



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 03:16 PM UTC

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

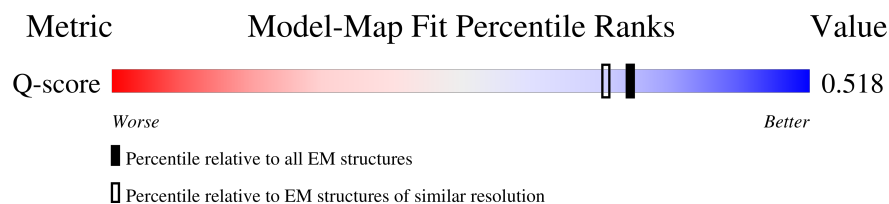
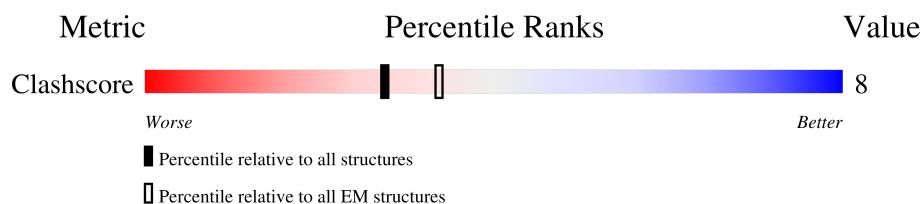
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.



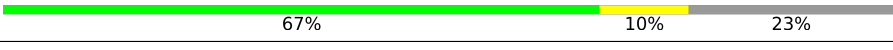
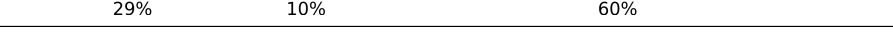
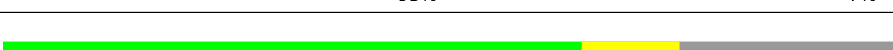
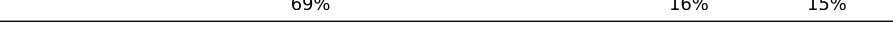
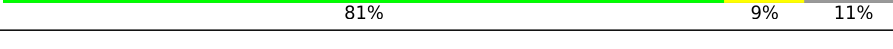
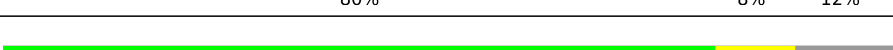
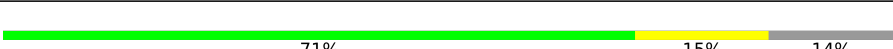
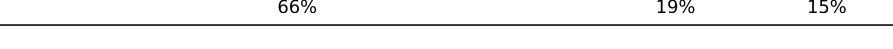
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	14474 (2.66 - 3.66)

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% 20% ..
4	D	196	 62% 10% . 27%
5	E	97	 60% 5% 35%
6	F	227	 65% 7% 27%

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Mol	Chain	Length	Quality of chain
7	G	126	
8	H	130	
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	4	604	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	7	602	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	A	808	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	B	813	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	U	603	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	Z	611	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CHL	Y	605	X	-	-	-
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		

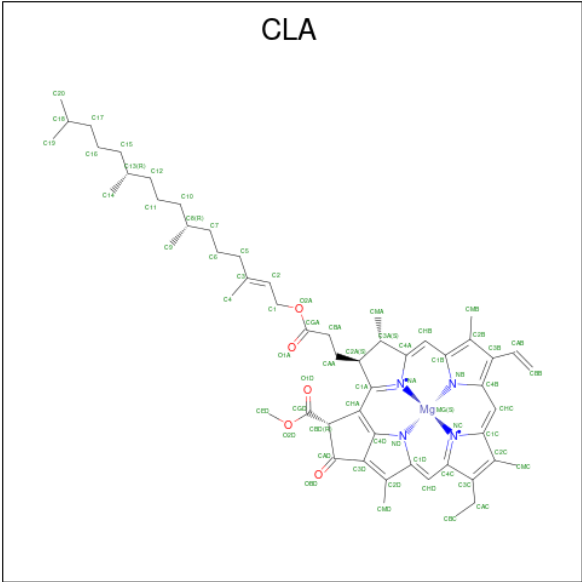
- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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

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

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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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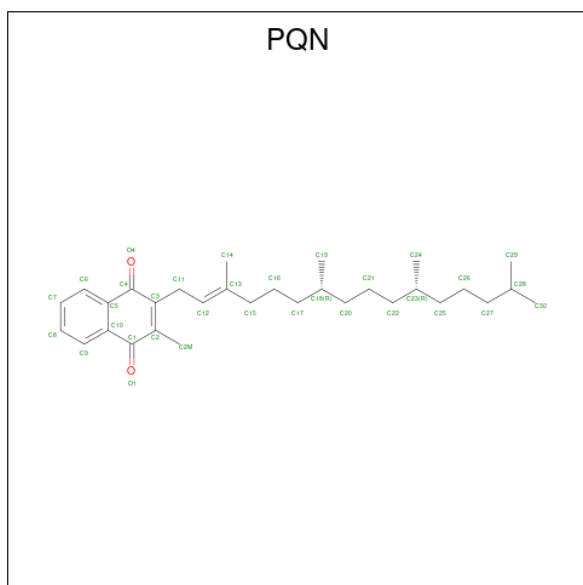
Mol	Chain	Residues	Atoms					AltConf
26	Z	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			49	40	1	4	4	
26	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
26	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	Z	1	Total	C	Mg	N	O	0
			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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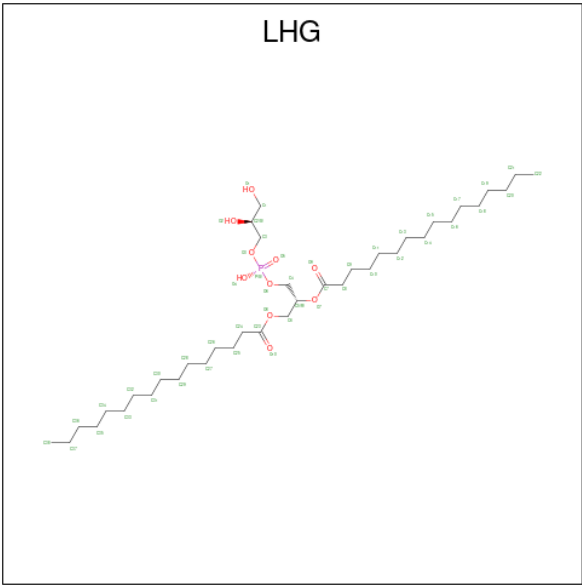
Mol	Chain	Residues	Atoms					AltConf
26	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
26	W	1	Total	C	Mg	N	O	0
			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).



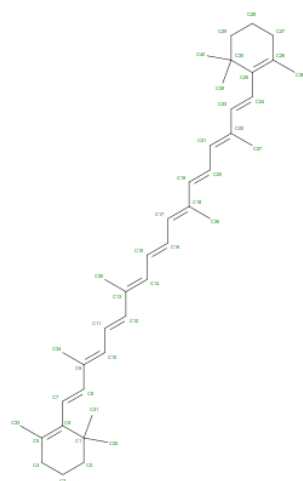
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			49	38	10	1	
28	A	1	Total	C	O	P	0
			30	19	10	1	
28	A	1	Total	C	O	P	0
			49	38	10	1	
28	B	1	Total	C	O	P	0
			38	27	10	1	
28	H	1	Total	C	O	P	0
			49	38	10	1	
28	O	1	Total	C	O	P	0
			36	25	10	1	
28	1	1	Total	C	O	P	0
			49	38	10	1	
28	a	1	Total	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: $C_{40}H_{56}$).



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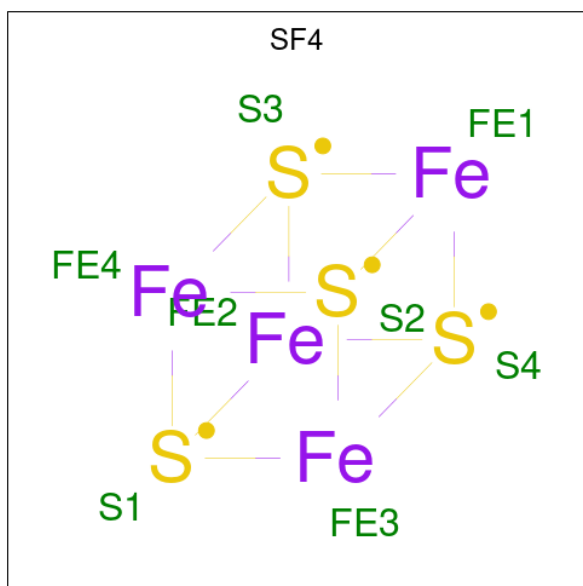
Mol	Chain	Residues	Atoms	AltConf
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	F	1	Total C 40 40	0
29	G	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	O	1	Total C 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).



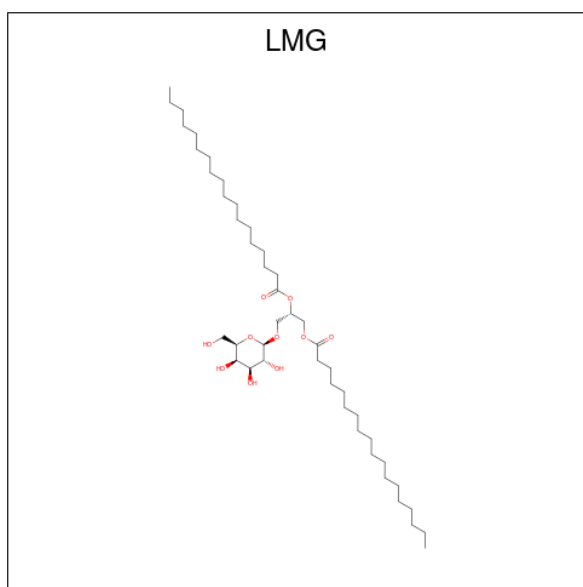
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total Fe S 8 4 4	0
30	C	1	Total Fe S 8 4 4	0
30	C	1	Total Fe S 8 4 4	0

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



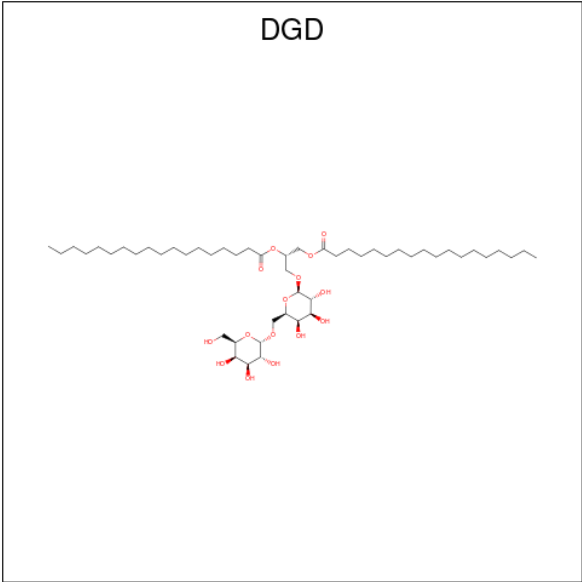
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total 35	C 24	O 11	0
31	A	1	Total 34	C 24	O 10	0
31	K	1	Total 35	C 24	O 11	0
31	1	1	Total 35	C 24	O 11	0
31	5	1	Total 33	C 22	O 11	0
31	5	1	Total 32	C 21	O 11	0
31	8	1	Total 35	C 24	O 11	0

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



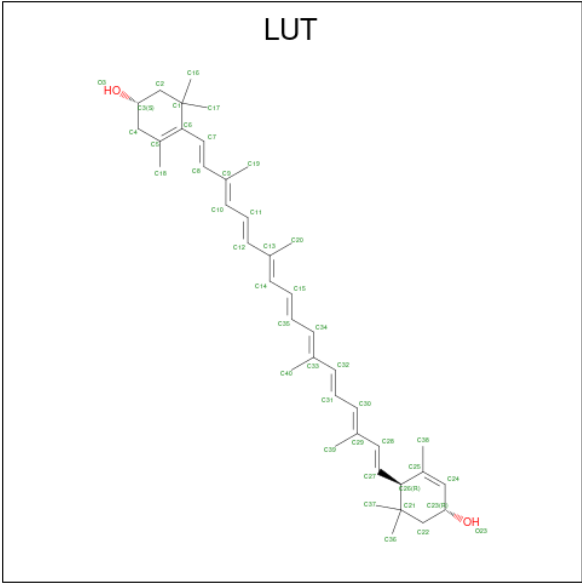
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			40	30	10	
32	H	1	Total	C	O	0
			55	45	10	
32	J	1	Total	C	O	0
			42	32	10	
32	J	1	Total	C	O	0
			40	30	10	
32	L	1	Total	C	O	0
			37	27	10	
32	4	1	Total	C	O	0
			40	30	10	
32	4	1	Total	C	O	0
			40	30	10	
32	5	1	Total	C	O	0
			40	30	10	
32	8	1	Total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



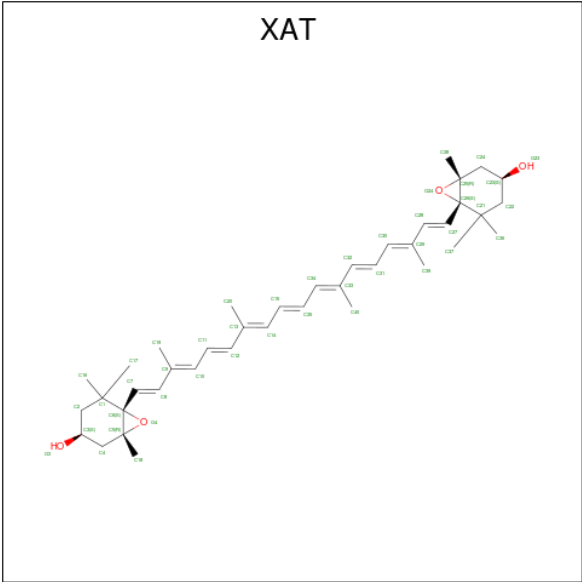
Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total	C	O	0
			42	40	2	
34	a	1	Total	C	O	0
			42	40	2	

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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).



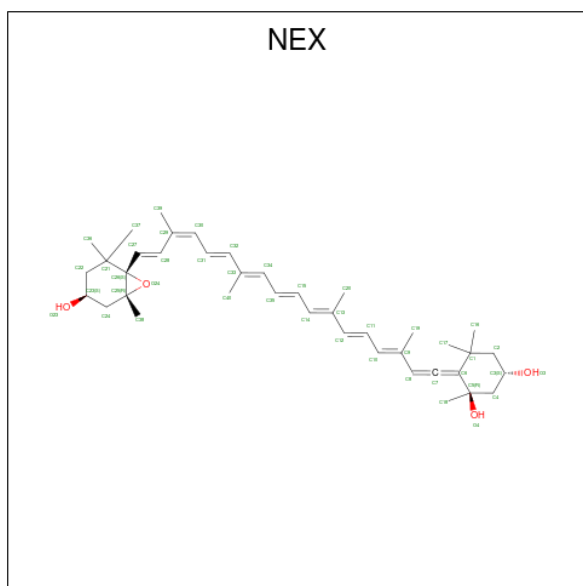
Mol	Chain	Residues	Atoms			AltConf
35	1	1	Total	C	O	0
			44	40	4	
35	a	1	Total	C	O	0
			44	40	4	
35	2	1	Total	C	O	0
			44	40	4	
35	3	1	Total	C	O	0
			44	40	4	
35	4	1	Total	C	O	0
			44	40	4	
35	5	1	Total	C	O	0
			44	40	4	
35	6	1	Total	C	O	0
			44	40	4	
35	7	1	Total	C	O	0
			44	40	4	
35	8	1	Total	C	O	0
			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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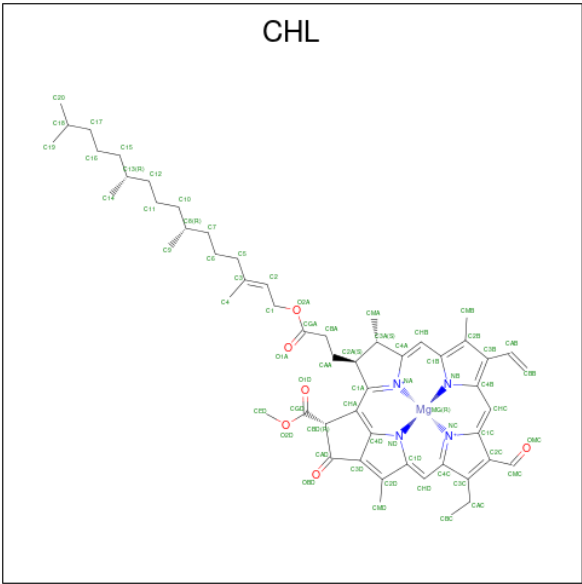
Mol	Chain	Residues	Atoms			AltConf
35	V	1	Total	C	O	0
			44	40	4	
35	W	1	Total	C	O	0
			44	40	4	

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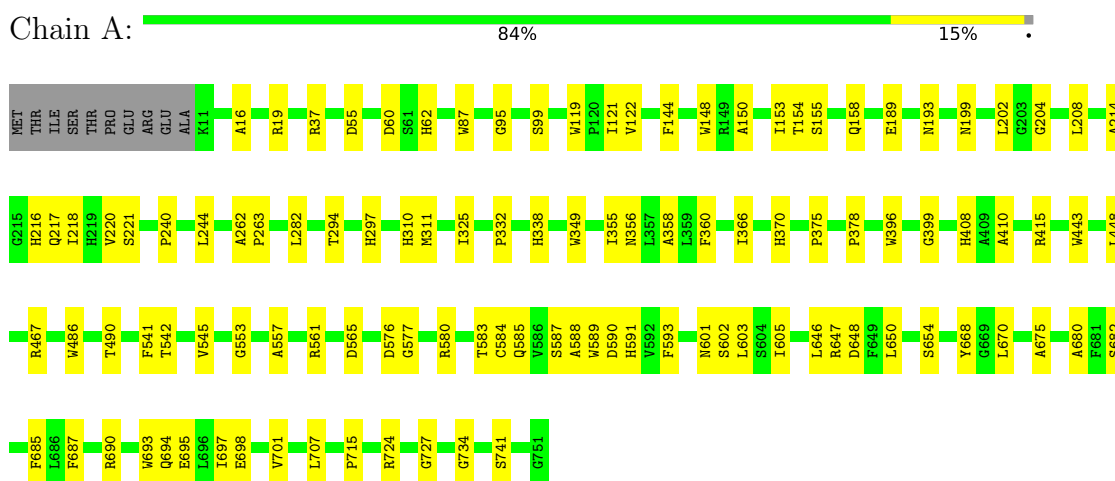
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Mol	Chain	Residues	Atoms					AltConf
37	W	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
37	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

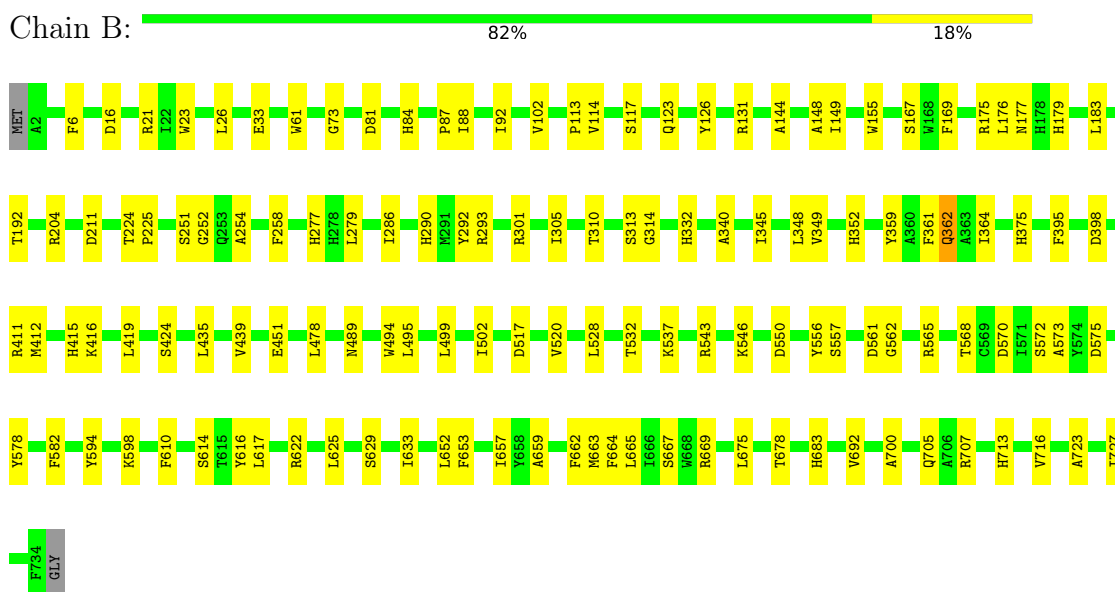
3 Residue-property plots

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.

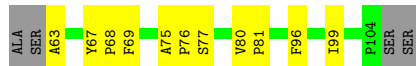
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

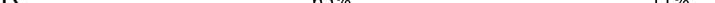


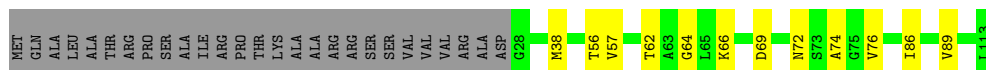
- Molecule 3: Photosystem I iron-sulfur center



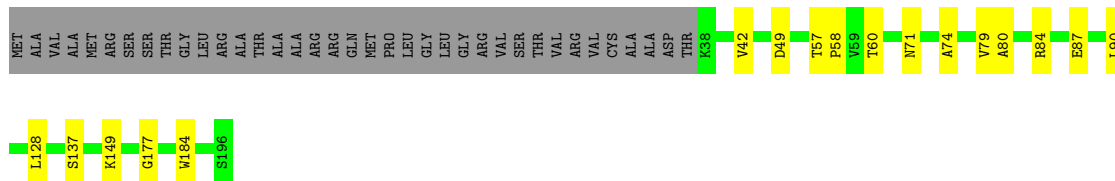
- Chain J:  93% 7%



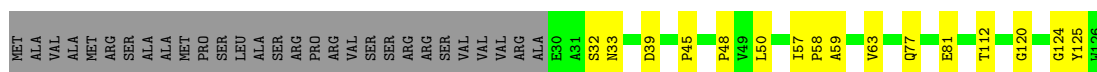
- Chain K:  65% 11% 24%



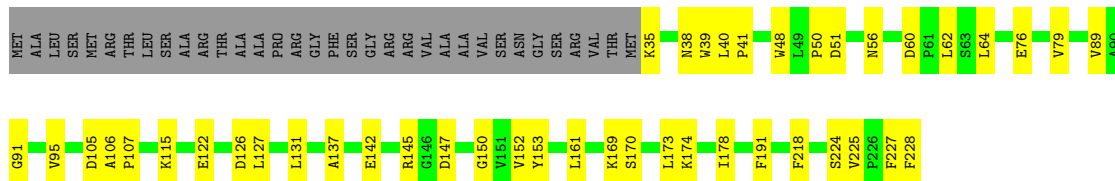
- Chain L: 72% 9% 19%

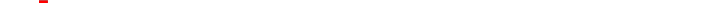


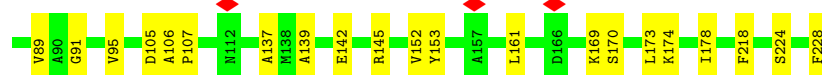
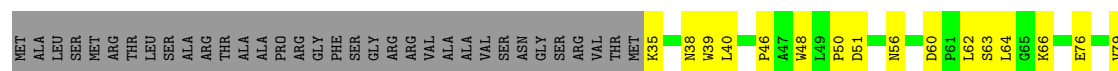
- Chain 0: 64% 13% 23%



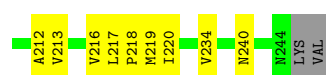
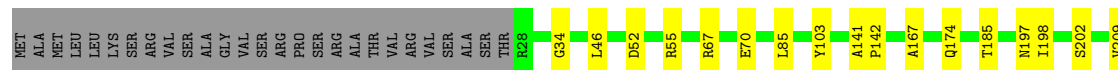
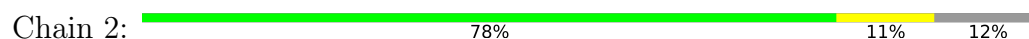
- Chain 1: 66% 19% 15%



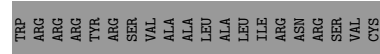
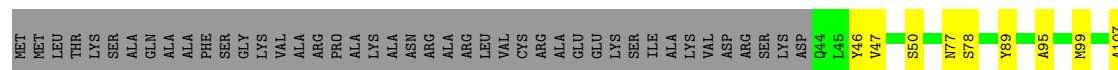
- Chain a:  69% 16% 15%



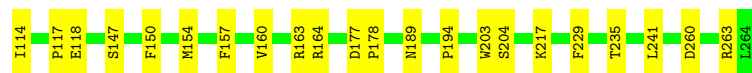
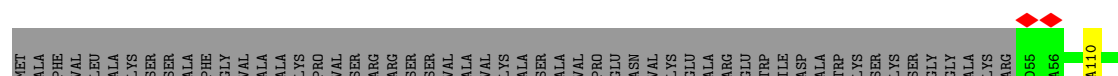
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



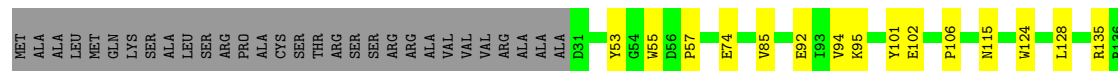
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



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

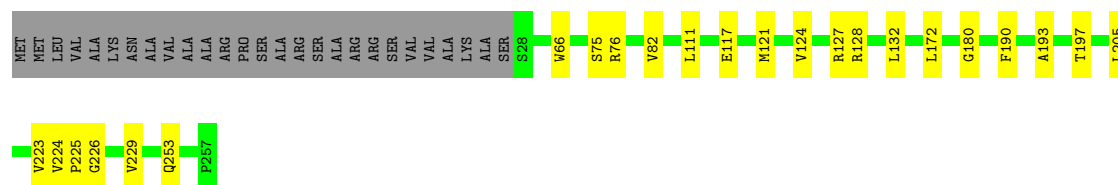


- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



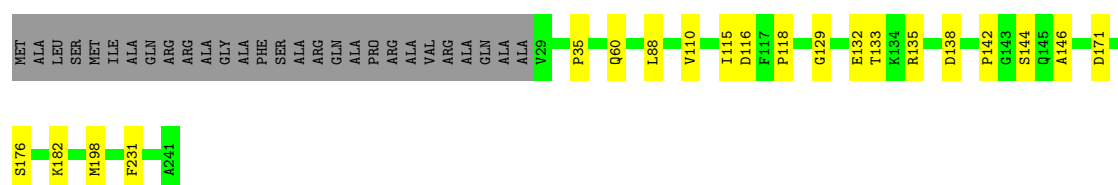
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 6:  81% 9% 11%



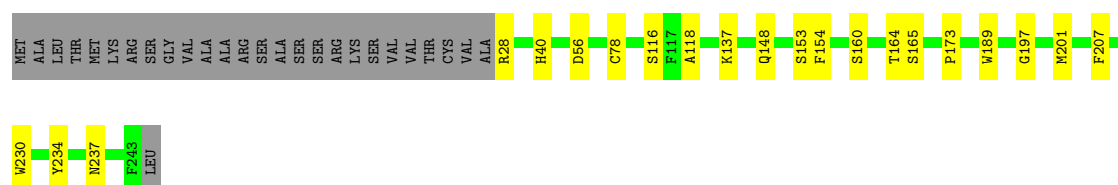
- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 7:  80% 8% 12%



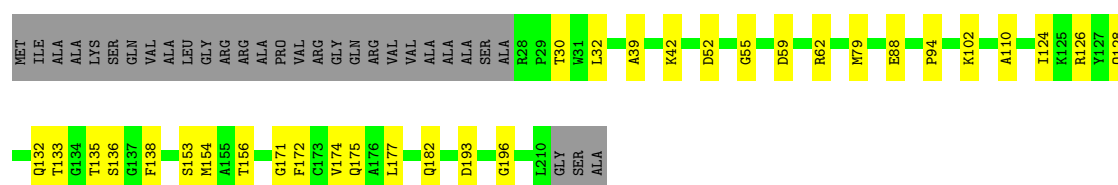
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 8:  80% 9% 11%



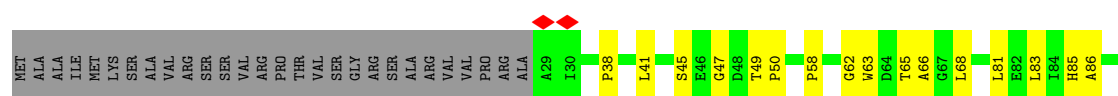
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain 9:  71% 15% 14%

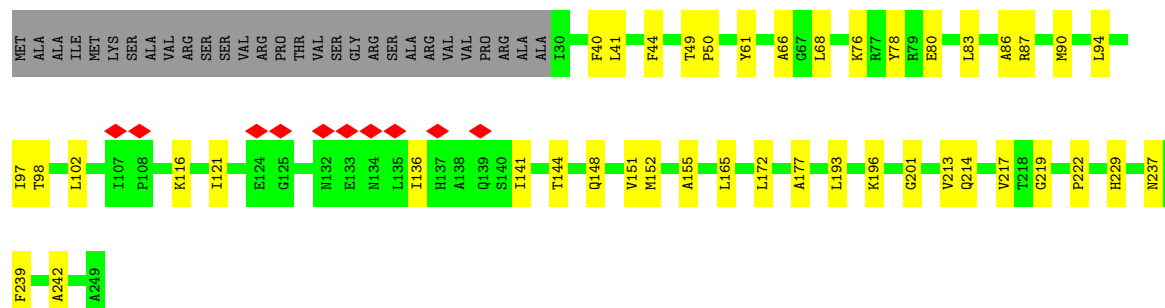


- Molecule 23: Chlorophyll a-b binding protein, chloroplastic

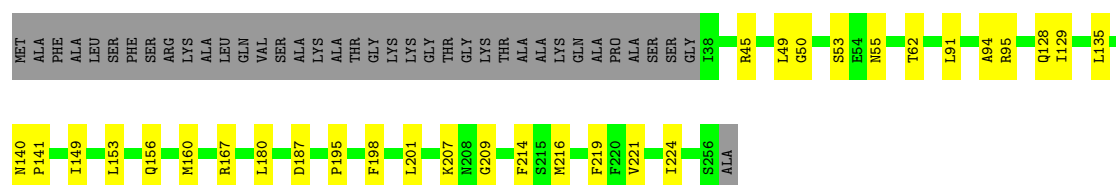
Chain X:  71% 18% 11%



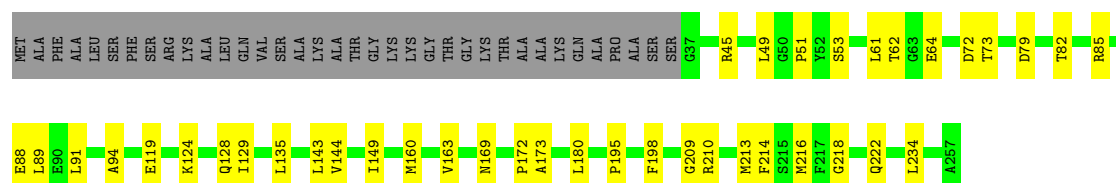
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic



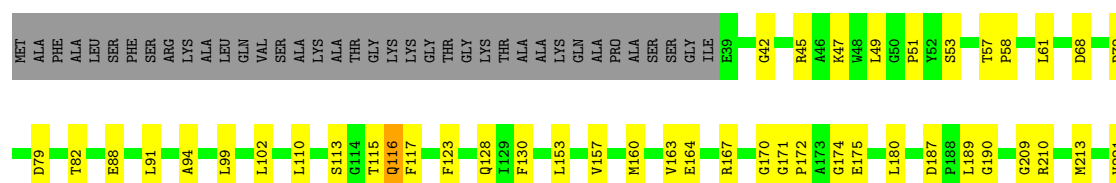
- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

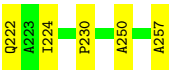


- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

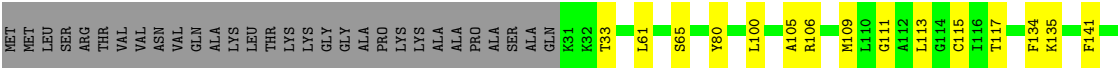


- Molecule 24: Chlorophyll a-b binding protein, chloroplastic





● 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: DGD, CHL, LMU, PQN, XAT, SF4, LHG, TPO, LMG, BCR, CLA, NEX, LUT

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

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 [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

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	1.61	1 (12%)	10,14,16	2.14	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	3.43	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	-5.83	107.48	123.33
25	V	33	TPO	CG2-CB-CA	-2.63	108.14	113.26

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
26	CLA	Y	612	24	49,53,73	1.39	7 (14%)	58,89,113	1.30	6 (10%)
26	CLA	A	808	-	54,58,73	1.30	7 (12%)	64,95,113	1.33	6 (9%)
26	CLA	4	606	-	43,48,73	1.43	8 (18%)	49,83,113	1.24	4 (8%)
29	BCR	3	620	-	41,41,41	0.78	0	56,56,56	2.41	23 (41%)
26	CLA	9	611	28	46,50,73	1.39	7 (15%)	53,85,113	1.22	2 (3%)
26	CLA	Z	602	24	62,66,73	1.22	8 (12%)	73,104,113	1.21	7 (9%)
26	CLA	B	832	-	64,68,73	1.24	8 (12%)	76,107,113	1.29	7 (9%)
34	LUT	W	1620	-	42,43,43	0.70	0	51,60,60	1.70	12 (23%)
26	CLA	A	811	-	69,73,73	1.20	7 (10%)	82,113,113	1.22	5 (6%)
31	LMU	K	208	-	36,36,36	1.14	2 (5%)	47,47,47	1.01	3 (6%)
26	CLA	3	612	16	47,51,73	1.39	8 (17%)	55,86,113	1.23	5 (9%)
26	CLA	a	601	14	57,62,73	1.27	8 (14%)	67,100,113	1.20	5 (7%)
34	LUT	Y	1621	-	42,43,43	0.87	1 (2%)	51,60,60	1.88	16 (31%)
26	CLA	X	614	-	46,50,73	1.42	7 (15%)	53,85,113	1.27	4 (7%)
35	XAT	V	1622	-	41,47,47	0.91	1 (2%)	54,74,74	2.60	22 (40%)
26	CLA	9	602	22	64,68,73	1.22	8 (12%)	76,107,113	1.27	8 (10%)
29	BCR	6	622	-	41,41,41	0.78	1 (2%)	56,56,56	2.49	25 (44%)
37	CHL	V	607	-	40,54,74	4.15	19 (47%)	34,90,114	2.36	13 (38%)
29	BCR	B	852	-	41,41,41	0.75	1 (2%)	56,56,56	4.24	30 (53%)
36	NEX	Z	1623	-	40,46,46	1.11	3 (7%)	50,70,70	2.51	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	A	823	-	46,50,73	1.37	8 (17%)	53,85,113	1.33	3 (5%)
29	BCR	B	801	-	41,41,41	0.86	0	56,56,56	2.15	17 (30%)
26	CLA	a	616	14	49,53,73	1.36	6 (12%)	58,89,113	1.37	6 (10%)
26	CLA	A	803	-	69,73,73	1.23	9 (13%)	82,113,113	1.19	4 (4%)
26	CLA	7	604	-	54,58,73	1.30	8 (14%)	63,95,113	1.22	6 (9%)
26	CLA	8	612	21	44,49,73	1.41	6 (13%)	50,84,113	1.32	3 (6%)
35	XAT	U	1622	-	41,47,47	0.94	2 (4%)	54,74,74	4.33	22 (40%)
37	CHL	X	609	23	60,74,74	3.44	20 (33%)	58,114,114	2.38	15 (25%)
29	BCR	L	309	-	41,41,41	0.73	0	56,56,56	2.43	24 (42%)
26	CLA	4	618	17	43,48,73	1.51	7 (16%)	51,83,113	1.29	4 (7%)
31	LMU	A	858	-	35,35,36	1.25	3 (8%)	44,45,47	1.00	2 (4%)
28	LHG	6	623	26	47,47,48	0.91	2 (4%)	50,53,54	0.98	3 (6%)
29	BCR	O	2004	-	41,41,41	0.85	0	56,56,56	1.97	13 (23%)
26	CLA	6	603	-	55,59,73	1.39	9 (16%)	66,96,113	1.38	5 (7%)
26	CLA	2	612	15	48,52,73	1.39	7 (14%)	57,88,113	1.27	3 (5%)
35	XAT	5	621	-	41,47,47	0.94	2 (4%)	54,74,74	2.39	19 (35%)
37	CHL	W	605	23	40,54,74	4.25	19 (47%)	34,90,114	2.84	11 (32%)
37	CHL	Y	609	24	60,74,74	3.44	20 (33%)	58,114,114	2.36	15 (25%)
26	CLA	A	807	1	69,73,73	1.21	10 (14%)	82,113,113	1.24	5 (6%)
26	CLA	Y	613	24	69,73,73	1.17	7 (10%)	82,113,113	1.18	5 (6%)
26	CLA	1	610	14	43,47,73	1.44	7 (16%)	50,81,113	1.41	8 (16%)
26	CLA	3	604	-	69,73,73	1.18	8 (11%)	82,113,113	1.17	8 (9%)
35	XAT	7	620	-	41,47,47	0.96	4 (9%)	54,74,74	2.37	19 (35%)
26	CLA	6	611	28	46,50,73	1.37	6 (13%)	53,85,113	1.28	4 (7%)
26	CLA	F	304	6	45,49,73	1.41	7 (15%)	54,84,113	1.32	5 (9%)
26	CLA	W	610	23	59,63,73	1.24	7 (11%)	70,101,113	1.24	8 (11%)
26	CLA	1	611	28	61,65,73	1.24	8 (13%)	72,103,113	1.16	6 (8%)
26	CLA	5	612	18	44,49,73	1.40	6 (13%)	50,84,113	1.26	4 (8%)
26	CLA	4	604	-	58,62,73	1.35	8 (13%)	71,100,113	1.28	6 (8%)
37	CHL	Z	601	24	60,74,74	3.42	19 (31%)	58,114,114	2.27	14 (24%)
28	LHG	U	2630	26	48,48,48	0.94	2 (4%)	51,54,54	1.10	4 (7%)
26	CLA	W	614	-	49,53,73	1.37	5 (10%)	58,89,113	1.36	4 (6%)
37	CHL	W	601	23	60,74,74	3.46	20 (33%)	58,114,114	2.20	13 (22%)
26	CLA	H	202	-	42,47,73	1.45	6 (14%)	50,82,113	1.21	3 (6%)
26	CLA	2	604	-	46,50,73	1.37	7 (15%)	54,85,113	1.31	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	F	303	-	46,50,73	1.42	9 (19%)	53,85,113	1.35	4 (7%)
26	CLA	K	201	11	49,53,73	1.36	6 (12%)	58,89,113	1.22	4 (6%)
26	CLA	3	615	-	43,48,73	1.41	6 (13%)	49,83,113	1.28	4 (8%)
29	BCR	J	102	-	41,41,41	0.87	1 (2%)	56,56,56	2.43	23 (41%)
26	CLA	A	814	-	69,73,73	1.17	10 (14%)	82,113,113	1.39	10 (12%)
26	CLA	A	806	-	69,73,73	1.22	11 (15%)	82,113,113	1.37	8 (9%)
26	CLA	X	612	23	47,51,73	1.38	6 (12%)	55,86,113	1.35	5 (9%)
26	CLA	B	827	-	66,70,73	1.19	9 (13%)	78,109,113	1.31	8 (10%)
26	CLA	Y	611	28	47,51,73	1.38	6 (12%)	55,86,113	1.23	3 (5%)
36	NEX	U	1623	-	40,46,46	1.03	3 (7%)	50,70,70	2.50	19 (38%)
26	CLA	V	613	25	69,73,73	1.16	8 (11%)	82,113,113	1.16	4 (4%)
26	CLA	U	613	24	63,67,73	1.22	8 (12%)	74,105,113	1.16	5 (6%)
26	CLA	B	818	-	64,68,73	1.23	9 (14%)	76,107,113	1.33	6 (7%)
26	CLA	4	610	17	65,69,73	1.18	7 (10%)	77,108,113	1.19	6 (7%)
28	LHG	7	622	26	36,36,48	1.05	2 (5%)	39,42,54	1.03	3 (7%)
30	SF4	A	853	1,2	0,12,12	-	-	-	-	-
34	LUT	9	619	-	42,43,43	0.87	1 (2%)	51,60,60	2.01	14 (27%)
37	CHL	V	601	25	60,74,74	3.46	19 (31%)	58,114,114	2.32	16 (27%)
37	CHL	Y	607	-	60,74,74	3.35	19 (31%)	58,114,114	2.19	13 (22%)
35	XAT	2	620	-	41,47,47	1.00	3 (7%)	54,74,74	2.43	27 (50%)
26	CLA	6	607	-	45,49,73	1.50	8 (17%)	54,84,113	1.32	5 (9%)
35	XAT	Z	1622	-	41,47,47	0.89	2 (4%)	54,74,74	2.78	21 (38%)
35	XAT	W	1622	-	41,47,47	0.93	2 (4%)	54,74,74	4.21	26 (48%)
29	BCR	B	848	-	41,41,41	0.78	0	56,56,56	2.57	14 (25%)
26	CLA	A	802	-	69,73,73	1.19	8 (11%)	82,113,113	1.37	9 (10%)
26	CLA	7	616	20	47,51,73	1.51	10 (21%)	58,87,113	1.33	5 (8%)
26	CLA	9	601	22	49,53,73	1.38	7 (14%)	58,89,113	1.29	4 (6%)
26	CLA	9	613	22	69,73,73	1.19	7 (10%)	82,113,113	1.23	5 (6%)
26	CLA	8	607	-	45,49,73	1.52	10 (22%)	54,84,113	1.30	5 (9%)
26	CLA	W	604	-	51,55,73	1.36	7 (13%)	60,91,113	1.26	7 (11%)
26	CLA	4	614	-	60,64,73	1.24	8 (13%)	71,102,113	1.22	5 (7%)
35	XAT	6	621	-	41,47,47	0.96	3 (7%)	54,74,74	2.33	23 (42%)
26	CLA	5	604	-	67,71,73	1.29	8 (11%)	82,111,113	1.18	6 (7%)
26	CLA	6	612	19	44,49,73	1.40	7 (15%)	50,84,113	1.21	3 (6%)
37	CHL	Z	606	-	40,54,74	4.17	20 (50%)	34,90,114	3.00	15 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	A	835	-	65,69,73	1.22	8 (12%)	77,108,113	1.25	6 (7%)
37	CHL	V	609	25	55,69,74	3.56	19 (34%)	52,108,114	2.62	15 (28%)
26	CLA	B	830	-	47,51,73	1.39	7 (14%)	55,86,113	1.31	6 (10%)
26	CLA	a	611	28	41,46,73	1.56	9 (21%)	51,81,113	1.34	7 (13%)
34	LUT	U	1621	-	42,43,43	0.73	0	51,60,60	1.63	11 (21%)
26	CLA	2	610	15	59,63,73	1.27	8 (13%)	70,101,113	1.20	7 (10%)
31	LMU	1	621	-	36,36,36	1.15	2 (5%)	47,47,47	1.01	1 (2%)
26	CLA	a	603	-	58,62,73	1.26	7 (12%)	68,99,113	1.31	3 (4%)
31	LMU	5	628	-	34,34,36	1.19	2 (5%)	45,45,47	1.16	5 (11%)
26	CLA	X	610	23	69,73,73	1.17	7 (10%)	82,113,113	1.15	7 (8%)
26	CLA	B	810	-	68,72,73	1.18	10 (14%)	80,111,113	1.39	9 (11%)
26	CLA	B	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.17	5 (6%)
26	CLA	8	608	-	55,59,73	1.31	8 (14%)	64,96,113	1.38	6 (9%)
26	CLA	W	611	28	61,65,73	1.23	7 (11%)	72,103,113	1.12	5 (6%)
29	BCR	L	305	-	41,41,41	0.85	0	56,56,56	2.53	26 (46%)
26	CLA	9	614	-	49,53,73	1.37	8 (16%)	58,89,113	1.20	4 (6%)
29	BCR	B	843	-	41,41,41	0.96	2 (4%)	56,56,56	1.96	17 (30%)
26	CLA	A	819	-	63,67,73	1.24	10 (15%)	74,105,113	1.34	6 (8%)
26	CLA	A	827	-	62,66,73	1.23	7 (11%)	73,104,113	1.16	4 (5%)
26	CLA	A	833	-	49,53,73	1.38	9 (18%)	58,89,113	1.47	9 (15%)
37	CHL	X	606	-	38,52,74	4.28	17 (44%)	31,87,114	3.00	13 (41%)
26	CLA	9	606	-	43,48,73	1.46	9 (20%)	49,83,113	1.28	4 (8%)
26	CLA	7	609	20	46,52,73	1.40	8 (17%)	57,87,113	1.21	4 (7%)
26	CLA	B	814	-	68,72,73	1.17	7 (10%)	80,111,113	1.28	5 (6%)
34	LUT	7	619	-	42,43,43	0.90	2 (4%)	51,60,60	2.10	16 (31%)
29	BCR	A	849	-	41,41,41	0.83	0	56,56,56	2.23	21 (37%)
26	CLA	a	607	-	49,53,73	1.41	9 (18%)	58,89,113	1.17	4 (6%)
37	CHL	W	606	-	40,54,74	4.08	20 (50%)	34,90,114	3.01	13 (38%)
26	CLA	A	820	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	8 (9%)
26	CLA	6	610	19	69,73,73	1.19	7 (10%)	82,113,113	1.15	5 (6%)
26	CLA	Y	610	24	69,73,73	1.17	8 (11%)	82,113,113	1.12	5 (6%)
36	NEX	X	1623	-	40,46,46	1.00	3 (7%)	50,70,70	4.29	19 (38%)
26	CLA	7	606	-	45,49,73	1.42	9 (20%)	52,84,113	1.27	4 (7%)
26	CLA	B	812	-	47,51,73	1.36	7 (14%)	55,86,113	1.24	5 (9%)
26	CLA	5	614	-	48,52,73	1.39	8 (16%)	53,87,113	1.27	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CHL	Y	605	24	36,50,74	4.52	17 (47%)	29,85,114	2.53	11 (37%)
26	CLA	1	614	-	40,45,73	1.58	10 (25%)	47,79,113	1.46	6 (12%)
29	BCR	A	856	-	41,41,41	0.86	1 (2%)	56,56,56	1.99	19 (33%)
29	BCR	A	850	-	41,41,41	0.94	1 (2%)	56,56,56	2.04	13 (23%)
29	BCR	B	846	-	41,41,41	0.80	1 (2%)	56,56,56	2.38	21 (37%)
26	CLA	1	606	-	41,47,73	1.49	8 (19%)	50,80,113	1.41	5 (10%)
26	CLA	8	610	21	64,68,73	1.19	7 (10%)	76,107,113	1.29	8 (10%)
29	BCR	A	852	-	41,41,41	0.89	2 (4%)	56,56,56	2.55	27 (48%)
29	BCR	7	621	-	41,41,41	0.83	1 (2%)	56,56,56	2.31	22 (39%)
26	CLA	4	612	17	44,49,73	1.42	7 (15%)	50,84,113	1.23	3 (6%)
26	CLA	A	830	-	69,73,73	1.18	8 (11%)	82,113,113	1.21	7 (8%)
26	CLA	7	603	-	47,52,73	1.43	8 (17%)	55,88,113	1.46	3 (5%)
36	NEX	Y	1623	-	40,46,46	1.12	3 (7%)	50,70,70	2.39	17 (34%)
26	CLA	3	609	16	64,68,73	1.25	7 (10%)	76,107,113	1.24	6 (7%)
37	CHL	Y	608	-	43,57,74	4.01	19 (44%)	37,93,114	2.85	15 (40%)
26	CLA	L	307	8	43,48,73	1.41	7 (16%)	49,83,113	1.40	6 (12%)
26	CLA	1	607	-	43,48,73	1.46	9 (20%)	51,83,113	1.19	5 (9%)
32	LMG	J	104	-	40,40,55	1.02	2 (5%)	48,48,63	1.30	5 (10%)
26	CLA	4	609	17	61,65,73	1.24	5 (8%)	72,103,113	1.16	5 (6%)
26	CLA	6	620	-	68,72,73	1.16	7 (10%)	80,111,113	1.18	5 (6%)
29	BCR	B	849	-	41,41,41	0.94	2 (4%)	56,56,56	2.58	19 (33%)
26	CLA	A	831	-	69,73,73	1.20	10 (14%)	82,113,113	1.21	7 (8%)
26	CLA	6	606	-	43,48,73	1.44	7 (16%)	49,83,113	1.22	4 (8%)
37	CHL	U	609	24	54,68,74	3.53	19 (35%)	50,106,114	2.56	13 (26%)
26	CLA	7	611	28	63,67,73	1.21	7 (11%)	74,105,113	1.18	7 (9%)
29	BCR	8	621	-	41,41,41	0.75	0	56,56,56	2.83	24 (42%)
26	CLA	B	834	-	64,68,73	1.20	8 (12%)	76,107,113	1.21	6 (7%)
26	CLA	5	618	18	43,48,73	1.53	9 (20%)	51,83,113	1.32	5 (9%)
32	LMG	H	205	-	55,55,55	0.86	2 (3%)	63,63,63	1.13	6 (9%)
34	LUT	X	1621	-	42,43,43	0.74	1 (2%)	51,60,60	1.85	15 (29%)
29	BCR	K	202	-	41,41,41	0.87	1 (2%)	56,56,56	2.29	21 (37%)
34	LUT	2	619	-	42,43,43	0.90	2 (4%)	51,60,60	2.09	15 (29%)
34	LUT	a	617	-	42,43,43	0.79	1 (2%)	51,60,60	2.04	18 (35%)
26	CLA	1	604	-	53,57,73	1.31	7 (13%)	61,93,113	1.25	4 (6%)
26	CLA	A	832	-	54,58,73	1.35	8 (14%)	64,95,113	1.43	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	J	103	-	42,42,55	0.99	2 (4%)	50,50,63	1.23	7 (14%)
37	CHL	Z	609	24	60,74,74	3.44	20 (33%)	58,114,114	2.30	17 (29%)
26	CLA	4	603	17	48,52,73	1.48	9 (18%)	59,88,113	1.37	6 (10%)
26	CLA	2	602	15	59,69,73	1.32	7 (11%)	70,102,113	1.31	4 (5%)
37	CHL	W	609	23	60,74,74	3.47	20 (33%)	58,114,114	2.12	16 (27%)
28	LHG	9	624	-	48,48,48	0.94	2 (4%)	51,54,54	0.88	2 (3%)
26	CLA	G	204	7	49,53,73	1.39	8 (16%)	58,89,113	1.29	4 (6%)
34	LUT	Z	1621	-	42,43,43	0.77	0	51,60,60	1.51	9 (17%)
26	CLA	7	614	-	46,50,73	1.38	8 (17%)	53,85,113	1.27	4 (7%)
34	LUT	X	1620	-	42,43,43	0.70	0	51,60,60	1.66	11 (21%)
26	CLA	B	821	-	47,51,73	1.44	8 (17%)	54,86,113	1.29	4 (7%)
26	CLA	8	604	-	54,58,73	1.29	7 (12%)	64,95,113	1.36	9 (14%)
26	CLA	U	603	-	56,60,73	1.29	7 (12%)	65,97,113	1.36	6 (9%)
37	CHL	Y	601	24	60,74,74	3.46	20 (33%)	58,114,114	2.14	14 (24%)
26	CLA	B	808	-	69,73,73	1.18	8 (11%)	82,113,113	1.22	9 (10%)
26	CLA	B	838	-	50,54,73	1.35	8 (16%)	59,90,113	1.36	6 (10%)
26	CLA	4	611	28	46,50,73	1.35	6 (13%)	53,85,113	1.30	6 (11%)
34	LUT	5	620	-	42,43,43	0.83	1 (2%)	51,60,60	2.03	15 (29%)
26	CLA	A	816	-	69,73,73	1.18	9 (13%)	82,113,113	1.28	5 (6%)
26	CLA	B	825	-	53,57,73	1.31	7 (13%)	61,93,113	1.33	7 (11%)
26	CLA	B	826	-	66,70,73	1.21	8 (12%)	78,109,113	1.44	6 (7%)
26	CLA	a	610	14	63,67,73	1.21	7 (11%)	75,106,113	1.14	8 (10%)
26	CLA	L	302	12	49,53,73	1.42	7 (14%)	58,89,113	1.31	5 (8%)
37	CHL	V	606	-	38,52,74	4.08	18 (47%)	31,87,114	3.25	14 (45%)
26	CLA	7	615	-	44,50,73	1.53	9 (20%)	57,85,113	1.32	5 (8%)
35	XAT	8	620	-	41,47,47	0.97	3 (7%)	54,74,74	2.38	25 (46%)
26	CLA	A	825	-	69,73,73	1.18	7 (10%)	82,113,113	1.16	4 (4%)
26	CLA	3	607	16	60,64,73	1.31	8 (13%)	73,102,113	1.20	7 (9%)
26	CLA	3	617	16	43,48,73	1.41	7 (16%)	51,83,113	1.35	4 (7%)
37	CHL	W	608	-	41,55,74	4.14	19 (46%)	35,91,114	2.80	13 (37%)
26	CLA	4	601	17	69,73,73	1.15	7 (10%)	82,113,113	1.22	5 (6%)
37	CHL	U	608	-	38,52,74	4.19	18 (47%)	31,87,114	2.76	11 (35%)
29	BCR	G	205	-	41,41,41	0.80	1 (2%)	56,56,56	1.98	15 (26%)
26	CLA	3	614	-	43,48,73	1.43	8 (18%)	51,83,113	1.31	4 (7%)
26	CLA	U	614	-	46,50,73	1.38	6 (13%)	53,85,113	1.33	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	BCR	a	619	-	41,41,41	0.86	0	56,56,56	2.41	22 (39%)
26	CLA	A	810	1	54,58,73	1.35	7 (12%)	64,95,113	1.36	8 (12%)
26	CLA	F	301	-	61,65,73	1.26	8 (13%)	72,103,113	1.15	4 (5%)
26	CLA	A	840	-	56,60,73	1.30	9 (16%)	65,97,113	1.39	7 (10%)
26	CLA	1	601	14	57,62,73	1.26	8 (14%)	67,100,113	1.19	5 (7%)
26	CLA	K	203	-	60,64,73	1.27	8 (13%)	71,102,113	1.36	8 (11%)
26	CLA	B	829	-	69,73,73	1.21	10 (14%)	82,113,113	1.28	7 (8%)
26	CLA	9	610	22	61,65,73	1.26	8 (13%)	72,103,113	1.24	6 (8%)
37	CHL	Z	605	24	36,50,74	4.34	18 (50%)	29,85,114	3.08	12 (41%)
29	BCR	B	847	-	41,41,41	0.91	2 (4%)	56,56,56	2.22	19 (33%)
26	CLA	Y	603	-	59,63,73	1.27	6 (10%)	70,101,113	1.38	6 (8%)
26	CLA	7	610	20	69,73,73	1.20	7 (10%)	82,113,113	1.09	5 (6%)
30	SF4	C	101	3	0,12,12	-	-	-	-	-
26	CLA	B	802	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	7 (8%)
26	CLA	Z	610	24	69,73,73	1.15	8 (11%)	82,113,113	1.16	8 (9%)
29	BCR	B	845	-	41,41,41	0.87	1 (2%)	56,56,56	2.45	24 (42%)
37	CHL	X	607	-	60,74,74	3.38	19 (31%)	58,114,114	2.36	15 (25%)
26	CLA	9	607	-	49,53,73	1.35	7 (14%)	58,89,113	1.24	4 (6%)
26	CLA	9	604	-	54,58,73	1.40	8 (14%)	65,95,113	1.27	6 (9%)
26	CLA	B	805	-	69,73,73	1.18	8 (11%)	82,113,113	1.23	8 (9%)
26	CLA	V	604	-	54,58,73	1.29	7 (12%)	64,95,113	1.30	6 (9%)
26	CLA	3	602	16	64,68,73	1.20	7 (10%)	76,107,113	1.18	8 (10%)
26	CLA	A	854	-	69,73,73	1.20	10 (14%)	82,113,113	1.30	8 (9%)
26	CLA	8	609	21	49,53,73	1.37	7 (14%)	58,89,113	1.31	4 (6%)
26	CLA	A	805	-	56,60,73	1.31	10 (17%)	65,97,113	1.47	8 (12%)
26	CLA	B	836	-	54,58,73	1.32	10 (18%)	64,95,113	1.46	7 (10%)
26	CLA	A	841	-	69,73,73	1.16	7 (10%)	82,113,113	1.18	5 (6%)
26	CLA	A	815	-	54,58,73	1.32	8 (14%)	64,95,113	1.32	5 (7%)
26	CLA	A	829	-	69,73,73	1.17	7 (10%)	82,113,113	1.32	7 (8%)
26	CLA	4	602	17	64,68,73	1.23	9 (14%)	76,107,113	1.19	6 (7%)
26	CLA	A	826	-	68,72,73	1.19	10 (14%)	80,111,113	1.25	7 (8%)
26	CLA	7	608	-	54,58,73	1.31	9 (16%)	64,95,113	1.32	6 (9%)
26	CLA	5	609	18	69,73,73	1.20	7 (10%)	82,113,113	1.18	6 (7%)
26	CLA	A	801	-	69,73,73	1.19	9 (13%)	82,113,113	1.26	7 (8%)
26	CLA	7	601	20	64,68,73	1.23	8 (12%)	76,107,113	1.28	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CHL	X	605	-	40,54,74	4.36	19 (47%)	34,90,114	2.35	10 (29%)
32	LMG	4	624	-	40,40,55	1.04	2 (5%)	48,48,63	1.16	4 (8%)
26	CLA	7	613	20	69,73,73	1.18	7 (10%)	82,113,113	1.22	4 (4%)
26	CLA	6	614	-	64,68,73	1.21	7 (10%)	76,107,113	1.16	5 (6%)
26	CLA	O	2003	-	43,48,73	1.43	8 (18%)	49,83,113	1.26	3 (6%)
28	LHG	X	2630	26	48,48,48	0.92	2 (4%)	51,54,54	1.03	3 (5%)
29	BCR	L	301	-	41,41,41	0.77	0	56,56,56	2.26	25 (44%)
34	LUT	Z	1620	-	42,43,43	0.70	0	51,60,60	1.92	14 (27%)
26	CLA	1	613	-	69,73,73	1.19	9 (13%)	82,113,113	1.12	5 (6%)
26	CLA	V	610	25	66,70,73	1.17	8 (12%)	78,109,113	1.18	7 (8%)
29	BCR	7	623	-	41,41,41	0.89	1 (2%)	56,56,56	2.03	17 (30%)
26	CLA	X	604	-	53,57,73	1.33	5 (9%)	61,93,113	1.22	5 (8%)
26	CLA	8	614	-	57,61,73	1.29	9 (15%)	67,98,113	1.29	6 (8%)
26	CLA	6	608	-	49,53,73	1.37	8 (16%)	58,89,113	1.30	6 (10%)
26	CLA	A	813	-	58,62,73	1.29	9 (15%)	68,99,113	1.29	5 (7%)
37	CHL	X	608	-	57,73,74	3.40	16 (28%)	54,112,114	2.13	18 (33%)
26	CLA	B	835	-	49,53,73	1.39	8 (16%)	58,89,113	1.30	5 (8%)
26	CLA	1	609	14	44,48,73	1.49	8 (18%)	55,83,113	1.45	7 (12%)
26	CLA	6	618	19	43,48,73	1.51	8 (18%)	51,83,113	1.39	5 (9%)
29	BCR	A	851	-	41,41,41	0.82	1 (2%)	56,56,56	2.34	24 (42%)
26	CLA	B	828	-	69,73,73	1.19	7 (10%)	82,113,113	1.15	4 (4%)
37	CHL	V	608	-	42,56,74	3.99	19 (45%)	36,92,114	3.01	13 (36%)
28	LHG	Y	2630	26	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
26	CLA	a	612	14	49,53,73	1.38	8 (16%)	58,89,113	1.35	4 (6%)
26	CLA	B	815	-	47,51,73	1.37	7 (14%)	55,86,113	1.23	3 (5%)
26	CLA	W	613	23	69,73,73	1.16	7 (10%)	82,113,113	1.12	4 (4%)
35	XAT	a	618	-	41,47,47	0.89	3 (7%)	54,74,74	2.37	25 (46%)
27	PQN	A	844	-	34,34,34	3.39	10 (29%)	43,45,45	1.99	4 (9%)
28	LHG	B	851	26	37,37,48	1.05	2 (5%)	40,43,54	1.16	4 (10%)
28	LHG	2	622	26	35,35,48	1.05	2 (5%)	38,41,54	1.18	3 (7%)
37	CHL	U	606	-	38,52,74	4.12	17 (44%)	31,87,114	3.17	12 (38%)
28	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	0.88	2 (3%)
26	CLA	5	602	18	69,73,73	1.18	8 (11%)	82,113,113	1.17	6 (7%)
26	CLA	L	306	-	43,48,73	1.42	7 (16%)	49,83,113	1.32	3 (6%)
26	CLA	2	613	15	69,73,73	1.15	6 (8%)	82,113,113	1.10	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	4	607	-	49,53,73	1.38	7 (14%)	58,89,113	1.23	4 (6%)
26	CLA	6	604	-	69,73,73	1.15	6 (8%)	82,113,113	1.07	4 (4%)
26	CLA	1	603	-	56,61,73	1.27	7 (12%)	65,98,113	1.30	3 (4%)
26	CLA	O	2001	-	41,46,73	1.49	7 (17%)	47,80,113	1.38	5 (10%)
29	BCR	B	844	-	41,41,41	0.92	3 (7%)	56,56,56	2.65	26 (46%)
26	CLA	U	602	24	63,67,73	1.22	7 (11%)	74,105,113	1.18	6 (8%)
34	LUT	V	1621	-	42,43,43	0.76	0	51,60,60	2.04	16 (31%)
26	CLA	G	203	-	46,50,73	1.38	7 (15%)	53,85,113	1.34	4 (7%)
26	CLA	J	101	10	46,50,73	1.40	7 (15%)	53,85,113	1.26	4 (7%)
34	LUT	6	619	-	42,43,43	0.75	1 (2%)	51,60,60	2.18	20 (39%)
26	CLA	a	606	-	46,52,73	1.43	8 (17%)	57,87,113	1.23	2 (3%)
26	CLA	B	824	-	69,73,73	1.18	8 (11%)	82,113,113	1.16	5 (6%)
28	LHG	8	623	-	39,39,48	1.03	2 (5%)	42,45,54	1.08	2 (4%)
29	BCR	5	622	-	41,41,41	0.91	2 (4%)	56,56,56	2.32	19 (33%)
35	XAT	4	620	-	41,47,47	0.93	3 (7%)	54,74,74	2.40	23 (42%)
26	CLA	B	806	2	69,73,73	1.20	10 (14%)	82,113,113	1.37	8 (9%)
26	CLA	8	603	-	48,52,73	1.50	8 (16%)	59,88,113	1.47	5 (8%)
35	XAT	1	618	-	41,47,47	0.90	3 (7%)	54,74,74	2.37	24 (44%)
26	CLA	5	617	-	54,58,73	1.31	9 (16%)	64,95,113	1.23	5 (7%)
26	CLA	a	613	-	58,62,73	1.29	8 (13%)	68,99,113	1.20	5 (7%)
34	LUT	V	1620	-	42,43,43	0.70	0	51,60,60	1.77	12 (23%)
29	BCR	F	305	-	41,41,41	0.86	1 (2%)	56,56,56	2.31	22 (39%)
26	CLA	Y	604	-	54,58,73	1.33	7 (12%)	64,95,113	1.21	4 (6%)
36	NEX	V	1623	-	40,46,46	1.00	3 (7%)	50,70,70	2.21	19 (38%)
26	CLA	U	610	24	60,64,73	1.23	6 (10%)	71,102,113	1.27	5 (7%)
26	CLA	B	804	-	45,49,73	1.36	8 (17%)	54,84,113	1.34	4 (7%)
26	CLA	5	603	-	58,62,73	1.35	10 (17%)	71,100,113	1.33	7 (9%)
26	CLA	U	612	24	46,50,73	1.40	6 (13%)	53,85,113	1.39	4 (7%)
29	BCR	3	621	-	41,41,41	0.84	1 (2%)	56,56,56	1.87	17 (30%)
26	CLA	4	616	17	47,51,73	1.49	8 (17%)	58,87,113	1.27	4 (6%)
26	CLA	9	612	22	44,49,73	1.41	6 (13%)	50,84,113	1.18	4 (8%)
26	CLA	2	616	-	47,51,73	1.49	8 (17%)	58,87,113	1.31	6 (10%)
26	CLA	2	609	15	49,53,73	1.40	8 (16%)	58,89,113	1.23	5 (8%)
26	CLA	A	828	-	69,73,73	1.18	8 (11%)	82,113,113	1.29	8 (9%)
26	CLA	a	602	14	65,69,73	1.23	10 (15%)	77,108,113	1.23	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	A	821	-	57,61,73	1.27	7 (12%)	67,98,113	1.28	6 (8%)
26	CLA	W	612	23	49,53,73	1.39	7 (14%)	58,89,113	1.39	5 (8%)
37	CHL	X	601	23	60,74,74	3.45	20 (33%)	58,114,114	2.15	15 (25%)
26	CLA	7	612	20	48,52,73	1.40	7 (14%)	57,88,113	1.28	4 (7%)
29	BCR	3	622	-	41,41,41	0.83	1 (2%)	56,56,56	2.24	21 (37%)
26	CLA	6	601	19	69,73,73	1.14	7 (10%)	82,113,113	1.11	6 (7%)
26	CLA	B	823	-	49,53,73	1.38	8 (16%)	58,89,113	1.32	5 (8%)
26	CLA	B	803	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
26	CLA	1	612	14	49,53,73	1.37	8 (16%)	58,89,113	1.35	3 (5%)
36	NEX	5	624	-	40,46,46	1.30	3 (7%)	50,70,70	2.29	20 (40%)
29	BCR	O	2005	-	41,41,41	0.92	1 (2%)	56,56,56	3.13	22 (39%)
26	CLA	3	606	-	57,62,73	1.26	7 (12%)	67,100,113	1.32	7 (10%)
26	CLA	3	613	16	56,61,73	1.30	8 (14%)	65,98,113	1.15	5 (7%)
26	CLA	6	609	19	49,53,73	1.39	8 (16%)	58,89,113	1.27	4 (6%)
26	CLA	A	834	-	69,73,73	1.21	10 (14%)	82,113,113	1.32	10 (12%)
26	CLA	X	602	23	69,73,73	1.16	8 (11%)	82,113,113	1.18	5 (6%)
26	CLA	K	206	11	49,53,73	1.39	7 (14%)	58,89,113	1.24	4 (6%)
26	CLA	2	603	15	47,52,73	1.41	8 (17%)	55,88,113	1.26	5 (9%)
28	LHG	5	625	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
26	CLA	Z	604	-	53,57,73	1.43	8 (15%)	64,93,113	1.31	7 (10%)
32	LMG	5	627	-	40,40,55	1.03	2 (5%)	48,48,63	1.02	3 (6%)
26	CLA	A	812	-	69,73,73	1.17	7 (10%)	82,113,113	1.16	5 (6%)
26	CLA	U	611	28	46,50,73	1.40	6 (13%)	53,85,113	1.31	3 (5%)
26	CLA	1	602	14	65,69,73	1.23	9 (13%)	77,108,113	1.24	7 (9%)
26	CLA	W	602	23	64,68,73	1.22	8 (12%)	76,107,113	1.16	7 (9%)
26	CLA	K	204	-	49,53,73	1.39	7 (14%)	58,89,113	1.43	4 (6%)
34	LUT	8	619	-	42,43,43	0.86	1 (2%)	51,60,60	1.98	12 (23%)
26	CLA	3	603	-	59,63,73	1.27	9 (15%)	70,101,113	1.36	5 (7%)
26	CLA	2	611	28	46,50,73	1.37	7 (15%)	53,85,113	1.32	4 (7%)
26	CLA	8	606	-	68,72,73	1.19	8 (11%)	81,112,113	1.11	5 (6%)
26	CLA	X	611	28	49,53,73	1.37	7 (14%)	58,89,113	1.25	4 (6%)
26	CLA	8	613	21	69,73,73	1.18	8 (11%)	82,113,113	1.13	5 (6%)
26	CLA	Z	612	24	49,53,73	1.38	7 (14%)	58,89,113	1.30	5 (8%)
28	LHG	A	847	26	29,29,48	1.17	3 (10%)	32,35,54	1.06	3 (9%)
26	CLA	V	612	25	49,53,73	1.38	7 (14%)	58,89,113	1.35	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	A	836	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	7 (8%)
26	CLA	3	611	28	41,46,73	1.54	7 (17%)	51,81,113	1.29	4 (7%)
26	CLA	A	843	-	68,72,73	1.20	9 (13%)	80,111,113	1.23	8 (10%)
31	LMU	5	629	-	33,33,36	1.21	2 (6%)	44,44,47	1.28	6 (13%)
26	CLA	2	606	-	47,51,73	1.39	8 (17%)	55,86,113	1.31	6 (10%)
28	LHG	a	620	26	42,42,48	0.99	2 (4%)	45,48,54	0.84	2 (4%)
26	CLA	8	601	21	69,73,73	1.21	7 (10%)	82,113,113	1.15	4 (4%)
36	NEX	W	1623	-	40,46,46	0.98	3 (7%)	50,70,70	2.37	13 (26%)
37	CHL	U	605	24	37,51,74	4.38	17 (45%)	30,86,114	2.59	13 (43%)
26	CLA	B	817	-	63,67,73	1.23	7 (11%)	74,105,113	1.28	5 (6%)
26	CLA	2	614	-	45,50,73	1.42	8 (17%)	52,85,113	1.31	5 (9%)
26	CLA	W	603	-	56,60,73	1.29	6 (10%)	65,97,113	1.39	7 (10%)
26	CLA	X	603	-	66,70,73	1.21	7 (10%)	78,109,113	1.28	5 (6%)
26	CLA	5	601	18	60,64,73	1.25	6 (10%)	71,102,113	1.27	4 (5%)
28	LHG	3	623	-	44,44,48	0.93	2 (4%)	47,50,54	1.02	3 (6%)
34	LUT	Y	1620	-	42,43,43	0.76	0	51,60,60	3.19	19 (37%)
26	CLA	L	303	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	8 (9%)
26	CLA	B	841	28	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
26	CLA	5	606	-	43,48,73	1.45	7 (16%)	49,83,113	1.27	4 (8%)
26	CLA	8	611	28	46,50,73	1.39	6 (13%)	53,85,113	1.26	3 (5%)
37	CHL	U	607	-	40,54,74	4.17	19 (47%)	34,90,114	2.55	12 (35%)
26	CLA	2	607	-	47,52,73	1.38	8 (17%)	55,88,113	1.34	5 (9%)
29	BCR	A	848	-	41,41,41	1.05	3 (7%)	56,56,56	2.25	16 (28%)
26	CLA	7	602	20	69,73,73	1.21	9 (13%)	82,113,113	1.20	7 (8%)
32	LMG	A	860	-	40,40,55	1.01	2 (5%)	48,48,63	1.10	4 (8%)
32	LMG	V	2631	-	55,55,55	0.88	2 (3%)	63,63,63	1.12	5 (7%)
26	CLA	5	616	18	44,50,73	1.53	10 (22%)	57,85,113	1.30	5 (8%)
26	CLA	4	608	-	69,73,73	1.16	6 (8%)	82,113,113	1.16	6 (7%)
26	CLA	Y	614	-	52,56,73	1.32	7 (13%)	61,92,113	1.25	5 (8%)
26	CLA	A	845	28	54,58,73	1.32	9 (16%)	64,95,113	1.35	6 (9%)
26	CLA	B	840	-	69,73,73	1.23	8 (11%)	82,113,113	1.24	4 (4%)
26	CLA	A	838	-	54,58,73	1.33	10 (18%)	64,95,113	1.34	5 (7%)
26	CLA	6	617	-	49,53,73	1.36	7 (14%)	58,89,113	1.26	5 (8%)
34	LUT	4	619	-	42,43,43	0.80	1 (2%)	51,60,60	2.14	17 (33%)
26	CLA	8	616	21	47,51,73	1.50	7 (14%)	58,87,113	1.35	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	8	602	21	64,68,73	1.24	8 (12%)	76,107,113	1.30	8 (10%)
26	CLA	B	809	2	69,73,73	1.20	8 (11%)	82,113,113	1.26	5 (6%)
26	CLA	H	203	-	69,73,73	1.16	7 (10%)	82,113,113	1.21	4 (4%)
26	CLA	a	608	-	47,52,73	1.40	7 (14%)	55,88,113	1.27	5 (9%)
28	LHG	V	2630	26	35,35,48	1.07	2 (5%)	38,41,54	1.09	2 (5%)
26	CLA	a	609	14	67,72,73	1.18	6 (8%)	79,112,113	1.15	4 (5%)
26	CLA	6	602	19	69,73,73	1.18	8 (11%)	82,113,113	1.16	6 (7%)
26	CLA	Y	602	24	62,66,73	1.22	7 (11%)	73,104,113	1.22	7 (9%)
26	CLA	B	822	-	46,50,73	1.37	8 (17%)	53,85,113	1.25	3 (5%)
32	LMG	9	625	-	55,55,55	0.89	2 (3%)	63,63,63	1.04	6 (9%)
26	CLA	B	816	-	58,62,73	1.24	8 (13%)	68,99,113	1.28	6 (8%)
26	CLA	5	613	18	68,72,73	1.14	8 (11%)	80,111,113	1.25	7 (8%)
26	CLA	A	822	-	69,73,73	1.21	10 (14%)	82,113,113	1.24	8 (9%)
26	CLA	V	602	25	64,68,73	1.19	7 (10%)	76,107,113	1.21	6 (7%)
28	LHG	4	622	26	48,48,48	0.91	2 (4%)	51,54,54	0.83	2 (3%)
37	CHL	Z	608	-	43,57,74	4.06	20 (46%)	37,93,114	2.41	12 (32%)
26	CLA	9	609	22	65,69,73	1.21	7 (10%)	77,108,113	1.19	4 (5%)
26	CLA	5	619	-	47,51,73	1.53	8 (17%)	58,87,113	1.40	7 (12%)
26	CLA	U	604	-	52,56,73	1.45	9 (17%)	61,91,113	1.34	8 (13%)
26	CLA	B	837	-	69,73,73	1.19	9 (13%)	82,113,113	1.29	7 (8%)
29	BCR	2	623	-	41,41,41	0.88	1 (2%)	56,56,56	2.38	22 (39%)
26	CLA	1	608	-	47,52,73	1.40	8 (17%)	55,88,113	1.26	5 (9%)
33	DGD	B	850	-	63,63,67	0.84	2 (3%)	77,77,81	1.25	7 (9%)
26	CLA	a	614	-	58,62,73	1.27	8 (13%)	65,99,113	1.27	4 (6%)
26	CLA	1	616	14	47,51,73	1.49	7 (14%)	58,87,113	1.41	7 (12%)
26	CLA	a	604	-	53,57,73	1.30	7 (13%)	61,93,113	1.24	4 (6%)
28	LHG	H	204	-	48,48,48	0.93	2 (4%)	51,54,54	0.95	2 (3%)
28	LHG	Z	2630	26	48,48,48	0.93	2 (4%)	51,54,54	0.97	2 (3%)
35	XAT	X	1622	-	41,47,47	0.89	1 (2%)	54,74,74	2.52	21 (38%)
26	CLA	L	304	-	49,53,73	1.36	6 (12%)	58,89,113	1.27	5 (8%)
26	CLA	3	610	16	69,73,73	1.18	7 (10%)	82,113,113	1.13	6 (7%)
29	BCR	4	621	-	41,41,41	0.86	1 (2%)	56,56,56	2.05	17 (30%)
28	LHG	W	2630	26	33,33,48	1.14	2 (6%)	36,39,54	1.19	3 (8%)
29	BCR	K	207	-	41,41,41	0.84	1 (2%)	56,56,56	2.80	22 (39%)
26	CLA	A	818	-	64,68,73	1.21	9 (14%)	76,107,113	1.25	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LMG	8	626	-	46,46,55	0.97	3 (6%)	54,54,63	1.11	4 (7%)
35	XAT	Y	1622	-	41,47,47	0.90	2 (4%)	54,74,74	2.66	22 (40%)
28	LHG	9	622	26	29,29,48	1.18	2 (6%)	32,35,54	1.04	1 (3%)
26	CLA	3	608	-	59,63,73	1.28	9 (15%)	70,101,113	1.16	3 (4%)
26	CLA	Z	613	24	69,73,73	1.18	7 (10%)	82,113,113	1.18	5 (6%)
26	CLA	4	613	17	69,73,73	1.20	9 (13%)	82,113,113	1.26	7 (8%)
26	CLA	A	809	1	69,73,73	1.19	9 (13%)	82,113,113	1.29	7 (8%)
35	XAT	9	620	-	41,47,47	0.95	3 (7%)	54,74,74	2.40	19 (35%)
26	CLA	A	842	-	69,73,73	1.22	9 (13%)	82,113,113	1.33	10 (12%)
37	CHL	U	601	24	60,74,74	3.49	19 (31%)	58,114,114	1.94	13 (22%)
36	NEX	6	624	-	40,46,46	1.25	5 (12%)	50,70,70	2.50	18 (36%)
26	CLA	2	601	15	69,73,73	1.14	9 (13%)	82,113,113	1.32	7 (8%)
26	CLA	B	813	-	69,73,73	1.21	10 (14%)	82,113,113	1.19	6 (7%)
26	CLA	B	819	-	59,63,73	1.27	7 (11%)	70,101,113	1.19	8 (11%)
26	CLA	5	611	28	46,50,73	1.37	6 (13%)	53,85,113	1.23	4 (7%)
26	CLA	B	833	-	69,73,73	1.16	7 (10%)	82,113,113	1.13	6 (7%)
35	XAT	3	619	-	41,47,47	0.94	3 (7%)	54,74,74	2.51	20 (37%)
26	CLA	Z	603	-	59,63,73	1.26	7 (11%)	70,101,113	1.40	8 (11%)
28	LHG	3	624	26	48,48,48	0.91	2 (4%)	51,54,54	0.98	3 (5%)
26	CLA	6	613	-	67,72,73	1.21	8 (11%)	79,112,113	1.19	8 (10%)
31	LMU	8	625	-	36,36,36	1.10	2 (5%)	47,47,47	1.25	3 (6%)
29	BCR	B	853	-	41,41,41	0.84	2 (4%)	56,56,56	1.82	14 (25%)
26	CLA	B	820	-	54,58,73	1.31	9 (16%)	64,95,113	1.35	5 (7%)
27	PQN	B	842	-	34,34,34	3.42	8 (23%)	43,45,45	1.94	7 (16%)
26	CLA	A	804	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
37	CHL	W	607	-	59,73,74	3.31	19 (32%)	59,113,114	1.90	16 (27%)
26	CLA	A	837	1	49,53,73	1.42	9 (18%)	58,89,113	1.46	4 (6%)
26	CLA	Z	611	28	46,50,73	1.46	8 (17%)	56,85,113	1.37	6 (10%)
26	CLA	B	807	-	56,60,73	1.35	10 (17%)	65,97,113	1.37	6 (9%)
34	LUT	3	618	-	42,43,43	0.82	1 (2%)	51,60,60	2.11	13 (25%)
26	CLA	X	613	23	69,73,73	1.16	7 (10%)	82,113,113	1.12	4 (4%)
26	CLA	A	824	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
26	CLA	9	603	22	48,52,73	1.51	11 (22%)	59,88,113	1.36	4 (6%)
26	CLA	B	839	-	69,73,73	1.18	9 (13%)	82,113,113	1.14	6 (7%)
32	LMG	4	623	-	40,40,55	1.08	2 (5%)	48,48,63	1.16	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CHL	Z	607	-	60,74,74	3.42	19 (31%)	58,114,114	2.07	12 (20%)
30	SF4	C	102	3	0,12,12	-	-	-	-	-
28	LHG	1	620	26	48,48,48	0.93	2 (4%)	51,54,54	0.80	2 (3%)
29	BCR	L	308	-	41,41,41	0.82	0	56,56,56	2.36	23 (41%)
26	CLA	B	811	-	56,60,73	1.46	10 (17%)	70,97,113	1.32	8 (11%)
26	CLA	A	839	-	59,63,73	1.29	8 (13%)	70,101,113	1.30	6 (8%)
32	LMG	L	2631	-	37,37,55	1.08	2 (5%)	45,45,63	1.19	4 (8%)
34	LUT	W	1621	-	42,43,43	0.64	0	51,60,60	1.84	14 (27%)
26	CLA	A	817	-	49,53,73	1.40	8 (16%)	58,89,113	1.37	6 (10%)
26	CLA	5	607	-	69,73,73	1.17	8 (11%)	82,113,113	1.19	5 (6%)
28	LHG	O	2631	-	35,35,48	1.07	2 (5%)	38,41,54	1.13	3 (7%)
28	LHG	A	861	-	48,48,48	0.94	2 (4%)	51,54,54	1.01	2 (3%)
29	BCR	9	621	-	41,41,41	0.72	0	56,56,56	2.94	18 (32%)
26	CLA	O	2002	-	41,46,73	1.56	8 (19%)	51,81,113	1.34	7 (13%)
26	CLA	V	603	-	49,53,73	1.37	6 (12%)	58,89,113	1.45	4 (6%)
37	CHL	Y	606	-	40,54,74	4.07	19 (47%)	34,90,114	2.92	14 (41%)
26	CLA	V	611	28	47,51,73	1.39	7 (14%)	55,86,113	1.22	3 (5%)
37	CHL	V	605	25	38,52,74	4.27	18 (47%)	31,87,114	2.80	13 (41%)
31	LMU	A	857	-	36,36,36	1.09	2 (5%)	47,47,47	1.38	8 (17%)
26	CLA	5	610	18	58,62,73	1.26	8 (13%)	68,99,113	1.20	5 (7%)
28	LHG	8	622	26	48,48,48	0.91	2 (4%)	51,54,54	0.87	2 (3%)
34	LUT	U	1620	-	42,43,43	0.70	0	51,60,60	1.71	11 (21%)
26	CLA	6	616	19	69,73,73	1.17	9 (13%)	82,113,113	1.28	9 (10%)
28	LHG	5	623	26	48,48,48	0.93	2 (4%)	51,54,54	0.88	2 (3%)
28	LHG	9	623	-	48,48,48	0.91	2 (4%)	51,54,54	0.97	2 (3%)
34	LUT	1	617	-	42,43,43	0.78	1 (2%)	51,60,60	2.04	18 (35%)
29	BCR	1	619	-	41,41,41	0.85	0	56,56,56	2.41	22 (39%)
26	CLA	Z	614	-	52,56,73	1.34	6 (11%)	61,92,113	1.25	4 (6%)
26	CLA	V	614	-	49,53,73	1.36	7 (14%)	58,89,113	1.30	4 (6%)
26	CLA	5	608	-	54,58,73	1.33	7 (12%)	63,95,113	1.18	4 (6%)
26	CLA	7	607	-	46,50,73	1.37	7 (15%)	53,85,113	1.19	3 (5%)

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
26	CLA	Y	612	24	1/1/11/20	6/15/91/115	-
26	CLA	A	808	-	1/1/12/20	1/21/97/115	-
26	CLA	4	606	-	1/1/10/20	4/8/84/115	-
29	BCR	3	620	-	-	4/29/63/63	0/2/2/2
26	CLA	9	611	28	1/1/10/20	3/12/88/115	-
26	CLA	Z	602	24	1/1/13/20	7/31/107/115	-
26	CLA	B	832	-	1/1/14/20	12/33/109/115	-
34	LUT	W	1620	-	-	6/29/67/67	0/2/2/2
26	CLA	A	811	-	1/1/15/20	11/39/115/115	-
31	LMU	K	208	-	-	10/21/61/61	0/2/2/2
26	CLA	3	612	16	1/1/10/20	4/13/89/115	-
26	CLA	a	601	14	-	4/25/101/115	-
34	LUT	Y	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	X	614	-	1/1/10/20	4/12/88/115	-
35	XAT	V	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	9	602	22	1/1/14/20	6/33/109/115	-
29	BCR	6	622	-	-	2/29/63/63	0/2/2/2
37	CHL	V	607	-	3/3/16/26	8/15/113/137	-
29	BCR	B	852	-	-	6/29/63/63	0/2/2/2
36	NEX	Z	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	A	823	-	1/1/10/20	3/12/88/115	-
29	BCR	B	801	-	-	2/29/63/63	0/2/2/2
26	CLA	a	616	14	1/1/11/20	5/15/91/115	-
26	CLA	A	803	-	1/1/15/20	8/39/115/115	-
26	CLA	7	604	-	1/1/12/20	7/21/97/115	-
26	CLA	8	612	21	1/1/10/20	2/10/86/115	-
37	CHL	X	609	23	3/3/20/26	22/39/137/137	-
35	XAT	U	1622	-	-	4/31/93/93	0/4/4/4
29	BCR	L	309	-	-	3/29/63/63	0/2/2/2
26	CLA	4	618	17	1/1/10/20	2/8/84/115	-
31	LMU	A	858	-	-	10/21/57/61	0/2/2/2
28	LHG	6	623	26	-	19/52/52/53	-
29	BCR	O	2004	-	-	2/29/63/63	0/2/2/2
26	CLA	6	603	-	1/1/12/20	6/22/98/115	-
26	CLA	2	612	15	1/1/11/20	7/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	XAT	5	621	-	-	0/31/93/93	0/4/4/4
37	CHL	W	605	23	3/3/16/26	8/15/113/137	-
37	CHL	Y	609	24	3/3/20/26	16/39/137/137	-
26	CLA	A	807	1	1/1/15/20	19/39/115/115	-
26	CLA	Y	613	24	-	14/39/115/115	-
26	CLA	1	610	14	1/1/9/20	3/8/80/115	-
26	CLA	3	604	-	1/1/15/20	6/39/115/115	-
35	XAT	7	620	-	-	0/31/93/93	0/4/4/4
26	CLA	6	611	28	1/1/10/20	3/12/88/115	-
26	CLA	W	610	23	1/1/13/20	6/27/103/115	-
26	CLA	F	304	6	-	4/10/86/115	-
26	CLA	1	611	28	1/1/13/20	5/30/106/115	-
26	CLA	5	612	18	1/1/10/20	2/10/86/115	-
26	CLA	4	604	-	1/1/13/20	7/25/101/115	-
37	CHL	Z	601	24	3/3/20/26	18/39/137/137	-
28	LHG	U	2630	26	-	20/53/53/53	-
26	CLA	W	614	-	1/1/11/20	7/15/91/115	-
37	CHL	W	601	23	3/3/20/26	21/39/137/137	-
26	CLA	H	202	-	1/1/10/20	4/6/82/115	-
26	CLA	2	604	-	1/1/10/20	3/11/87/115	-
26	CLA	3	615	-	1/1/10/20	3/8/84/115	-
26	CLA	K	201	11	1/1/11/20	6/15/91/115	-
26	CLA	F	303	-	-	6/12/88/115	-
29	BCR	J	102	-	-	2/29/63/63	0/2/2/2
26	CLA	A	814	-	1/1/15/20	17/39/115/115	-
26	CLA	A	806	-	1/1/15/20	11/39/115/115	-
26	CLA	X	612	23	1/1/10/20	8/13/89/115	-
26	CLA	B	827	-	1/1/14/20	11/36/112/115	-
26	CLA	Y	611	28	1/1/10/20	8/13/89/115	-
36	NEX	U	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	V	613	25	1/1/15/20	18/39/115/115	-
26	CLA	U	613	24	1/1/13/20	11/32/108/115	-
26	CLA	B	818	-	-	11/33/109/115	-
26	CLA	4	610	17	1/1/14/20	7/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	7	622	26	-	18/41/41/53	-
30	SF4	A	853	1,2	-	-	0/6/5/5
34	LUT	9	619	-	-	4/29/67/67	0/2/2/2
37	CHL	V	601	25	3/3/20/26	9/39/137/137	-
37	CHL	Y	607	-	3/3/20/26	19/39/137/137	-
35	XAT	2	620	-	-	0/31/93/93	0/4/4/4
26	CLA	6	607	-	1/1/10/20	0/10/86/115	-
35	XAT	Z	1622	-	-	4/31/93/93	0/4/4/4
35	XAT	W	1622	-	-	1/31/93/93	0/4/4/4
29	BCR	B	848	-	-	4/29/63/63	0/2/2/2
26	CLA	A	802	-	1/1/15/20	11/39/115/115	-
26	CLA	7	616	20	1/1/11/20	6/11/87/115	-
26	CLA	9	601	22	1/1/11/20	6/15/91/115	-
26	CLA	9	613	22	1/1/15/20	12/39/115/115	-
26	CLA	8	607	-	1/1/10/20	2/10/86/115	-
26	CLA	W	604	-	1/1/11/20	4/18/94/115	-
26	CLA	4	614	-	-	10/29/105/115	-
35	XAT	6	621	-	-	0/31/93/93	0/4/4/4
26	CLA	5	604	-	1/1/15/20	10/35/111/115	-
26	CLA	6	612	19	1/1/10/20	4/10/86/115	-
37	CHL	Z	606	-	3/3/16/26	7/15/113/137	-
26	CLA	A	835	-	-	12/35/111/115	-
37	CHL	V	609	25	3/3/19/26	14/33/131/137	-
26	CLA	B	830	-	1/1/10/20	4/13/89/115	-
26	CLA	a	611	28	1/1/10/20	0/4/80/115	-
34	LUT	U	1621	-	-	5/29/67/67	0/2/2/2
26	CLA	2	610	15	1/1/13/20	4/27/103/115	-
31	LMU	1	621	-	-	7/21/61/61	0/2/2/2
26	CLA	a	603	-	1/1/12/20	9/25/101/115	-
31	LMU	5	628	-	-	10/19/59/61	0/2/2/2
26	CLA	X	610	23	1/1/15/20	12/39/115/115	-
26	CLA	B	810	-	1/1/14/20	18/37/113/115	-
26	CLA	B	831	-	1/1/15/20	12/39/115/115	-
26	CLA	8	608	-	-	7/23/99/115	-
26	CLA	W	611	28	1/1/13/20	9/30/106/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	L	305	-	-	2/29/63/63	0/2/2/2
26	CLA	9	614	-	1/1/11/20	5/15/91/115	-
29	BCR	B	843	-	-	4/29/63/63	0/2/2/2
26	CLA	A	819	-	1/1/13/20	5/32/108/115	-
26	CLA	A	827	-	1/1/13/20	5/31/107/115	-
26	CLA	A	833	-	1/1/11/20	5/15/91/115	-
37	CHL	X	606	-	3/3/15/26	4/13/111/137	-
26	CLA	9	606	-	1/1/10/20	3/8/84/115	-
26	CLA	7	609	20	1/1/10/20	6/12/88/115	-
26	CLA	B	814	-	1/1/14/20	13/38/114/115	-
34	LUT	7	619	-	-	2/29/67/67	0/2/2/2
29	BCR	A	849	-	-	5/29/63/63	0/2/2/2
26	CLA	a	607	-	1/1/11/20	6/15/91/115	-
37	CHL	W	606	-	3/3/16/26	1/15/113/137	-
26	CLA	A	820	-	1/1/15/20	7/39/115/115	-
26	CLA	6	610	19	1/1/15/20	11/39/115/115	-
26	CLA	Y	610	24	1/1/15/20	10/39/115/115	-
36	NEX	X	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	7	606	-	1/1/10/20	2/10/86/115	-
26	CLA	B	812	-	1/1/10/20	4/13/89/115	-
26	CLA	5	614	-	1/1/10/20	8/15/87/115	-
37	CHL	Y	605	24	3/3/15/26	2/10/108/137	-
26	CLA	1	614	-	1/1/9/20	0/4/76/115	-
29	BCR	A	856	-	-	2/29/63/63	0/2/2/2
29	BCR	A	850	-	-	2/29/63/63	0/2/2/2
29	BCR	B	846	-	-	0/29/63/63	0/2/2/2
26	CLA	1	606	-	1/1/8/20	3/7/79/115	-
26	CLA	8	610	21	1/1/14/20	9/33/109/115	-
29	BCR	A	852	-	-	8/29/63/63	0/2/2/2
29	BCR	7	621	-	-	2/29/63/63	0/2/2/2
26	CLA	4	612	17	1/1/10/20	3/10/86/115	-
26	CLA	A	830	-	1/1/15/20	13/39/115/115	-
26	CLA	7	603	-	1/1/11/20	6/13/89/115	-
37	CHL	Y	608	-	3/3/16/26	6/19/117/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	3	609	16	1/1/14/20	14/33/109/115	-
36	NEX	Y	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	L	307	8	1/1/10/20	2/8/84/115	-
26	CLA	1	607	-	1/1/10/20	4/8/84/115	-
32	LMG	J	104	-	-	12/35/55/70	0/1/1/1
26	CLA	4	609	17	1/1/13/20	4/30/106/115	-
26	CLA	6	620	-	1/1/14/20	11/37/113/115	-
29	BCR	B	849	-	-	5/29/63/63	0/2/2/2
26	CLA	A	831	-	1/1/15/20	17/39/115/115	-
26	CLA	6	606	-	1/1/10/20	2/8/84/115	-
37	CHL	U	609	24	3/3/18/26	14/32/130/137	-
26	CLA	7	611	28	1/1/13/20	4/31/107/115	-
29	BCR	8	621	-	-	2/29/63/63	0/2/2/2
26	CLA	B	834	-	1/1/14/20	4/33/109/115	-
26	CLA	5	618	18	1/1/10/20	3/8/84/115	-
32	LMG	H	205	-	-	14/50/70/70	0/1/1/1
34	LUT	X	1621	-	-	3/29/67/67	0/2/2/2
29	BCR	K	202	-	-	4/29/63/63	0/2/2/2
34	LUT	2	619	-	-	2/29/67/67	0/2/2/2
34	LUT	a	617	-	-	4/29/67/67	0/2/2/2
26	CLA	1	604	-	1/1/11/20	6/20/96/115	-
26	CLA	A	832	-	1/1/12/20	11/21/97/115	-
32	LMG	J	103	-	-	10/37/57/70	0/1/1/1
37	CHL	Z	609	24	3/3/20/26	17/39/137/137	-
26	CLA	4	603	17	1/1/11/20	4/13/89/115	-
26	CLA	2	602	15	1/1/15/20	17/49/99/115	-
37	CHL	W	609	23	3/3/20/26	12/39/137/137	-
28	LHG	9	624	-	-	17/53/53/53	-
26	CLA	G	204	7	1/1/11/20	7/15/91/115	-
34	LUT	Z	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	7	614	-	1/1/10/20	3/12/88/115	-
34	LUT	X	1620	-	-	4/29/67/67	0/2/2/2
26	CLA	B	821	-	1/1/11/20	6/13/89/115	-
26	CLA	8	604	-	1/1/12/20	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	U	603	-	1/1/12/20	9/24/100/115	-
37	CHL	Y	601	24	3/3/20/26	19/39/137/137	-
26	CLA	B	808	-	1/1/15/20	13/39/115/115	-
26	CLA	B	838	-	1/1/11/20	2/17/93/115	-
26	CLA	4	611	28	1/1/10/20	6/12/88/115	-
34	LUT	5	620	-	-	0/29/67/67	0/2/2/2
26	CLA	A	816	-	1/1/15/20	14/39/115/115	-
26	CLA	B	825	-	-	3/20/96/115	-
26	CLA	B	826	-	1/1/14/20	11/36/112/115	-
26	CLA	a	610	14	1/1/14/20	8/31/107/115	-
26	CLA	L	302	12	1/1/11/20	6/15/91/115	-
37	CHL	V	606	-	3/3/15/26	5/13/111/137	-
26	CLA	7	615	-	1/1/10/20	6/8/84/115	-
35	XAT	8	620	-	-	0/31/93/93	0/4/4/4
26	CLA	A	825	-	1/1/15/20	16/39/115/115	-
26	CLA	3	607	16	1/1/13/20	6/28/104/115	-
26	CLA	3	617	16	1/1/10/20	0/8/84/115	-
37	CHL	W	608	-	3/3/16/26	9/17/115/137	-
26	CLA	4	601	17	1/1/15/20	15/39/115/115	-
37	CHL	U	608	-	3/3/15/26	5/13/111/137	-
29	BCR	G	205	-	-	2/29/63/63	0/2/2/2
26	CLA	3	614	-	1/1/10/20	2/8/84/115	-
26	CLA	U	614	-	1/1/10/20	5/12/88/115	-
29	BCR	a	619	-	-	2/29/63/63	0/2/2/2
26	CLA	A	810	1	-	7/21/97/115	-
26	CLA	F	301	-	1/1/13/20	13/30/106/115	-
26	CLA	A	840	-	-	7/24/100/115	-
26	CLA	9	610	22	1/1/13/20	5/30/106/115	-
26	CLA	K	203	-	-	10/29/105/115	-
26	CLA	B	829	-	1/1/15/20	9/39/115/115	-
26	CLA	1	601	14	-	4/25/101/115	-
37	CHL	Z	605	24	3/3/15/26	4/10/108/137	-
29	BCR	B	847	-	-	2/29/63/63	0/2/2/2
26	CLA	Y	603	-	1/1/13/20	12/27/103/115	-
26	CLA	7	610	20	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SF4	C	101	3	-	-	0/6/5/5
26	CLA	B	802	-	1/1/15/20	17/39/115/115	-
26	CLA	Z	610	24	1/1/15/20	9/39/115/115	-
29	BCR	B	845	-	-	9/29/63/63	0/2/2/2
37	CHL	X	607	-	3/3/20/26	23/39/137/137	-
26	CLA	9	607	-	-	9/15/91/115	-
26	CLA	9	604	-	1/1/12/20	8/20/96/115	-
26	CLA	B	805	-	1/1/15/20	9/39/115/115	-
26	CLA	V	604	-	1/1/12/20	7/21/97/115	-
26	CLA	3	602	16	1/1/14/20	4/33/109/115	-
26	CLA	A	854	-	1/1/15/20	7/39/115/115	-
26	CLA	8	609	21	1/1/11/20	2/15/91/115	-
26	CLA	A	805	-	-	6/24/100/115	-
26	CLA	B	836	-	1/1/12/20	5/21/97/115	-
26	CLA	A	841	-	1/1/15/20	15/39/115/115	-
26	CLA	A	815	-	1/1/12/20	11/21/97/115	-
26	CLA	A	829	-	1/1/15/20	10/39/115/115	-
26	CLA	4	602	17	1/1/14/20	8/33/109/115	-
26	CLA	A	826	-	1/1/14/20	8/37/113/115	-
26	CLA	7	608	-	-	4/21/97/115	-
26	CLA	5	609	18	1/1/15/20	12/39/115/115	-
26	CLA	A	801	-	1/1/15/20	10/39/115/115	-
26	CLA	7	601	20	1/1/14/20	6/33/109/115	-
37	CHL	X	605	-	3/3/16/26	9/15/113/137	-
32	LMG	4	624	-	-	5/35/55/70	0/1/1/1
26	CLA	7	613	20	1/1/15/20	15/39/115/115	-
26	CLA	6	614	-	1/1/14/20	8/33/109/115	-
26	CLA	O	2003	-	1/1/10/20	5/8/84/115	-
28	LHG	X	2630	26	-	12/53/53/53	-
29	BCR	L	301	-	-	4/29/63/63	0/2/2/2
34	LUT	Z	1620	-	-	5/29/67/67	0/2/2/2
26	CLA	1	613	-	1/1/15/20	15/39/115/115	-
26	CLA	V	610	25	1/1/14/20	9/36/112/115	-
29	BCR	7	623	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	X	604	-	1/1/11/20	11/20/96/115	-
26	CLA	8	614	-	1/1/12/20	6/25/101/115	-
26	CLA	A	813	-	1/1/12/20	7/26/102/115	-
26	CLA	6	608	-	-	8/15/91/115	-
37	CHL	X	608	-	3/3/19/26	21/39/133/137	-
26	CLA	B	835	-	1/1/11/20	2/15/91/115	-
26	CLA	1	609	14	1/1/10/20	2/8/84/115	-
26	CLA	6	618	19	1/1/10/20	1/8/84/115	-
29	BCR	A	851	-	-	2/29/63/63	0/2/2/2
26	CLA	B	828	-	1/1/15/20	14/39/115/115	-
37	CHL	V	608	-	3/3/16/26	4/18/116/137	-
28	LHG	Y	2630	26	-	12/53/53/53	-
26	CLA	a	612	14	1/1/11/20	4/15/91/115	-
26	CLA	B	815	-	1/1/10/20	2/13/89/115	-
26	CLA	W	613	23	1/1/15/20	20/39/115/115	-
35	XAT	a	618	-	-	0/31/93/93	0/4/4/4
27	PQN	A	844	-	-	7/23/43/43	0/2/2/2
28	LHG	B	851	26	-	13/42/42/53	-
28	LHG	2	622	26	-	9/40/40/53	-
37	CHL	U	606	-	3/3/15/26	6/13/111/137	-
28	LHG	A	846	-	-	15/53/53/53	-
26	CLA	5	602	18	1/1/15/20	8/39/115/115	-
26	CLA	L	306	-	1/1/10/20	1/8/84/115	-
26	CLA	2	613	15	1/1/15/20	9/39/115/115	-
26	CLA	4	607	-	1/1/11/20	5/15/91/115	-
26	CLA	6	604	-	1/1/15/20	14/39/115/115	-
26	CLA	1	603	-	1/1/12/20	7/23/99/115	-
26	CLA	O	2001	-	1/1/9/20	2/6/78/115	-
29	BCR	B	844	-	-	2/29/63/63	0/2/2/2
26	CLA	U	602	24	1/1/13/20	17/32/108/115	-
34	LUT	V	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	G	203	-	1/1/10/20	4/12/88/115	-
26	CLA	J	101	10	1/1/10/20	5/12/88/115	-
34	LUT	6	619	-	-	4/29/67/67	0/2/2/2
26	CLA	a	606	-	1/1/10/20	8/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	824	-	1/1/15/20	13/39/115/115	-
28	LHG	8	623	-	-	10/44/44/53	-
29	BCR	5	622	-	-	1/29/63/63	0/2/2/2
35	XAT	4	620	-	-	2/31/93/93	0/4/4/4
26	CLA	B	806	2	1/1/15/20	18/39/115/115	-
26	CLA	8	603	-	1/1/11/20	5/13/89/115	-
35	XAT	1	618	-	-	0/31/93/93	0/4/4/4
26	CLA	5	617	-	1/1/12/20	10/21/97/115	-
26	CLA	a	613	-	1/1/12/20	7/26/102/115	-
34	LUT	V	1620	-	-	4/29/67/67	0/2/2/2
29	BCR	F	305	-	-	6/29/63/63	0/2/2/2
26	CLA	Y	604	-	1/1/12/20	8/21/97/115	-
36	NEX	V	1623	-	-	7/27/83/83	0/3/3/3
26	CLA	U	610	24	1/1/13/20	4/29/105/115	-
26	CLA	B	804	-	1/1/10/20	2/10/86/115	-
26	CLA	5	603	-	1/1/13/20	5/25/101/115	-
26	CLA	U	612	24	1/1/10/20	4/12/88/115	-
29	BCR	3	621	-	-	0/29/63/63	0/2/2/2
26	CLA	4	616	17	1/1/11/20	4/11/87/115	-
26	CLA	9	612	22	1/1/10/20	2/10/86/115	-
26	CLA	2	616	-	1/1/11/20	2/11/87/115	-
26	CLA	2	609	15	1/1/11/20	3/15/91/115	-
26	CLA	A	828	-	1/1/15/20	16/39/115/115	-
26	CLA	a	602	14	1/1/14/20	4/35/111/115	-
26	CLA	A	821	-	-	13/25/101/115	-
26	CLA	W	612	23	1/1/11/20	7/15/91/115	-
37	CHL	X	601	23	3/3/20/26	14/39/137/137	-
26	CLA	7	612	20	1/1/11/20	4/13/89/115	-
29	BCR	3	622	-	-	2/29/63/63	0/2/2/2
26	CLA	6	601	19	1/1/15/20	16/39/115/115	-
26	CLA	B	823	-	1/1/11/20	5/15/91/115	-
26	CLA	B	803	-	1/1/15/20	11/39/115/115	-
26	CLA	1	612	14	1/1/11/20	4/15/91/115	-
36	NEX	5	624	-	-	2/27/83/83	0/3/3/3
29	BCR	O	2005	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	3	606	-	1/1/13/20	3/25/101/115	-
26	CLA	3	613	16	1/1/12/20	8/23/99/115	-
26	CLA	6	609	19	1/1/11/20	7/15/91/115	-
26	CLA	A	834	-	1/1/15/20	12/39/115/115	-
26	CLA	X	602	23	1/1/15/20	9/39/115/115	-
26	CLA	K	206	11	1/1/11/20	6/15/91/115	-
26	CLA	2	603	15	1/1/11/20	7/13/89/115	-
28	LHG	5	625	-	-	12/53/53/53	-
26	CLA	Z	604	-	1/1/11/20	4/21/93/115	-
32	LMG	5	627	-	-	7/35/55/70	0/1/1/1
26	CLA	A	812	-	1/1/15/20	9/39/115/115	-
26	CLA	U	611	28	1/1/10/20	2/12/88/115	-
26	CLA	1	602	14	1/1/14/20	4/35/111/115	-
26	CLA	W	602	23	1/1/14/20	12/33/109/115	-
26	CLA	K	204	-	1/1/11/20	5/15/91/115	-
34	LUT	8	619	-	-	4/29/67/67	0/2/2/2
26	CLA	3	603	-	1/1/13/20	10/27/103/115	-
26	CLA	2	611	28	1/1/10/20	2/12/88/115	-
26	CLA	8	606	-	1/1/15/20	5/37/113/115	-
26	CLA	X	611	28	1/1/11/20	4/15/91/115	-
26	CLA	8	613	21	1/1/15/20	14/39/115/115	-
26	CLA	Z	612	24	1/1/11/20	7/15/91/115	-
28	LHG	A	847	26	-	6/34/34/53	-
26	CLA	V	612	25	1/1/11/20	6/15/91/115	-
26	CLA	A	836	-	1/1/15/20	9/39/115/115	-
26	CLA	3	611	28	1/1/10/20	2/4/80/115	-
26	CLA	A	843	-	1/1/14/20	13/37/113/115	-
31	LMU	5	629	-	-	11/18/58/61	0/2/2/2
26	CLA	2	606	-	1/1/10/20	2/13/89/115	-
28	LHG	a	620	26	-	7/47/47/53	-
26	CLA	8	601	21	1/1/15/20	15/39/115/115	-
36	NEX	W	1623	-	-	6/27/83/83	0/3/3/3
37	CHL	U	605	24	3/3/15/26	2/12/110/137	-
26	CLA	B	817	-	1/1/13/20	8/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	2	614	-	1/1/10/20	0/11/87/115	-
26	CLA	W	603	-	1/1/12/20	9/24/100/115	-
26	CLA	X	603	-	1/1/14/20	15/36/112/115	-
26	CLA	5	601	18	1/1/13/20	3/29/105/115	-
28	LHG	3	623	-	-	15/49/49/53	-
34	LUT	Y	1620	-	-	5/29/67/67	0/2/2/2
26	CLA	L	303	-	-	12/39/115/115	-
26	CLA	B	841	28	1/1/15/20	13/39/115/115	-
26	CLA	5	606	-	-	3/8/84/115	-
26	CLA	8	611	28	1/1/10/20	6/12/88/115	-
37	CHL	U	607	-	3/3/16/26	8/15/113/137	-
26	CLA	2	607	-	1/1/11/20	2/13/89/115	-
29	BCR	A	848	-	-	3/29/63/63	0/2/2/2
26	CLA	7	602	20	1/1/15/20	9/39/115/115	-
32	LMG	A	860	-	-	9/35/55/70	0/1/1/1
32	LMG	V	2631	-	-	12/50/70/70	0/1/1/1
26	CLA	5	616	18	1/1/10/20	3/8/84/115	-
26	CLA	4	608	-	1/1/15/20	11/39/115/115	-
26	CLA	Y	614	-	1/1/11/20	10/19/95/115	-
26	CLA	A	845	28	1/1/12/20	6/21/97/115	-
26	CLA	B	840	-	1/1/15/20	8/39/115/115	-
26	CLA	A	838	-	1/1/12/20	7/21/97/115	-
26	CLA	6	617	-	1/1/11/20	9/15/91/115	-
34	LUT	4	619	-	-	4/29/67/67	0/2/2/2
26	CLA	8	616	21	1/1/11/20	4/11/87/115	-
26	CLA	8	602	21	-	12/33/109/115	-
26	CLA	B	809	2	1/1/15/20	11/39/115/115	-
26	CLA	H	203	-	1/1/15/20	17/39/115/115	-
26	CLA	a	608	-	1/1/11/20	4/13/89/115	-
28	LHG	V	2630	26	-	5/40/40/53	-
26	CLA	a	609	14	1/1/15/20	14/37/113/115	-
26	CLA	Y	602	24	1/1/13/20	12/31/107/115	-
26	CLA	6	602	19	-	8/39/115/115	-
26	CLA	B	822	-	-	4/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	9	625	-	-	12/50/70/70	0/1/1/1
26	CLA	B	816	-	1/1/12/20	9/25/101/115	-
26	CLA	5	613	18	1/1/14/20	16/37/113/115	-
26	CLA	A	822	-	1/1/15/20	6/39/115/115	-
26	CLA	V	602	25	1/1/14/20	6/33/109/115	-
28	LHG	4	622	26	-	6/53/53/53	-
37	CHL	Z	608	-	3/3/16/26	5/19/117/137	-
26	CLA	9	609	22	1/1/14/20	3/35/111/115	-
26	CLA	5	619	-	1/1/11/20	9/11/87/115	-
26	CLA	U	604	-	1/1/10/20	7/20/92/115	-
26	CLA	B	837	-	-	10/39/115/115	-
29	BCR	2	623	-	-	4/29/63/63	0/2/2/2
26	CLA	1	608	-	1/1/11/20	4/13/89/115	-
33	DGD	B	850	-	-	15/51/91/95	0/2/2/2
26	CLA	a	614	-	1/1/12/20	5/27/99/115	-
26	CLA	1	616	14	1/1/11/20	5/11/87/115	-
26	CLA	a	604	-	1/1/11/20	6/20/96/115	-
28	LHG	H	204	-	-	14/53/53/53	-
28	LHG	Z	2630	26	-	18/53/53/53	-
35	XAT	X	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	L	304	-	1/1/11/20	2/15/91/115	-
26	CLA	3	610	16	1/1/15/20	12/39/115/115	-
29	BCR	4	621	-	-	2/29/63/63	0/2/2/2
28	LHG	W	2630	26	-	11/38/38/53	-
29	BCR	K	207	-	-	1/29/63/63	0/2/2/2
26	CLA	A	818	-	-	14/33/109/115	-
32	LMG	8	626	-	-	15/41/61/70	0/1/1/1
35	XAT	Y	1622	-	-	2/31/93/93	0/4/4/4
28	LHG	9	622	26	-	10/34/34/53	-
26	CLA	3	608	-	1/1/13/20	9/27/103/115	-
26	CLA	Z	613	24	1/1/15/20	8/39/115/115	-
26	CLA	4	613	17	1/1/15/20	13/39/115/115	-
26	CLA	A	809	1	1/1/15/20	11/39/115/115	-
35	XAT	9	620	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	842	-	1/1/15/20	18/39/115/115	-
37	CHL	U	601	24	3/3/20/26	20/39/137/137	-
36	NEX	6	624	-	-	3/27/83/83	0/3/3/3
26	CLA	2	601	15	1/1/15/20	8/39/115/115	-
26	CLA	B	813	-	1/1/15/20	19/39/115/115	-
26	CLA	B	819	-	1/1/13/20	8/27/103/115	-
26	CLA	5	611	28	1/1/10/20	2/12/88/115	-
26	CLA	B	833	-	1/1/15/20	13/39/115/115	-
35	XAT	3	619	-	-	0/31/93/93	0/4/4/4
26	CLA	Z	603	-	1/1/13/20	10/27/103/115	-
28	LHG	3	624	26	-	13/53/53/53	-
26	CLA	6	613	-	-	13/37/113/115	-
31	LMU	8	625	-	-	12/21/61/61	0/2/2/2
29	BCR	B	853	-	-	4/29/63/63	0/2/2/2
26	CLA	B	820	-	1/1/12/20	3/21/97/115	-
27	PQN	B	842	-	-	7/23/43/43	0/2/2/2
26	CLA	A	804	-	1/1/15/20	15/39/115/115	-
37	CHL	W	607	-	3/3/20/26	20/37/135/137	-
26	CLA	A	837	1	1/1/11/20	7/15/91/115	-
26	CLA	Z	611	28	1/1/10/20	4/11/87/115	-
26	CLA	B	807	-	-	4/24/100/115	-
34	LUT	3	618	-	-	4/29/67/67	0/2/2/2
26	CLA	X	613	23	1/1/15/20	12/39/115/115	-
26	CLA	A	824	-	1/1/15/20	9/39/115/115	-
26	CLA	9	603	22	1/1/11/20	5/13/89/115	-
26	CLA	B	839	-	1/1/15/20	13/39/115/115	-
32	LMG	4	623	-	-	7/35/55/70	0/1/1/1
37	CHL	Z	607	-	3/3/20/26	20/39/137/137	-
30	SF4	C	102	3	-	-	0/6/5/5
28	LHG	1	620	26	-	9/53/53/53	-
29	BCR	L	308	-	-	6/29/63/63	0/2/2/2
26	CLA	B	811	-	1/1/12/20	11/23/95/115	-
26	CLA	A	839	-	1/1/13/20	9/27/103/115	-
32	LMG	L	2631	-	-	4/32/52/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LUT	W	1621	-	-	5/29/67/67	0/2/2/2
26	CLA	A	817	-	-	2/15/91/115	-
26	CLA	5	607	-	1/1/15/20	13/39/115/115	-
28	LHG	O	2631	-	-	12/40/40/53	-
28	LHG	A	861	-	-	19/53/53/53	-
29	BCR	9	621	-	-	4/29/63/63	0/2/2/2
26	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
26	CLA	V	603	-	1/1/11/20	6/15/91/115	-
37	CHL	Y	606	-	3/3/16/26	8/15/113/137	-
26	CLA	V	611	28	1/1/10/20	6/13/89/115	-
37	CHL	V	605	25	3/3/15/26	4/13/111/137	-
31	LMU	A	857	-	-	9/21/61/61	0/2/2/2
26	CLA	5	610	18	1/1/12/20	5/26/102/115	-
28	LHG	8	622	26	-	11/53/53/53	-
34	LUT	U	1620	-	-	7/29/67/67	0/2/2/2
26	CLA	6	616	19	1/1/15/20	16/39/115/115	-
28	LHG	5	623	26	-	15/53/53/53	-
28	LHG	9	623	-	-	20/53/53/53	-
34	LUT	1	617	-	-	4/29/67/67	0/2/2/2
29	BCR	1	619	-	-	2/29/63/63	0/2/2/2
26	CLA	Z	614	-	1/1/11/20	8/19/95/115	-
26	CLA	V	614	-	1/1/11/20	5/15/91/115	-
26	CLA	5	608	-	1/1/12/20	6/21/97/115	-
26	CLA	7	607	-	1/1/10/20	1/12/88/115	-

The worst 5 of 3223 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	605	CHL	C2C-C3C	11.23	1.47	1.36
37	Y	605	CHL	C2C-C3C	11.17	1.47	1.36
37	X	609	CHL	C2C-C3C	10.97	1.47	1.36
37	U	605	CHL	C2C-C3C	10.95	1.47	1.36
37	Y	609	CHL	C2C-C3C	10.95	1.47	1.36

The worst 5 of 3934 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	-17.67	81.69	107.37
35	W	1622	XAT	C37-C21-C36	-17.66	81.72	107.37
29	B	852	BCR	C32-C1-C6	-16.83	83.85	110.24
35	U	1622	XAT	C37-C21-C22	-15.27	82.13	108.97

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 3468 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
26	A	808	CLA	2	0
26	4	606	CLA	1	0
29	3	620	BCR	8	0
26	Z	602	CLA	4	0
34	W	1620	LUT	4	0
26	3	612	CLA	1	0
26	a	601	CLA	3	0
34	Y	1621	LUT	4	0
26	X	614	CLA	1	0
35	V	1622	XAT	6	0
29	6	622	BCR	1	0
37	V	607	CHL	4	0
29	B	852	BCR	6	0
36	Z	1623	NEX	3	0
29	B	801	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	803	CLA	3	0
26	7	604	CLA	1	0
26	8	612	CLA	2	0
35	U	1622	XAT	5	0
37	X	609	CHL	4	0
29	L	309	BCR	4	0
26	4	618	CLA	1	0
29	O	2004	BCR	3	0
35	5	621	XAT	2	0
37	W	605	CHL	2	0
37	Y	609	CHL	3	0
26	A	807	CLA	3	0
26	Y	613	CLA	4	0
35	7	620	XAT	1	0
26	F	304	CLA	1	0
26	W	610	CLA	1	0
26	1	611	CLA	1	0
37	Z	601	CHL	4	0
28	U	2630	LHG	1	0
26	W	614	CLA	4	0
37	W	601	CHL	3	0
26	F	303	CLA	4	0
29	J	102	BCR	8	0
26	A	806	CLA	2	0
26	X	612	CLA	1	0
26	B	827	CLA	1	0
26	V	613	CLA	4	0
26	U	613	CLA	3	0
26	B	818	CLA	1	0
34	9	619	LUT	5	0
37	V	601	CHL	4	0
37	Y	607	CHL	3	0
35	2	620	XAT	1	0
26	6	607	CLA	1	0
35	Z	1622	XAT	5	0
35	W	1622	XAT	3	0
29	B	848	BCR	2	0
26	A	802	CLA	3	0
26	7	616	CLA	1	0
26	9	613	CLA	2	0
35	6	621	XAT	1	0
37	Z	606	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	835	CLA	2	0
37	V	609	CHL	3	0
26	B	830	CLA	1	0
26	a	611	CLA	1	0
34	U	1621	LUT	2	0
26	a	603	CLA	1	0
26	X	610	CLA	3	0
29	L	305	BCR	8	0
29	B	843	BCR	9	0
26	A	819	CLA	2	0
26	A	827	CLA	1	0
26	7	609	CLA	1	0
34	7	619	LUT	3	0
29	A	849	BCR	5	0
26	a	607	CLA	1	0
37	W	606	CHL	1	0
26	A	820	CLA	2	0
26	6	610	CLA	3	0
26	Y	610	CLA	2	0
36	X	1623	NEX	2	0
37	Y	605	CHL	1	0
29	A	856	BCR	10	0
29	A	850	BCR	8	0
29	B	846	BCR	3	0
26	1	606	CLA	1	0
26	8	610	CLA	1	0
29	A	852	BCR	10	0
29	7	621	BCR	3	0
26	A	830	CLA	1	0
36	Y	1623	NEX	2	0
37	Y	608	CHL	2	0
26	L	307	CLA	2	0
26	1	607	CLA	1	0
26	4	609	CLA	1	0
29	B	849	BCR	2	0
26	A	831	CLA	1	0
26	6	606	CLA	1	0
37	U	609	CHL	3	0
26	7	611	CLA	4	0
29	8	621	BCR	3	0
26	B	834	CLA	3	0
34	X	1621	LUT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	K	202	BCR	5	0
34	2	619	LUT	7	0
34	a	617	LUT	5	0
26	1	604	CLA	1	0
37	Z	609	CHL	3	0
37	W	609	CHL	1	0
34	Z	1621	LUT	4	0
26	7	614	CLA	2	0
34	X	1620	LUT	6	0
26	B	821	CLA	3	0
26	8	604	CLA	1	0
37	Y	601	CHL	6	0
26	B	808	CLA	3	0
26	4	611	CLA	1	0
34	5	620	LUT	4	0
26	A	816	CLA	1	0
26	B	825	CLA	2	0
26	L	302	CLA	3	0
37	V	606	CHL	2	0
26	7	615	CLA	1	0
35	8	620	XAT	1	0
26	A	825	CLA	3	0
26	4	601	CLA	1	0
37	U	608	CHL	3	0
29	G	205	BCR	4	0
29	a	619	BCR	3	0
26	F	301	CLA	1	0
26	A	840	CLA	1	0
26	1	601	CLA	2	0
26	K	203	CLA	1	0
26	9	610	CLA	1	0
29	B	847	BCR	4	0
26	Y	603	CLA	3	0
26	B	802	CLA	1	0
26	Z	610	CLA	5	0
29	B	845	BCR	3	0
37	X	607	CHL	2	0
26	A	854	CLA	5	0
26	A	805	CLA	1	0
26	A	841	CLA	4	0
26	A	815	CLA	2	0
26	A	829	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	7	601	CLA	1	0
26	7	613	CLA	2	0
26	6	614	CLA	2	0
28	X	2630	LHG	6	0
29	L	301	BCR	10	0
34	Z	1620	LUT	6	0
26	1	613	CLA	1	0
26	V	610	CLA	3	0
29	7	623	BCR	5	0
26	X	604	CLA	1	0
26	6	608	CLA	1	0
37	X	608	CHL	3	0
26	B	835	CLA	1	0
29	A	851	BCR	6	0
26	B	828	CLA	2	0
37	V	608	CHL	2	0
28	Y	2630	LHG	6	0
26	W	613	CLA	4	0
35	a	618	XAT	3	0
27	A	844	PQN	2	0
37	U	606	CHL	2	0
26	5	602	CLA	2	0
26	2	613	CLA	3	0
26	4	607	CLA	1	0
29	B	844	BCR	6	0
26	U	602	CLA	1	0
34	V	1621	LUT	5	0
34	6	619	LUT	5	0
26	a	606	CLA	1	0
26	B	824	CLA	1	0
29	5	622	BCR	2	0
35	4	620	XAT	3	0
35	1	618	XAT	3	0
26	a	613	CLA	1	0
34	V	1620	LUT	5	0
29	F	305	BCR	7	0
36	V	1623	NEX	11	0
26	U	610	CLA	4	0
26	5	603	CLA	1	0
29	3	621	BCR	4	0
26	4	616	CLA	1	0
26	A	821	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	W	612	CLA	1	0
37	X	601	CHL	7	0
29	3	622	BCR	7	0
26	6	601	CLA	1	0
26	B	803	CLA	2	0
36	5	624	NEX	1	0
29	O	2005	BCR	6	0
26	3	606	CLA	1	0
26	3	613	CLA	1	0
26	6	609	CLA	1	0
26	A	834	CLA	2	0
26	X	602	CLA	4	0
32	5	627	LMG	1	0
26	A	812	CLA	1	0
26	W	602	CLA	2	0
26	K	204	CLA	2	0
34	8	619	LUT	6	0
26	8	606	CLA	1	0
26	X	611	CLA	2	0
26	8	613	CLA	2	0
26	Z	612	CLA	1	0
26	V	612	CLA	2	0
26	A	843	CLA	2	0
26	2	606	CLA	1	0
28	a	620	LHG	1	0
36	W	1623	NEX	2	0
37	U	605	CHL	1	0
26	B	817	CLA	1	0
26	W	603	CLA	2	0
26	X	603	CLA	1	0
28	3	623	LHG	1	0
34	Y	1620	LUT	5	0
26	L	303	CLA	2	0
26	8	611	CLA	2	0
37	U	607	CHL	2	0
29	A	848	BCR	3	0
26	7	602	CLA	1	0
32	A	860	LMG	1	0
32	V	2631	LMG	2	0
26	B	840	CLA	1	0
34	4	619	LUT	3	0
28	V	2630	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	6	602	CLA	1	0
26	Y	602	CLA	2	0
26	B	822	CLA	1	0
32	9	625	LMG	2	0
26	B	816	CLA	1	0
26	5	613	CLA	1	0
26	A	822	CLA	4	0
26	V	602	CLA	3	0
37	Z	608	CHL	2	0
26	9	609	CLA	1	0
26	5	619	CLA	3	0
26	U	604	CLA	3	0
26	B	837	CLA	2	0
29	2	623	BCR	5	0
33	B	850	DGD	1	0
26	a	604	CLA	1	0
28	Z	2630	LHG	9	0
35	X	1622	XAT	3	0
26	3	610	CLA	1	0
29	4	621	BCR	5	0
28	W	2630	LHG	1	0
29	K	207	BCR	3	0
26	A	818	CLA	1	0
32	8	626	LMG	3	0
35	Y	1622	XAT	3	0
28	9	622	LHG	1	0
26	3	608	CLA	1	0
26	Z	613	CLA	4	0
26	A	809	CLA	1	0
37	U	601	CHL	4	0
36	6	624	NEX	6	0
26	B	813	CLA	2	0
26	B	819	CLA	1	0
26	5	611	CLA	7	0
26	B	833	CLA	2	0
35	3	619	XAT	2	0
26	Z	603	CLA	1	0
28	3	624	LHG	2	0
29	B	853	BCR	3	0
27	B	842	PQN	3	0
37	W	607	CHL	3	0
26	A	837	CLA	1	0

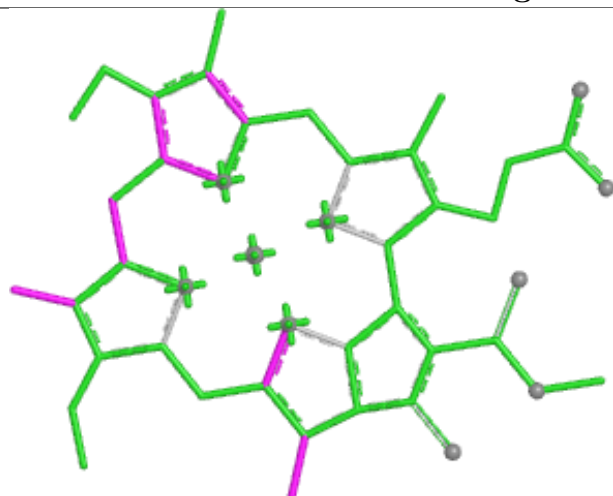
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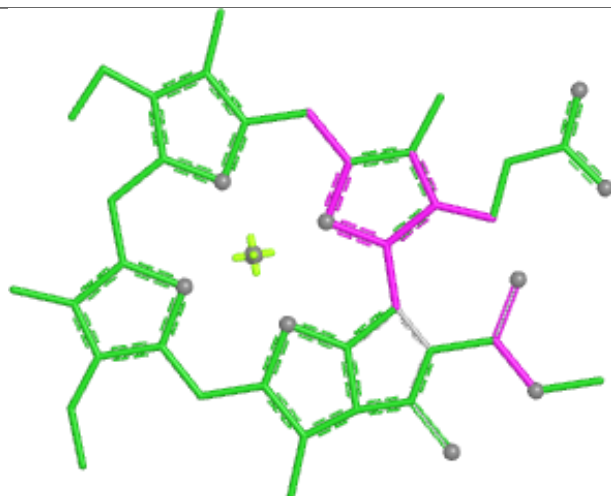
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Z	611	CLA	3	0
34	3	618	LUT	7	0
26	X	613	CLA	4	0
26	A	824	CLA	2	0
26	B	839	CLA	1	0
37	Z	607	CHL	3	0
30	C	102	SF4	1	0
29	L	308	BCR	7	0
34	W	1621	LUT	4	0
26	5	607	CLA	2	0
28	O	2631	LHG	1	0
29	9	621	BCR	7	0
37	Y	606	CHL	2	0
37	V	605	CHL	1	0
31	A	857	LMU	1	0
26	5	610	CLA	1	0
34	U	1620	LUT	6	0
26	6	616	CLA	1	0
28	5	623	LHG	6	0
34	1	617	LUT	6	0
29	1	619	BCR	2	0
26	Z	614	CLA	1	0
26	V	614	CLA	1	0

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

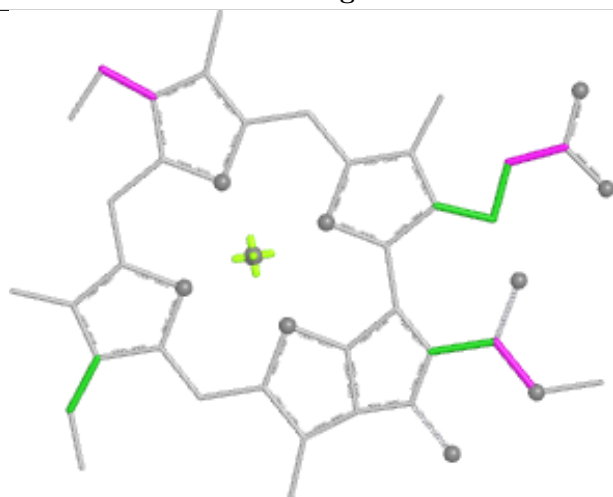
Ligand CLA Y 612



Bond lengths



Bond angles

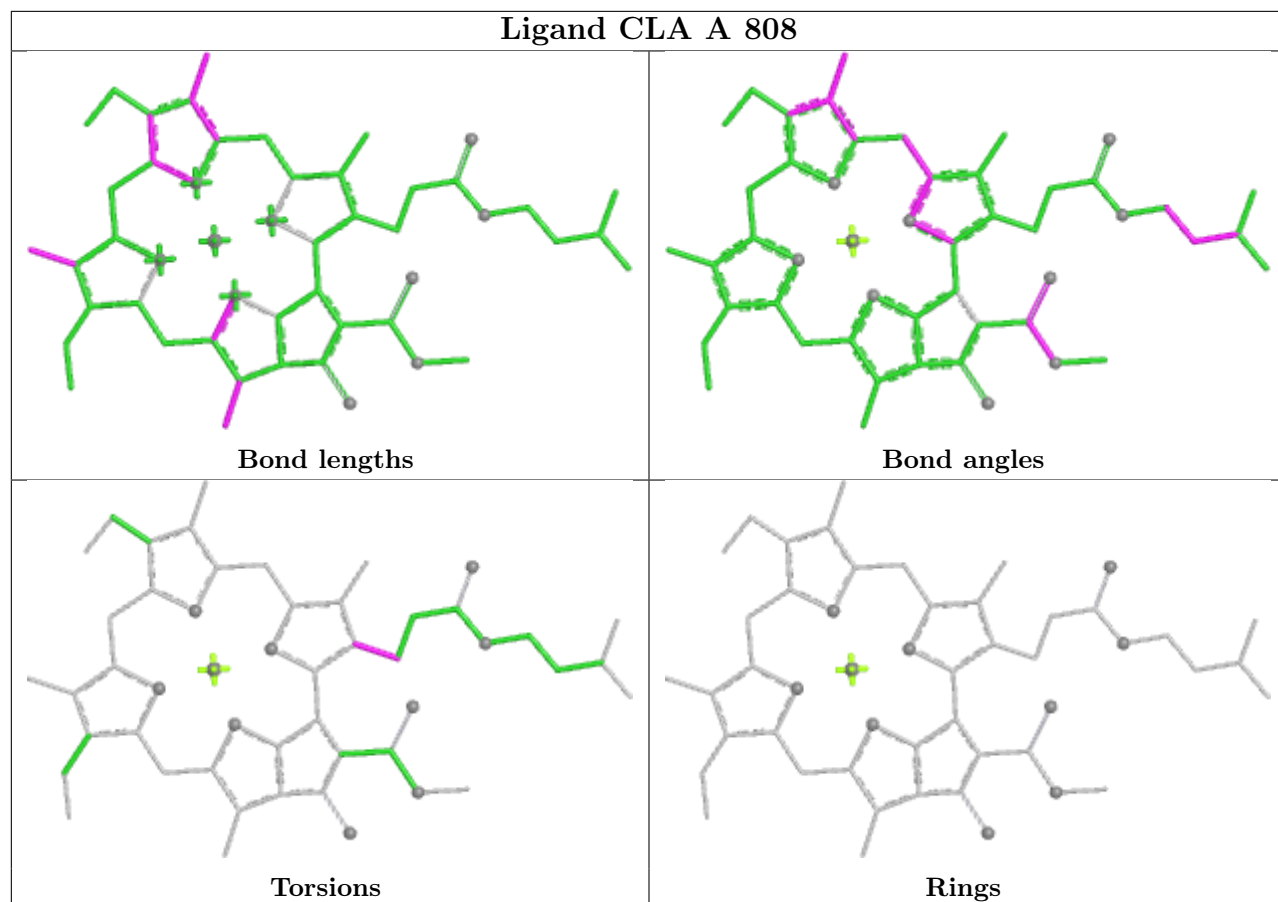


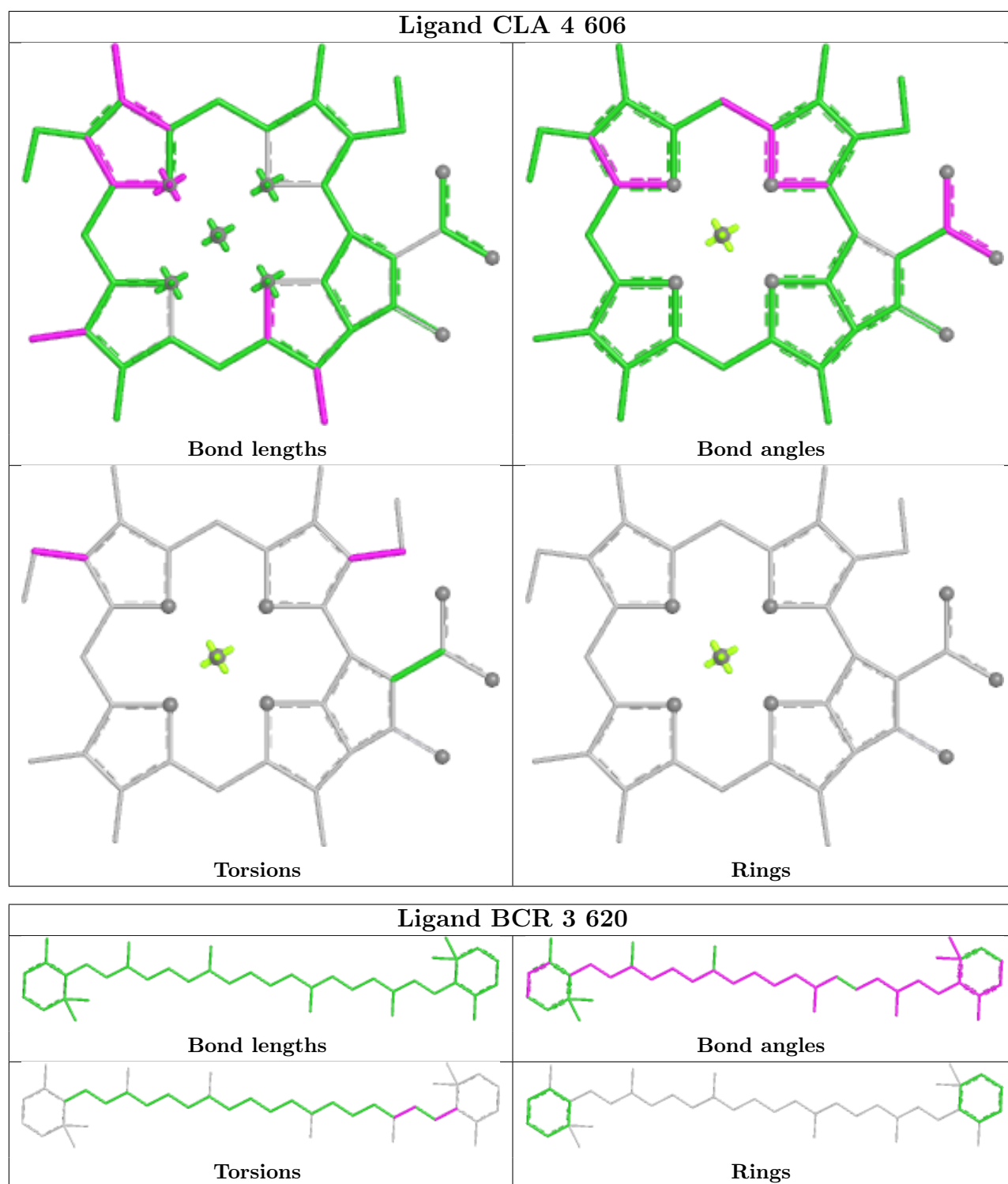
Torsions



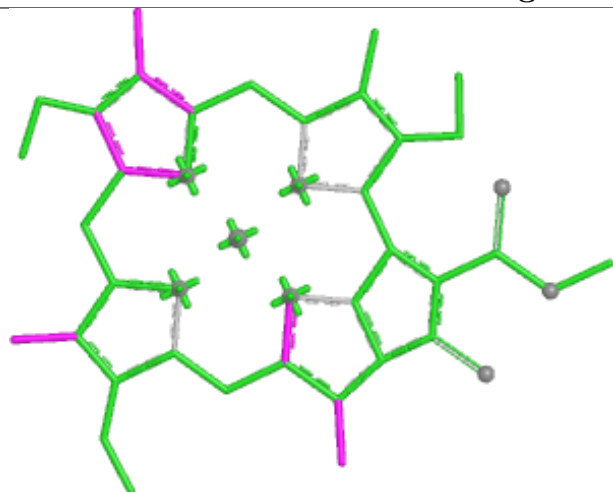
Rings

Ligand CLA A 808

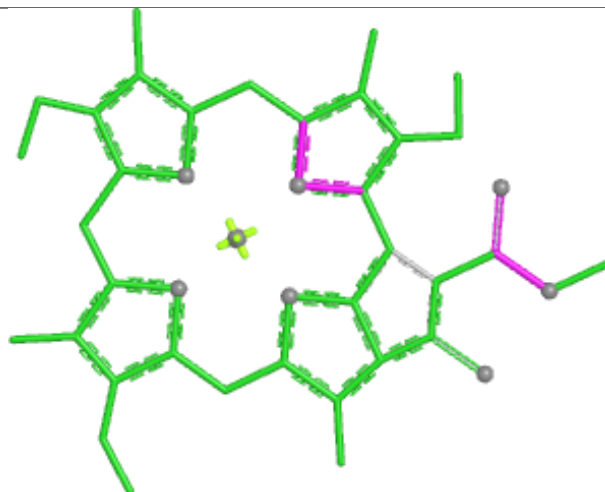




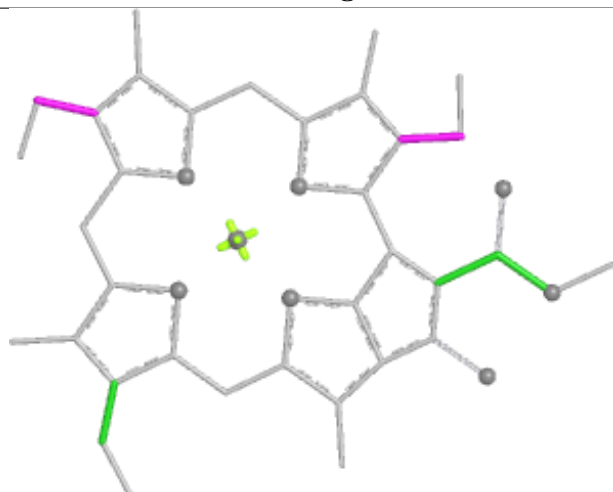
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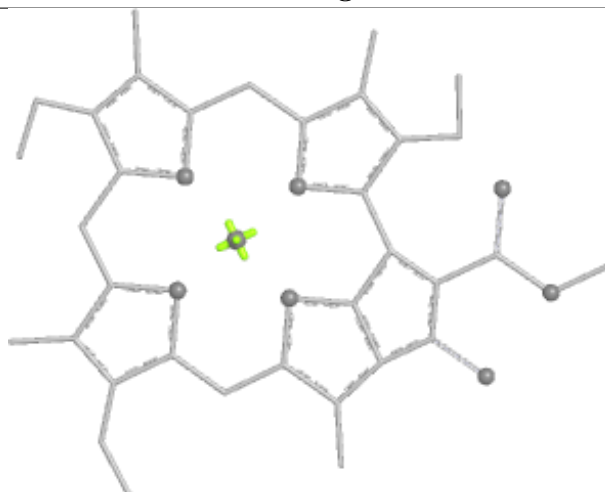
Bond lengths



Bond angles

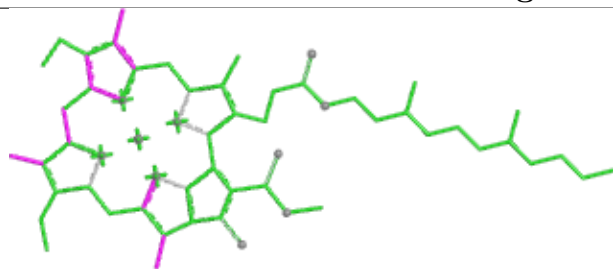


Torsions

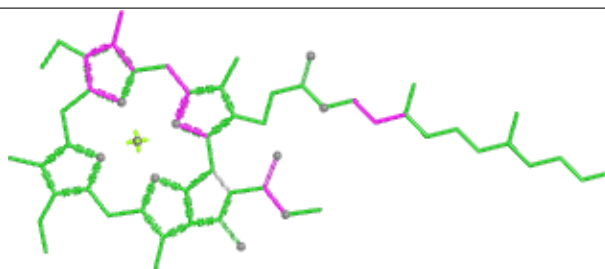


Rings

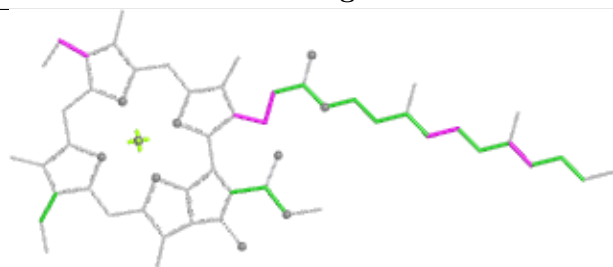
Ligand CLA Z 602



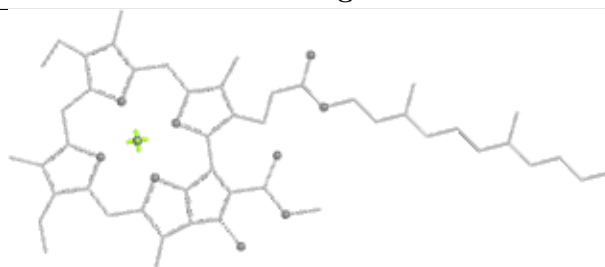
Bond lengths



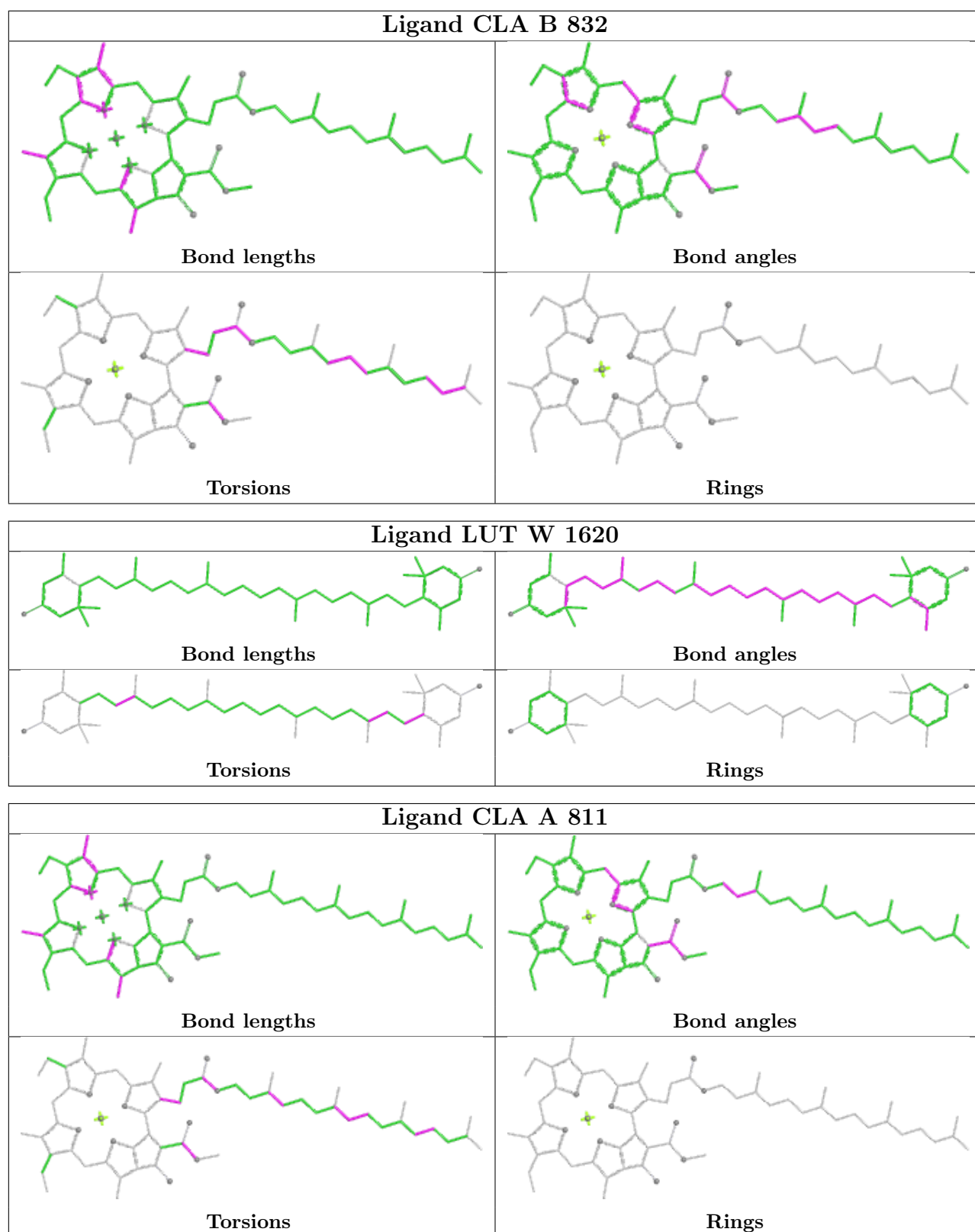
Bond angles

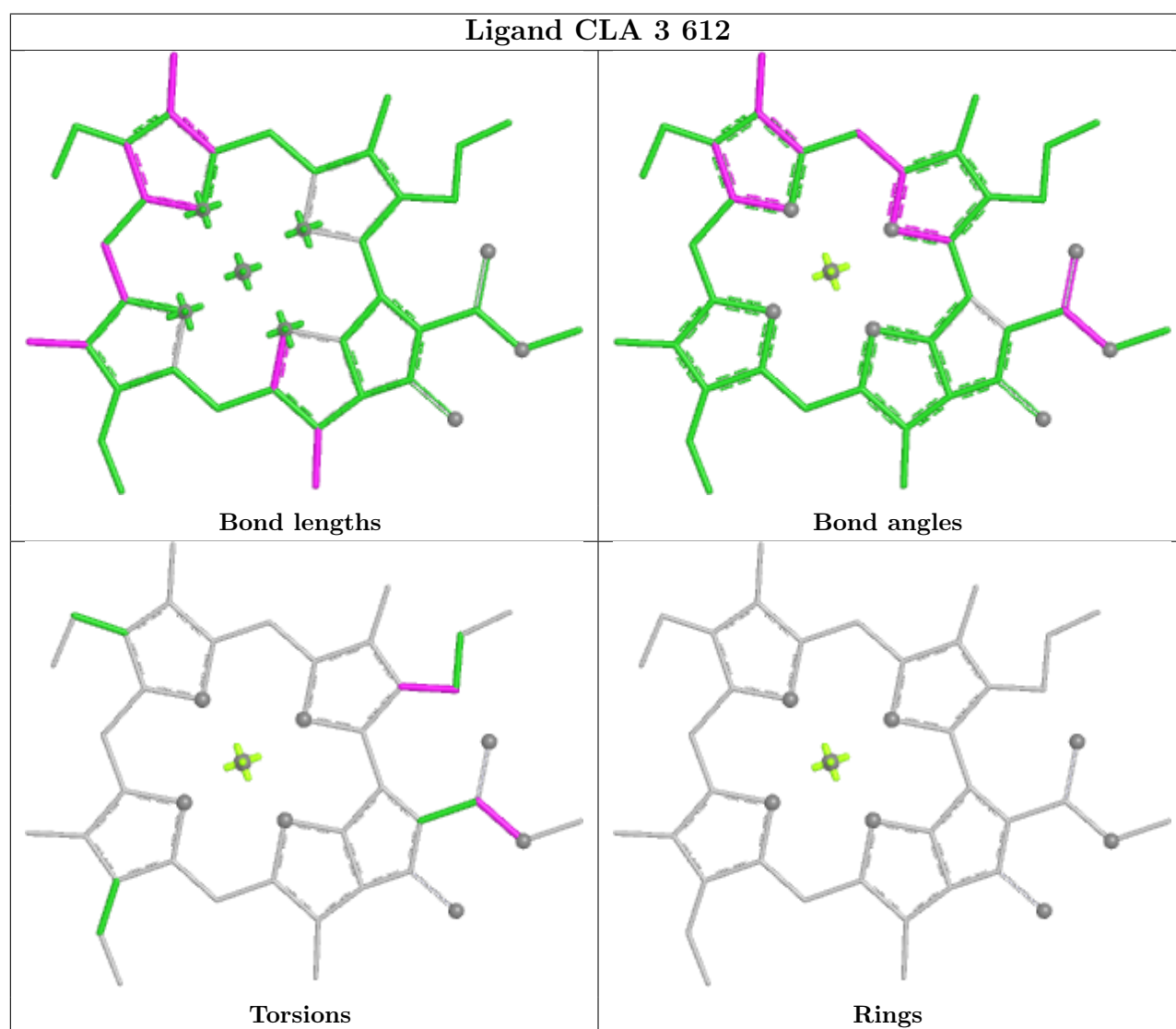
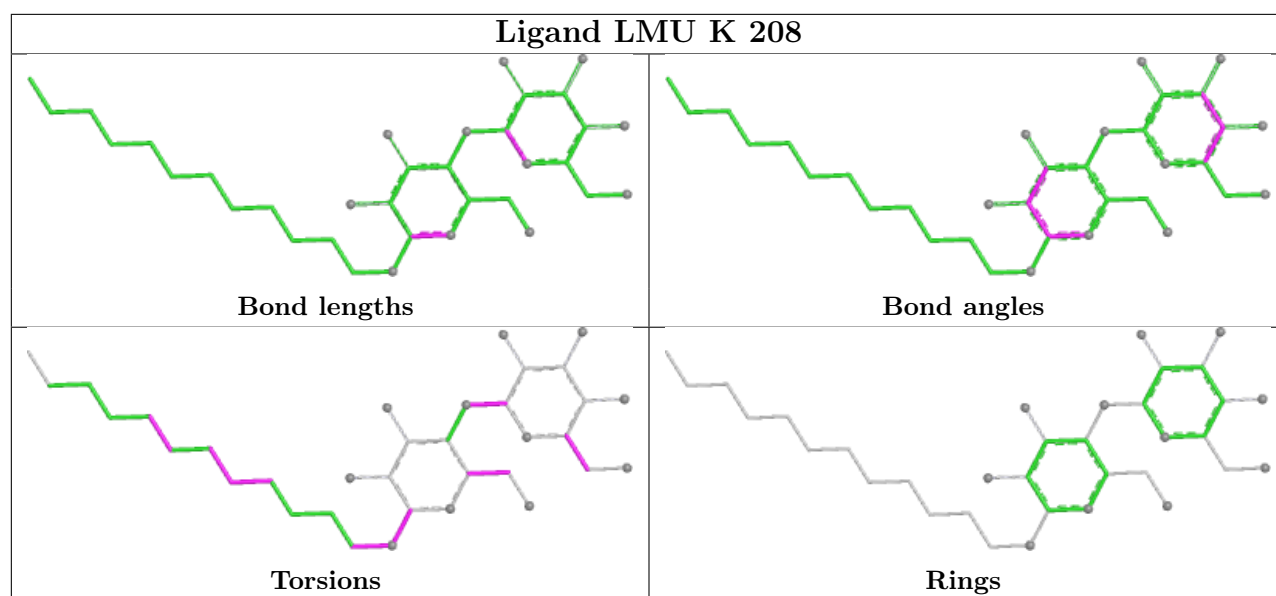


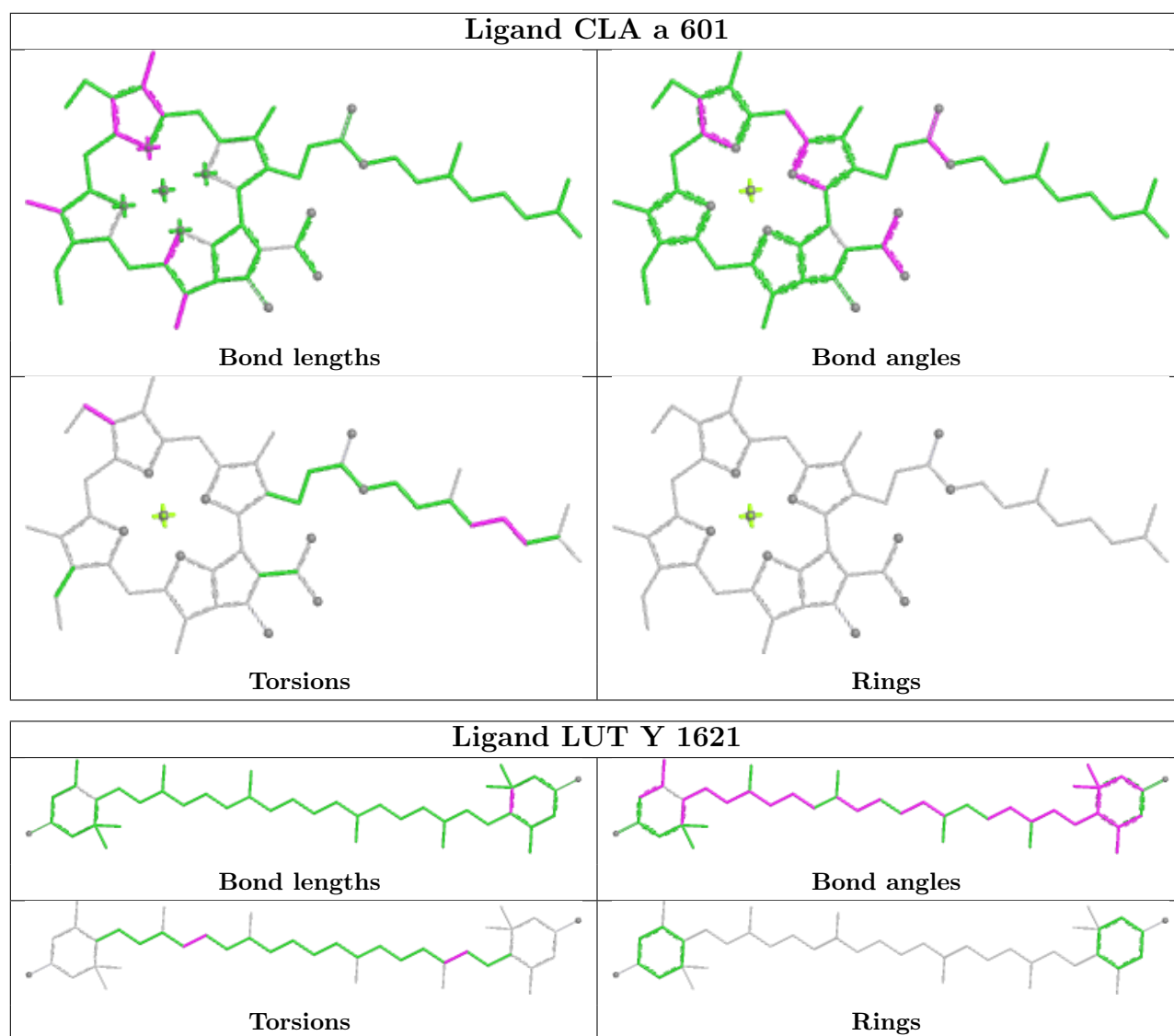
Torsions



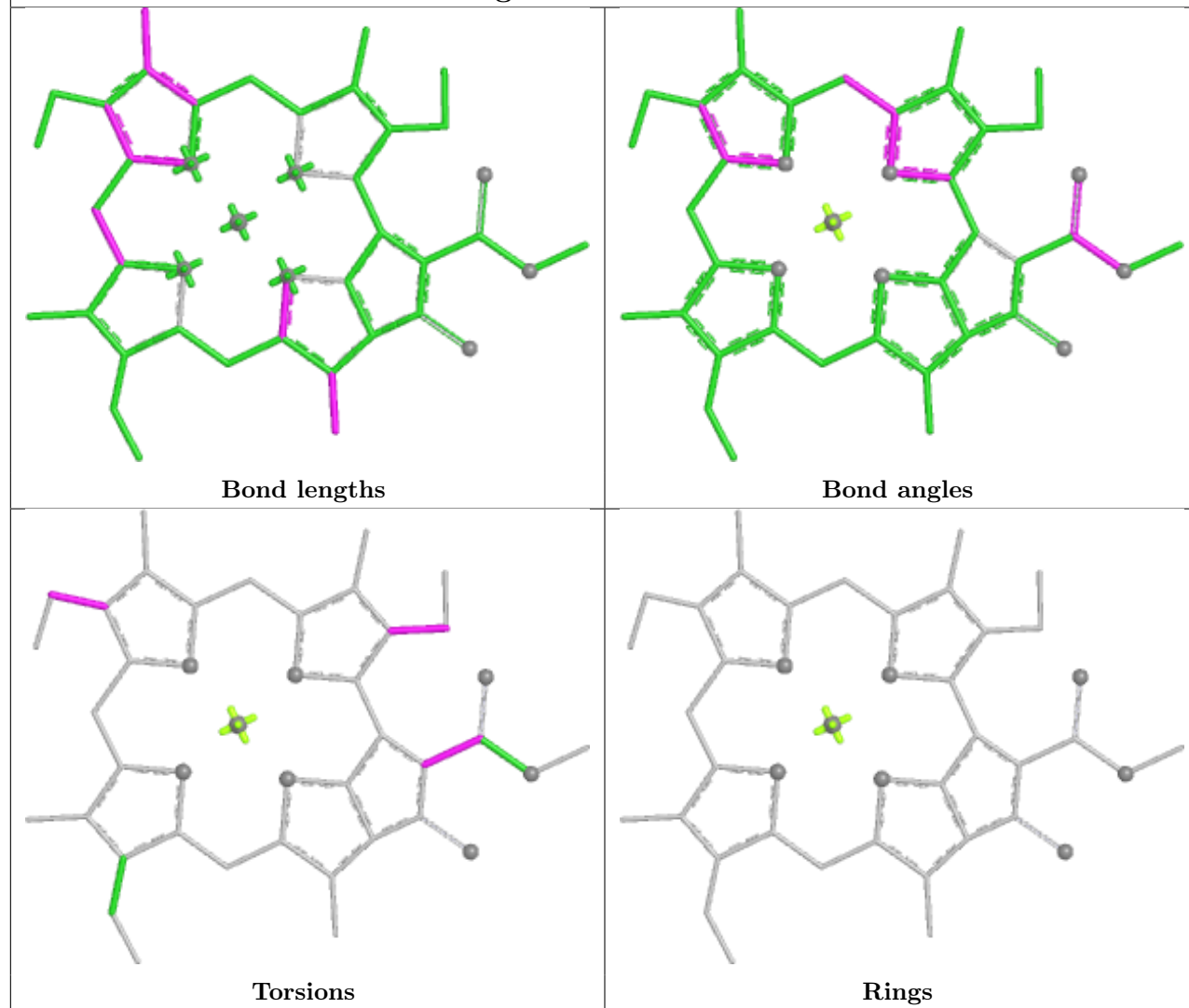
Rings



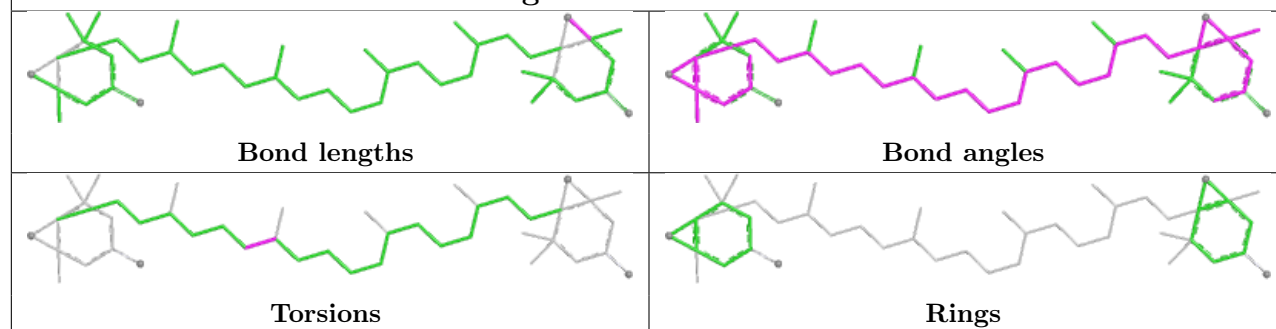


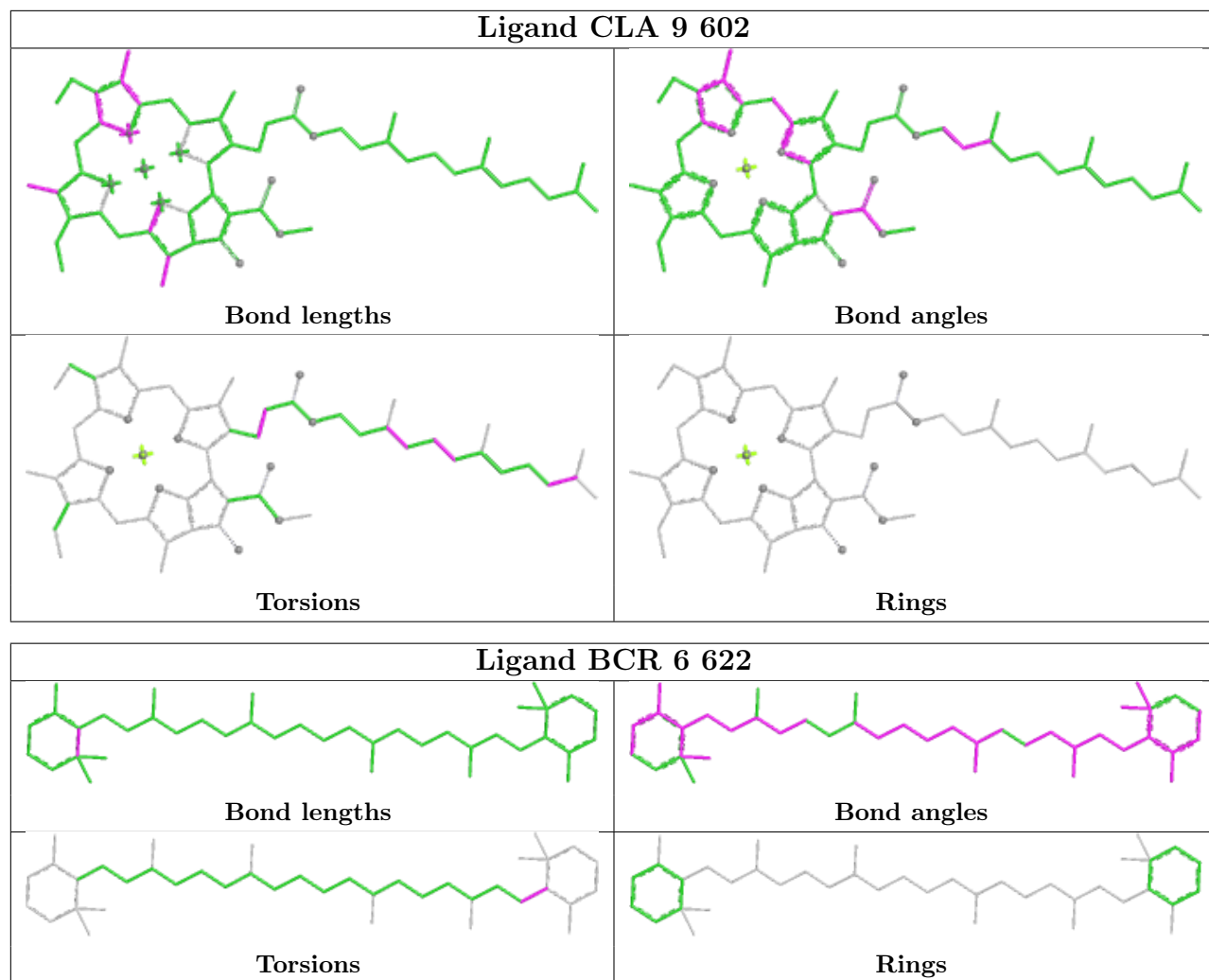


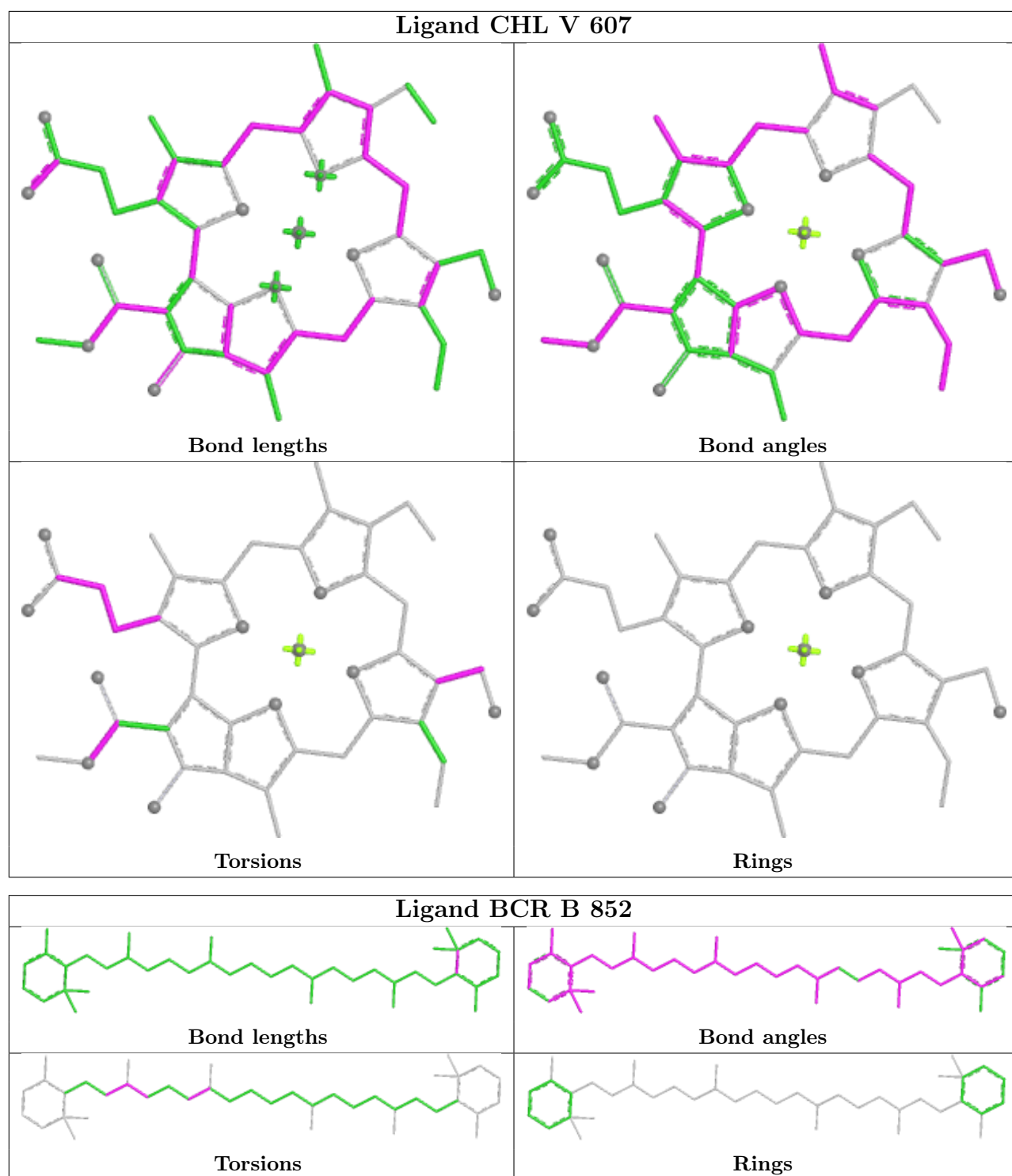
Ligand CLA X 614

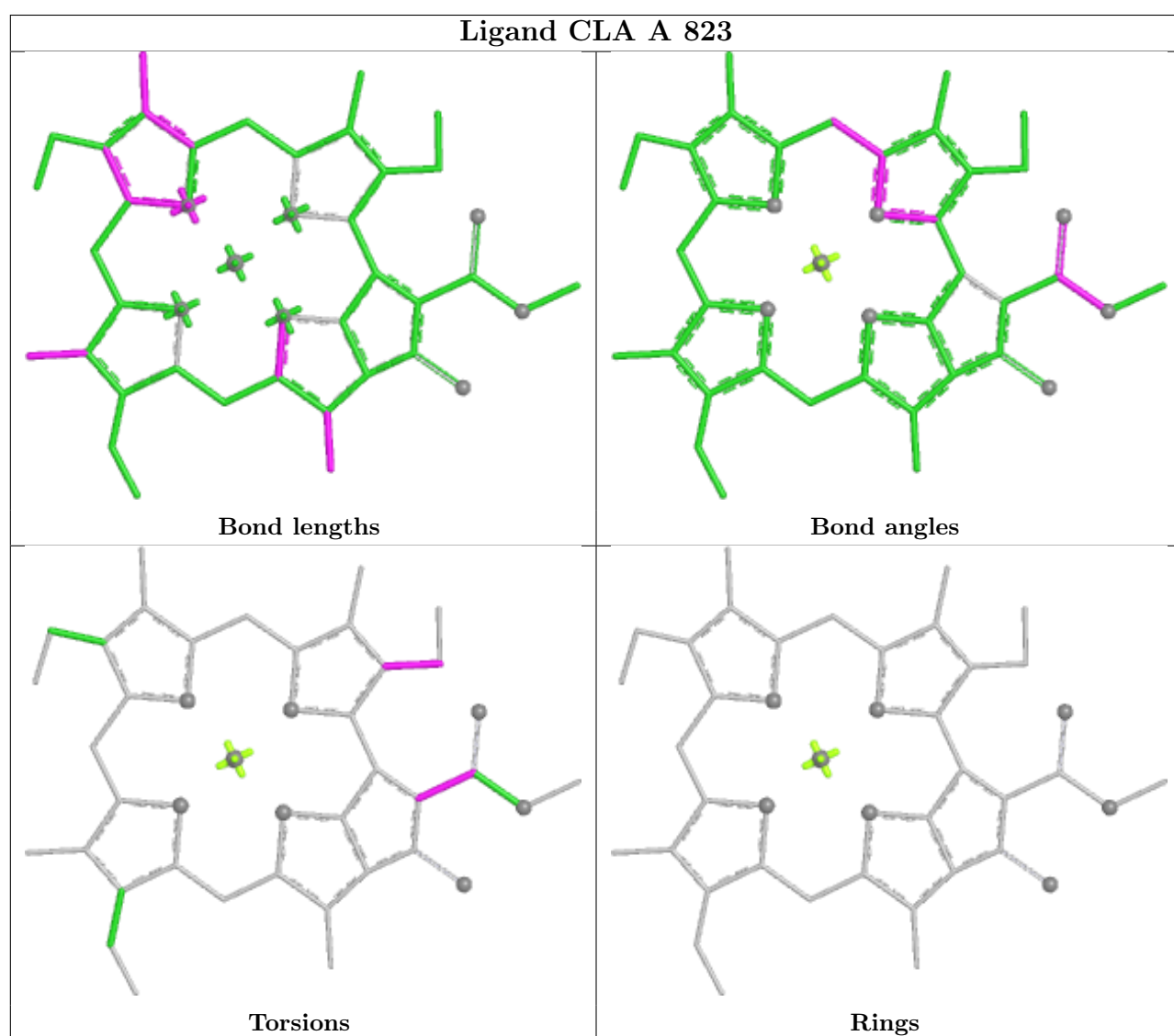
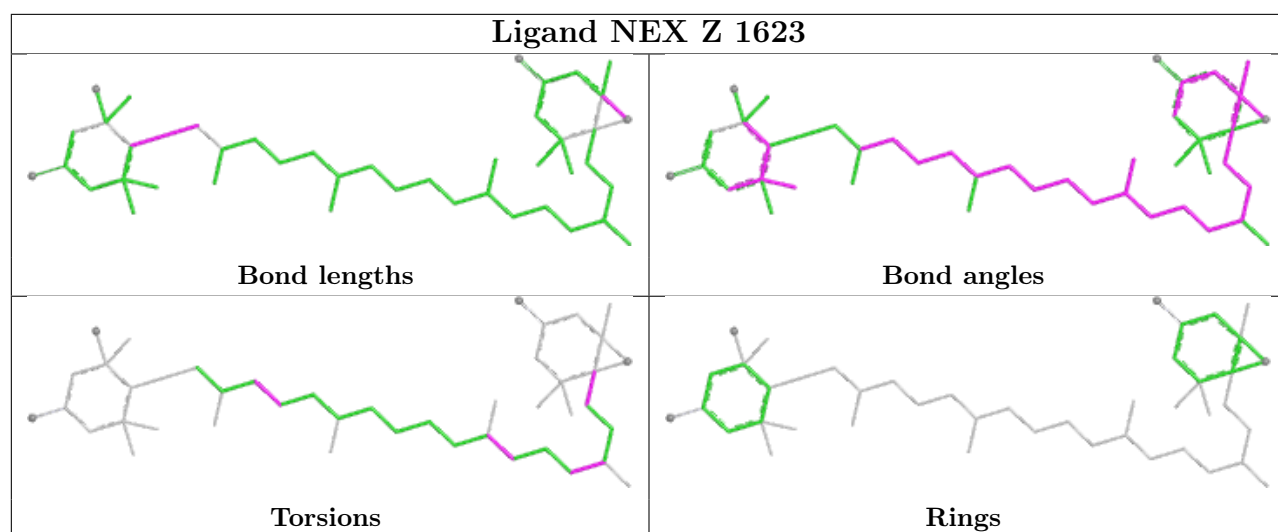


