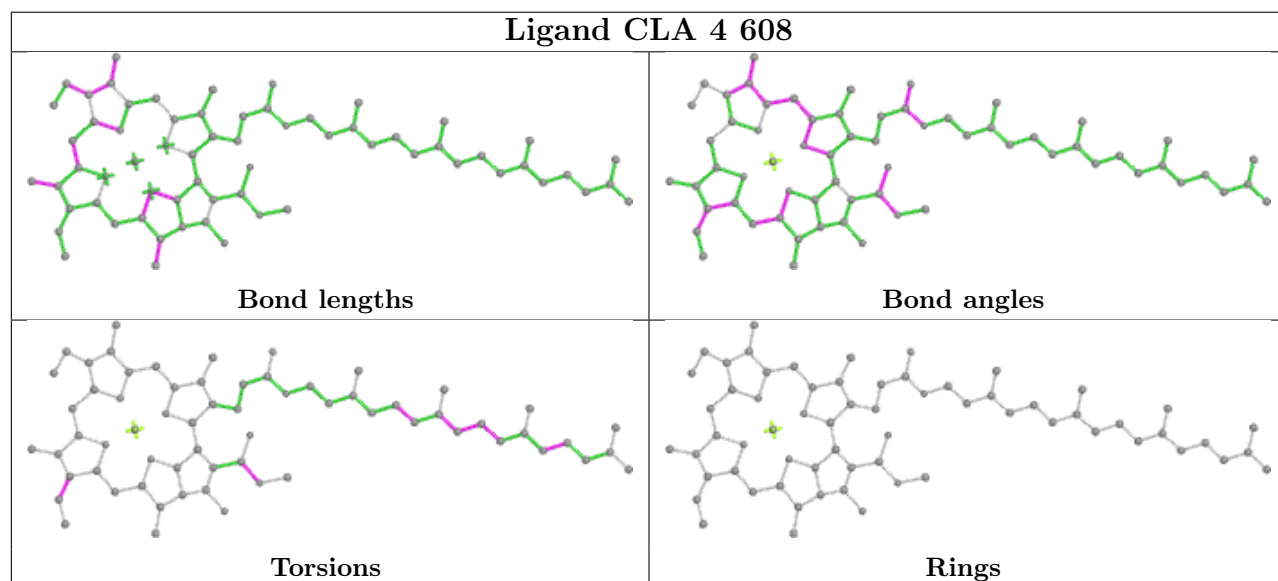
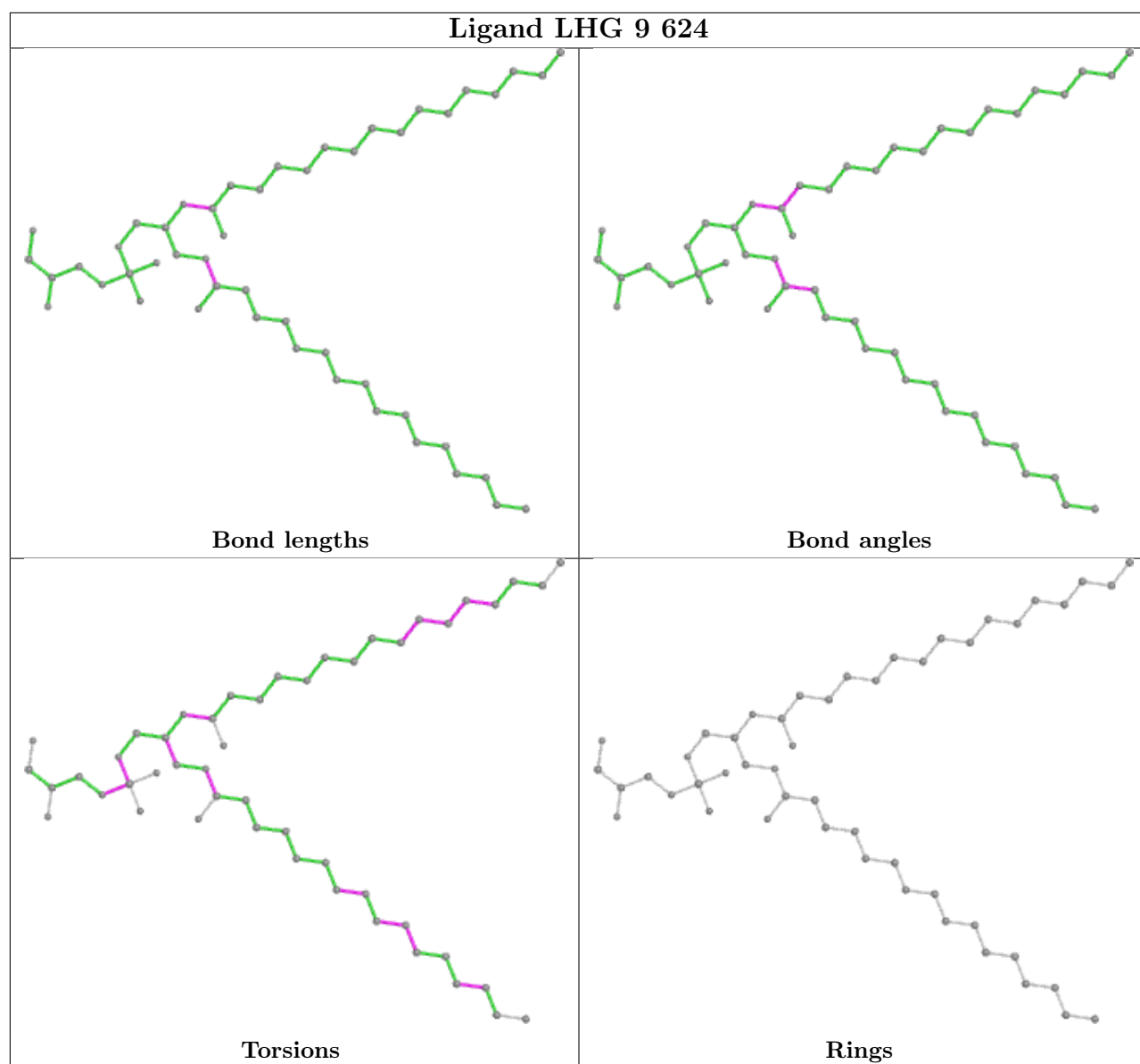


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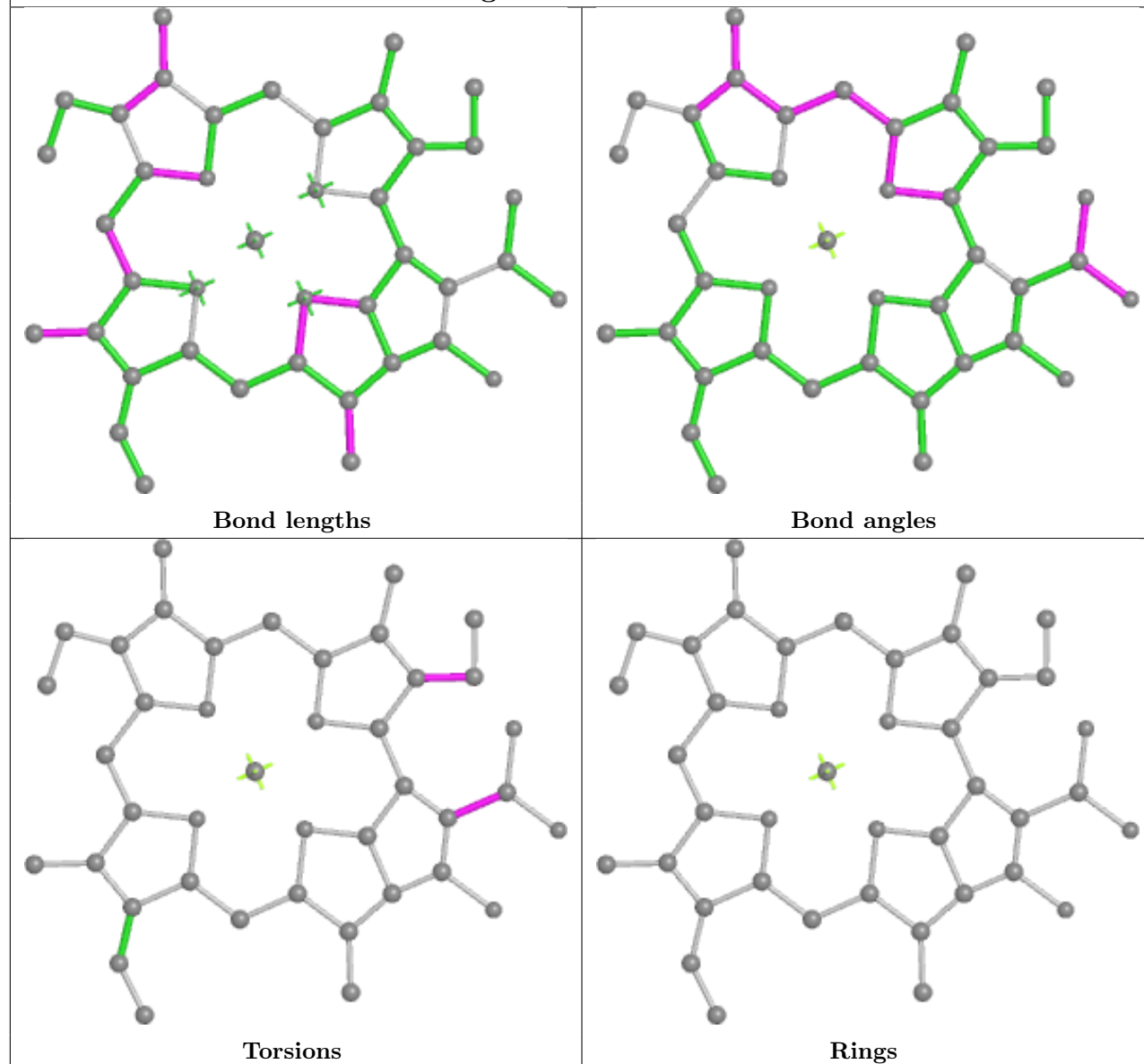


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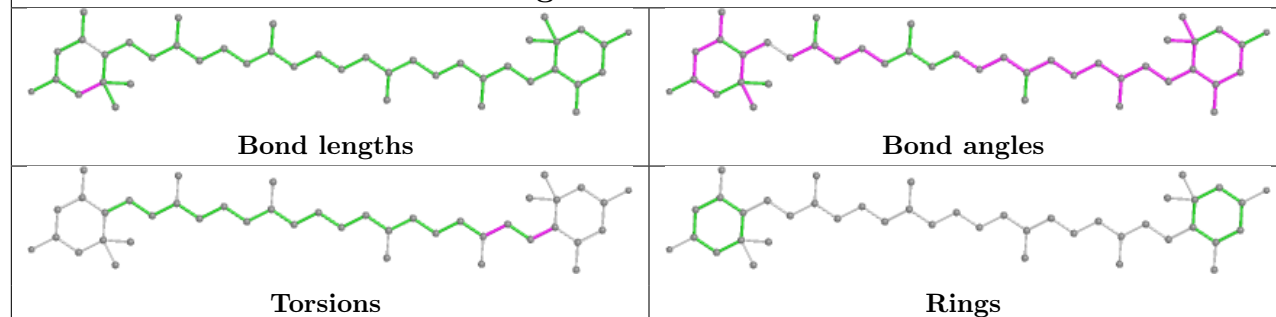


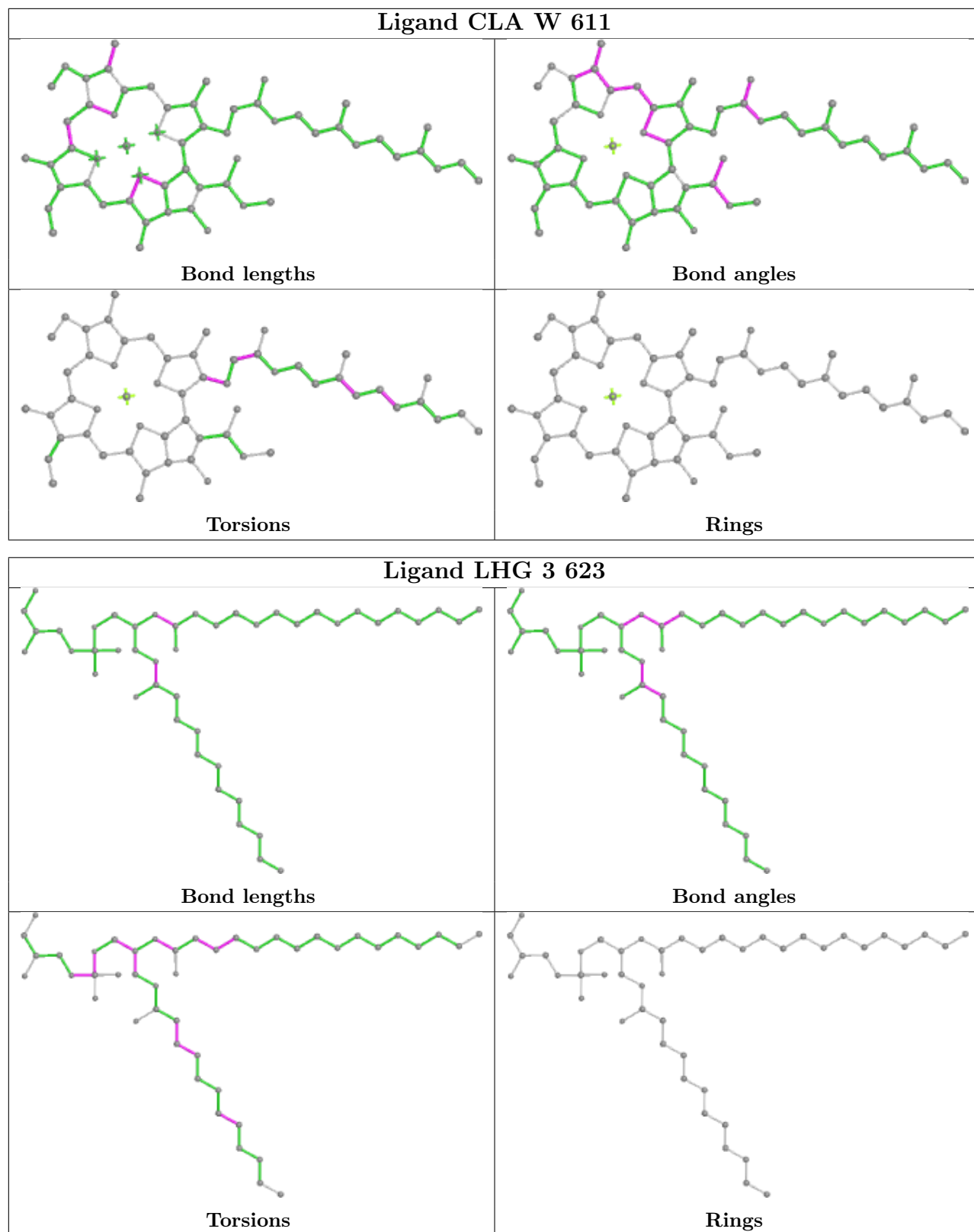


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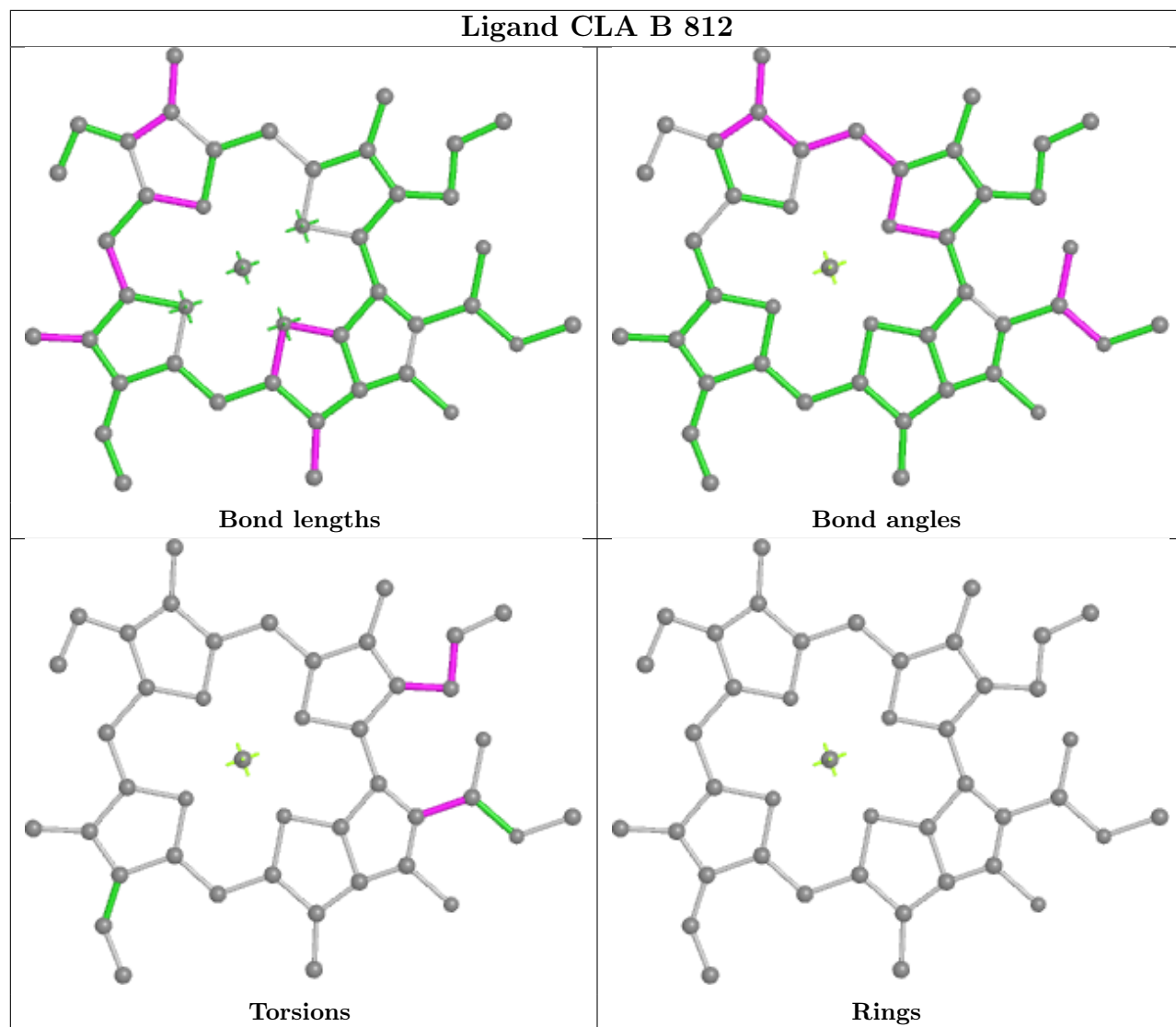


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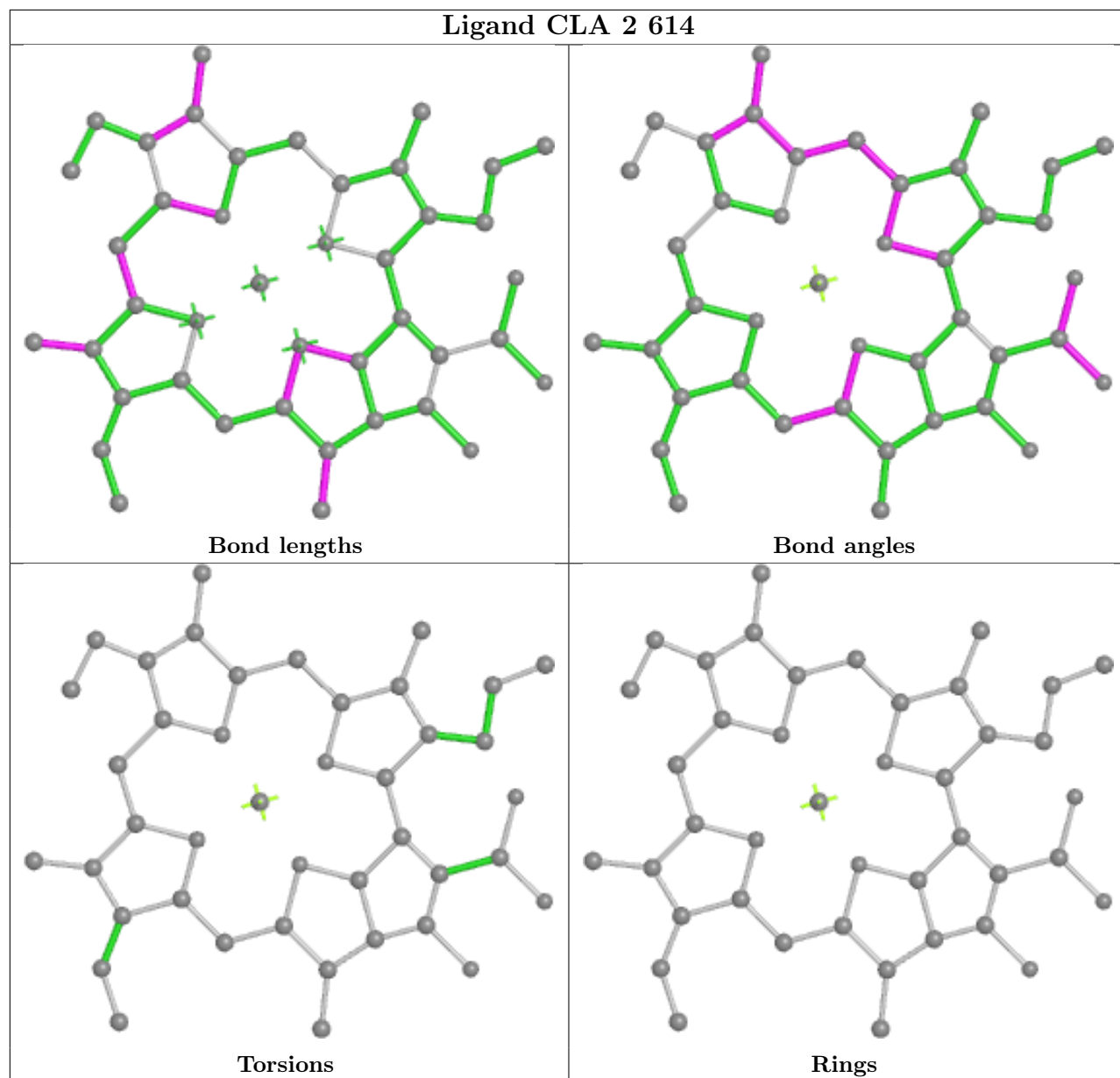




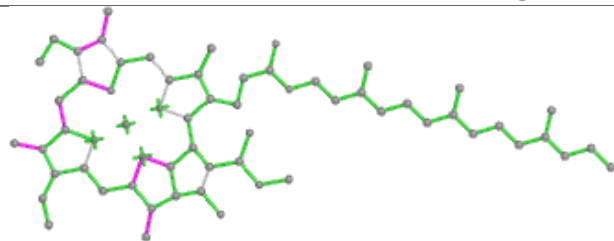
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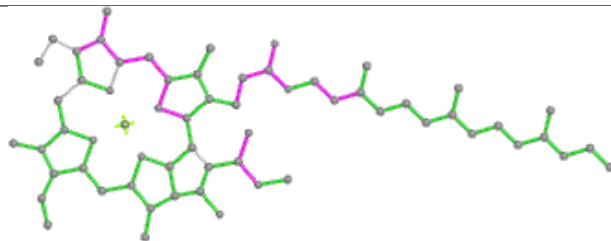
Ligand CLA 2 614



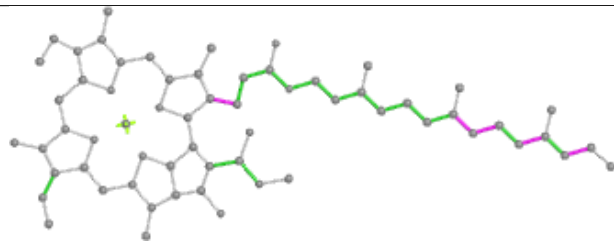
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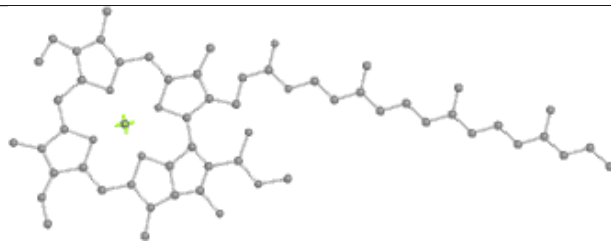
Bond lengths



Bond angles

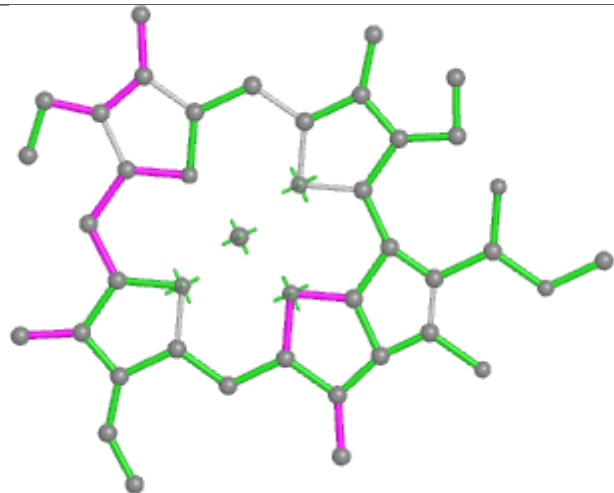


Torsions

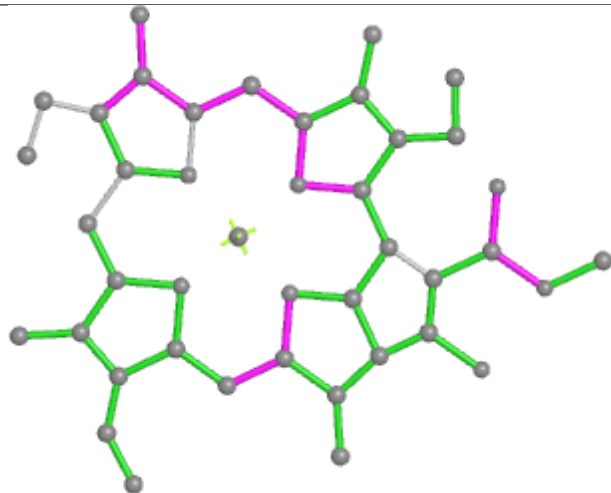


Rings

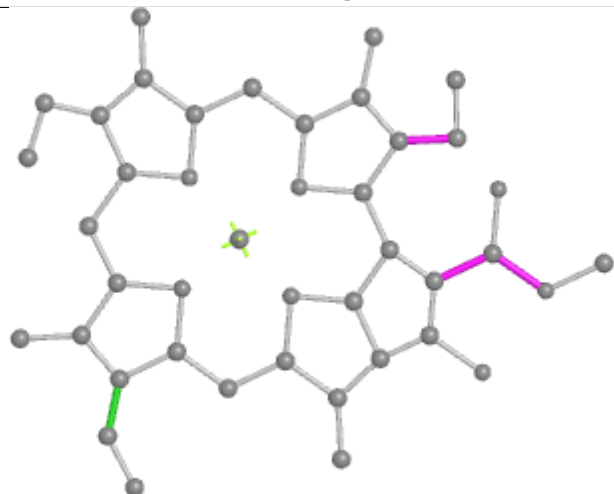
Ligand CLA B 822



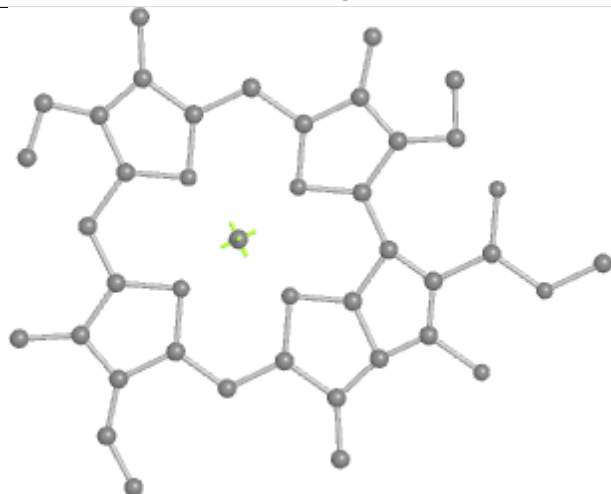
Bond lengths



Bond angles

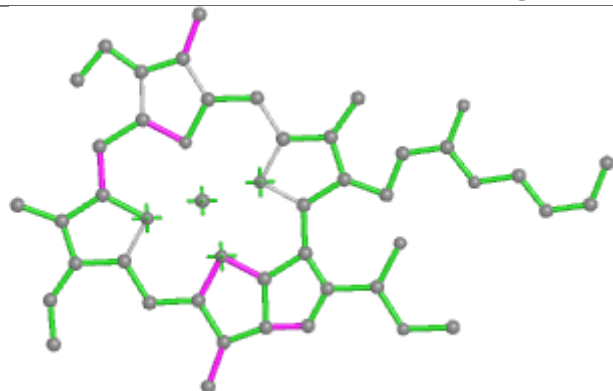


Torsions

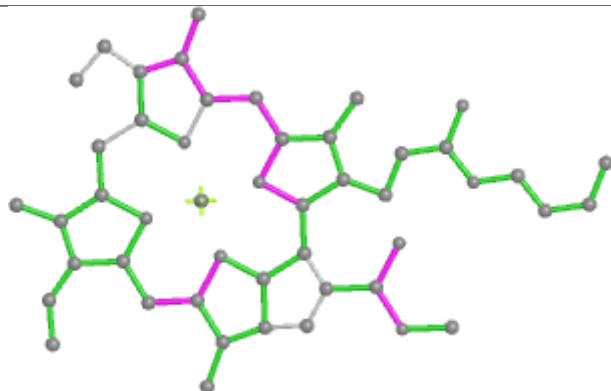


Rings

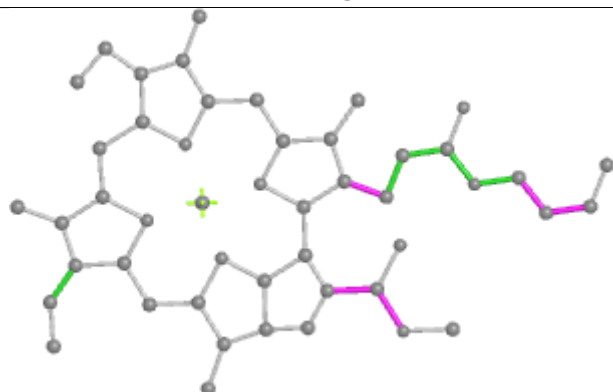
Ligand CLA U 604



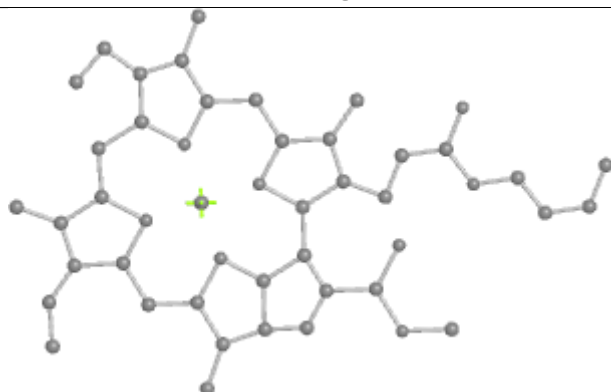
Bond lengths



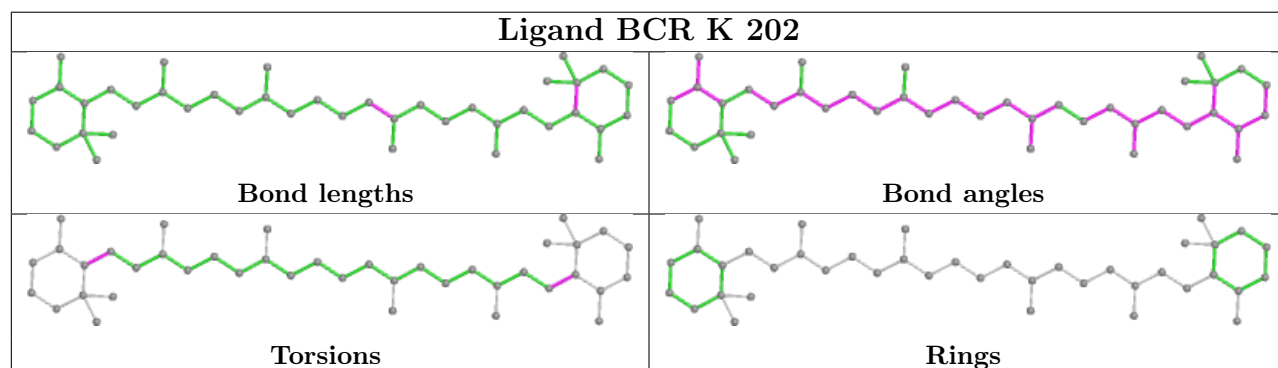
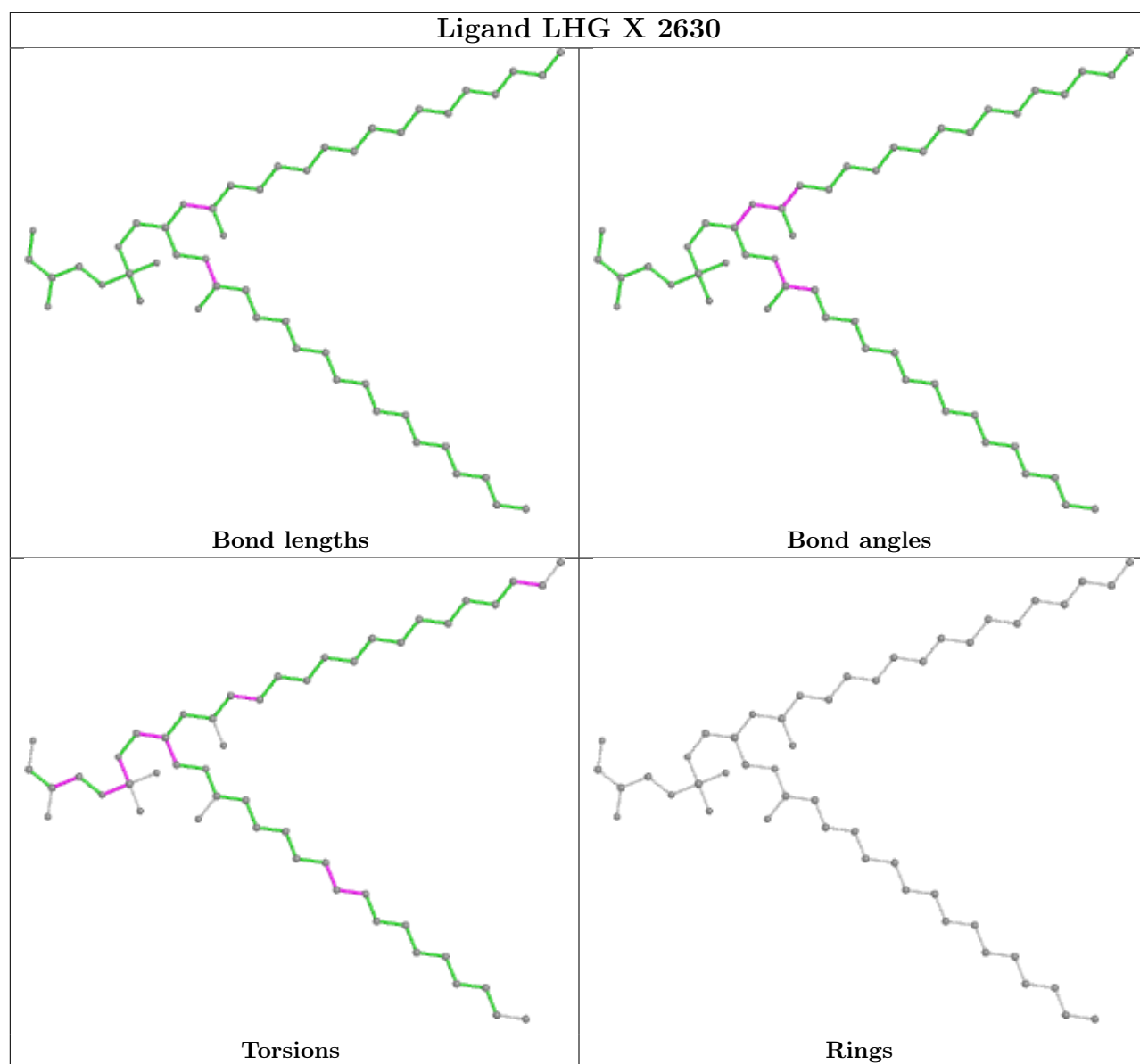
Bond angles



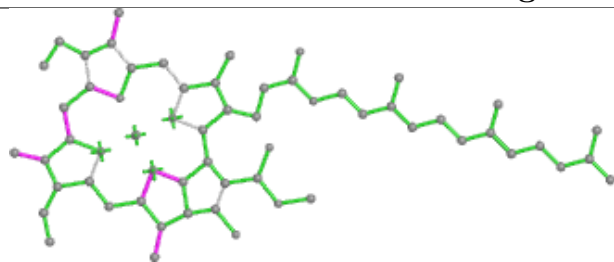
Torsions



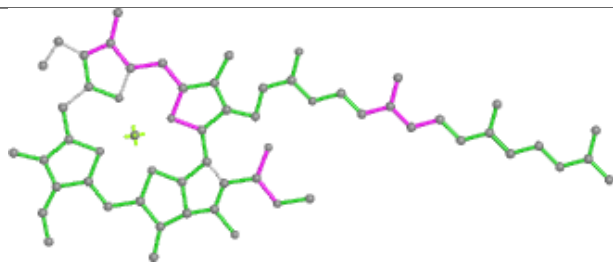
Rings



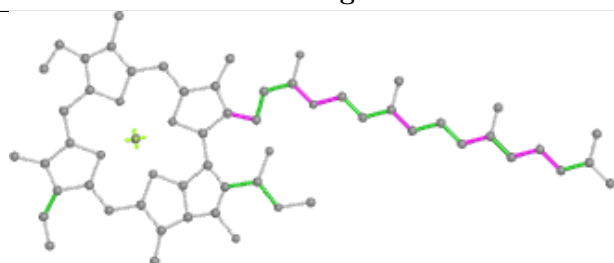
Ligand CLA 8 610



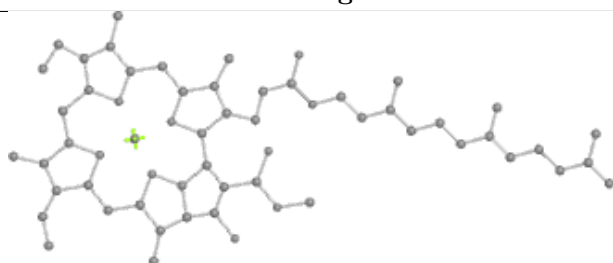
Bond lengths



Bond angles

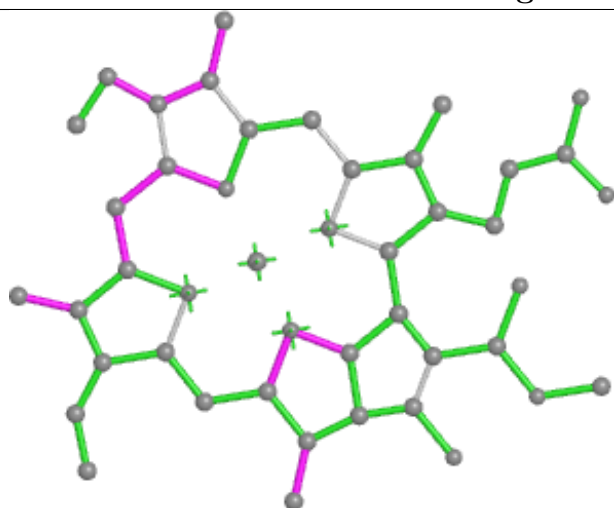


Torsions

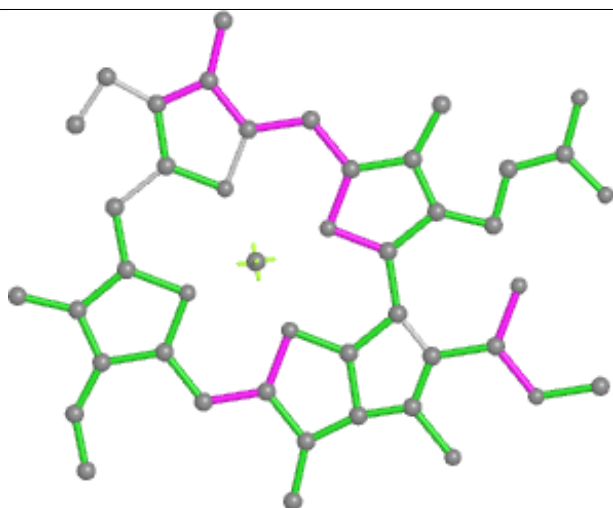


Rings

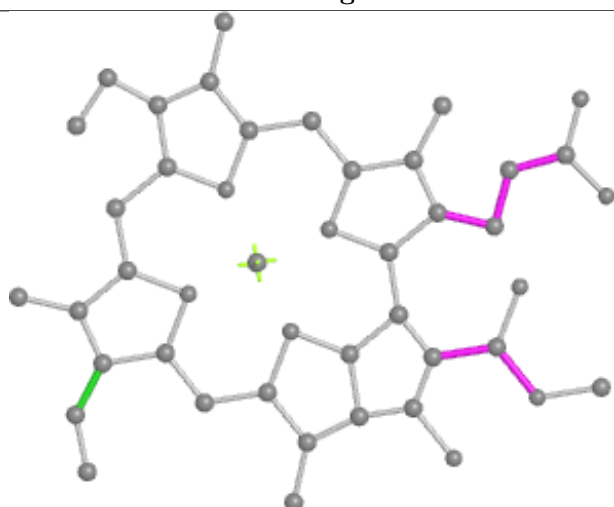
Ligand CLA L 302



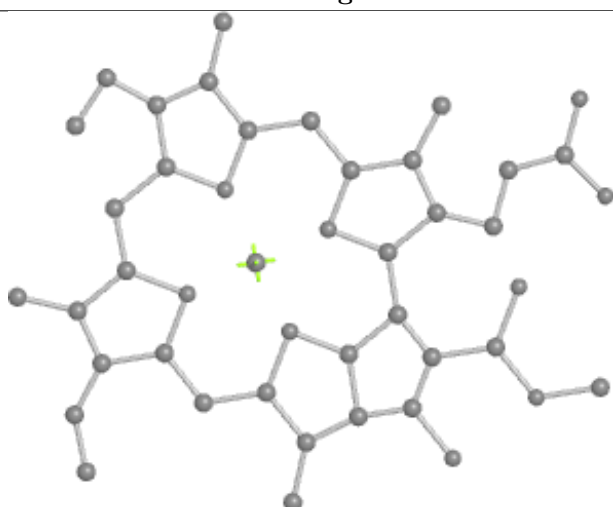
Bond lengths



Bond angles

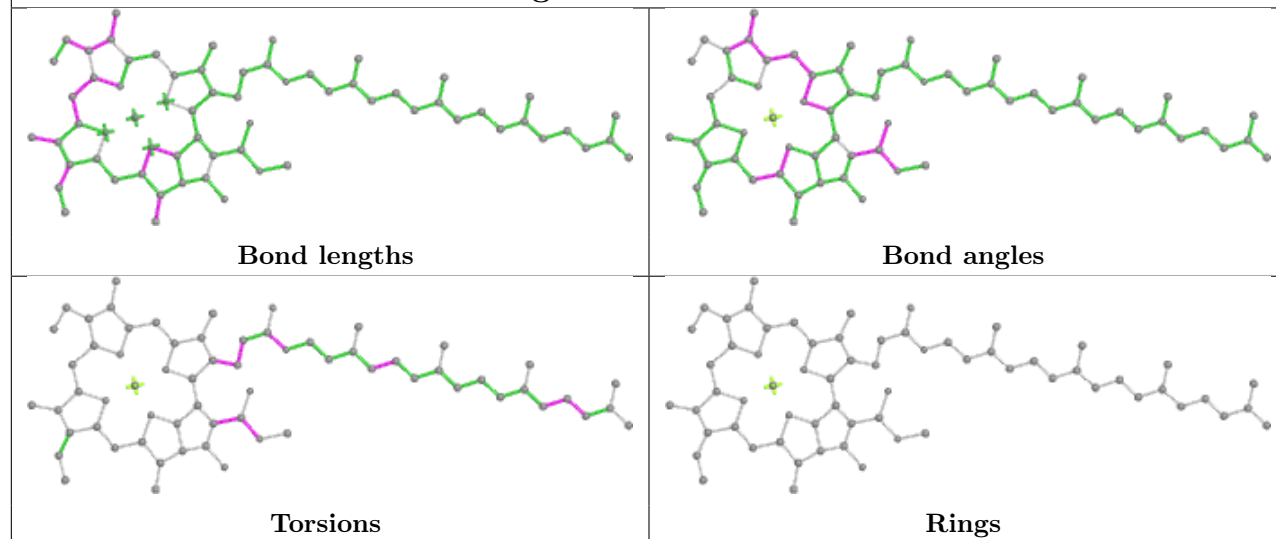


Torsions

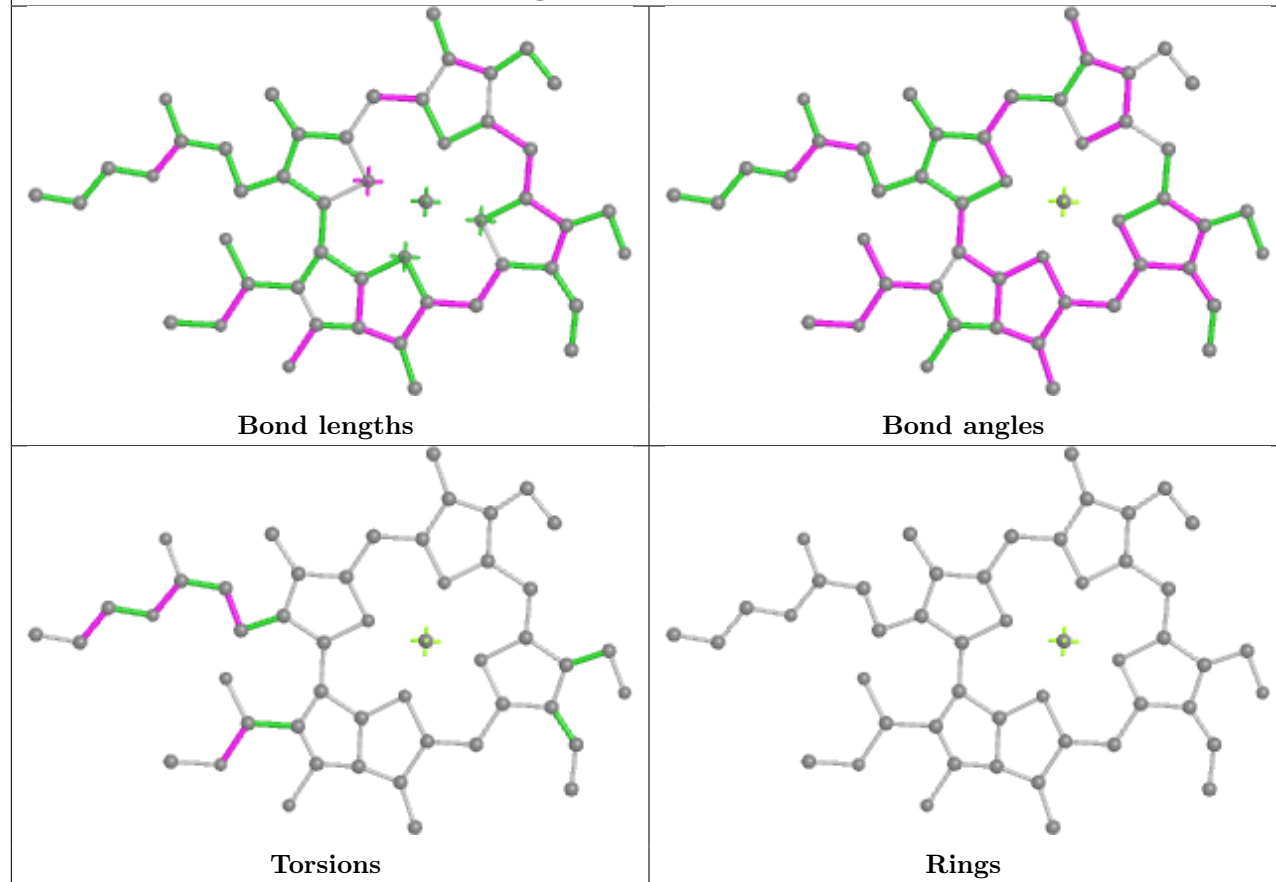


Rings

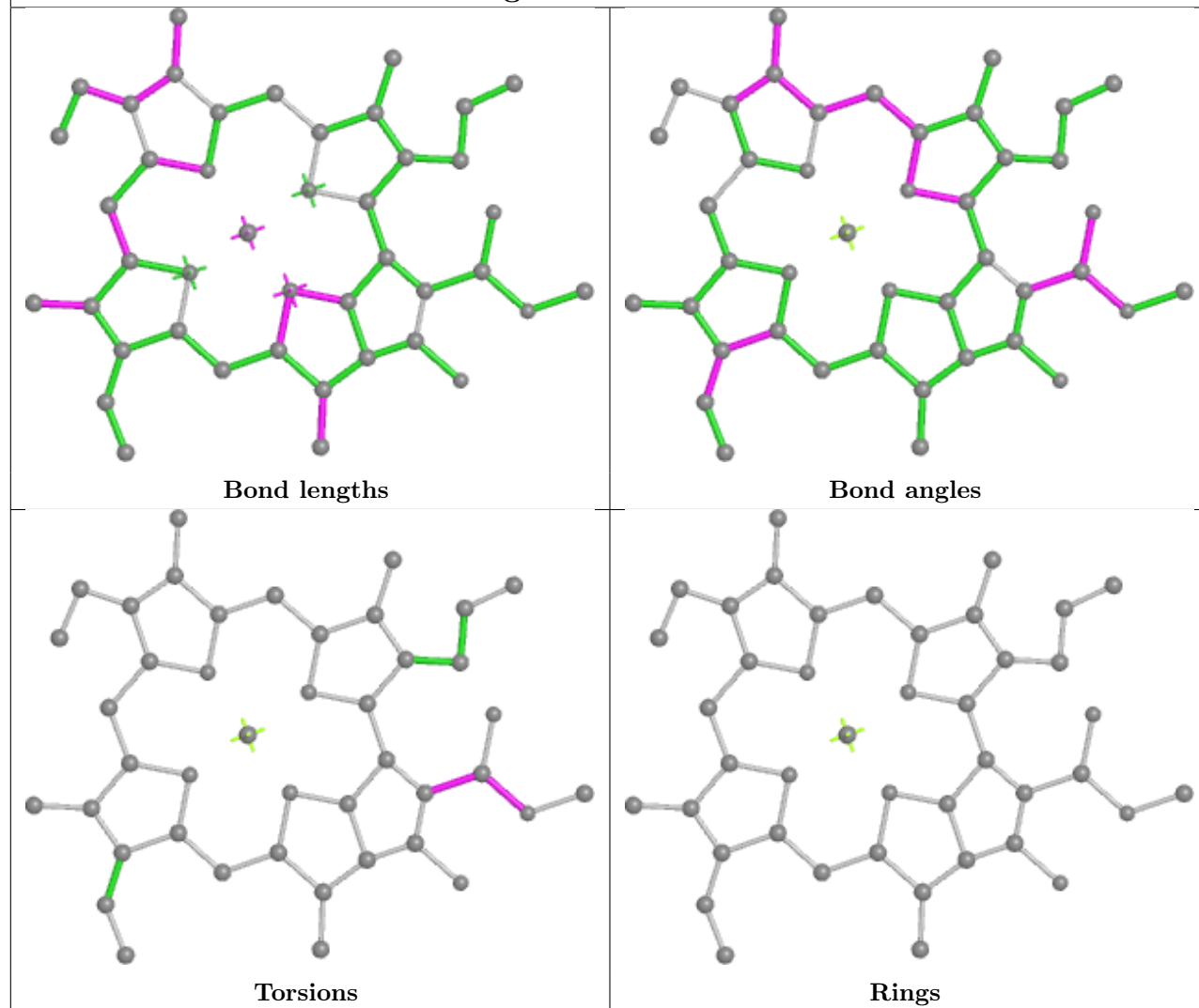
Ligand CLA B 809



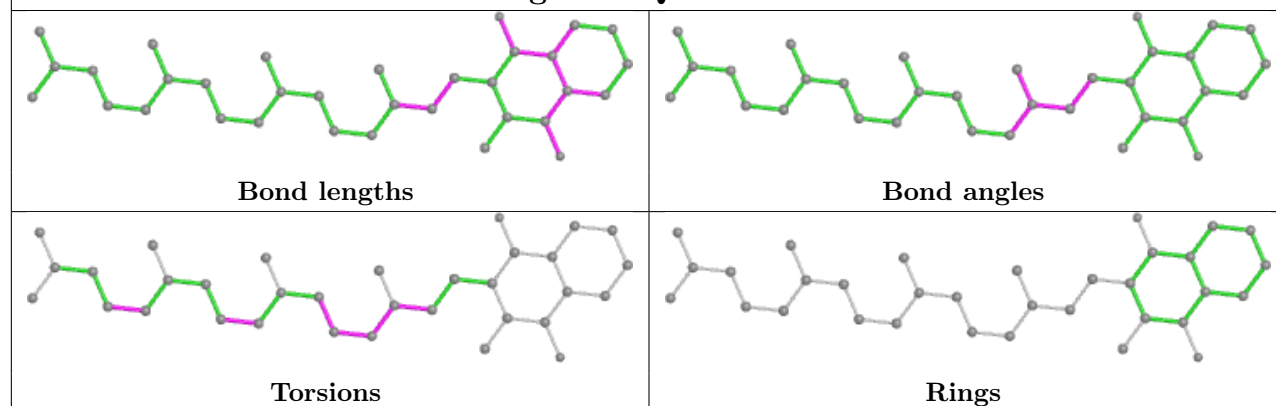
Ligand CHL Y 608



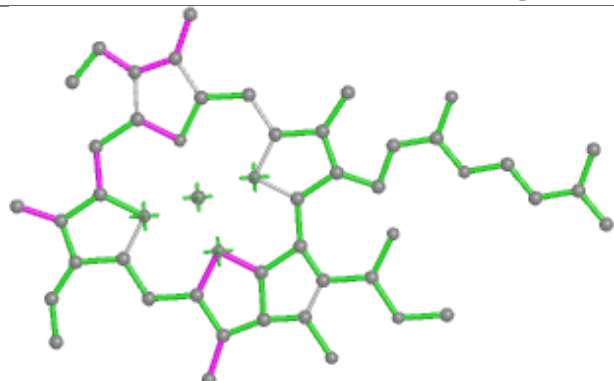
Ligand CLA 2 606



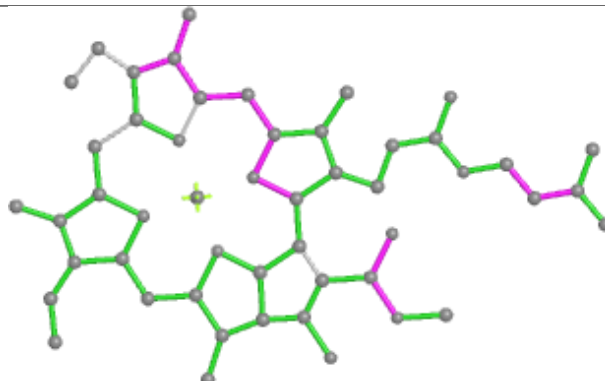
Ligand PQN A 844



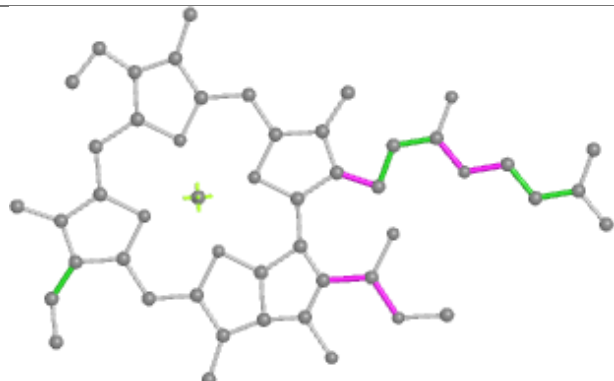
Ligand CLA A 815



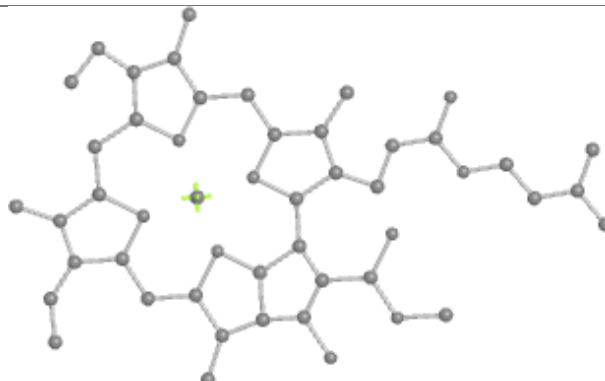
Bond lengths



Bond angles

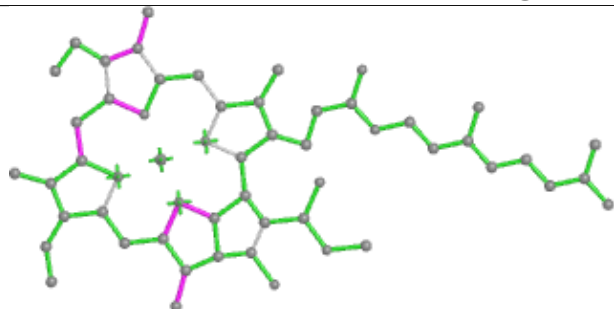


Torsions

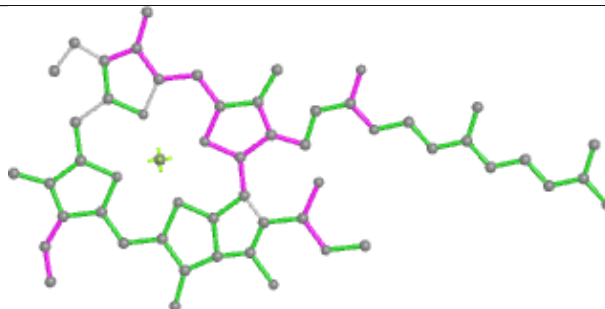


Rings

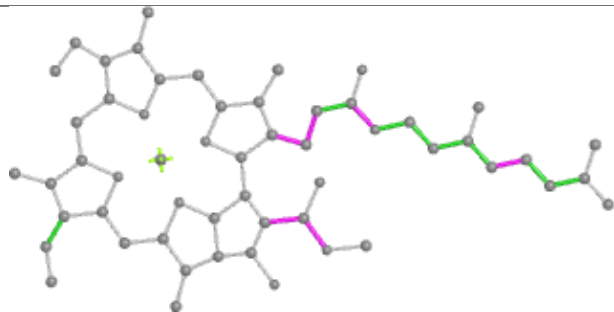
Ligand CLA Z 603



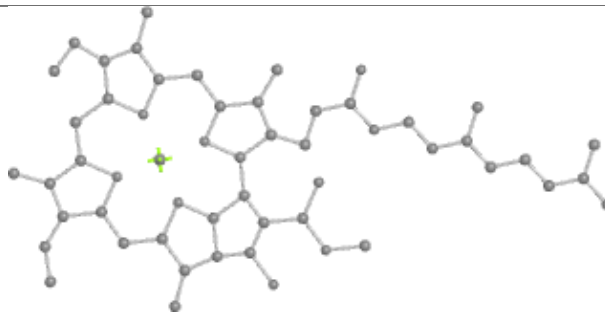
Bond lengths



Bond angles

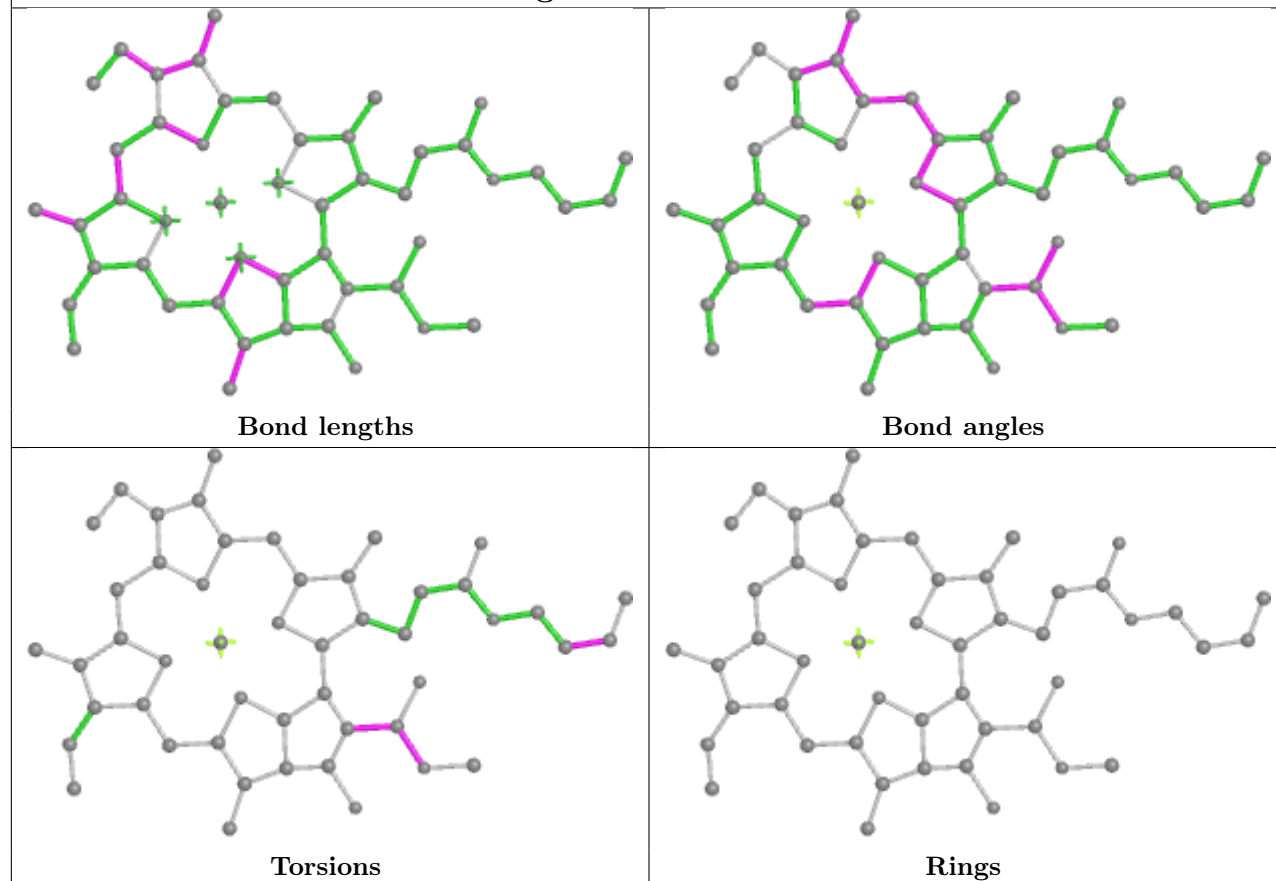


Torsions

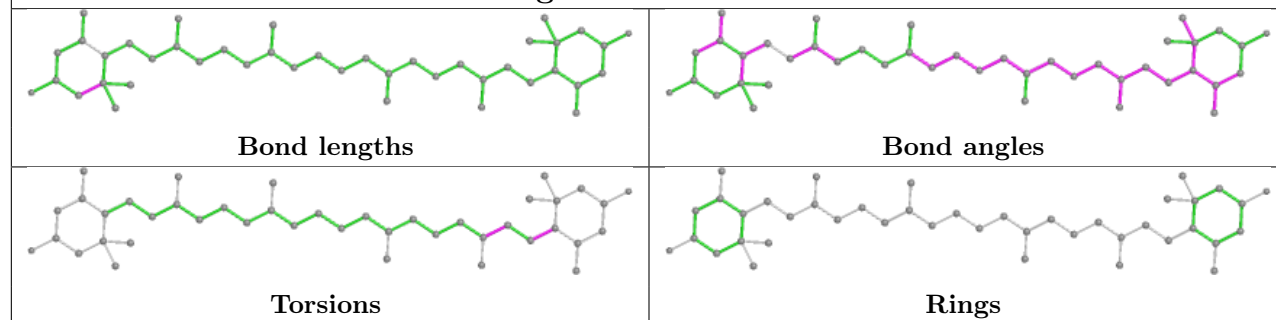


Rings

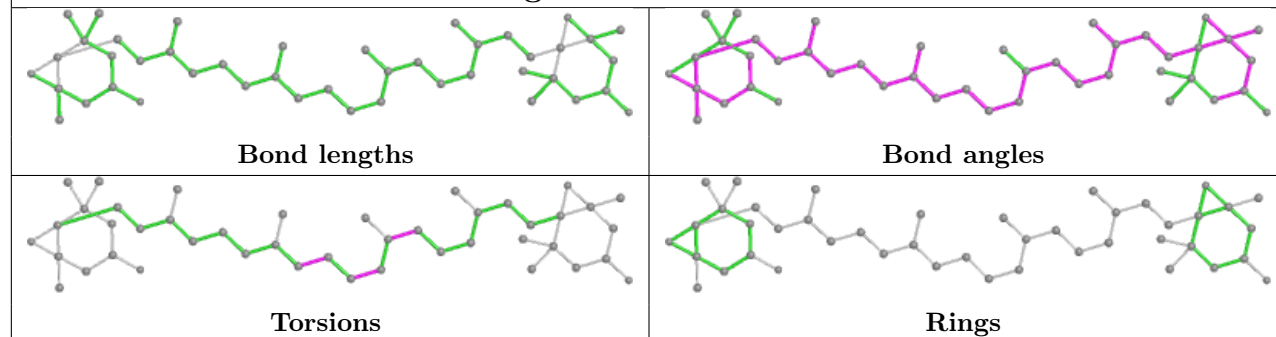
Ligand CLA 1 604

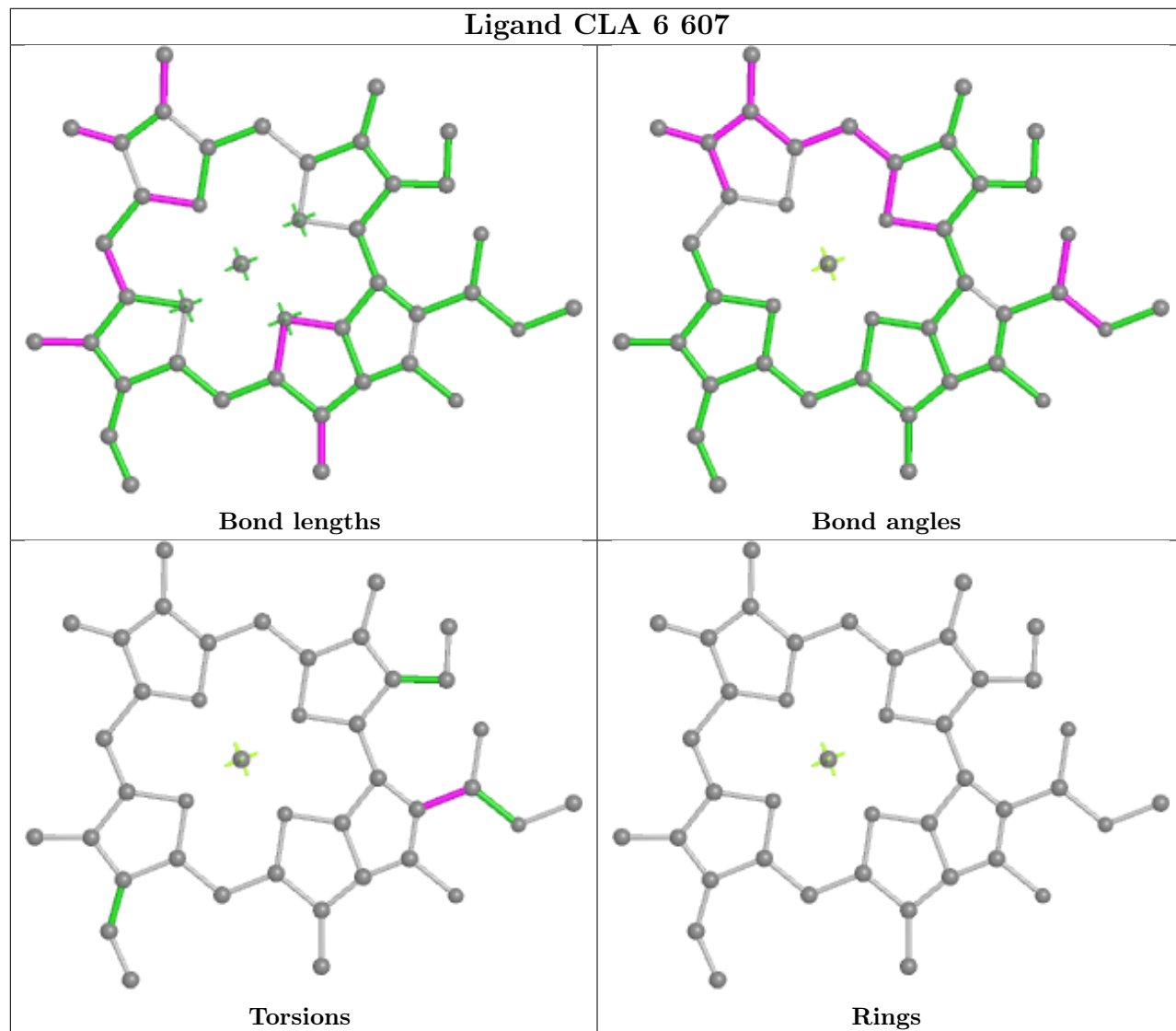
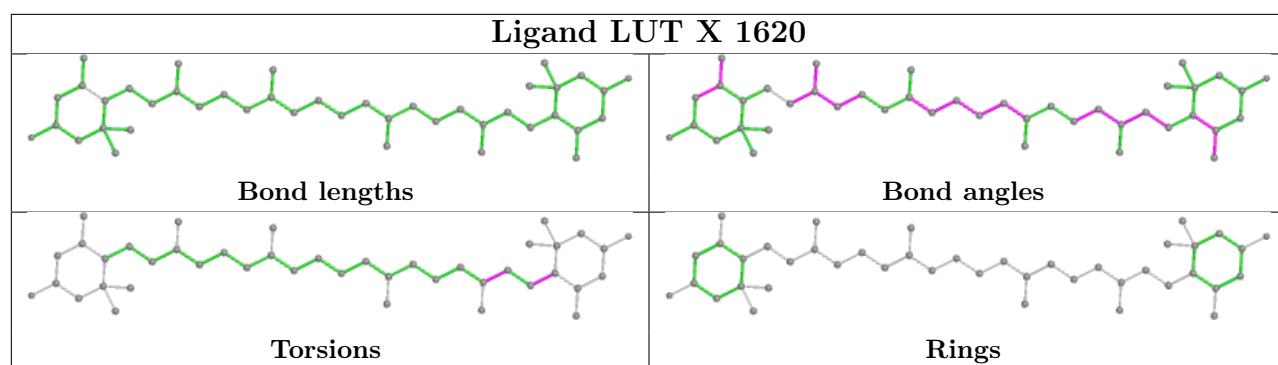


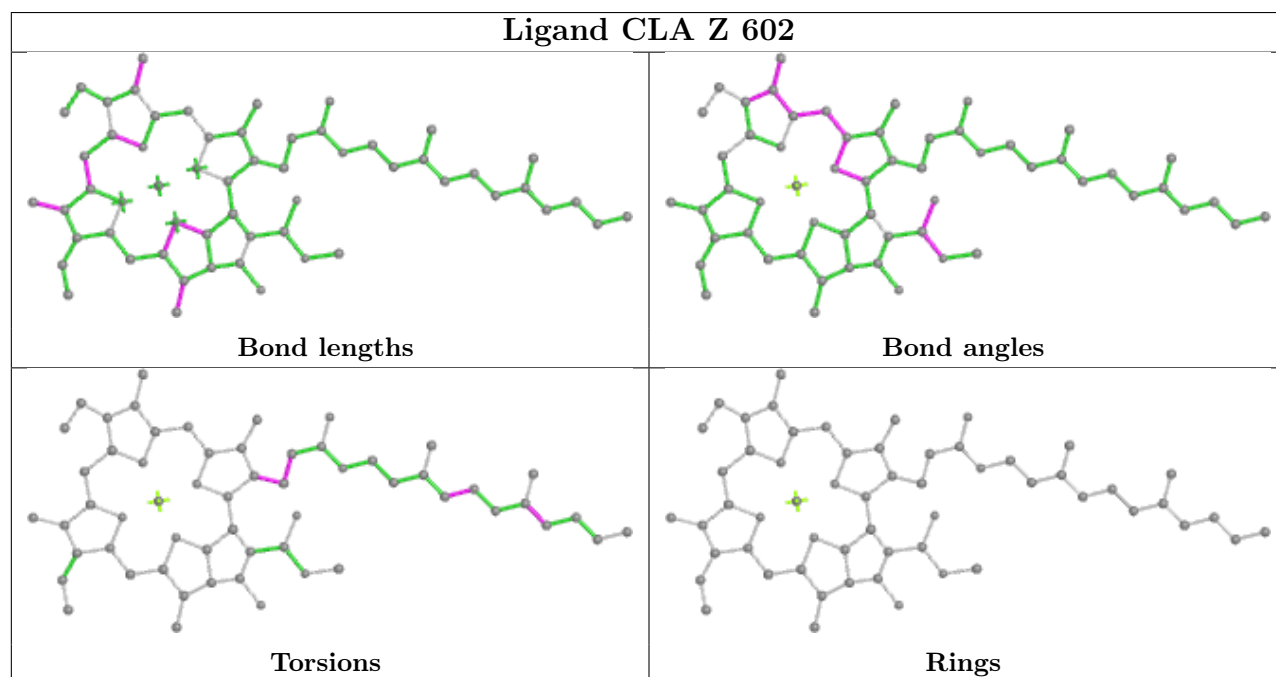
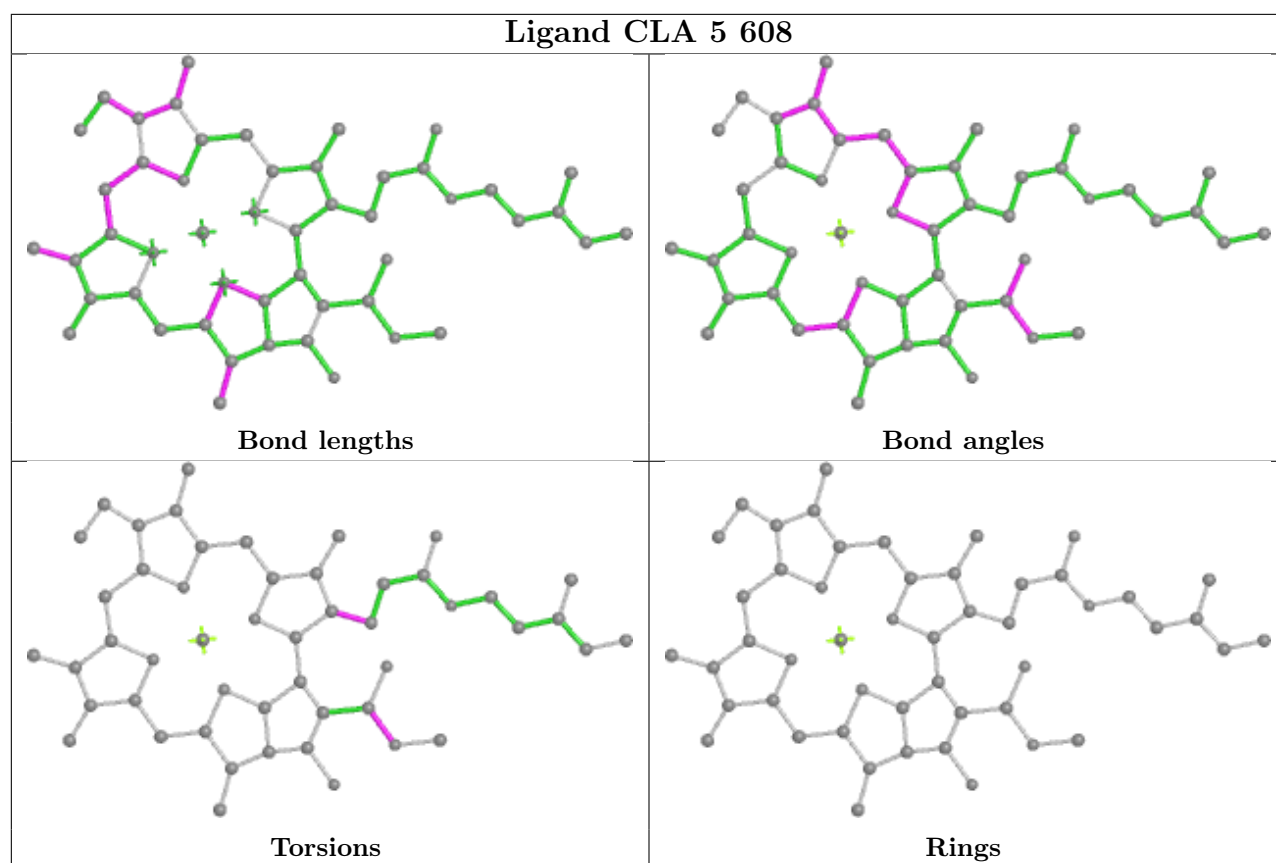
Ligand LUT 1 617

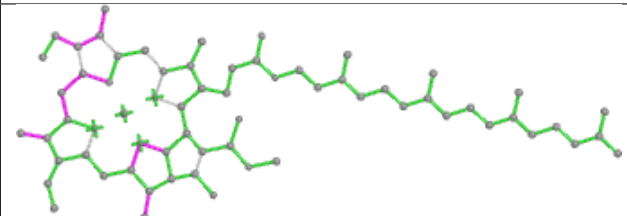
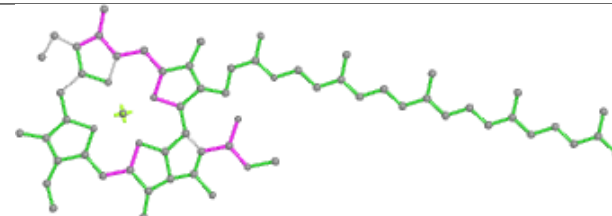
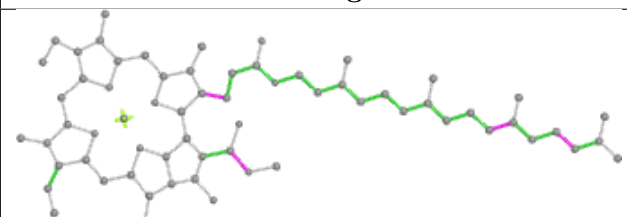
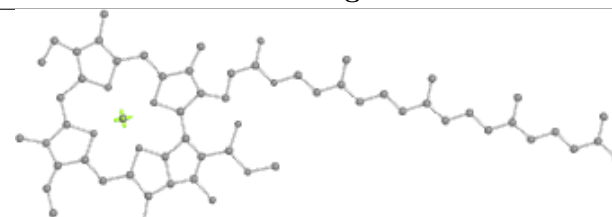


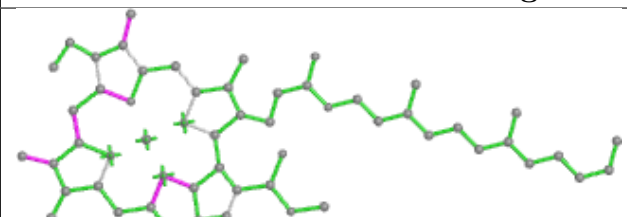
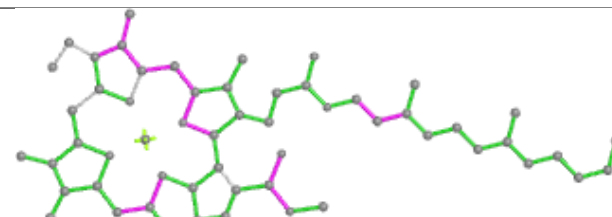
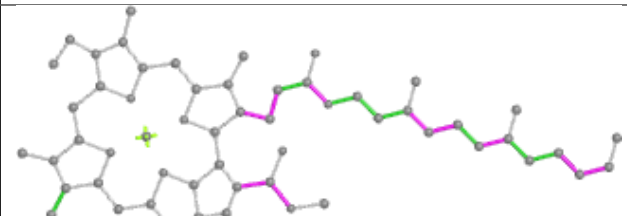
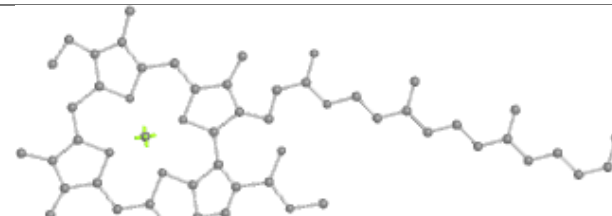
Ligand XAT Z 1622

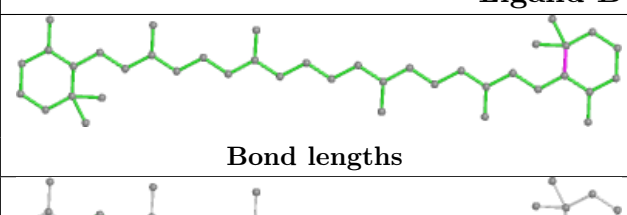
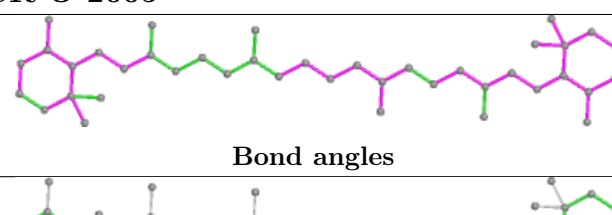






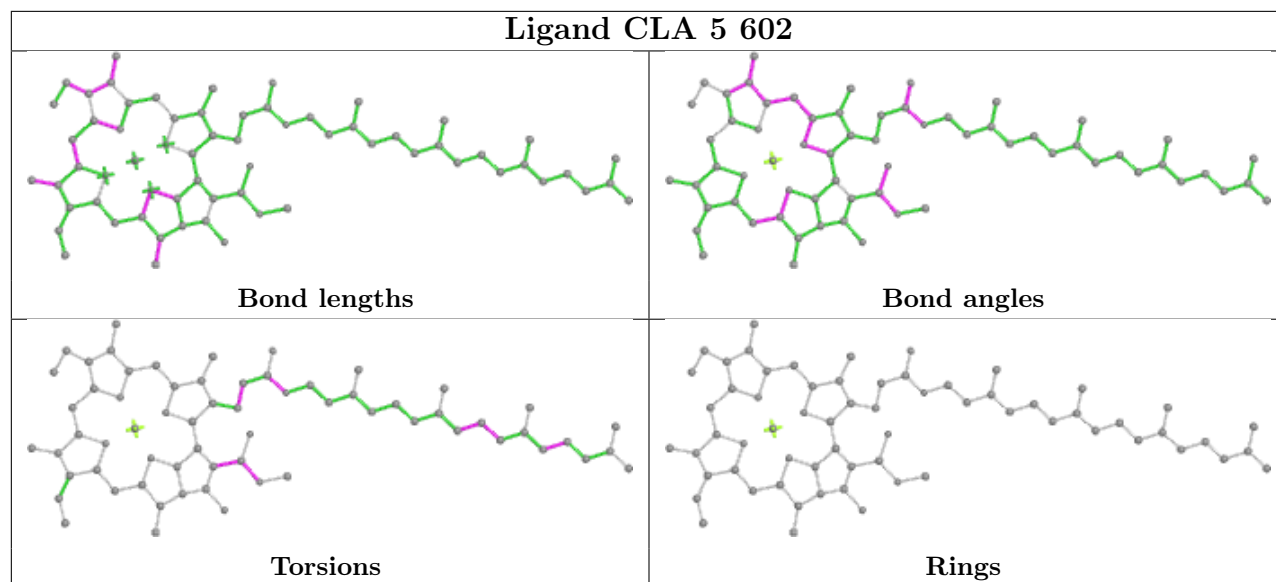


Ligand CLA A 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

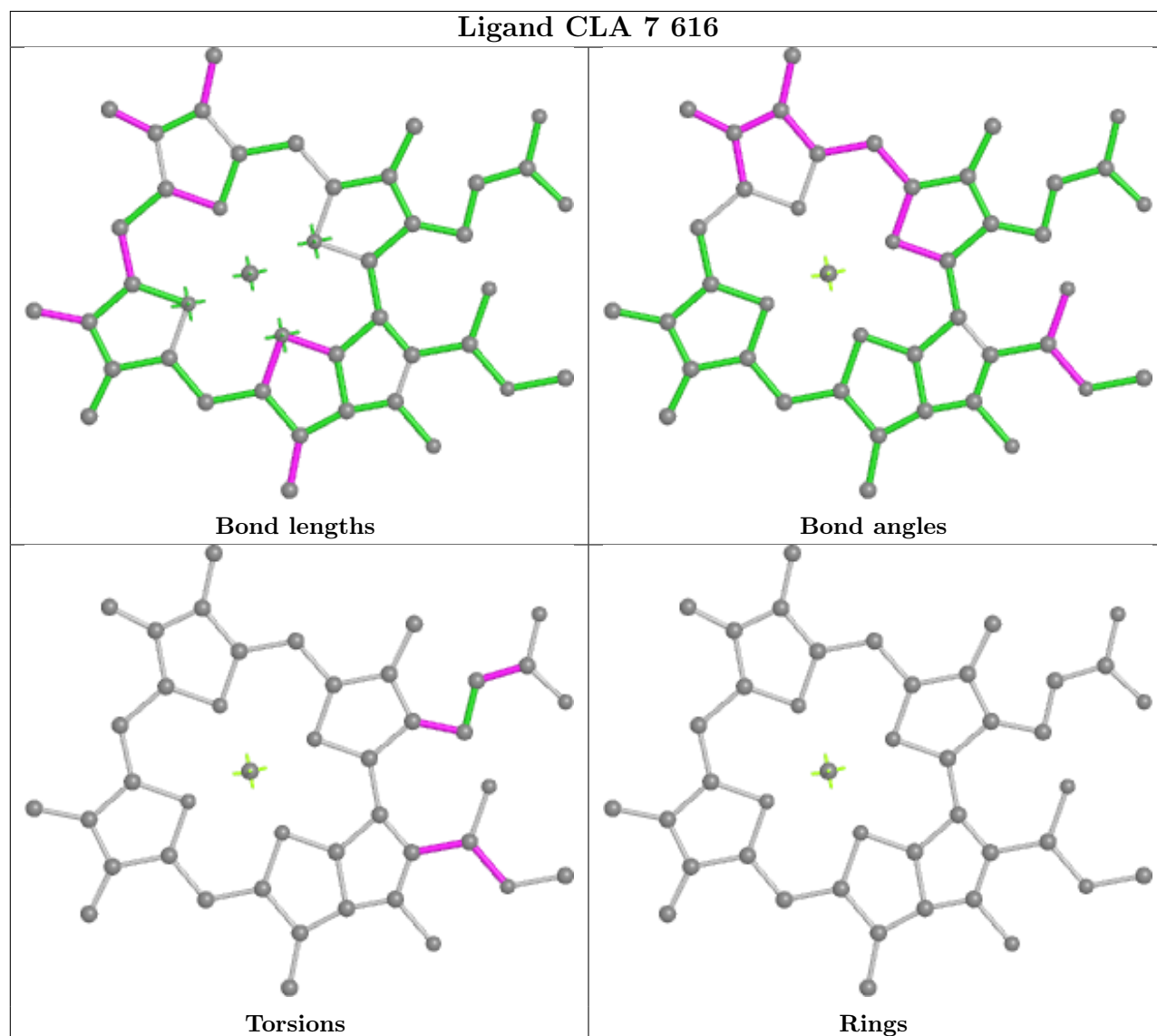
Ligand CLA U 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

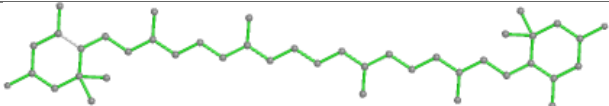
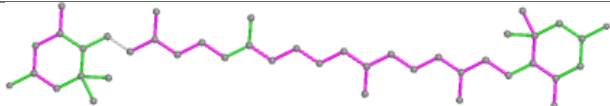
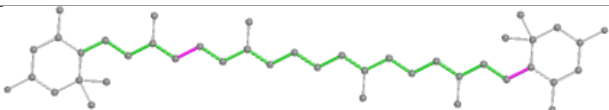
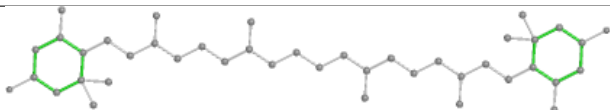
Ligand BCR O 2005	
	
Bond lengths	Bond angles
	
Torsions	Rings

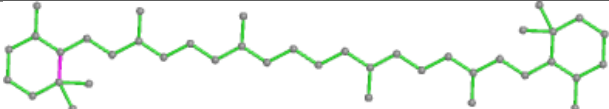
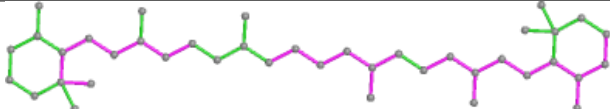
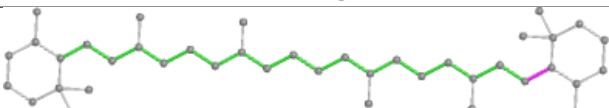
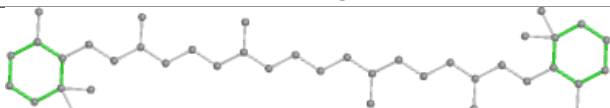
Ligand CLA 5 602

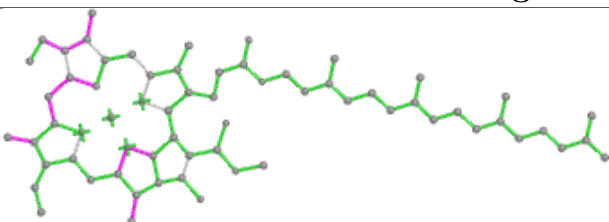
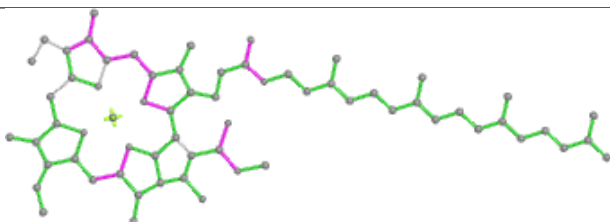
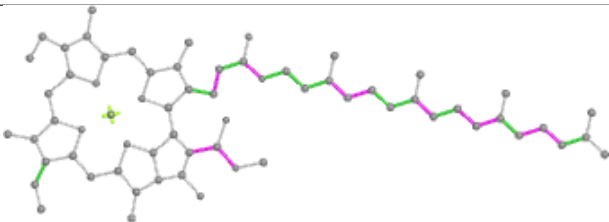
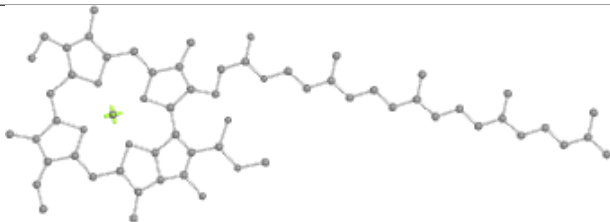


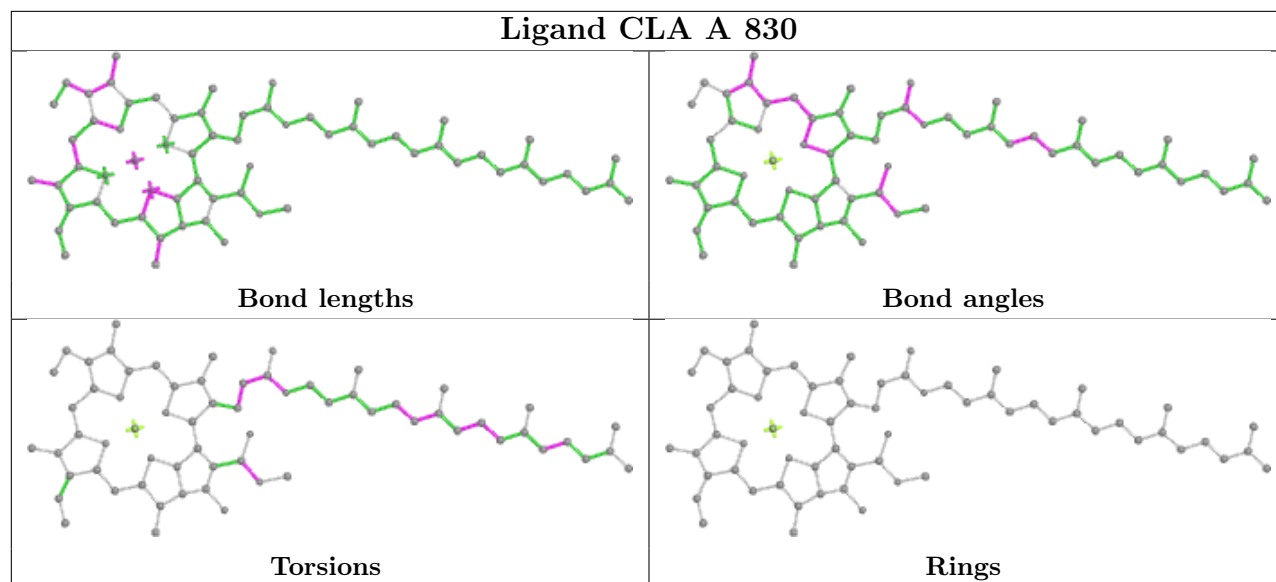
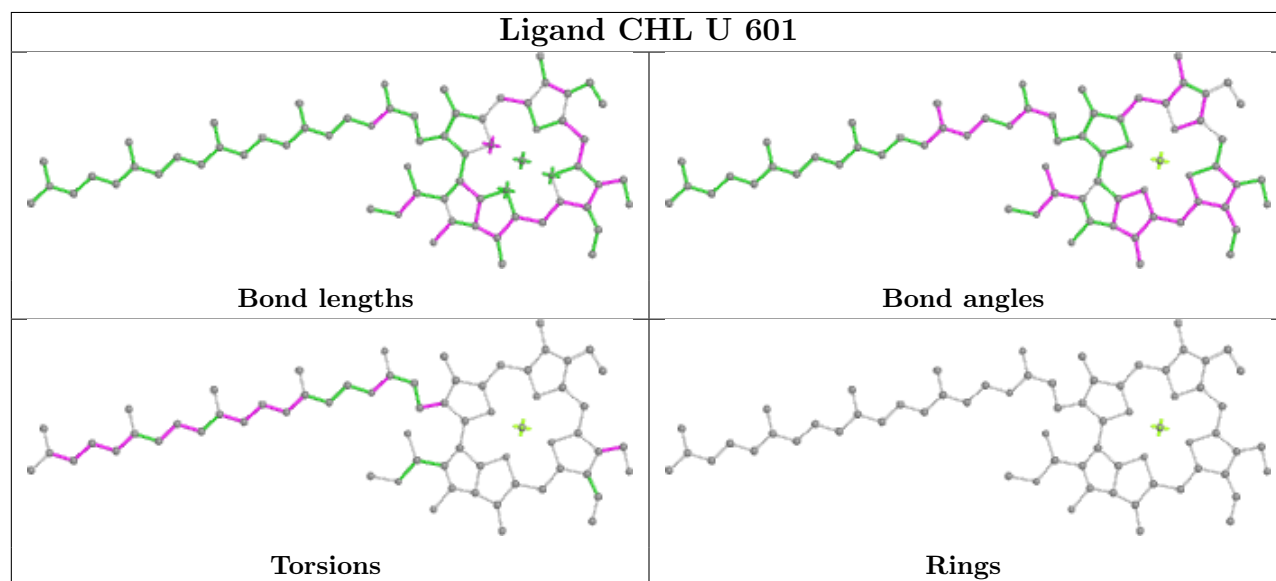
Ligand CLA 7 616



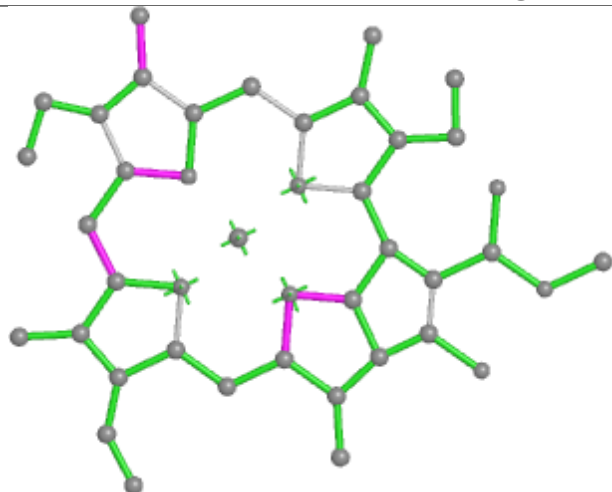
Ligand LUT X 1621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR G 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

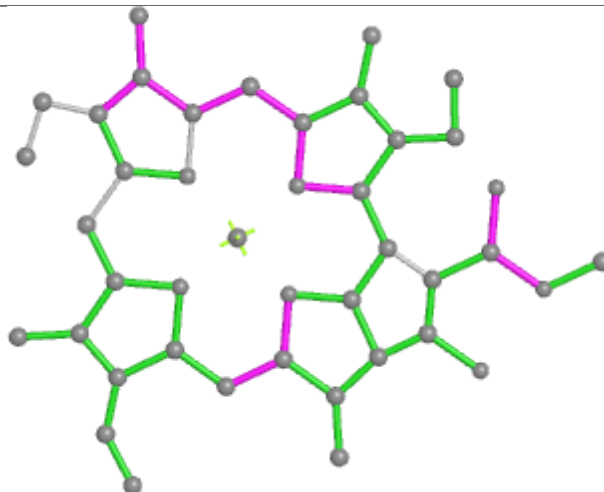
Ligand CLA 7 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 830**Ligand CHL U 601**

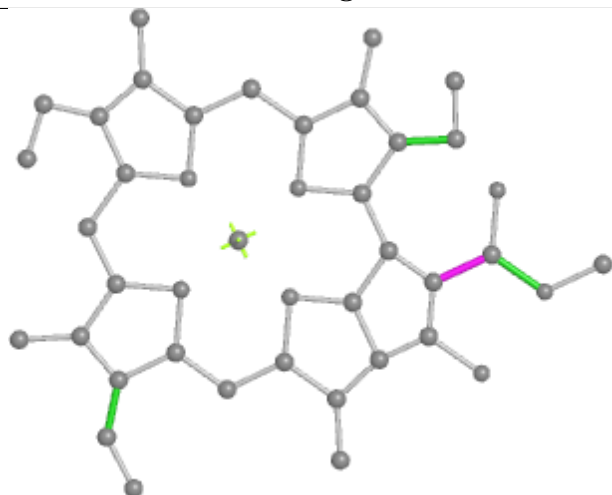
Ligand CLA U 611



Bond lengths



Bond angles

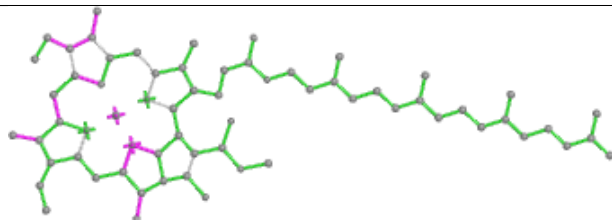


Torsions

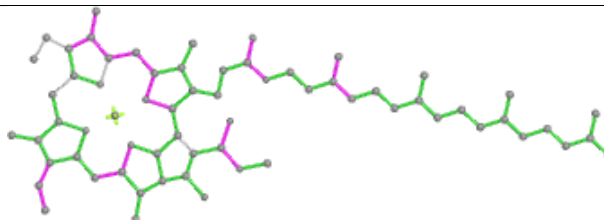


Rings

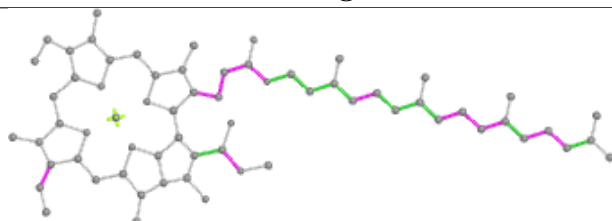
Ligand CLA 6 616



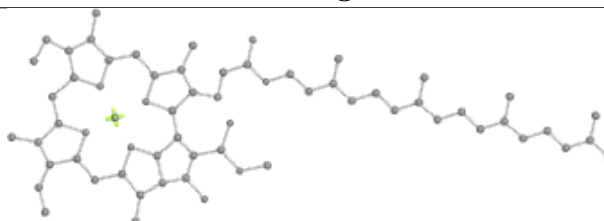
Bond lengths



Bond angles

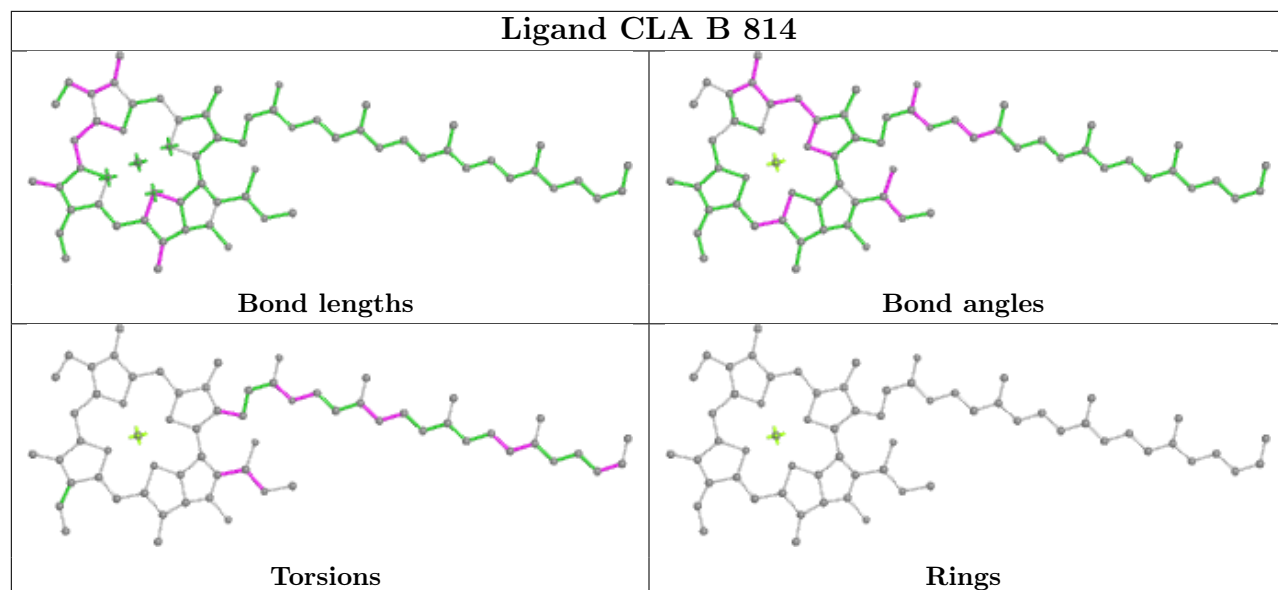


Torsions

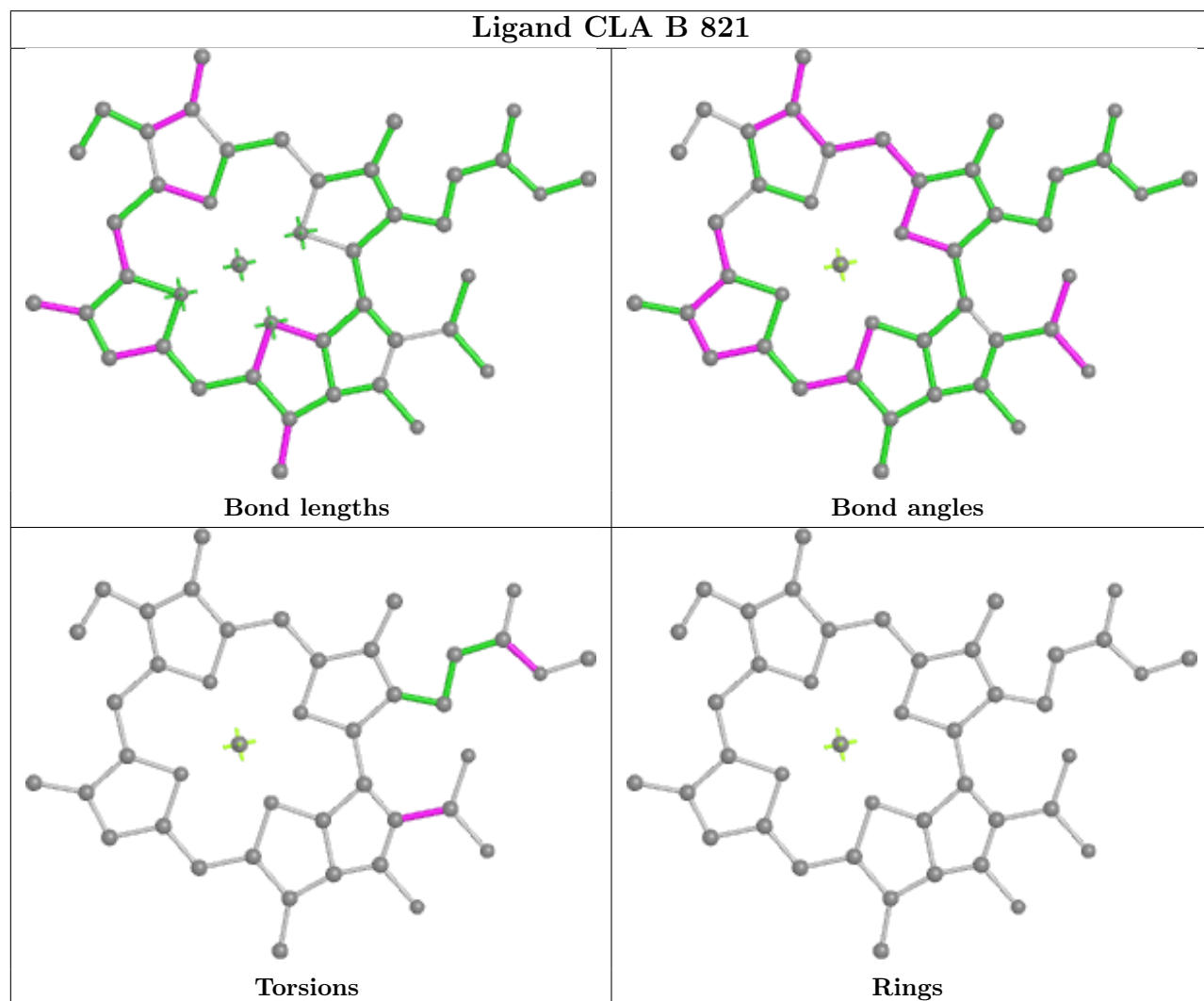


Rings

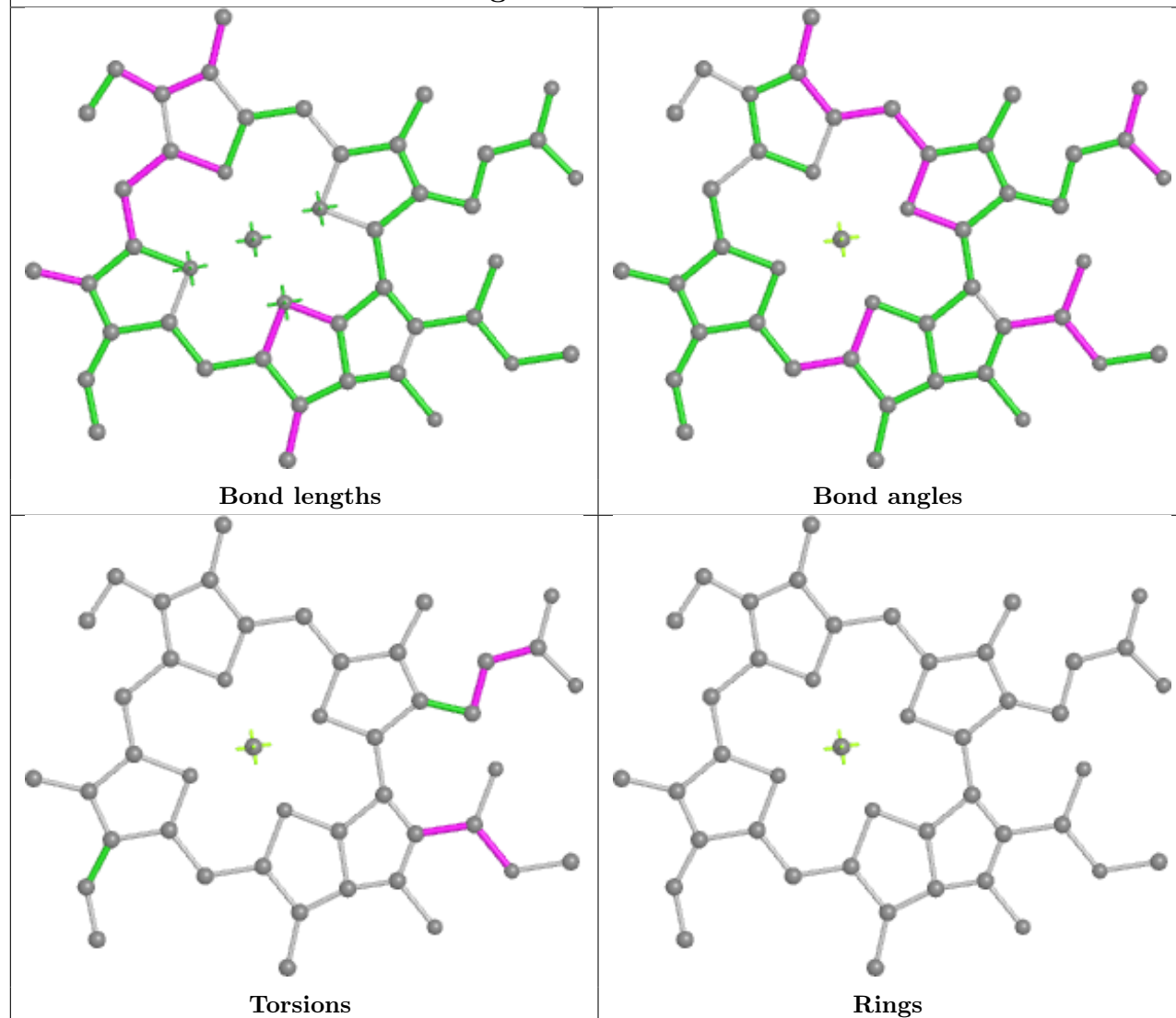
Ligand CLA B 814



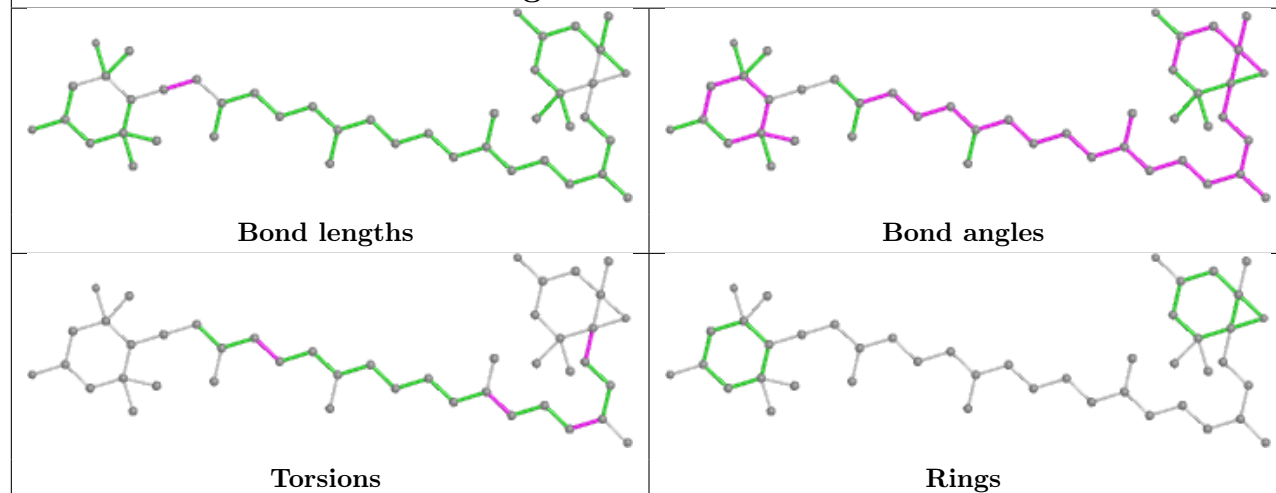
Ligand CLA B 821



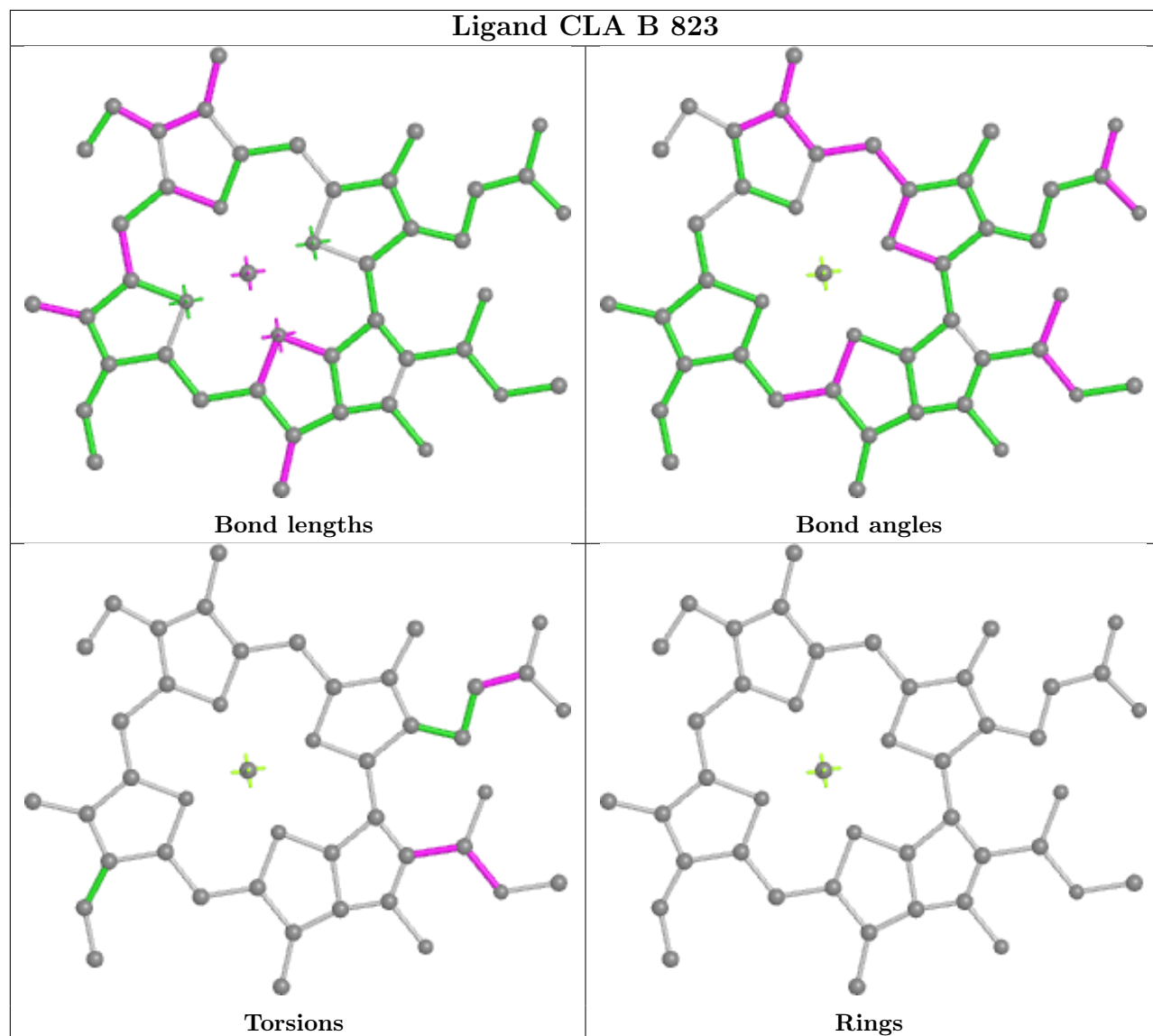
Ligand CLA A 837



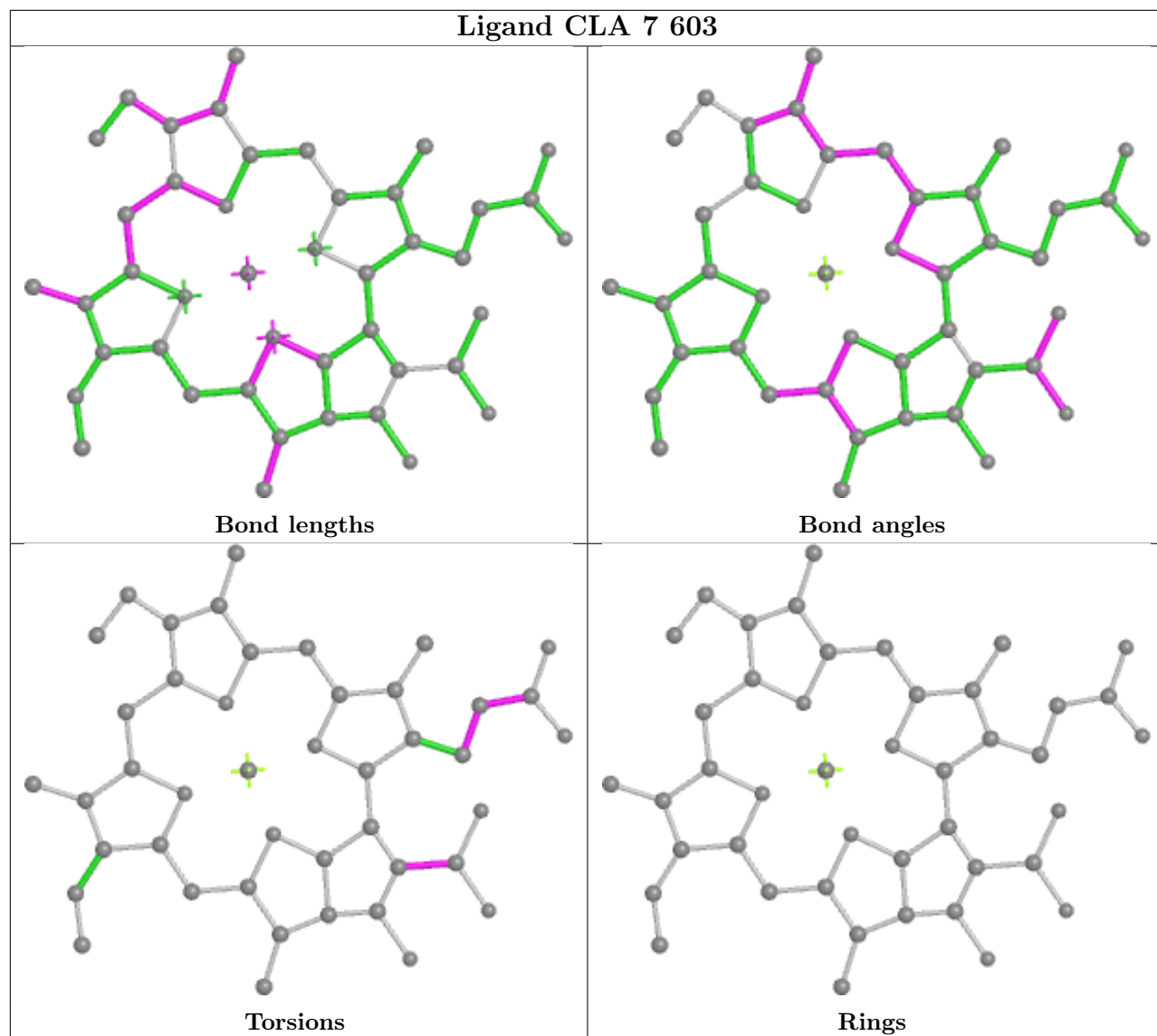
Ligand NEX Z 1623



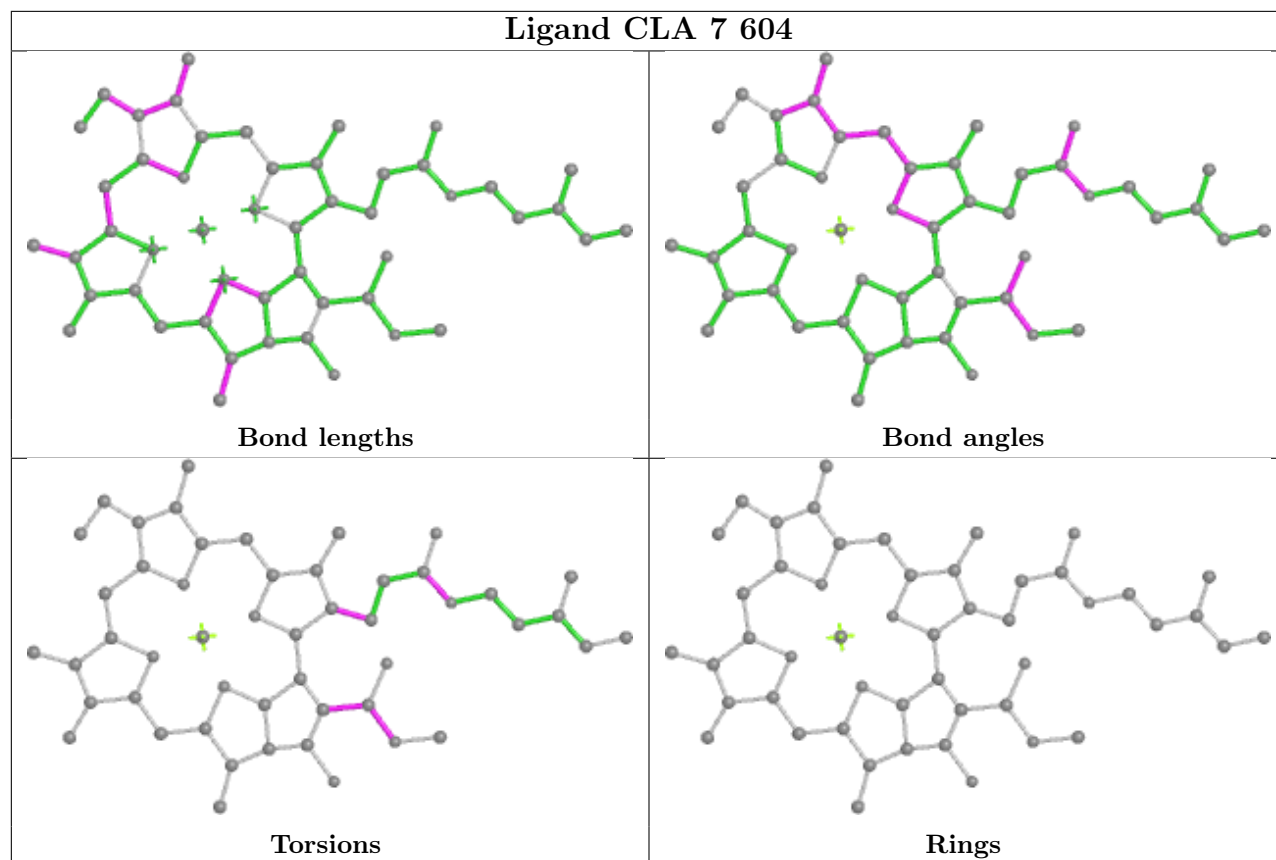
Ligand CLA B 823



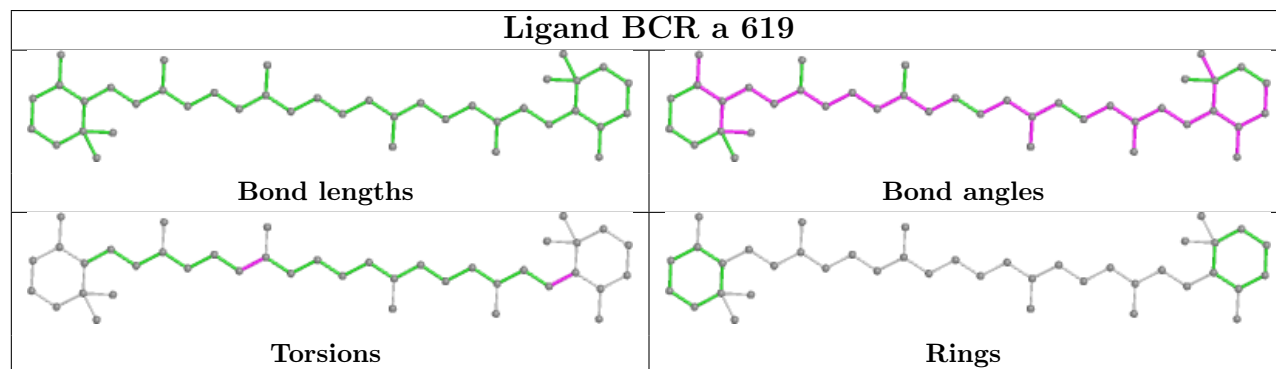
Ligand CLA 7 603



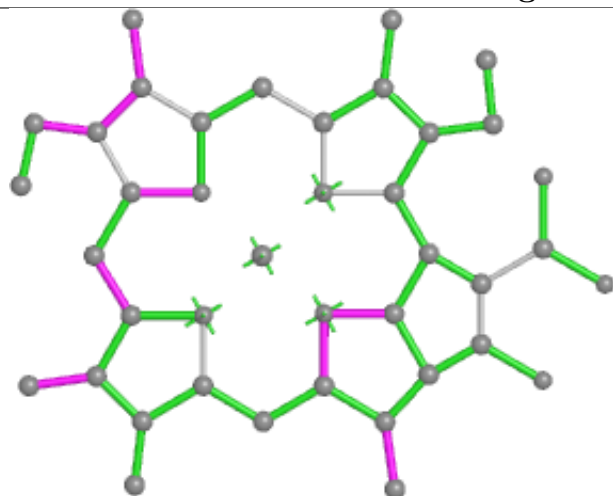
Ligand CLA 7 604



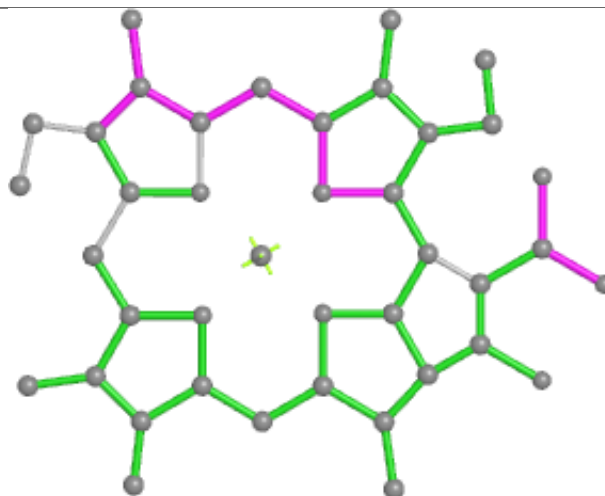
Ligand BCR a 619



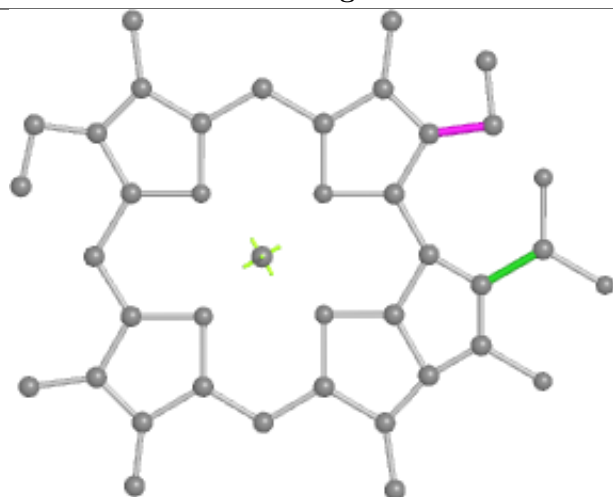
Ligand CLA 4 606



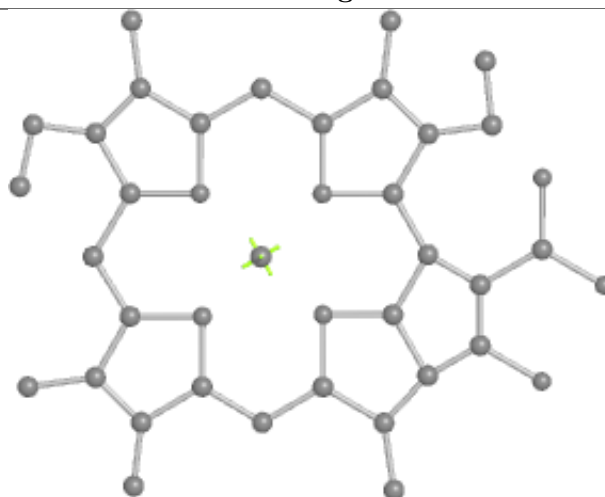
Bond lengths



Bond angles

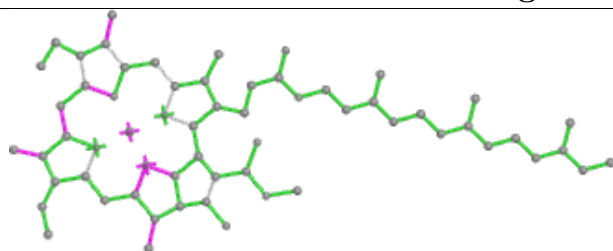


Torsions

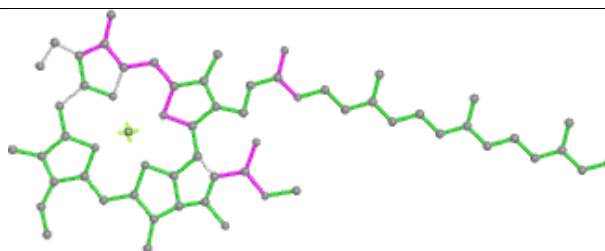


Rings

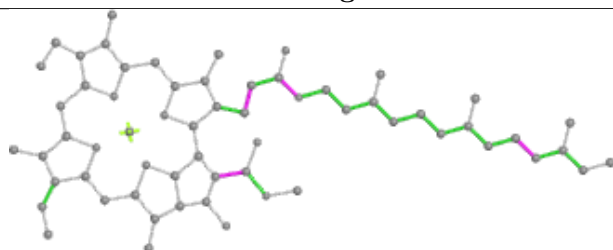
Ligand CLA a 602



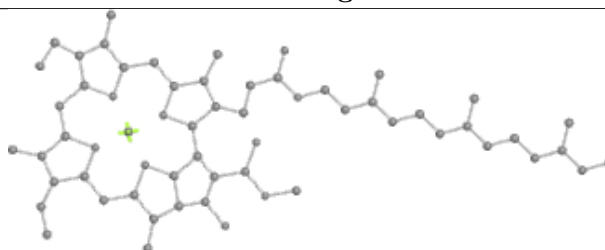
Bond lengths



Bond angles

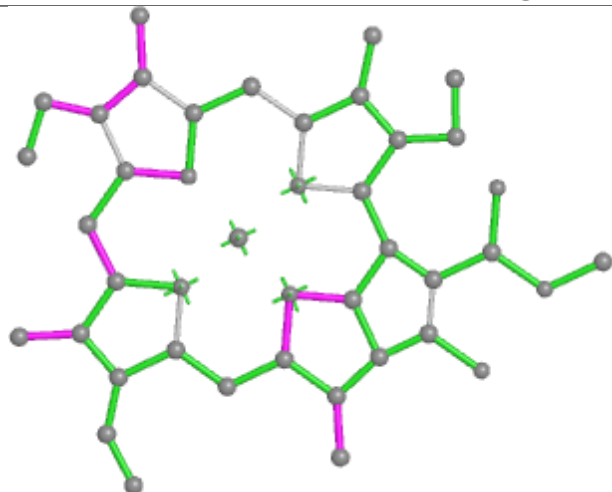


Torsions

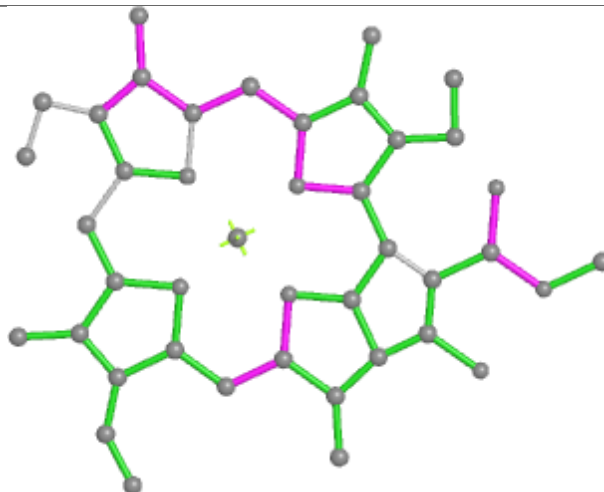


Rings

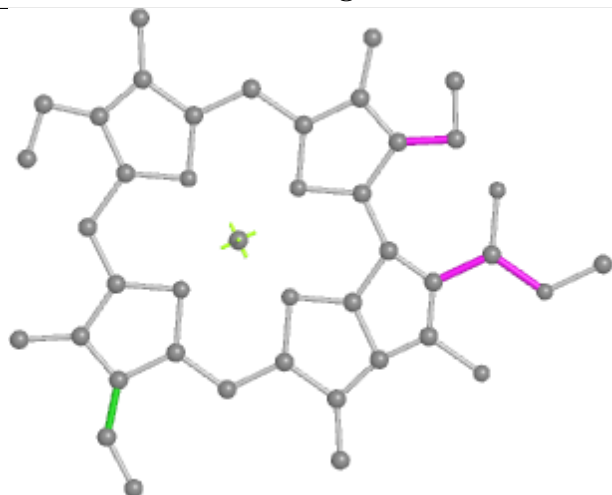
Ligand CLA J 101



Bond lengths



Bond angles

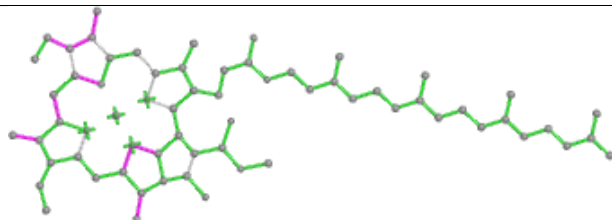


Torsions

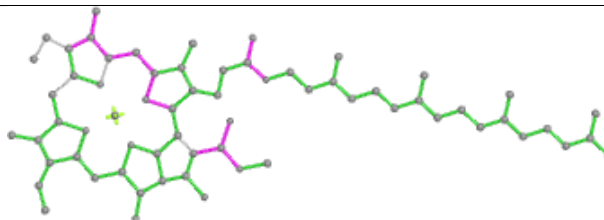


Rings

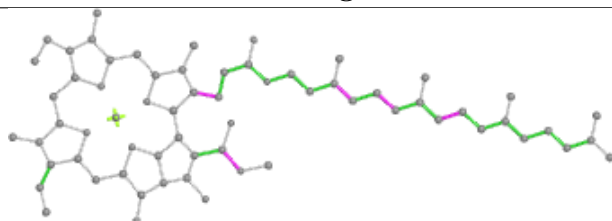
Ligand CLA Z 610



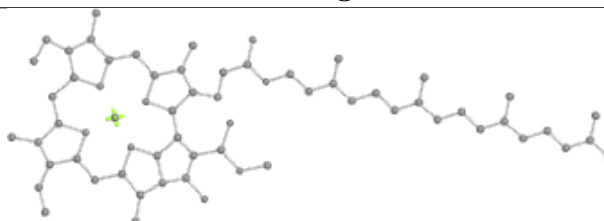
Bond lengths



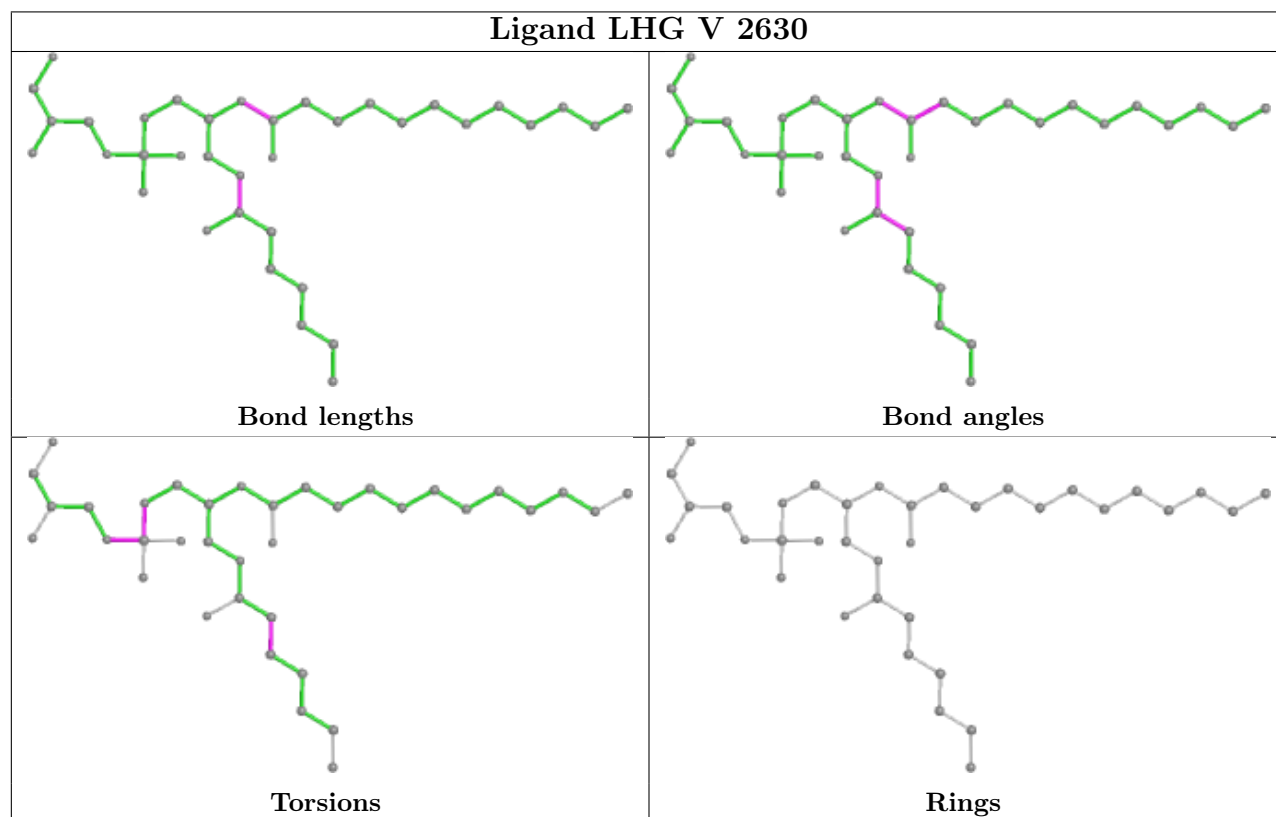
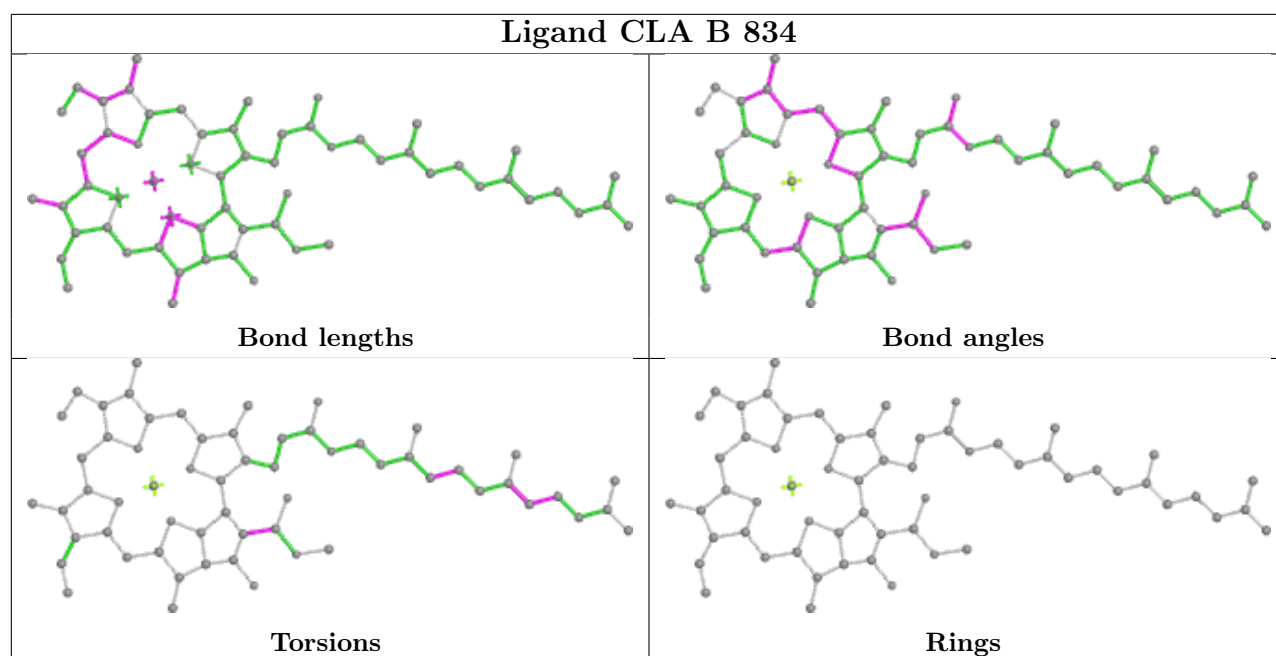
Bond angles

