



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 05:57 PM JST

PDB ID : 7DZ7
EMDB ID : EMD-30925
Title : State transition supercomplex PSI-LHCI-LHCII from double phosphatase mutant pph1;pbcp of green alga Chlamydomonas reinhardtii
Authors : Pan, X.W.; Li, A.J.; Liu, Z.F.; Li, M.
Deposited on : 2021-01-23
Resolution : 2.84 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:

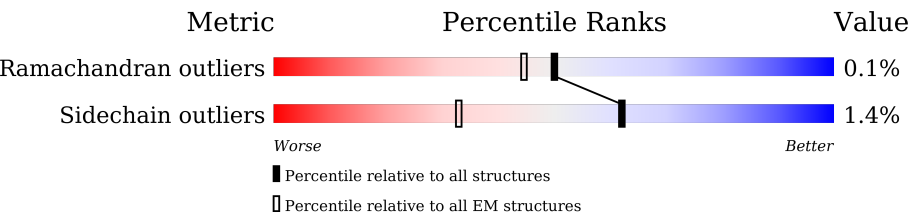
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.84 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	751	
2	B	735	
3	C	81	
4	D	196	
5	E	97	
6	F	227	
7	G	126	
8	H	130	
9	I	106	

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Mol	Chain	Length	Quality of chain
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	
25	Z	256	
26	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
27	CLA	1	602	X	-	-	-
27	CLA	1	603	X	-	-	-
27	CLA	1	604	X	-	-	-

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	7	602	X	-	-	-
27	CLA	7	603	X	-	-	-
27	CLA	7	604	X	-	-	-
27	CLA	7	607	X	-	-	-
27	CLA	7	608	X	-	-	-
27	CLA	7	609	X	-	-	-
27	CLA	7	610	X	-	-	-
27	CLA	7	611	X	-	-	-
27	CLA	7	612	X	-	-	-
27	CLA	7	613	X	-	-	-
27	CLA	7	614	X	-	-	-
27	CLA	7	615	X	-	-	-
27	CLA	7	616	X	-	-	-
27	CLA	8	601	X	-	-	-
27	CLA	8	602	X	-	-	-
27	CLA	8	603	X	-	-	-
27	CLA	8	604	X	-	-	-
27	CLA	8	606	X	-	-	-
27	CLA	8	607	X	-	-	-
27	CLA	8	608	X	-	-	-
27	CLA	8	609	X	-	-	-
27	CLA	8	610	X	-	-	-
27	CLA	8	611	X	-	-	-
27	CLA	8	612	X	-	-	-
27	CLA	8	613	X	-	-	-
27	CLA	8	614	X	-	-	-
27	CLA	8	616	X	-	-	-
27	CLA	9	601	X	-	-	-
27	CLA	9	603	X	-	-	-
27	CLA	9	604	X	-	-	-
27	CLA	9	606	X	-	-	-
27	CLA	9	609	X	-	-	-
27	CLA	9	610	X	-	-	-
27	CLA	9	611	X	-	-	-
27	CLA	9	612	X	-	-	-
27	CLA	9	613	X	-	-	-
27	CLA	9	614	X	-	-	-
27	CLA	A	801	X	-	-	-
27	CLA	A	802	X	-	-	-
27	CLA	A	803	X	-	-	-
27	CLA	A	804	X	-	-	-
27	CLA	A	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	807	X	-	-	-
27	CLA	A	809	X	-	-	-
27	CLA	A	810	X	-	-	-
27	CLA	A	811	X	-	-	-
27	CLA	A	812	X	-	-	-
27	CLA	A	813	X	-	-	-
27	CLA	A	814	X	-	-	-
27	CLA	A	815	X	-	-	-
27	CLA	A	816	X	-	-	-
27	CLA	A	819	X	-	-	-
27	CLA	A	820	X	-	-	-
27	CLA	A	821	X	-	-	-
27	CLA	A	822	X	-	-	-
27	CLA	A	823	X	-	-	-
27	CLA	A	824	X	-	-	-
27	CLA	A	825	X	-	-	-
27	CLA	A	826	X	-	-	-
27	CLA	A	827	X	-	-	-
27	CLA	A	828	X	-	-	-
27	CLA	A	829	X	-	-	-
27	CLA	A	830	X	-	-	-
27	CLA	A	831	X	-	-	-
27	CLA	A	832	X	-	-	-
27	CLA	A	833	X	-	-	-
27	CLA	A	834	X	-	-	-
27	CLA	A	836	X	-	-	-
27	CLA	A	838	X	-	-	-
27	CLA	A	839	X	-	-	-
27	CLA	A	841	X	-	-	-
27	CLA	A	842	X	-	-	-
27	CLA	A	843	X	-	-	-
27	CLA	A	845	X	-	-	-
27	CLA	A	854	X	-	-	-
27	CLA	B	802	X	-	-	-
27	CLA	B	803	X	-	-	-
27	CLA	B	804	X	-	-	-
27	CLA	B	805	X	-	-	-
27	CLA	B	806	X	-	-	-
27	CLA	B	808	X	-	-	-
27	CLA	B	809	X	-	-	-
27	CLA	B	810	X	-	-	-
27	CLA	B	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	812	X	-	-	-
27	CLA	B	813	X	-	-	-
27	CLA	B	814	X	-	-	-
27	CLA	B	815	X	-	-	-
27	CLA	B	816	X	-	-	-
27	CLA	B	817	X	-	-	-
27	CLA	B	819	X	-	-	-
27	CLA	B	820	X	-	-	-
27	CLA	B	821	X	-	-	-
27	CLA	B	823	X	-	-	-
27	CLA	B	824	X	-	-	-
27	CLA	B	826	X	-	-	-
27	CLA	B	827	X	-	-	-
27	CLA	B	828	X	-	-	-
27	CLA	B	829	X	-	-	-
27	CLA	B	830	X	-	-	-
27	CLA	B	831	X	-	-	-
27	CLA	B	833	X	-	-	-
27	CLA	B	834	X	-	-	-
27	CLA	B	835	X	-	-	-
27	CLA	B	836	X	-	-	-
27	CLA	B	839	X	-	-	-
27	CLA	B	840	X	-	-	-
27	CLA	B	841	X	-	-	-
27	CLA	F	301	X	-	-	-
27	CLA	G	203	X	-	-	-
27	CLA	G	204	X	-	-	-
27	CLA	H	202	X	-	-	-
27	CLA	J	101	X	-	-	-
27	CLA	K	201	X	-	-	-
27	CLA	K	204	X	-	-	-
27	CLA	K	206	X	-	-	-
27	CLA	L	302	X	-	-	-
27	CLA	L	304	X	-	-	-
27	CLA	L	306	X	-	-	-
27	CLA	L	307	X	-	-	-
27	CLA	O	2001	X	-	-	-
27	CLA	O	2002	X	-	-	-
27	CLA	O	2003	X	-	-	-
27	CLA	U	602	X	-	-	-
27	CLA	U	603	X	-	-	-
27	CLA	U	604	X	-	-	-

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

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

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

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 69647 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	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
14	1	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	217	Total	C	N	O	S	0	0
			1649	1073	280	292	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	220	Total	C	N	O	S	0	0
			1675	1088	273	309	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	220	Total	C	N	O	S	0	0
			1679	1086	273	315	5		
24	U	219	Total	C	N	O	S	0	0
			1670	1080	272	313	5		

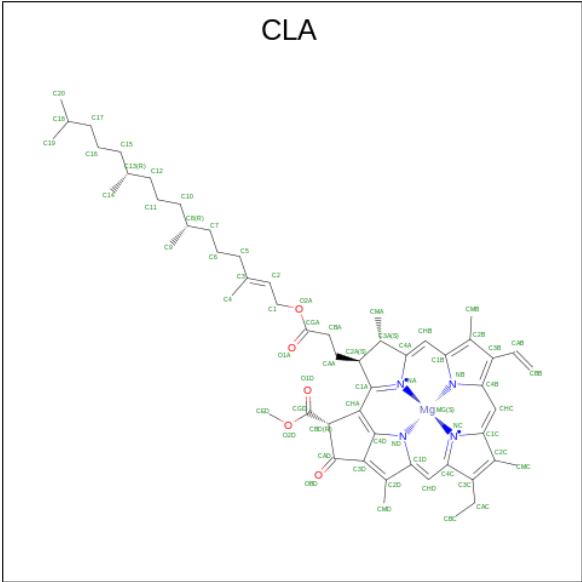
- Molecule 25 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	232	Total	C	N	O	P S	0	0
			1780	1154	291	329	1 5		

- Molecule 26 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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

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



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

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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
27	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	L	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	L	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
27	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
27	O	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	a	1	Total 54	C 45	Mg 1	N 4	O 4	0
27	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	a	1	Total 44	C 35	Mg 1	N 4	O 4	0
27	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	a	1	Total 44	C 34	Mg 1	N 4	O 5	0
27	a	1	Total 64	C 54	Mg 1	N 4	O 5	0
27	a	1	Total 59	C 49	Mg 1	N 4	O 5	0
27	a	1	Total 38	C 30	Mg 1	N 4	O 3	0
27	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	1	1	Total 53	C 44	Mg 1	N 4	O 4	0
27	1	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	1	1	Total 39	C 32	Mg 1	N 4	O 2	0
27	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
27	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	1	1	Total 39	C 31	Mg 1	N 4	O 3	0
27	1	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	1	1	Total 37	C 29	Mg 1	N 4	O 3	0
27	1	1	Total 43	C 33	Mg 1	N 4	O 5	0
27	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	2	1	Total 64	C 54	Mg 1	N 4	O 5	0
27	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
27	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	2	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	2	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
27	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
27	3	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
27	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	4	1	Total 44	C 34	Mg 1	N 4	O 5	0
27	4	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	4	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	4	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	4	1	Total 61	C 51	Mg 1	N 4	O 5	0
27	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	4	1	Total 43	C 33	Mg 1	N 4	O 5	0
27	4	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	5	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	5	1	Total 63	C 53	Mg 1	N 4	O 5	0
27	5	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	5	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	5	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	5	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	5	1	Total 64	C 55	Mg 1	N 4	O 4	0
27	5	1	Total 44	C 34	Mg 1	N 4	O 5	0
27	5	1	Total 42	C 33	Mg 1	N 4	O 4	0
27	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	5	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	5	1	Total 43	C 33	Mg 1	N 4	O 5	0
27	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	6	1	Total 51	C 41	Mg 1	N 4	O 5	0
27	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	6	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
27	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	7	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
27	7	1	Total	C	Mg	N	O	0
			43	33	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	9	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	9	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	X	1	Total 62	C 52	Mg 1	N 4	O 5	0
27	X	1	Total 49	C 39	Mg 1	N 4	O 5	0
27	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	X	1	Total 43	C 35	Mg 1	N 4	O 3	0
27	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	X	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	Y	1	Total 58	C 48	Mg 1	N 4	O 5	0
27	Y	1	Total 55	C 45	Mg 1	N 4	O 5	0
27	Y	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Y	1	Total 43	C 35	Mg 1	N 4	O 3	0
27	Y	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Y	1	Total 48	C 38	Mg 1	N 4	O 5	0

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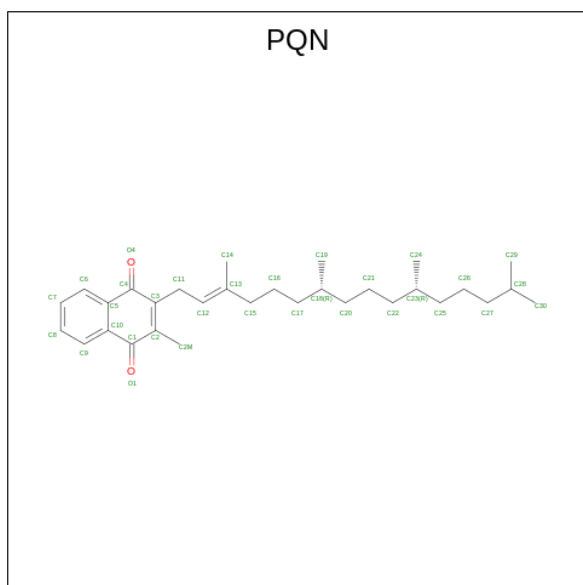
Mol	Chain	Residues	Atoms					AltConf
27	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Z	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Z	1	Total 54	C 44	Mg 1	N 4	O 5	0
27	U	1	Total 59	C 49	Mg 1	N 4	O 5	0
27	U	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	U	1	Total 48	C 39	Mg 1	N 4	O 4	0
27	U	1	Total 56	C 46	Mg 1	N 4	O 5	0
27	U	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	U	1	Total 43	C 35	Mg 1	N 4	O 3	0
27	U	1	Total 59	C 49	Mg 1	N 4	O 5	0
27	U	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	V	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	V	1	Total 62	C 52	Mg 1	N 4	O 5	0
27	V	1	Total 43	C 35	Mg 1	N 4	O 3	0

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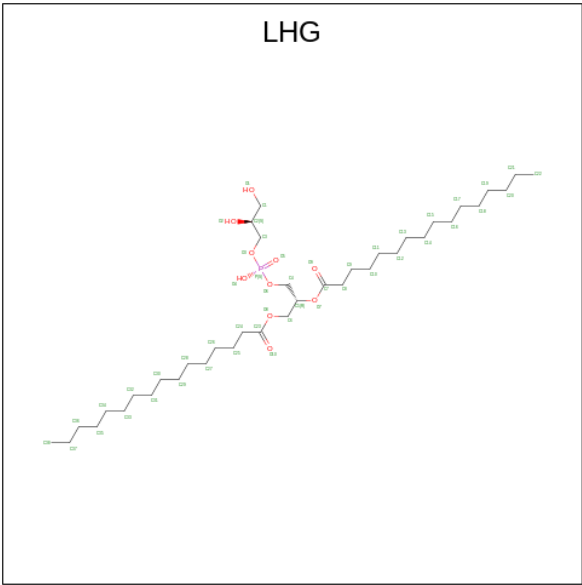
Mol	Chain	Residues	Atoms					AltConf
27	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	W	1	Total	C	Mg	N	O	0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

- Molecule 28 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



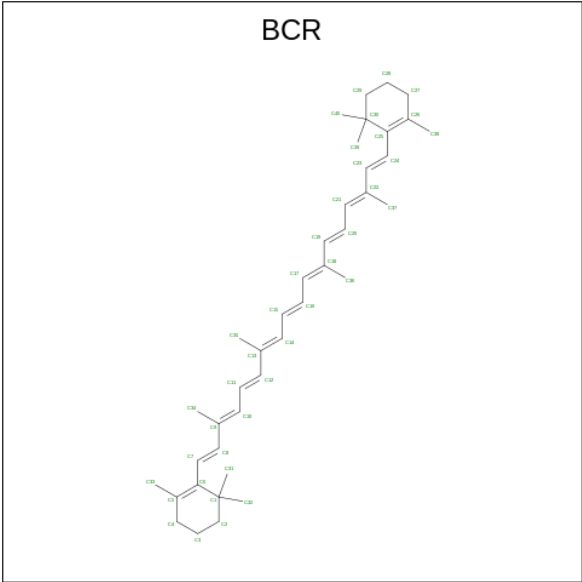
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	P	0
			49	38	10	1	
29	A	1	Total	C	O	P	0
			30	19	10	1	
29	B	1	Total	C	O	P	0
			38	27	10	1	
29	B	1	Total	C	O	P	0
			49	38	10	1	
29	H	1	Total	C	O	P	0
			49	38	10	1	
29	O	1	Total	C	O	P	0
			36	25	10	1	
29	a	1	Total	C	O	P	0
			43	32	10	1	
29	1	1	Total	C	O	P	0
			49	38	10	1	
29	2	1	Total	C	O	P	0
			36	25	10	1	

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Mol	Chain	Residues	Atoms				AltConf
29	3	1	Total	C	O	P	0
			45	34	10	1	
29	3	1	Total	C	O	P	0
			49	38	10	1	
29	4	1	Total	C	O	P	0
			49	38	10	1	
29	5	1	Total	C	O	P	0
			49	38	10	1	
29	5	1	Total	C	O	P	0
			49	38	10	1	
29	6	1	Total	C	O	P	0
			48	37	10	1	
29	7	1	Total	C	O	P	0
			37	26	10	1	
29	8	1	Total	C	O	P	0
			49	38	10	1	
29	8	1	Total	C	O	P	0
			40	29	10	1	
29	9	1	Total	C	O	P	0
			30	19	10	1	
29	9	1	Total	C	O	P	0
			49	38	10	1	
29	9	1	Total	C	O	P	0
			49	38	10	1	
29	X	1	Total	C	O	P	0
			49	38	10	1	
29	Y	1	Total	C	O	P	0
			49	38	10	1	
29	Z	1	Total	C	O	P	0
			49	38	10	1	
29	U	1	Total	C	O	P	0
			49	38	10	1	
29	V	1	Total	C	O	P	0
			48	37	10	1	
29	W	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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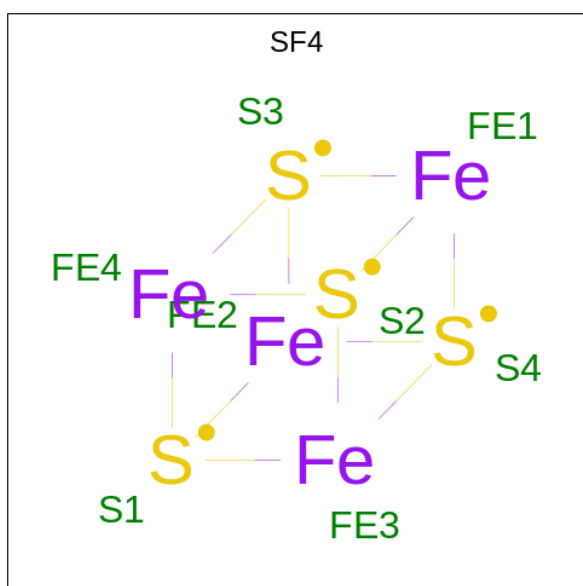
Mol	Chain	Residues	Atoms	AltConf
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	G	1	Total C 40 40	0
30	J	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	O	1	Total C 40 40	0
30	O	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	1	1	Total C 40 40	0
30	2	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	3	1	Total C 40 40	0
30	4	1	Total C 40 40	0
30	5	1	Total C 40 40	0

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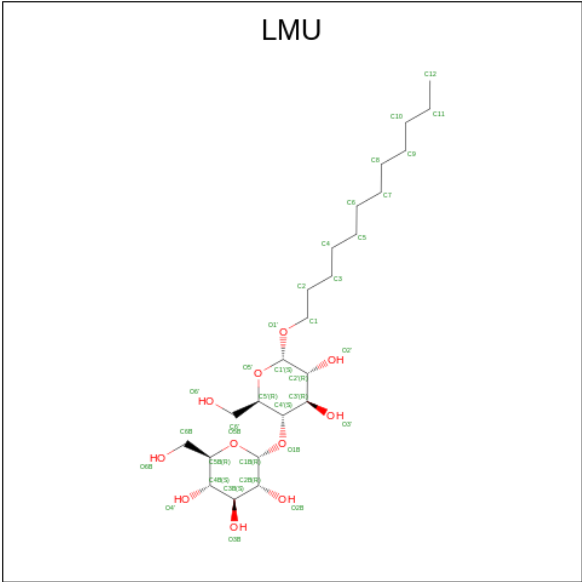
Mol	Chain	Residues	Atoms	AltConf
30	6	1	Total C 40 40	0
30	7	1	Total C 40 40	0
30	7	1	Total C 40 40	0
30	8	1	Total C 40 40	0
30	9	1	Total C 40 40	0

- Molecule 31 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



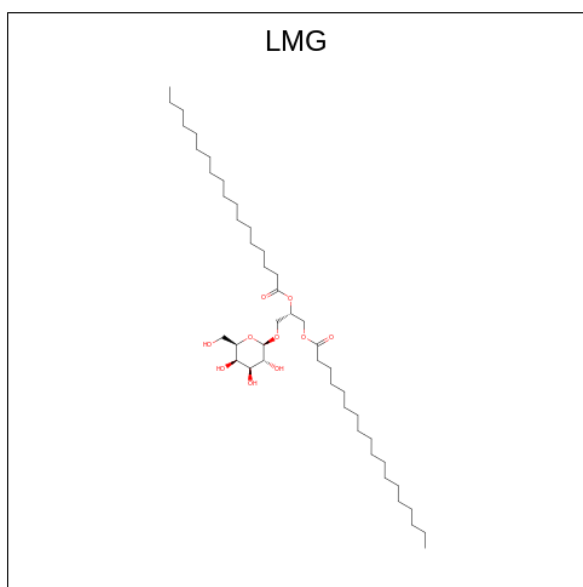
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total Fe S 8 4 4	0
31	C	1	Total Fe S 8 4 4	0
31	C	1	Total Fe S 8 4 4	0

- Molecule 32 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



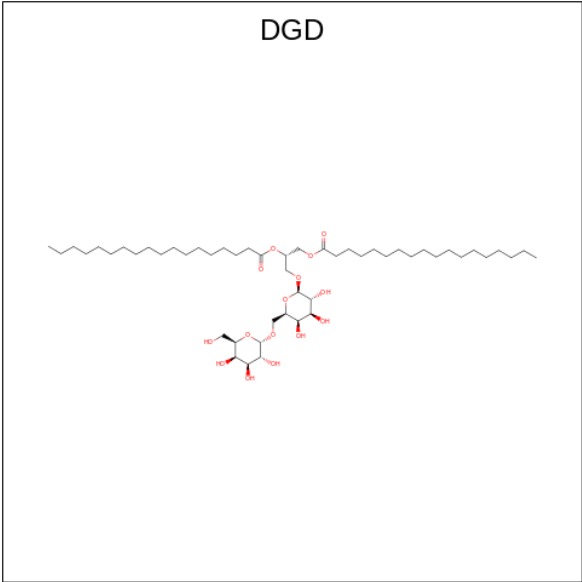
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			35	24	11	
32	A	1	Total	C	O	0
			34	24	10	
32	K	1	Total	C	O	0
			35	24	11	
32	1	1	Total	C	O	0
			35	24	11	
32	5	1	Total	C	O	0
			33	22	11	
32	5	1	Total	C	O	0
			32	21	11	
32	8	1	Total	C	O	0
			35	24	11	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



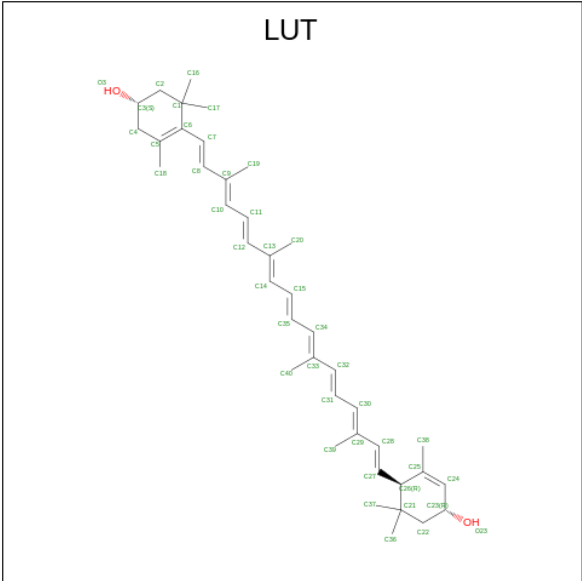
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			40	30	10	
33	H	1	Total	C	O	0
			55	45	10	
33	J	1	Total	C	O	0
			42	32	10	
33	J	1	Total	C	O	0
			40	30	10	
33	L	1	Total	C	O	0
			37	27	10	
33	4	1	Total	C	O	0
			40	30	10	
33	4	1	Total	C	O	0
			40	30	10	
33	5	1	Total	C	O	0
			40	30	10	
33	8	1	Total	C	O	0
			46	36	10	
33	9	1	Total	C	O	0
			55	45	10	
33	V	1	Total	C	O	0
			41	31	10	

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 35 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



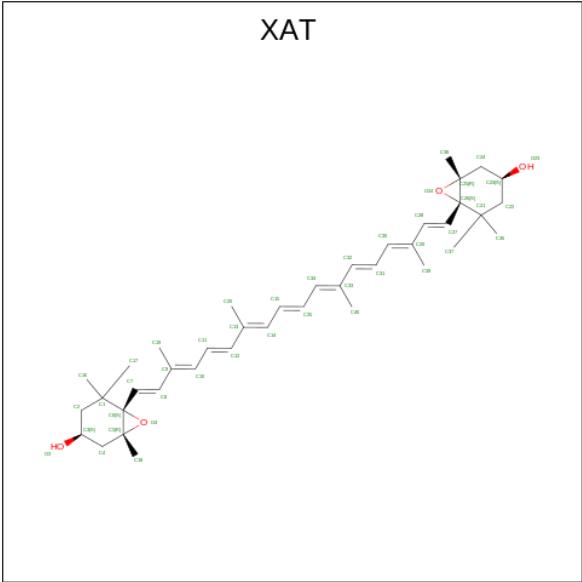
Mol	Chain	Residues	Atoms			AltConf
35	a	1	Total	C	O	0
			42	40	2	
35	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
35	2	1	Total	C	O	0
			42	40	2	
35	3	1	Total	C	O	0
			42	40	2	
35	4	1	Total	C	O	0
			42	40	2	
35	5	1	Total	C	O	0
			42	40	2	
35	6	1	Total	C	O	0
			42	40	2	
35	7	1	Total	C	O	0
			42	40	2	
35	8	1	Total	C	O	0
			42	40	2	
35	9	1	Total	C	O	0
			42	40	2	
35	X	1	Total	C	O	0
			42	40	2	
35	X	1	Total	C	O	0
			42	40	2	
35	Y	1	Total	C	O	0
			42	40	2	
35	Y	1	Total	C	O	0
			42	40	2	
35	Z	1	Total	C	O	0
			42	40	2	
35	Z	1	Total	C	O	0
			42	40	2	
35	U	1	Total	C	O	0
			42	40	2	
35	U	1	Total	C	O	0
			42	40	2	
35	V	1	Total	C	O	0
			42	40	2	
35	V	1	Total	C	O	0
			42	40	2	
35	W	1	Total	C	O	0
			42	40	2	
35	W	1	Total	C	O	0
			42	40	2	

- Molecule 36 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 (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



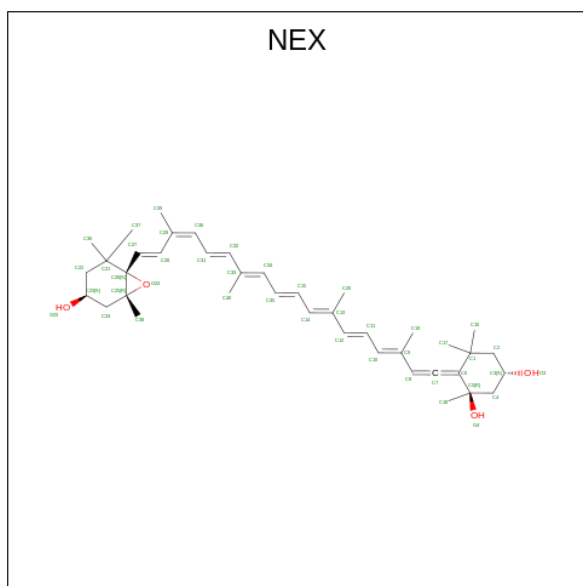
Mol	Chain	Residues	Atoms			AltConf
36	a	1	Total	C	O	0
			44	40	4	
36	1	1	Total	C	O	0
			44	40	4	
36	2	1	Total	C	O	0
			44	40	4	
36	3	1	Total	C	O	0
			44	40	4	
36	4	1	Total	C	O	0
			44	40	4	
36	5	1	Total	C	O	0
			44	40	4	
36	6	1	Total	C	O	0
			44	40	4	
36	7	1	Total	C	O	0
			44	40	4	
36	8	1	Total	C	O	0
			44	40	4	
36	9	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	

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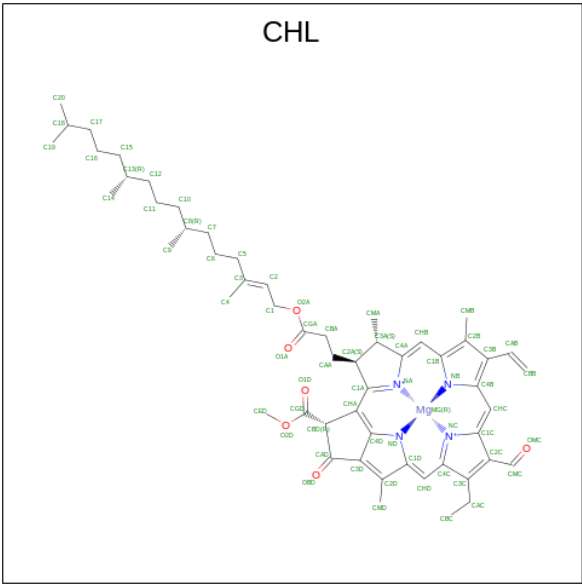
Mol	Chain	Residues	Atoms			AltConf
36	V	1	Total	C	O	0
			44	40	4	
36	W	1	Total	C	O	0
			44	40	4	

- Molecule 37 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
37	5	1	Total	C	O	0
			44	40	4	
37	6	1	Total	C	O	0
			44	40	4	
37	X	1	Total	C	O	0
			44	40	4	
37	Y	1	Total	C	O	0
			43	40	3	
37	Z	1	Total	C	O	0
			44	40	4	
37	U	1	Total	C	O	0
			44	40	4	
37	V	1	Total	C	O	0
			44	40	4	
37	W	1	Total	C	O	0
			44	40	4	

- Molecule 38 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
38	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	Z	1	Total 44	C 35	Mg 1	N 4	O 4	0
38	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
38	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	Z	1	Total 50	C 39	Mg 1	N 4	O 6	0
38	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	U	1	Total 43	C 34	Mg 1	N 4	O 4	0
38	U	1	Total 44	C 35	Mg 1	N 4	O 4	0
38	U	1	Total 46	C 35	Mg 1	N 4	O 6	0
38	U	1	Total 44	C 35	Mg 1	N 4	O 4	0
38	U	1	Total 60	C 49	Mg 1	N 4	O 6	0
38	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	V	1	Total 44	C 35	Mg 1	N 4	O 4	0
38	V	1	Total 44	C 35	Mg 1	N 4	O 4	0
38	V	1	Total 46	C 35	Mg 1	N 4	O 6	0
38	V	1	Total 48	C 37	Mg 1	N 4	O 6	0
38	V	1	Total 61	C 50	Mg 1	N 4	O 6	0
38	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
38	W	1	Total 46	C 35	Mg 1	N 4	O 6	0
38	W	1	Total 46	C 35	Mg 1	N 4	O 6	0

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

3 Residue-property plots [i](#)

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

Chain A:  98% ..



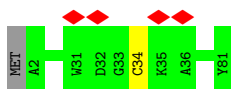
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  98% .



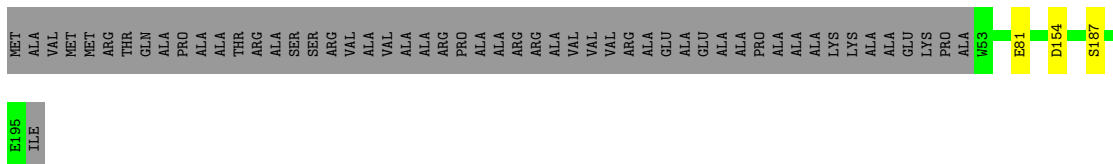
- Molecule 3: Photosystem I iron-sulfur center

Chain C:  5% 98% ..



- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

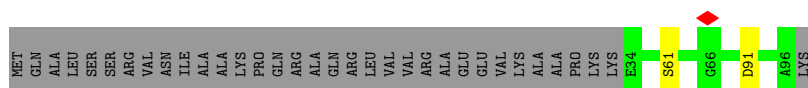
Chain D:  71% 27% .



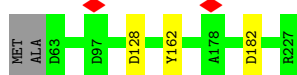
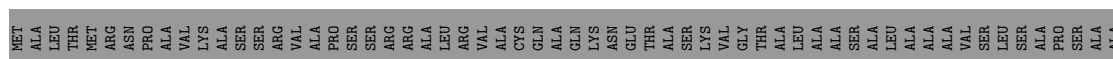
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:  63% 35% .

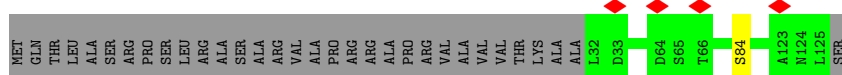
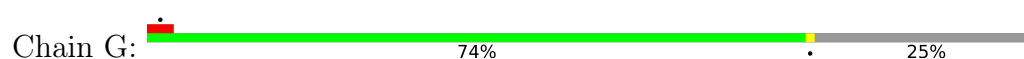




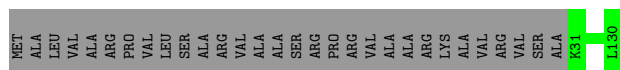
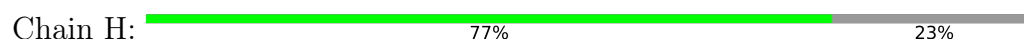
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



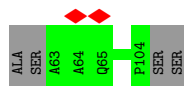
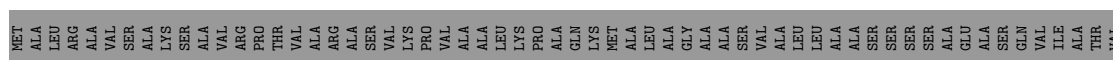
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



- Molecule 8: Photosystem I reaction center subunit VI, chloroplastic



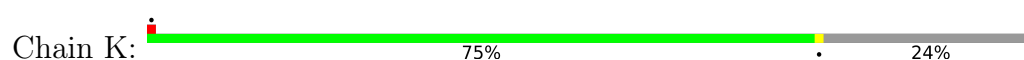
- Molecule 9: Photosystem I reaction center subunit VIII

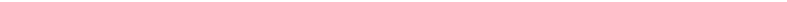


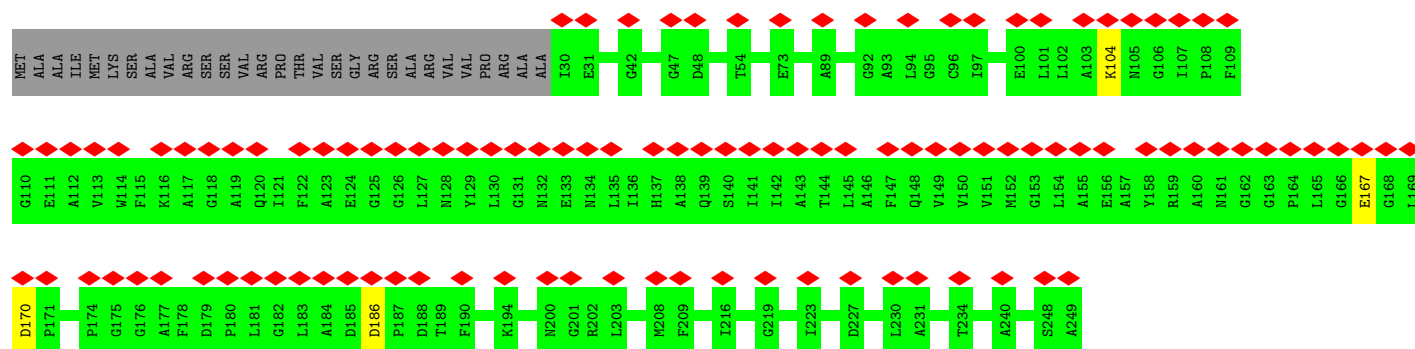
- Molecule 10: Photosystem I reaction center subunit IX



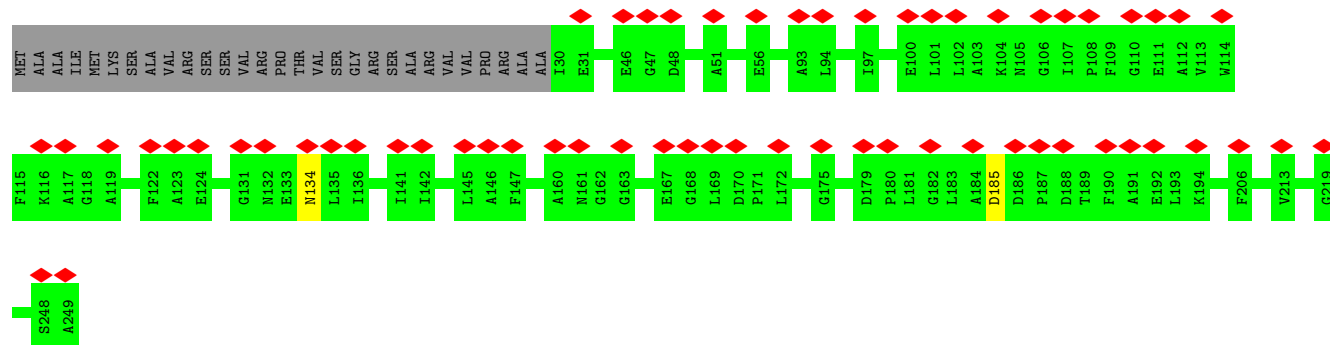
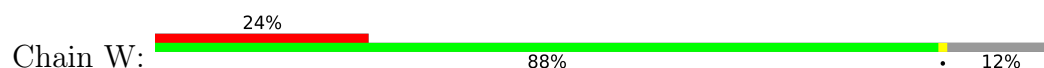
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic



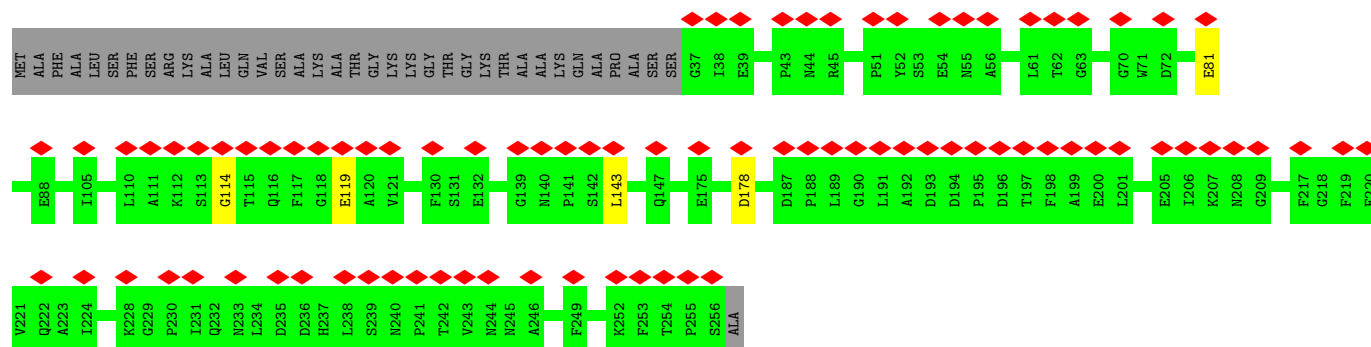
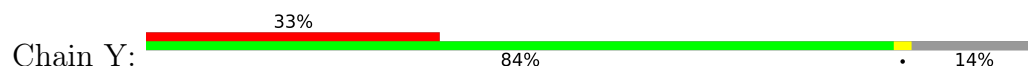
- Chain X:  44% 87% 12%



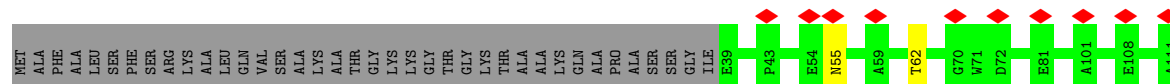
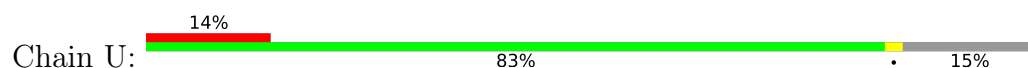
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic



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

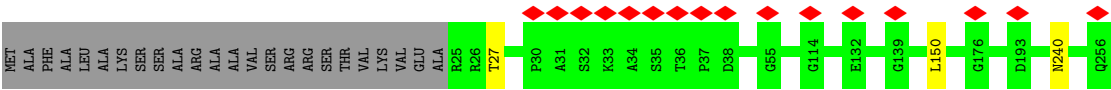
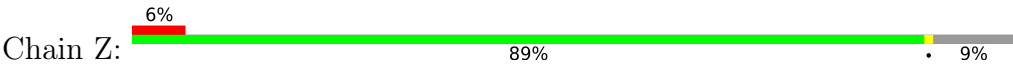


- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

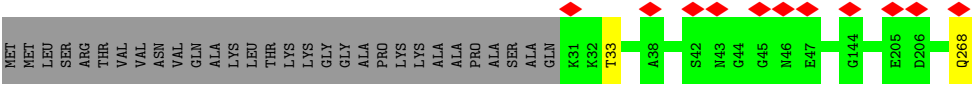
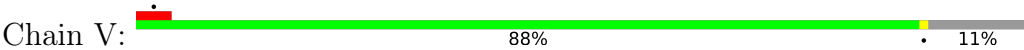




• Molecule 25: Chlorophyll a-b binding protein, chloroplastic



• Molecule 26: 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	56601	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	0.216	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	480, 480, 480	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: CLA, NEX, PQN, XAT, LMU, TPO, BCR, SF4, LUT, CHL, LHG, DGD, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/6015	0.43	0/8201
2	B	0.37	0/6036	0.44	0/8242
3	C	0.35	0/610	0.48	0/826
4	D	0.34	0/1152	0.47	0/1556
5	E	0.36	0/506	0.43	0/689
6	F	0.33	0/1291	0.43	0/1747
7	G	0.29	0/714	0.44	0/972
8	H	0.33	0/788	0.45	0/1059
9	I	0.38	0/329	0.43	0/456
10	J	0.37	0/349	0.42	0/478
11	K	0.30	0/587	0.46	0/795
12	L	0.36	0/1190	0.44	0/1628
13	O	0.33	0/784	0.45	0/1069
14	1	0.36	0/1490	0.45	0/2028
14	a	0.37	0/1490	0.46	0/2028
15	2	0.31	0/1730	0.44	0/2353
16	3	0.36	0/1726	0.42	0/2342
17	4	0.31	0/1686	0.41	0/2300
18	5	0.33	0/1829	0.43	0/2492
19	6	0.34	0/1833	0.43	0/2505
20	7	0.36	0/1701	0.41	0/2310
21	8	0.34	0/1700	0.43	0/2315
22	9	0.30	0/1444	0.45	0/1964
23	W	0.46	0/1721	0.47	0/2341
23	X	0.31	0/1725	0.50	0/2348
24	U	0.48	0/1718	0.48	0/2338
24	Y	0.31	0/1727	0.48	0/2350
25	Z	0.26	0/1822	0.42	0/2474
26	V	0.46	0/1856	0.46	0/2518
All	All	0.36	0/47549	0.44	0/64724

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	720 (97%)	19 (3%)	0	100	100
2	B	731/735 (100%)	714 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	141/196 (72%)	135 (96%)	6 (4%)	0	100	100
5	E	61/97 (63%)	59 (97%)	2 (3%)	0	100	100
6	F	163/227 (72%)	155 (95%)	8 (5%)	0	100	100
7	G	92/126 (73%)	86 (94%)	6 (6%)	0	100	100
8	H	98/130 (75%)	92 (94%)	6 (6%)	0	100	100
9	I	40/106 (38%)	35 (88%)	5 (12%)	0	100	100
10	J	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
11	K	84/113 (74%)	79 (94%)	5 (6%)	0	100	100
12	L	157/196 (80%)	150 (96%)	7 (4%)	0	100	100
13	O	95/126 (75%)	87 (92%)	8 (8%)	0	100	100
14	1	192/228 (84%)	185 (96%)	7 (4%)	0	100	100
14	a	192/228 (84%)	185 (96%)	7 (4%)	0	100	100
15	2	215/246 (87%)	202 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	3	218/298 (73%)	213 (98%)	5 (2%)	0	100	100
17	4	208/264 (79%)	201 (97%)	7 (3%)	0	100	100
18	5	225/257 (88%)	212 (94%)	13 (6%)	0	100	100
19	6	228/257 (89%)	206 (90%)	22 (10%)	0	100	100
20	7	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
21	8	215/243 (88%)	209 (97%)	6 (3%)	0	100	100
22	9	181/213 (85%)	167 (92%)	14 (8%)	0	100	100
23	W	218/249 (88%)	204 (94%)	14 (6%)	0	100	100
23	X	218/249 (88%)	204 (94%)	13 (6%)	1 (0%)	25	44
24	U	217/257 (84%)	197 (91%)	19 (9%)	1 (0%)	25	44
24	Y	218/257 (85%)	202 (93%)	15 (7%)	1 (0%)	25	44
25	Z	229/256 (90%)	223 (97%)	6 (3%)	0	100	100
26	V	235/268 (88%)	220 (94%)	15 (6%)	0	100	100
All	All	5938/6936 (86%)	5655 (95%)	280 (5%)	3 (0%)	50	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	X	167	GLU
24	Y	114	GLY
24	U	174	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/610 (98%)	596 (99%)	5 (1%)	79	90
2	B	596/597 (100%)	586 (98%)	10 (2%)	56	78
3	C	69/70 (99%)	68 (99%)	1 (1%)	62	82
4	D	120/152 (79%)	117 (98%)	3 (2%)	42	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	54/81 (67%)	52 (96%)	2 (4%)	29	54
6	F	127/169 (75%)	124 (98%)	3 (2%)	44	69
7	G	70/94 (74%)	69 (99%)	1 (1%)	62	82
8	H	81/102 (79%)	81 (100%)	0	100	100
9	I	33/76 (43%)	33 (100%)	0	100	100
10	J	37/37 (100%)	36 (97%)	1 (3%)	40	65
11	K	59/80 (74%)	58 (98%)	1 (2%)	56	78
12	L	121/148 (82%)	121 (100%)	0	100	100
13	O	78/101 (77%)	77 (99%)	1 (1%)	65	83
14	1	137/162 (85%)	136 (99%)	1 (1%)	81	91
14	a	137/162 (85%)	135 (98%)	2 (2%)	60	81
15	2	173/198 (87%)	170 (98%)	3 (2%)	56	78
16	3	167/230 (73%)	165 (99%)	2 (1%)	67	85
17	4	165/205 (80%)	164 (99%)	1 (1%)	84	92
18	5	184/206 (89%)	181 (98%)	3 (2%)	58	79
19	6	184/203 (91%)	180 (98%)	4 (2%)	47	71
20	7	164/181 (91%)	162 (99%)	2 (1%)	67	85
21	8	163/183 (89%)	161 (99%)	2 (1%)	67	85
22	9	140/159 (88%)	139 (99%)	1 (1%)	81	91
23	W	163/187 (87%)	161 (99%)	2 (1%)	67	85
23	X	165/187 (88%)	162 (98%)	3 (2%)	54	76
24	U	168/194 (87%)	164 (98%)	4 (2%)	44	69
24	Y	170/194 (88%)	166 (98%)	4 (2%)	44	69
25	Z	178/195 (91%)	176 (99%)	2 (1%)	70	86
26	V	178/201 (89%)	177 (99%)	1 (1%)	84	92
All	All	4682/5364 (87%)	4617 (99%)	65 (1%)	62	82

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	Z	240	ASN
24	U	62	THR
7	G	84	SER

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Mol	Chain	Res	Type
6	F	182	ASP
24	U	193	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
24	Y	140	ASN
24	U	169	ASN
26	V	158	GLN
26	V	156	HIS
10	J	30	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	TPO	V	33	26	8,10,11	1.54	1 (12%)	10,14,16	1.77	2 (20%)
25	TPO	Z	27	25	8,10,11	1.09	0	10,14,16	1.63	1 (10%)

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	TPO	V	33	26	-	5/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	TPO	Z	27	25	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	33	TPO	P-O1P	3.17	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V	33	TPO	P-OG1-CB	-4.60	109.31	123.21
25	Z	27	TPO	P-OG1-CB	-4.57	109.42	123.21
26	V	33	TPO	CG2-CB-CA	-2.26	108.70	113.16

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	V	33	TPO	N-CA-CB-CG2
26	V	33	TPO	CB-OG1-P-O1P
26	V	33	TPO	CB-OG1-P-O2P
26	V	33	TPO	CB-OG1-P-O3P
26	V	33	TPO	O-C-CA-CB

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	$\# Z > 2$
27	CLA	K	206	11	45,53,73	1.82	7 (15%)	52,89,113	1.47	7 (13%)
31	SF4	C	101	3	0,12,12	-	-	-		
27	CLA	A	811	-	65,73,73	1.48	8 (12%)	76,113,113	1.25	9 (11%)
27	CLA	a	611	29	37,46,73	2.01	8 (21%)	46,81,113	1.57	9 (19%)
27	CLA	K	201	11	45,53,73	1.81	7 (15%)	52,89,113	1.37	7 (13%)
27	CLA	A	809	1	65,73,73	1.45	9 (13%)	76,113,113	1.34	7 (9%)
27	CLA	2	601	15	65,73,73	1.46	6 (9%)	76,113,113	1.52	9 (11%)
27	CLA	4	616	17	43,51,73	1.93	7 (16%)	54,87,113	1.50	8 (14%)
27	CLA	K	204	-	45,53,73	1.76	8 (17%)	52,89,113	1.55	8 (15%)
27	CLA	A	841	-	65,73,73	1.48	9 (13%)	76,113,113	1.29	7 (9%)
27	CLA	1	603	-	52,61,73	1.64	7 (13%)	59,98,113	1.52	9 (15%)
27	CLA	B	831	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
27	CLA	1	611	29	57,65,73	1.61	8 (14%)	66,103,113	1.32	7 (10%)
27	CLA	6	616	19	65,73,73	1.48	8 (12%)	76,113,113	1.40	8 (10%)
27	CLA	X	604	-	49,57,73	1.77	6 (12%)	55,93,113	1.34	8 (14%)
30	BCR	L	308	-	41,41,41	0.82	2 (4%)	56,56,56	2.31	27 (48%)
27	CLA	9	614	-	45,53,73	1.80	8 (17%)	52,89,113	1.47	9 (17%)
38	CHL	U	606	-	44,52,74	2.18	14 (31%)	46,87,114	2.88	21 (45%)
27	CLA	5	612	18	40,49,73	1.86	7 (17%)	45,84,113	1.48	6 (13%)
27	CLA	6	620	-	64,72,73	1.50	7 (10%)	74,111,113	1.21	6 (8%)
27	CLA	6	613	-	63,72,73	1.56	8 (12%)	73,112,113	1.19	7 (9%)
27	CLA	B	835	-	45,53,73	1.80	7 (15%)	52,89,113	1.36	7 (13%)
27	CLA	B	826	-	62,70,73	1.52	7 (11%)	72,109,113	1.41	9 (12%)
27	CLA	A	840	-	52,60,73	1.66	8 (15%)	60,97,113	1.48	9 (15%)
38	CHL	V	605	26	44,52,74	2.25	14 (31%)	46,87,114	2.85	21 (45%)
27	CLA	8	614	-	53,61,73	1.66	8 (15%)	61,98,113	1.41	9 (14%)
27	CLA	1	604	-	49,57,73	1.74	8 (16%)	55,93,113	1.38	7 (12%)
27	CLA	2	604	-	42,50,73	1.86	8 (19%)	48,85,113	1.39	7 (14%)
29	LHG	3	624	27	48,48,48	0.92	2 (4%)	51,54,54	0.97	3 (5%)
38	CHL	W	606	-	46,54,74	2.25	16 (34%)	49,90,114	4.69	24 (48%)
27	CLA	5	619	-	43,51,73	1.91	7 (16%)	54,87,113	1.53	10 (18%)
30	BCR	5	622	-	41,41,41	0.73	0	56,56,56	2.34	21 (37%)
35	LUT	6	619	-	42,43,43	0.82	1 (2%)	51,60,60	1.83	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	4	612	17	40,49,73	1.87	8 (20%)	45,84,113	1.53	7 (15%)
27	CLA	6	618	19	39,48,73	1.93	8 (20%)	48,83,113	1.62	9 (18%)
27	CLA	F	301	-	57,65,73	1.64	7 (12%)	66,103,113	1.28	7 (10%)
29	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	0.90	2 (3%)
27	CLA	6	610	19	65,73,73	1.54	9 (13%)	76,113,113	1.18	8 (10%)
36	XAT	6	621	-	39,47,47	0.87	0	54,74,74	2.39	20 (37%)
27	CLA	6	608	-	45,53,73	1.82	9 (20%)	52,89,113	1.43	7 (13%)
30	BCR	3	620	-	41,41,41	0.85	0	56,56,56	4.30	30 (53%)
27	CLA	A	838	-	50,58,73	1.62	6 (12%)	58,95,113	1.57	9 (15%)
27	CLA	A	843	-	64,72,73	1.54	8 (12%)	74,111,113	1.23	8 (10%)
27	CLA	Y	604	-	50,58,73	1.76	6 (12%)	58,95,113	1.33	9 (15%)
27	CLA	B	837	-	65,73,73	1.52	8 (12%)	76,113,113	1.32	10 (13%)
32	LMU	5	629	-	33,33,36	1.18	2 (6%)	44,44,47	1.09	3 (6%)
35	LUT	2	619	-	42,43,43	0.82	1 (2%)	51,60,60	1.84	11 (21%)
30	BCR	B	847	-	41,41,41	0.82	0	56,56,56	2.08	15 (26%)
38	CHL	Z	606	-	46,54,74	2.38	15 (32%)	49,90,114	2.83	22 (44%)
29	LHG	V	2630	27	47,47,48	0.89	2 (4%)	50,53,54	1.12	3 (6%)
30	BCR	F	305	-	41,41,41	0.81	0	56,56,56	2.29	26 (46%)
27	CLA	3	602	16	60,68,73	1.55	9 (15%)	70,107,113	1.26	8 (11%)
38	CHL	W	609	23	66,74,74	1.94	15 (22%)	73,114,114	2.62	22 (30%)
35	LUT	X	1620	-	42,43,43	0.80	0	51,60,60	1.93	10 (19%)
27	CLA	a	604	-	49,57,73	1.73	8 (16%)	55,93,113	1.37	7 (12%)
27	CLA	A	815	-	50,58,73	1.68	9 (18%)	58,95,113	1.43	6 (10%)
27	CLA	a	601	14	53,62,73	1.65	9 (16%)	61,100,113	1.29	8 (13%)
27	CLA	8	606	-	64,72,73	1.50	9 (14%)	75,112,113	1.24	8 (10%)
38	CHL	W	605	23	46,54,74	2.29	14 (30%)	49,90,114	2.91	22 (44%)
32	LMU	A	857	-	36,36,36	1.14	2 (5%)	47,47,47	0.98	1 (2%)
27	CLA	A	828	-	65,73,73	1.48	9 (13%)	76,113,113	1.30	8 (10%)
32	LMU	K	208	-	36,36,36	1.15	2 (5%)	47,47,47	0.97	2 (4%)
38	CHL	Z	601	25	66,74,74	1.91	15 (22%)	73,114,114	2.65	20 (27%)
30	BCR	2	623	-	41,41,41	0.78	0	56,56,56	2.33	21 (37%)
27	CLA	V	614	-	45,53,73	1.81	8 (17%)	52,89,113	1.45	7 (13%)
27	CLA	W	614	-	45,53,73	1.78	9 (20%)	52,89,113	1.47	8 (15%)
29	LHG	2	622	27	35,35,48	1.08	2 (5%)	38,41,54	0.98	1 (2%)
27	CLA	3	611	29	37,46,73	2.02	8 (21%)	46,81,113	1.56	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	6	617	-	45,53,73	1.78	8 (17%)	52,89,113	1.42	7 (13%)
27	CLA	B	834	-	60,68,73	1.54	8 (13%)	70,107,113	1.35	8 (11%)
27	CLA	H	203	-	65,73,73	1.50	8 (12%)	76,113,113	1.34	8 (10%)
27	CLA	1	612	14	45,53,73	1.78	7 (15%)	52,89,113	1.45	7 (13%)
38	CHL	X	609	23	66,74,74	1.95	15 (22%)	73,114,114	2.62	22 (30%)
27	CLA	B	820	-	50,58,73	1.67	8 (16%)	58,95,113	1.46	9 (15%)
27	CLA	6	609	19	45,53,73	1.79	8 (17%)	52,89,113	1.47	7 (13%)
32	LMU	5	628	-	34,34,36	1.16	2 (5%)	45,45,47	1.16	6 (13%)
27	CLA	B	830	-	43,51,73	1.85	9 (20%)	49,86,113	1.42	7 (14%)
27	CLA	W	603	-	52,60,73	1.65	11 (21%)	60,97,113	1.48	8 (13%)
27	CLA	B	802	-	65,73,73	1.47	9 (13%)	76,113,113	1.19	6 (7%)
32	LMU	A	858	-	34,35,36	1.23	3 (8%)	42,45,47	0.92	1 (2%)
38	CHL	U	601	24	66,74,74	1.91	15 (22%)	73,114,114	2.68	22 (30%)
38	CHL	W	601	23	66,74,74	1.91	15 (22%)	73,114,114	2.68	23 (31%)
29	LHG	9	624	-	48,48,48	0.95	2 (4%)	51,54,54	1.00	2 (3%)
27	CLA	B	813	-	65,73,73	1.49	9 (13%)	76,113,113	1.34	8 (10%)
27	CLA	A	834	-	65,73,73	1.47	8 (12%)	76,113,113	1.33	8 (10%)
38	CHL	Y	605	24	42,50,74	2.45	16 (38%)	44,85,114	3.03	22 (50%)
38	CHL	V	608	-	48,56,74	2.20	16 (33%)	51,92,114	2.70	21 (41%)
27	CLA	a	609	14	63,72,73	1.52	8 (12%)	73,112,113	1.25	9 (12%)
35	LUT	Y	1621	-	42,43,43	0.78	0	51,60,60	1.75	13 (25%)
30	BCR	B	849	-	41,41,41	0.72	0	56,56,56	2.49	24 (42%)
36	XAT	W	1622	-	39,47,47	1.01	3 (7%)	54,74,74	3.94	24 (44%)
27	CLA	X	610	23	65,73,73	1.58	7 (10%)	76,113,113	1.23	9 (11%)
27	CLA	9	609	22	61,69,73	1.54	8 (13%)	71,108,113	1.29	7 (9%)
37	NEX	6	624	-	38,46,46	1.09	1 (2%)	50,70,70	2.10	15 (30%)
27	CLA	A	807	1	65,73,73	1.50	9 (13%)	76,113,113	1.32	8 (10%)
27	CLA	4	603	17	44,52,73	1.88	8 (18%)	55,88,113	1.56	8 (14%)
36	XAT	4	620	-	39,47,47	0.88	0	54,74,74	2.49	23 (42%)
27	CLA	A	804	-	65,73,73	1.45	7 (10%)	76,113,113	1.39	8 (10%)
35	LUT	U	1621	-	42,43,43	0.96	2 (4%)	51,60,60	1.70	11 (21%)
27	CLA	3	612	16	43,51,73	1.86	8 (18%)	49,86,113	1.48	7 (14%)
27	CLA	4	607	-	45,53,73	1.78	9 (20%)	52,89,113	1.45	7 (13%)
27	CLA	V	610	26	62,70,73	1.52	10 (16%)	72,109,113	1.33	8 (11%)
27	CLA	L	307	-	39,48,73	1.92	8 (20%)	44,83,113	1.52	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	B	808	-	65,73,73	1.50	9 (13%)	76,113,113	1.22	9 (11%)
35	LUT	V	1621	-	42,43,43	0.97	2 (4%)	51,60,60	1.74	12 (23%)
27	CLA	7	602	20	65,73,73	1.47	8 (12%)	76,113,113	1.25	6 (7%)
27	CLA	5	611	29	42,50,73	1.83	8 (19%)	48,85,113	1.39	7 (14%)
27	CLA	4	606	-	39,48,73	1.92	7 (17%)	44,83,113	1.43	7 (15%)
27	CLA	B	824	-	65,73,73	1.49	9 (13%)	76,113,113	1.27	6 (7%)
27	CLA	A	810	1	50,58,73	1.71	9 (18%)	58,95,113	1.47	9 (15%)
27	CLA	4	608	-	65,73,73	1.49	8 (12%)	76,113,113	1.28	8 (10%)
36	XAT	Y	1622	-	39,47,47	0.89	1 (2%)	54,74,74	3.87	25 (46%)
27	CLA	B	841	29	65,73,73	1.50	9 (13%)	76,113,113	1.28	7 (9%)
27	CLA	5	601	18	56,64,73	1.59	8 (14%)	65,102,113	1.46	9 (13%)
33	LMG	A	860	-	40,40,55	1.04	2 (5%)	48,48,63	1.10	4 (8%)
38	CHL	V	609	26	61,69,74	2.05	15 (24%)	67,108,114	2.66	20 (29%)
27	CLA	A	826	-	64,72,73	1.47	7 (10%)	74,111,113	1.43	6 (8%)
27	CLA	B	821	-	43,51,73	1.91	8 (18%)	48,86,113	1.49	9 (18%)
27	CLA	Z	612	25	65,73,73	1.52	5 (7%)	76,113,113	1.25	7 (9%)
34	DGD	B	850	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	4 (5%)
27	CLA	2	602	15	63,72,73	1.49	8 (12%)	73,112,113	1.29	6 (8%)
30	BCR	J	102	-	41,41,41	0.76	0	56,56,56	2.18	23 (41%)
27	CLA	V	603	-	45,53,73	1.75	9 (20%)	52,89,113	1.56	6 (11%)
27	CLA	B	805	-	65,73,73	1.47	8 (12%)	76,113,113	1.36	8 (10%)
27	CLA	G	203	-	42,50,73	1.83	7 (16%)	48,85,113	1.50	7 (14%)
27	CLA	Y	613	24	65,73,73	1.56	6 (9%)	76,113,113	1.27	11 (14%)
36	XAT	Z	1622	-	39,47,47	0.90	1 (2%)	54,74,74	3.78	25 (46%)
38	CHL	Y	609	24	66,74,74	1.95	15 (22%)	73,114,114	2.58	21 (28%)
38	CHL	X	605	23	46,54,74	2.35	16 (34%)	49,90,114	2.88	23 (46%)
36	XAT	7	620	-	39,47,47	0.91	1 (2%)	54,74,74	2.48	22 (40%)
27	CLA	1	610	14	38,47,73	1.87	7 (18%)	44,81,113	1.77	9 (20%)
27	CLA	V	602	26	60,68,73	1.54	10 (16%)	70,107,113	1.37	8 (11%)
35	LUT	W	1621	-	42,43,43	0.96	2 (4%)	51,60,60	1.70	12 (23%)
27	CLA	8	609	21	45,53,73	1.79	9 (20%)	52,89,113	1.41	7 (13%)
32	LMU	8	625	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	3 (6%)
36	XAT	V	1622	-	39,47,47	0.97	2 (5%)	54,74,74	2.58	19 (35%)
27	CLA	A	845	29	50,58,73	1.69	8 (16%)	58,95,113	1.35	7 (12%)
27	CLA	7	611	29	59,67,73	1.55	8 (13%)	68,105,113	1.27	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LUT	1	617	-	42,43,43	0.83	1 (2%)	51,60,60	1.77	14 (27%)
27	CLA	2	603	15	43,52,73	1.87	8 (18%)	49,88,113	1.48	6 (12%)
27	CLA	Y	610	24	65,73,73	1.57	7 (10%)	76,113,113	1.23	9 (11%)
33	LMG	4	624	-	40,40,55	1.05	2 (5%)	48,48,63	1.20	7 (14%)
30	BCR	4	621	-	41,41,41	0.78	1 (2%)	56,56,56	2.47	24 (42%)
27	CLA	Z	603	-	65,73,73	1.48	6 (9%)	76,113,113	1.32	6 (7%)
27	CLA	U	612	24	43,51,73	1.81	8 (18%)	49,86,113	1.46	6 (12%)
27	CLA	2	607	-	45,53,73	1.78	9 (20%)	52,89,113	1.48	7 (13%)
27	CLA	a	607	-	45,53,73	1.80	8 (17%)	52,89,113	1.44	8 (15%)
27	CLA	6	602	19	65,73,73	1.51	9 (13%)	76,113,113	1.26	8 (10%)
27	CLA	B	816	-	54,62,73	1.62	8 (14%)	62,99,113	1.36	8 (12%)
27	CLA	2	612	15	44,52,73	1.83	8 (18%)	51,88,113	1.43	6 (11%)
27	CLA	6	612	19	40,49,73	1.85	7 (17%)	45,84,113	1.50	8 (17%)
27	CLA	Z	602	25	60,68,73	1.61	6 (10%)	70,107,113	1.25	7 (10%)
33	LMG	L	2631	-	37,37,55	1.10	2 (5%)	45,45,63	1.11	3 (6%)
38	CHL	U	605	24	43,51,74	2.27	12 (27%)	45,86,114	3.00	22 (48%)
27	CLA	1	607	-	39,48,73	1.88	9 (23%)	44,83,113	1.51	8 (18%)
27	CLA	F	303	-	42,50,73	1.89	8 (19%)	48,85,113	1.47	7 (14%)
29	LHG	U	2630	27	48,48,48	0.92	2 (4%)	51,54,54	0.92	2 (3%)
38	CHL	Y	606	-	46,54,74	2.32	15 (32%)	49,90,114	2.81	21 (42%)
29	LHG	A	847	27	29,29,48	1.17	2 (6%)	32,35,54	1.04	2 (6%)
27	CLA	B	815	-	43,51,73	1.81	9 (20%)	49,86,113	1.43	7 (14%)
29	LHG	1	620	27	48,48,48	0.91	2 (4%)	51,54,54	0.97	3 (5%)
30	BCR	B	846	-	41,41,41	0.76	1 (2%)	56,56,56	2.23	21 (37%)
27	CLA	L	304	-	45,53,73	1.77	8 (17%)	52,89,113	1.42	7 (13%)
27	CLA	9	611	29	42,50,73	1.86	7 (16%)	48,85,113	1.44	7 (14%)
27	CLA	B	825	-	49,57,73	1.69	8 (16%)	55,93,113	1.42	9 (16%)
27	CLA	5	617	-	50,58,73	1.68	10 (20%)	58,95,113	1.39	9 (15%)
30	BCR	1	619	-	41,41,41	0.72	0	56,56,56	2.42	22 (39%)
27	CLA	G	204	7	45,53,73	1.81	8 (17%)	52,89,113	1.49	8 (15%)
27	CLA	U	613	24	59,67,73	1.57	9 (15%)	68,105,113	1.35	9 (13%)
27	CLA	9	606	-	39,48,73	1.94	9 (23%)	44,83,113	1.52	8 (18%)
27	CLA	8	611	29	42,50,73	1.83	9 (21%)	48,85,113	1.39	7 (14%)
33	LMG	V	2631	-	41,41,55	1.01	2 (4%)	49,49,63	1.16	4 (8%)
27	CLA	6	603	-	51,59,73	1.72	7 (13%)	63,96,113	1.45	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	3	613	16	52,61,73	1.69	8 (15%)	59,98,113	1.31	8 (13%)
27	CLA	A	830	-	65,73,73	1.47	9 (13%)	76,113,113	1.33	7 (9%)
36	XAT	2	620	-	39,47,47	0.93	0	54,74,74	2.50	21 (38%)
27	CLA	5	609	18	65,73,73	1.50	9 (13%)	76,113,113	1.27	7 (9%)
30	BCR	7	621	-	41,41,41	0.75	0	56,56,56	2.34	23 (41%)
27	CLA	A	803	-	65,73,73	1.49	9 (13%)	76,113,113	1.34	6 (7%)
27	CLA	7	616	20	43,51,73	1.90	7 (16%)	54,87,113	1.49	9 (16%)
27	CLA	U	614	-	42,50,73	1.83	9 (21%)	48,85,113	1.45	7 (14%)
27	CLA	Z	611	29	65,73,73	1.49	5 (7%)	76,113,113	1.26	7 (9%)
27	CLA	B	804	-	41,49,73	1.83	8 (19%)	47,84,113	1.46	7 (14%)
27	CLA	A	823	-	42,50,73	1.86	9 (21%)	48,85,113	1.44	7 (14%)
27	CLA	a	612	14	45,53,73	1.79	8 (17%)	52,89,113	1.46	7 (13%)
27	CLA	H	202	8	38,47,73	1.94	9 (23%)	43,82,113	1.43	7 (16%)
38	CHL	X	601	23	66,74,74	1.91	15 (22%)	73,114,114	2.69	21 (28%)
30	BCR	A	848	-	41,41,41	0.82	0	56,56,56	1.97	14 (25%)
27	CLA	B	803	-	65,73,73	1.47	9 (13%)	76,113,113	1.25	6 (7%)
27	CLA	A	836	-	65,73,73	1.49	9 (13%)	76,113,113	1.29	9 (11%)
27	CLA	B	809	2	65,73,73	1.50	9 (13%)	76,113,113	1.32	7 (9%)
27	CLA	3	609	16	60,68,73	1.55	9 (15%)	70,107,113	1.45	10 (14%)
27	CLA	U	610	24	56,64,73	1.66	9 (16%)	65,102,113	1.27	8 (12%)
27	CLA	1	613	-	65,73,73	1.51	8 (12%)	76,113,113	1.23	9 (11%)
27	CLA	A	805	-	52,60,73	1.67	9 (17%)	60,97,113	1.54	8 (13%)
30	BCR	A	852	-	41,41,41	0.85	1 (2%)	56,56,56	2.47	25 (44%)
29	LHG	X	2630	27	48,48,48	0.96	2 (4%)	51,54,54	0.97	2 (3%)
27	CLA	3	610	16	65,73,73	1.50	9 (13%)	76,113,113	1.28	7 (9%)
27	CLA	a	610	14	59,67,73	1.55	7 (11%)	69,106,113	1.42	8 (11%)
33	LMG	9	625	-	55,55,55	0.89	2 (3%)	63,63,63	0.95	2 (3%)
27	CLA	2	606	-	45,53,73	1.78	8 (17%)	52,89,113	1.55	7 (13%)
27	CLA	1	602	14	61,69,73	1.53	9 (14%)	71,108,113	1.29	8 (11%)
27	CLA	A	822	-	65,73,73	1.49	8 (12%)	76,113,113	1.47	10 (13%)
27	CLA	7	612	20	44,52,73	1.82	8 (18%)	51,88,113	1.51	6 (11%)
38	CHL	Z	607	-	66,74,74	1.90	15 (22%)	73,114,114	2.73	20 (27%)
27	CLA	B	829	-	65,73,73	1.48	9 (13%)	76,113,113	1.32	8 (10%)
27	CLA	V	604	-	50,58,73	1.71	9 (18%)	58,95,113	1.46	7 (12%)
27	CLA	7	614	-	42,50,73	1.85	9 (21%)	48,85,113	1.36	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	A	819	-	59,67,73	1.52	10 (16%)	68,105,113	1.42	7 (10%)
27	CLA	A	817	-	45,53,73	1.76	8 (17%)	52,89,113	1.62	8 (15%)
27	CLA	W	604	-	47,55,73	1.75	8 (17%)	54,91,113	1.41	8 (14%)
27	CLA	1	616	14	43,51,73	1.86	7 (16%)	54,87,113	1.60	9 (16%)
27	CLA	6	607	-	41,49,73	1.87	8 (19%)	51,84,113	1.56	9 (17%)
37	NEX	W	1623	-	38,46,46	0.91	1 (2%)	50,70,70	2.48	16 (32%)
29	LHG	5	625	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
33	LMG	H	205	-	55,55,55	0.89	2 (3%)	63,63,63	1.12	6 (9%)
27	CLA	X	602	23	65,73,73	1.56	7 (10%)	76,113,113	1.22	6 (7%)
27	CLA	A	808	-	50,58,73	1.69	9 (18%)	58,95,113	1.43	8 (13%)
37	NEX	5	624	-	38,46,46	1.04	1 (2%)	50,70,70	2.16	13 (26%)
27	CLA	A	806	-	65,73,73	1.46	8 (12%)	76,113,113	1.42	9 (11%)
33	LMG	4	623	-	40,40,55	1.05	2 (5%)	48,48,63	1.14	4 (8%)
27	CLA	A	820	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	8 (10%)
27	CLA	3	607	16	56,64,73	1.63	8 (14%)	69,102,113	1.47	11 (15%)
27	CLA	Y	612	24	45,53,73	1.85	6 (13%)	52,89,113	1.45	7 (13%)
27	CLA	A	802	-	65,73,73	1.48	9 (13%)	76,113,113	1.36	8 (10%)
27	CLA	9	603	22	44,52,73	1.86	9 (20%)	55,88,113	1.45	8 (14%)
38	CHL	V	601	26	66,74,74	1.91	15 (22%)	73,114,114	2.66	21 (28%)
36	XAT	9	620	-	39,47,47	0.92	1 (2%)	54,74,74	2.41	20 (37%)
29	LHG	a	620	27	42,42,48	0.98	2 (4%)	45,48,54	1.01	2 (4%)
27	CLA	7	615	-	41,50,73	1.93	7 (17%)	50,85,113	1.50	8 (16%)
27	CLA	9	601	22	45,53,73	1.81	8 (17%)	52,89,113	1.43	8 (15%)
27	CLA	A	821	-	53,61,73	1.66	8 (15%)	61,98,113	1.40	8 (13%)
27	CLA	B	836	-	50,58,73	1.67	7 (14%)	58,95,113	1.52	6 (10%)
29	LHG	6	623	27	47,47,48	0.93	2 (4%)	50,53,54	0.90	3 (6%)
28	PQN	B	842	-	34,34,34	3.39	10 (29%)	42,45,45	1.59	6 (14%)
30	BCR	a	619	-	41,41,41	0.73	0	56,56,56	2.41	22 (39%)
32	LMU	1	621	-	36,36,36	1.17	2 (5%)	47,47,47	0.95	1 (2%)
27	CLA	A	801	-	65,73,73	1.50	9 (13%)	76,113,113	1.29	10 (13%)
27	CLA	A	818	-	60,68,73	1.52	7 (11%)	70,107,113	1.39	8 (11%)
27	CLA	B	840	-	65,73,73	1.53	8 (12%)	76,113,113	1.32	8 (10%)
27	CLA	Y	603	-	55,63,73	1.68	7 (12%)	64,101,113	1.35	8 (12%)
27	CLA	O	2001	-	36,46,73	1.97	8 (22%)	41,80,113	1.49	8 (19%)
27	CLA	B	832	-	60,68,73	1.56	8 (13%)	70,107,113	1.32	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	B	833	-	65,73,73	1.51	9 (13%)	76,113,113	1.27	11 (14%)
35	LUT	Z	1621	-	42,43,43	0.76	0	51,60,60	1.77	13 (25%)
36	XAT	3	619	-	39,47,47	0.89	1 (2%)	54,74,74	2.56	22 (40%)
27	CLA	X	611	29	45,53,73	1.84	6 (13%)	52,89,113	1.49	9 (17%)
27	CLA	X	613	23	65,73,73	1.55	6 (9%)	76,113,113	1.27	11 (14%)
27	CLA	5	603	-	54,62,73	1.70	8 (14%)	67,100,113	1.45	11 (16%)
27	CLA	Z	604	-	57,65,73	1.64	5 (8%)	66,103,113	1.33	7 (10%)
27	CLA	8	601	21	65,73,73	1.45	7 (10%)	76,113,113	1.36	7 (9%)
27	CLA	8	616	-	43,51,73	1.94	7 (16%)	54,87,113	1.50	9 (16%)
27	CLA	B	838	-	46,54,73	1.74	8 (17%)	53,90,113	1.50	8 (15%)
27	CLA	4	604	-	54,62,73	1.68	8 (14%)	67,100,113	1.40	10 (14%)
27	CLA	A	842	-	65,73,73	1.50	8 (12%)	76,113,113	1.37	10 (13%)
27	CLA	a	613	-	54,62,73	1.65	8 (14%)	62,99,113	1.30	8 (12%)
29	LHG	B	854	-	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
27	CLA	Z	610	25	65,73,73	1.51	6 (9%)	76,113,113	1.34	9 (11%)
30	BCR	O	2004	-	41,41,41	0.77	0	56,56,56	2.38	19 (33%)
35	LUT	U	1620	-	42,43,43	0.90	1 (2%)	51,60,60	1.83	10 (19%)
29	LHG	Y	2630	27	48,48,48	0.95	2 (4%)	51,54,54	0.97	2 (3%)
38	CHL	Y	607	-	66,74,74	1.96	16 (24%)	73,114,114	2.66	25 (34%)
27	CLA	3	615	-	39,48,73	1.90	7 (17%)	44,83,113	1.70	7 (15%)
27	CLA	a	602	14	61,69,73	1.53	9 (14%)	71,108,113	1.29	8 (11%)
35	LUT	3	618	-	42,43,43	0.82	1 (2%)	51,60,60	1.67	12 (23%)
27	CLA	5	607	-	65,73,73	1.49	9 (13%)	76,113,113	1.38	7 (9%)
27	CLA	8	607	-	41,49,73	1.89	8 (19%)	51,84,113	1.56	9 (17%)
36	XAT	8	620	-	39,47,47	0.95	1 (2%)	54,74,74	2.56	26 (48%)
27	CLA	5	610	18	54,62,73	1.62	7 (12%)	62,99,113	1.45	8 (12%)
35	LUT	4	619	-	42,43,43	0.78	0	51,60,60	1.76	16 (31%)
27	CLA	B	811	-	53,60,73	1.74	9 (16%)	62,97,113	1.38	9 (14%)
27	CLA	6	614	-	60,68,73	1.58	8 (13%)	70,107,113	1.28	9 (12%)
30	BCR	9	621	-	41,41,41	0.76	0	56,56,56	2.08	18 (32%)
27	CLA	4	611	29	42,50,73	1.84	8 (19%)	48,85,113	1.45	7 (14%)
29	LHG	9	622	27	29,29,48	1.19	2 (6%)	32,35,54	1.03	1 (3%)
29	LHG	7	622	27	36,36,48	1.05	2 (5%)	39,42,54	0.85	2 (5%)
38	CHL	X	606	-	44,52,74	2.28	14 (31%)	46,87,114	2.90	21 (45%)
27	CLA	A	832	-	50,58,73	1.75	9 (18%)	58,95,113	1.38	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	CHL	W	608	-	47,55,74	2.23	14 (29%)	50,91,114	2.73	21 (42%)
29	LHG	9	623	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
27	CLA	Y	602	24	58,66,73	1.65	6 (10%)	67,104,113	1.27	6 (8%)
27	CLA	a	603	-	54,62,73	1.63	8 (14%)	62,99,113	1.52	9 (14%)
30	BCR	A	850	-	41,41,41	0.78	1 (2%)	56,56,56	2.16	22 (39%)
35	LUT	8	619	-	42,43,43	0.81	1 (2%)	51,60,60	1.66	13 (25%)
37	NEX	V	1623	-	38,46,46	0.90	2 (5%)	50,70,70	2.25	12 (24%)
30	BCR	O	2005	-	41,41,41	0.80	1 (2%)	56,56,56	3.00	25 (44%)
27	CLA	X	612	23	43,51,73	1.86	6 (13%)	49,86,113	1.45	7 (14%)
27	CLA	3	603	-	55,63,73	1.60	7 (12%)	64,101,113	1.62	9 (14%)
27	CLA	8	608	-	51,59,73	1.68	9 (17%)	59,96,113	1.43	8 (13%)
28	PQN	A	844	-	34,34,34	3.46	11 (32%)	42,45,45	1.59	4 (9%)
38	CHL	X	607	-	66,74,74	1.92	14 (21%)	73,114,114	2.72	22 (30%)
27	CLA	6	606	-	39,48,73	1.91	7 (17%)	44,83,113	1.39	7 (15%)
27	CLA	3	617	16	39,48,73	1.88	9 (23%)	44,83,113	1.56	7 (15%)
38	CHL	U	609	24	60,68,74	2.04	15 (25%)	65,106,114	2.74	22 (33%)
27	CLA	V	612	26	45,53,73	1.78	10 (22%)	52,89,113	1.53	9 (17%)
27	CLA	Z	614	-	54,62,73	1.67	6 (11%)	62,99,113	1.30	7 (11%)
29	LHG	8	623	-	39,39,48	1.02	2 (5%)	42,45,54	1.09	3 (7%)
30	BCR	L	309	-	41,41,41	0.68	0	56,56,56	1.97	18 (32%)
36	XAT	1	618	-	39,47,47	0.90	0	54,74,74	2.51	22 (40%)
27	CLA	3	614	-	39,48,73	1.91	8 (20%)	44,83,113	1.47	6 (13%)
27	CLA	A	831	-	65,73,73	1.50	10 (15%)	76,113,113	1.26	7 (9%)
38	CHL	U	608	-	44,52,74	2.22	14 (31%)	46,87,114	2.80	19 (41%)
27	CLA	7	608	-	50,58,73	1.69	8 (16%)	58,95,113	1.40	7 (12%)
27	CLA	8	610	21	60,68,73	1.52	7 (11%)	70,107,113	1.52	8 (11%)
35	LUT	7	619	-	42,43,43	0.85	2 (4%)	51,60,60	1.82	11 (21%)
30	BCR	B	848	-	41,41,41	0.78	0	56,56,56	2.20	20 (35%)
27	CLA	Y	611	29	43,51,73	1.87	6 (13%)	49,86,113	1.46	7 (14%)
27	CLA	A	835	-	61,69,73	1.54	9 (14%)	71,108,113	1.29	8 (11%)
29	LHG	O	2631	-	35,35,48	1.08	2 (5%)	38,41,54	1.07	3 (7%)
30	BCR	6	622	-	41,41,41	0.72	1 (2%)	56,56,56	3.46	27 (48%)
27	CLA	A	812	-	65,73,73	1.49	8 (12%)	76,113,113	1.27	8 (10%)
27	CLA	A	854	-	65,73,73	1.51	9 (13%)	76,113,113	1.41	10 (13%)
27	CLA	V	611	29	43,51,73	1.81	10 (23%)	49,86,113	1.51	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	W	611	29	57,65,73	1.57	8 (14%)	66,103,113	1.37	8 (12%)
37	NEX	Z	1623	-	38,46,46	1.14	2 (5%)	50,70,70	2.34	15 (30%)
29	LHG	3	623	-	44,44,48	0.96	2 (4%)	47,50,54	1.05	3 (6%)
27	CLA	W	610	23	55,63,73	1.65	9 (16%)	64,101,113	1.27	8 (12%)
30	BCR	8	621	-	41,41,41	0.83	0	56,56,56	2.52	17 (30%)
29	LHG	8	622	27	48,48,48	0.92	2 (4%)	51,54,54	0.85	2 (3%)
27	CLA	5	616	18	41,50,73	1.90	8 (19%)	50,85,113	1.46	9 (18%)
27	CLA	6	601	19	65,73,73	1.50	9 (13%)	76,113,113	1.32	9 (11%)
38	CHL	Z	609	25	66,74,74	2.01	15 (22%)	73,114,114	2.55	22 (30%)
27	CLA	B	817	-	59,67,73	1.58	9 (15%)	68,105,113	1.43	10 (14%)
27	CLA	a	606	-	43,52,73	1.81	8 (18%)	48,87,113	1.42	6 (12%)
33	LMG	8	626	-	46,46,55	0.97	2 (4%)	54,54,63	1.10	4 (7%)
27	CLA	5	613	18	64,72,73	1.51	8 (12%)	74,111,113	1.26	7 (9%)
27	CLA	4	614	-	56,64,73	1.62	7 (12%)	65,102,113	1.35	10 (15%)
30	BCR	L	305	-	41,41,41	0.75	0	56,56,56	2.07	23 (41%)
27	CLA	B	823	-	45,53,73	1.84	9 (20%)	52,89,113	1.34	8 (15%)
38	CHL	Y	608	-	49,57,74	2.28	15 (30%)	52,93,114	2.72	23 (44%)
30	BCR	A	856	-	41,41,41	0.77	0	56,56,56	2.14	19 (33%)
27	CLA	1	608	-	43,52,73	1.84	8 (18%)	49,88,113	1.43	8 (16%)
27	CLA	5	602	18	65,73,73	1.48	9 (13%)	76,113,113	1.25	7 (9%)
27	CLA	6	604	-	65,73,73	1.49	8 (12%)	76,113,113	1.22	9 (11%)
37	NEX	Y	1623	-	40,45,46	1.03	2 (5%)	50,67,70	2.47	16 (32%)
30	BCR	L	301	-	41,41,41	0.72	0	56,56,56	2.26	27 (48%)
30	BCR	K	207	-	41,41,41	0.75	0	56,56,56	2.93	23 (41%)
30	BCR	B	844	-	41,41,41	0.87	1 (2%)	56,56,56	2.11	20 (35%)
27	CLA	X	603	-	62,70,73	1.58	7 (11%)	72,109,113	1.29	8 (11%)
30	BCR	3	621	-	41,41,41	0.81	0	56,56,56	1.79	14 (25%)
27	CLA	L	302	12	45,53,73	1.81	9 (20%)	52,89,113	1.49	8 (15%)
27	CLA	5	606	-	39,48,73	1.92	9 (23%)	44,83,113	1.35	6 (13%)
31	SF4	A	853	1,2	0,12,12	-	-	-	-	-
29	LHG	B	851	27	37,37,48	1.08	2 (5%)	40,43,54	1.13	3 (7%)
27	CLA	B	819	-	55,63,73	1.64	9 (16%)	64,101,113	1.37	8 (12%)
38	CHL	V	606	-	44,52,74	2.17	15 (34%)	46,87,114	2.94	19 (41%)
27	CLA	J	101	10	42,50,73	1.89	9 (21%)	48,85,113	1.46	8 (16%)
27	CLA	2	609	15	45,53,73	1.81	8 (17%)	52,89,113	1.42	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	B	843	-	41,41,41	0.78	0	56,56,56	1.80	16 (28%)
30	BCR	G	205	-	41,41,41	0.79	0	56,56,56	1.96	15 (26%)
36	XAT	5	621	-	39,47,47	0.89	1 (2%)	54,74,74	2.52	22 (40%)
27	CLA	B	822	-	42,50,73	1.83	9 (21%)	48,85,113	1.42	8 (16%)
27	CLA	9	612	22	40,49,73	1.87	6 (15%)	45,84,113	1.54	8 (17%)
27	CLA	7	604	-	50,58,73	1.72	9 (18%)	58,95,113	1.35	8 (13%)
27	CLA	4	601	17	65,73,73	1.49	7 (10%)	76,113,113	1.34	9 (11%)
27	CLA	1	609	14	40,48,73	1.93	8 (20%)	50,83,113	1.60	10 (20%)
35	LUT	X	1621	-	42,43,43	0.79	1 (2%)	51,60,60	1.75	13 (25%)
27	CLA	9	602	22	60,68,73	1.54	8 (13%)	70,107,113	1.38	8 (11%)
27	CLA	B	839	-	65,73,73	1.49	8 (12%)	76,113,113	1.24	7 (9%)
27	CLA	7	603	-	43,52,73	1.79	9 (20%)	49,88,113	1.58	7 (14%)
38	CHL	Z	608	-	50,58,74	2.24	14 (28%)	52,94,114	2.73	22 (42%)
27	CLA	1	606	-	37,47,73	1.90	8 (21%)	41,80,113	1.57	8 (19%)
27	CLA	U	603	-	52,60,73	1.64	11 (21%)	60,97,113	1.47	8 (13%)
27	CLA	A	839	-	55,63,73	1.63	9 (16%)	64,101,113	1.34	9 (14%)
27	CLA	A	827	-	58,66,73	1.56	9 (15%)	67,104,113	1.34	8 (11%)
27	CLA	X	614	-	42,50,73	1.88	6 (14%)	48,85,113	1.43	7 (14%)
27	CLA	W	613	23	65,73,73	1.48	9 (13%)	76,113,113	1.31	9 (11%)
38	CHL	X	608	-	66,74,74	1.95	16 (24%)	73,114,114	2.62	19 (26%)
27	CLA	A	829	-	65,73,73	1.46	7 (10%)	76,113,113	1.32	7 (9%)
27	CLA	Y	614	-	48,56,73	1.80	6 (12%)	55,92,113	1.38	8 (14%)
27	CLA	U	602	24	59,67,73	1.55	9 (15%)	68,105,113	1.38	6 (8%)
27	CLA	O	2003	-	39,48,73	1.94	8 (20%)	44,83,113	1.45	7 (15%)
37	NEX	X	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.44	16 (32%)
27	CLA	W	612	23	45,53,73	1.78	8 (17%)	52,89,113	1.45	6 (11%)
27	CLA	9	607	-	45,53,73	1.81	9 (20%)	52,89,113	1.43	7 (13%)
27	CLA	L	303	-	65,73,73	1.49	8 (12%)	76,113,113	1.32	9 (11%)
36	XAT	U	1622	-	39,47,47	1.02	3 (7%)	54,74,74	3.93	24 (44%)
27	CLA	2	611	29	42,50,73	1.85	8 (19%)	48,85,113	1.46	7 (14%)
27	CLA	9	604	-	50,58,73	1.74	8 (16%)	62,95,113	1.42	10 (16%)
33	LMG	5	627	-	40,40,55	1.05	2 (5%)	48,48,63	1.01	2 (4%)
27	CLA	A	824	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	9 (11%)
30	BCR	B	801	-	41,41,41	0.84	0	56,56,56	2.10	20 (35%)
27	CLA	a	614	-	55,62,73	1.71	9 (16%)	60,99,113	1.43	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	B	818	-	60,68,73	1.54	9 (15%)	70,107,113	1.48	9 (12%)
35	LUT	Y	1620	-	42,43,43	0.80	1 (2%)	51,60,60	1.94	11 (21%)
27	CLA	B	814	-	62,70,73	1.50	8 (12%)	72,109,113	1.27	9 (12%)
27	CLA	4	613	17	65,73,73	1.51	8 (12%)	76,113,113	1.24	8 (10%)
29	LHG	H	204	-	48,48,48	0.90	2 (4%)	51,54,54	0.90	1 (1%)
27	CLA	B	810	-	64,72,73	1.51	8 (12%)	74,111,113	1.27	7 (9%)
29	LHG	W	2630	27	43,43,48	0.96	2 (4%)	46,49,54	0.96	2 (4%)
37	NEX	U	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.48	15 (30%)
27	CLA	3	606	-	53,62,73	1.63	8 (15%)	61,100,113	1.32	7 (11%)
27	CLA	a	608	-	43,52,73	1.84	8 (18%)	49,88,113	1.42	8 (16%)
33	LMG	J	104	-	40,40,55	1.06	2 (5%)	48,48,63	1.17	4 (8%)
35	LUT	Z	1620	-	42,43,43	0.75	1 (2%)	51,60,60	1.78	12 (23%)
27	CLA	B	828	-	65,73,73	1.48	9 (13%)	76,113,113	1.27	9 (11%)
27	CLA	8	612	21	40,49,73	1.87	8 (20%)	45,84,113	1.55	7 (15%)
27	CLA	4	609	17	57,65,73	1.59	8 (14%)	66,103,113	1.34	9 (13%)
38	CHL	V	607	-	46,54,74	2.23	16 (34%)	49,90,114	2.74	22 (44%)
35	LUT	9	619	-	42,43,43	0.79	0	51,60,60	1.73	14 (27%)
27	CLA	4	602	17	60,68,73	1.54	7 (11%)	70,107,113	1.44	8 (11%)
38	CHL	Z	605	25	44,52,74	2.31	15 (34%)	46,87,114	2.86	23 (50%)
27	CLA	U	611	29	42,50,73	1.79	9 (21%)	48,85,113	1.49	7 (14%)
38	CHL	Y	601	24	66,74,74	1.90	15 (22%)	73,114,114	2.67	22 (30%)
27	CLA	4	610	17	61,69,73	1.52	8 (13%)	71,108,113	1.31	9 (12%)
27	CLA	8	602	21	60,68,73	1.55	9 (15%)	70,107,113	1.31	8 (11%)
27	CLA	B	806	2	65,73,73	1.48	9 (13%)	76,113,113	1.32	7 (9%)
35	LUT	V	1620	-	42,43,43	0.91	1 (2%)	51,60,60	1.65	11 (21%)
27	CLA	6	611	29	42,50,73	1.84	8 (19%)	48,85,113	1.45	7 (14%)
30	BCR	A	851	-	41,41,41	0.88	1 (2%)	56,56,56	2.08	21 (37%)
27	CLA	A	837	1	45,53,73	1.79	8 (17%)	52,89,113	1.50	7 (13%)
27	CLA	O	2002	-	37,46,73	2.03	8 (21%)	46,81,113	1.53	8 (17%)
27	CLA	K	203	-	56,64,73	1.62	8 (14%)	65,102,113	1.43	11 (16%)
27	CLA	A	816	-	65,73,73	1.51	8 (12%)	76,113,113	1.35	8 (10%)
27	CLA	2	614	-	41,50,73	1.86	8 (19%)	46,85,113	1.41	7 (15%)
29	LHG	Z	2630	27	48,48,48	0.94	2 (4%)	51,54,54	0.85	2 (3%)
30	BCR	B	852	-	41,41,41	0.80	0	56,56,56	3.56	24 (42%)
29	LHG	4	622	27	48,48,48	0.92	2 (4%)	51,54,54	0.89	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	5	604	-	63,71,73	1.57	8 (12%)	78,111,113	1.31	11 (14%)
30	BCR	3	622	-	41,41,41	0.73	0	56,56,56	2.30	19 (33%)
38	CHL	U	607	-	46,54,74	2.21	13 (28%)	49,90,114	2.80	25 (51%)
35	LUT	5	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.97	11 (21%)
35	LUT	W	1620	-	42,43,43	0.90	1 (2%)	51,60,60	1.83	9 (17%)
27	CLA	8	604	-	50,58,73	1.66	7 (14%)	58,95,113	1.46	9 (15%)
27	CLA	7	613	20	65,73,73	1.49	8 (12%)	76,113,113	1.22	8 (10%)
38	CHL	W	607	-	65,73,74	1.95	16 (24%)	73,113,114	2.55	22 (30%)
27	CLA	1	614	-	37,45,73	2.12	9 (24%)	44,79,113	1.68	11 (25%)
27	CLA	A	813	-	54,62,73	1.61	8 (14%)	62,99,113	1.45	8 (12%)
29	LHG	5	623	27	48,48,48	0.92	2 (4%)	51,54,54	0.83	2 (3%)
27	CLA	A	814	-	65,73,73	1.47	9 (13%)	76,113,113	1.40	9 (11%)
27	CLA	a	616	14	45,53,73	1.78	6 (13%)	52,89,113	1.46	7 (13%)
31	SF4	C	102	3	0,12,12	-	-	-	-	-
27	CLA	5	614	-	45,52,73	1.90	9 (20%)	48,87,113	1.45	8 (16%)
27	CLA	8	603	-	44,52,73	1.83	8 (18%)	55,88,113	1.60	9 (16%)
27	CLA	7	609	20	43,52,73	1.79	7 (16%)	48,87,113	1.44	6 (12%)
27	CLA	2	613	15	65,73,73	1.47	7 (10%)	76,113,113	1.27	8 (10%)
30	BCR	B	853	-	41,41,41	0.75	0	56,56,56	1.70	13 (23%)
30	BCR	A	849	-	41,41,41	0.82	0	56,56,56	2.24	19 (33%)
30	BCR	K	202	-	41,41,41	0.83	0	56,56,56	2.16	18 (32%)
27	CLA	9	613	22	65,73,73	1.51	8 (12%)	76,113,113	1.26	7 (9%)
27	CLA	5	608	-	50,58,73	1.71	9 (18%)	58,95,113	1.37	8 (13%)
33	LMG	J	103	-	42,42,55	1.01	2 (4%)	50,50,63	1.09	2 (4%)
27	CLA	V	613	26	65,73,73	1.50	10 (15%)	76,113,113	1.29	7 (9%)
27	CLA	3	604	-	65,73,73	1.48	8 (12%)	76,113,113	1.29	8 (10%)
27	CLA	5	618	18	39,48,73	1.96	7 (17%)	48,83,113	1.62	9 (18%)
27	CLA	U	604	-	49,56,73	1.79	10 (20%)	50,91,113	1.47	8 (16%)
36	XAT	X	1622	-	39,47,47	0.91	1 (2%)	54,74,74	3.87	25 (46%)
27	CLA	7	601	20	60,68,73	1.49	7 (11%)	70,107,113	1.51	8 (11%)
27	CLA	2	610	15	55,63,73	1.59	7 (12%)	64,101,113	1.52	8 (12%)
36	XAT	a	618	-	39,47,47	0.89	1 (2%)	54,74,74	2.51	22 (40%)
30	BCR	B	845	-	41,41,41	0.81	0	56,56,56	2.13	22 (39%)
27	CLA	8	613	21	65,73,73	1.53	9 (13%)	76,113,113	1.25	8 (10%)
27	CLA	W	602	23	60,68,73	1.53	9 (15%)	70,107,113	1.37	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	7	607	-	42,50,73	1.82	9 (21%)	48,85,113	1.44	7 (14%)
27	CLA	B	827	-	62,70,73	1.51	8 (12%)	72,109,113	1.35	8 (11%)
27	CLA	4	618	17	39,48,73	1.94	7 (17%)	48,83,113	1.62	9 (18%)
27	CLA	L	306	-	39,48,73	1.89	8 (20%)	44,83,113	1.55	7 (15%)
27	CLA	9	610	22	57,65,73	1.61	8 (14%)	66,103,113	1.32	10 (15%)
27	CLA	7	610	20	65,73,73	1.46	7 (10%)	76,113,113	1.37	9 (11%)
27	CLA	2	616	-	43,51,73	1.89	8 (18%)	54,87,113	1.49	9 (16%)
27	CLA	3	608	-	55,63,73	1.71	9 (16%)	64,101,113	1.32	7 (10%)
27	CLA	A	825	-	65,73,73	1.48	9 (13%)	76,113,113	1.27	8 (10%)
35	LUT	a	617	-	42,43,43	0.82	1 (2%)	51,60,60	1.77	14 (27%)
27	CLA	Z	613	25	65,73,73	1.54	6 (9%)	76,113,113	1.25	9 (11%)
27	CLA	7	606	-	41,49,73	1.84	9 (21%)	47,84,113	1.45	7 (14%)
27	CLA	B	812	-	43,51,73	1.85	8 (18%)	49,86,113	1.45	8 (16%)
27	CLA	F	304	6	41,49,73	1.86	8 (19%)	47,84,113	1.47	7 (14%)
27	CLA	1	601	14	53,62,73	1.67	9 (16%)	61,100,113	1.29	8 (13%)
27	CLA	B	807	-	52,60,73	1.66	10 (19%)	60,97,113	1.43	10 (16%)
30	BCR	7	623	-	41,41,41	0.68	0	56,56,56	2.22	26 (46%)
27	CLA	A	833	-	45,53,73	1.79	9 (20%)	52,89,113	1.51	8 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	K	206	11	1/1/11/20	5/13/91/115	-
31	SF4	C	101	3	-	-	0/6/5/5
27	CLA	A	811	-	1/1/15/20	11/37/115/115	-
27	CLA	a	611	29	1/1/10/20	3/4/80/115	-
27	CLA	K	201	11	1/1/11/20	4/13/91/115	-
27	CLA	A	809	1	1/1/15/20	11/37/115/115	-
27	CLA	2	601	15	1/1/15/20	14/37/115/115	-
27	CLA	4	616	17	1/1/11/20	9/11/87/115	-
27	CLA	K	204	-	1/1/11/20	5/13/91/115	-
27	CLA	A	841	-	1/1/15/20	16/37/115/115	-
27	CLA	1	603	-	1/1/12/20	4/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	831	-	1/1/15/20	15/37/115/115	-
27	CLA	1	611	29	1/1/13/20	5/28/106/115	-
27	CLA	6	616	19	1/1/15/20	22/37/115/115	-
27	CLA	X	604	-	1/1/11/20	5/18/96/115	-
30	BCR	L	308	-	-	2/29/63/63	0/2/2/2
27	CLA	9	614	-	1/1/11/20	4/13/91/115	-
38	CHL	U	606	-	3/3/15/26	0/13/111/137	-
27	CLA	5	612	18	1/1/10/20	3/8/86/115	-
27	CLA	6	620	-	1/1/14/20	11/35/113/115	-
27	CLA	6	613	-	1/1/15/20	14/35/113/115	-
27	CLA	B	835	-	1/1/11/20	4/13/91/115	-
27	CLA	B	826	-	1/1/14/20	6/34/112/115	-
38	CHL	V	605	26	3/3/15/26	0/13/111/137	-
27	CLA	A	840	-	-	5/22/100/115	-
27	CLA	8	614	-	1/1/12/20	9/23/101/115	-
27	CLA	1	604	-	1/1/11/20	9/18/96/115	-
27	CLA	2	604	-	1/1/10/20	5/9/87/115	-
38	CHL	W	606	-	3/3/16/26	2/15/113/137	-
29	LHG	3	624	27	-	23/53/53/53	-
27	CLA	5	619	-	1/1/11/20	6/11/87/115	-
30	BCR	5	622	-	-	3/29/63/63	0/2/2/2
35	LUT	6	619	-	-	0/29/67/67	0/2/2/2
27	CLA	4	612	17	1/1/10/20	2/8/86/115	-
27	CLA	6	618	19	1/1/10/20	0/8/84/115	-
27	CLA	F	301	-	1/1/13/20	8/28/106/115	-
29	LHG	A	846	-	-	14/53/53/53	-
27	CLA	6	610	19	1/1/15/20	8/37/115/115	-
36	XAT	6	621	-	-	0/31/93/93	0/4/4/4
27	CLA	6	608	-	1/1/11/20	4/13/91/115	-
30	BCR	3	620	-	-	4/29/63/63	0/2/2/2
27	CLA	A	838	-	1/1/12/20	7/19/97/115	-
27	CLA	A	843	-	1/1/14/20	12/35/113/115	-
27	CLA	Y	604	-	1/1/12/20	3/19/97/115	-
27	CLA	B	837	-	-	12/37/115/115	-
32	LMU	5	629	-	-	11/18/58/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LUT	2	619	-	-	1/29/67/67	0/2/2/2
30	BCR	B	847	-	-	2/29/63/63	0/2/2/2
38	CHL	Z	606	-	3/3/16/26	4/15/113/137	-
29	LHG	V	2630	27	-	9/52/52/53	-
30	BCR	F	305	-	-	6/29/63/63	0/2/2/2
27	CLA	3	602	16	1/1/14/20	4/31/109/115	-
38	CHL	W	609	23	3/3/20/26	16/39/137/137	-
35	LUT	X	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	a	604	-	1/1/11/20	9/18/96/115	-
27	CLA	A	815	-	1/1/12/20	8/19/97/115	-
27	CLA	a	601	14	-	2/23/101/115	-
27	CLA	8	606	-	1/1/15/20	7/35/113/115	-
38	CHL	W	605	23	3/3/16/26	5/15/113/137	-
32	LMU	A	857	-	-	3/21/61/61	0/2/2/2
27	CLA	A	828	-	1/1/15/20	9/37/115/115	-
32	LMU	K	208	-	-	14/21/61/61	0/2/2/2
38	CHL	Z	601	25	3/3/20/26	21/39/137/137	-
30	BCR	2	623	-	-	4/29/63/63	0/2/2/2
27	CLA	V	614	-	1/1/11/20	3/13/91/115	-
27	CLA	W	614	-	1/1/11/20	3/13/91/115	-
29	LHG	2	622	27	-	13/40/40/53	-
27	CLA	3	611	29	1/1/10/20	2/4/80/115	-
27	CLA	6	617	-	1/1/11/20	7/13/91/115	-
27	CLA	B	834	-	1/1/14/20	7/31/109/115	-
27	CLA	H	203	-	-	12/37/115/115	-
27	CLA	1	612	14	1/1/11/20	5/13/91/115	-
38	CHL	X	609	23	3/3/20/26	17/39/137/137	-
27	CLA	B	820	-	1/1/12/20	1/19/97/115	-
27	CLA	6	609	19	1/1/11/20	2/13/91/115	-
32	LMU	5	628	-	-	9/19/59/61	0/2/2/2
27	CLA	B	830	-	1/1/10/20	2/11/89/115	-
27	CLA	W	603	-	1/1/12/20	8/22/100/115	-
27	CLA	B	802	-	1/1/15/20	20/37/115/115	-
32	LMU	A	858	-	-	12/21/57/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	U	601	24	3/3/20/26	21/39/137/137	-
38	CHL	W	601	23	3/3/20/26	18/39/137/137	-
29	LHG	9	624	-	-	20/53/53/53	-
27	CLA	B	813	-	1/1/15/20	19/37/115/115	-
27	CLA	A	834	-	1/1/15/20	13/37/115/115	-
38	CHL	Y	605	24	3/3/15/26	2/10/108/137	-
38	CHL	V	608	-	3/3/16/26	5/18/116/137	-
27	CLA	a	609	14	1/1/15/20	12/35/113/115	-
35	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
30	BCR	B	849	-	-	3/29/63/63	0/2/2/2
36	XAT	W	1622	-	-	1/31/93/93	0/4/4/4
27	CLA	X	610	23	1/1/15/20	7/37/115/115	-
27	CLA	9	609	22	1/1/14/20	8/33/111/115	-
37	NEX	6	624	-	-	2/27/83/83	0/3/3/3
27	CLA	A	807	1	1/1/15/20	18/37/115/115	-
27	CLA	4	603	17	1/1/11/20	2/13/89/115	-
36	XAT	4	620	-	-	0/31/93/93	0/4/4/4
27	CLA	A	804	-	1/1/15/20	16/37/115/115	-
35	LUT	U	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	3	612	16	1/1/10/20	1/11/89/115	-
27	CLA	4	607	-	1/1/11/20	4/13/91/115	-
27	CLA	V	610	26	1/1/14/20	7/34/112/115	-
27	CLA	L	307	-	1/1/10/20	0/6/84/115	-
27	CLA	B	808	-	1/1/15/20	14/37/115/115	-
35	LUT	V	1621	-	-	2/29/67/67	0/2/2/2
27	CLA	7	602	20	1/1/15/20	13/37/115/115	-
27	CLA	5	611	29	1/1/10/20	5/10/88/115	-
27	CLA	4	606	-	1/1/10/20	2/6/84/115	-
27	CLA	B	824	-	1/1/15/20	12/37/115/115	-
27	CLA	A	810	1	1/1/12/20	8/19/97/115	-
27	CLA	4	608	-	1/1/15/20	14/37/115/115	-
36	XAT	Y	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	B	841	29	1/1/15/20	10/37/115/115	-
27	CLA	5	601	18	1/1/13/20	2/27/105/115	-
33	LMG	A	860	-	-	9/35/55/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	V	609	26	3/3/19/26	16/33/131/137	-
27	CLA	A	826	-	1/1/14/20	10/35/113/115	-
27	CLA	B	821	-	1/1/11/20	2/11/89/115	-
27	CLA	Z	612	25	1/1/15/20	6/37/115/115	-
34	DGD	B	850	-	-	16/51/91/95	0/2/2/2
27	CLA	2	602	15	1/1/15/20	9/35/113/115	-
30	BCR	J	102	-	-	3/29/63/63	0/2/2/2
27	CLA	V	603	-	1/1/11/20	3/13/91/115	-
27	CLA	B	805	-	1/1/15/20	15/37/115/115	-
27	CLA	G	203	-	1/1/10/20	2/10/88/115	-
27	CLA	Y	613	24	1/1/15/20	16/37/115/115	-
38	CHL	Y	609	24	3/3/20/26	14/39/137/137	-
36	XAT	Z	1622	-	-	0/31/93/93	0/4/4/4
38	CHL	X	605	23	3/3/16/26	3/15/113/137	-
36	XAT	7	620	-	-	0/31/93/93	0/4/4/4
27	CLA	1	610	14	1/1/9/20	0/6/80/115	-
27	CLA	V	602	26	1/1/14/20	4/31/109/115	-
35	LUT	W	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	8	609	21	1/1/11/20	4/13/91/115	-
32	LMU	8	625	-	-	9/21/61/61	0/2/2/2
36	XAT	V	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	A	845	29	1/1/12/20	4/19/97/115	-
27	CLA	7	611	29	1/1/13/20	5/29/107/115	-
35	LUT	1	617	-	-	0/29/67/67	0/2/2/2
27	CLA	2	603	15	1/1/11/20	4/11/89/115	-
27	CLA	Y	610	24	1/1/15/20	7/37/115/115	-
33	LMG	4	624	-	-	8/35/55/70	0/1/1/1
30	BCR	4	621	-	-	4/29/63/63	0/2/2/2
27	CLA	Z	603	-	1/1/15/20	20/37/115/115	-
27	CLA	U	612	24	1/1/10/20	2/11/89/115	-
27	CLA	2	607	-	1/1/11/20	3/13/91/115	-
27	CLA	a	607	-	1/1/11/20	3/13/91/115	-
27	CLA	6	602	19	1/1/15/20	10/37/115/115	-
27	CLA	B	816	-	1/1/12/20	12/23/101/115	-
27	CLA	2	612	15	1/1/11/20	5/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	6	612	19	1/1/10/20	2/8/86/115	-
27	CLA	Z	602	25	1/1/14/20	4/31/109/115	-
38	CHL	U	605	24	3/3/15/26	3/12/110/137	-
33	LMG	L	2631	-	-	8/32/52/70	0/1/1/1
27	CLA	1	607	-	1/1/10/20	1/6/84/115	-
27	CLA	F	303	-	-	5/10/88/115	-
29	LHG	U	2630	27	-	12/53/53/53	-
38	CHL	Y	606	-	3/3/16/26	2/15/113/137	-
29	LHG	A	847	27	-	7/34/34/53	-
27	CLA	B	815	-	1/1/10/20	0/11/89/115	-
29	LHG	1	620	27	-	11/53/53/53	-
30	BCR	B	846	-	-	2/29/63/63	0/2/2/2
27	CLA	L	304	-	1/1/11/20	1/13/91/115	-
27	CLA	9	611	29	1/1/10/20	3/10/88/115	-
27	CLA	B	825	-	-	4/18/96/115	-
27	CLA	5	617	-	1/1/12/20	7/19/97/115	-
30	BCR	1	619	-	-	4/29/63/63	0/2/2/2
27	CLA	G	204	7	1/1/11/20	5/13/91/115	-
27	CLA	U	613	24	1/1/13/20	12/30/108/115	-
27	CLA	9	606	-	1/1/10/20	2/6/84/115	-
27	CLA	8	611	29	1/1/10/20	2/10/88/115	-
33	LMG	V	2631	-	-	9/36/56/70	0/1/1/1
27	CLA	6	603	-	1/1/12/20	4/22/98/115	-
27	CLA	3	613	16	1/1/12/20	7/21/99/115	-
27	CLA	A	830	-	1/1/15/20	11/37/115/115	-
36	XAT	2	620	-	-	0/31/93/93	0/4/4/4
27	CLA	5	609	18	1/1/15/20	12/37/115/115	-
30	BCR	7	621	-	-	5/29/63/63	0/2/2/2
27	CLA	A	803	-	1/1/15/20	3/37/115/115	-
27	CLA	7	616	20	1/1/11/20	2/11/87/115	-
27	CLA	U	614	-	1/1/10/20	4/10/88/115	-
27	CLA	Z	611	29	1/1/15/20	6/37/115/115	-
27	CLA	B	804	-	1/1/10/20	0/8/86/115	-
27	CLA	A	823	-	1/1/10/20	2/10/88/115	-
27	CLA	a	612	14	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	H	202	8	1/1/10/20	1/4/82/115	-
38	CHL	X	601	23	3/3/20/26	22/39/137/137	-
30	BCR	A	848	-	-	1/29/63/63	0/2/2/2
27	CLA	B	803	-	1/1/15/20	11/37/115/115	-
27	CLA	A	836	-	1/1/15/20	5/37/115/115	-
27	CLA	B	809	2	1/1/15/20	15/37/115/115	-
27	CLA	3	609	16	1/1/14/20	15/31/109/115	-
27	CLA	U	610	24	1/1/13/20	5/27/105/115	-
27	CLA	1	613	-	1/1/15/20	13/37/115/115	-
27	CLA	A	805	-	-	5/22/100/115	-
30	BCR	A	852	-	-	8/29/63/63	0/2/2/2
29	LHG	X	2630	27	-	11/53/53/53	-
27	CLA	3	610	16	1/1/15/20	12/37/115/115	-
27	CLA	a	610	14	1/1/14/20	1/29/107/115	-
33	LMG	9	625	-	-	16/50/70/70	0/1/1/1
27	CLA	2	606	-	1/1/11/20	5/13/91/115	-
27	CLA	1	602	14	1/1/14/20	3/33/111/115	-
27	CLA	A	822	-	1/1/15/20	7/37/115/115	-
27	CLA	7	612	20	1/1/11/20	5/11/89/115	-
38	CHL	Z	607	-	3/3/20/26	19/39/137/137	-
27	CLA	B	829	-	1/1/15/20	11/37/115/115	-
27	CLA	V	604	-	1/1/12/20	4/19/97/115	-
27	CLA	7	614	-	1/1/10/20	3/10/88/115	-
27	CLA	A	819	-	1/1/13/20	6/30/108/115	-
27	CLA	A	817	-	-	4/13/91/115	-
27	CLA	W	604	-	1/1/11/20	4/16/94/115	-
27	CLA	1	616	14	1/1/11/20	5/11/87/115	-
27	CLA	6	607	-	1/1/10/20	5/10/86/115	-
37	NEX	W	1623	-	-	4/27/83/83	0/3/3/3
29	LHG	5	625	-	-	16/53/53/53	-
33	LMG	H	205	-	-	8/50/70/70	0/1/1/1
27	CLA	X	602	23	1/1/15/20	10/37/115/115	-
27	CLA	A	808	-	-	3/19/97/115	-
37	NEX	5	624	-	-	2/27/83/83	0/3/3/3
27	CLA	A	806	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	4	623	-	-	5/35/55/70	0/1/1/1
27	CLA	A	820	-	1/1/15/20	13/37/115/115	-
27	CLA	3	607	16	1/1/13/20	10/28/104/115	-
27	CLA	Y	612	24	1/1/11/20	4/13/91/115	-
27	CLA	A	802	-	1/1/15/20	9/37/115/115	-
27	CLA	9	603	22	1/1/11/20	2/13/89/115	-
38	CHL	V	601	26	3/3/20/26	14/39/137/137	-
36	XAT	9	620	-	-	0/31/93/93	0/4/4/4
29	LHG	a	620	27	-	10/47/47/53	-
27	CLA	7	615	-	1/1/10/20	6/8/84/115	-
27	CLA	9	601	22	1/1/11/20	2/13/91/115	-
27	CLA	A	821	-	1/1/12/20	12/23/101/115	-
27	CLA	B	836	-	1/1/12/20	4/19/97/115	-
29	LHG	6	623	27	-	25/52/52/53	-
28	PQN	B	842	-	-	5/23/43/43	0/2/2/2
30	BCR	a	619	-	-	4/29/63/63	0/2/2/2
32	LMU	1	621	-	-	7/21/61/61	0/2/2/2
27	CLA	A	801	-	1/1/15/20	9/37/115/115	-
27	CLA	A	818	-	-	14/31/109/115	-
27	CLA	B	840	-	1/1/15/20	4/37/115/115	-
27	CLA	Y	603	-	1/1/13/20	7/25/103/115	-
27	CLA	O	2001	-	1/1/9/20	1/4/78/115	-
27	CLA	B	833	-	1/1/15/20	8/37/115/115	-
27	CLA	B	832	-	-	9/31/109/115	-
35	LUT	Z	1621	-	-	2/29/67/67	0/2/2/2
36	XAT	3	619	-	-	0/31/93/93	0/4/4/4
27	CLA	X	611	29	1/1/11/20	8/13/91/115	-
27	CLA	X	613	23	1/1/15/20	16/37/115/115	-
27	CLA	5	603	-	1/1/13/20	6/25/101/115	-
27	CLA	Z	604	-	1/1/13/20	6/28/106/115	-
27	CLA	8	601	21	1/1/15/20	16/37/115/115	-
27	CLA	8	616	-	1/1/11/20	4/11/87/115	-
27	CLA	B	838	-	-	3/15/93/115	-
27	CLA	4	604	-	1/1/13/20	8/25/101/115	-
27	CLA	A	842	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	613	-	1/1/12/20	8/24/102/115	-
29	LHG	B	854	-	-	17/53/53/53	-
27	CLA	Z	610	25	1/1/15/20	11/37/115/115	-
30	BCR	O	2004	-	-	3/29/63/63	0/2/2/2
35	LUT	U	1620	-	-	2/29/67/67	0/2/2/2
38	CHL	Y	607	-	3/3/20/26	21/39/137/137	-
29	LHG	Y	2630	27	-	11/53/53/53	-
27	CLA	3	615	-	1/1/10/20	2/6/84/115	-
27	CLA	a	602	14	1/1/14/20	3/33/111/115	-
35	LUT	3	618	-	-	0/29/67/67	0/2/2/2
27	CLA	5	607	-	1/1/15/20	14/37/115/115	-
27	CLA	8	607	-	1/1/10/20	5/10/86/115	-
36	XAT	8	620	-	-	0/31/93/93	0/4/4/4
27	CLA	5	610	18	1/1/12/20	4/24/102/115	-
35	LUT	4	619	-	-	4/29/67/67	0/2/2/2
27	CLA	B	811	-	1/1/12/20	8/23/95/115	-
27	CLA	6	614	-	1/1/14/20	9/31/109/115	-
30	BCR	9	621	-	-	4/29/63/63	0/2/2/2
27	CLA	4	611	29	1/1/10/20	2/10/88/115	-
29	LHG	9	622	27	-	12/34/34/53	-
29	LHG	7	622	27	-	21/41/41/53	-
38	CHL	X	606	-	3/3/15/26	0/13/111/137	-
38	CHL	W	608	-	3/3/16/26	5/17/115/137	-
27	CLA	A	832	-	1/1/12/20	6/19/97/115	-
29	LHG	9	623	-	-	16/53/53/53	-
27	CLA	Y	602	24	1/1/13/20	7/29/107/115	-
27	CLA	a	603	-	1/1/12/20	3/23/101/115	-
30	BCR	A	850	-	-	2/29/63/63	0/2/2/2
35	LUT	8	619	-	-	1/29/67/67	0/2/2/2
37	NEX	V	1623	-	-	4/27/83/83	0/3/3/3
30	BCR	O	2005	-	-	5/29/63/63	0/2/2/2
27	CLA	X	612	23	1/1/10/20	2/11/89/115	-
27	CLA	3	603	-	1/1/13/20	6/25/103/115	-
27	CLA	8	608	-	1/1/12/20	7/21/99/115	-
28	PQN	A	844	-	-	11/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	X	607	-	3/3/20/26	17/39/137/137	-
27	CLA	6	606	-	1/1/10/20	0/6/84/115	-
27	CLA	3	617	16	1/1/10/20	0/6/84/115	-
38	CHL	U	609	24	3/3/18/26	11/32/130/137	-
27	CLA	V	612	26	1/1/11/20	2/13/91/115	-
27	CLA	Z	614	-	1/1/12/20	7/24/102/115	-
29	LHG	8	623	-	-	10/44/44/53	-
30	BCR	L	309	-	-	1/29/63/63	0/2/2/2
36	XAT	1	618	-	-	0/31/93/93	0/4/4/4
27	CLA	3	614	-	1/1/10/20	1/6/84/115	-
27	CLA	A	831	-	1/1/15/20	12/37/115/115	-
38	CHL	U	608	-	3/3/15/26	3/13/111/137	-
27	CLA	7	608	-	1/1/12/20	3/19/97/115	-
27	CLA	8	610	21	1/1/14/20	8/31/109/115	-
35	LUT	7	619	-	-	1/29/67/67	0/2/2/2
30	BCR	B	848	-	-	3/29/63/63	0/2/2/2
27	CLA	Y	611	29	1/1/10/20	6/11/89/115	-
27	CLA	A	835	-	-	11/33/111/115	-
29	LHG	O	2631	-	-	17/40/40/53	-
30	BCR	6	622	-	-	5/29/63/63	0/2/2/2
27	CLA	A	812	-	1/1/15/20	6/37/115/115	-
27	CLA	A	854	-	1/1/15/20	13/37/115/115	-
27	CLA	V	611	29	1/1/10/20	5/11/89/115	-
27	CLA	W	611	29	1/1/13/20	12/28/106/115	-
37	NEX	Z	1623	-	-	3/27/83/83	0/3/3/3
29	LHG	3	623	-	-	20/49/49/53	-
27	CLA	W	610	23	1/1/13/20	5/25/103/115	-
30	BCR	8	621	-	-	4/29/63/63	0/2/2/2
29	LHG	8	622	27	-	9/53/53/53	-
27	CLA	5	616	18	1/1/10/20	3/8/84/115	-
27	CLA	6	601	19	1/1/15/20	14/37/115/115	-
38	CHL	Z	609	25	3/3/20/26	18/39/137/137	-
27	CLA	B	817	-	1/1/13/20	7/30/108/115	-
27	CLA	a	606	-	1/1/10/20	4/10/88/115	-
33	LMG	8	626	-	-	15/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	5	613	18	1/1/14/20	16/35/113/115	-
27	CLA	4	614	-	1/1/13/20	9/27/105/115	-
30	BCR	L	305	-	-	2/29/63/63	0/2/2/2
27	CLA	B	823	-	1/1/11/20	6/13/91/115	-
38	CHL	Y	608	-	3/3/16/26	6/19/117/137	-
30	BCR	A	856	-	-	2/29/63/63	0/2/2/2
27	CLA	1	608	-	1/1/11/20	3/11/89/115	-
27	CLA	5	602	18	-	14/37/115/115	-
27	CLA	6	604	-	-	13/37/115/115	-
37	NEX	Y	1623	-	-	3/27/80/83	0/3/3/3
30	BCR	L	301	-	-	4/29/63/63	0/2/2/2
30	BCR	K	207	-	-	1/29/63/63	0/2/2/2
30	BCR	B	844	-	-	2/29/63/63	0/2/2/2
27	CLA	X	603	-	1/1/14/20	7/34/112/115	-
30	BCR	3	621	-	-	0/29/63/63	0/2/2/2
27	CLA	L	302	12	1/1/11/20	4/13/91/115	-
27	CLA	5	606	-	-	1/6/84/115	-
31	SF4	A	853	1,2	-	-	0/6/5/5
29	LHG	B	851	27	-	11/42/42/53	-
27	CLA	B	819	-	1/1/13/20	7/25/103/115	-
38	CHL	V	606	-	3/3/15/26	3/13/111/137	-
27	CLA	J	101	10	1/1/10/20	4/10/88/115	-
27	CLA	2	609	15	1/1/11/20	2/13/91/115	-
30	BCR	B	843	-	-	4/29/63/63	0/2/2/2
30	BCR	G	205	-	-	1/29/63/63	0/2/2/2
36	XAT	5	621	-	-	0/31/93/93	0/4/4/4
27	CLA	B	822	-	-	4/10/88/115	-
27	CLA	9	612	22	1/1/10/20	2/8/86/115	-
27	CLA	7	604	-	1/1/12/20	7/19/97/115	-
27	CLA	4	601	17	1/1/15/20	15/37/115/115	-
27	CLA	1	609	14	1/1/10/20	3/8/84/115	-
35	LUT	X	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	9	602	22	-	7/31/109/115	-
27	CLA	B	839	-	1/1/15/20	14/37/115/115	-
27	CLA	7	603	-	1/1/11/20	3/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	1	606	-	1/1/8/20	3/5/79/115	-
27	CLA	U	603	-	1/1/12/20	8/22/100/115	-
27	CLA	A	839	-	1/1/13/20	6/25/103/115	-
27	CLA	A	827	-	1/1/13/20	7/29/107/115	-
27	CLA	X	614	-	1/1/10/20	4/10/88/115	-
27	CLA	W	613	23	1/1/15/20	14/37/115/115	-
38	CHL	X	608	-	3/3/20/26	21/39/137/137	-
27	CLA	A	829	-	1/1/15/20	15/37/115/115	-
27	CLA	Y	614	-	1/1/11/20	7/17/95/115	-
27	CLA	U	602	24	1/1/13/20	7/30/108/115	-
27	CLA	O	2003	-	1/1/10/20	3/6/84/115	-
37	NEX	X	1623	-	-	3/27/83/83	0/3/3/3
27	CLA	W	612	23	1/1/11/20	4/13/91/115	-
27	CLA	9	607	-	-	6/13/91/115	-
27	CLA	L	303	-	-	13/37/115/115	-
36	XAT	U	1622	-	-	1/31/93/93	0/4/4/4
27	CLA	2	611	29	1/1/10/20	3/10/88/115	-
27	CLA	9	604	-	1/1/12/20	3/20/96/115	-
33	LMG	5	627	-	-	11/35/55/70	0/1/1/1
27	CLA	A	824	-	1/1/15/20	10/37/115/115	-
30	BCR	B	801	-	-	4/29/63/63	0/2/2/2
27	CLA	a	614	-	1/1/12/20	9/25/99/115	-
27	CLA	B	818	-	-	13/31/109/115	-
35	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	B	814	-	1/1/14/20	10/34/112/115	-
27	CLA	4	613	17	1/1/15/20	12/37/115/115	-
29	LHG	H	204	-	-	17/53/53/53	-
27	CLA	B	810	-	1/1/14/20	15/35/113/115	-
29	LHG	W	2630	27	-	10/48/48/53	-
37	NEX	U	1623	-	-	4/27/83/83	0/3/3/3
27	CLA	3	606	-	1/1/13/20	6/23/101/115	-
27	CLA	a	608	-	1/1/11/20	3/11/89/115	-
33	LMG	J	104	-	-	15/35/55/70	0/1/1/1
35	LUT	Z	1620	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	828	-	1/1/15/20	15/37/115/115	-
27	CLA	8	612	21	1/1/10/20	2/8/86/115	-
27	CLA	4	609	17	1/1/13/20	4/28/106/115	-
38	CHL	V	607	-	3/3/16/26	2/15/113/137	-
38	CHL	Z	605	25	3/3/15/26	1/13/111/137	-
27	CLA	4	602	17	1/1/14/20	5/31/109/115	-
35	LUT	9	619	-	-	1/29/67/67	0/2/2/2
27	CLA	U	611	29	1/1/10/20	6/10/88/115	-
38	CHL	Y	601	24	3/3/20/26	22/39/137/137	-
27	CLA	4	610	17	1/1/14/20	8/33/111/115	-
27	CLA	8	602	21	1/1/14/20	8/31/109/115	-
27	CLA	B	806	2	1/1/15/20	16/37/115/115	-
35	LUT	V	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	6	611	29	1/1/10/20	2/10/88/115	-
30	BCR	A	851	-	-	2/29/63/63	0/2/2/2
27	CLA	A	837	1	-	9/13/91/115	-
27	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
27	CLA	K	203	-	-	6/27/105/115	-
27	CLA	A	816	-	1/1/15/20	10/37/115/115	-
27	CLA	2	614	-	1/1/10/20	0/9/87/115	-
29	LHG	Z	2630	27	-	17/53/53/53	-
30	BCR	B	852	-	-	7/29/63/63	0/2/2/2
29	LHG	4	622	27	-	10/53/53/53	-
27	CLA	5	604	-	1/1/15/20	18/35/111/115	-
30	BCR	3	622	-	-	2/29/63/63	0/2/2/2
38	CHL	U	607	-	3/3/16/26	5/15/113/137	-
35	LUT	5	620	-	-	1/29/67/67	0/2/2/2
35	LUT	W	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	8	604	-	1/1/12/20	4/19/97/115	-
27	CLA	7	613	20	1/1/15/20	11/37/115/115	-
38	CHL	W	607	-	3/3/20/26	25/37/135/137	-
27	CLA	1	614	-	1/1/9/20	2/4/76/115	-
27	CLA	A	813	-	1/1/12/20	6/24/102/115	-
29	LHG	5	623	27	-	14/53/53/53	-
27	CLA	A	814	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	616	14	1/1/11/20	5/13/91/115	-
31	SF4	C	102	3	-	-	0/6/5/5
27	CLA	5	614	-	1/1/10/20	8/13/87/115	-
27	CLA	8	603	-	1/1/11/20	4/13/89/115	-
27	CLA	7	609	20	1/1/10/20	4/10/88/115	-
27	CLA	2	613	15	1/1/15/20	7/37/115/115	-
30	BCR	B	853	-	-	4/29/63/63	0/2/2/2
30	BCR	A	849	-	-	5/29/63/63	0/2/2/2
30	BCR	K	202	-	-	4/29/63/63	0/2/2/2
27	CLA	9	613	22	1/1/15/20	6/37/115/115	-
27	CLA	5	608	-	1/1/12/20	6/19/97/115	-
33	LMG	J	103	-	-	5/37/57/70	0/1/1/1
27	CLA	V	613	26	1/1/15/20	18/37/115/115	-
27	CLA	3	604	-	1/1/15/20	9/37/115/115	-
27	CLA	5	618	18	1/1/10/20	0/8/84/115	-
27	CLA	U	604	-	1/1/10/20	6/18/92/115	-
36	XAT	X	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	7	601	20	1/1/14/20	10/31/109/115	-
27	CLA	2	610	15	1/1/13/20	8/25/103/115	-
36	XAT	a	618	-	-	0/31/93/93	0/4/4/4
30	BCR	B	845	-	-	9/29/63/63	0/2/2/2
27	CLA	8	613	21	1/1/15/20	14/37/115/115	-
27	CLA	W	602	23	1/1/14/20	7/31/109/115	-
27	CLA	A	833	-	1/1/11/20	5/13/91/115	-
27	CLA	7	607	-	1/1/10/20	2/10/88/115	-
27	CLA	B	827	-	1/1/14/20	17/34/112/115	-
27	CLA	4	618	17	1/1/10/20	2/8/84/115	-
27	CLA	L	306	-	1/1/10/20	0/6/84/115	-
27	CLA	9	610	22	1/1/13/20	5/28/106/115	-
27	CLA	7	610	20	1/1/15/20	2/37/115/115	-
27	CLA	2	616	-	1/1/11/20	4/11/87/115	-
27	CLA	3	608	-	1/1/13/20	2/25/103/115	-
27	CLA	A	825	-	1/1/15/20	19/37/115/115	-
35	LUT	a	617	-	-	0/29/67/67	0/2/2/2
27	CLA	Z	613	25	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	7	606	-	-	2/8/86/115	-
27	CLA	B	812	-	1/1/10/20	3/11/89/115	-
27	CLA	F	304	6	-	4/8/86/115	-
27	CLA	1	601	14	-	2/23/101/115	-
27	CLA	B	807	-	-	1/22/100/115	-
30	BCR	7	623	-	-	4/29/63/63	0/2/2/2
38	CHL	Z	608	-	3/3/16/26	6/20/118/137	-

The worst 5 of 3112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	844	PQN	C12-C13	9.80	1.56	1.33
28	B	842	PQN	C12-C13	9.64	1.56	1.33
27	X	602	CLA	C4B-NB	8.26	1.42	1.35
27	Y	610	CLA	C4B-NB	8.25	1.42	1.35
27	X	610	CLA	C4B-NB	8.24	1.42	1.35

The worst 5 of 4865 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	W	606	CHL	O2A-CGA-O1A	-17.62	79.39	123.30
30	B	852	BCR	C32-C1-C6	-14.75	86.38	110.30
38	W	606	CHL	O2A-CGA-CBA	14.42	160.37	114.03
30	6	622	BCR	C40-C30-C25	-14.02	87.56	110.30
36	U	1622	XAT	C37-C21-C36	-14.00	86.72	107.37

5 of 379 chirality outliers are listed below:

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

5 of 3214 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	801	CLA	CBD-CGD-O2D-CED
27	A	801	CLA	O1D-CGD-O2D-CED

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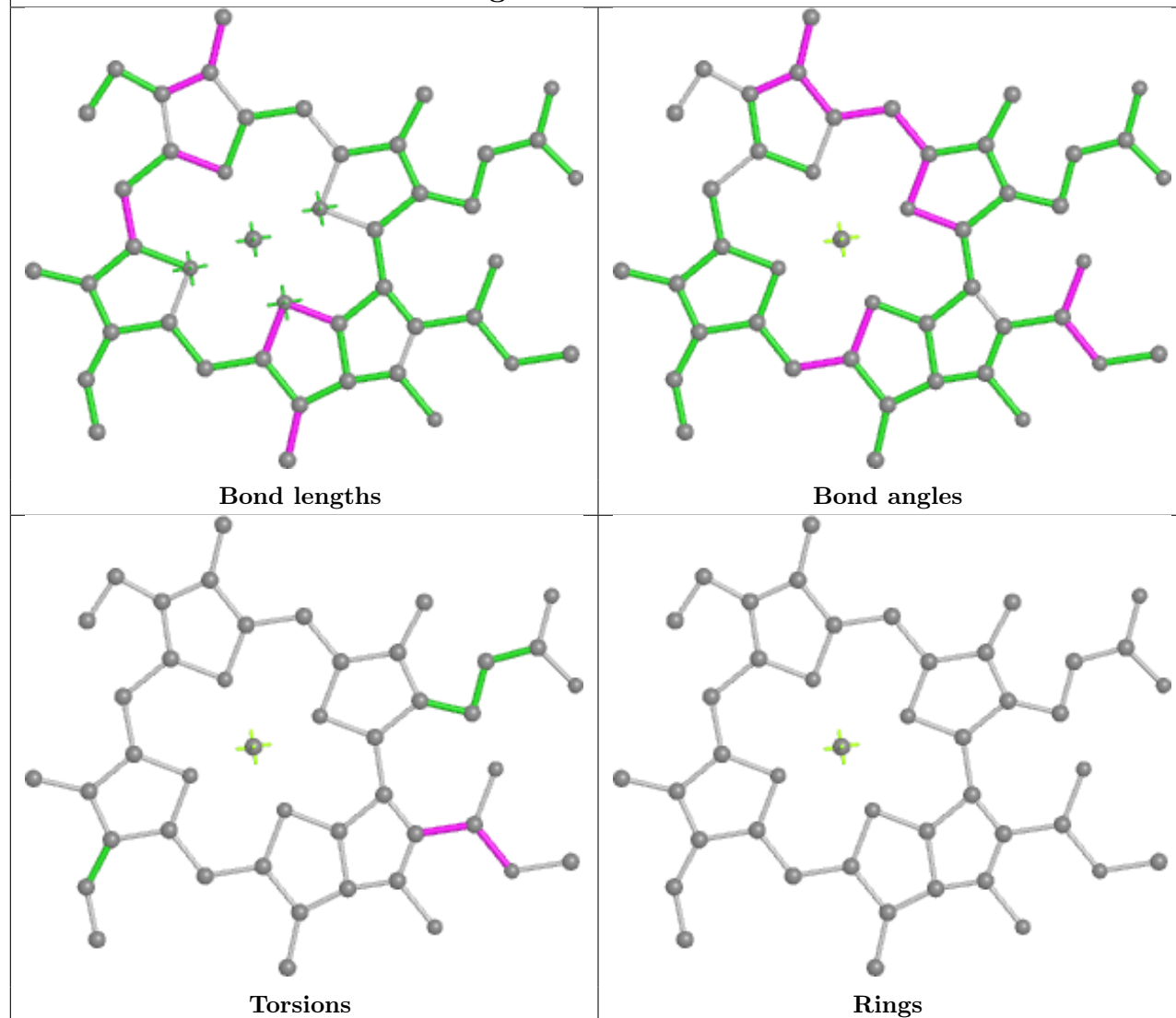
Mol	Chain	Res	Type	Atoms
27	A	804	CLA	C1A-C2A-CAA-CBA
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27	A	805	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

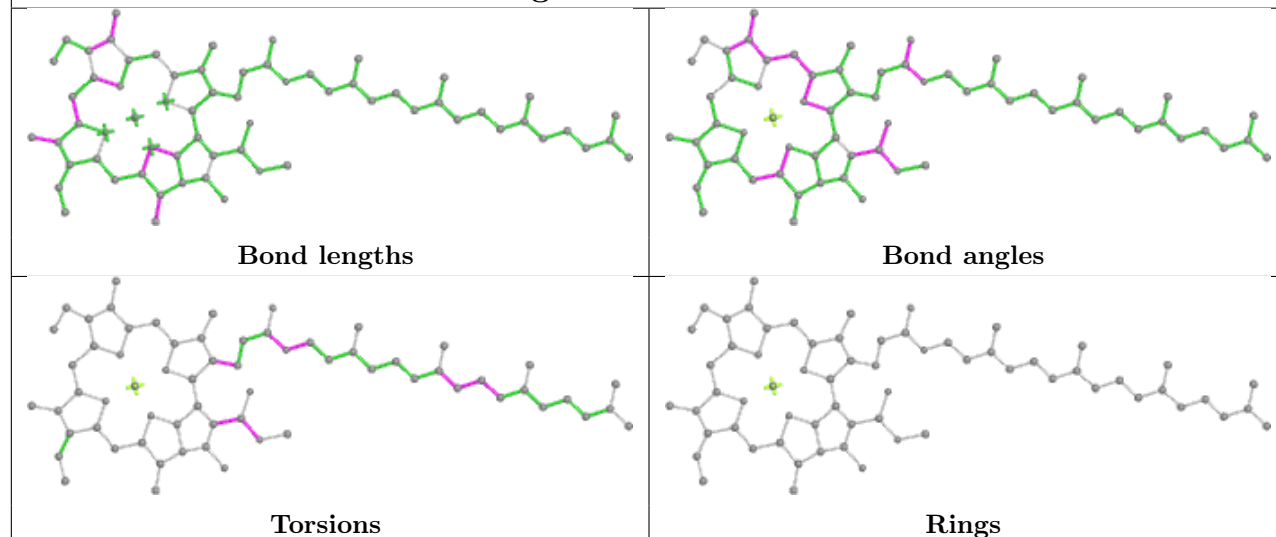
No monomer is involved in short contacts.