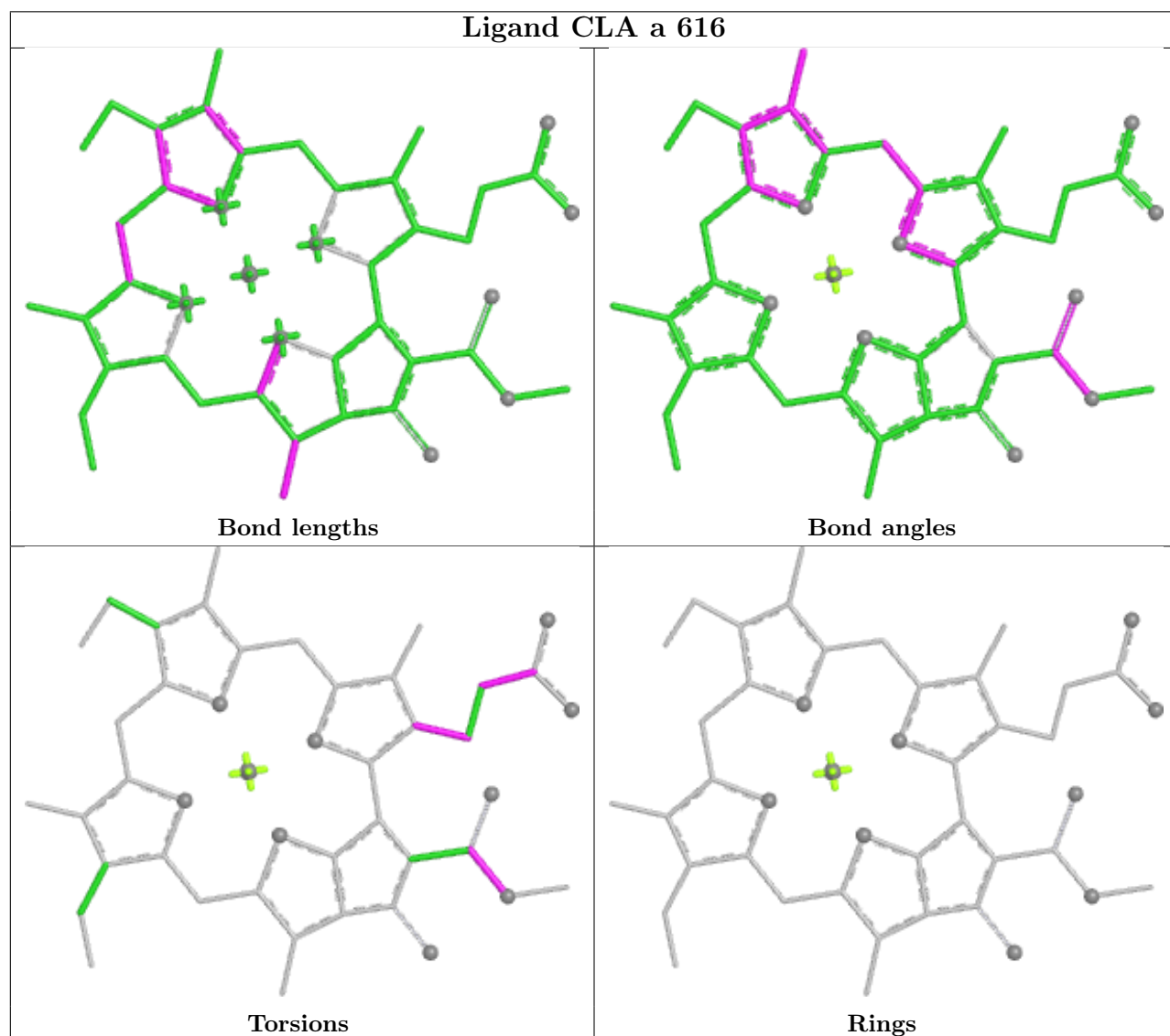
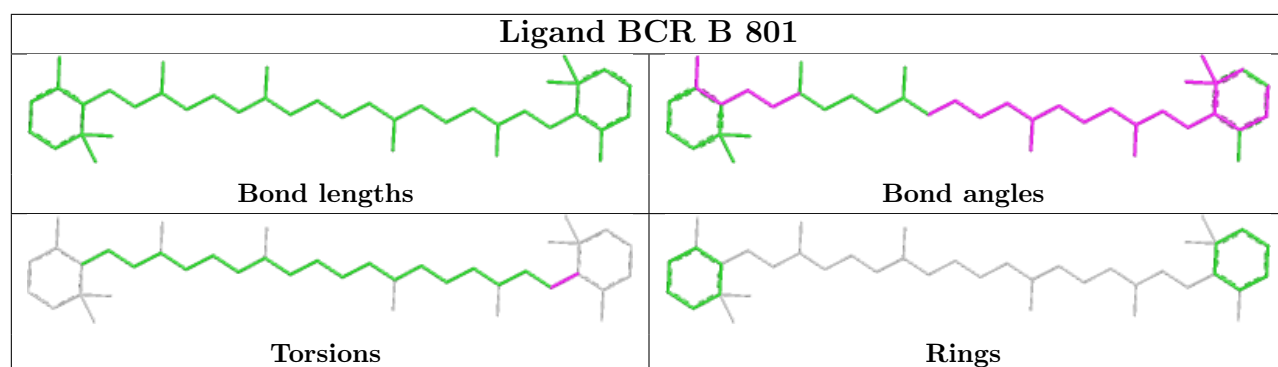
Ligand XAT V 1622



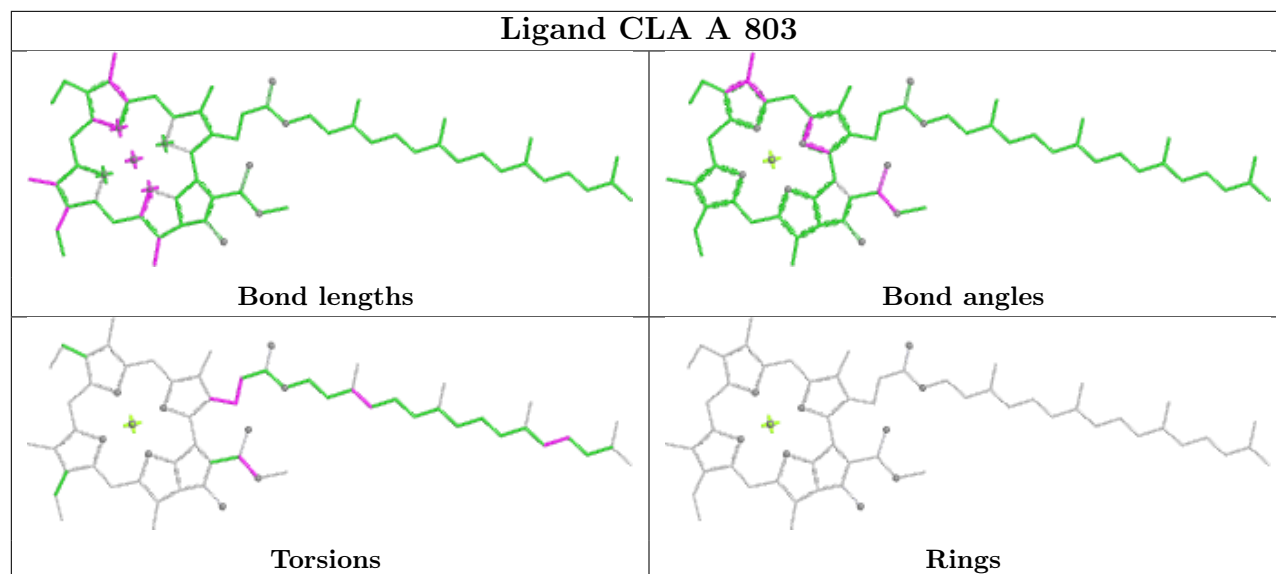




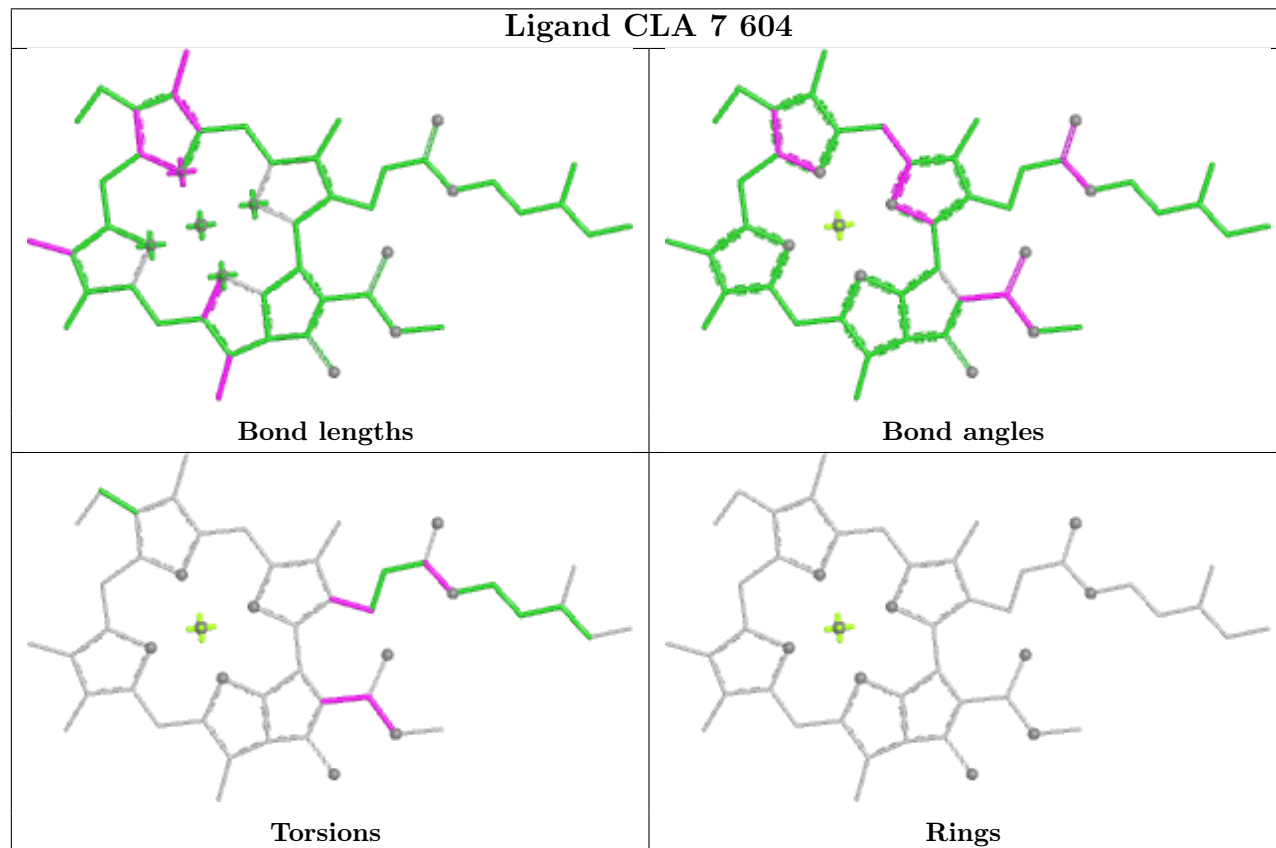




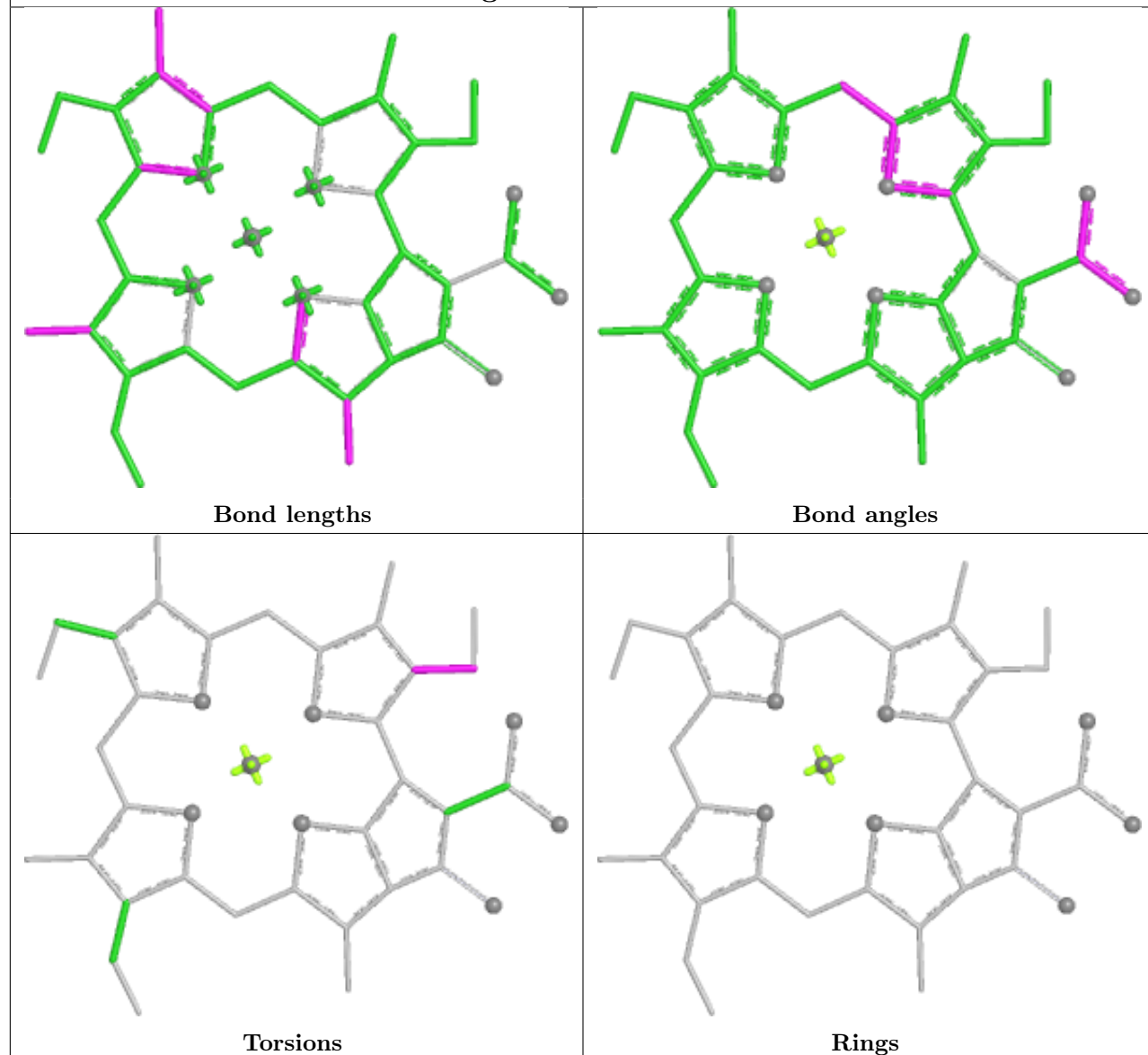
Ligand CLA A 803



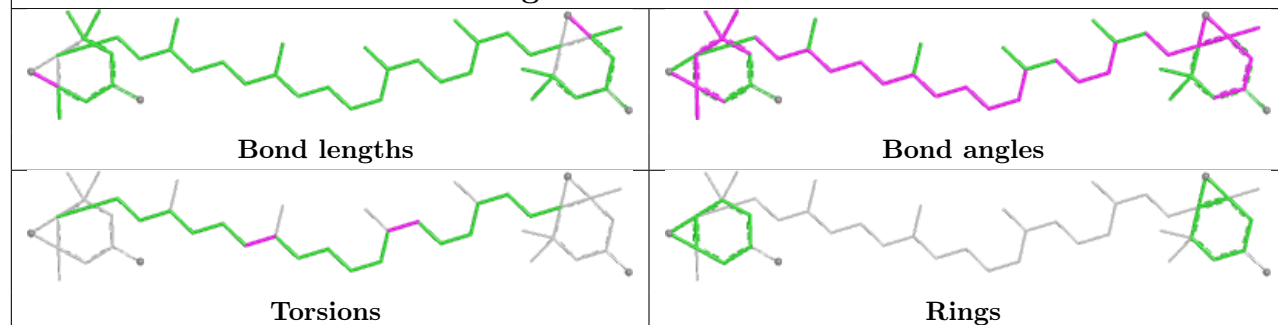
Ligand CLA 7 604

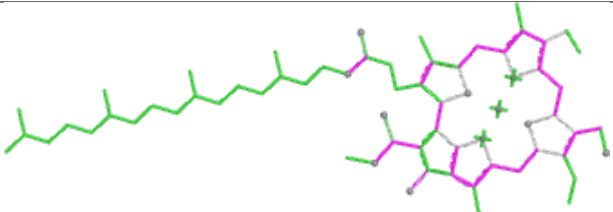
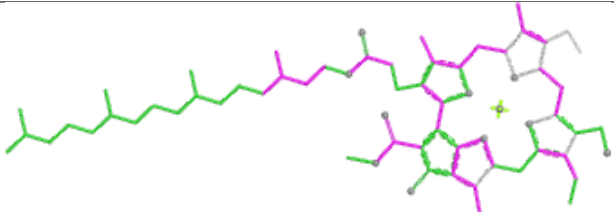
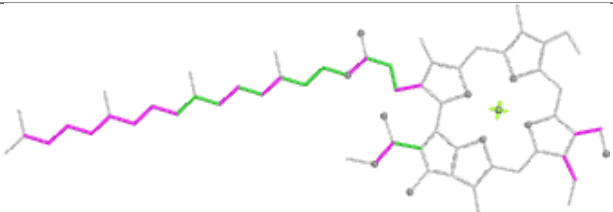
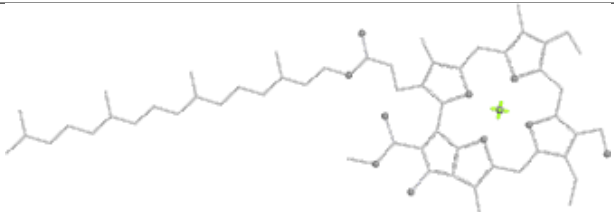


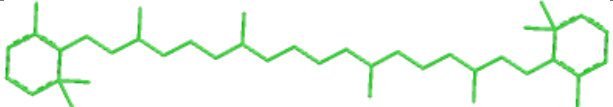
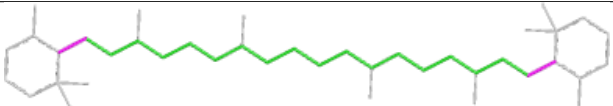
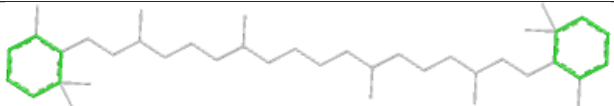
Ligand CLA 8 612



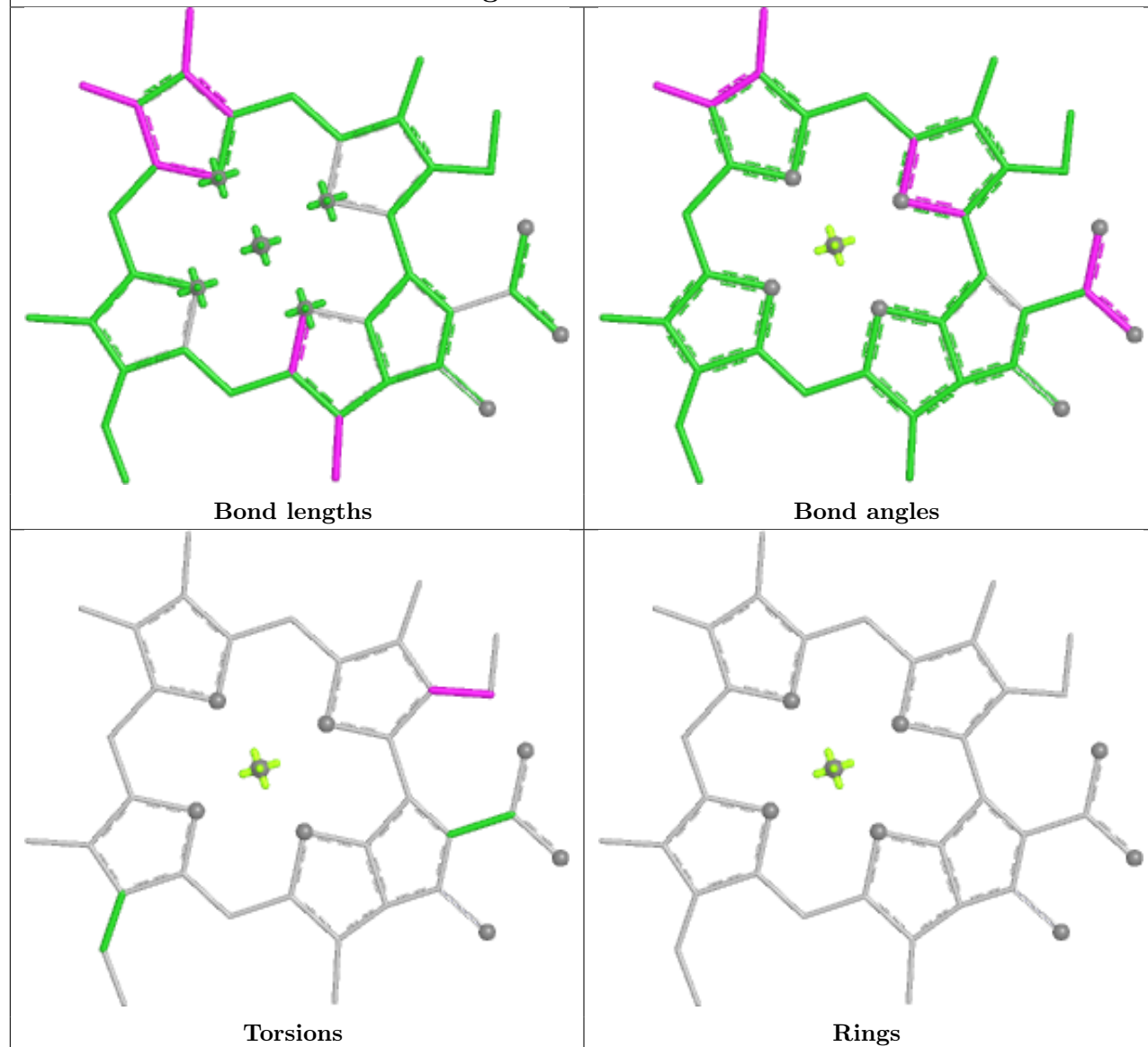
Ligand XAT U 1622



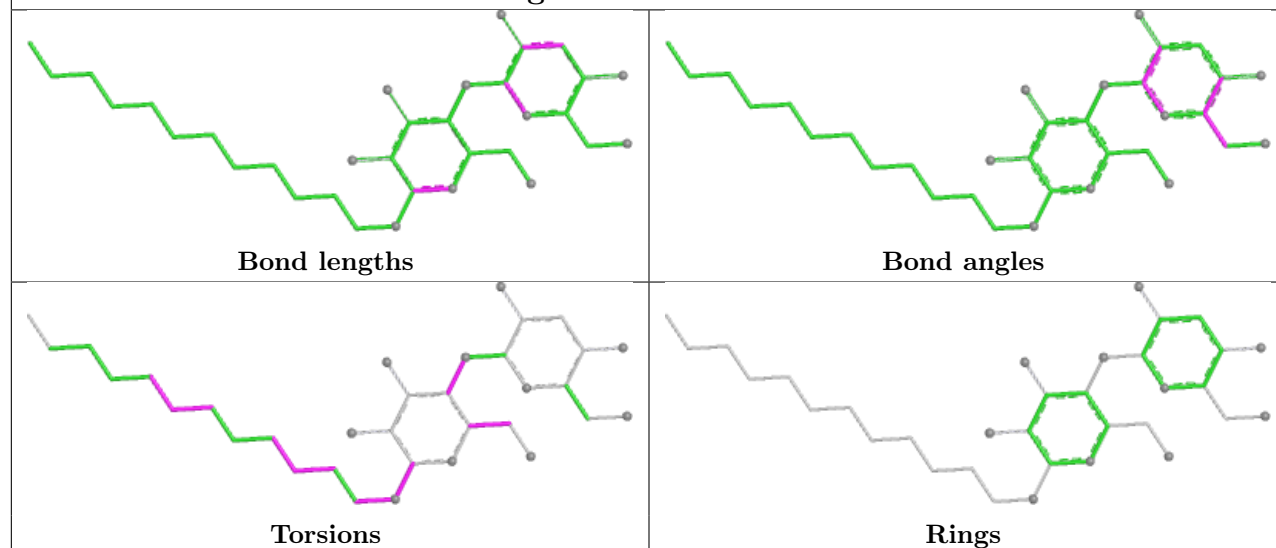
Ligand CHL X 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

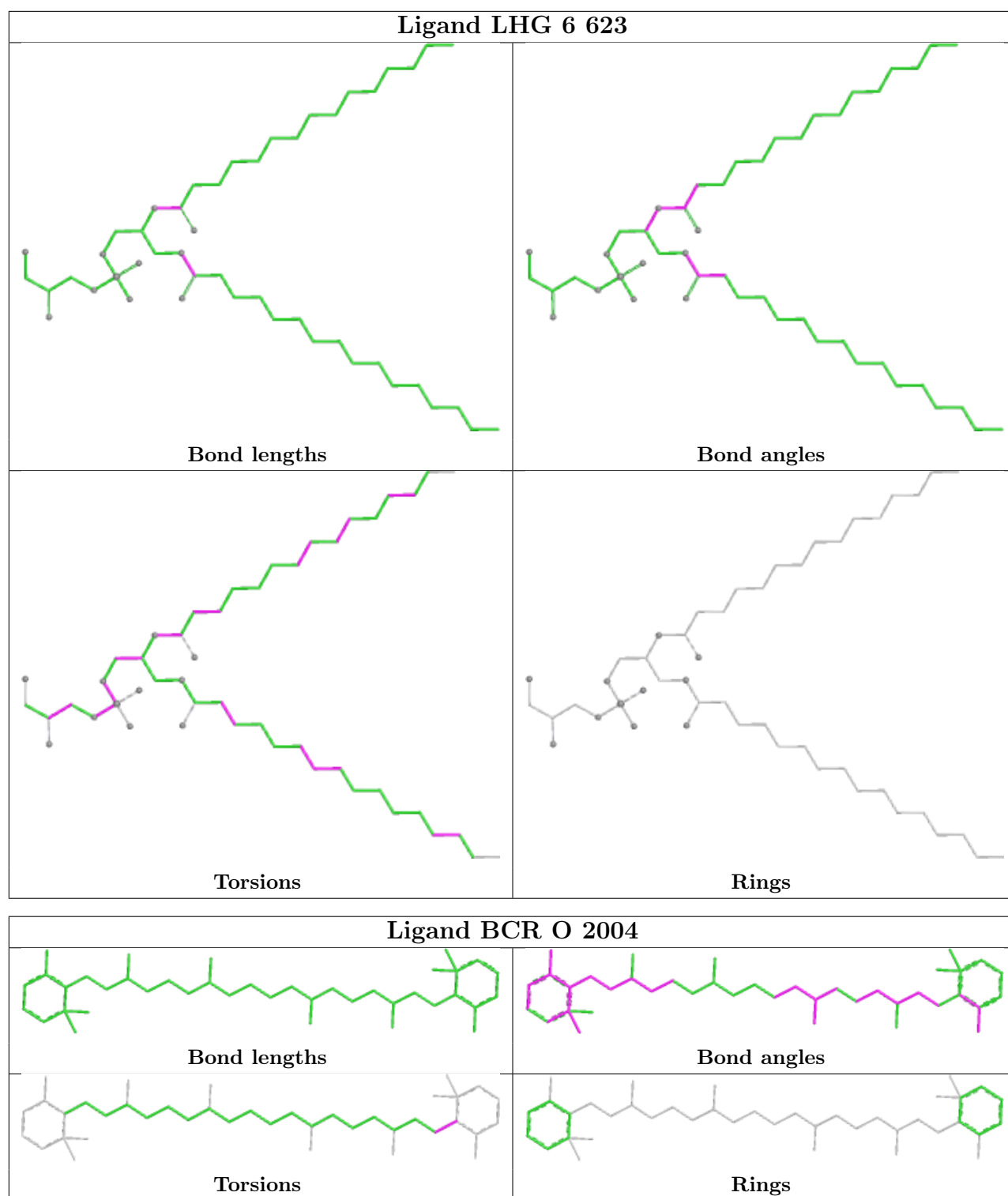
Ligand BCR L 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

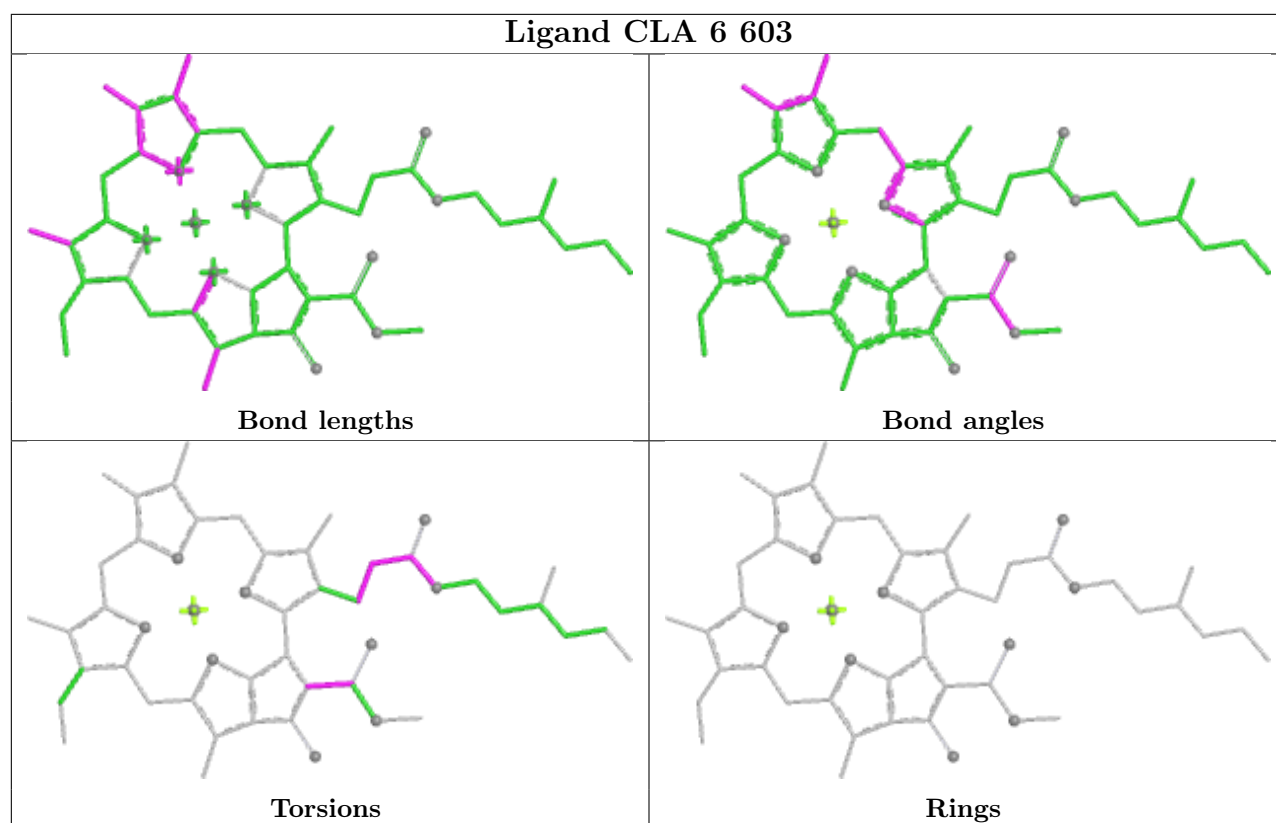
Ligand CLA 4 618



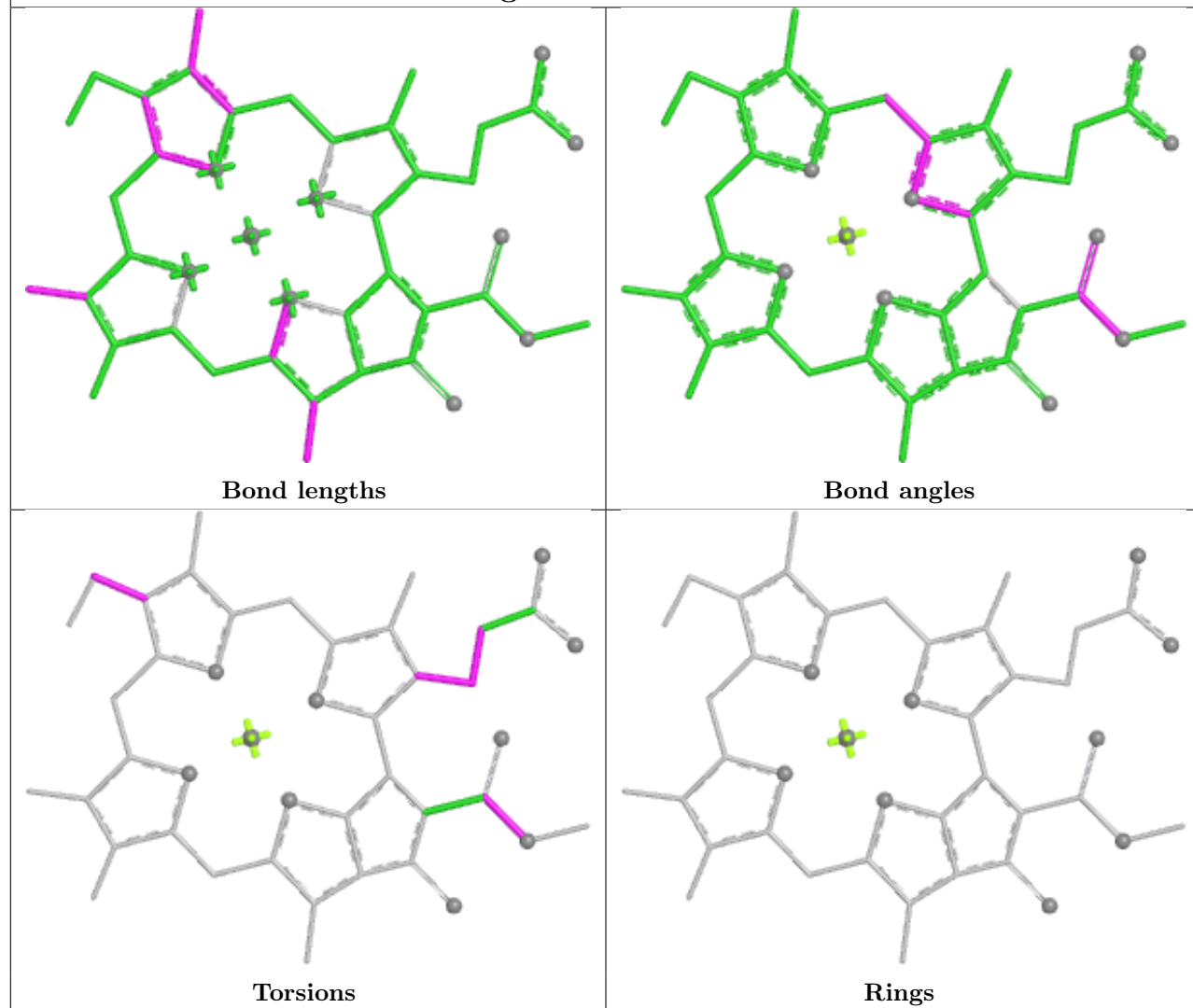
Ligand LMU A 858



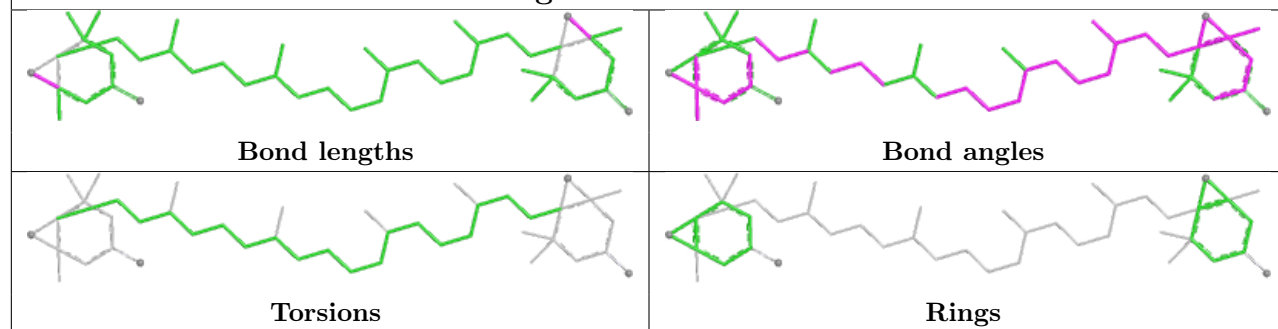


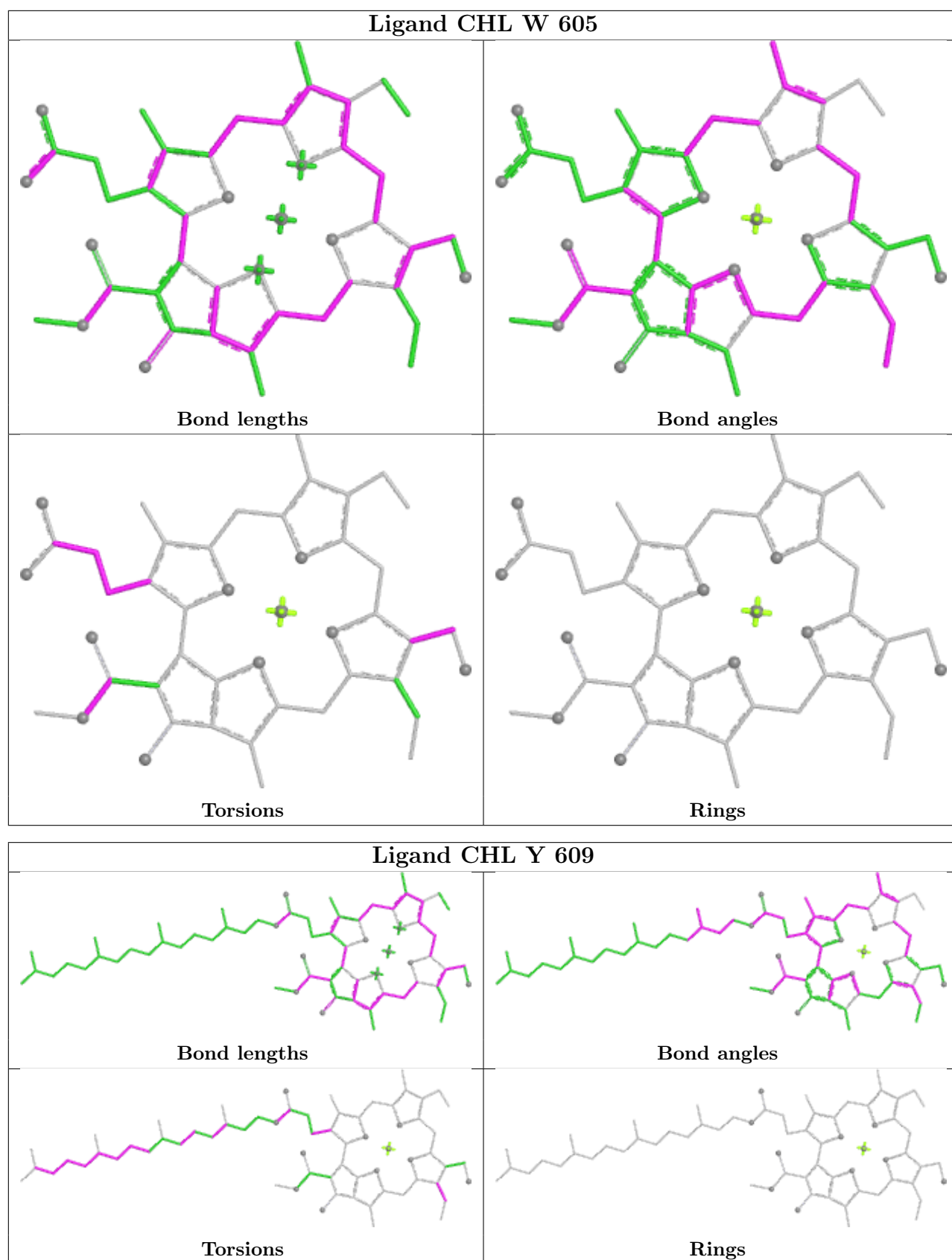


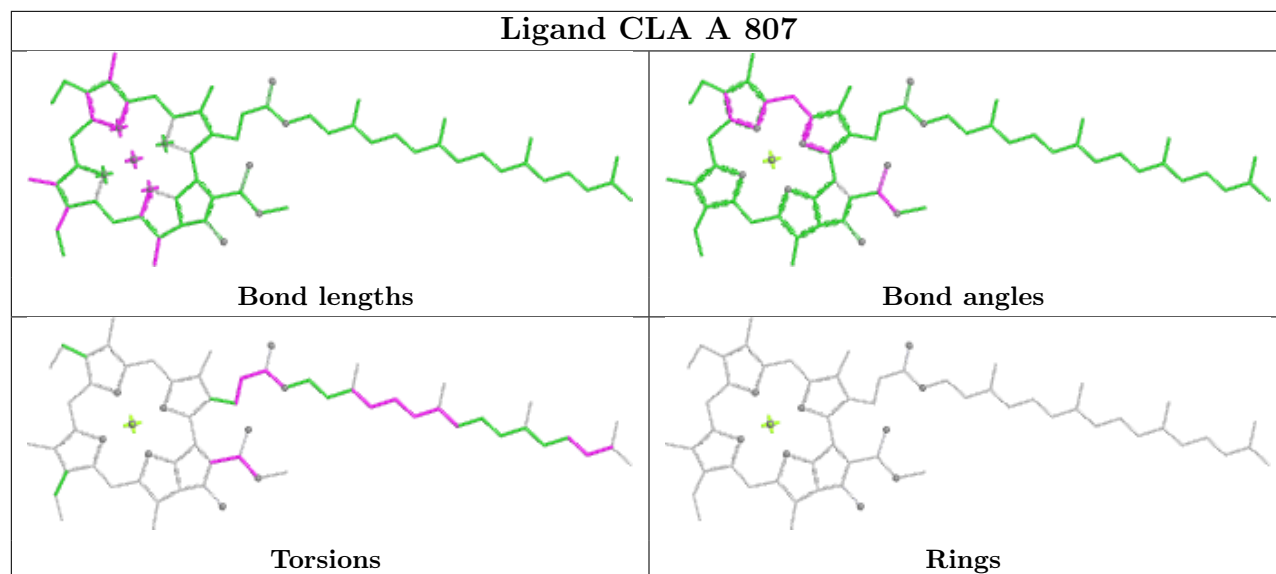
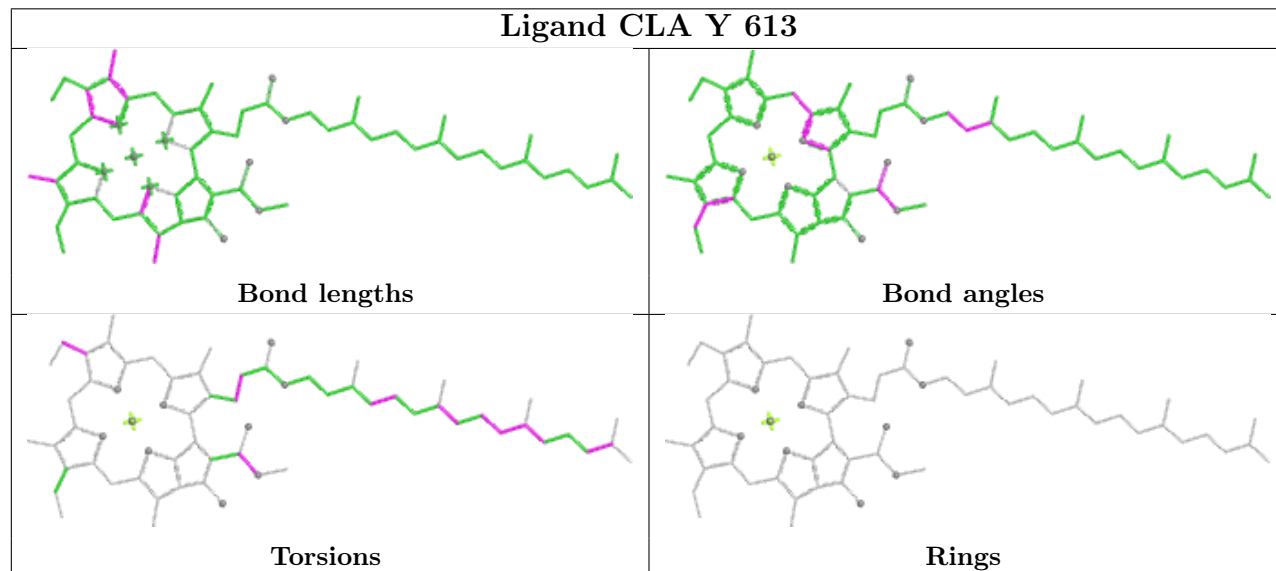
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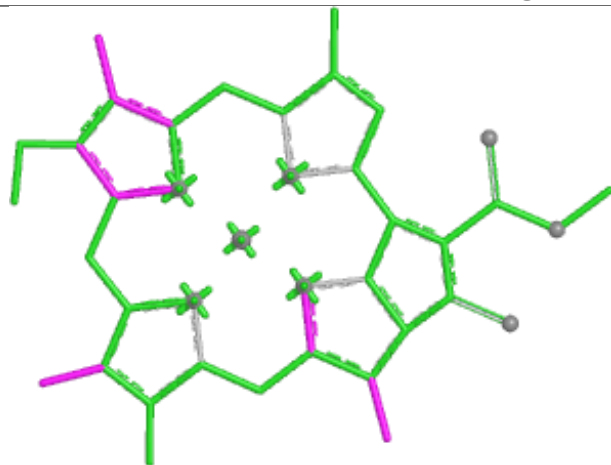
Ligand XAT 5 621



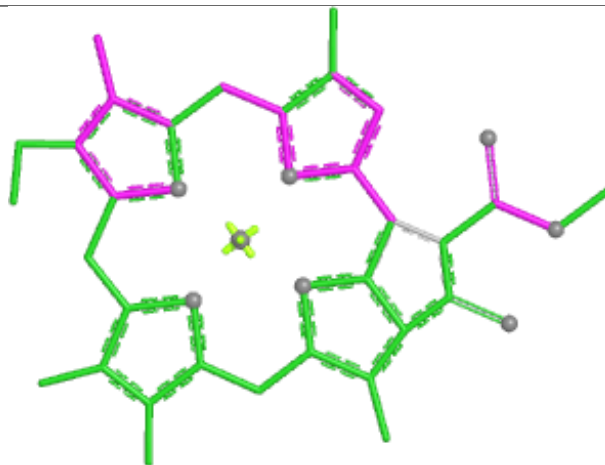


Ligand CLA A 807**Ligand CLA Y 613**

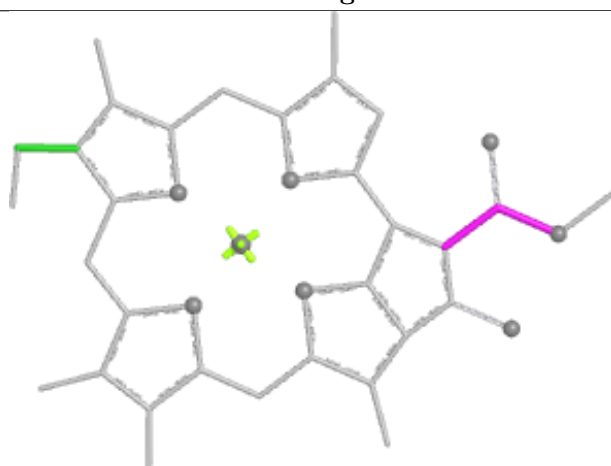
Ligand CLA 1 610



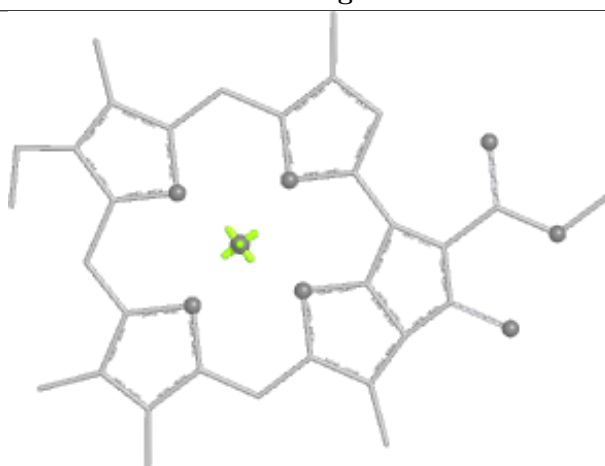
Bond lengths



Bond angles

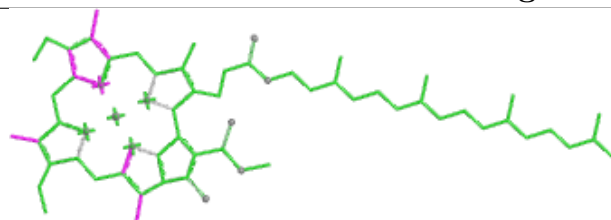


Torsions

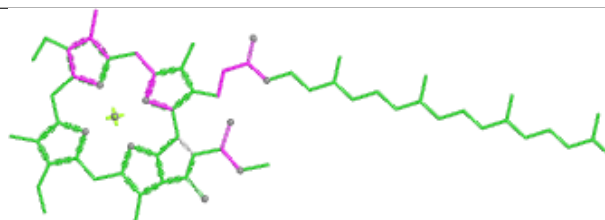


Rings

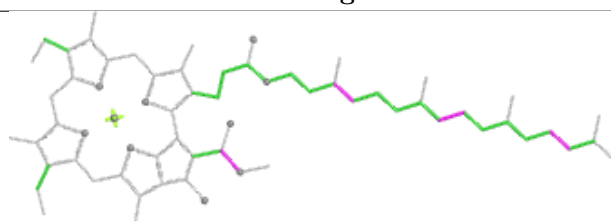
Ligand CLA 3 604



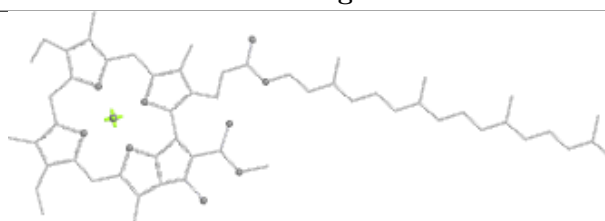
Bond lengths



Bond angles

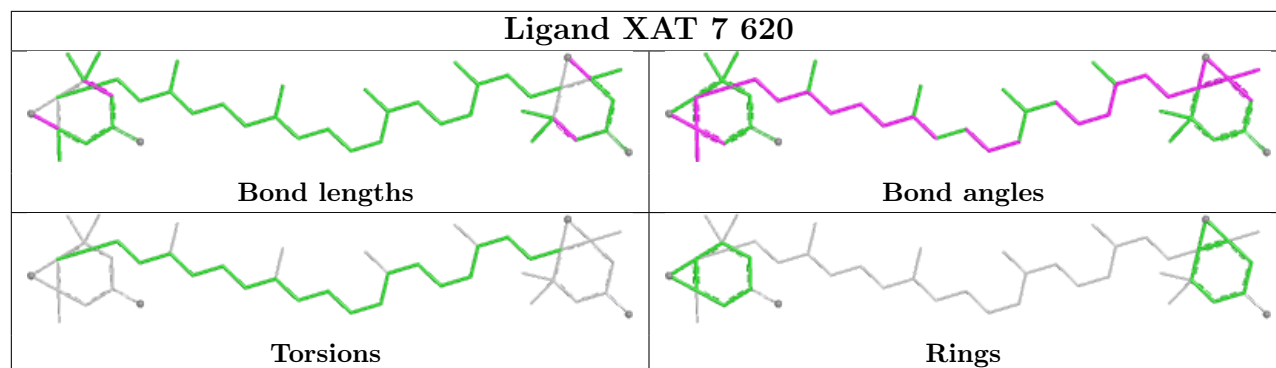


Torsions

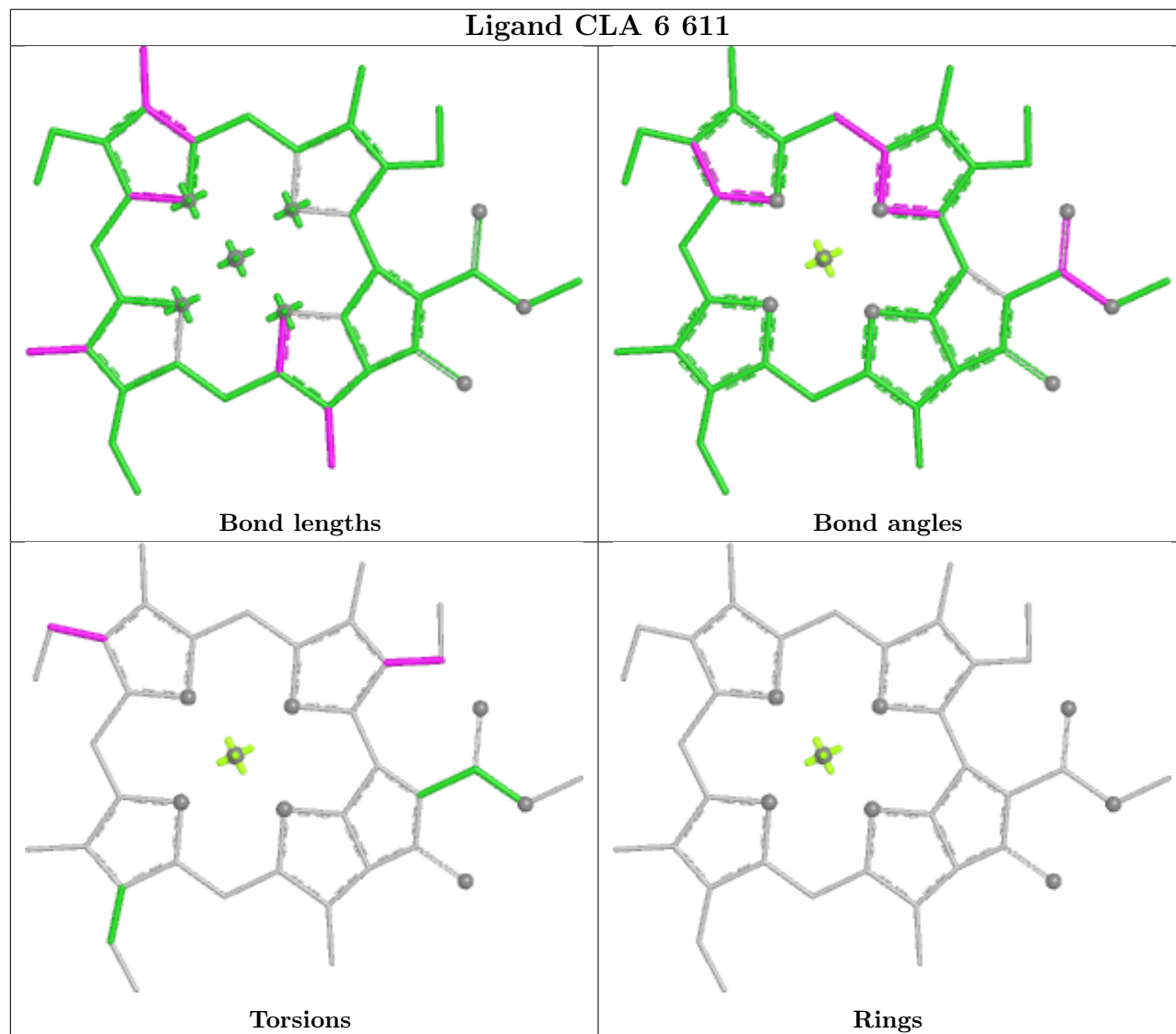


Rings

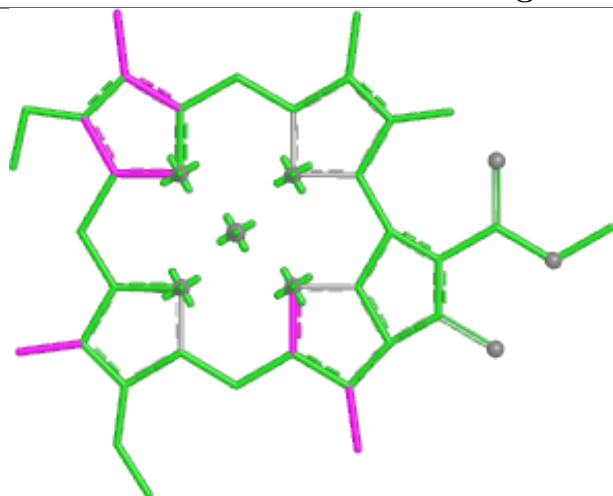
Ligand XAT 7 620



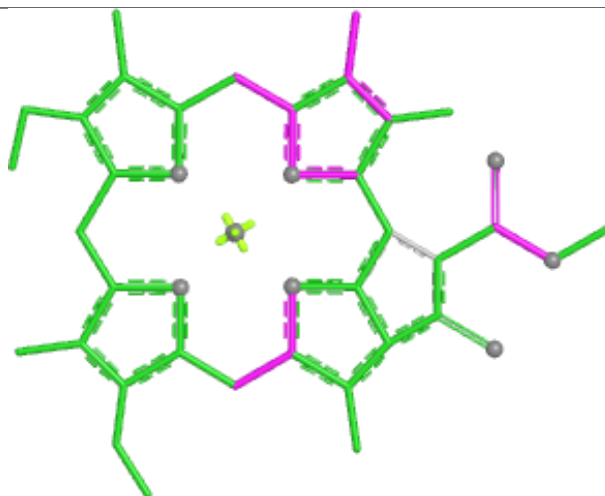
Ligand CLA 6 611



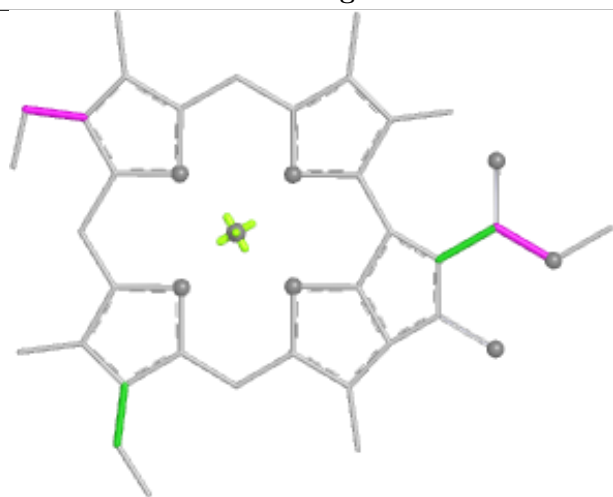
Ligand CLA F 304



Bond lengths



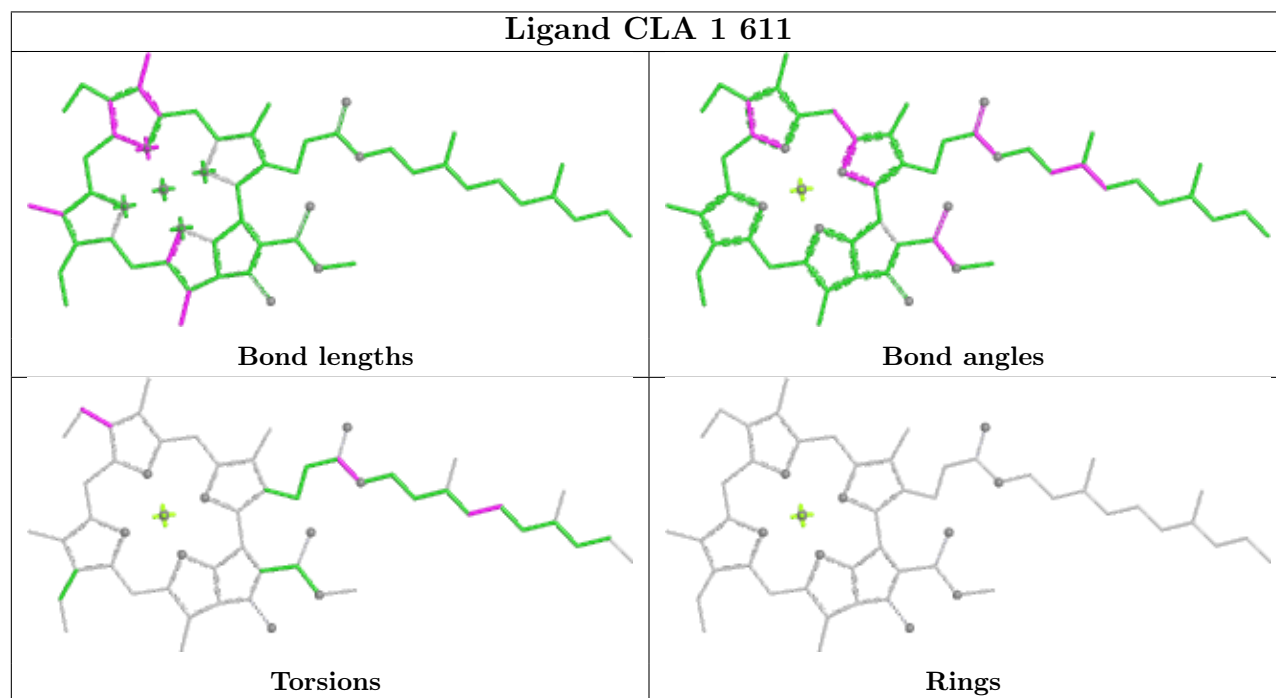
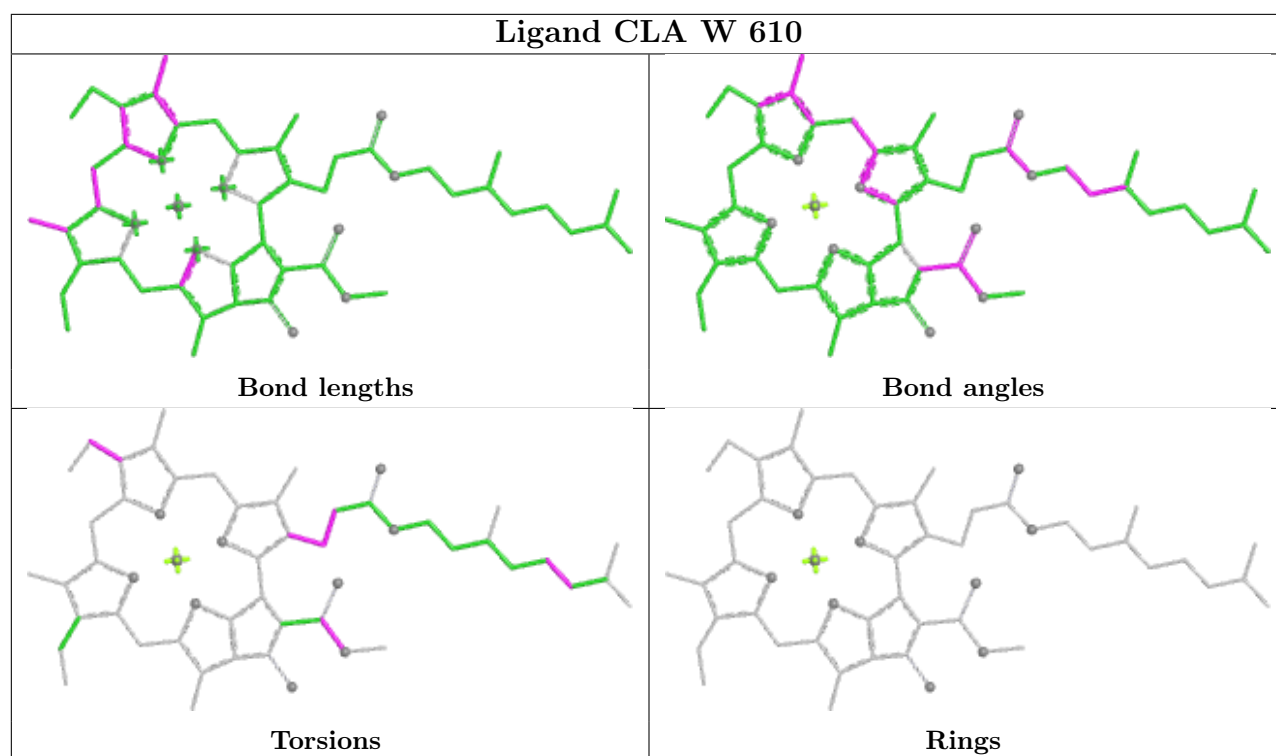
Bond angles



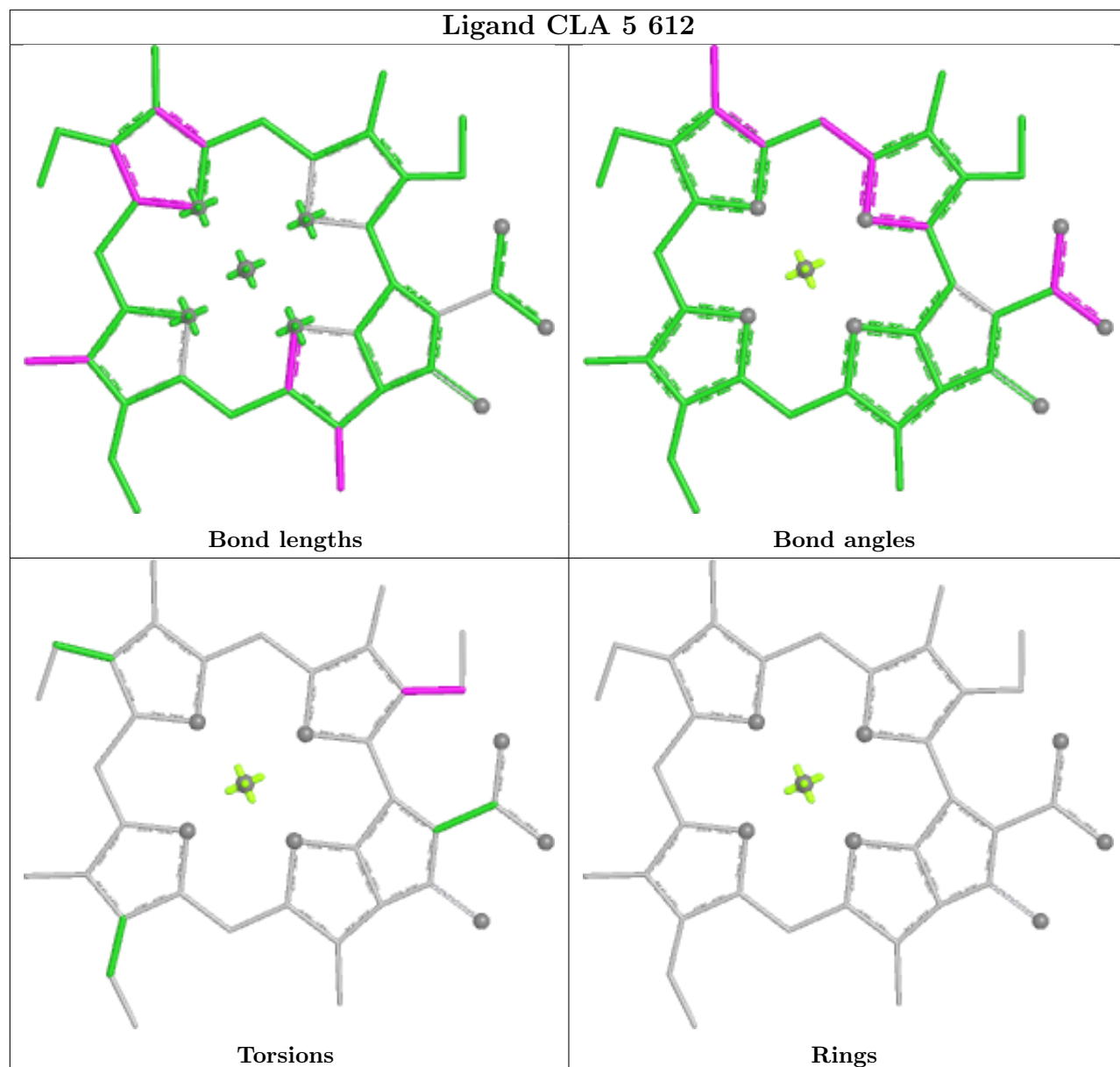
Torsions



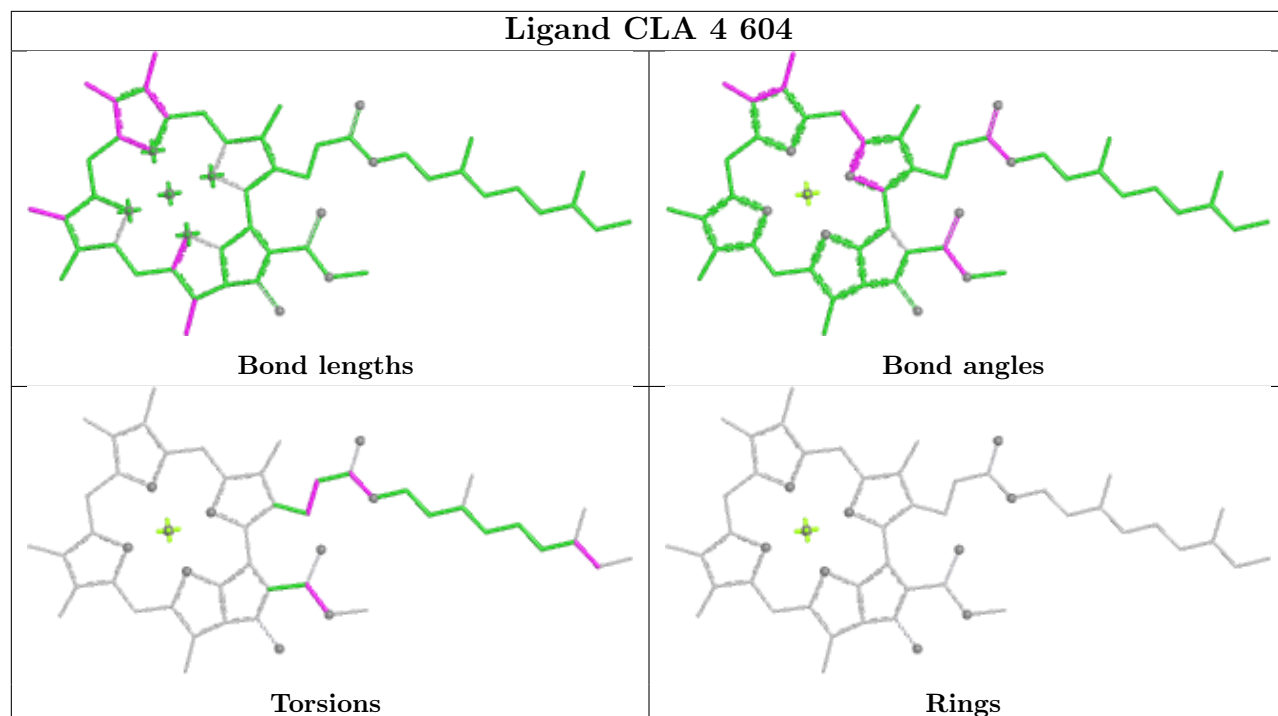
Rings



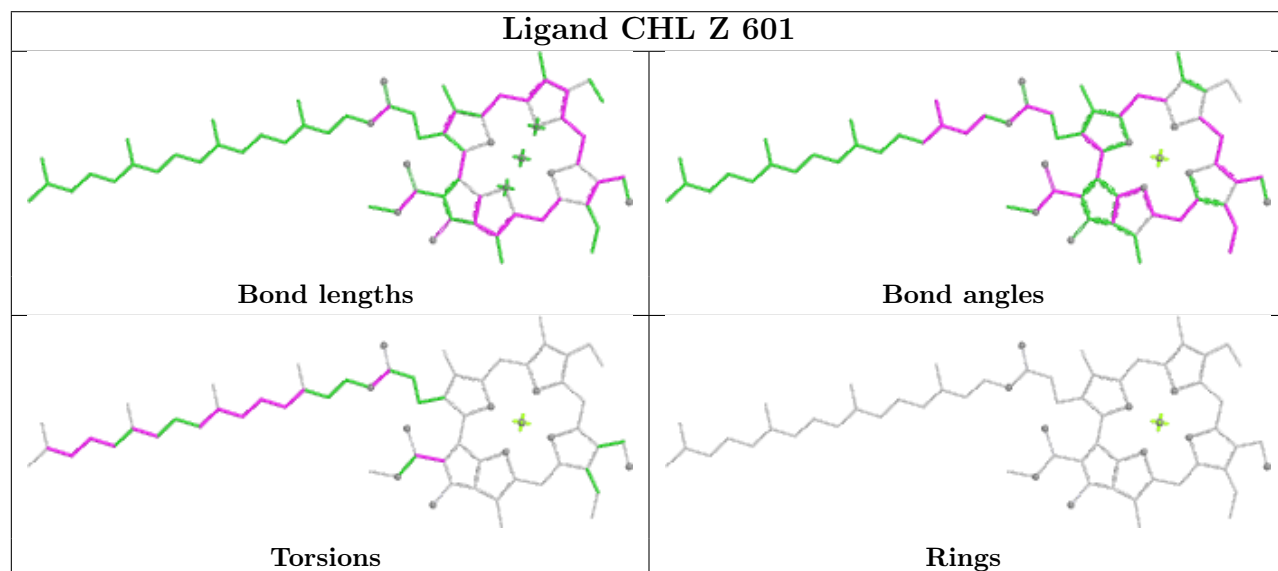
Ligand CLA 5 612

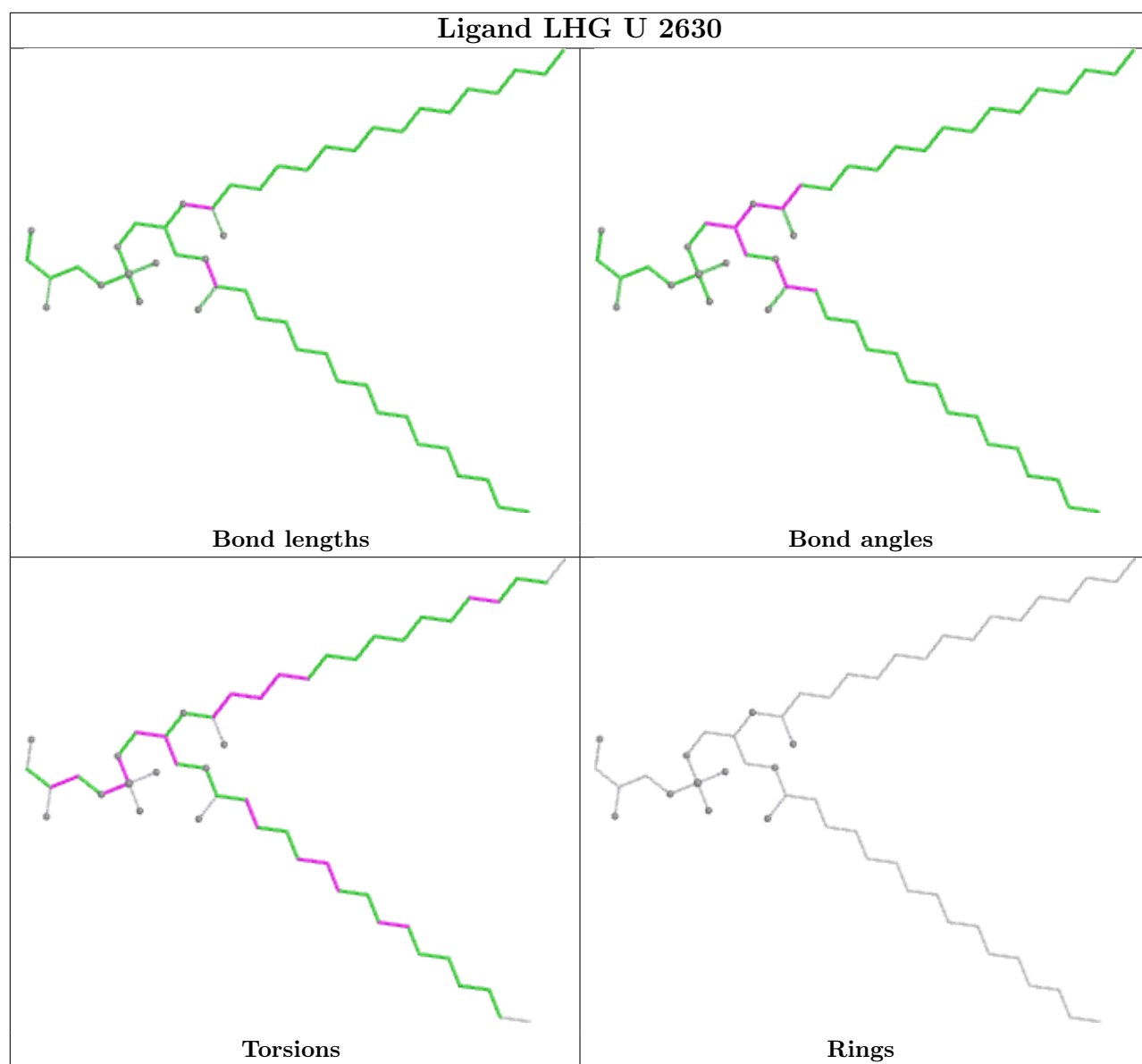


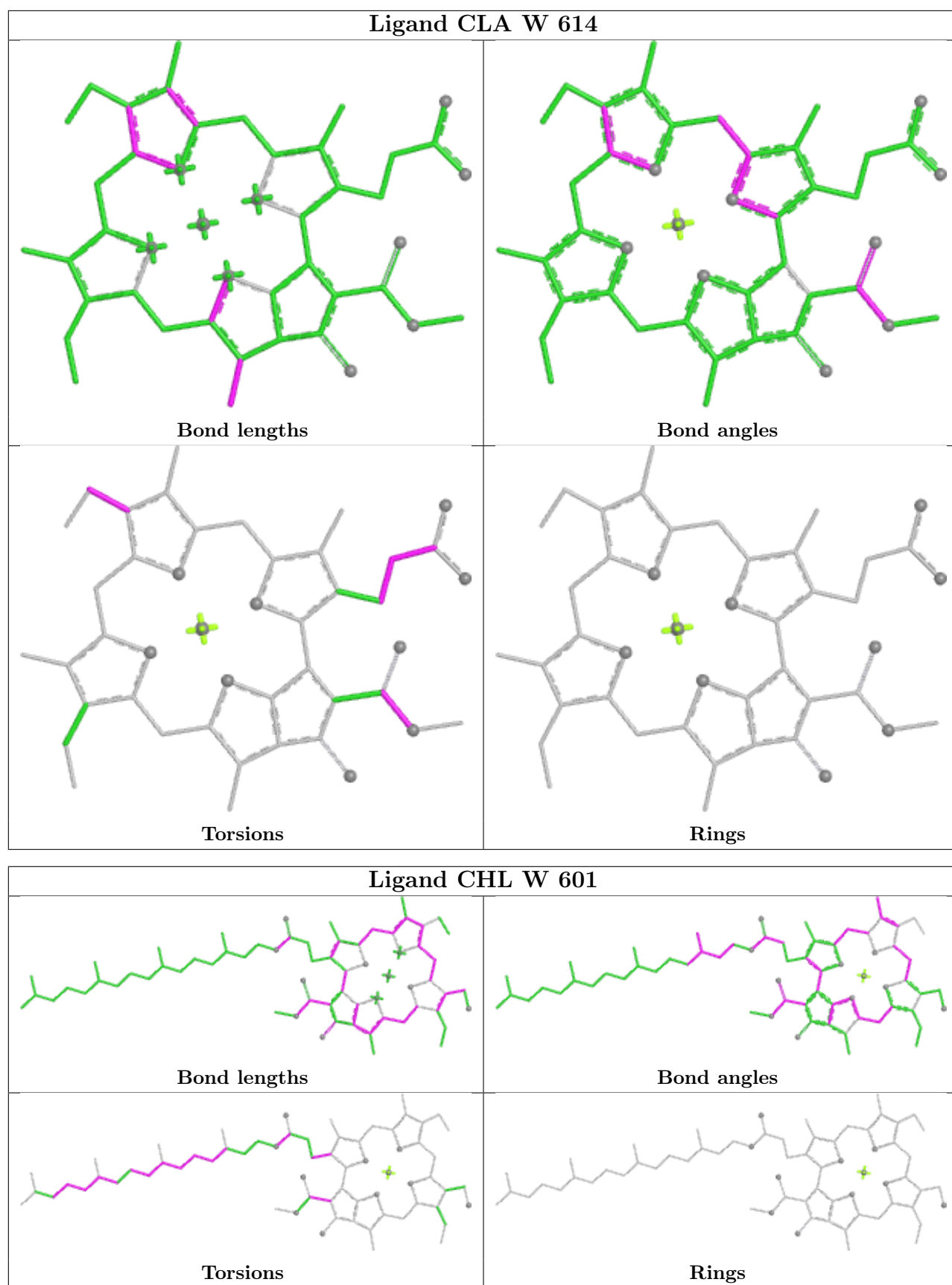
Ligand CLA 4 604



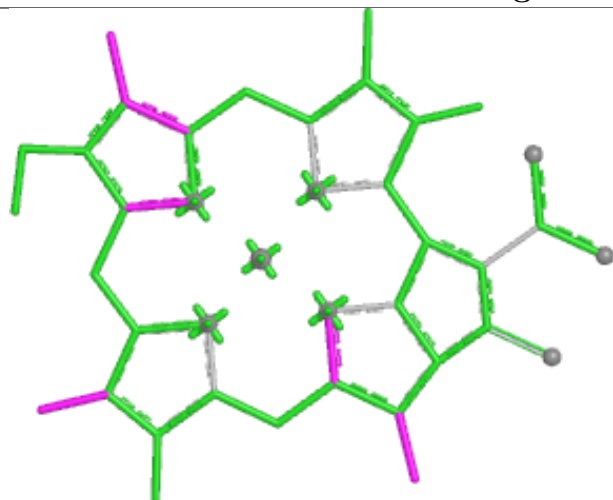
Ligand CHL Z 601



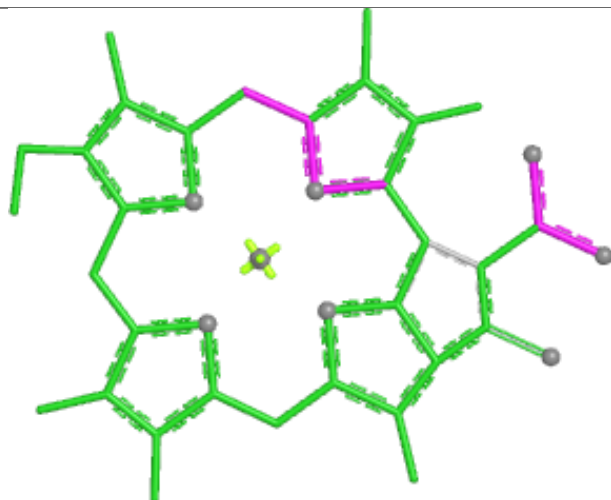




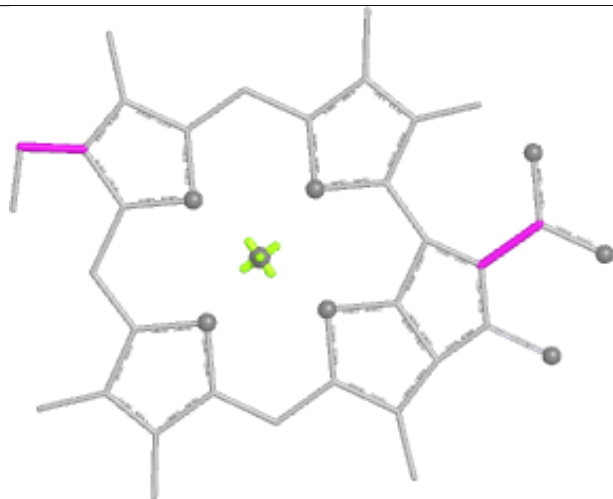
Ligand CLA H 202



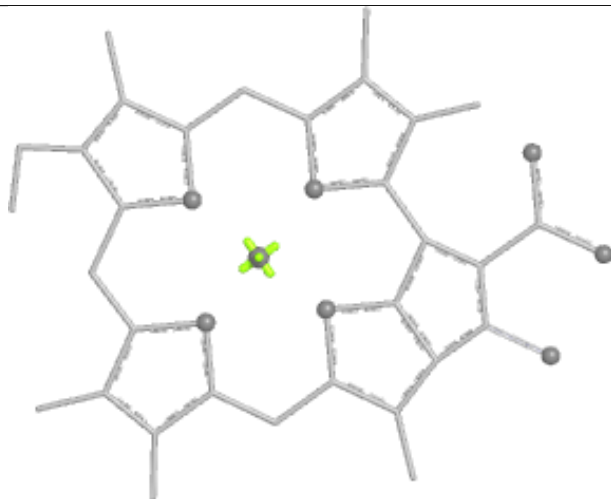
Bond lengths



Bond angles

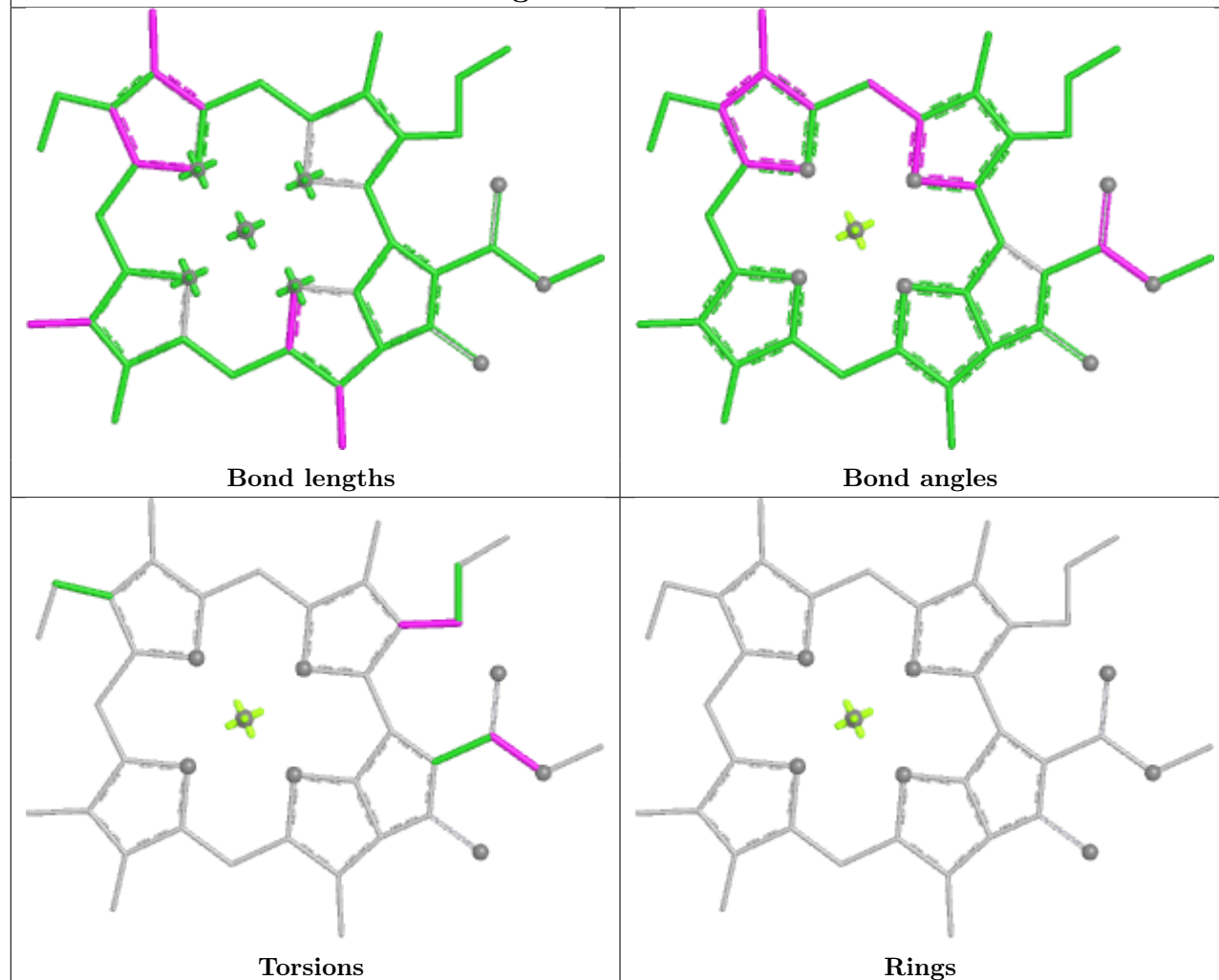


Torsions

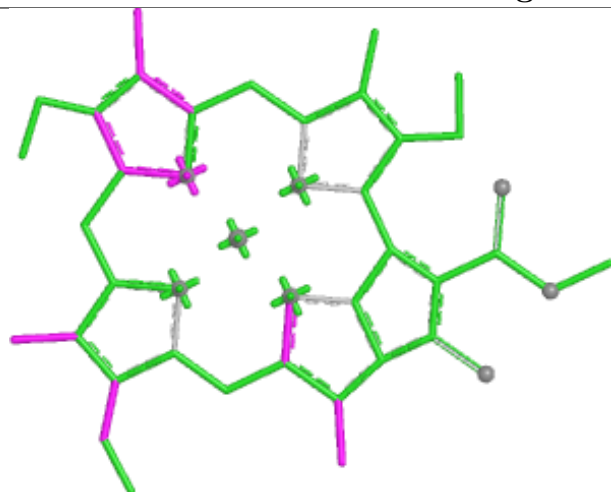


Rings

Ligand CLA 2 604



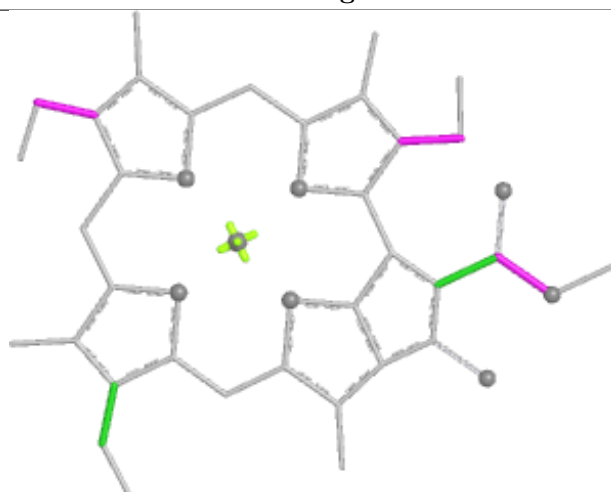
Ligand CLA F 303



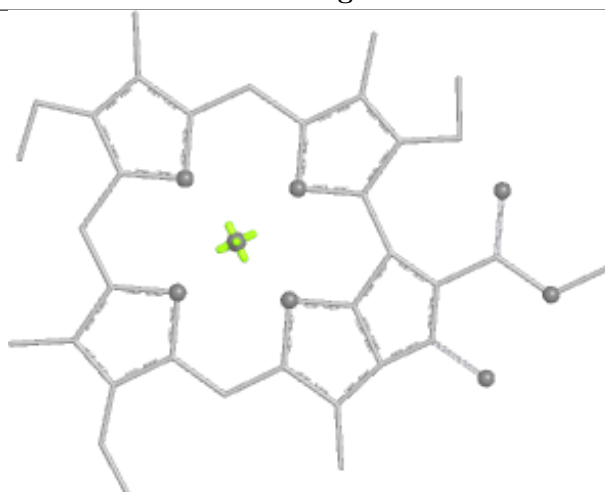
Bond lengths



Bond angles

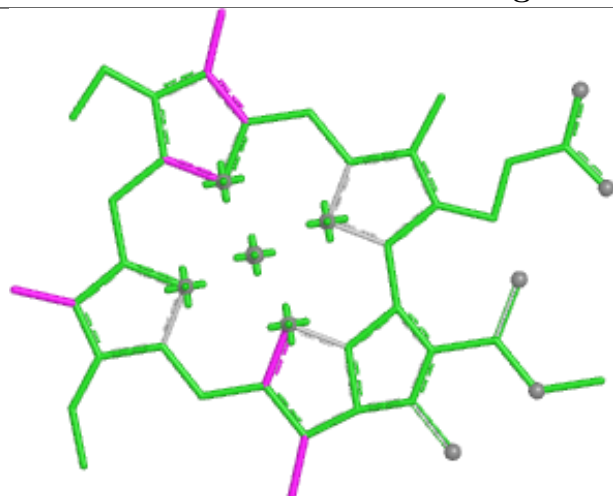


Torsions

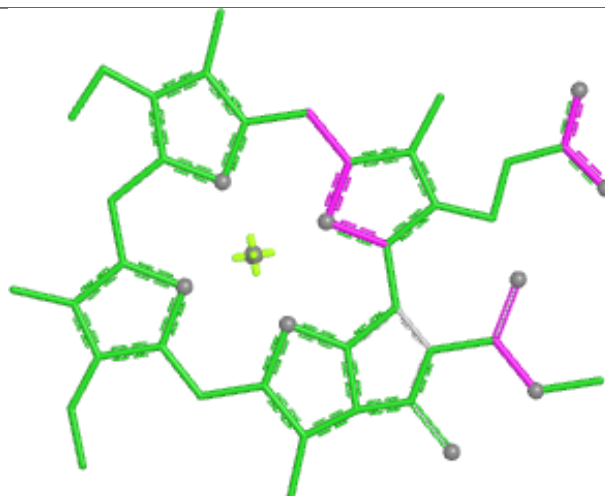


Rings

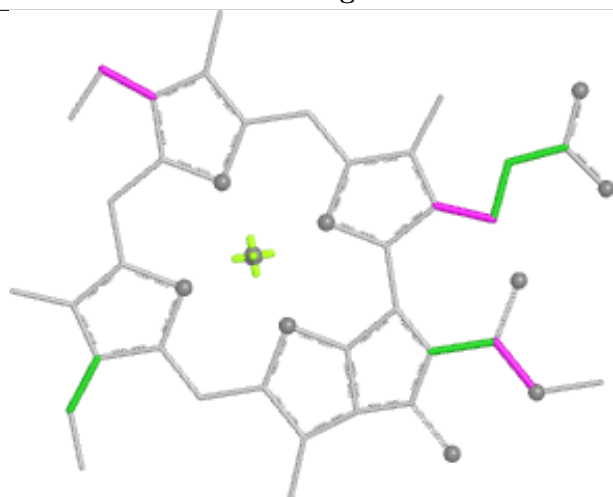
Ligand CLA K 201



Bond lengths



Bond angles

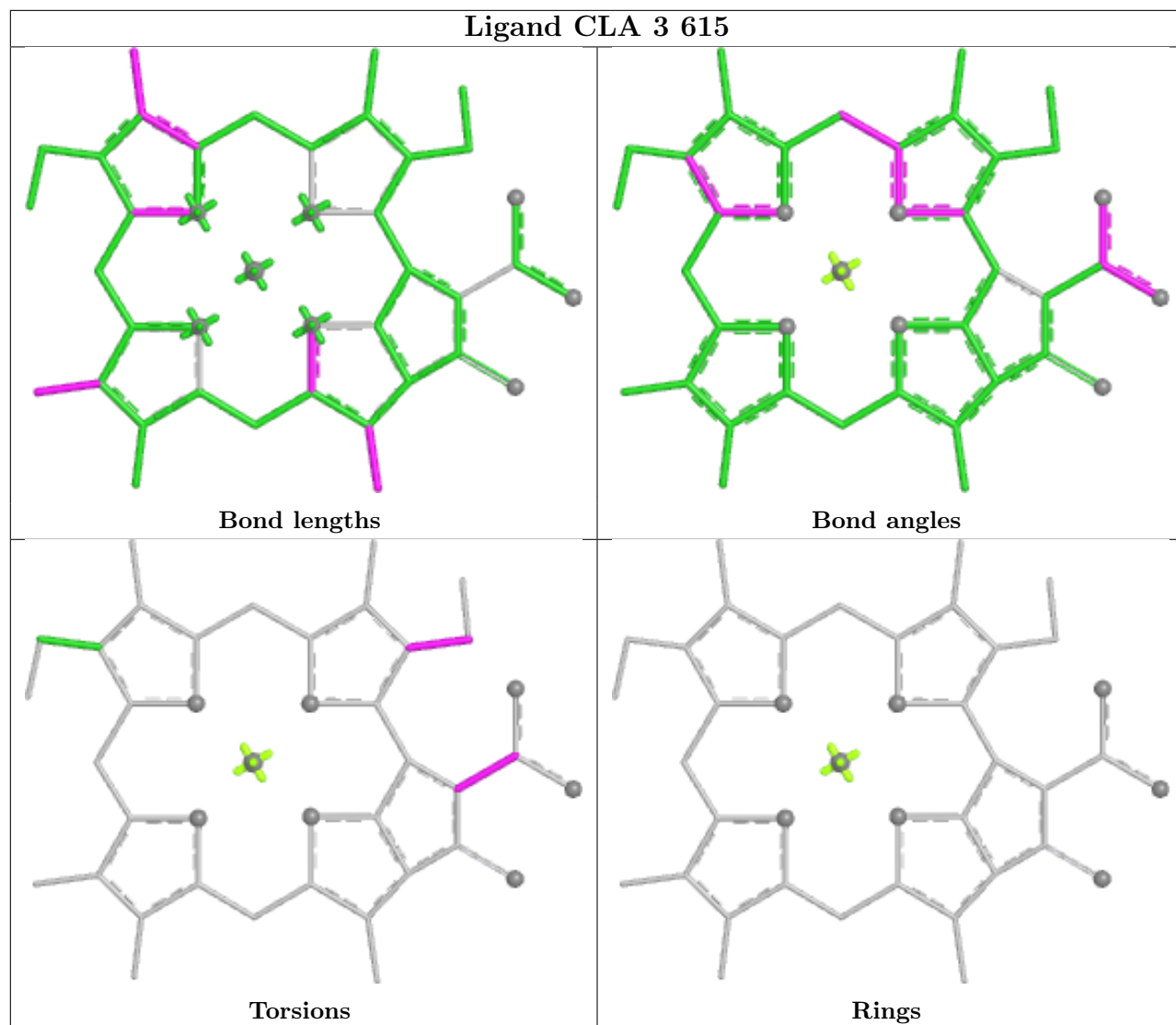


Torsions

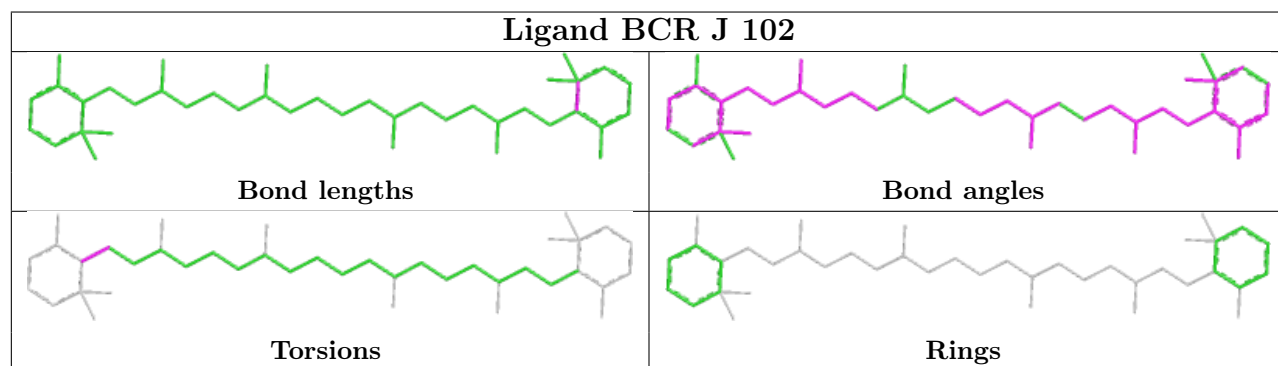


Rings

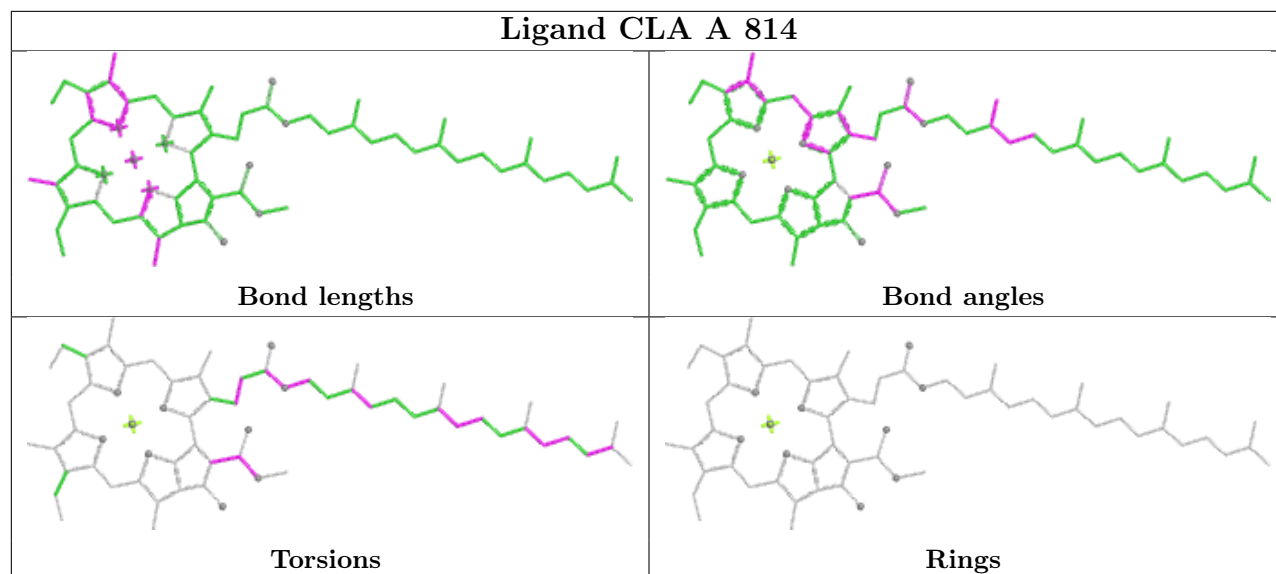
Ligand CLA 3 615



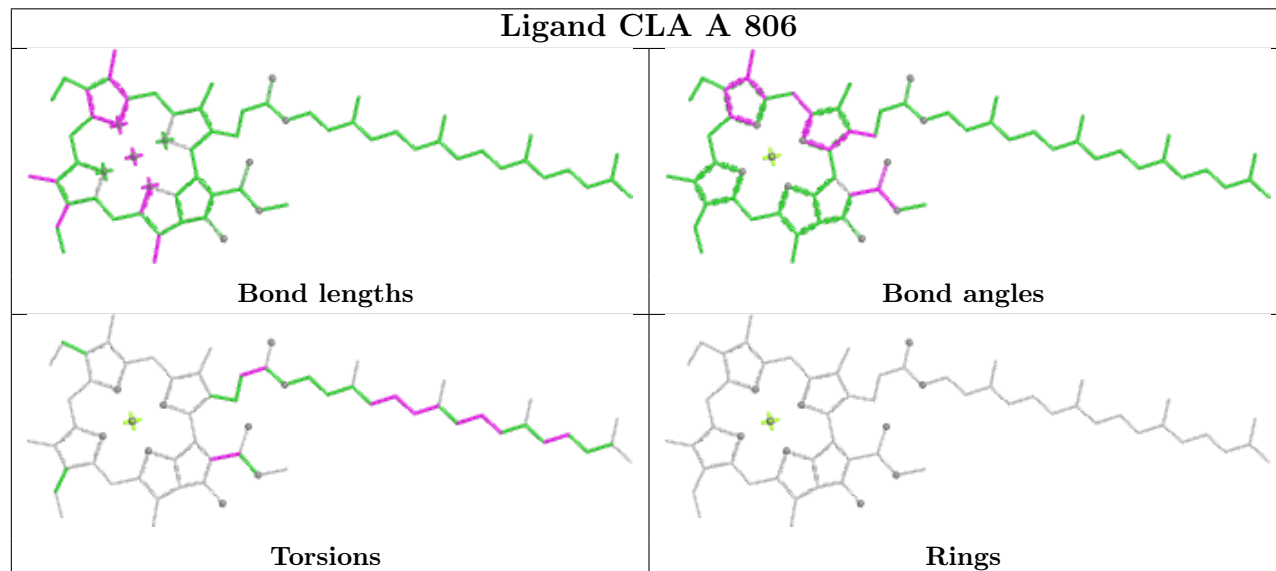
Ligand BCR J 102



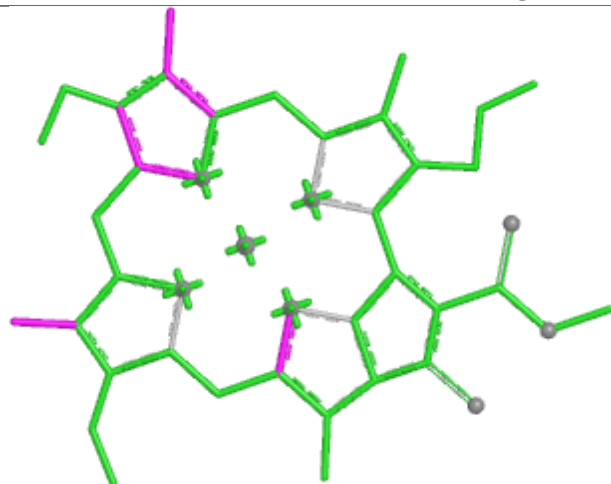
Ligand CLA A 814



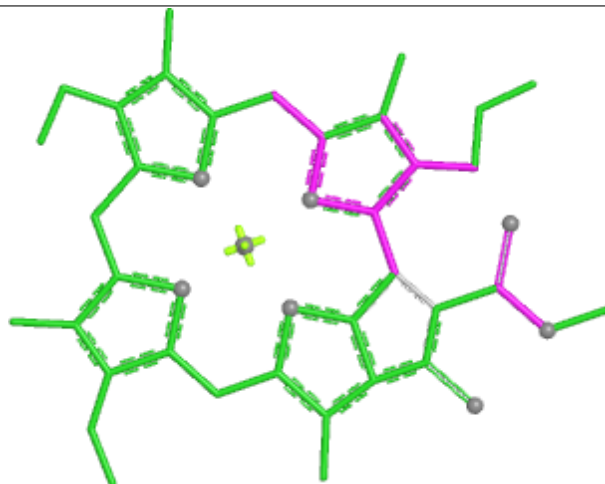
Ligand CLA A 806



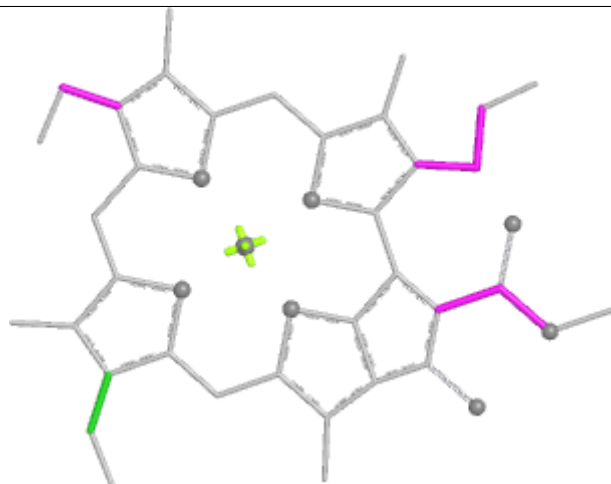
Ligand CLA X 612



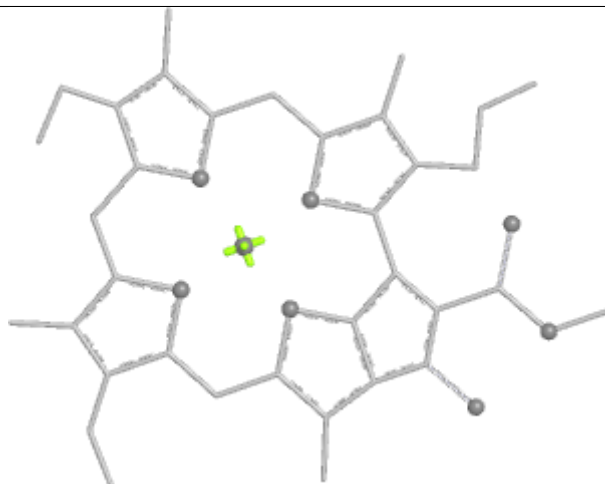
Bond lengths



Bond angles

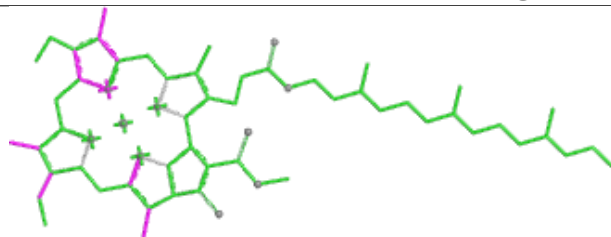


Torsions

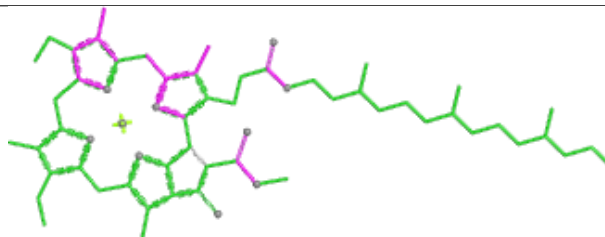


Rings

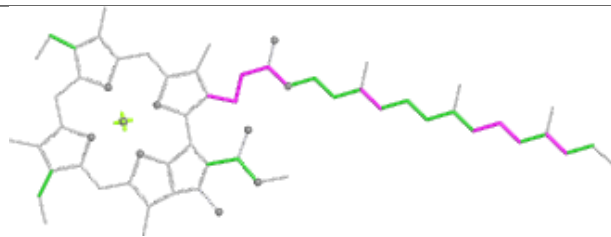
Ligand CLA B 827



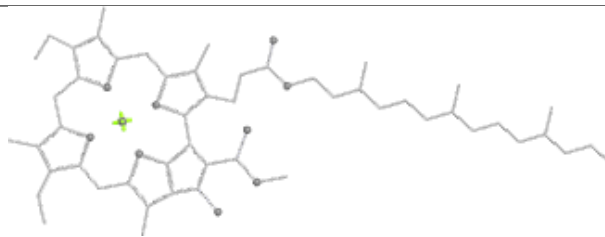
Bond lengths



Bond angles

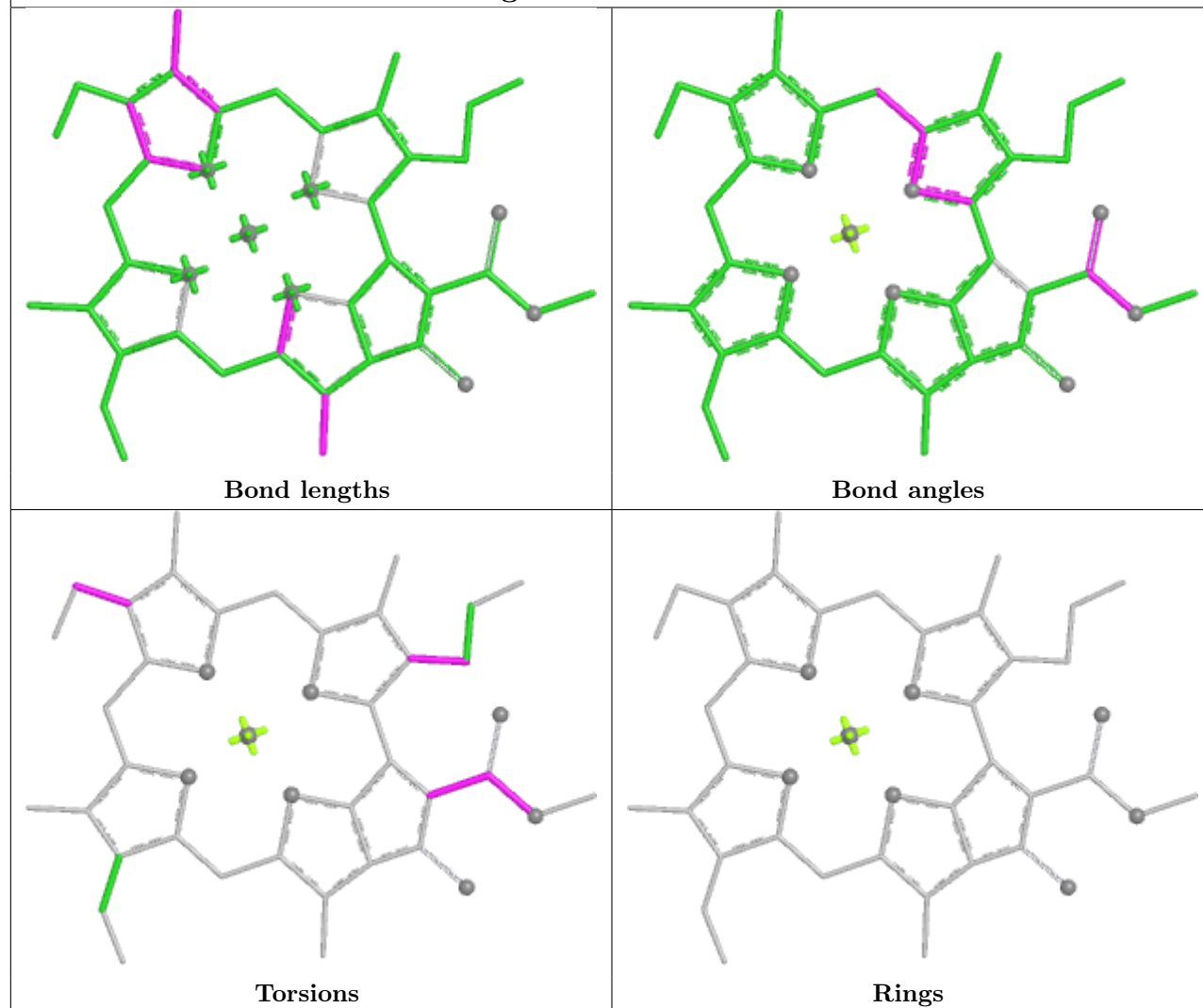


Torsions

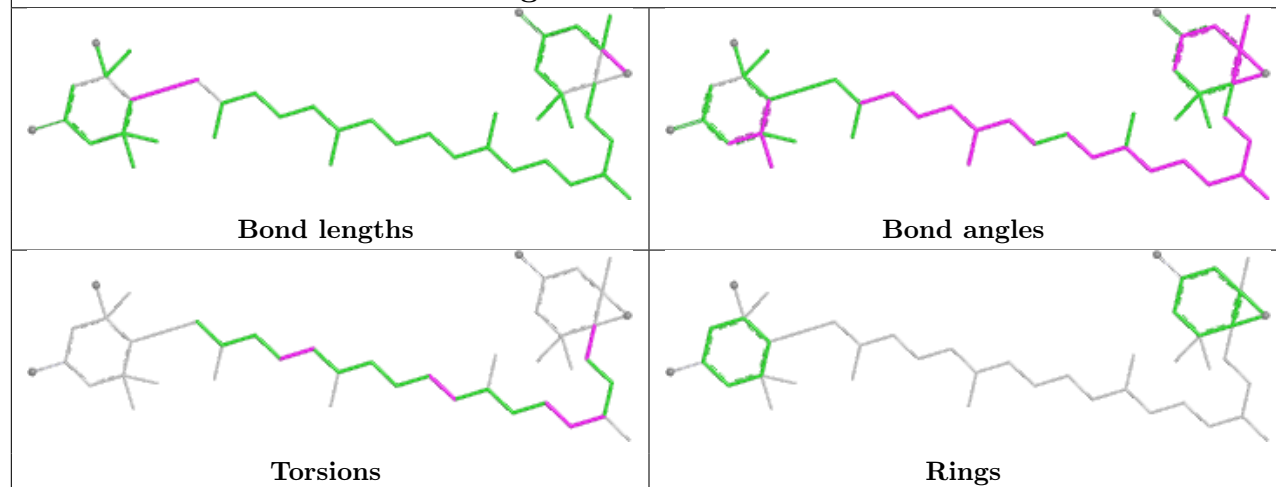


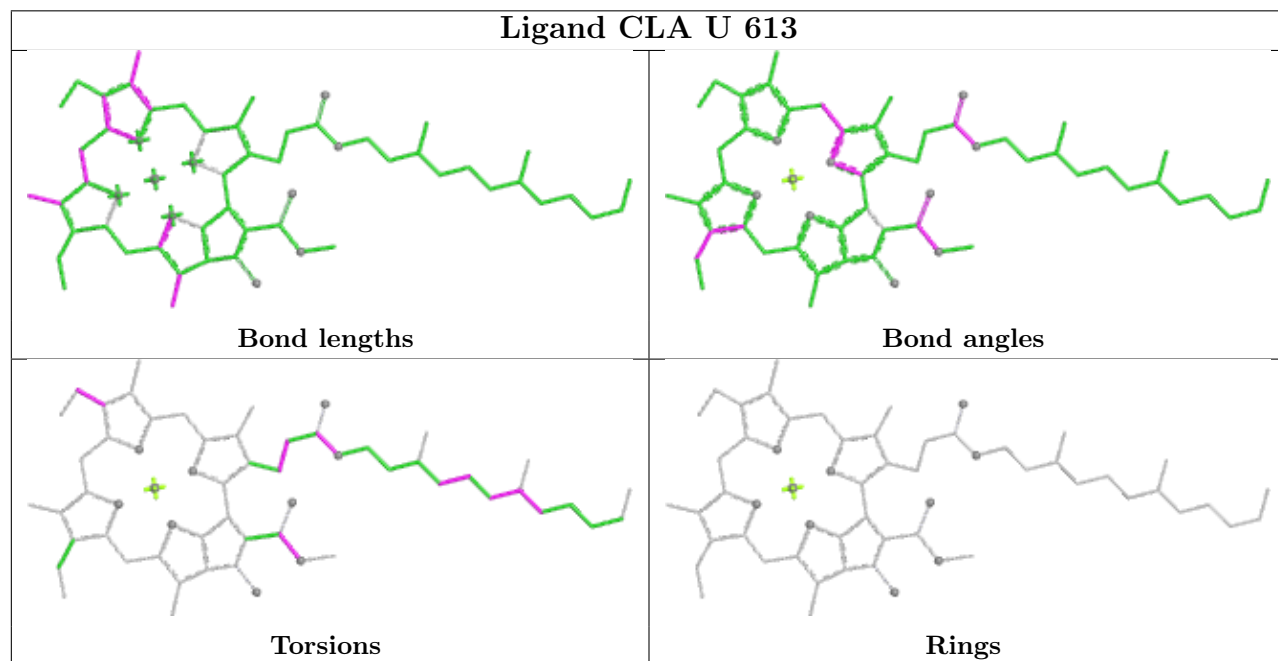
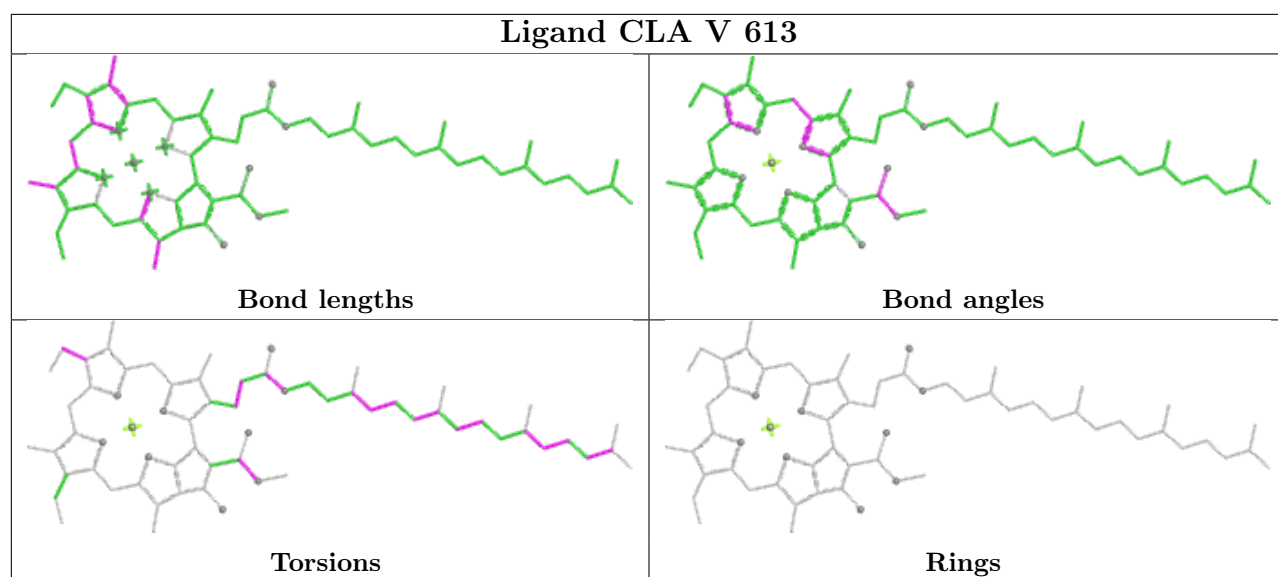
Rings

Ligand CLA Y 611

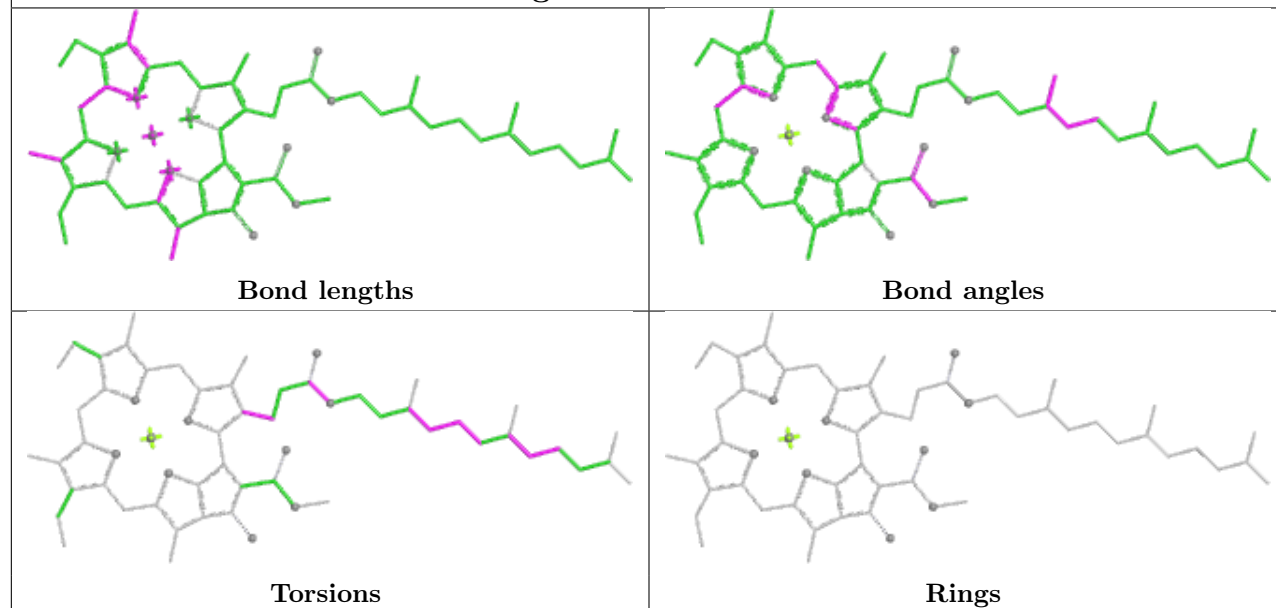


Ligand NEX U 1623

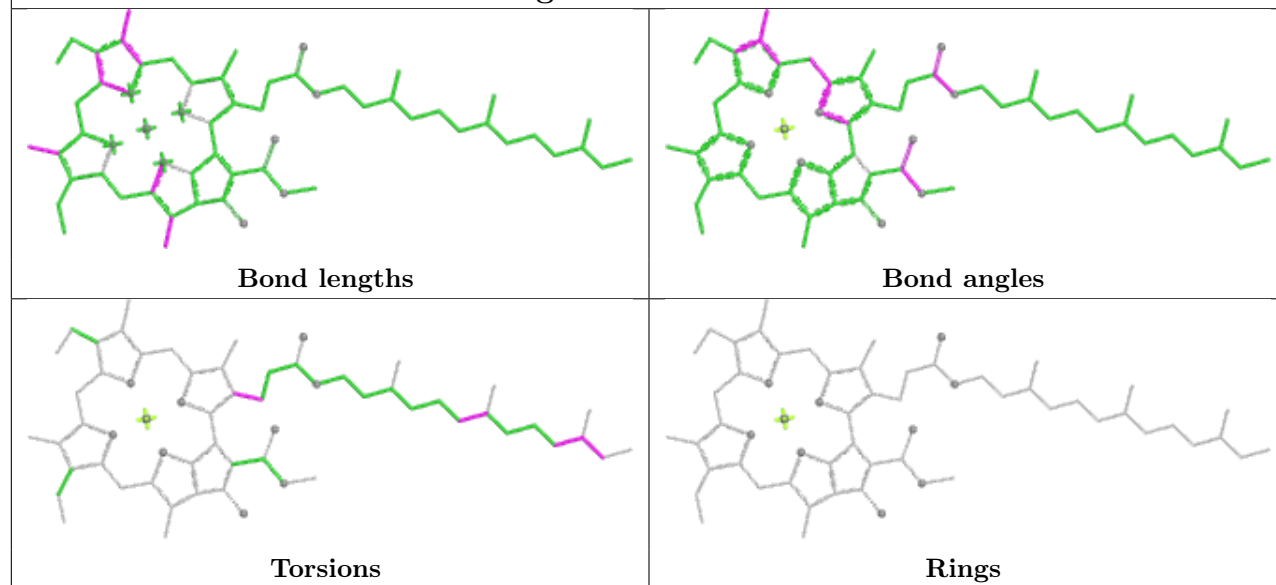


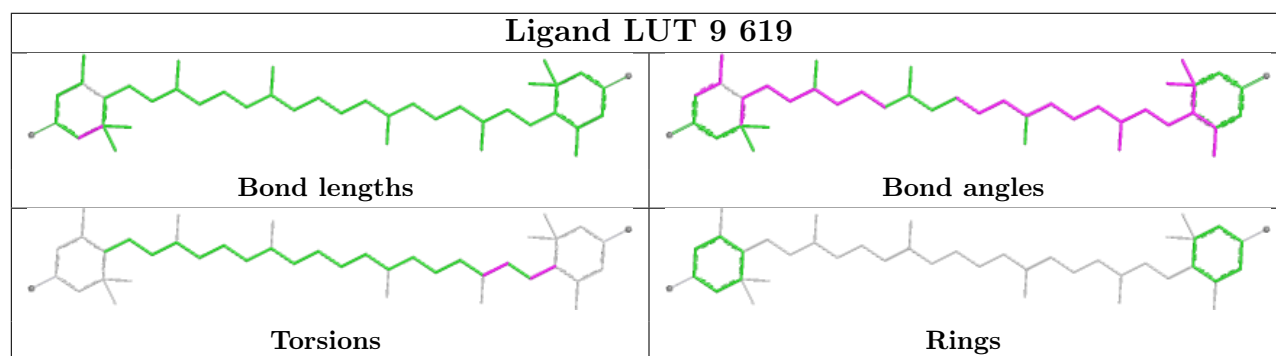
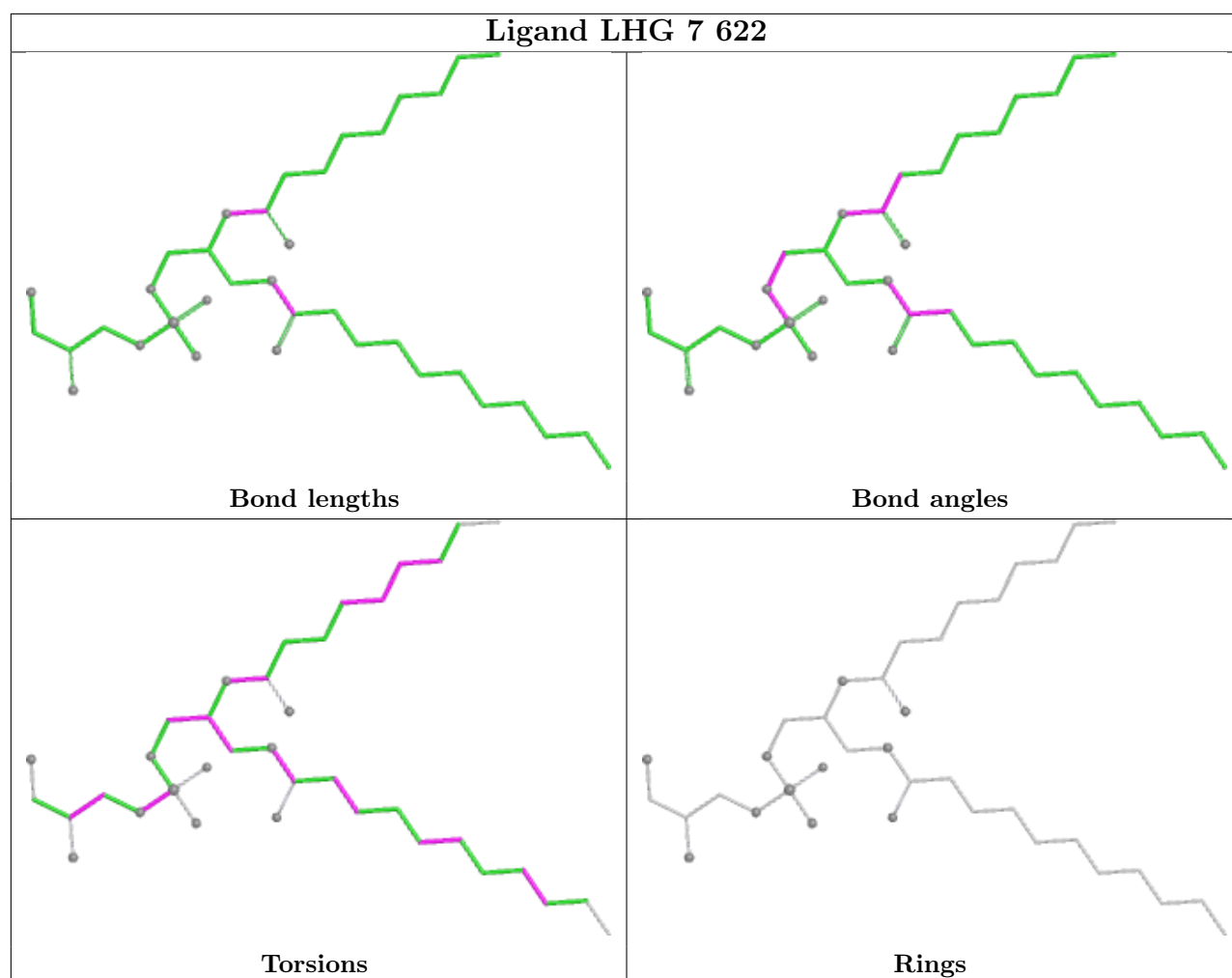


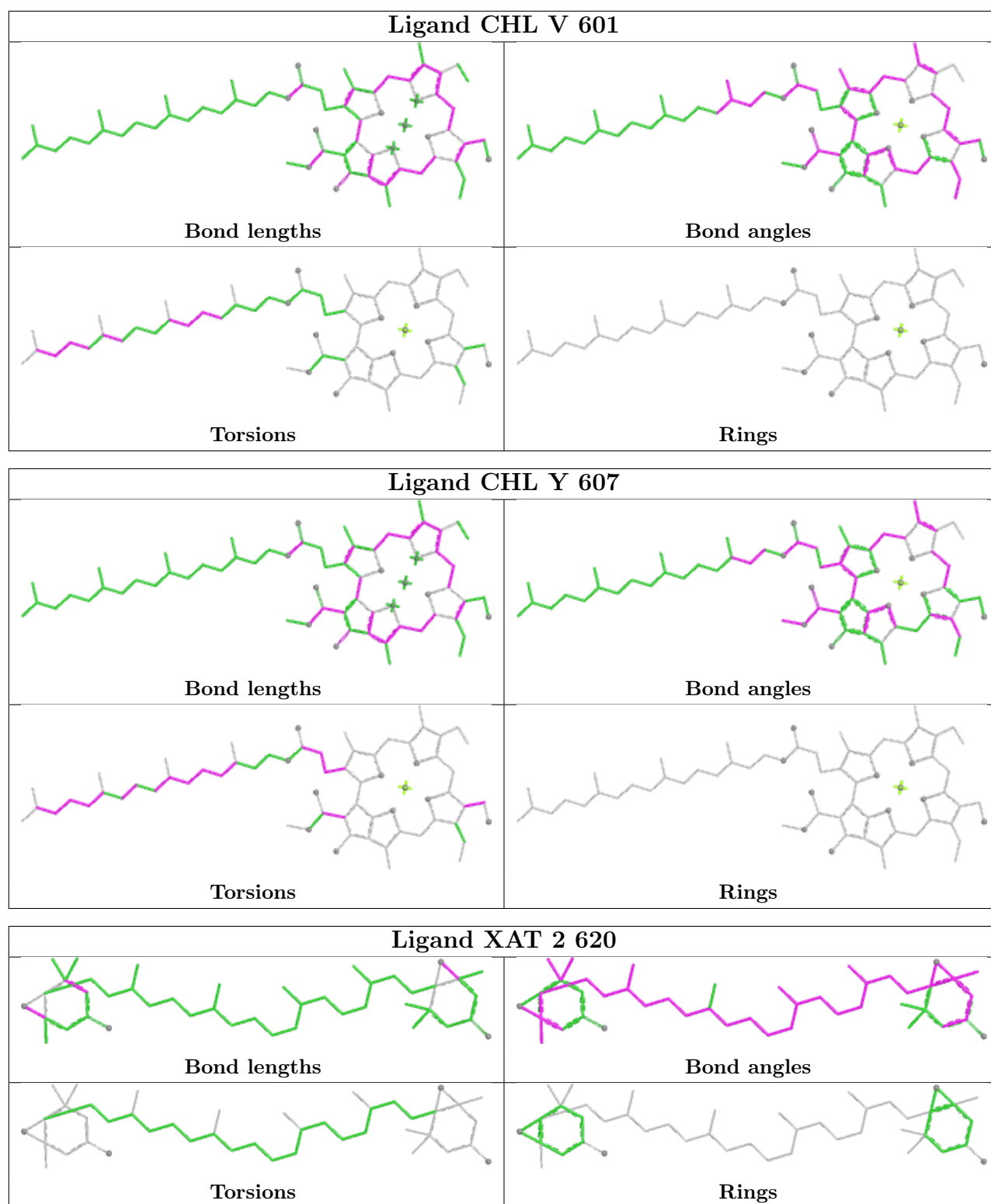
Ligand CLA B 818



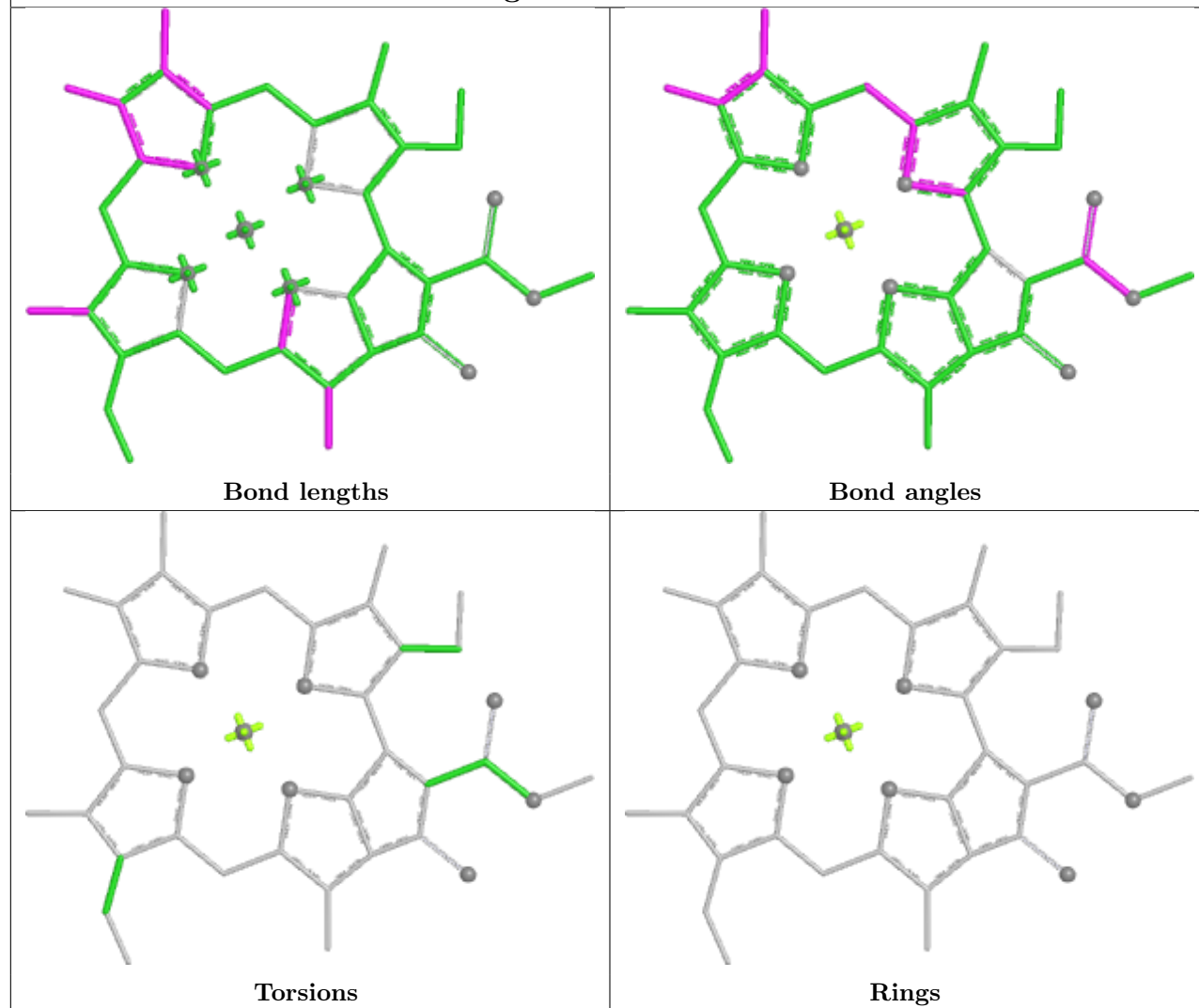
Ligand CLA 4 610



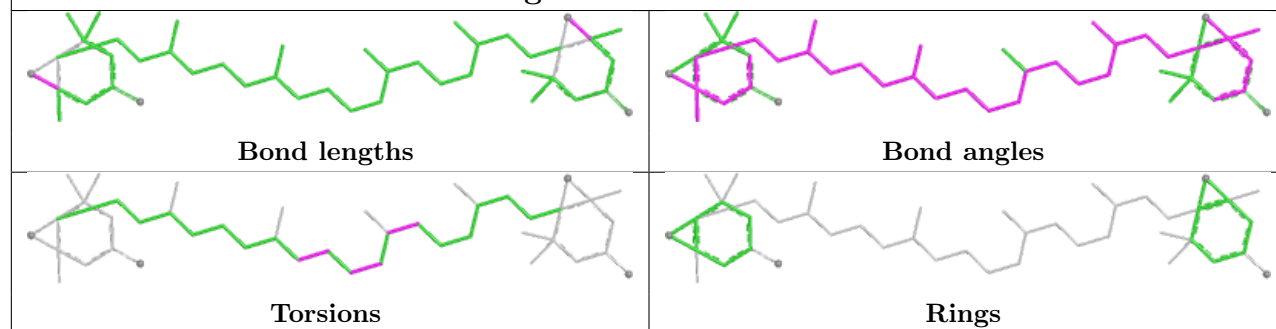


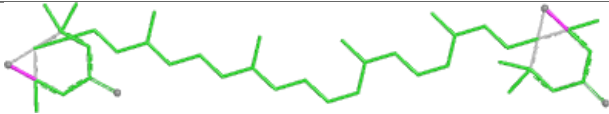
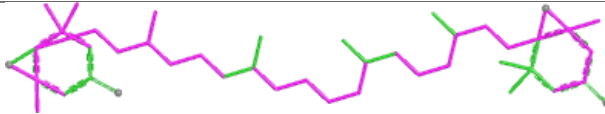
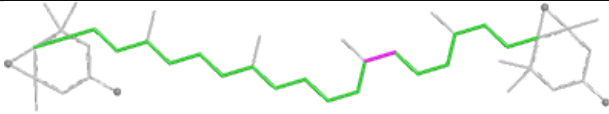
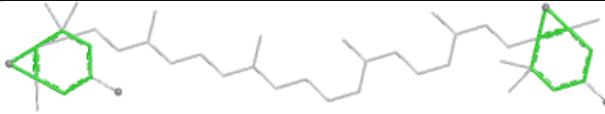


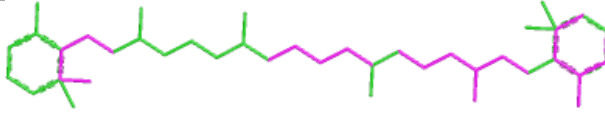
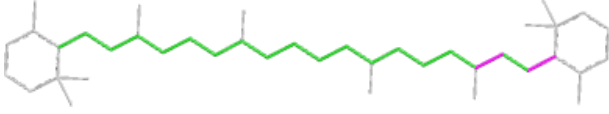
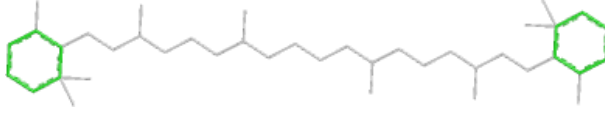
Ligand CLA 6 607

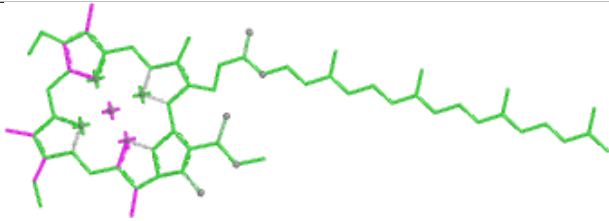
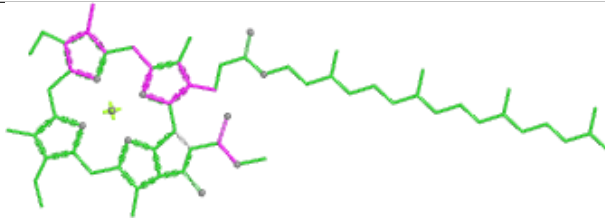
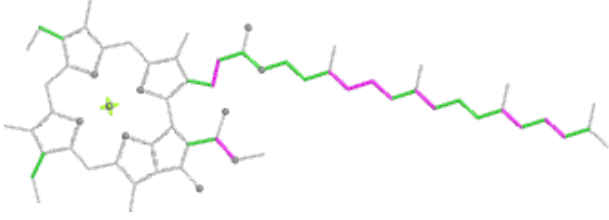
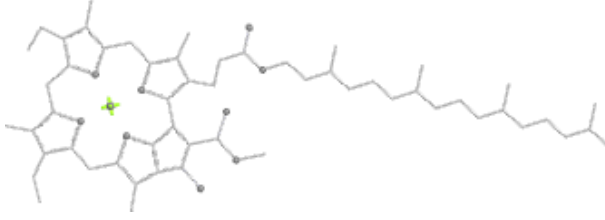


Ligand XAT Z 1622

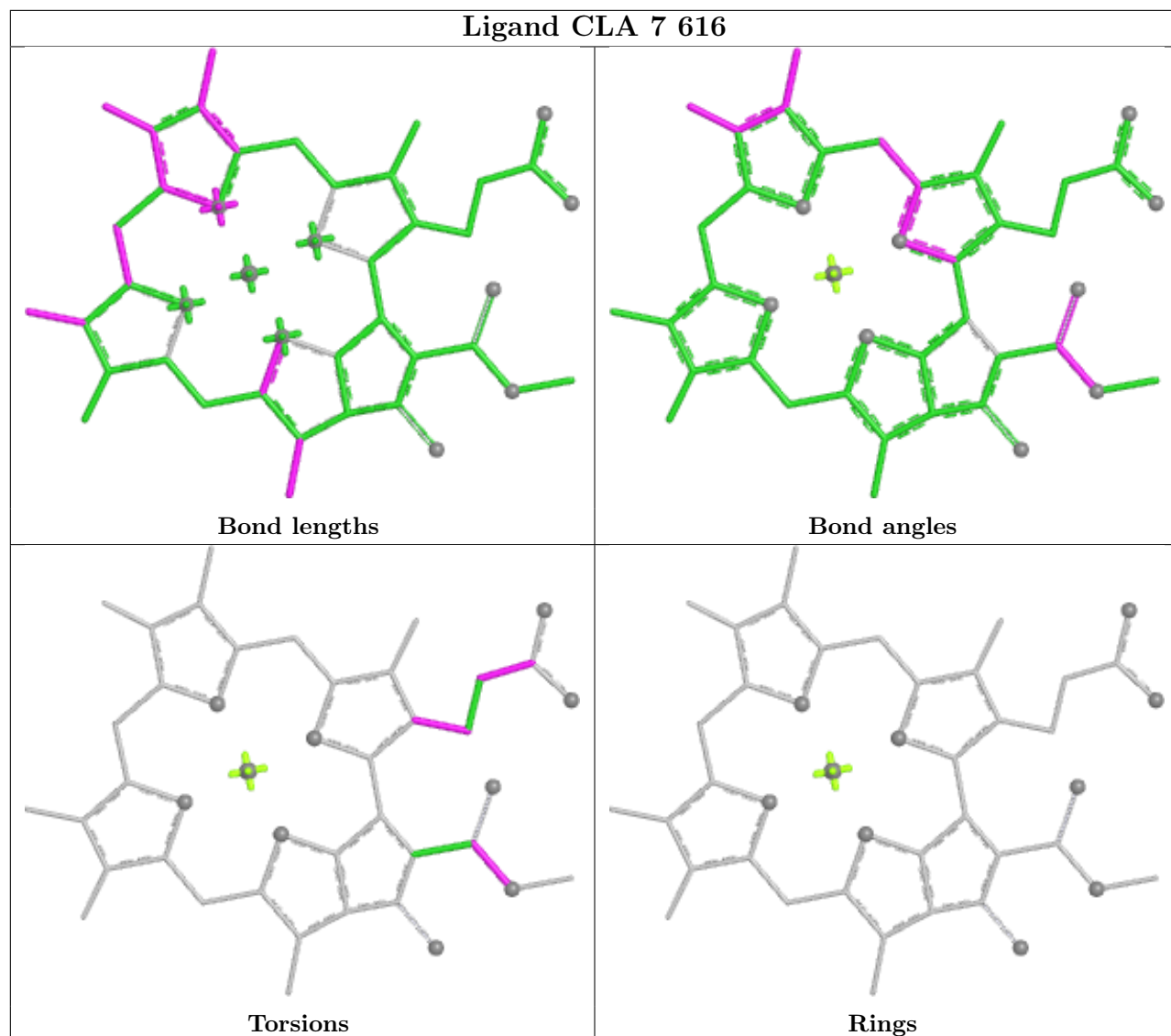


Ligand XAT W 1622	
	
Bond lengths	Bond angles
	
Torsions	Rings

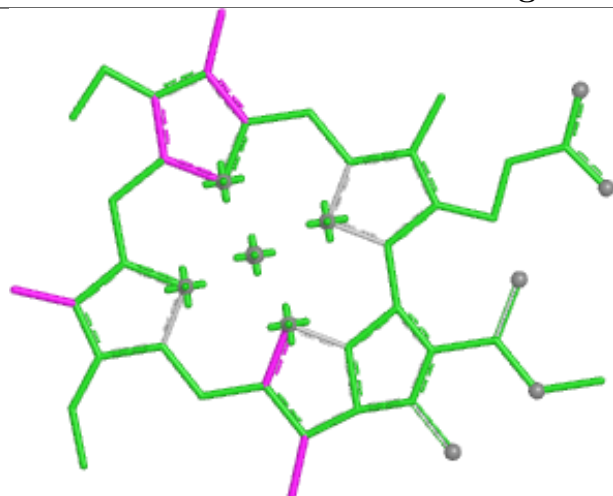
Ligand BCR B 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

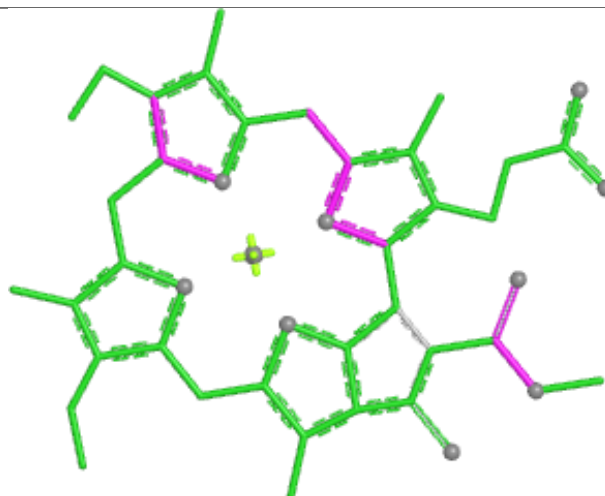
Ligand CLA 7 616



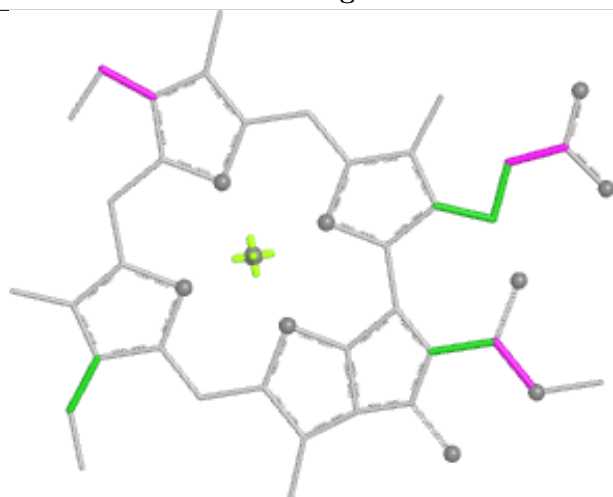
Ligand CLA 9 601



Bond lengths



Bond angles

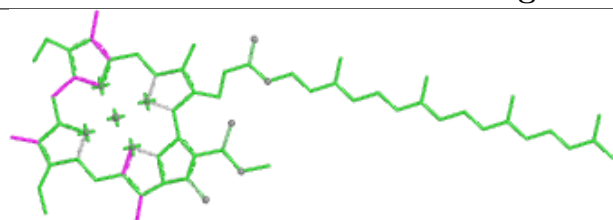


Torsions

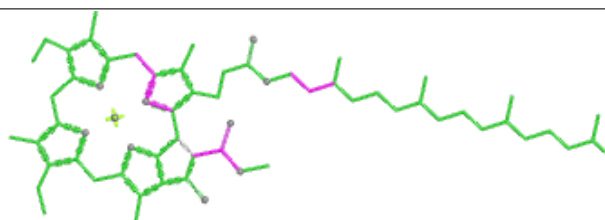


Rings

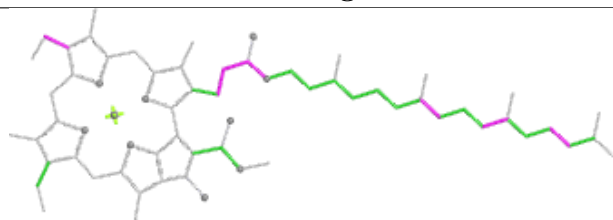
Ligand CLA 9 613



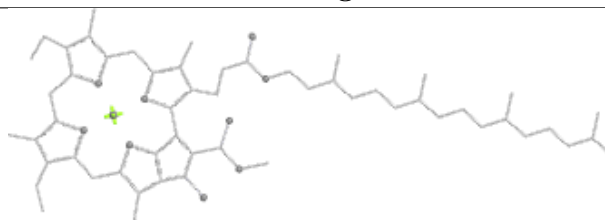
Bond lengths



Bond angles

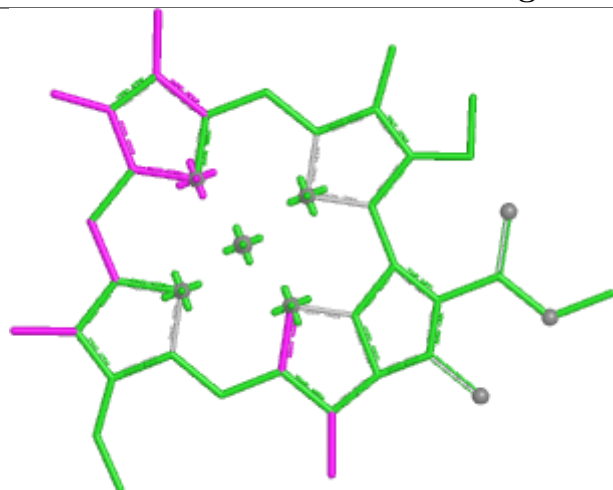


Torsions



Rings

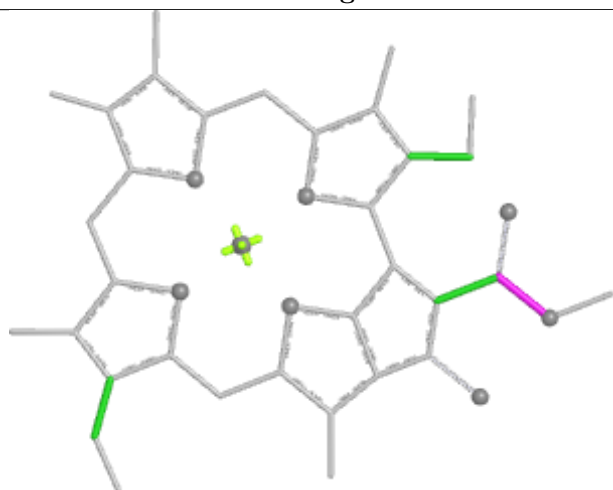
Ligand CLA 8 607



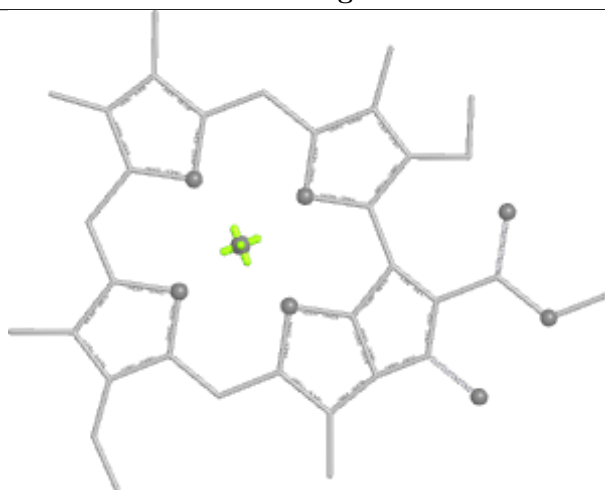
Bond lengths



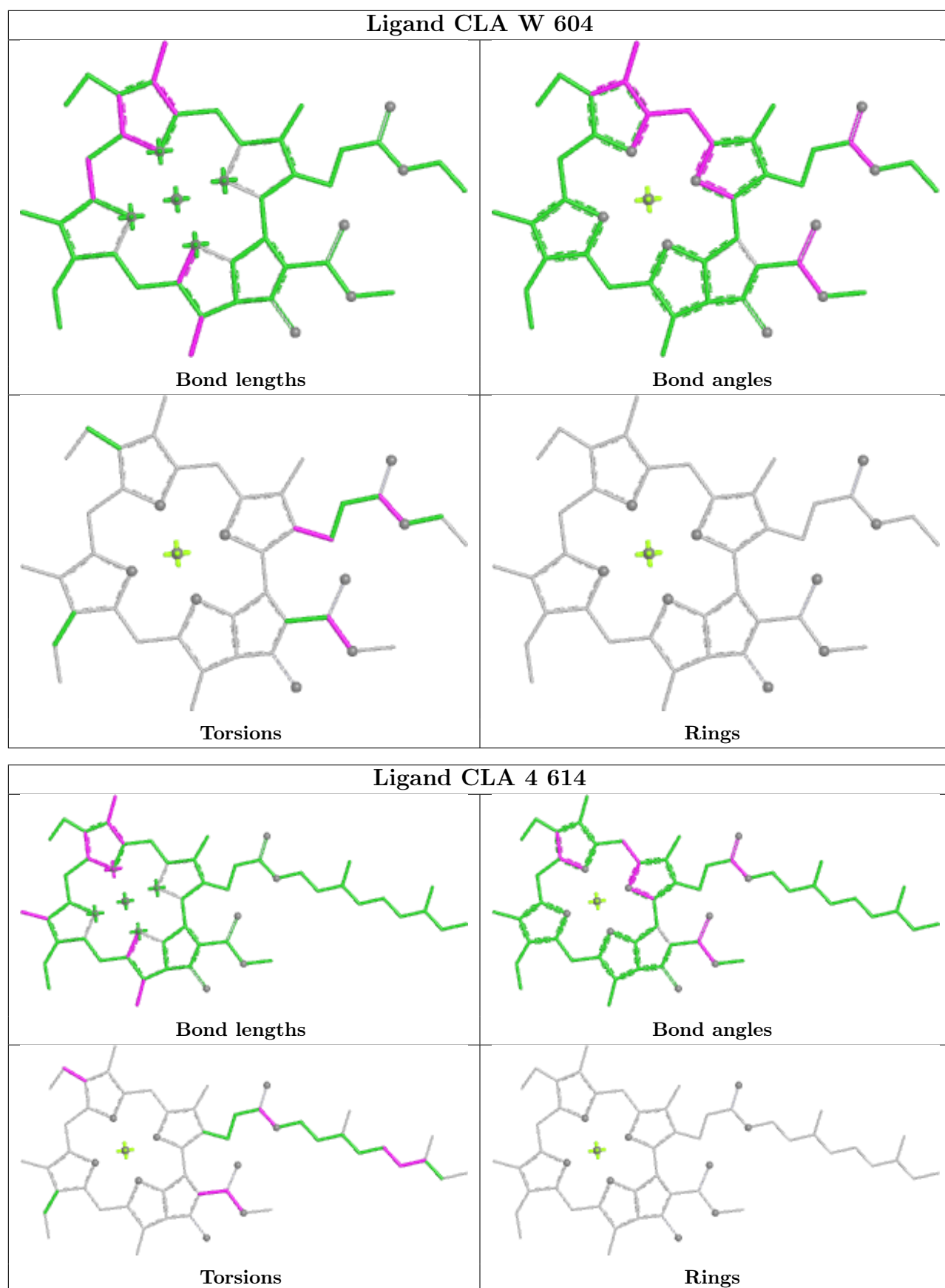
Bond angles

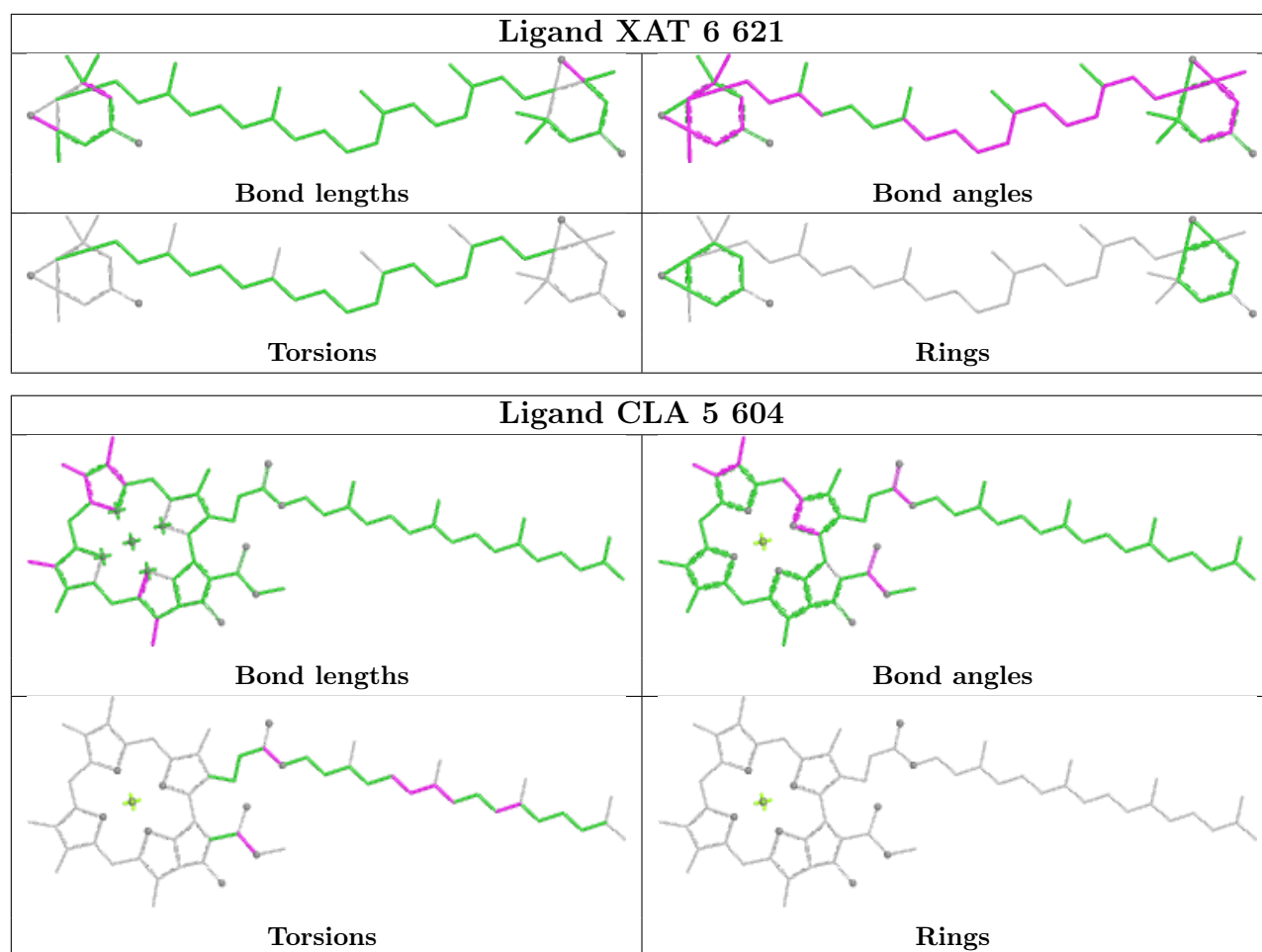


Torsions

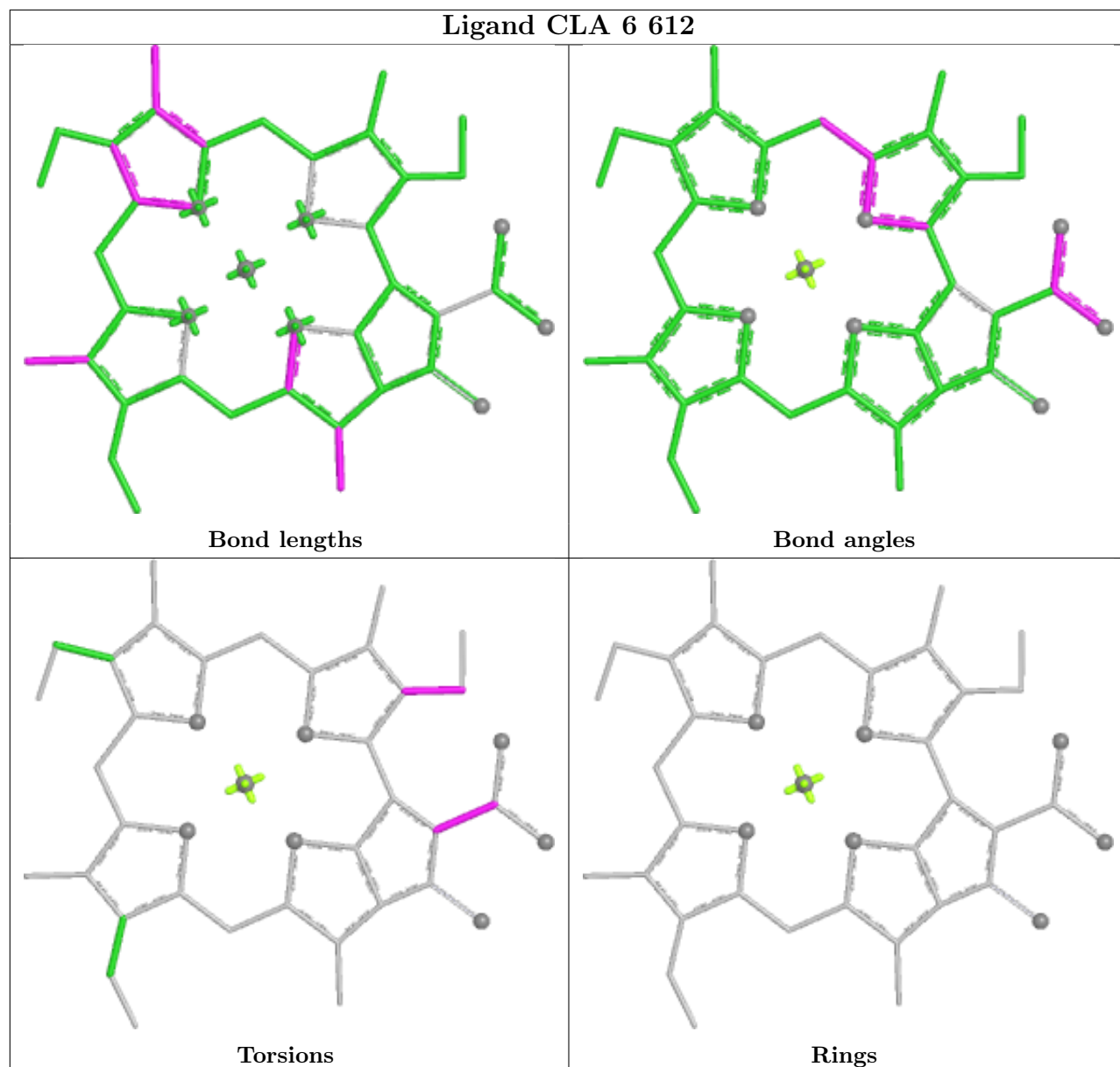


Rings

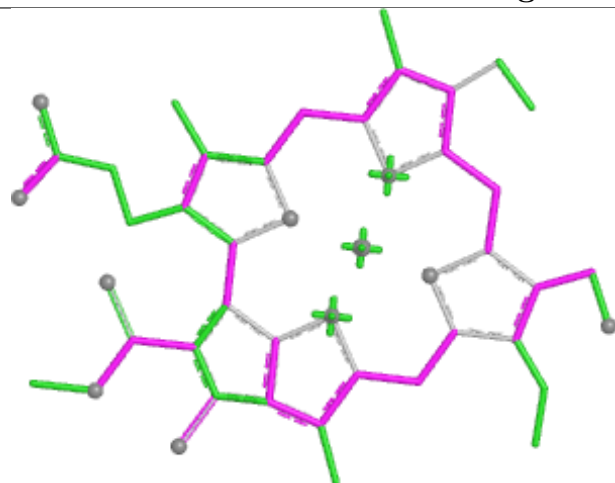




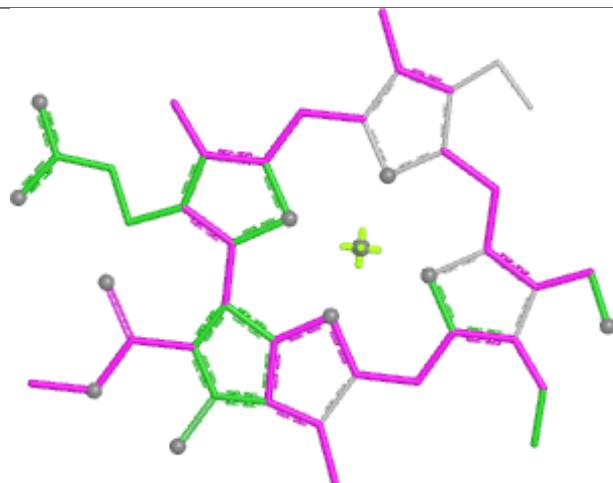
Ligand CLA 6 612



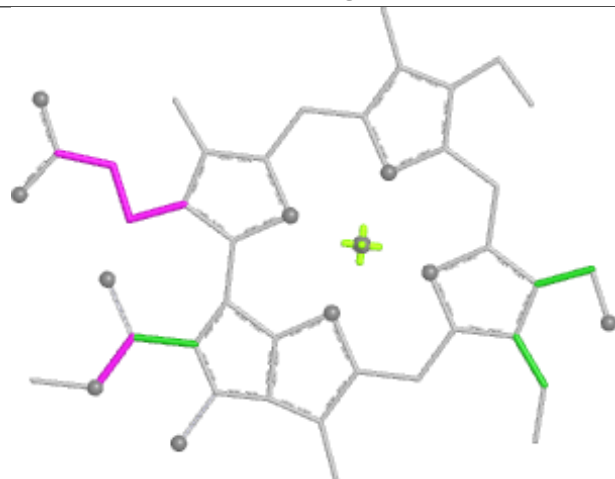
Ligand CHL Z 606



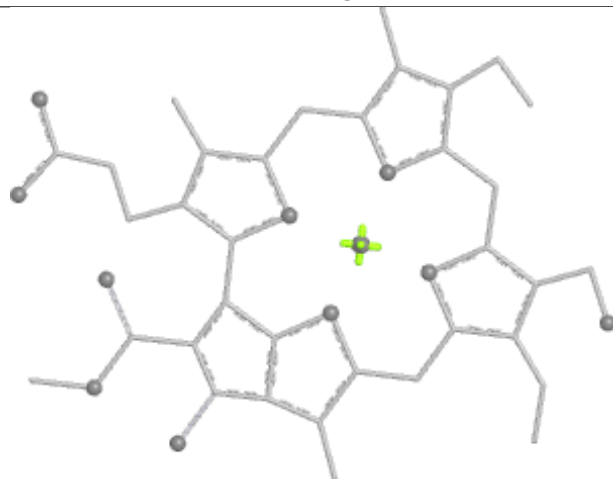
Bond lengths



Bond angles

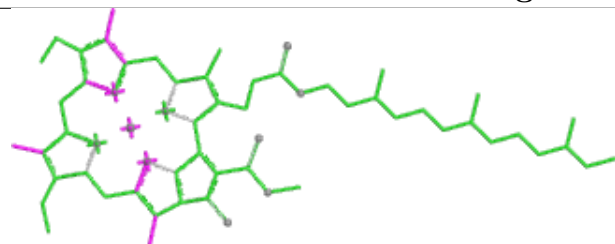


Torsions

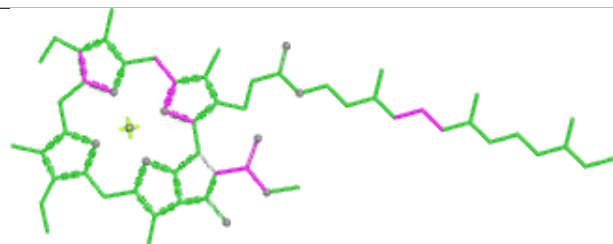


Rings

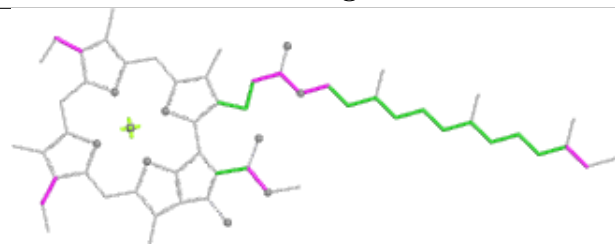
Ligand CLA A 835



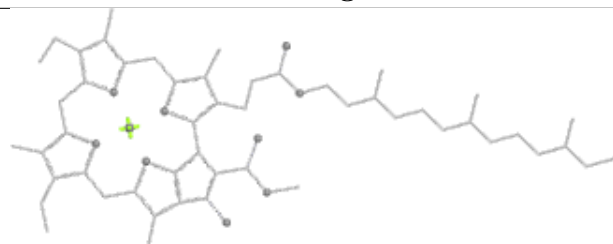
Bond lengths



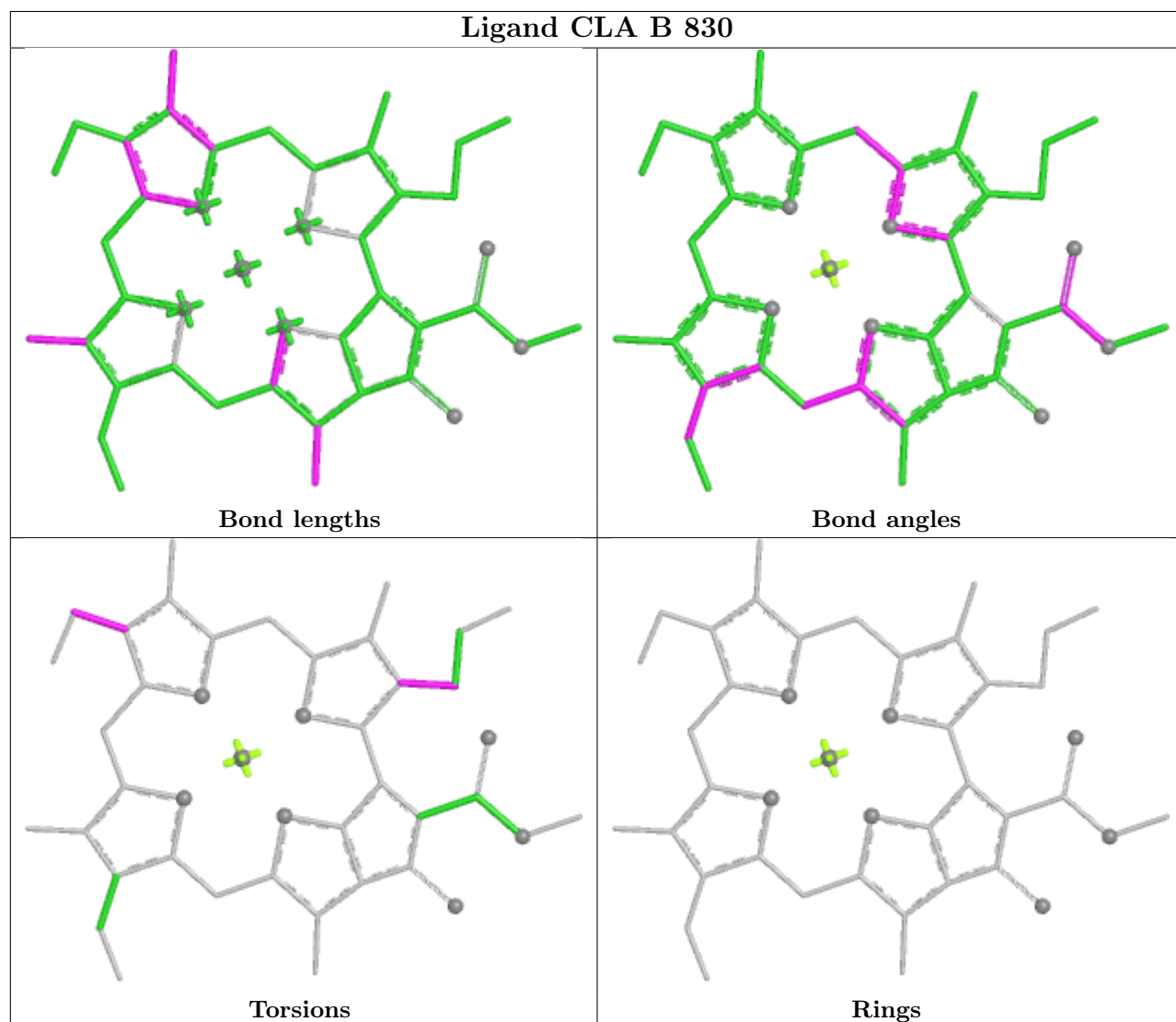
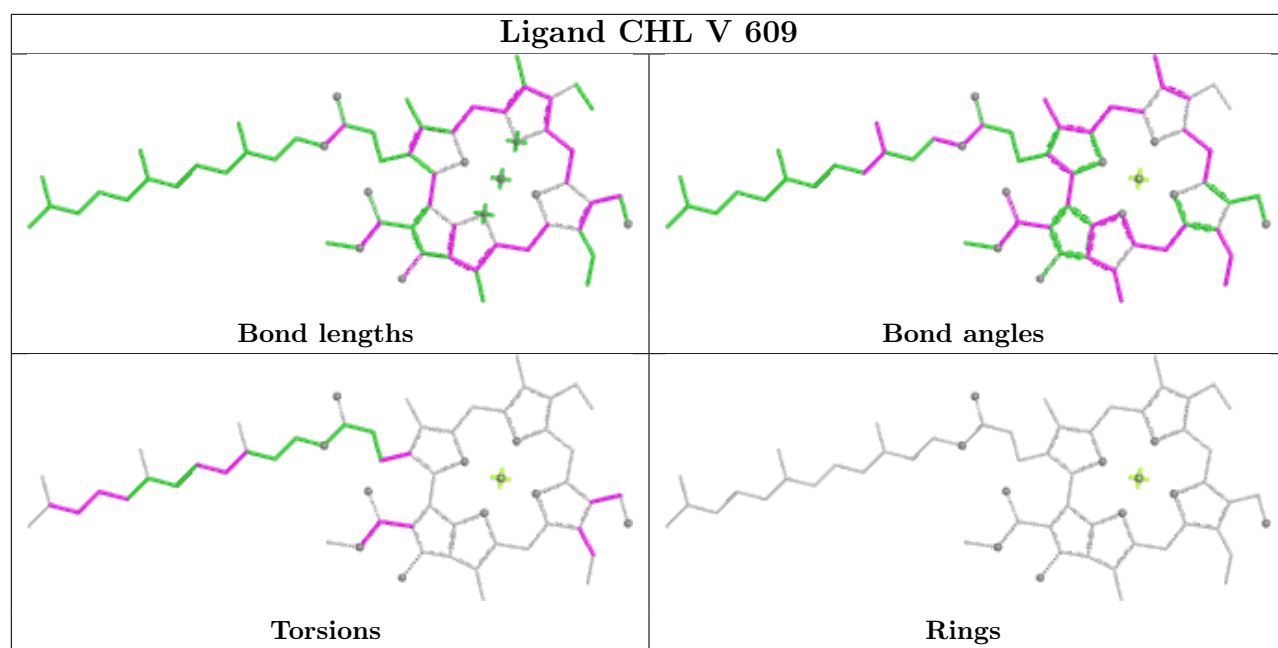
Bond angles