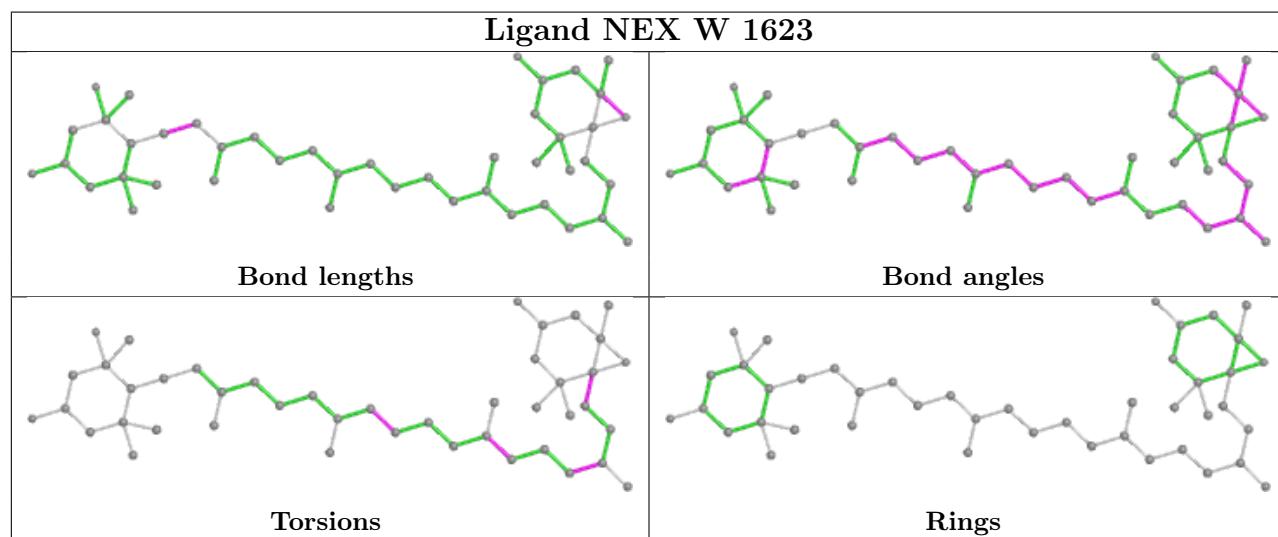
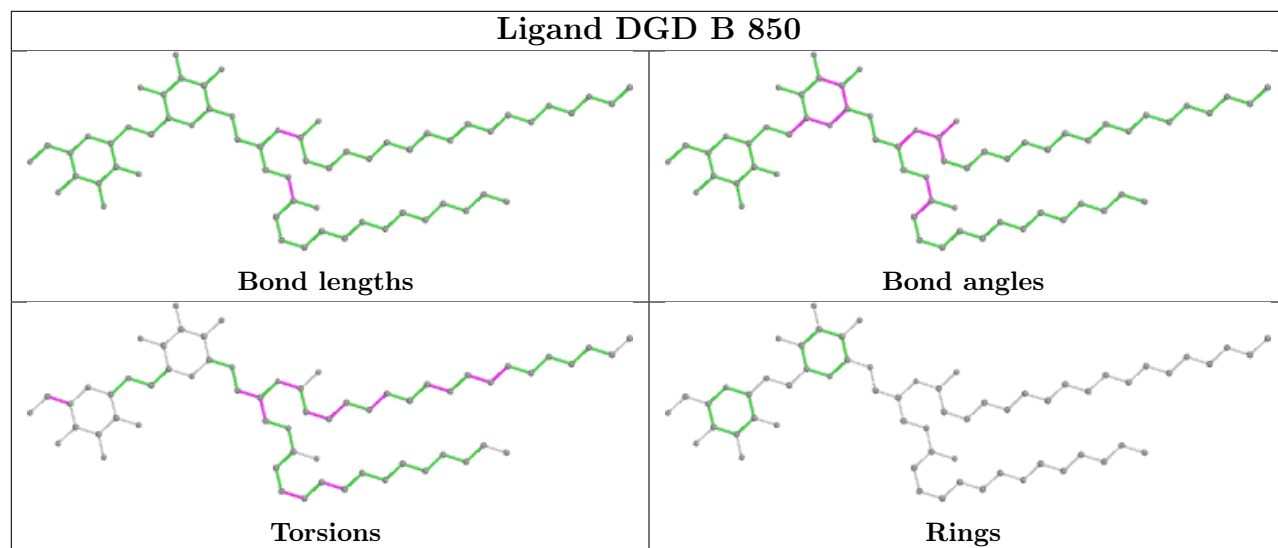
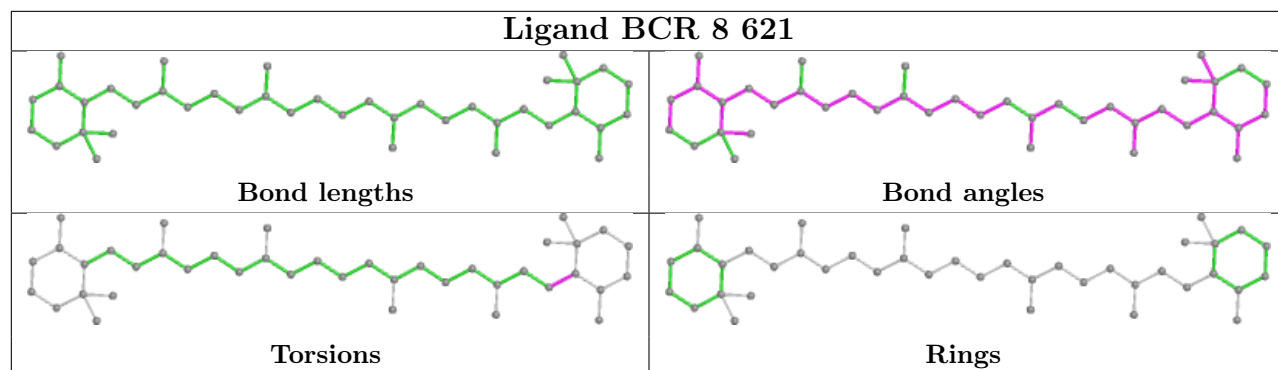


Torsions

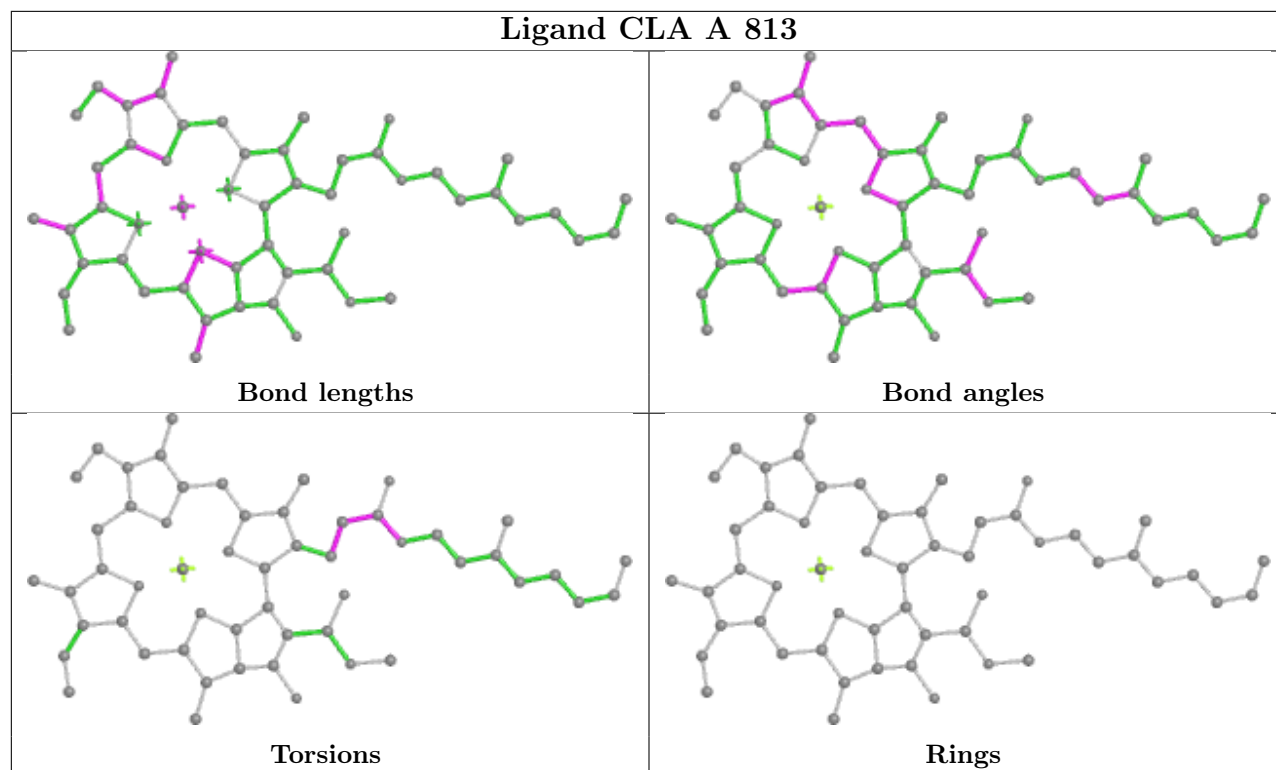


Rings

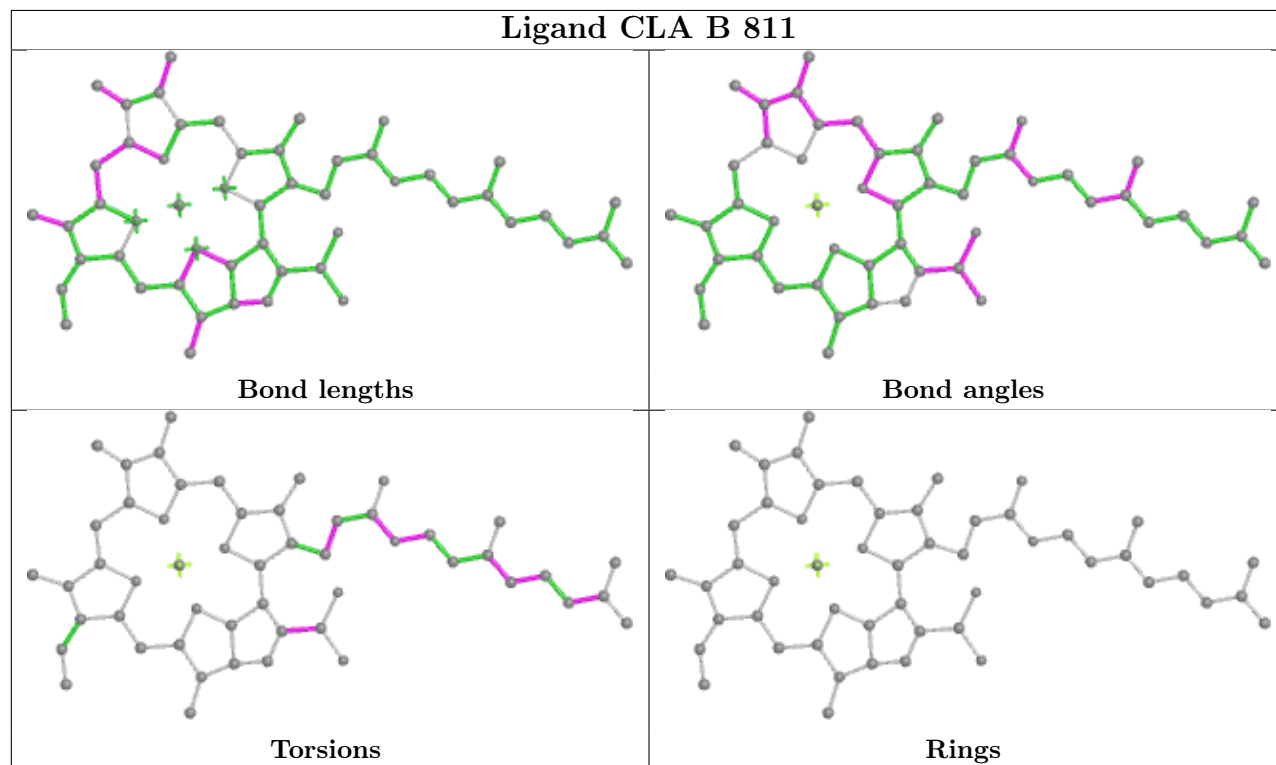


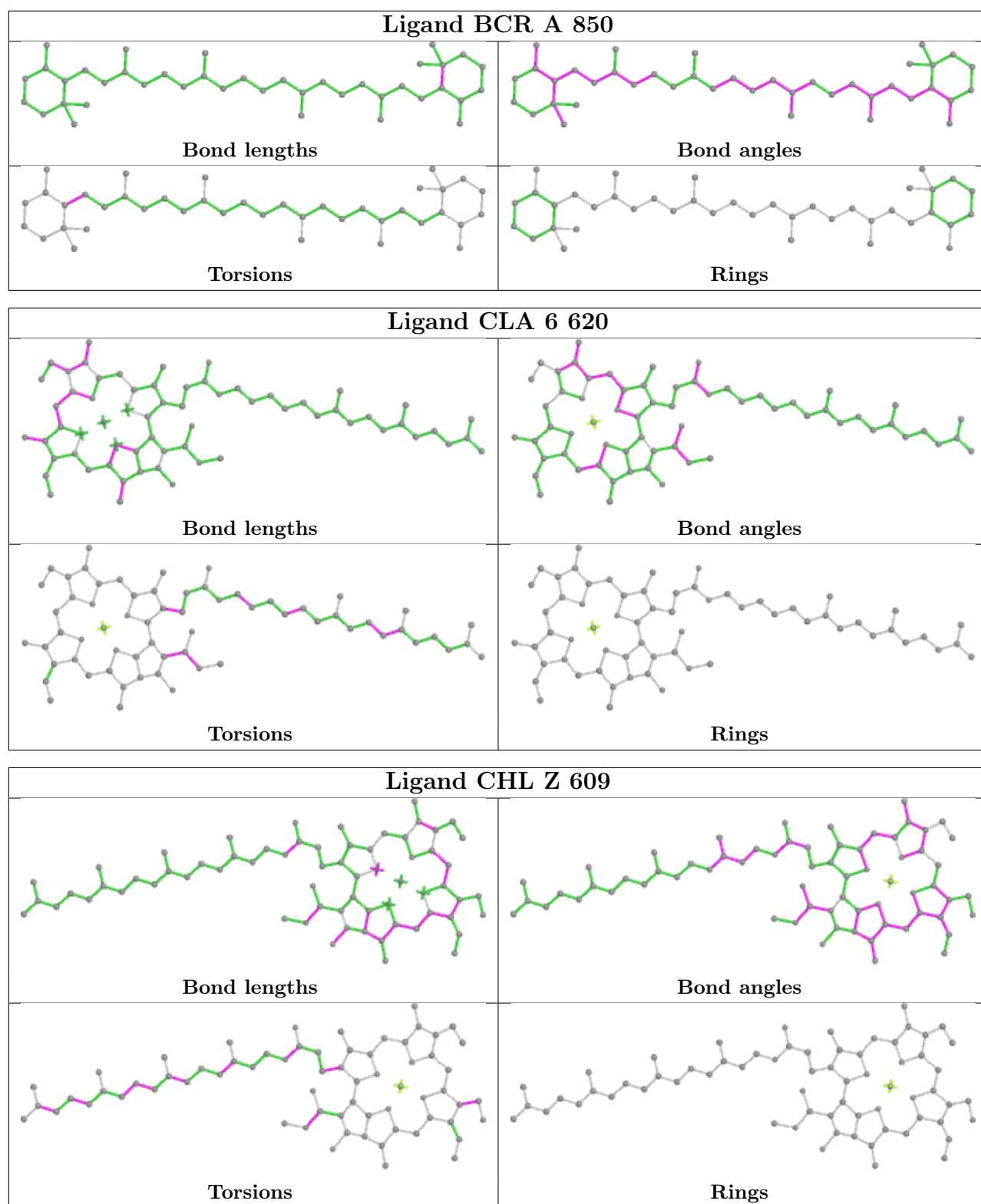


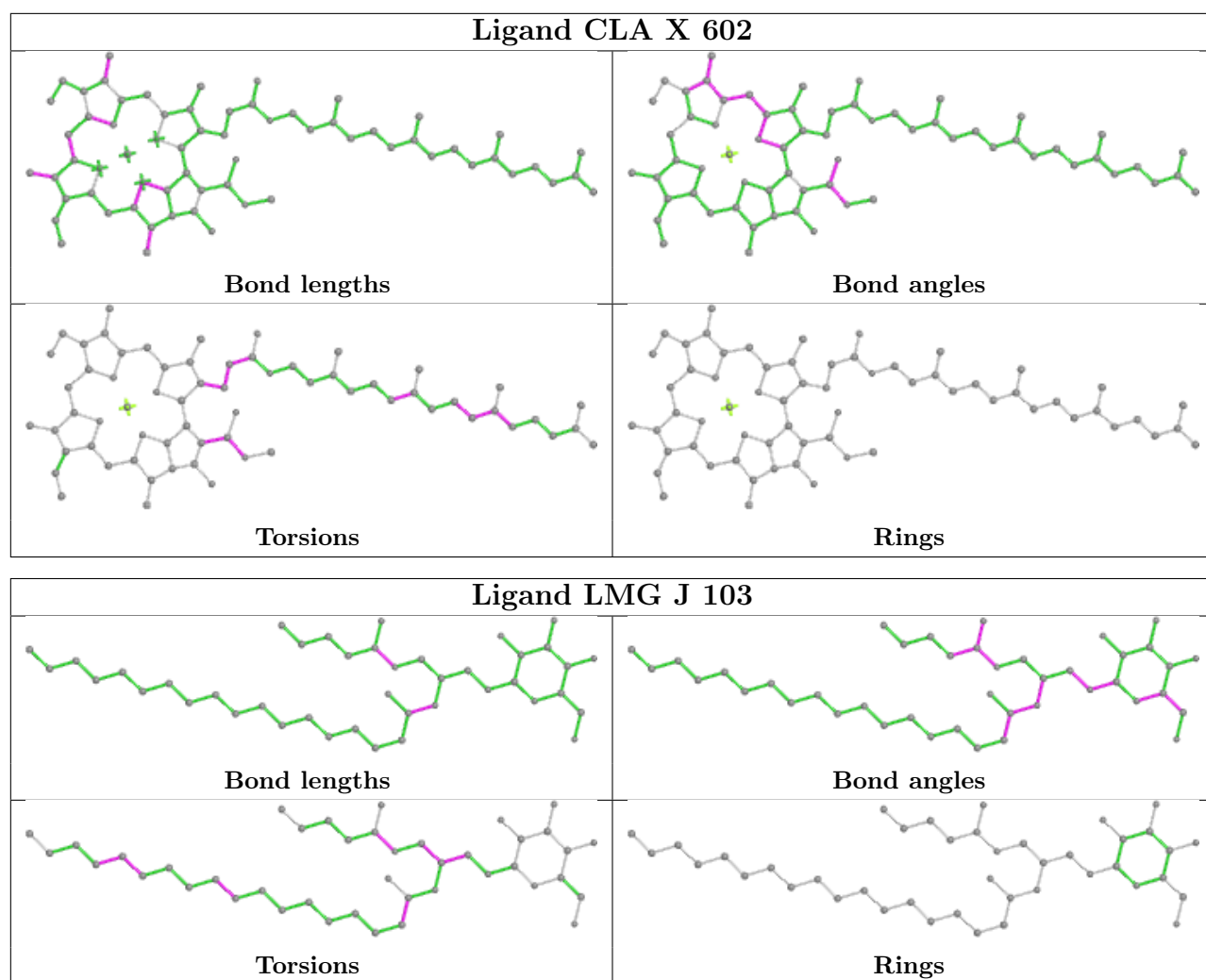
Ligand CLA A 813



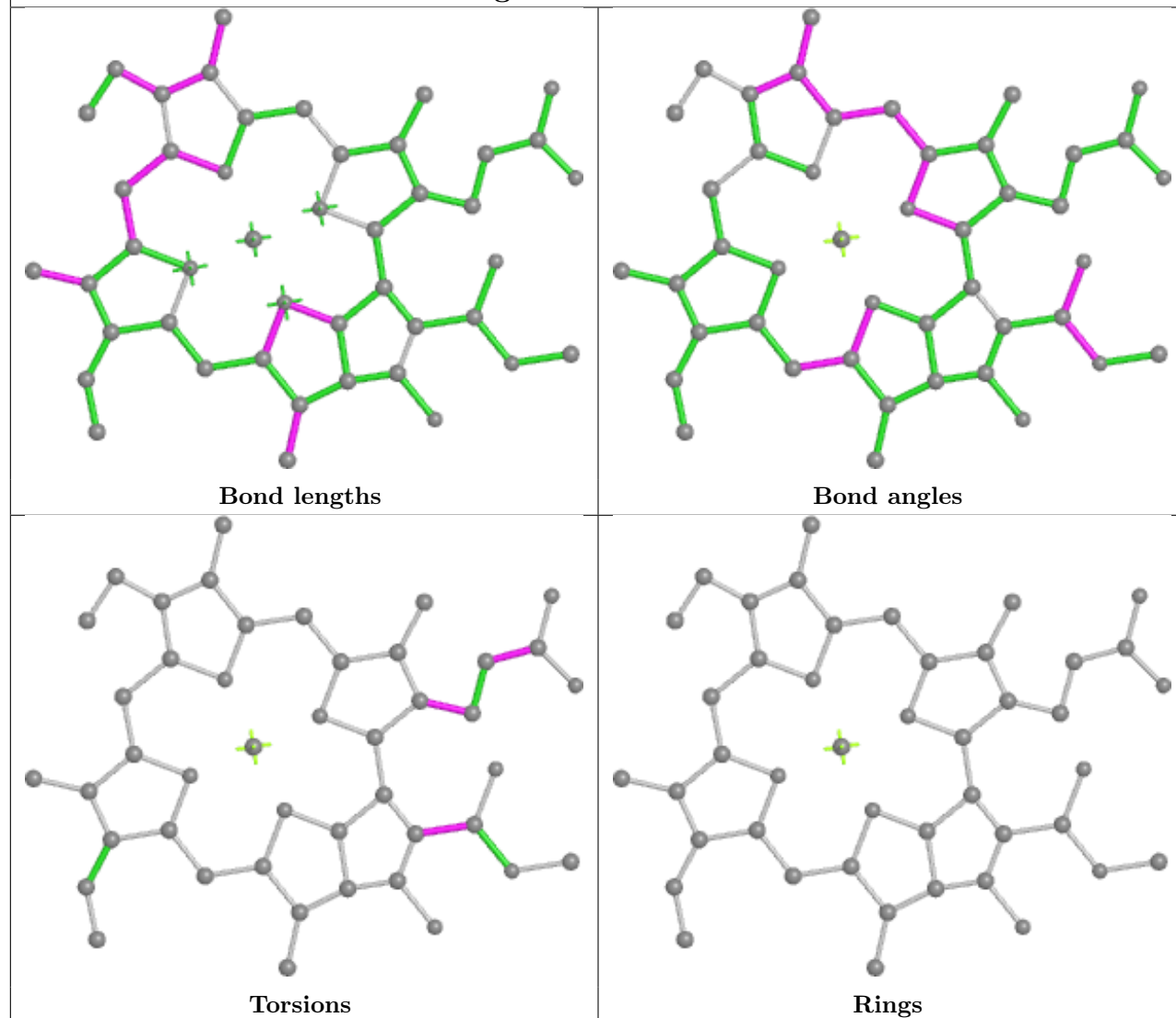
Ligand CLA B 811



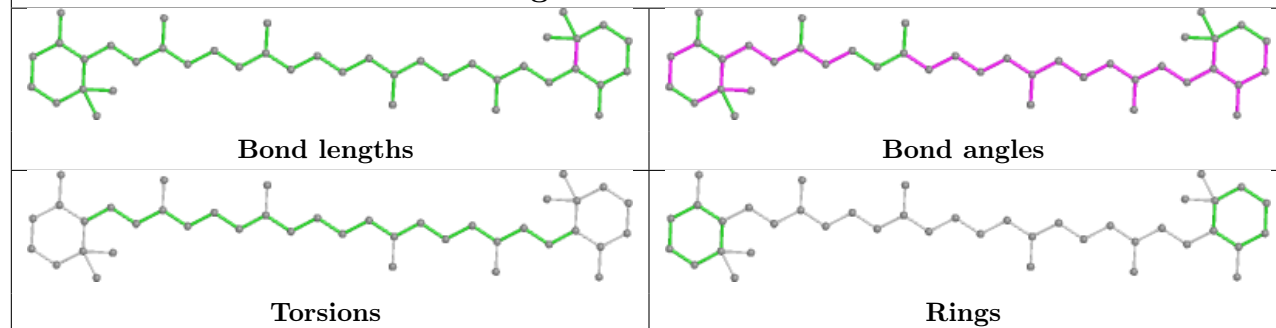


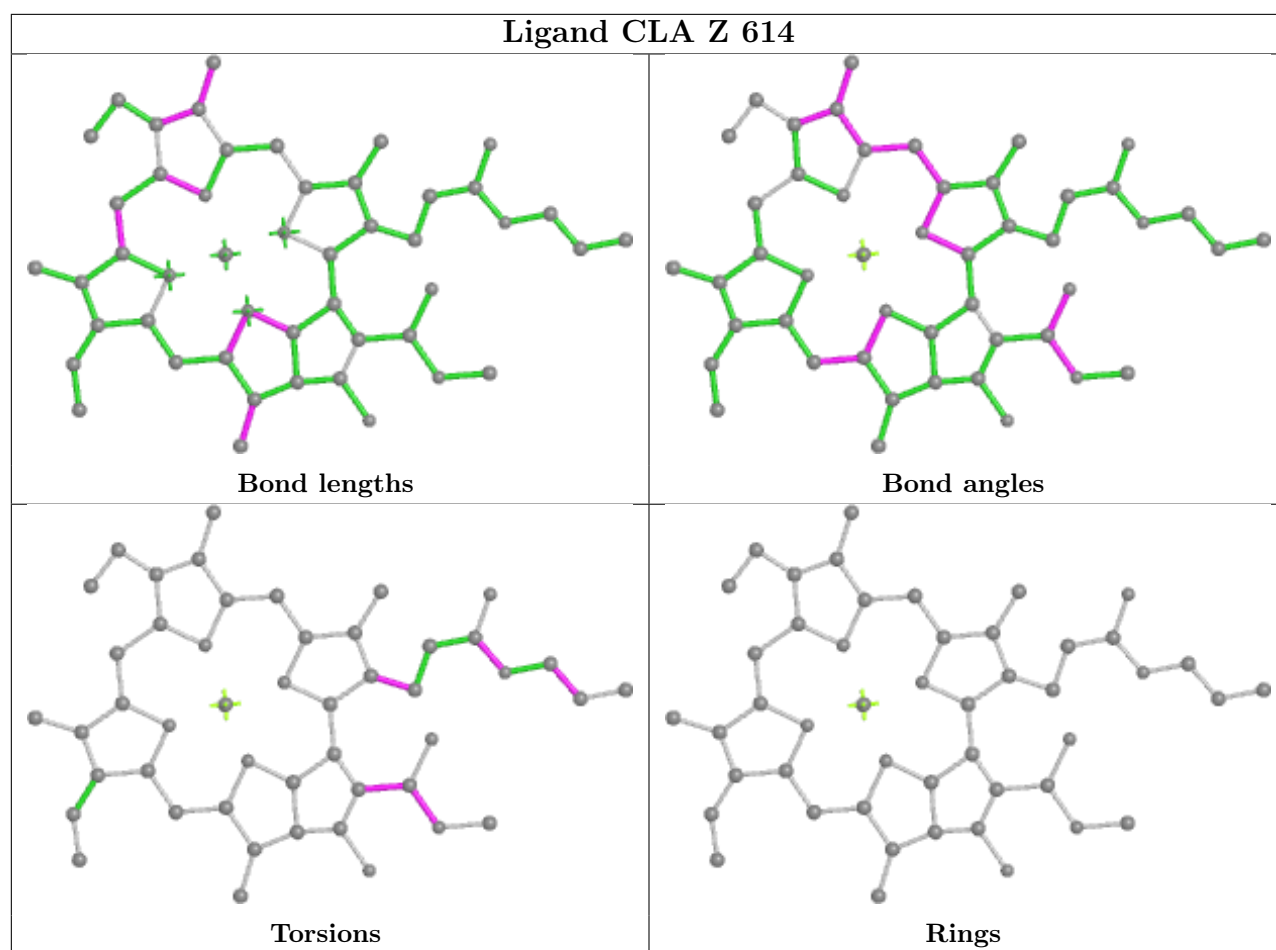


Ligand CLA 6 609

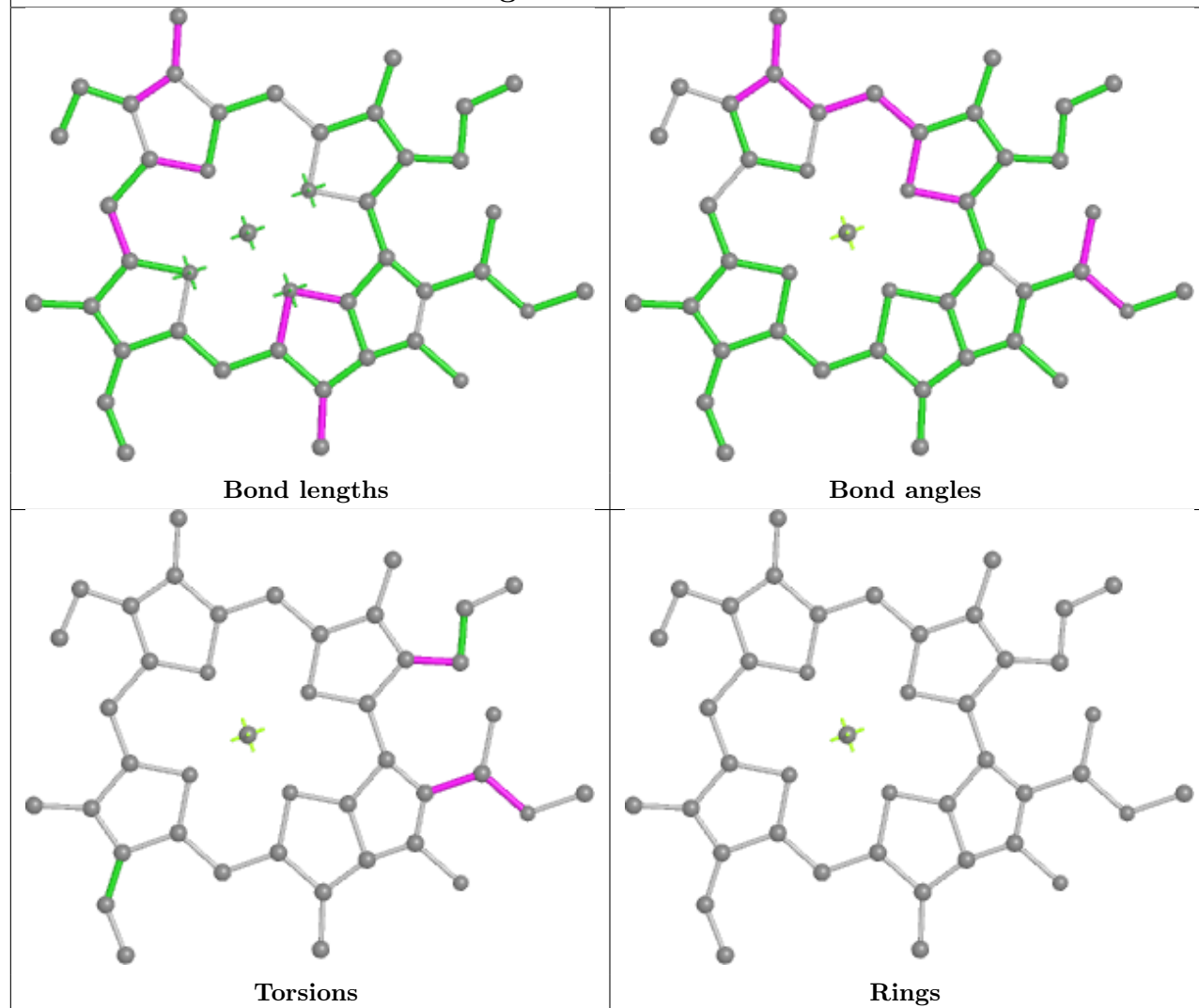


Ligand BCR B 846

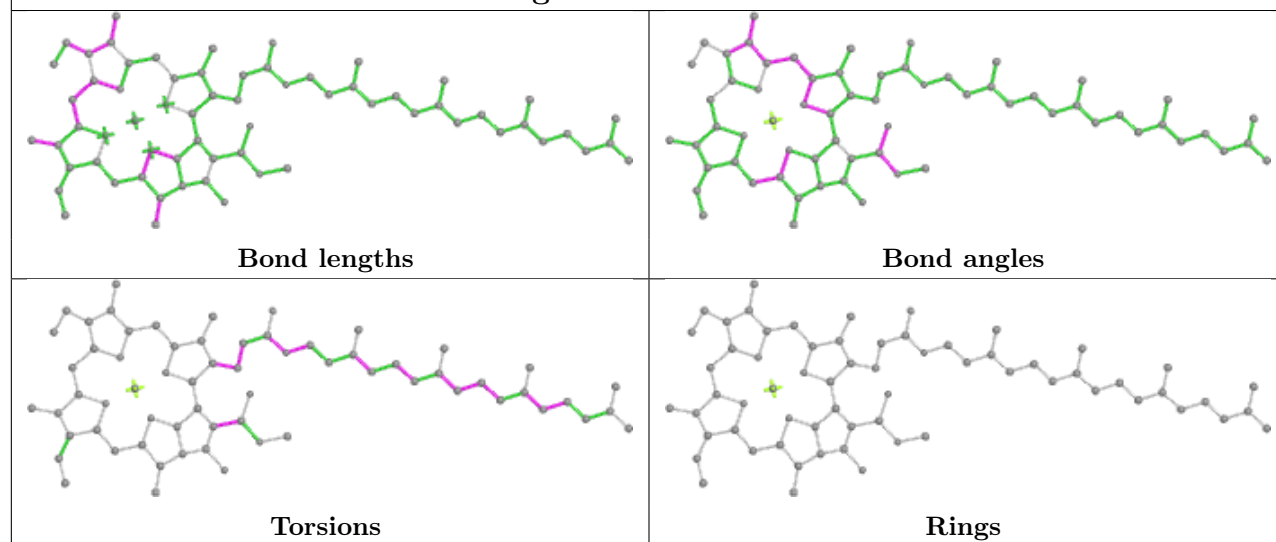


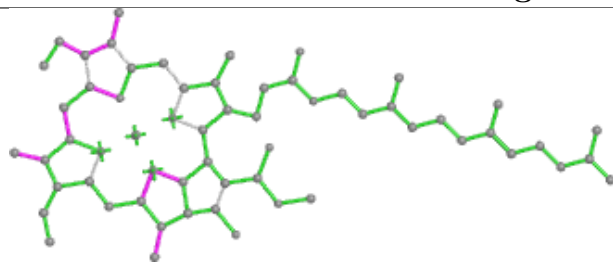
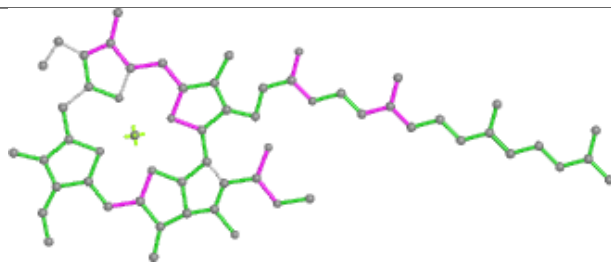
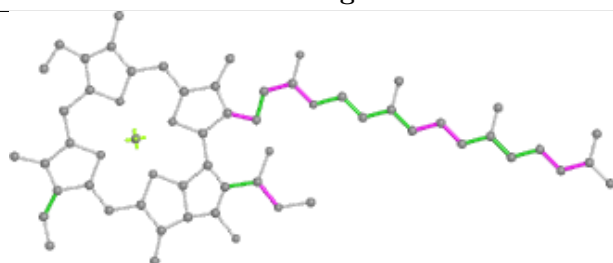
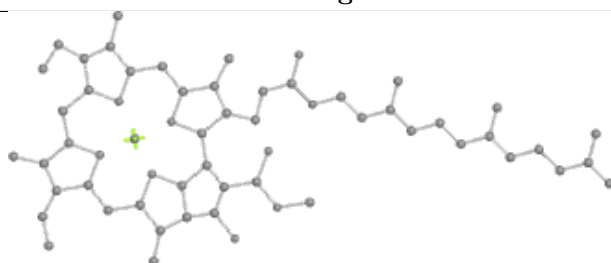
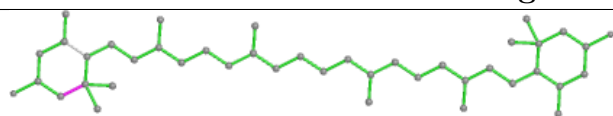
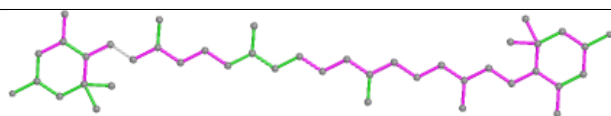
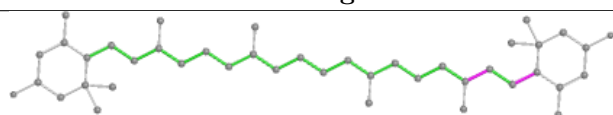
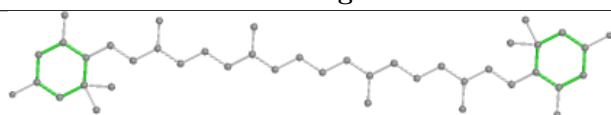


Ligand CLA Y 611

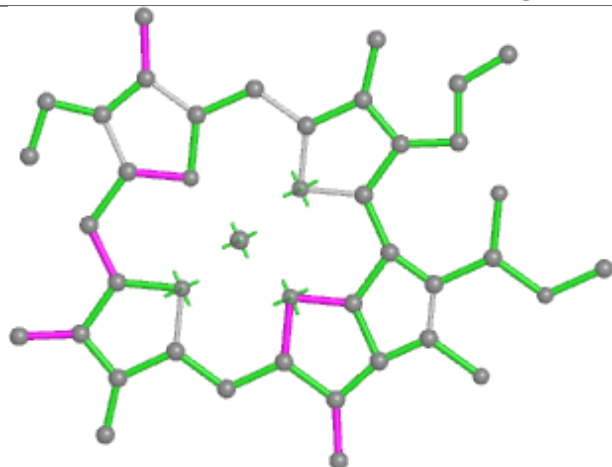


Ligand CLA B 828

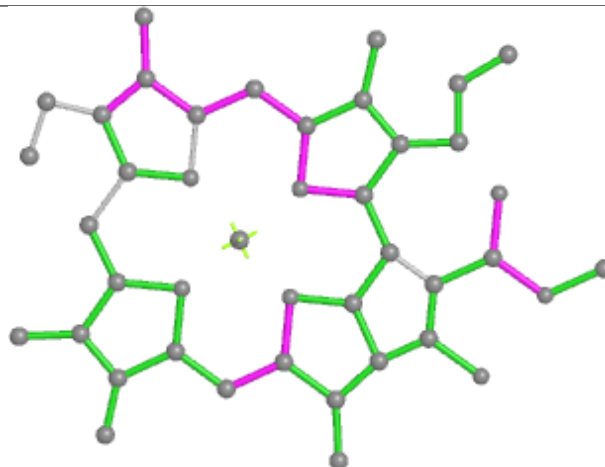


Ligand CLA B 832**Bond lengths****Bond angles****Torsions****Rings****Ligand LUT 9 619****Bond lengths****Bond angles****Torsions****Rings**

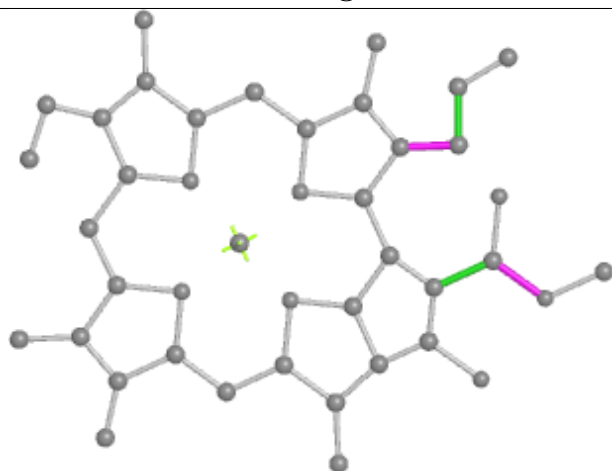
Ligand CLA 2 604



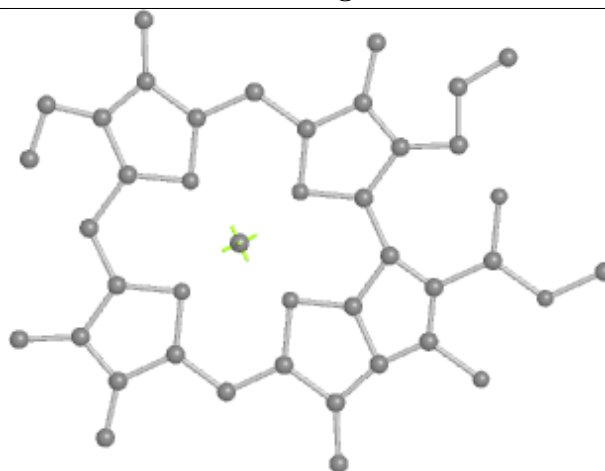
Bond lengths



Bond angles

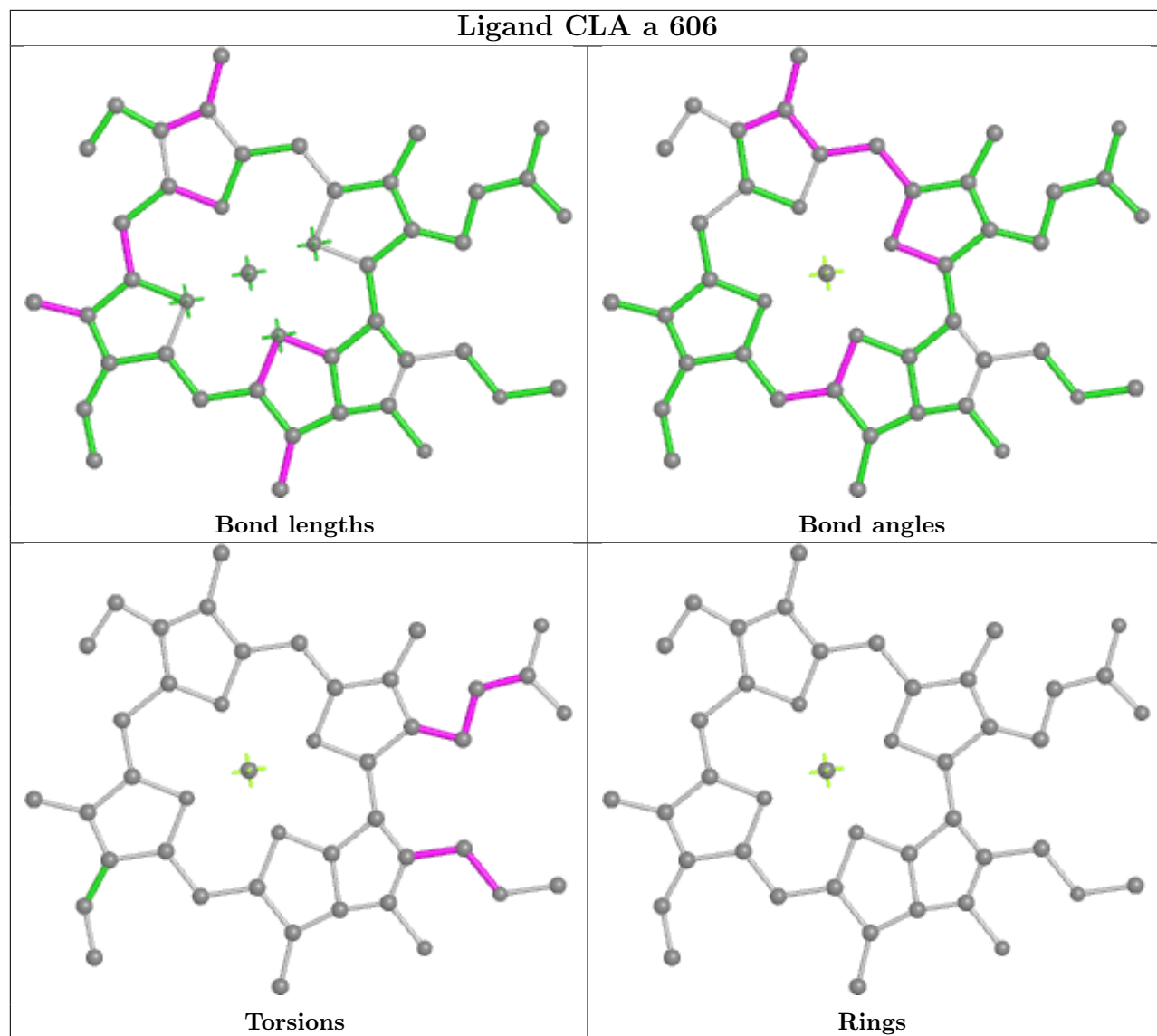


Torsions

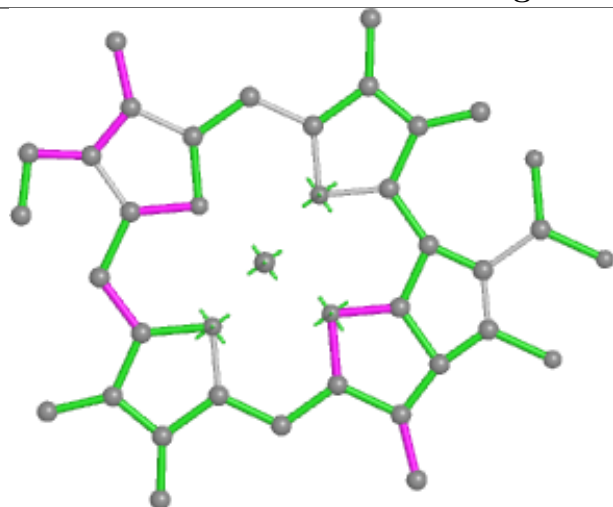


Rings

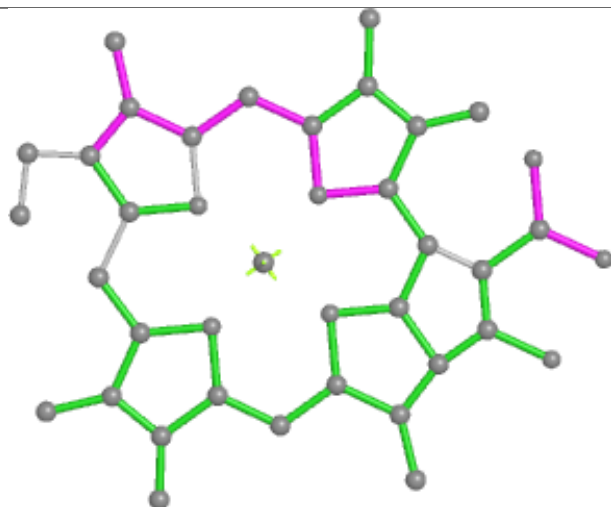
Ligand CLA a 606



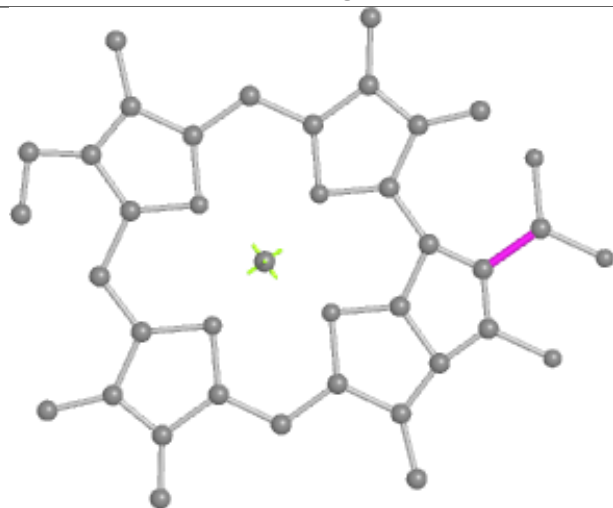
Ligand CLA H 202



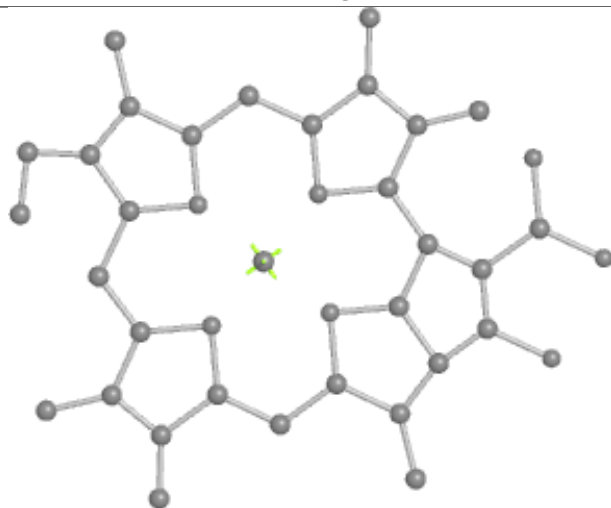
Bond lengths



Bond angles

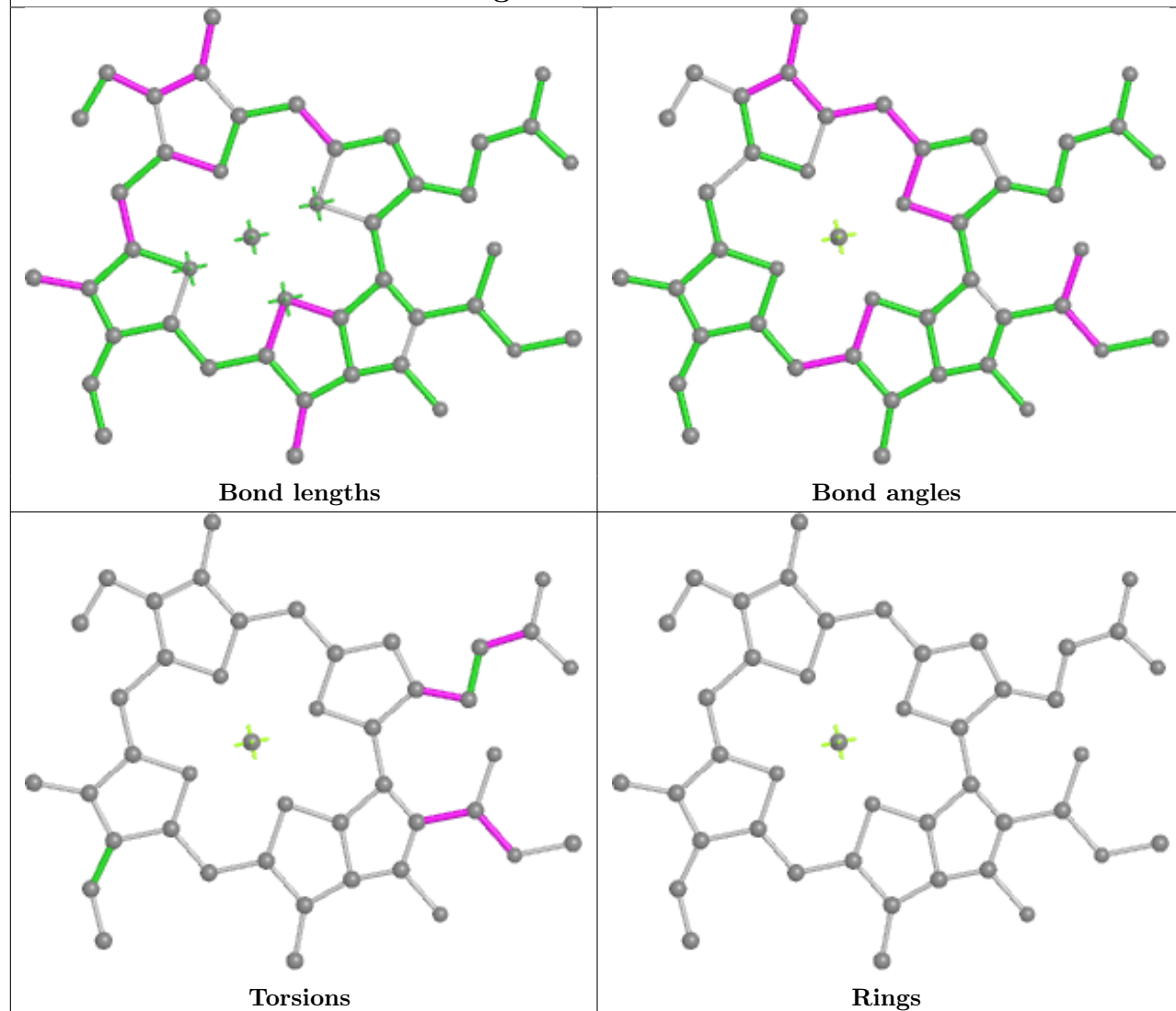


Torsions

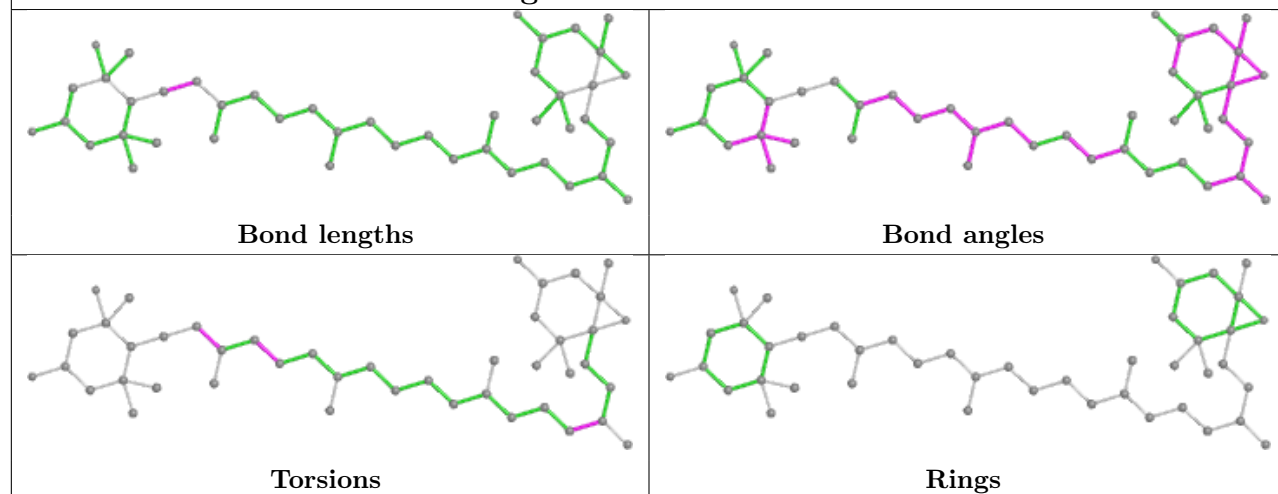


Rings

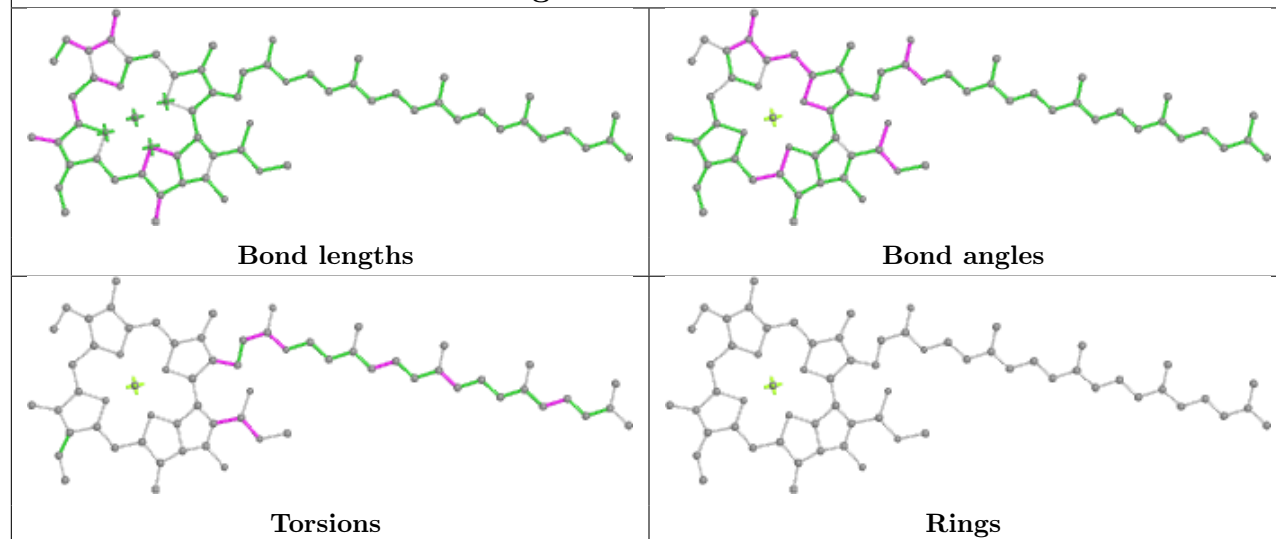
Ligand CLA 5 614



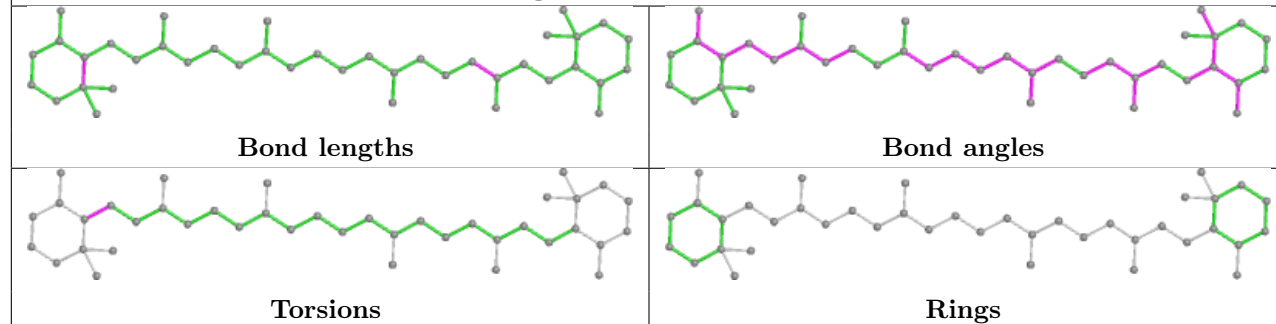
Ligand NEX X 1623



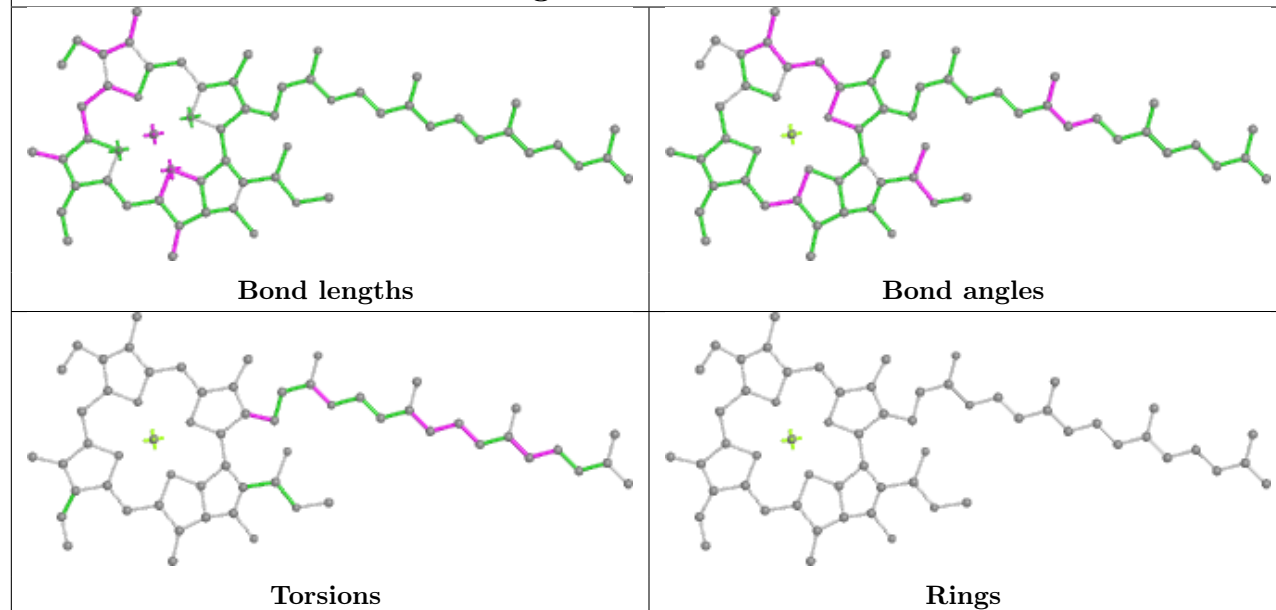
Ligand CLA B 841

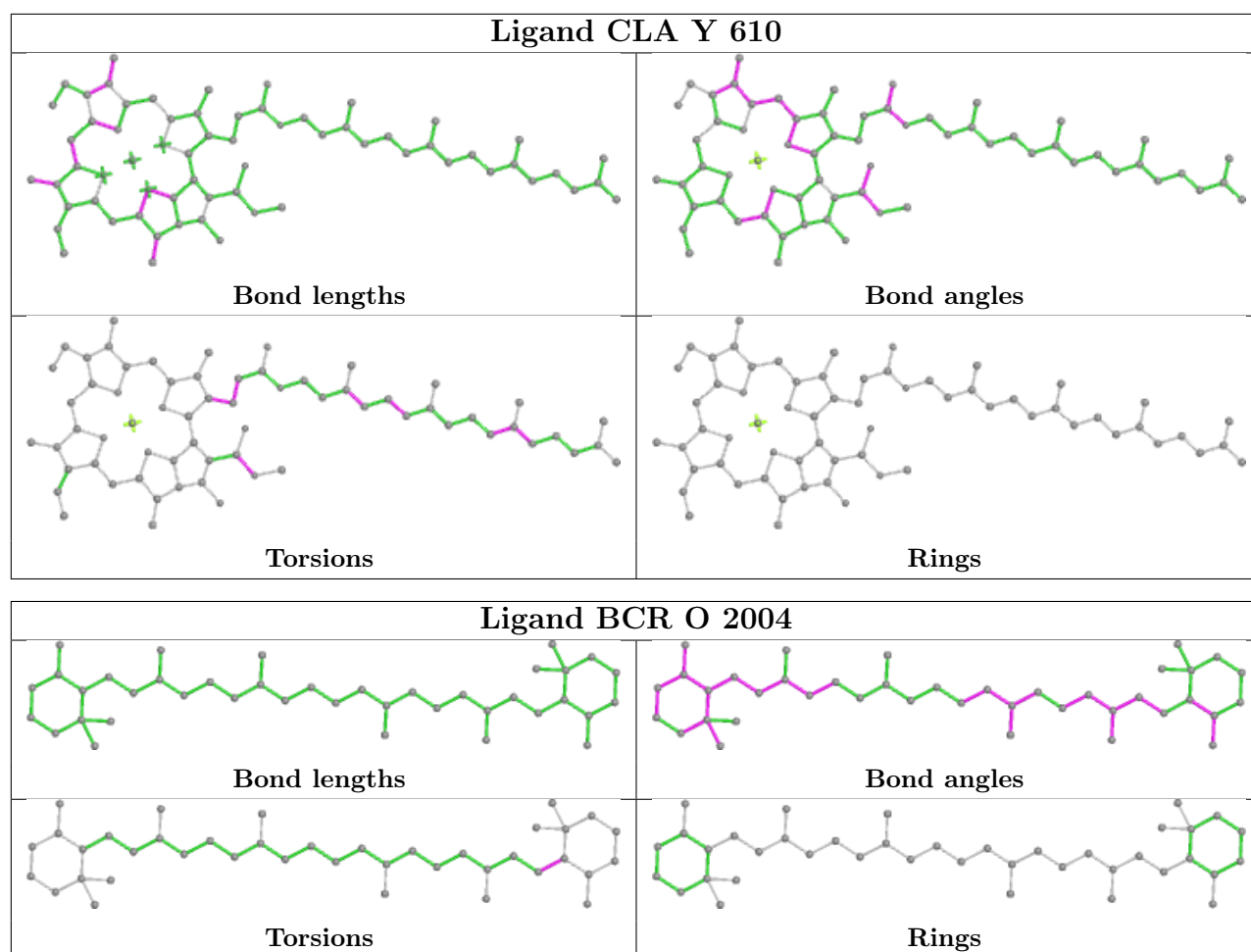


Ligand BCR A 856

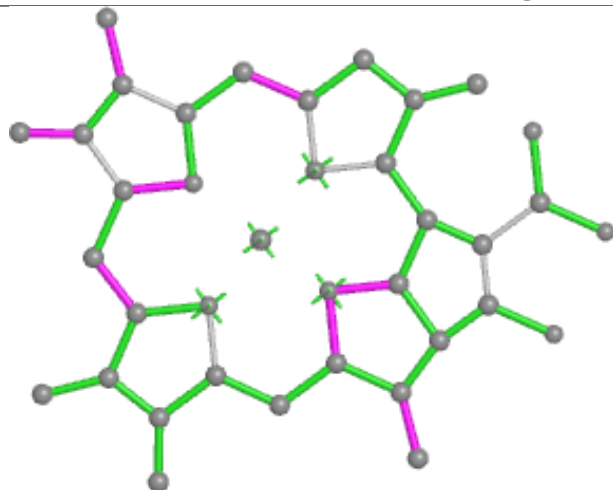


Ligand CLA B 818

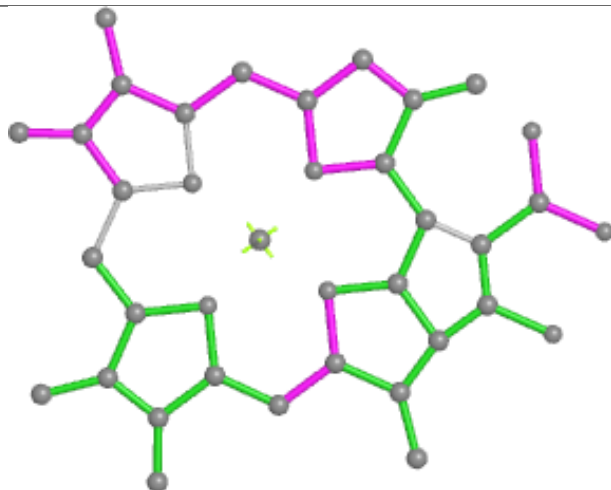




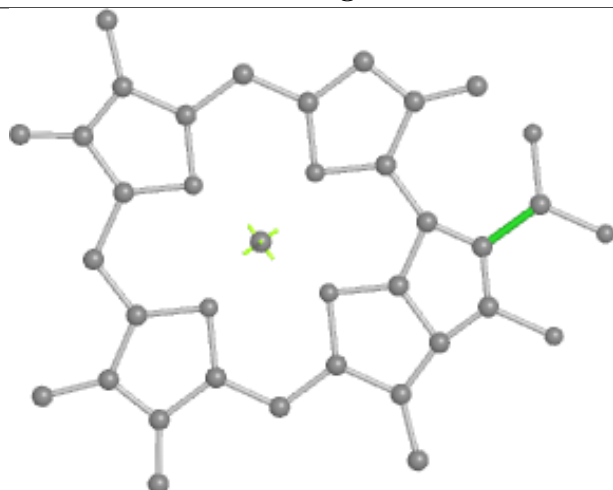
Ligand CLA 1 614



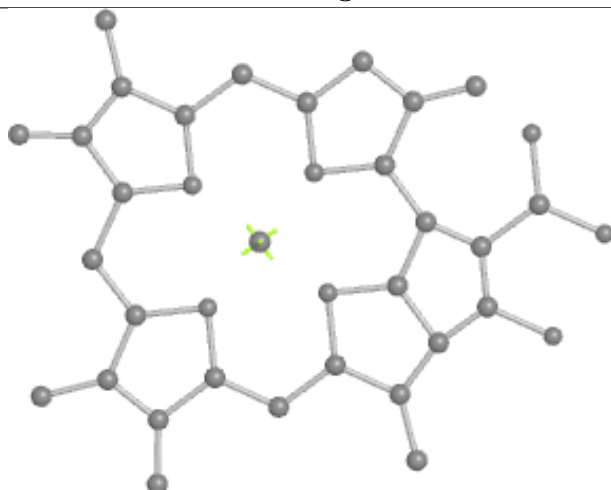
Bond lengths



Bond angles

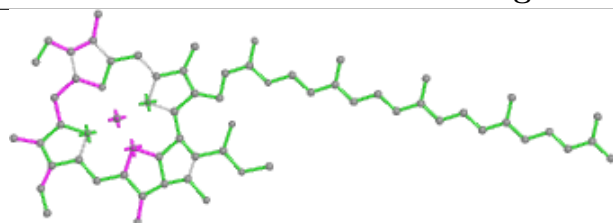


Torsions

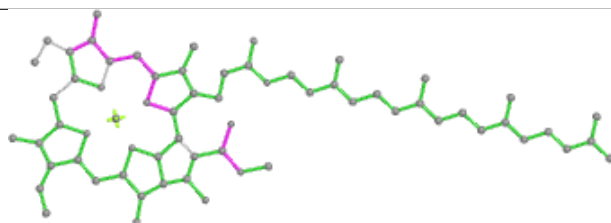


Rings

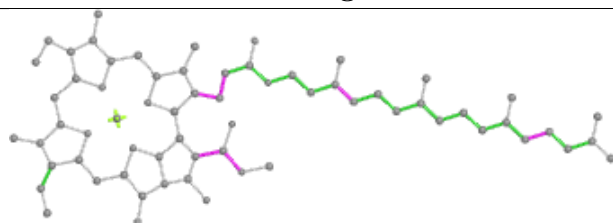
Ligand CLA A 803



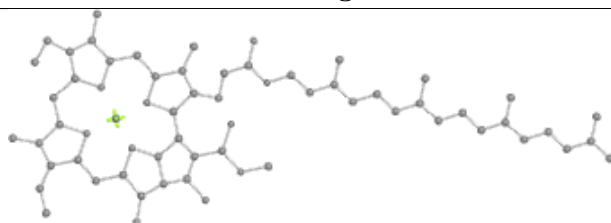
Bond lengths



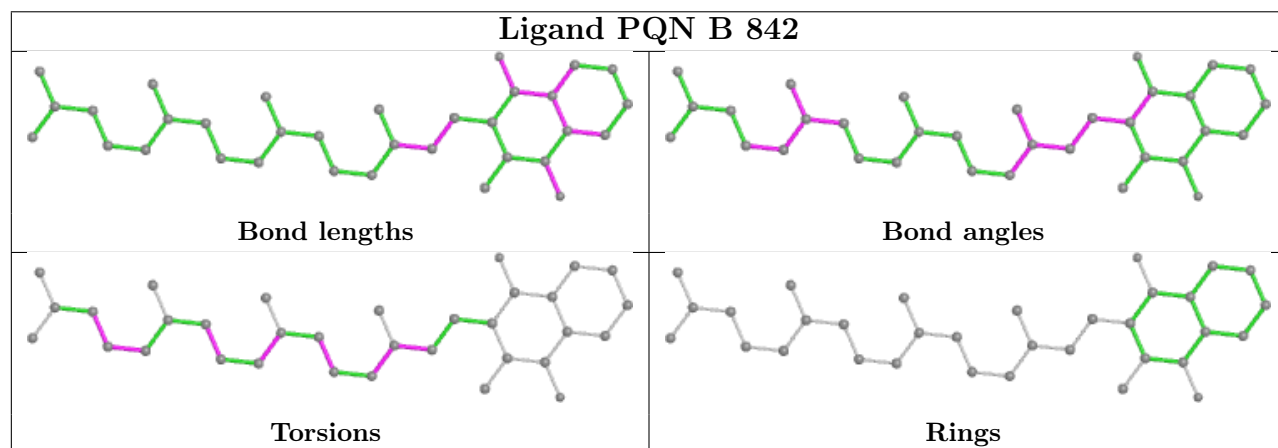
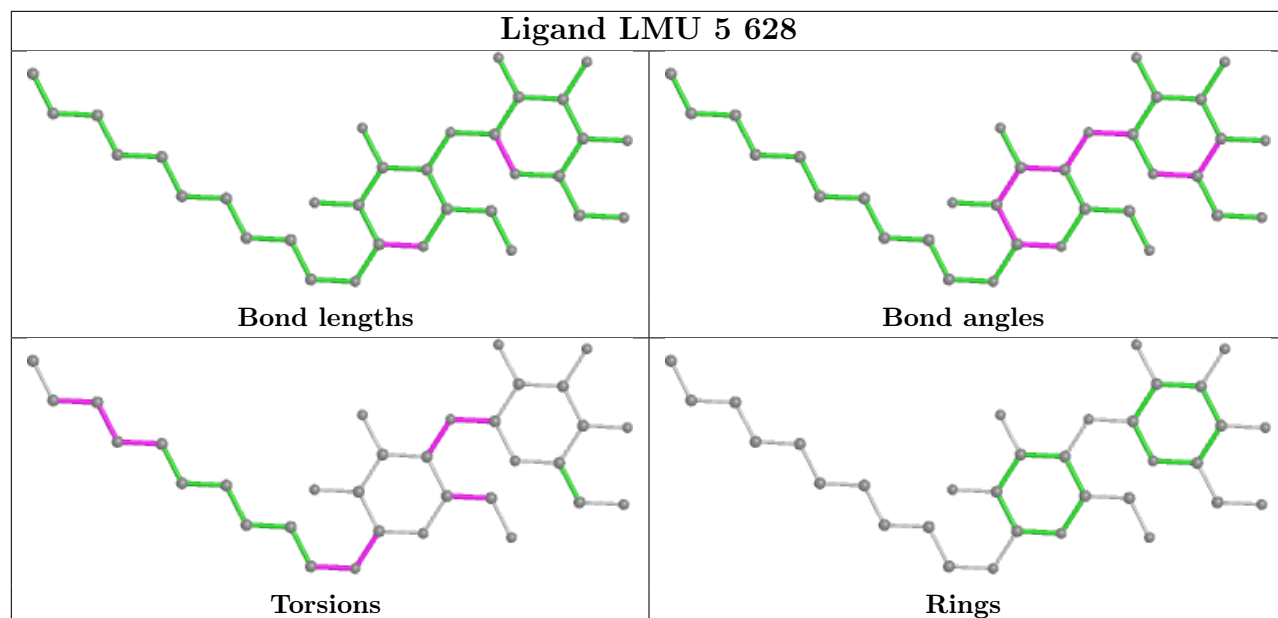
Bond angles



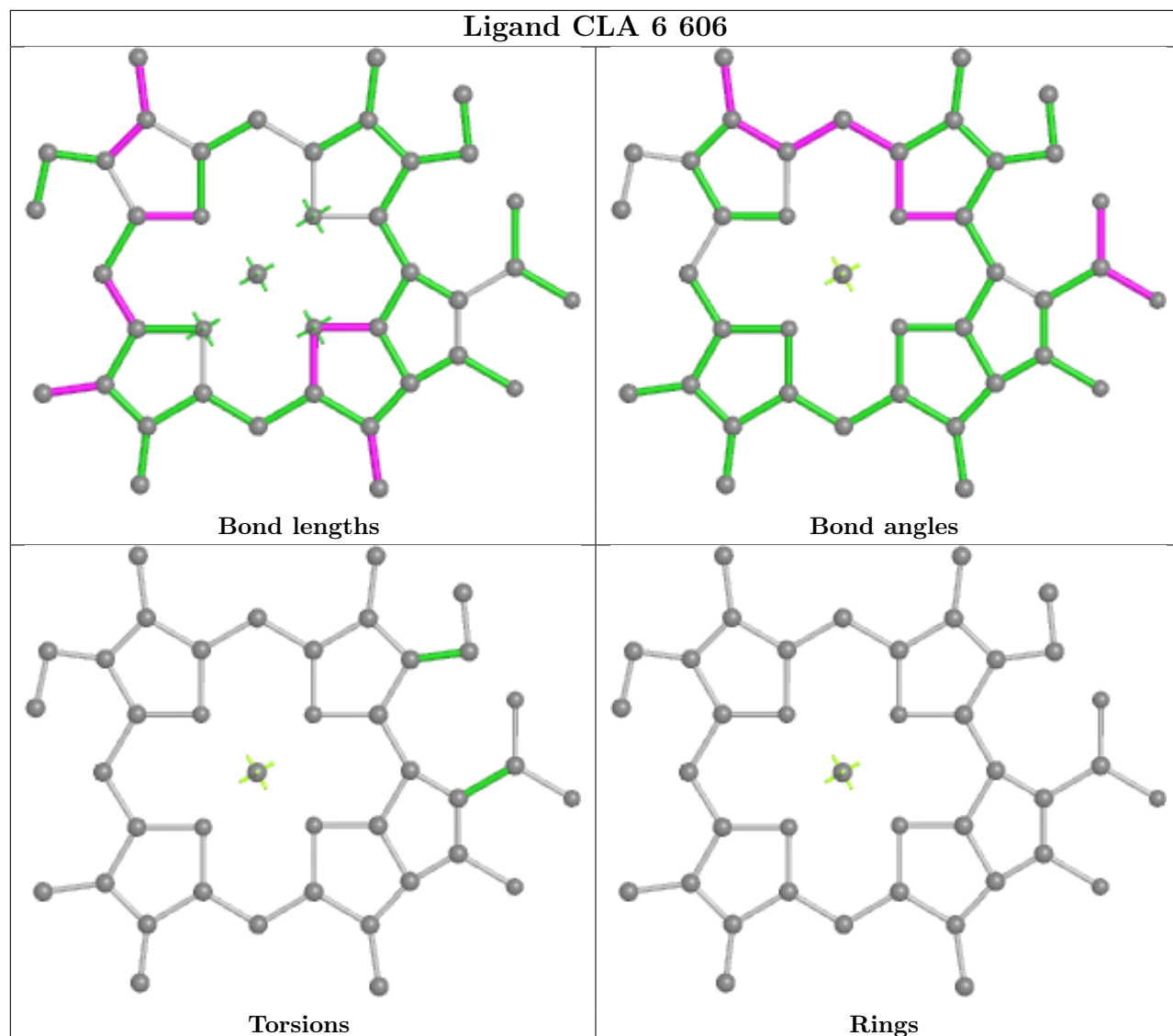
Torsions



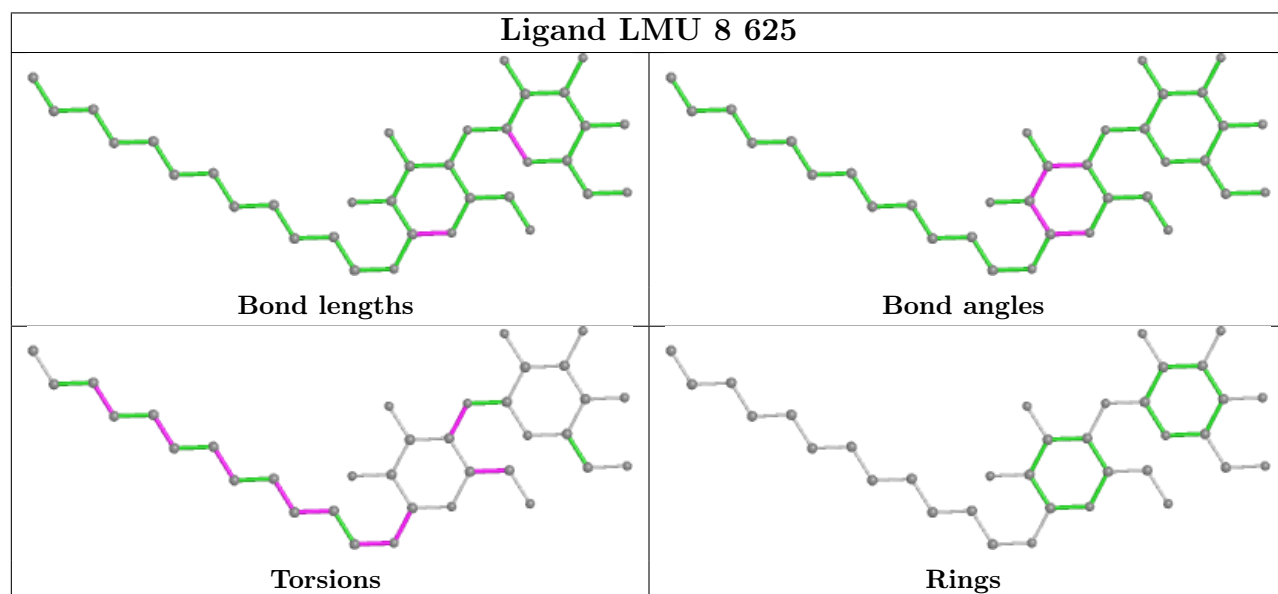
Rings

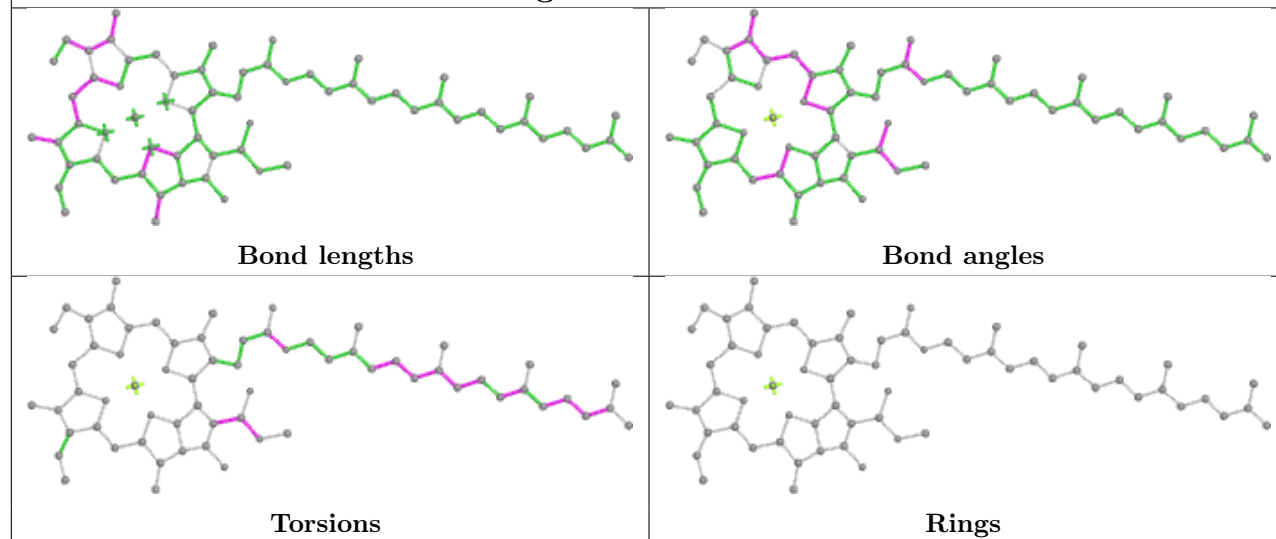
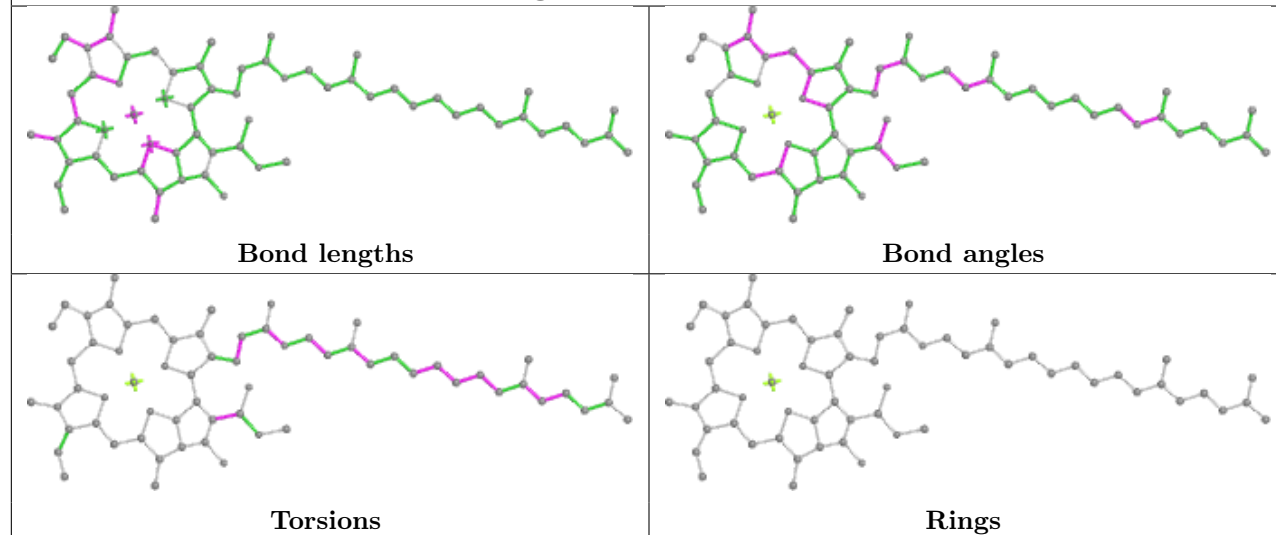


Ligand CLA 6 606

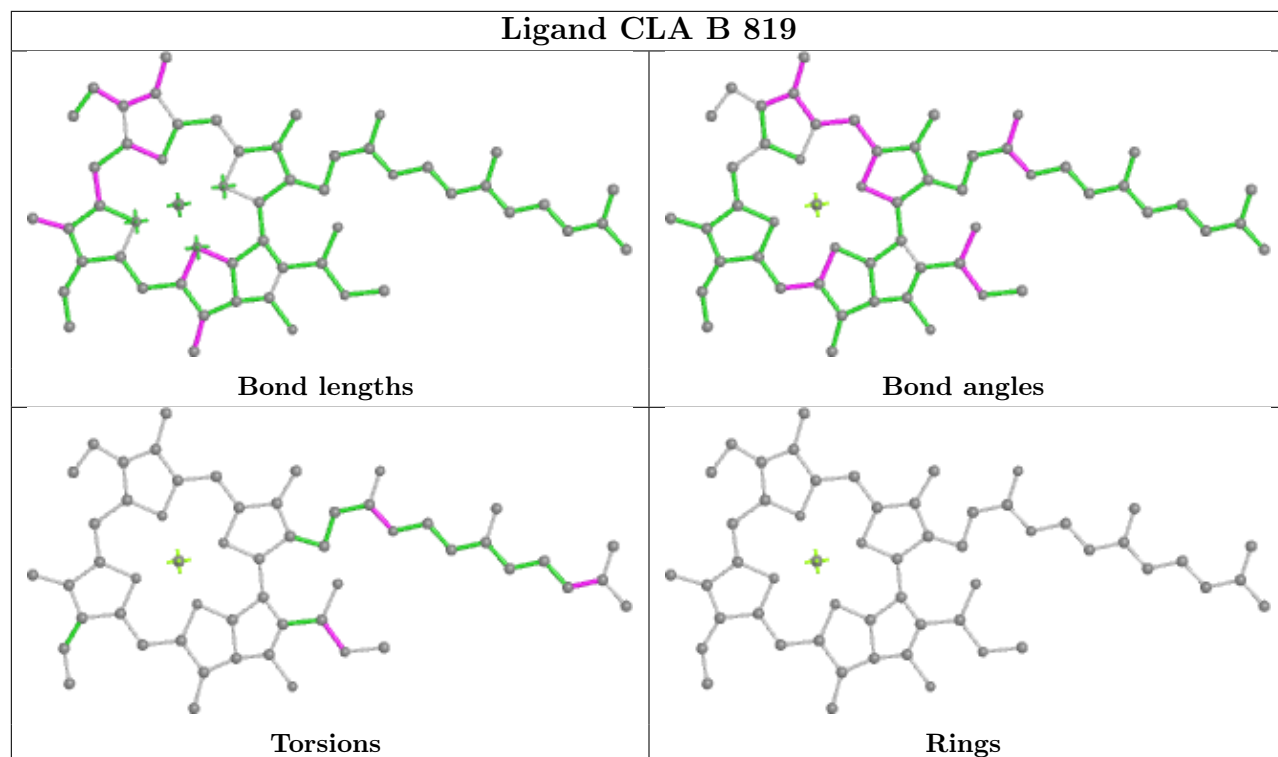


Ligand LMU 8 625

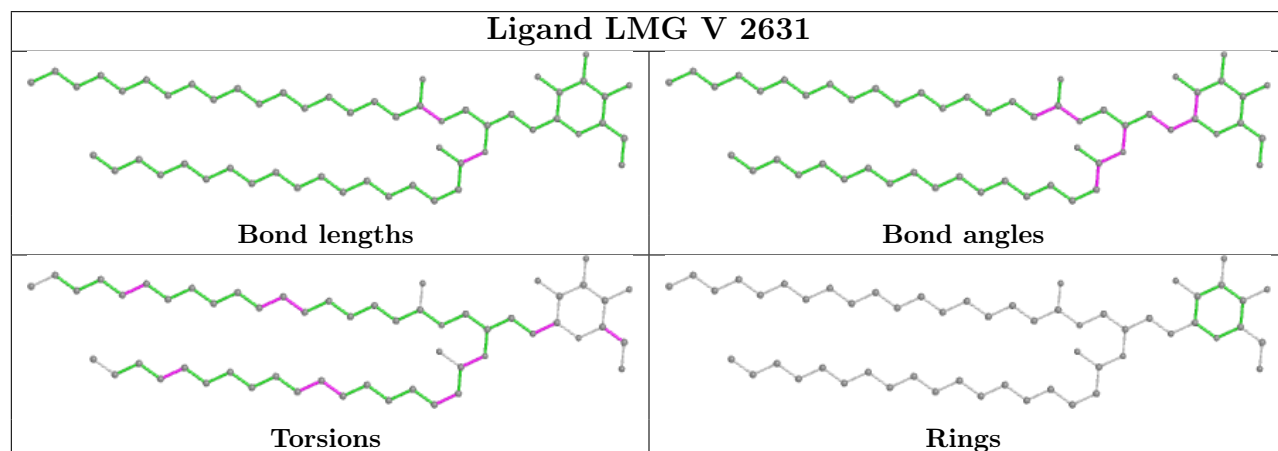


Ligand CLA 6 604**Ligand CLA A 843**

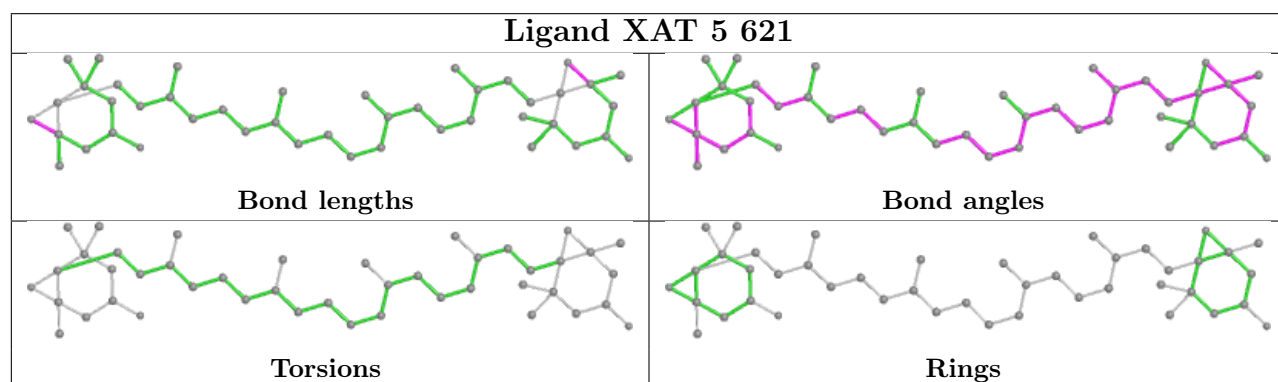
Ligand CLA B 819

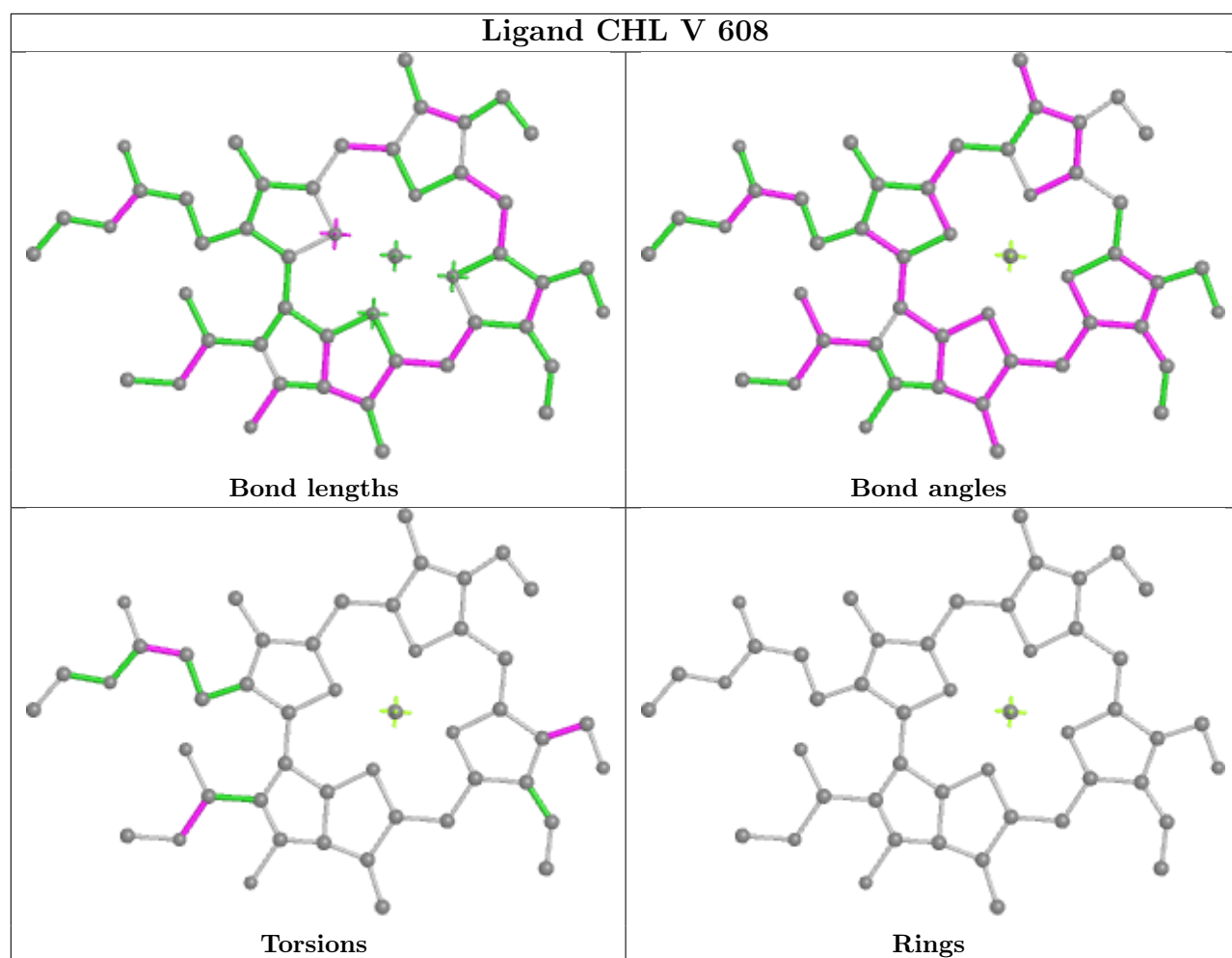


Ligand LMG V 2631

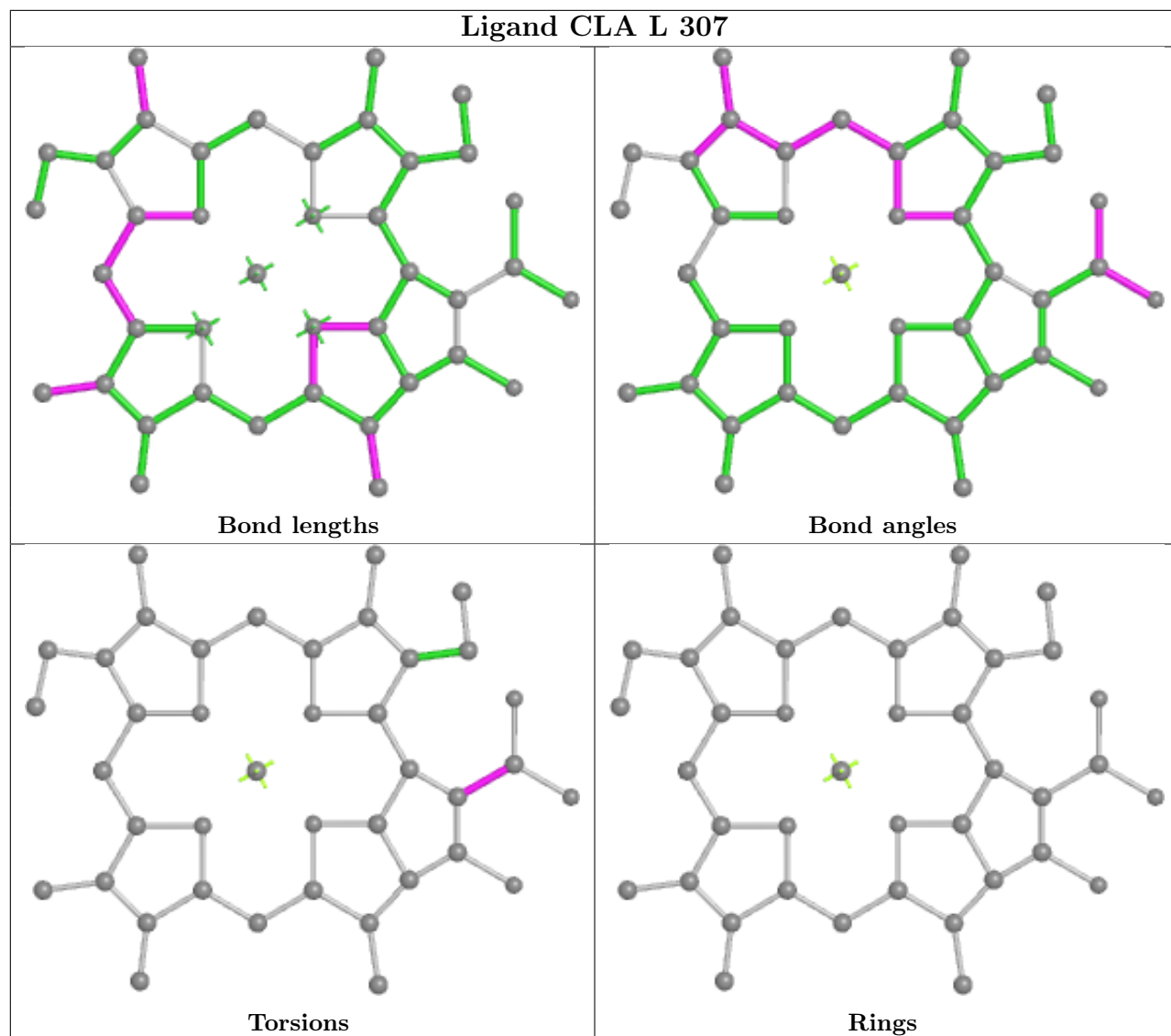


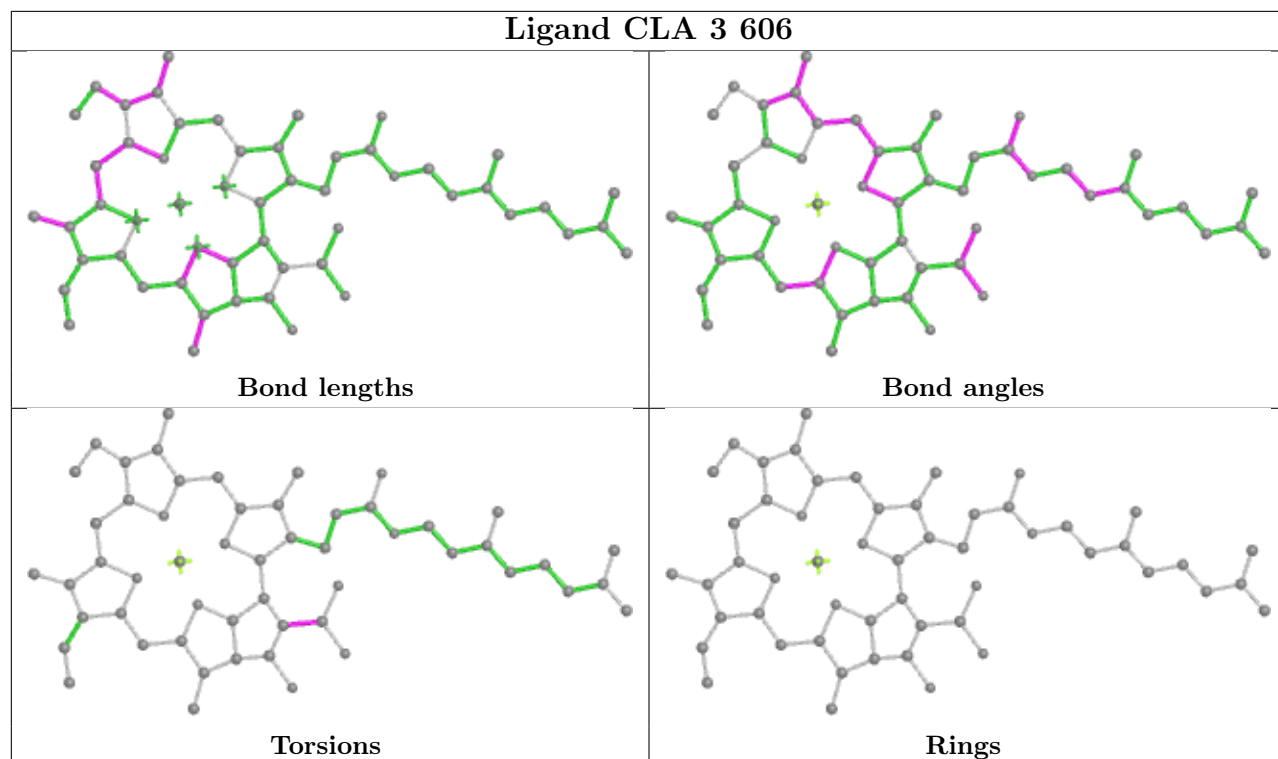
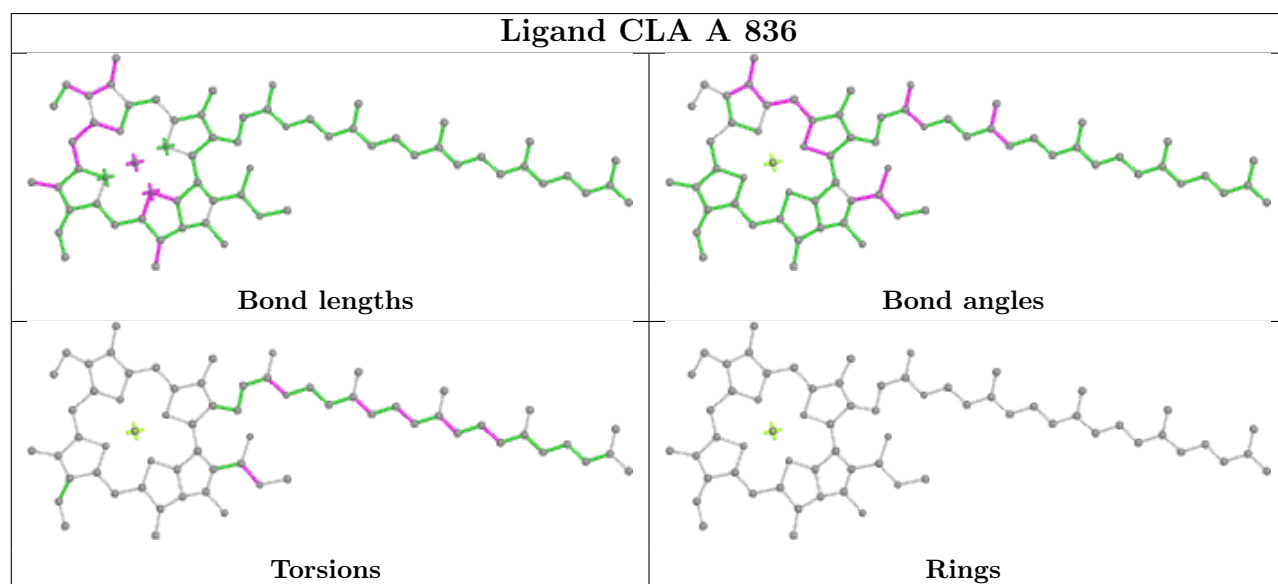
Ligand XAT 5 621

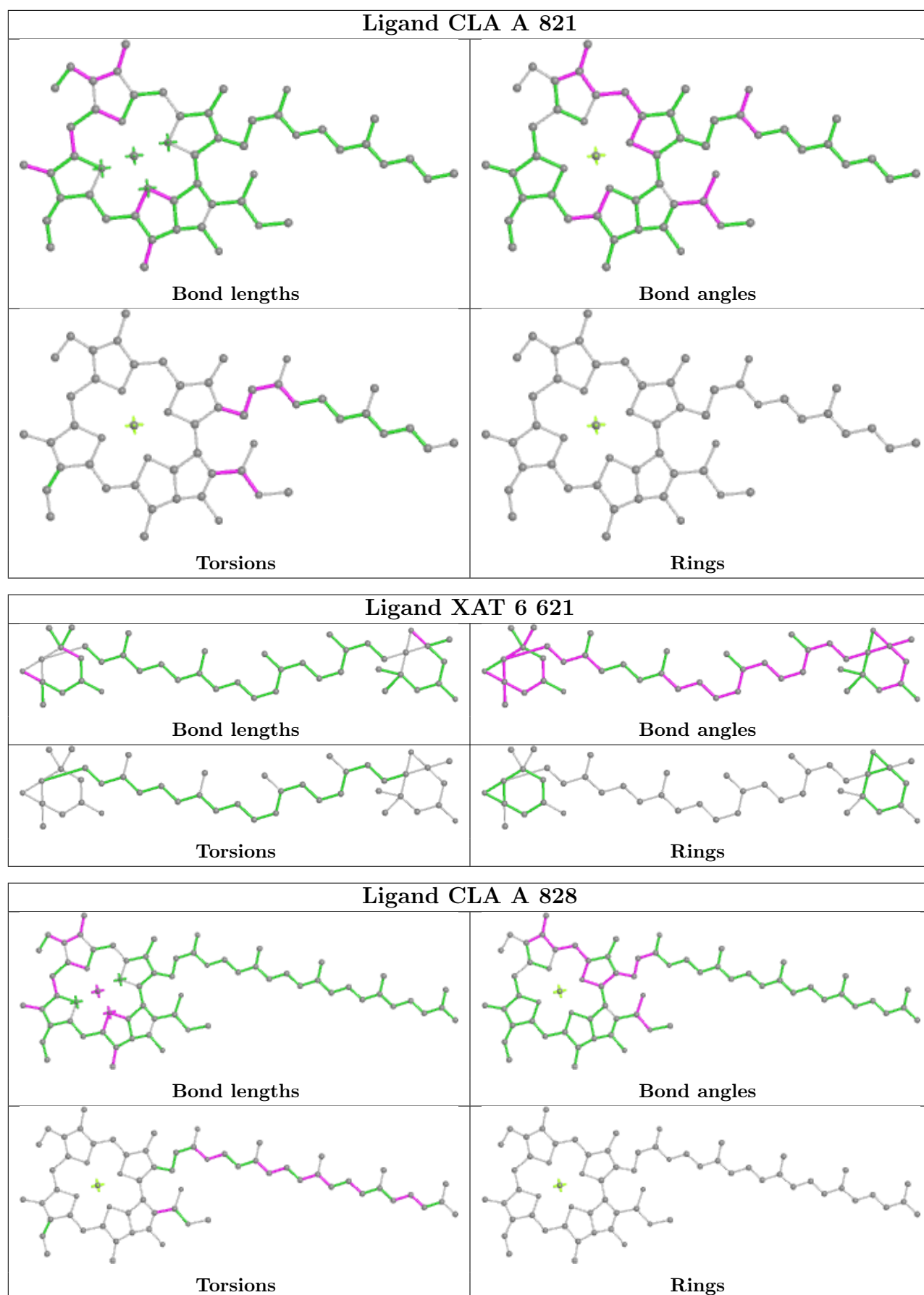


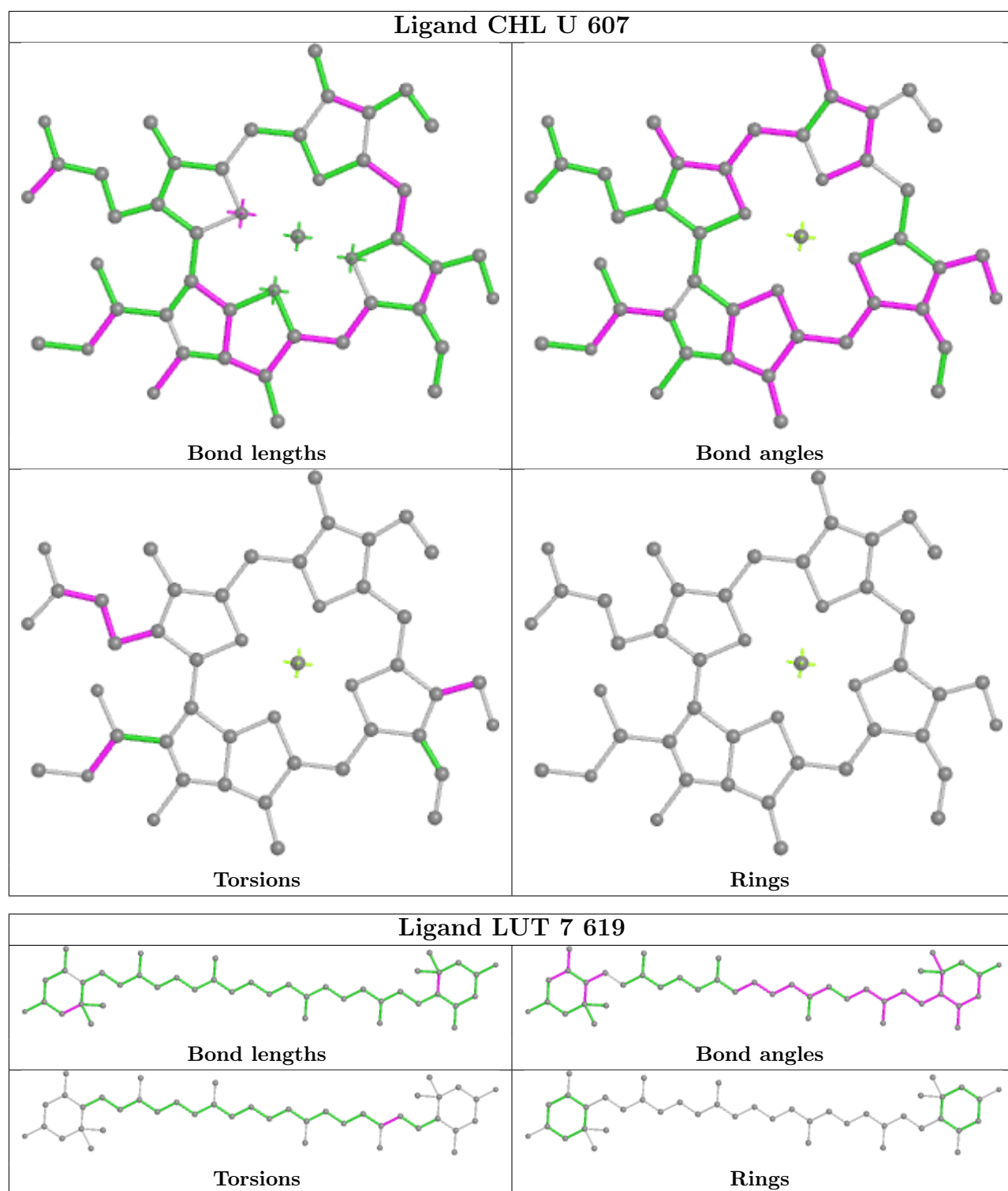


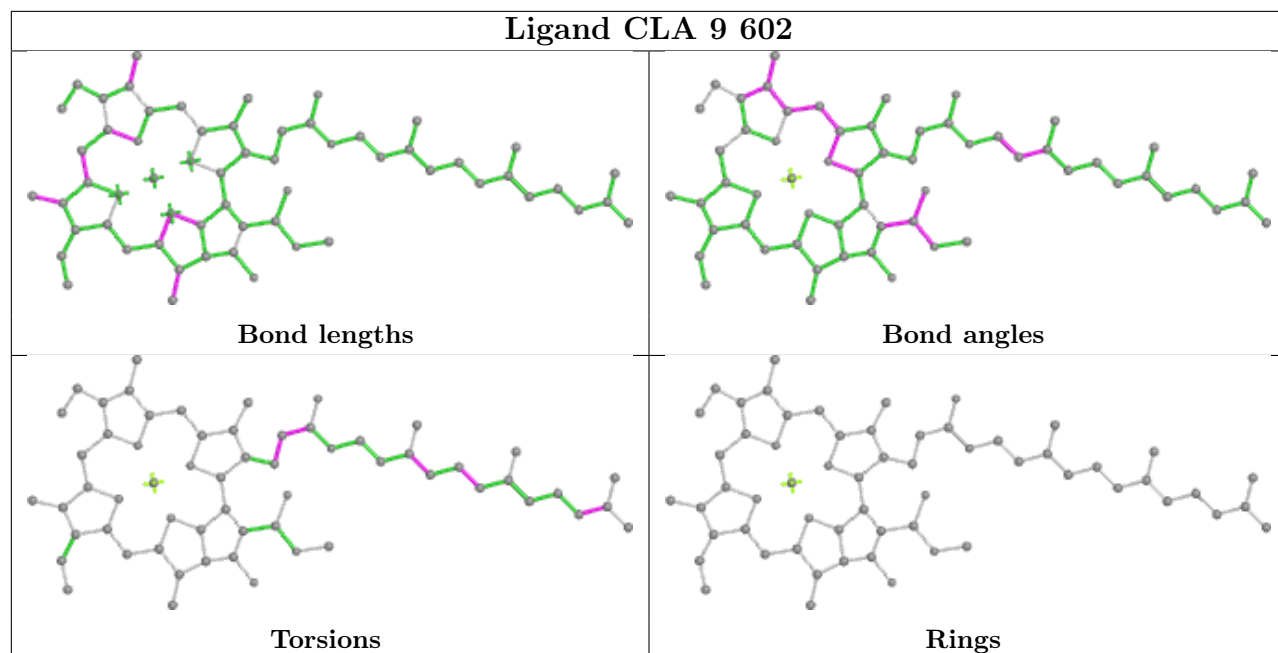
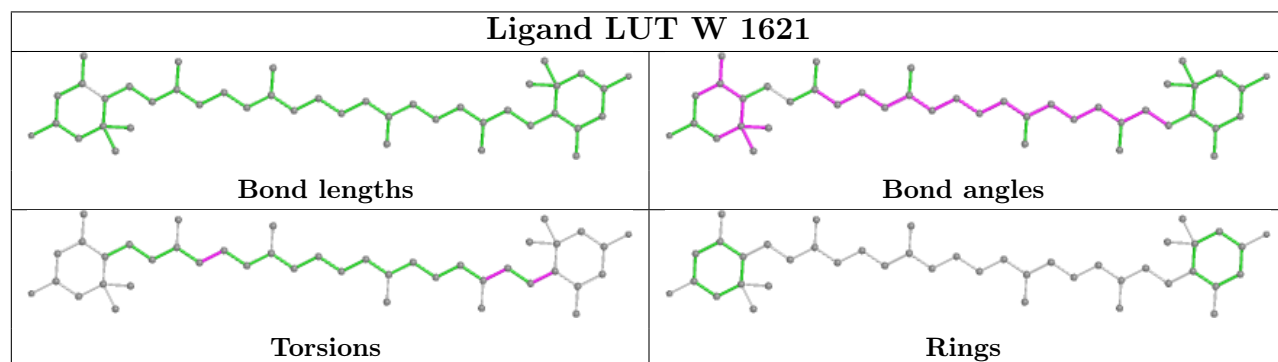
Ligand CLA L 307



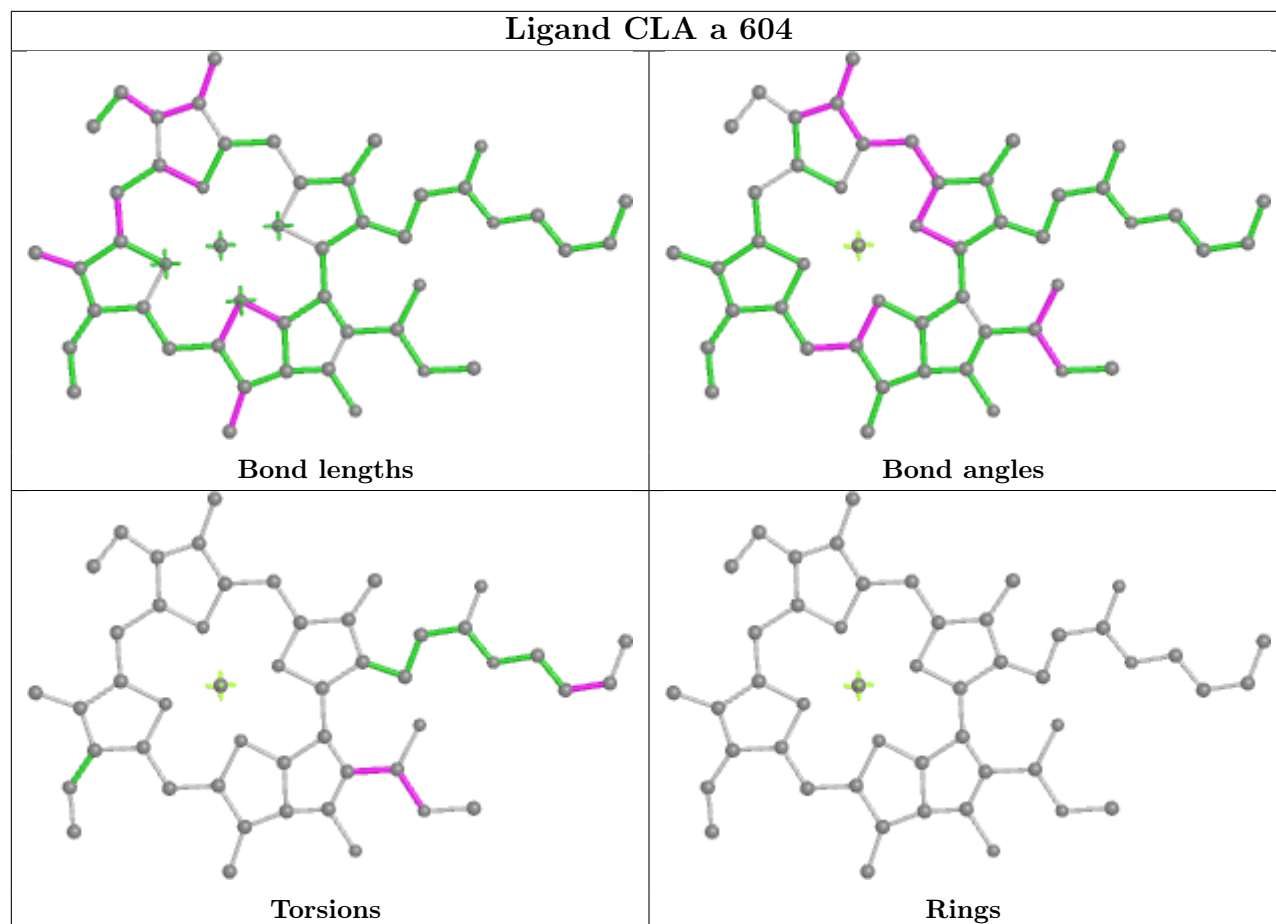
Ligand CLA 3 606**Ligand CLA A 836**



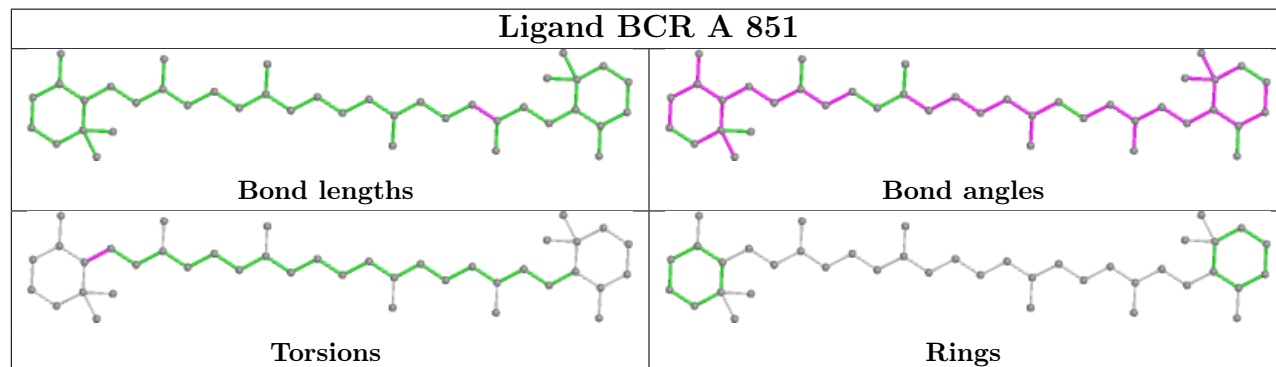


Ligand CLA 9 602**Ligand LUT W 1621**

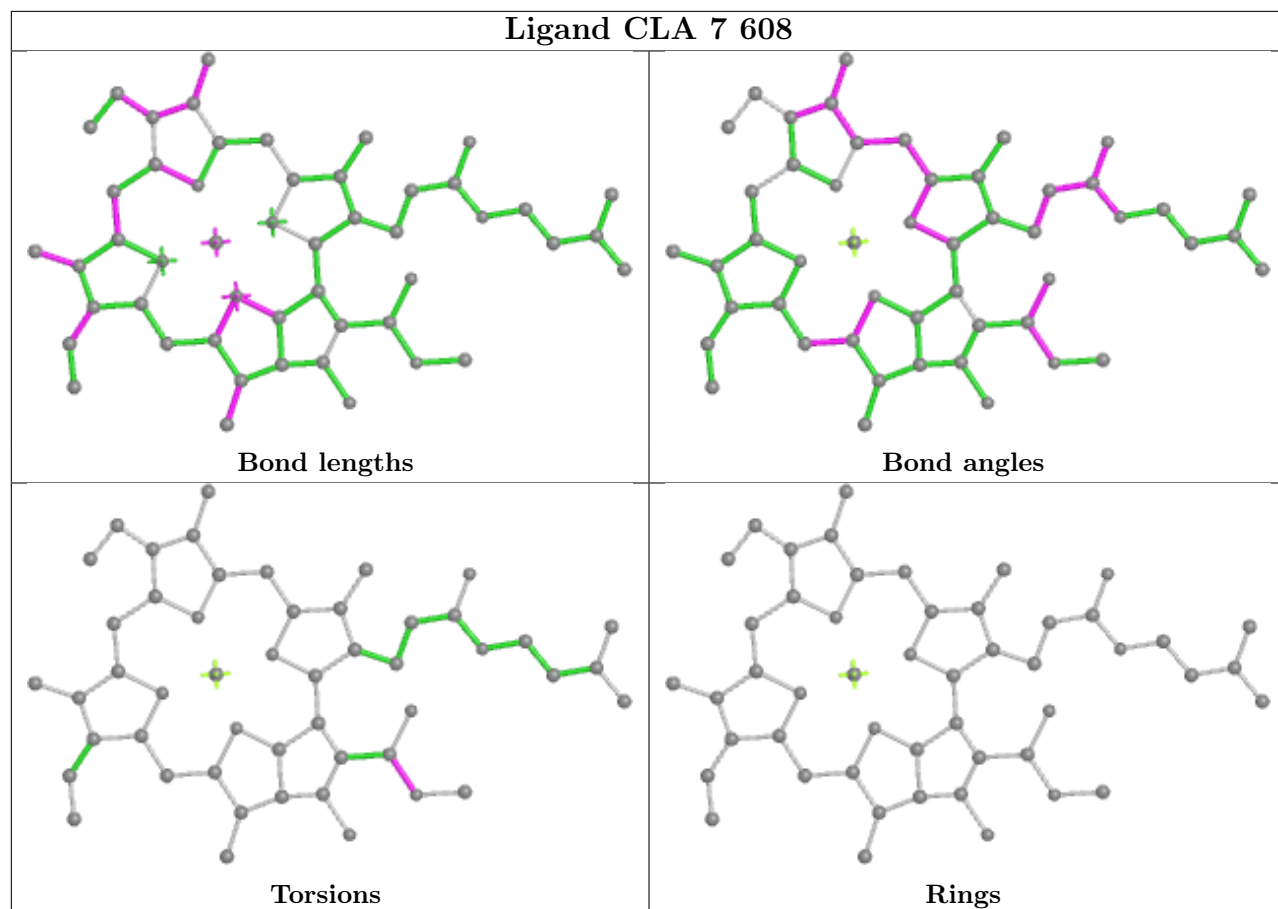
Ligand CLA a 604



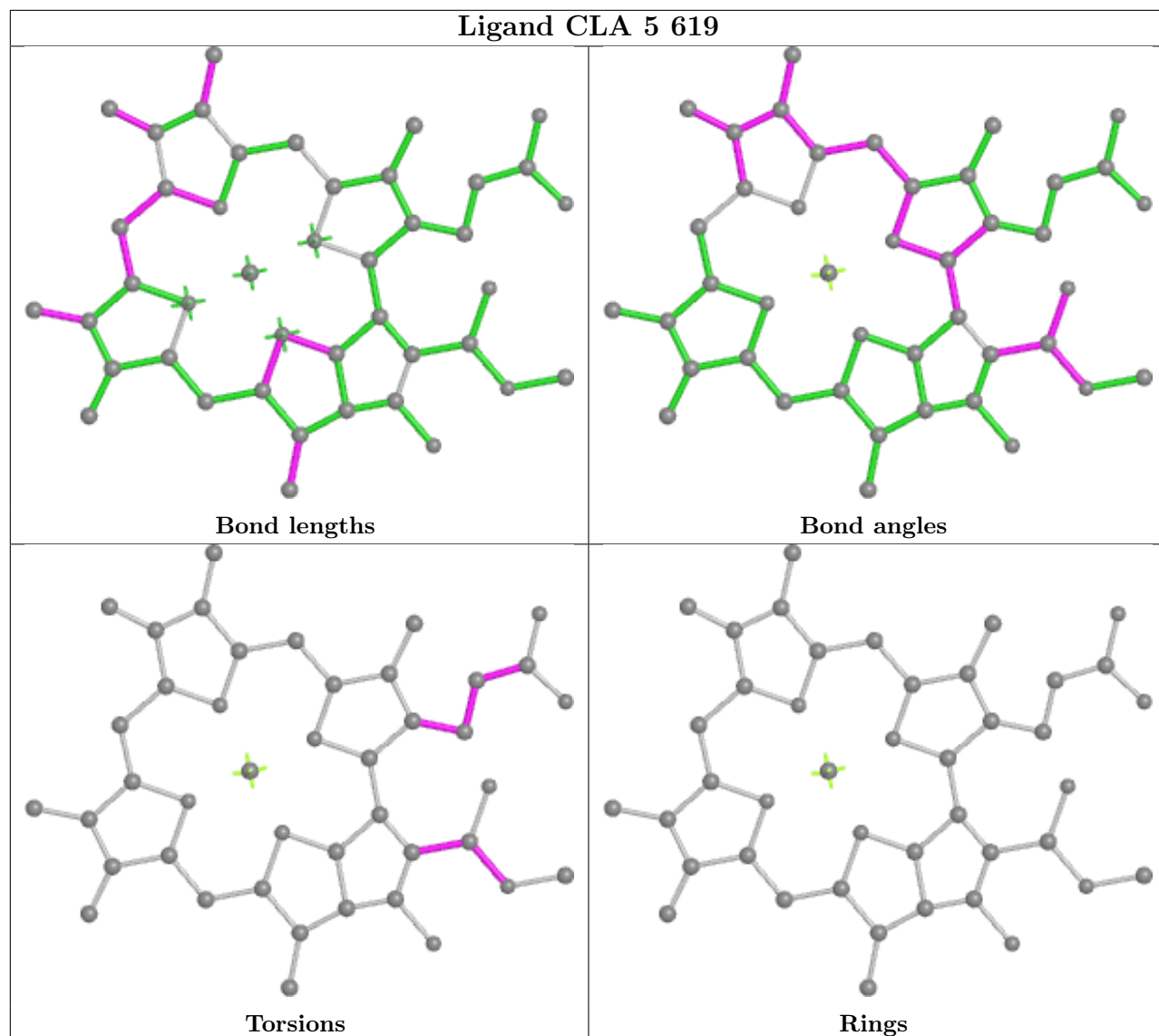
Ligand BCR A 851



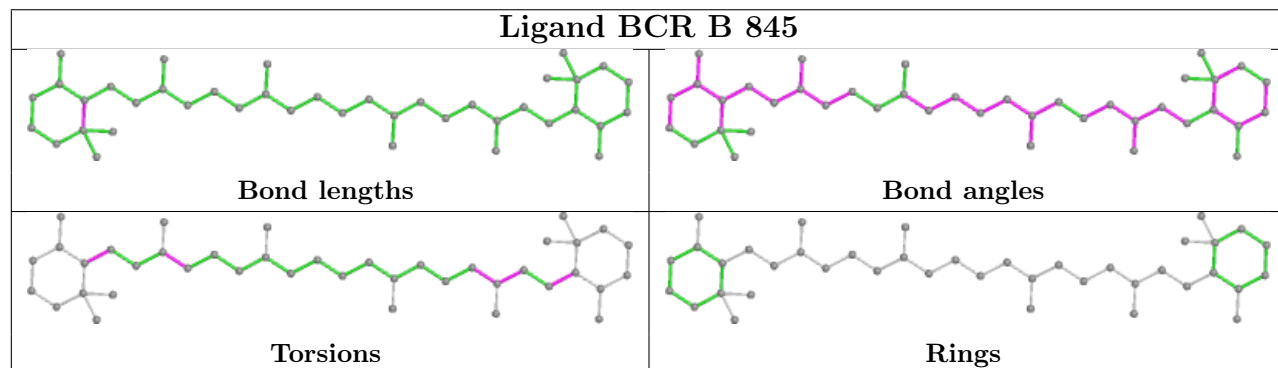
Ligand CLA 7 608

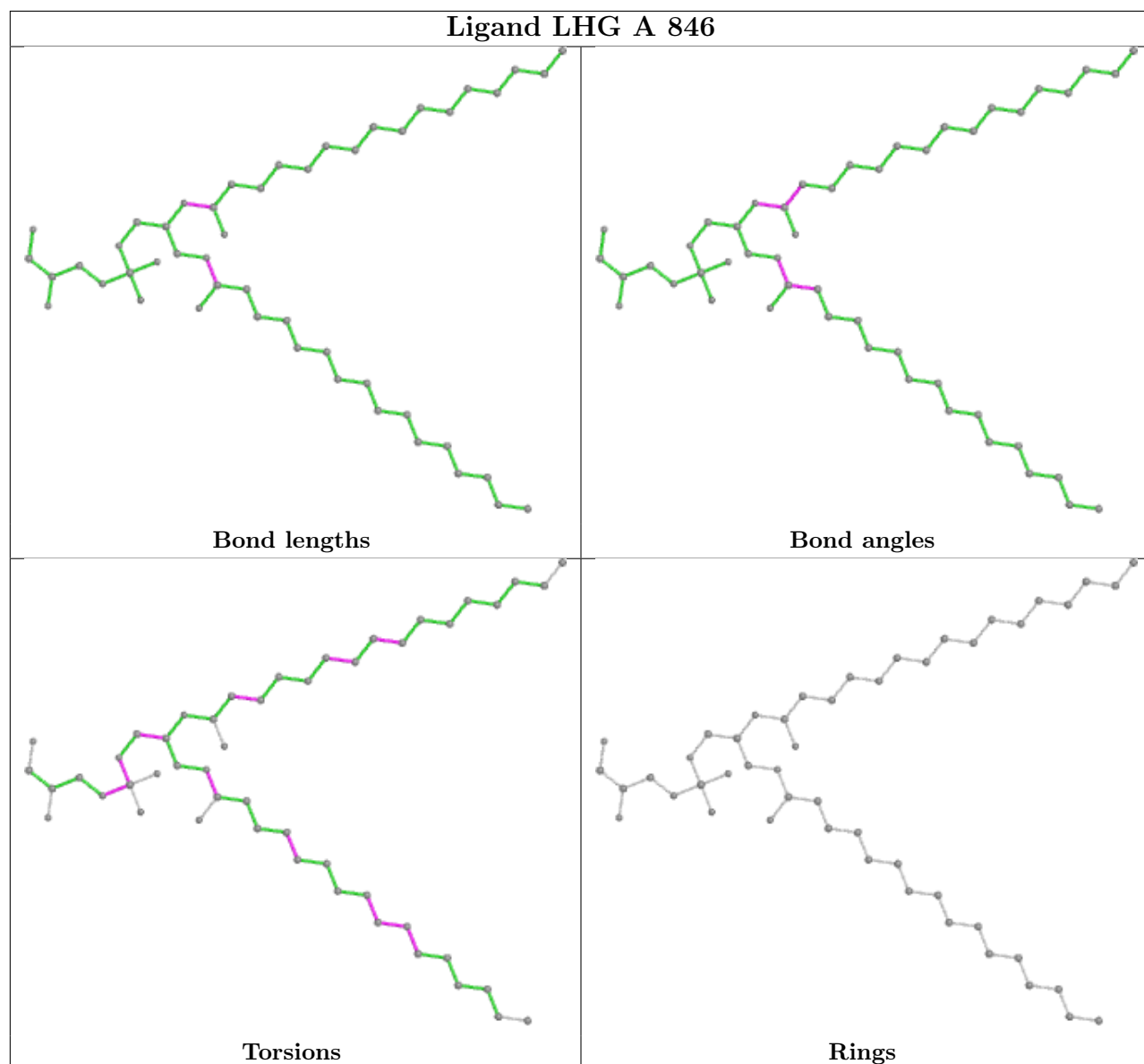
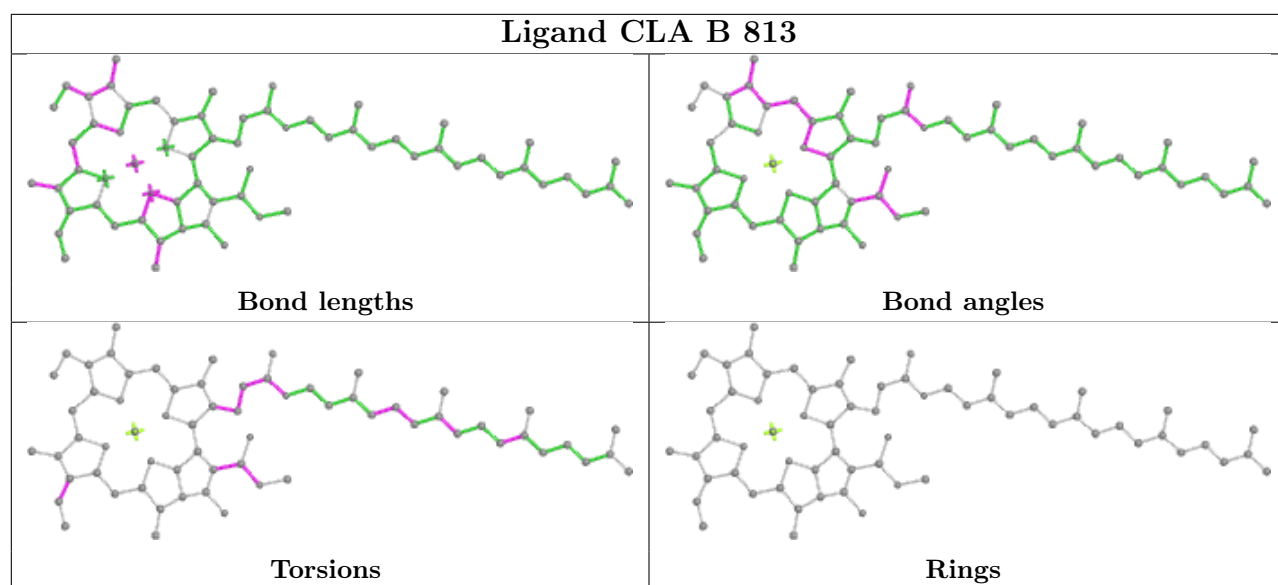


Ligand CLA 5 619

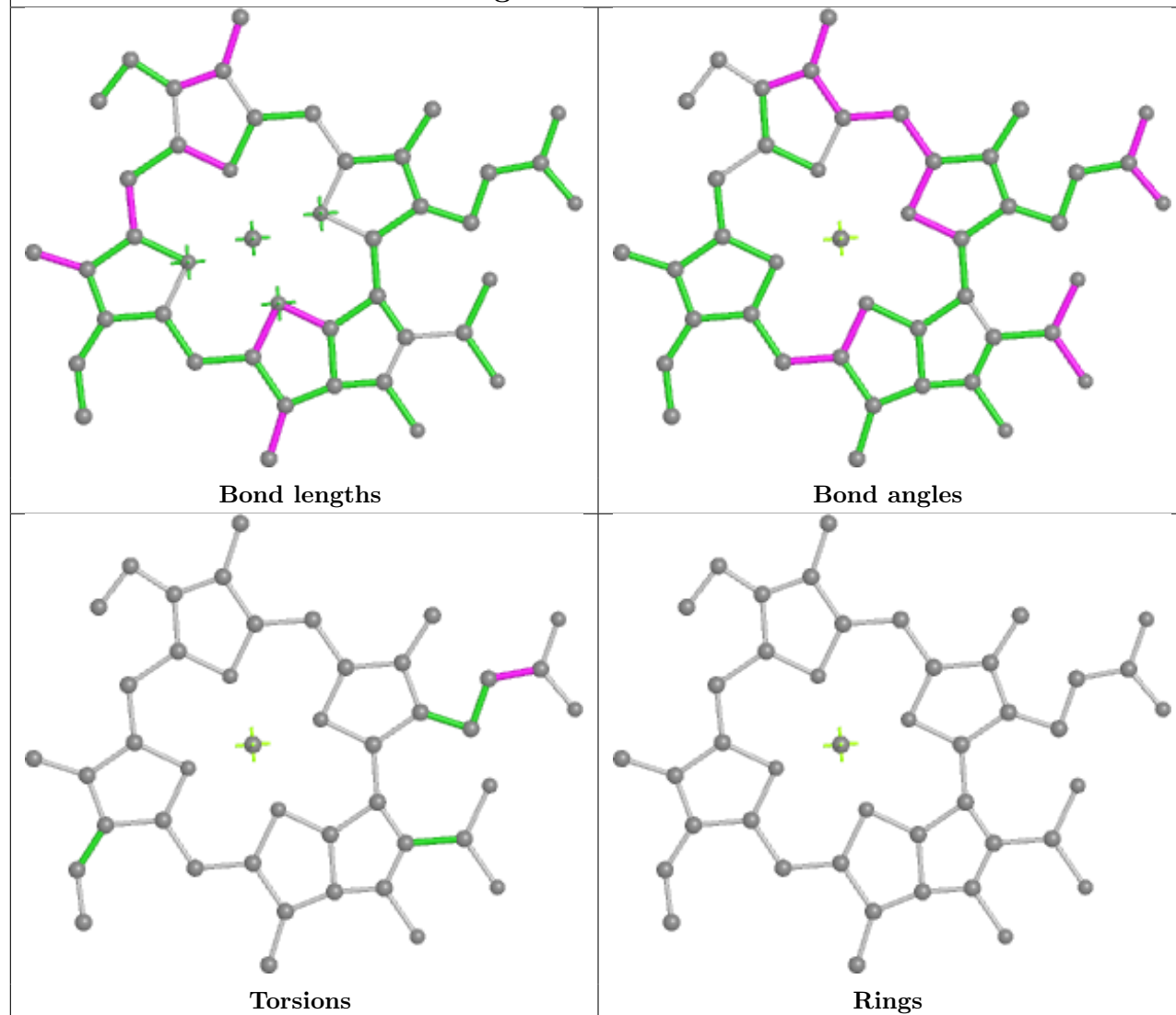


Ligand BCR B 845

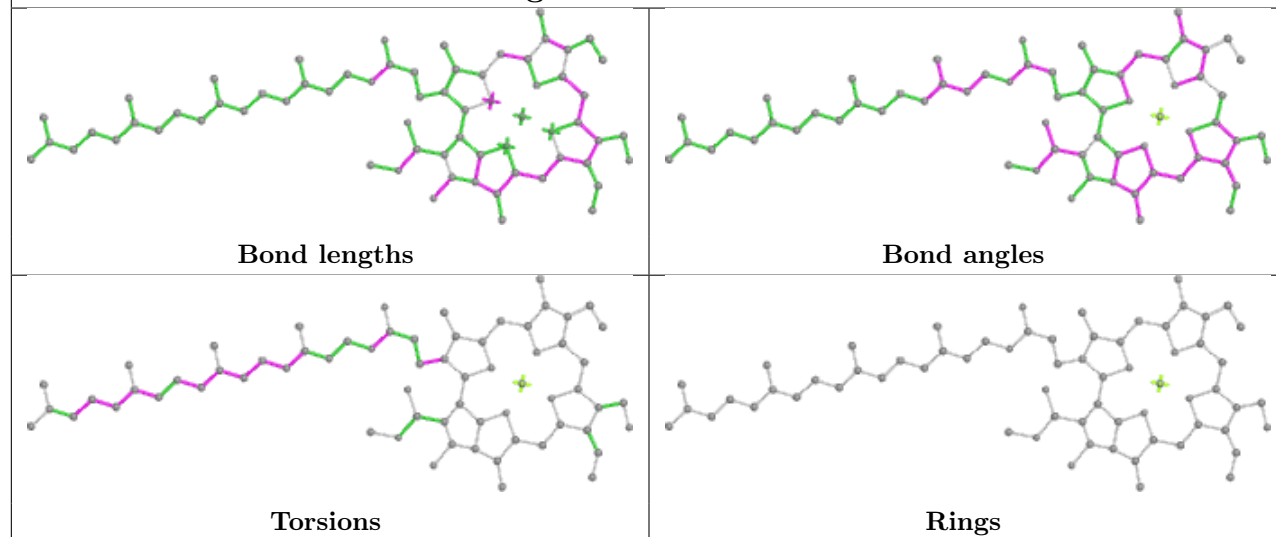


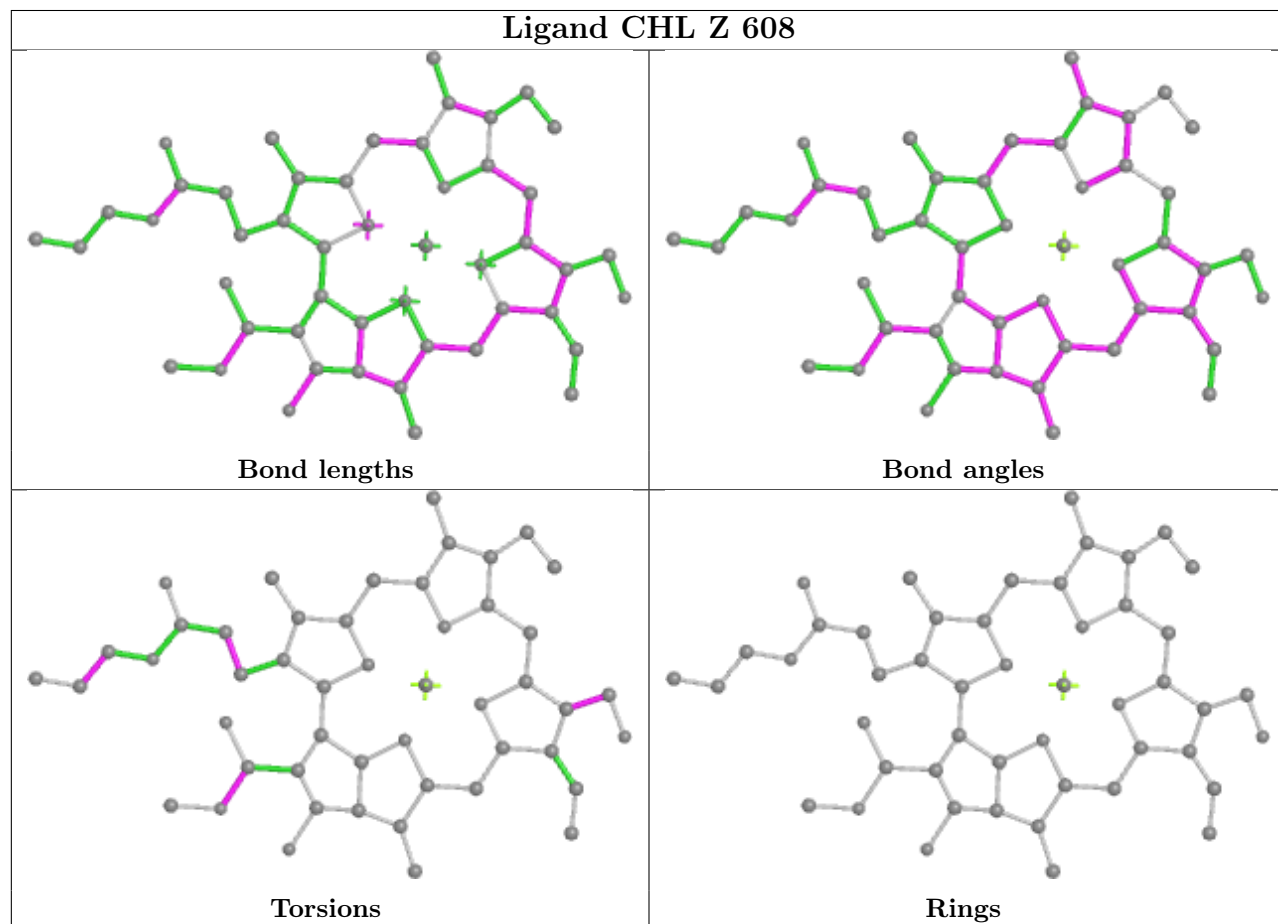
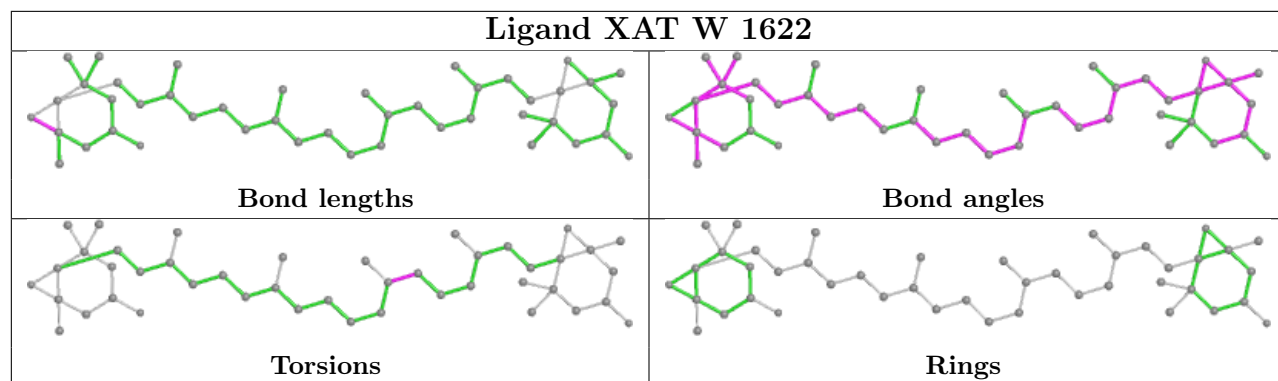