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.

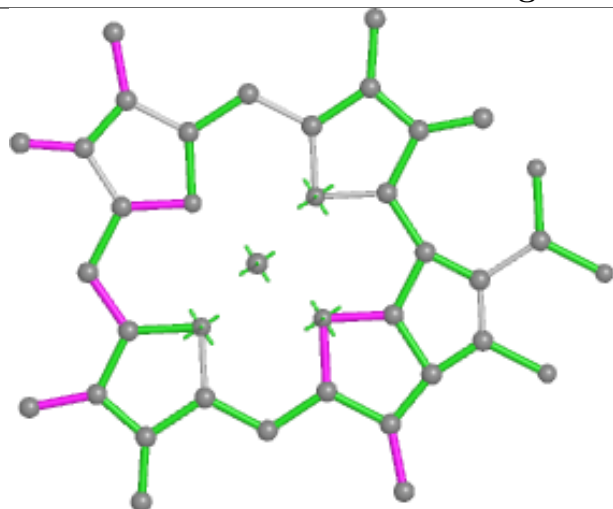
Ligand CLA K 206



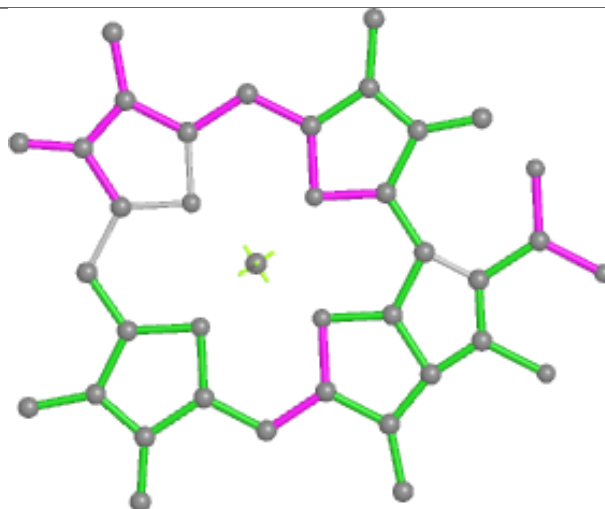
Ligand CLA A 811



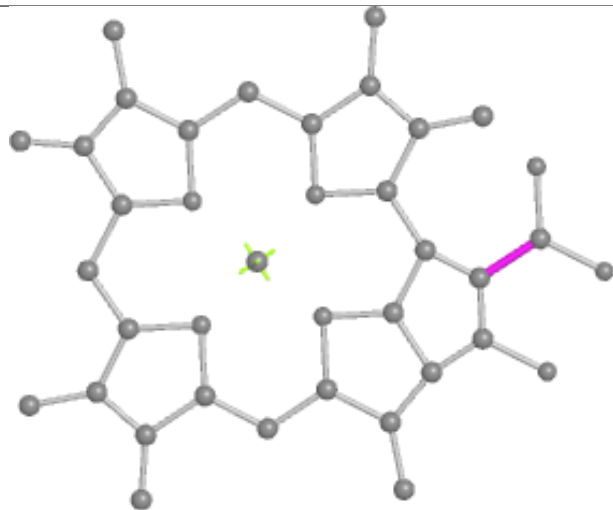
Ligand CLA a 611



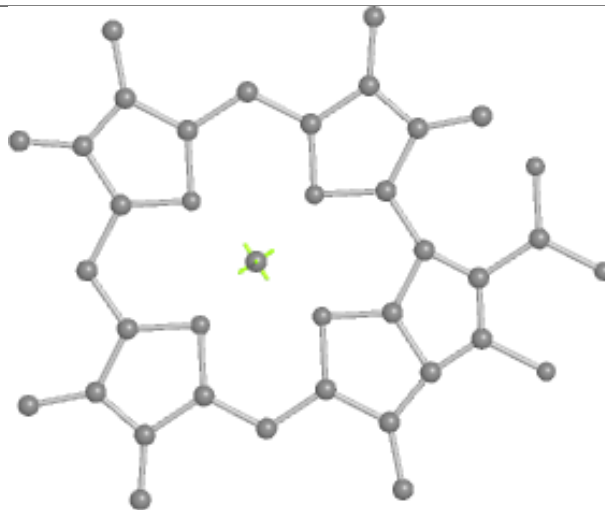
Bond lengths



Bond angles

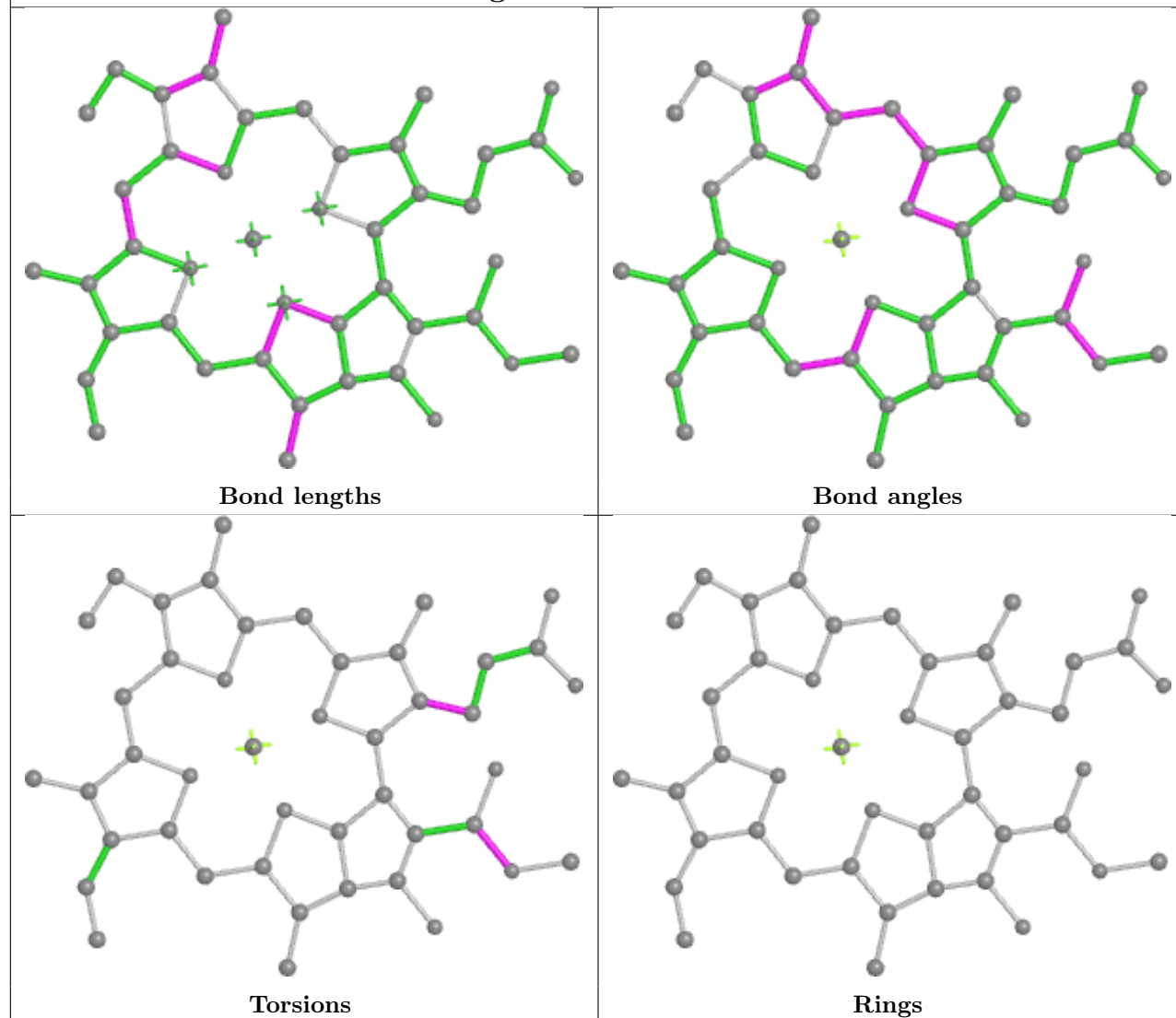


Torsions

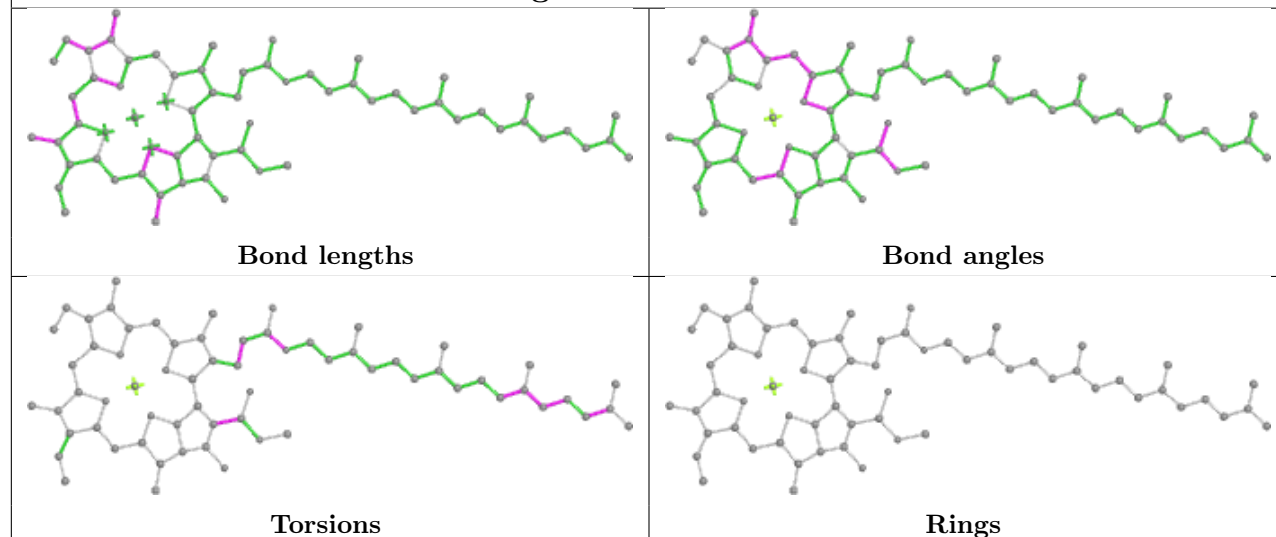


Rings

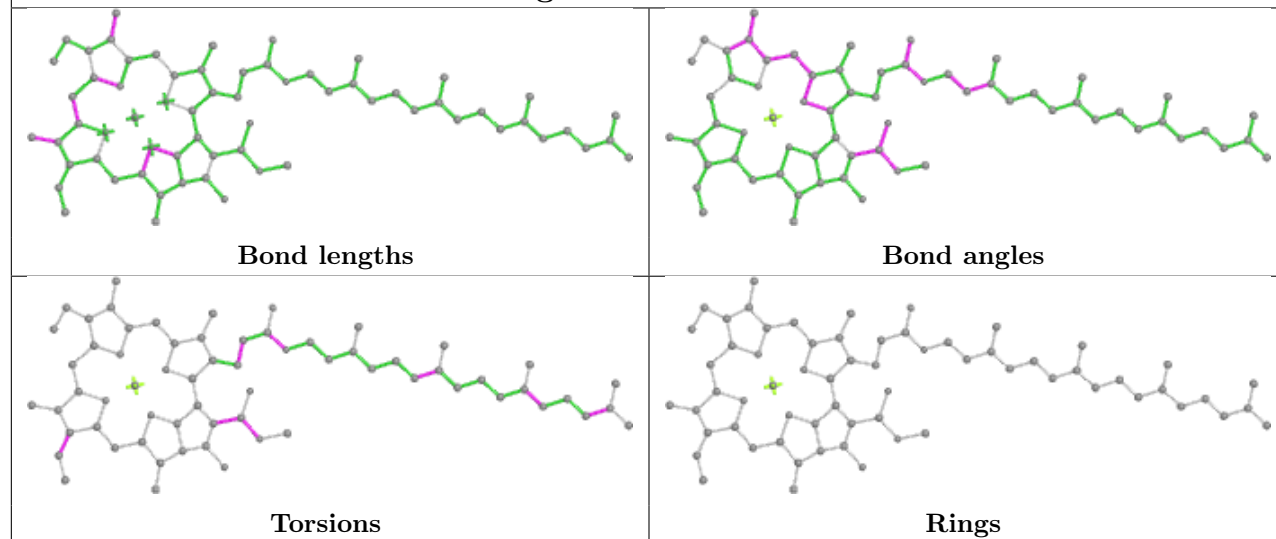
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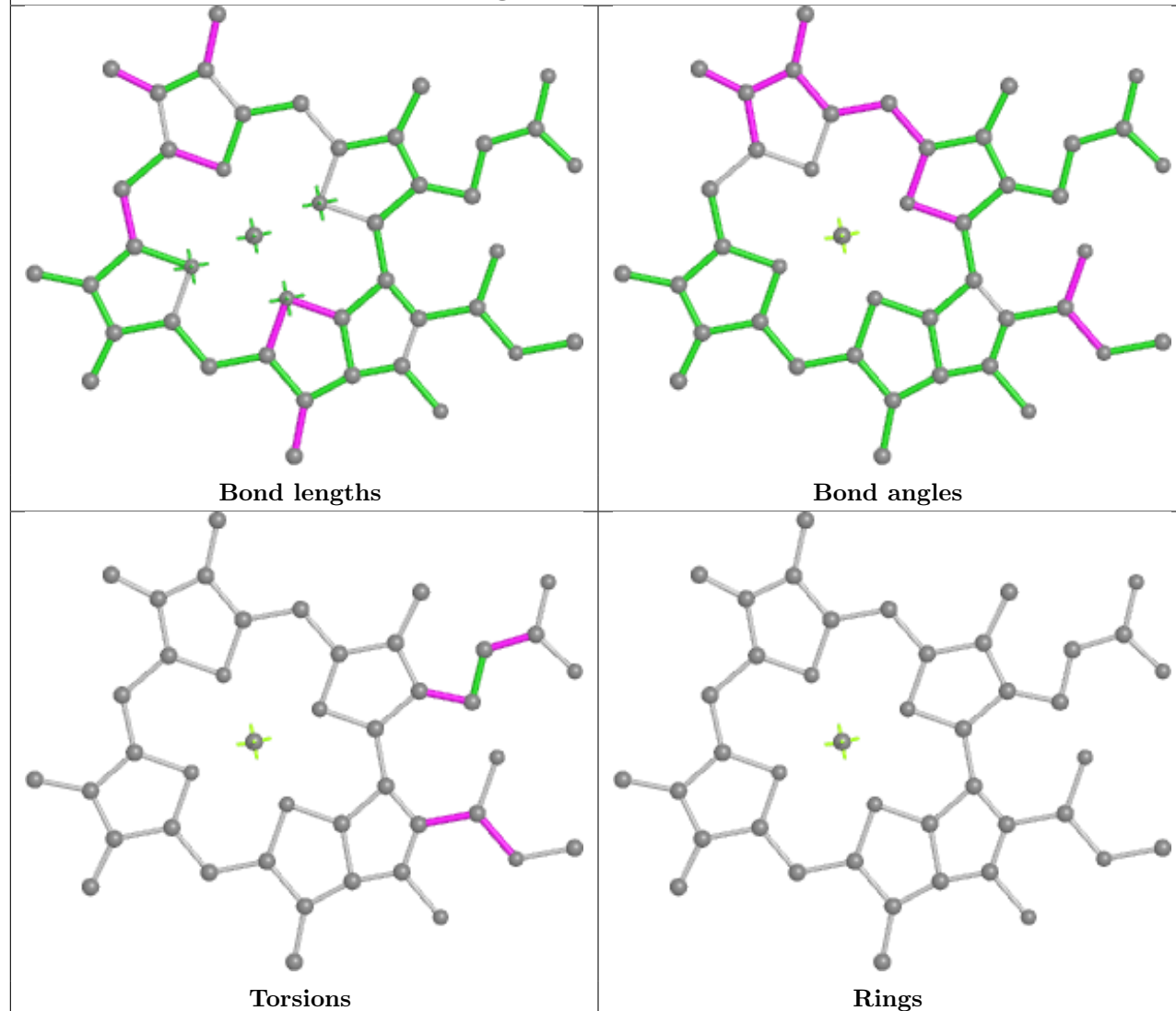
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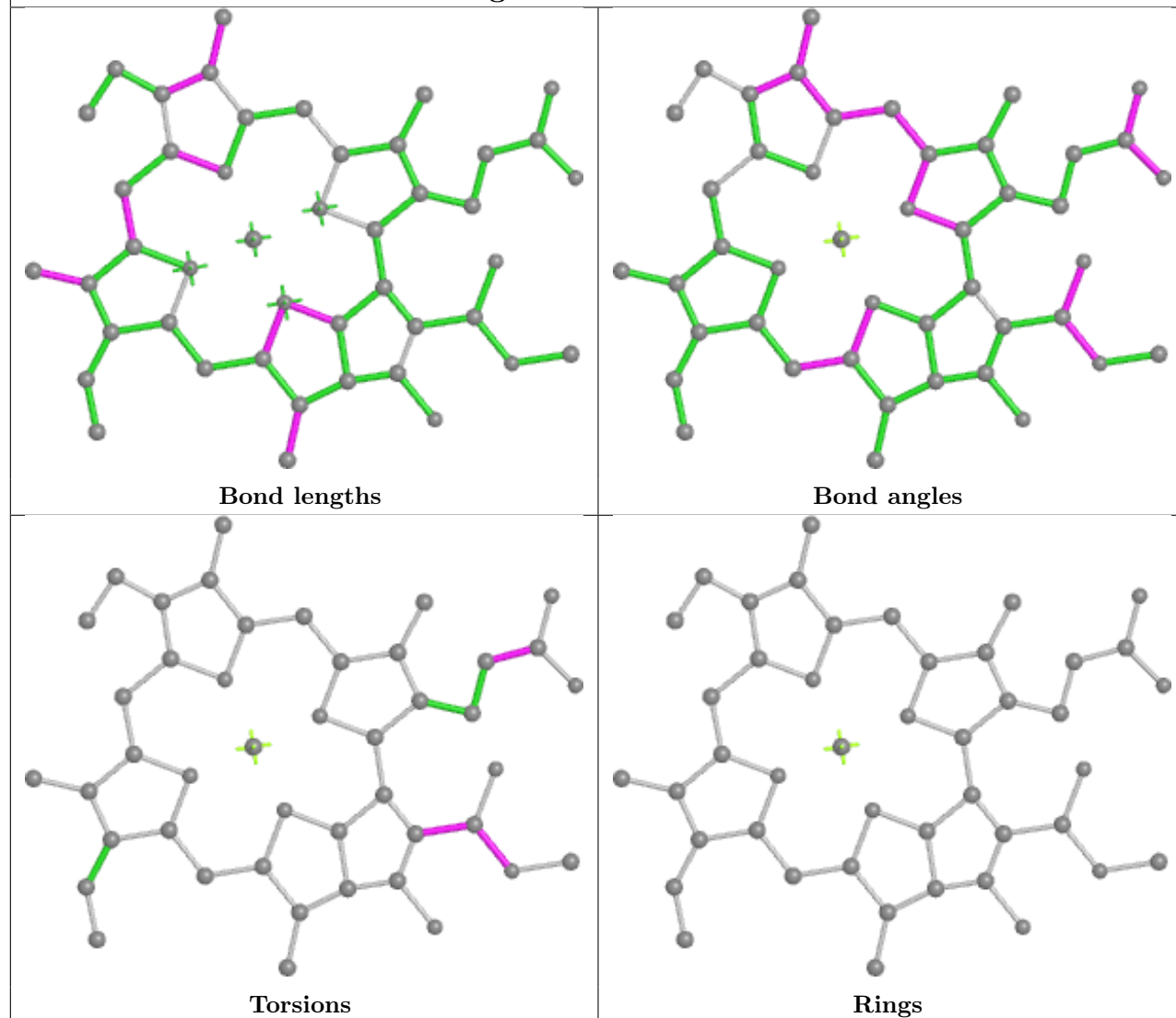
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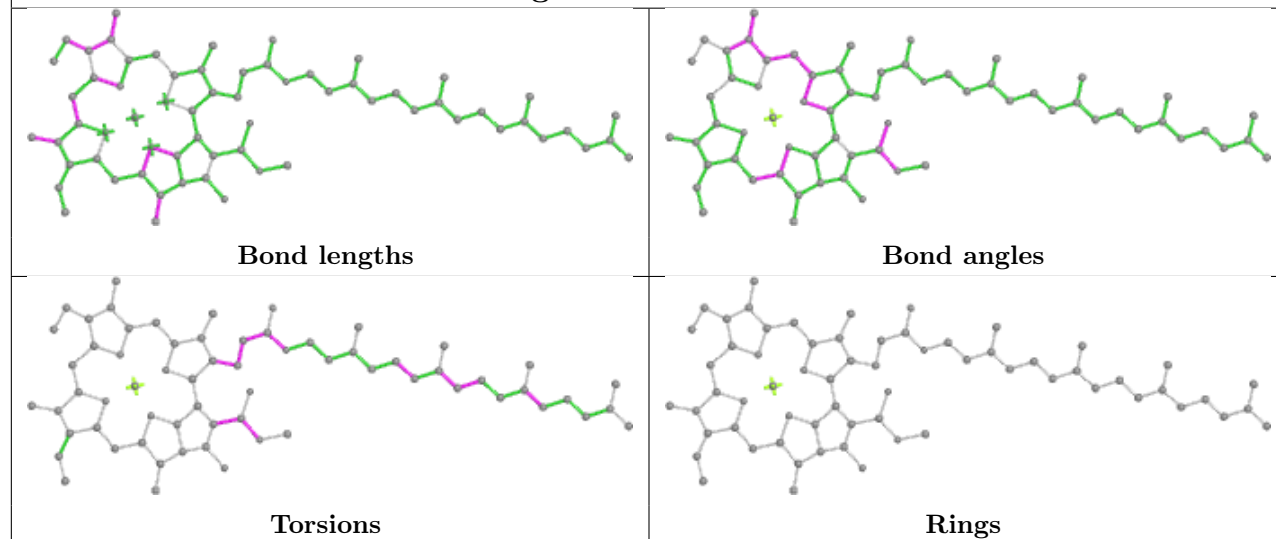
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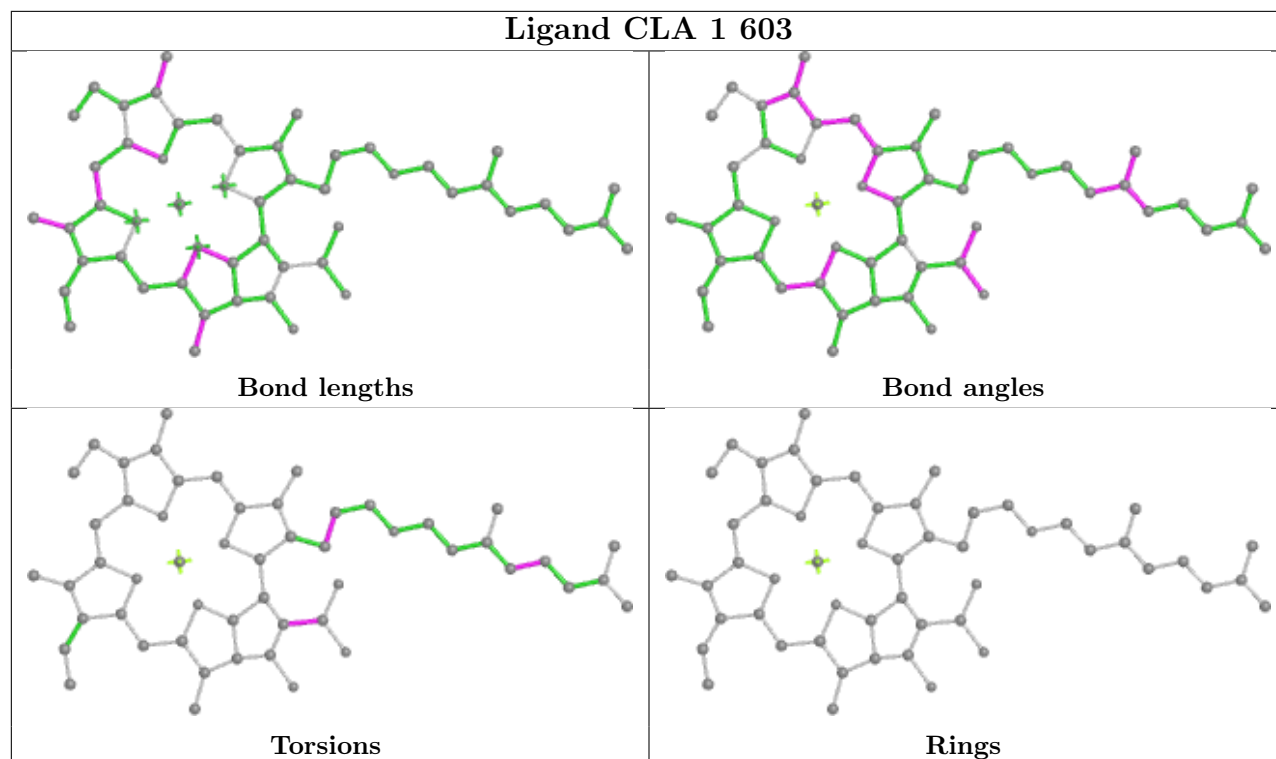
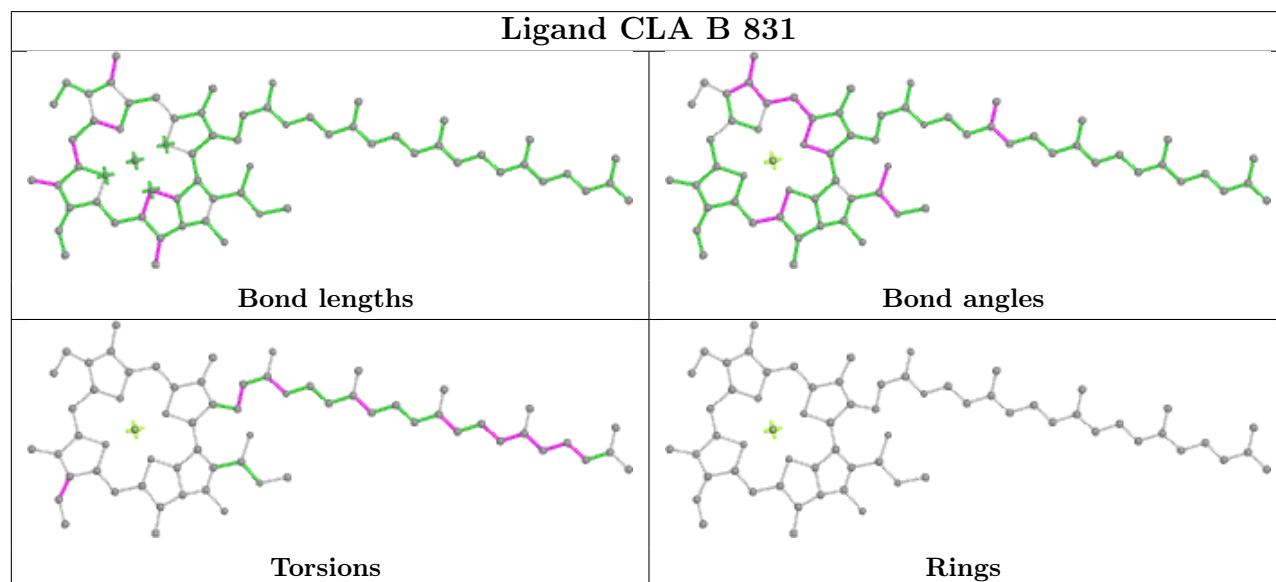


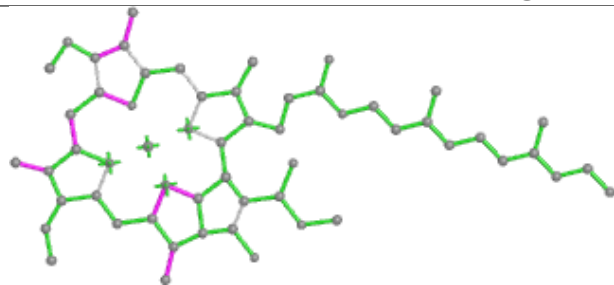
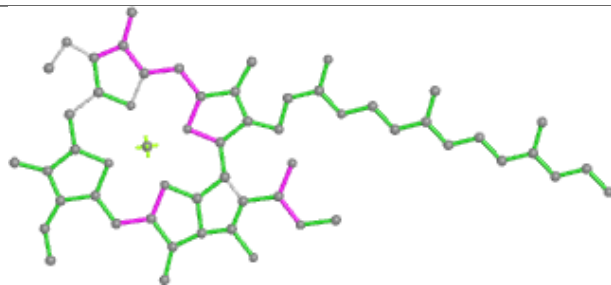
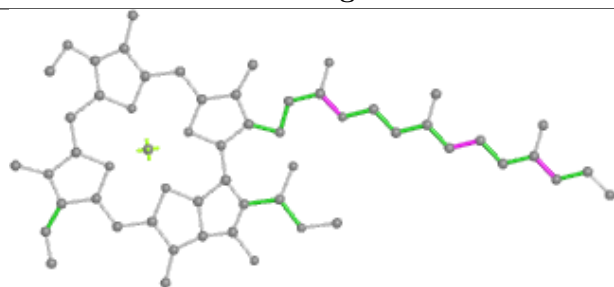
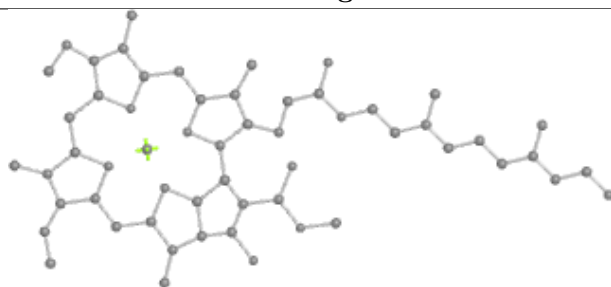
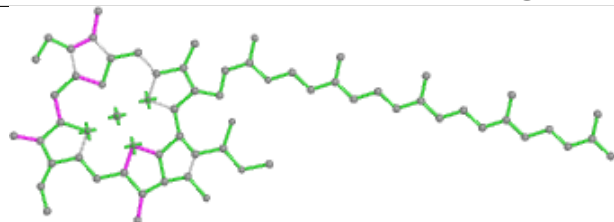
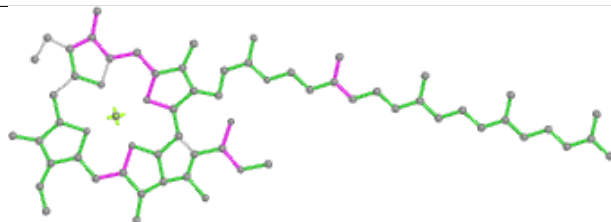
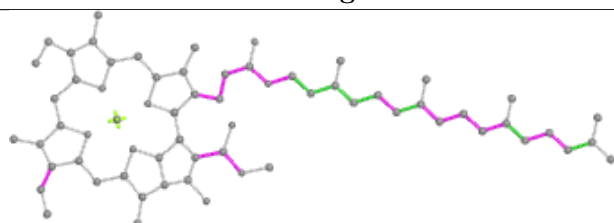
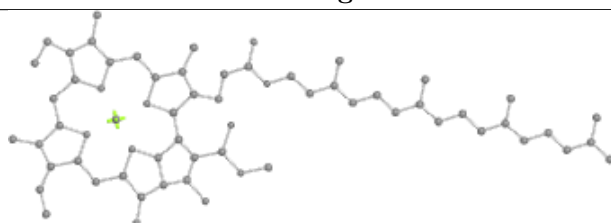
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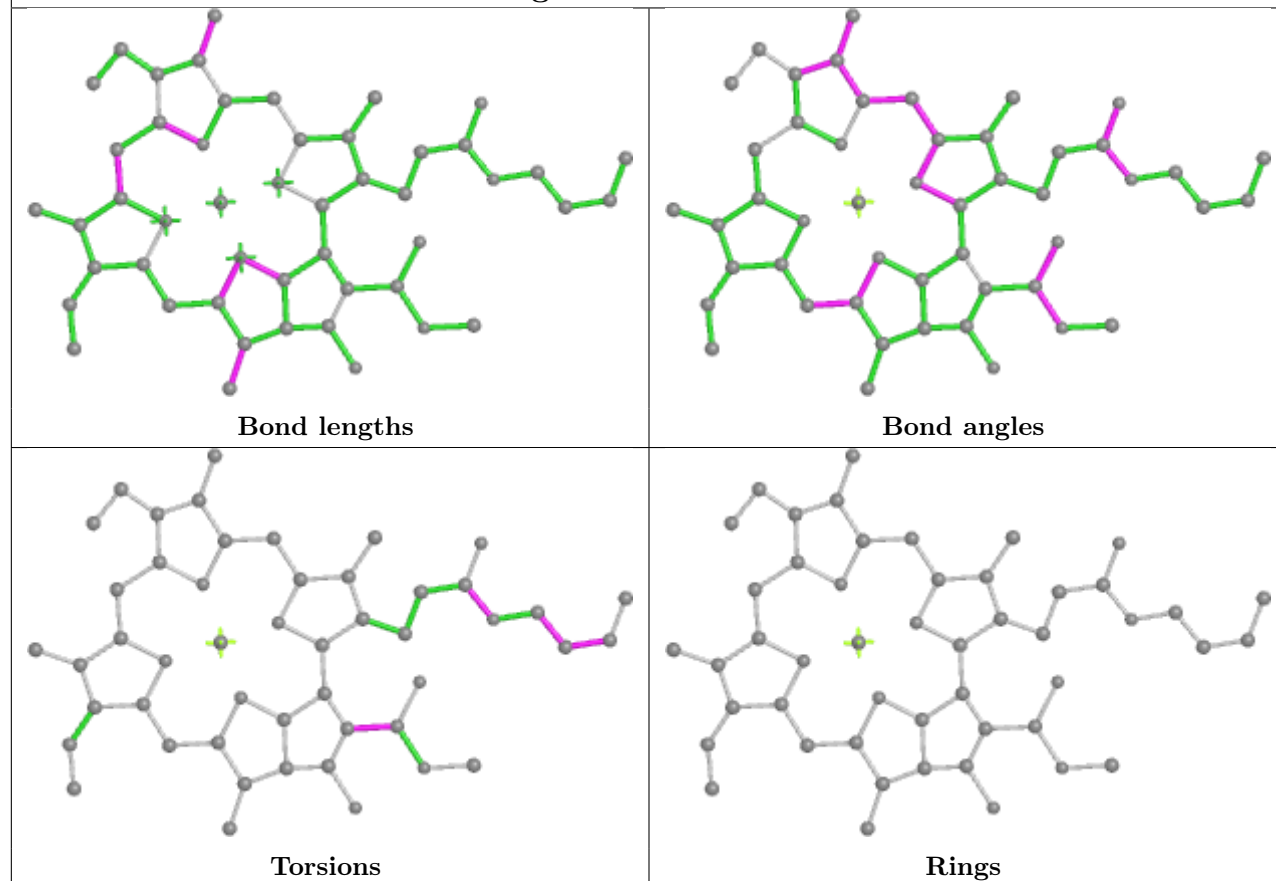
Ligand CLA A 841



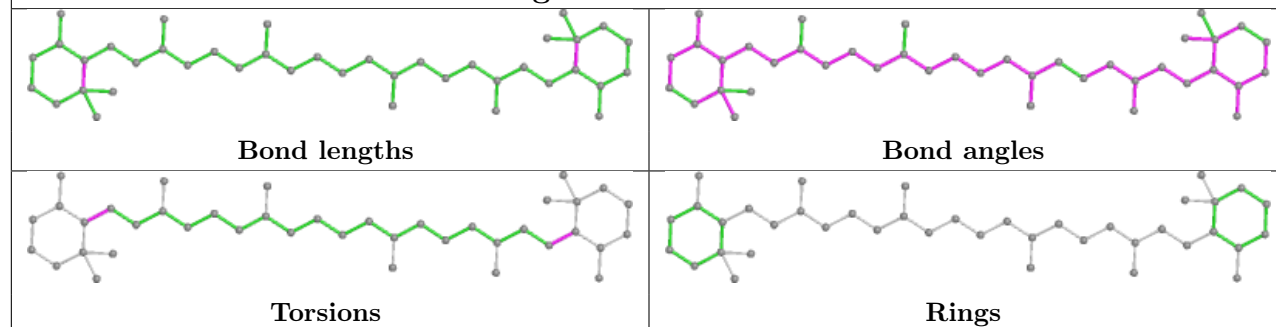
Ligand CLA 1 603**Ligand CLA B 831**

Ligand CLA 1 611**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 6 616****Bond lengths****Bond angles****Torsions****Rings**

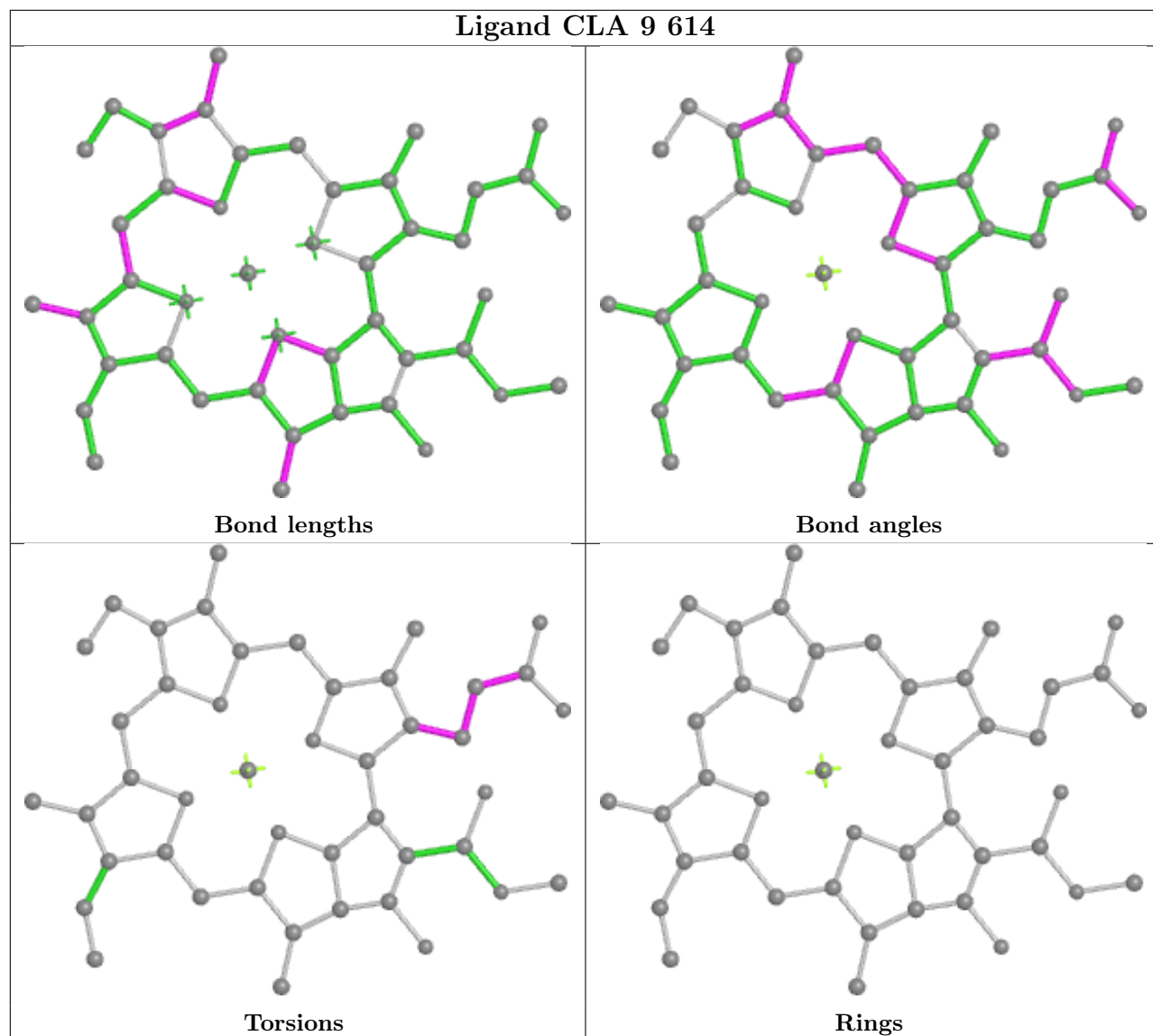
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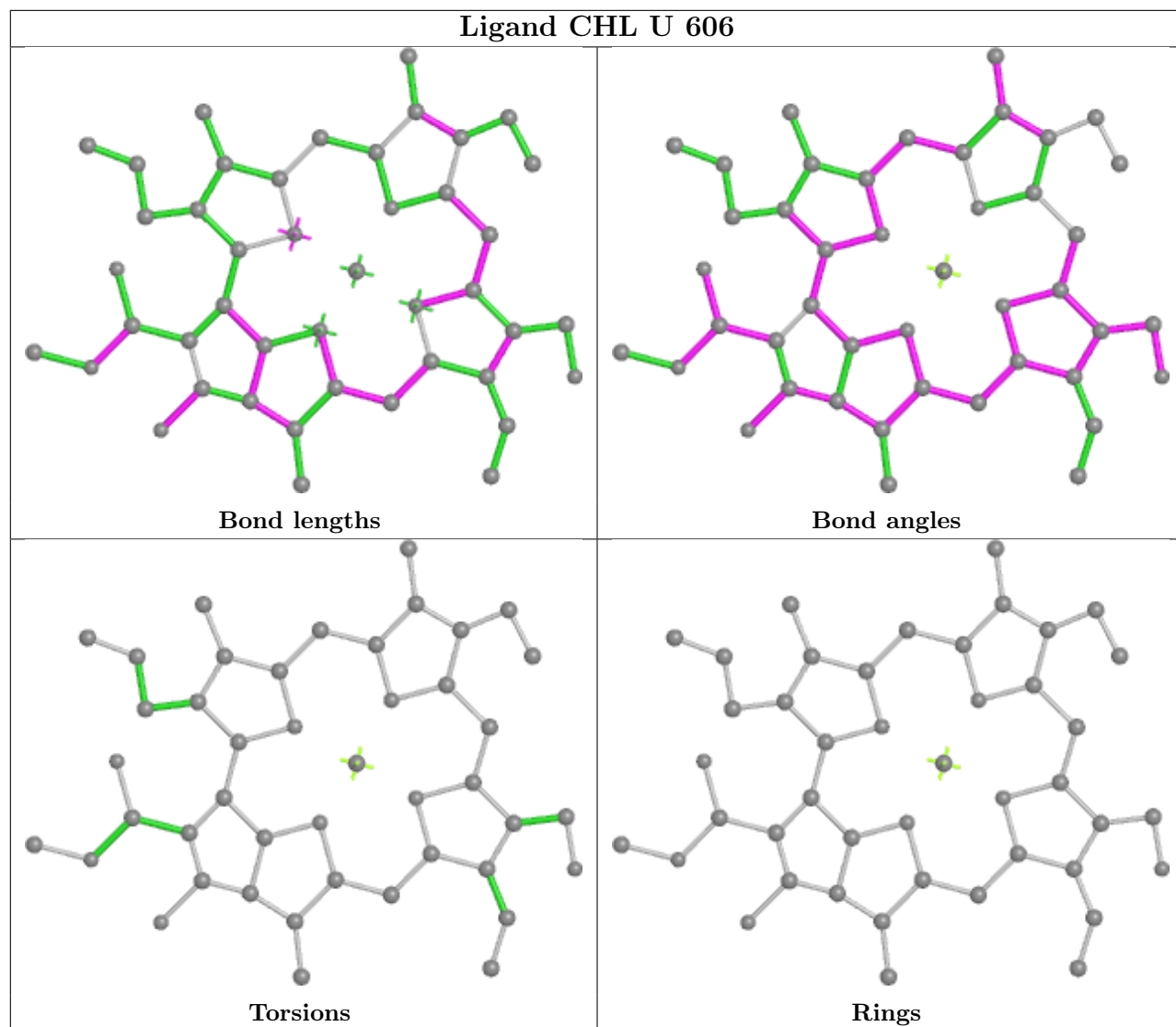


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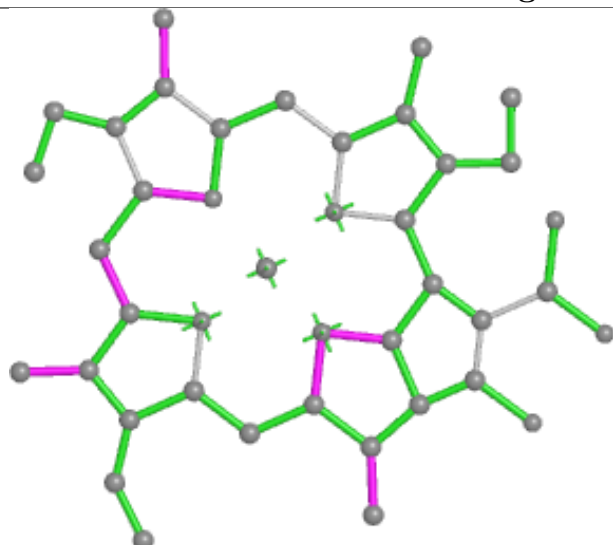


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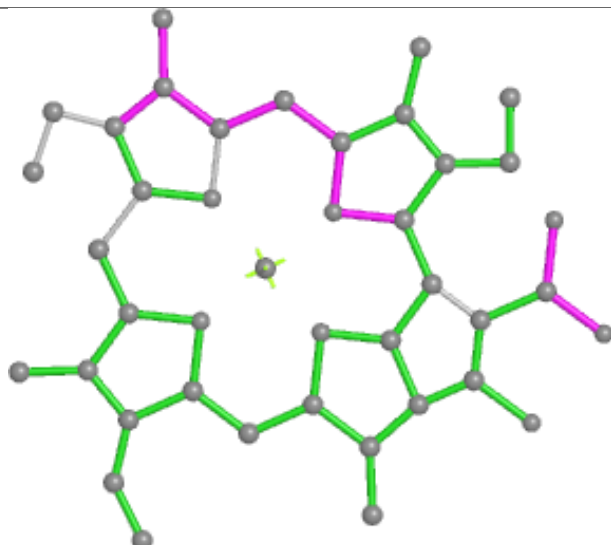




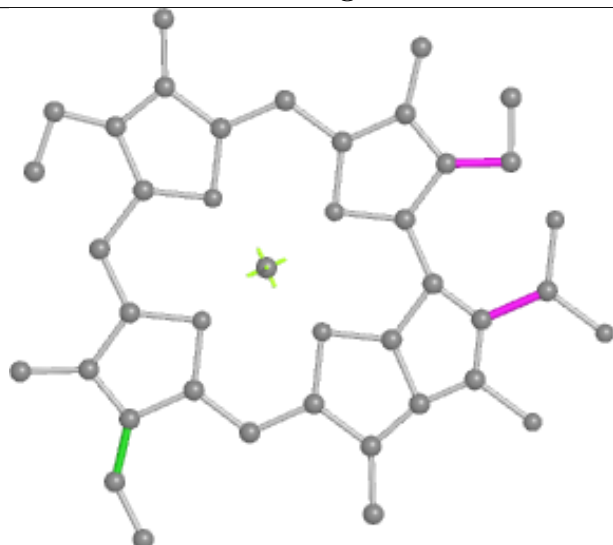
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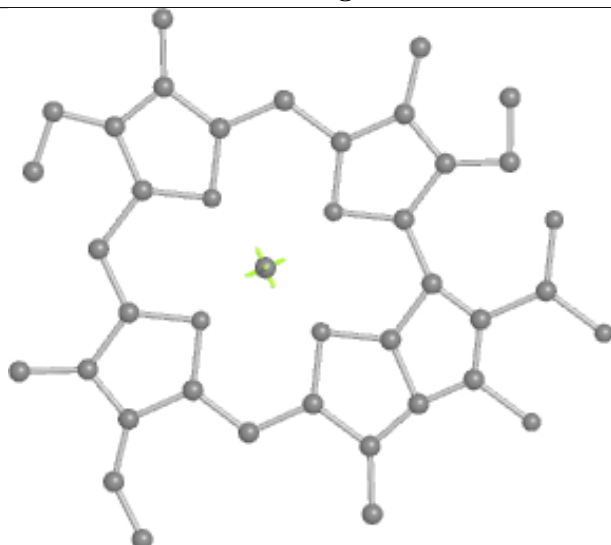
Bond lengths



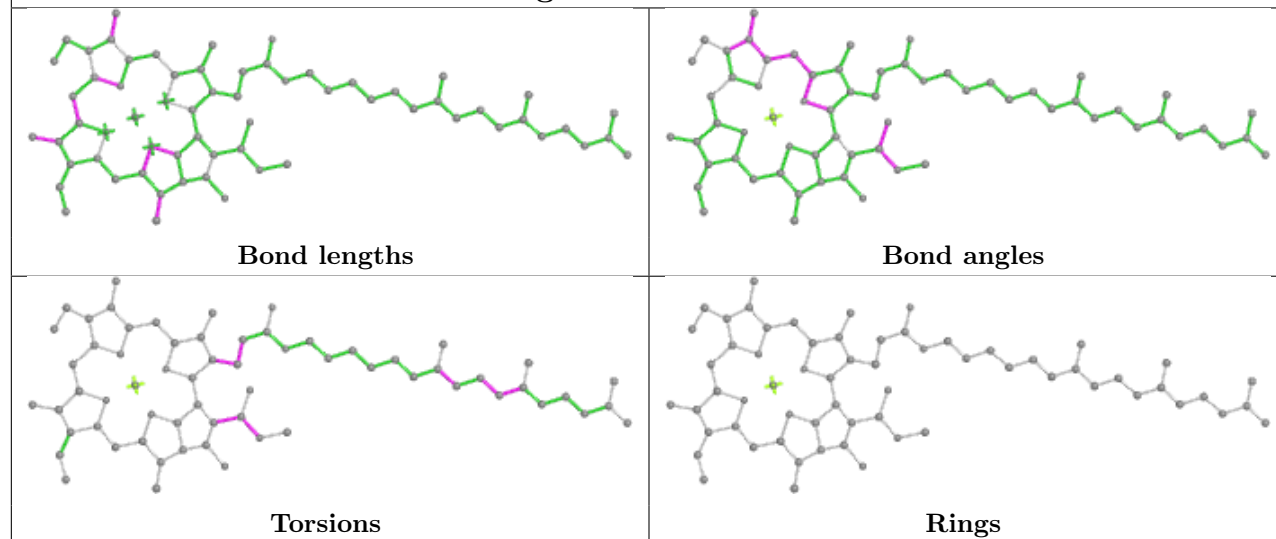
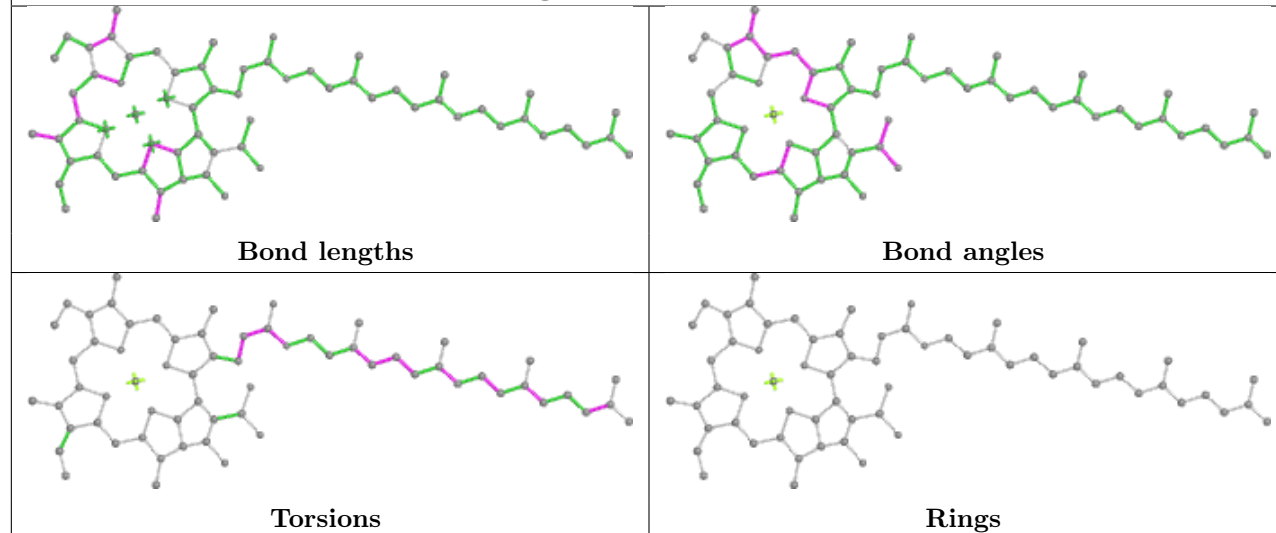
Bond angles



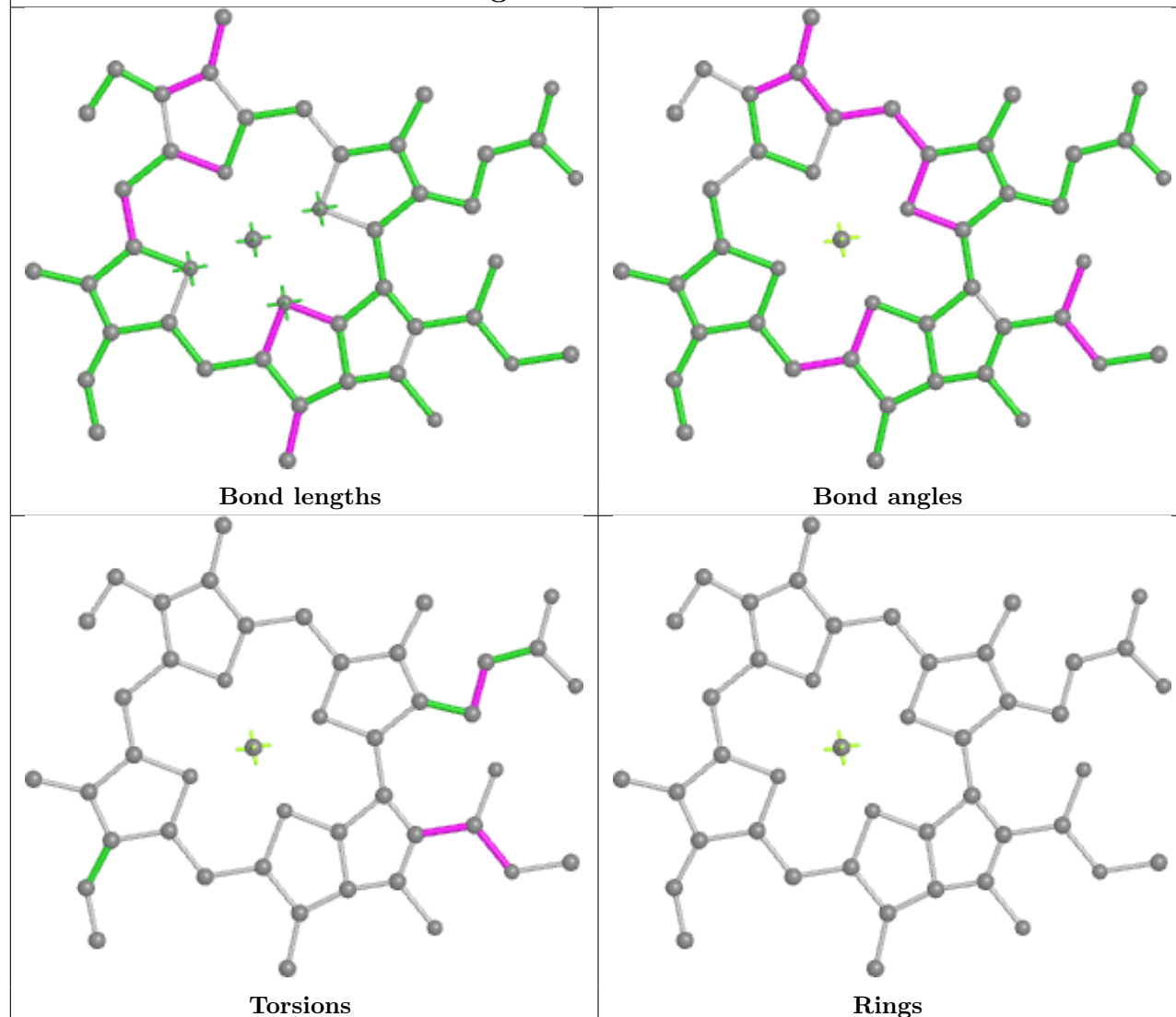
Torsions



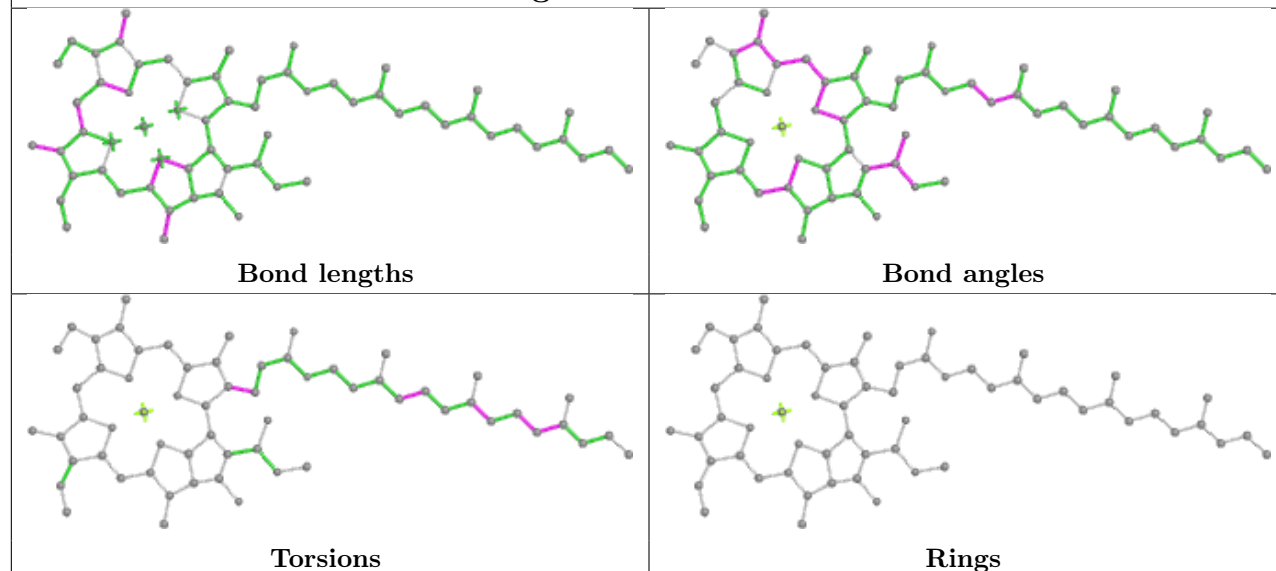
Rings

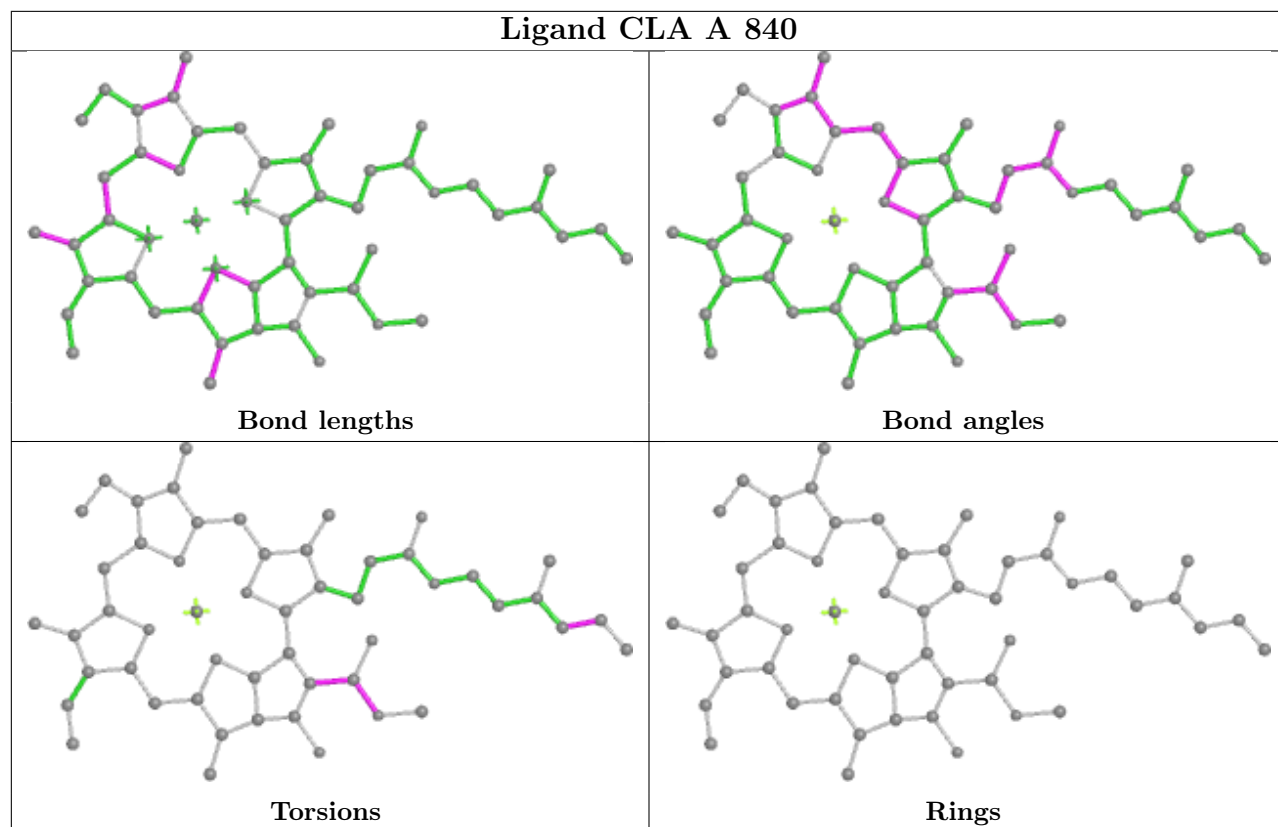
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Ligand CLA B 835

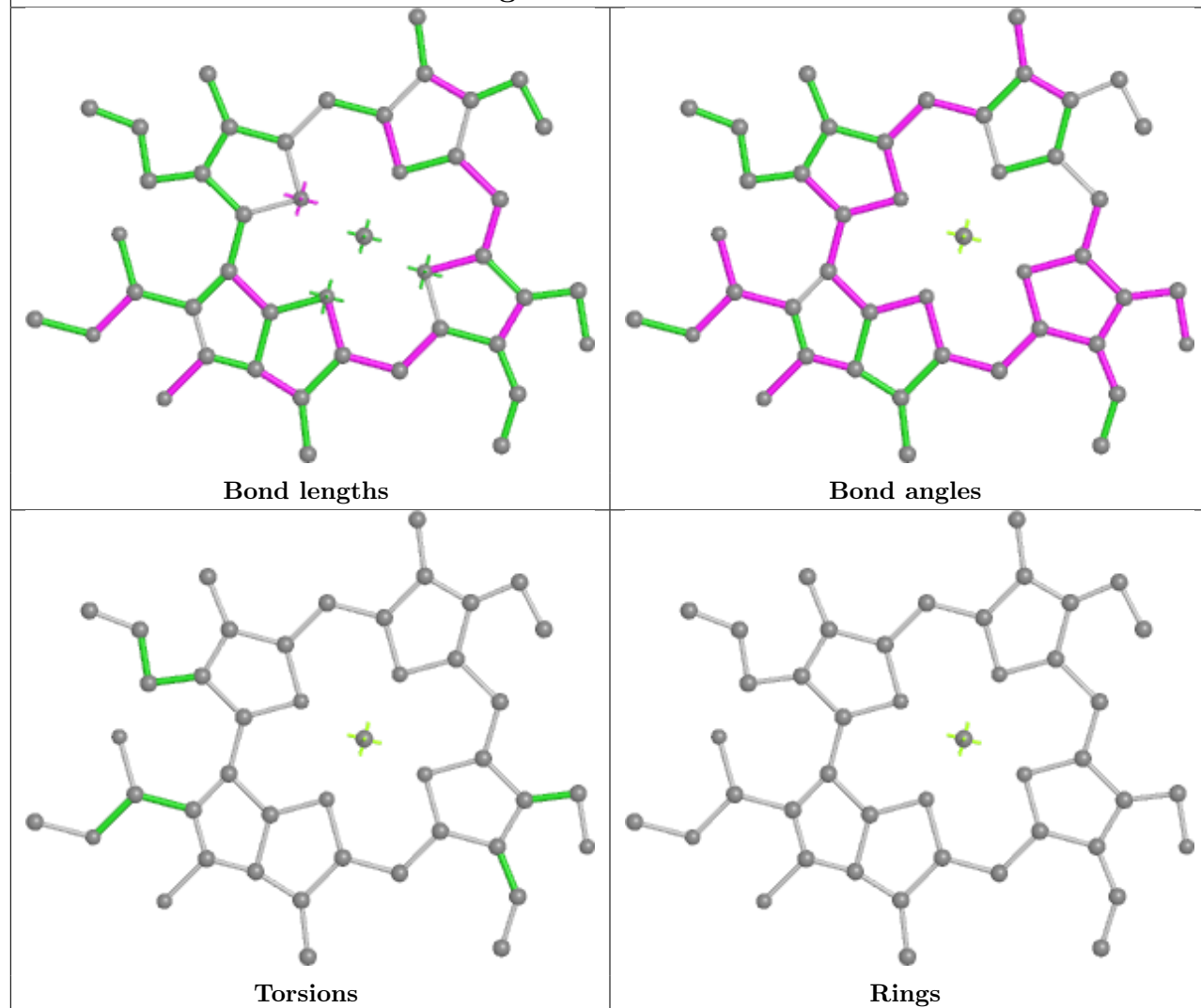


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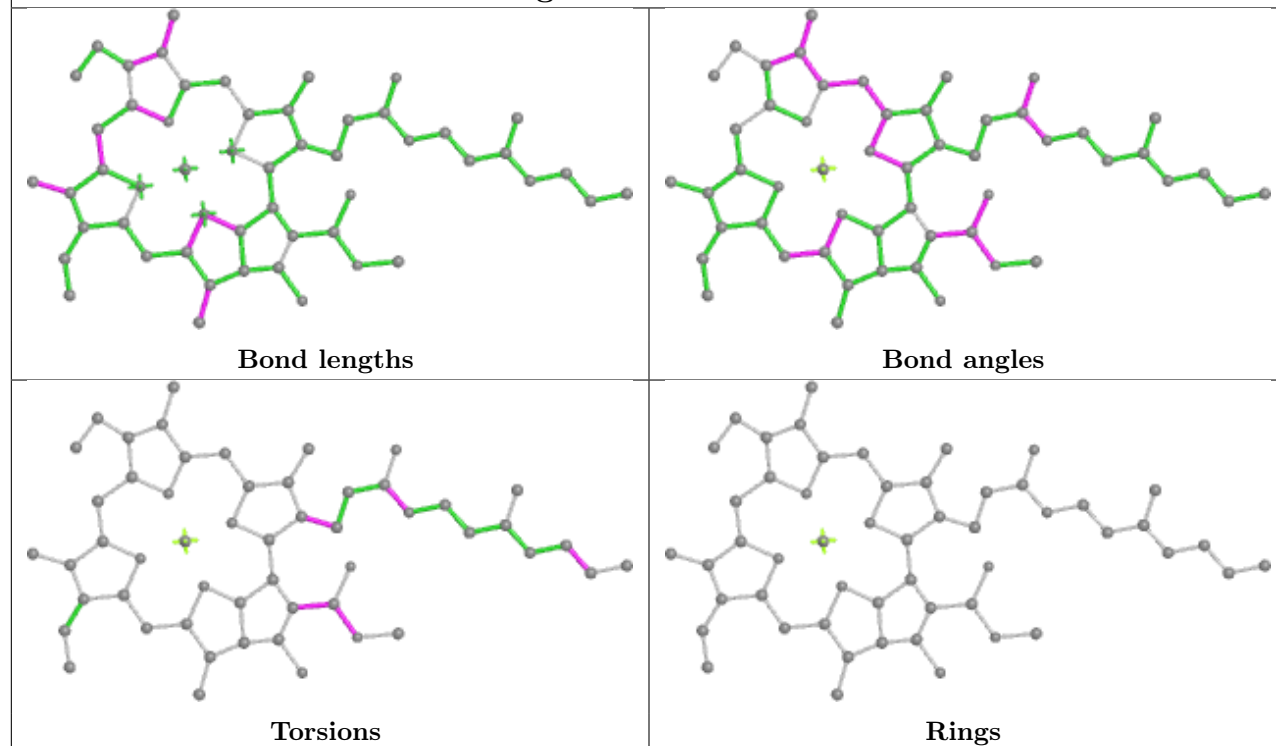




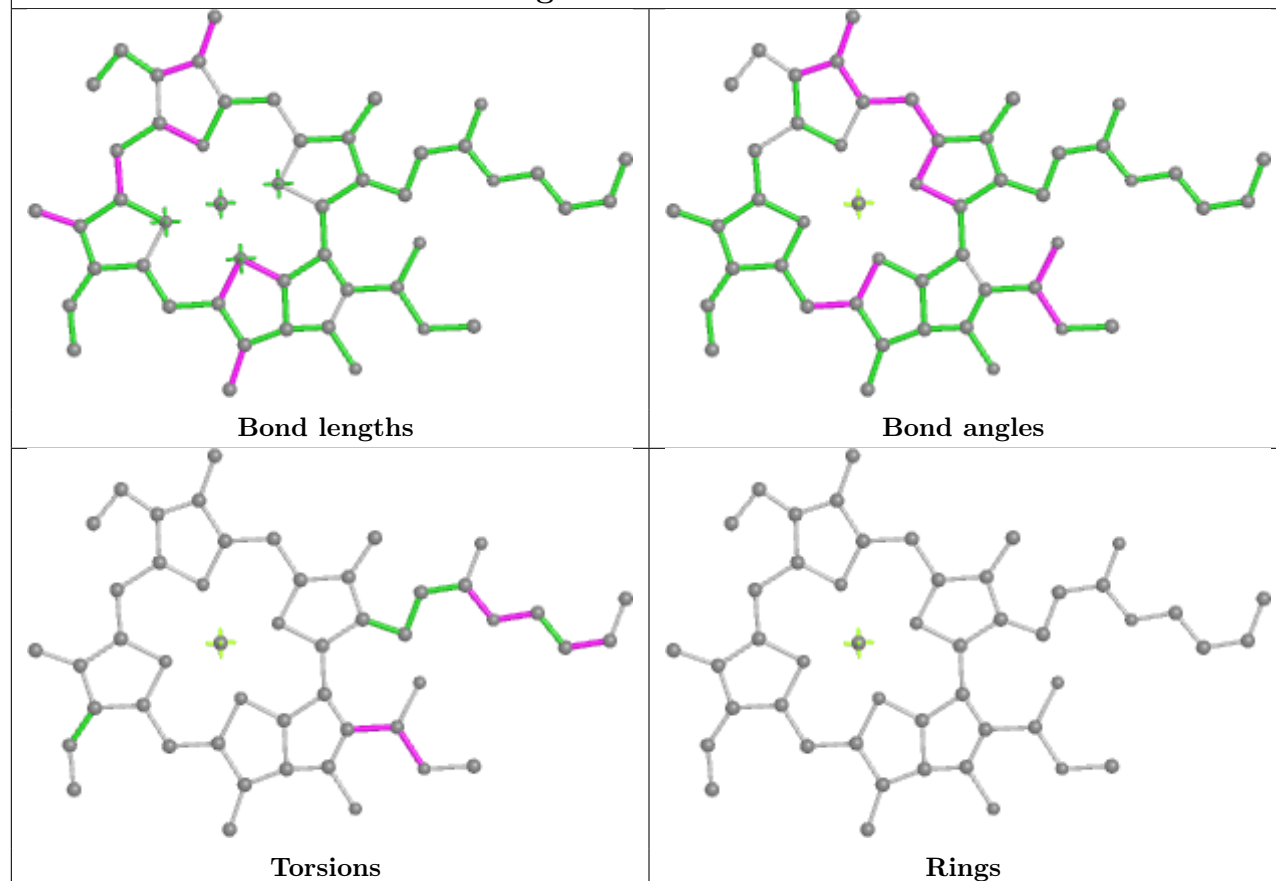
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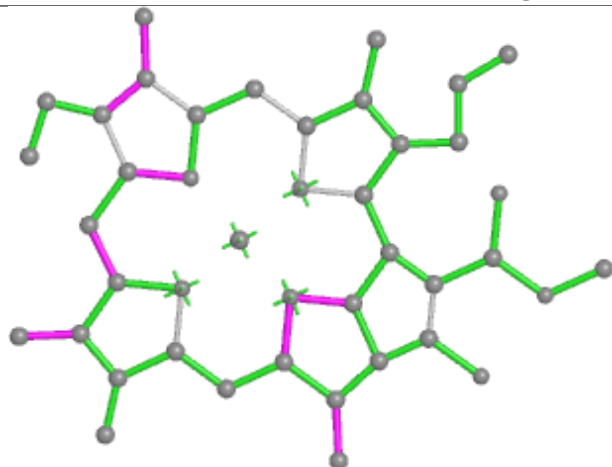
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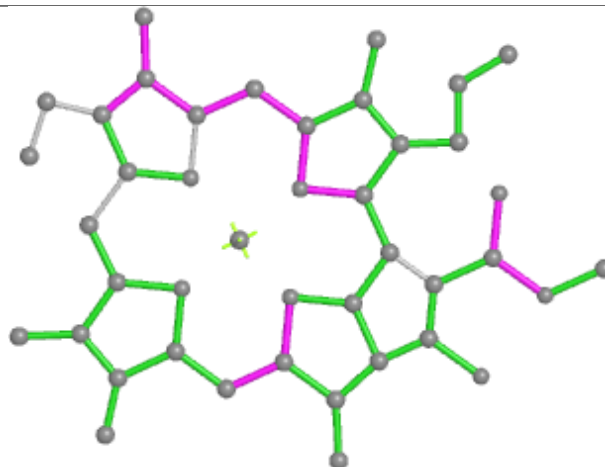
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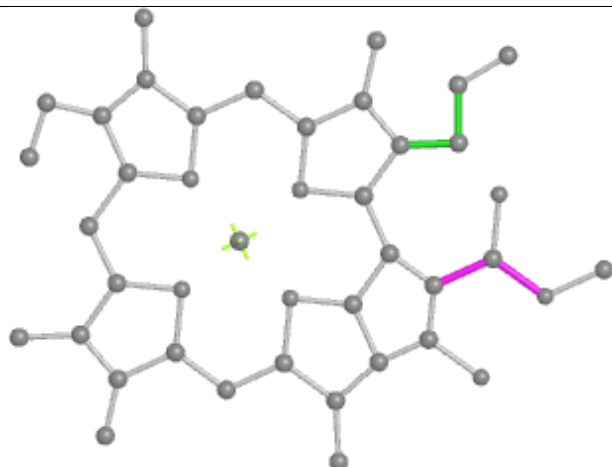
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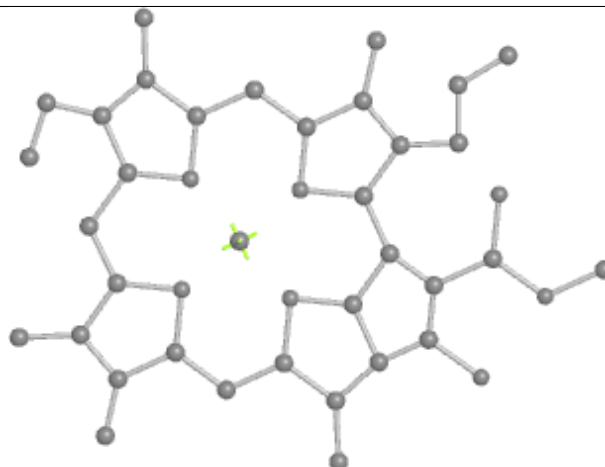
Bond lengths



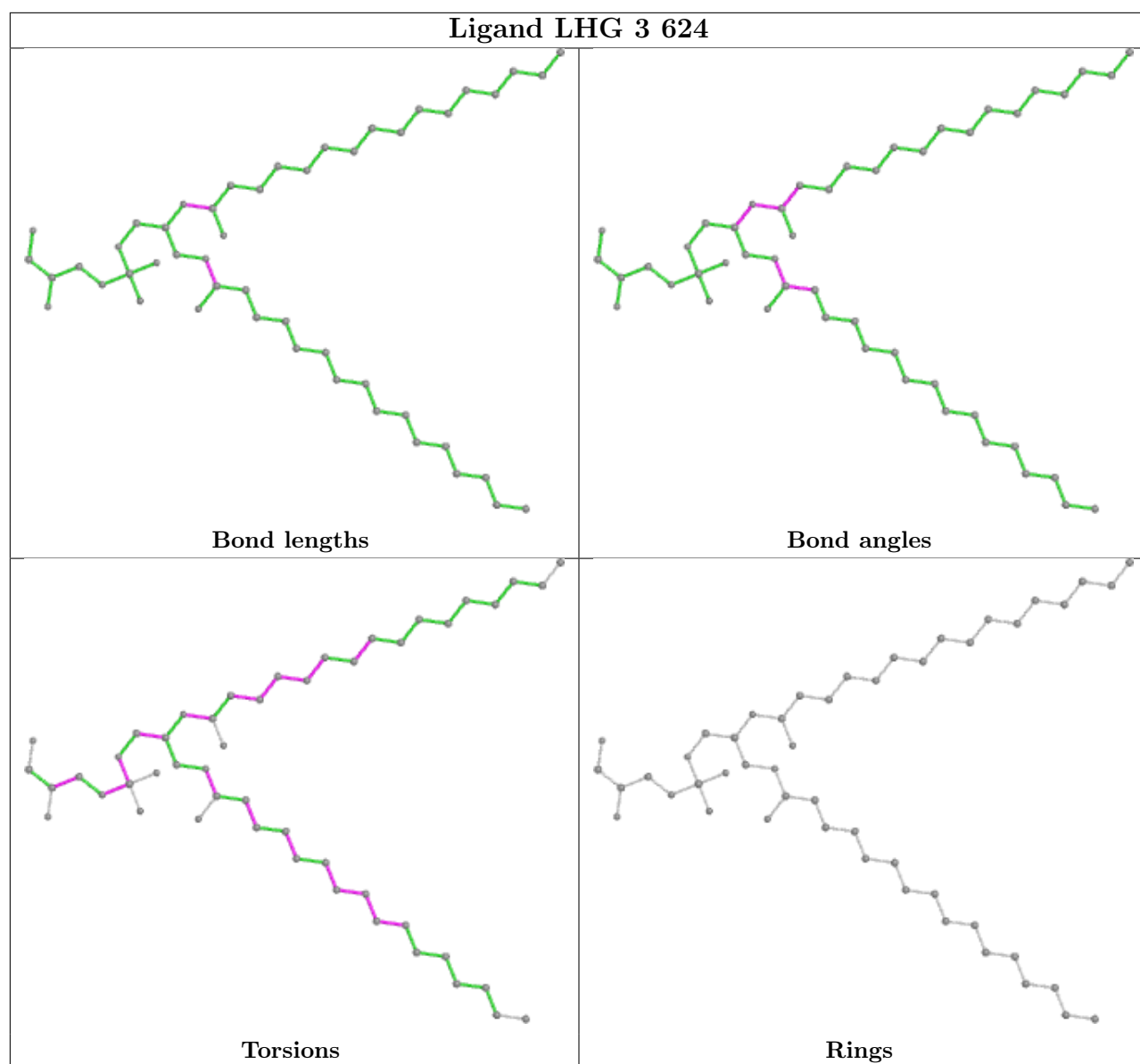
Bond angles

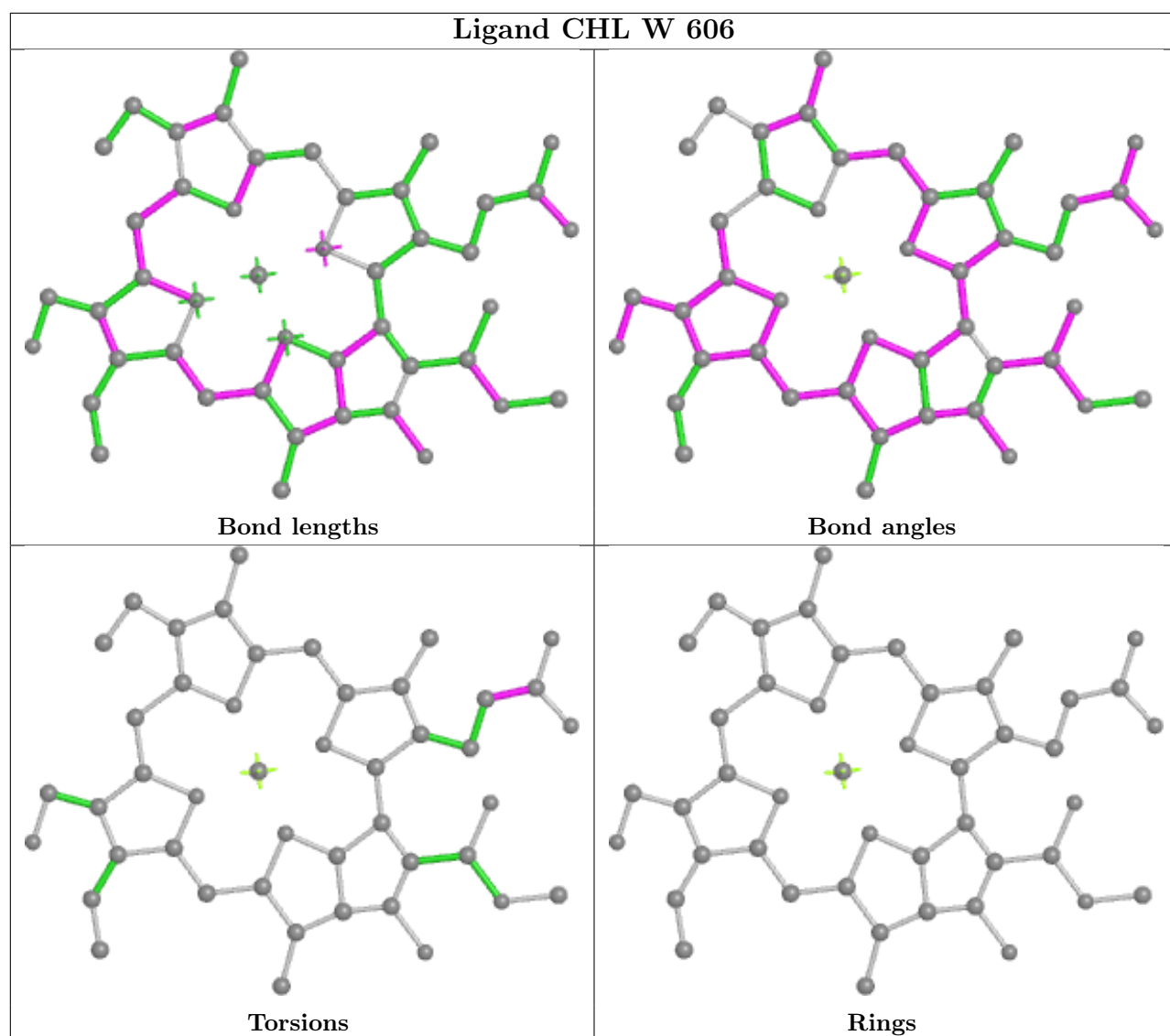


Torsions

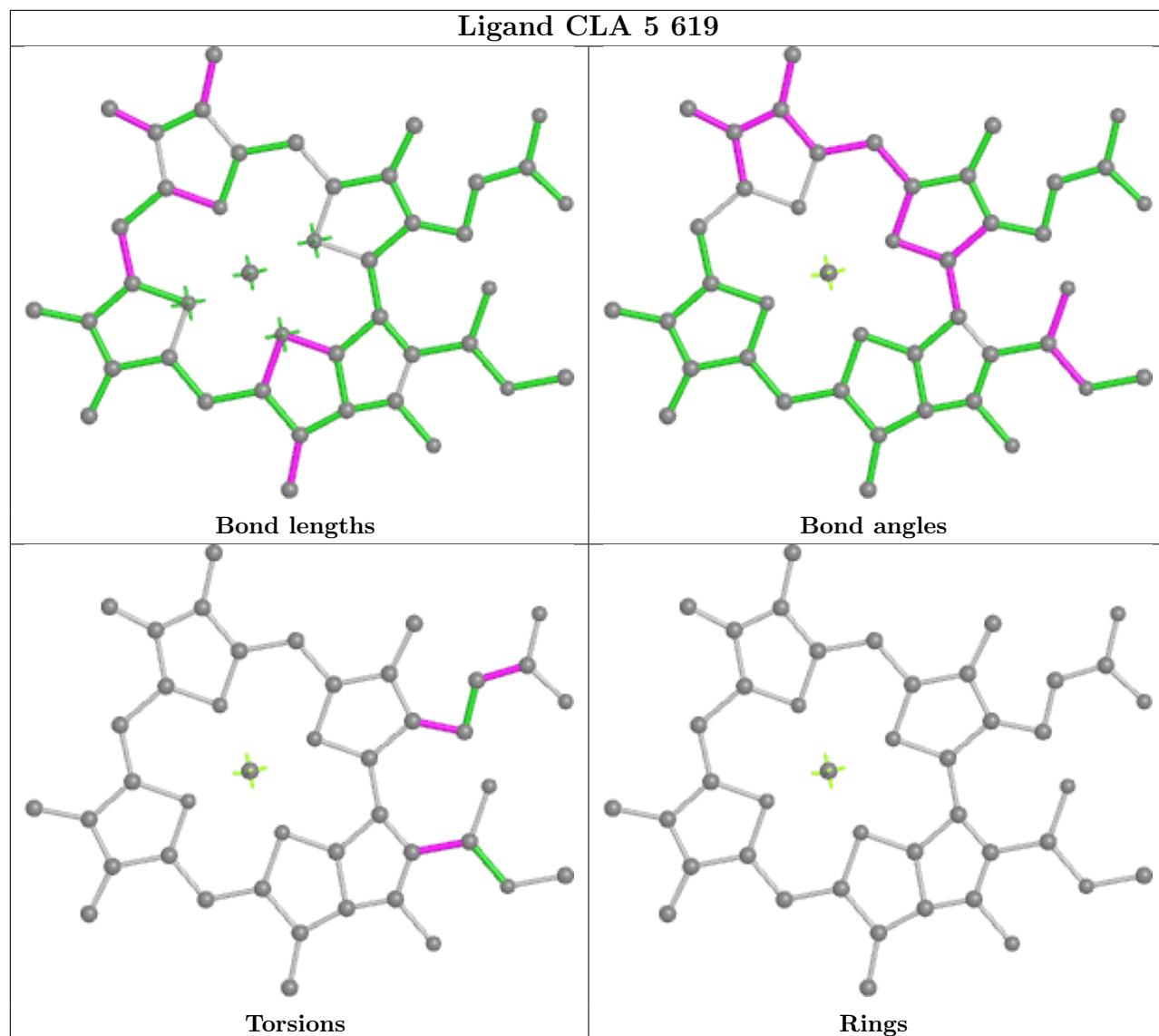


Rings

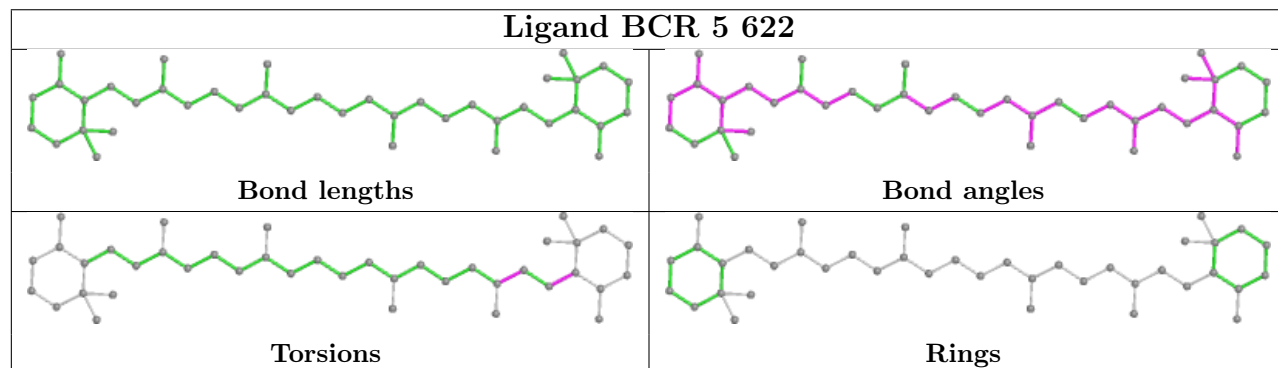


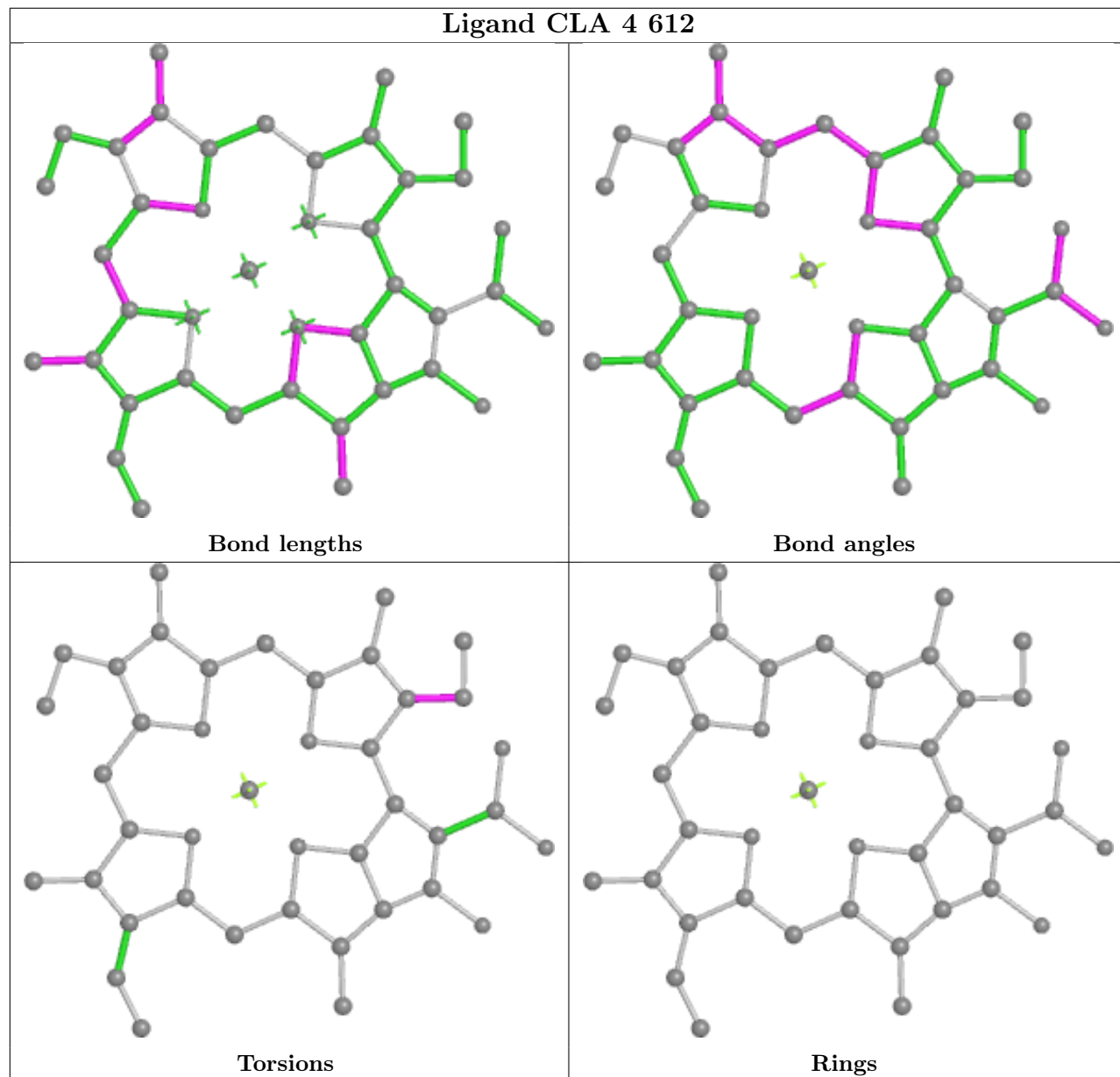
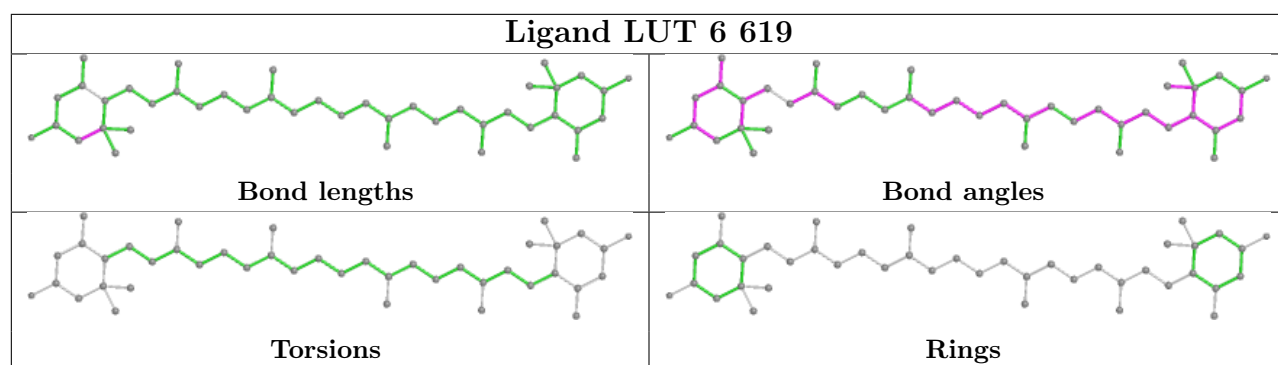


Ligand CLA 5 619

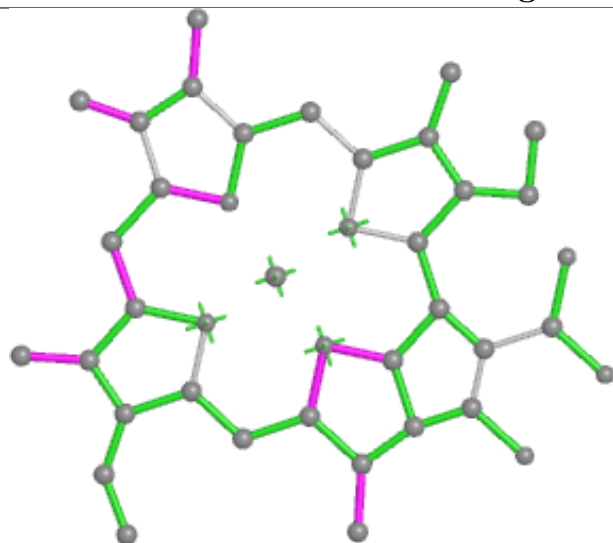


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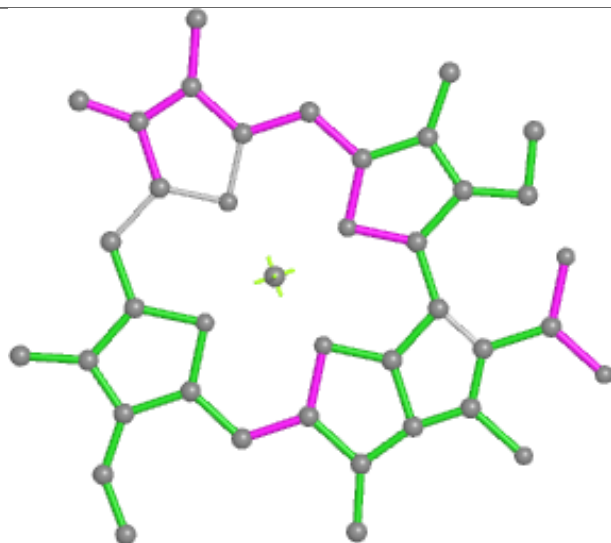




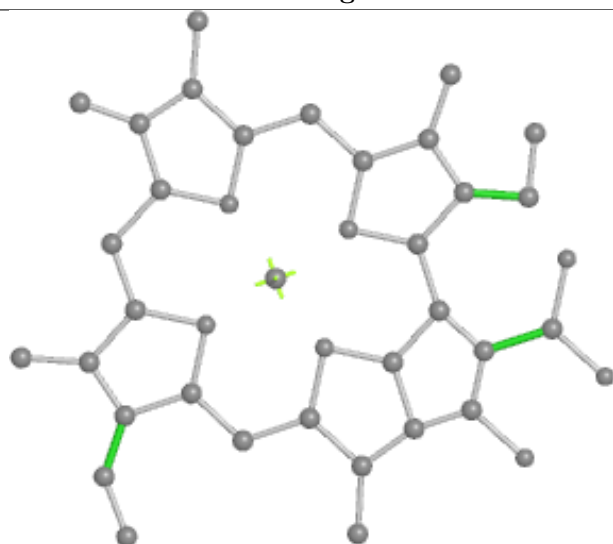
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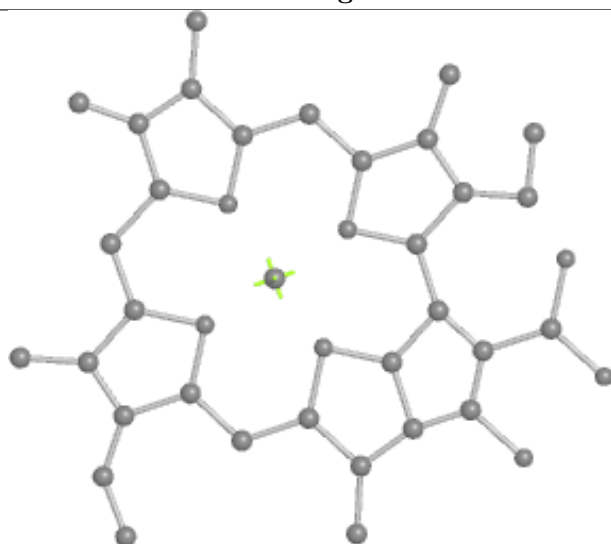
Bond lengths



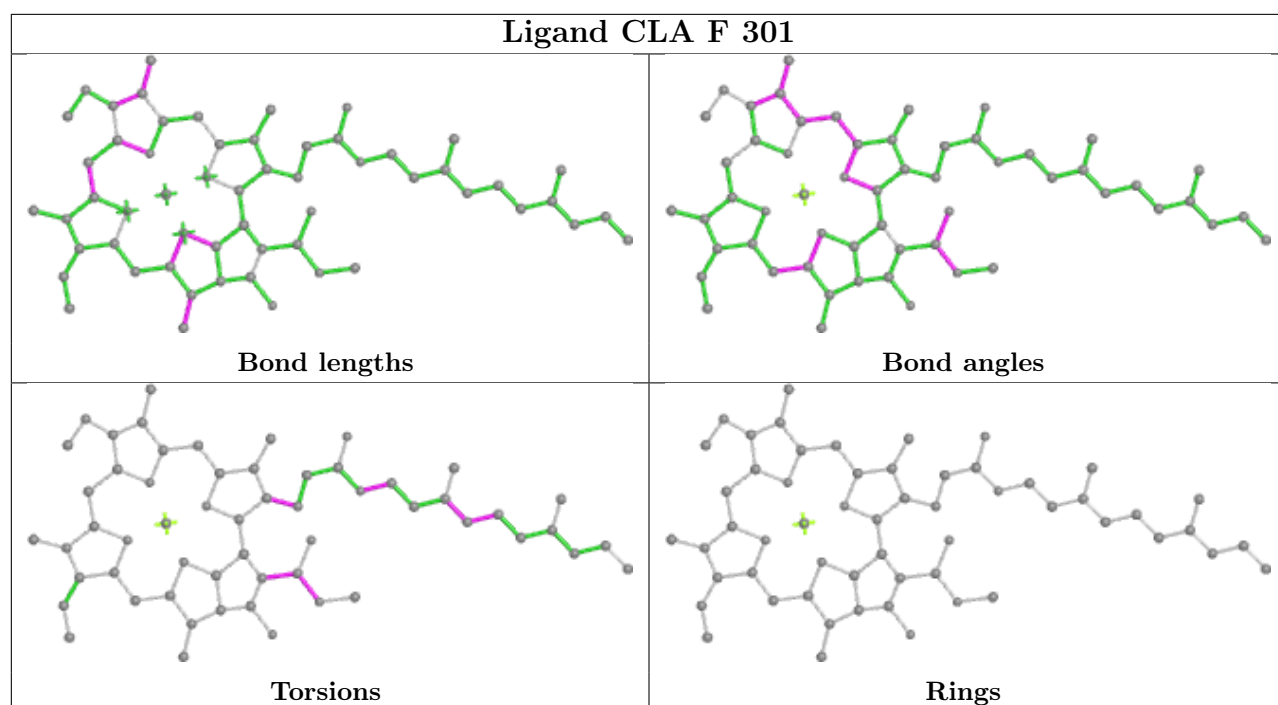
Bond angles

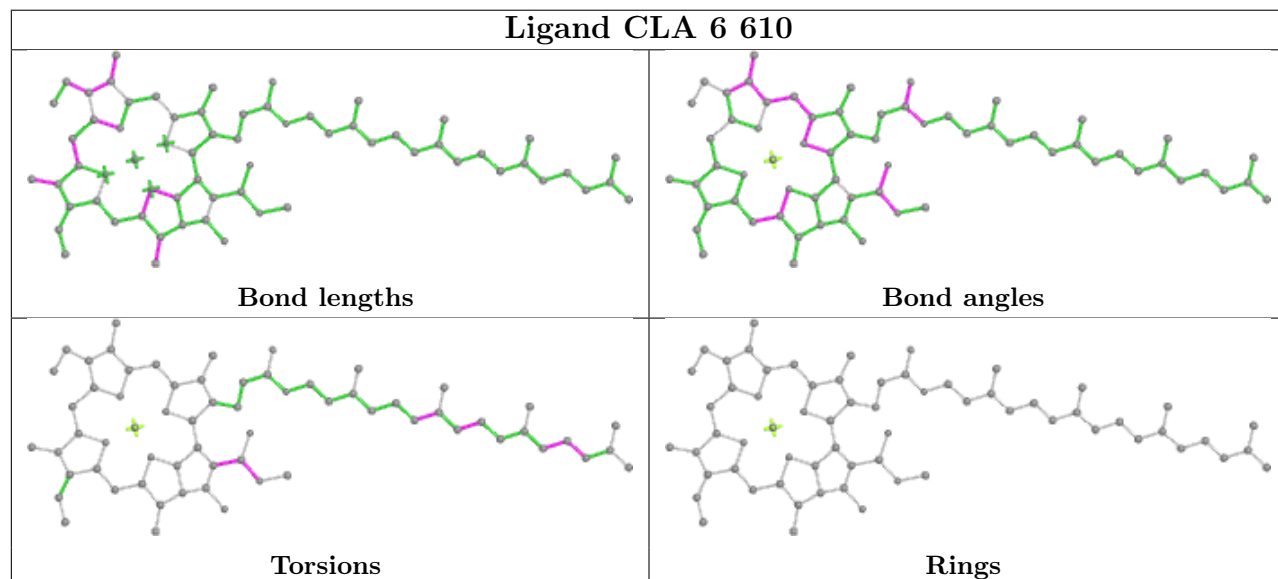
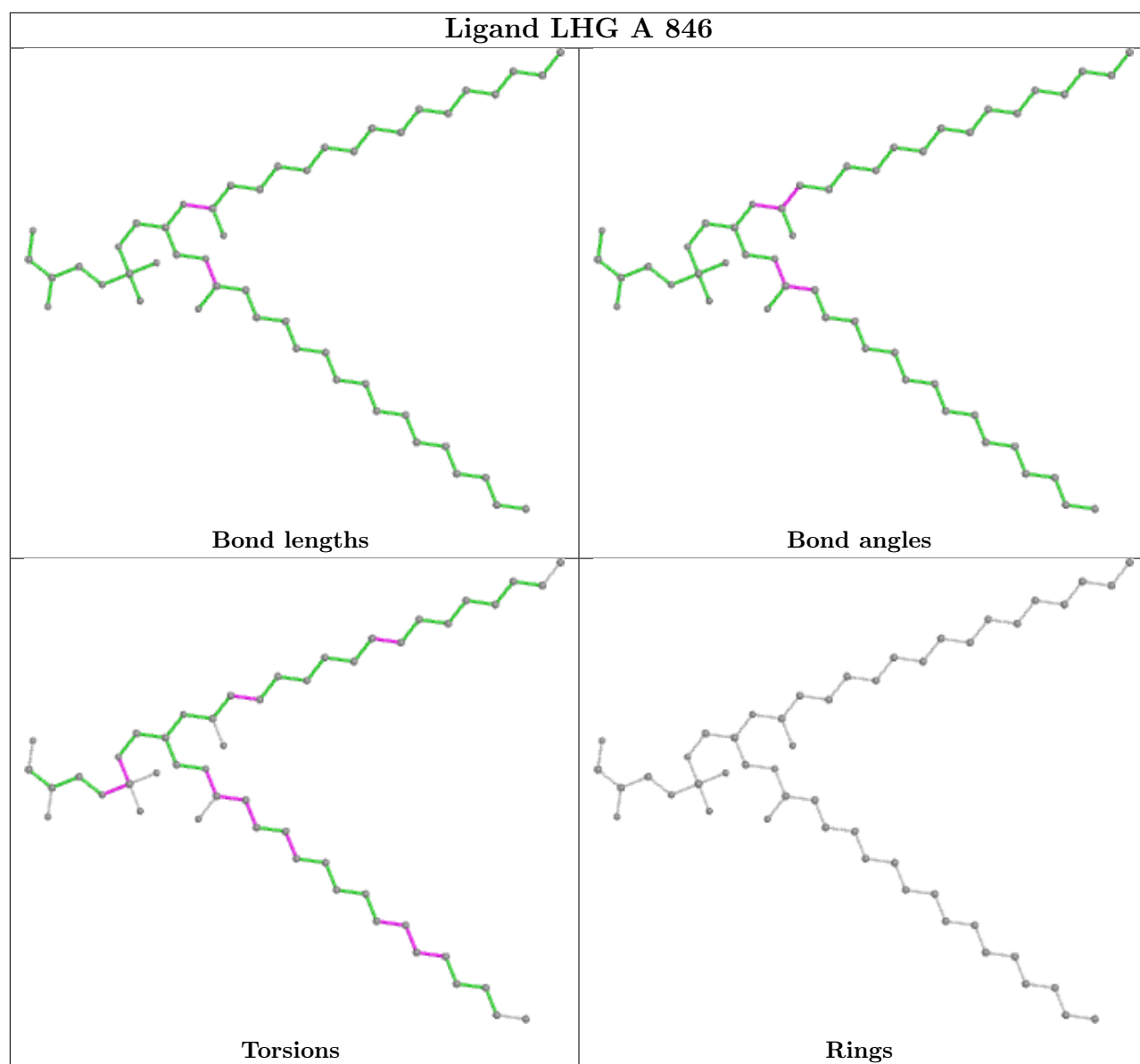


Torsions

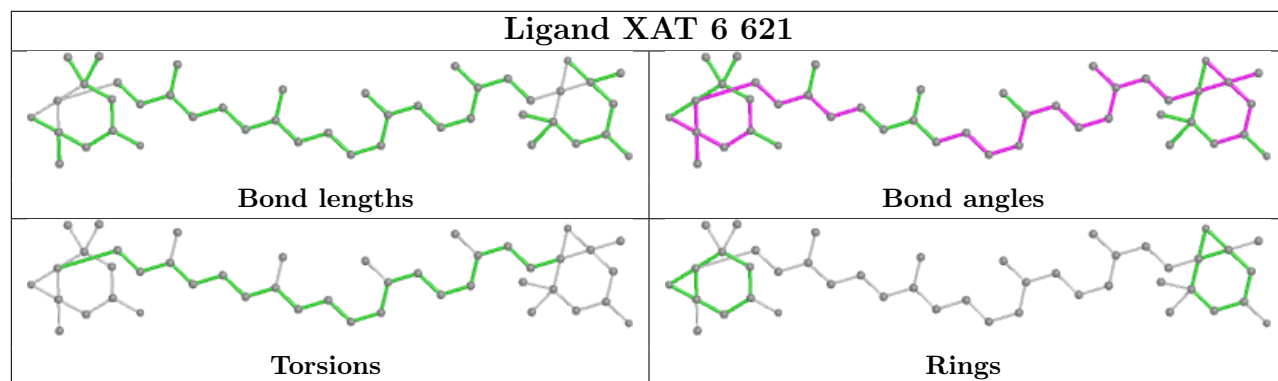


Rings

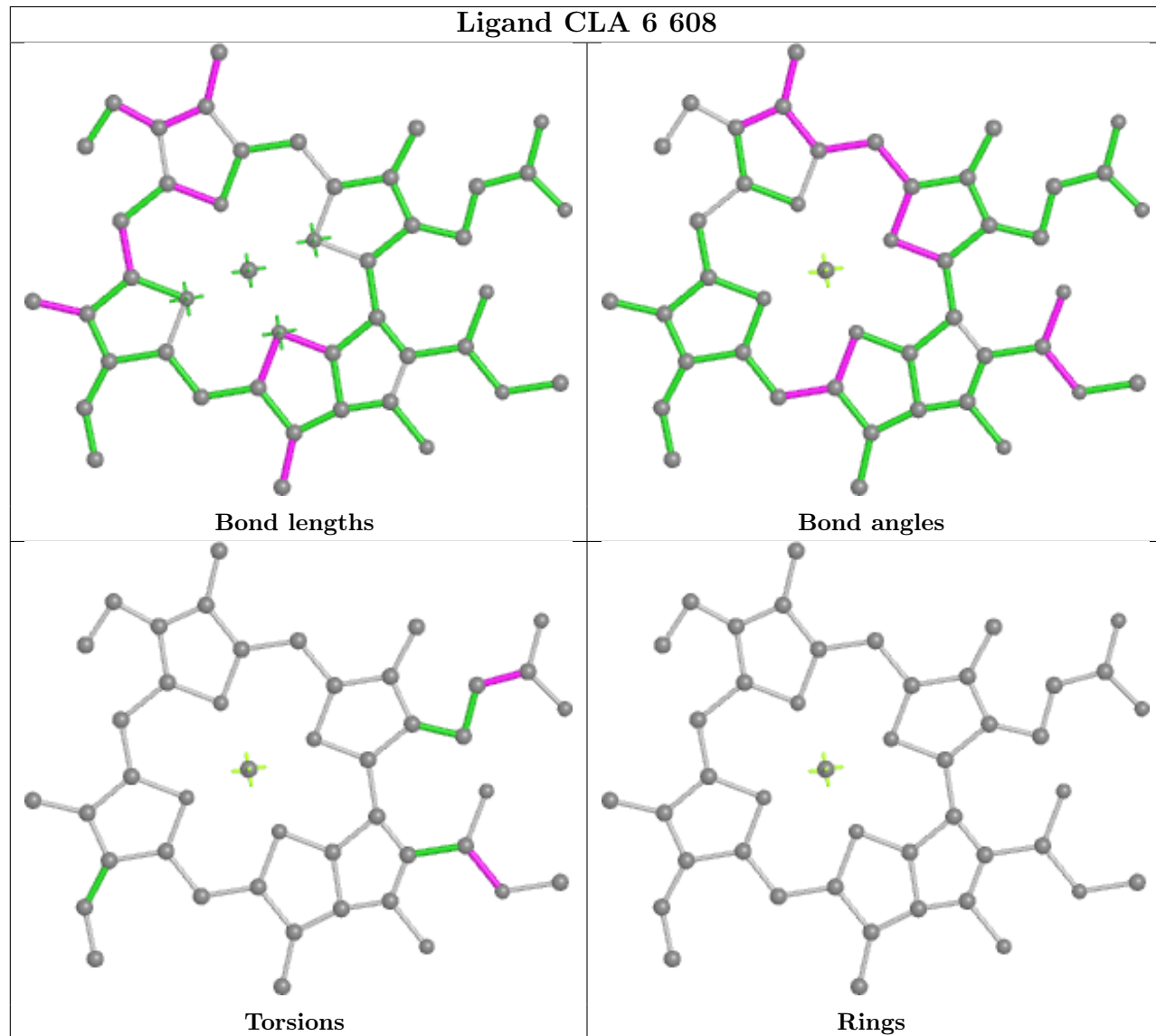


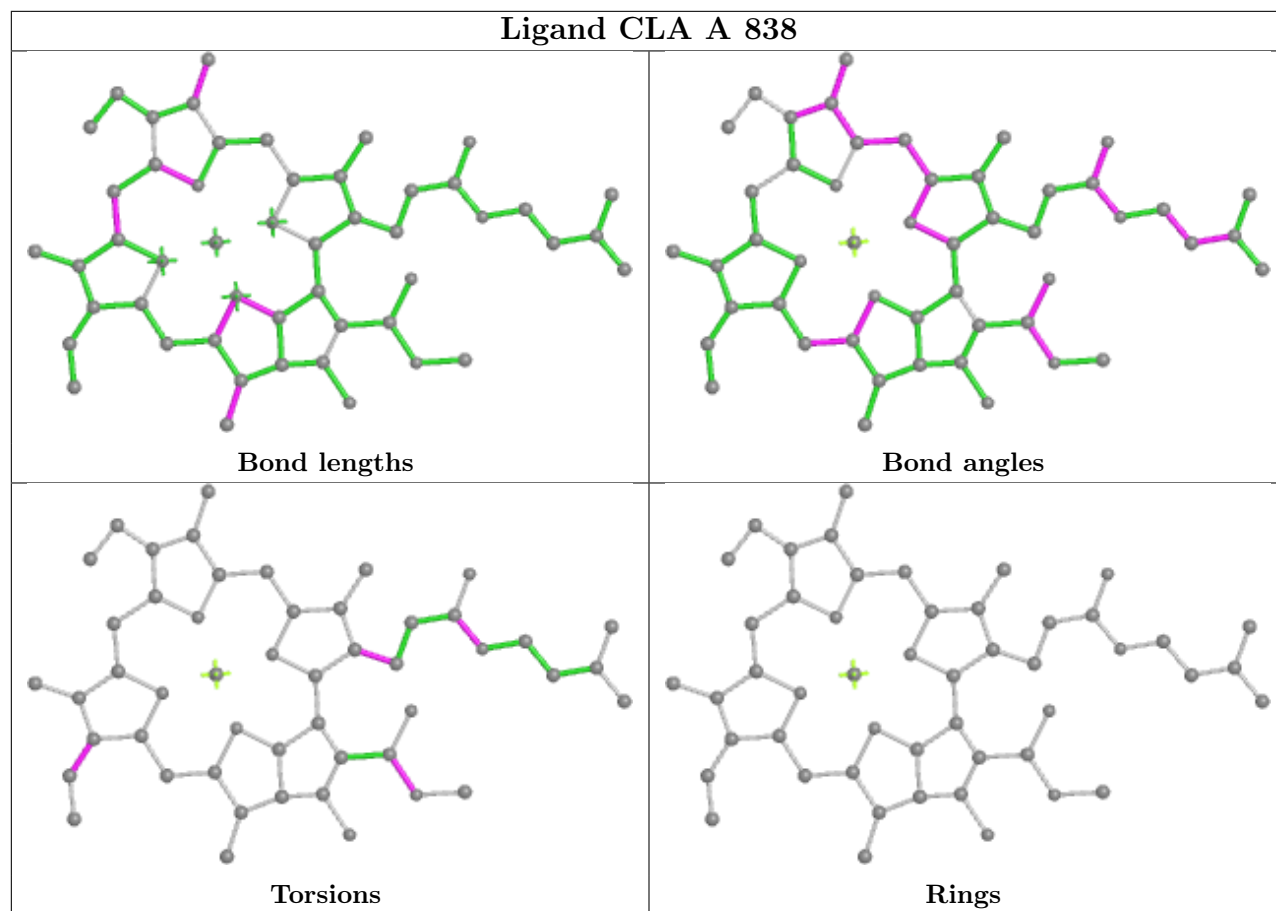
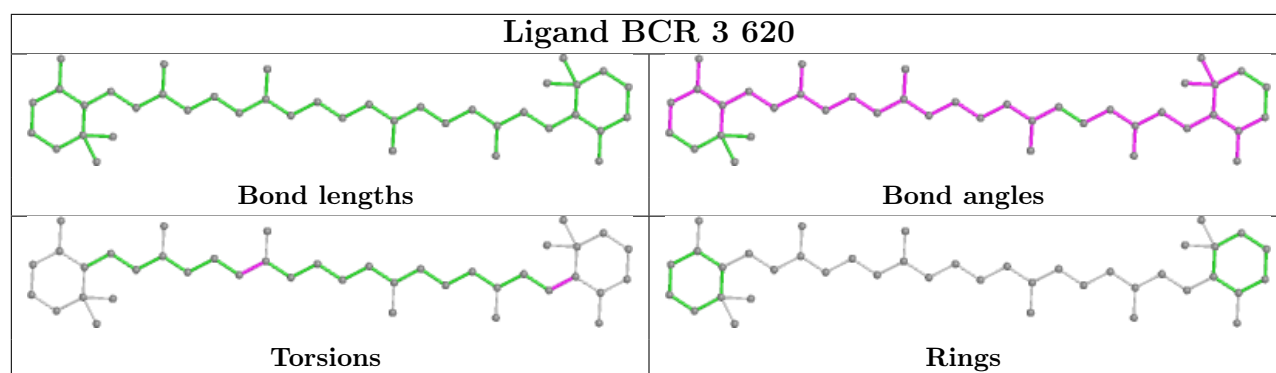


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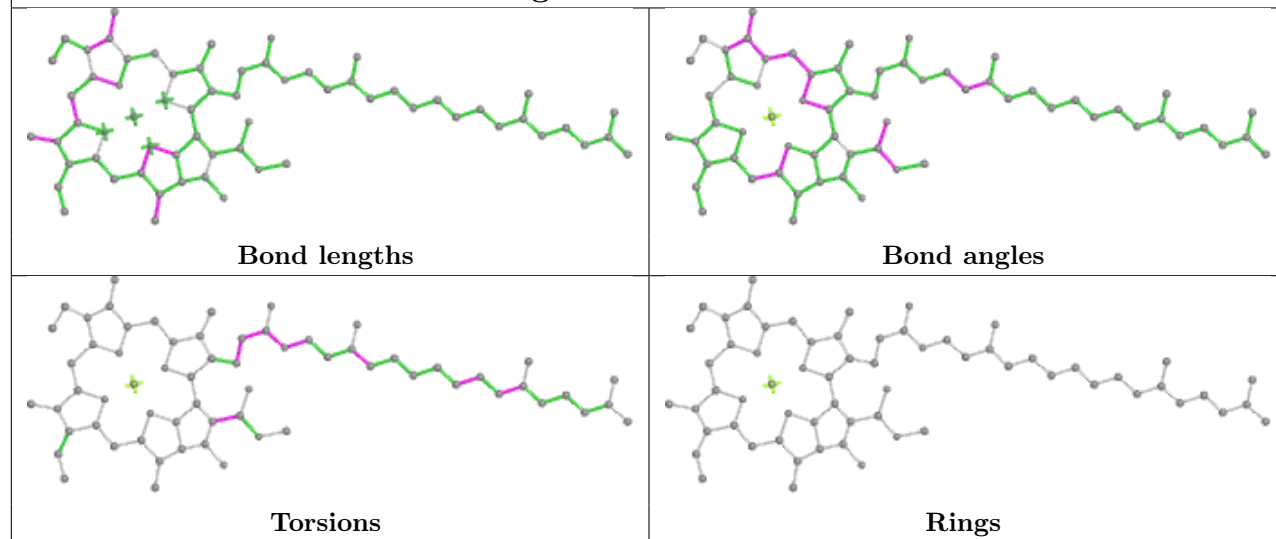