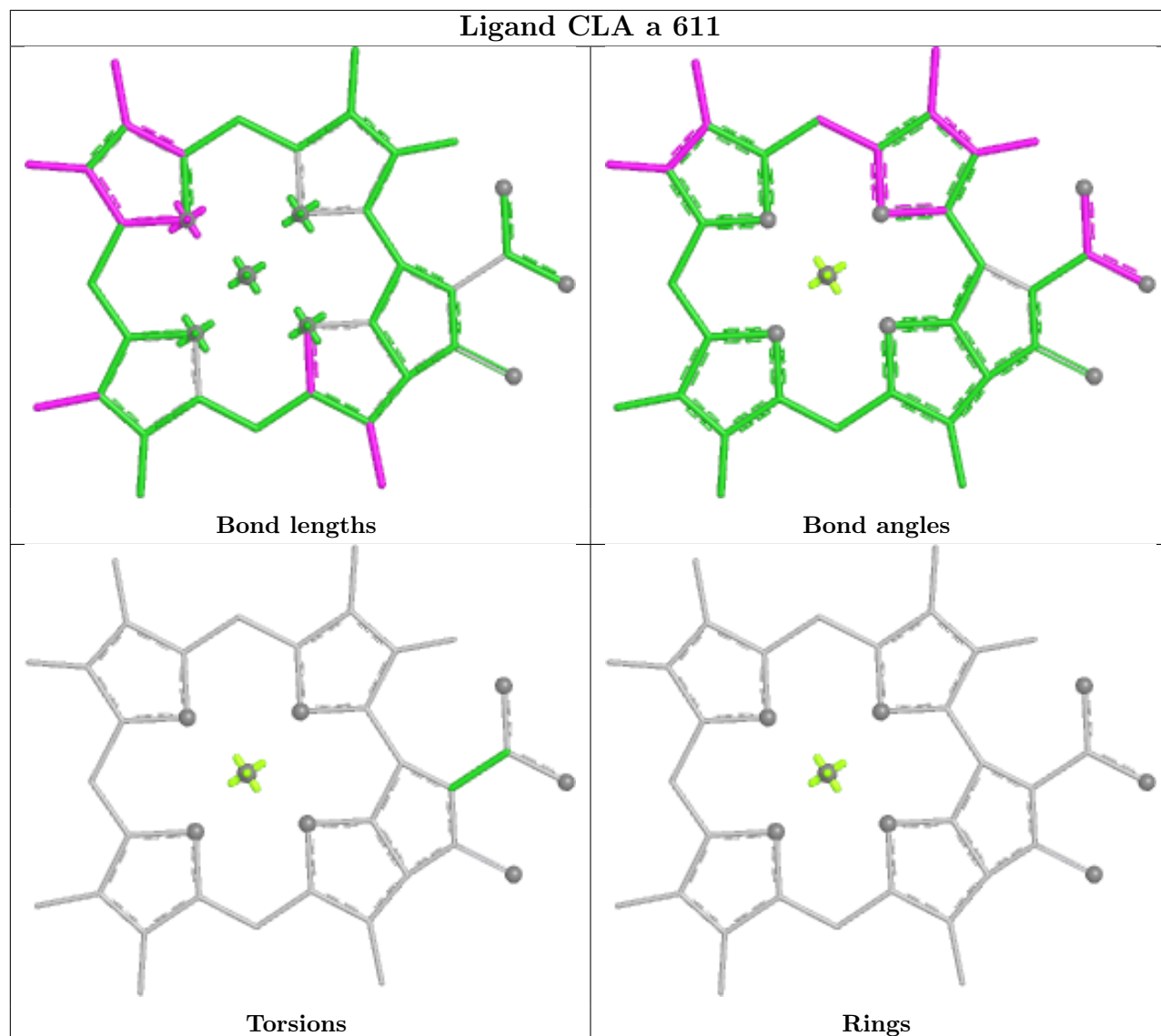
Torsions



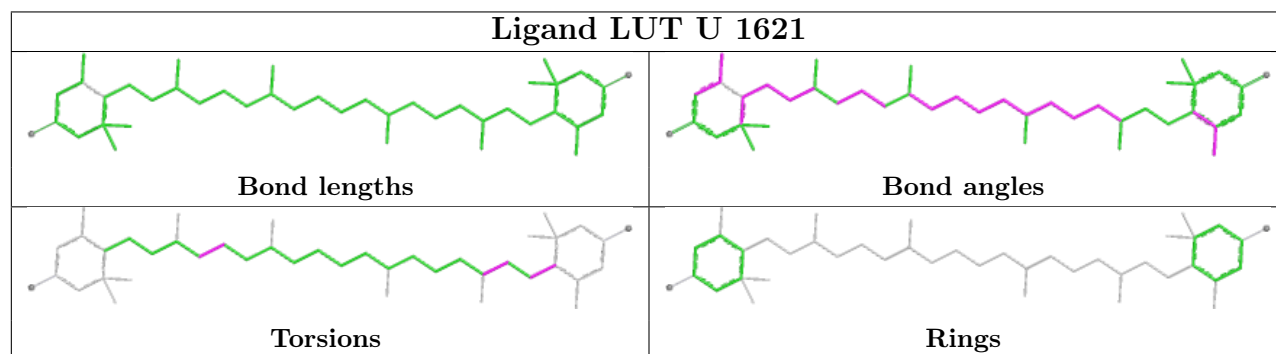
Rings

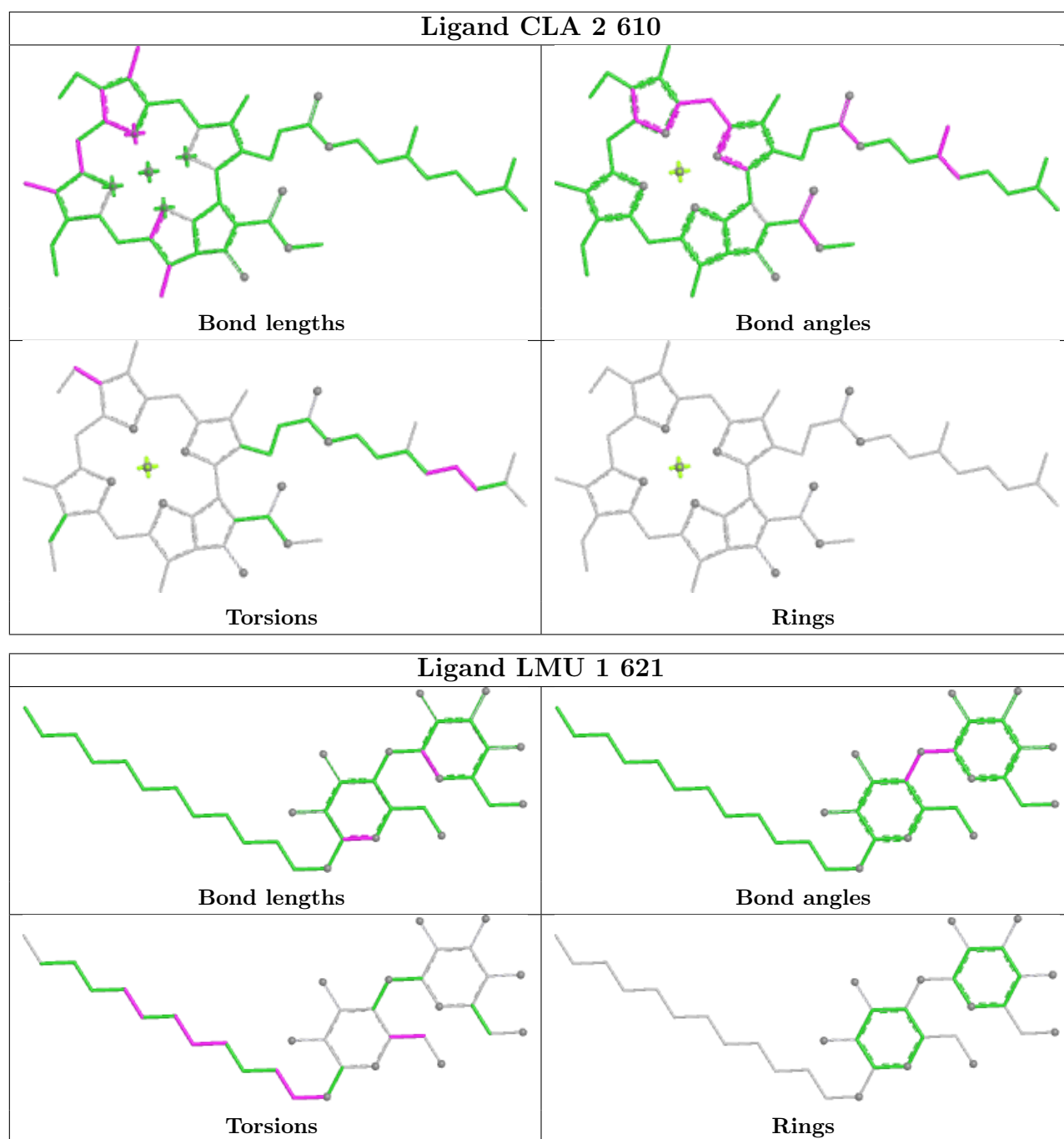


Ligand CLA a 611

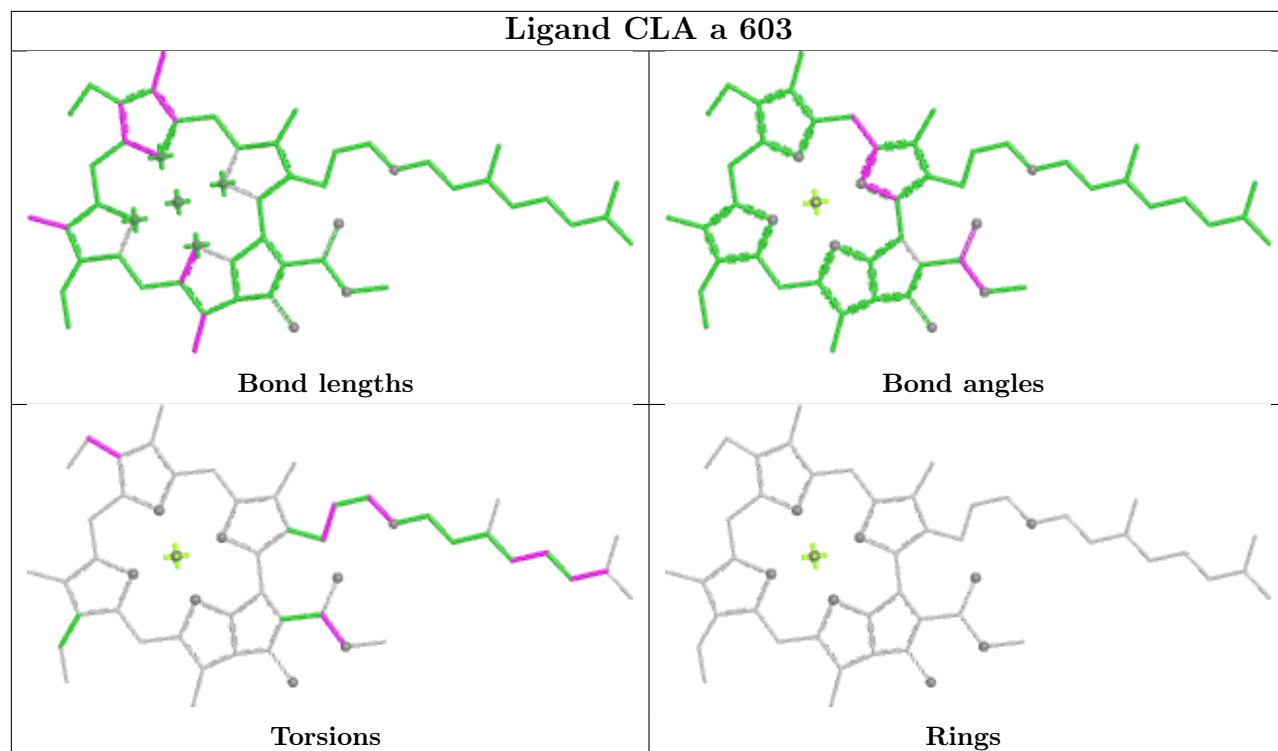


Ligand LUT U 1621

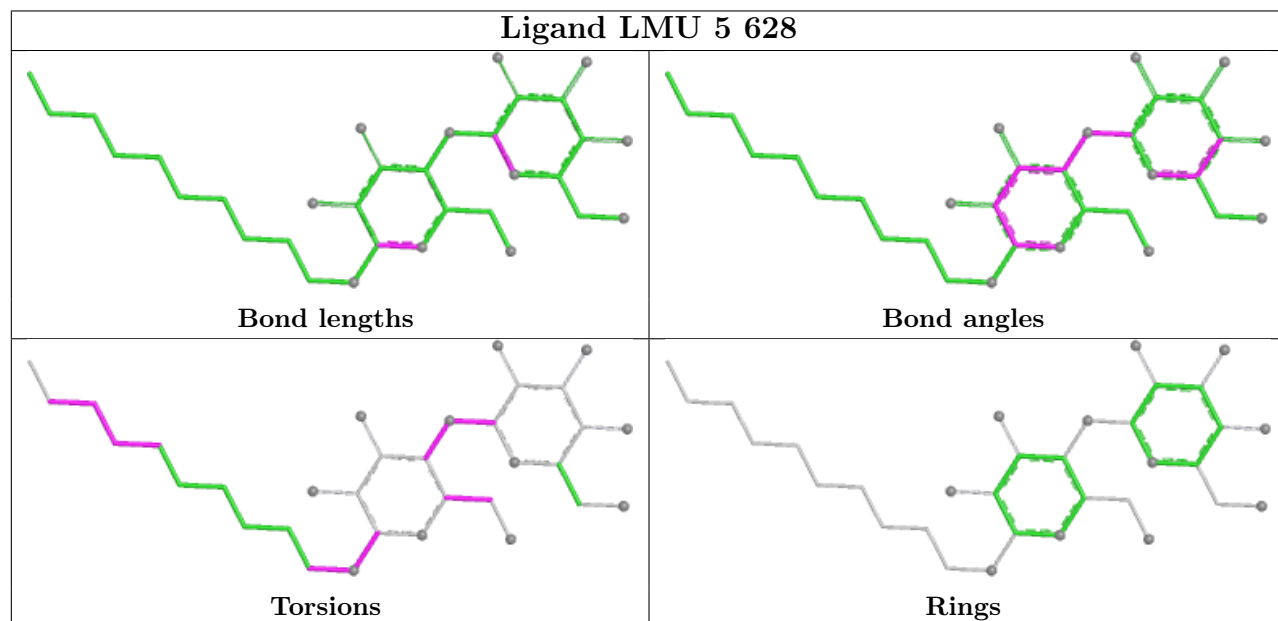


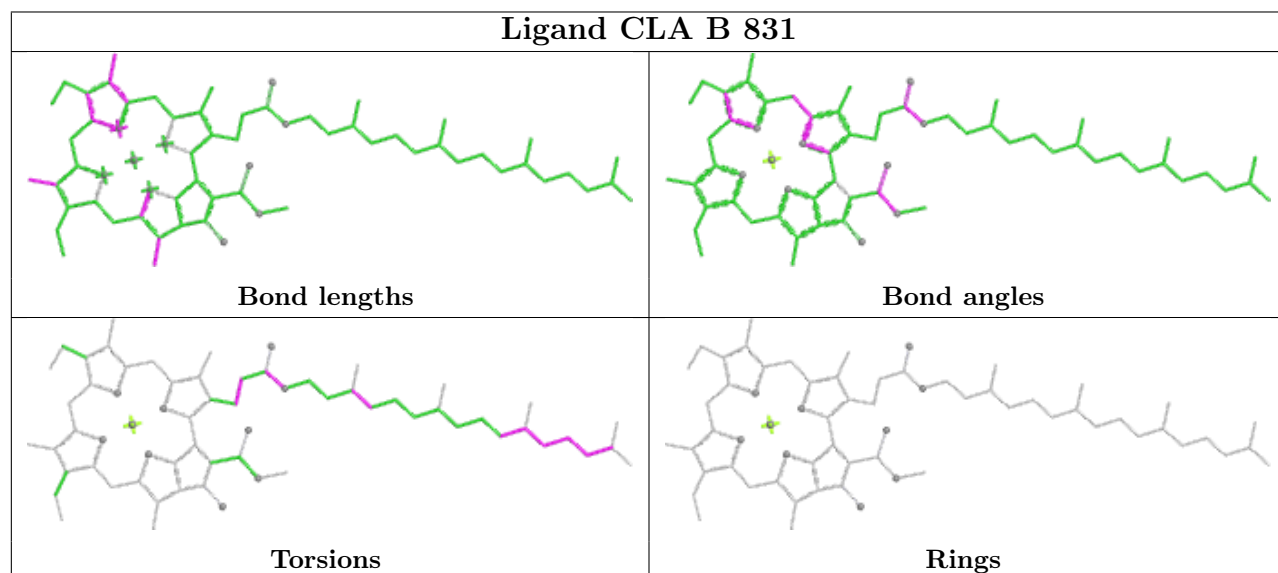
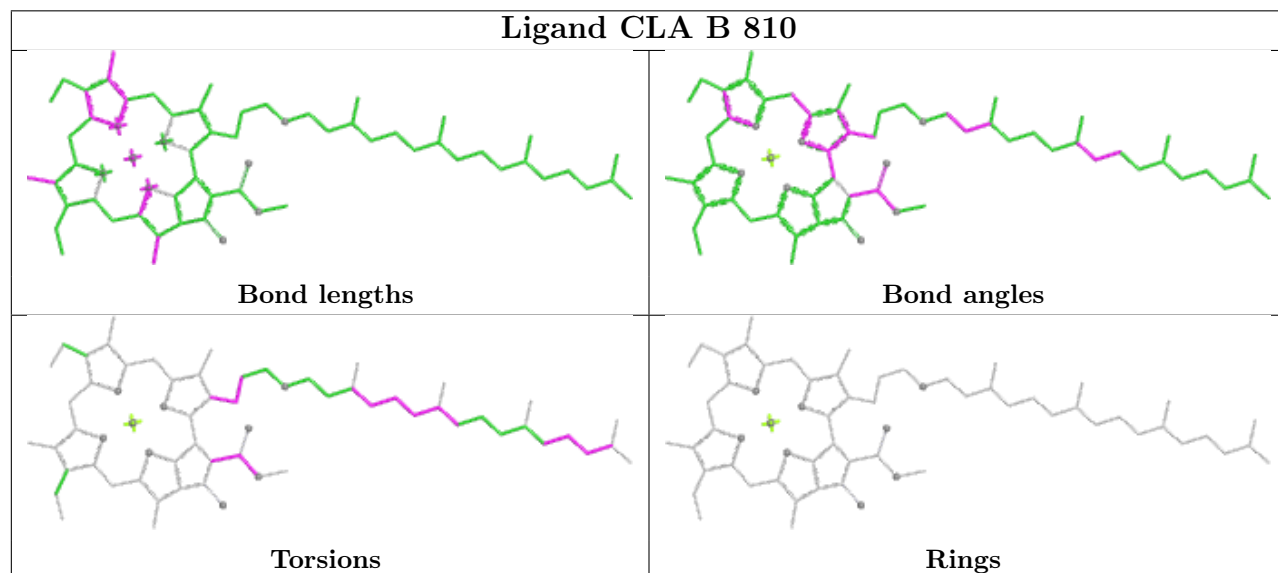
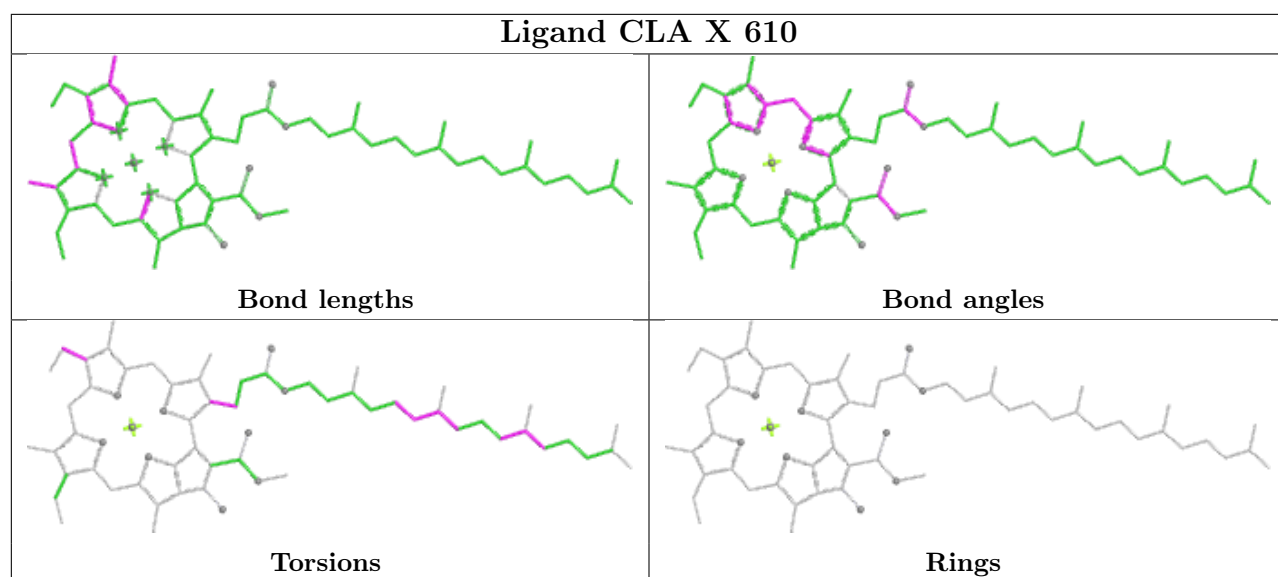


Ligand CLA a 603

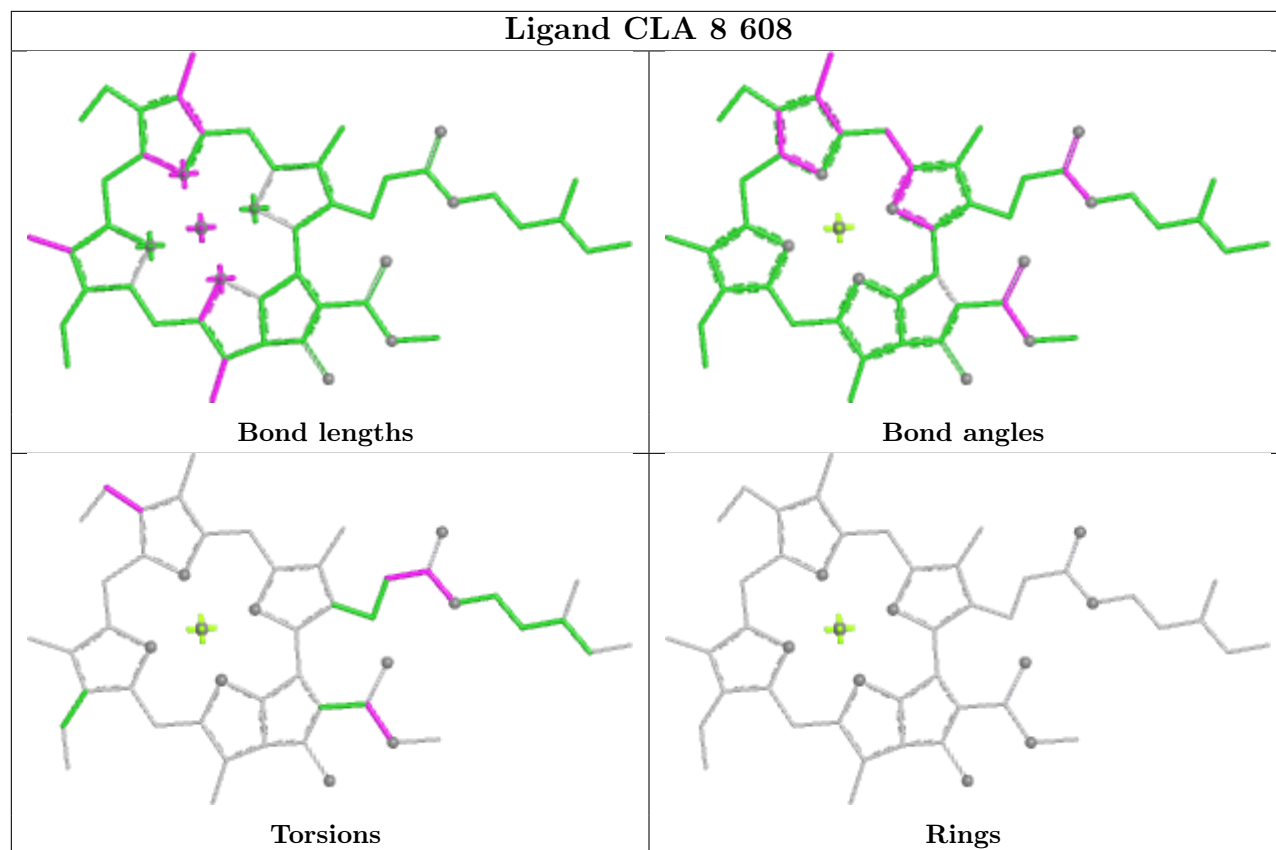


Ligand LMU 5 628

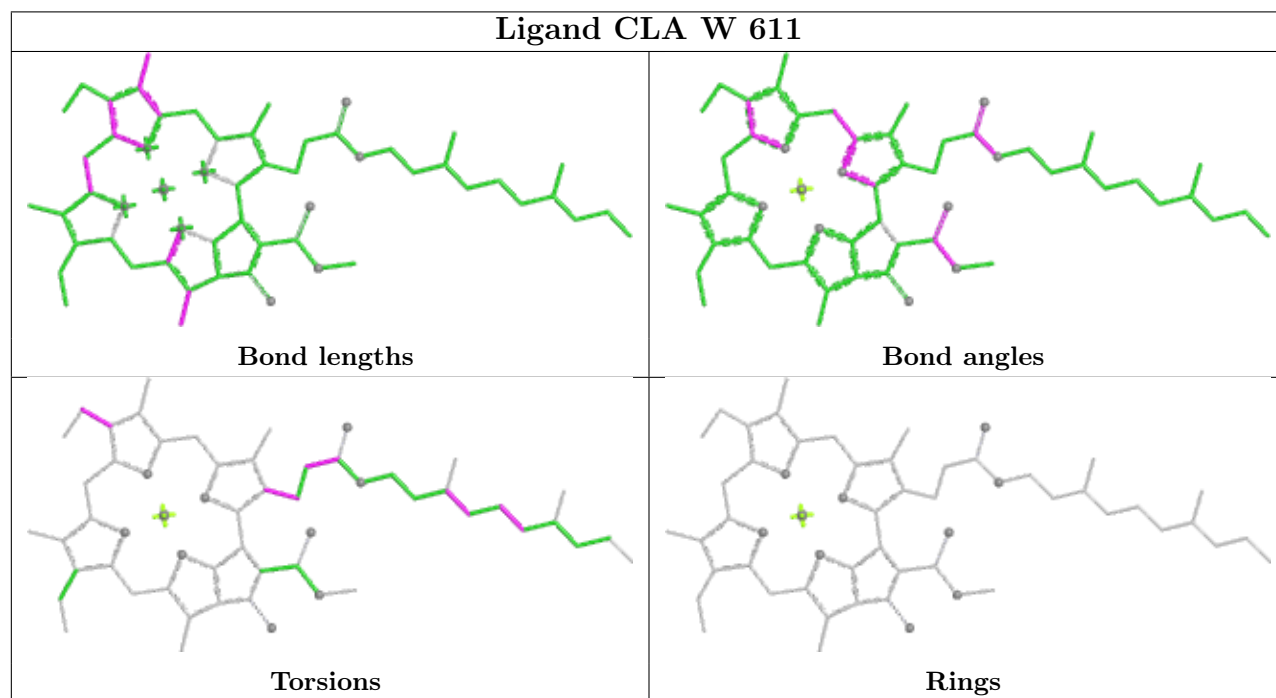


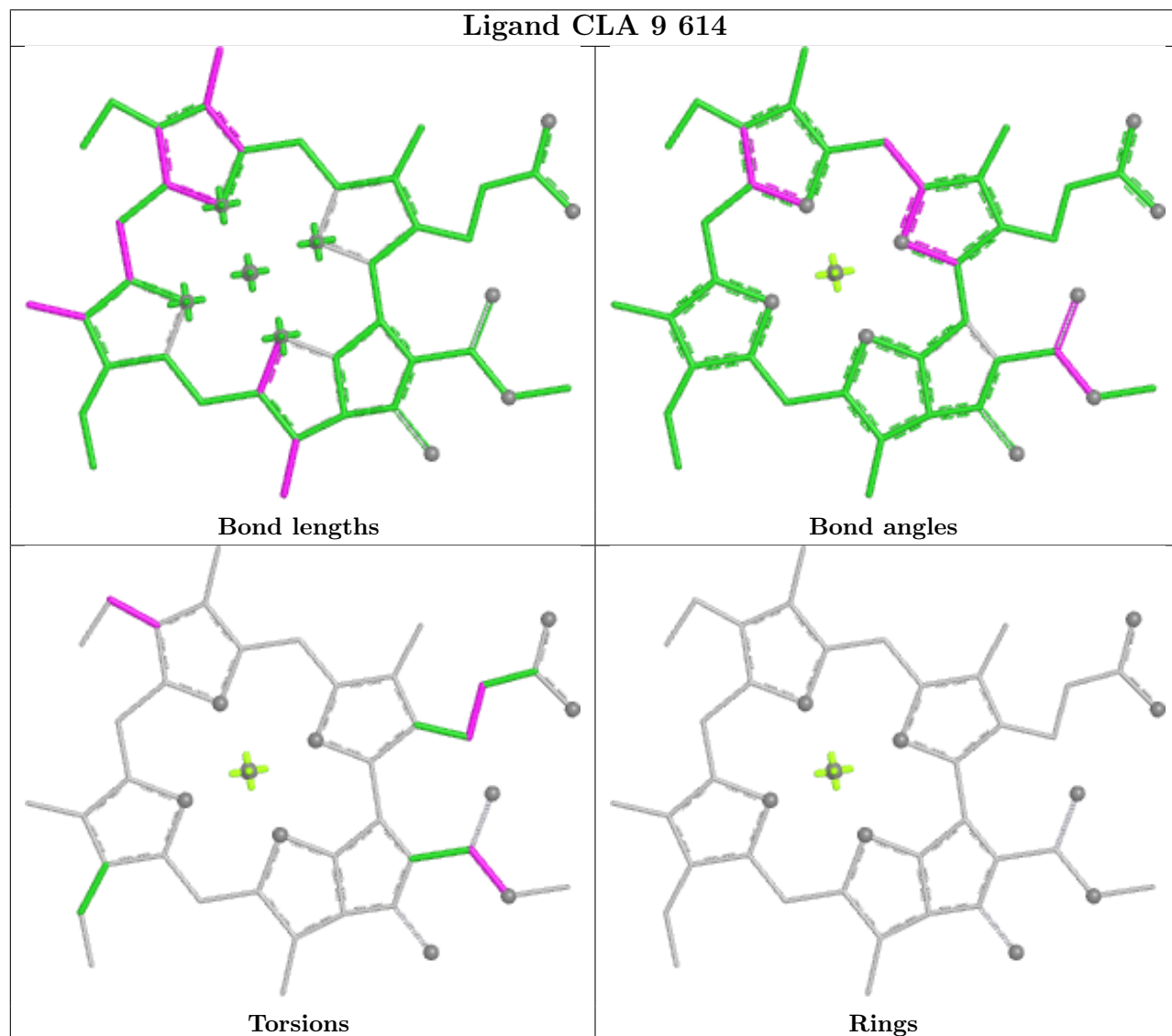
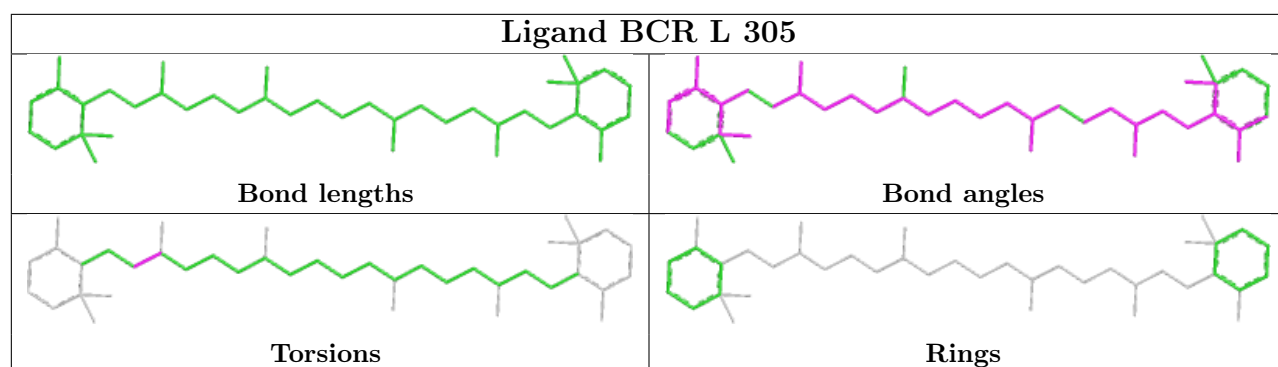


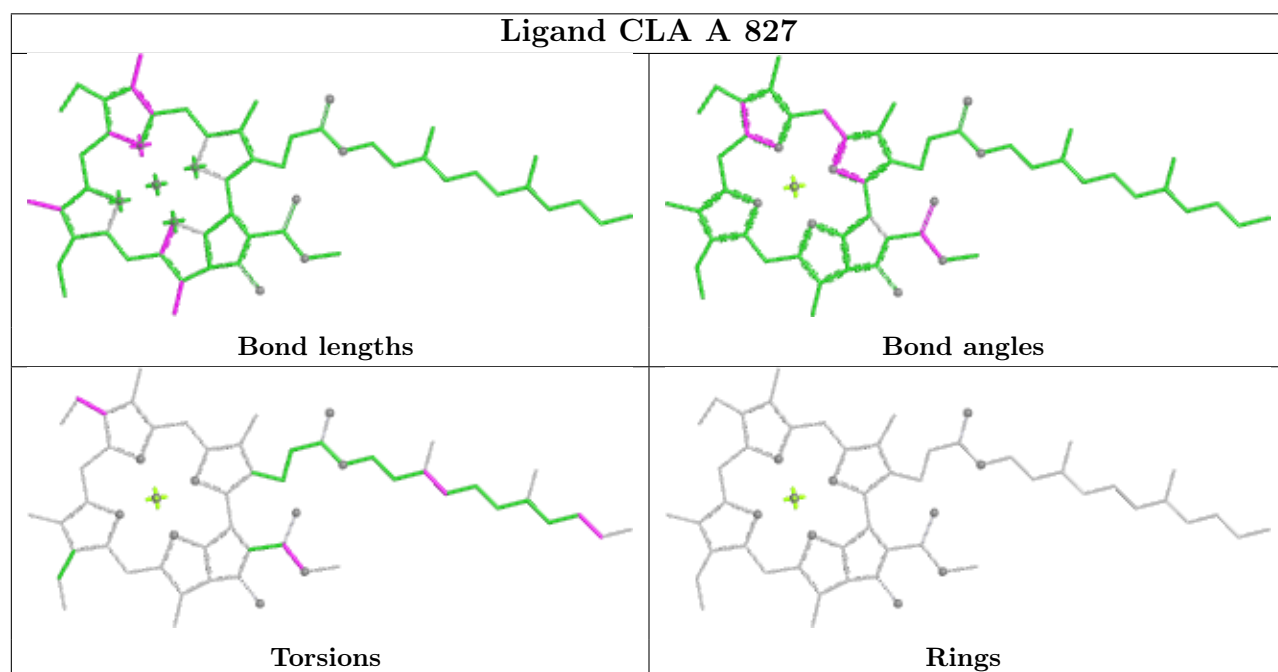
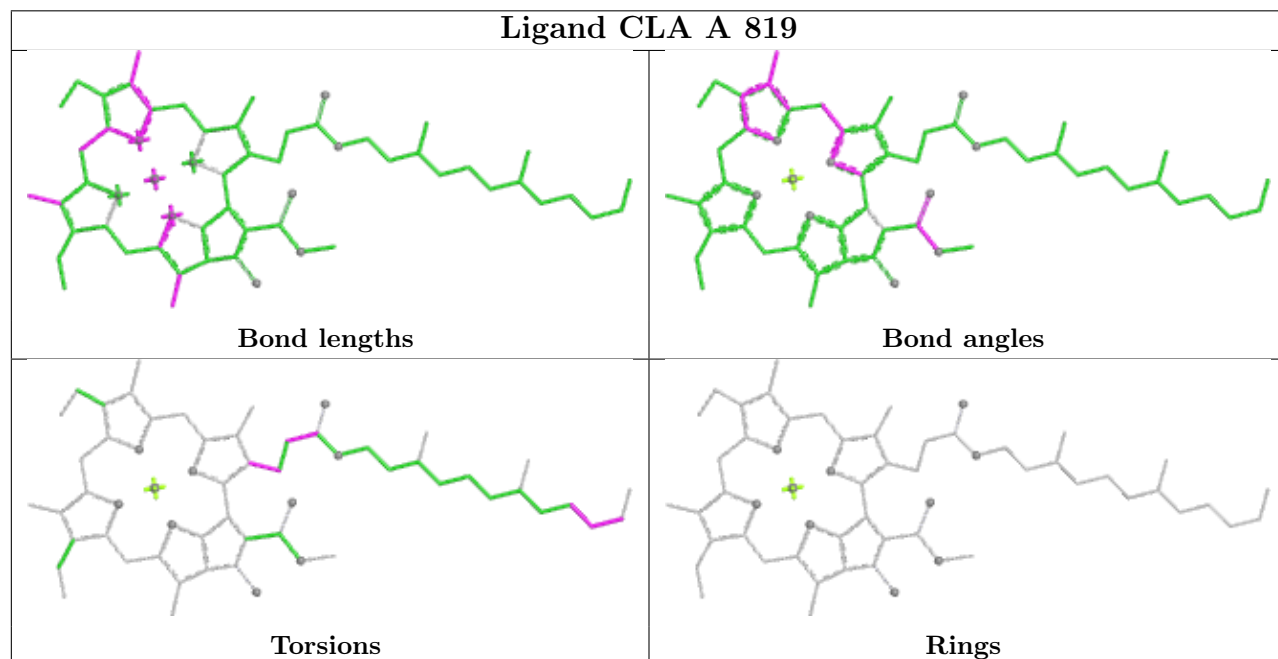
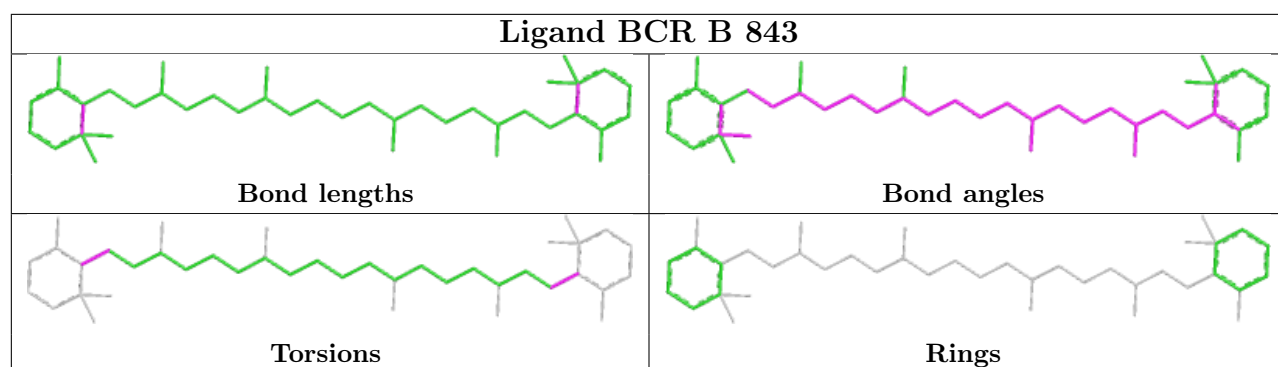
Ligand CLA 8 608



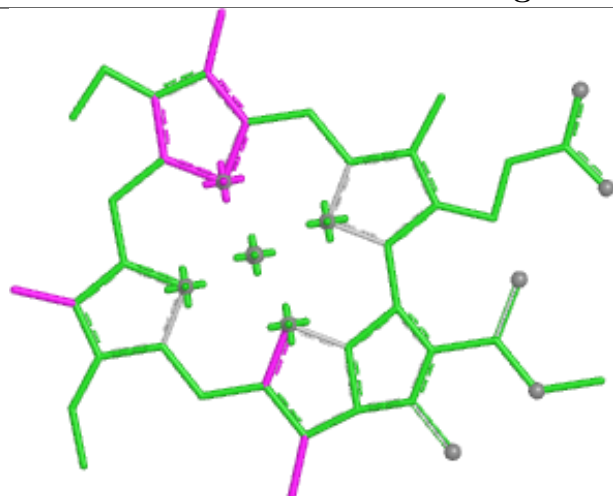
Ligand CLA W 611



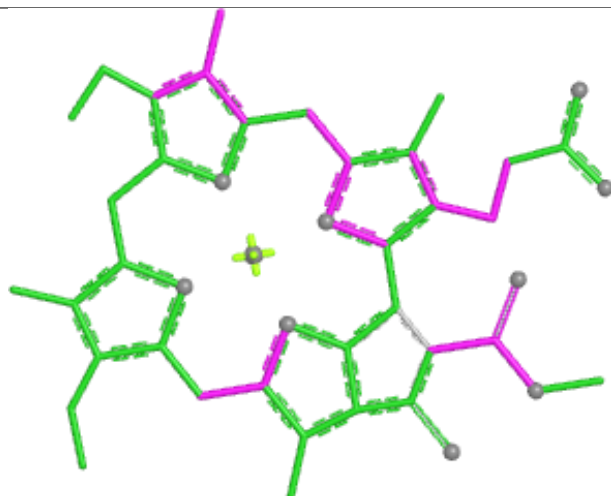




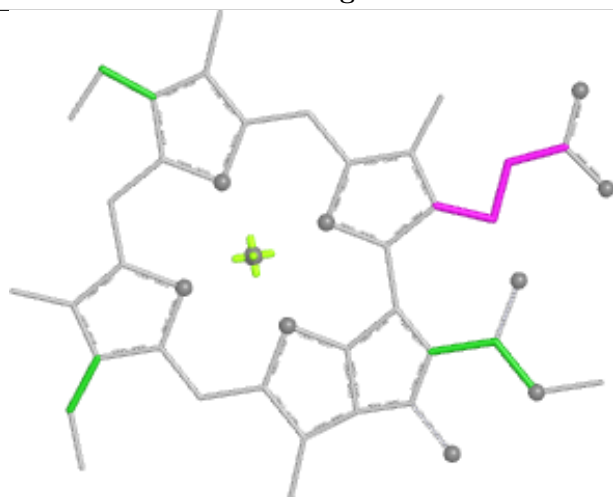
Ligand CLA A 833



Bond lengths



Bond angles

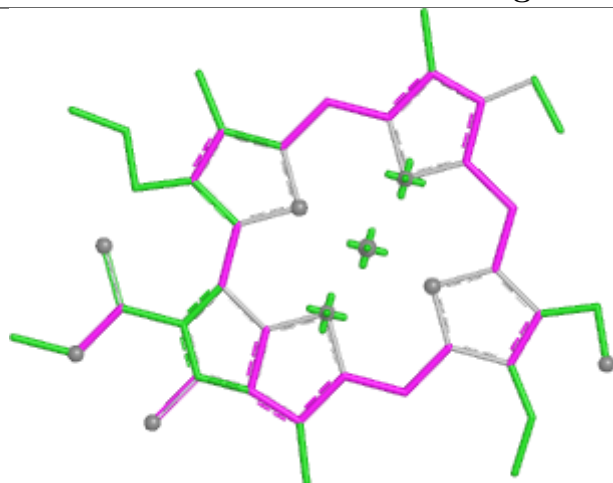


Torsions

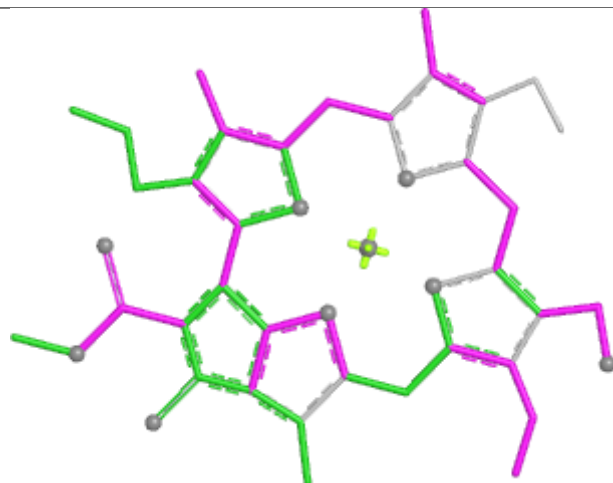


Rings

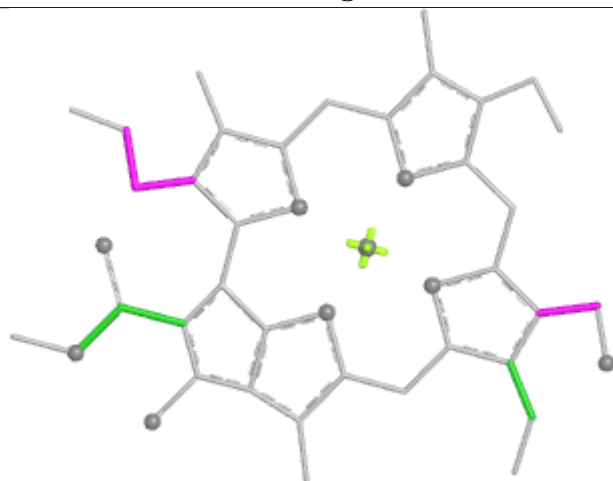
Ligand CHL X 606



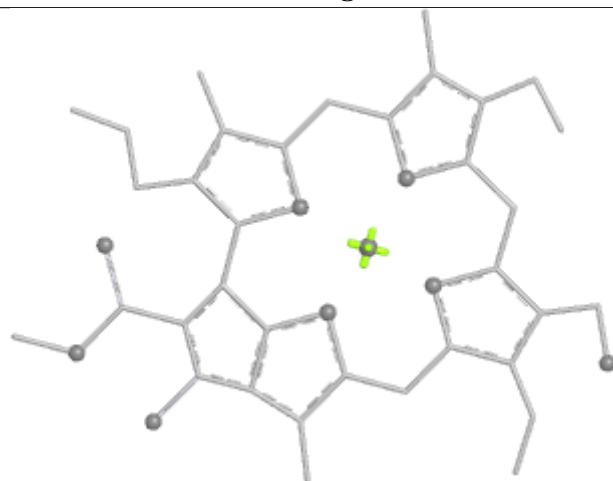
Bond lengths



Bond angles

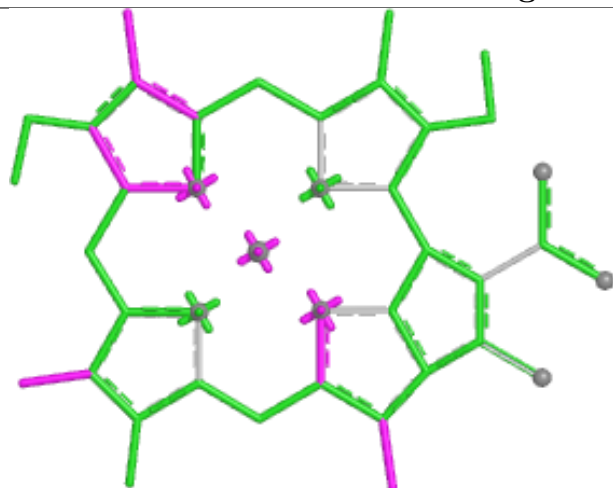


Torsions

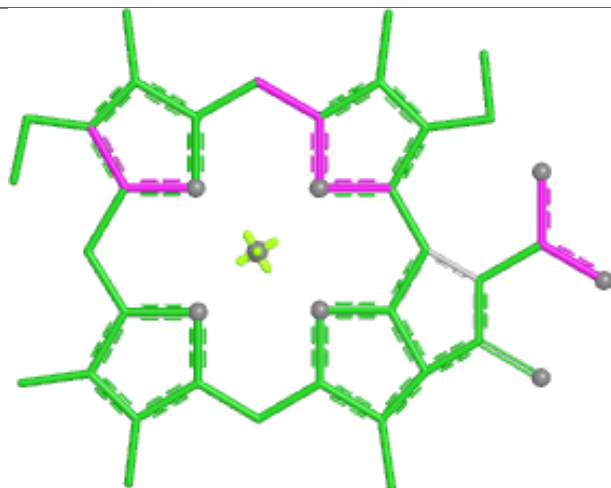


Rings

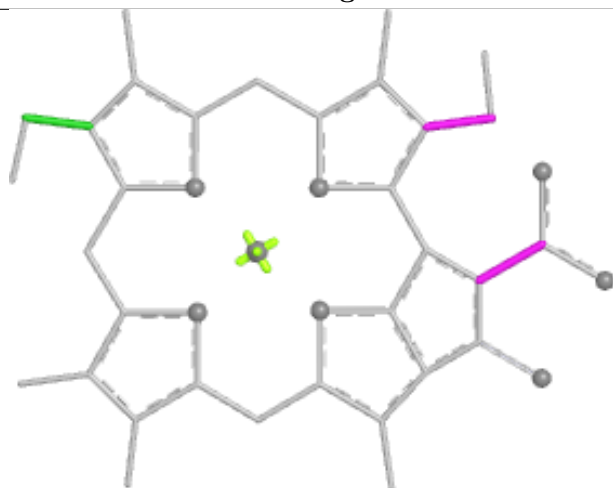
Ligand CLA 9 606



Bond lengths



Bond angles

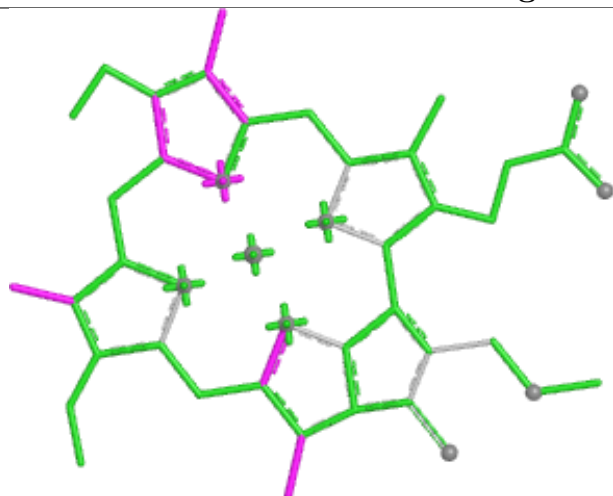


Torsions

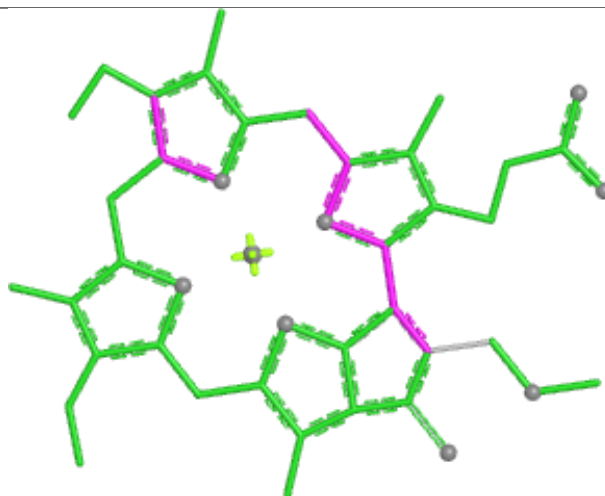


Rings

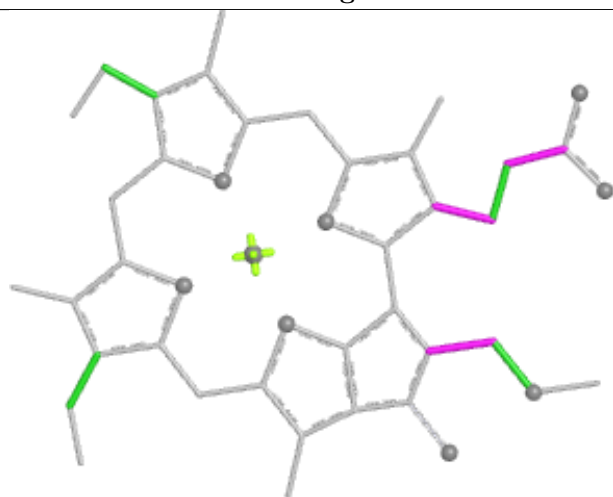
Ligand CLA 7 609



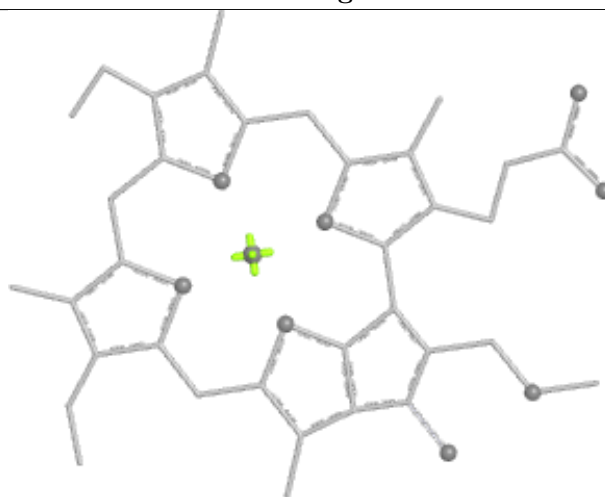
Bond lengths



Bond angles

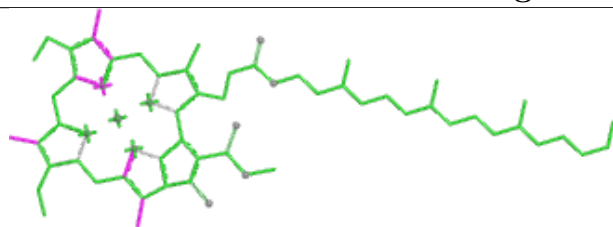


Torsions

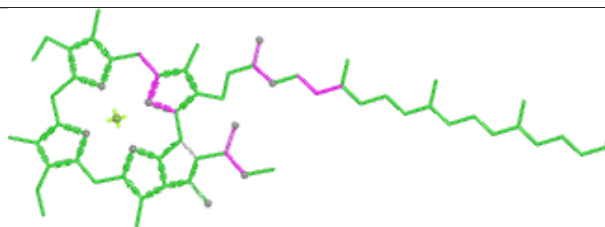


Rings

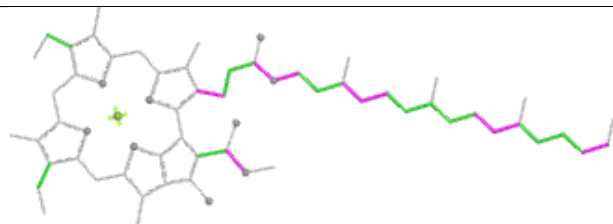
Ligand CLA B 814



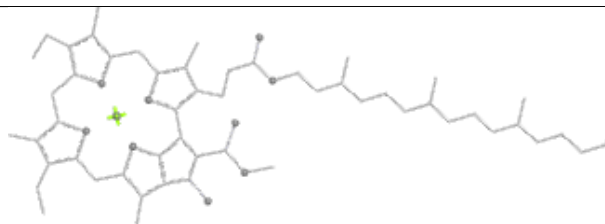
Bond lengths



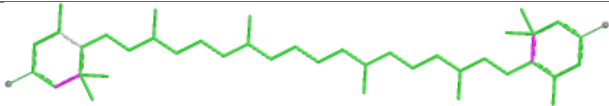
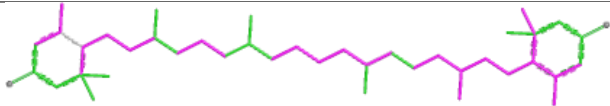
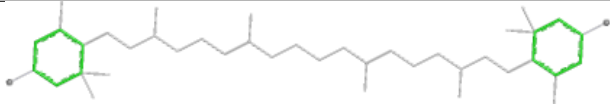
Bond angles

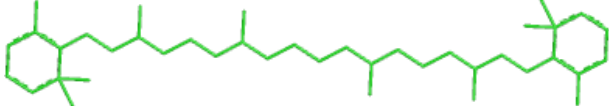
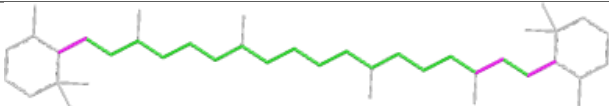
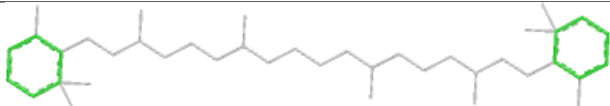


Torsions

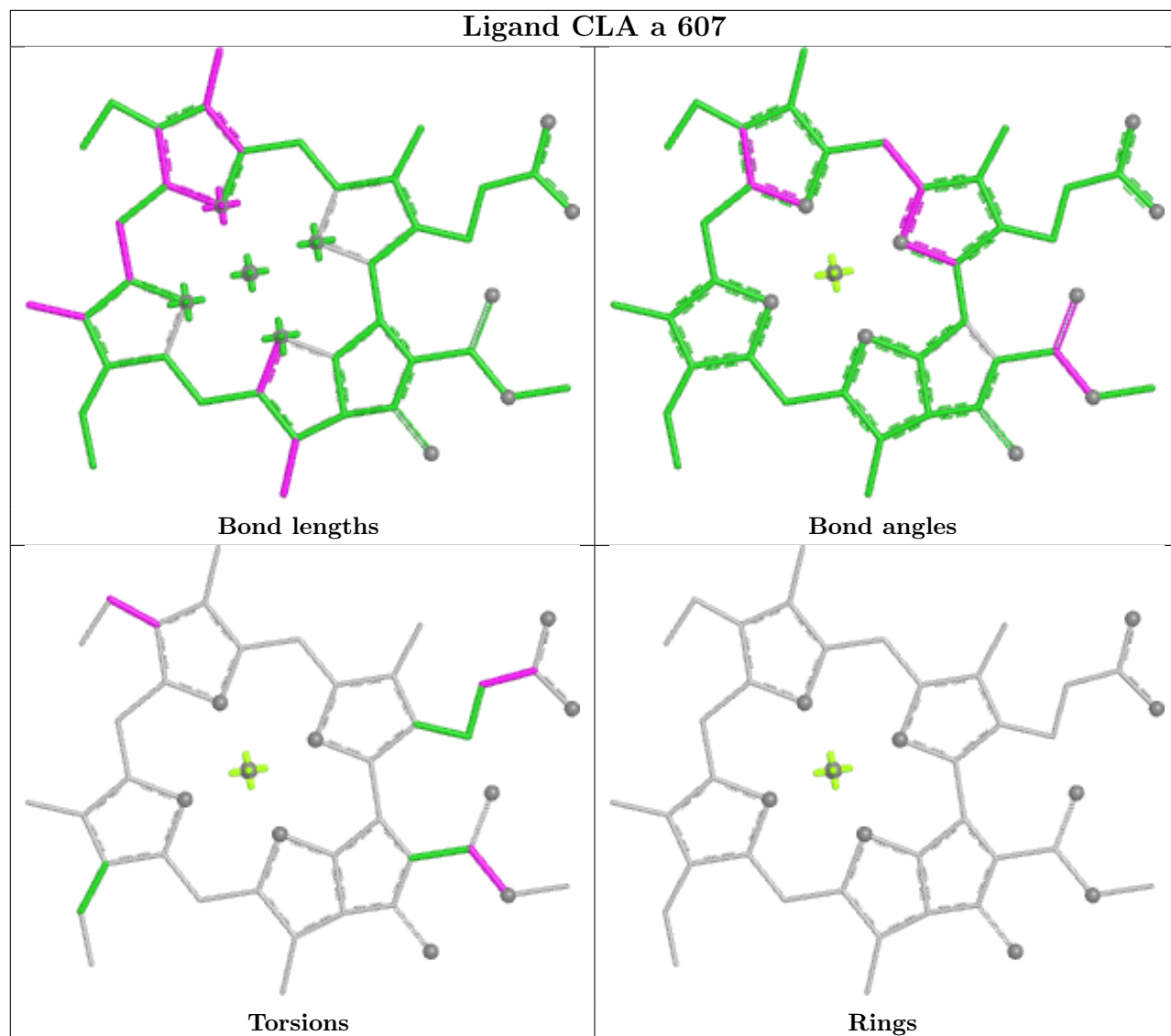


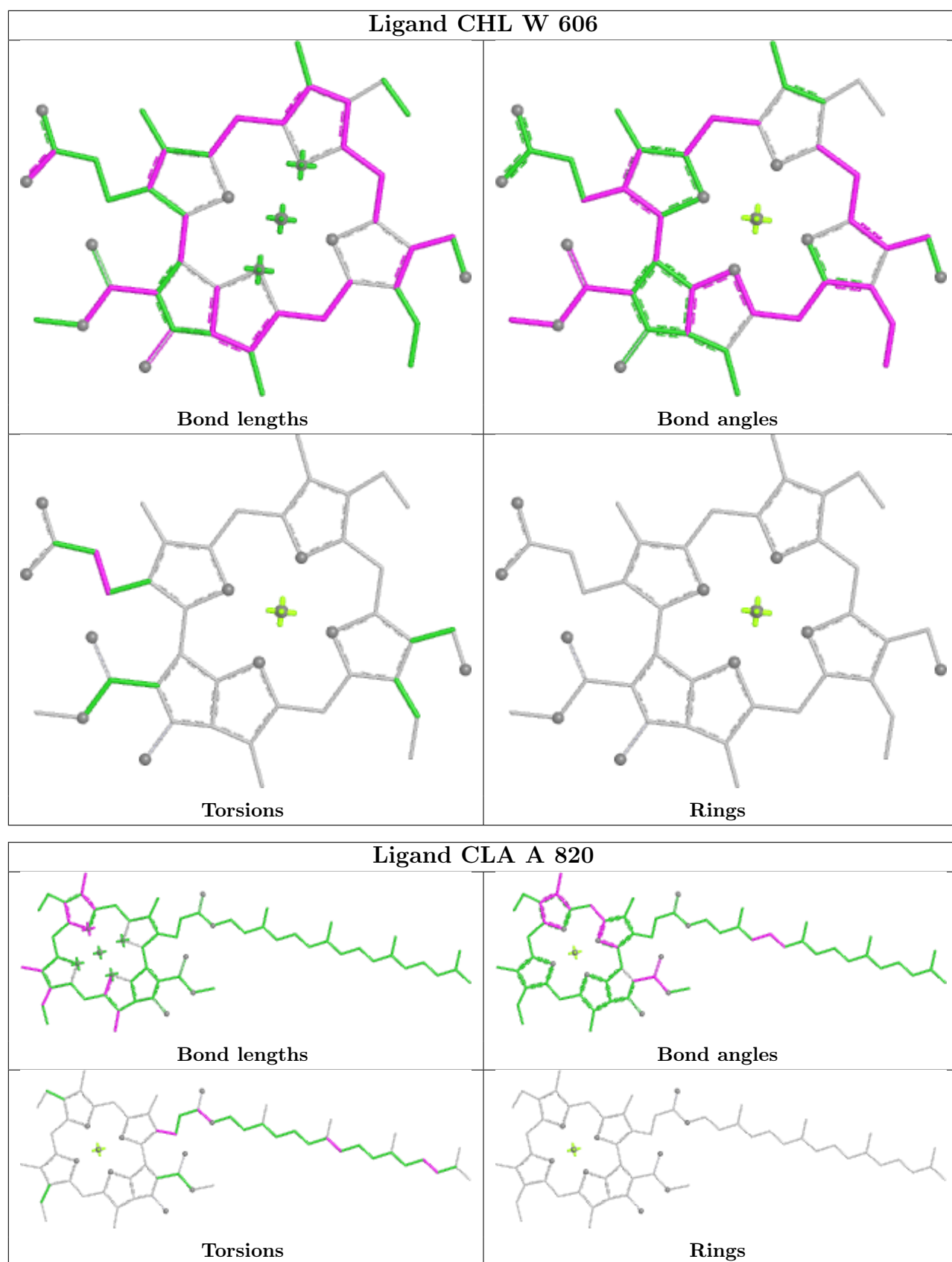
Rings

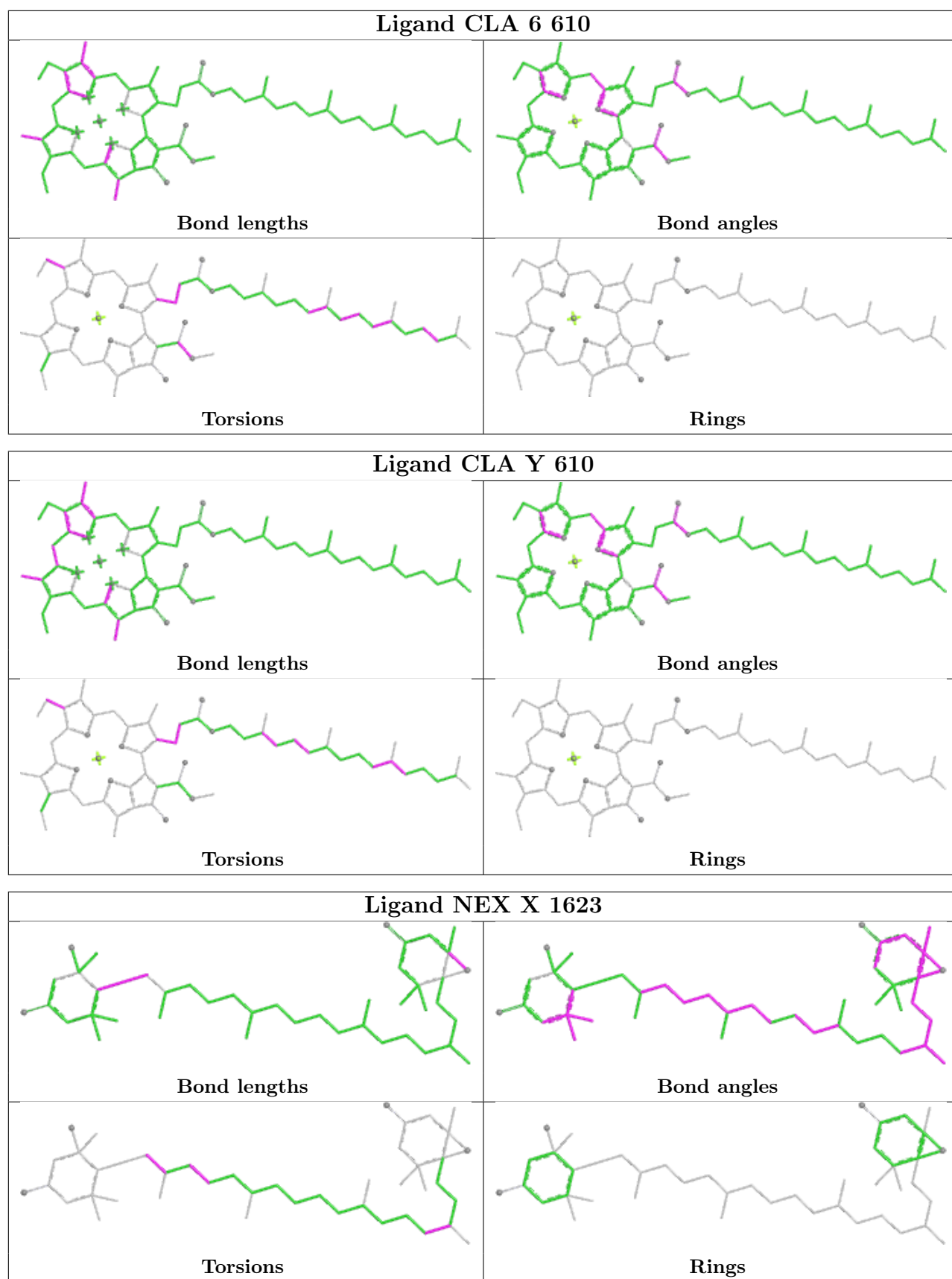
Ligand LUT 7 619	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand BCR A 849	
	Bond lengths
	Bond angles
	Torsions
	Rings

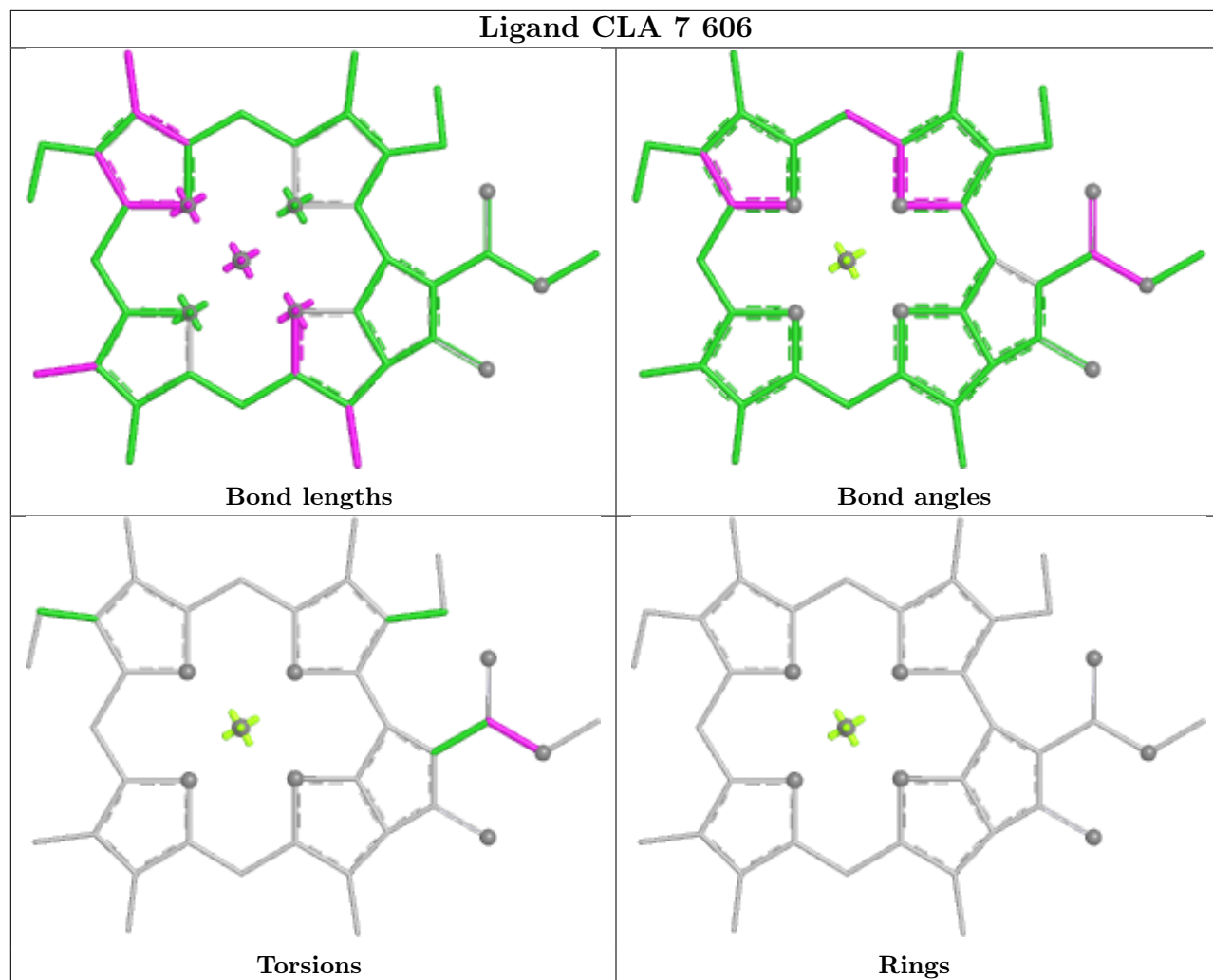
Ligand CLA a 607



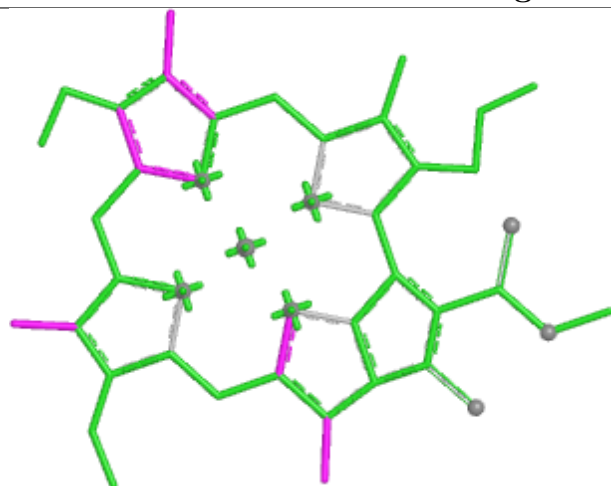




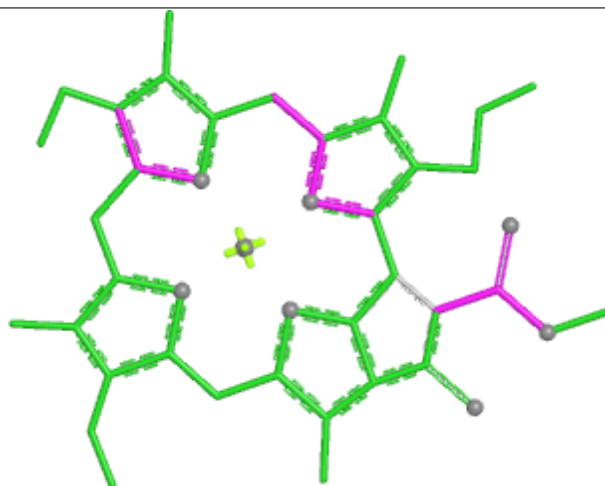
Ligand CLA 7 606



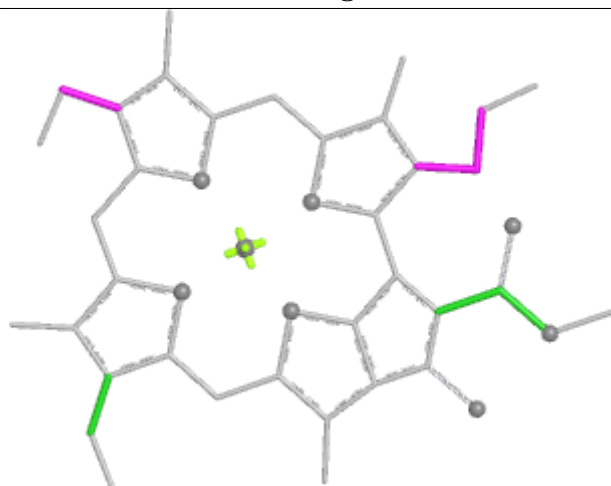
Ligand CLA B 812



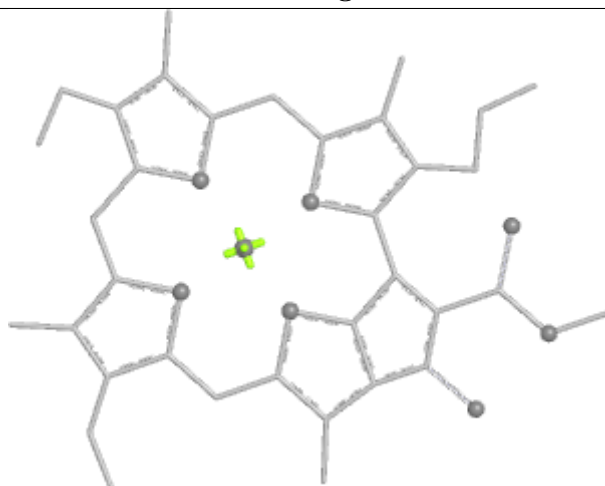
Bond lengths



Bond angles

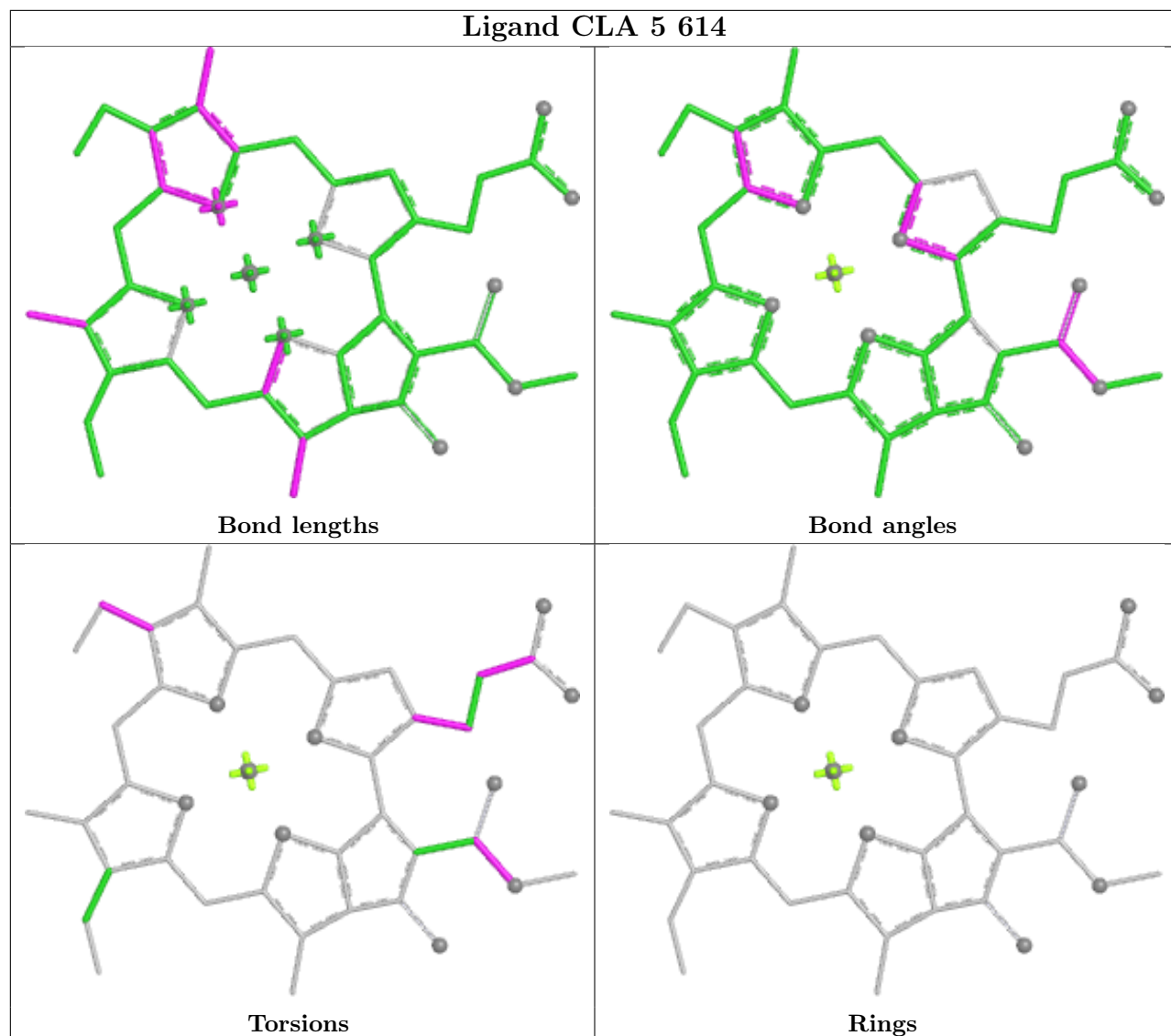


Torsions

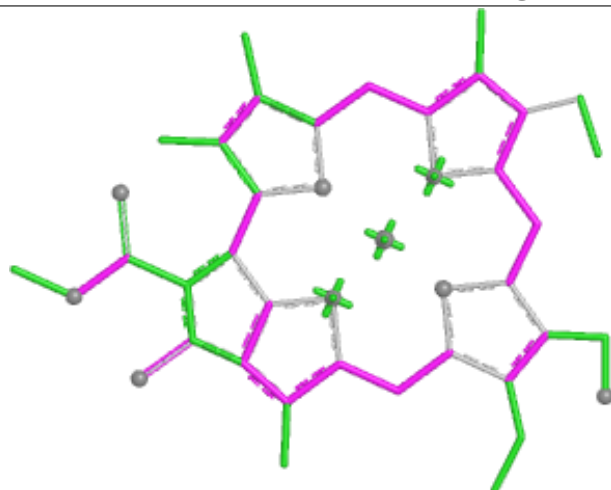


Rings

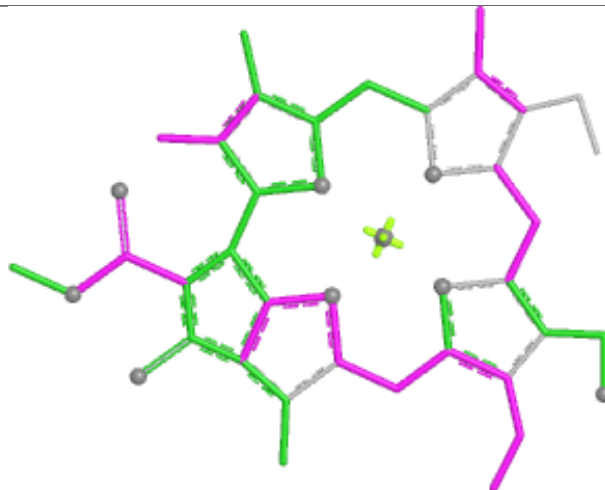
Ligand CLA 5 614



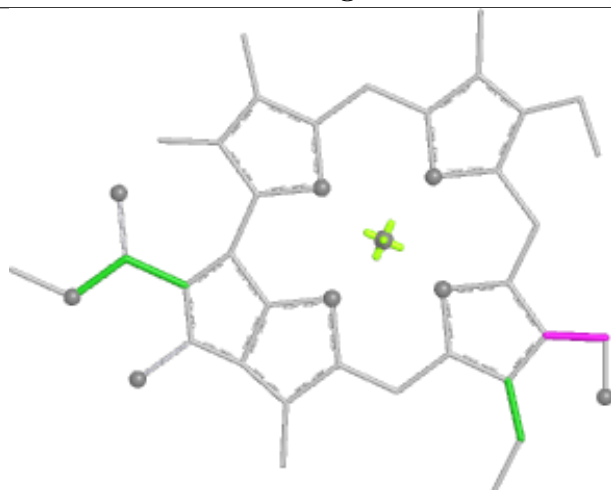
Ligand CHL Y 605



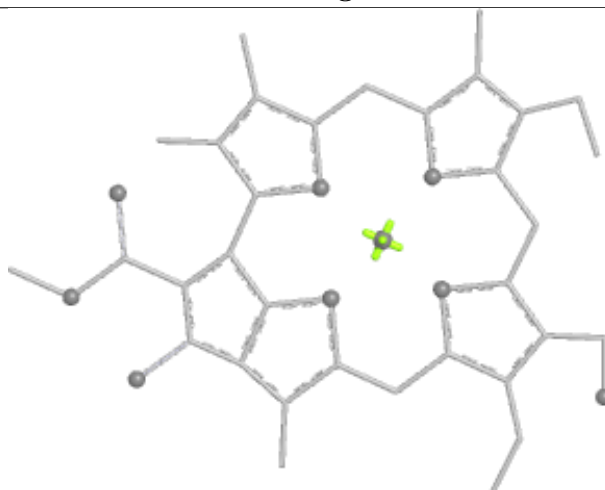
Bond lengths



Bond angles

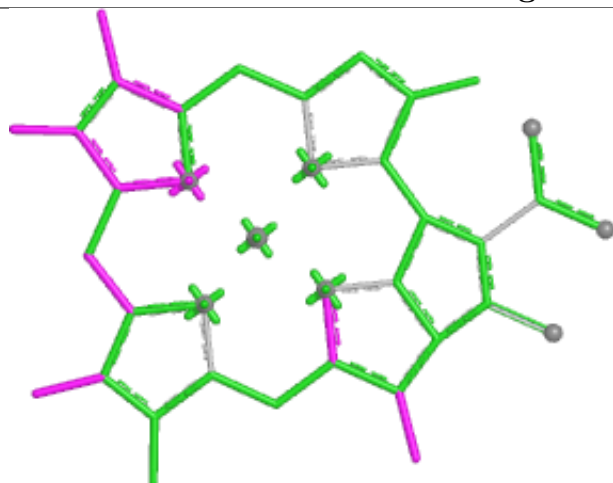


Torsions

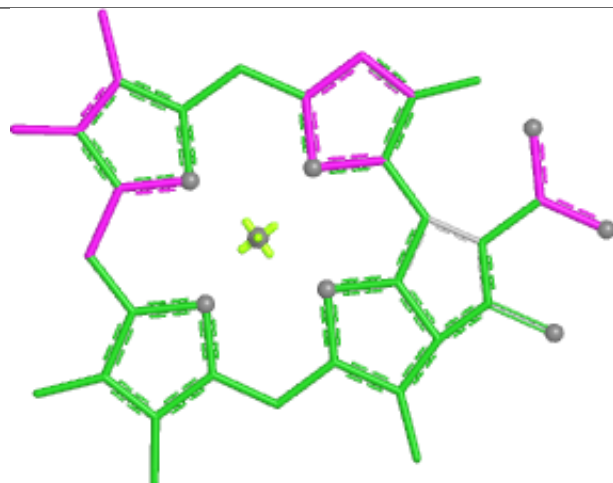


Rings

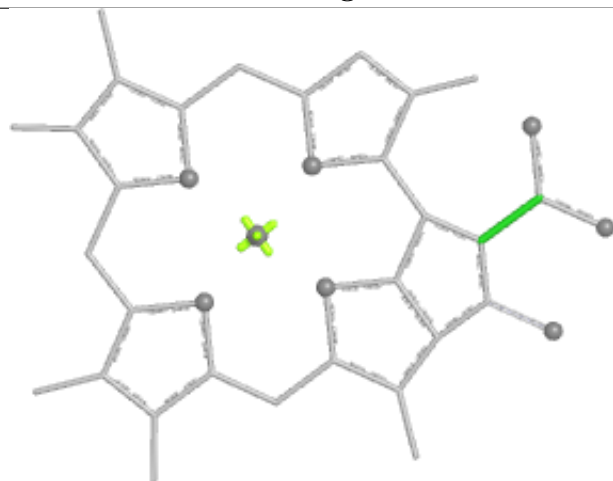
Ligand CLA 1 614



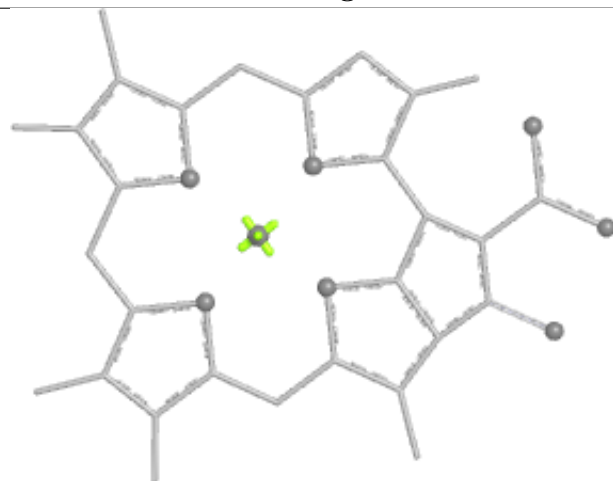
Bond lengths



Bond angles

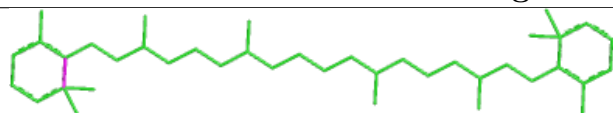


Torsions

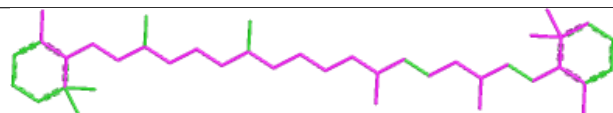


Rings

Ligand BCR A 856



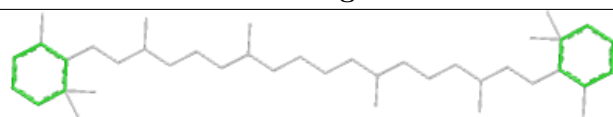
Bond lengths



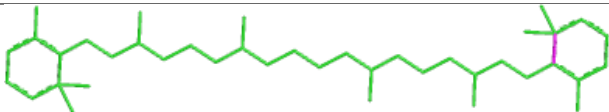
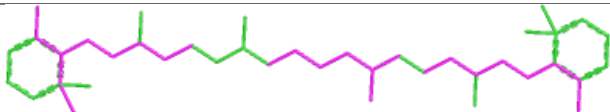
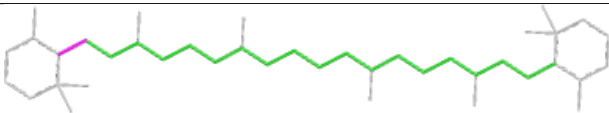
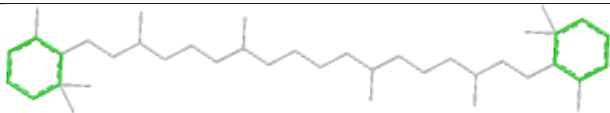
Bond angles

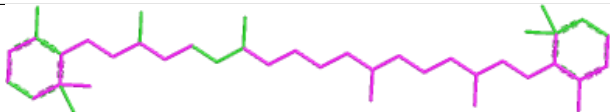
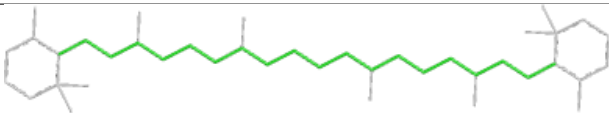
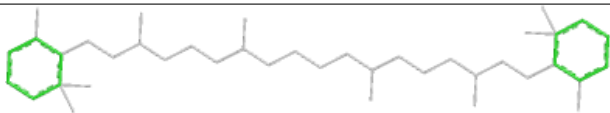


Torsions

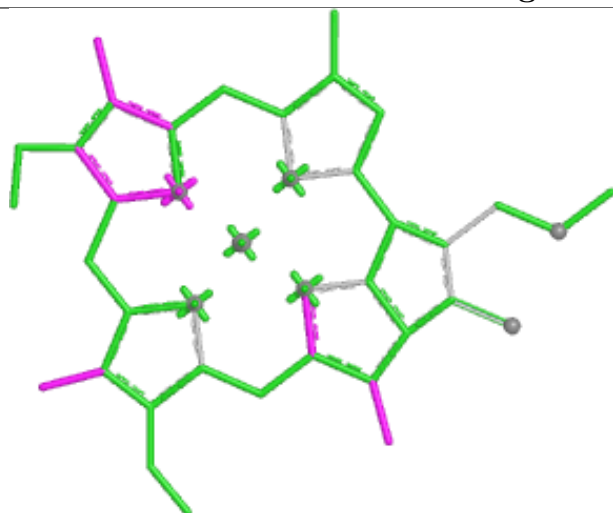


Rings

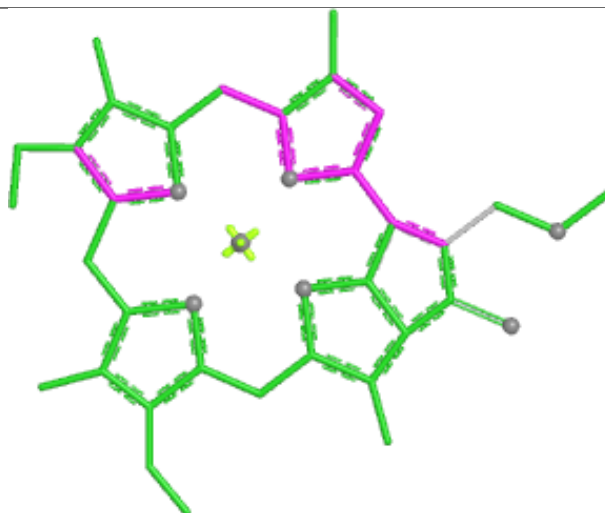
Ligand BCR A 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 606



Bond lengths



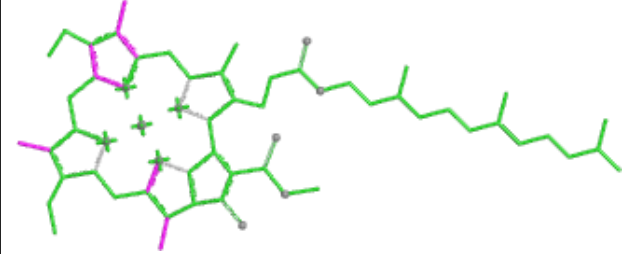
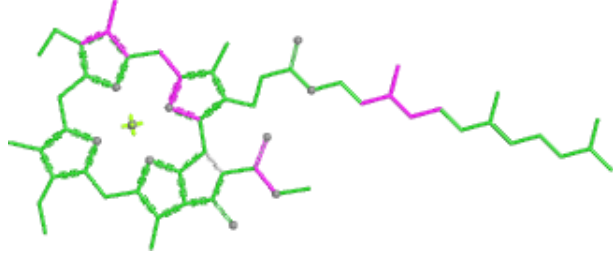
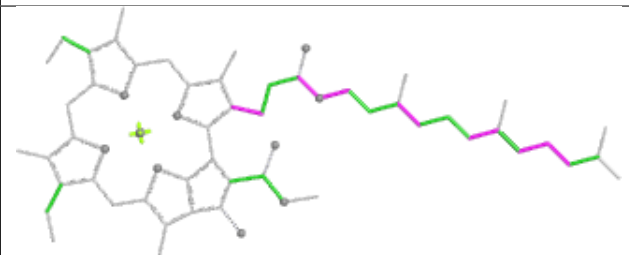
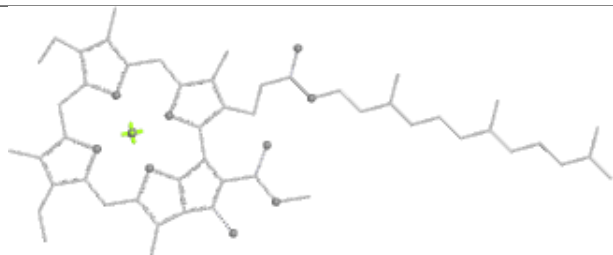
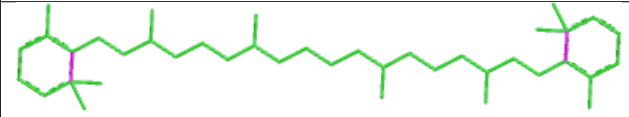
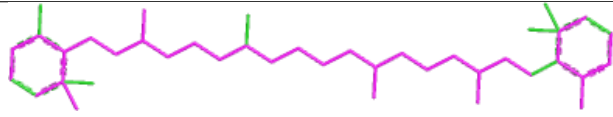
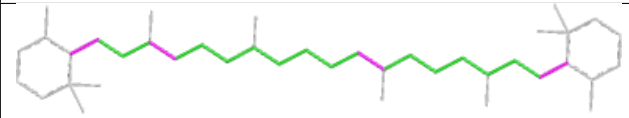
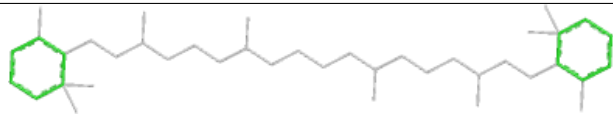
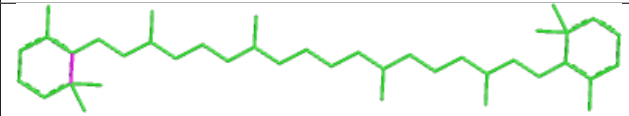
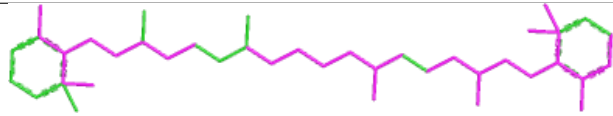
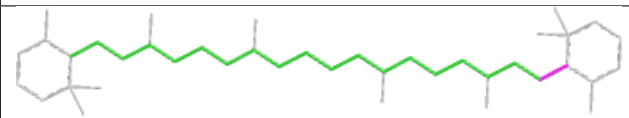
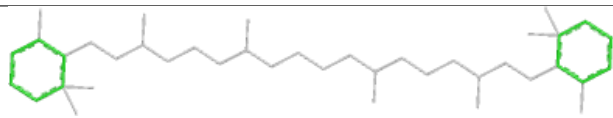
Bond angles



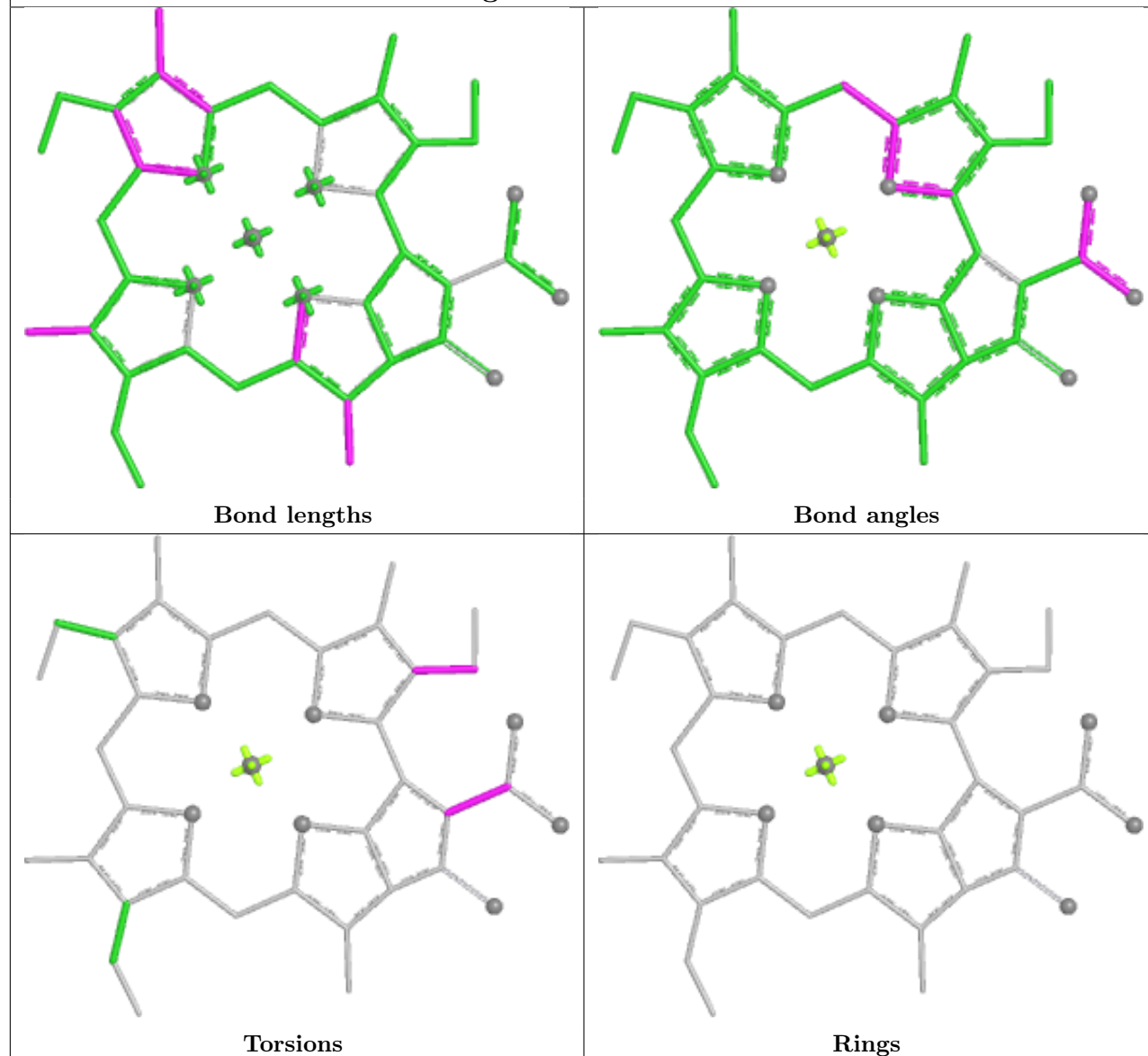
Torsions



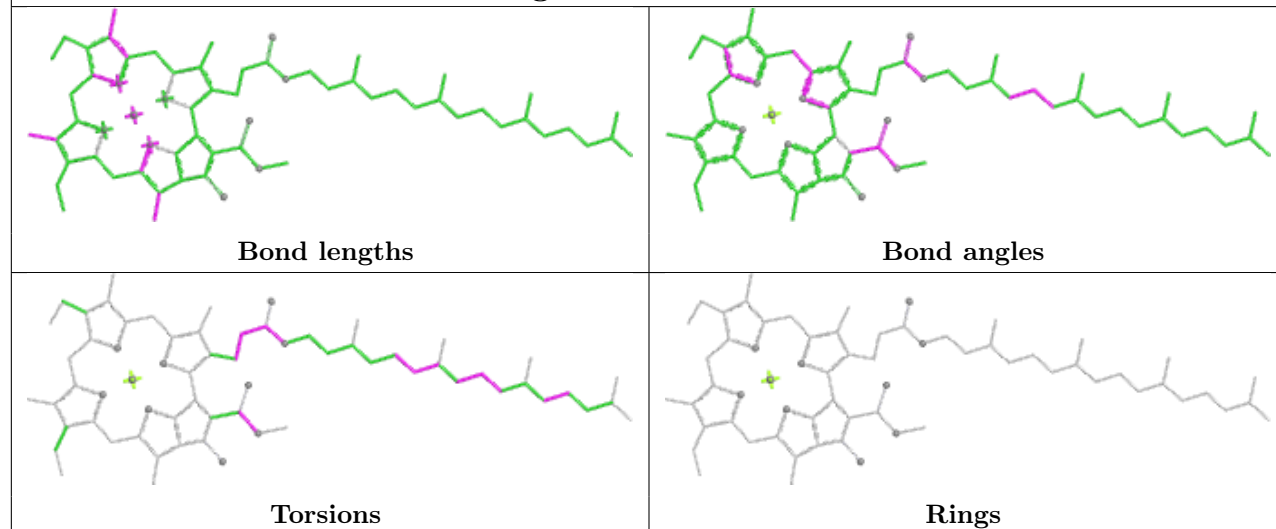
Rings

Ligand CLA 8 610	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 852	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 7 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

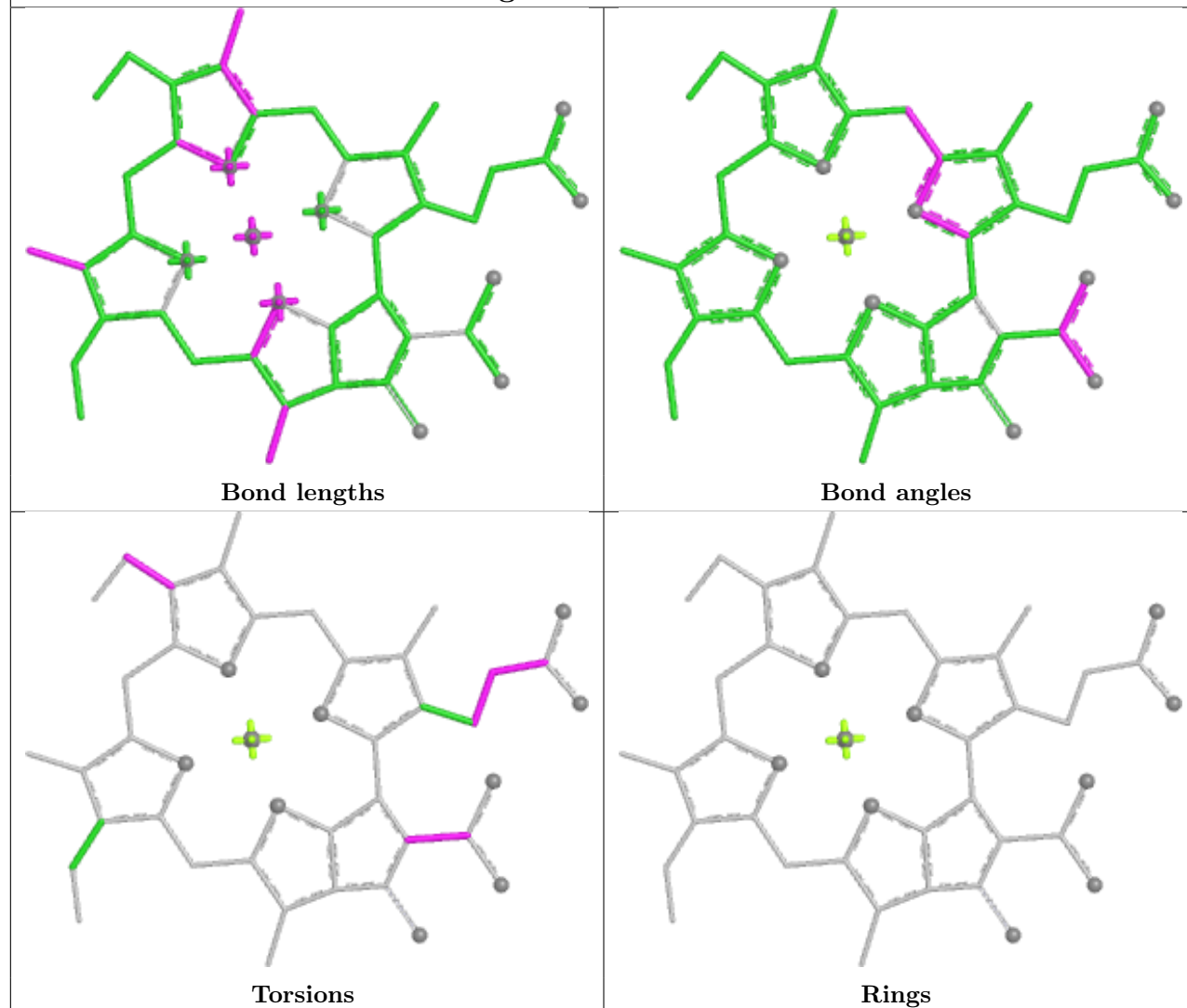
Ligand CLA 4 612



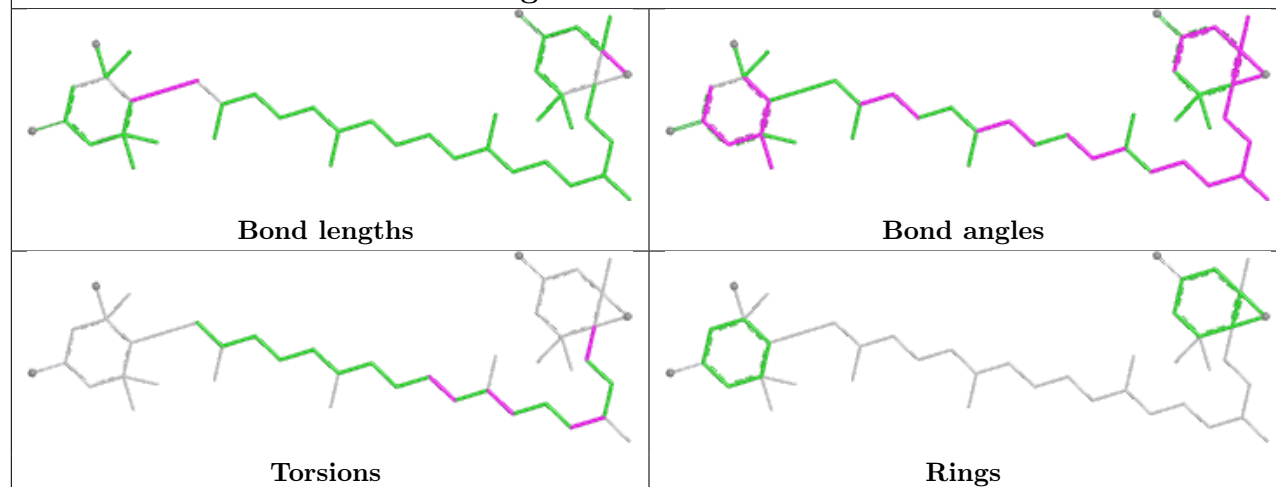
Ligand CLA A 830



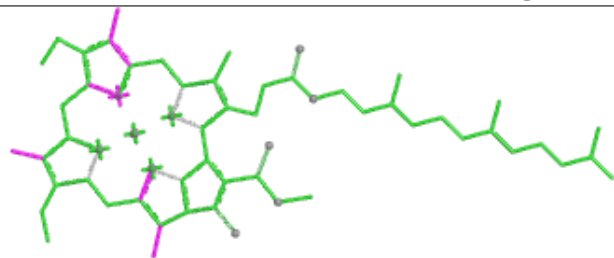
Ligand CLA 7 603



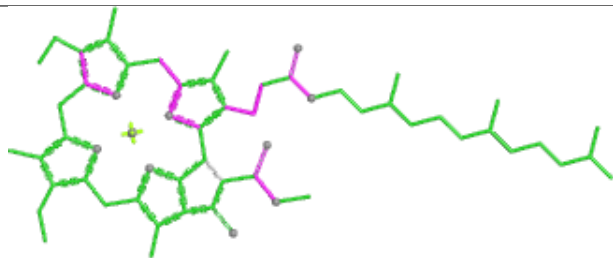
Ligand NEX Y 1623



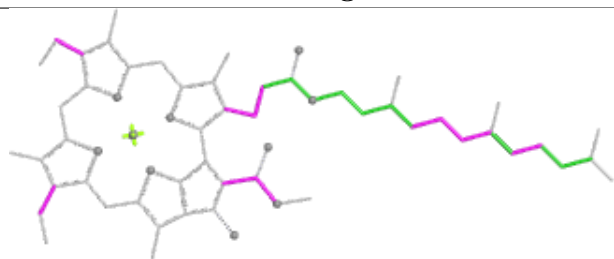
Ligand CLA 3 609



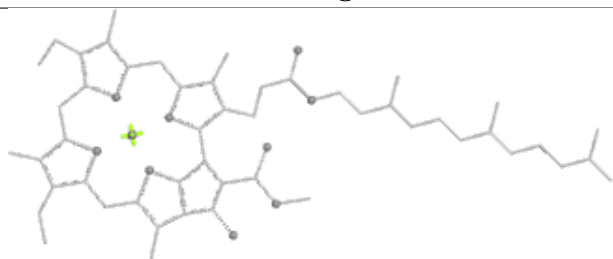
Bond lengths



Bond angles

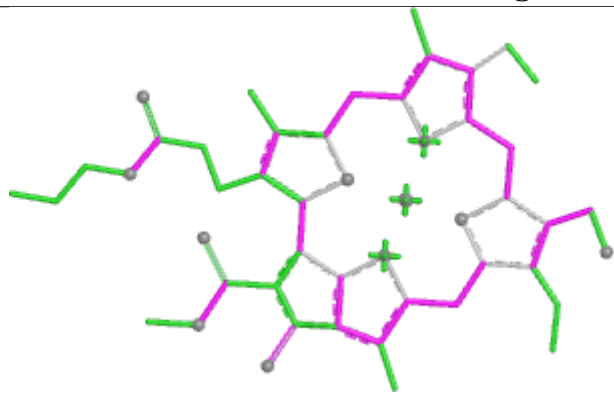


Torsions

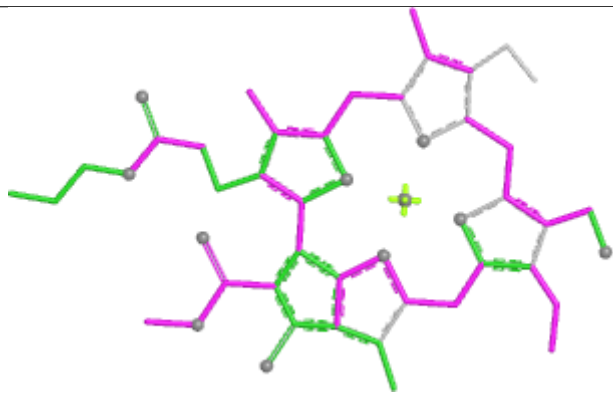


Rings

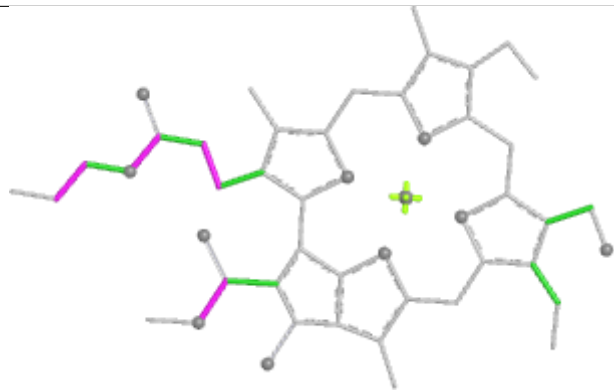
Ligand CHL Y 608



Bond lengths



Bond angles

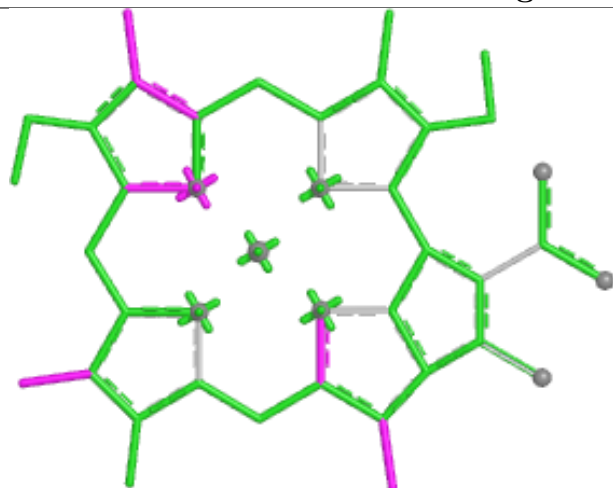


Torsions

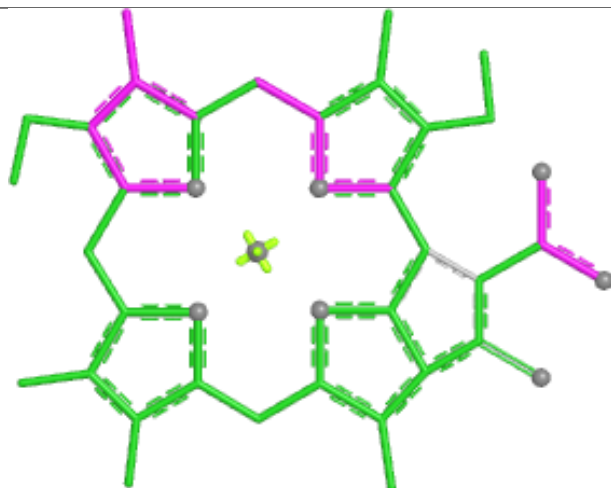


Rings

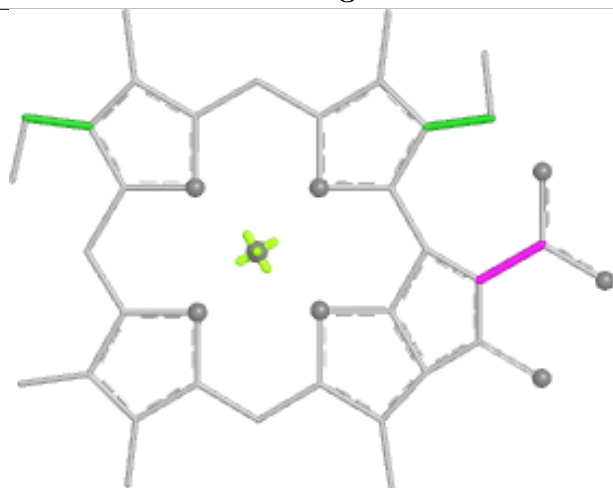
Ligand CLA L 307



Bond lengths



Bond angles

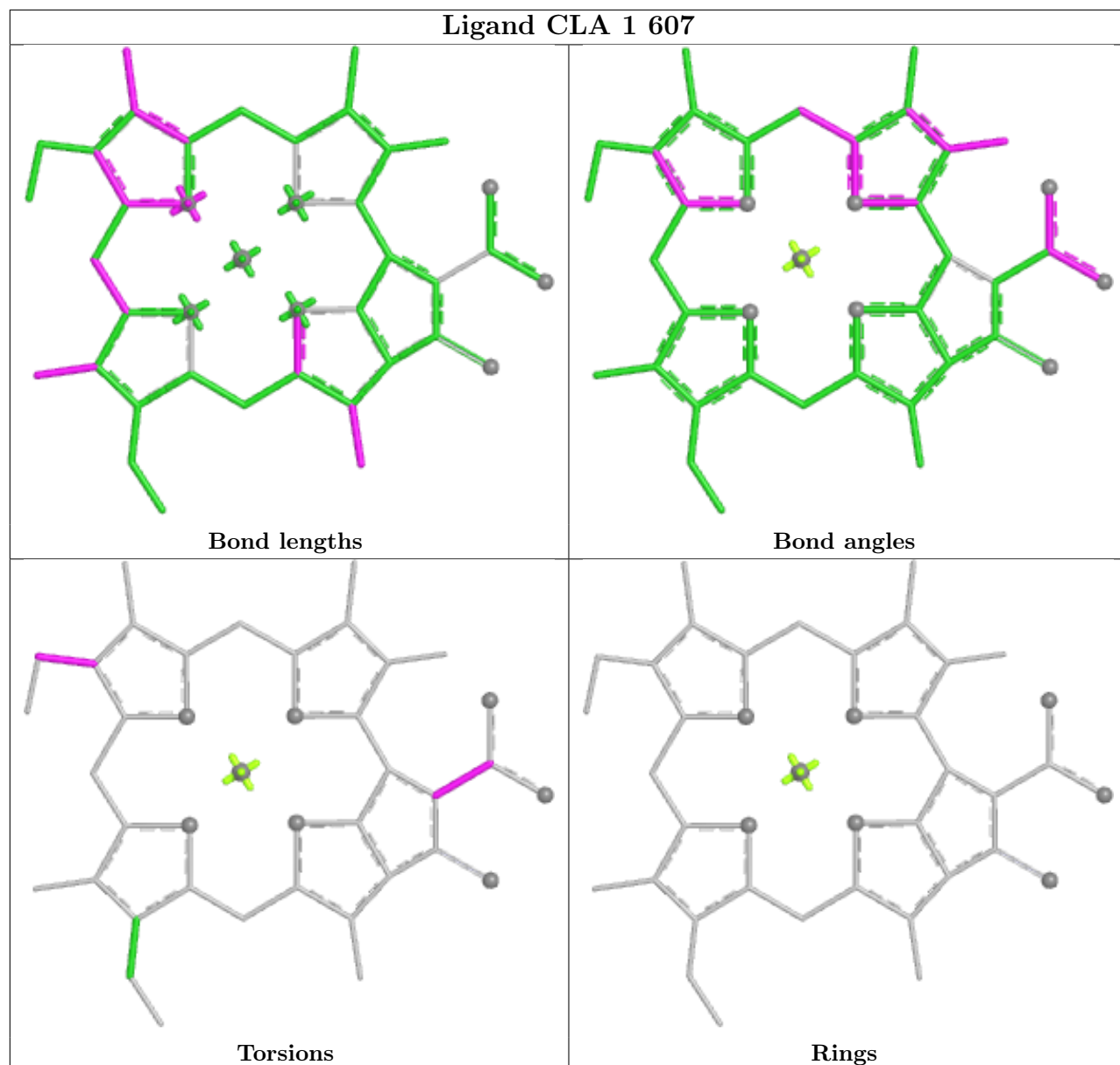


Torsions

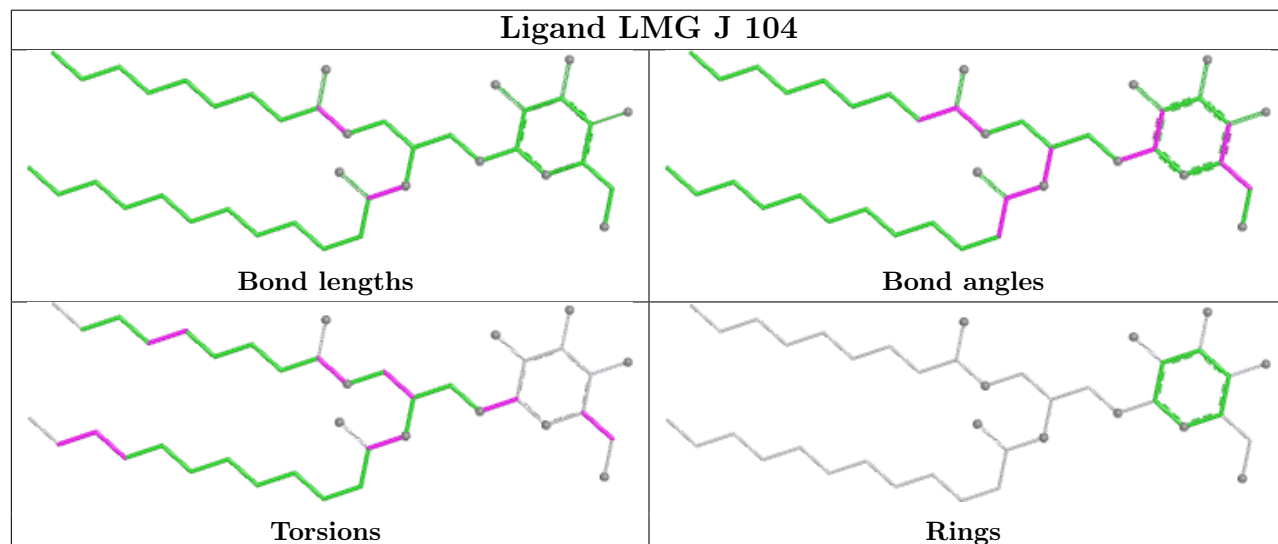


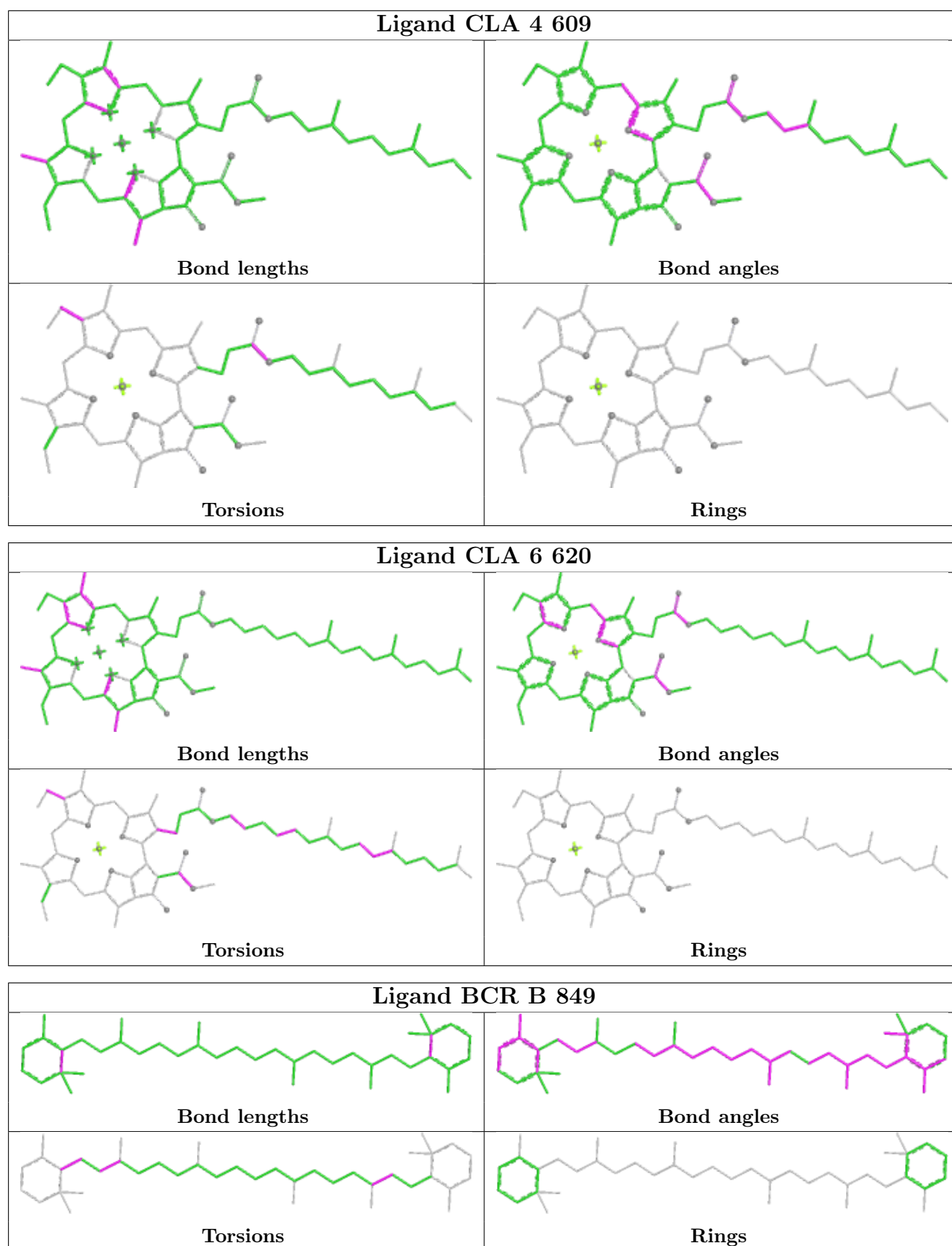
Rings

Ligand CLA 1 607

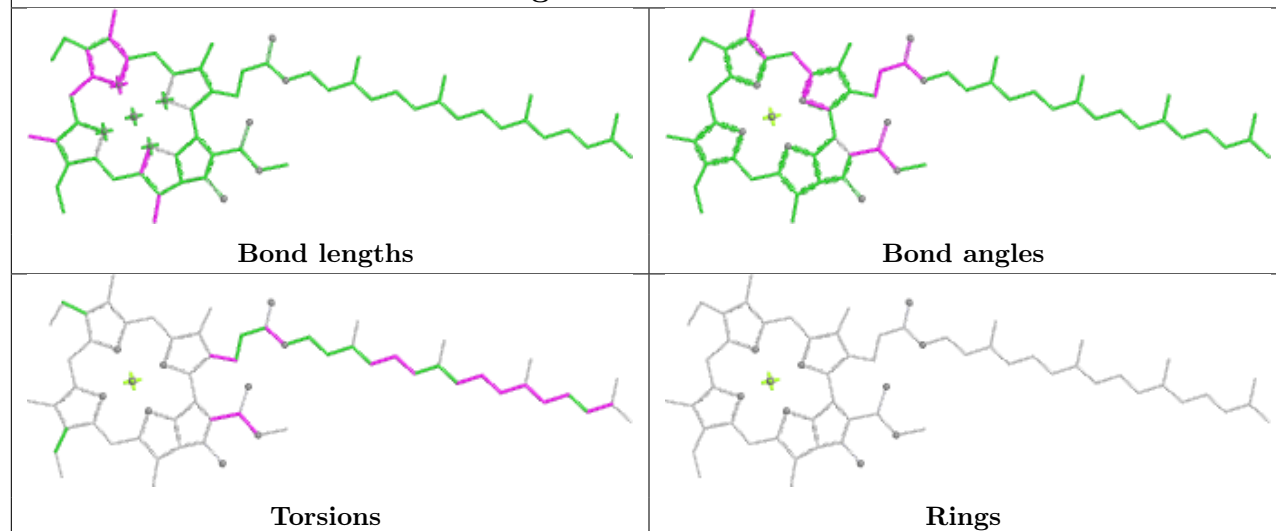


Ligand LMG J 104

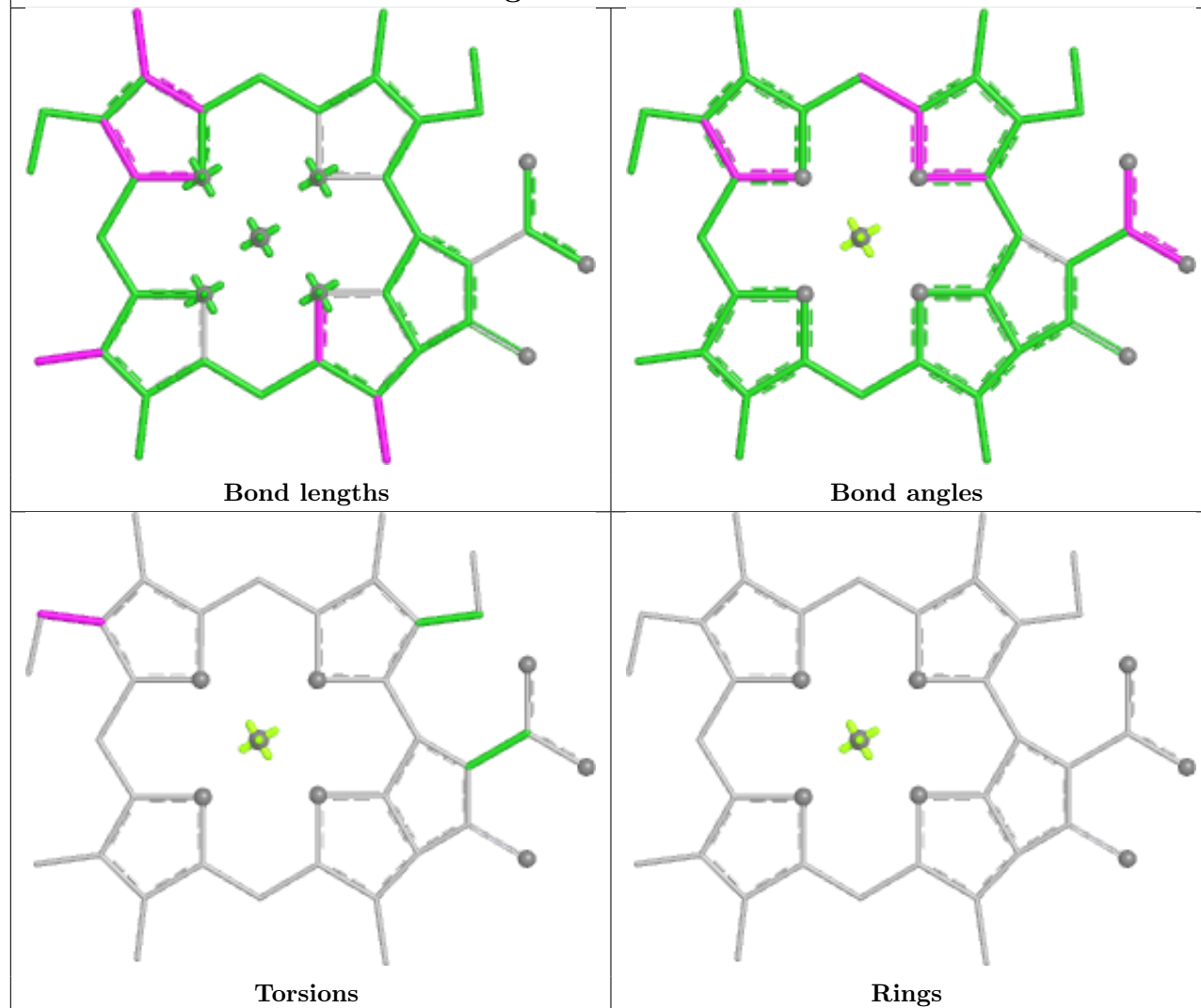


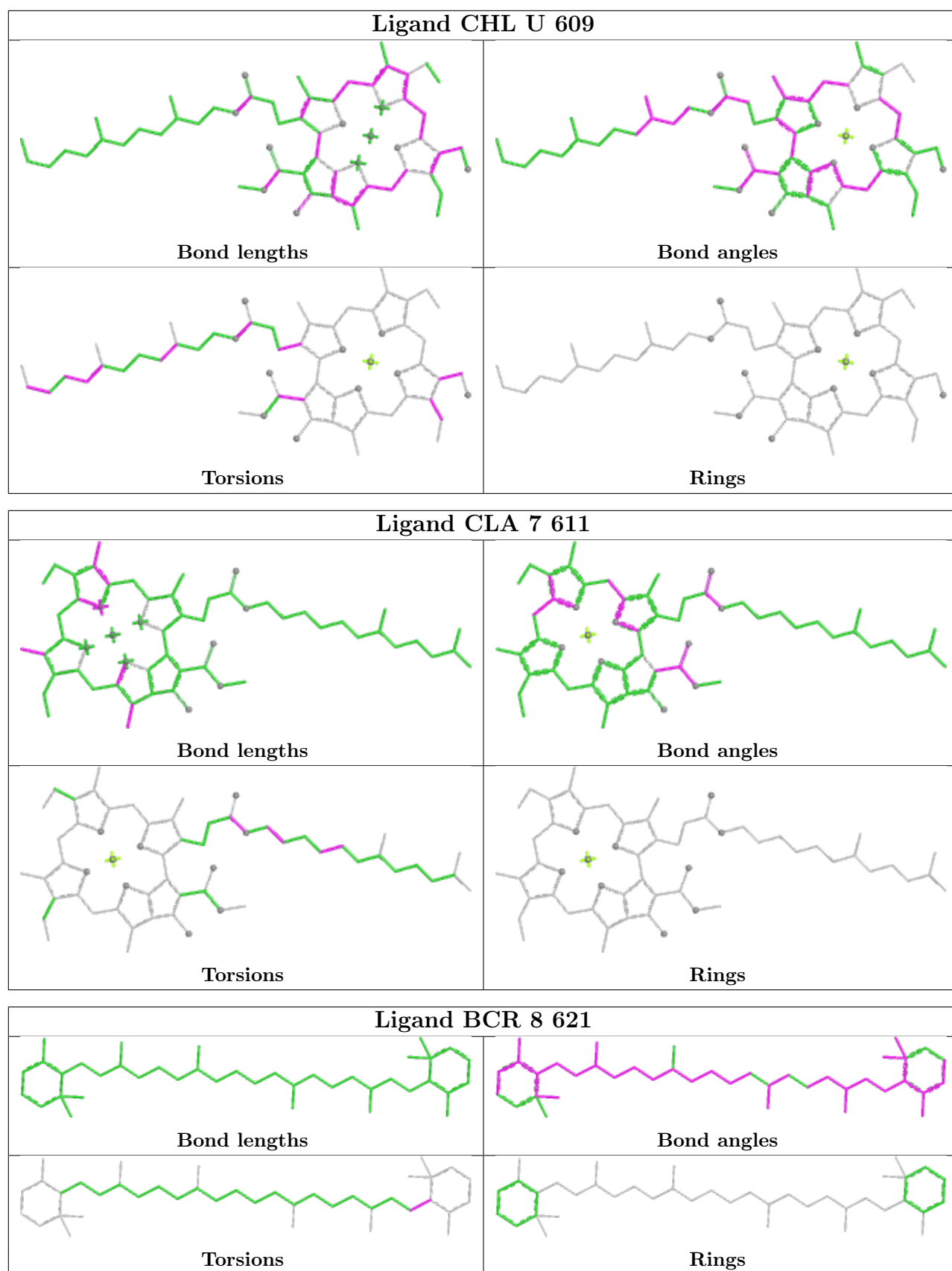


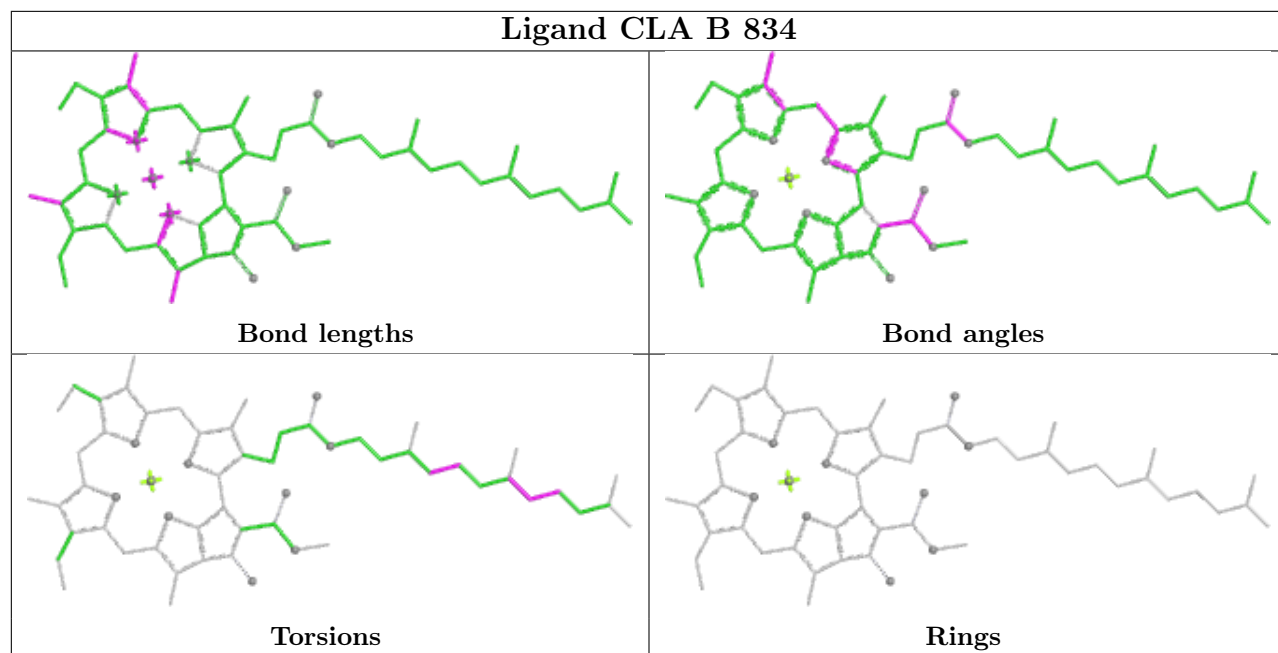
Ligand CLA A 831



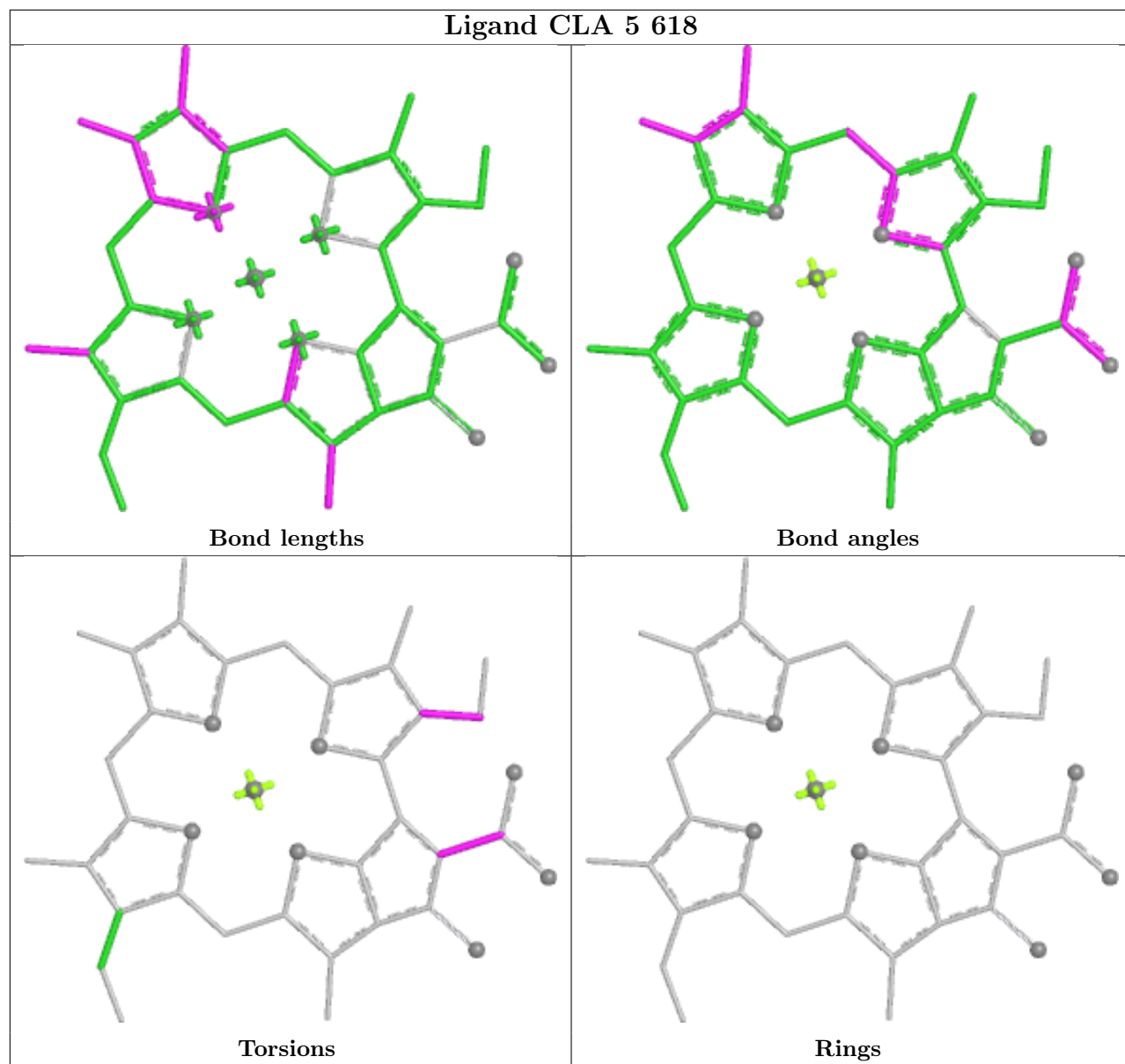
Ligand CLA 6 606



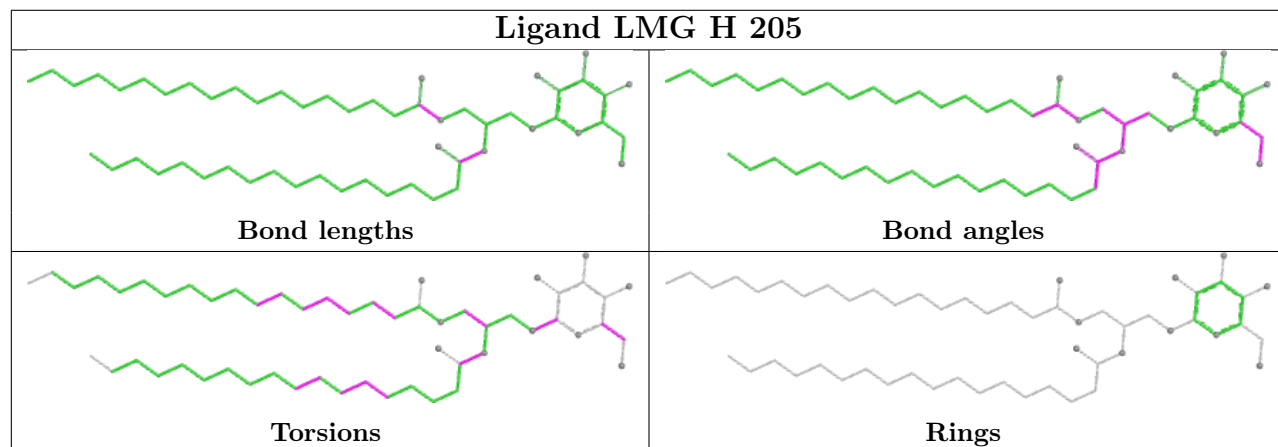


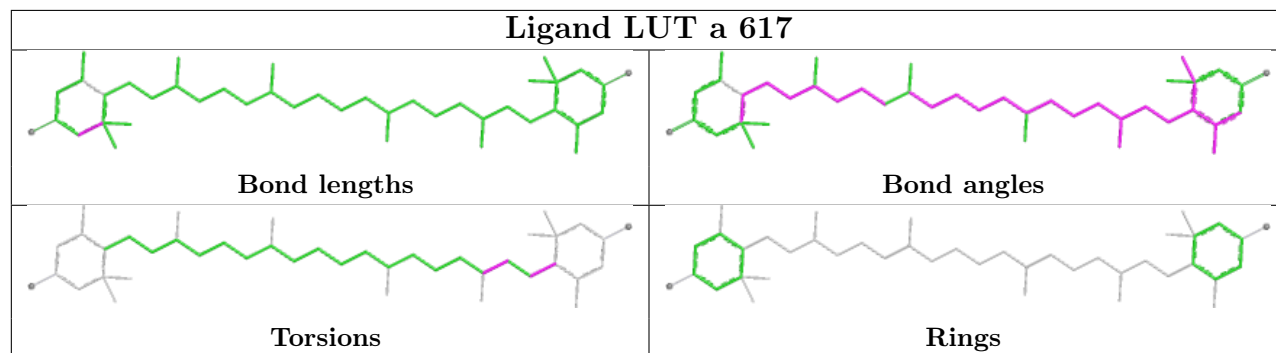
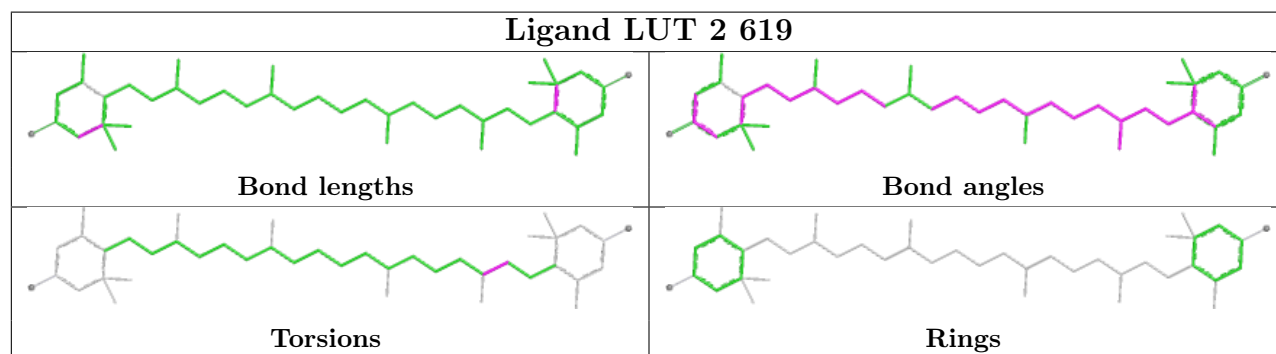
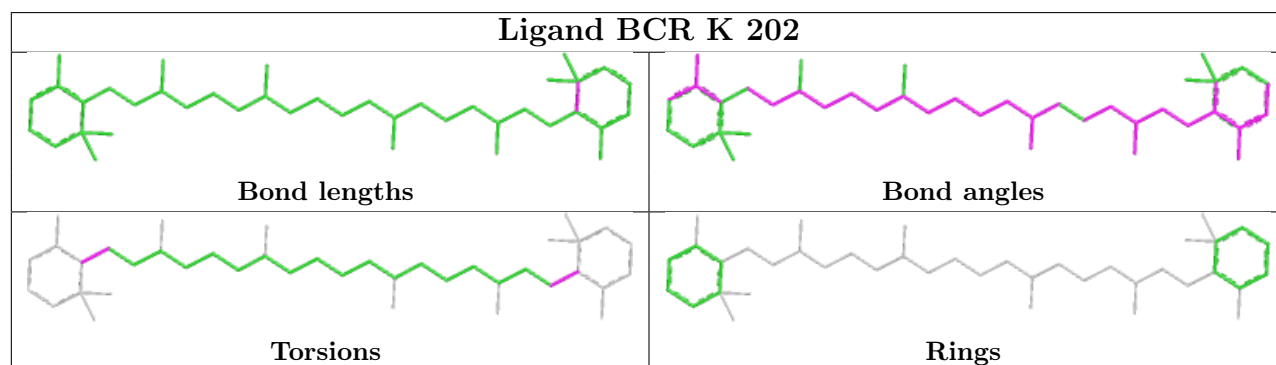
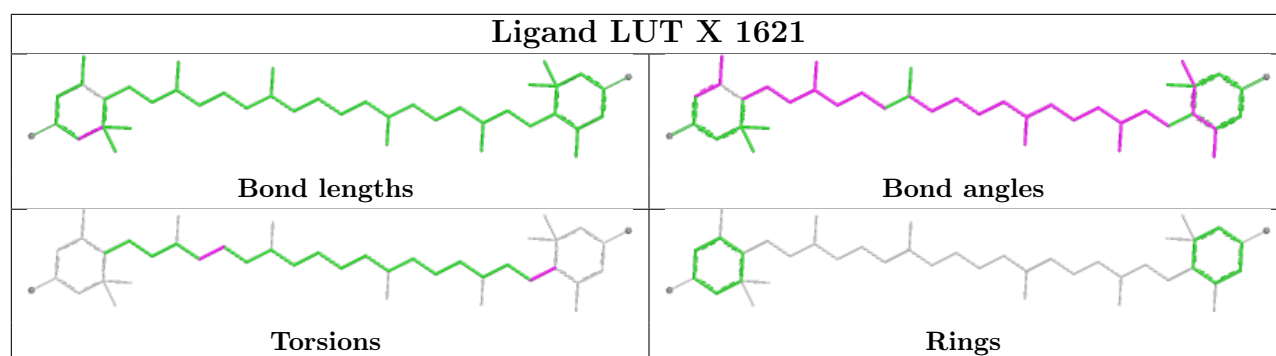