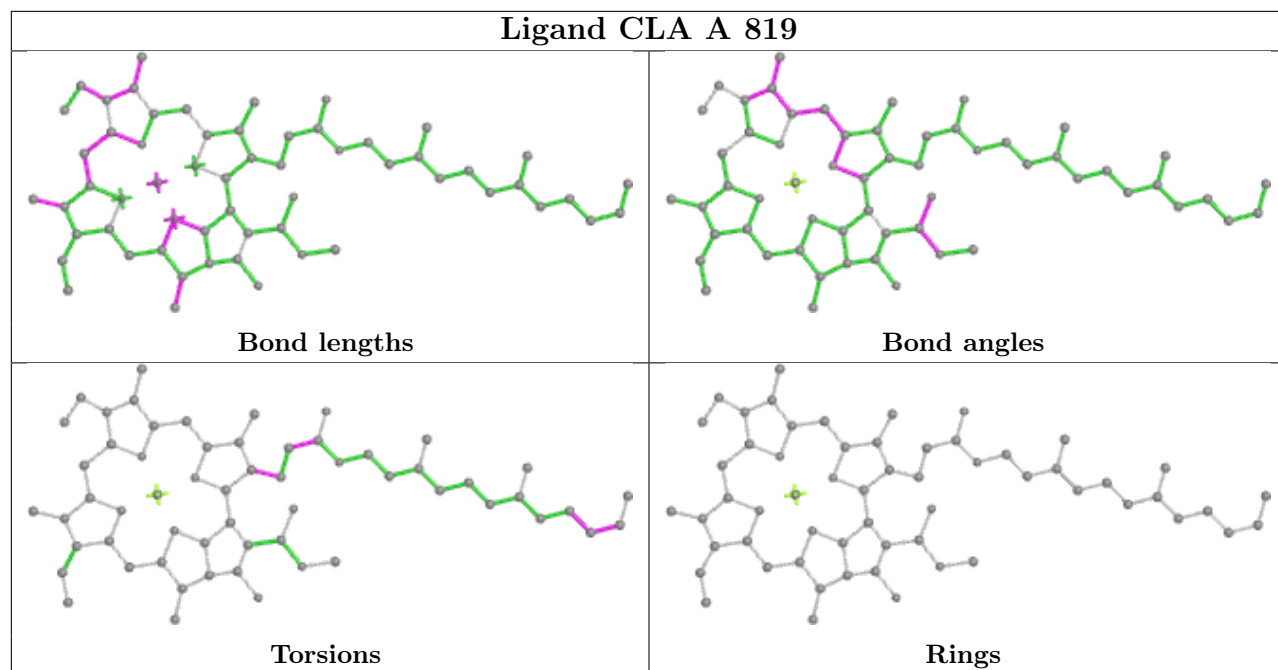
Ligand CLA 1 608



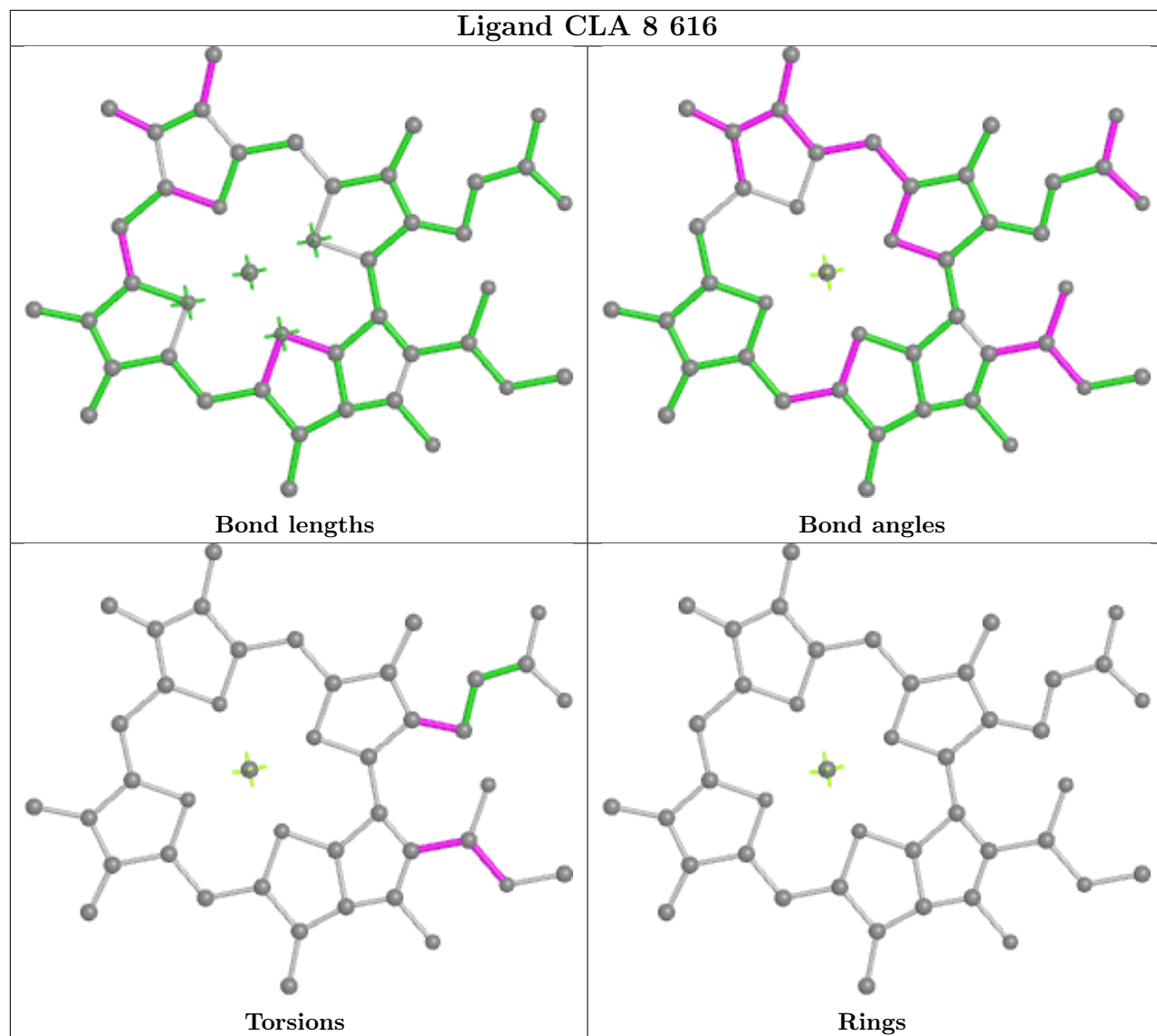
Ligand CHL W 601



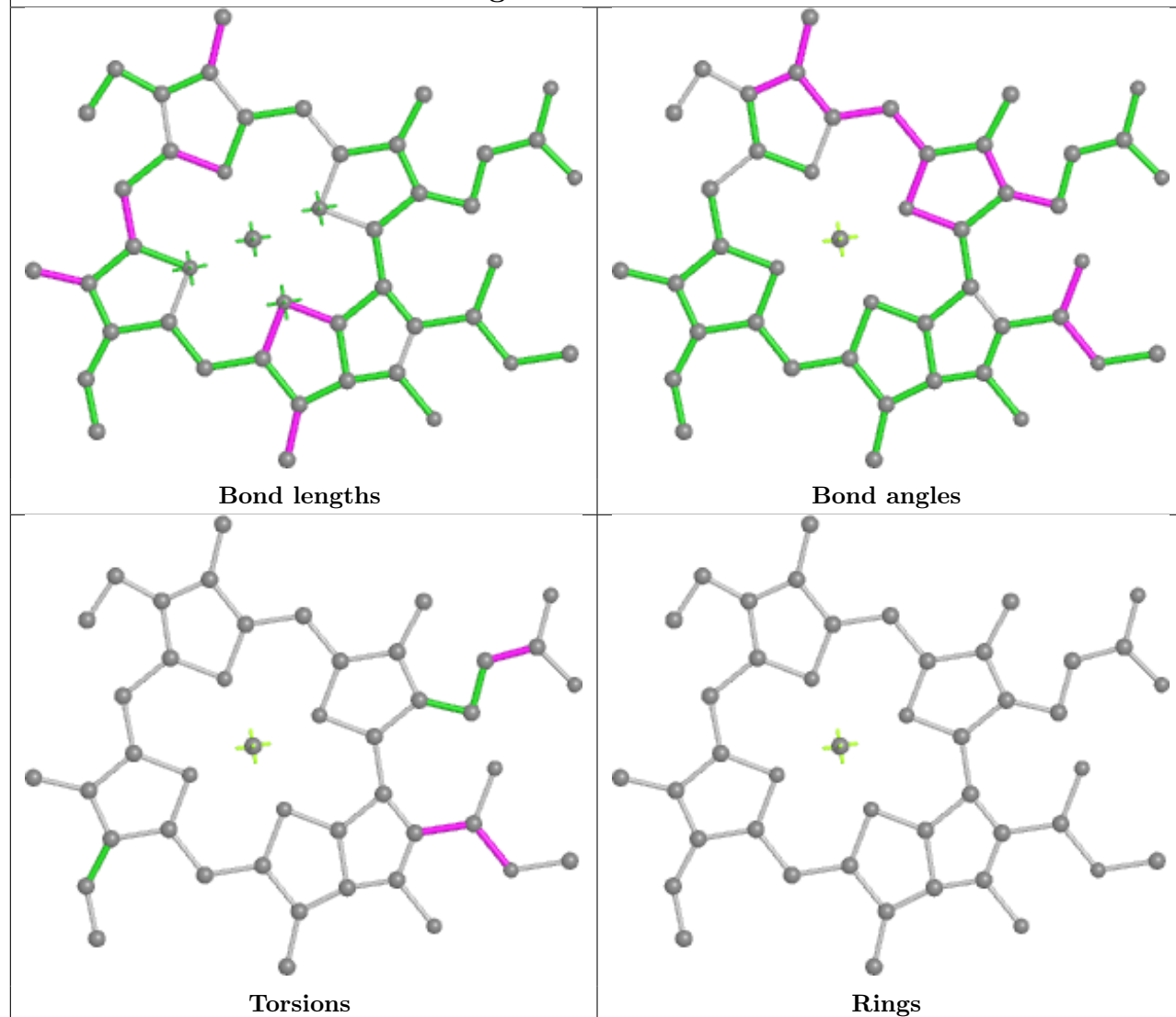




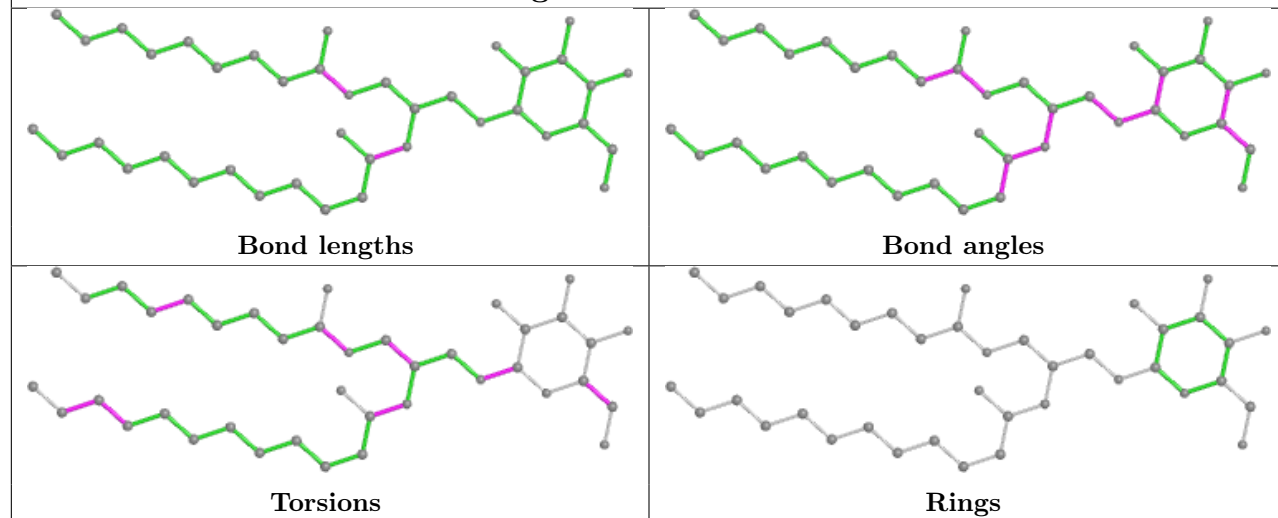
Ligand CLA 8 616



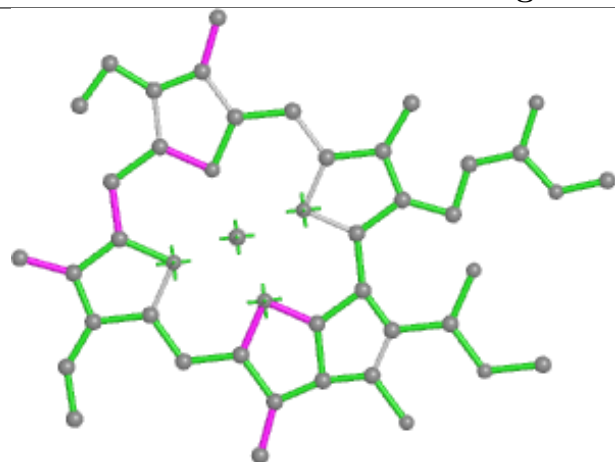
Ligand CLA Y 612



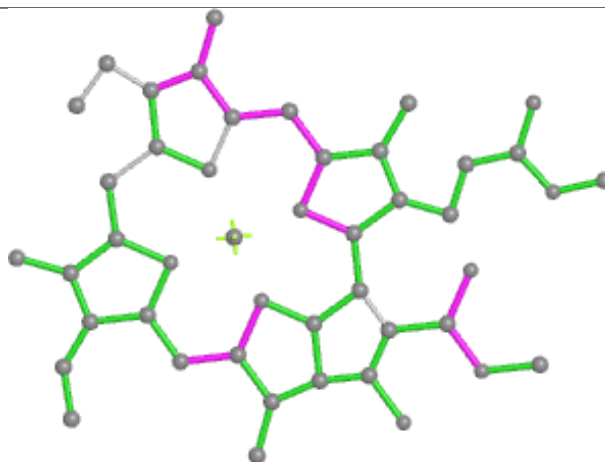
Ligand LMG J 104



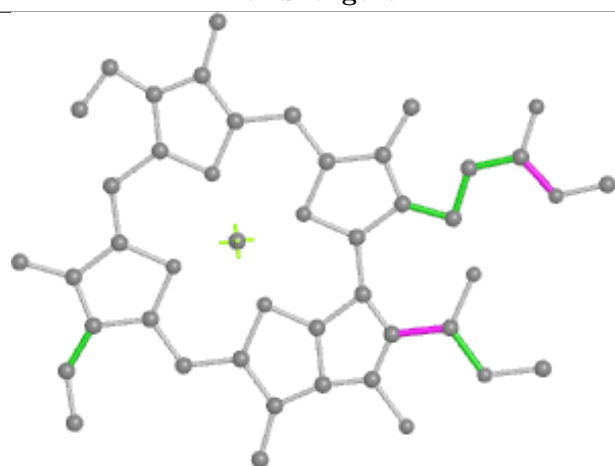
Ligand CLA B 838



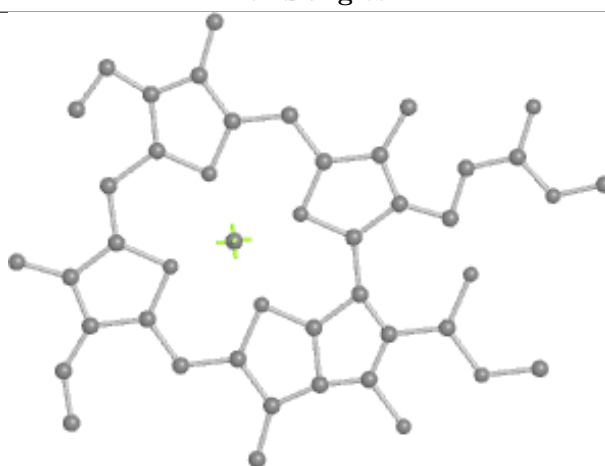
Bond lengths



Bond angles

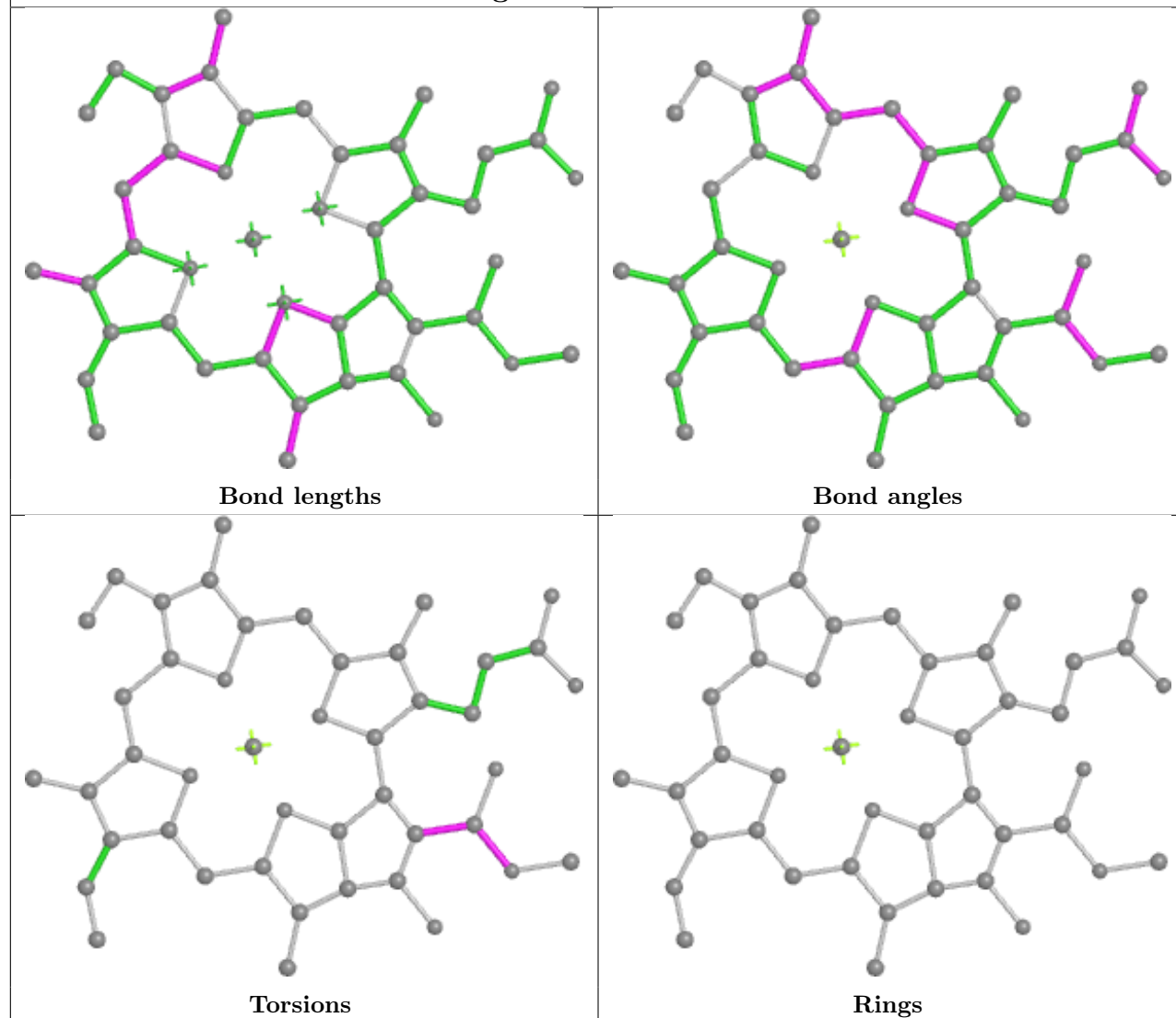


Torsions

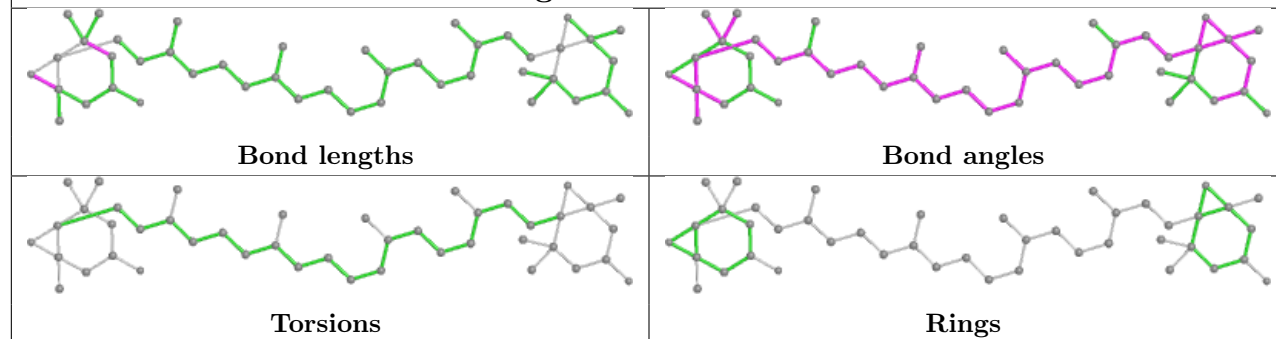


Rings

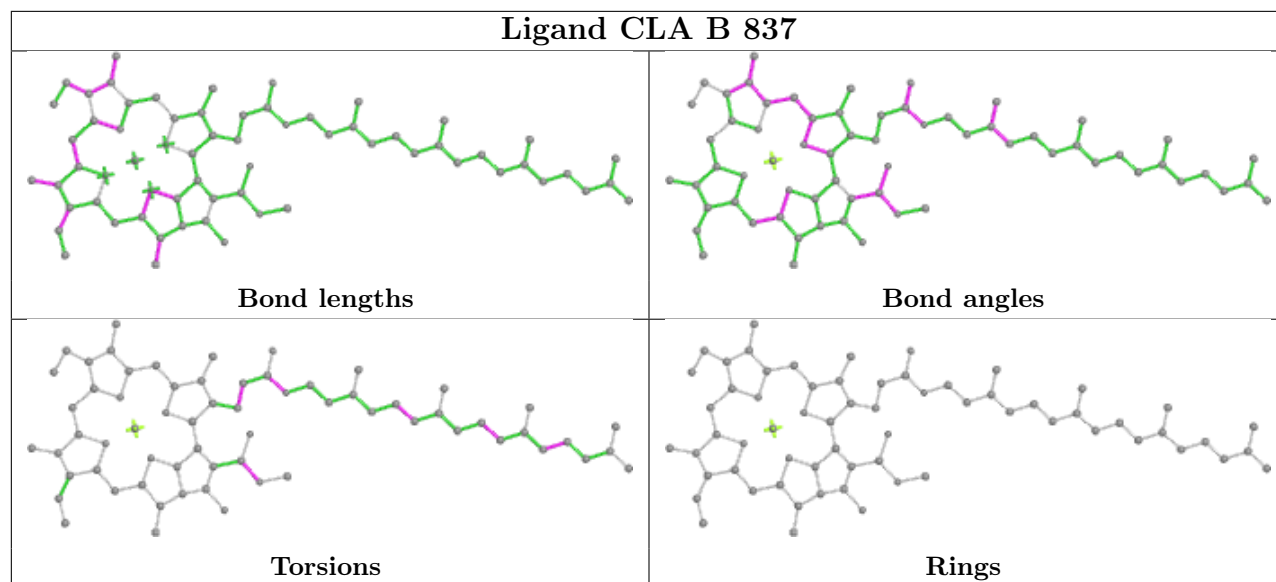
Ligand CLA L 304



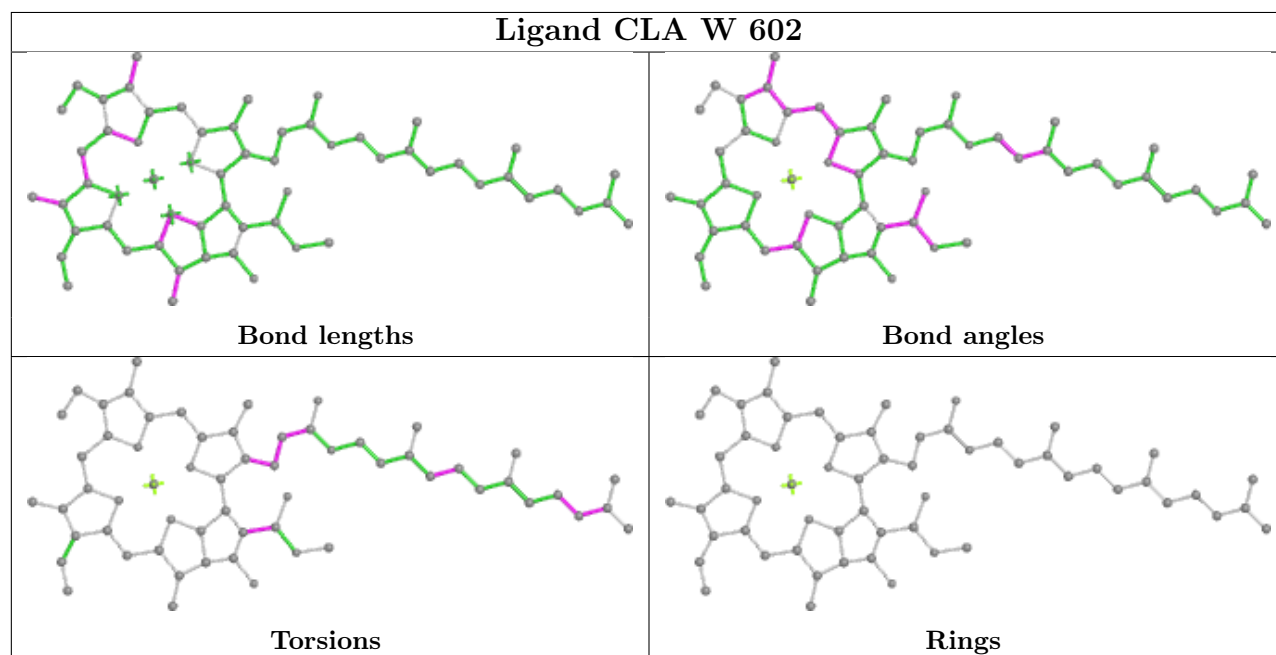
Ligand XAT 2 620

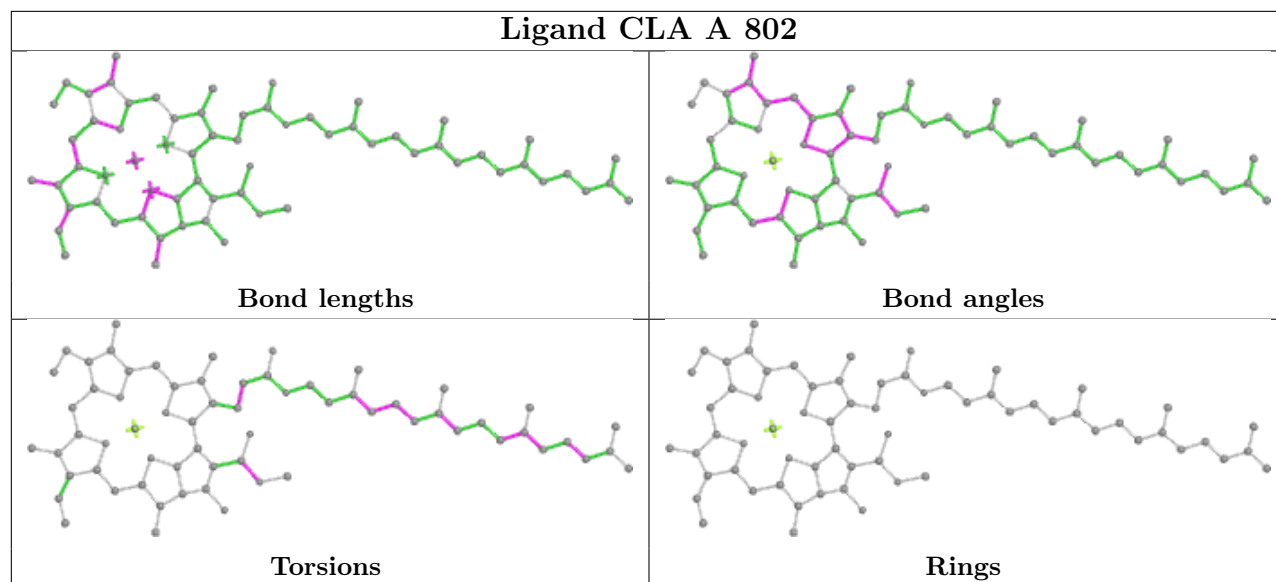
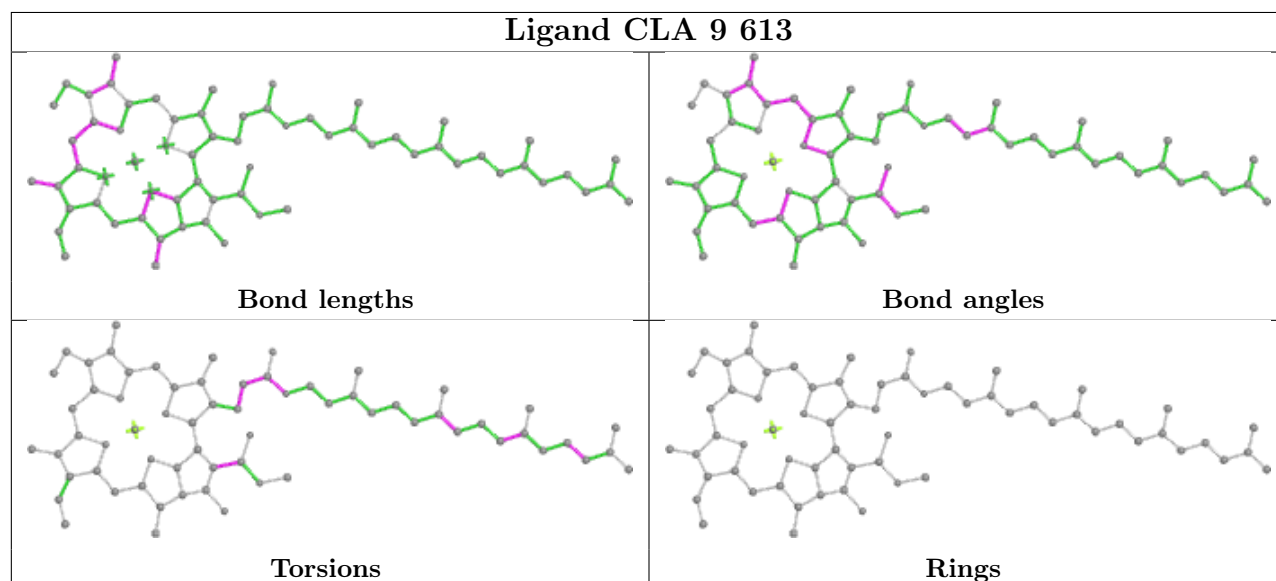
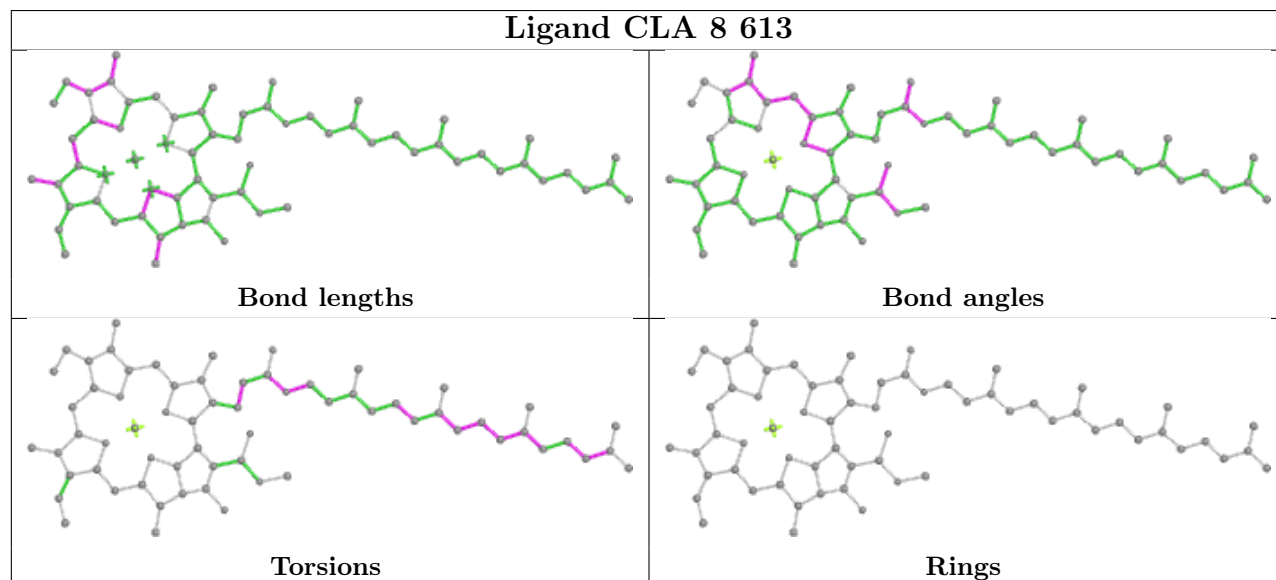


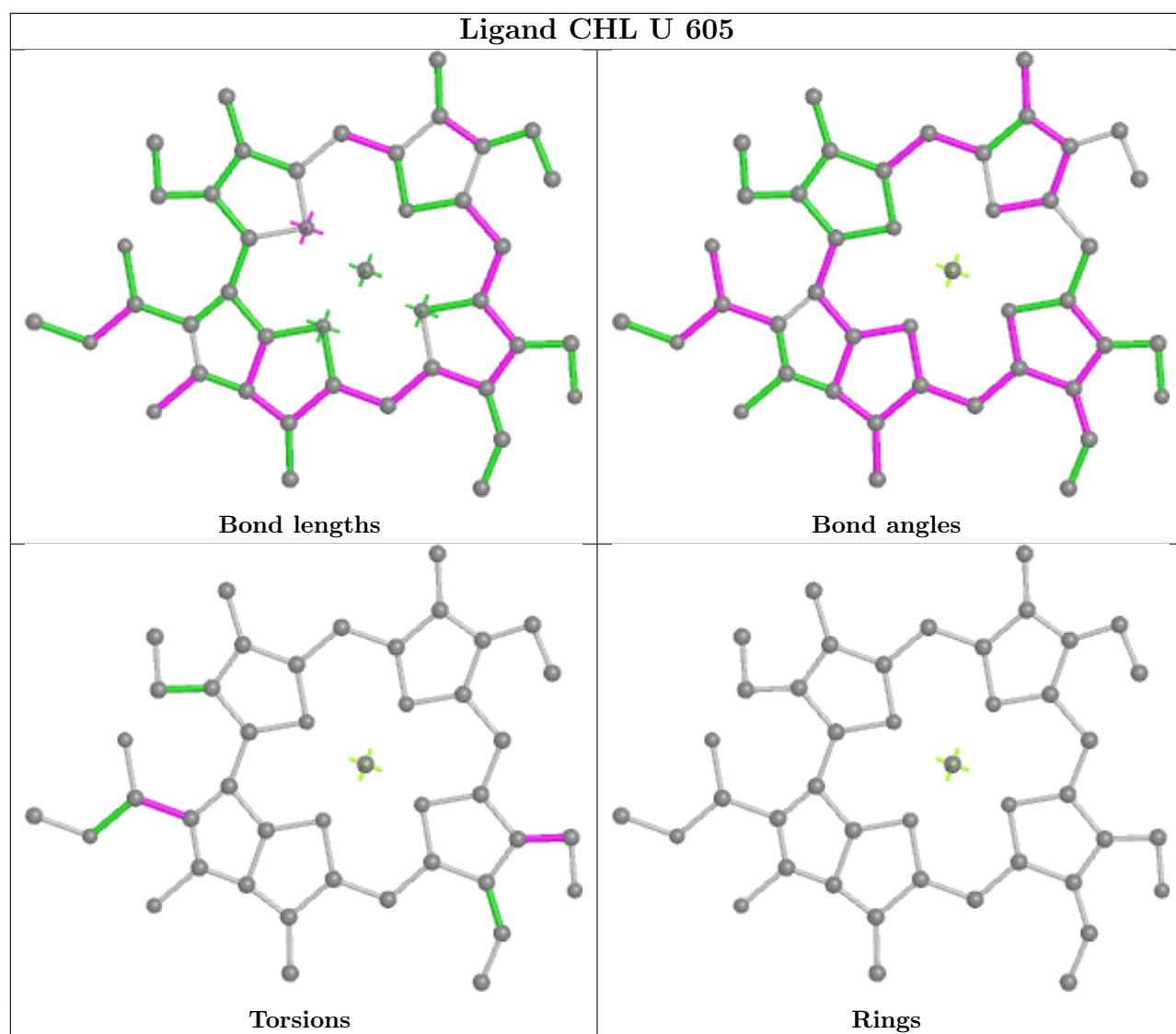
Ligand CLA B 837

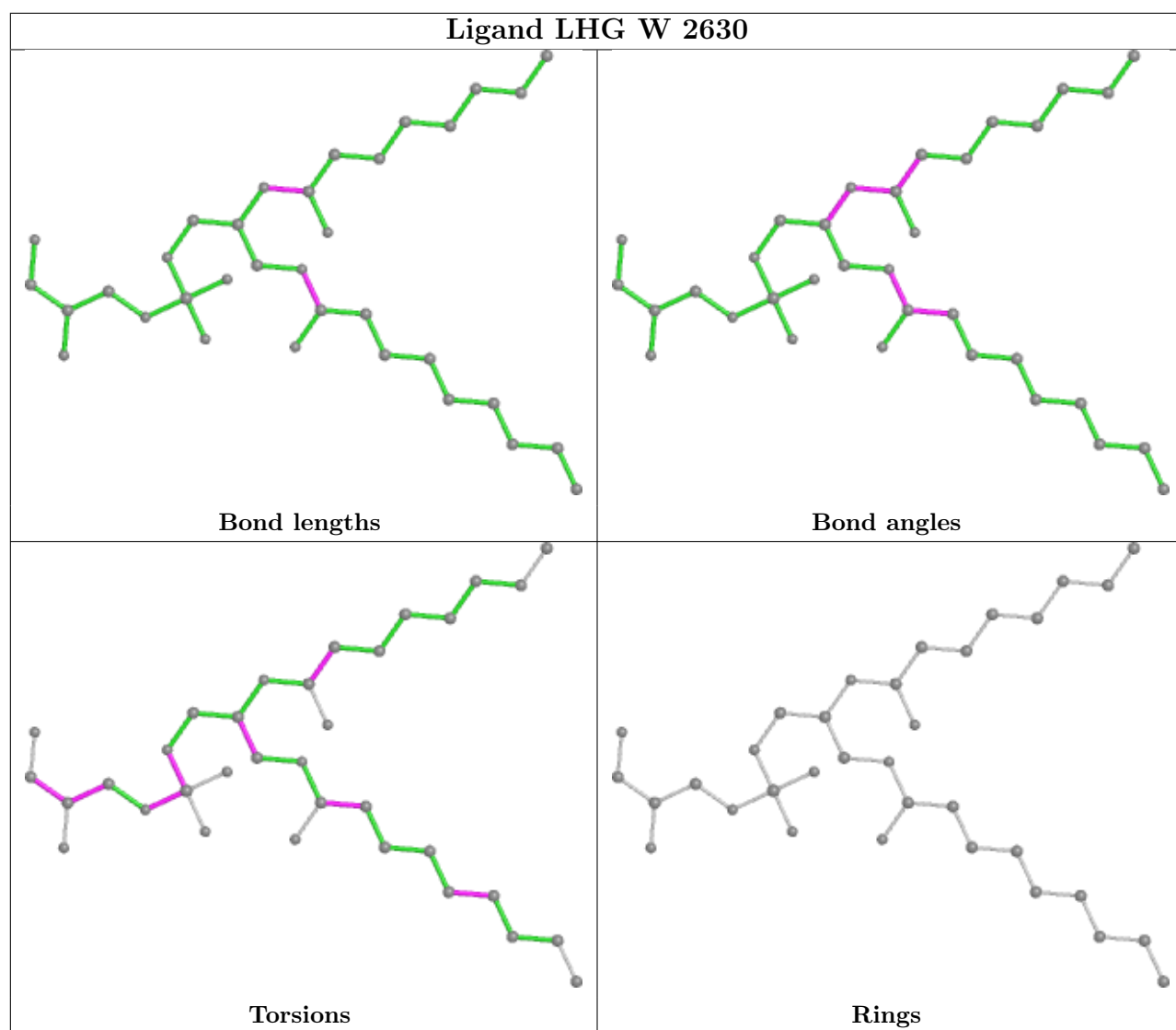


Ligand CLA W 602

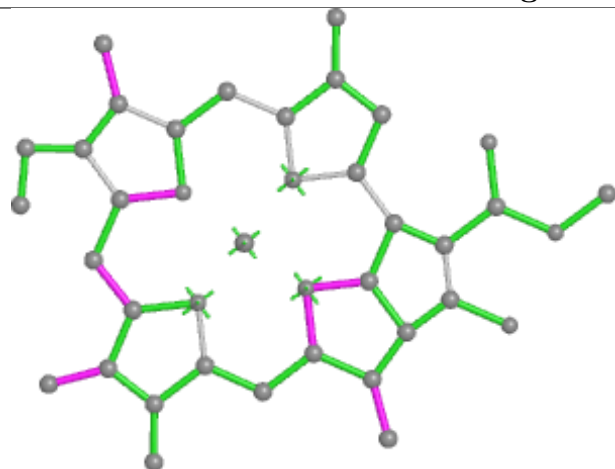


Ligand CLA A 802**Ligand CLA 9 613****Ligand CLA 8 613**

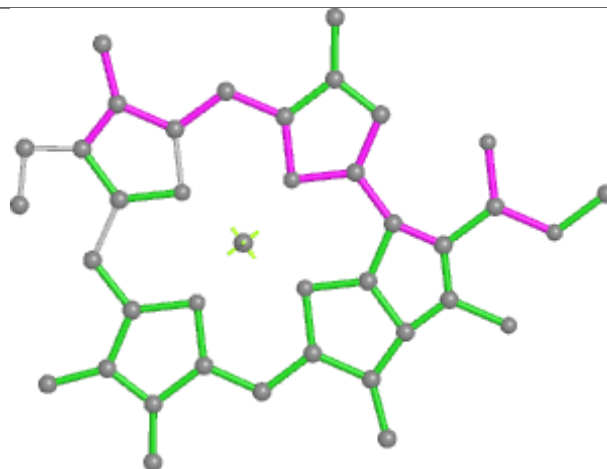




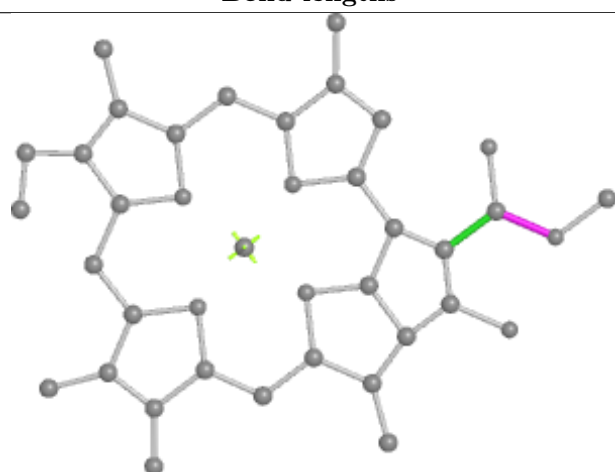
Ligand CLA 1 610



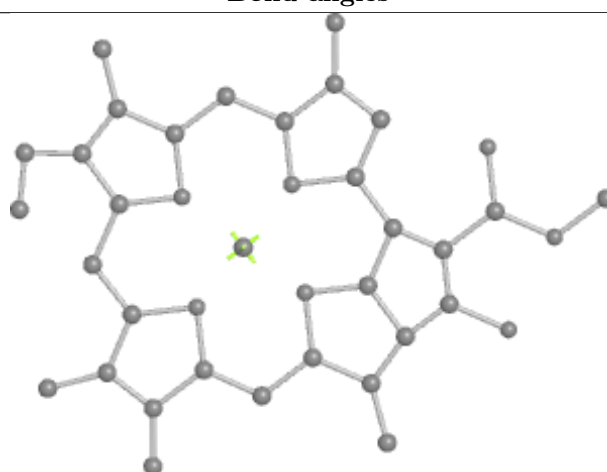
Bond lengths



Bond angles

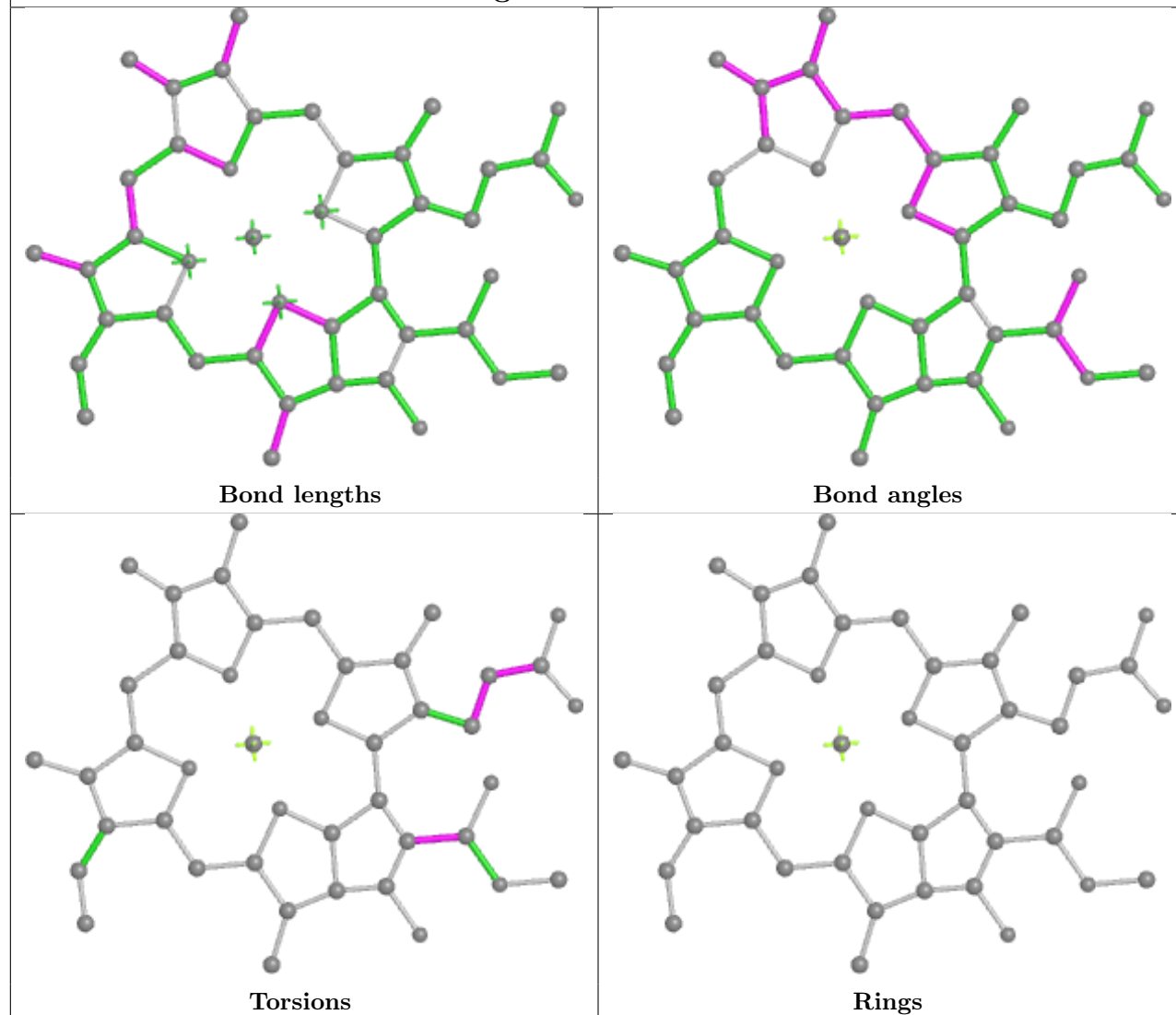


Torsions

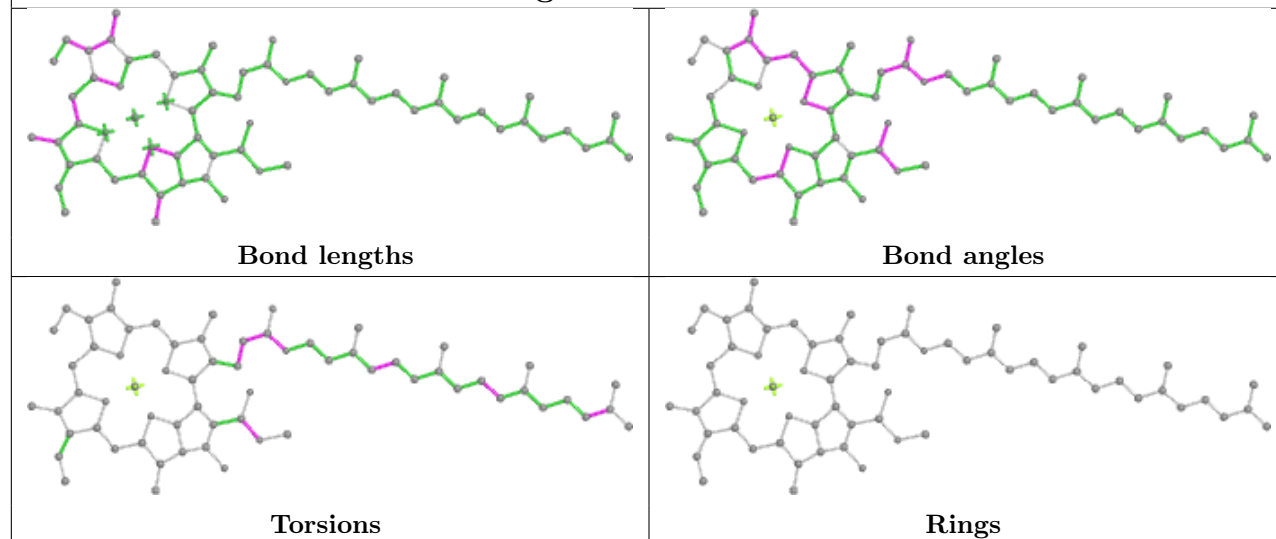


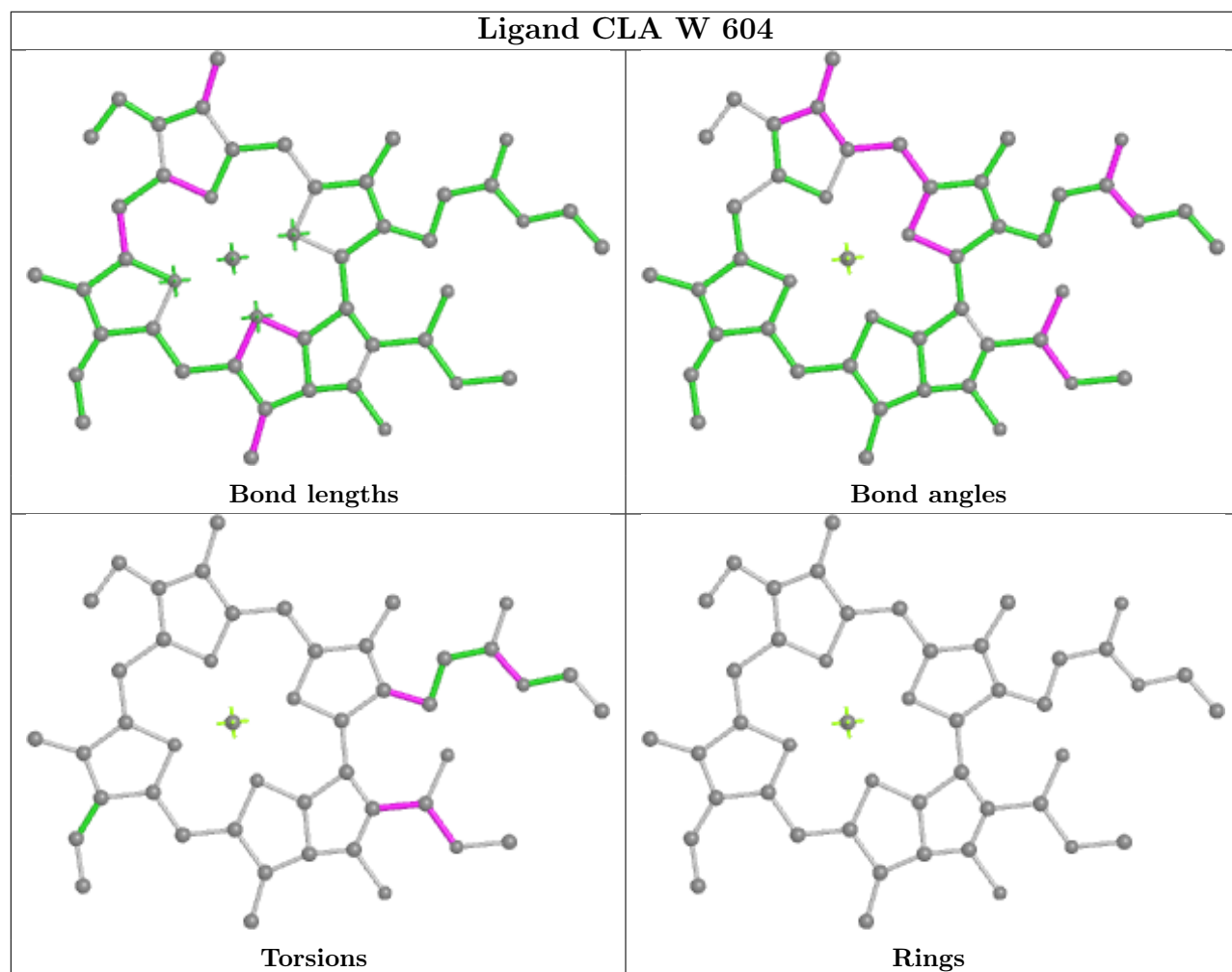
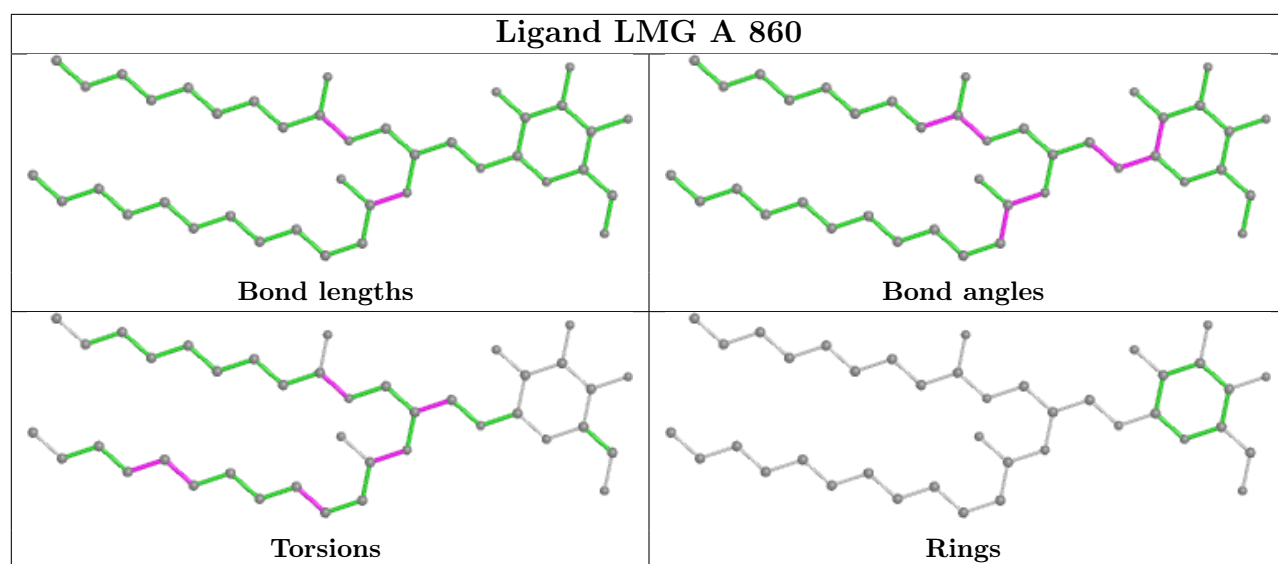
Rings

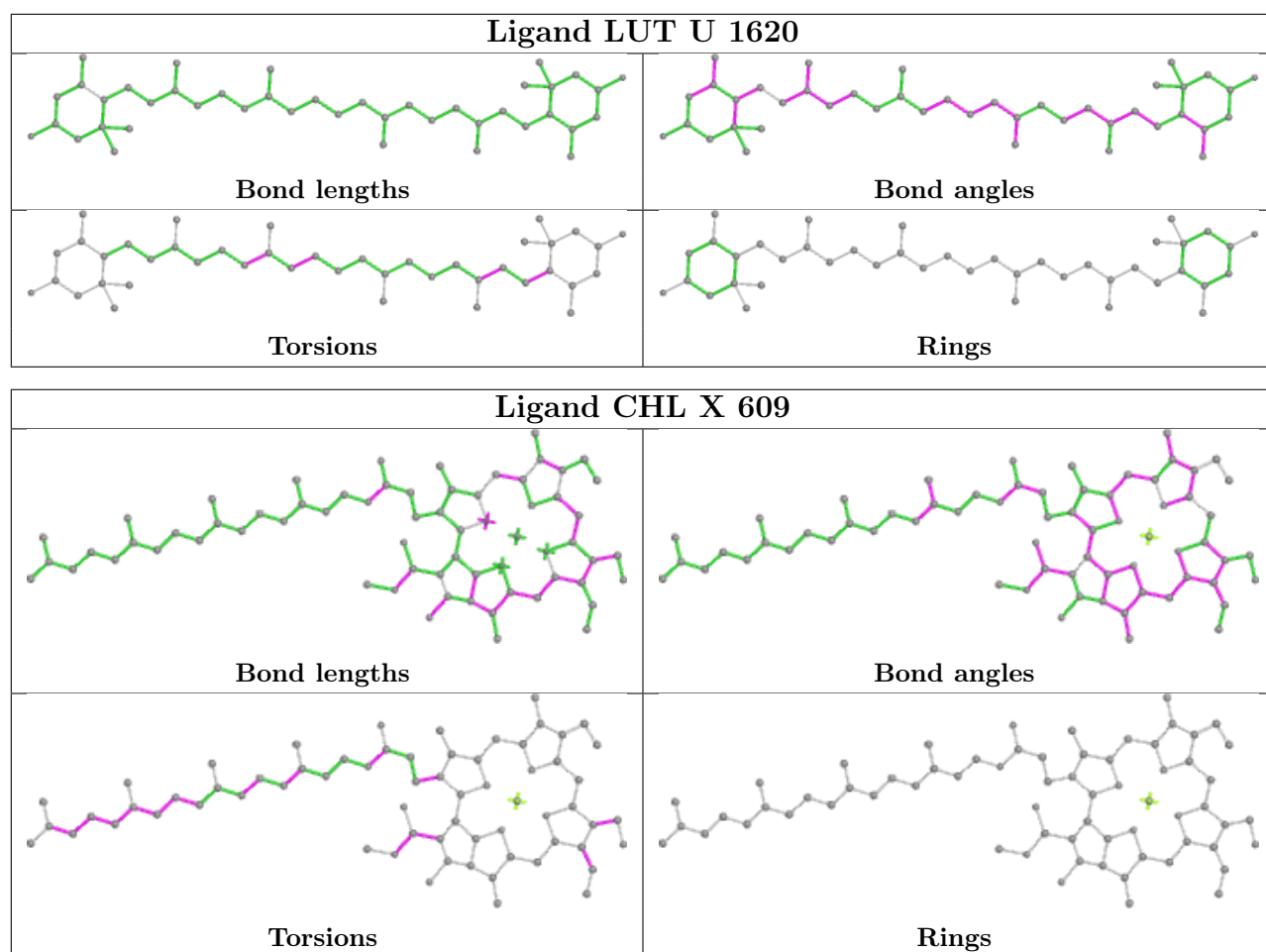
Ligand CLA 8 603

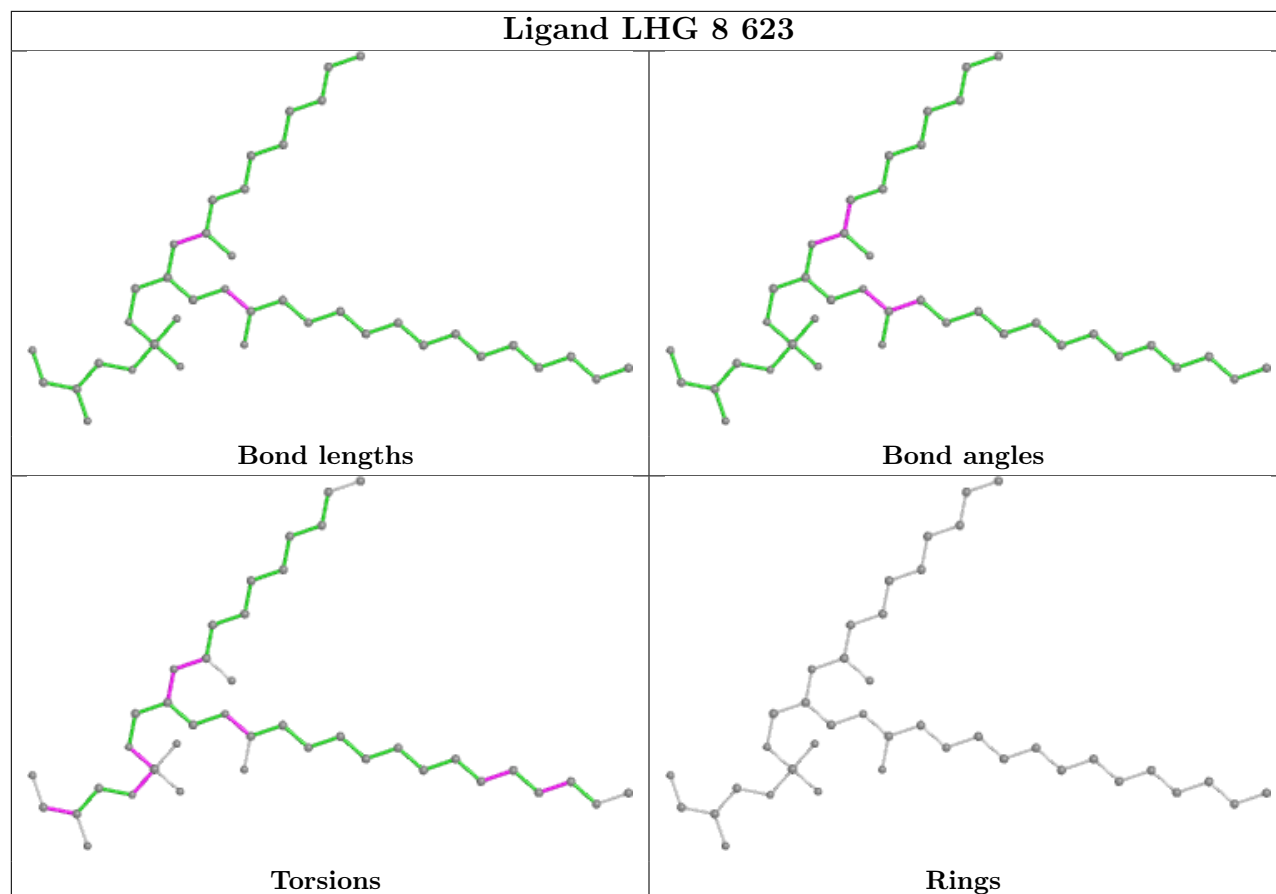
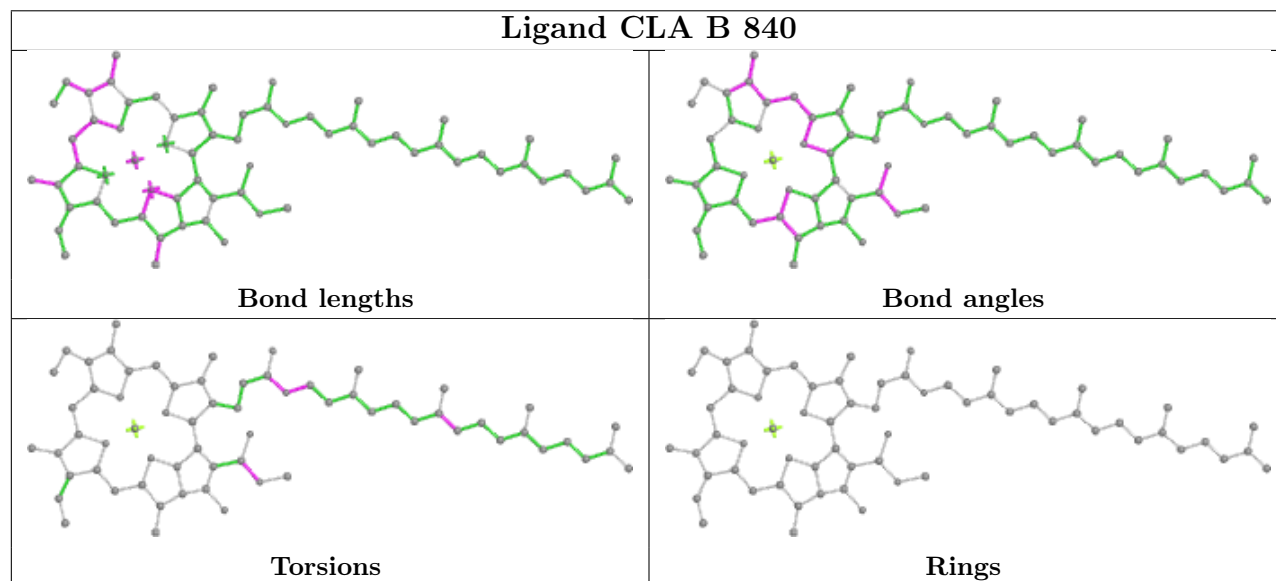


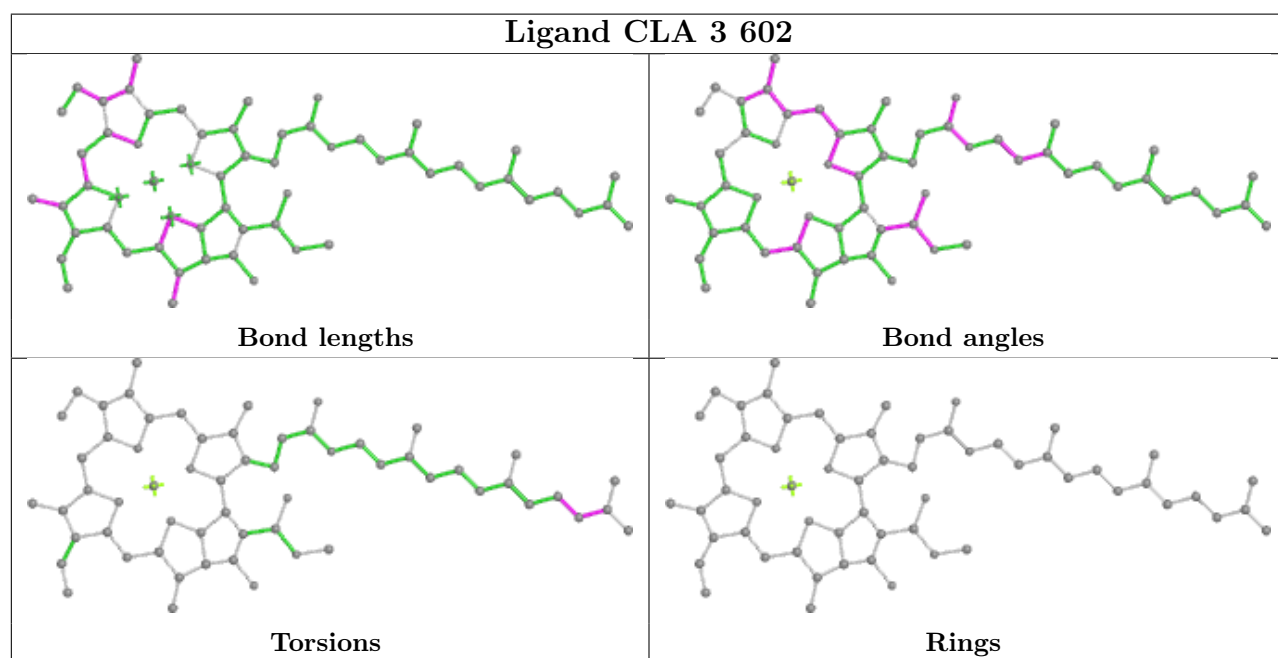
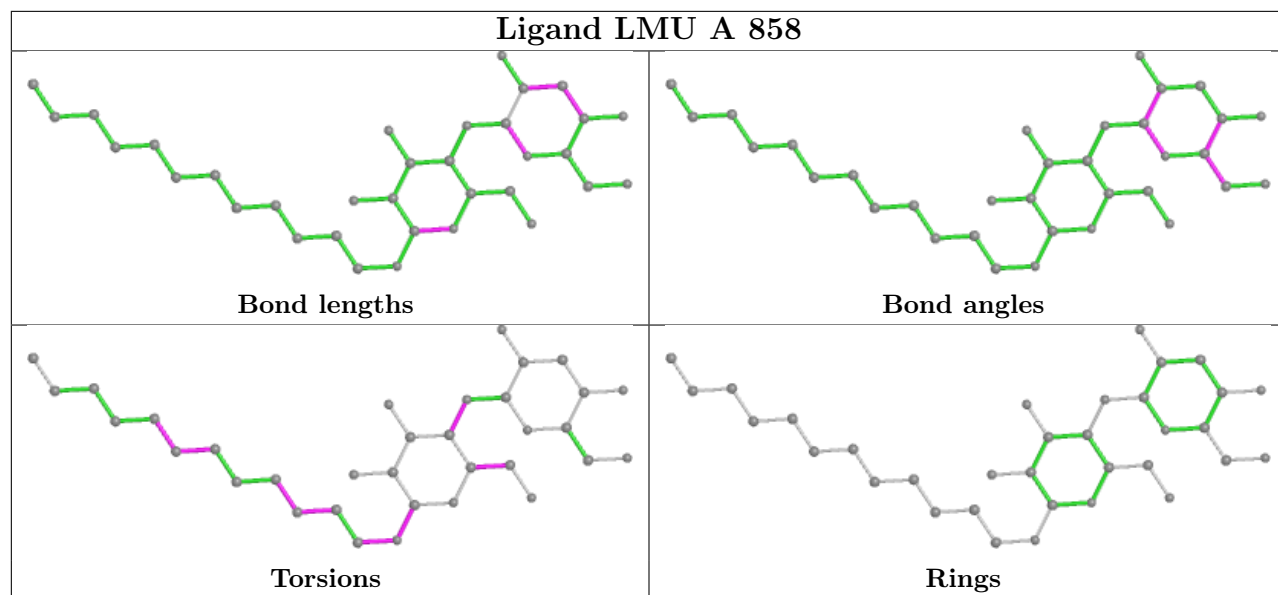
Ligand CLA 4 613

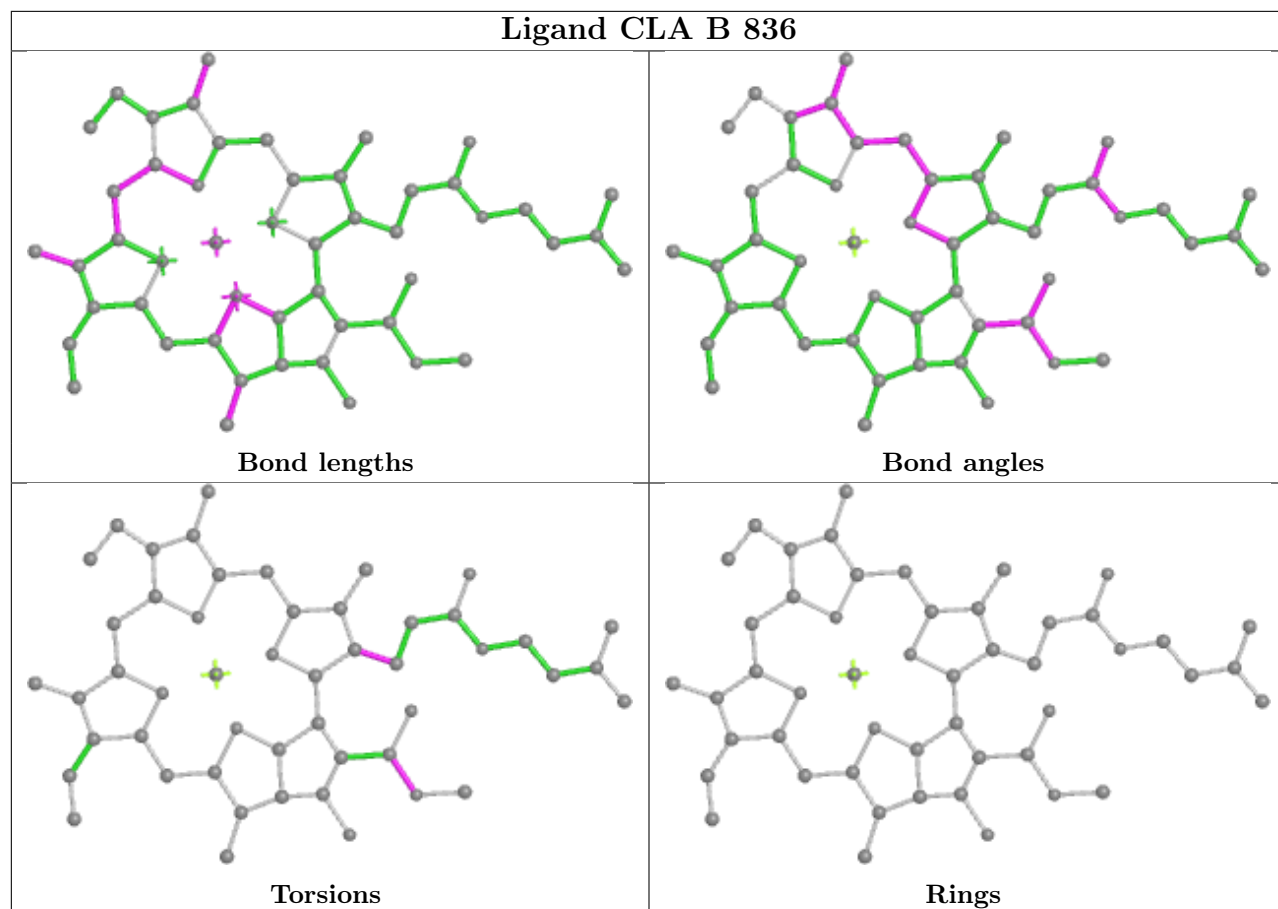




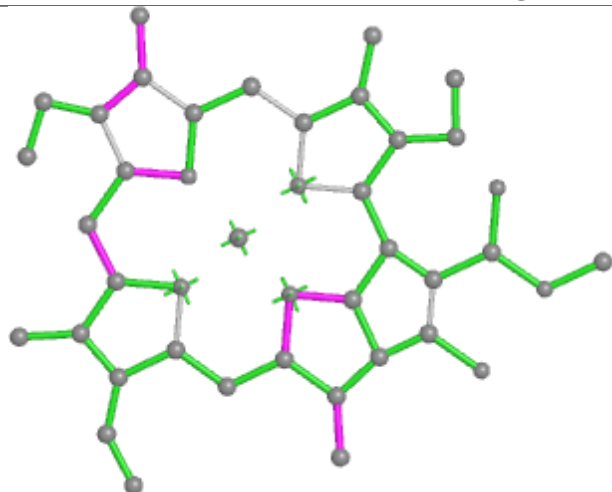


Ligand LHG 8 623**Ligand CLA B 840**

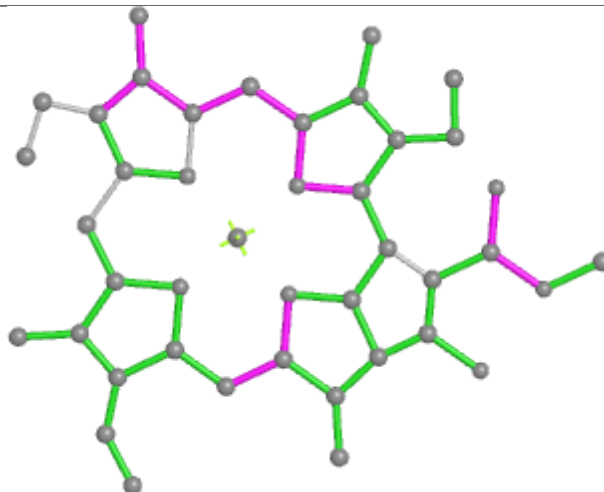




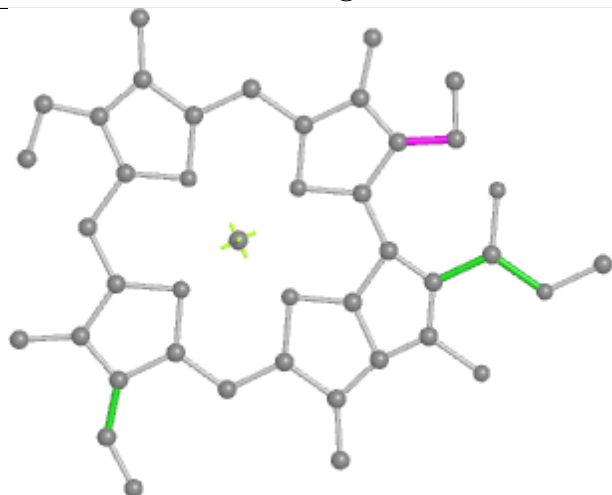
Ligand CLA X 614



Bond lengths



Bond angles

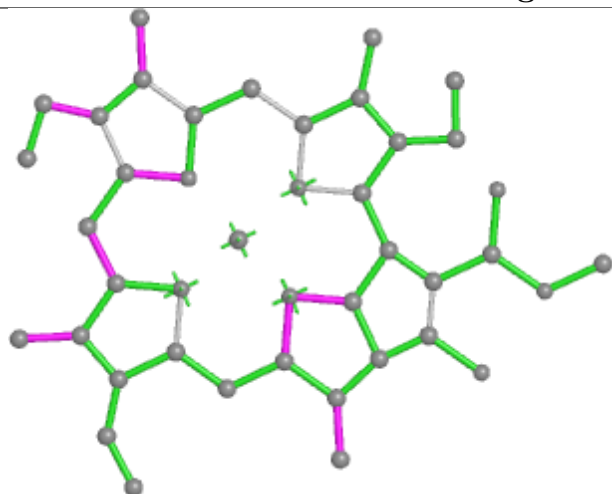


Torsions

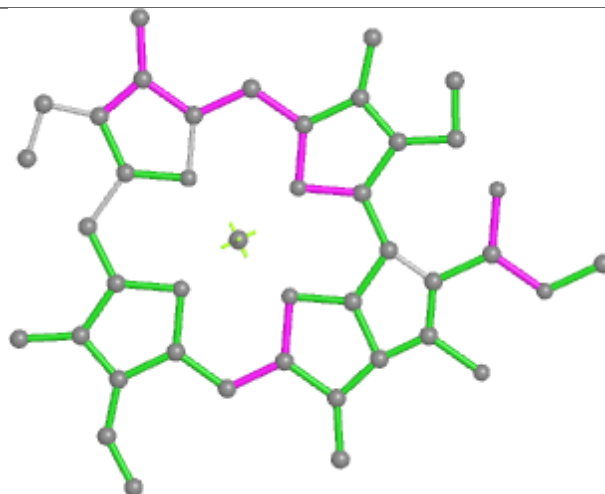


Rings

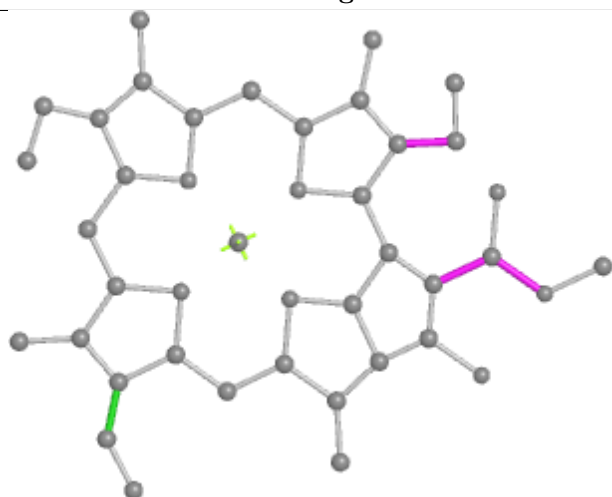
Ligand CLA 4 611



Bond lengths



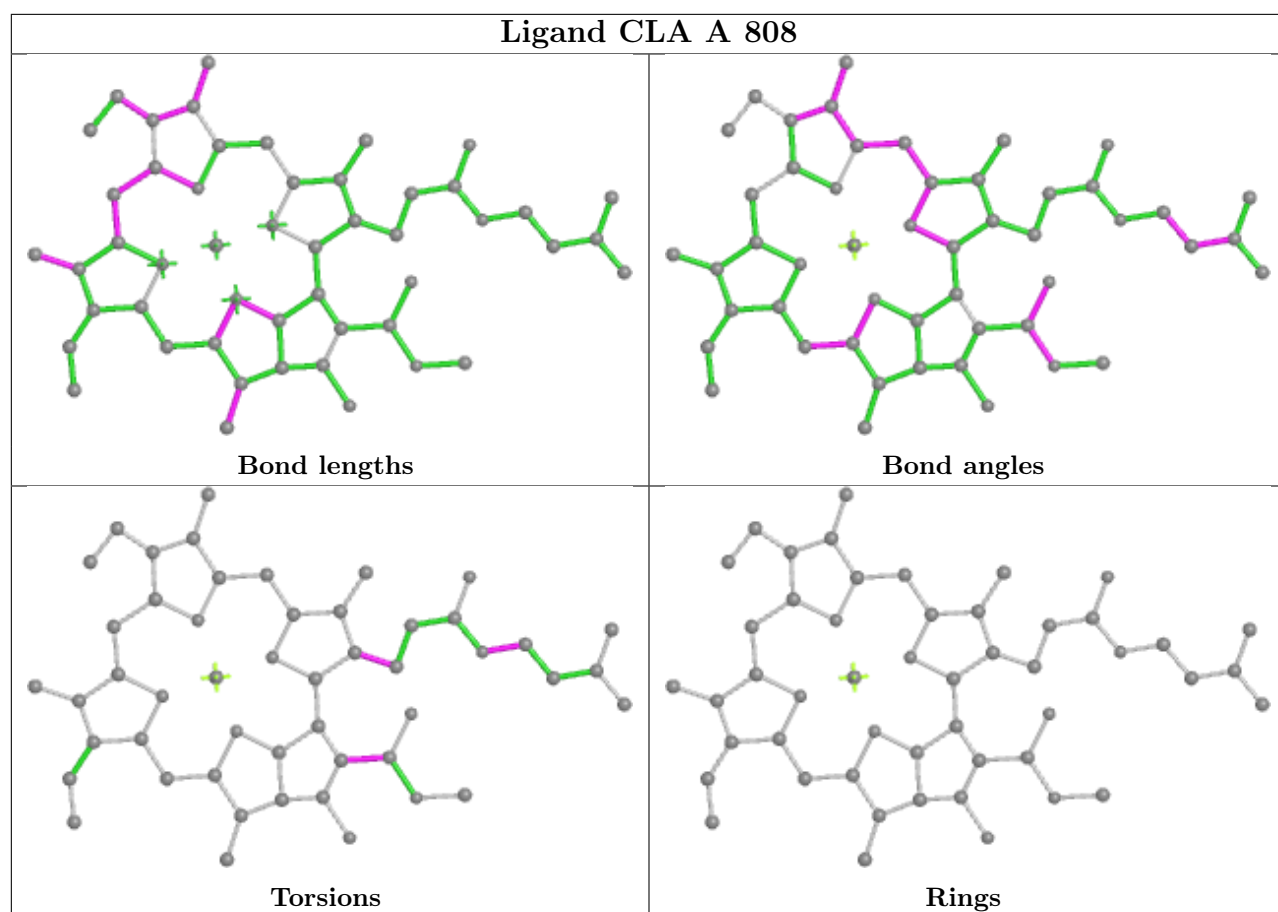
Bond angles



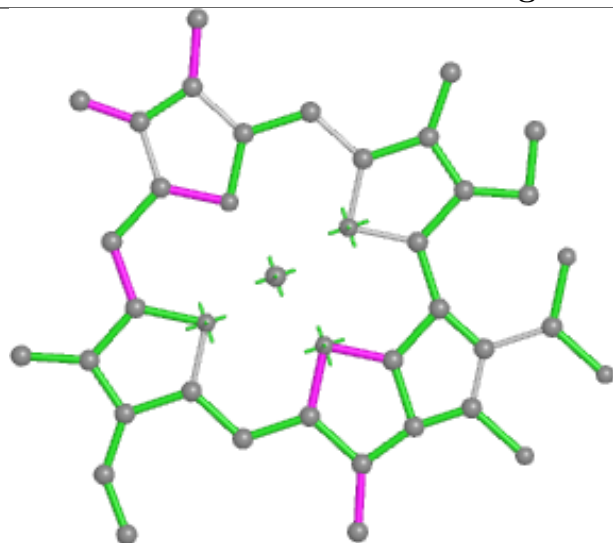
Torsions



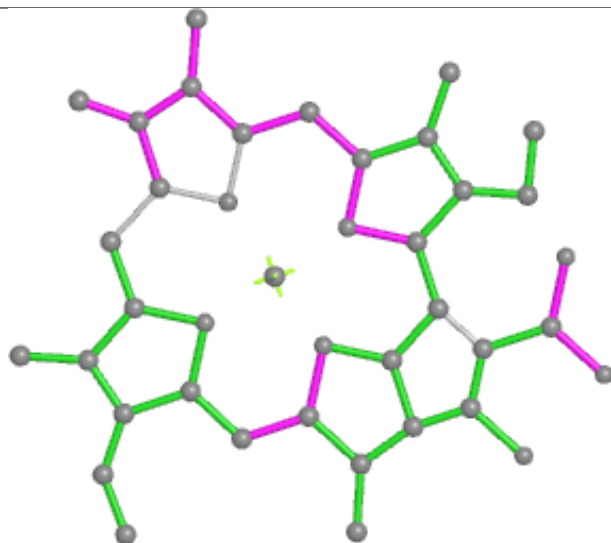
Rings



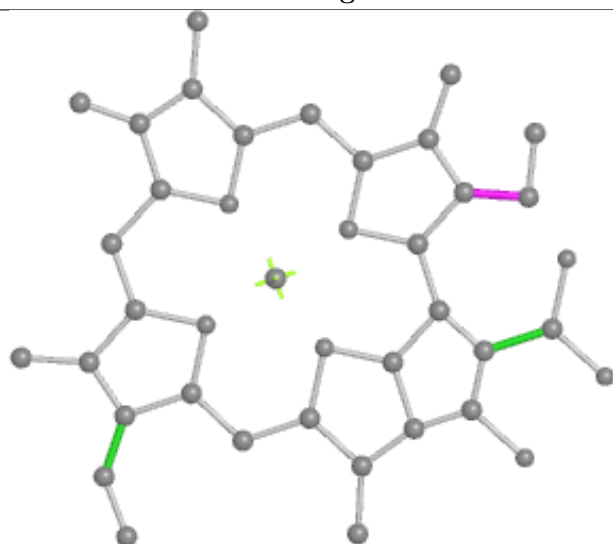
Ligand CLA 4 618



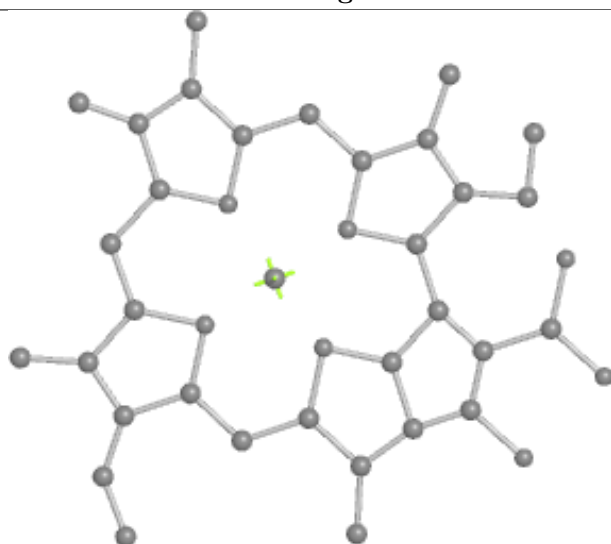
Bond lengths



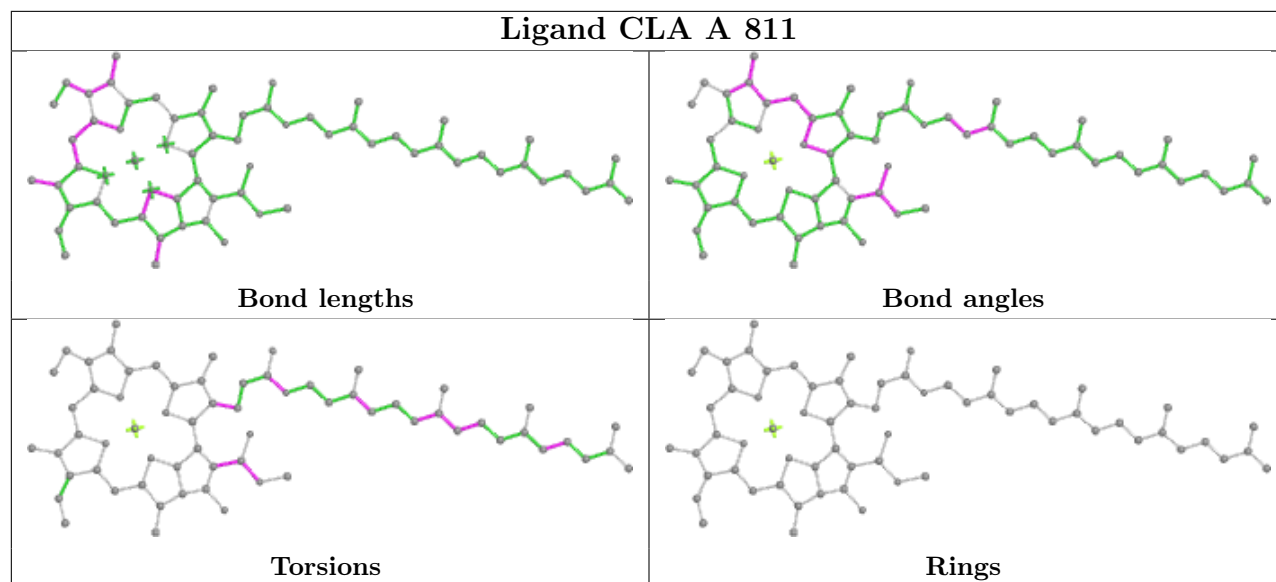
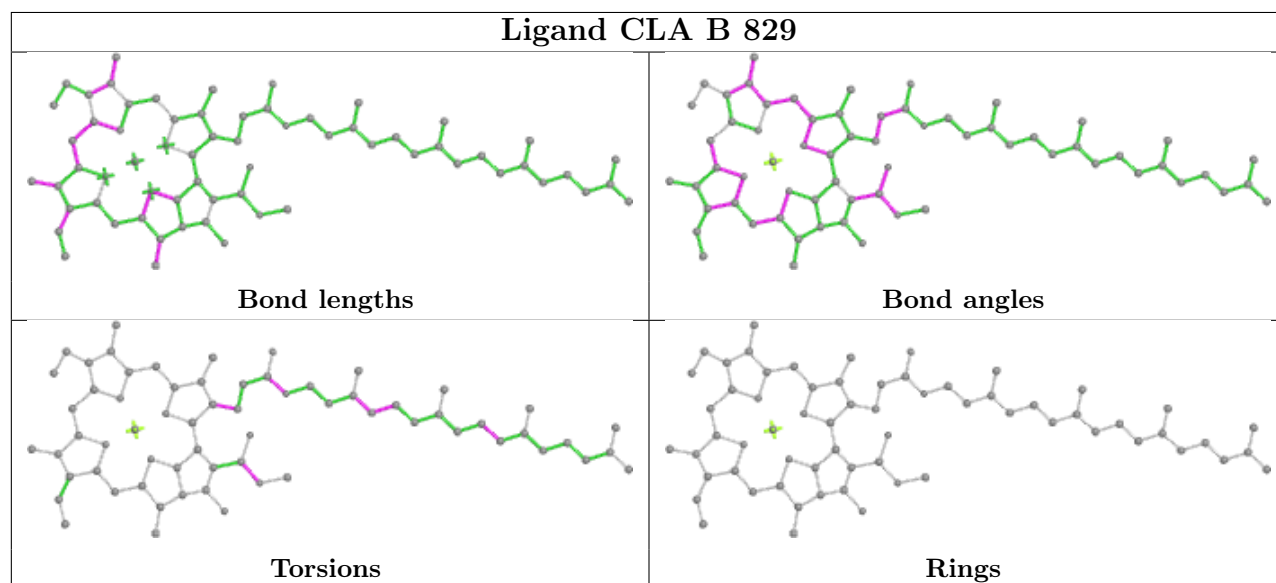
Bond angles



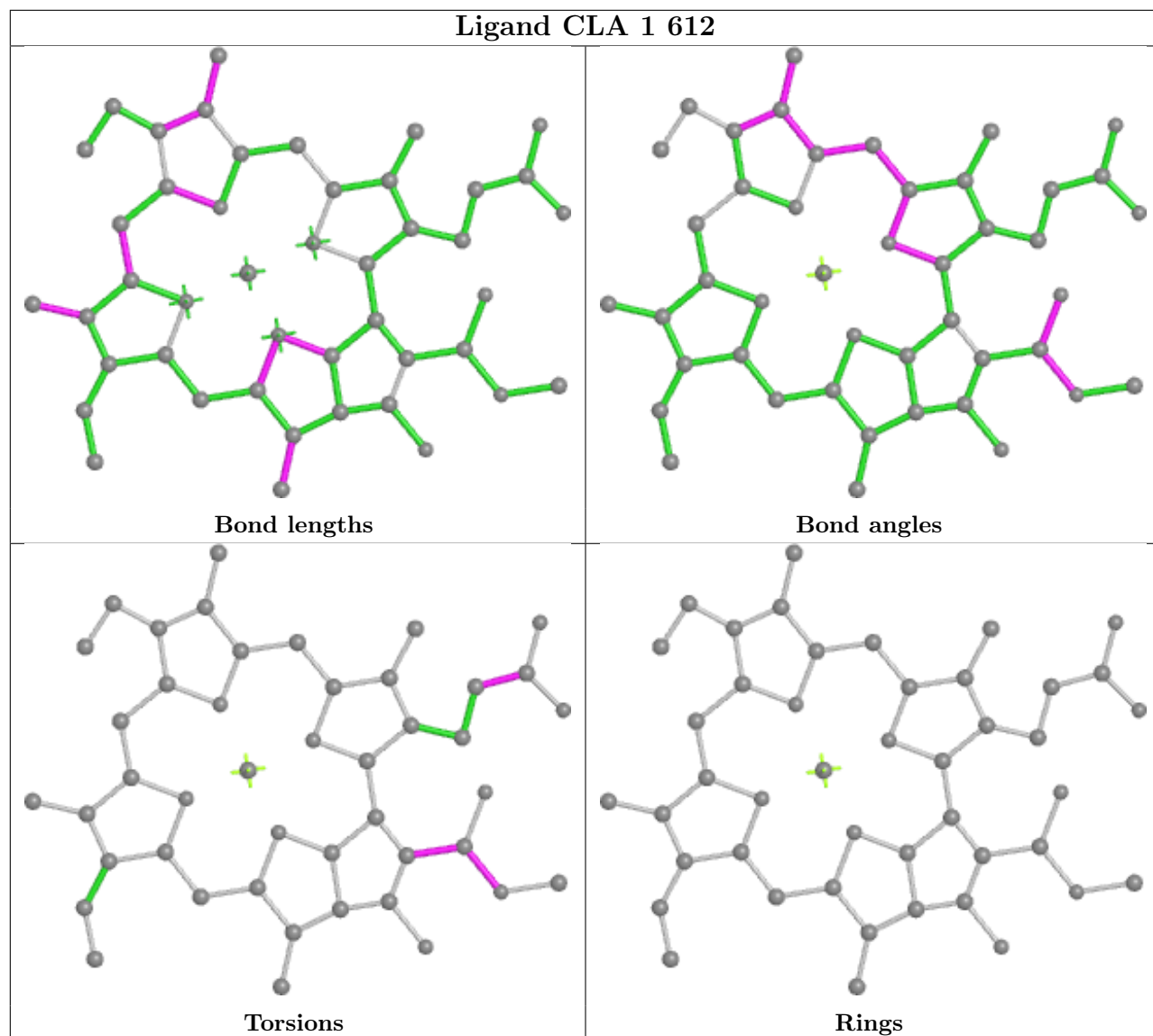
Torsions



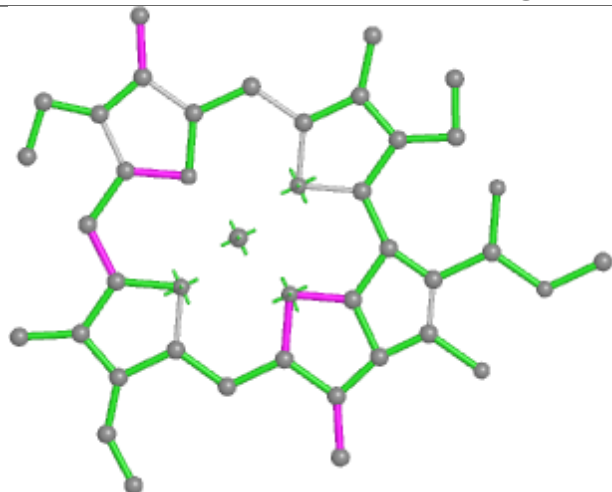
Rings

Ligand CLA A 811**Ligand CLA B 829**

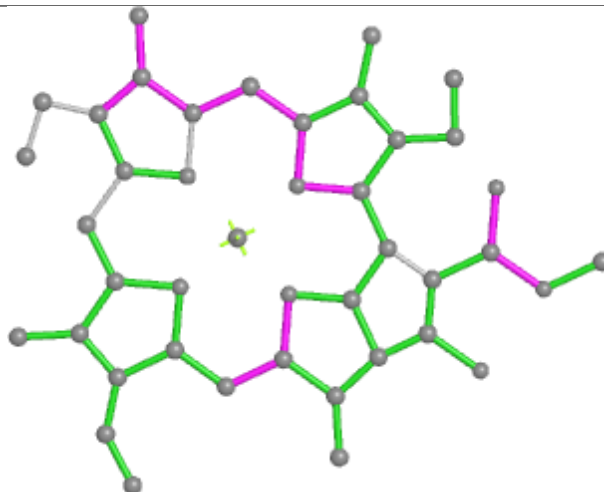
Ligand CLA 1 612



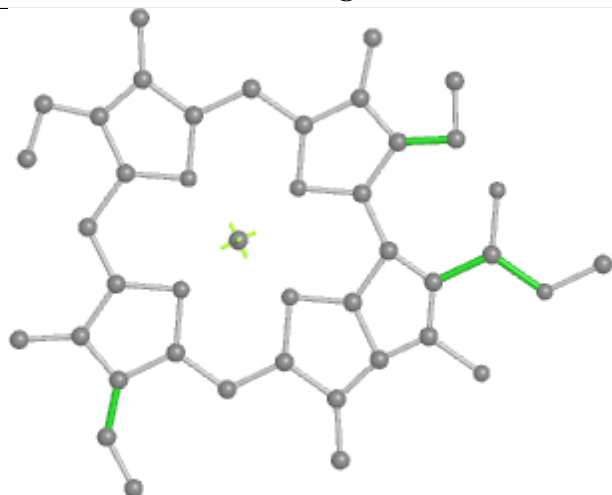
Ligand CLA 5 611



Bond lengths



Bond angles

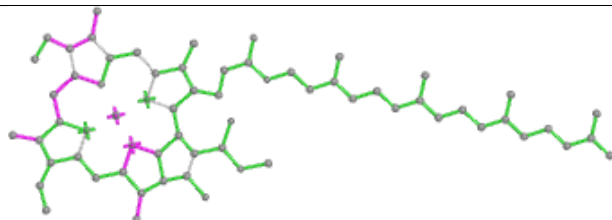


Torsions

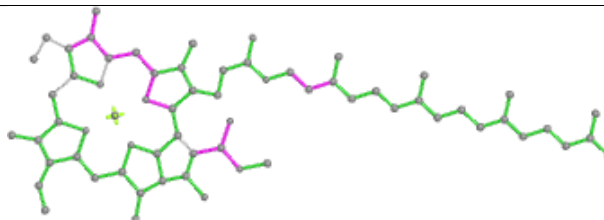


Rings

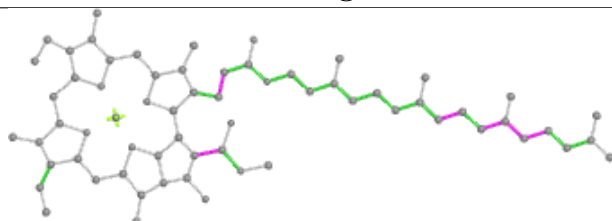
Ligand CLA A 809



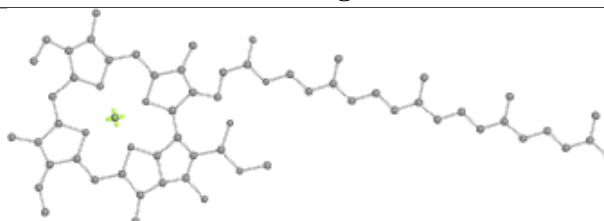
Bond lengths



Bond angles

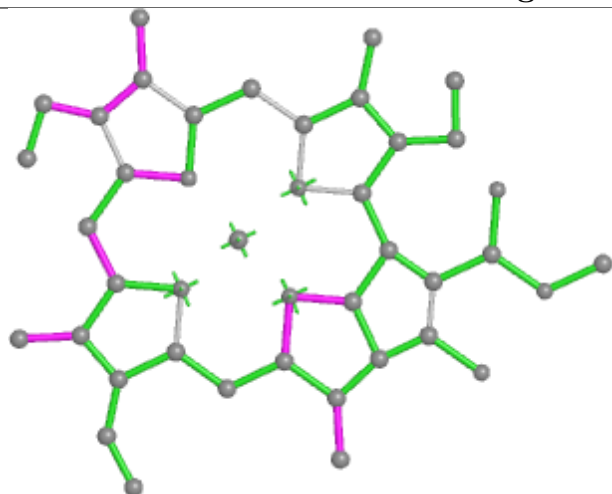


Torsions

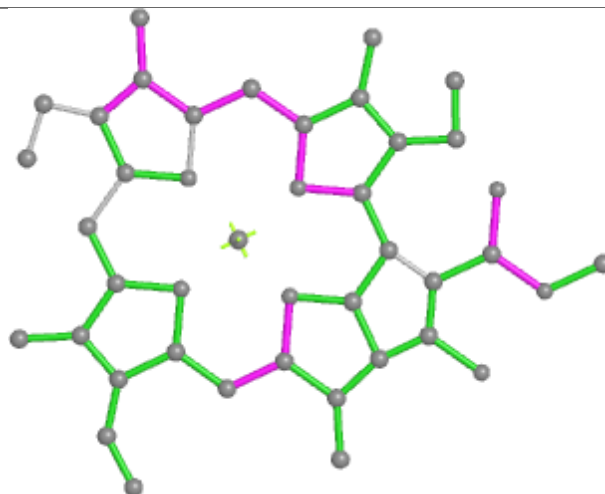


Rings

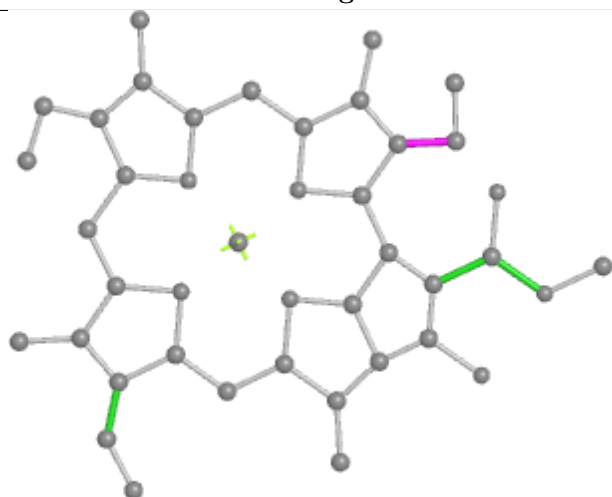
Ligand CLA 7 614



Bond lengths



Bond angles

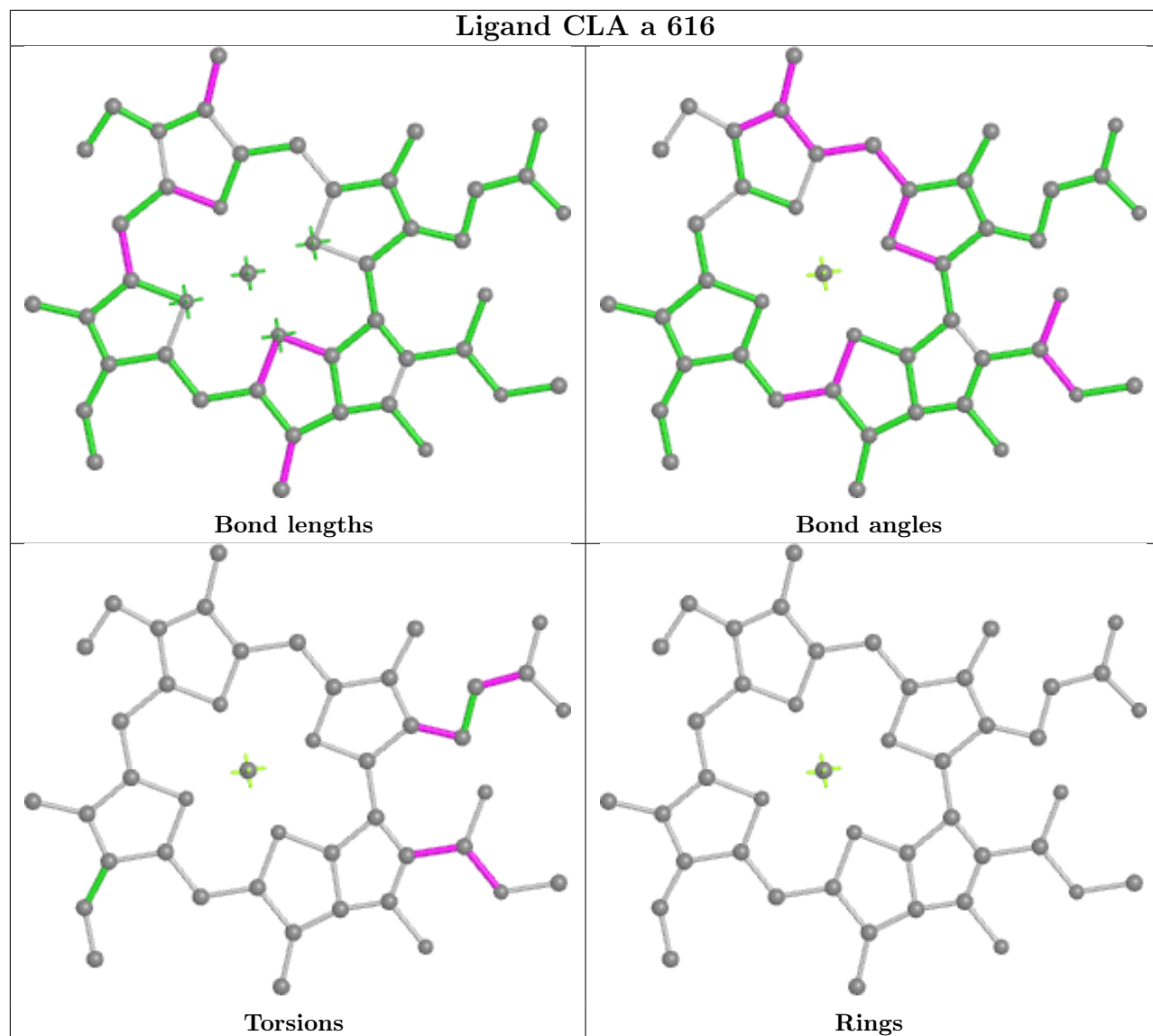


Torsions

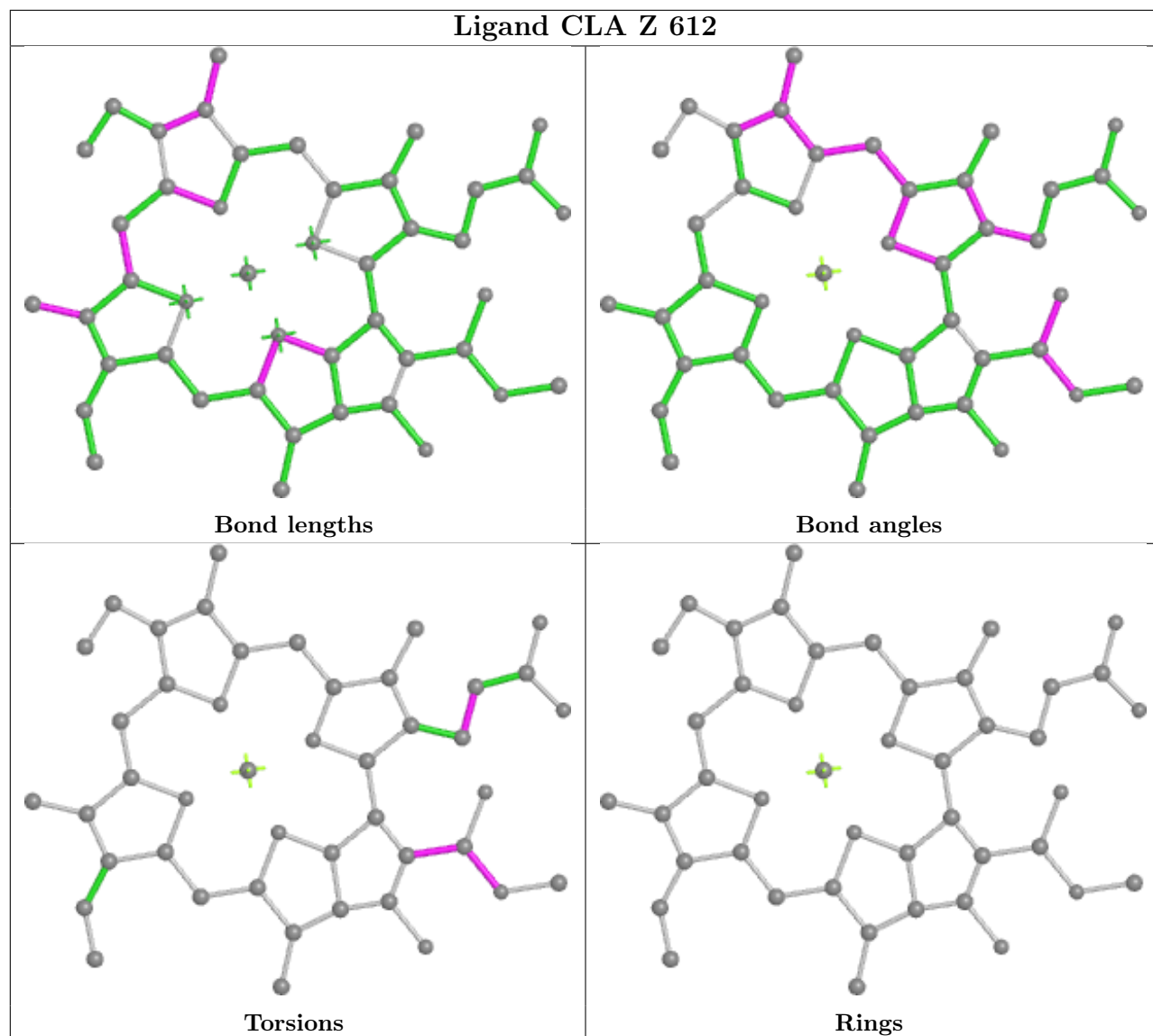


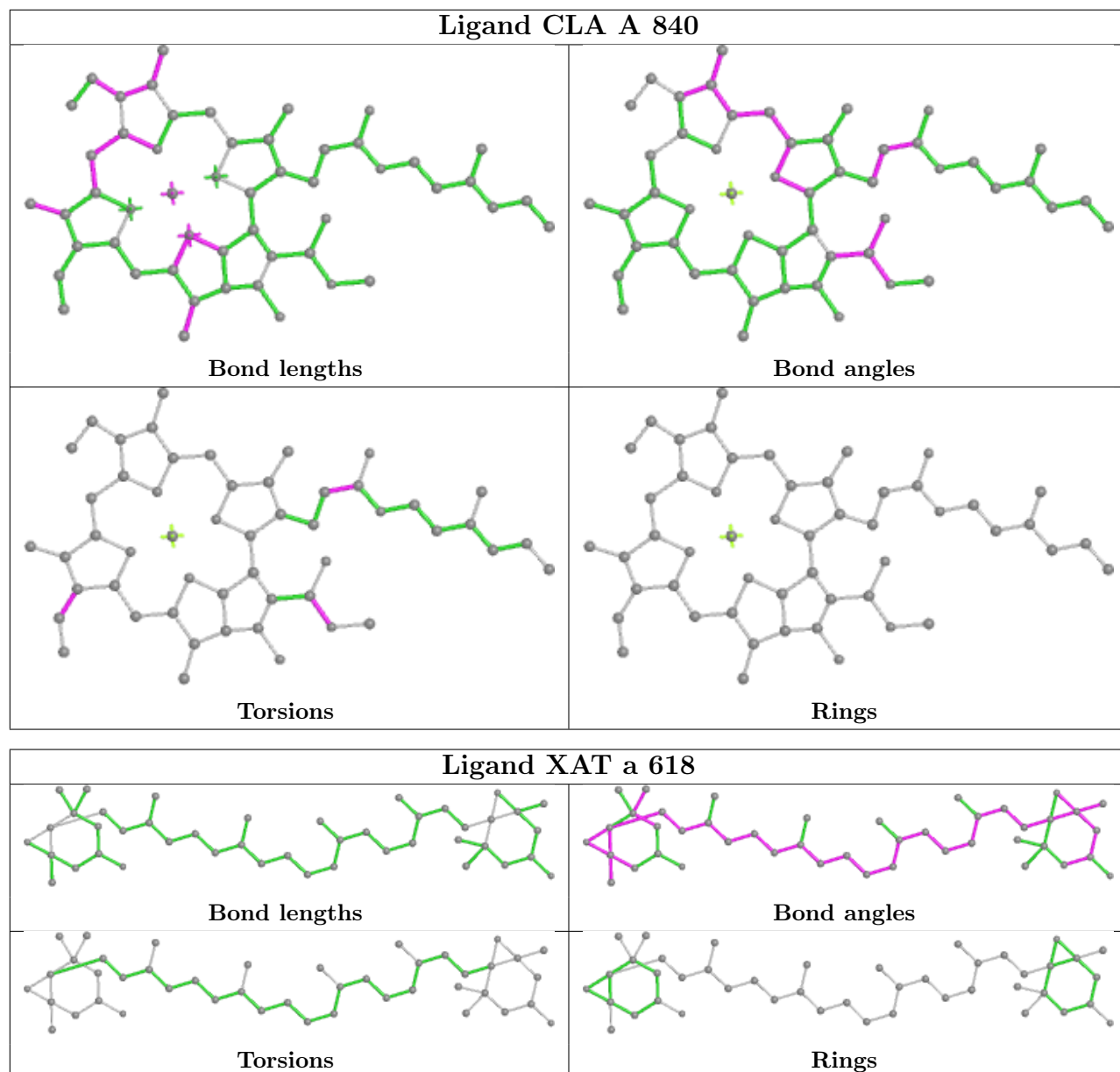
Rings

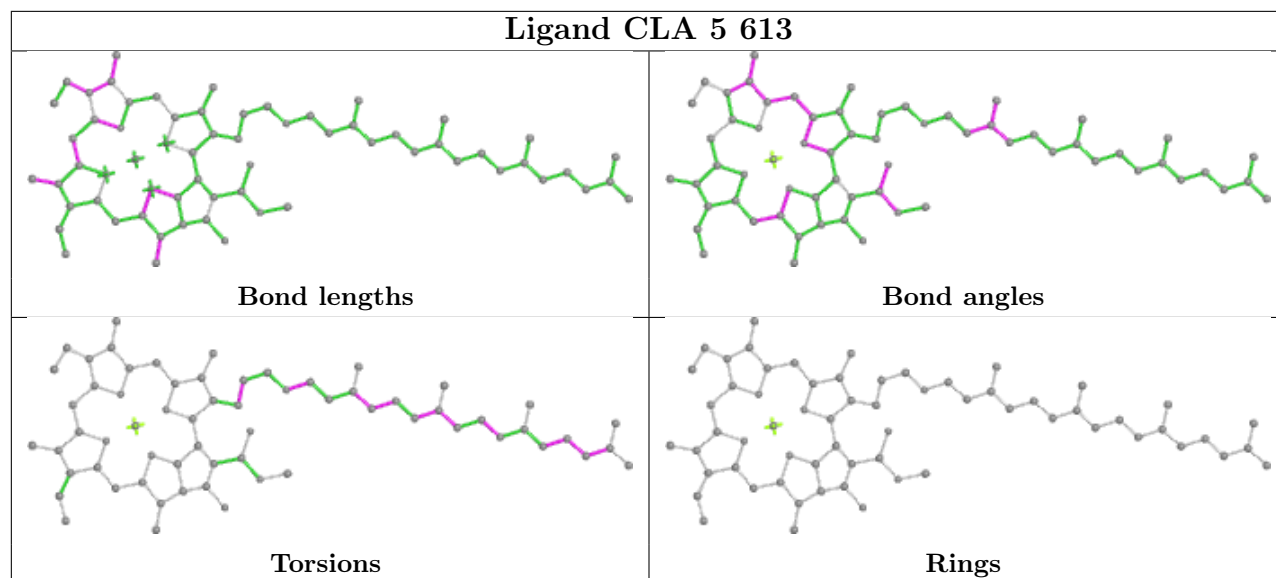
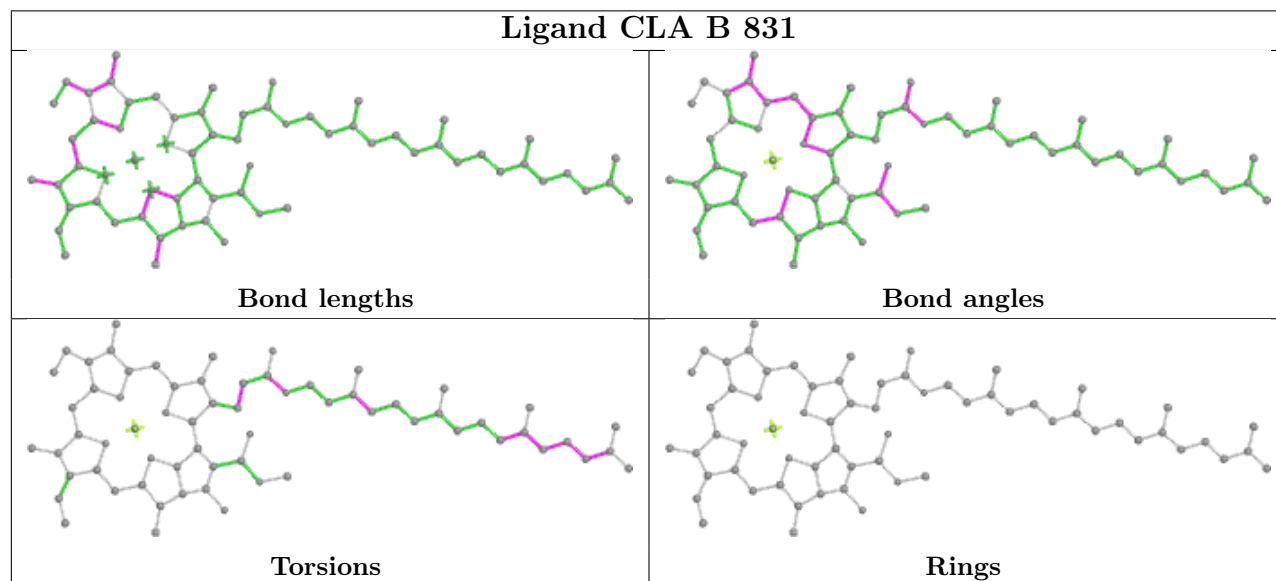
Ligand CLA a 616

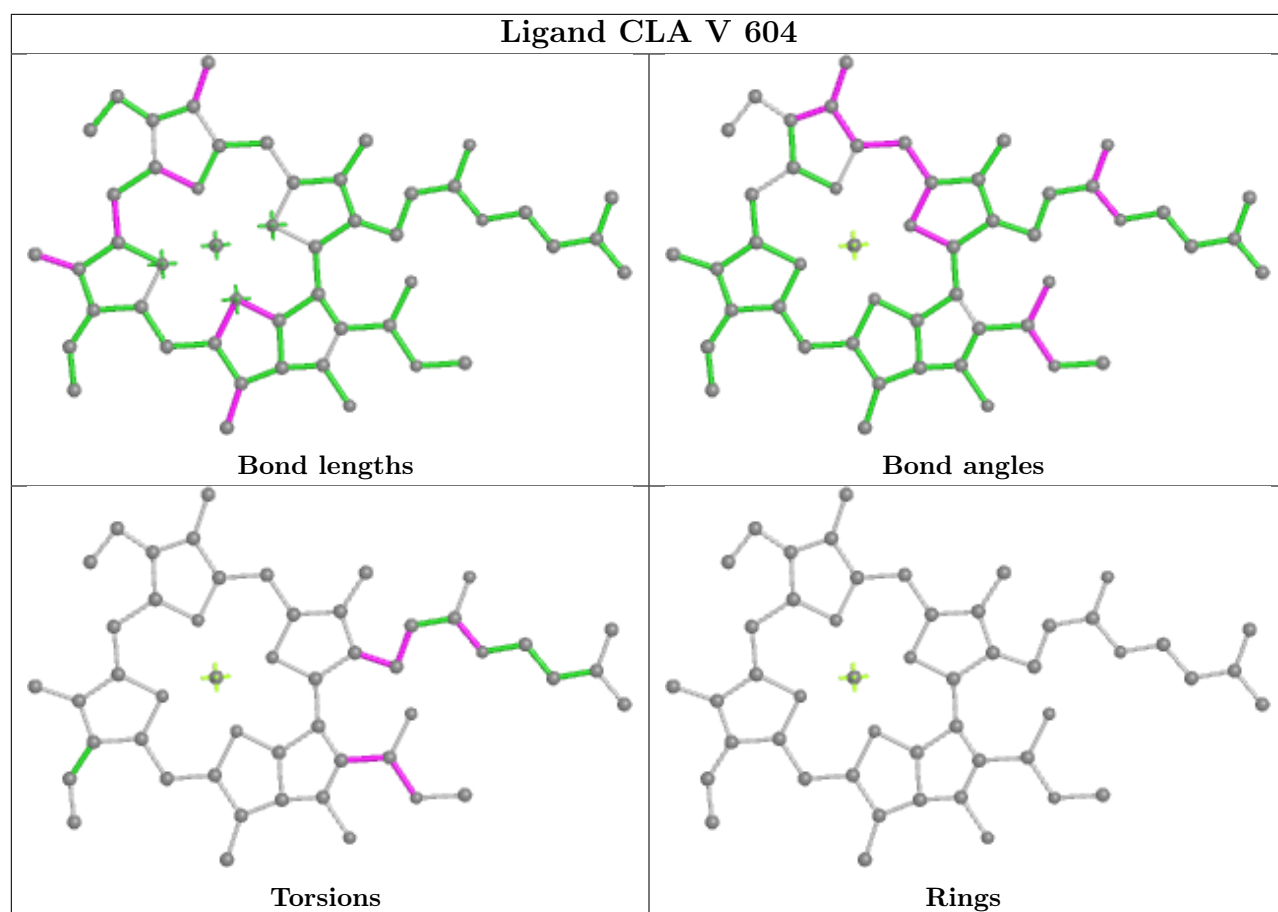


Ligand CLA Z 612

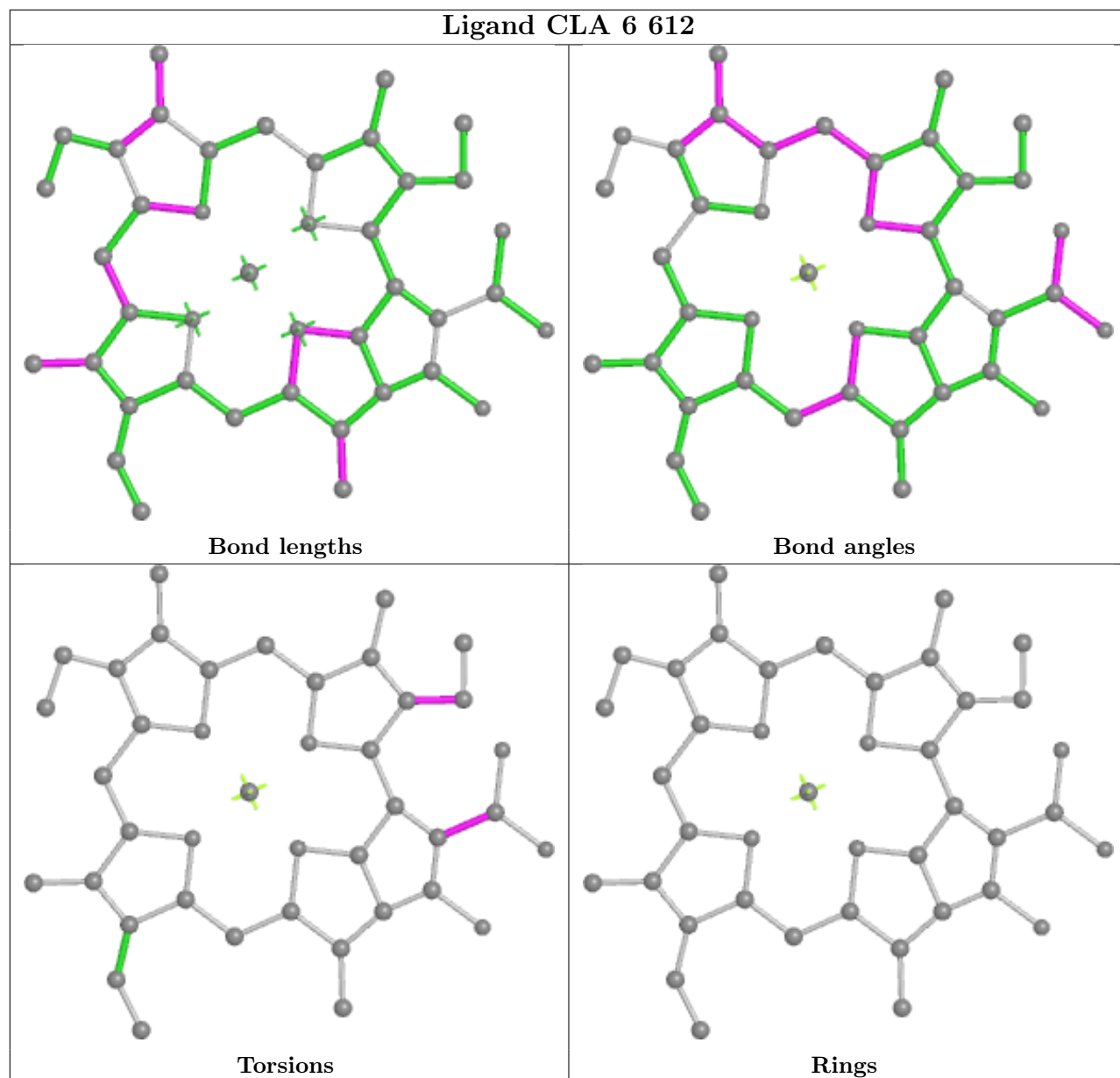


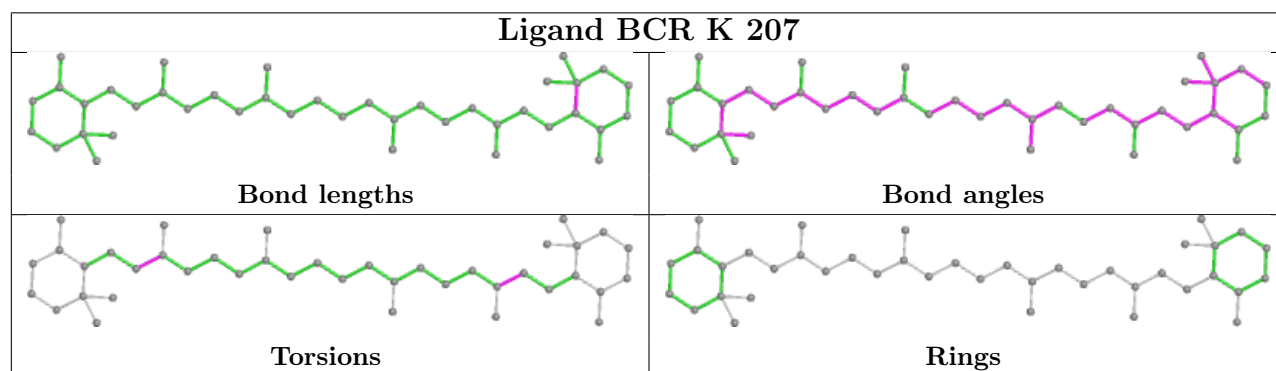
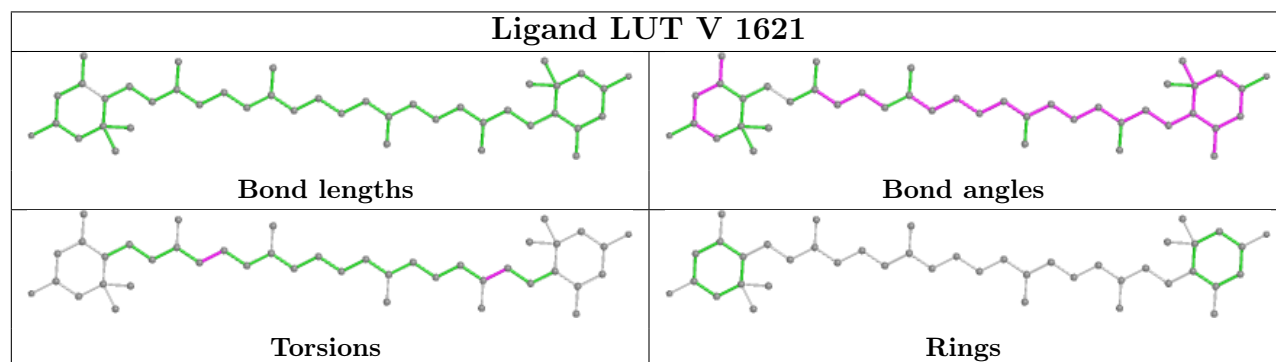
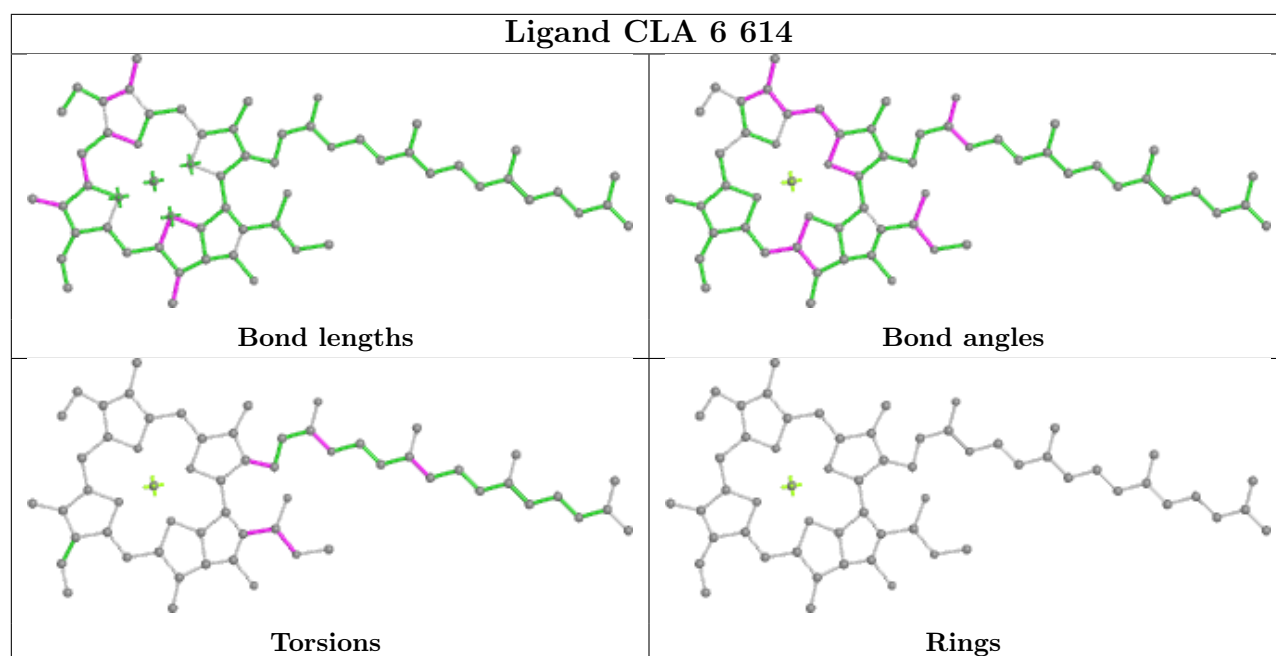


Ligand CLA 5 613**Ligand CLA B 831**

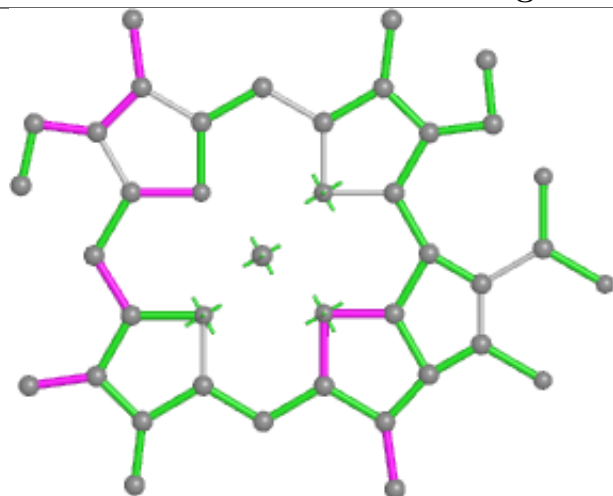


Ligand CLA 6 612

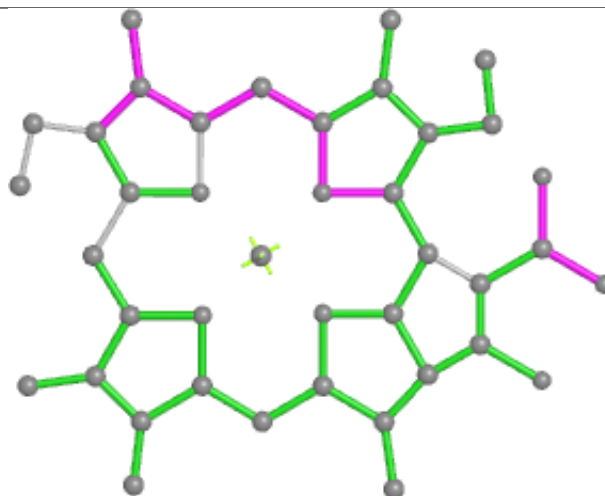




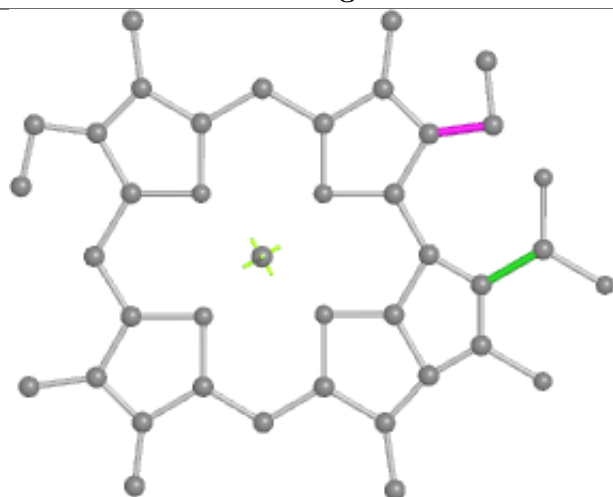
Ligand CLA L 306



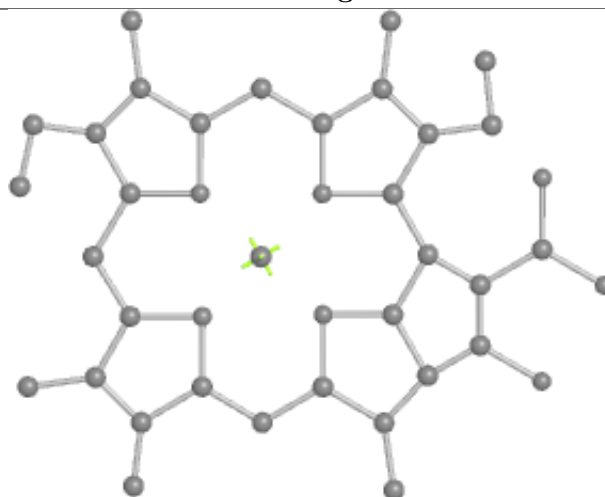
Bond lengths



Bond angles

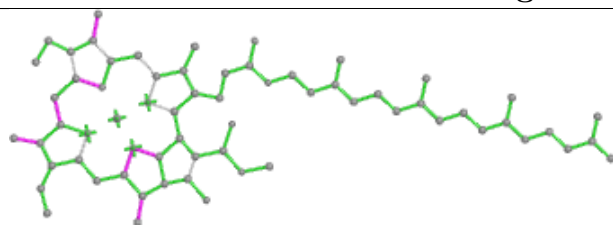


Torsions

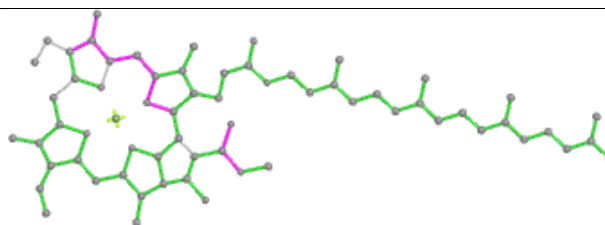


Rings

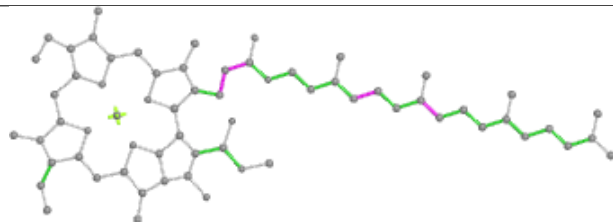
Ligand CLA Z 613



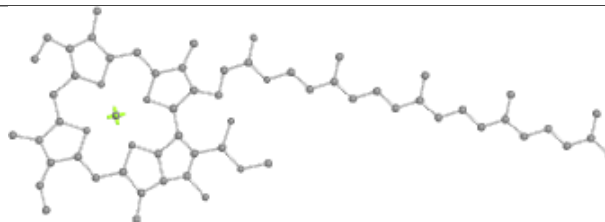
Bond lengths



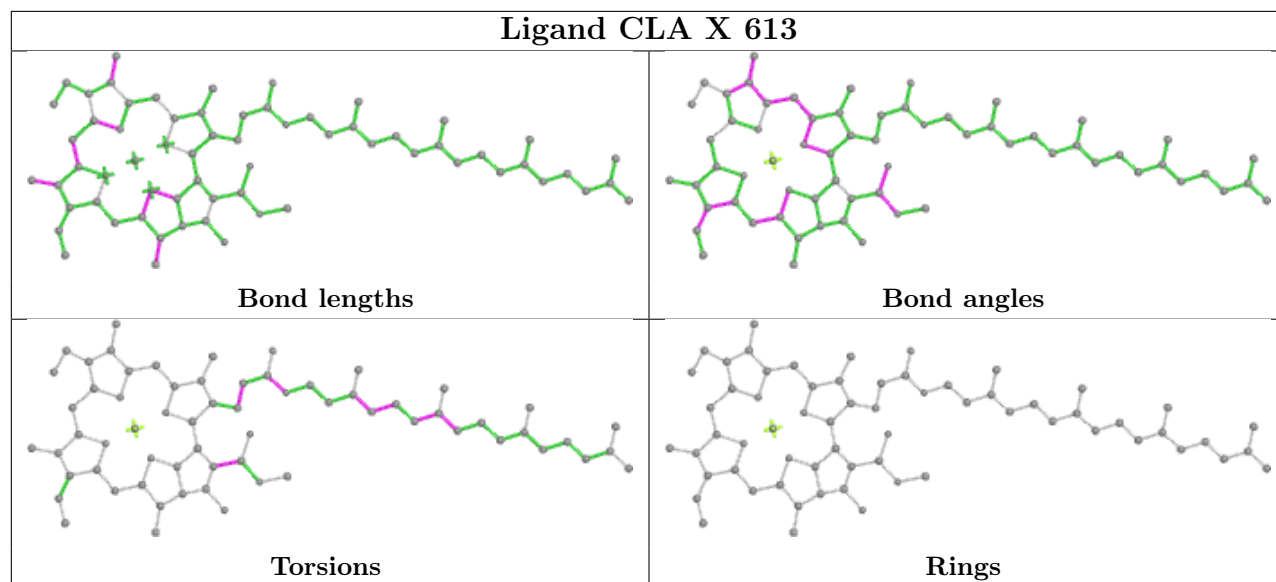
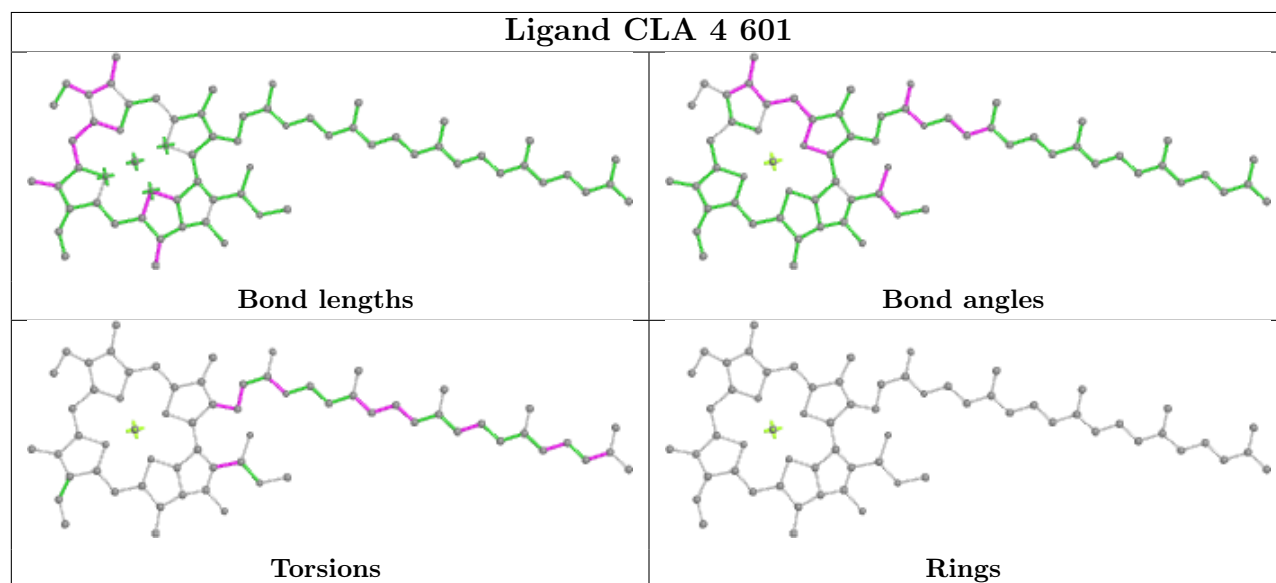
Bond angles