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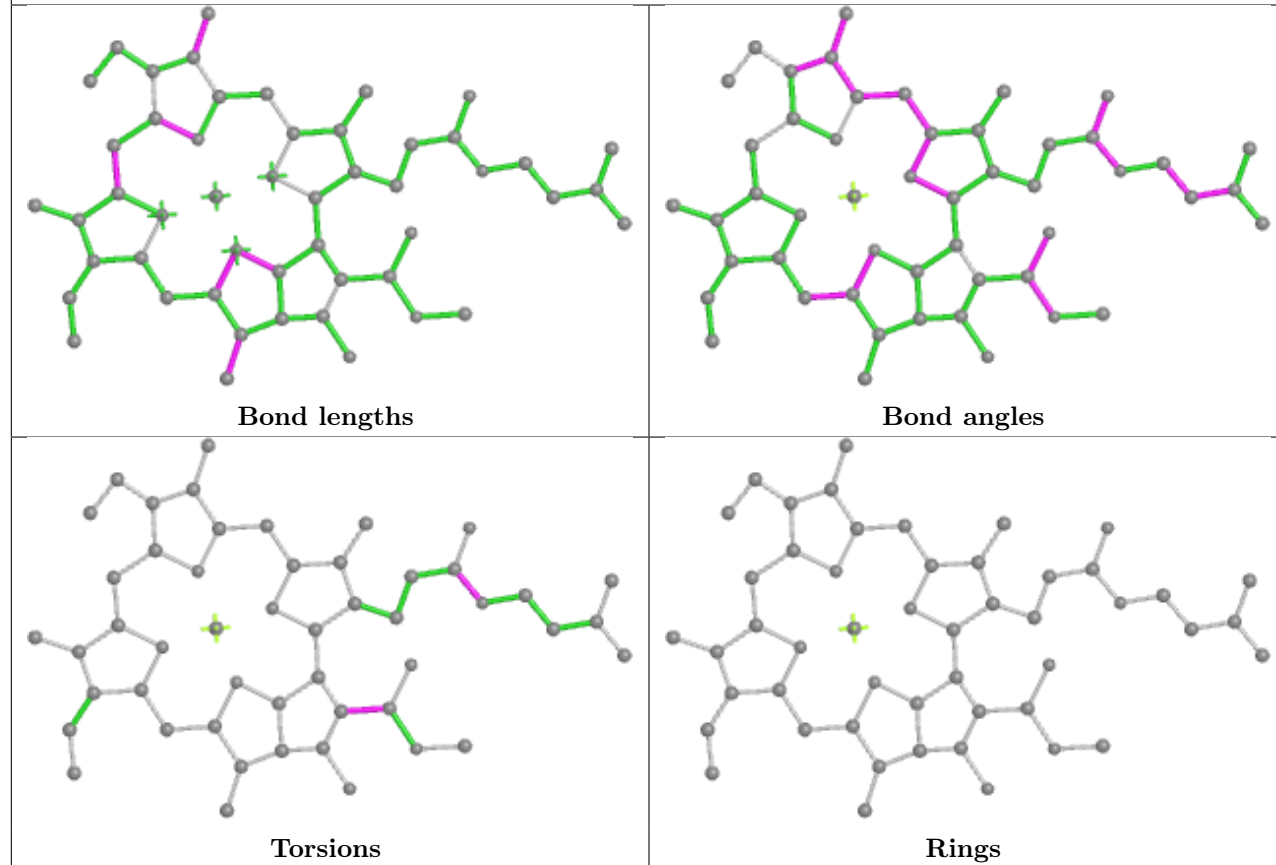




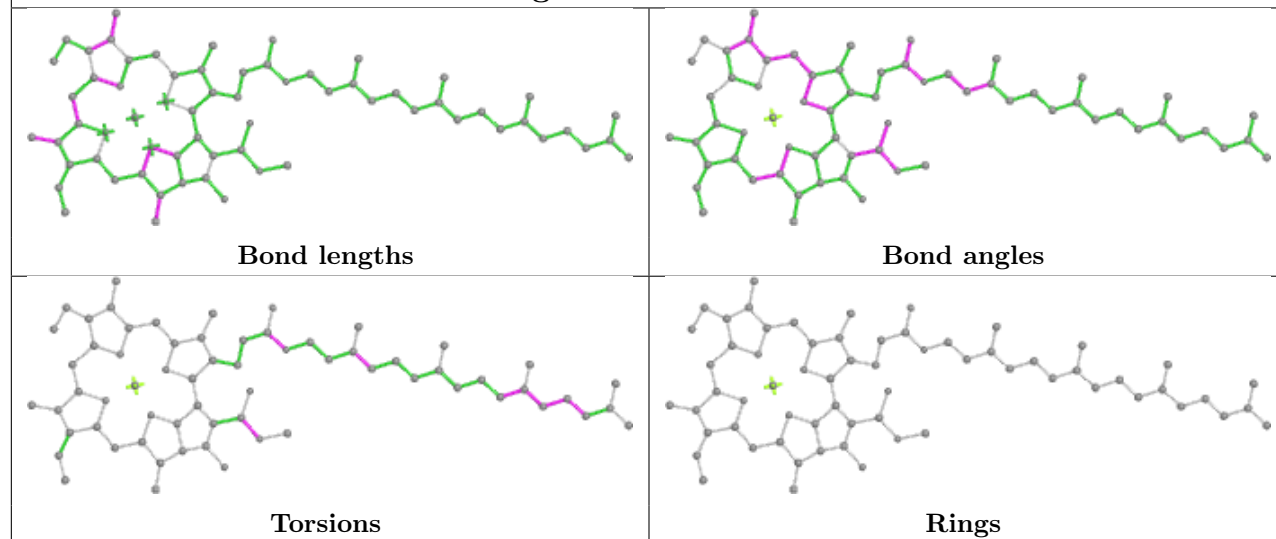
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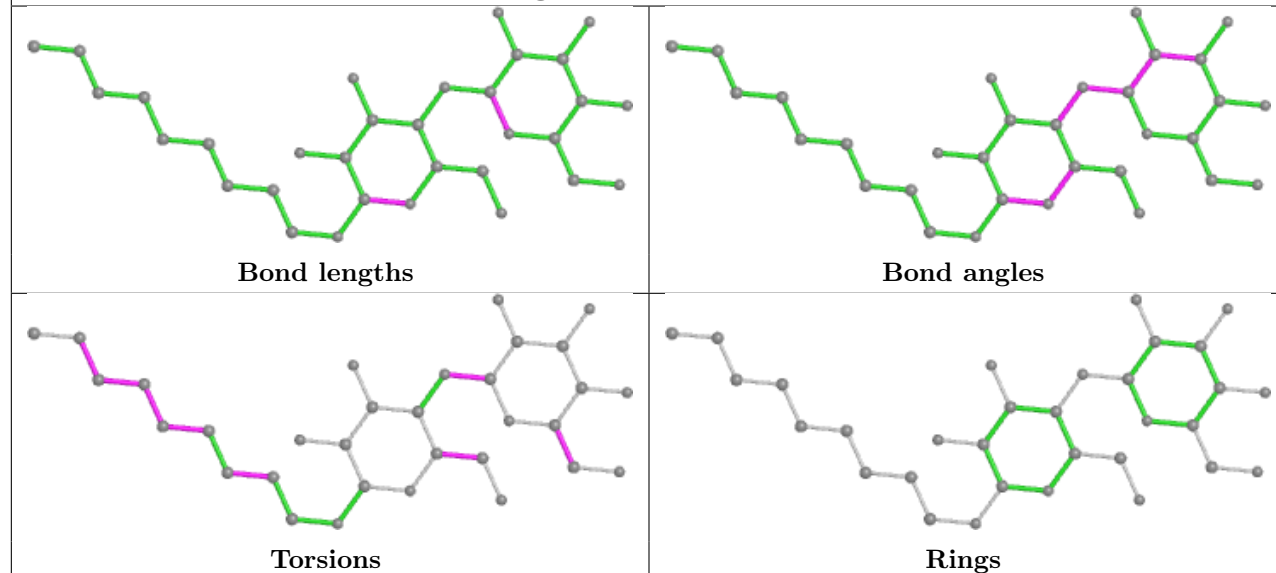
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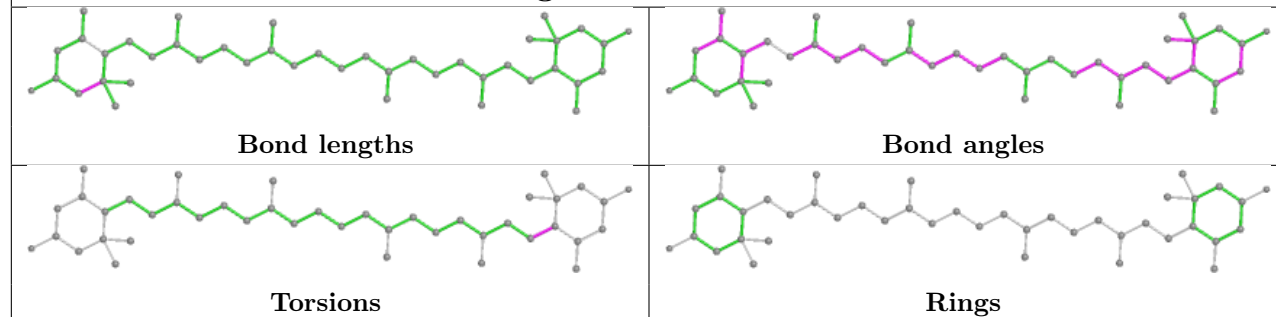
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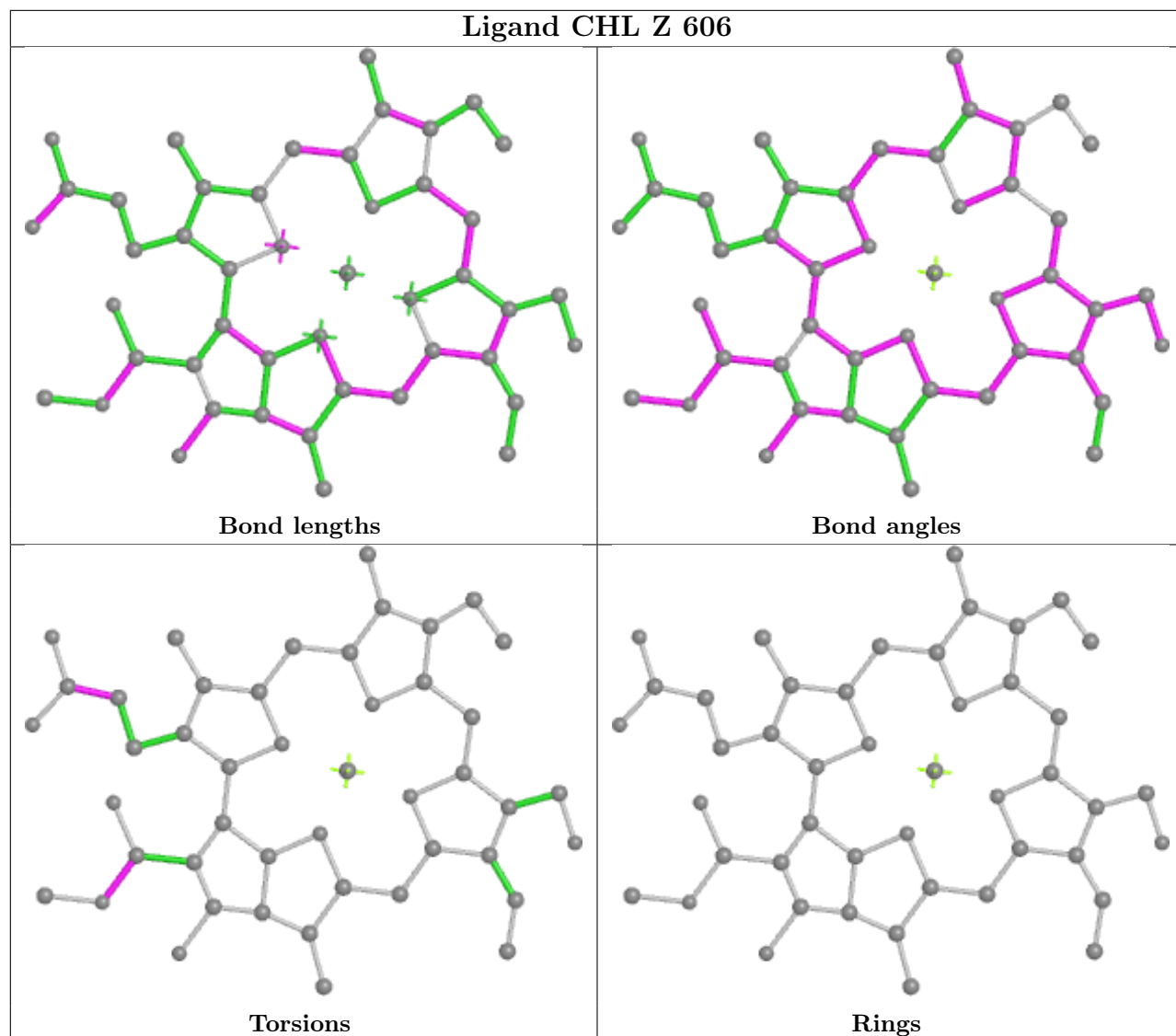
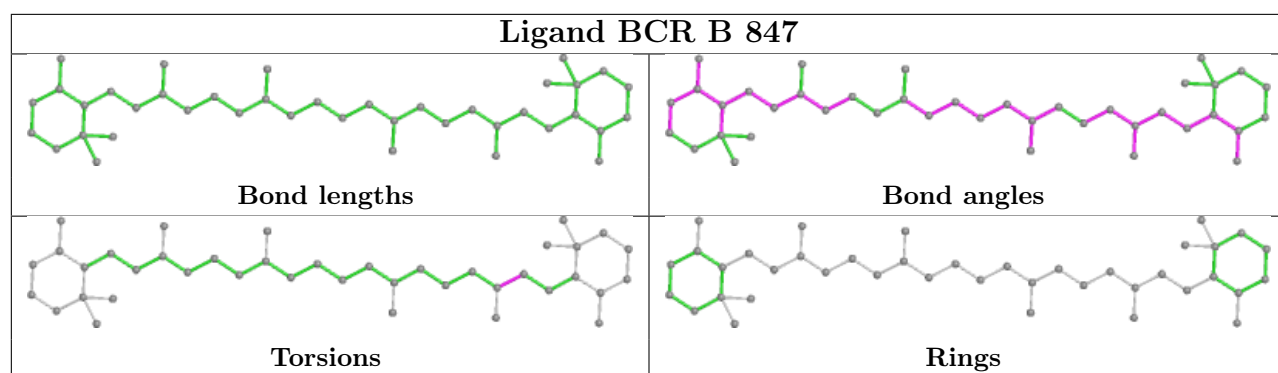


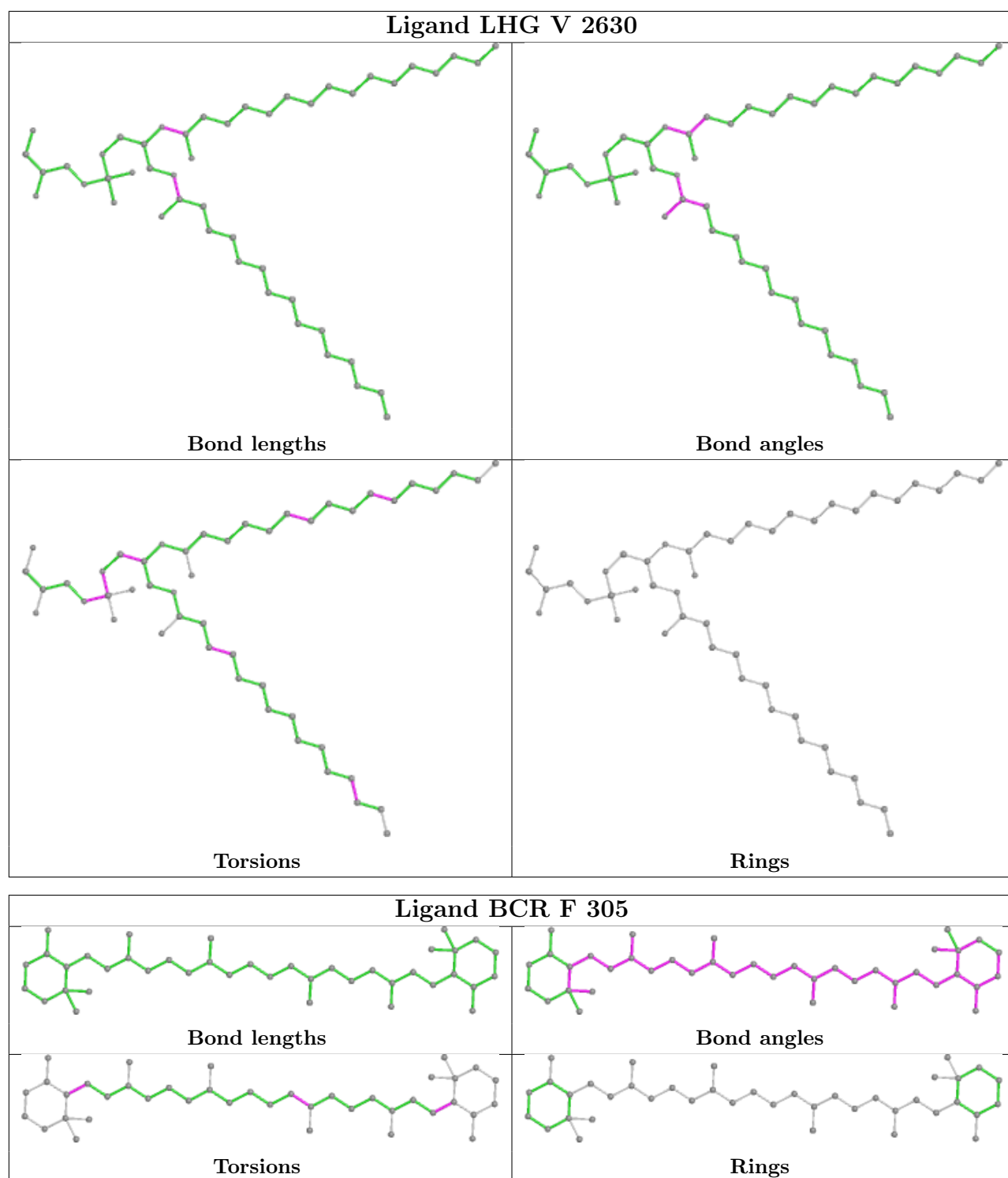
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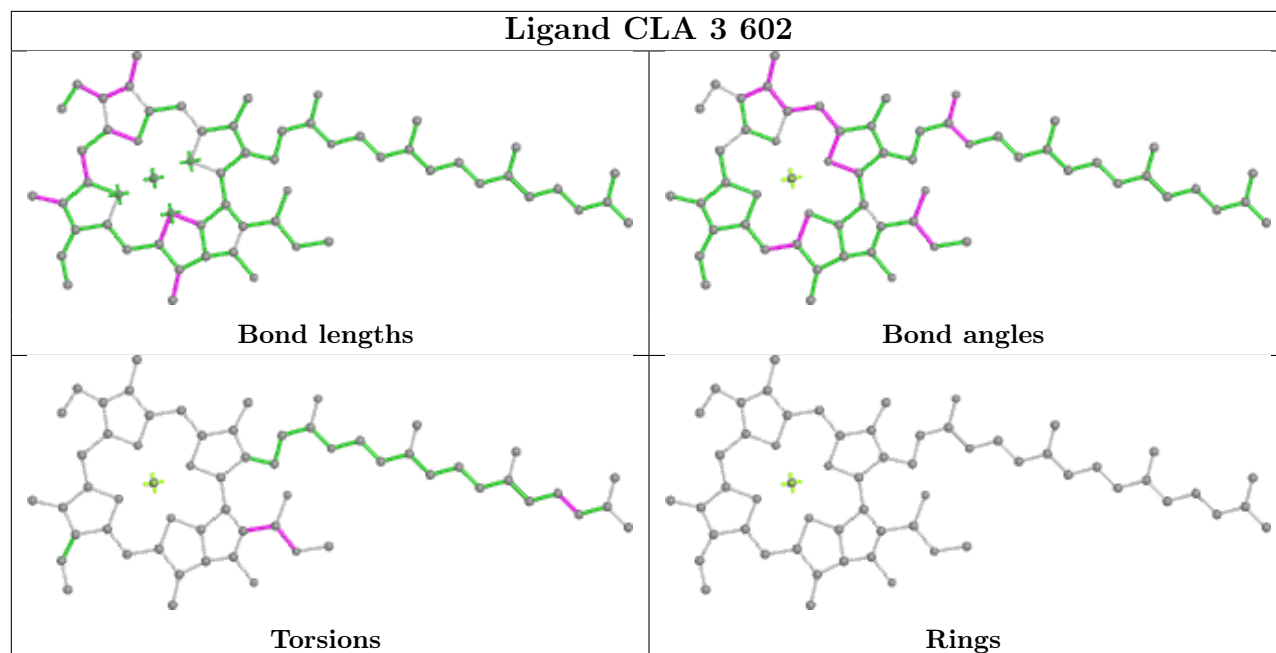
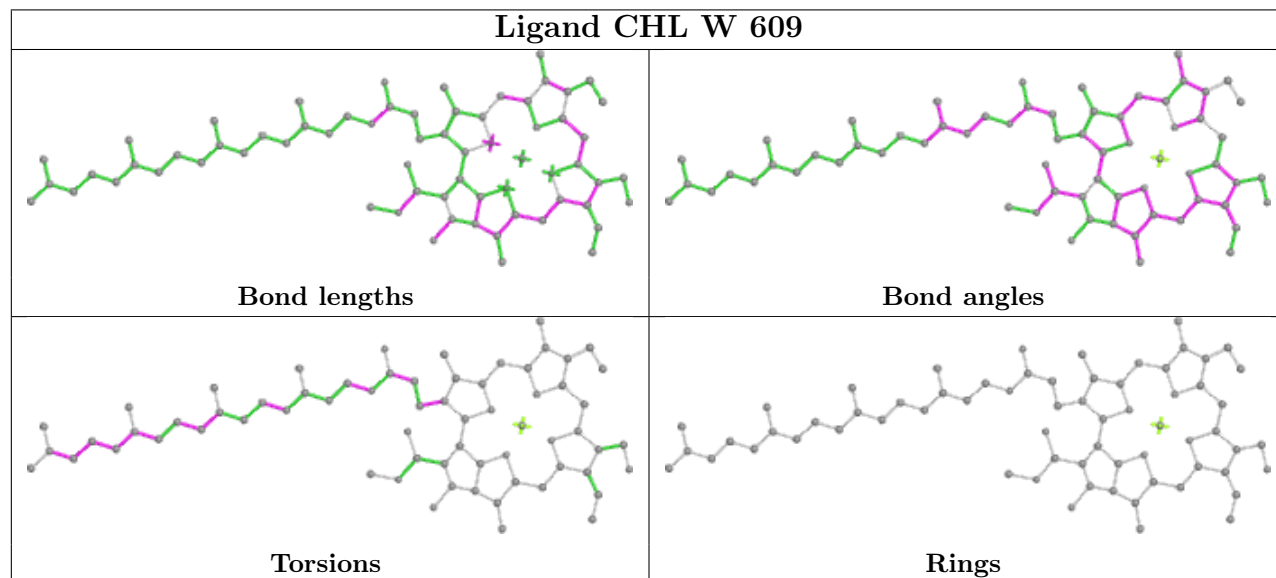
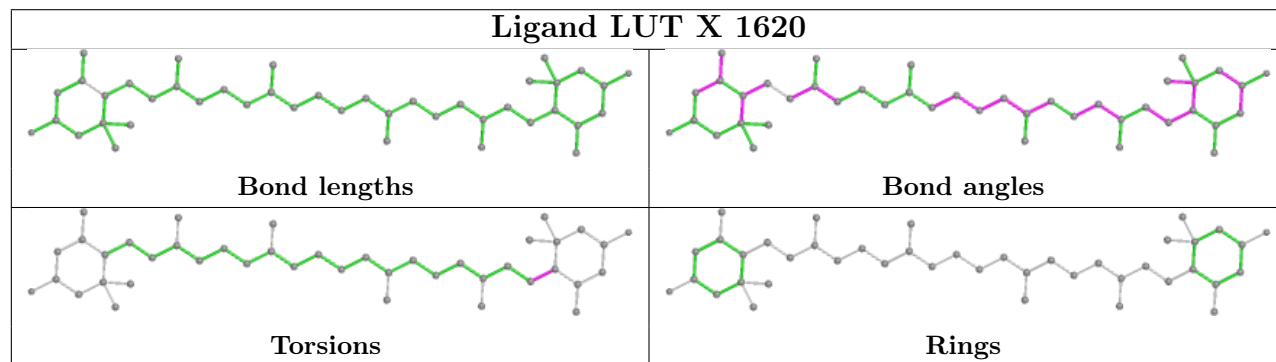


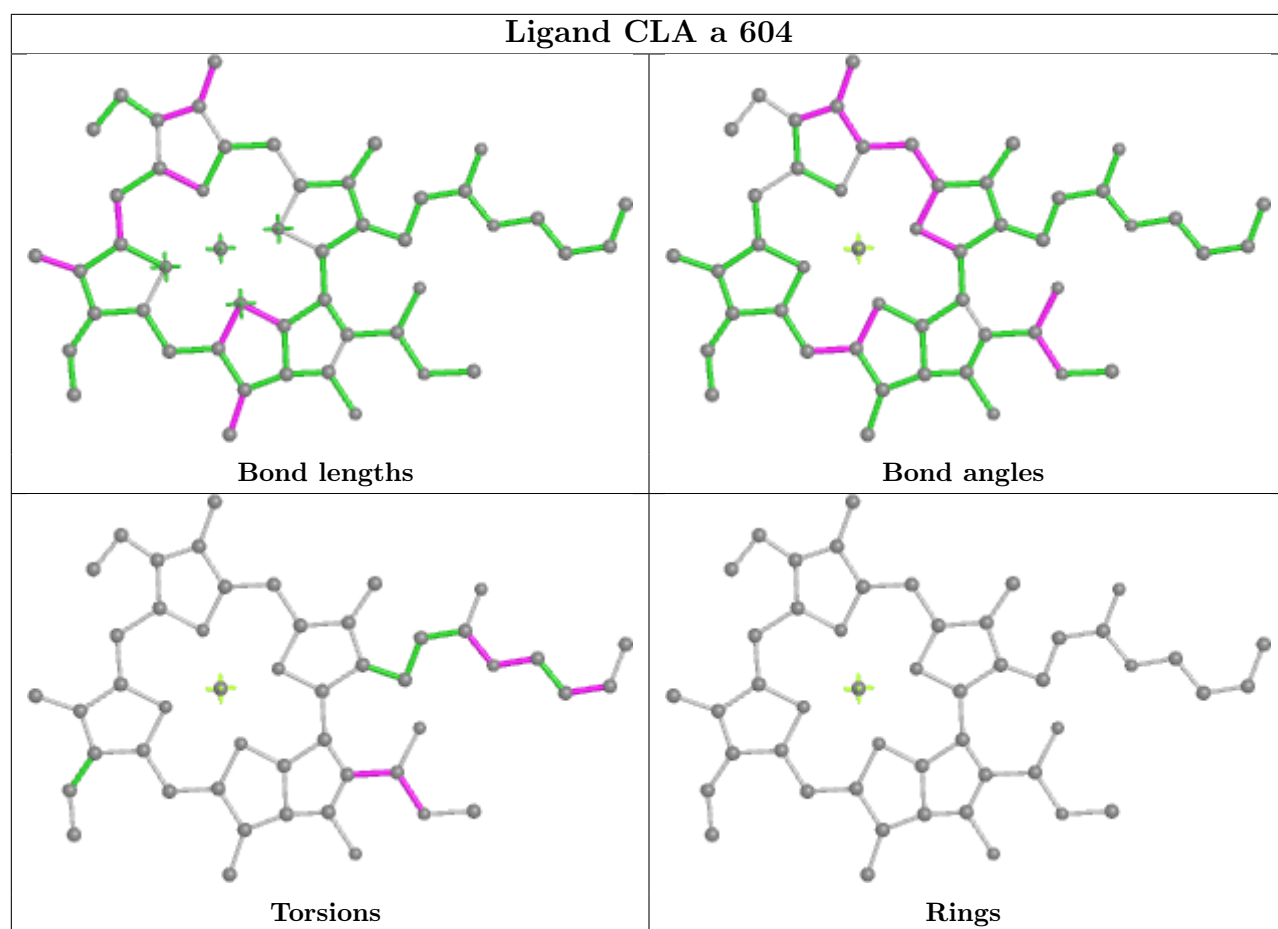
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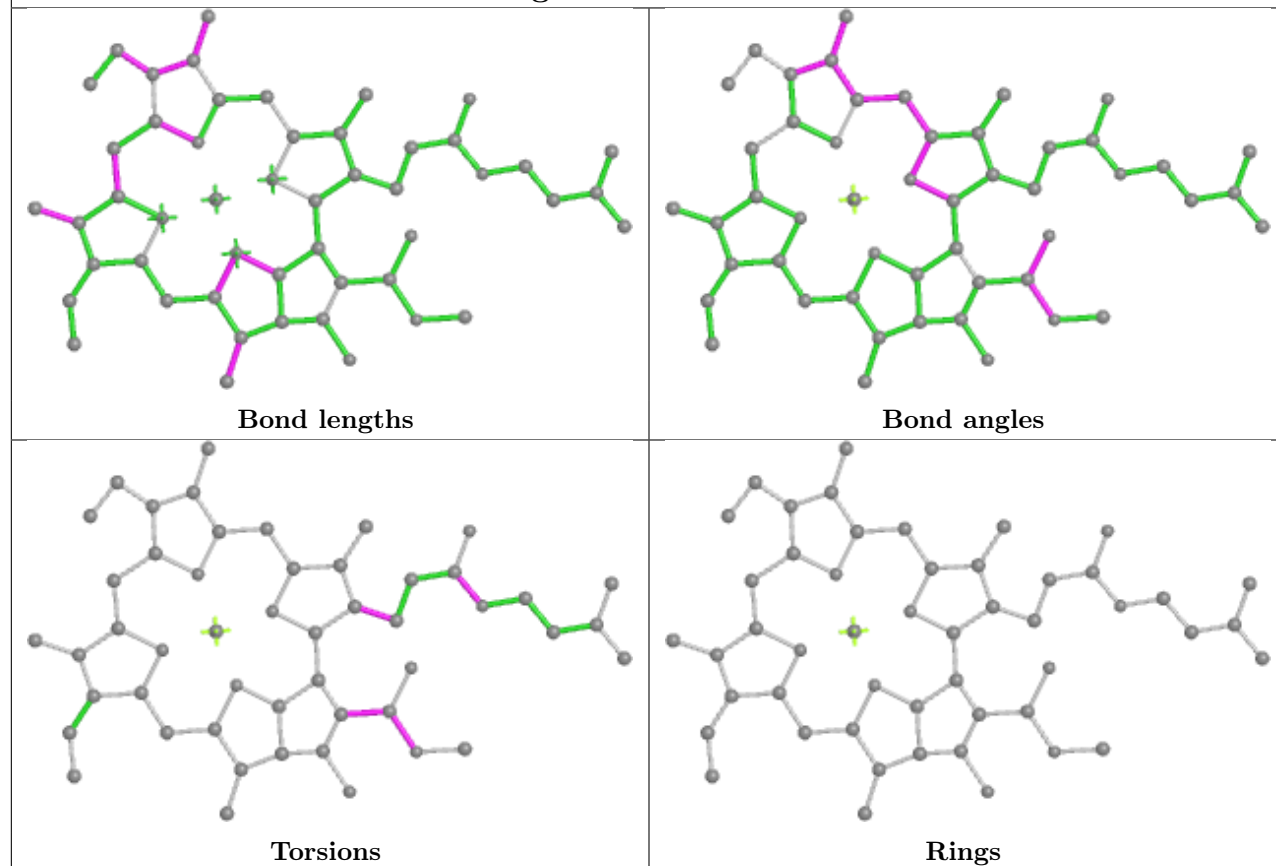




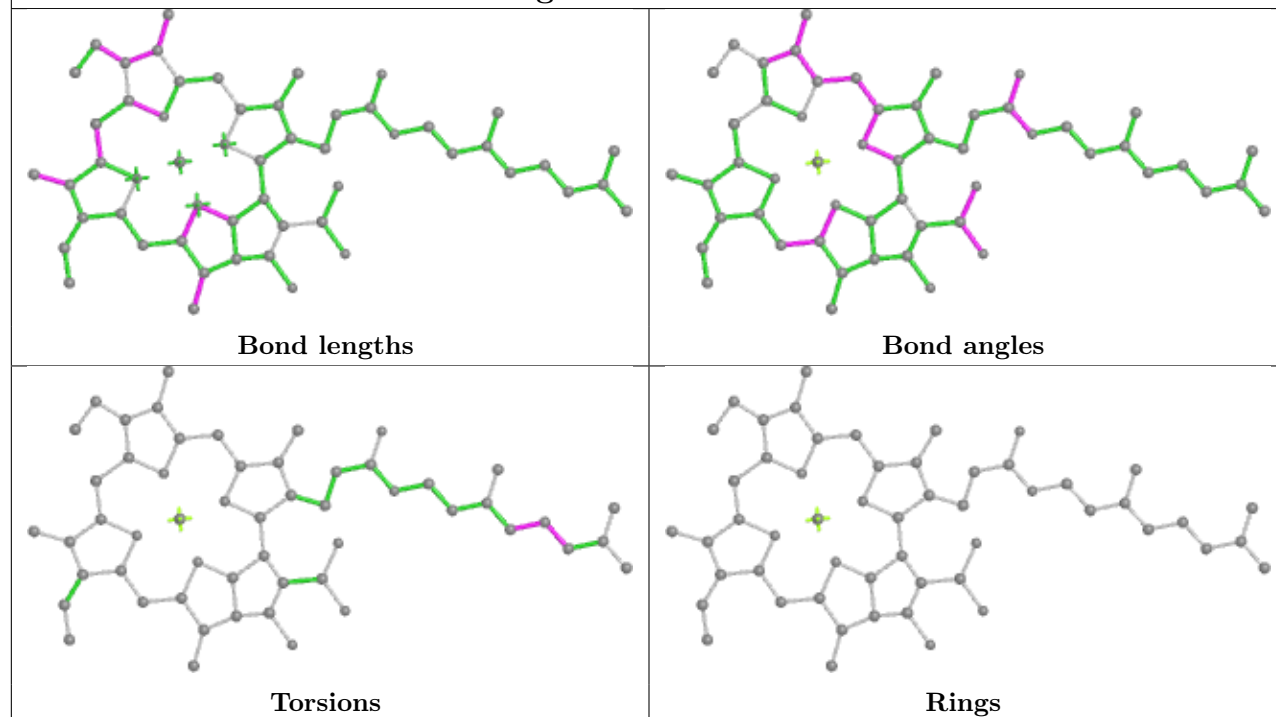
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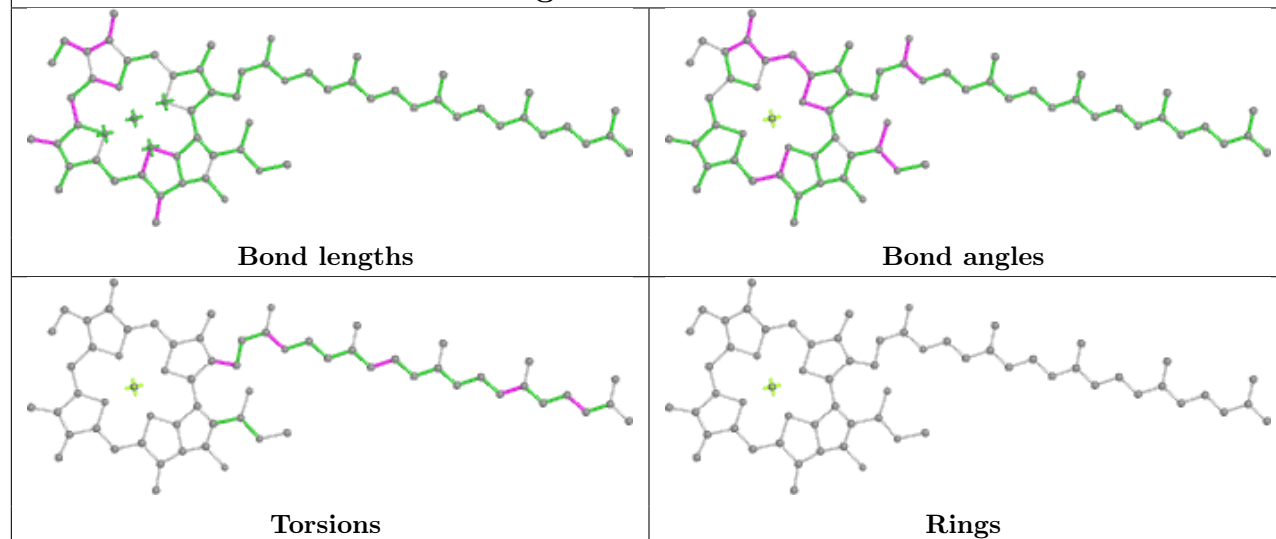
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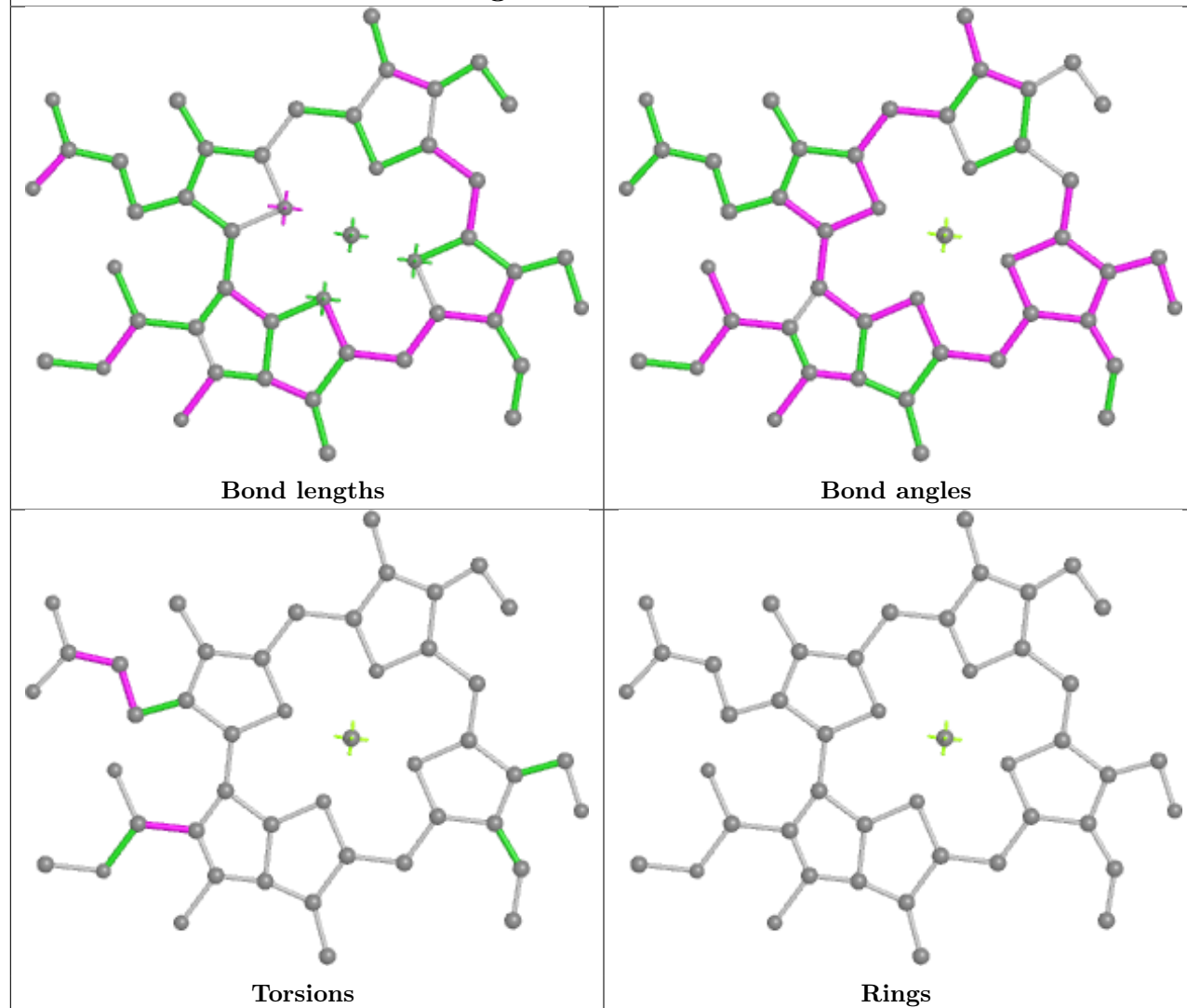
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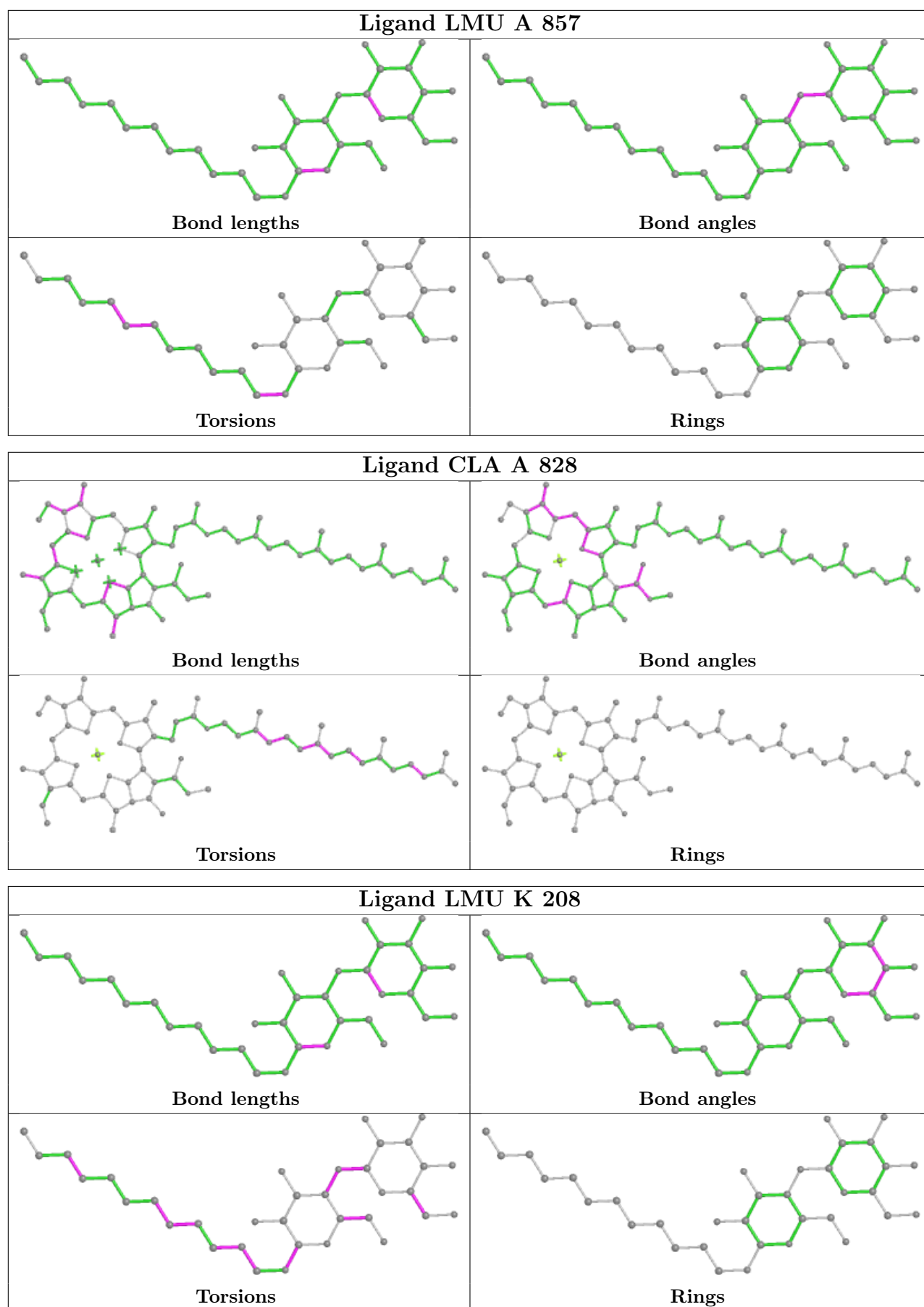


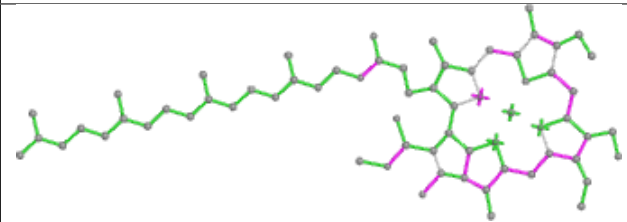
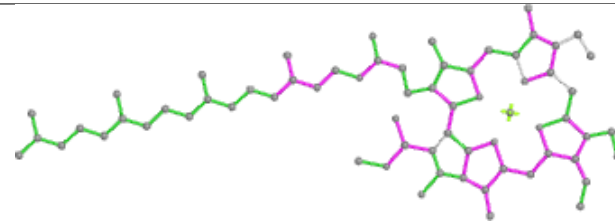
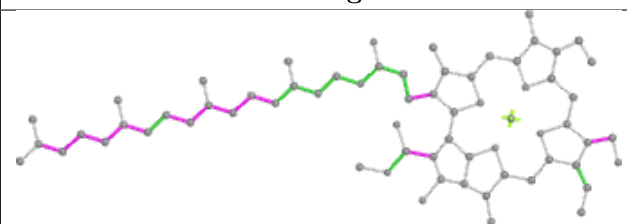
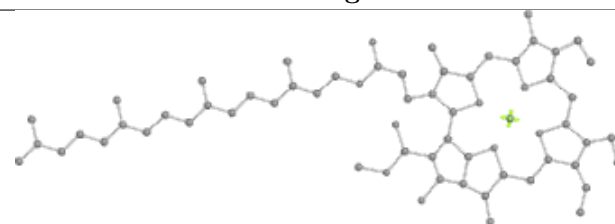
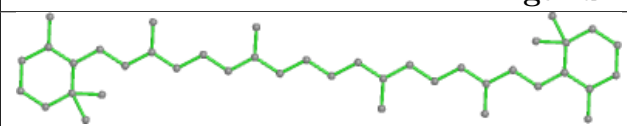
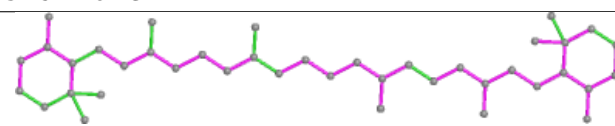
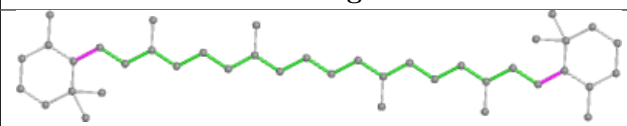
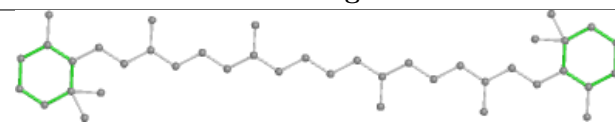
Ligand CLA 8 606



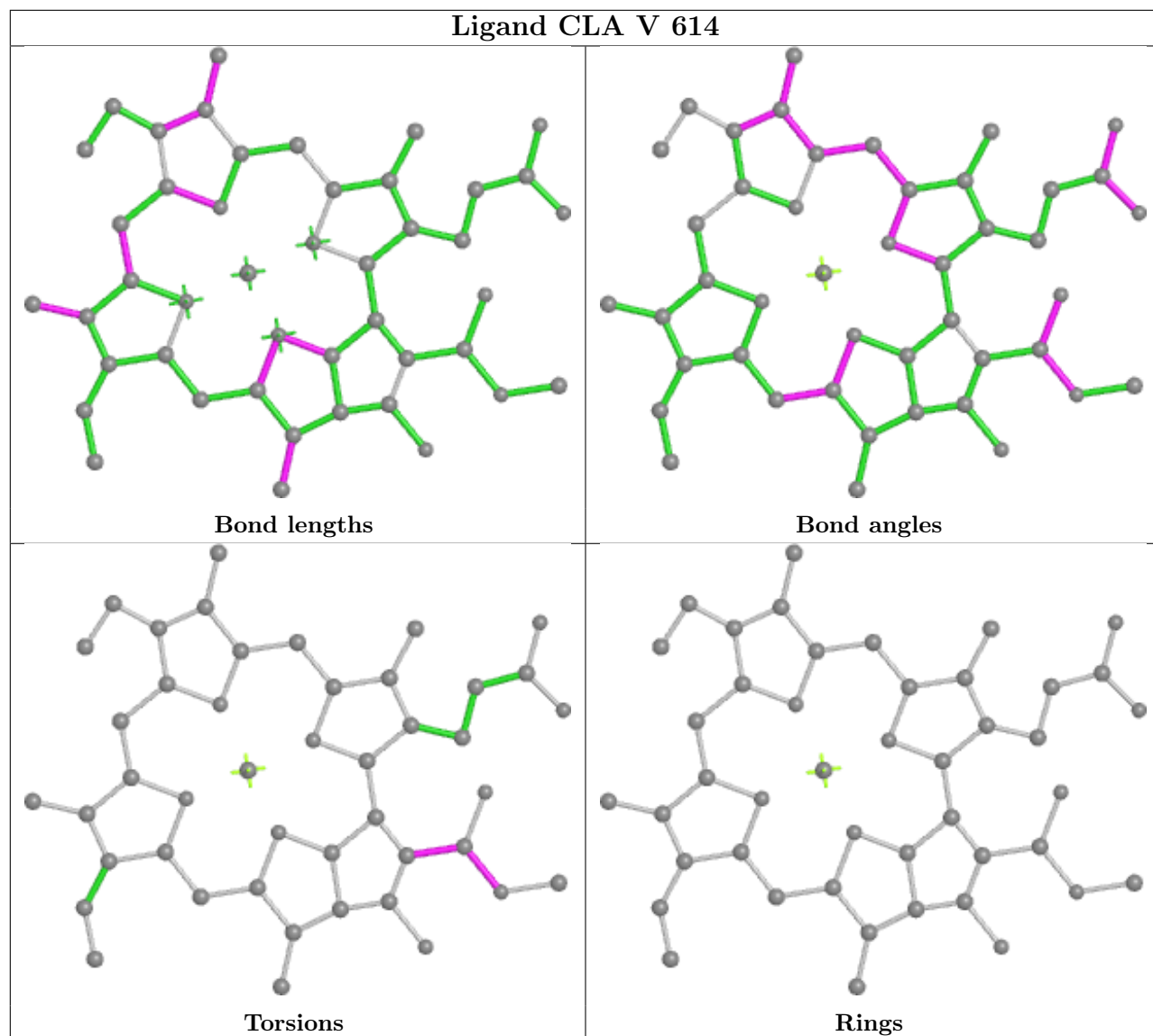
Ligand CHL W 605

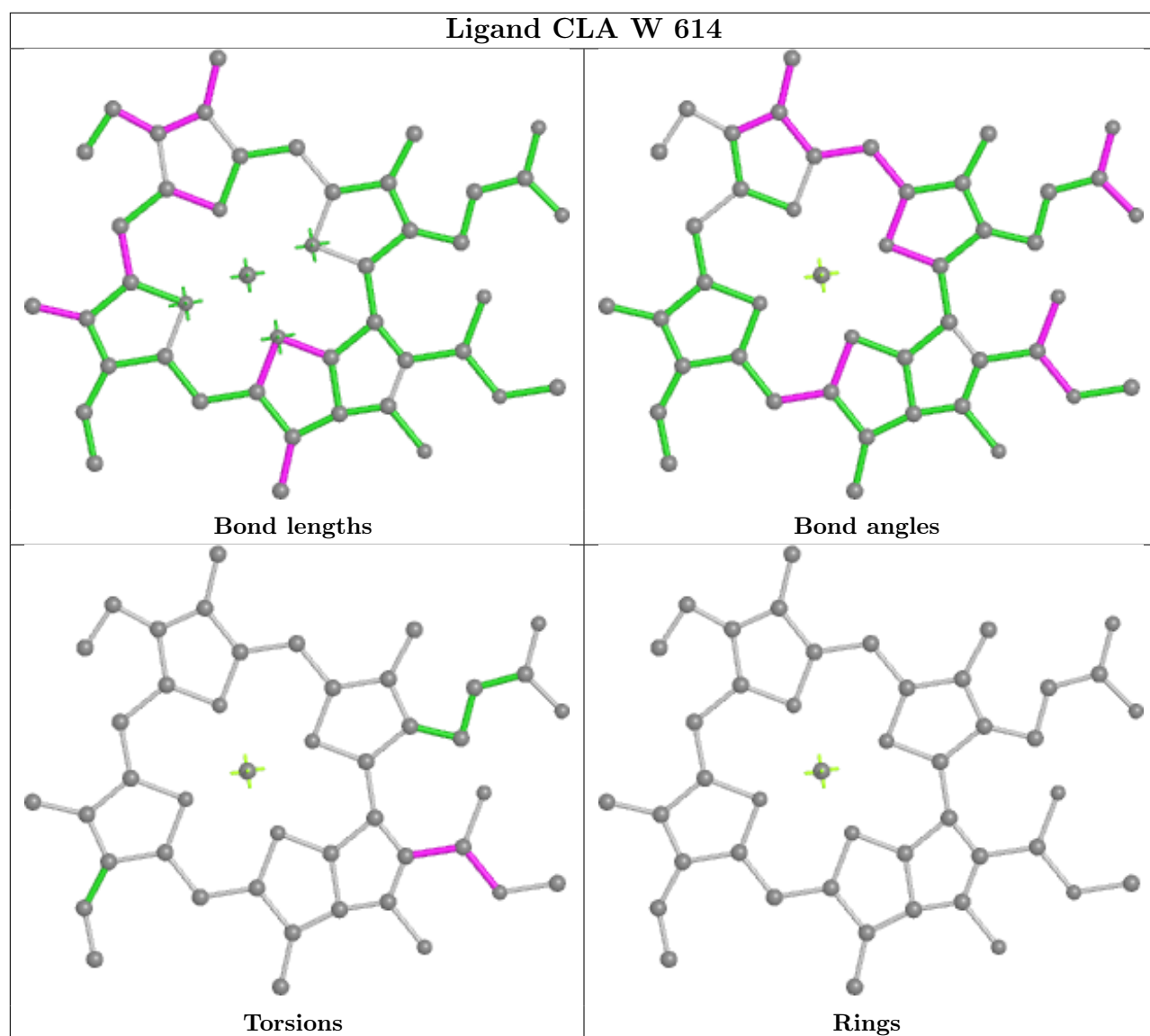


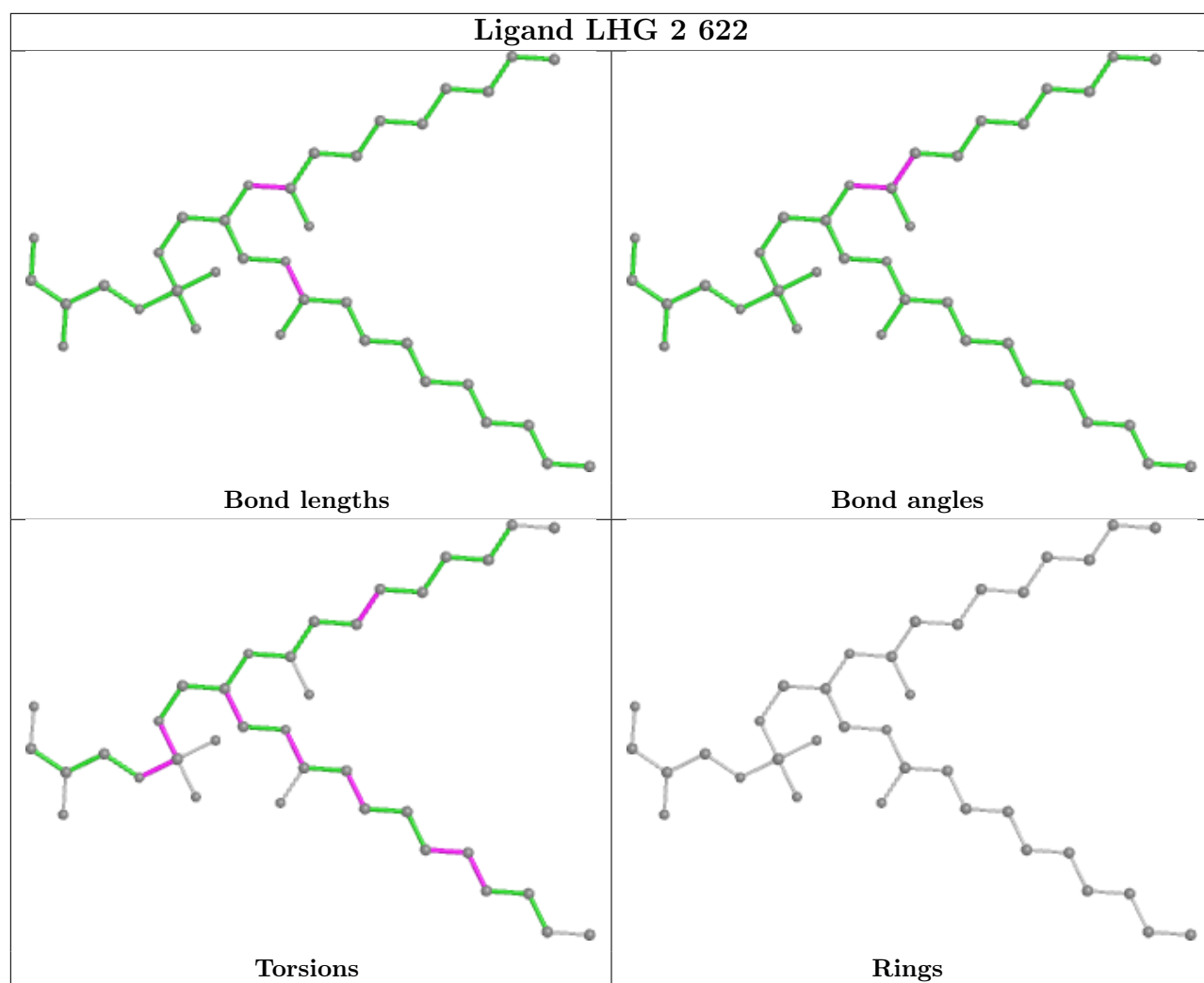


Ligand CHL Z 601	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR 2 623	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

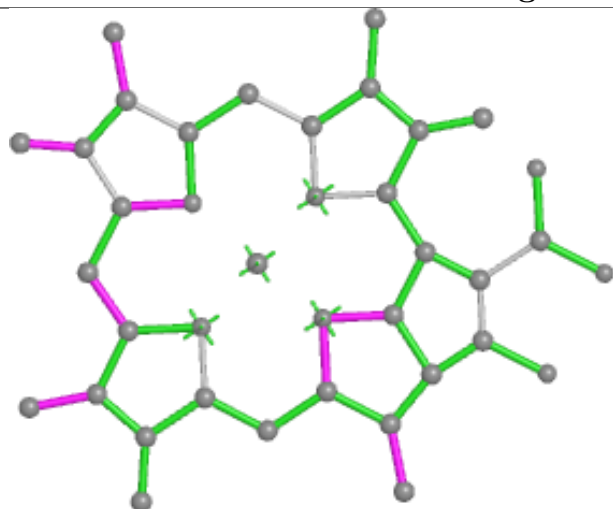
Ligand CLA V 614



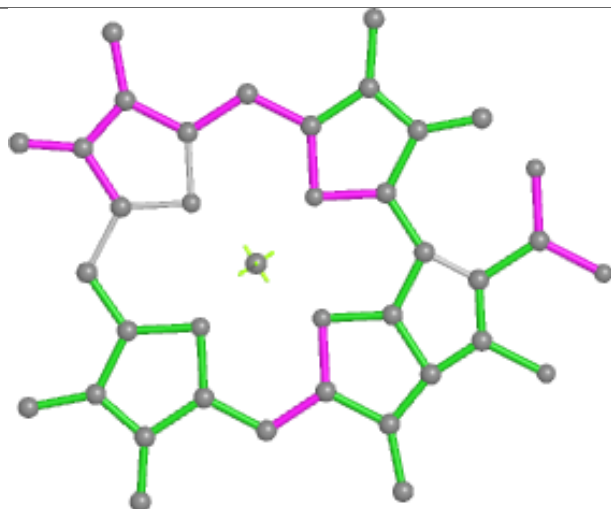




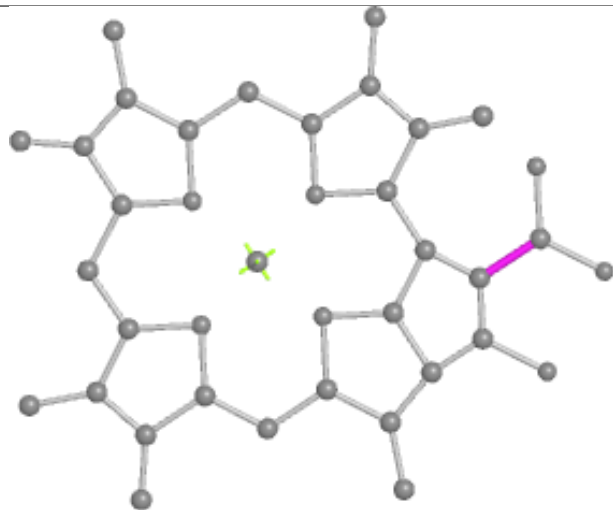
Ligand CLA 3 611



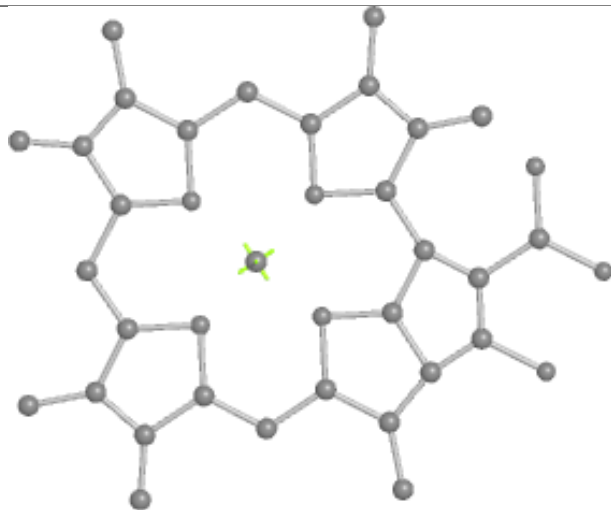
Bond lengths



Bond angles

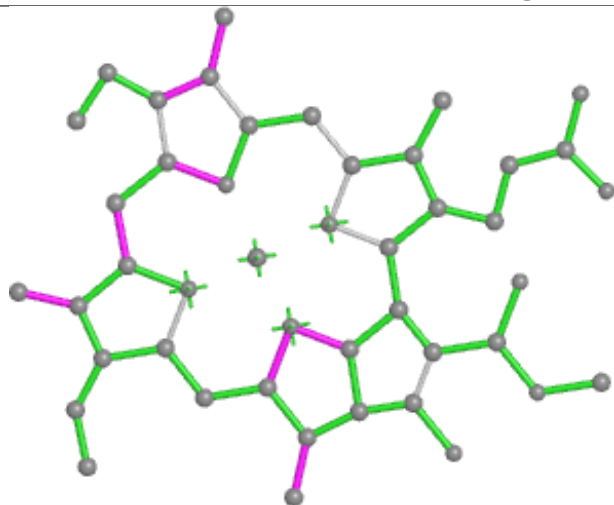


Torsions

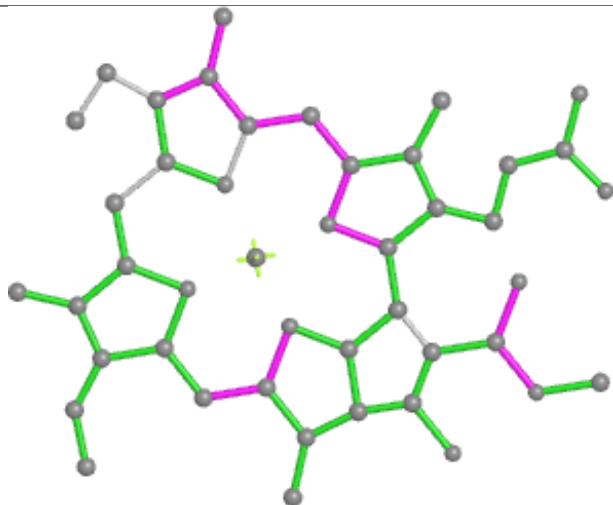


Rings

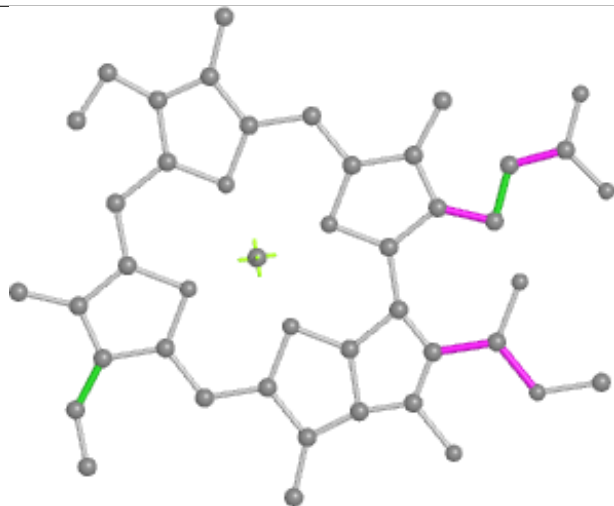
Ligand CLA 6 617



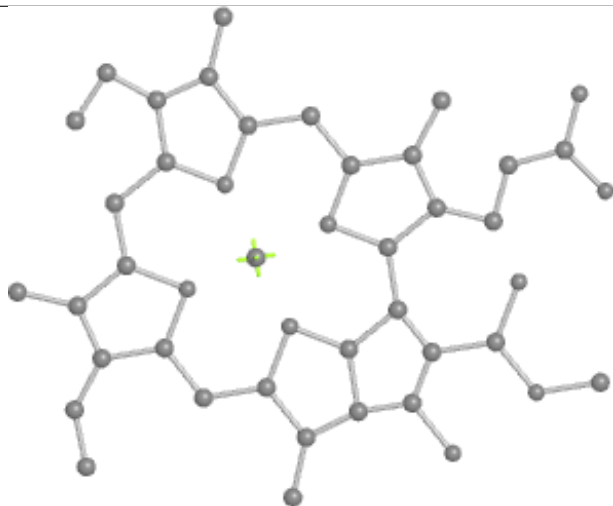
Bond lengths



Bond angles

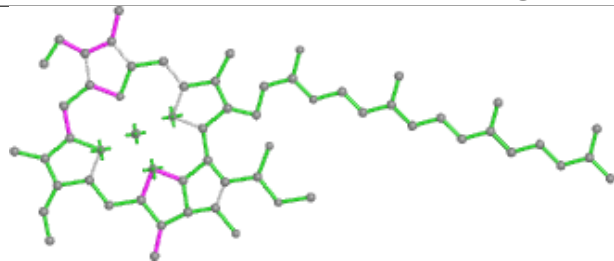


Torsions

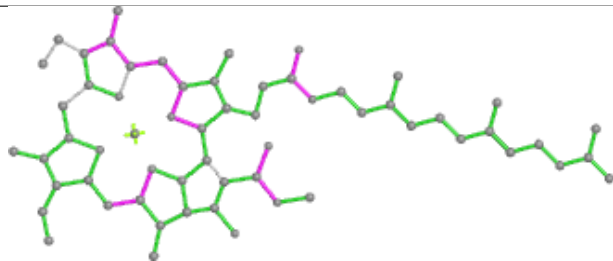


Rings

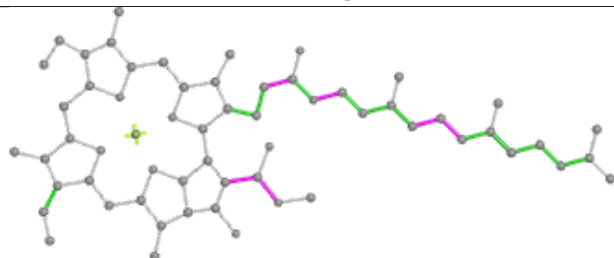
Ligand CLA B 834



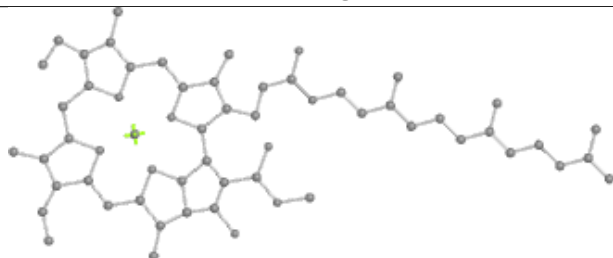
Bond lengths



Bond angles

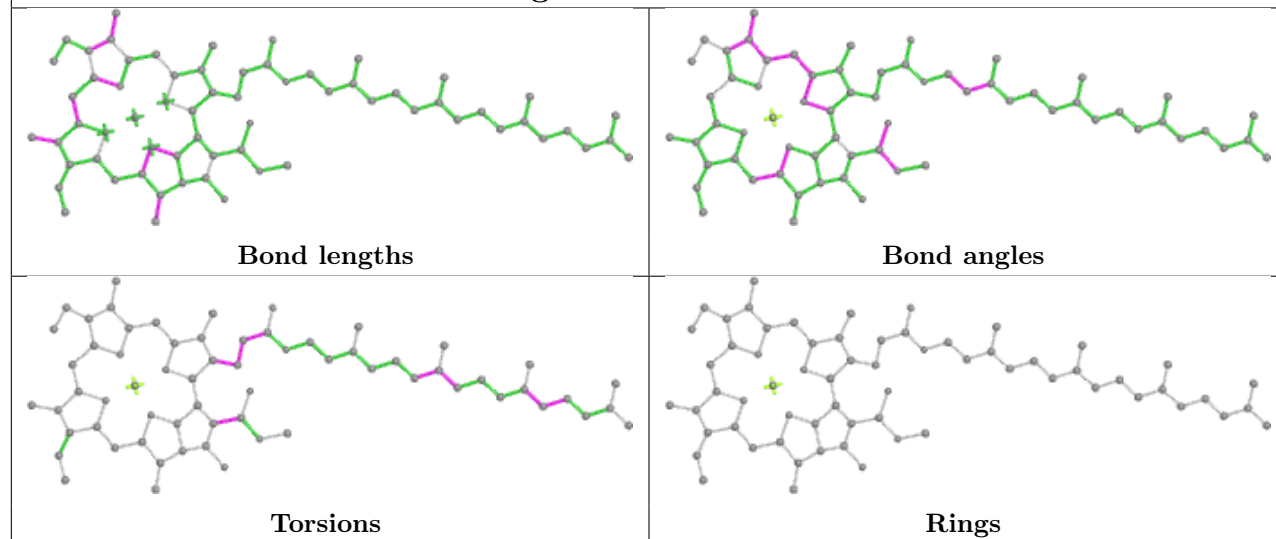


Torsions

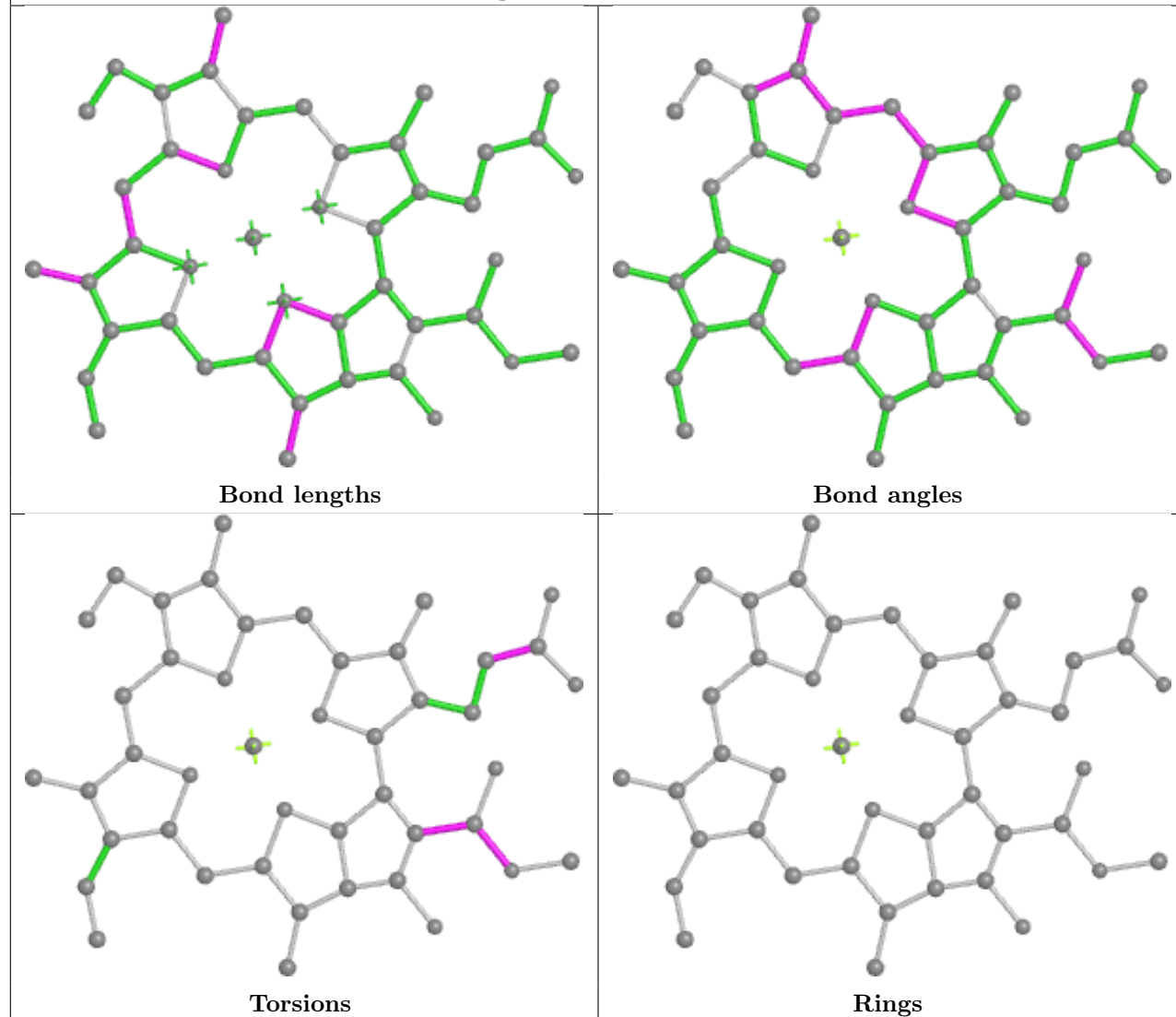


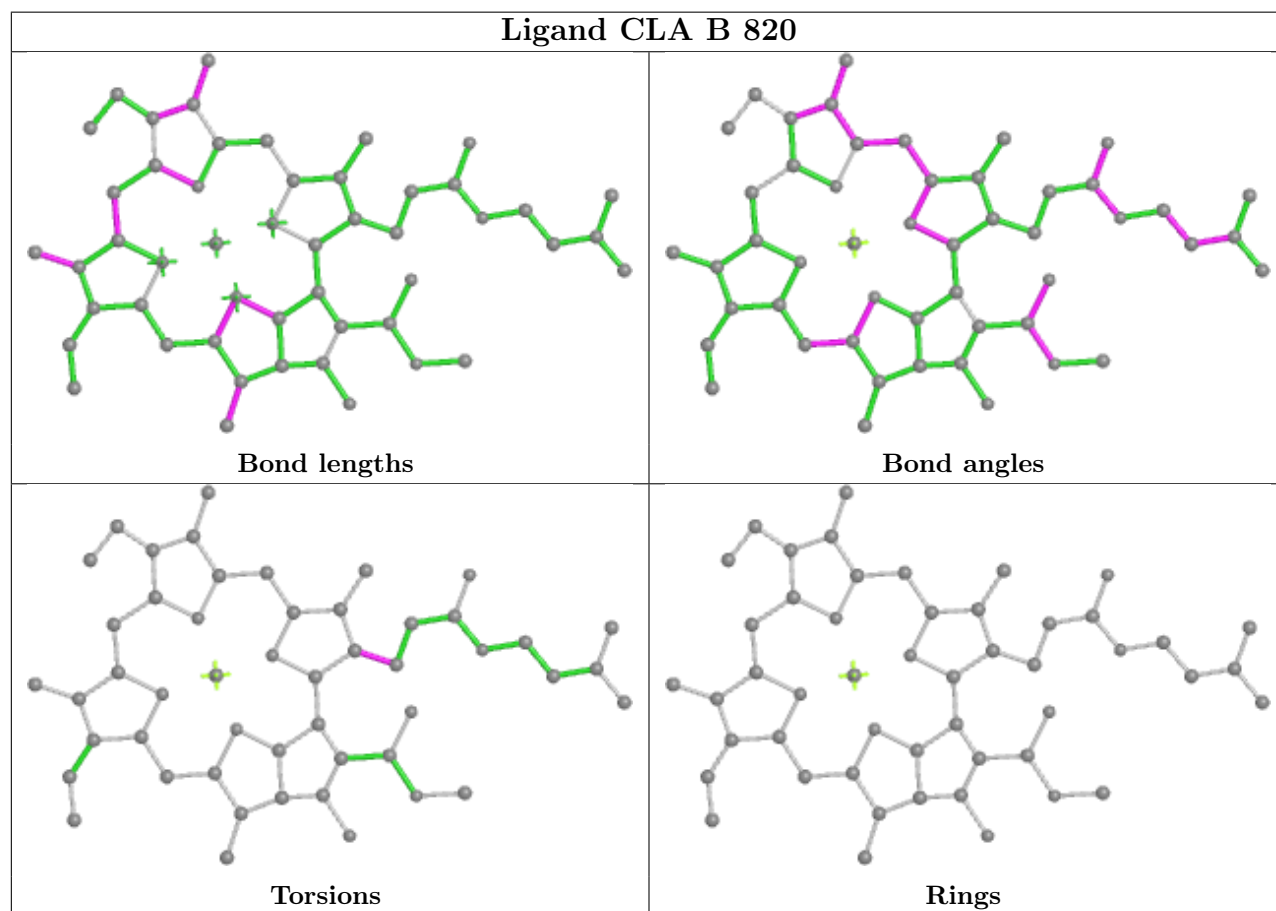
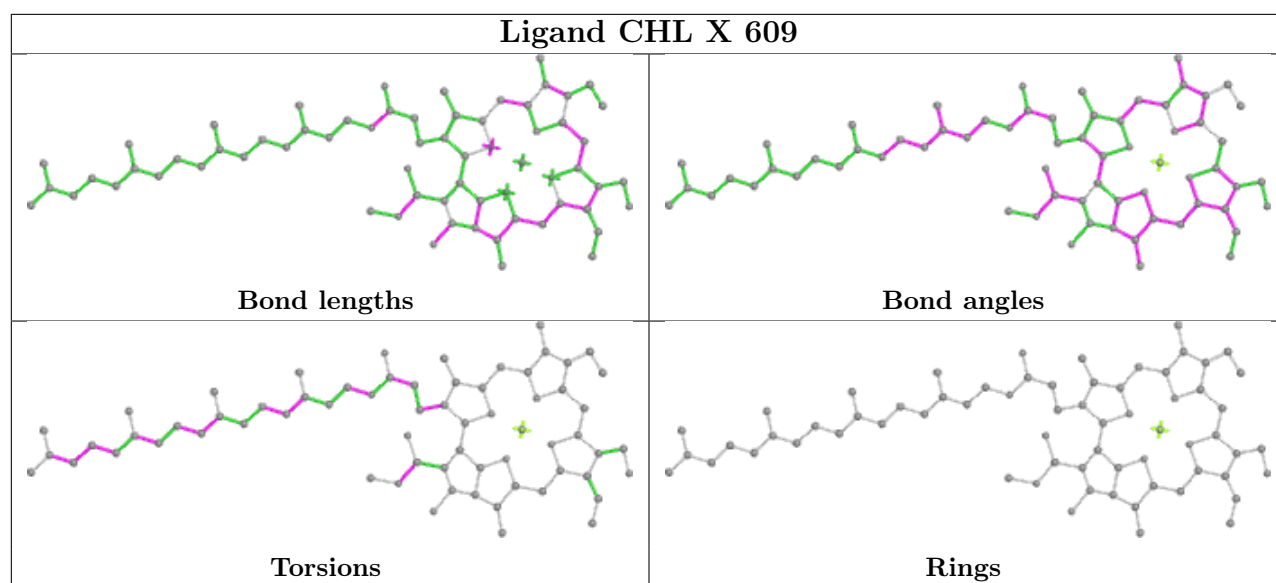
Rings

Ligand CLA H 203

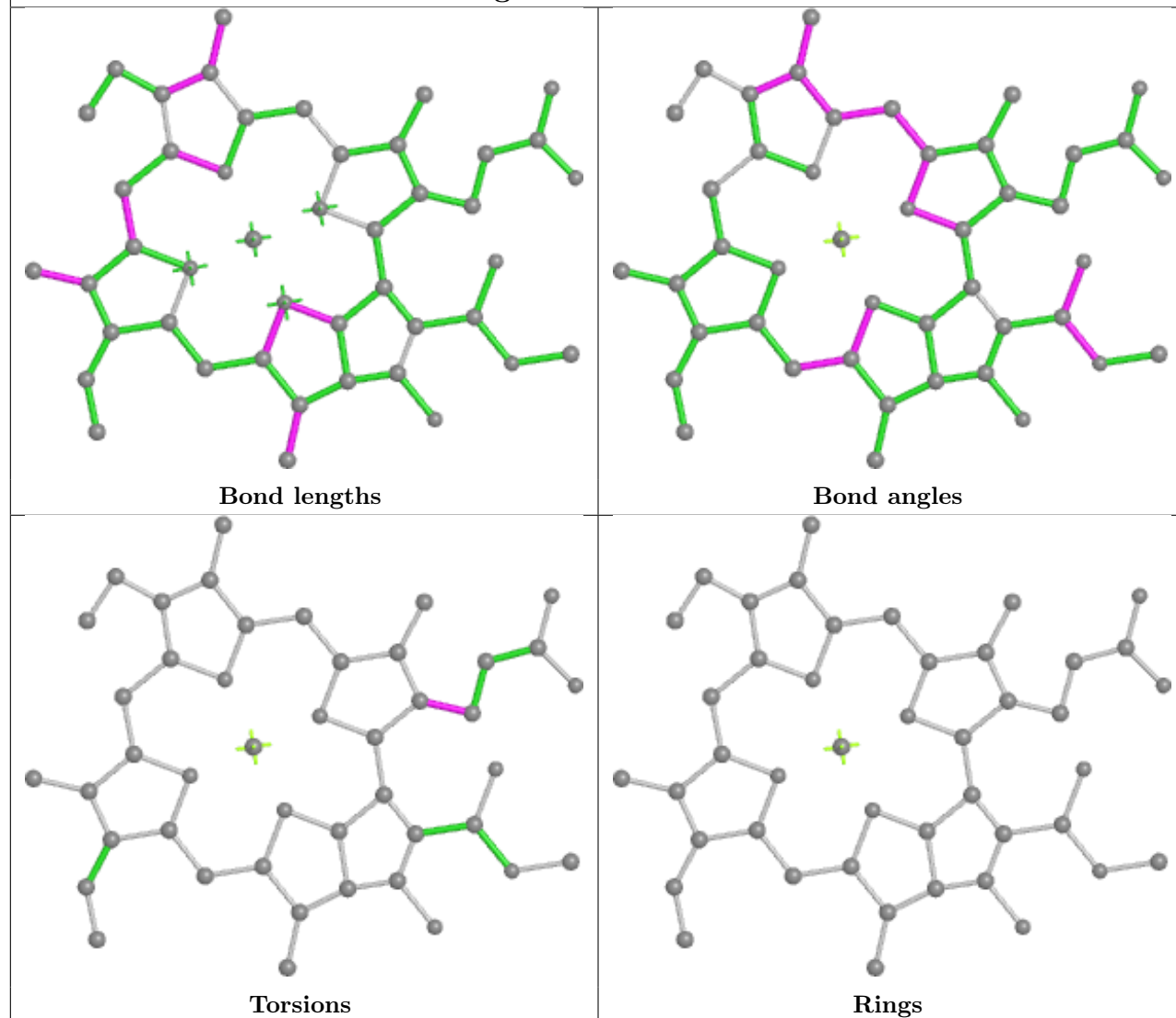


Ligand CLA 1 612

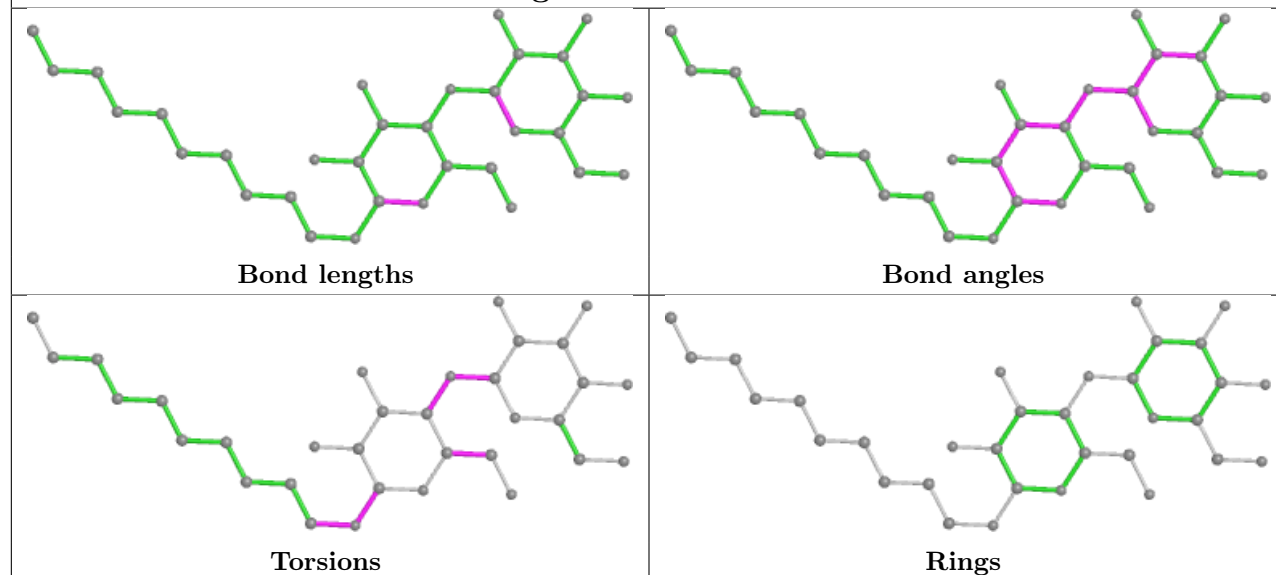




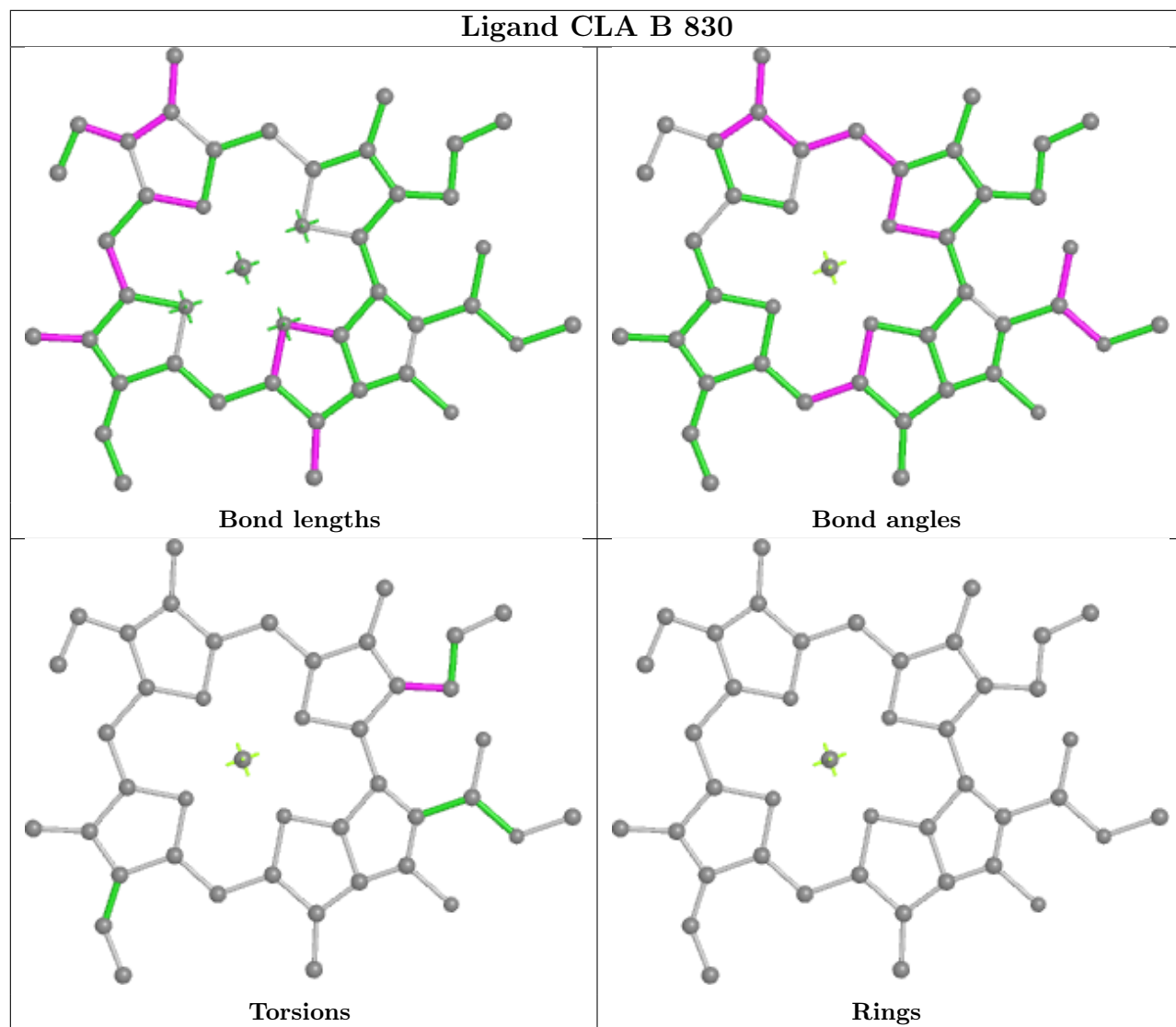
Ligand CLA 6 609

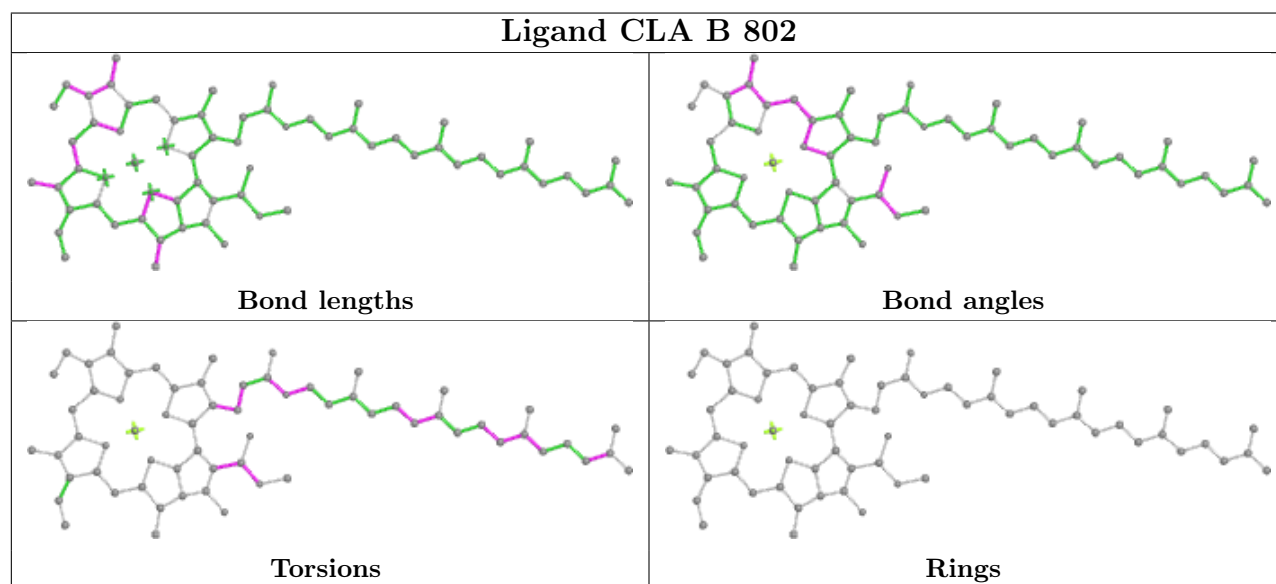
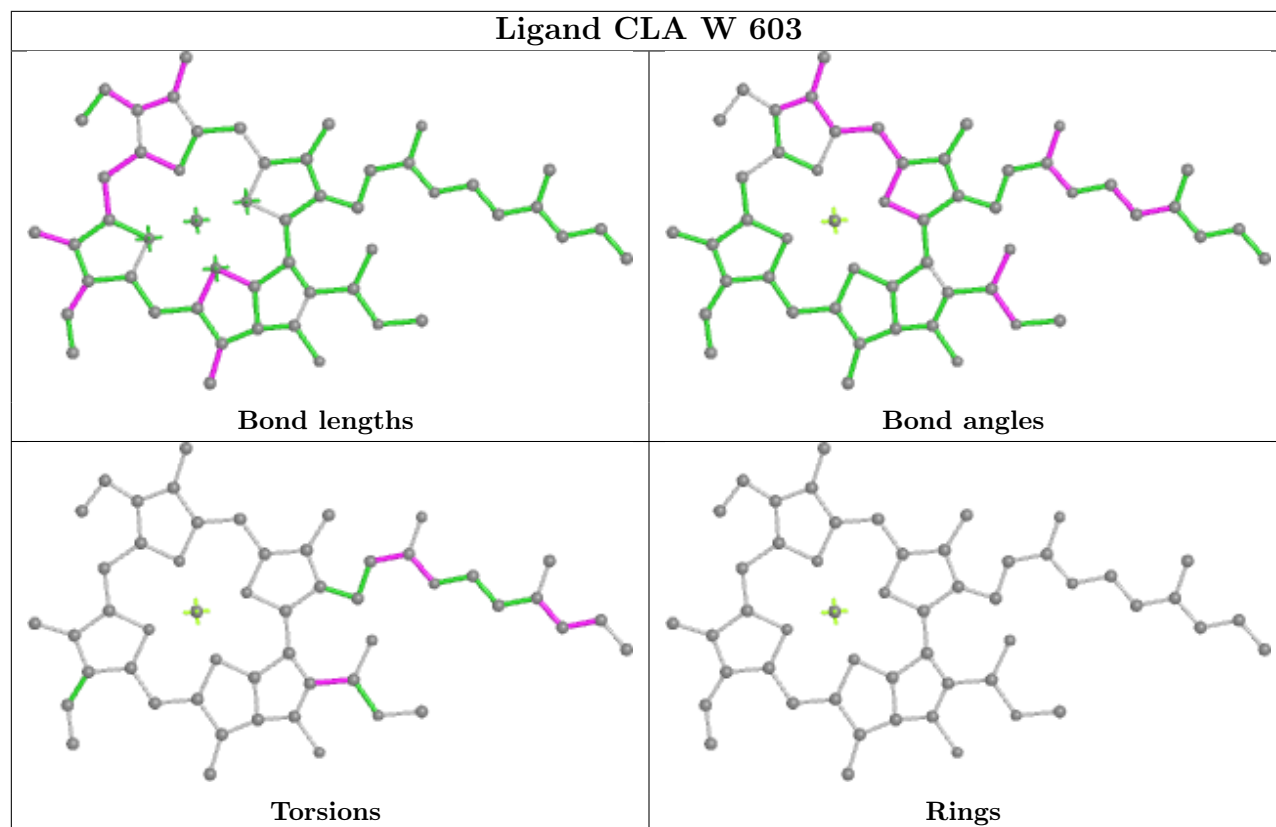


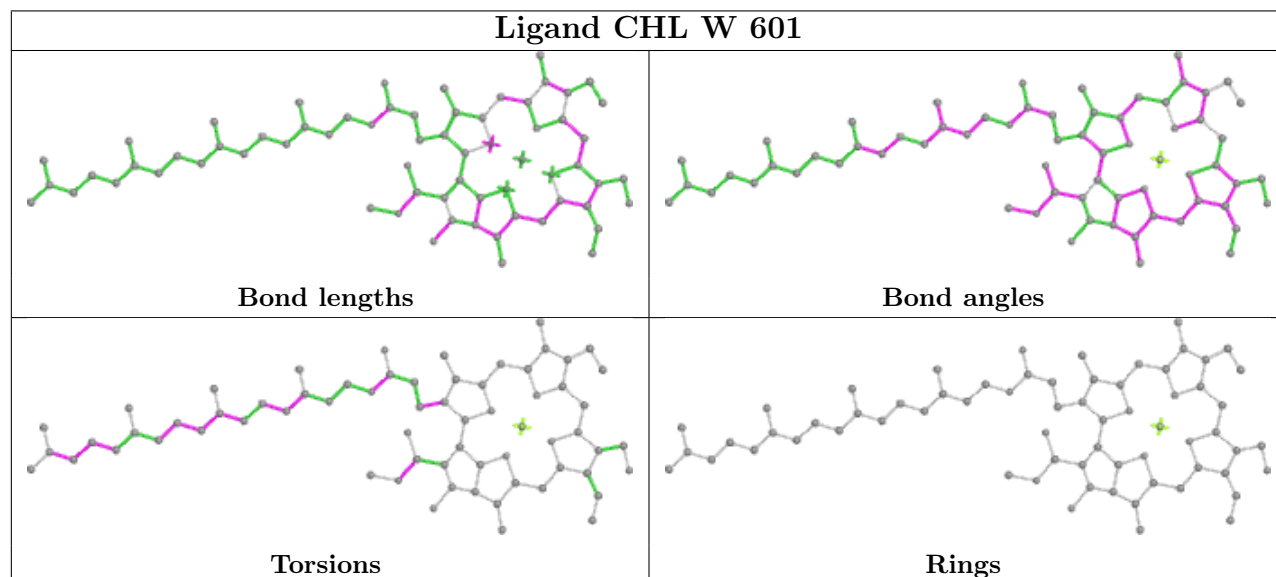
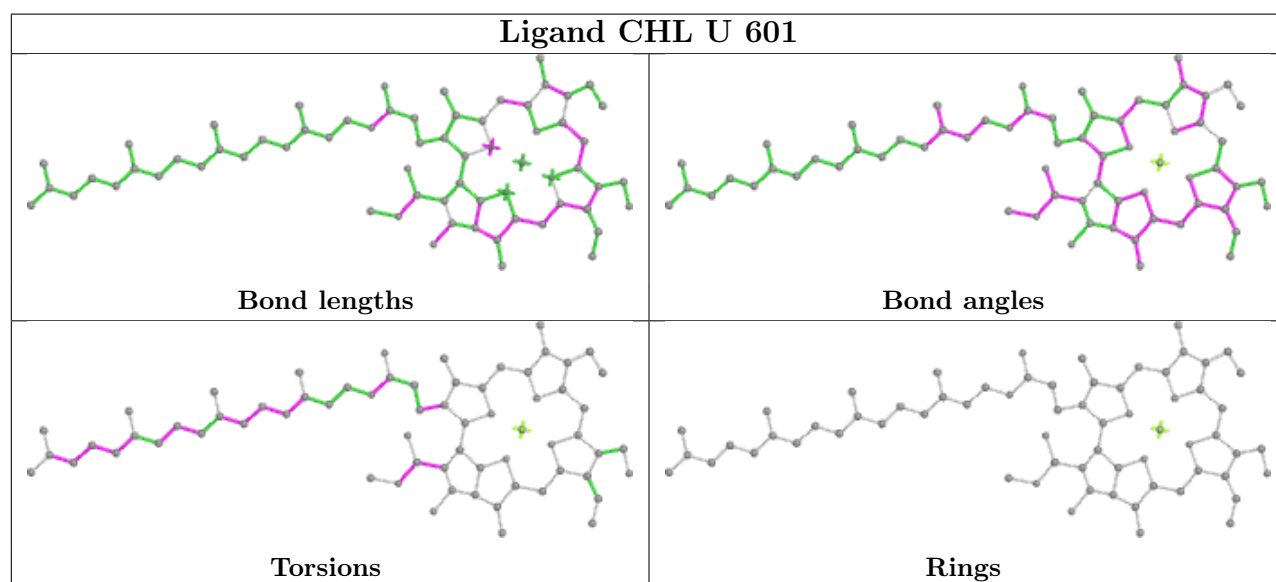
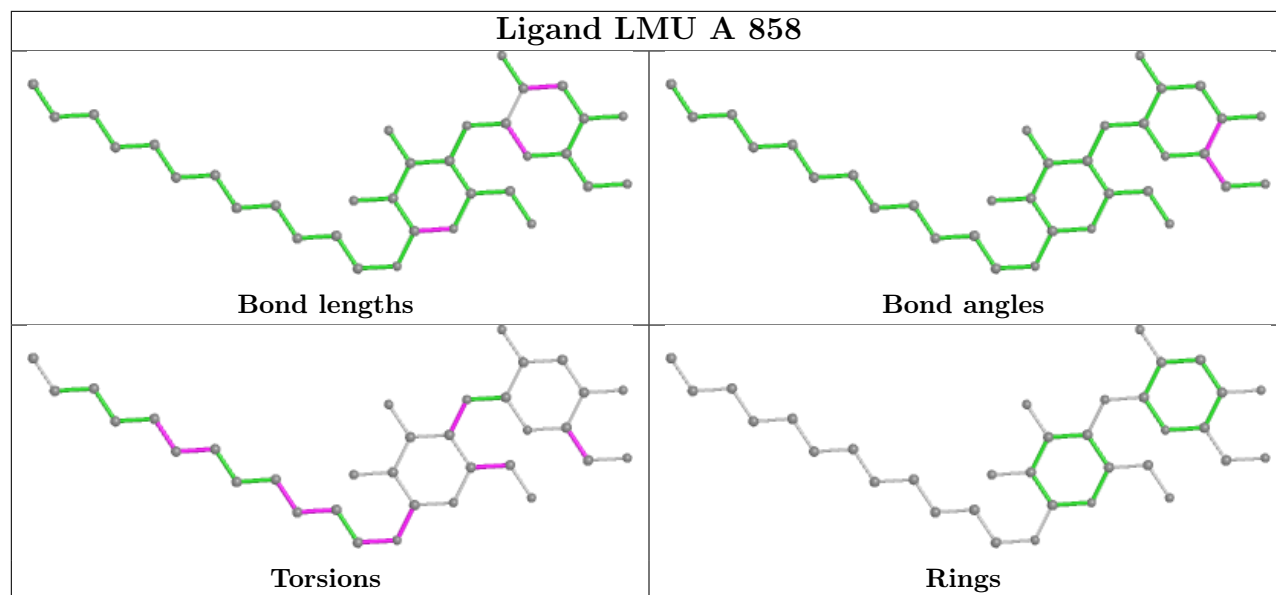
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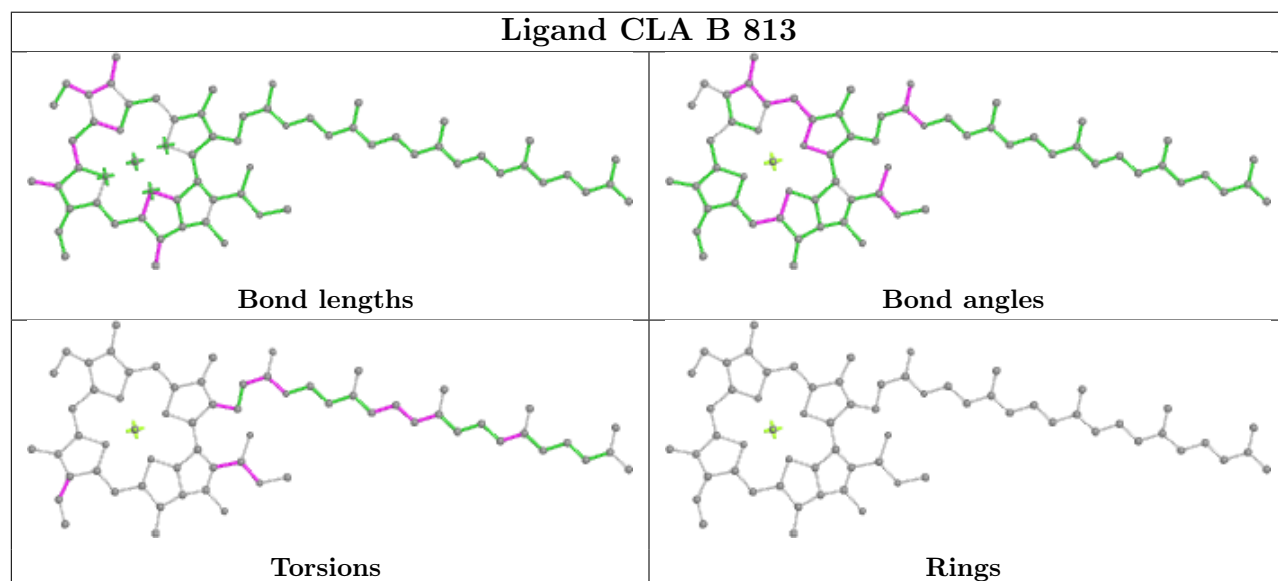
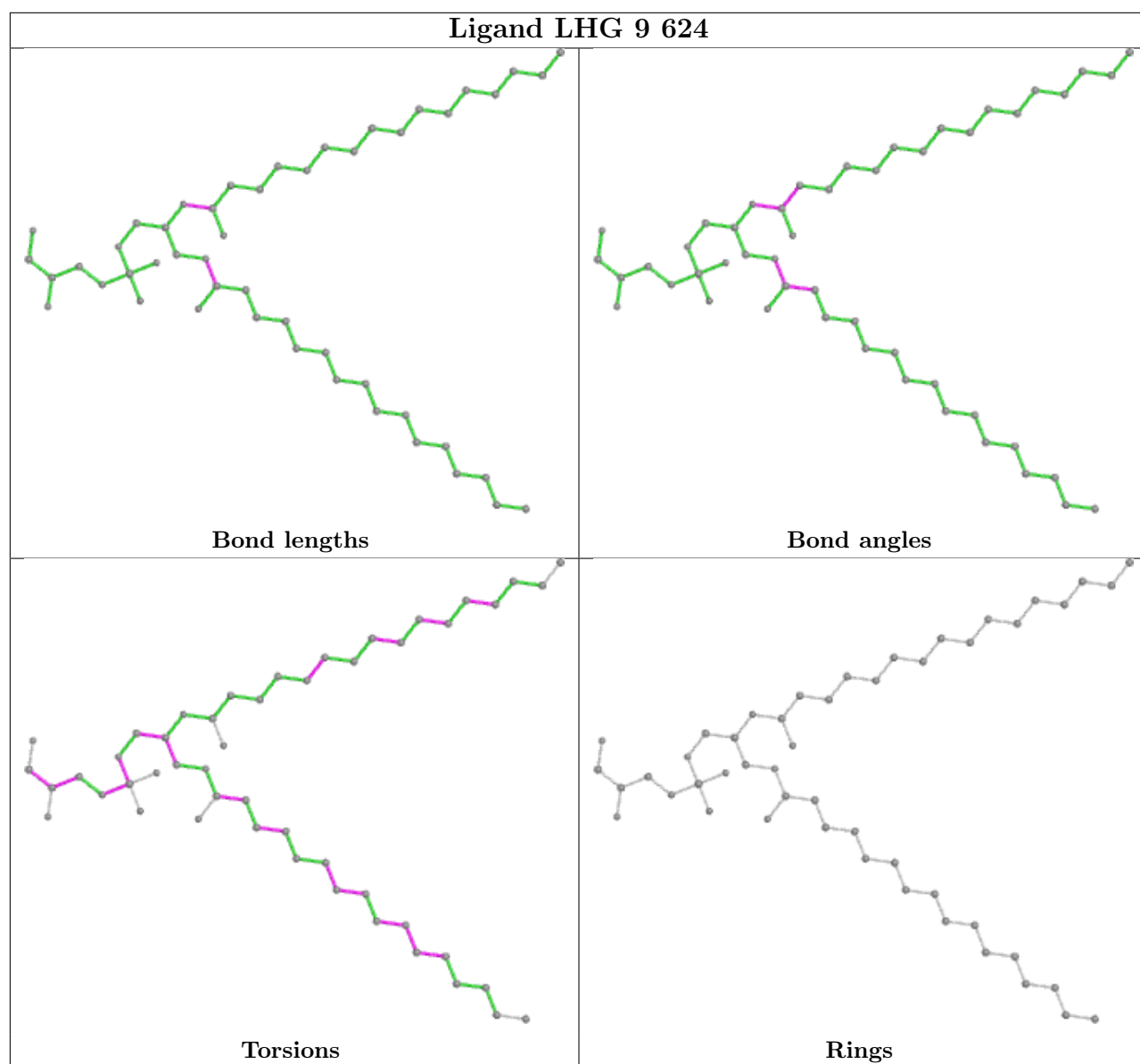