Ligand CLA 5 618

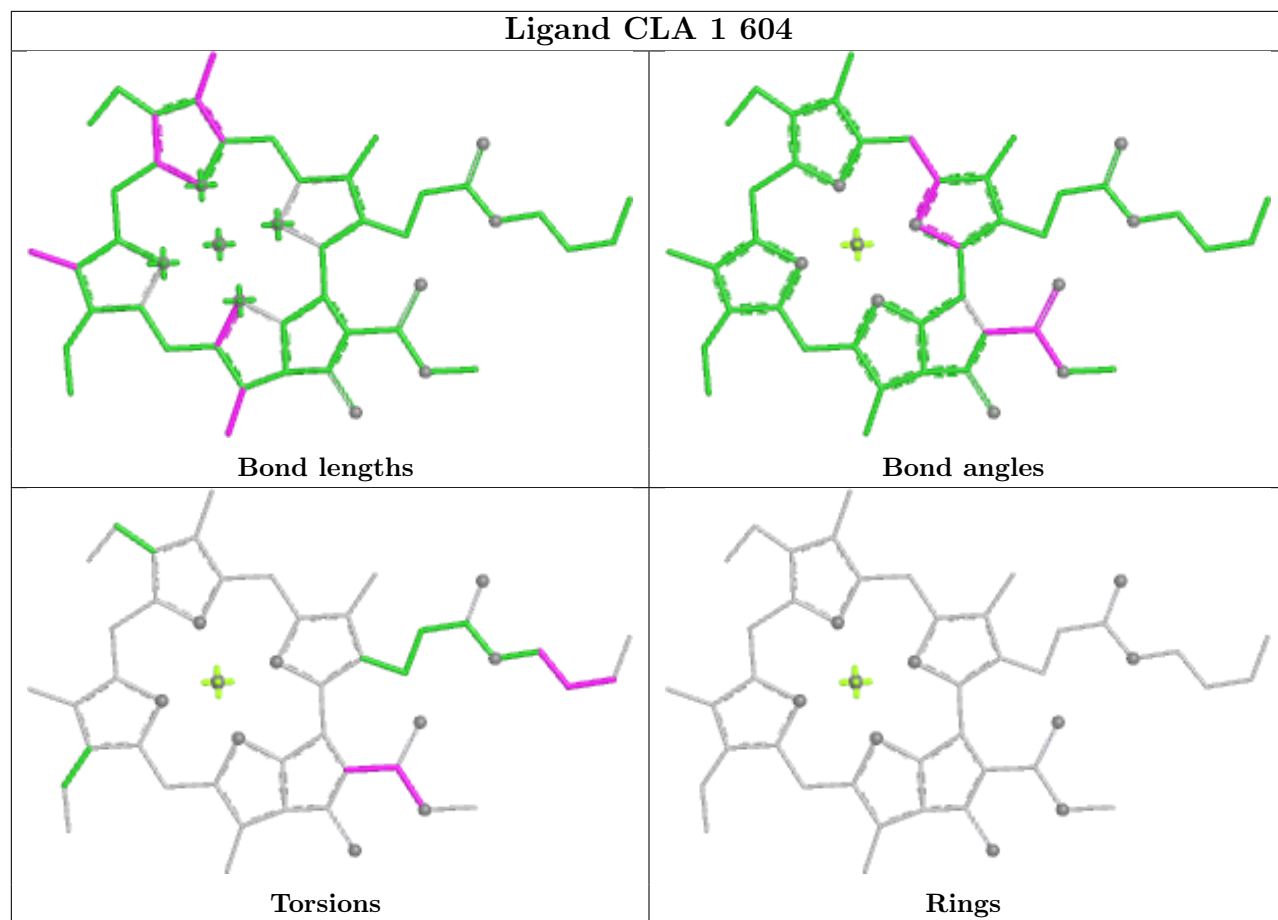


Ligand LMG H 205

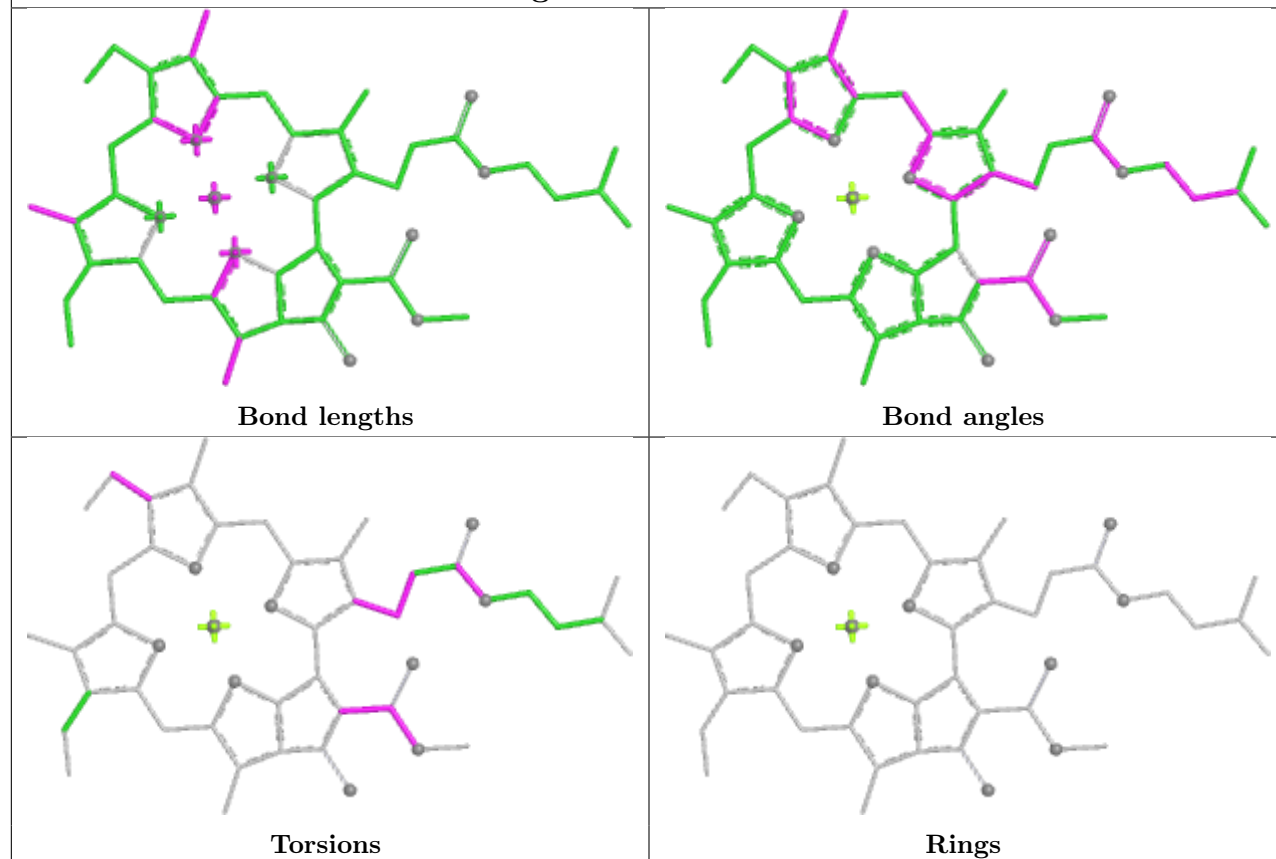




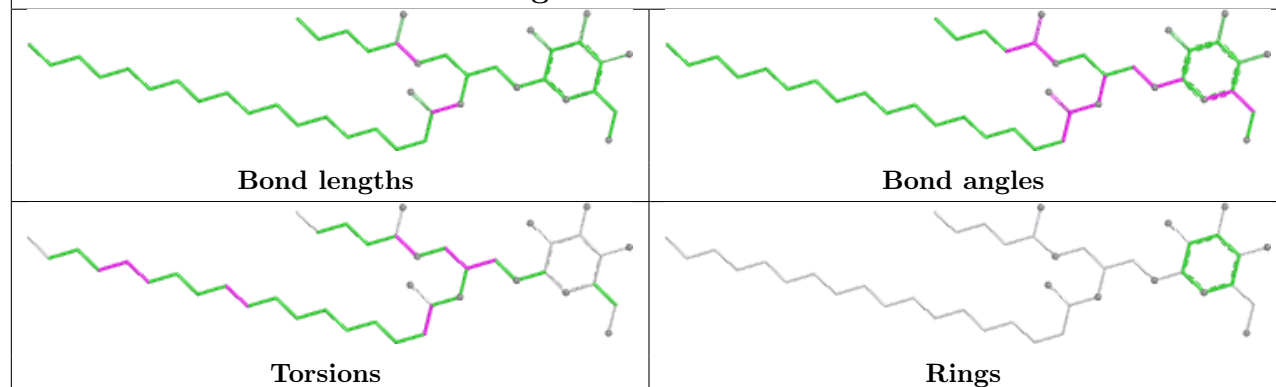
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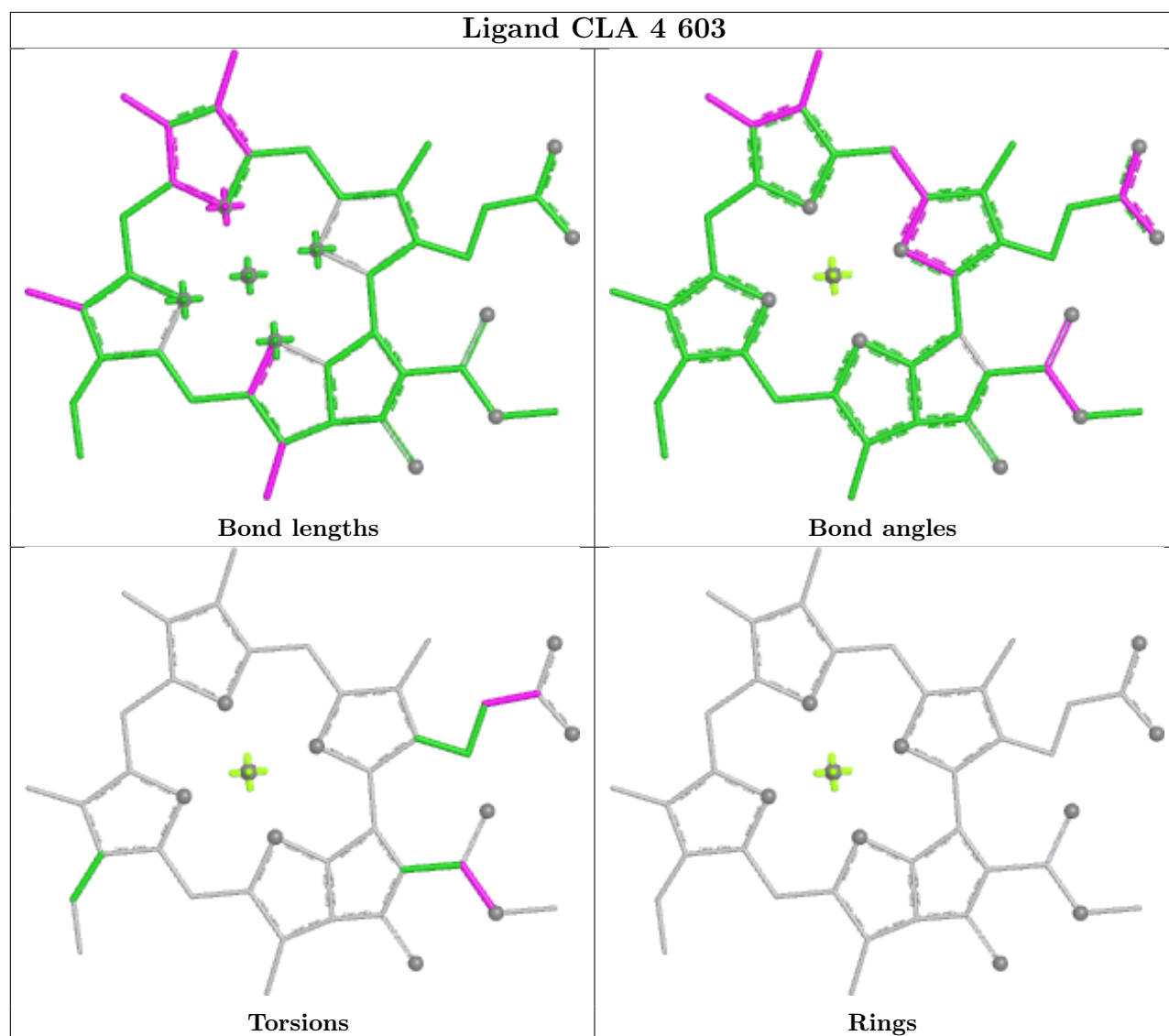
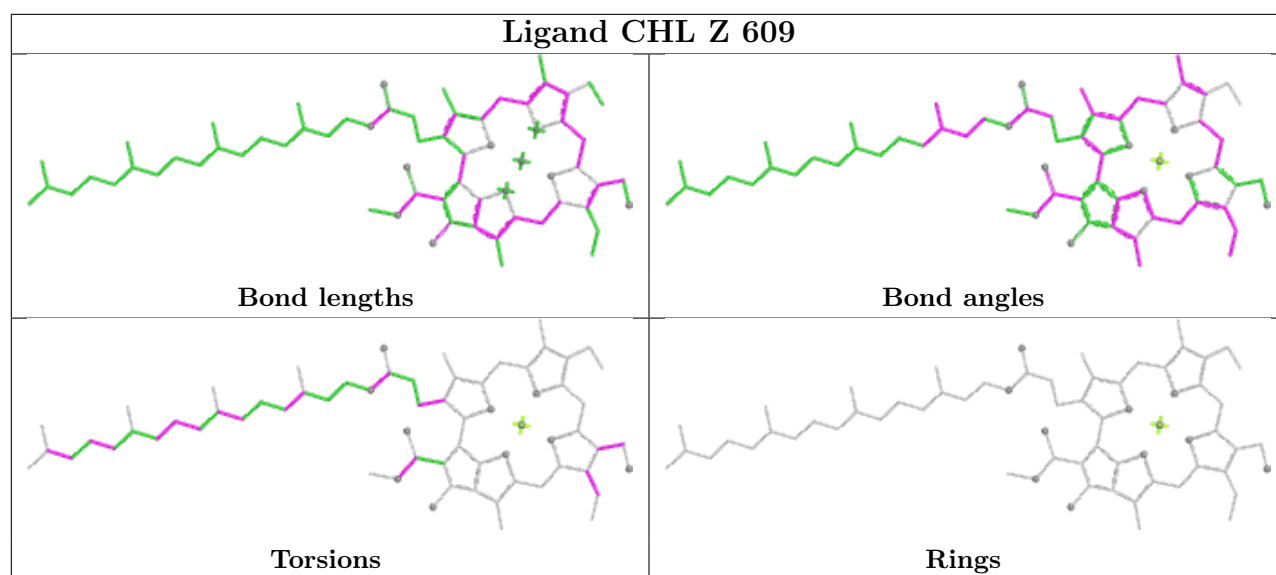


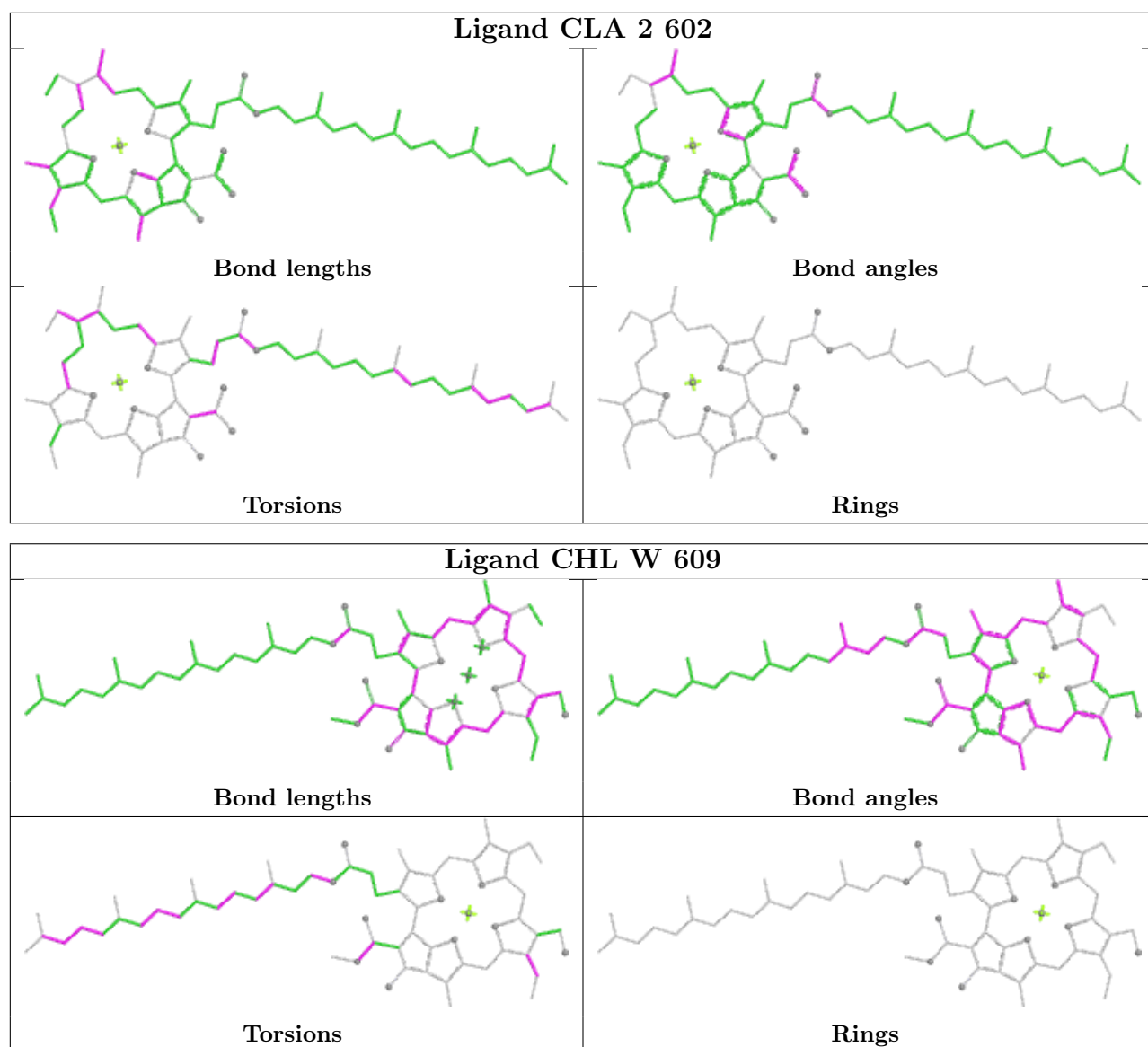
Ligand CLA A 832

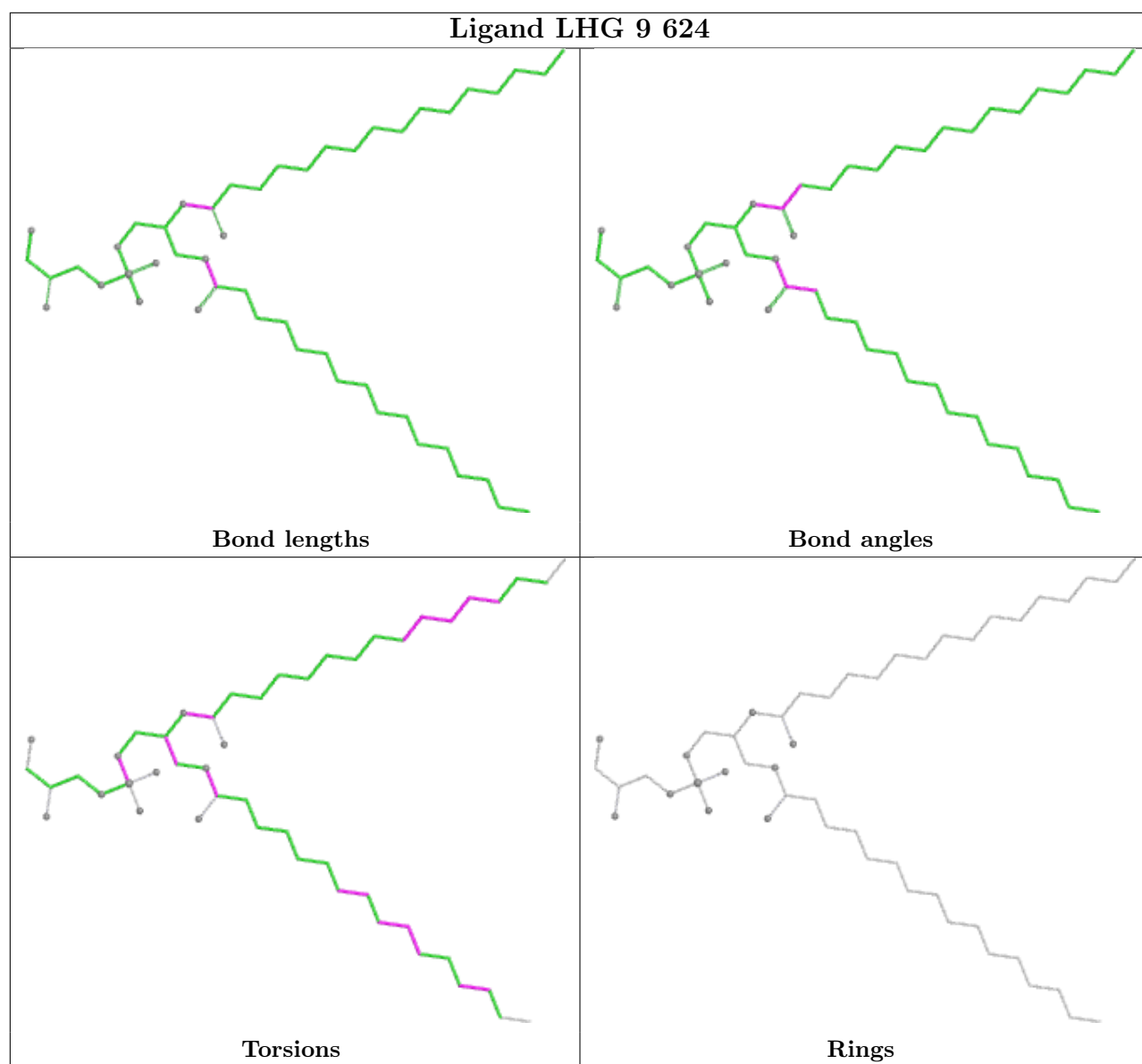


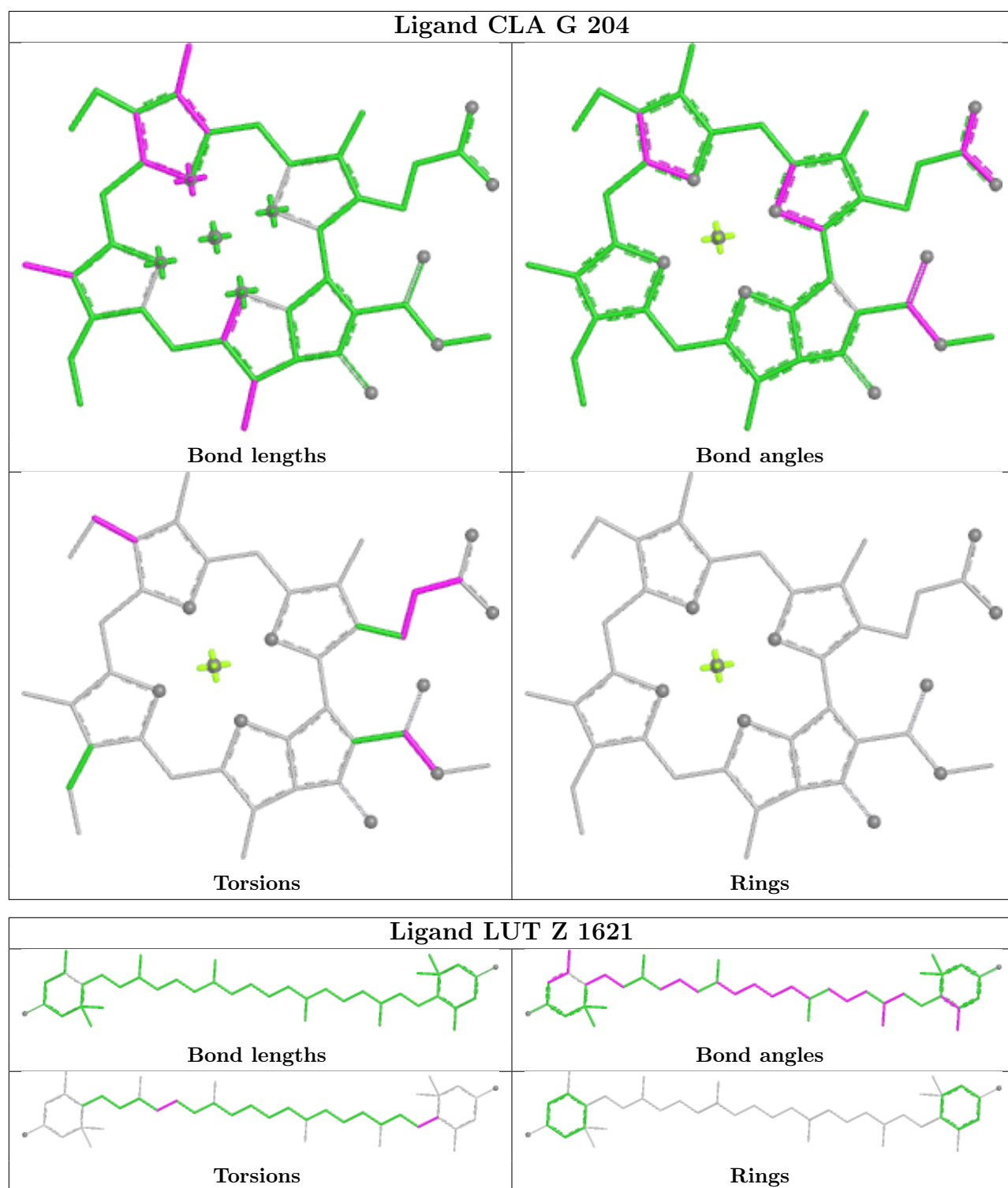
Ligand LMG J 103



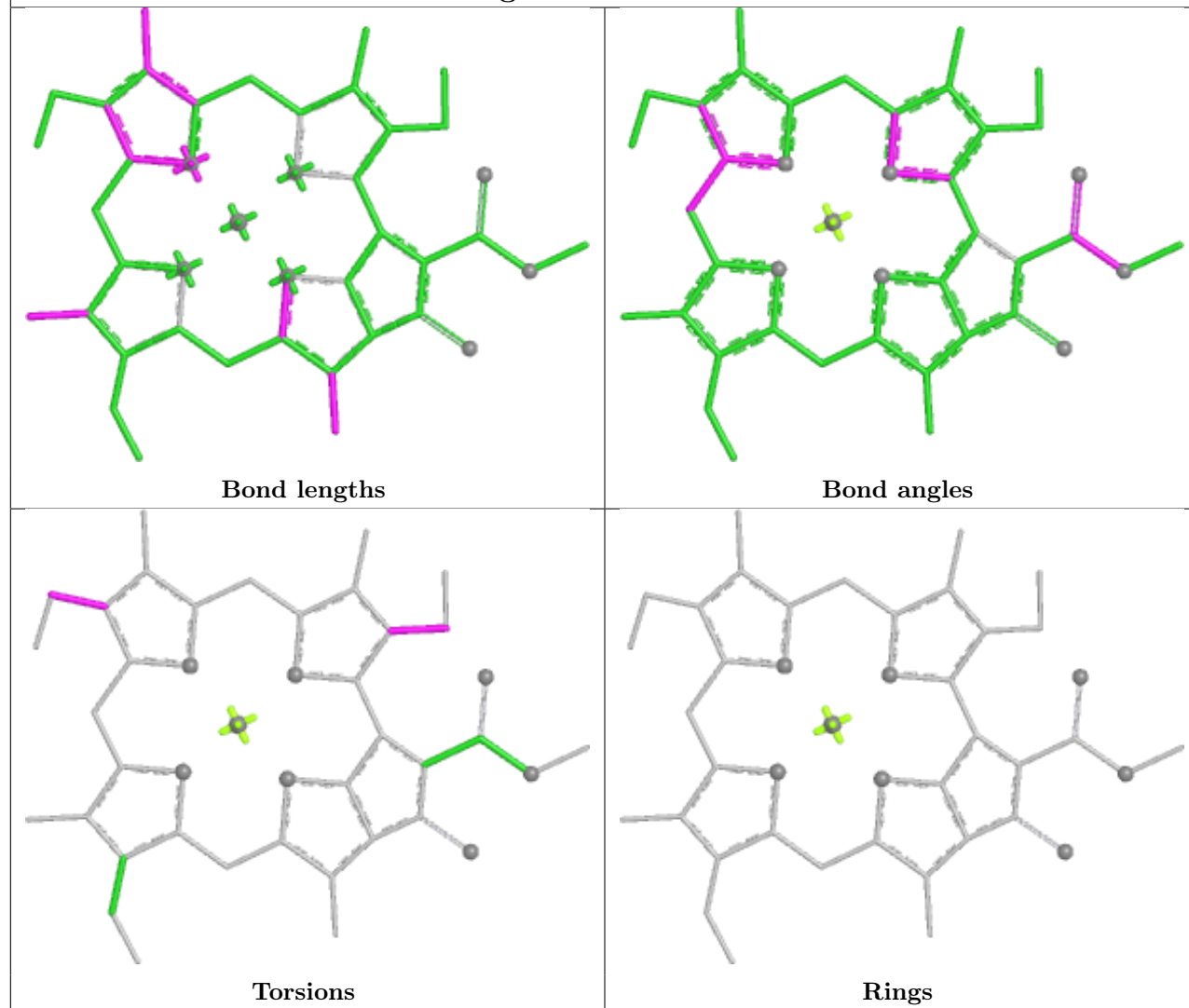




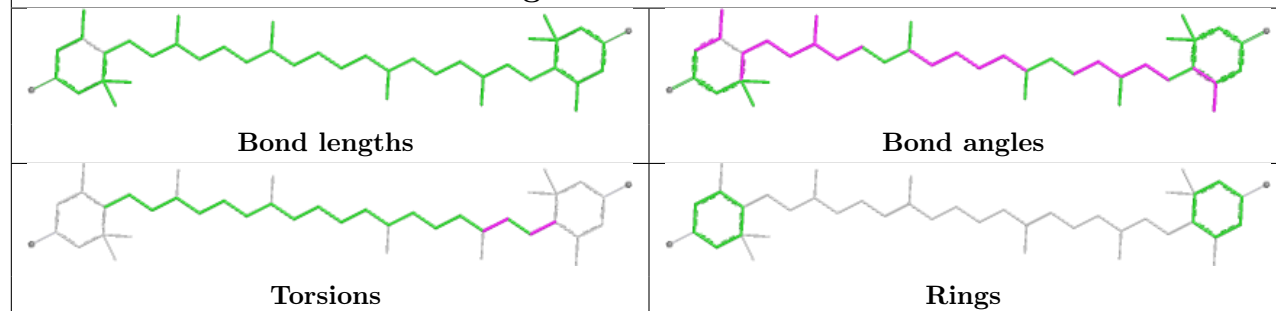




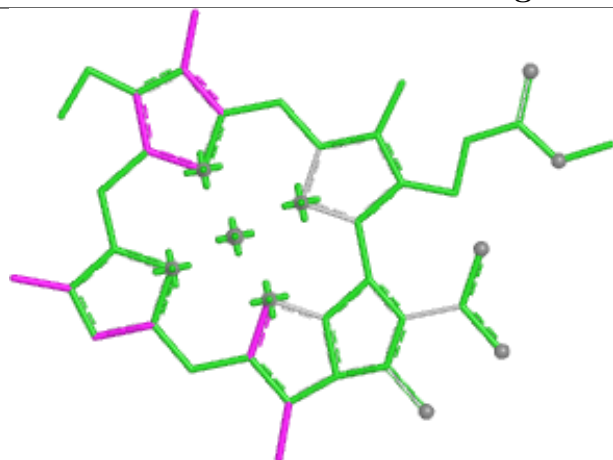
Ligand CLA 7 614



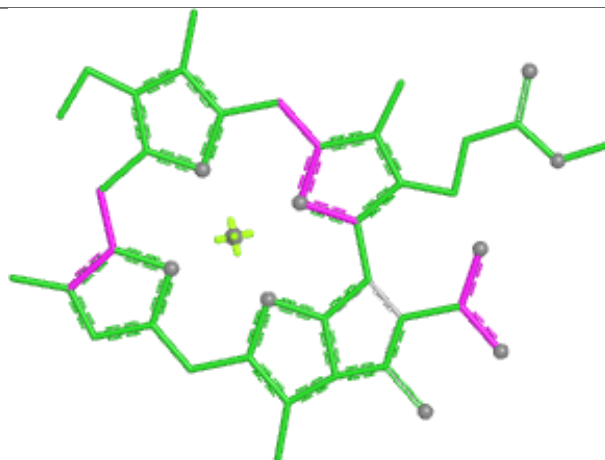
Ligand LUT X 1620



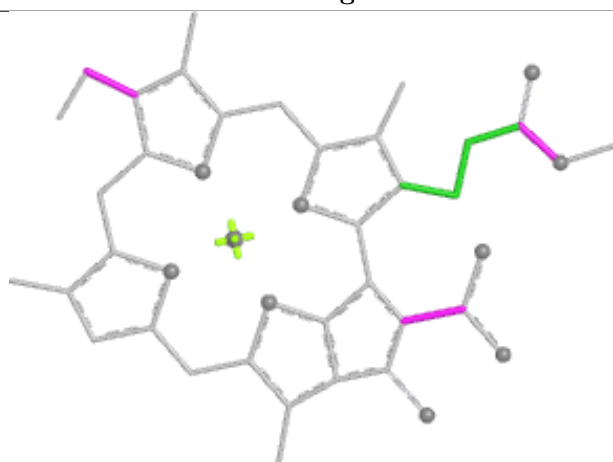
Ligand CLA B 821



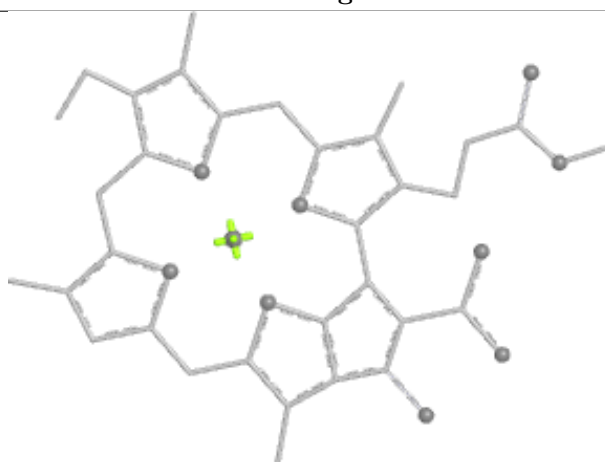
Bond lengths



Bond angles

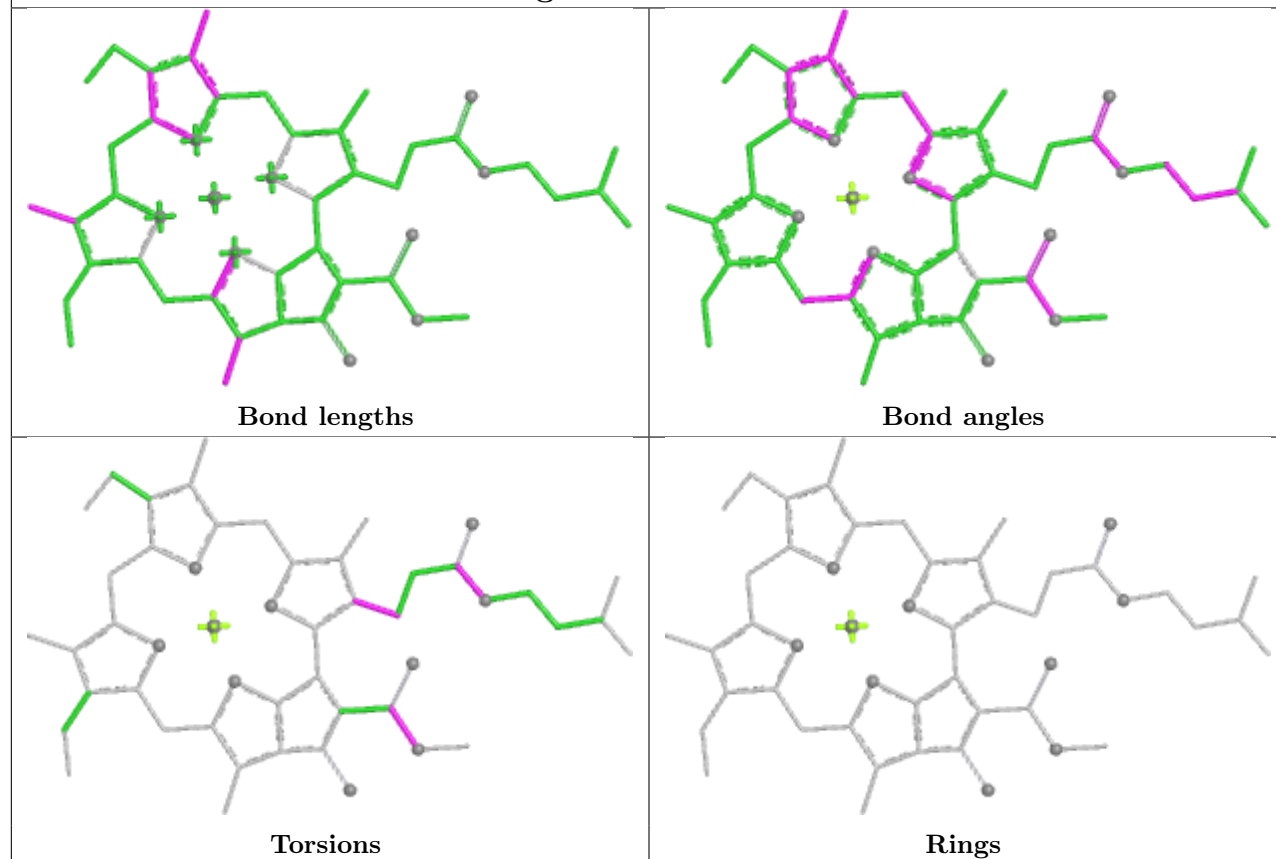


Torsions

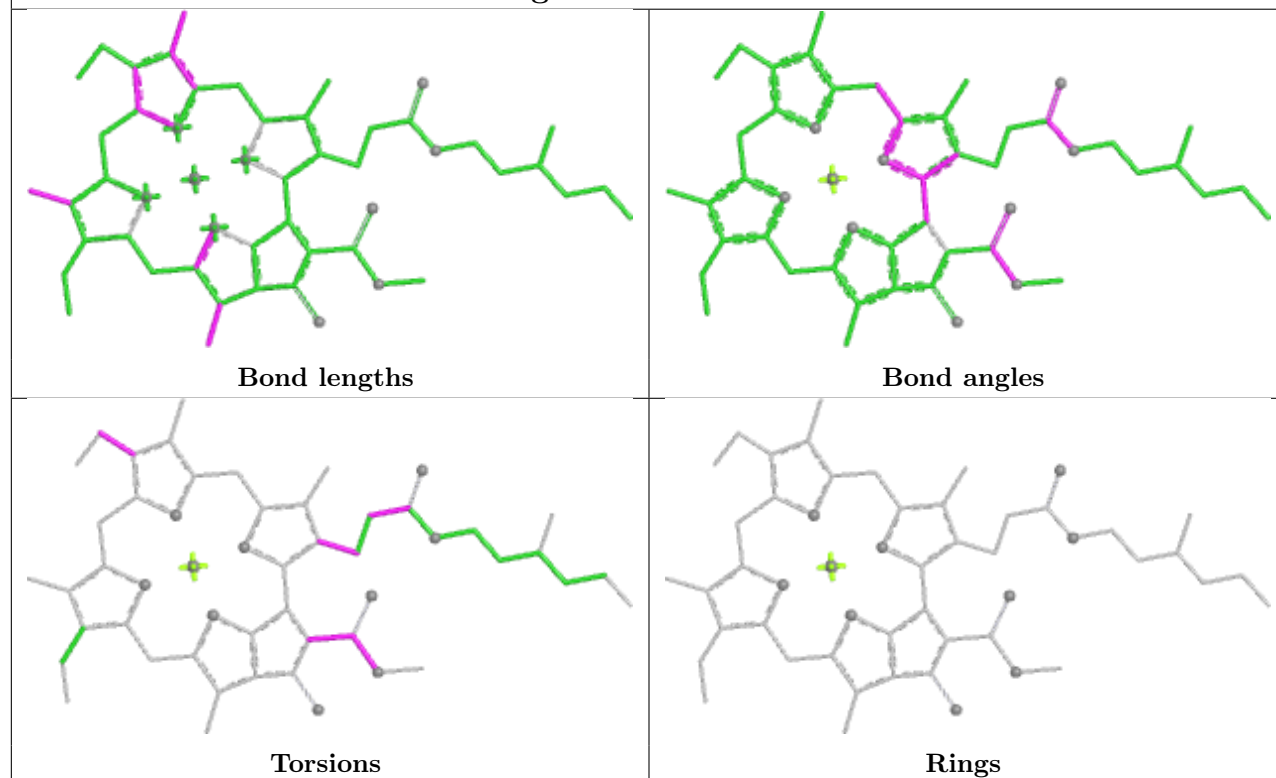


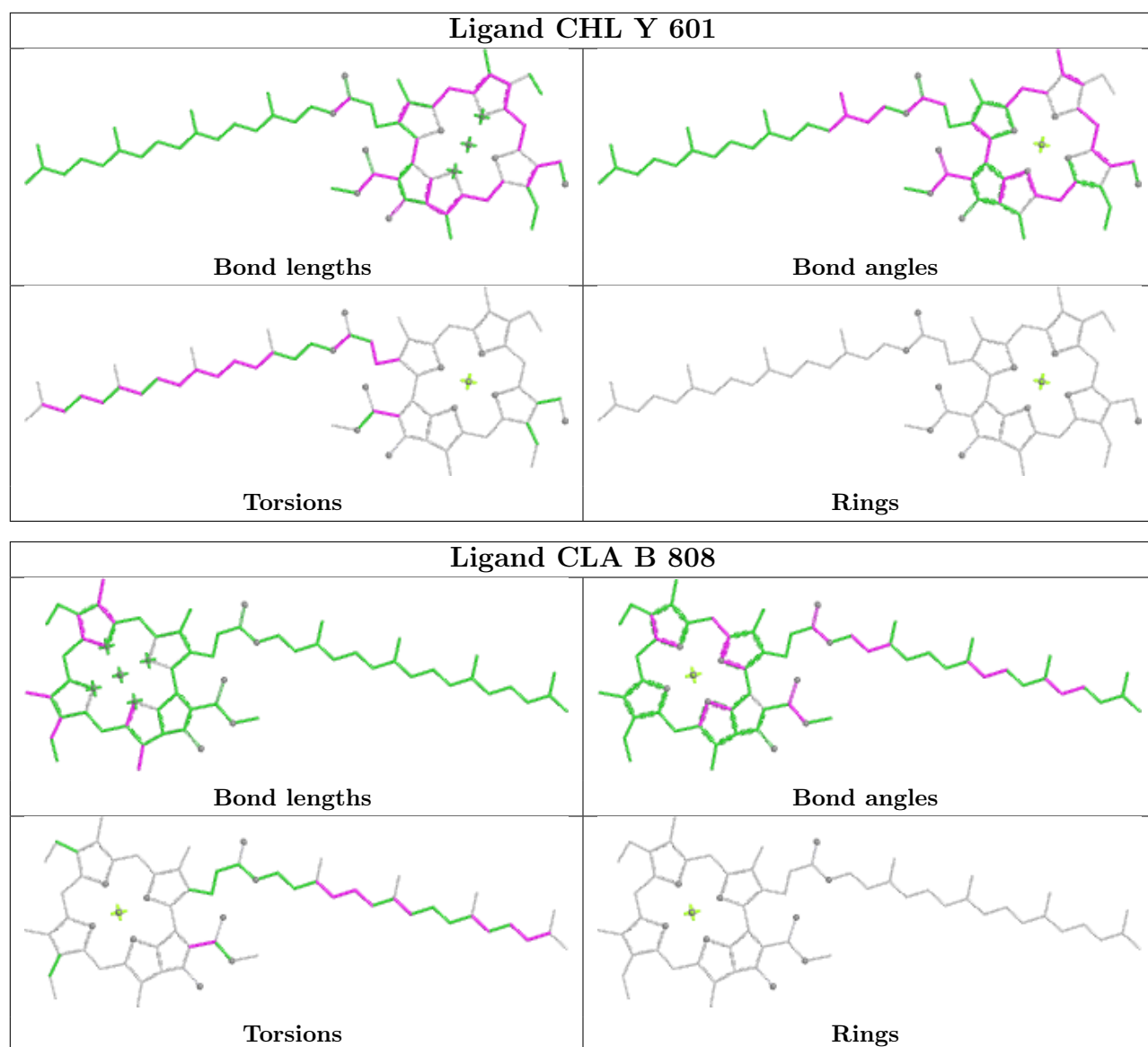
Rings

Ligand CLA 8 604

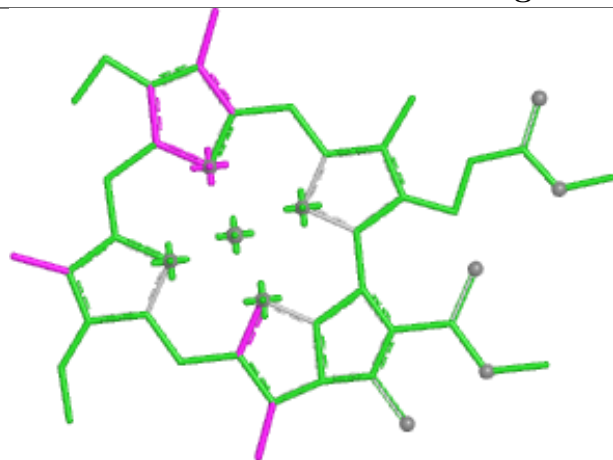


Ligand CLA U 603

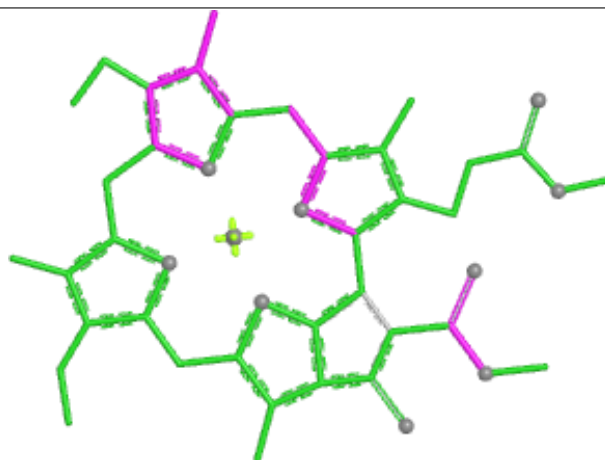




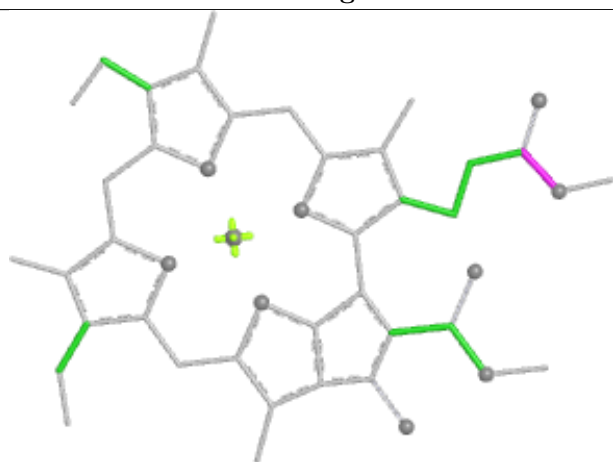
Ligand CLA B 838



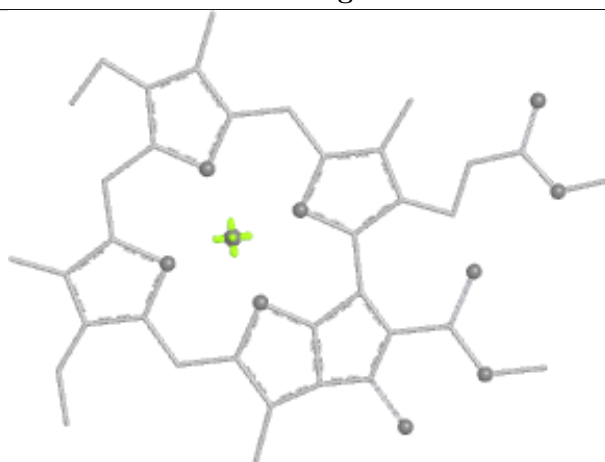
Bond lengths



Bond angles

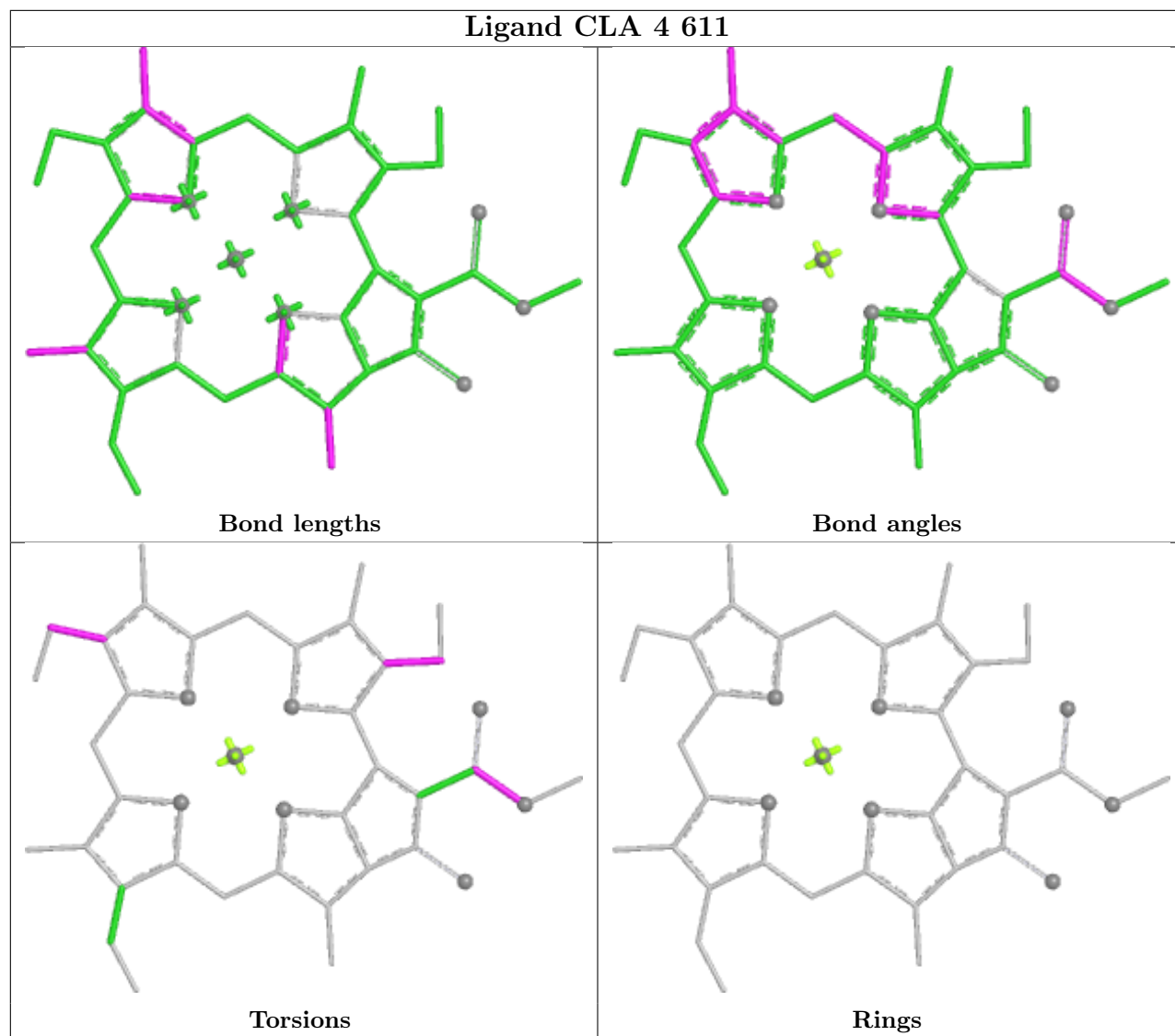


Torsions

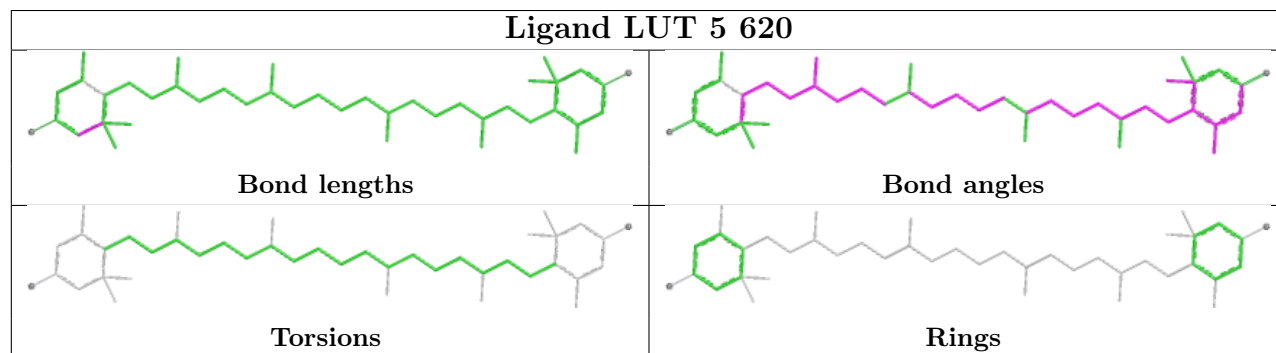


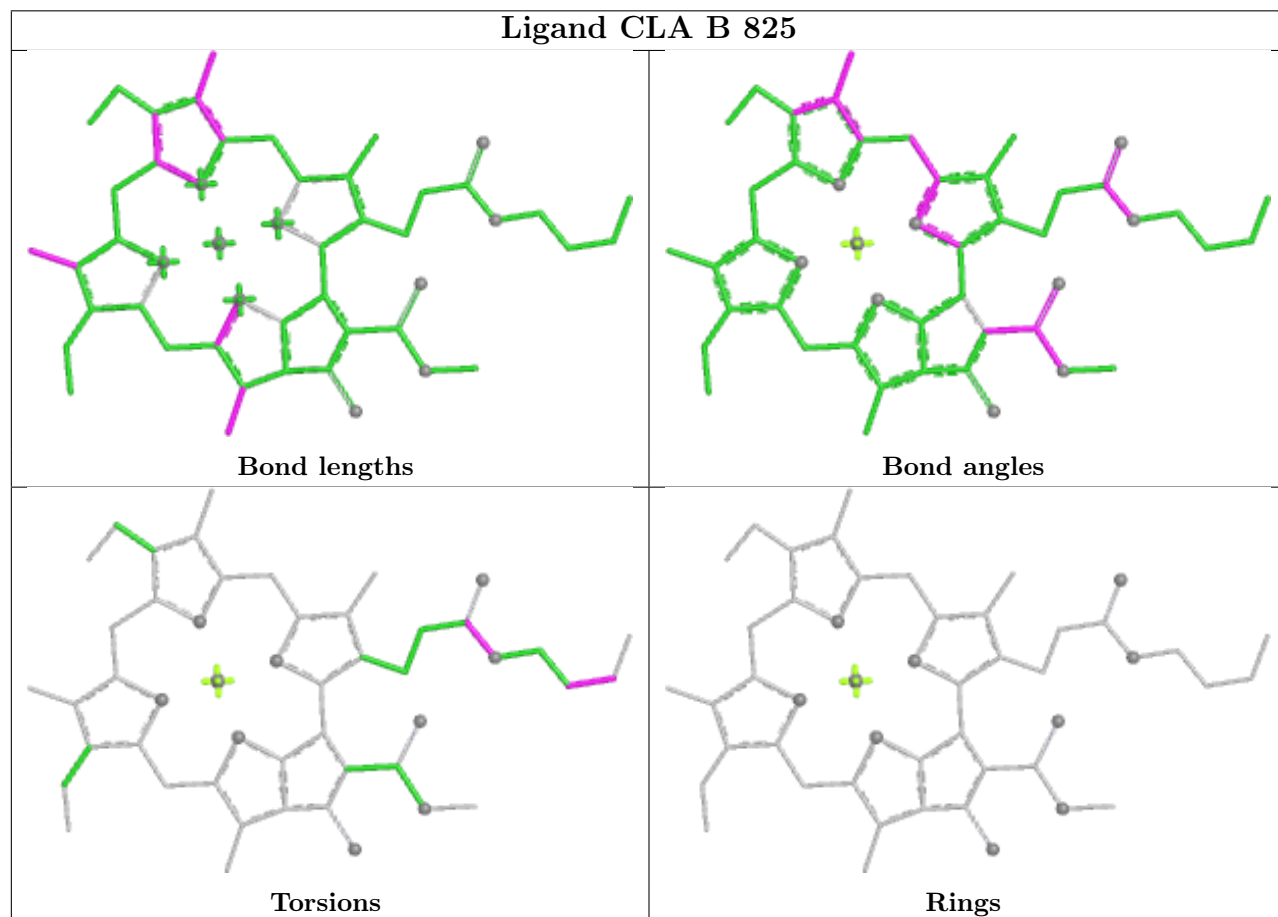
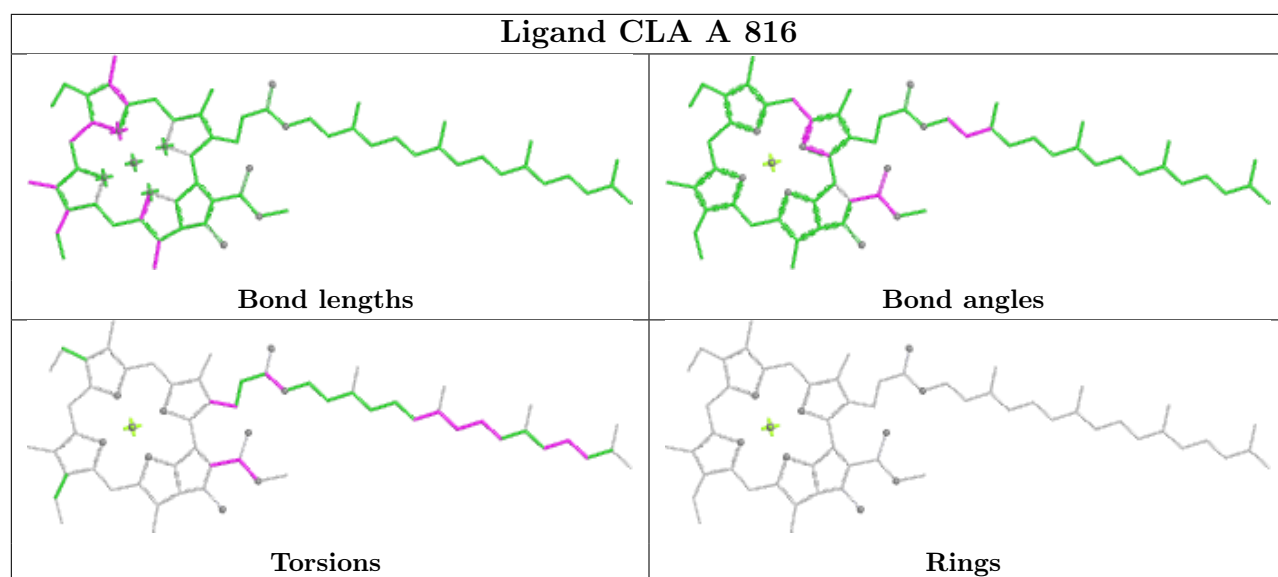
Rings

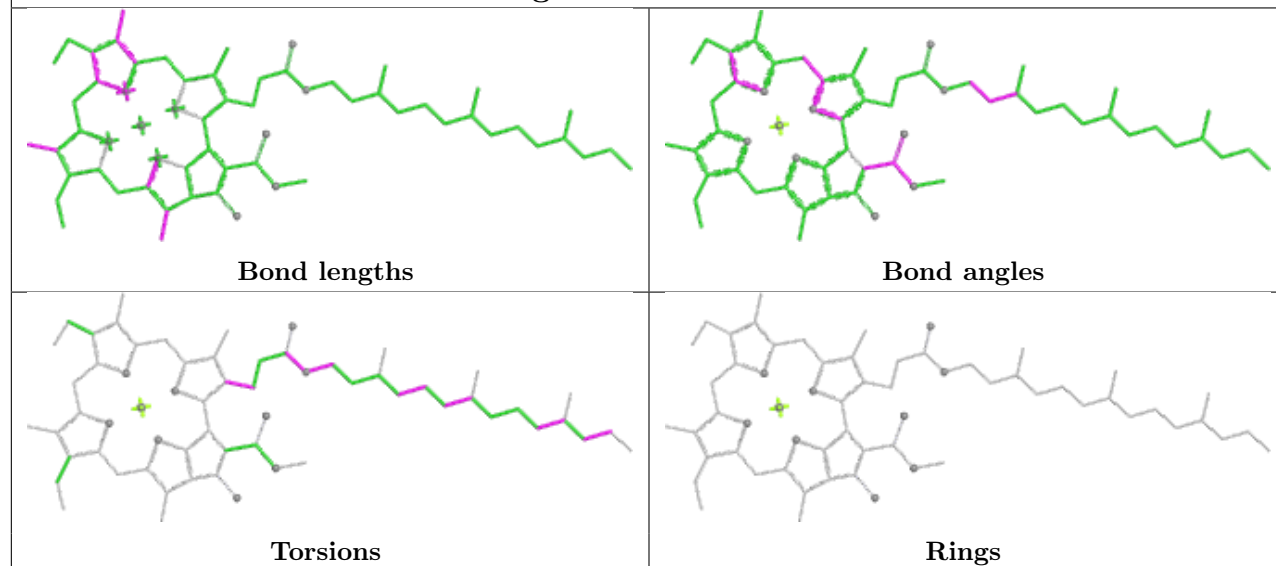
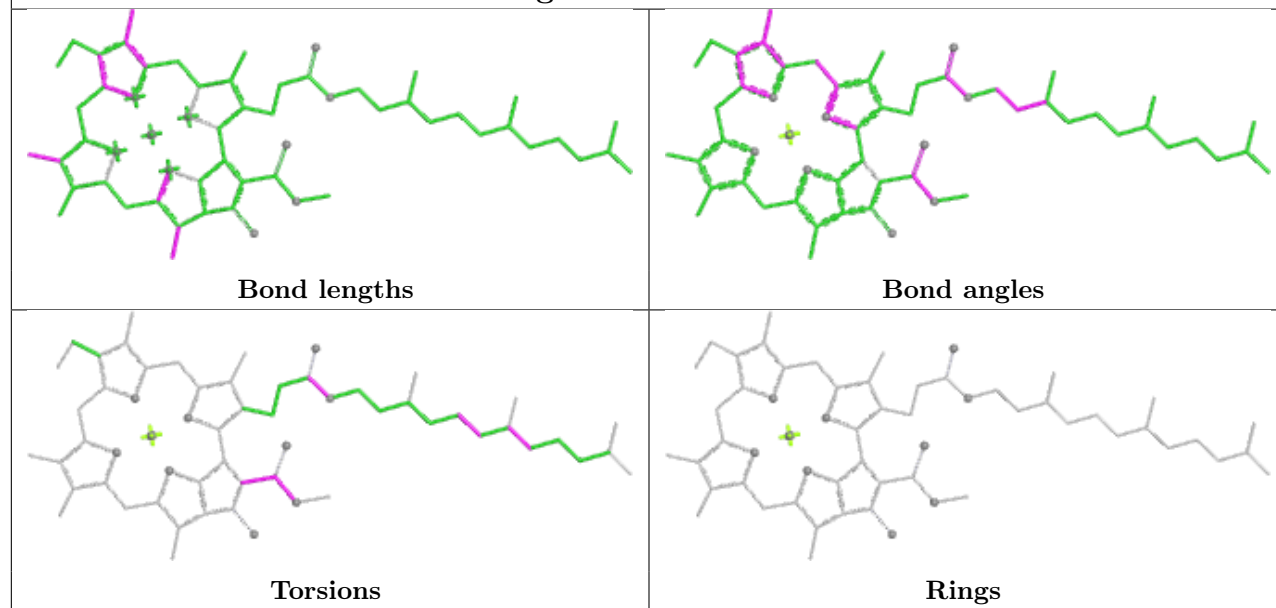
Ligand CLA 4 611



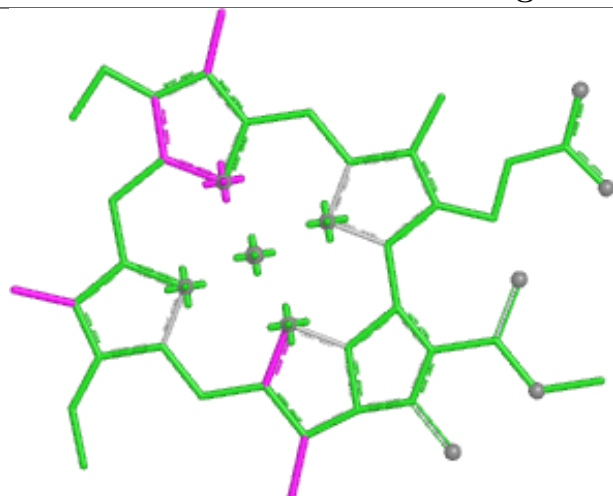
Ligand LUT 5 620



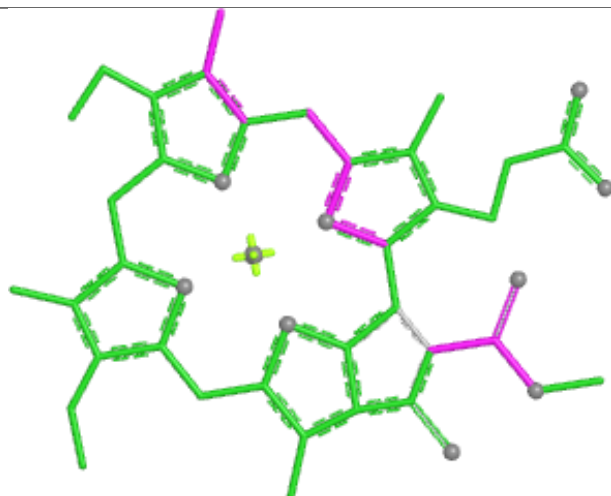


Ligand CLA B 826**Ligand CLA a 610**

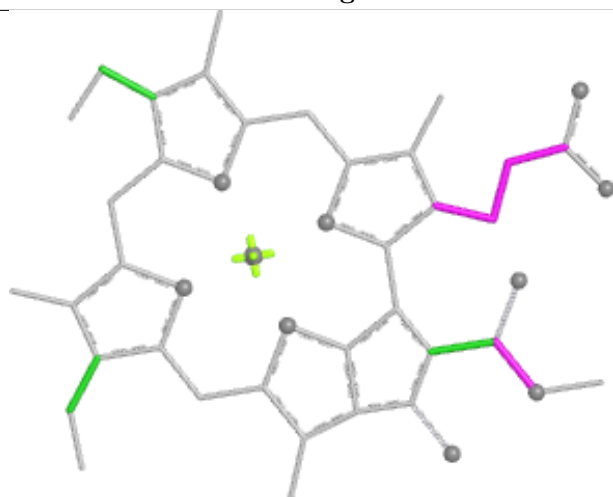
Ligand CLA L 302



Bond lengths



Bond angles

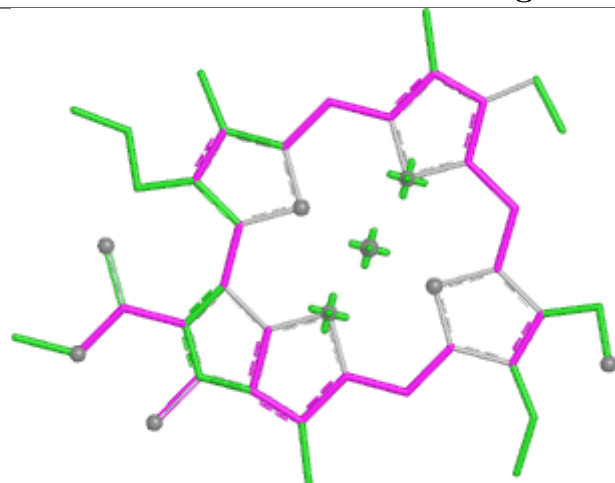


Torsions

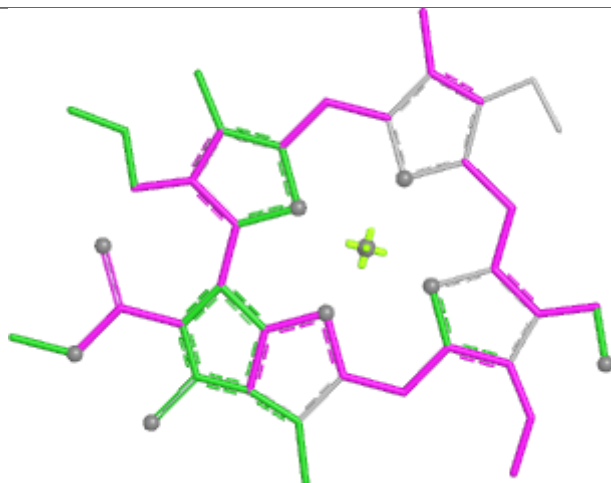


Rings

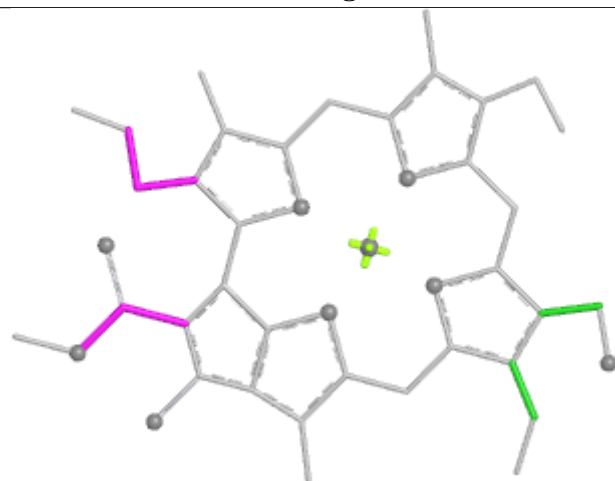
Ligand CHL V 606



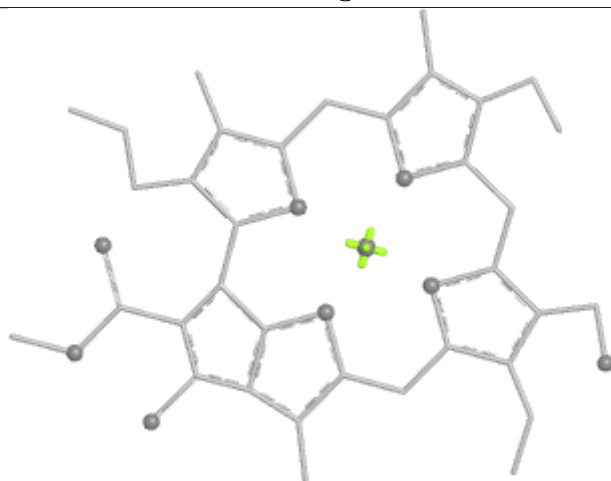
Bond lengths



Bond angles

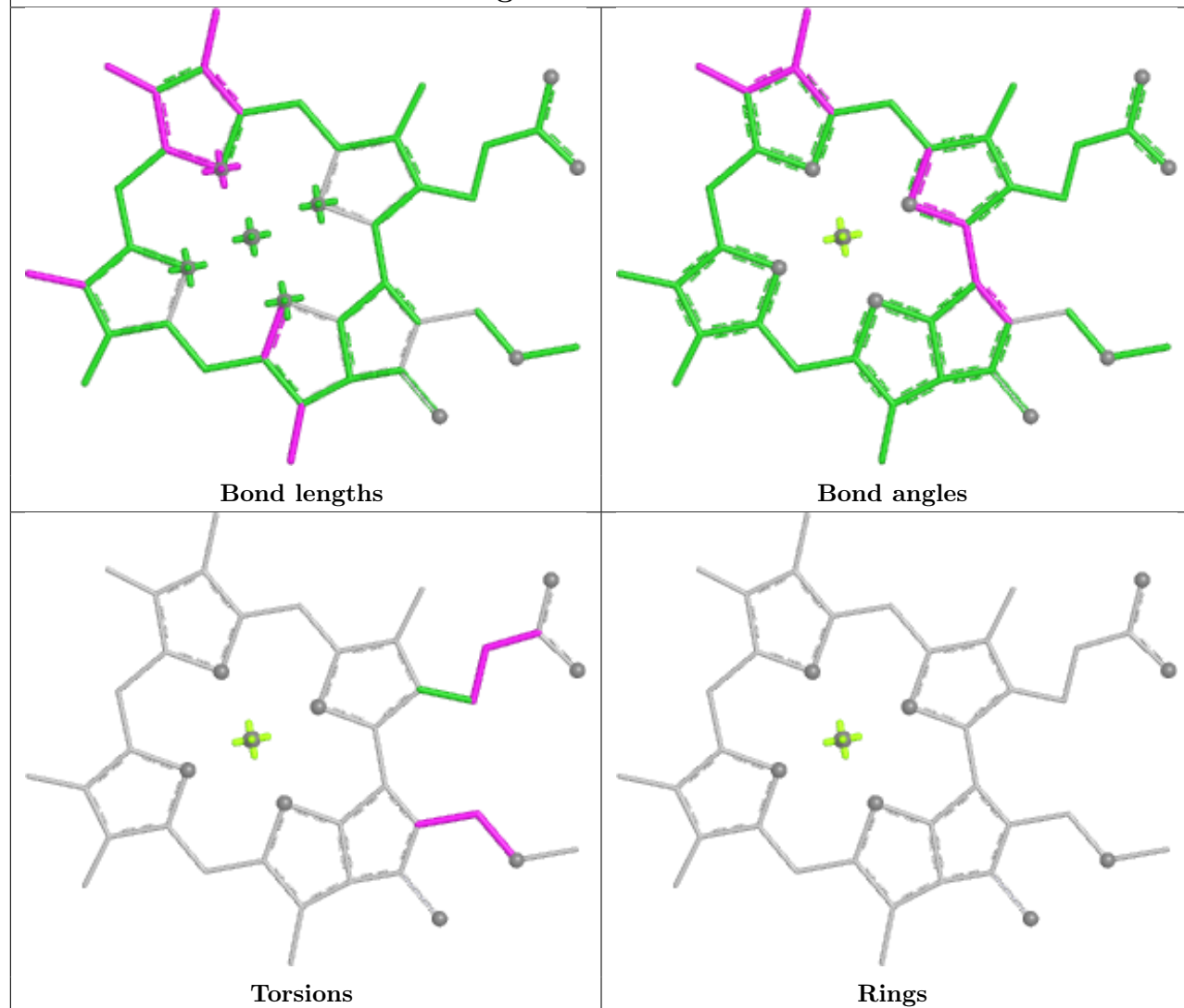


Torsions

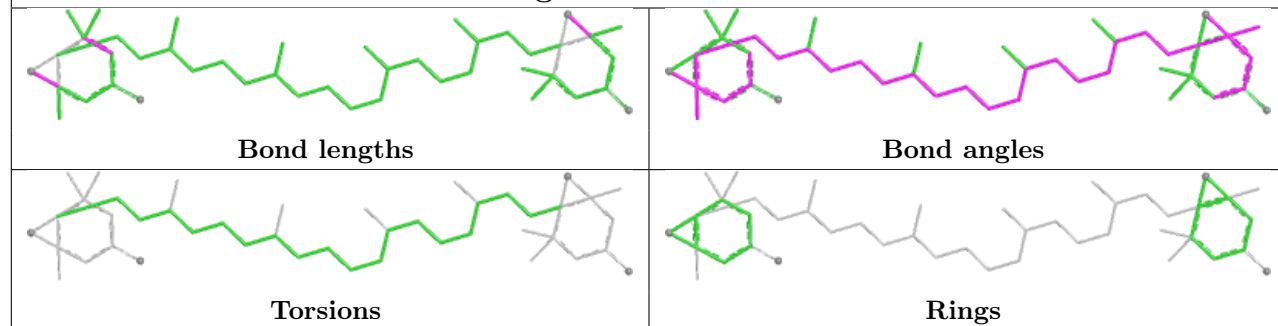


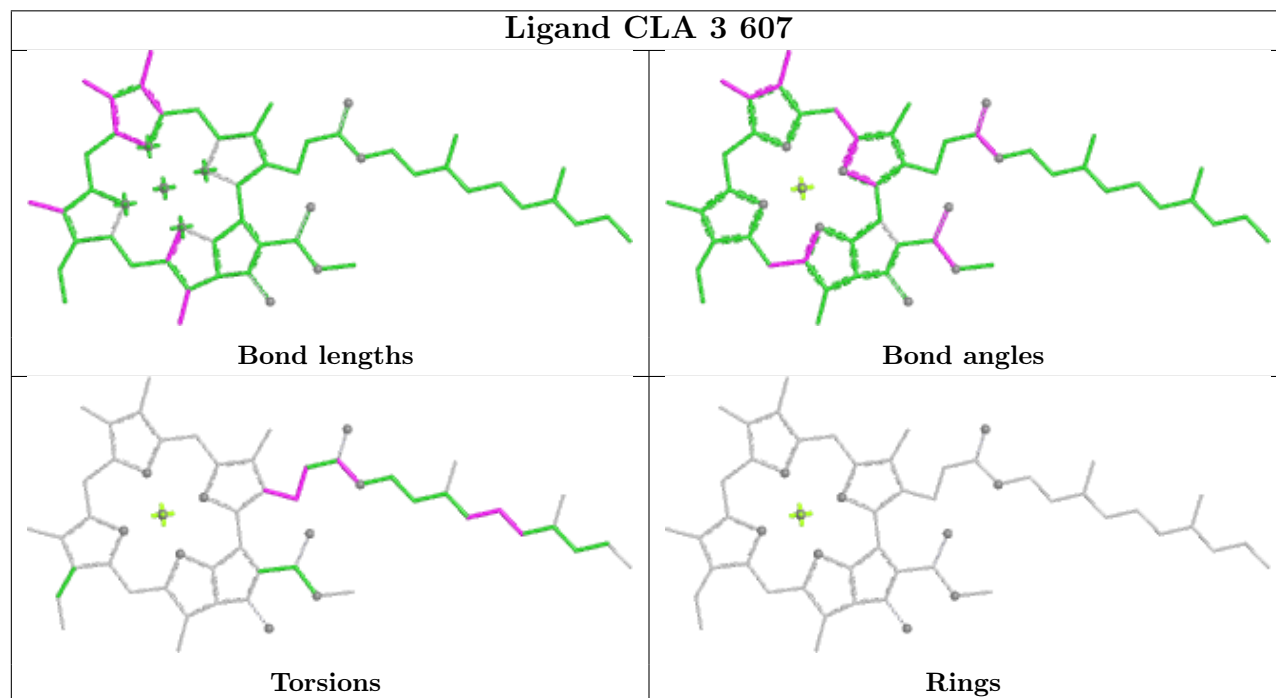
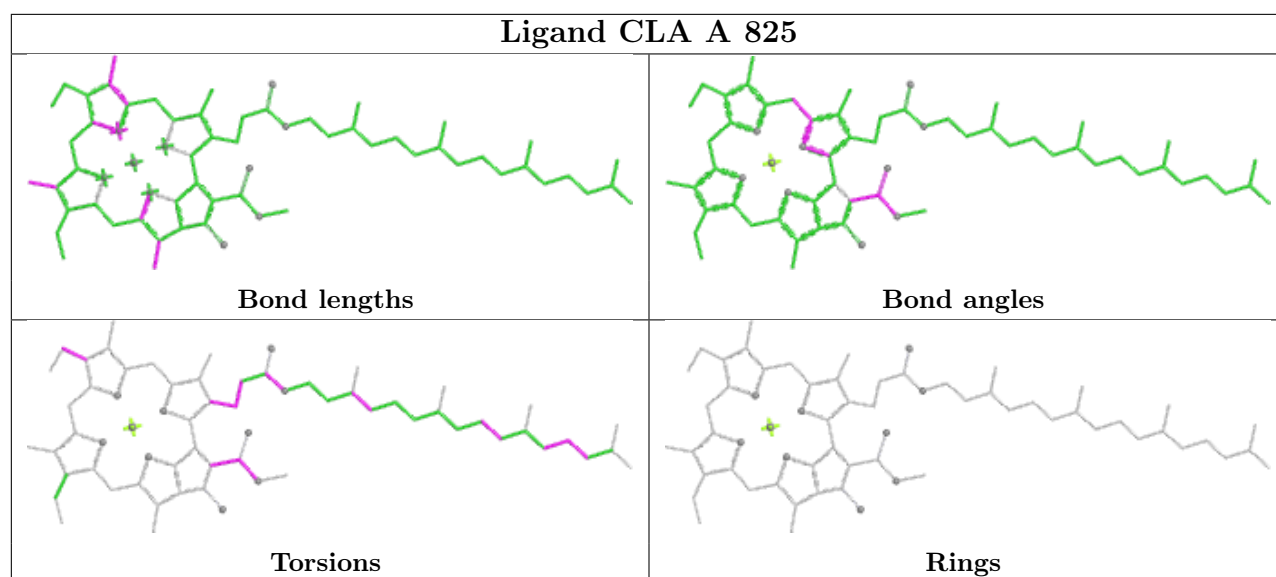
Rings

Ligand CLA 7 615

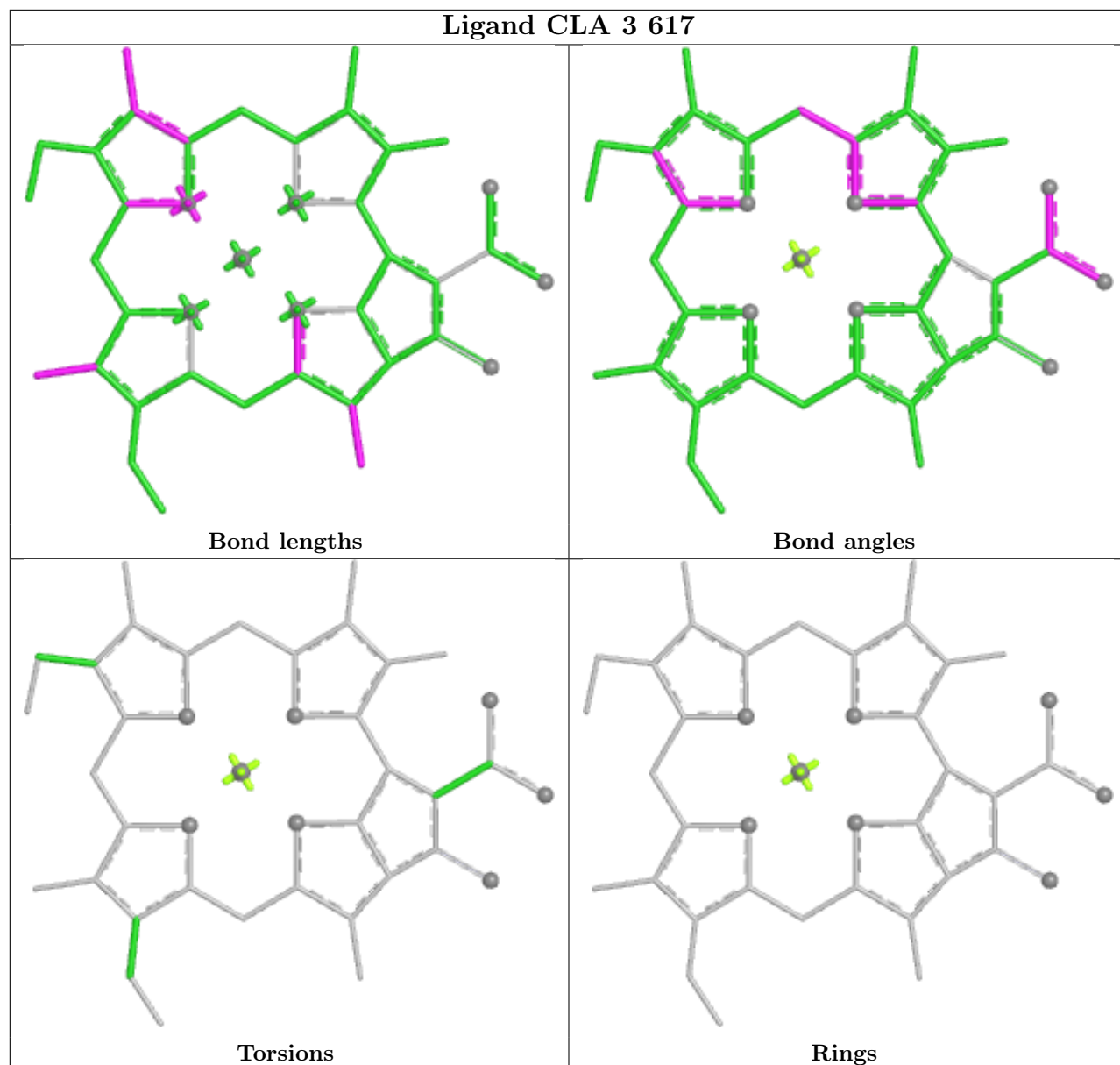


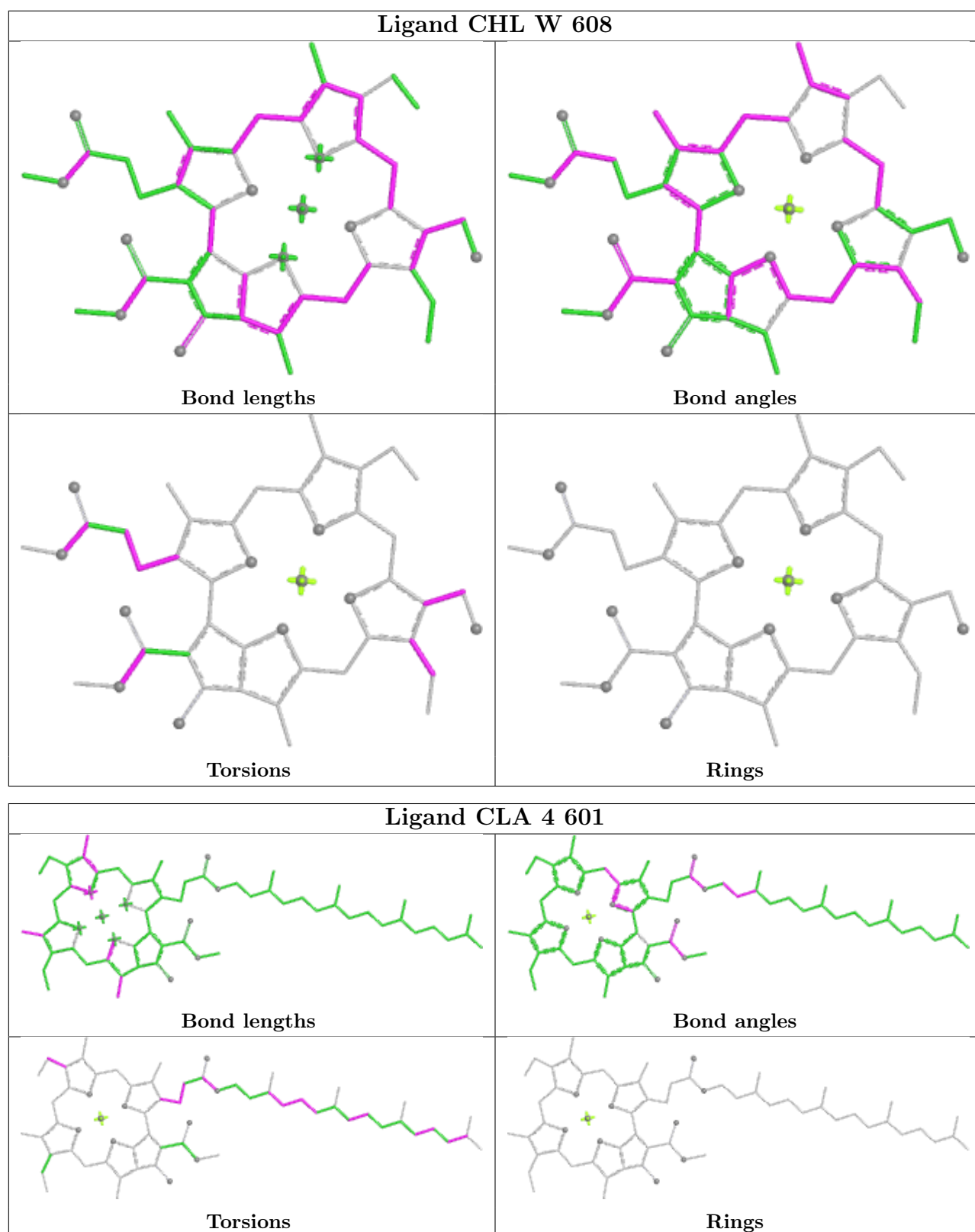
Ligand XAT 8 620



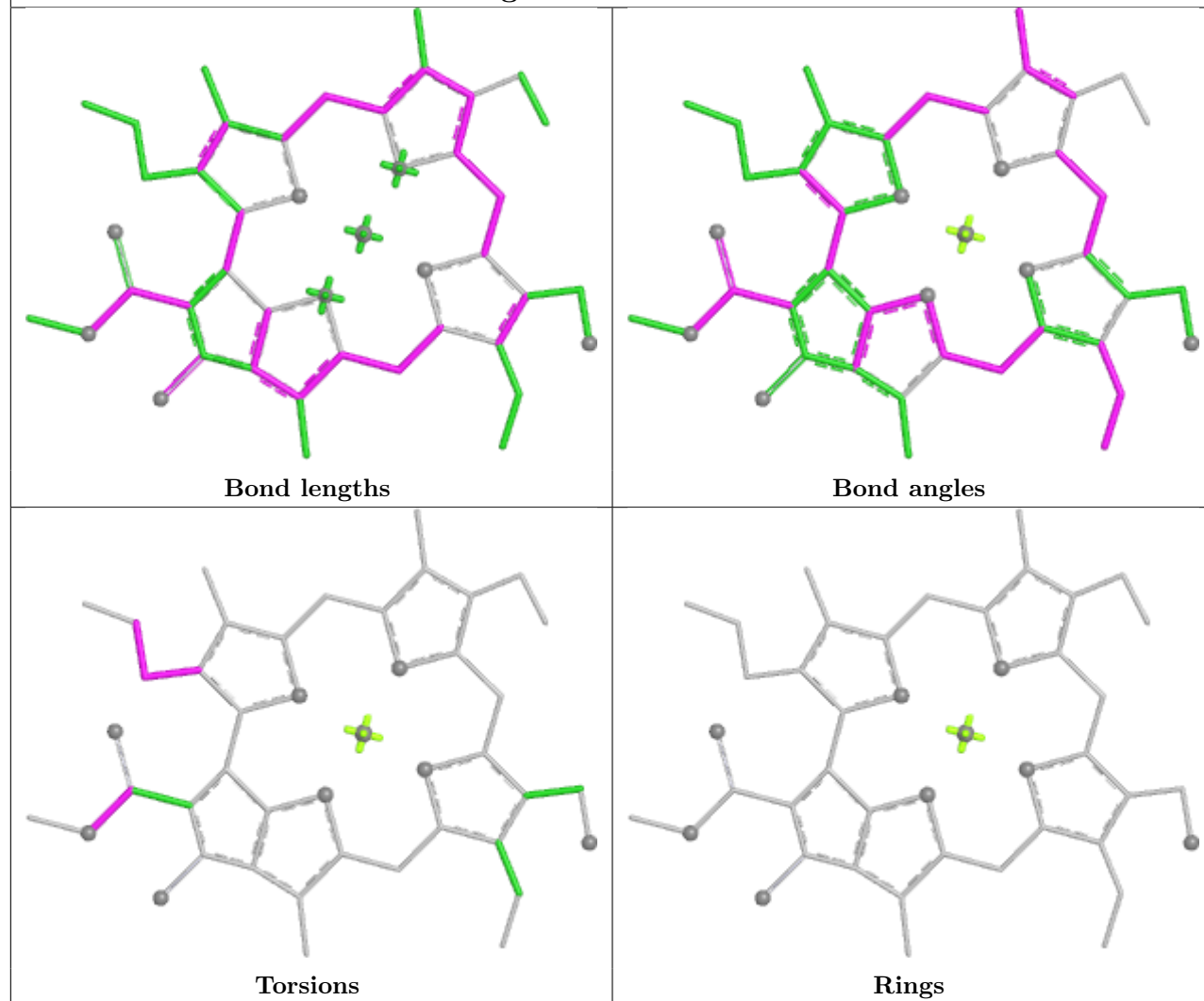


Ligand CLA 3 617

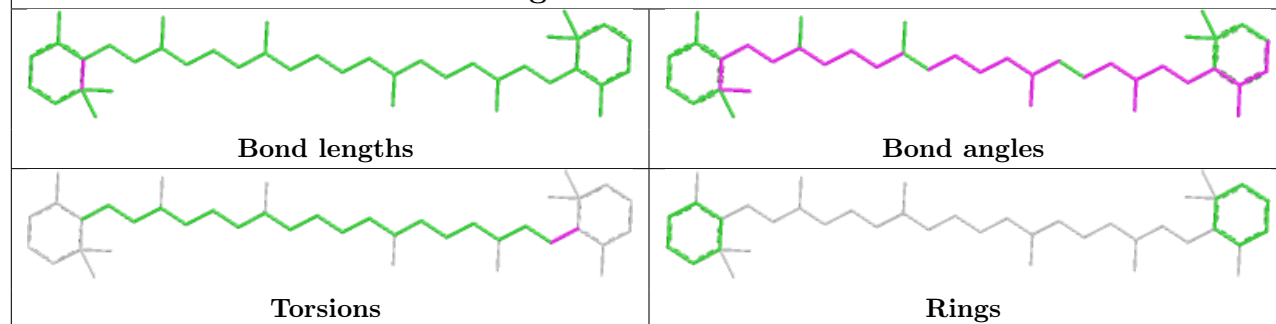




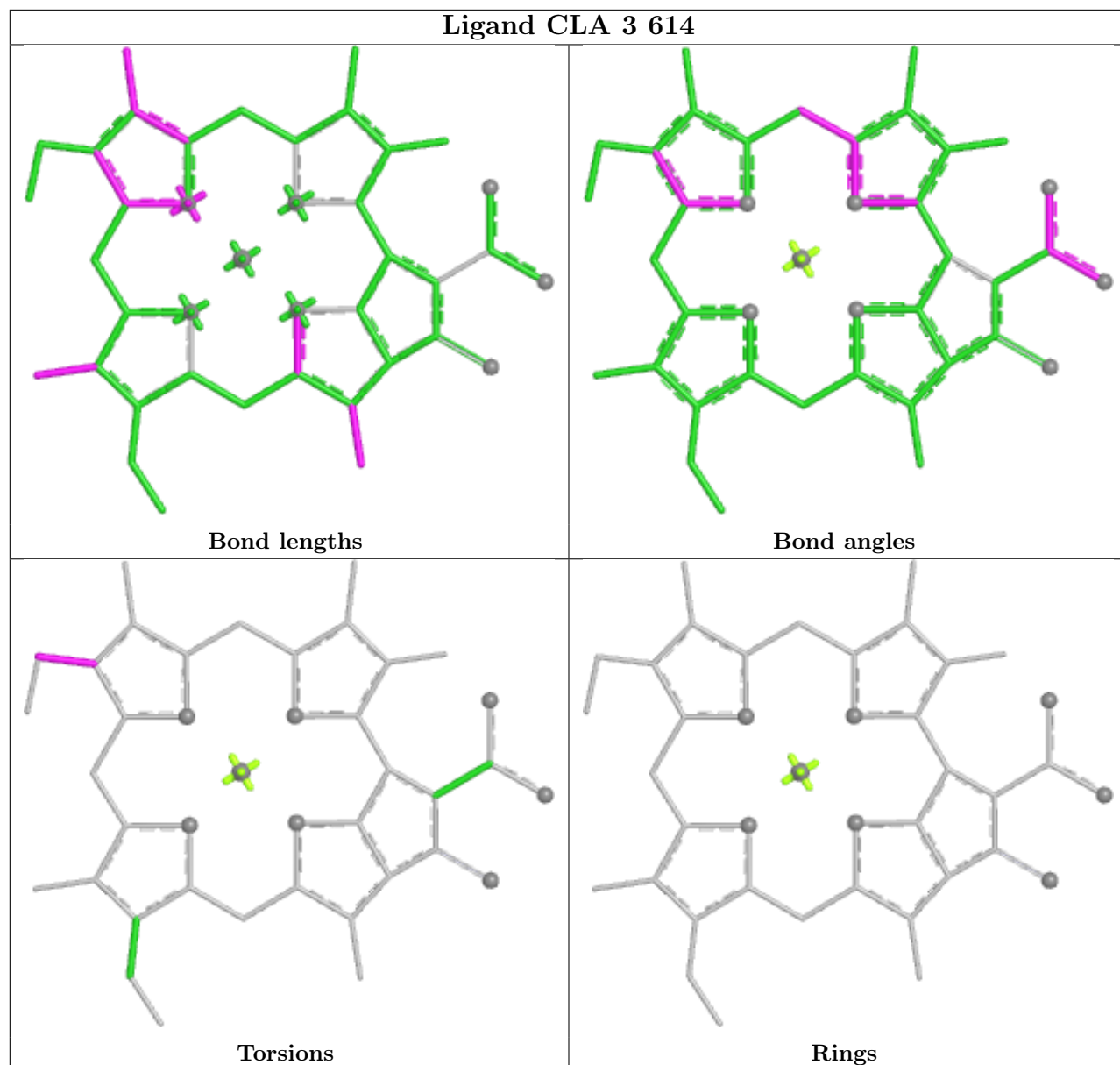
Ligand CHL U 608



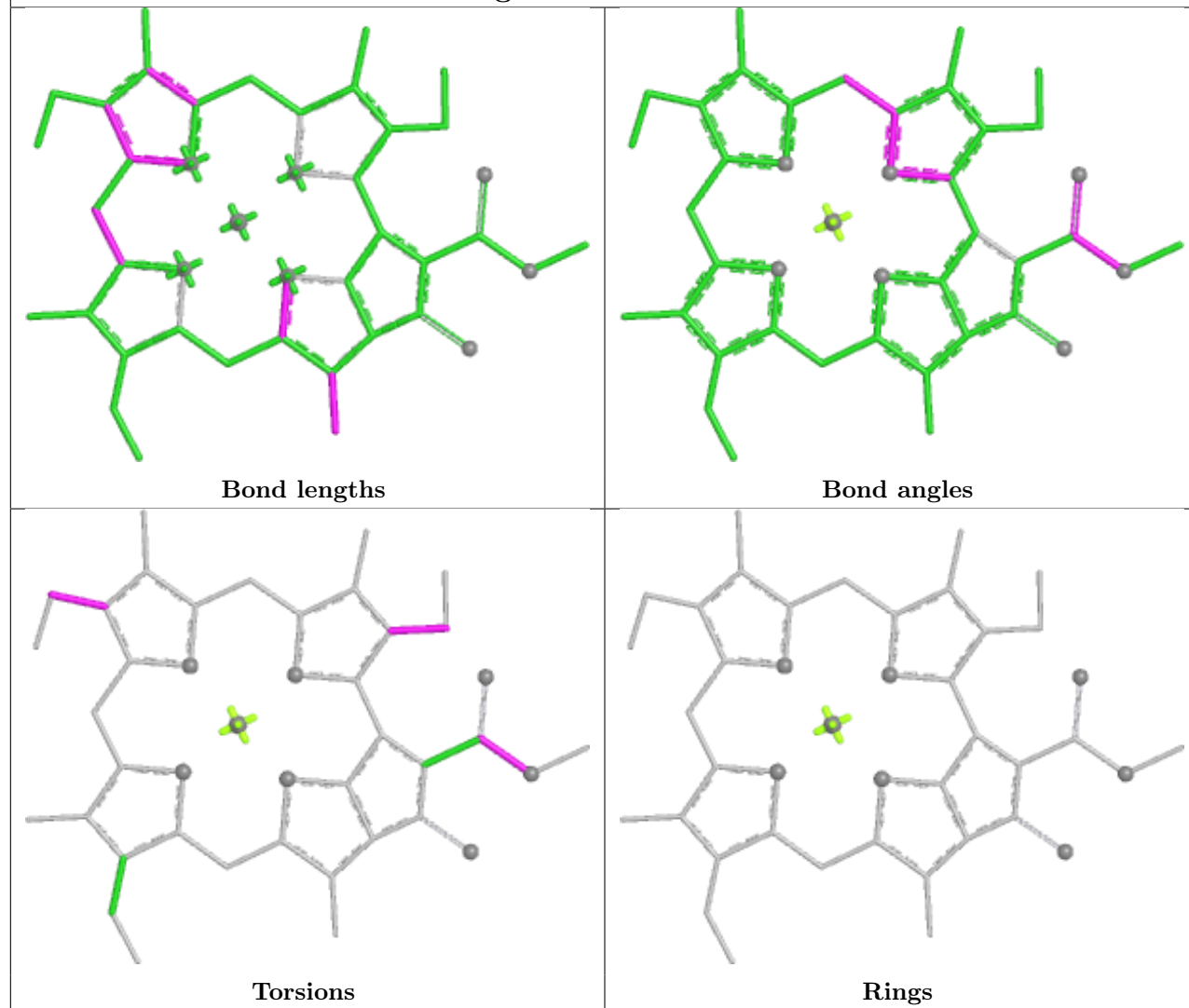
Ligand BCR G 205



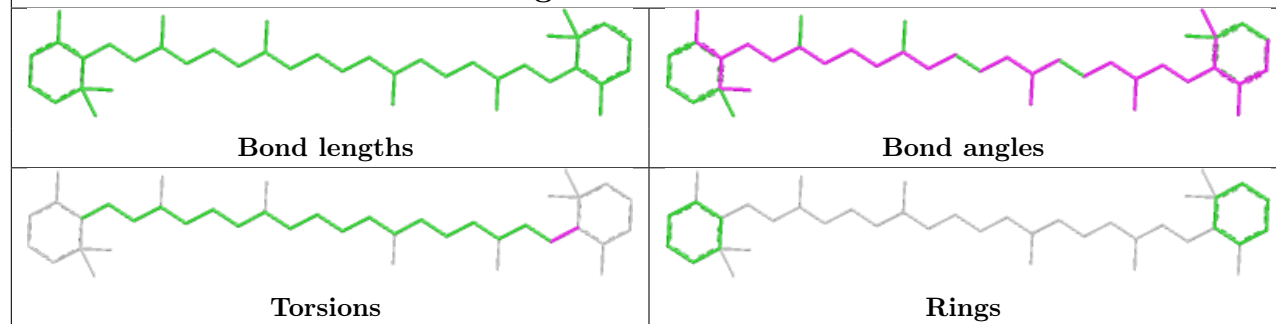
Ligand CLA 3 614



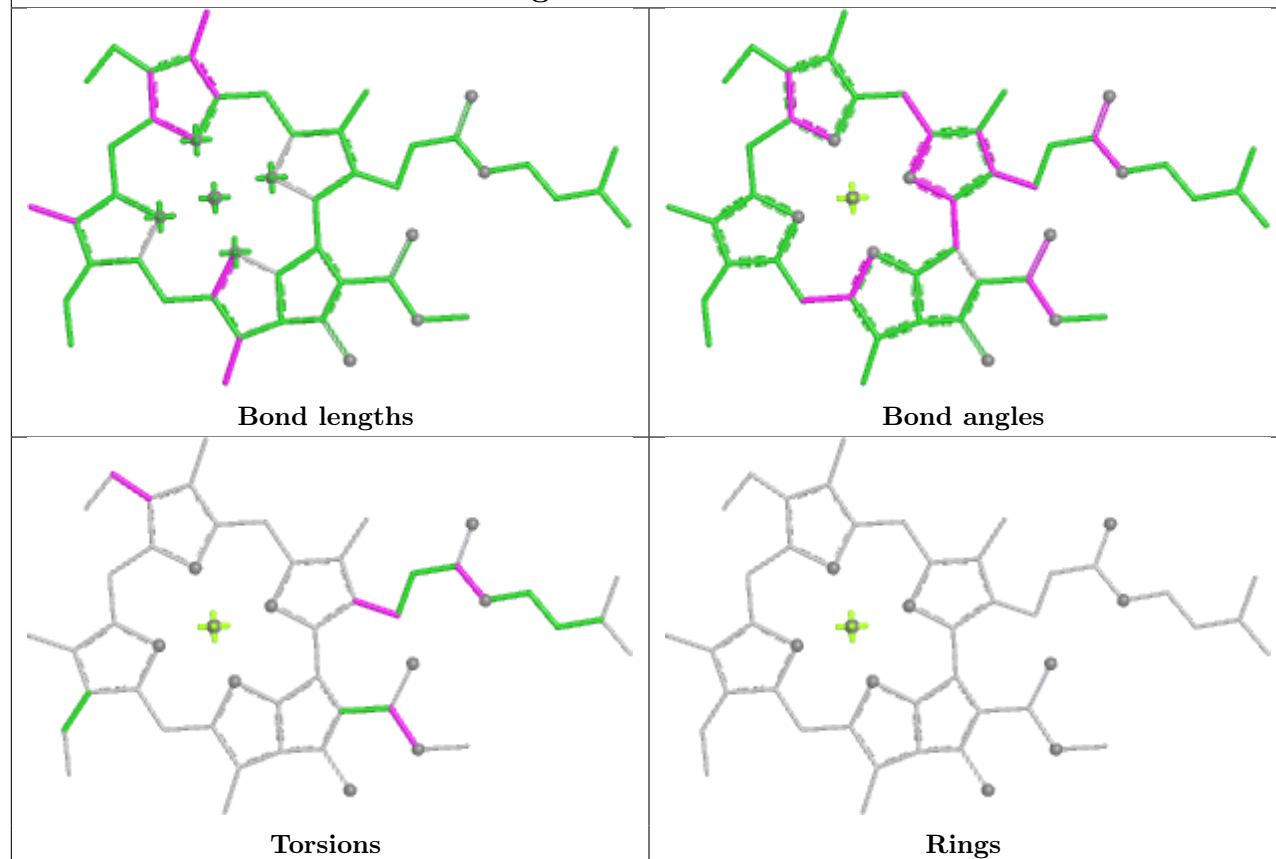
Ligand CLA U 614



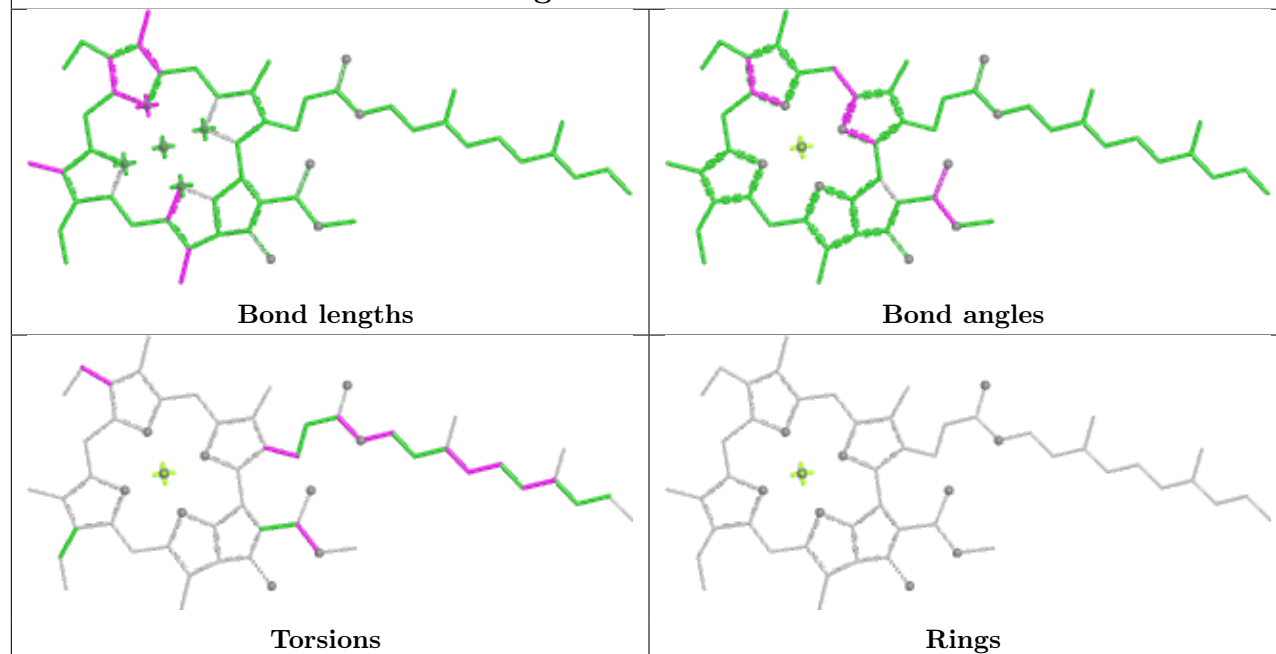
Ligand BCR a 619



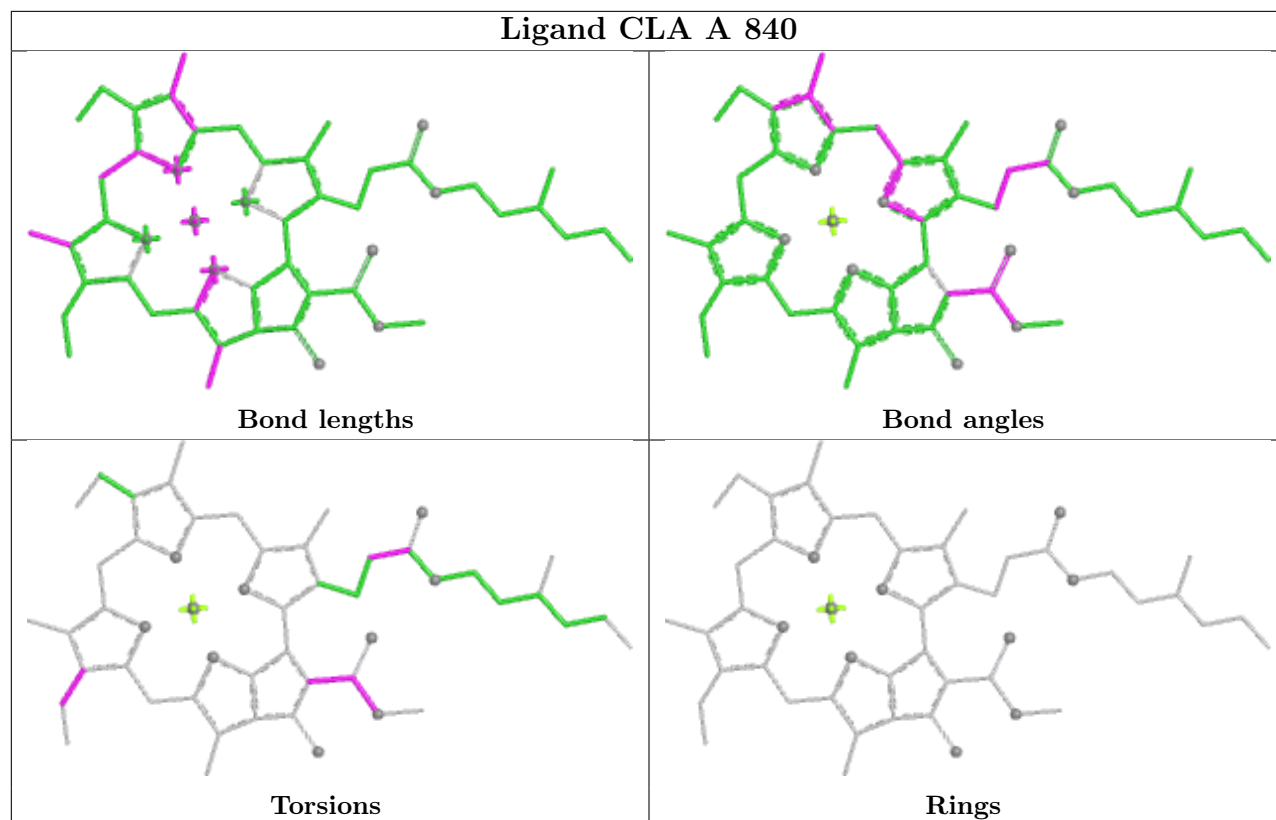
Ligand CLA A 810



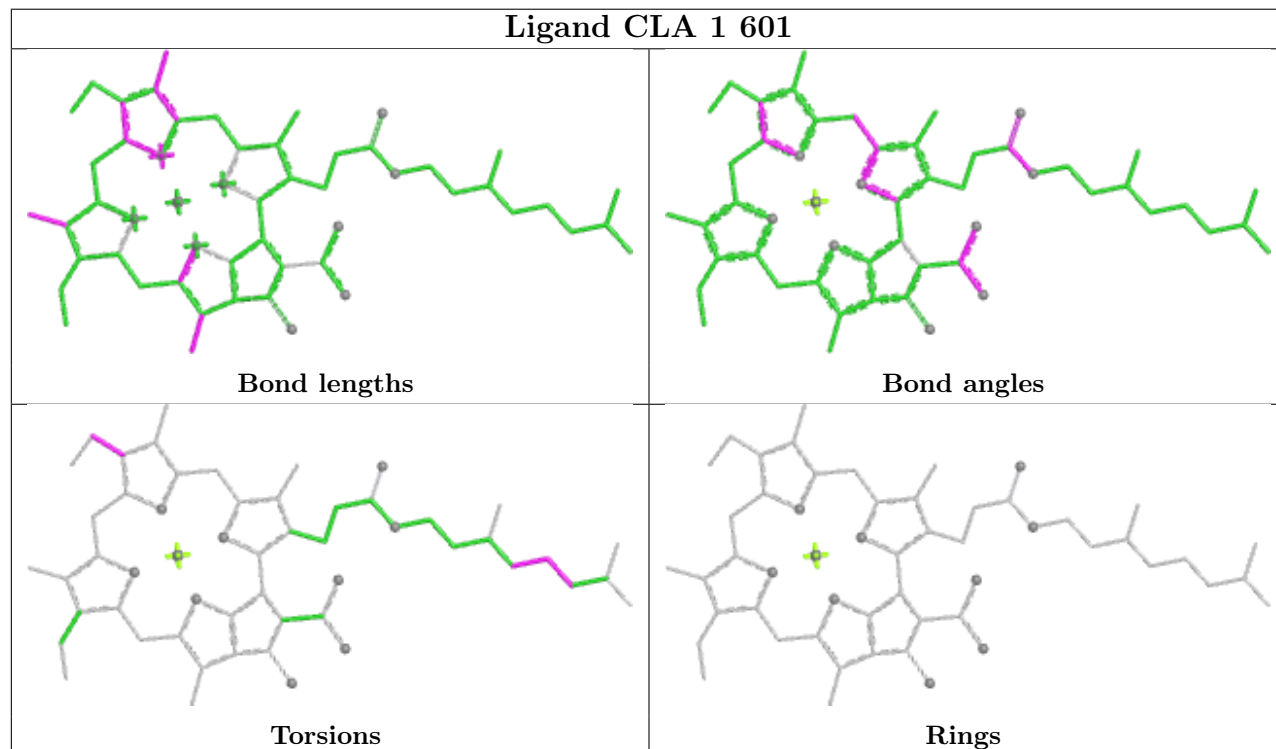
Ligand CLA F 301

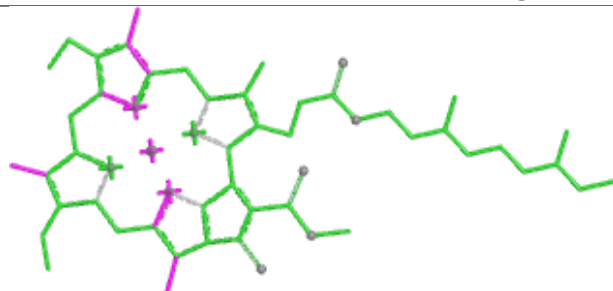


Ligand CLA A 840

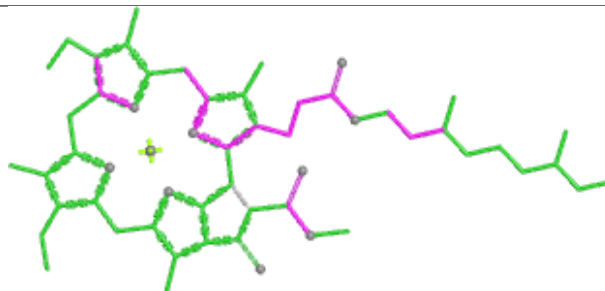


Ligand CLA 1 601

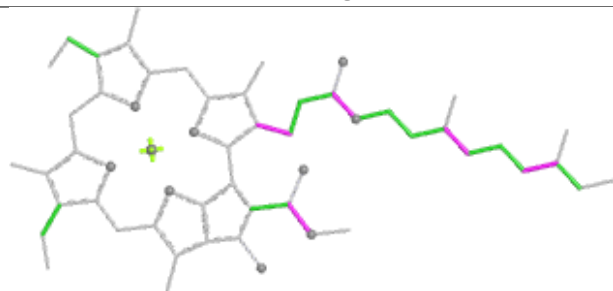


Ligand CLA K 203

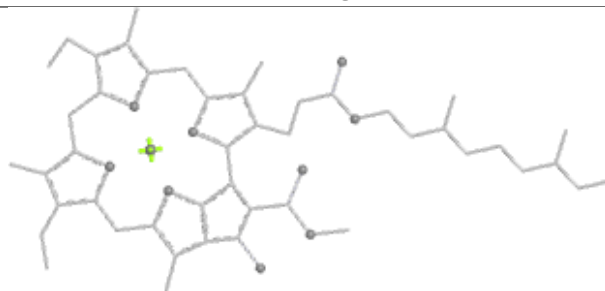
Bond lengths



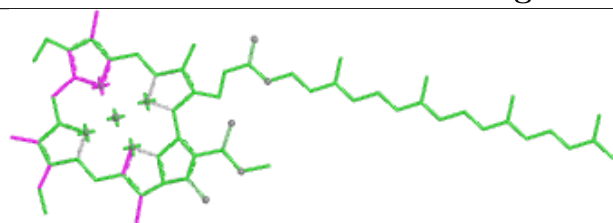
Bond angles



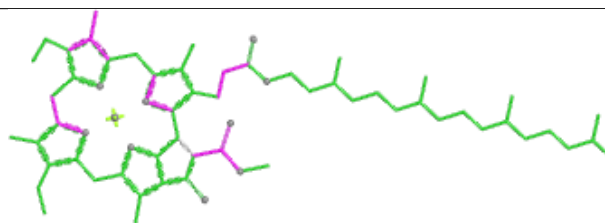
Torsions



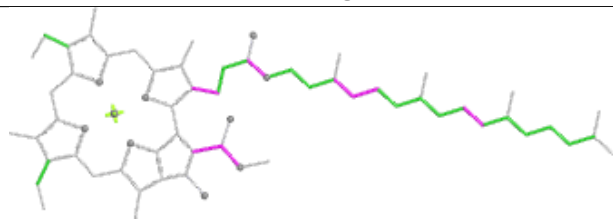
Rings

Ligand CLA B 829

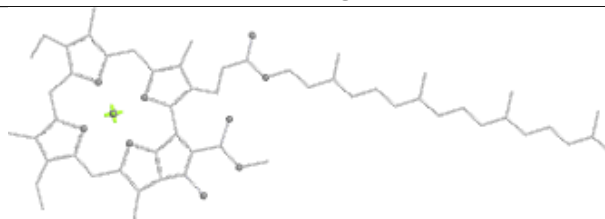
Bond lengths



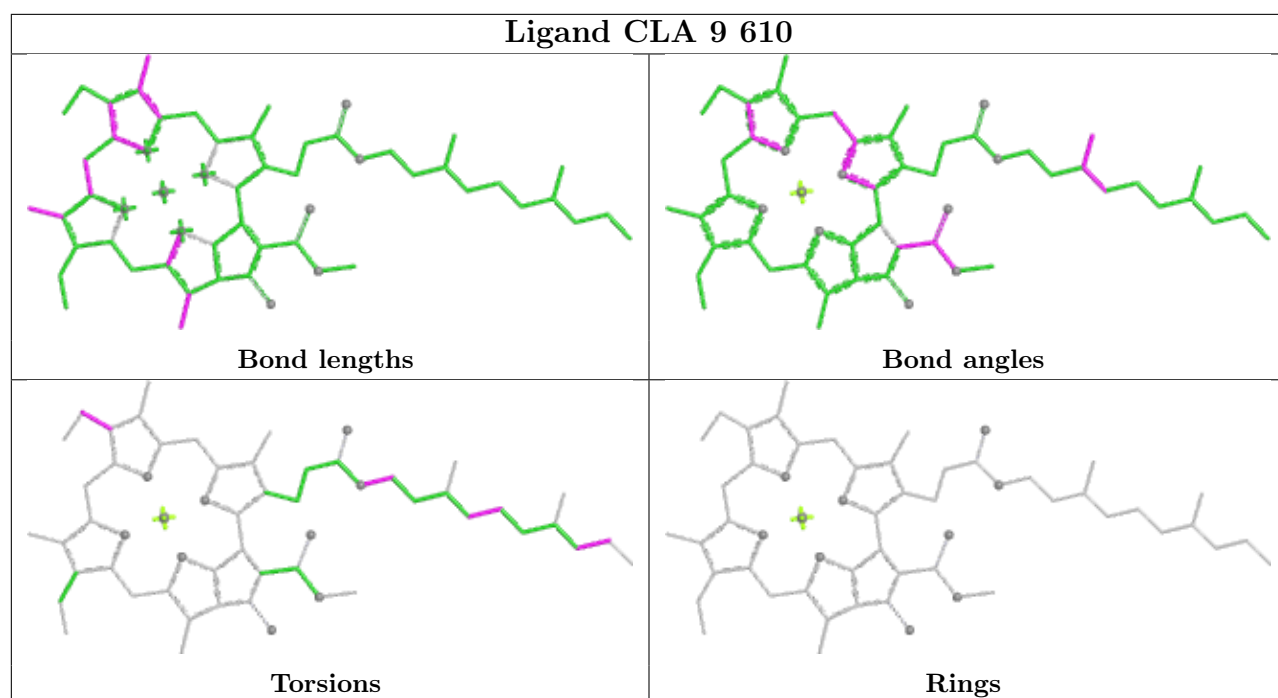
Bond angles



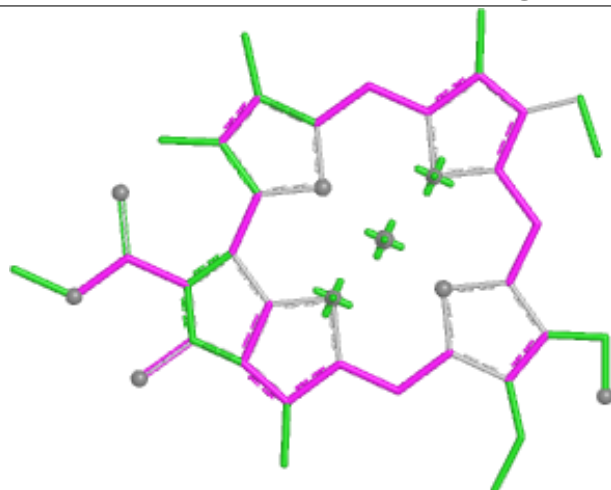
Torsions



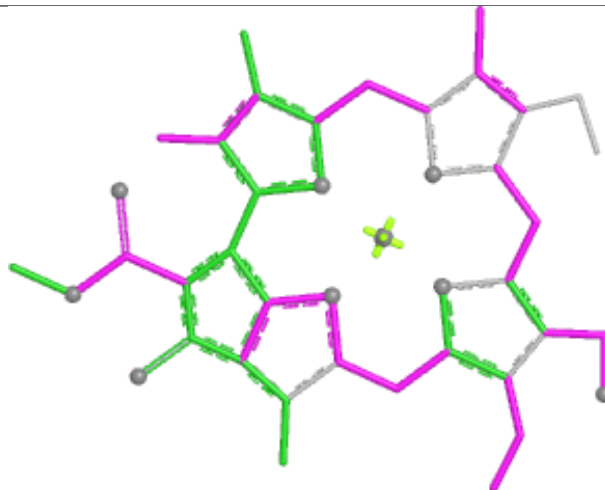
Rings



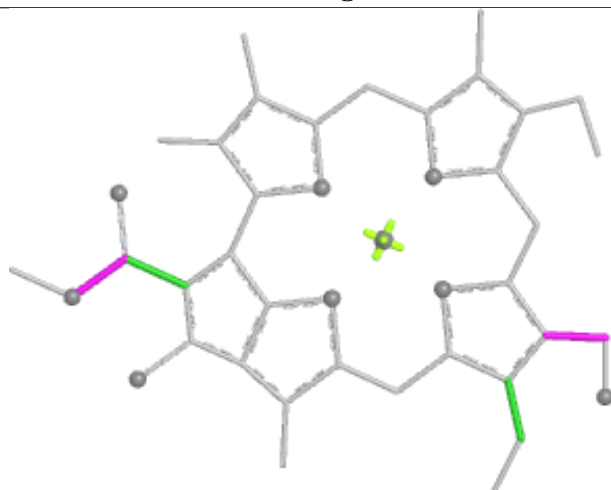
Ligand CHL Z 605



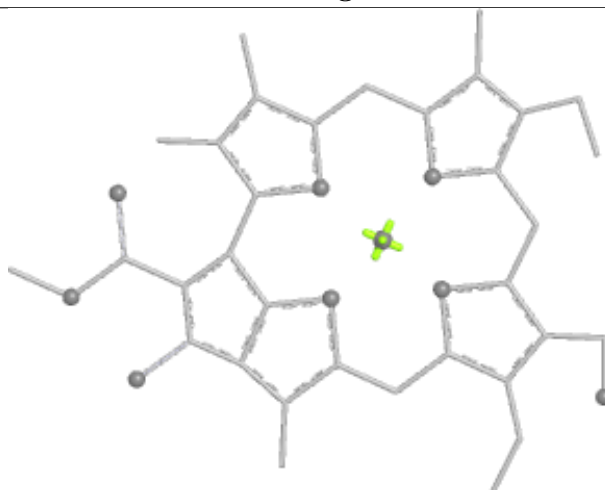
Bond lengths



Bond angles

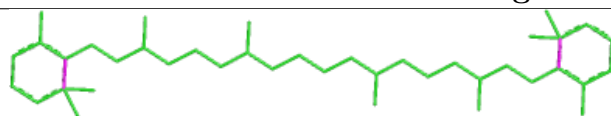


Torsions

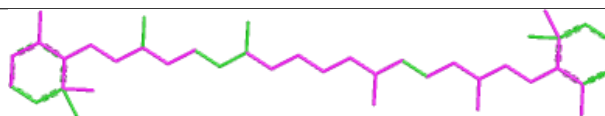


Rings

Ligand BCR B 847



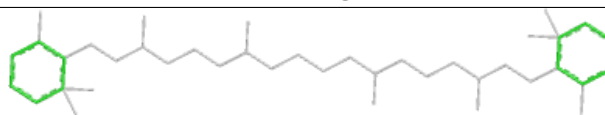
Bond lengths



Bond angles

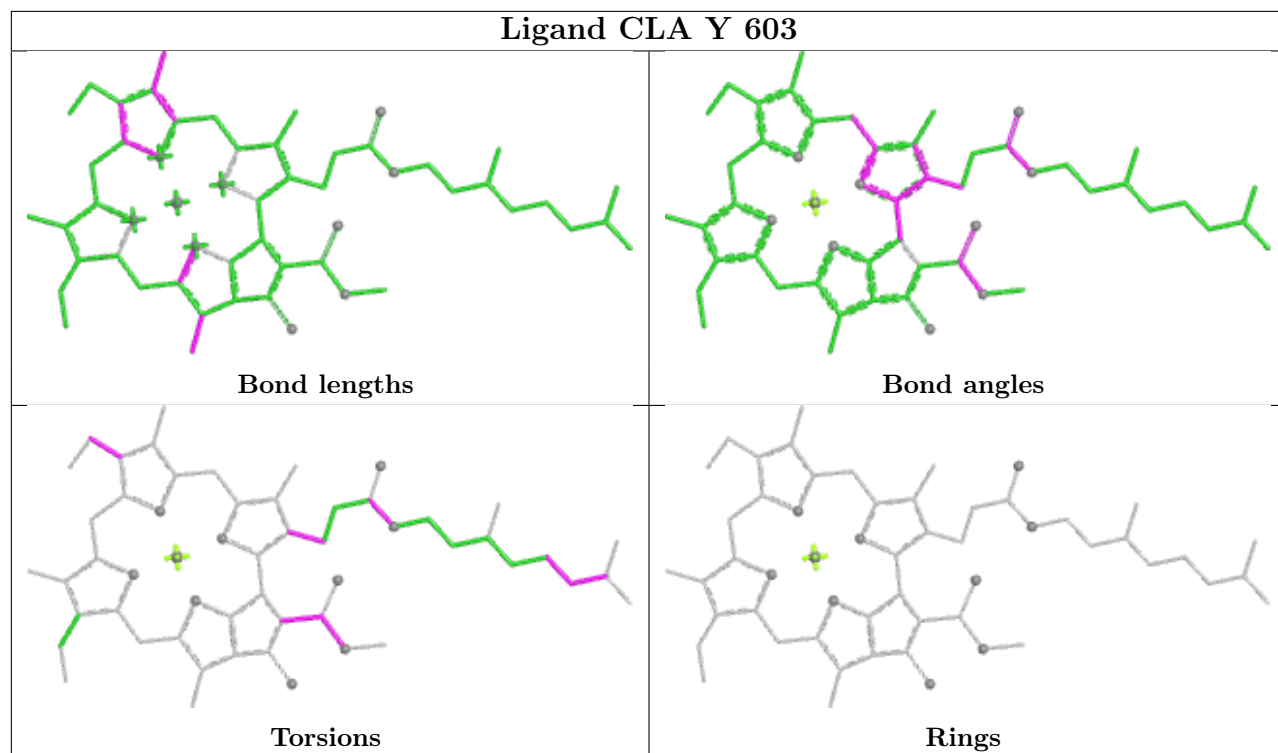


Torsions

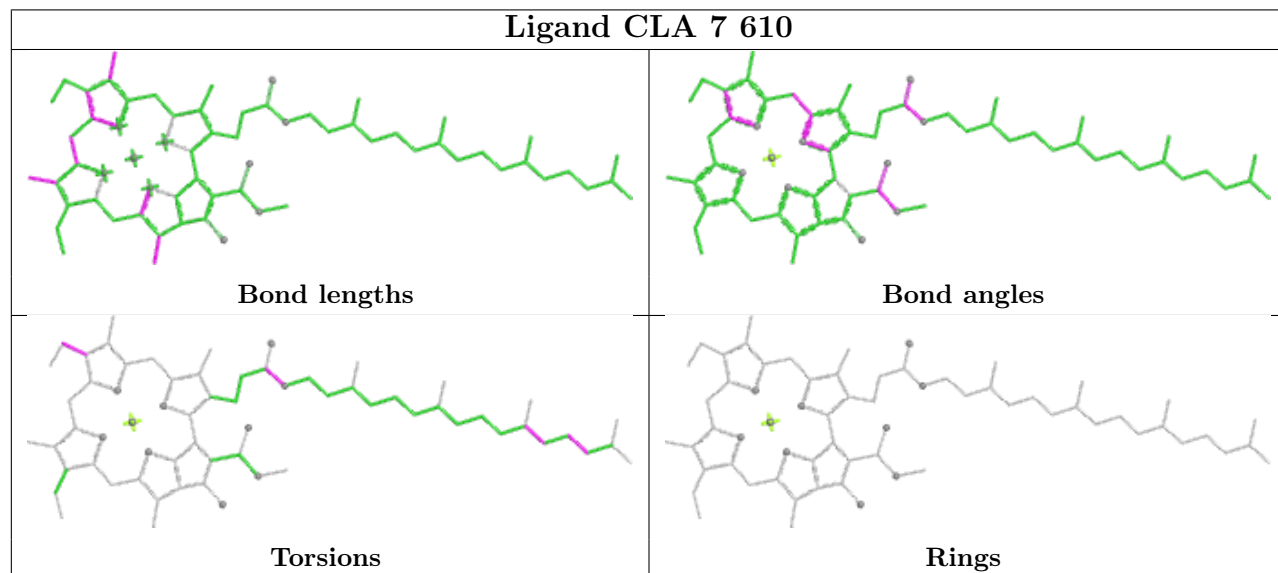


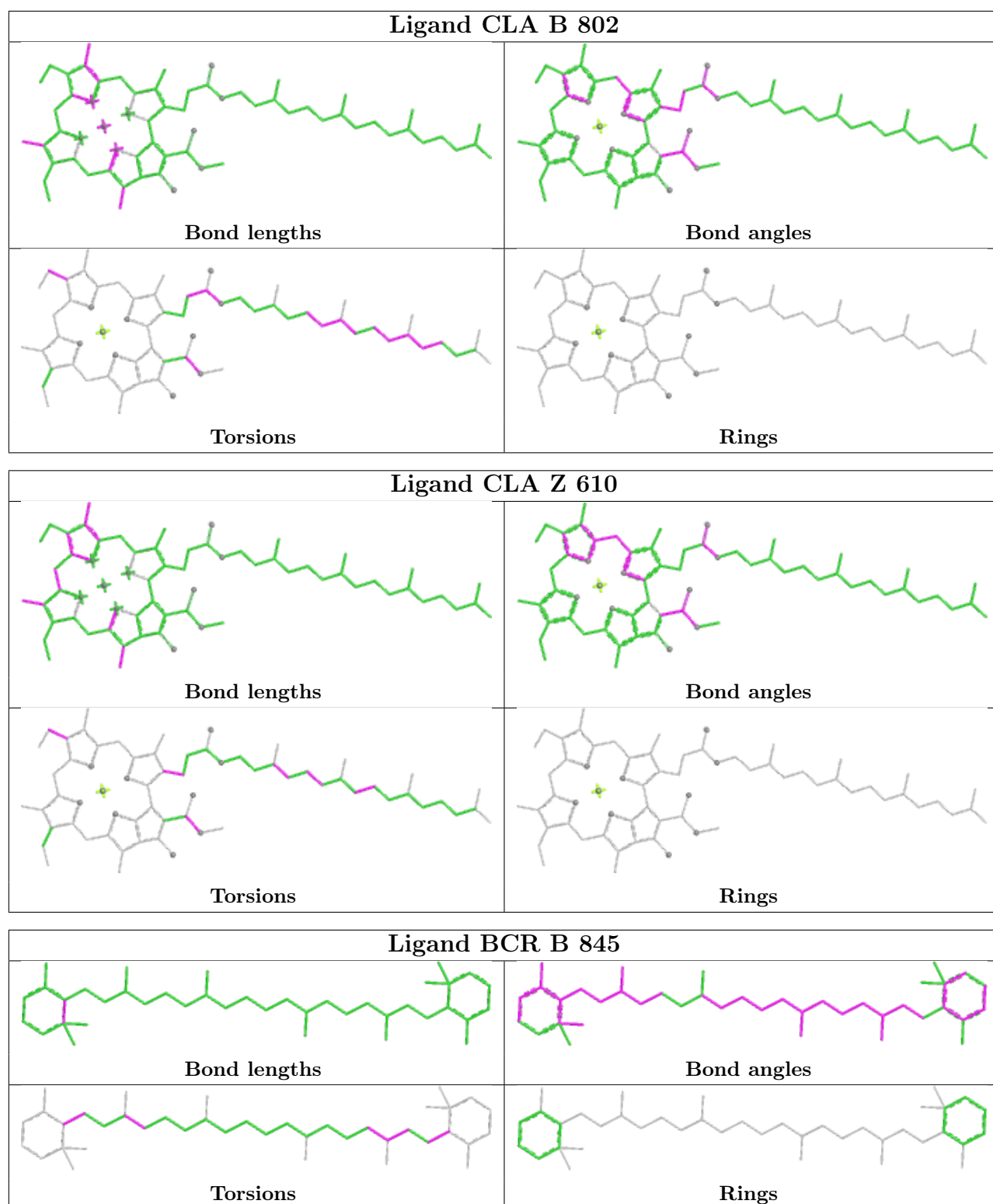
Rings

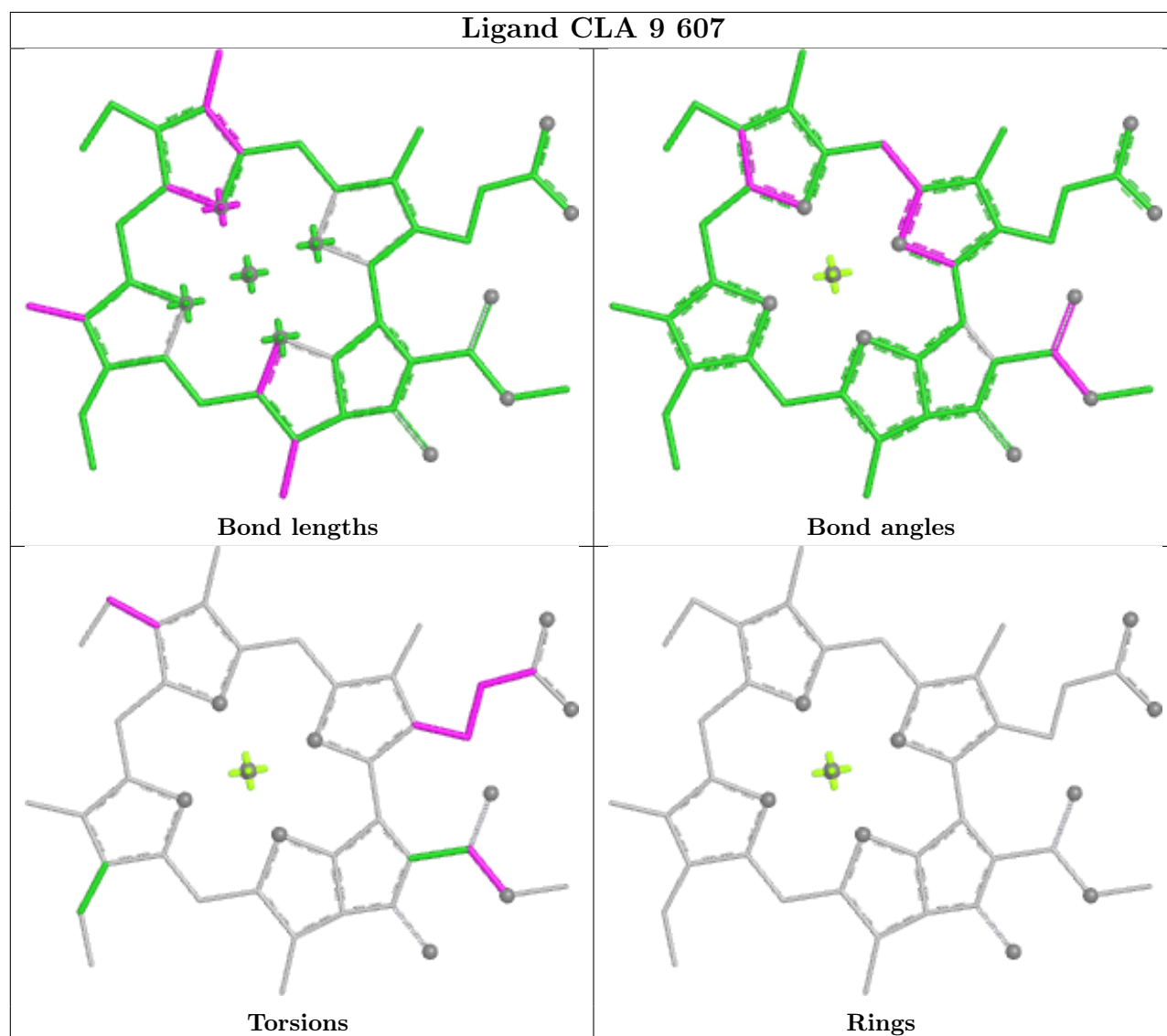
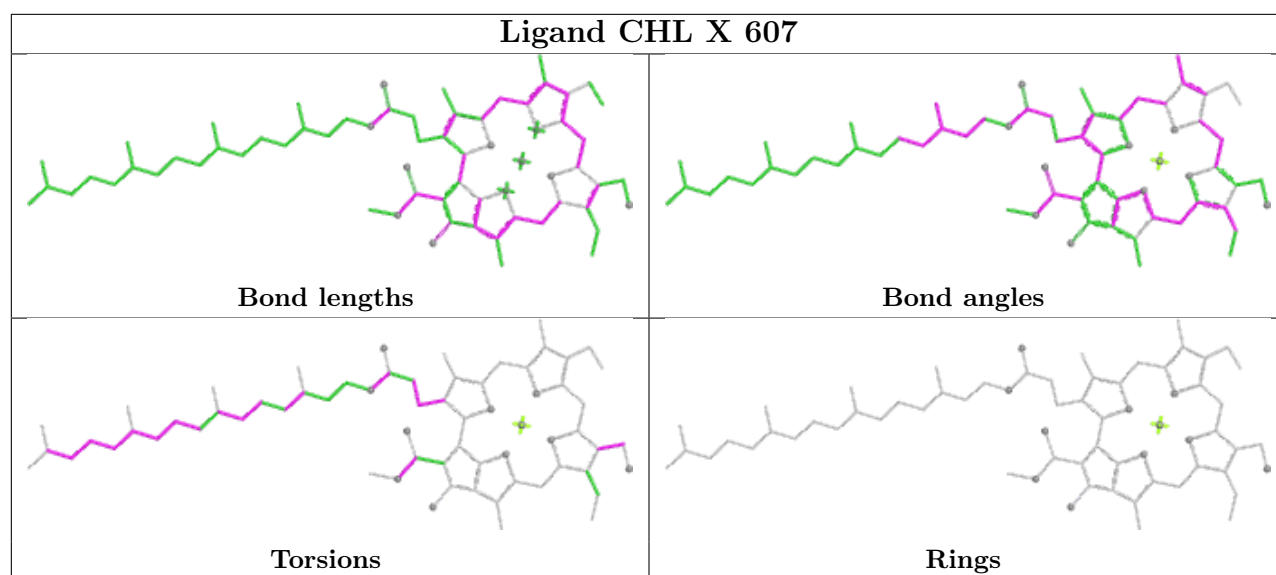
Ligand CLA Y 603

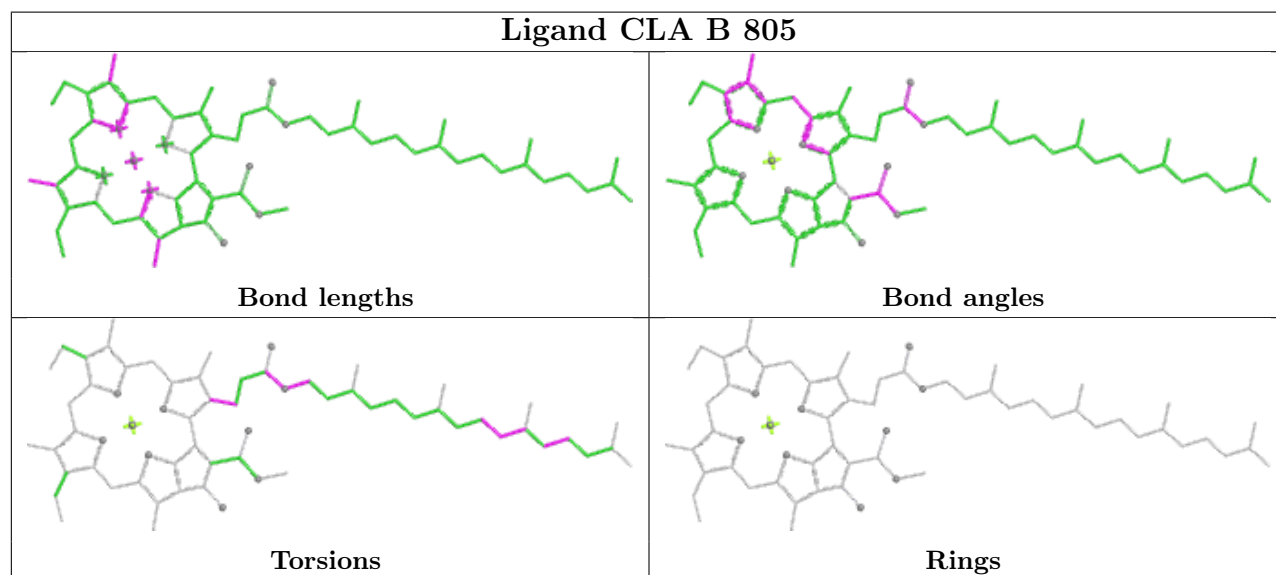
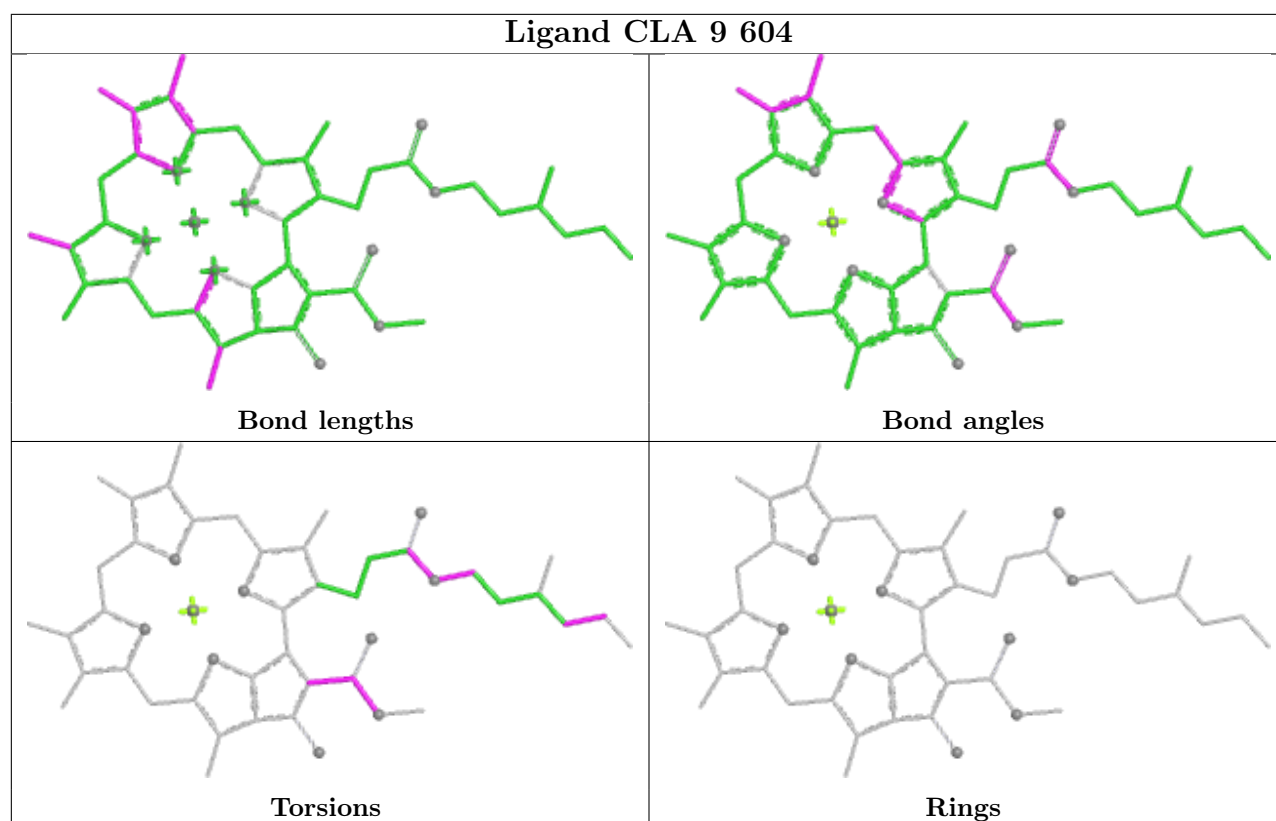


Ligand CLA 7 610

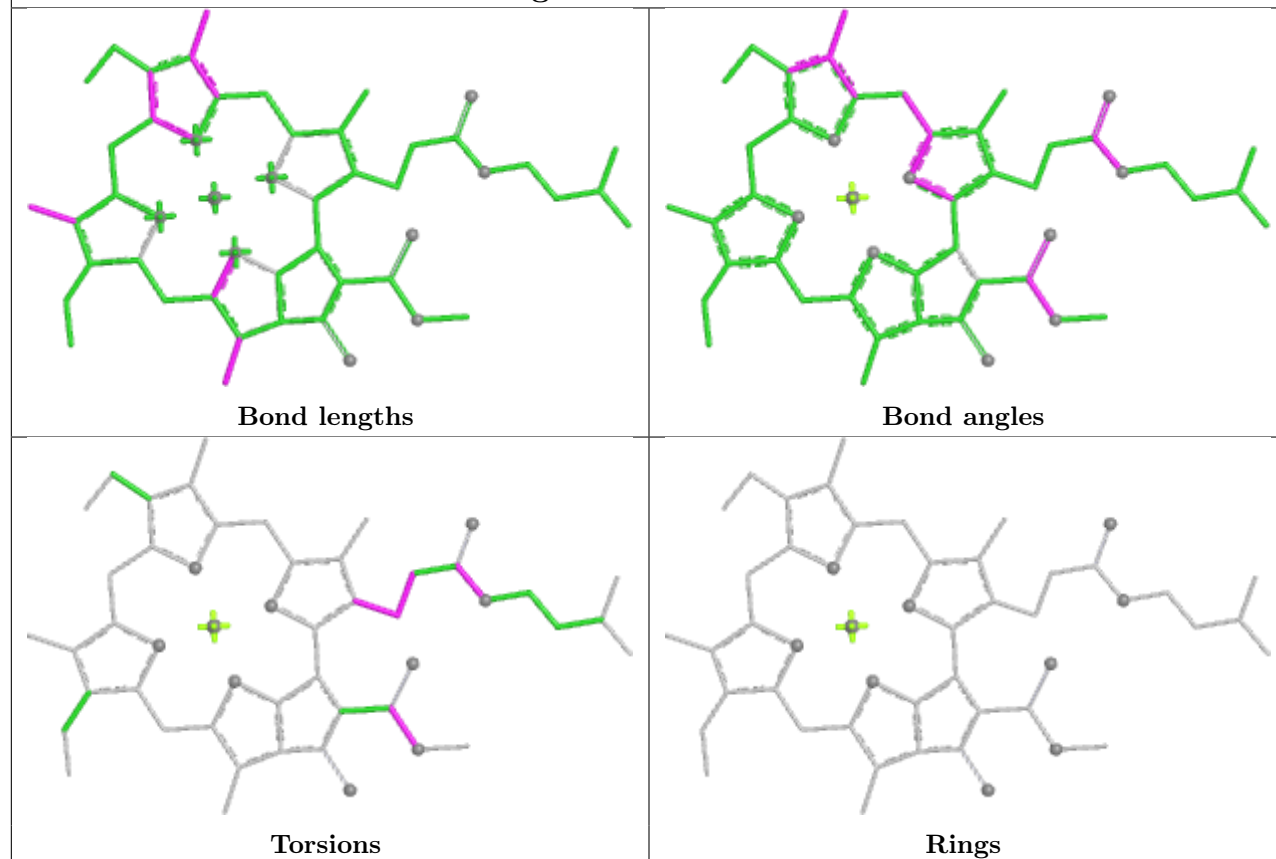




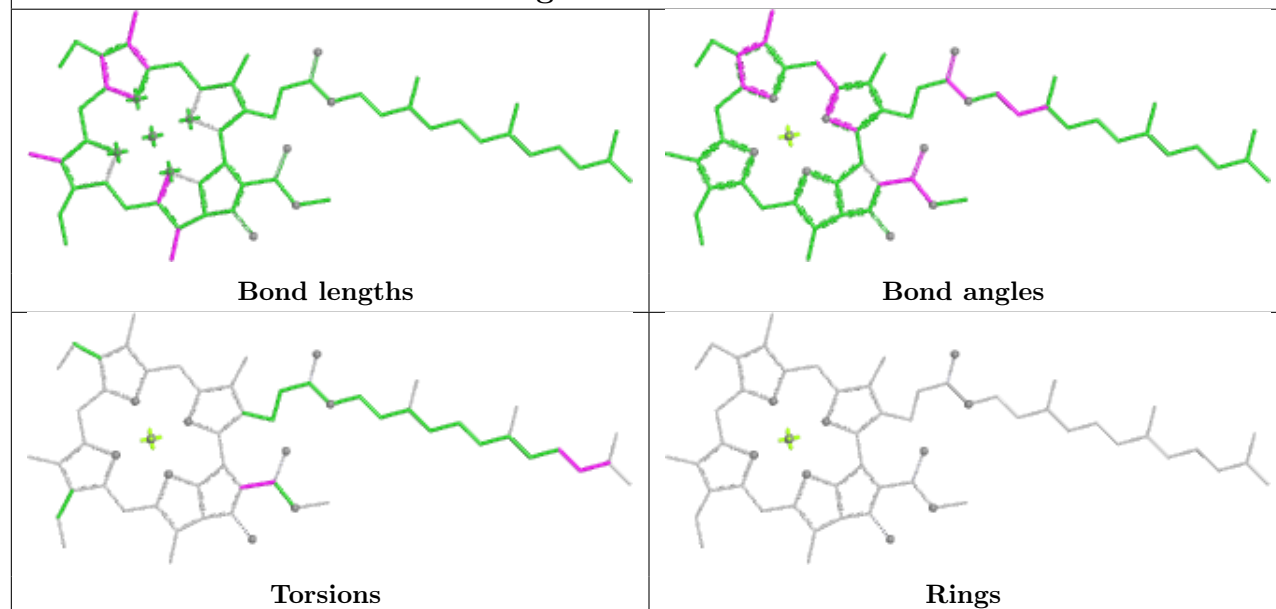


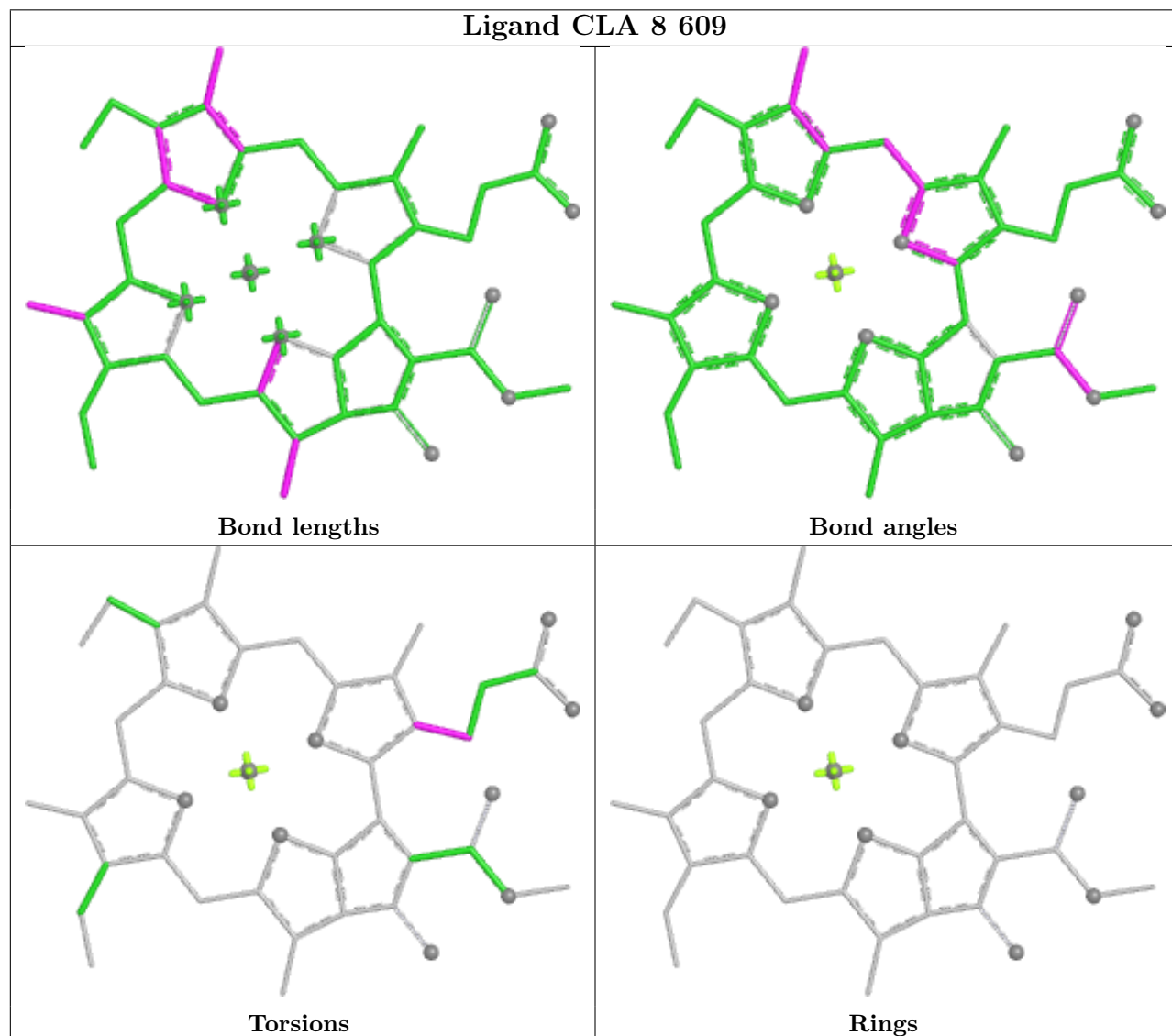
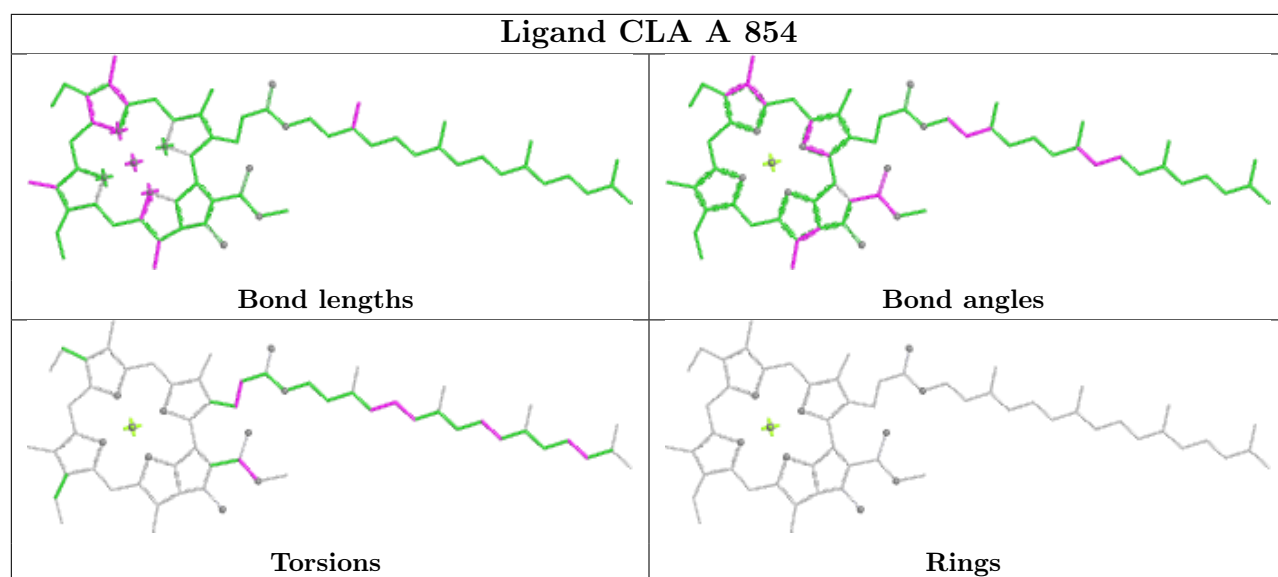


Ligand CLA V 604

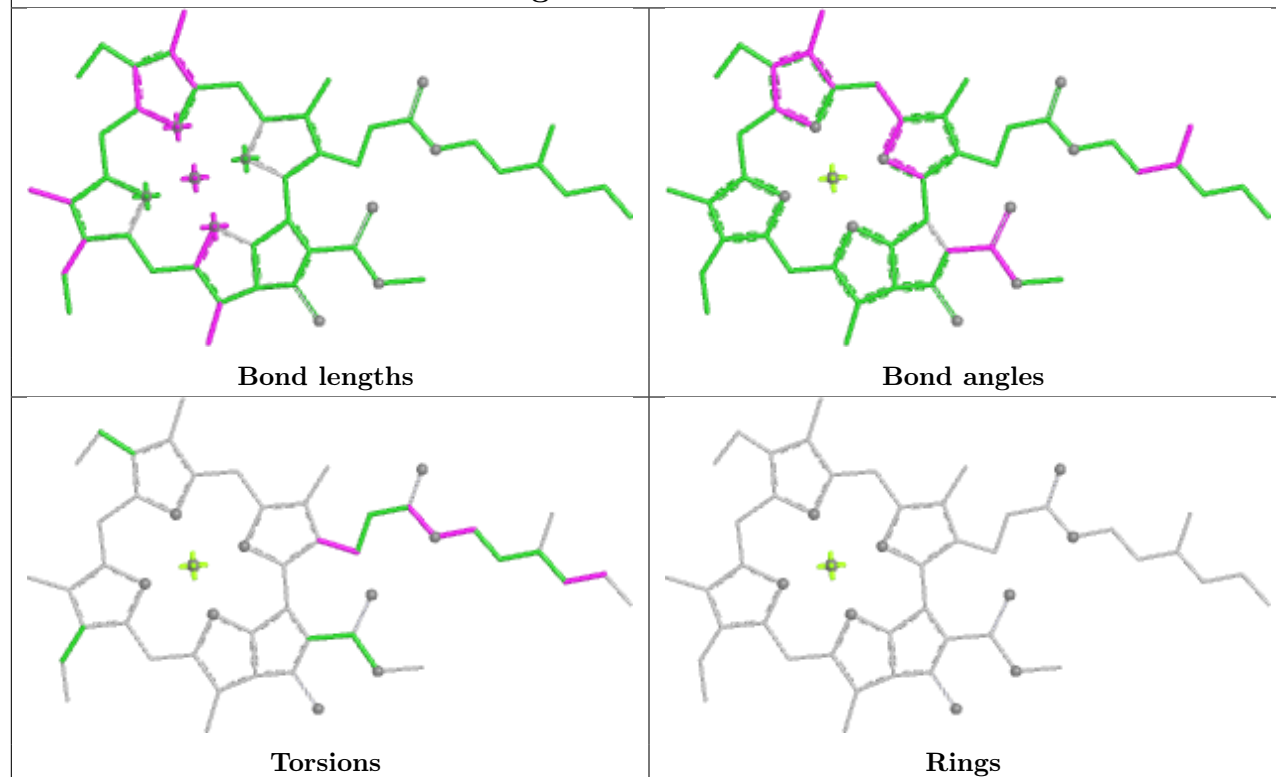


Ligand CLA 3 602

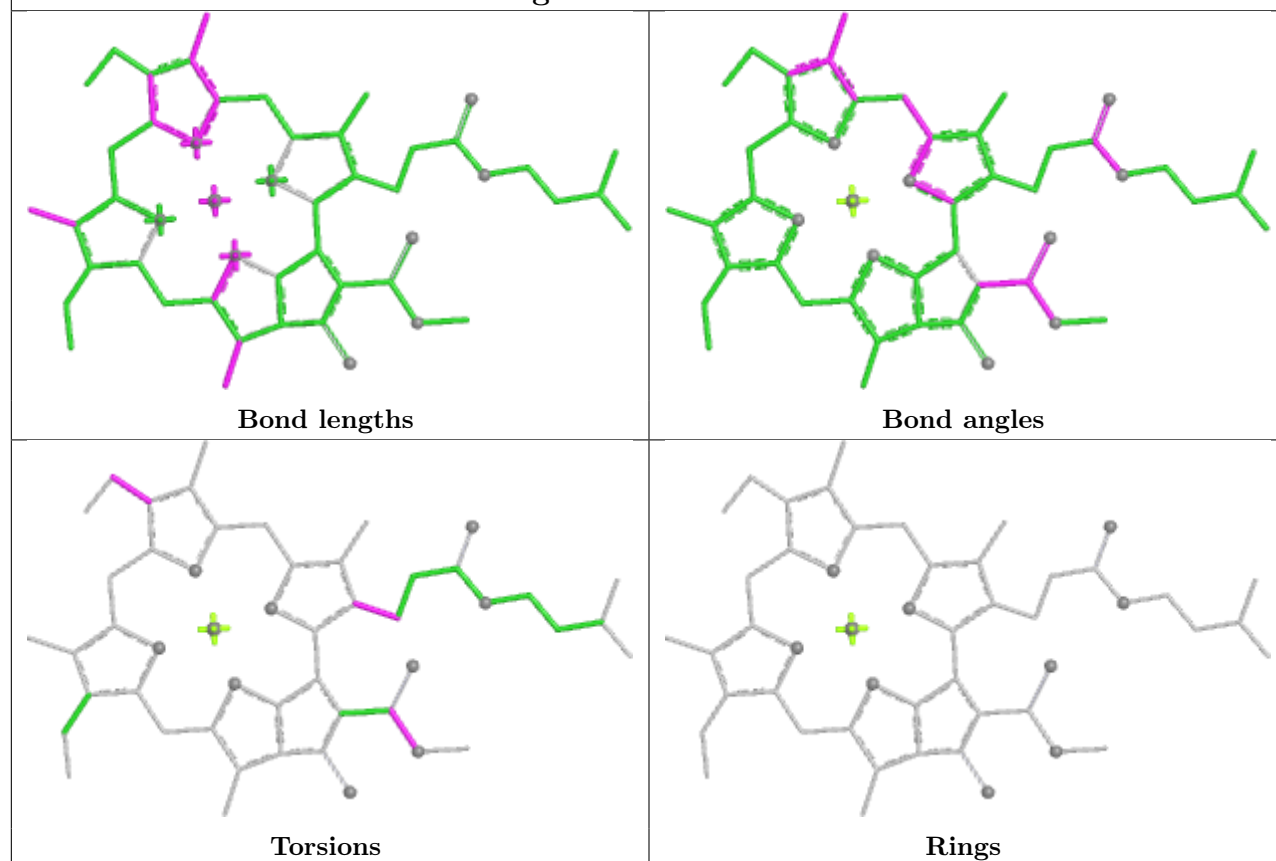




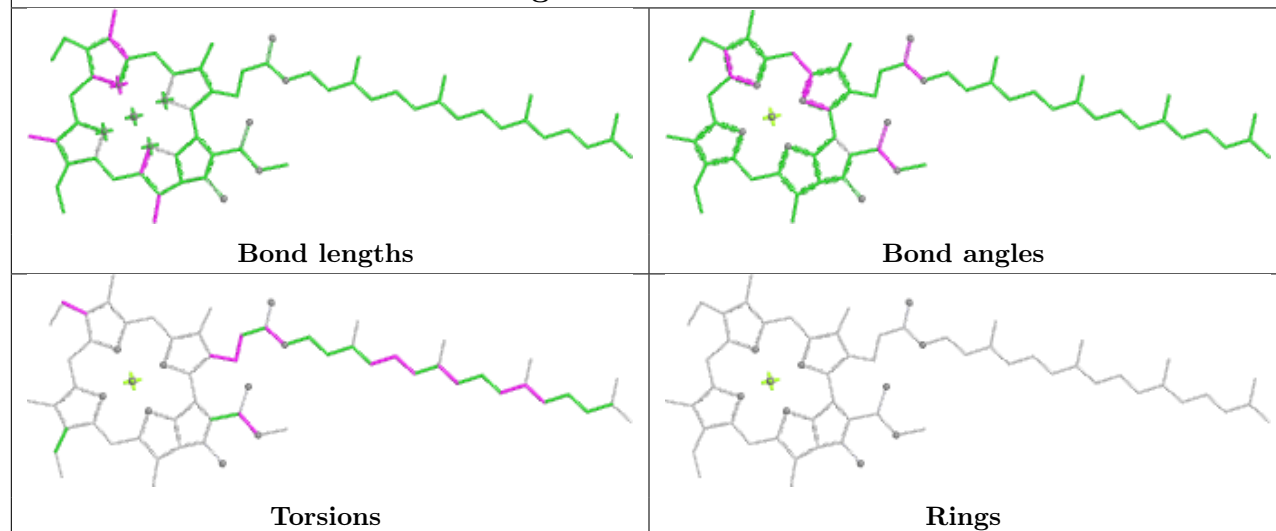
Ligand CLA A 805



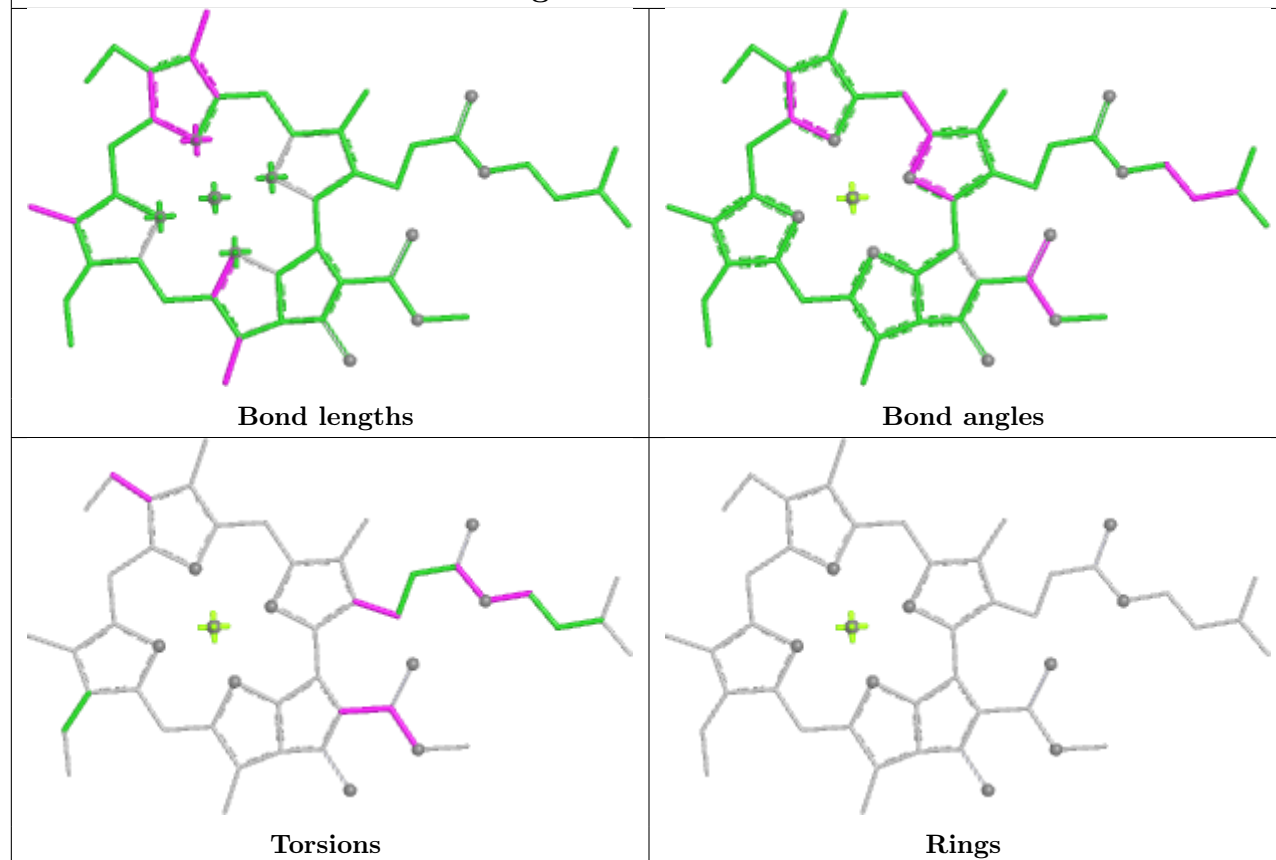
Ligand CLA B 836

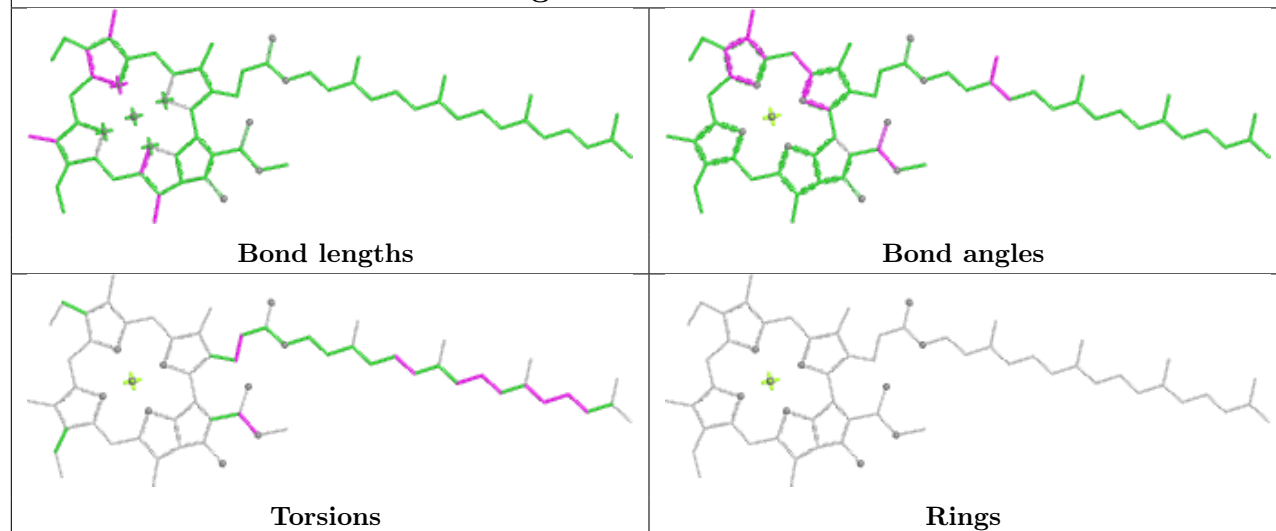
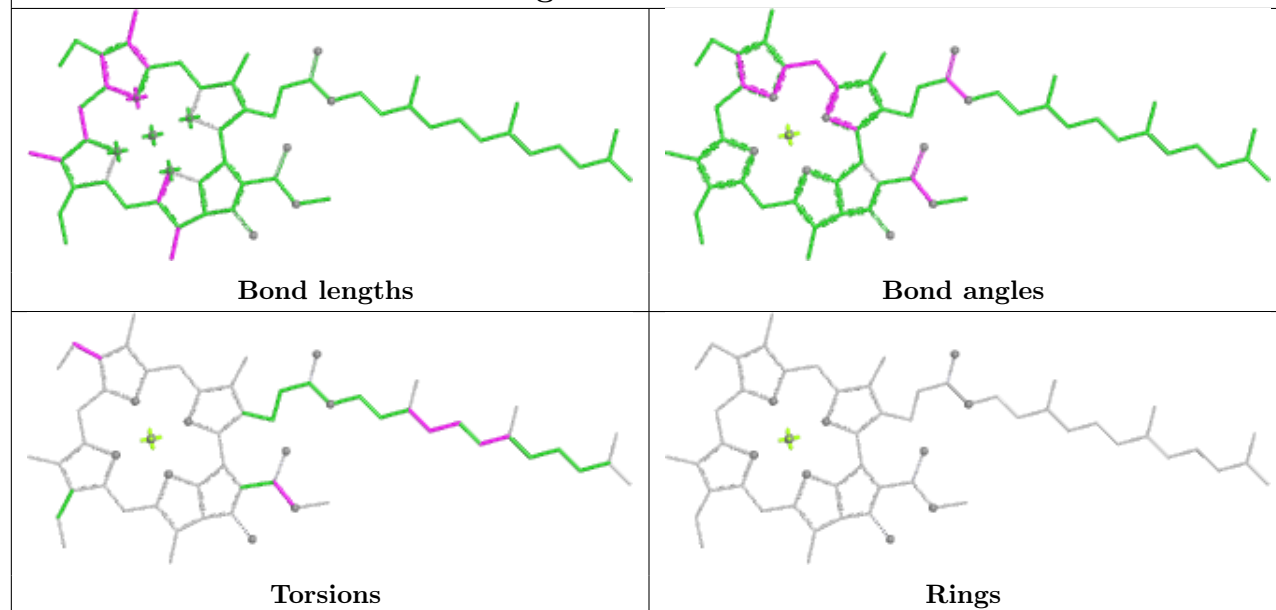