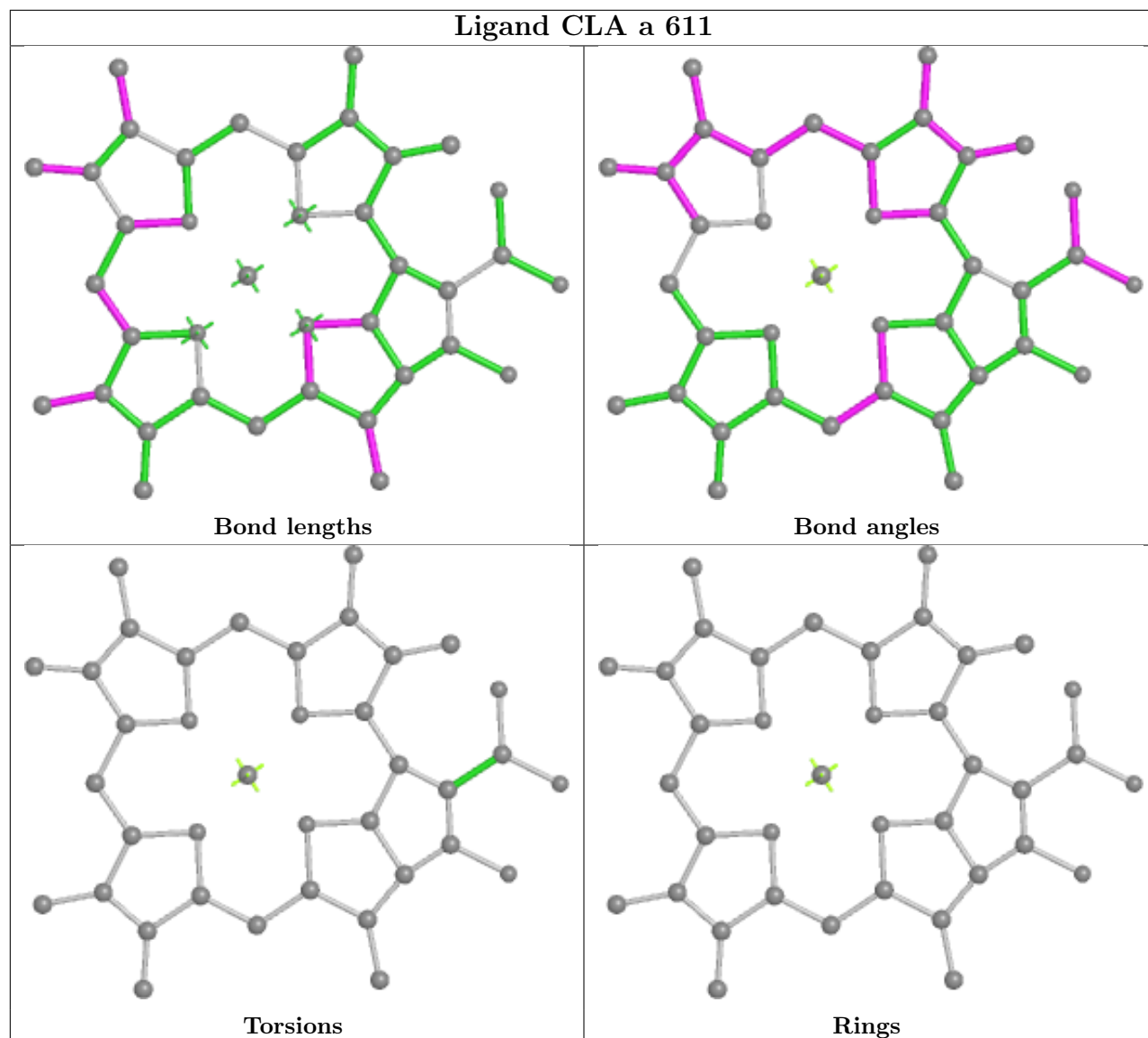
Torsions



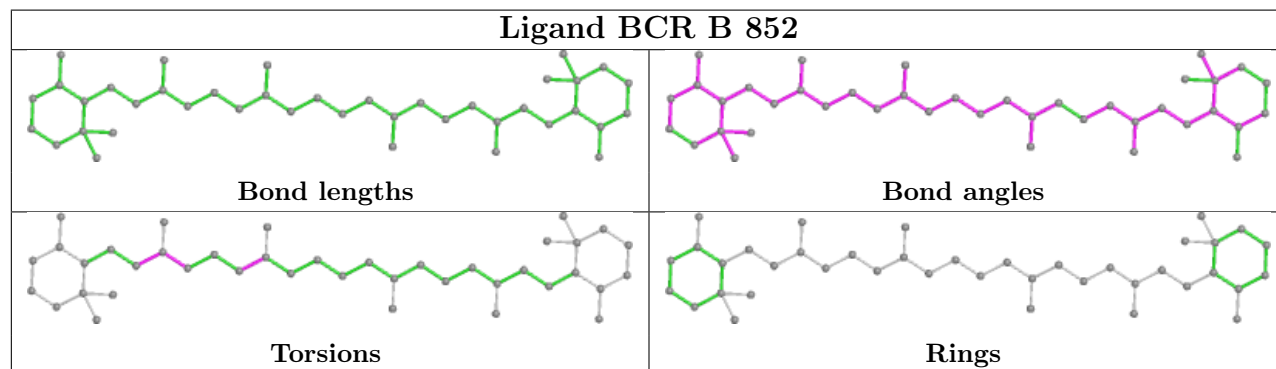
Rings

Ligand CLA X 613**Ligand CLA 4 601**

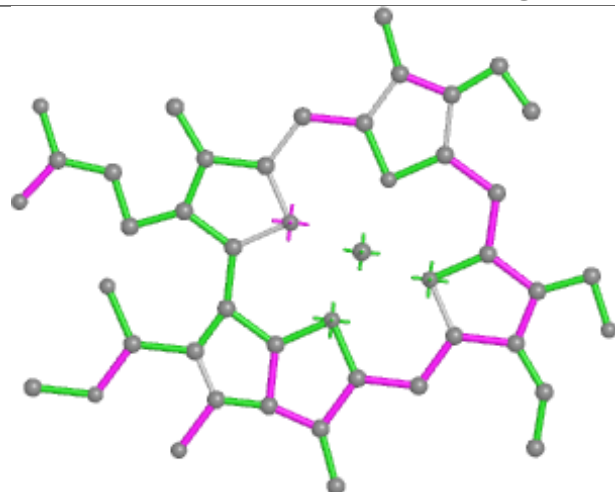
Ligand CLA a 611



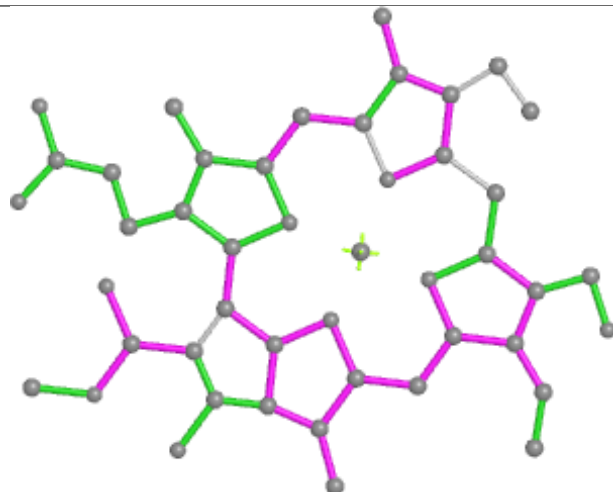
Ligand BCR B 852



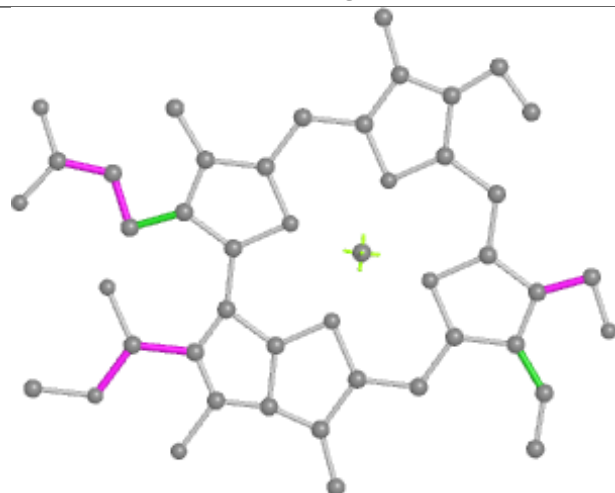
Ligand CHL X 605



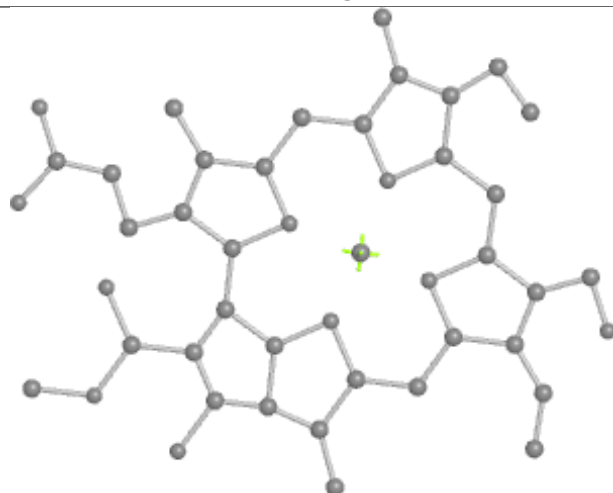
Bond lengths



Bond angles

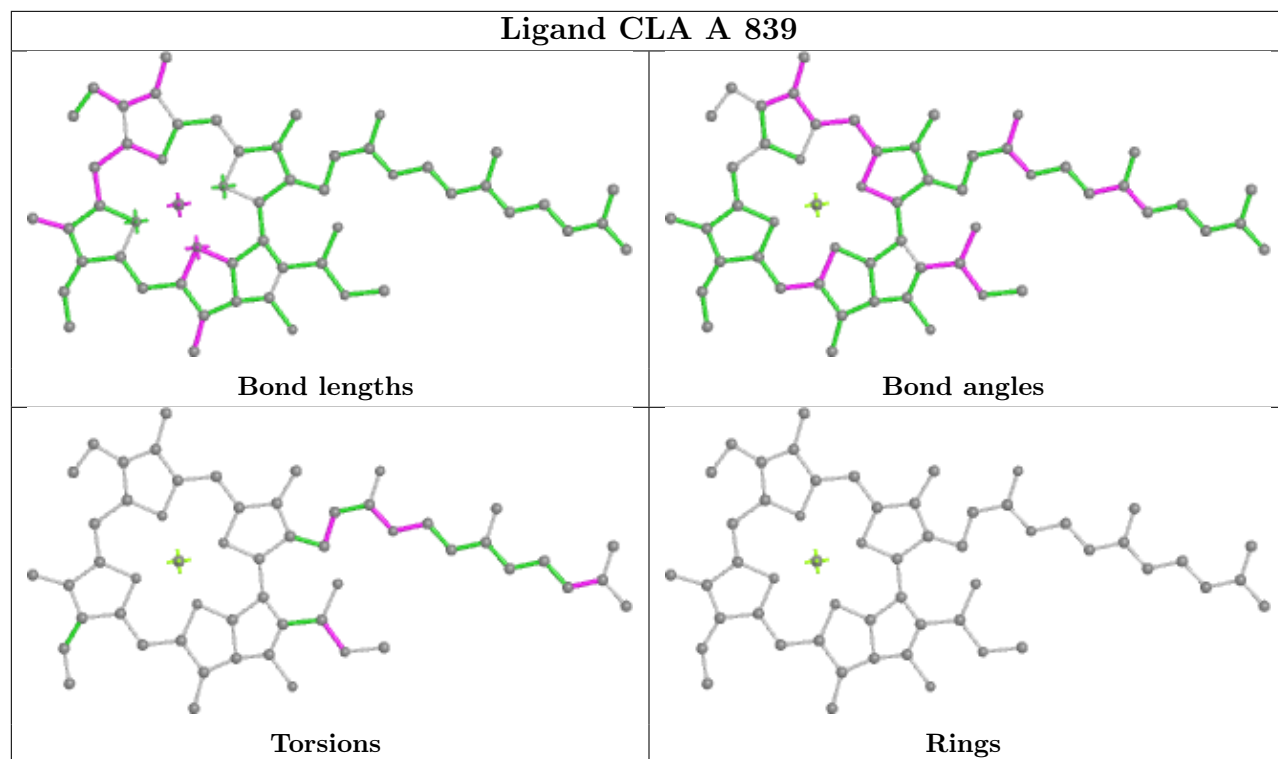


Torsions

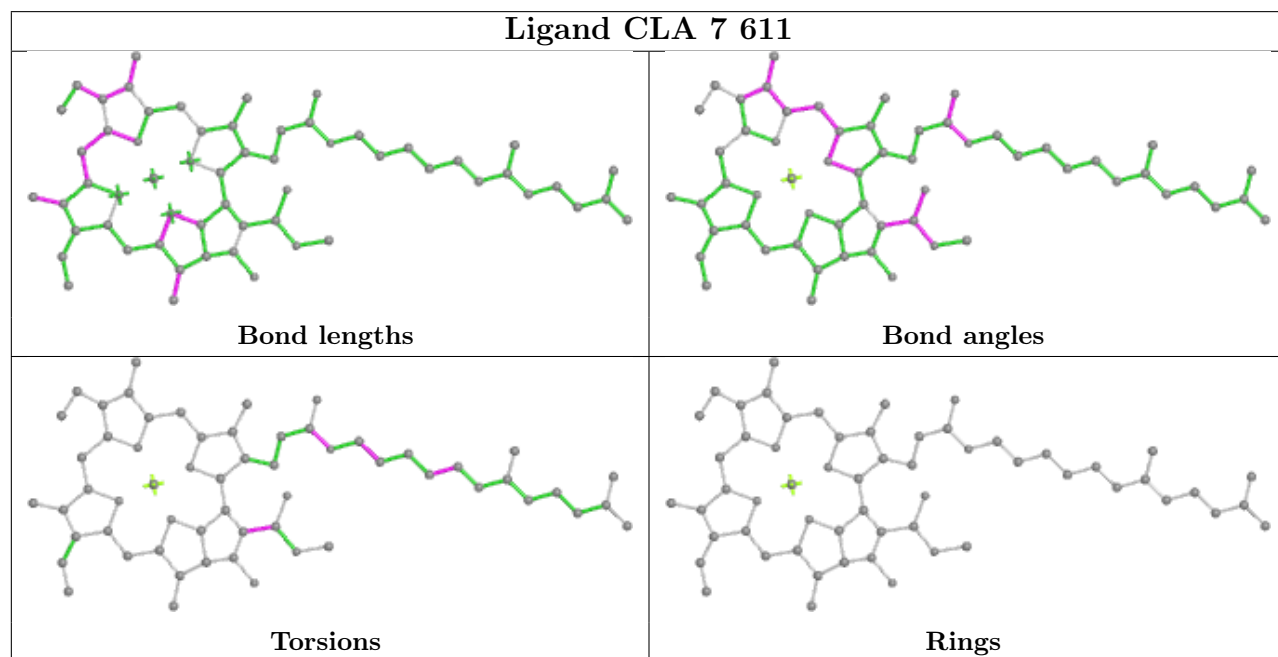


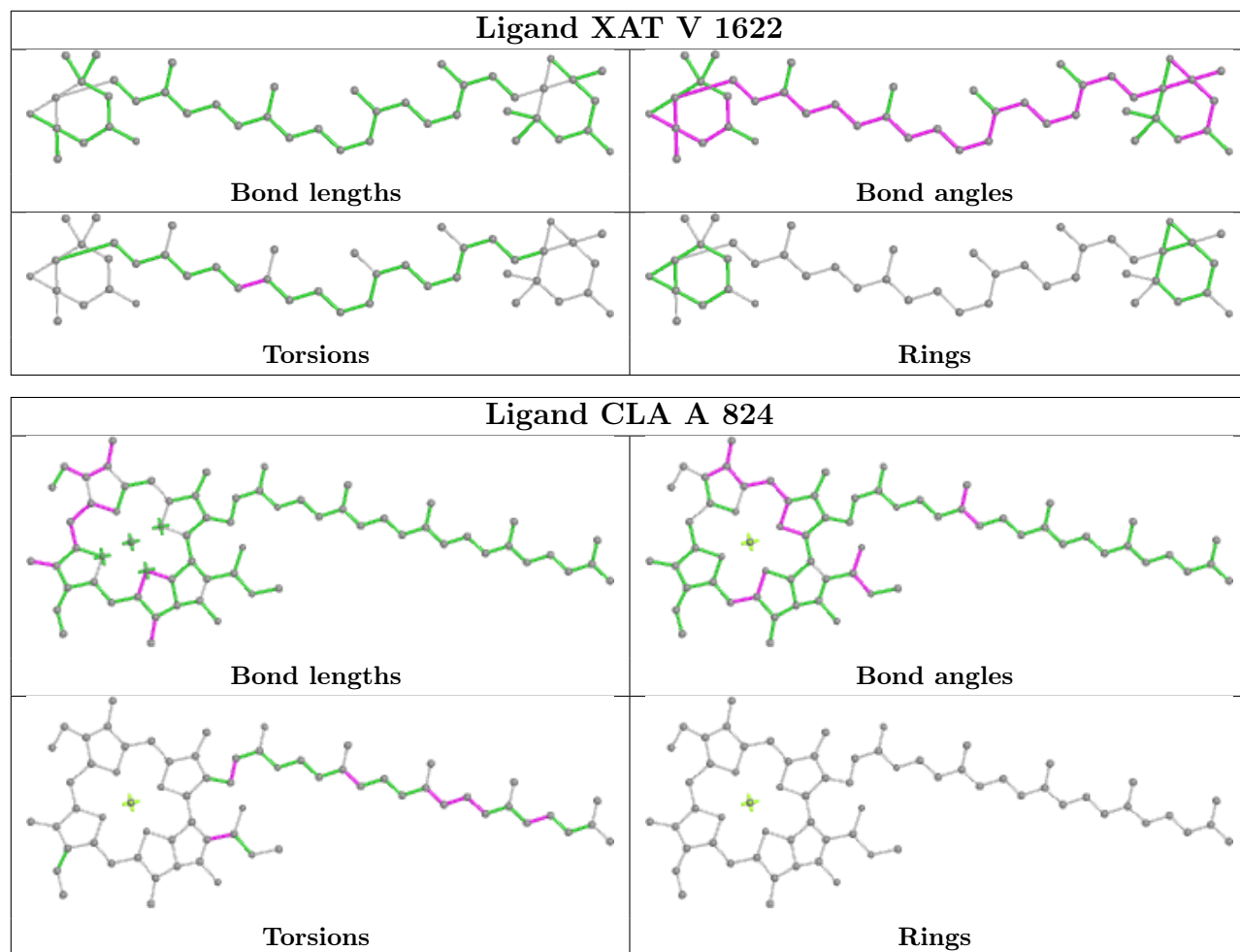
Rings

Ligand CLA A 839

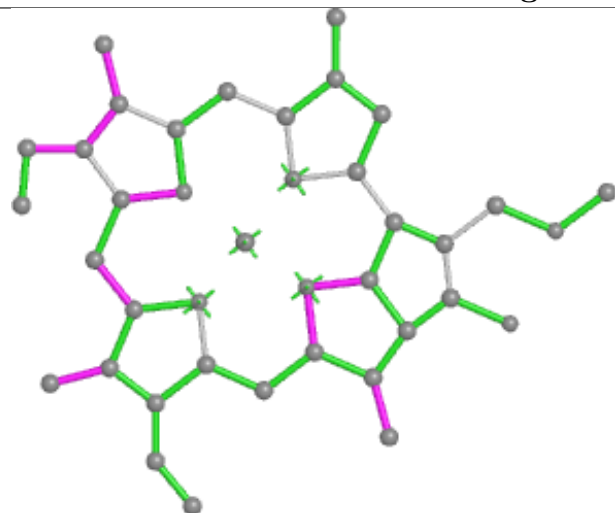


Ligand CLA 7 611

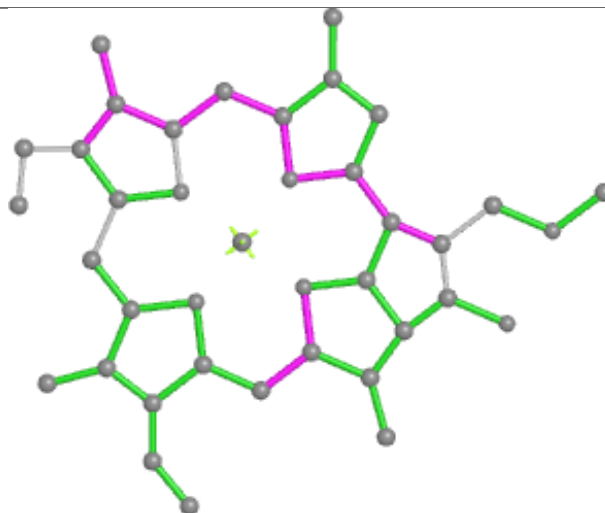




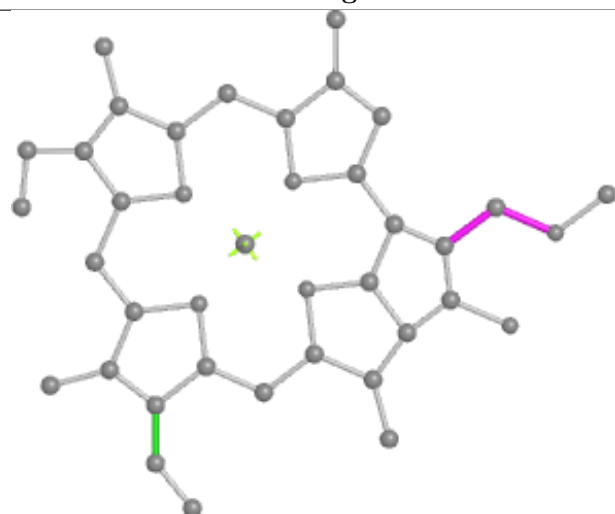
Ligand CLA 1 606



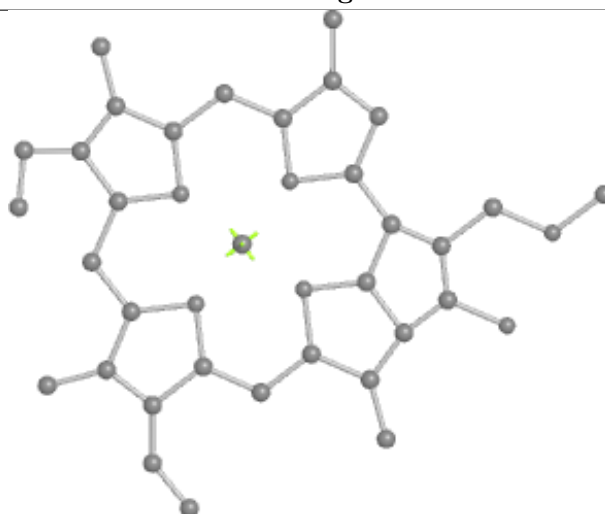
Bond lengths



Bond angles

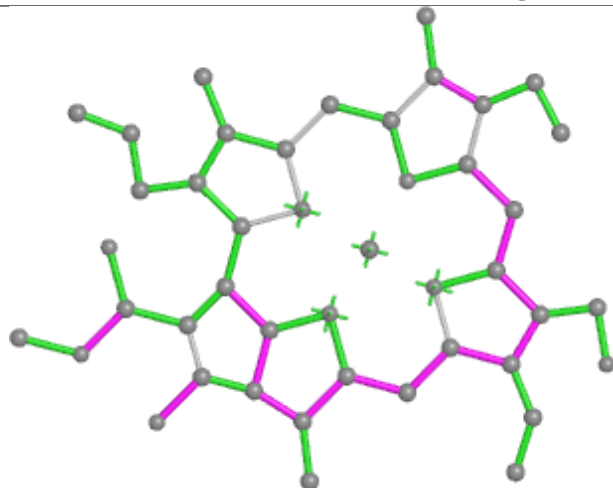


Torsions

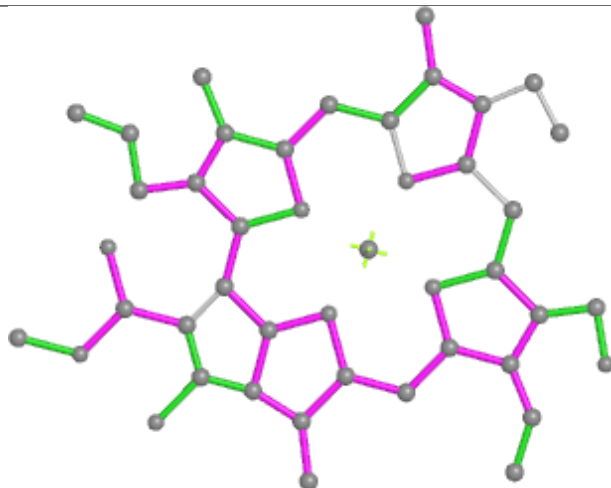


Rings

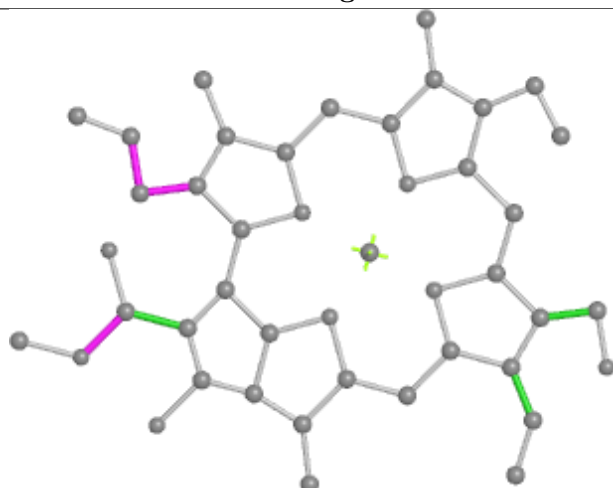
Ligand CHL V 606



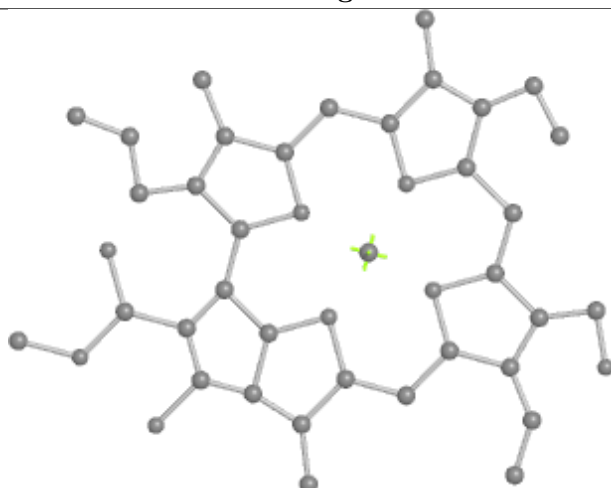
Bond lengths



Bond angles

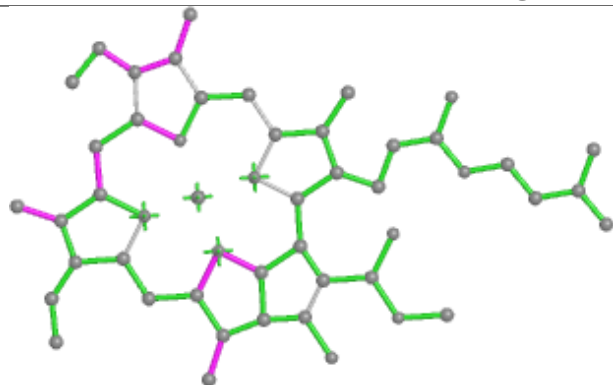


Torsions

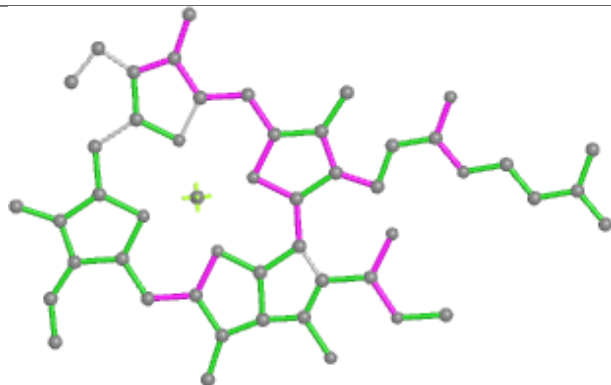


Rings

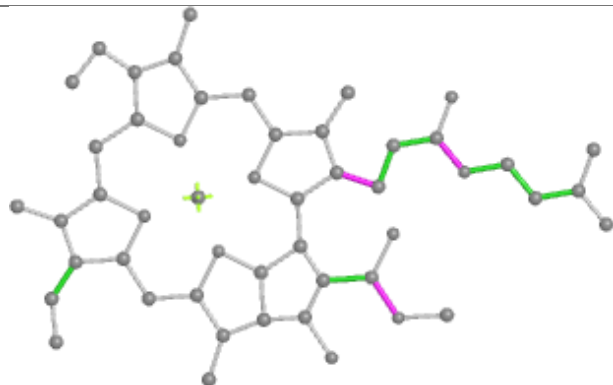
Ligand CLA A 810



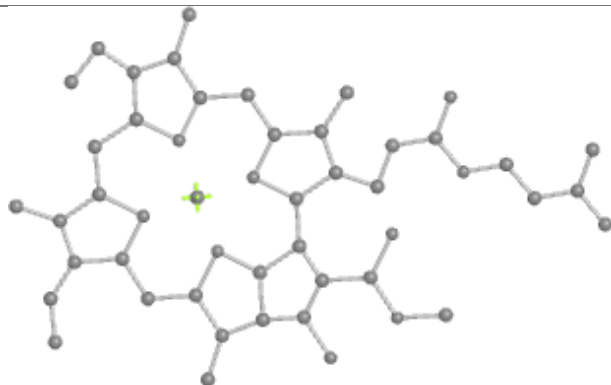
Bond lengths



Bond angles

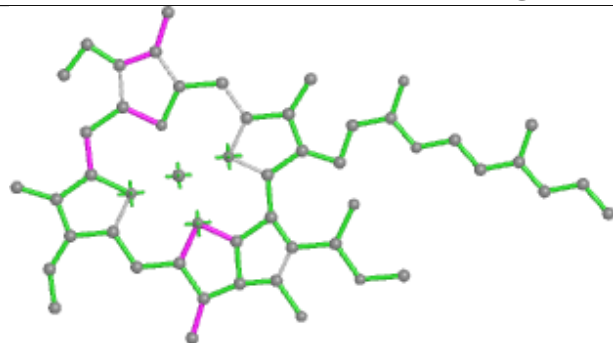


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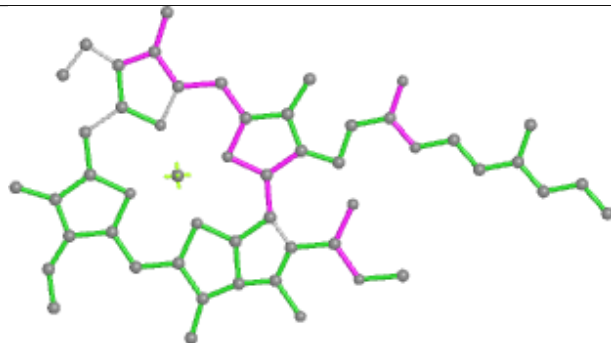


Rings

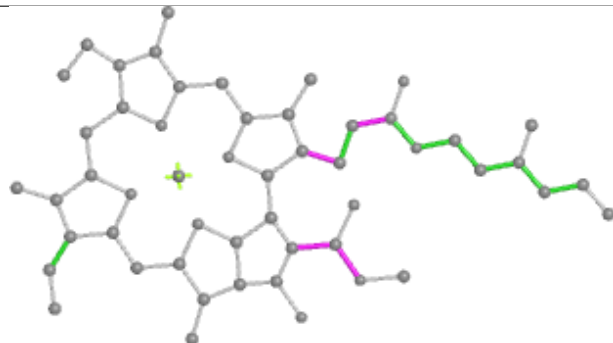
Ligand CLA U 603



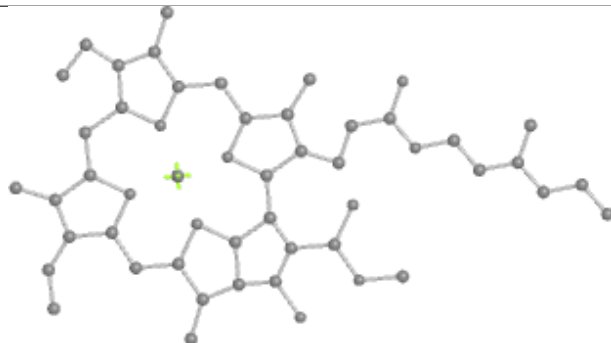
Bond lengths



Bond angles

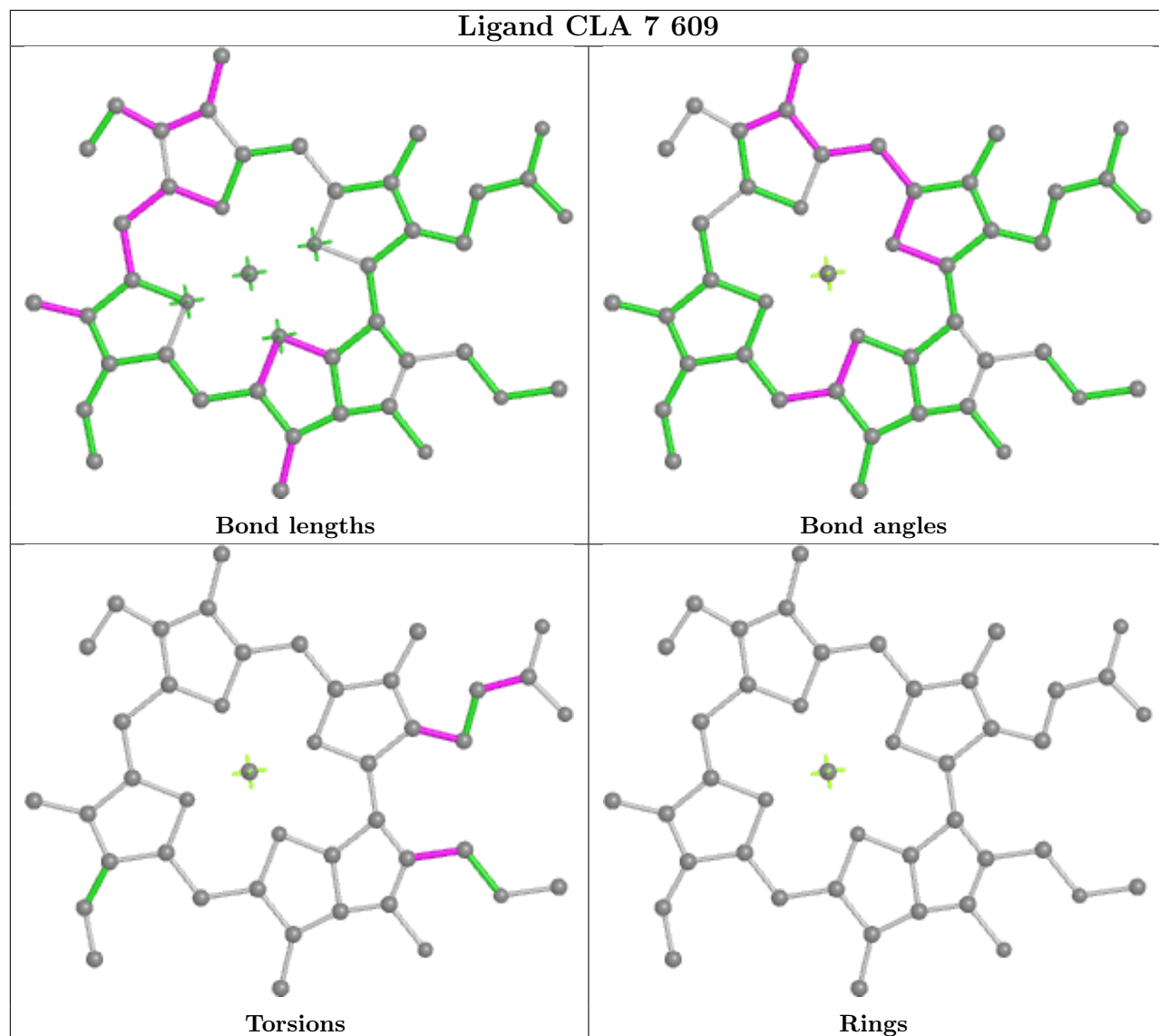


Torsions

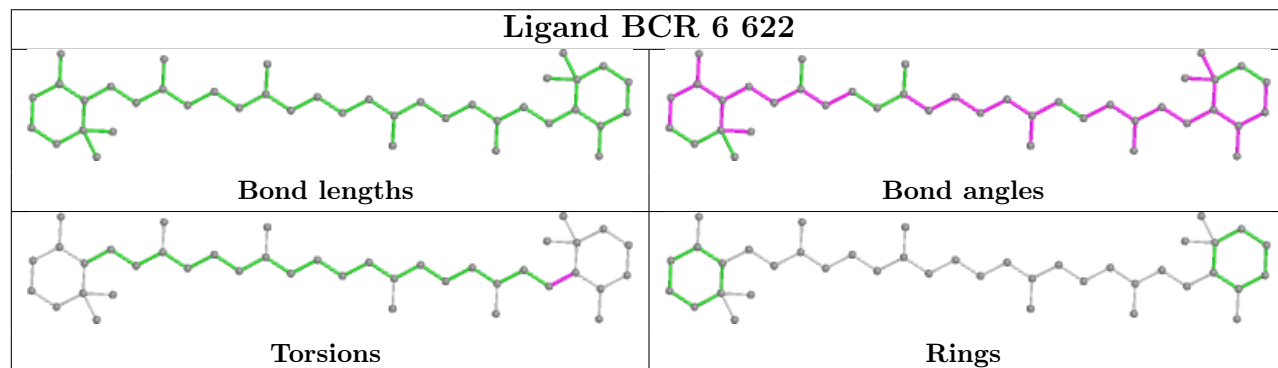


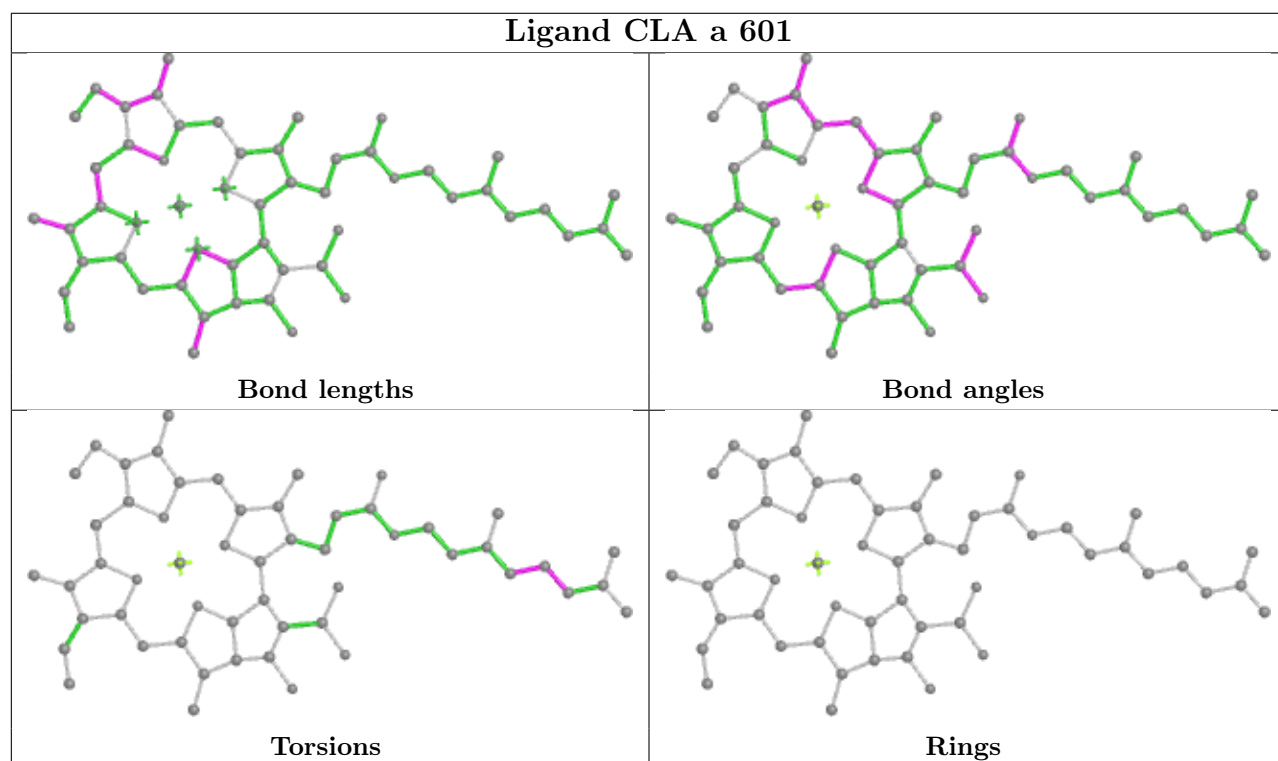
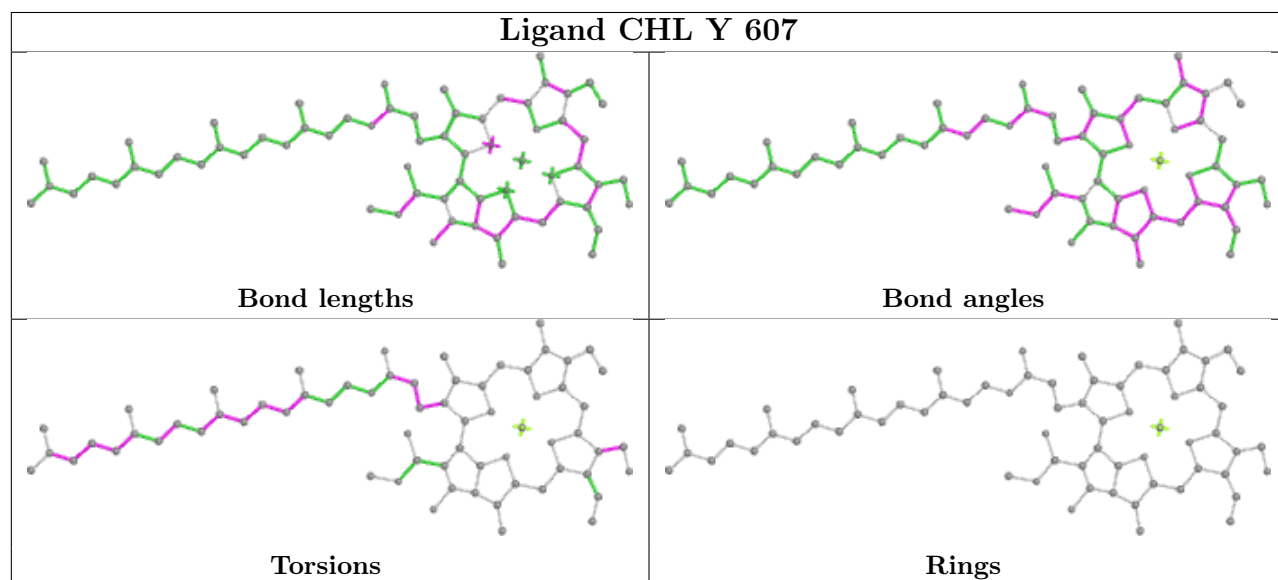
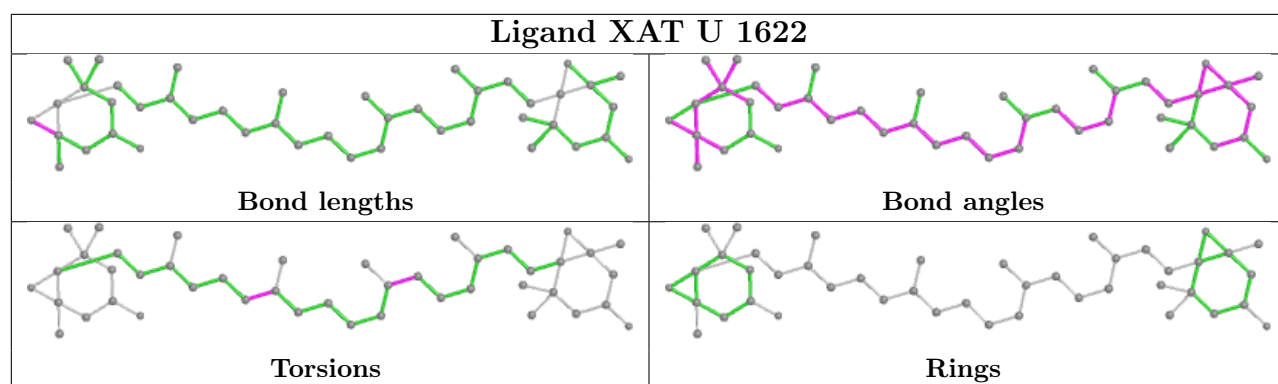
Rings

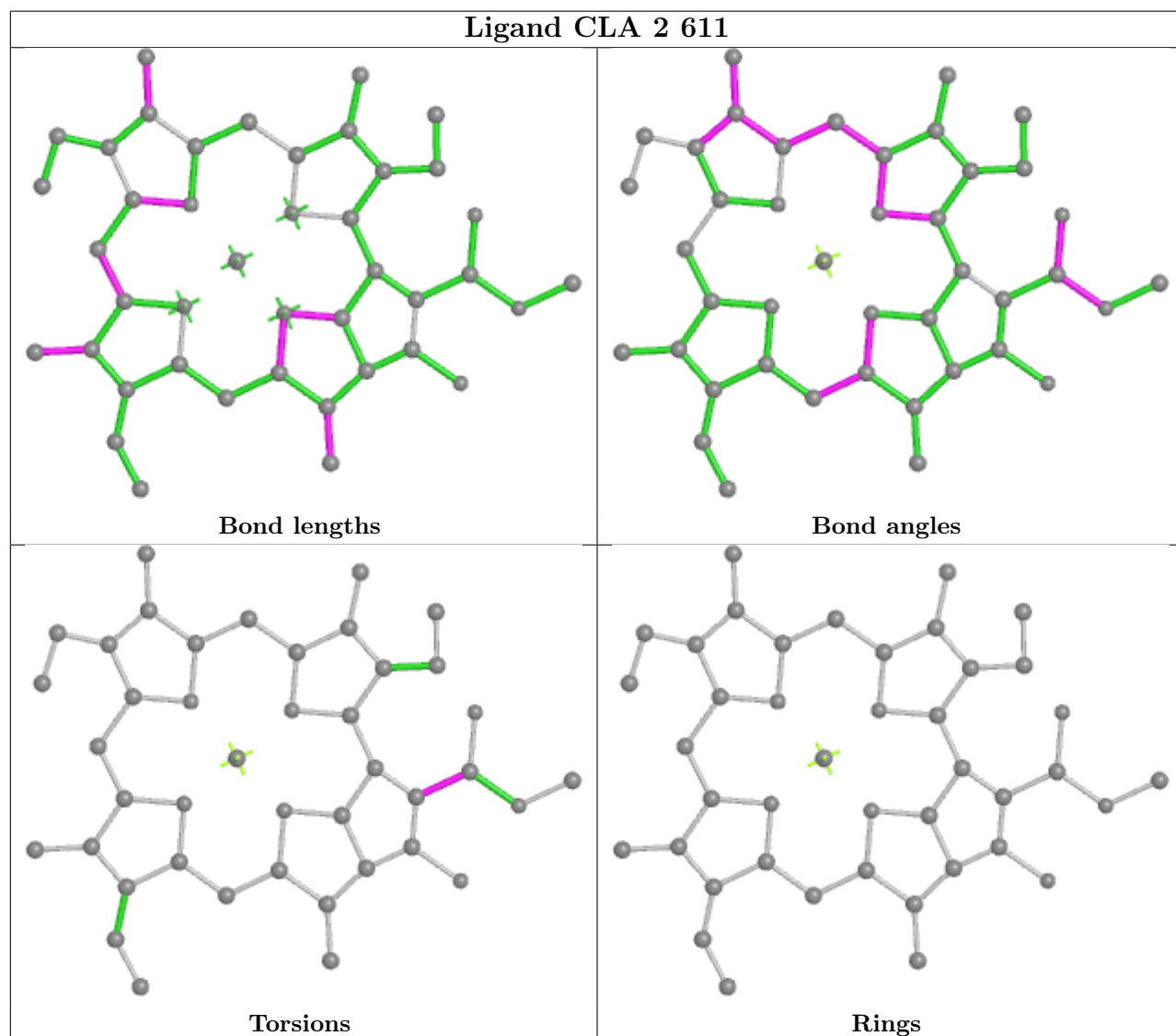
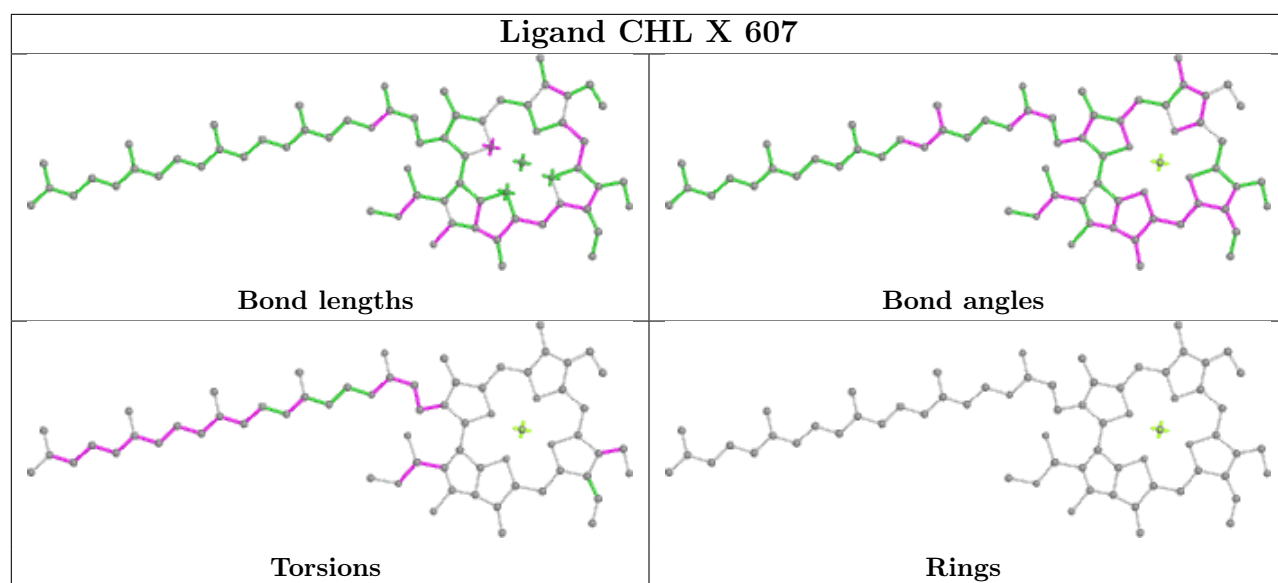
Ligand CLA 7 609

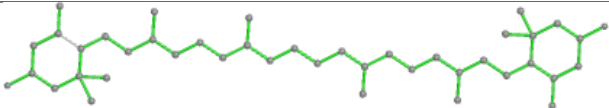
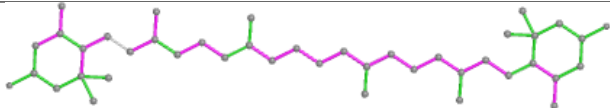
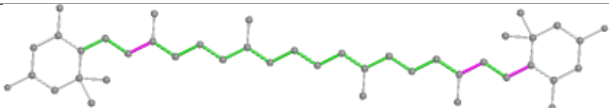
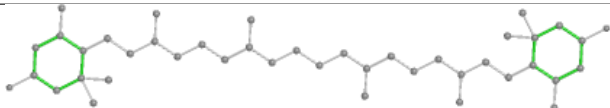


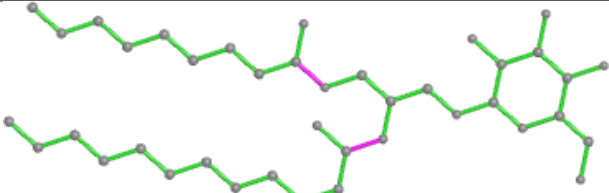
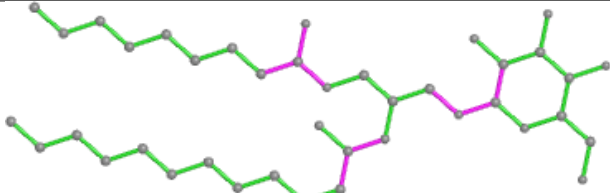
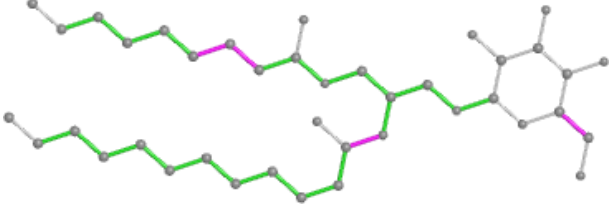
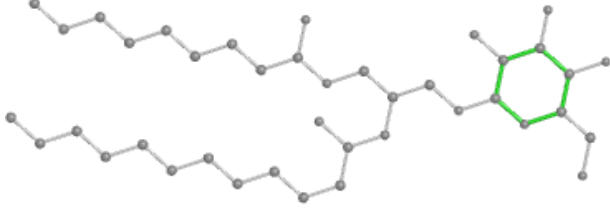
Ligand BCR 6 622

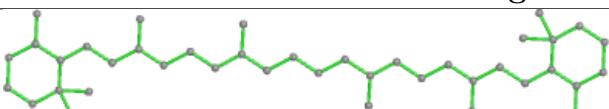
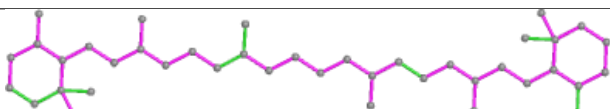
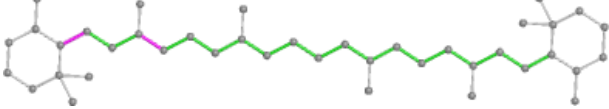



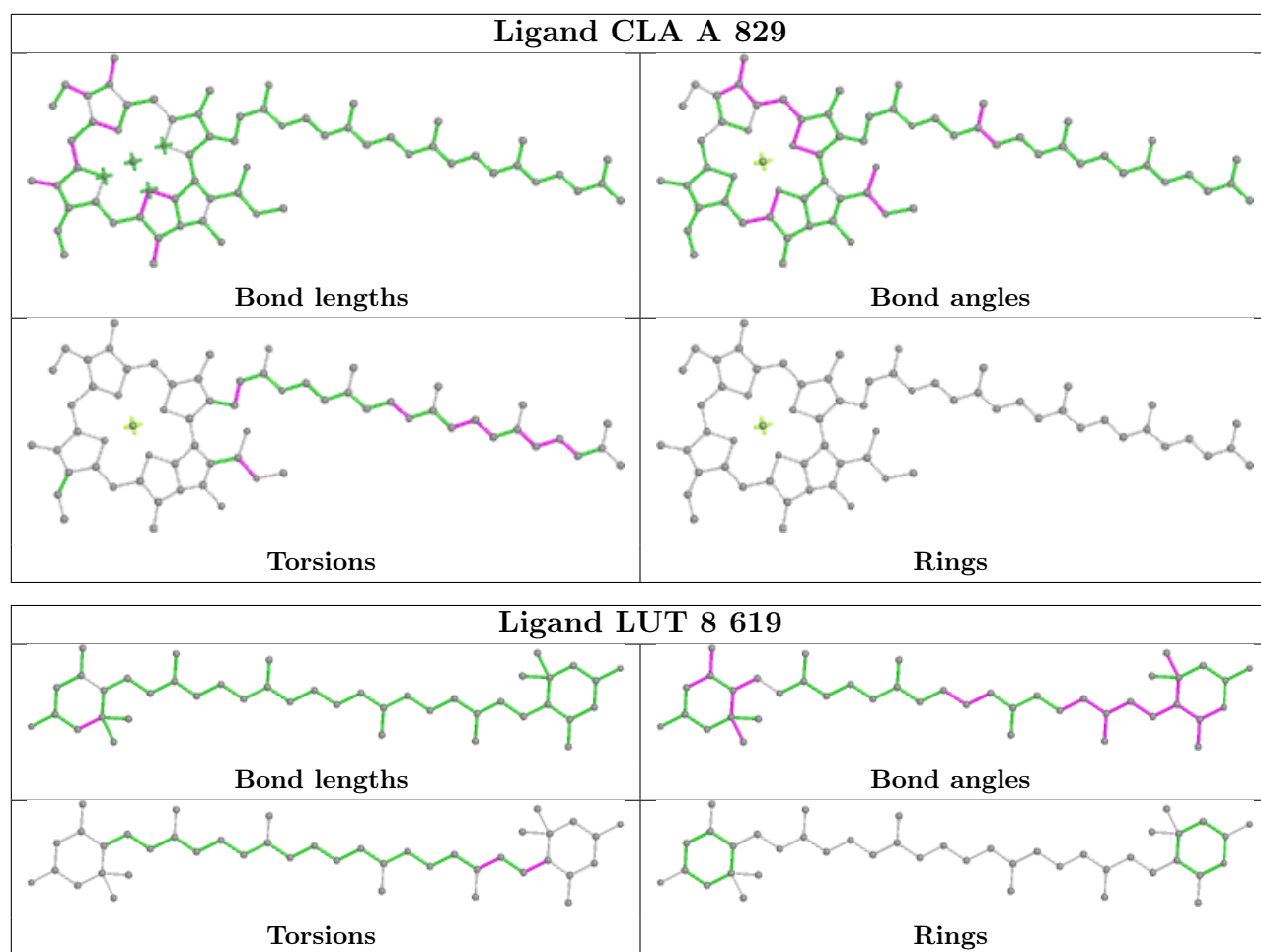




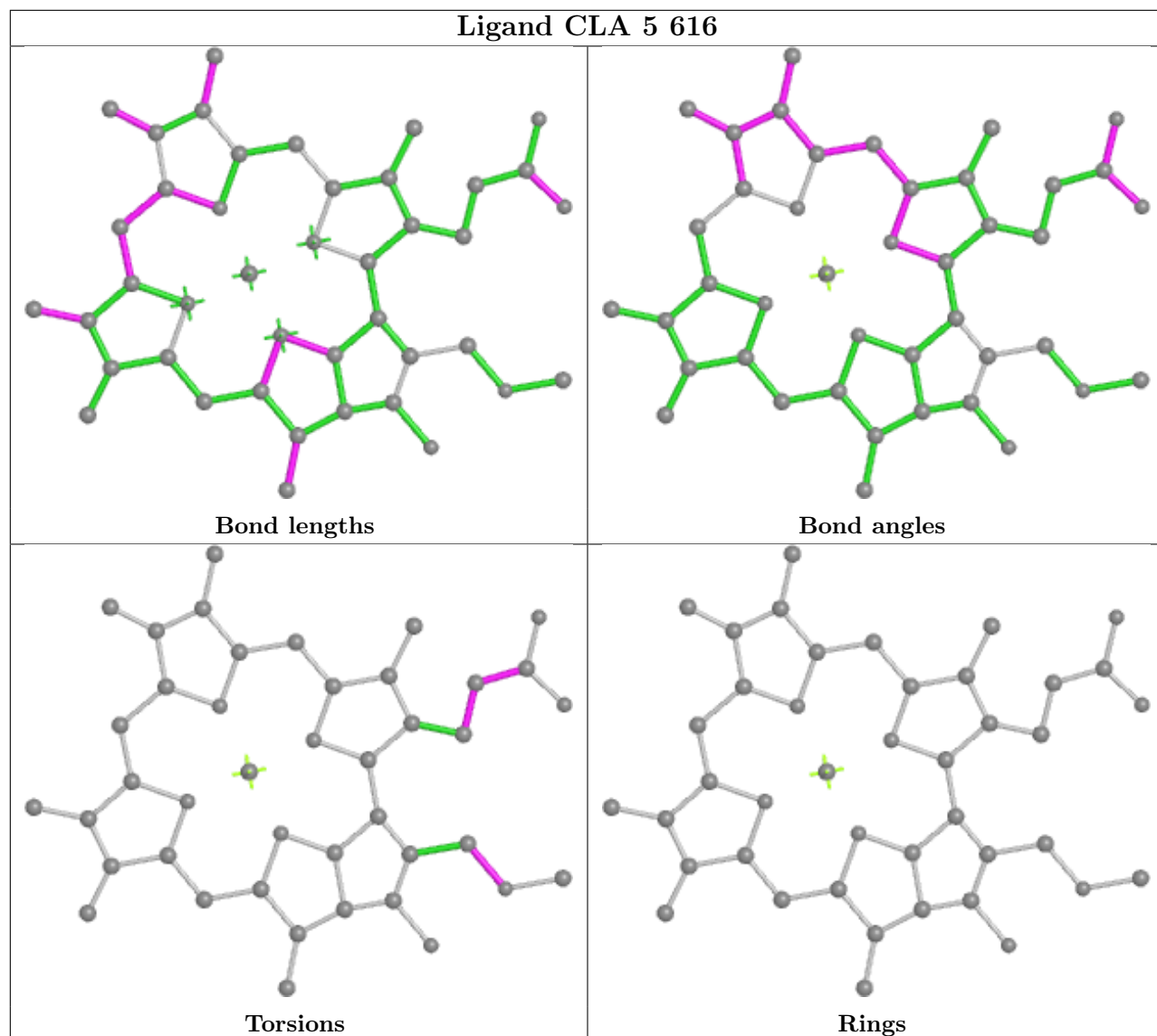
Ligand LUT W 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG 4 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

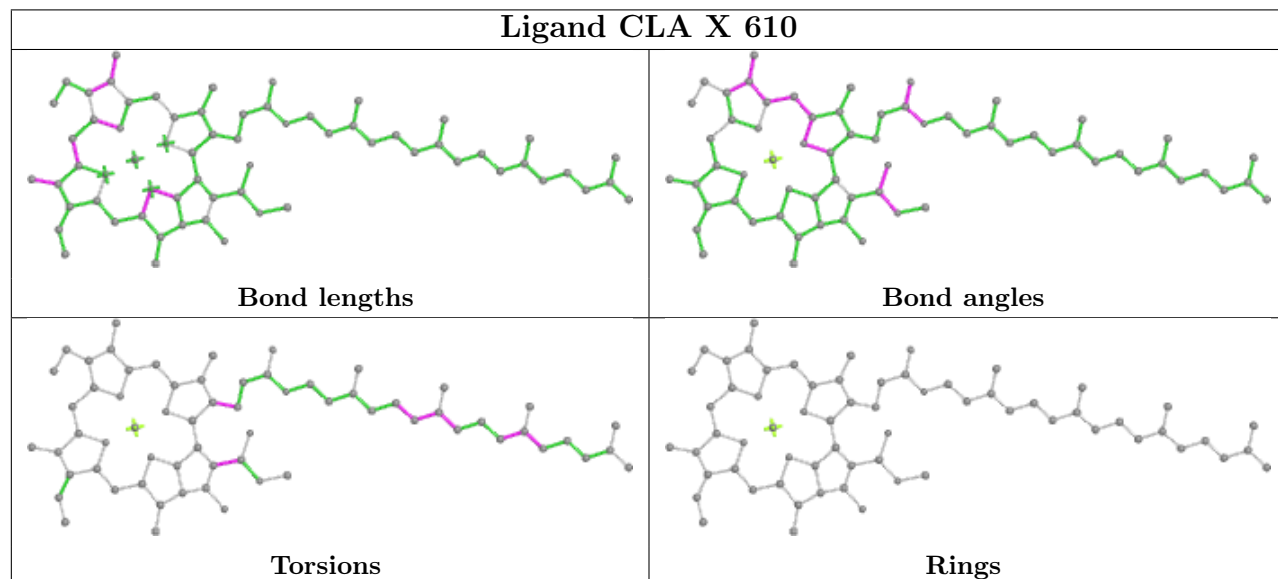
Ligand BCR L 301	
	
Bond lengths	Bond angles
	
Torsions	Rings



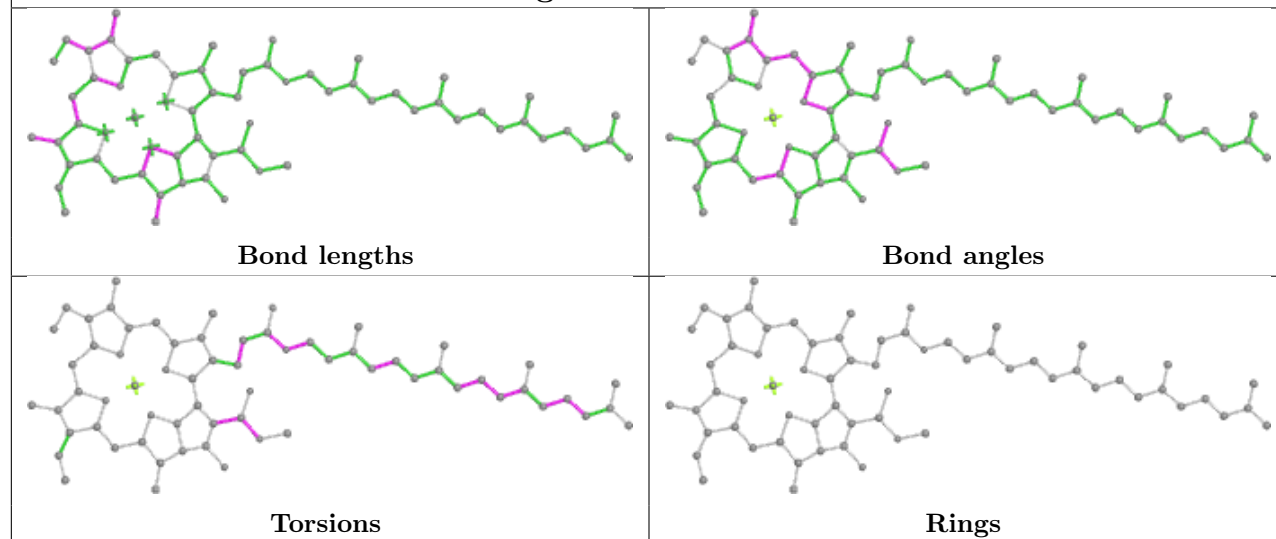
Ligand CLA 5 616



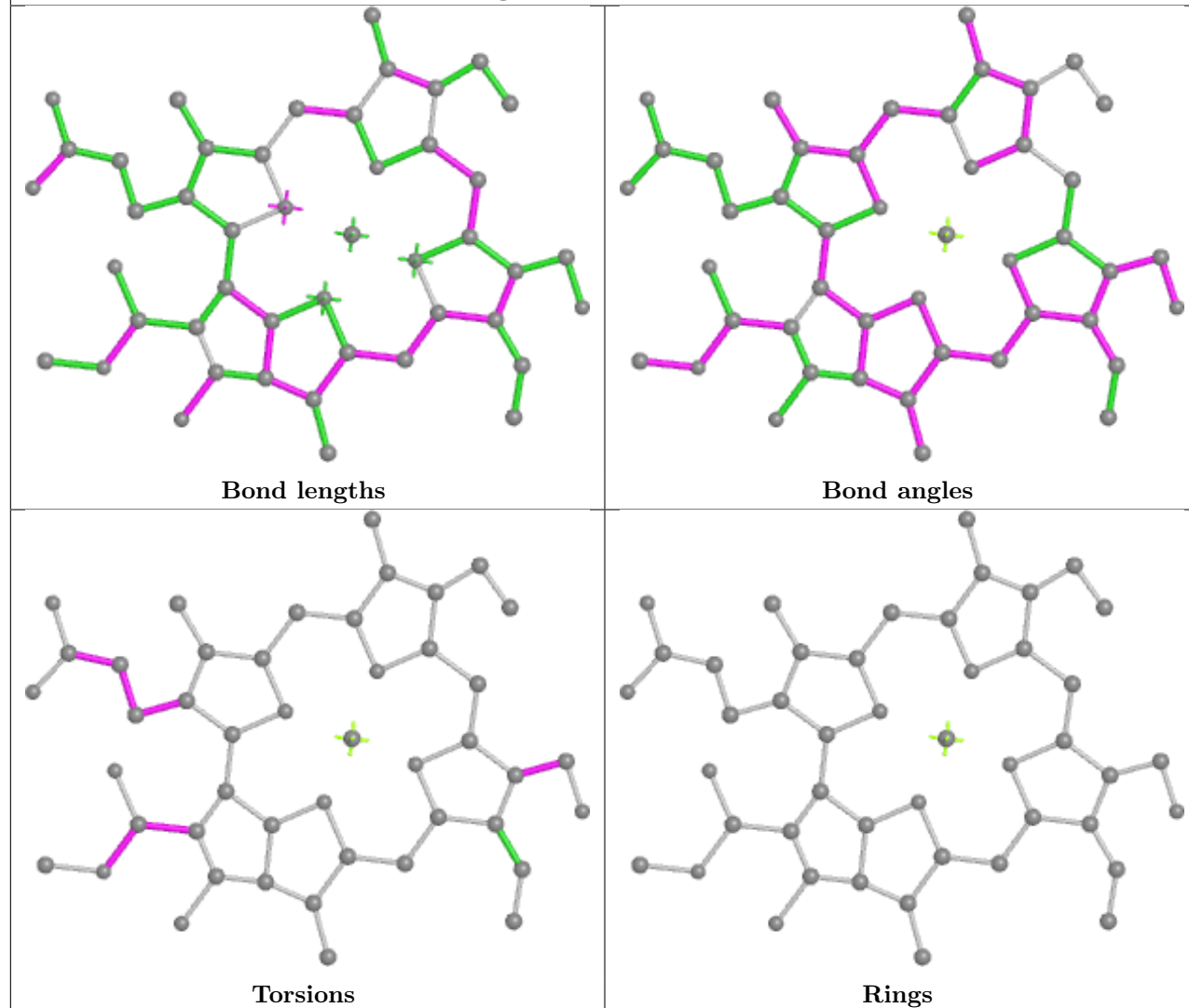
Ligand CLA X 610

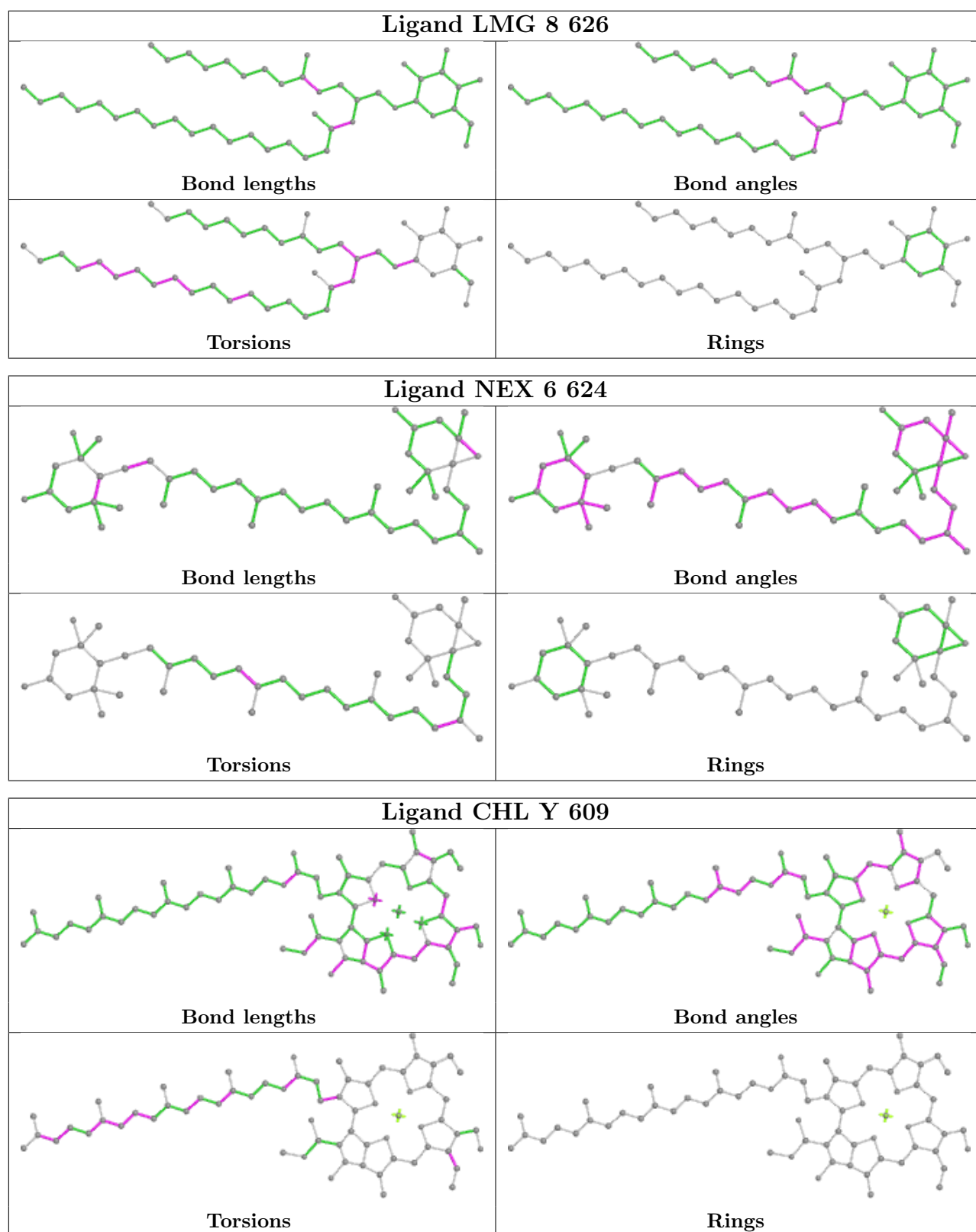


Ligand CLA 8 601

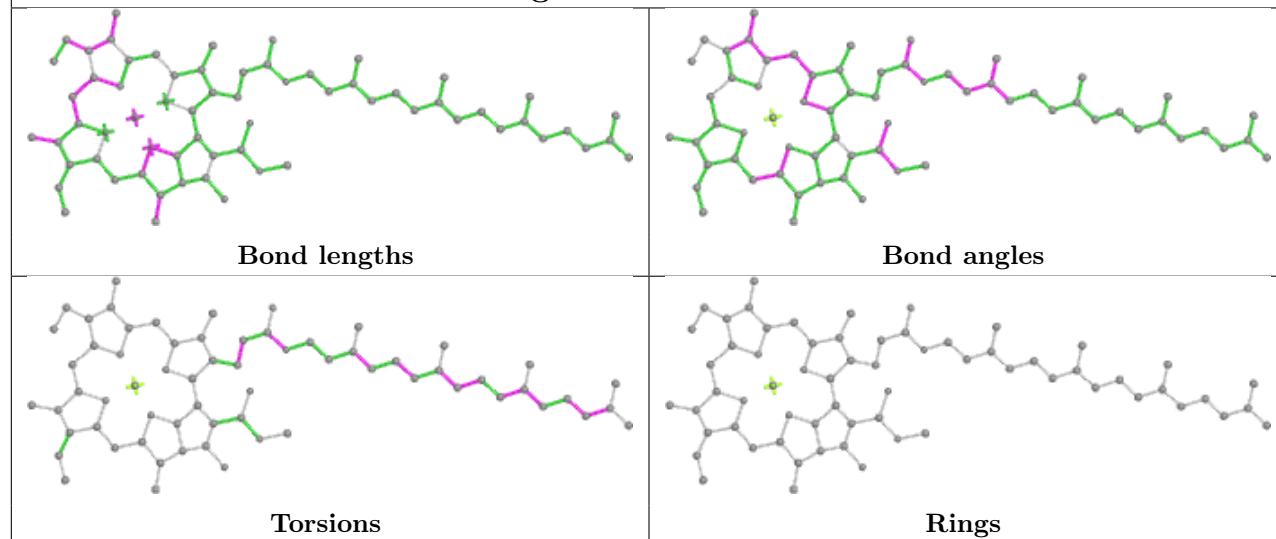


Ligand CHL V 607

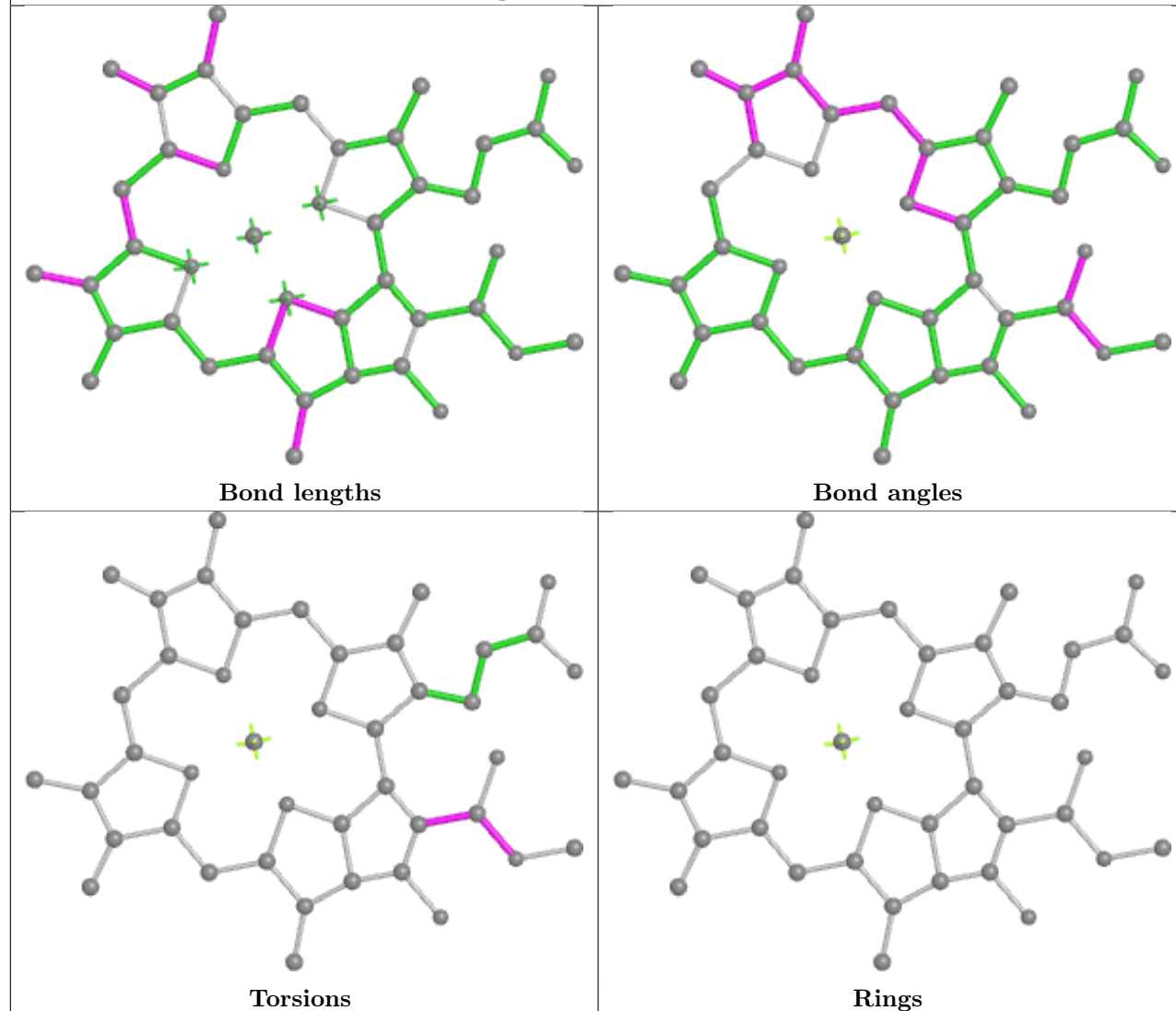




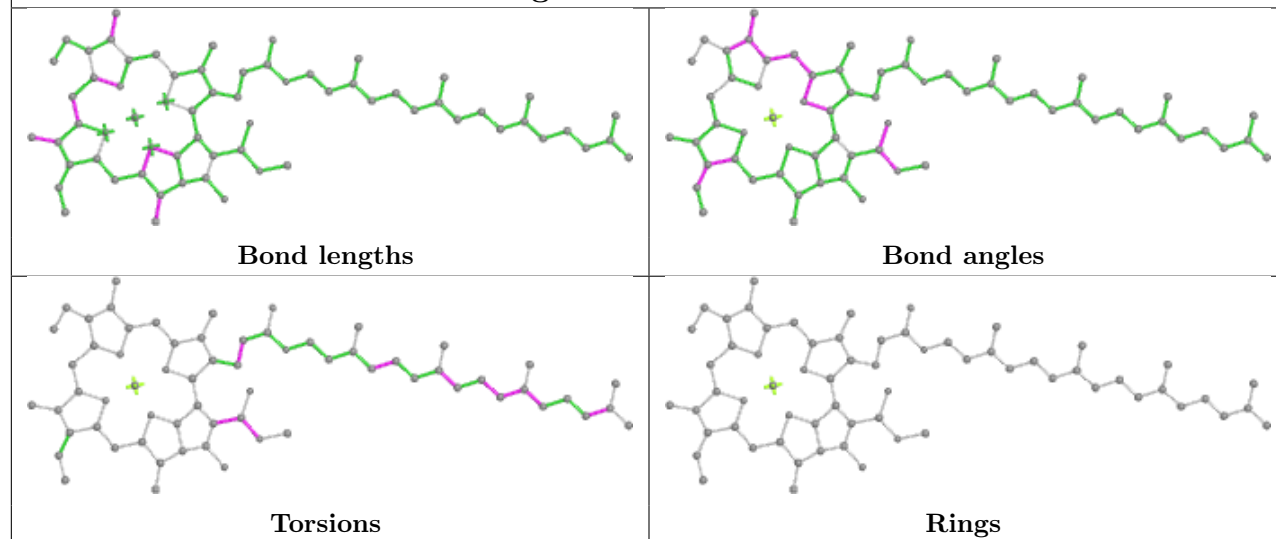
Ligand CLA A 842



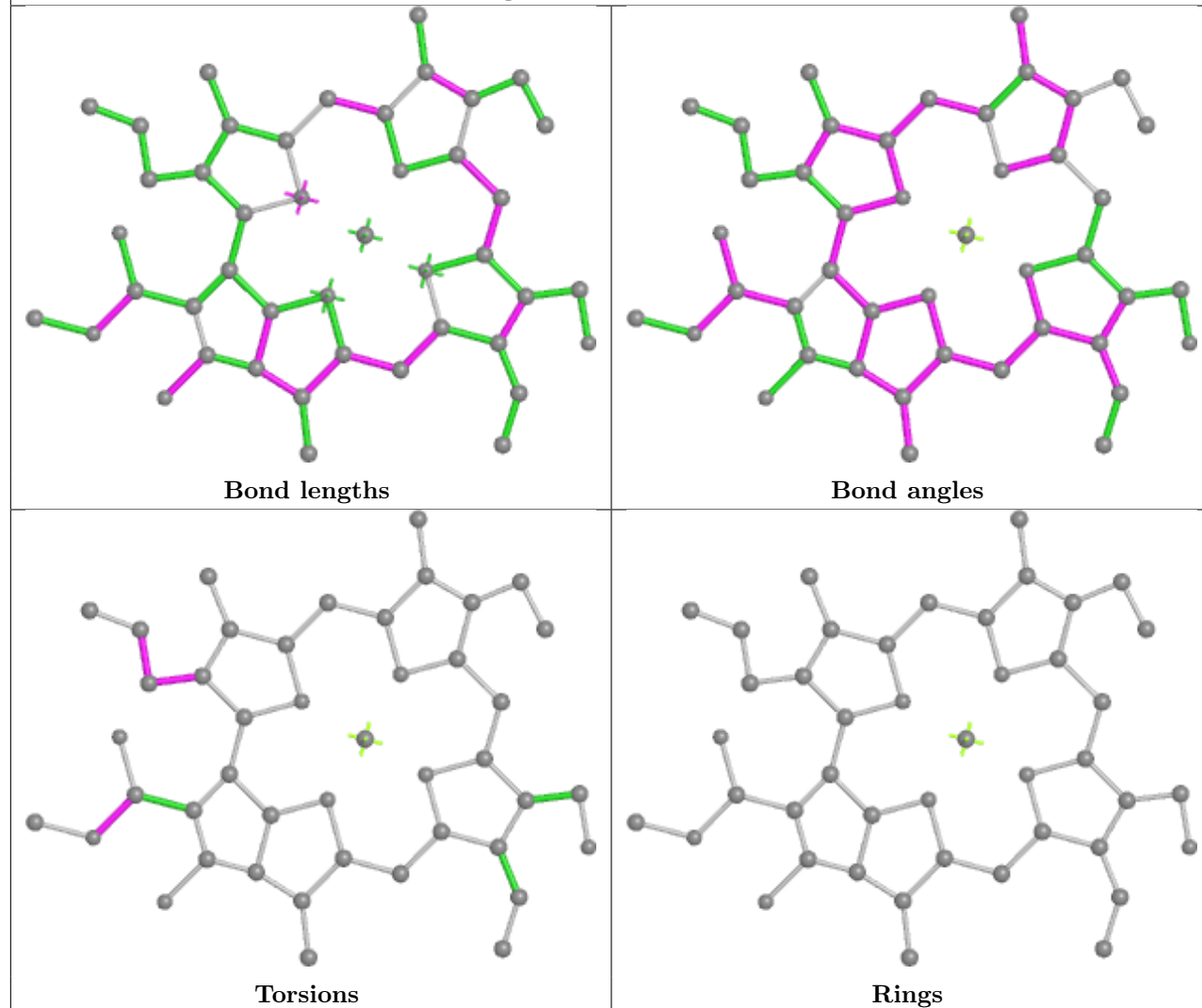
Ligand CLA 2 616

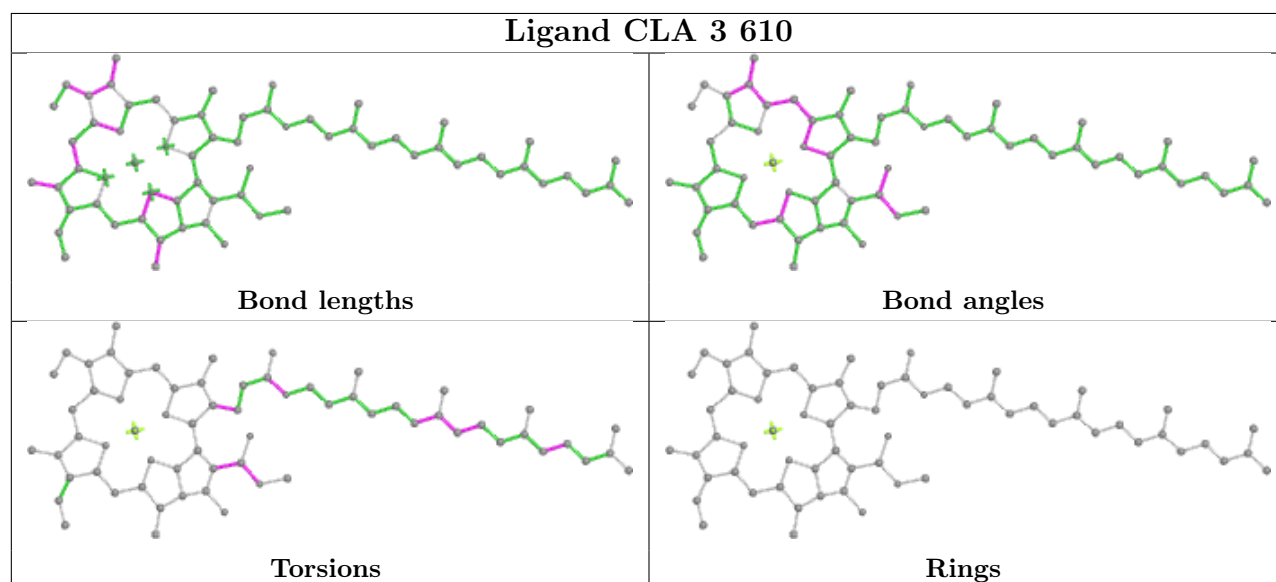
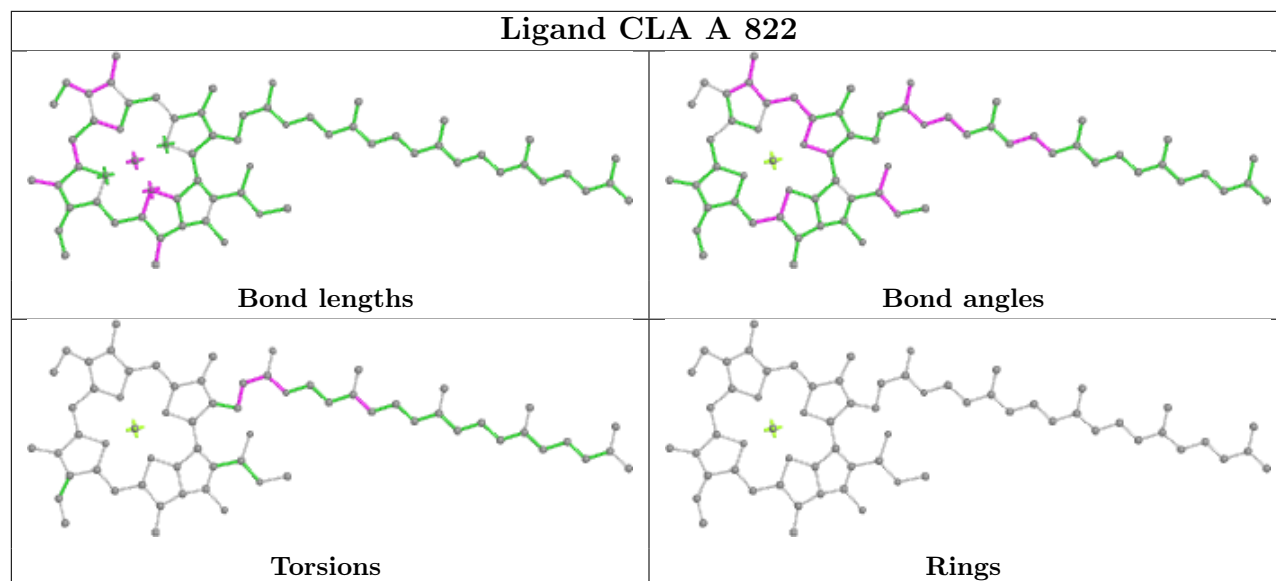
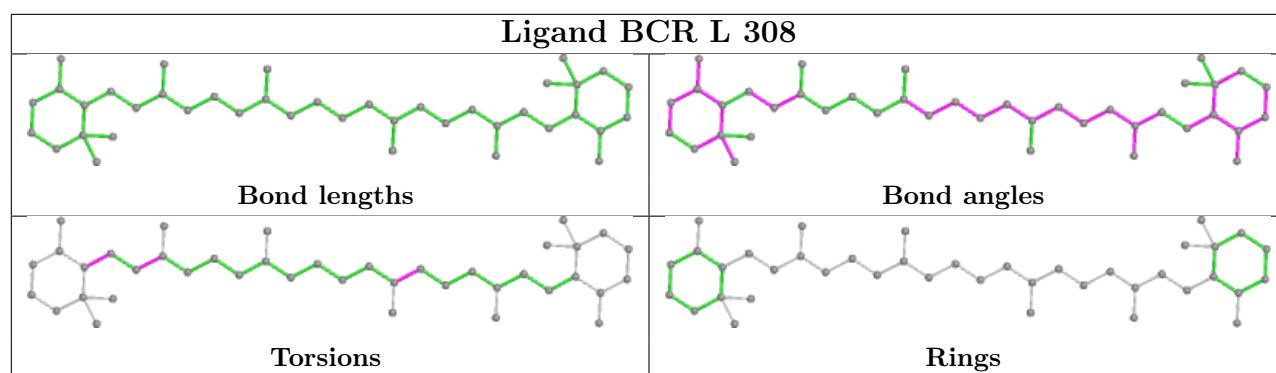


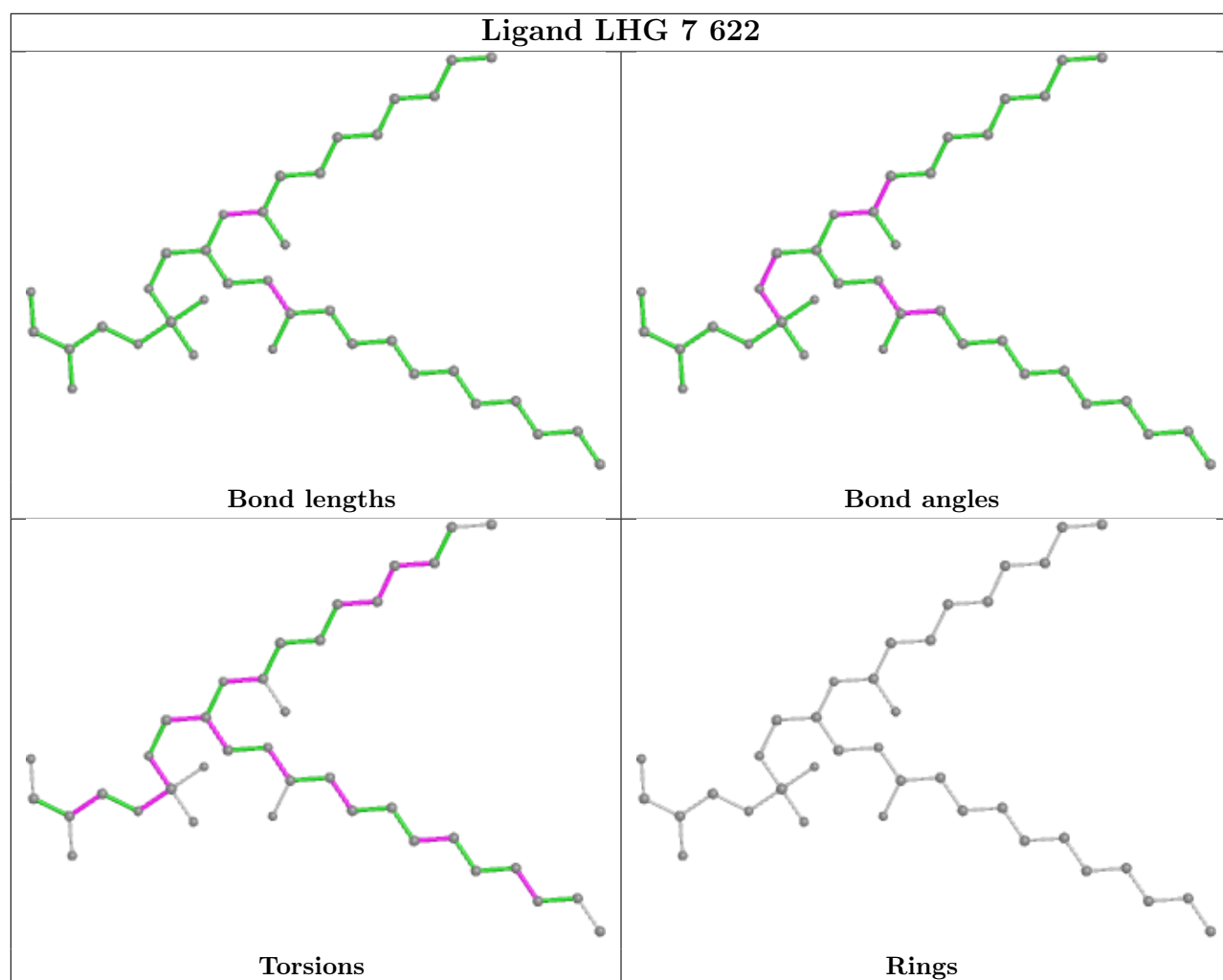
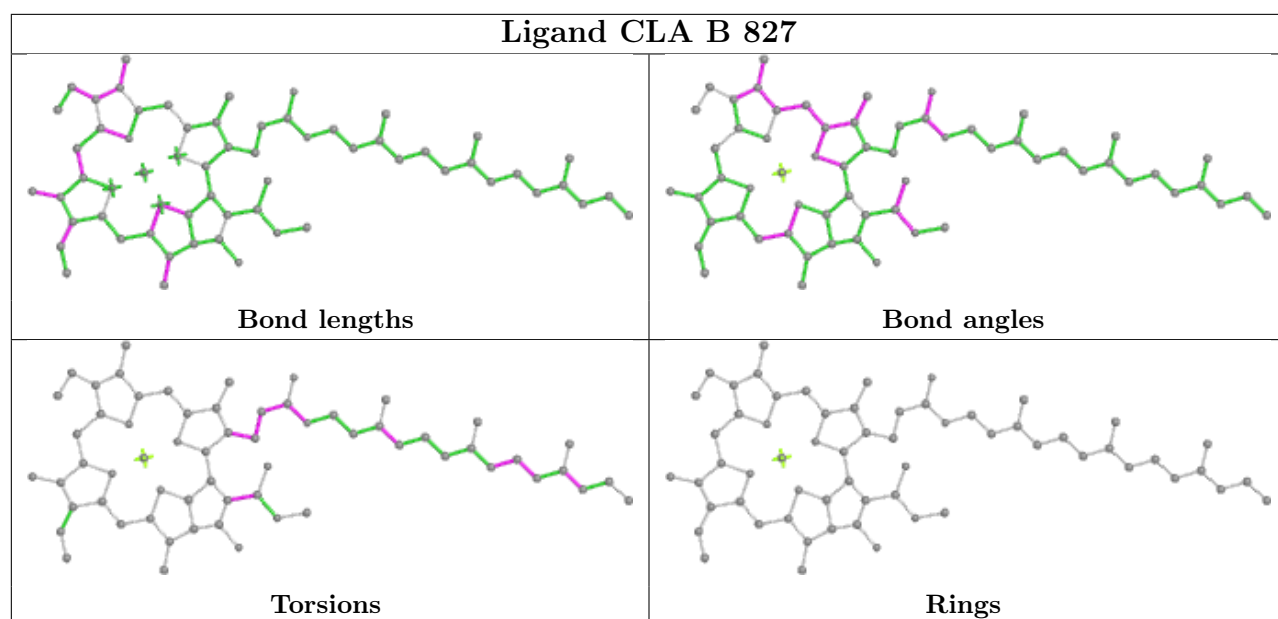
Ligand CLA Y 613



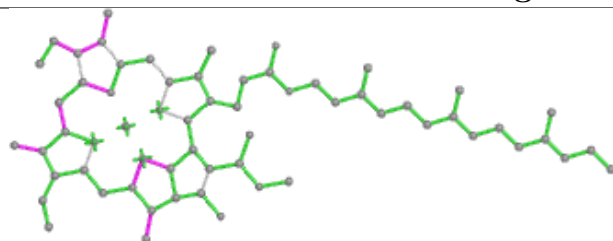
Ligand CHL U 608



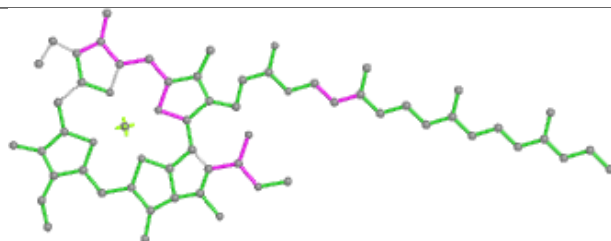




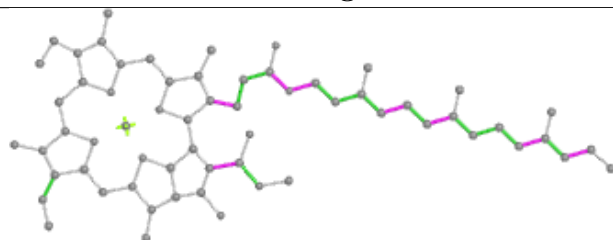
Ligand CLA B 826



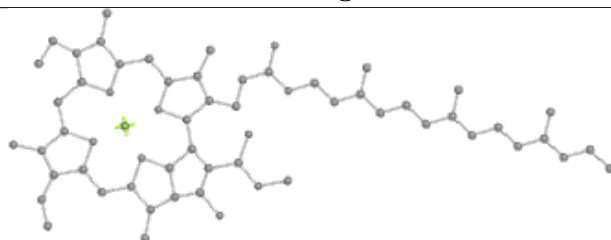
Bond lengths



Bond angles

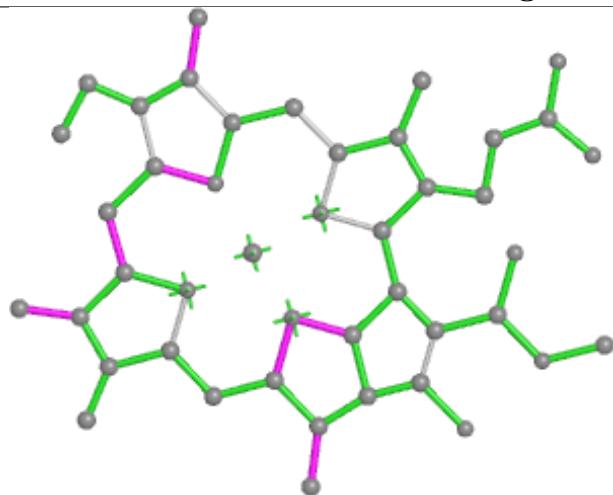


Torsions

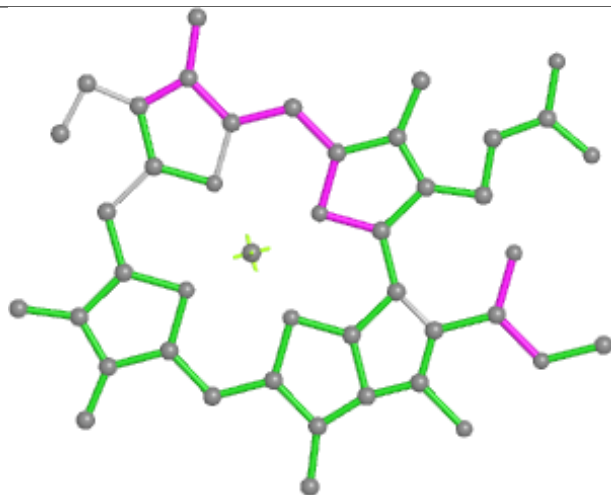


Rings

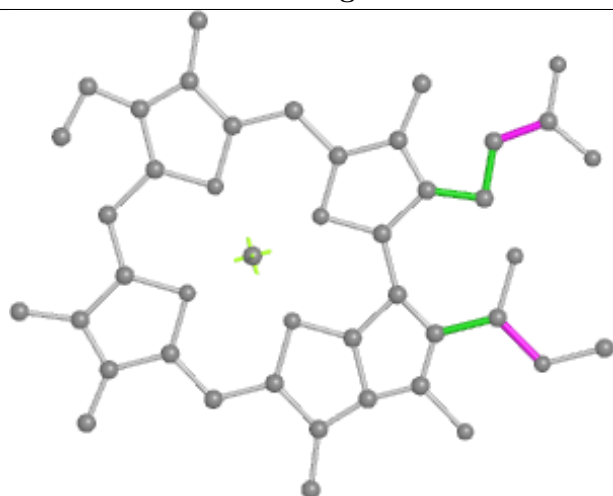
Ligand CLA 7 612



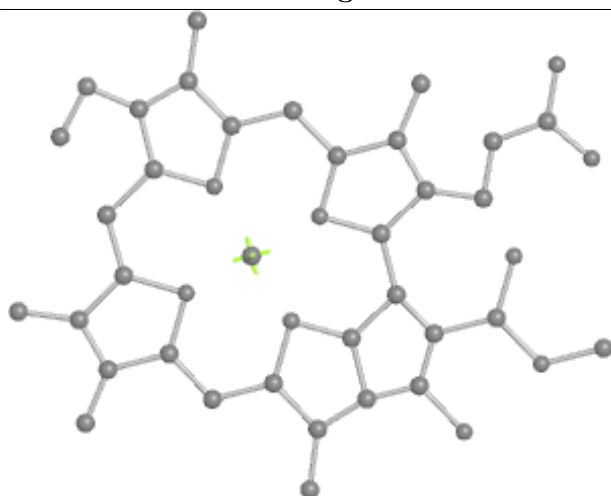
Bond lengths



Bond angles

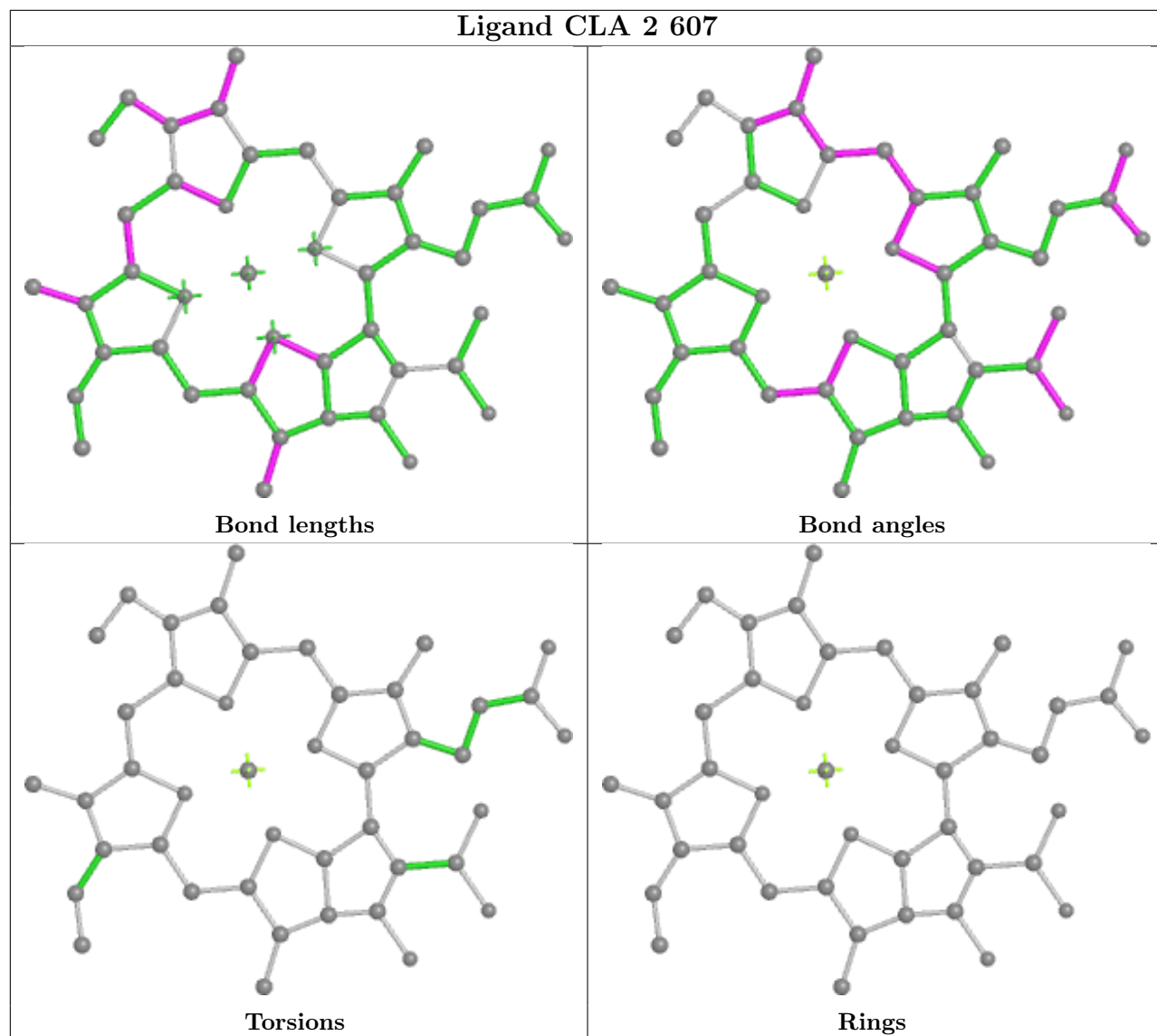


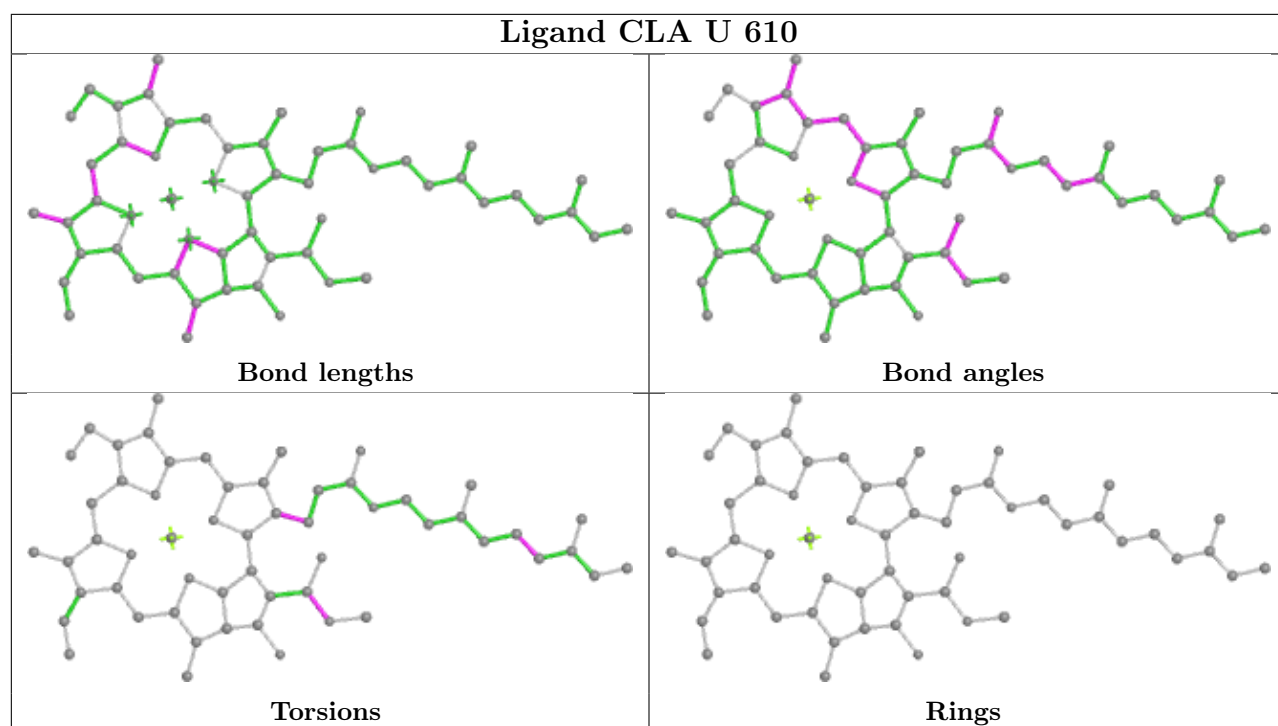
Torsions

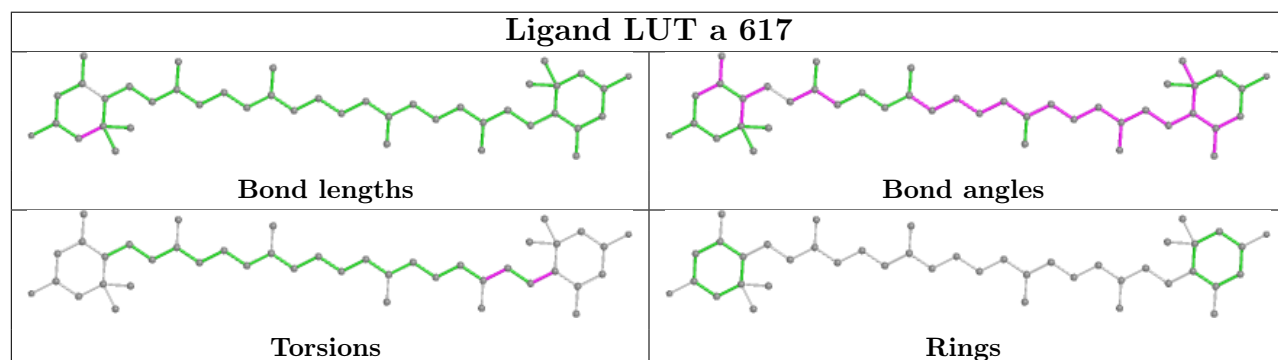
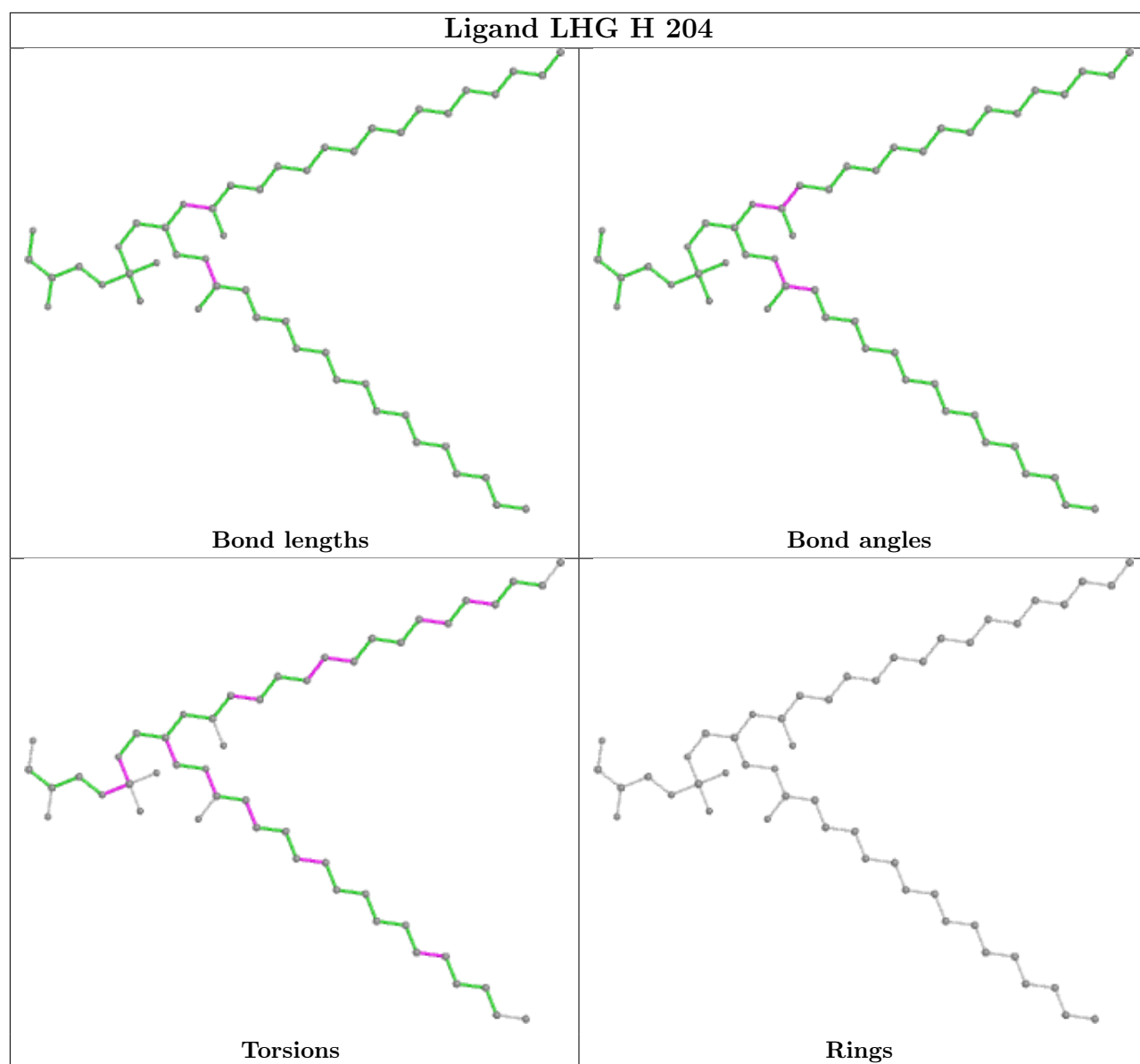


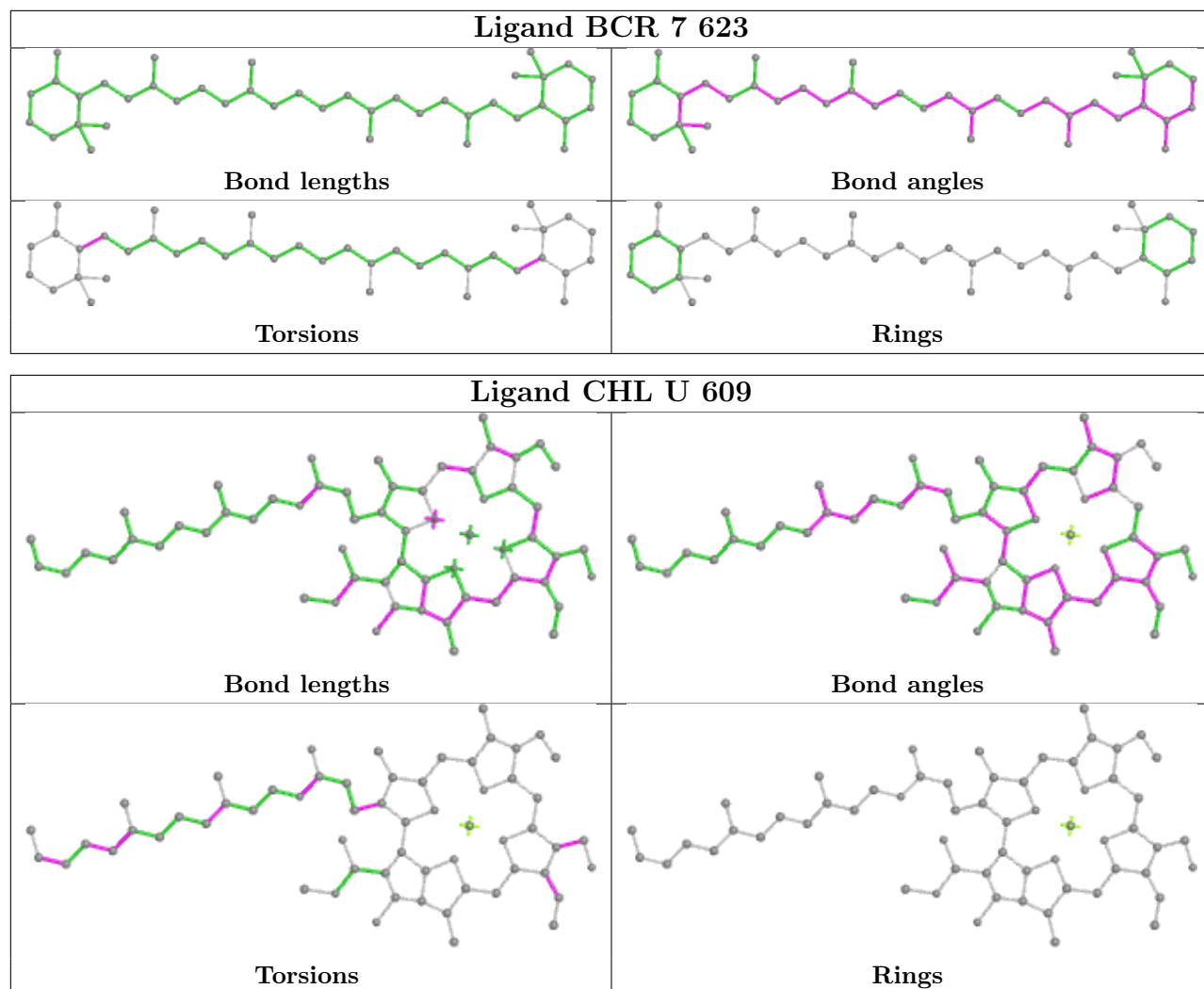
Rings

Ligand CLA 2 607

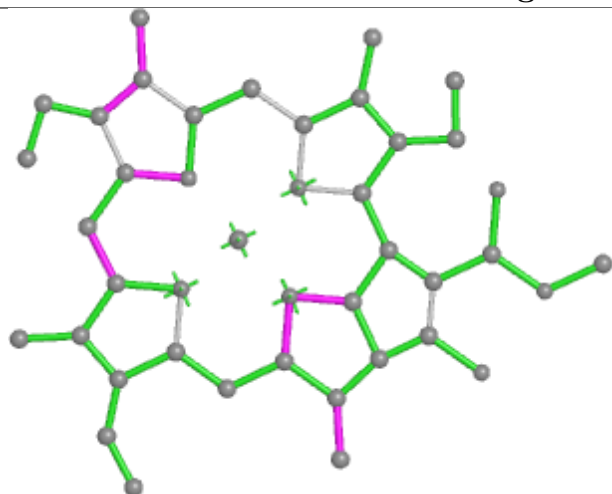




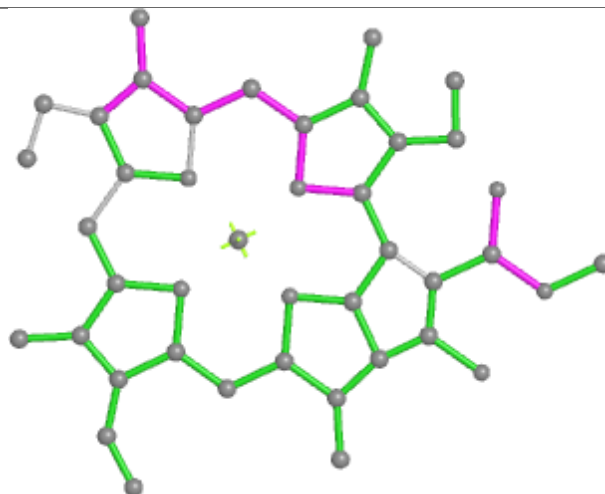




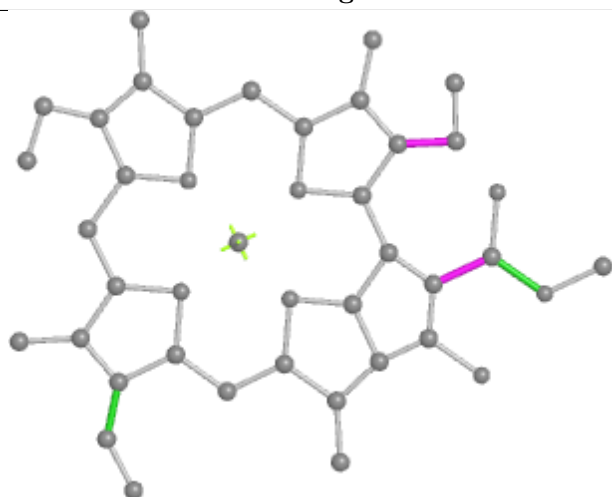
Ligand CLA 9 611



Bond lengths



Bond angles

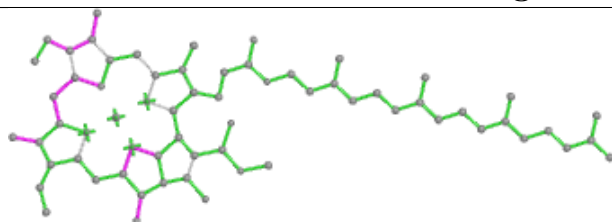


Torsions

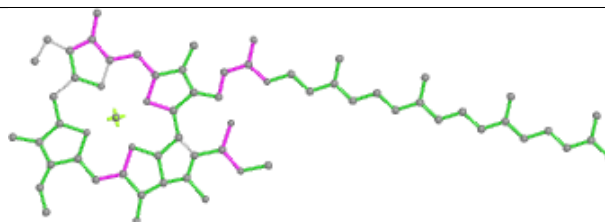


Rings

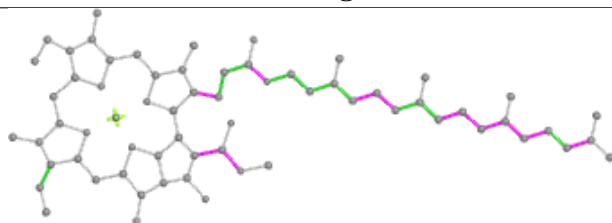
Ligand CLA A 831



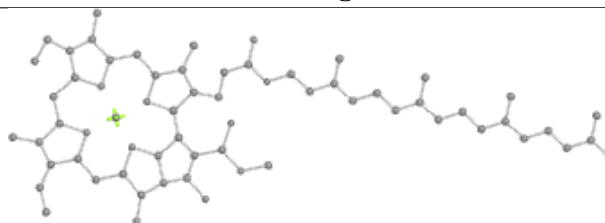
Bond lengths



Bond angles

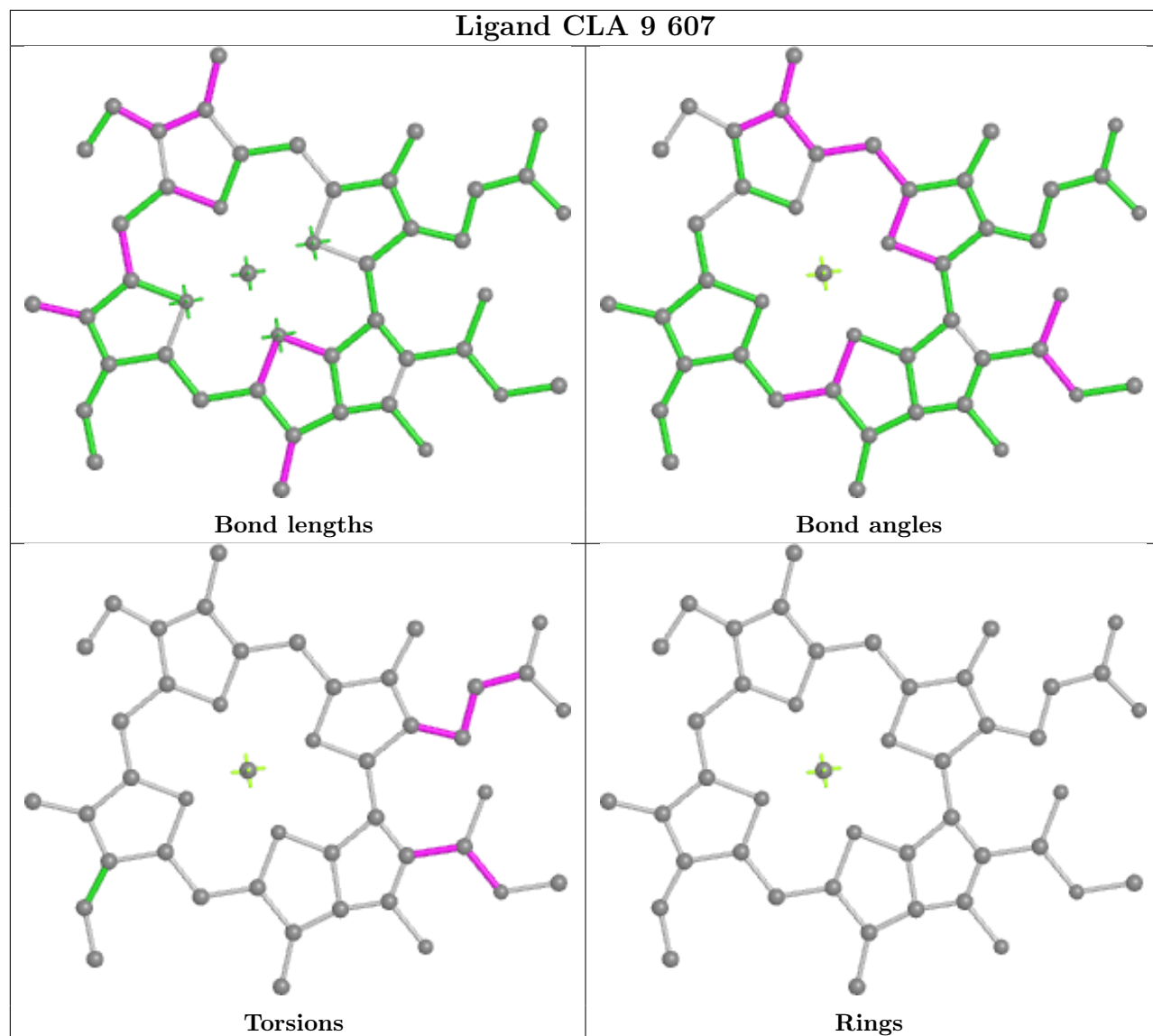


Torsions

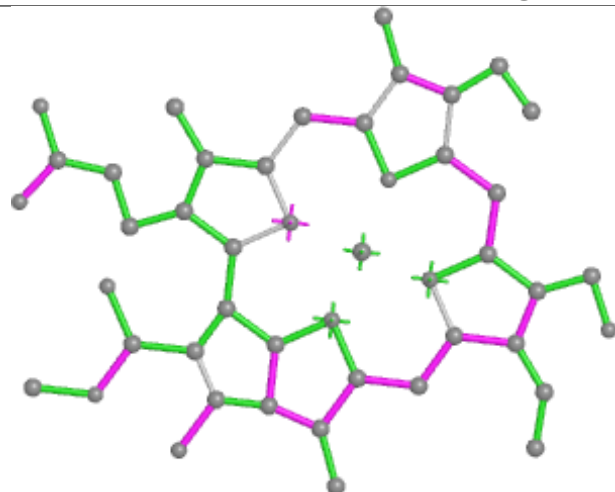


Rings

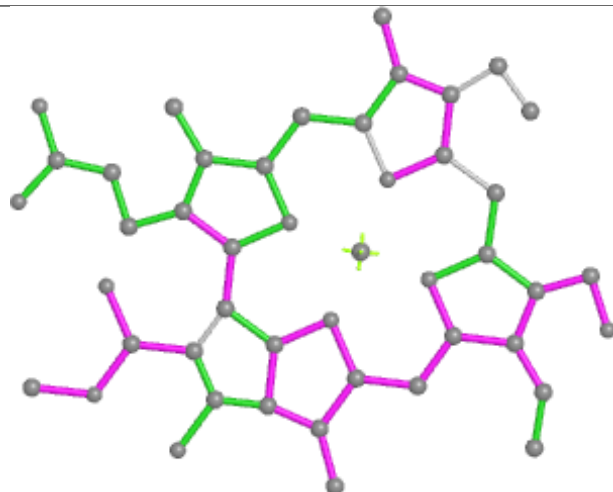
Ligand CLA 9 607



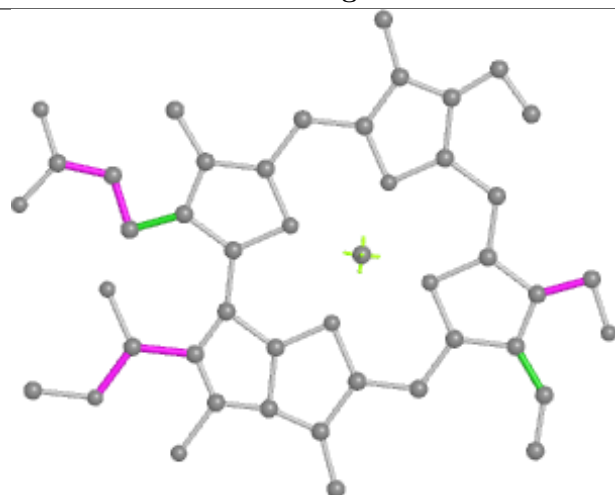
Ligand CHL Y 606



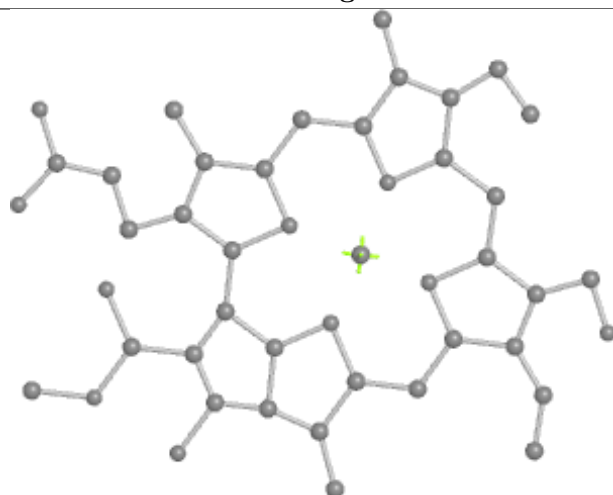
Bond lengths



Bond angles

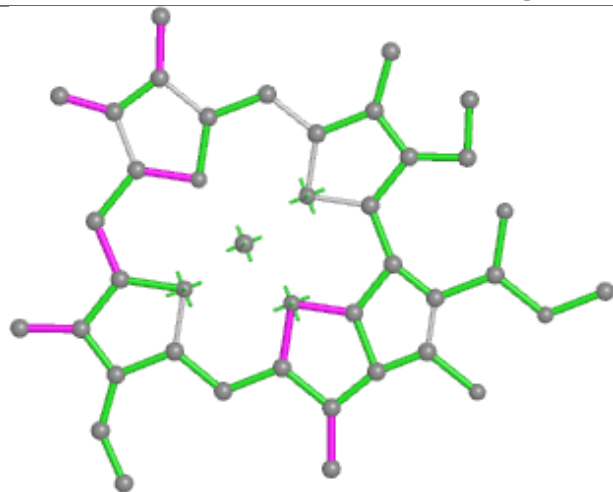


Torsions

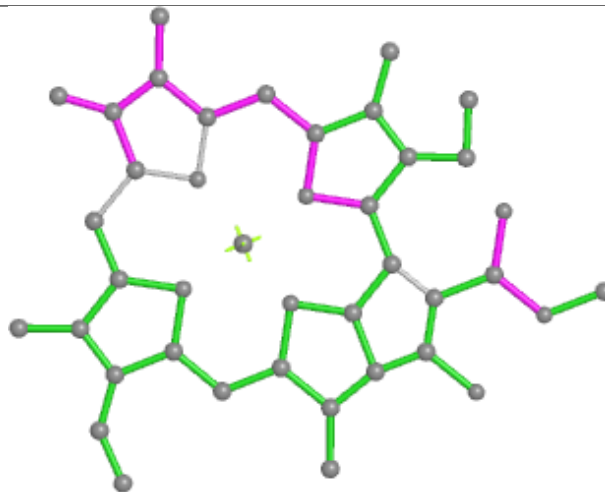


Rings

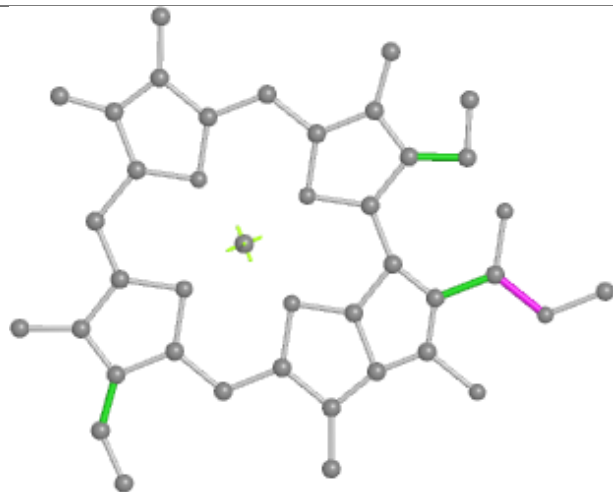
Ligand CLA 8 607



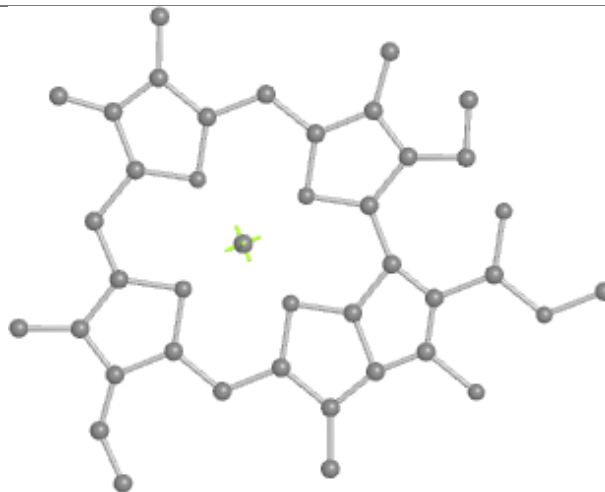
Bond lengths



Bond angles

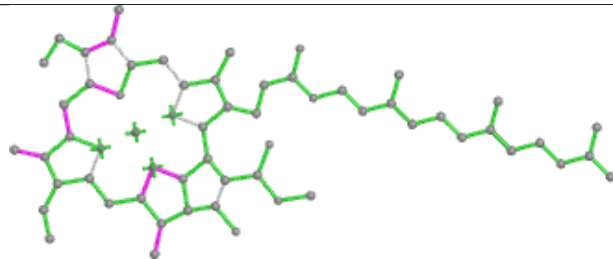


Torsions

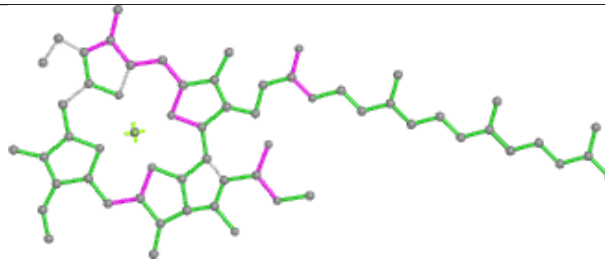


Rings

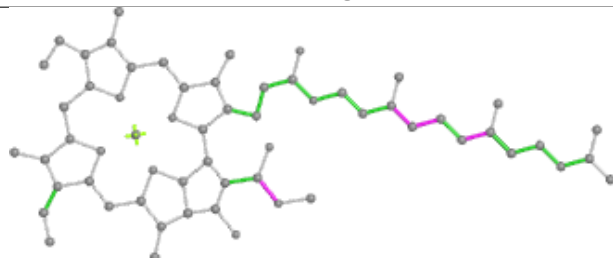
Ligand CLA 4 602



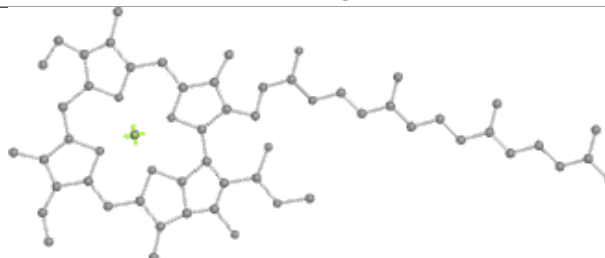
Bond lengths



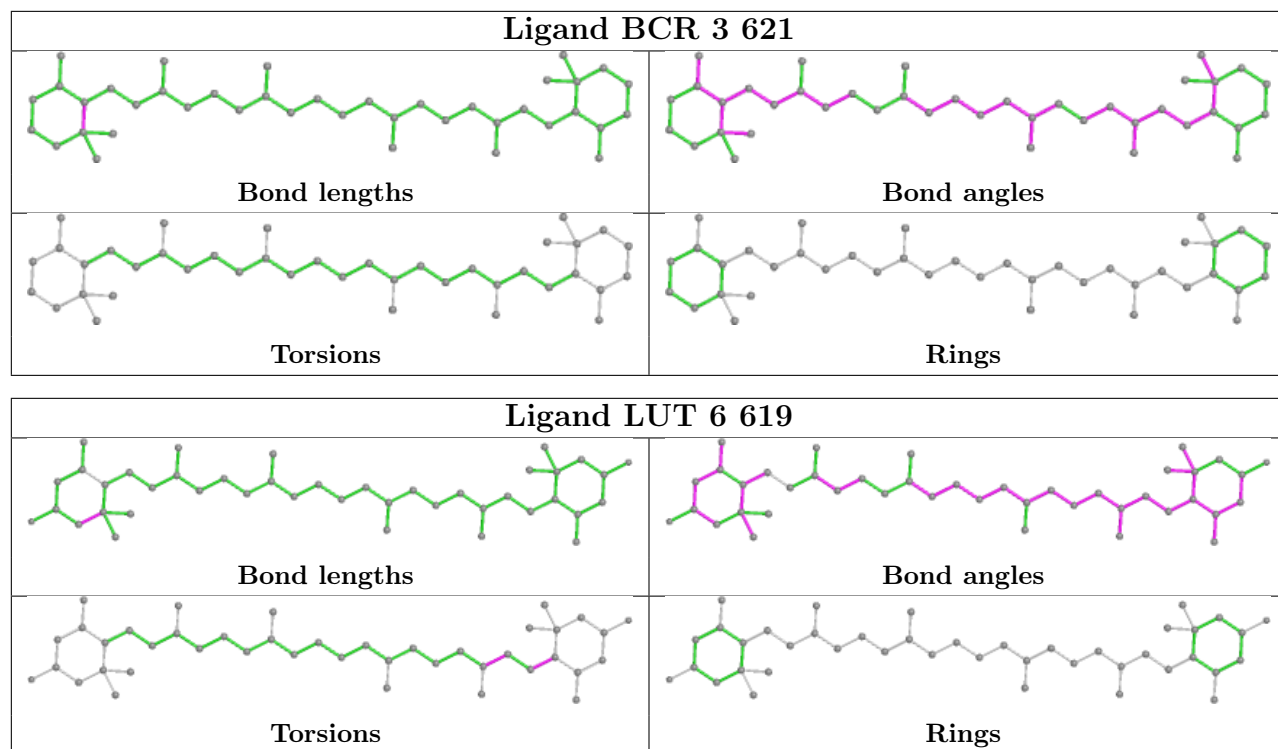
Bond angles



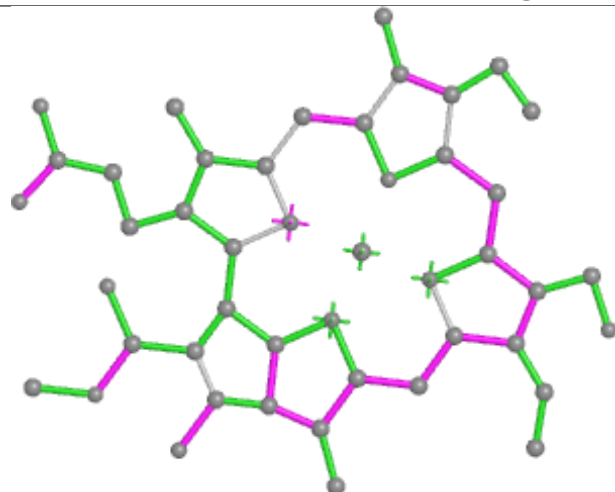
Torsions



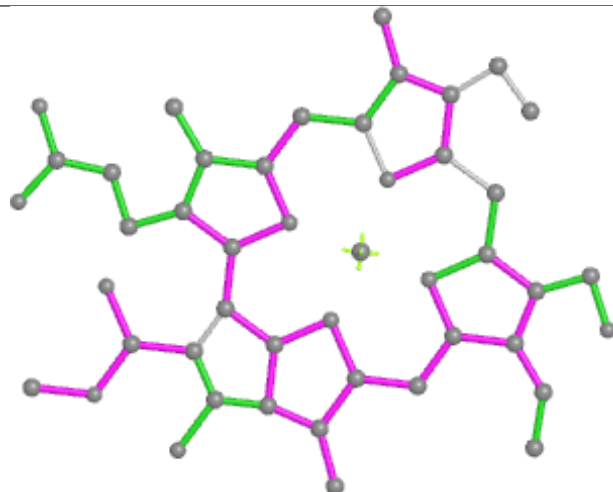
Rings



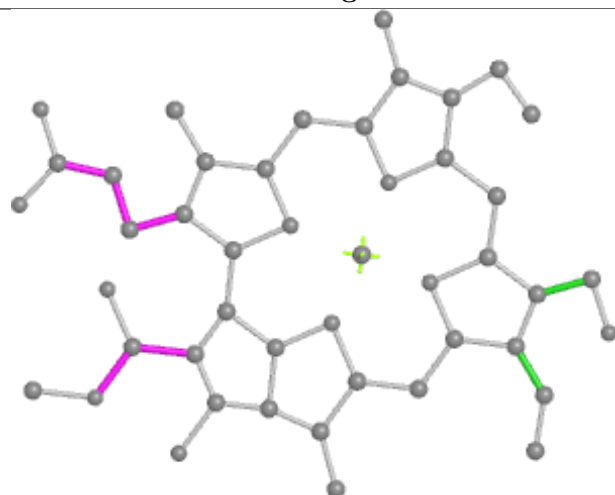
Ligand CHL Z 606



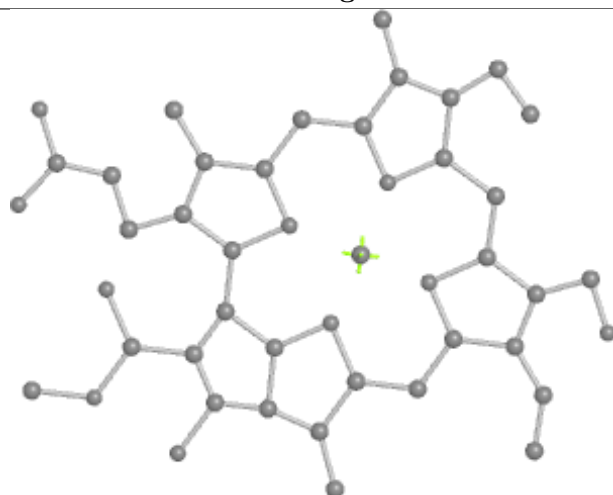
Bond lengths



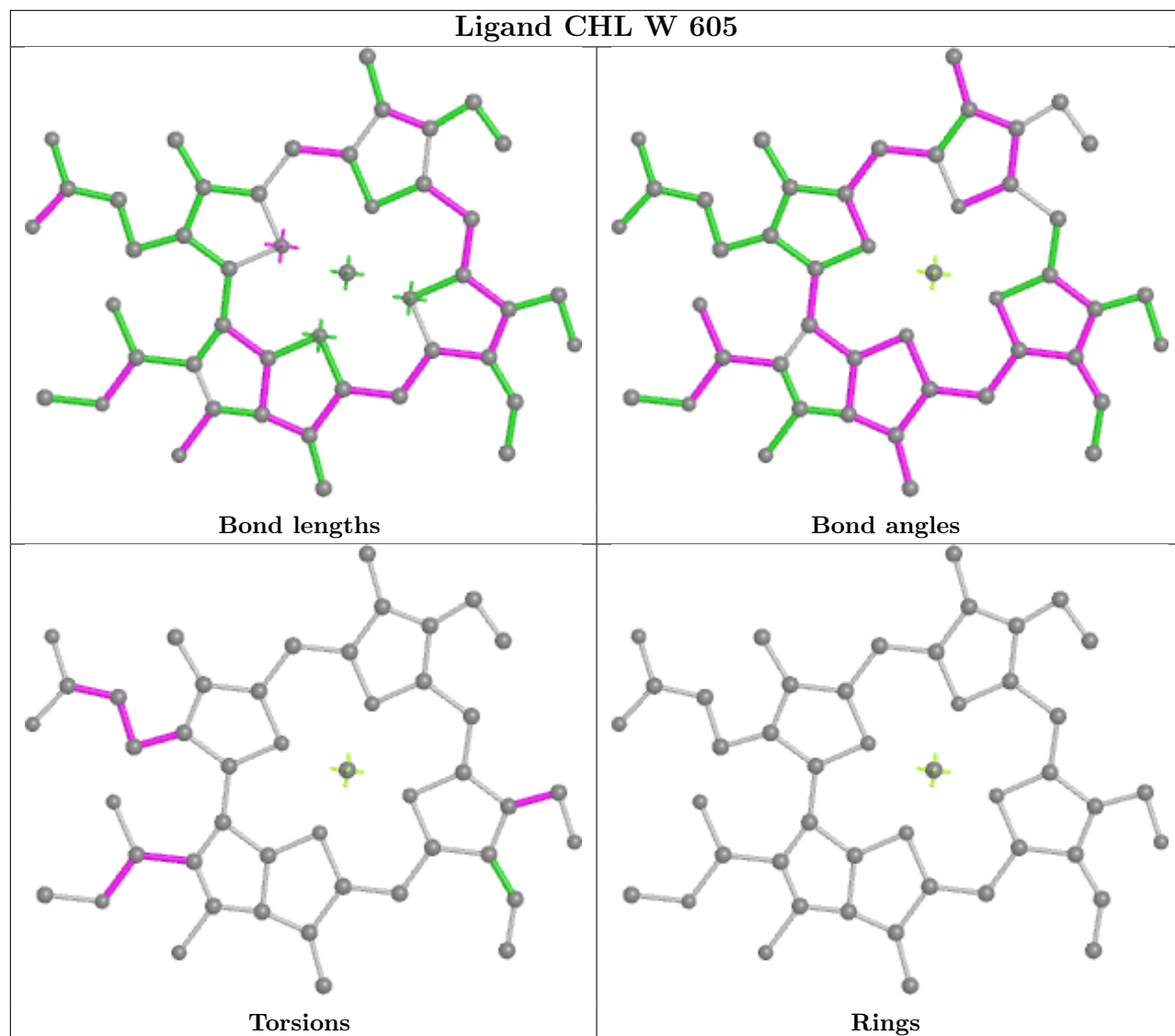
Bond angles

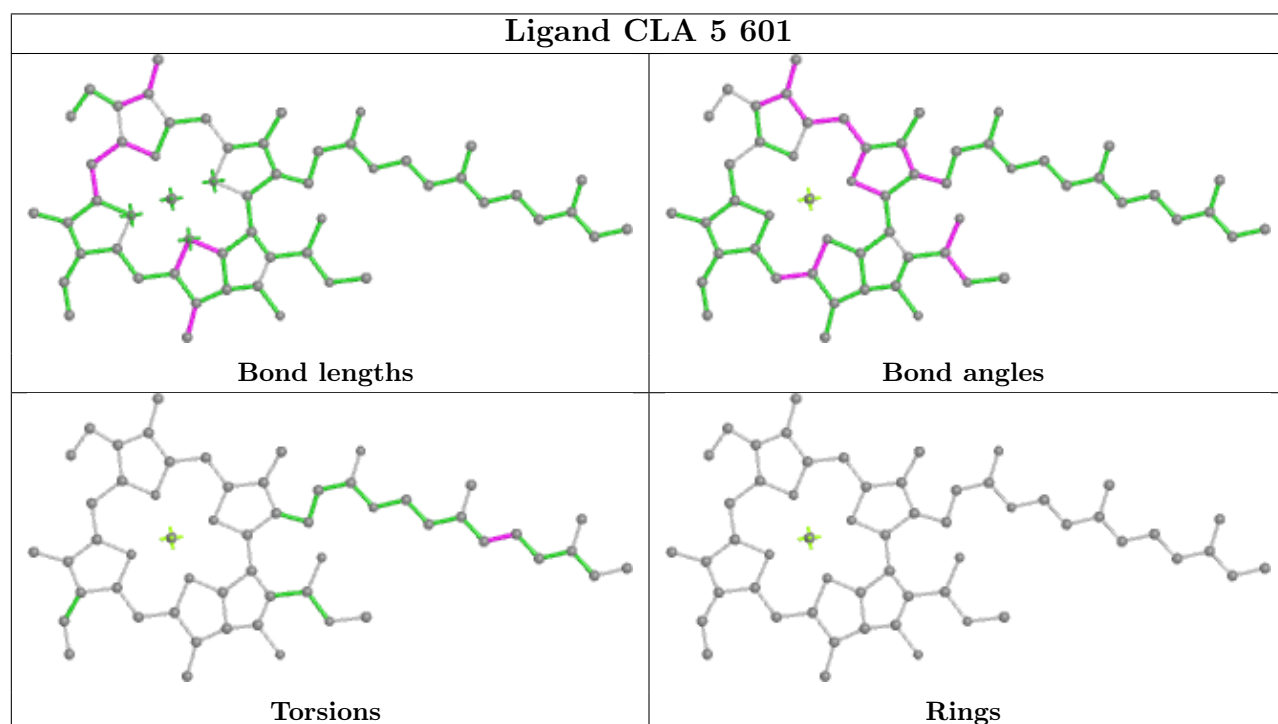
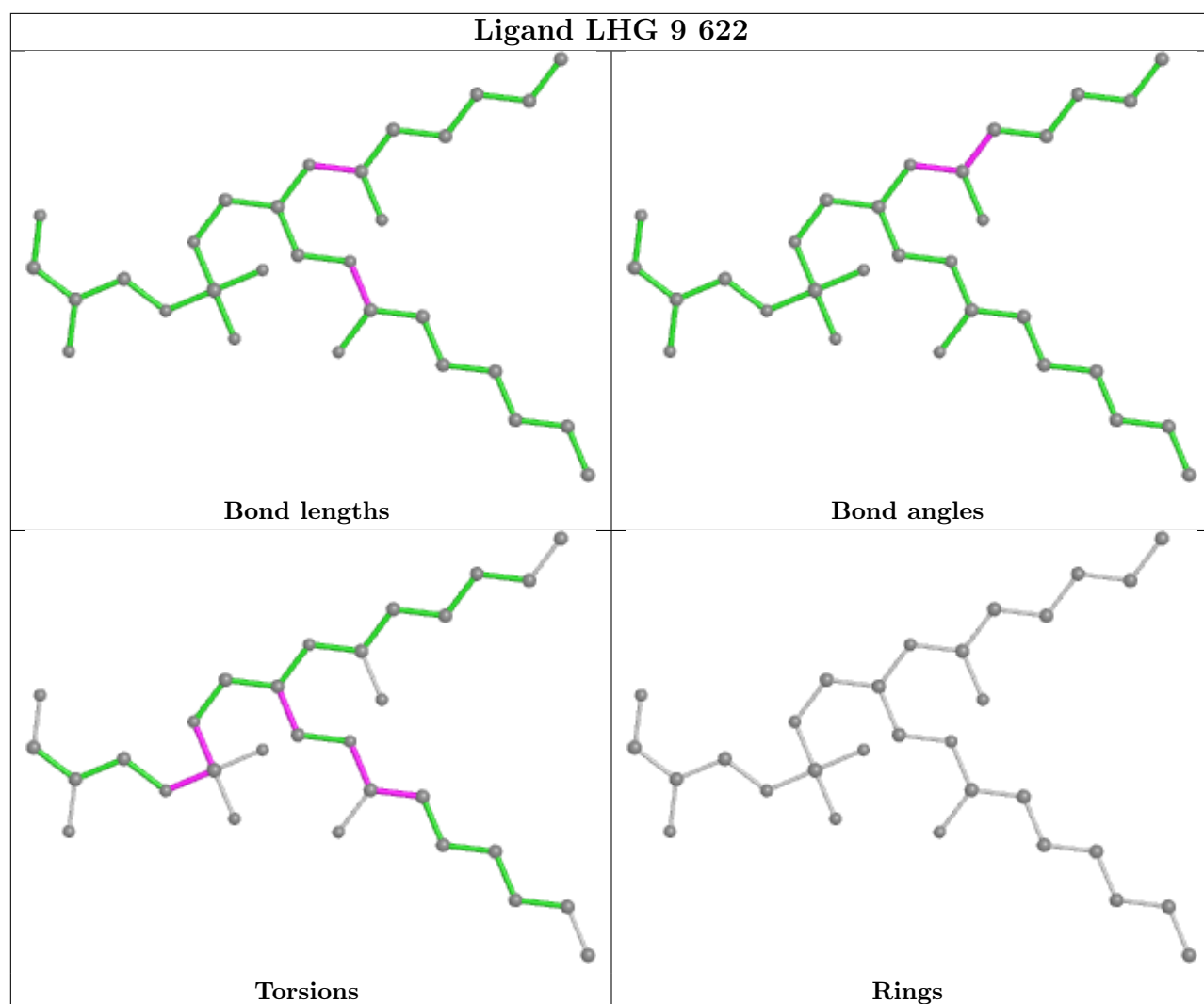