Ligand CLA B 830

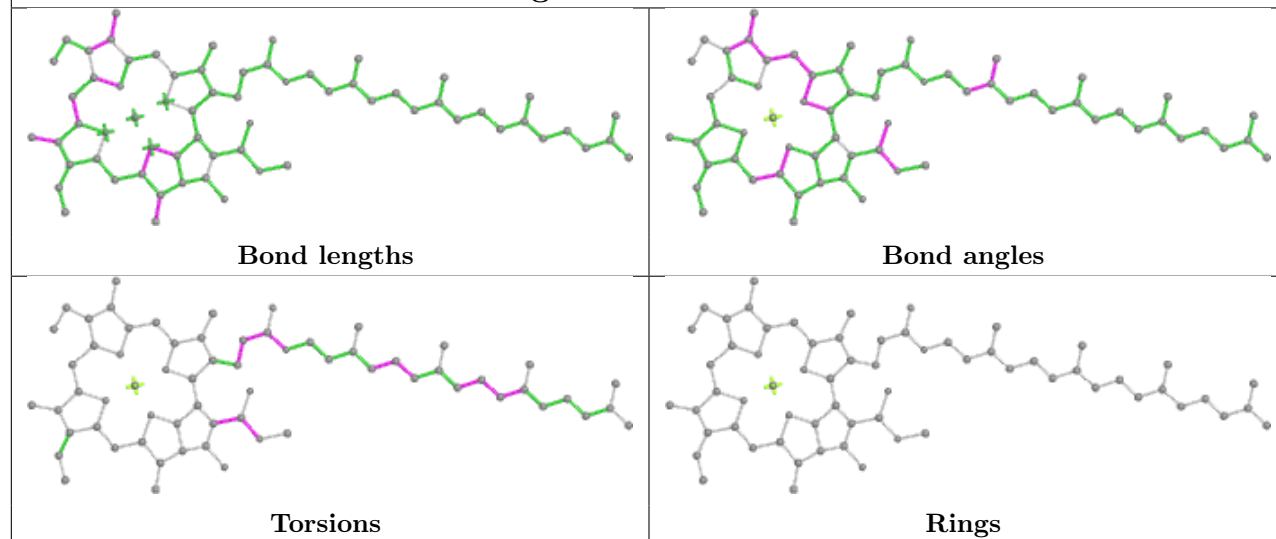




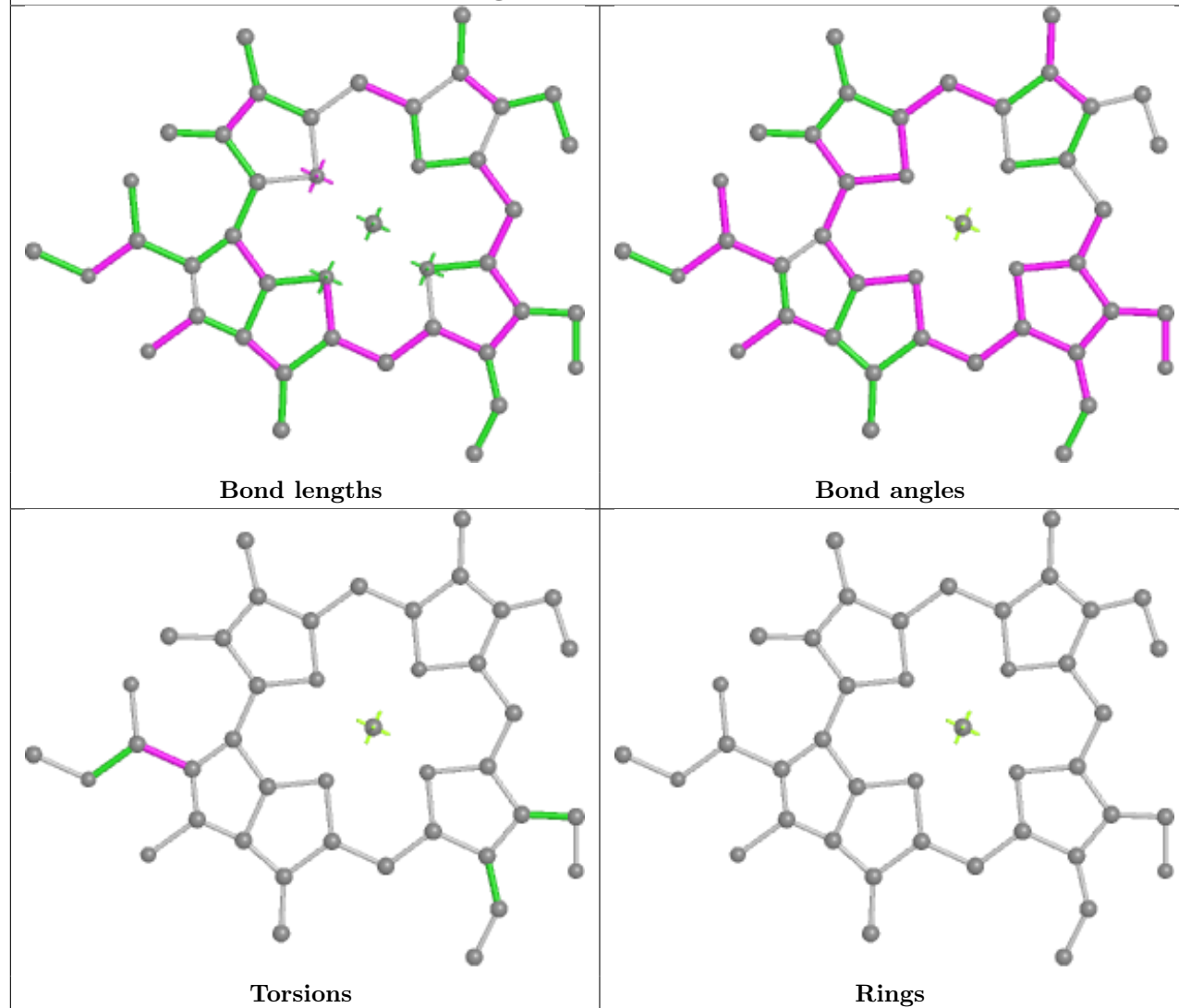




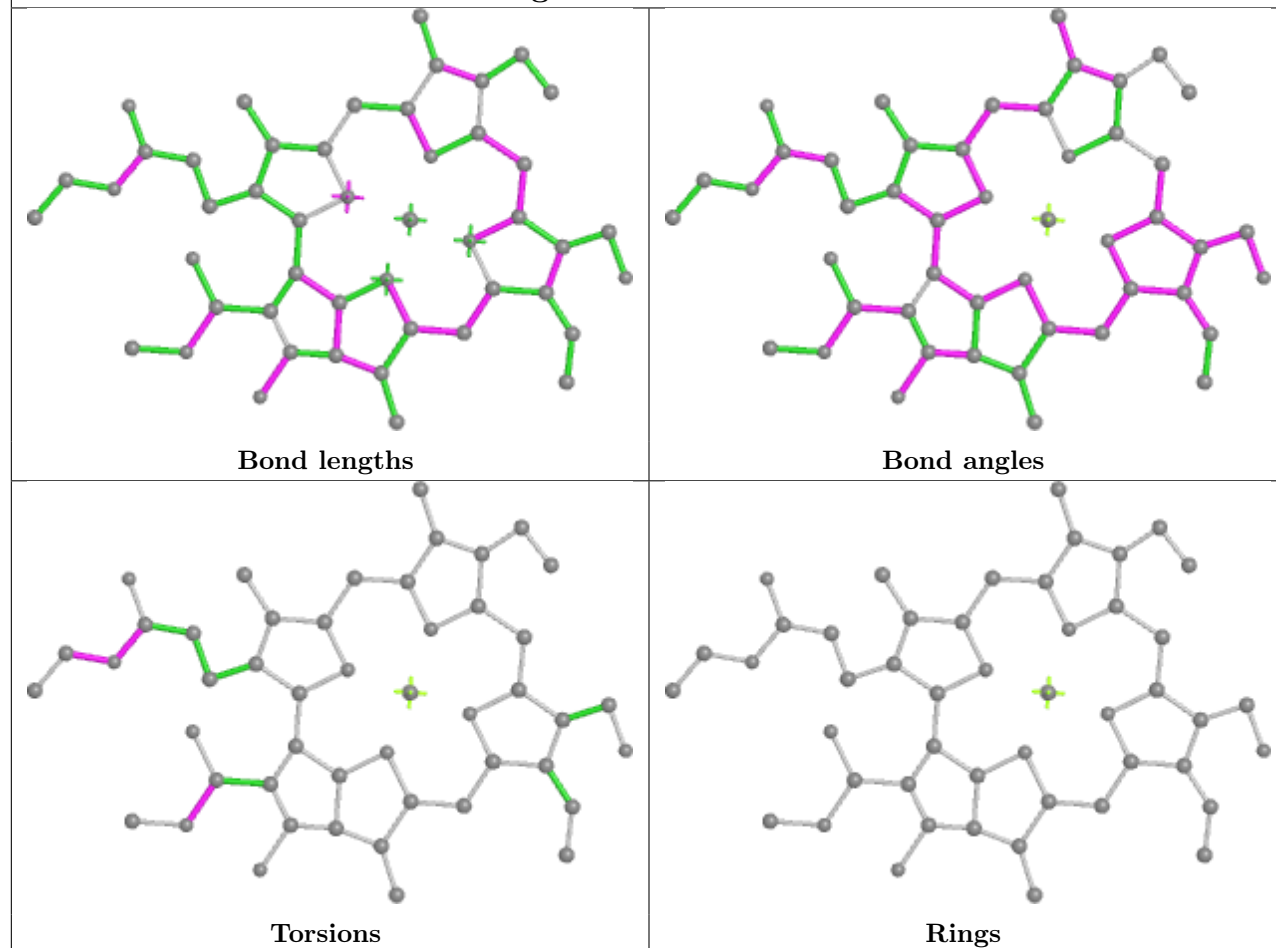
Ligand CLA A 834



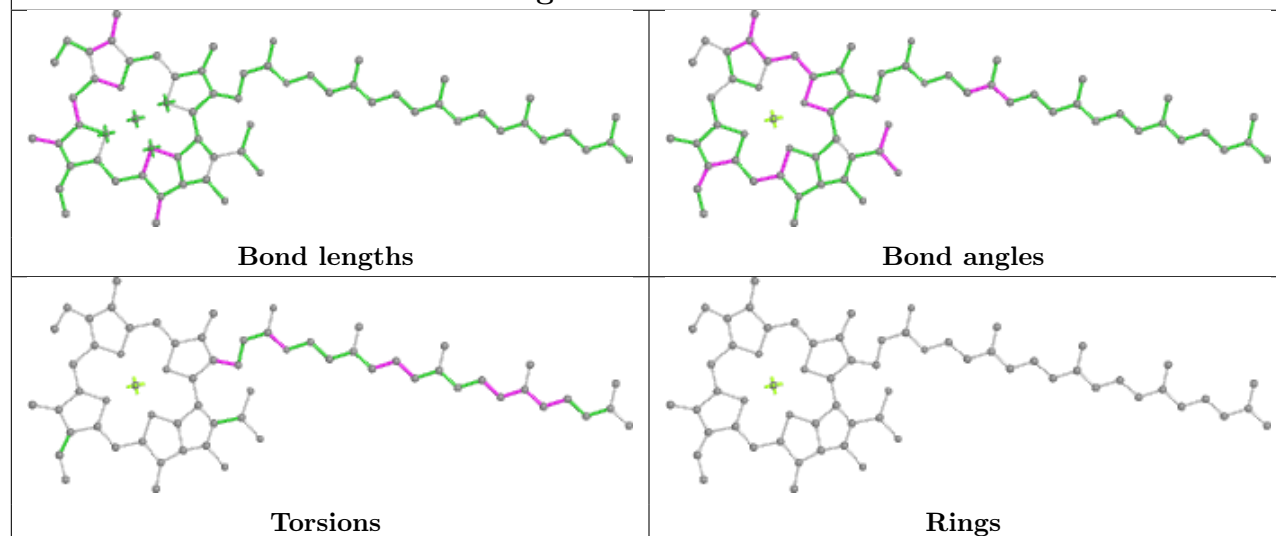
Ligand CHL Y 605

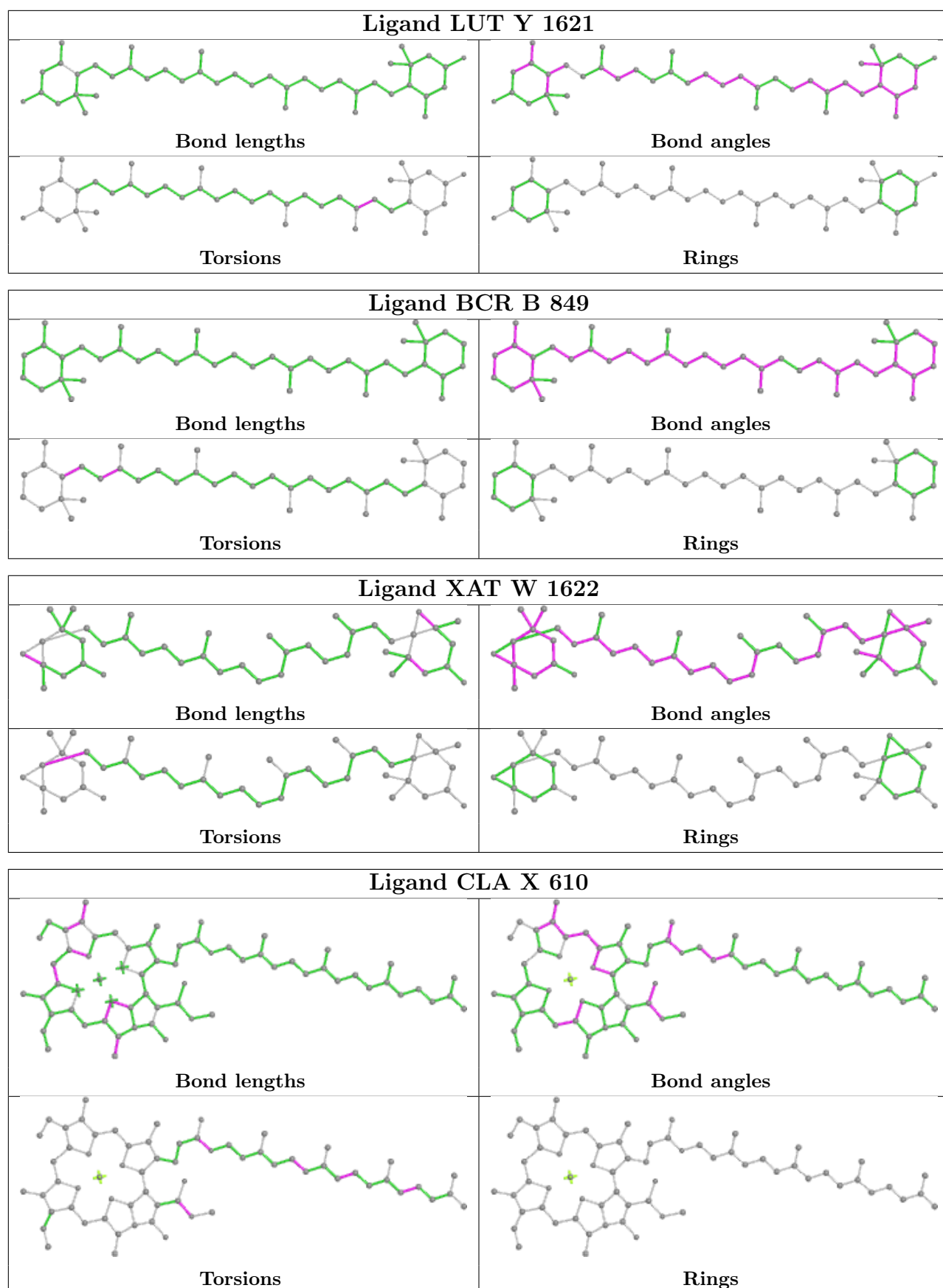


Ligand CHL V 608

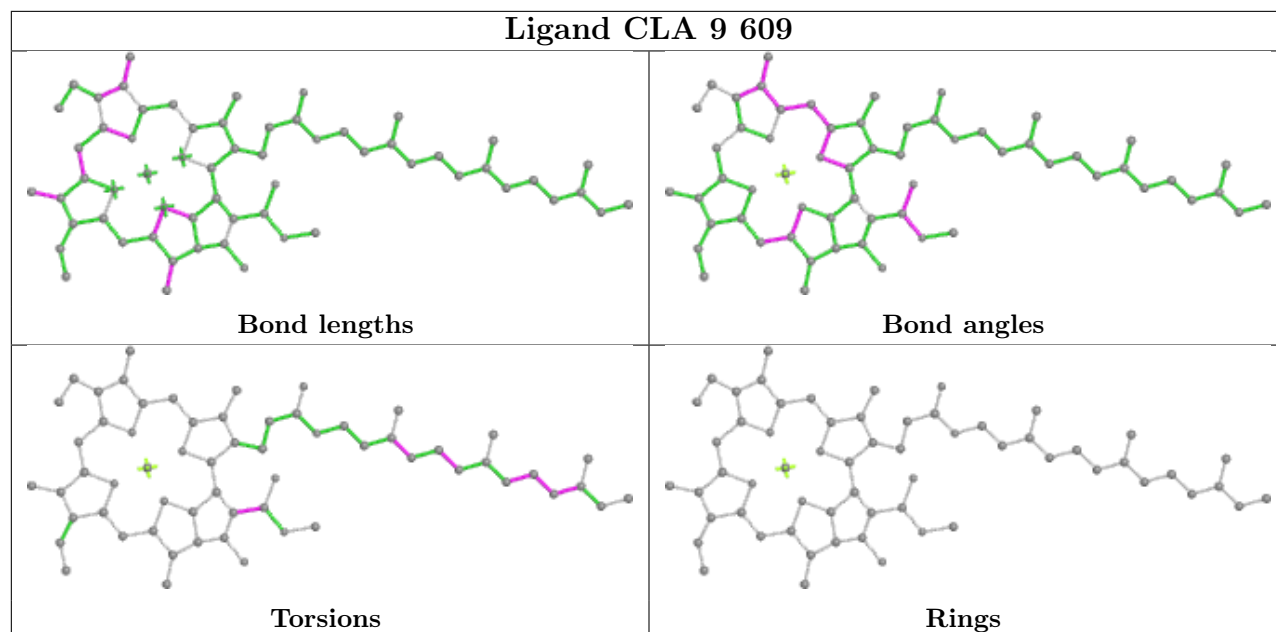


Ligand CLA a 609

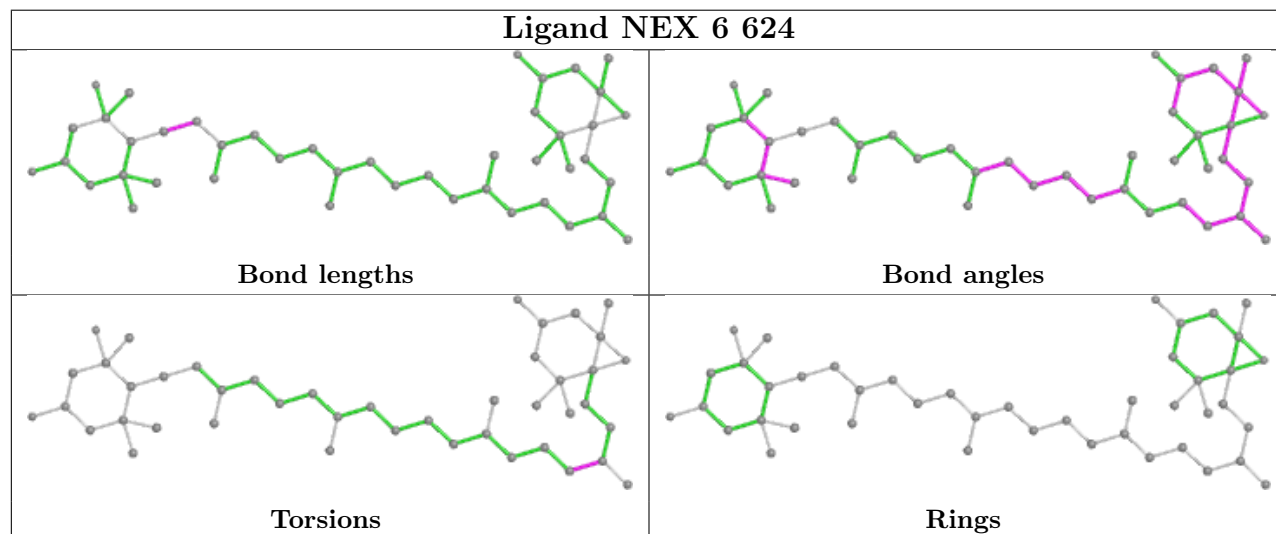




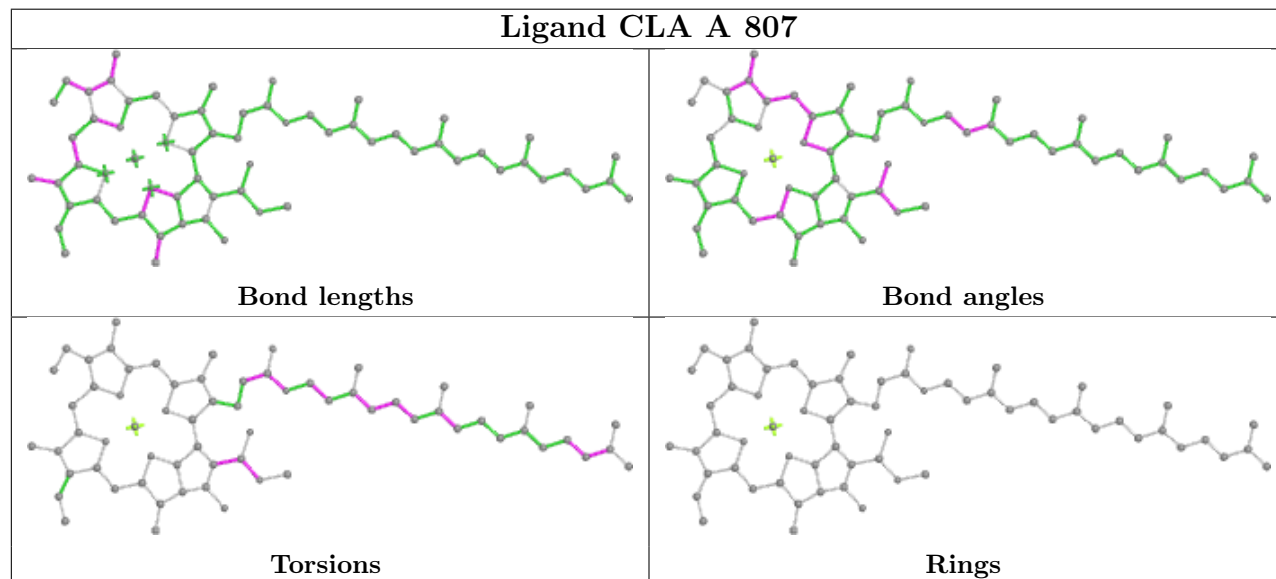
Ligand CLA 9 609



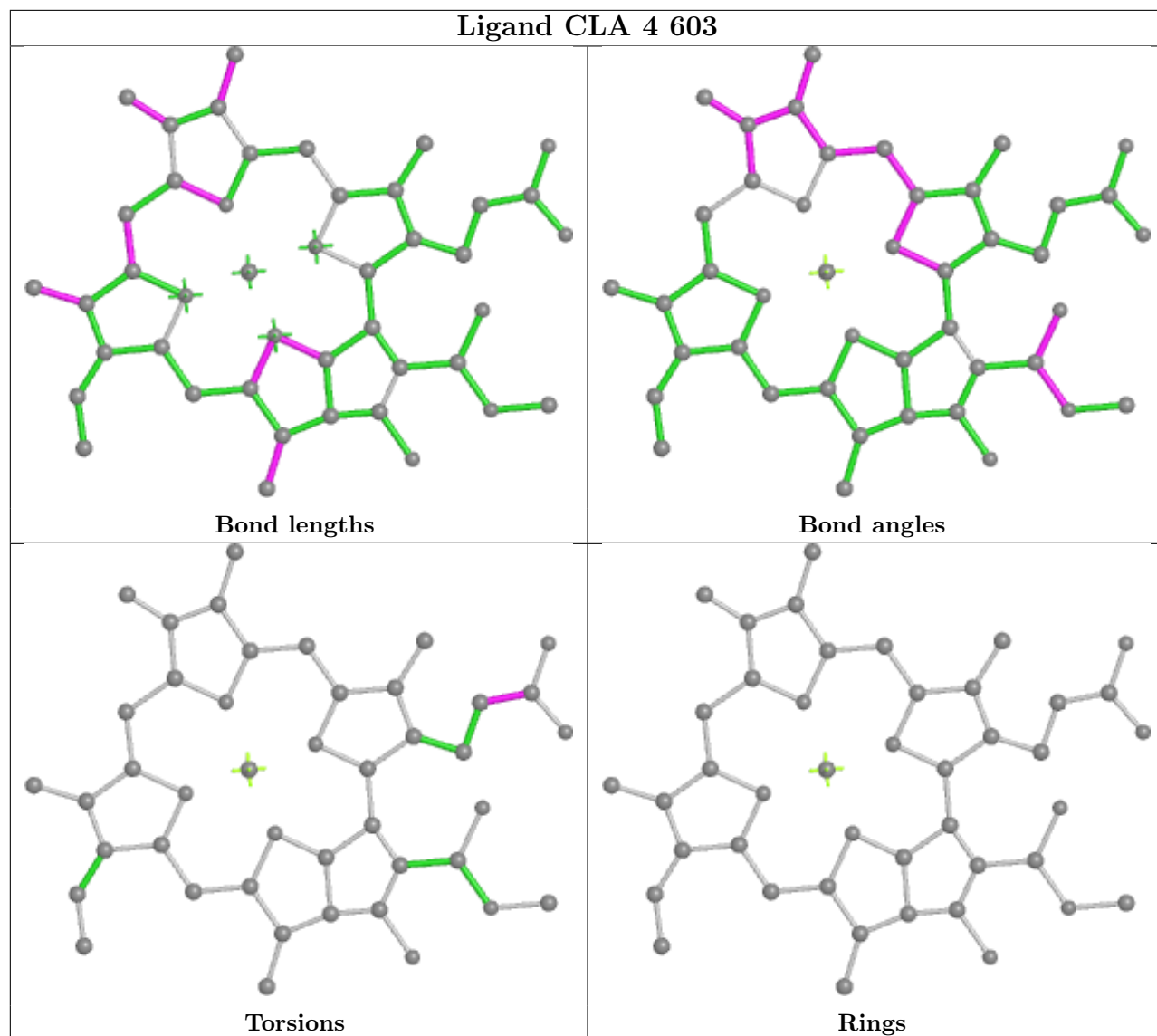
Ligand NEX 6 624



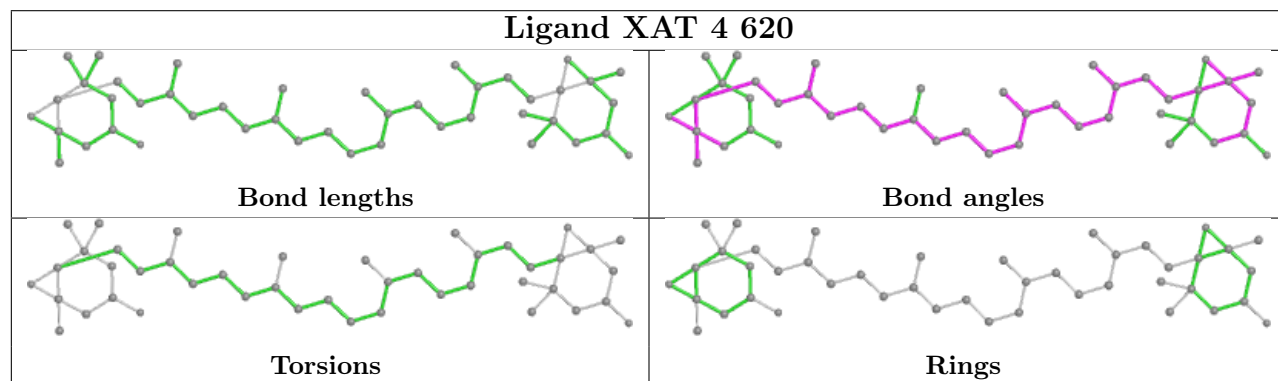
Ligand CLA A 807

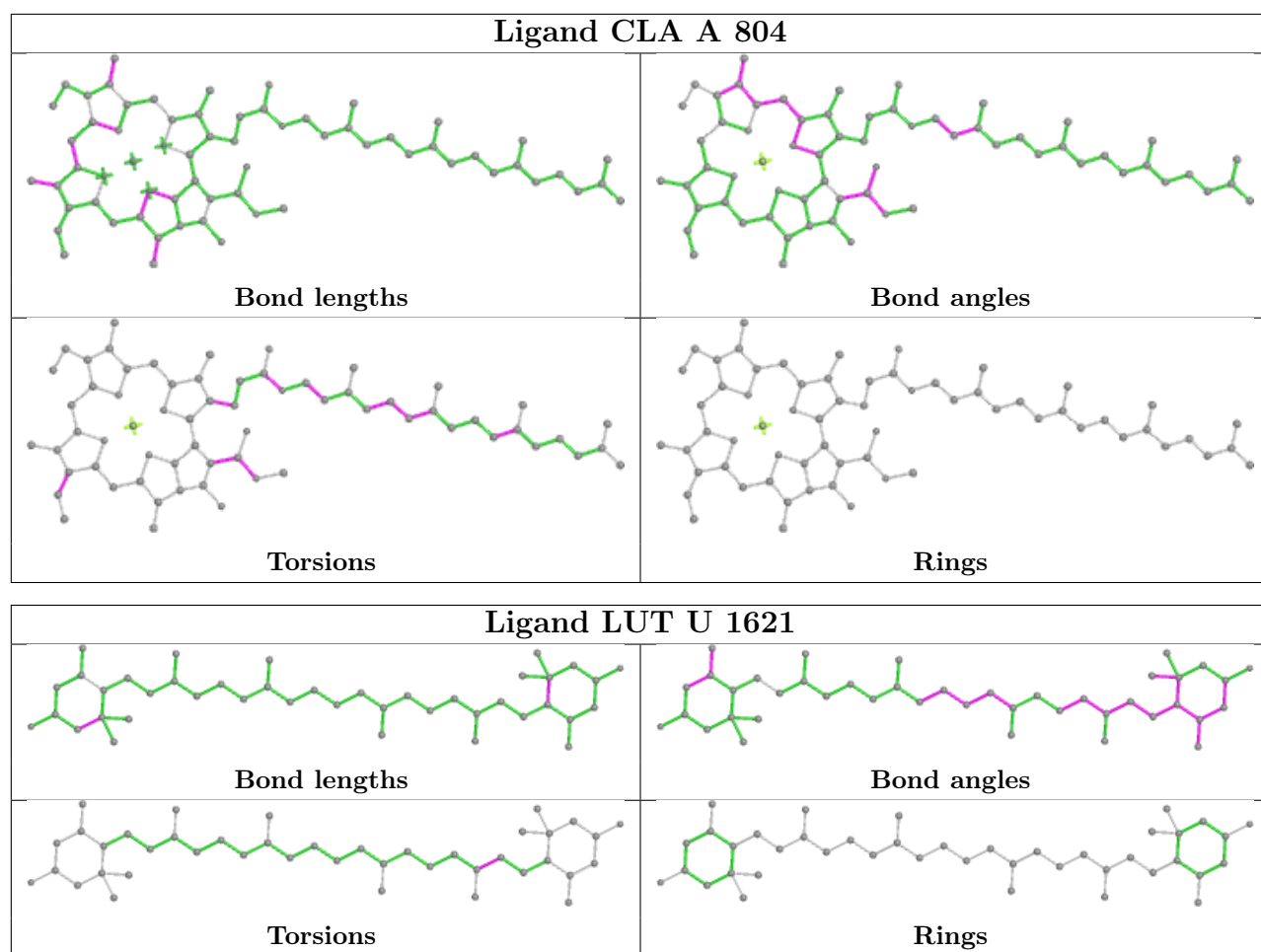


Ligand CLA 4 603

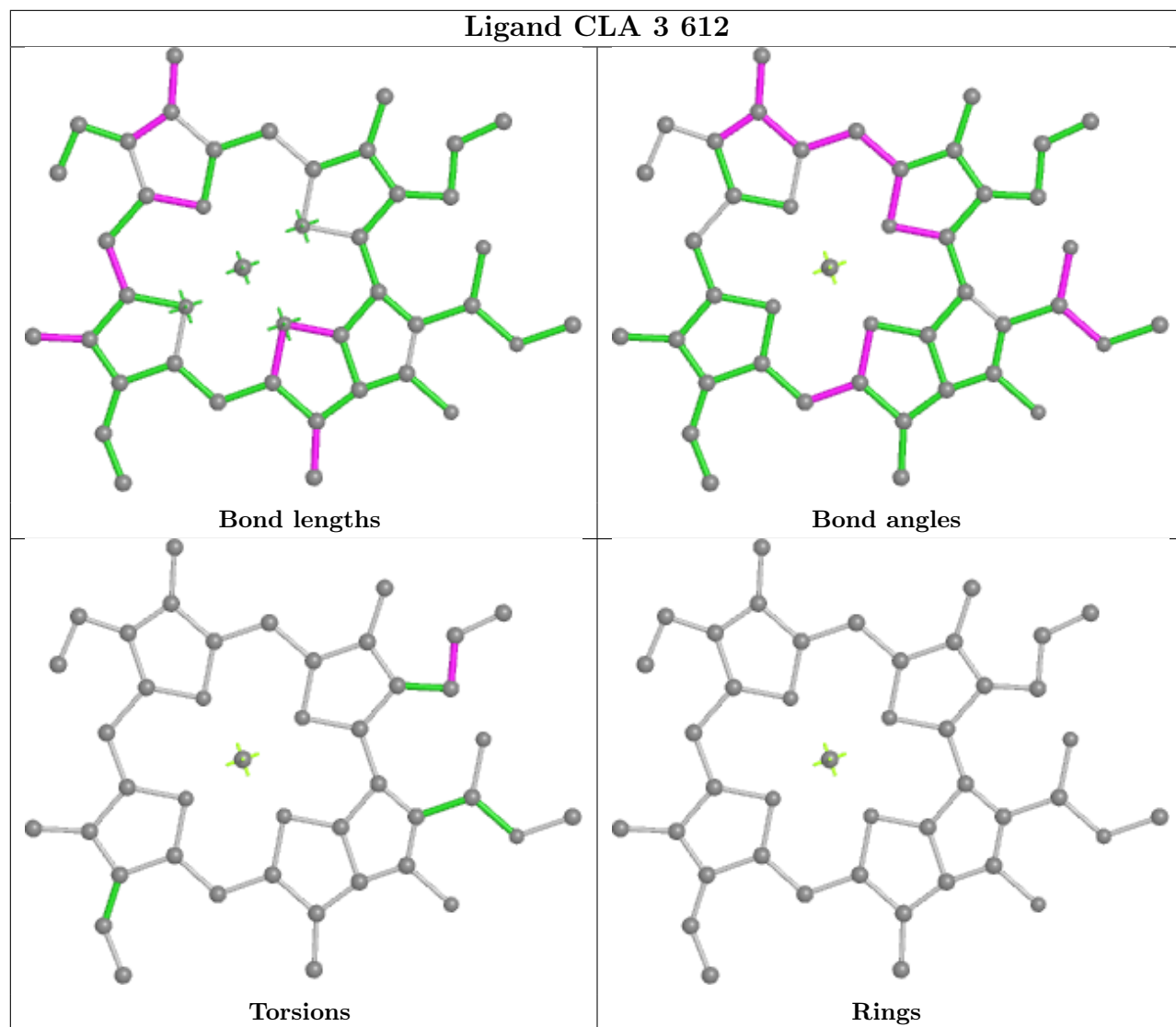


Ligand XAT 4 620

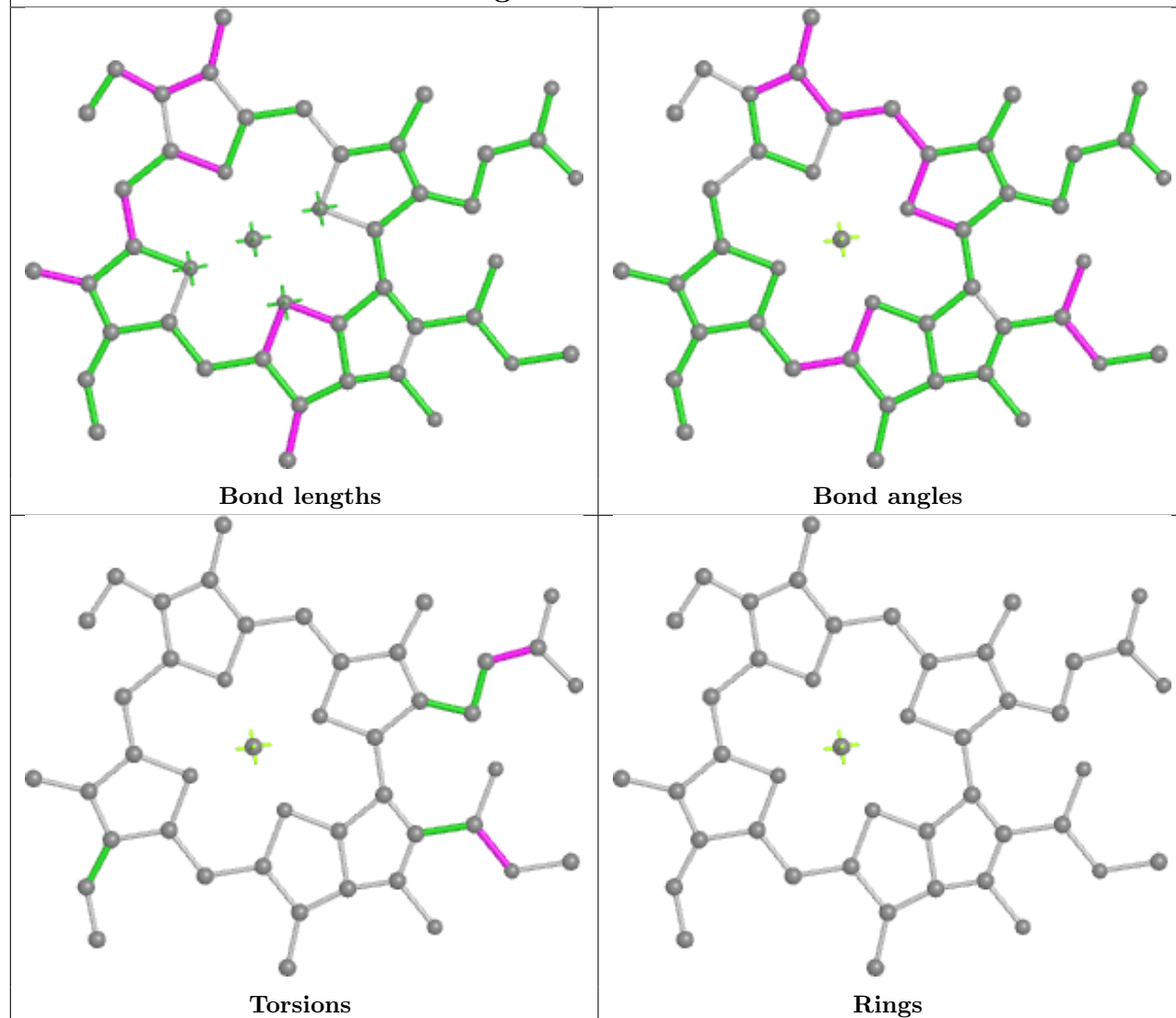




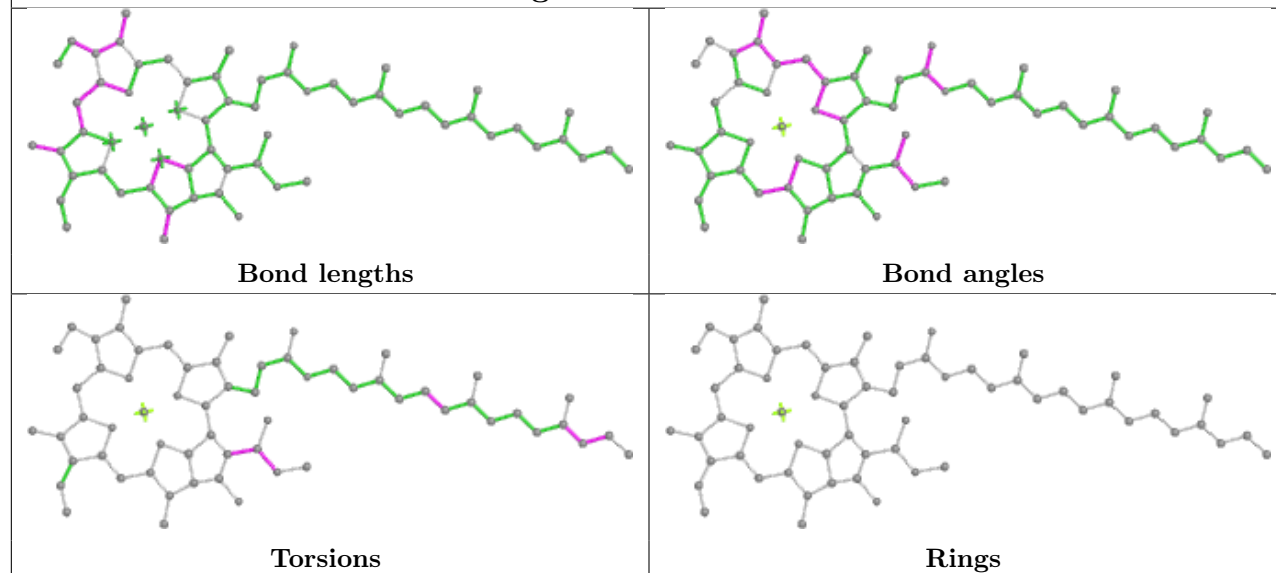
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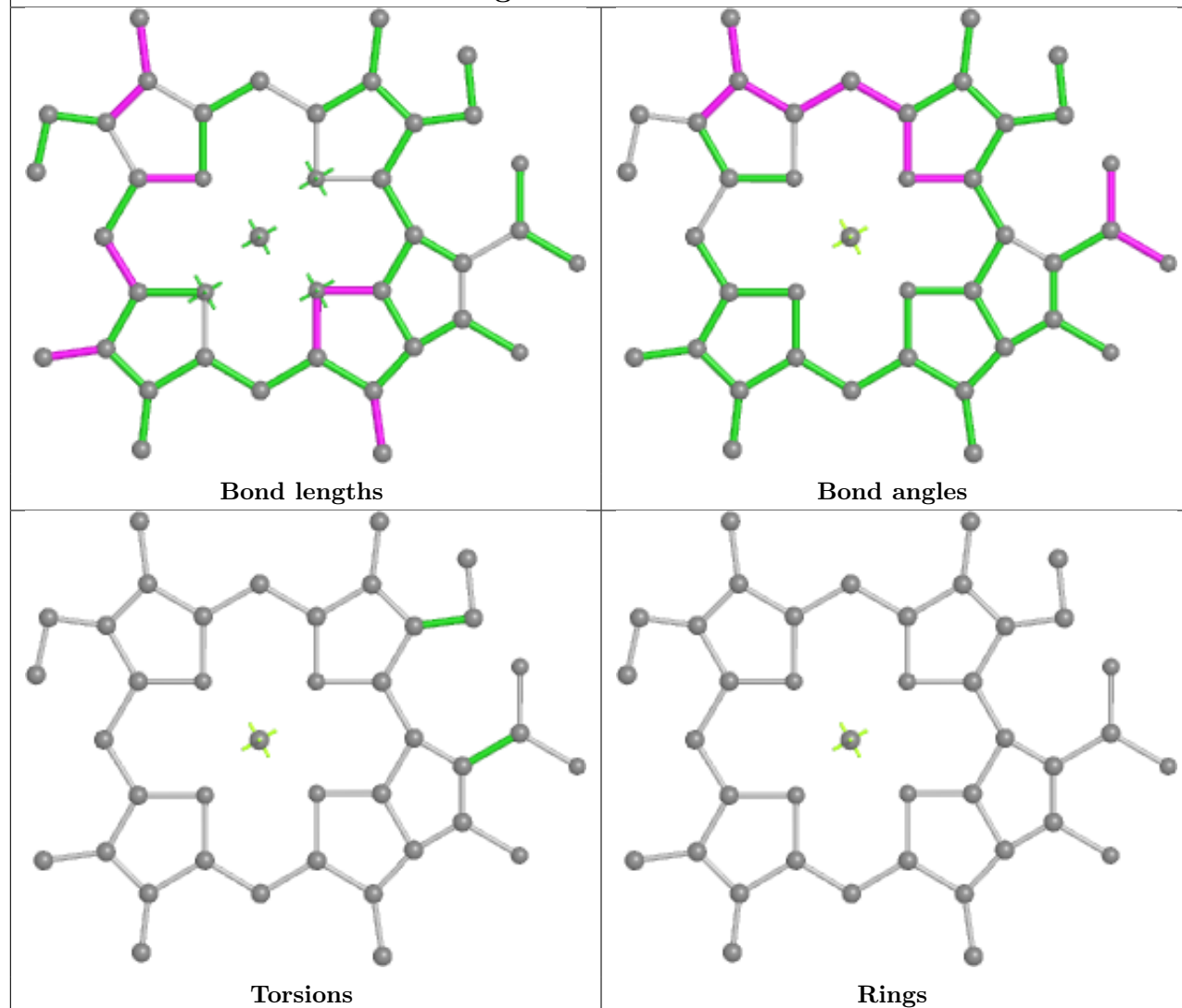
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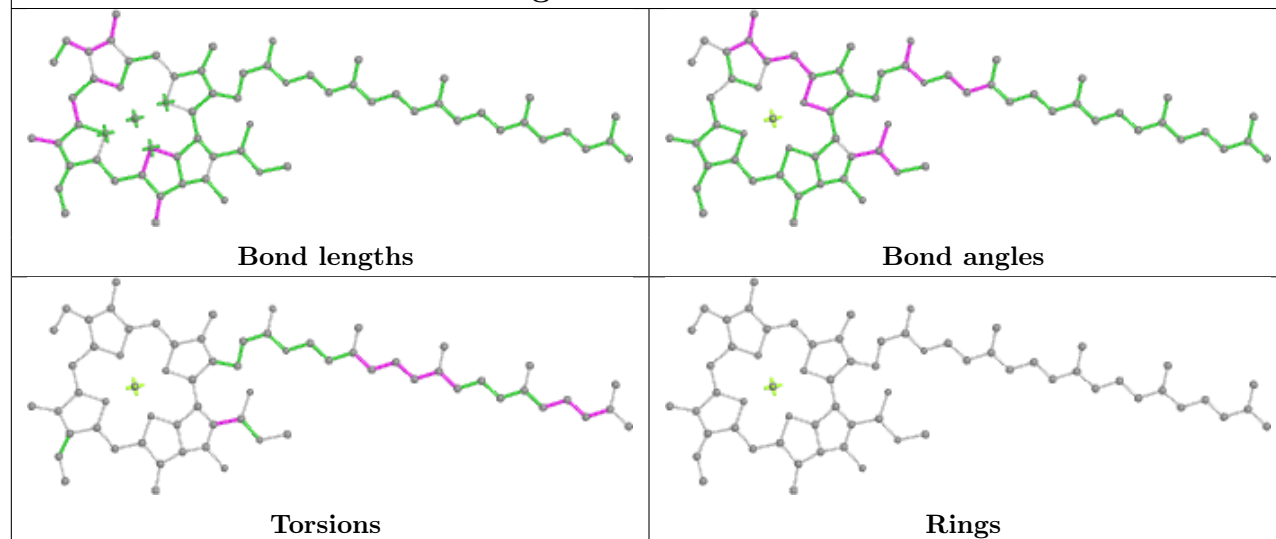
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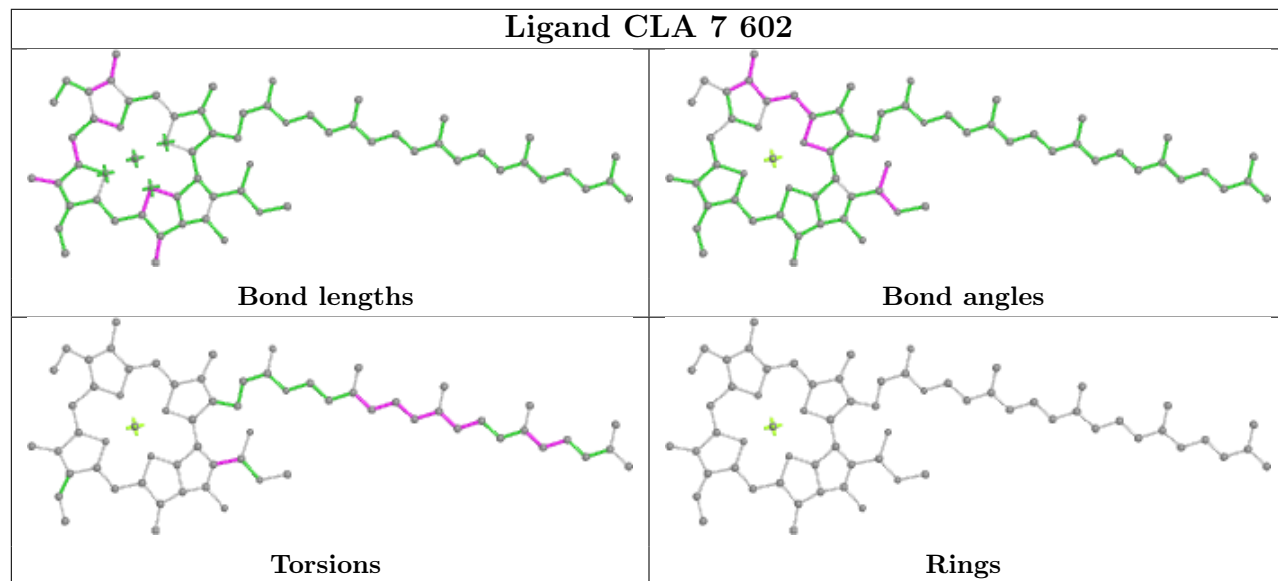
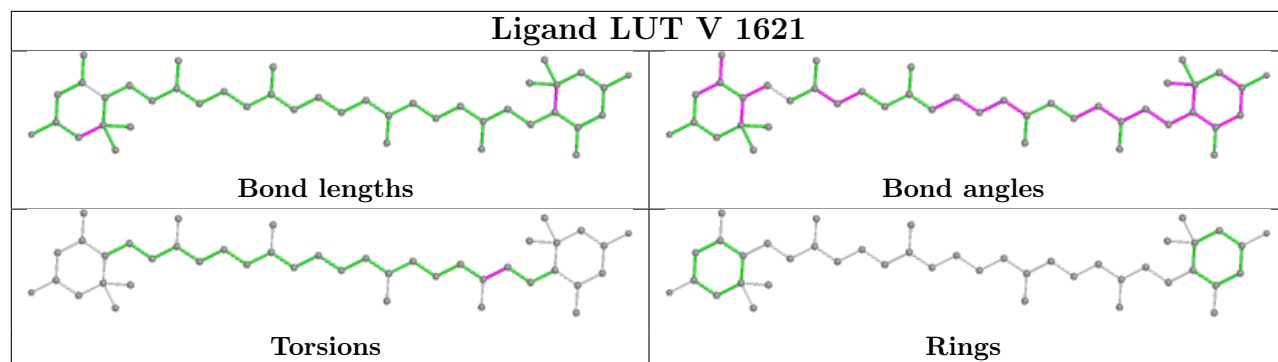


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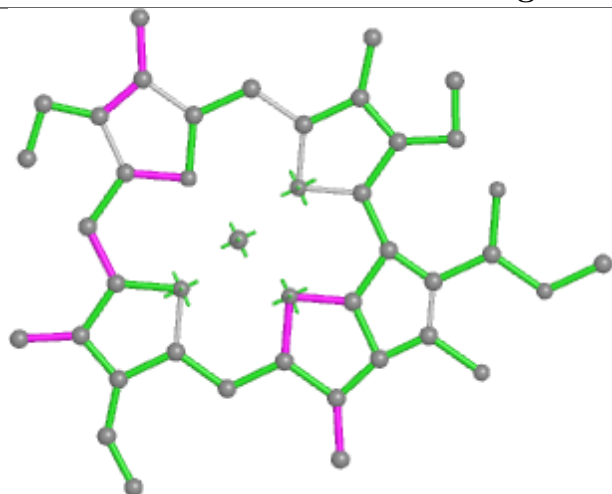


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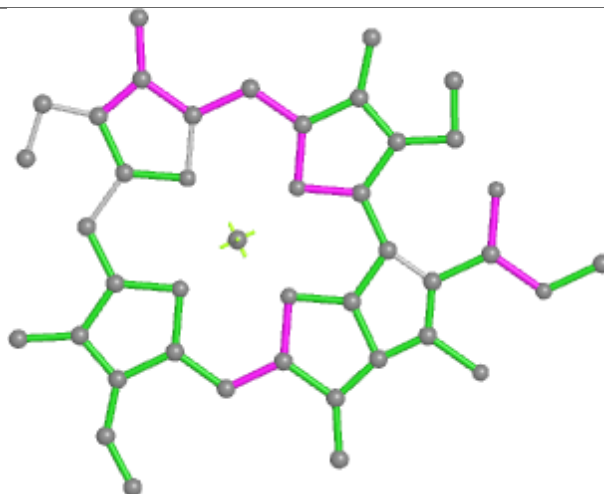




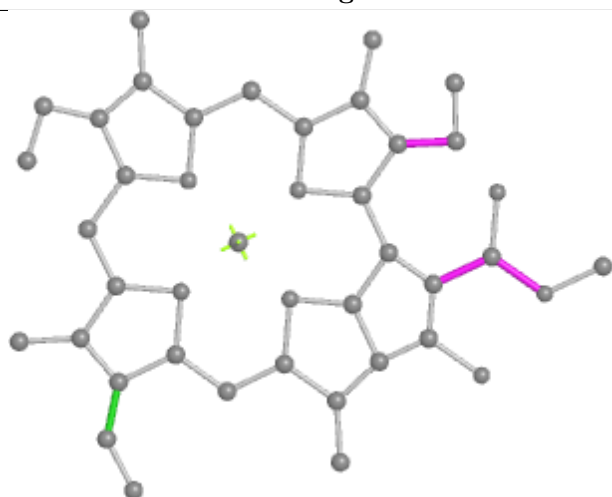
Ligand CLA 5 611



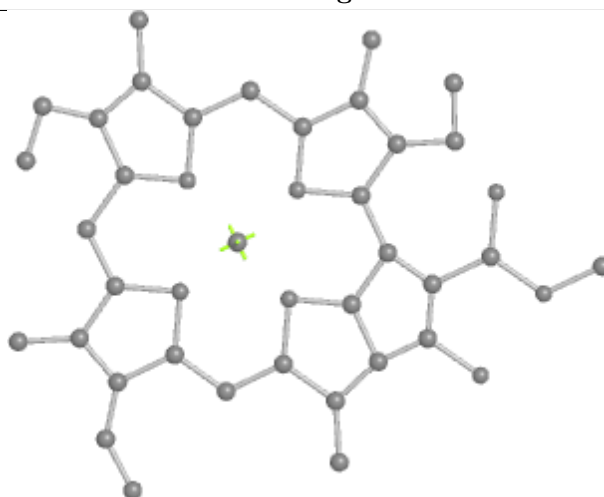
Bond lengths



Bond angles

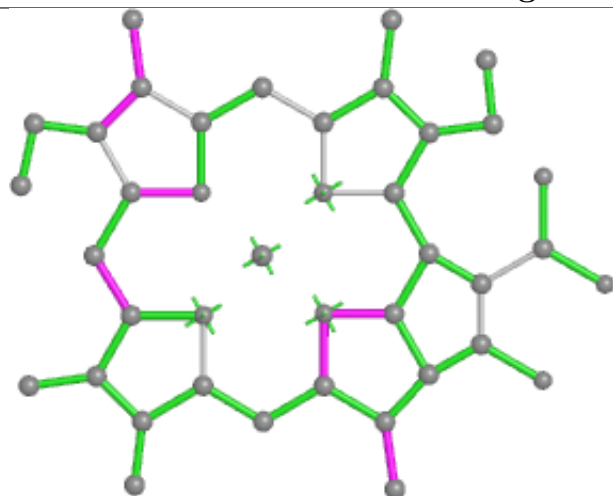


Torsions

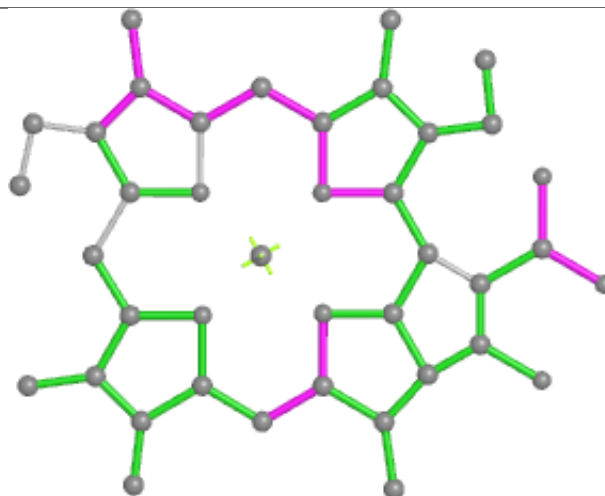


Rings

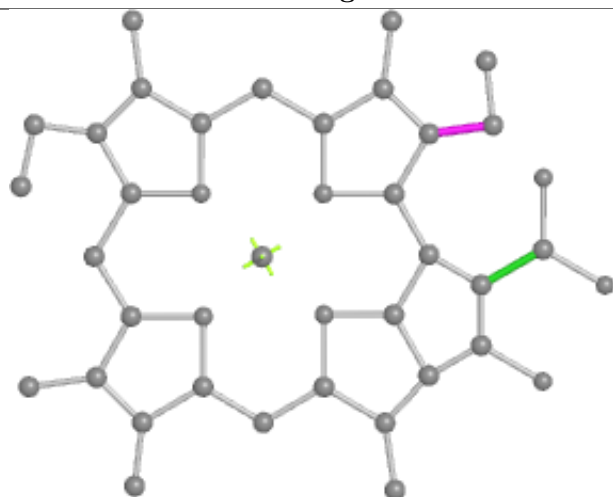
Ligand CLA 4 606



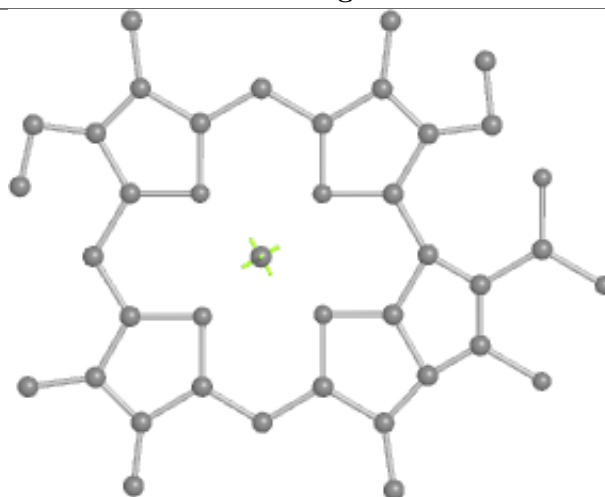
Bond lengths



Bond angles

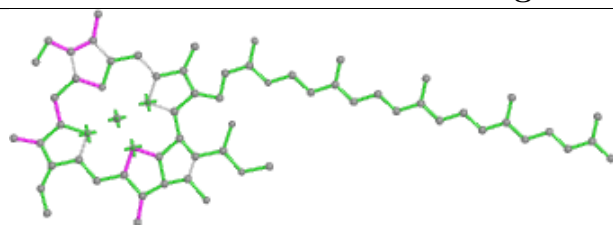


Torsions

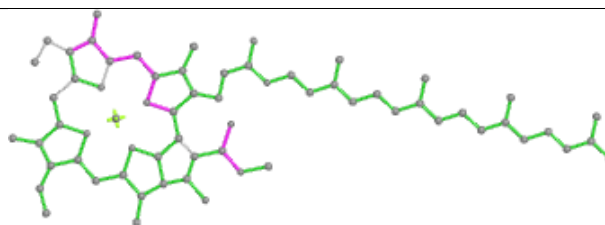


Rings

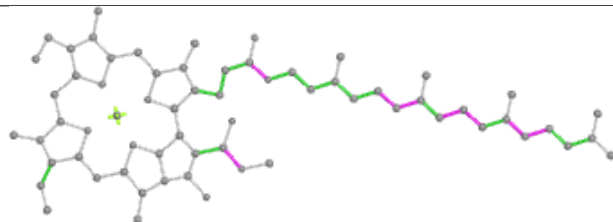
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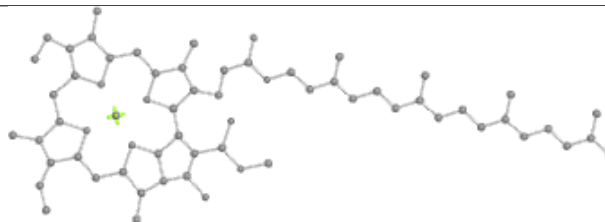
Bond lengths



Bond angles

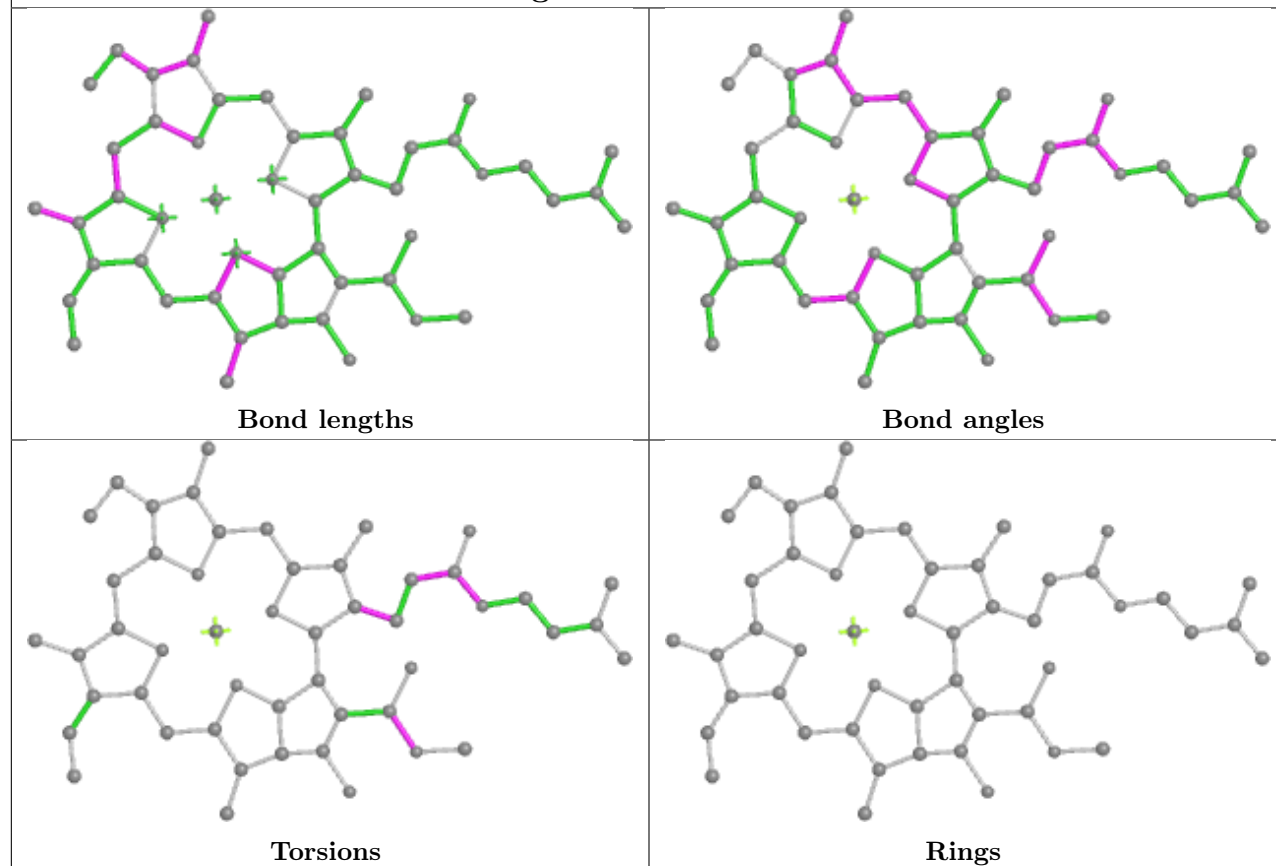


Torsions

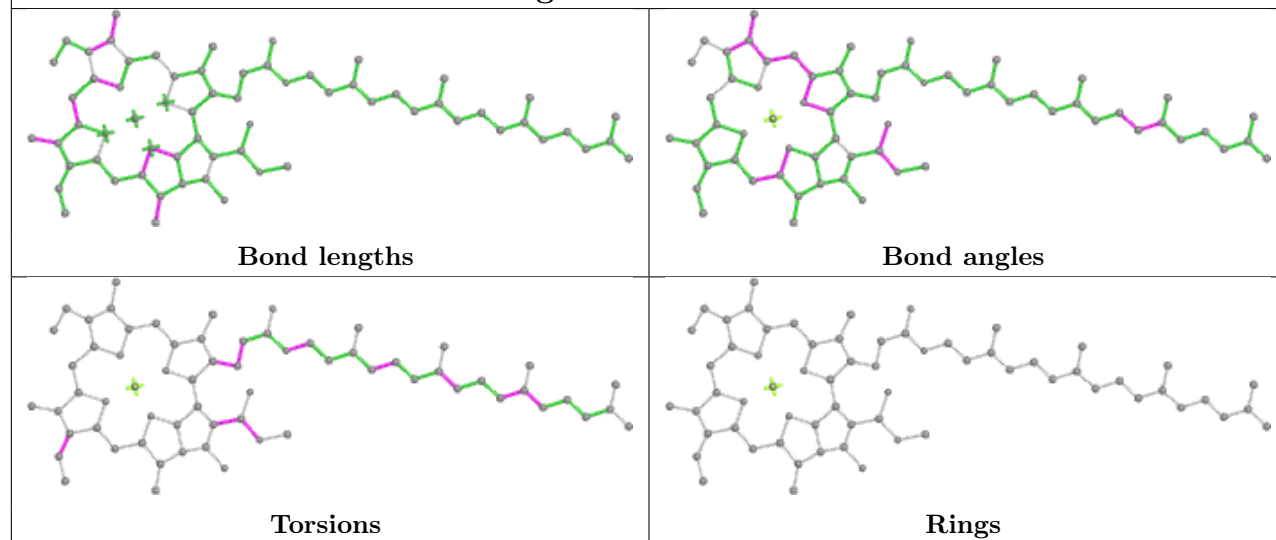


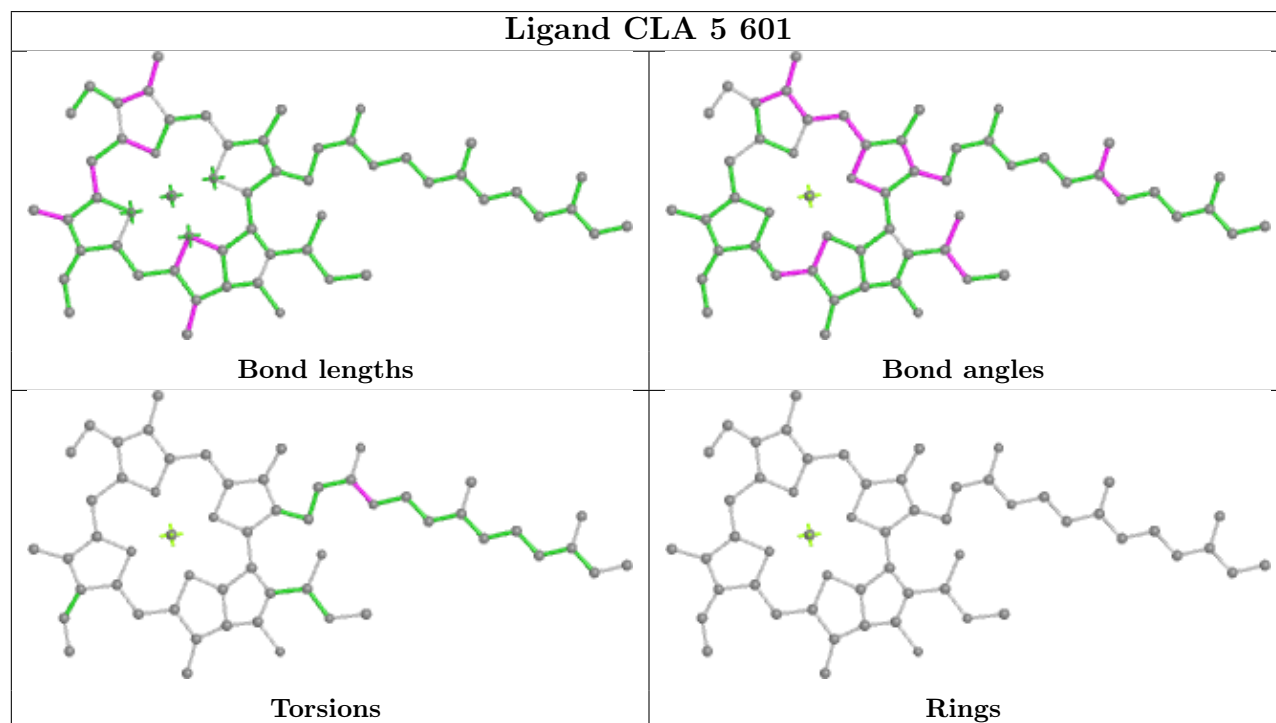
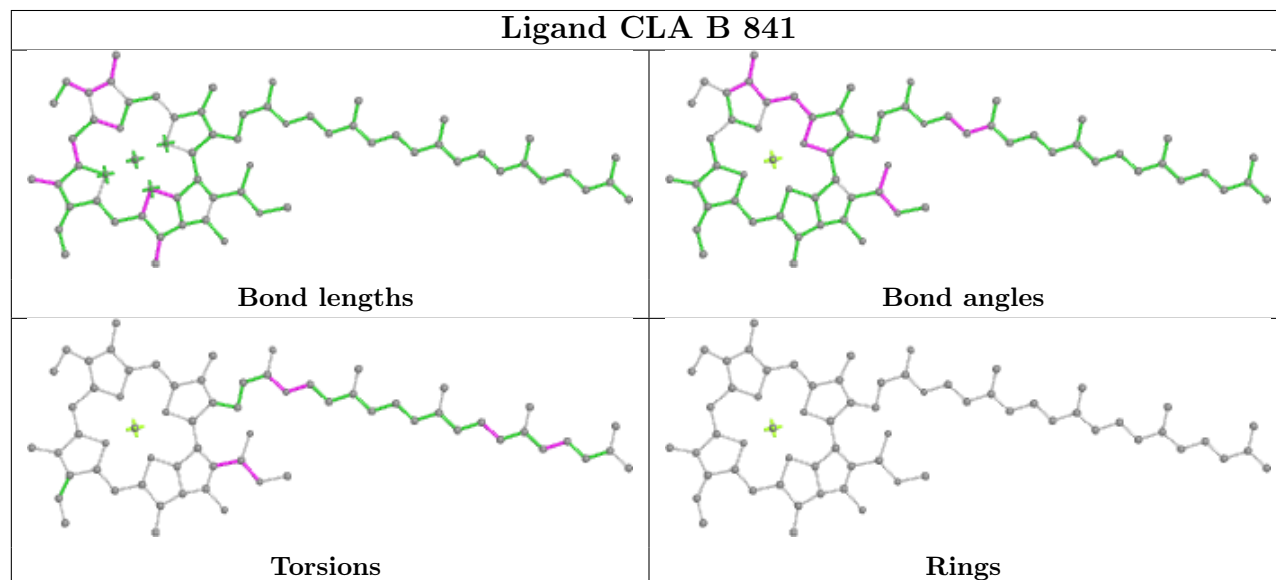
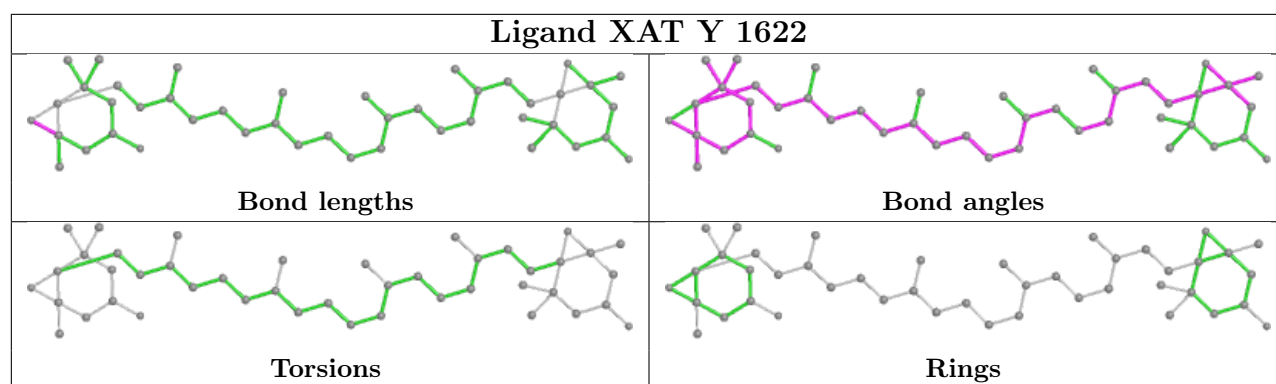
Rings

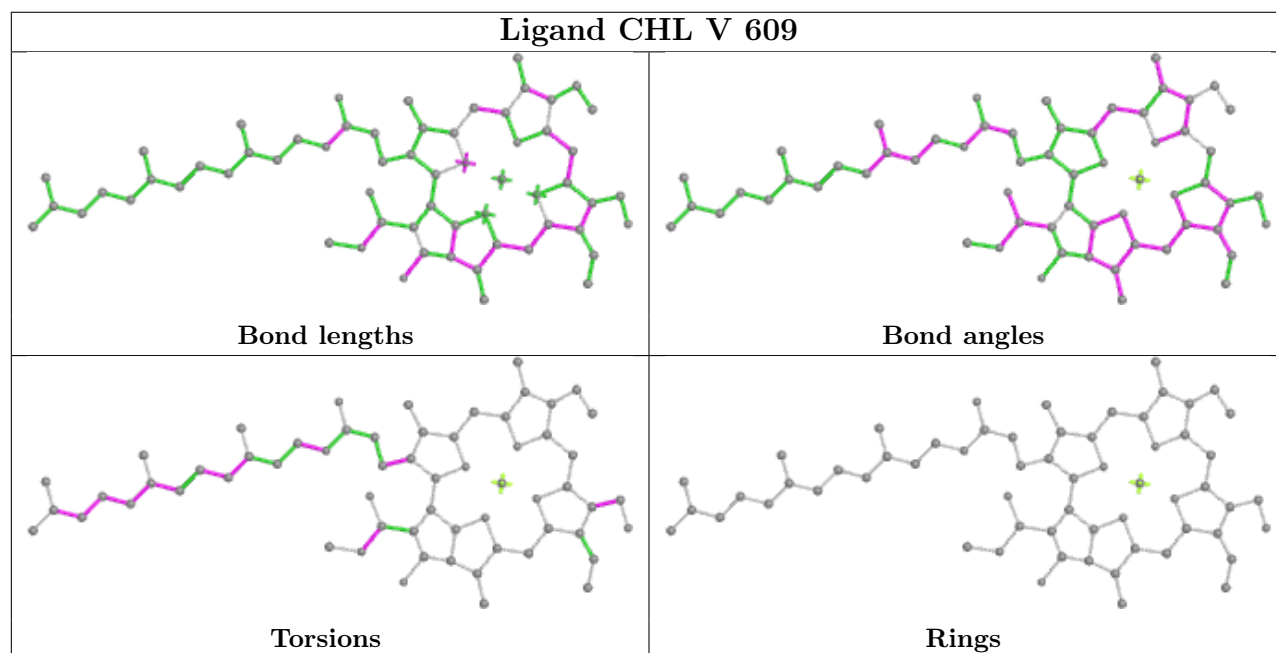
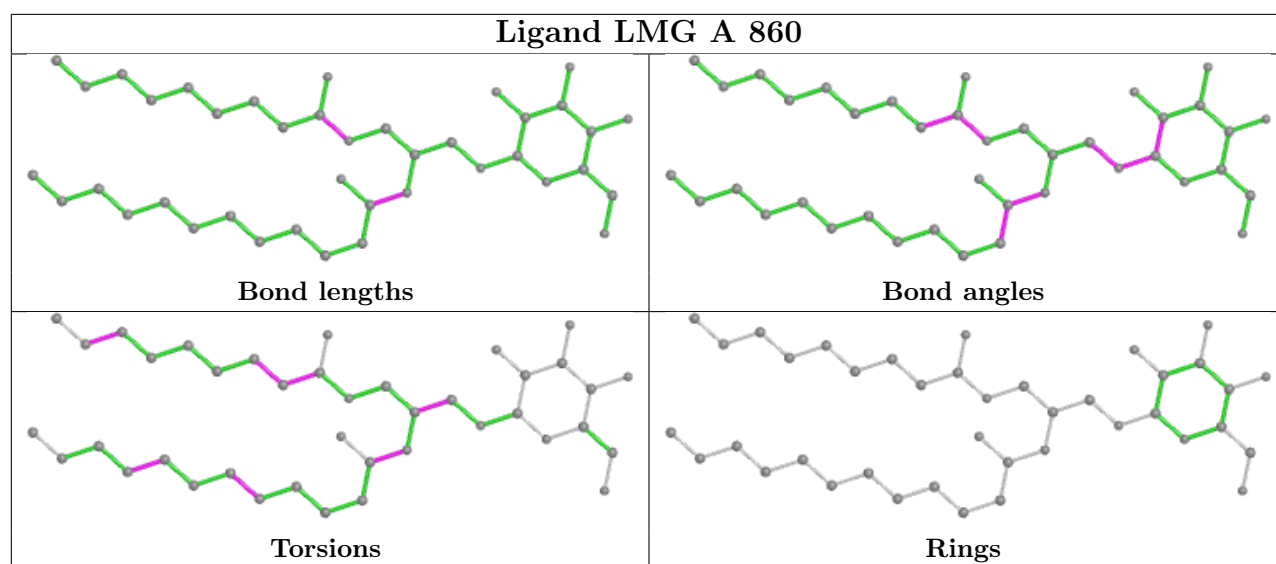
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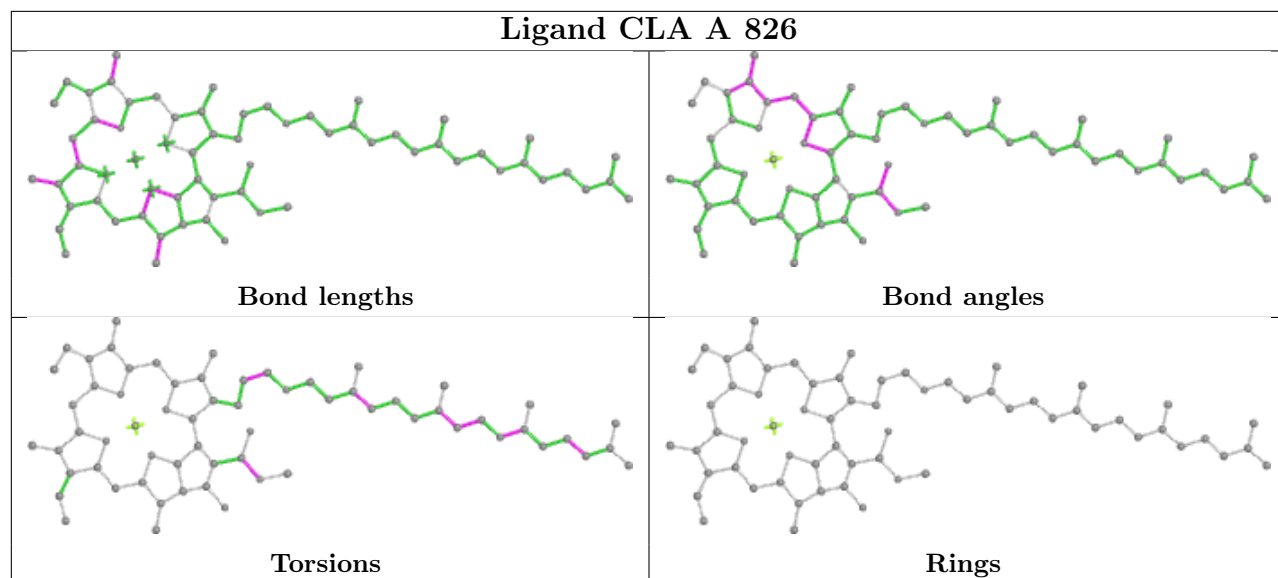
Ligand CLA 4 608



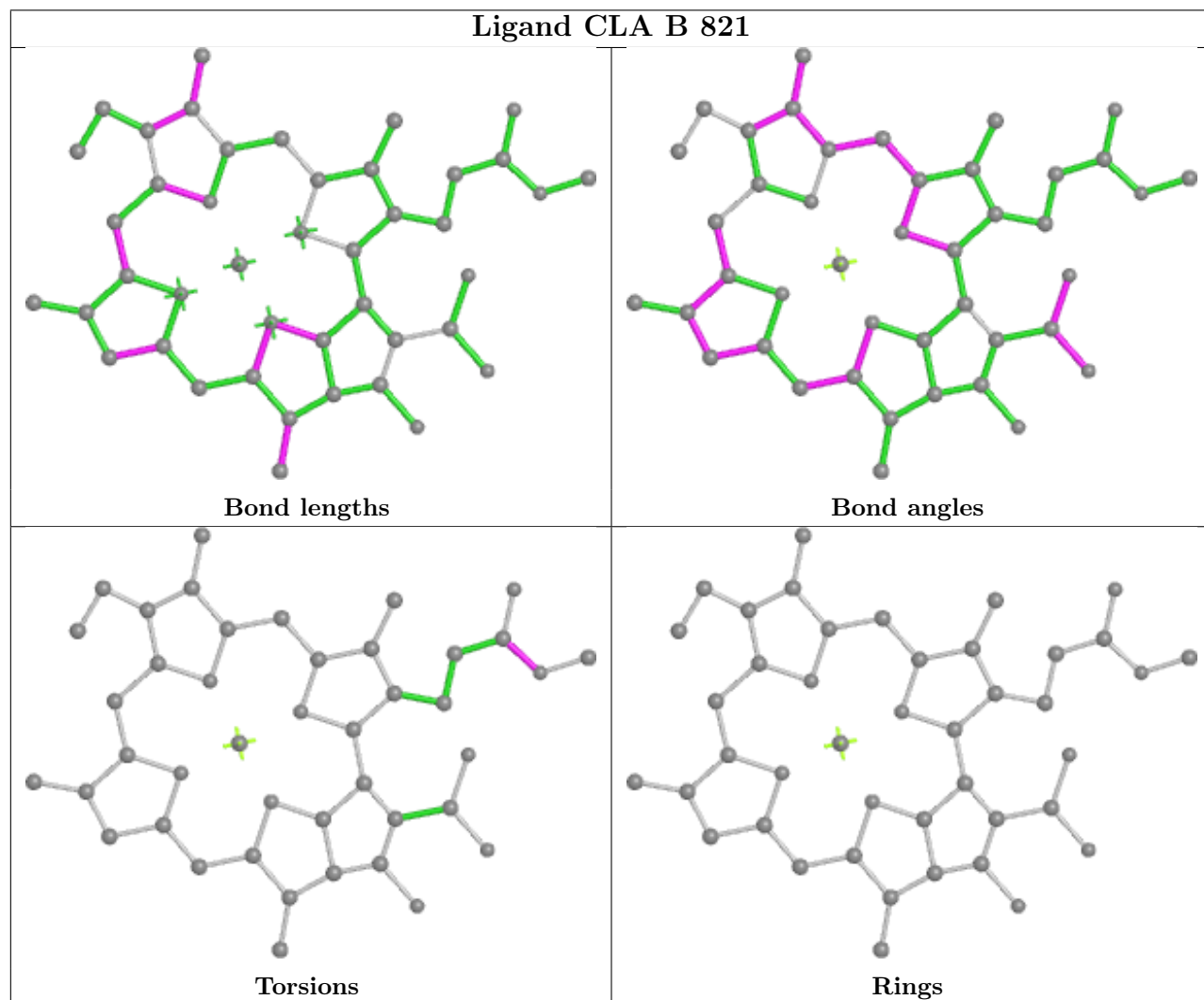




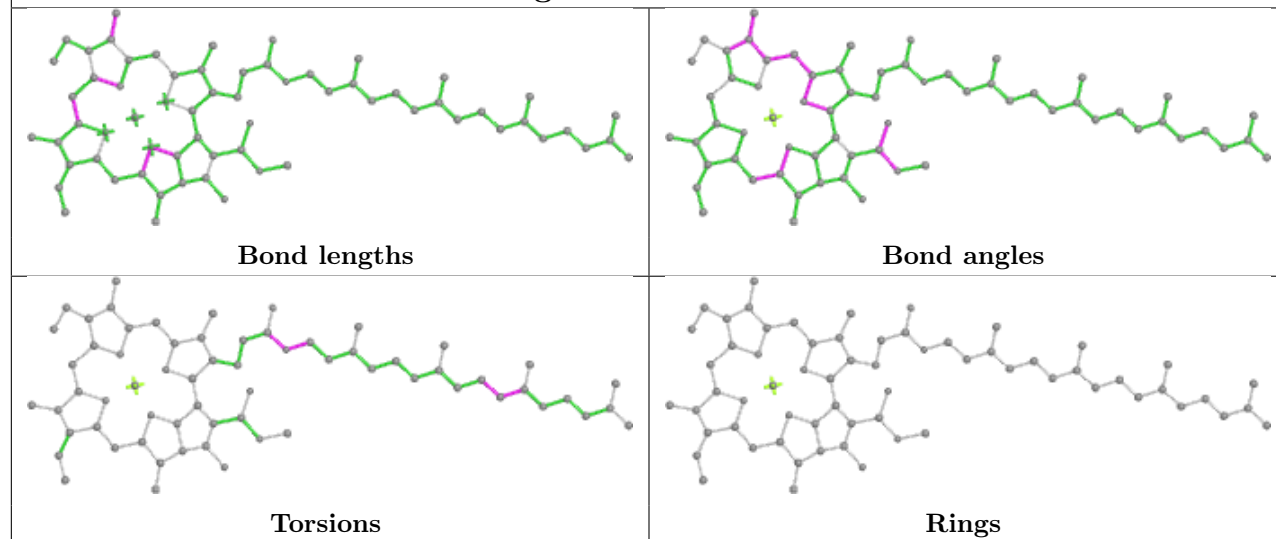
Ligand CLA A 826



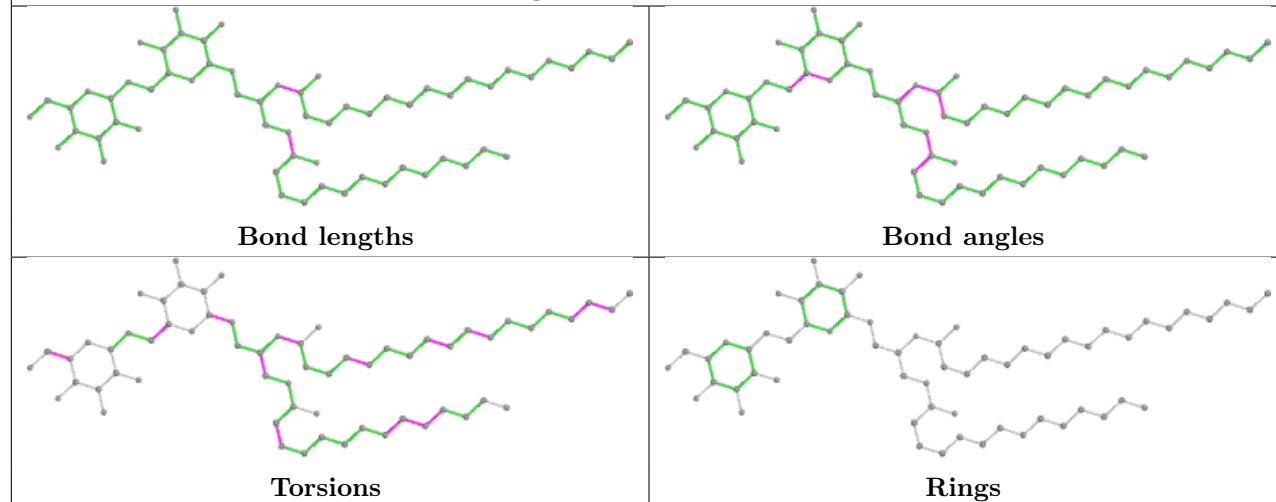
Ligand CLA B 821



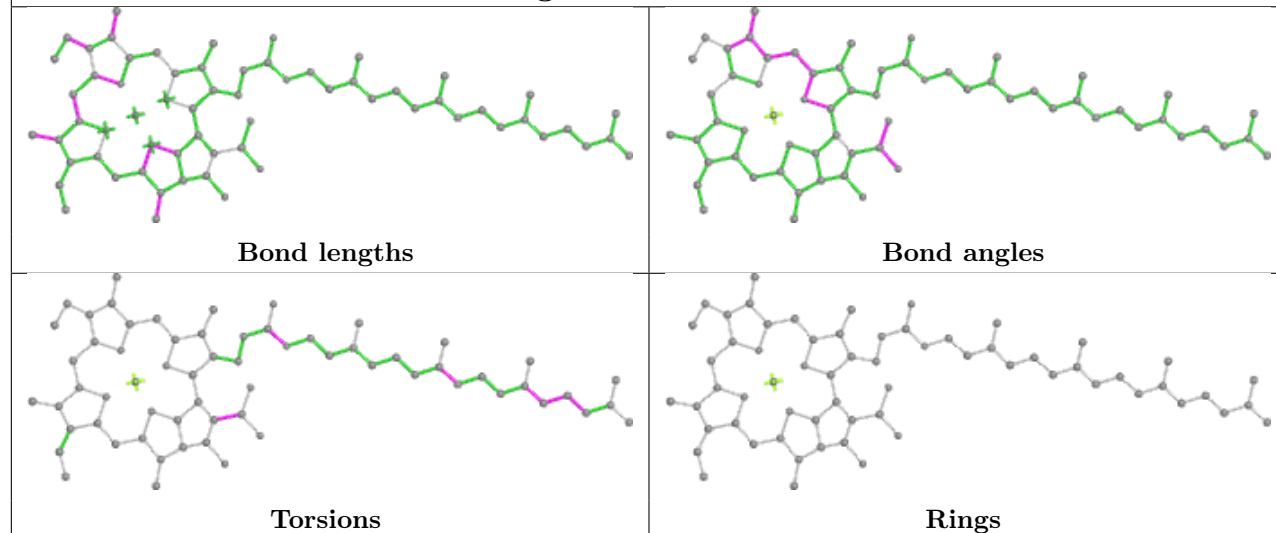
Ligand CLA Z 612



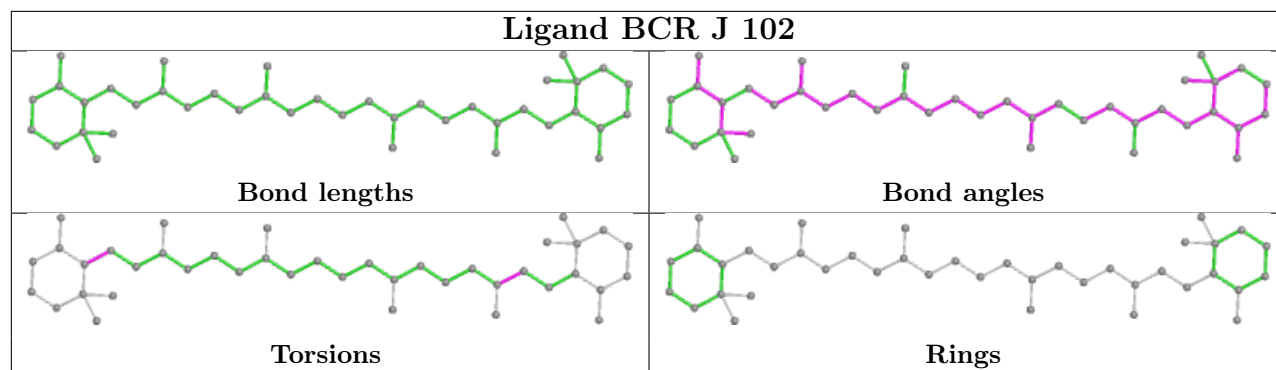
Ligand DGD B 850



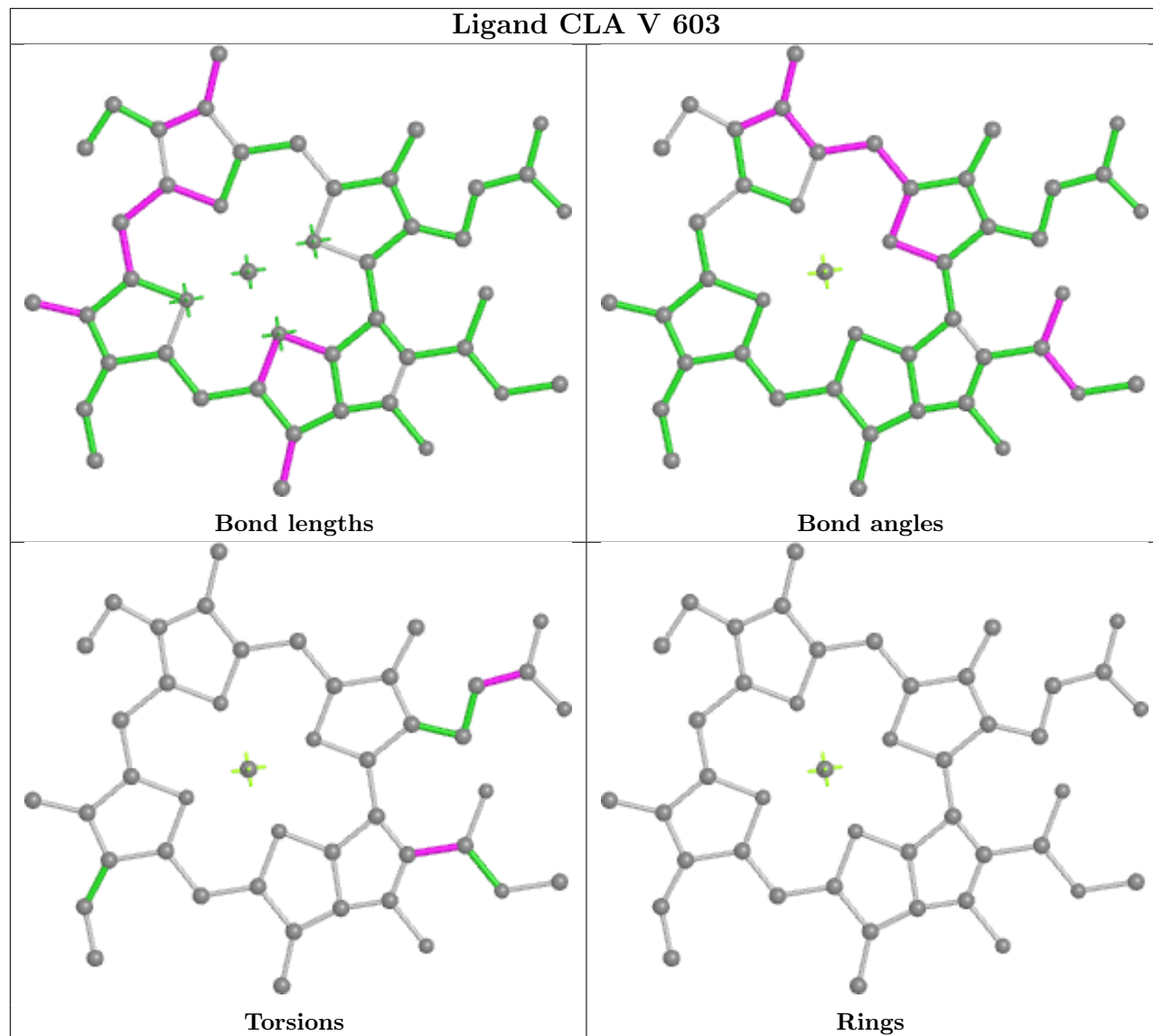
Ligand CLA 2 602



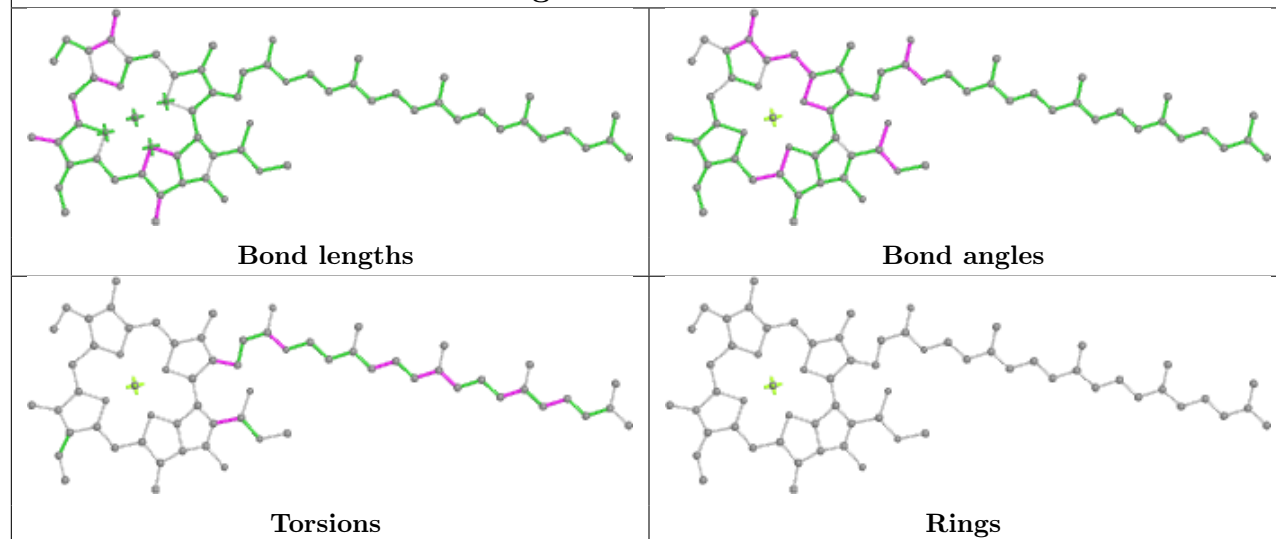
Ligand BCR J 102



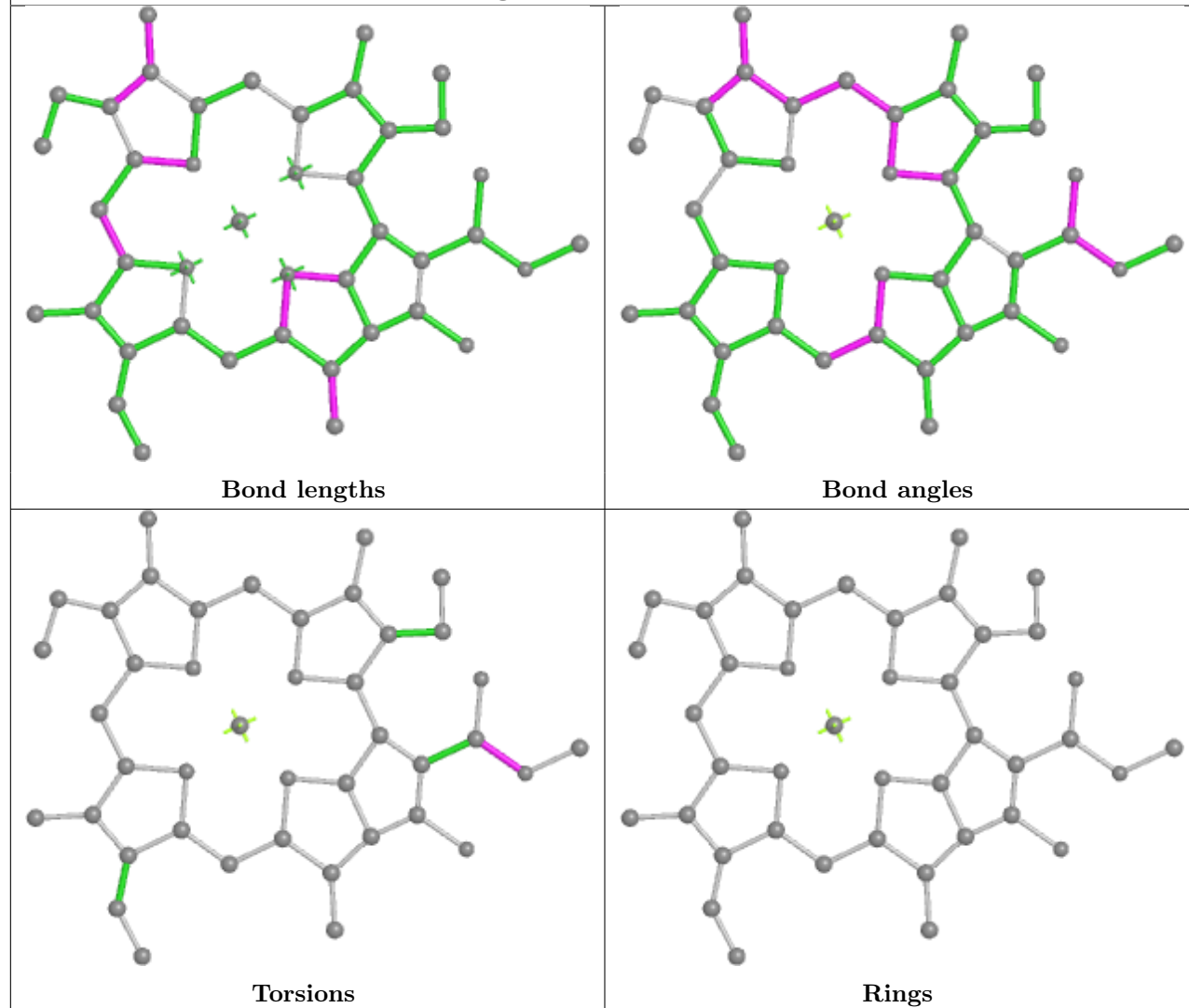
Ligand CLA V 603

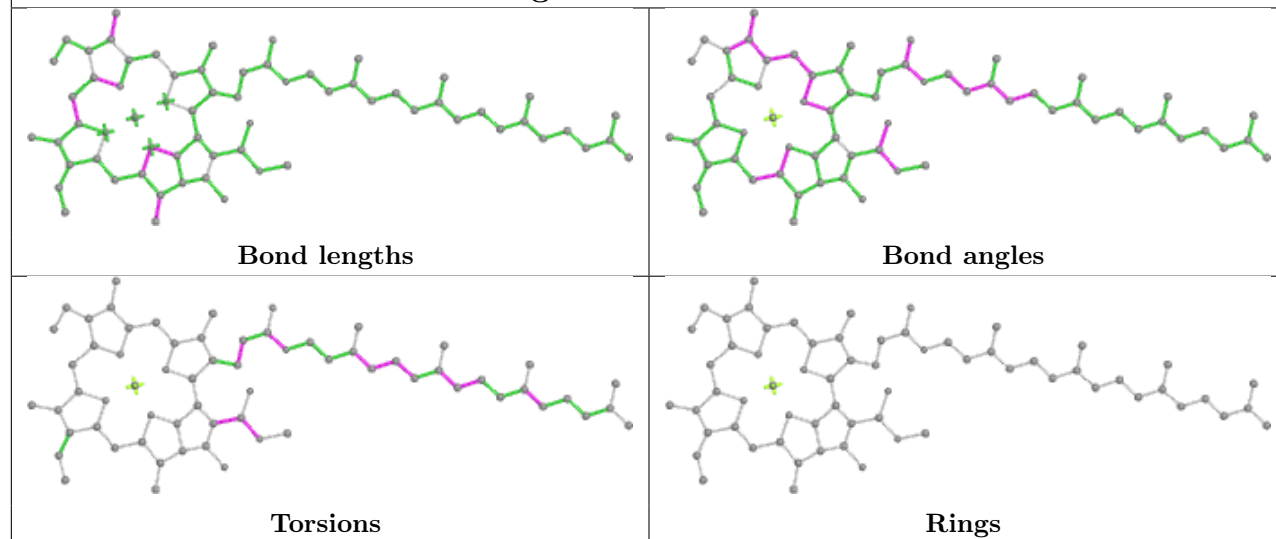
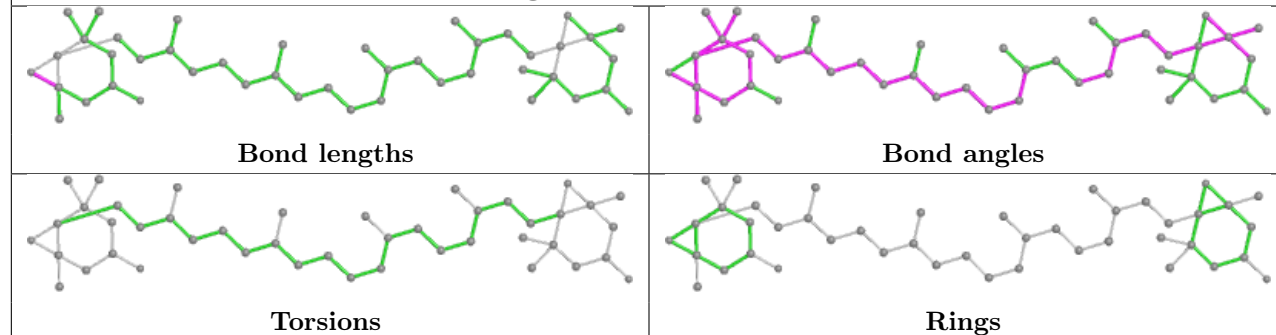
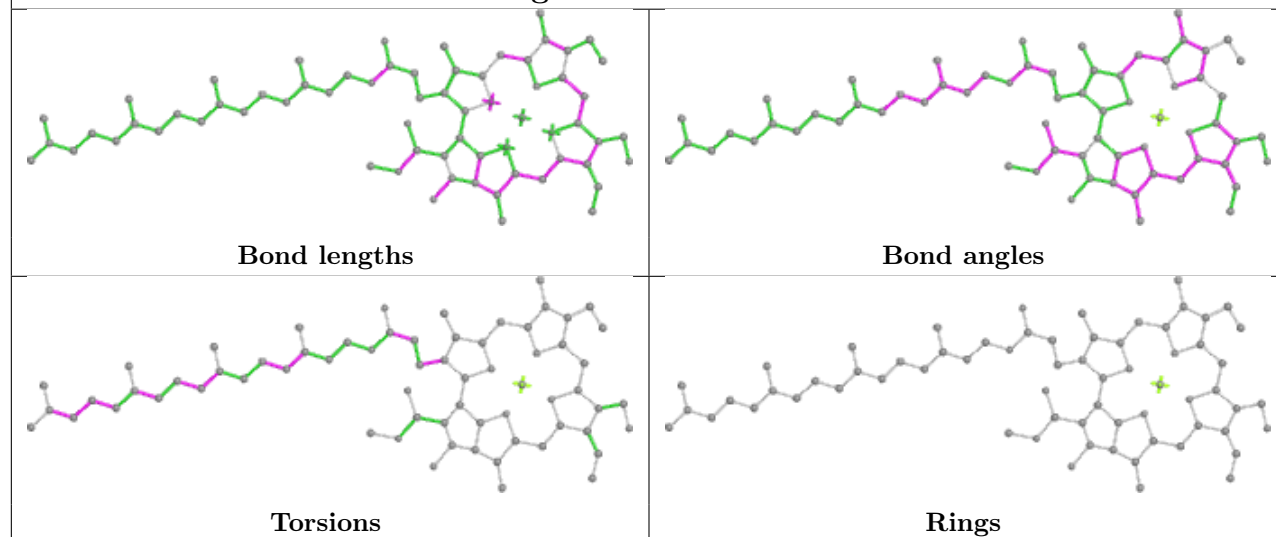


Ligand CLA B 805

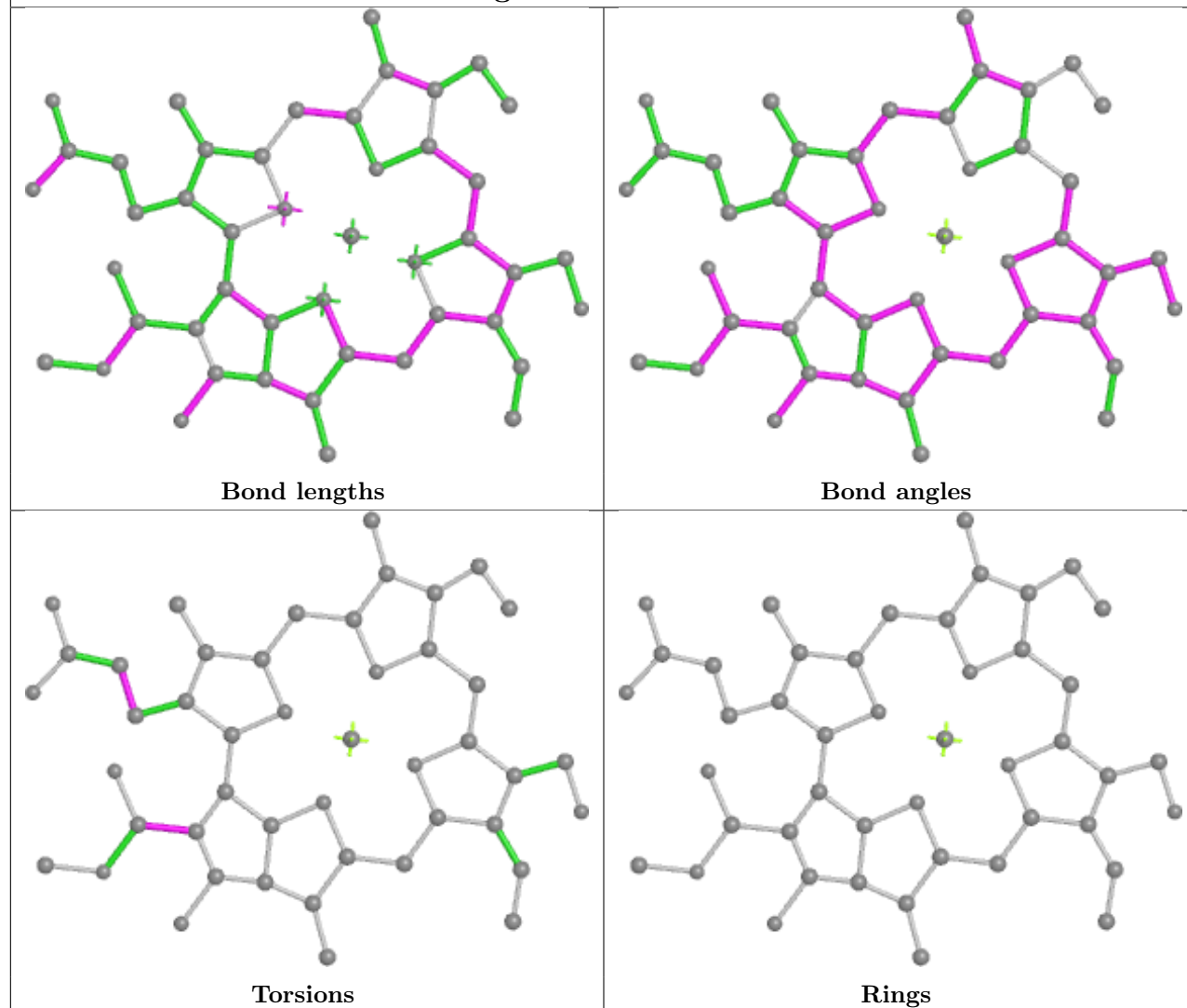


Ligand CLA G 203

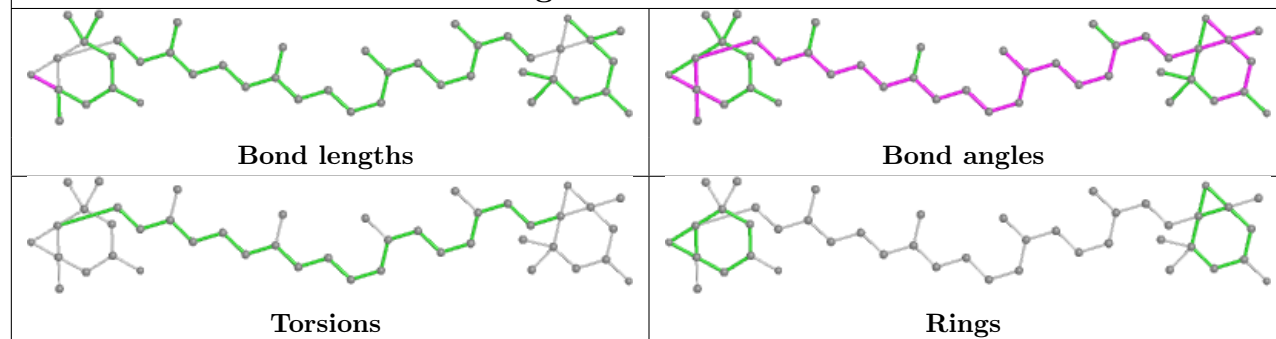


Ligand CLA Y 613**Ligand XAT Z 1622****Ligand CHL Y 609**

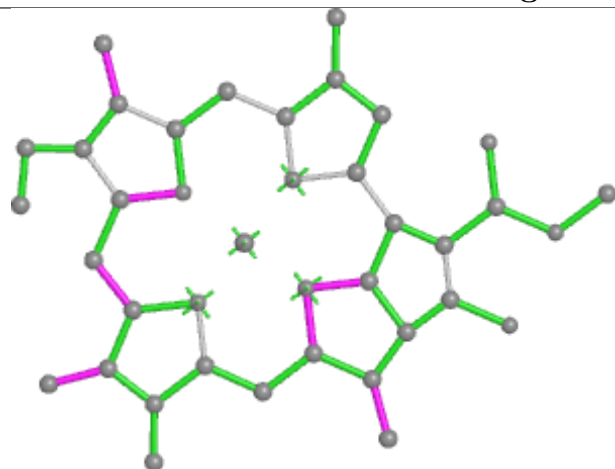
Ligand CHL X 605



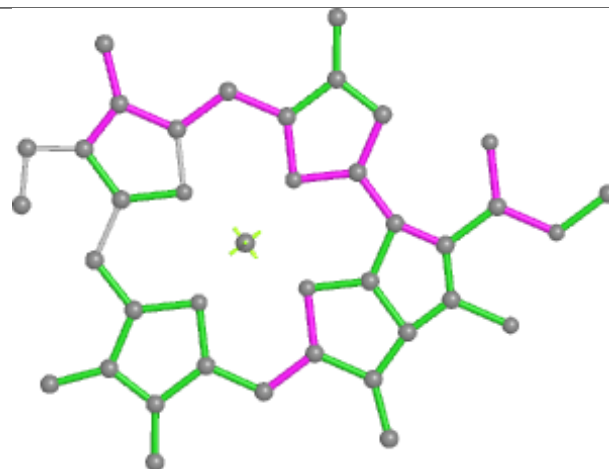
Ligand XAT 7 620



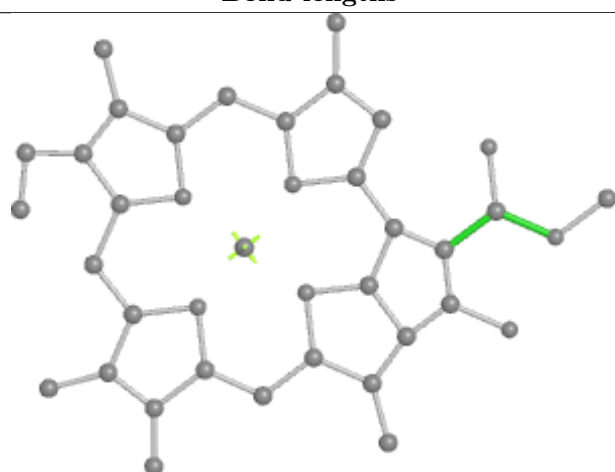
Ligand CLA 1 610



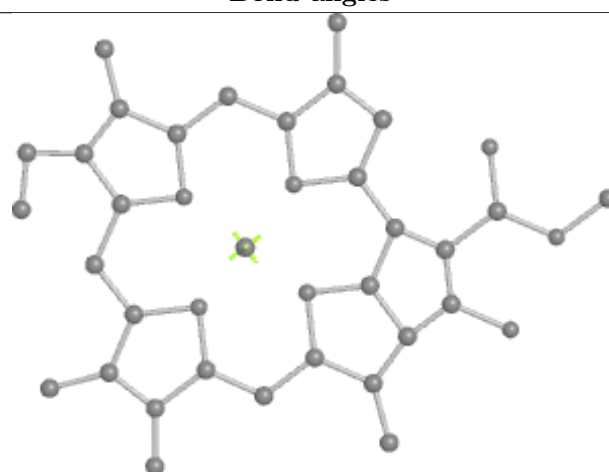
Bond lengths



Bond angles

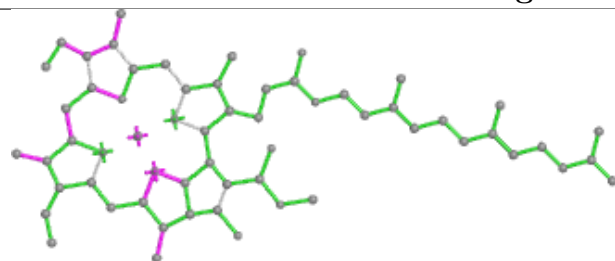


Torsions

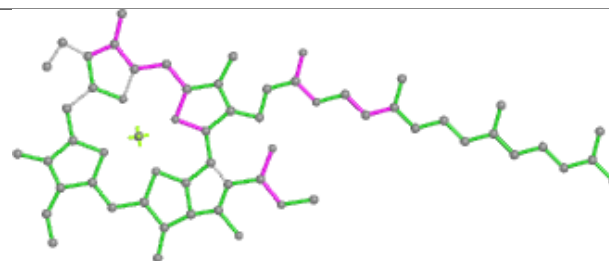


Rings

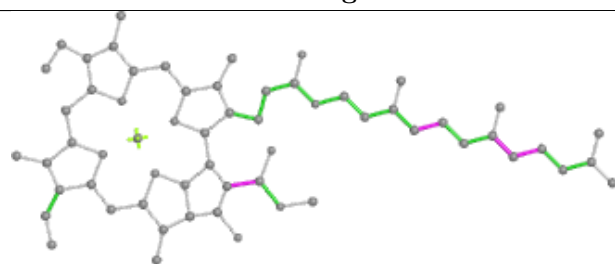
Ligand CLA V 602



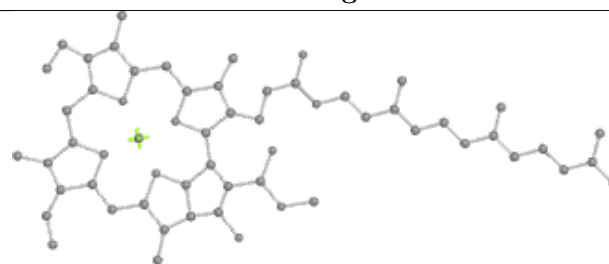
Bond lengths



Bond angles

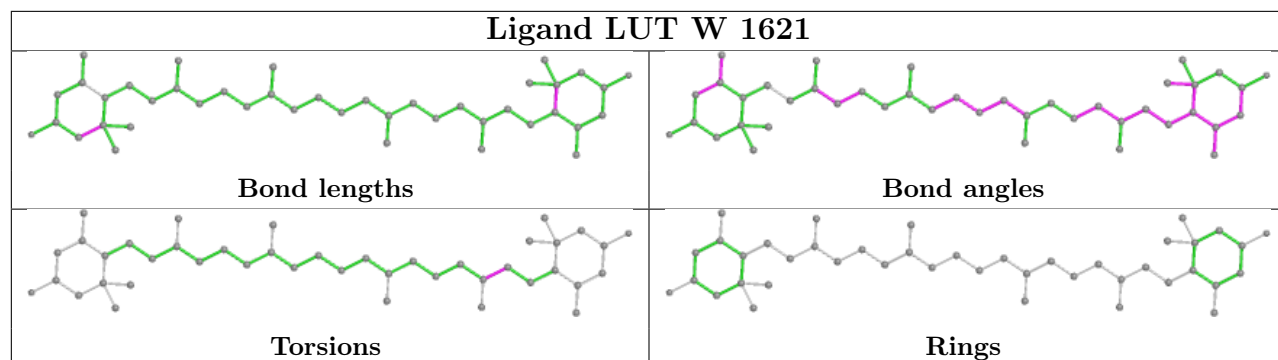


Torsions

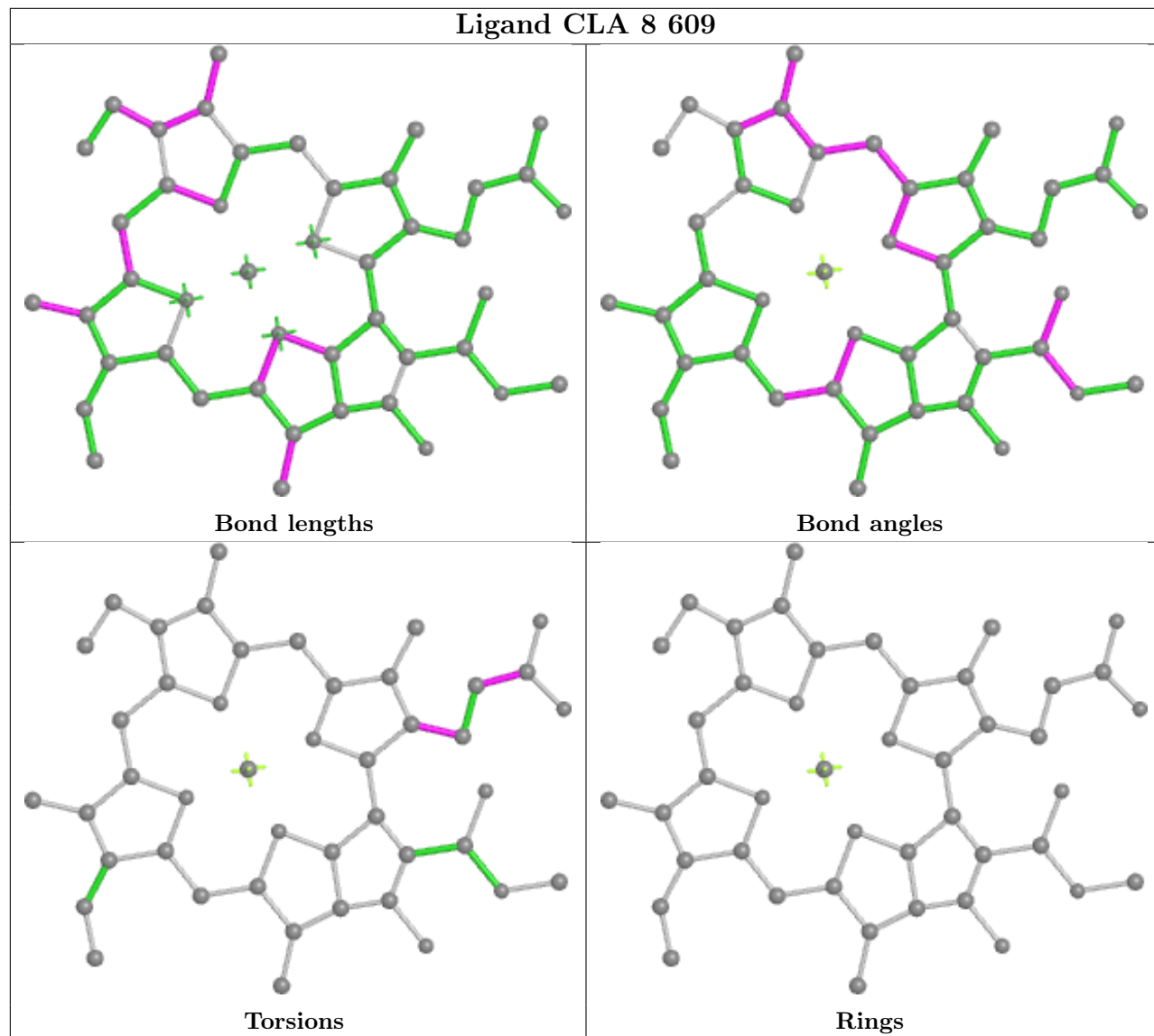


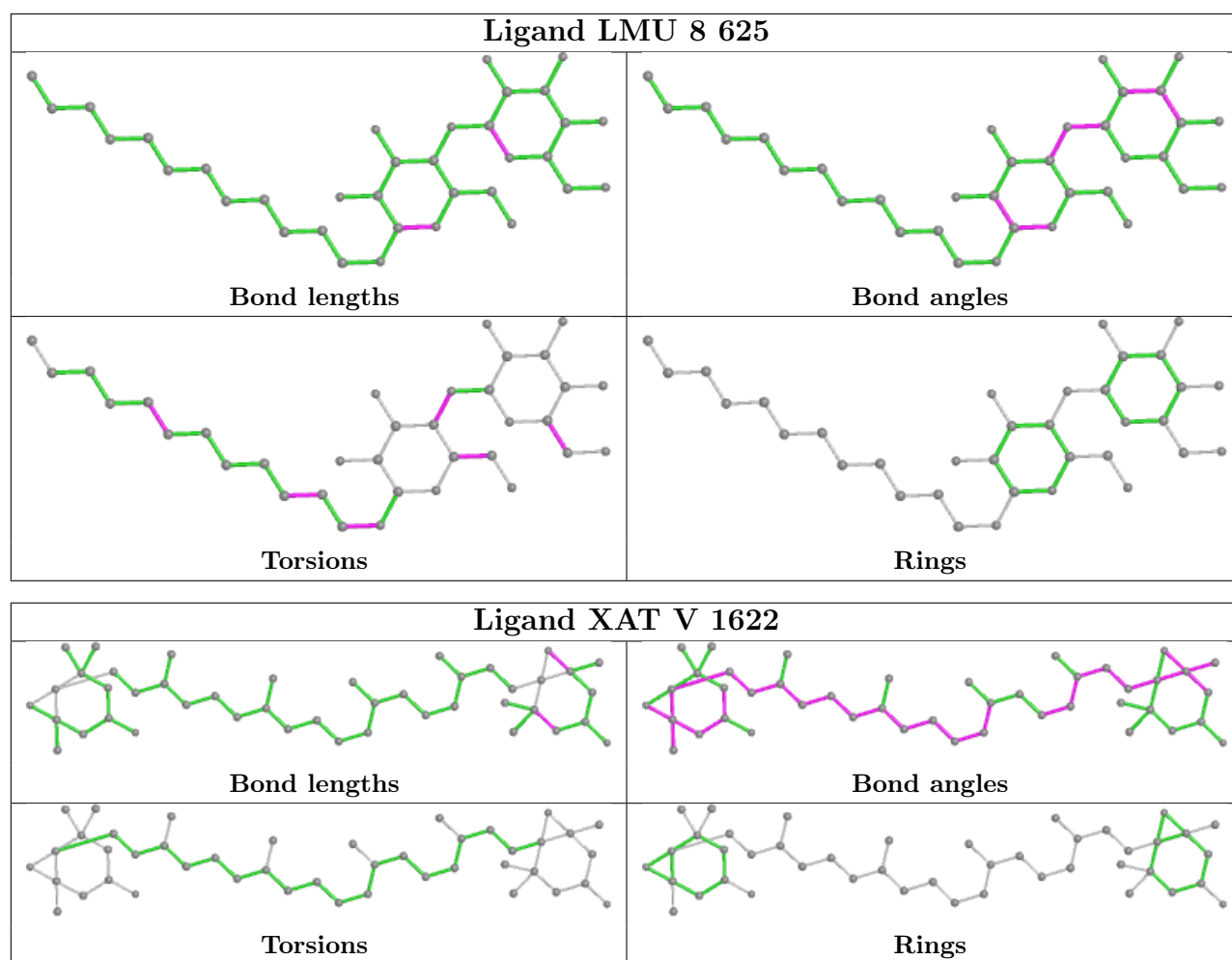
Rings

Ligand LUT W 1621

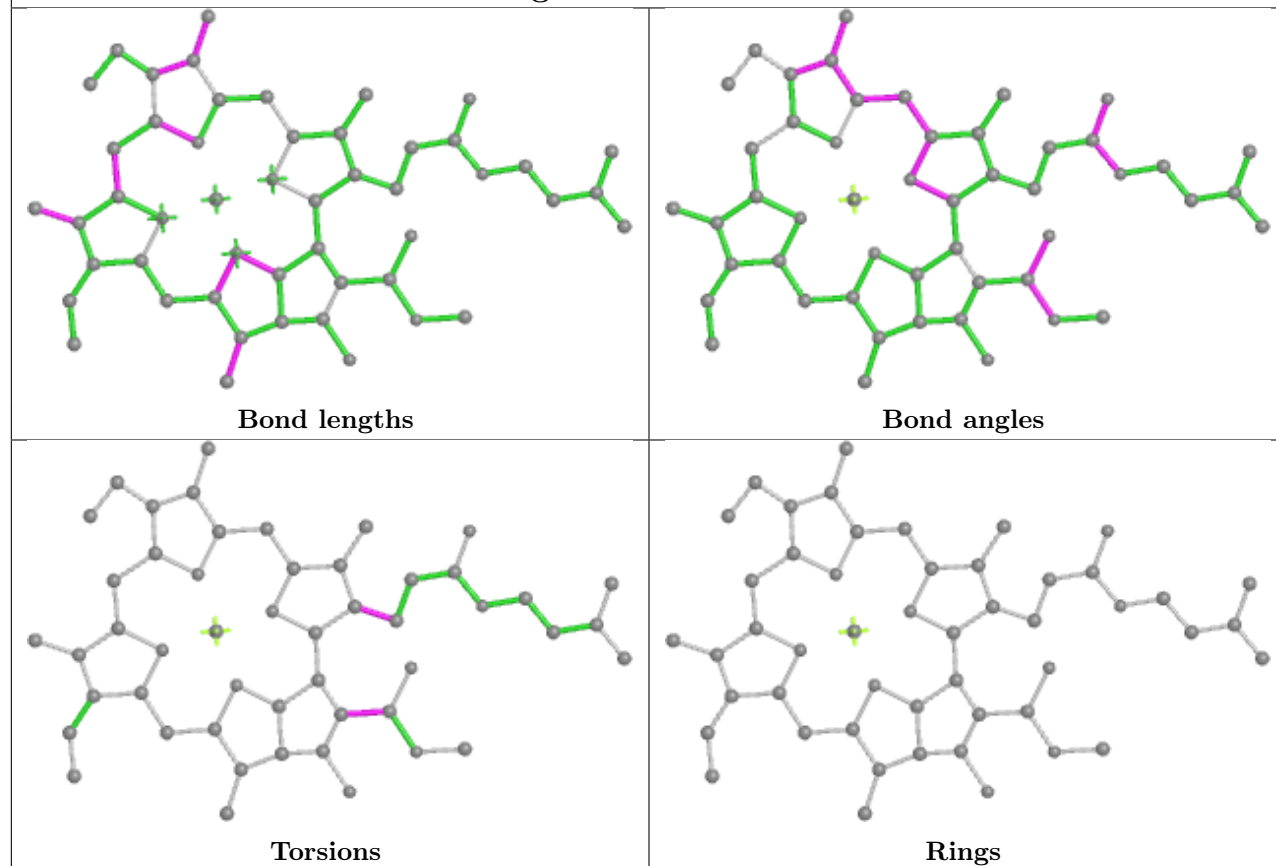


Ligand CLA 8 609

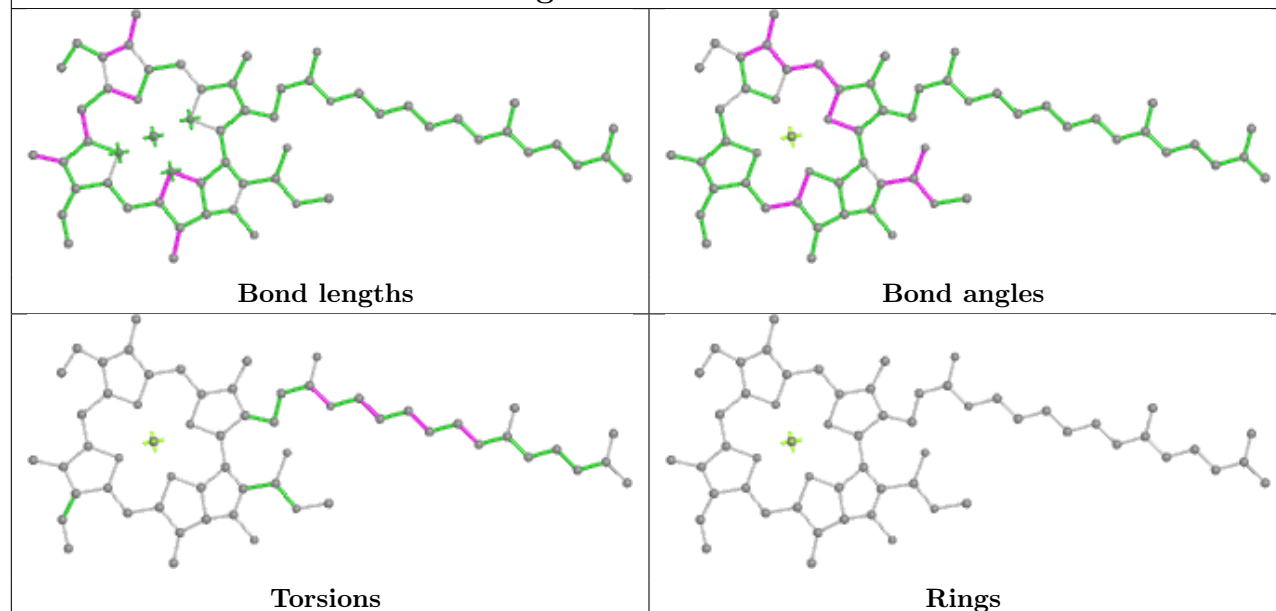




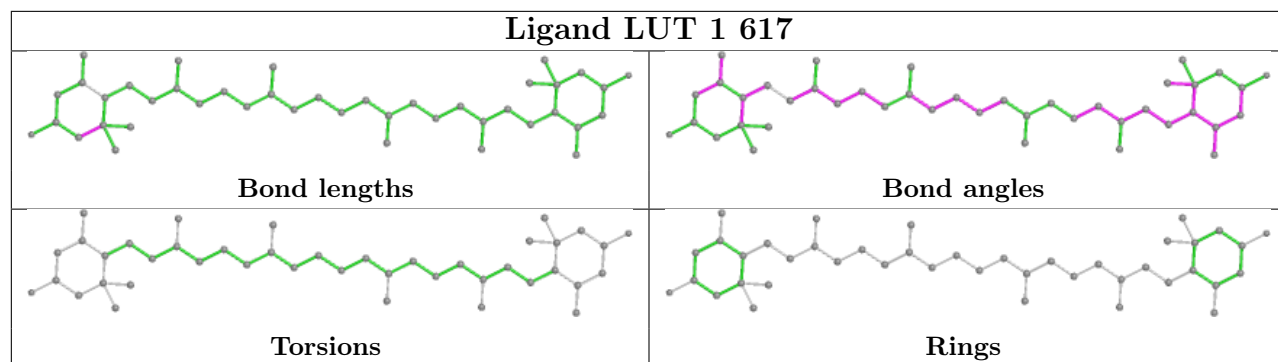
Ligand CLA A 845



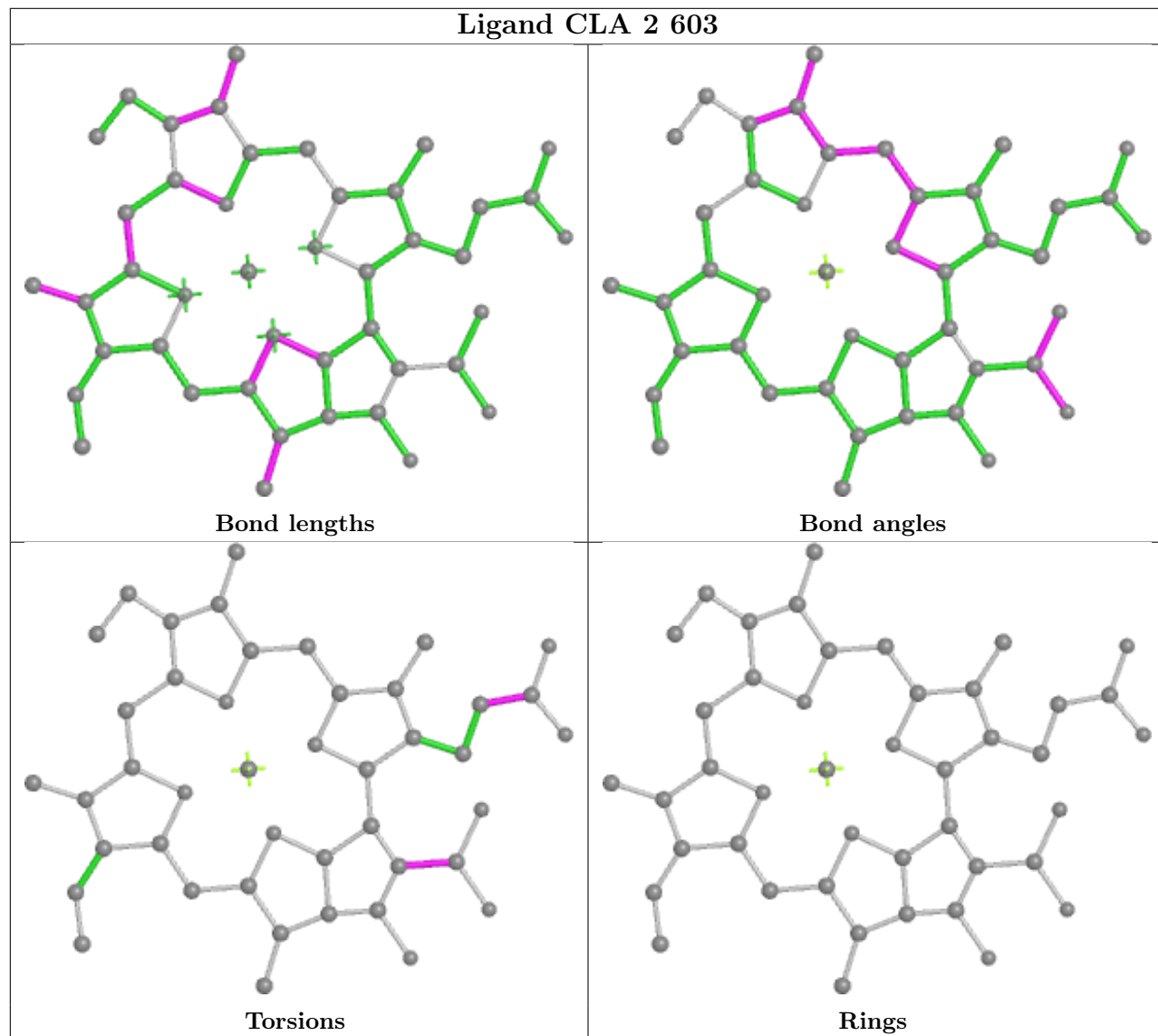
Ligand CLA 7 611



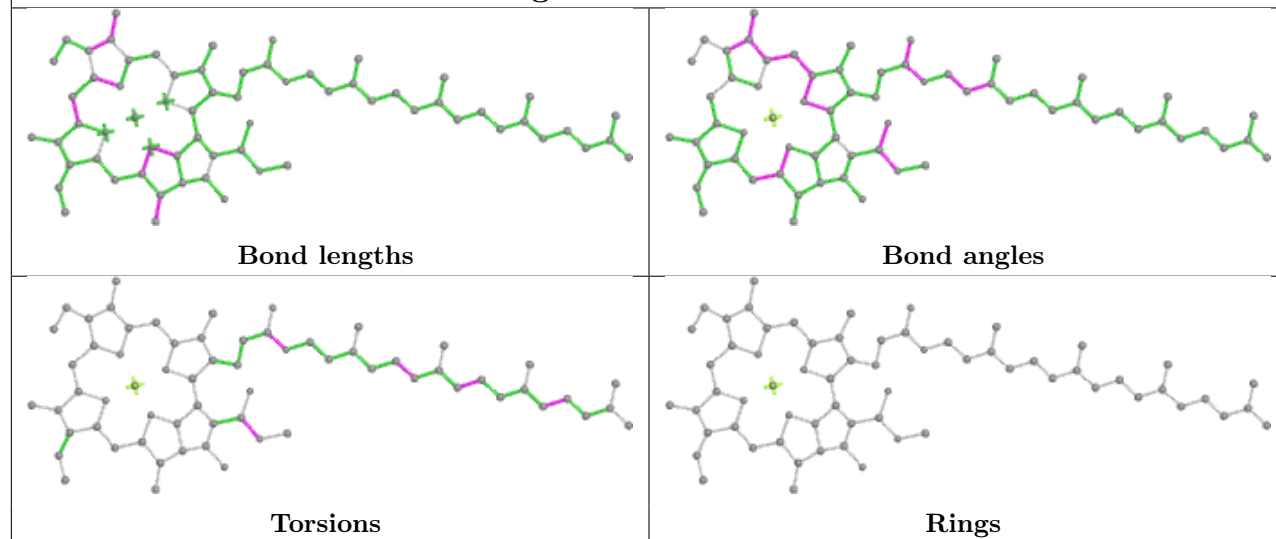
Ligand LUT 1 617



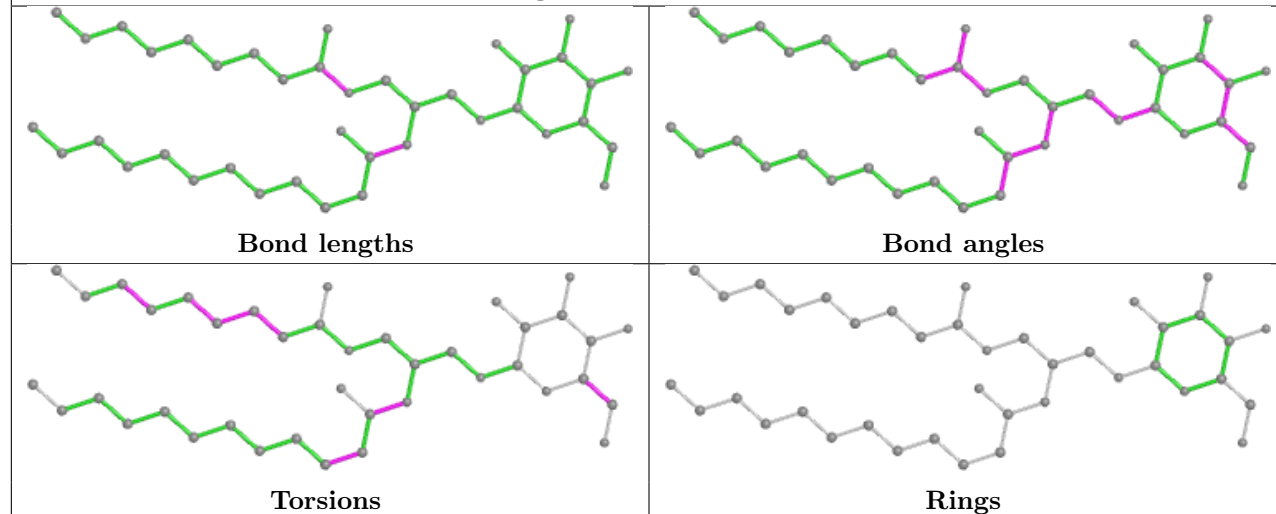
Ligand CLA 2 603



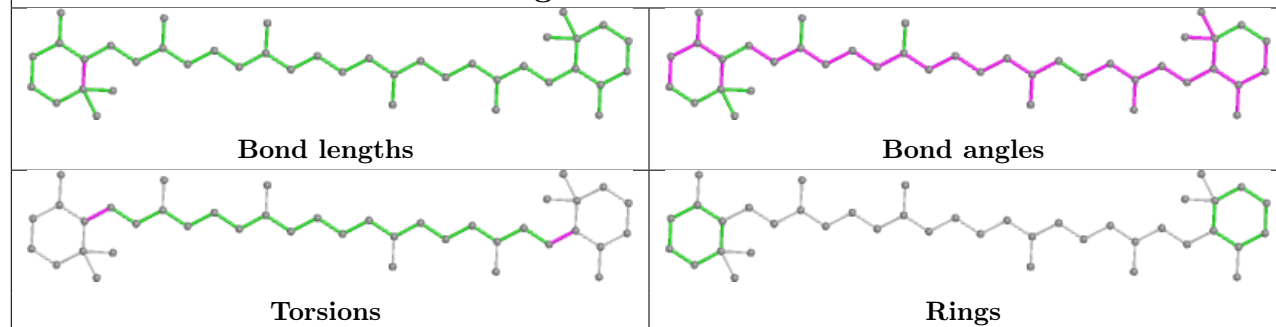
Ligand CLA Y 610



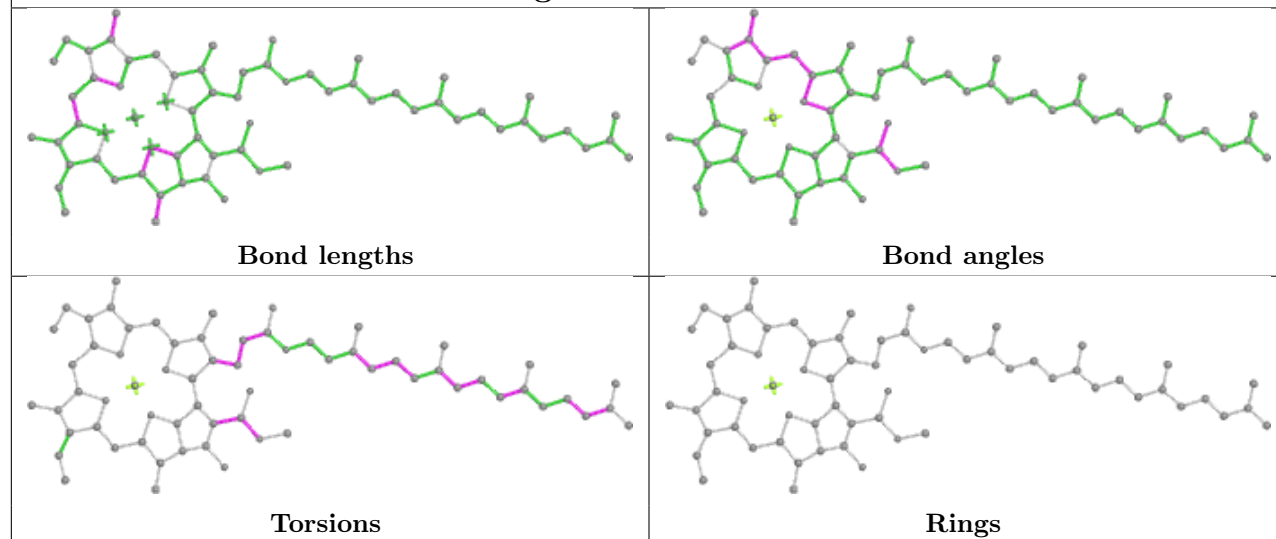
Ligand LMG 4 624



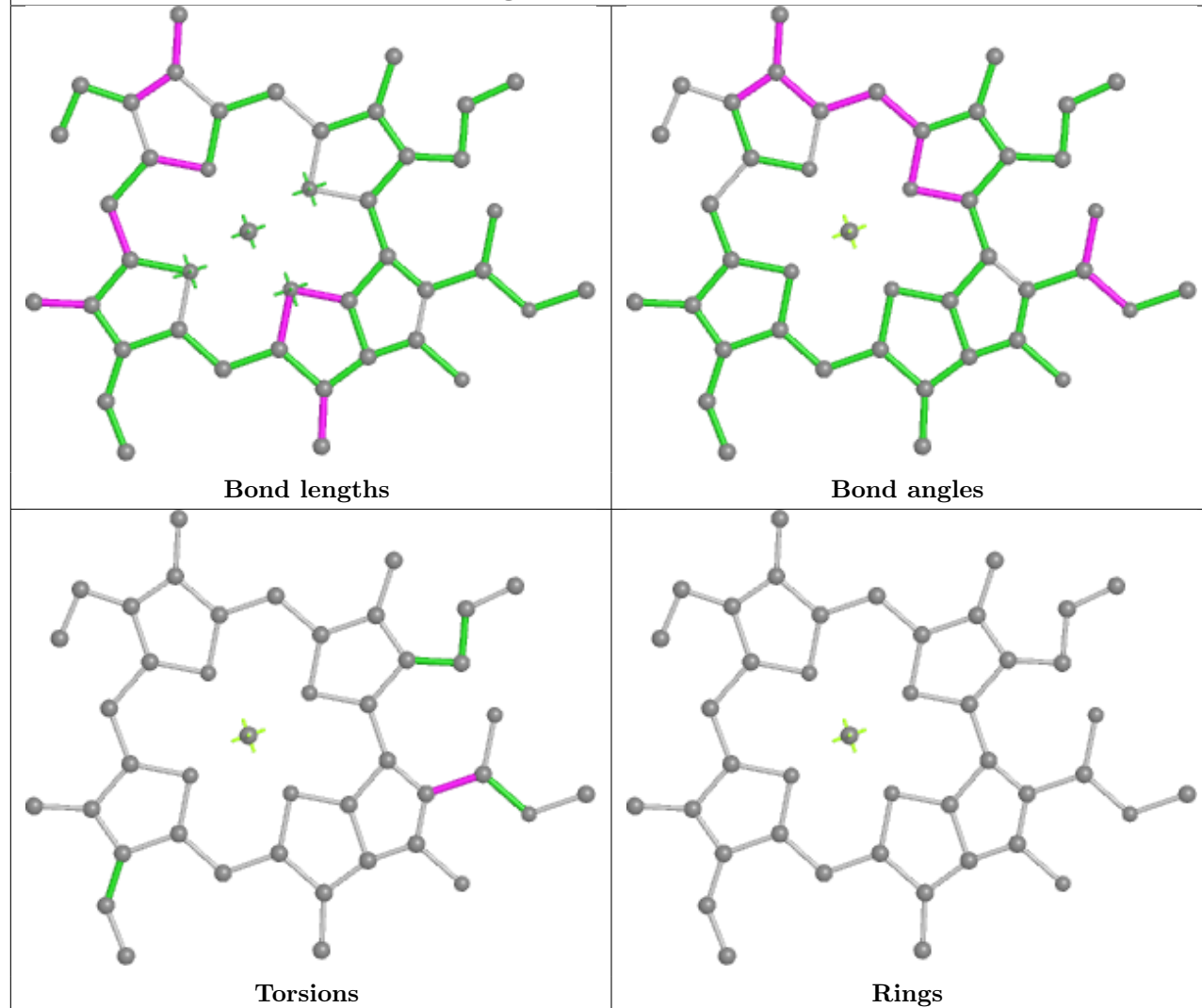
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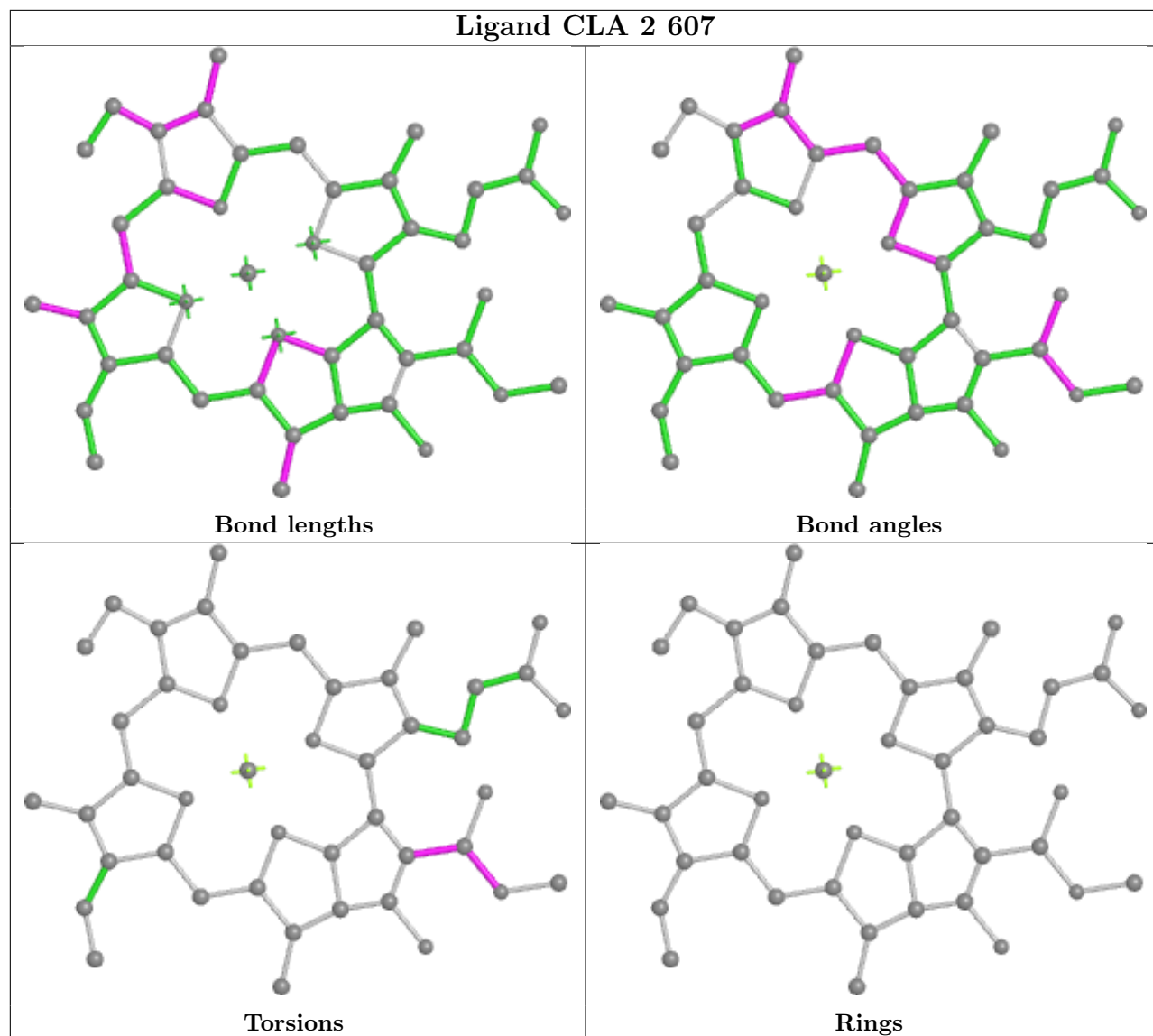
Ligand CLA Z 603