Ligand CLA A 841

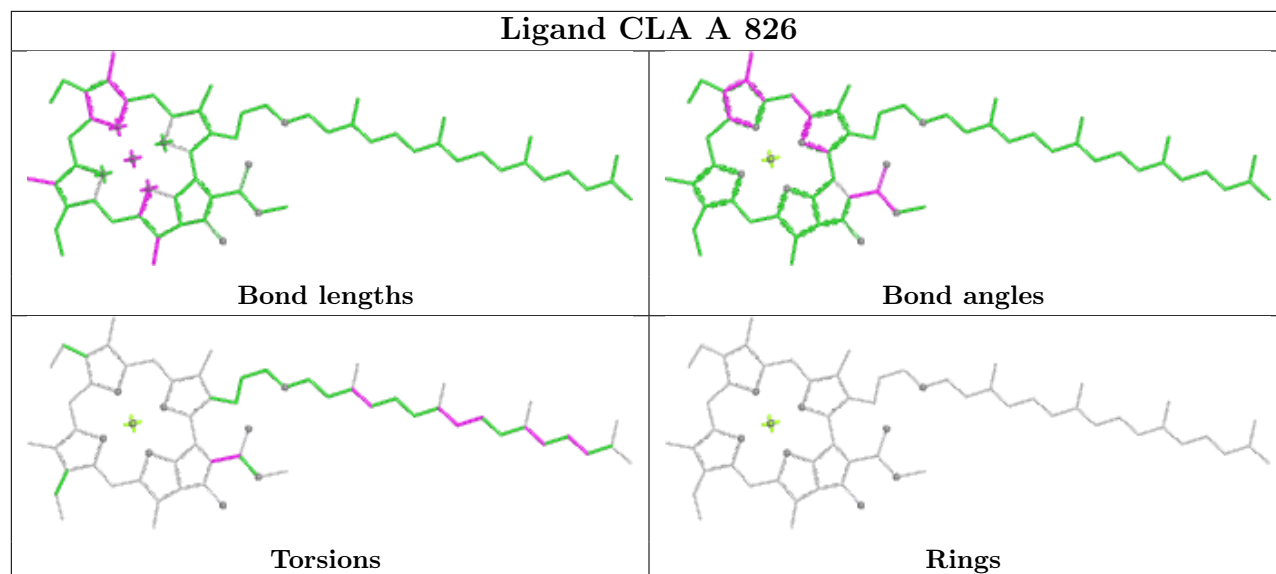


Ligand CLA A 815

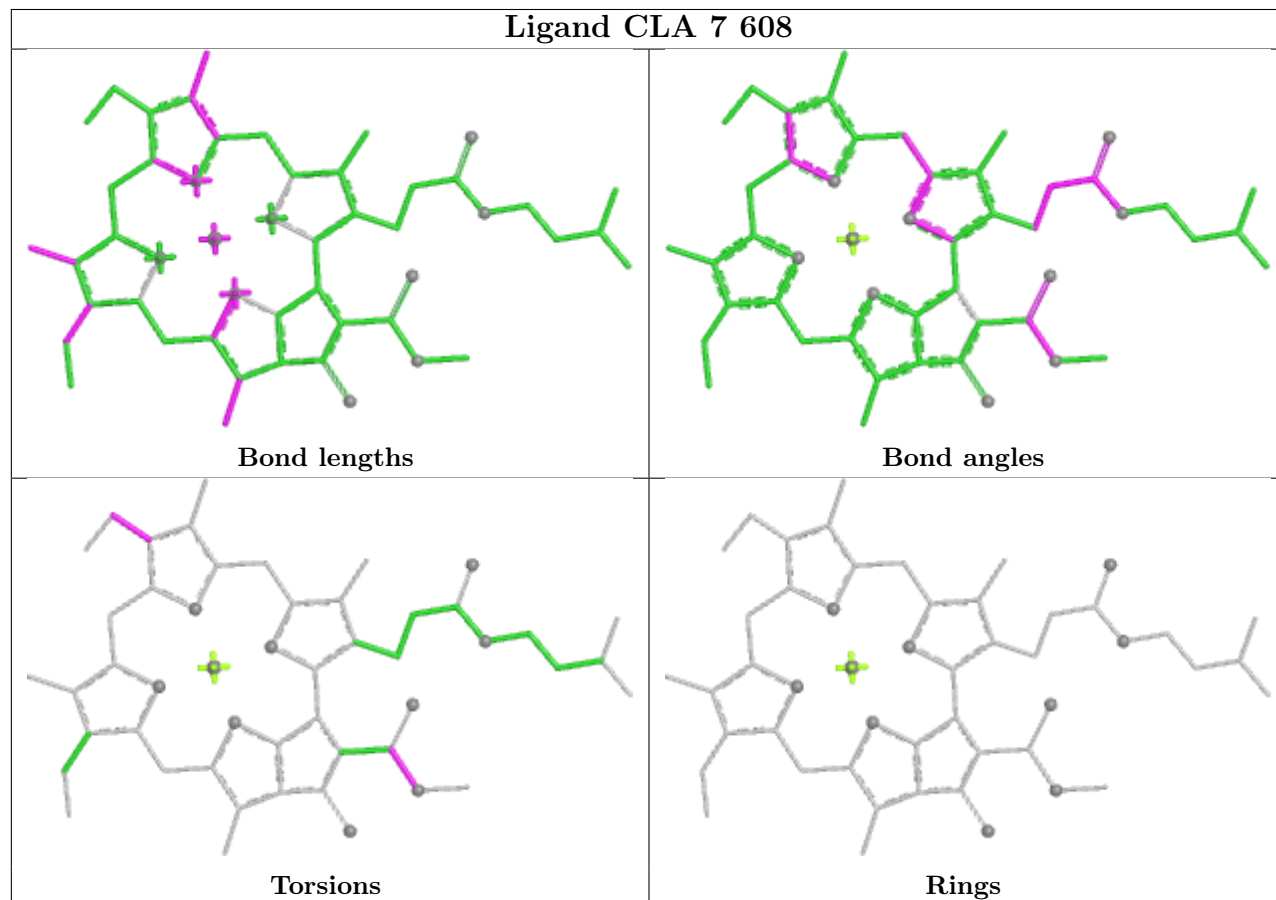


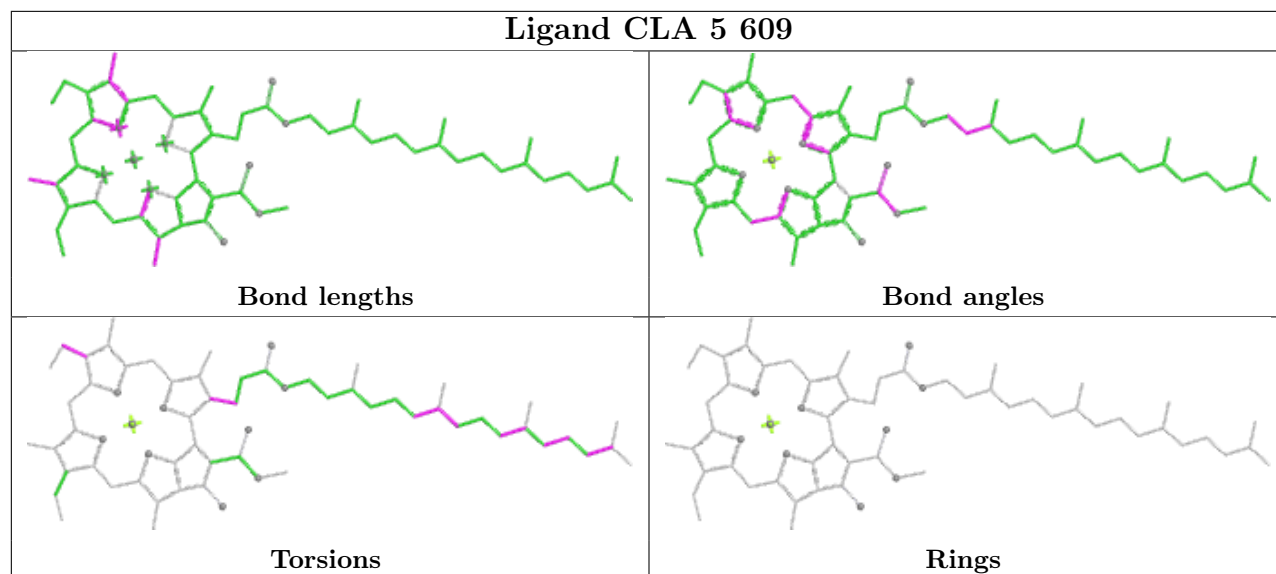
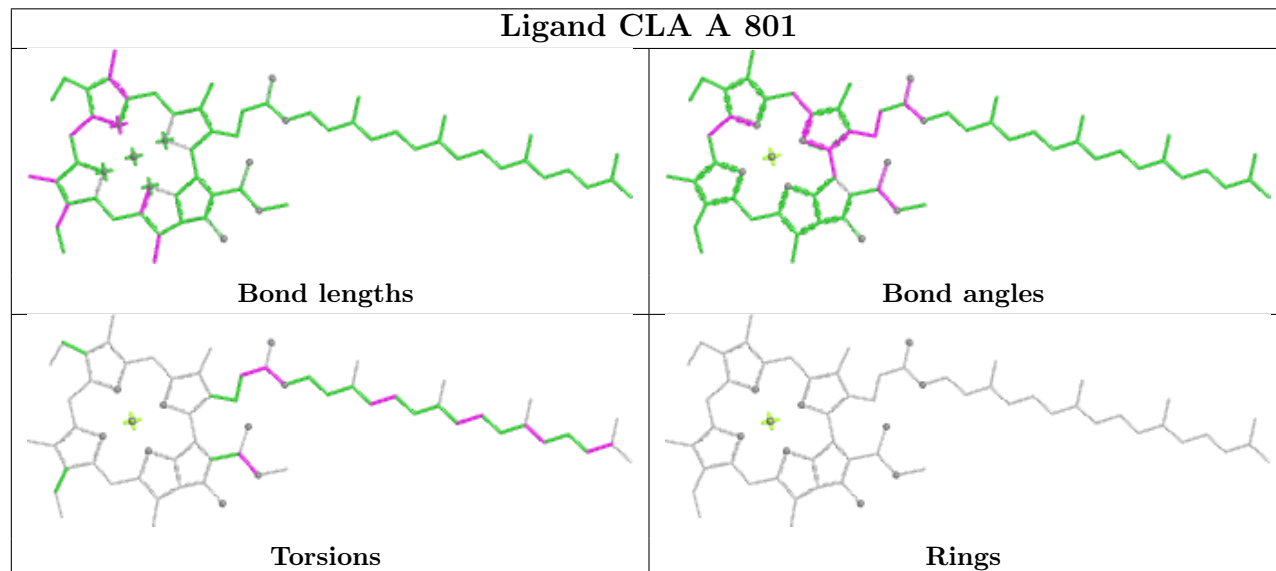
Ligand CLA A 829**Ligand CLA 4 602**

Ligand CLA A 826

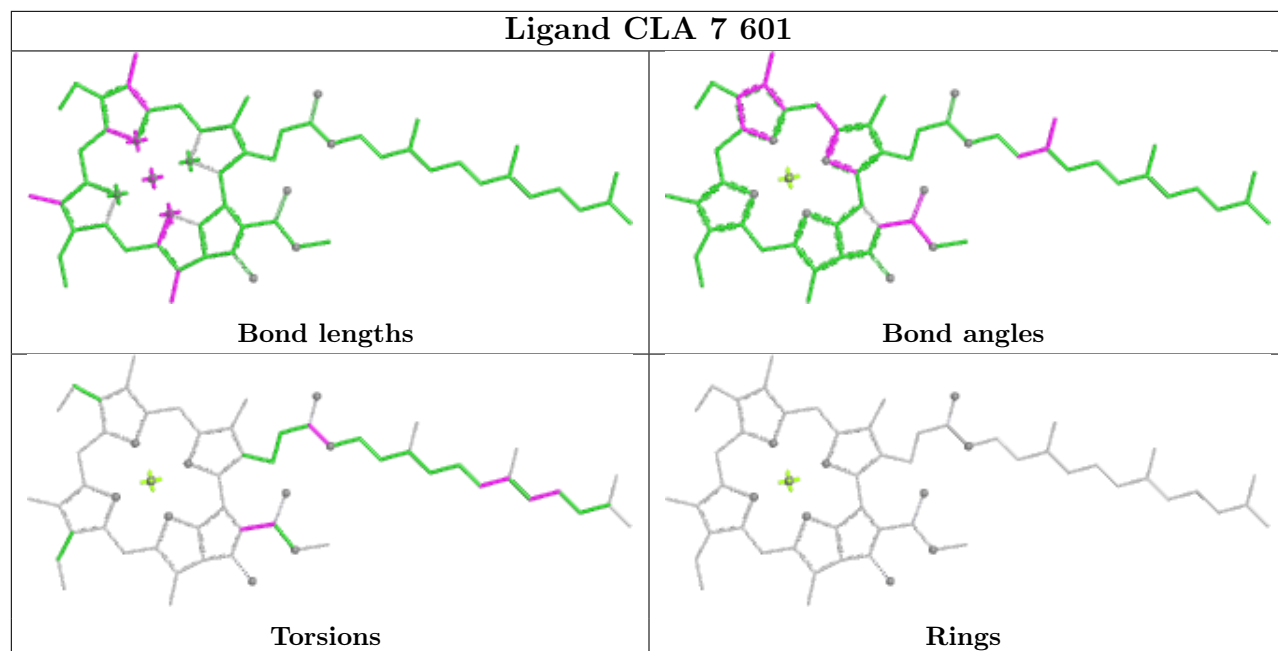


Ligand CLA 7 608

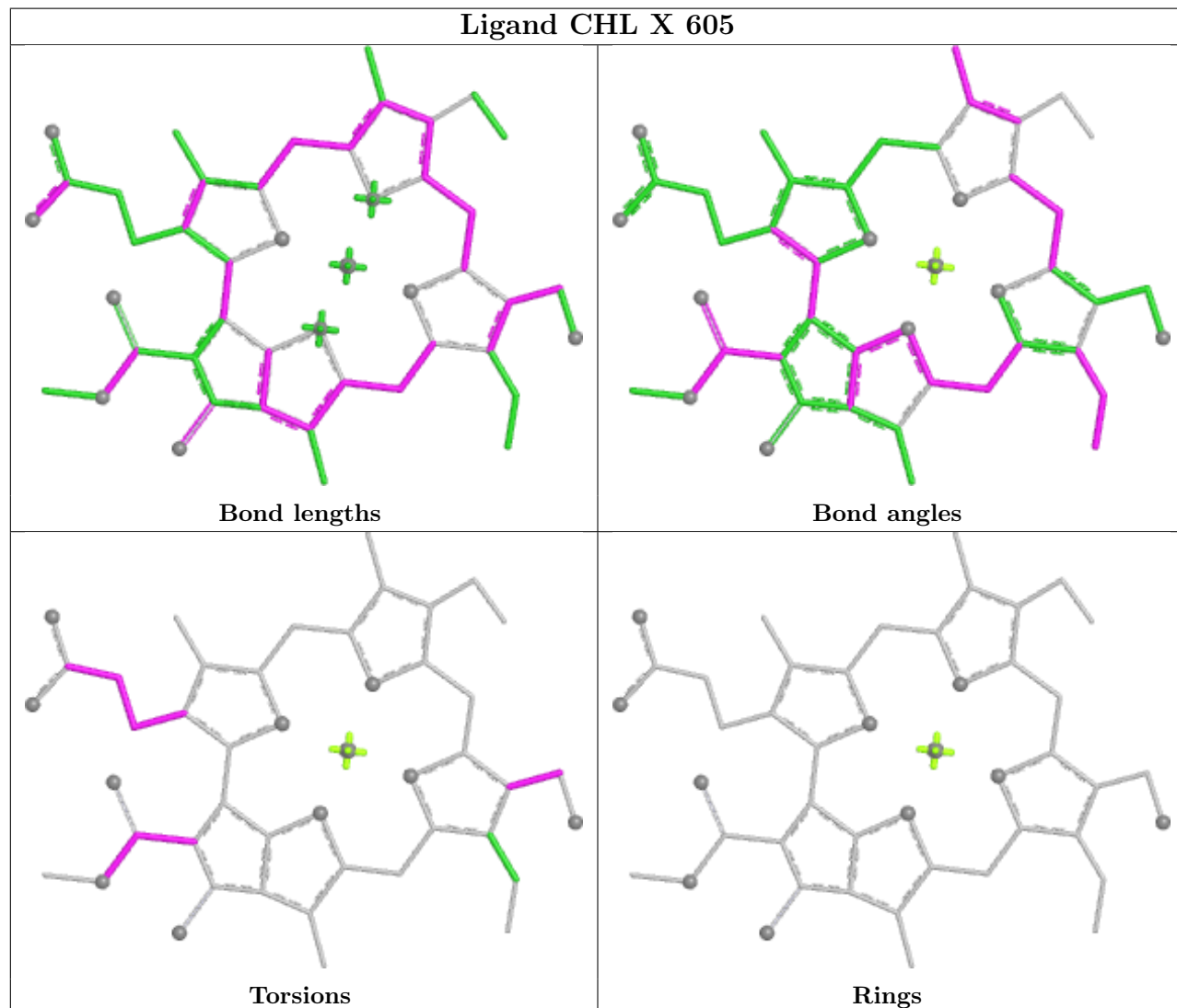


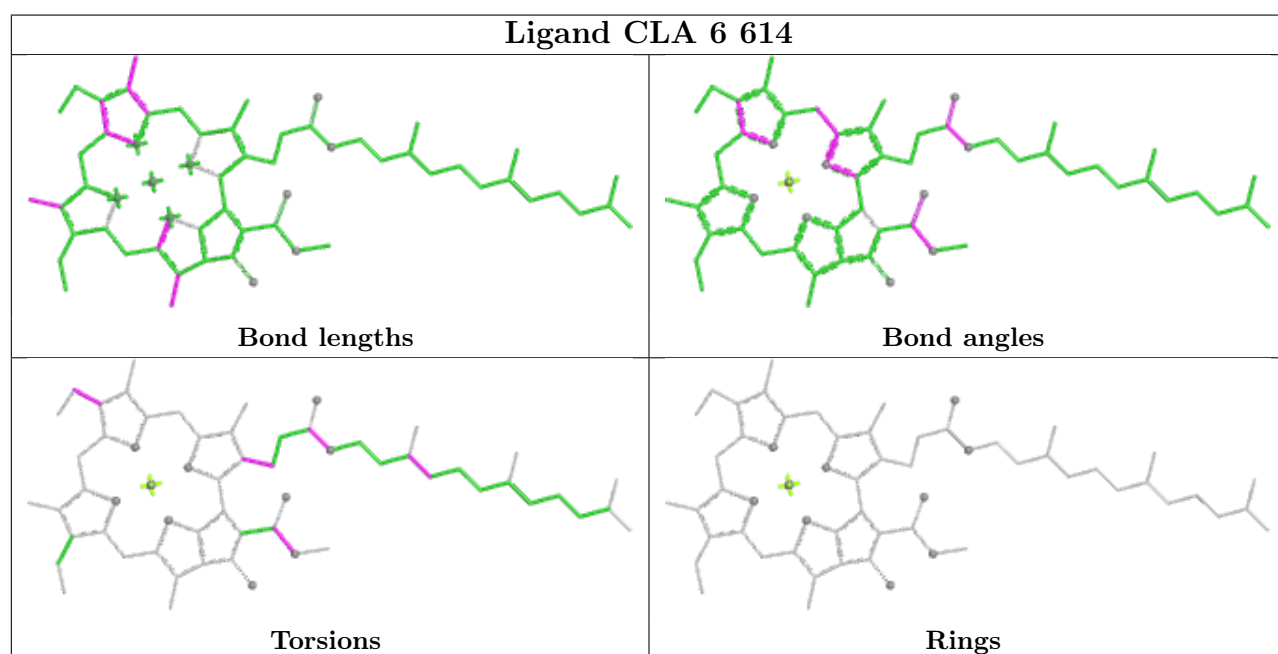
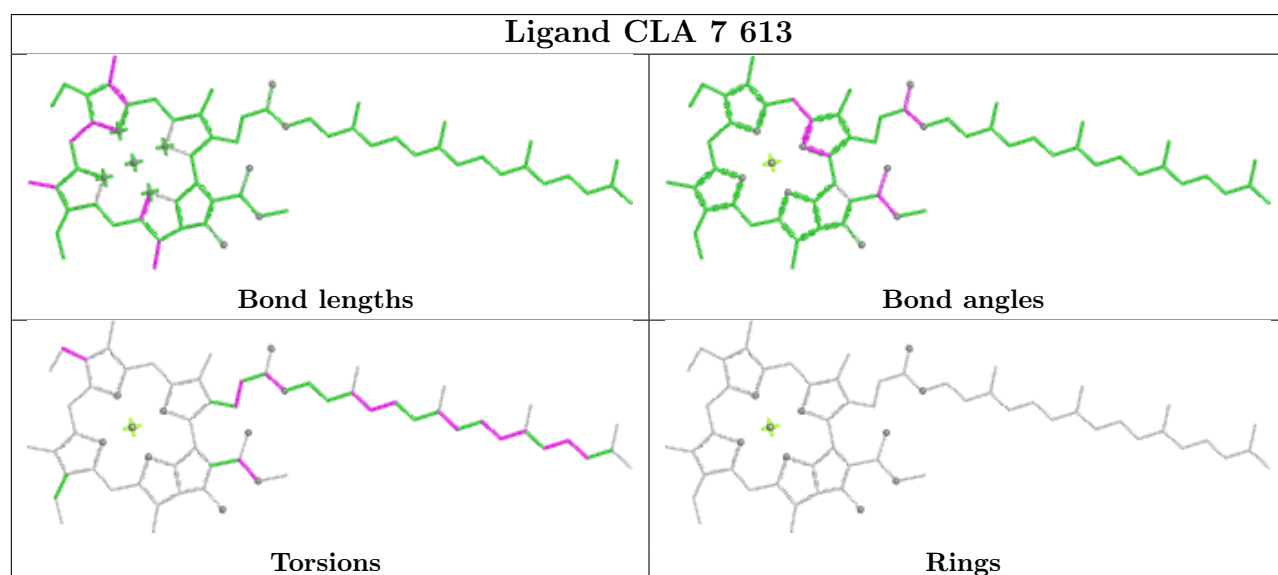
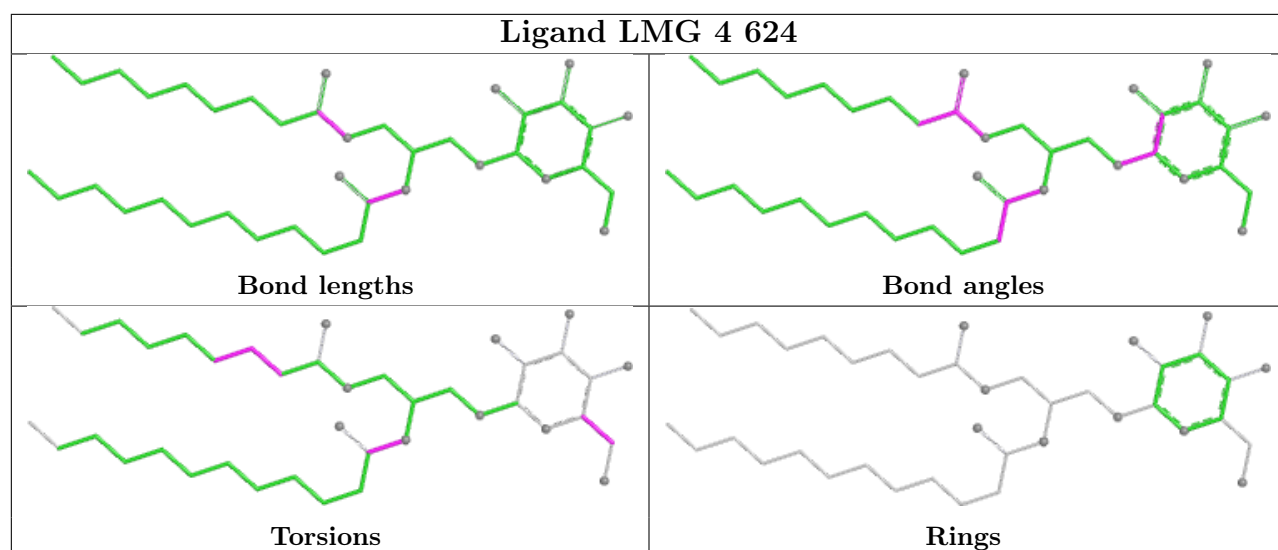
Ligand CLA 5 609**Ligand CLA A 801**

Ligand CLA 7 601

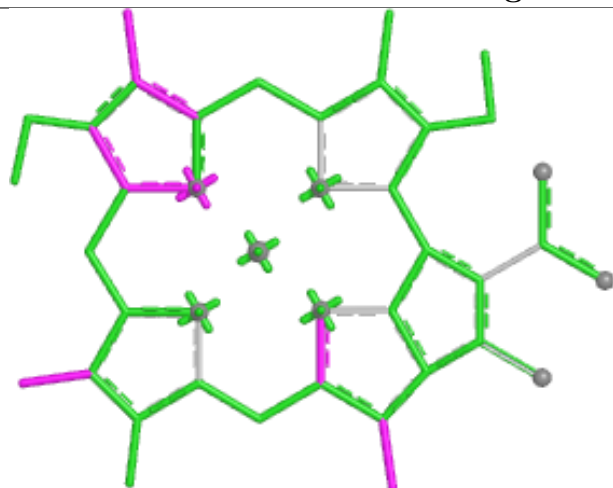


Ligand CHL X 605

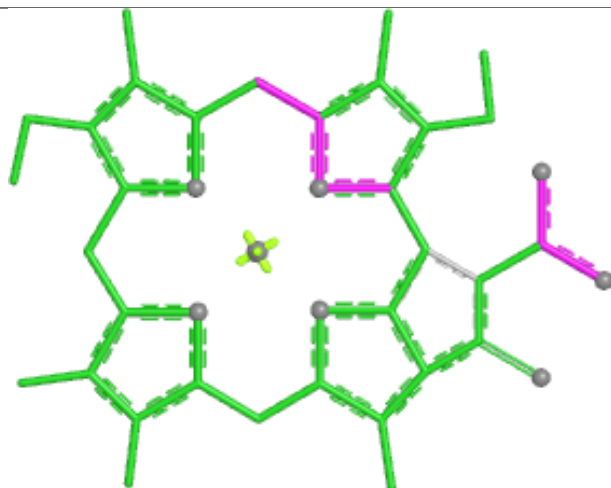




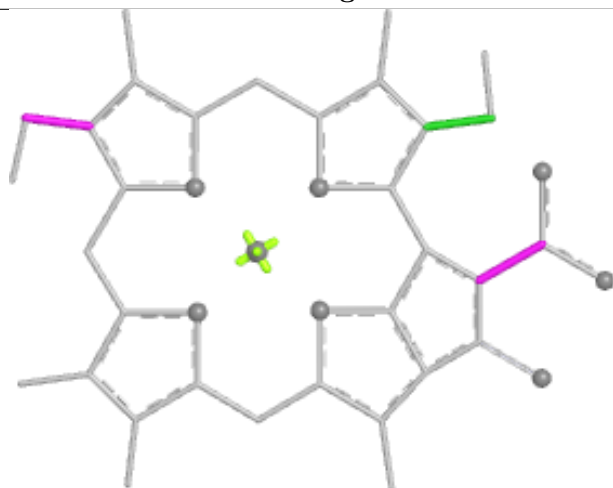
Ligand CLA O 2003



Bond lengths



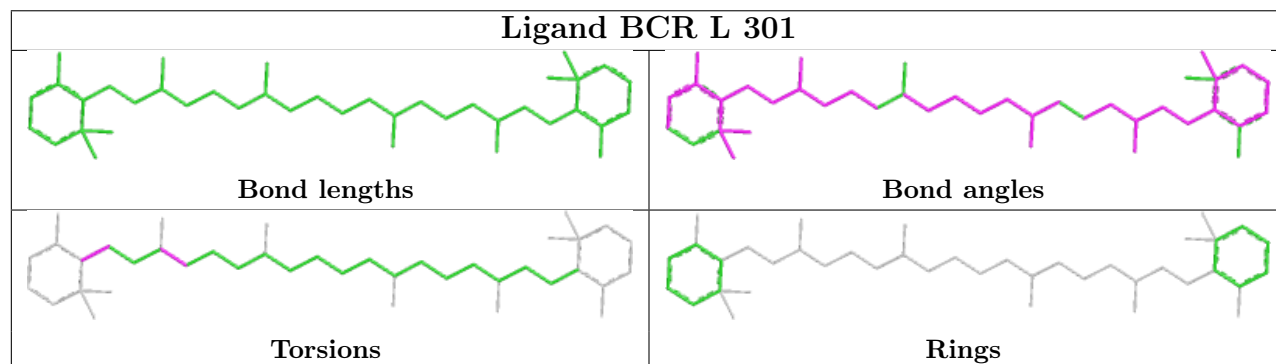
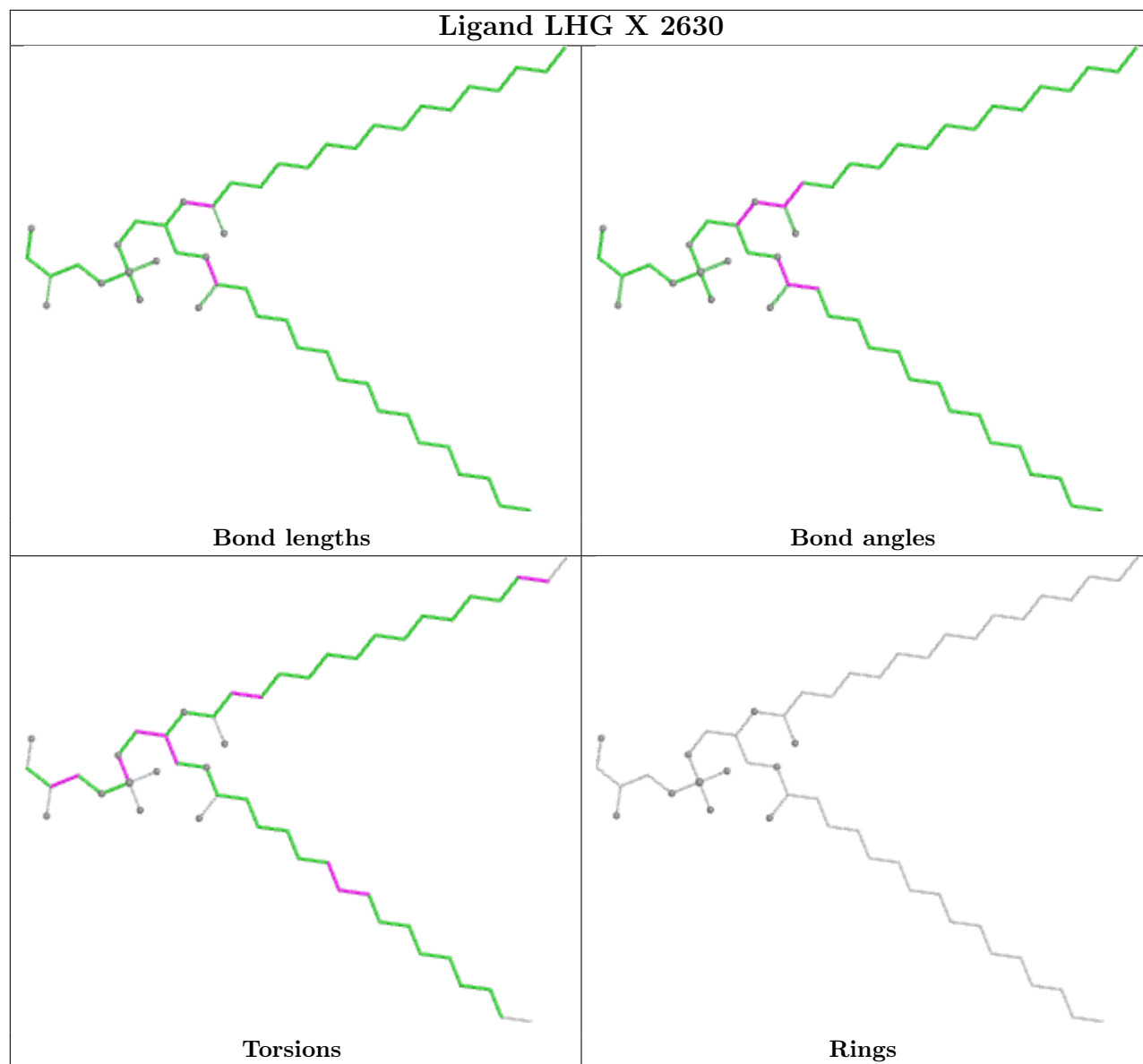
Bond angles

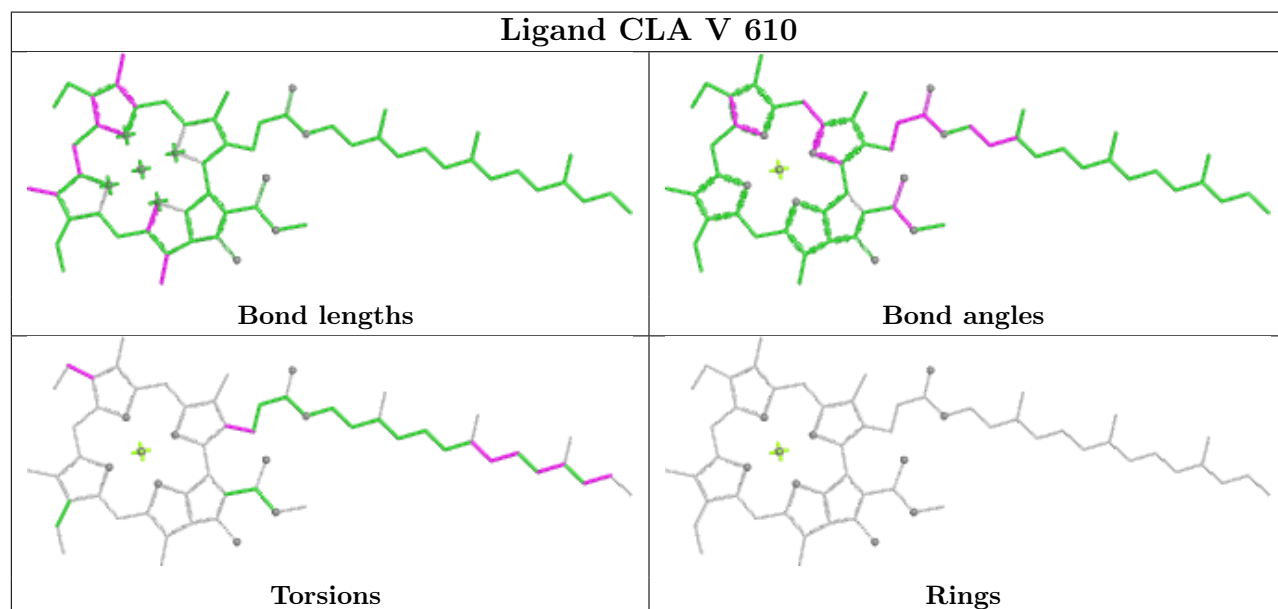
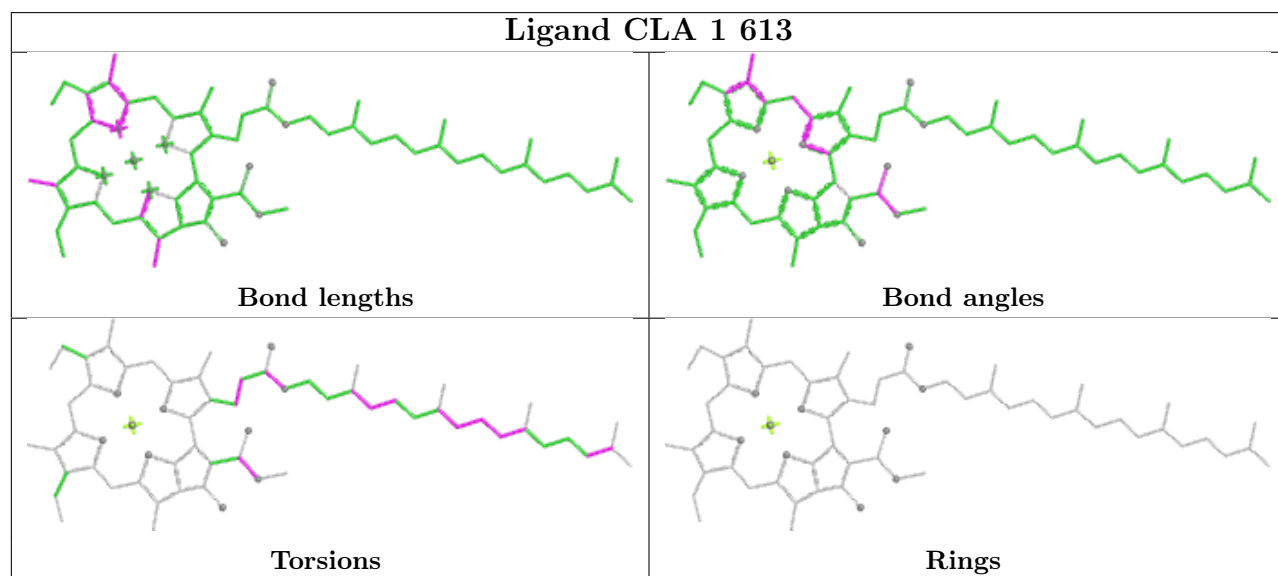
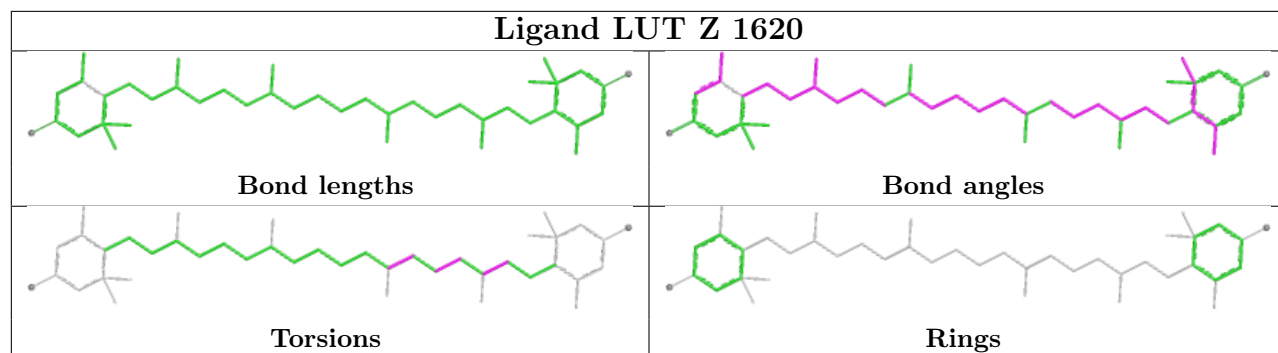


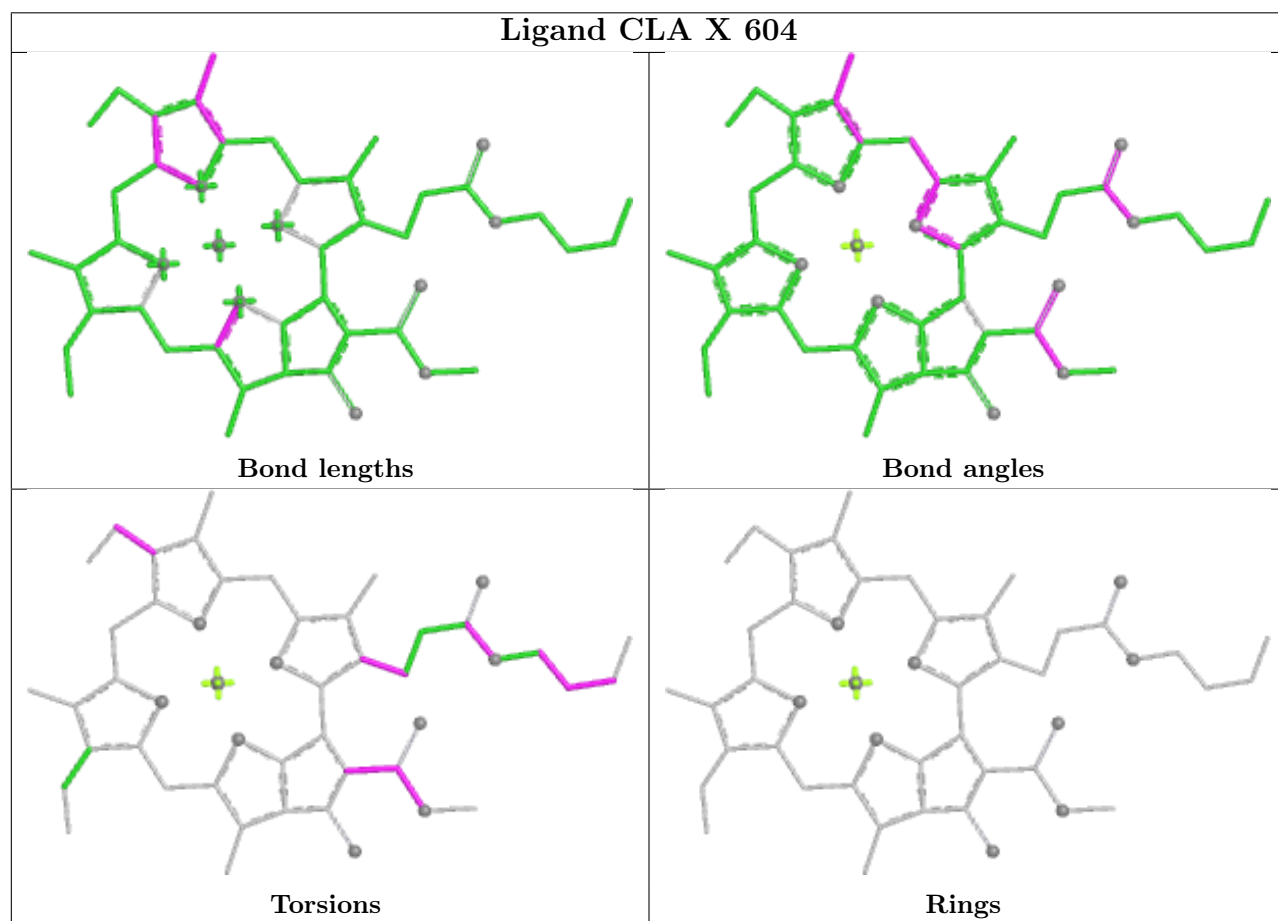
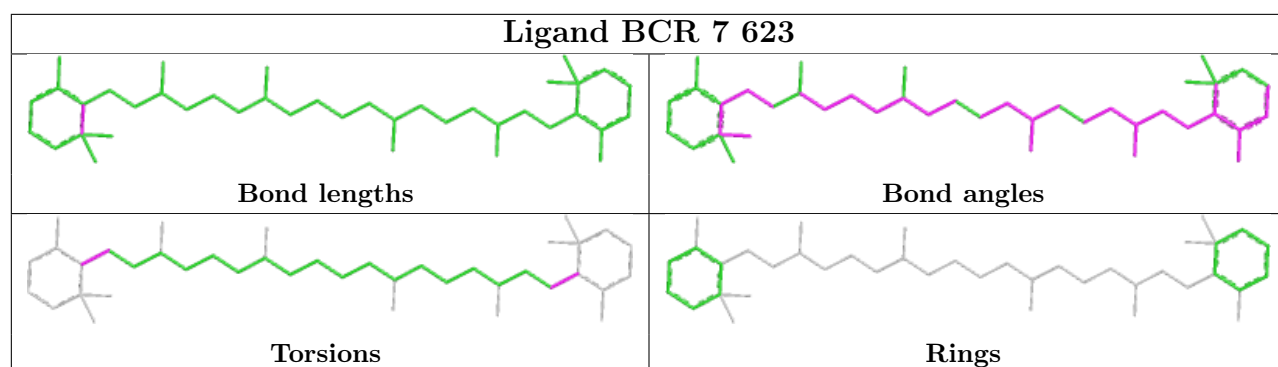
Torsions

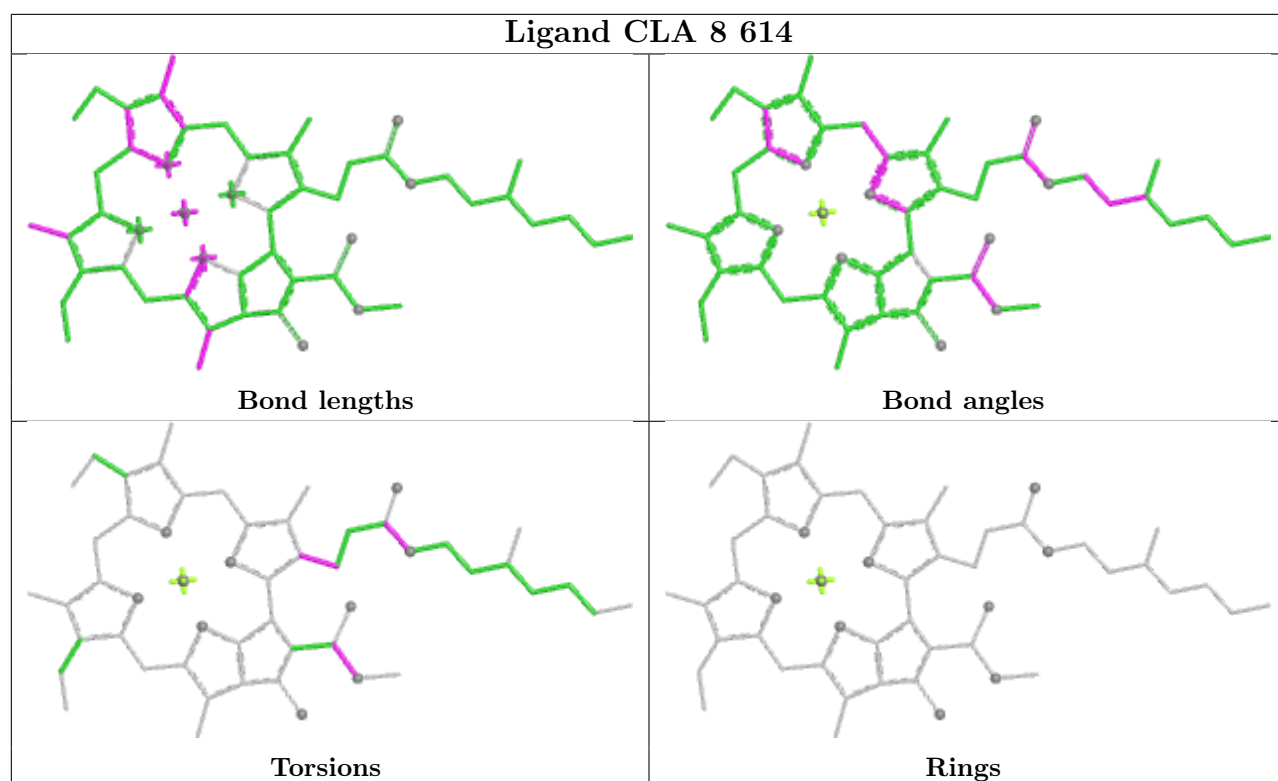


Rings

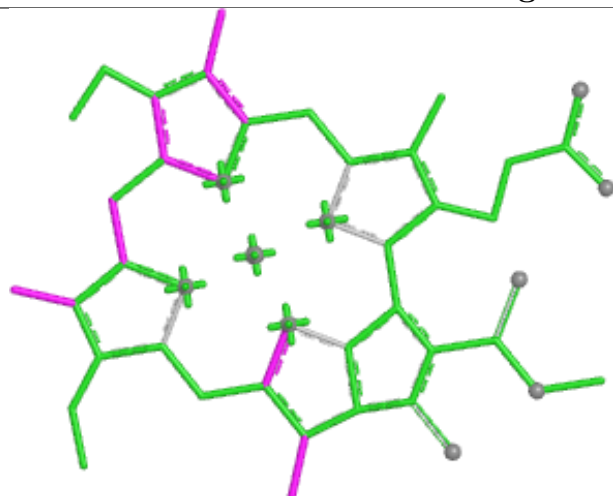




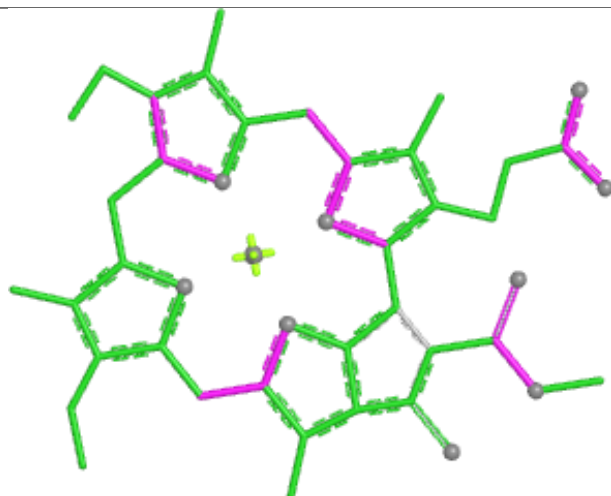




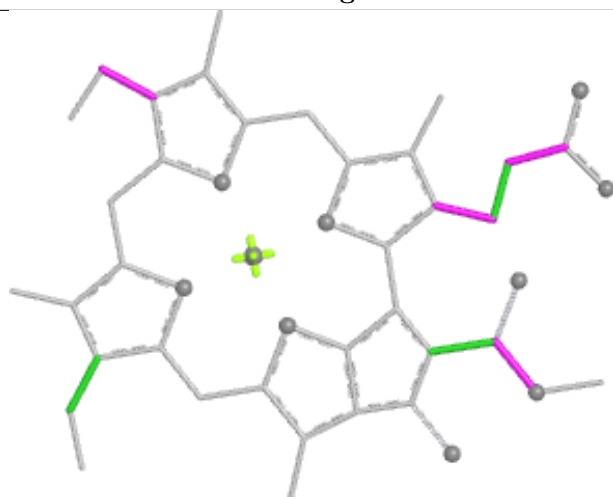
Ligand CLA 6 608



Bond lengths



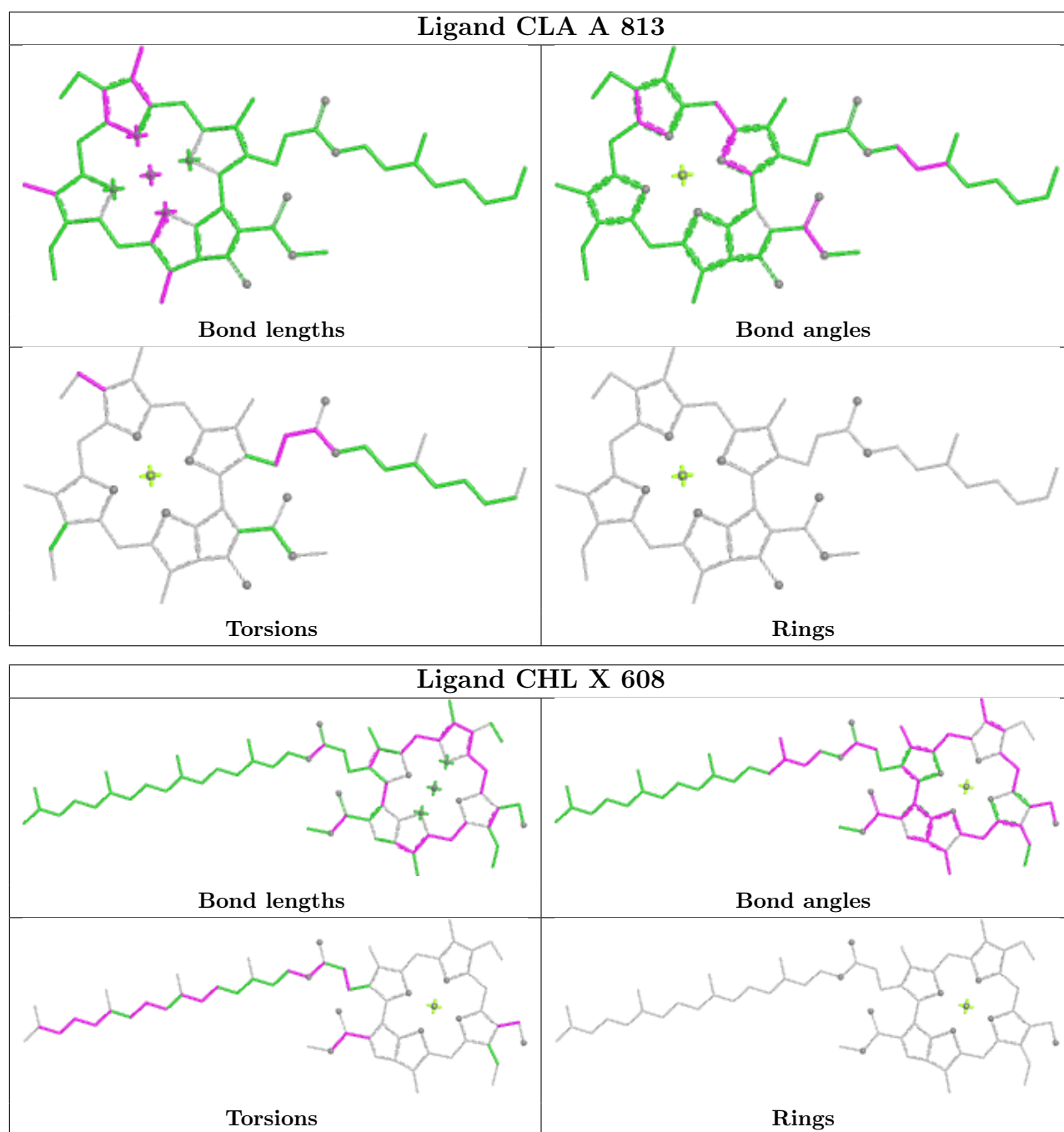
Bond angles



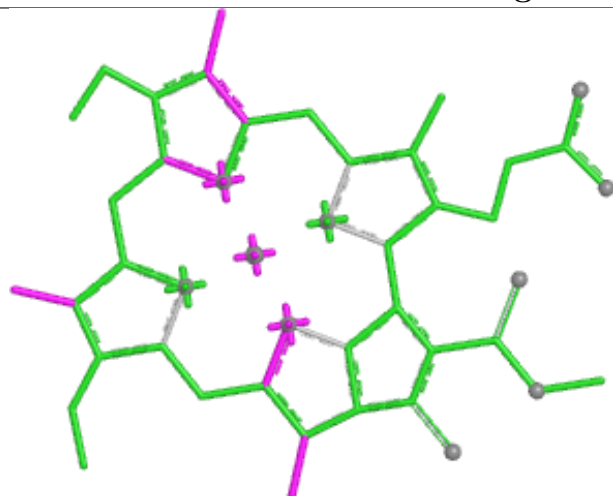
Torsions



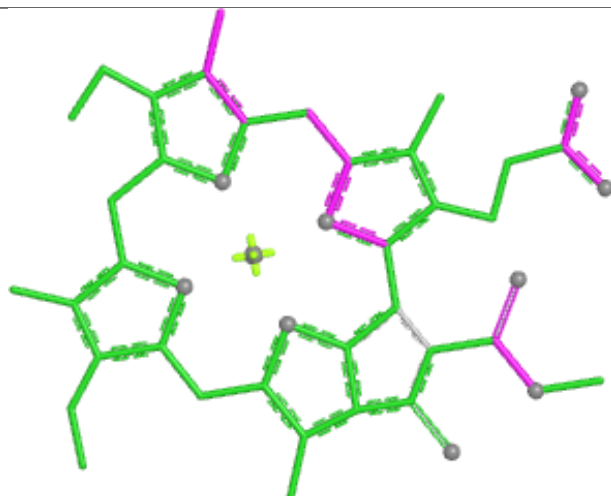
Rings



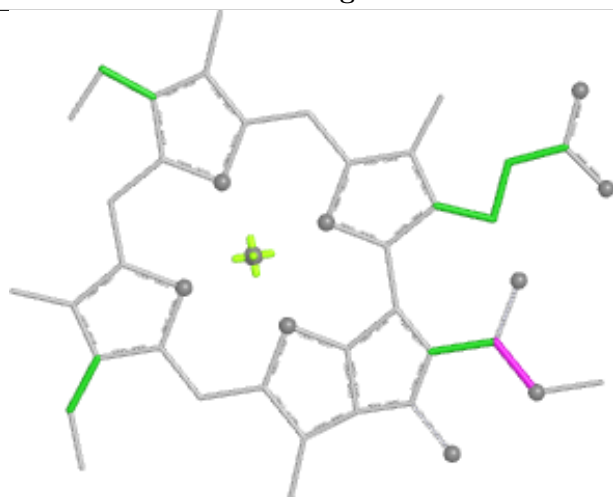
Ligand CLA B 835



Bond lengths



Bond angles

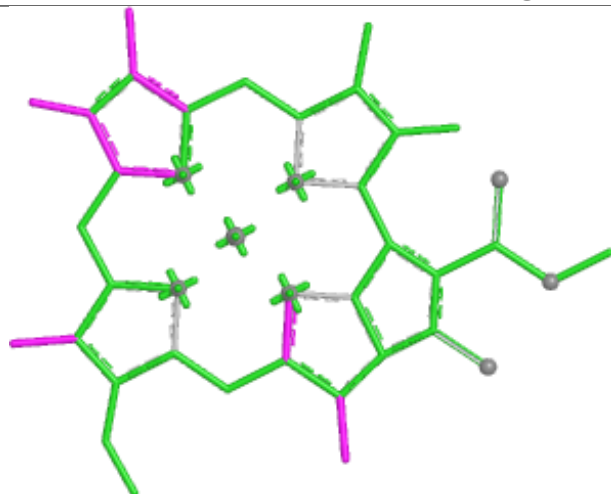


Torsions

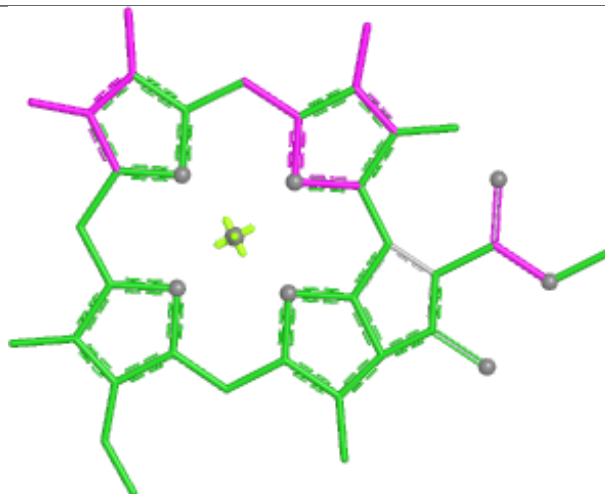


Rings

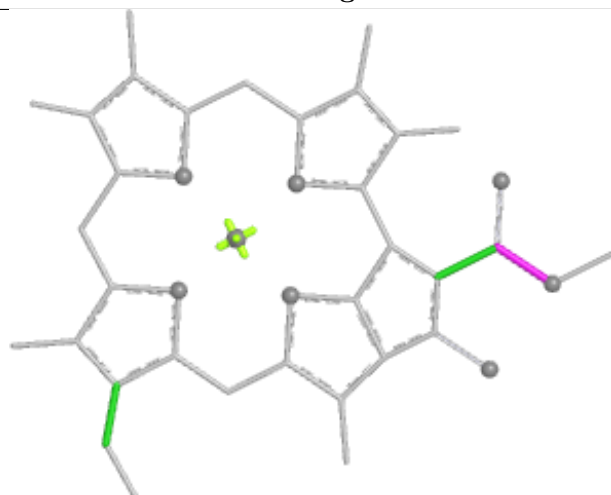
Ligand CLA 1 609



Bond lengths



Bond angles

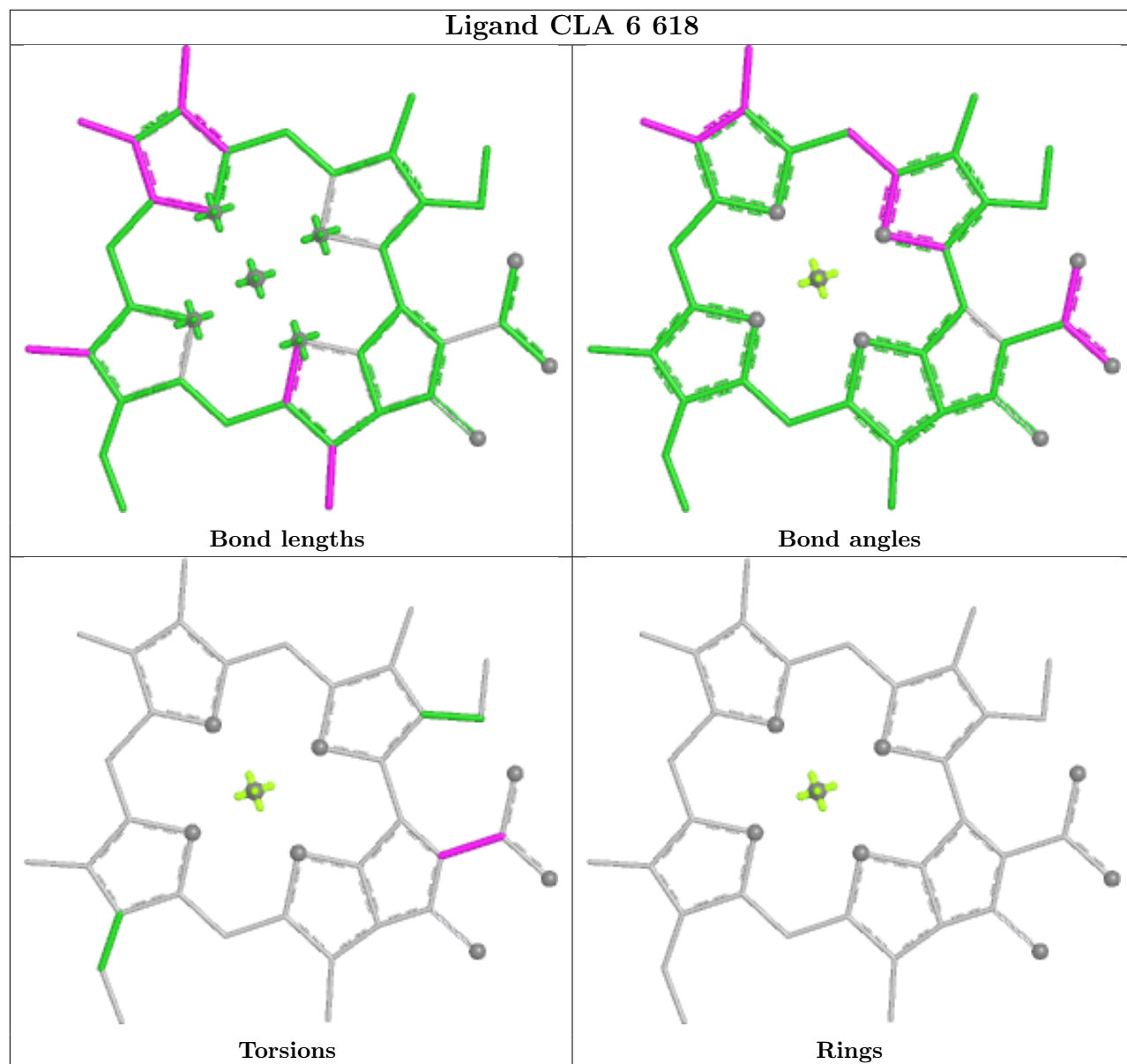


Torsions

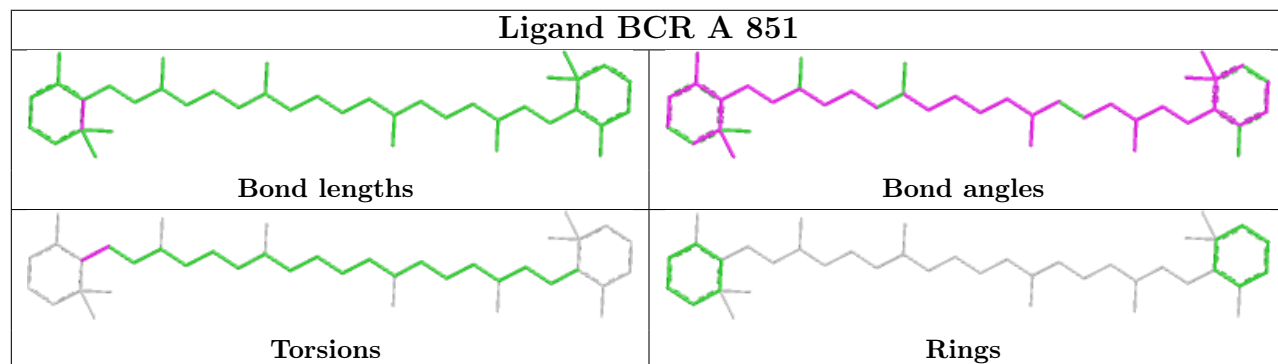


Rings

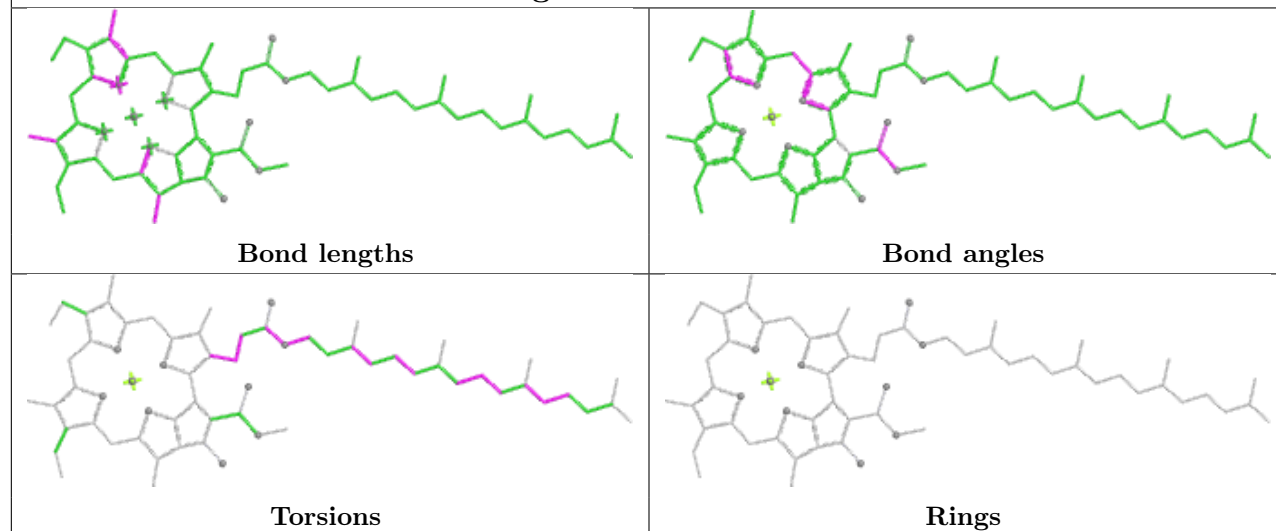
Ligand CLA 6 618



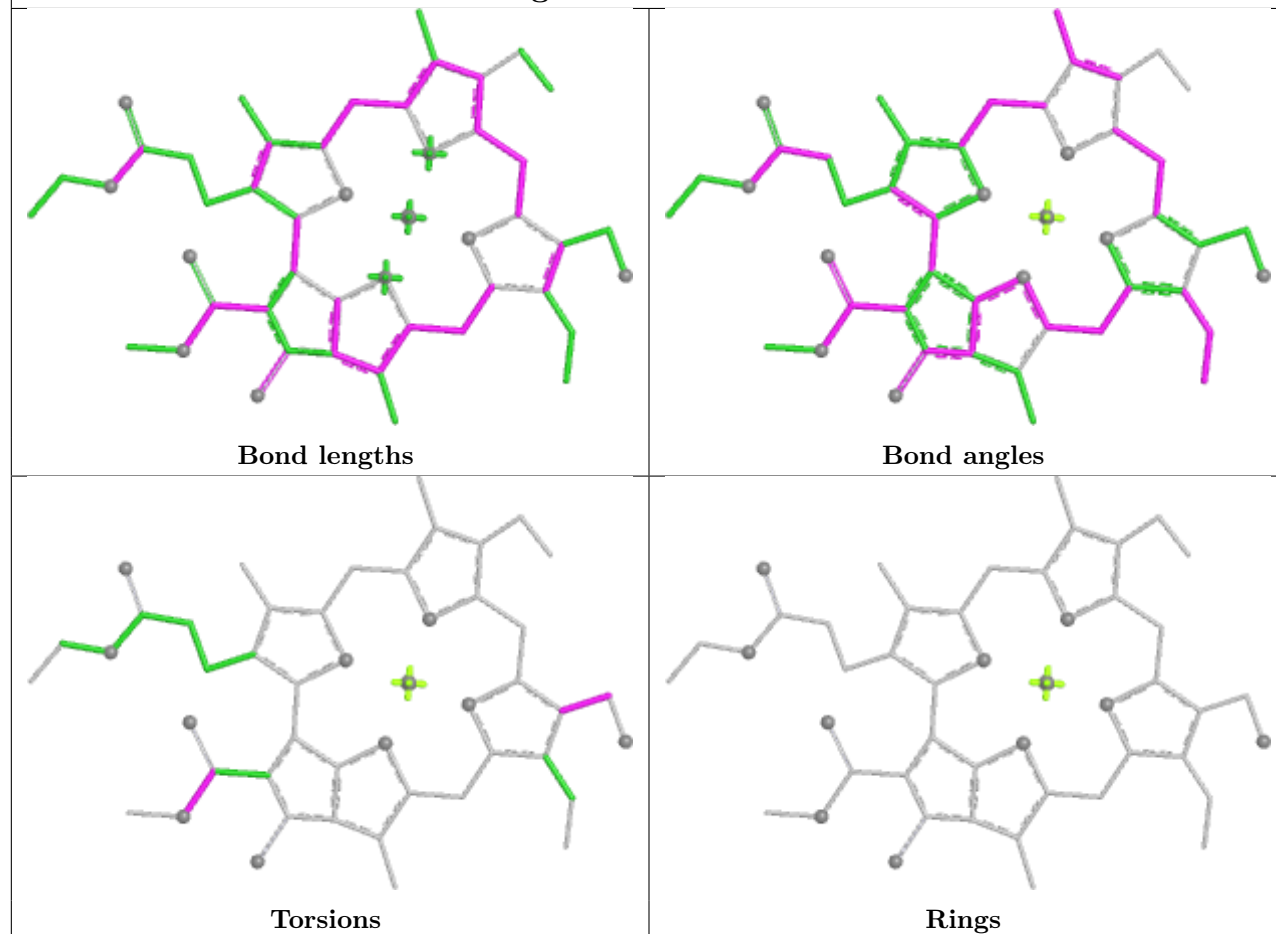
Ligand BCR A 851

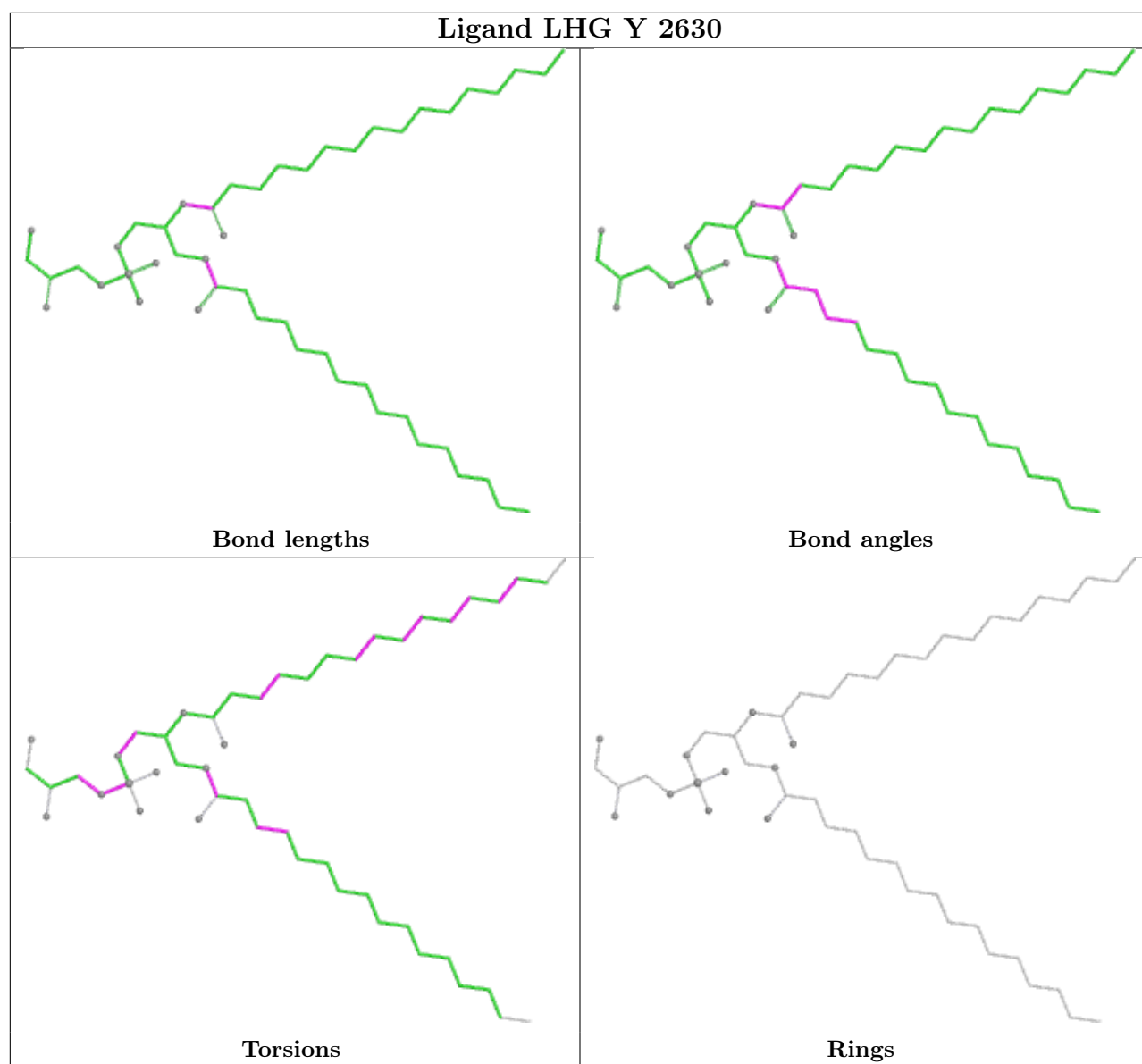


Ligand CLA B 828

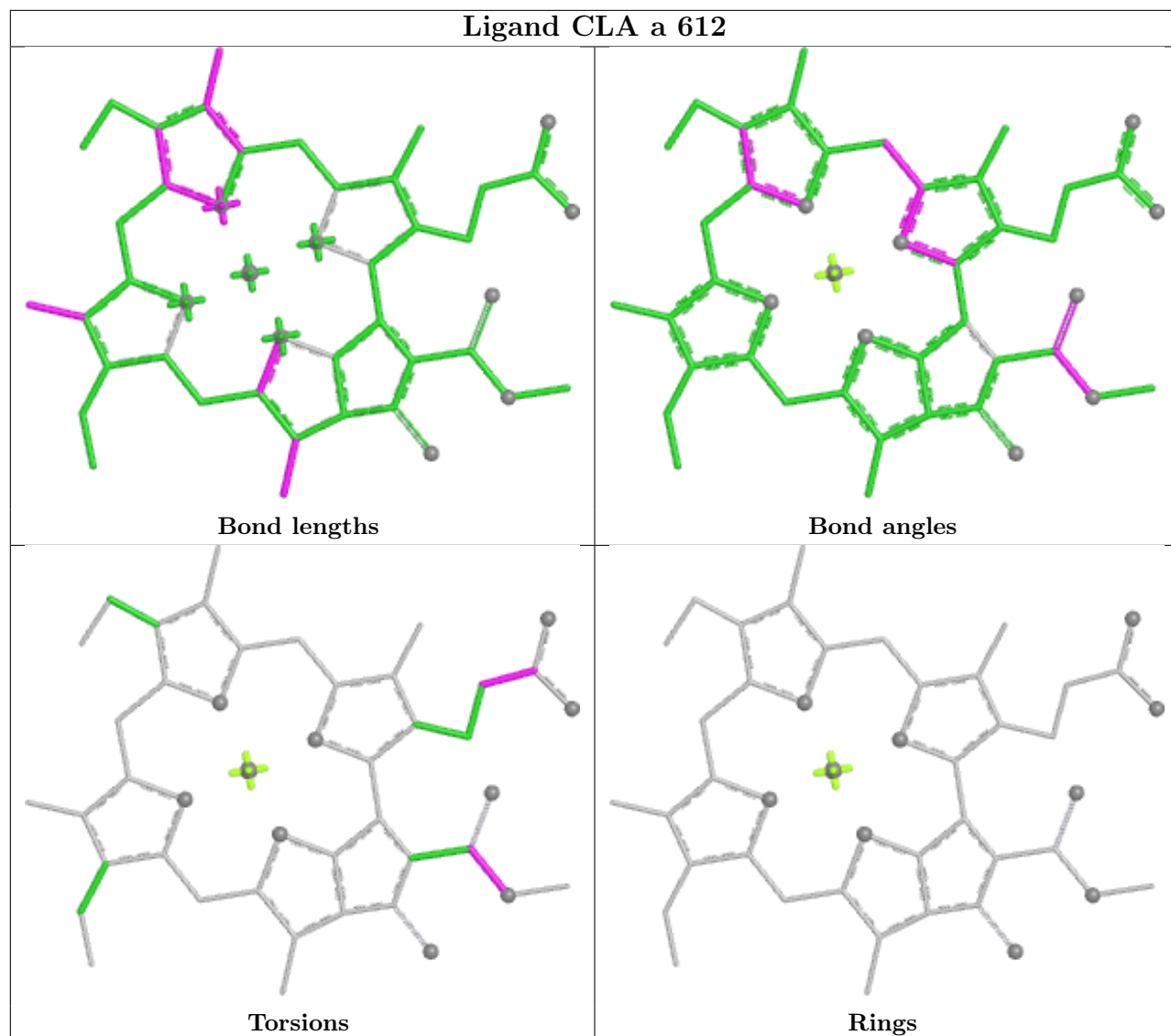


Ligand CHL V 608

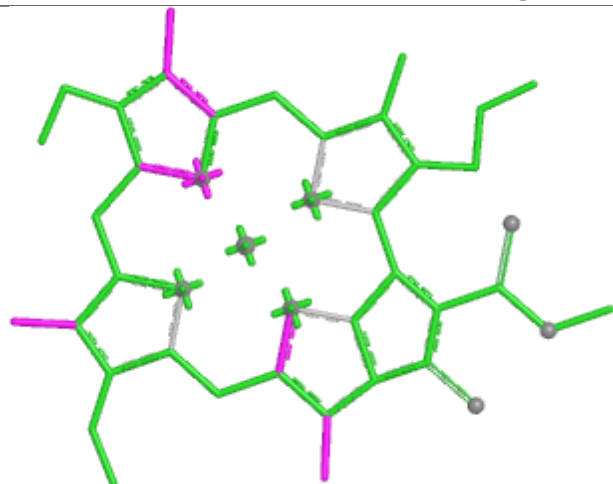




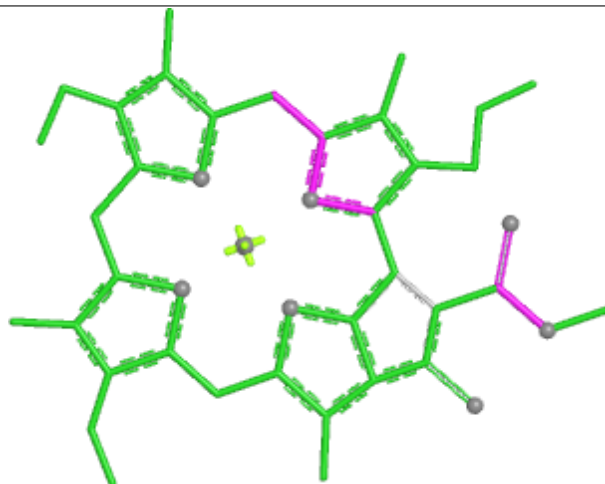
Ligand CLA a 612



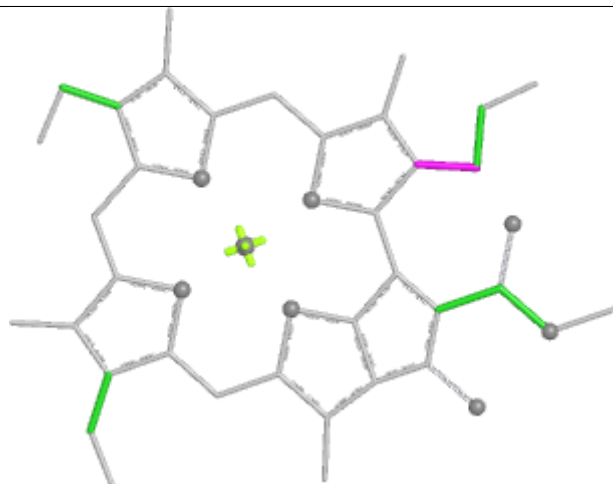
Ligand CLA B 815



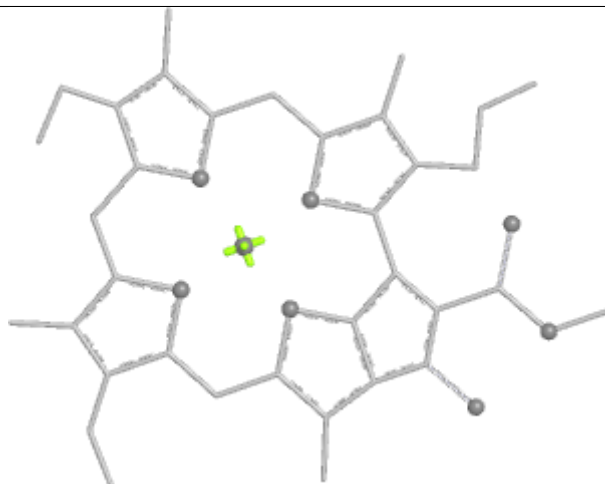
Bond lengths



Bond angles

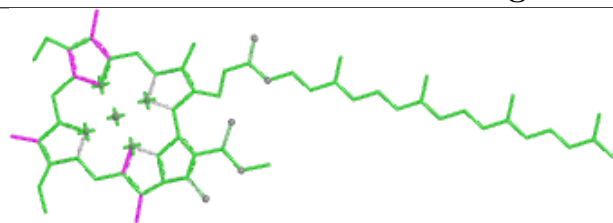


Torsions

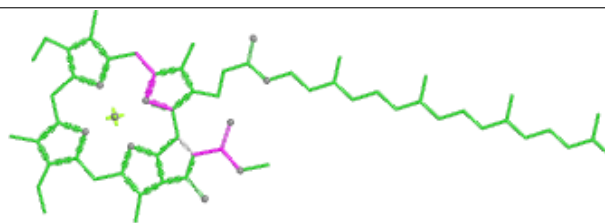


Rings

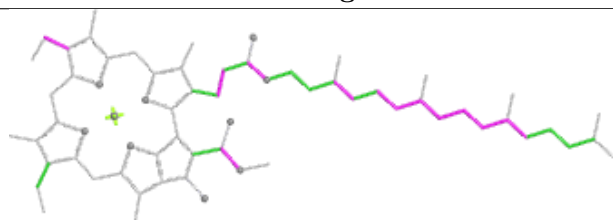
Ligand CLA W 613



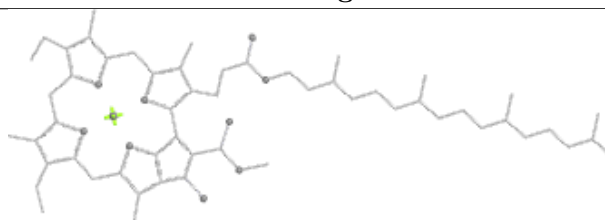
Bond lengths



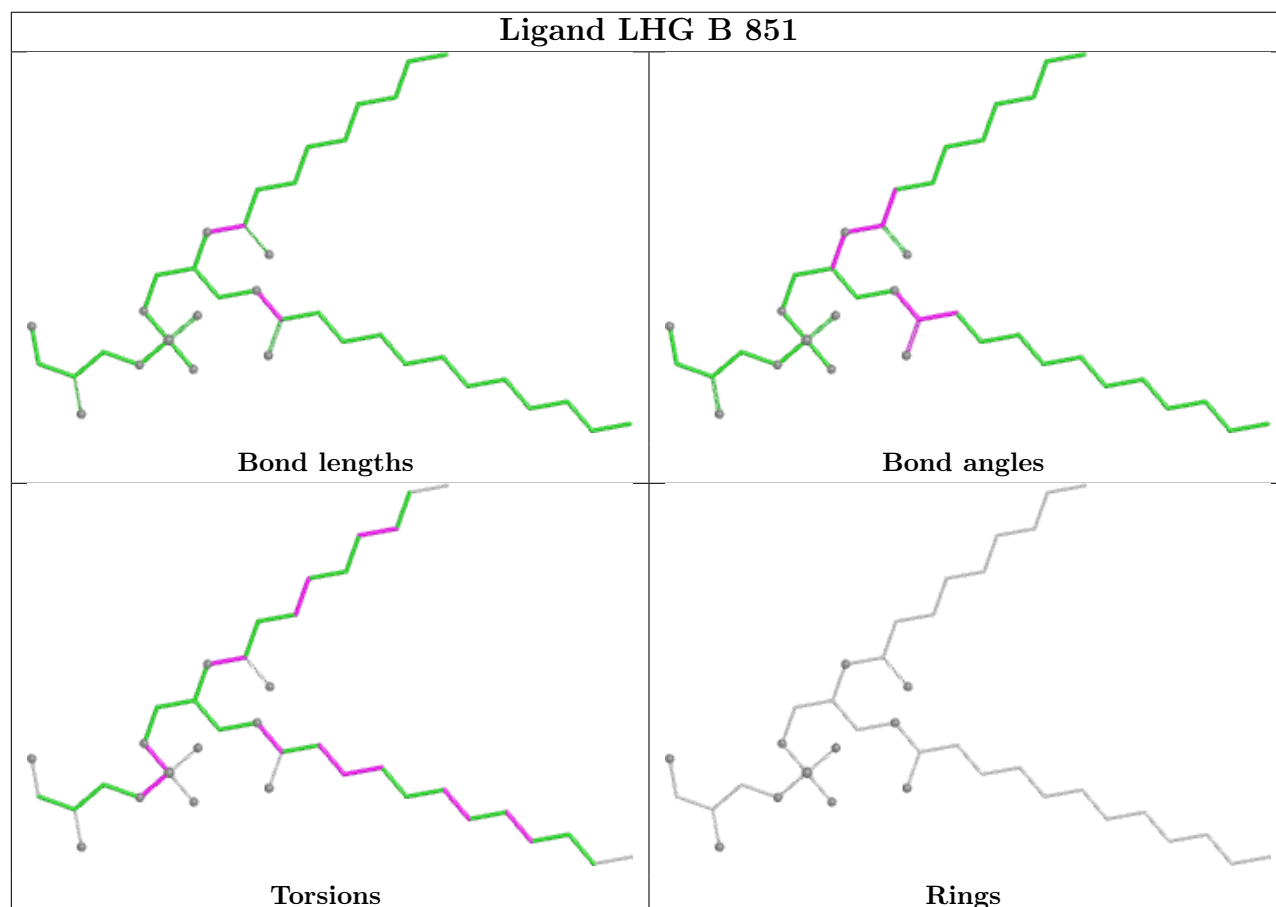
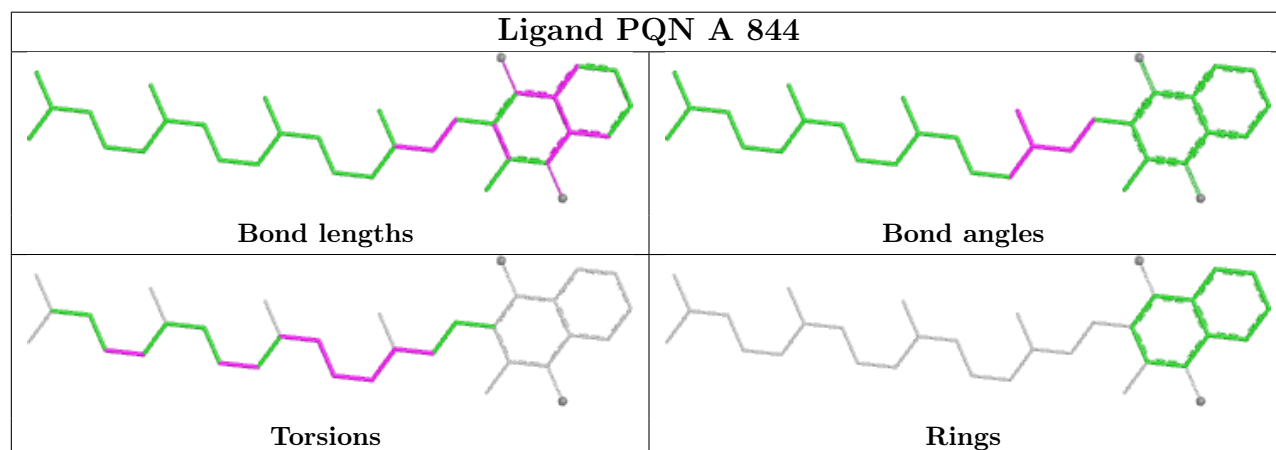
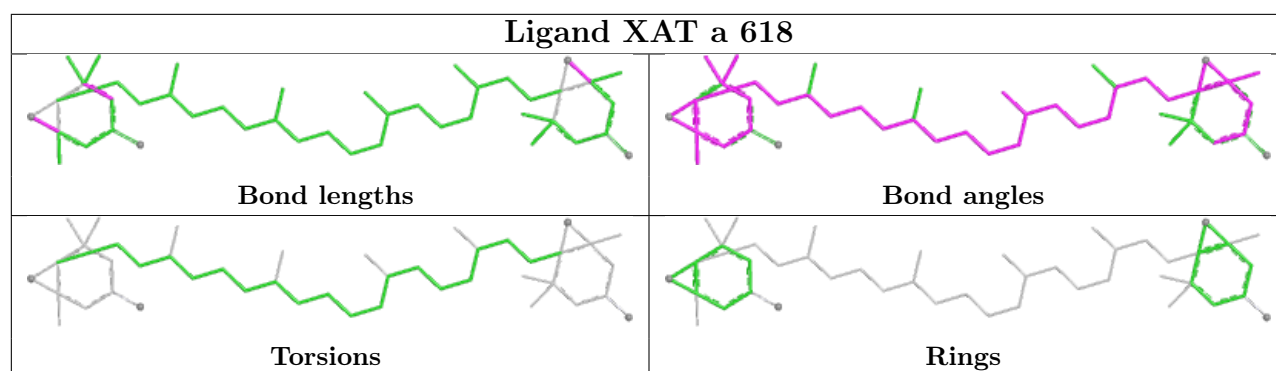
Bond angles

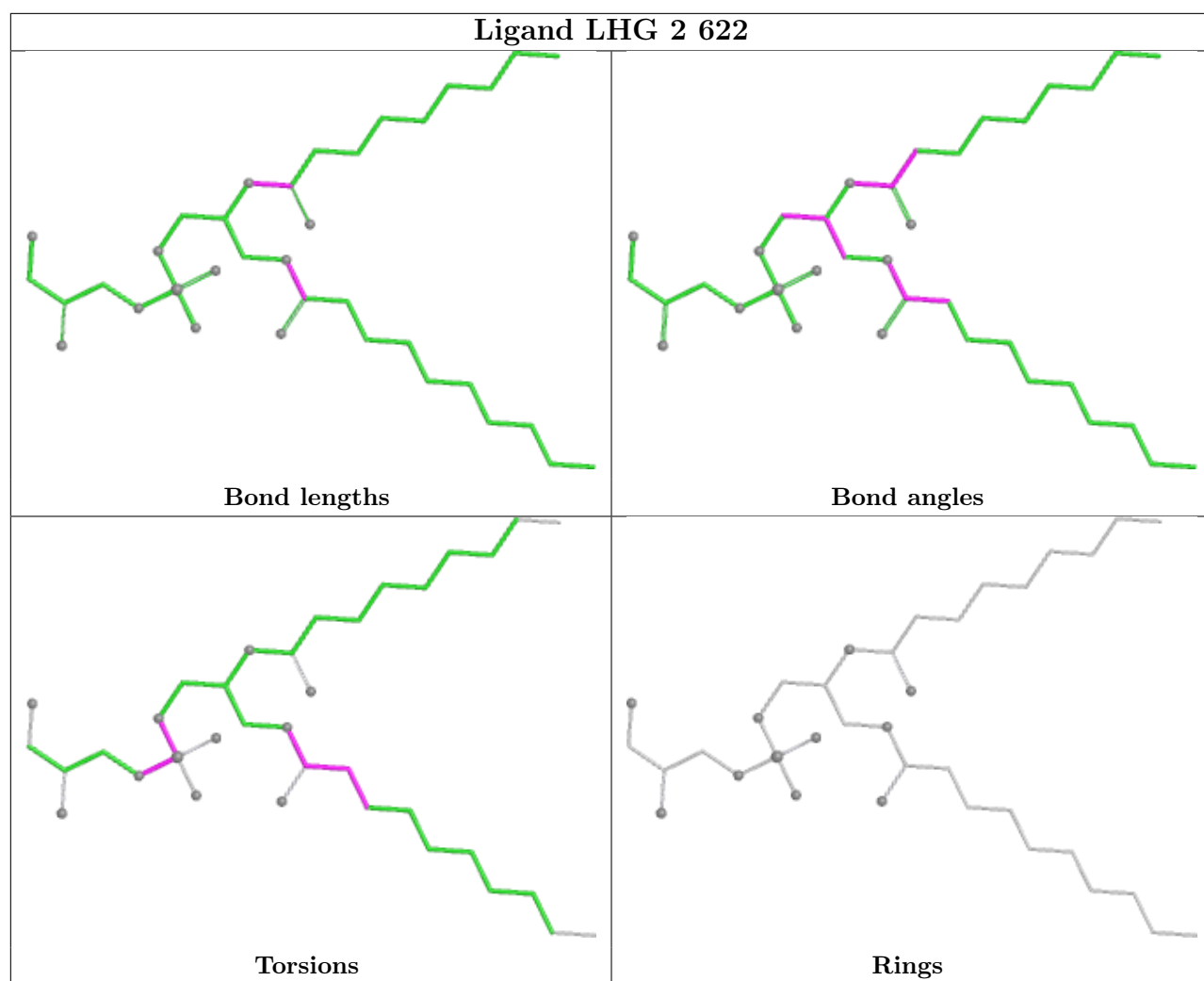


Torsions

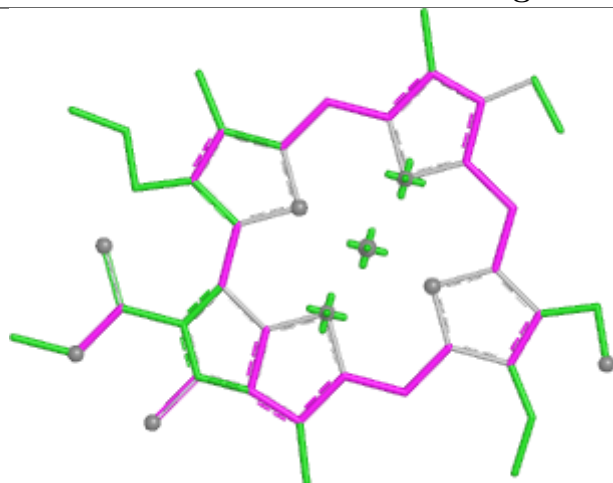


Rings

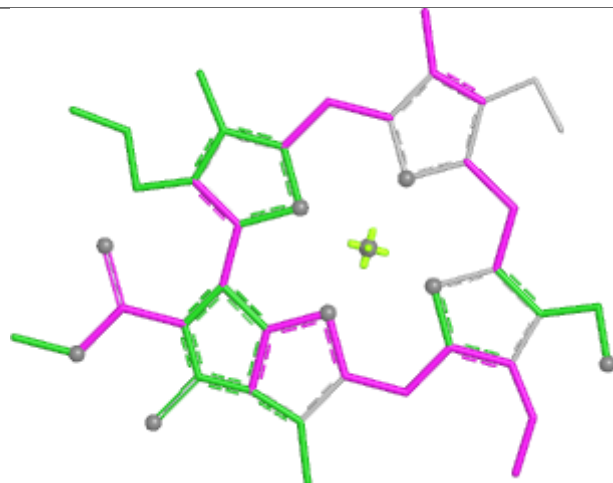




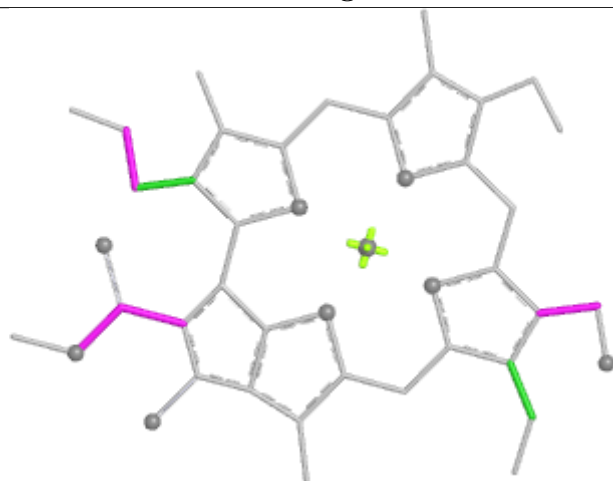
Ligand CHL U 606



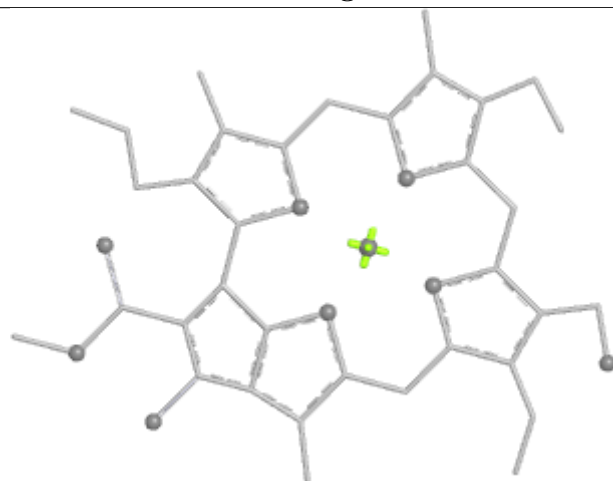
Bond lengths



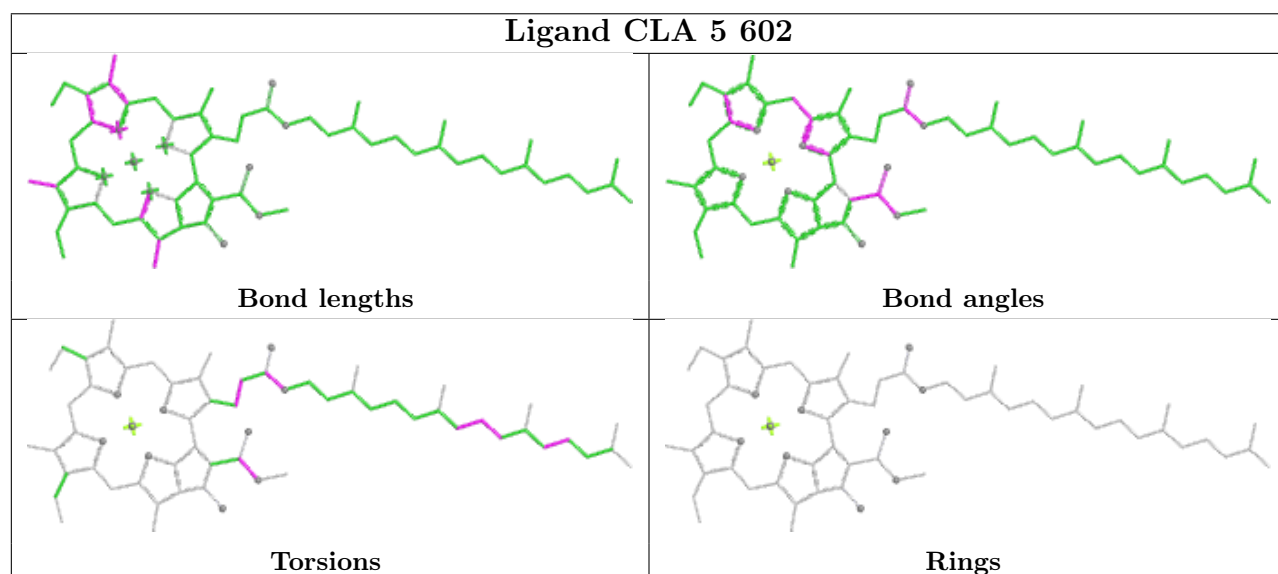
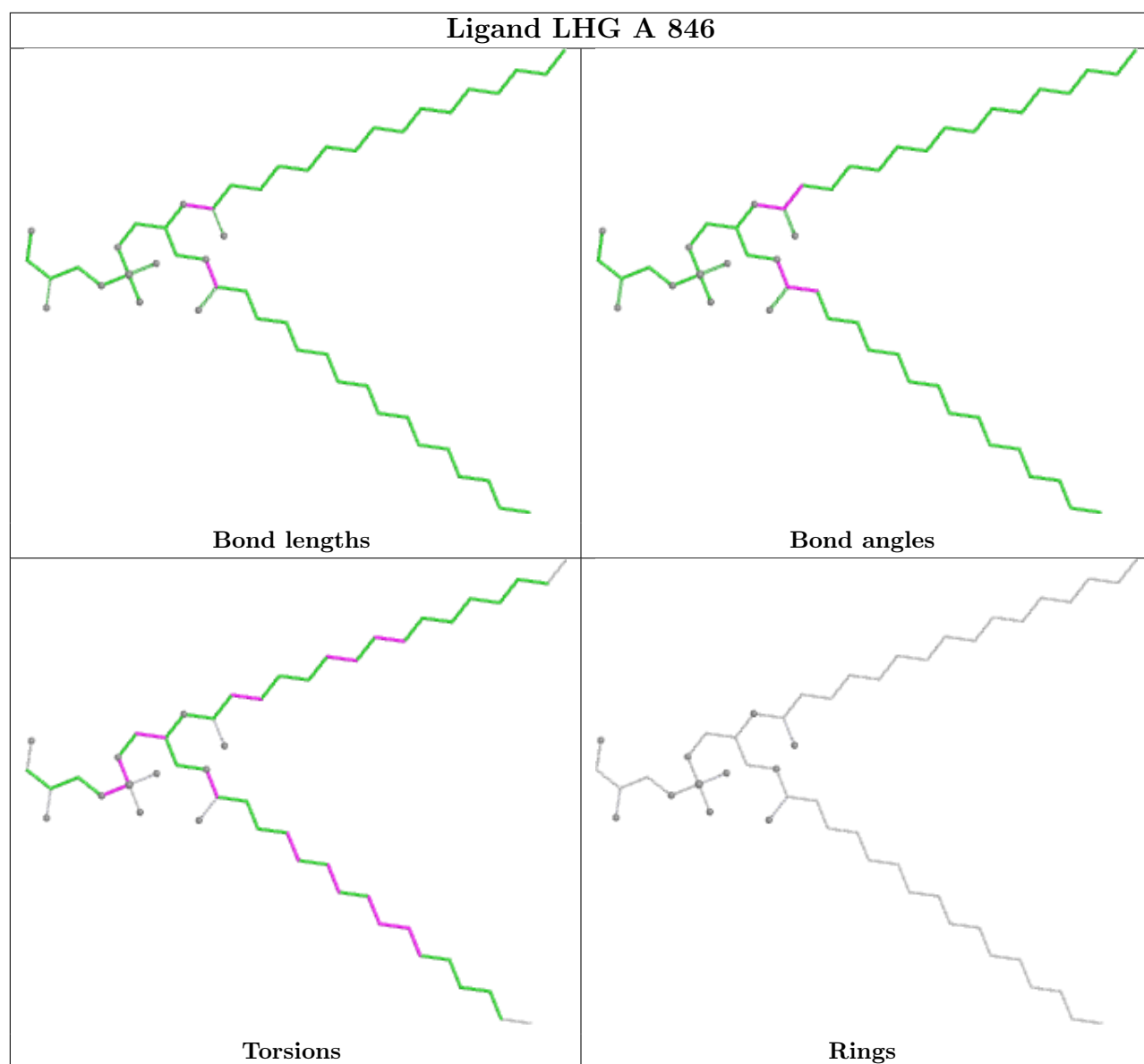
Bond angles



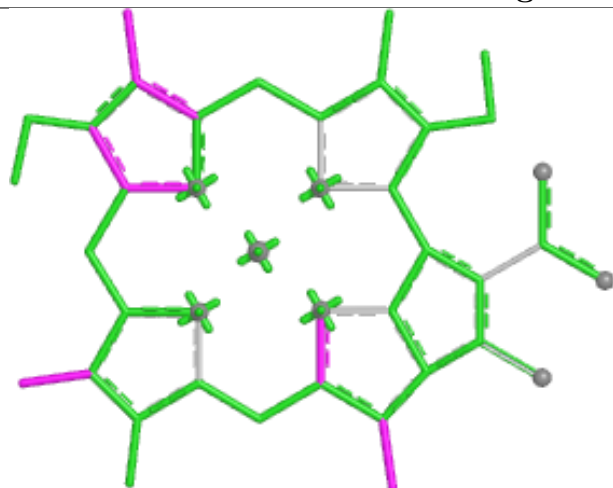
Torsions



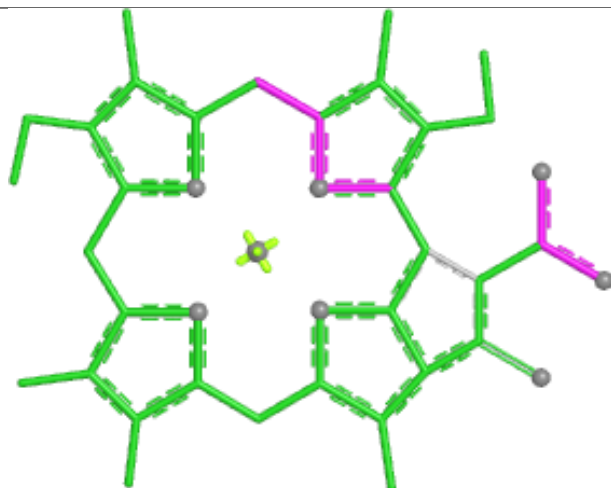
Rings



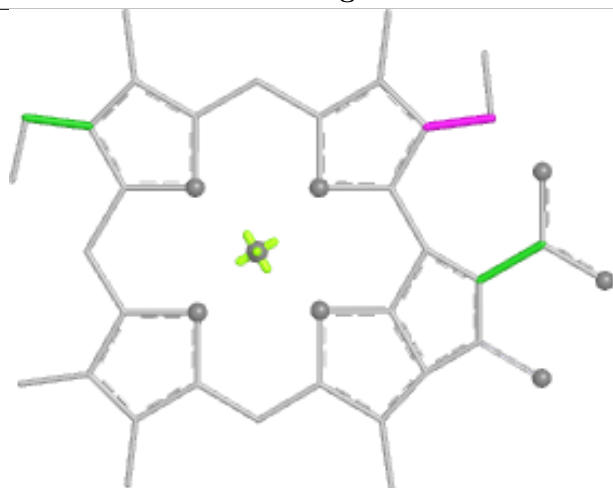
Ligand CLA L 306



Bond lengths



Bond angles

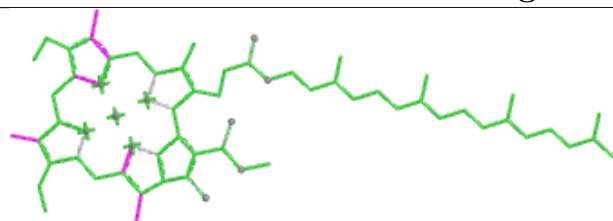


Torsions

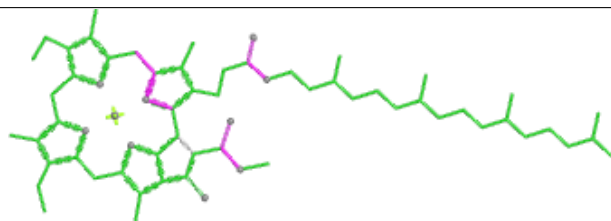


Rings

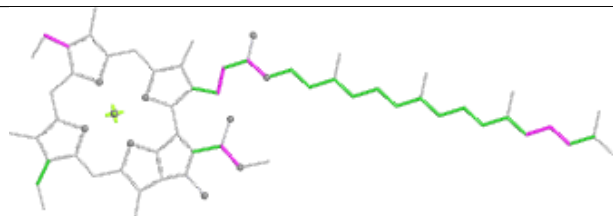
Ligand CLA 2 613



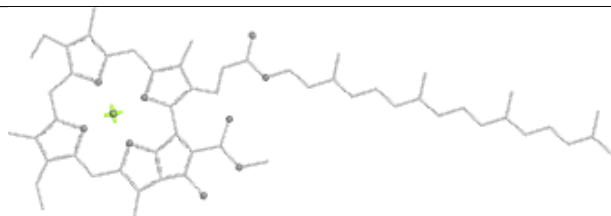
Bond lengths



Bond angles

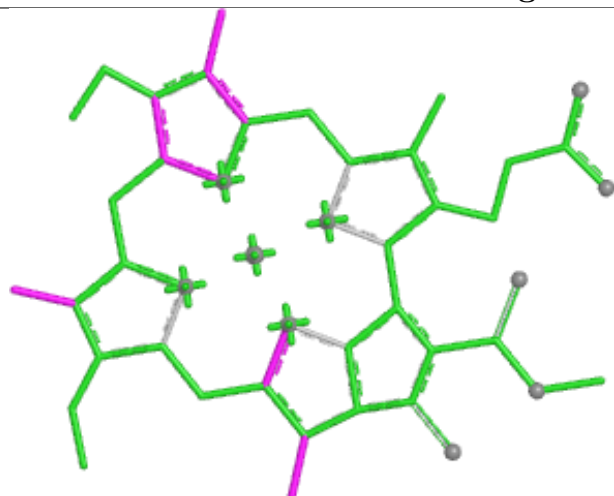


Torsions

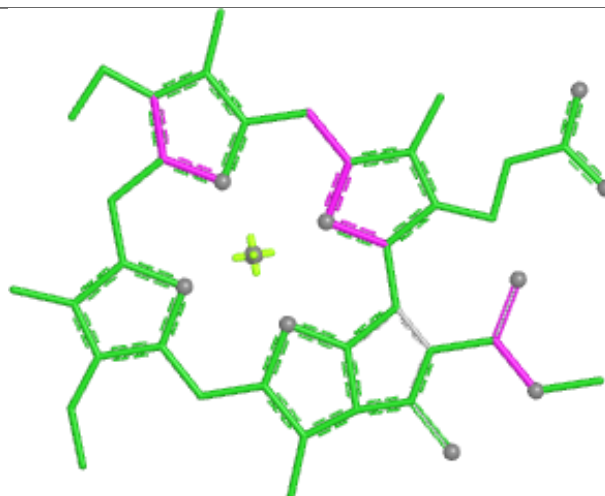


Rings

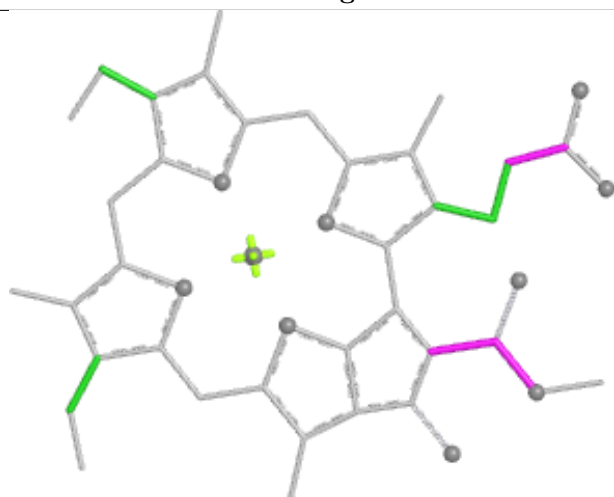
Ligand CLA 4 607



Bond lengths



Bond angles

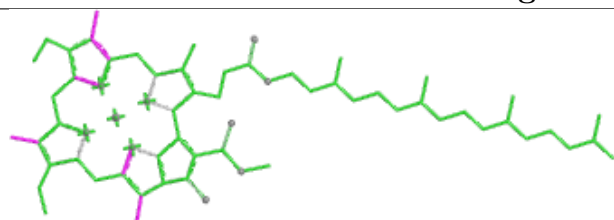


Torsions

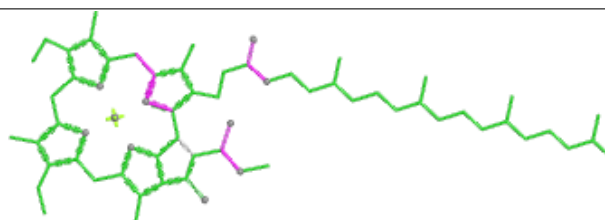


Rings

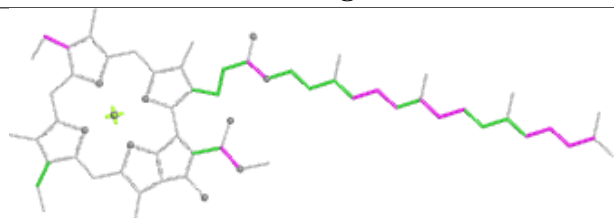
Ligand CLA 6 604



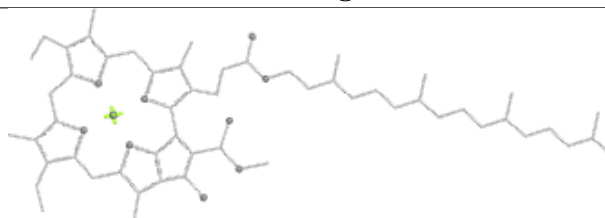
Bond lengths



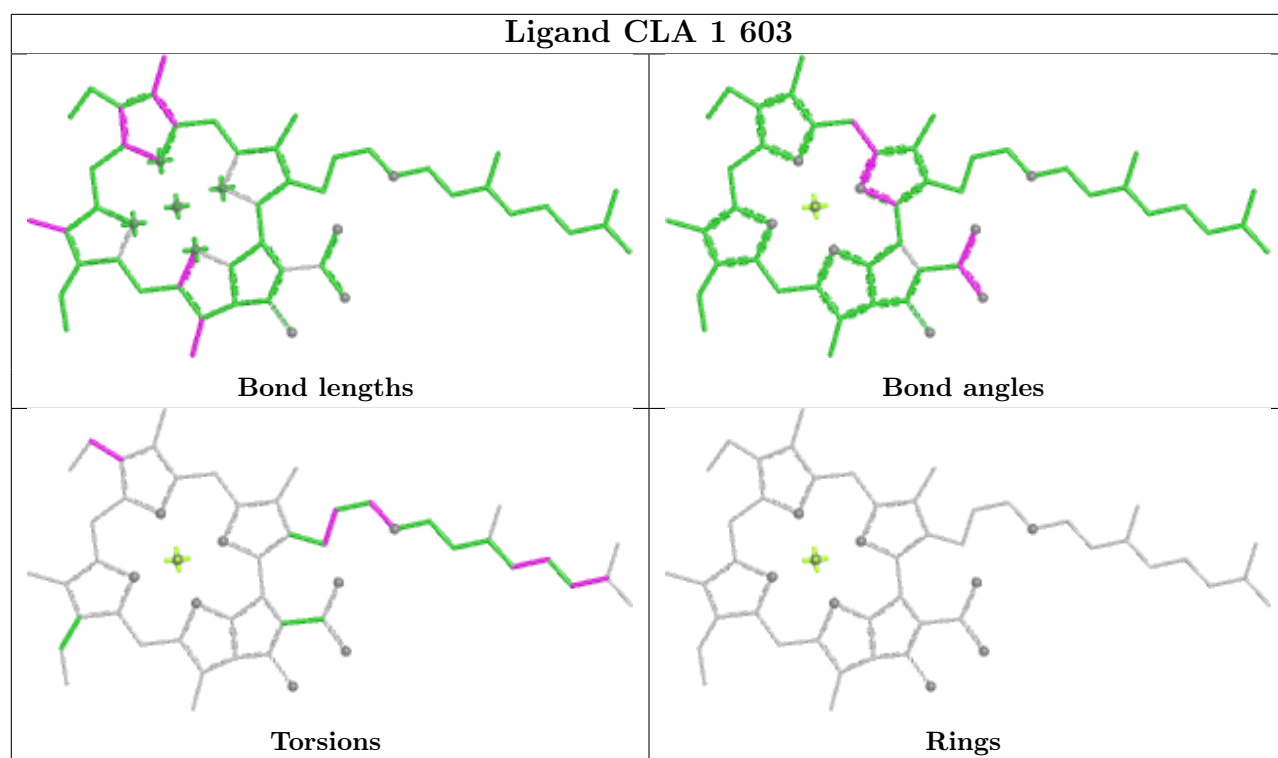
Bond angles



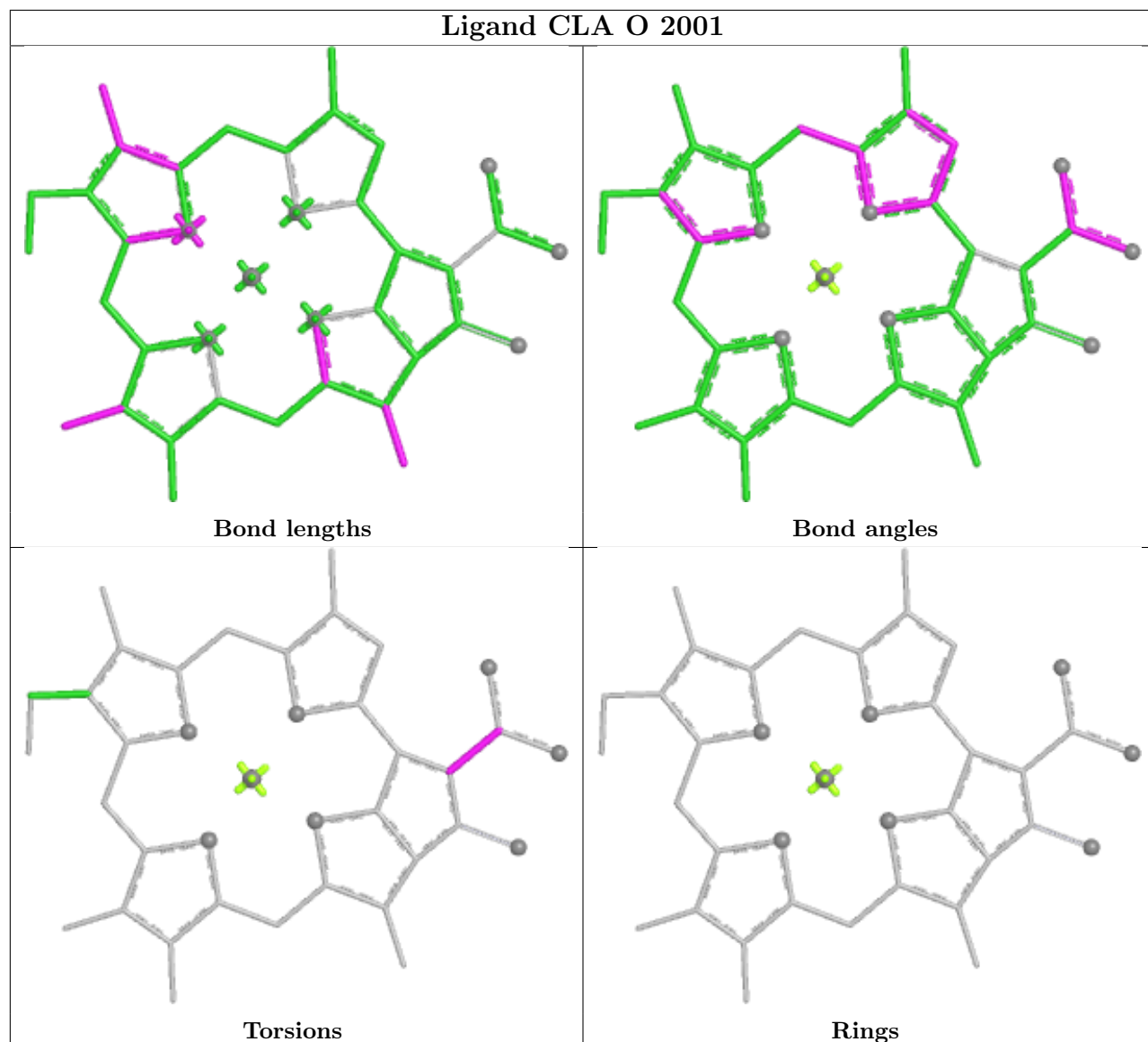
Torsions



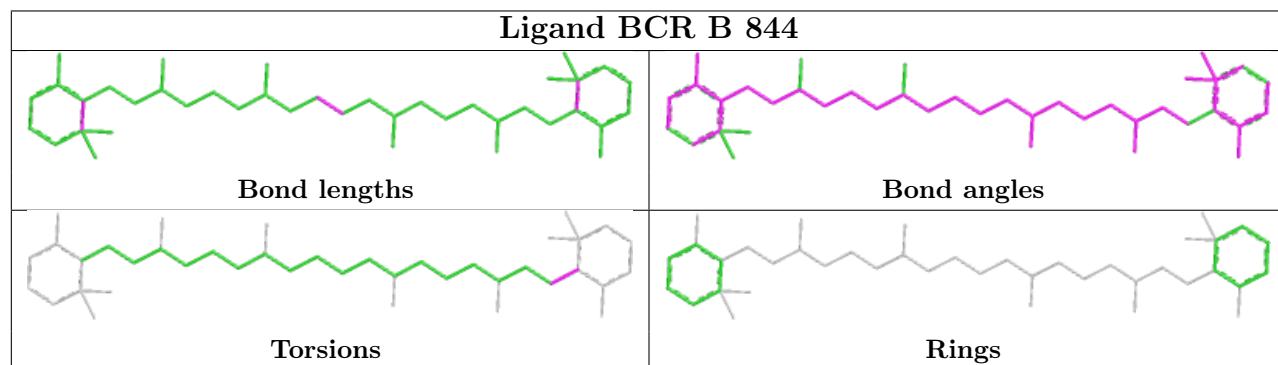
Rings

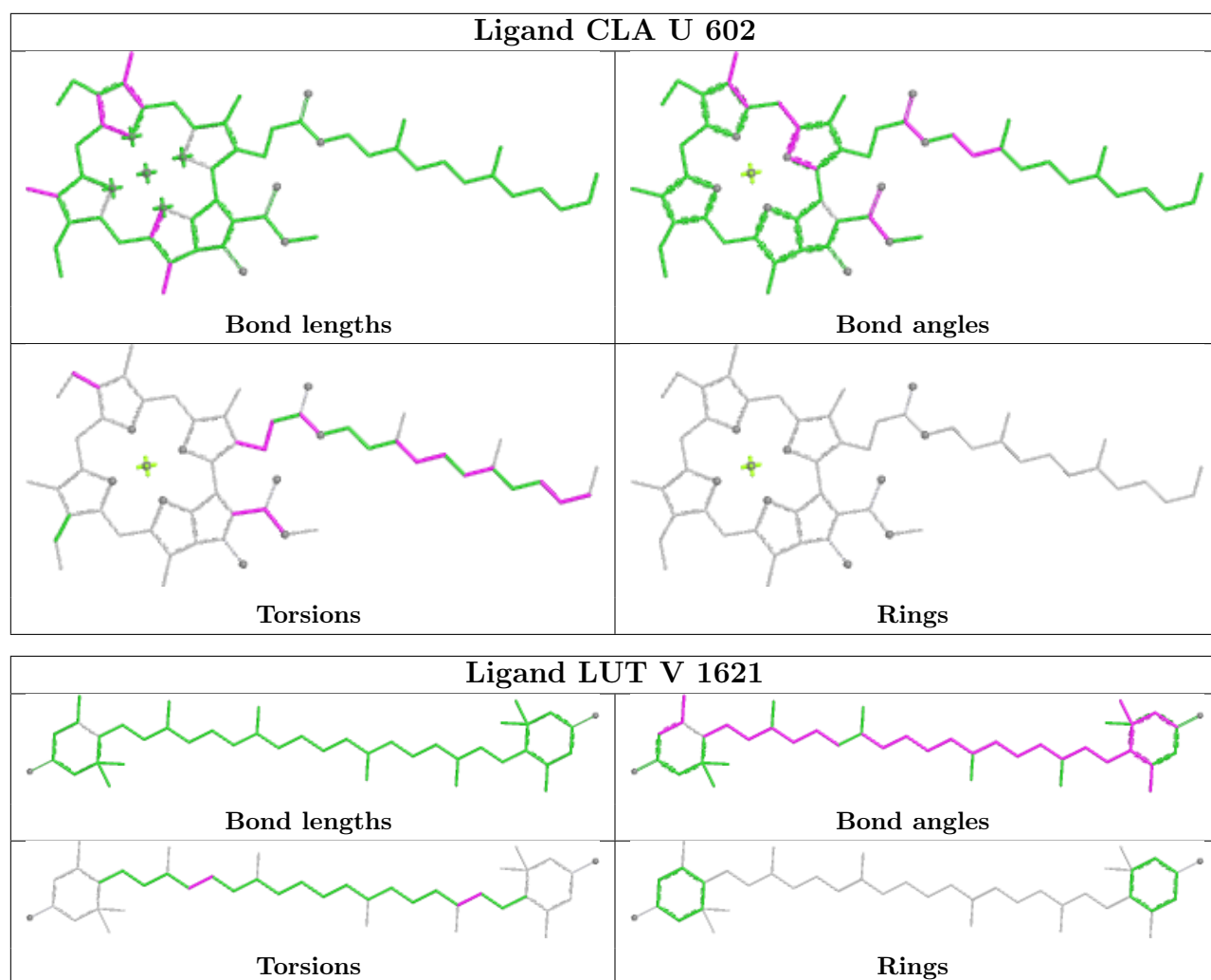


Ligand CLA O 2001

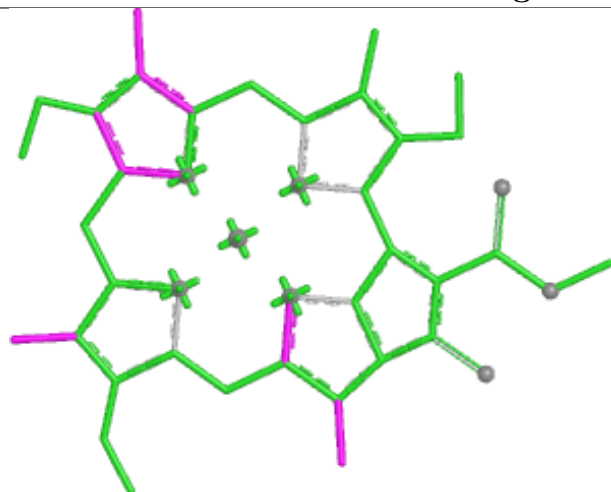


Ligand BCR B 844

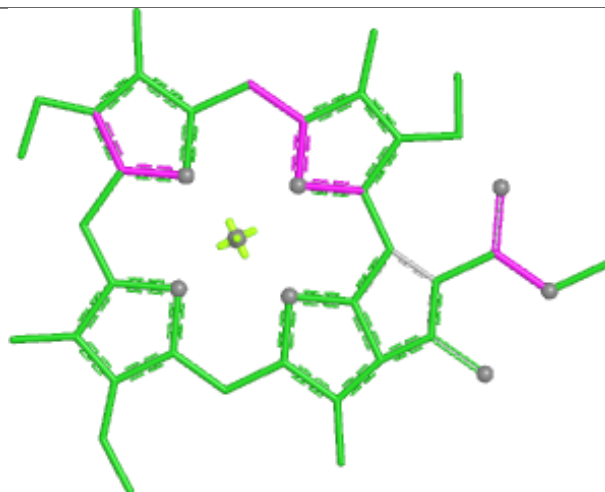




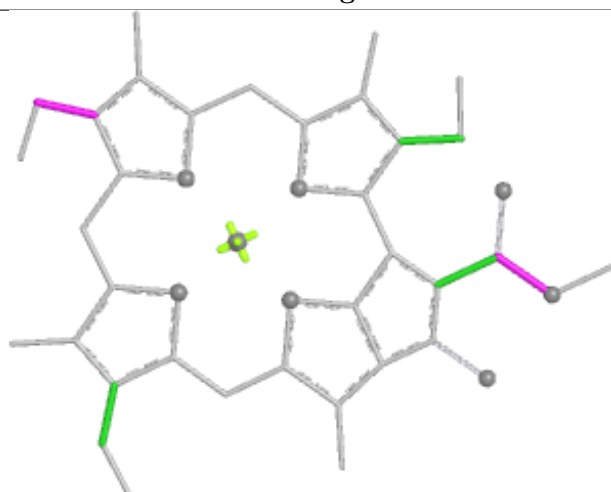
Ligand CLA G 203



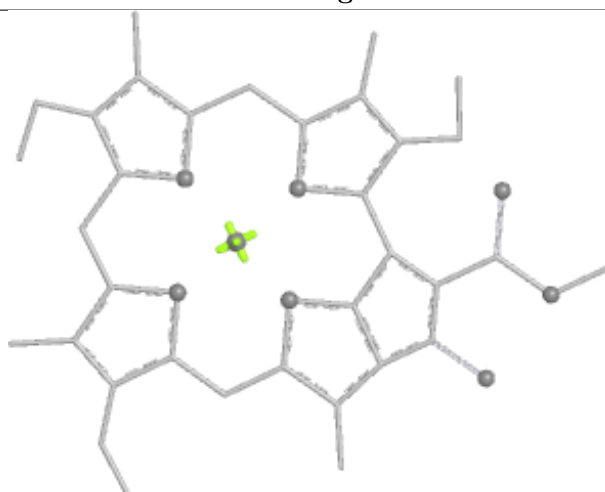
Bond lengths



Bond angles

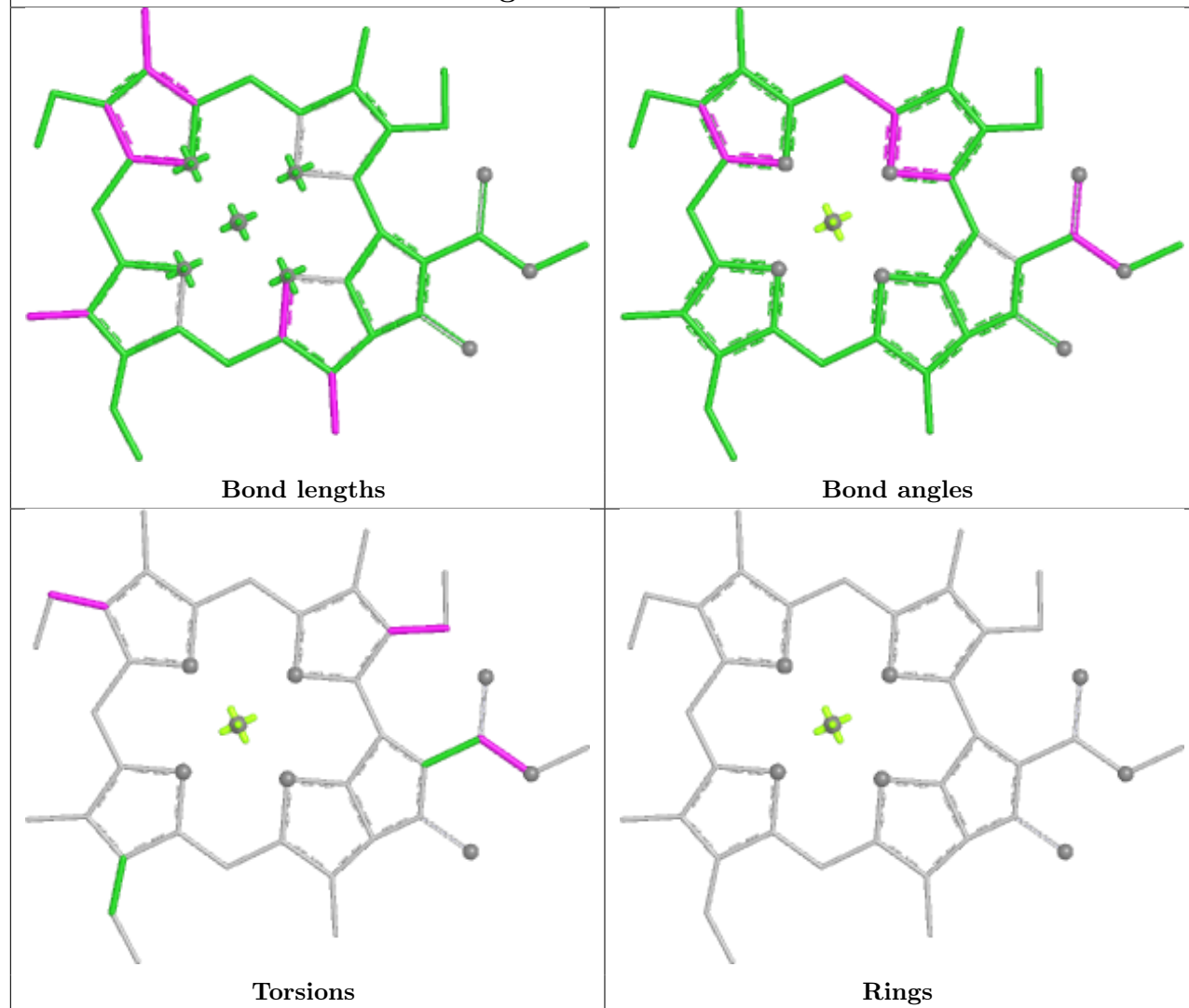


Torsions

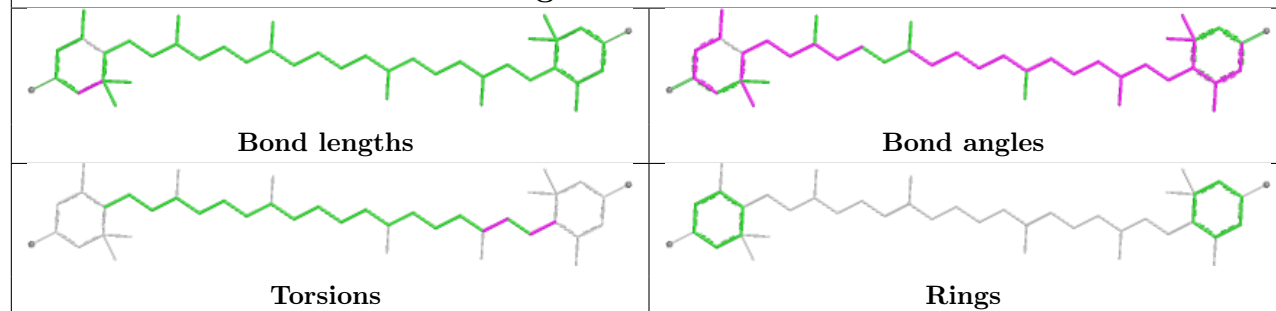


Rings

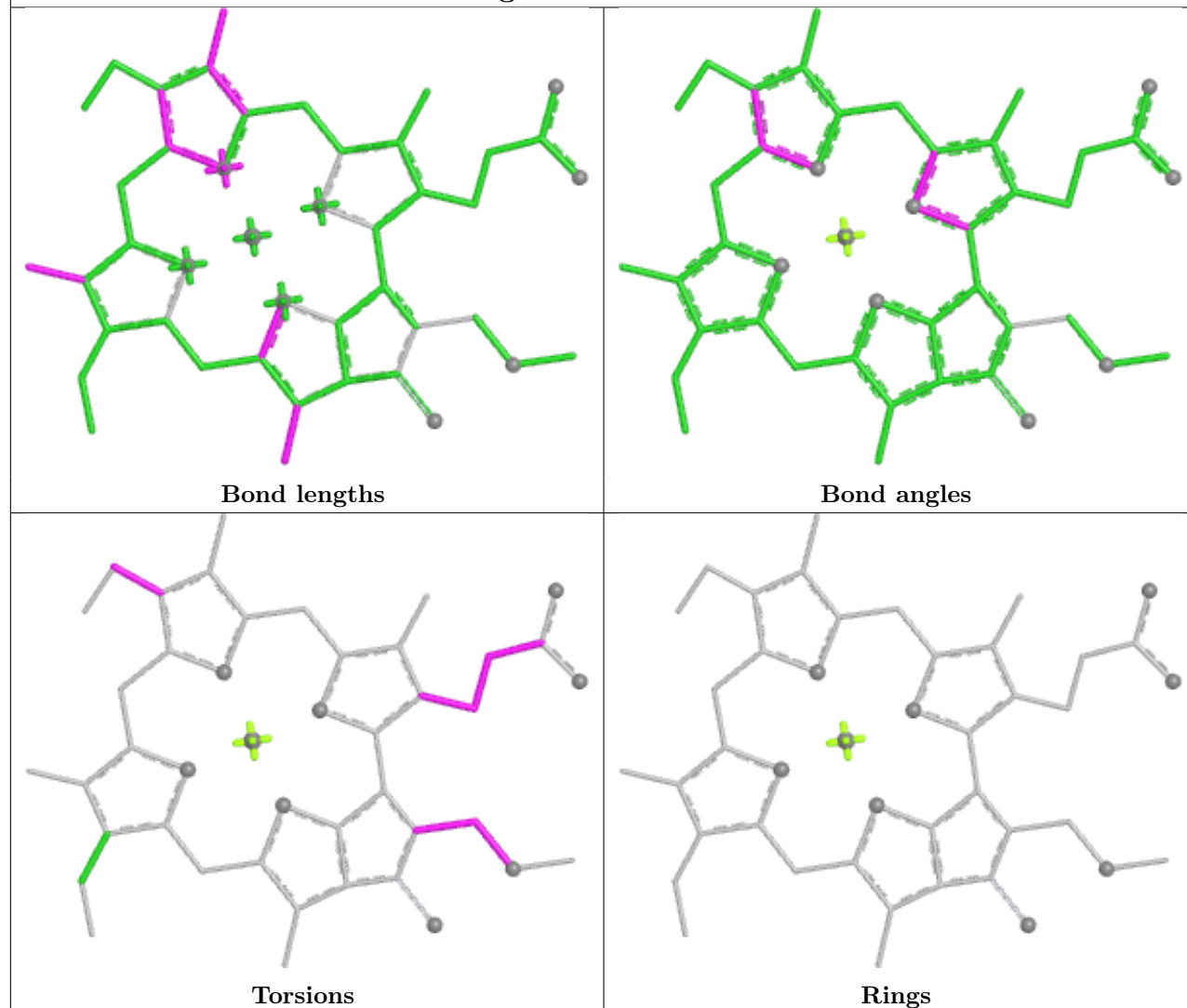
Ligand CLA J 101



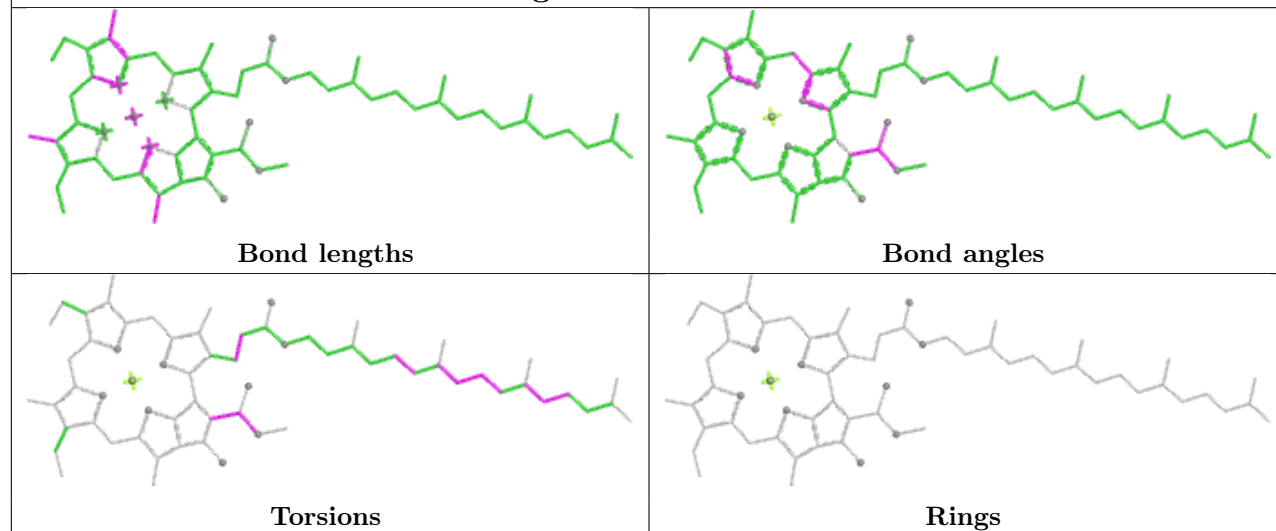
Ligand LUT 6 619

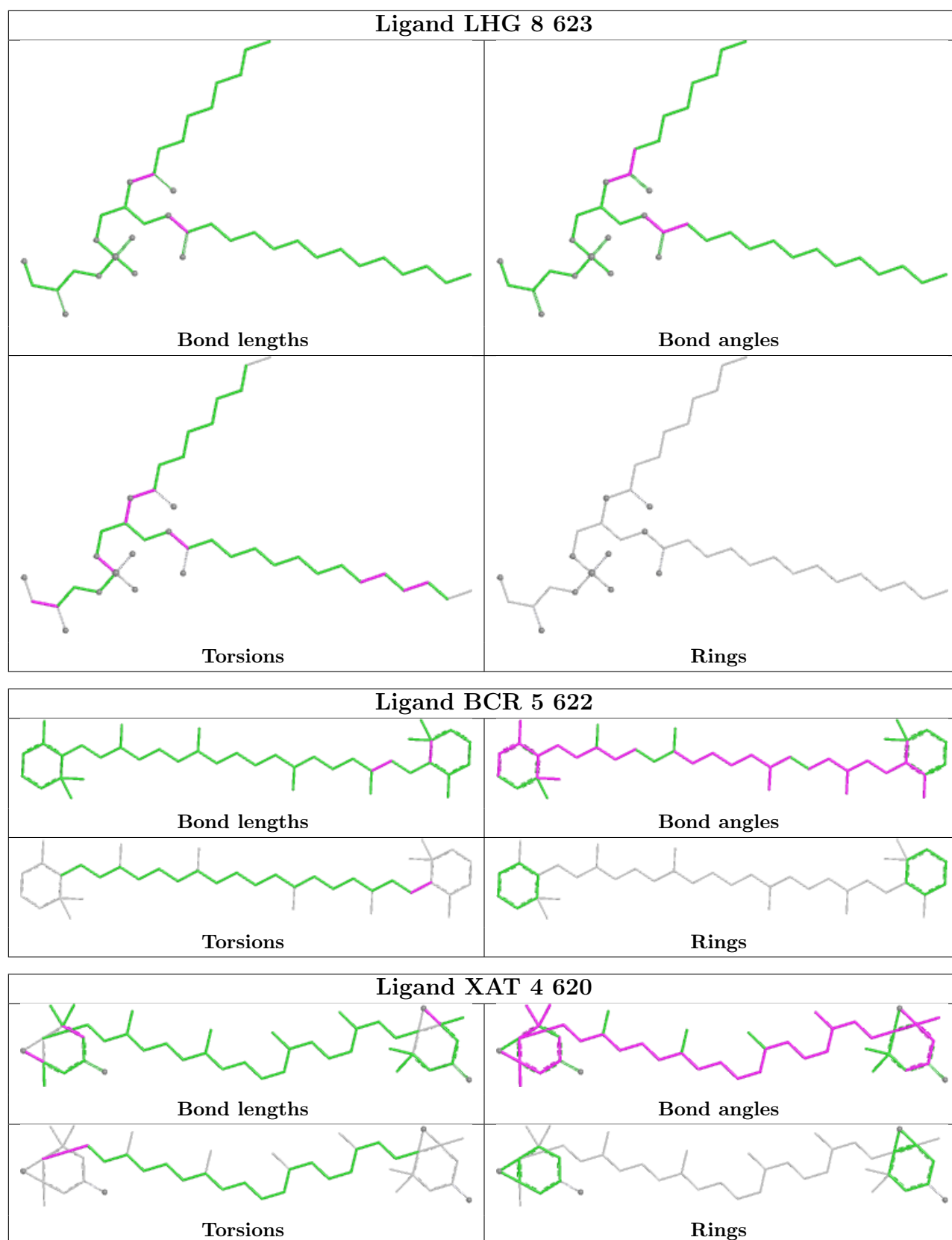


Ligand CLA a 606

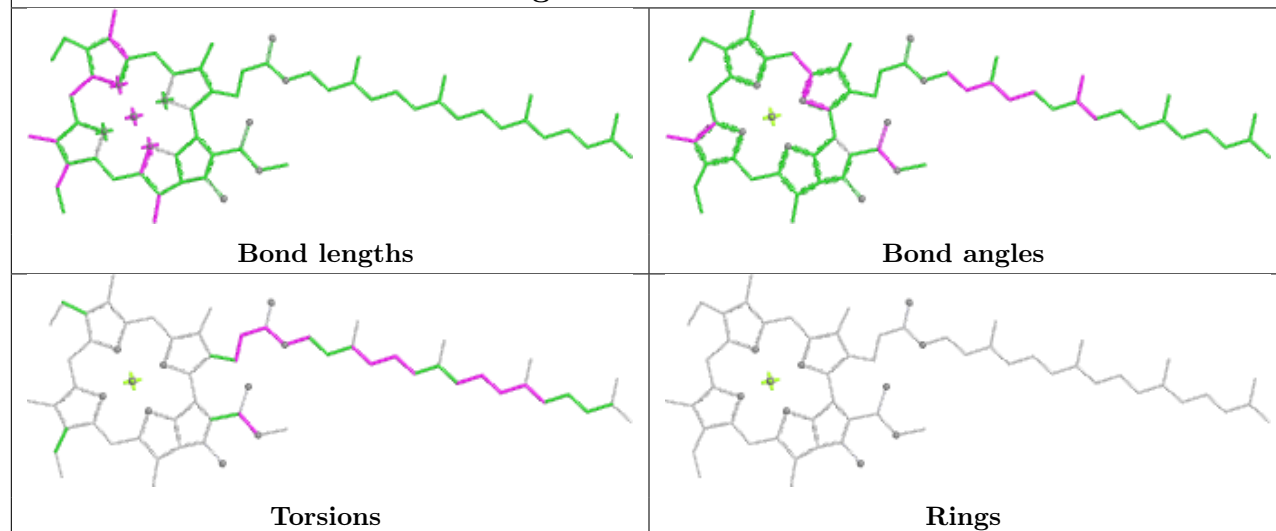


Ligand CLA B 824

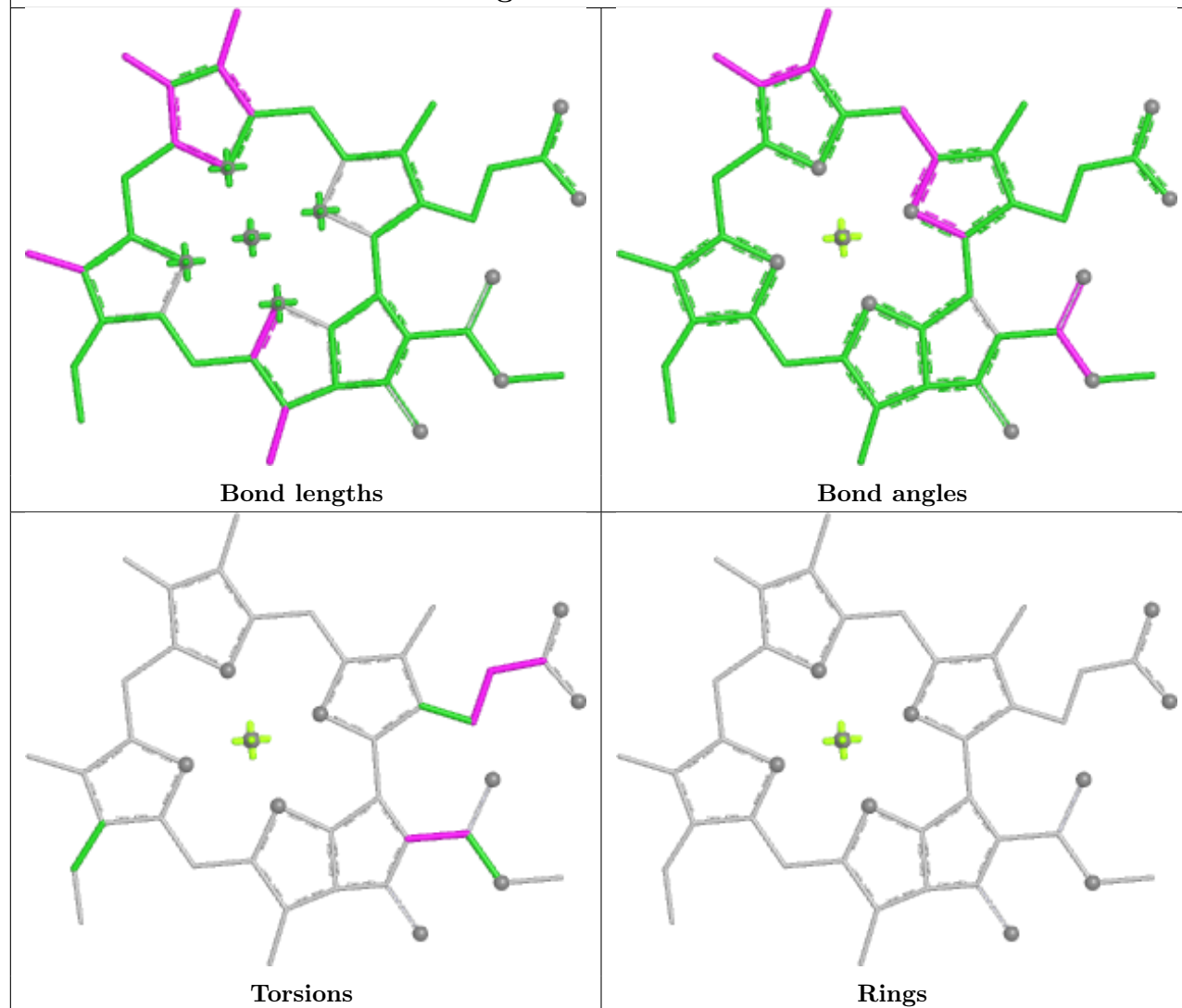


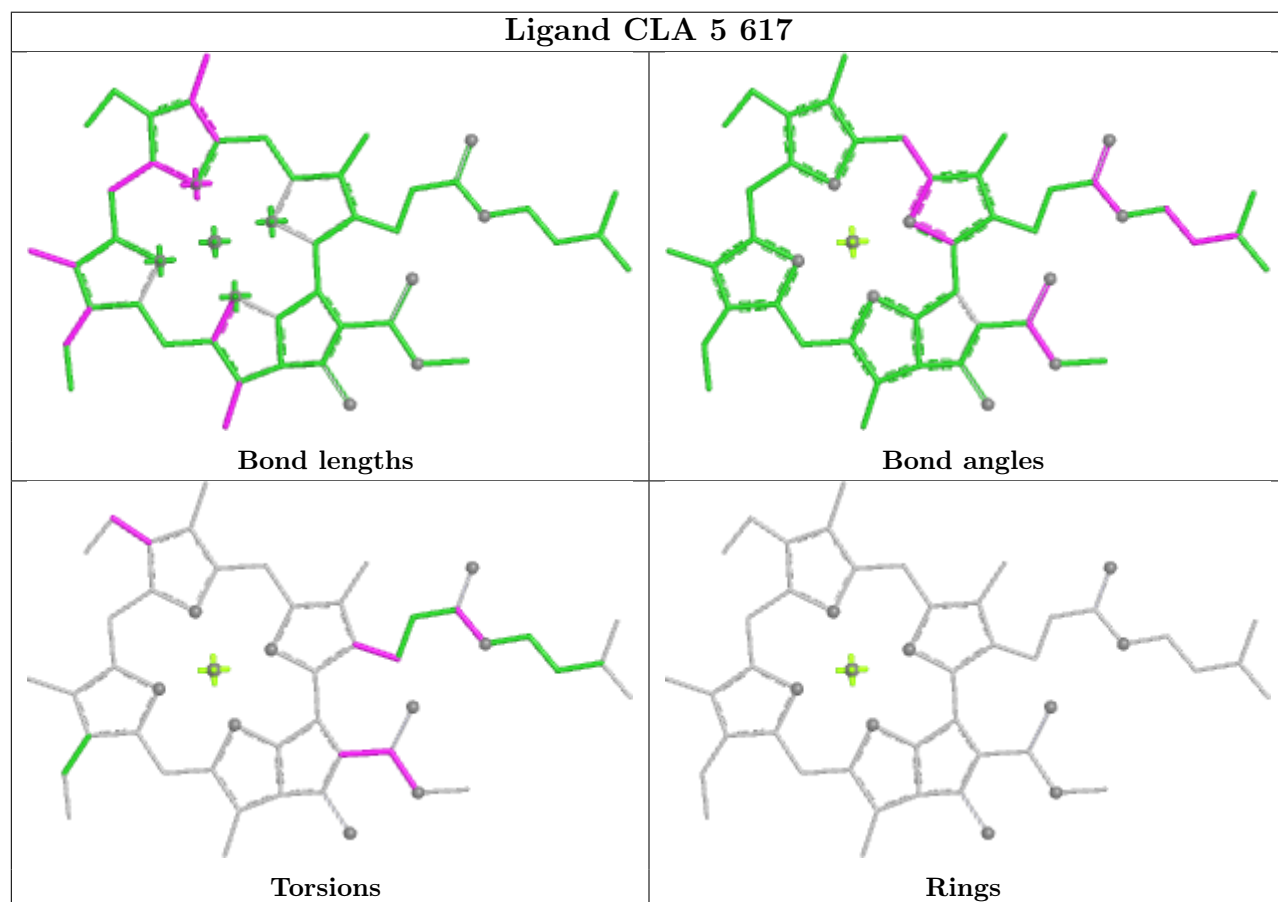
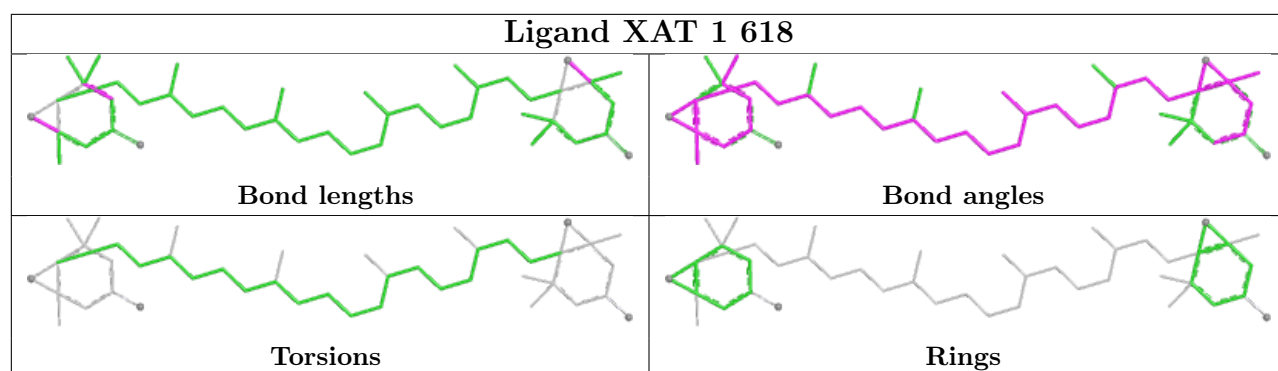


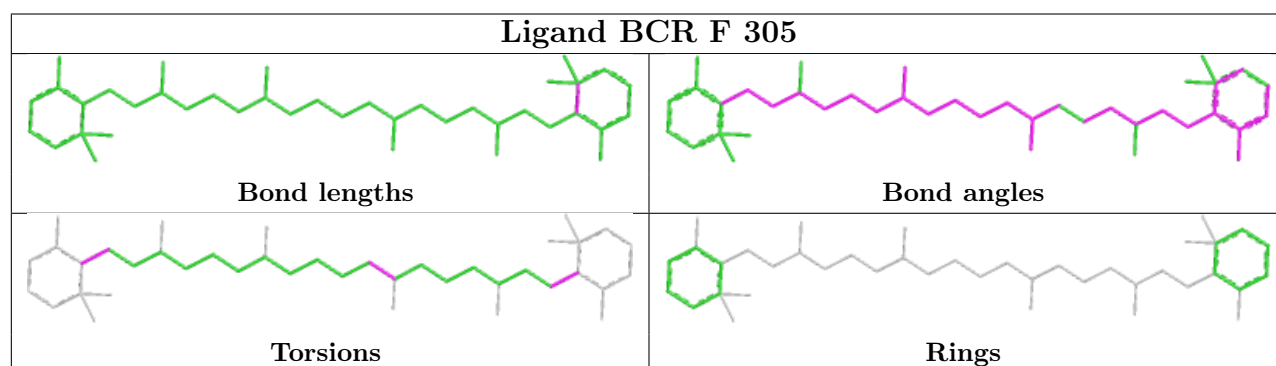
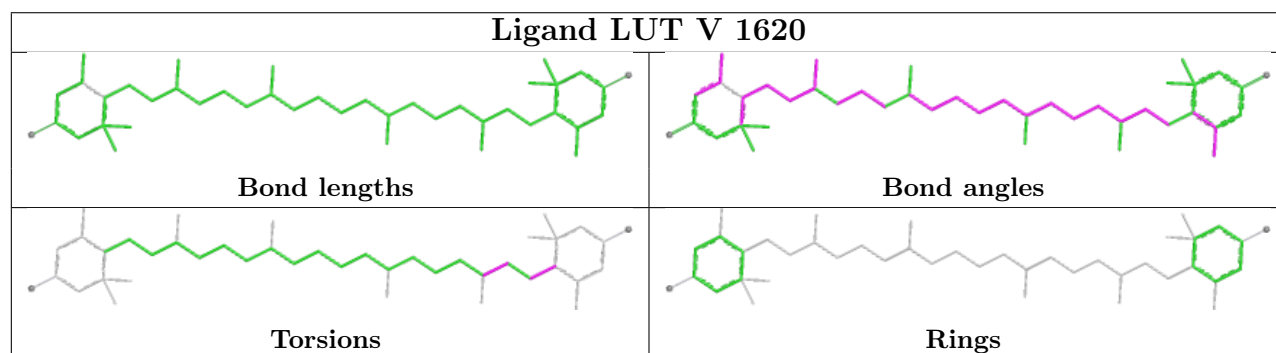
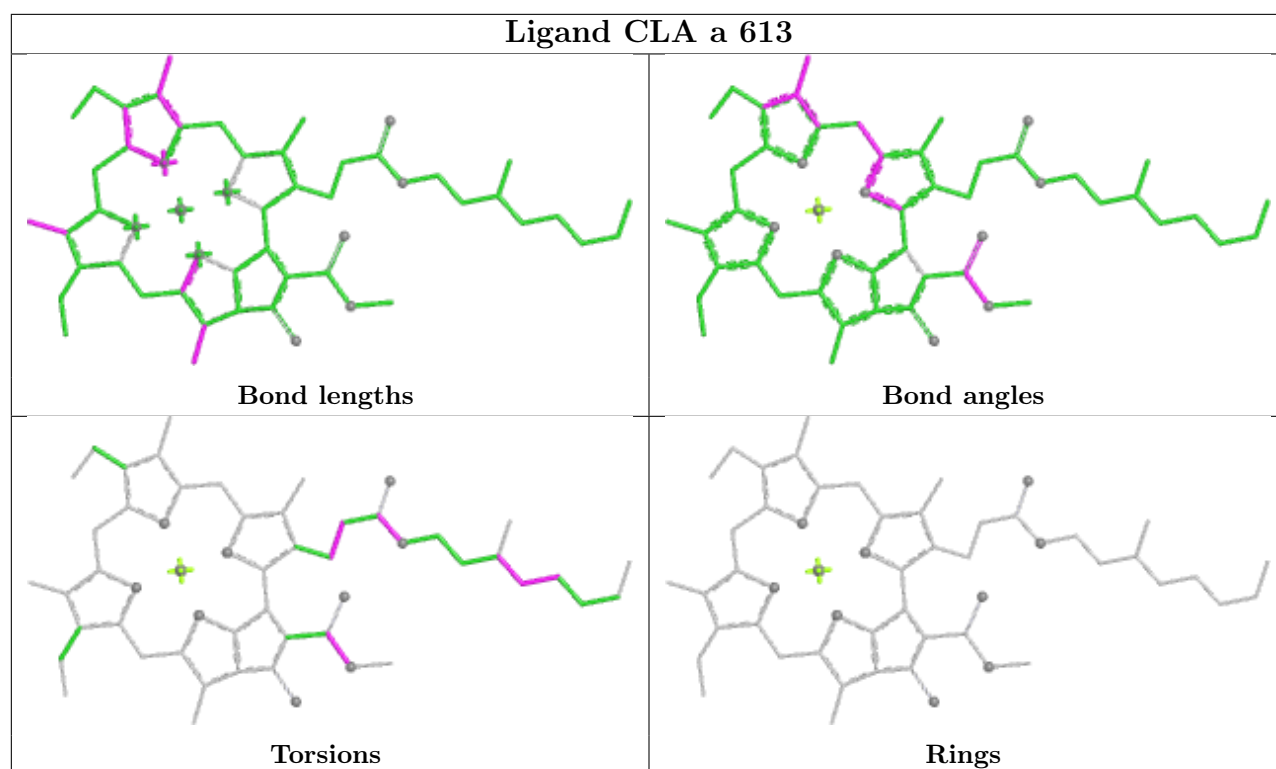
Ligand CLA B 806