Torsions

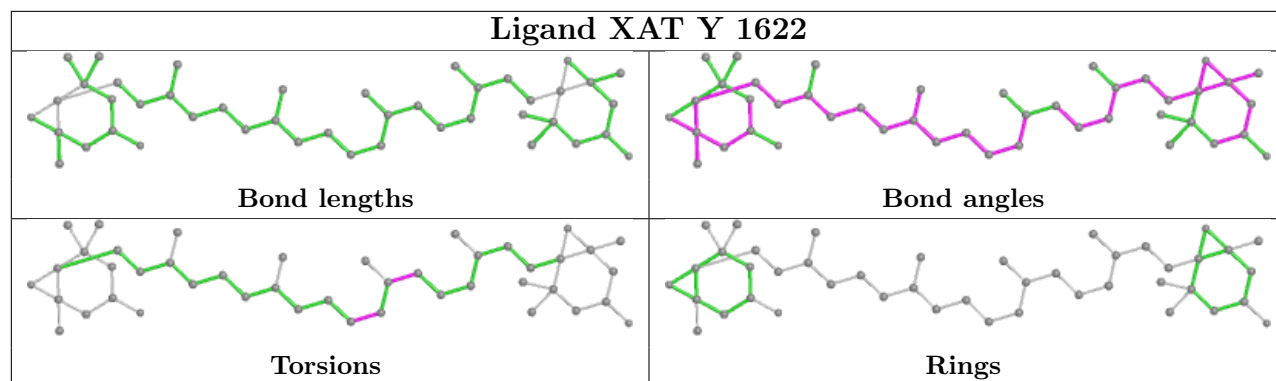


Rings

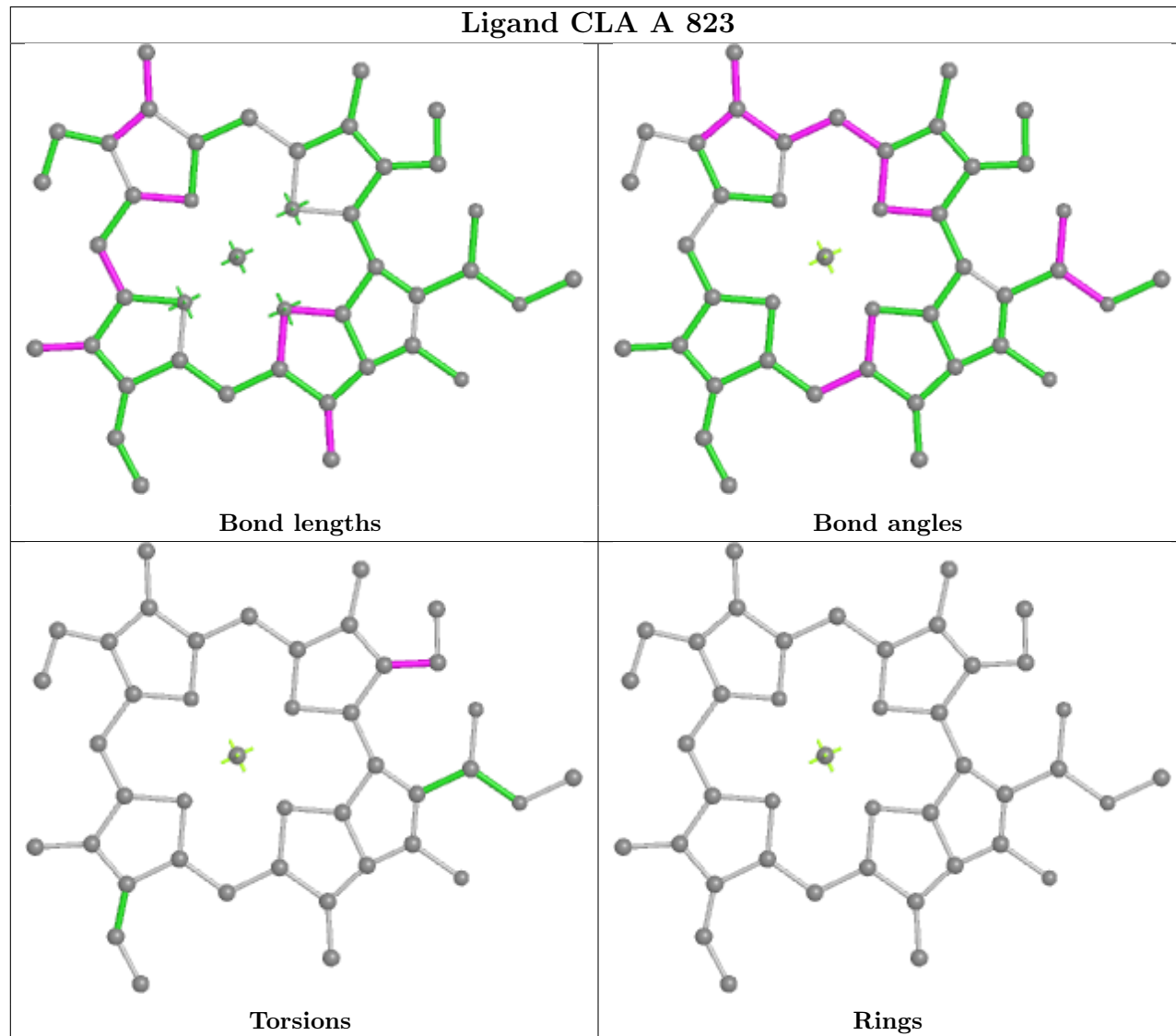




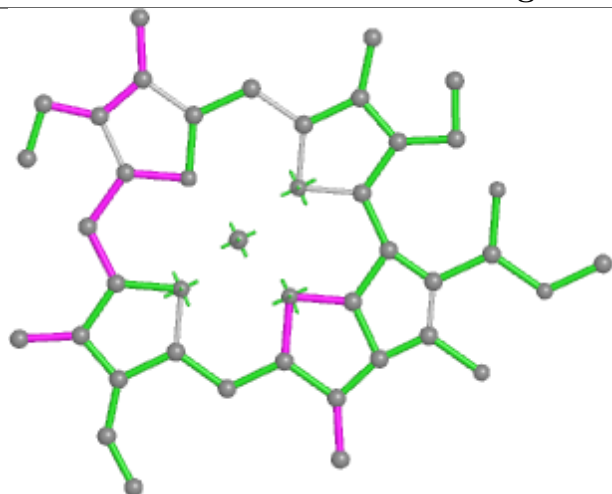
Ligand XAT Y 1622



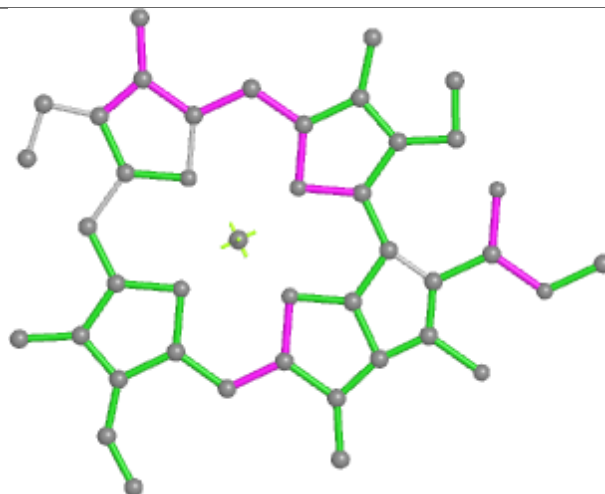
Ligand CLA A 823



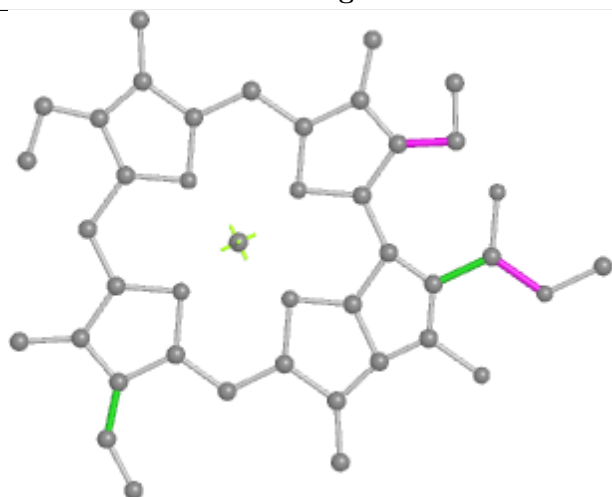
Ligand CLA 8 611



Bond lengths



Bond angles

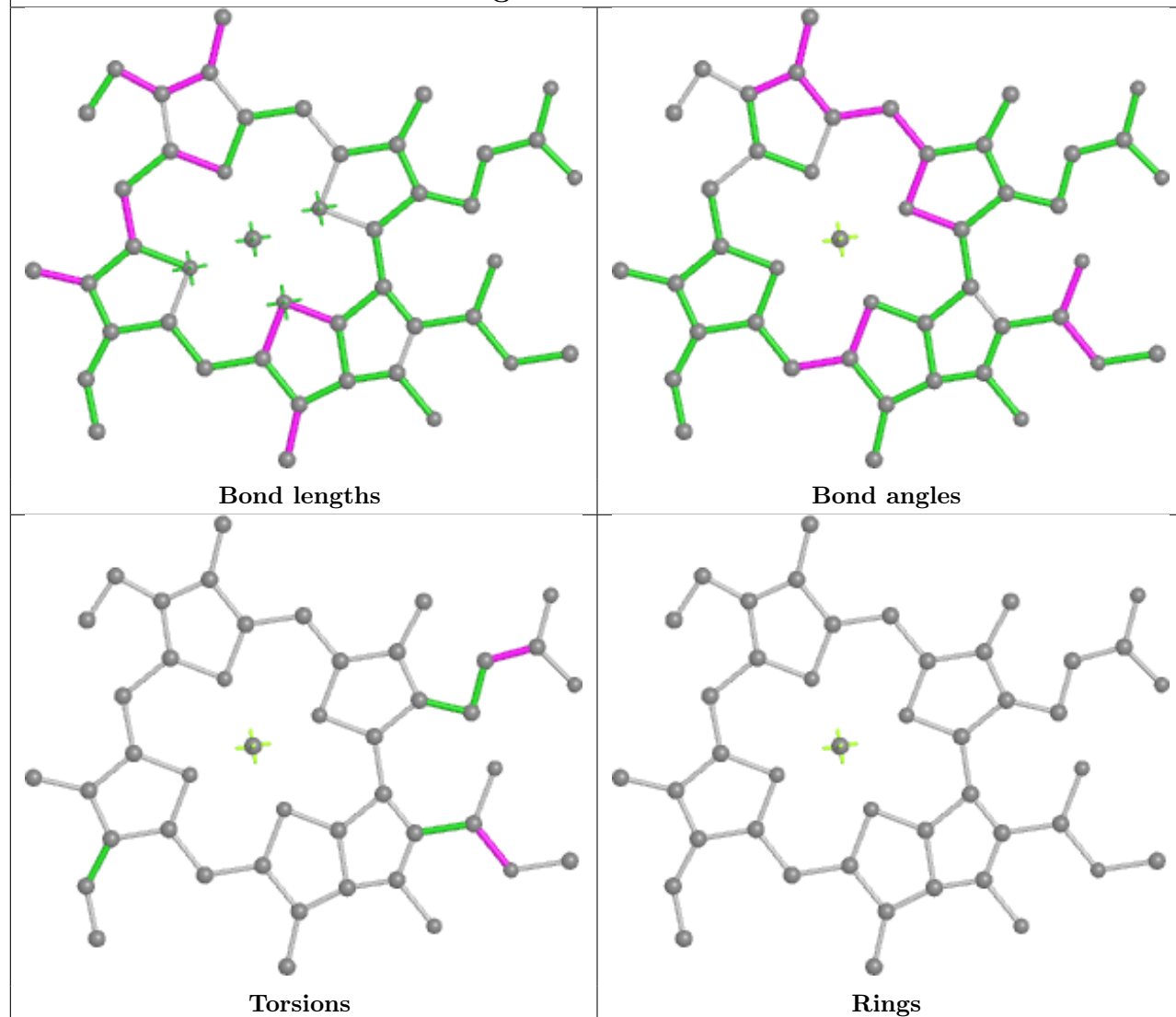


Torsions

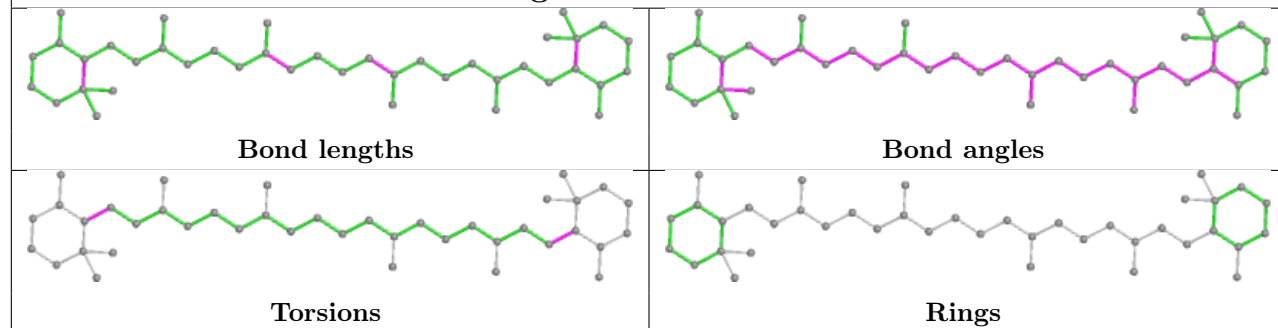


Rings

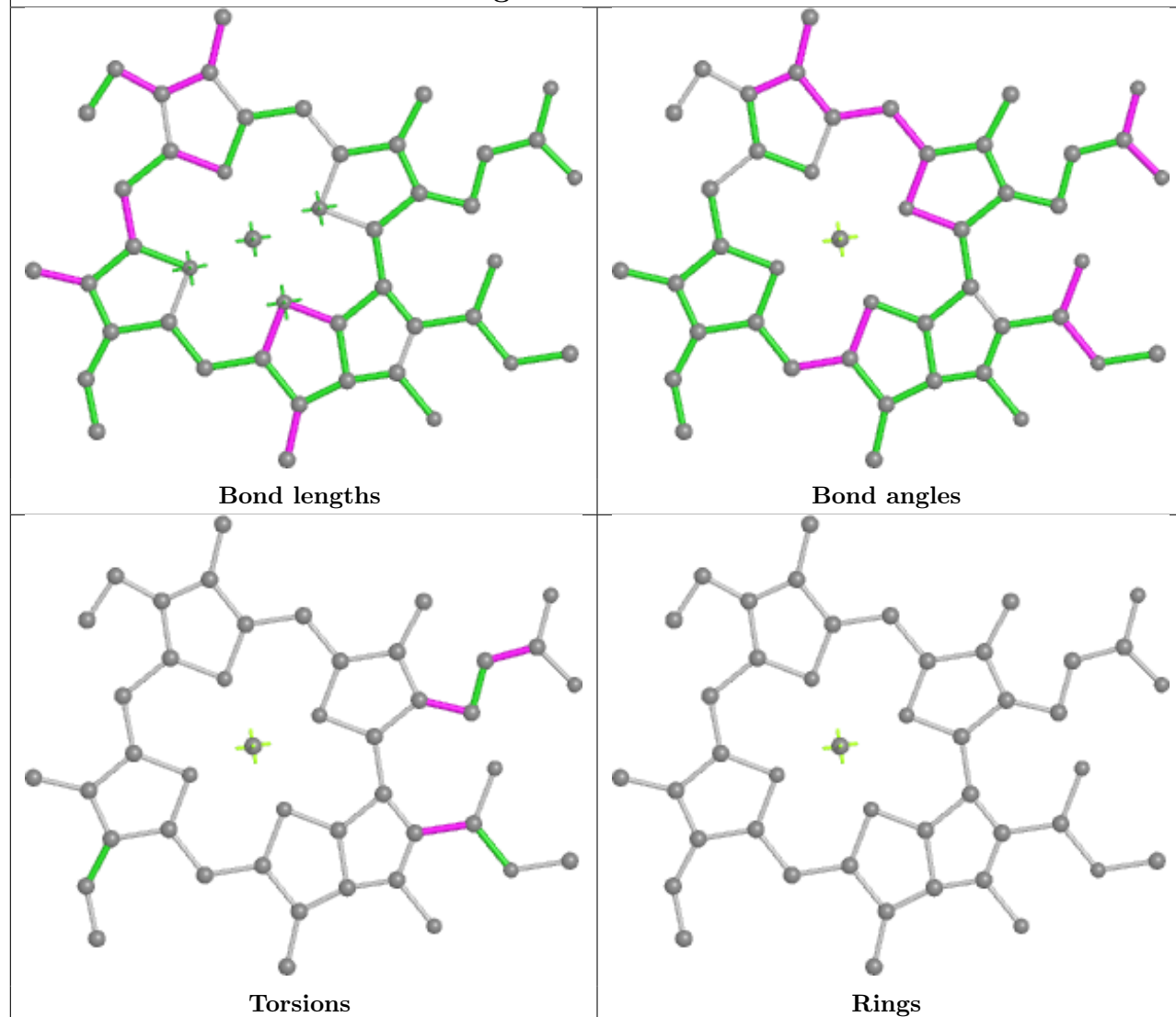
Ligand CLA a 607



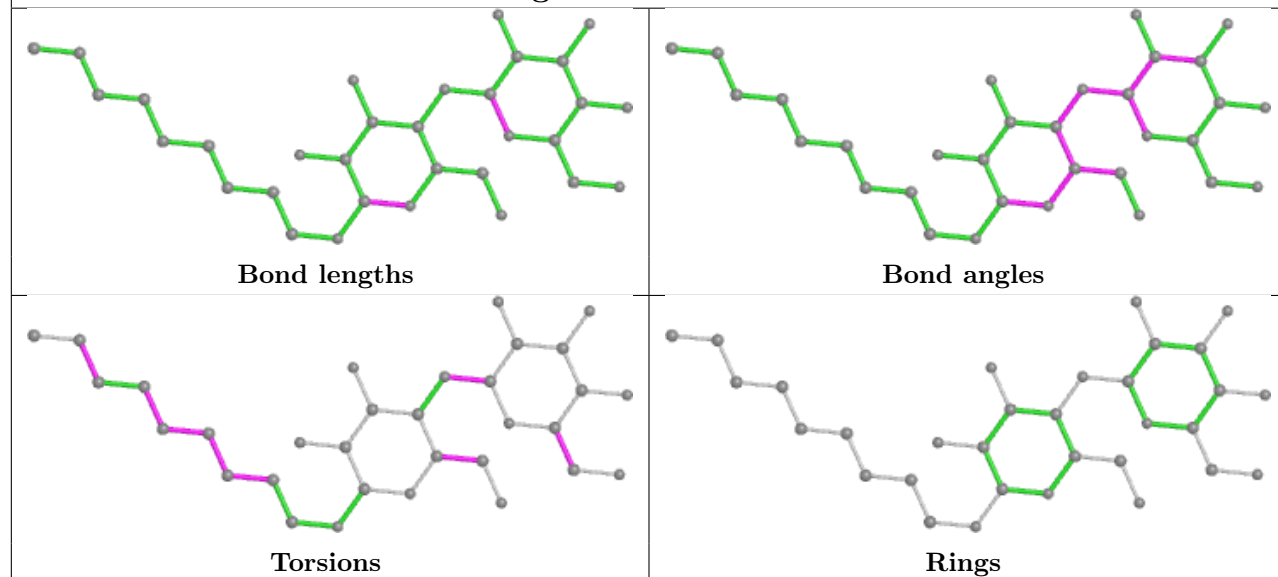
Ligand BCR B 843



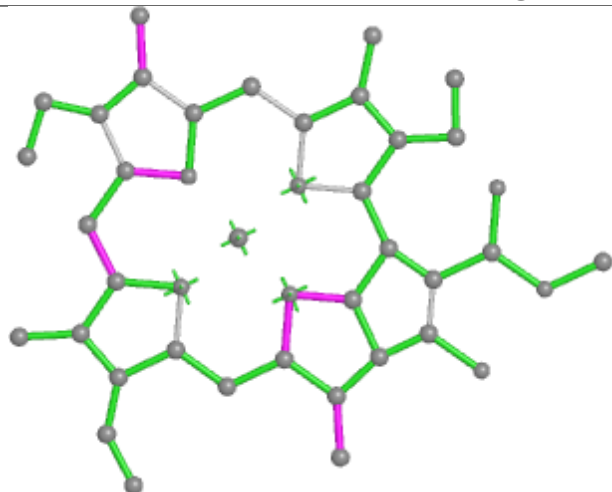
Ligand CLA 2 609



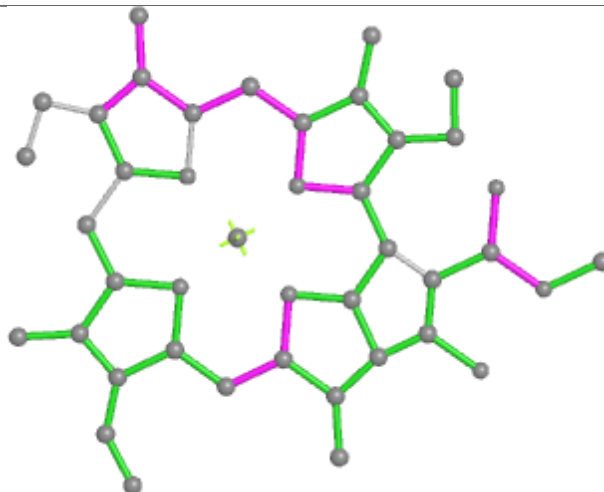
Ligand LMU 5 629



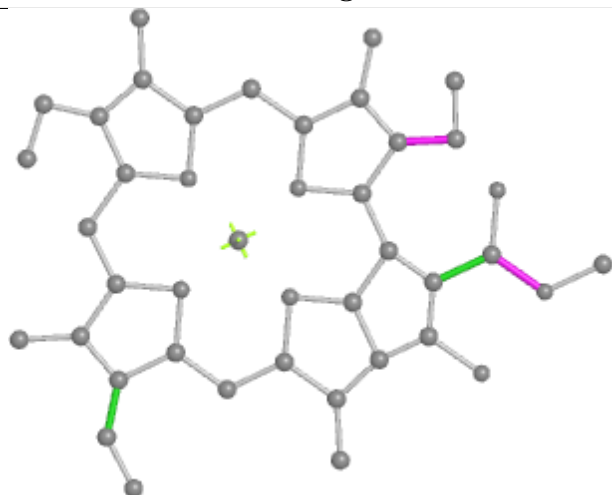
Ligand CLA U 614



Bond lengths



Bond angles

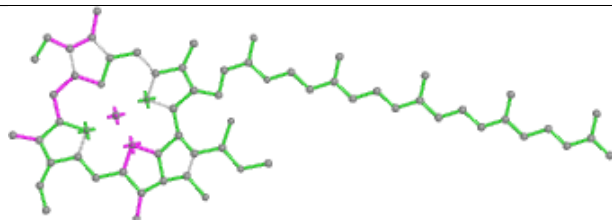


Torsions

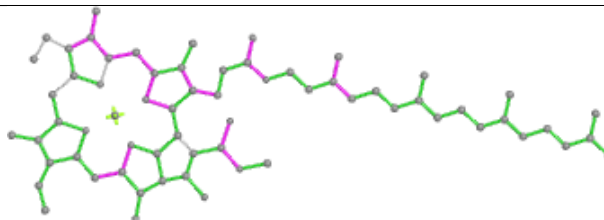


Rings

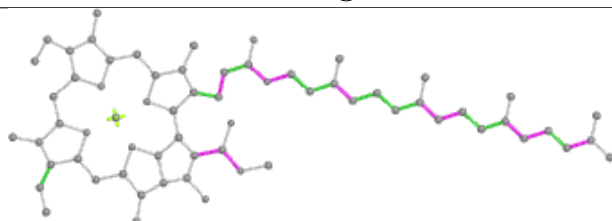
Ligand CLA A 814



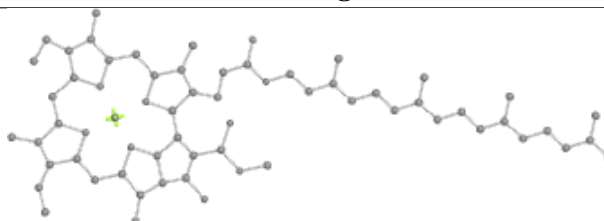
Bond lengths



Bond angles

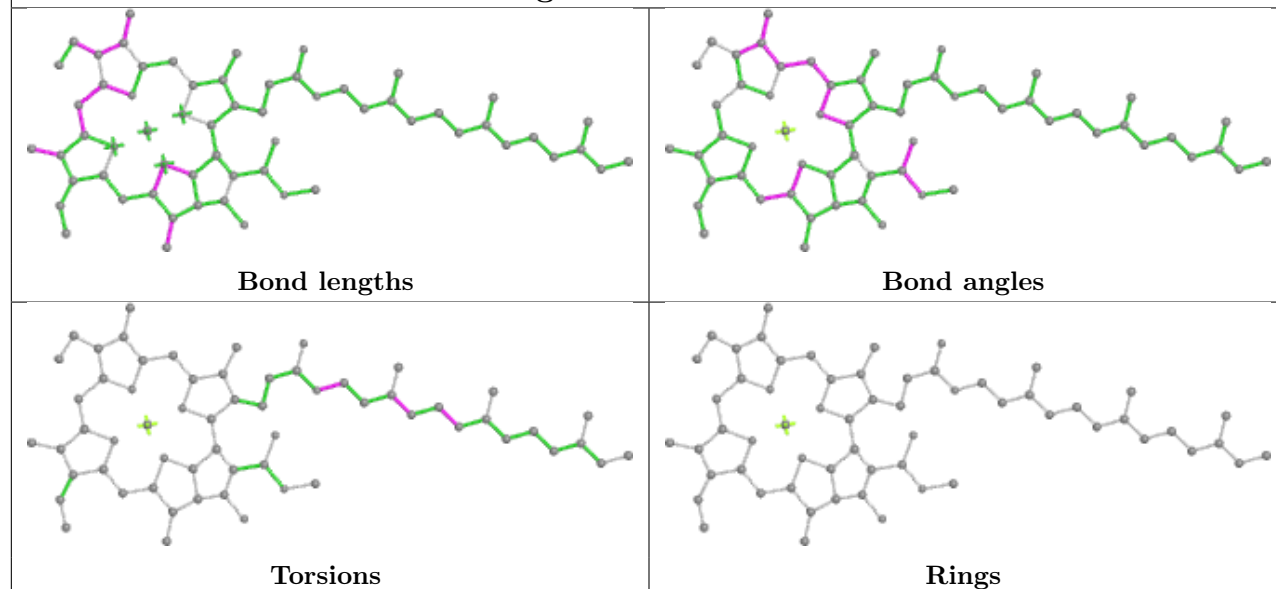


Torsions

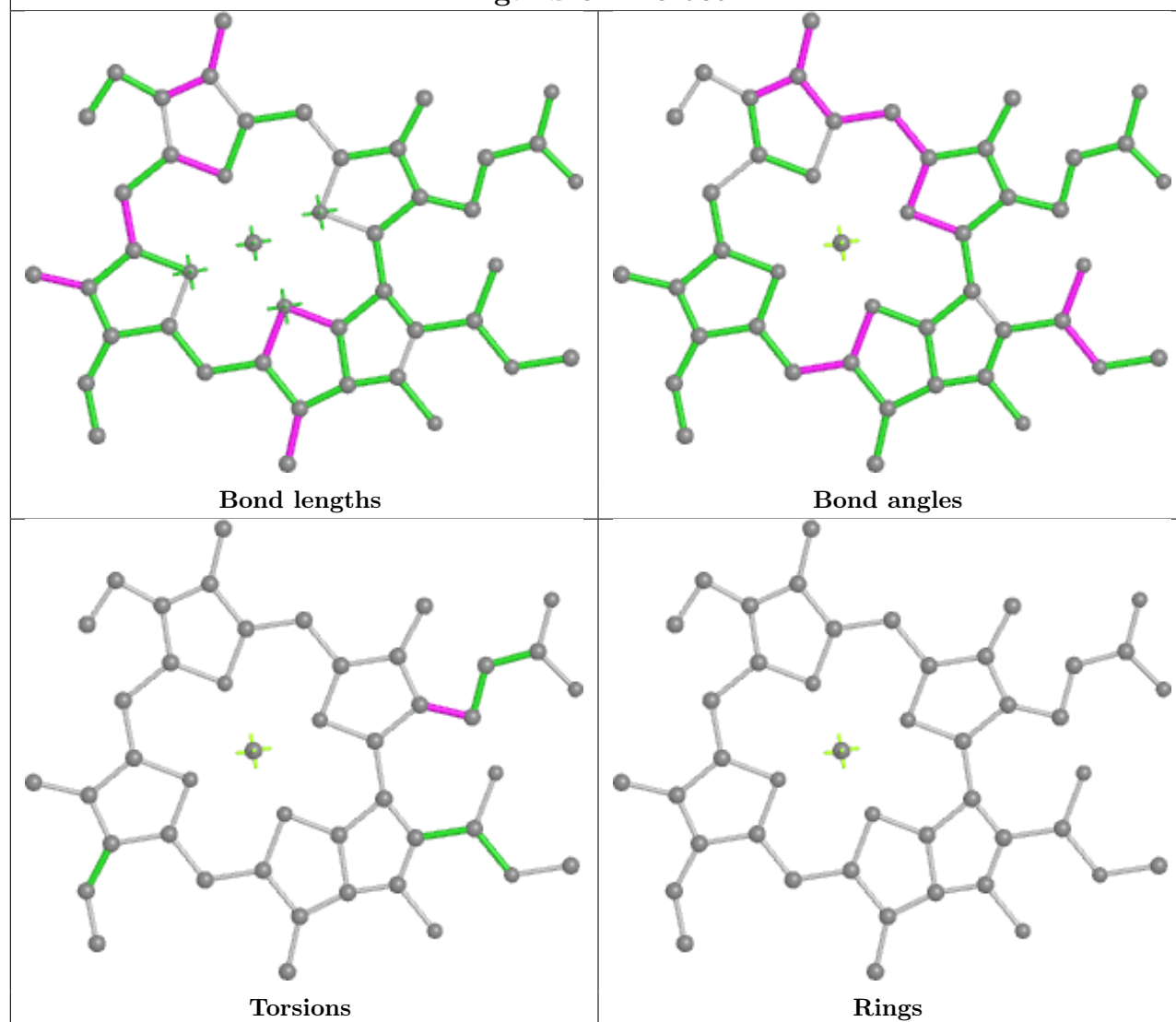


Rings

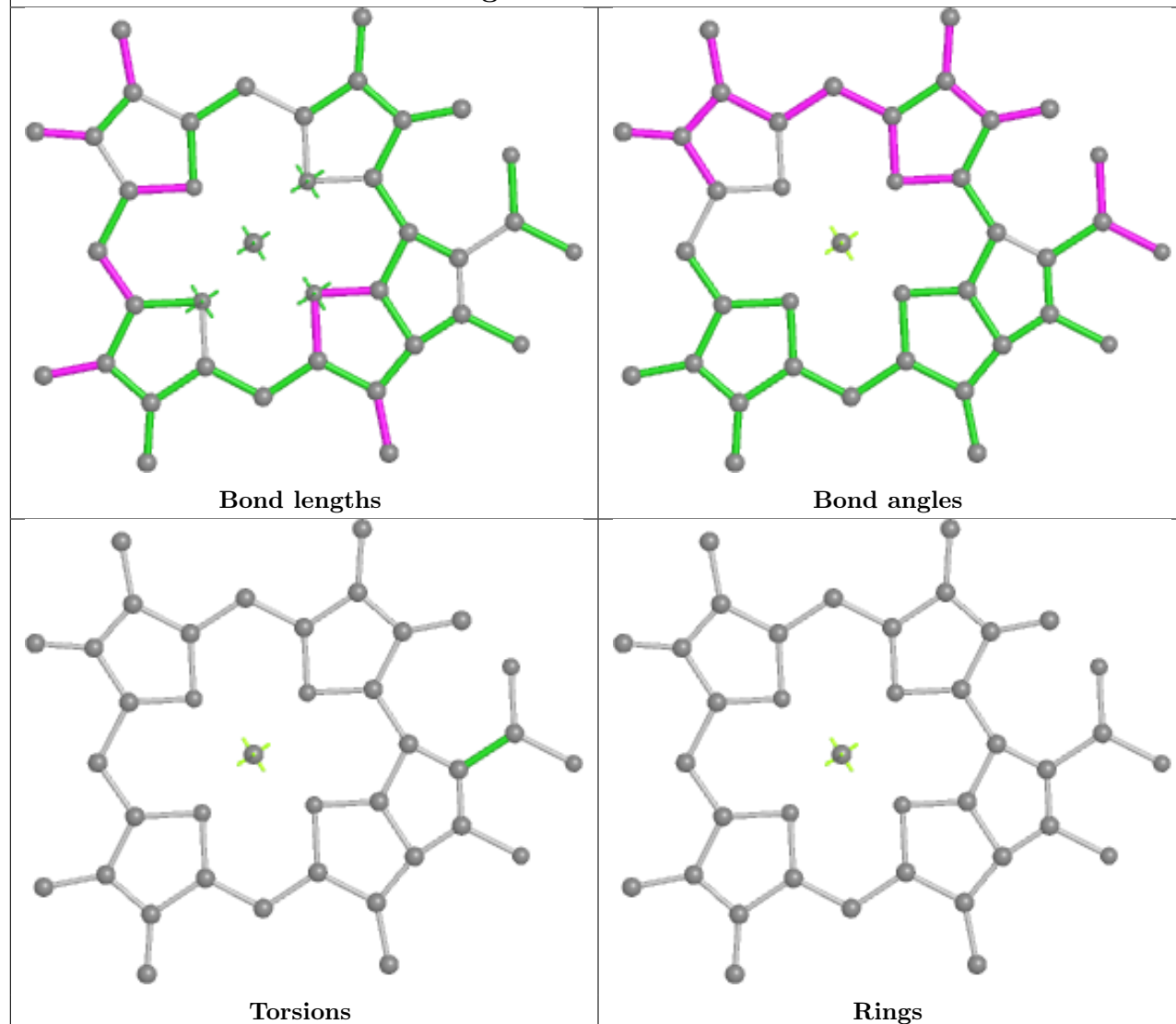
Ligand CLA 9 609



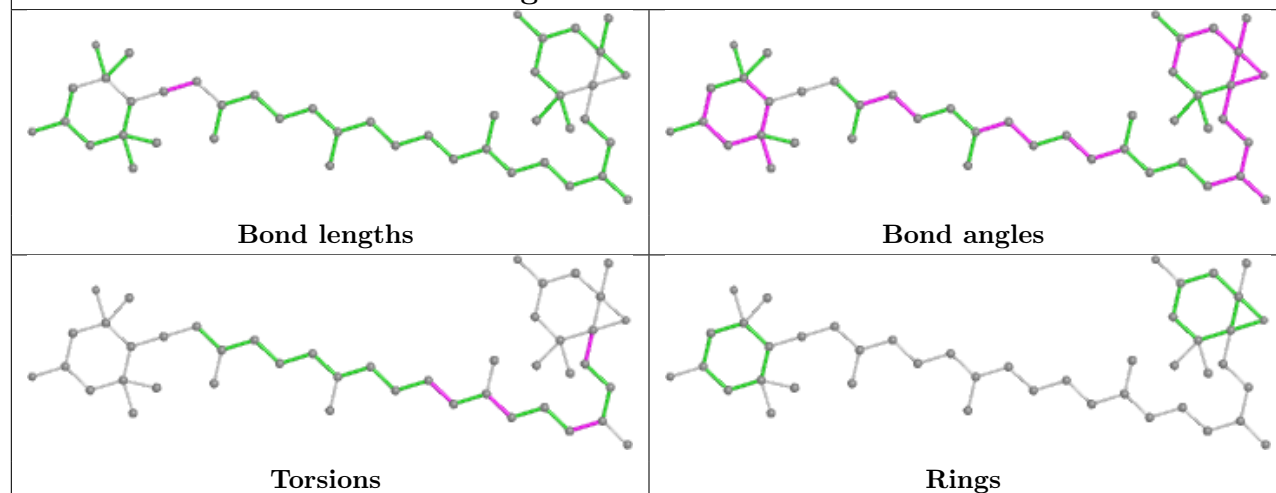
Ligand CLA 8 609

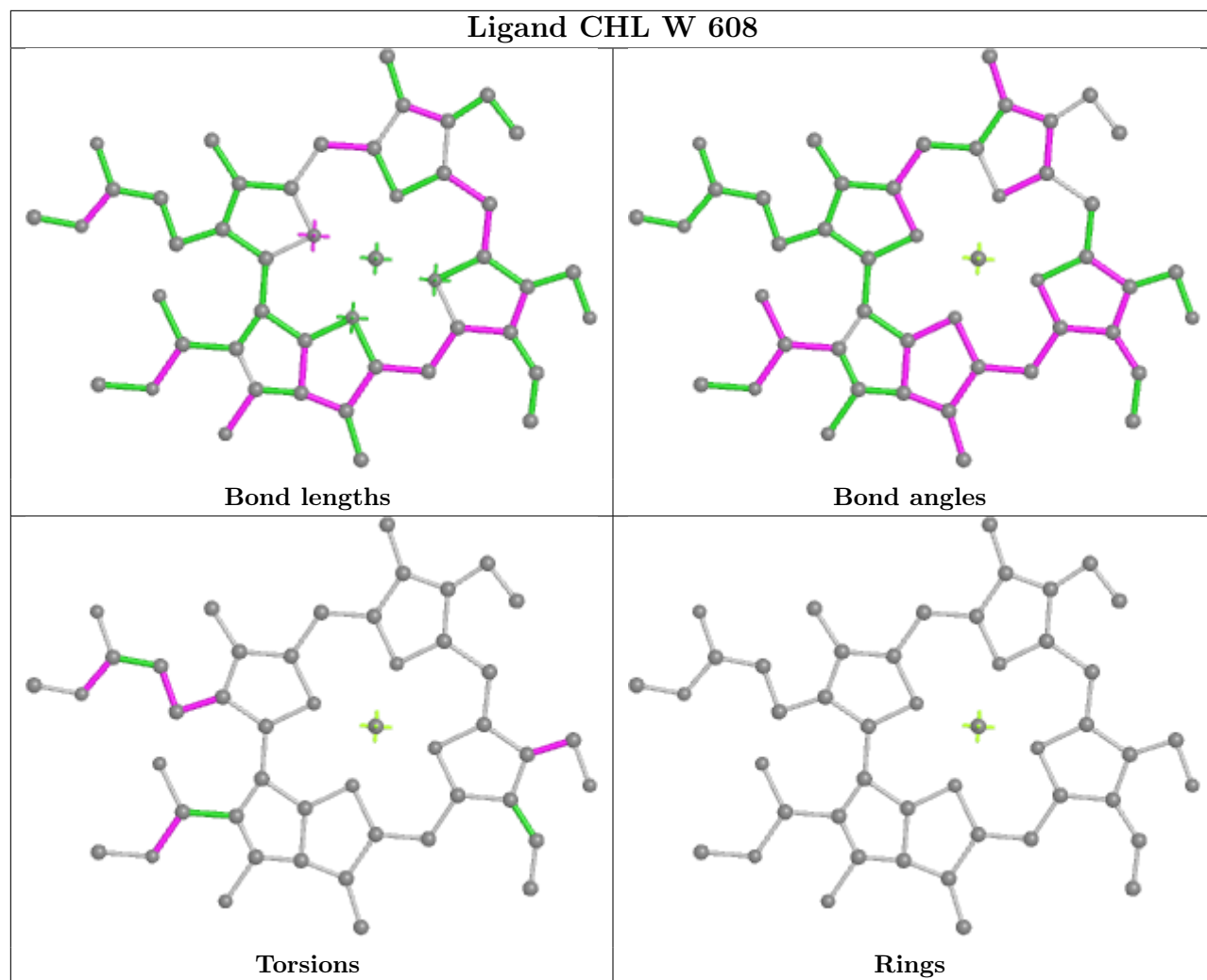


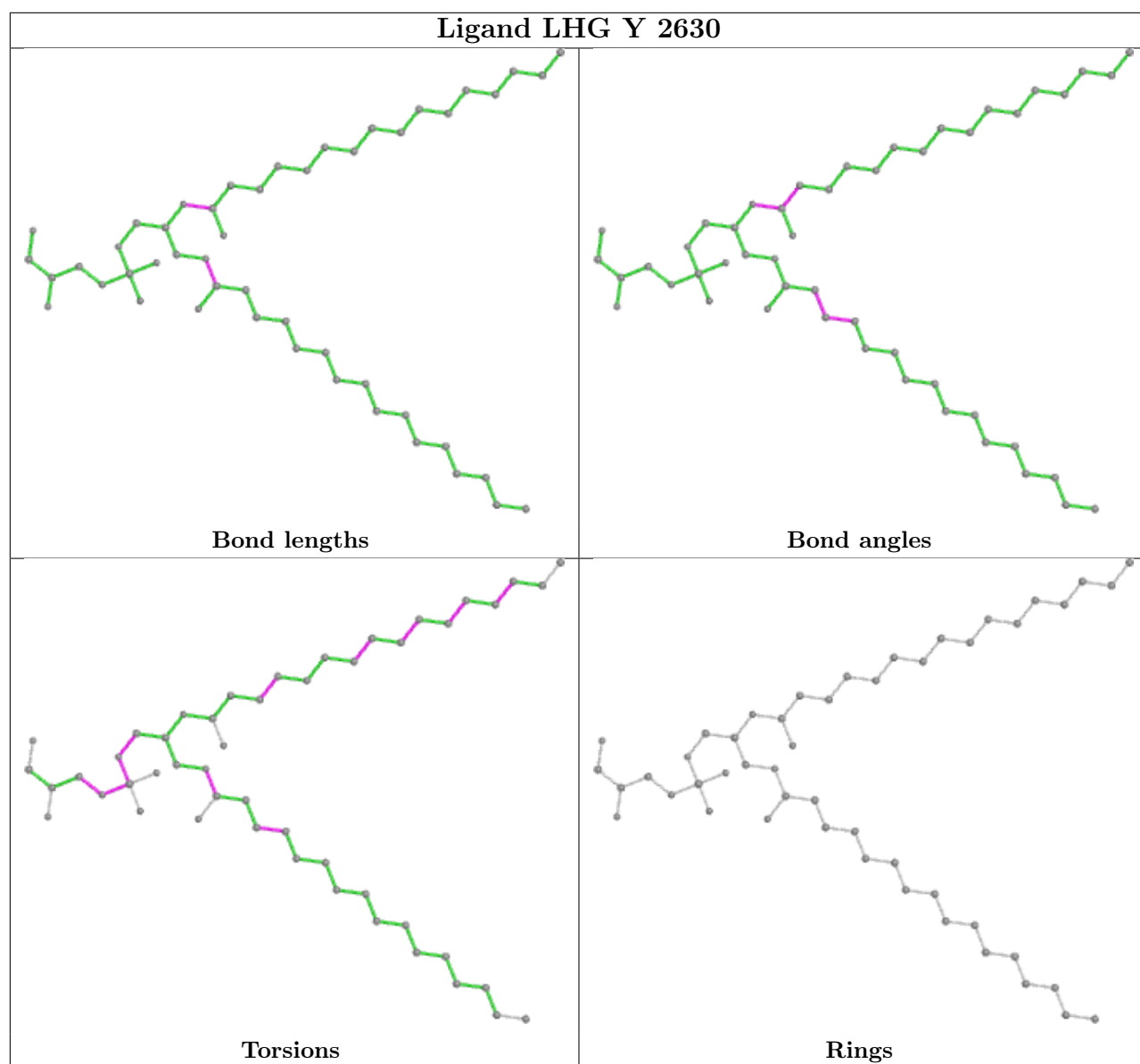
Ligand CLA O 2002

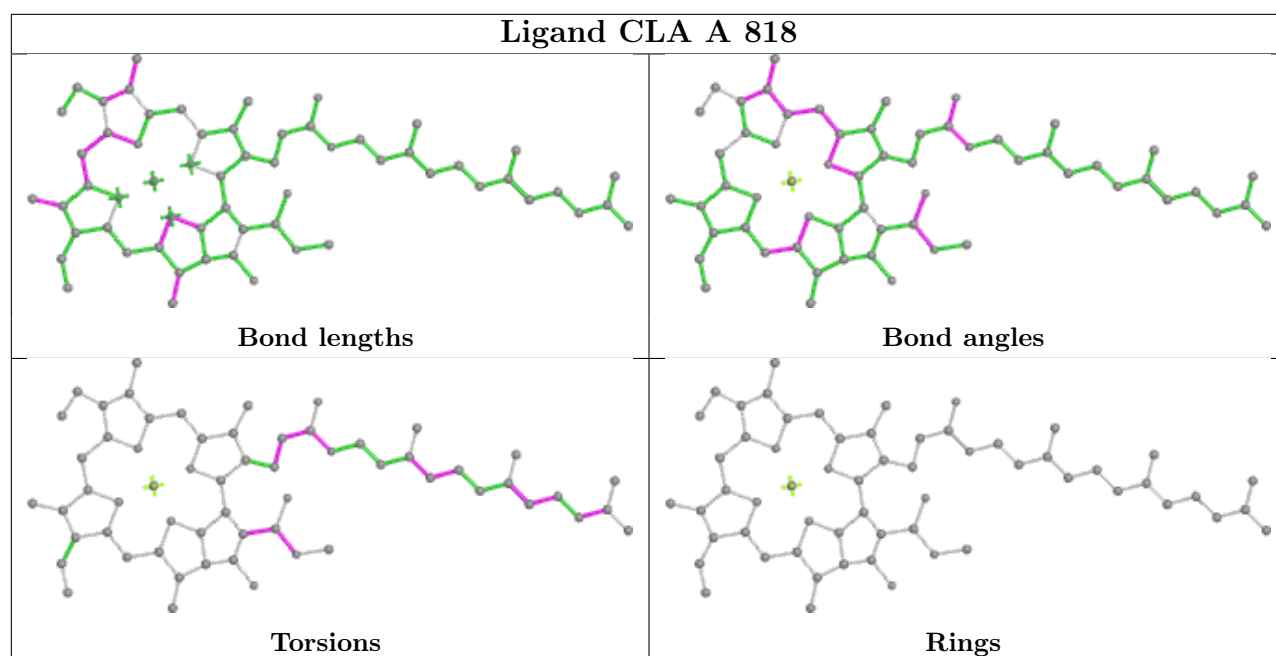


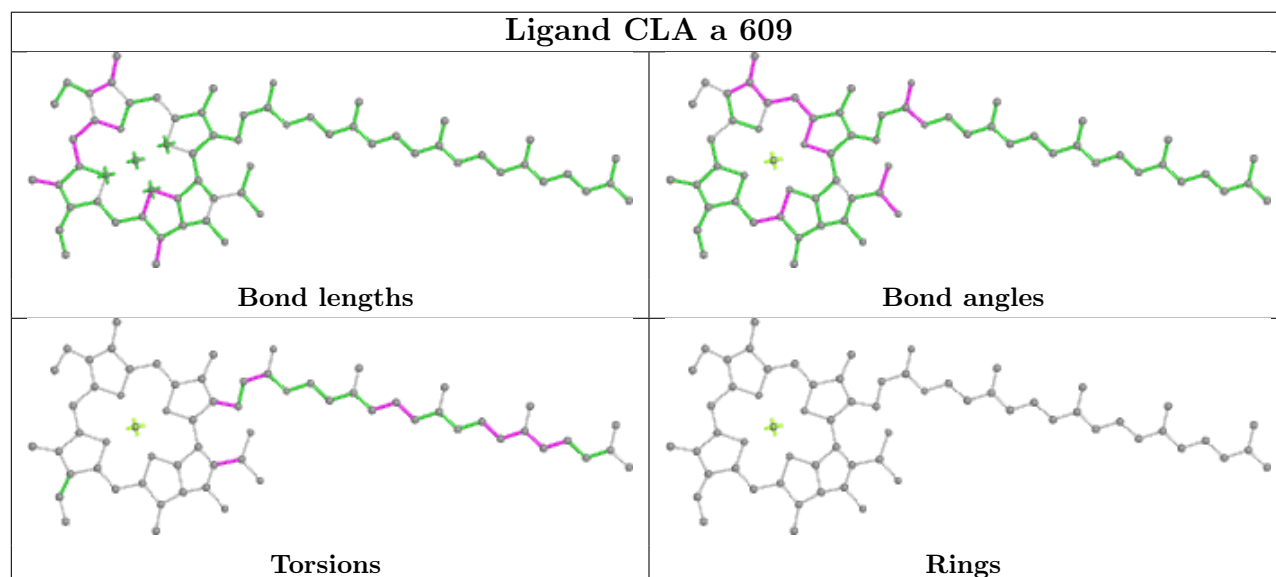
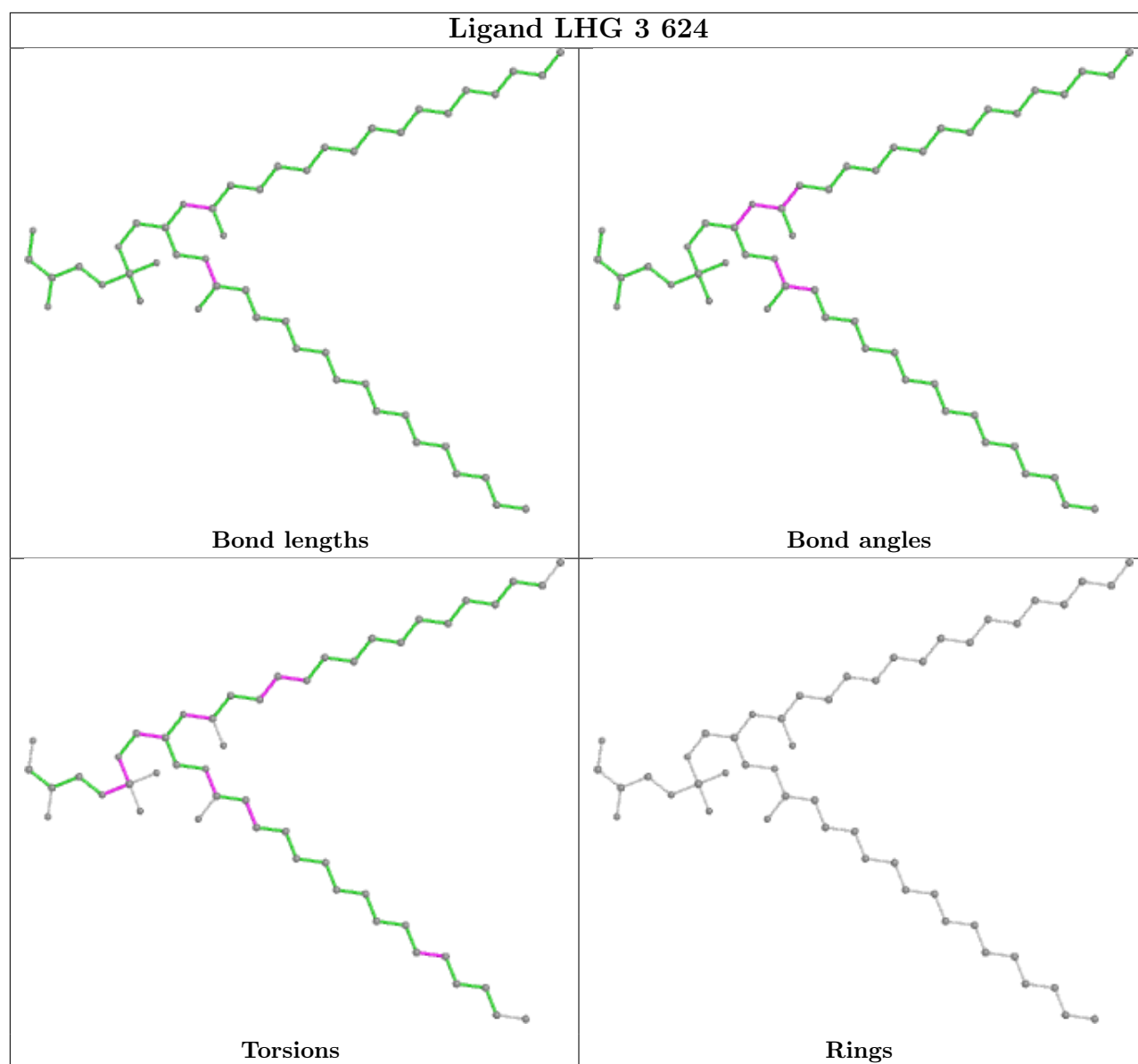
Ligand NEX Y 1623



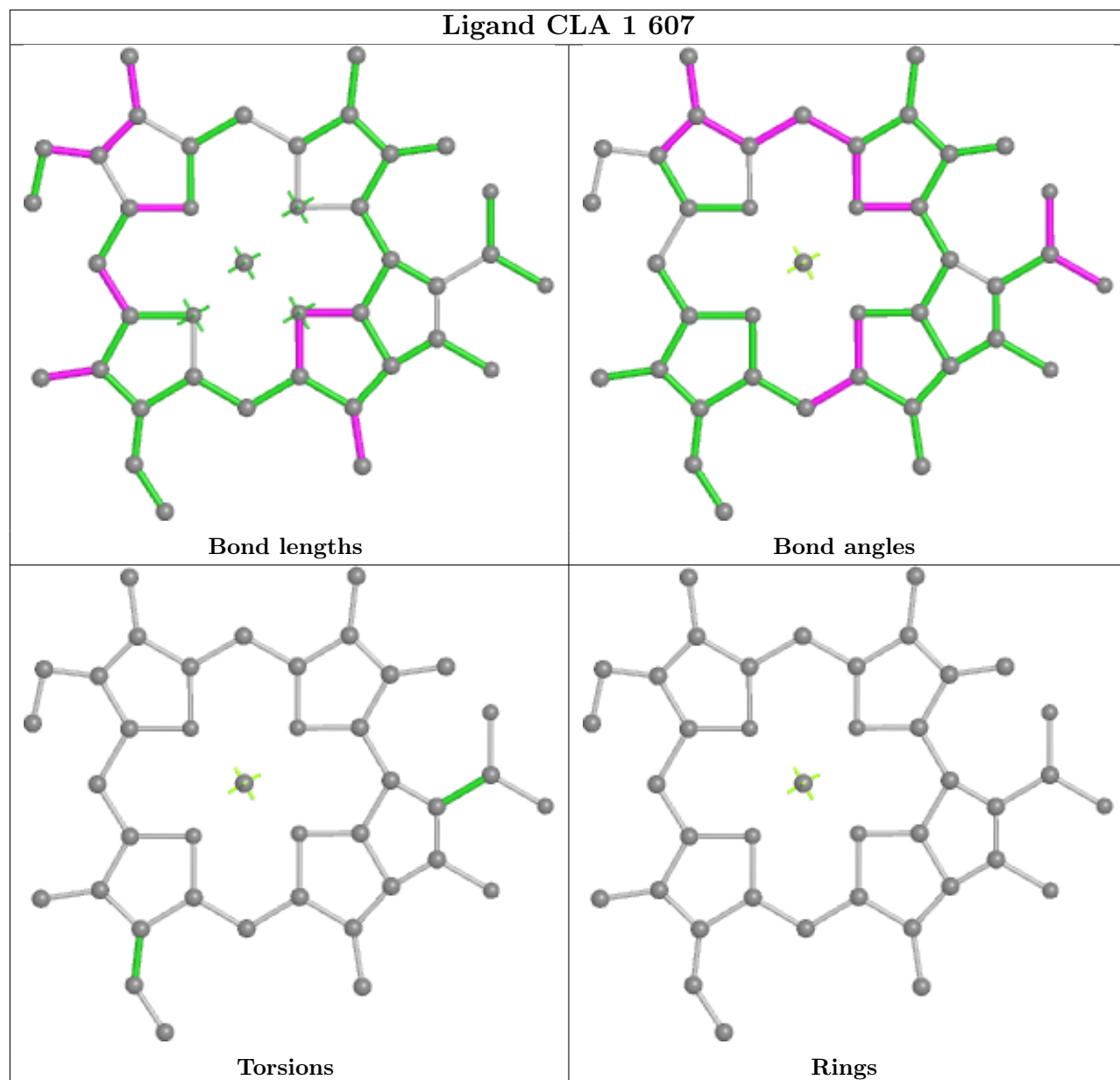


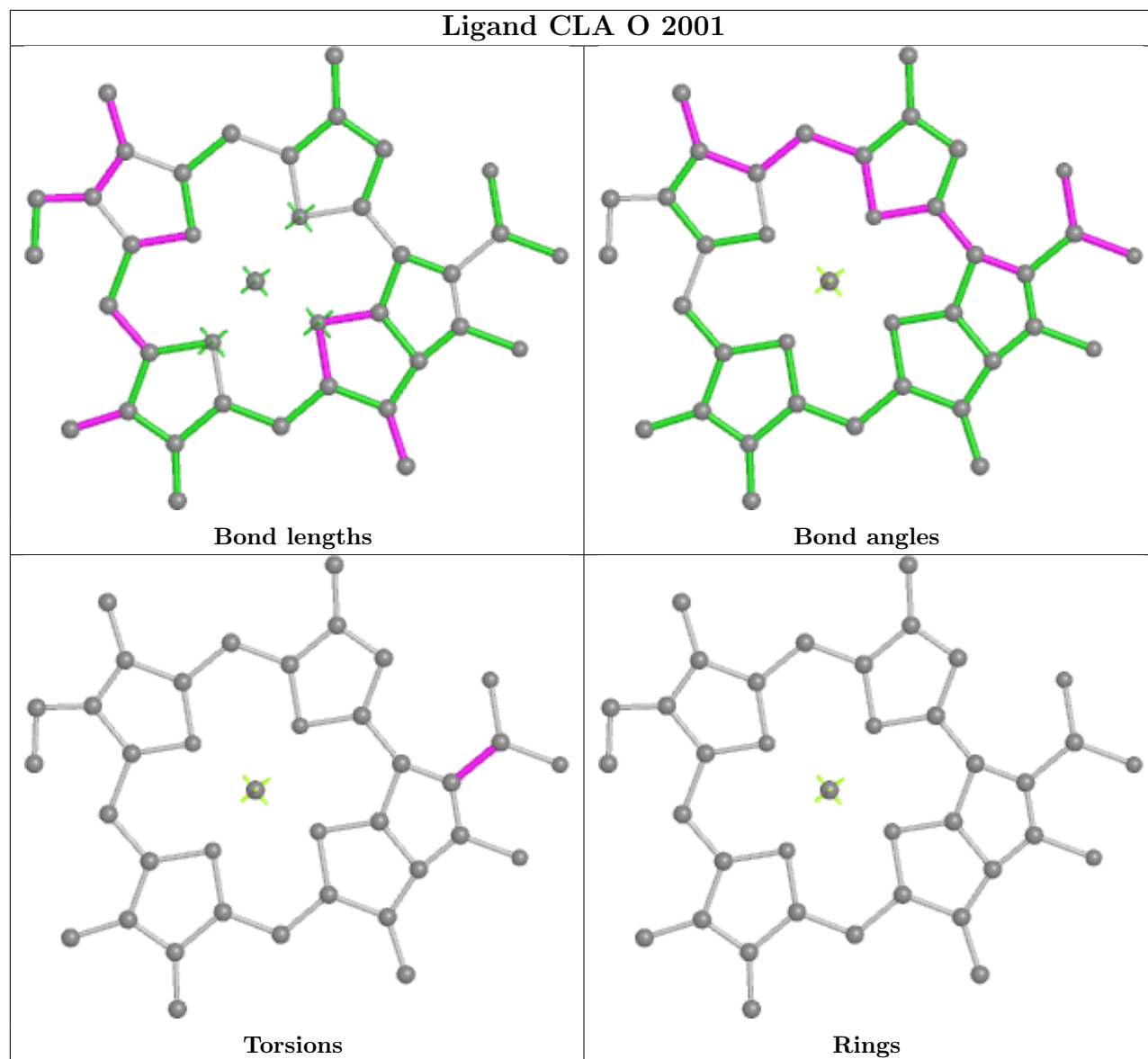


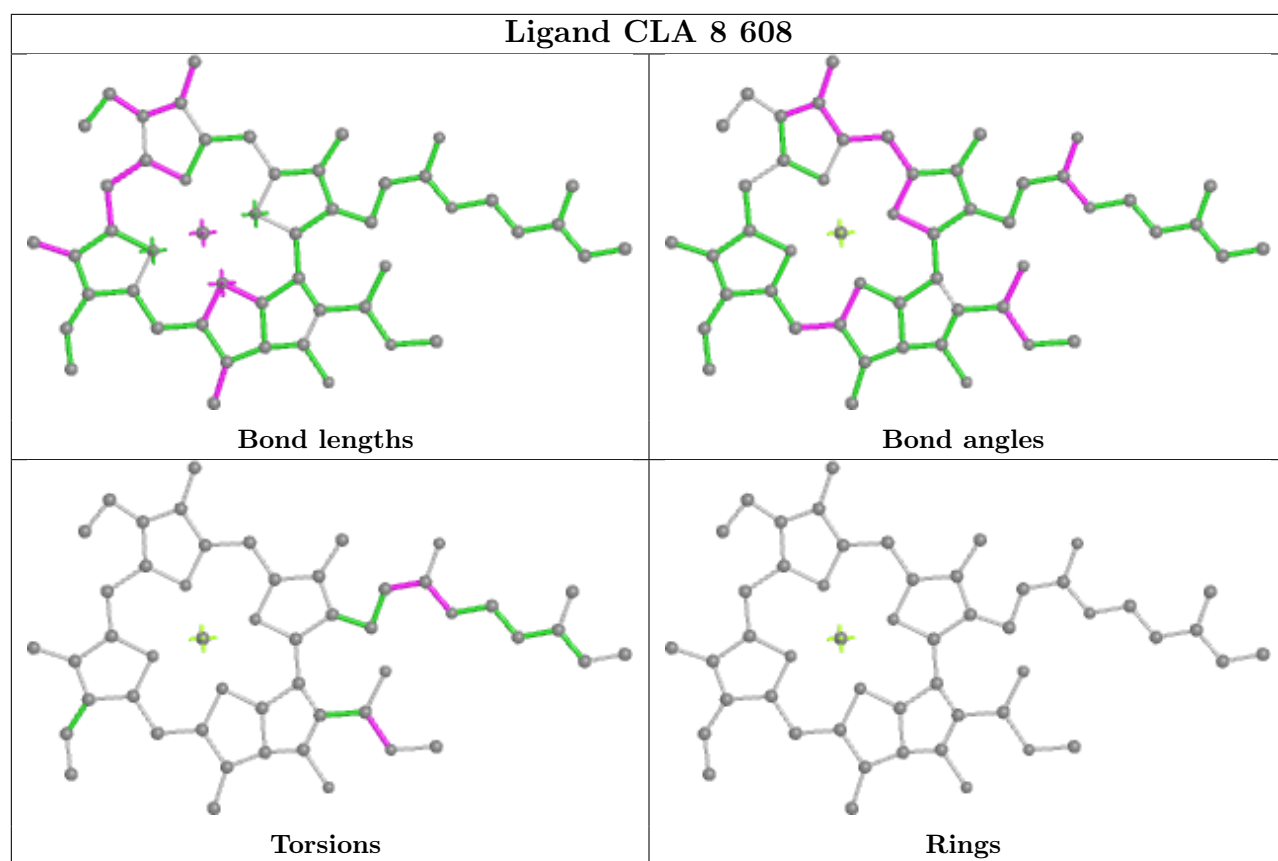




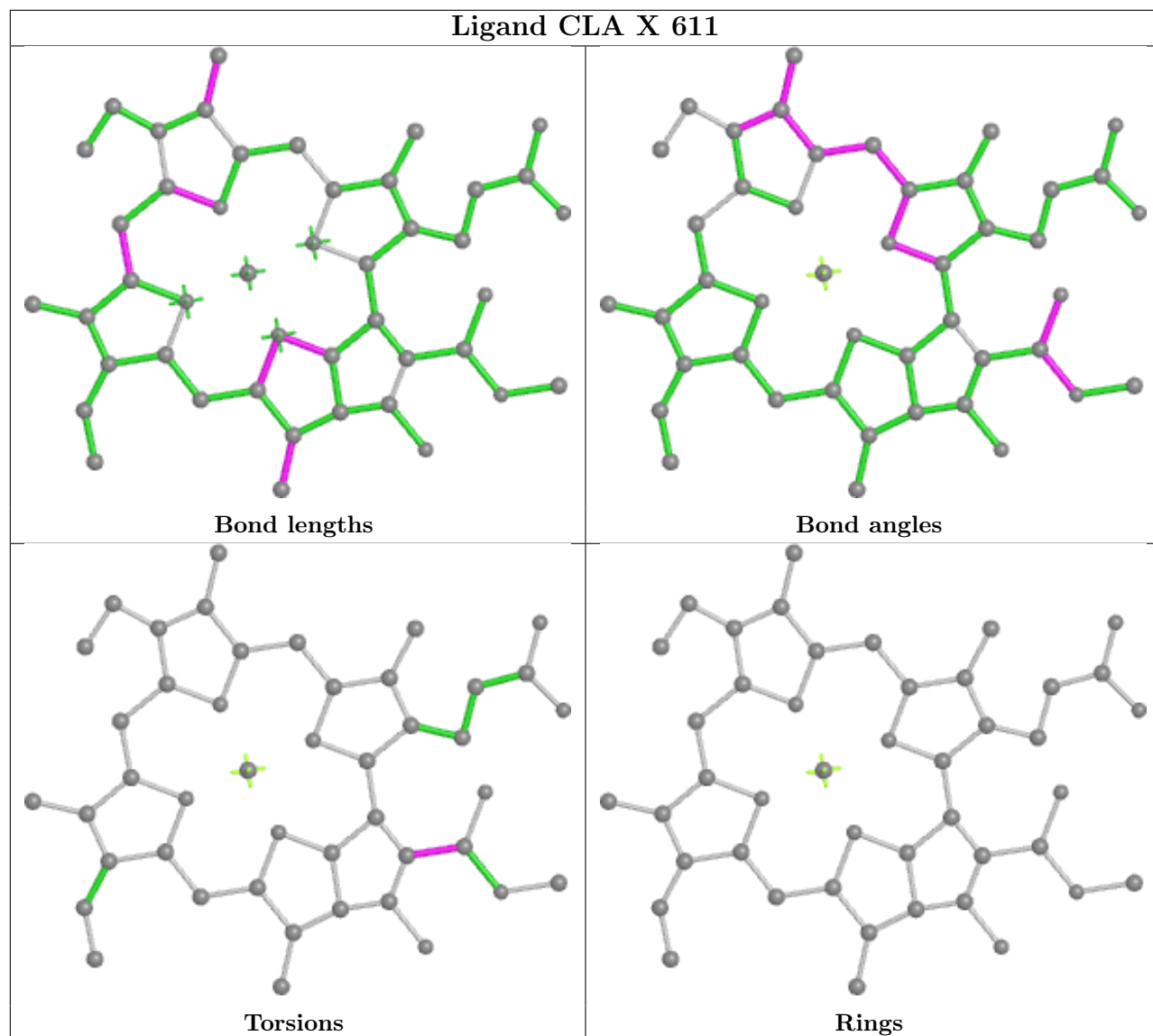
Ligand CLA 1 607

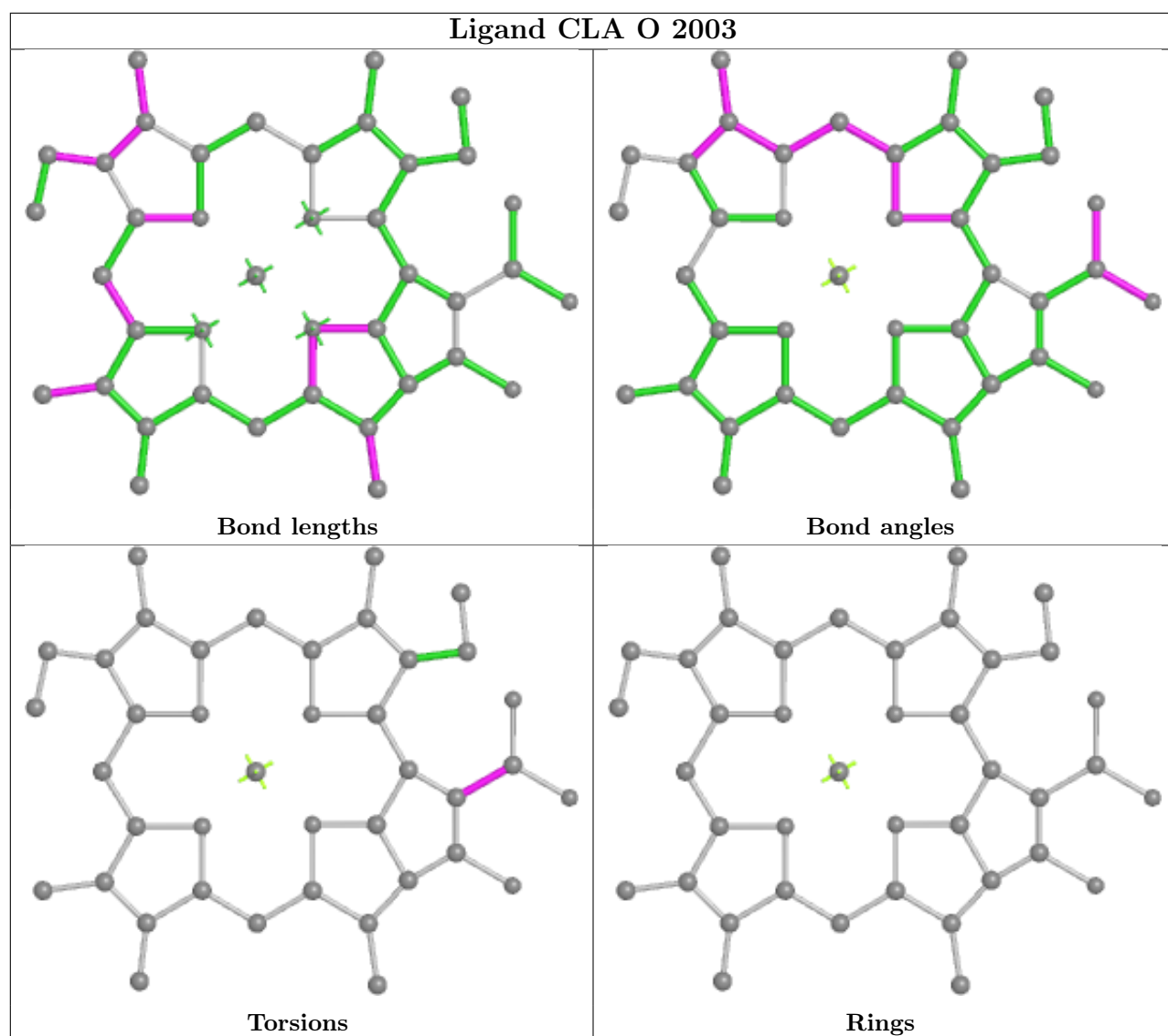




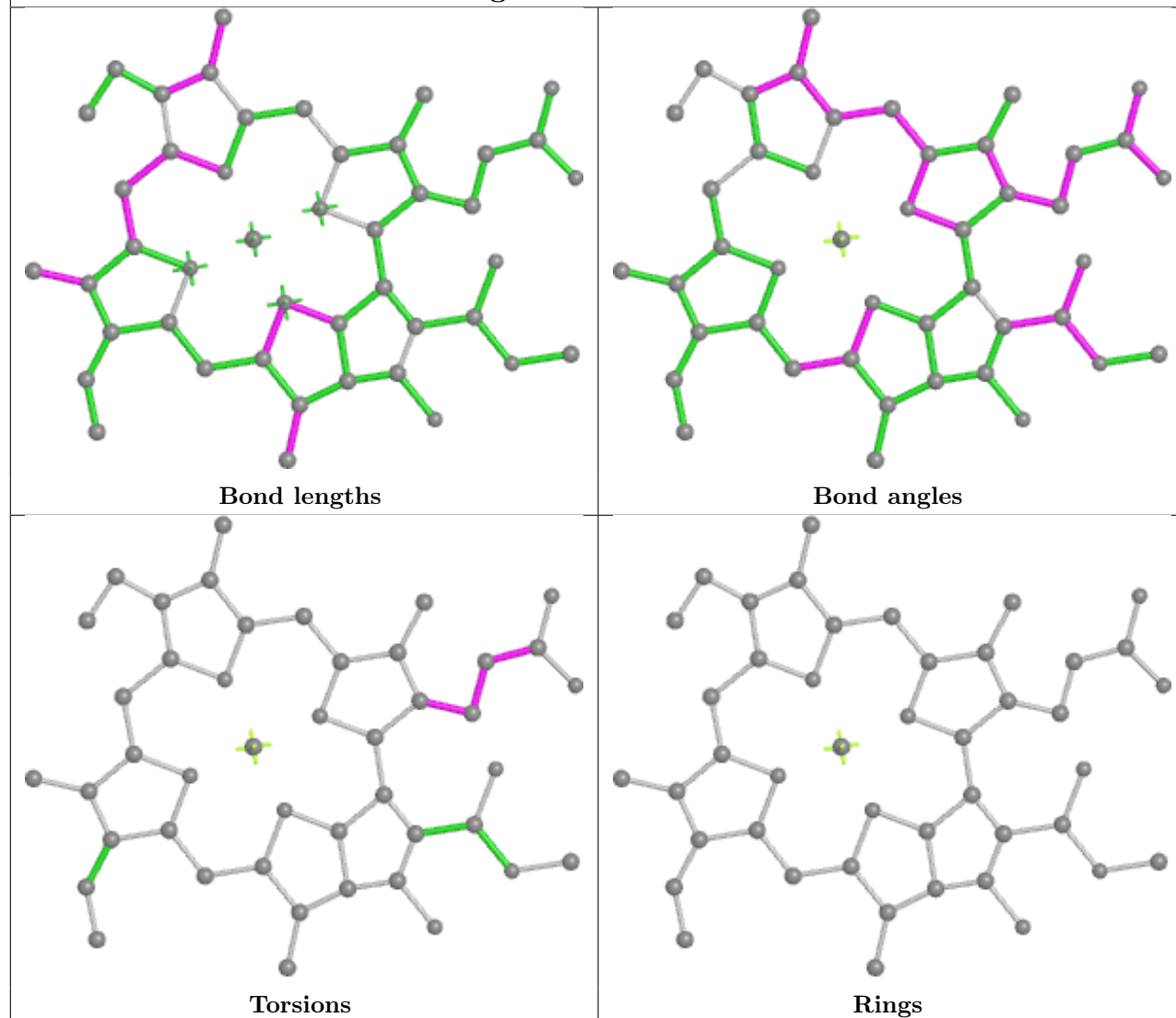


Ligand CLA X 611

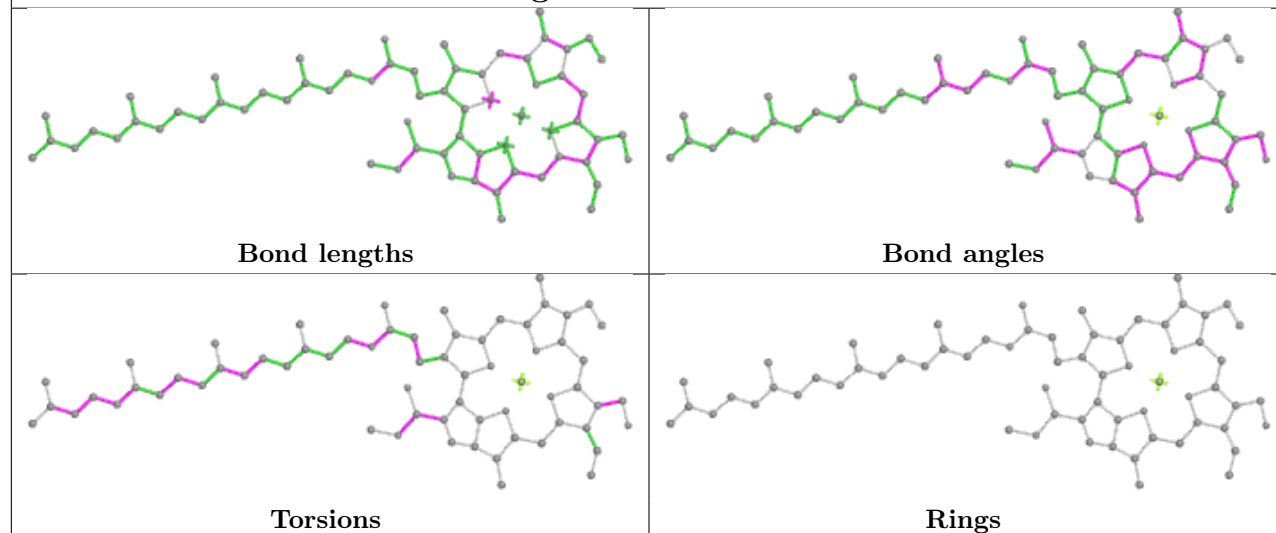


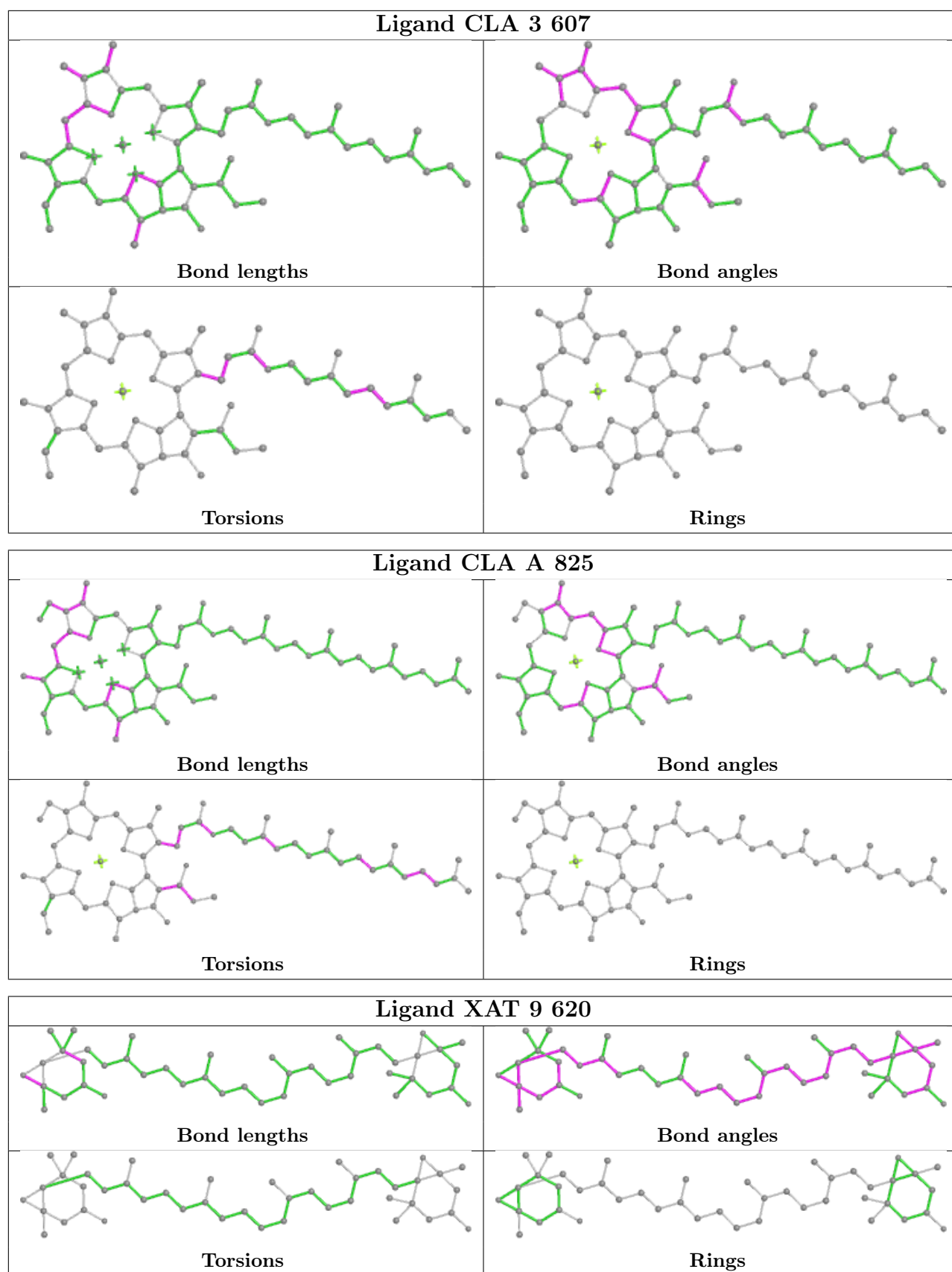


Ligand CLA A 833

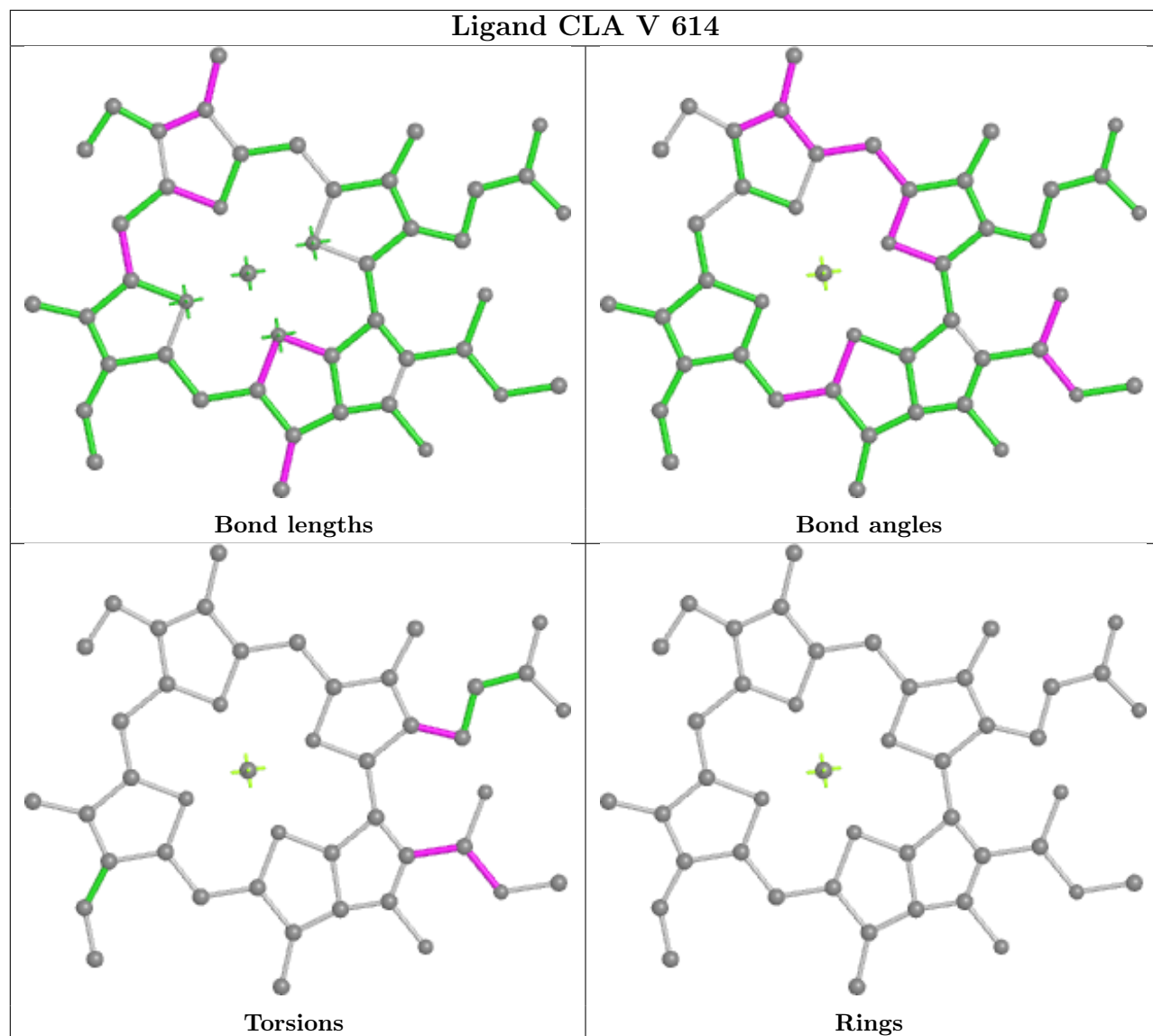


Ligand CHL X 608

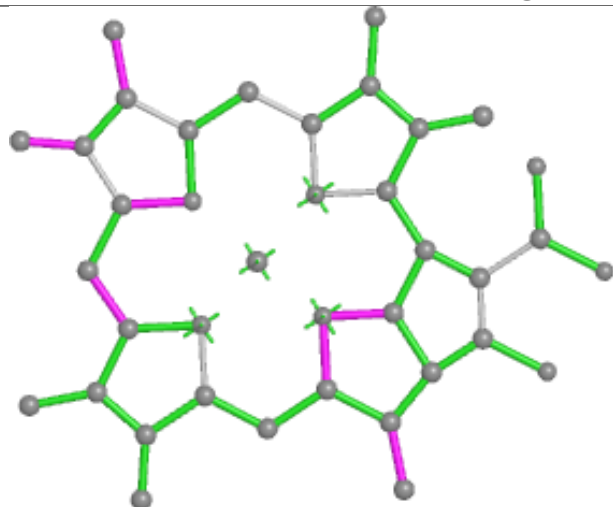




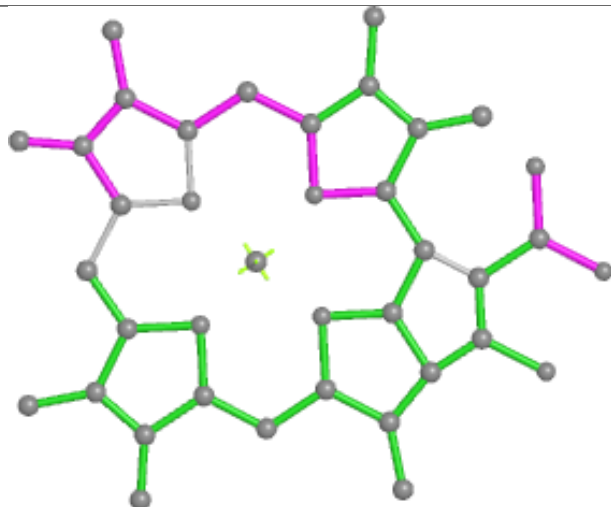
Ligand CLA V 614



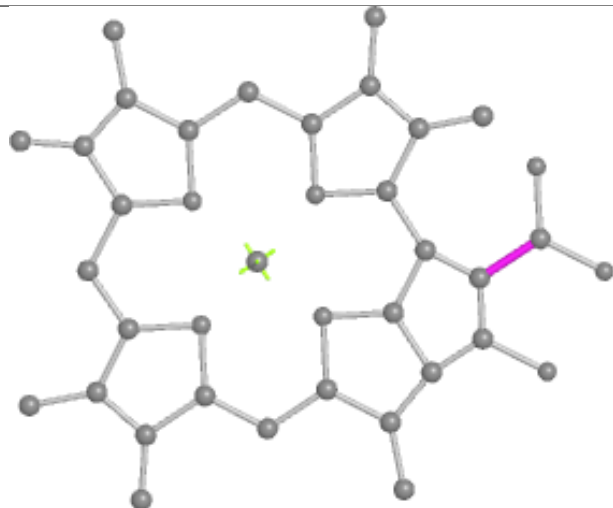
Ligand CLA 3 611



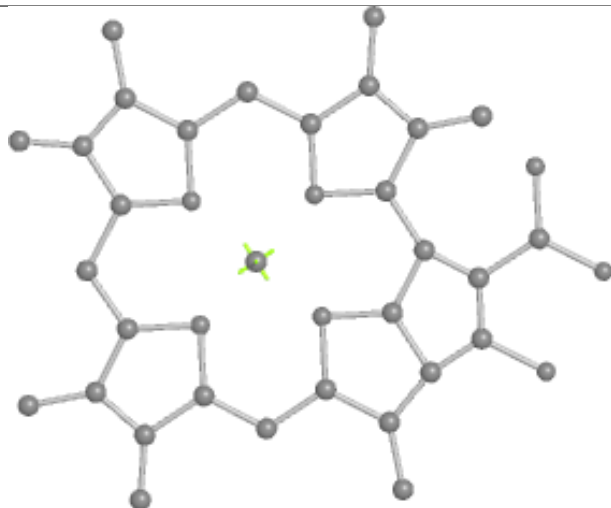
Bond lengths



Bond angles

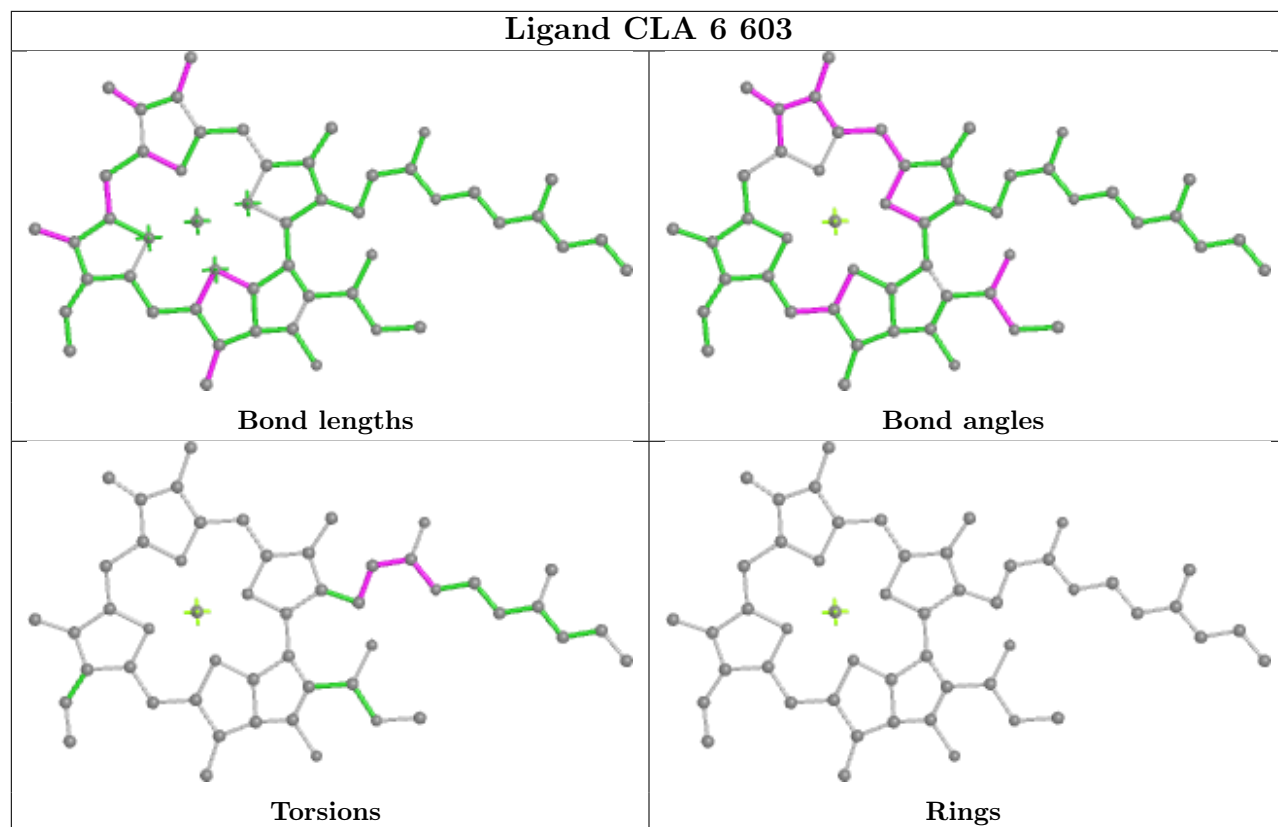


Torsions

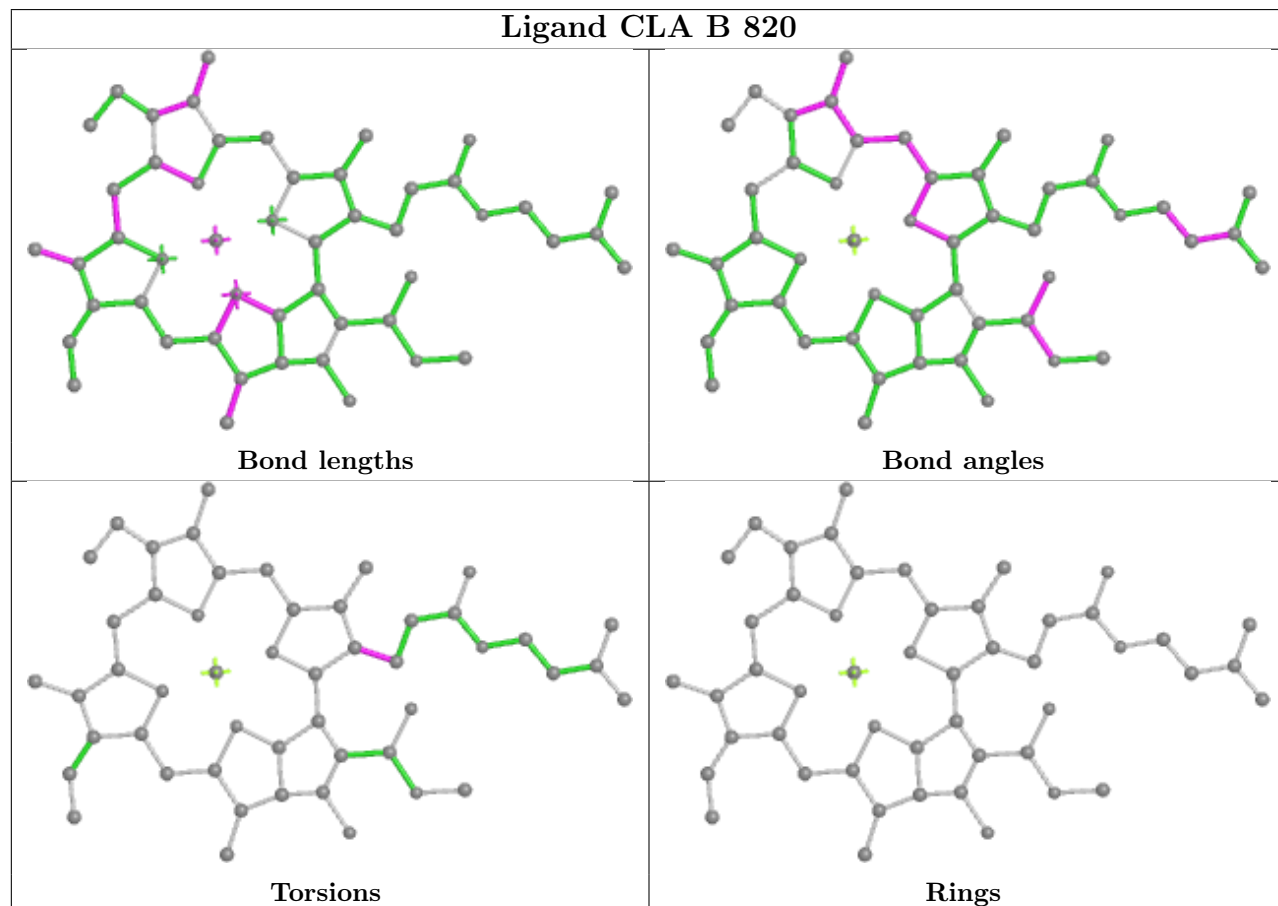


Rings

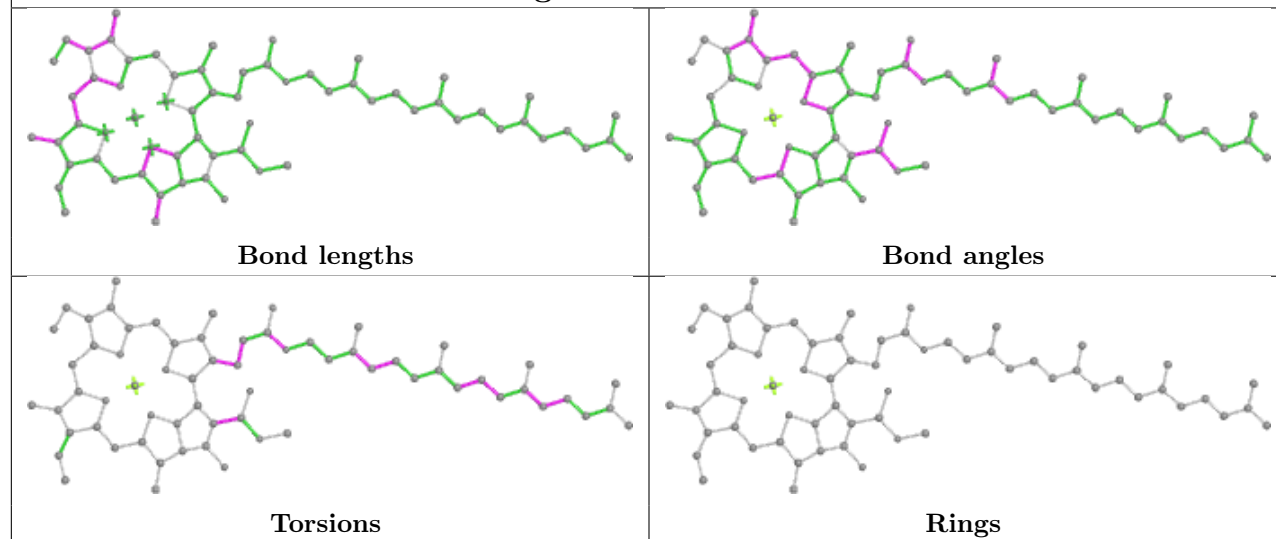
Ligand CLA 6 603



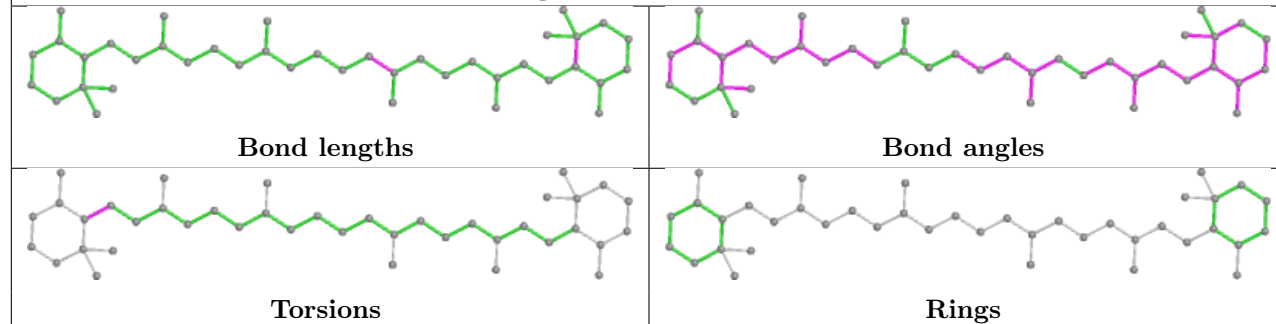
Ligand CLA B 820



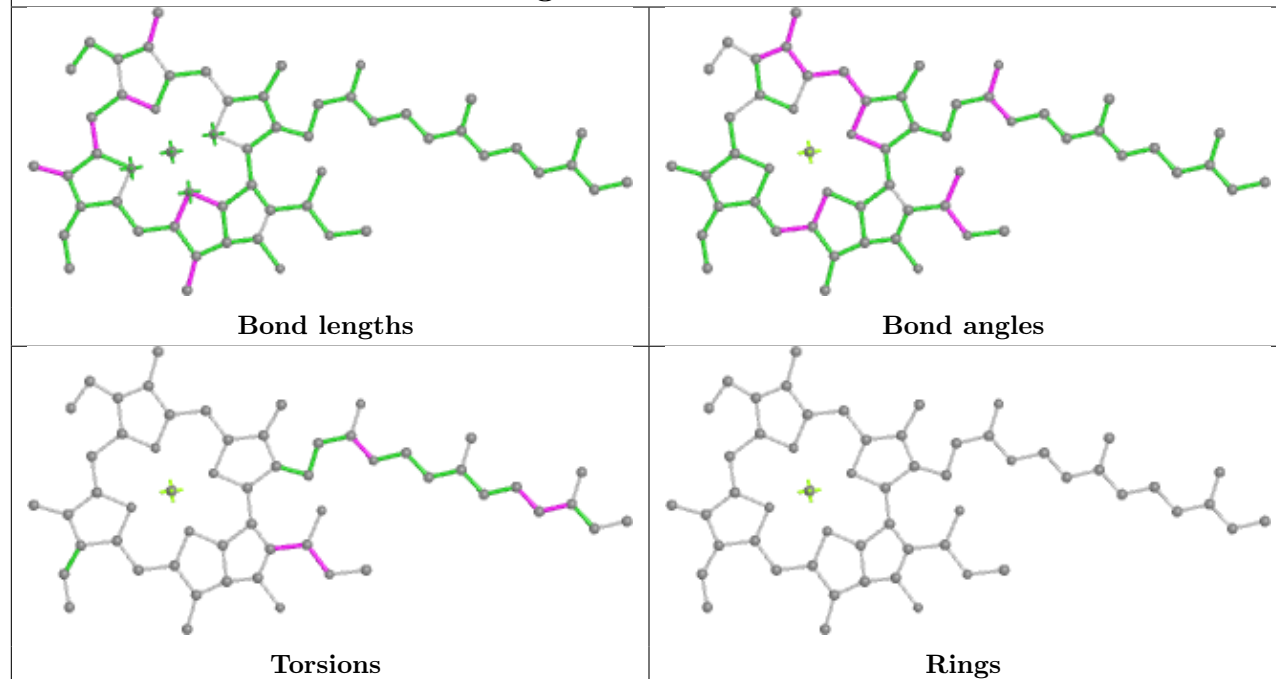
Ligand CLA L 303



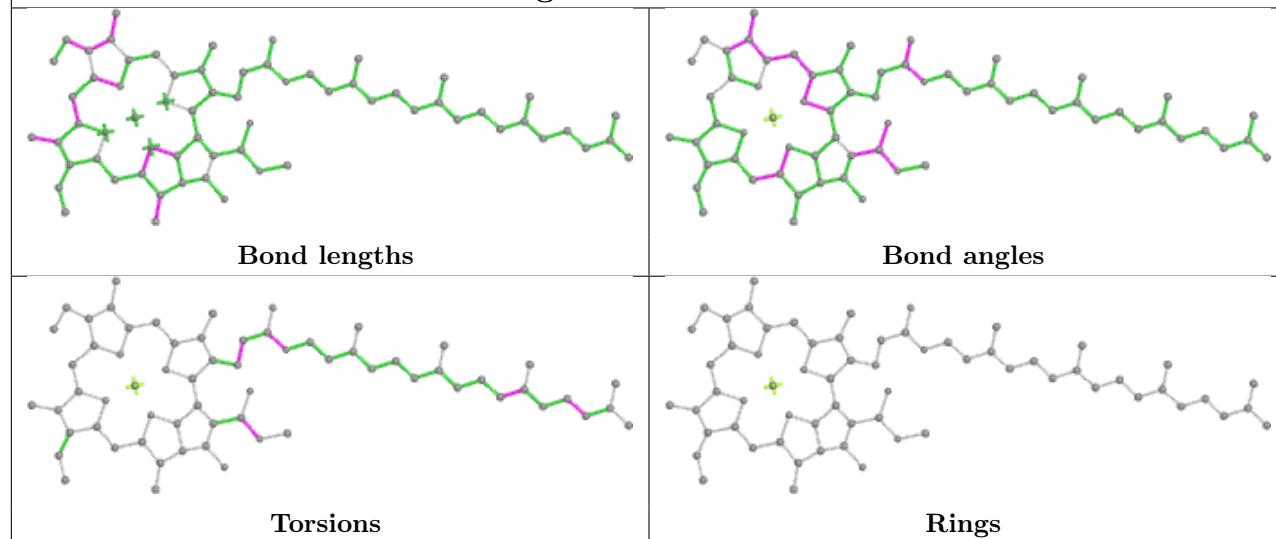
Ligand BCR J 102



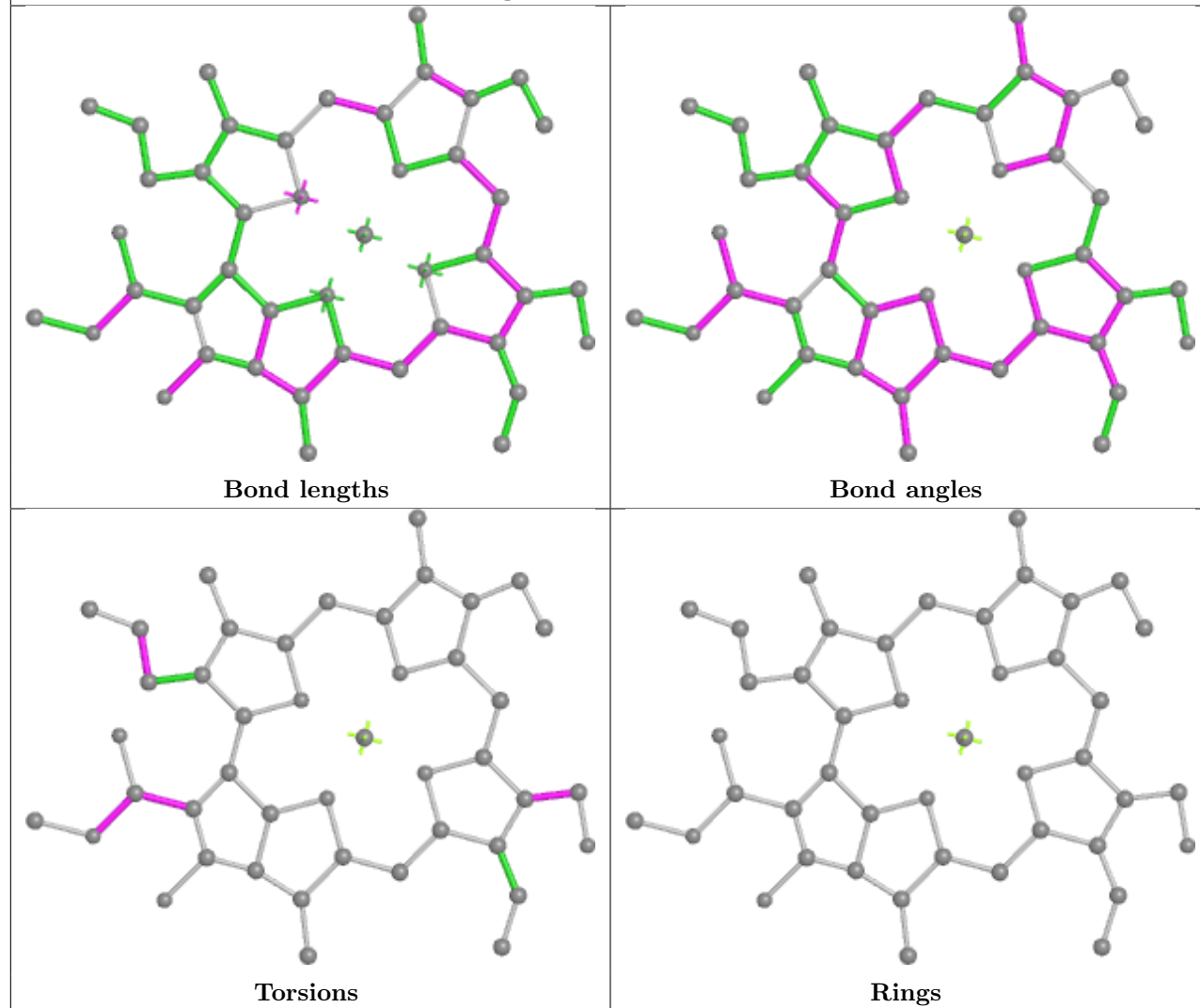
Ligand CLA 4 614

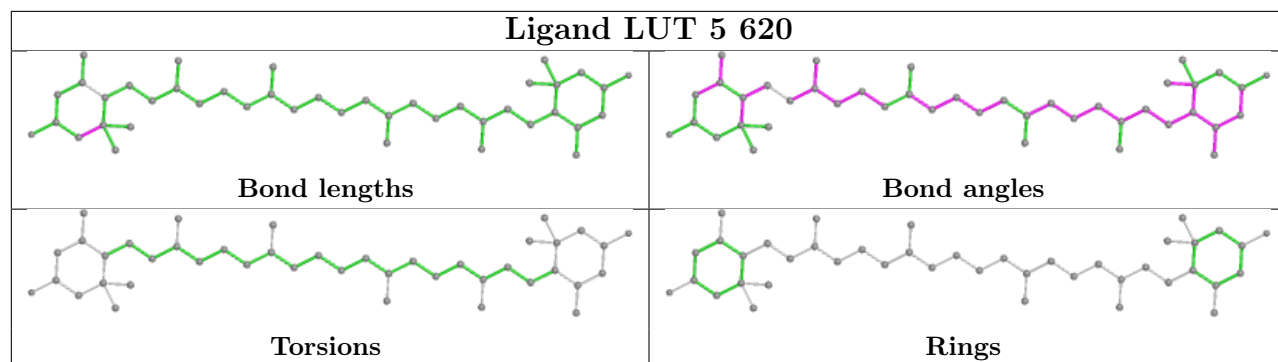
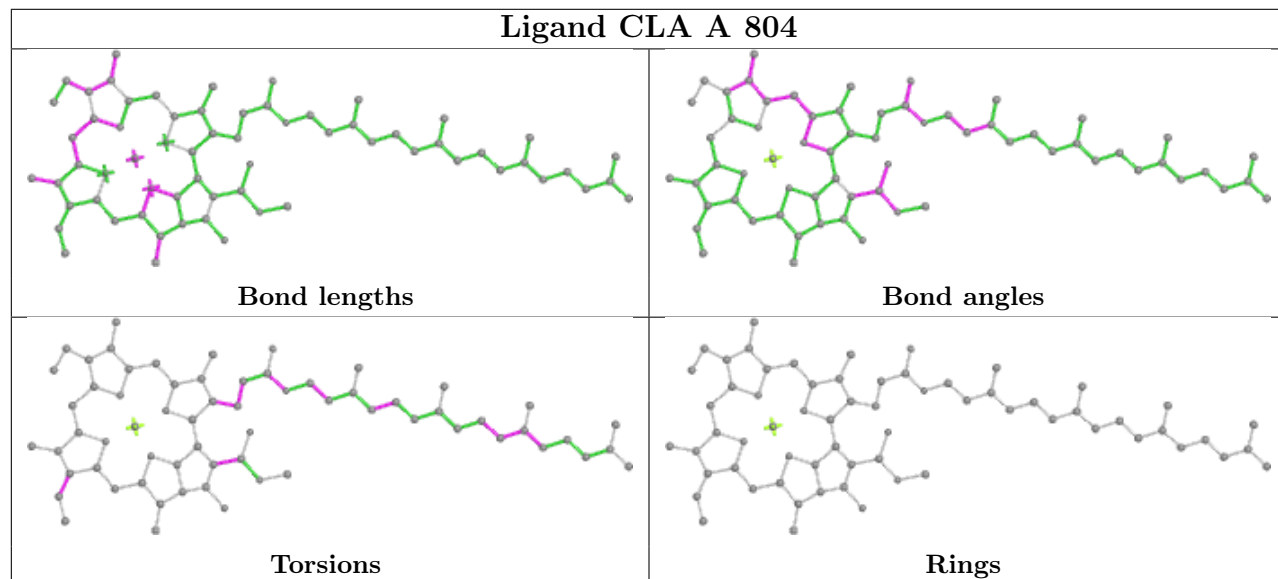
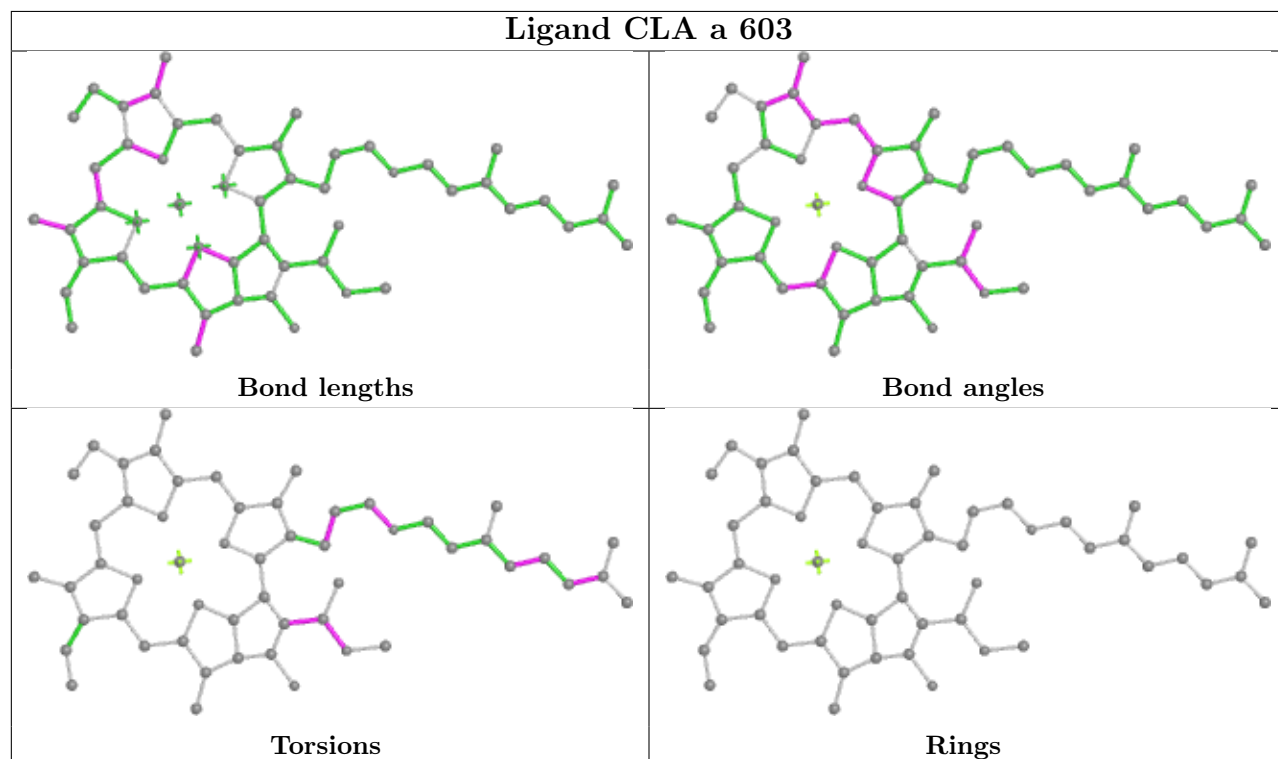


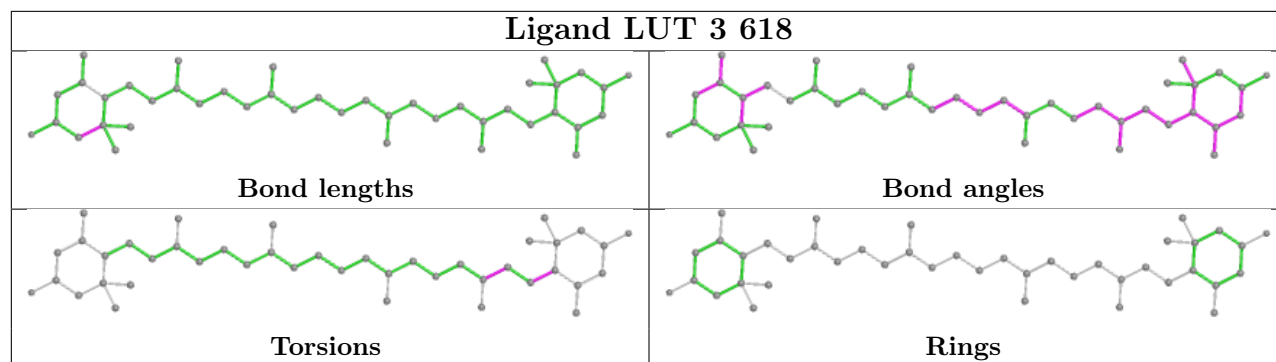
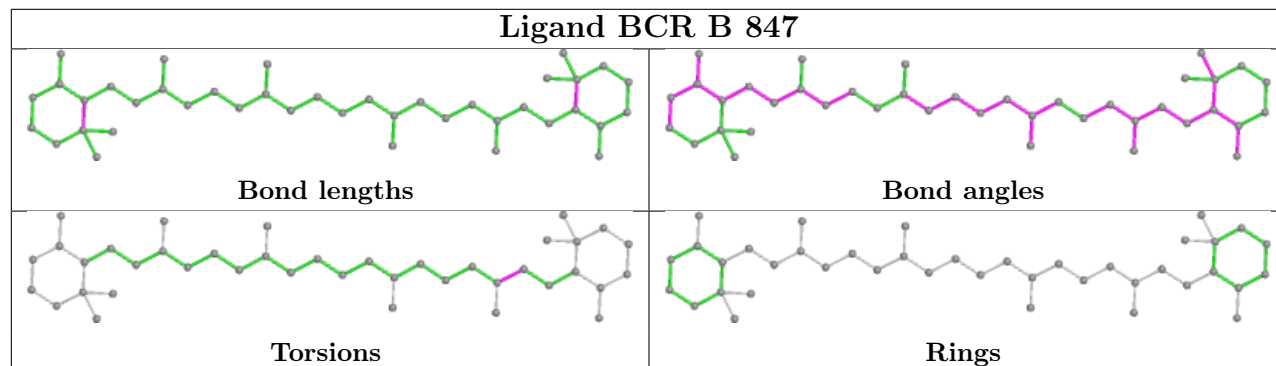
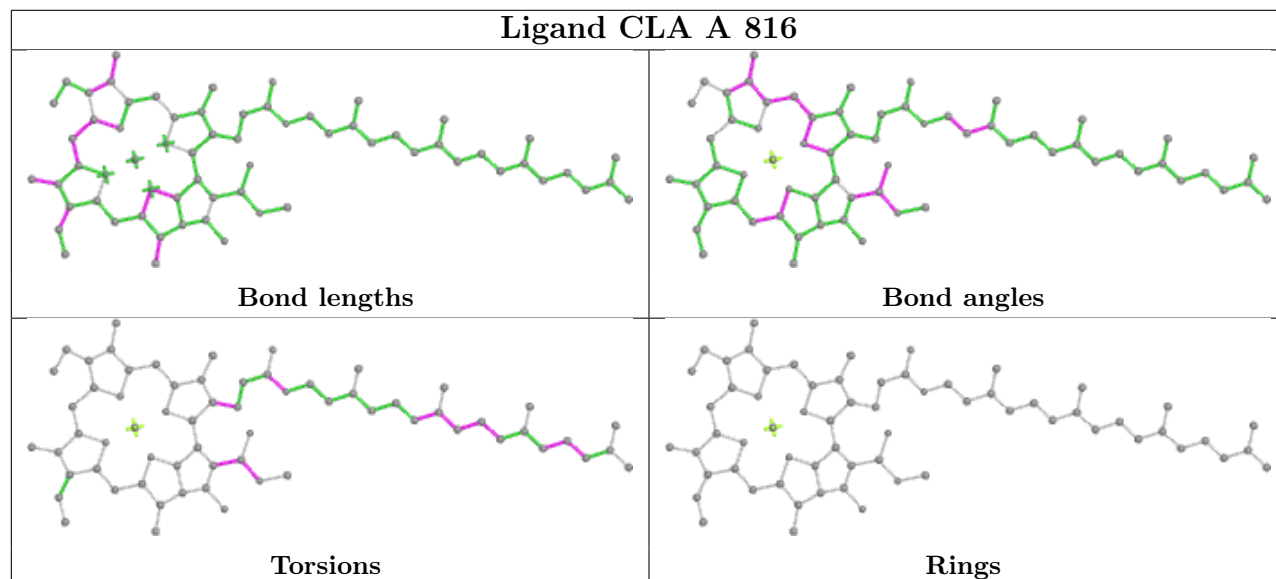
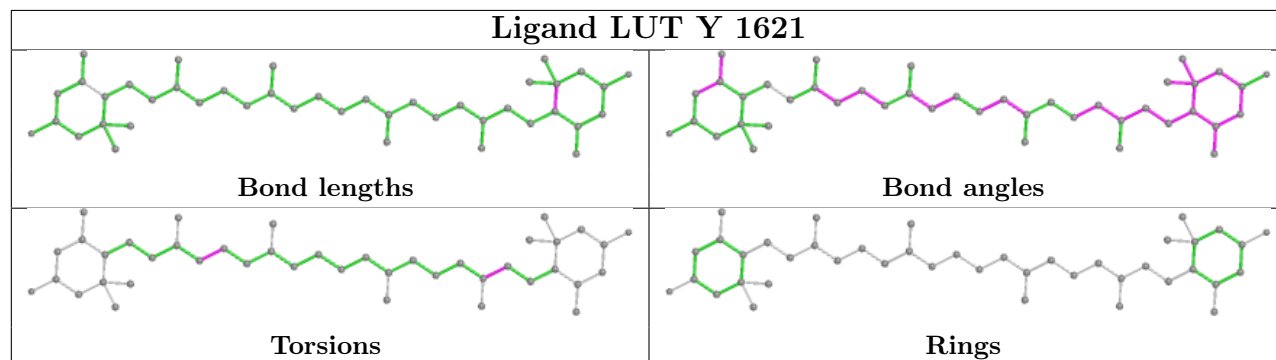
Ligand CLA 6 602

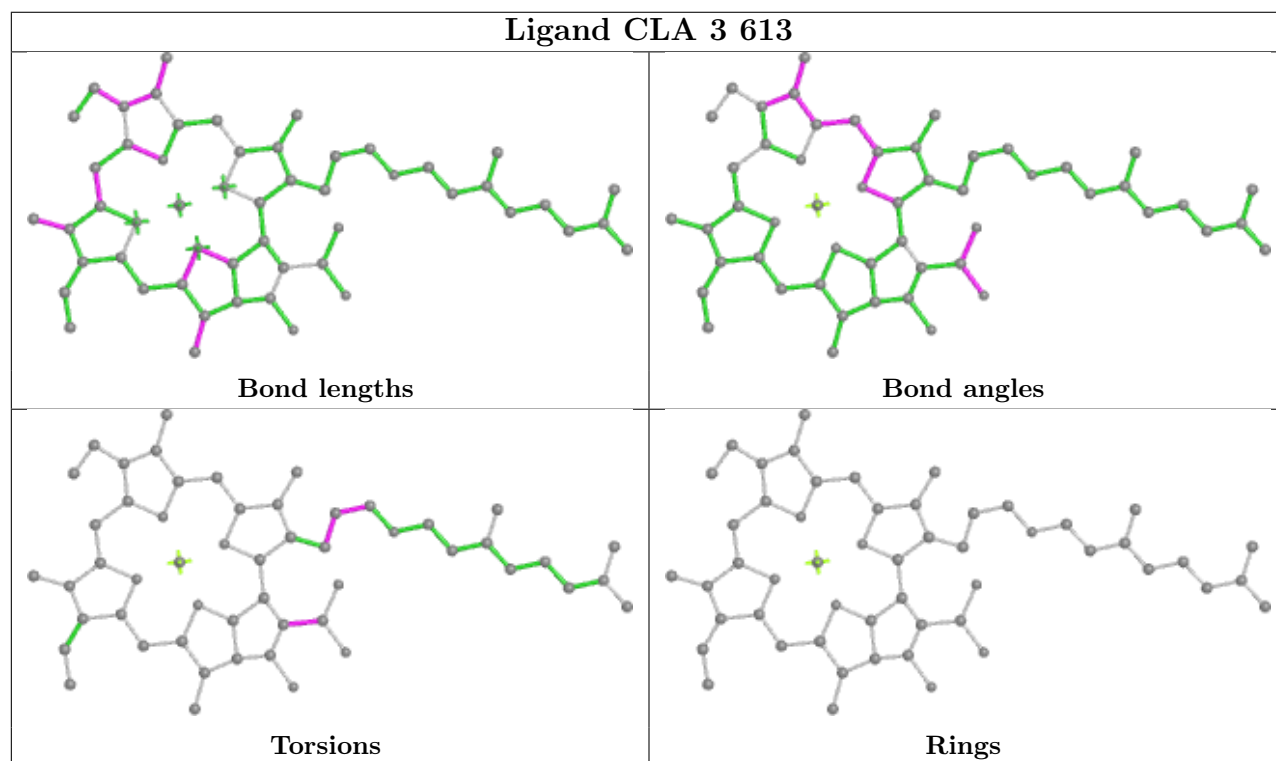
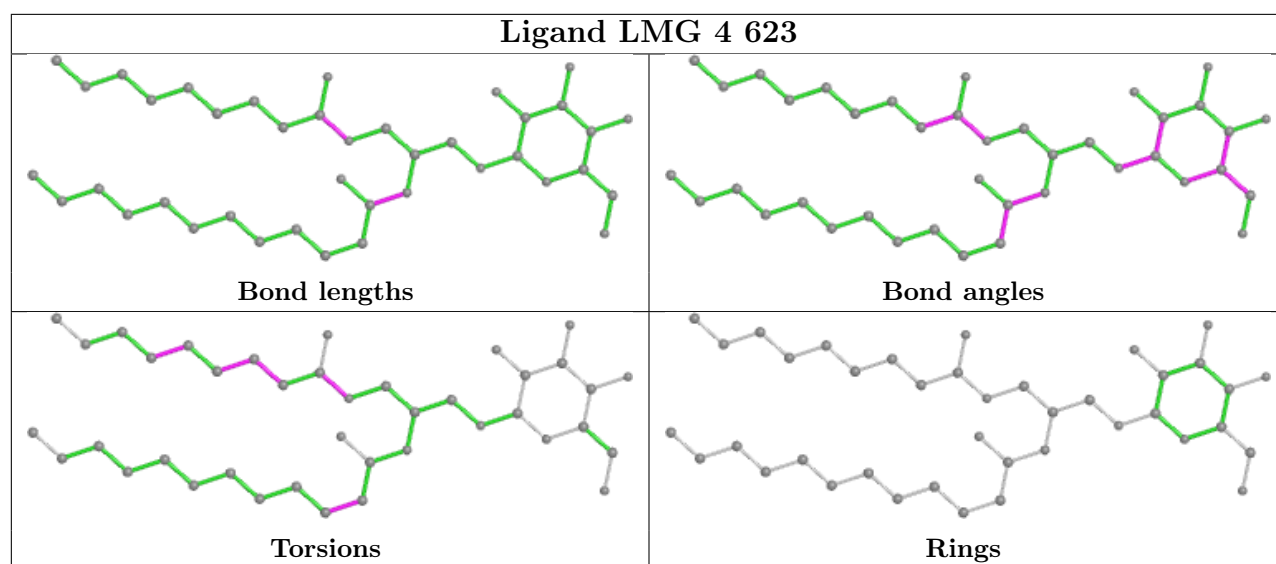