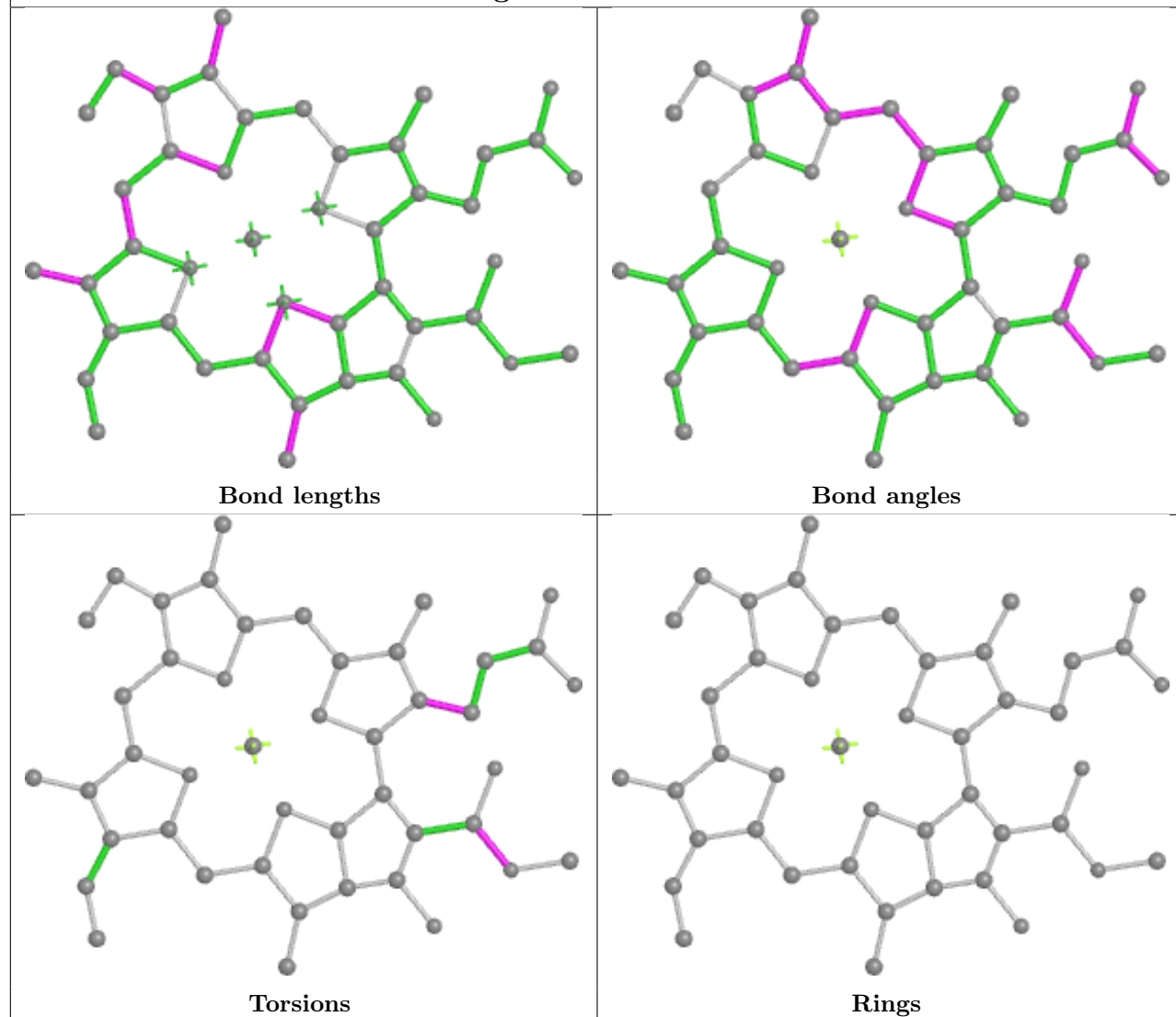
Ligand CLA U 612



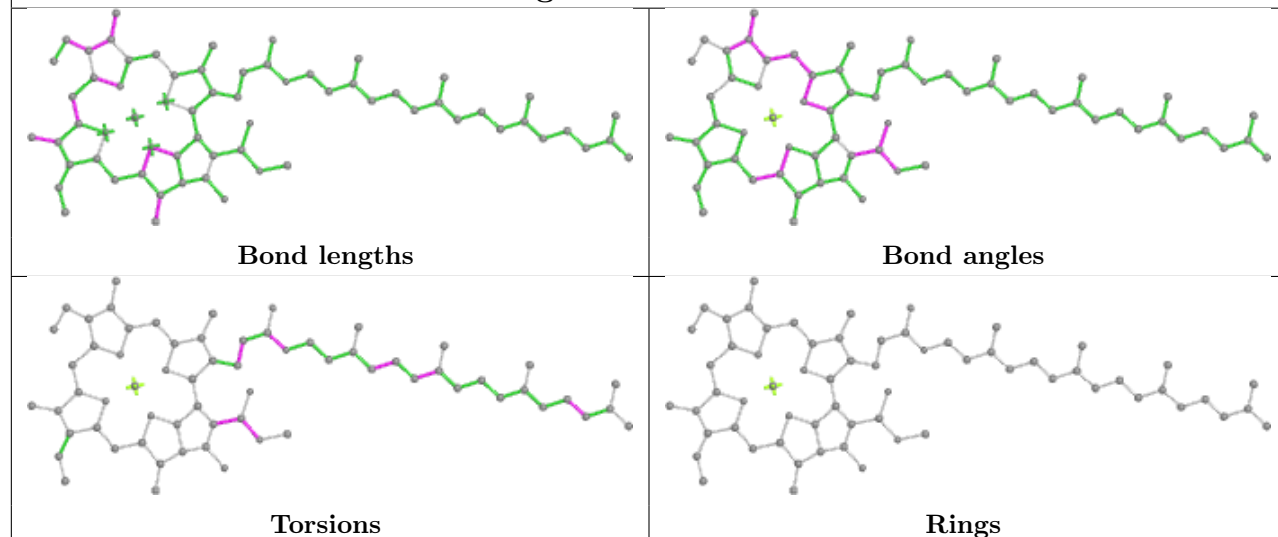
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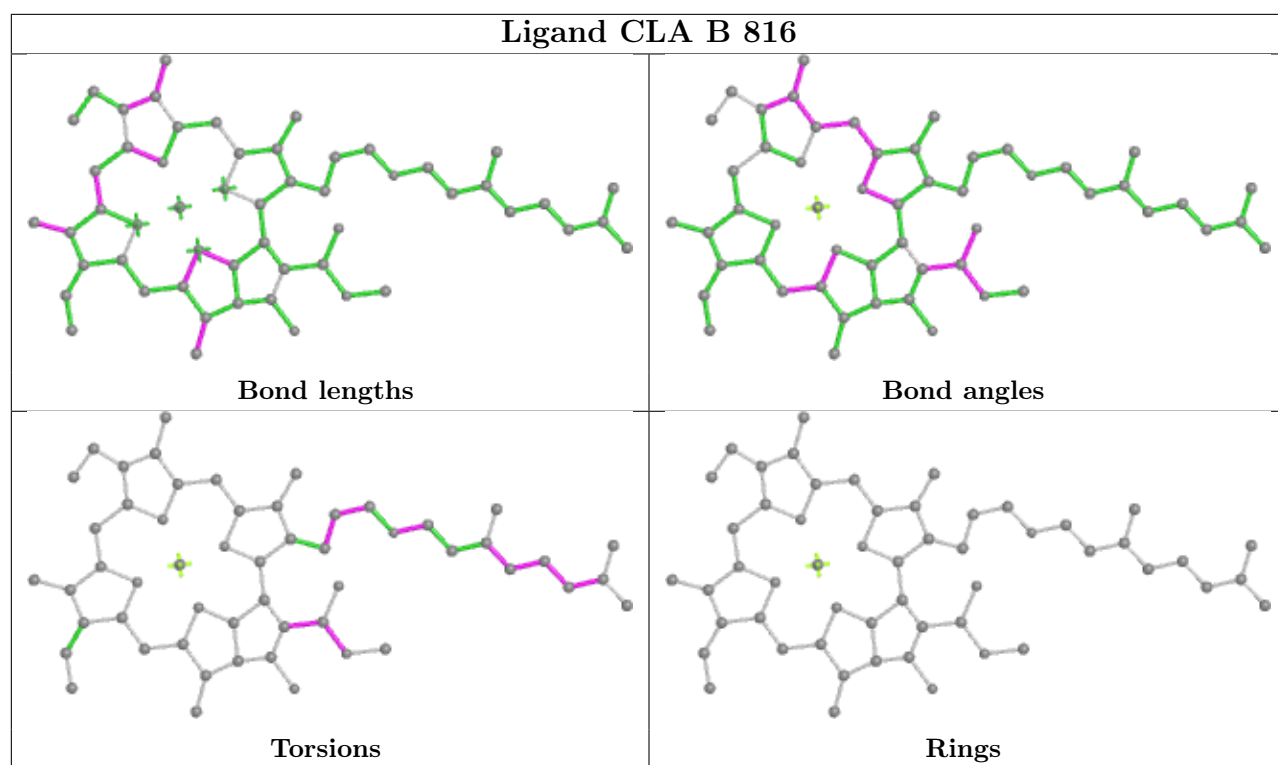


Ligand CLA a 607

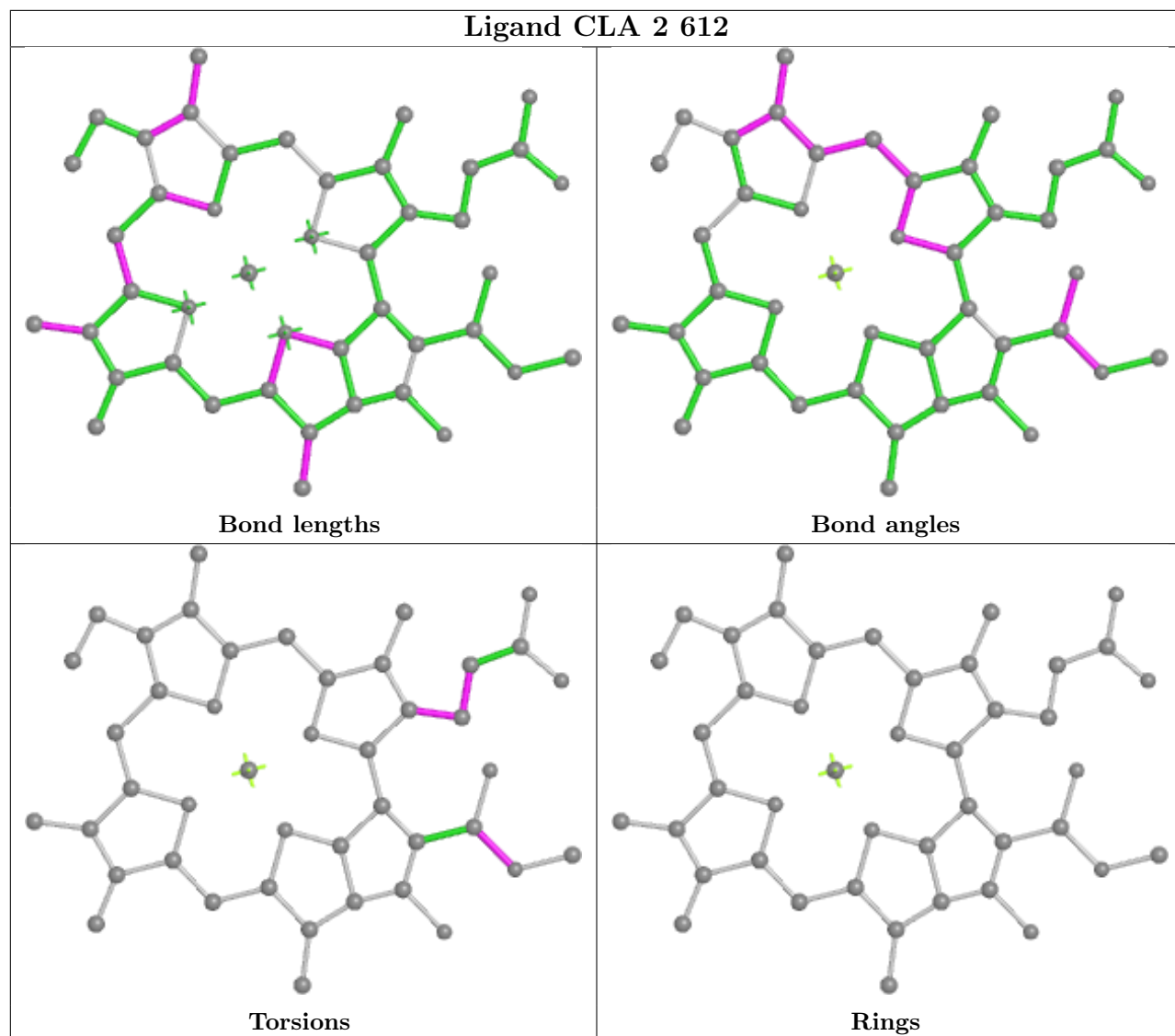


Ligand CLA 6 602

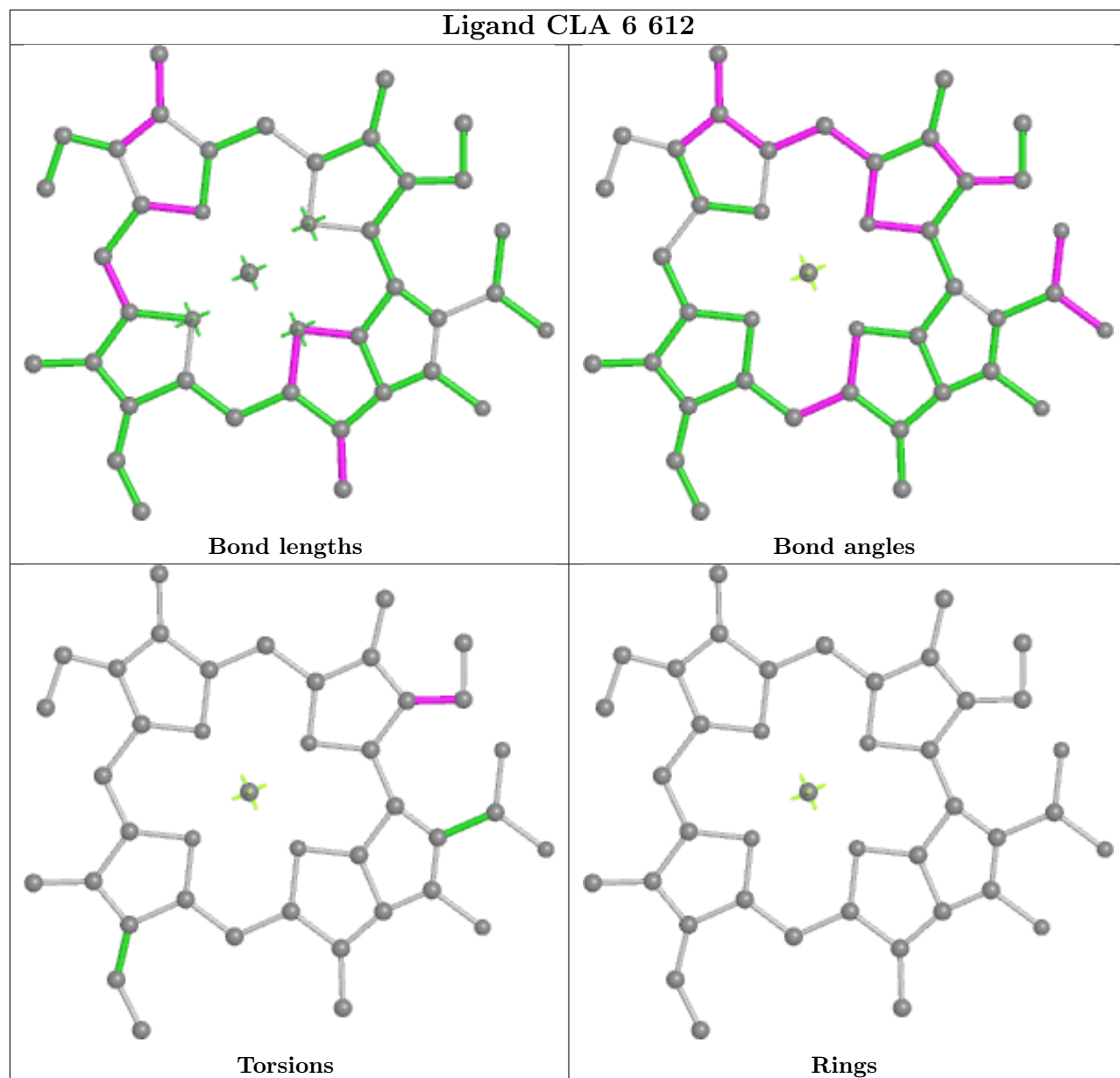


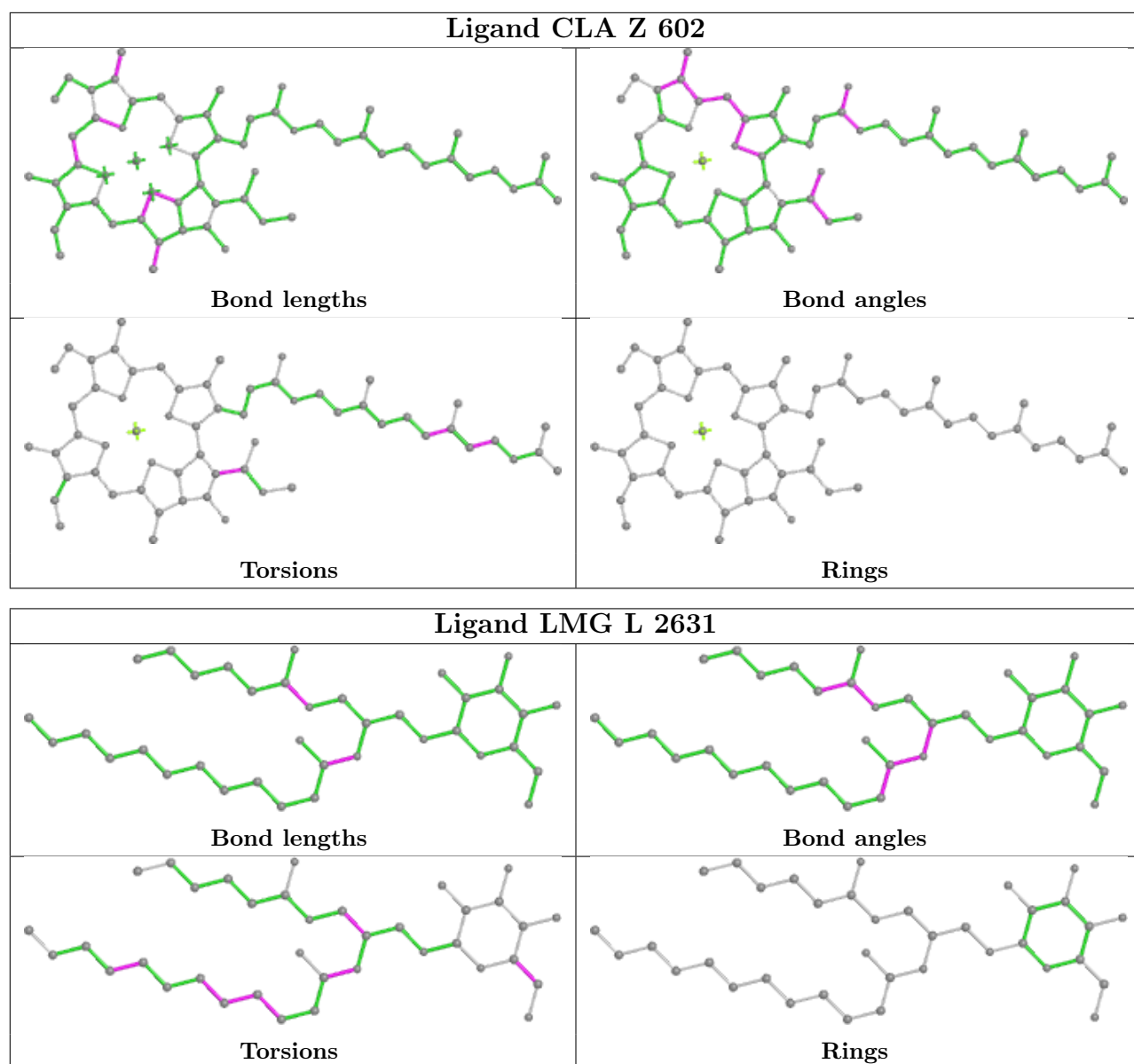


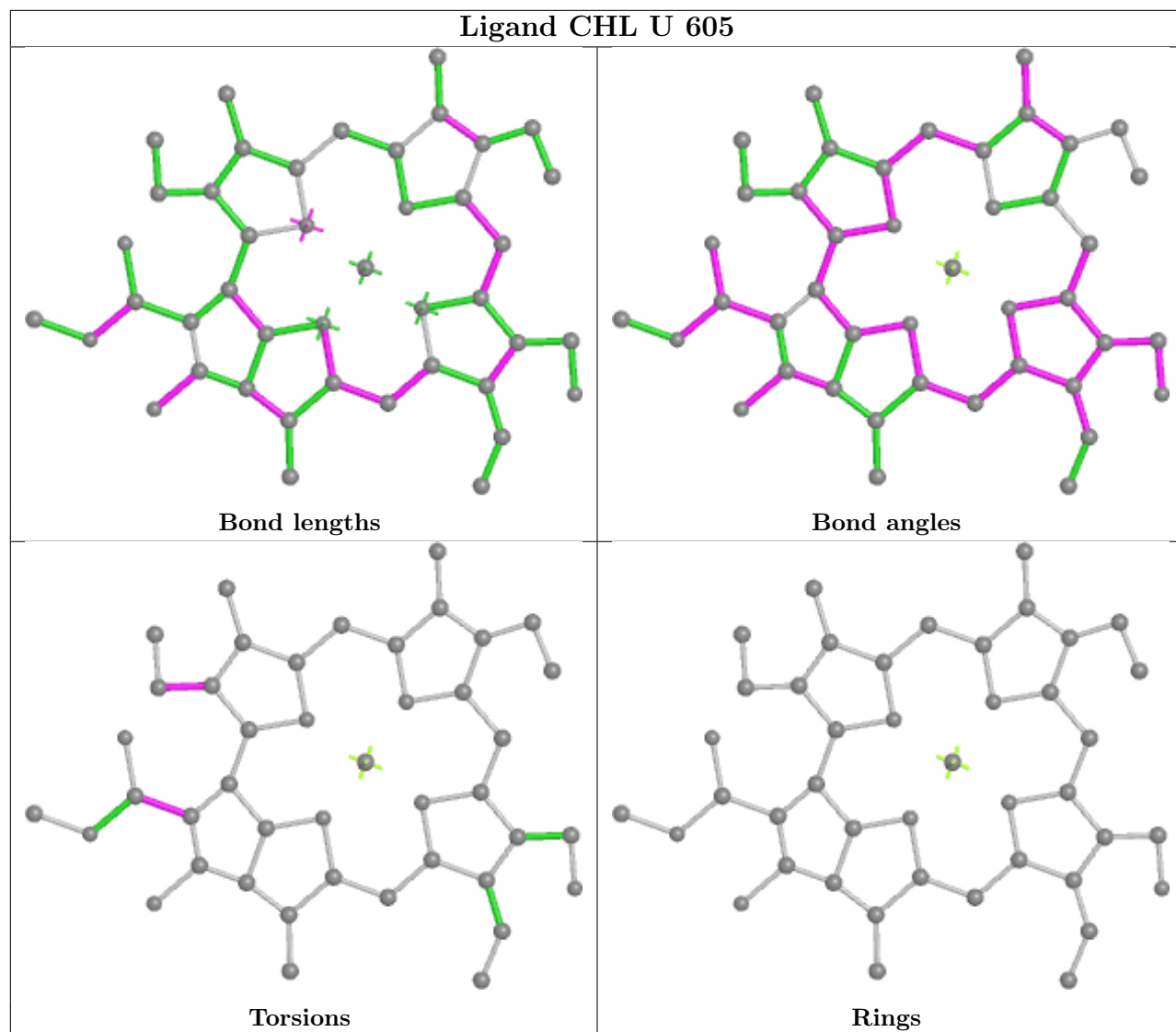
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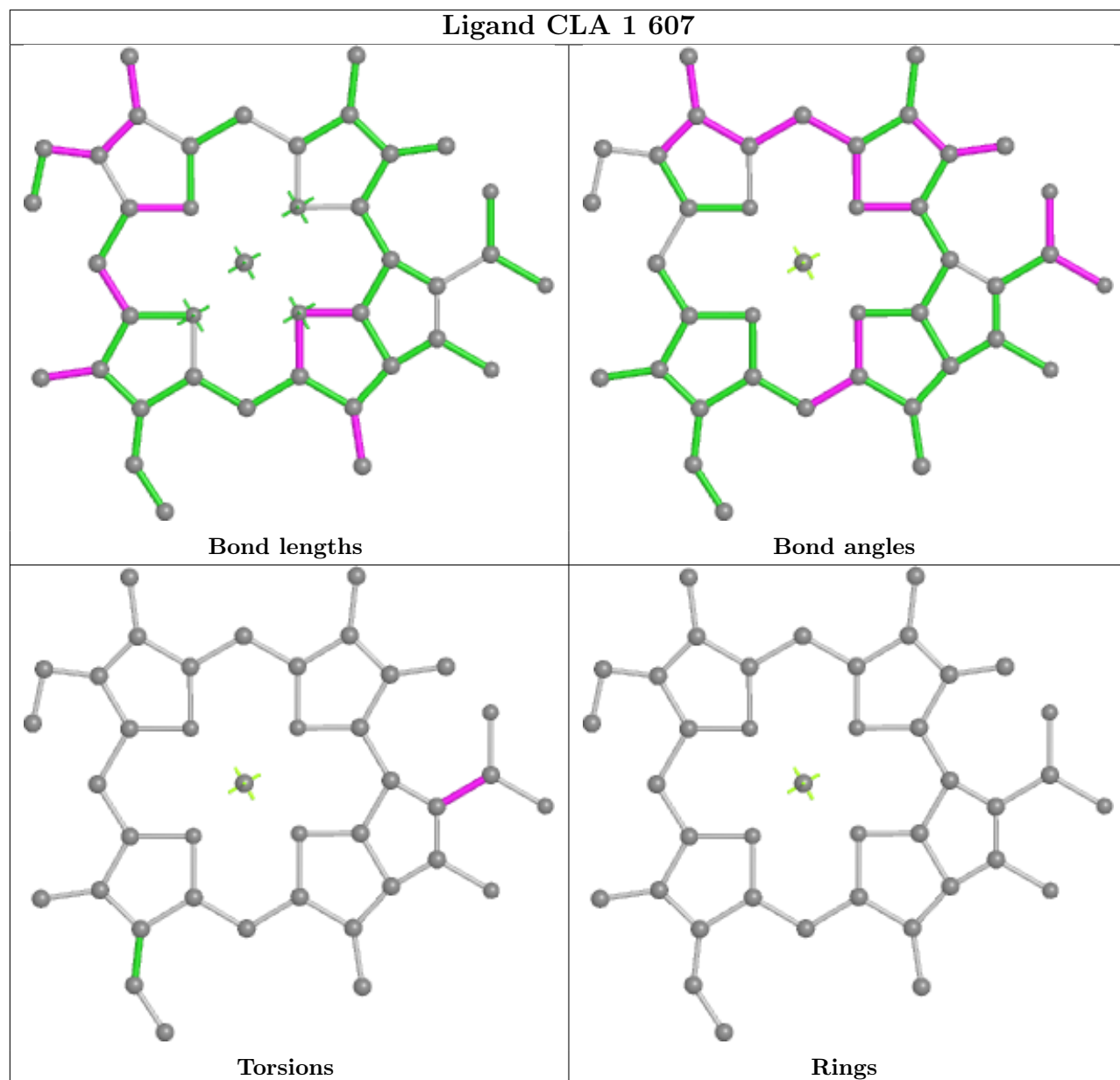
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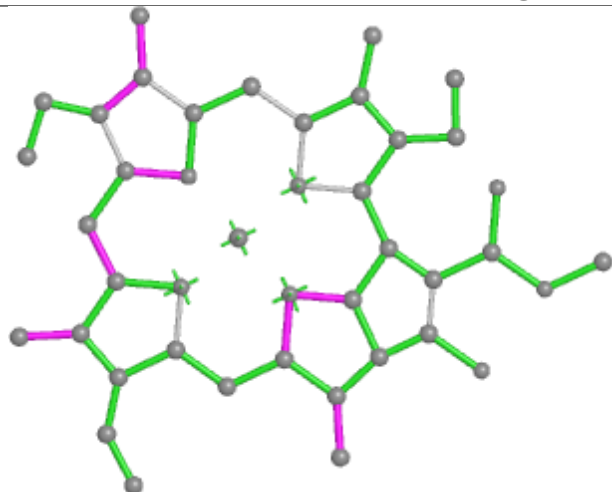




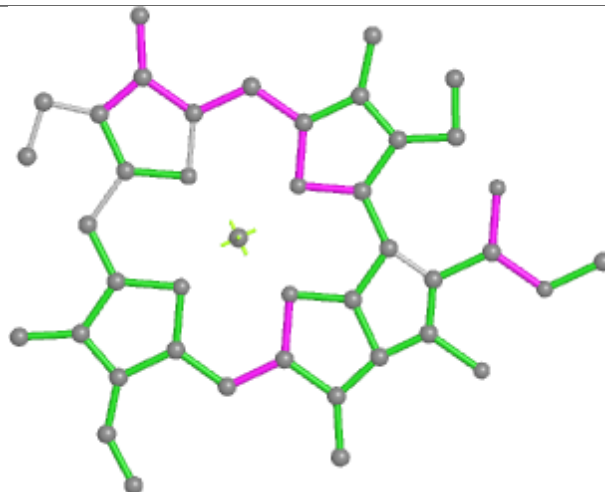
Ligand CLA 1 607



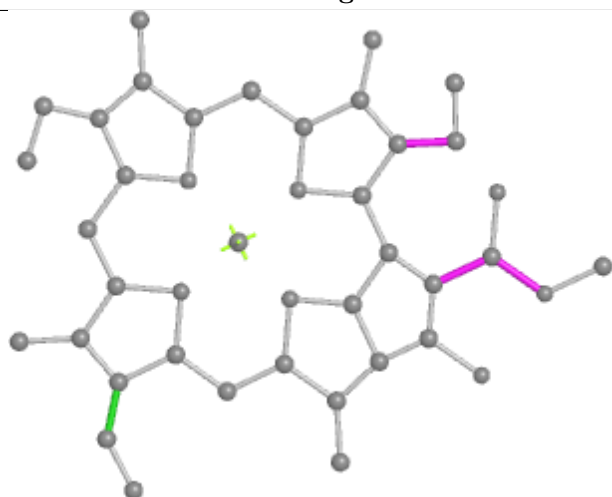
Ligand CLA F 303



Bond lengths



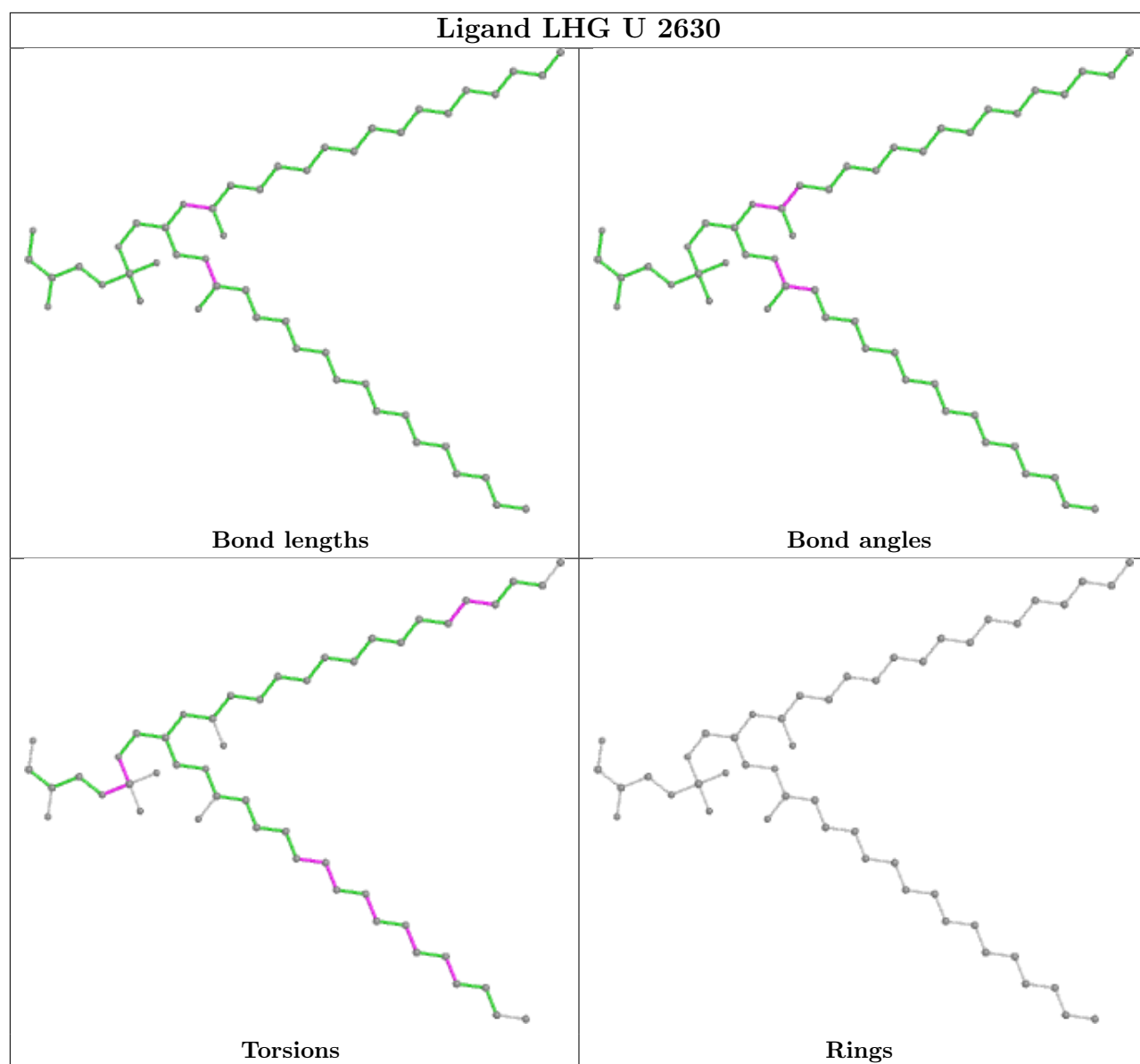
Bond angles



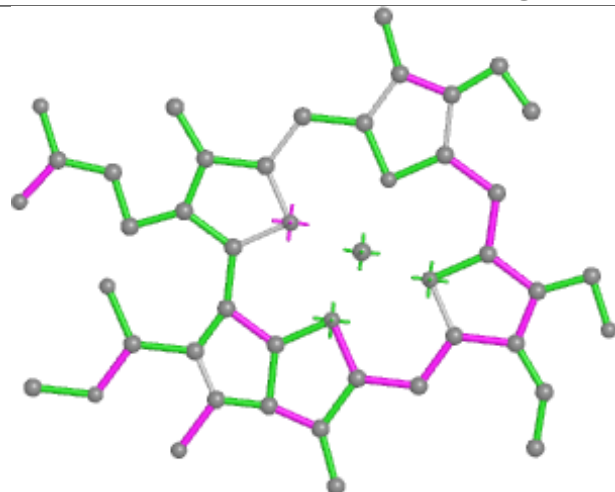
Torsions



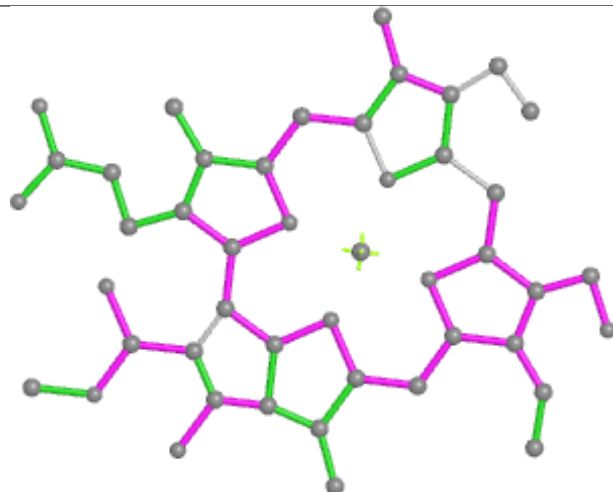
Rings



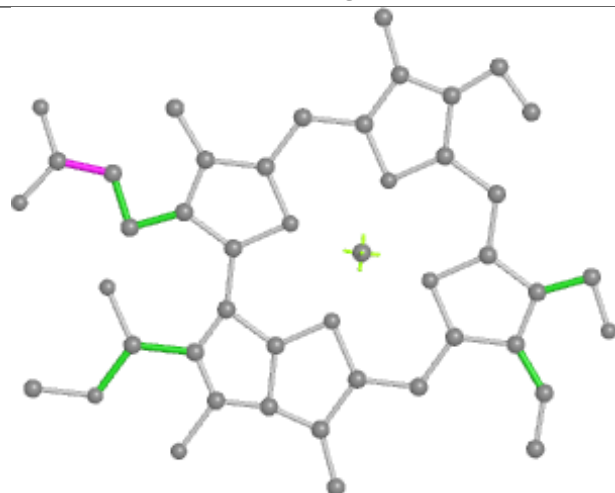
Ligand CHL Y 606



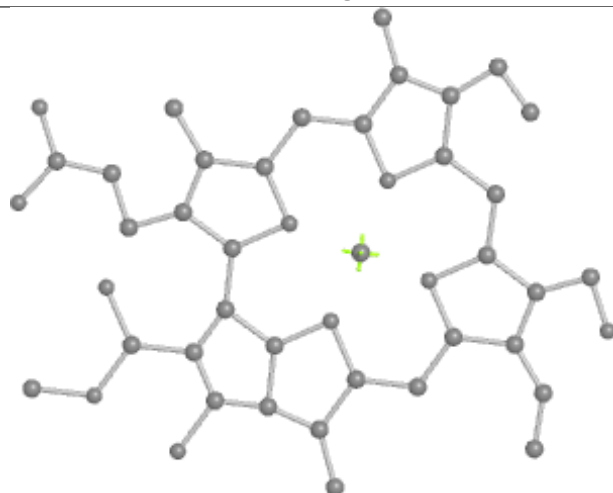
Bond lengths



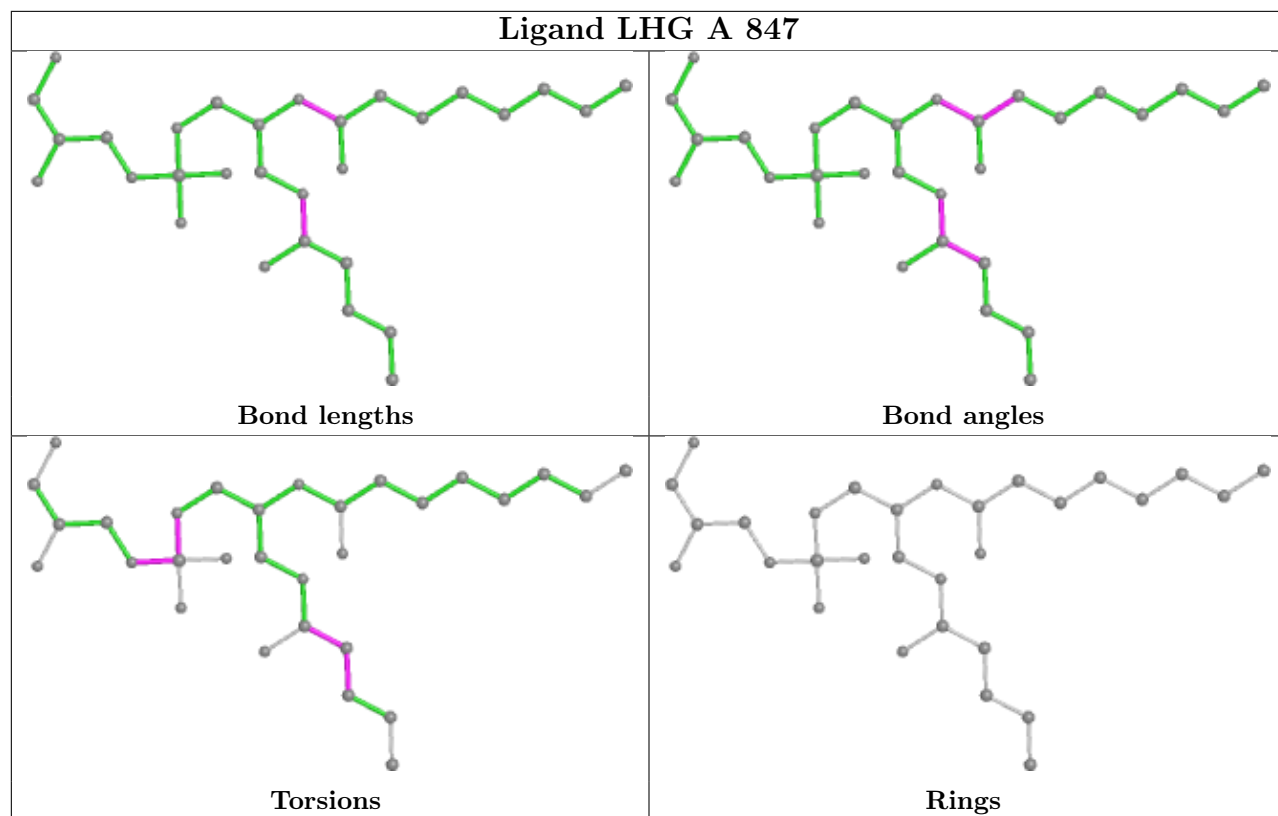
Bond angles



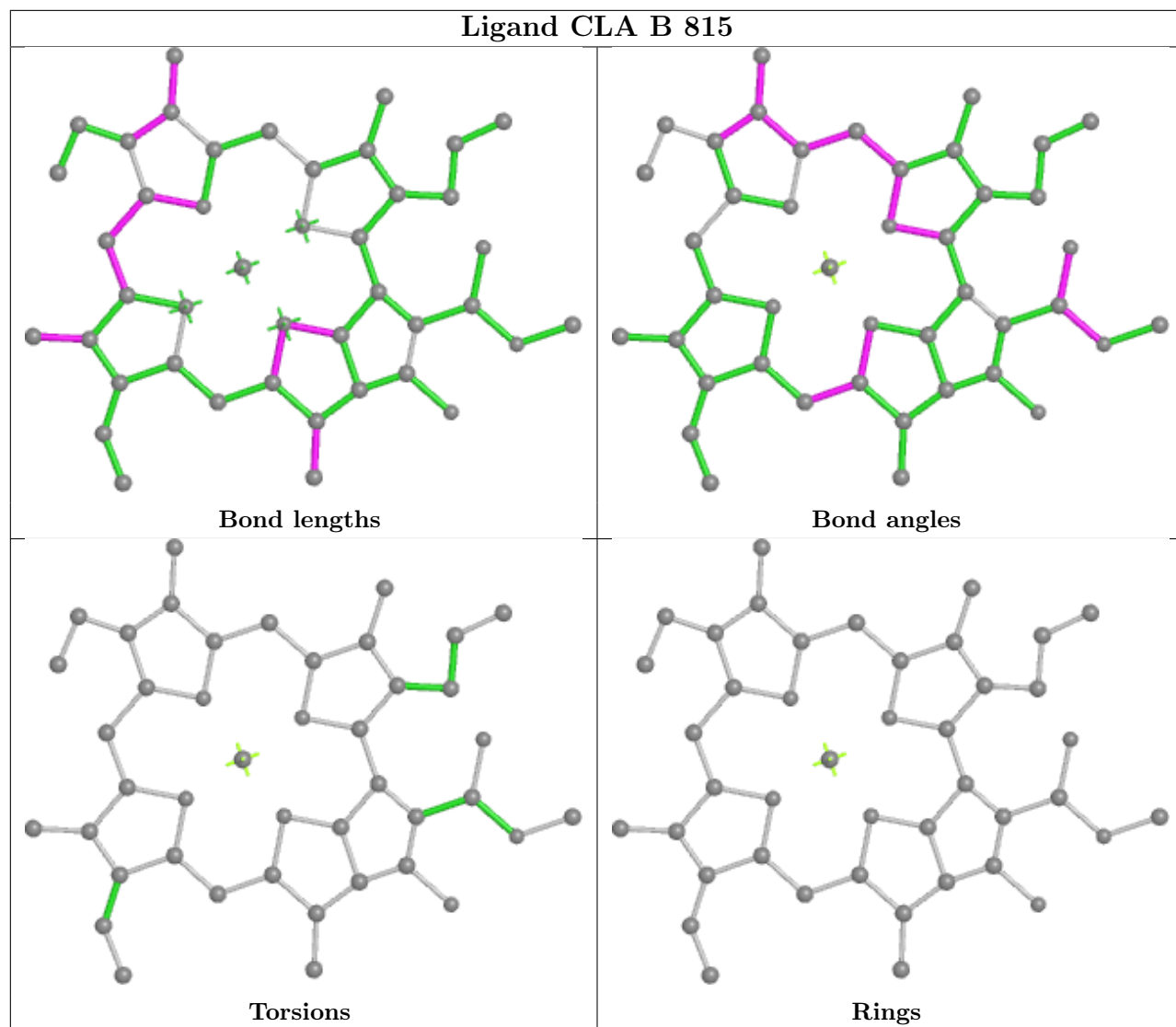
Torsions



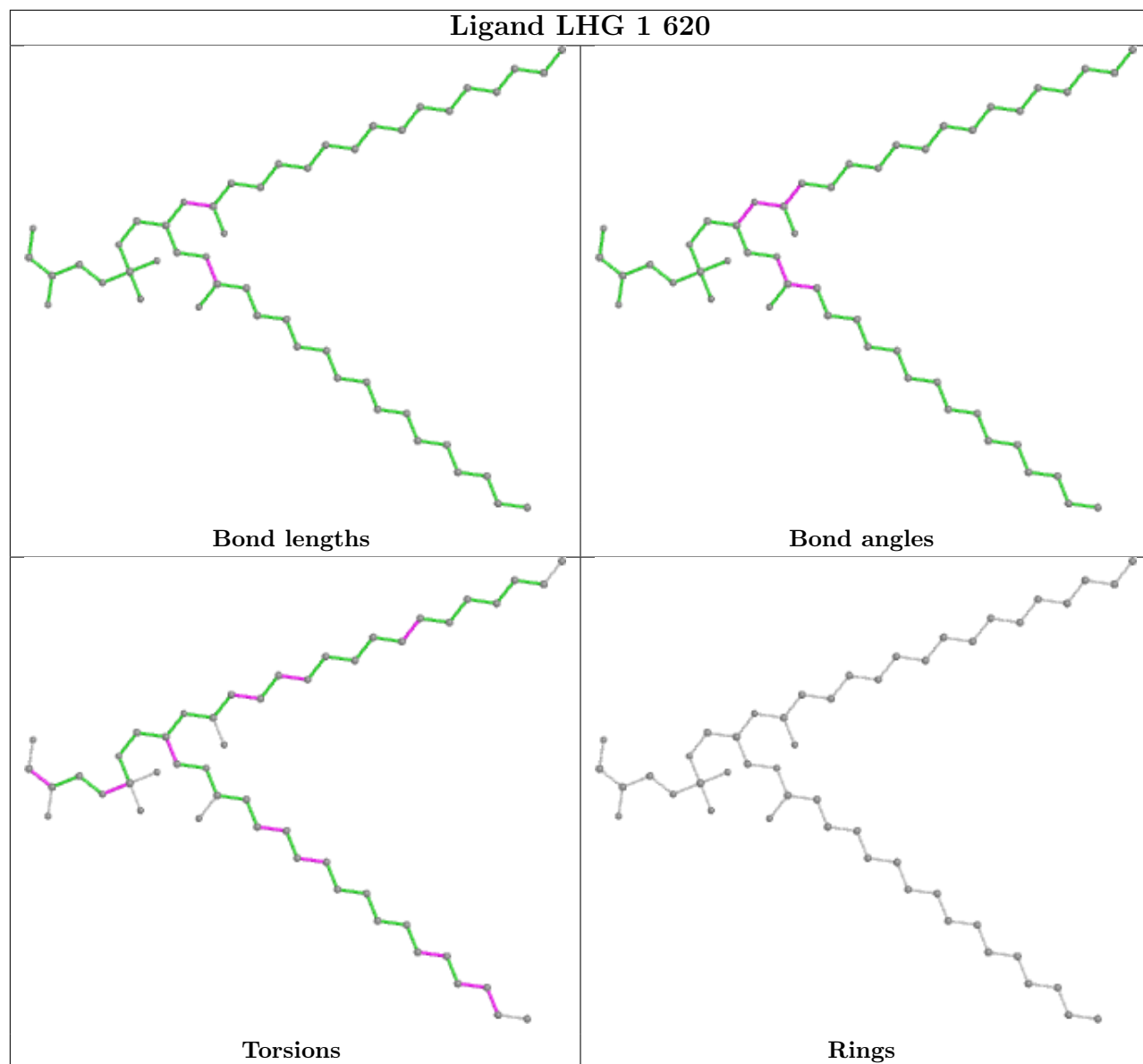
Rings



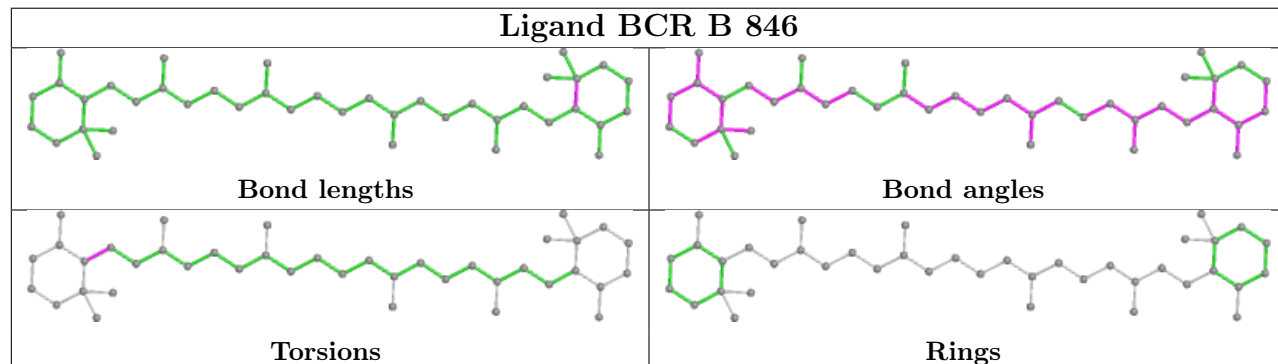
Ligand CLA B 815



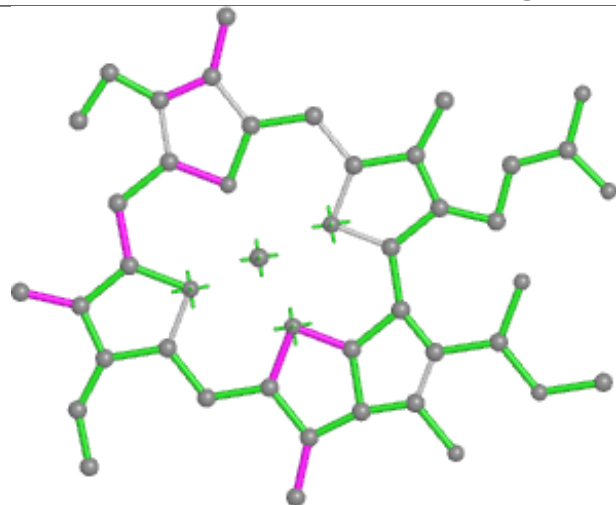
Ligand LHG 1 620



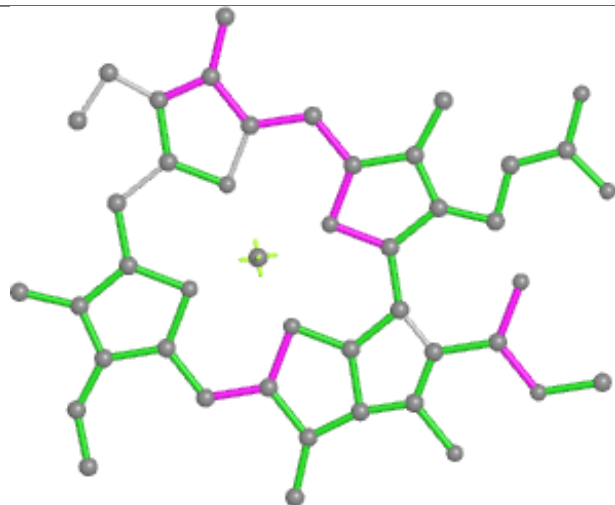
Ligand BCR B 846



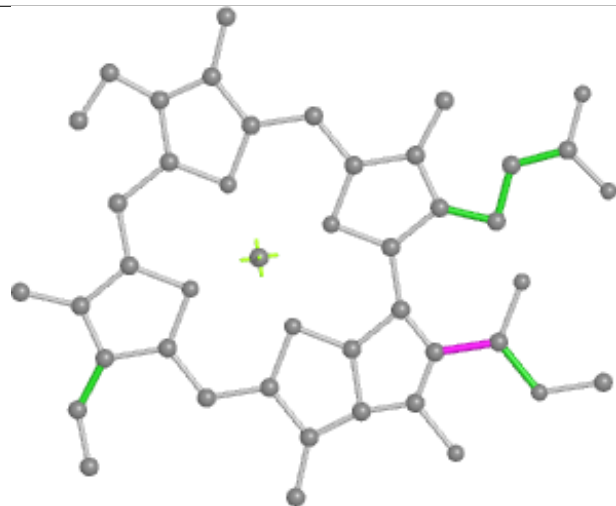
Ligand CLA L 304



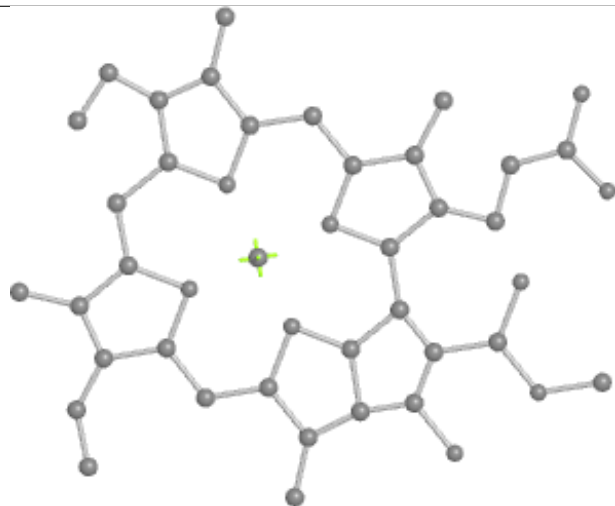
Bond lengths



Bond angles

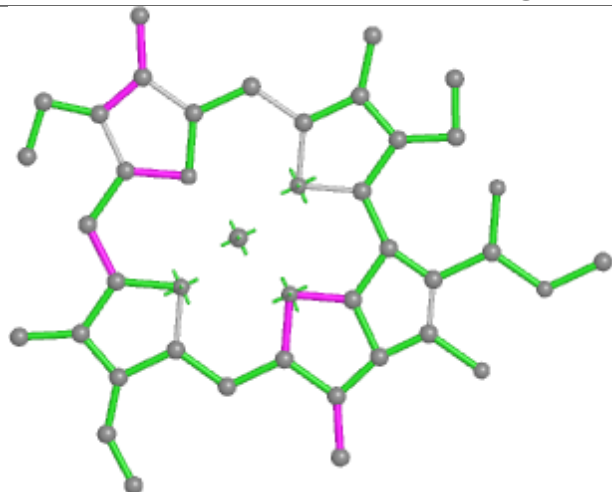


Torsions

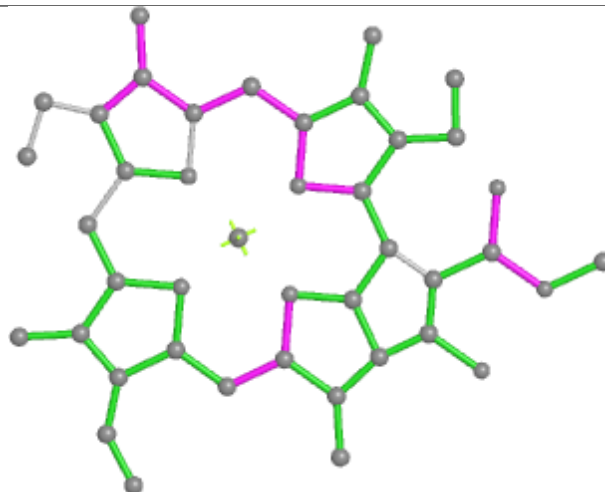


Rings

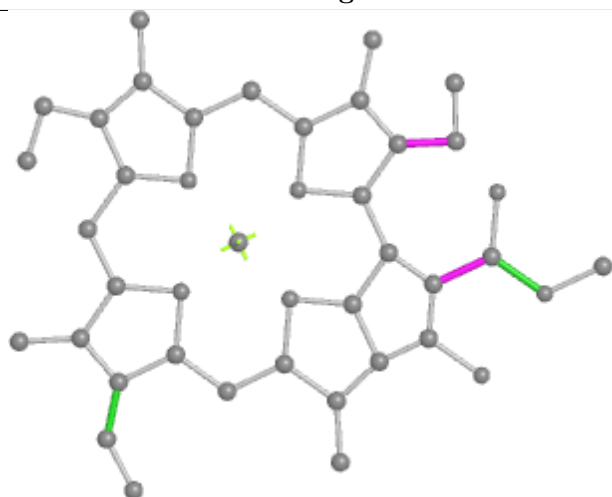
Ligand CLA 9 611



Bond lengths



Bond angles

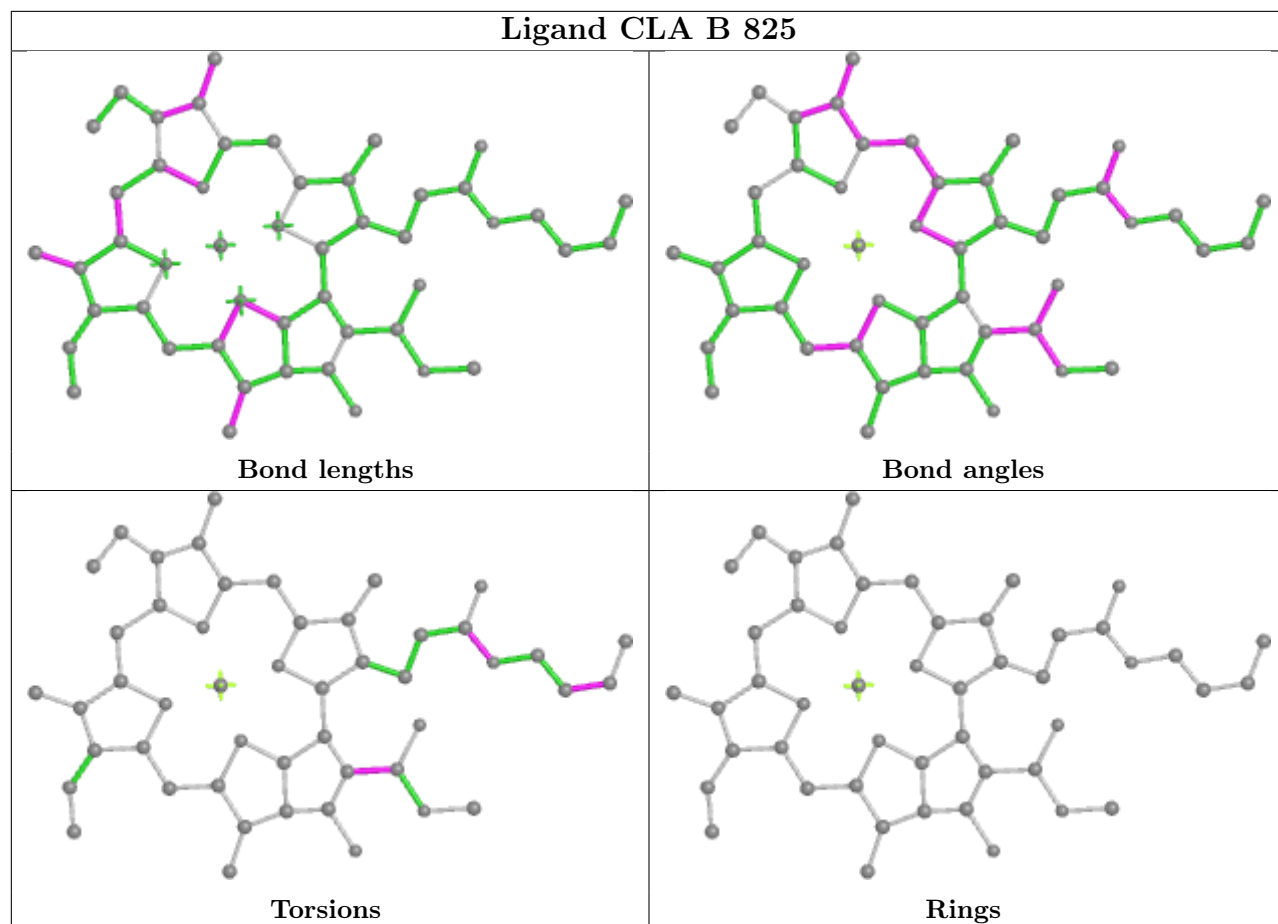


Torsions

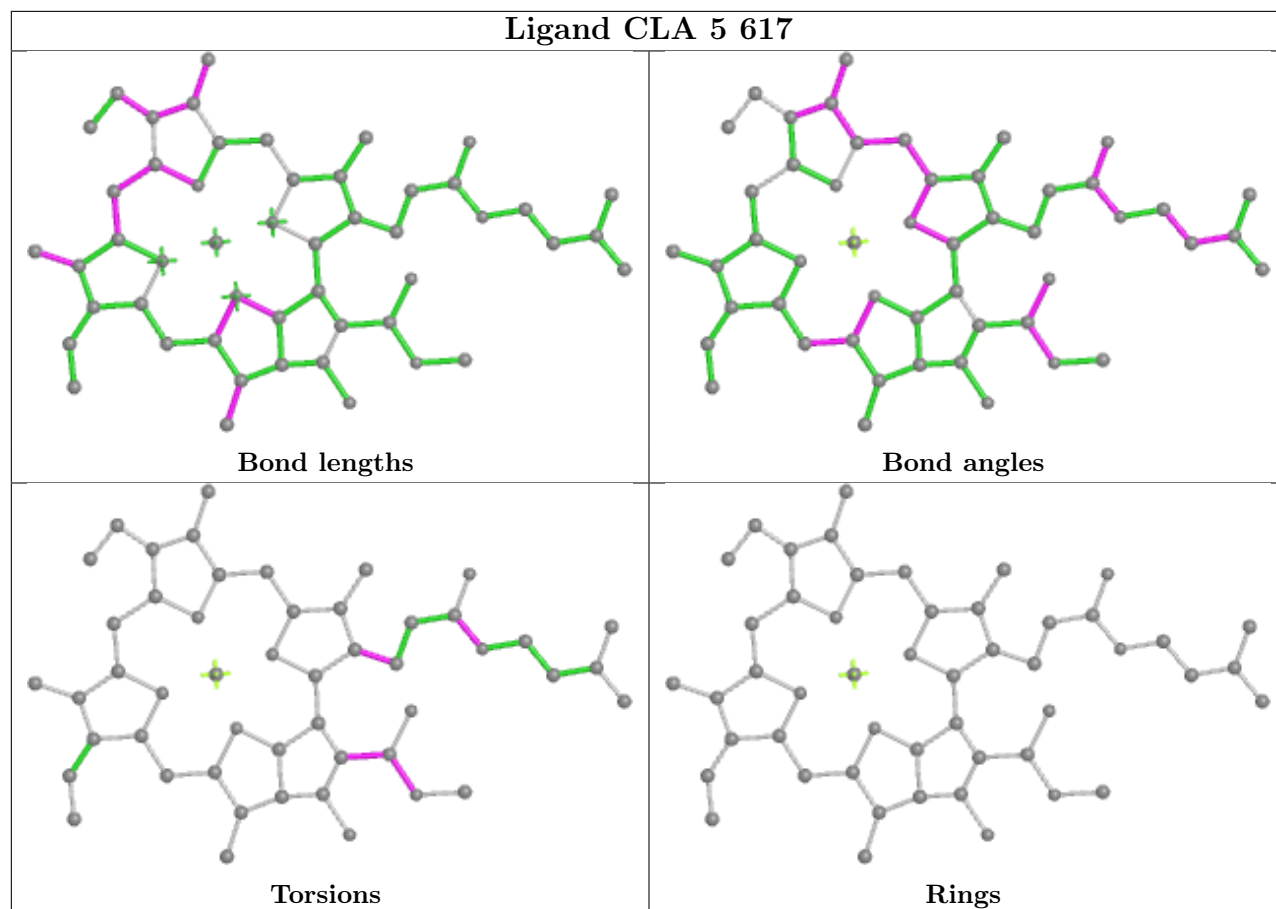


Rings

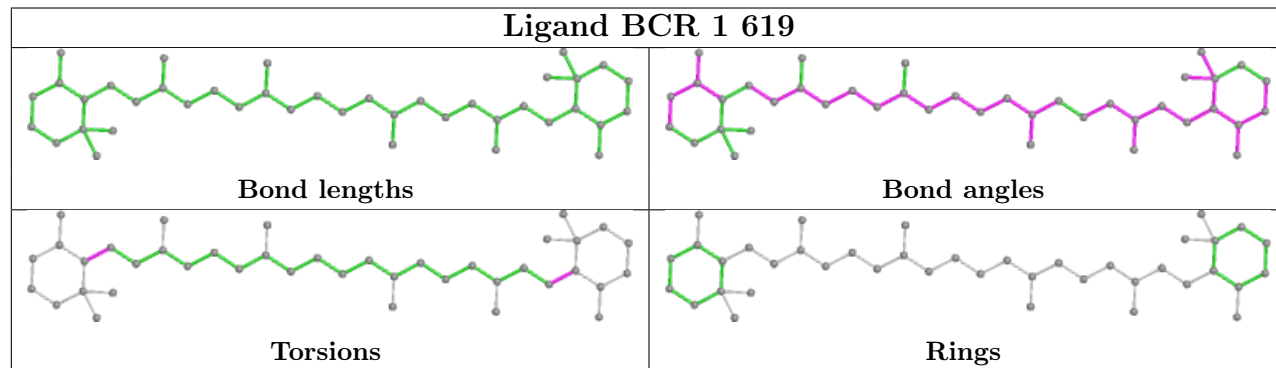
Ligand CLA B 825

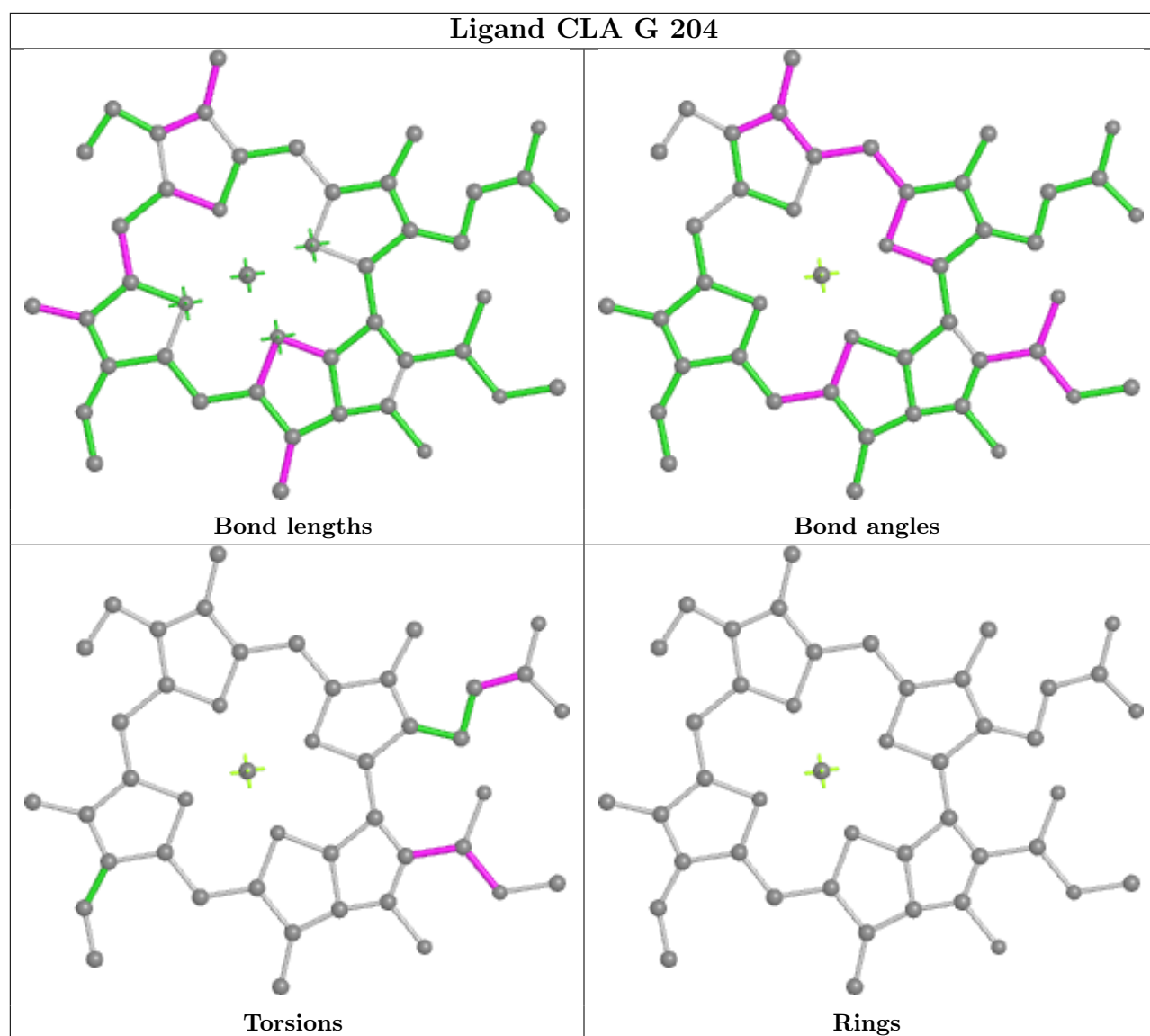


Ligand CLA 5 617

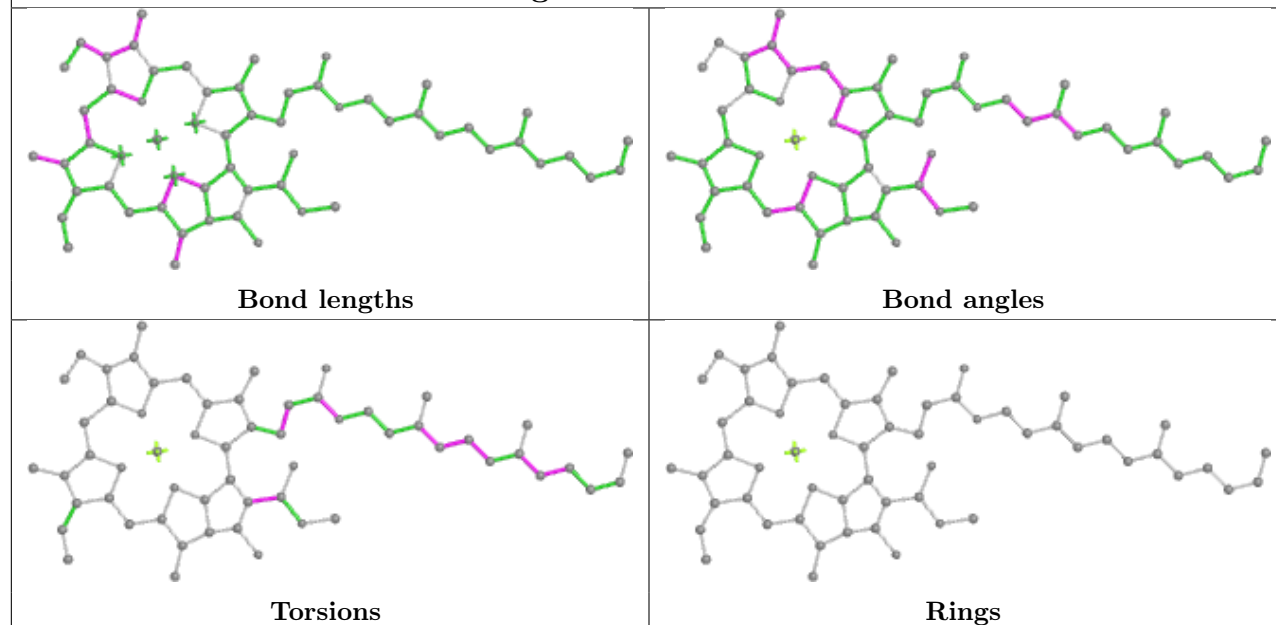


Ligand BCR 1 619

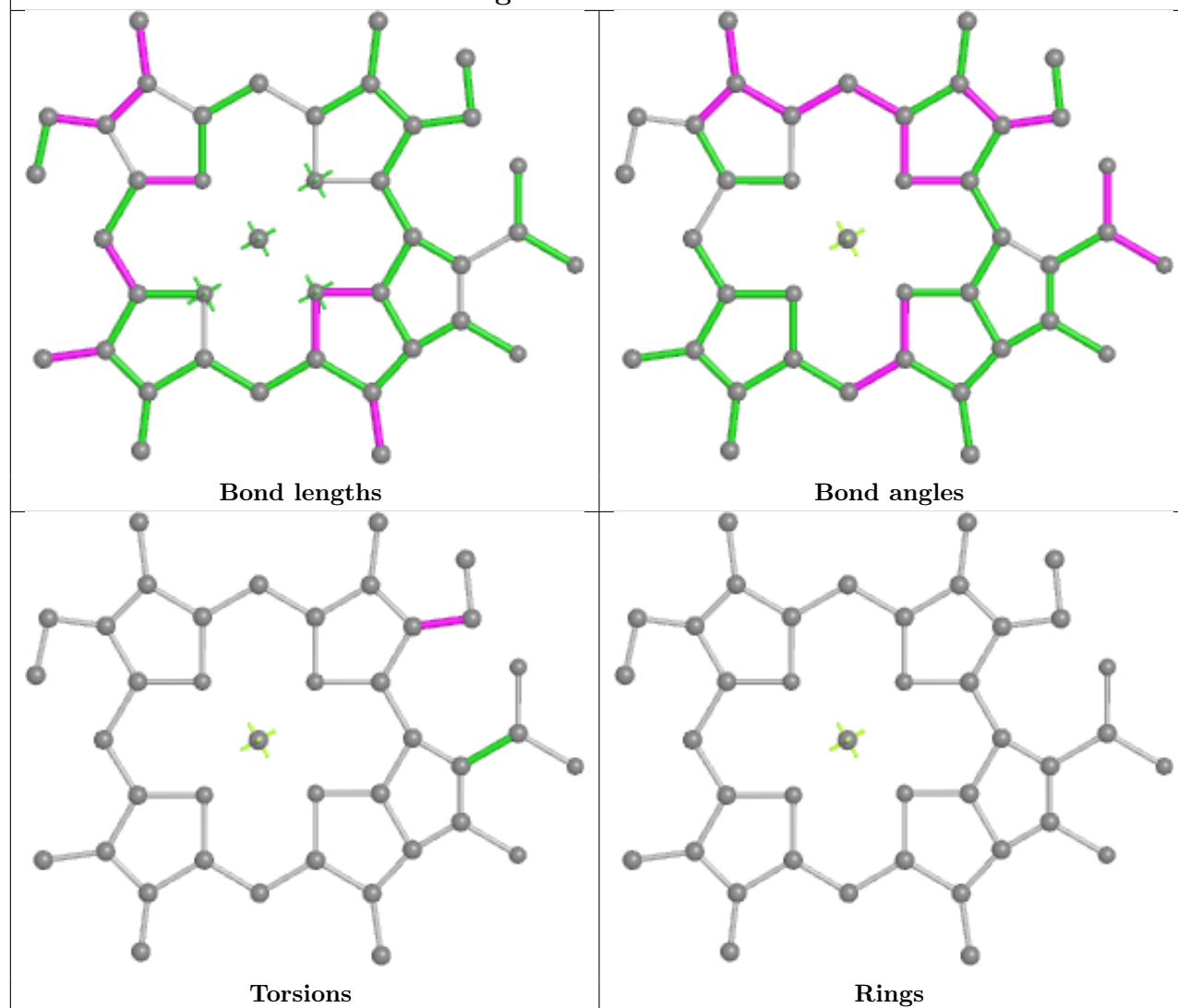




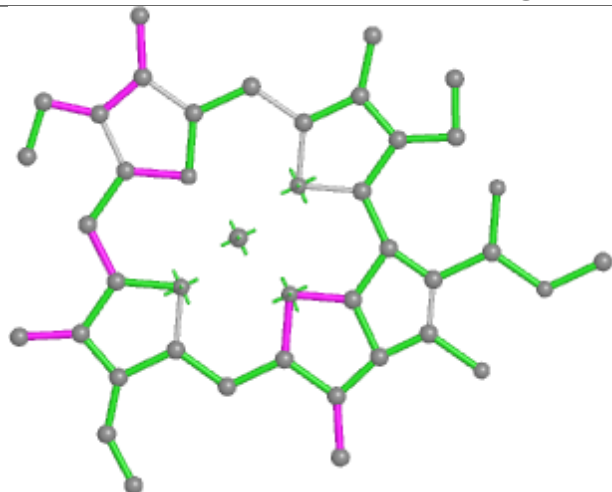
Ligand CLA U 613



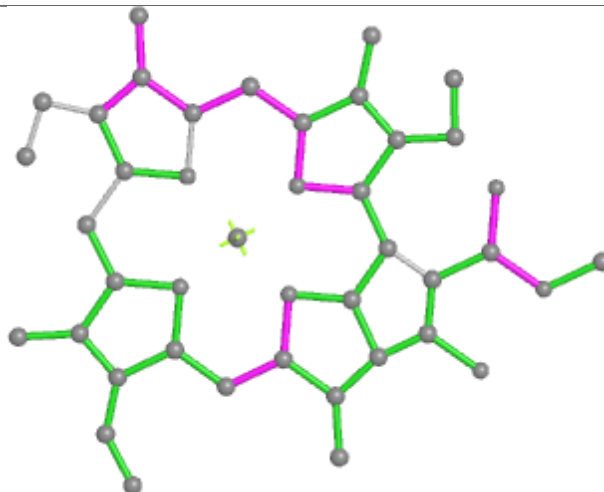
Ligand CLA 9 606



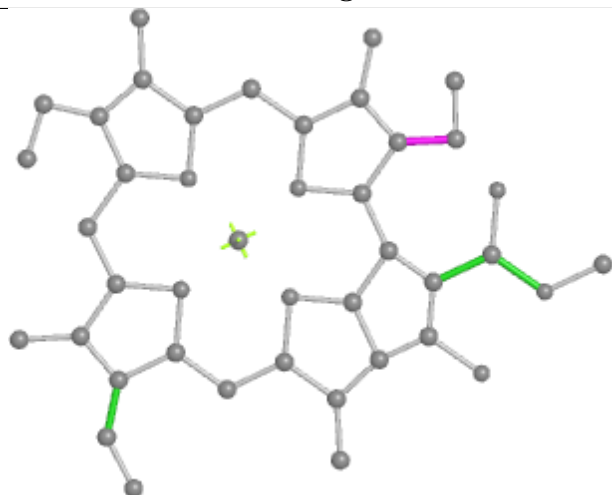
Ligand CLA 8 611



Bond lengths



Bond angles

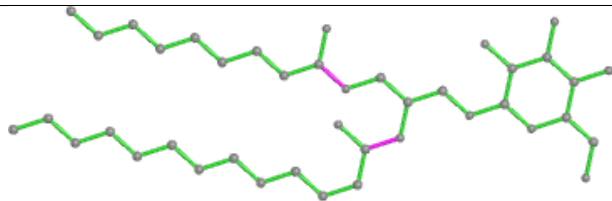


Torsions

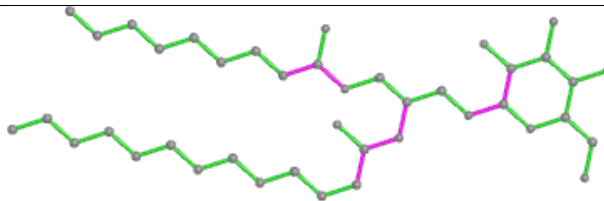


Rings

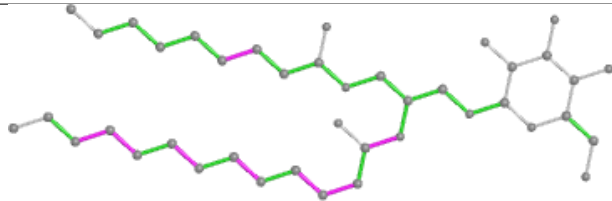
Ligand LMG V 2631



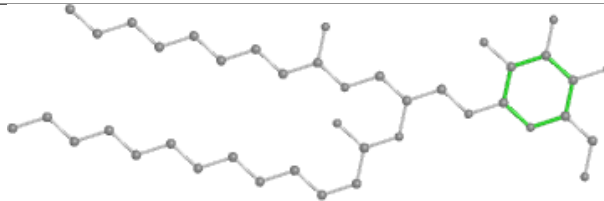
Bond lengths



Bond angles

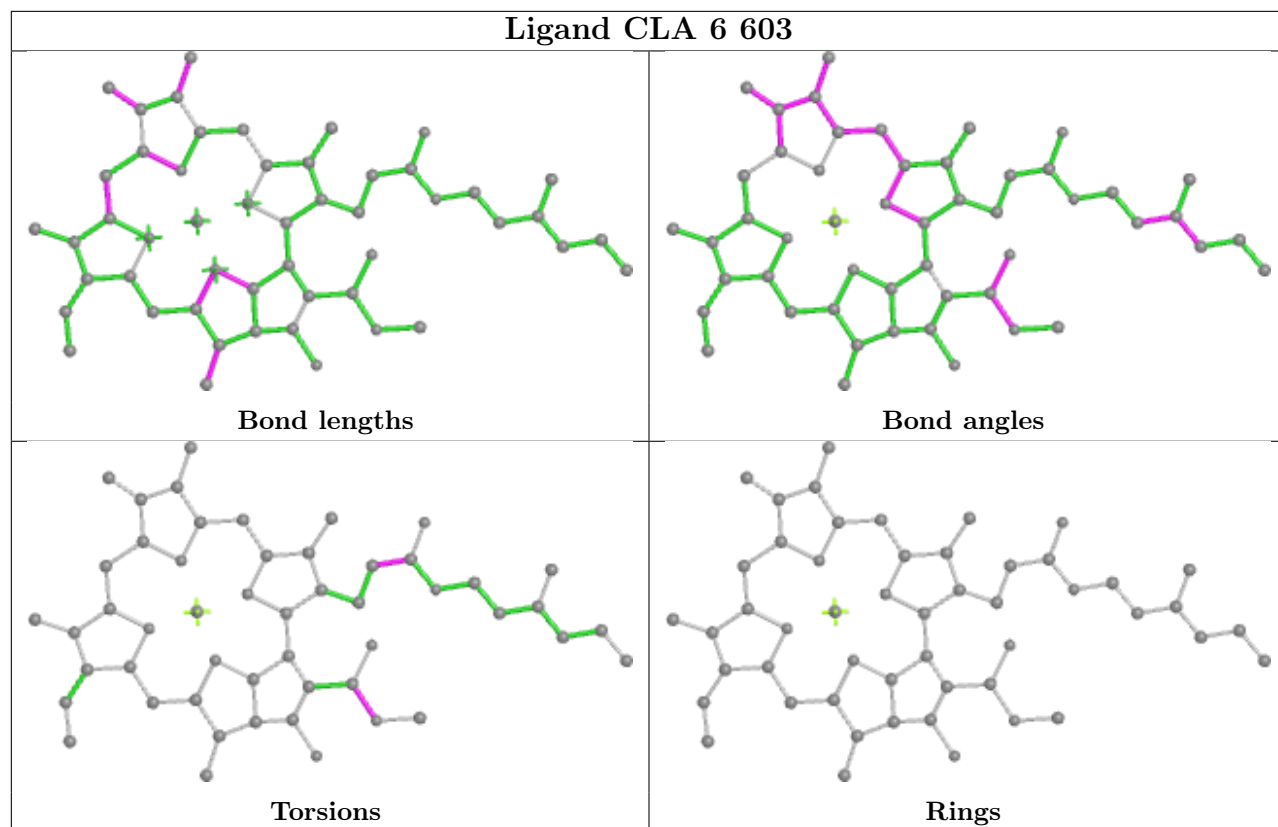


Torsions

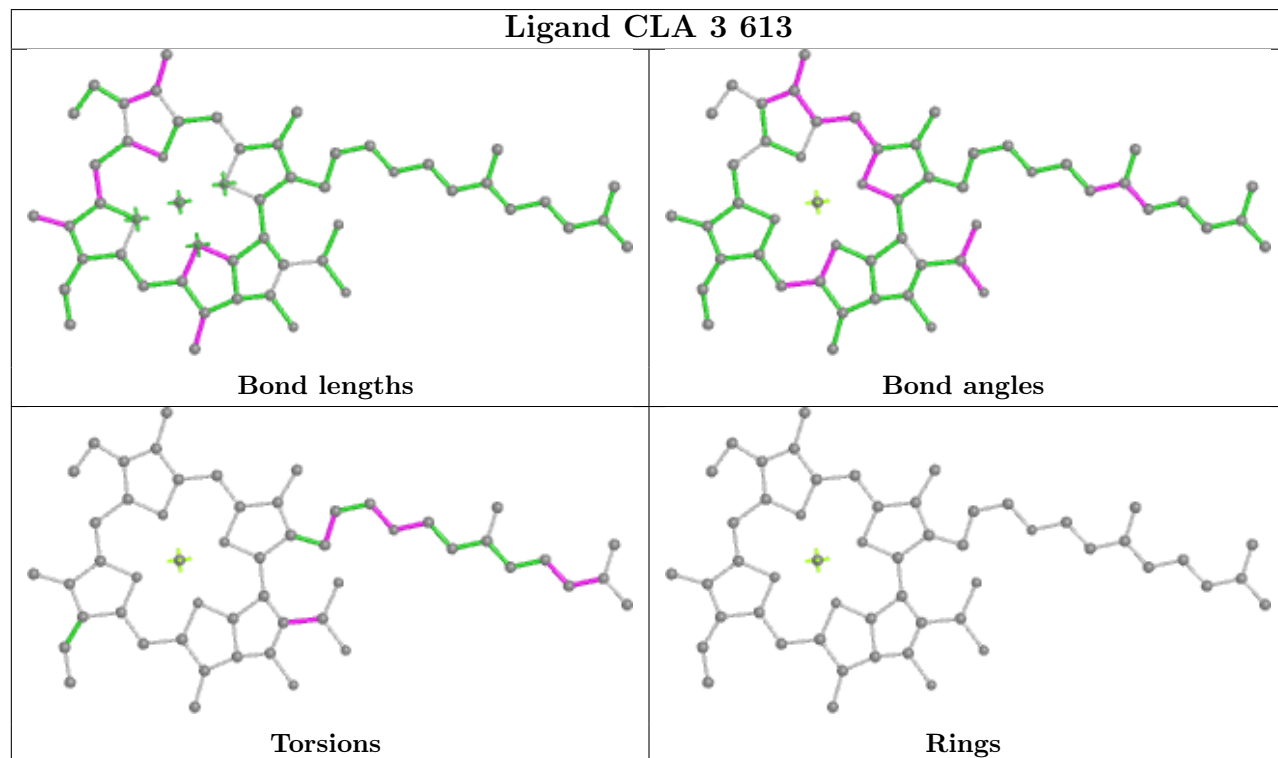


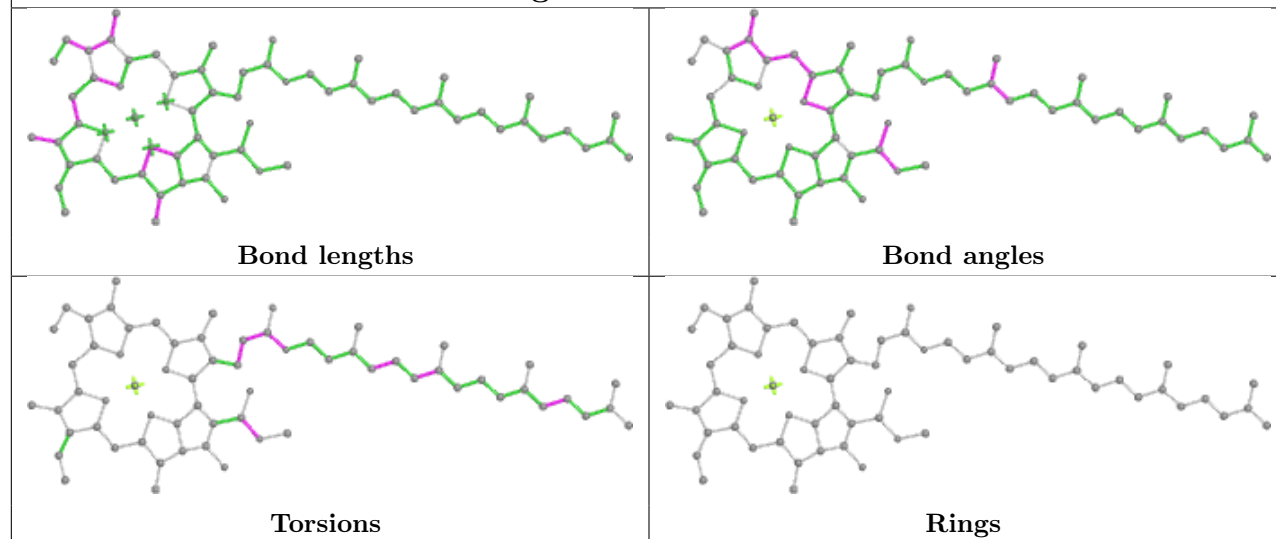
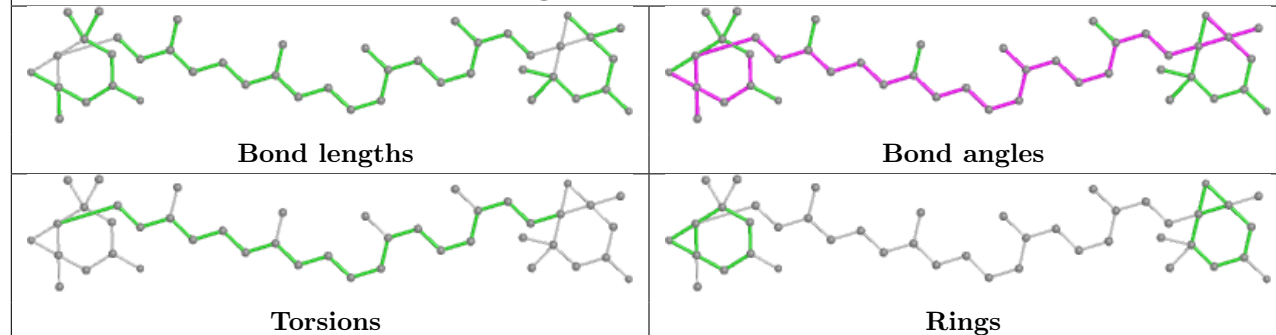
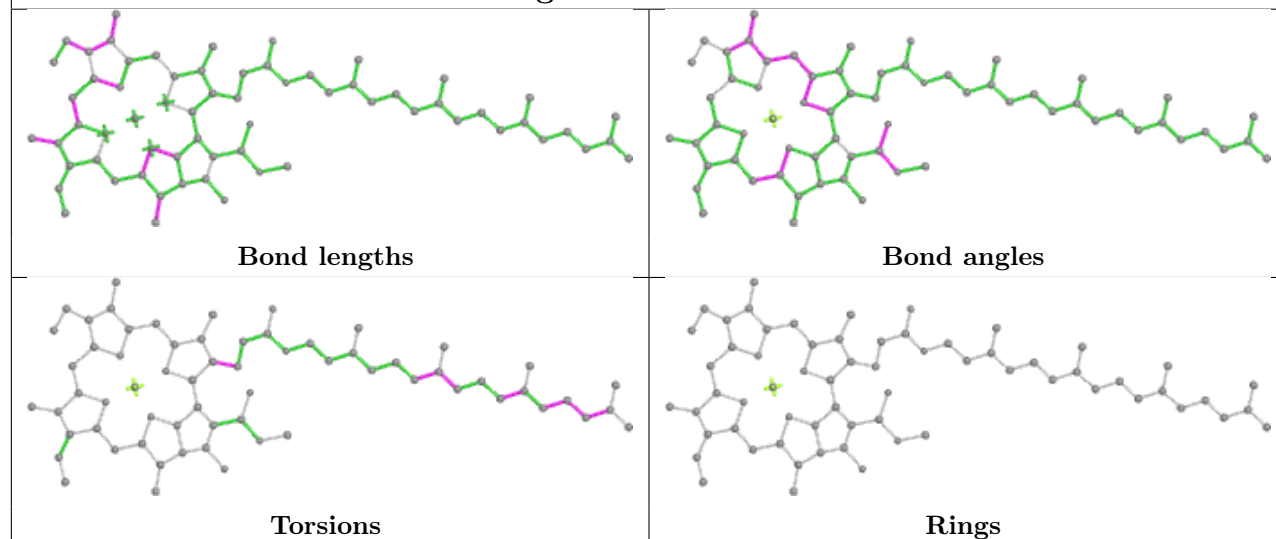
Rings

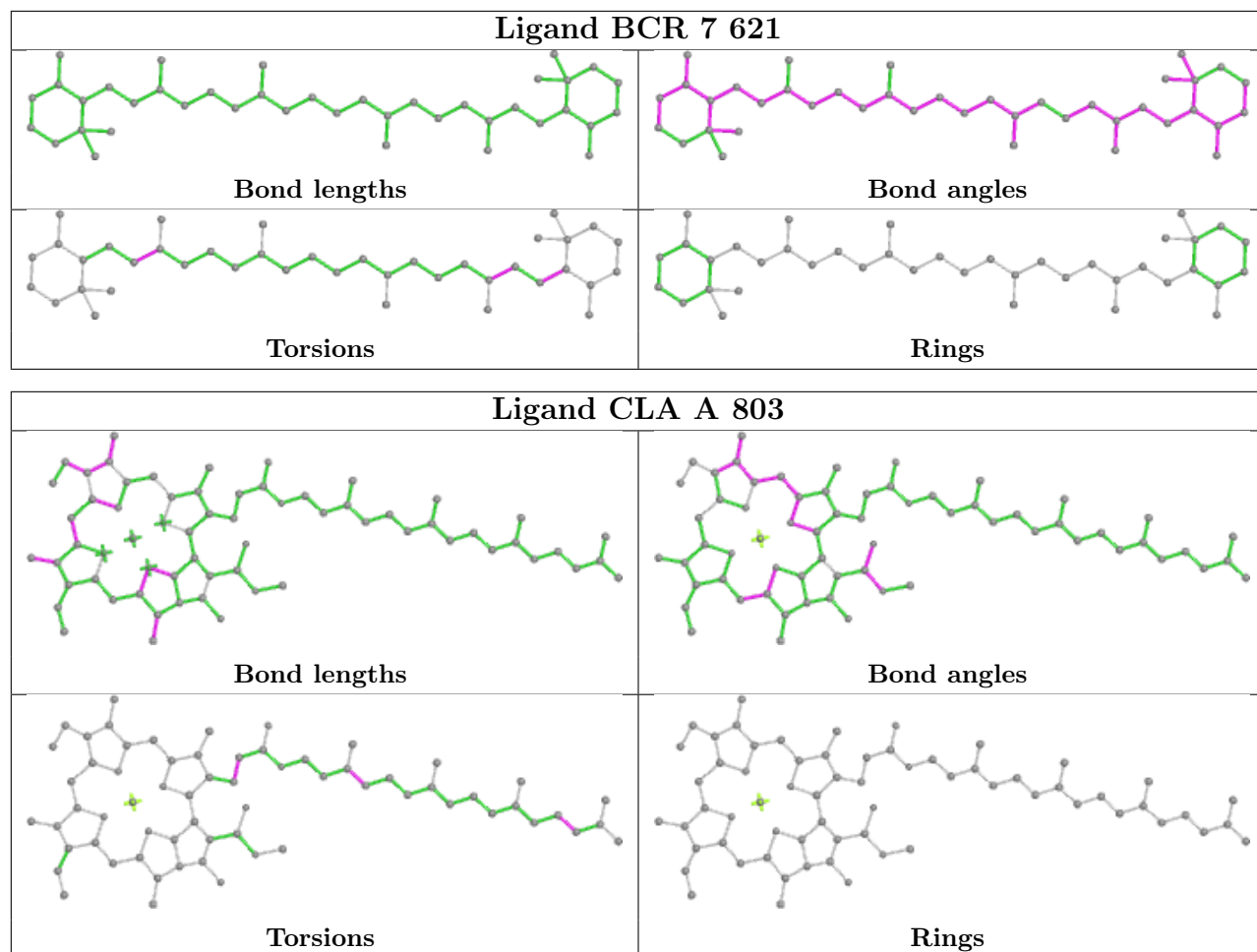
Ligand CLA 6 603



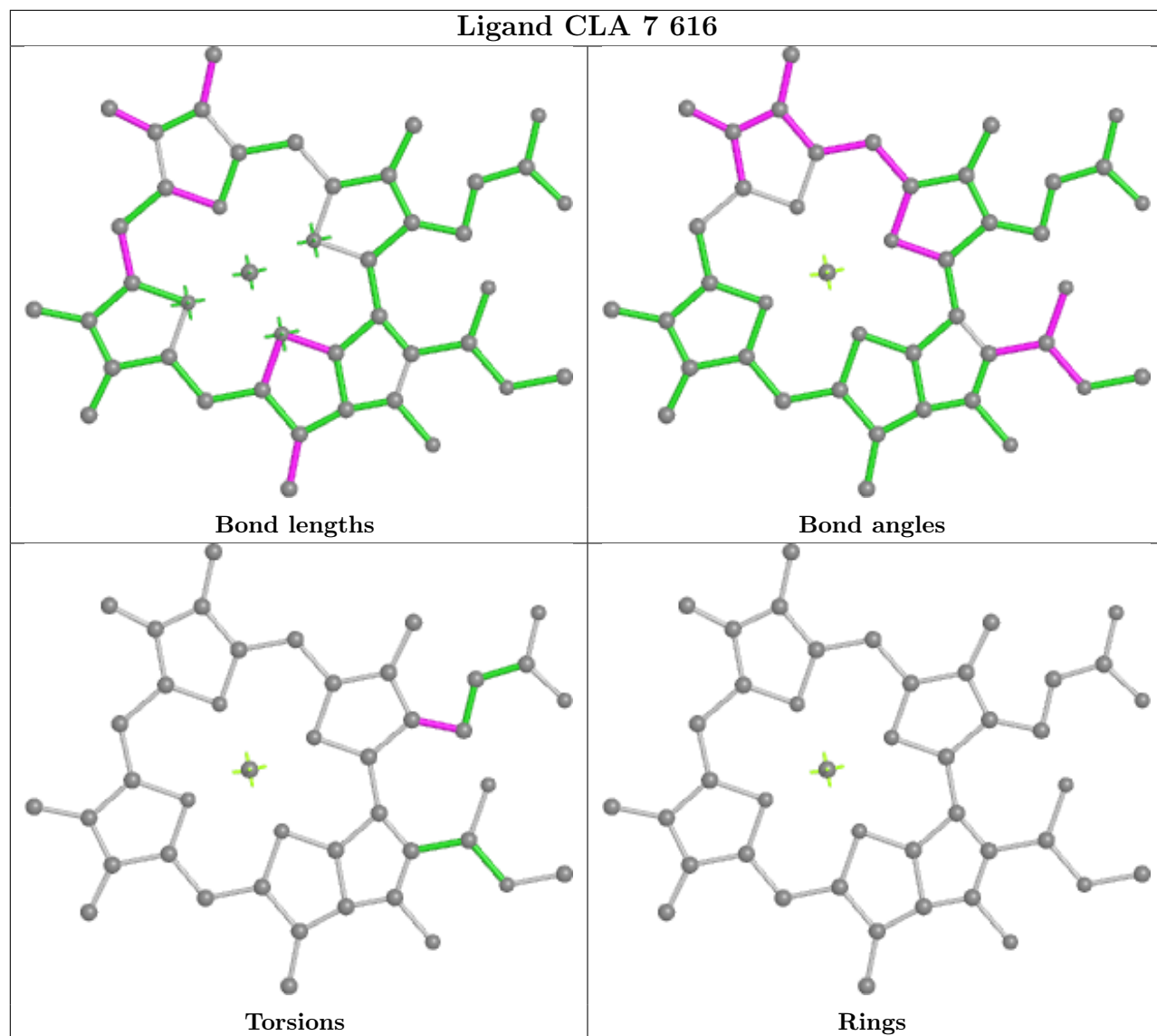
Ligand CLA 3 613



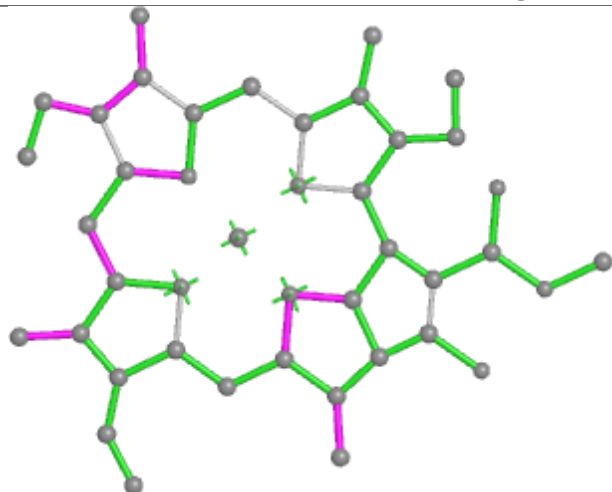
Ligand CLA A 830**Ligand XAT 2 620****Ligand CLA 5 609**



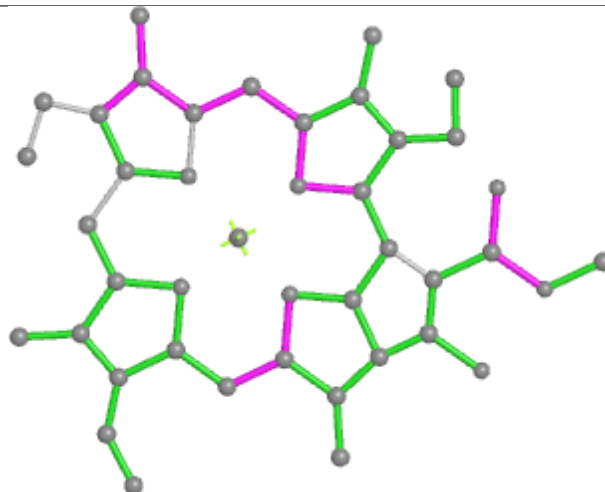
Ligand CLA 7 616



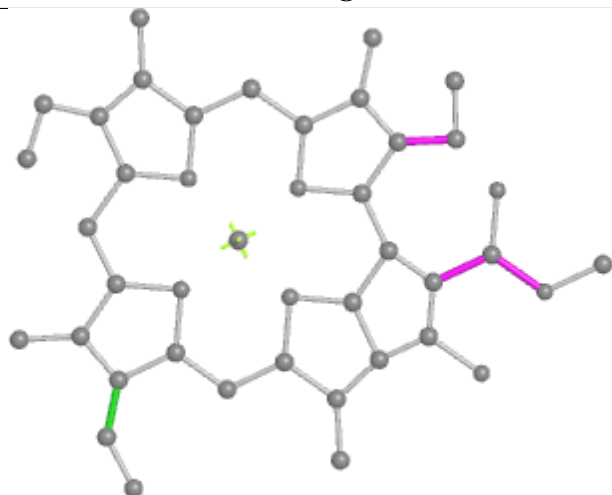
Ligand CLA U 614



Bond lengths



Bond angles

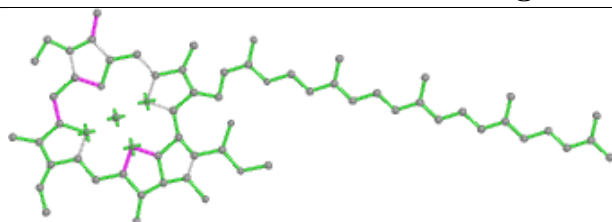


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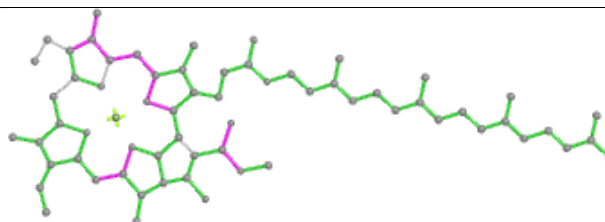


Rings

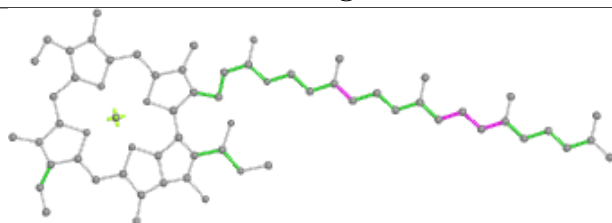
Ligand CLA Z 611



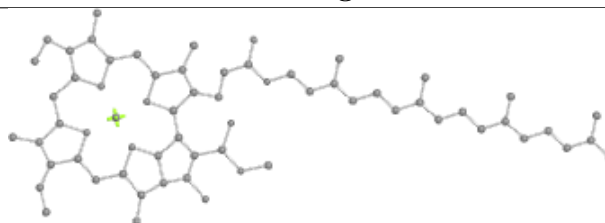
Bond lengths



Bond angles

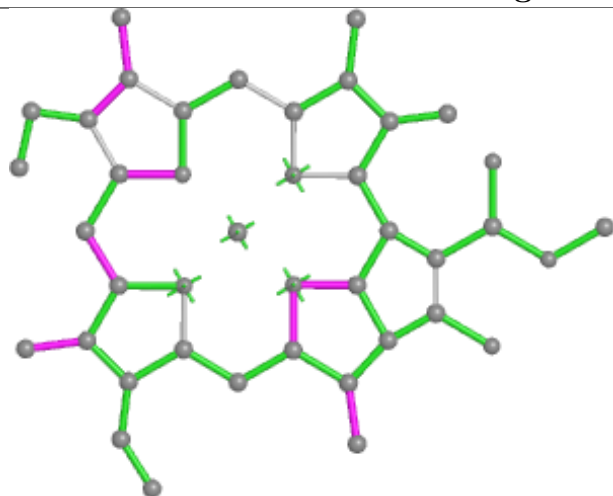


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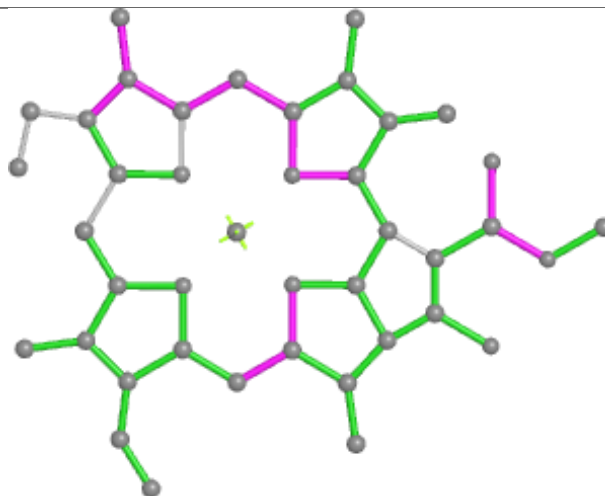


Rings

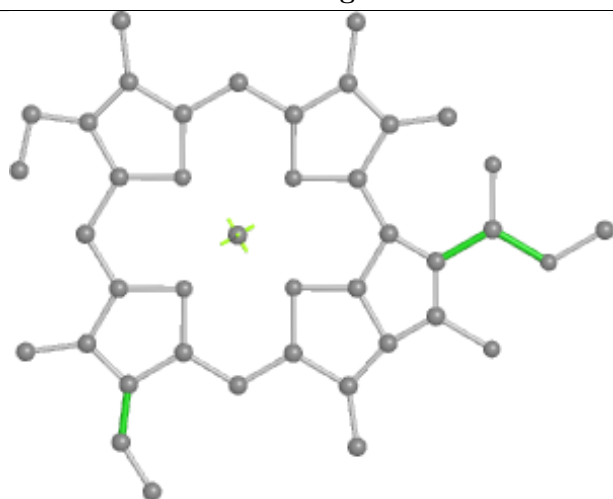
Ligand CLA B 804



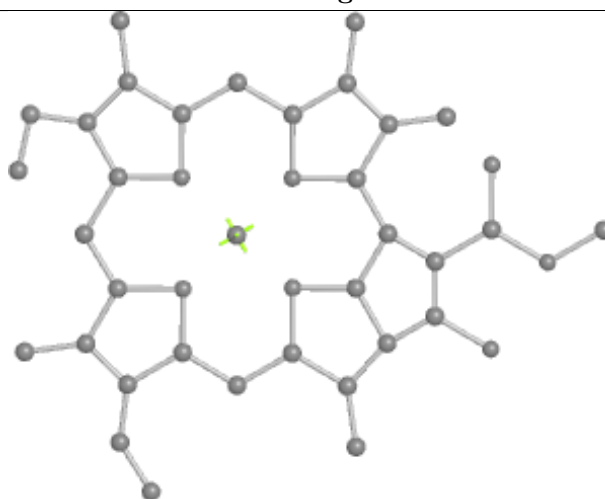
Bond lengths



Bond angles

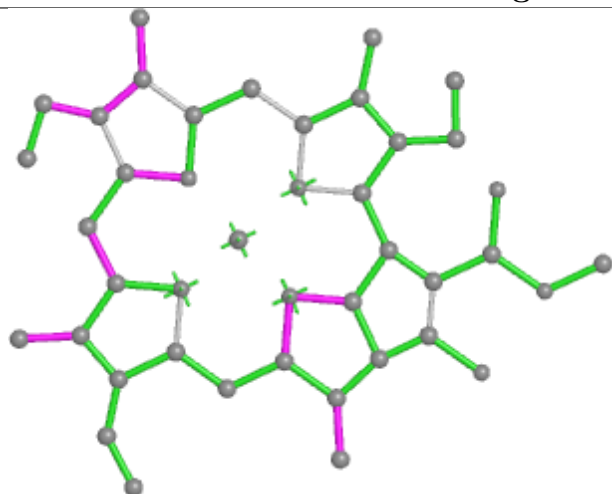


Torsions

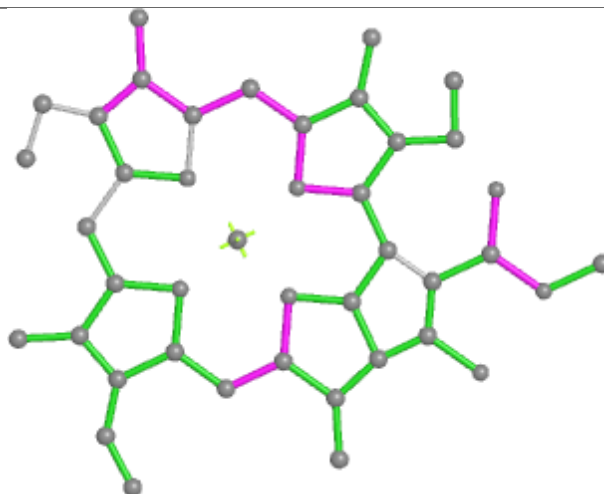


Rings

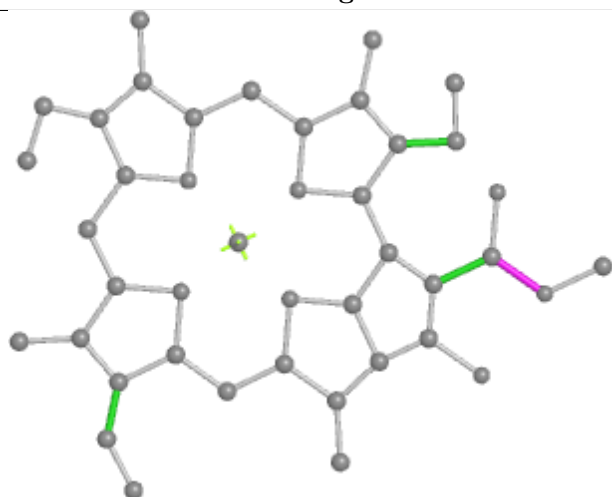
Ligand CLA A 823



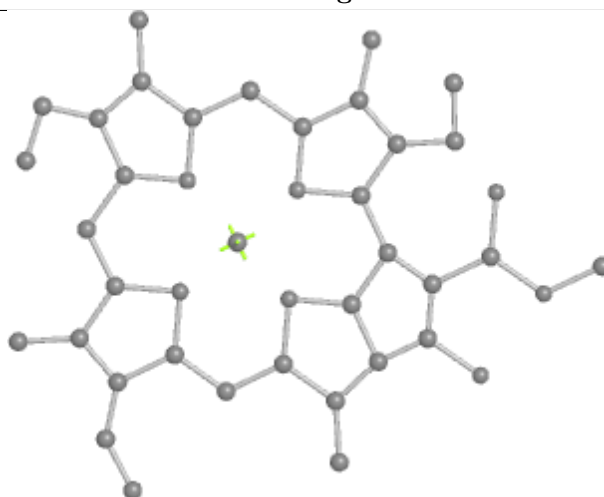
Bond lengths



Bond angles

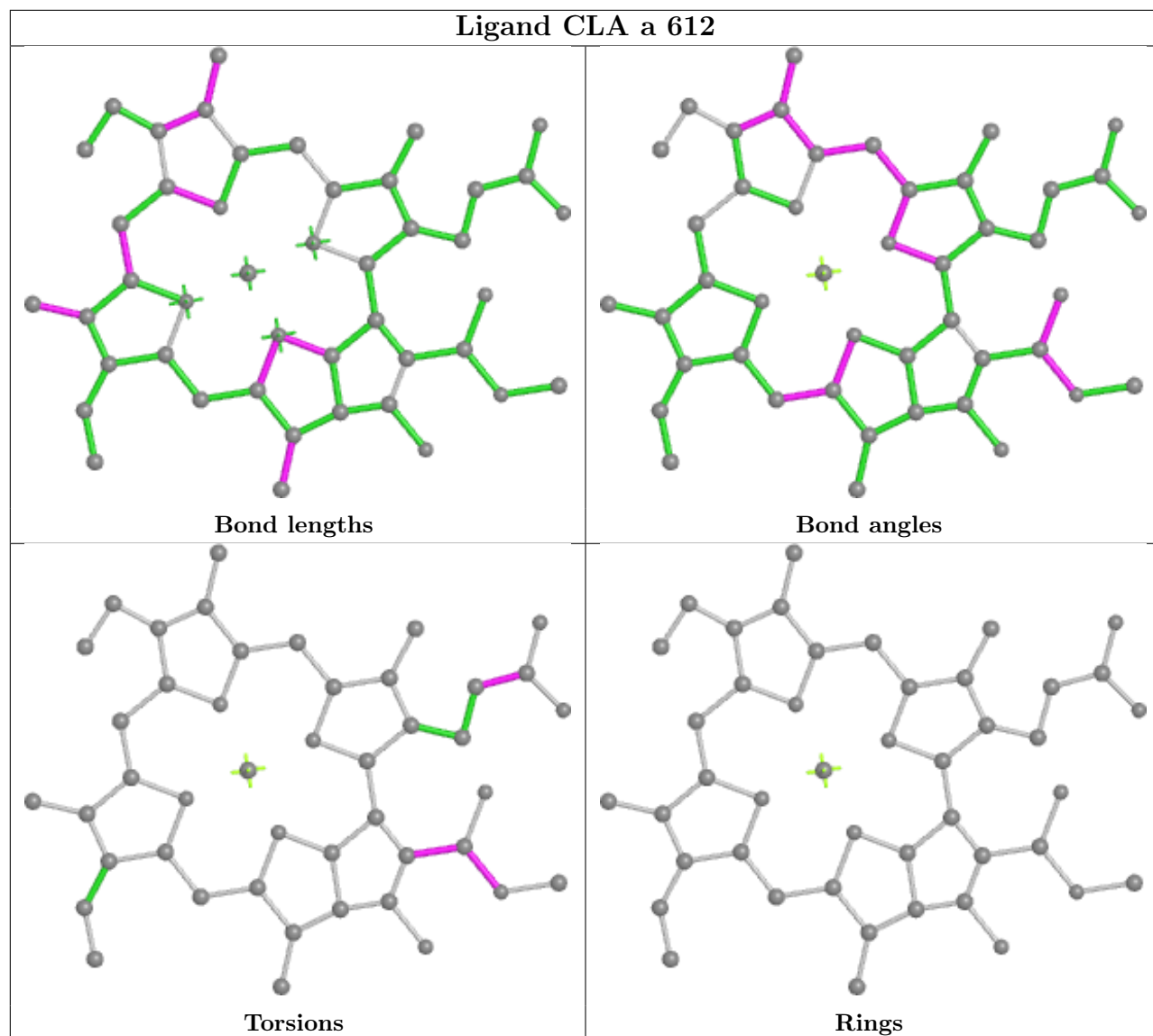


Torsions

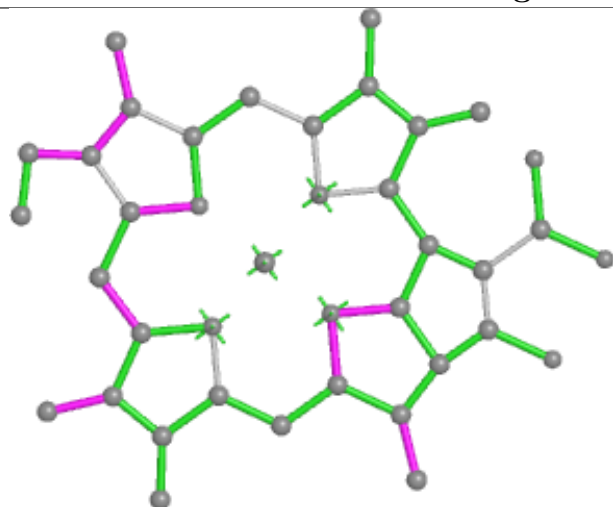


Rings

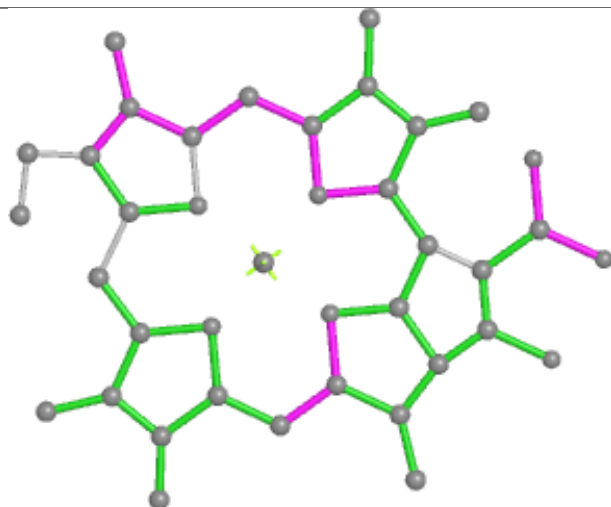
Ligand CLA a 612



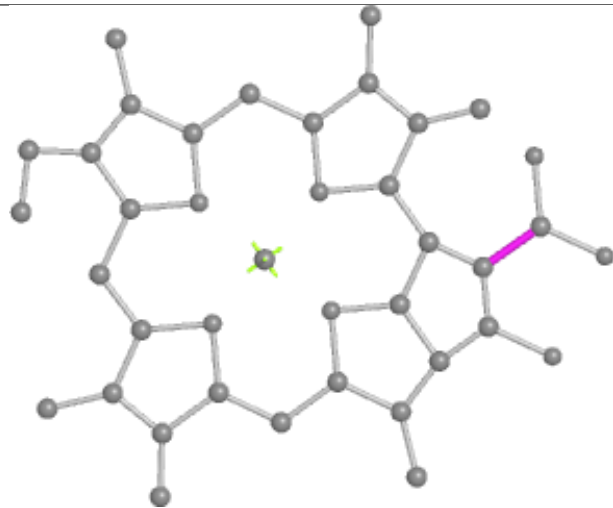
Ligand CLA H 202



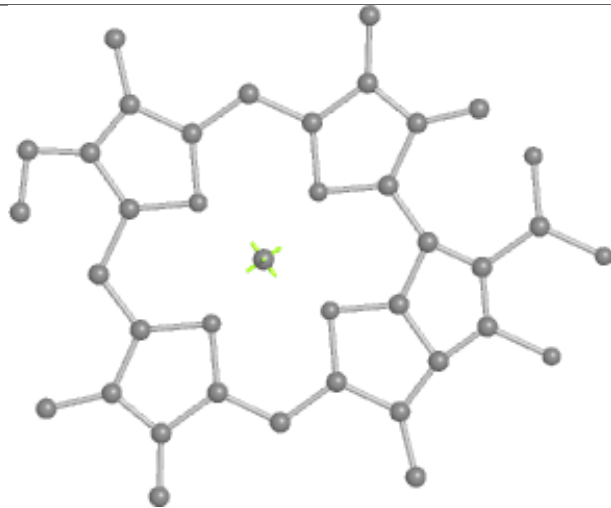
Bond lengths



Bond angles

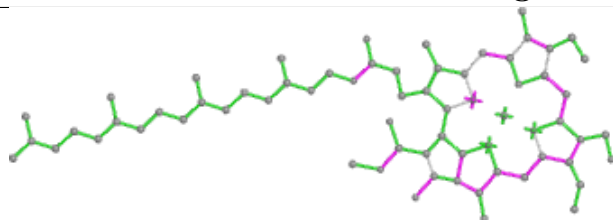


Torsions

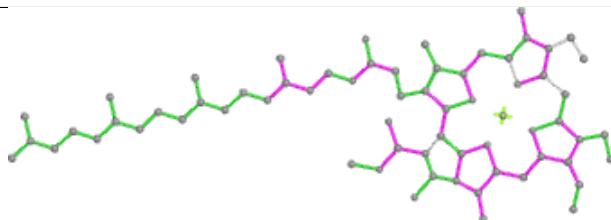


Rings

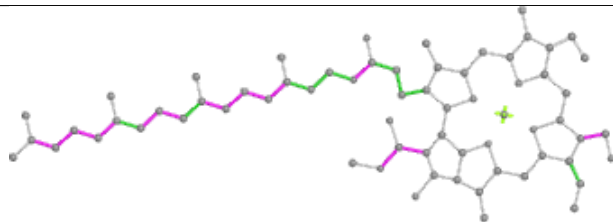
Ligand CHL X 601



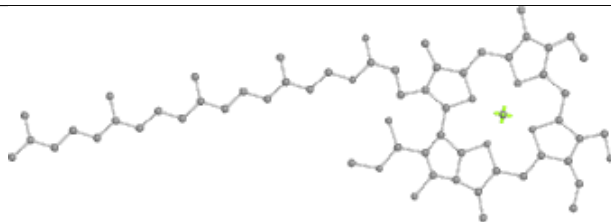
Bond lengths



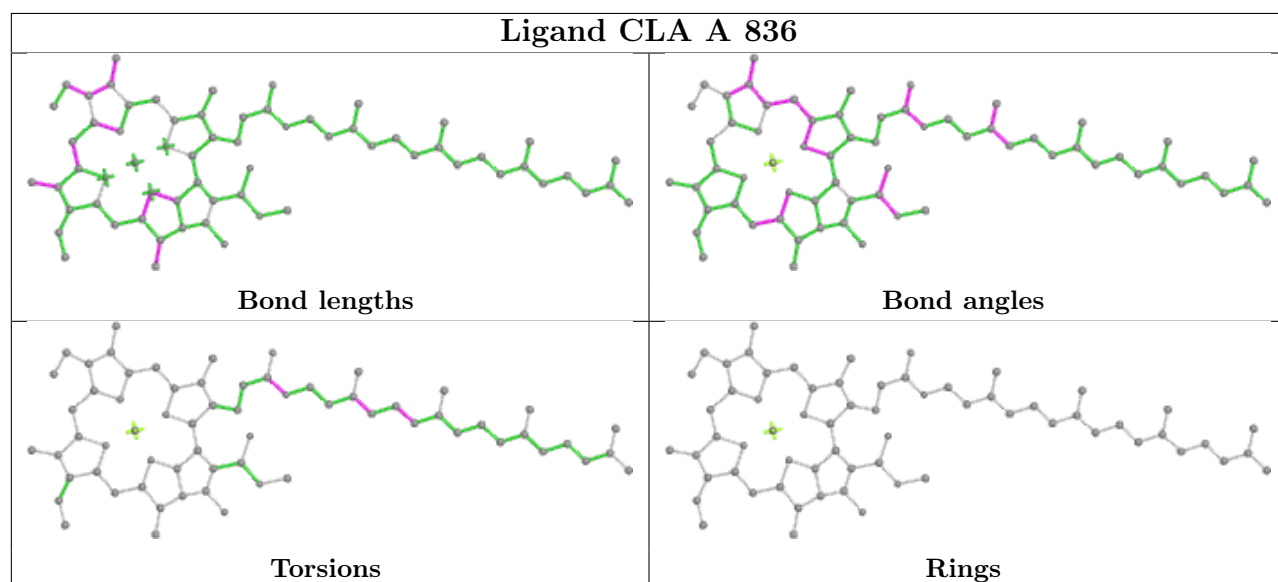
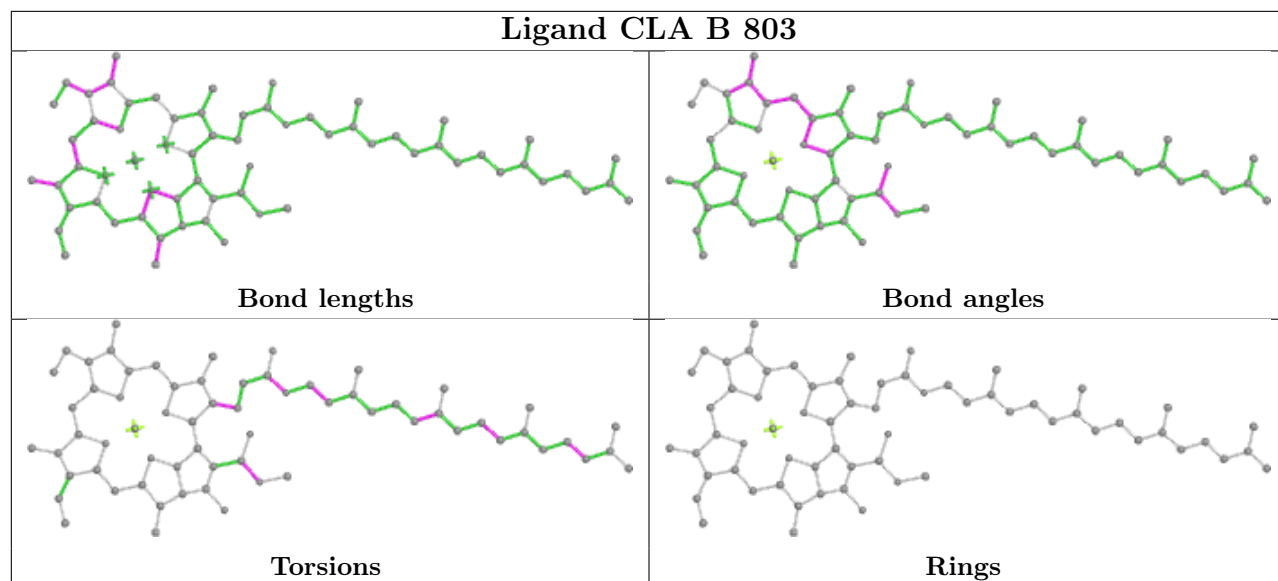
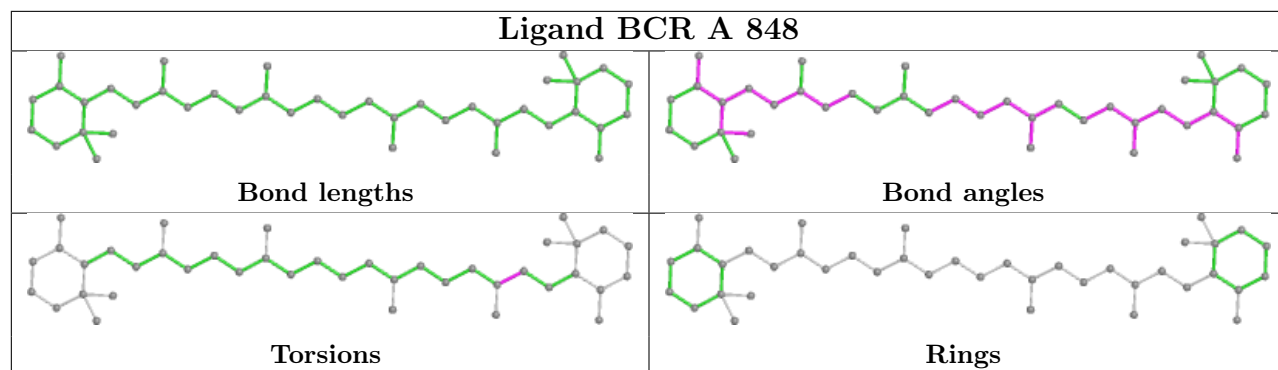
Bond angles