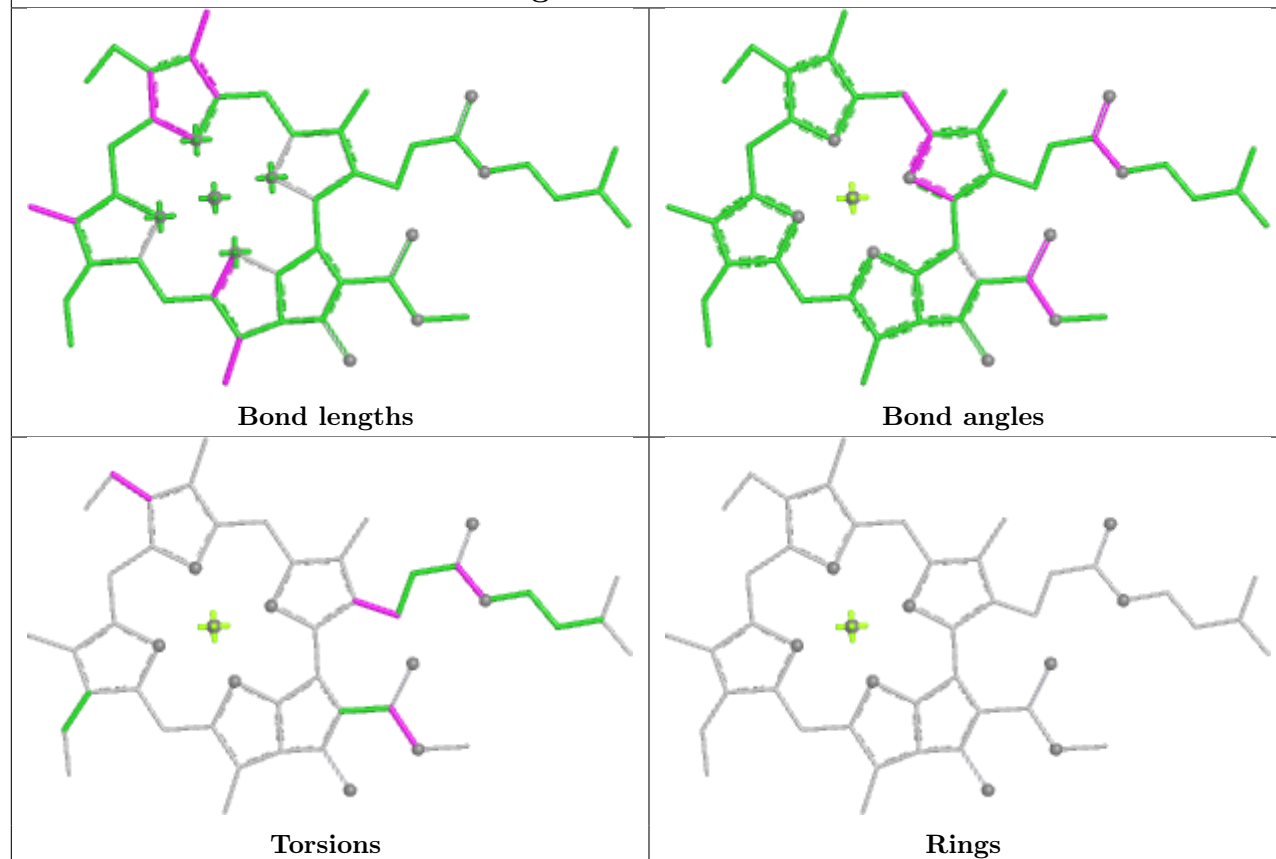
Ligand CLA 8 603



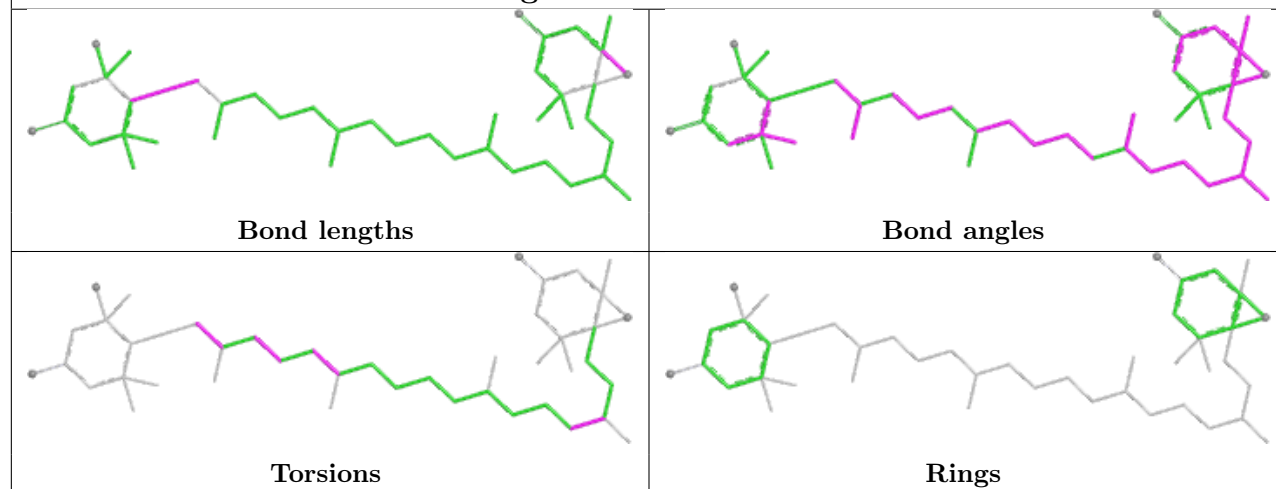


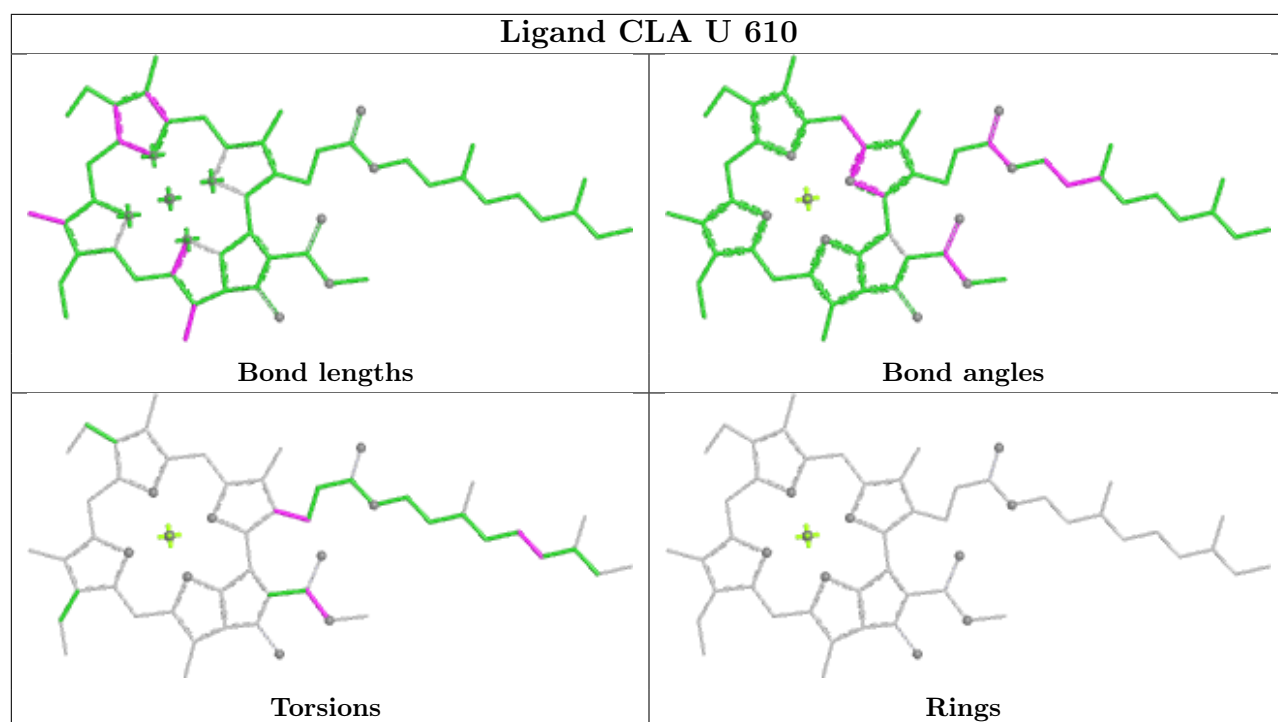


Ligand CLA Y 604

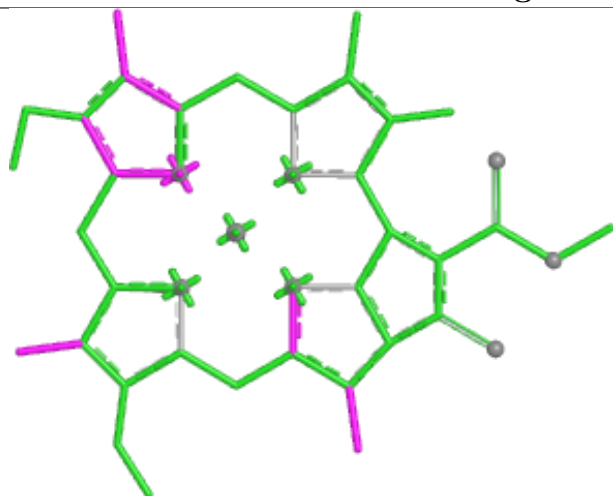


Ligand NEX V 1623

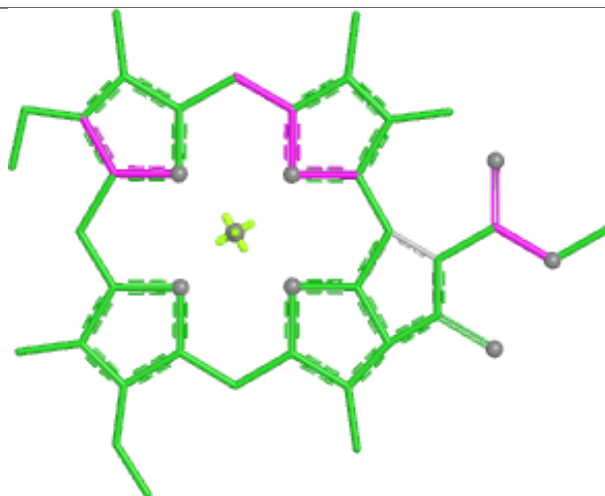




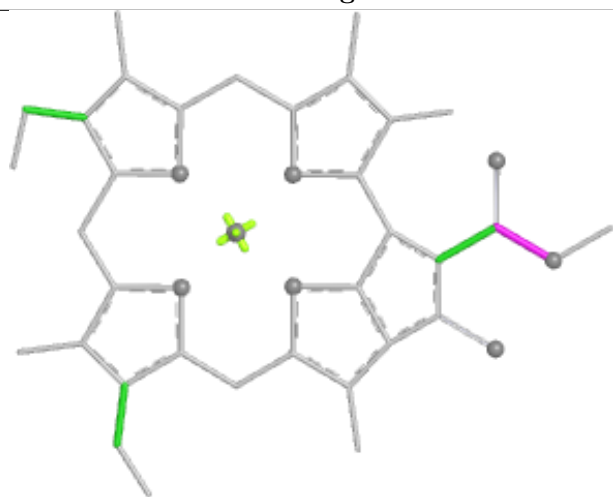
Ligand CLA B 804



Bond lengths



Bond angles

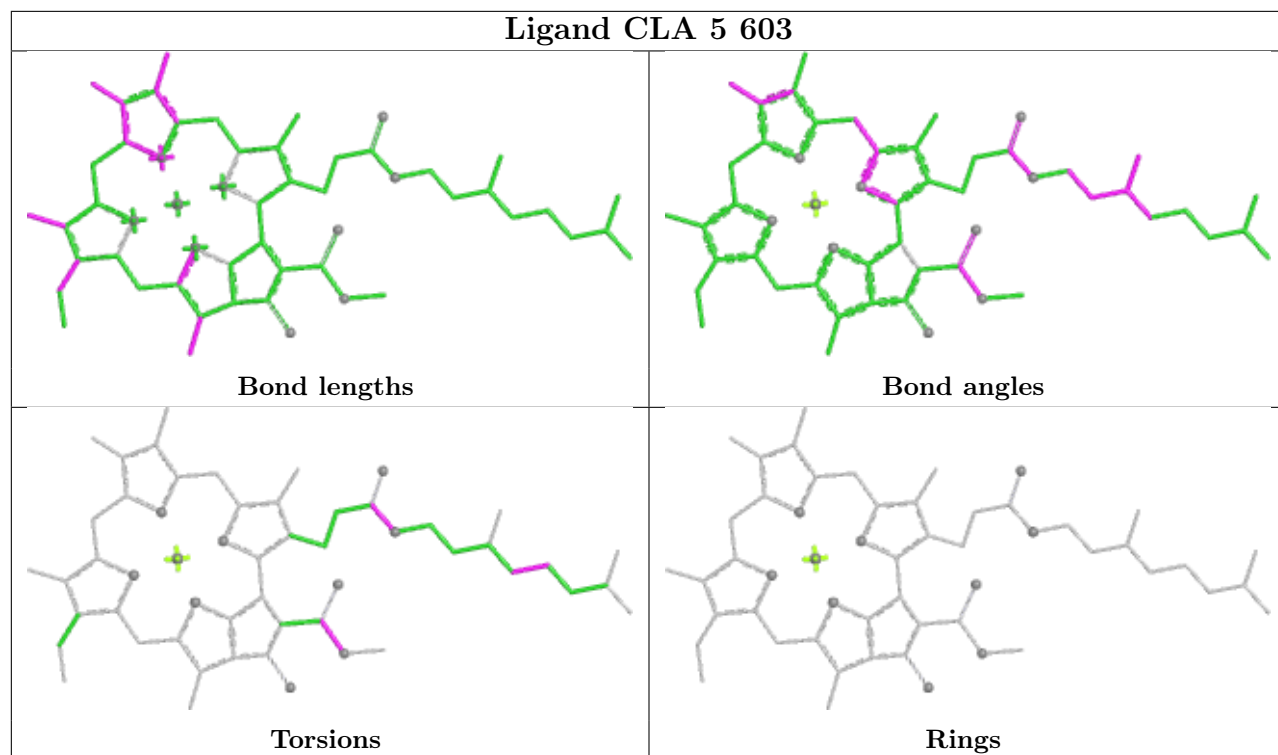


Torsions

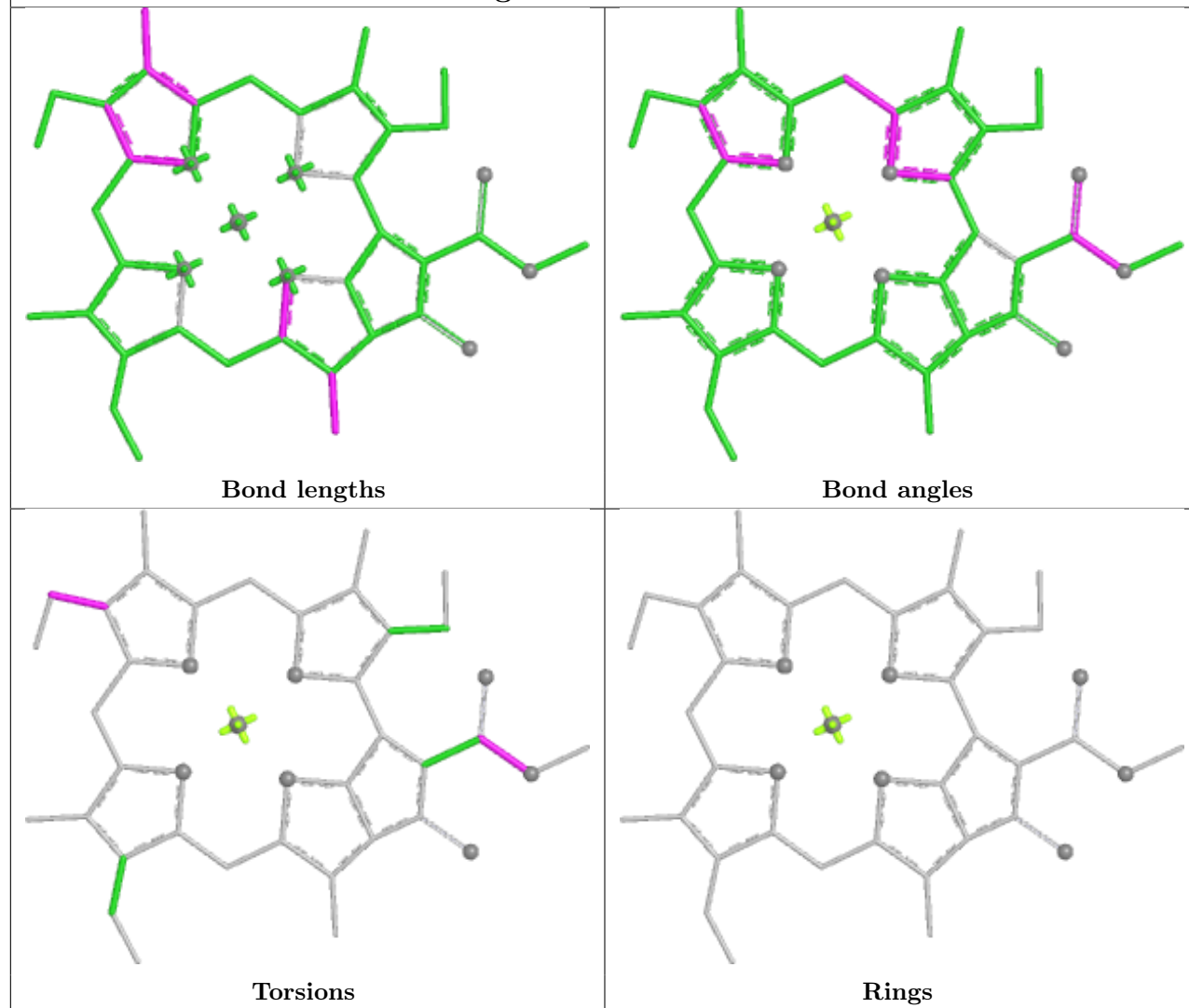


Rings

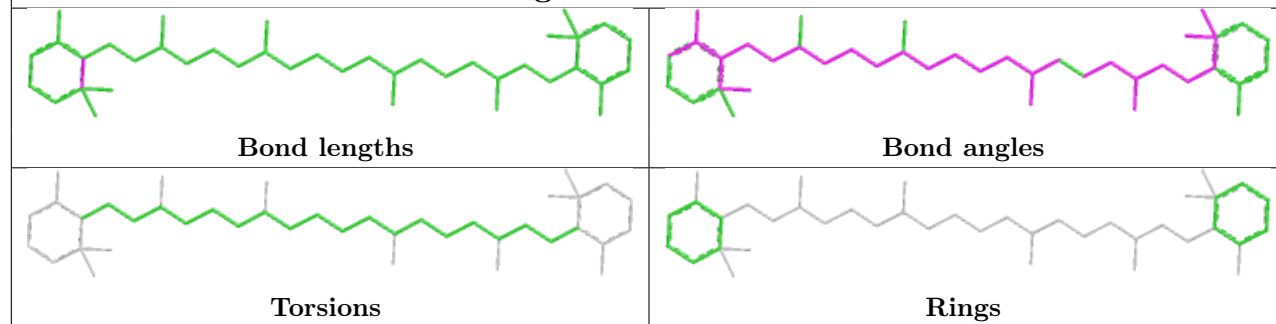
Ligand CLA 5 603



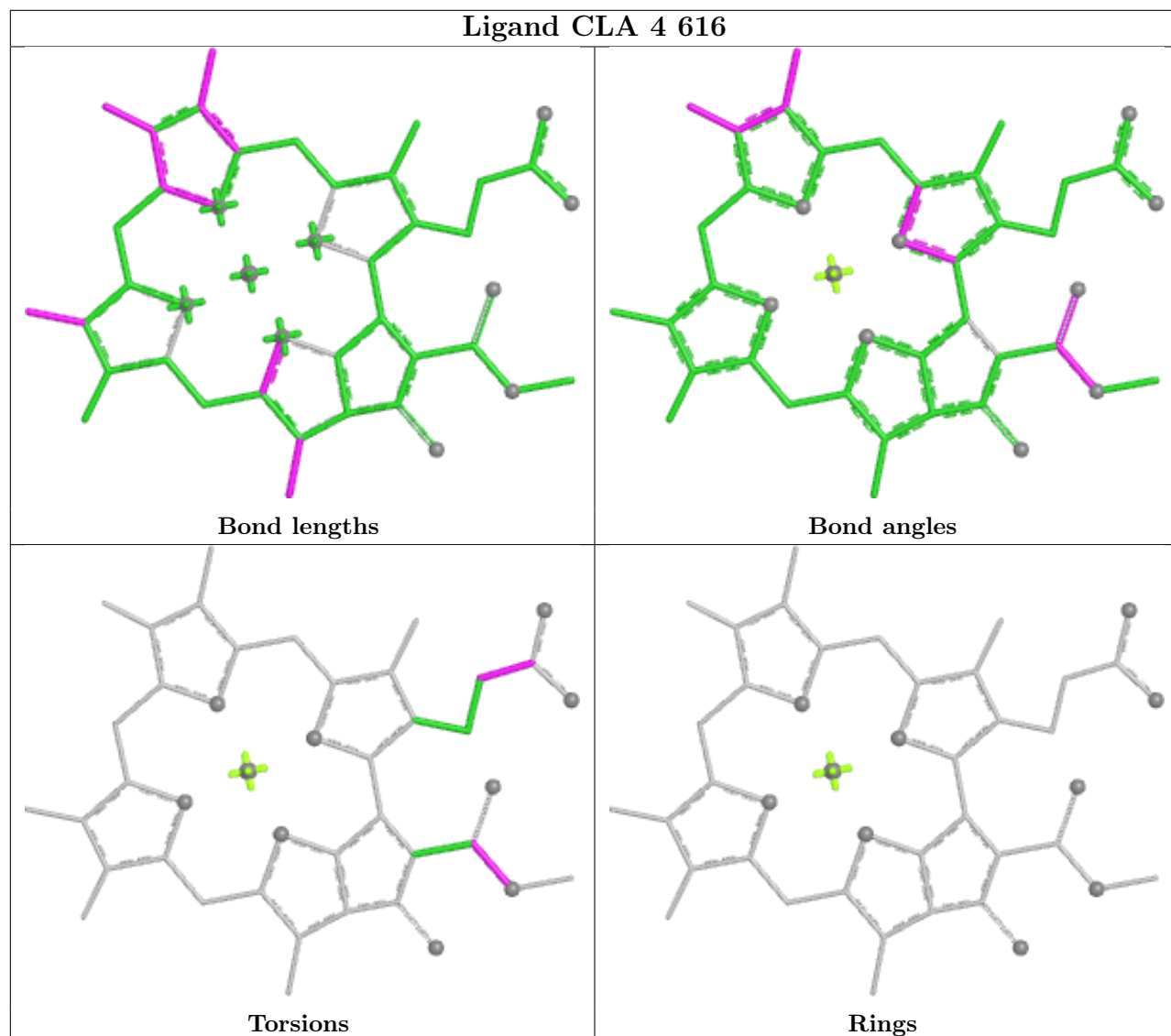
Ligand CLA U 612



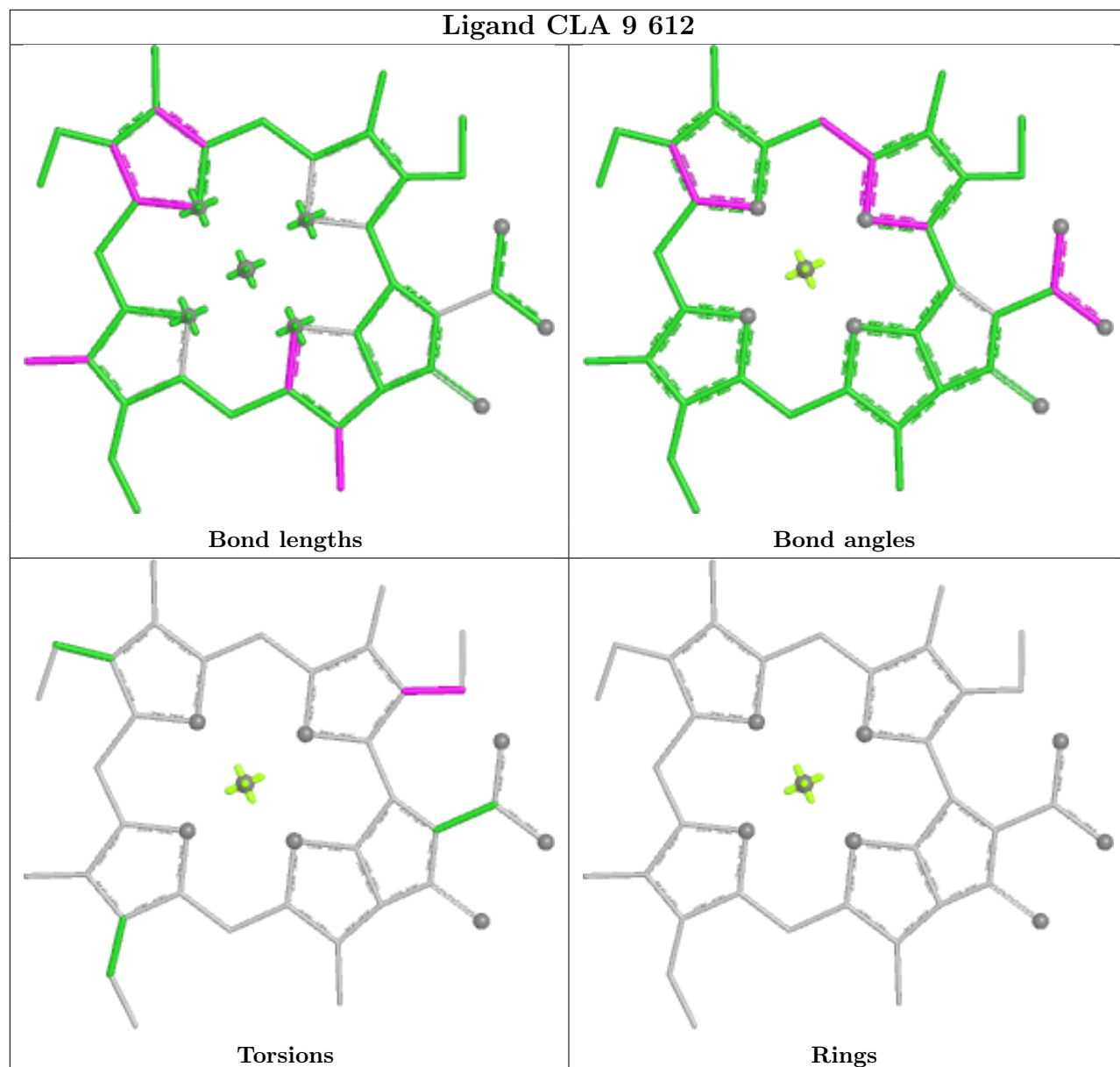
Ligand BCR 3 621



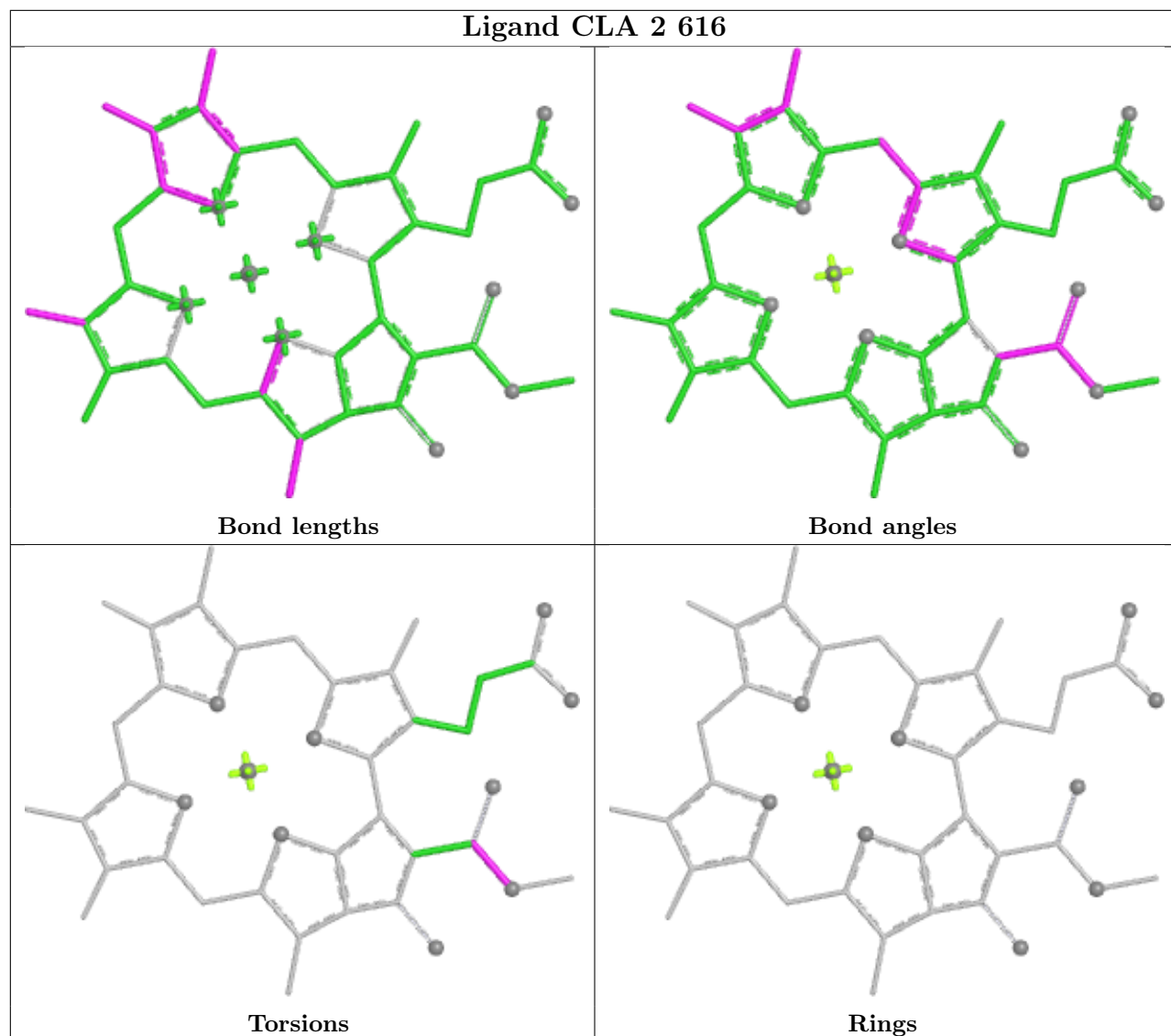
Ligand CLA 4 616



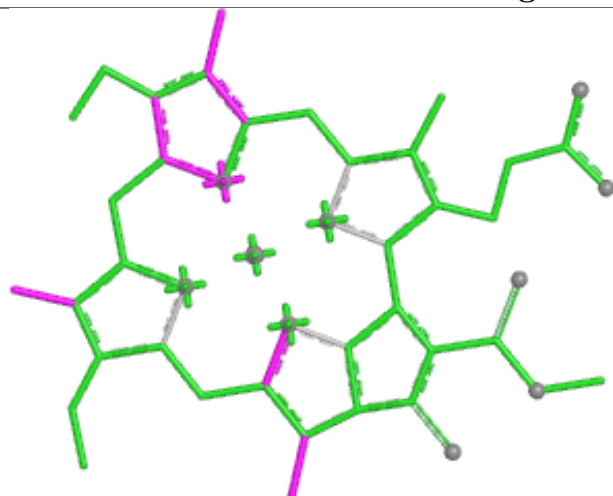
Ligand CLA 9 612



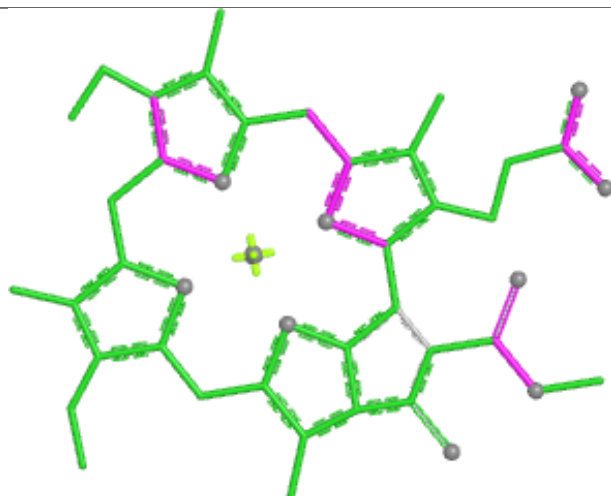
Ligand CLA 2 616



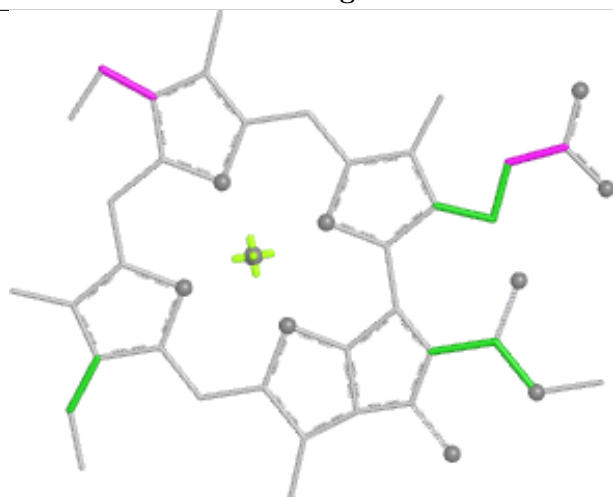
Ligand CLA 2 609



Bond lengths



Bond angles

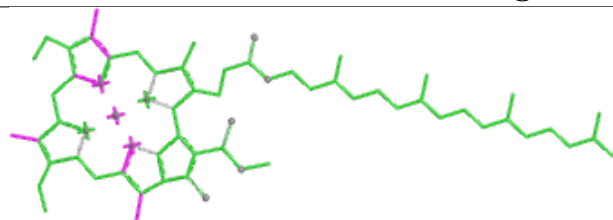


Torsions

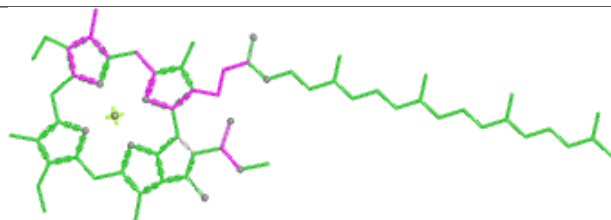


Rings

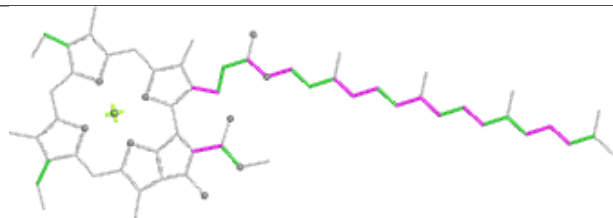
Ligand CLA A 828



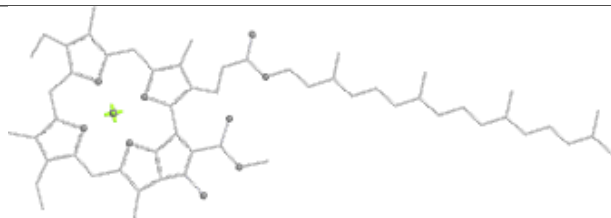
Bond lengths



Bond angles

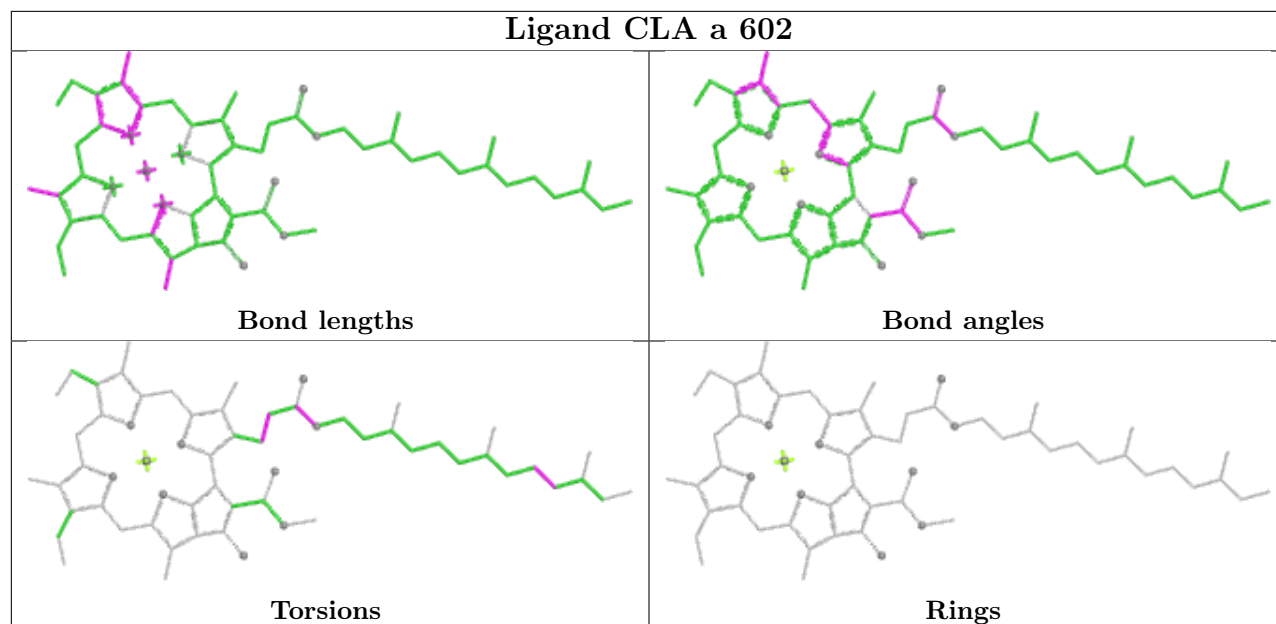


Torsions

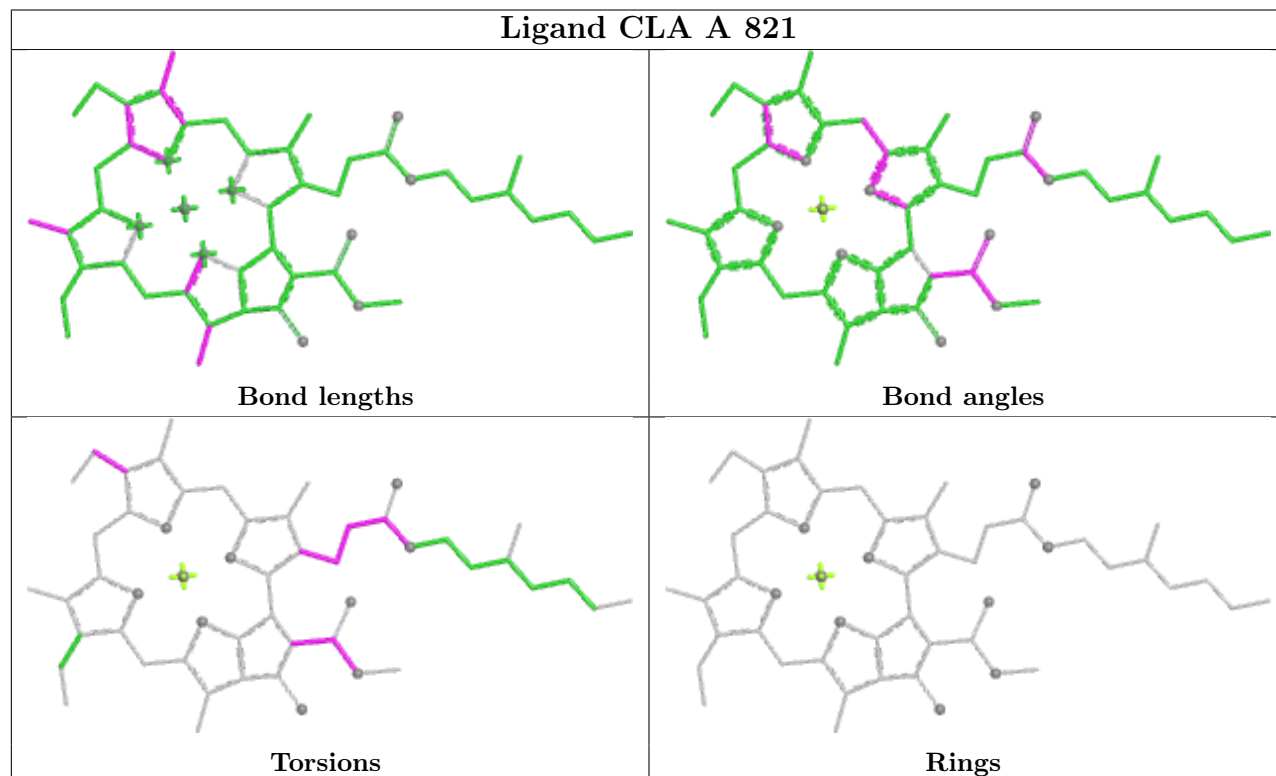


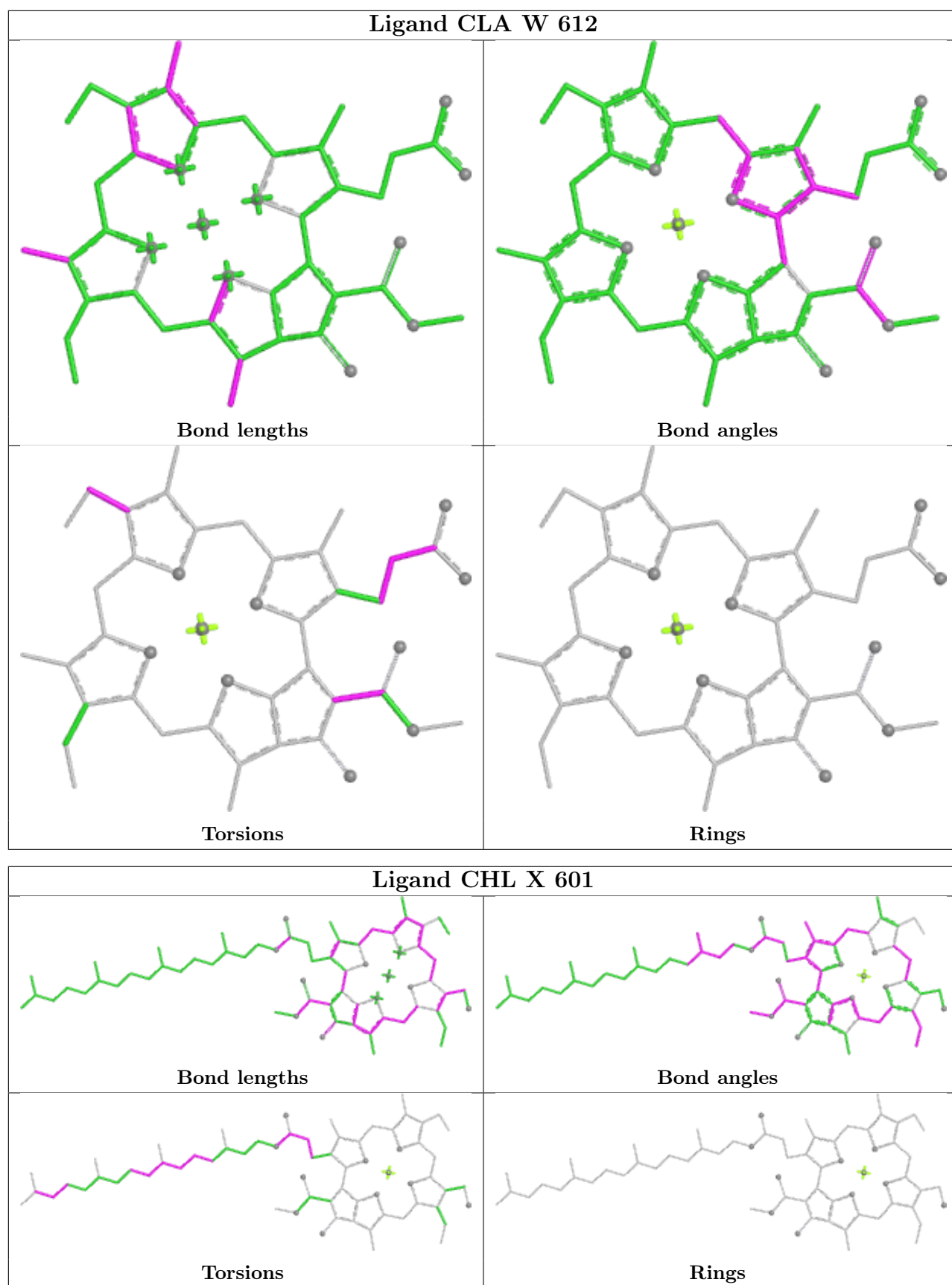
Rings

Ligand CLA a 602

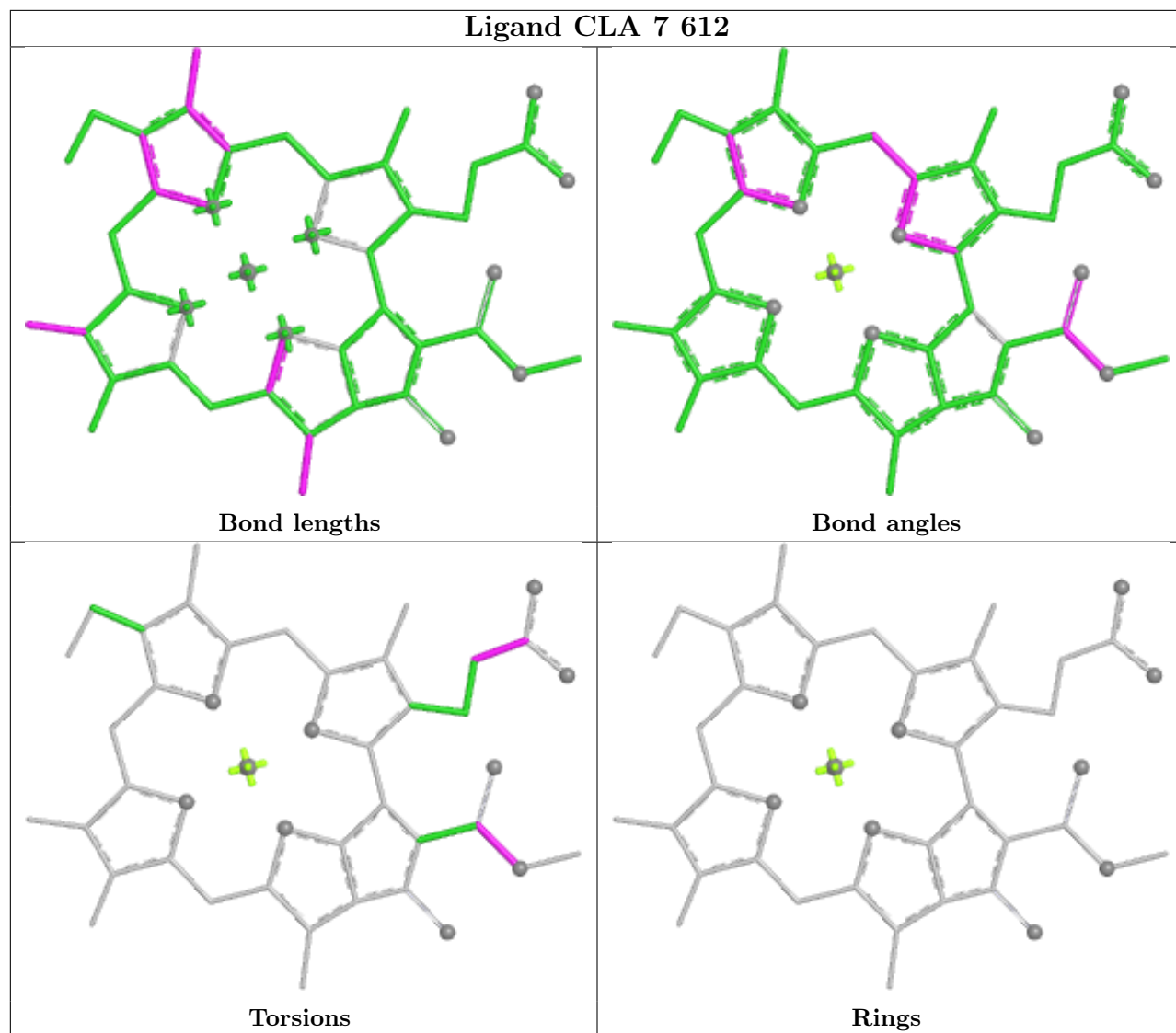


Ligand CLA A 821

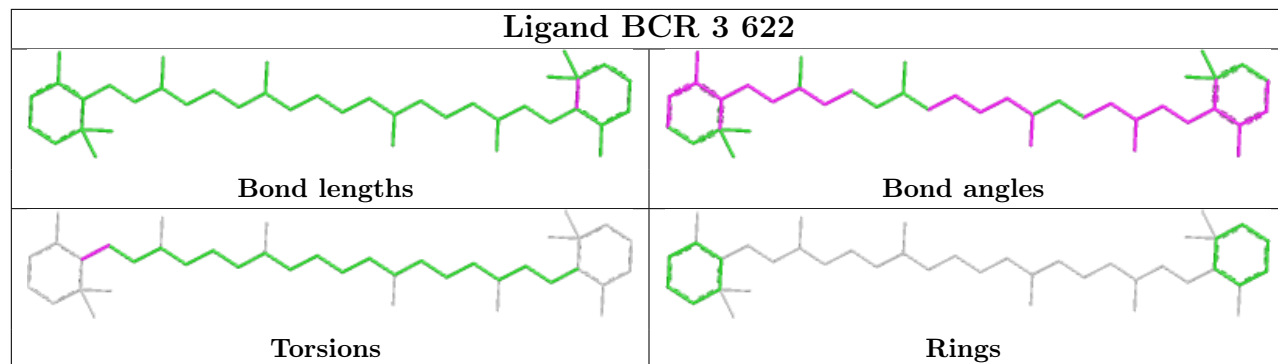




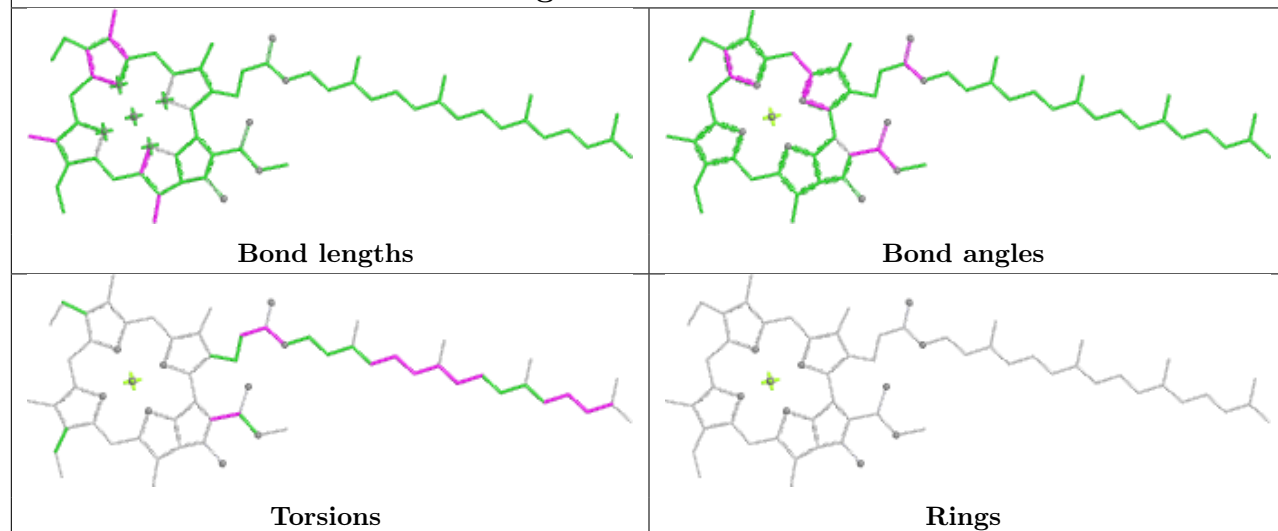
Ligand CLA 7 612



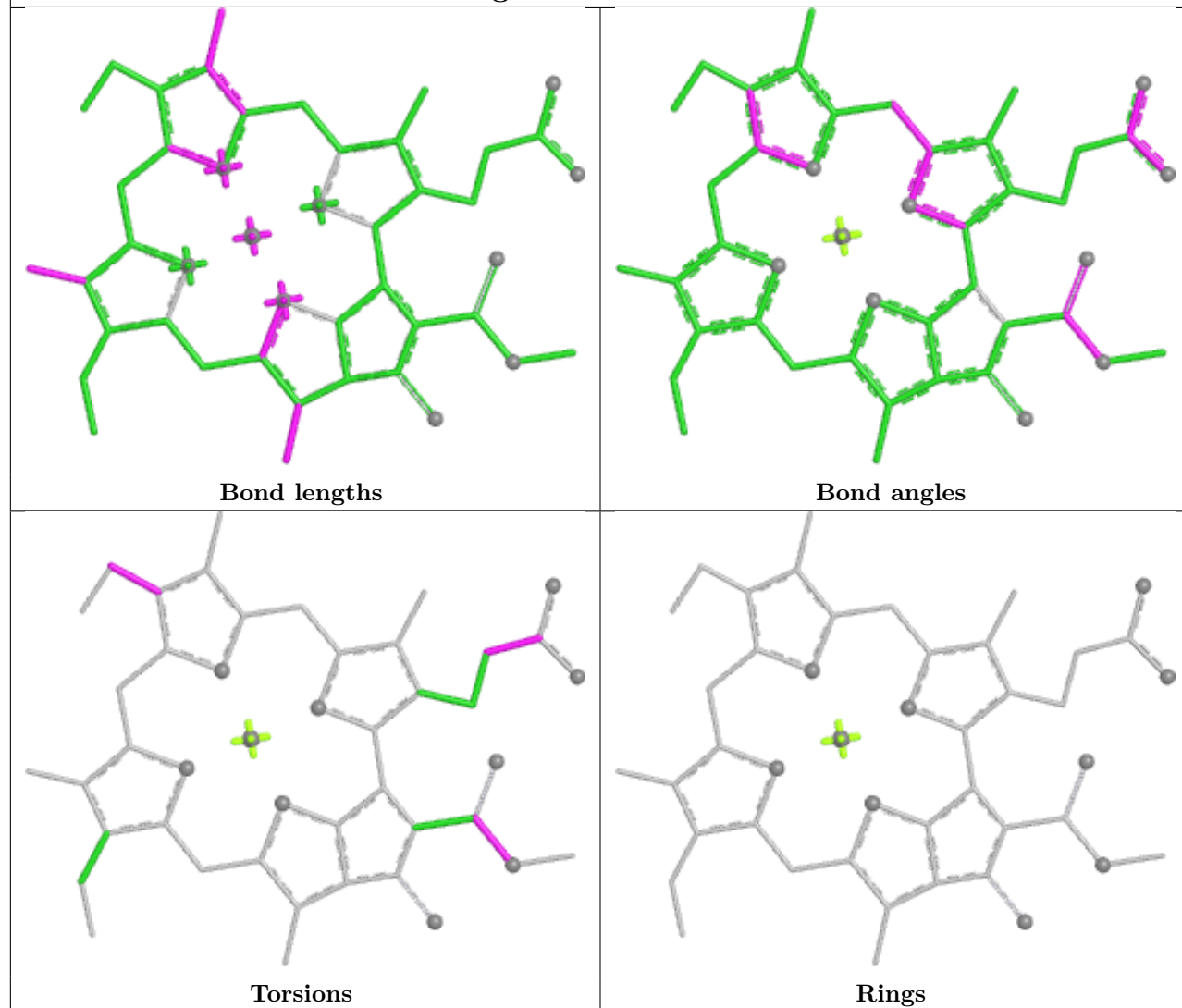
Ligand BCR 3 622



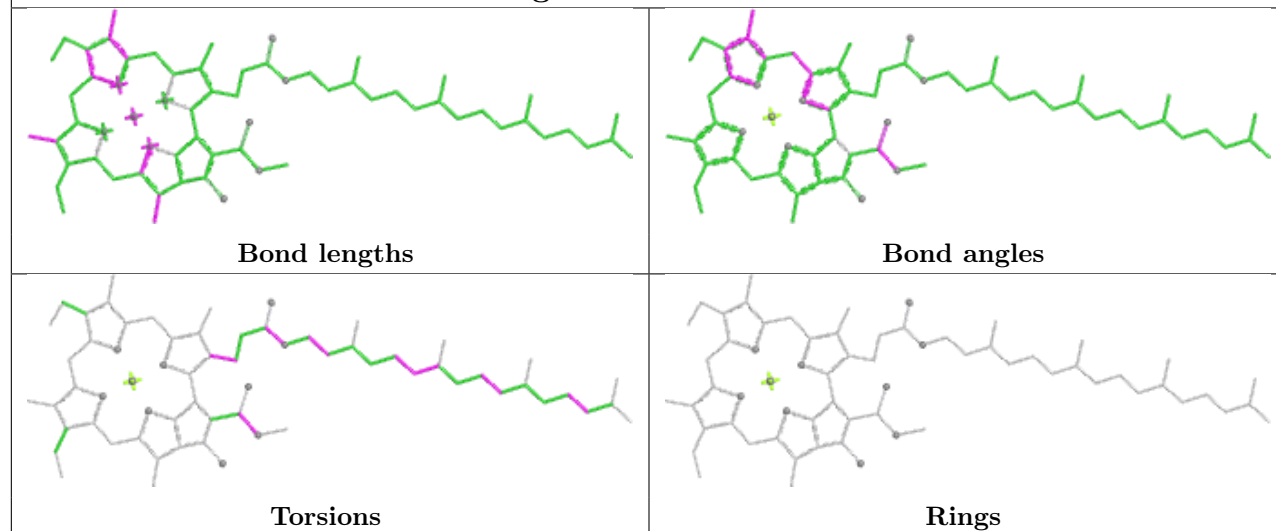
Ligand CLA 6 601



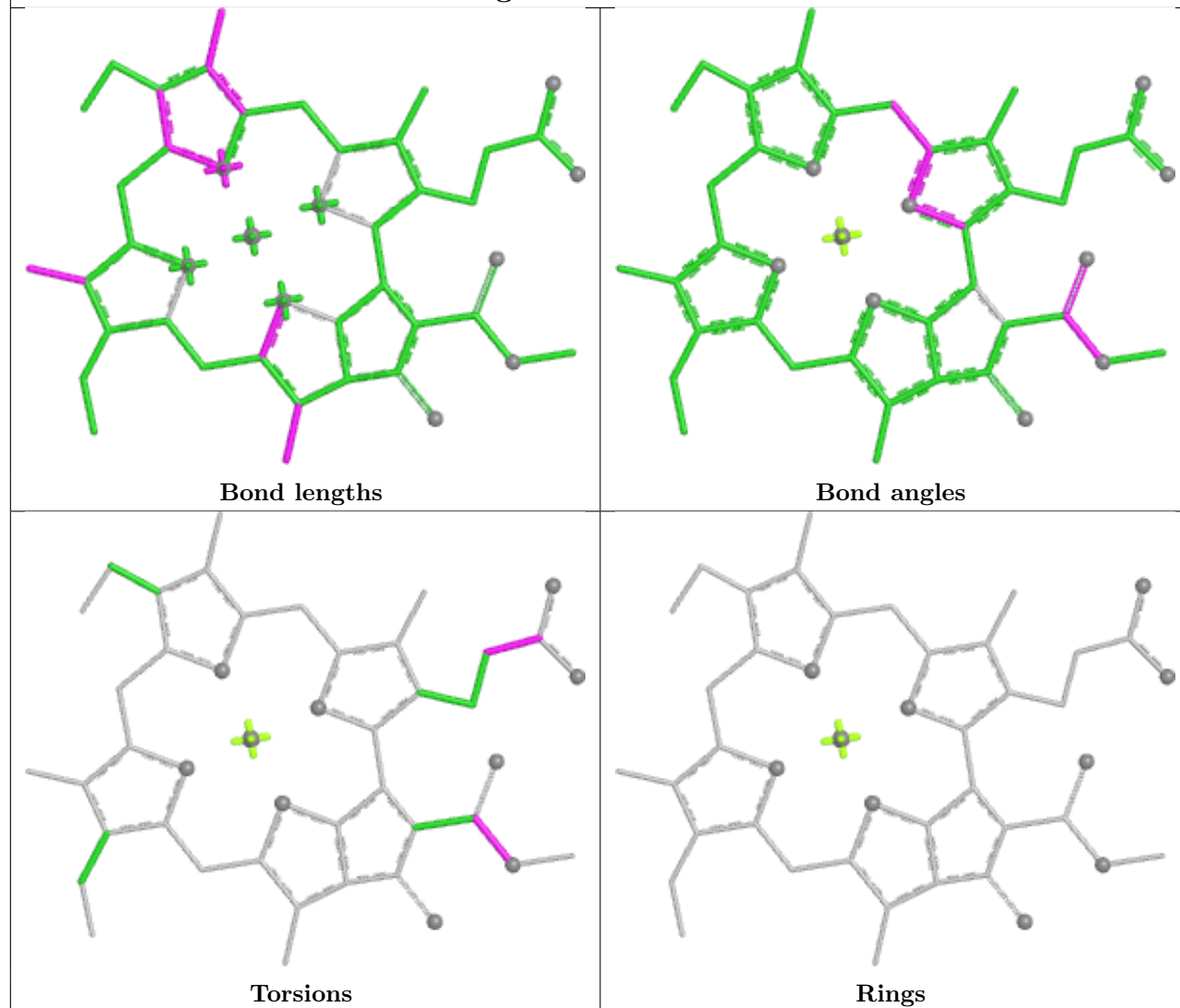
Ligand CLA B 823

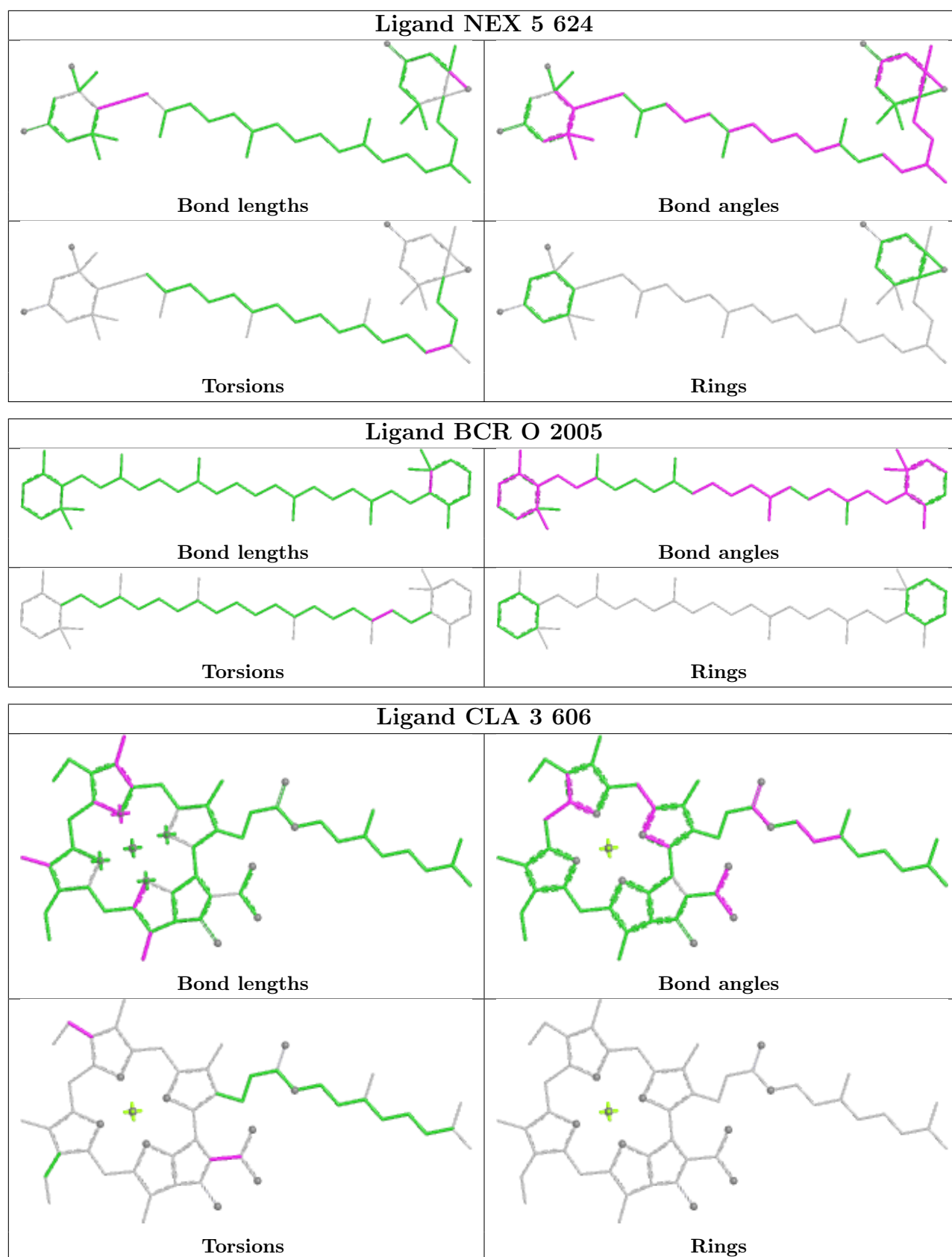


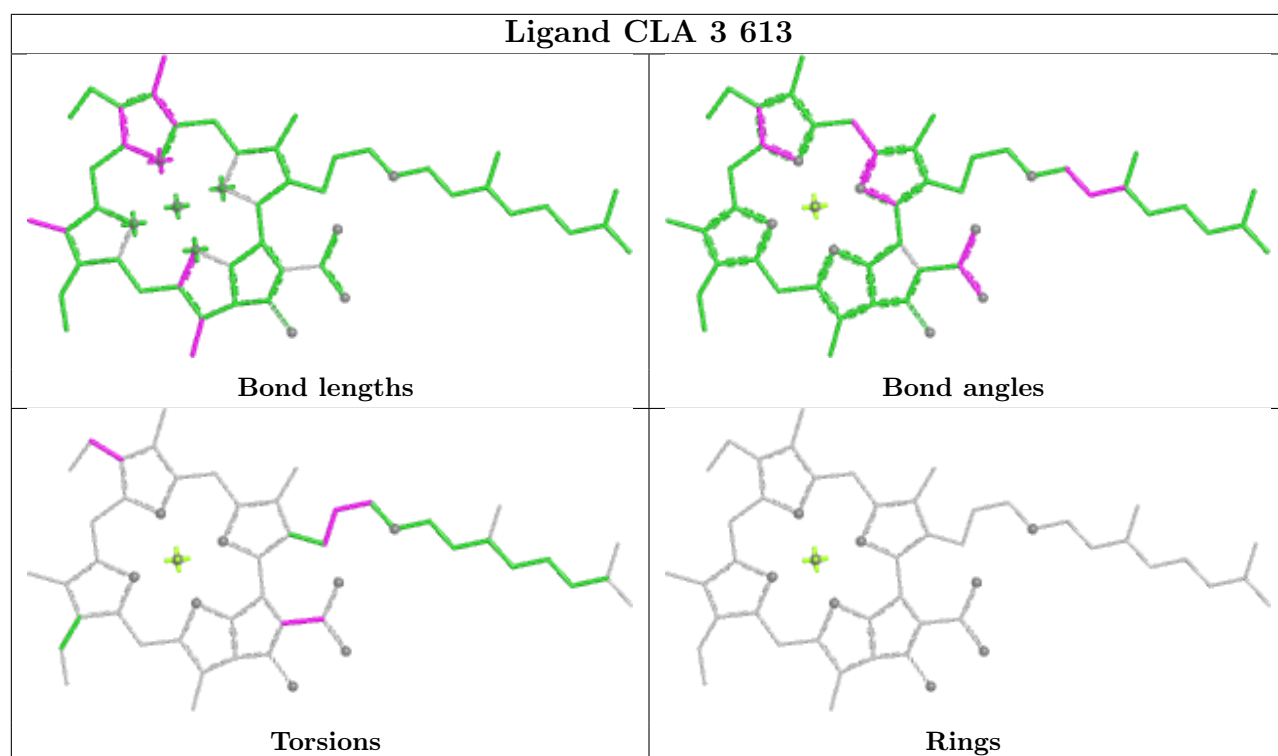
Ligand CLA B 803



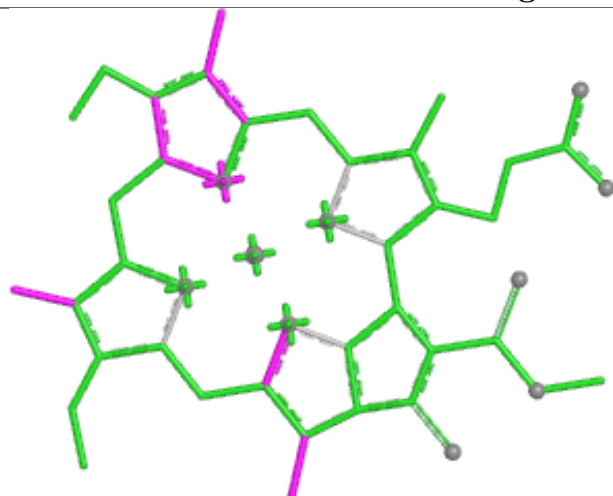
Ligand CLA 1 612



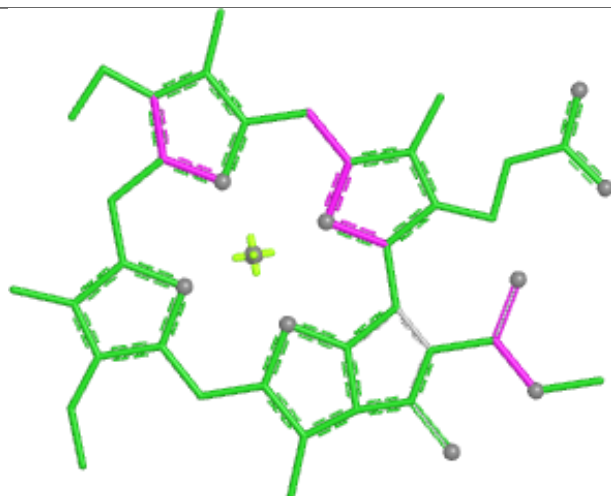




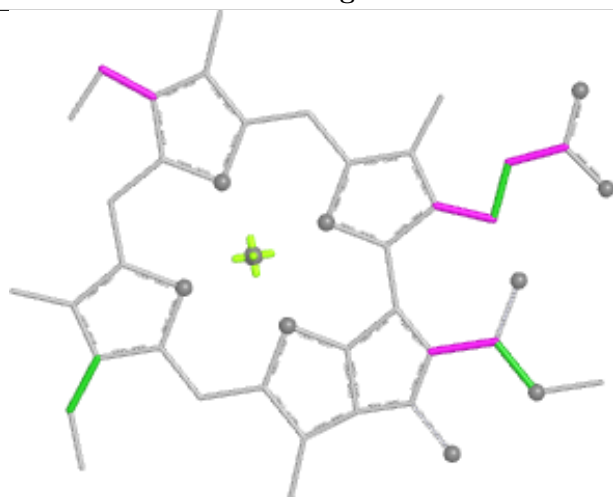
Ligand CLA 6 609



Bond lengths



Bond angles

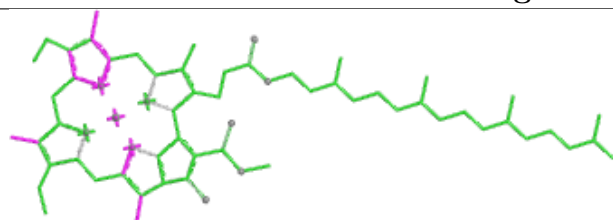


Torsions

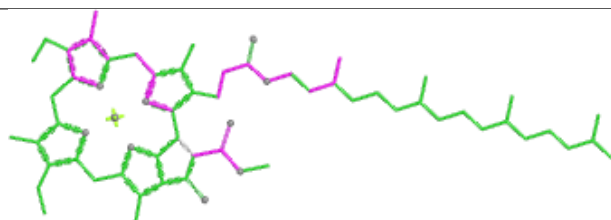


Rings

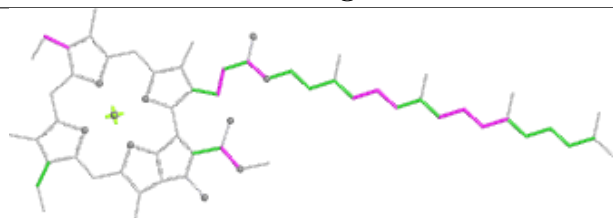
Ligand CLA A 834



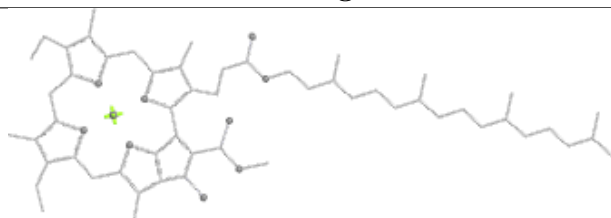
Bond lengths



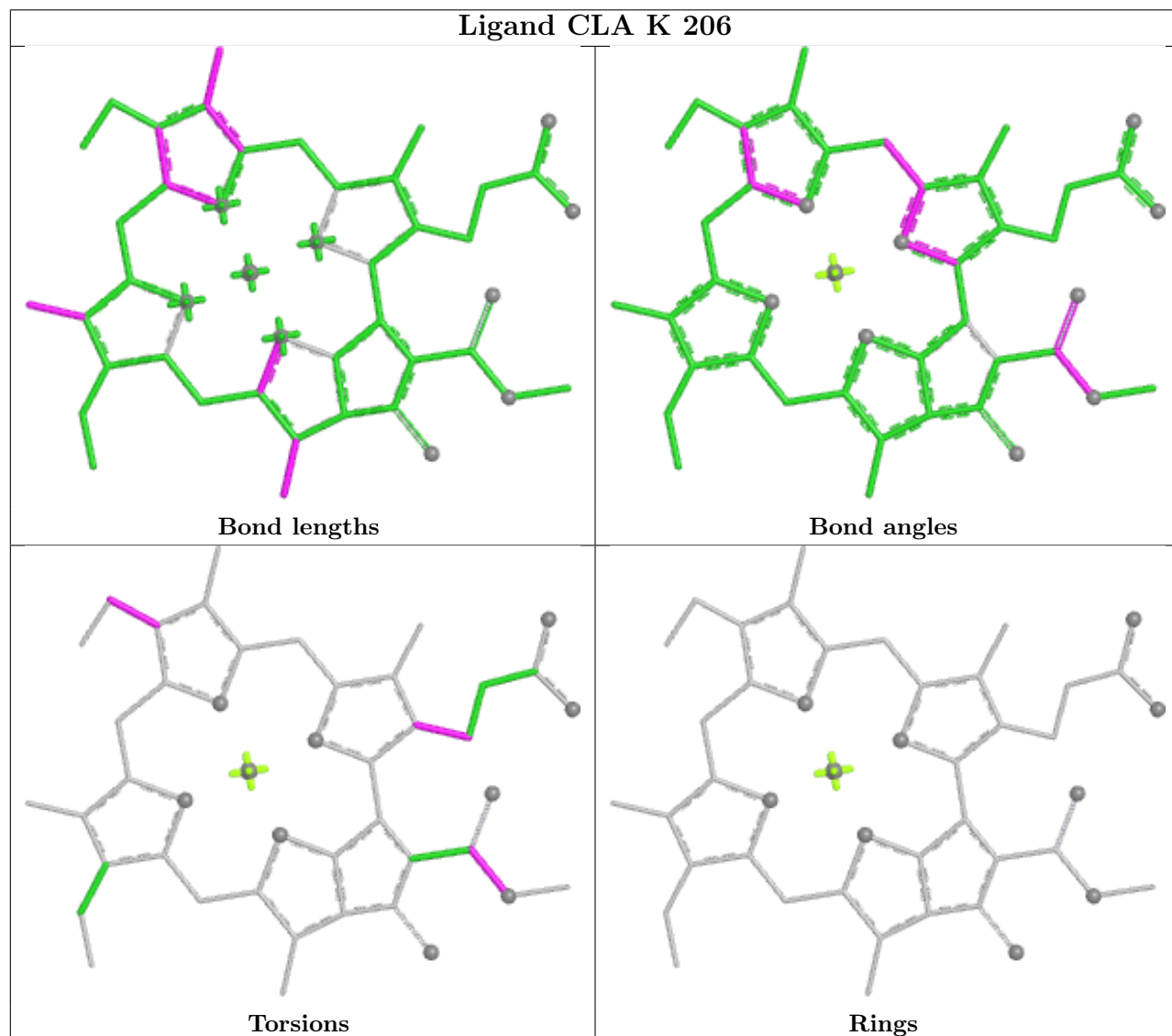
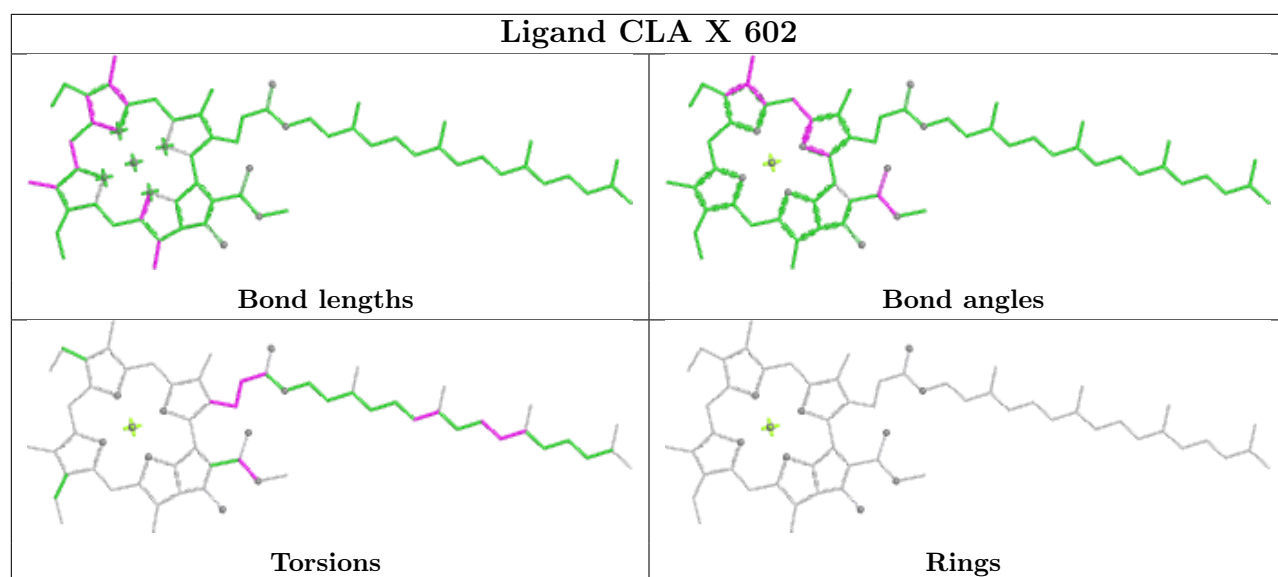
Bond angles



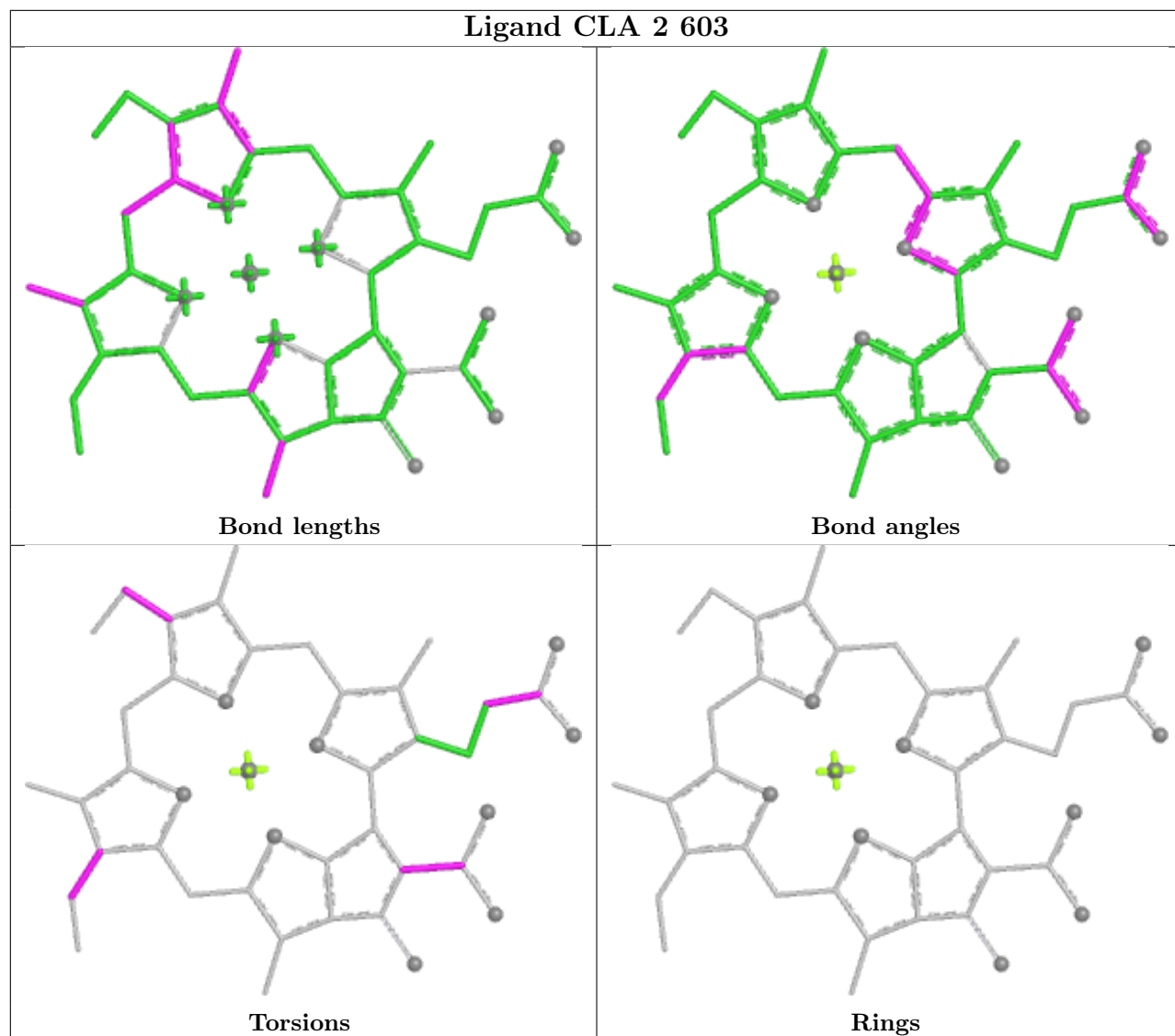
Torsions

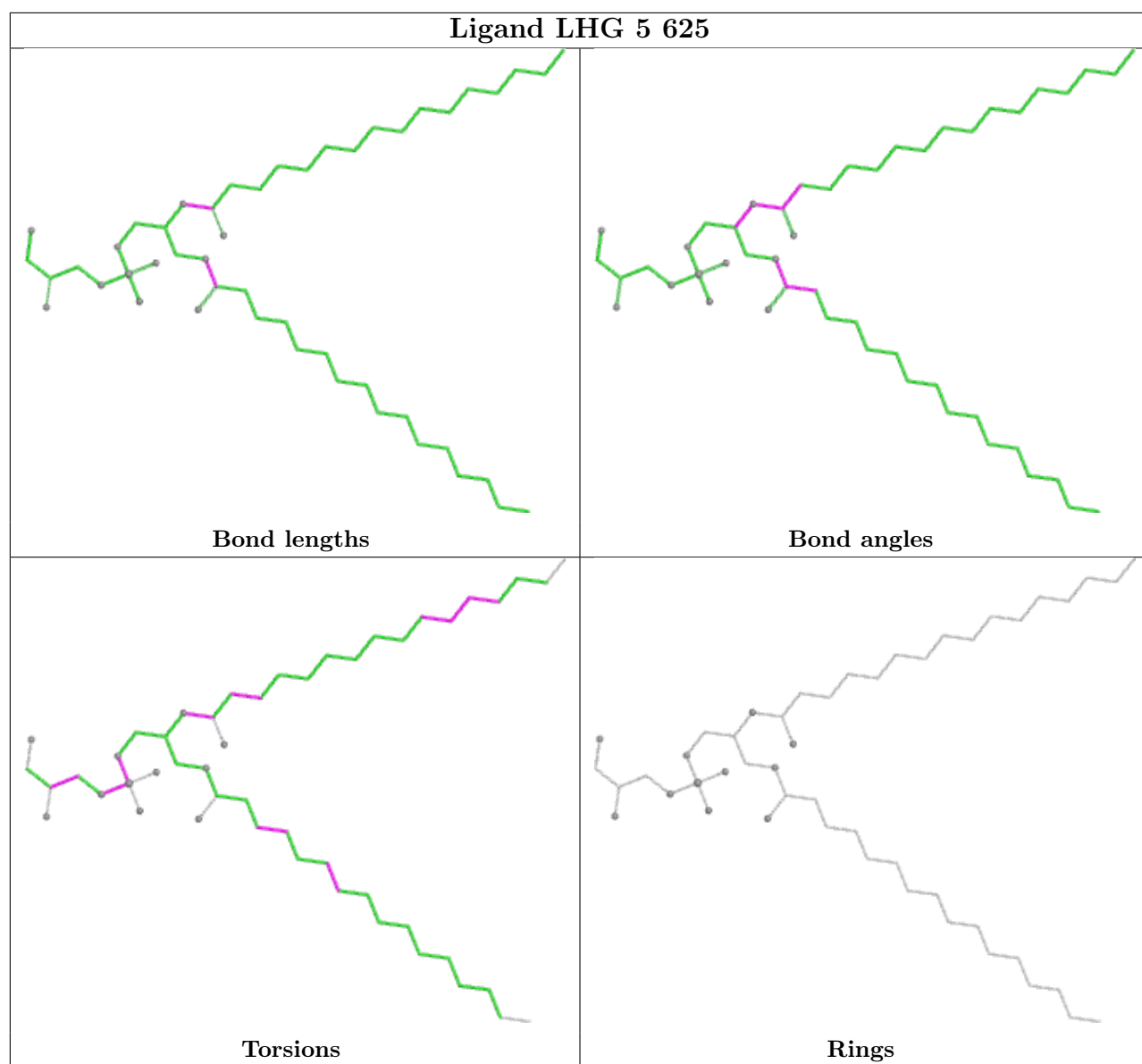


Rings

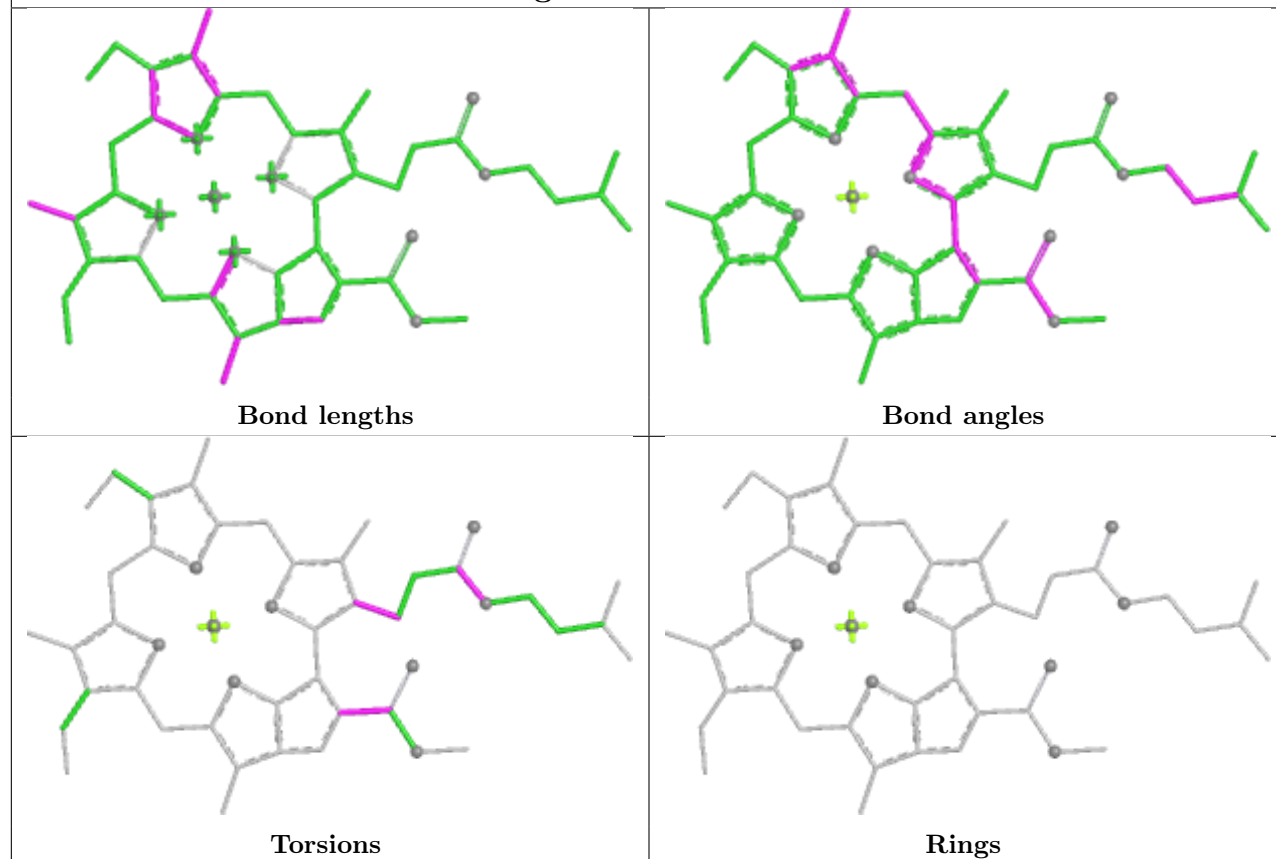


Ligand CLA 2 603

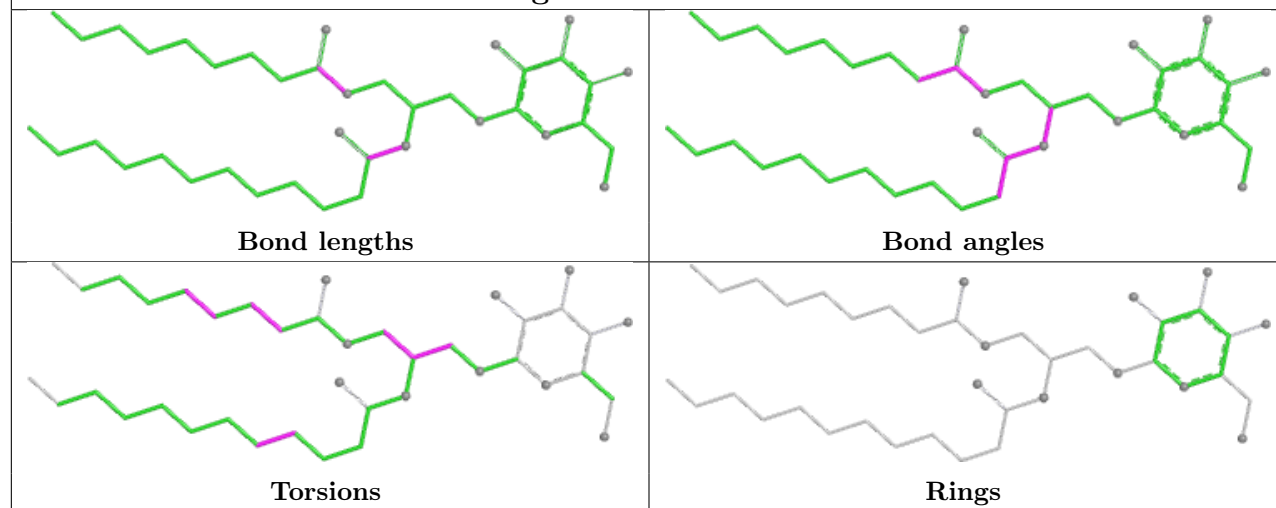


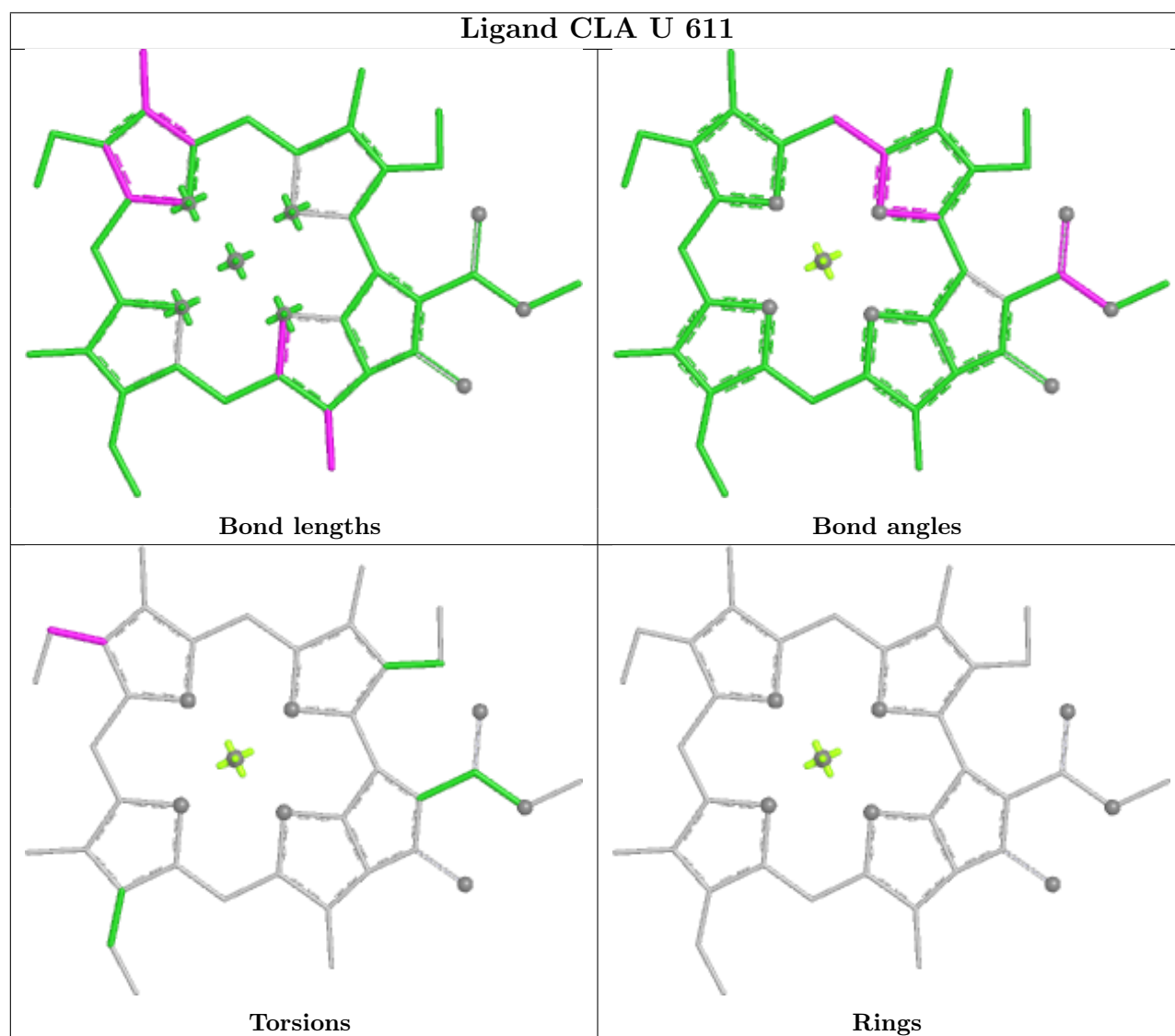
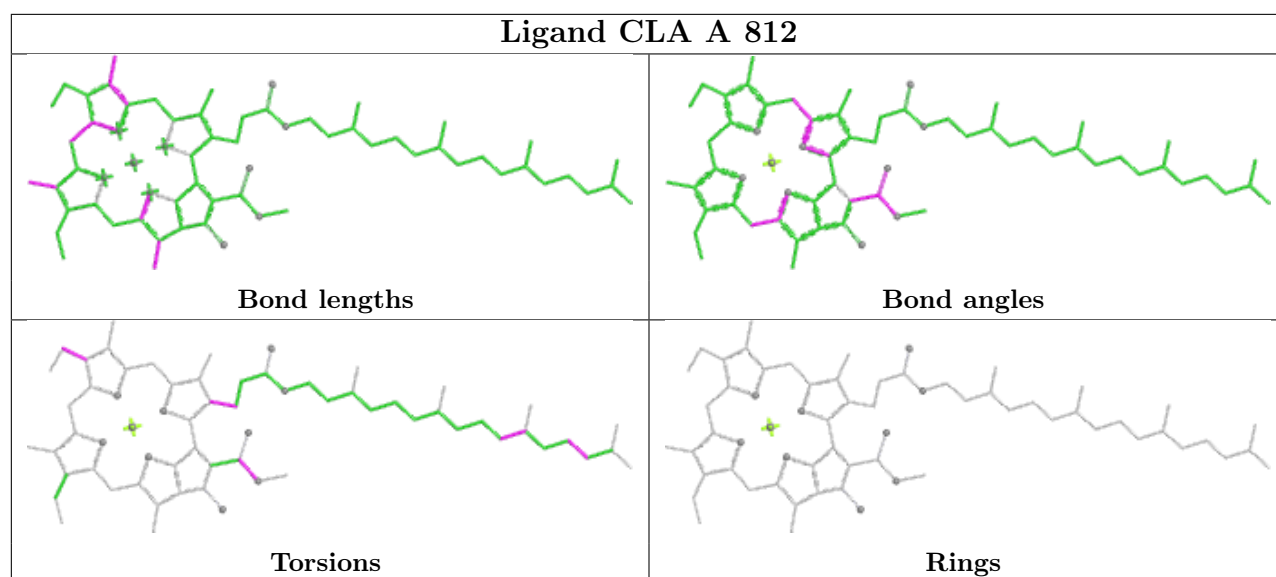


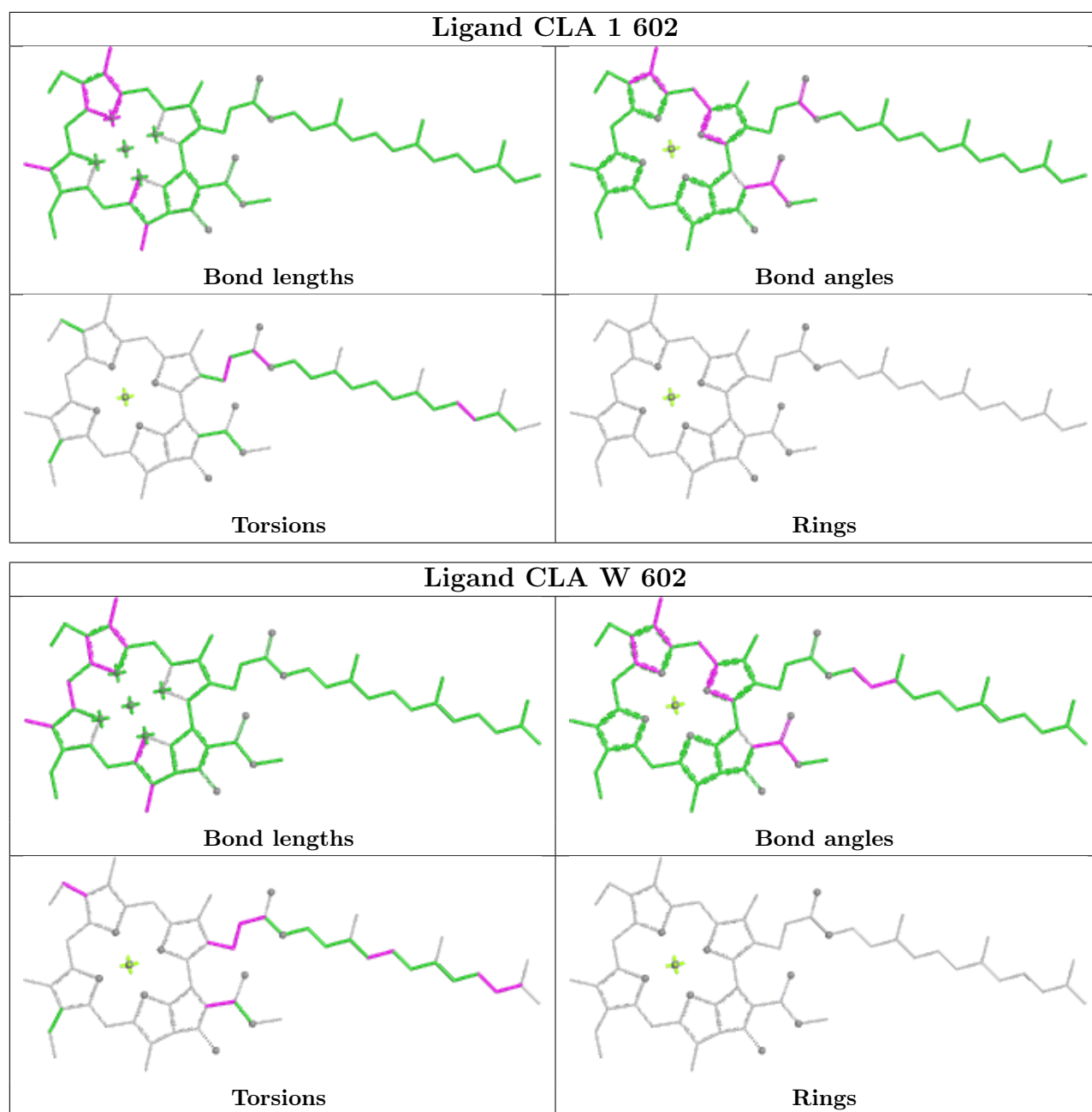
Ligand CLA Z 604



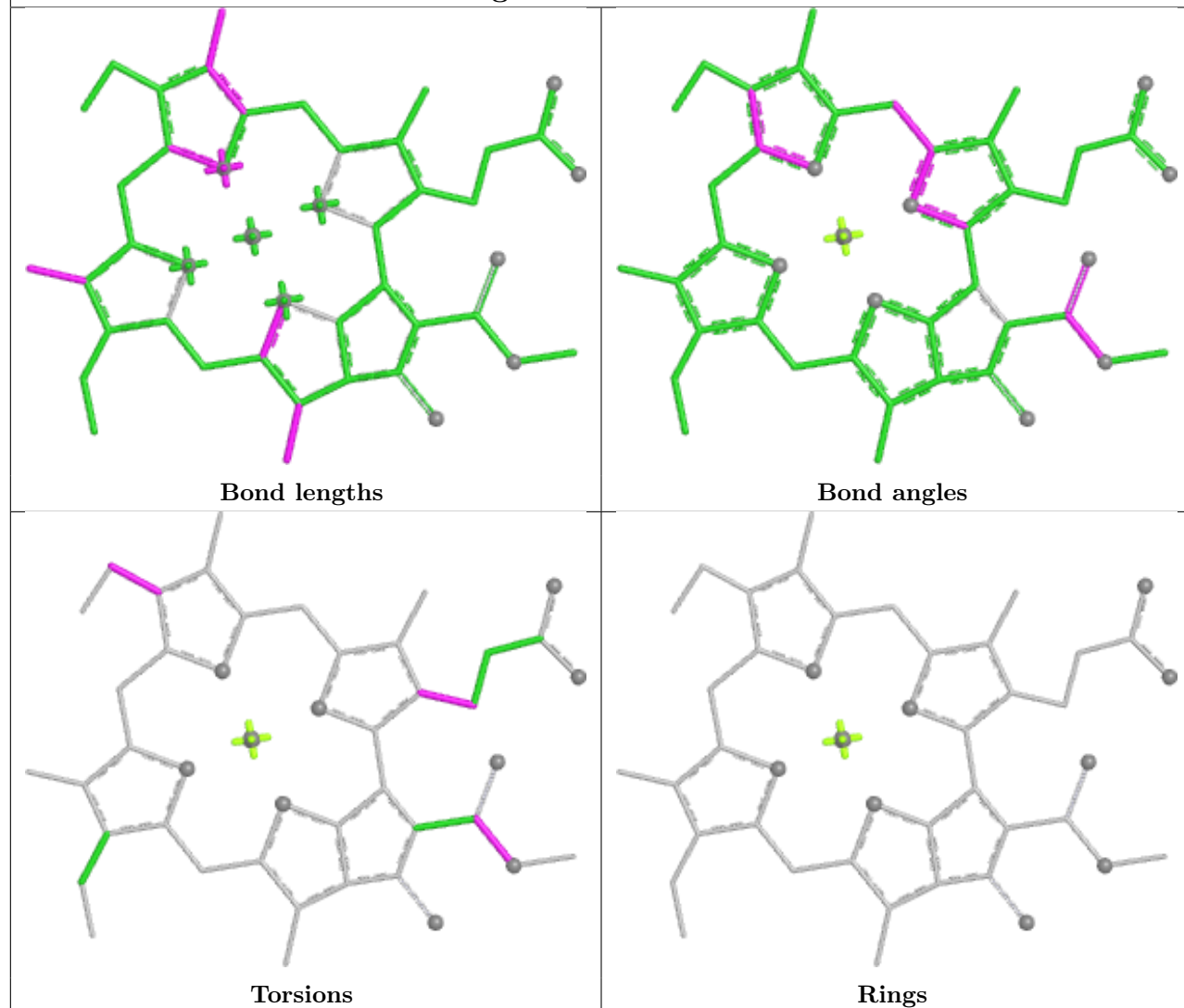
Ligand LMG 5 627



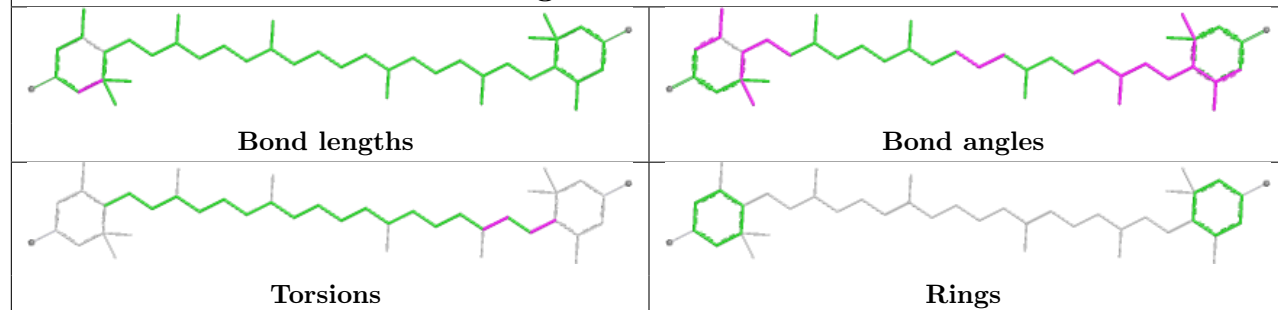


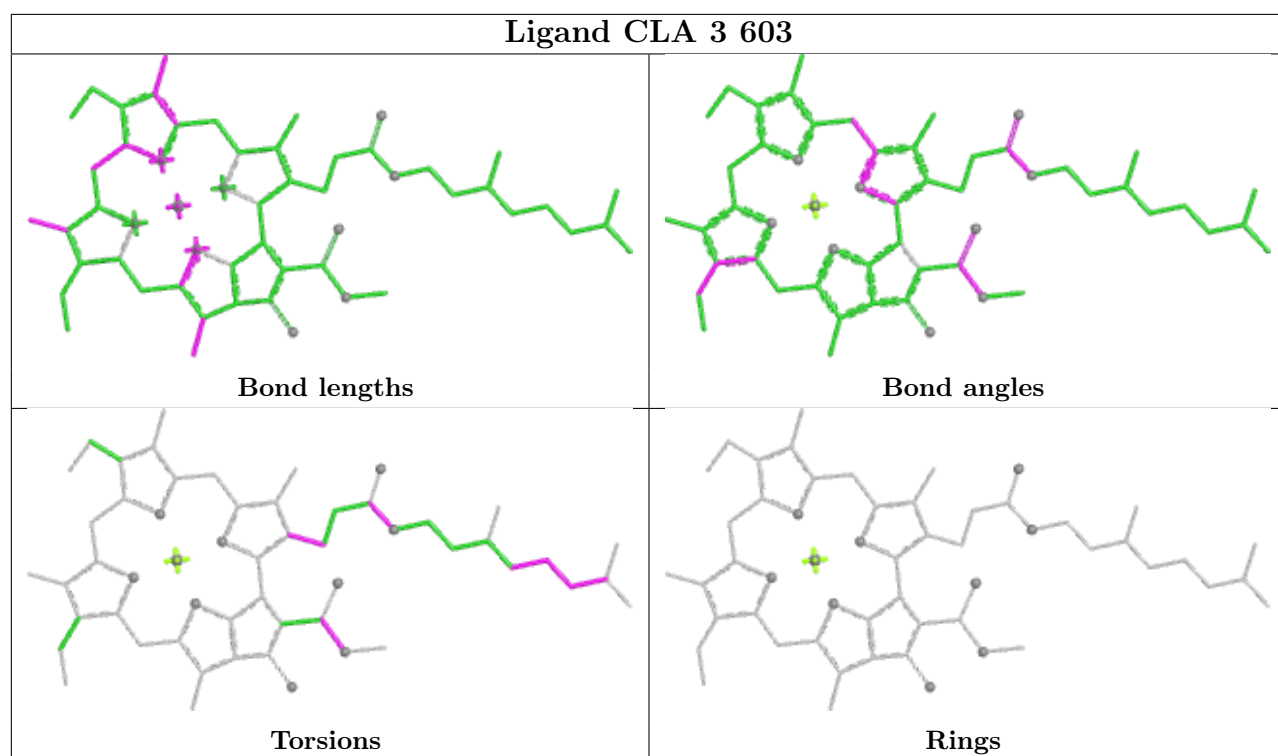


Ligand CLA K 204

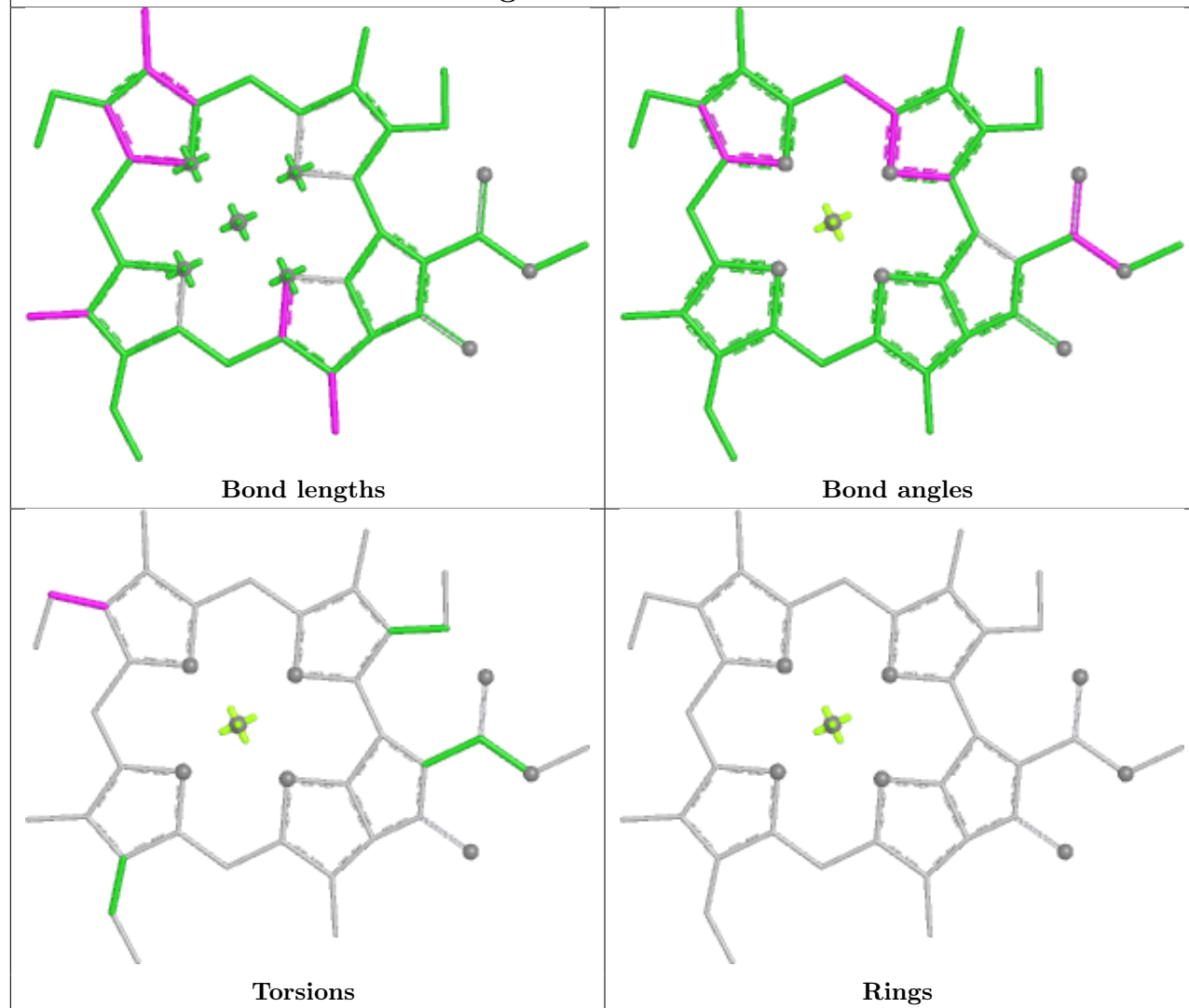


Ligand LUT 8 619

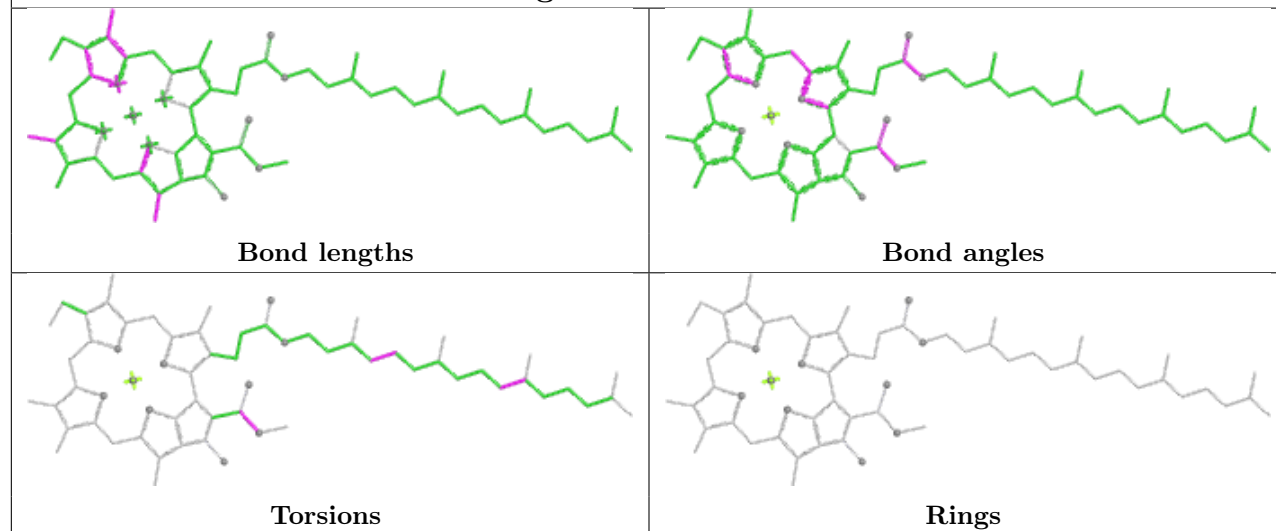




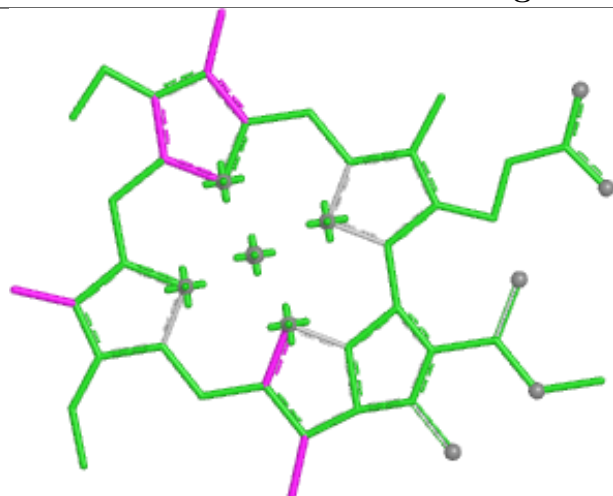
Ligand CLA 2 611



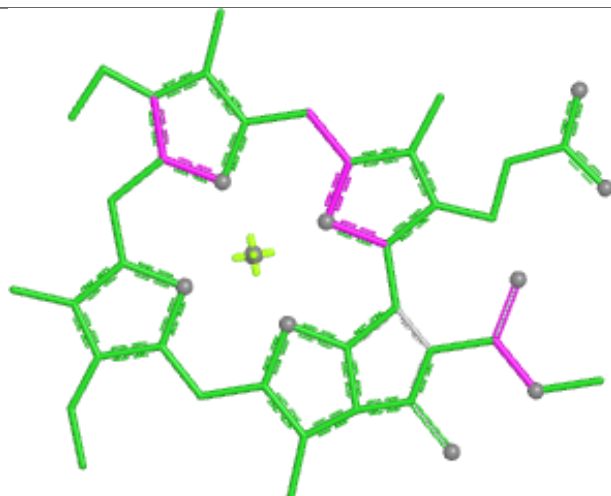
Ligand CLA 8 606



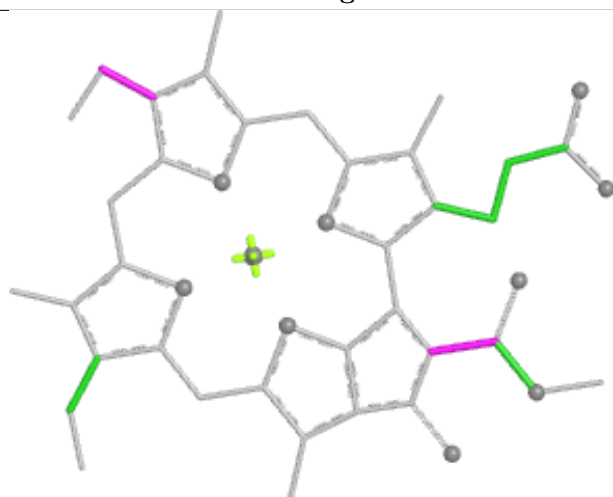
Ligand CLA X 611



Bond lengths



Bond angles

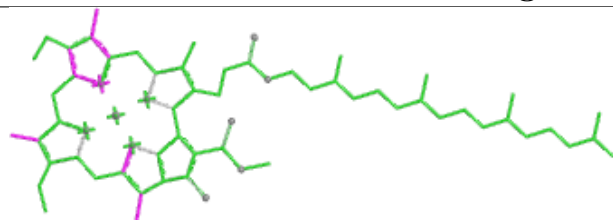


Torsions

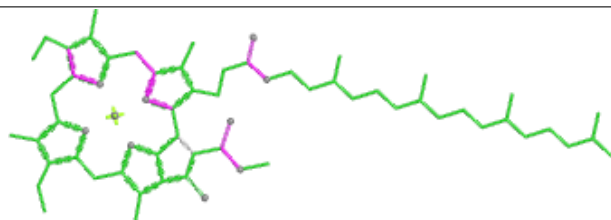


Rings

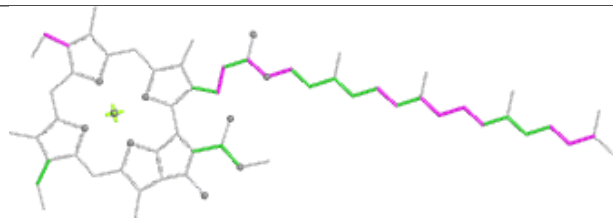
Ligand CLA 8 613



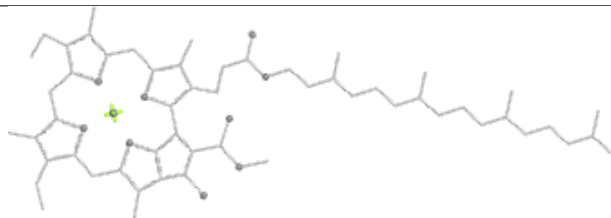
Bond lengths



Bond angles

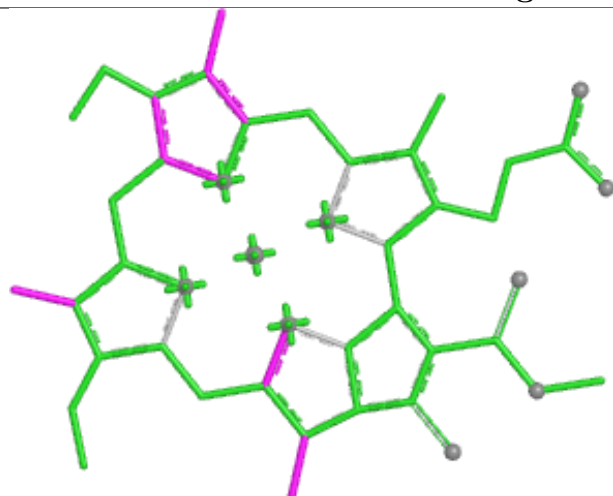


Torsions

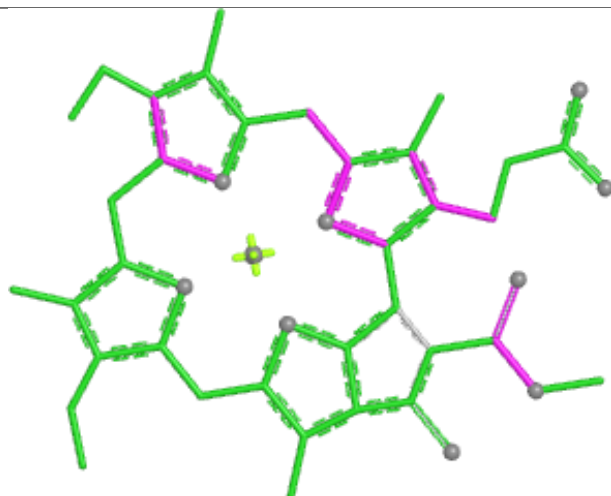


Rings

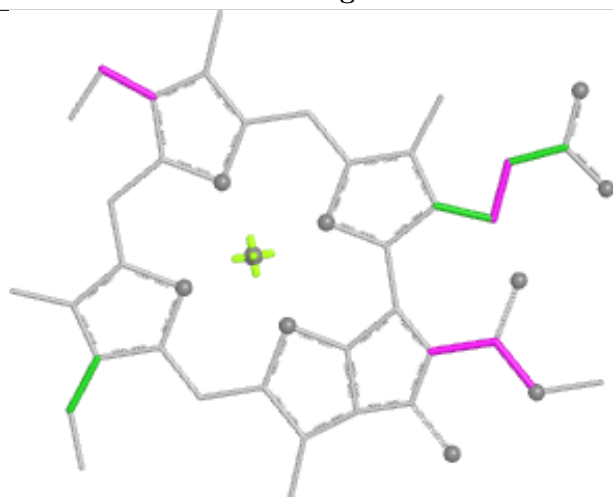
Ligand CLA Z 612



Bond lengths



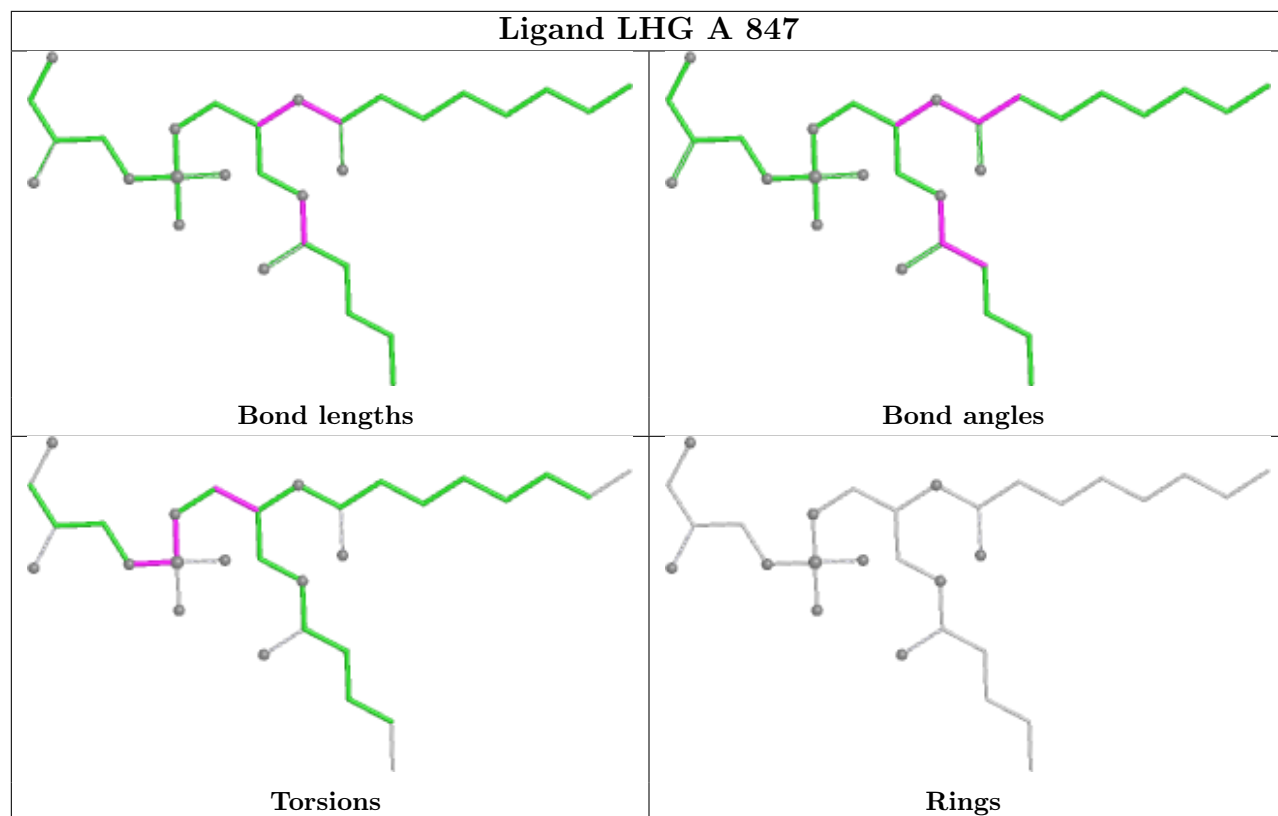
Bond angles



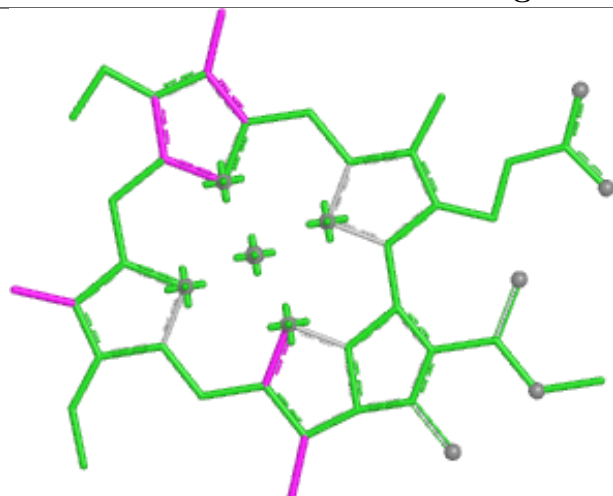
Torsions



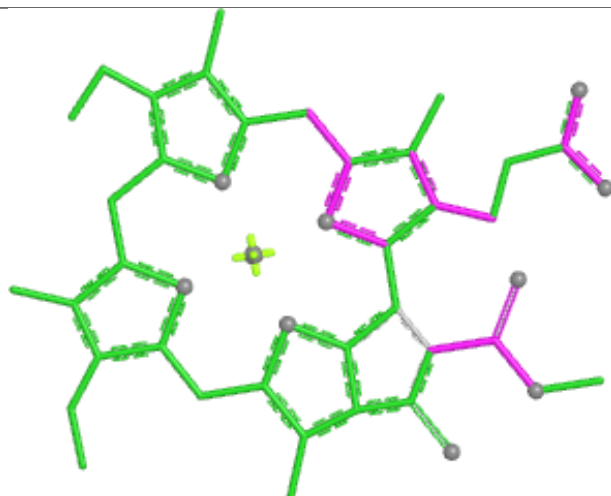
Rings



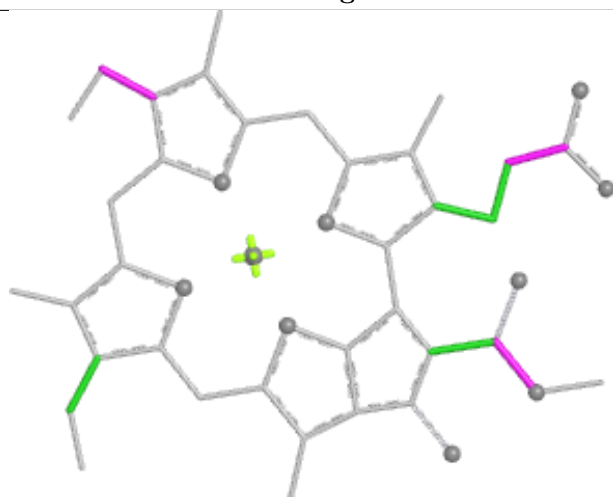
Ligand CLA V 612



Bond lengths



Bond angles

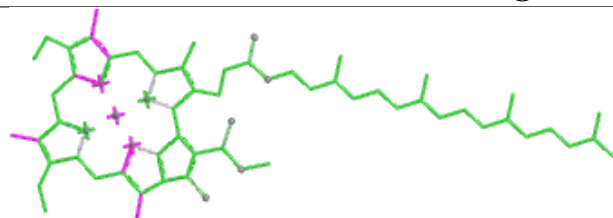


Torsions

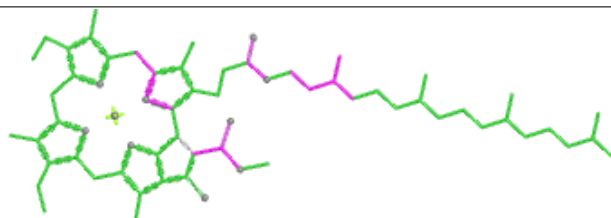


Rings

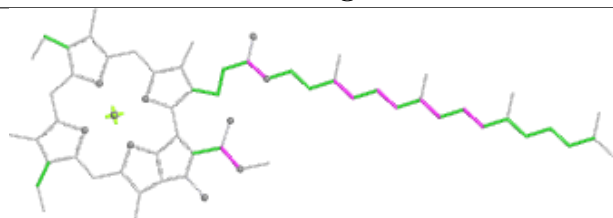
Ligand CLA A 836



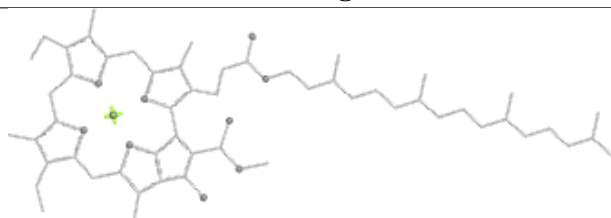
Bond lengths



Bond angles

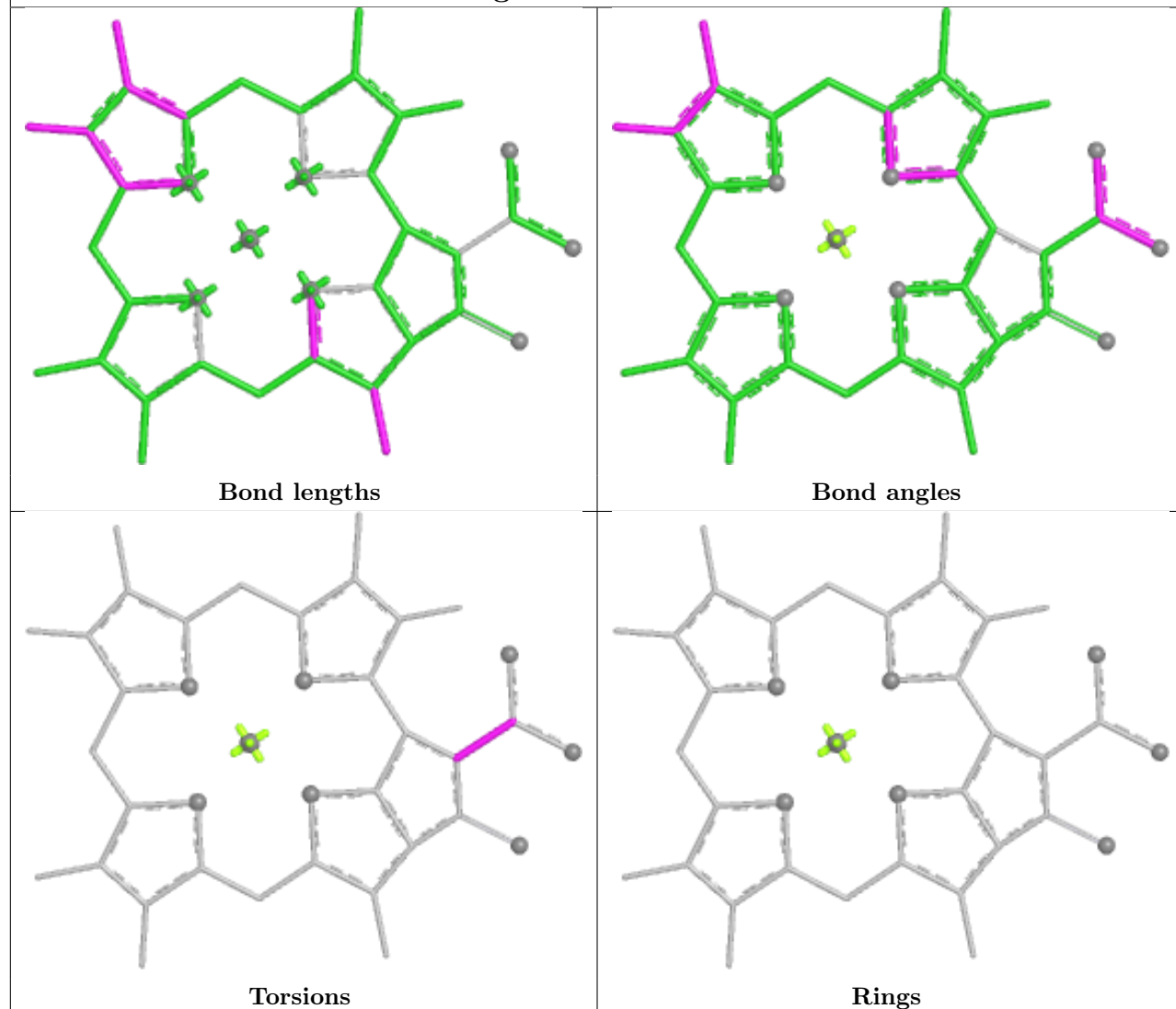


Torsions

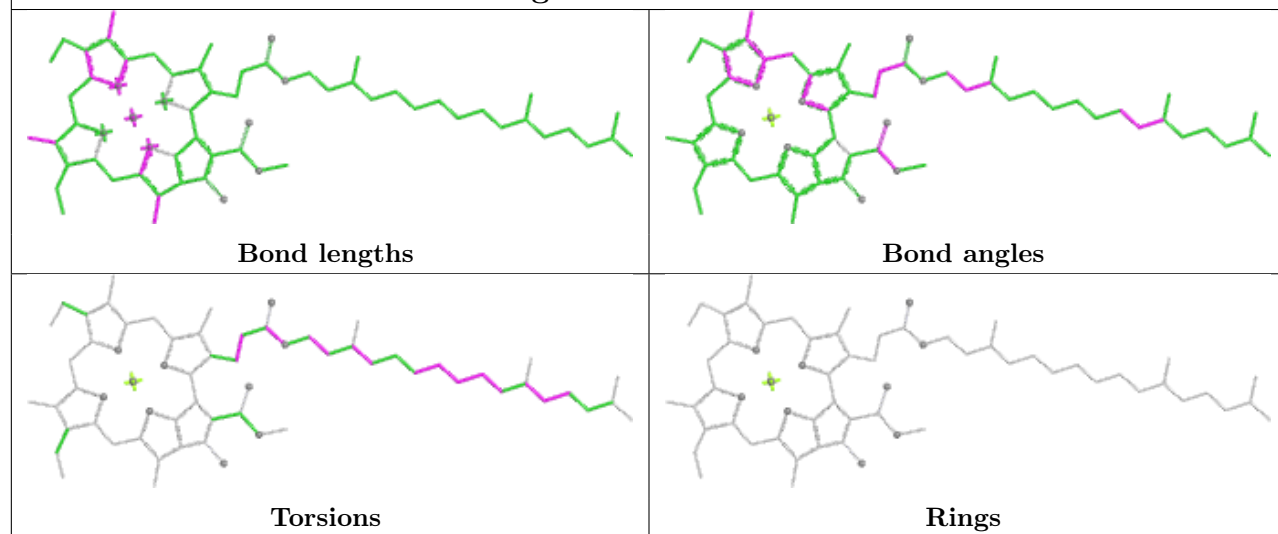


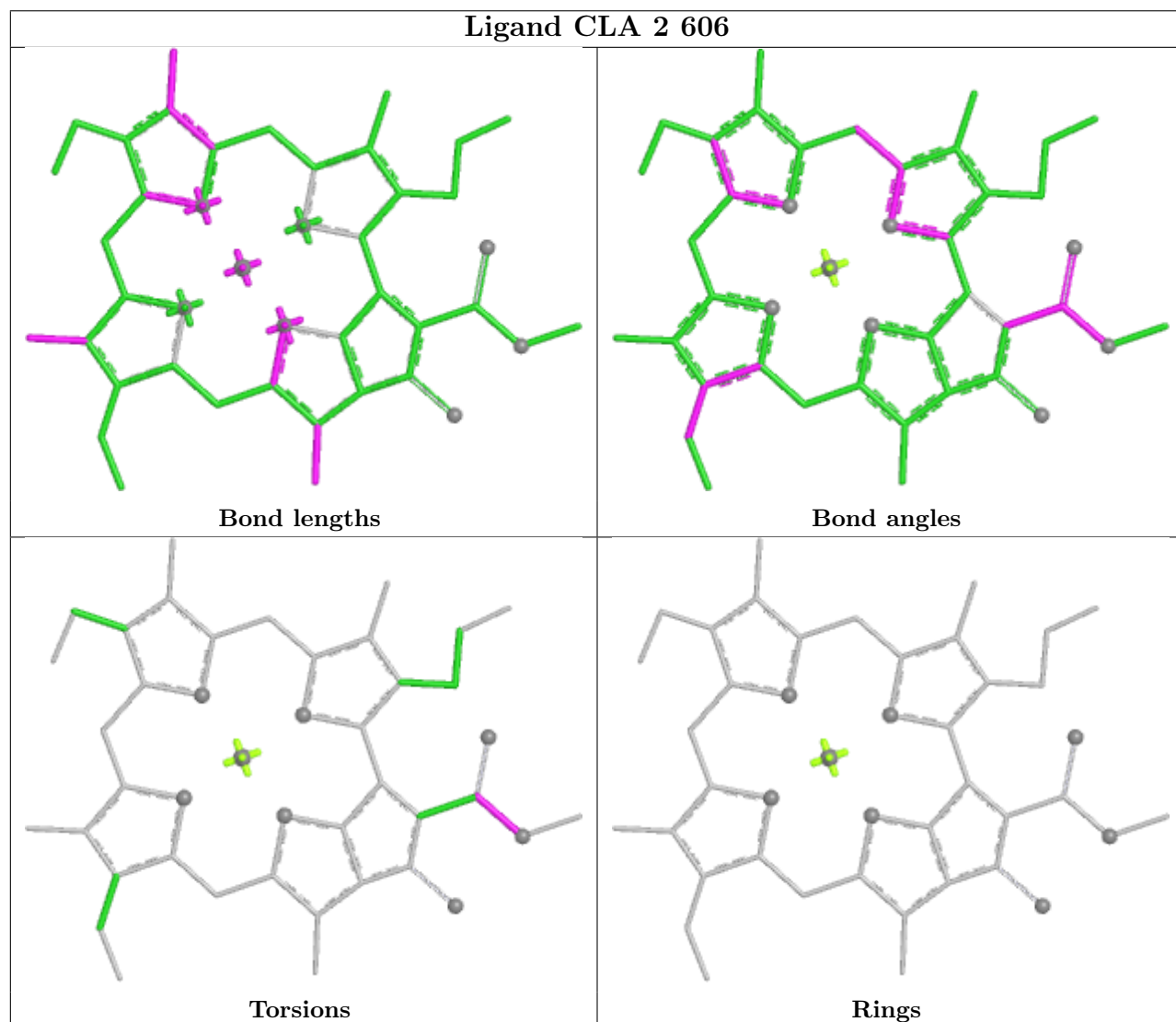
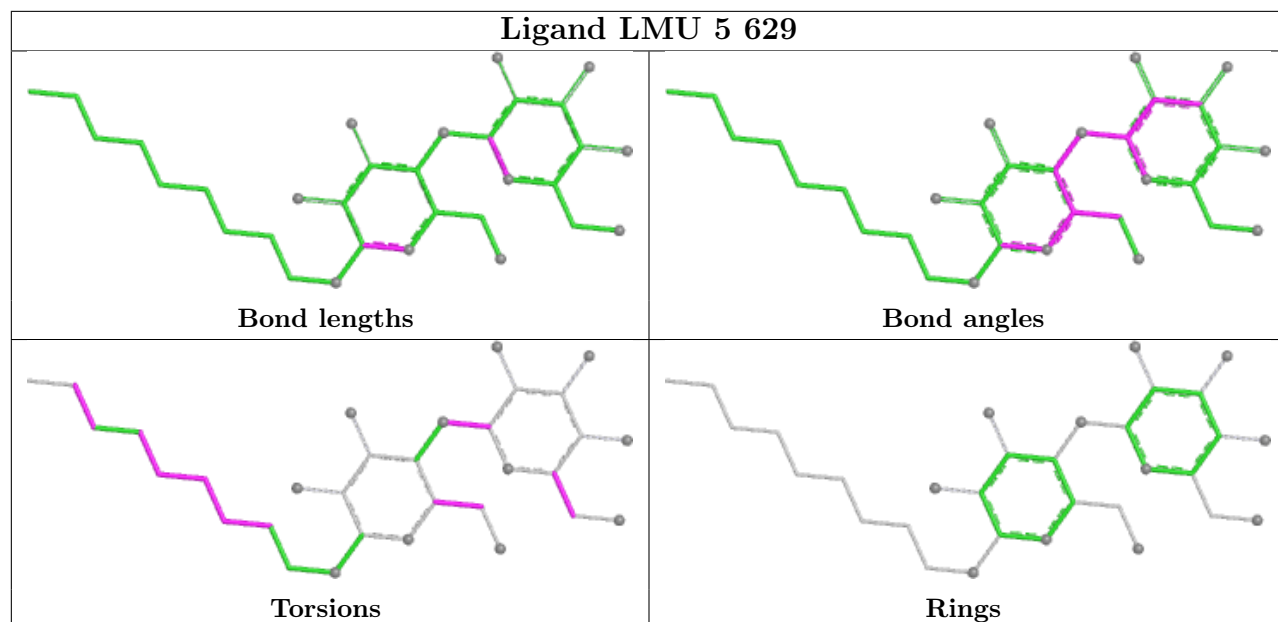
Rings

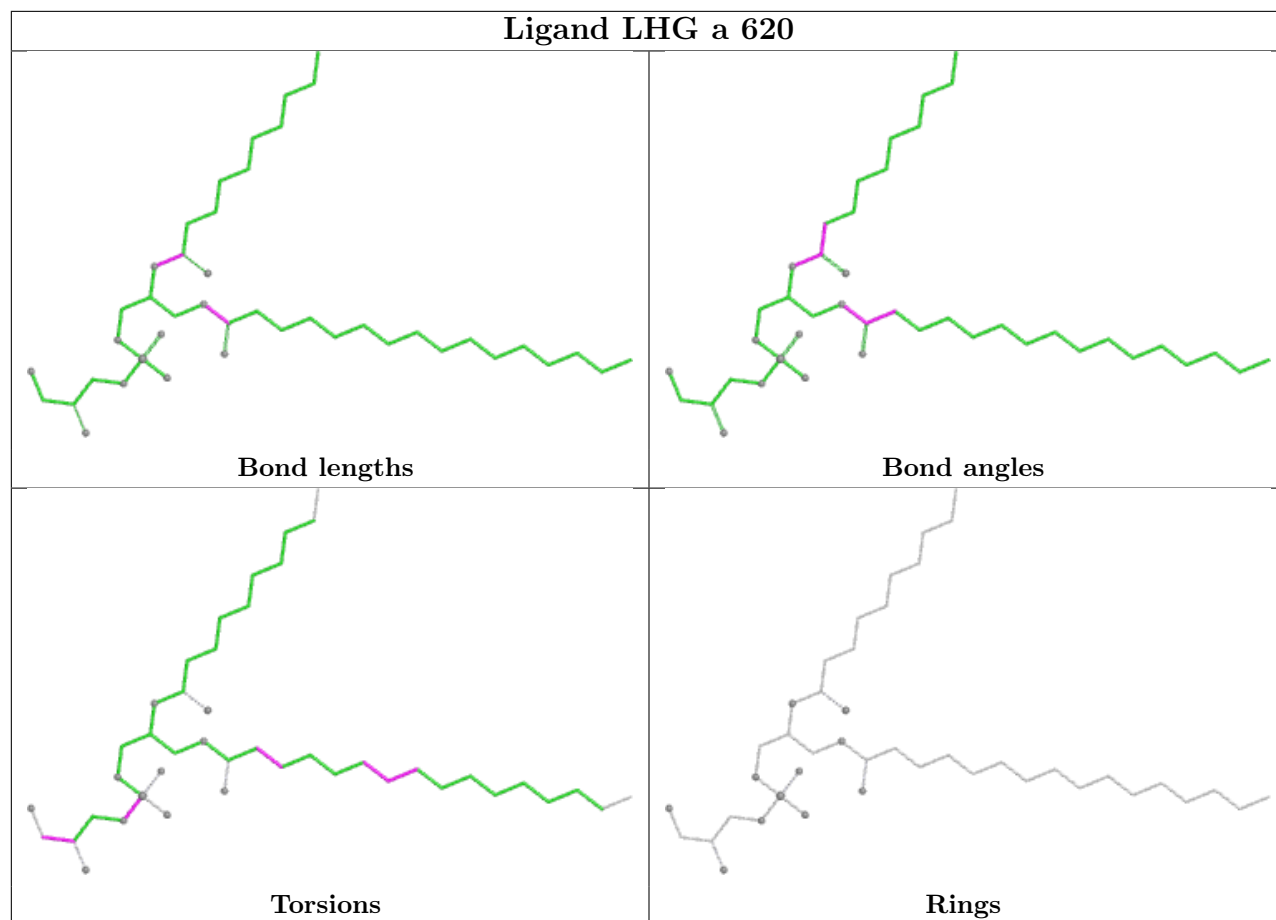
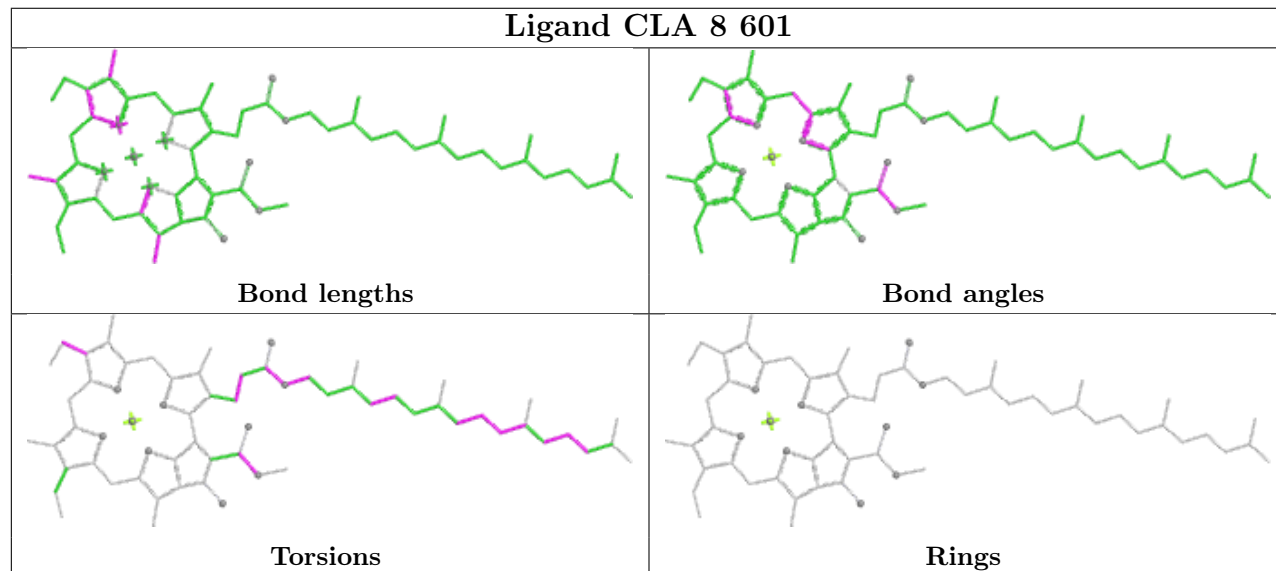
Ligand CLA 3 611



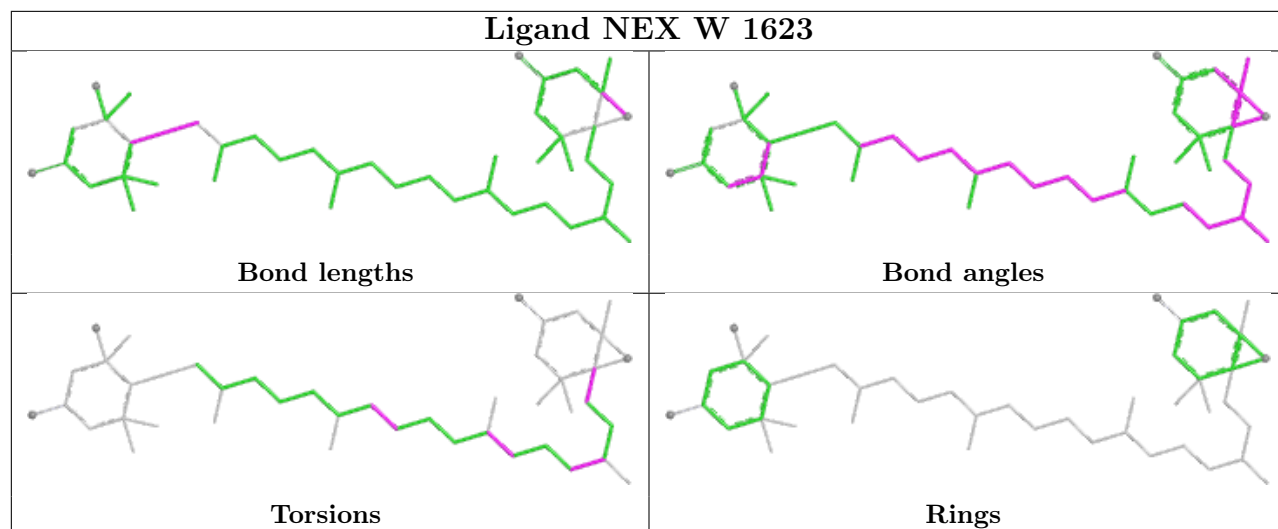
Ligand CLA A 843



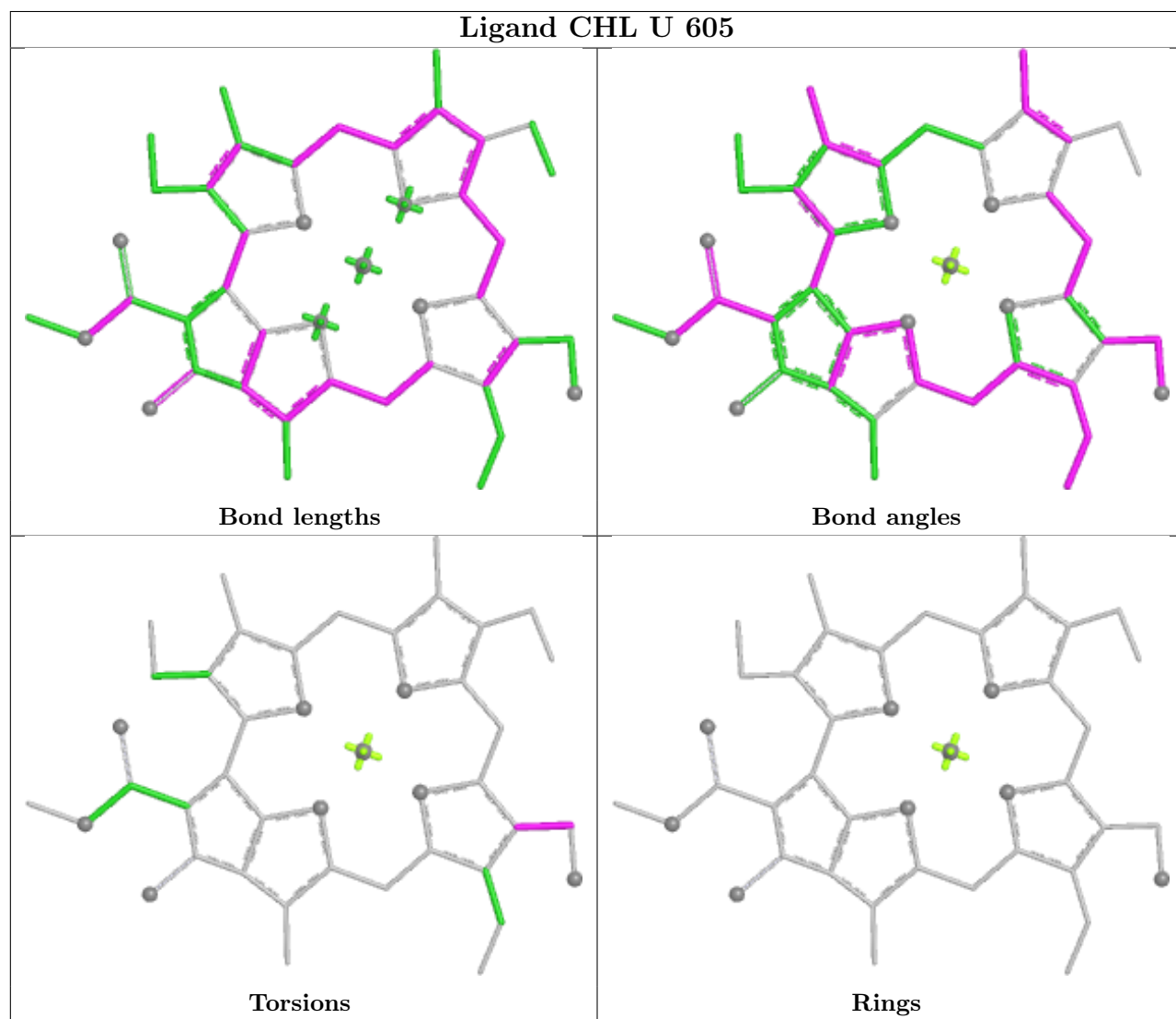


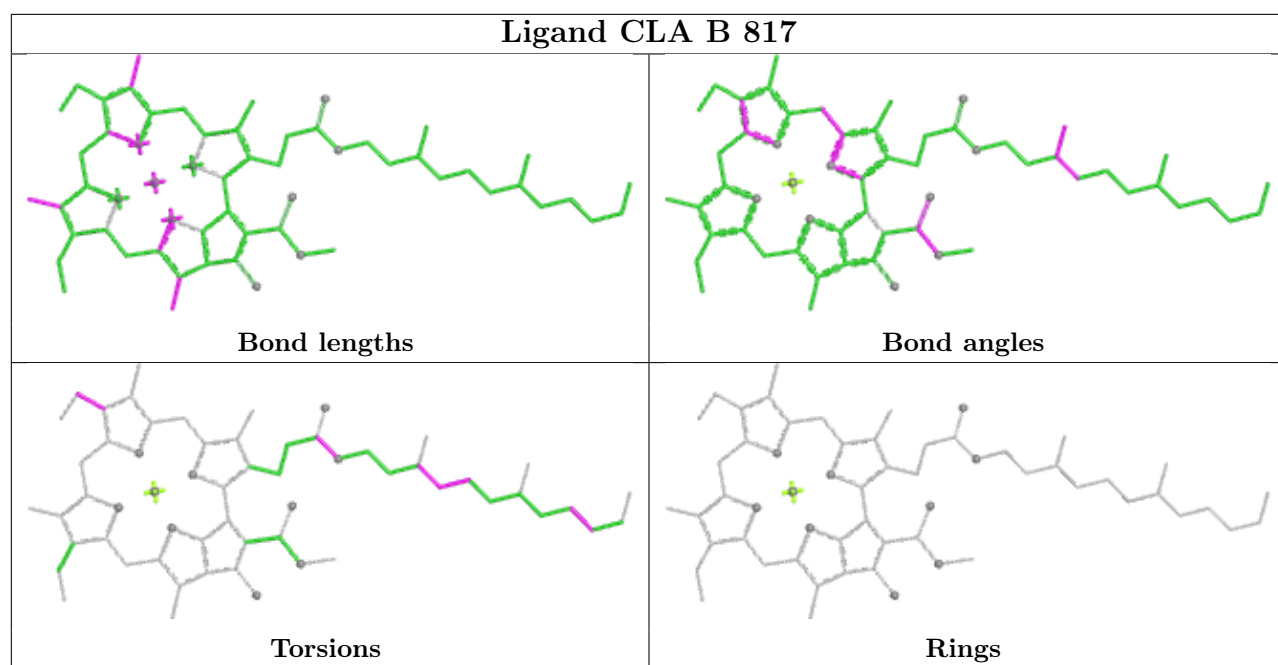
Ligand LHG a 620**Ligand CLA 8 601**

Ligand NEX W 1623

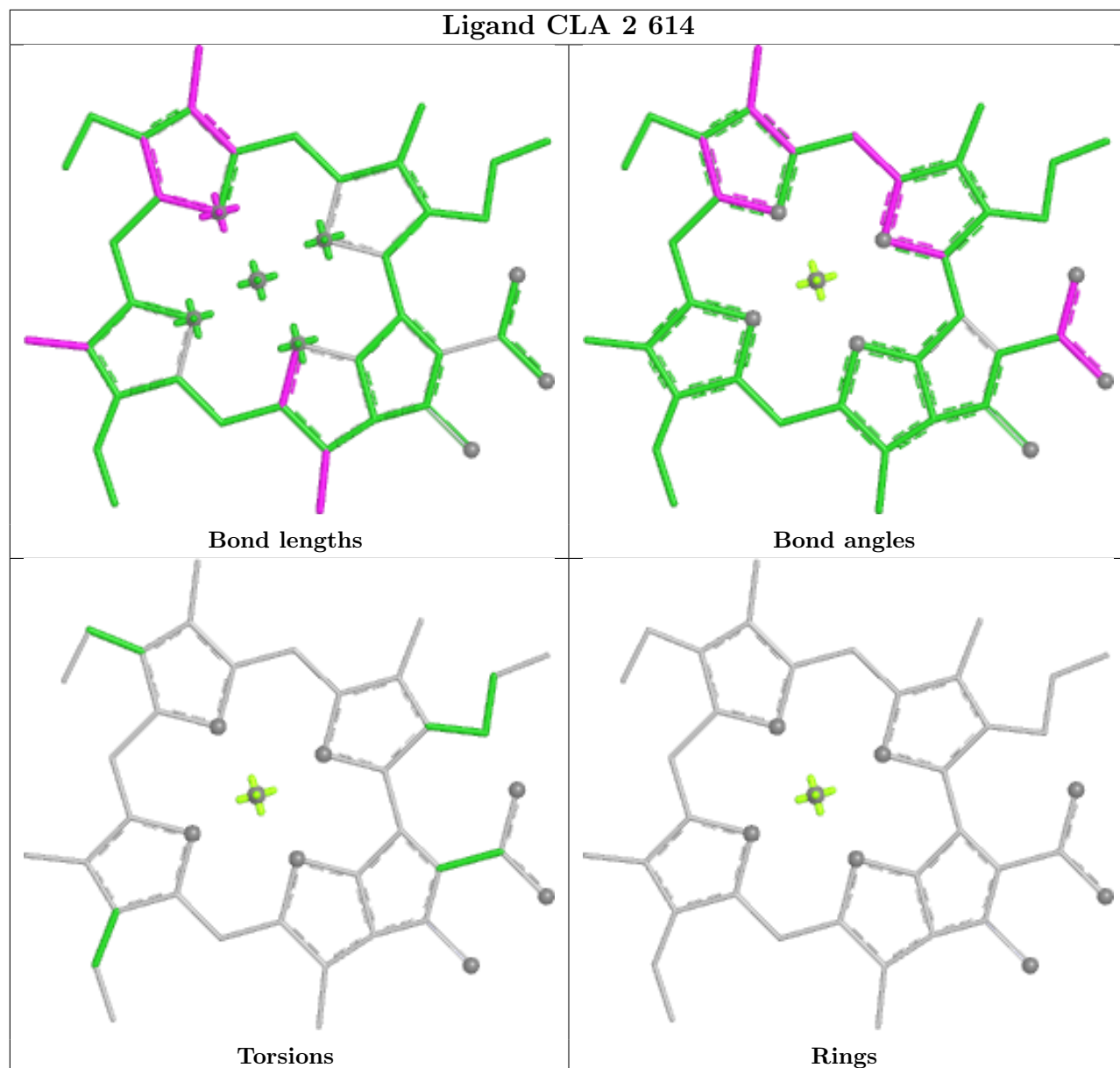


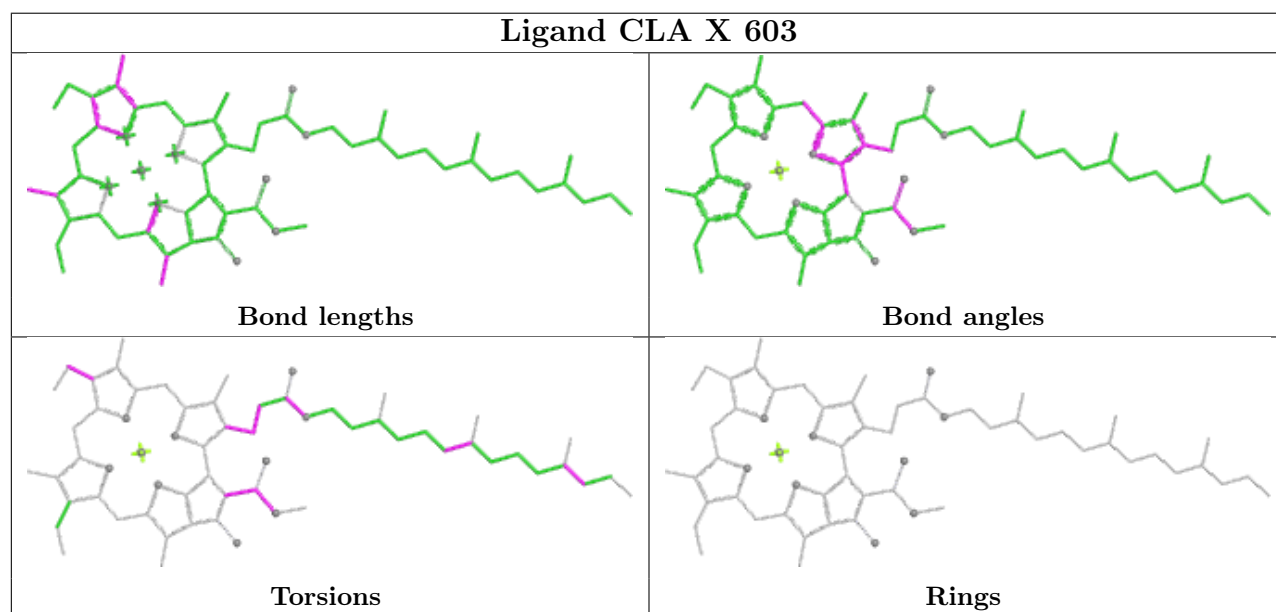
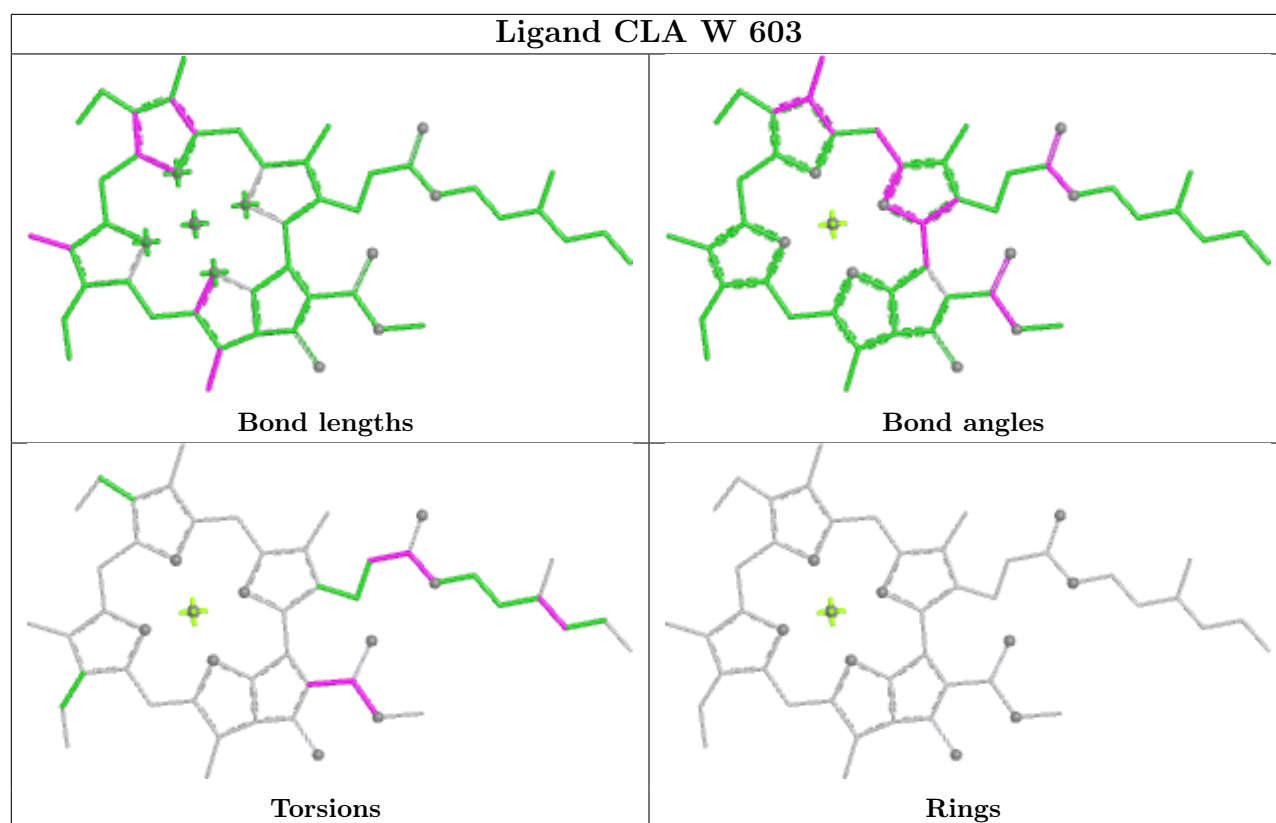
Ligand CHL U 605

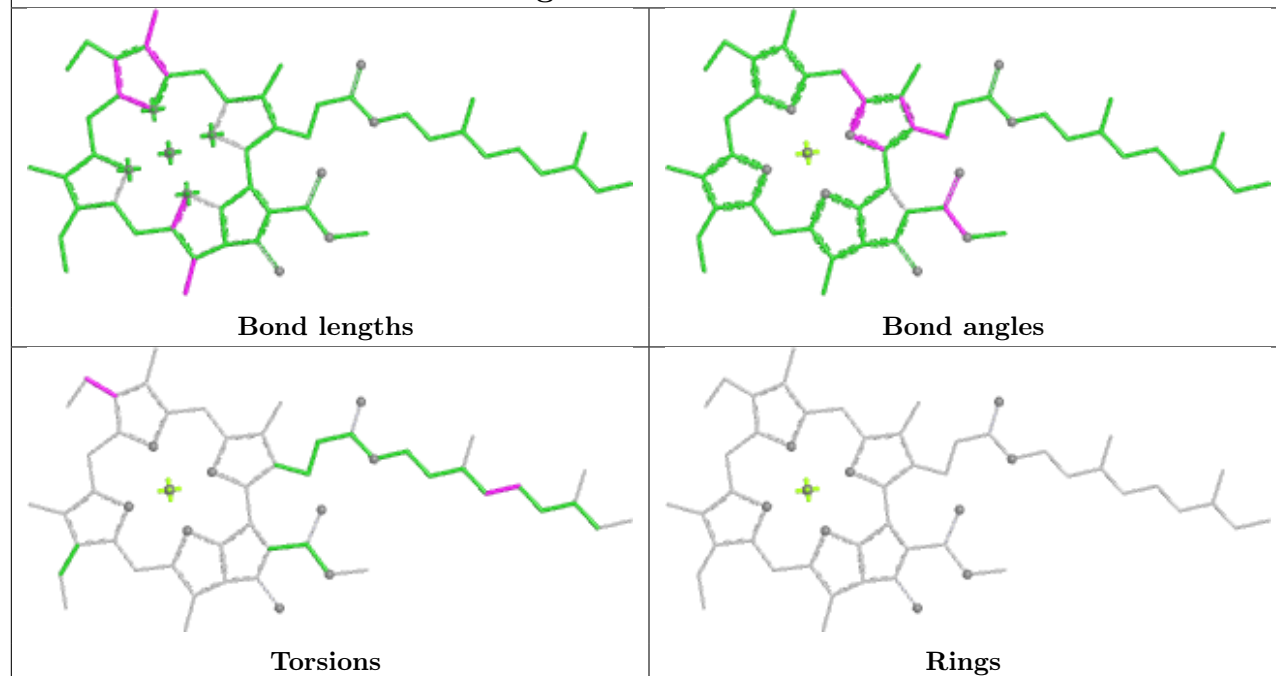
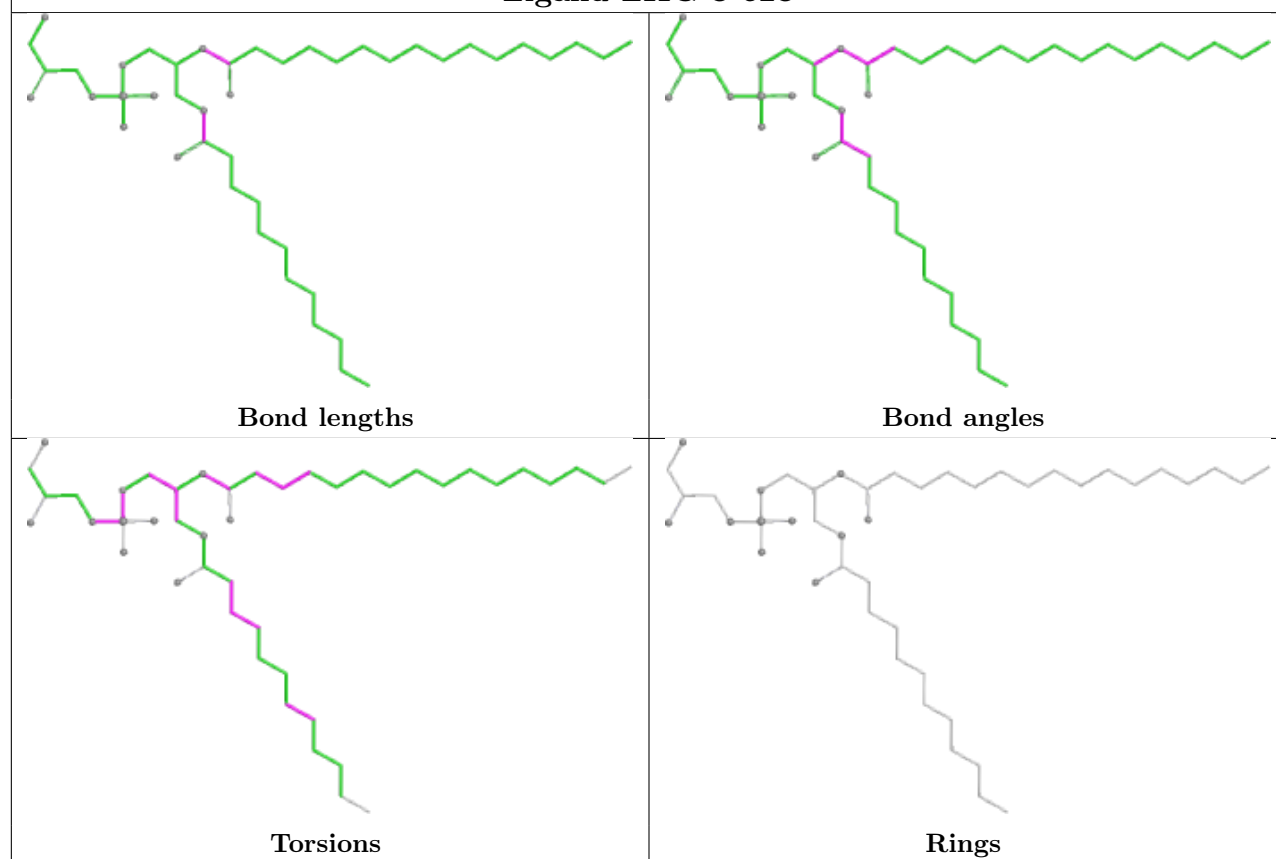