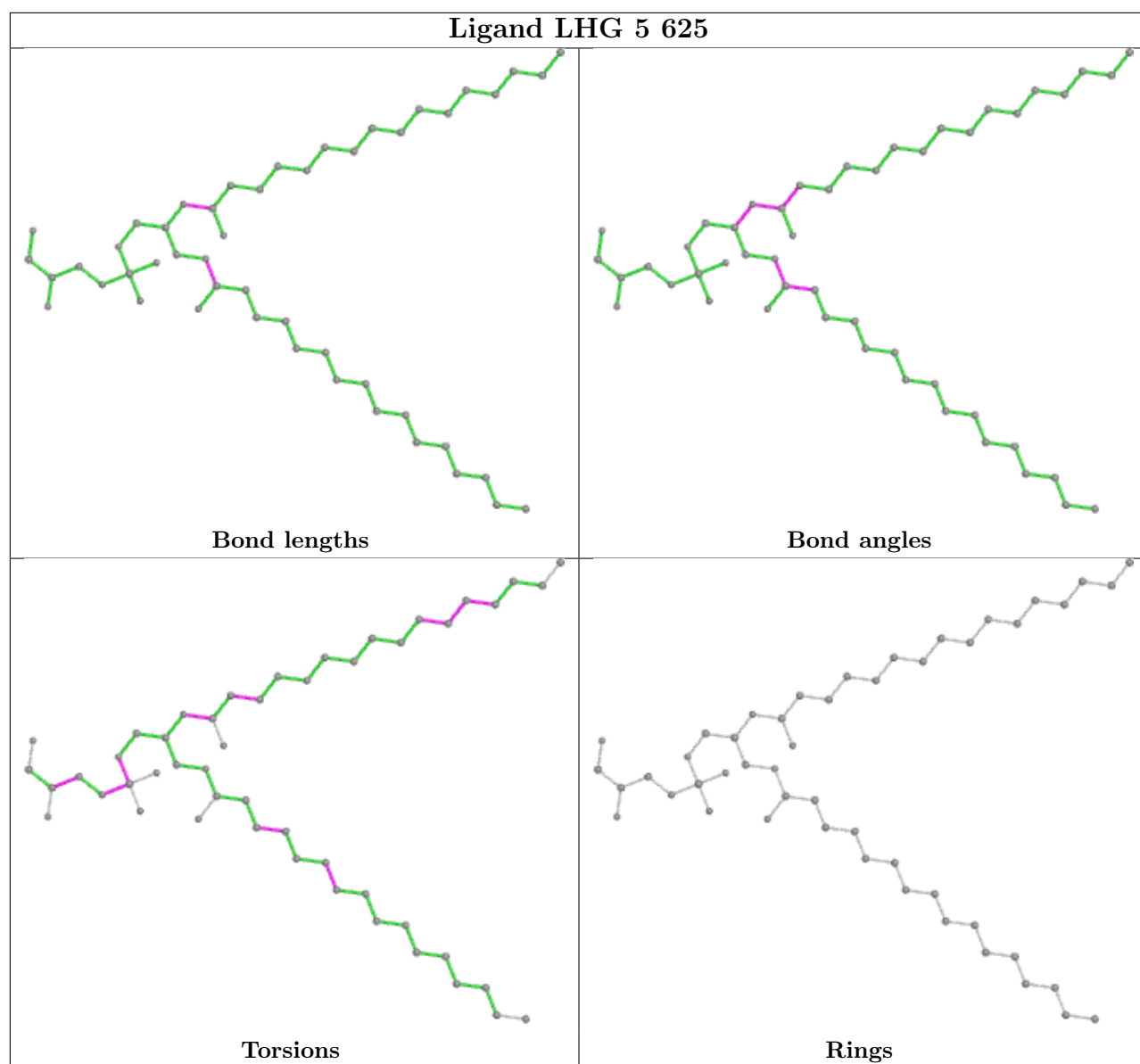
Ligand CHL U 606



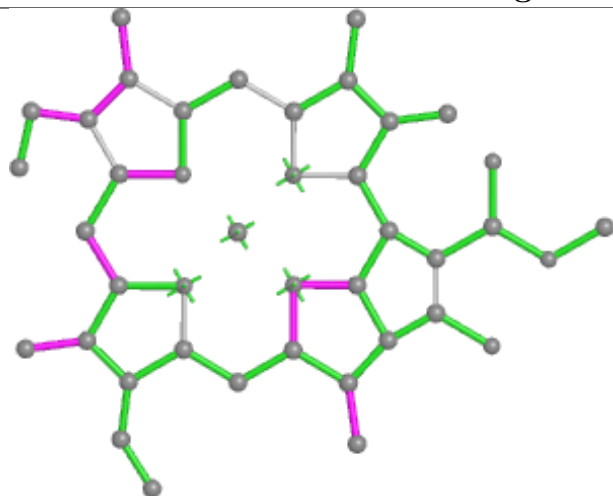
Ligand LUT 5 620**Ligand CLA A 804****Ligand CLA a 603**

Ligand LUT 3 618**Ligand BCR B 847****Ligand CLA A 816****Ligand LUT Y 1621**

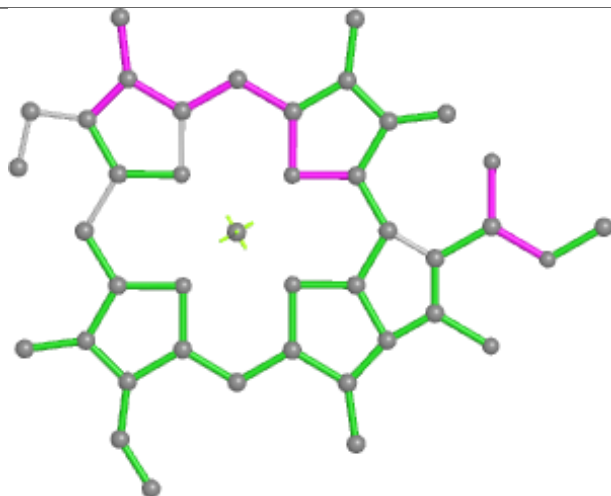




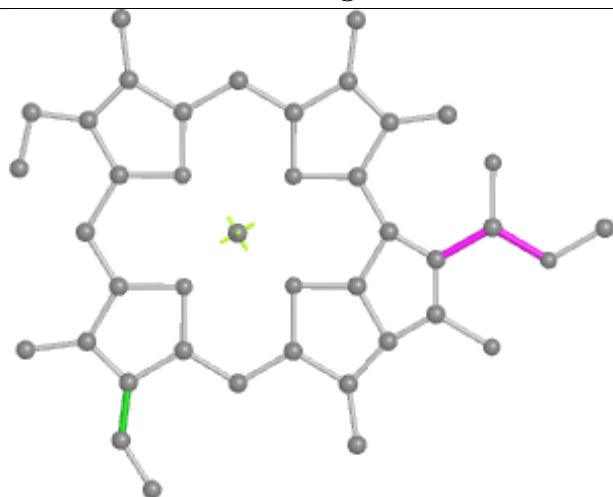
Ligand CLA B 804



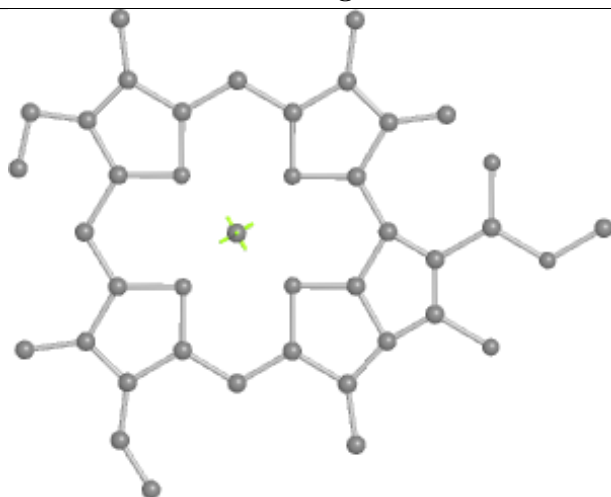
Bond lengths



Bond angles

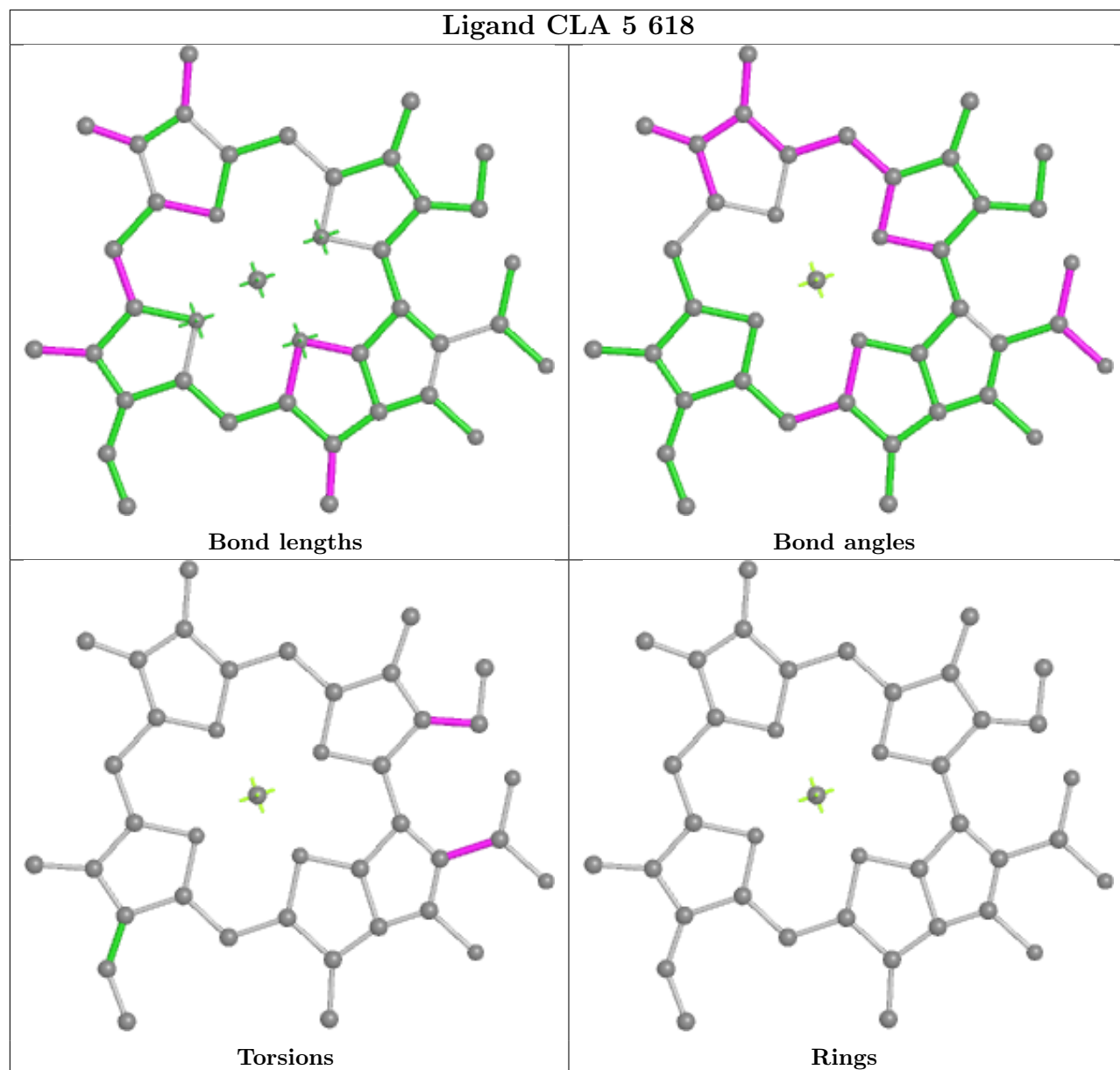


Torsions

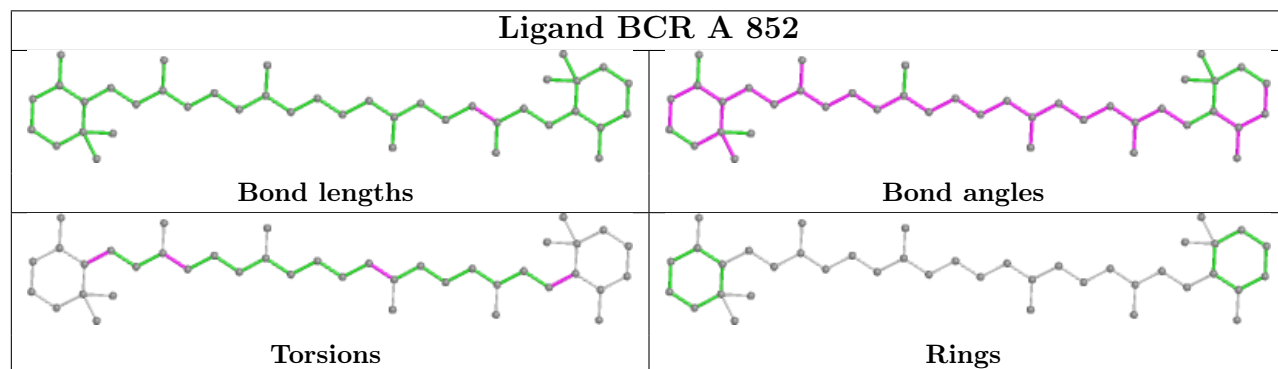


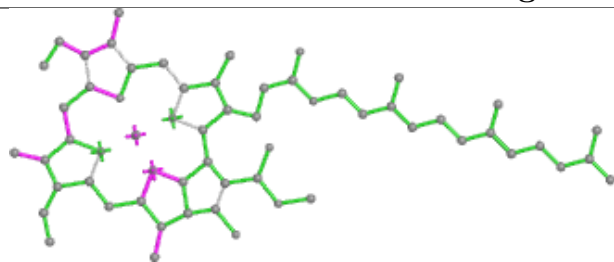
Rings

Ligand CLA 5 618

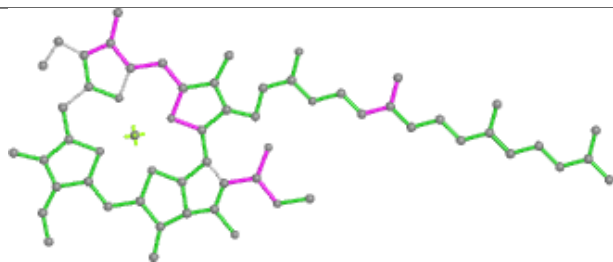


Ligand BCR A 852

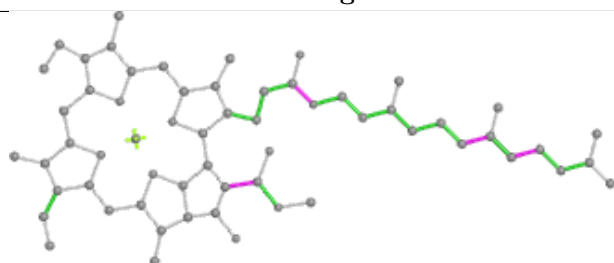


Ligand CLA 7 601

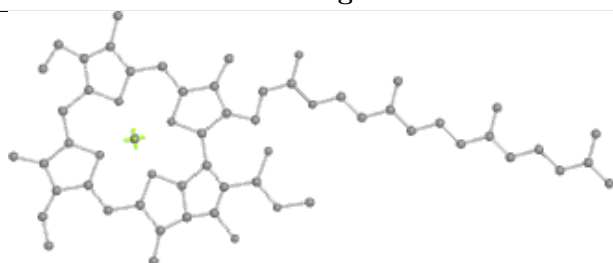
Bond lengths



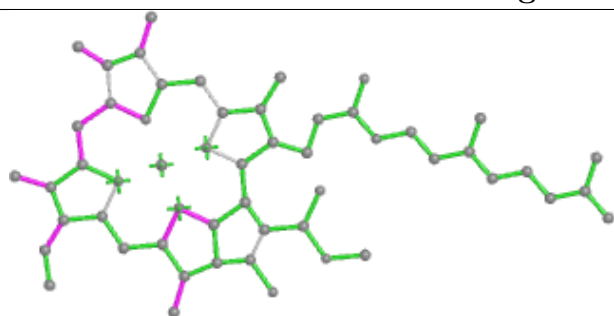
Bond angles



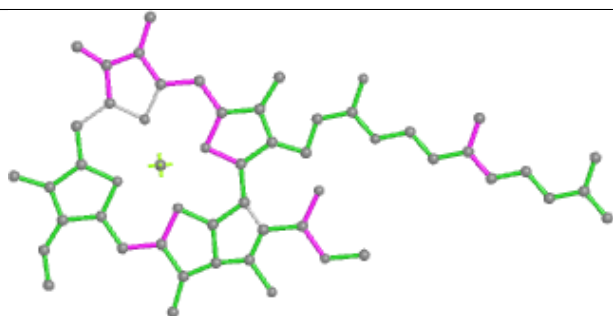
Torsions



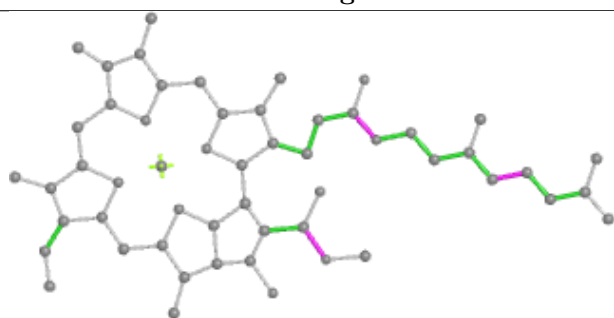
Rings

Ligand CLA 5 603

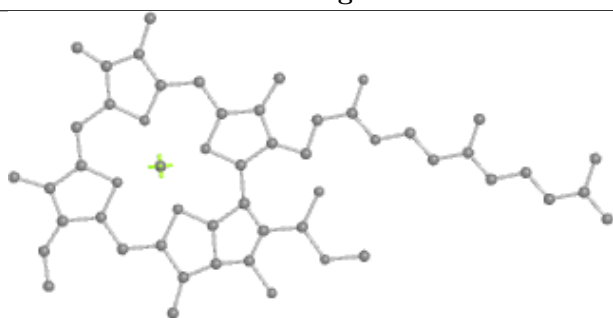
Bond lengths



Bond angles

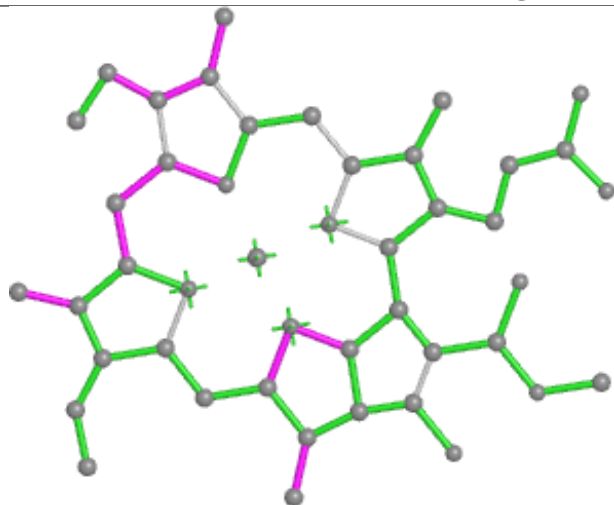


Torsions

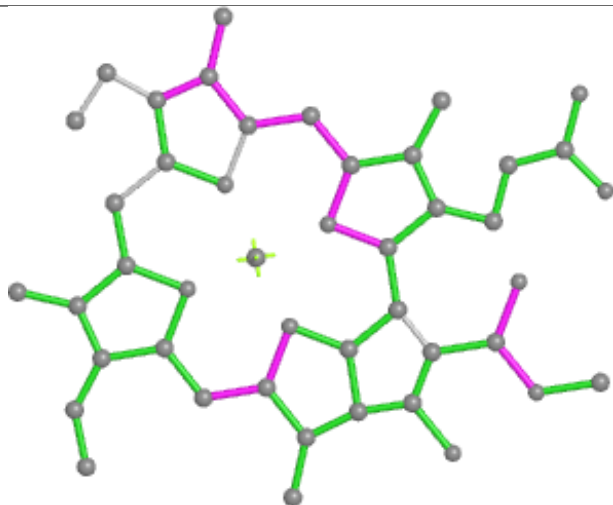


Rings

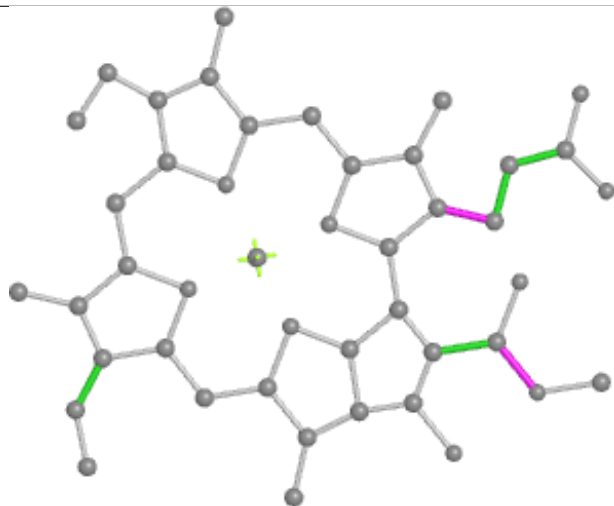
Ligand CLA K 204



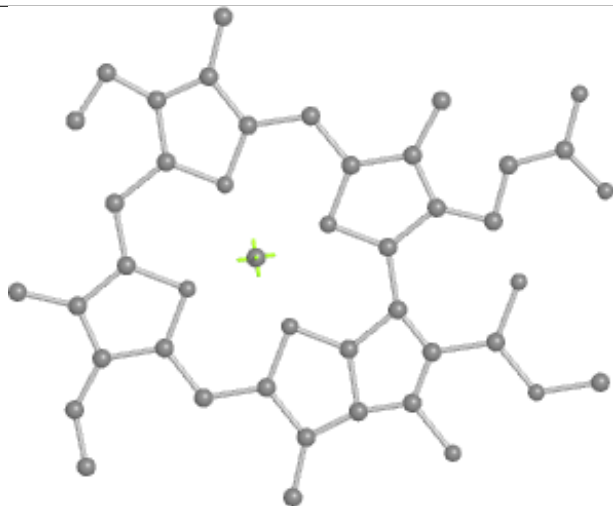
Bond lengths



Bond angles

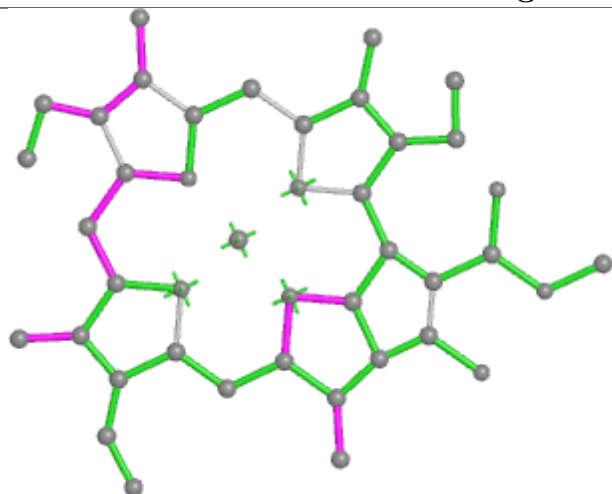


Torsions

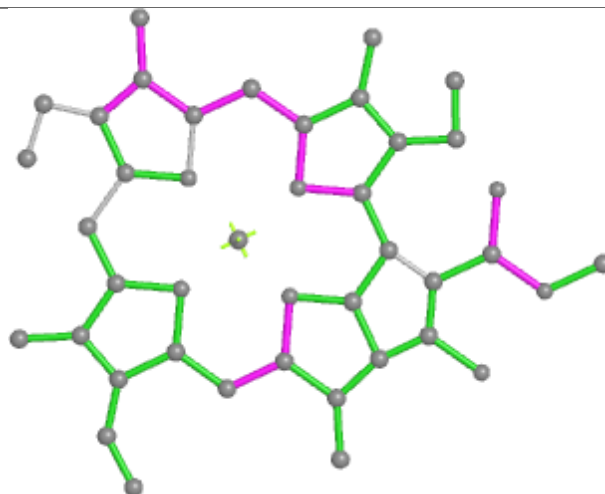


Rings

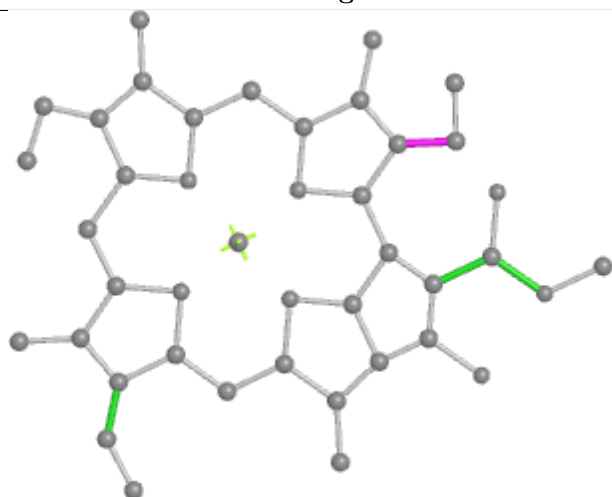
Ligand CLA 7 607



Bond lengths



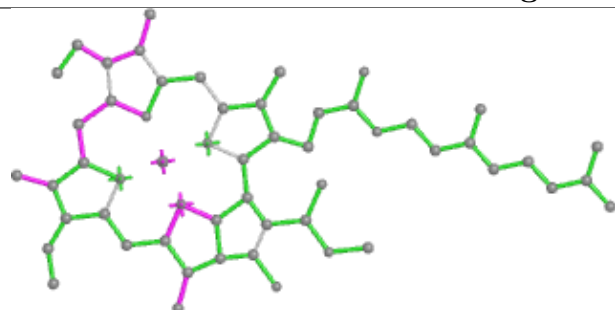
Bond angles



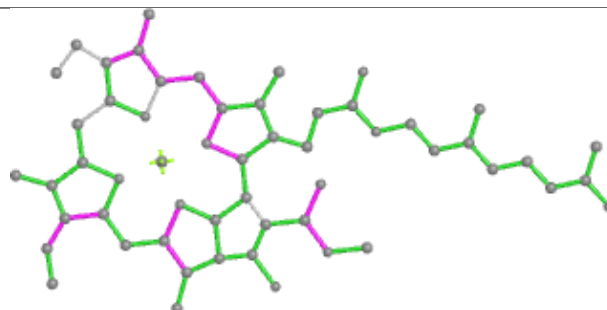
Torsions



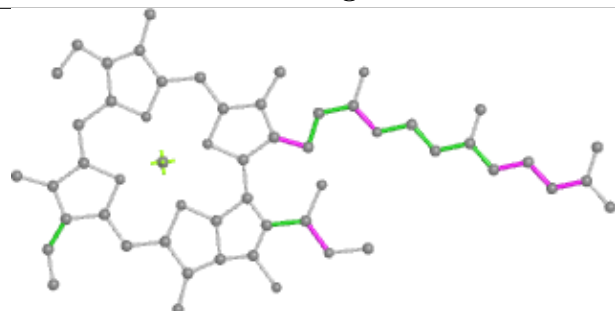
Rings

Ligand CLA 3 603

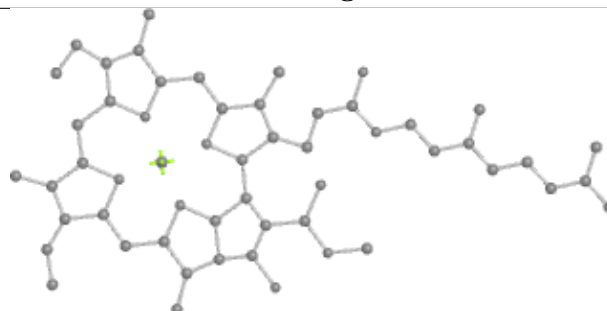
Bond lengths



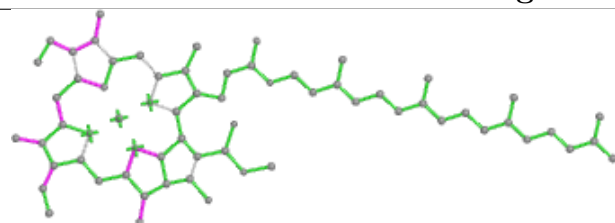
Bond angles



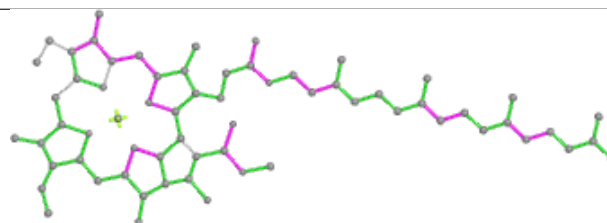
Torsions



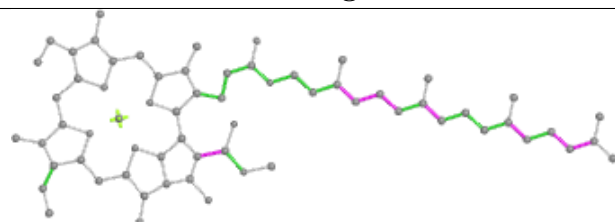
Rings

Ligand CLA B 808

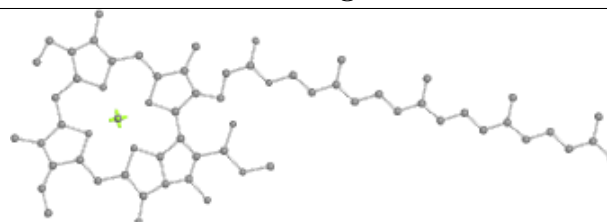
Bond lengths



Bond angles

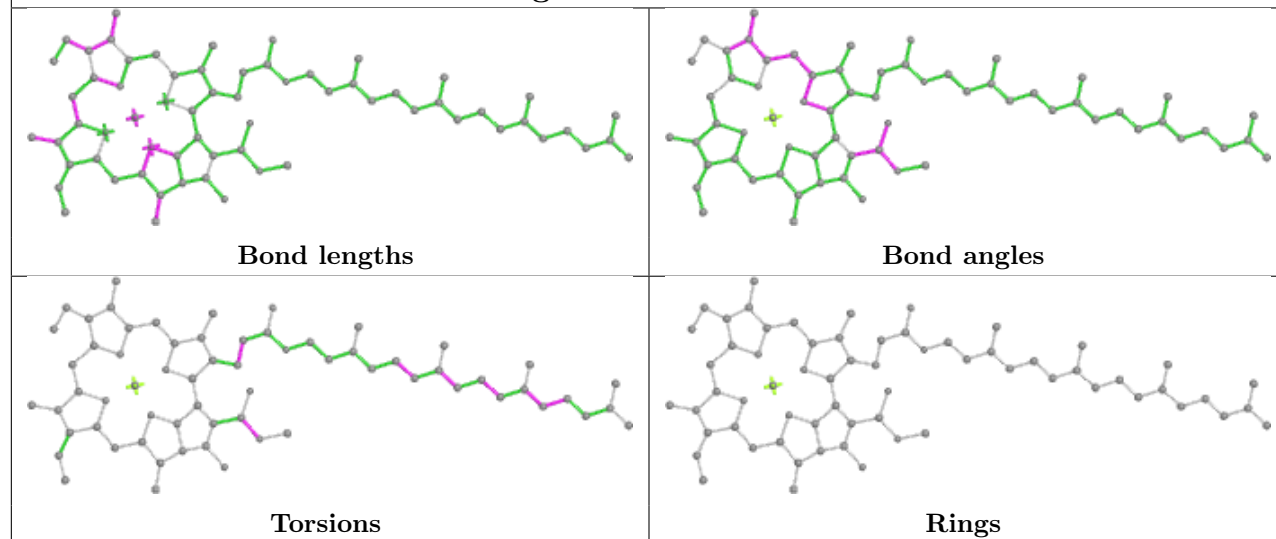


Torsions

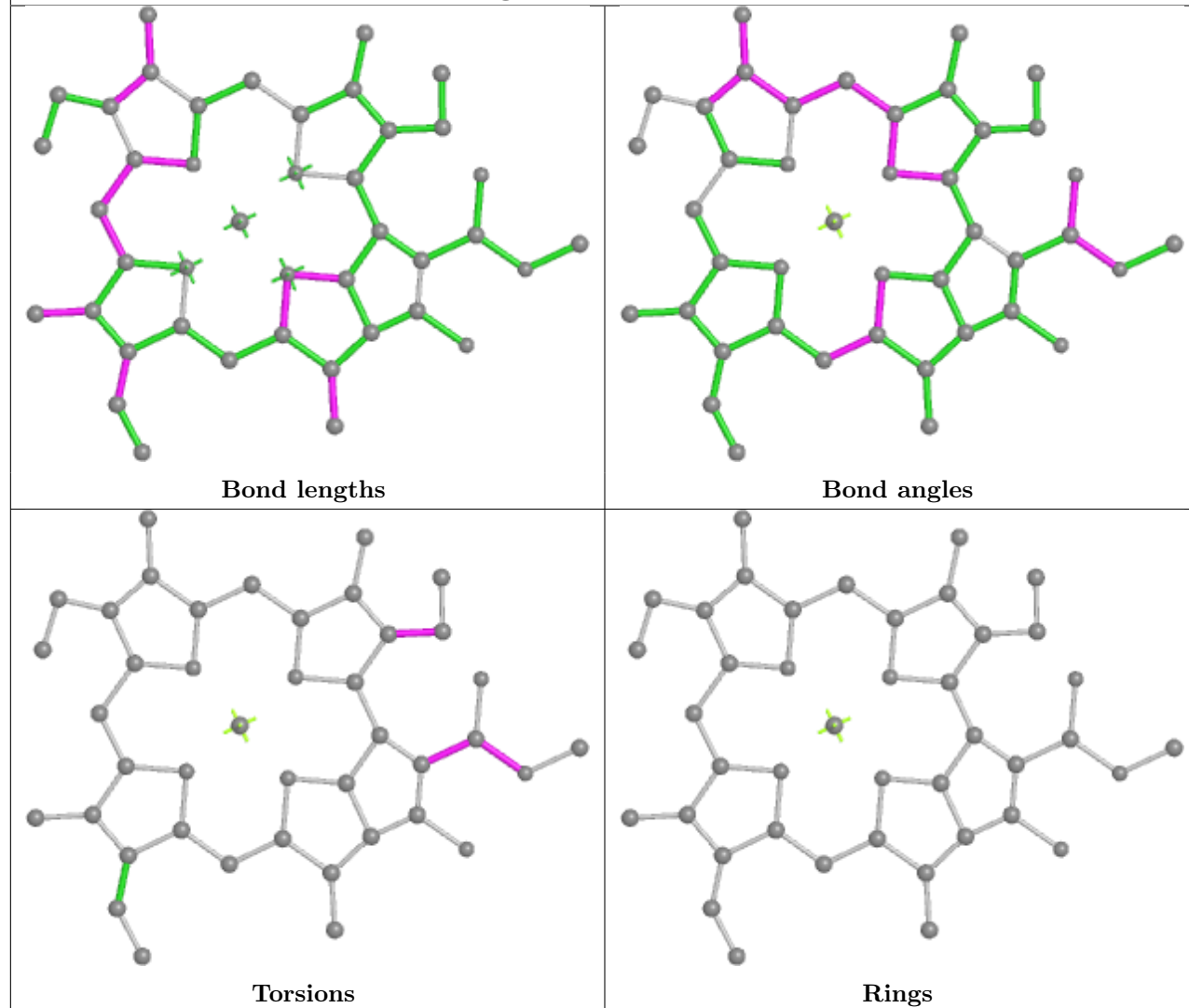


Rings

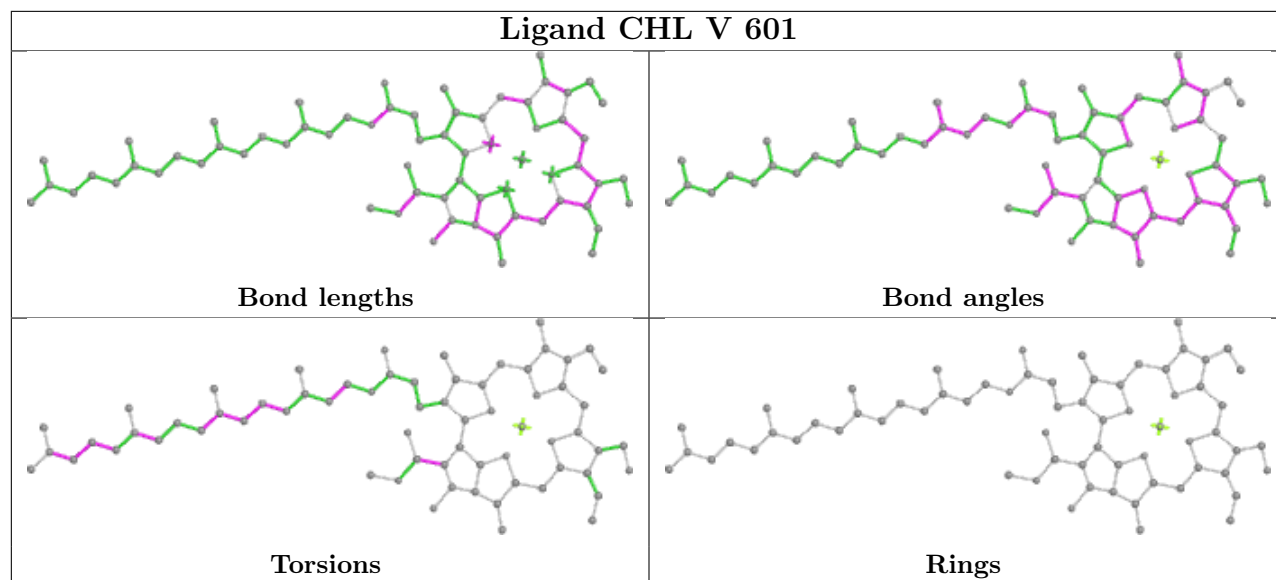
Ligand CLA B 824



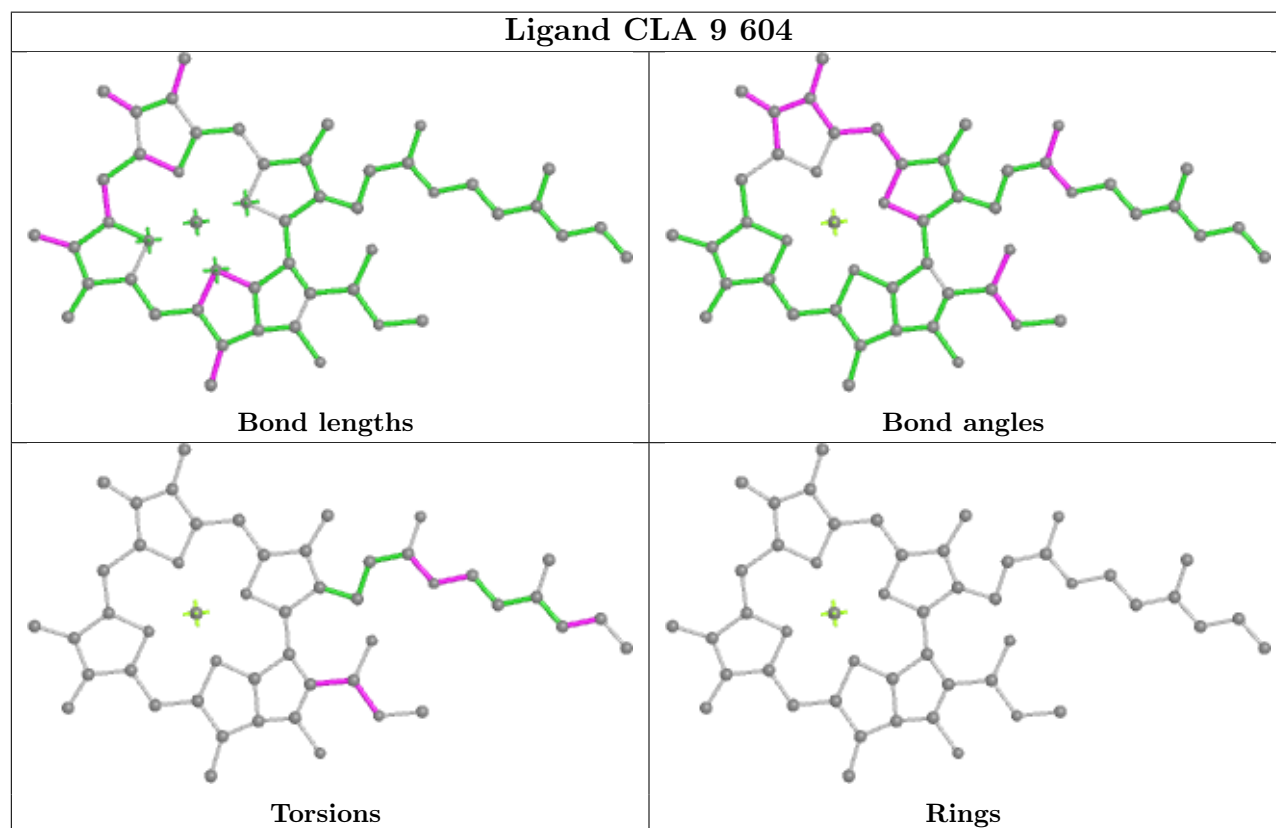
Ligand CLA F 303

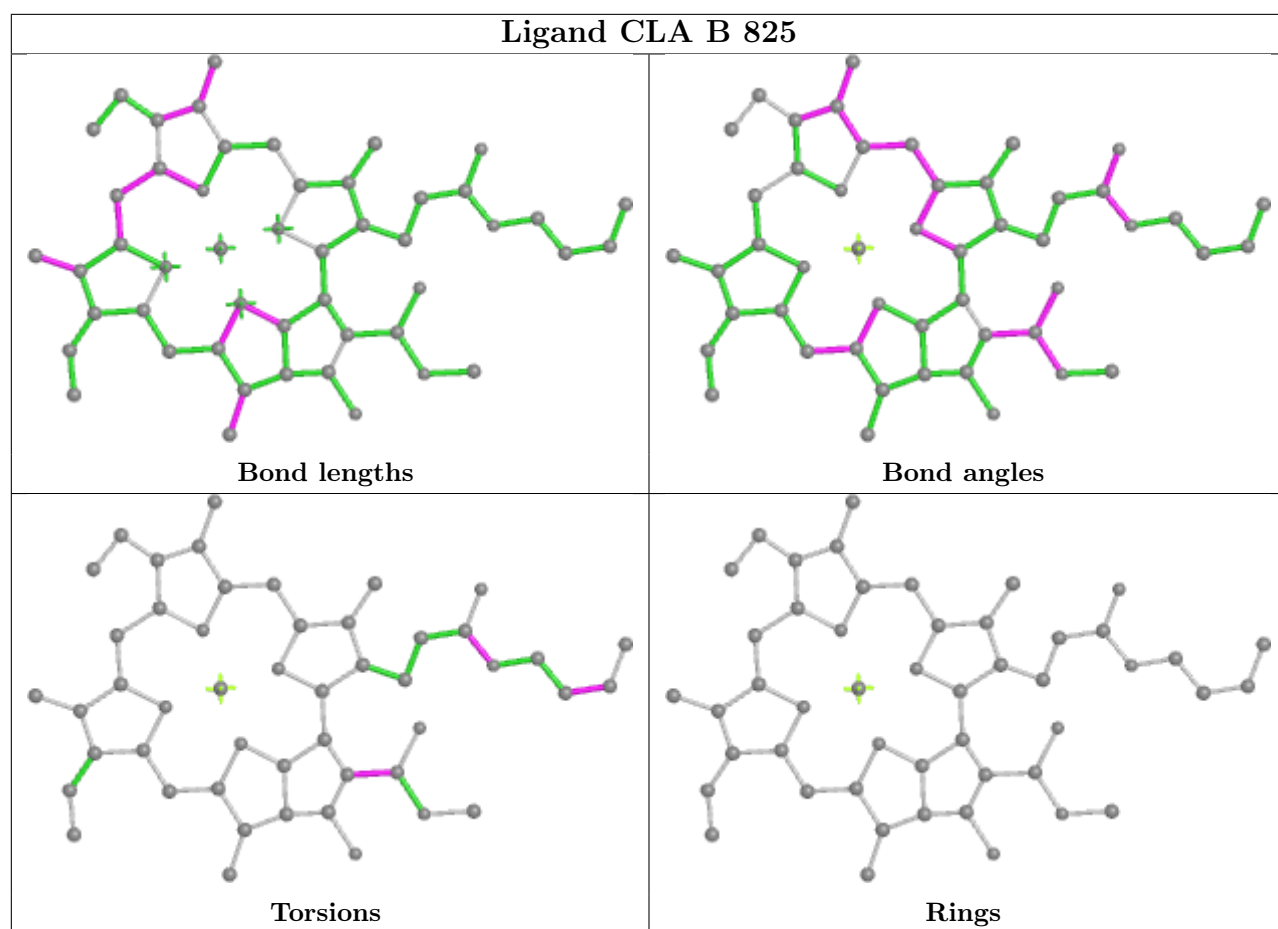


Ligand CHL V 601

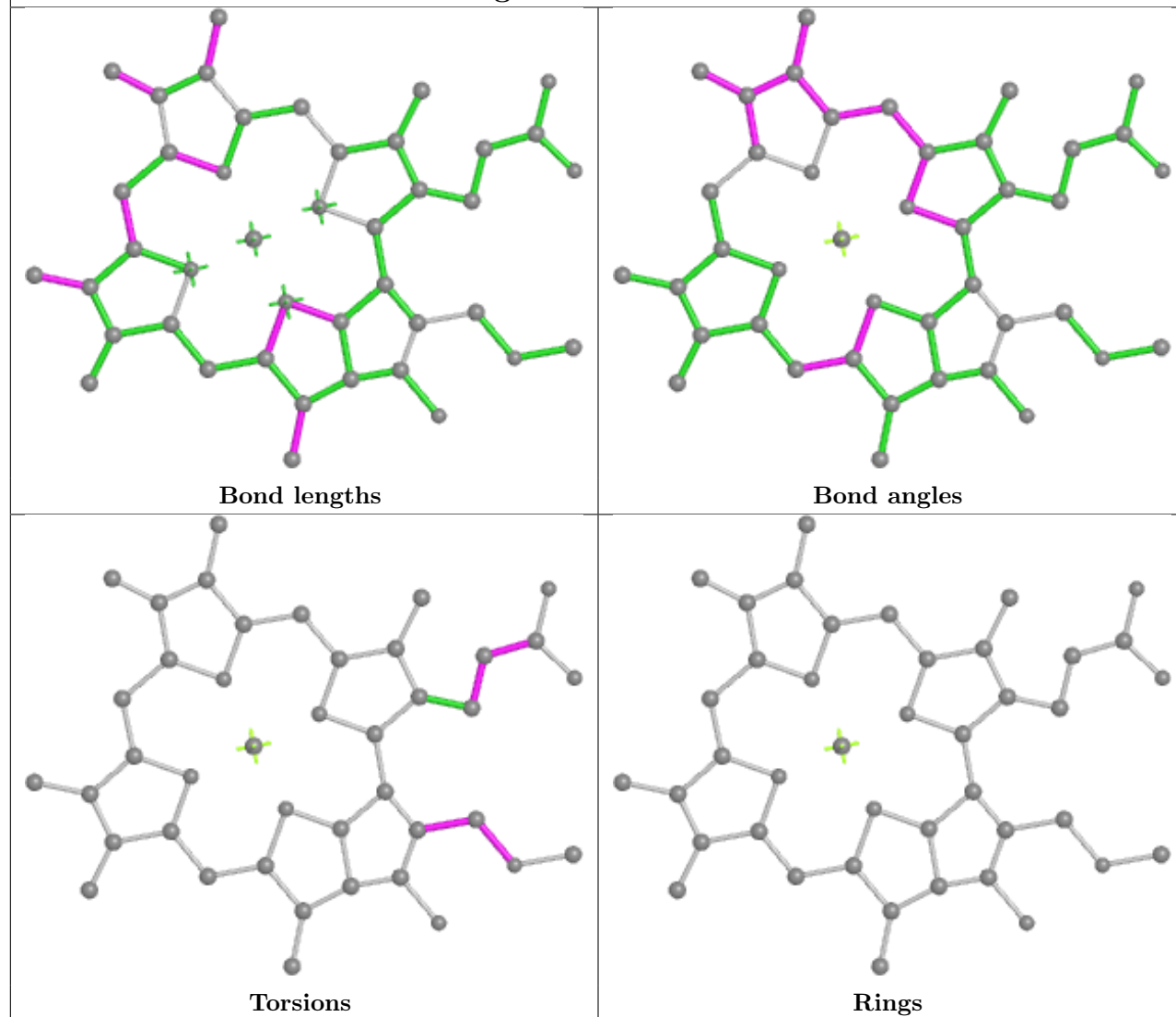


Ligand CLA 9 604

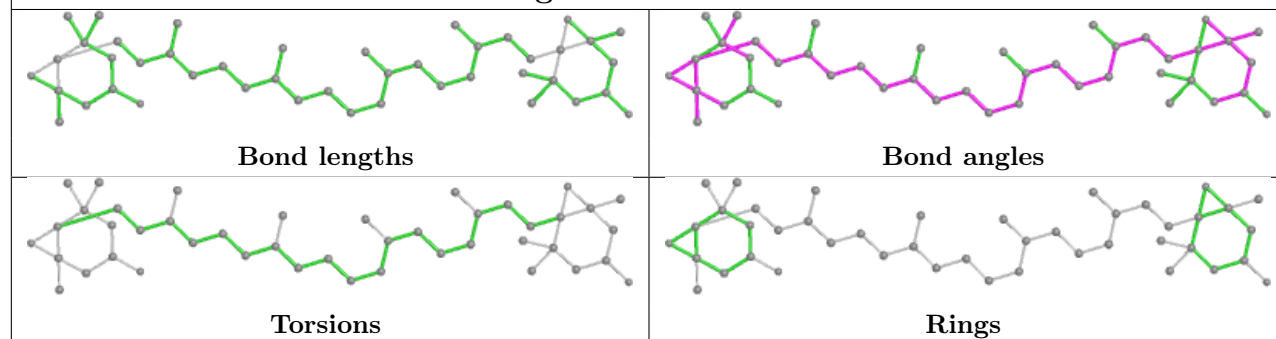


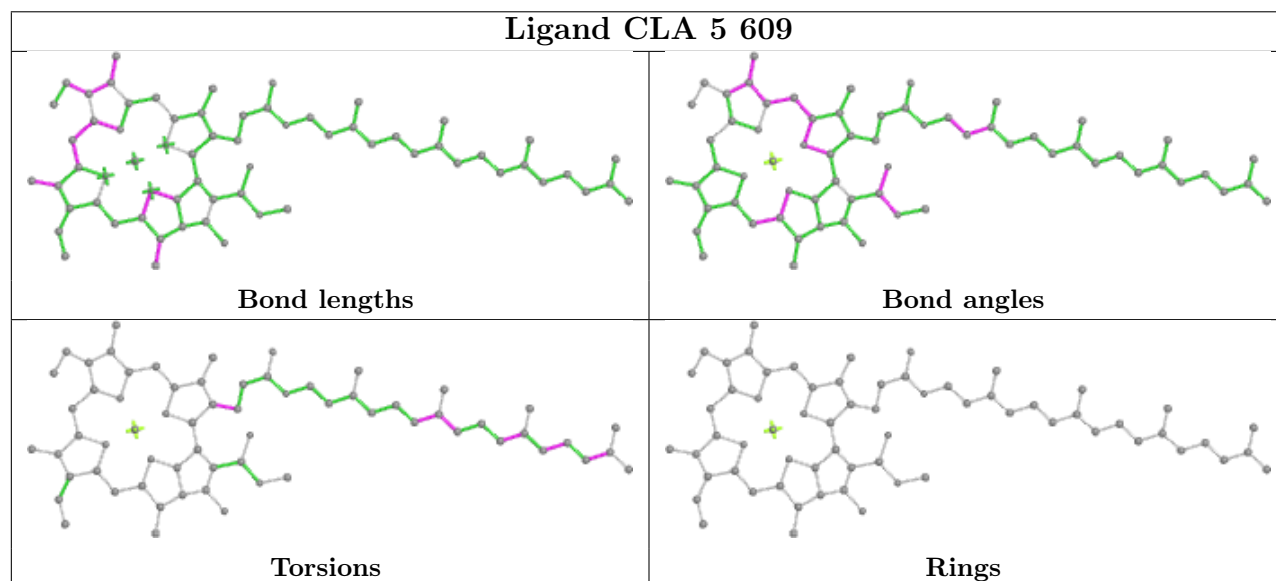
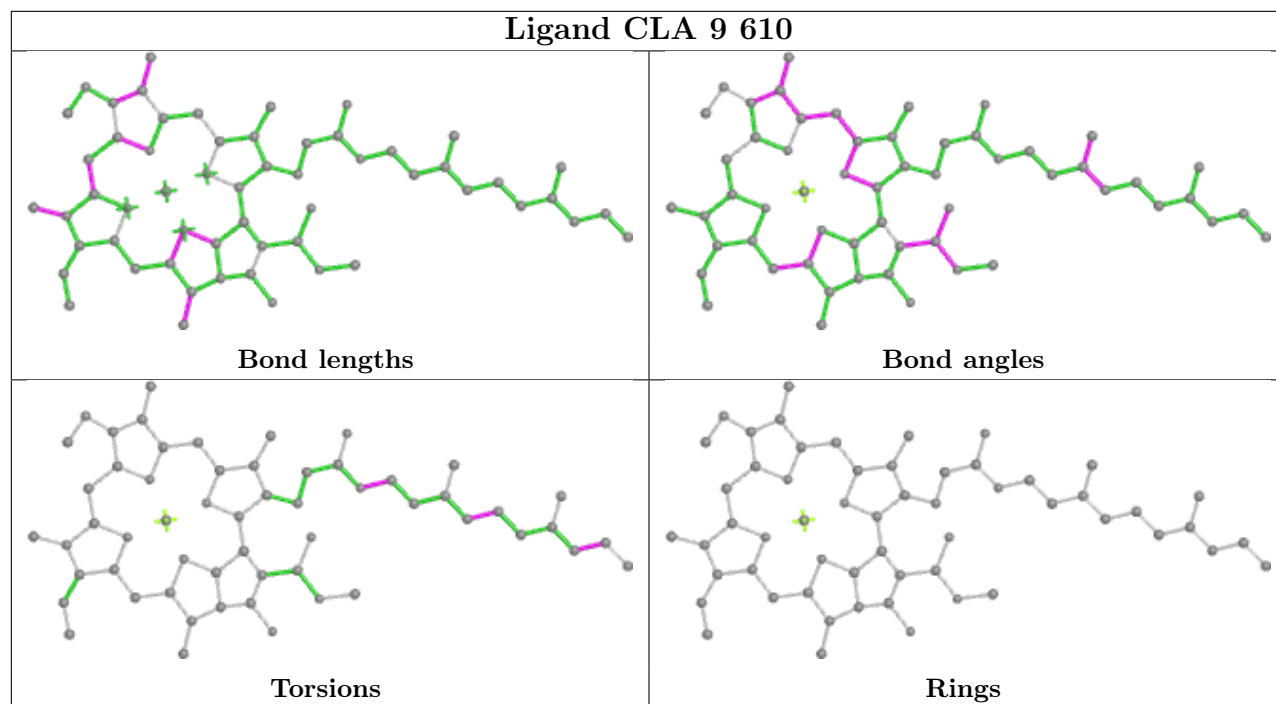
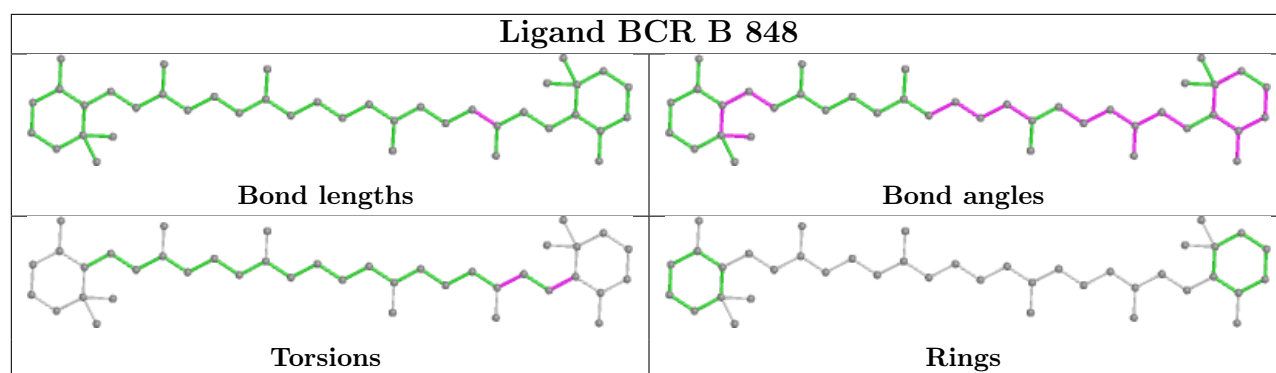


Ligand CLA 7 615

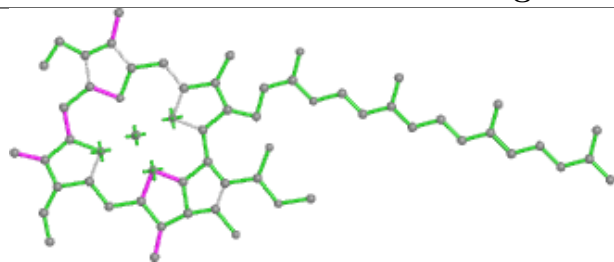


Ligand XAT 1 618

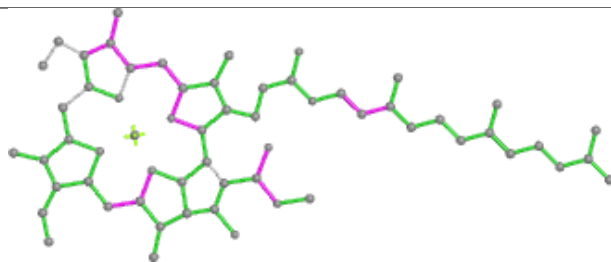




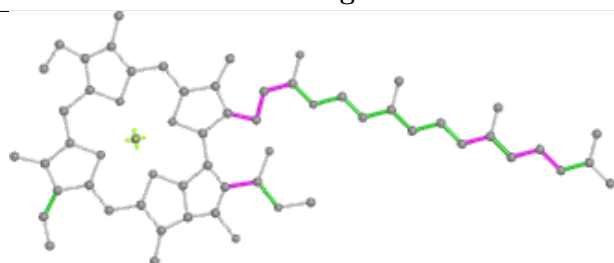
Ligand CLA V 602



Bond lengths



Bond angles

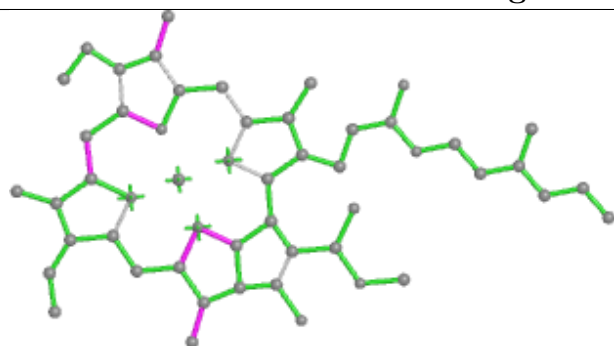


Torsions

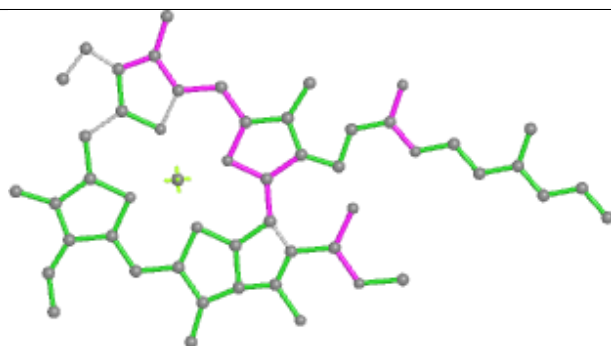


Rings

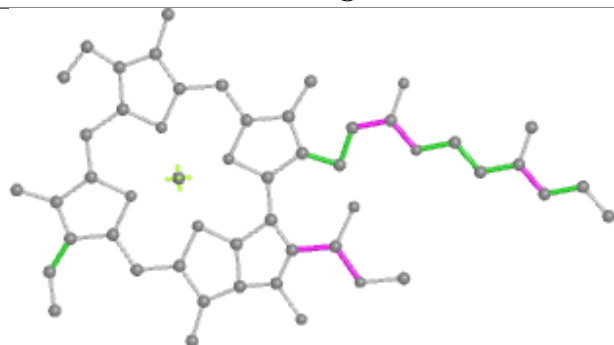
Ligand CLA W 603



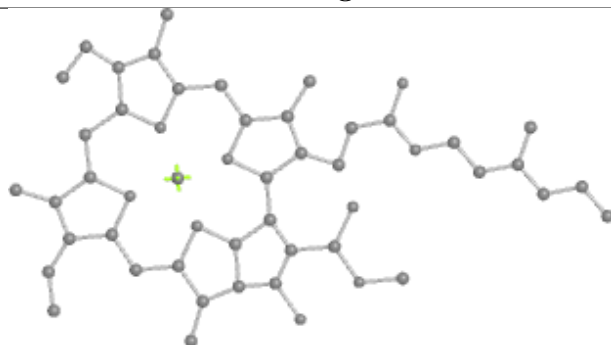
Bond lengths



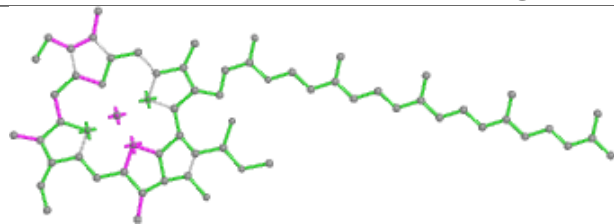
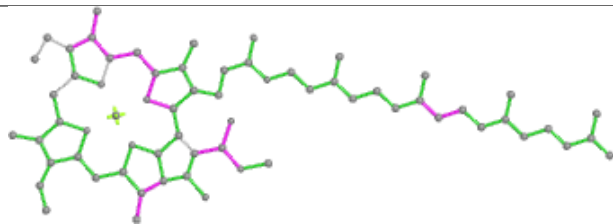
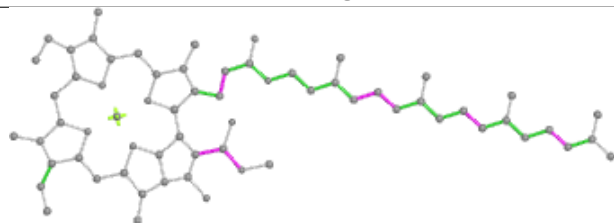
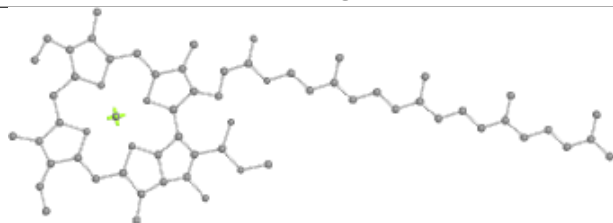
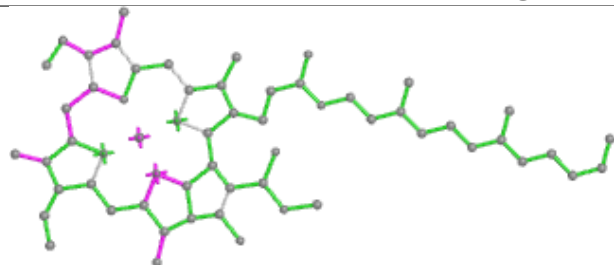
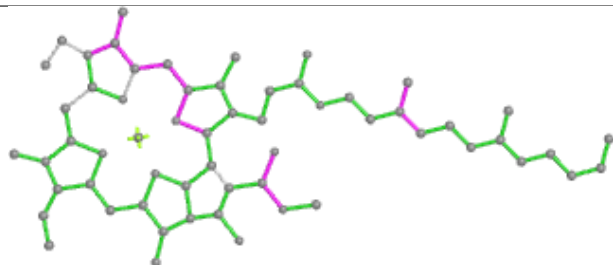
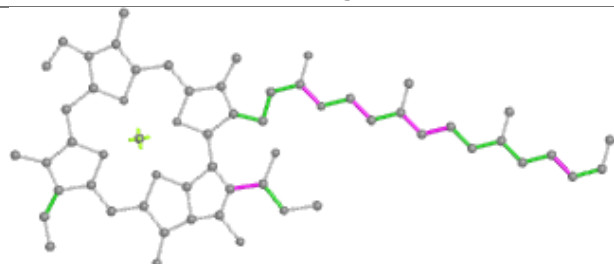
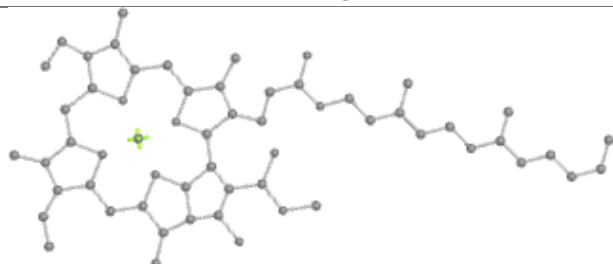
Bond angles

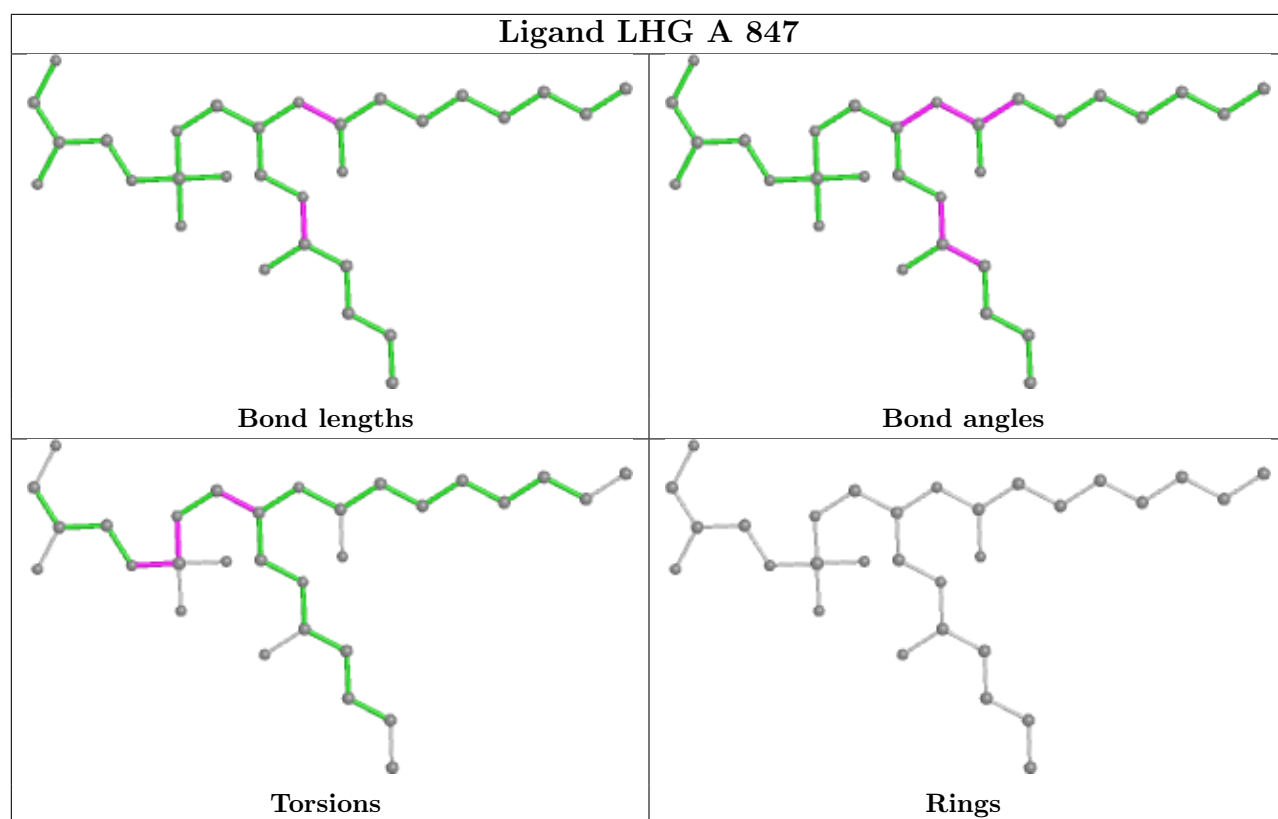


Torsions

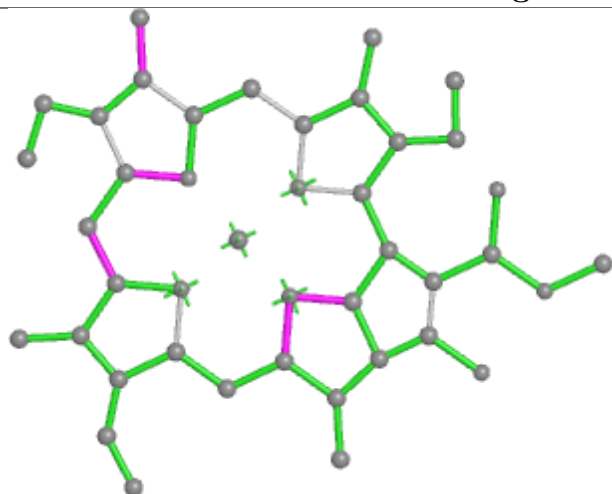


Rings

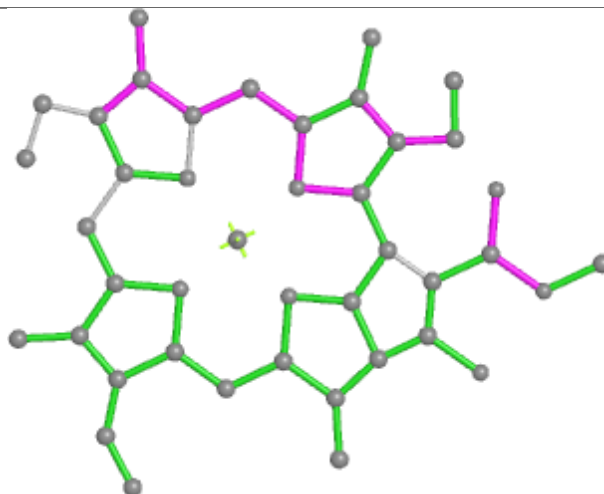
Ligand CLA A 854**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 817****Bond lengths****Bond angles****Torsions****Rings**



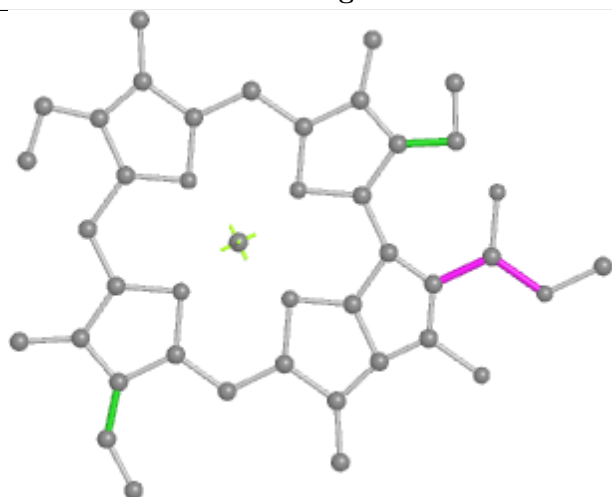
Ligand CLA U 612



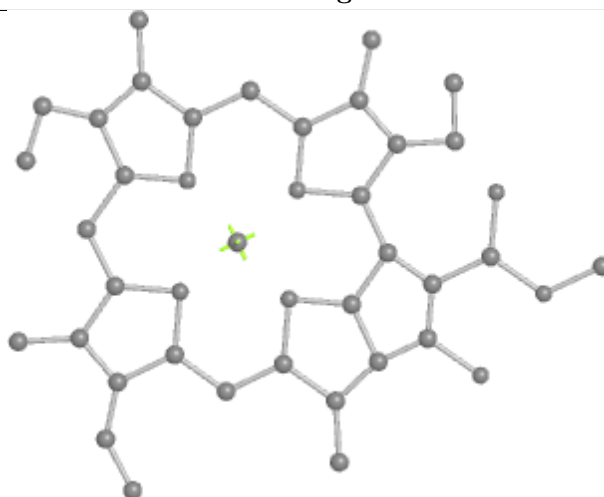
Bond lengths



Bond angles

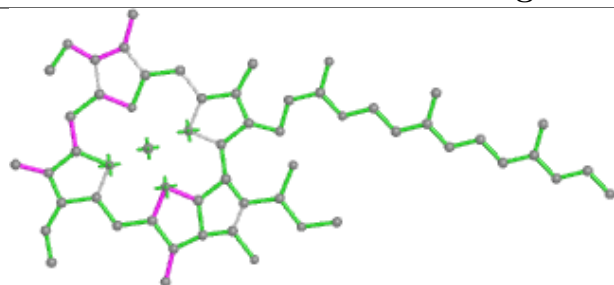


Torsions

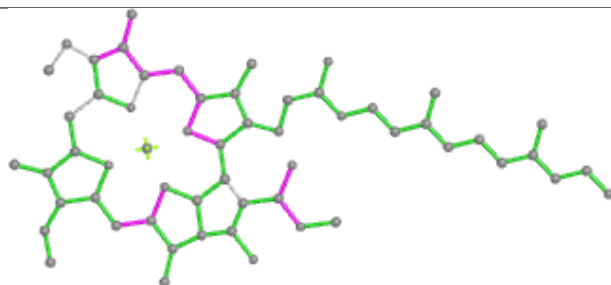


Rings

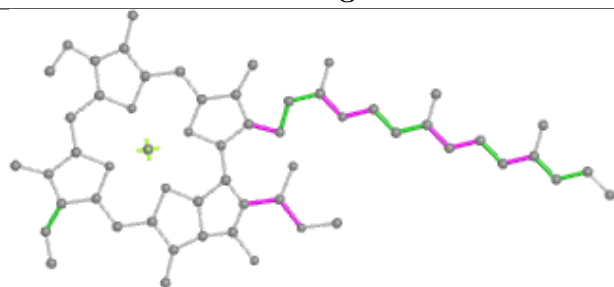
Ligand CLA F 301



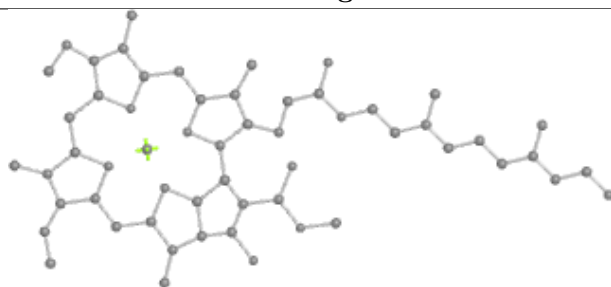
Bond lengths



Bond angles

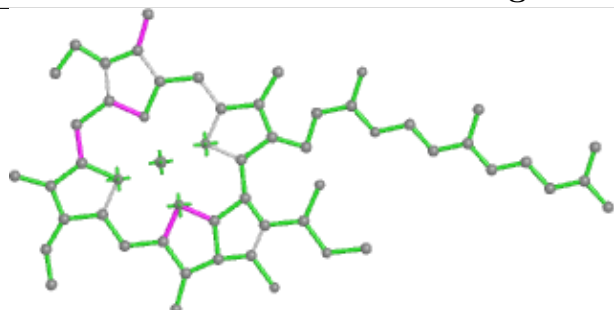


Torsions

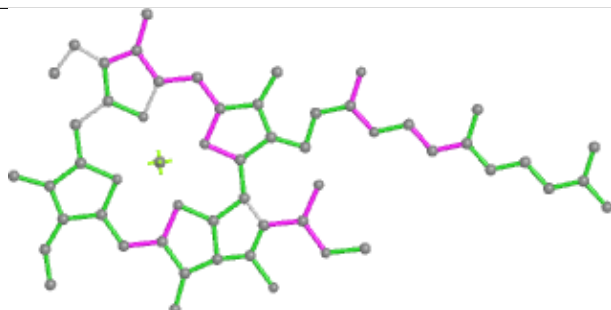


Rings

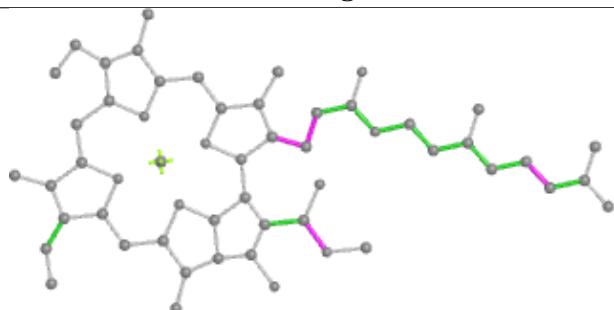
Ligand CLA W 610



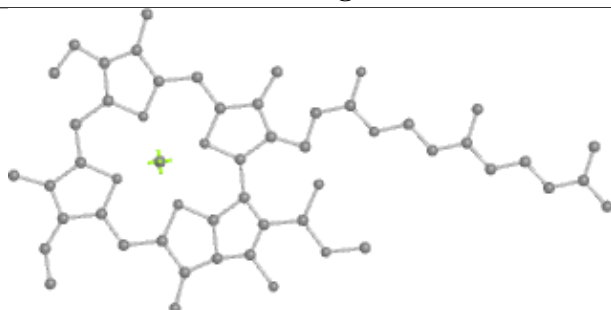
Bond lengths



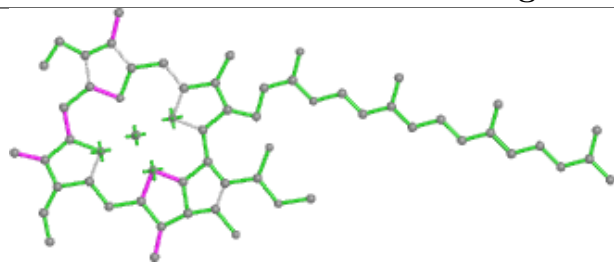
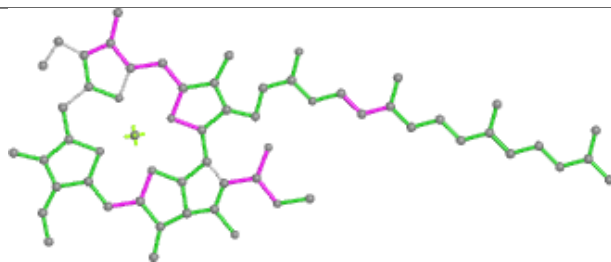
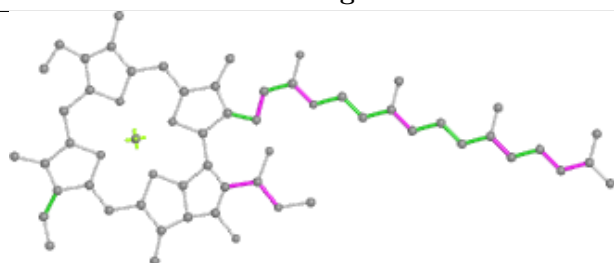
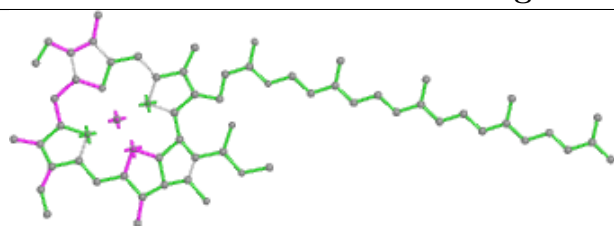
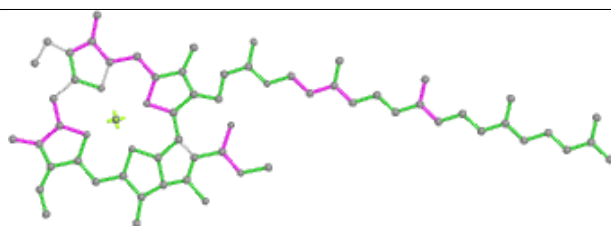
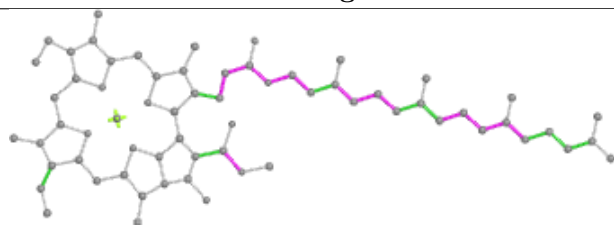
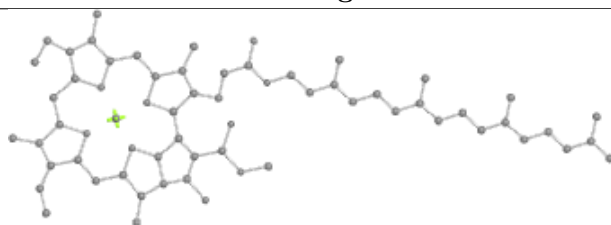
Bond angles



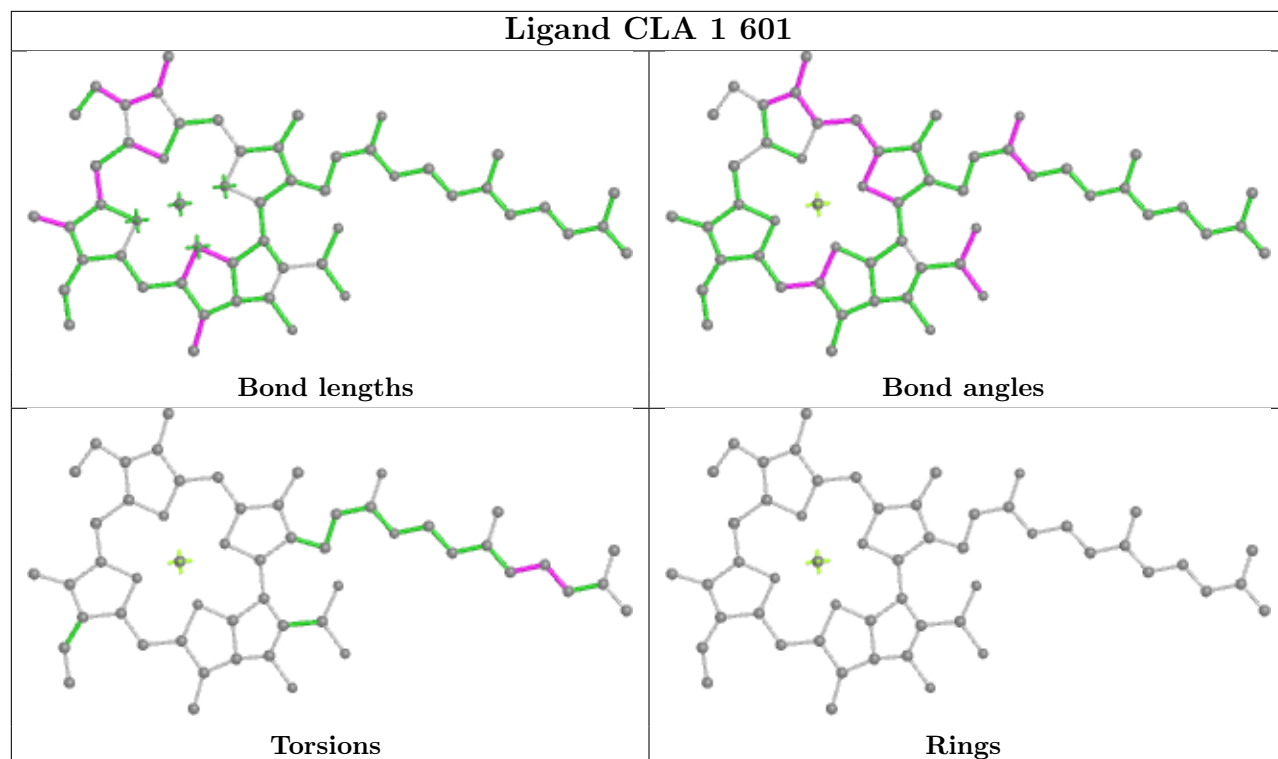
Torsions



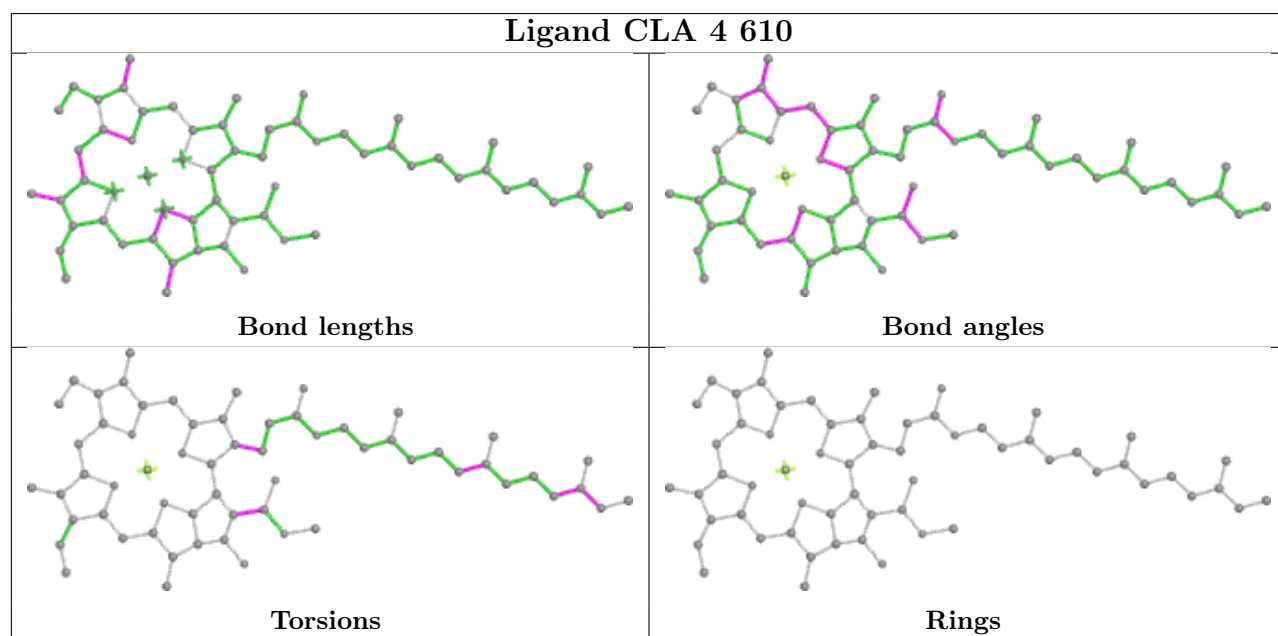
Rings

Ligand CLA 8 602**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 806****Bond lengths****Bond angles****Torsions****Rings**

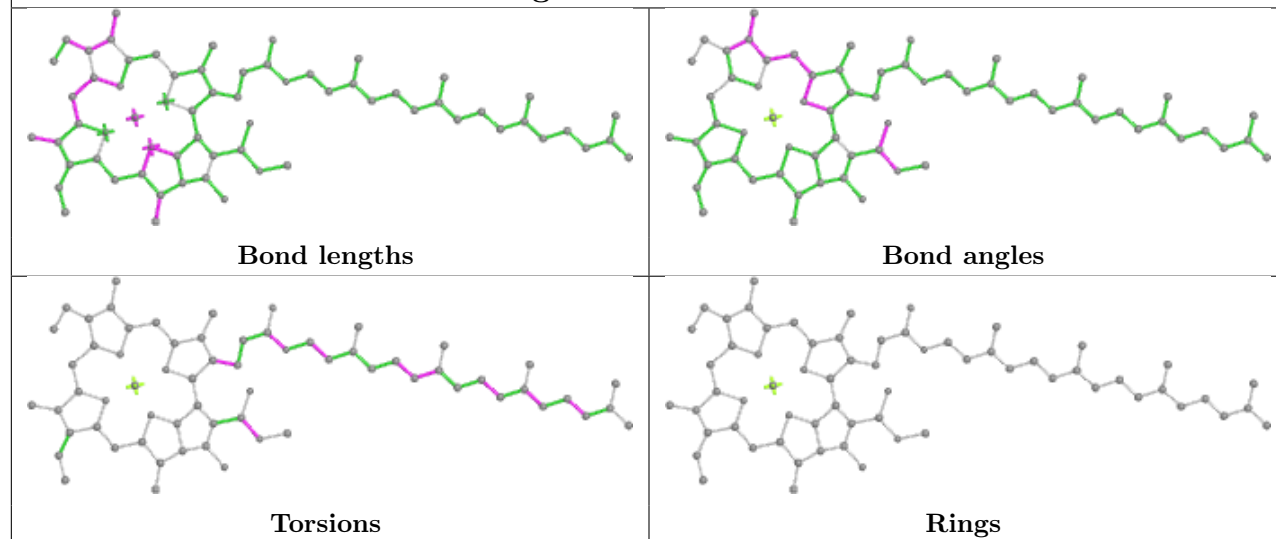
Ligand CLA 1 601



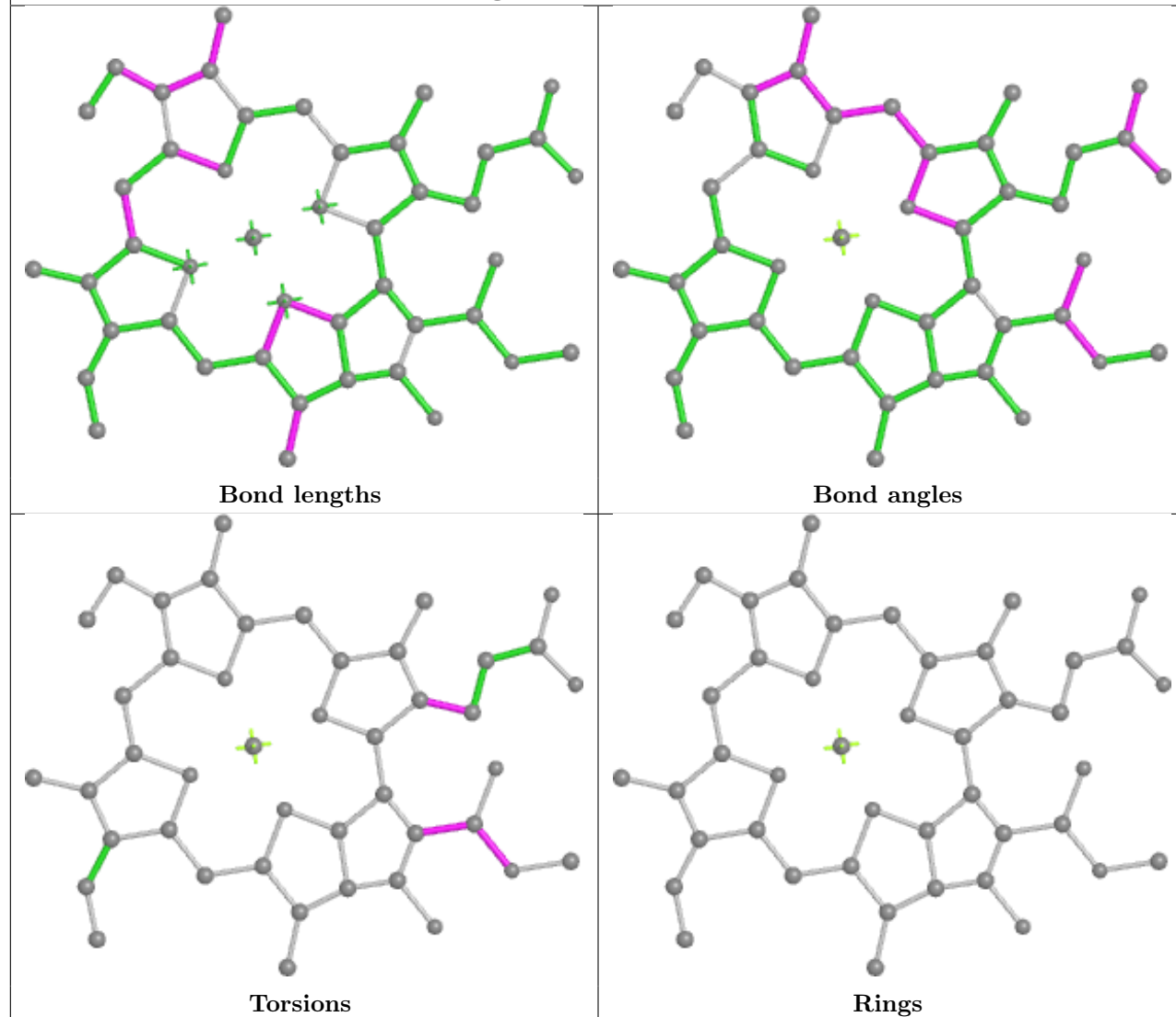
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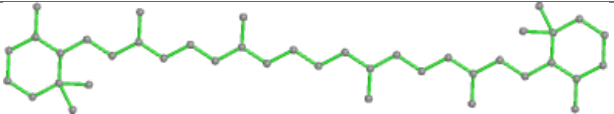
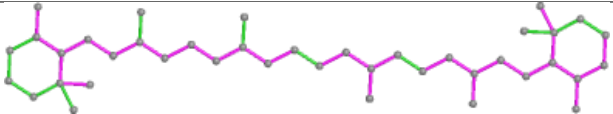
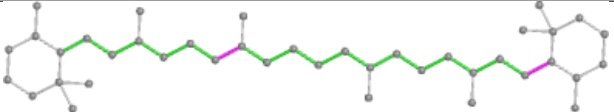
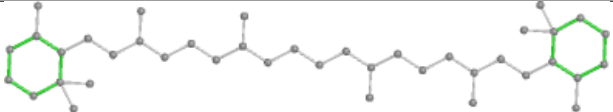


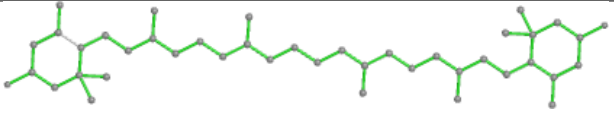
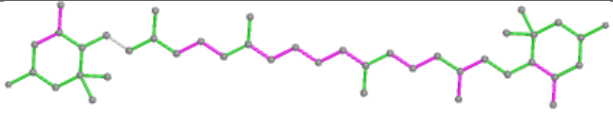
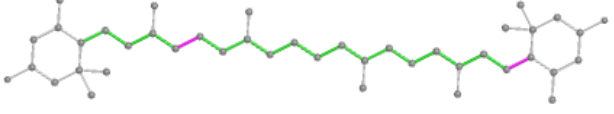
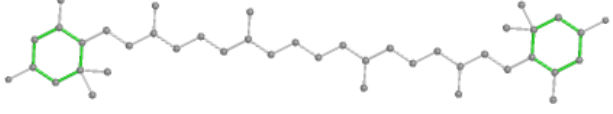
Ligand CLA B 803

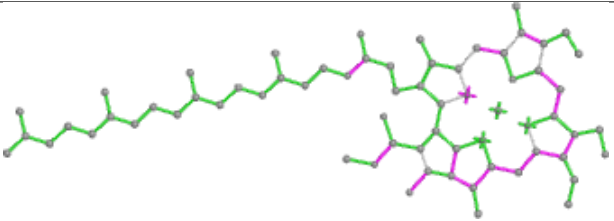
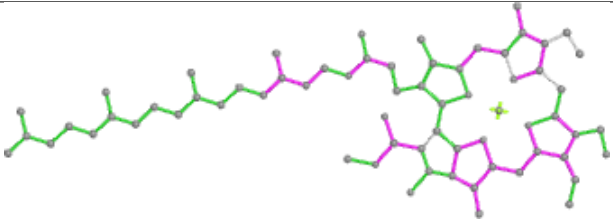
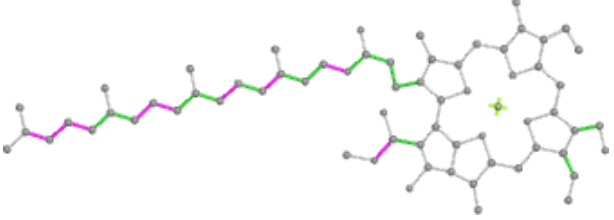
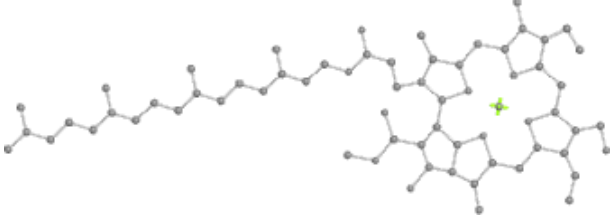


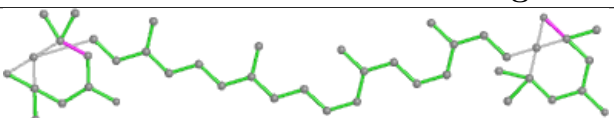
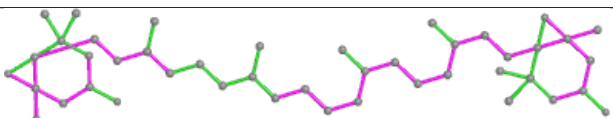
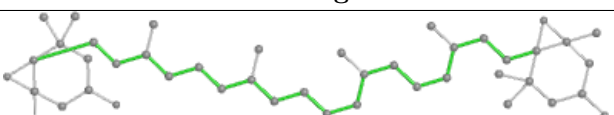
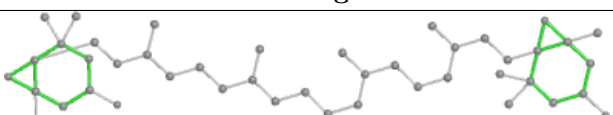
Ligand CLA K 201



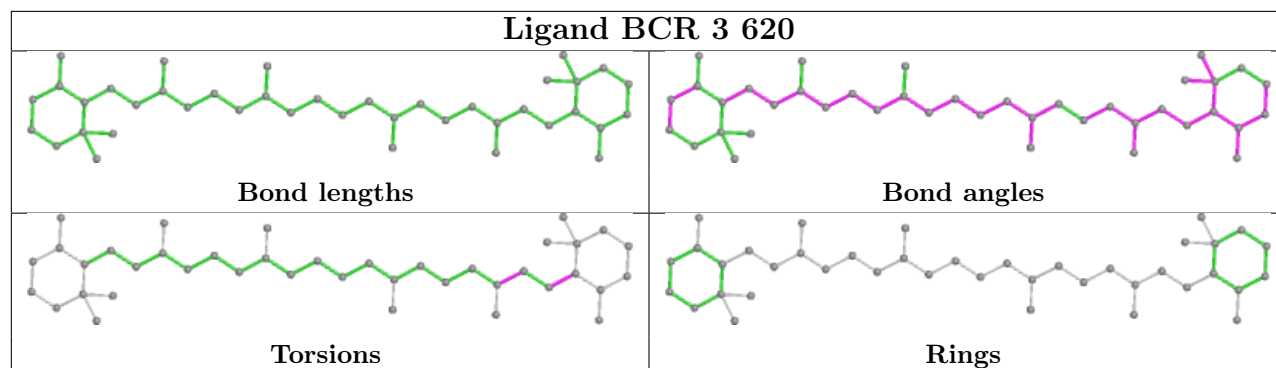
Ligand BCR 1 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT Z 1621	
 Bond lengths	 Bond angles
 Torsions	 Rings

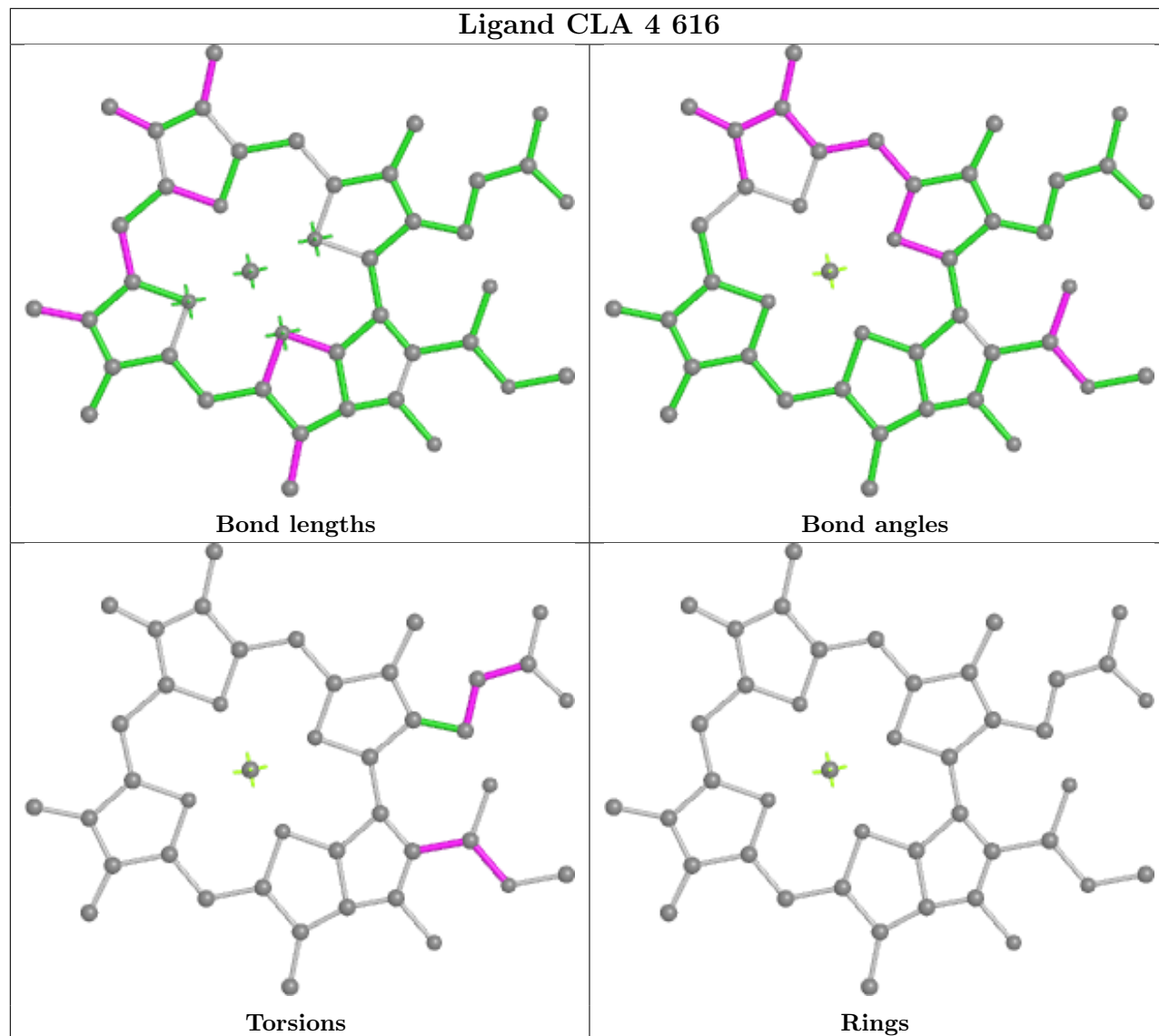
Ligand CHL W 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT 3 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

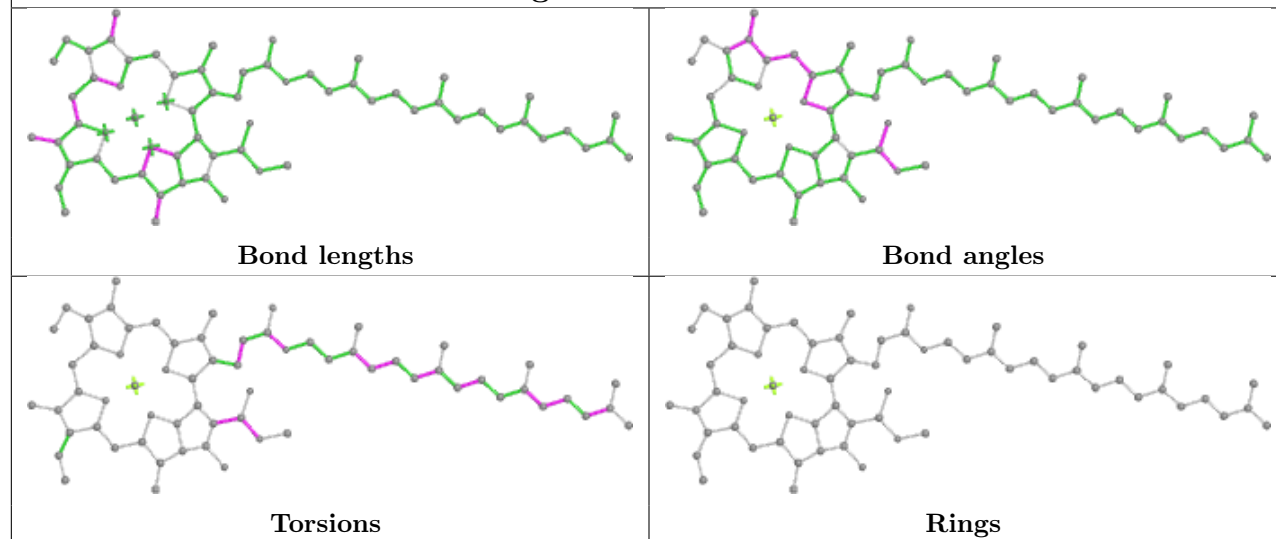
Ligand BCR 3 620



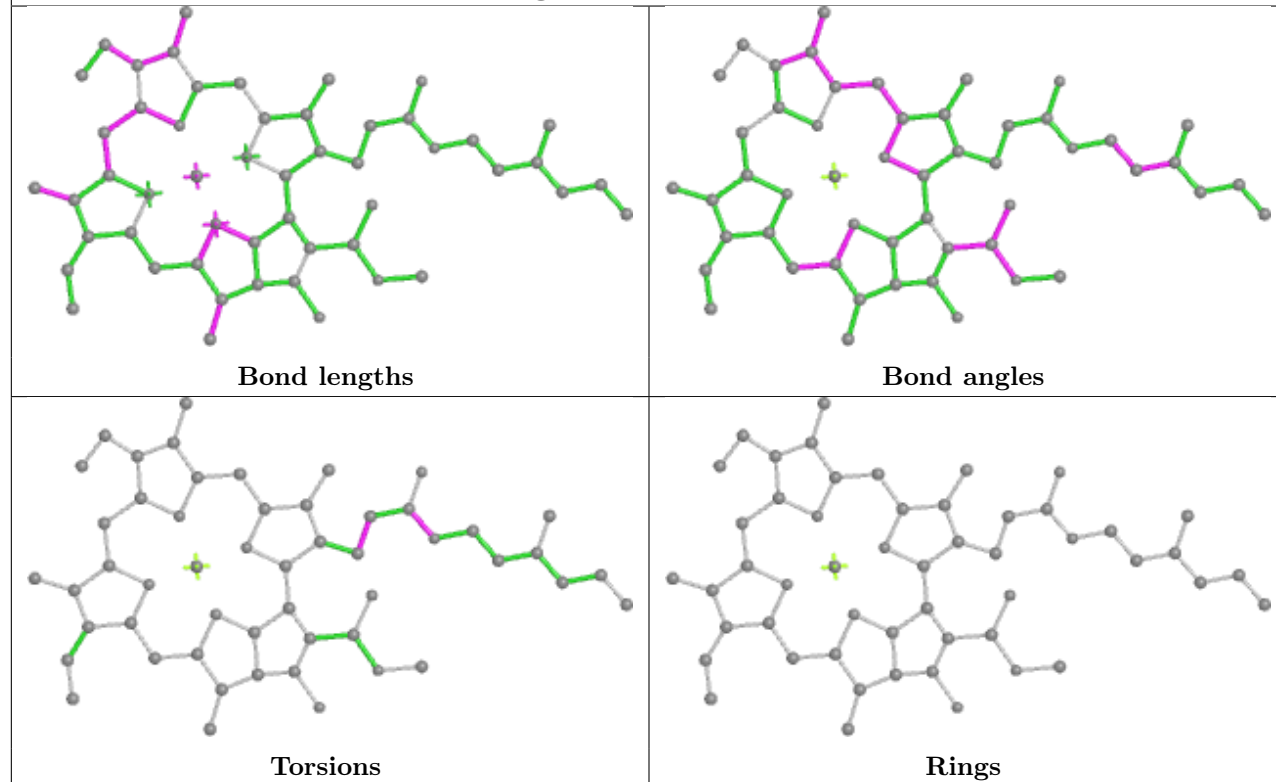
Ligand CLA 4 616



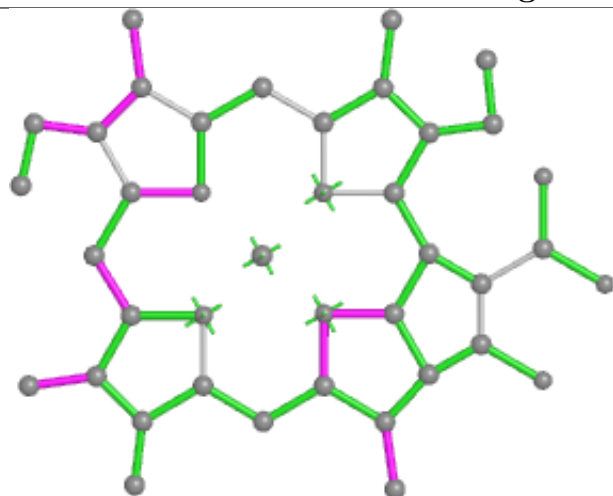
Ligand CLA V 613



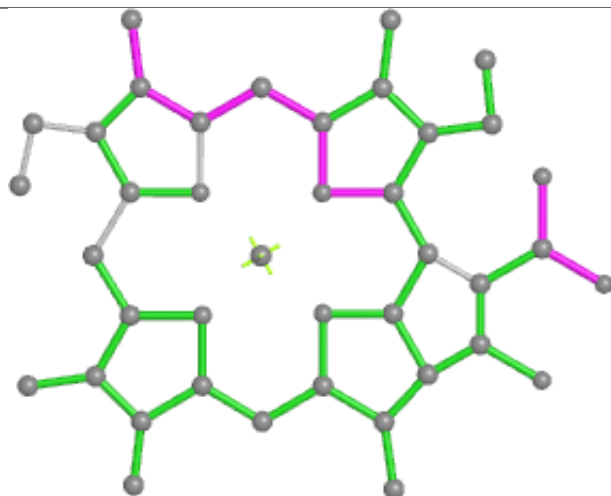
Ligand CLA B 807



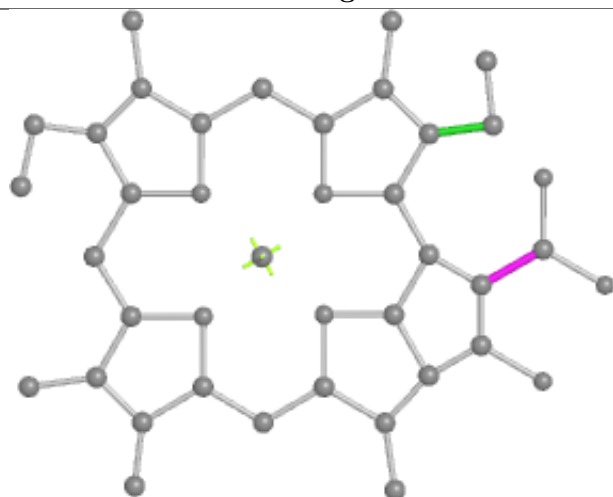
Ligand CLA 5 606



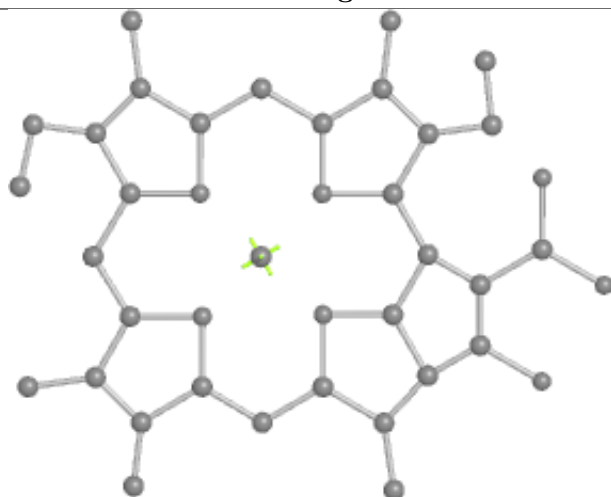
Bond lengths



Bond angles

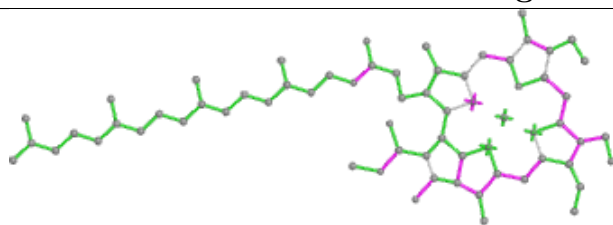


Torsions

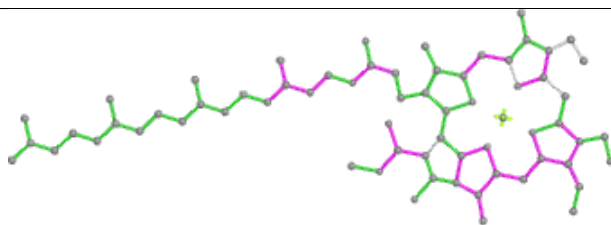


Rings

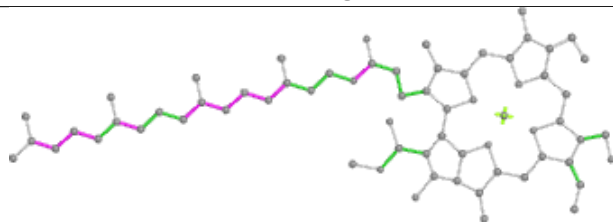
Ligand CHL Z 601



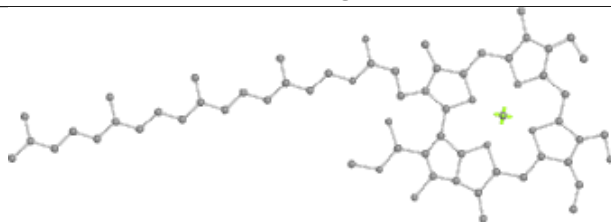
Bond lengths



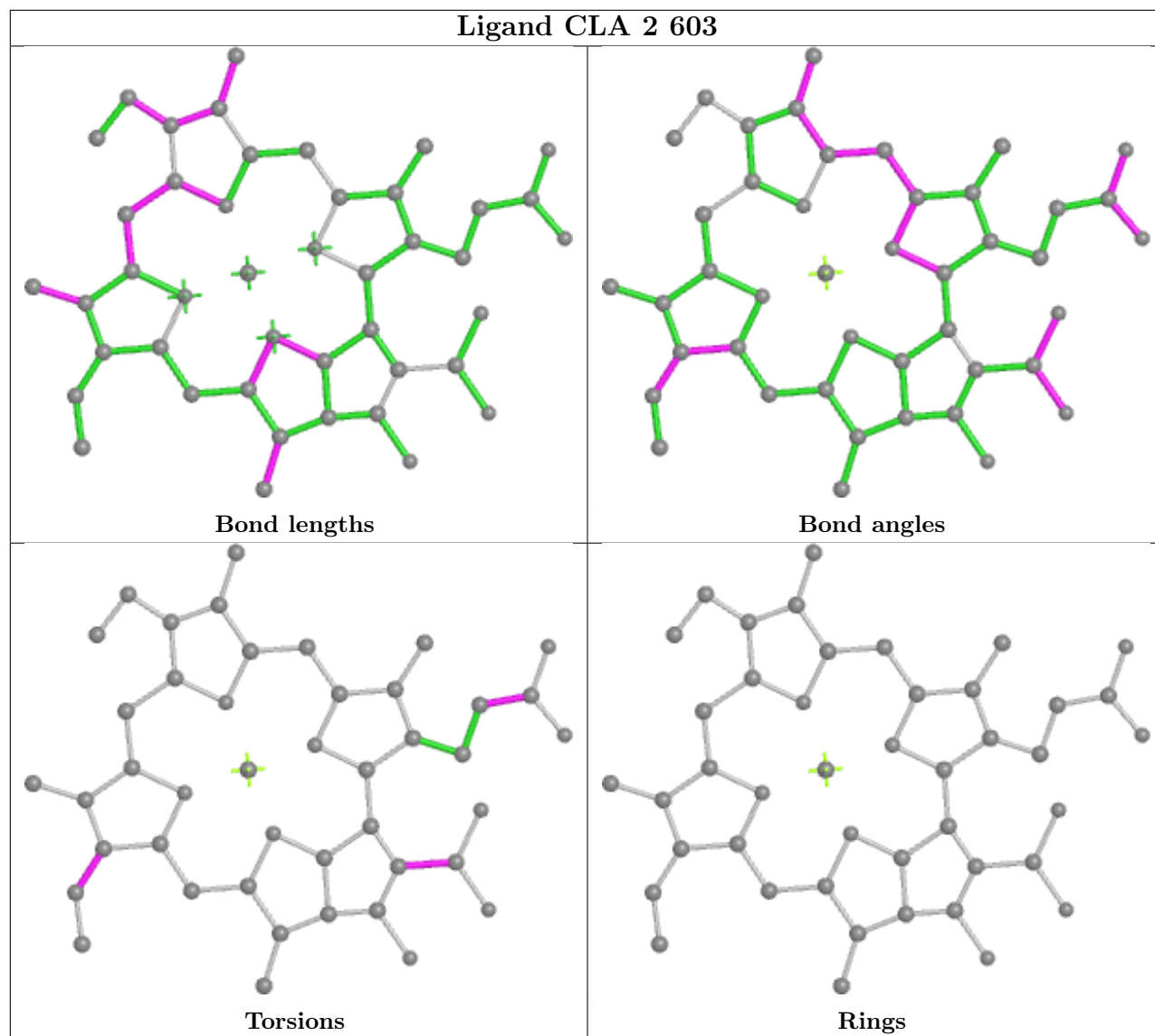
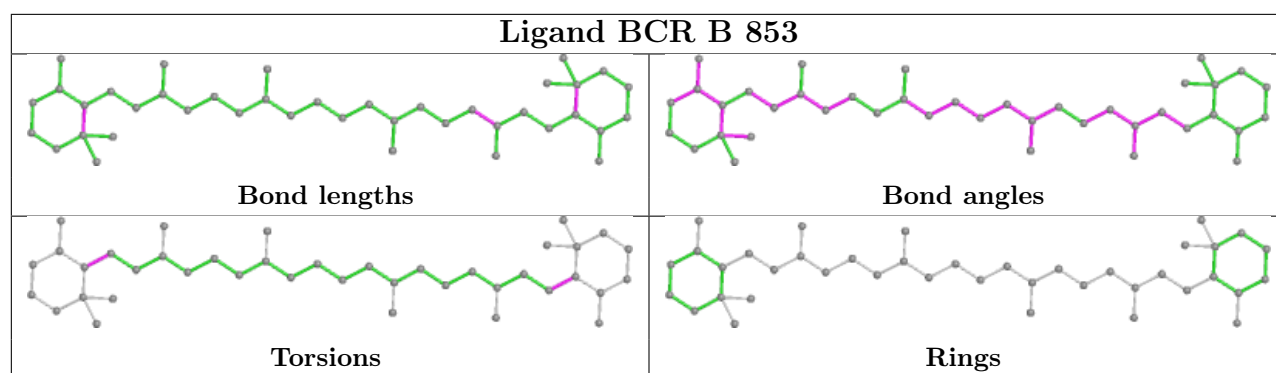
Bond angles



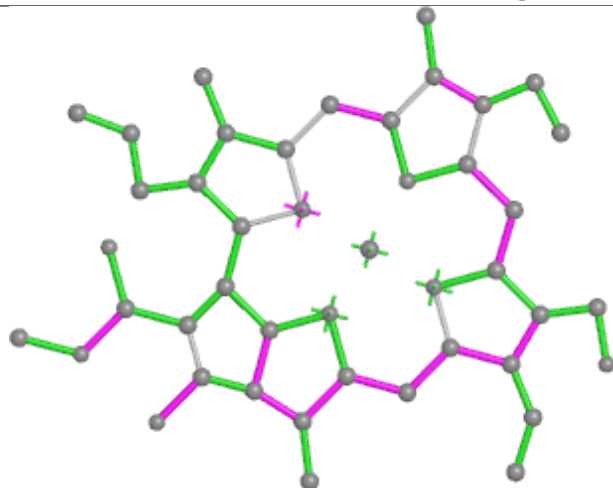
Torsions



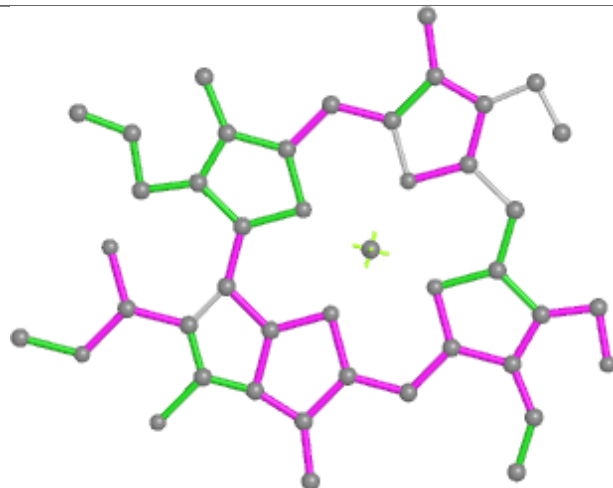
Rings



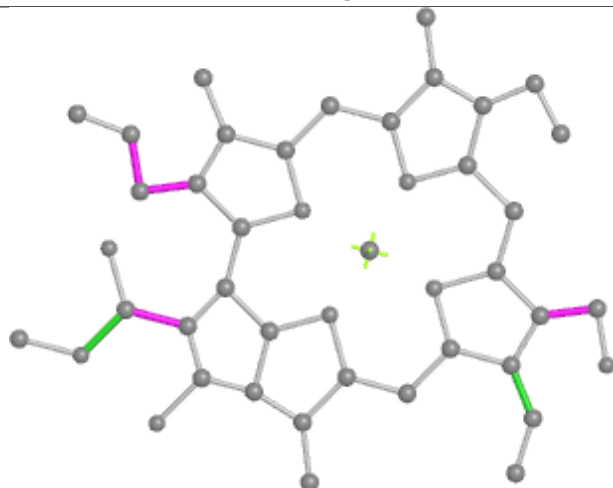
Ligand CHL X 606



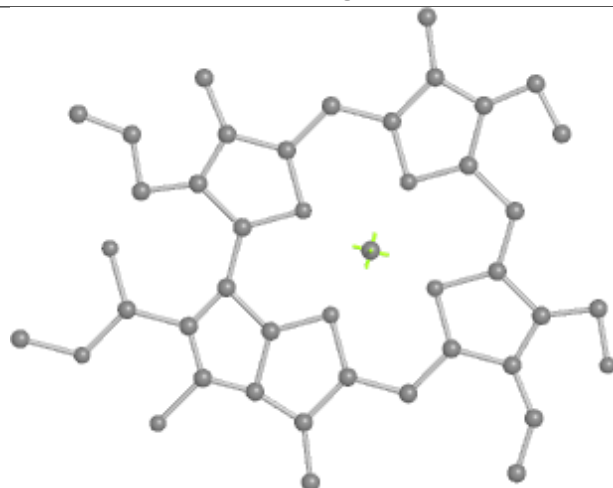
Bond lengths



Bond angles

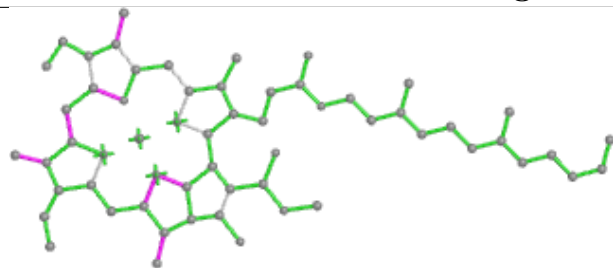


Torsions

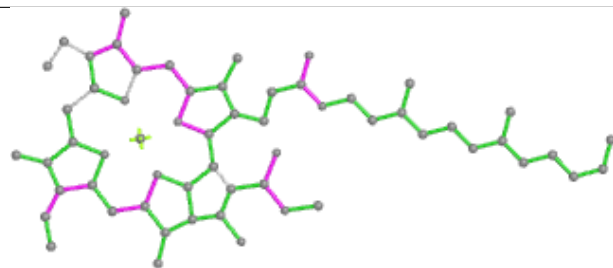


Rings

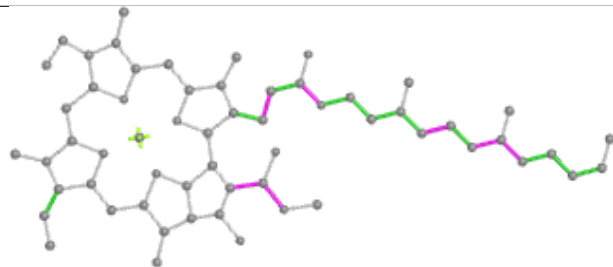
Ligand CLA U 613



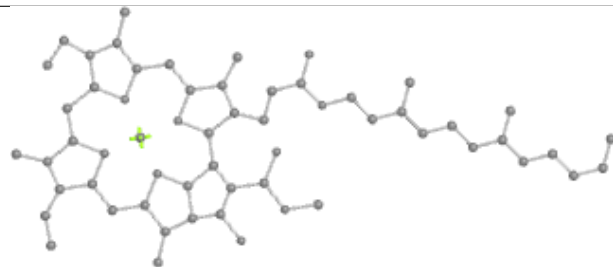
Bond lengths



Bond angles

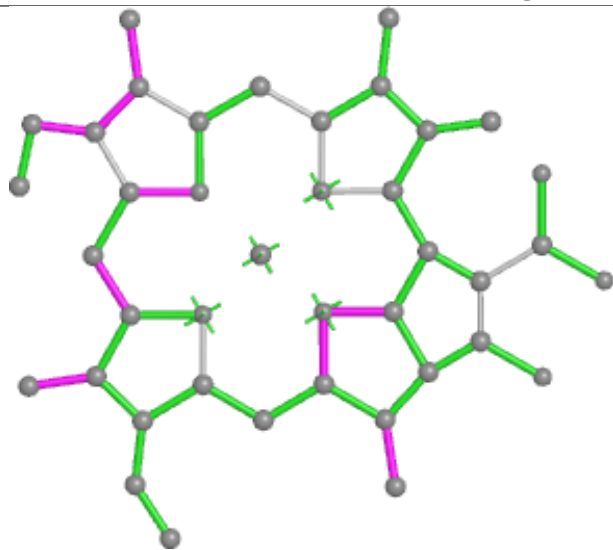


Torsions

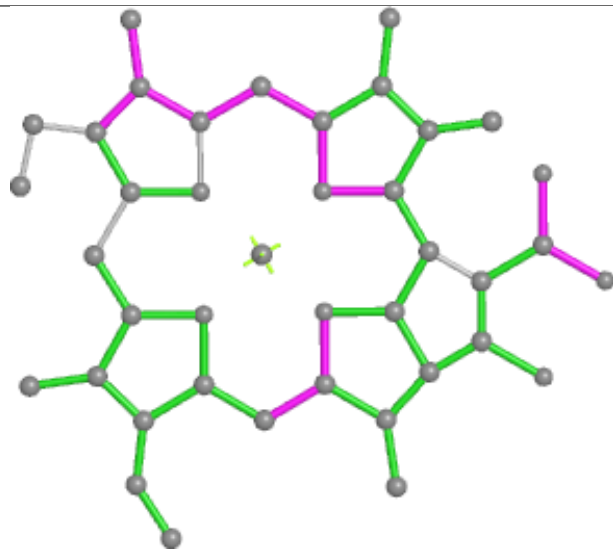


Rings

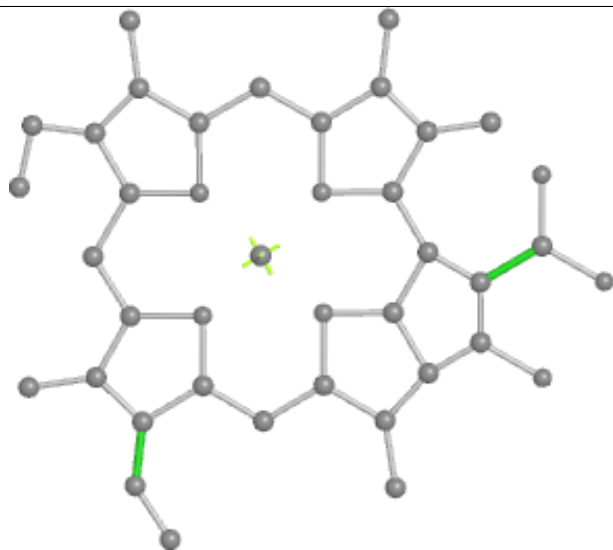
Ligand CLA 3 617



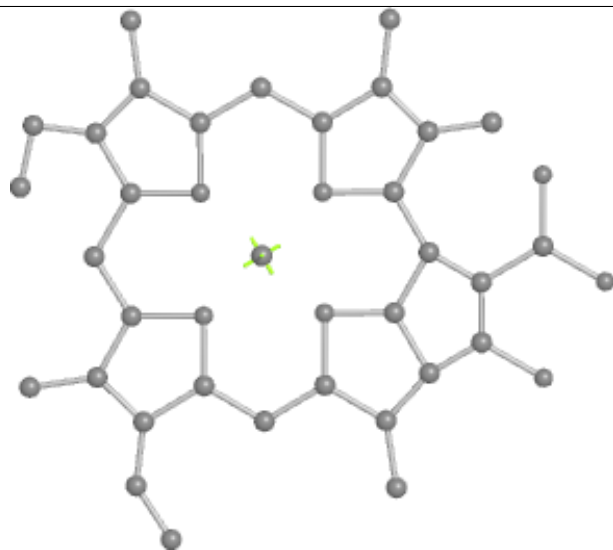
Bond lengths



Bond angles

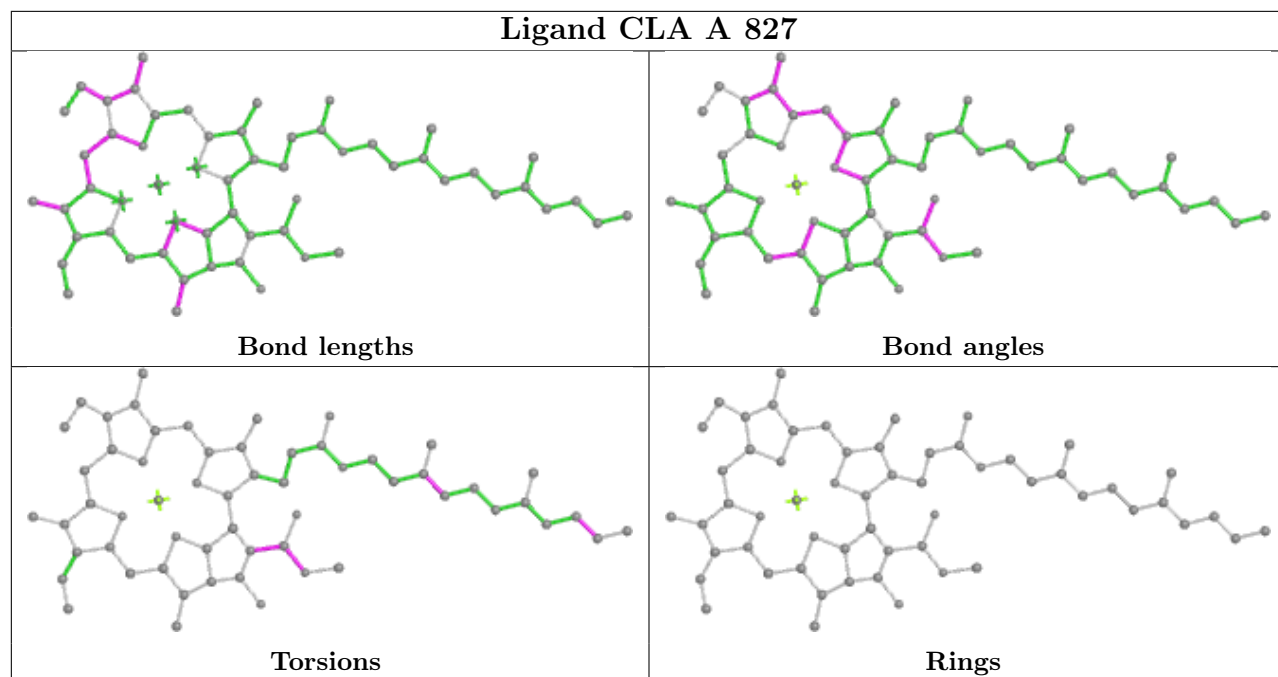


Torsions

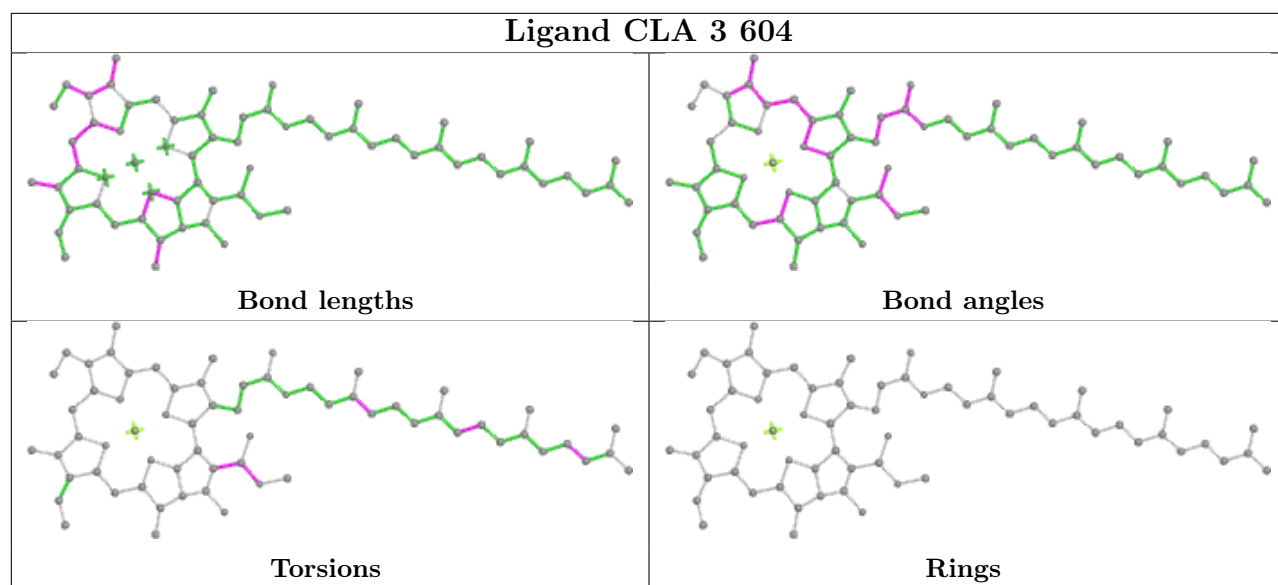


Rings

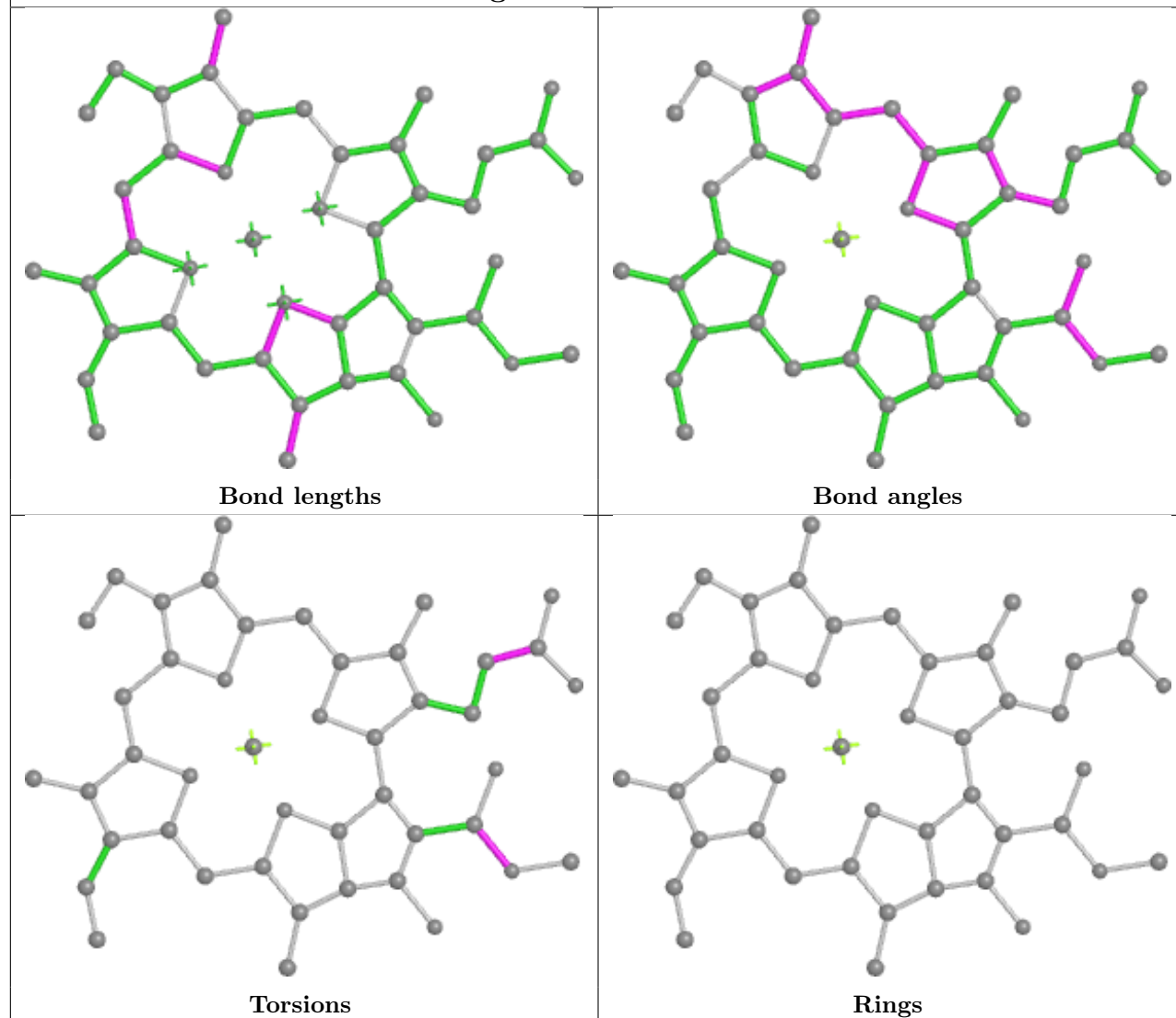
Ligand CLA A 827



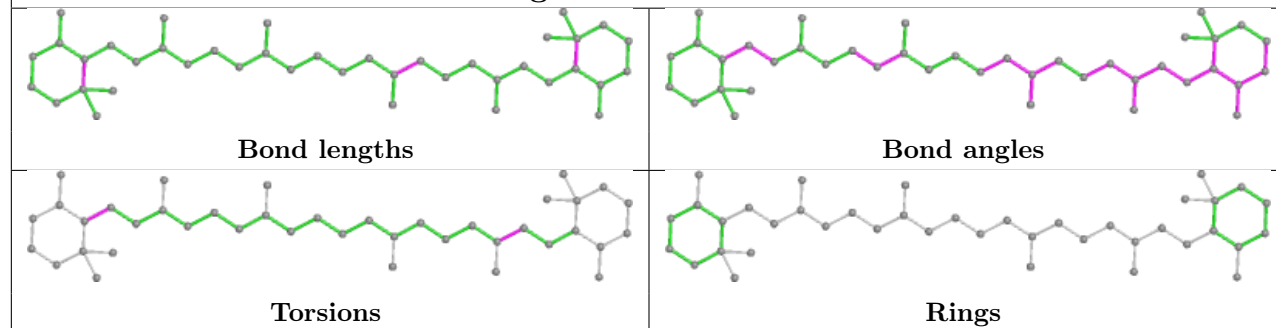
Ligand CLA 3 604

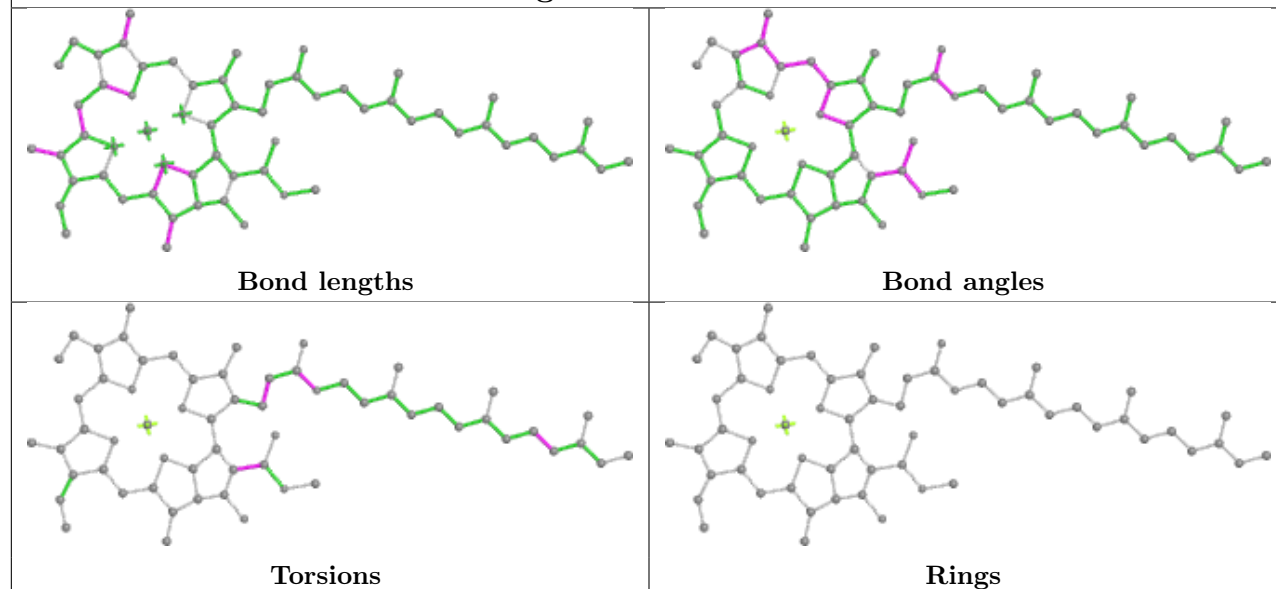
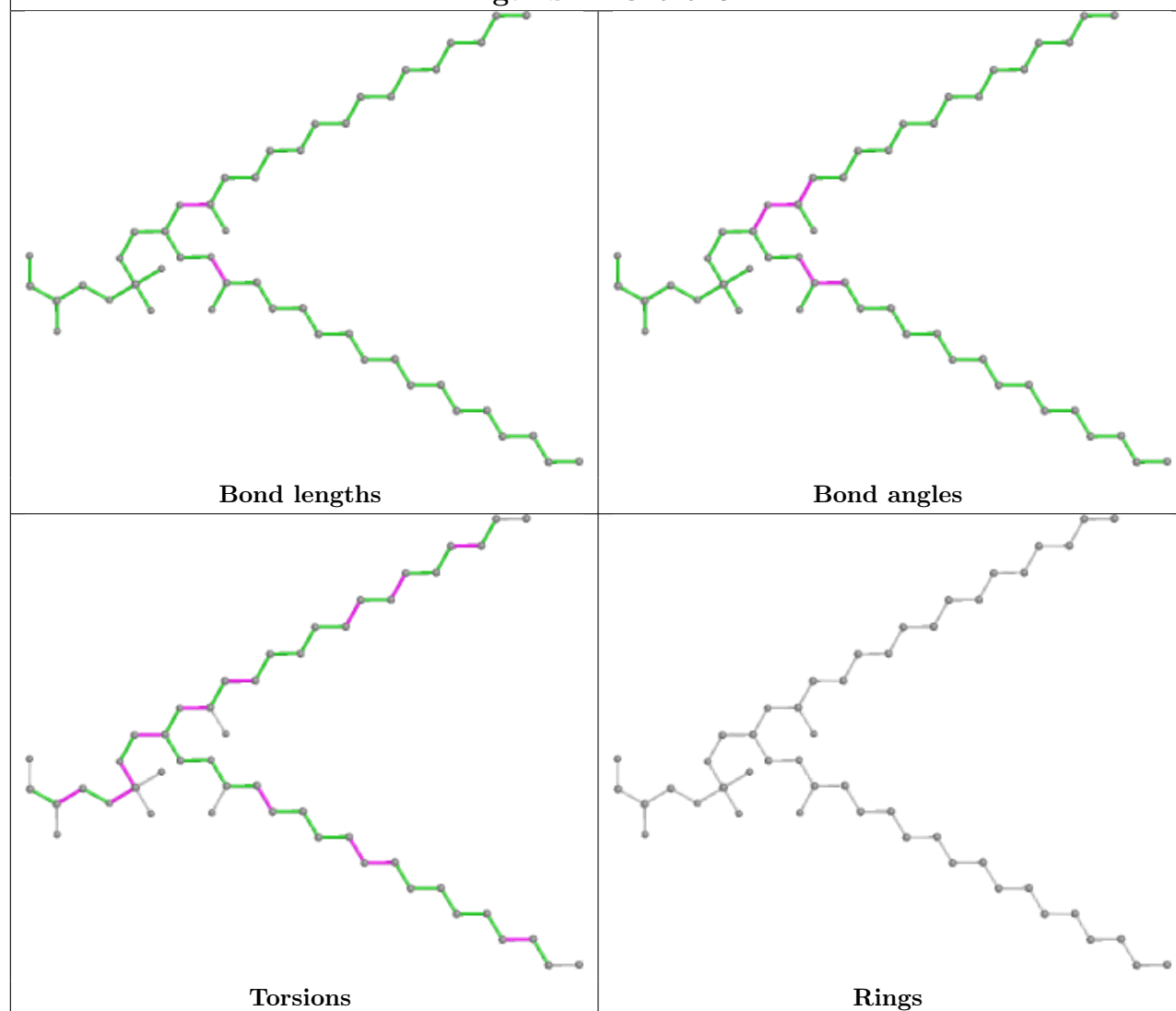