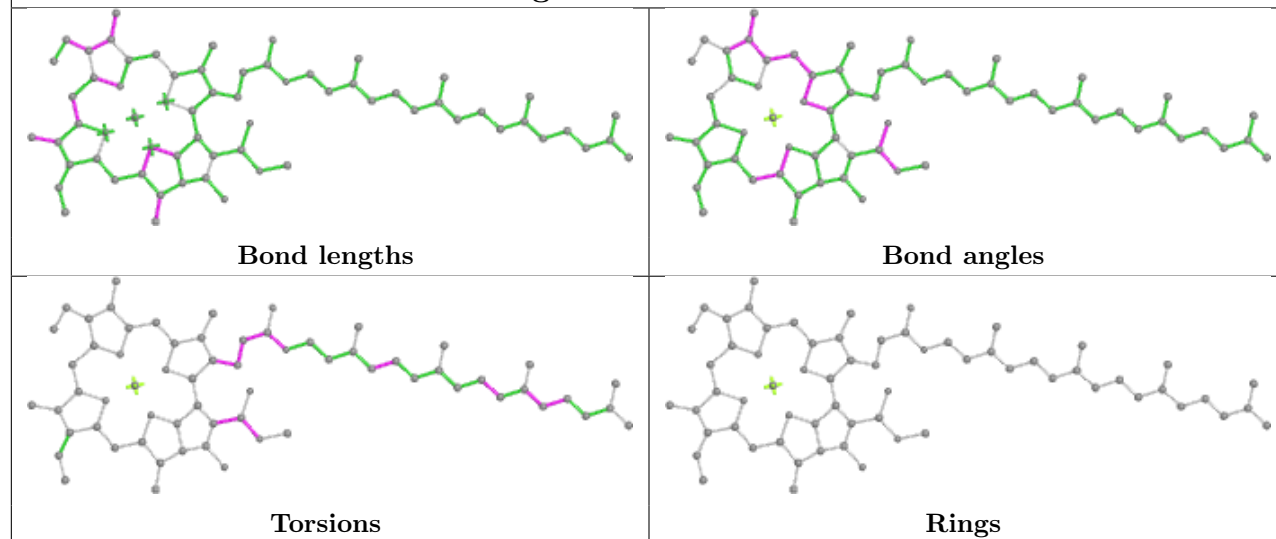
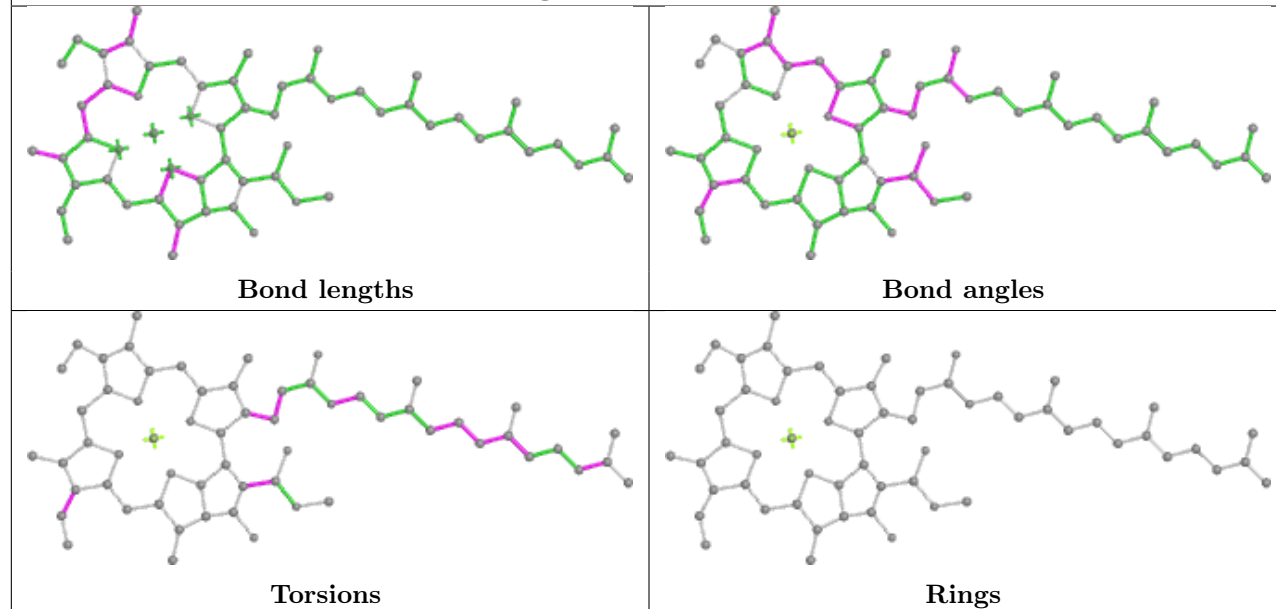


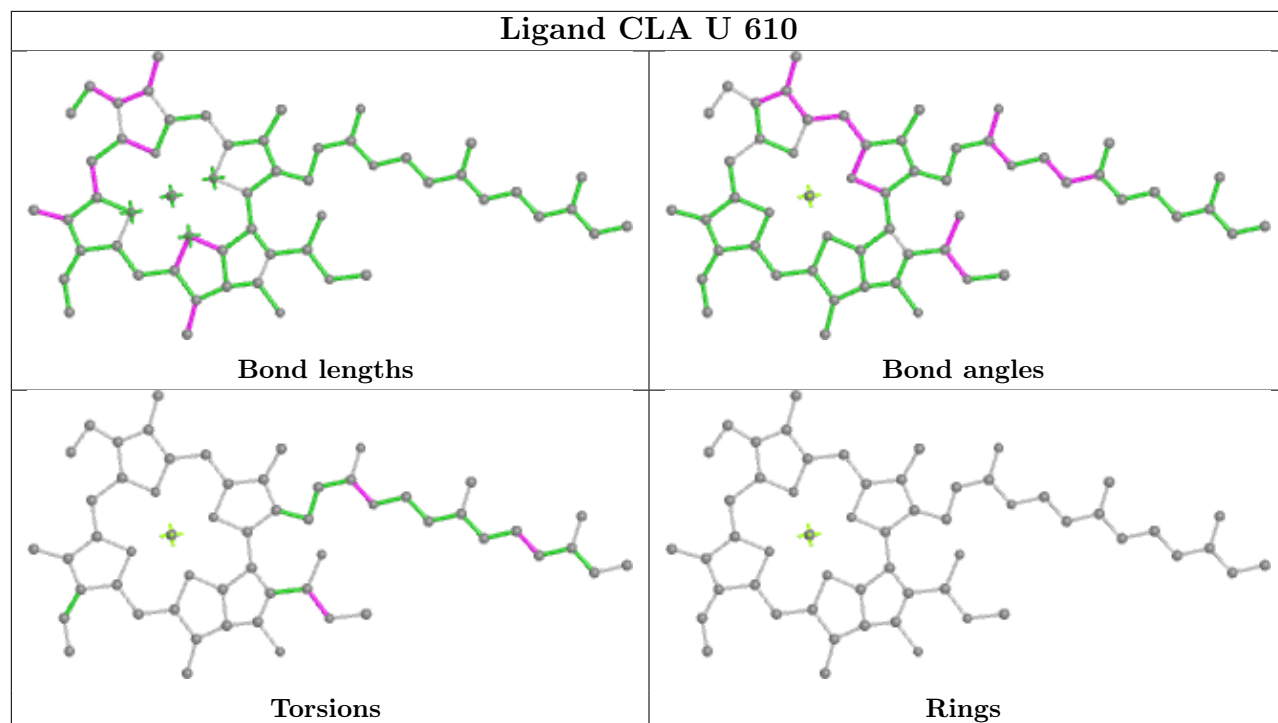
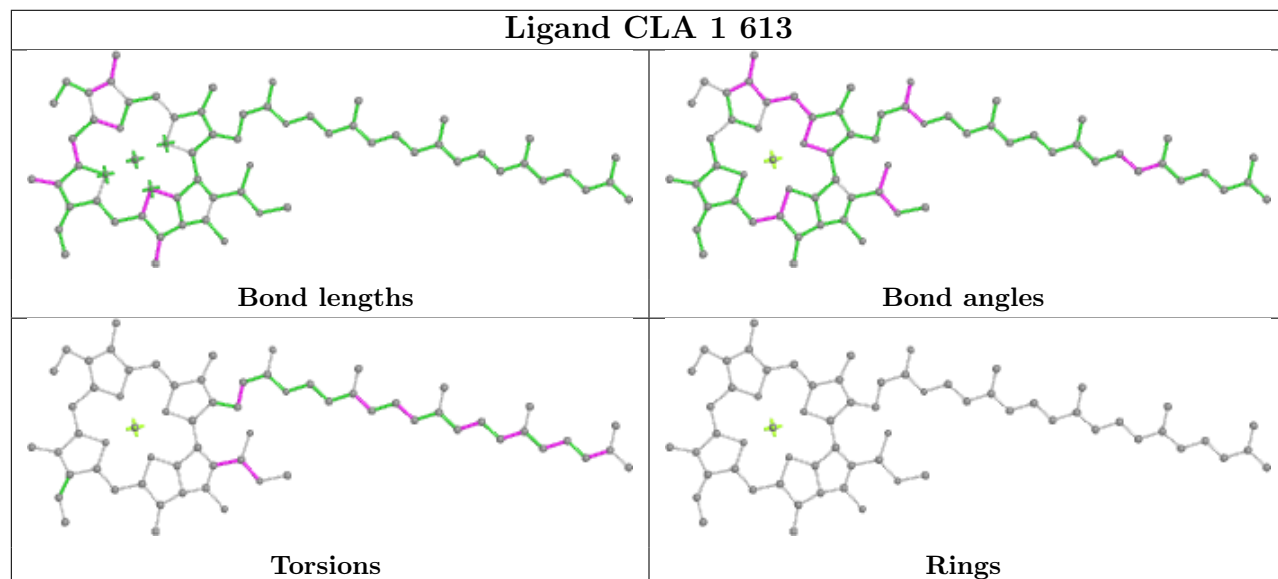
Torsions

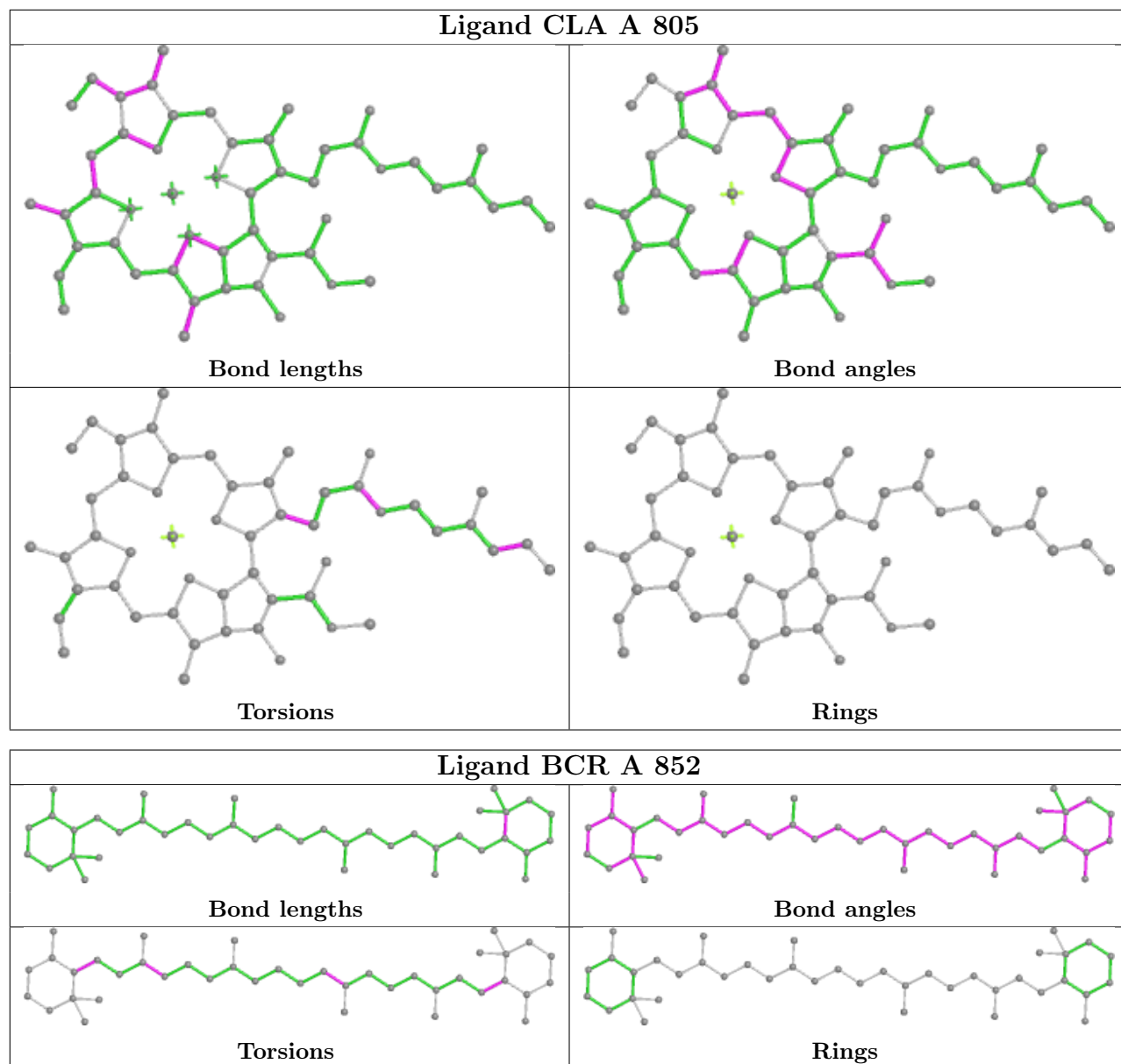


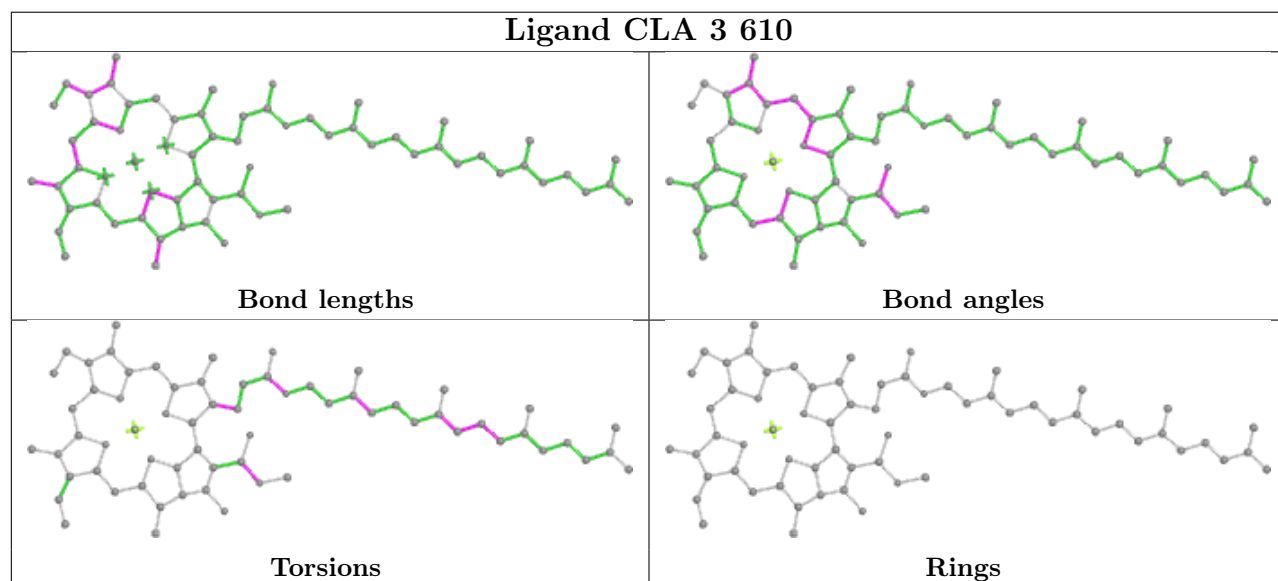
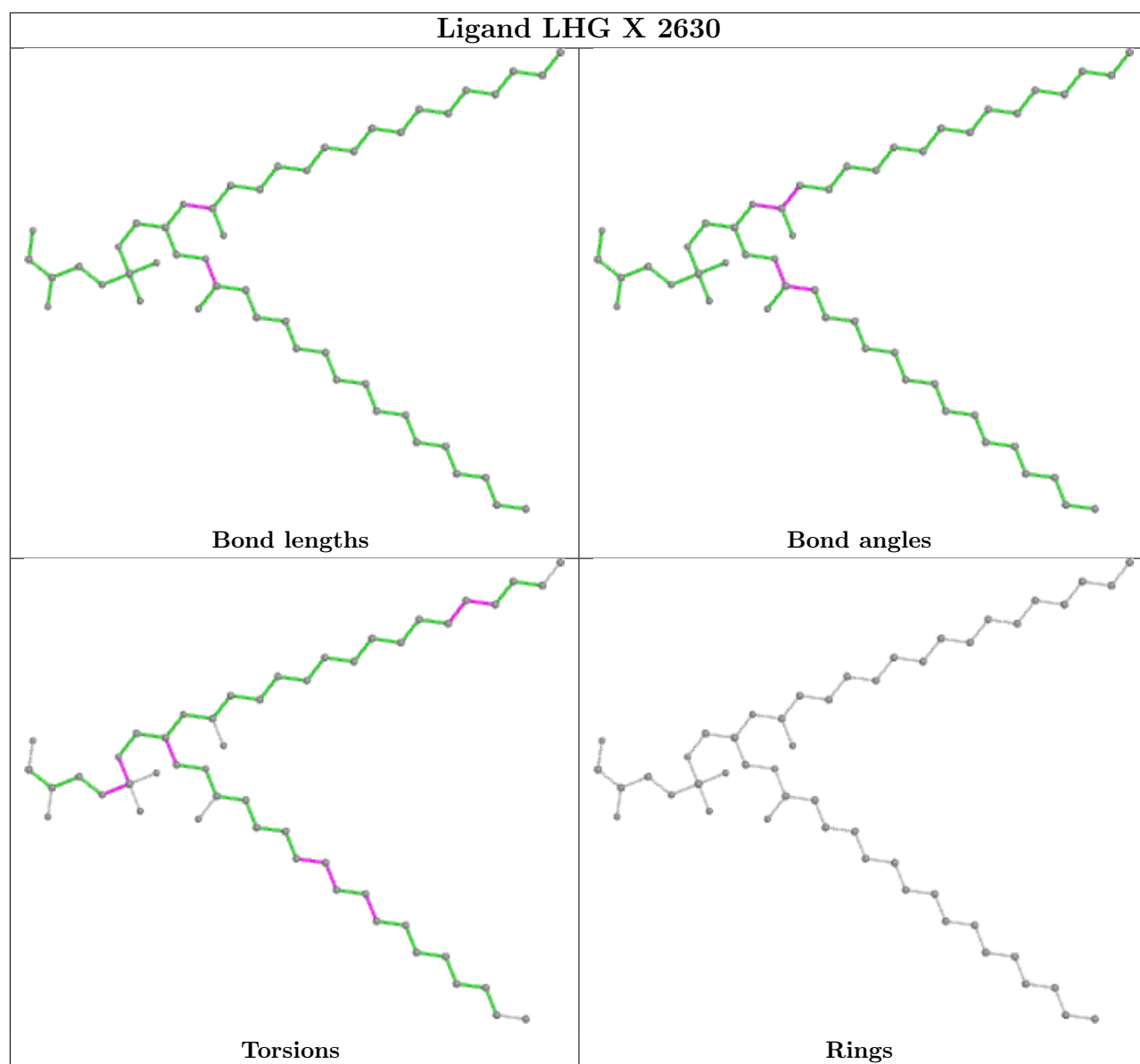
Rings

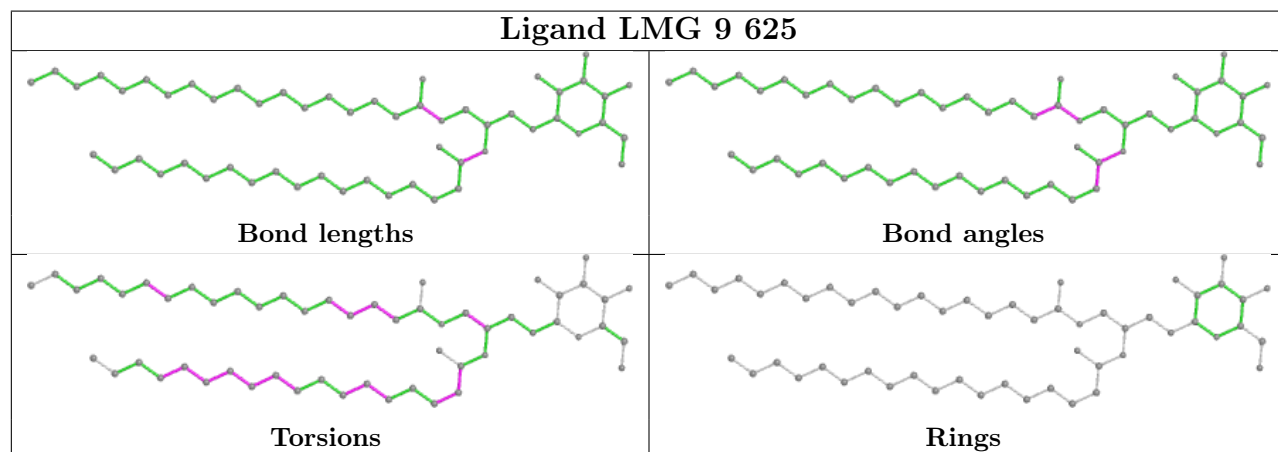
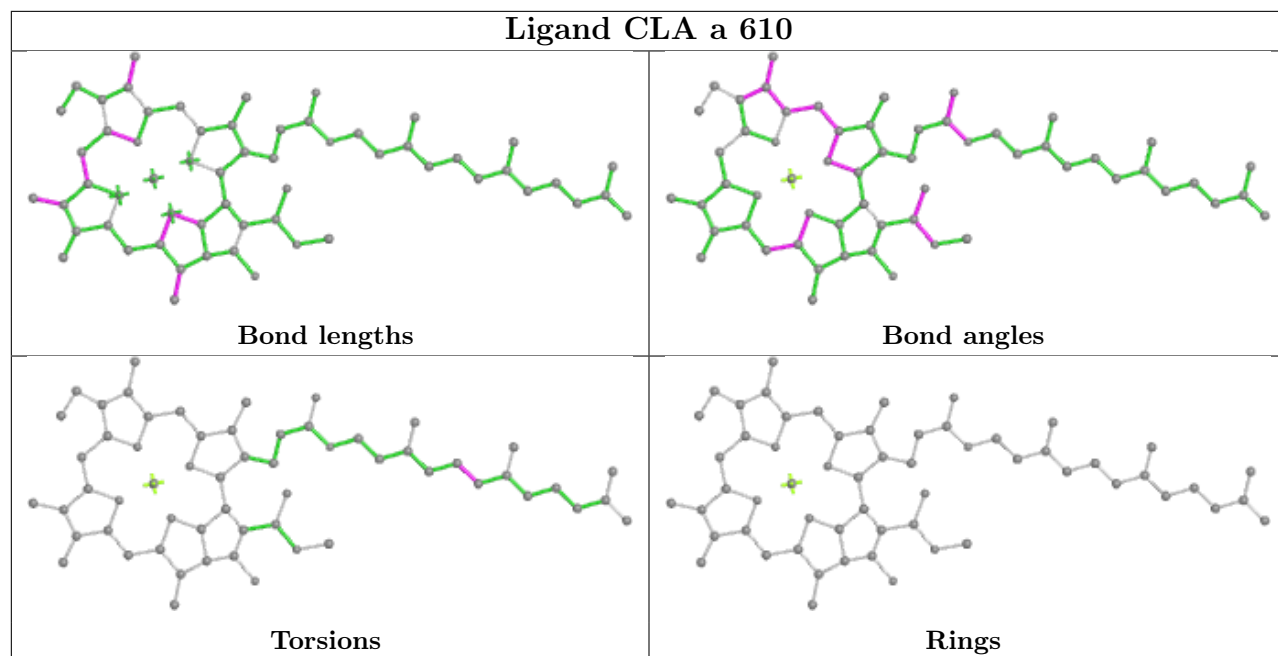


Ligand CLA B 809**Ligand CLA 3 609**

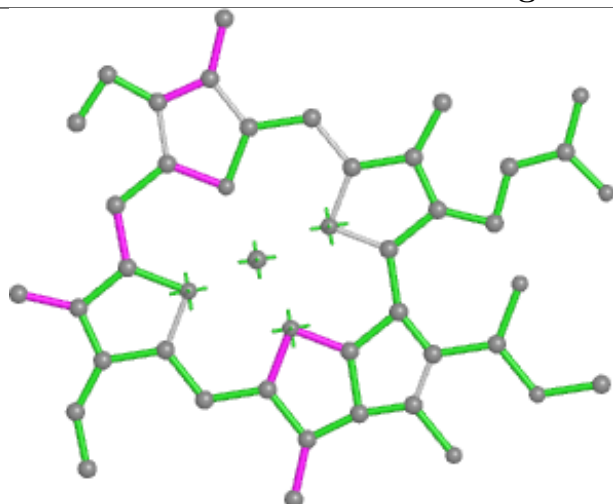
Ligand CLA U 610**Ligand CLA 1 613**



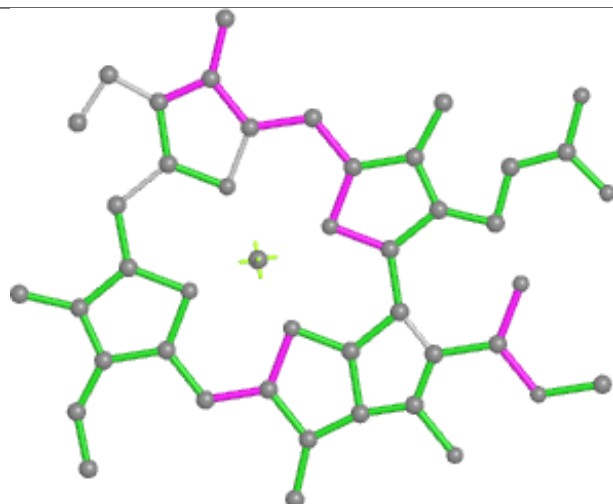




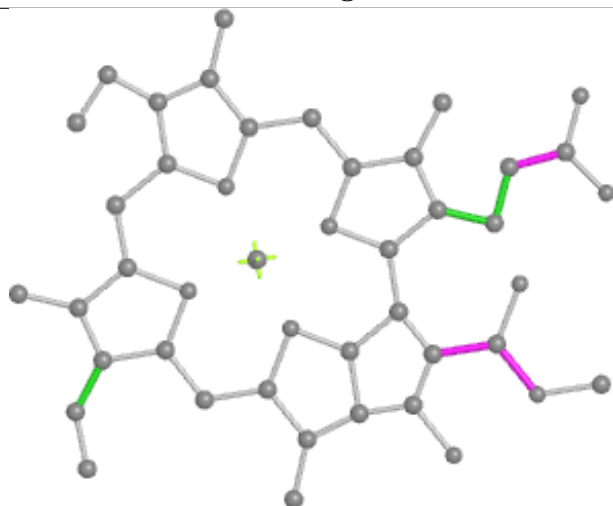
Ligand CLA 2 606



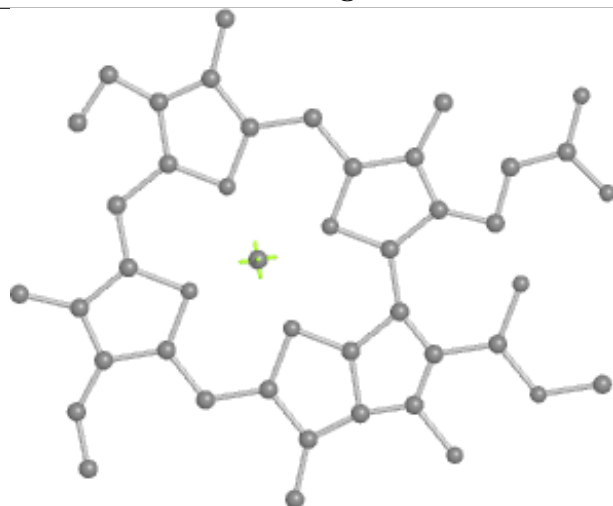
Bond lengths



Bond angles

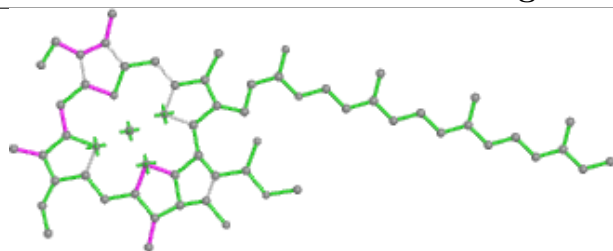


Torsions

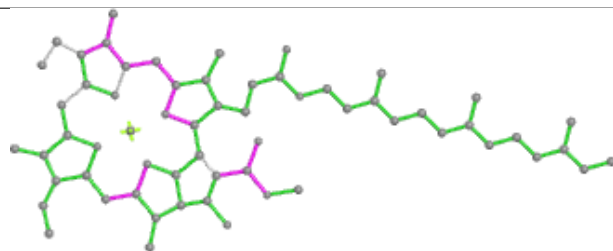


Rings

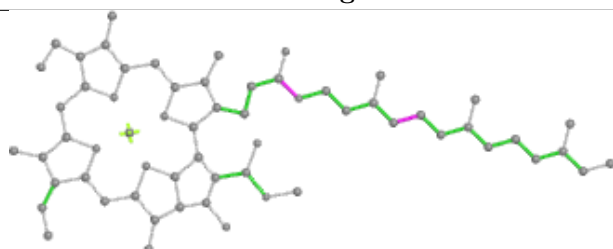
Ligand CLA 1 602



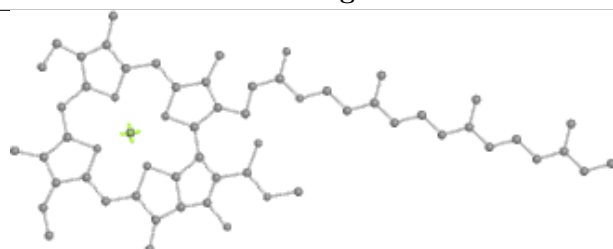
Bond lengths



Bond angles

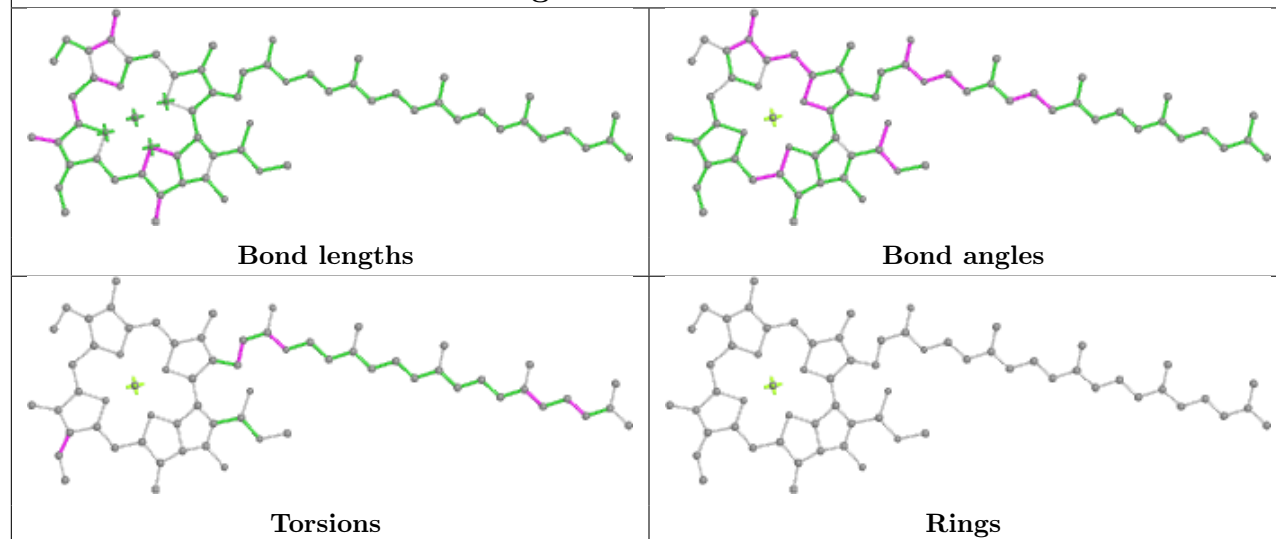


Torsions

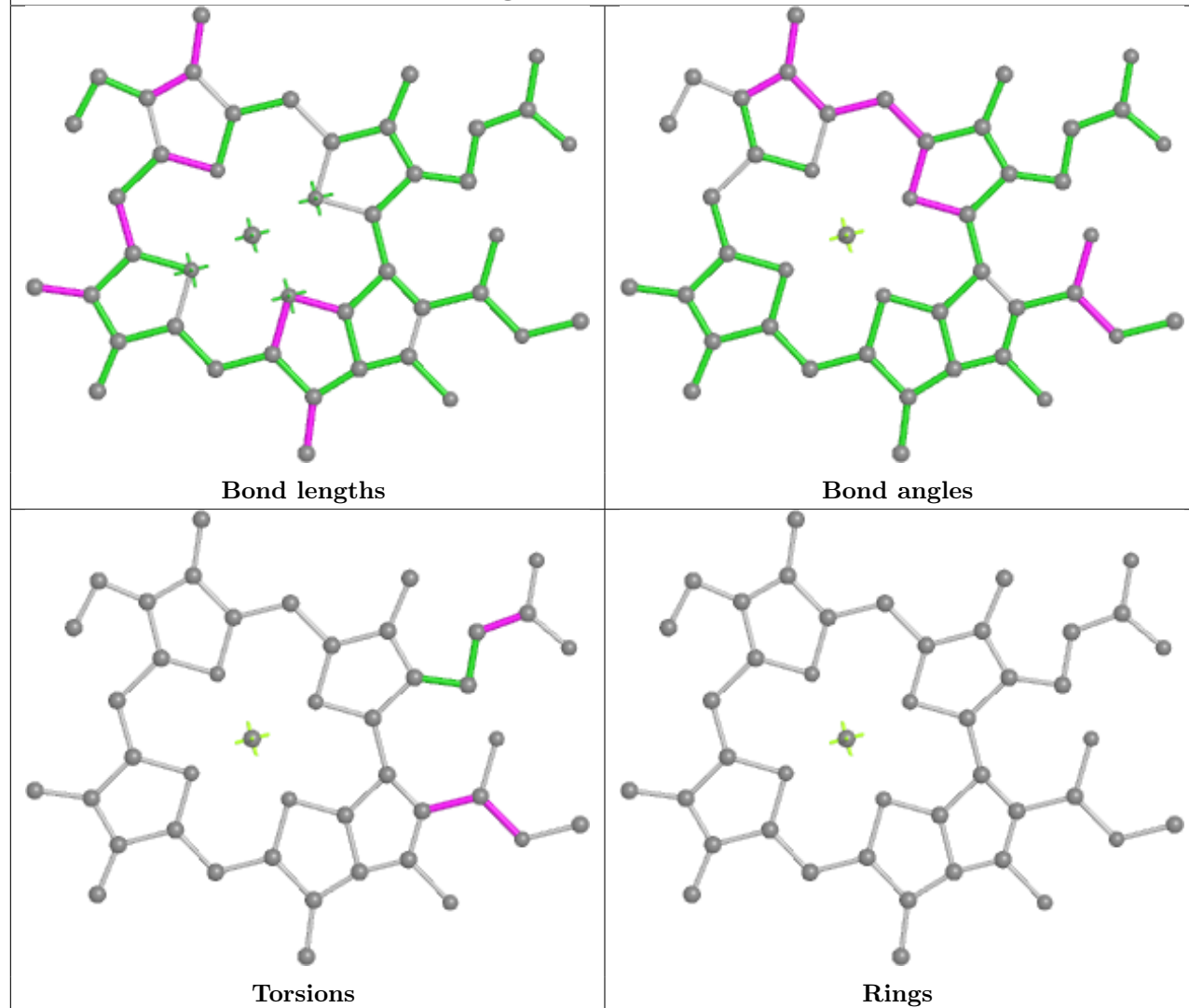


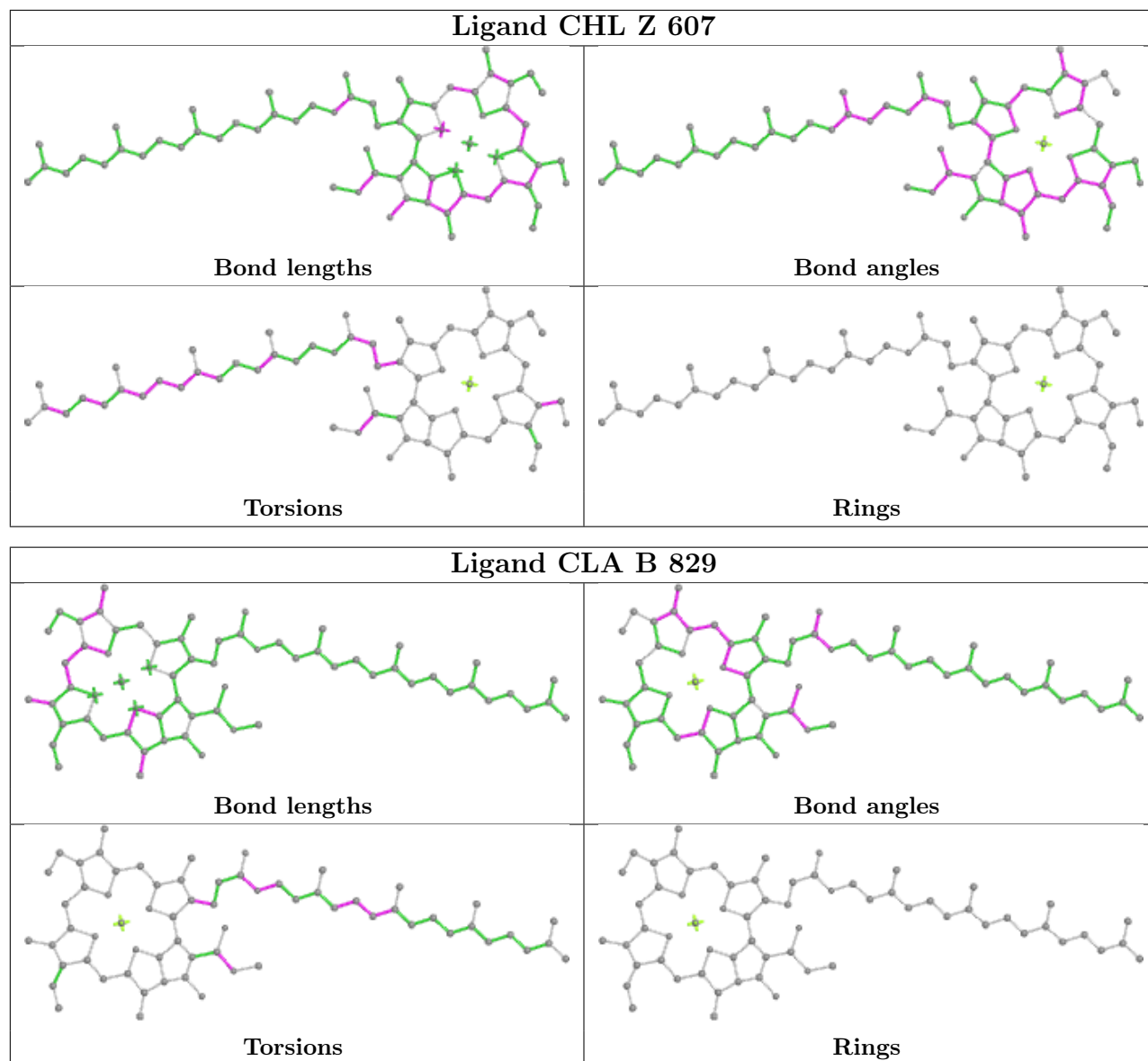
Rings

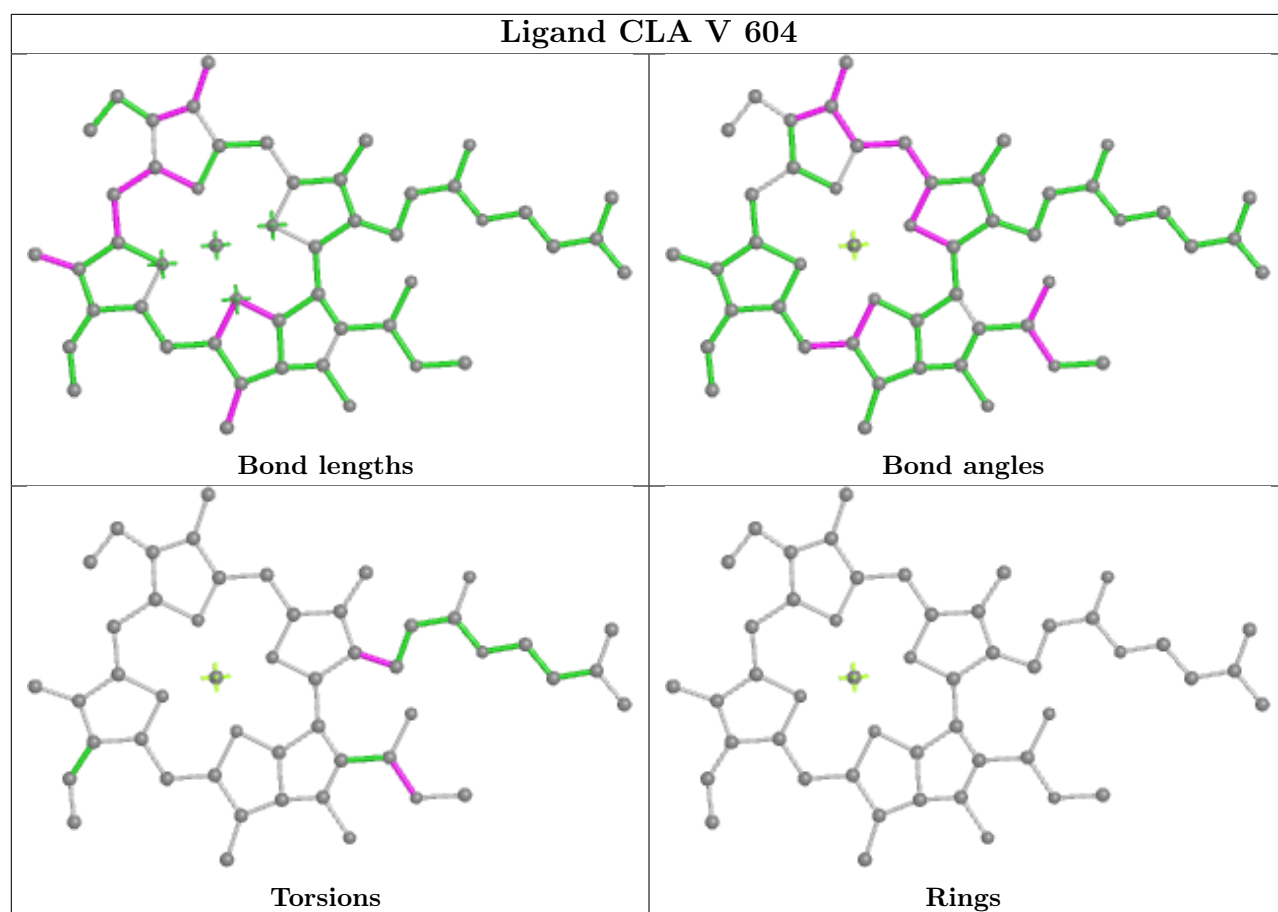
Ligand CLA A 822



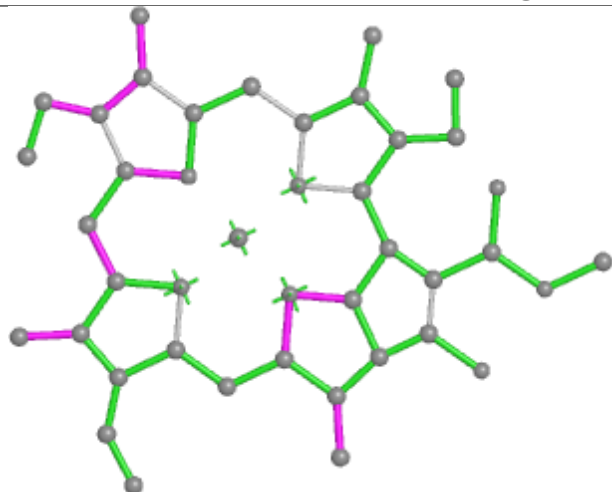
Ligand CLA 7 612



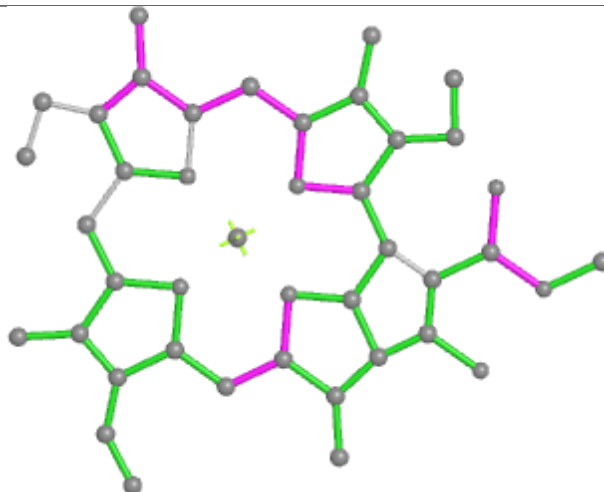




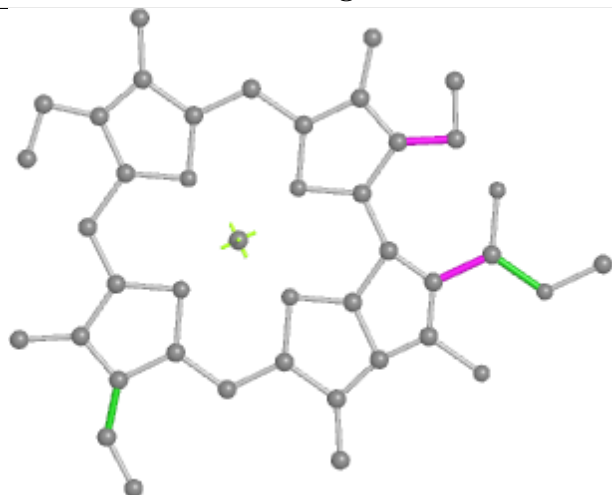
Ligand CLA 7 614



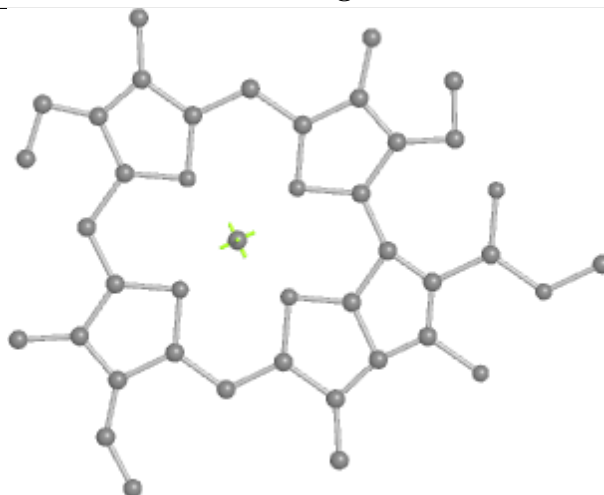
Bond lengths



Bond angles

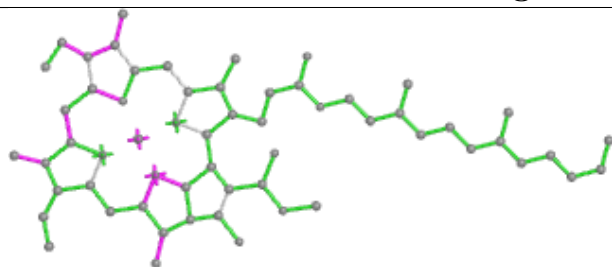


Torsions

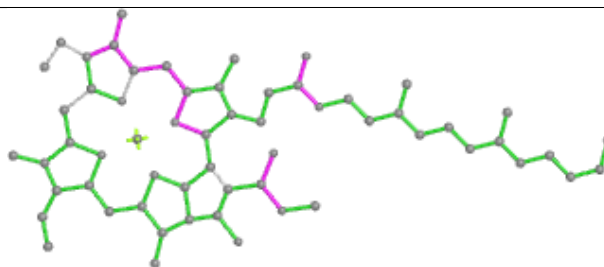


Rings

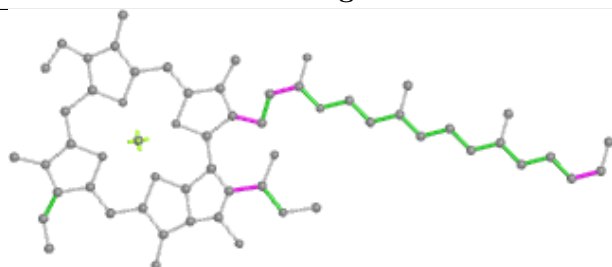
Ligand CLA A 819



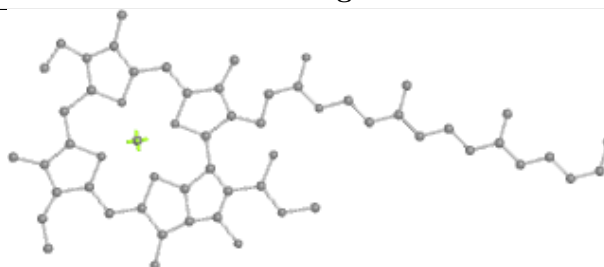
Bond lengths



Bond angles

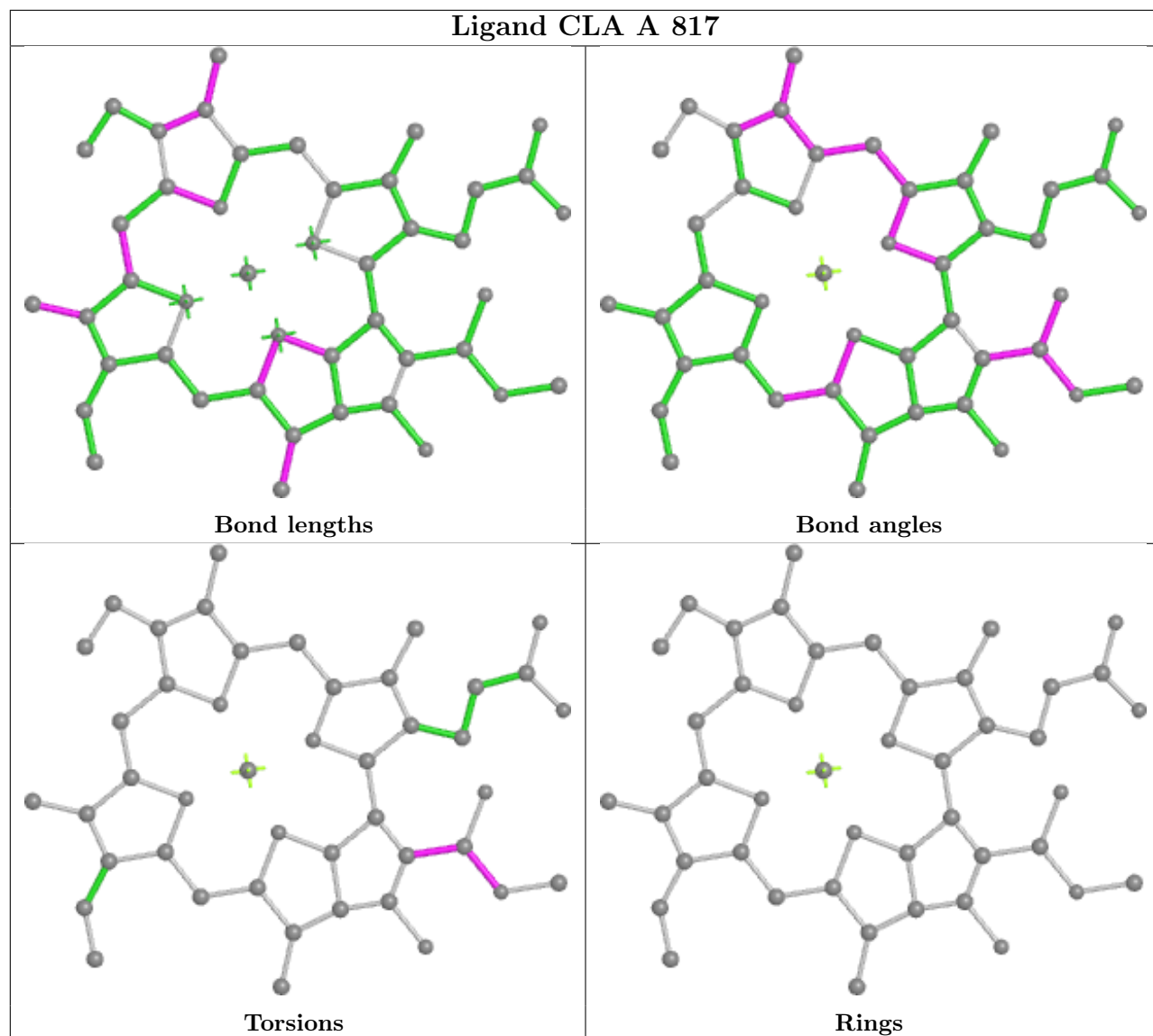


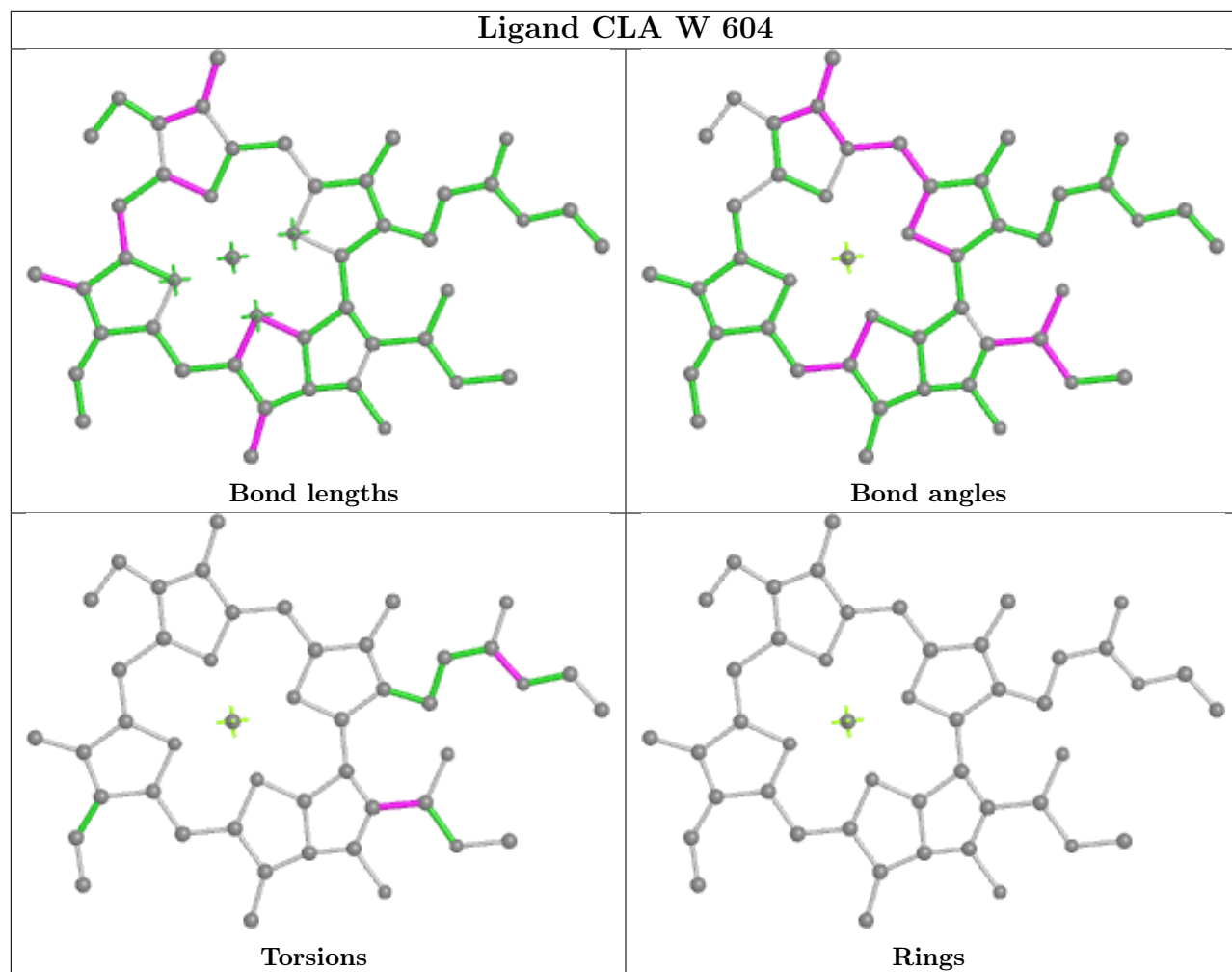
Torsions



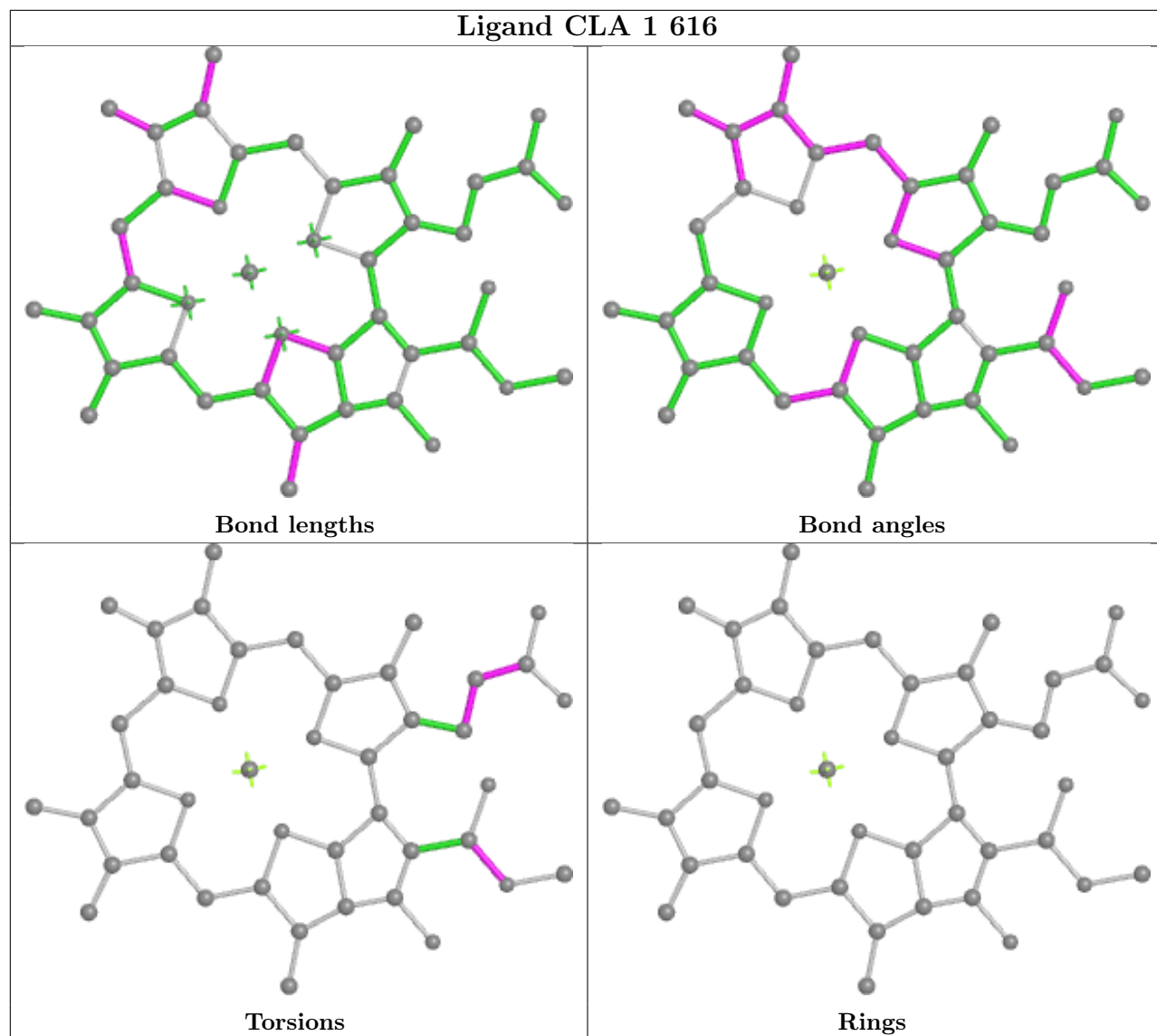
Rings

Ligand CLA A 817

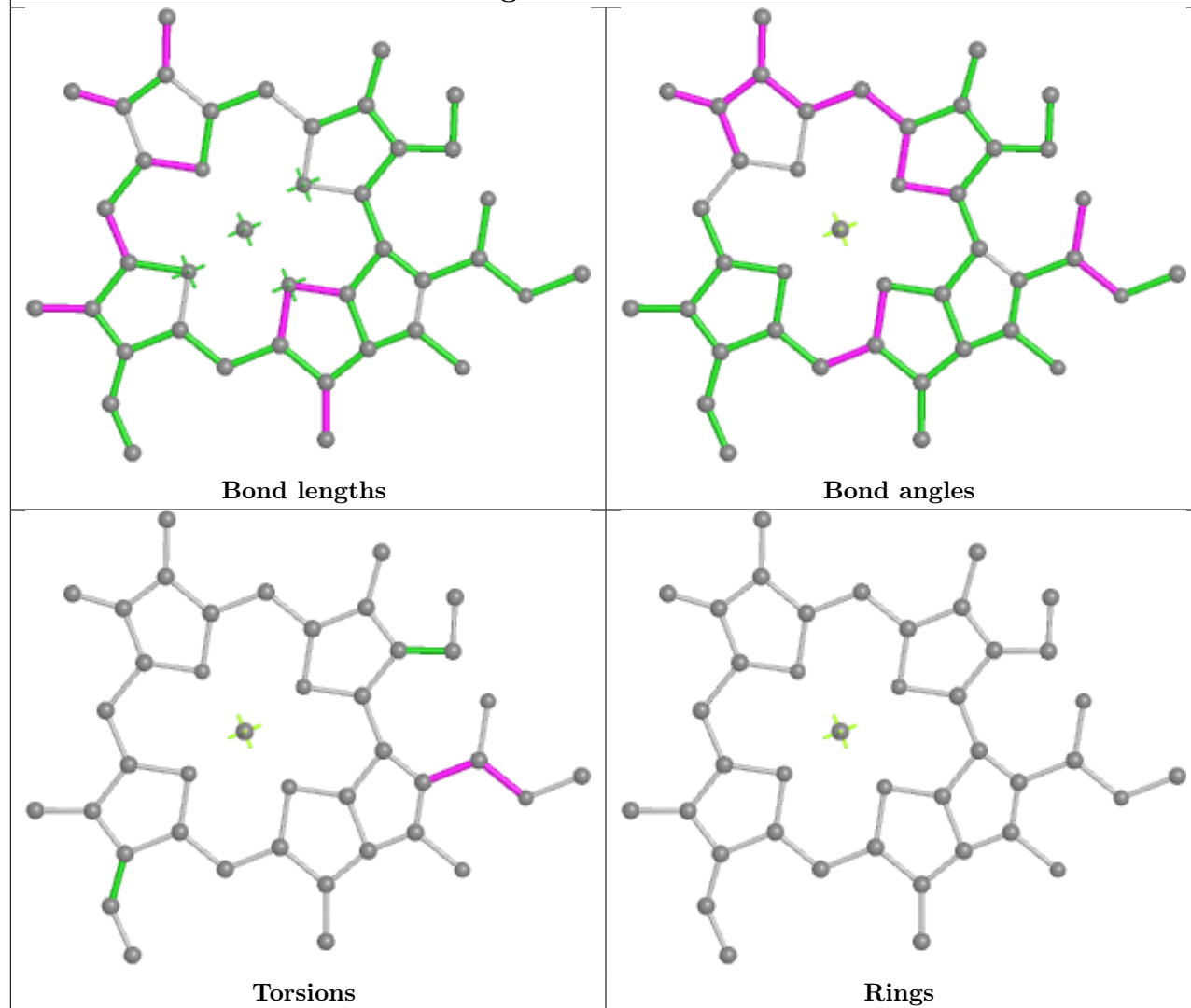




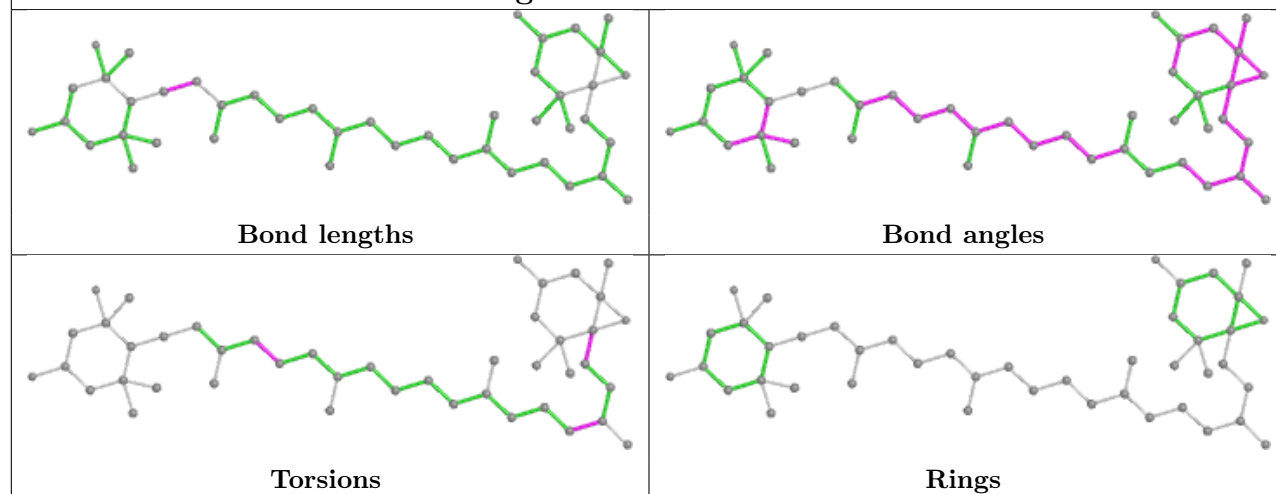
Ligand CLA 1 616

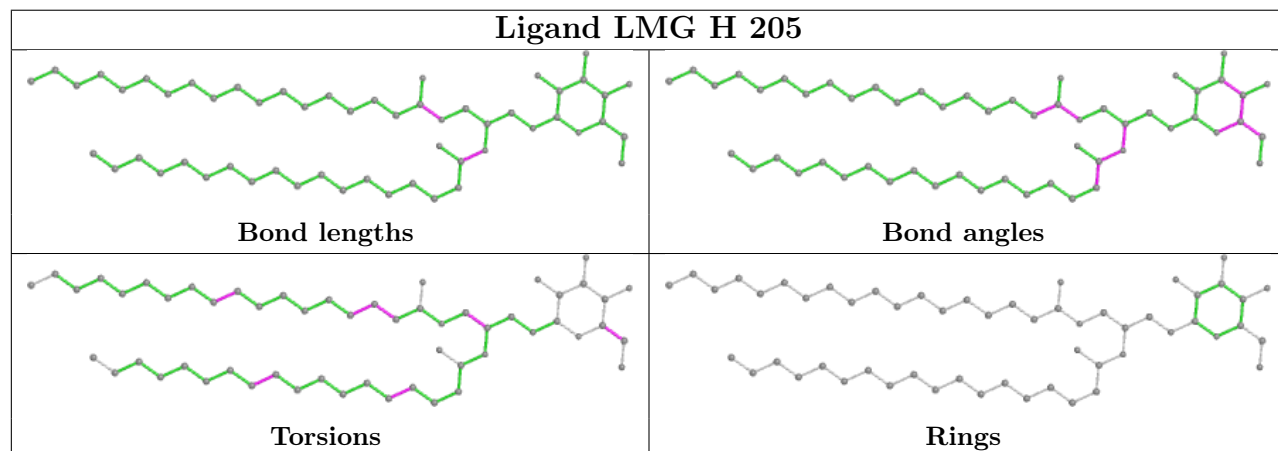
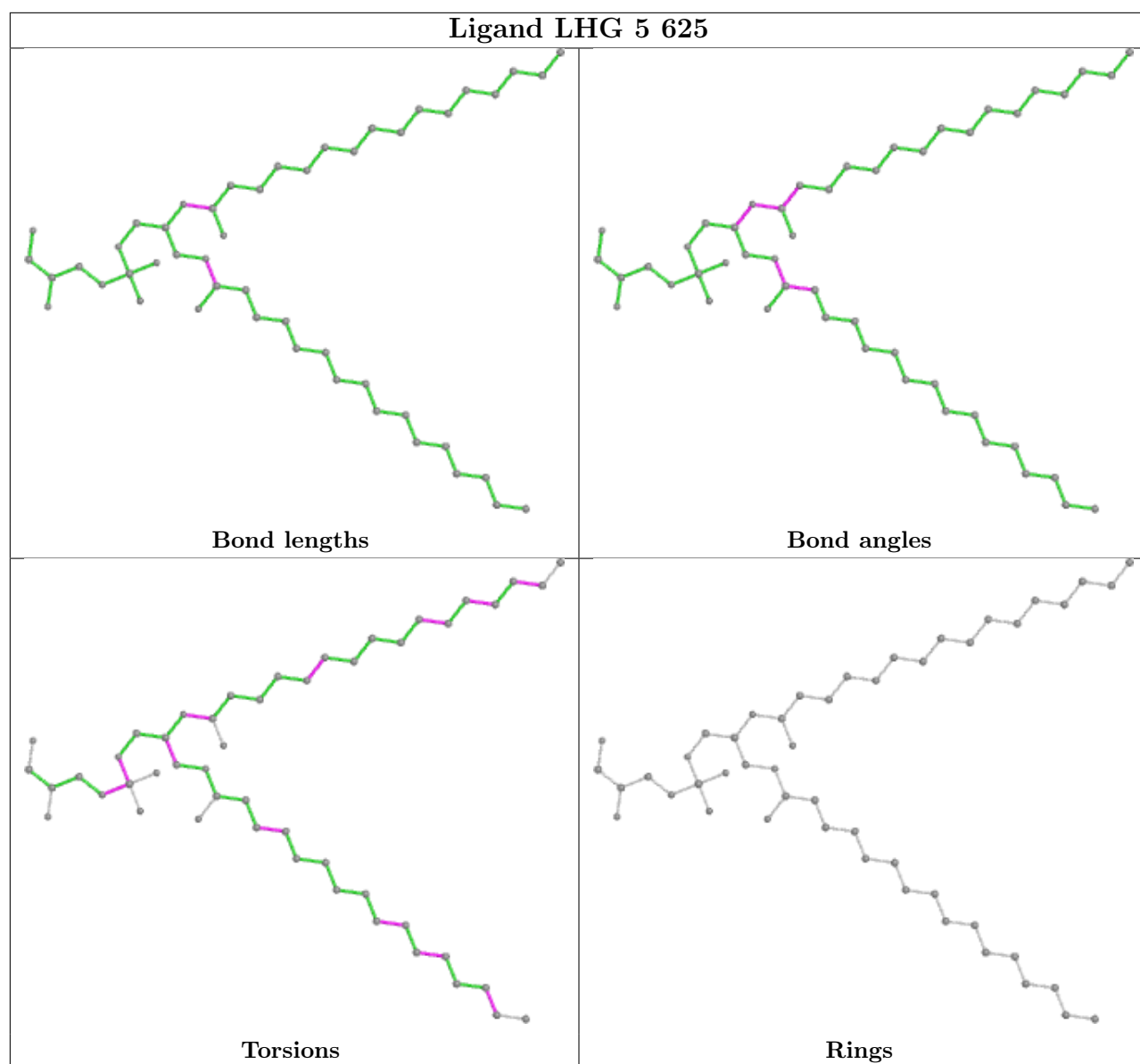


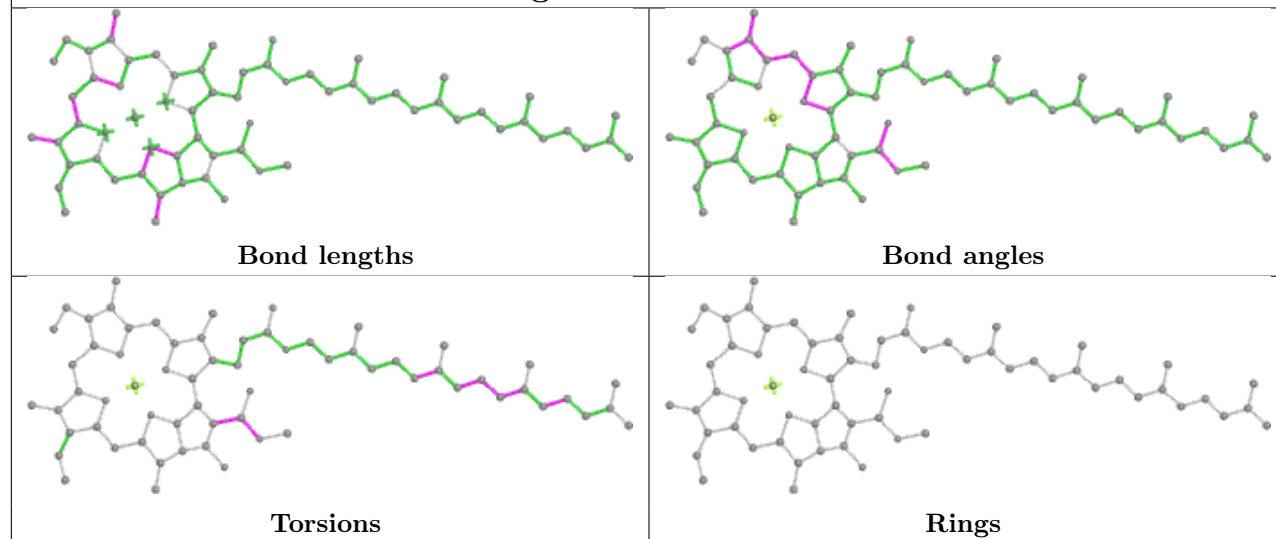
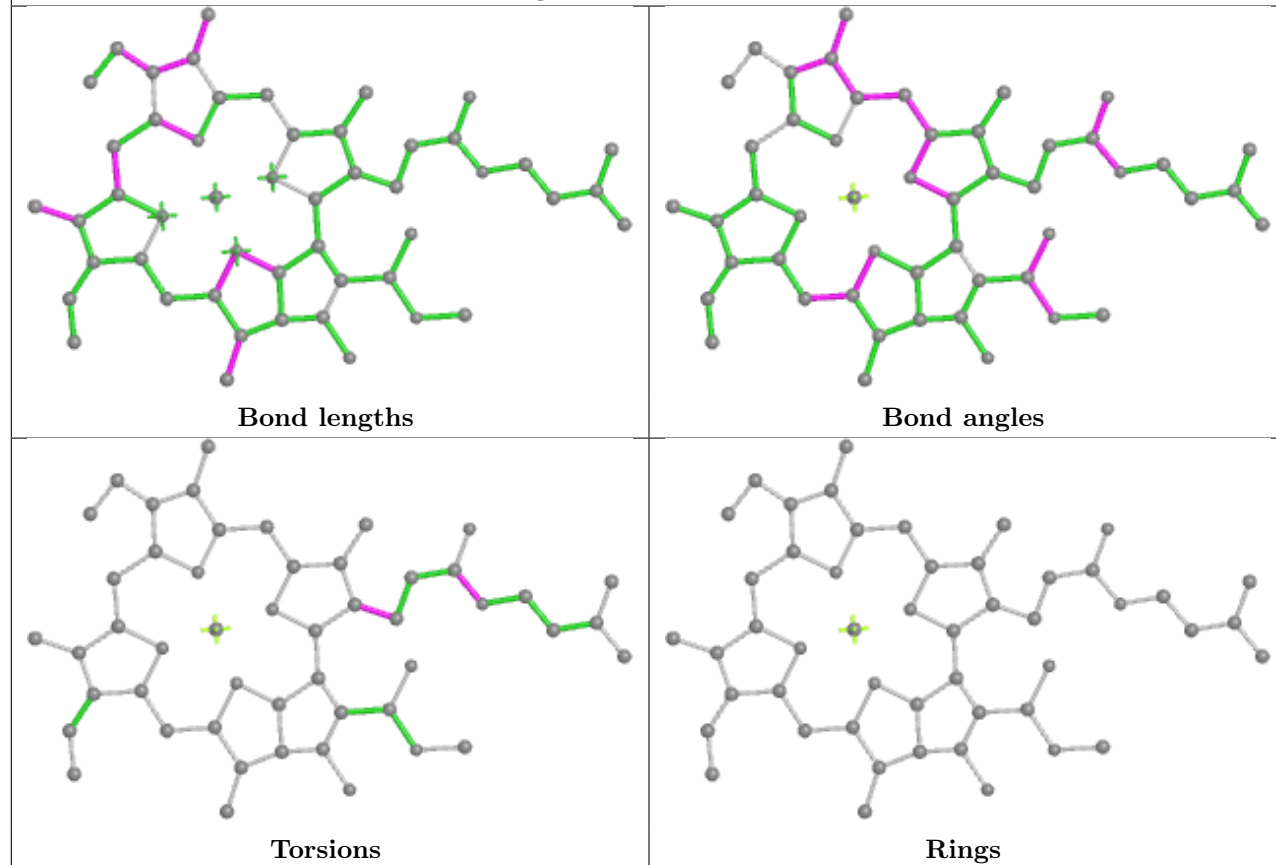
Ligand CLA 6 607

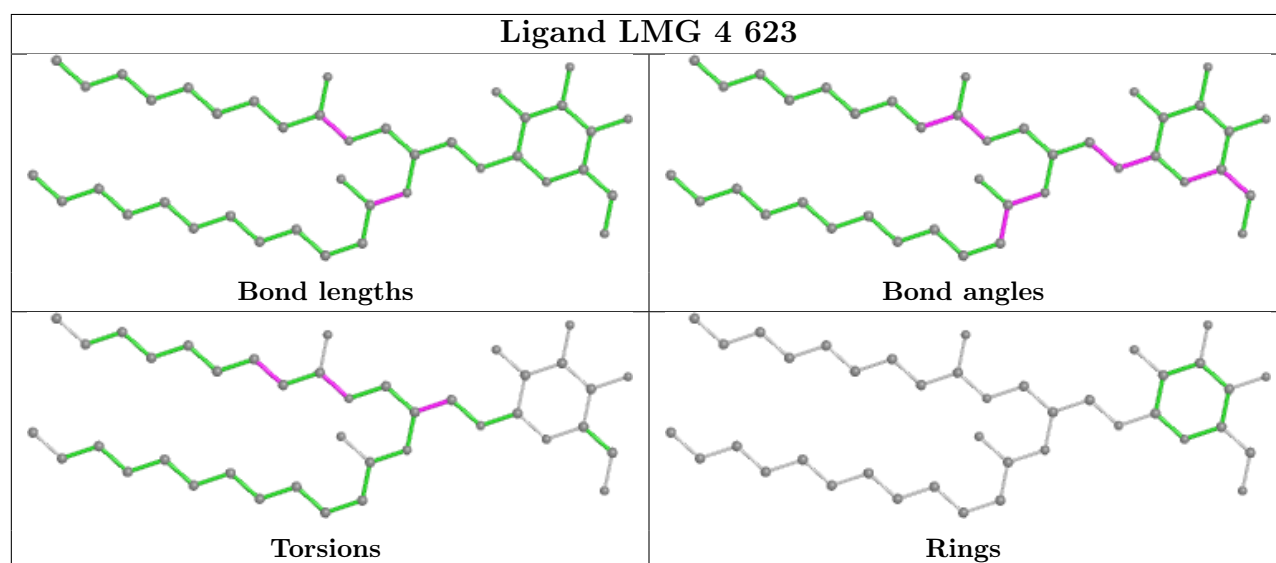
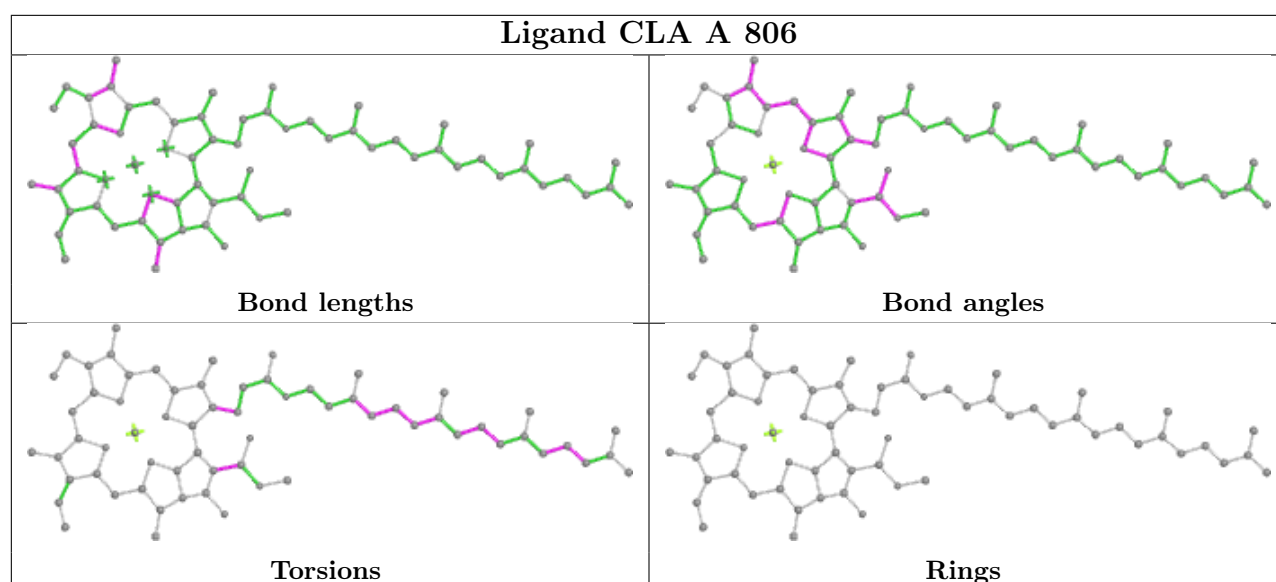
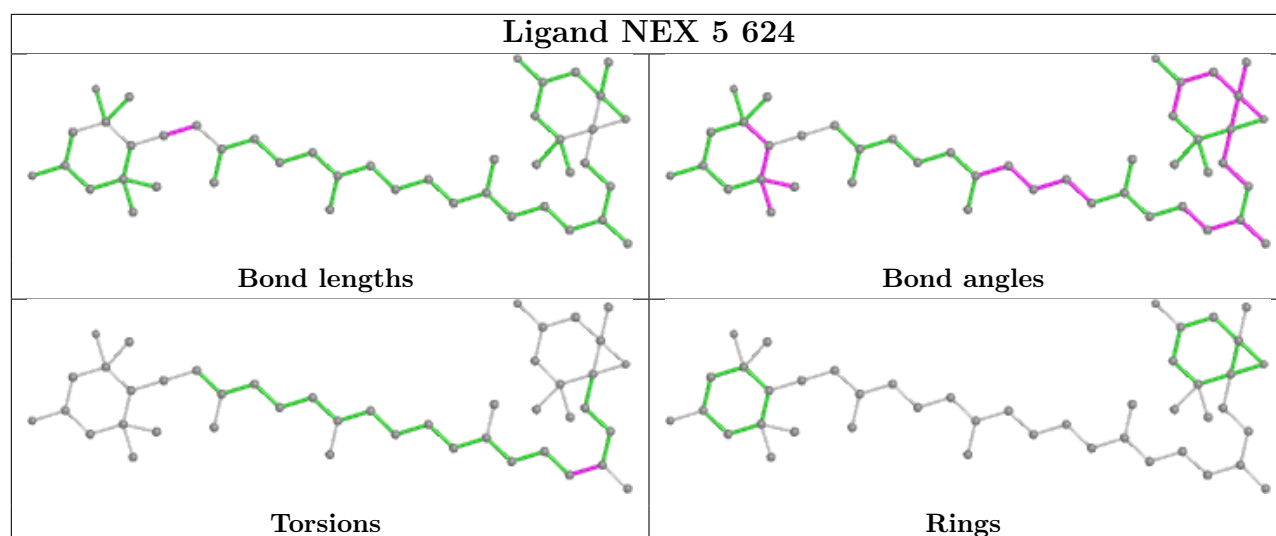


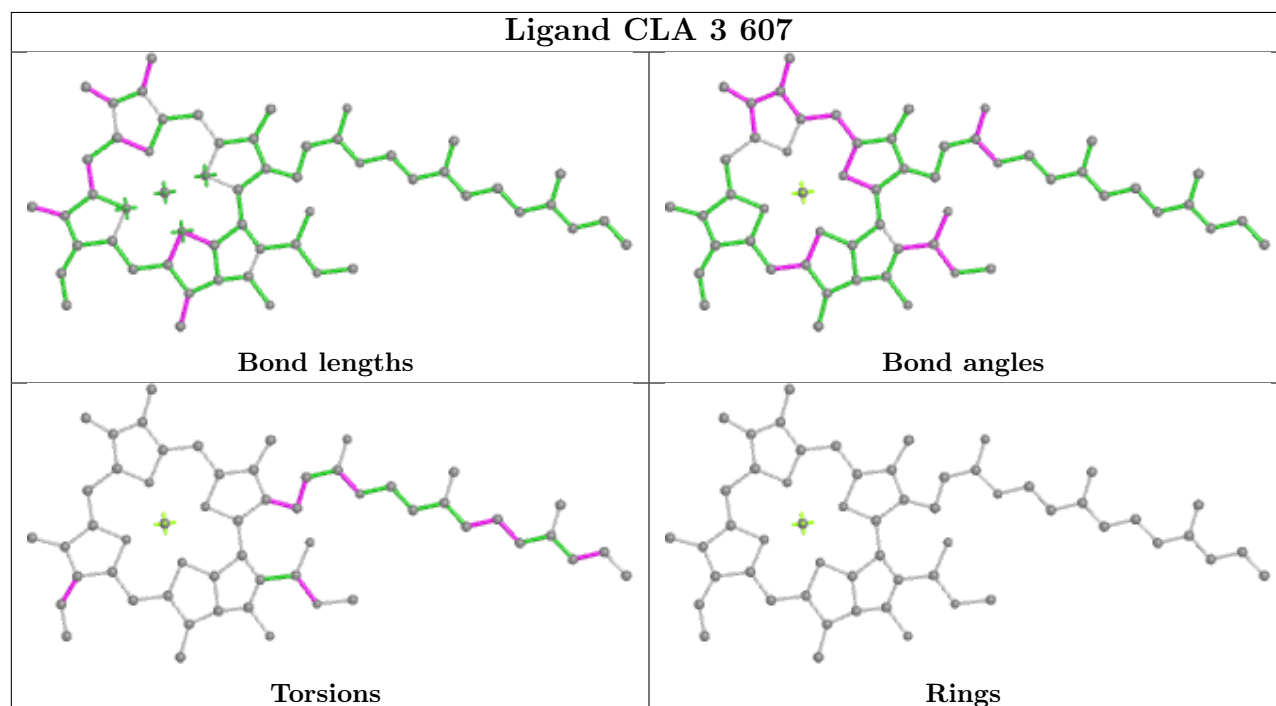
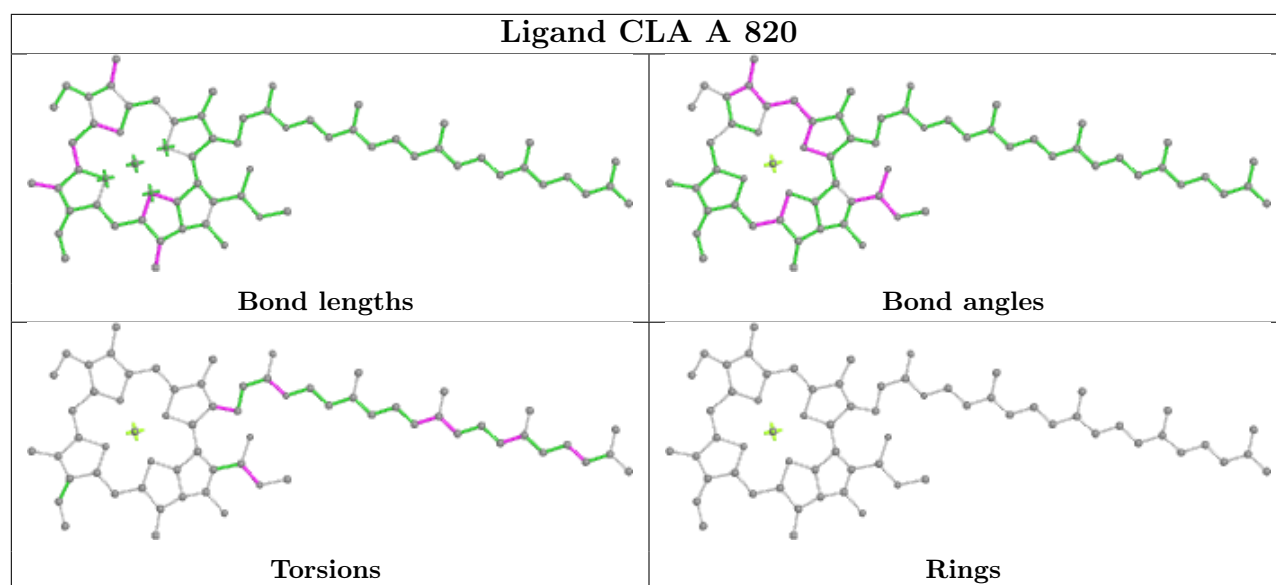
Ligand NEX W 1623



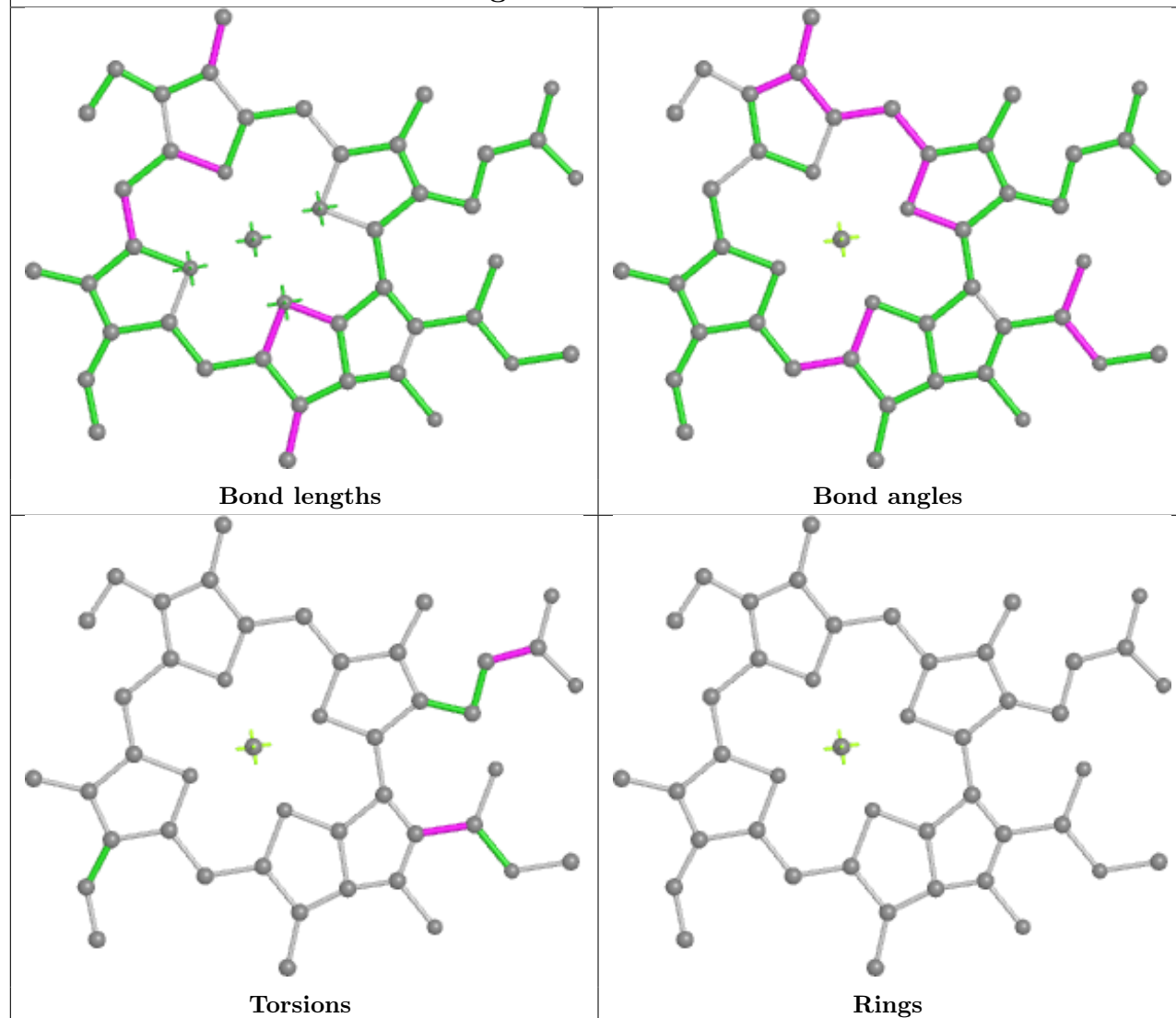


Ligand CLA X 602**Ligand CLA A 808**

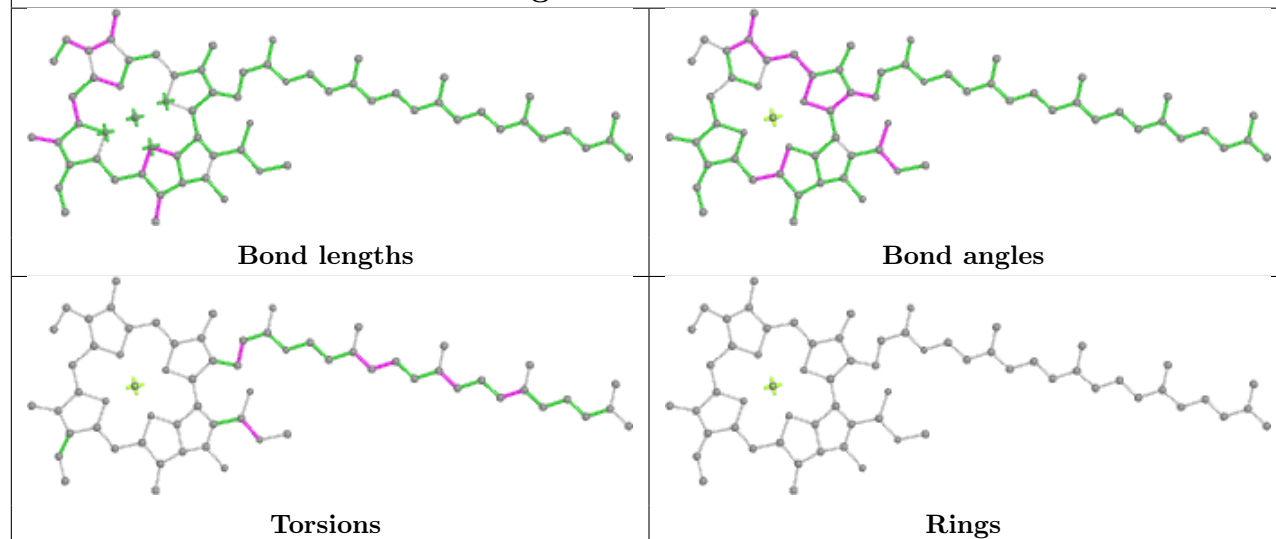




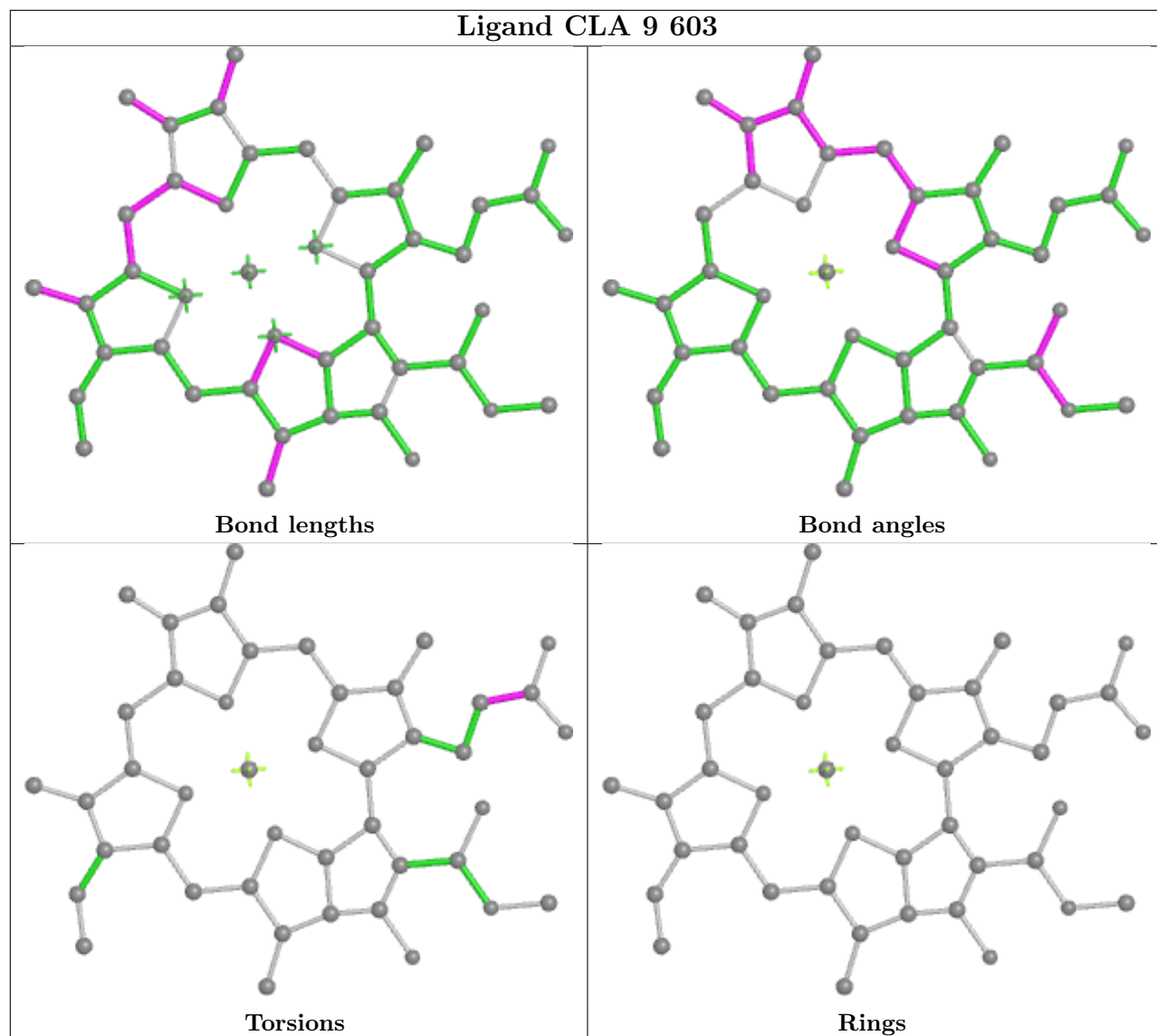
Ligand CLA Y 612



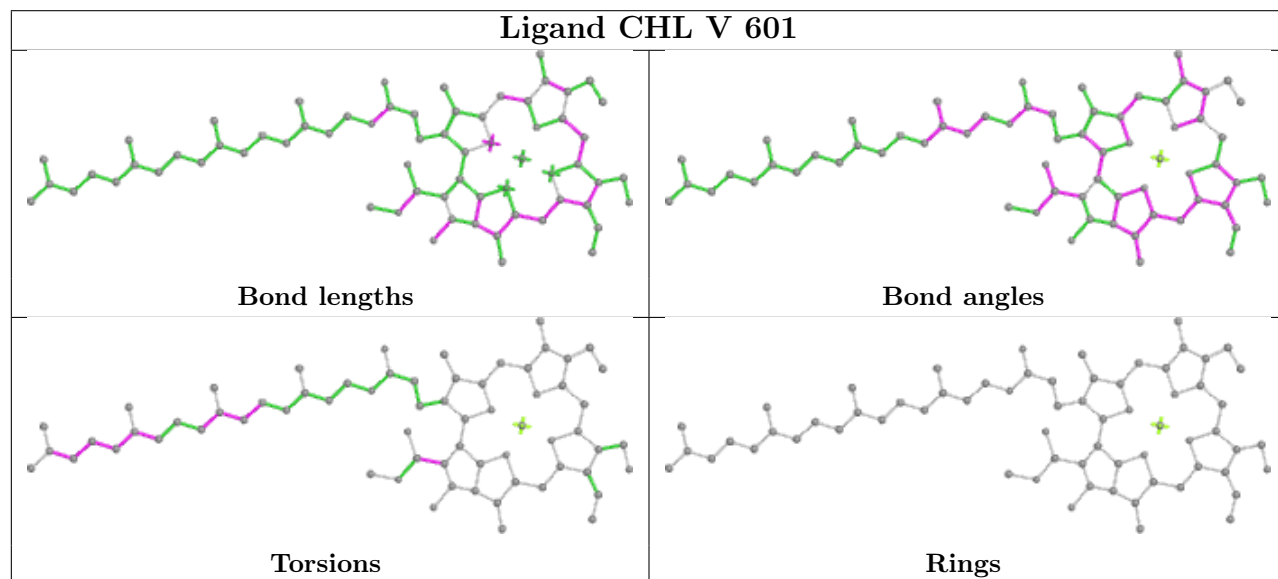
Ligand CLA A 802

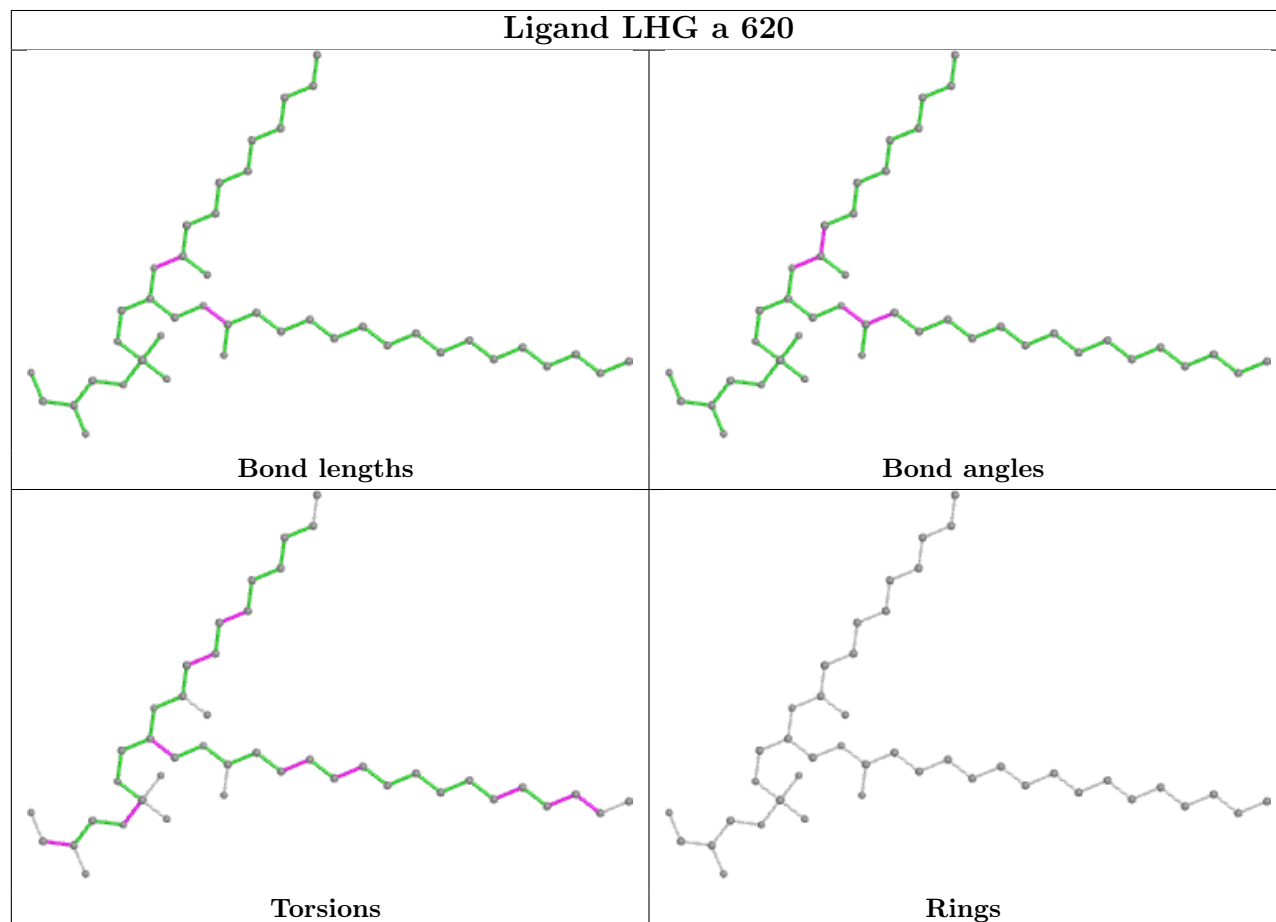
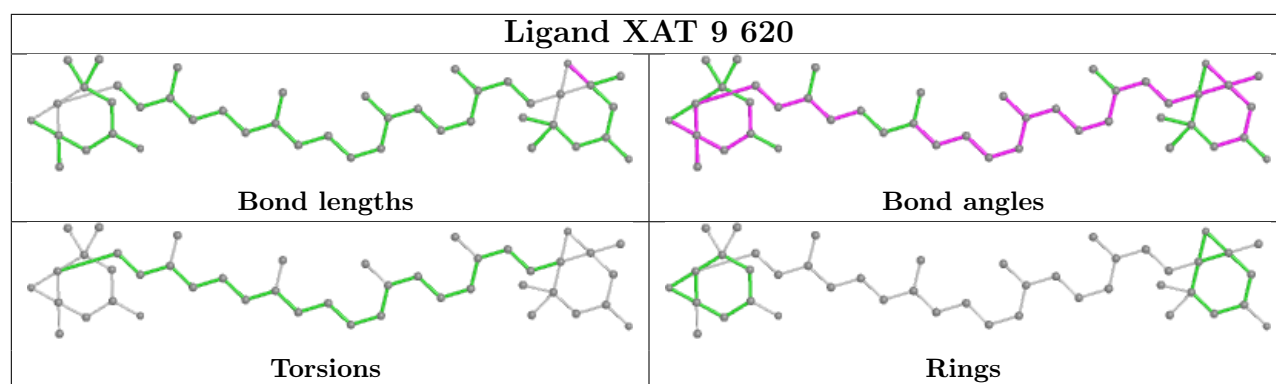


Ligand CLA 9 603

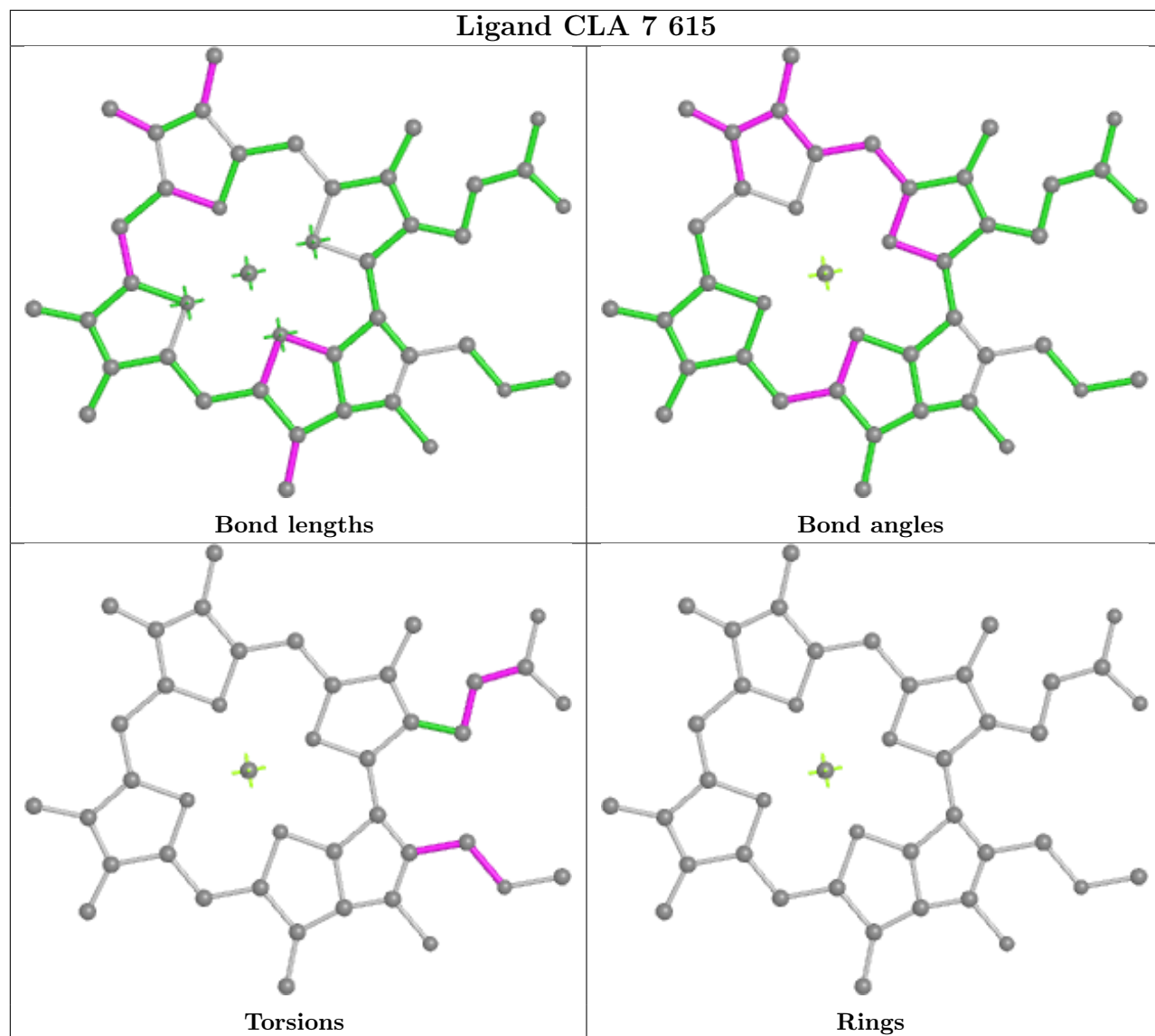


Ligand CHL V 601

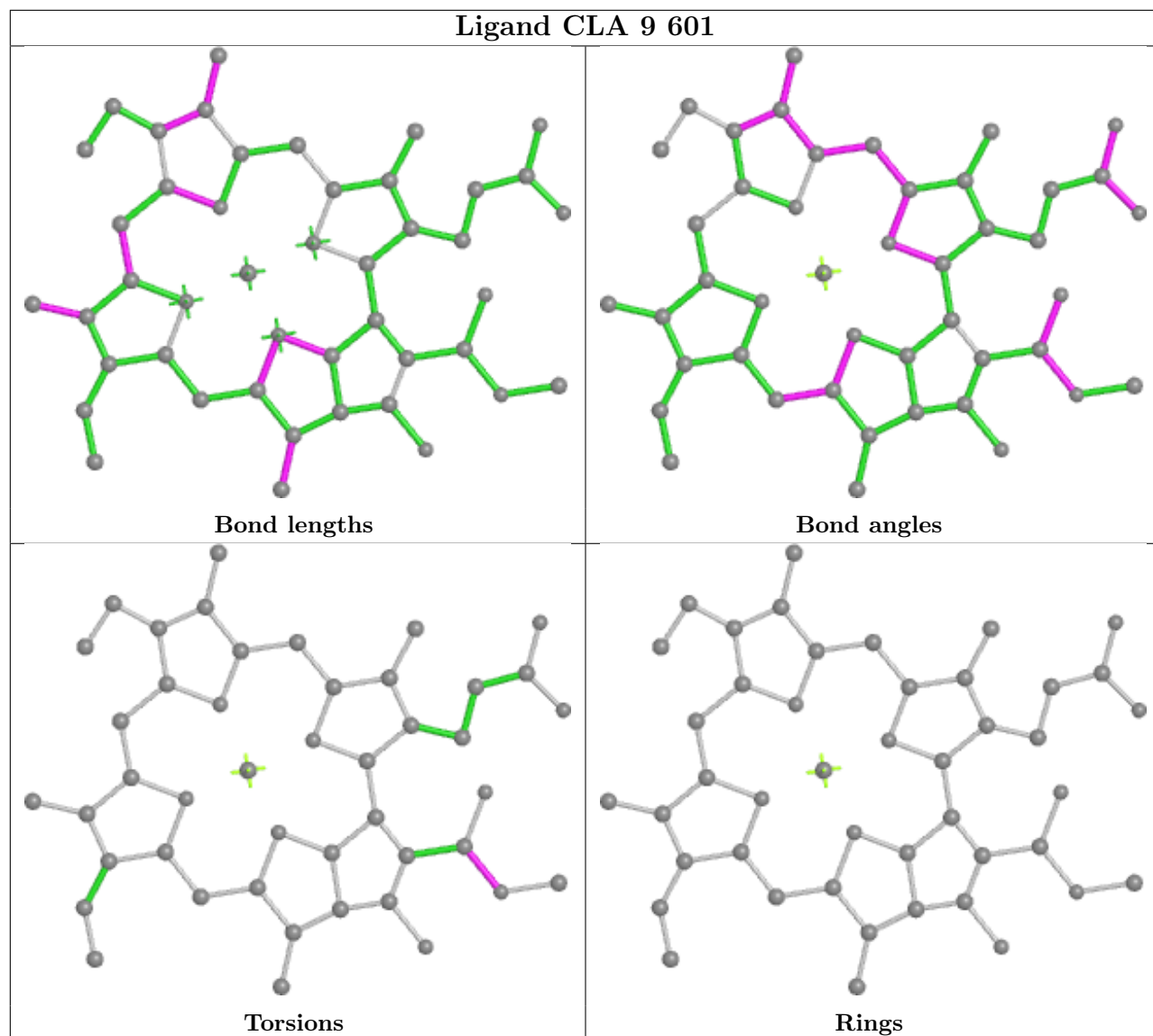




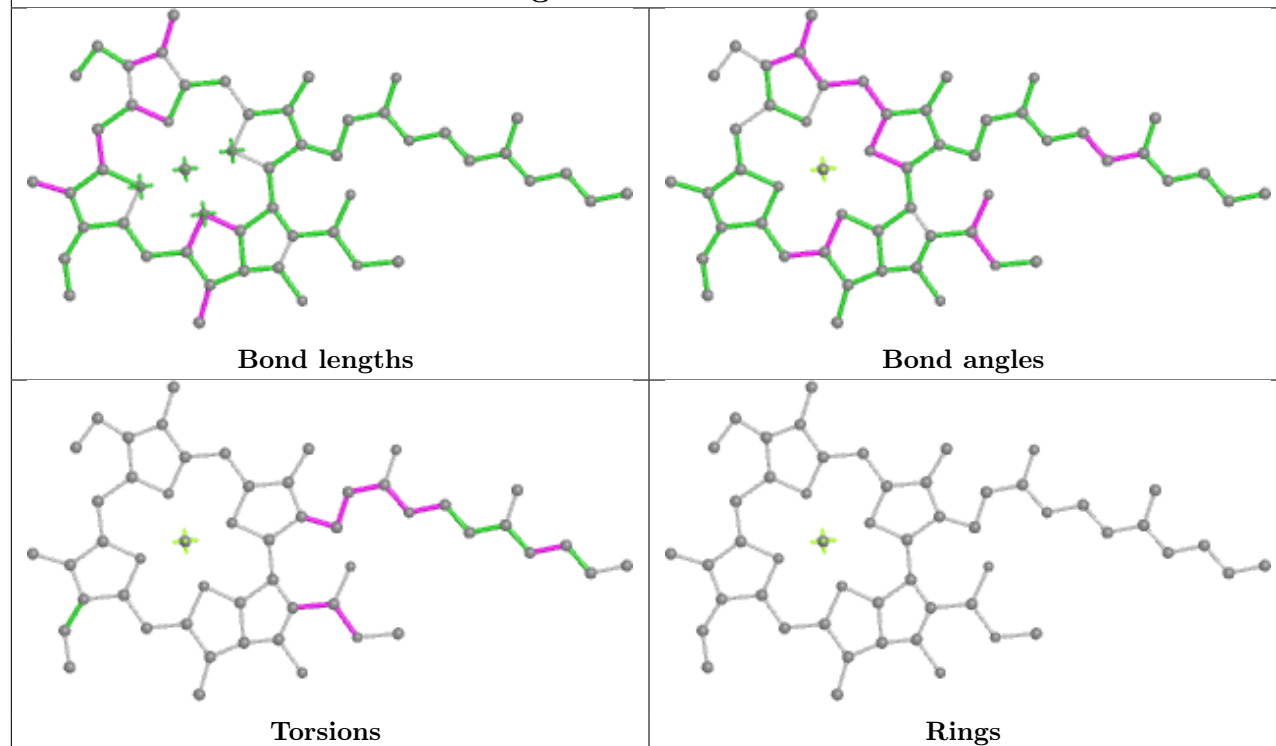
Ligand CLA 7 615



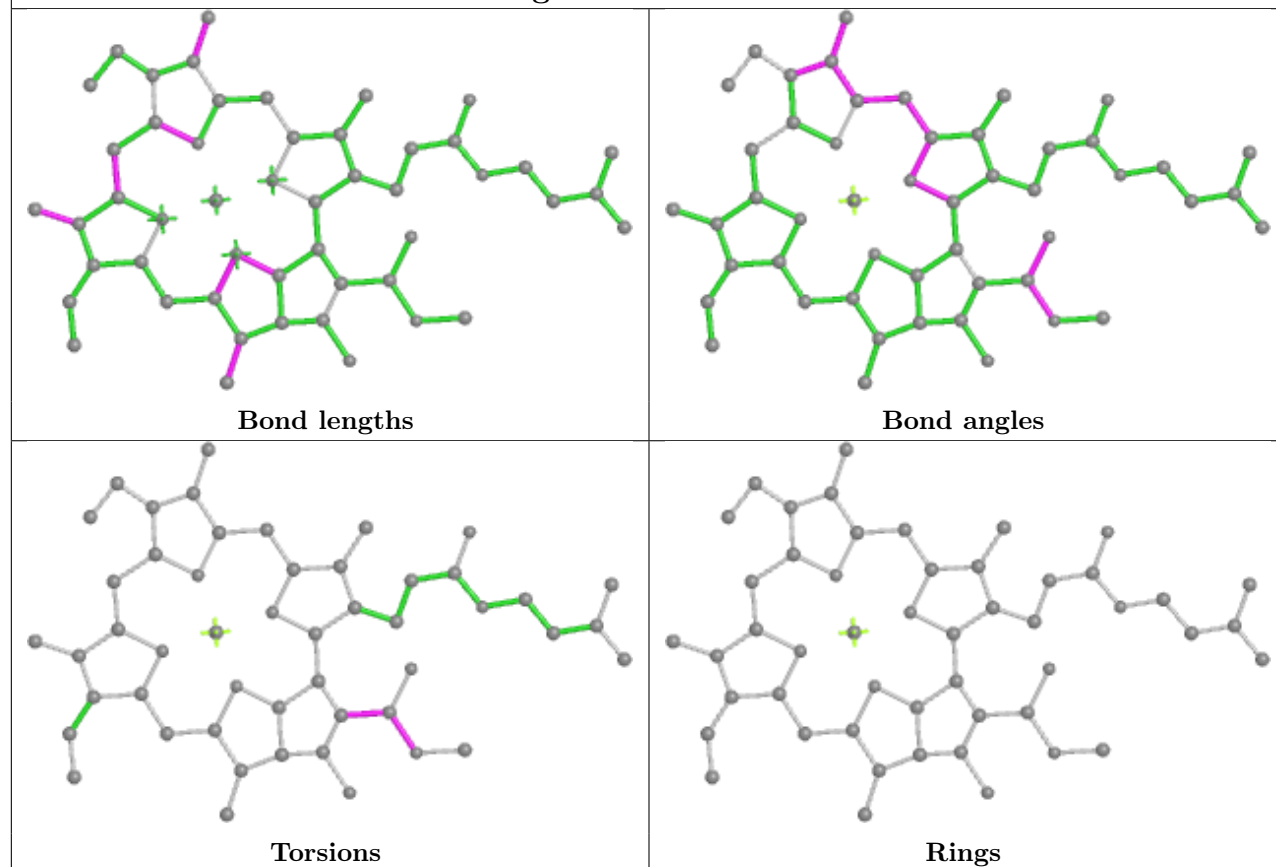
Ligand CLA 9 601

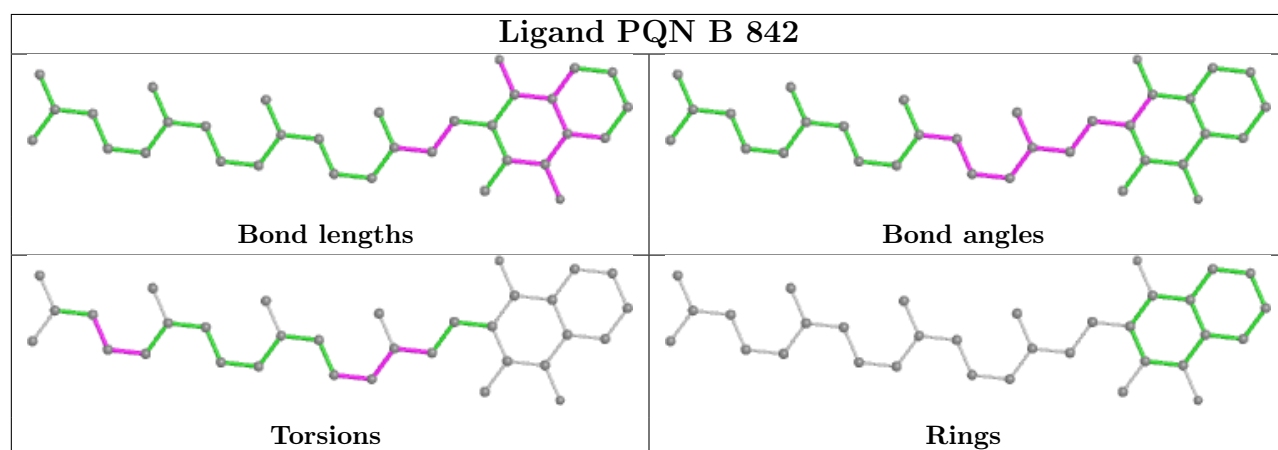
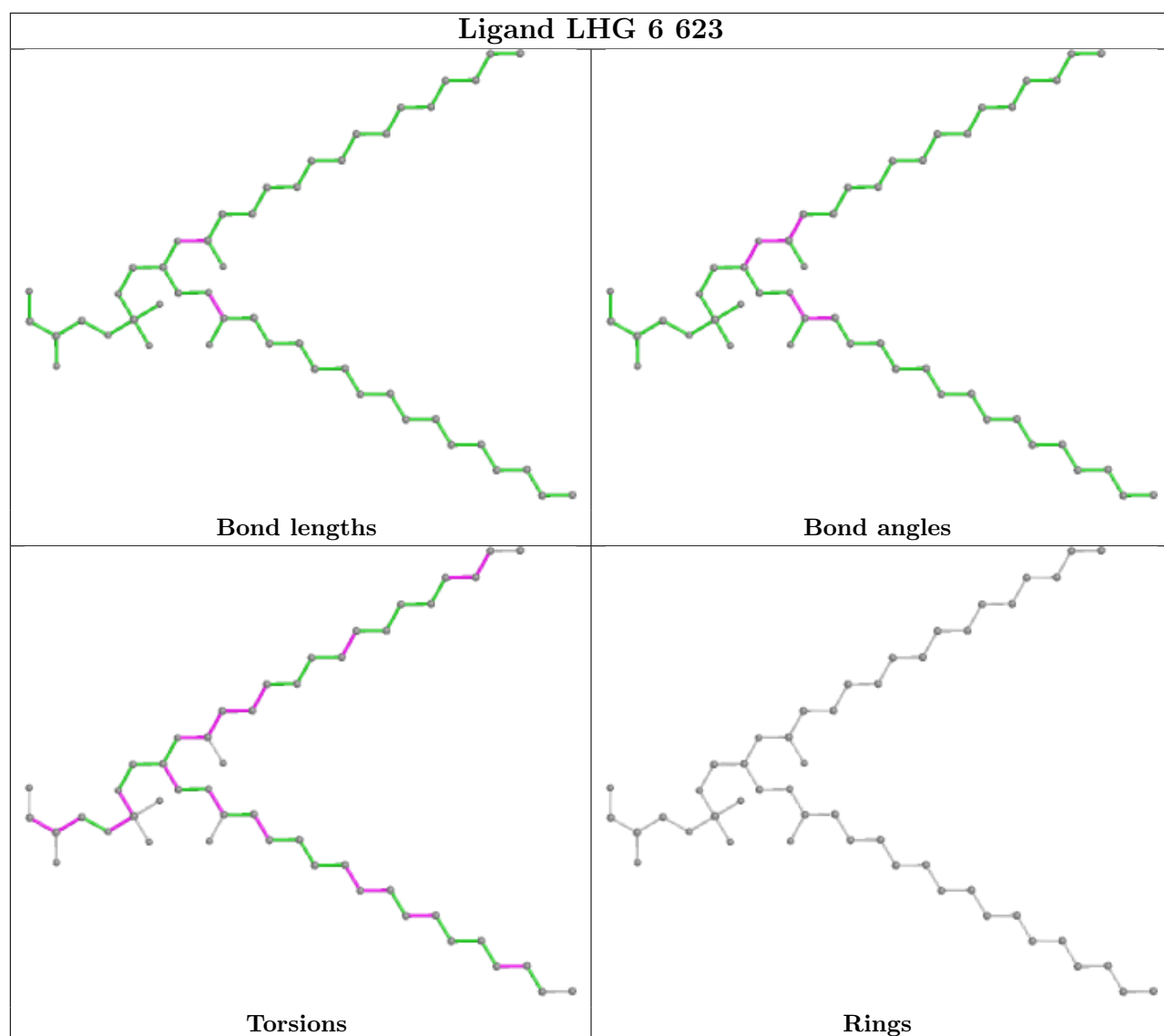