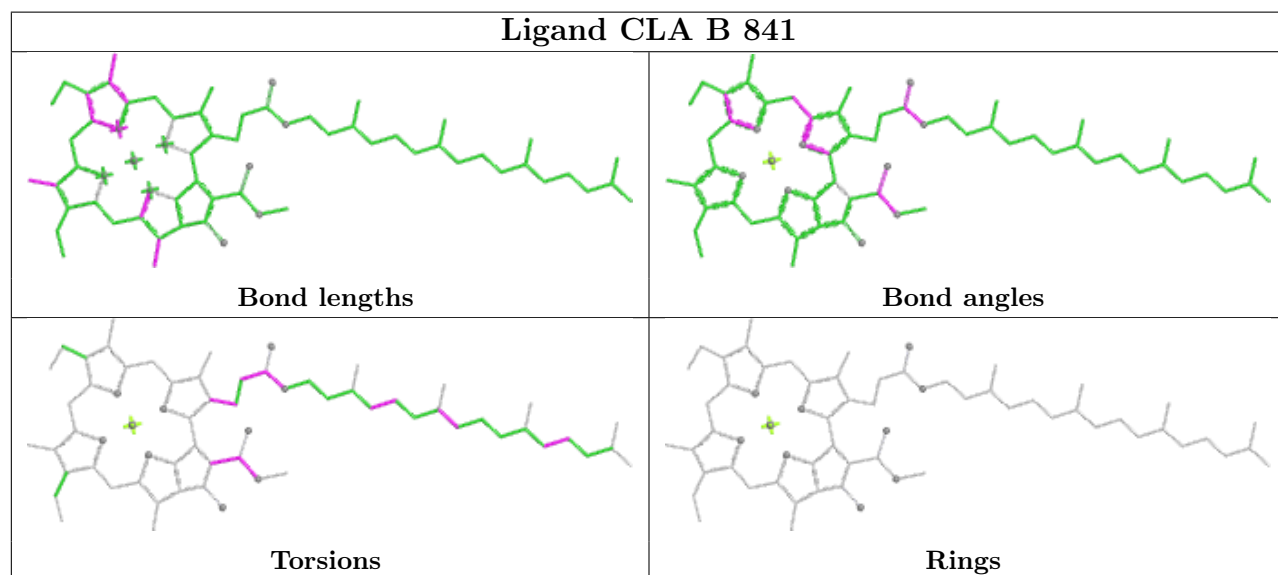
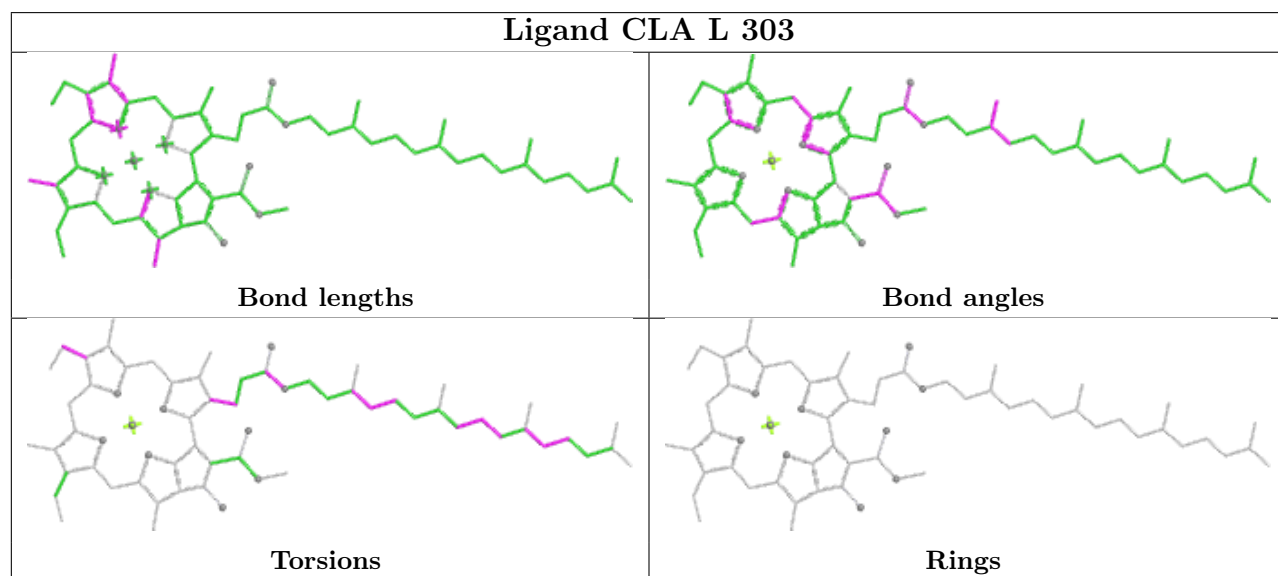
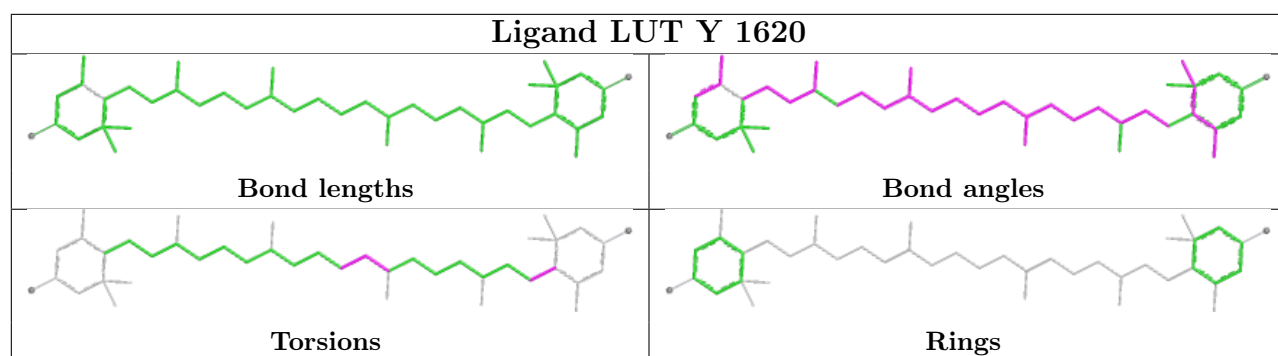


Ligand CLA 2 614

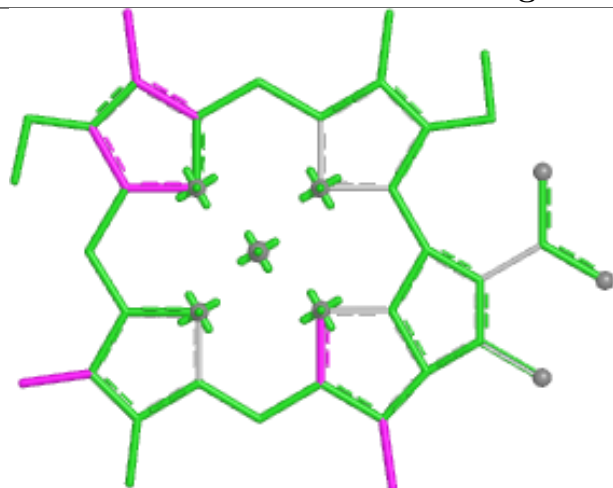




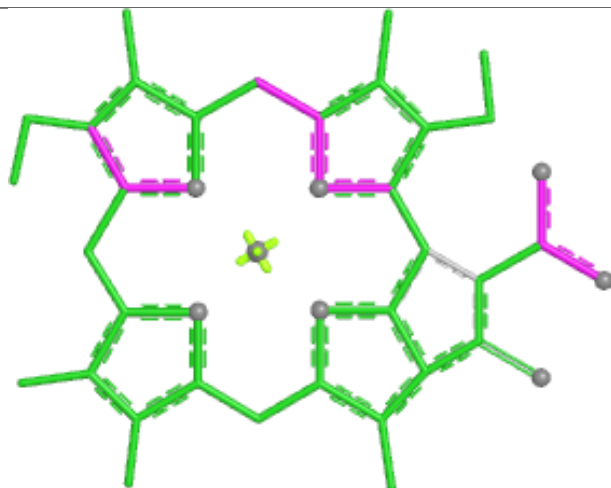
Ligand CLA 5 601**Ligand LHG 3 623**



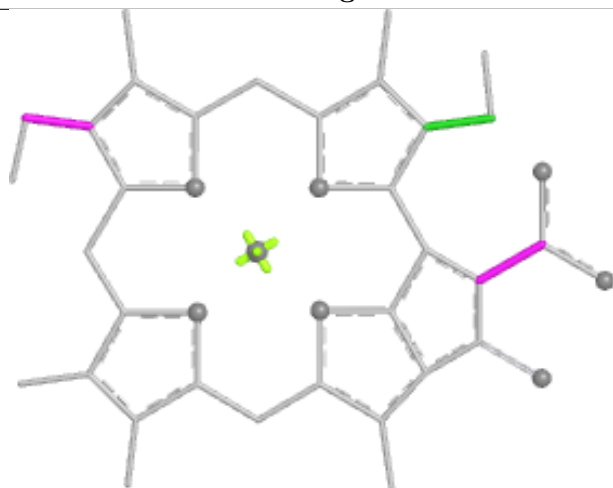
Ligand CLA 5 606



Bond lengths



Bond angles

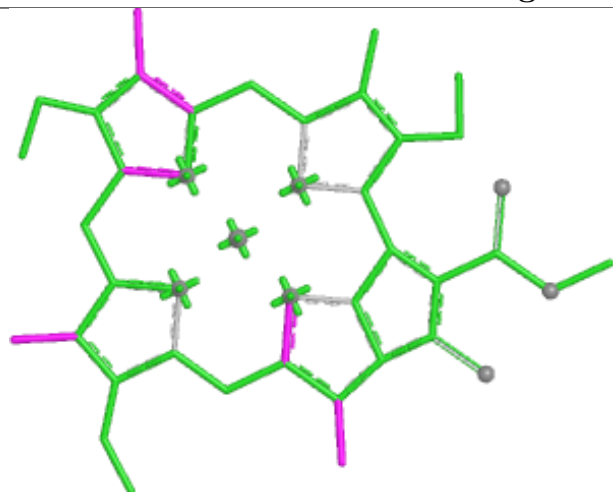


Torsions

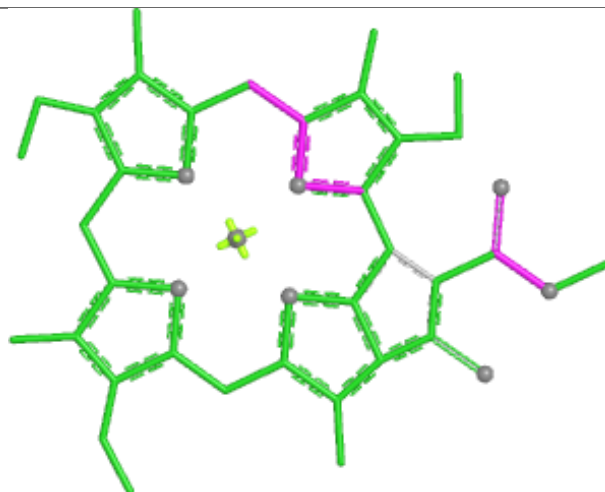


Rings

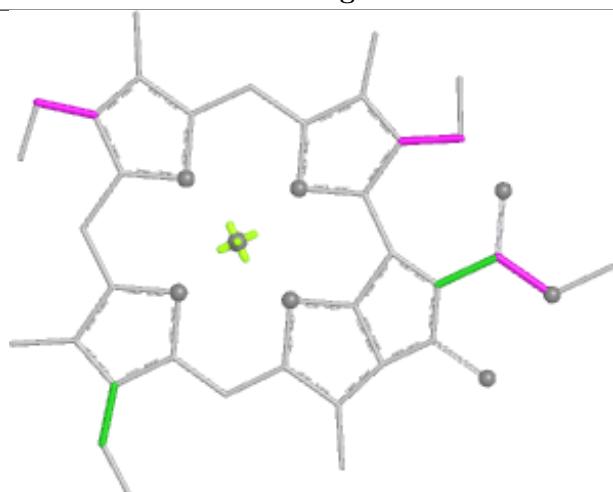
Ligand CLA 8 611



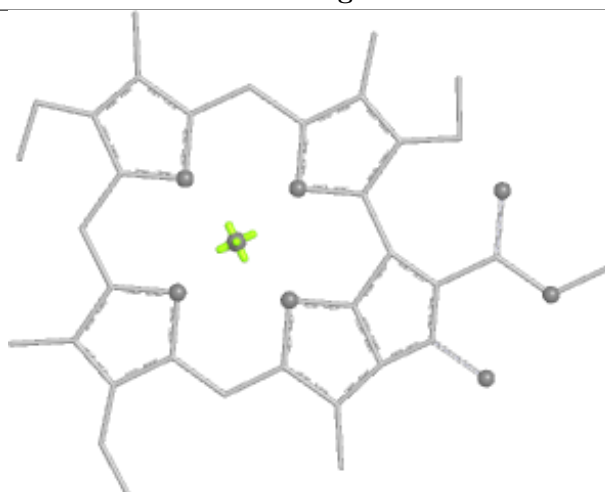
Bond lengths



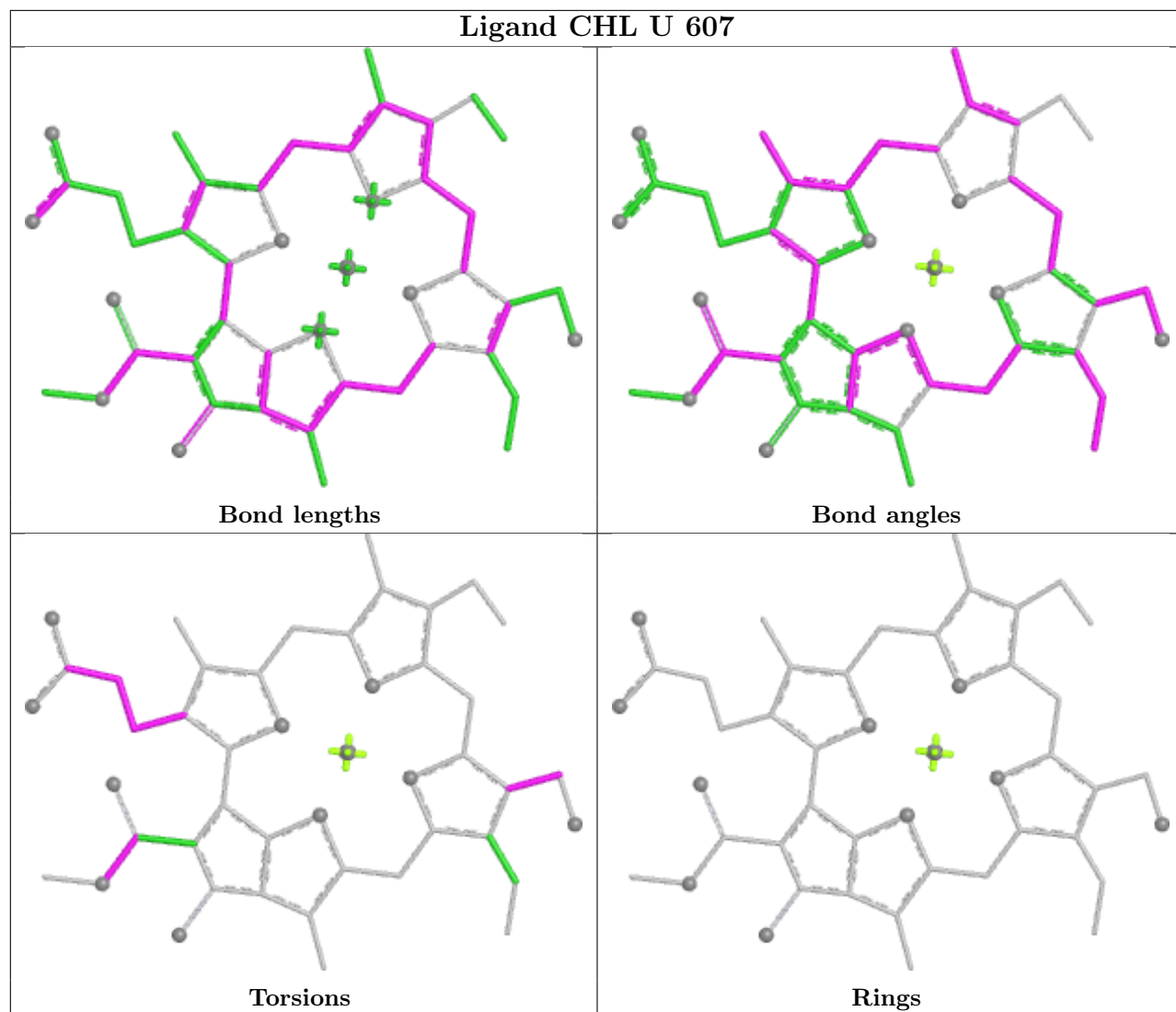
Bond angles



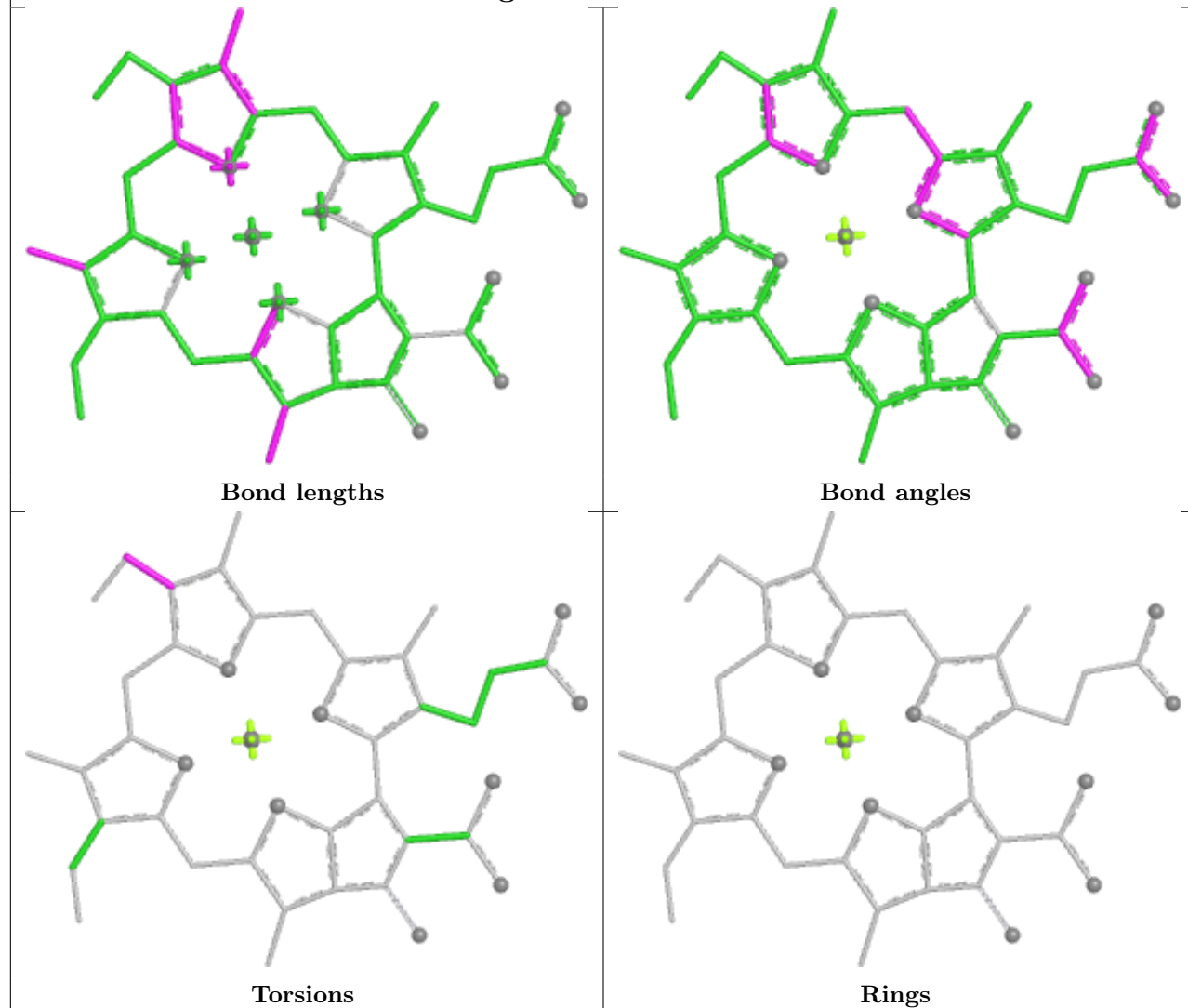
Torsions



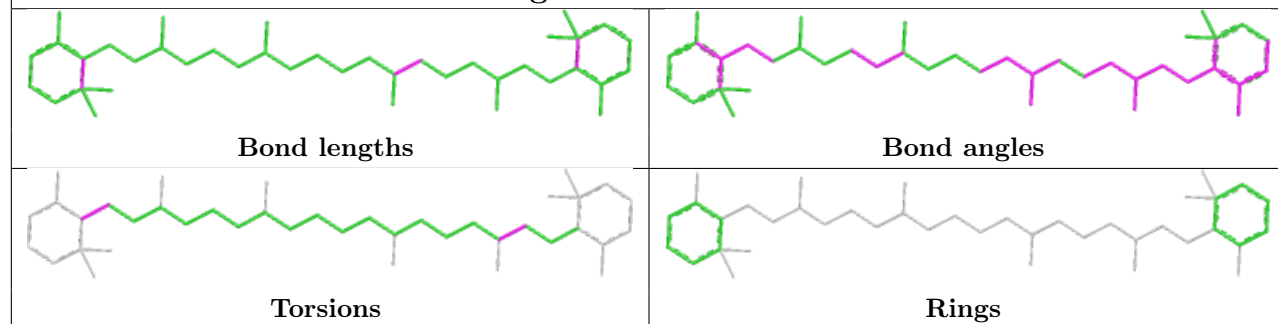
Rings

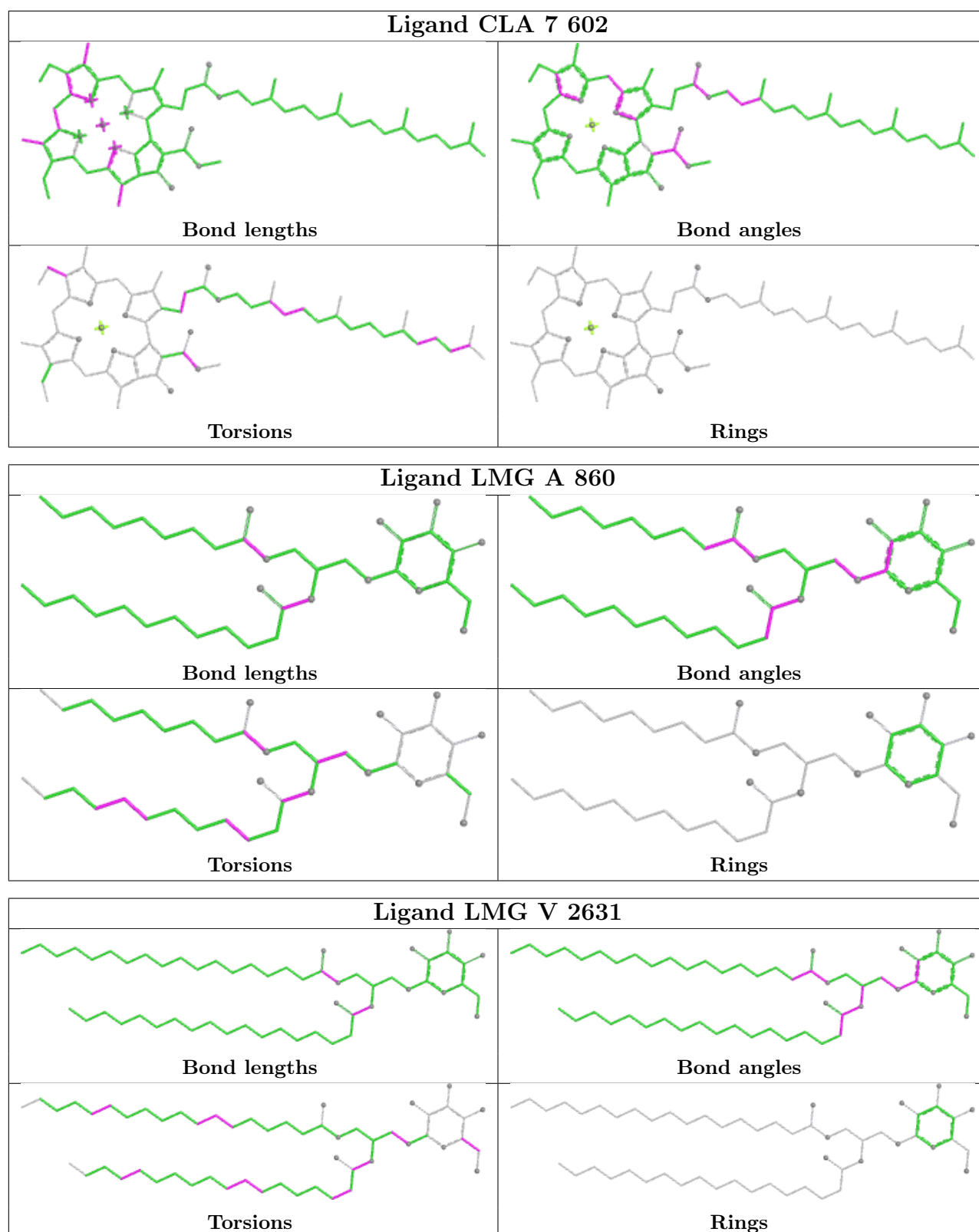


Ligand CLA 2 607

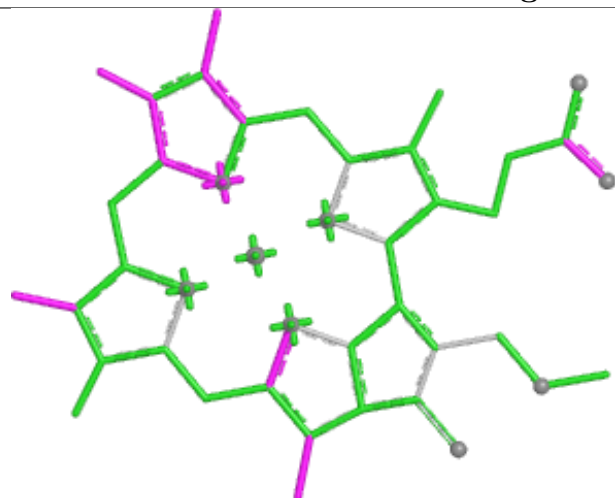


Ligand BCR A 848

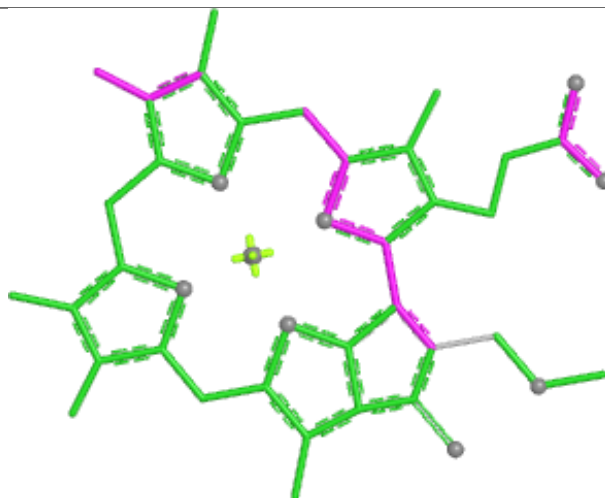




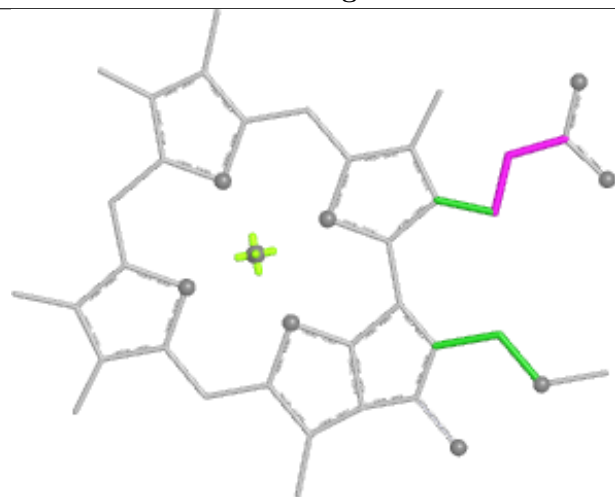
Ligand CLA 5 616



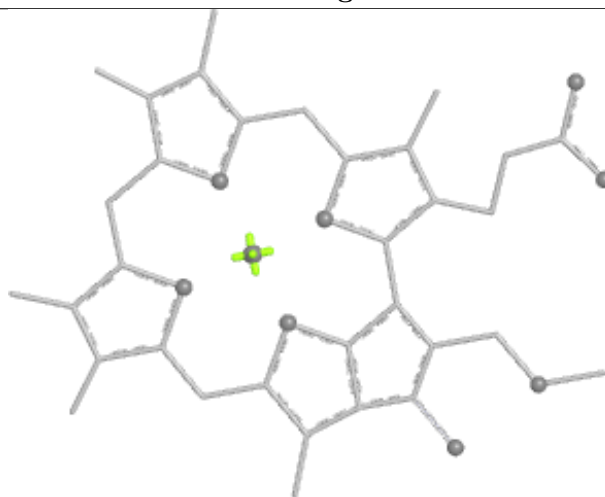
Bond lengths



Bond angles

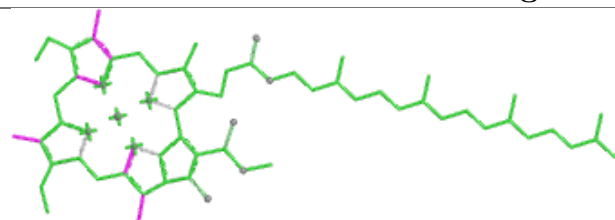


Torsions

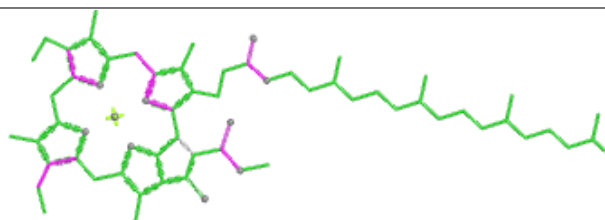


Rings

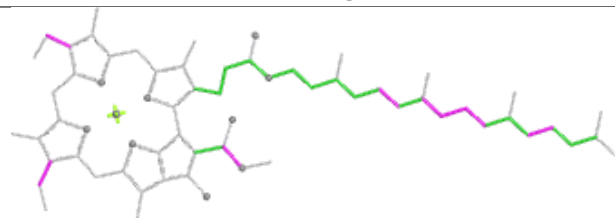
Ligand CLA 4 608



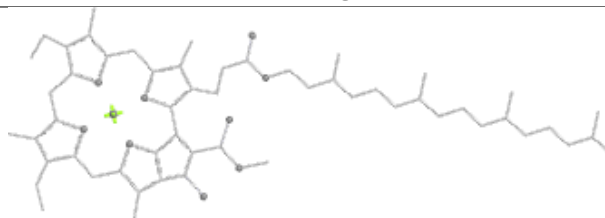
Bond lengths



Bond angles

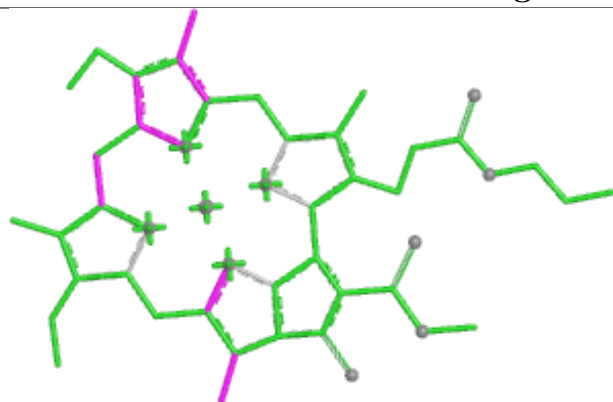


Torsions

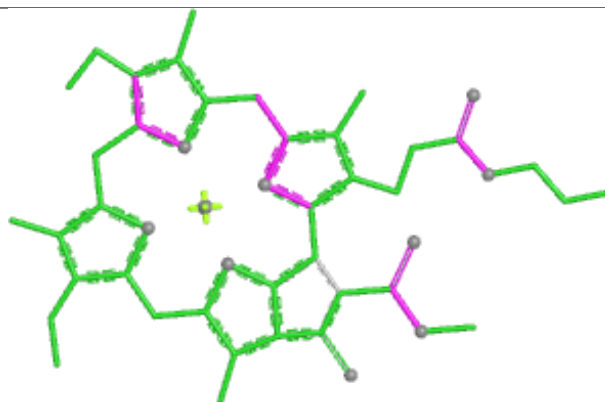


Rings

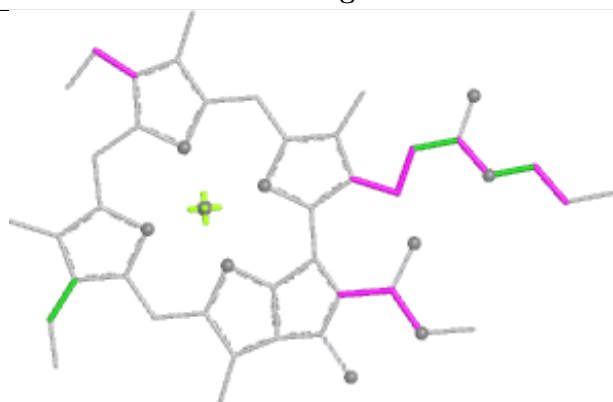
Ligand CLA Y 614



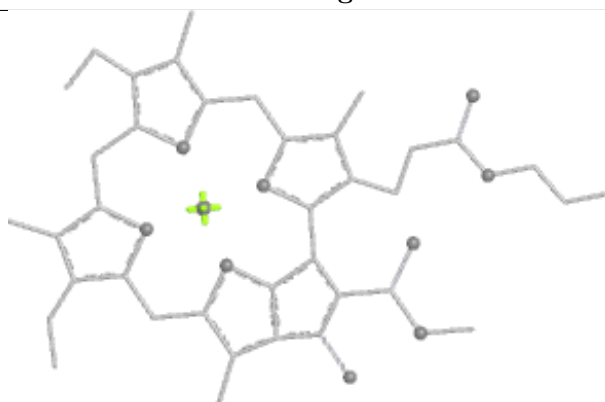
Bond lengths



Bond angles

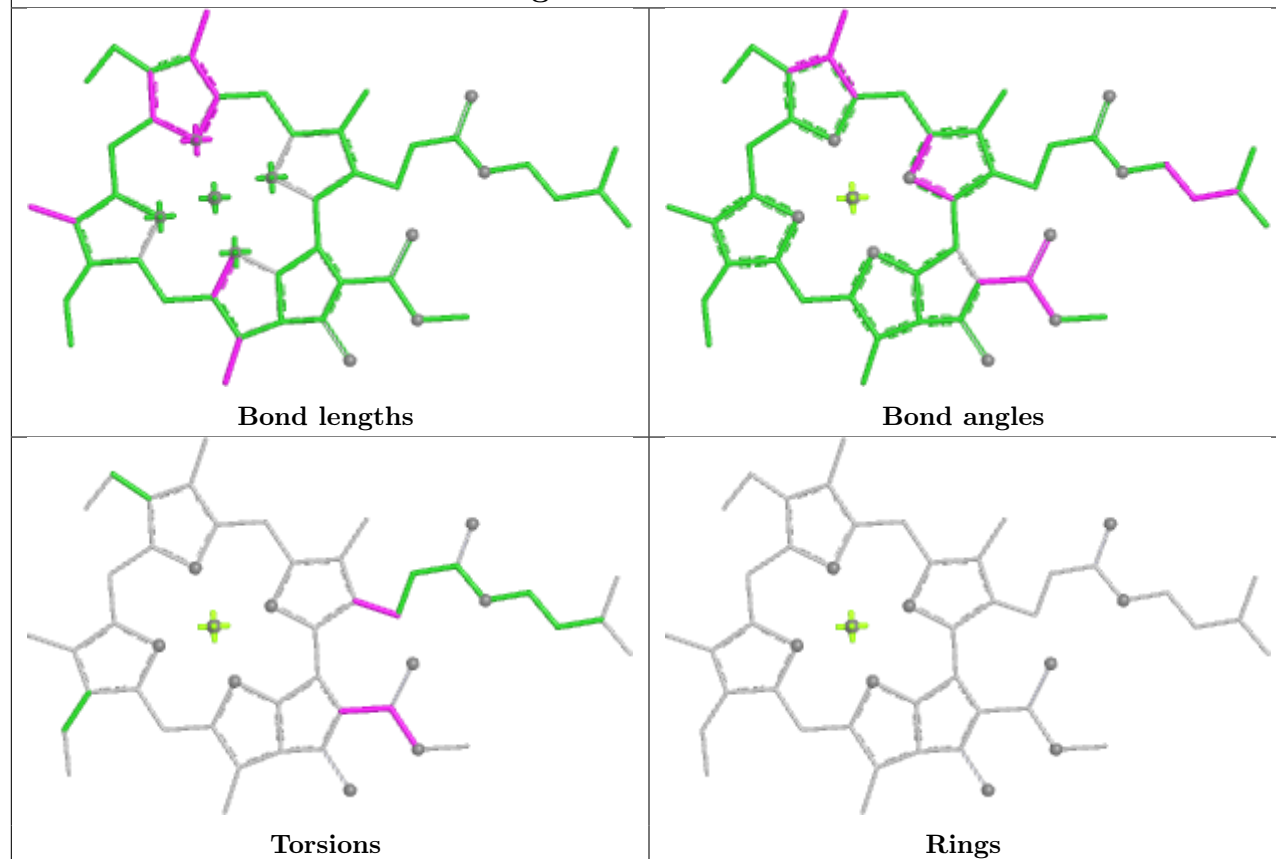


Torsions

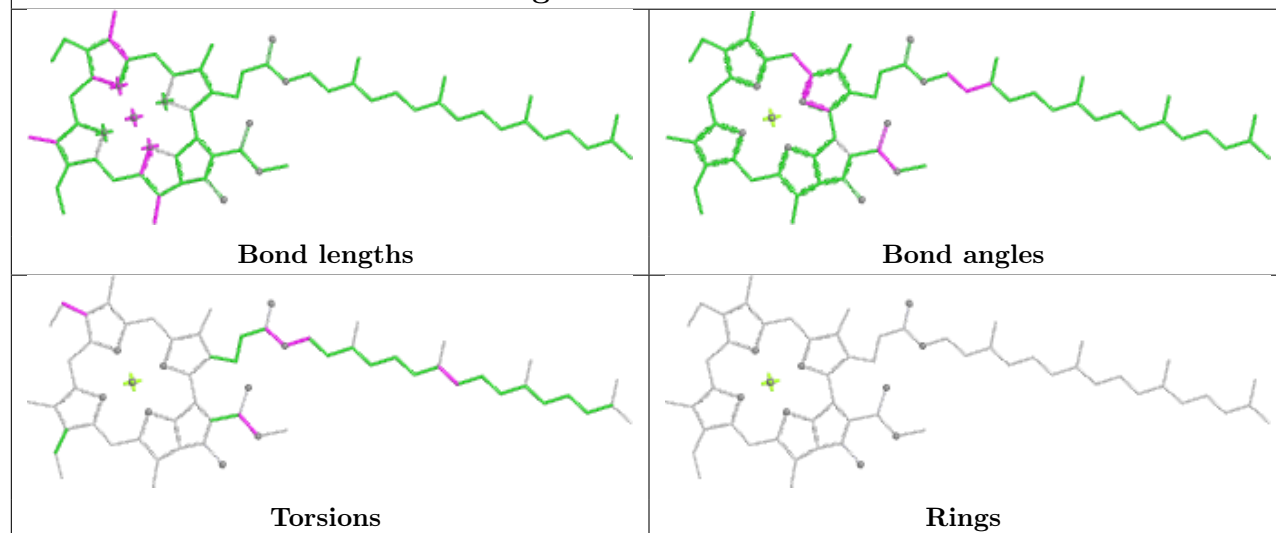


Rings

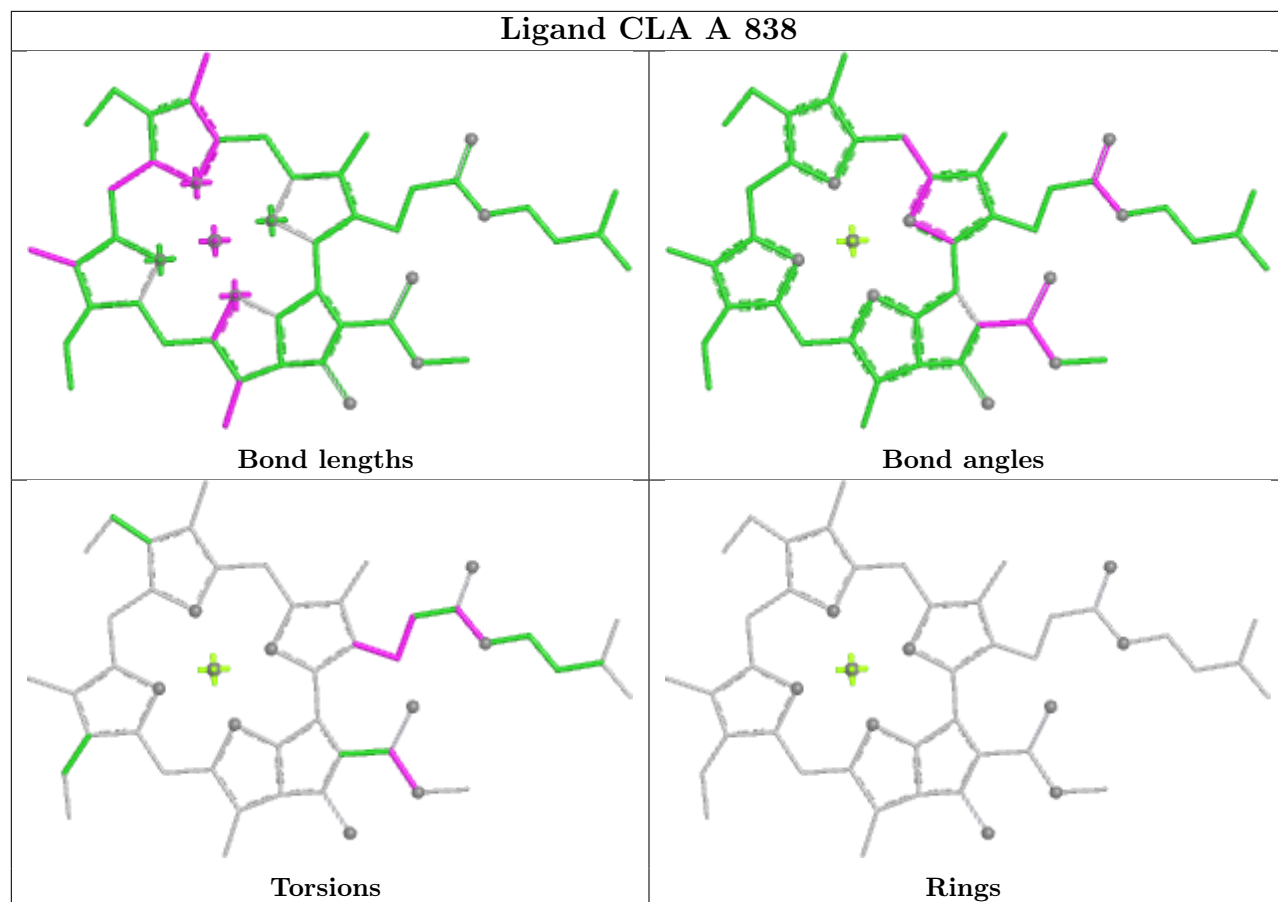
Ligand CLA A 845



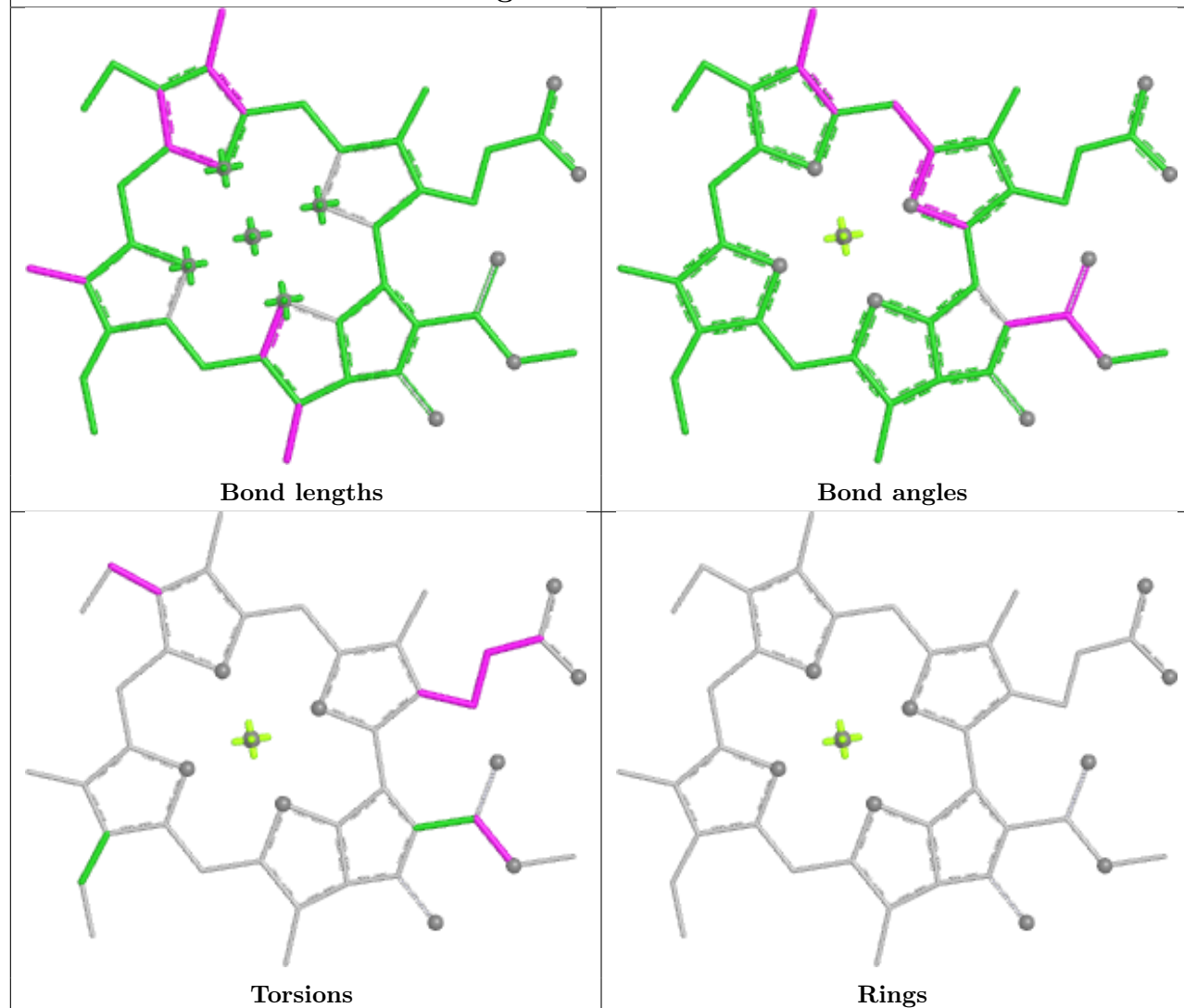
Ligand CLA B 840



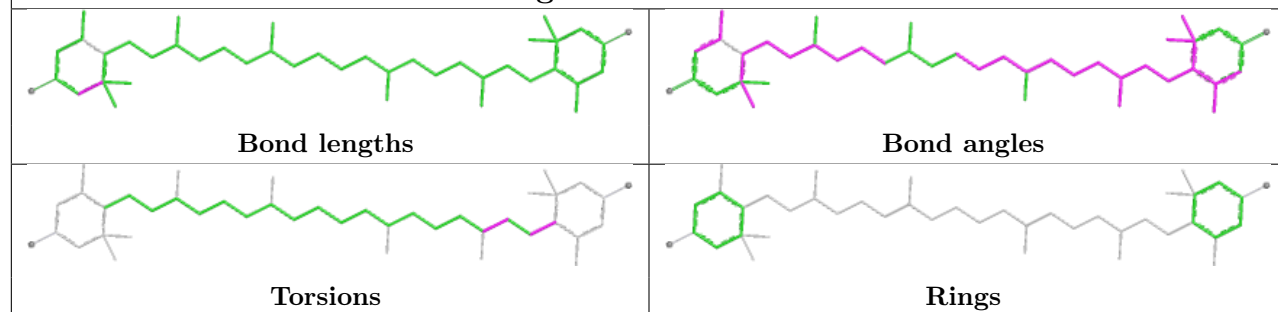
Ligand CLA A 838



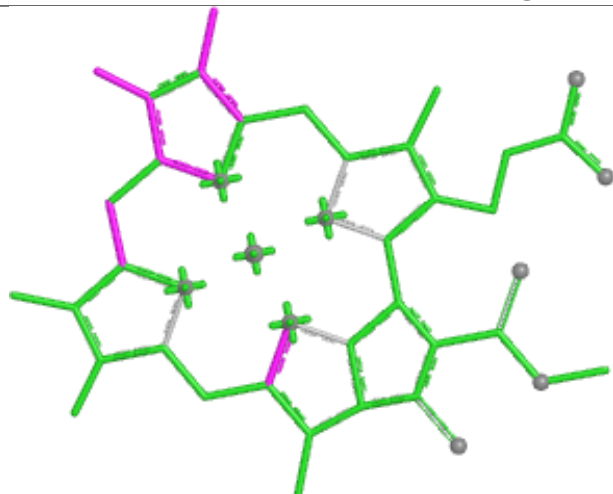
Ligand CLA 6 617



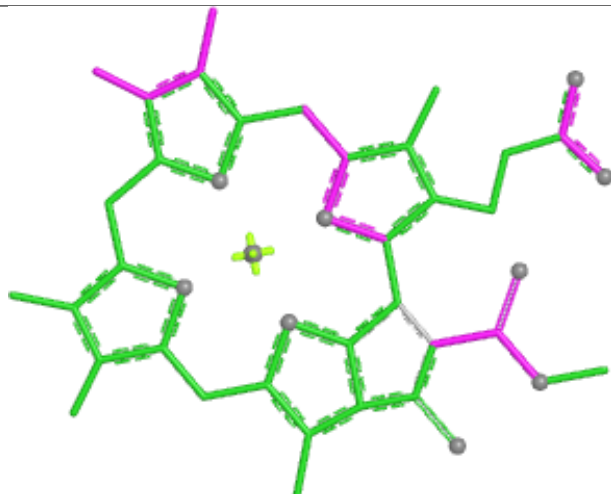
Ligand LUT 4 619



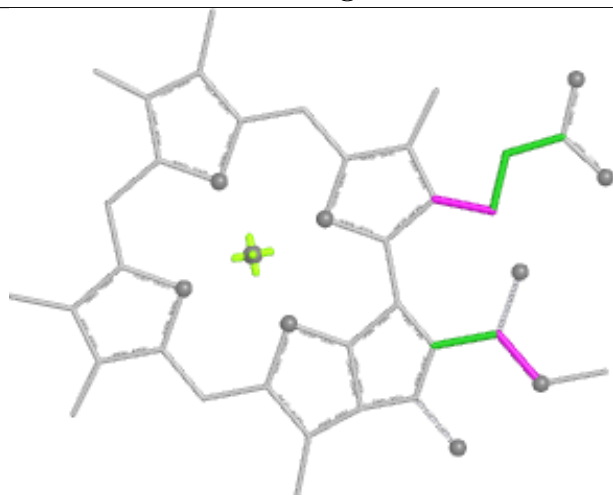
Ligand CLA 8 616



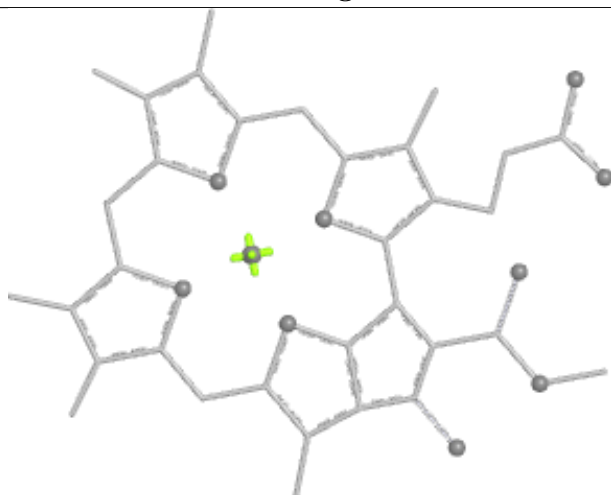
Bond lengths



Bond angles

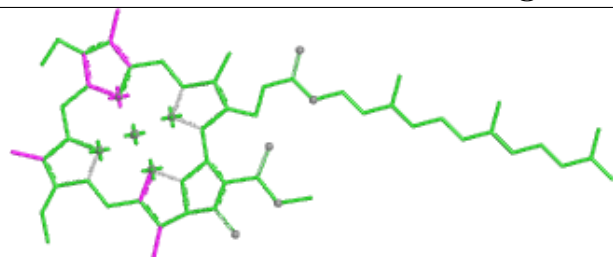


Torsions

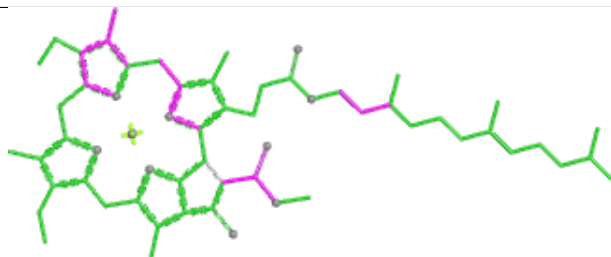


Rings

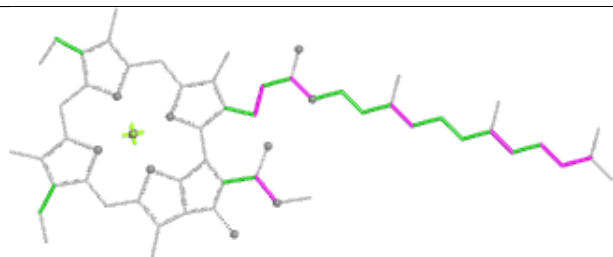
Ligand CLA 8 602



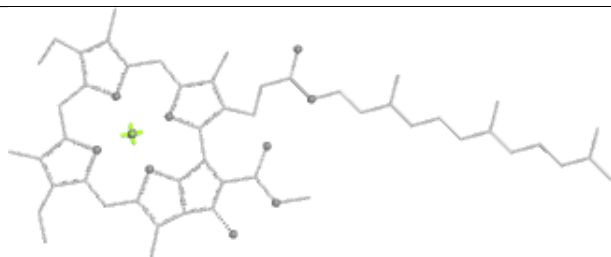
Bond lengths



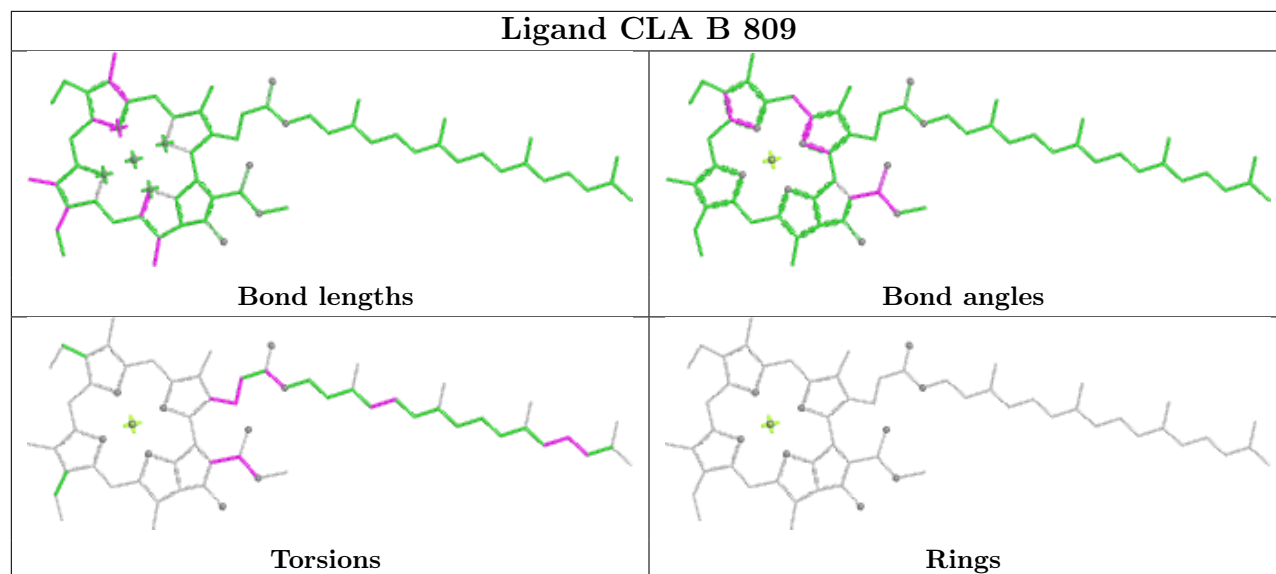
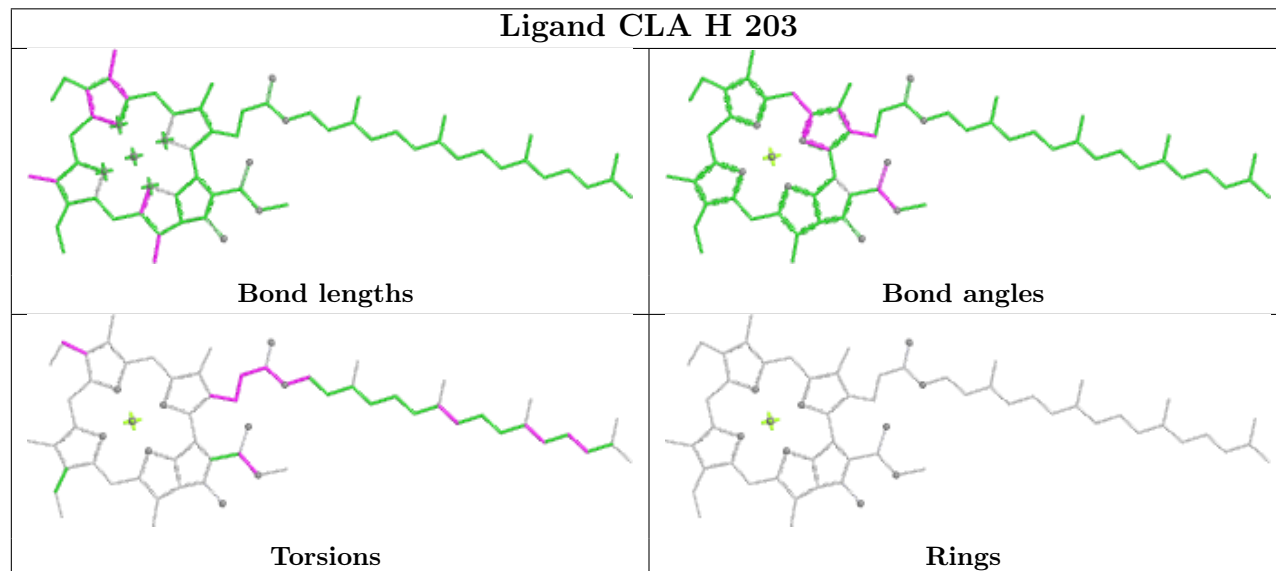
Bond angles



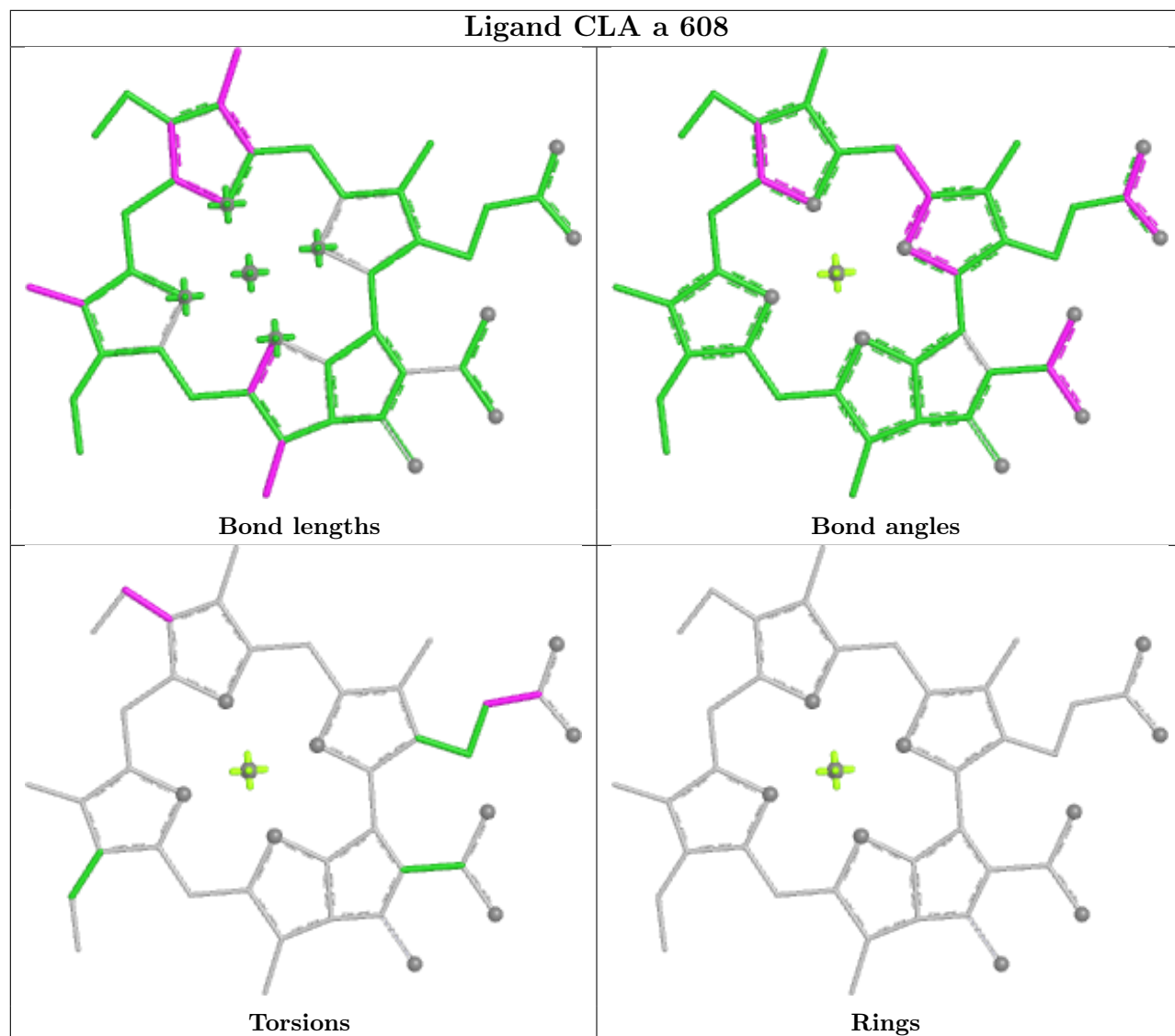
Torsions

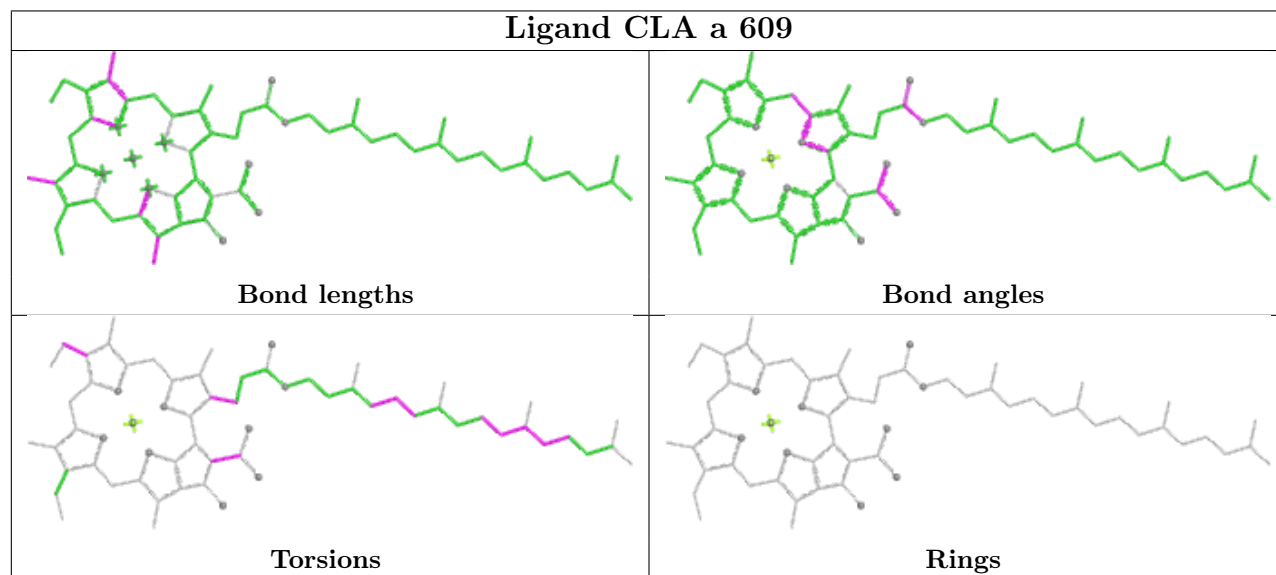
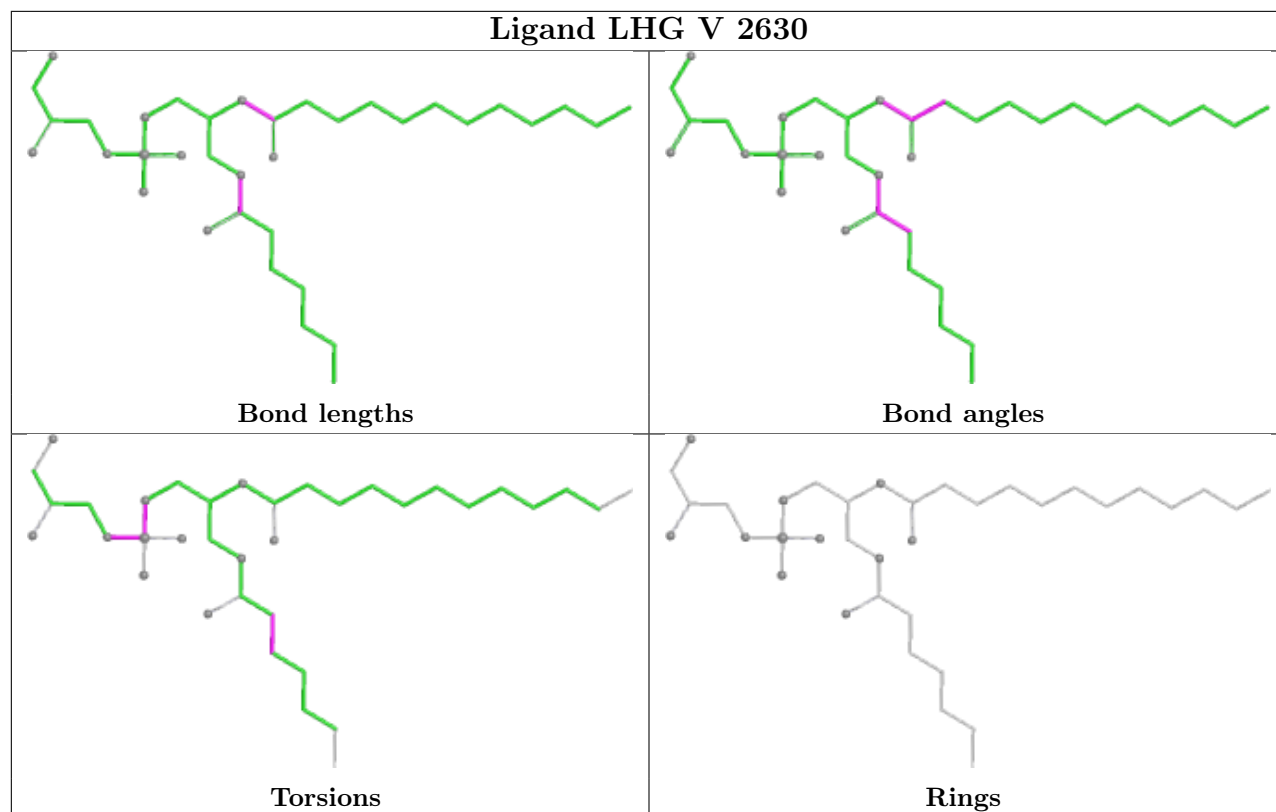


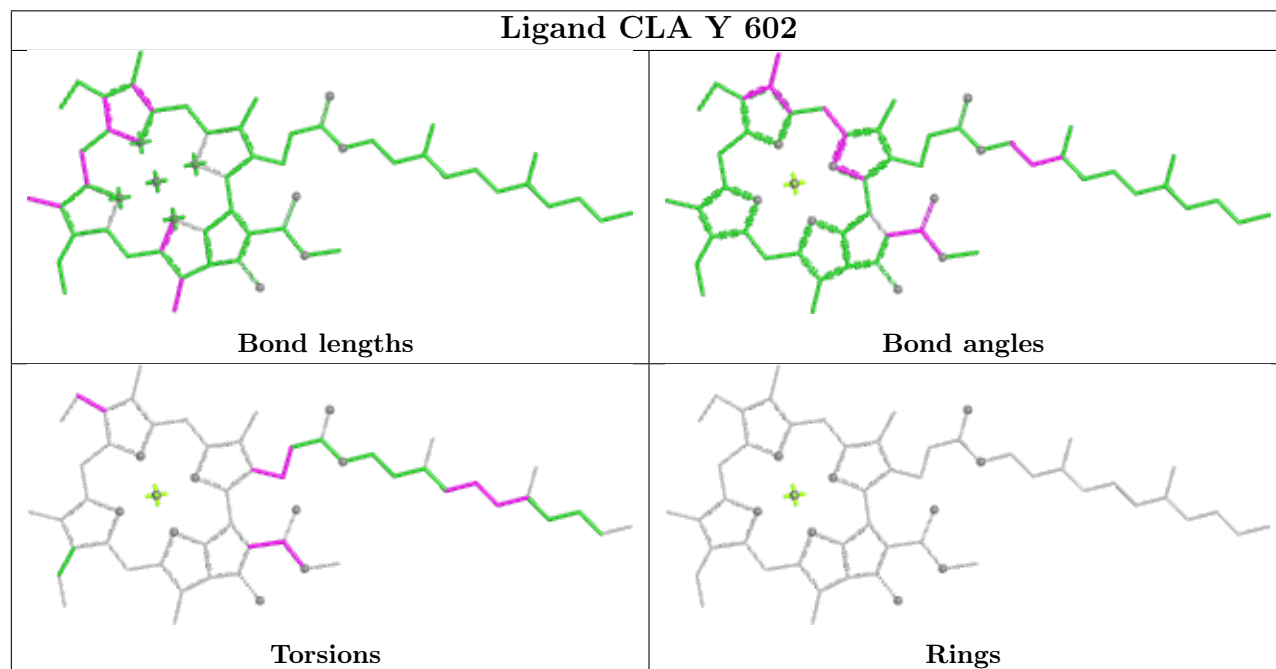
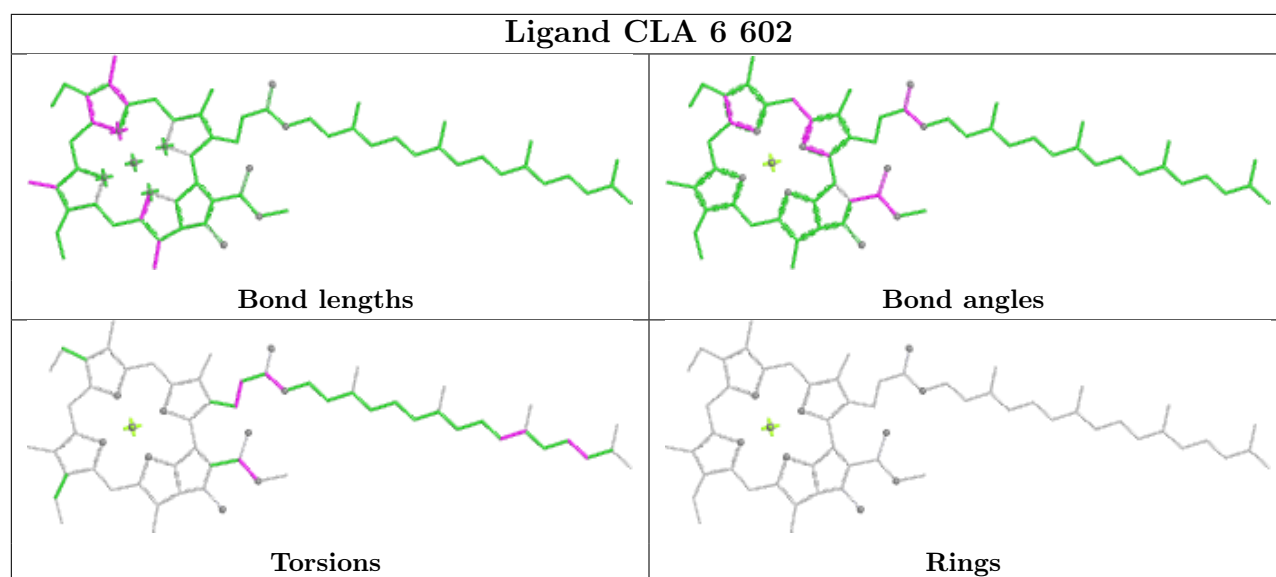
Rings

Ligand CLA B 809**Ligand CLA H 203**

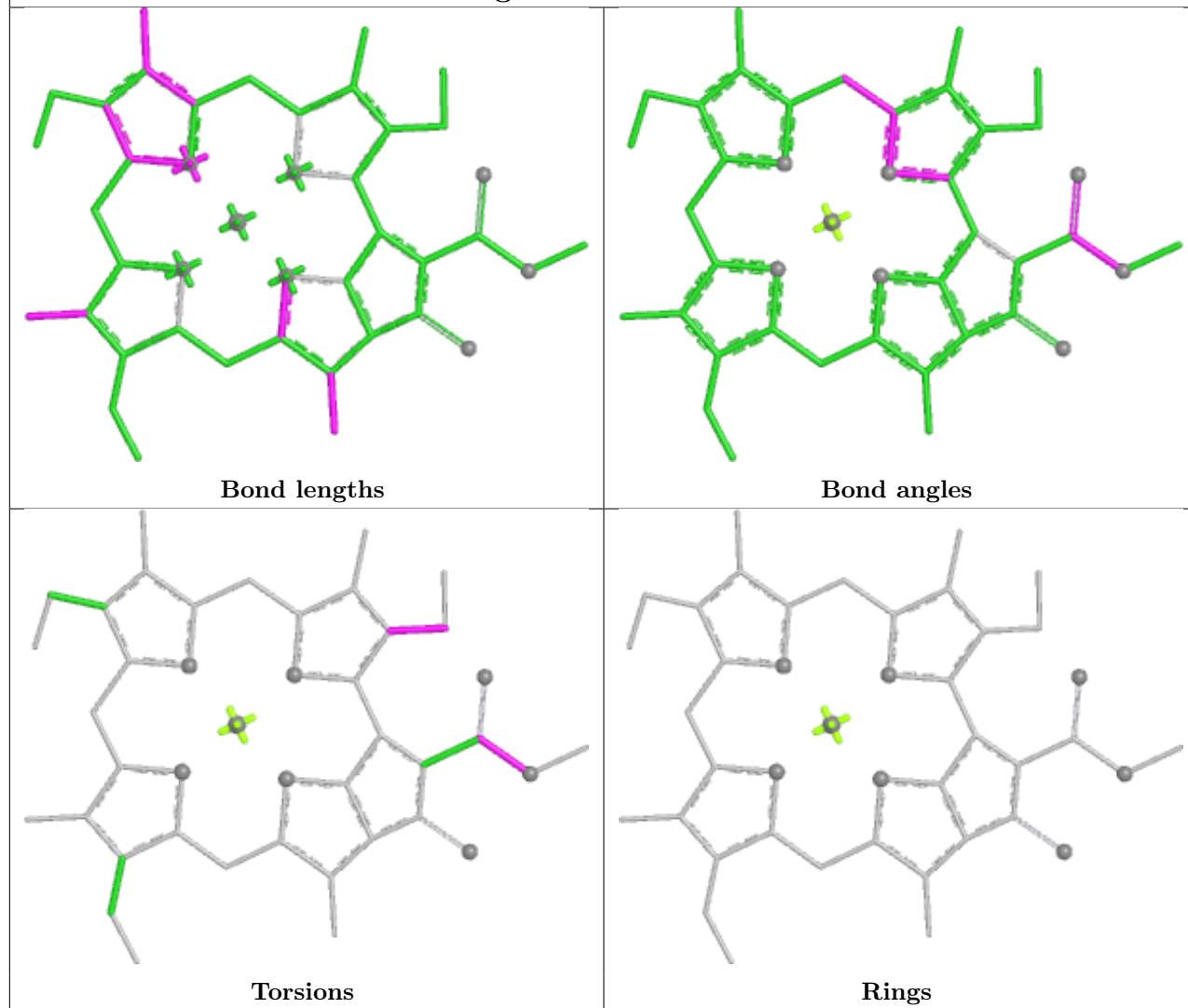
Ligand CLA a 608



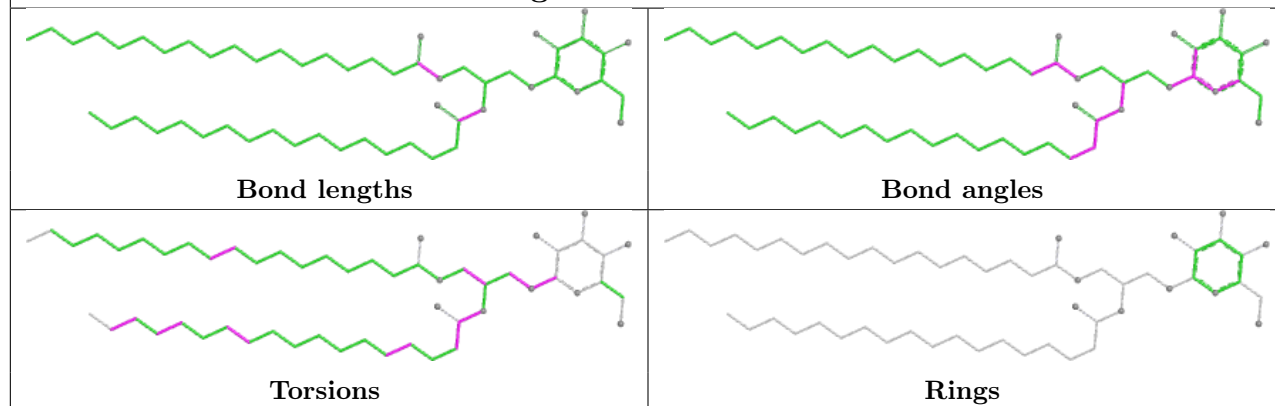




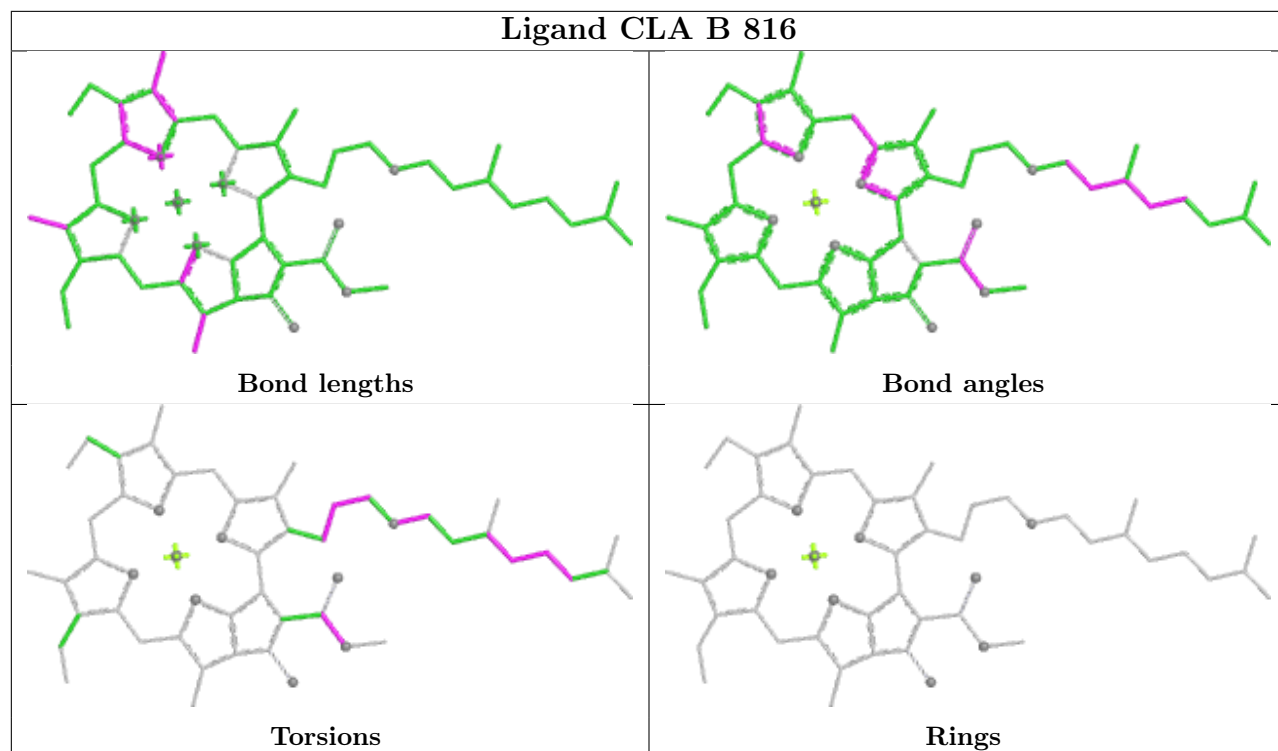
Ligand CLA B 822



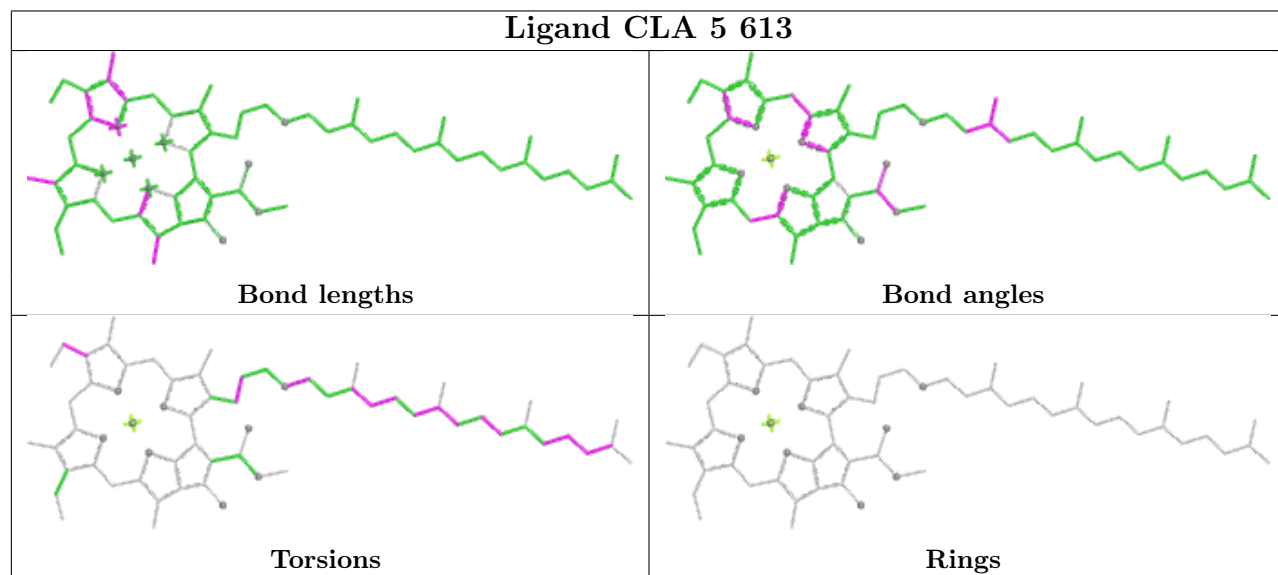
Ligand LMG 9 625

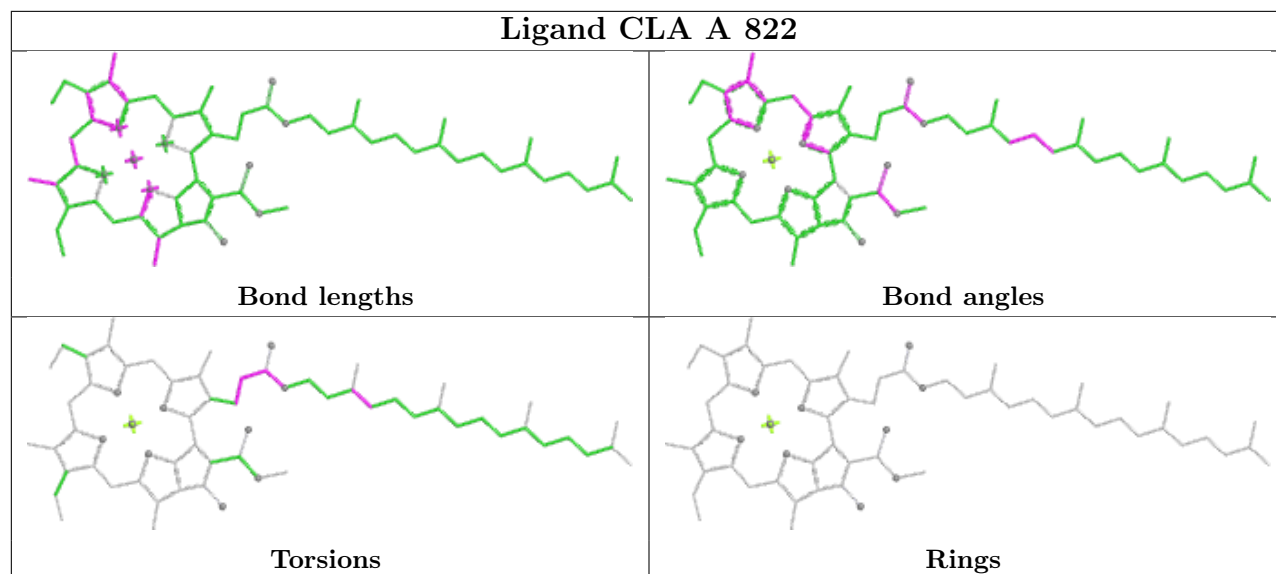
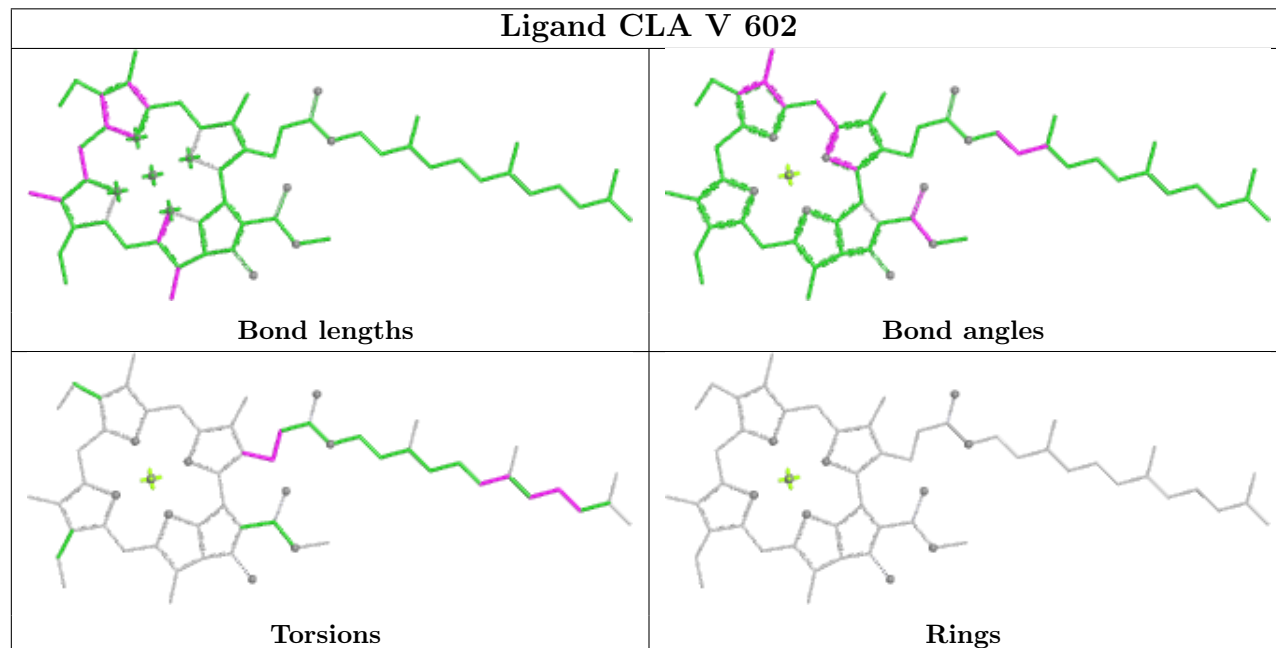


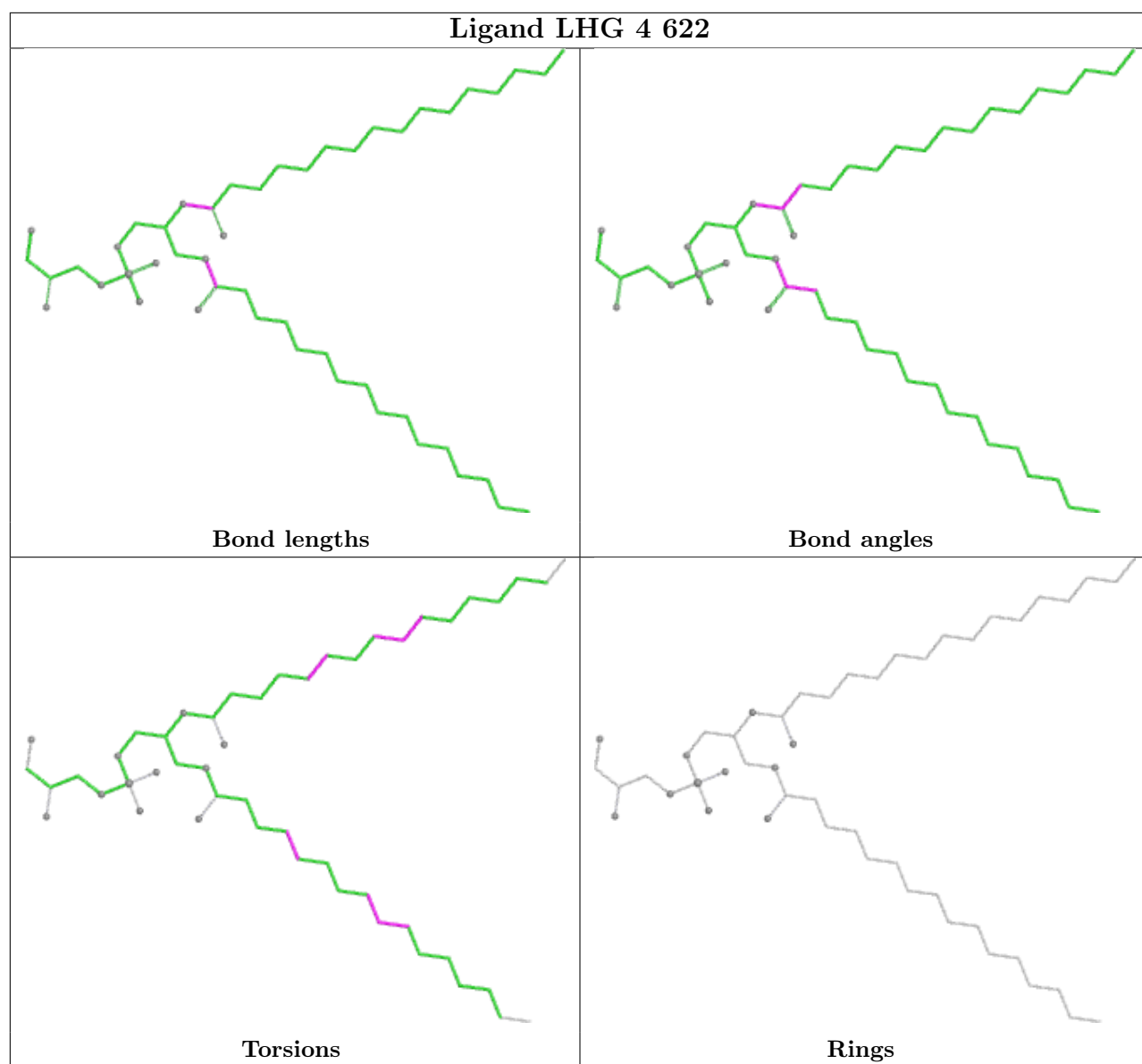
Ligand CLA B 816



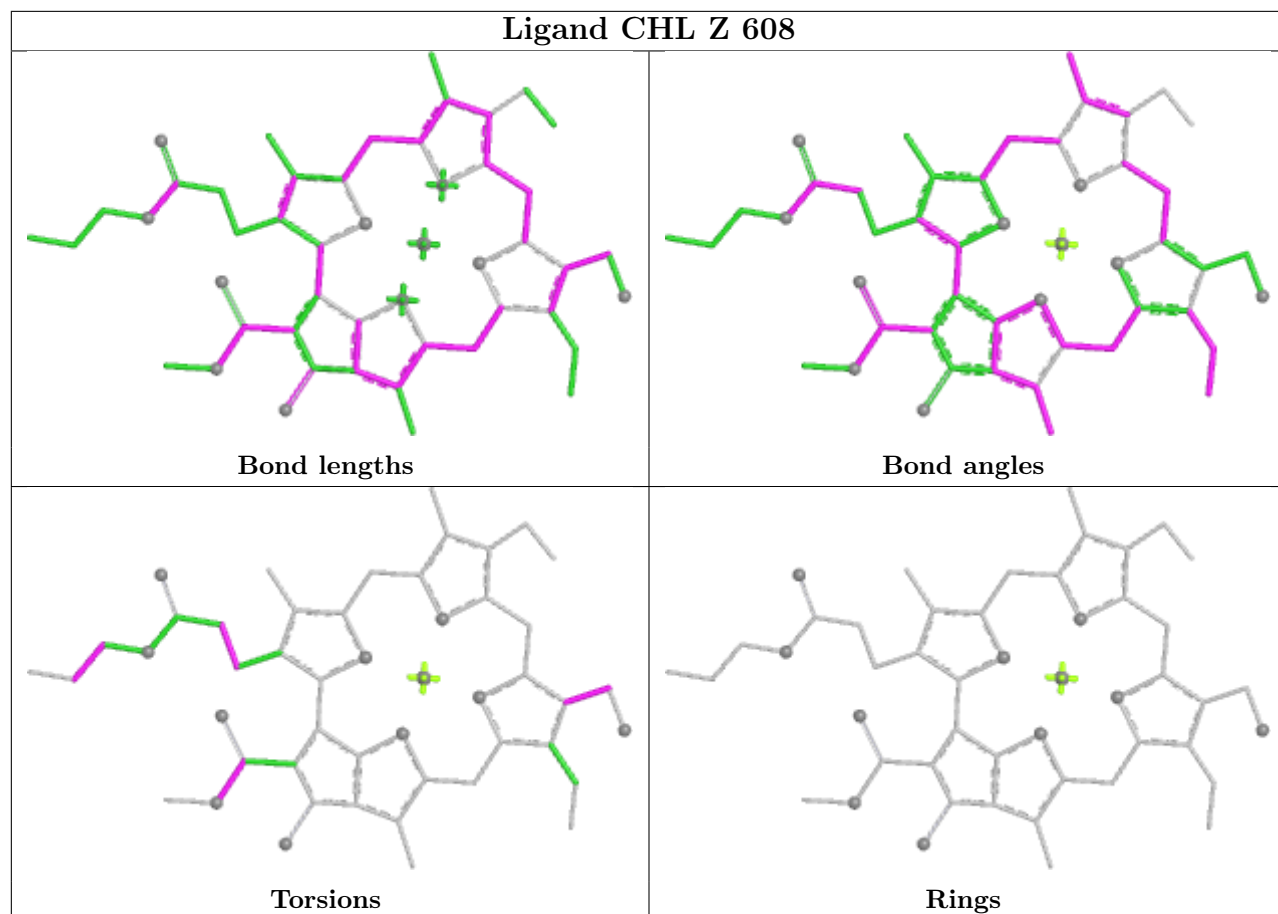
Ligand CLA 5 613



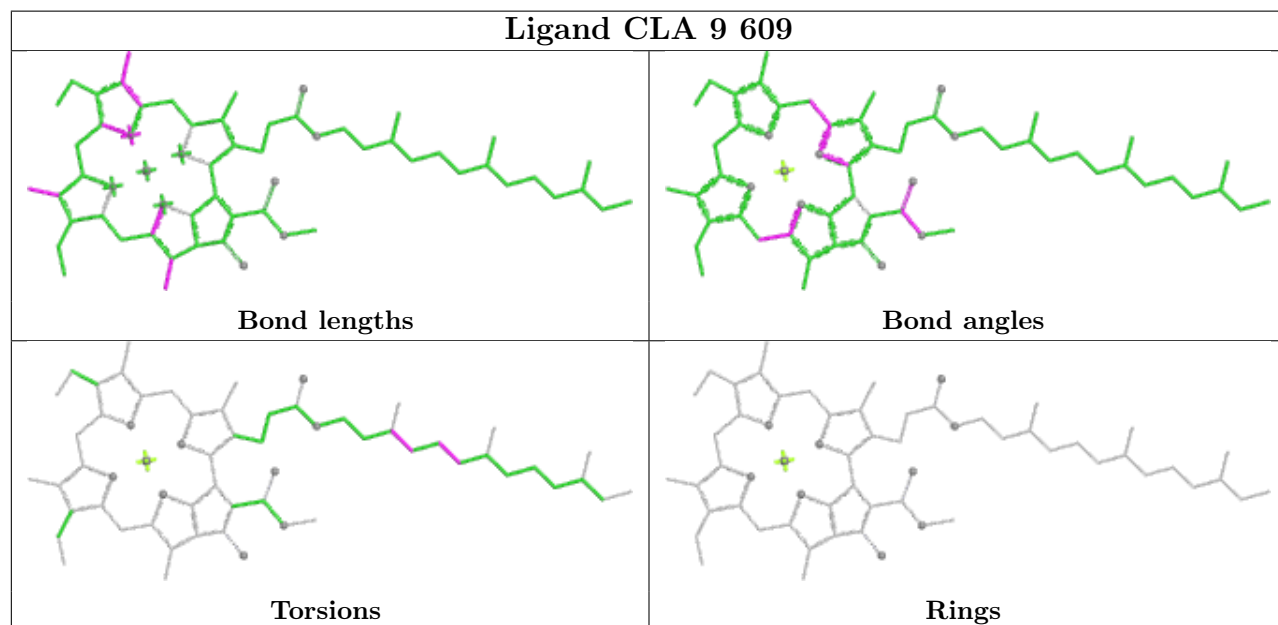
Ligand CLA A 822**Ligand CLA V 602**



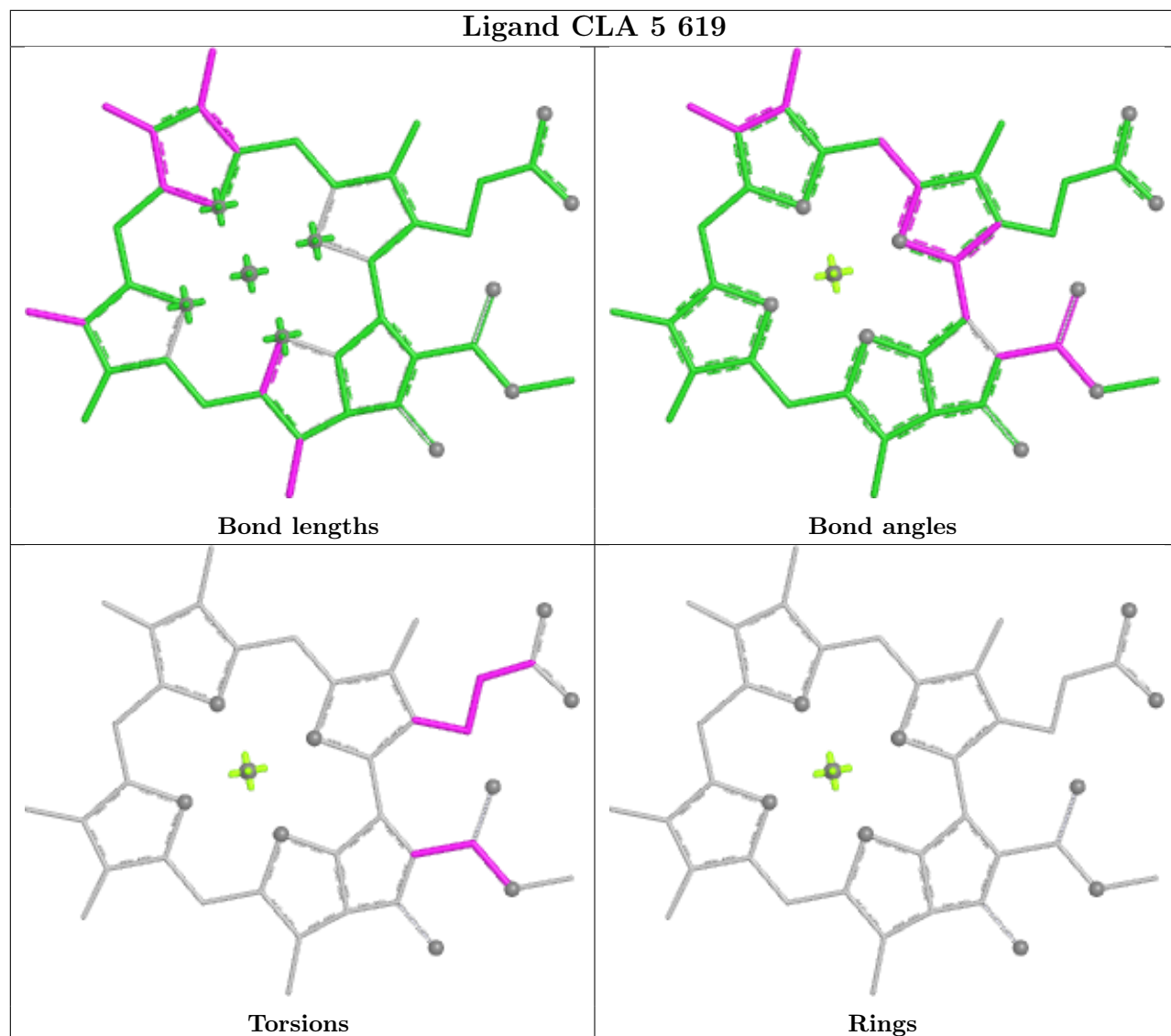
Ligand CHL Z 608



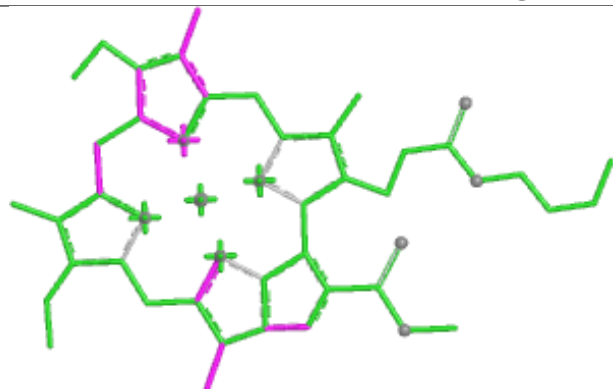
Ligand CLA 9 609



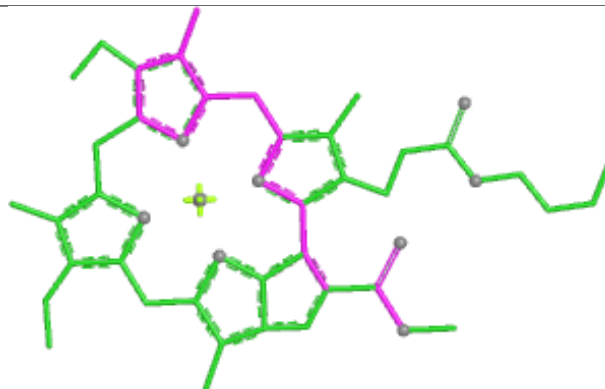
Ligand CLA 5 619



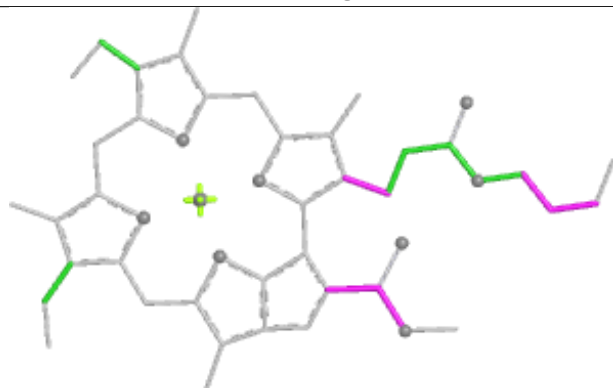
Ligand CLA U 604



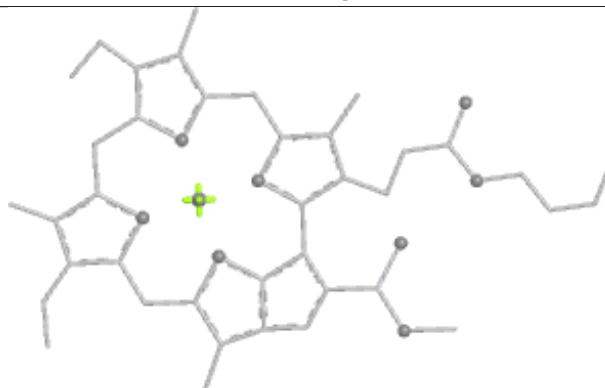
Bond lengths



Bond angles

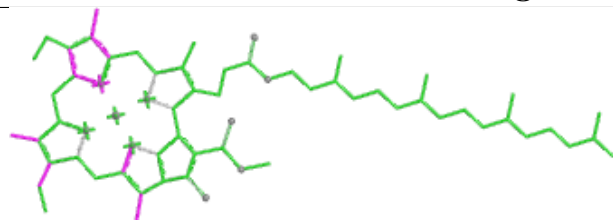


Torsions

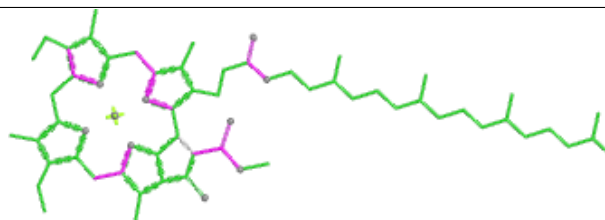


Rings

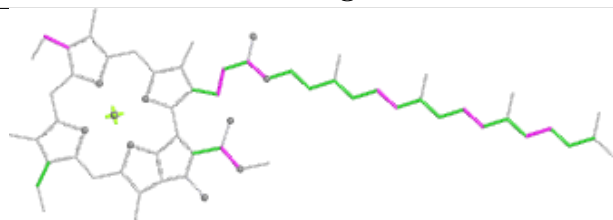
Ligand CLA B 837



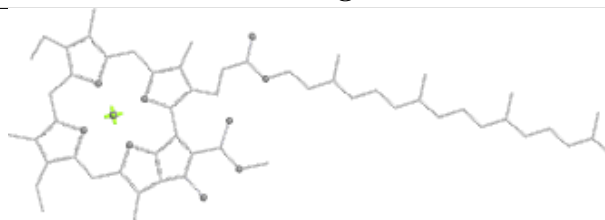
Bond lengths



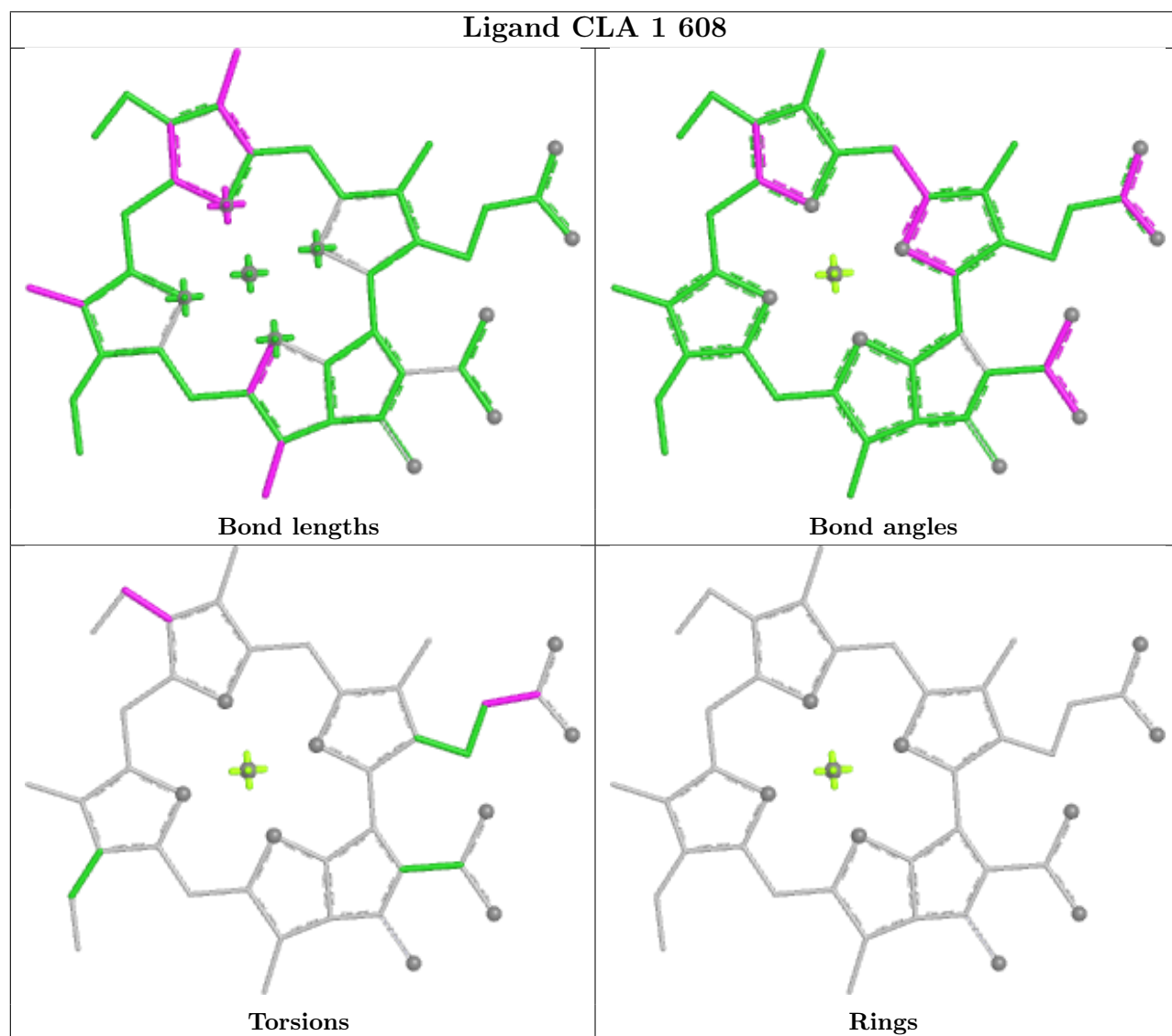
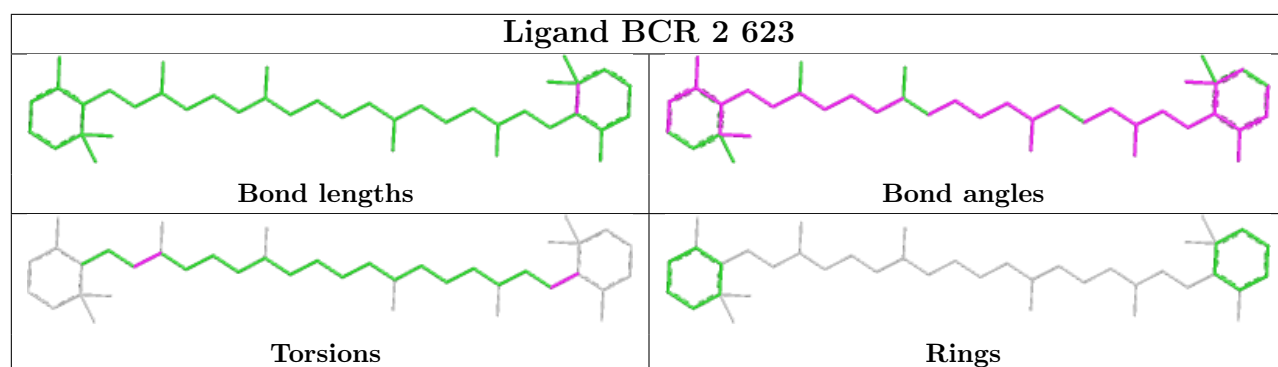
Bond angles

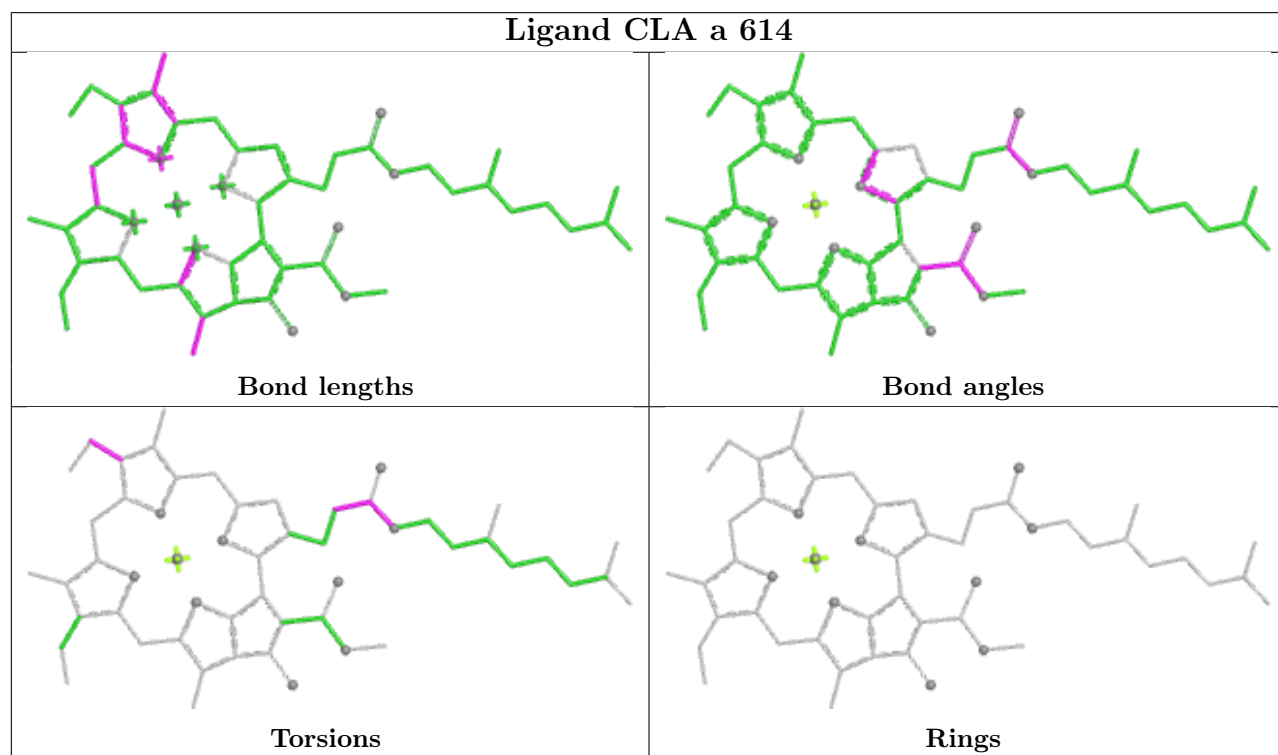
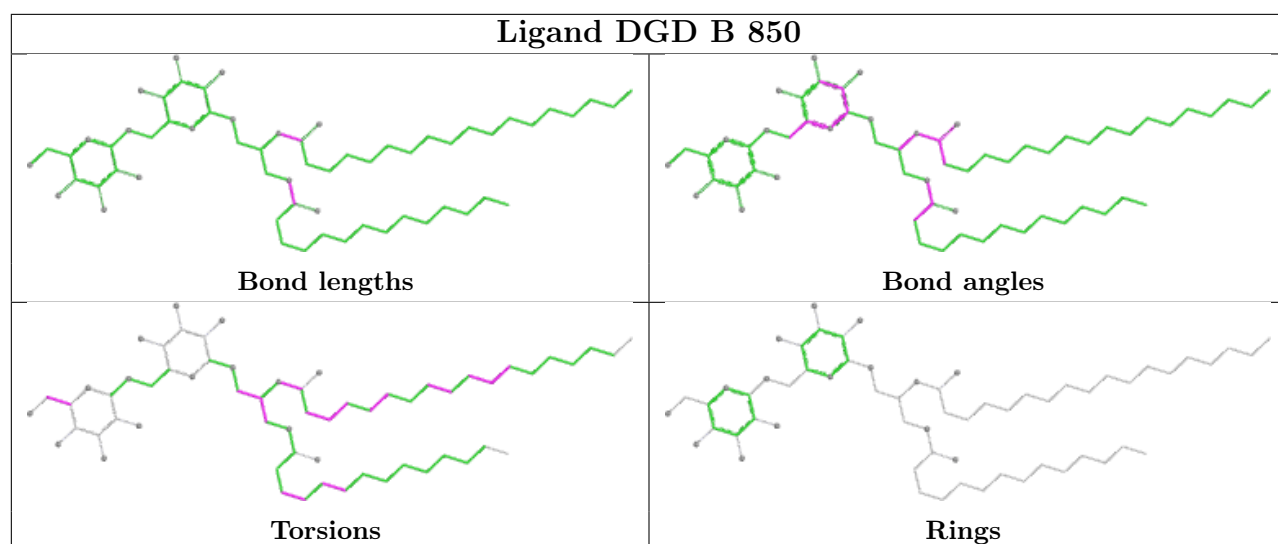


Torsions

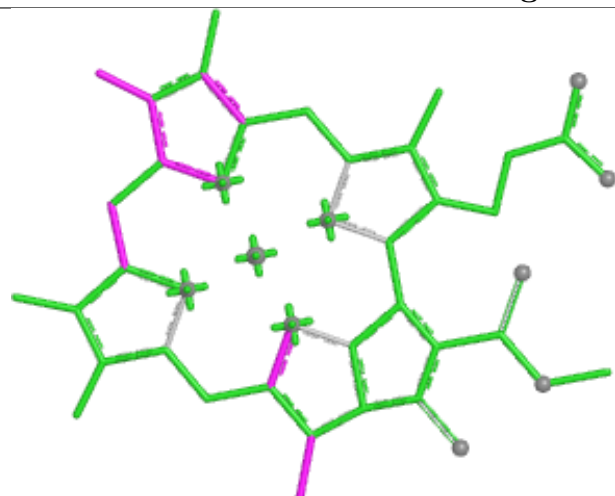


Rings

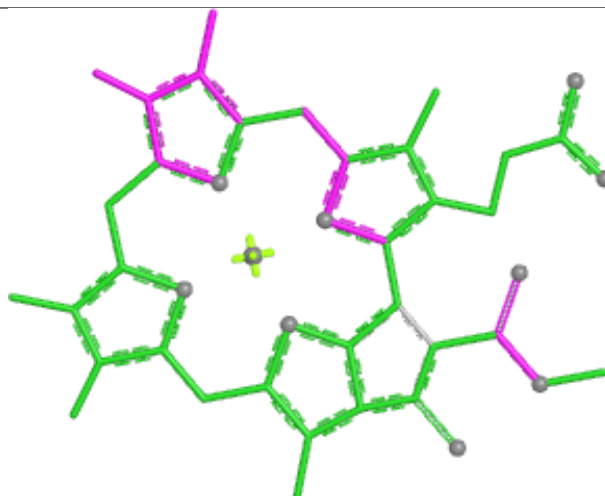




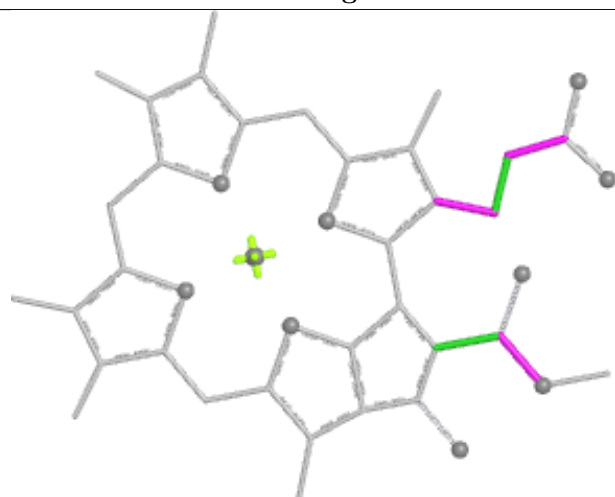
Ligand CLA 1 616



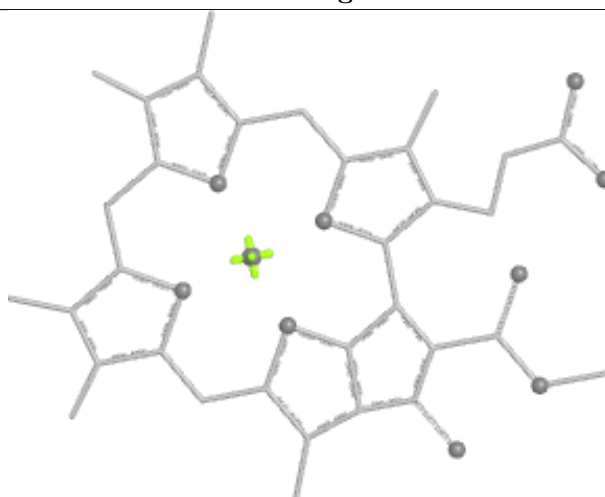
Bond lengths



Bond angles

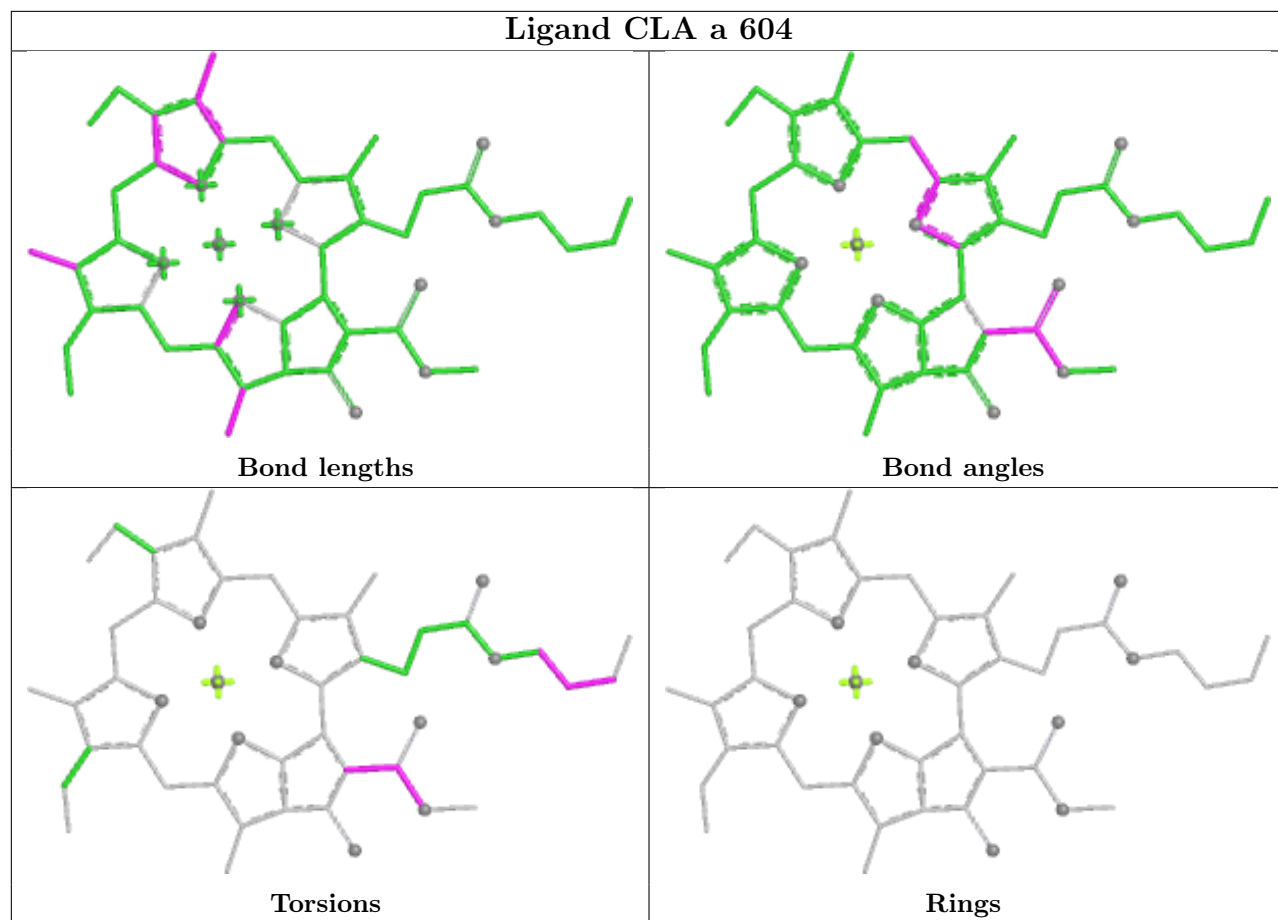


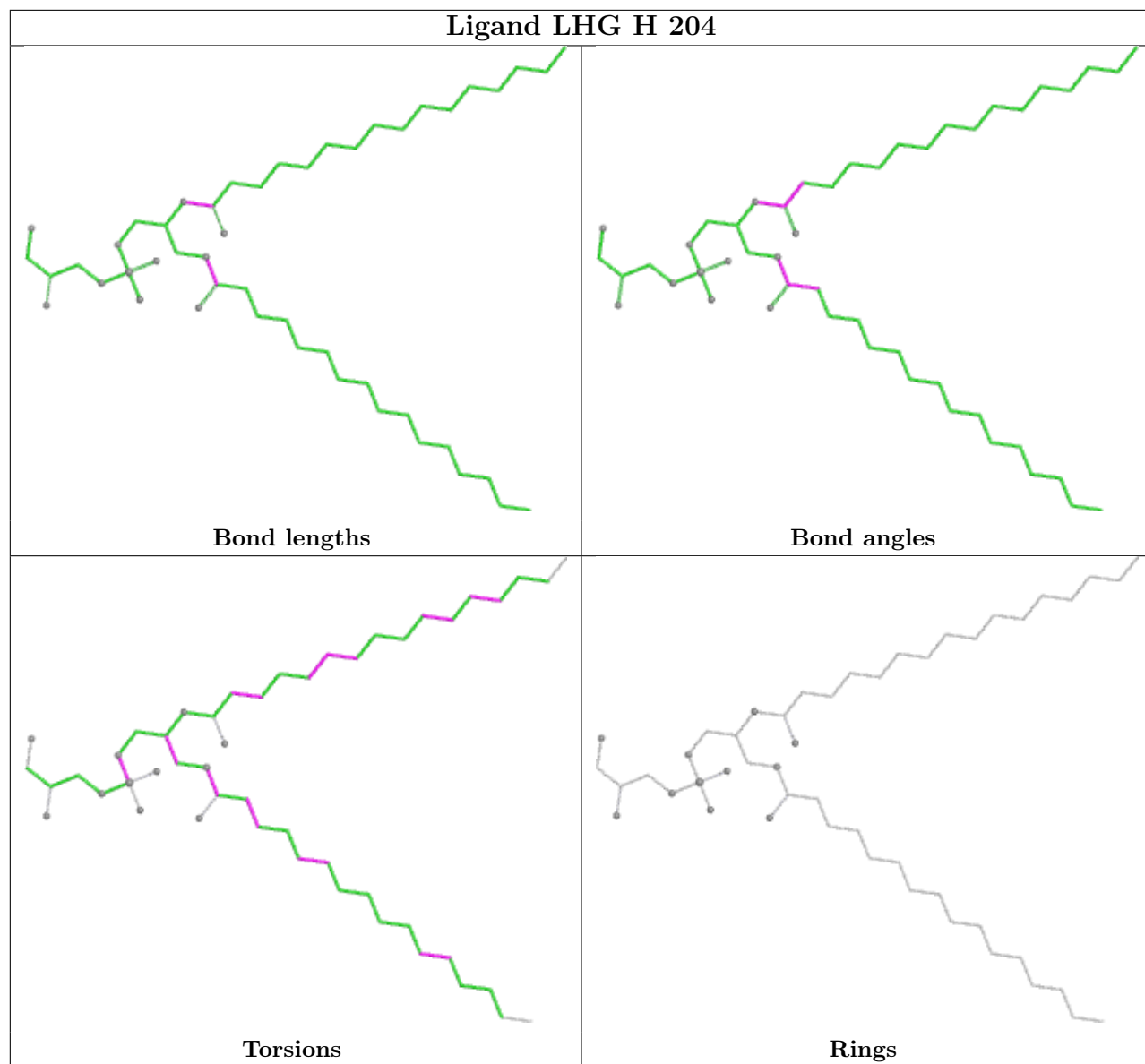
Torsions

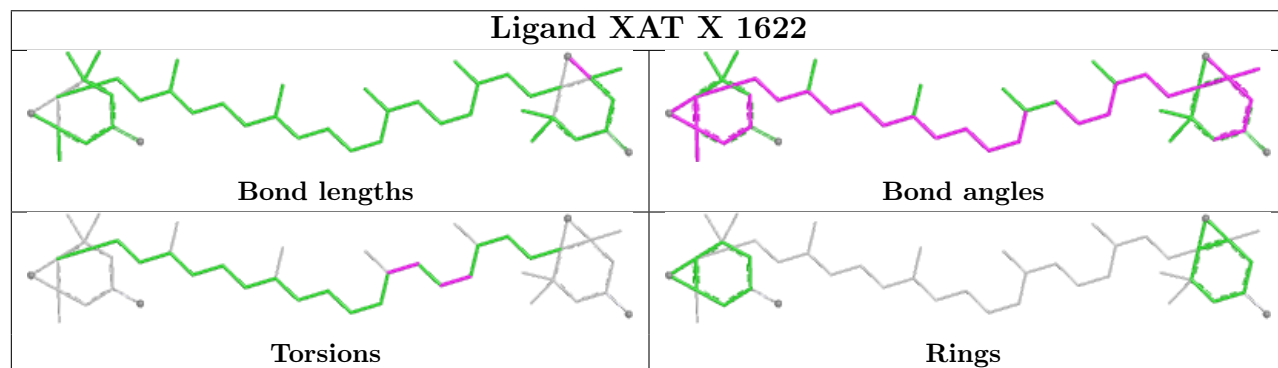
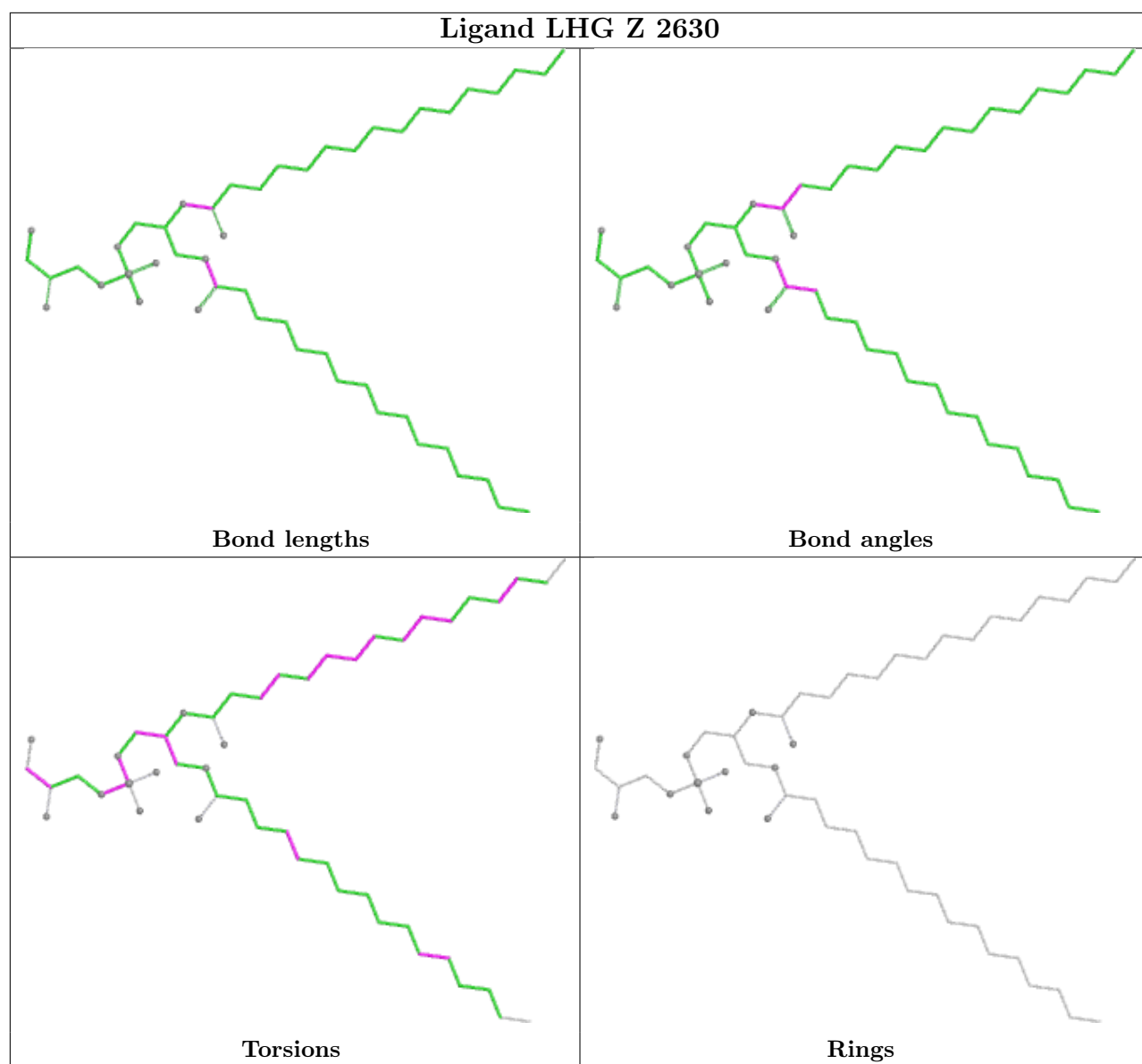


Rings

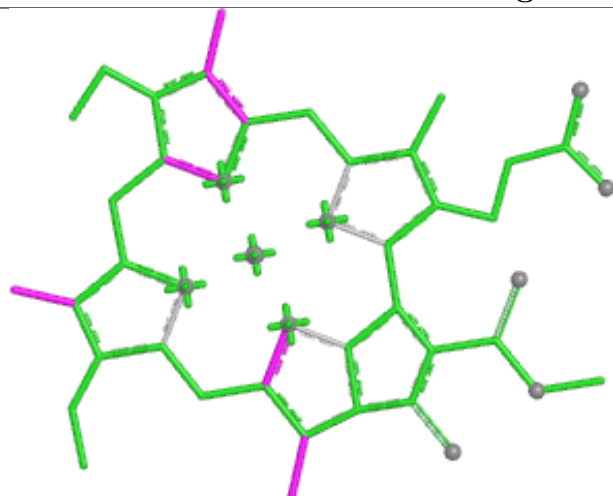
Ligand CLA a 604



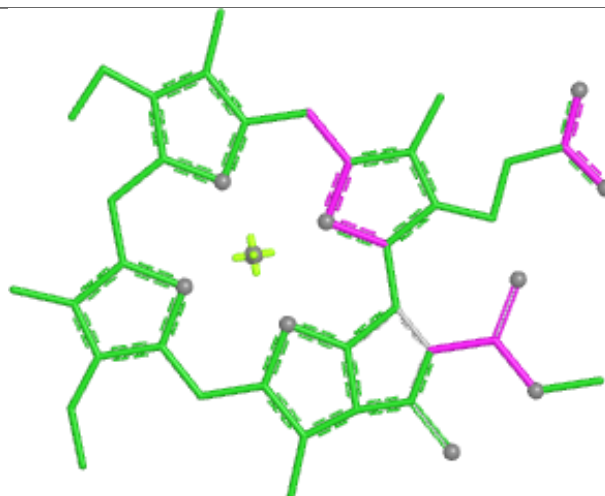




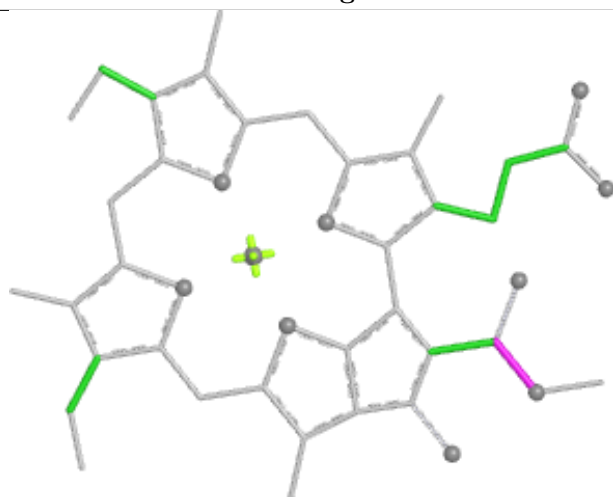
Ligand CLA L 304



Bond lengths



Bond angles

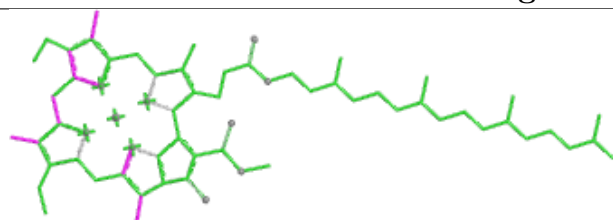


Torsions

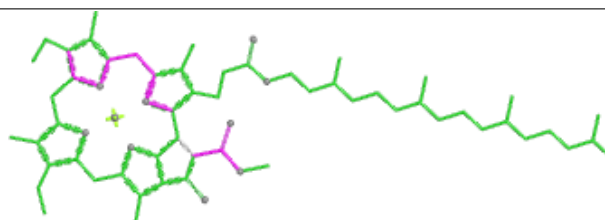


Rings

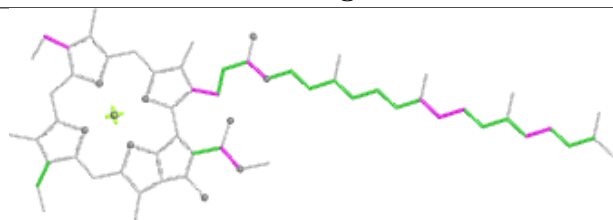
Ligand CLA 3 610



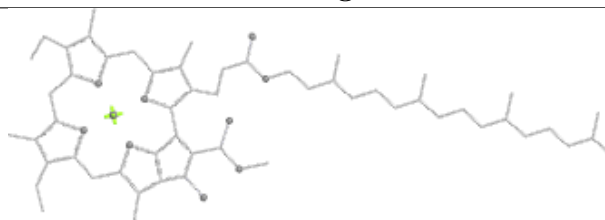
Bond lengths



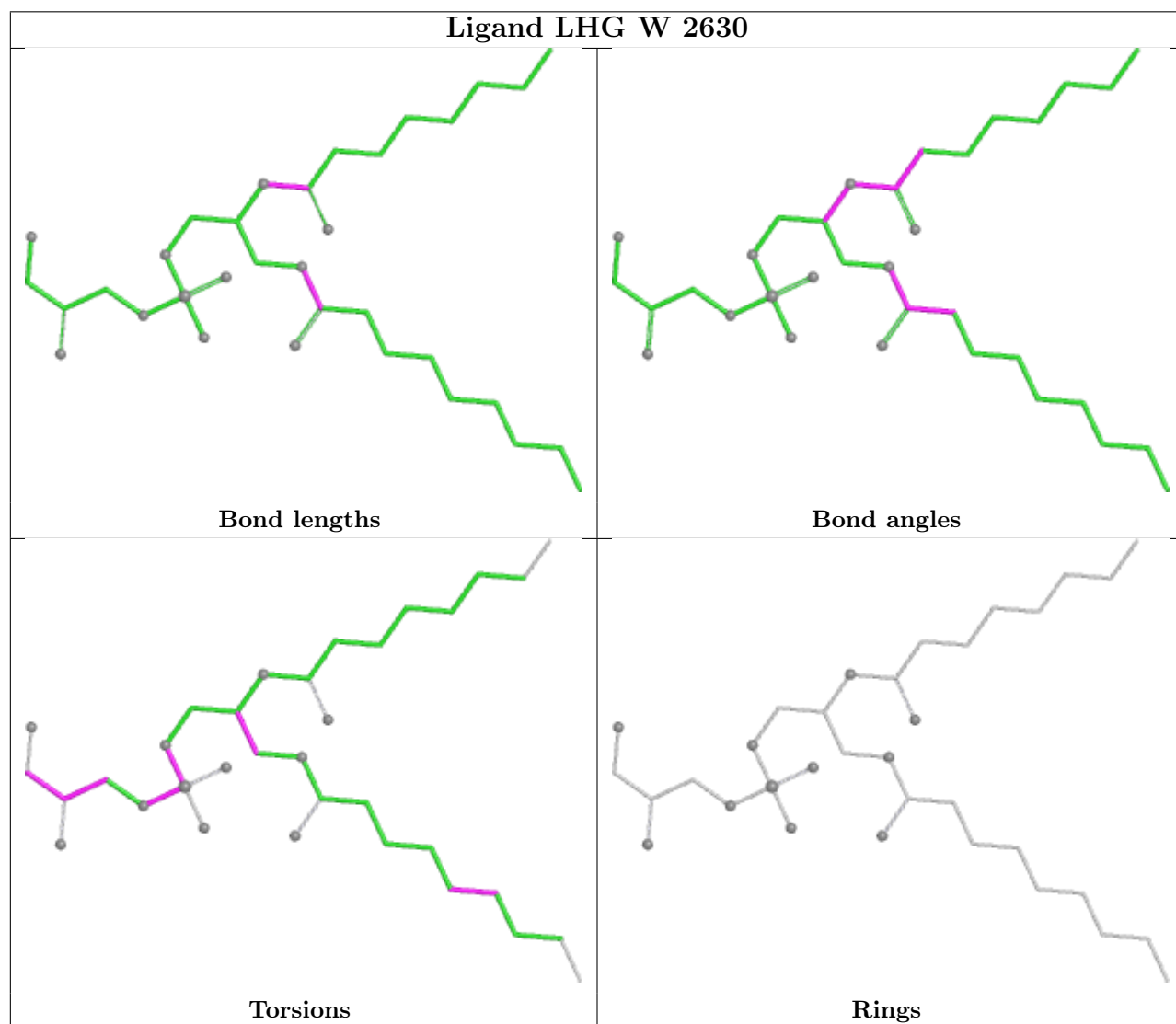
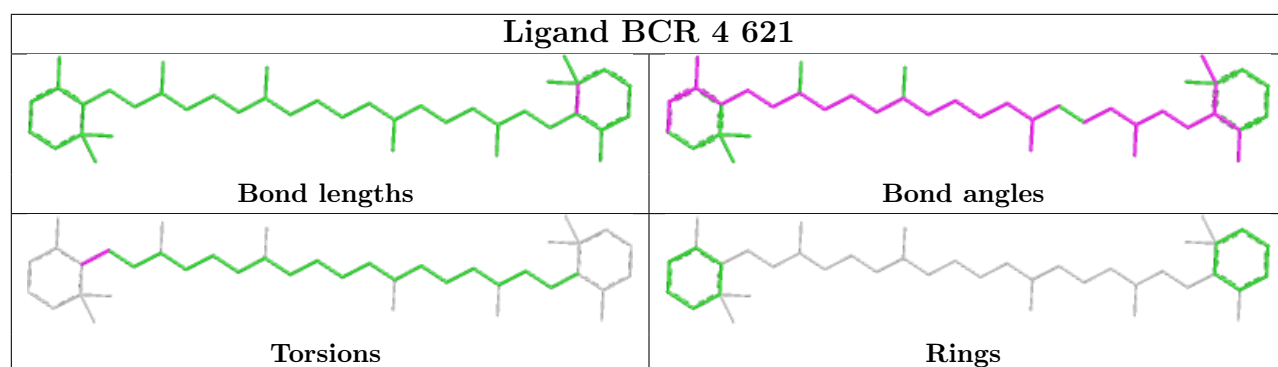
Bond angles

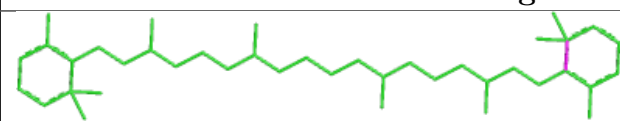
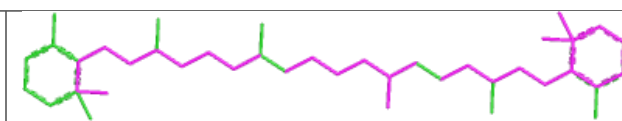
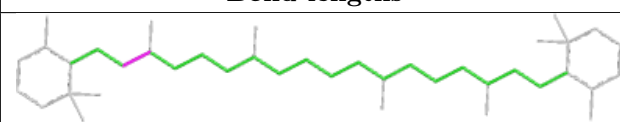
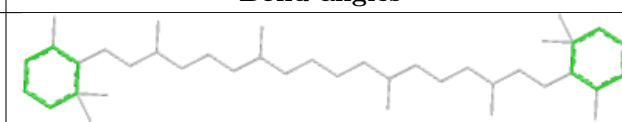


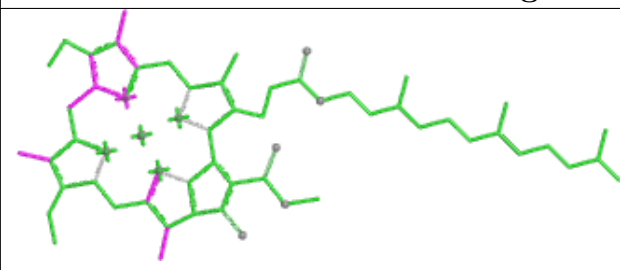
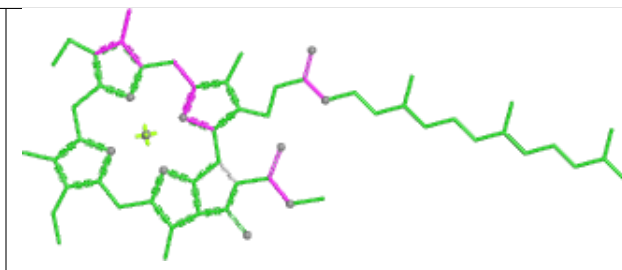
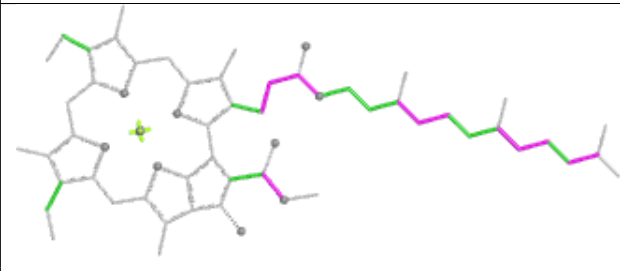
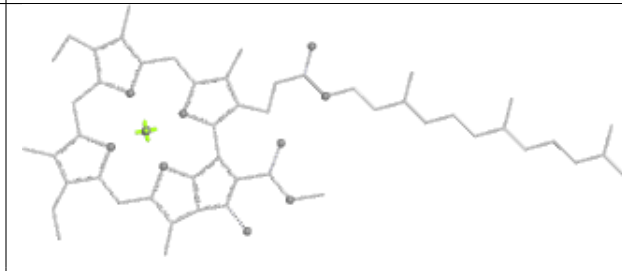
Torsions

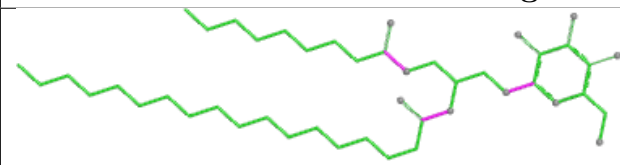
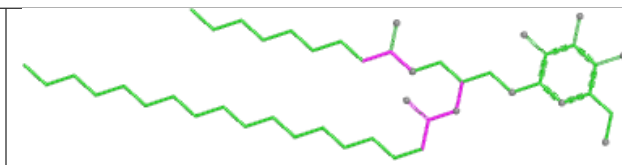
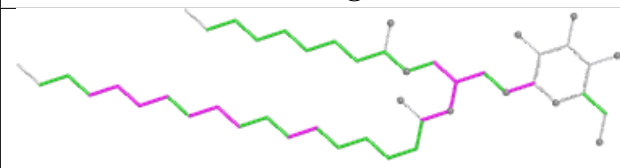
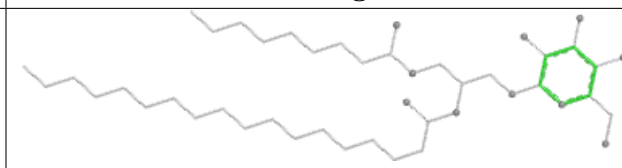


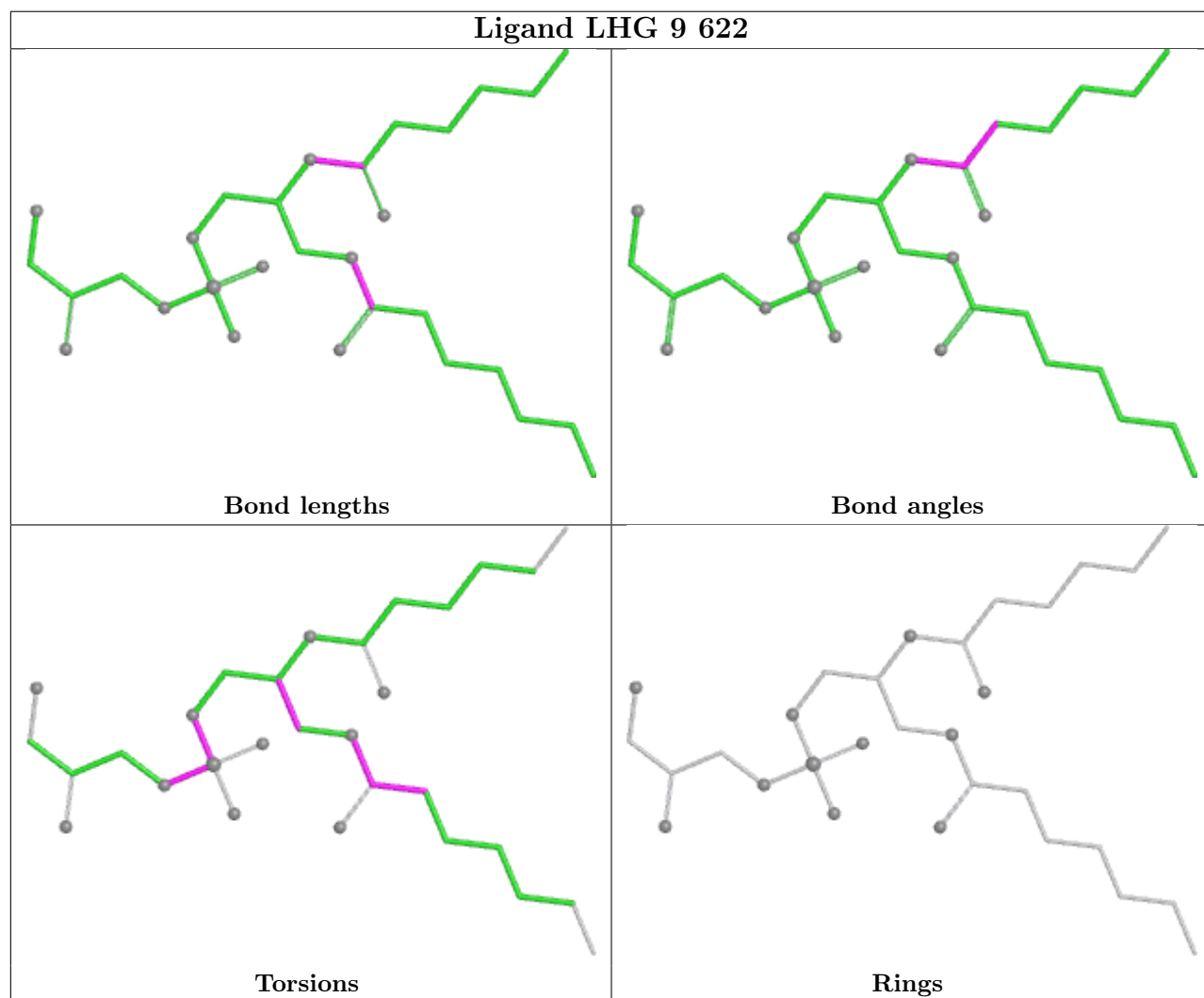
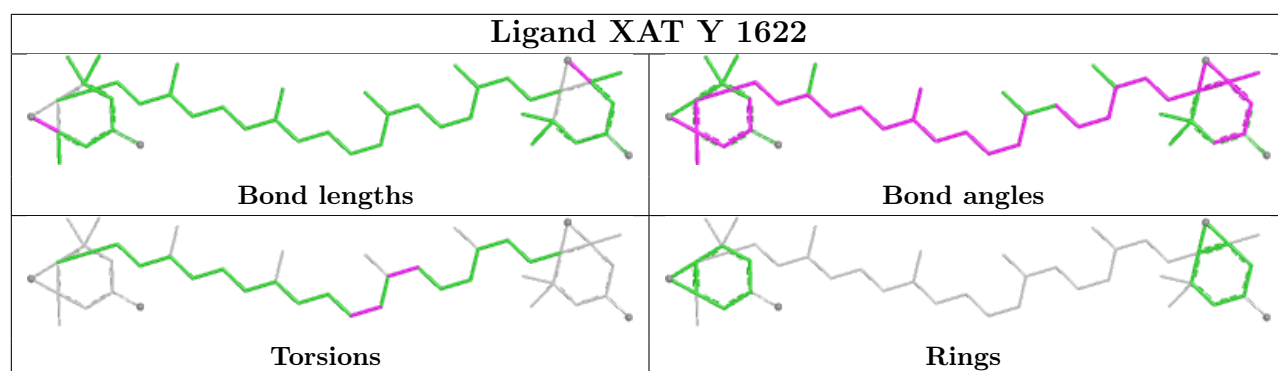
Rings

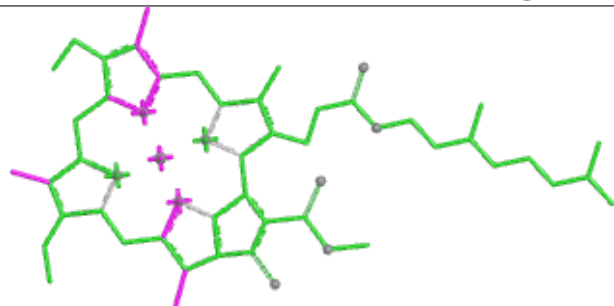


Ligand BCR K 207	
	
Bond lengths	Bond angles
	
Torsions	Rings

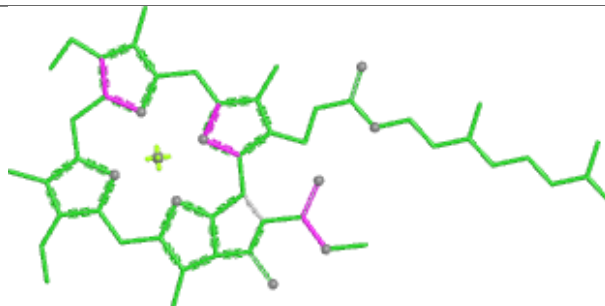
Ligand CLA A 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG 8 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

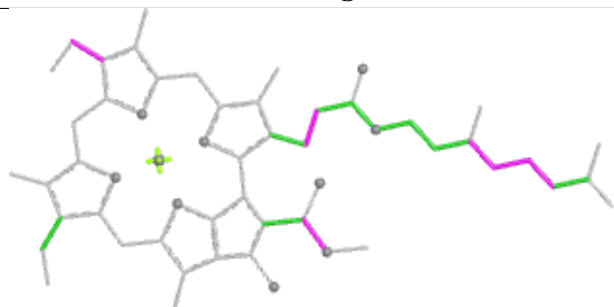


Ligand CLA 3 608

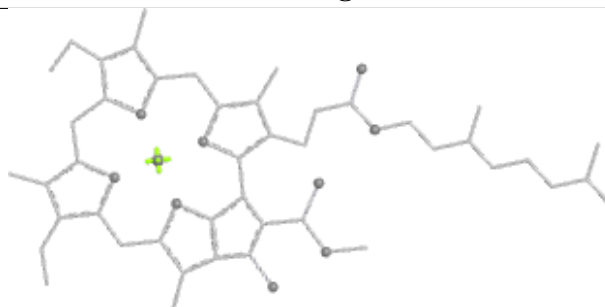
Bond lengths



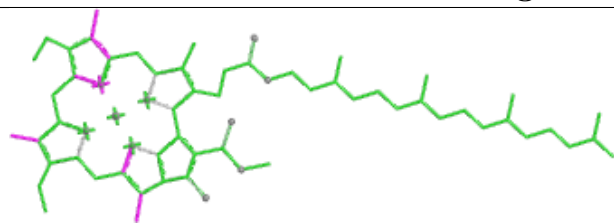
Bond angles



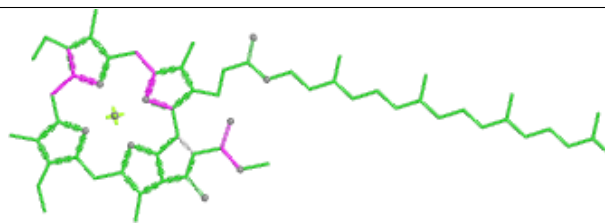
Torsions



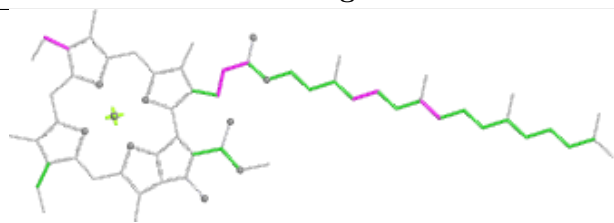
Rings

Ligand CLA Z 613

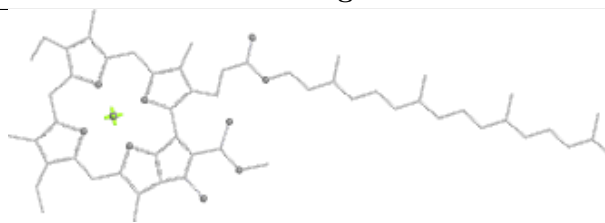
Bond lengths



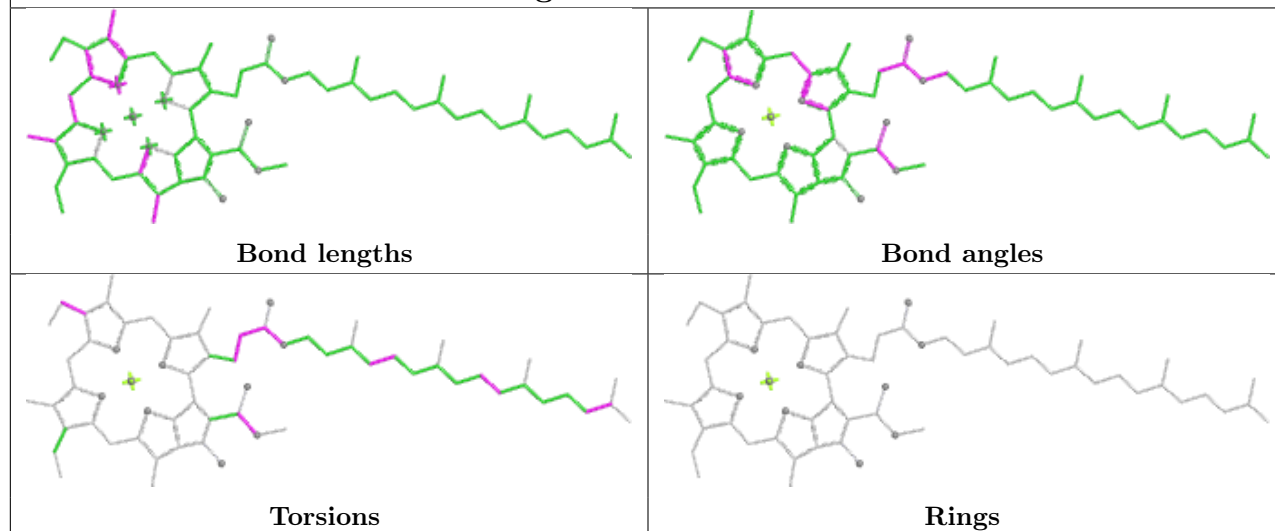
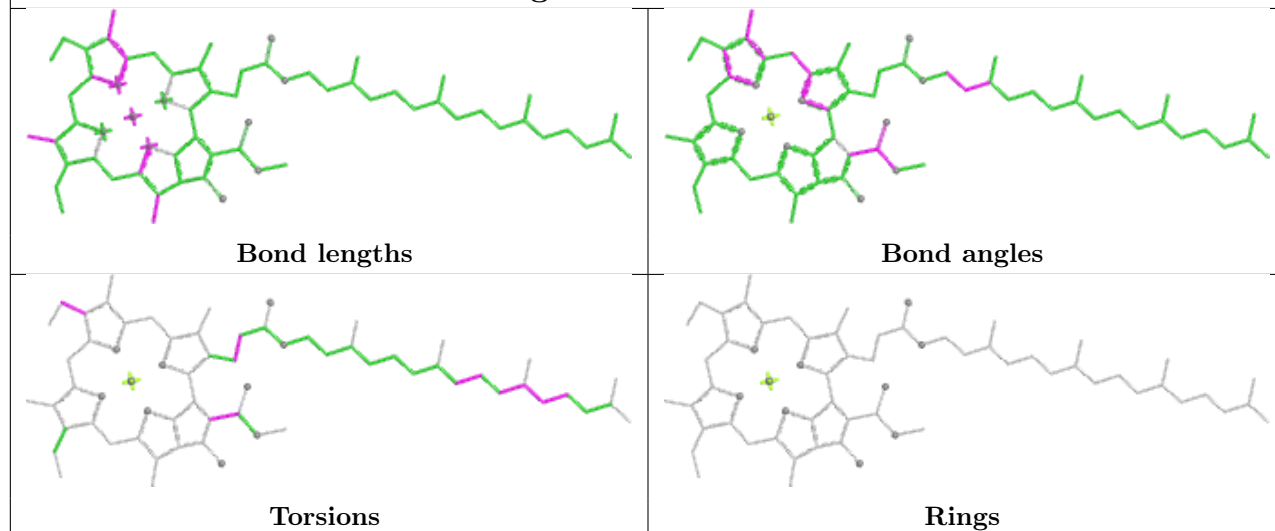
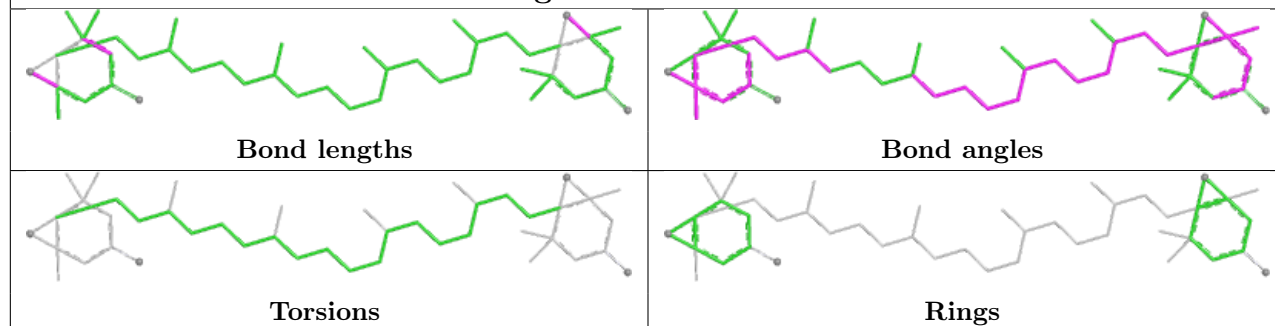
Bond angles