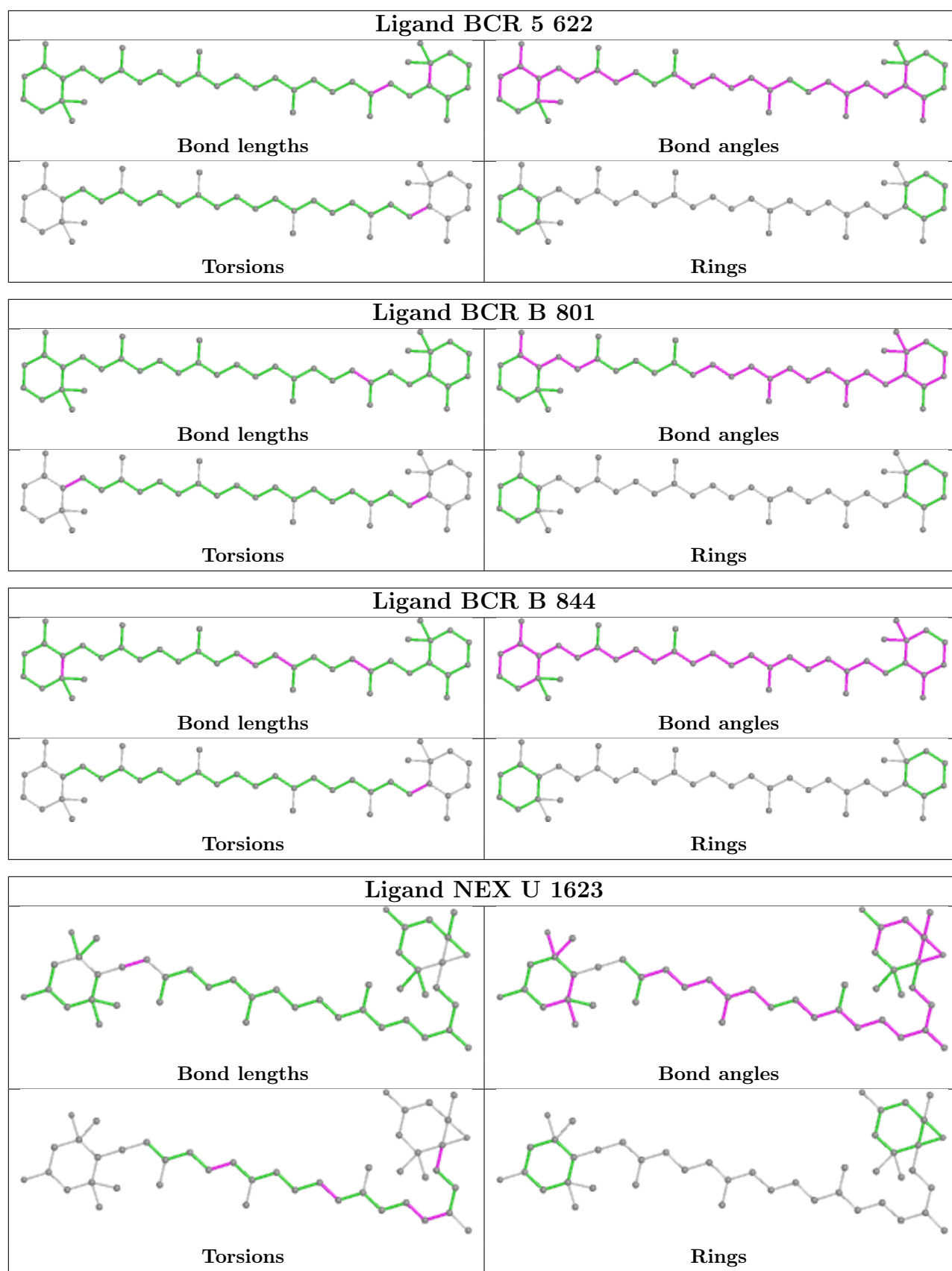
Ligand CLA V 603

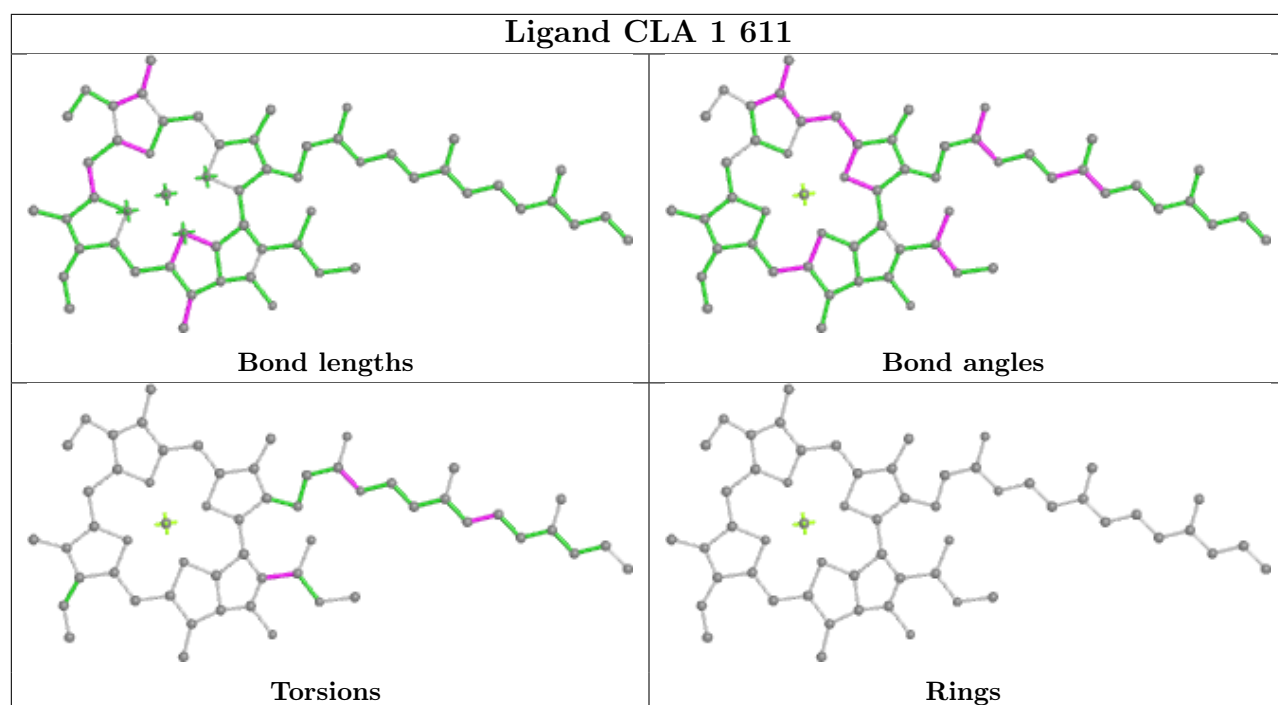


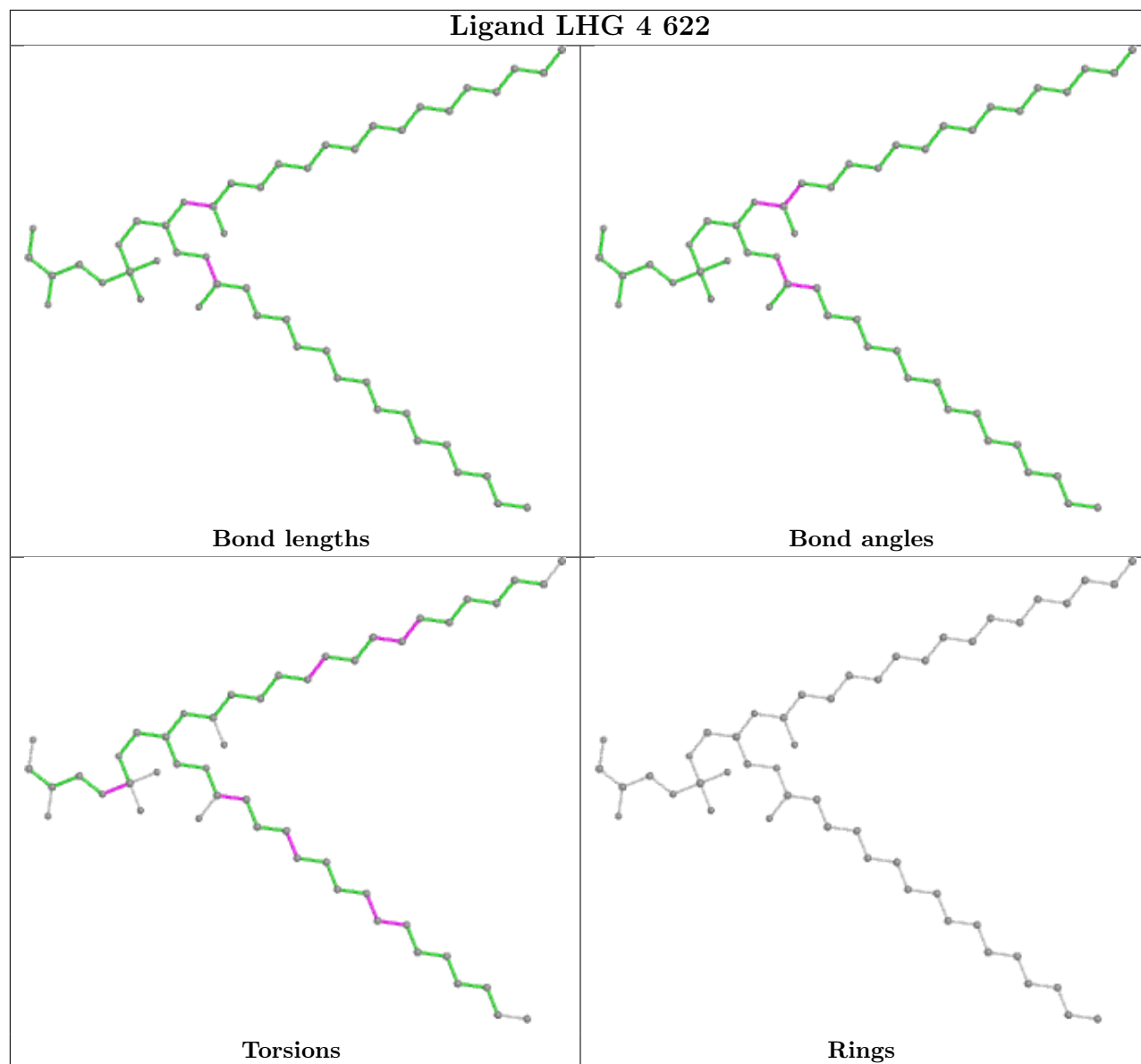
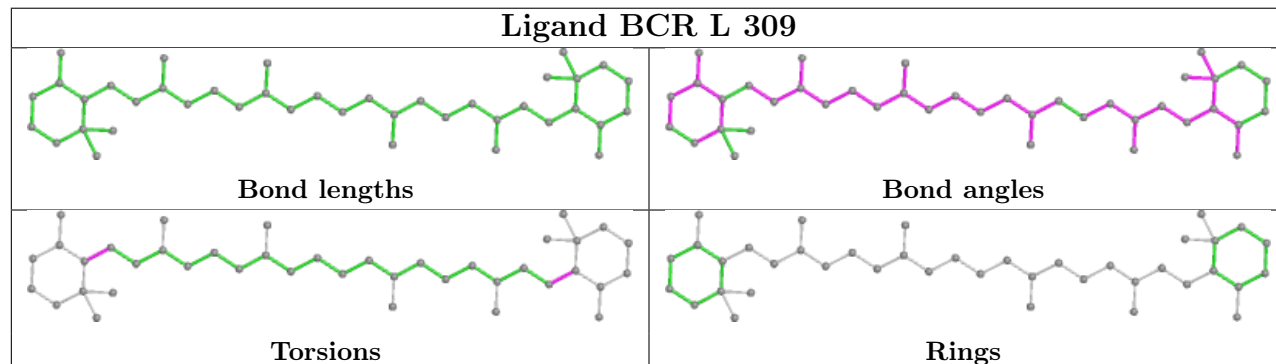
Ligand BCR A 848



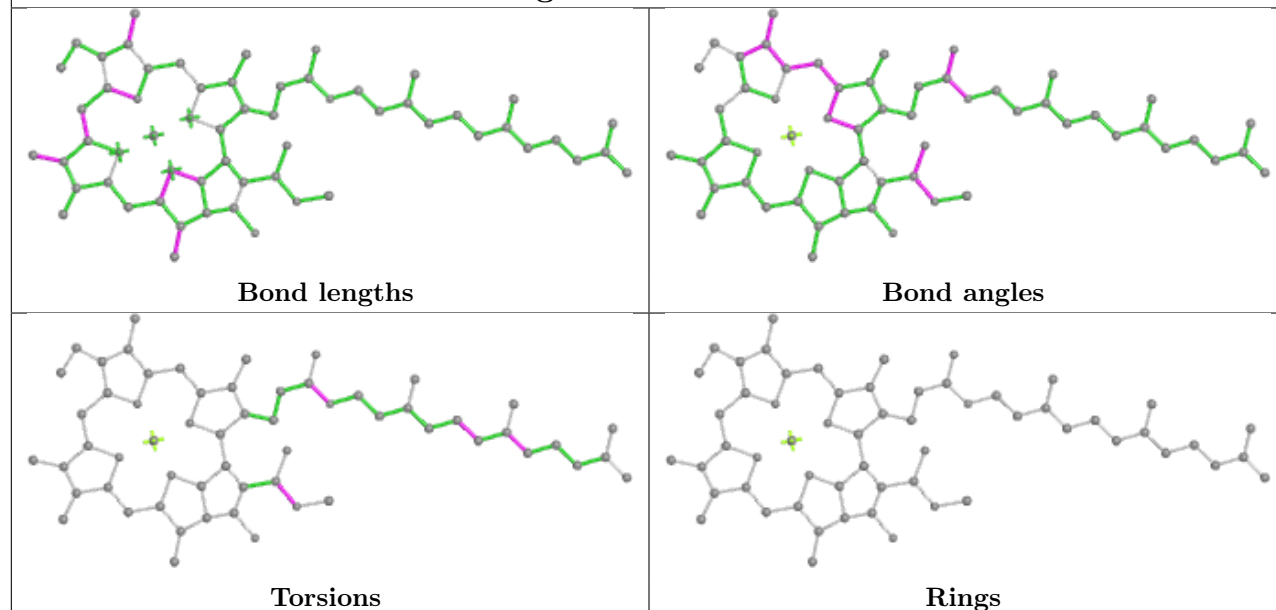
Ligand CLA 1 602**Ligand LHG 6 623**



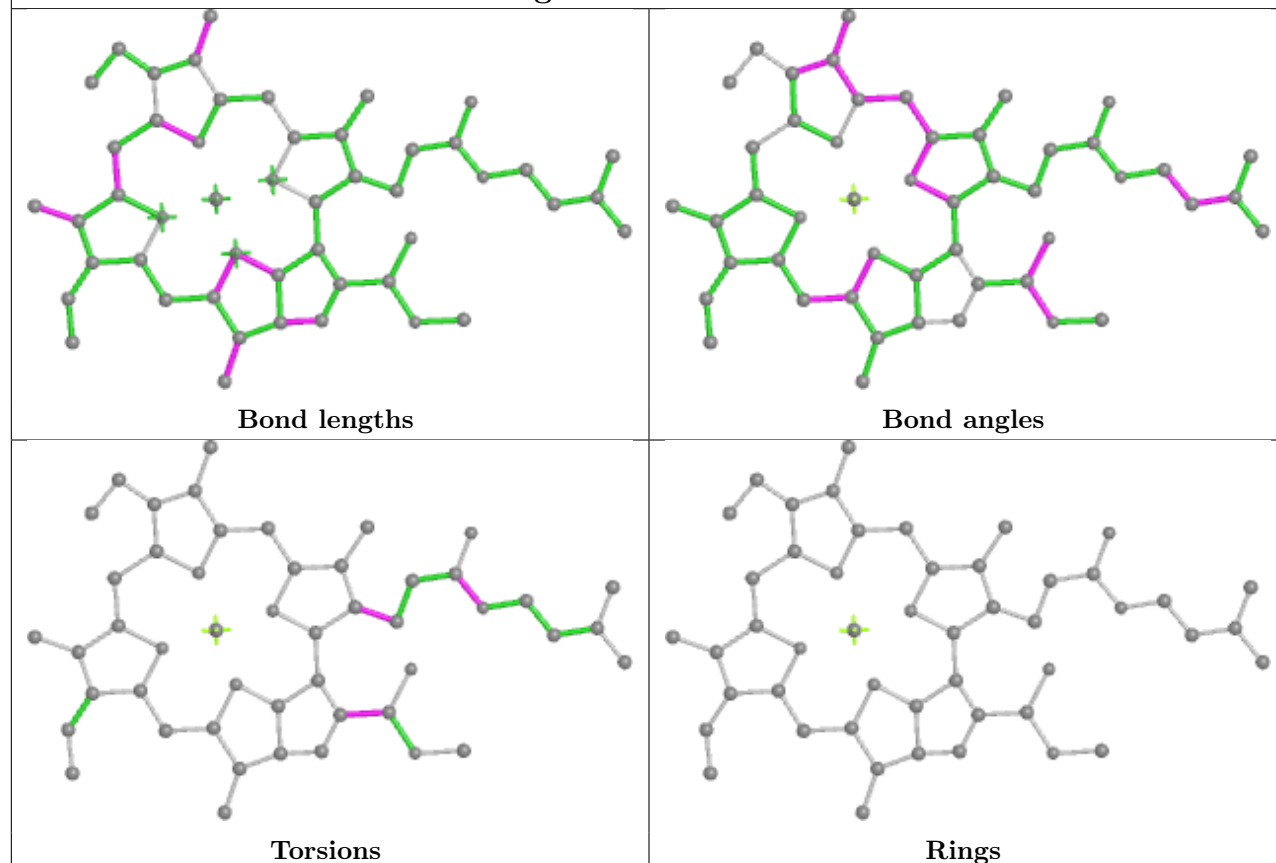


Ligand LHG 4 622**Ligand BCR L 309**

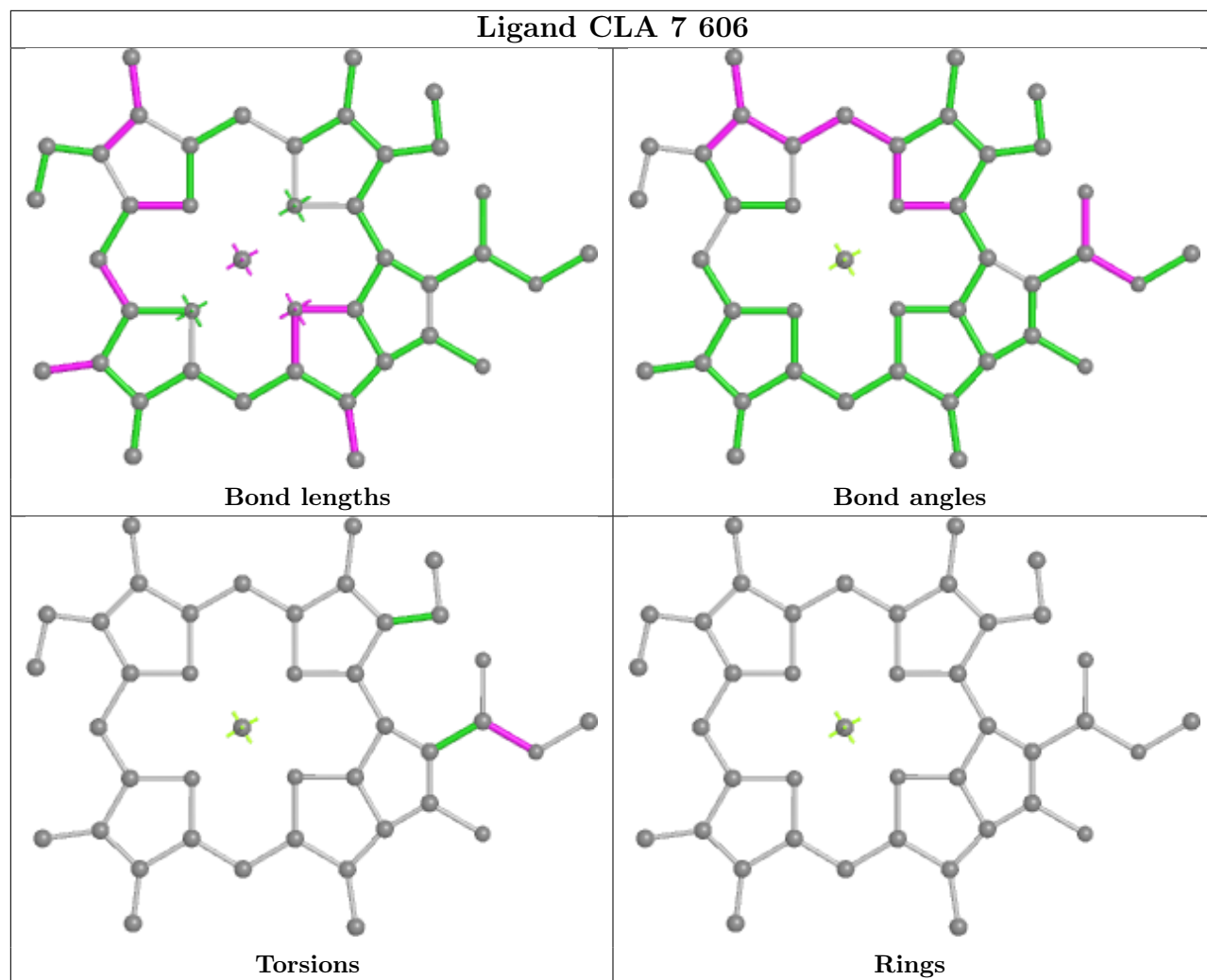
Ligand CLA a 610



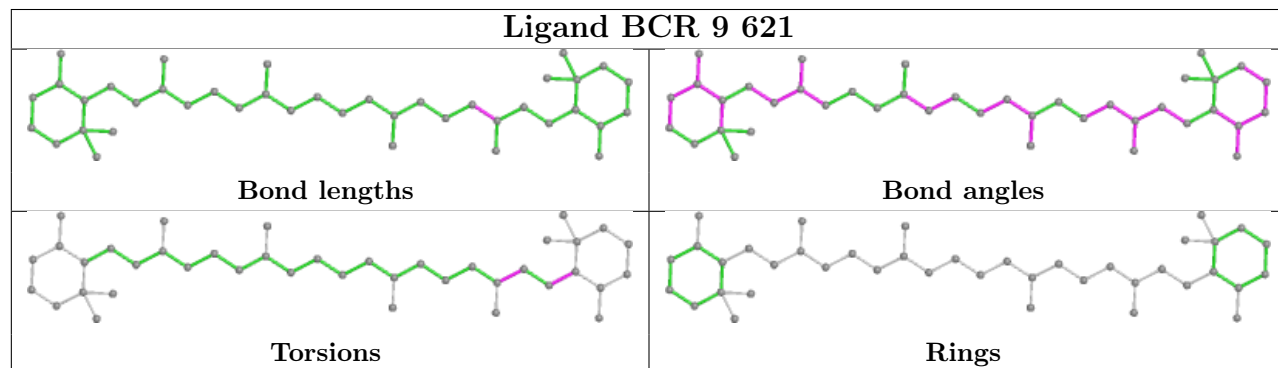
Ligand CLA Z 604



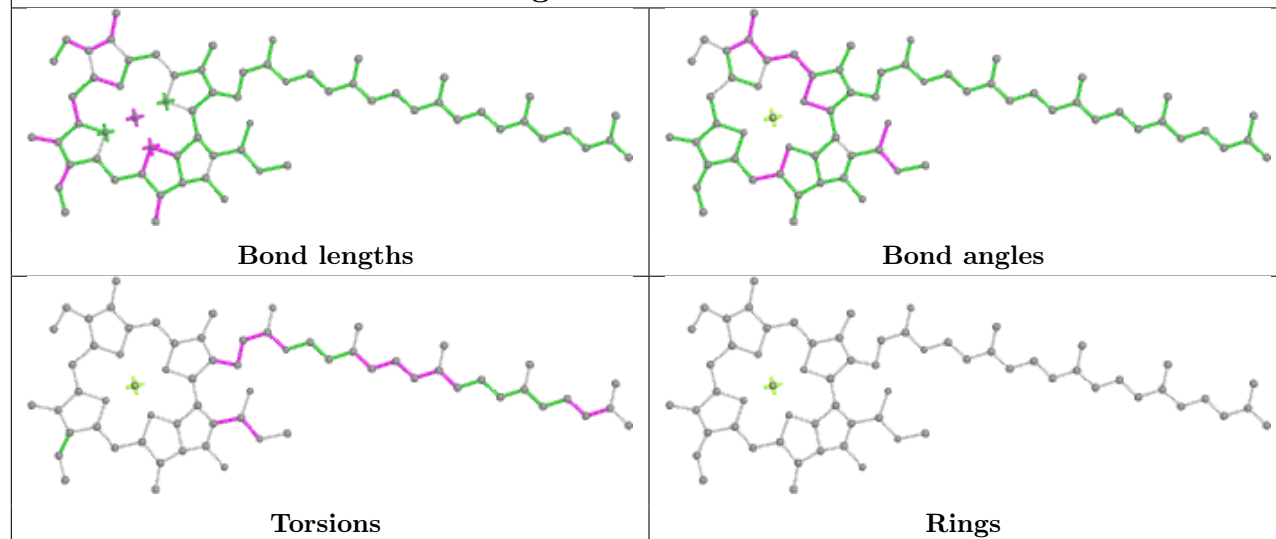
Ligand CLA 7 606



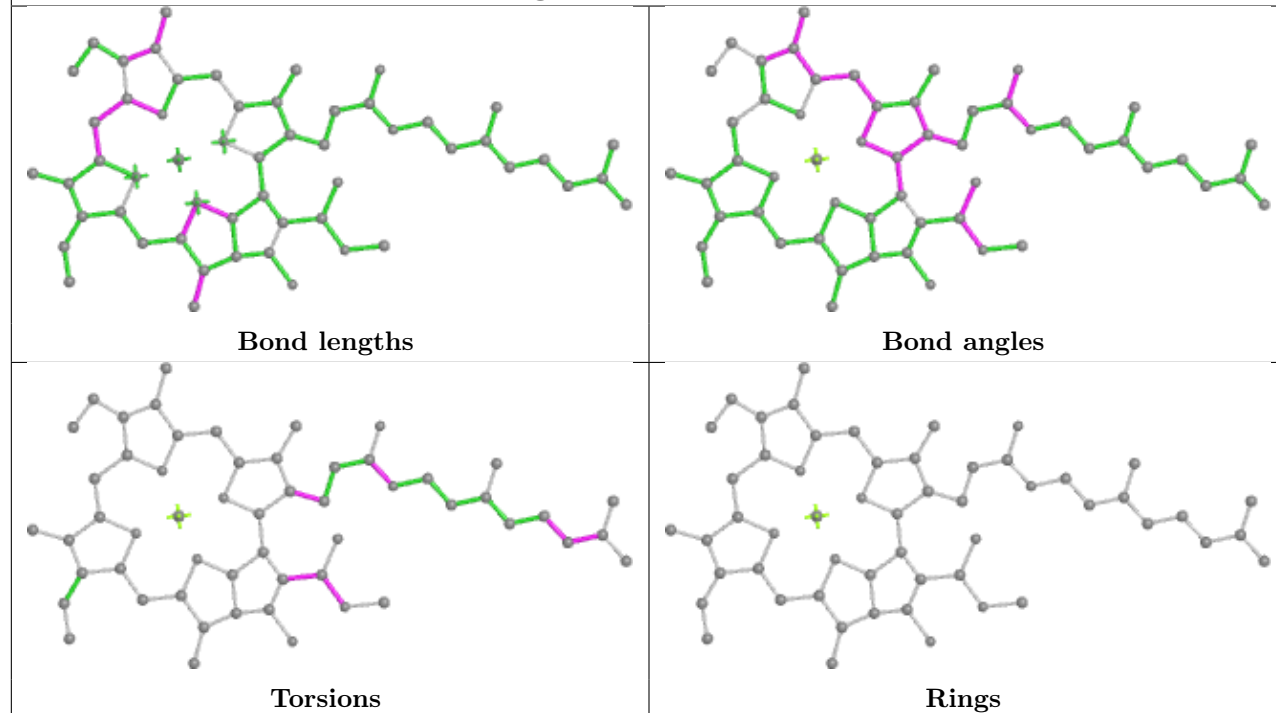
Ligand BCR 9 621



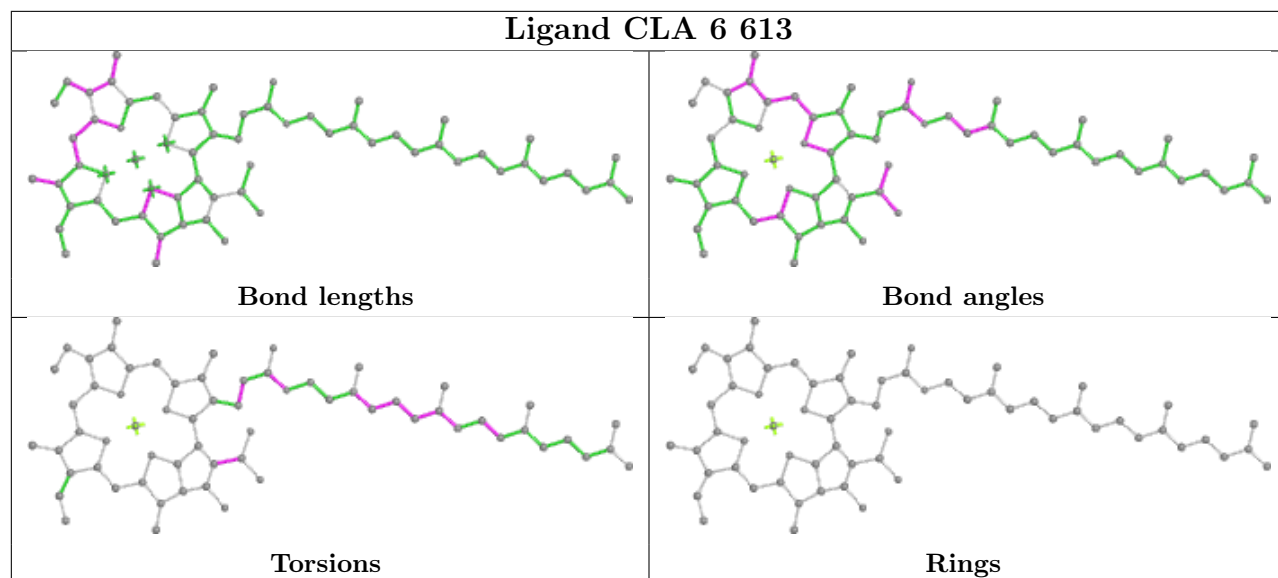
Ligand CLA A 807



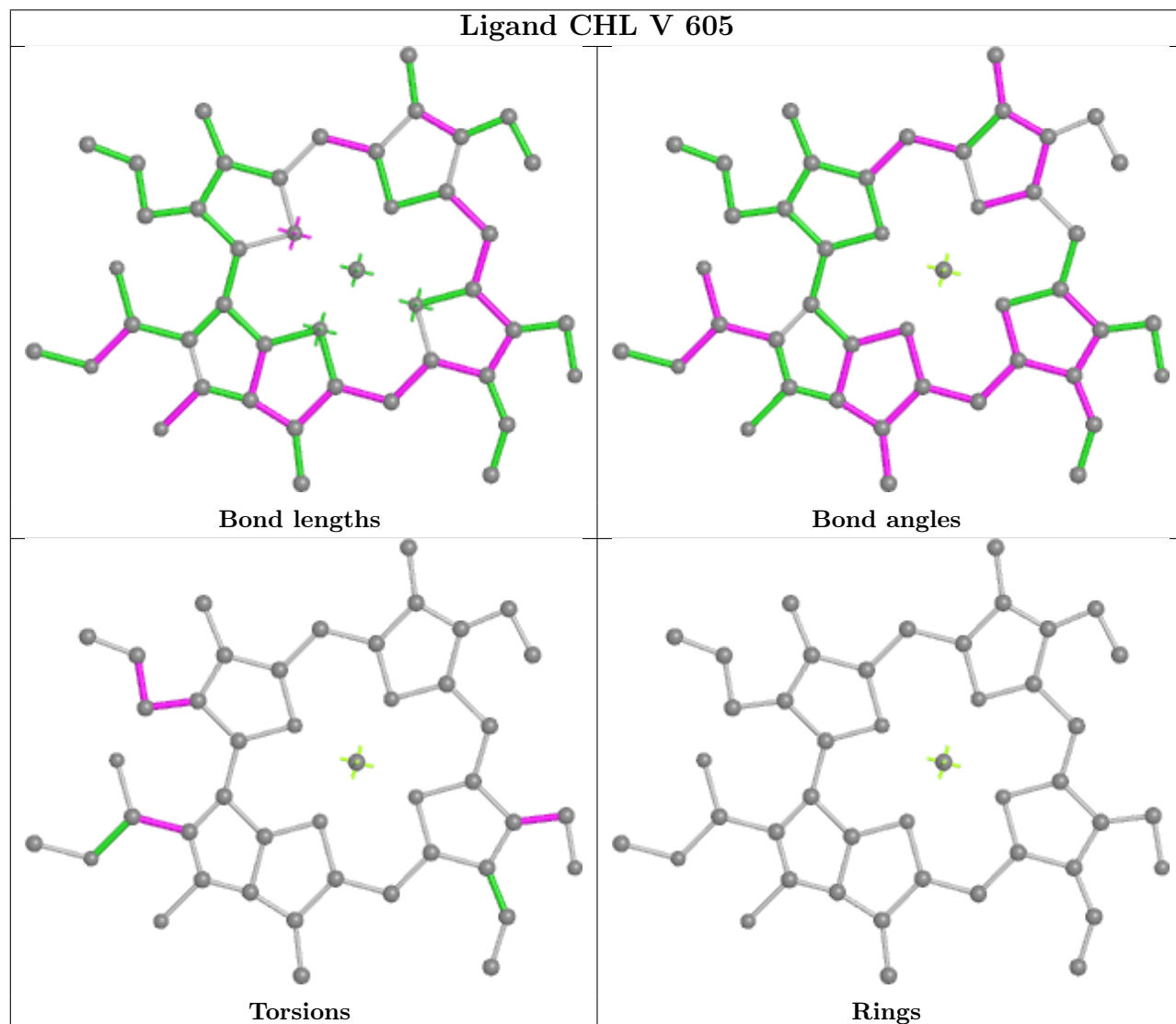
Ligand CLA Y 603



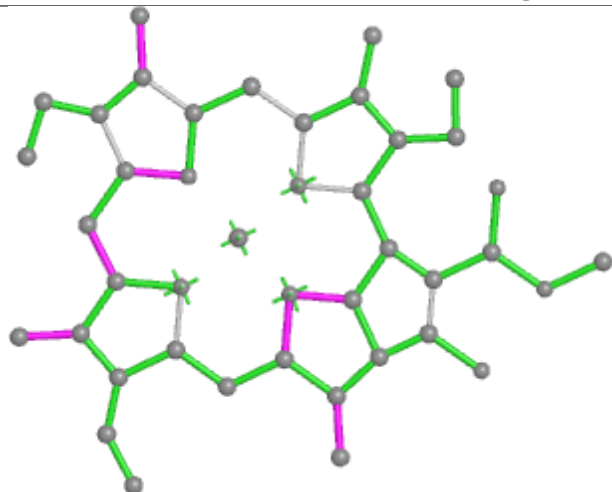
Ligand CLA 6 613



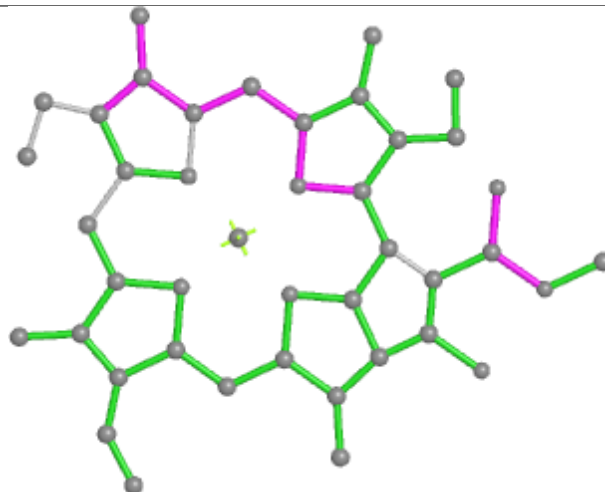
Ligand CHL V 605



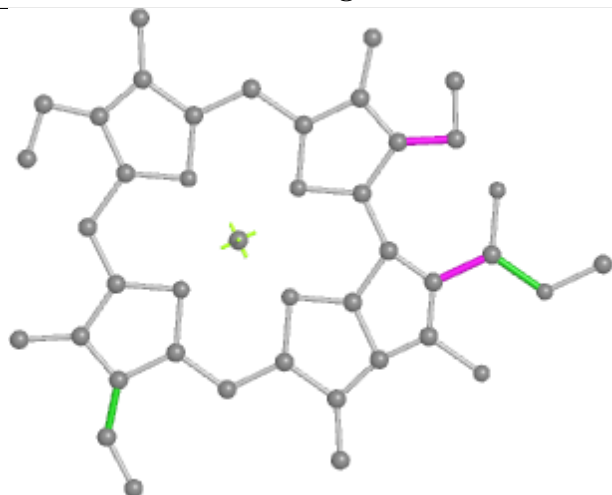
Ligand CLA 6 611



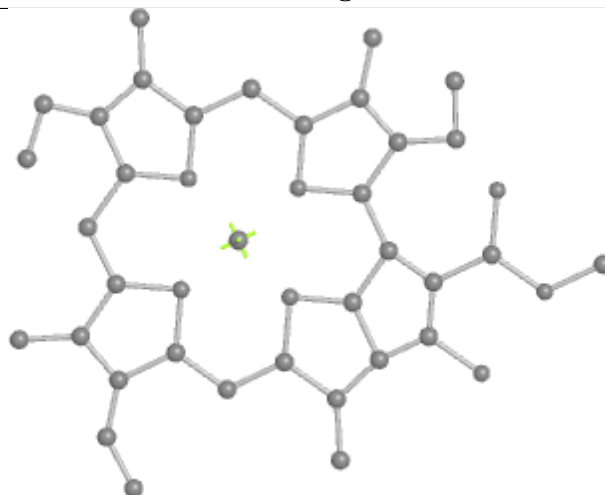
Bond lengths



Bond angles

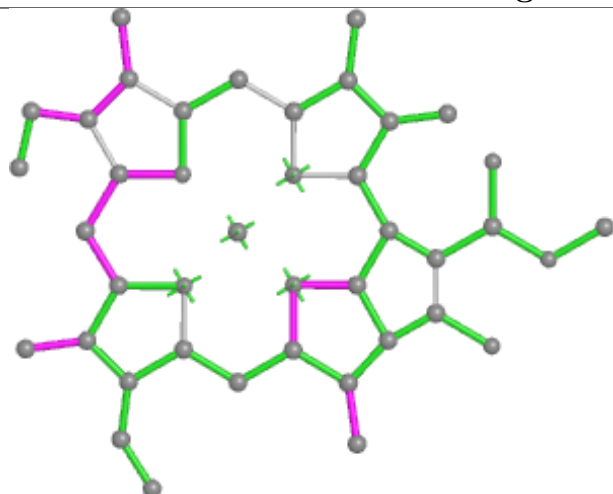


Torsions

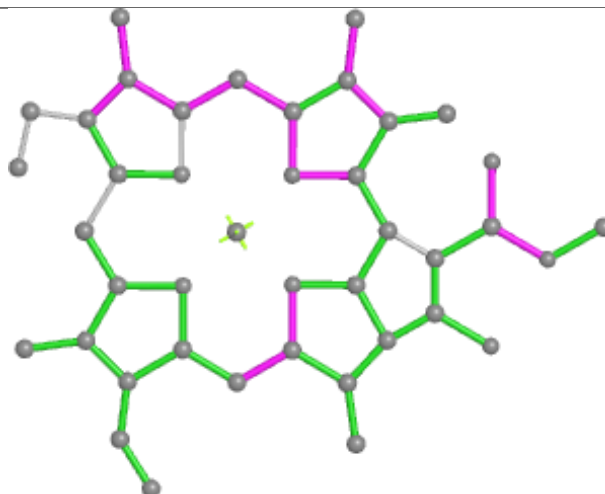


Rings

Ligand CLA F 304



Bond lengths



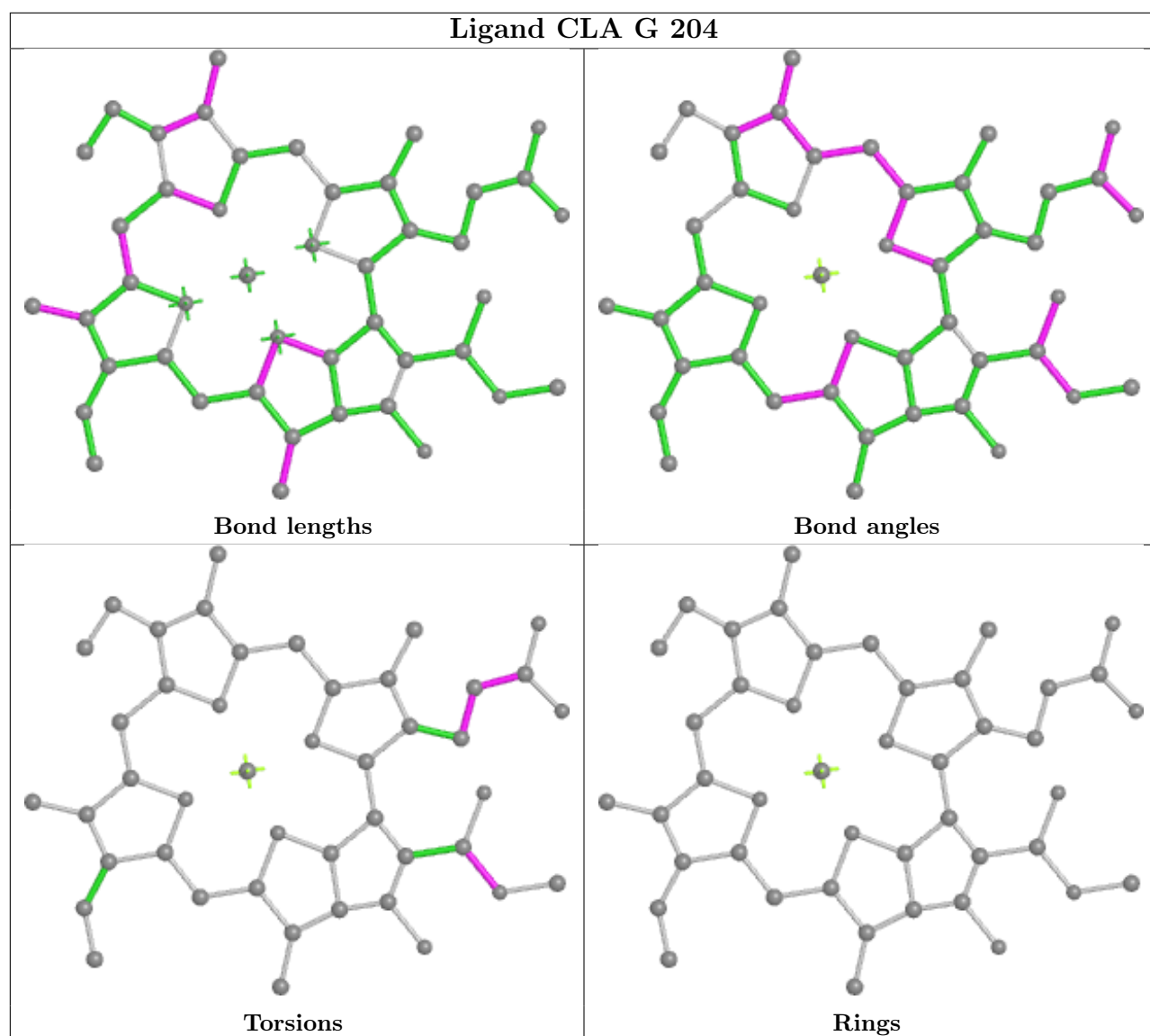
Bond angles

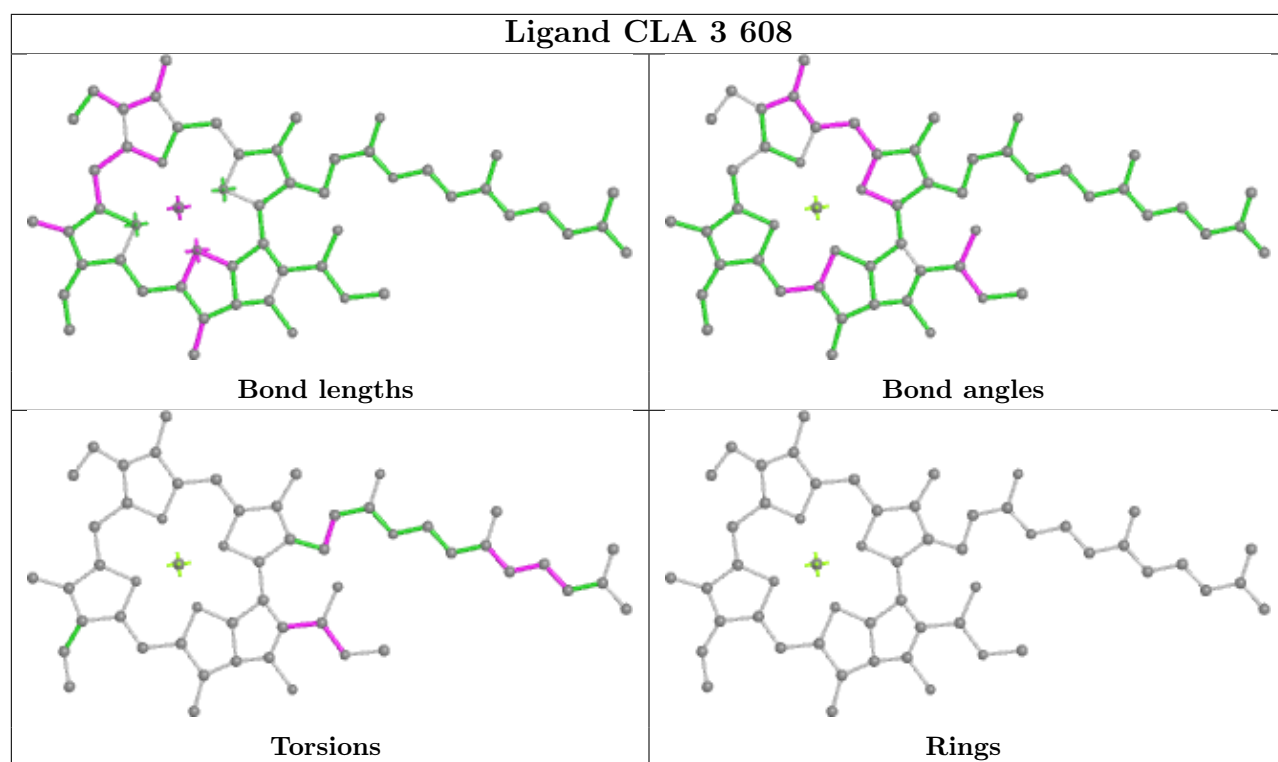


Torsions

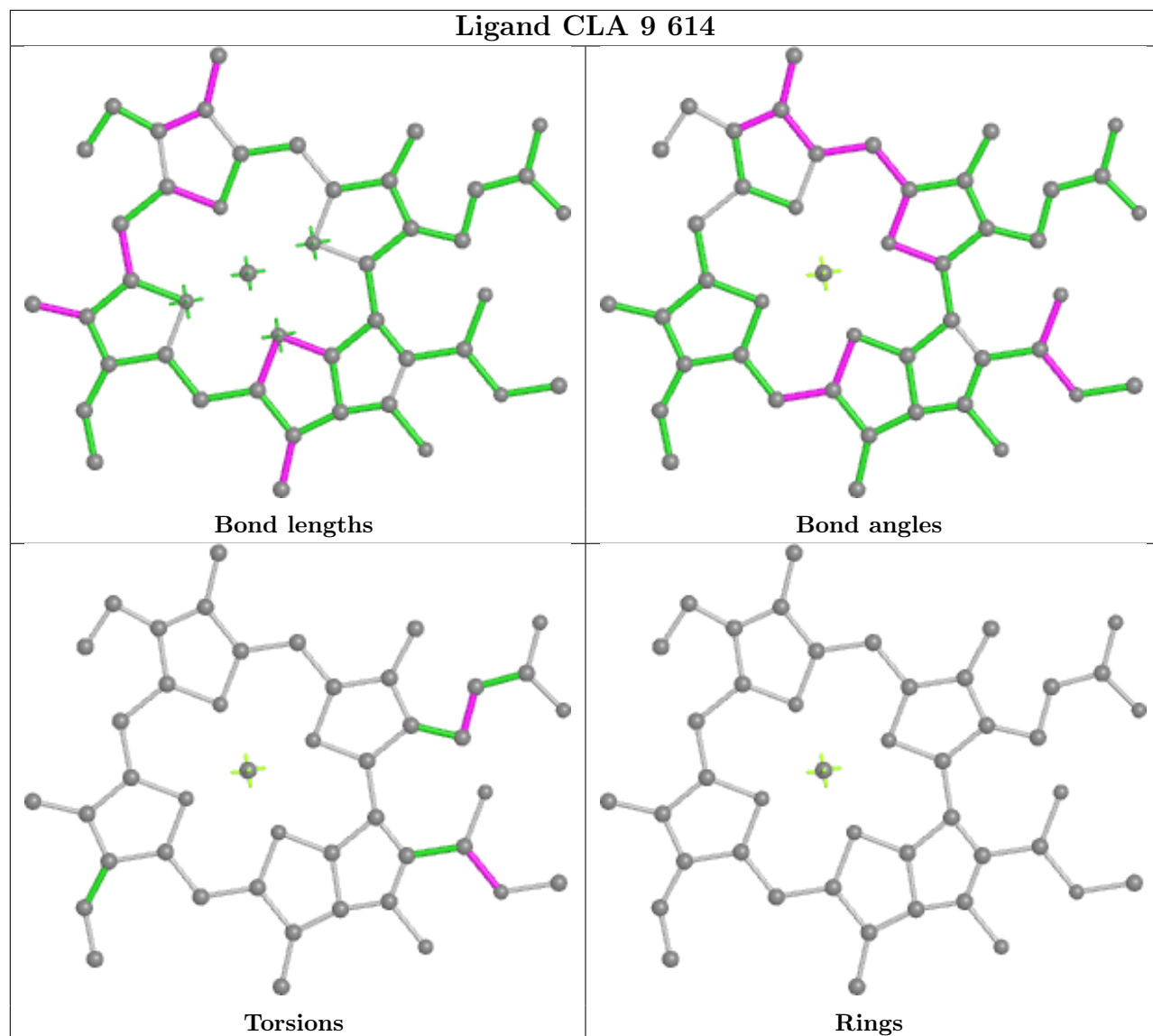


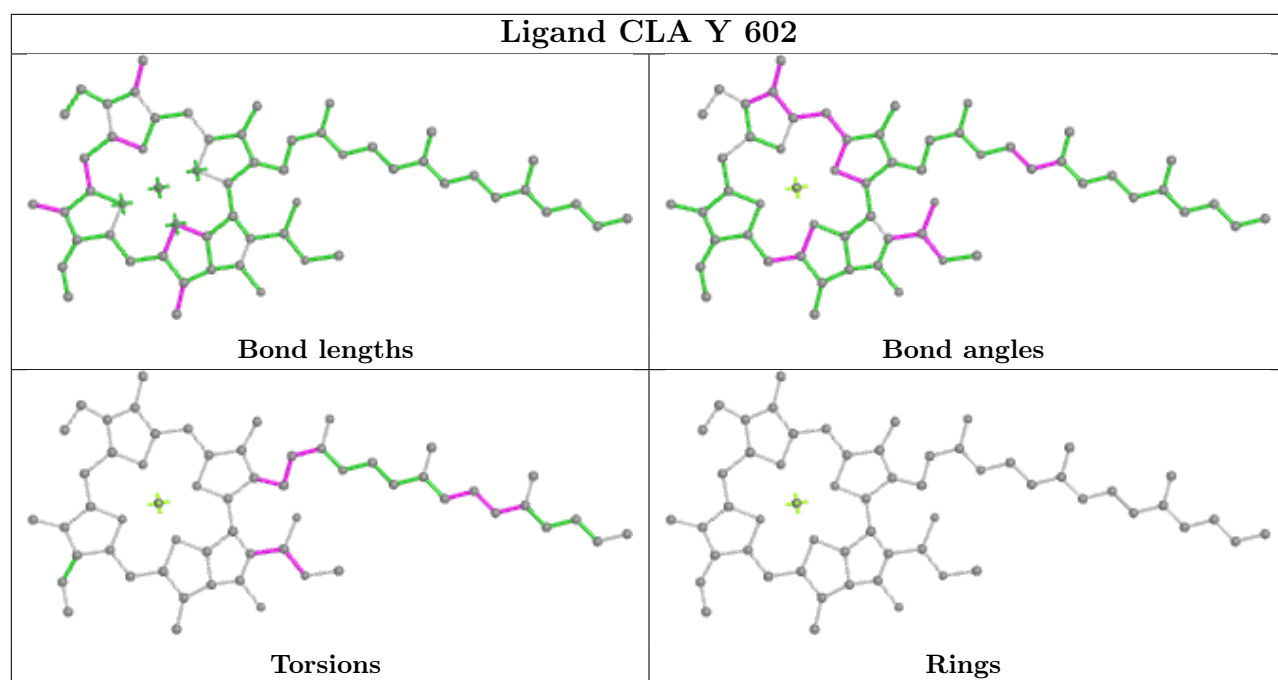
Rings



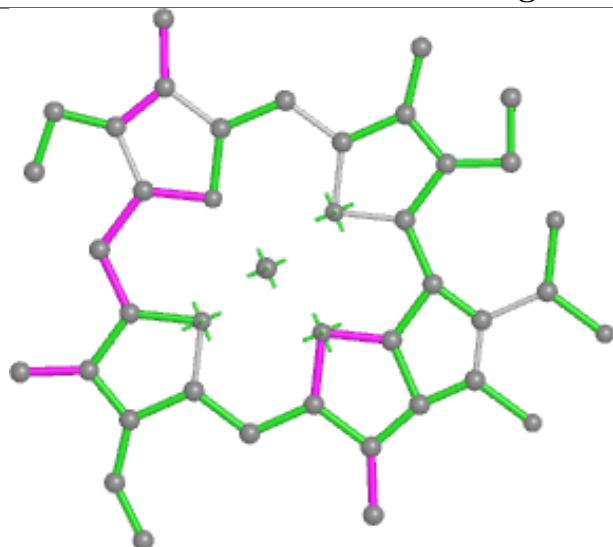


Ligand CLA 9 614

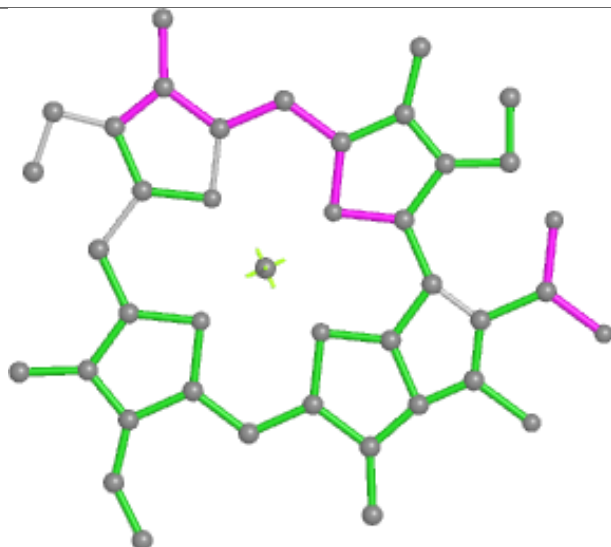




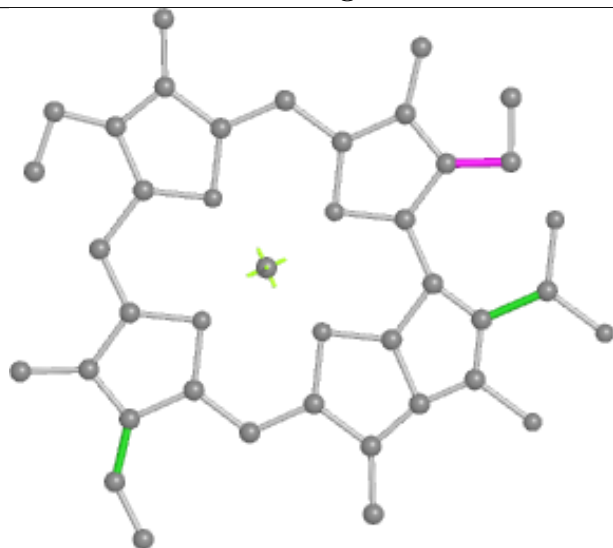
Ligand CLA 8 612



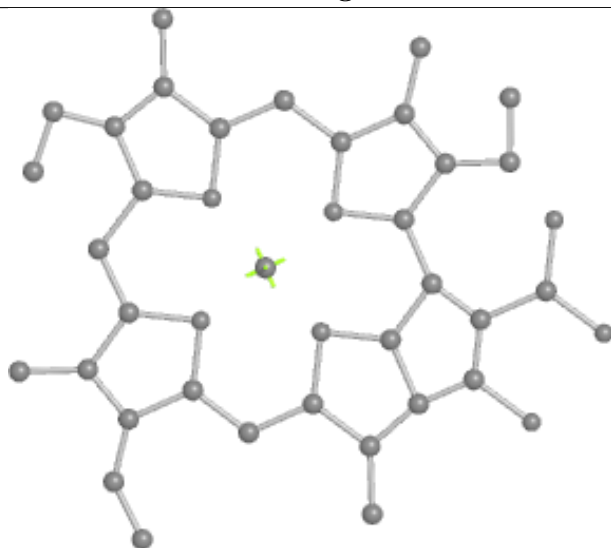
Bond lengths



Bond angles

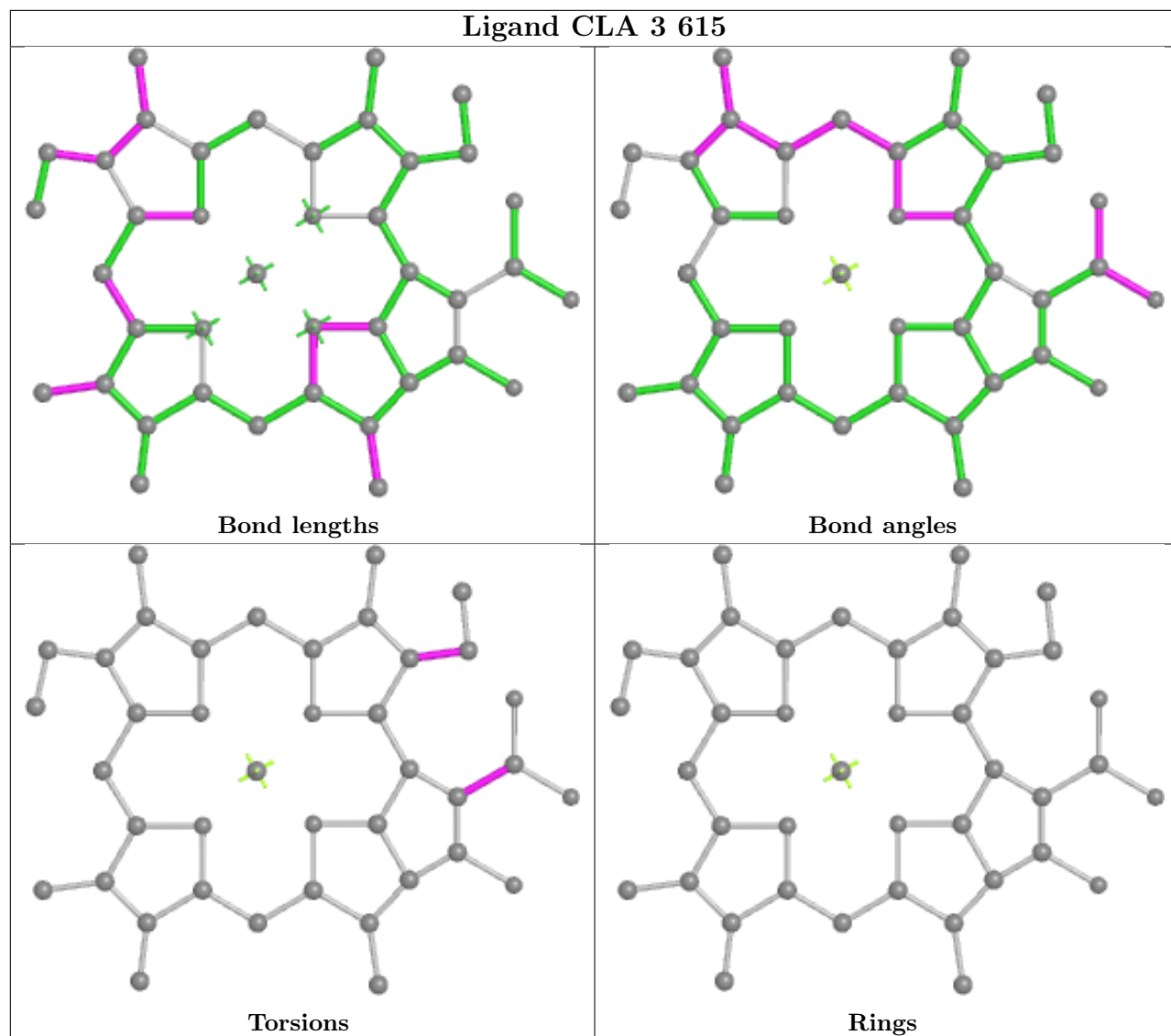


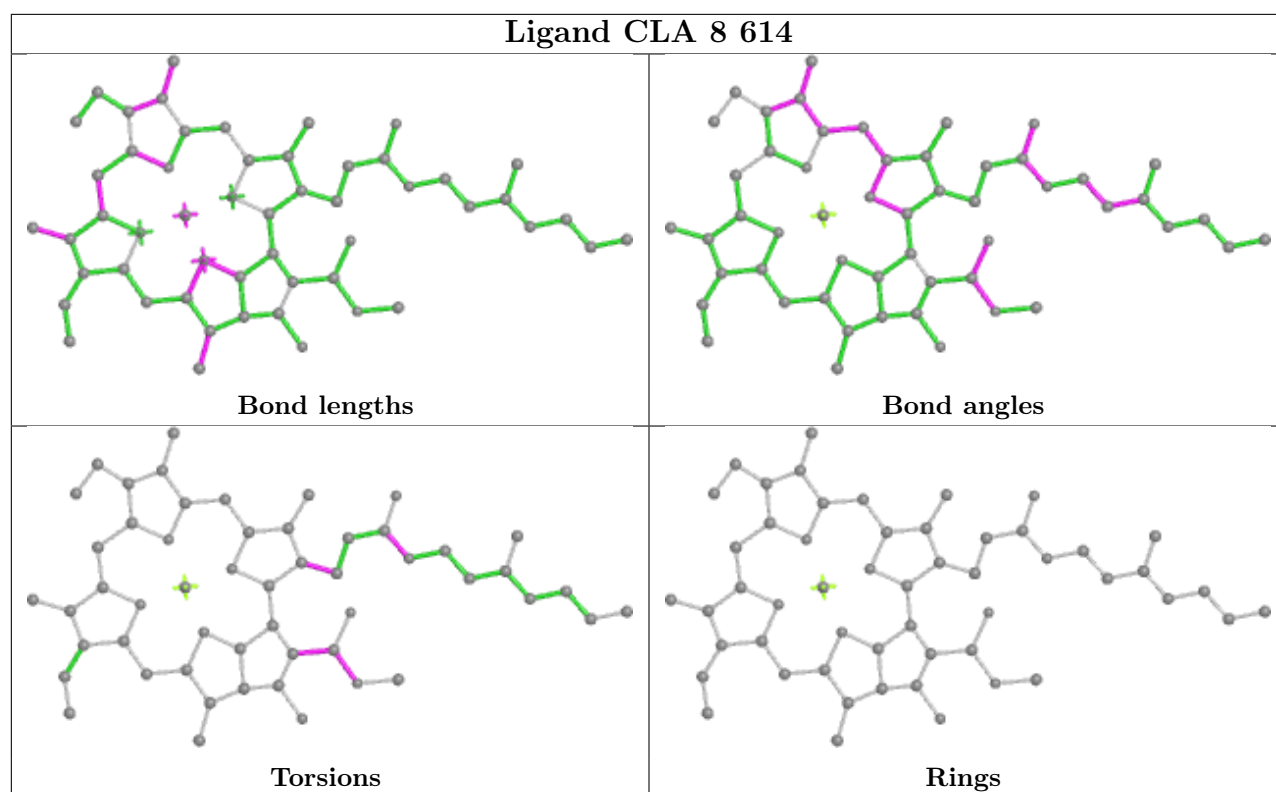
Torsions

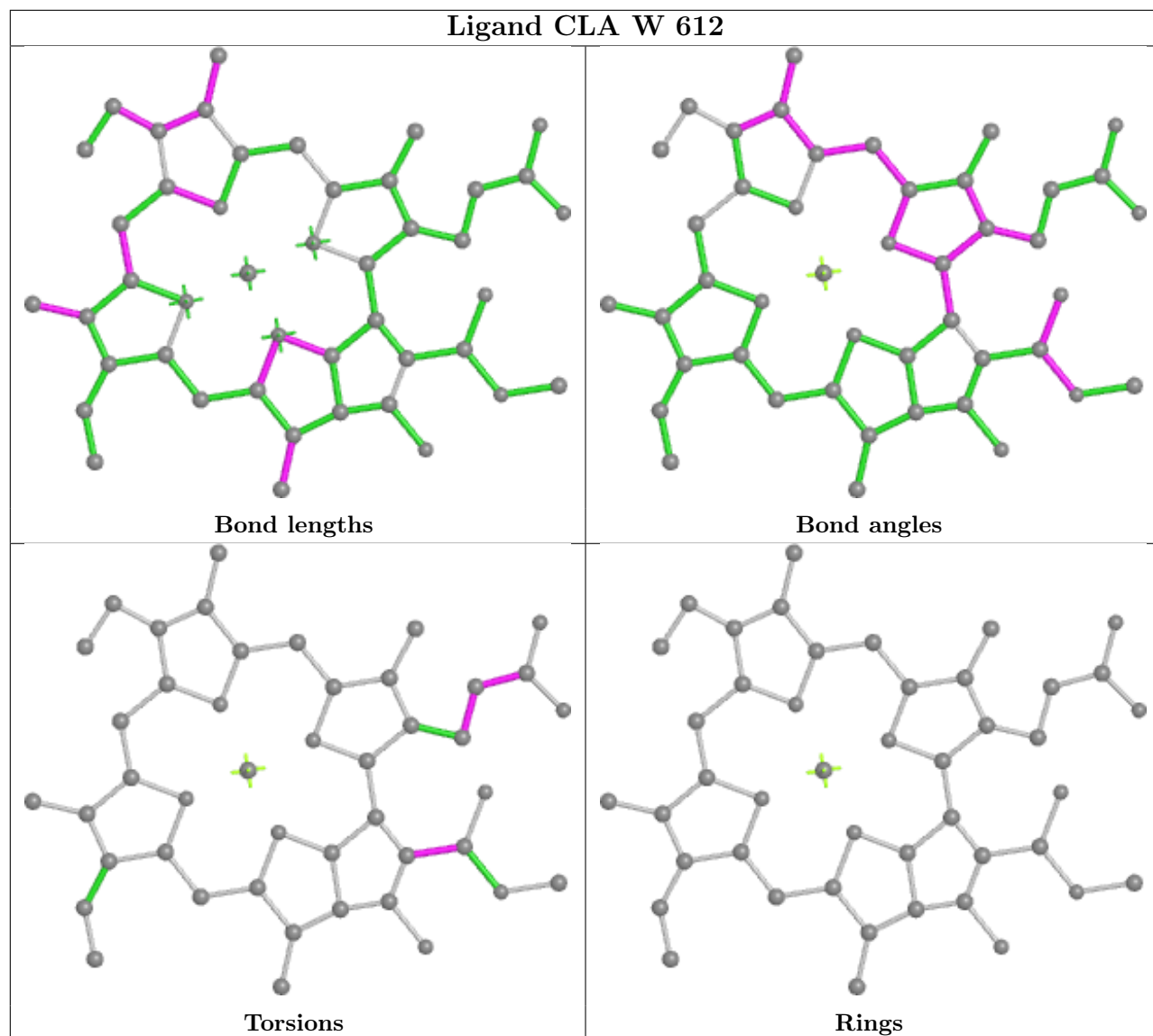


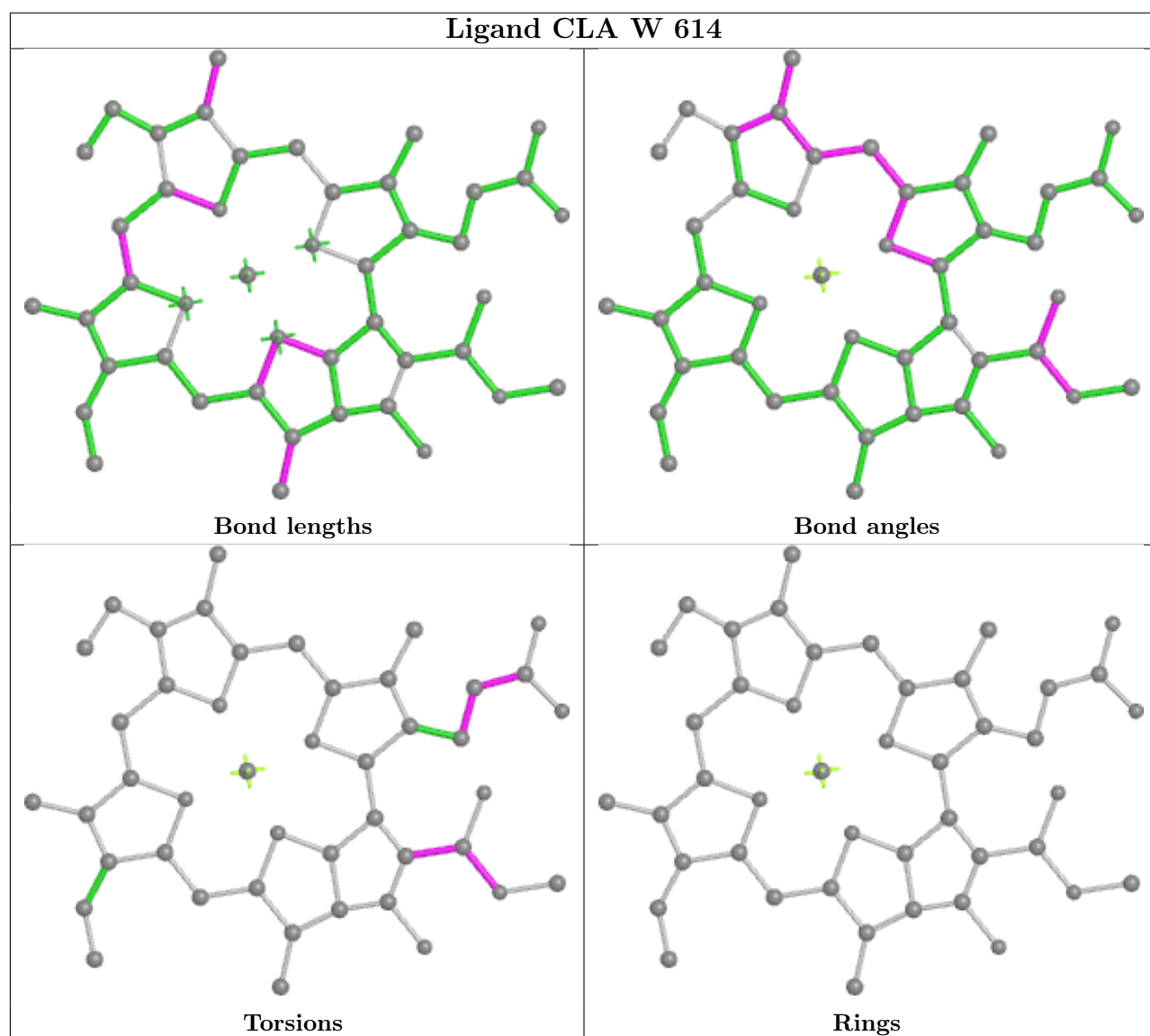
Rings

Ligand CLA 3 615

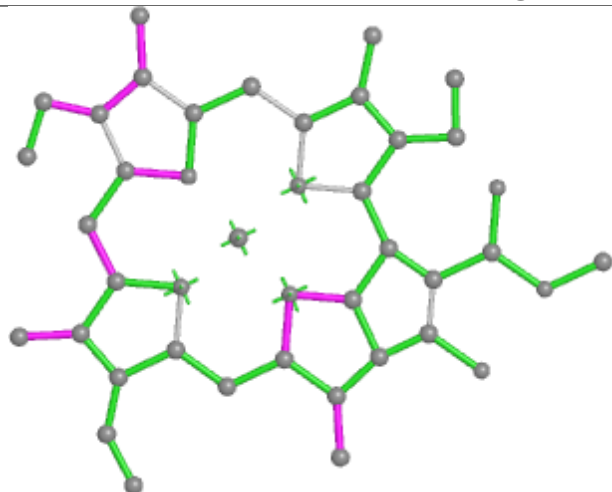




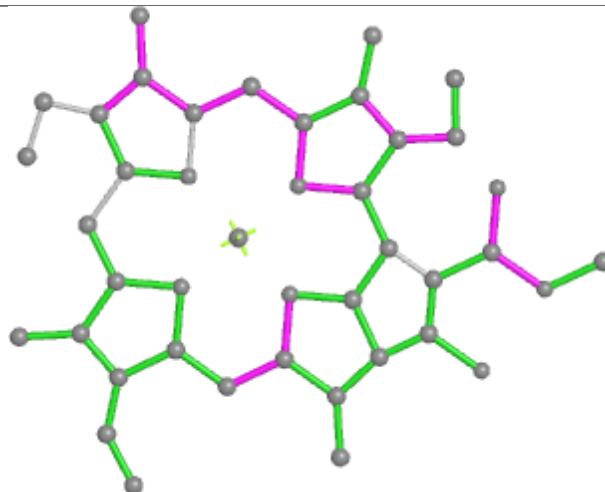




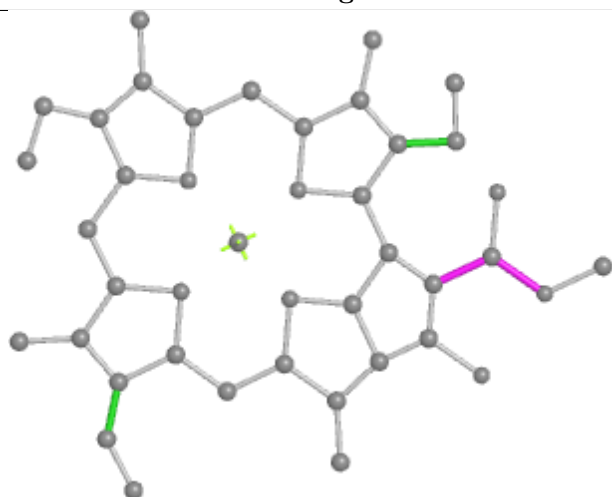
Ligand CLA G 203



Bond lengths



Bond angles

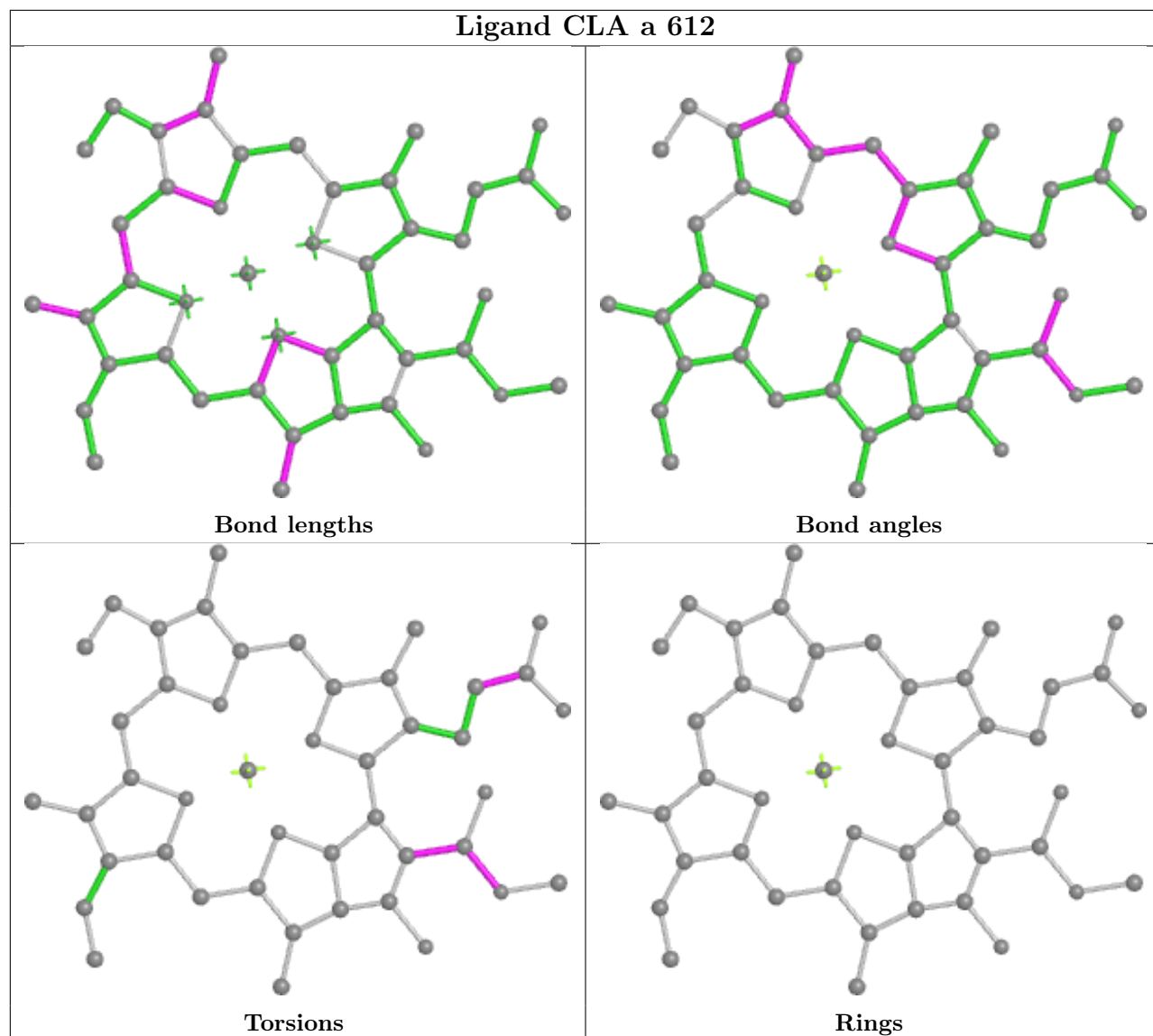


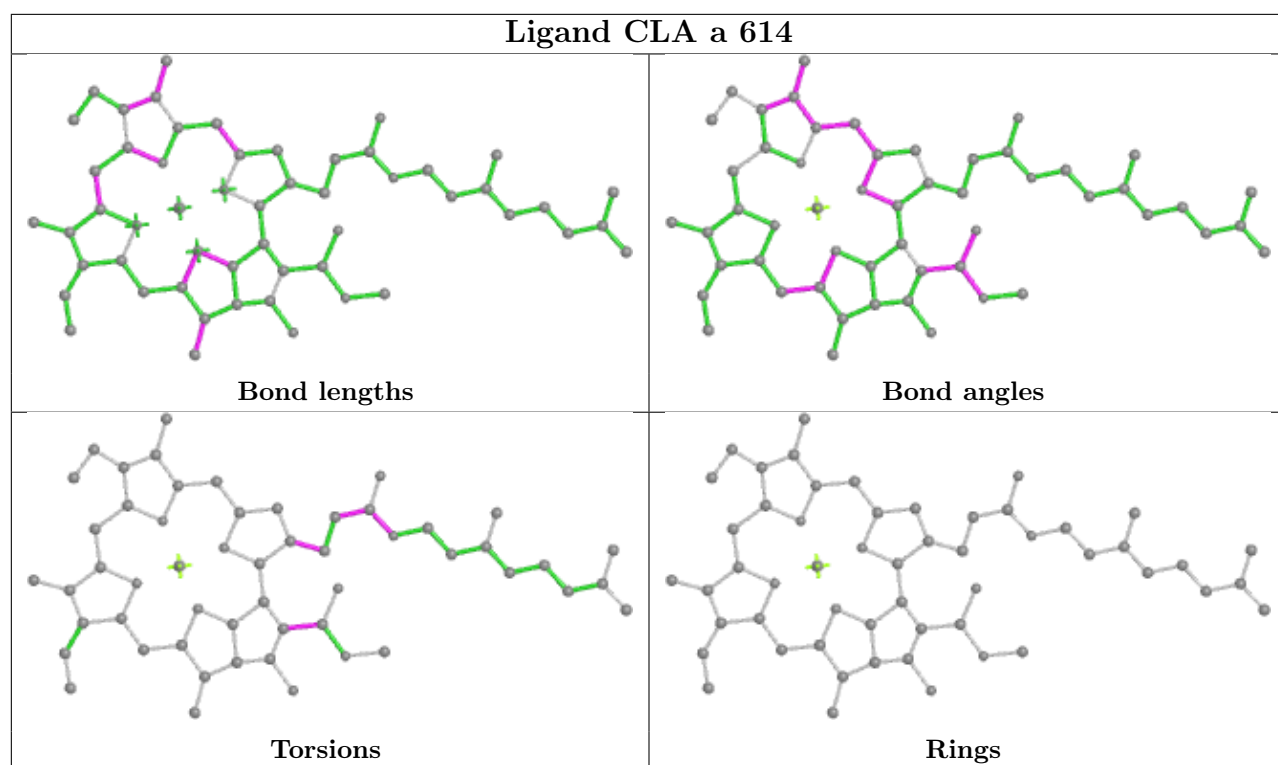
Torsions



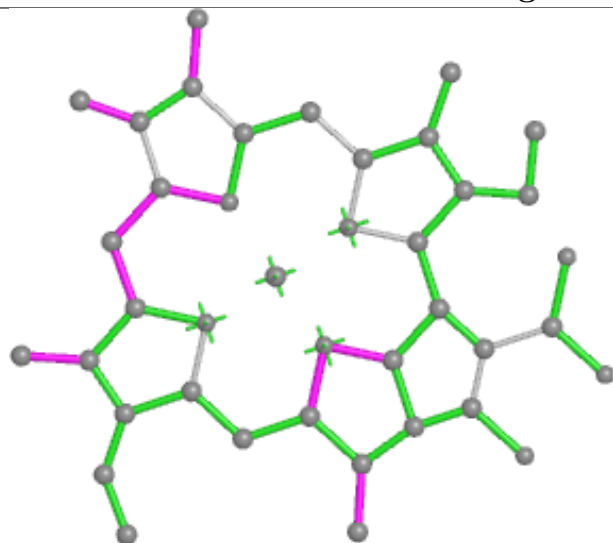
Rings

Ligand CLA a 612

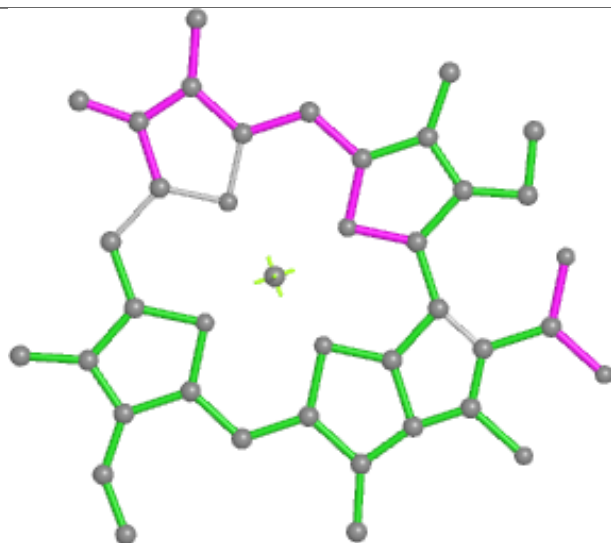




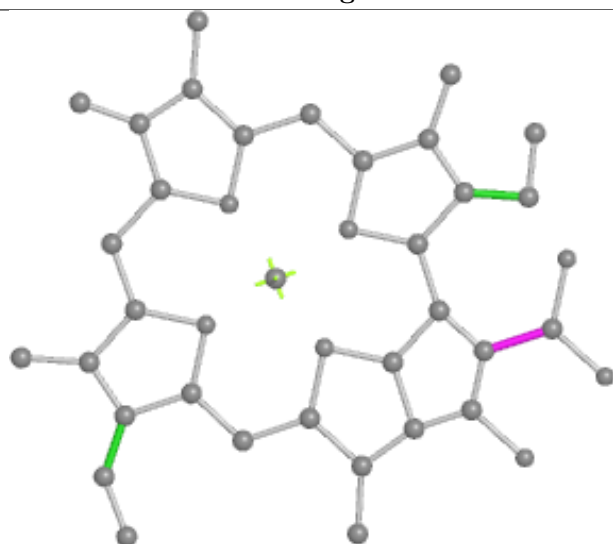
Ligand CLA 6 618



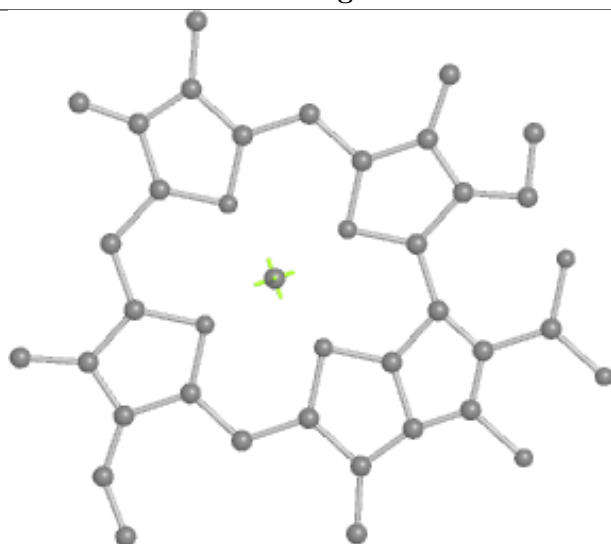
Bond lengths



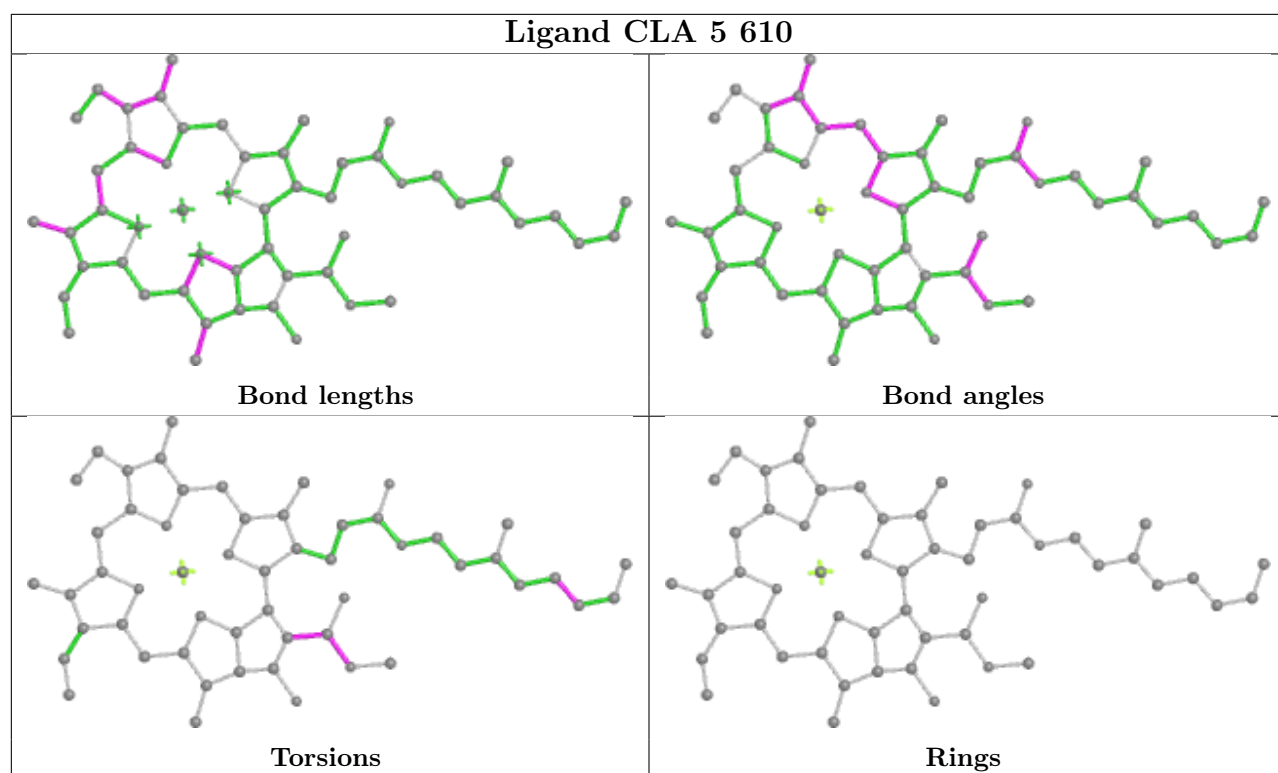
Bond angles



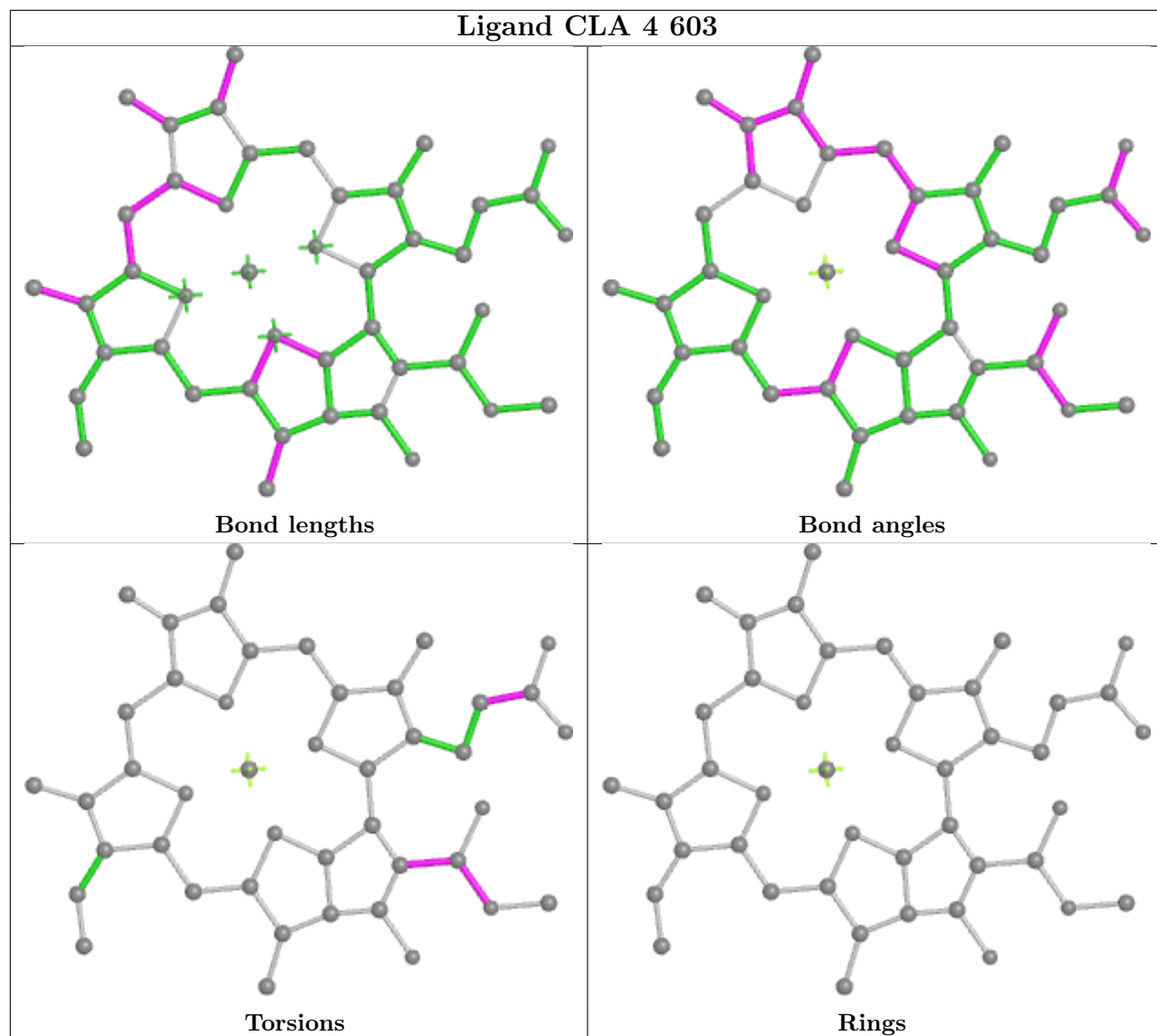
Torsions



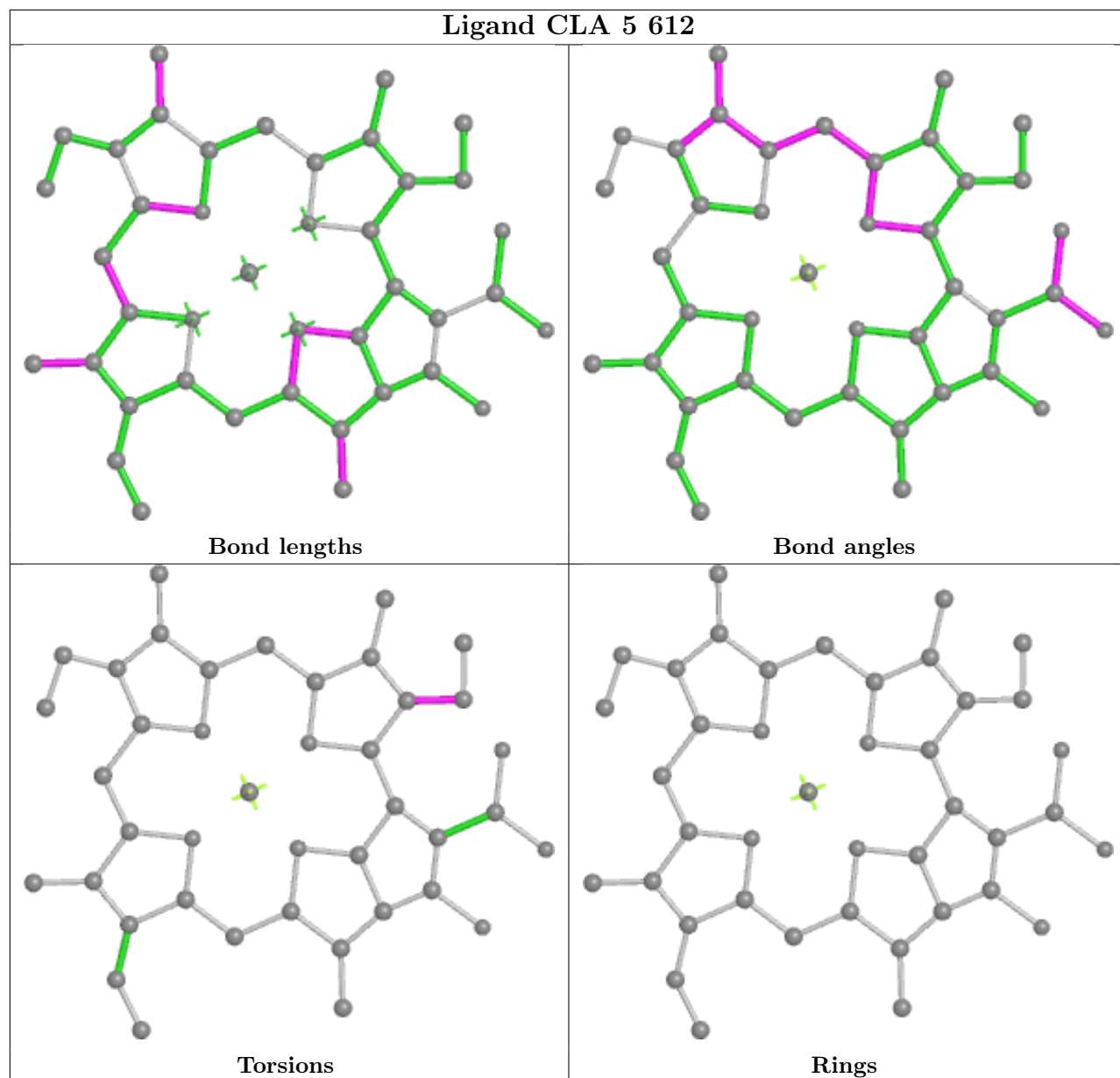
Rings

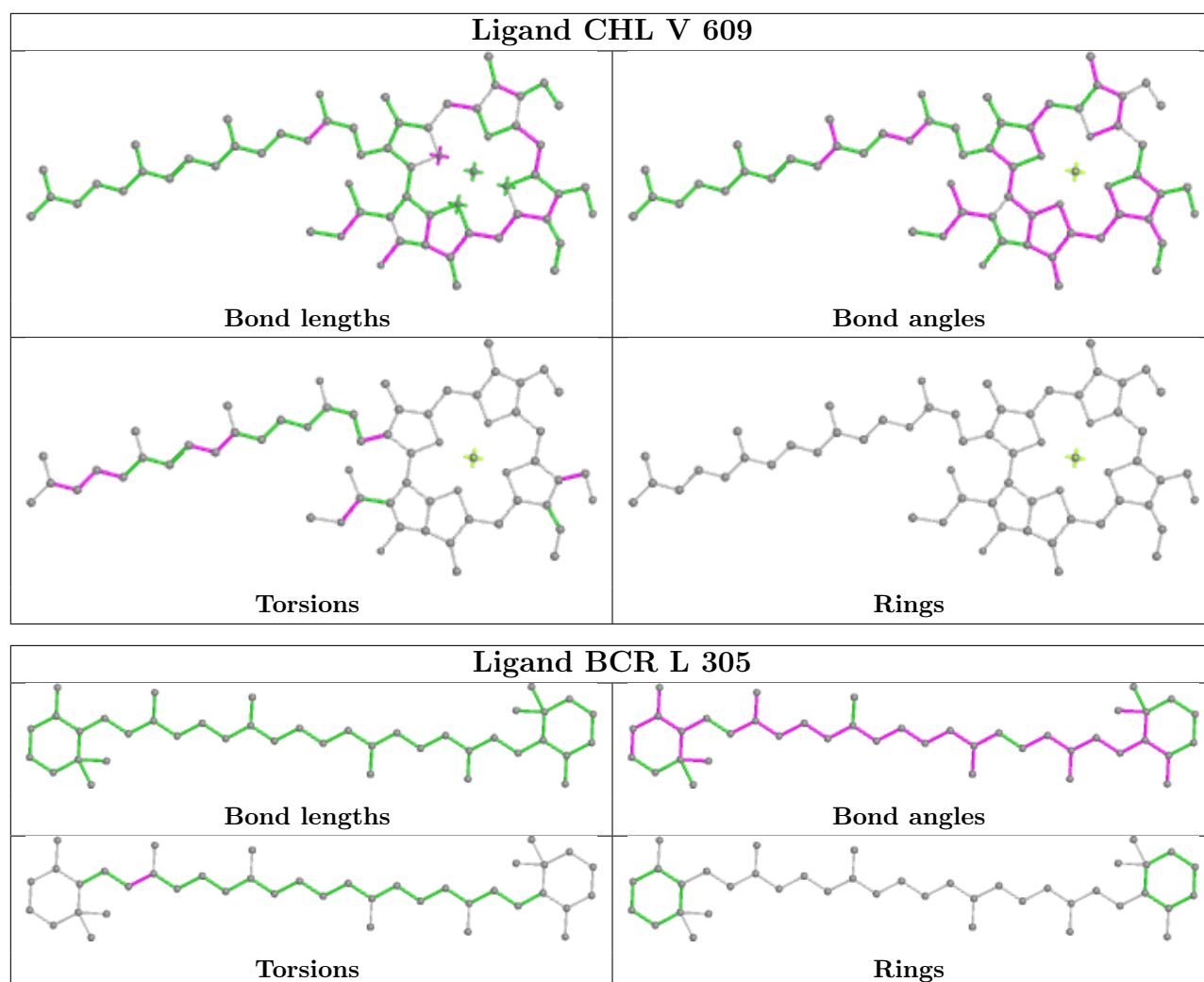


Ligand CLA 4 603

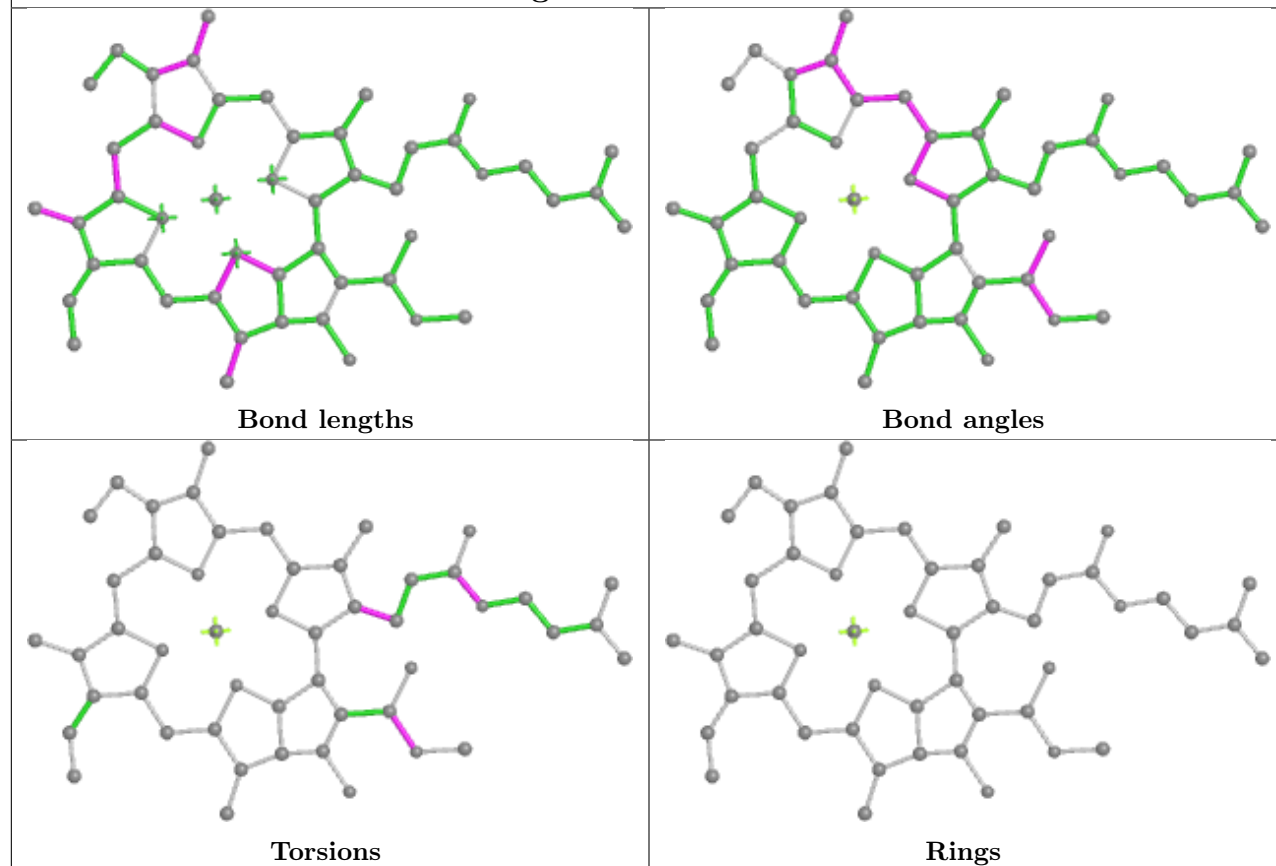


Ligand CLA 5 612

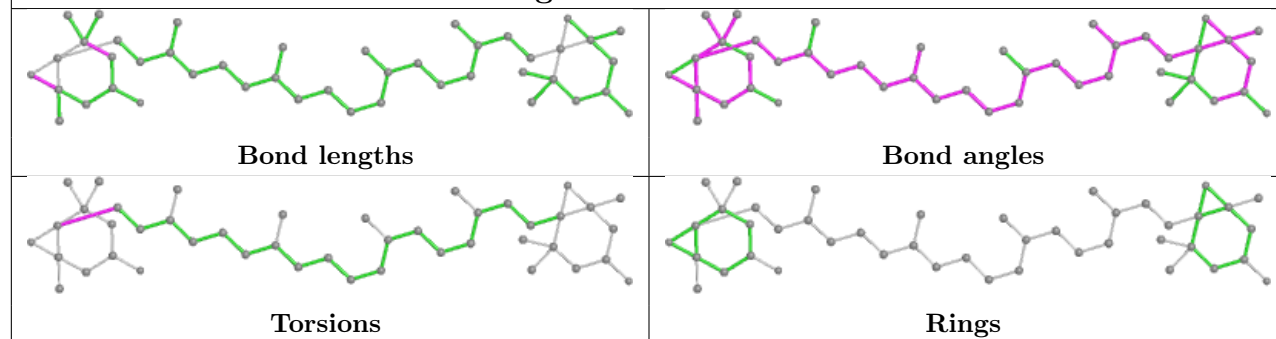


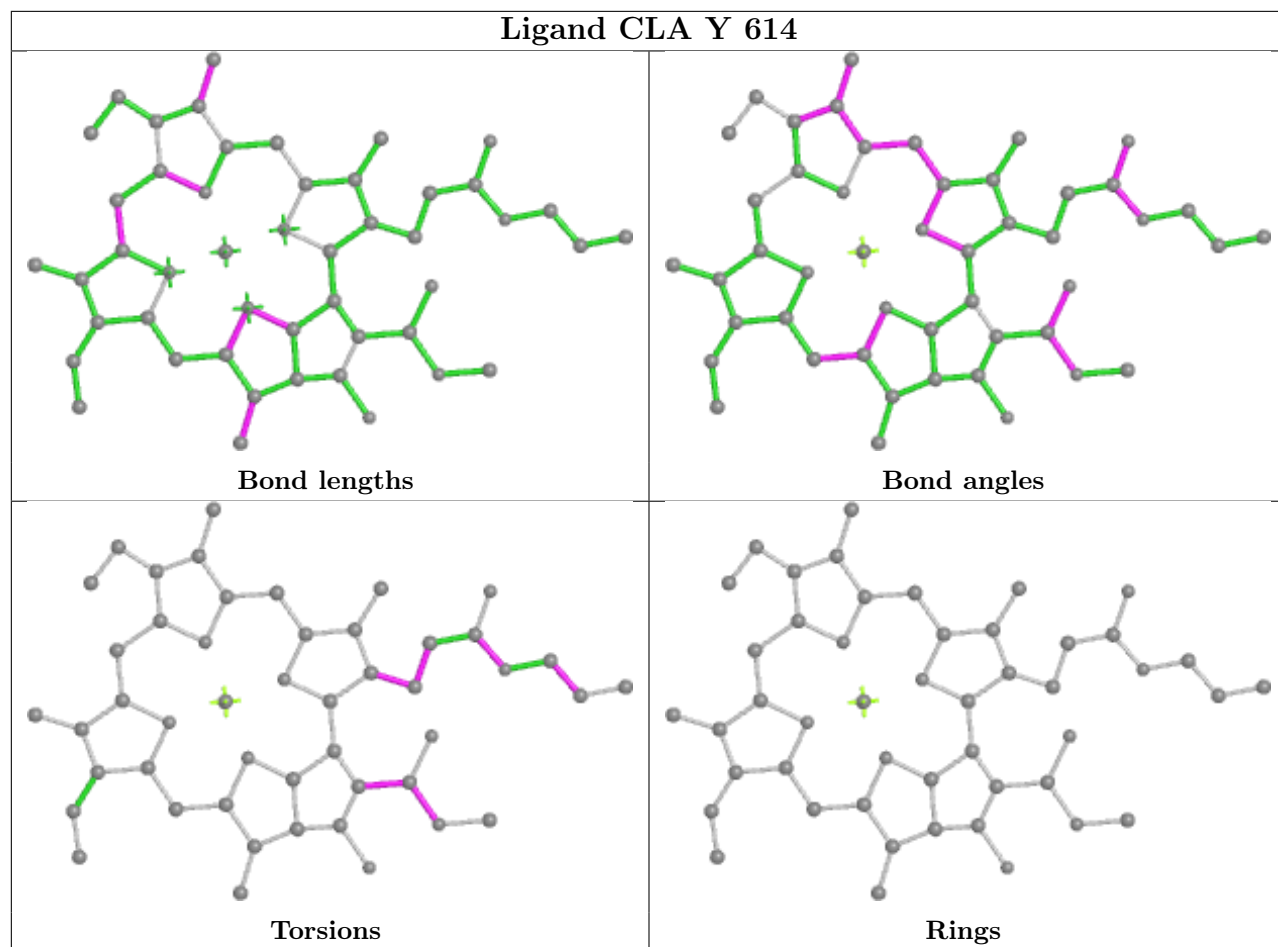


Ligand CLA Y 604

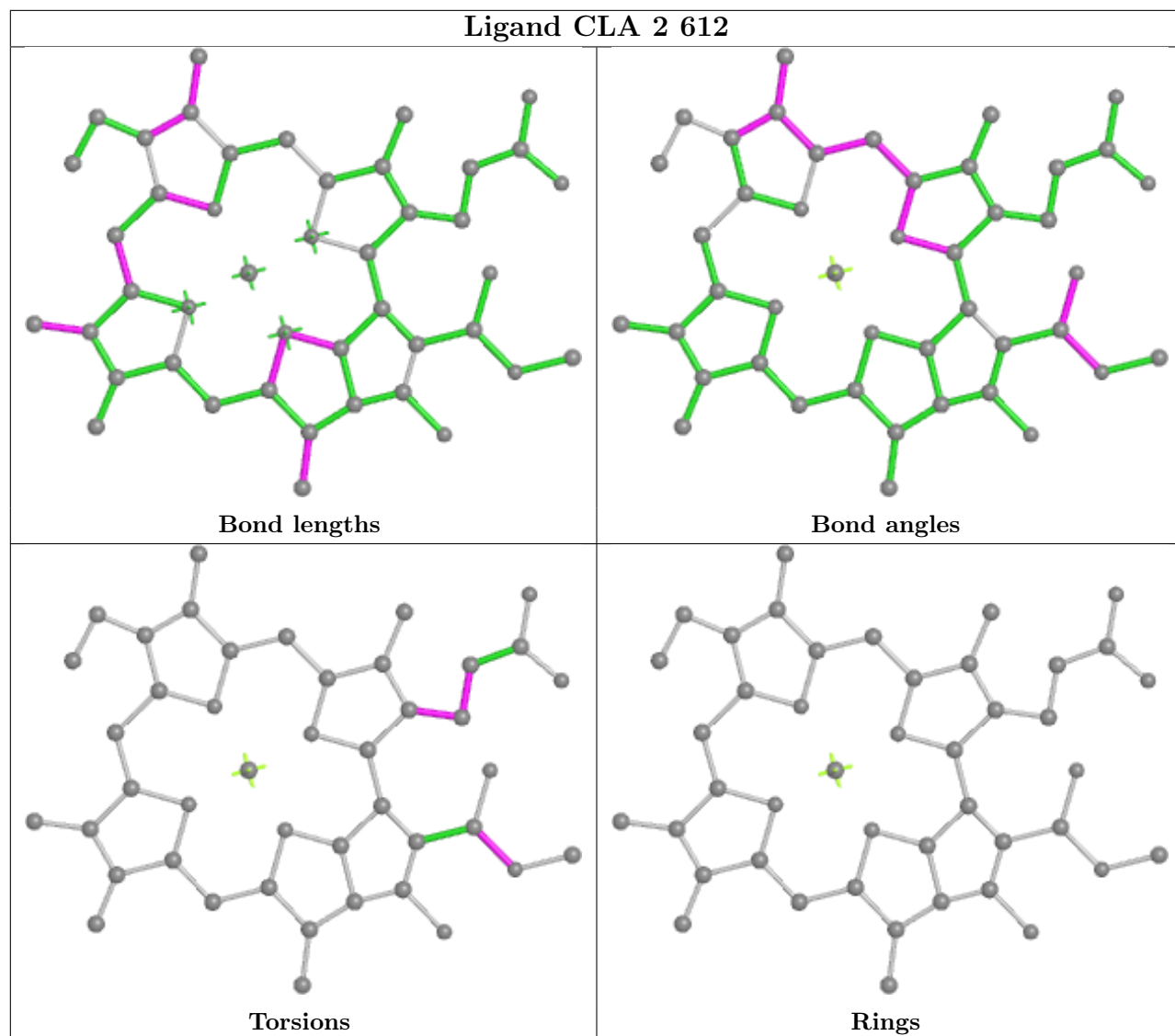


Ligand XAT 4 620

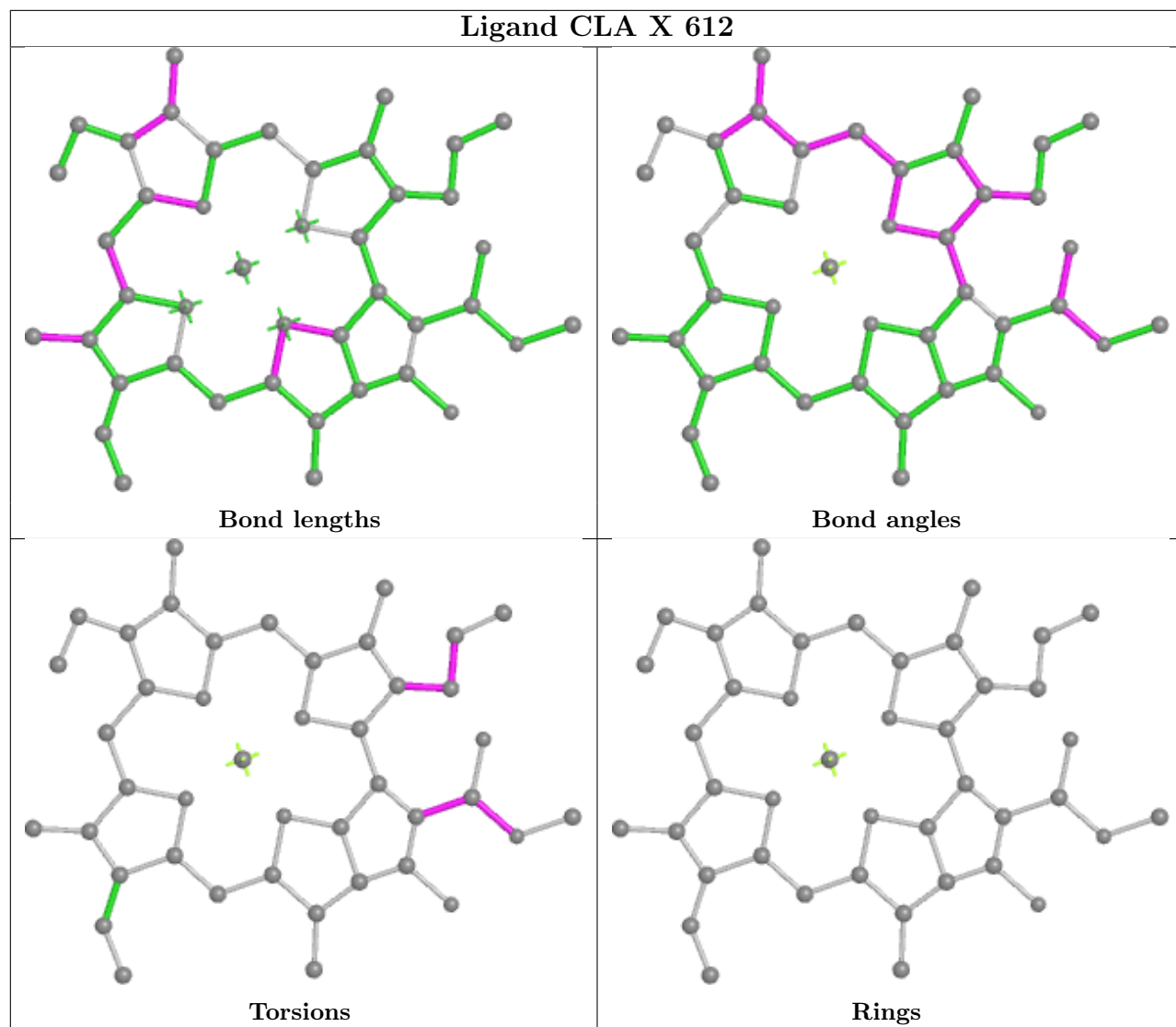




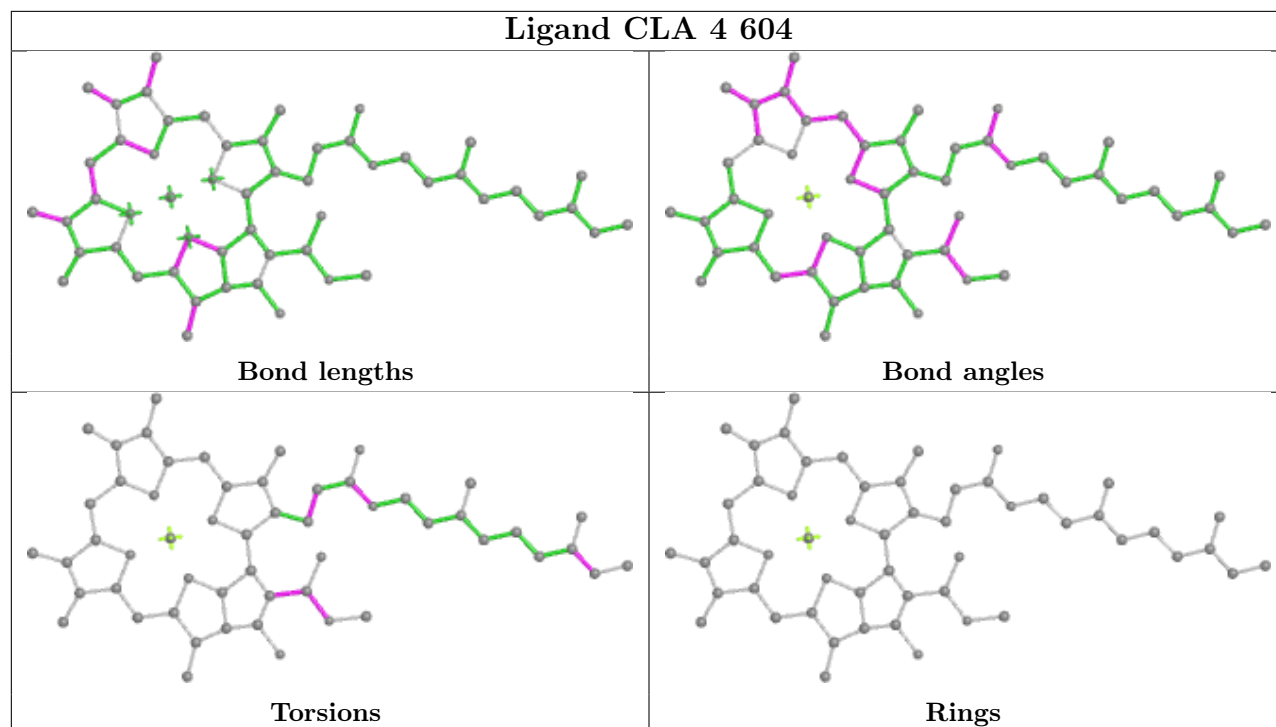
Ligand CLA 2 612



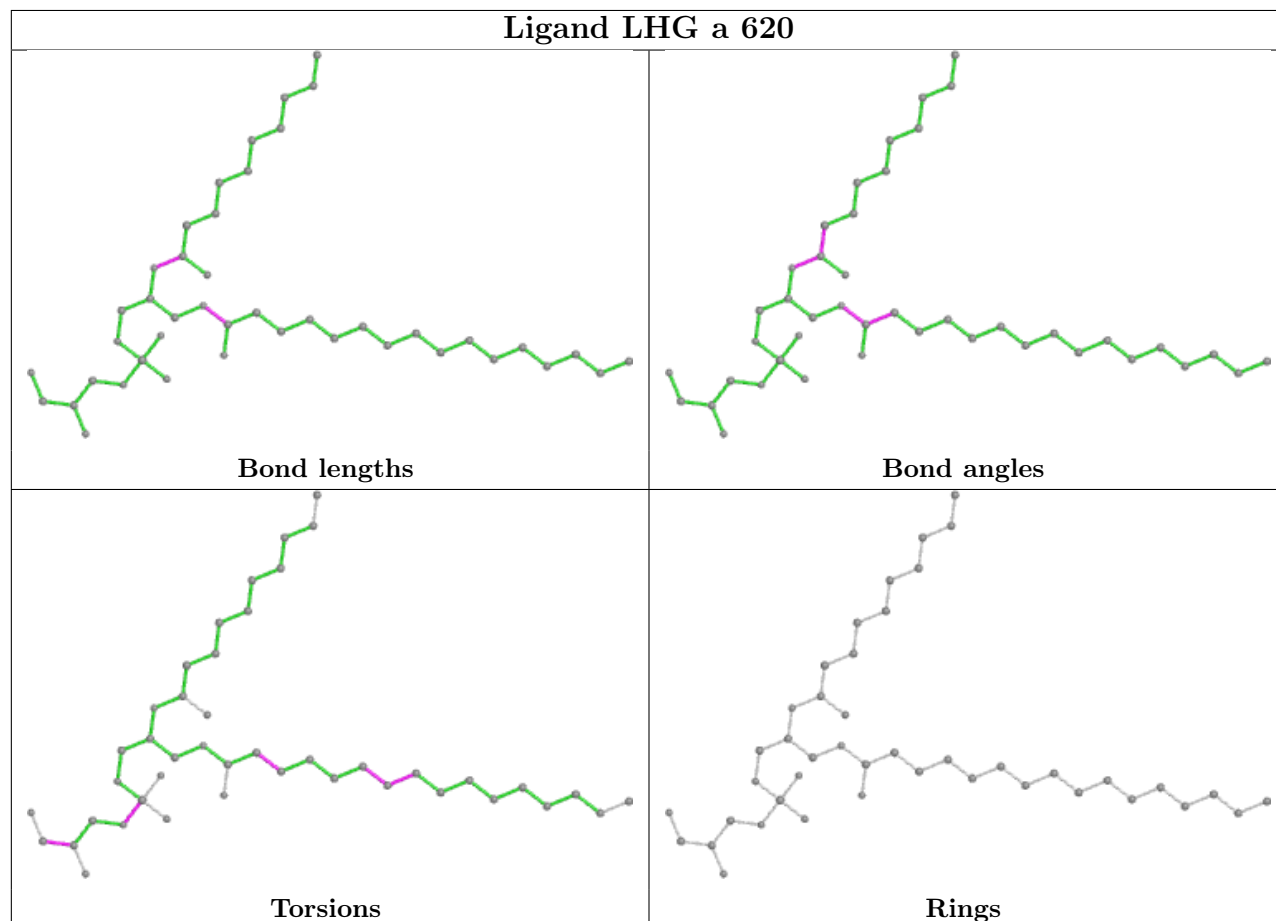
Ligand CLA X 612

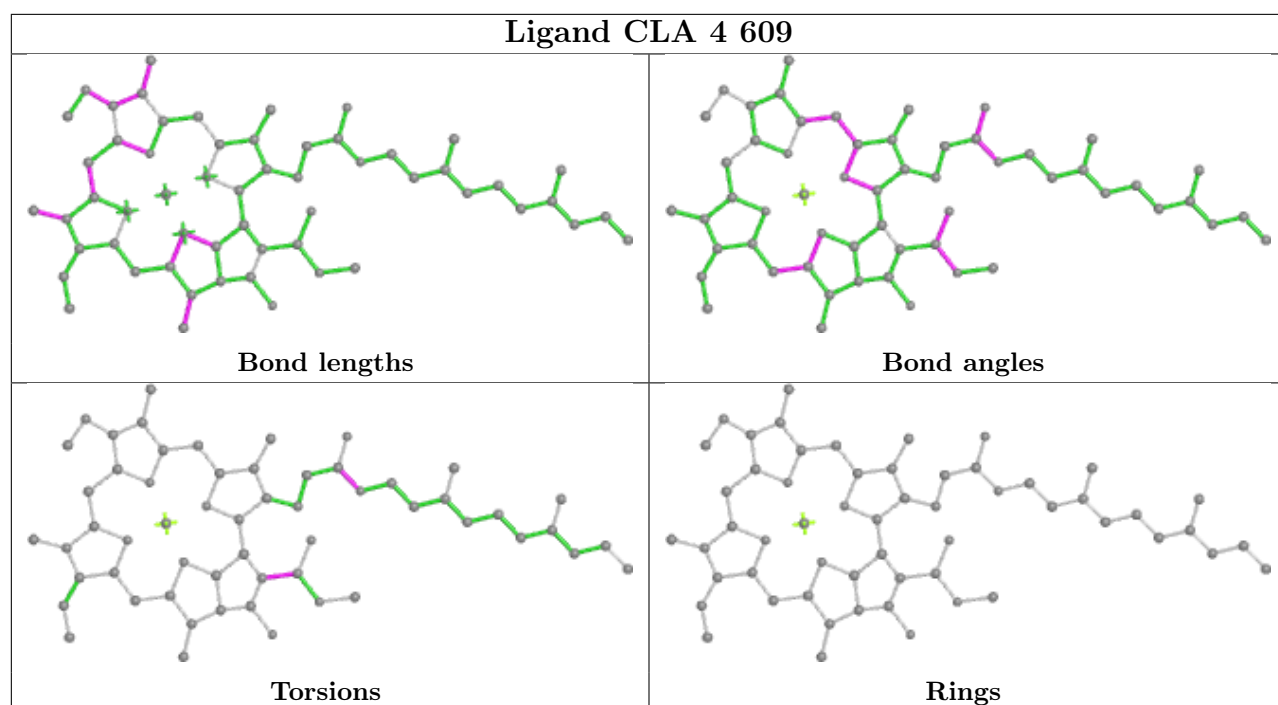


Ligand CLA 4 604

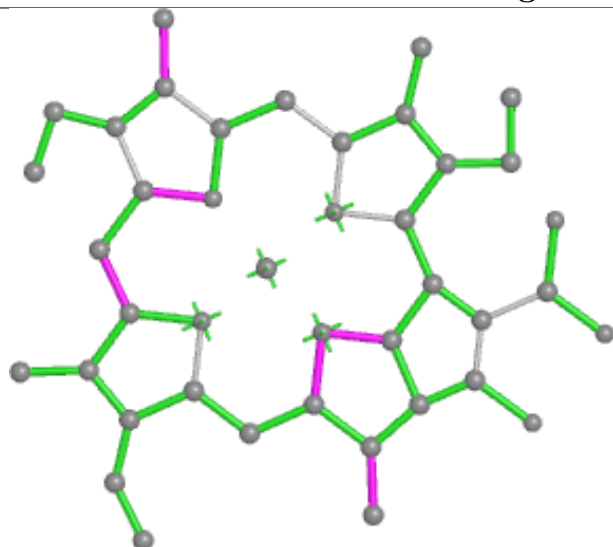


Ligand LHG a 620

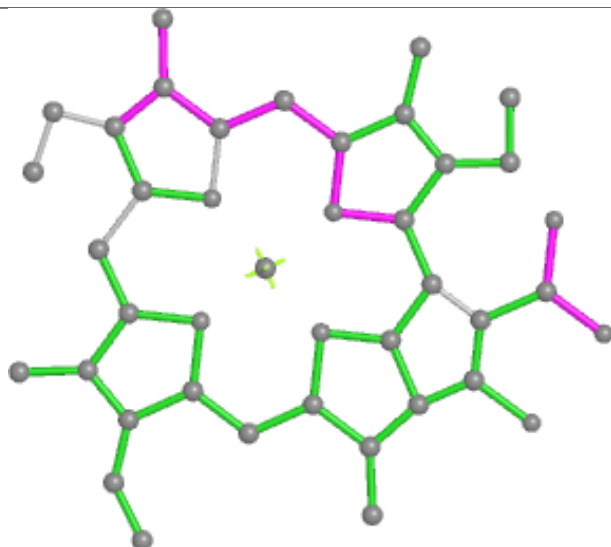




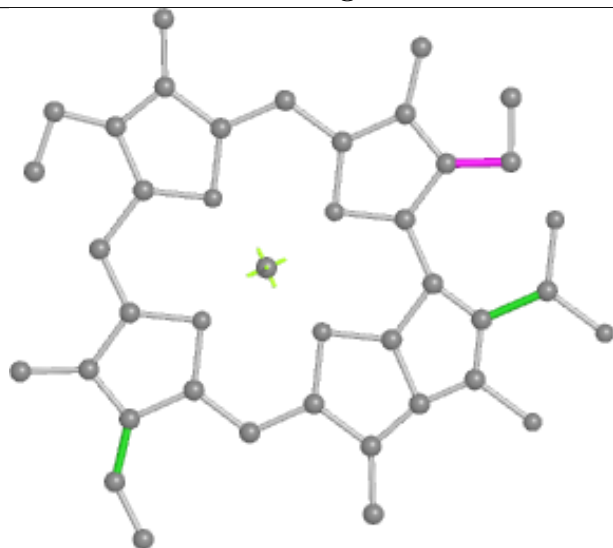
Ligand CLA 9 612



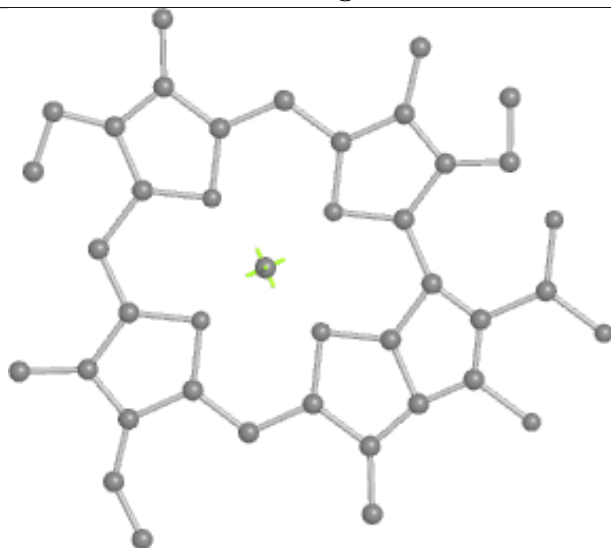
Bond lengths



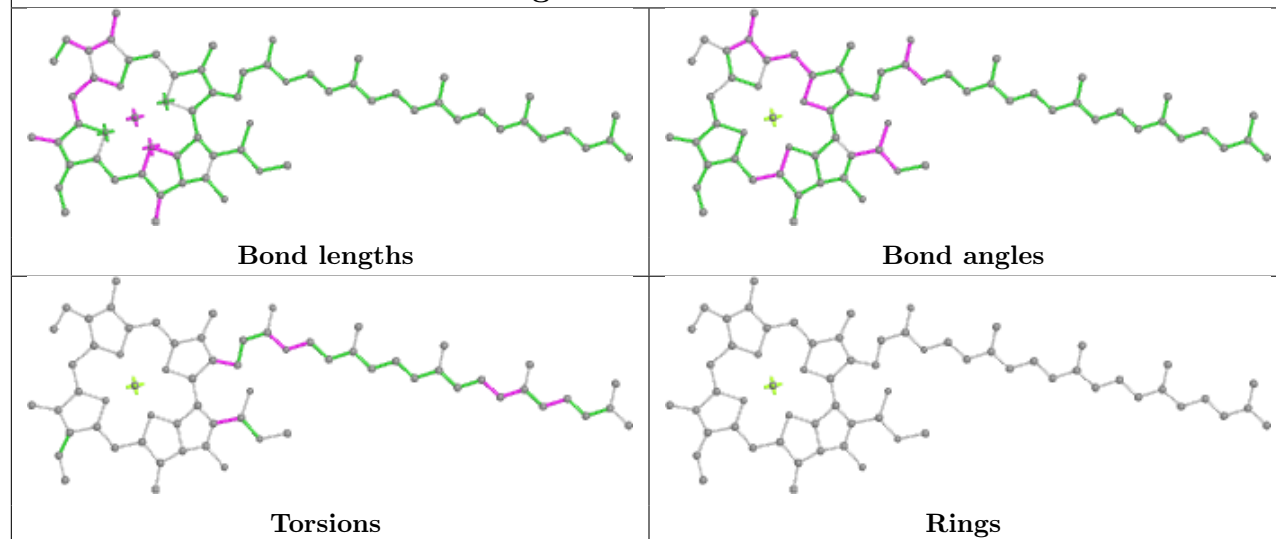
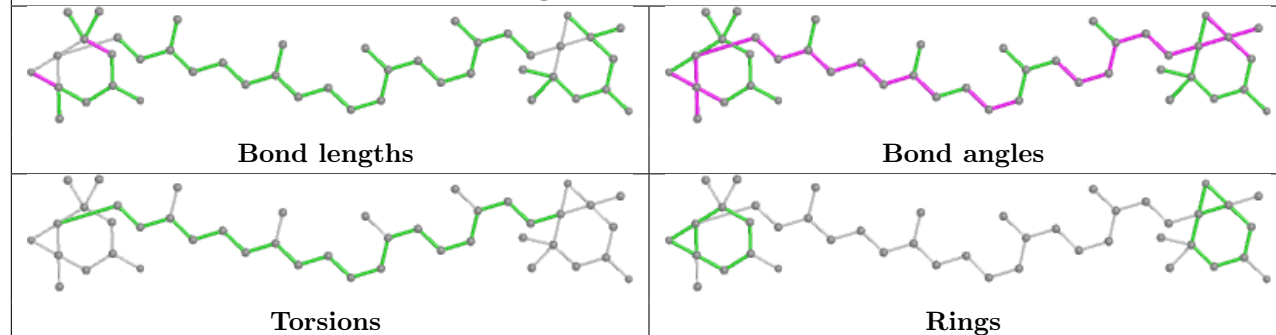
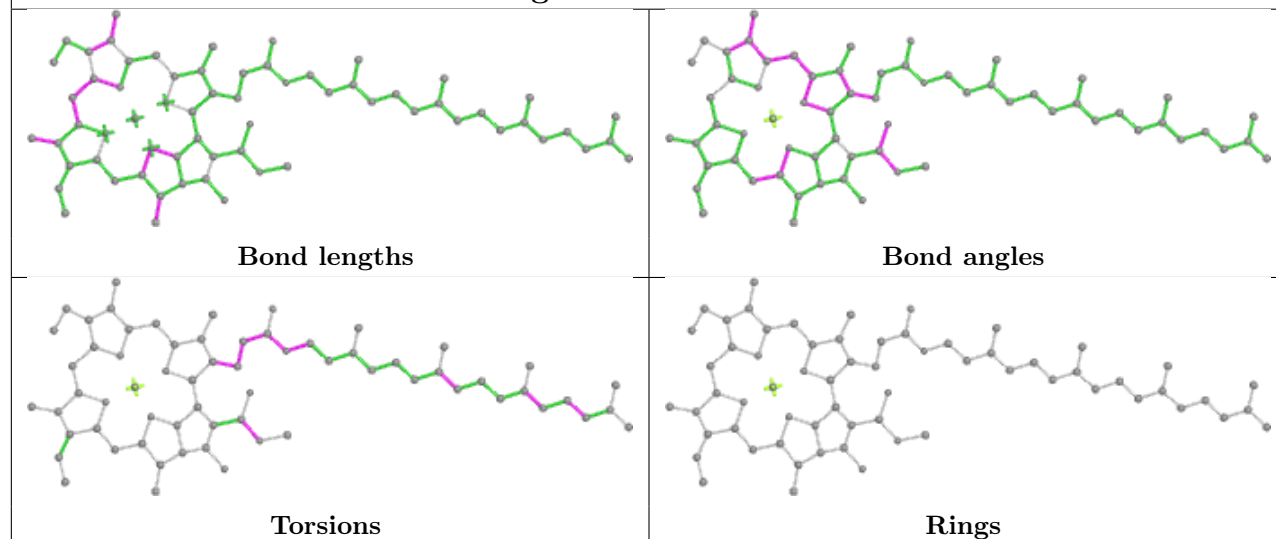
Bond angles



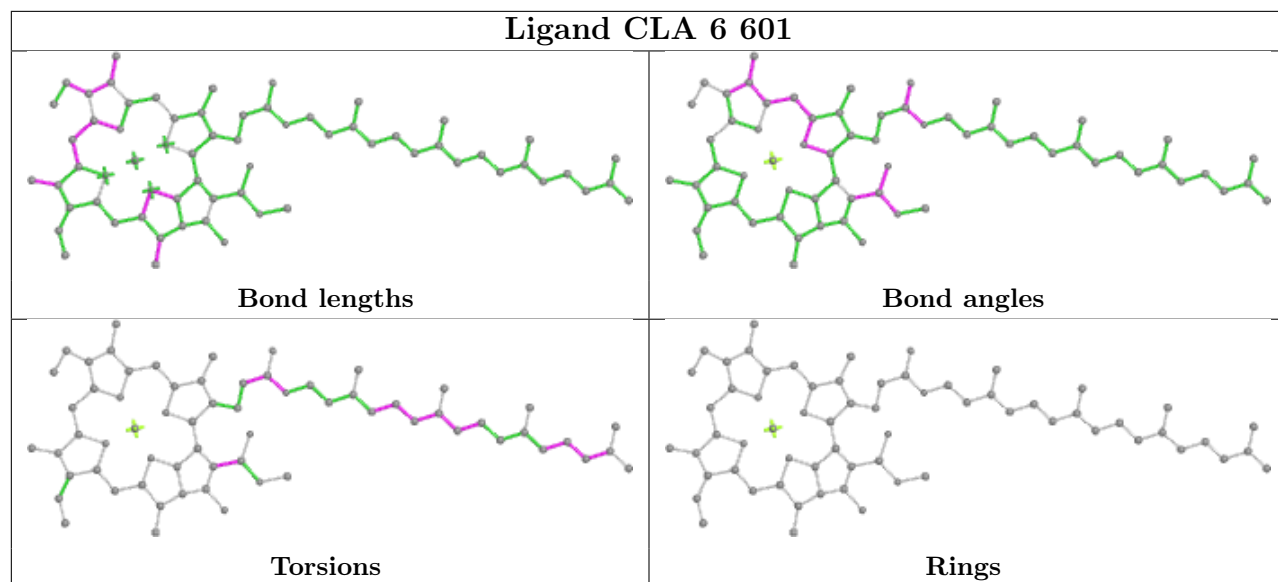
Torsions



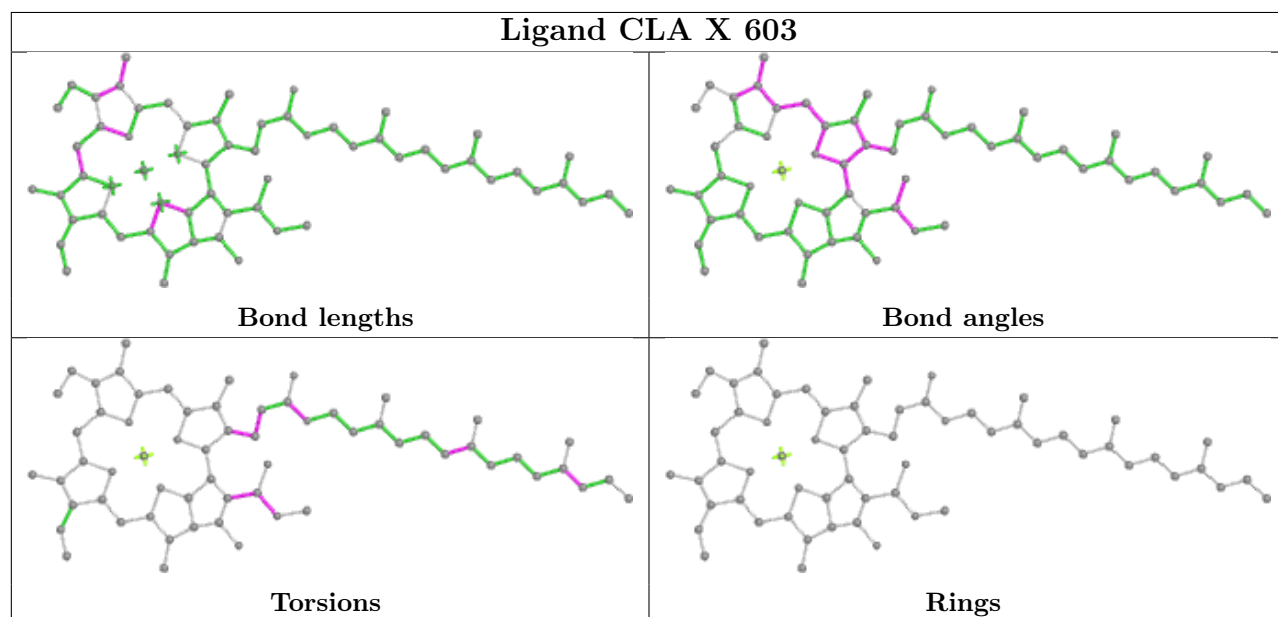
Rings

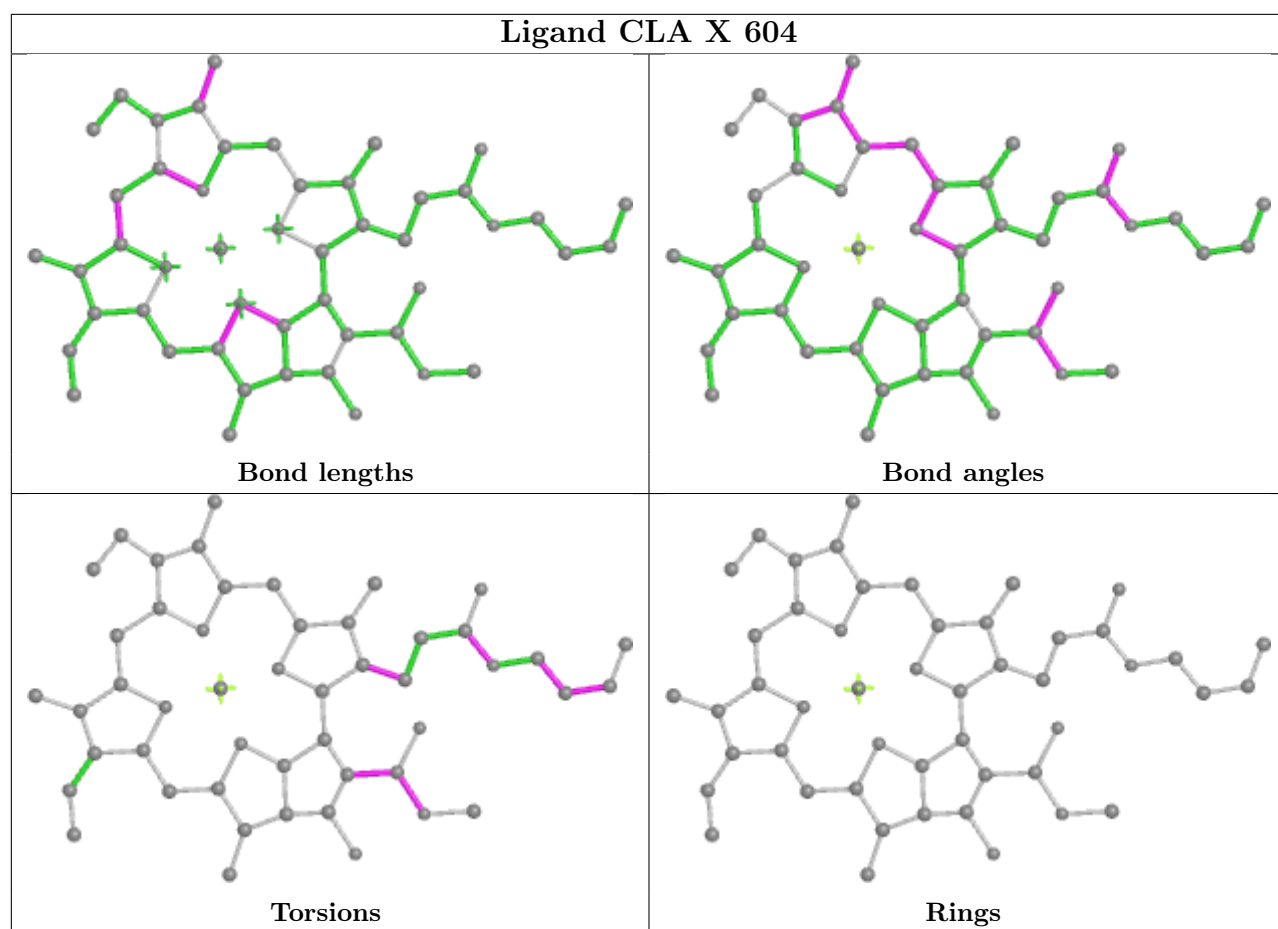
Ligand CLA B 805**Ligand XAT 7 620****Ligand CLA H 203**