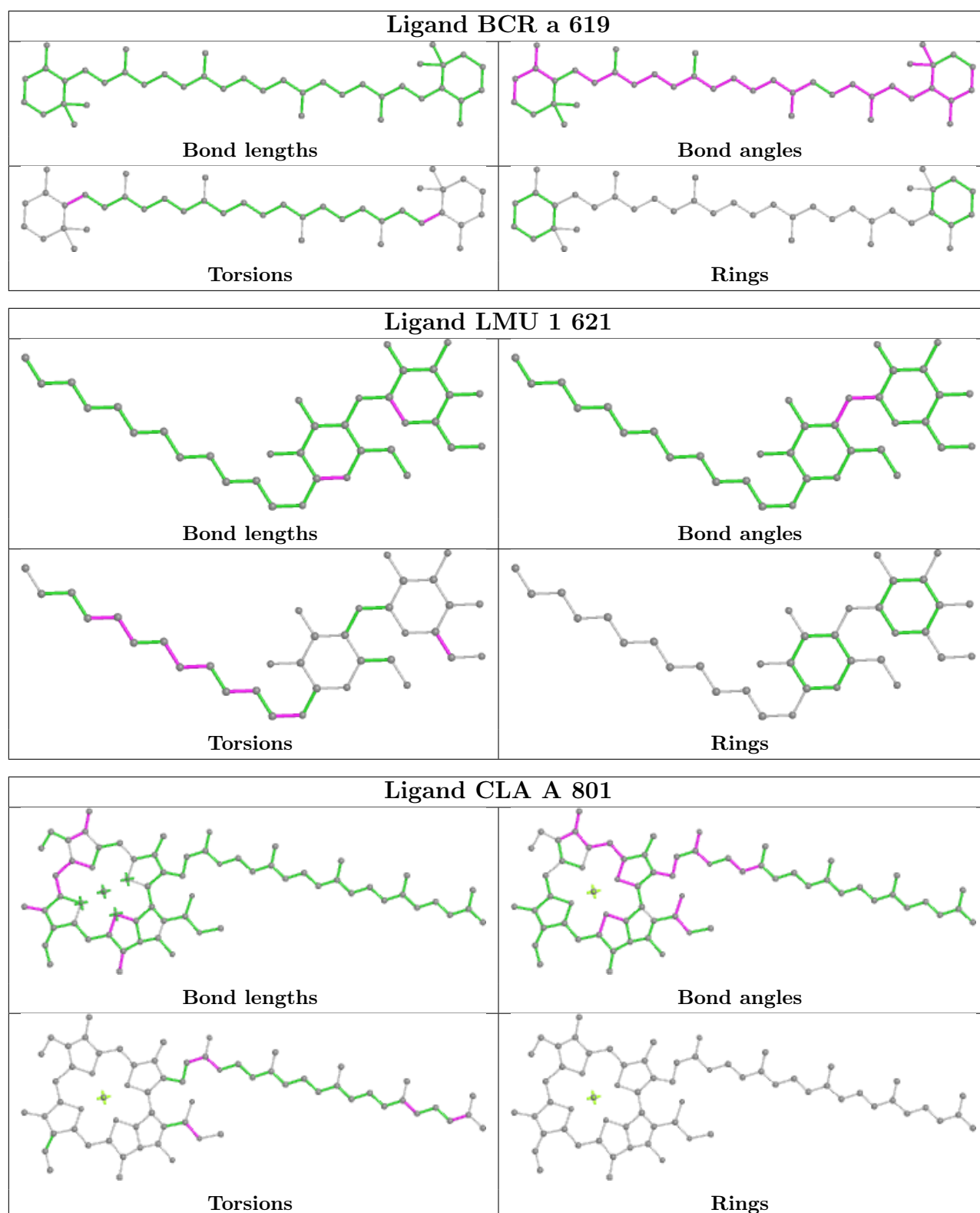
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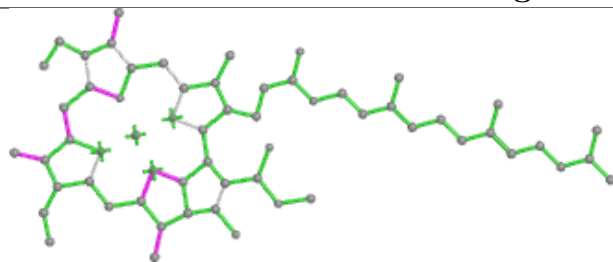
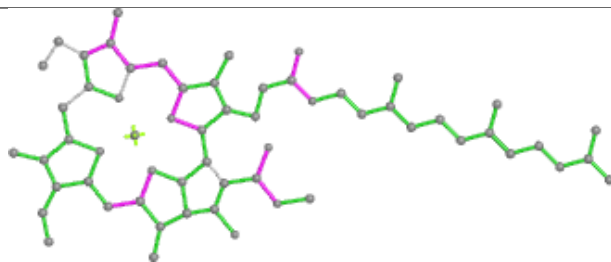
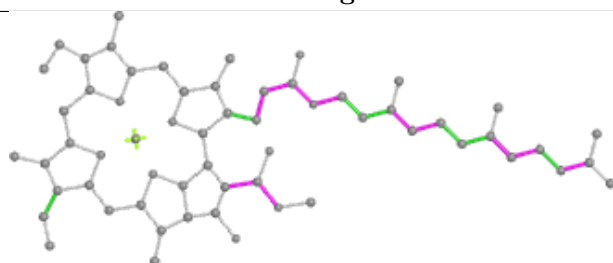
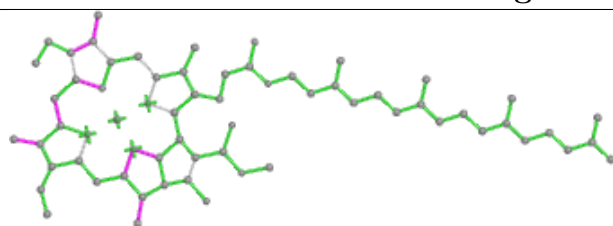
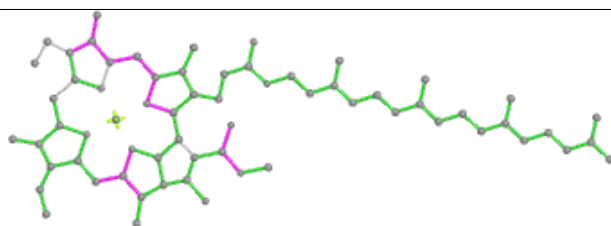
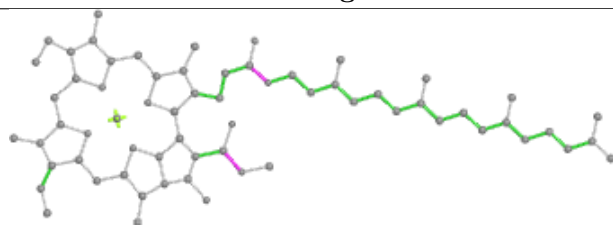
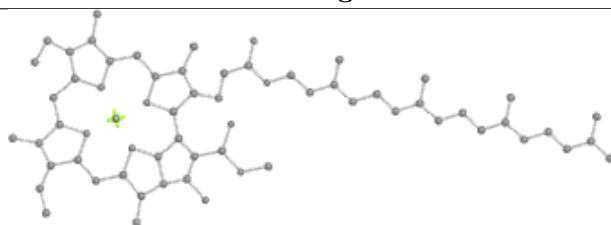


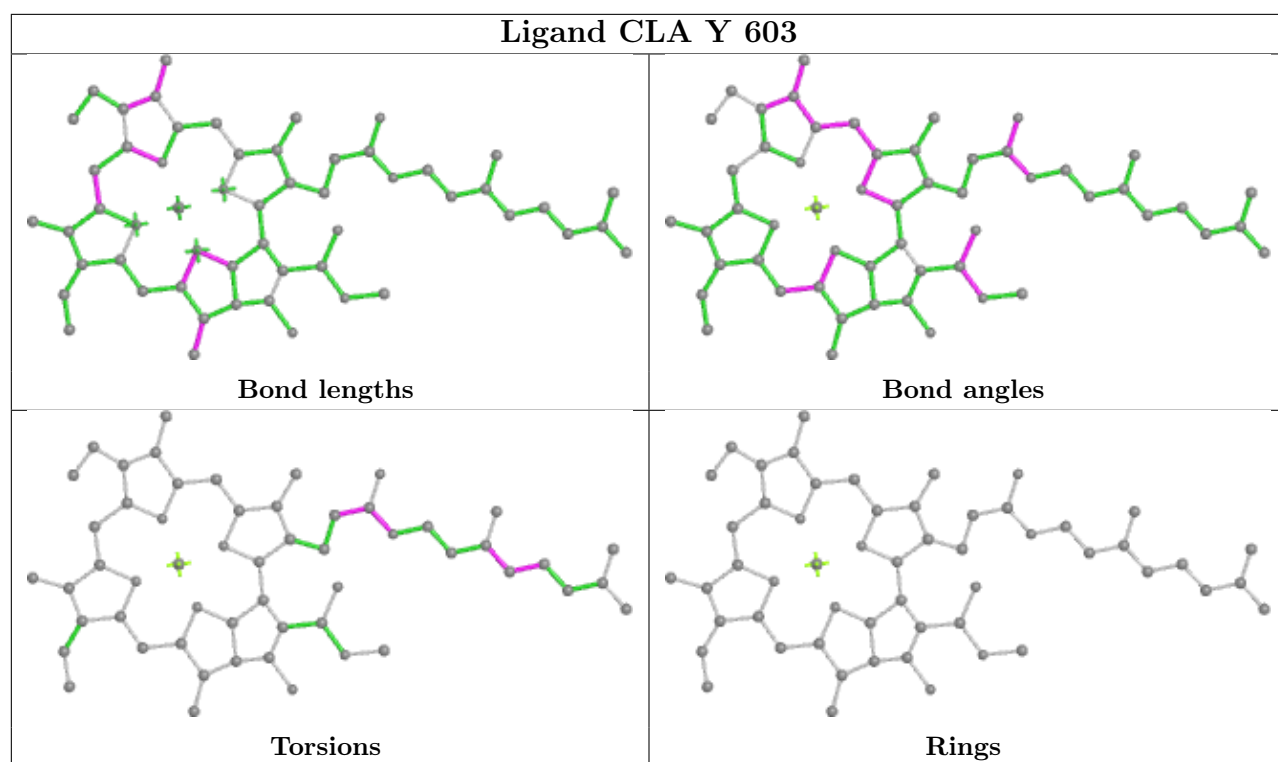
Ligand CLA B 836



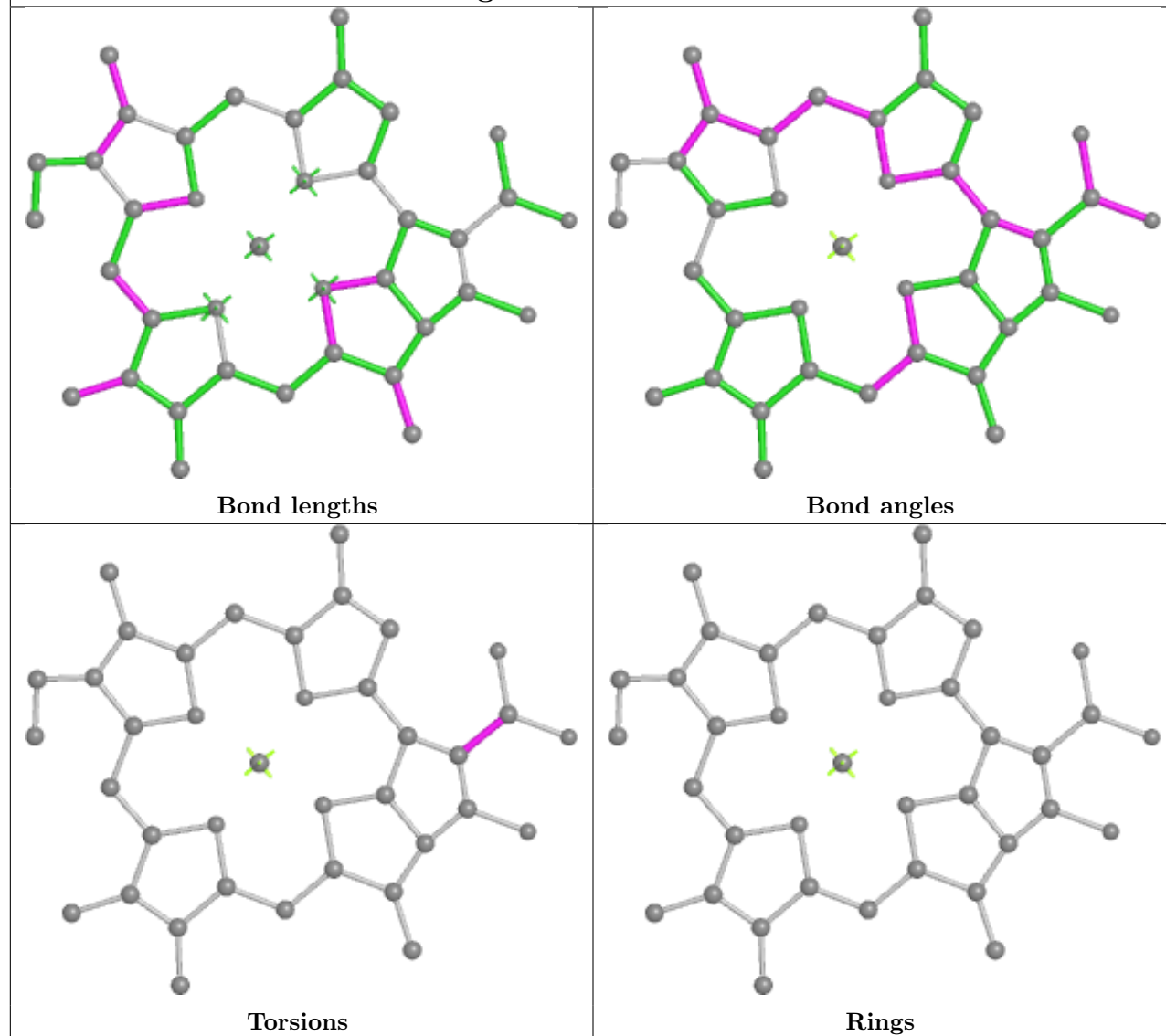


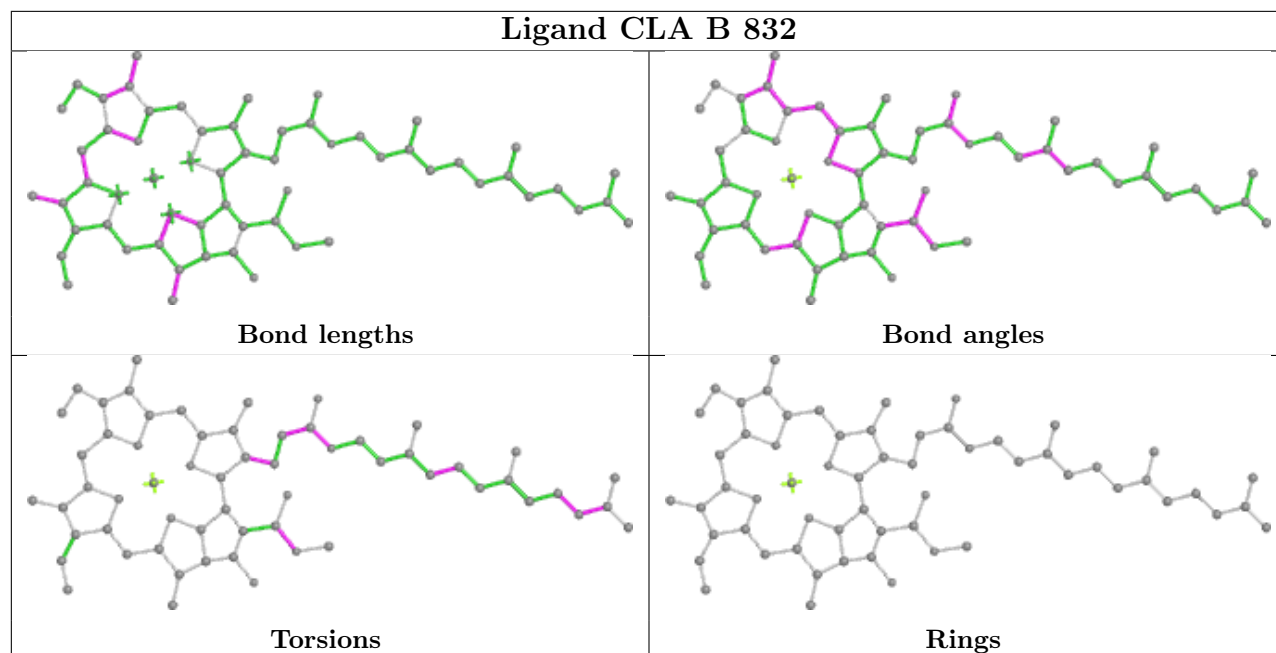
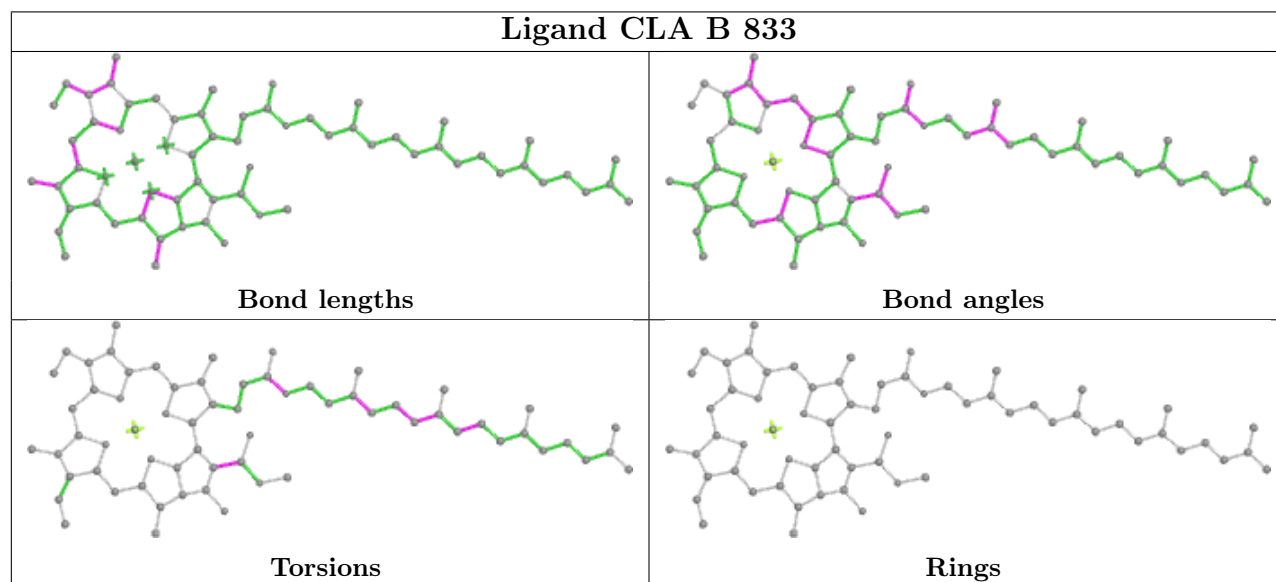
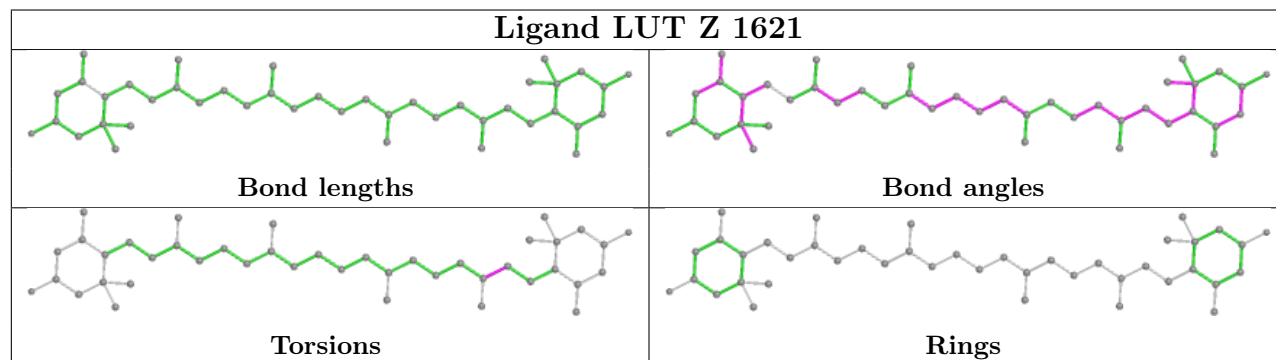


Ligand CLA A 818**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 840****Bond lengths****Bond angles****Torsions****Rings**

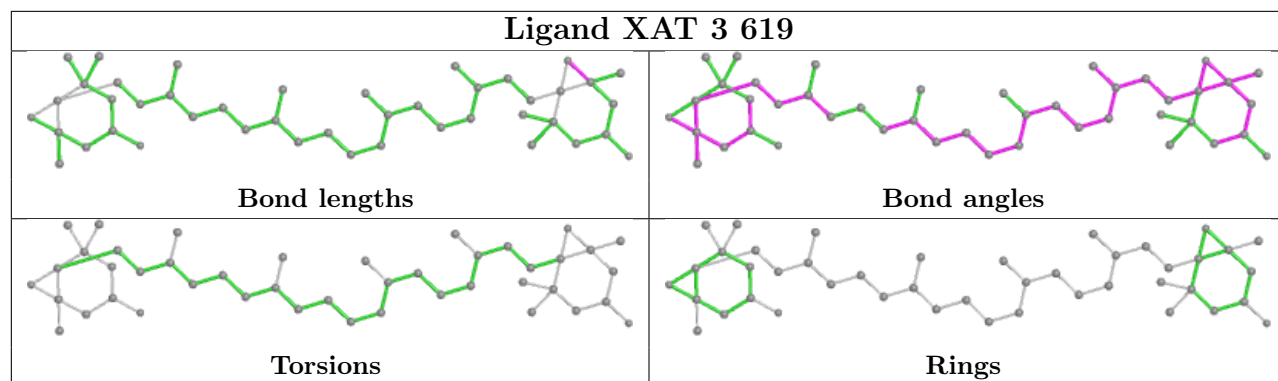


Ligand CLA O 2001

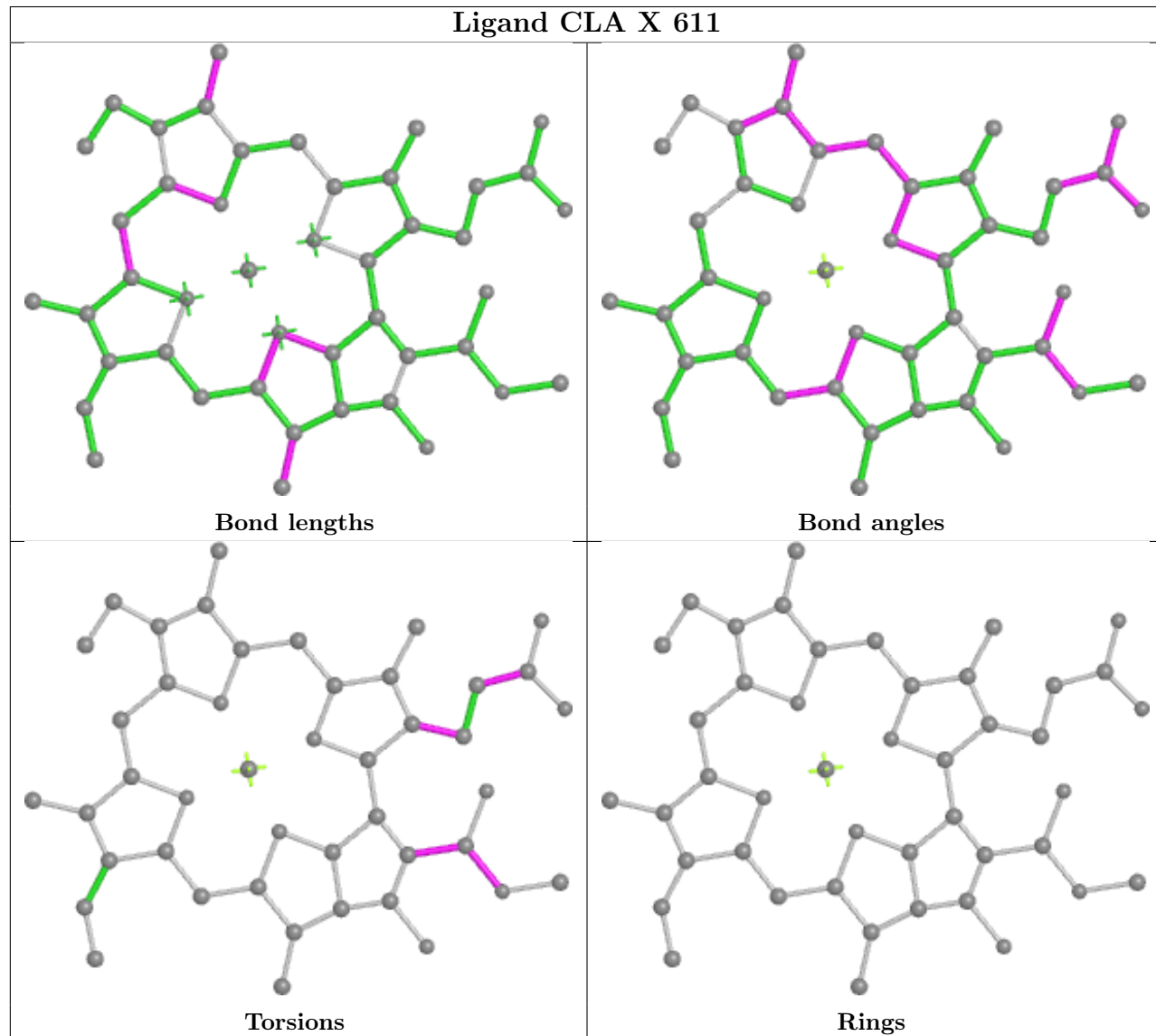


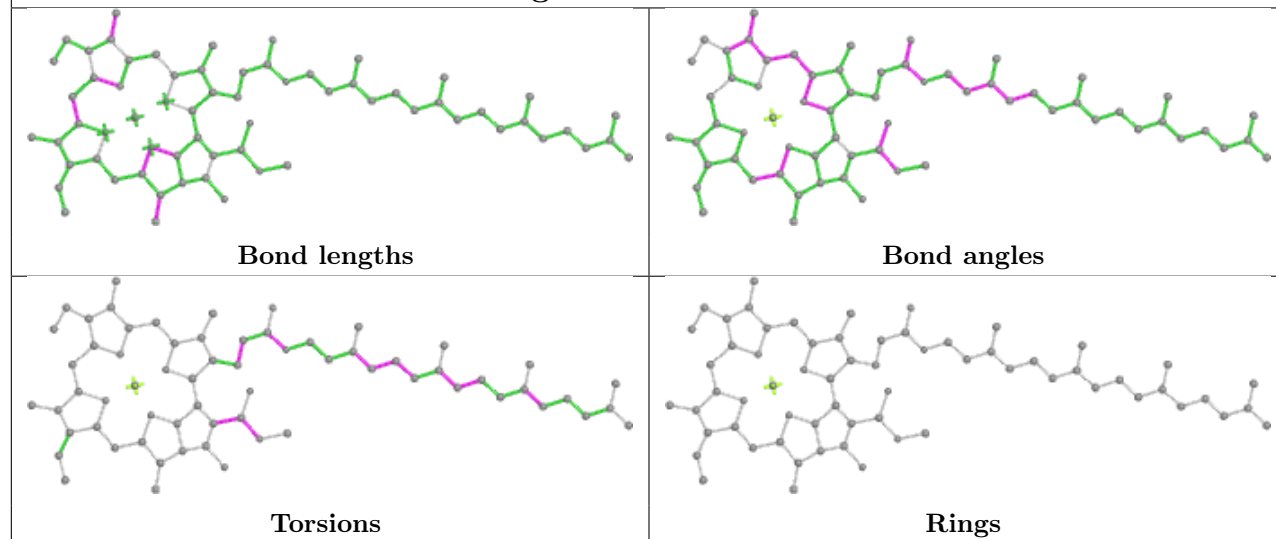
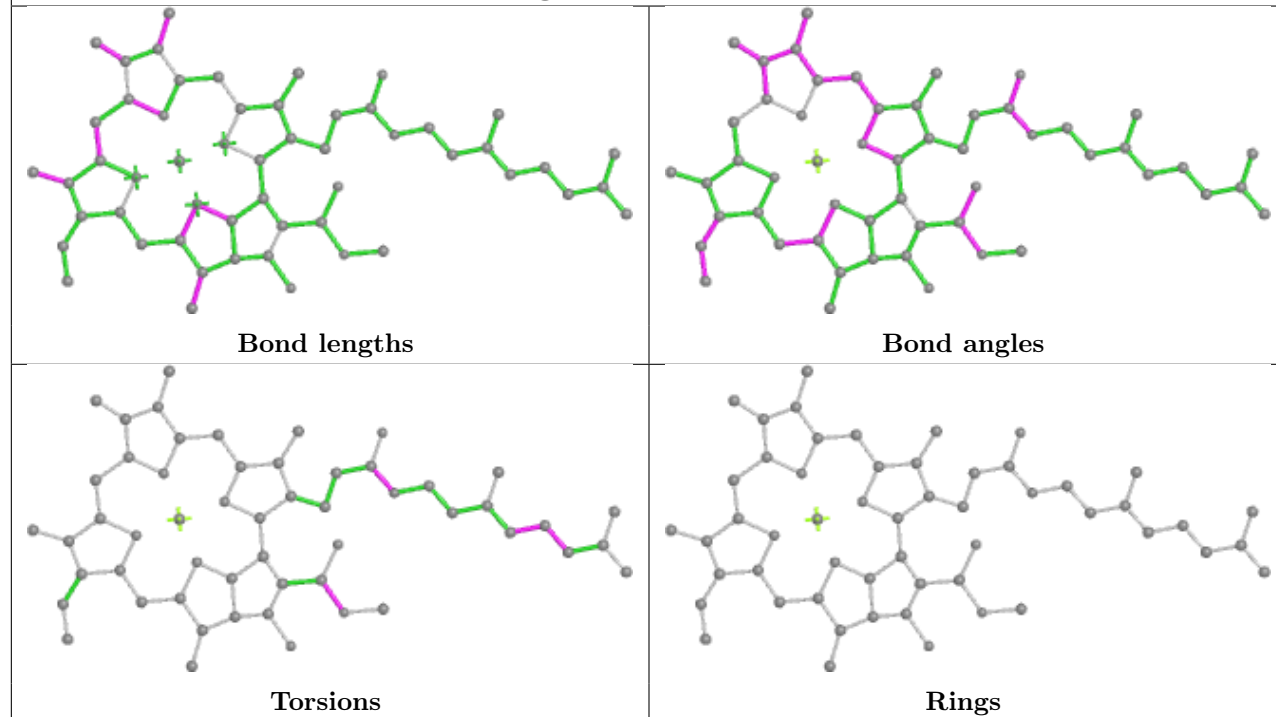
Ligand CLA B 832**Ligand CLA B 833****Ligand LUT Z 1621**

Ligand XAT 3 619

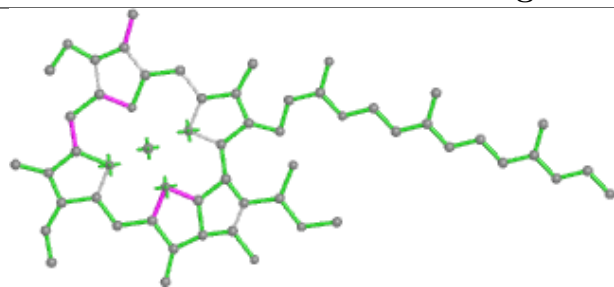


Ligand CLA X 611

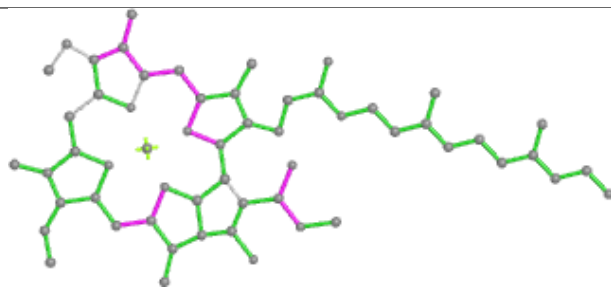


Ligand CLA X 613**Ligand CLA 5 603**

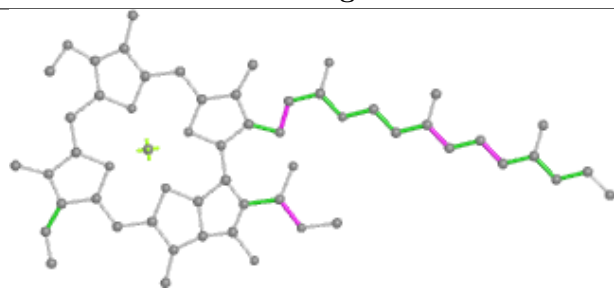
Ligand CLA Z 604



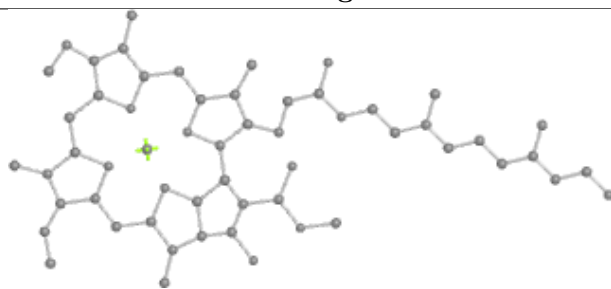
Bond lengths



Bond angles

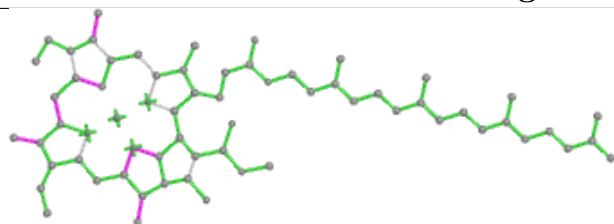


Torsions

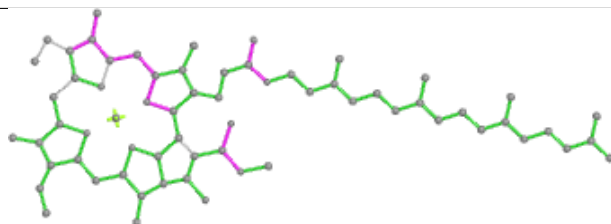


Rings

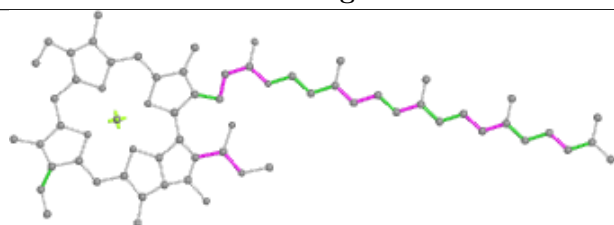
Ligand CLA 8 601



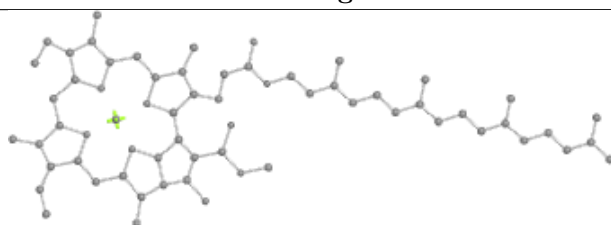
Bond lengths



Bond angles

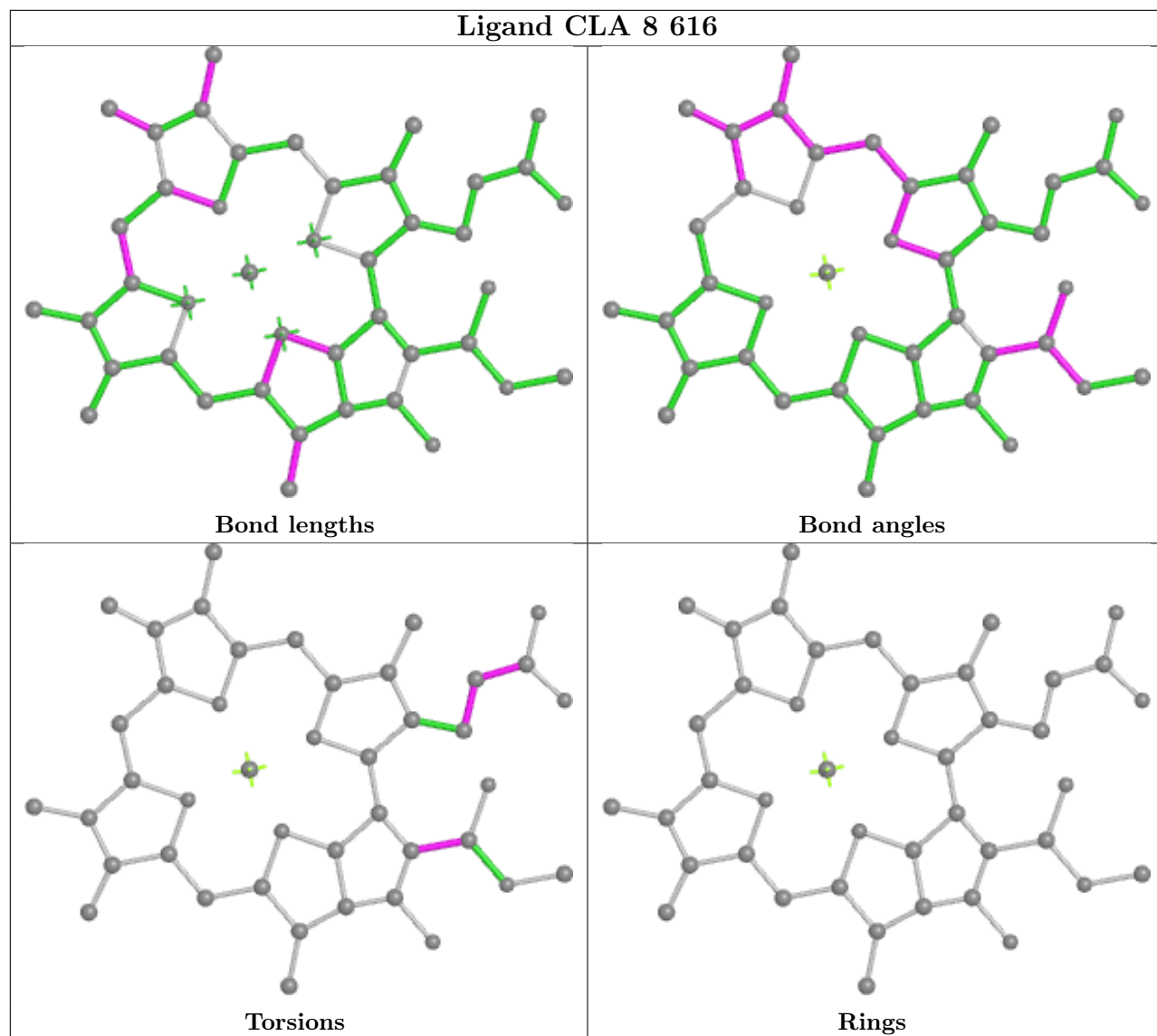


Torsions

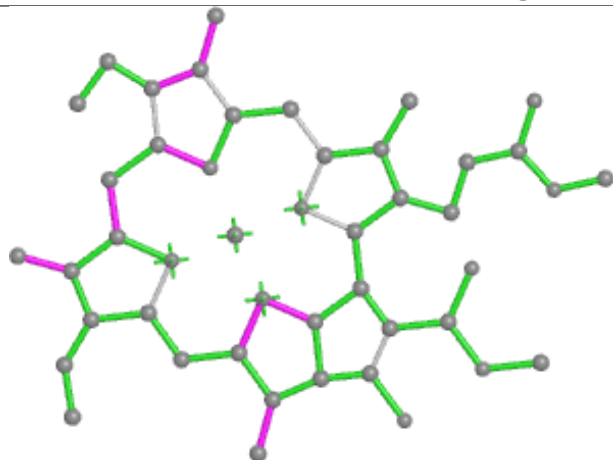


Rings

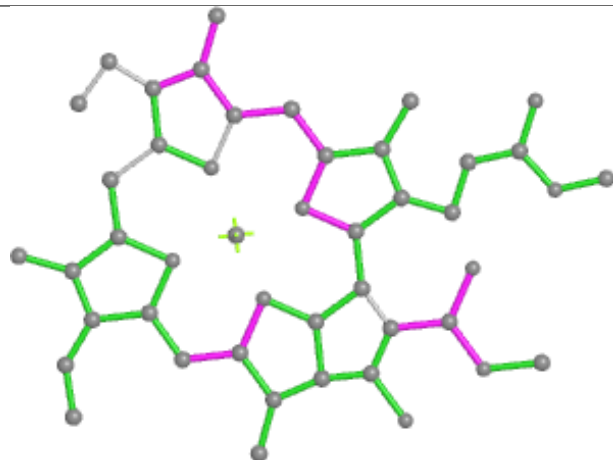
Ligand CLA 8 616



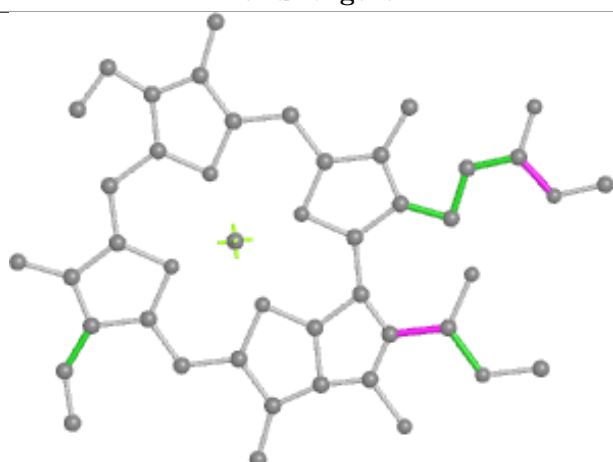
Ligand CLA B 838



Bond lengths



Bond angles

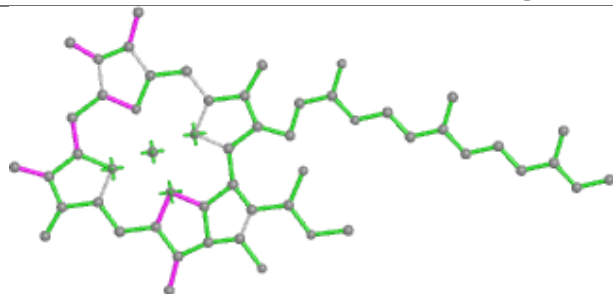


Torsions

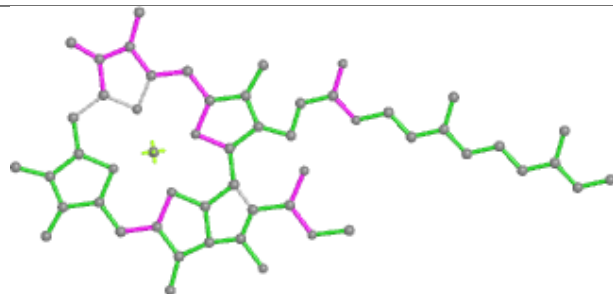


Rings

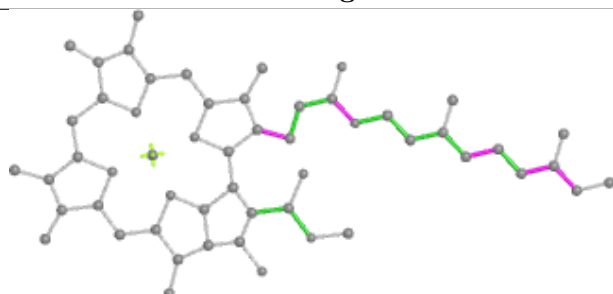
Ligand CLA 4 604



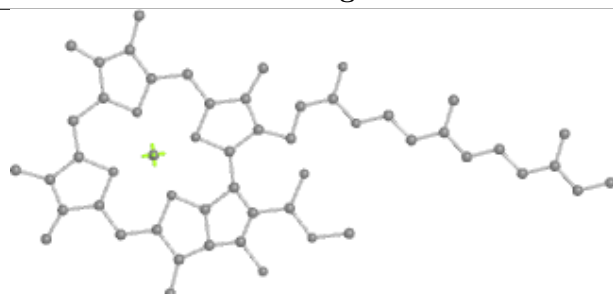
Bond lengths



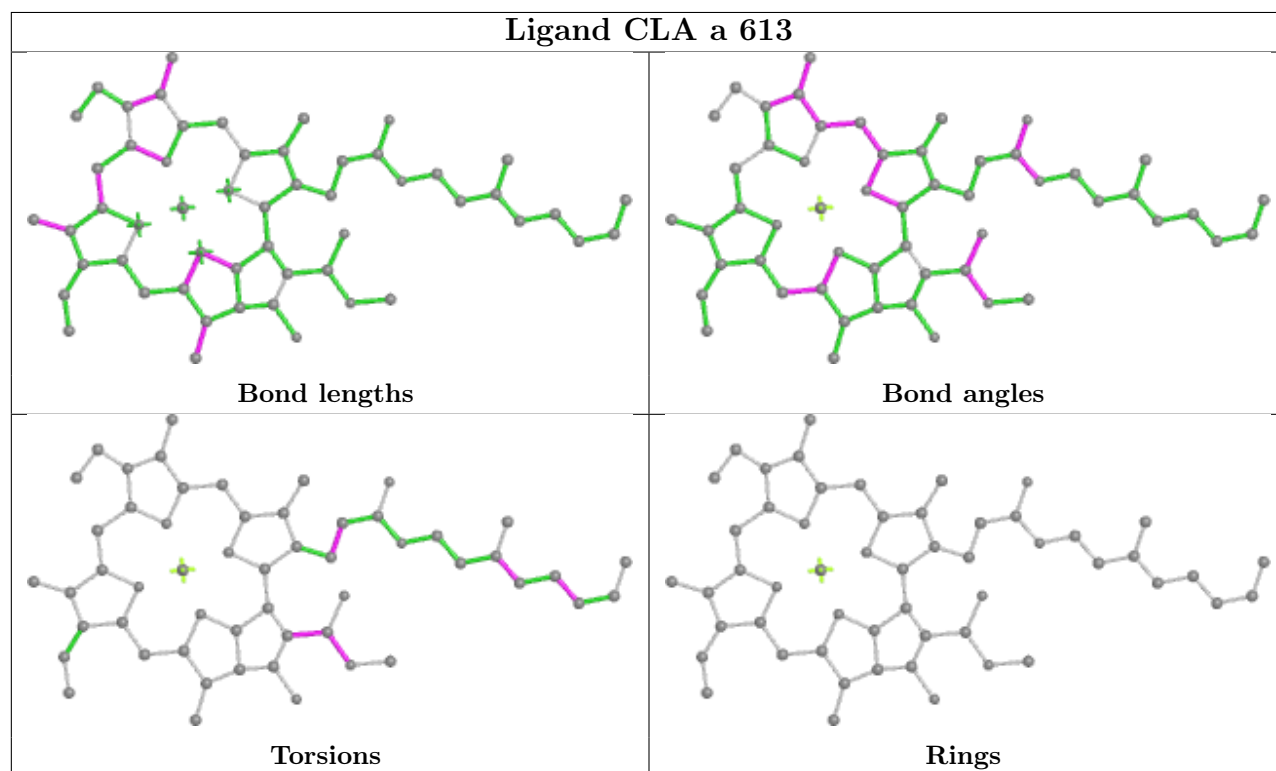
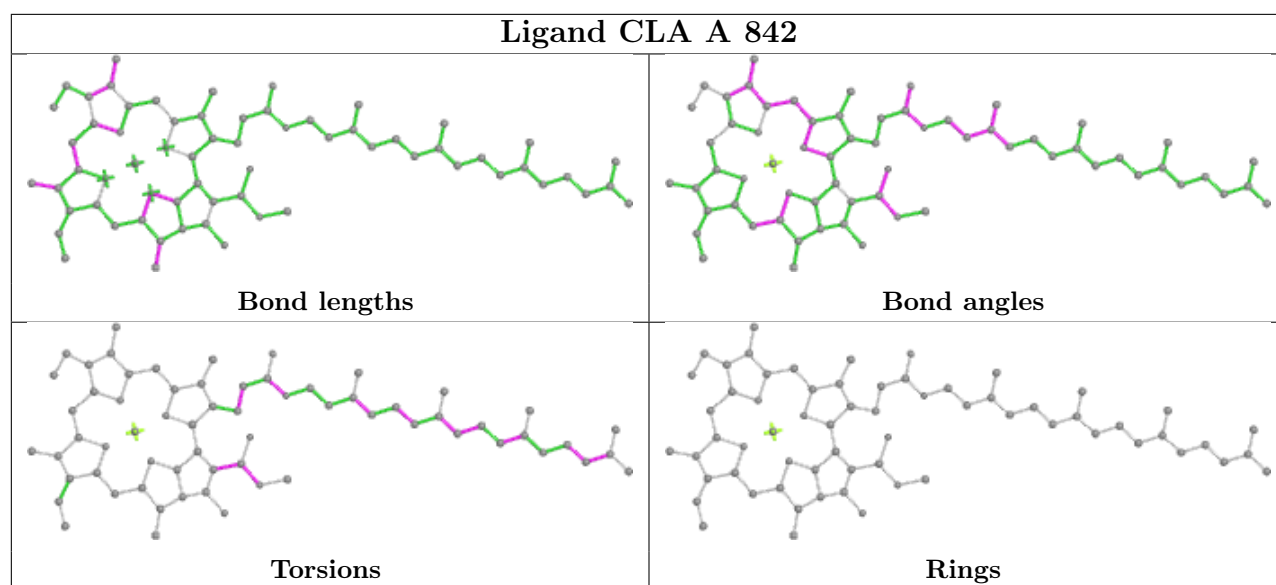
Bond angles

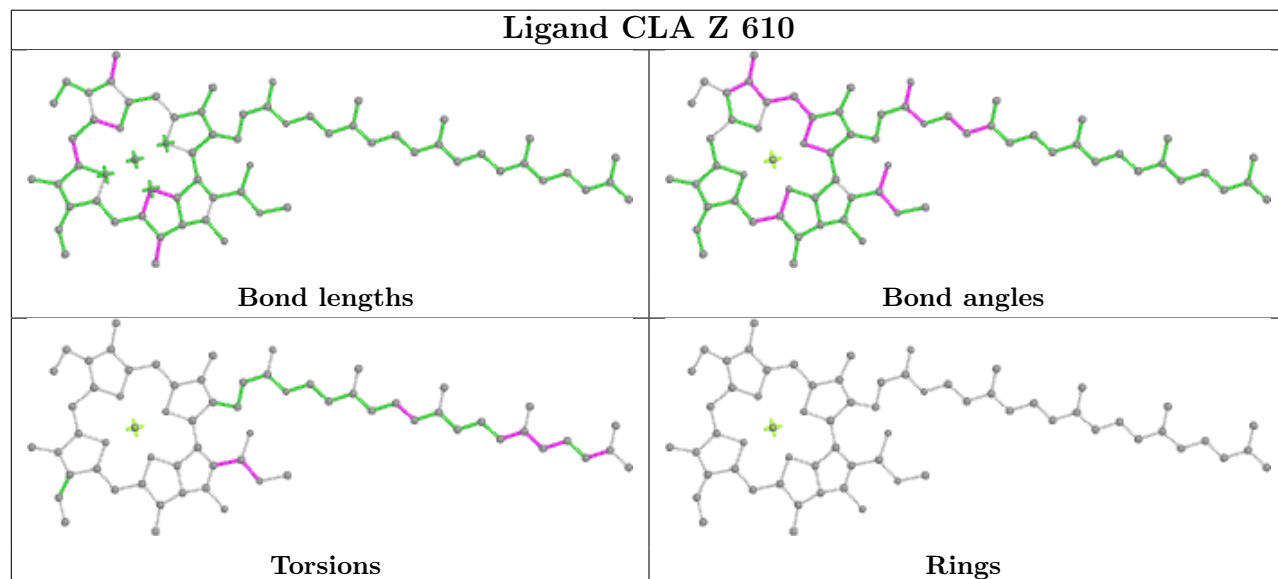
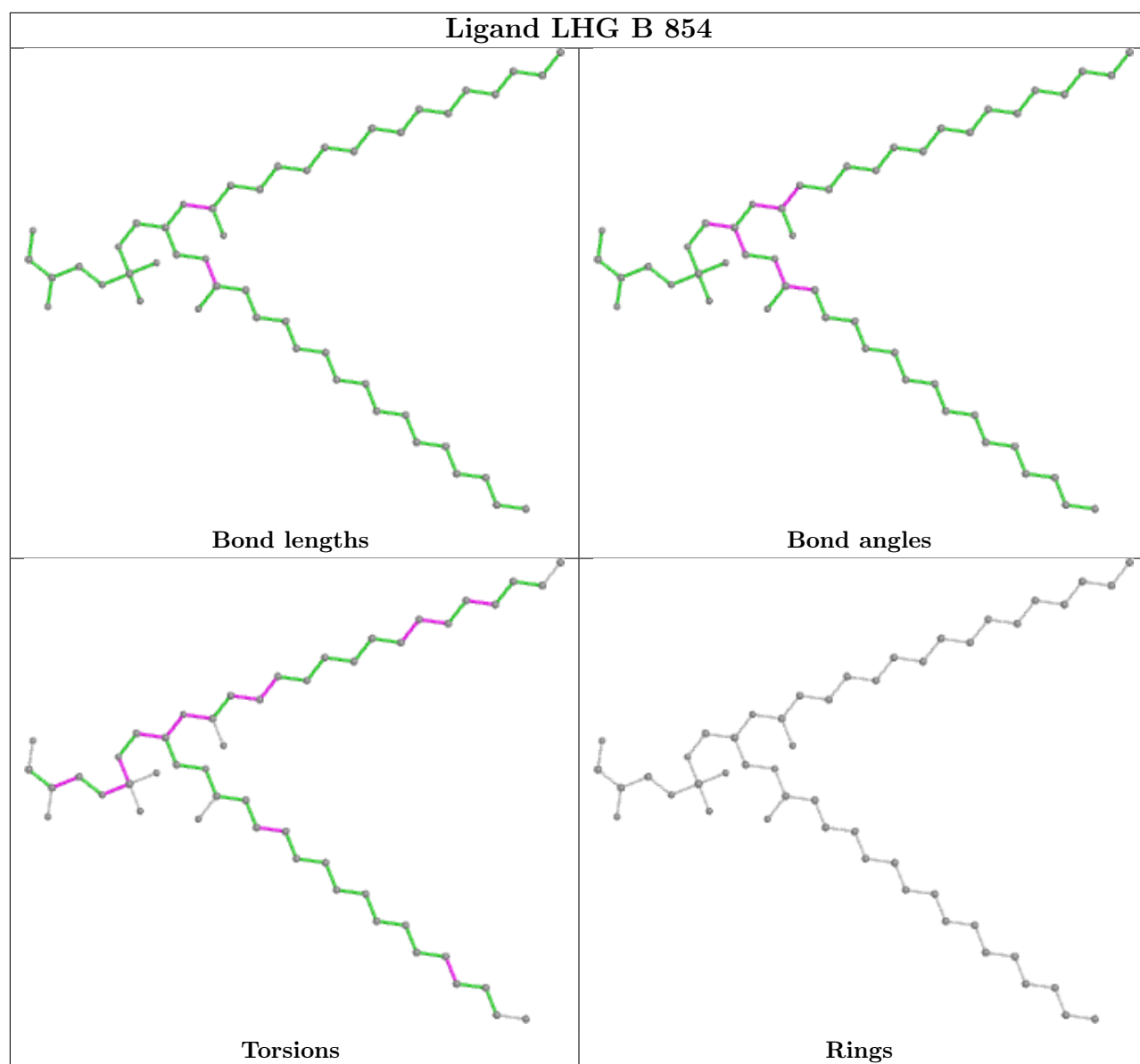


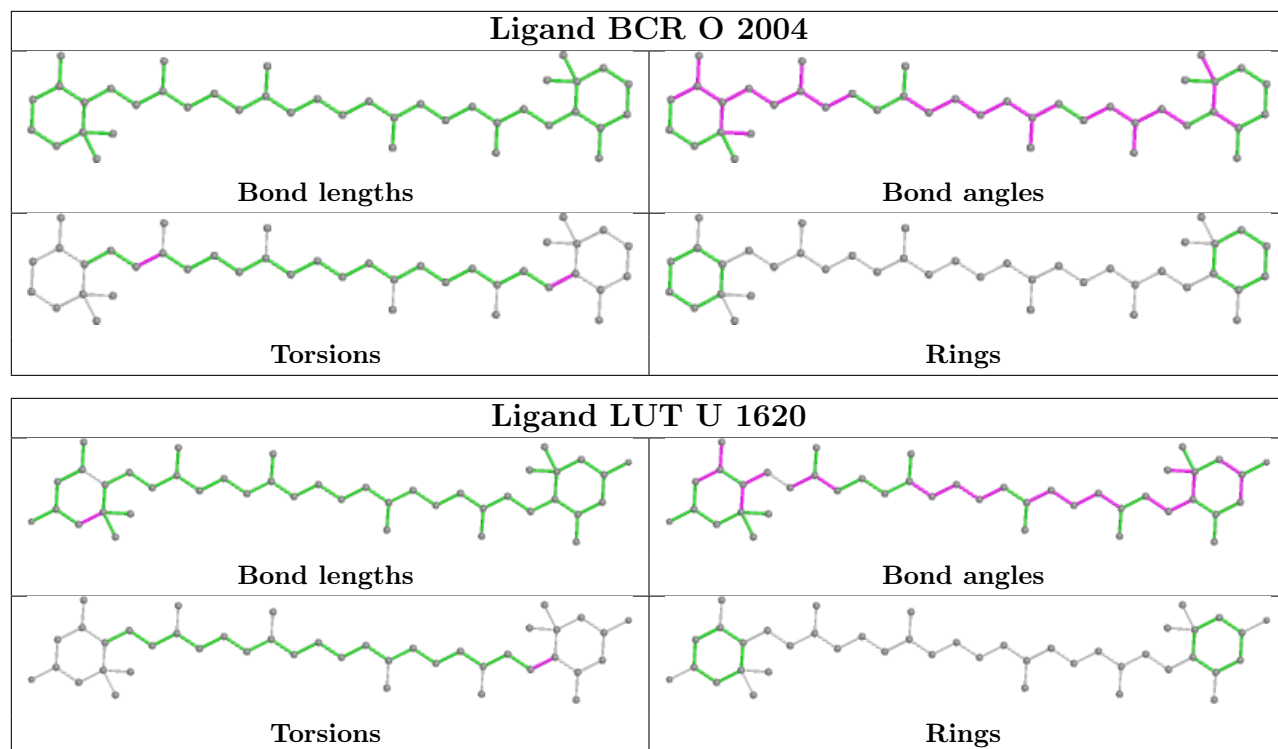
Torsions

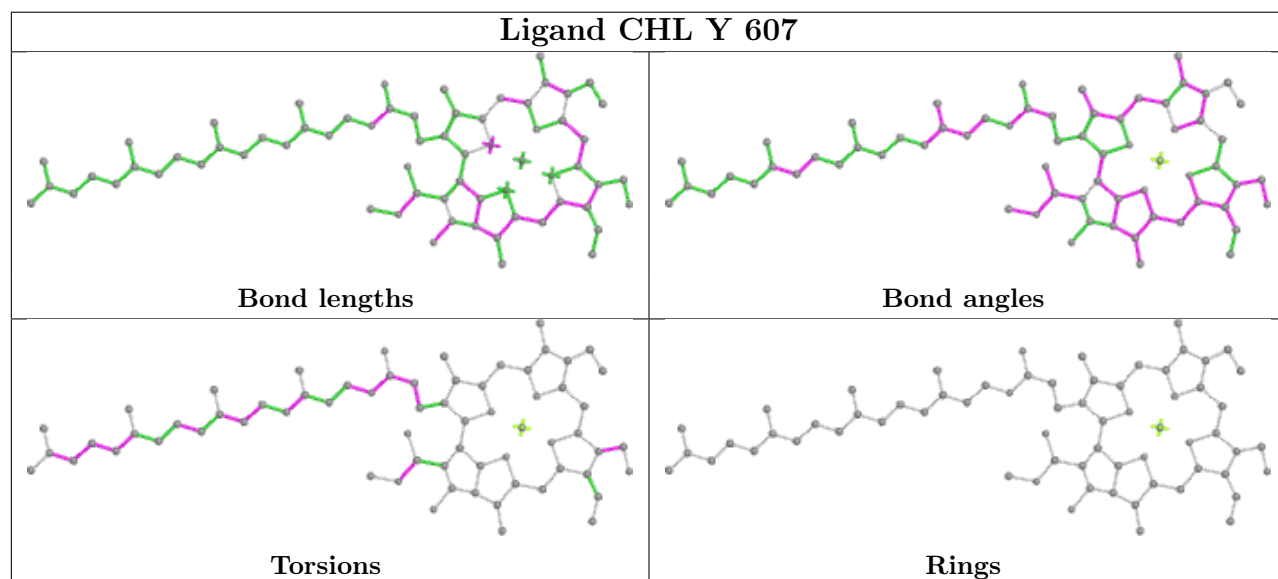
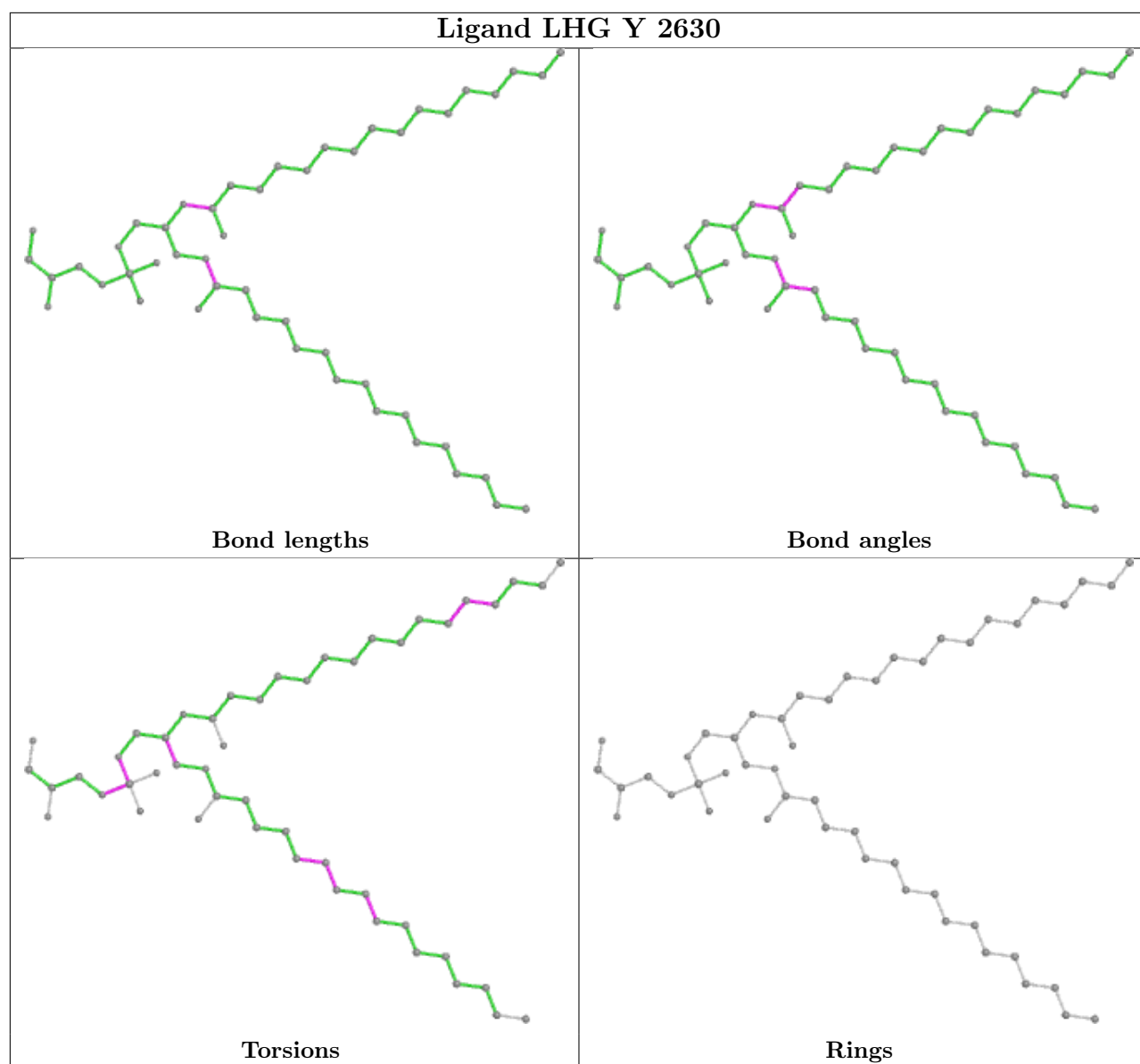


Rings

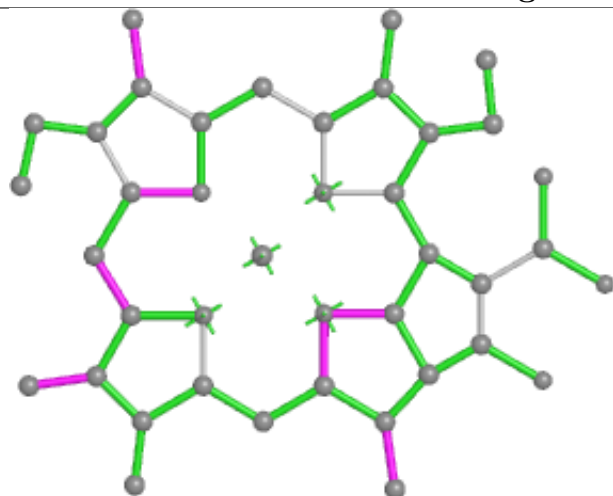




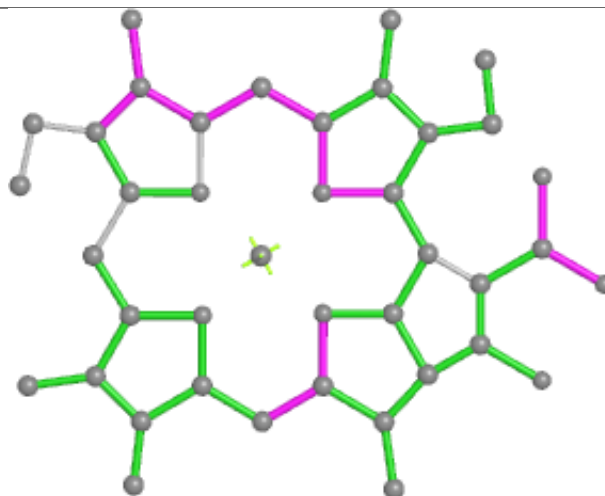




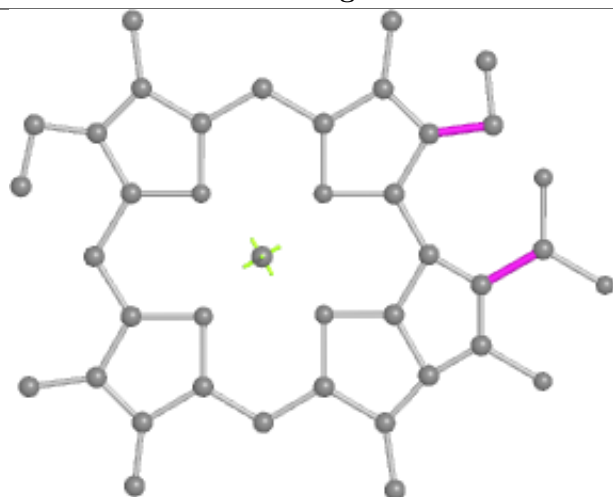
Ligand CLA 3 615



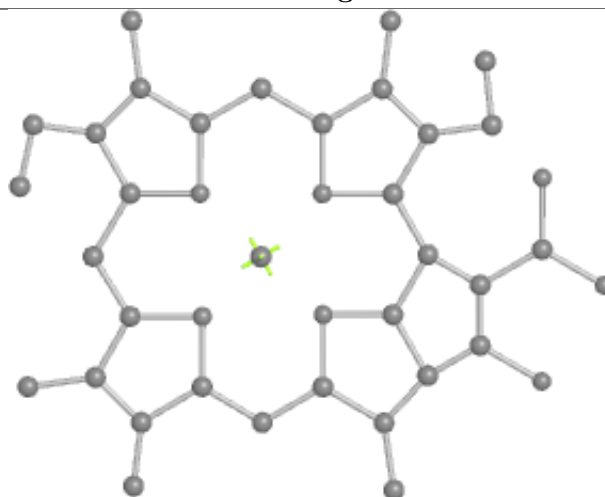
Bond lengths



Bond angles

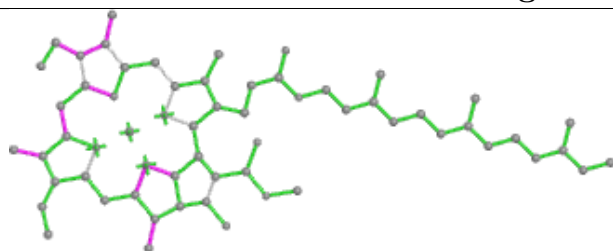


Torsions

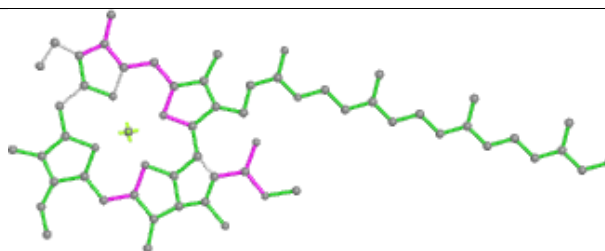


Rings

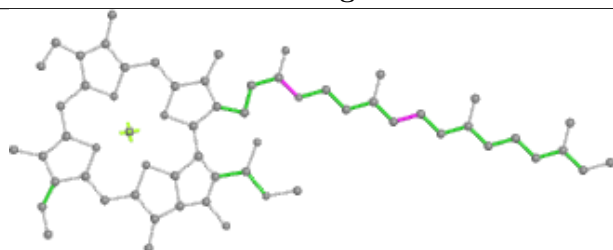
Ligand CLA a 602



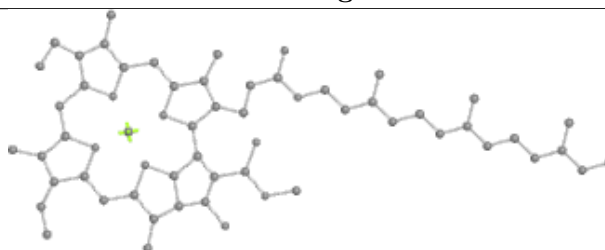
Bond lengths



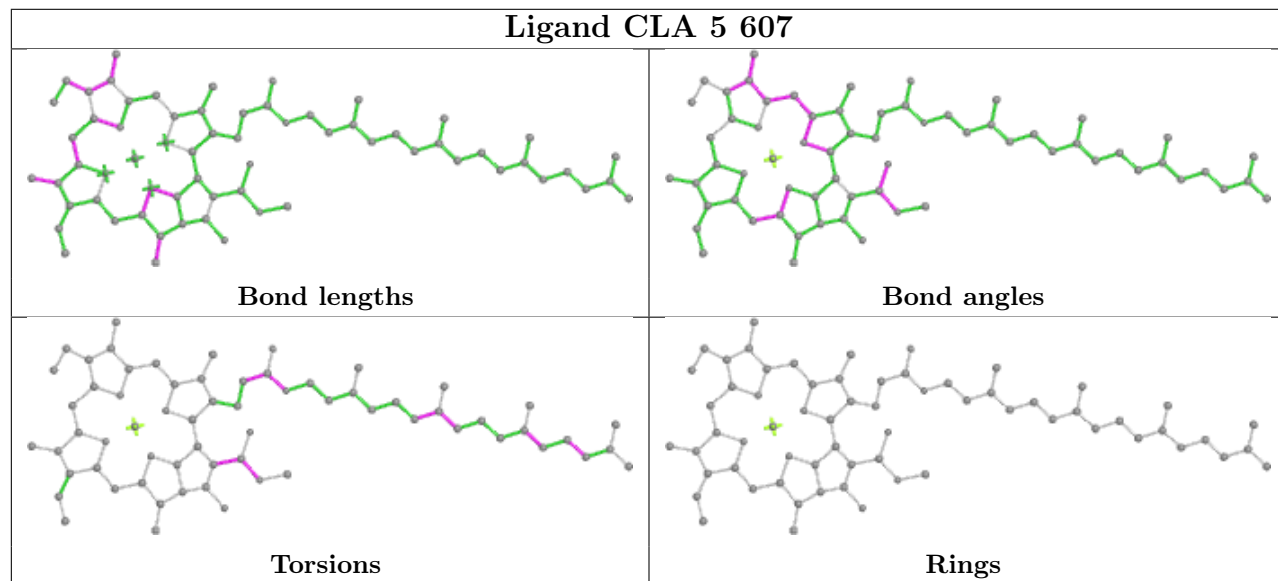
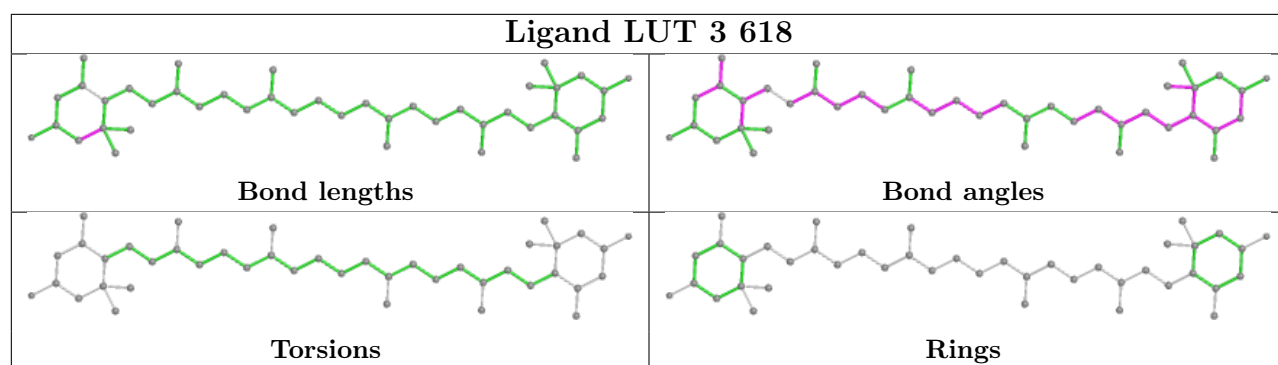
Bond angles



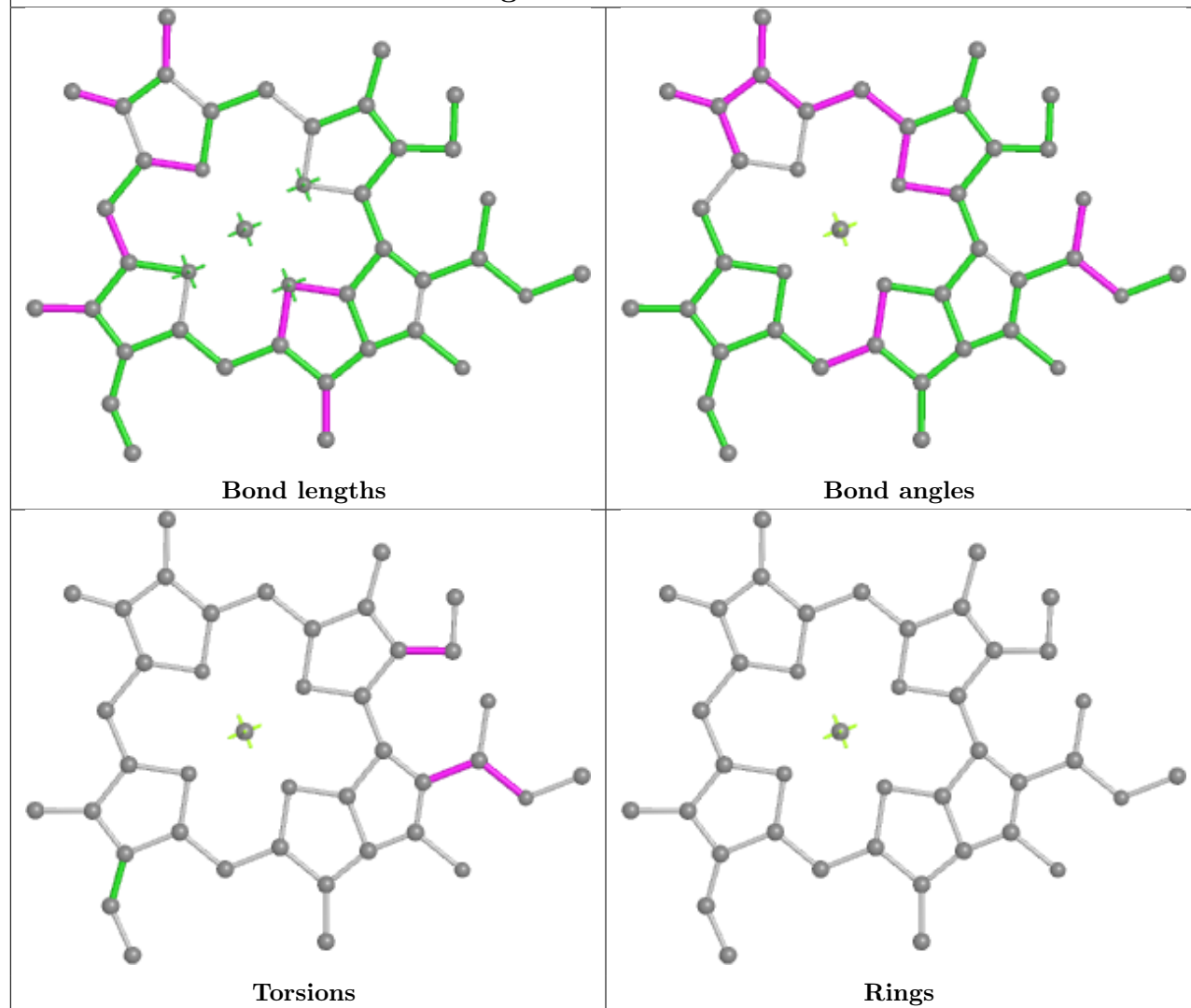
Torsions



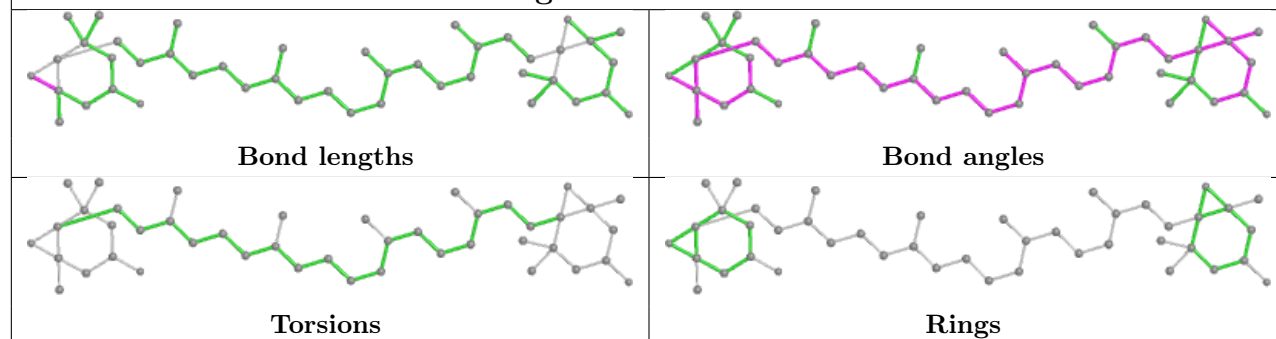
Rings

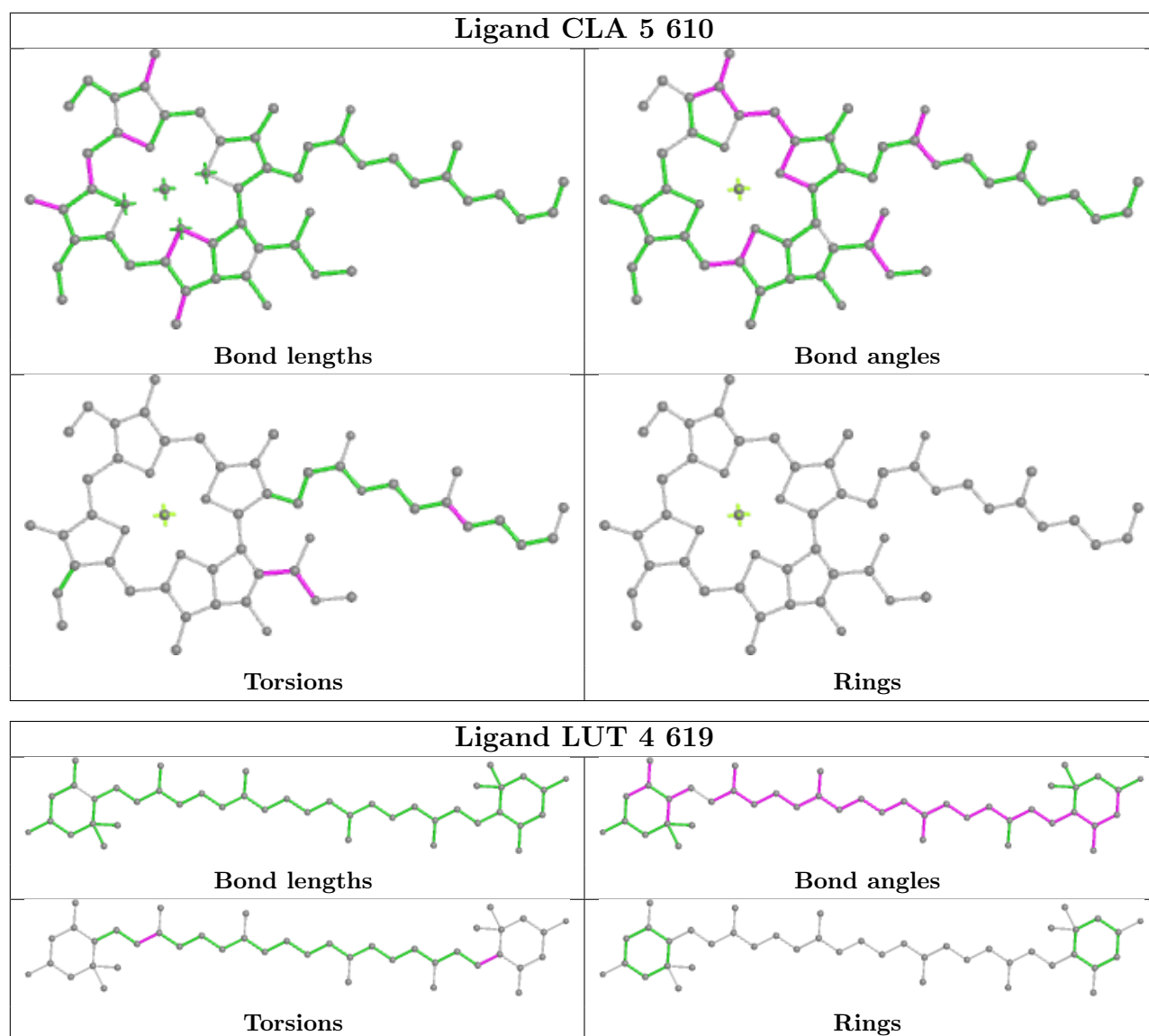


Ligand CLA 8 607

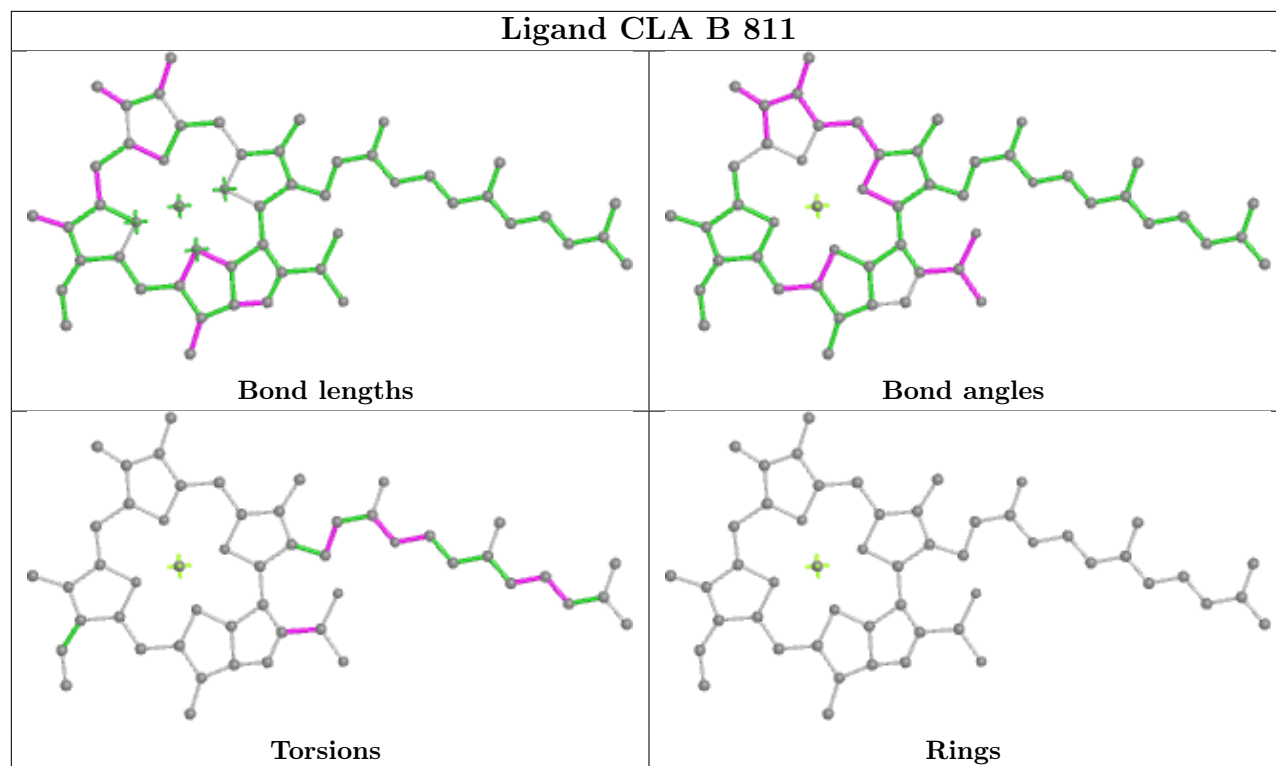


Ligand XAT 8 620

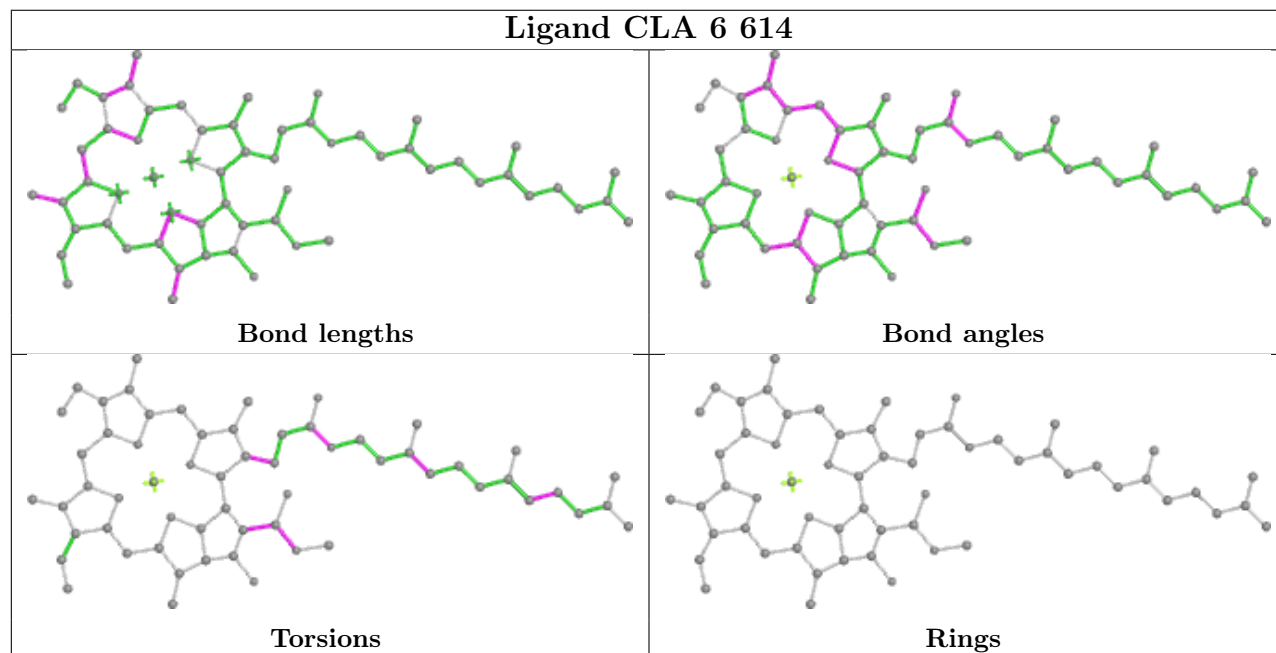




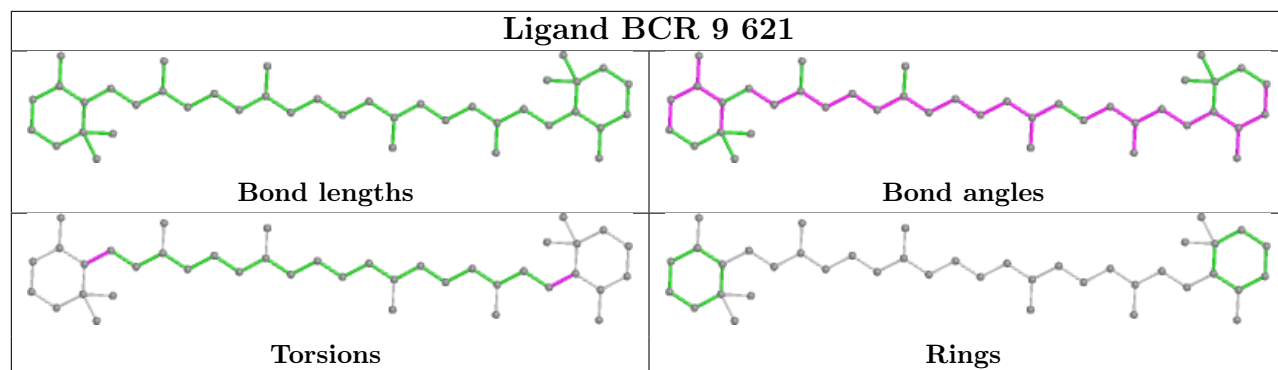
Ligand CLA B 811



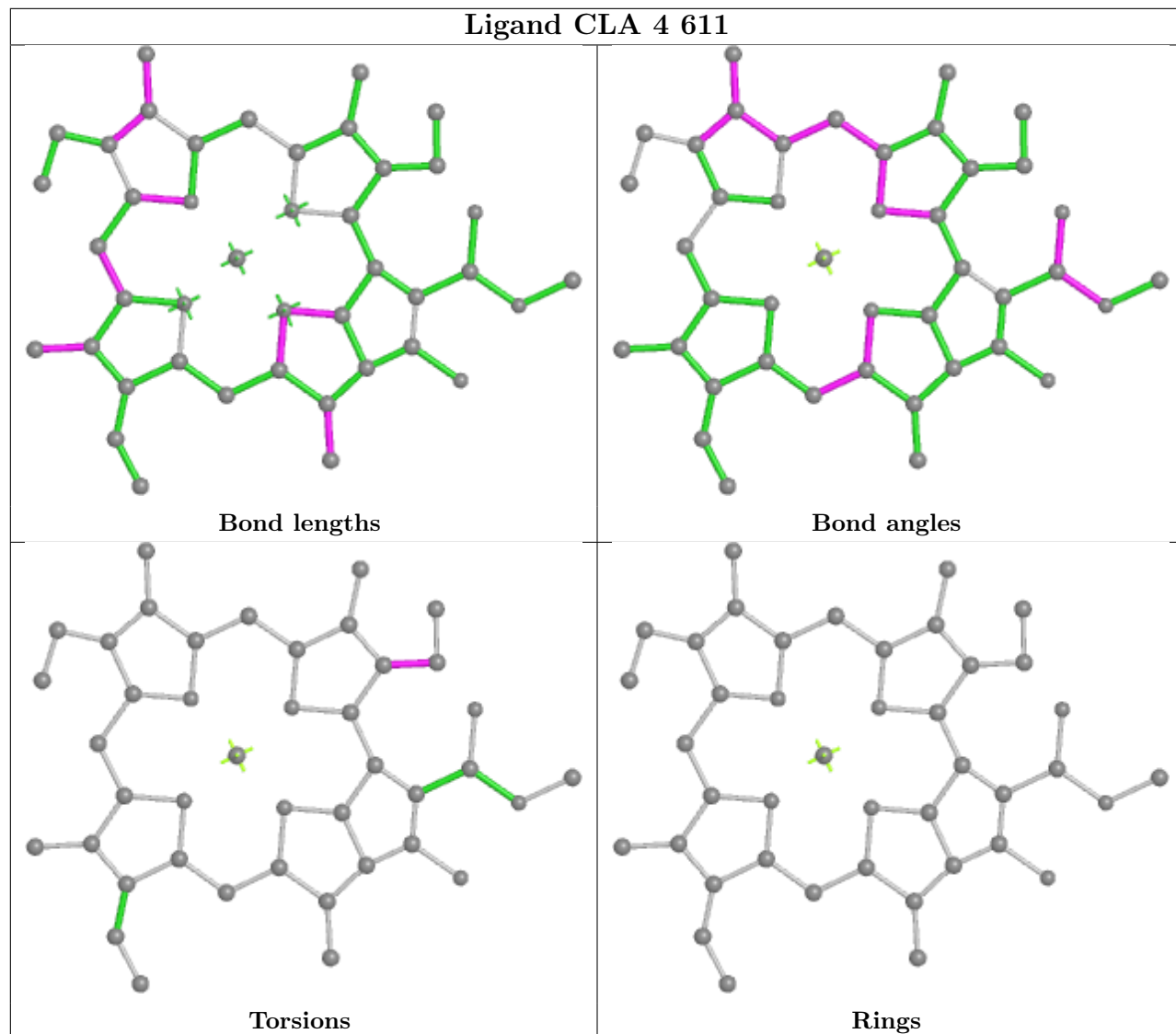
Ligand CLA 6 614

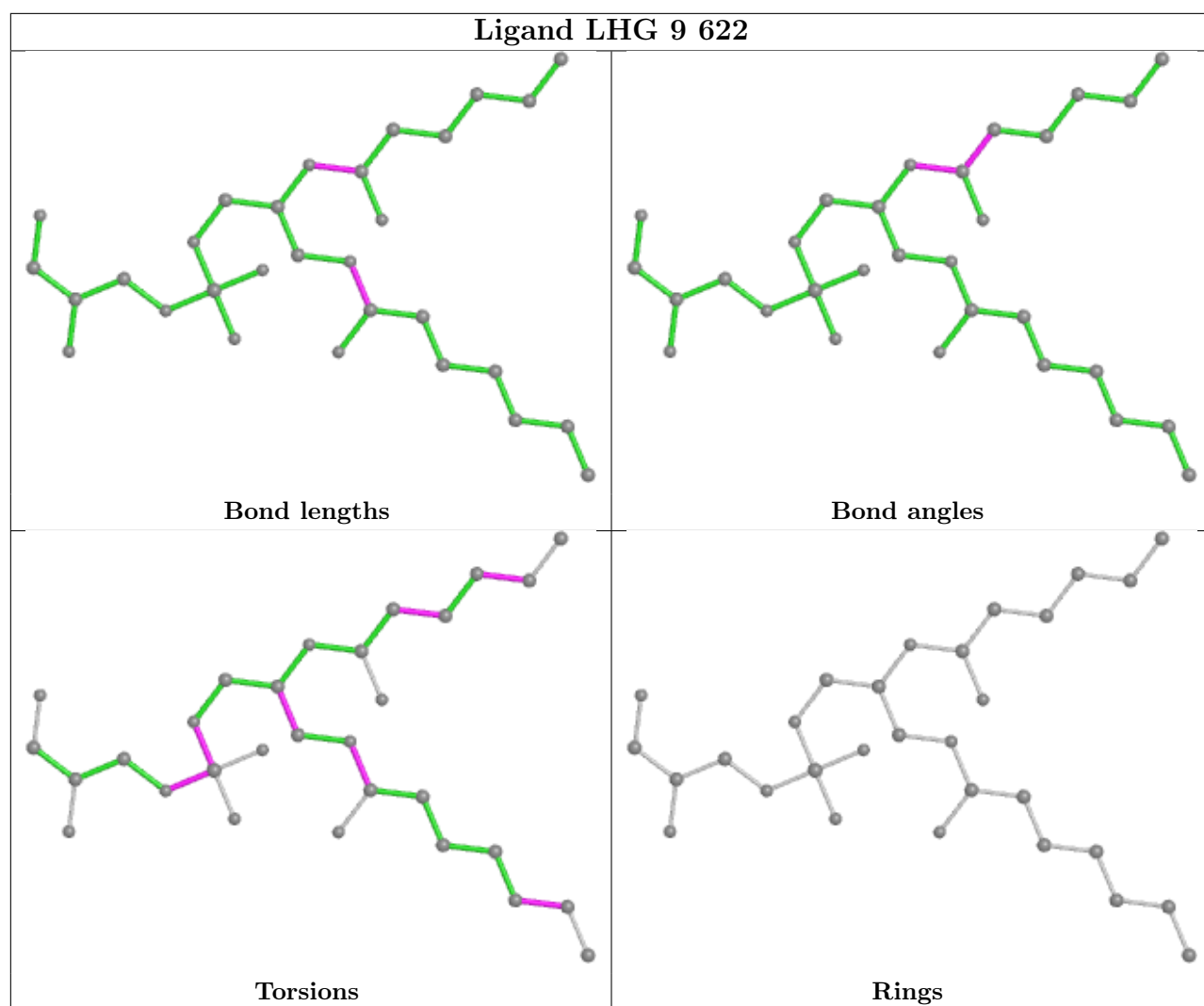


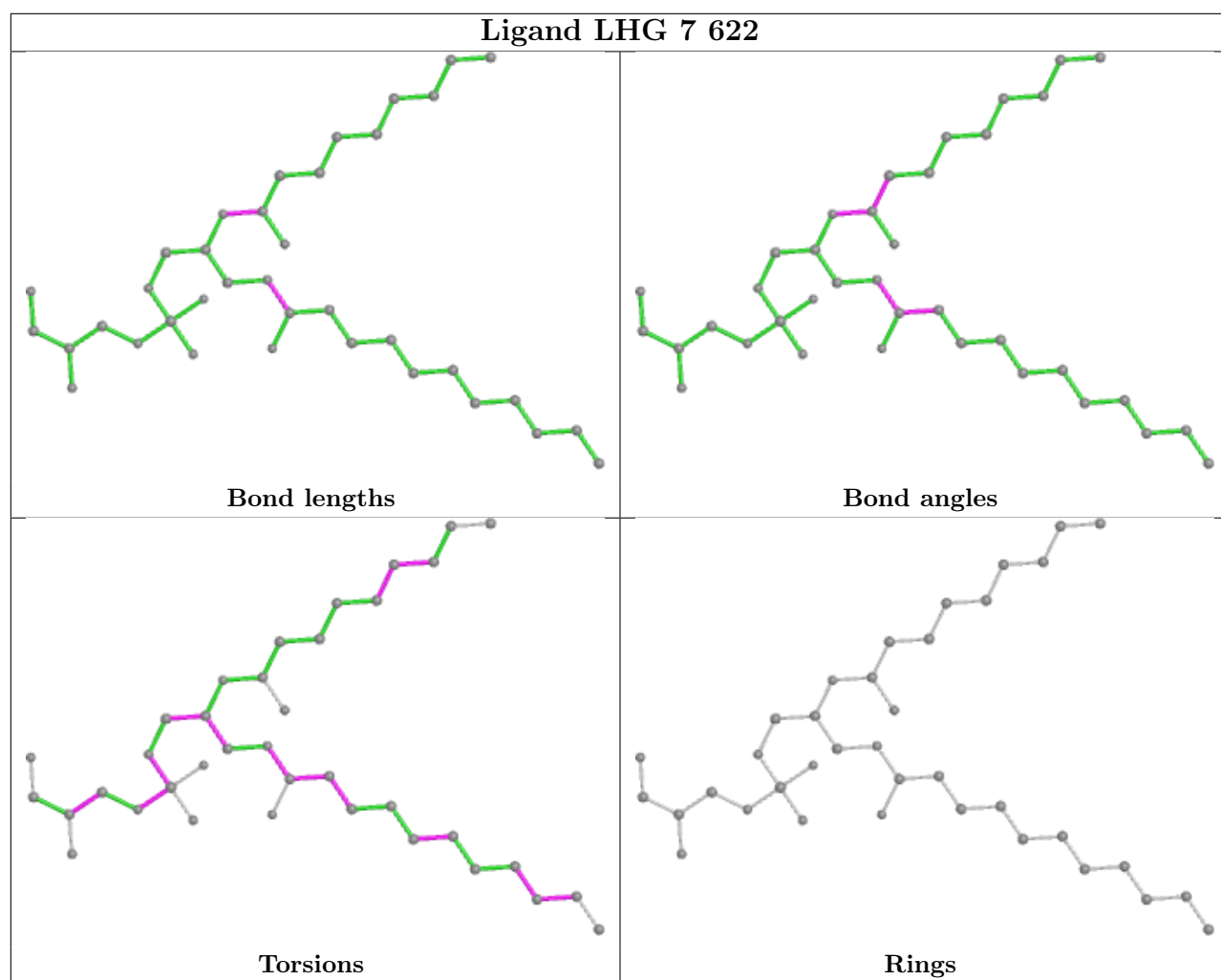
Ligand BCR 9 621



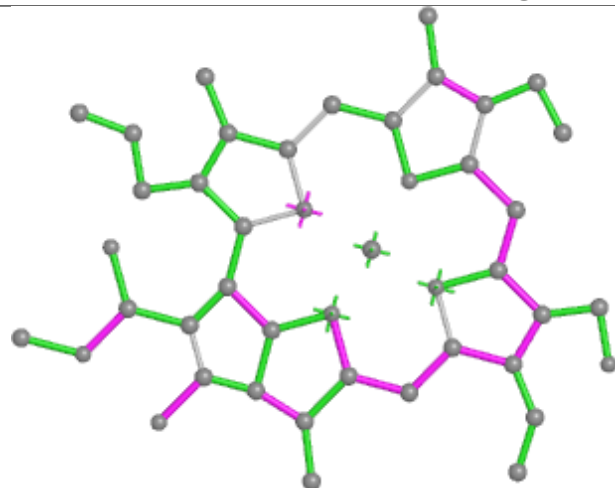
Ligand CLA 4 611



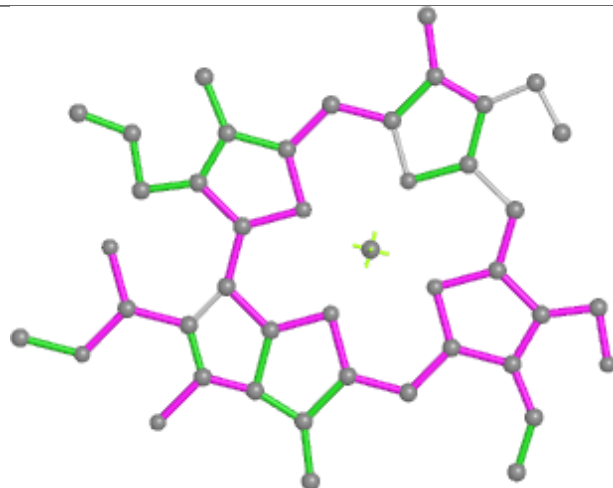




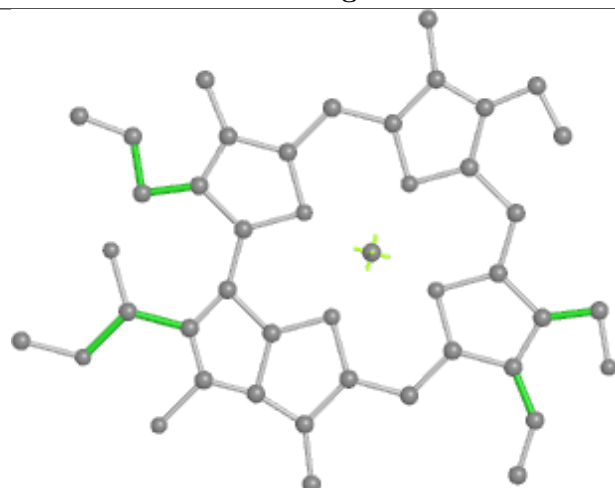
Ligand CHL X 606



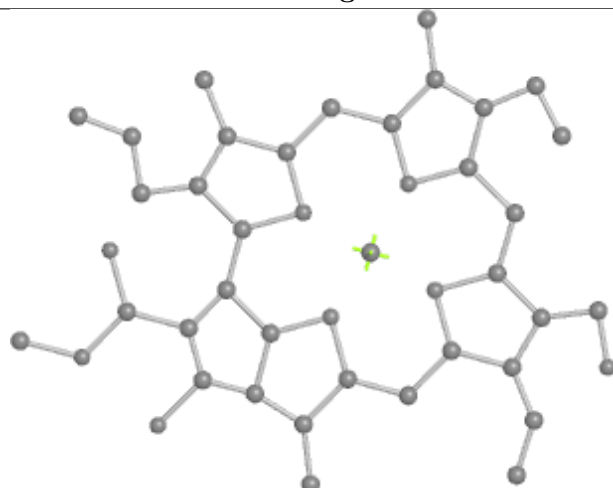
Bond lengths



Bond angles

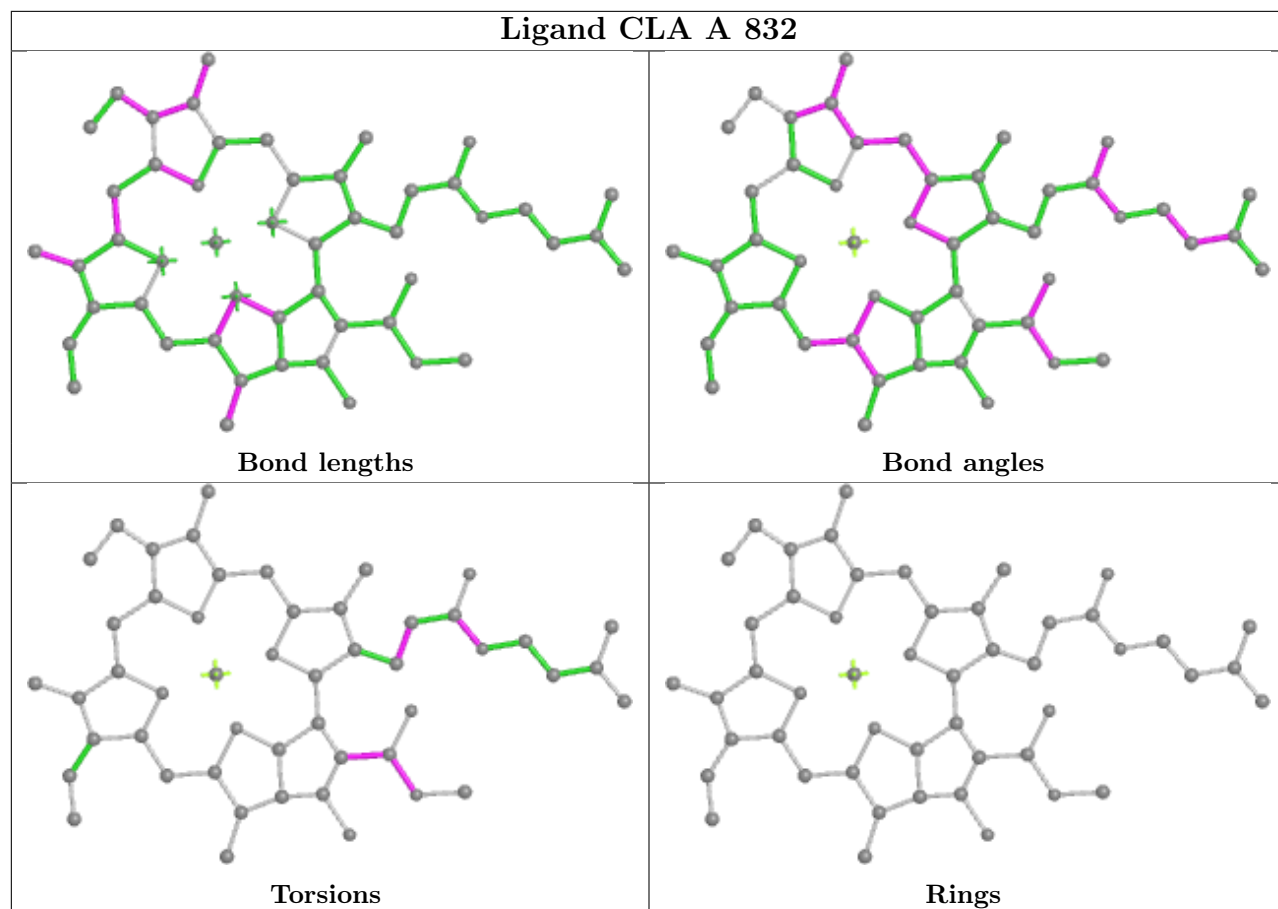


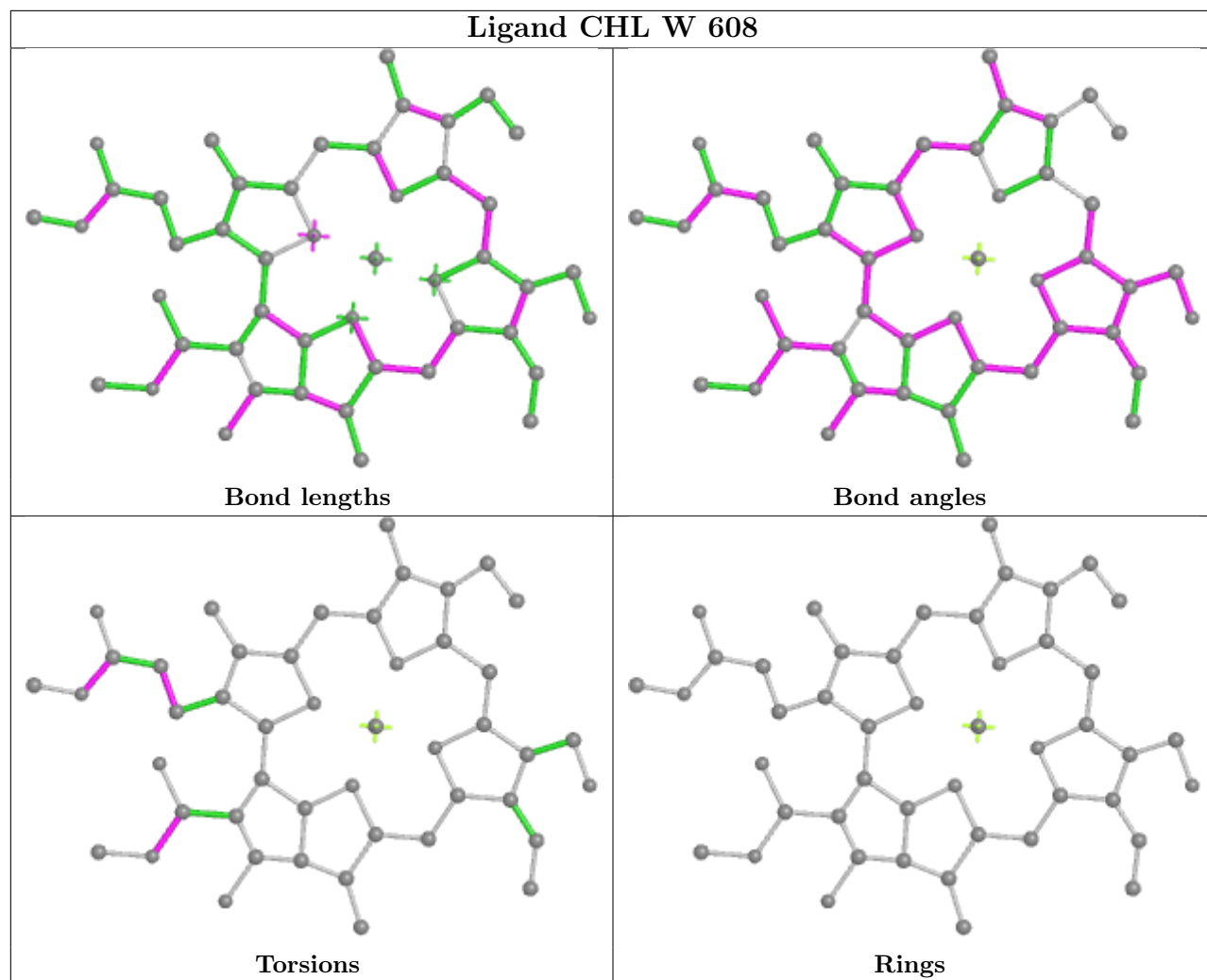
Torsions

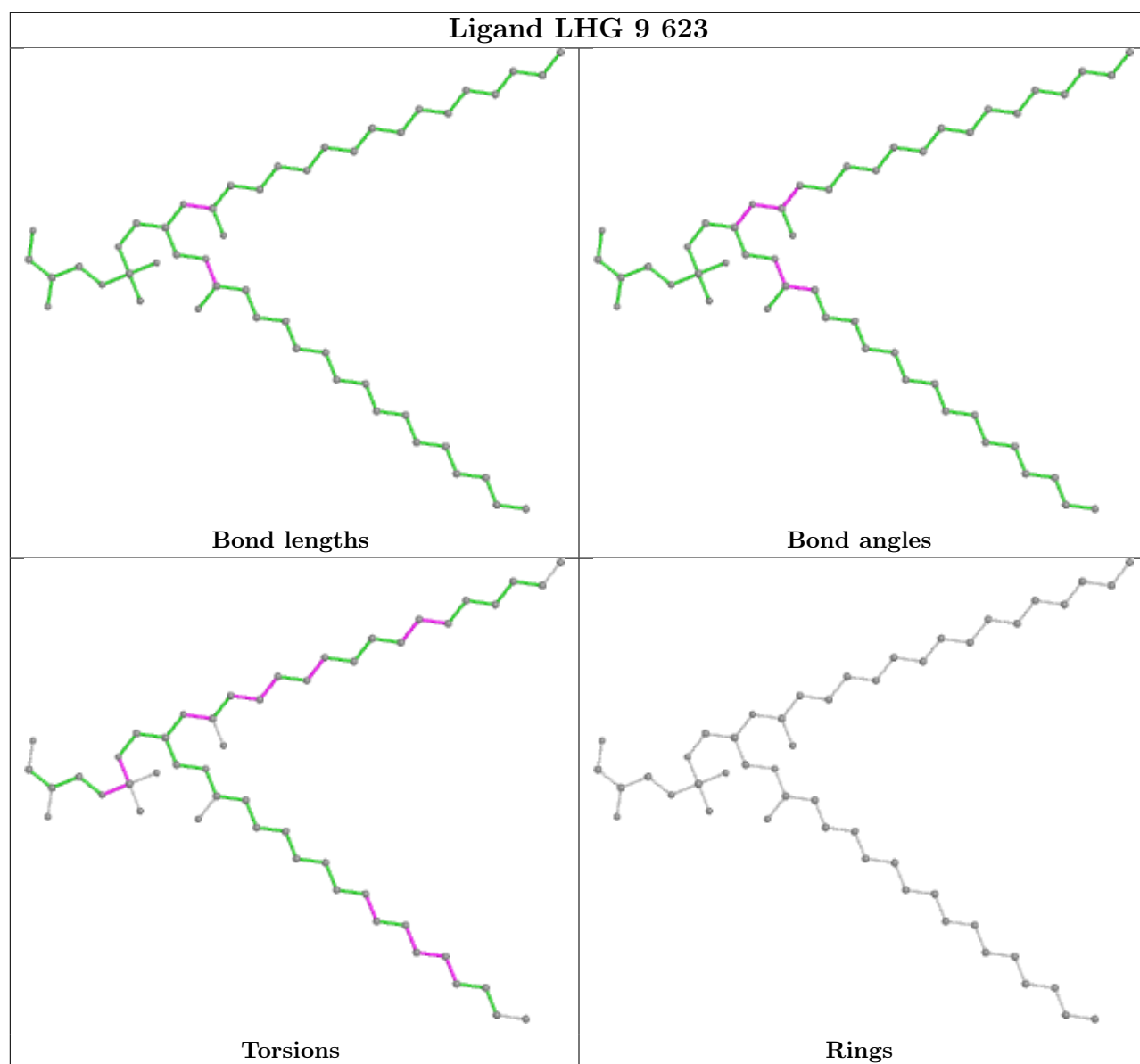


Rings

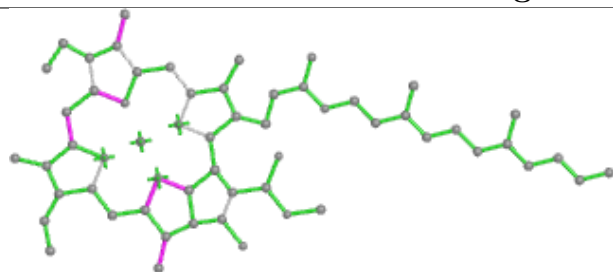
Ligand CLA A 832



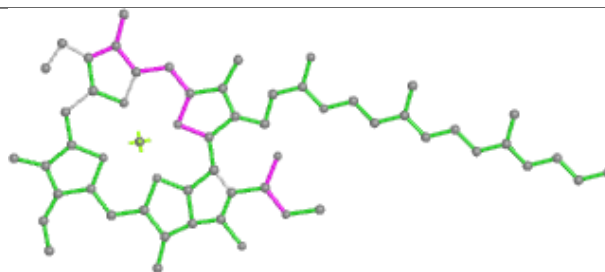




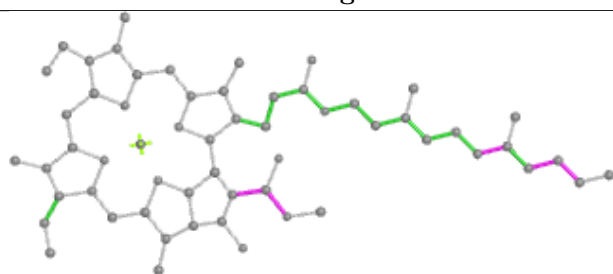
Ligand CLA Y 602



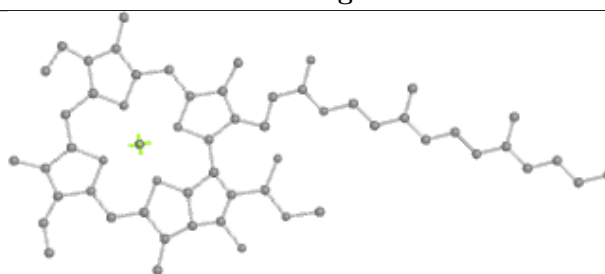
Bond lengths



Bond angles

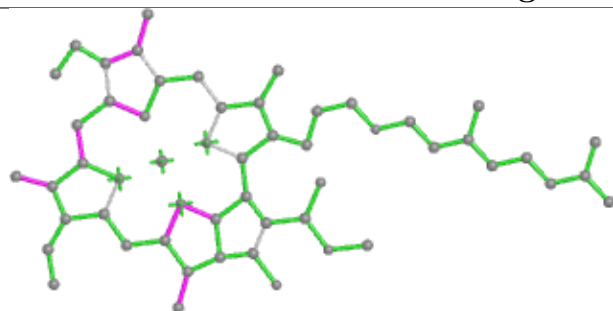


Torsions

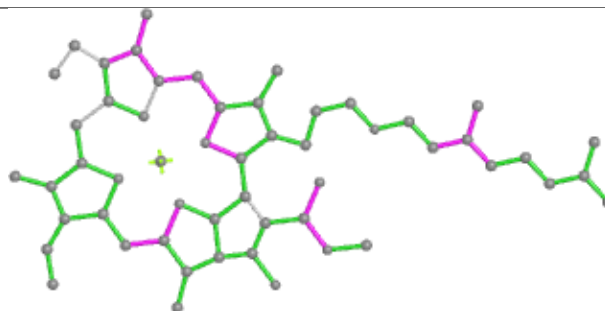


Rings

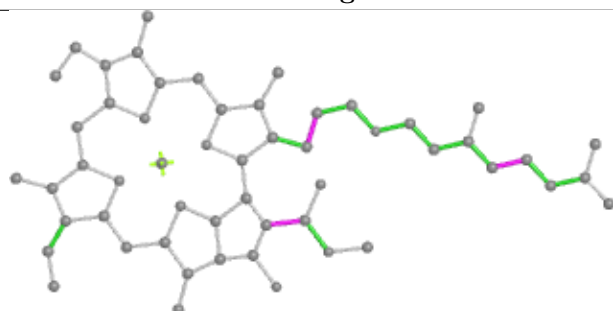
Ligand CLA a 603



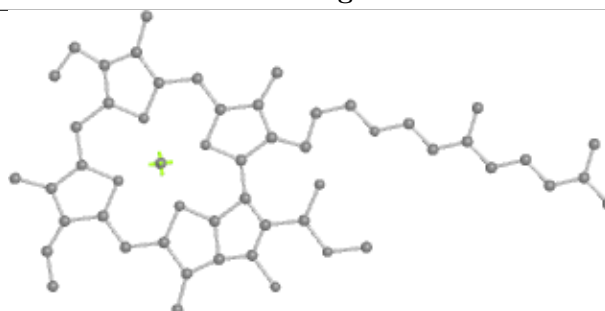
Bond lengths



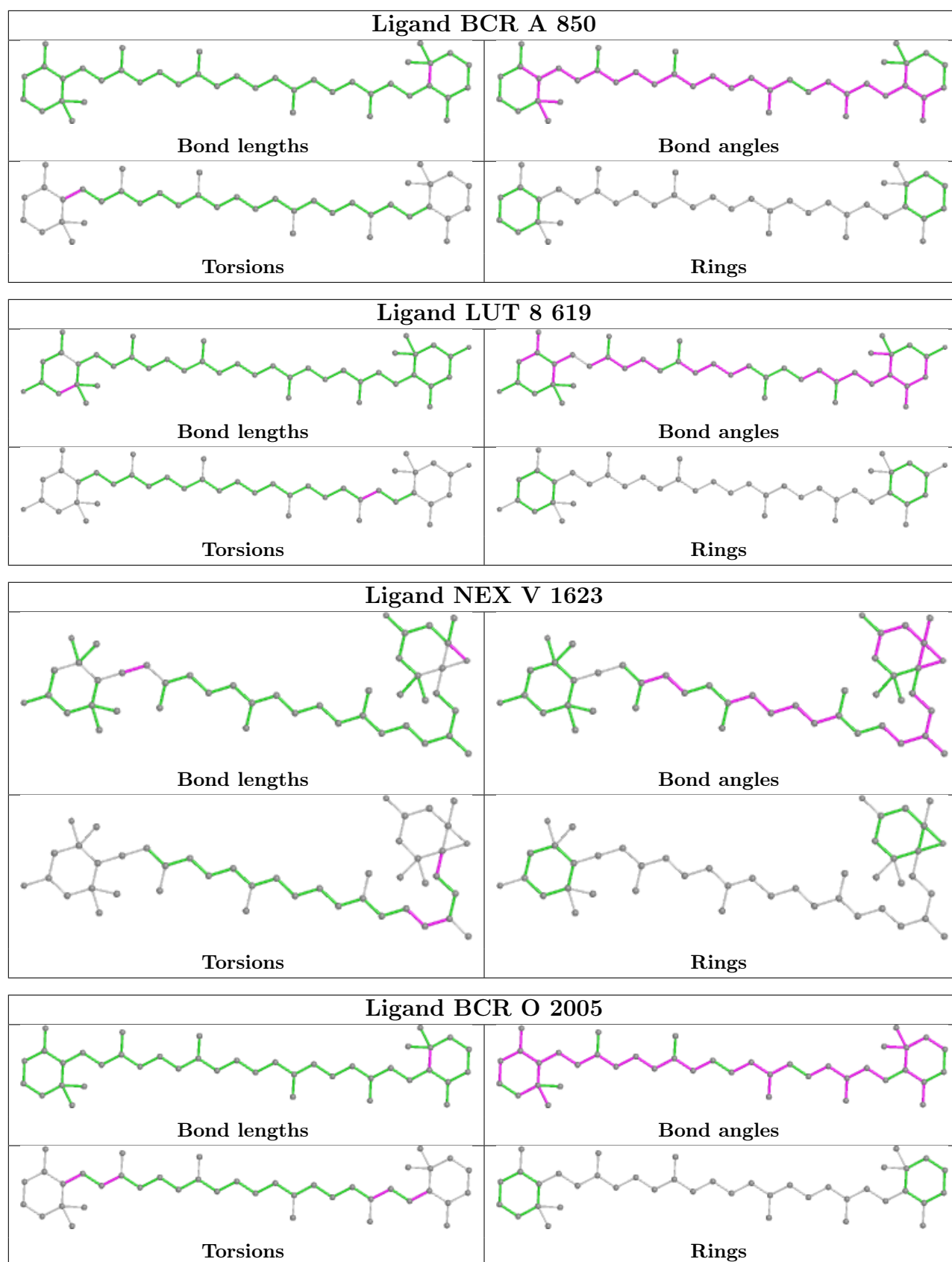
Bond angles



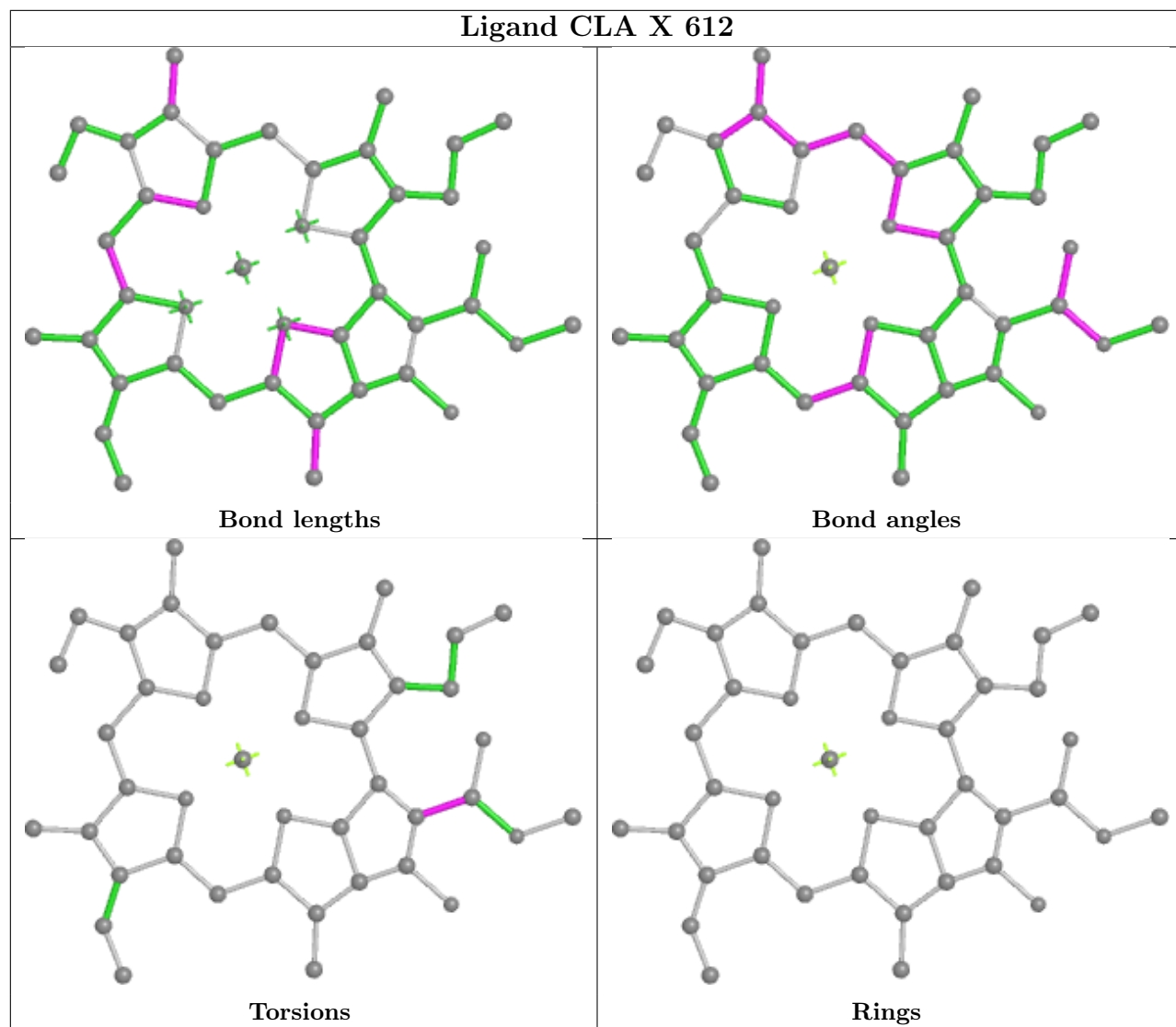
Torsions

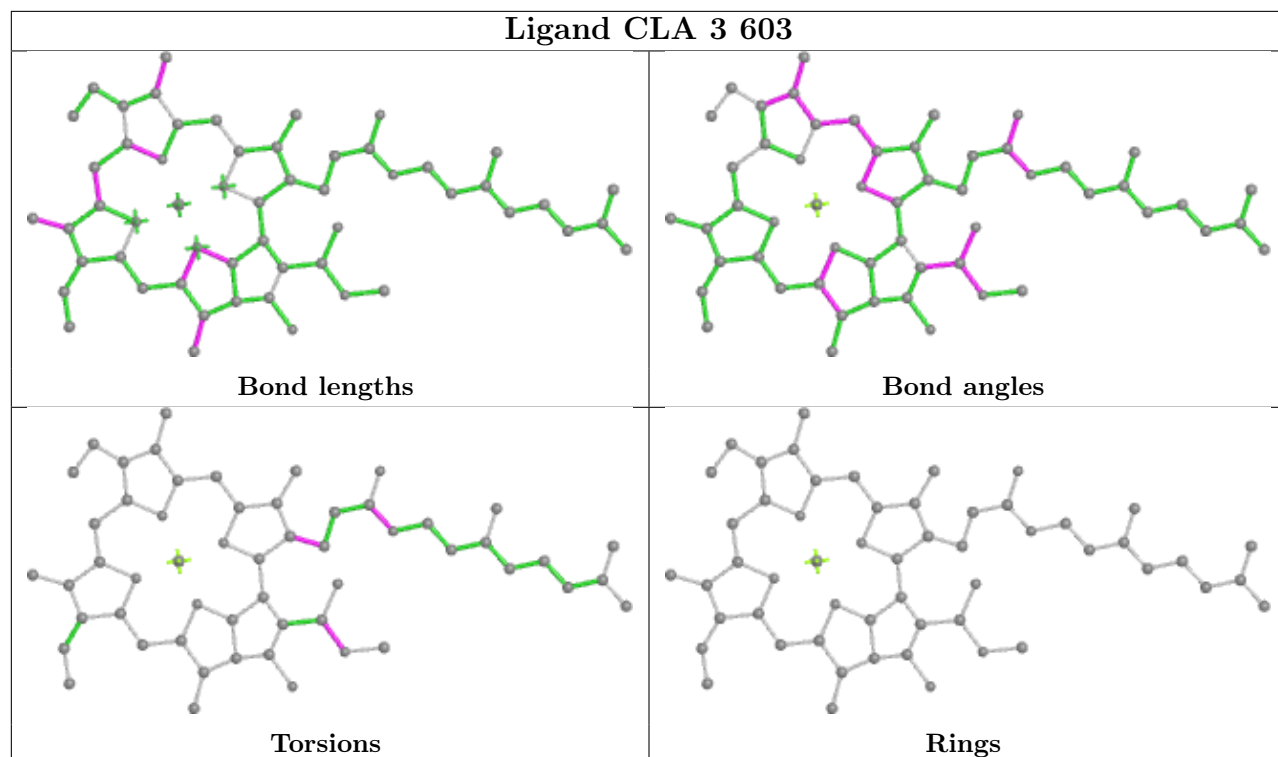
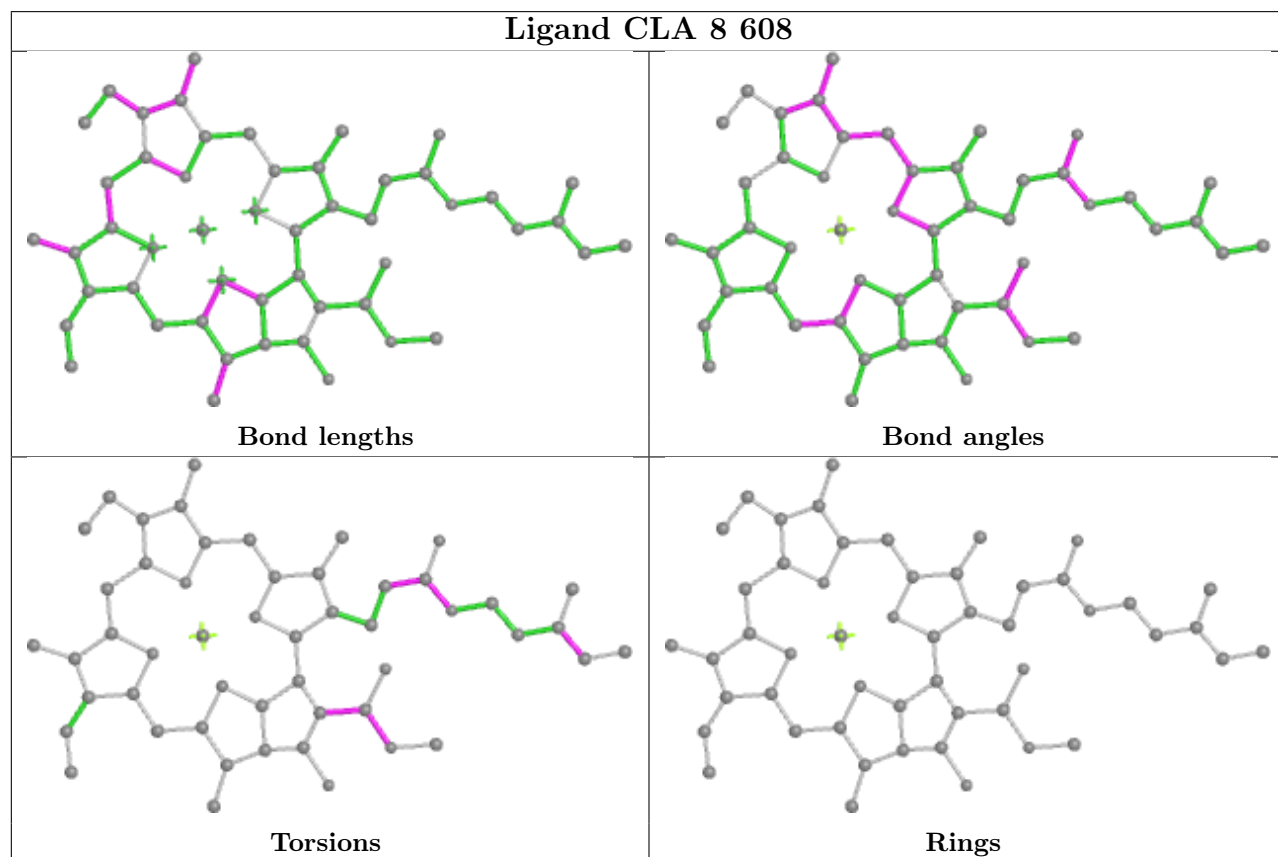