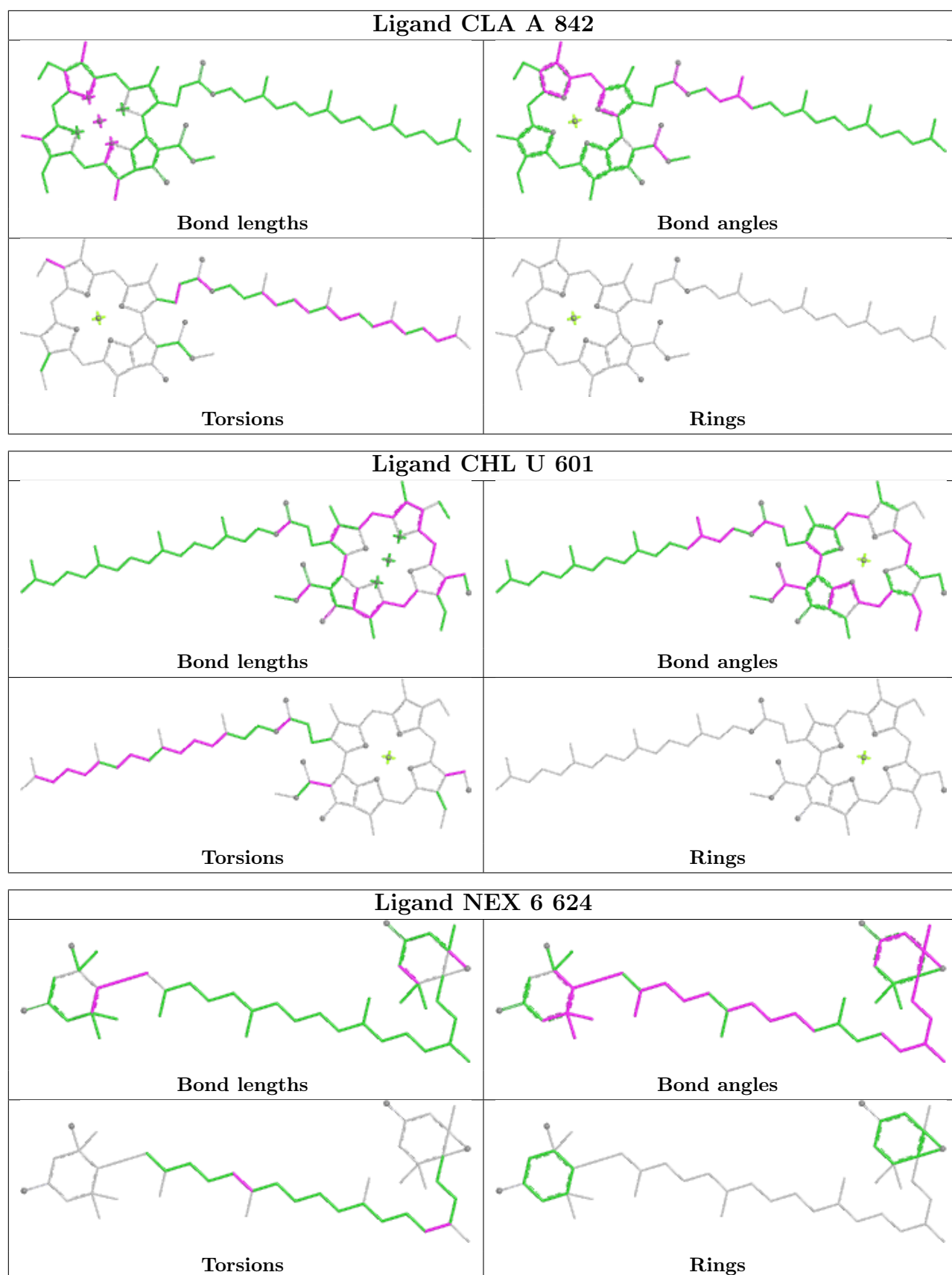


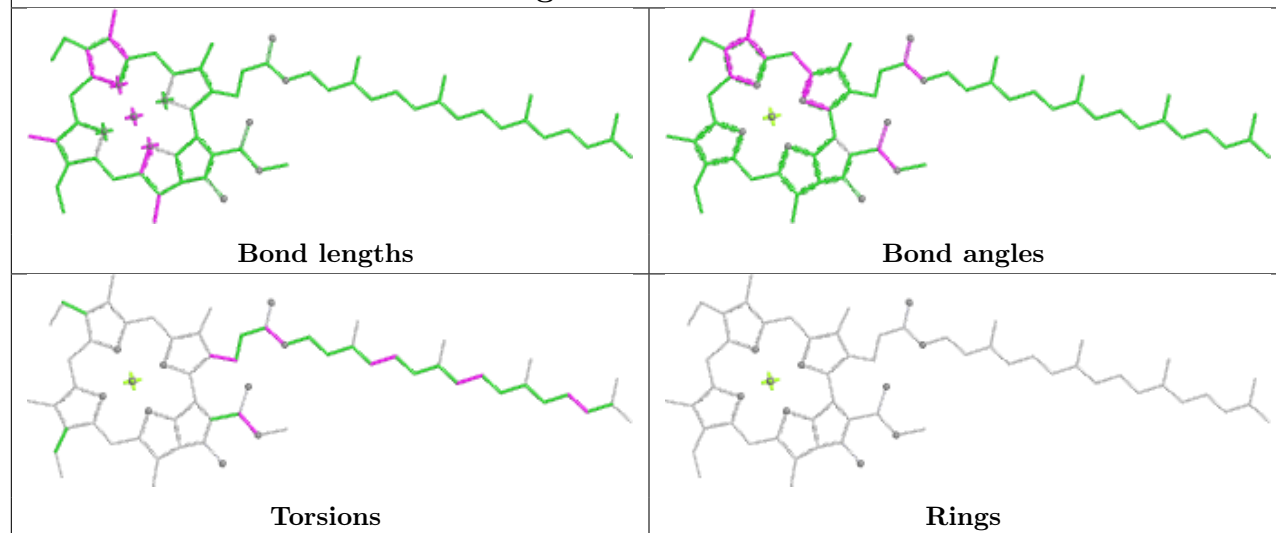
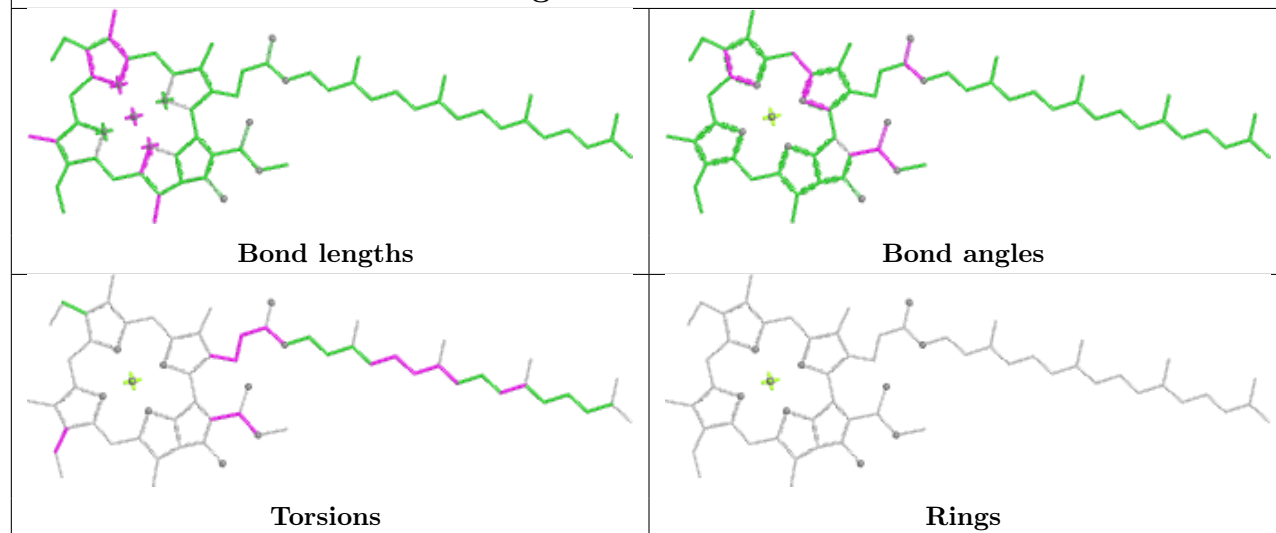
Torsions

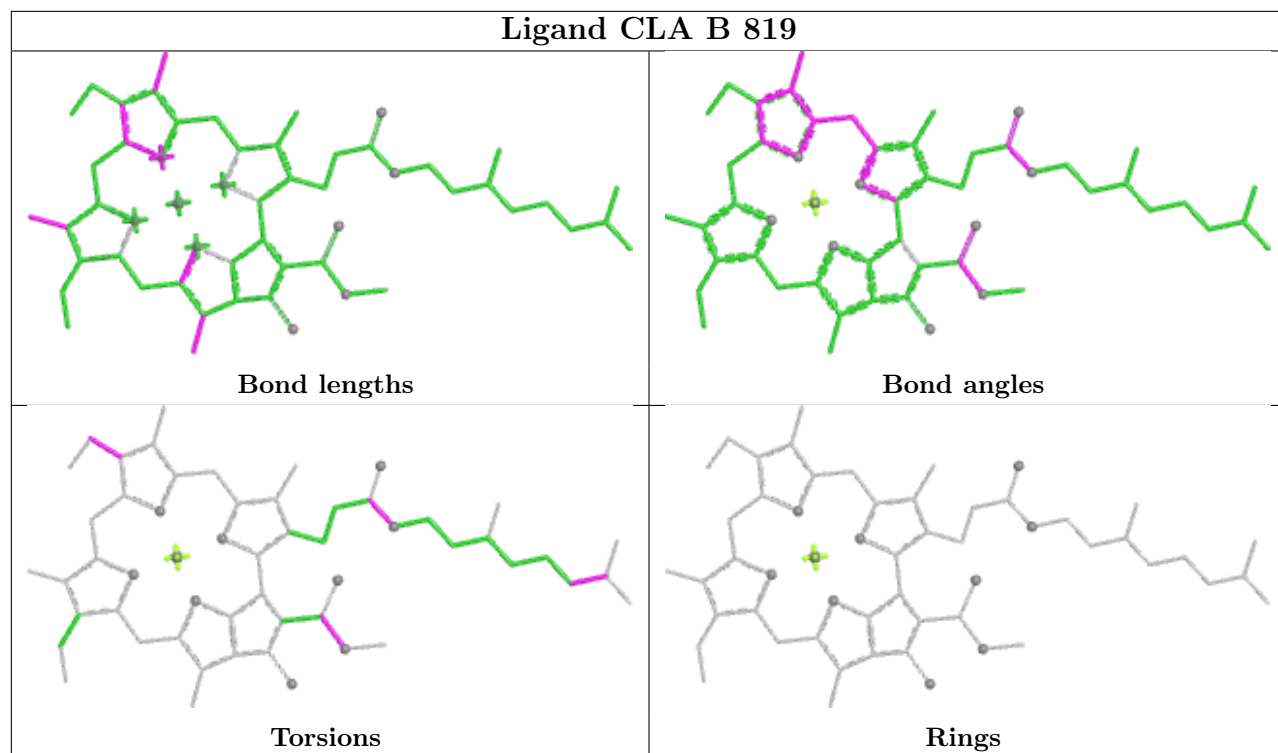


Rings

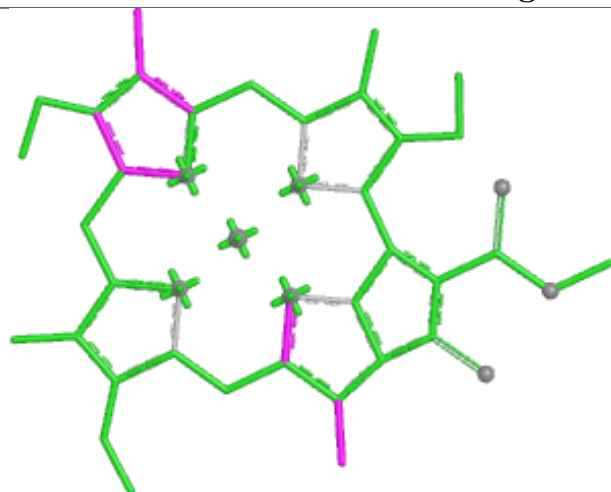
Ligand CLA 4 613**Ligand CLA A 809****Ligand XAT 9 620**



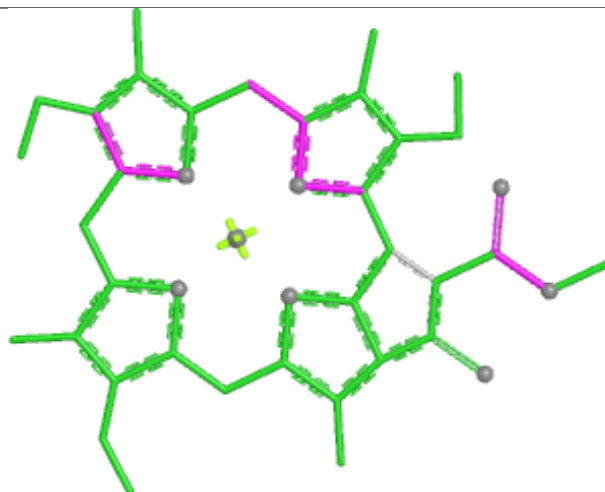
Ligand CLA 2 601**Ligand CLA B 813**



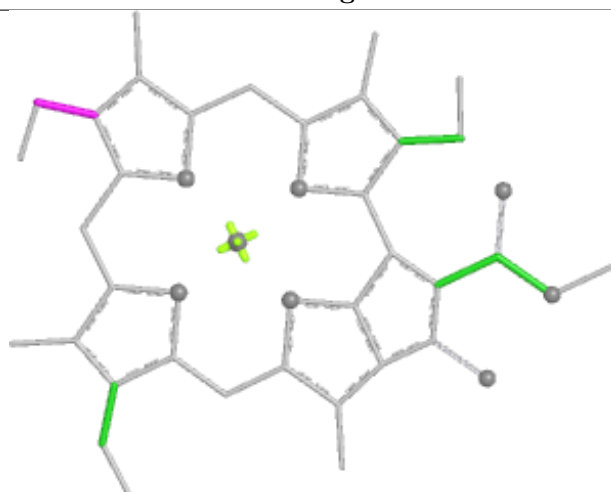
Ligand CLA 5 611



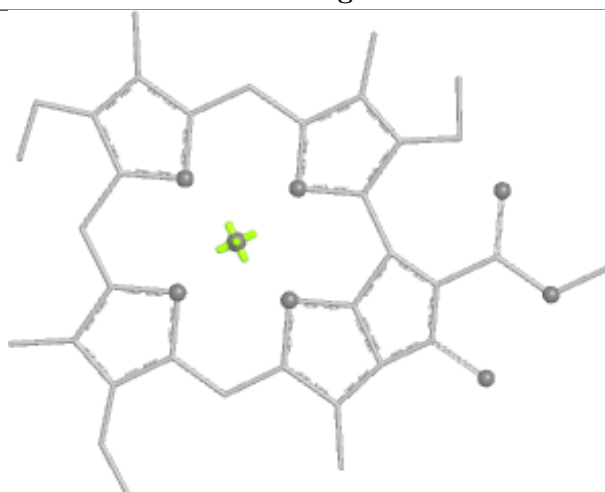
Bond lengths



Bond angles

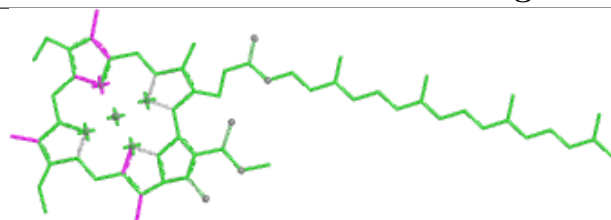


Torsions

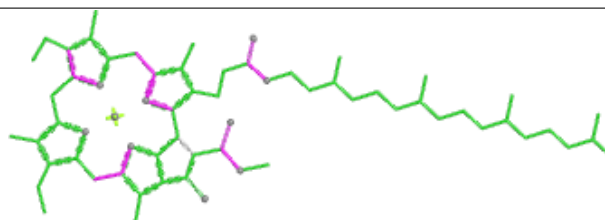


Rings

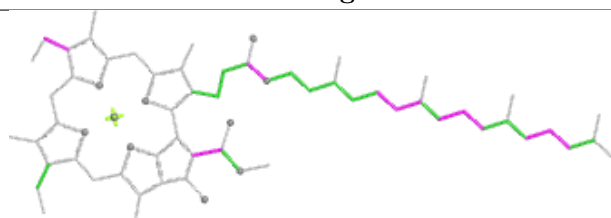
Ligand CLA B 833



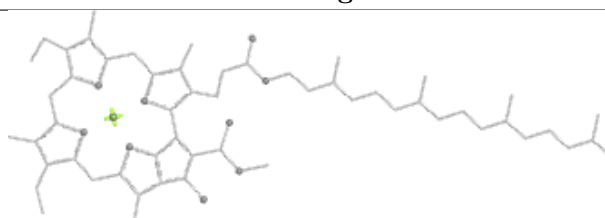
Bond lengths



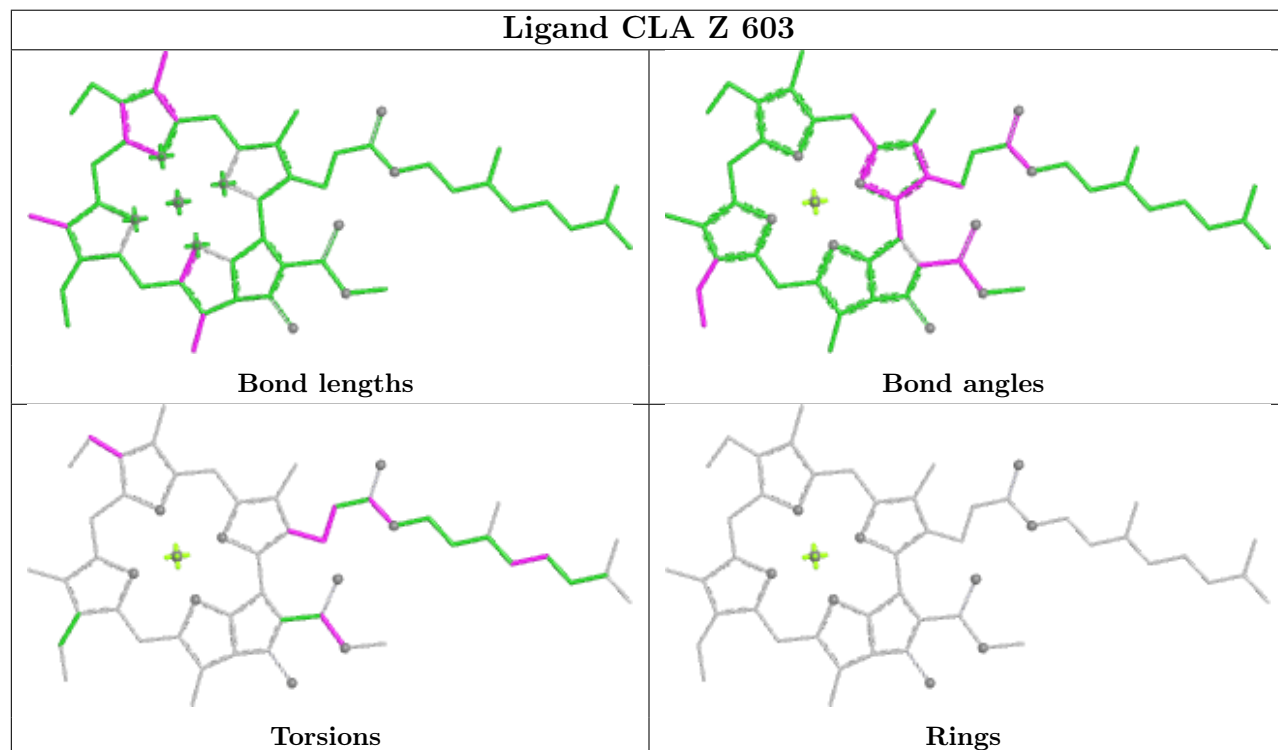
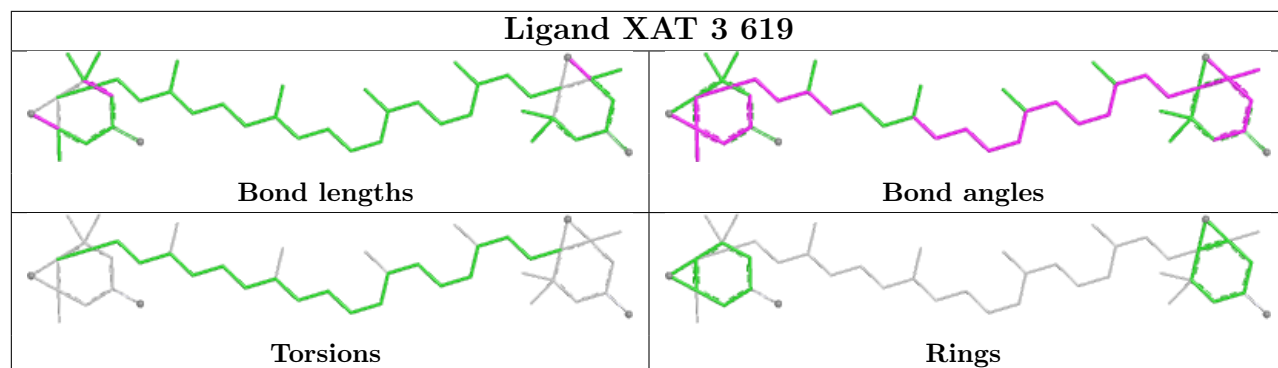
Bond angles



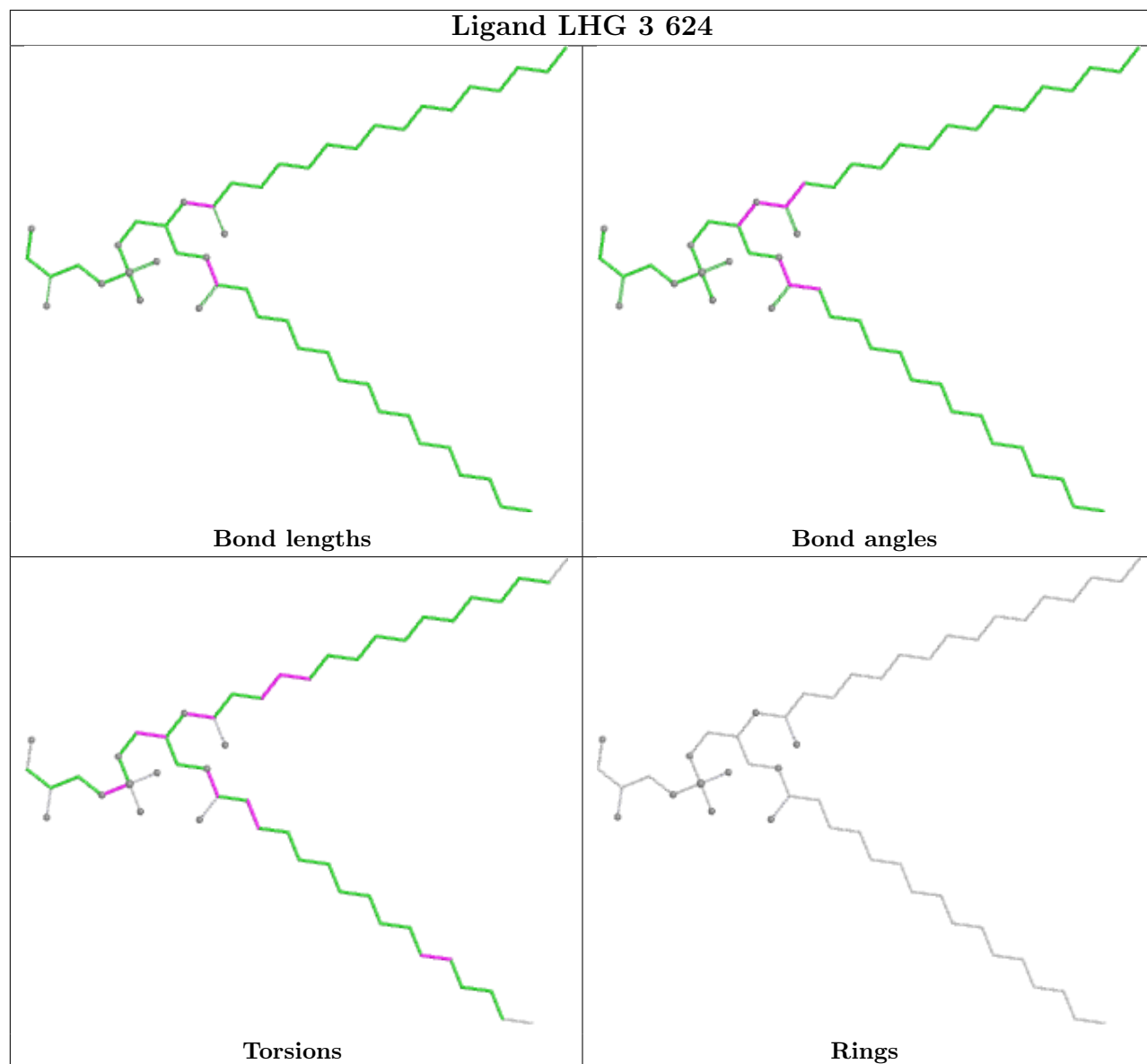
Torsions



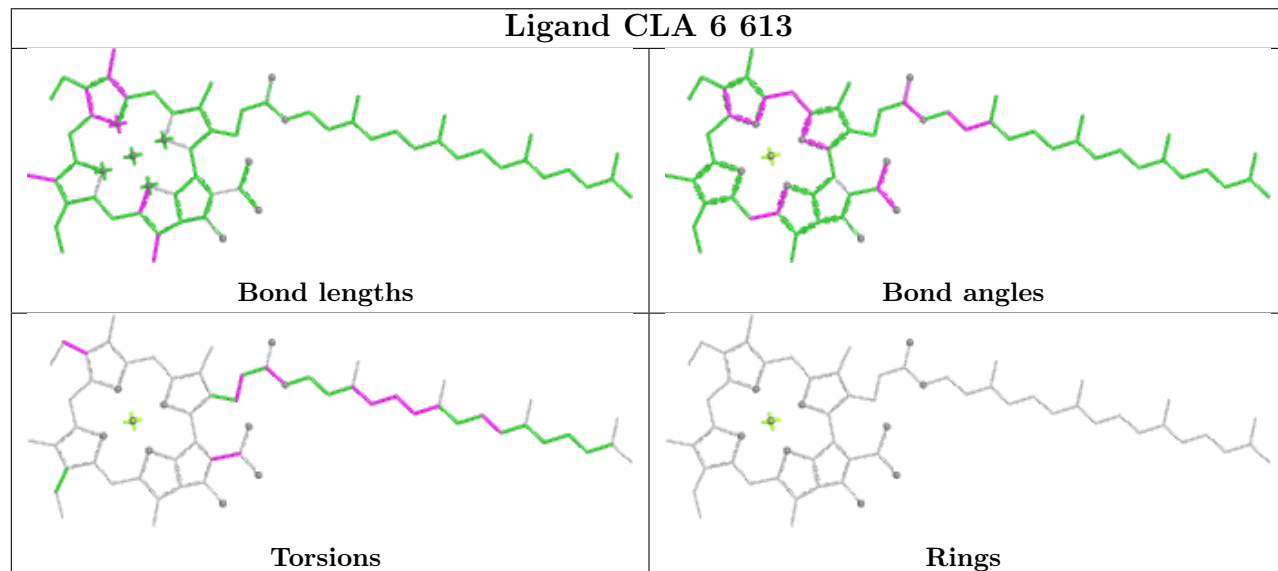
Rings

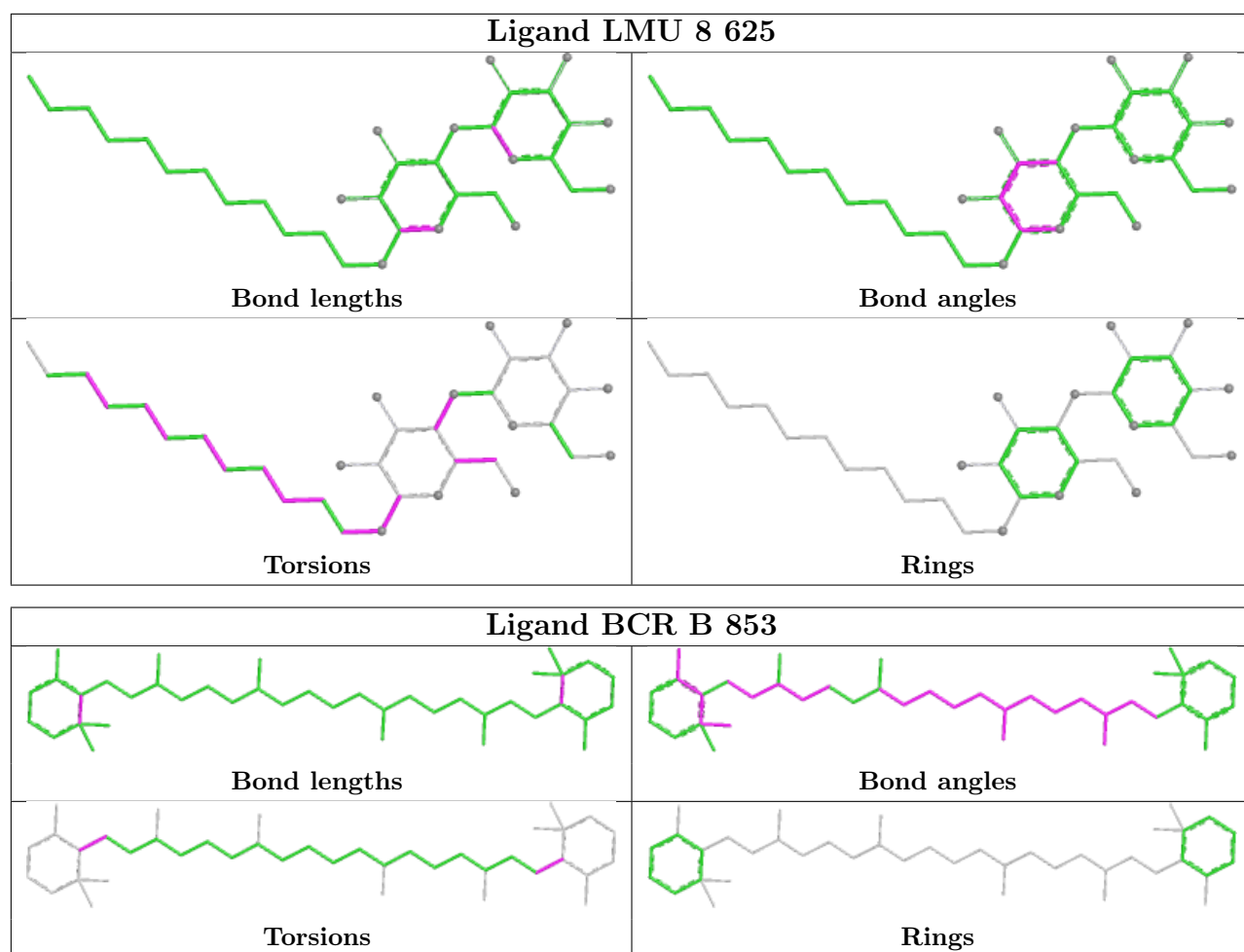


Ligand LHG 3 624

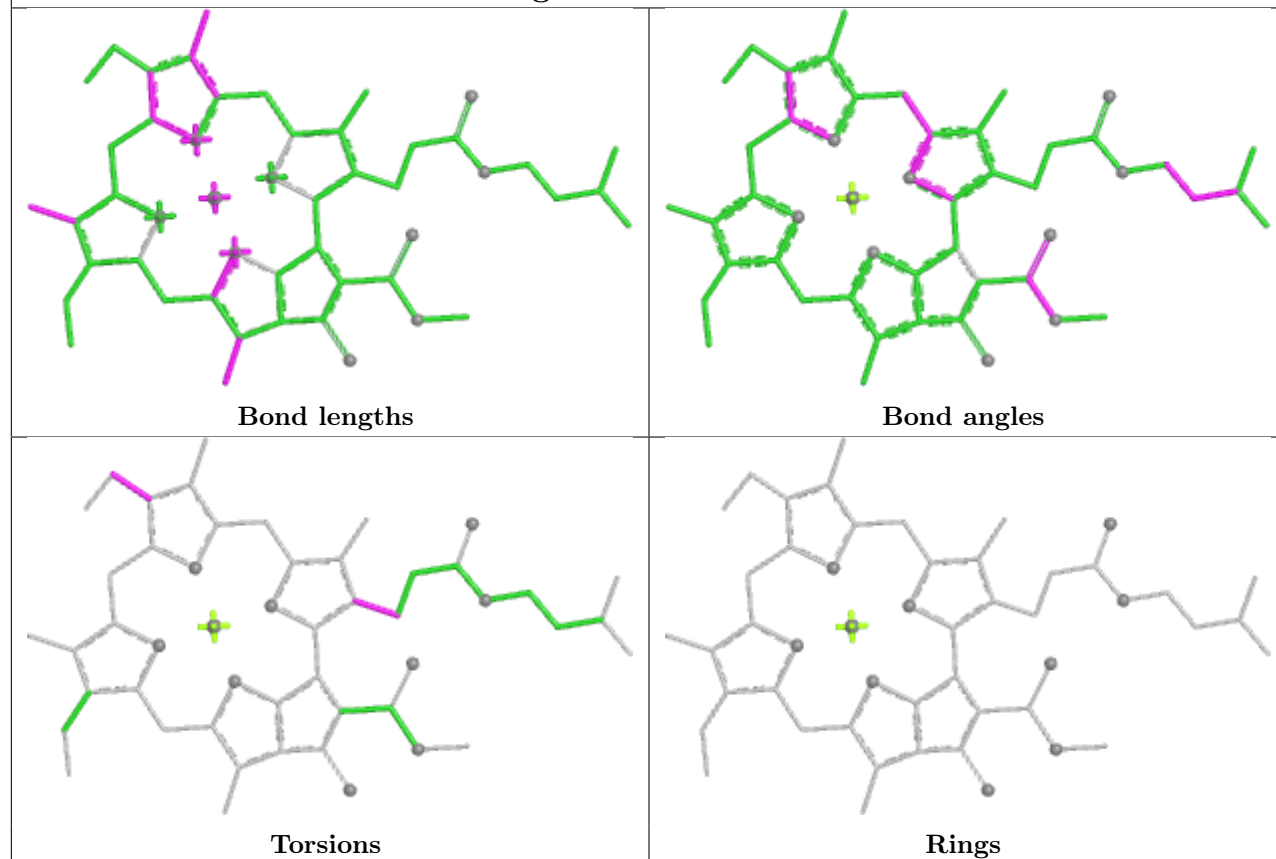


Ligand CLA 6 613

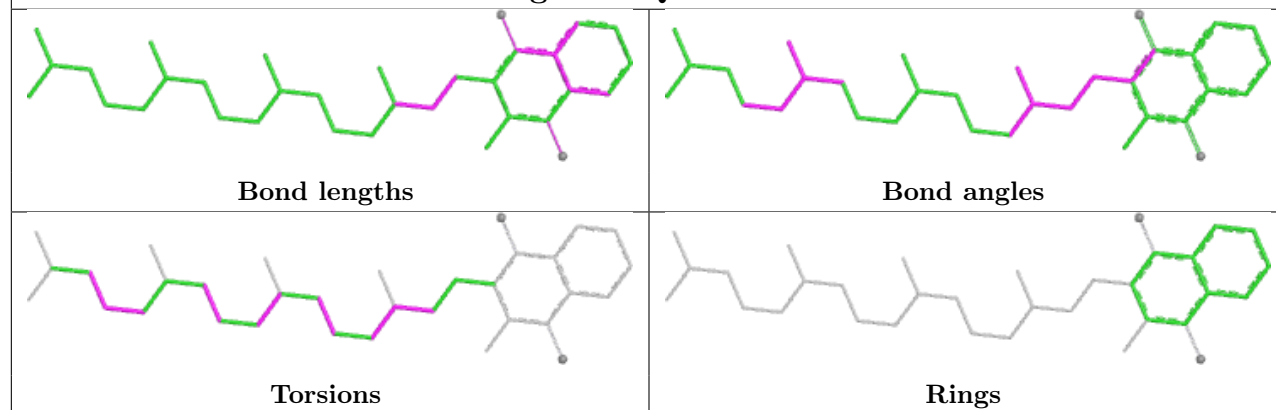


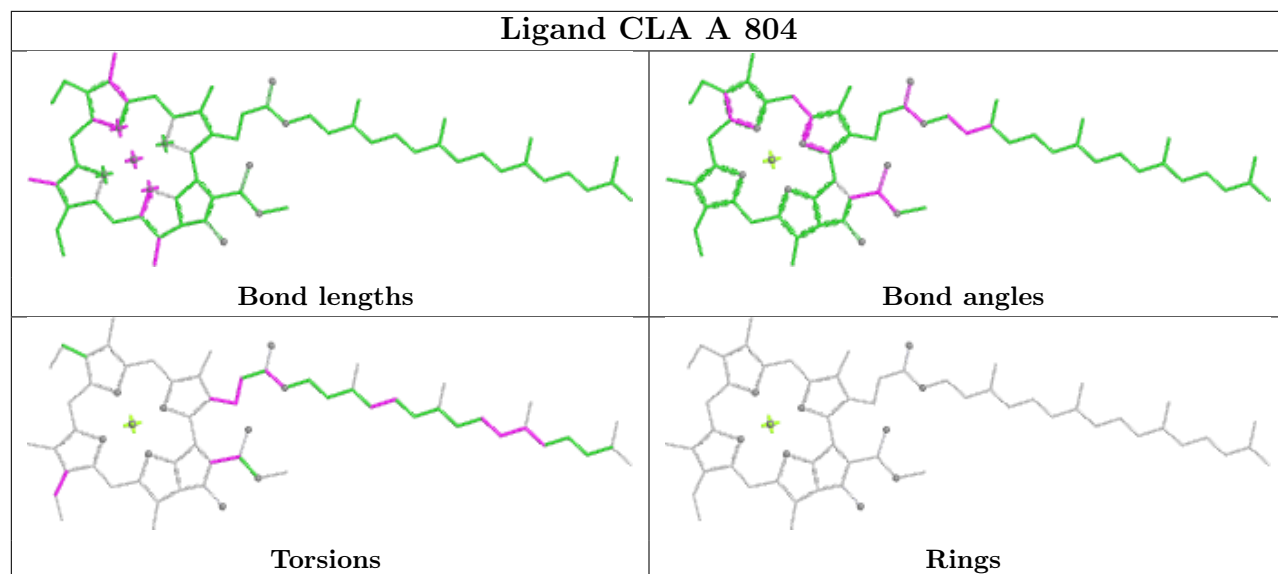
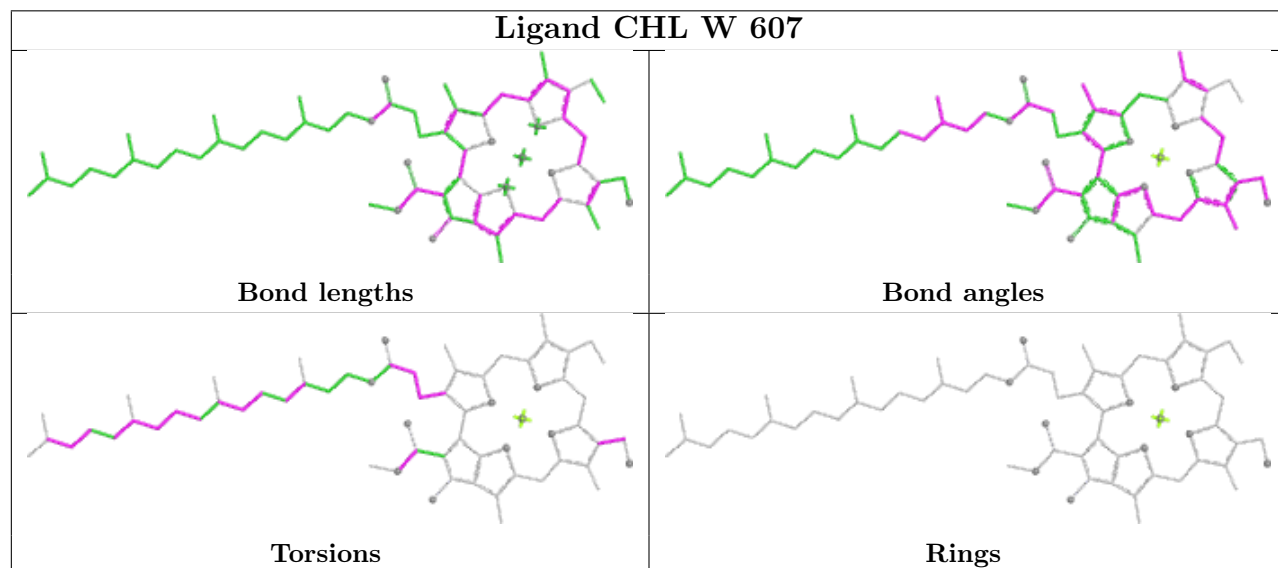


Ligand CLA B 820

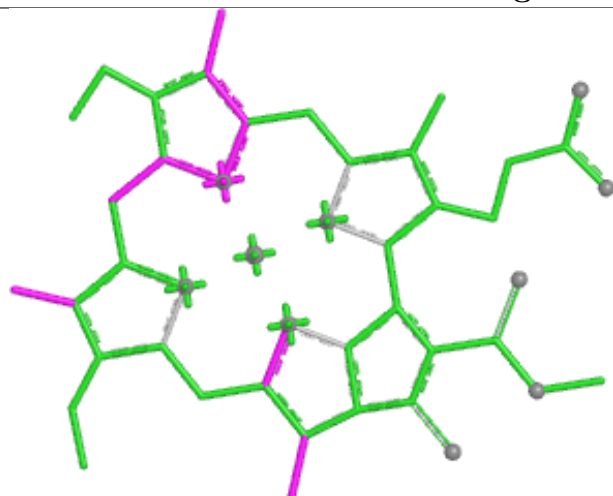


Ligand PQN B 842

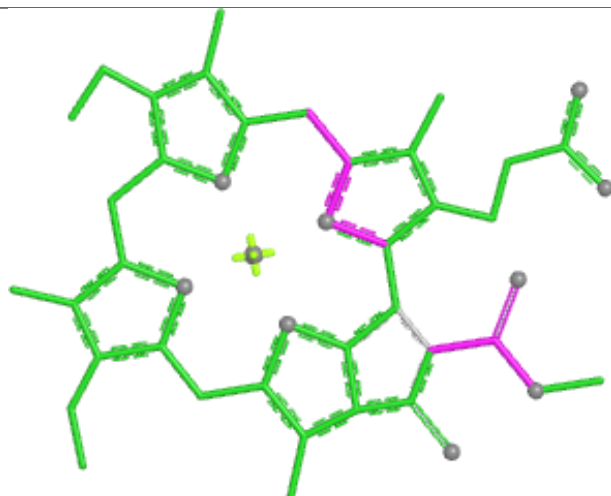


Ligand CLA A 804**Ligand CHL W 607**

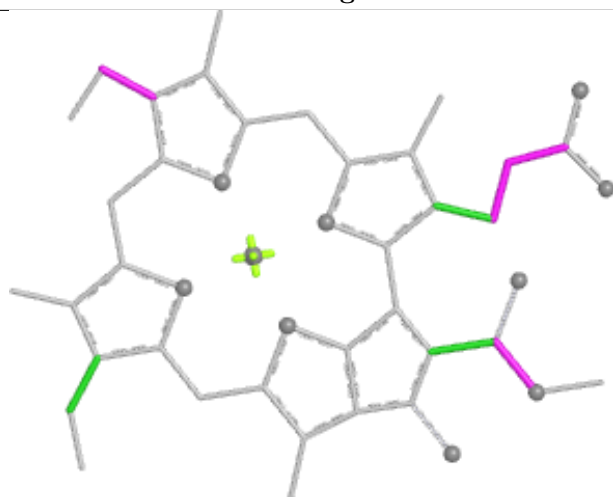
Ligand CLA A 837



Bond lengths



Bond angles

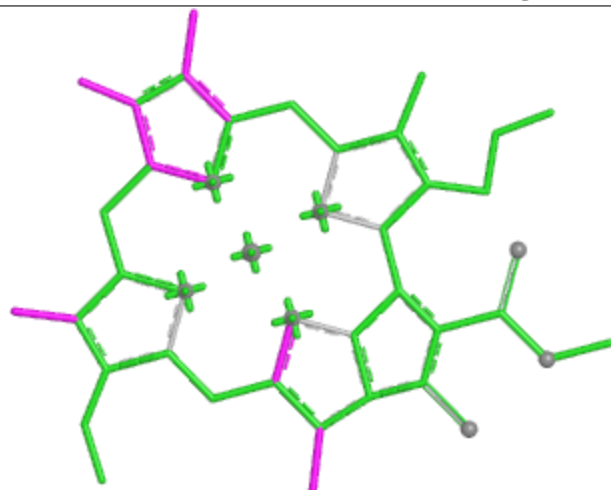


Torsions

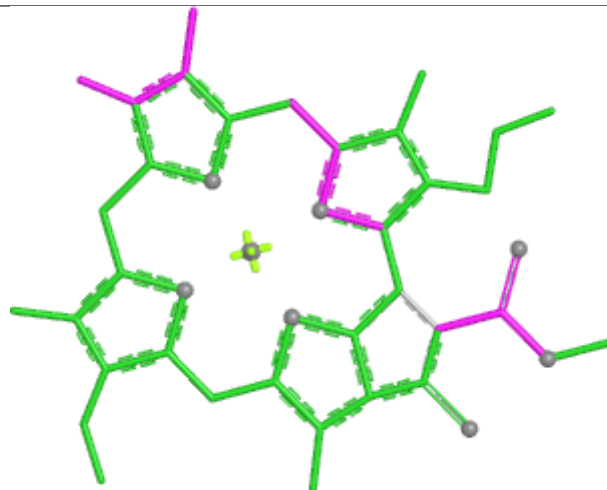


Rings

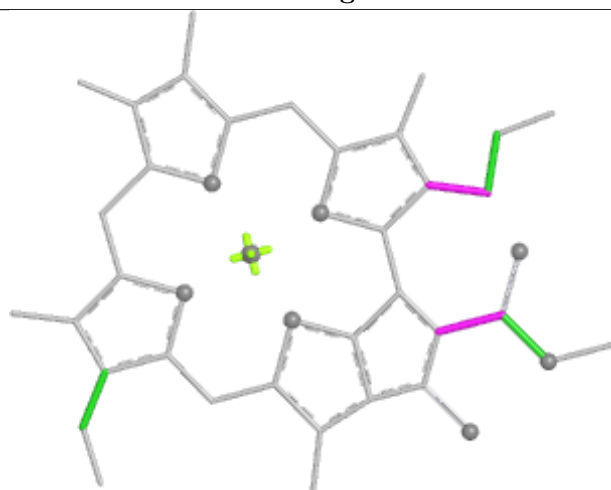
Ligand CLA Z 611



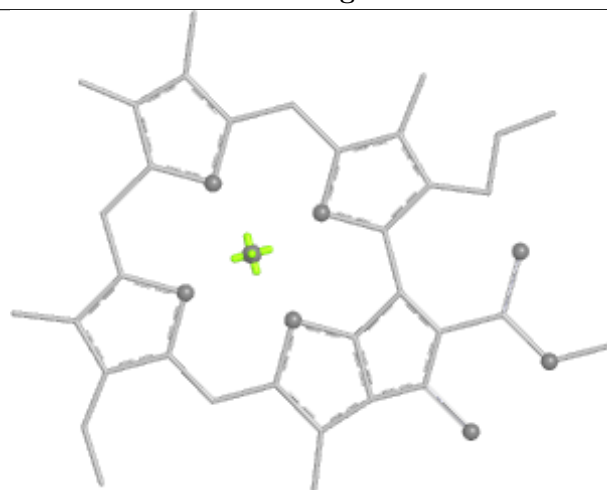
Bond lengths



Bond angles

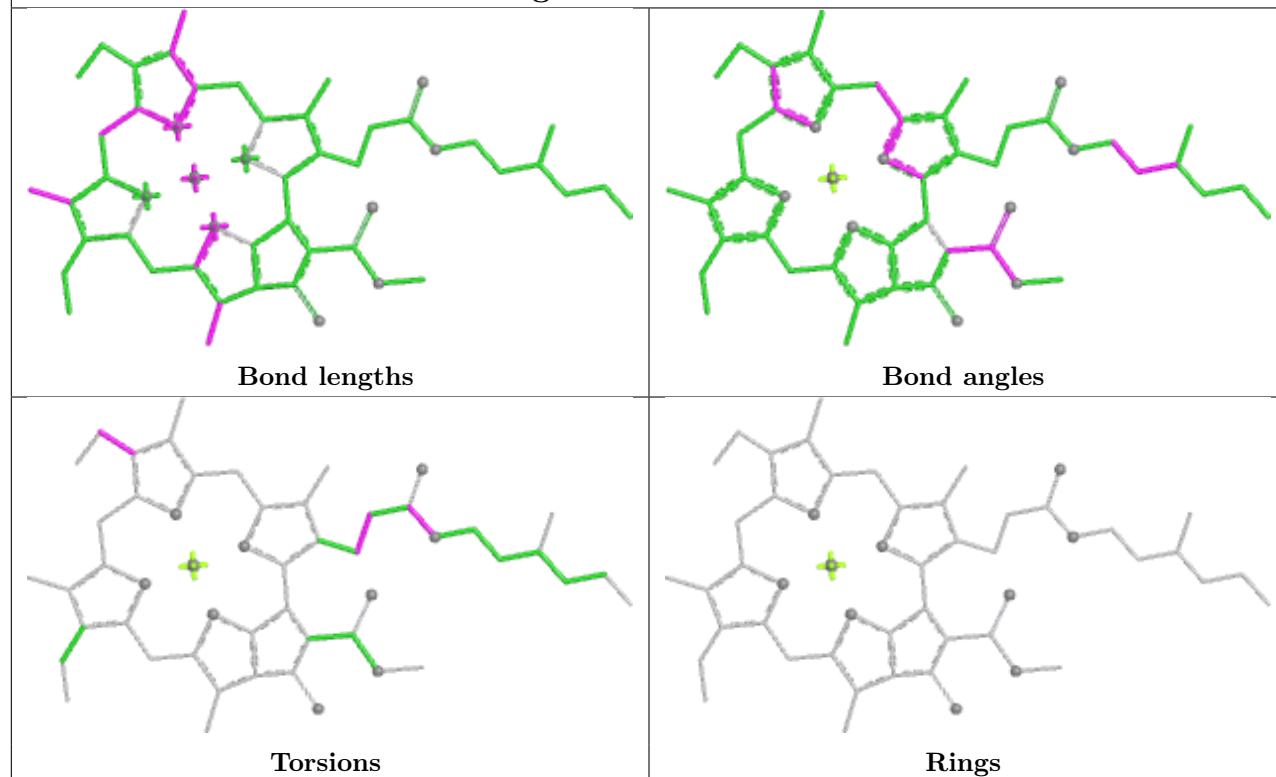


Torsions

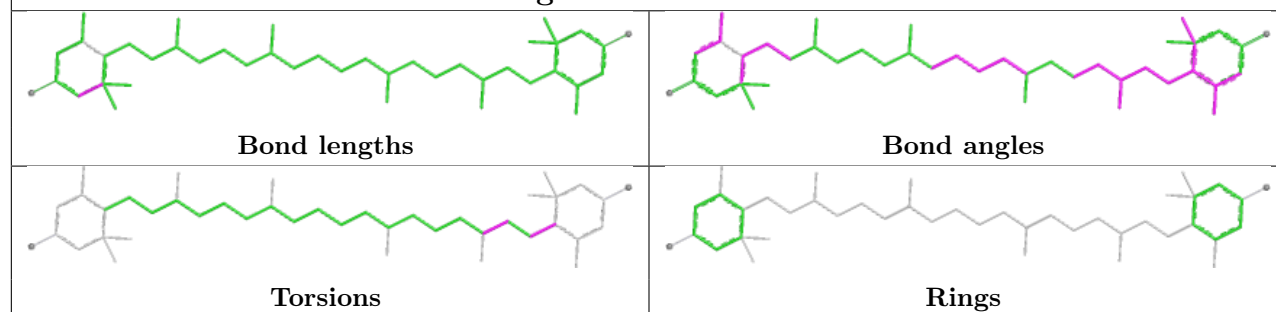


Rings

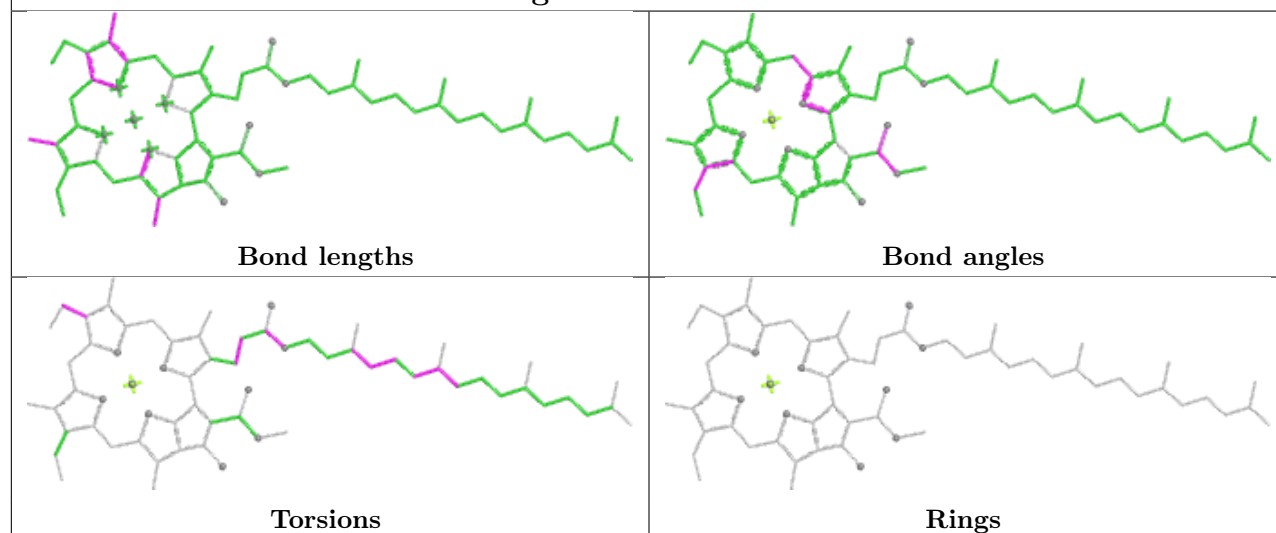
Ligand CLA B 807



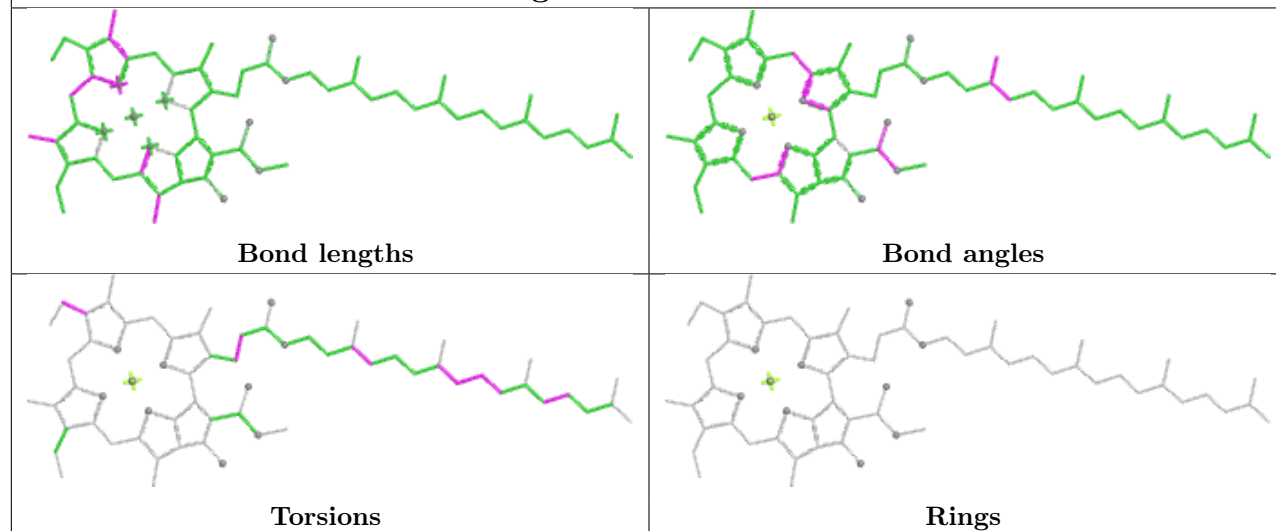
Ligand LUT 3 618



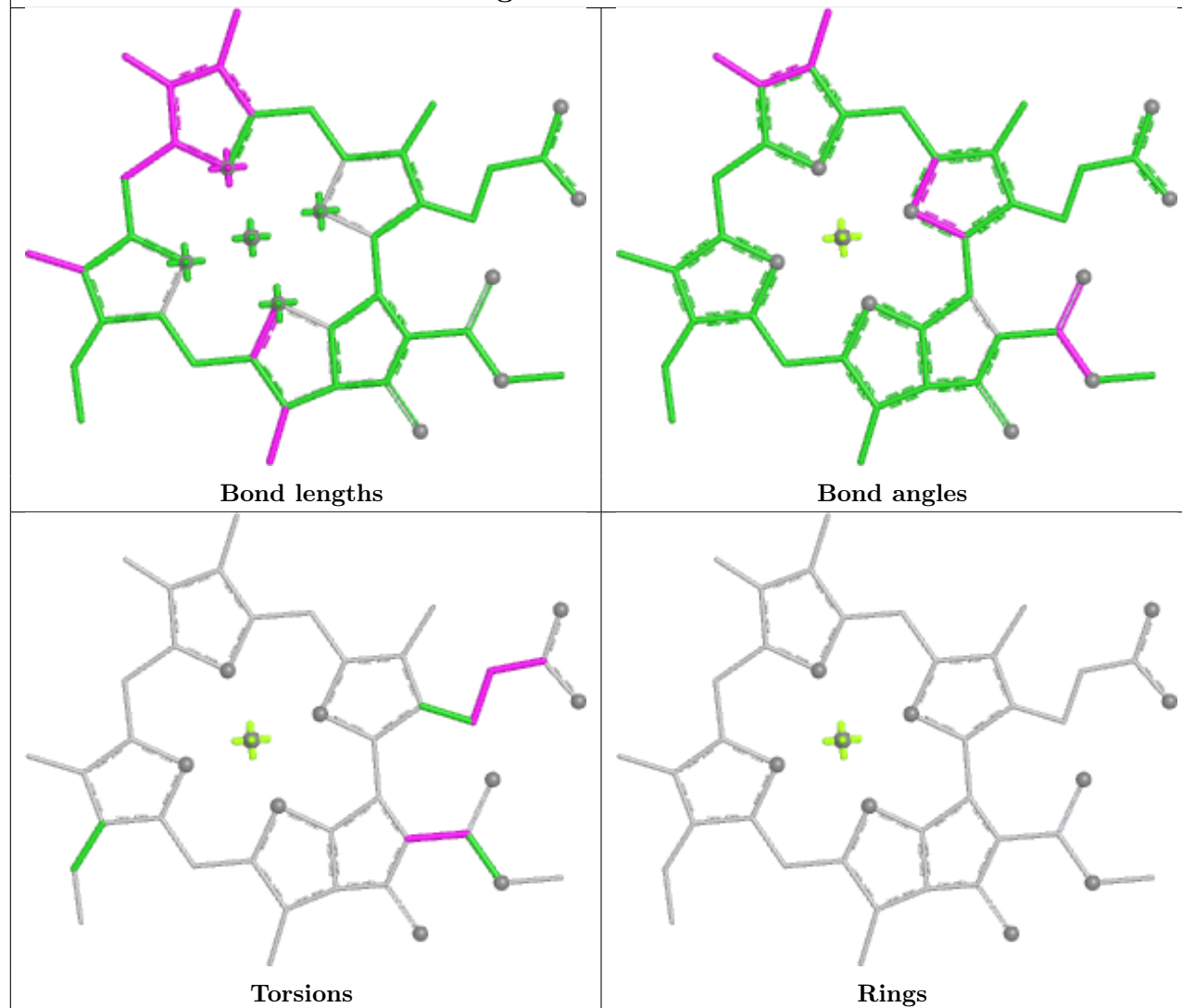
Ligand CLA X 613

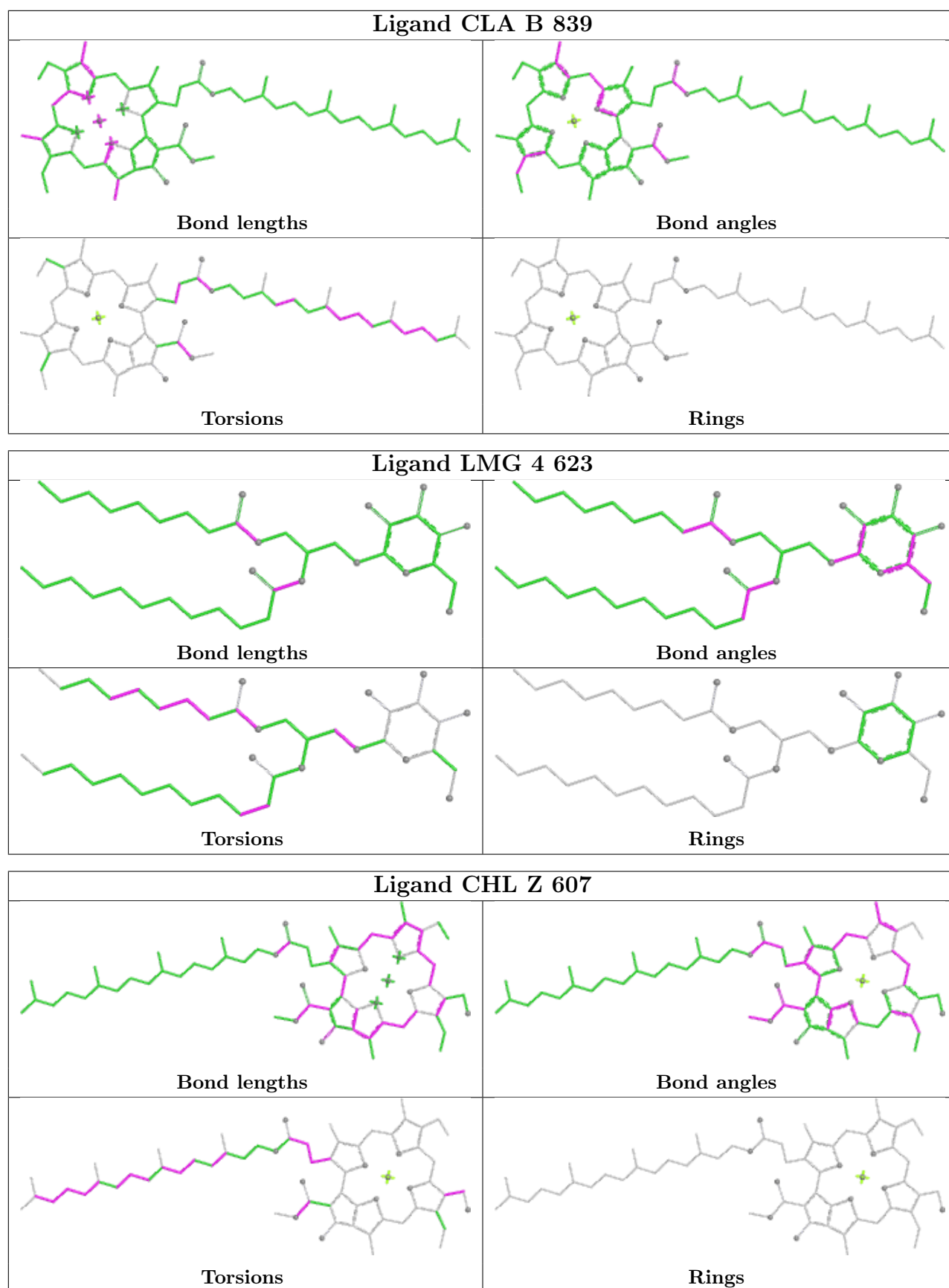


Ligand CLA A 824

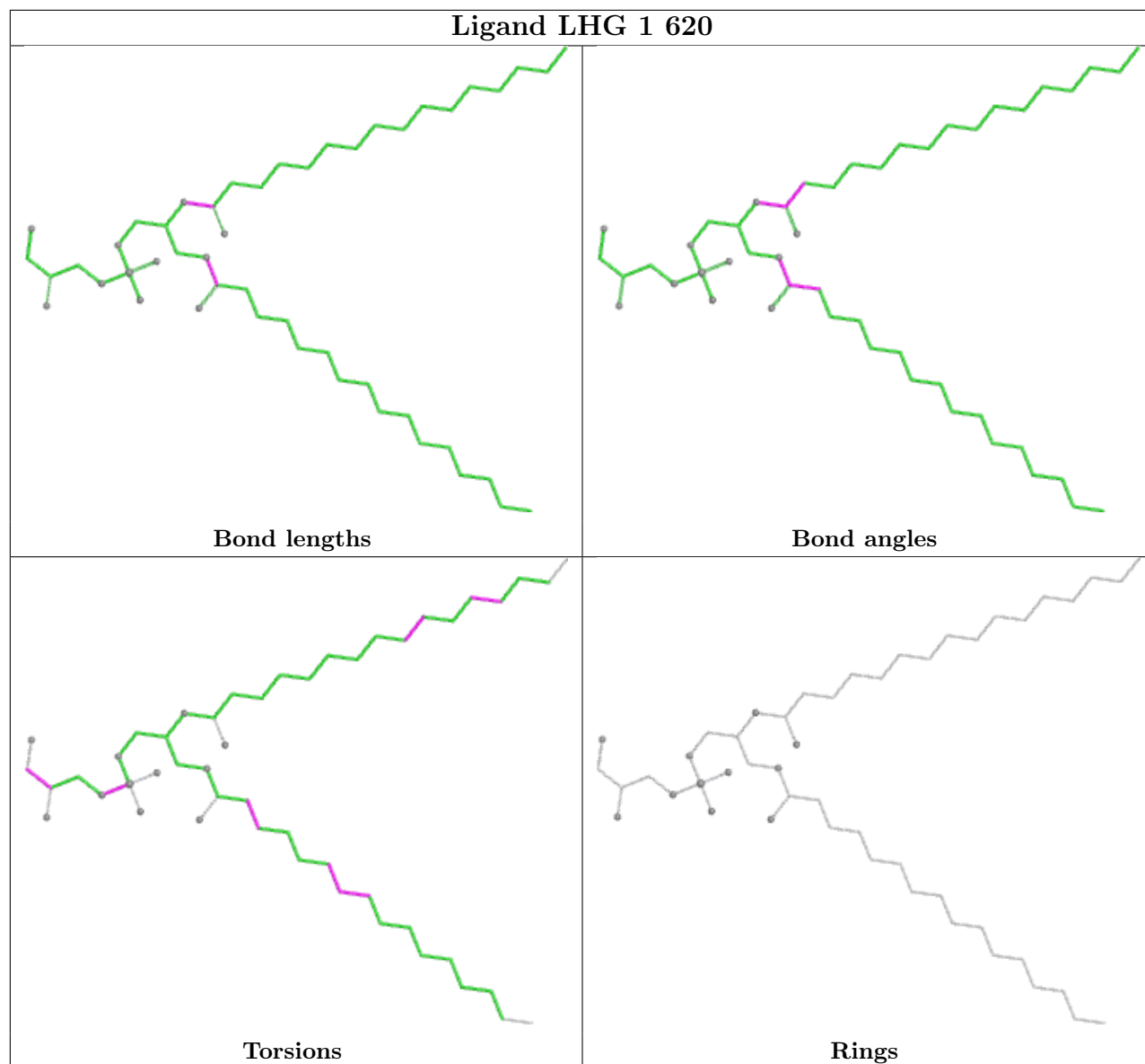


Ligand CLA 9 603

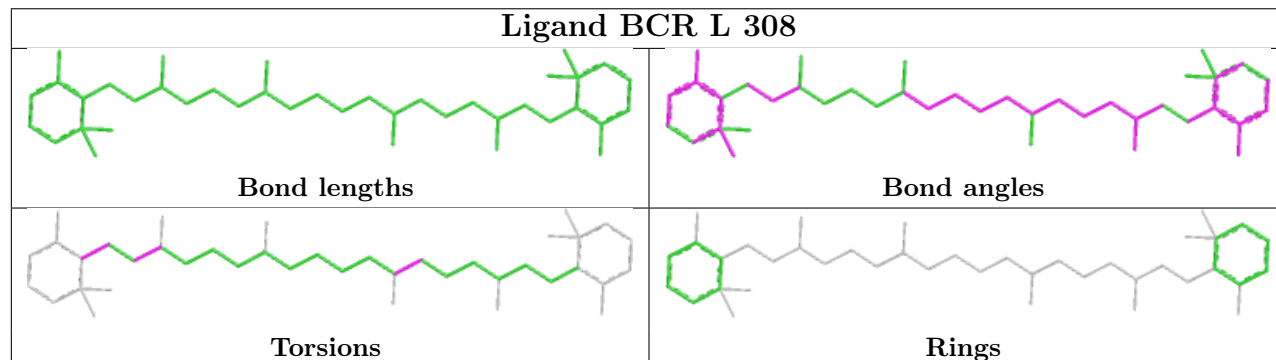




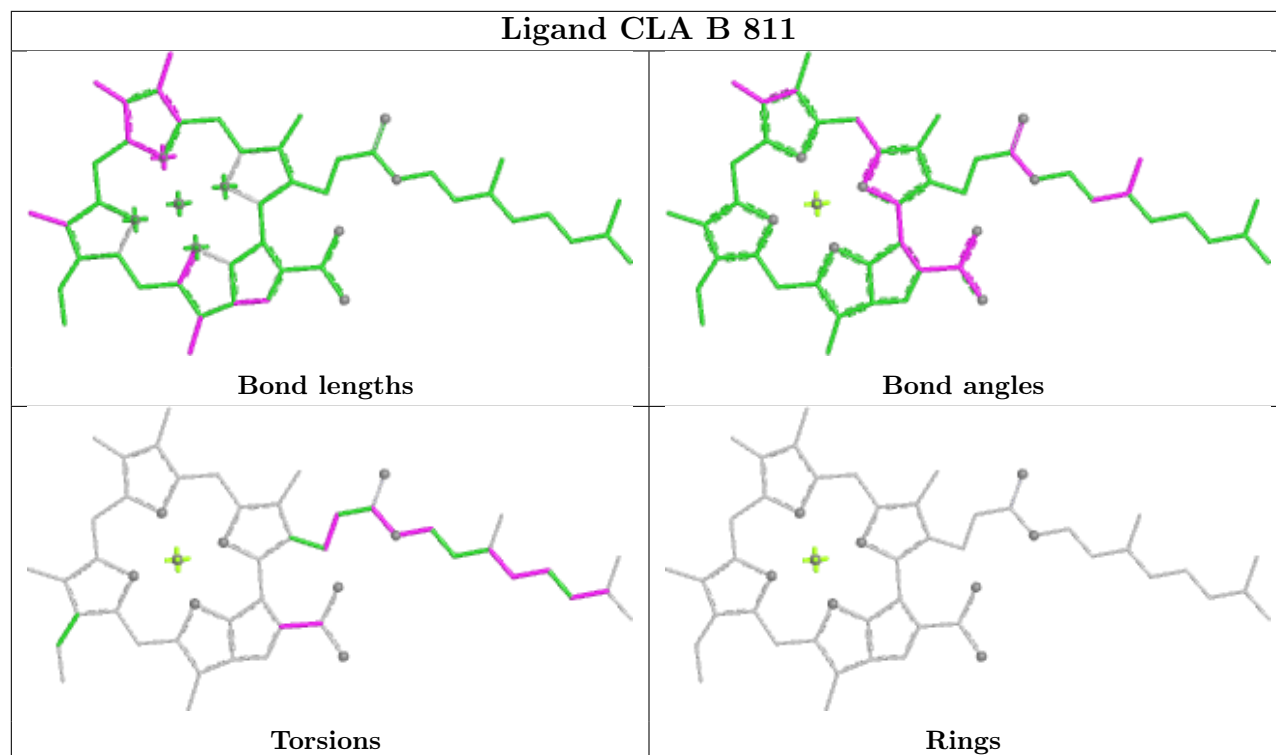
Ligand LHG 1 620



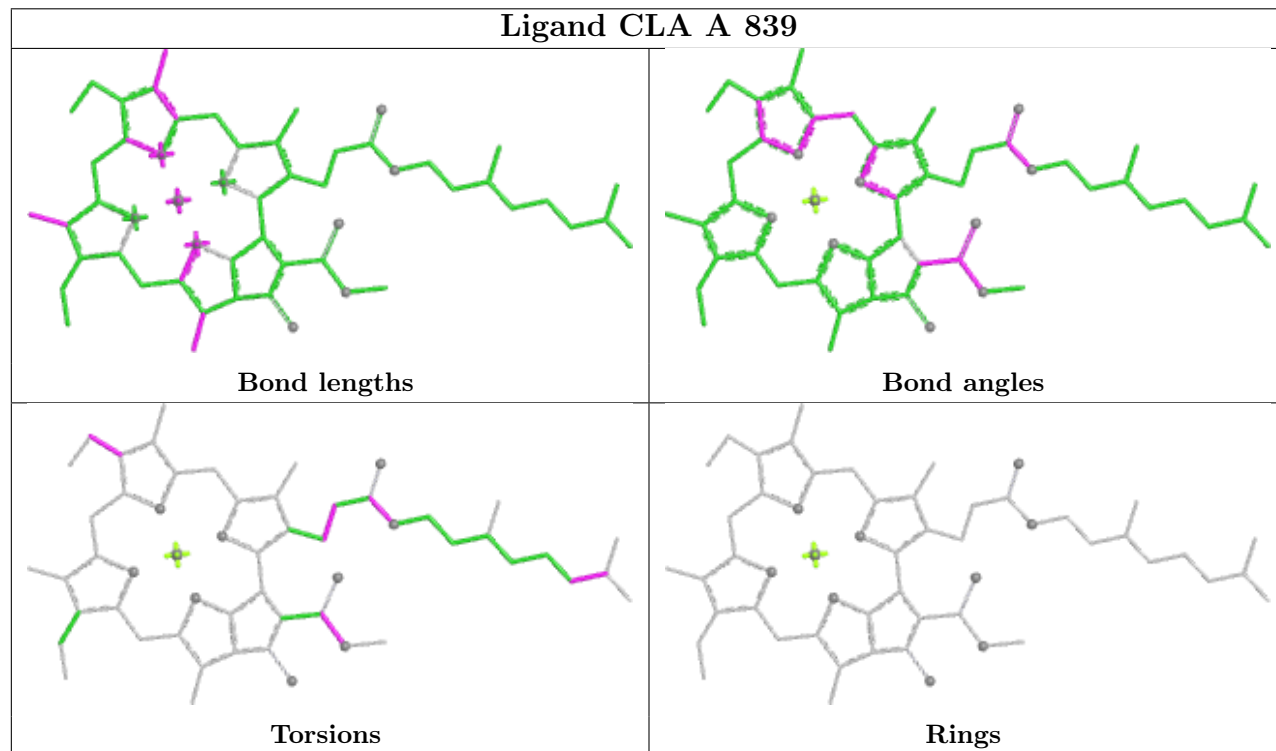
Ligand BCR L 308

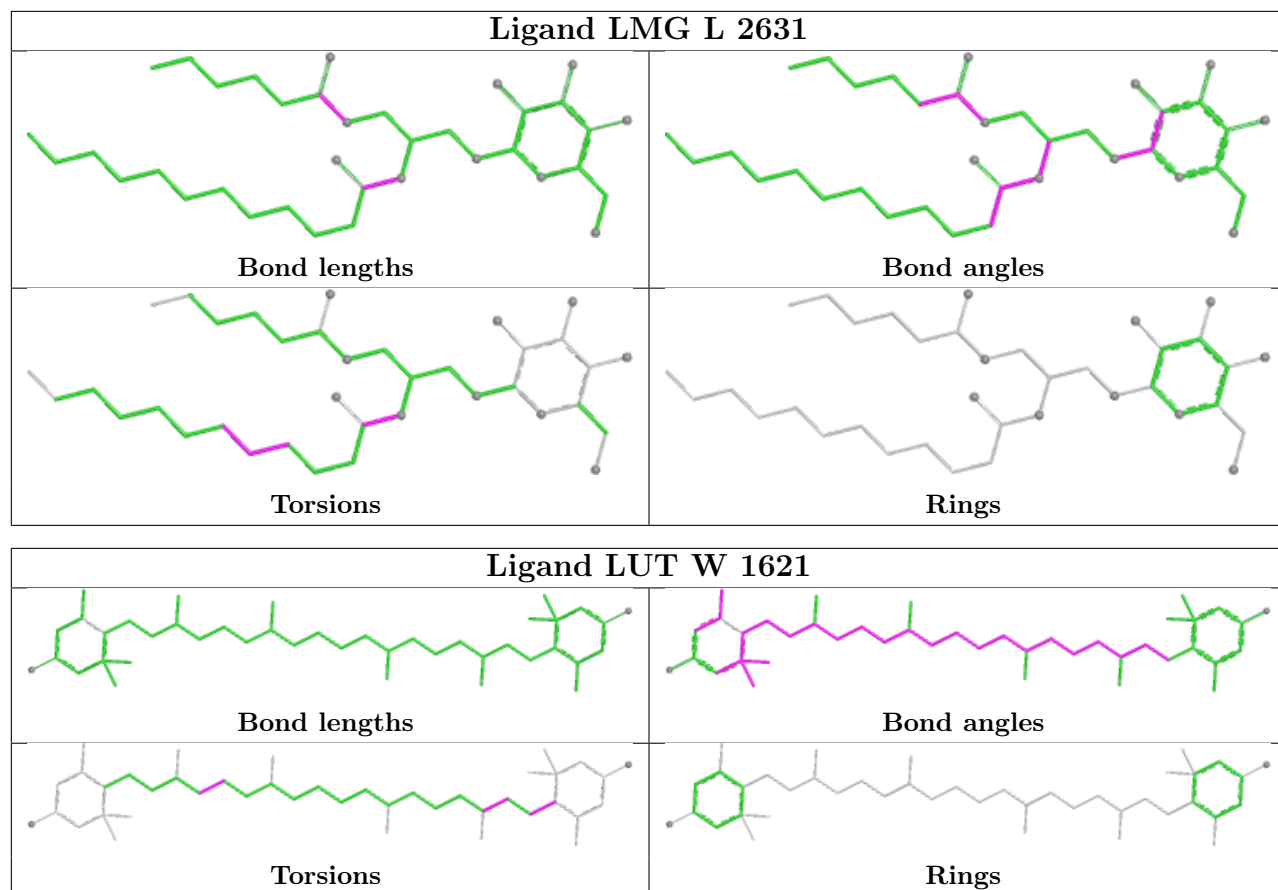


Ligand CLA B 811

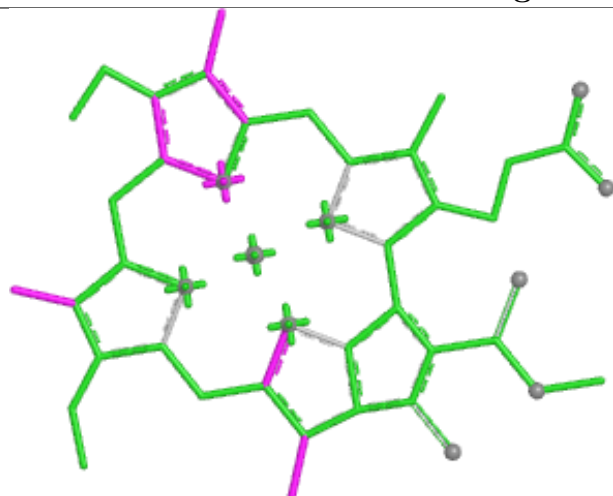


Ligand CLA A 839

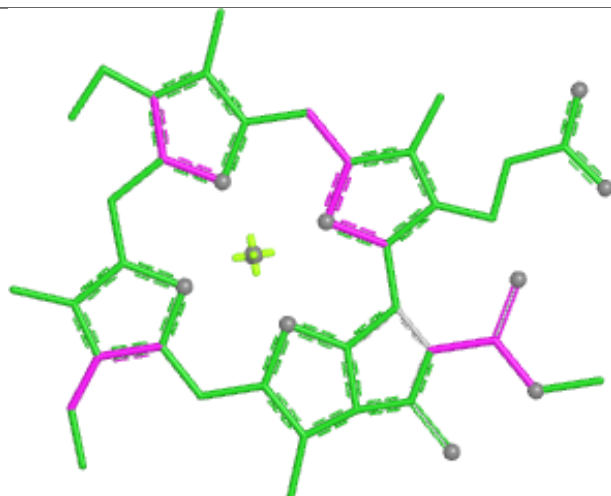




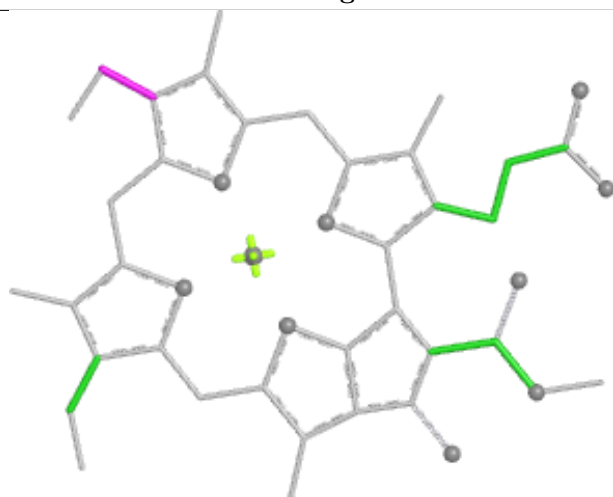
Ligand CLA A 817



Bond lengths



Bond angles

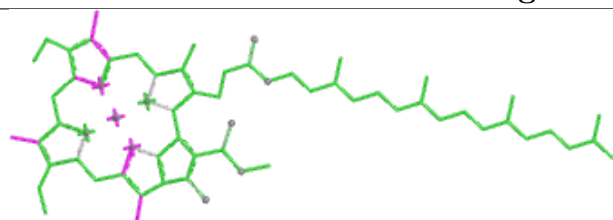


Torsions

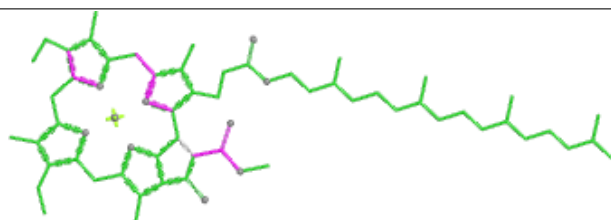


Rings

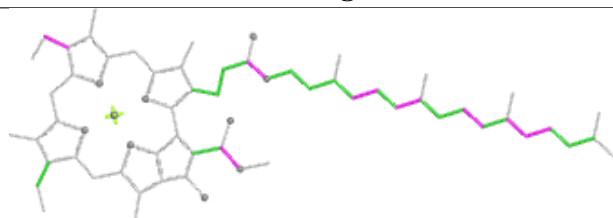
Ligand CLA 5 607



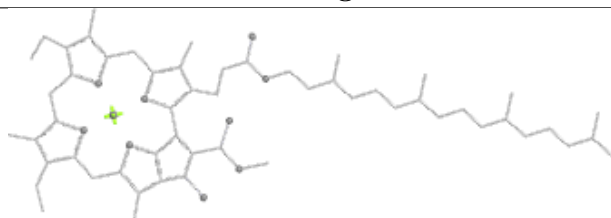
Bond lengths



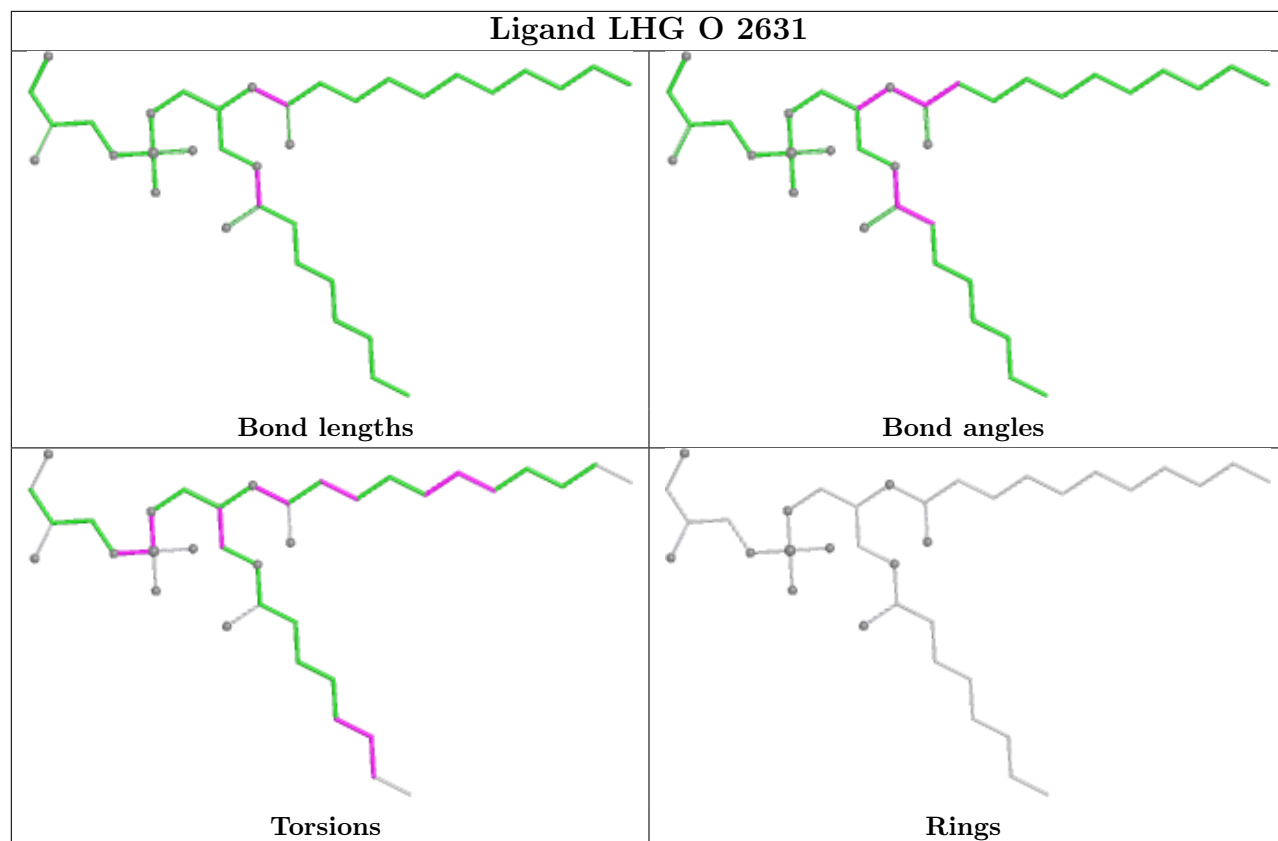
Bond angles

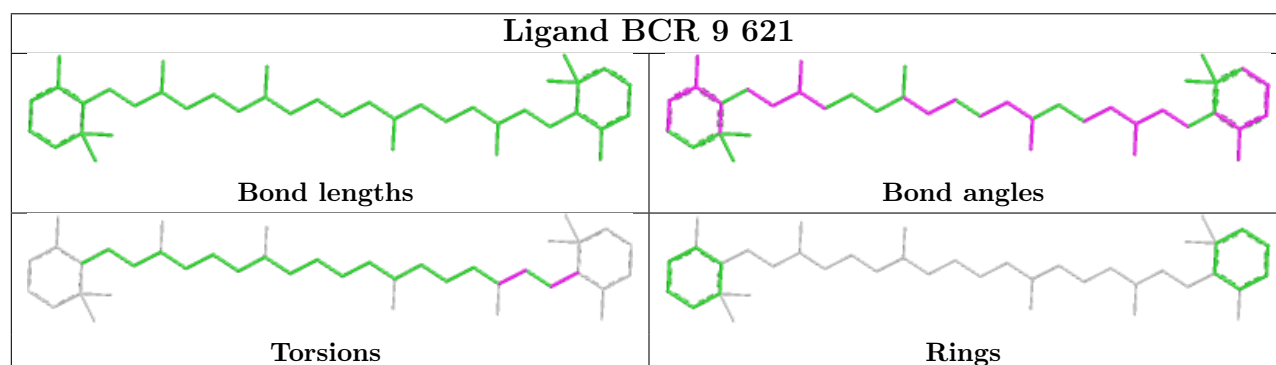
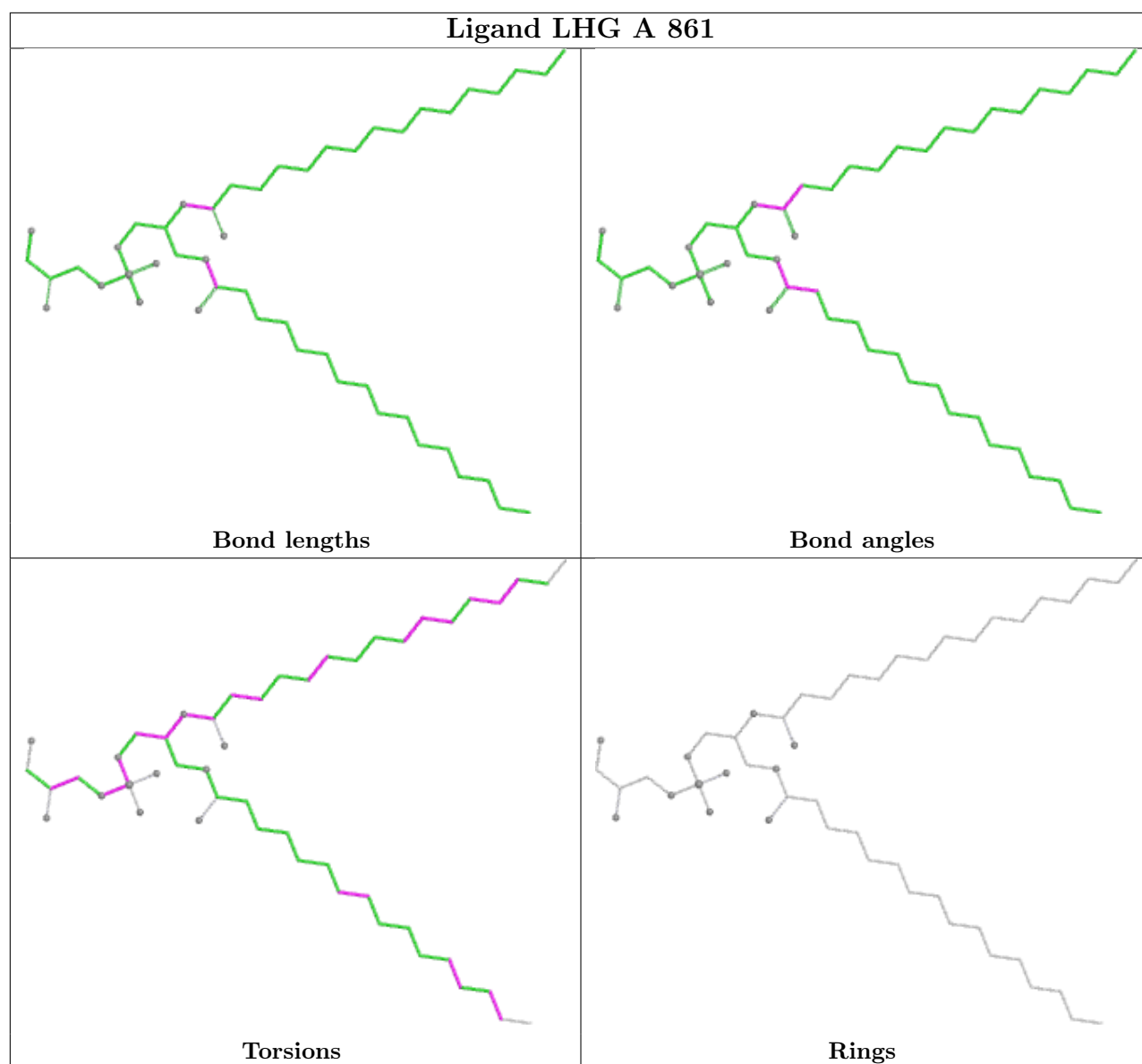


Torsions

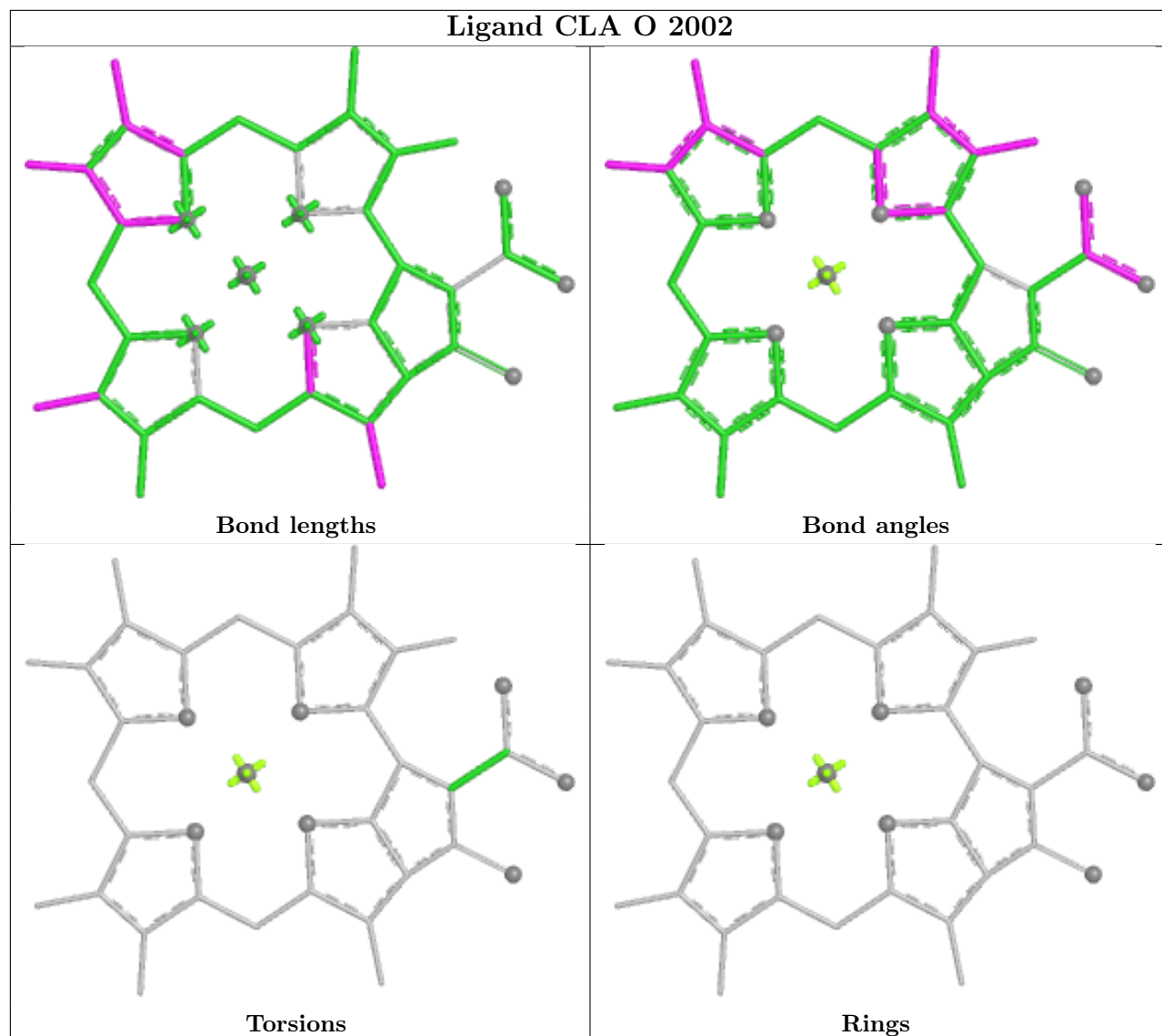


Rings

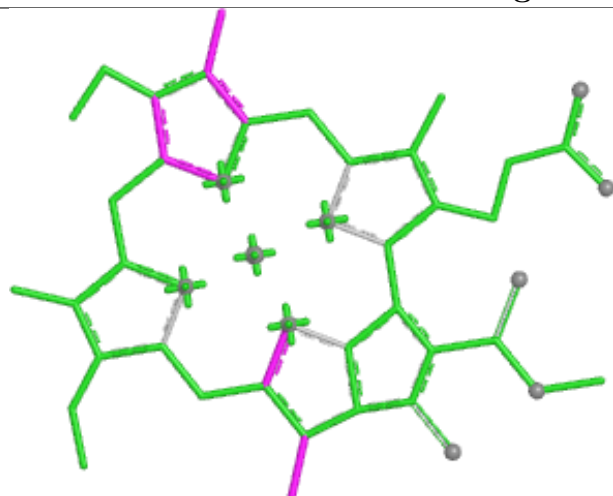




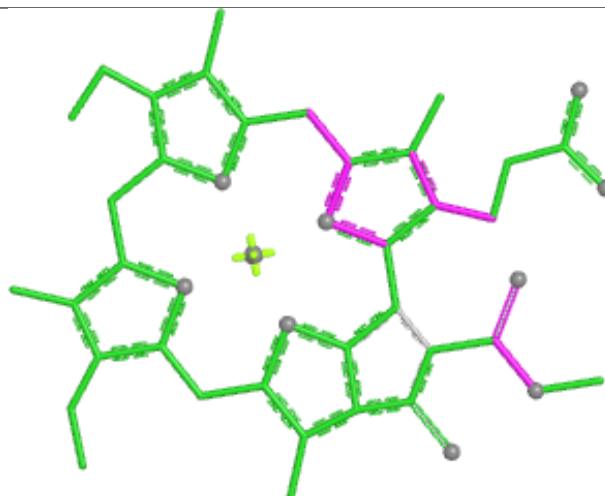
Ligand CLA O 2002



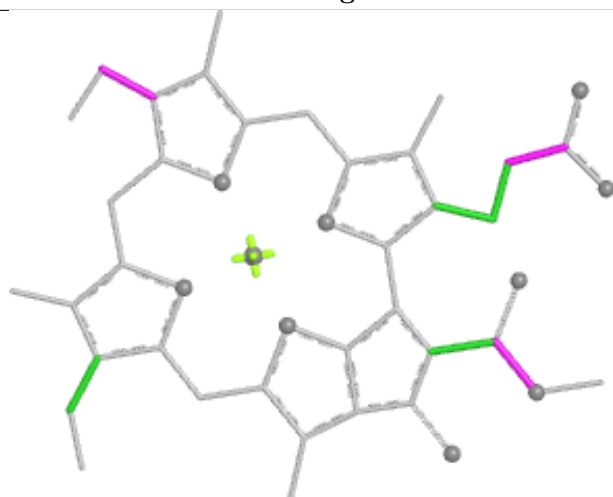
Ligand CLA V 603



Bond lengths



Bond angles

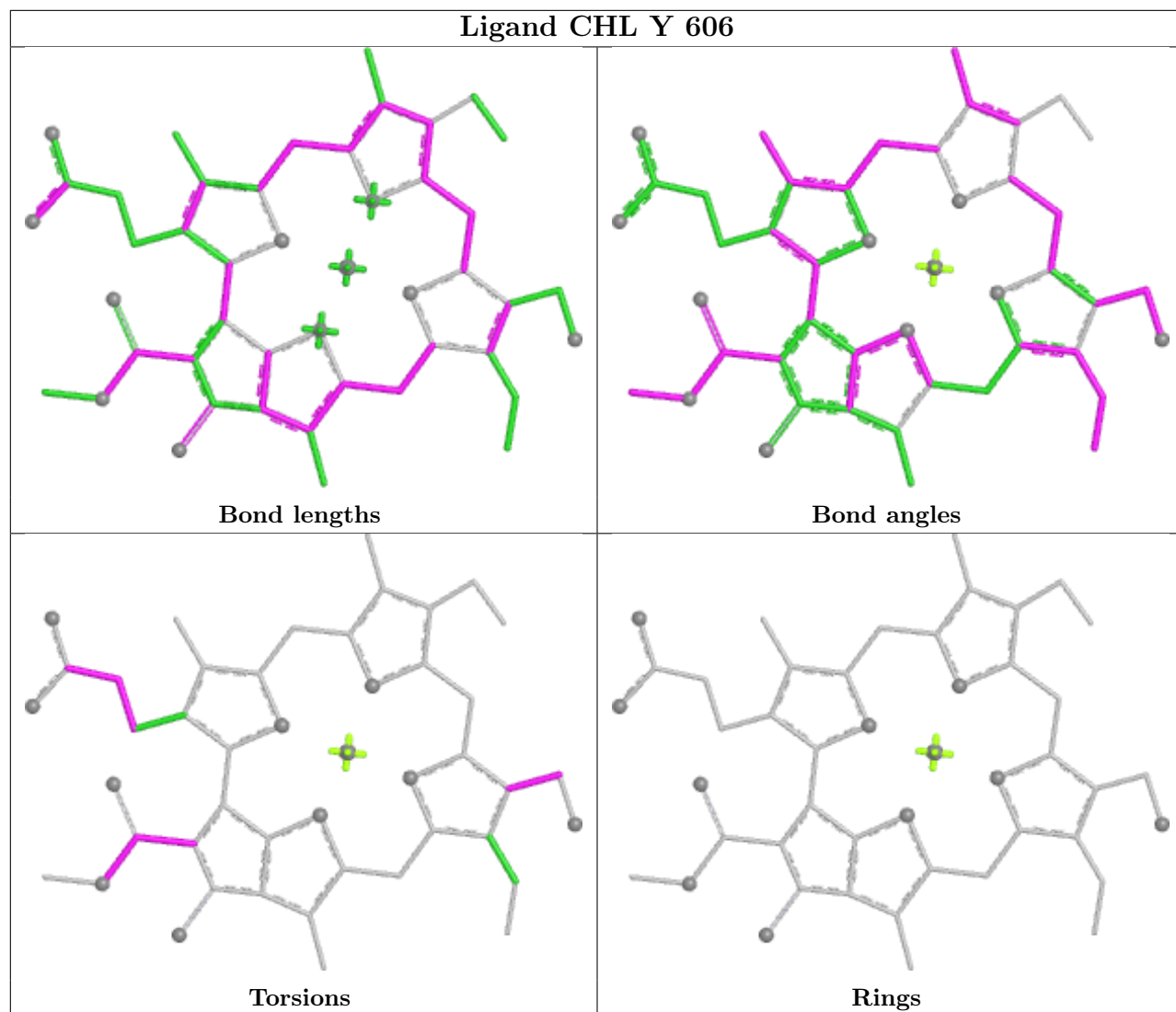


Torsions

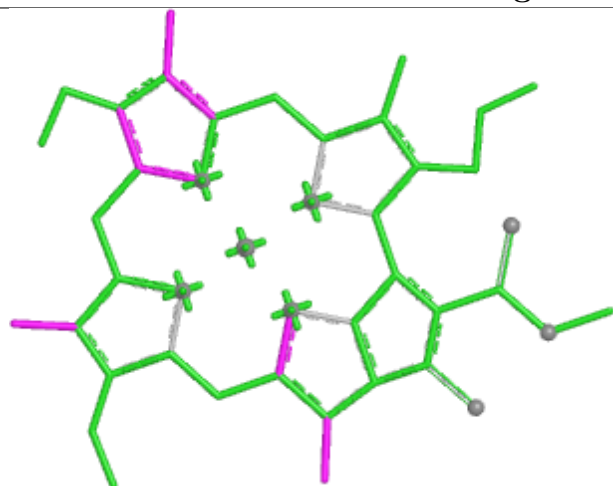


Rings

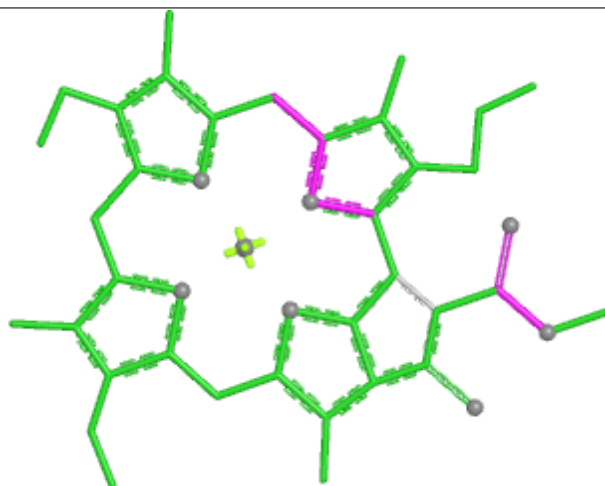
Ligand CHL Y 606



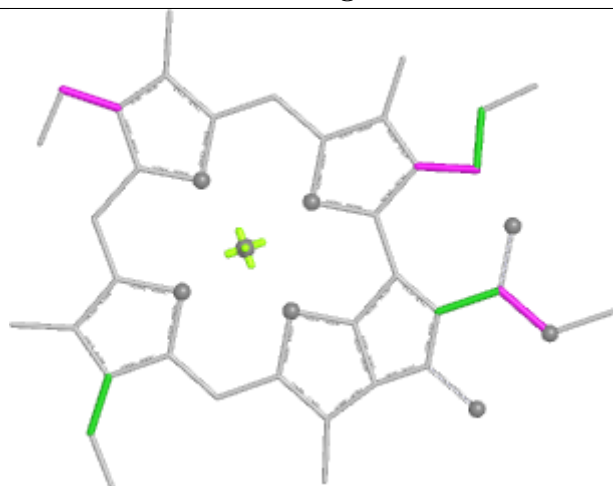
Ligand CLA V 611



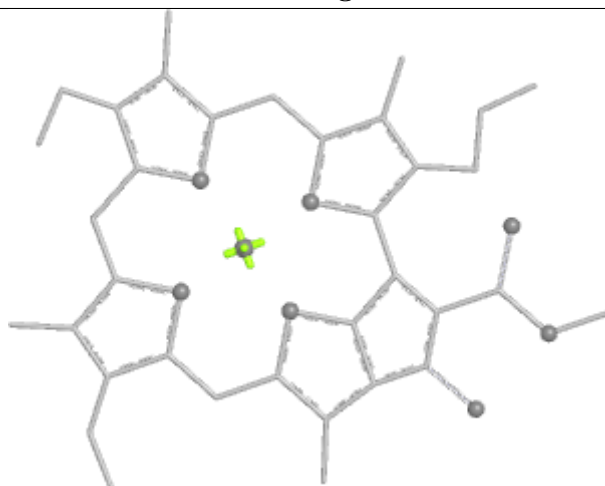
Bond lengths



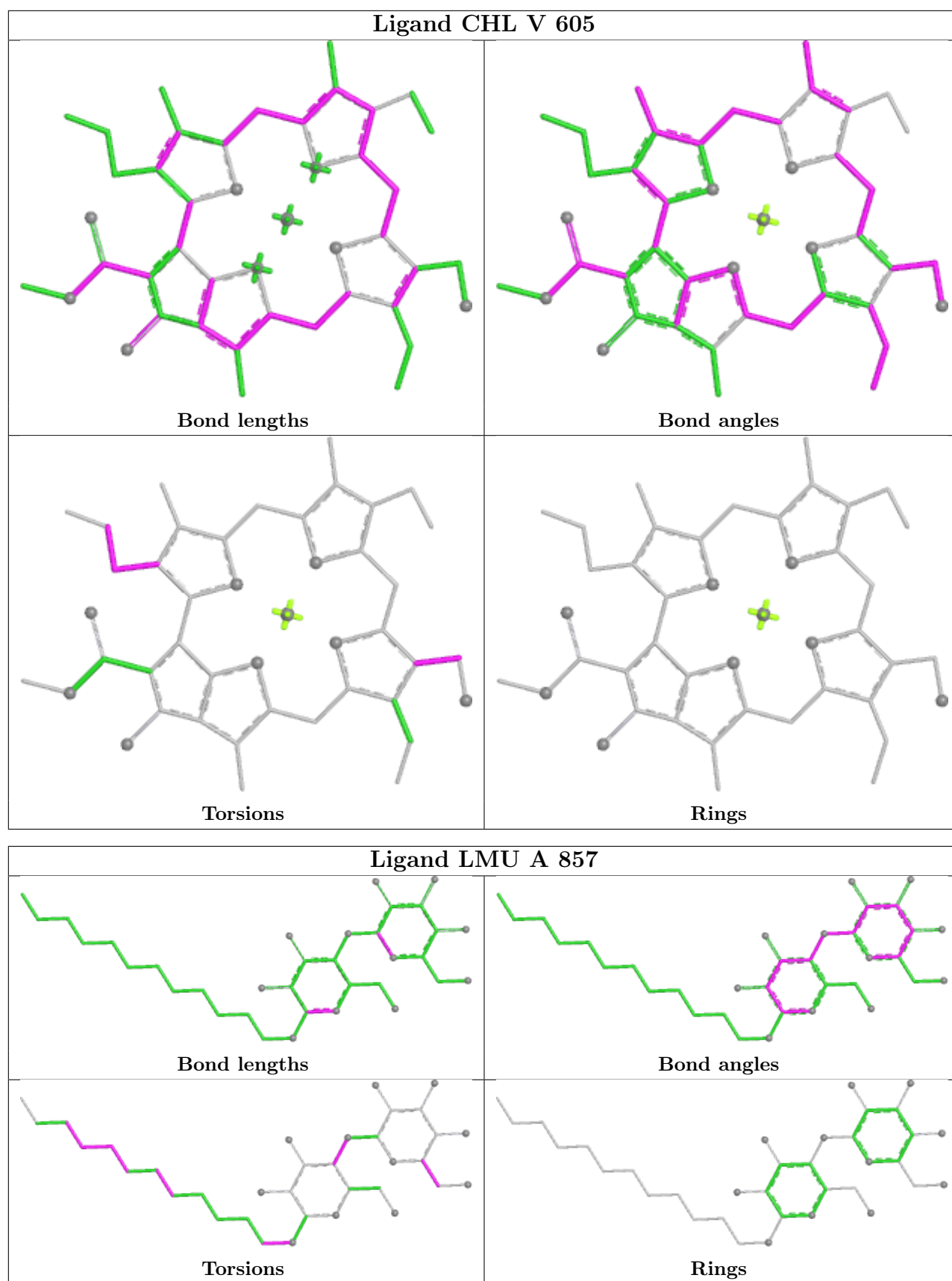
Bond angles

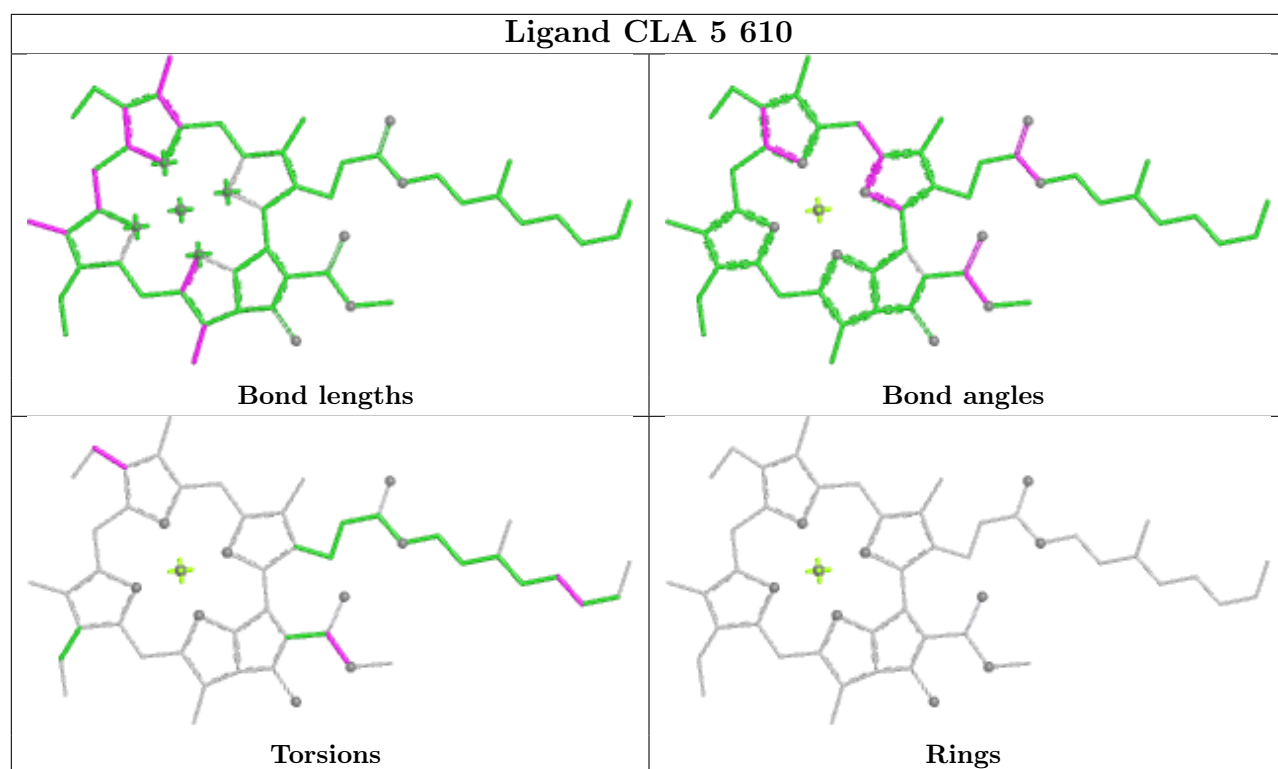


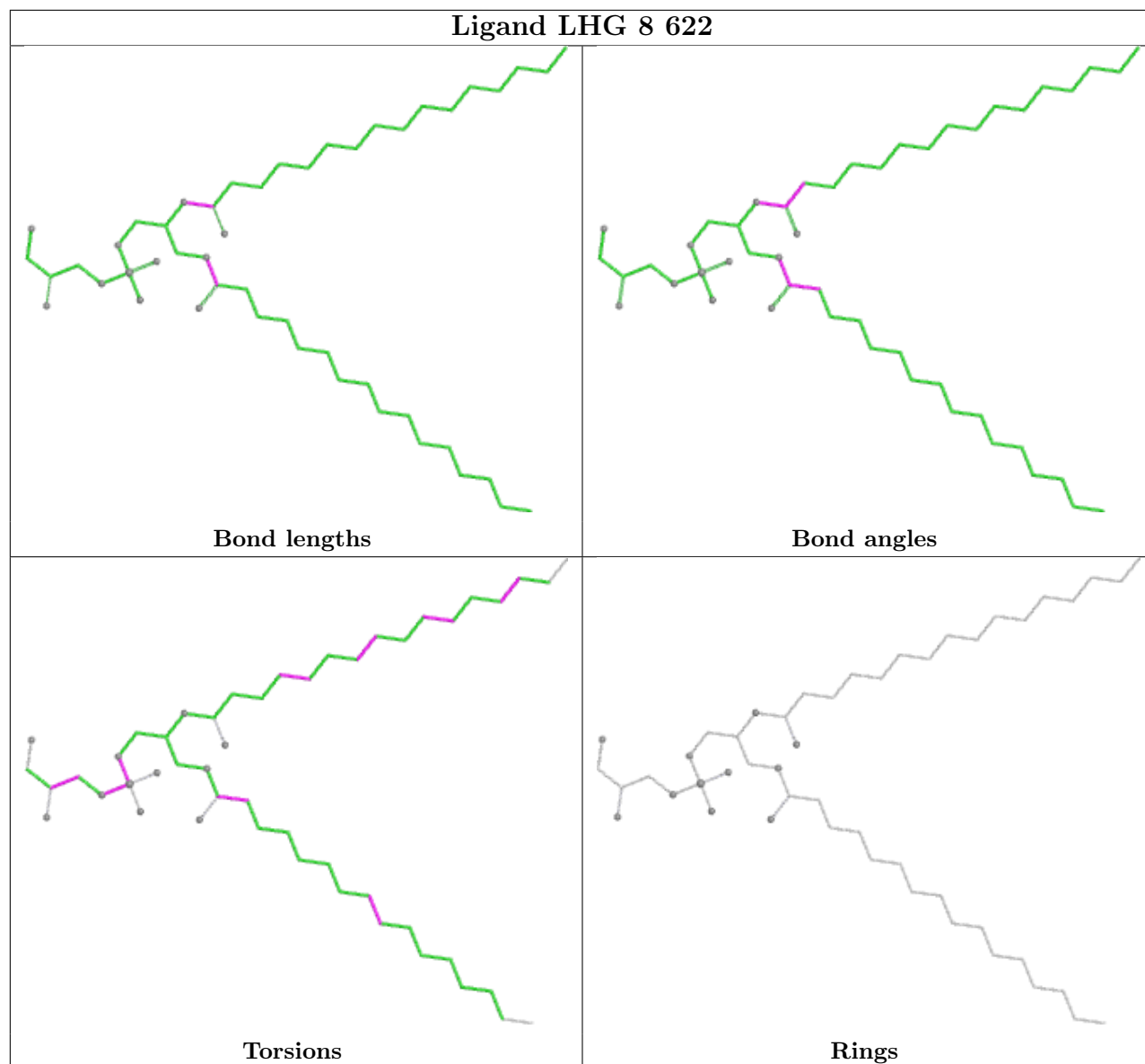
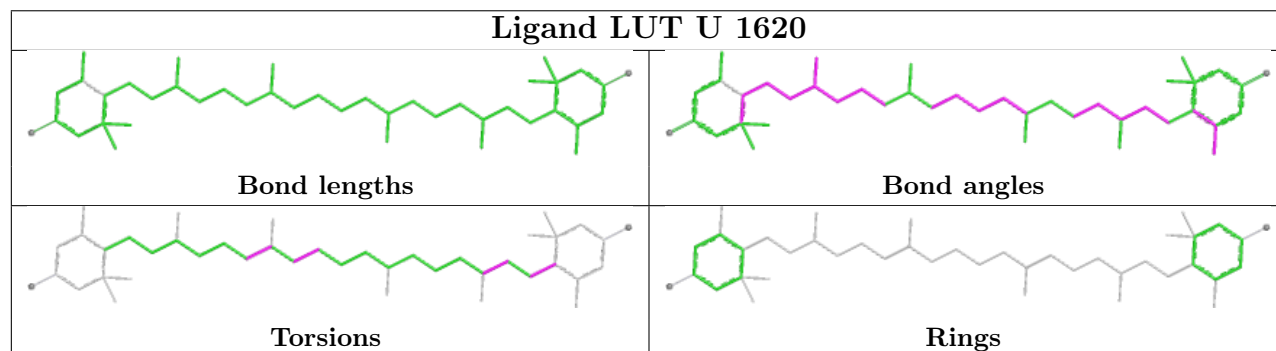
Torsions

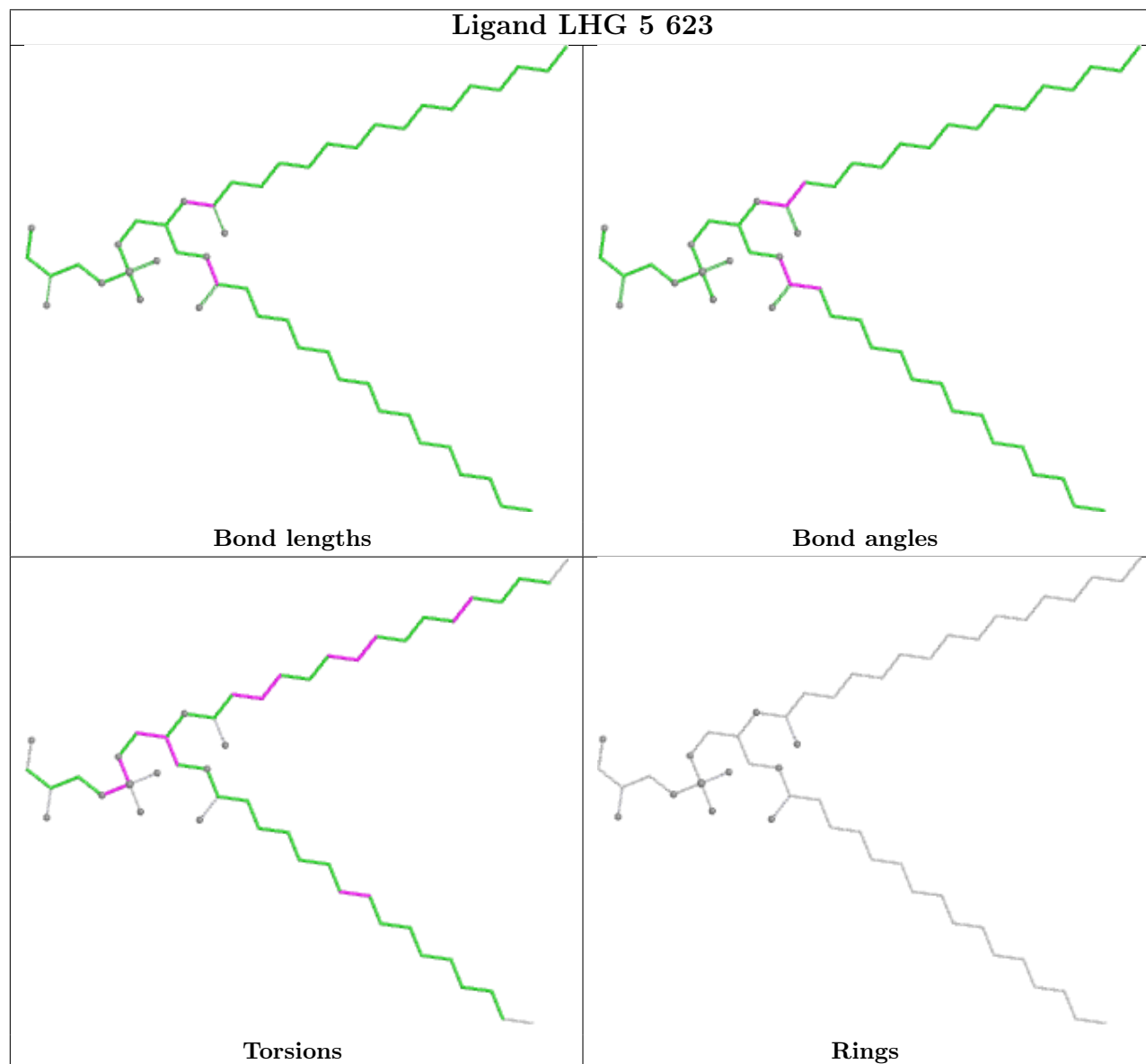
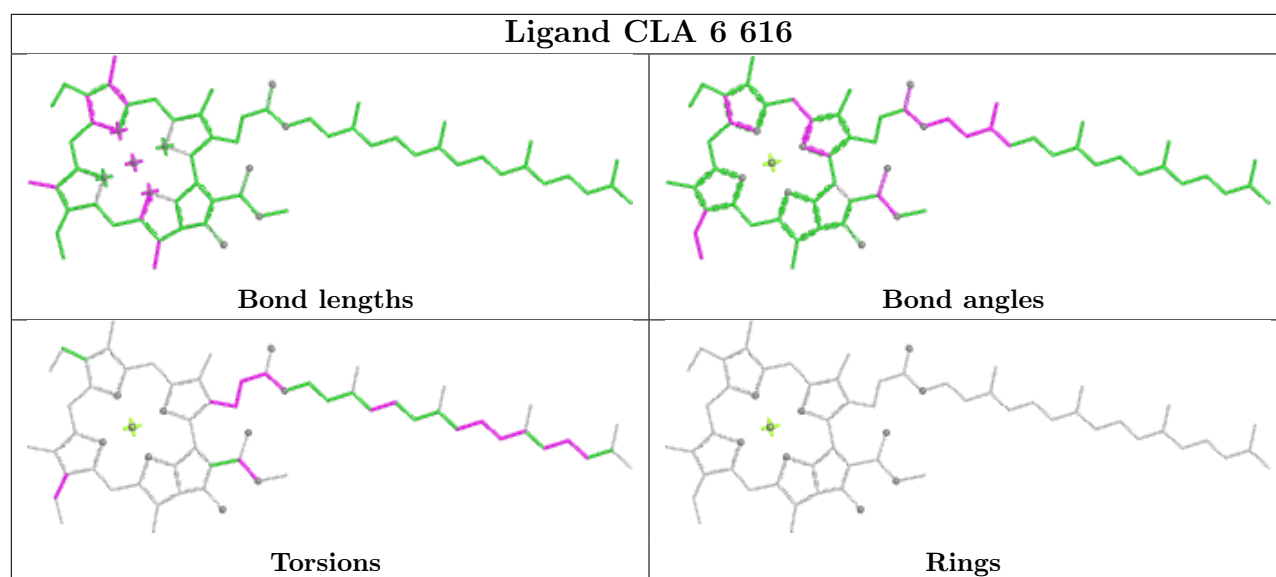


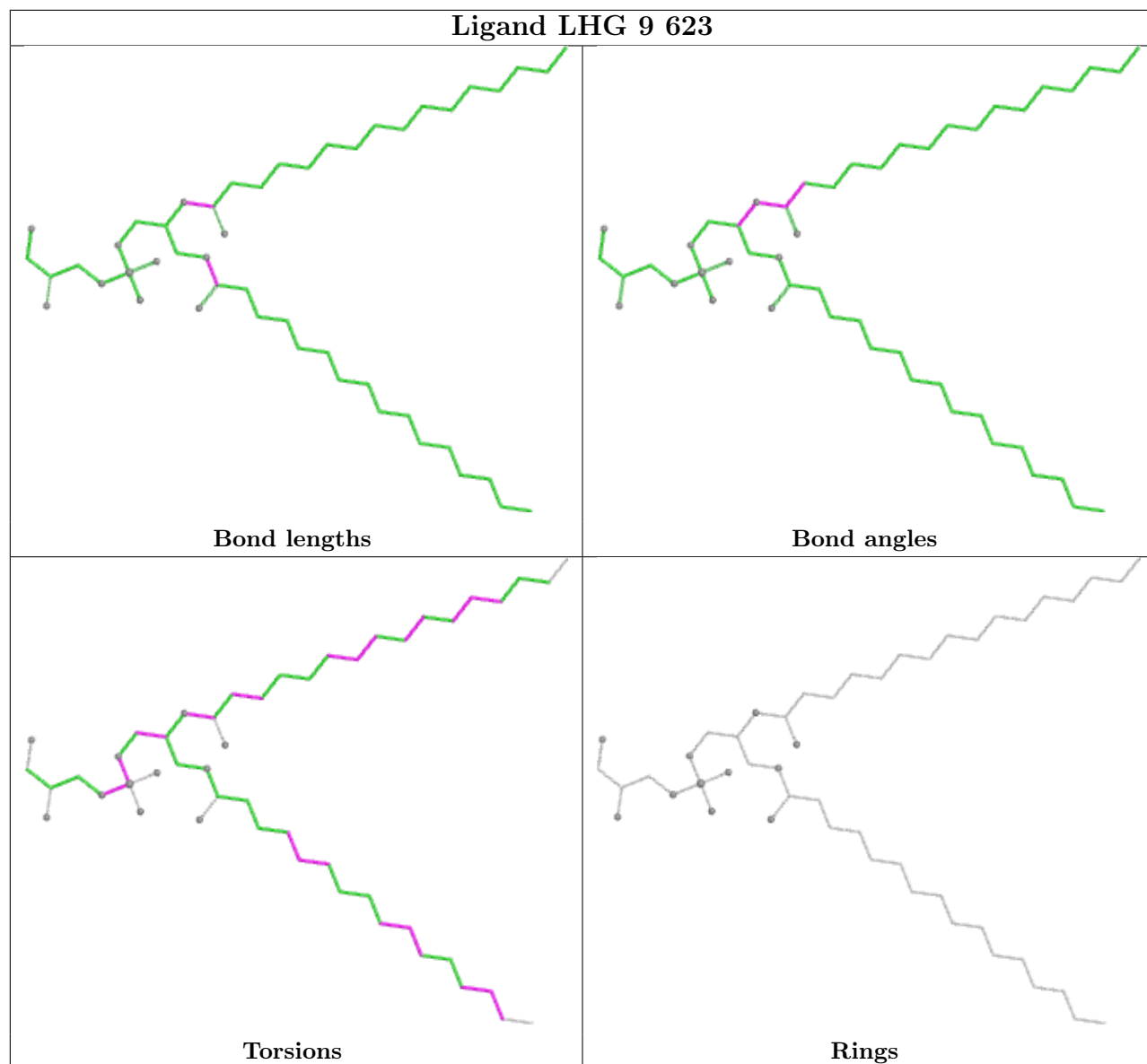
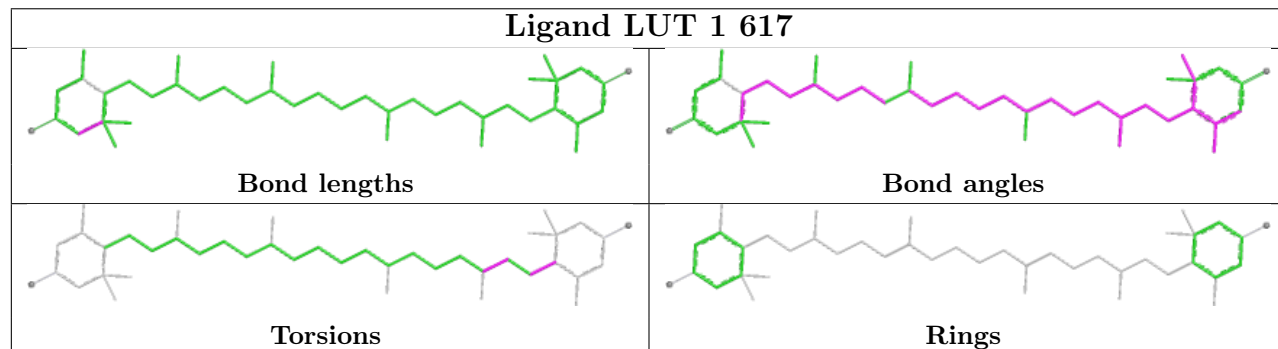
Rings

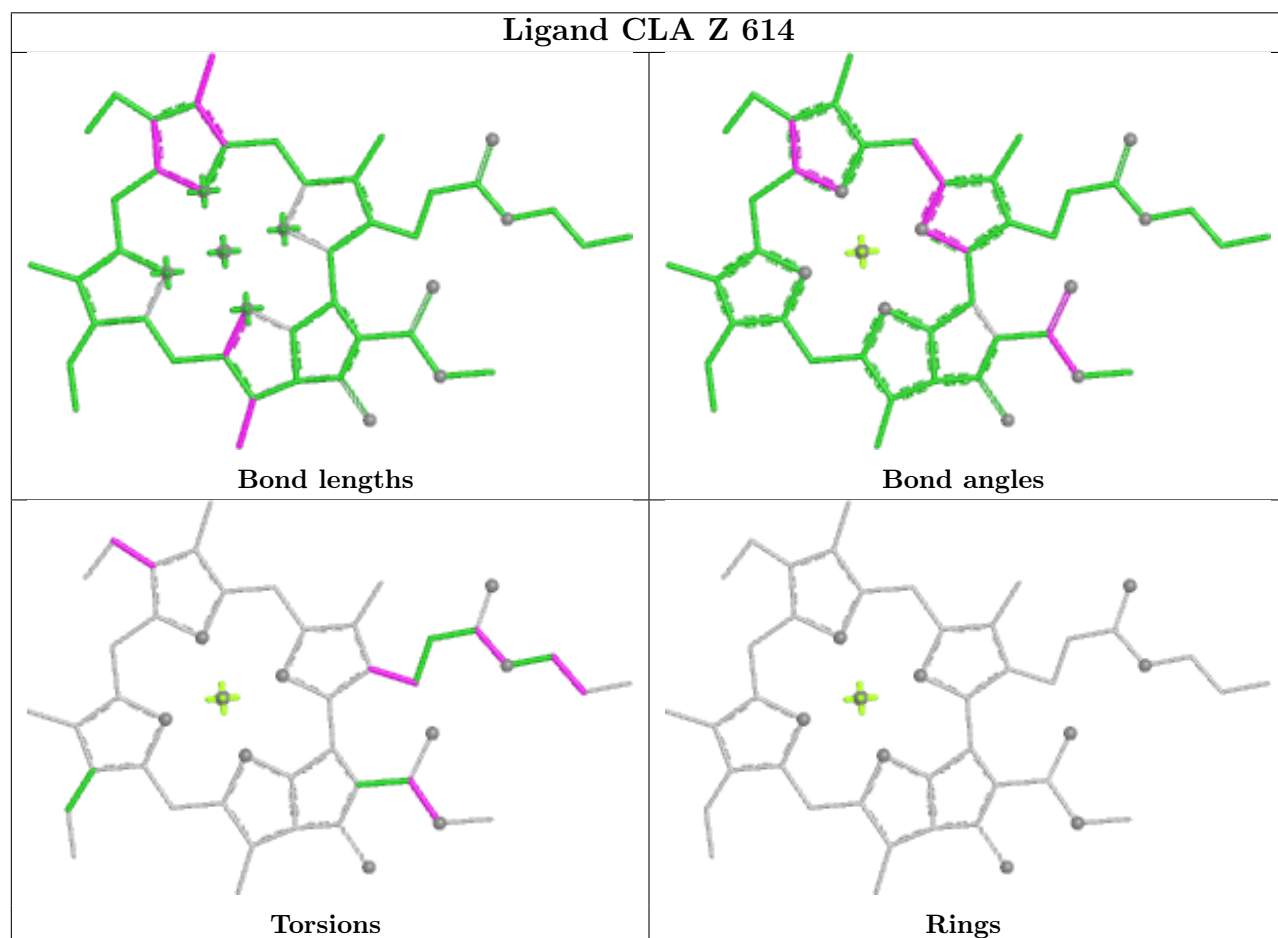
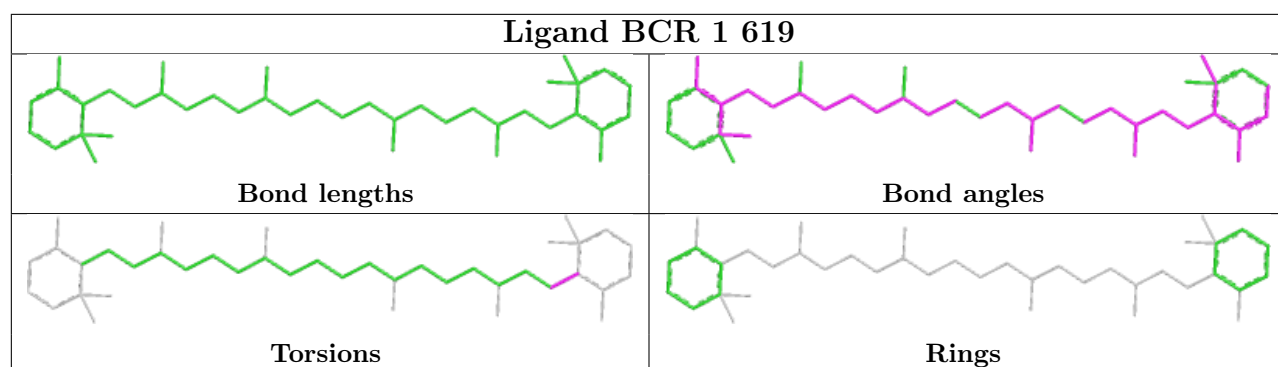




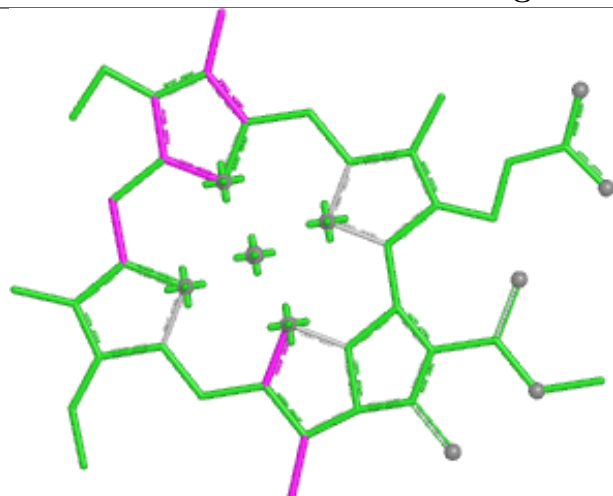
Ligand LHG 8 622**Ligand LUT U 1620**



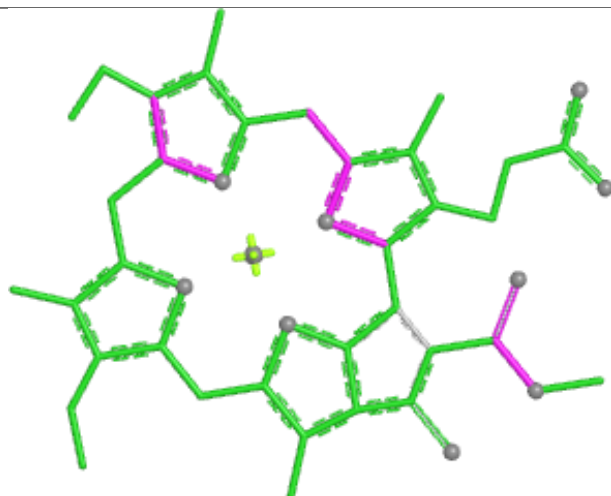
Ligand LHG 9 623**Ligand LUT 1 617**



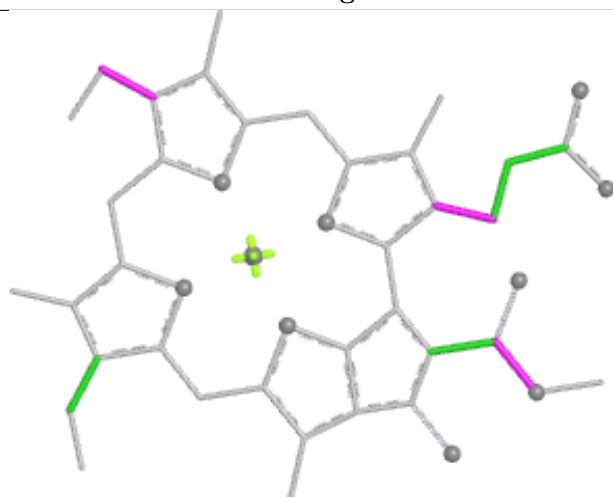
Ligand CLA V 614



Bond lengths



Bond angles

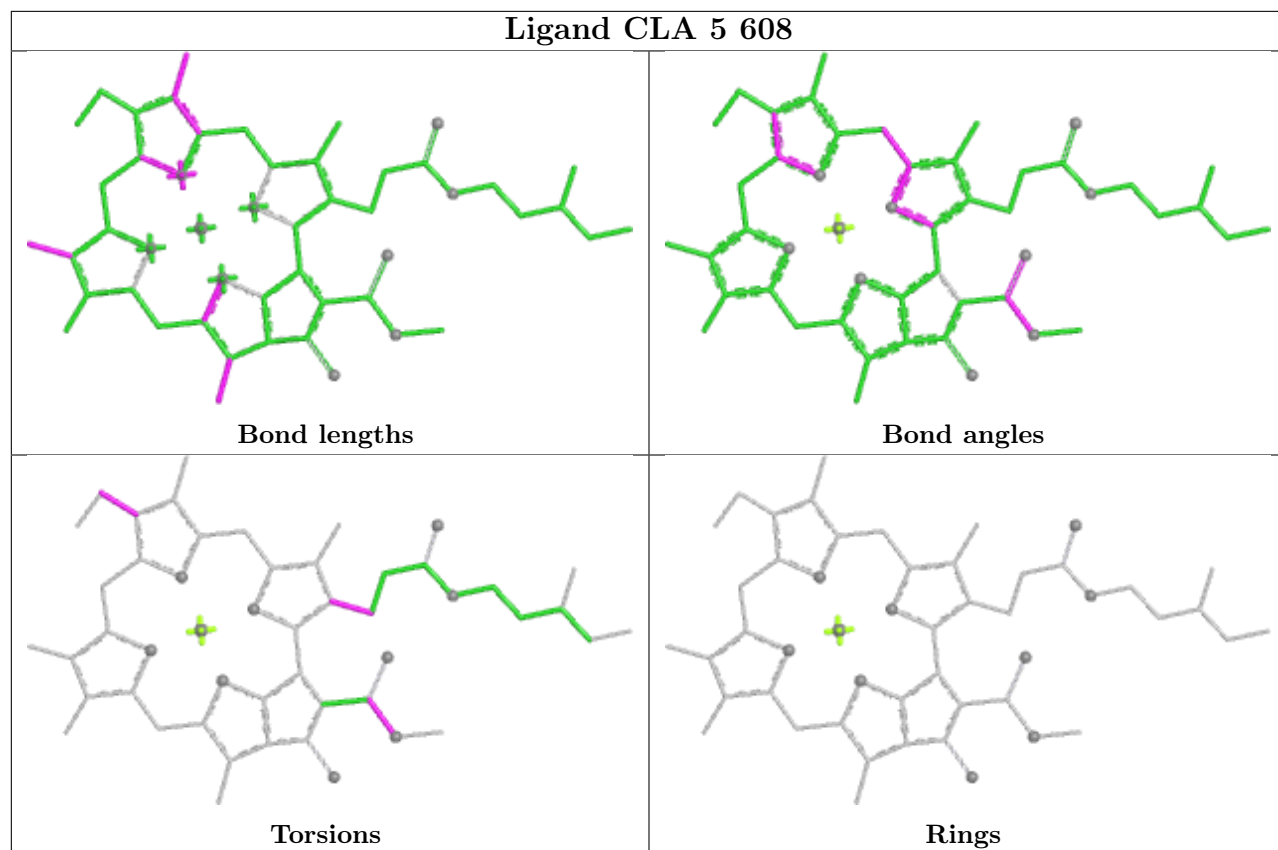


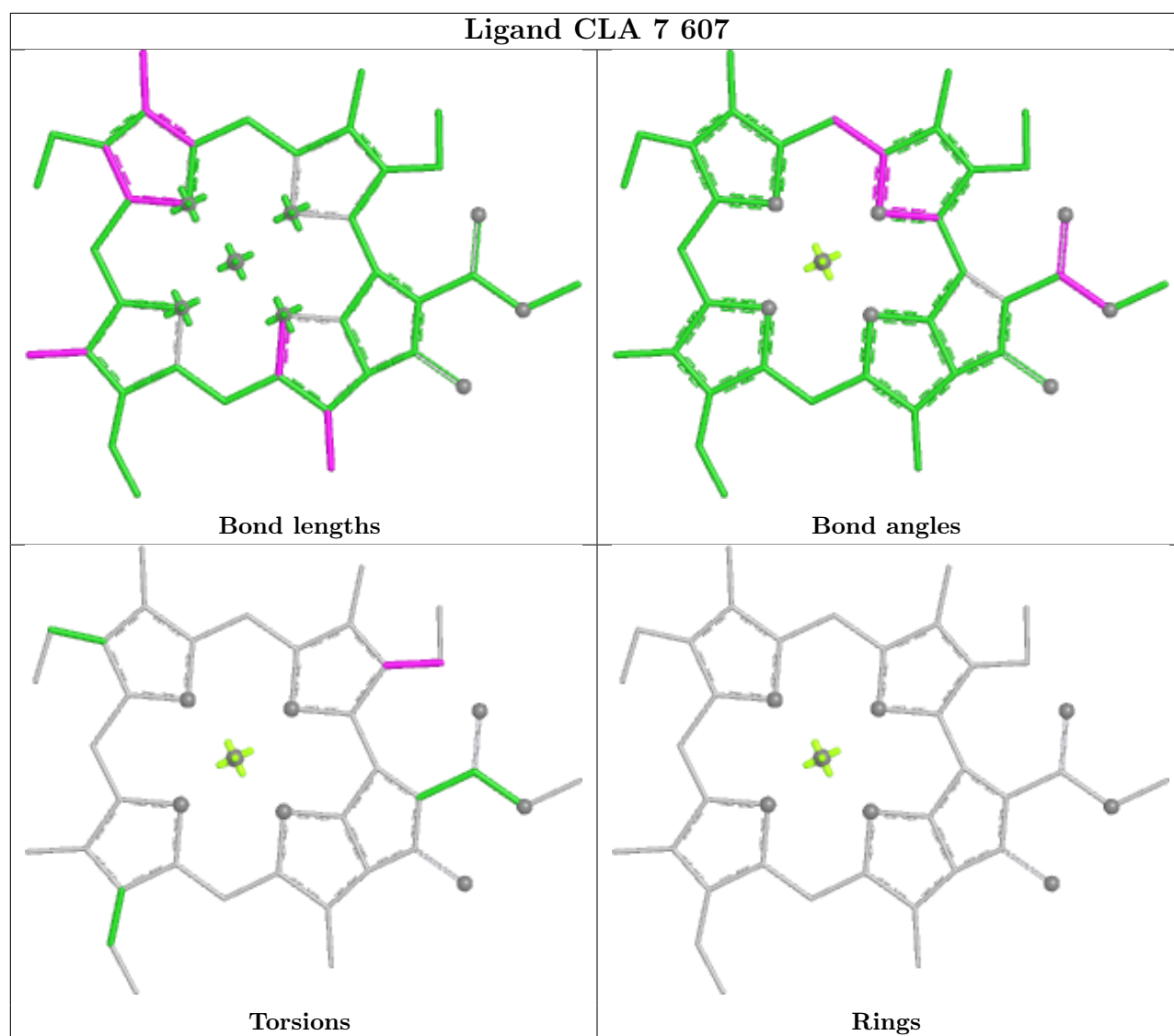
Torsions



Rings

Ligand CLA 5 608





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

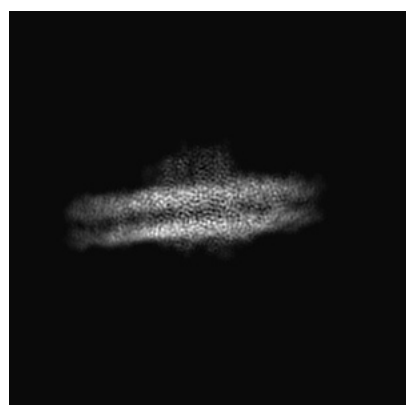
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-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](#)

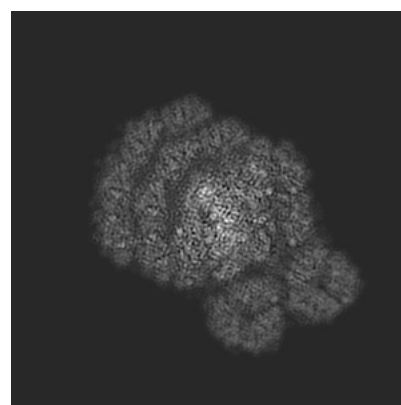
6.1.1 Primary map



X



Y

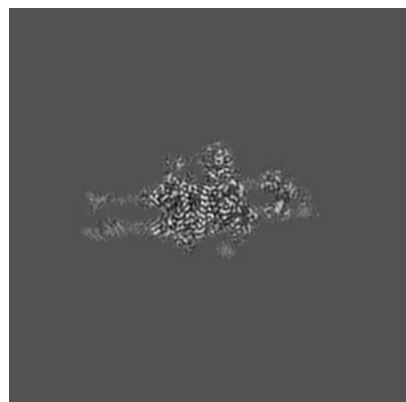


Z

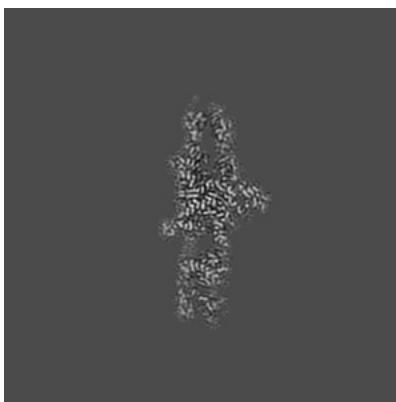
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

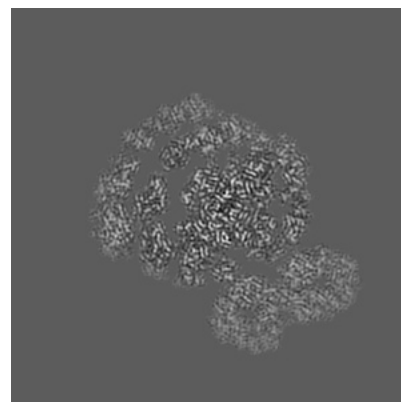
6.2.1 Primary map



X Index: 180



Y Index: 180

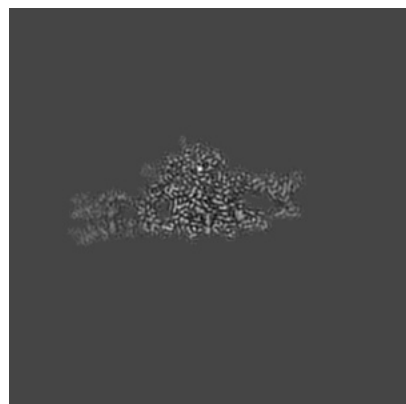


Z Index: 180

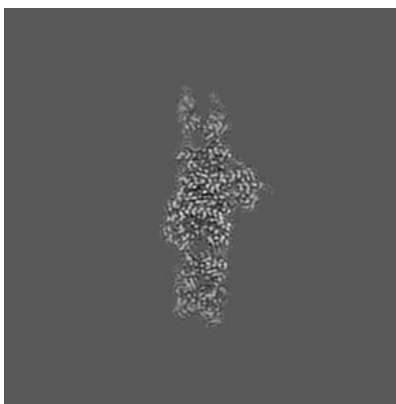
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

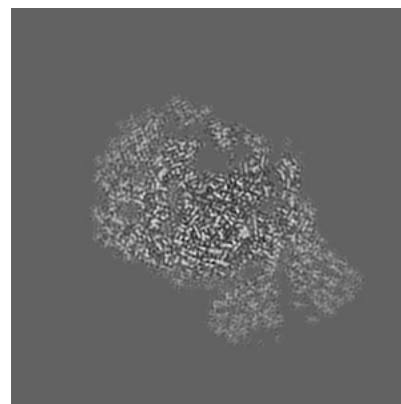
6.3.1 Primary map



X Index: 194



Y Index: 153

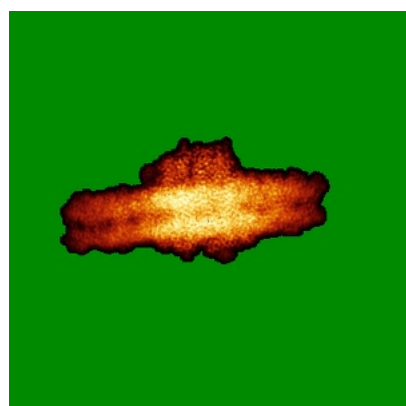


Z Index: 190

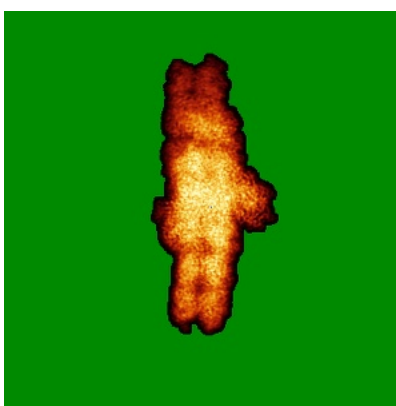
The images above show the largest variance slices of the map in three orthogonal directions.

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

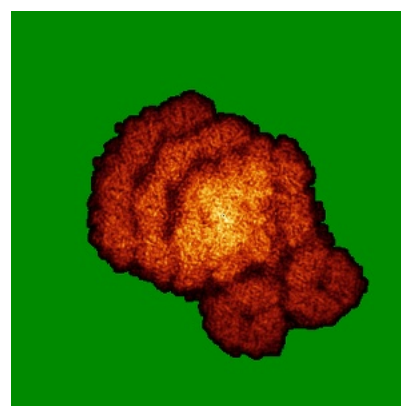
6.4.1 Primary map



X



Y

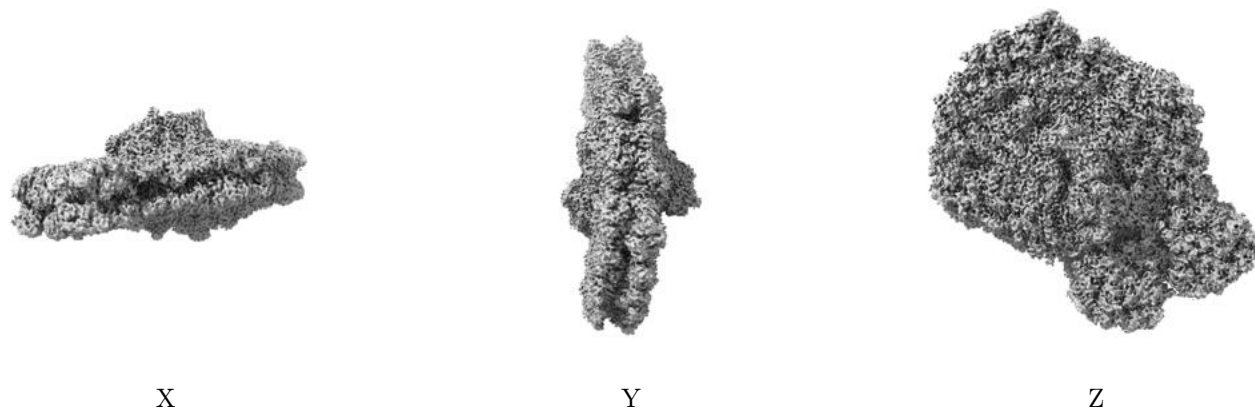


Z

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.

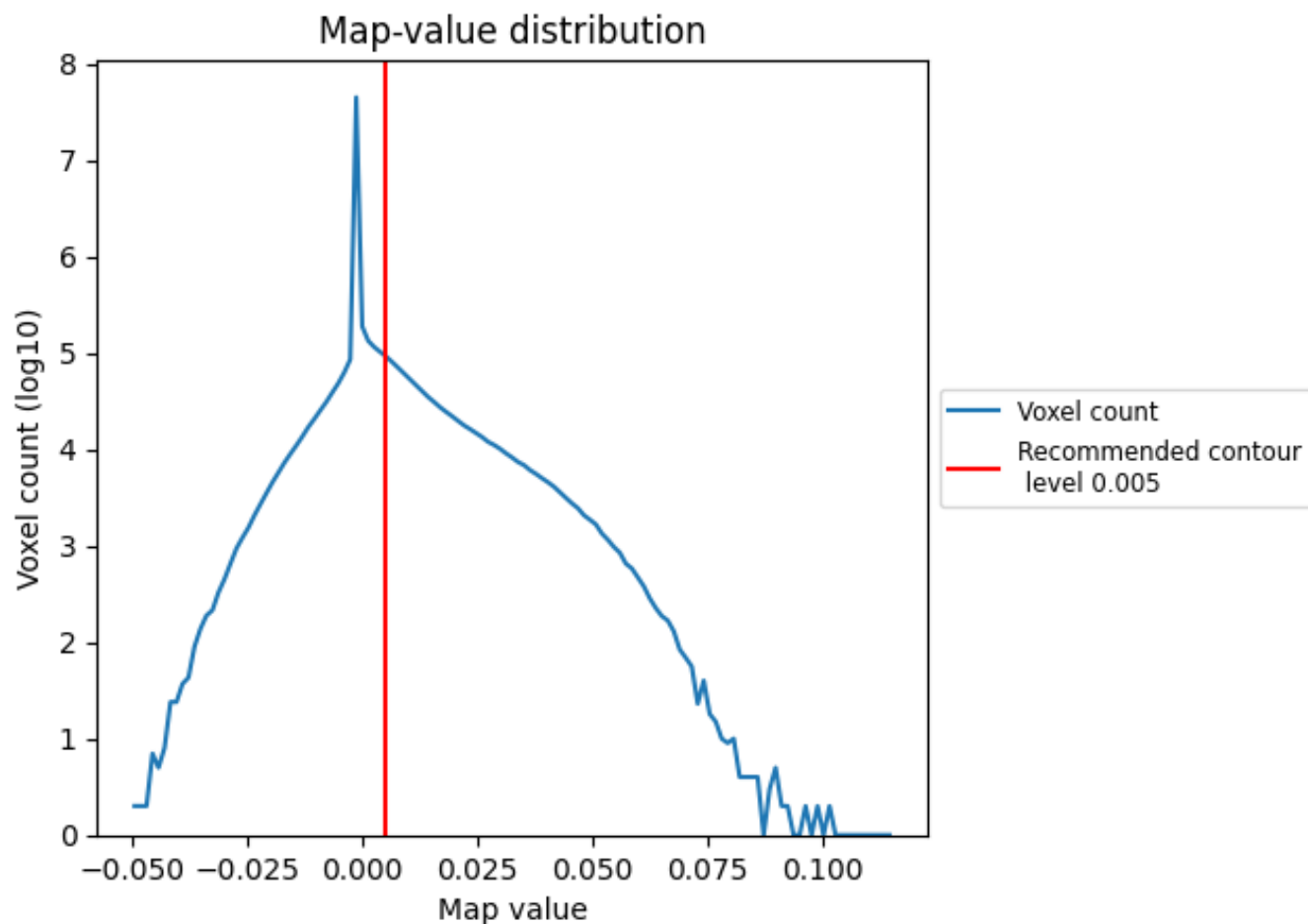
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

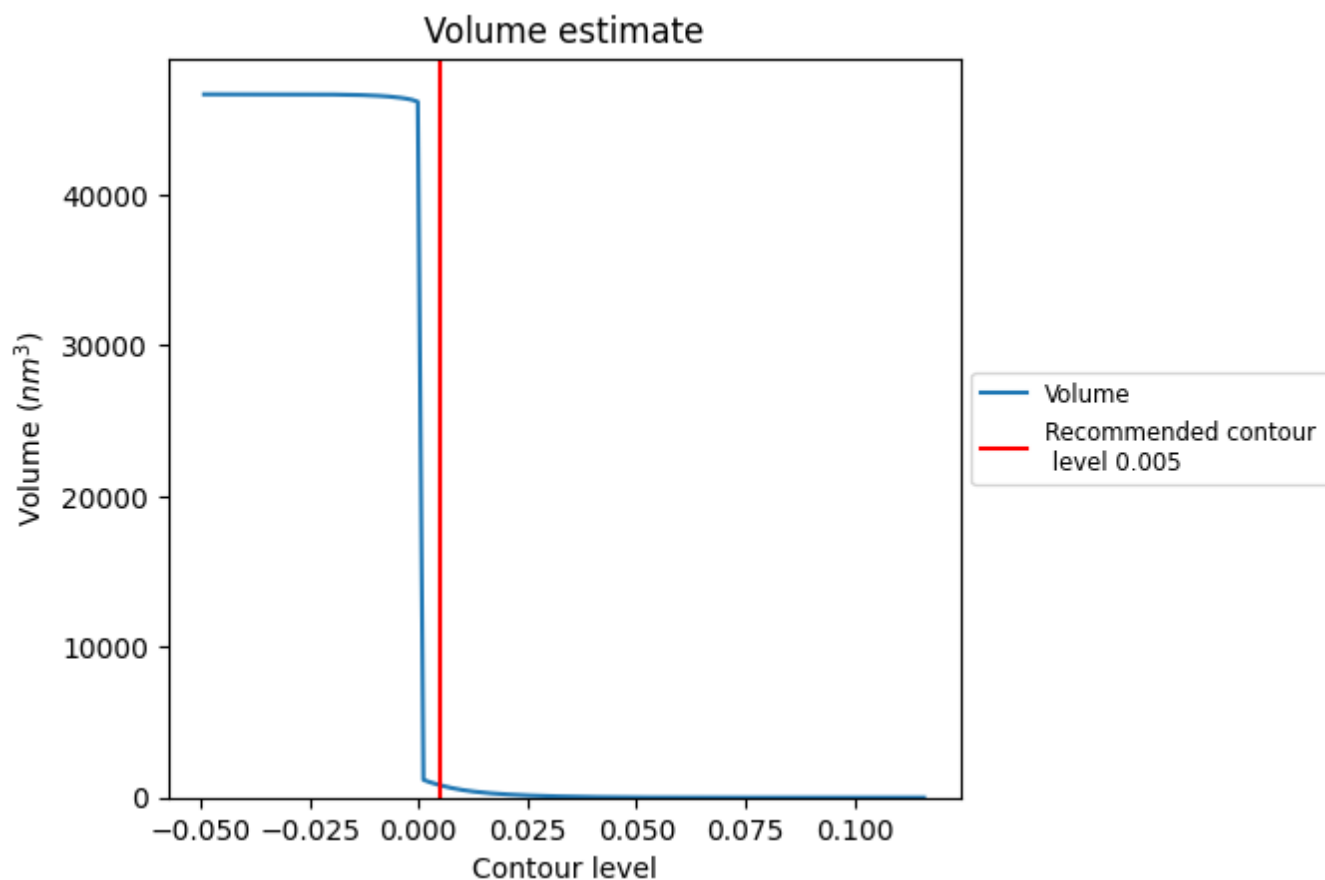
This section contains the results of statistical analysis of the map.

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.

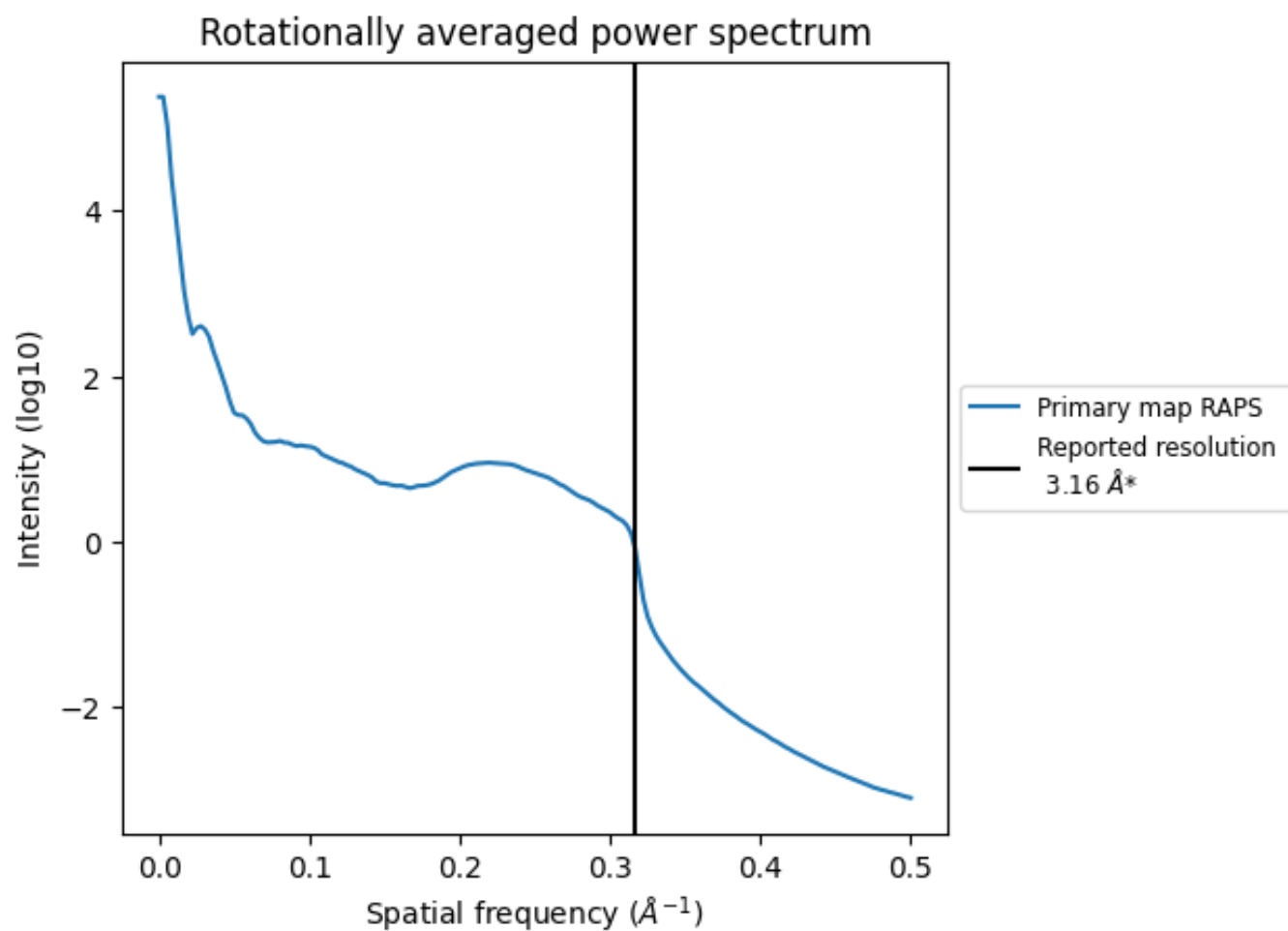
7.2 Volume estimate [i](#)



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

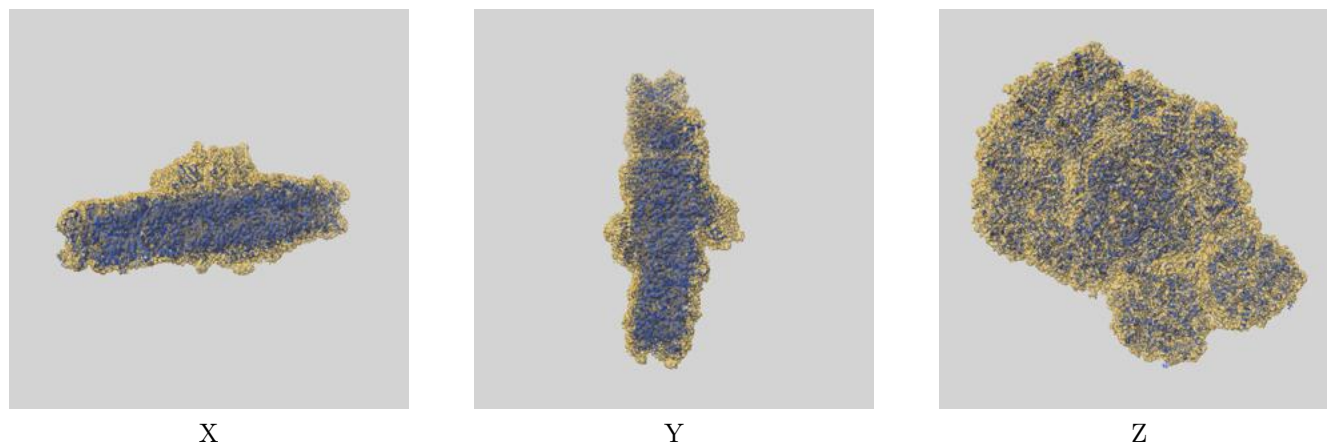
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

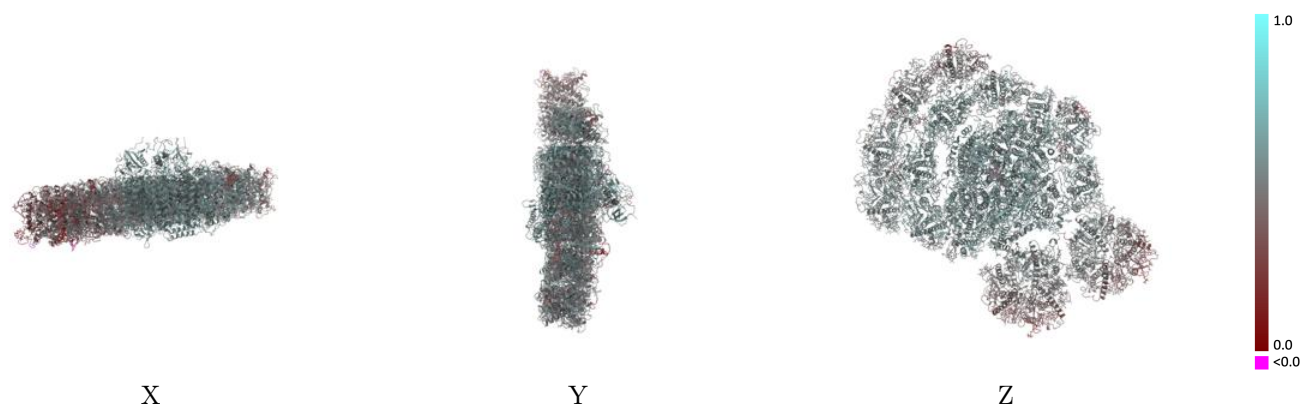
This section contains information regarding the fit between EMDB map EMD-30926 and PDB model 7DZ8. Per-residue inclusion information can be found in section [3](#) on page [45](#).

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](#)

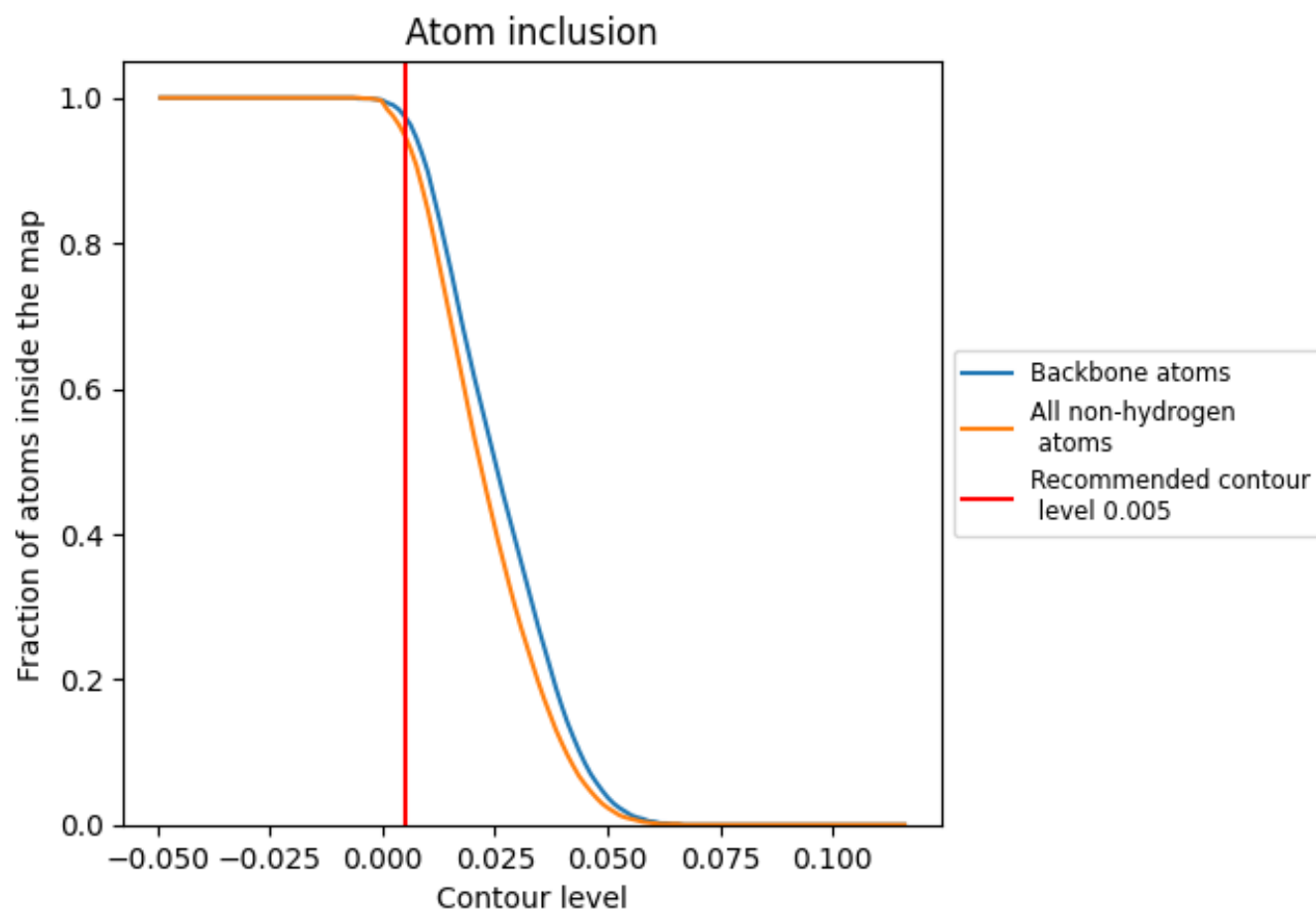


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



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