Ligand CLA 6 601

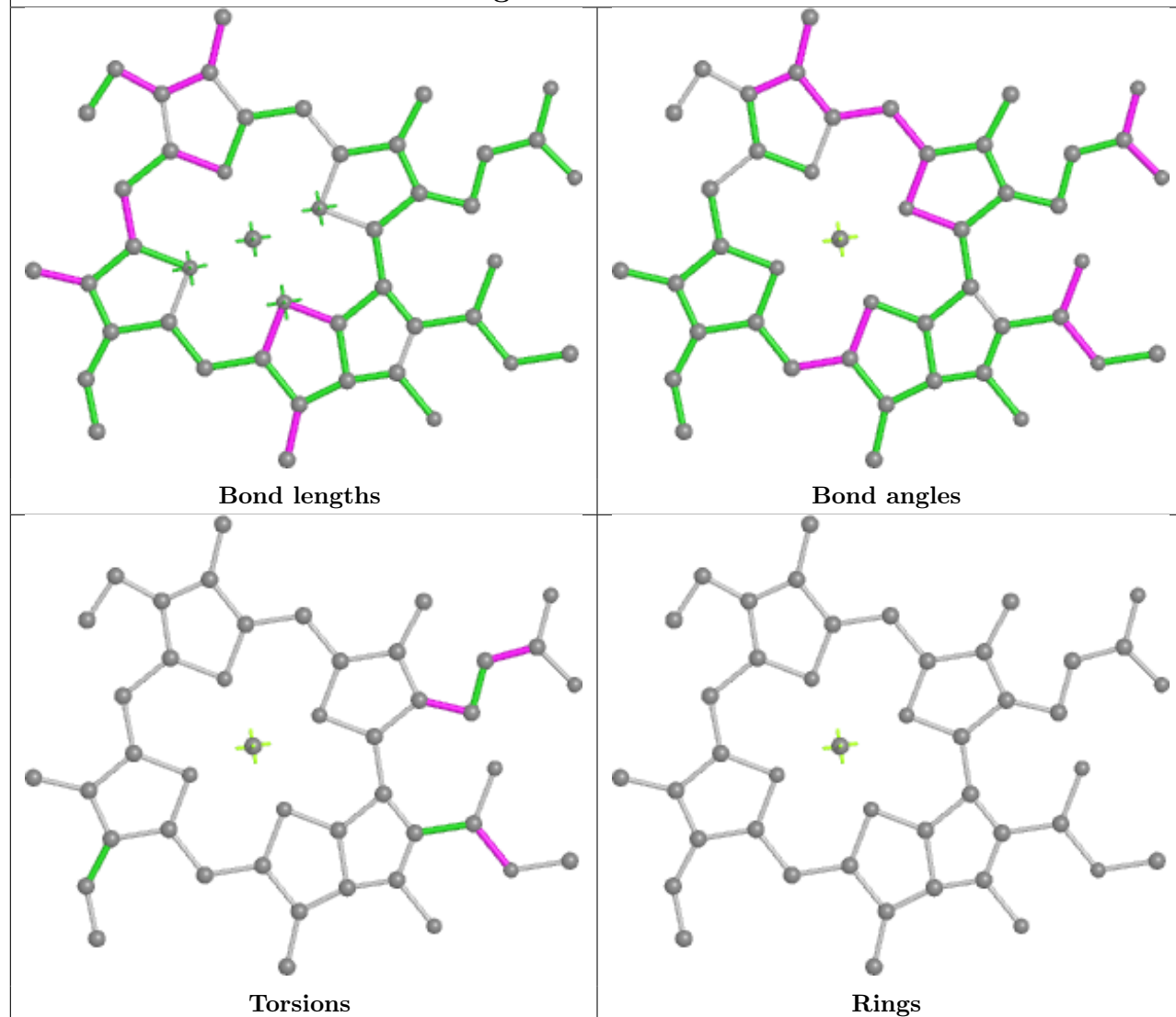


Ligand CLA X 603

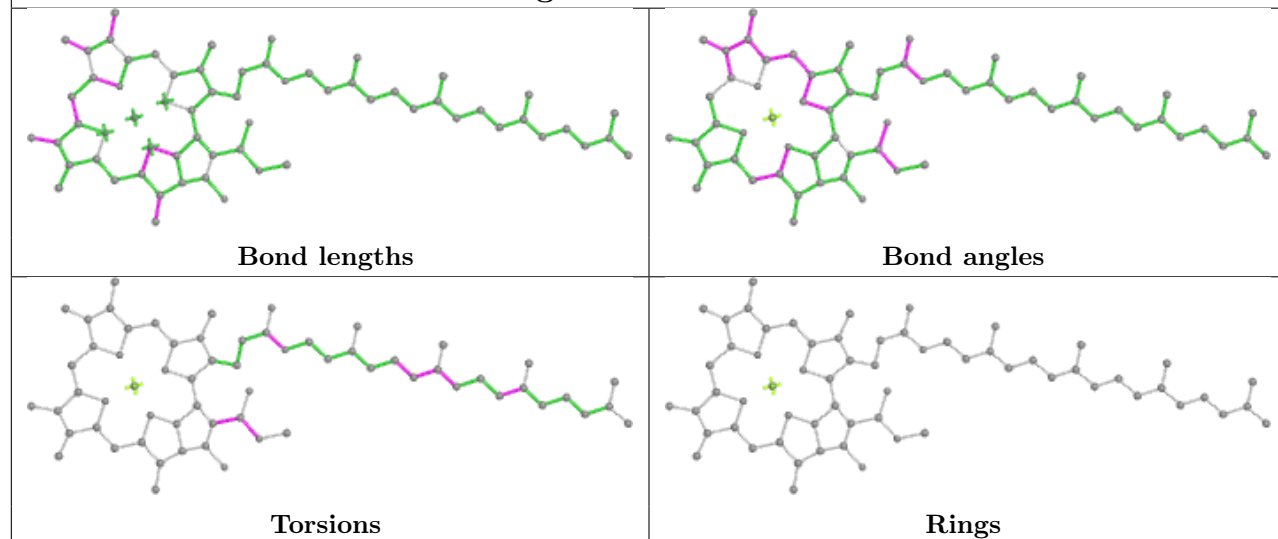




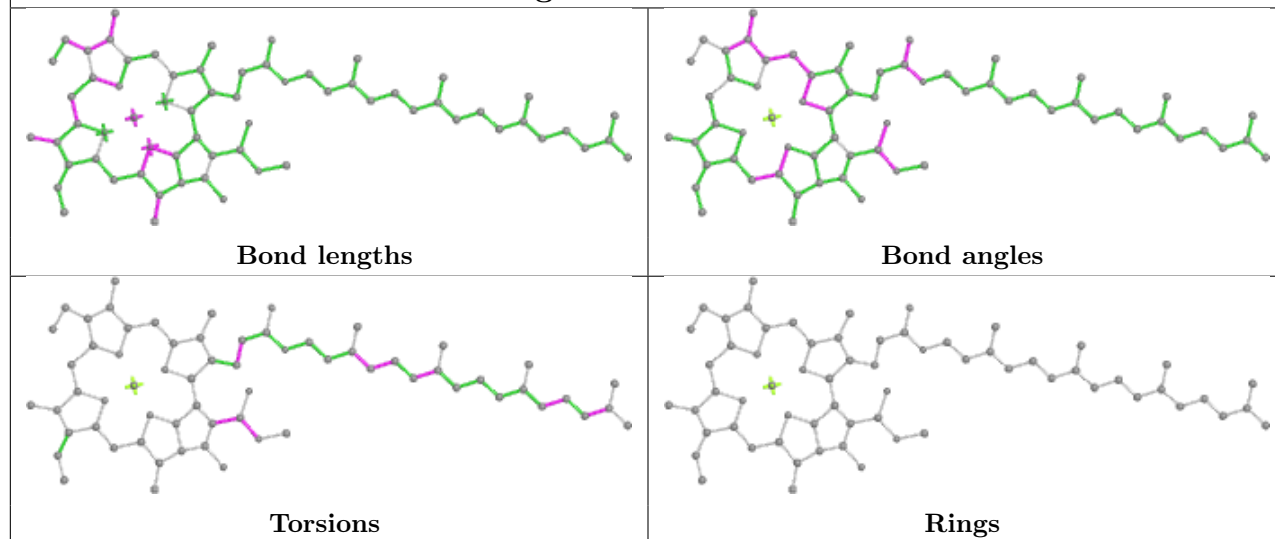
Ligand CLA 6 608



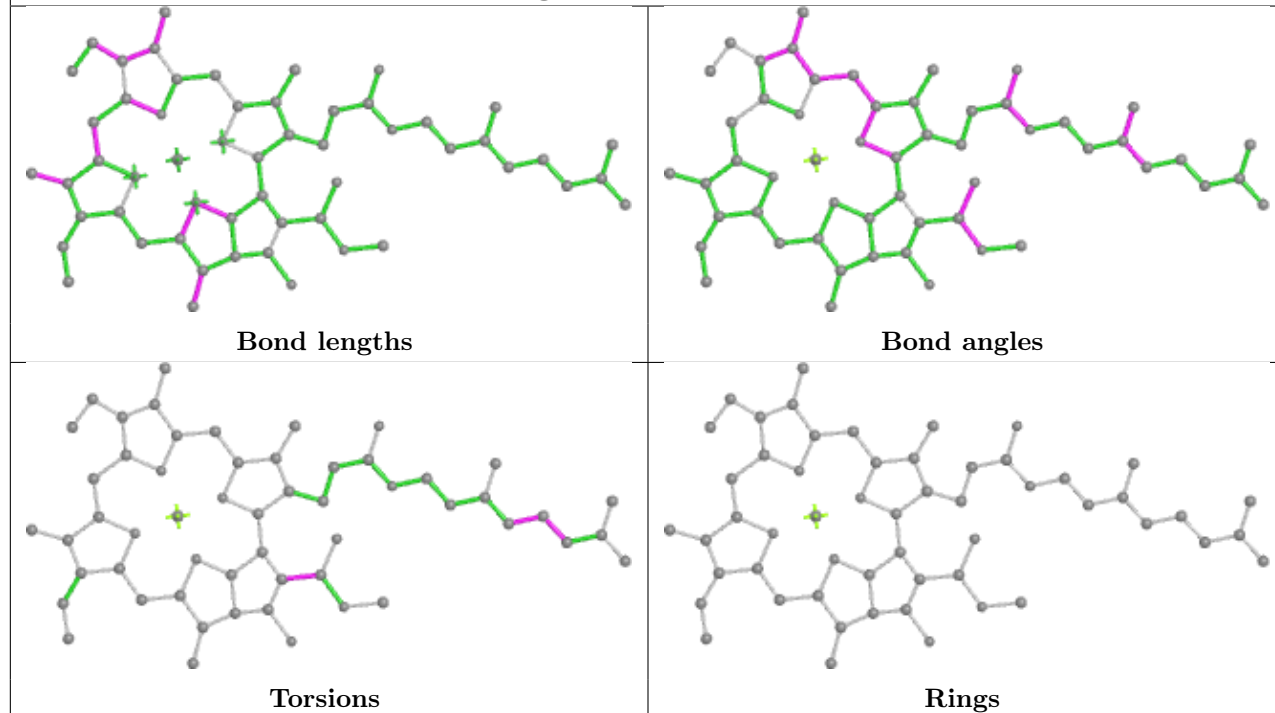
Ligand CLA 5 604



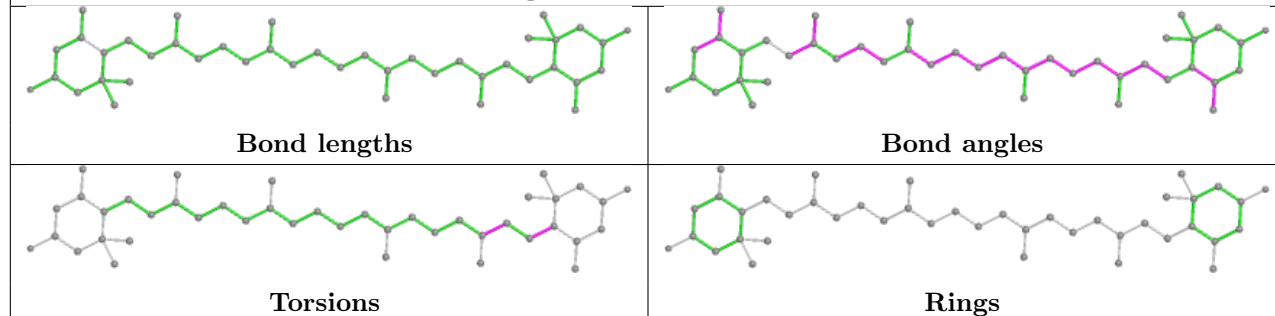
Ligand CLA 7 602

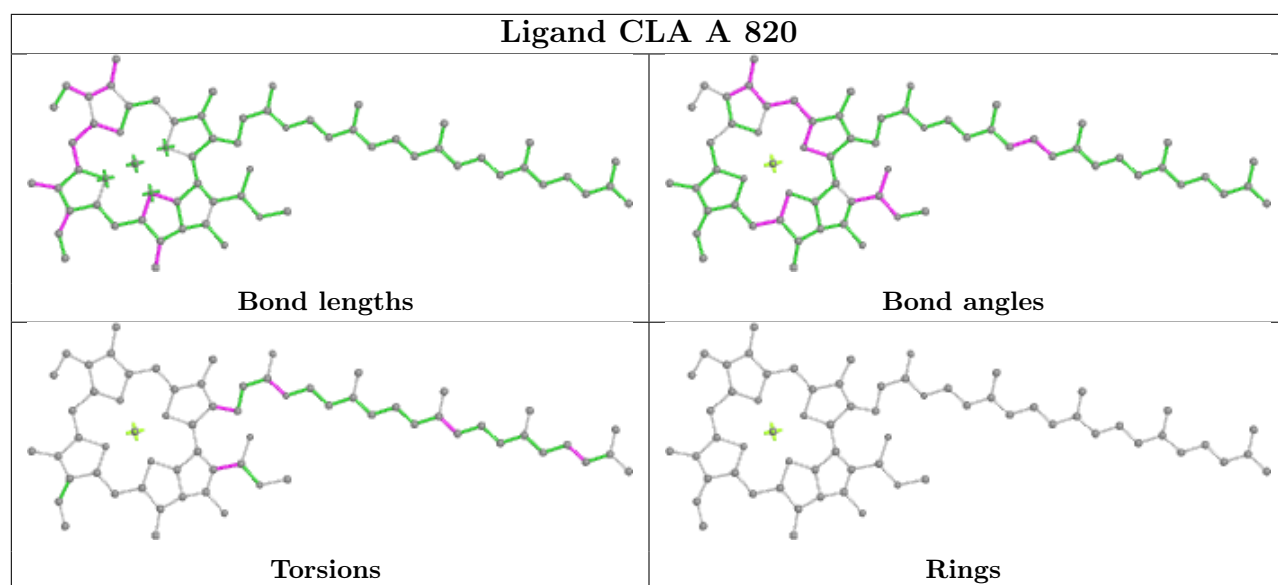


Ligand CLA 2 610

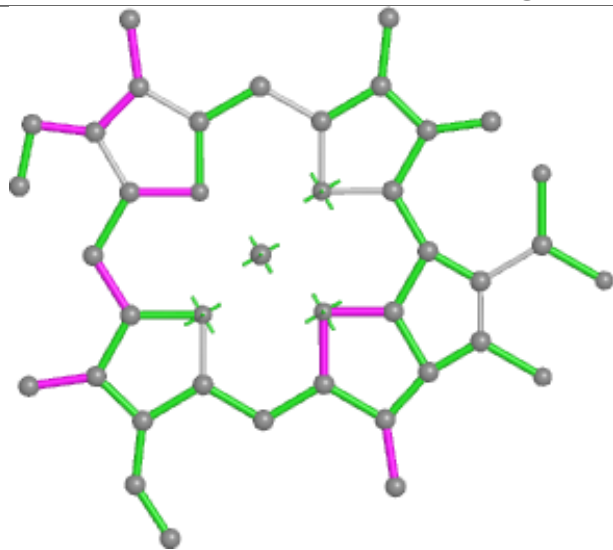


Ligand LUT V 1620

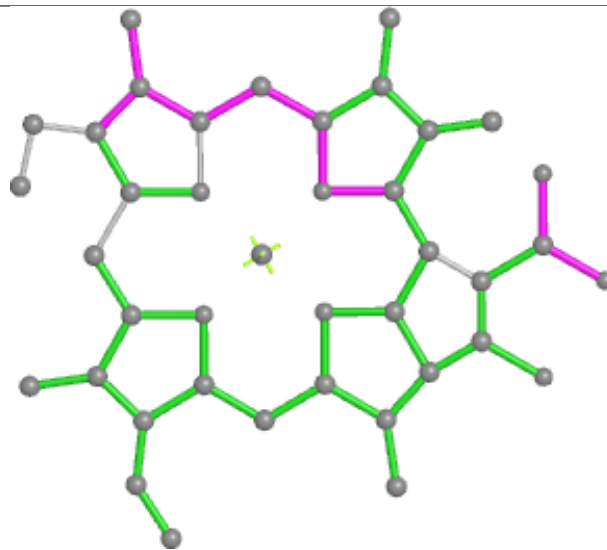




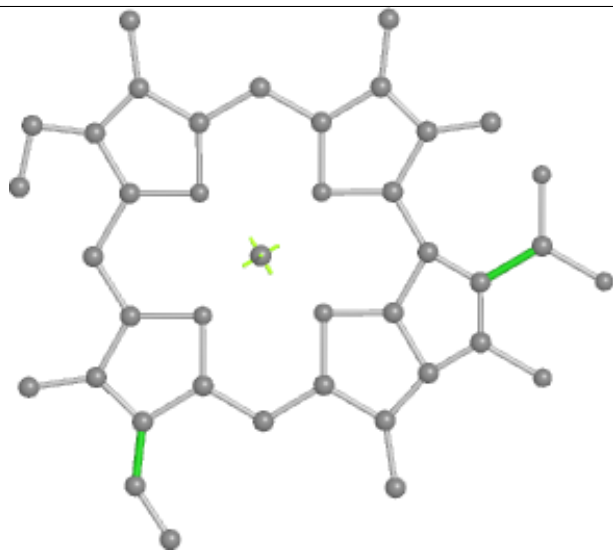
Ligand CLA 3 614



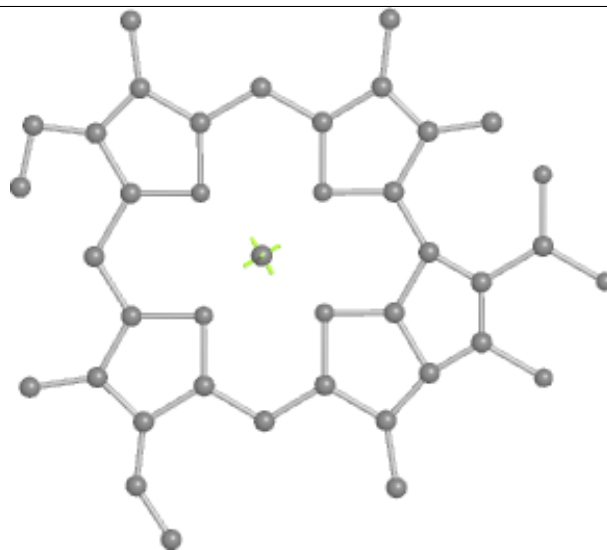
Bond lengths



Bond angles

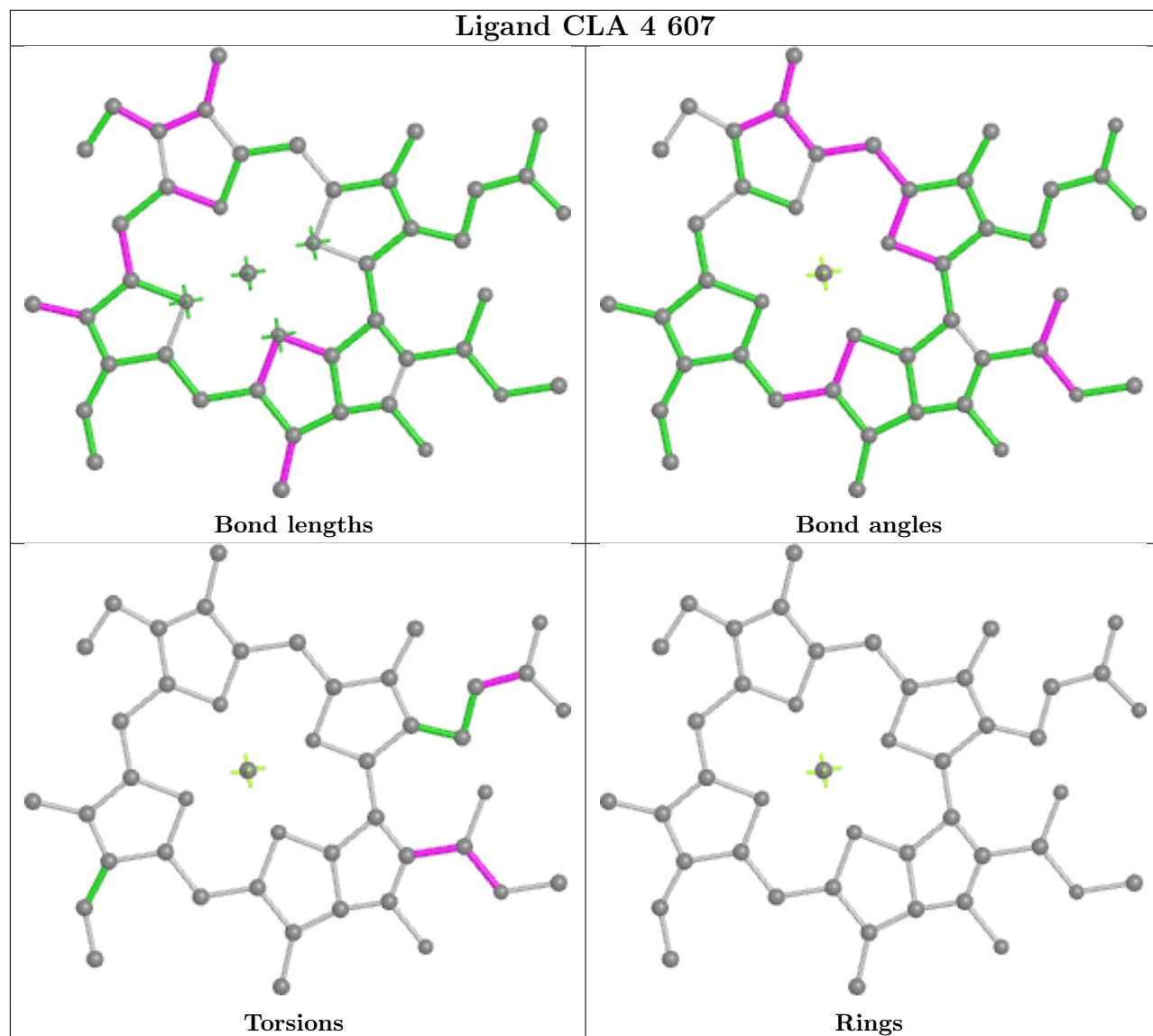


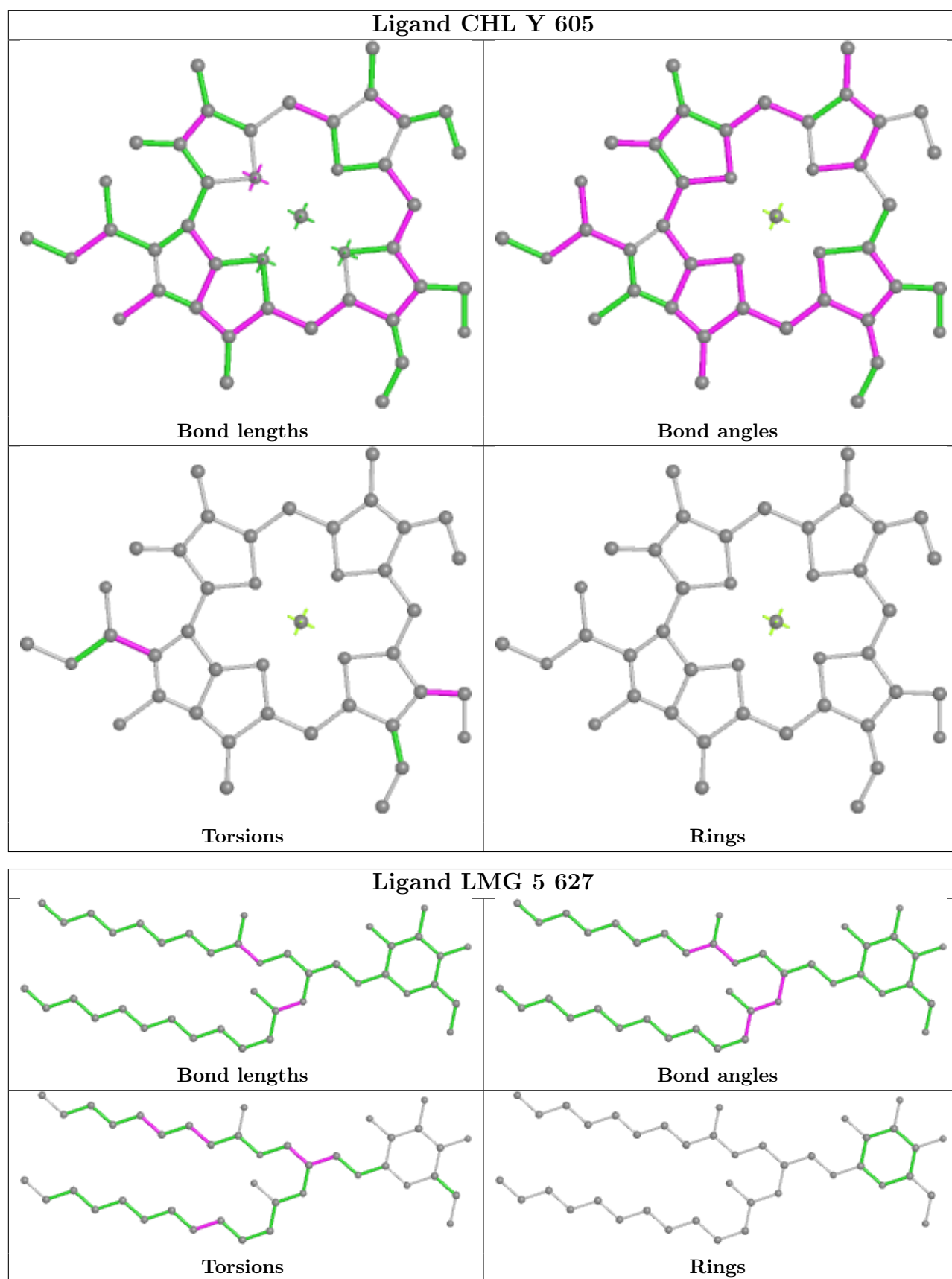
Torsions

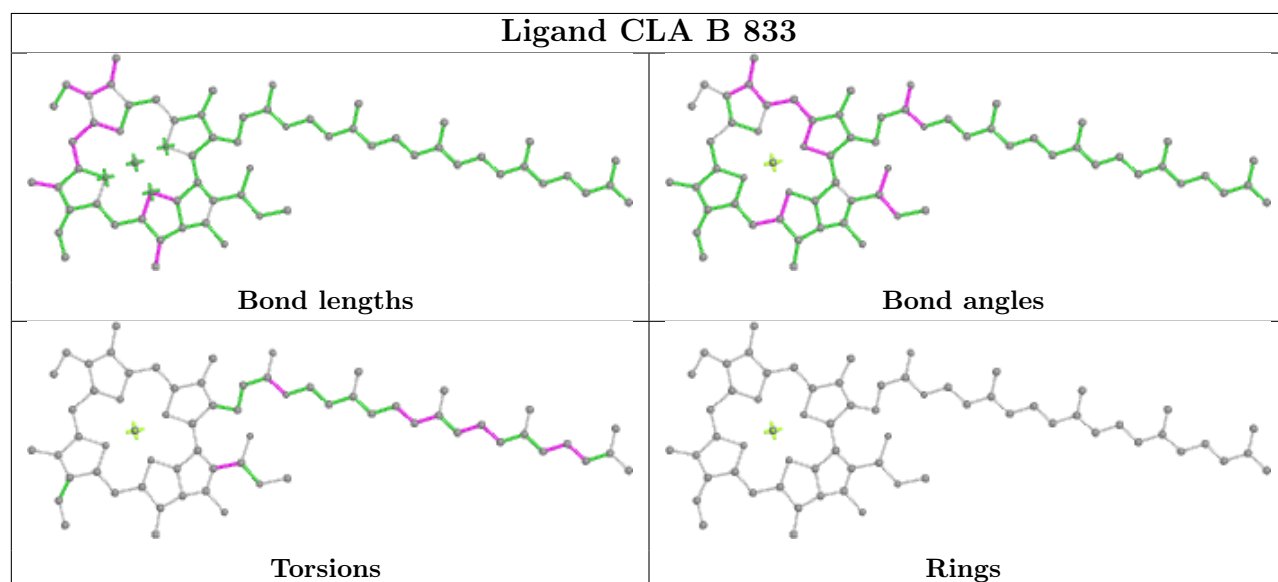
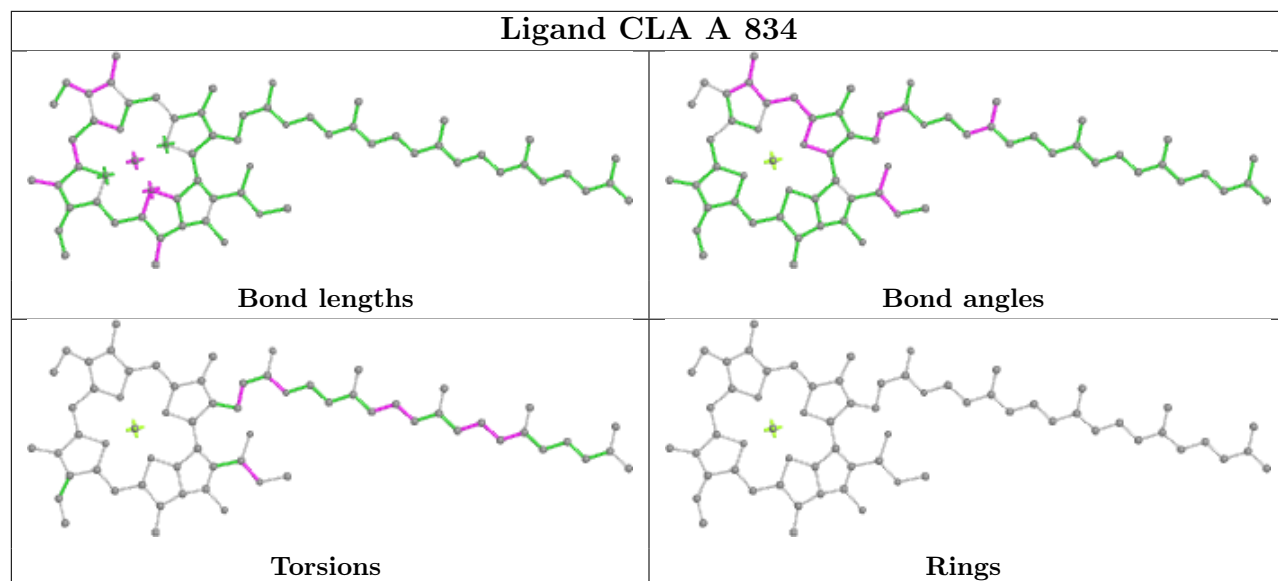
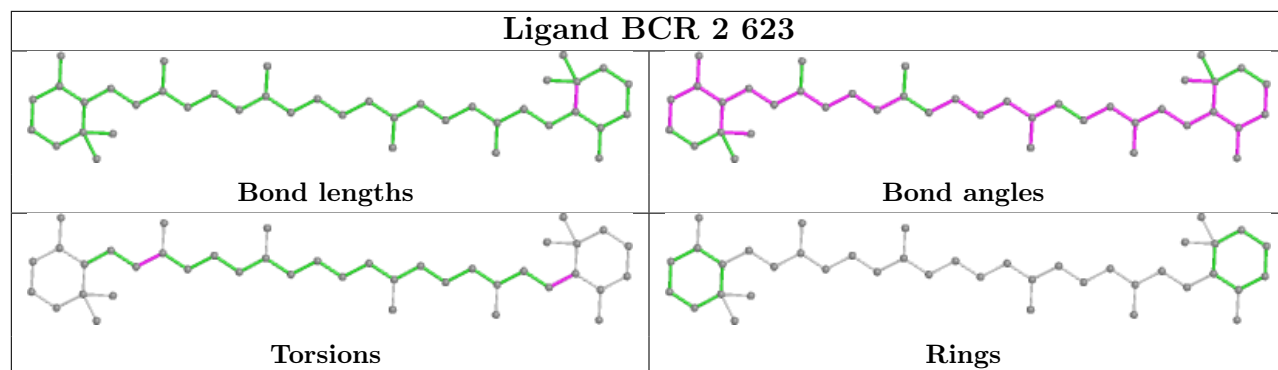


Rings

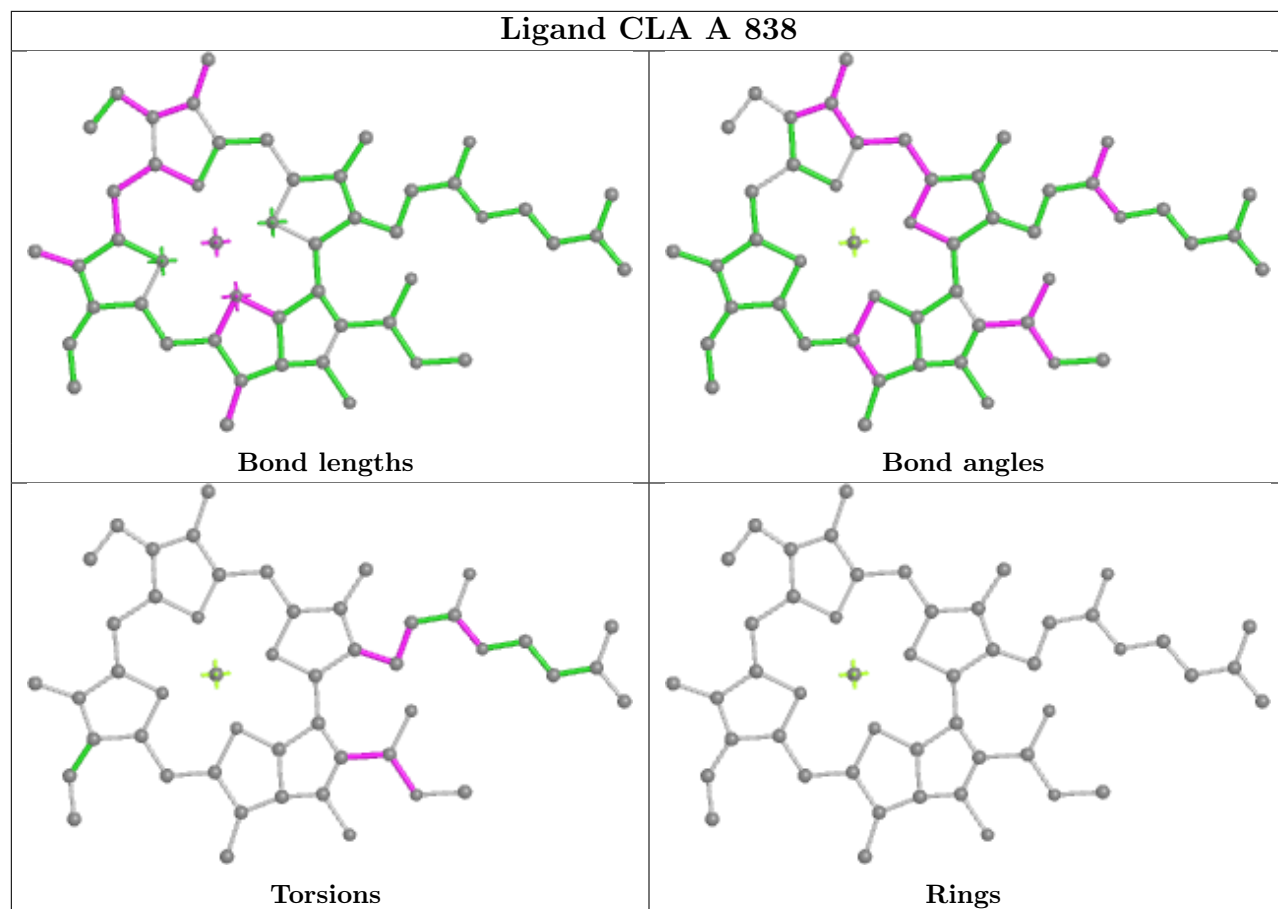
Ligand CLA 4 607



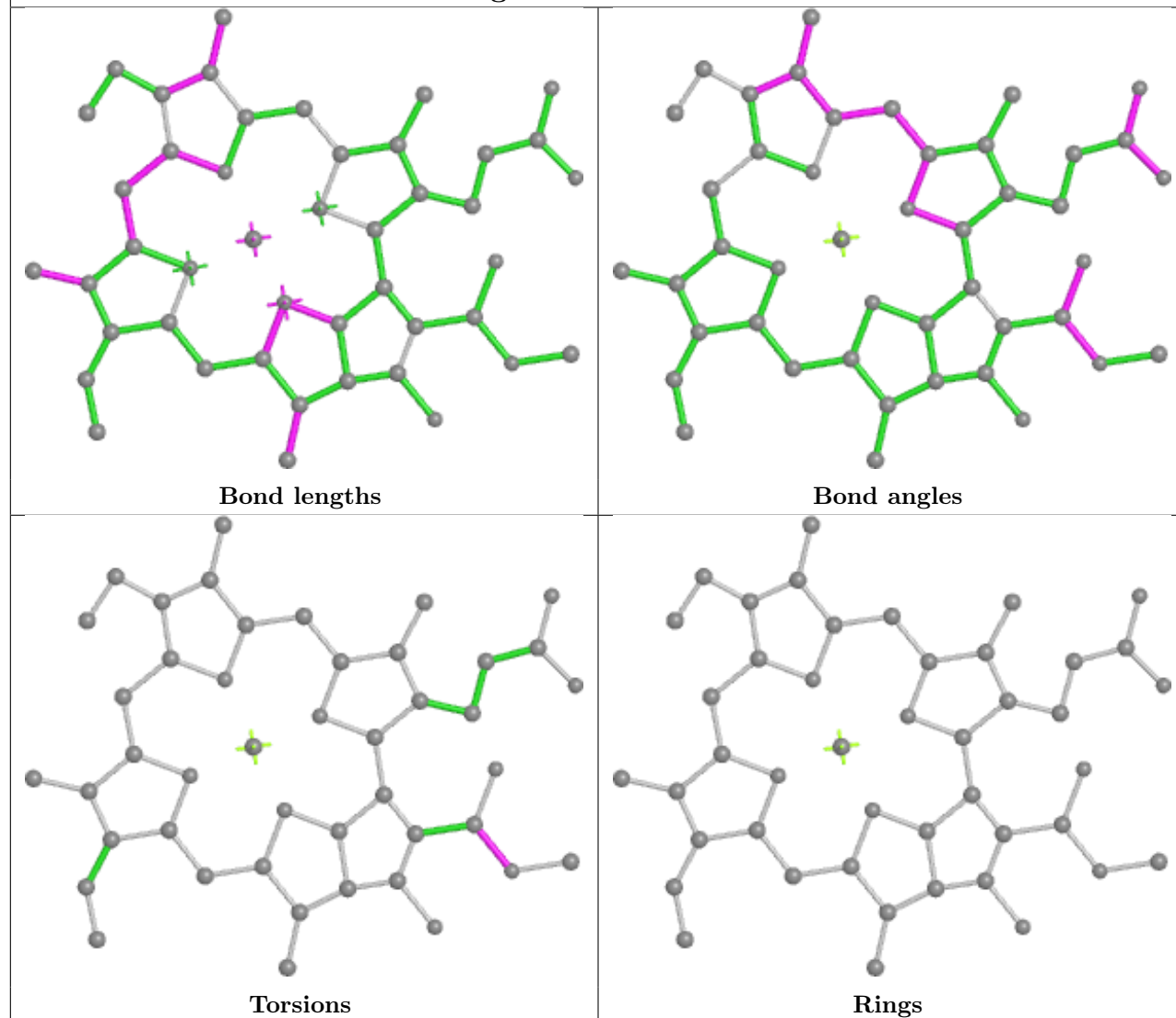




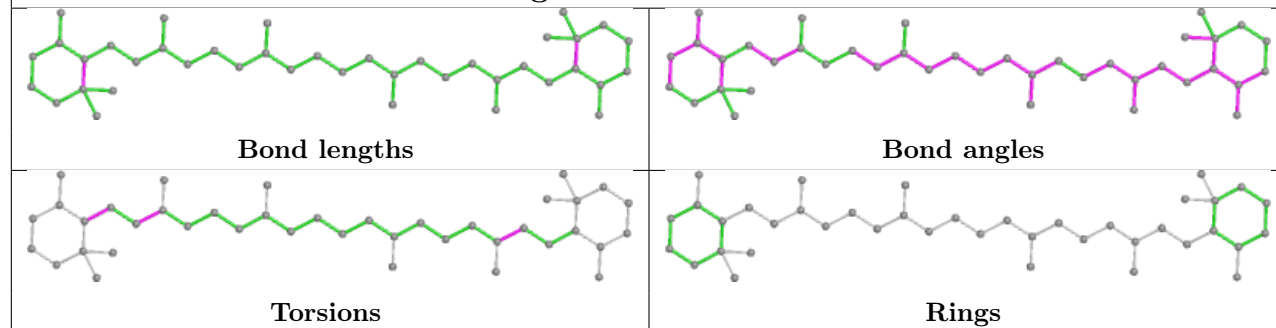
Ligand CLA A 838



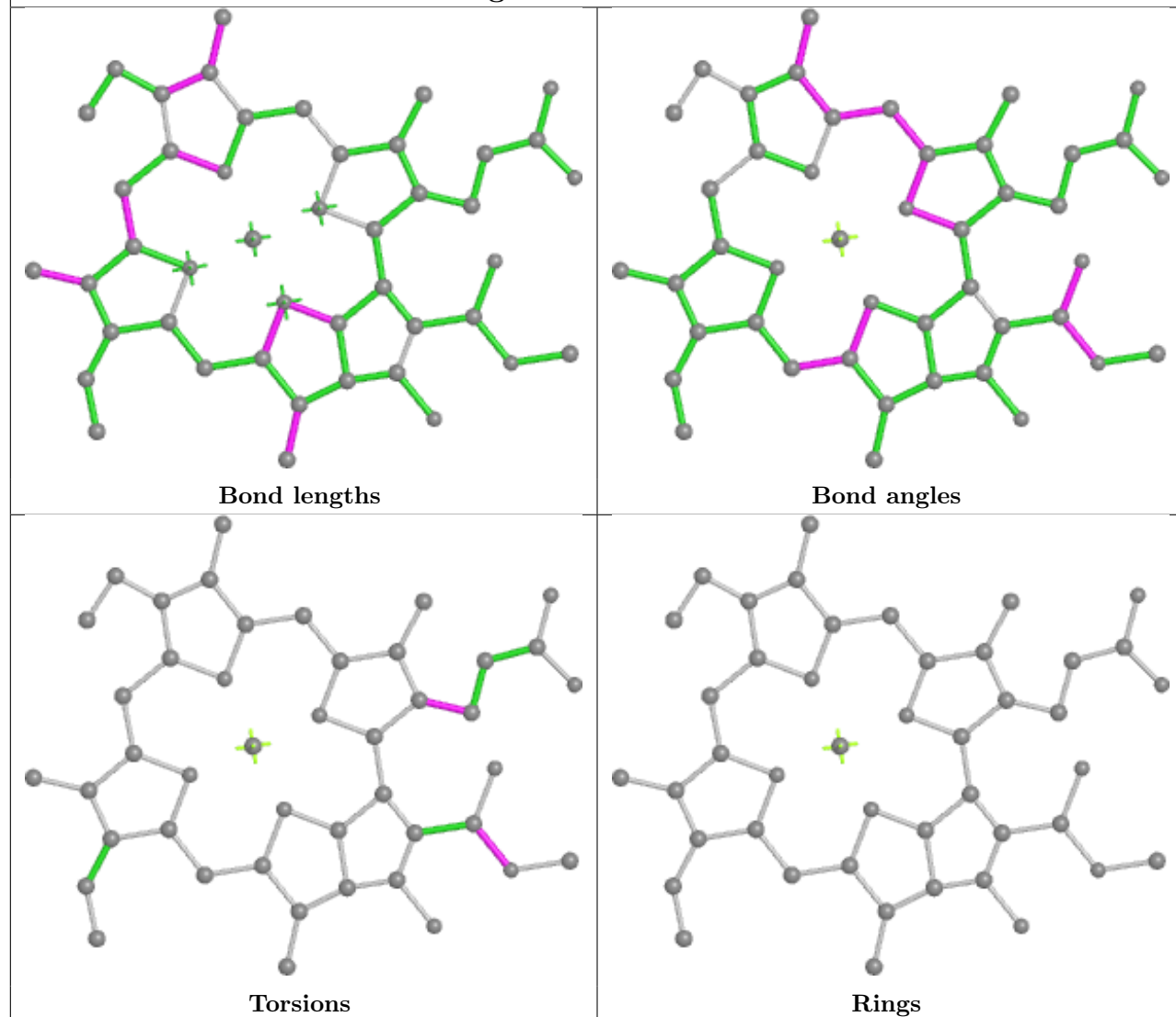
Ligand CLA B 835



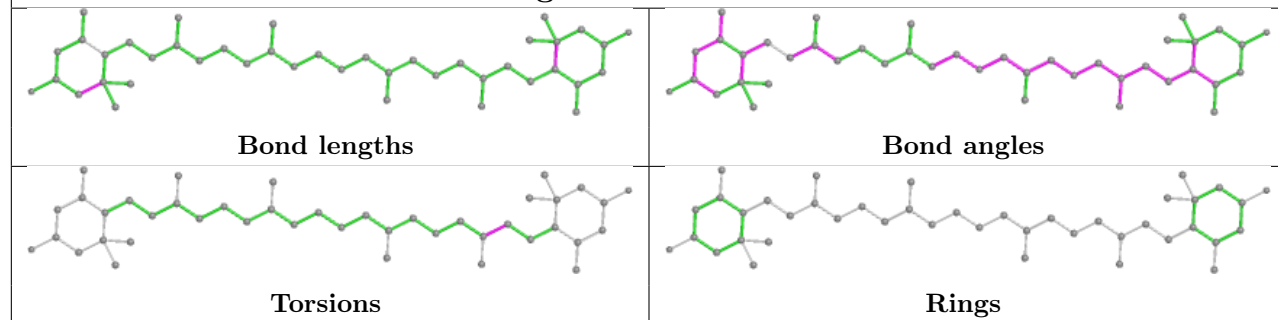
Ligand BCR B 849



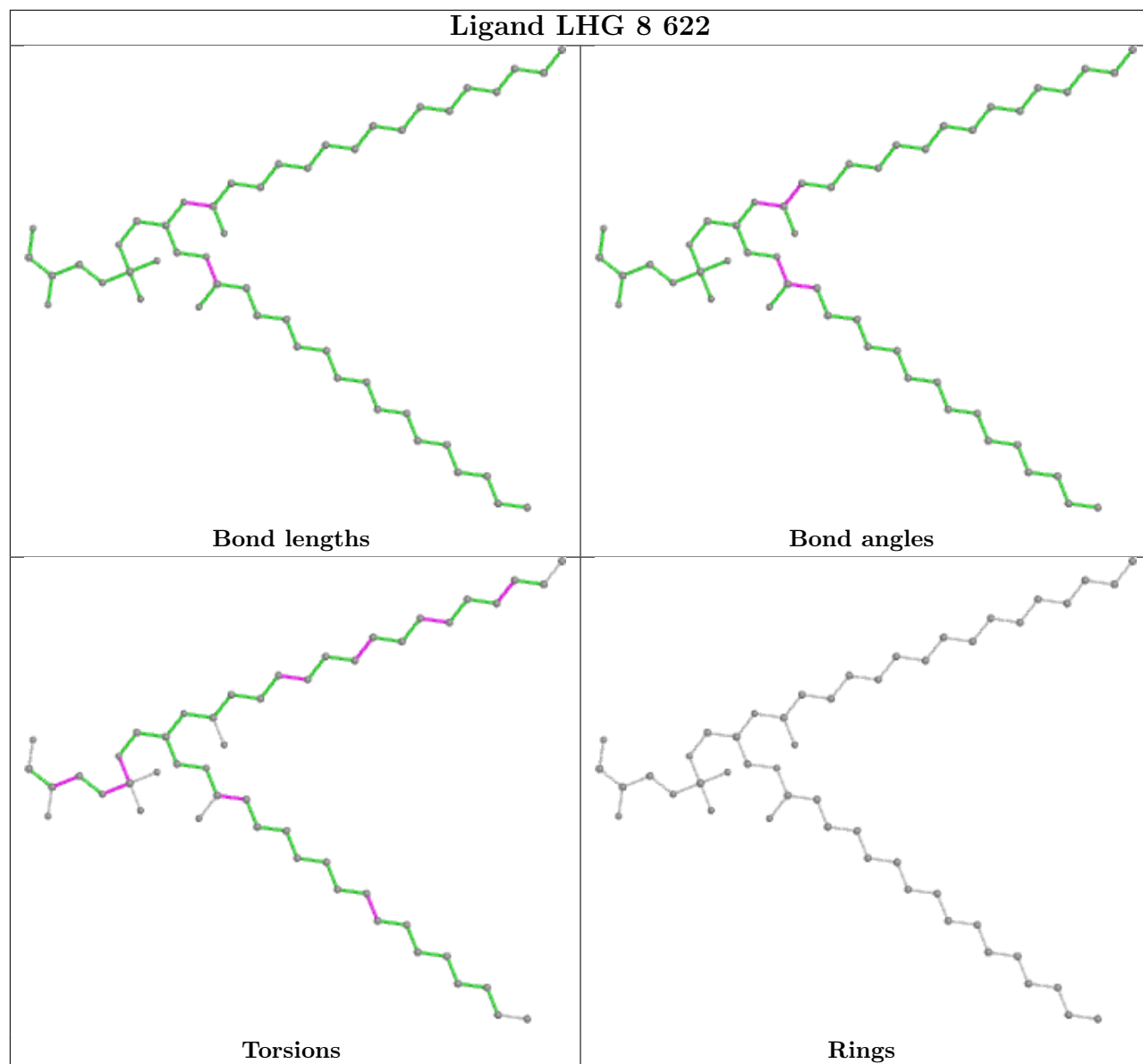
Ligand CLA K 206



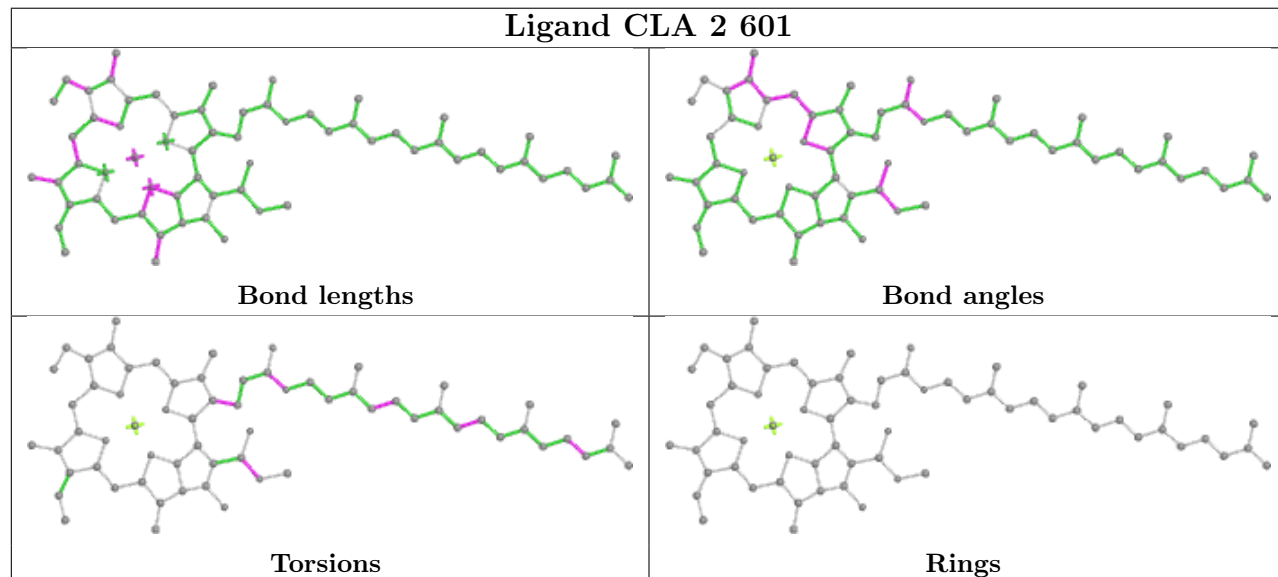
Ligand LUT 2 619

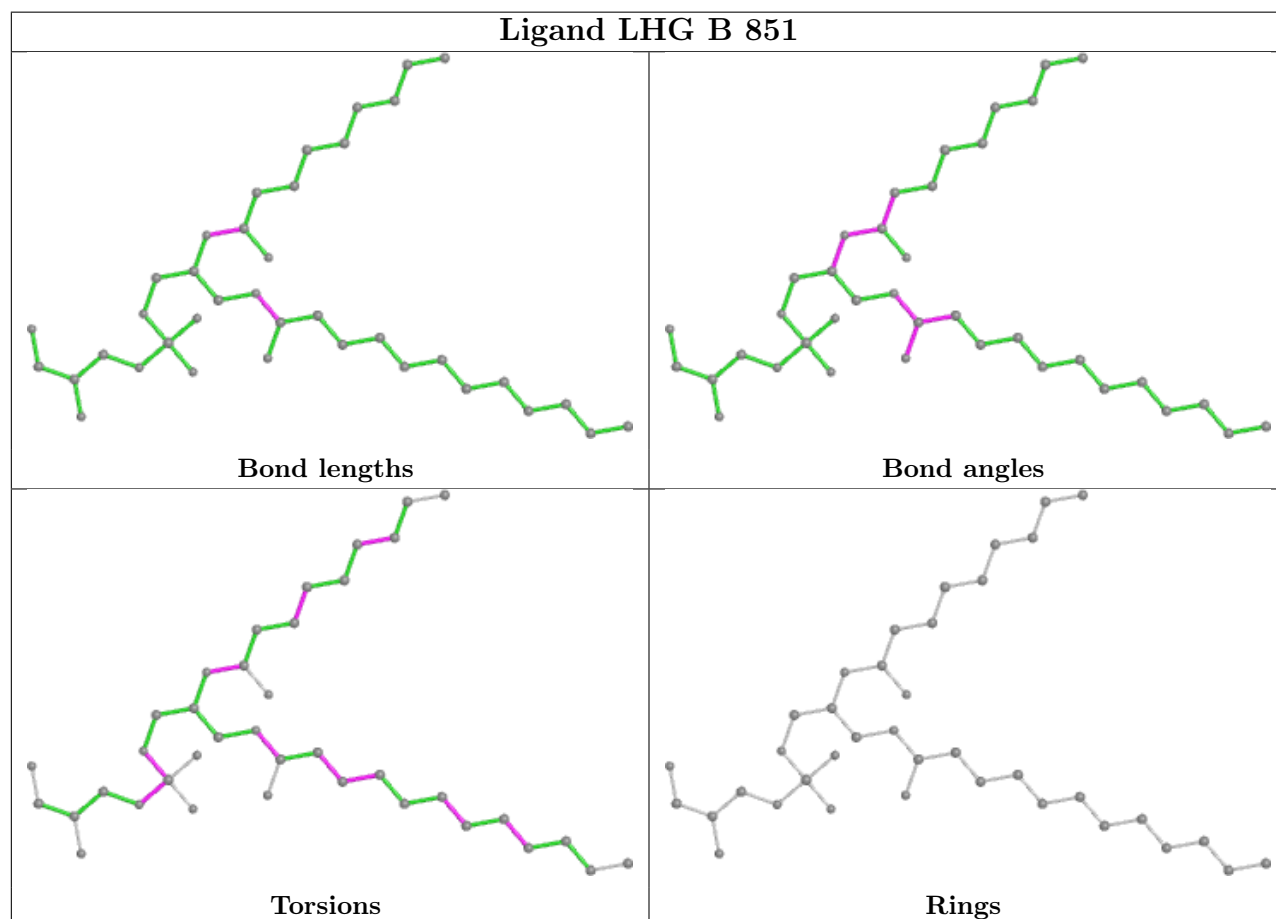
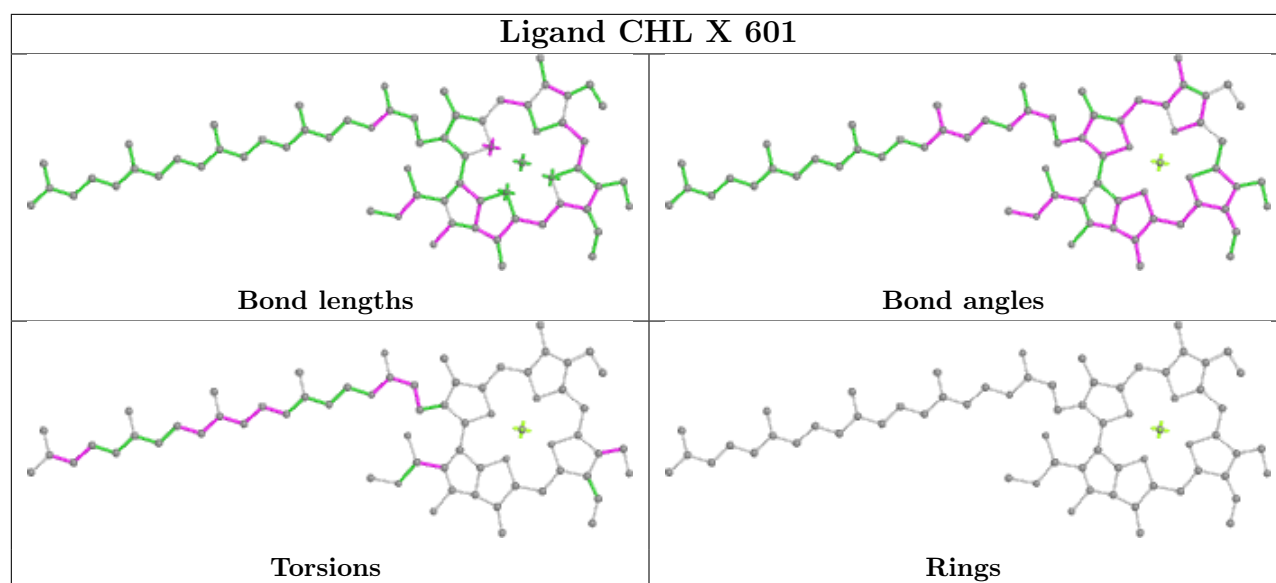


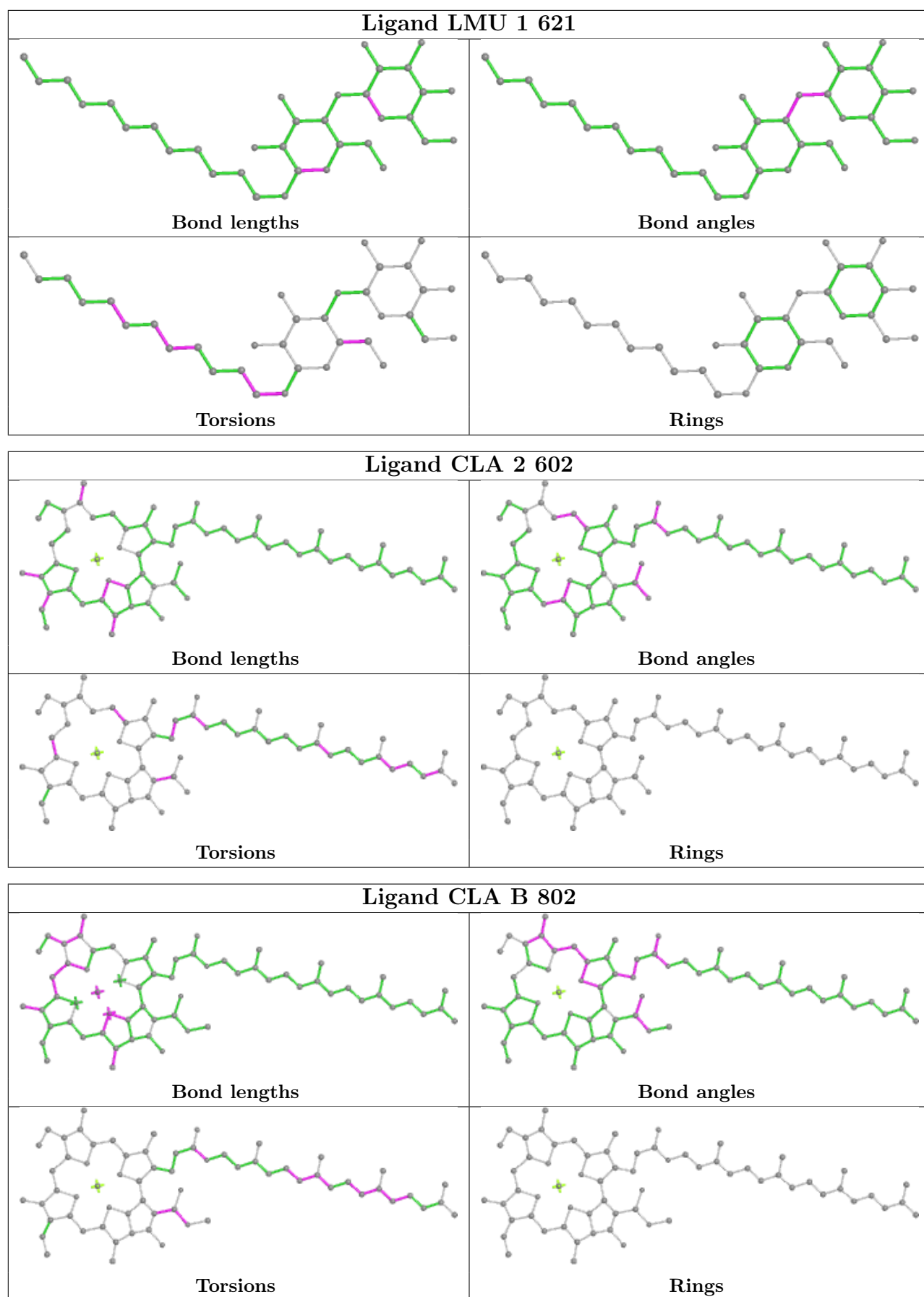
Ligand LHG 8 622

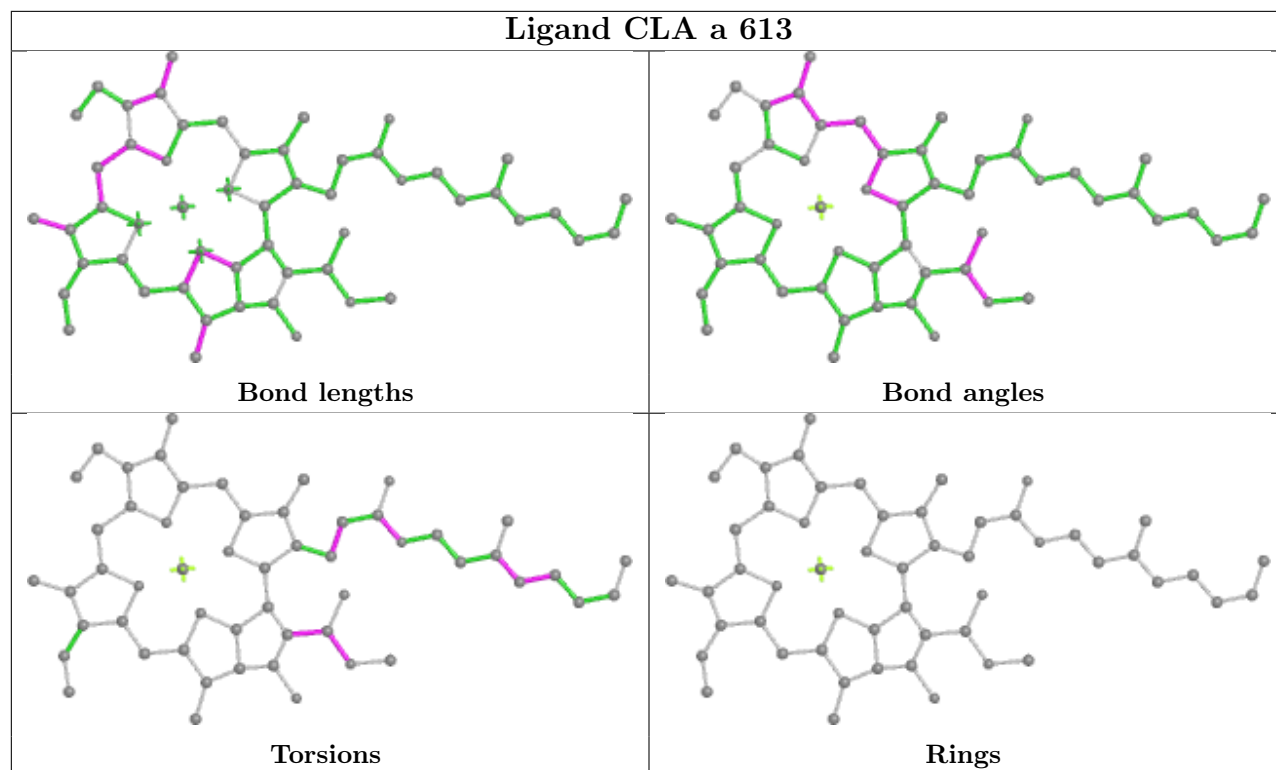
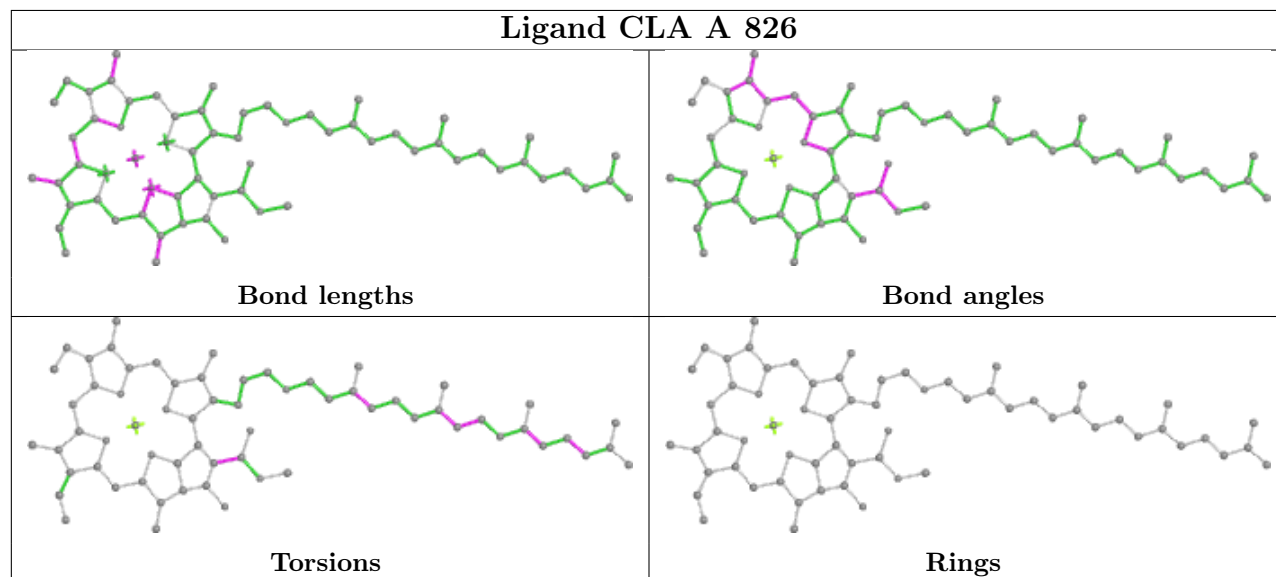


Ligand CLA 2 601

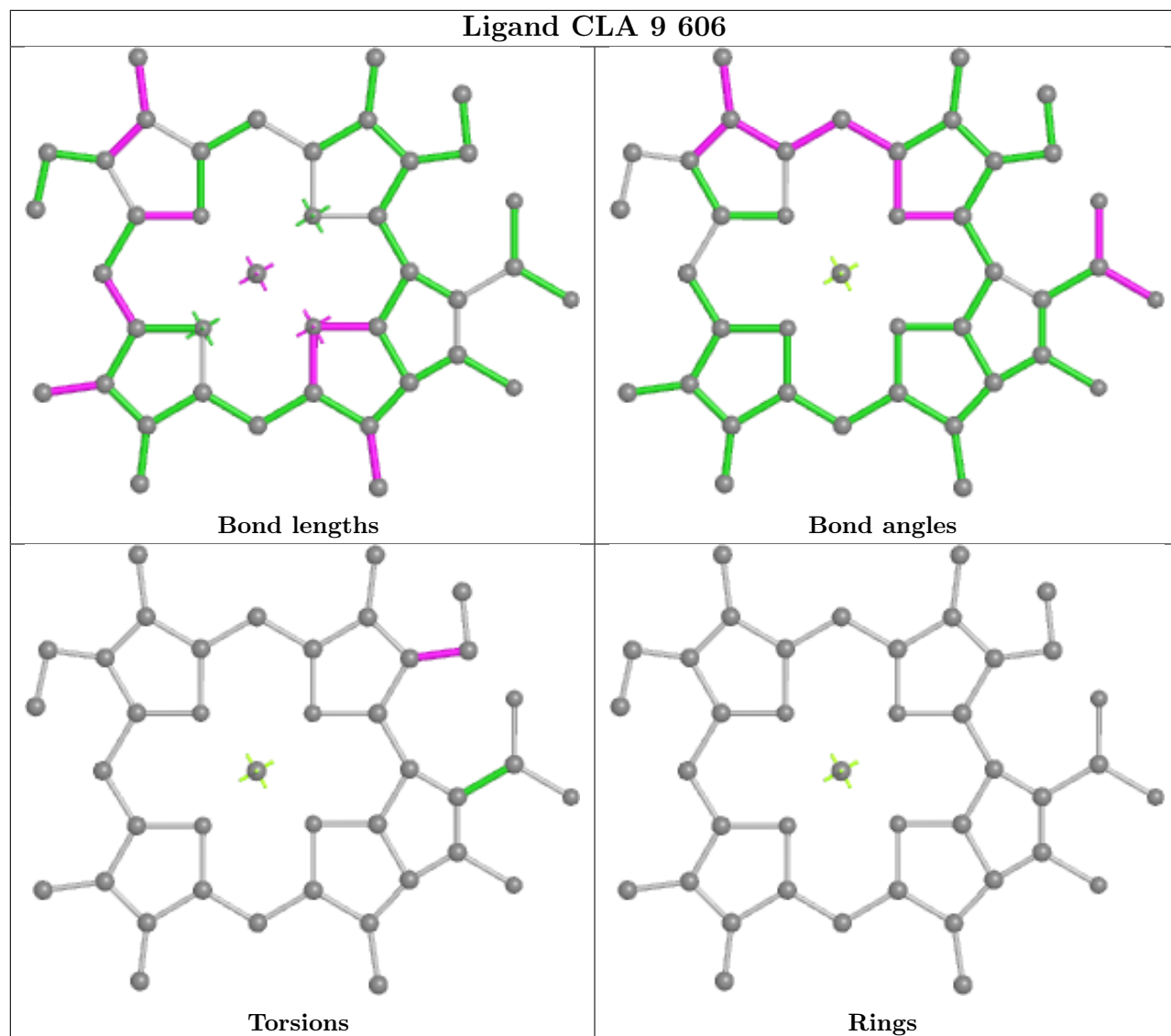




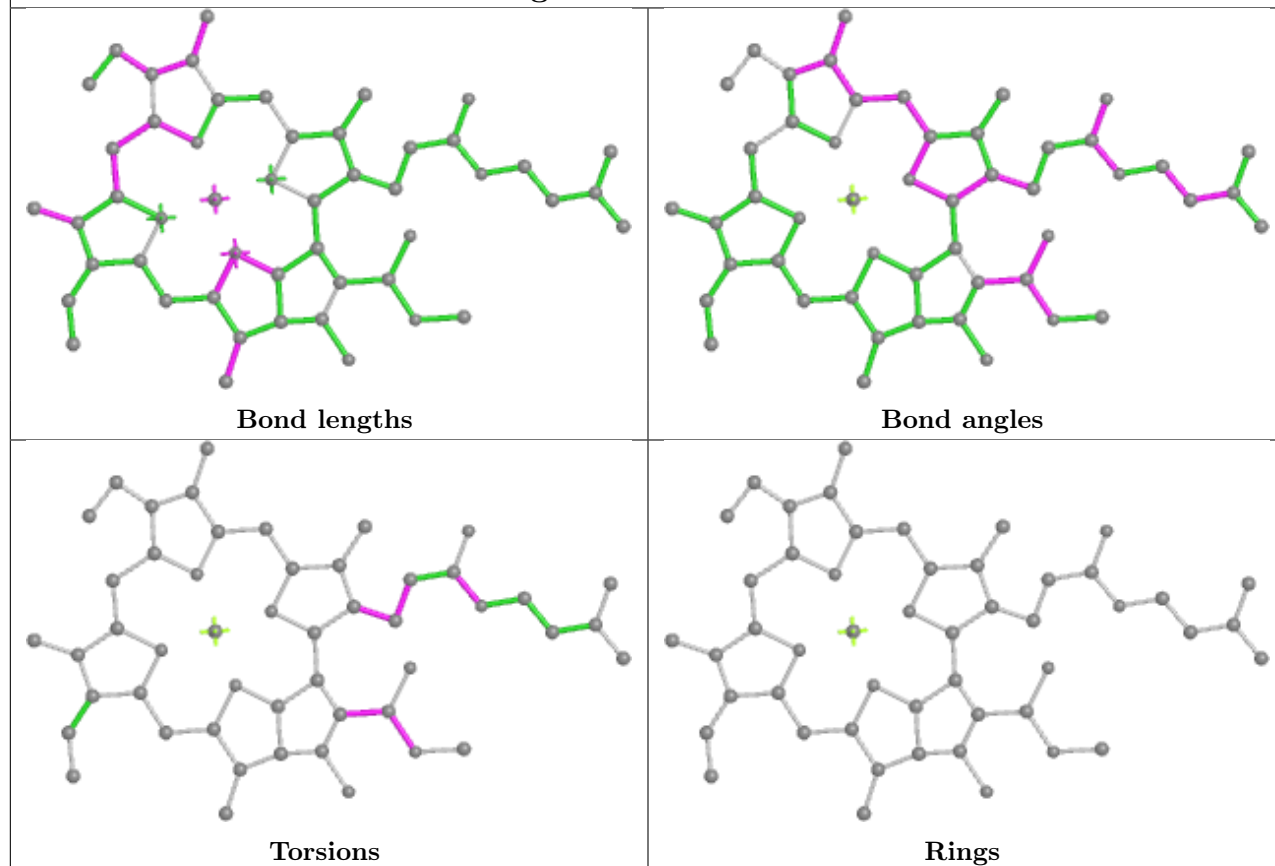


Ligand CLA a 613**Ligand CLA A 826**

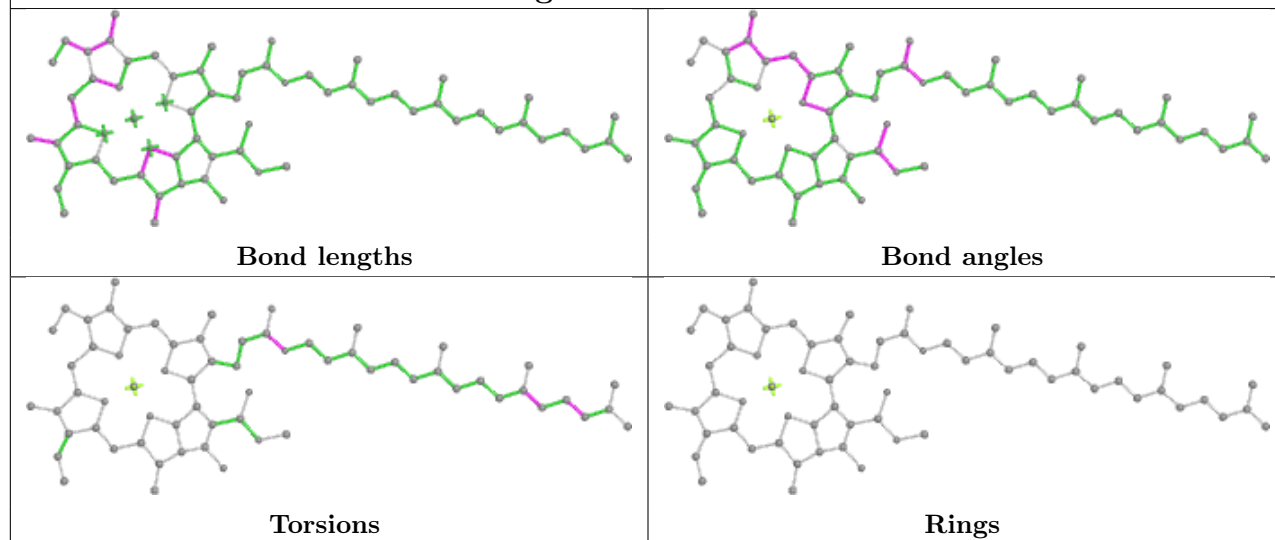
Ligand CLA 9 606

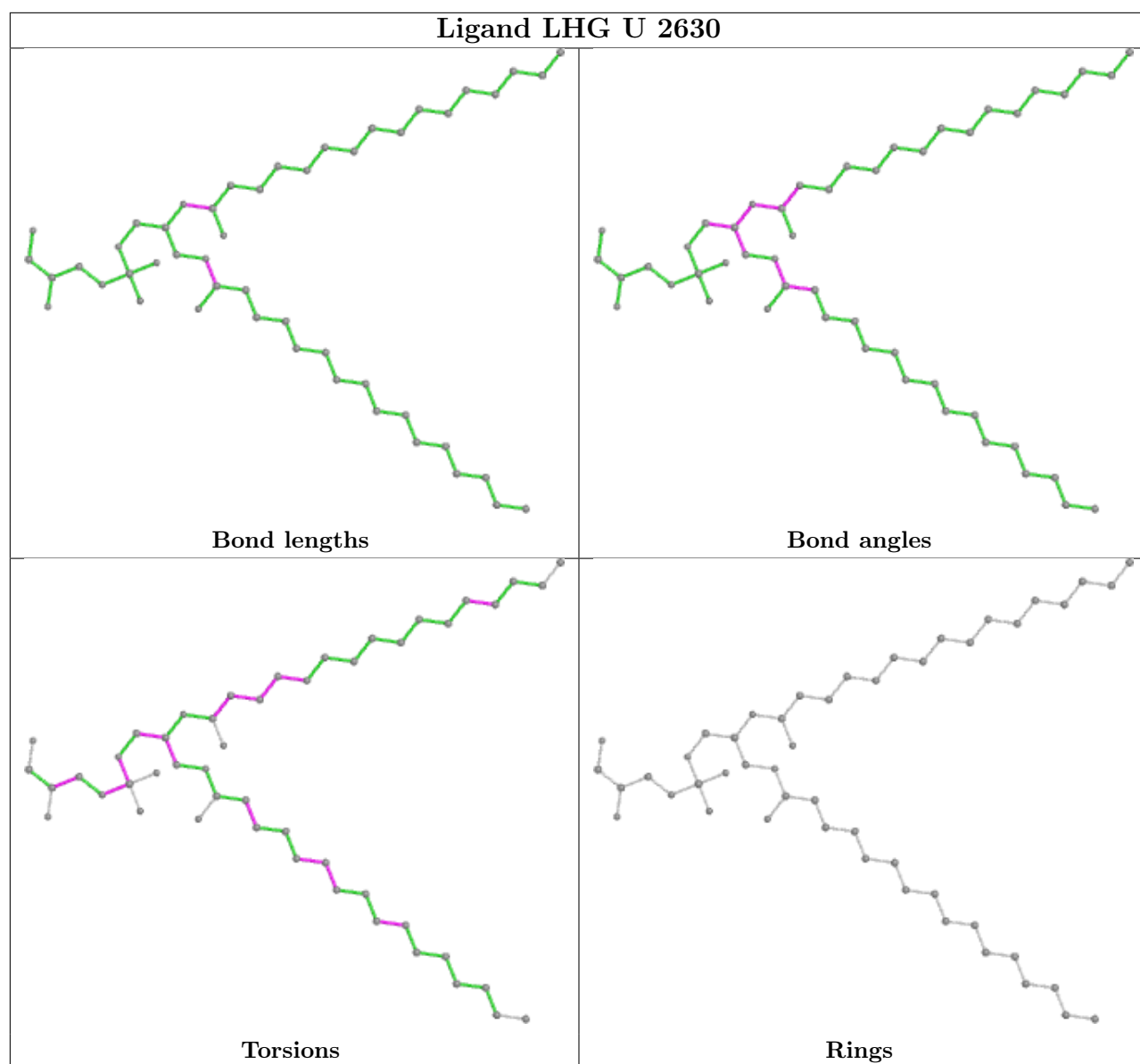


Ligand CLA A 832

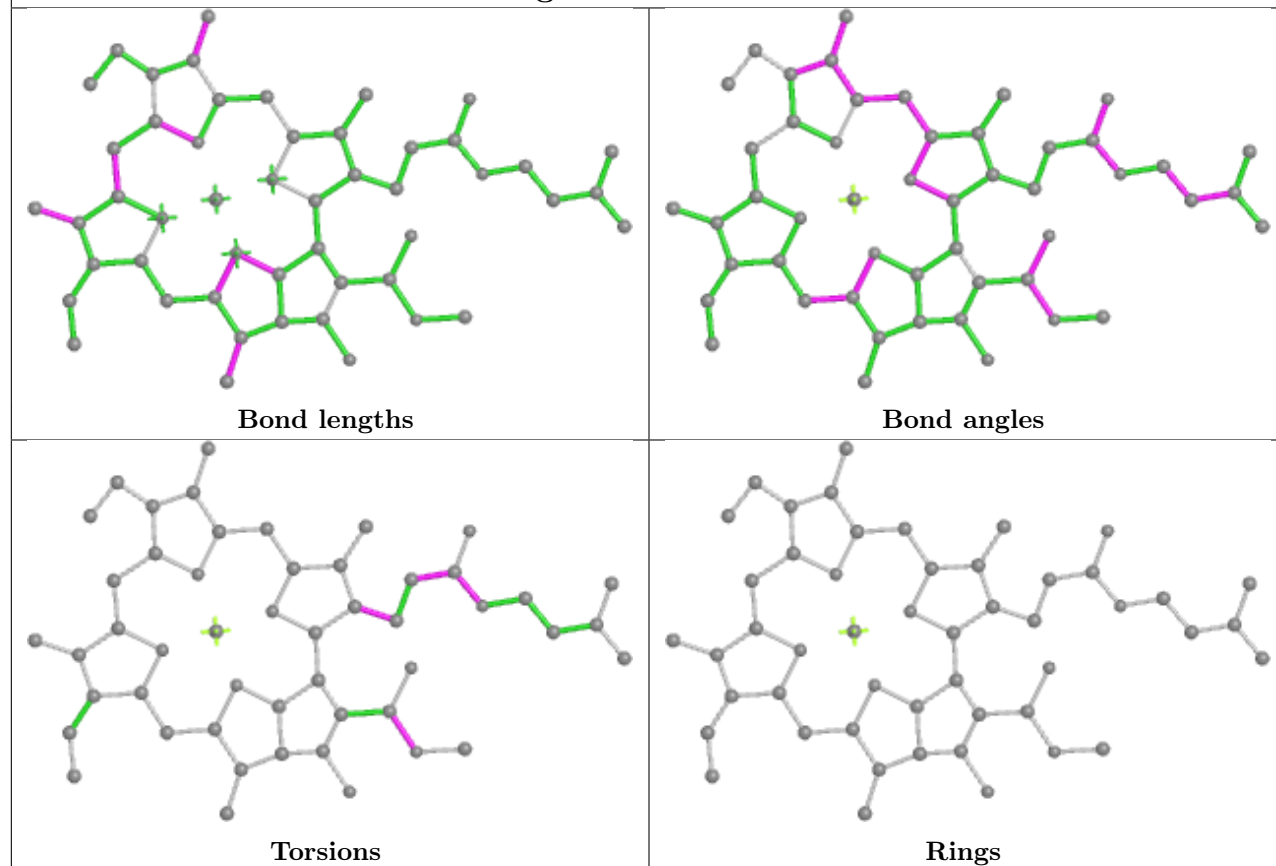


Ligand CLA 7 610

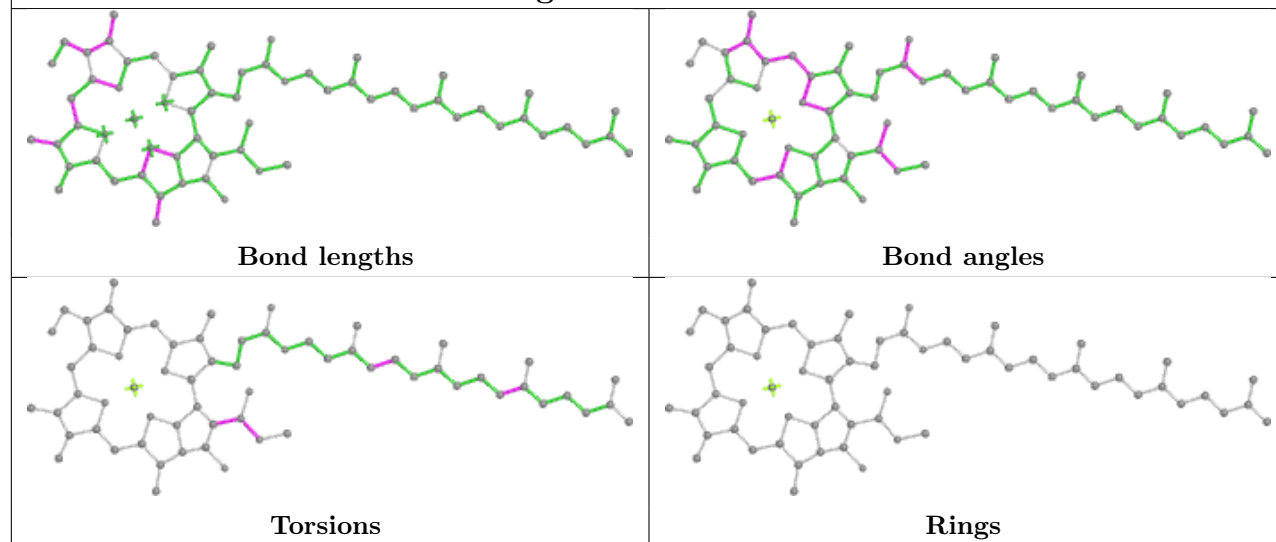




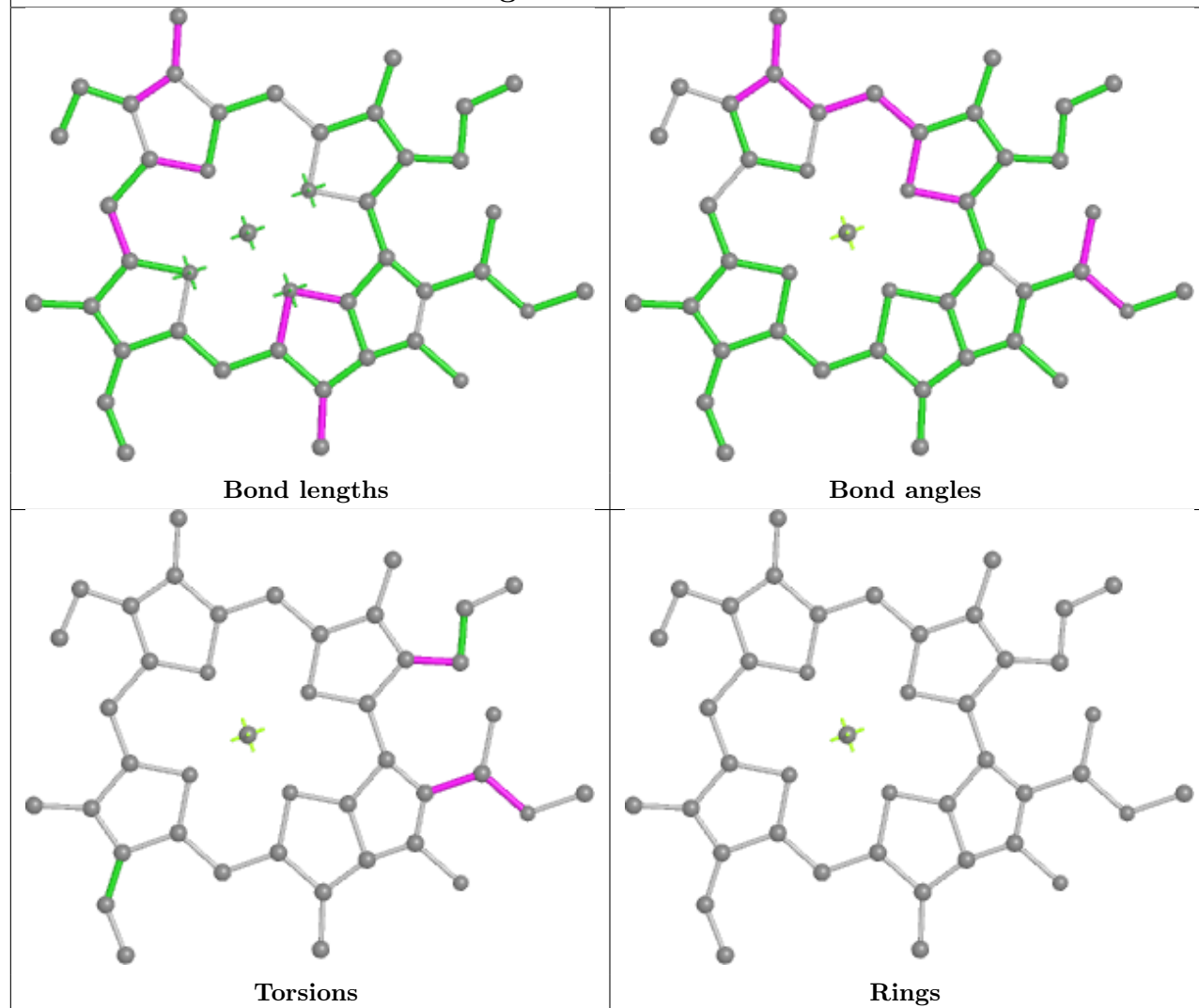
Ligand CLA 8 604



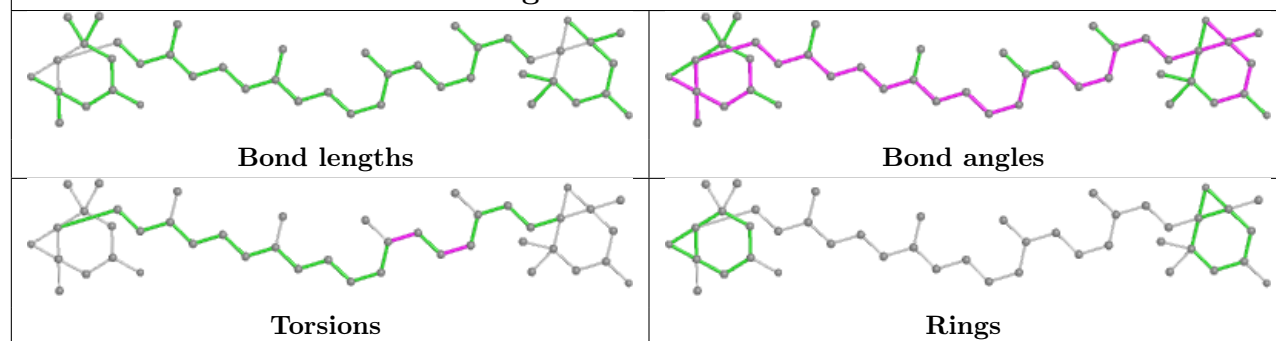
Ligand CLA 8 606

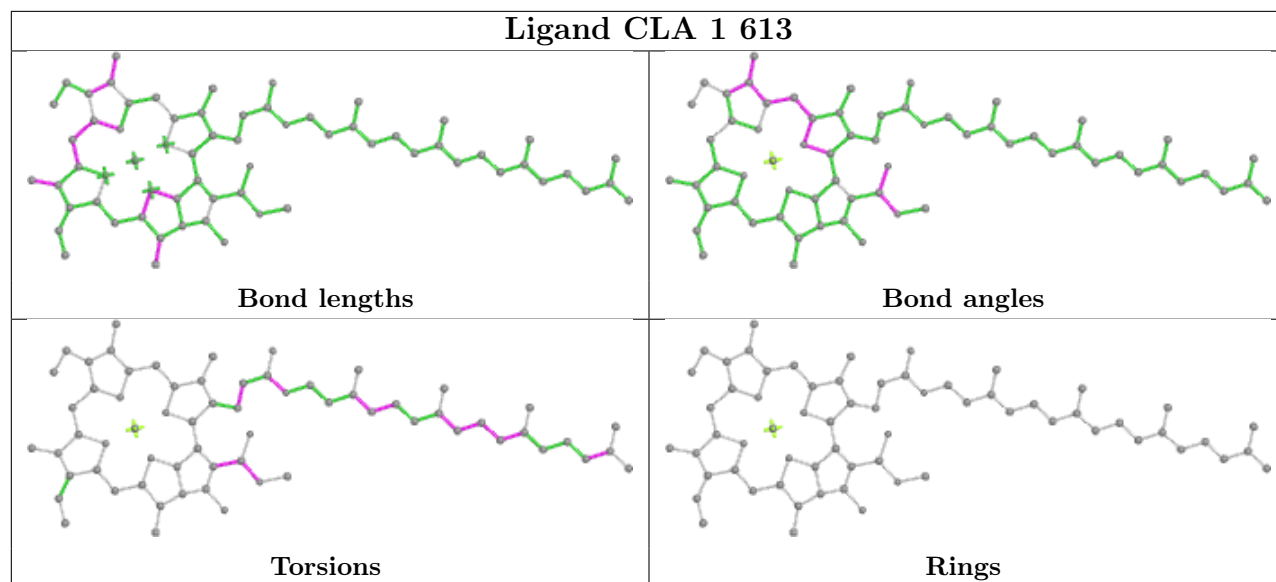
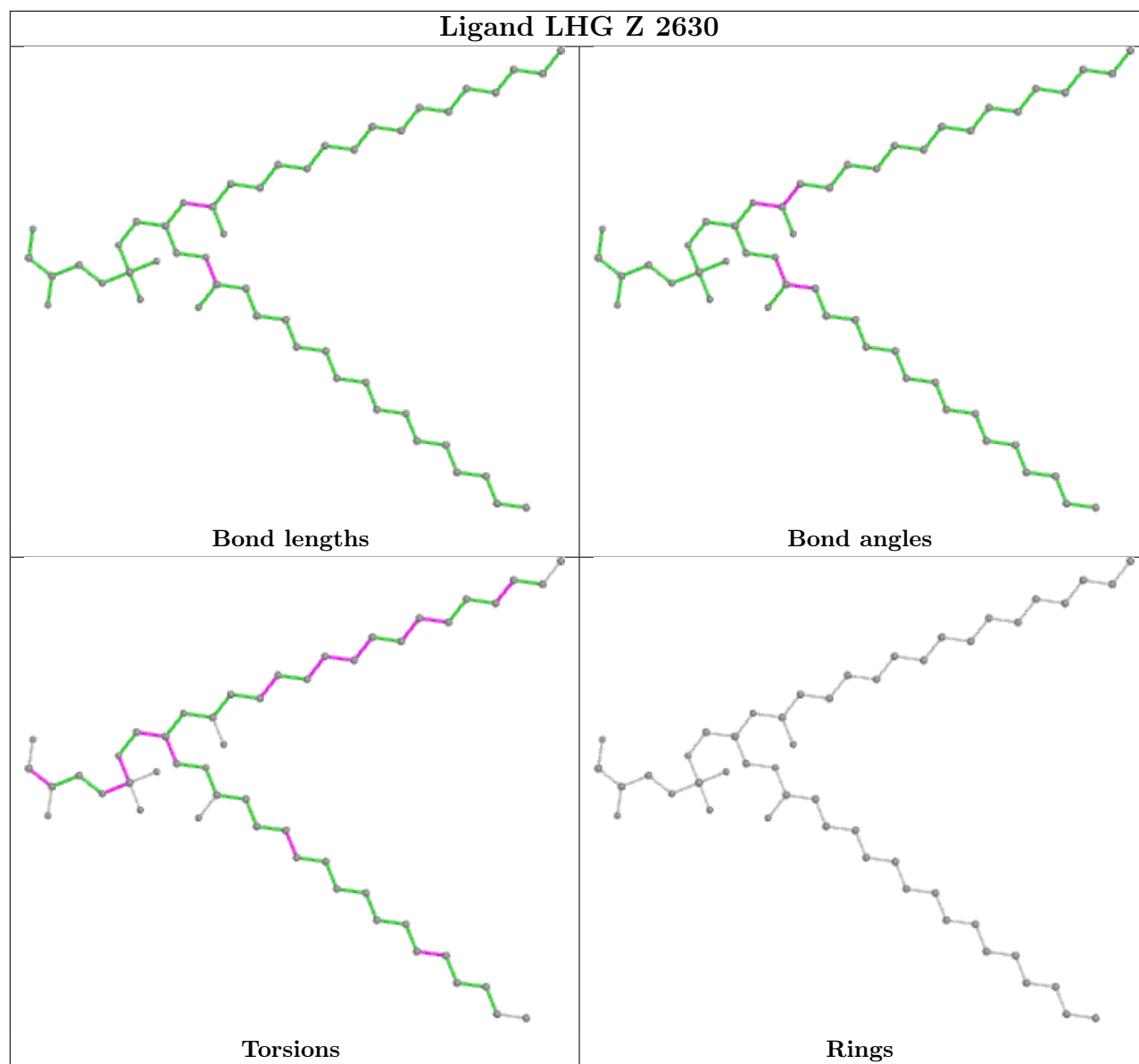


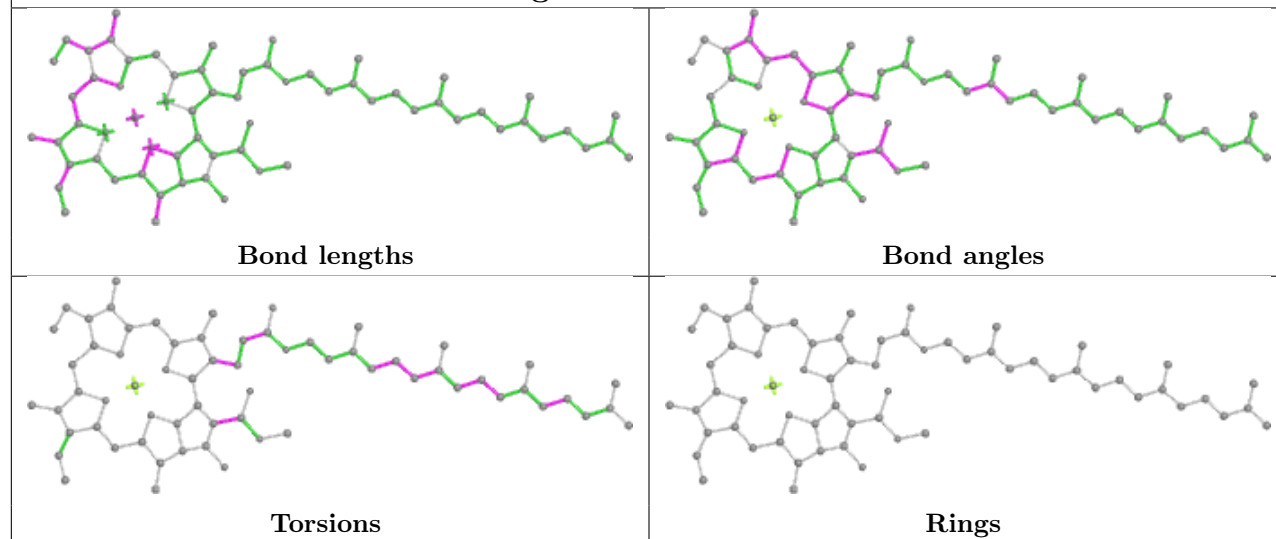
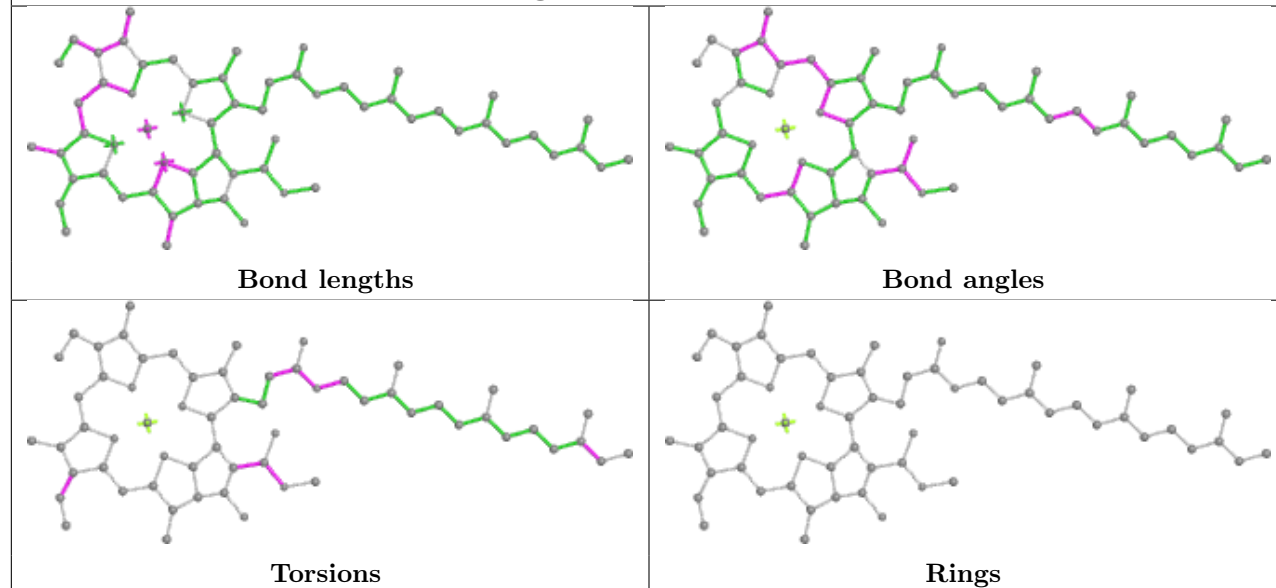
Ligand CLA V 611

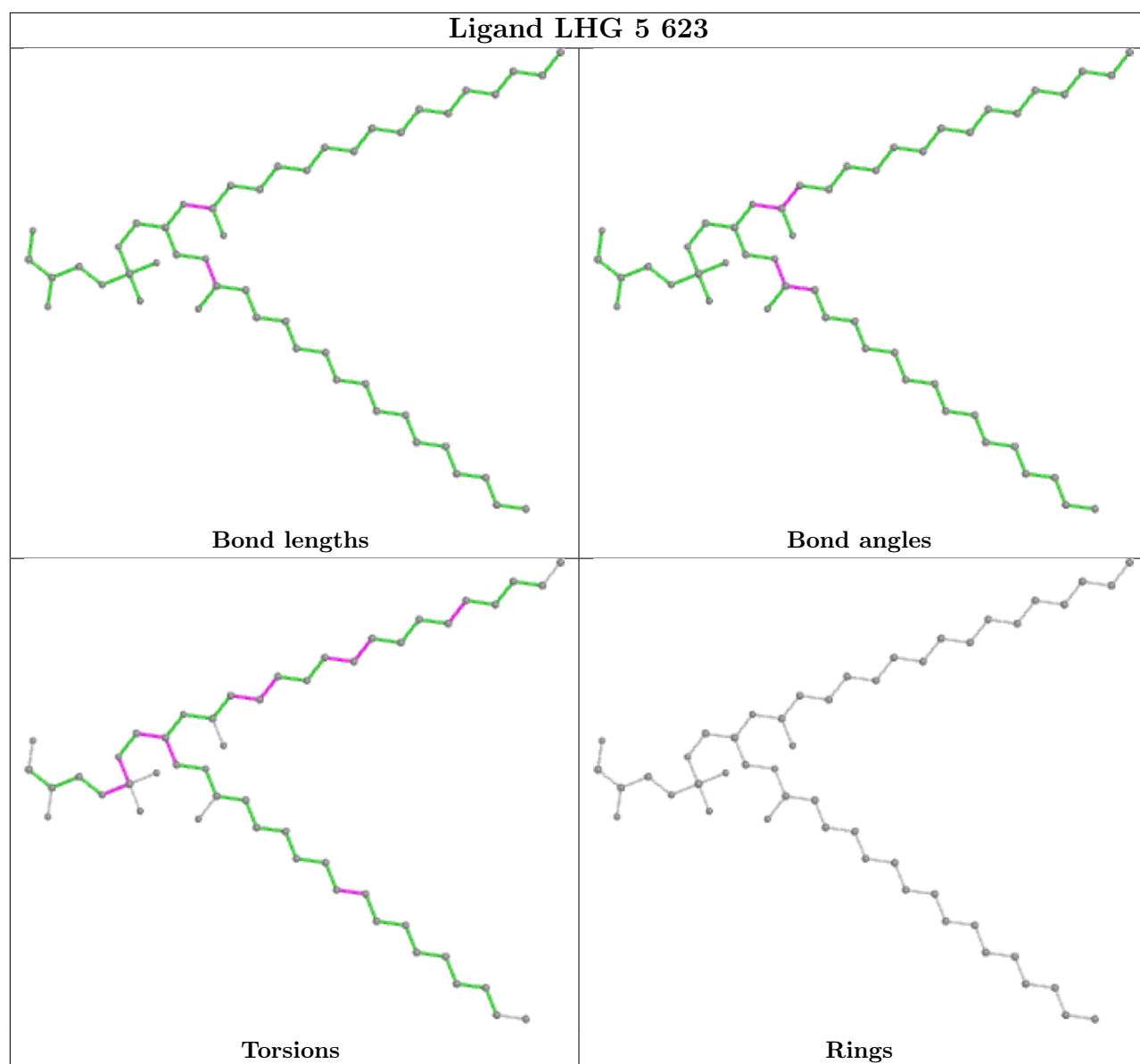


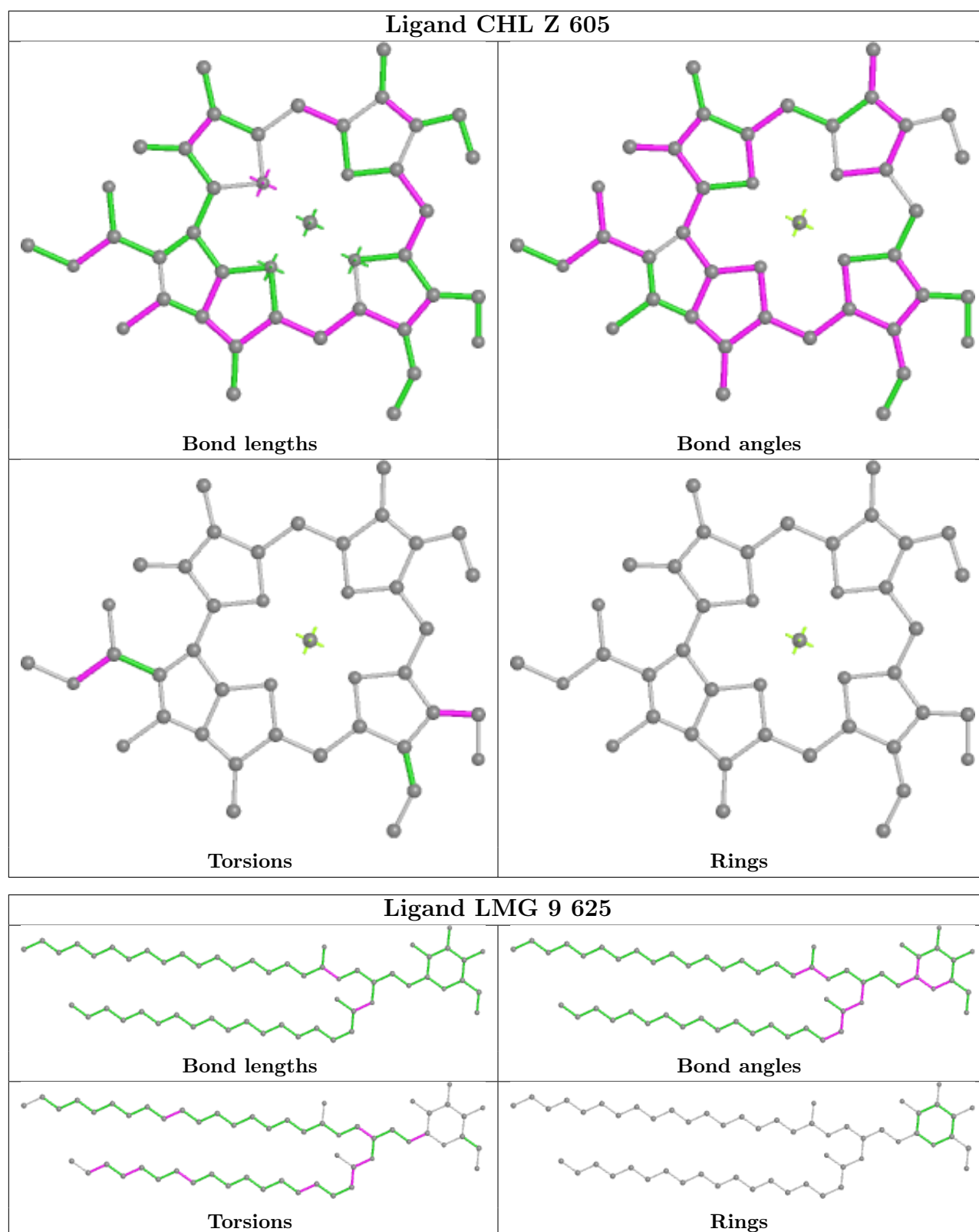
Ligand XAT X 1622



Ligand CLA 1 613**Ligand LHG Z 2630**

Ligand CLA A 806**Ligand CLA A 835**





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

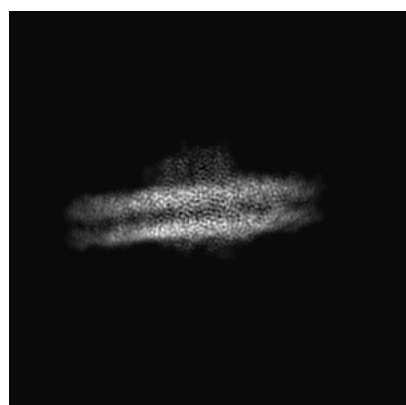
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30926. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

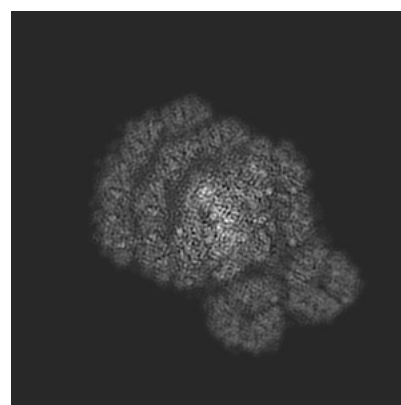
6.1.1 Primary map



X



Y

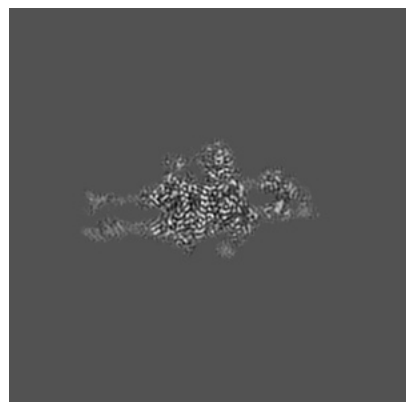


Z

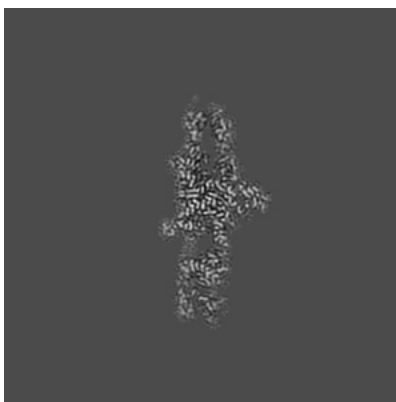
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

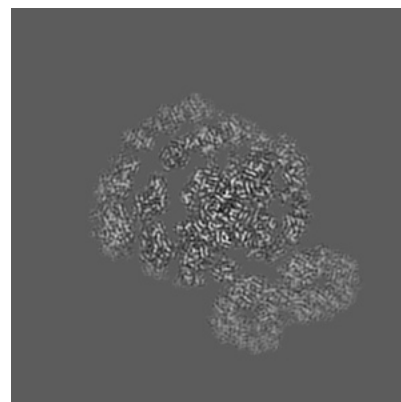
6.2.1 Primary map



X Index: 180



Y Index: 180

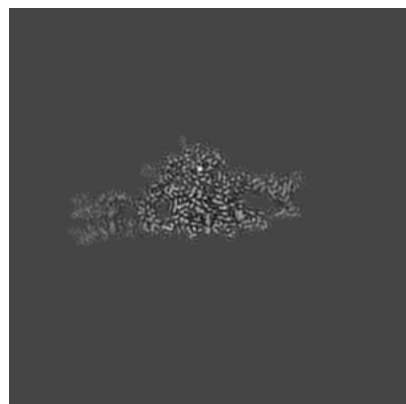


Z Index: 180

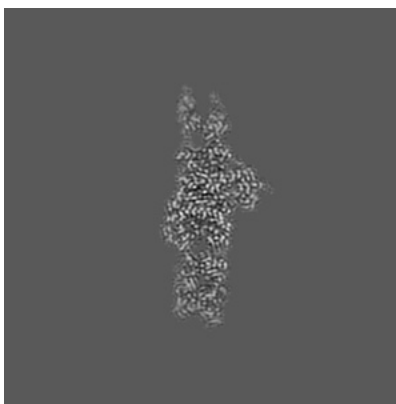
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

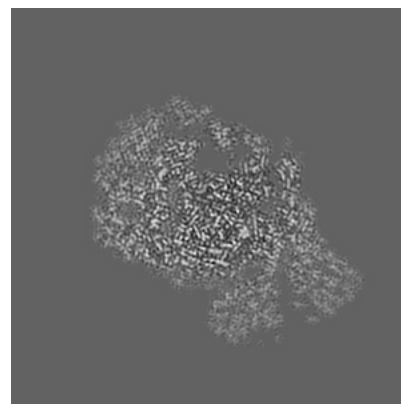
6.3.1 Primary map



X Index: 194



Y Index: 153

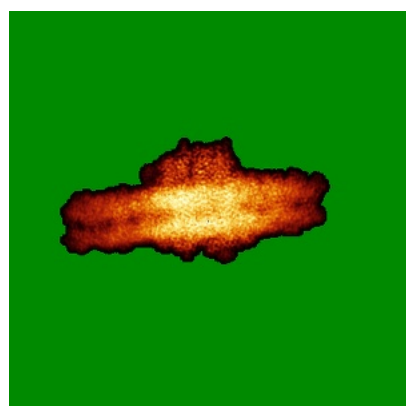


Z Index: 190

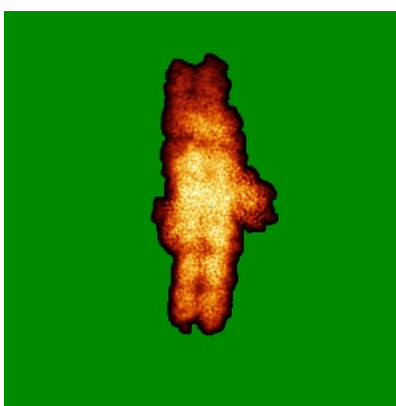
The images above show the largest variance slices of the map in three orthogonal directions.

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

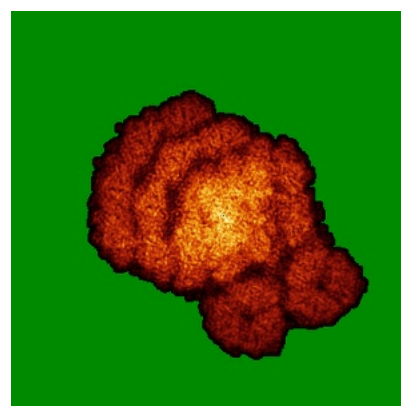
6.4.1 Primary map



X



Y

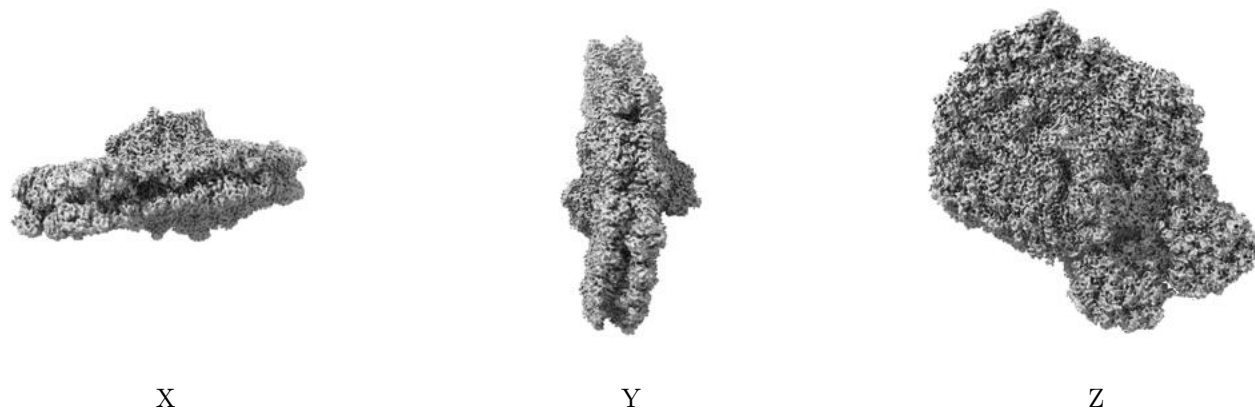


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

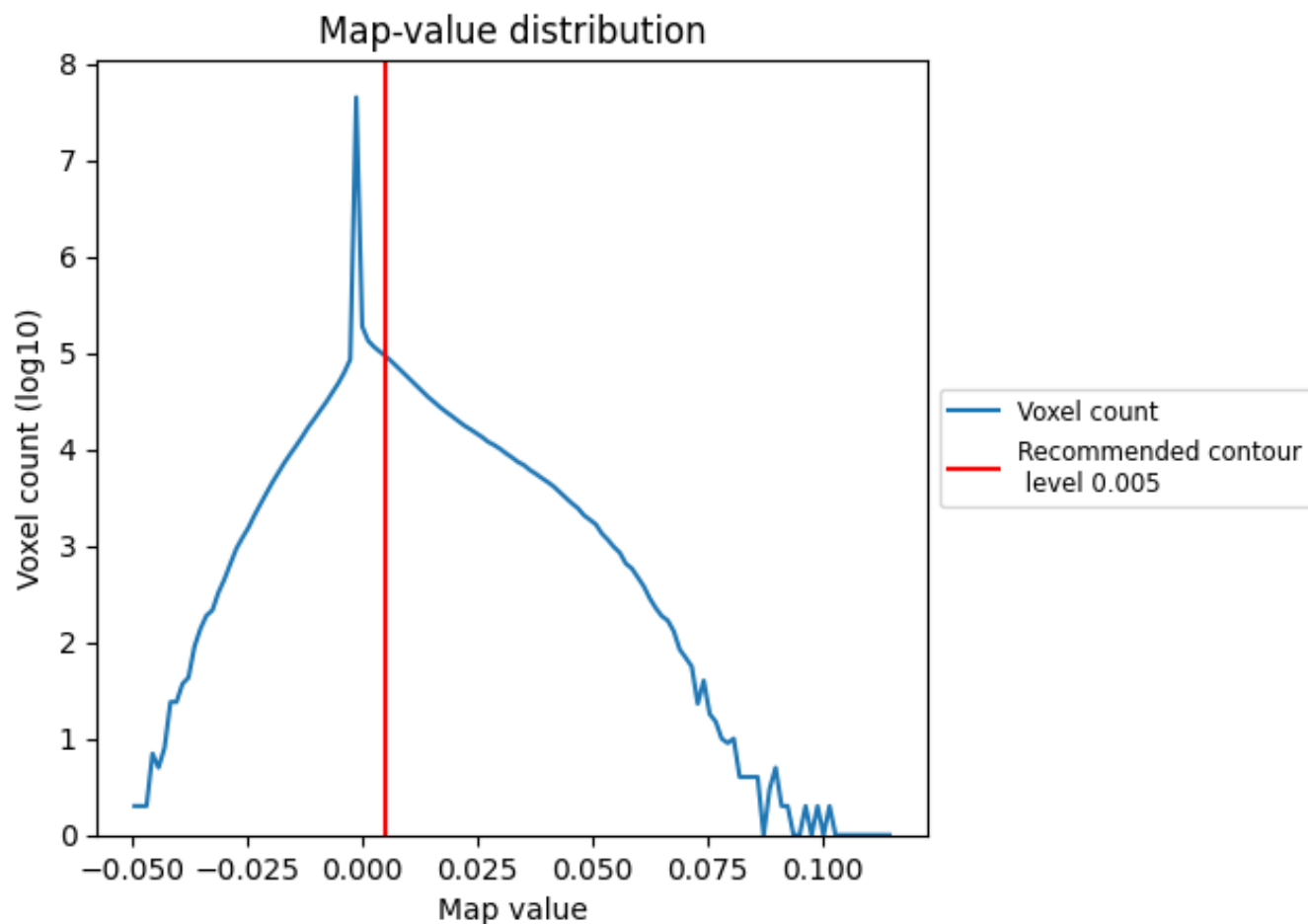
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

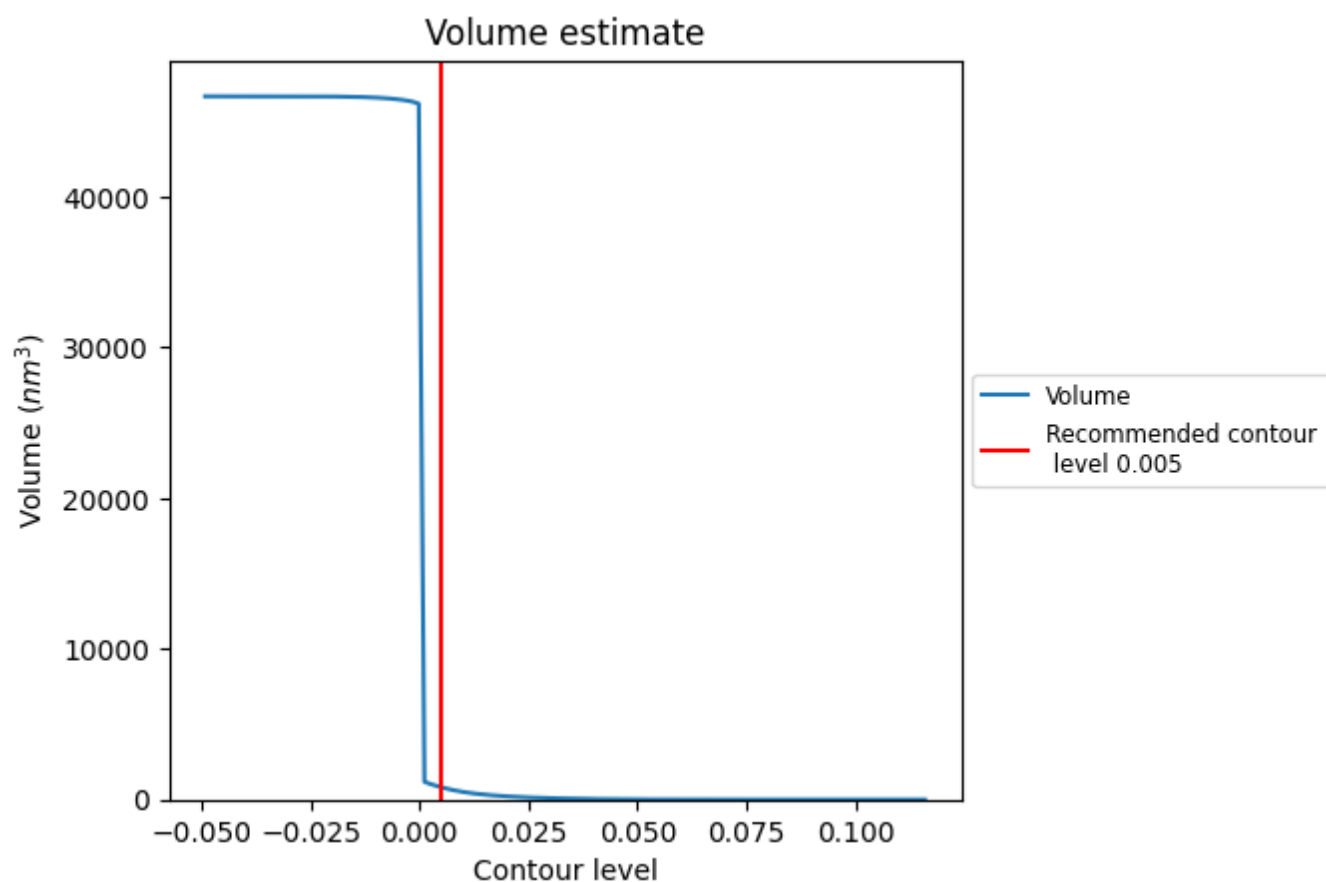
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

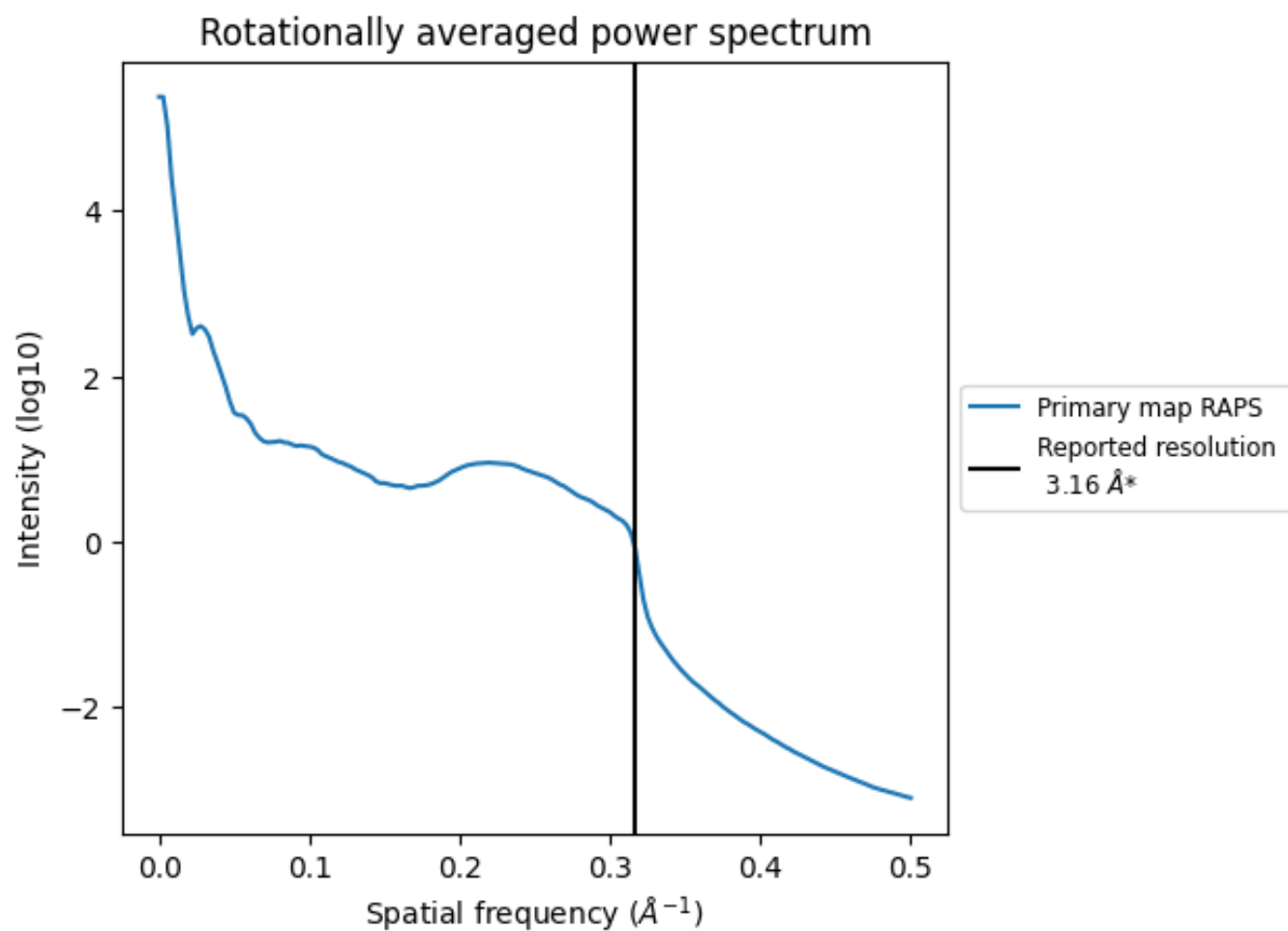
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 811 nm^3 ; this corresponds to an approximate mass of 733 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 0.316 Å⁻¹

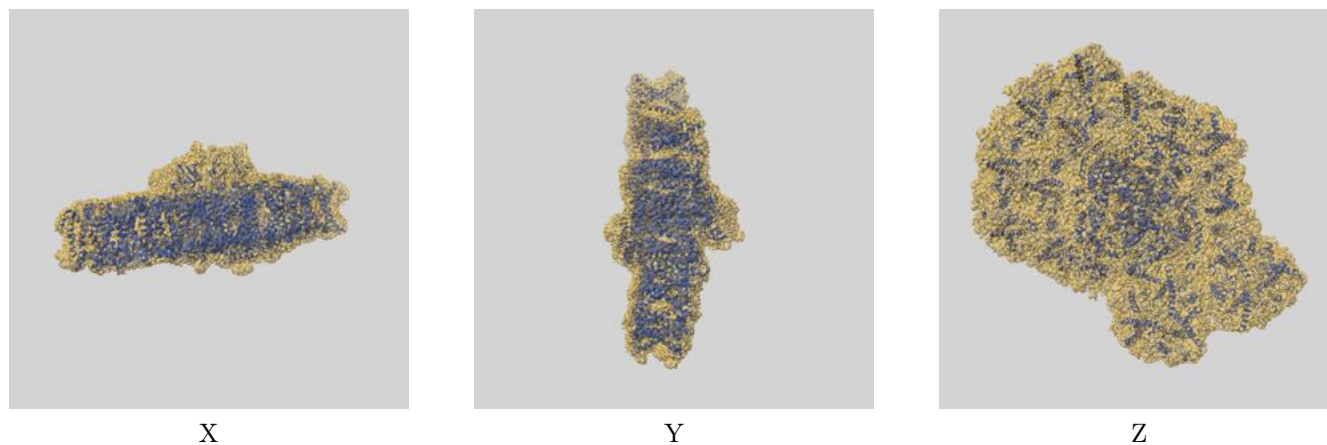
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

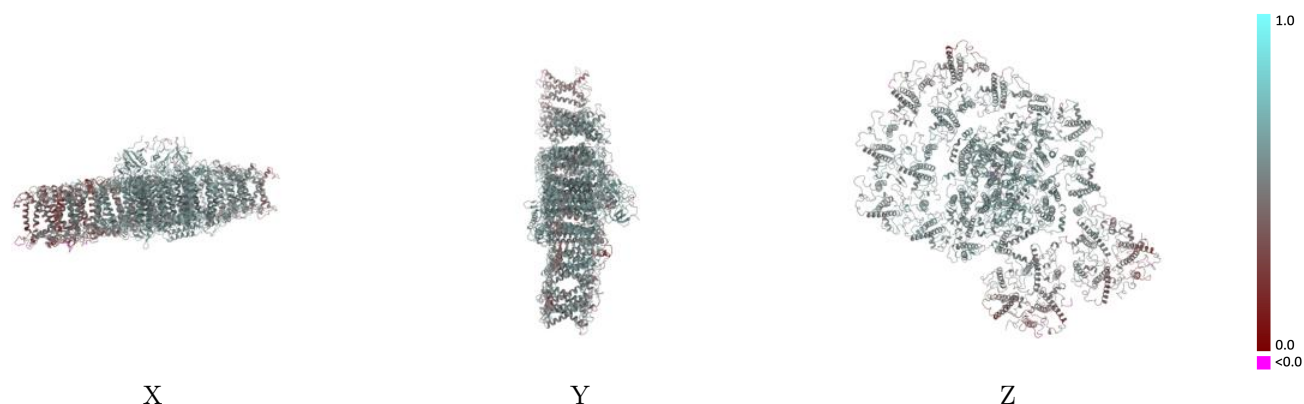
This section contains information regarding the fit between EMDB map EMD-30926 and PDB model 7DZ8. Per-residue inclusion information can be found in section [3](#) on page [45](#).

9.1 Map-model overlay [i](#)



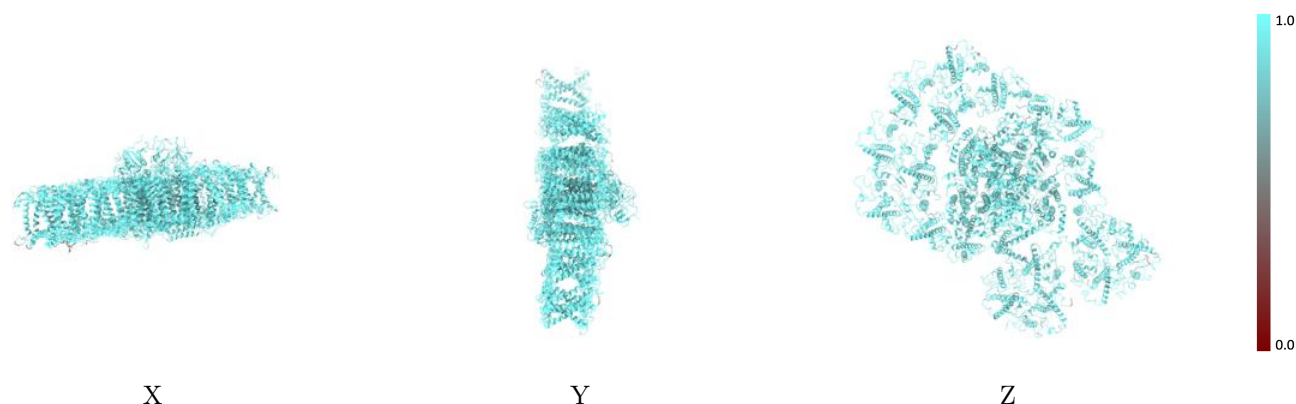
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



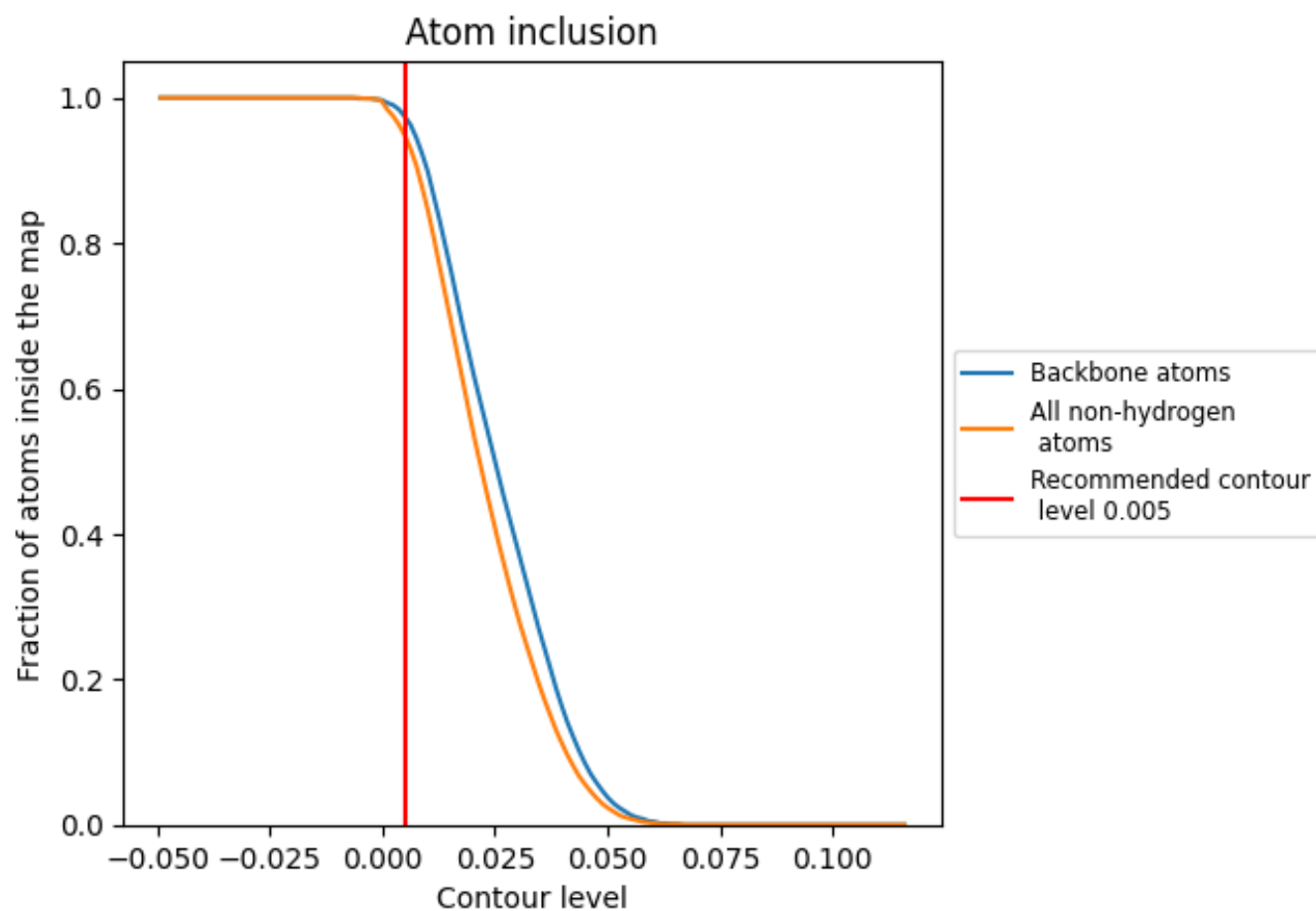
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9480	 0.5180
1	 0.9450	 0.5180
2	 0.9720	 0.5370
3	 0.9620	 0.5530
4	 0.9300	 0.4740
5	 0.9380	 0.5160
6	 0.9480	 0.5130
7	 0.9750	 0.5640
8	 0.9680	 0.5530
9	 0.9410	 0.5060
A	 0.9810	 0.5850
B	 0.9750	 0.5810
C	 0.9700	 0.5390
D	 0.9900	 0.5690
E	 0.9900	 0.5660
F	 0.9890	 0.5650
G	 0.9410	 0.5040
H	 0.9700	 0.5480
I	 0.9430	 0.5380
J	 0.9610	 0.5550
K	 0.9690	 0.5310
L	 0.9740	 0.5570
O	 0.9750	 0.5400
U	 0.9200	 0.4270
V	 0.9480	 0.4950
W	 0.8530	 0.3620
X	 0.8550	 0.3700
Y	 0.8830	 0.4070
Z	 0.9350	 0.4990
a	 0.8970	 0.4270