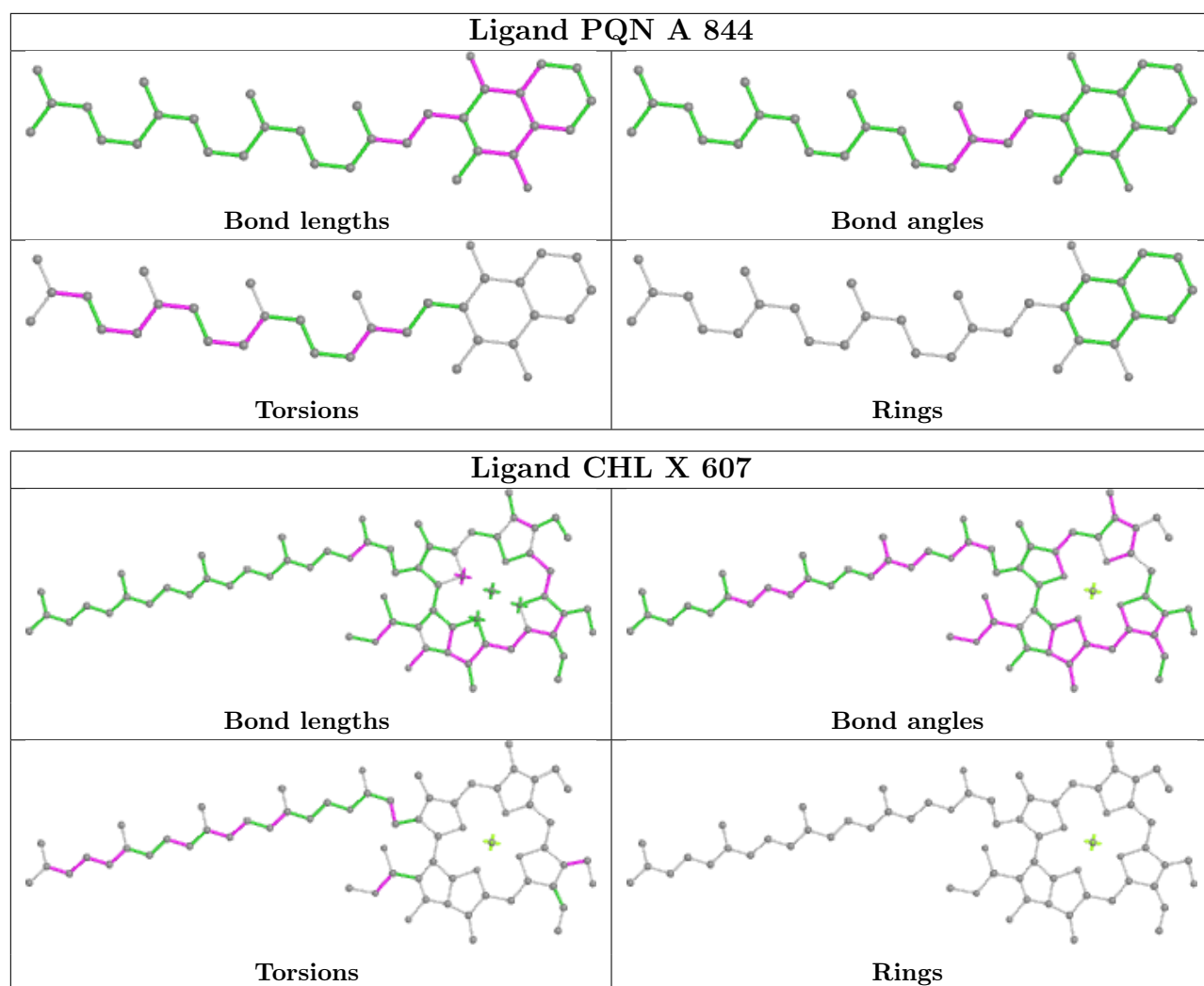
Rings



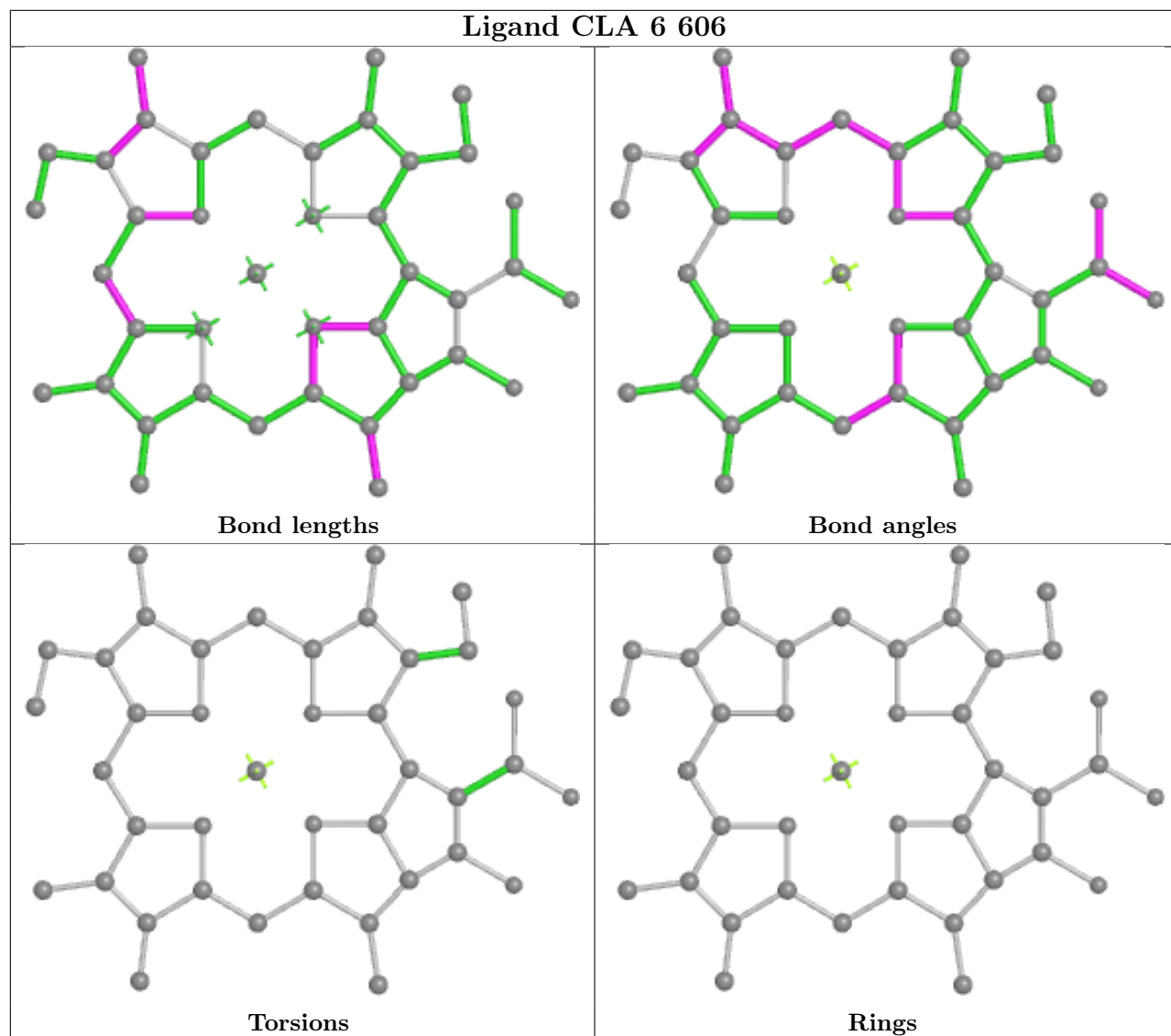
Ligand CLA X 612



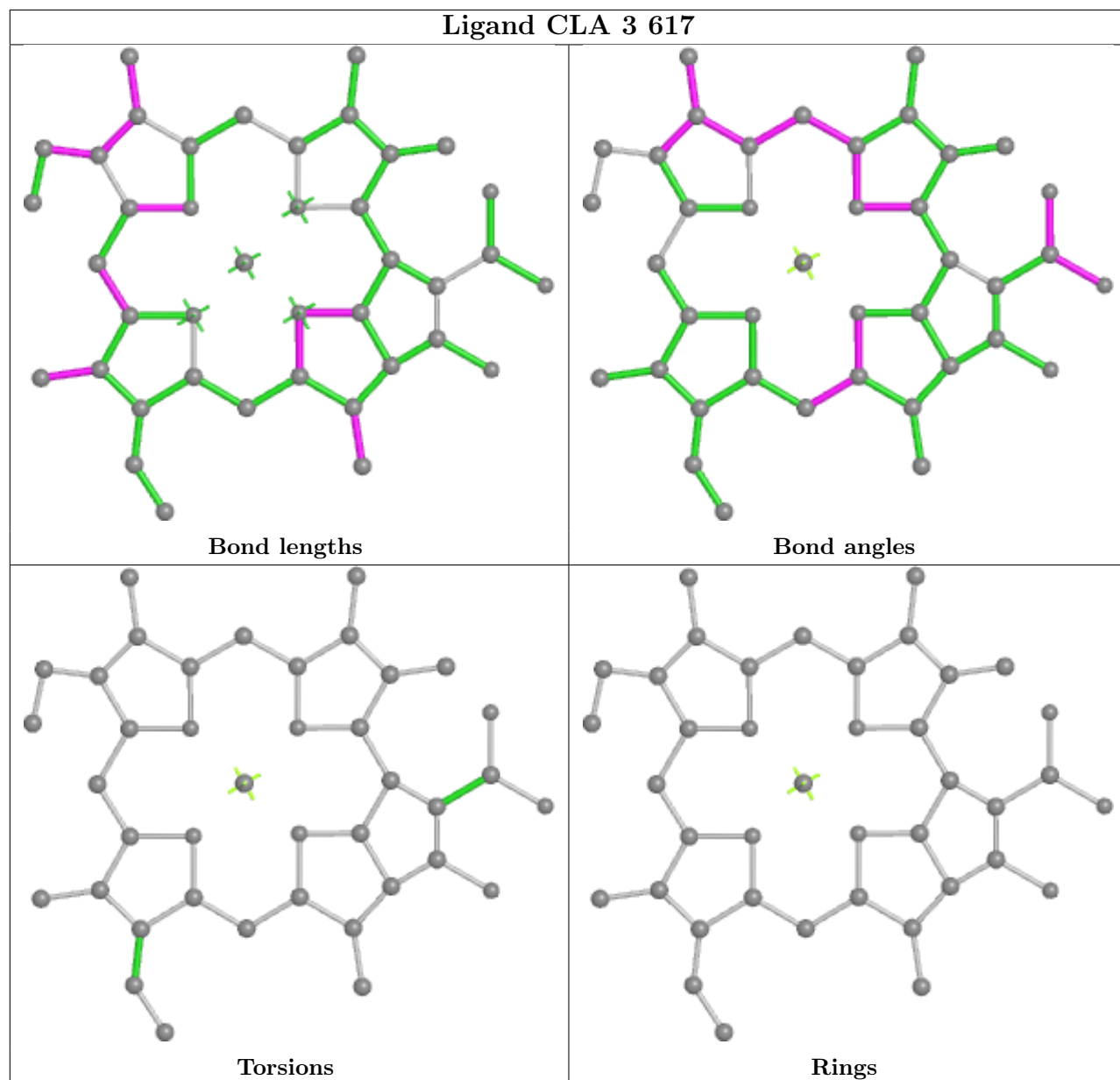
Ligand CLA 3 603**Ligand CLA 8 608**

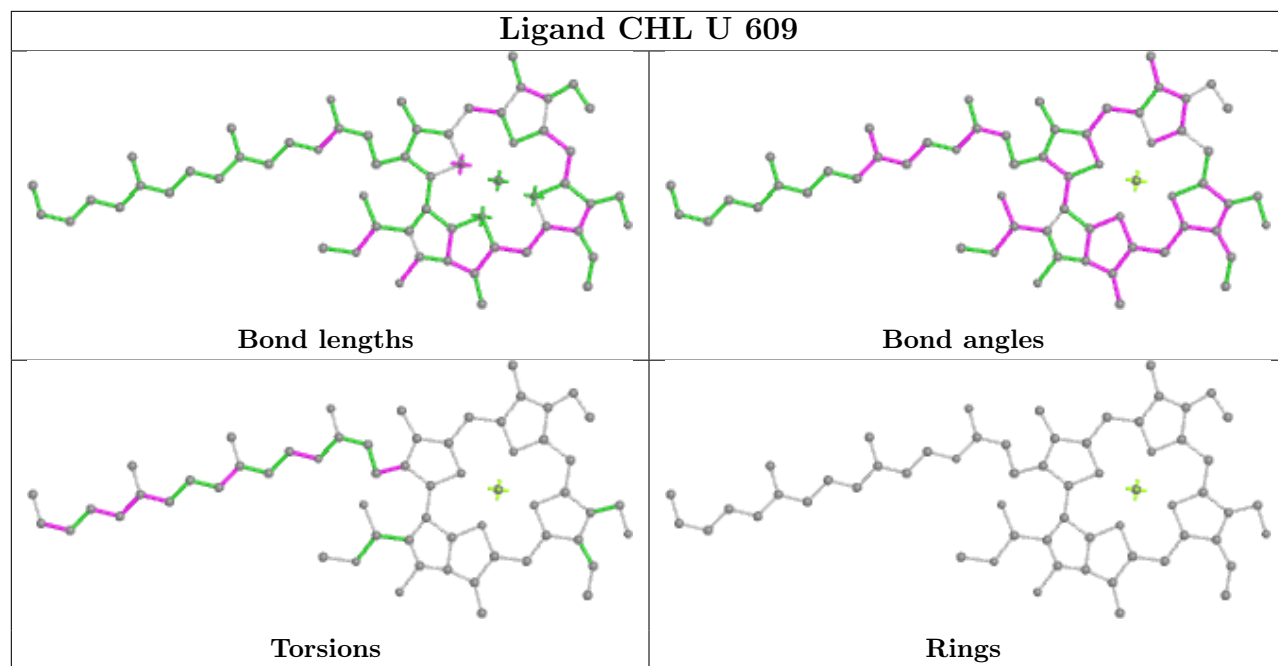


Ligand CLA 6 606

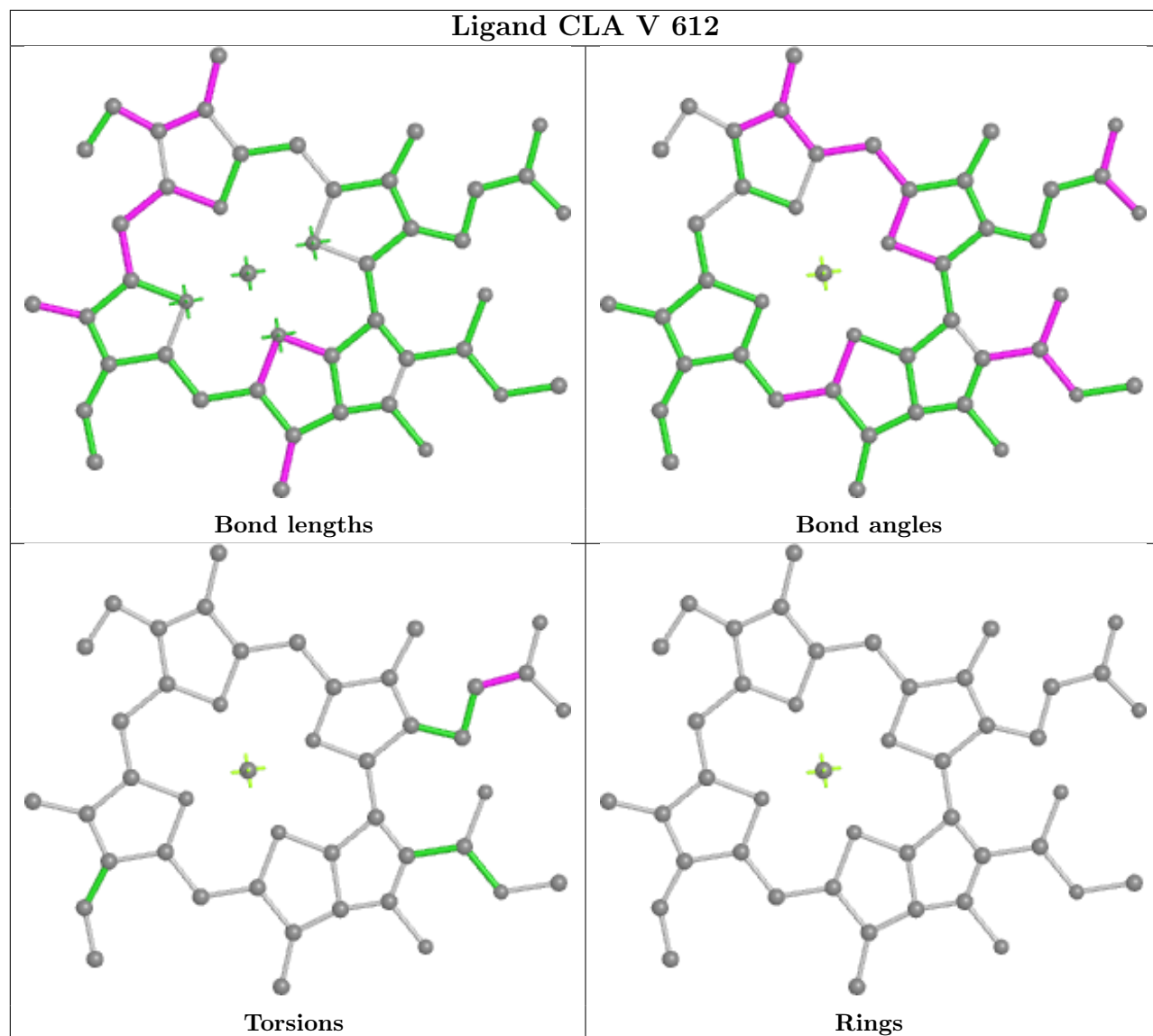


Ligand CLA 3 617

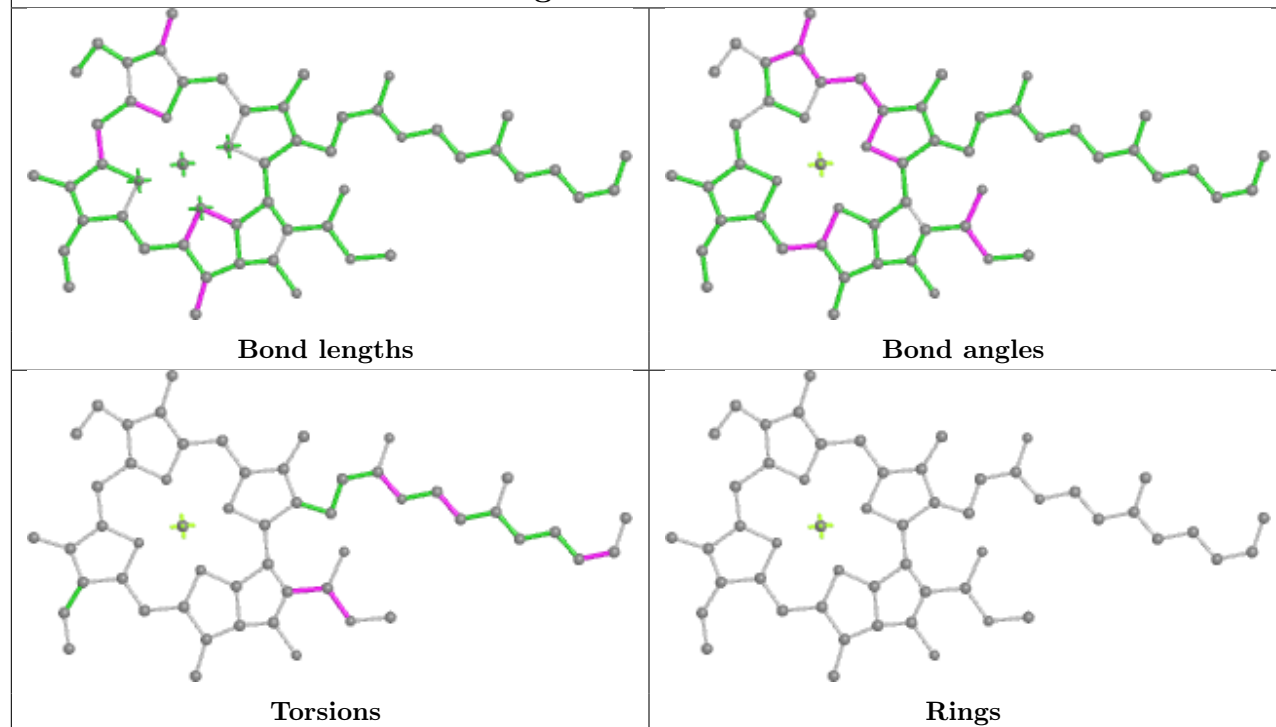




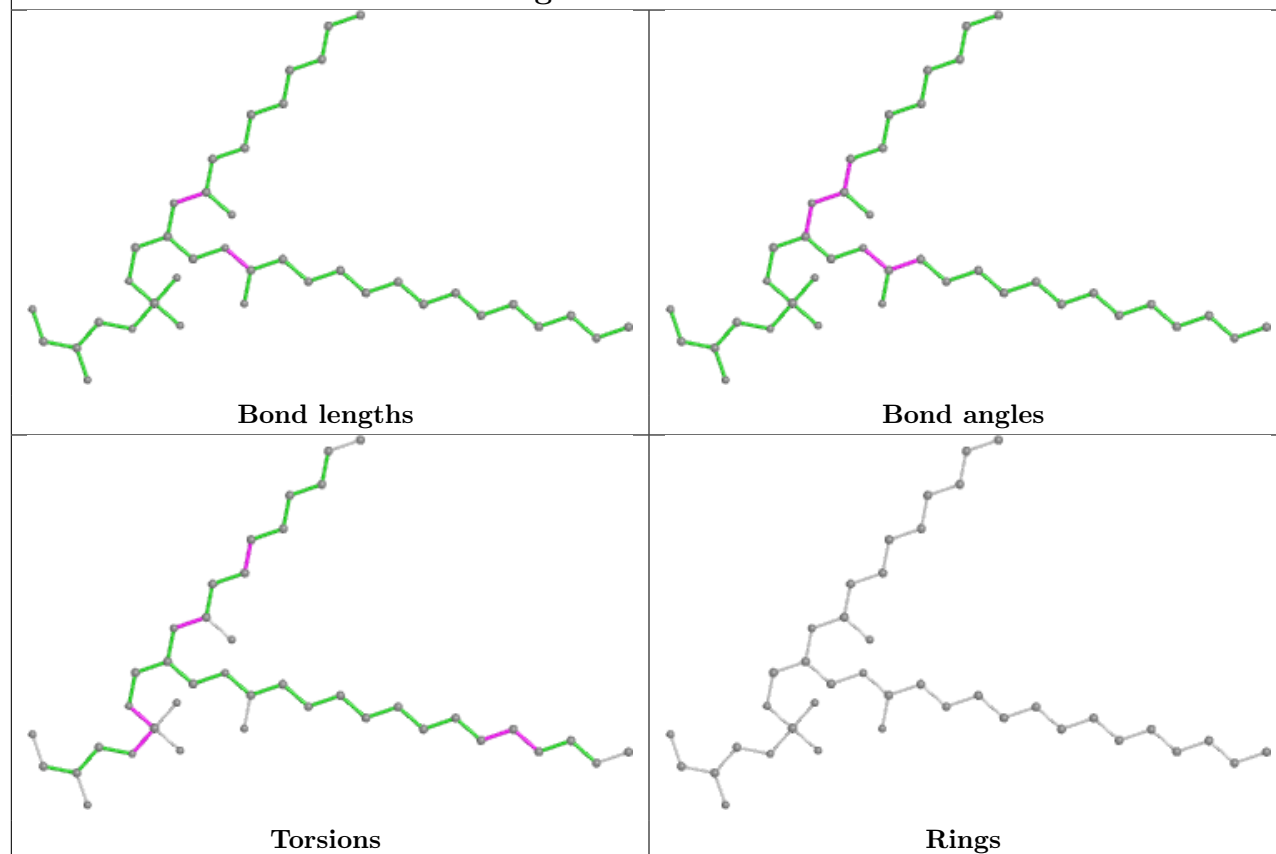
Ligand CLA V 612

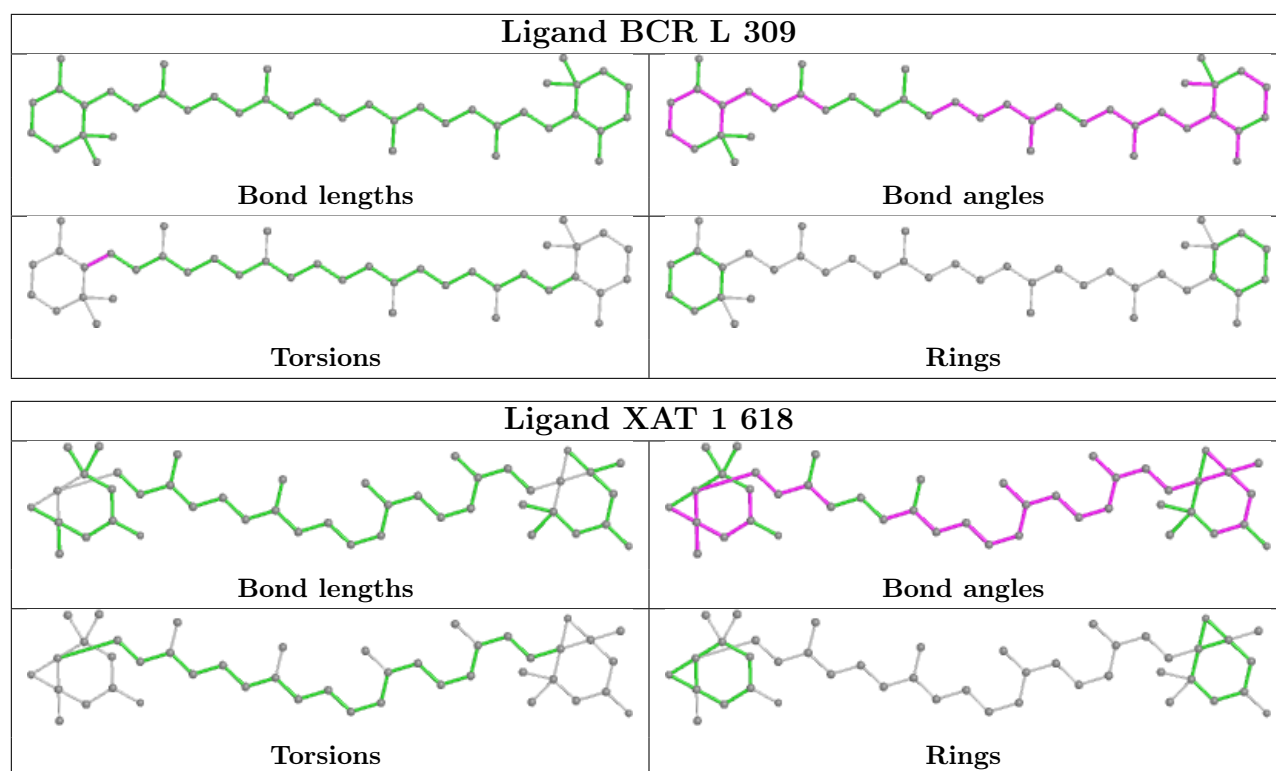


Ligand CLA Z 614

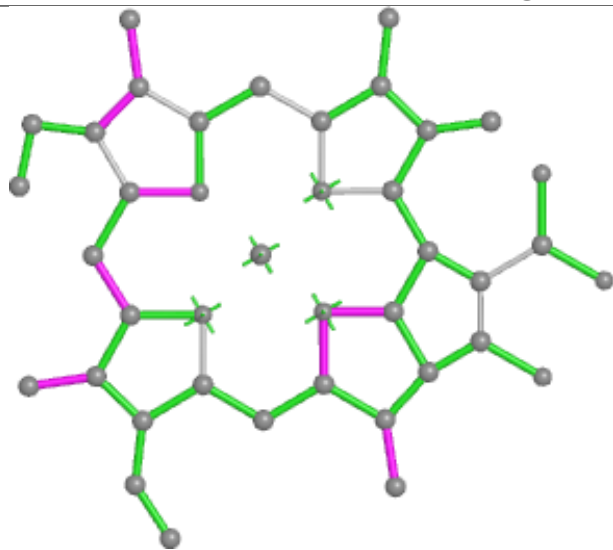


Ligand LHG 8 623

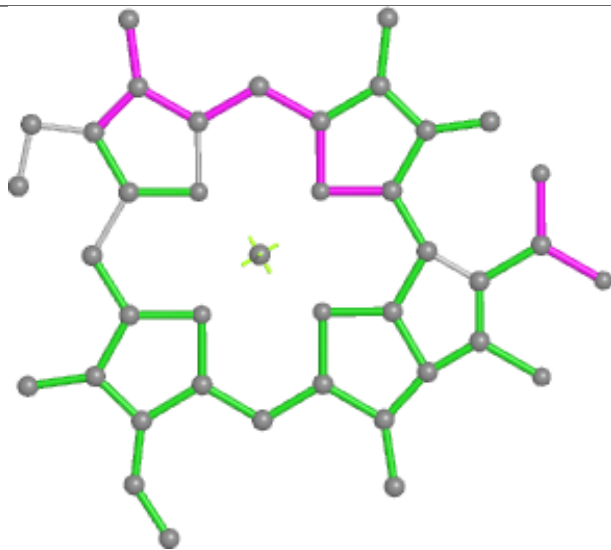




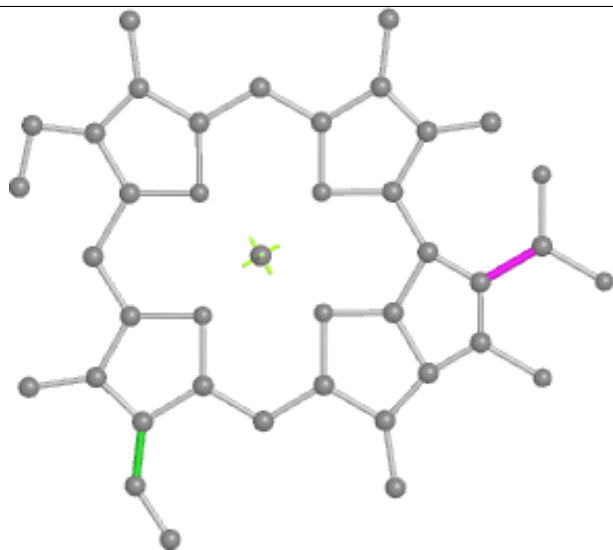
Ligand CLA 3 614



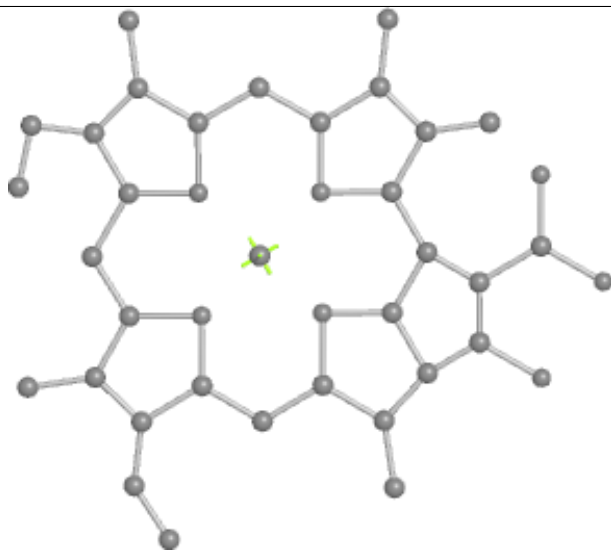
Bond lengths



Bond angles

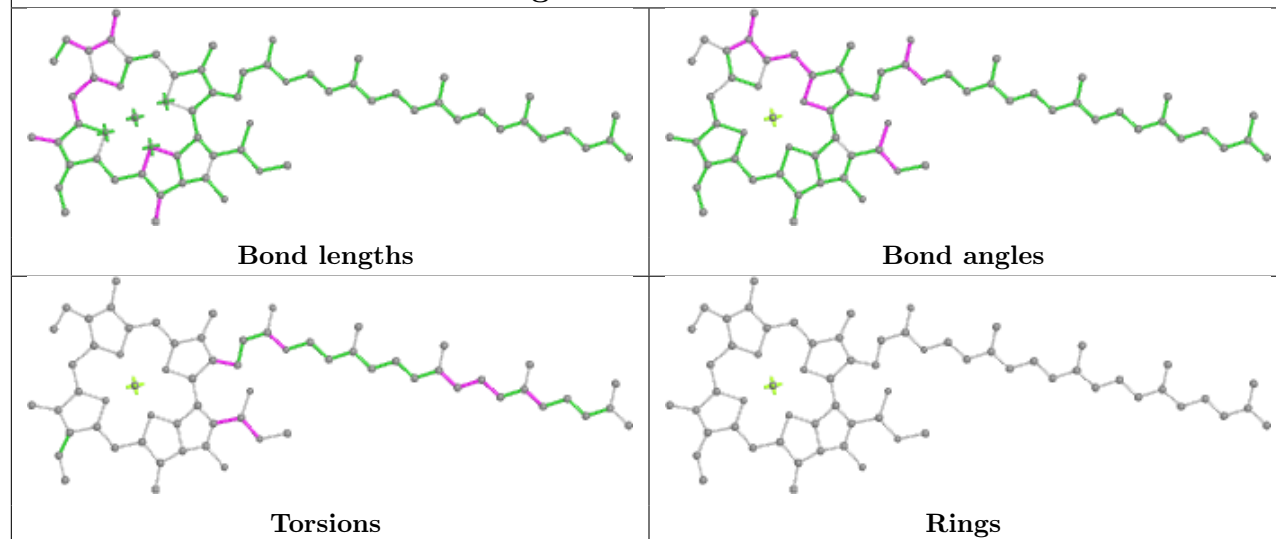


Torsions

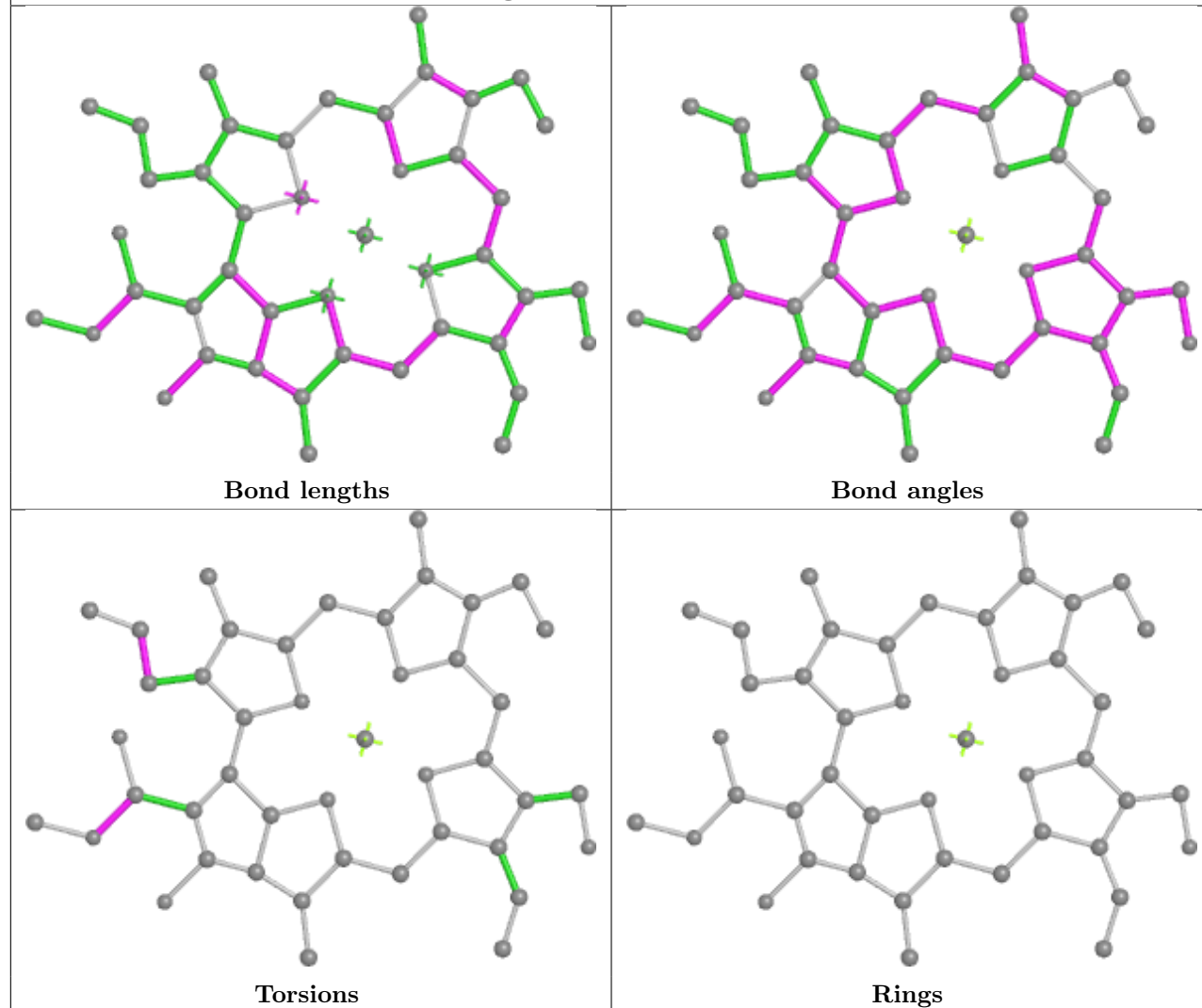


Rings

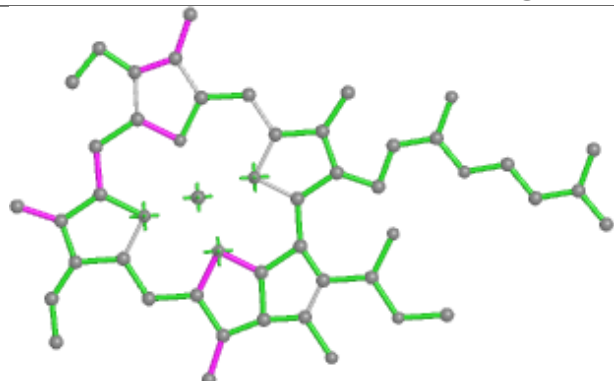
Ligand CLA A 831



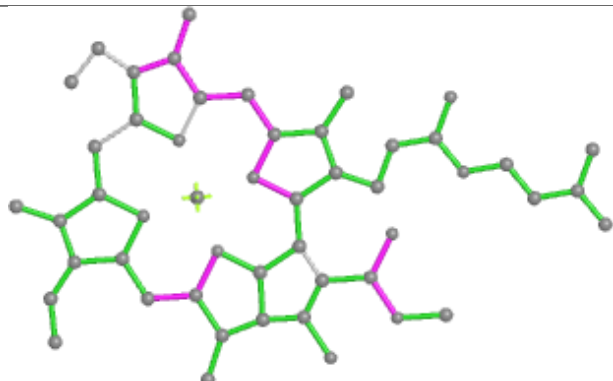
Ligand CHL U 608



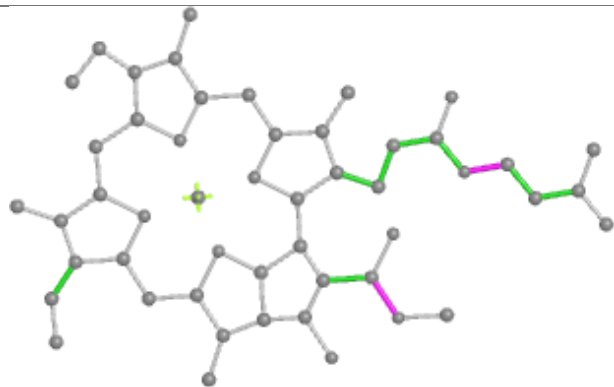
Ligand CLA 7 608



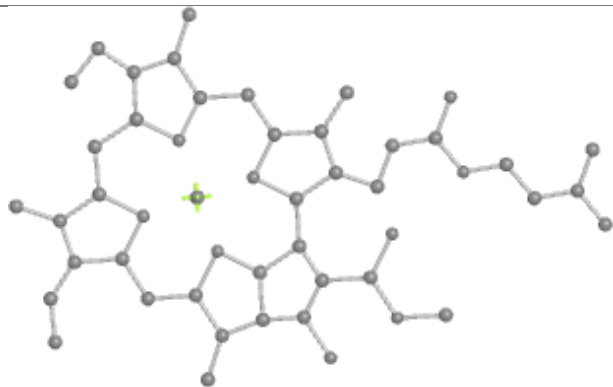
Bond lengths



Bond angles

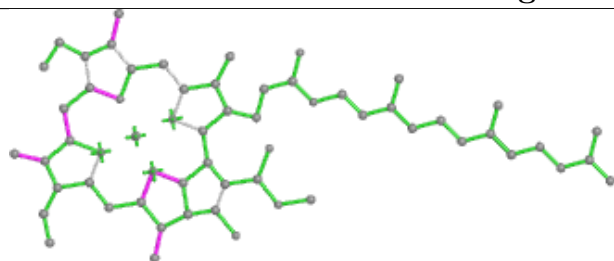


Torsions

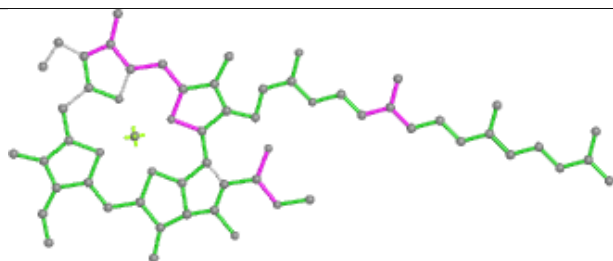


Rings

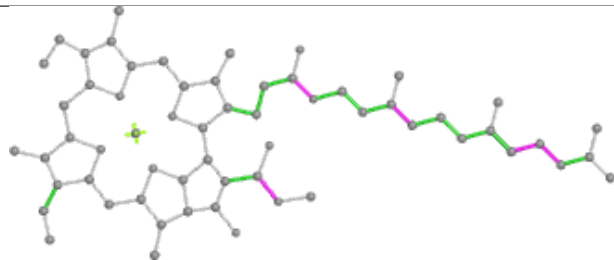
Ligand CLA 8 610



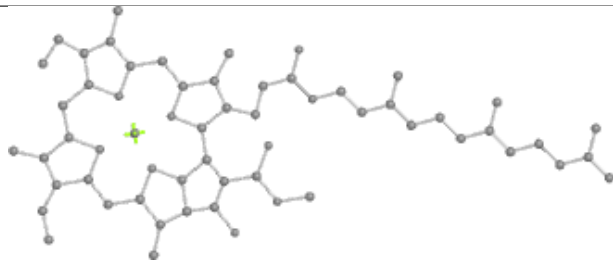
Bond lengths



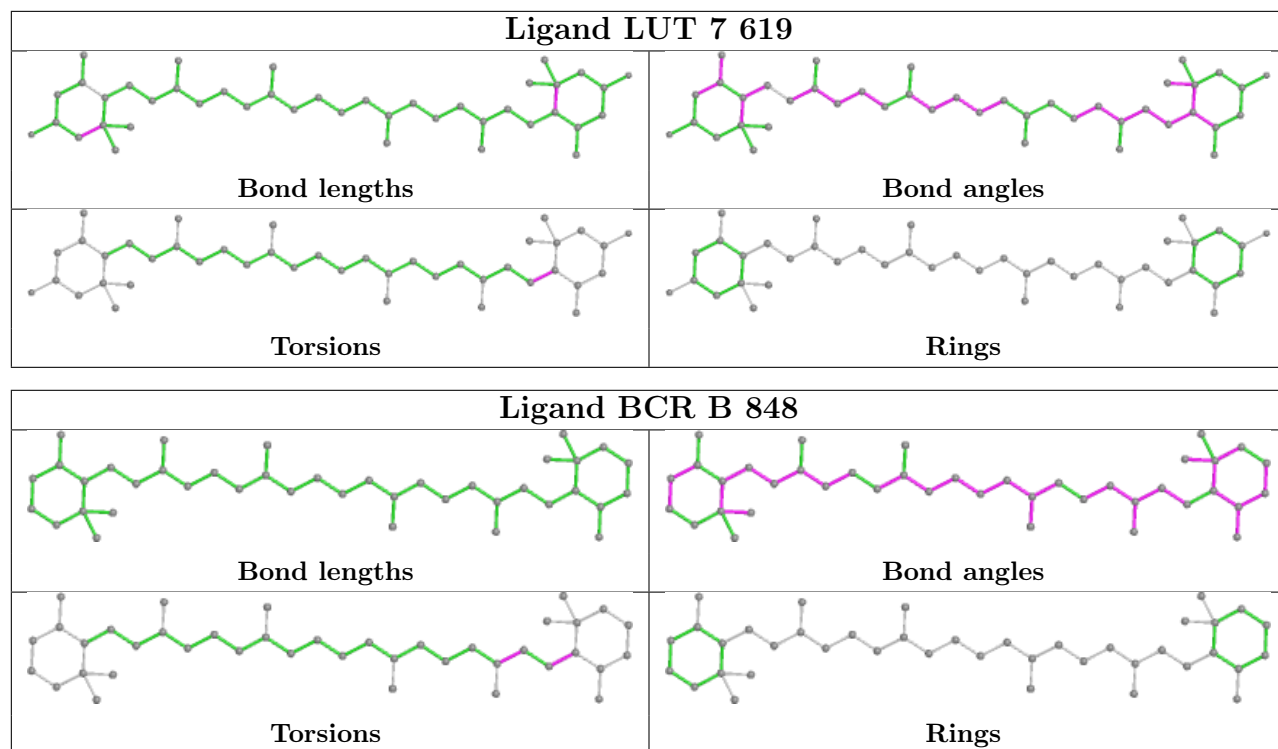
Bond angles



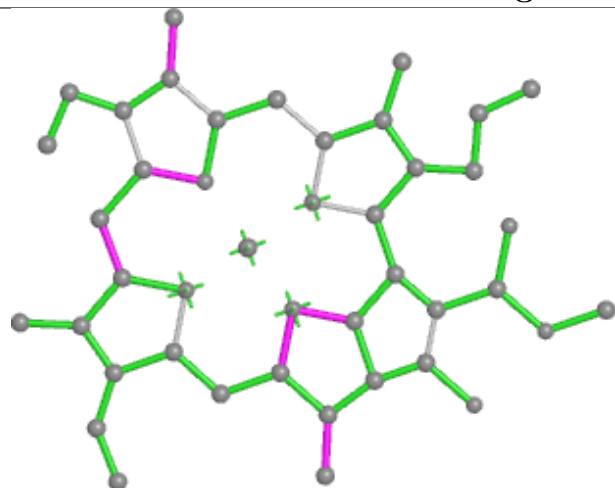
Torsions



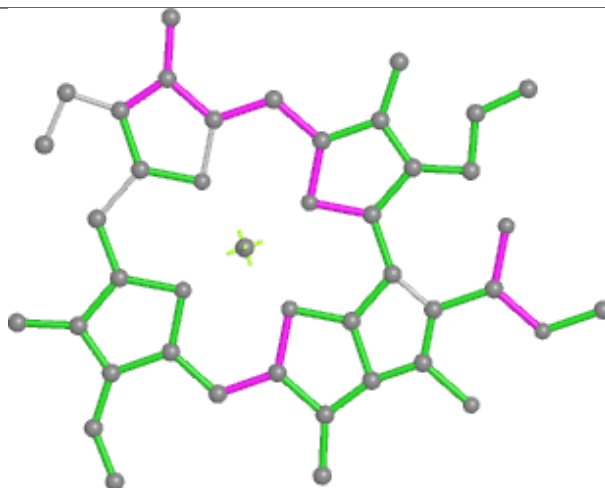
Rings



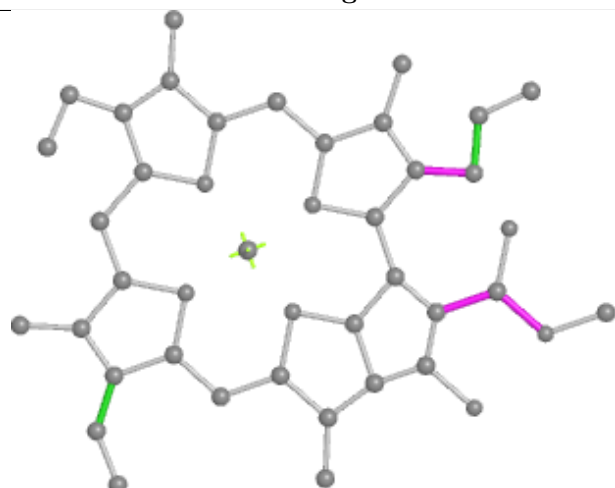
Ligand CLA Y 611



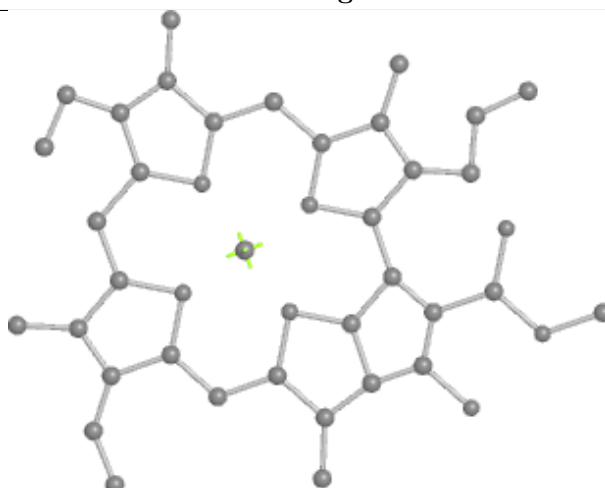
Bond lengths



Bond angles

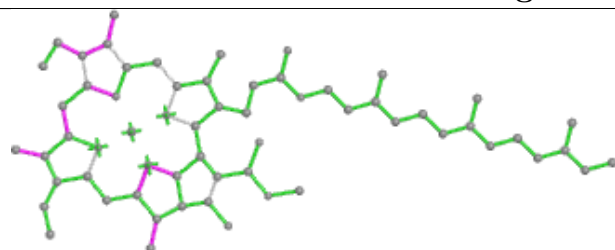


Torsions

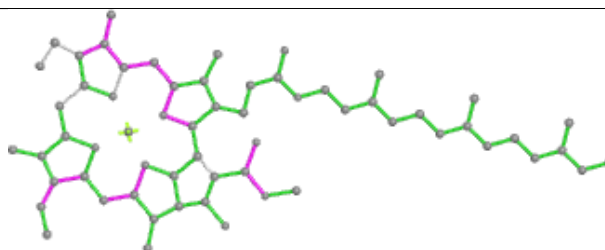


Rings

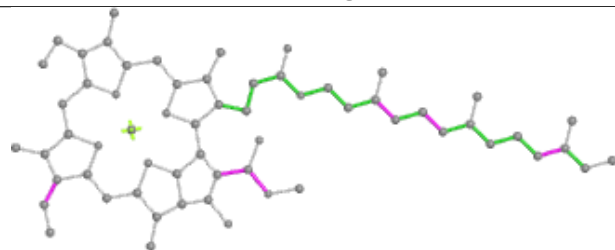
Ligand CLA A 835



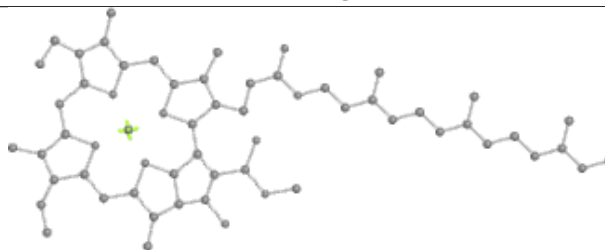
Bond lengths



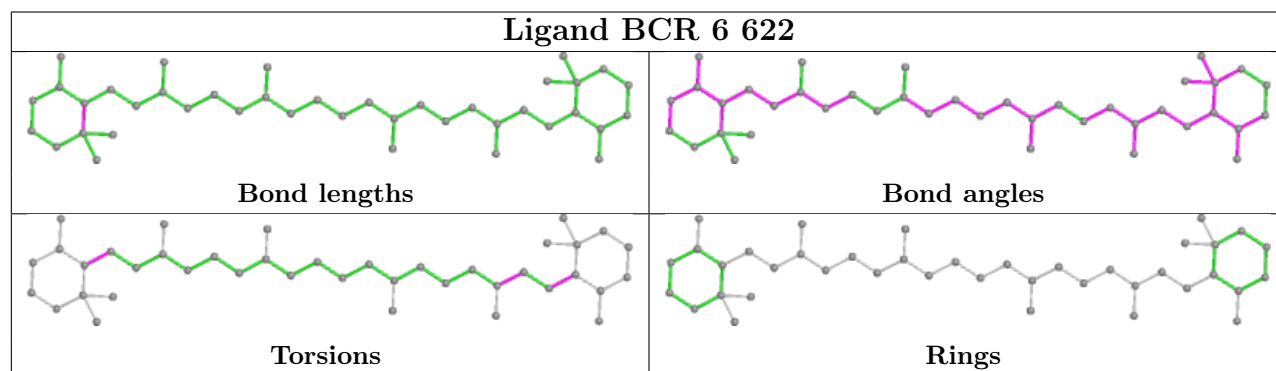
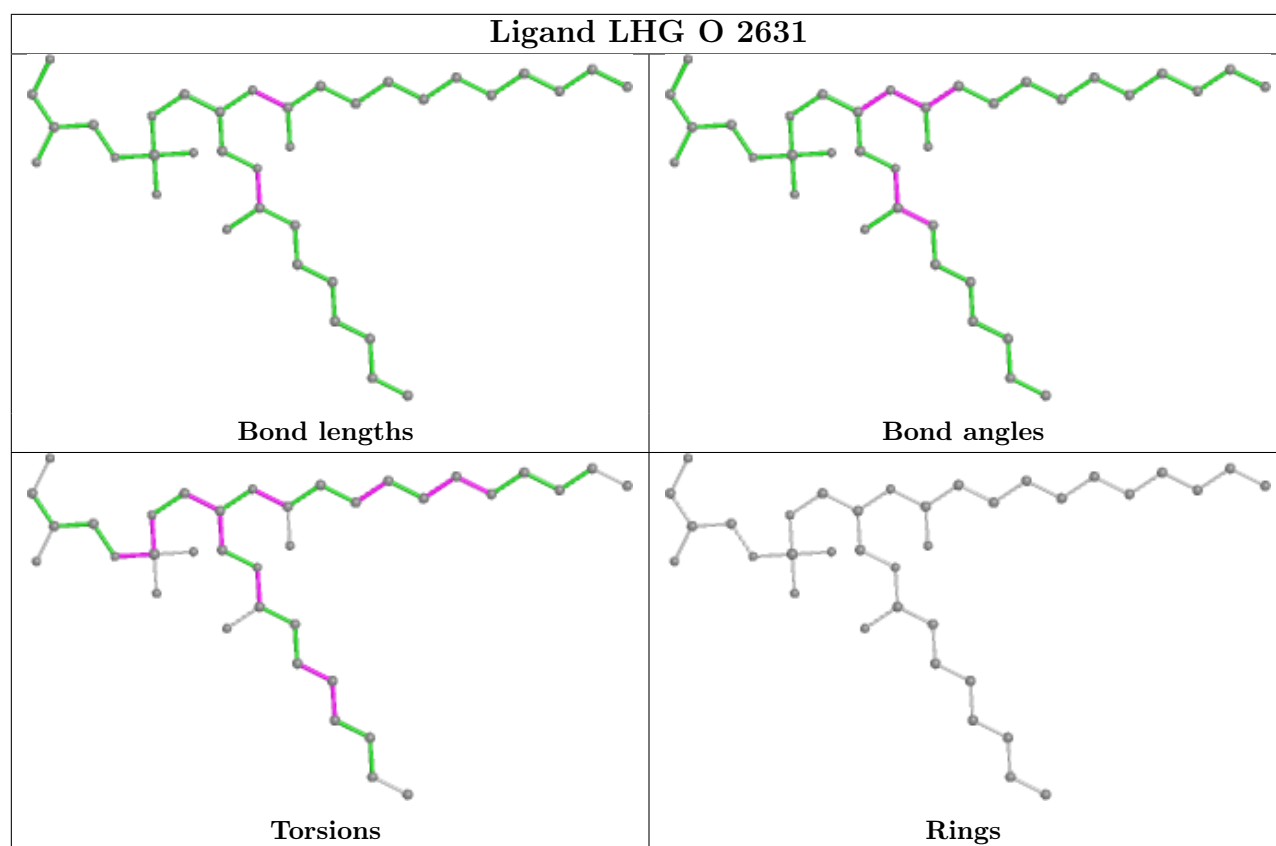
Bond angles

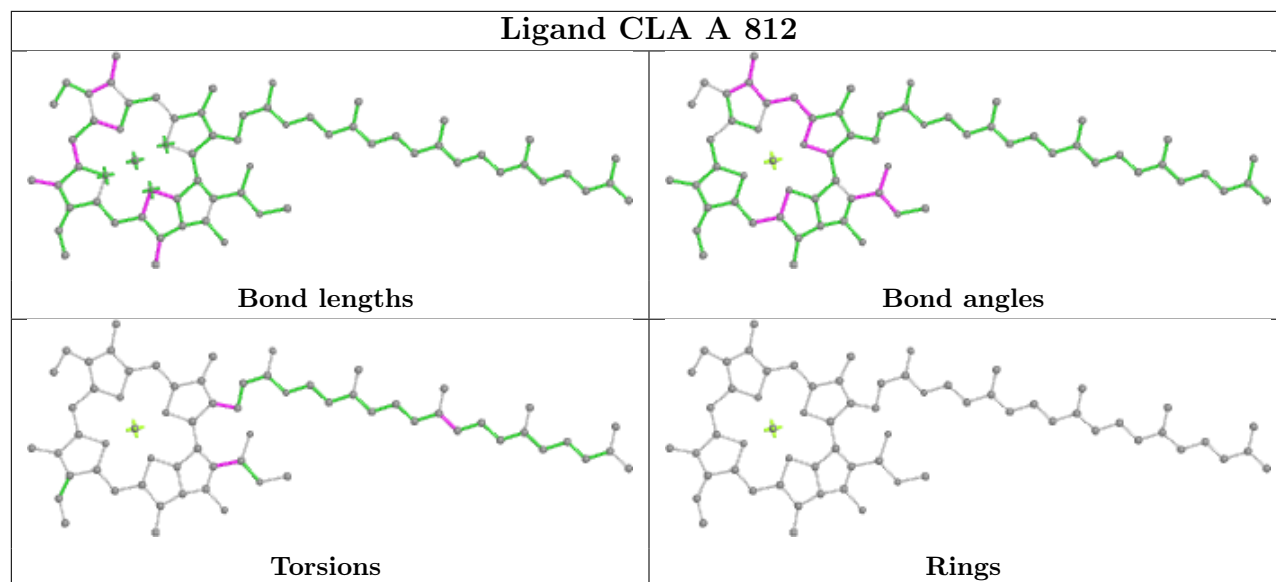
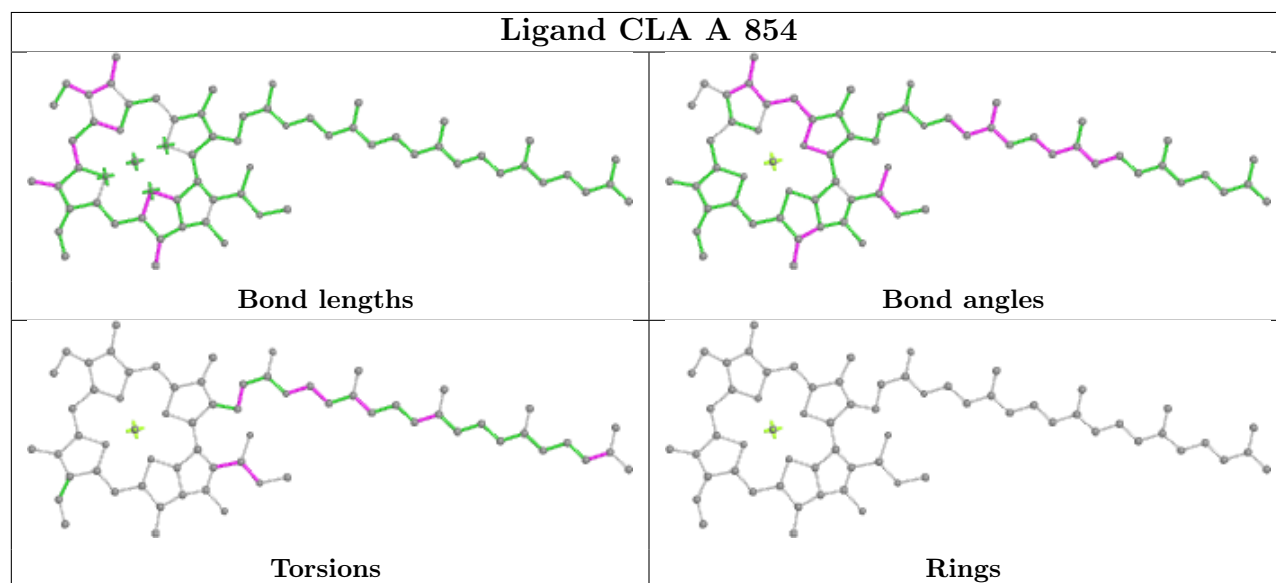


Torsions

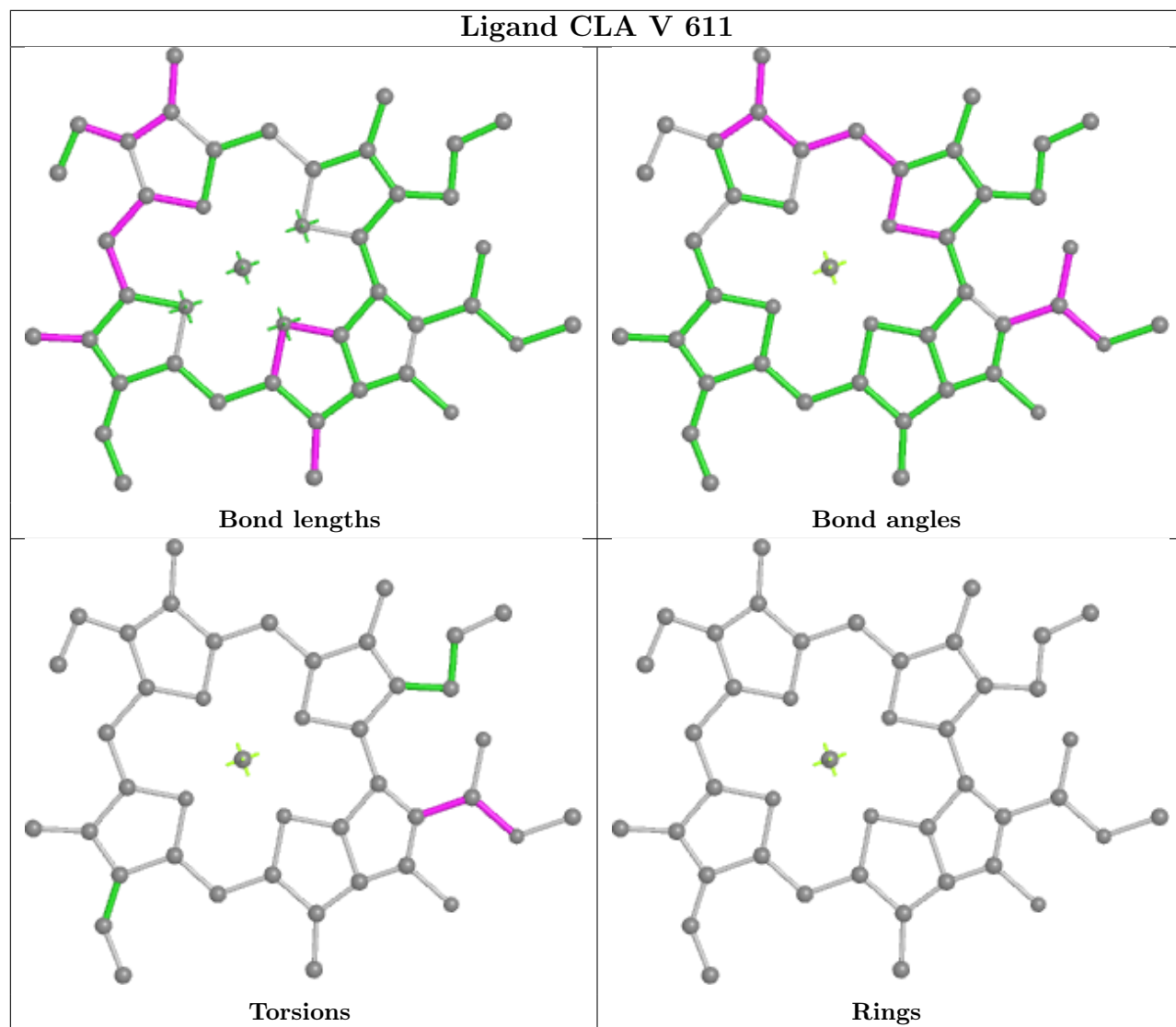


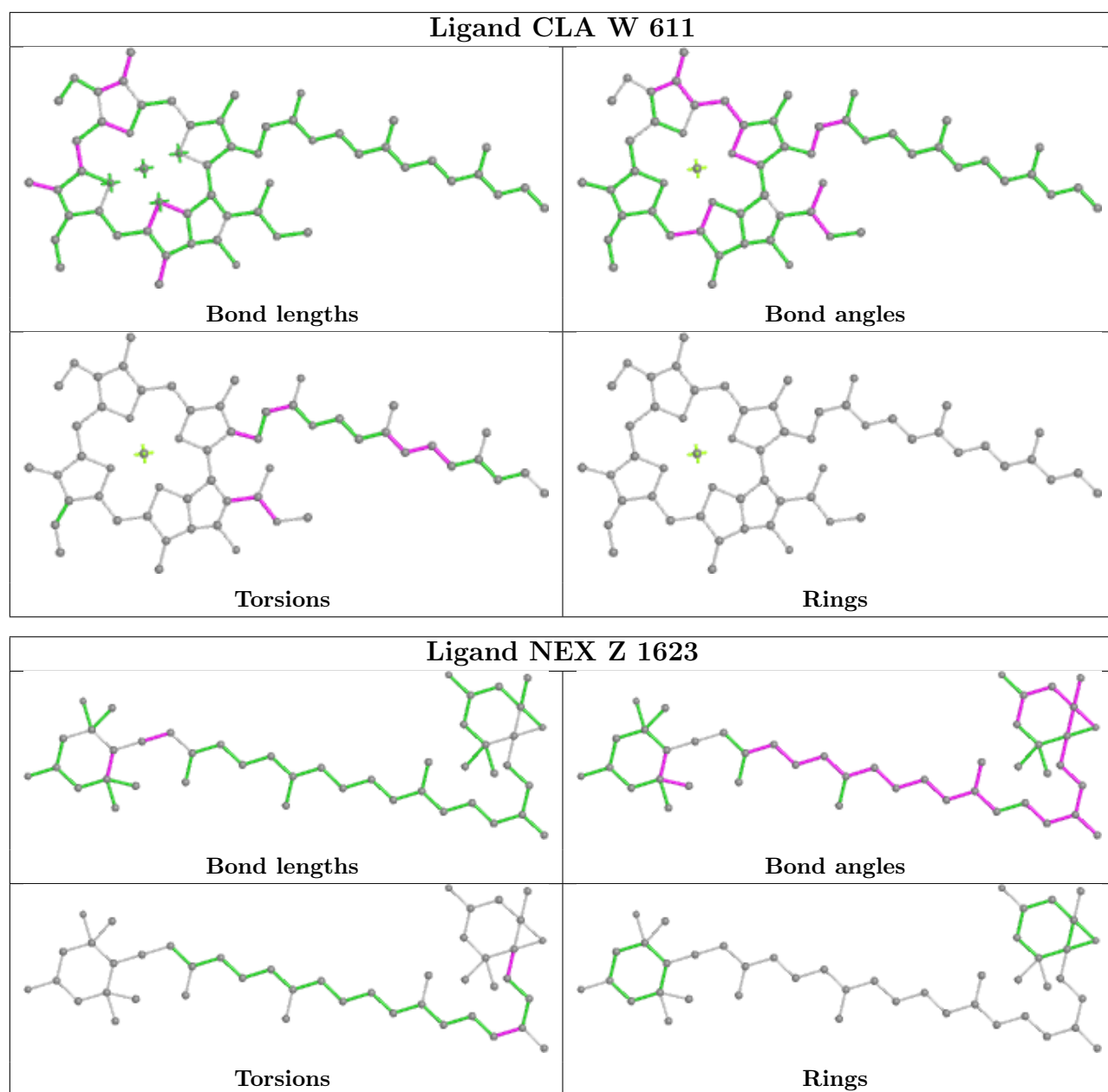
Rings



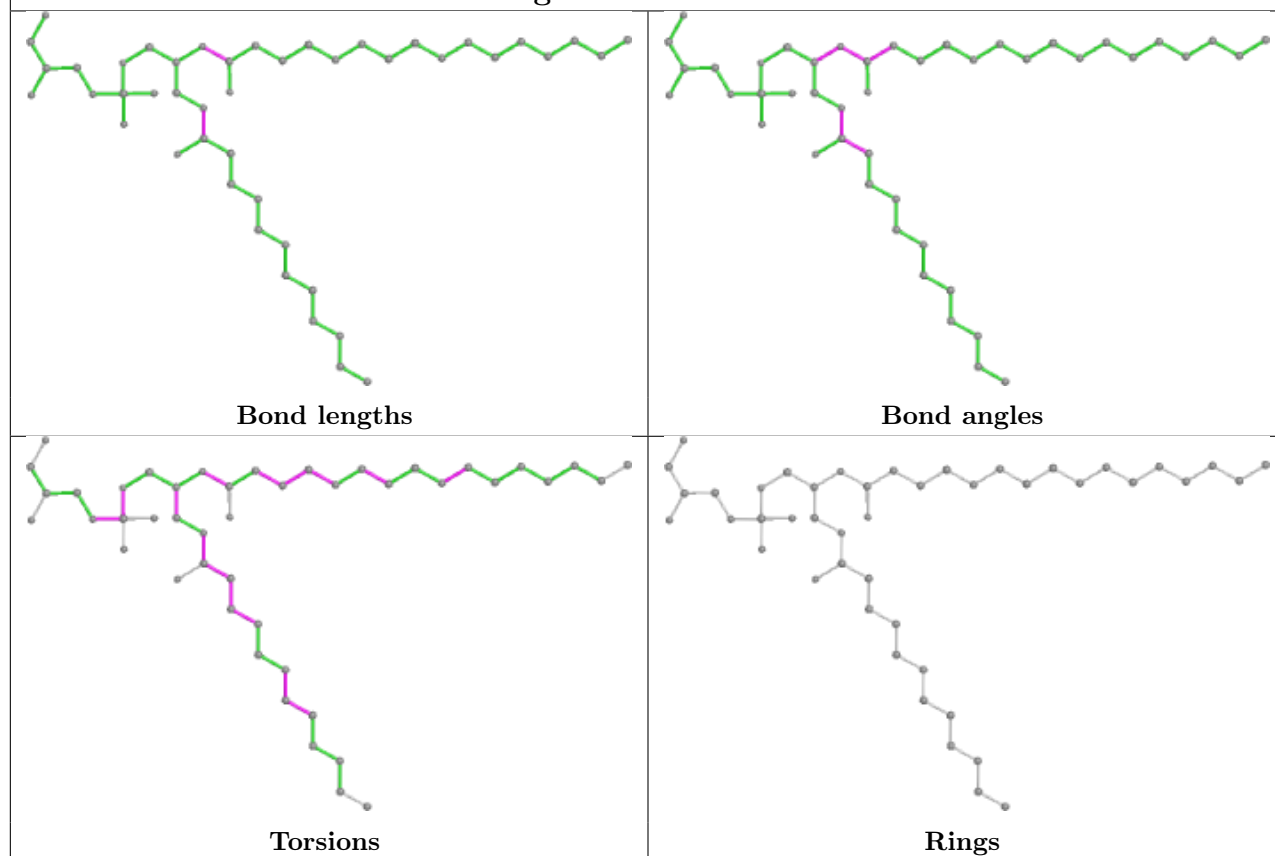
Ligand CLA A 812**Ligand CLA A 854**

Ligand CLA V 611

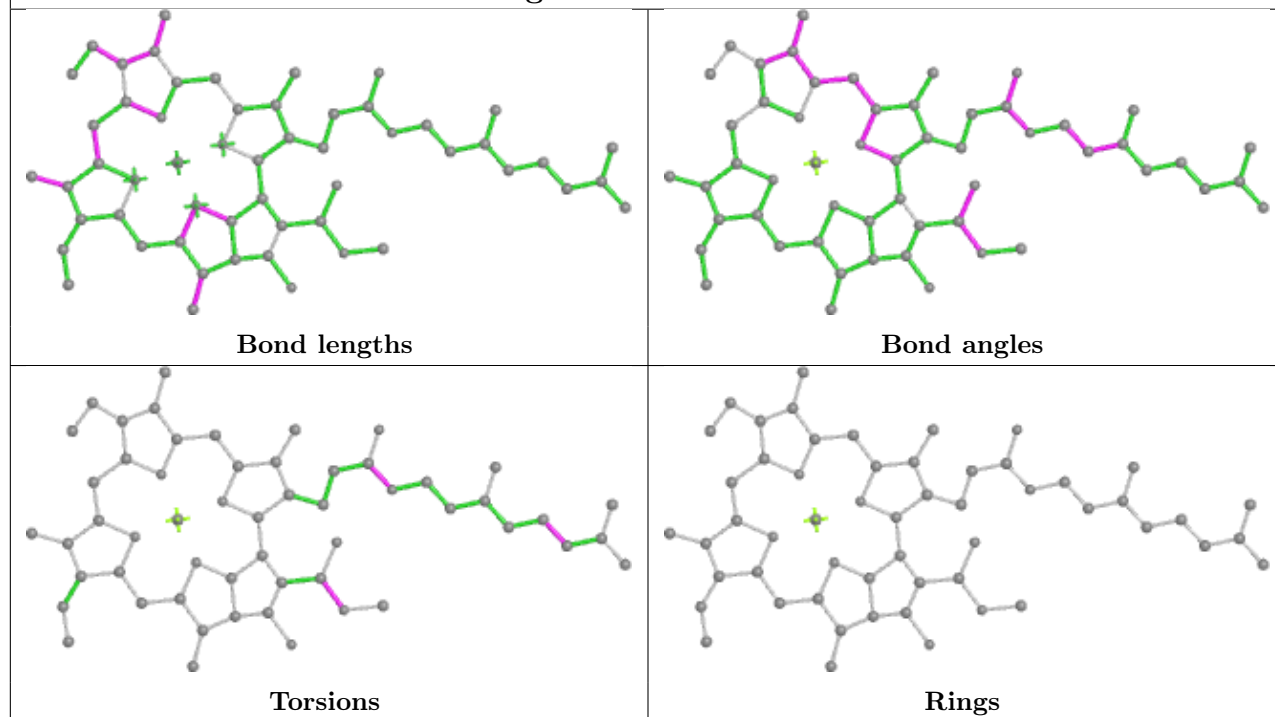


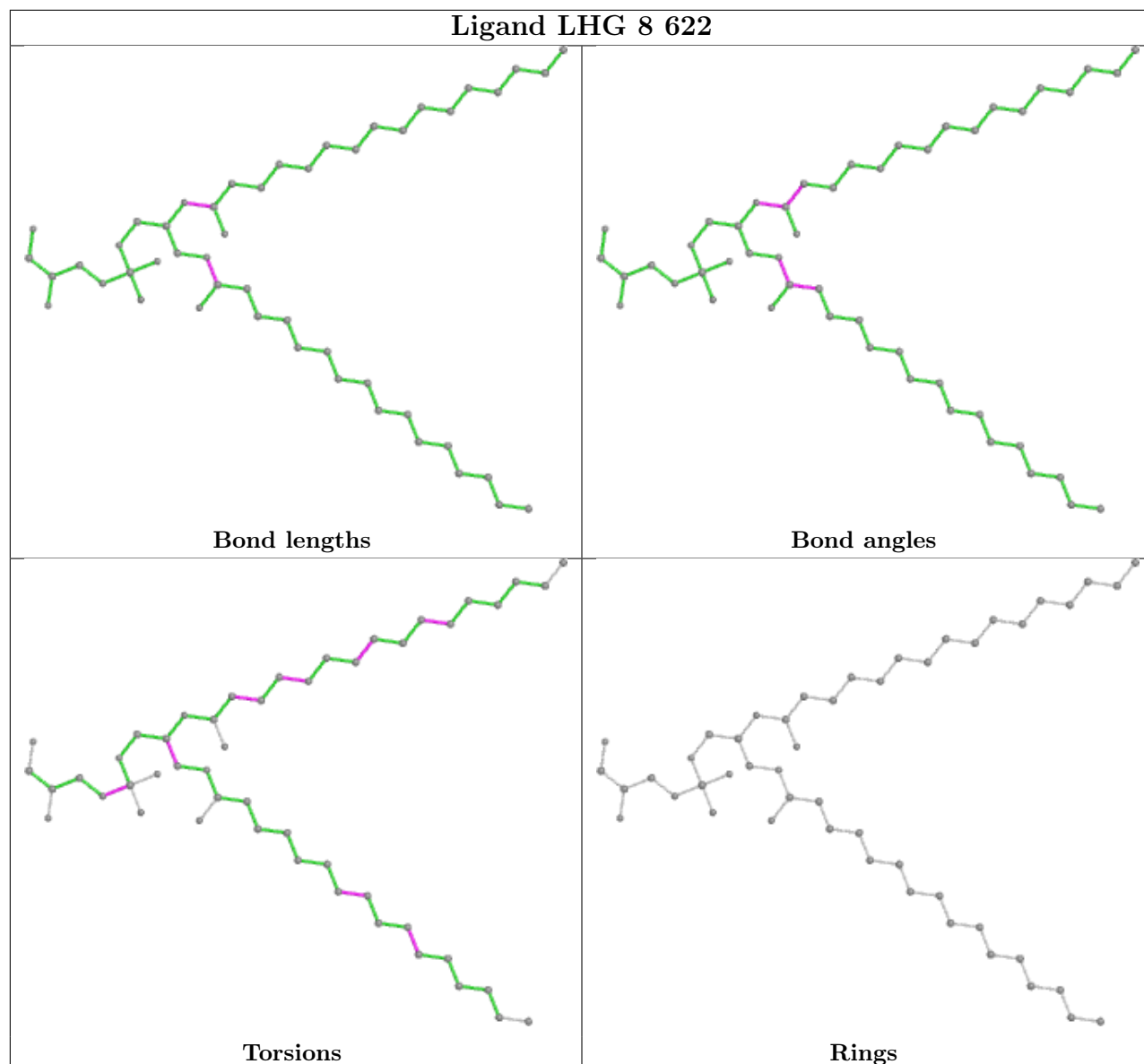
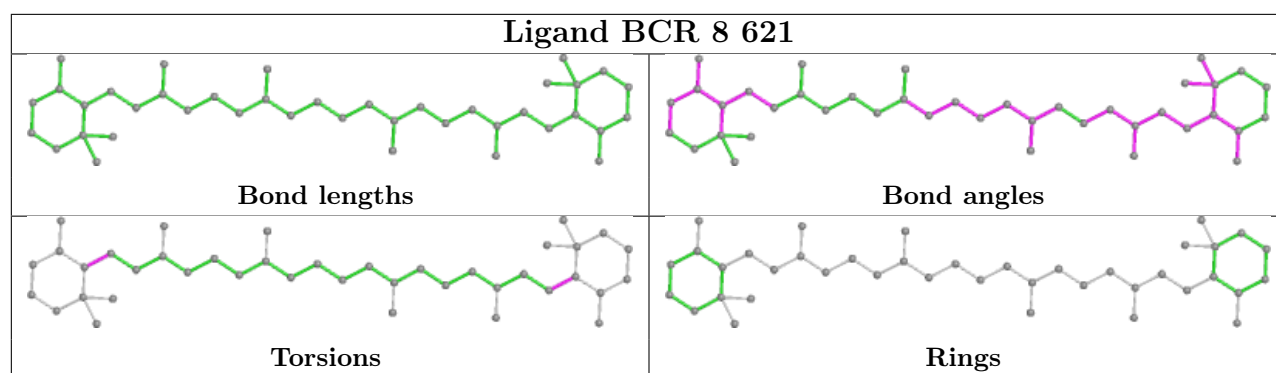


Ligand LHG 3 623

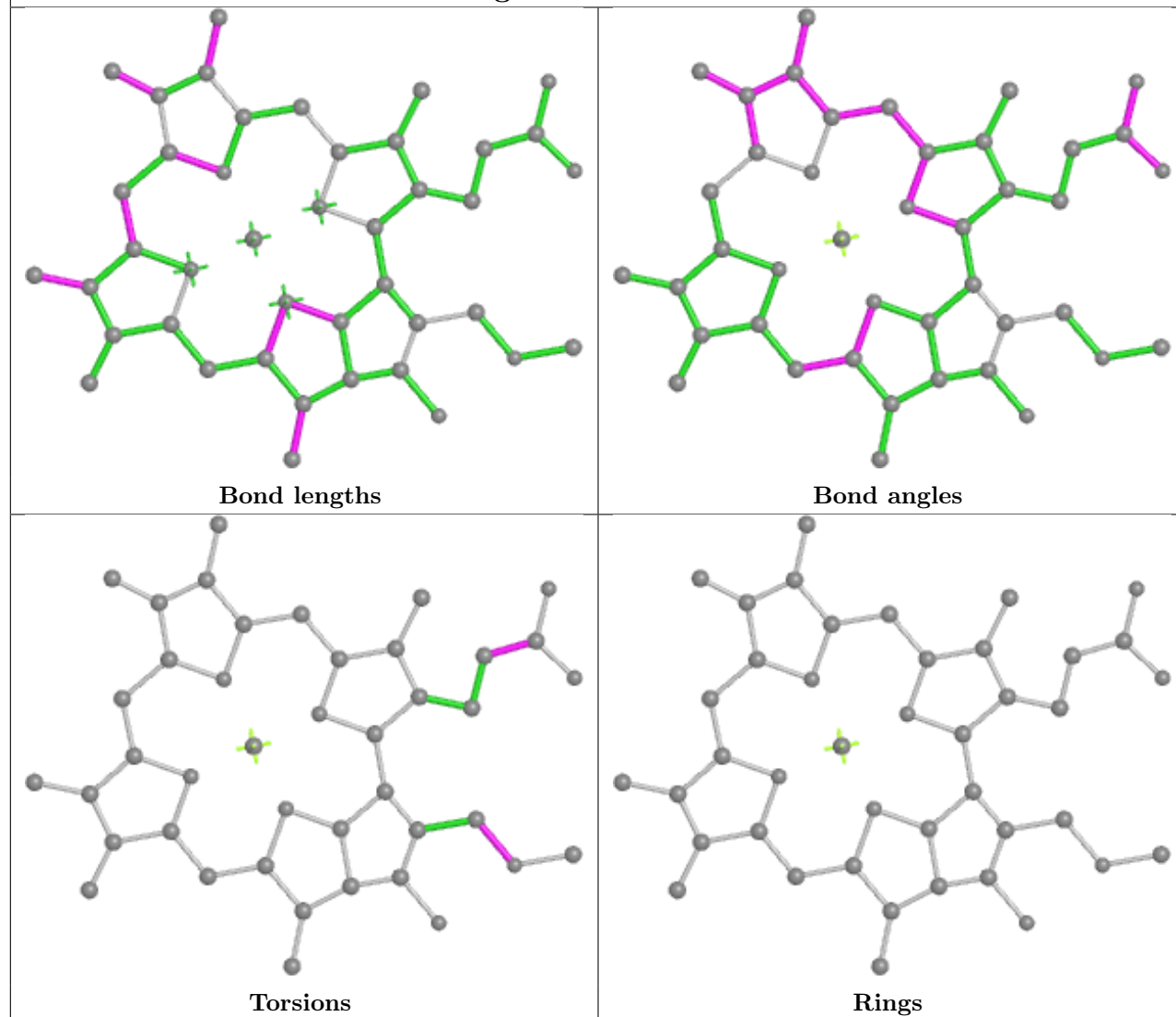


Ligand CLA W 610

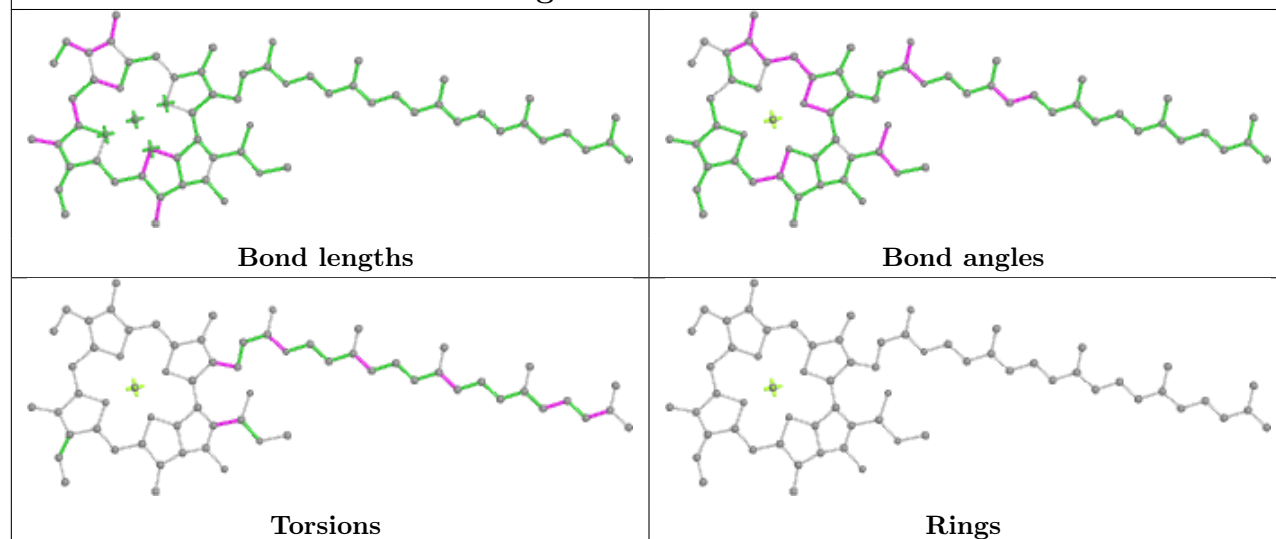


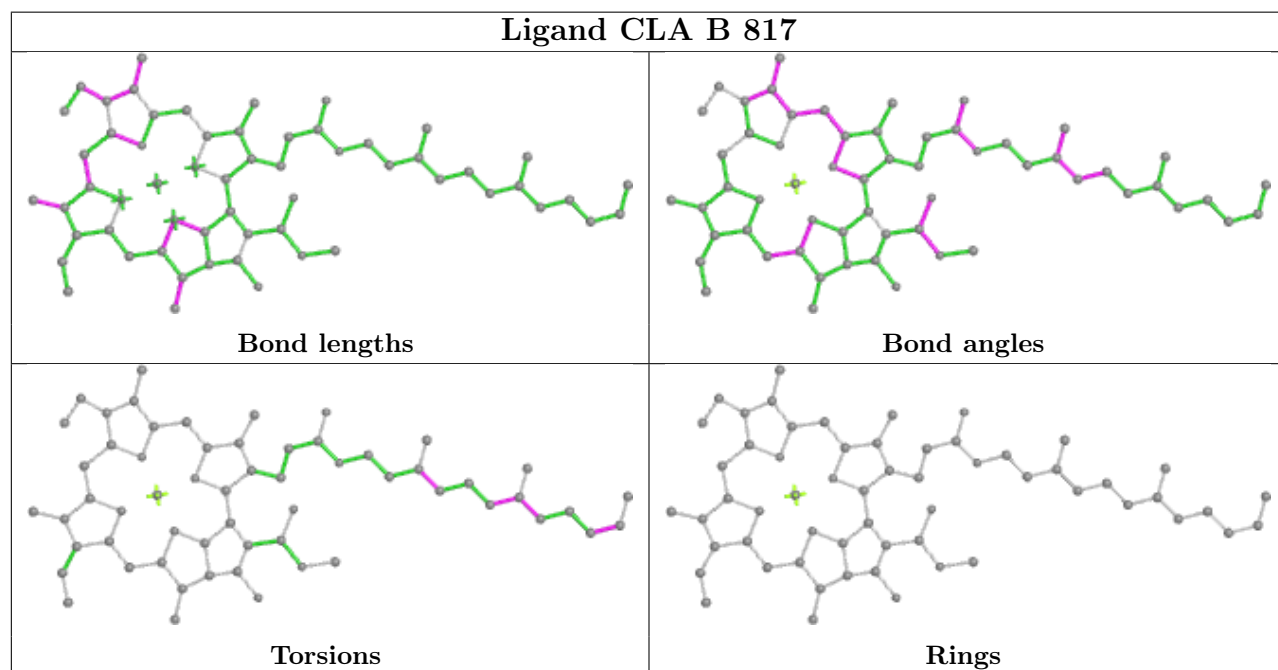
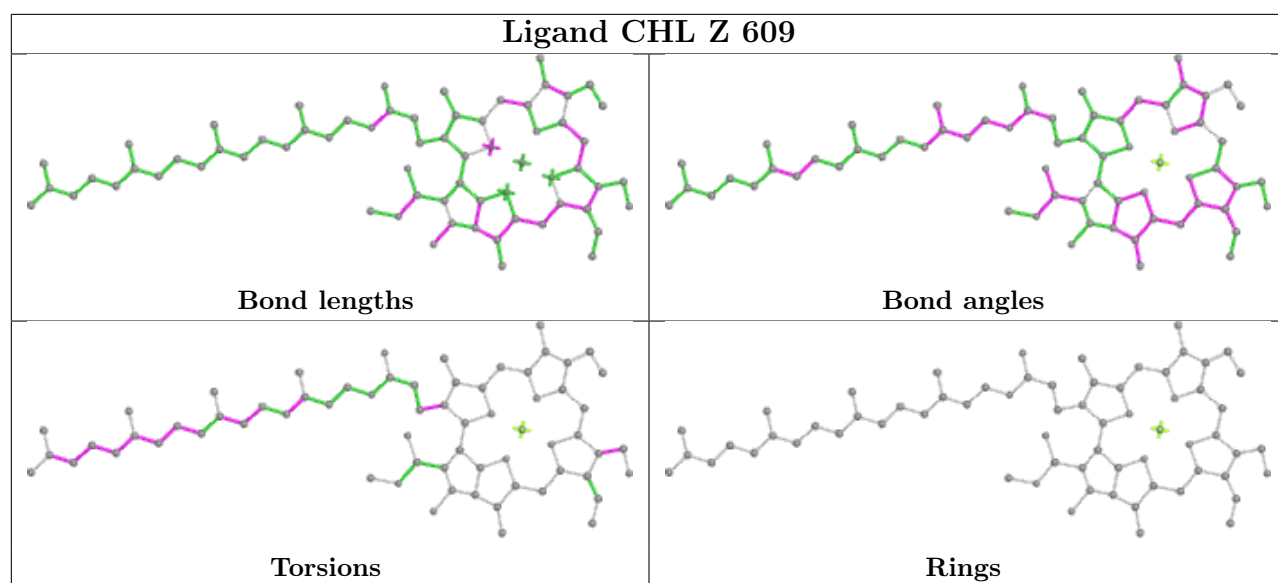


Ligand CLA 5 616

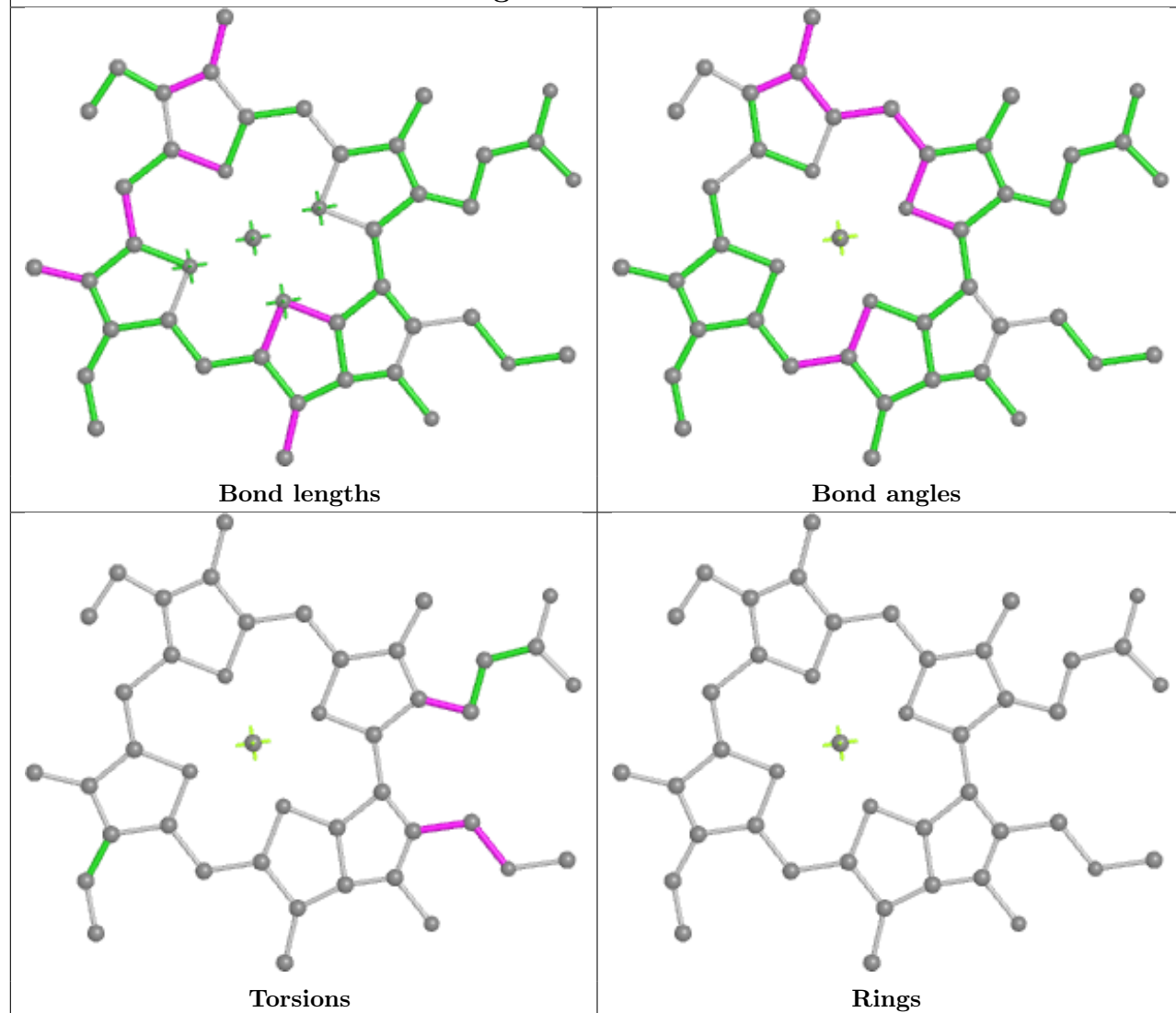


Ligand CLA 6 601

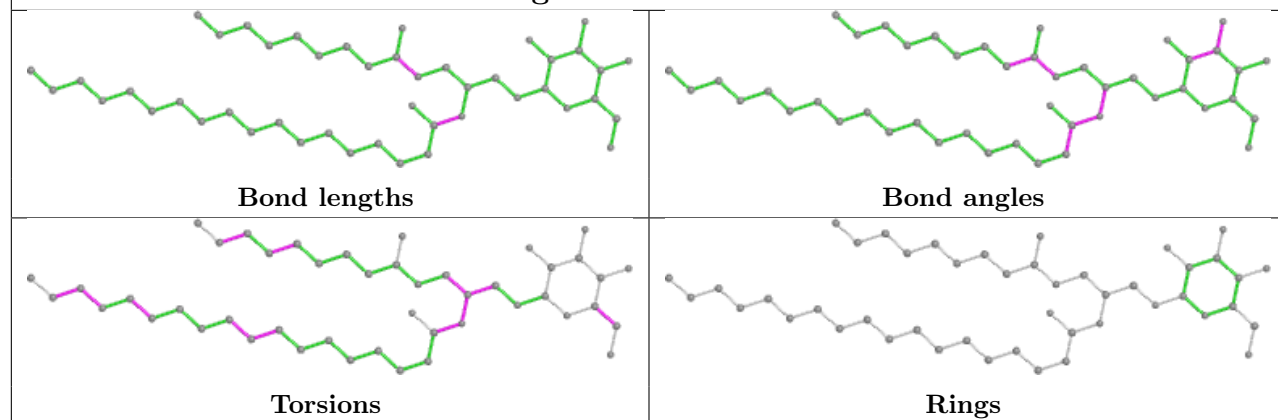




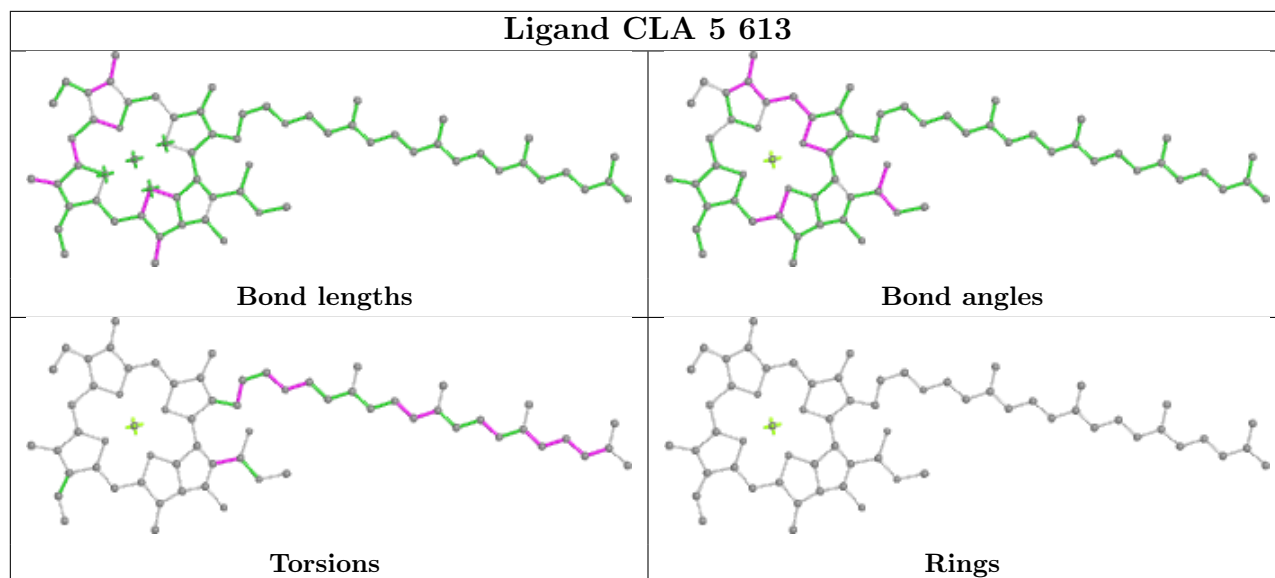
Ligand CLA a 606



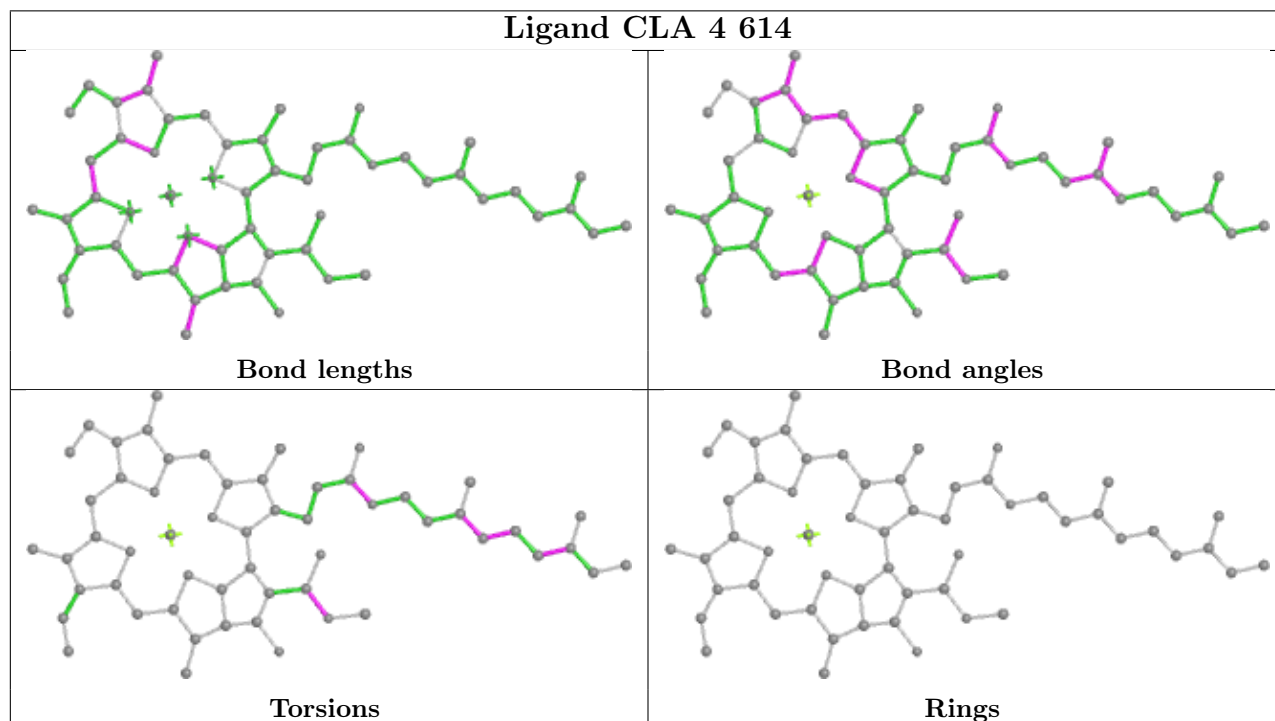
Ligand LMG 8 626



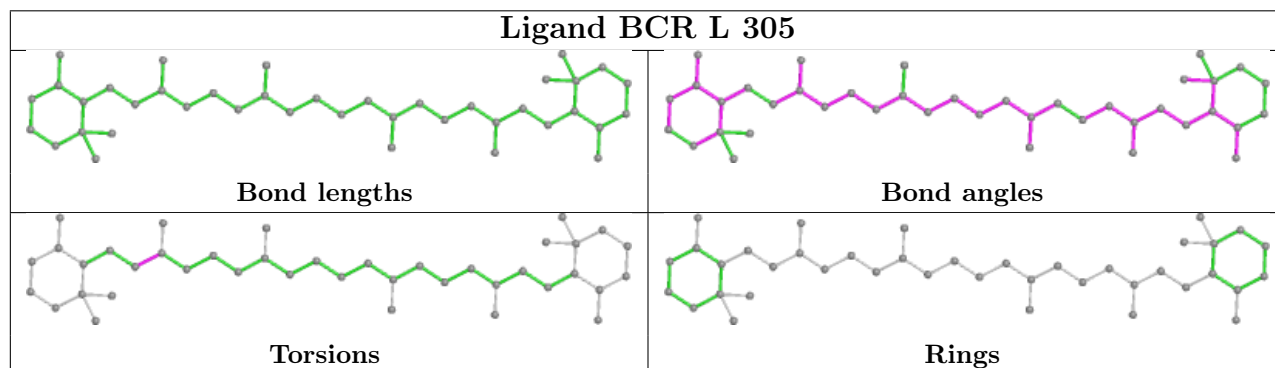
Ligand CLA 5 613



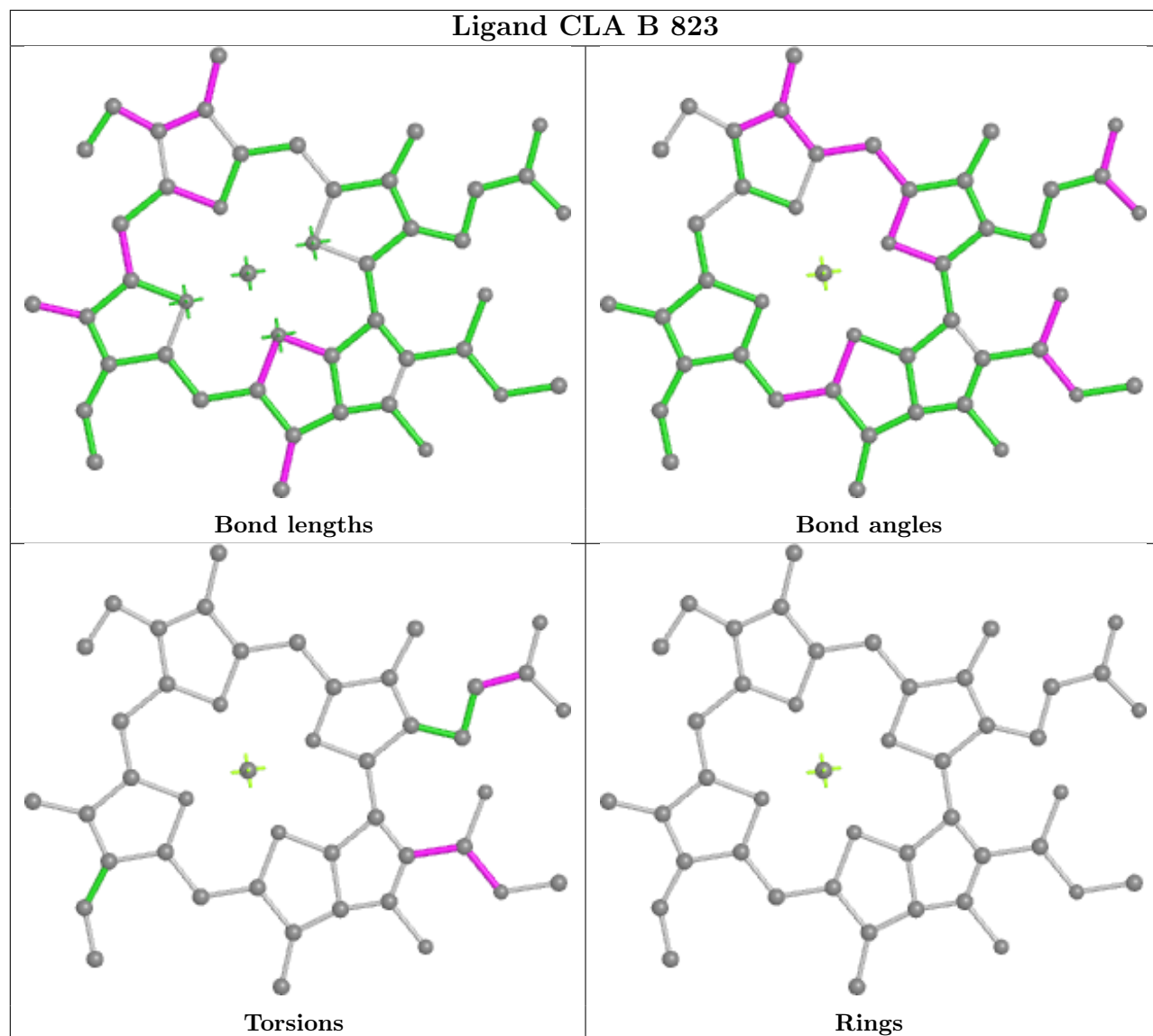
Ligand CLA 4 614

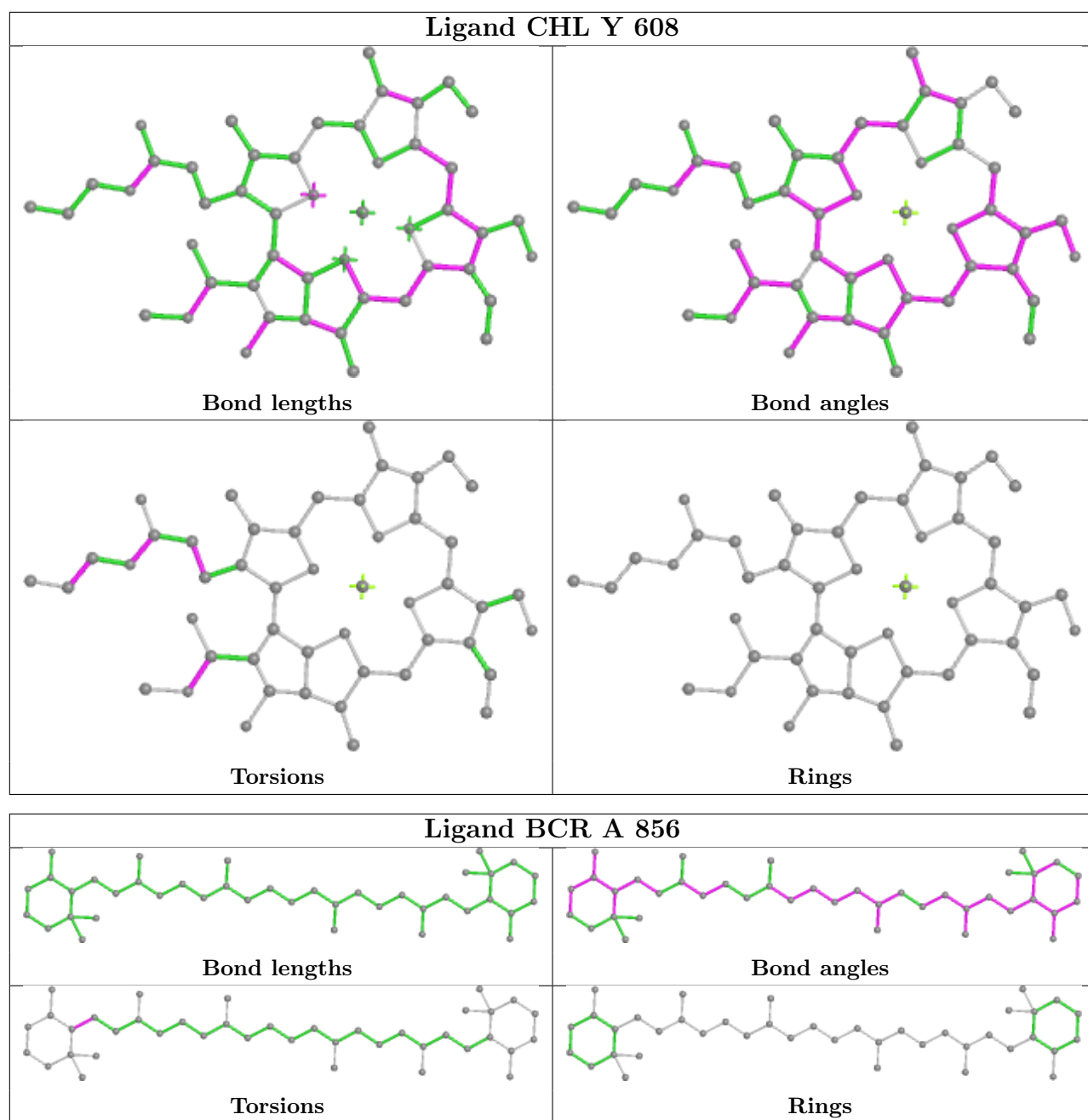


Ligand BCR L 305

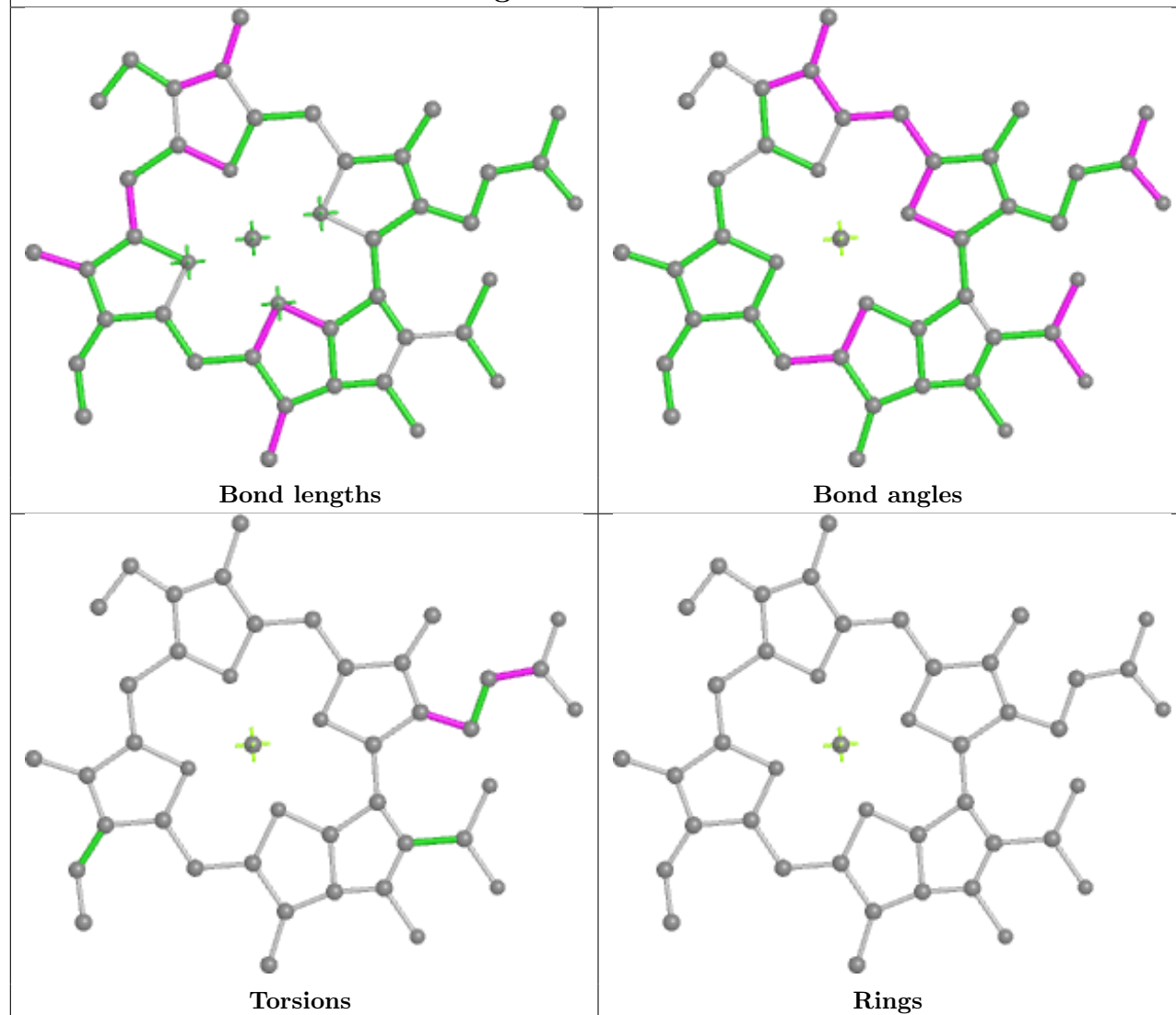


Ligand CLA B 823

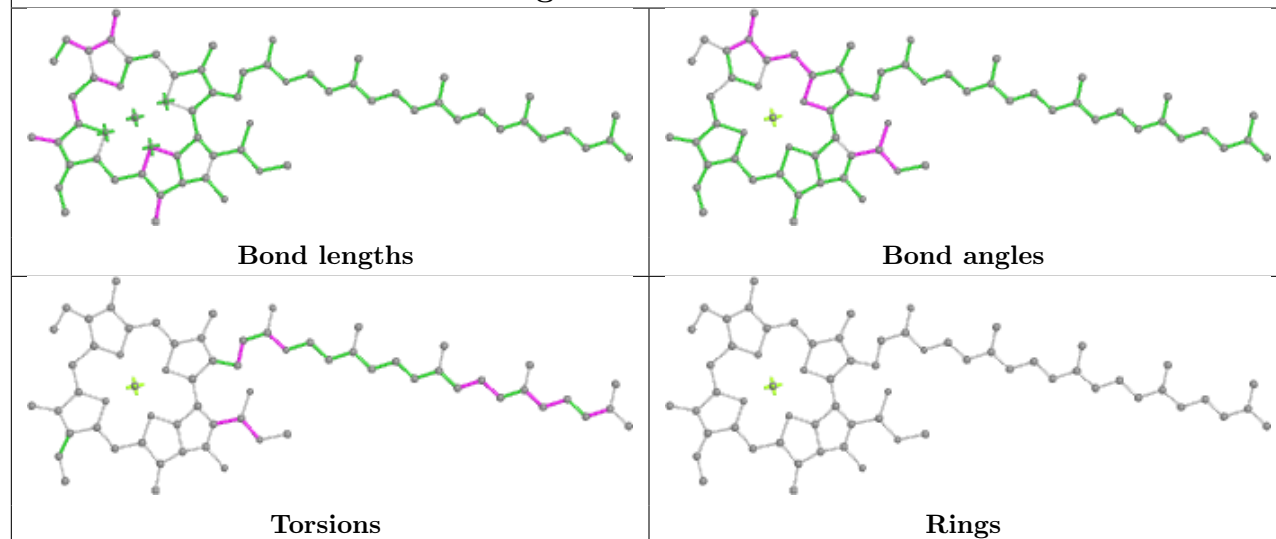


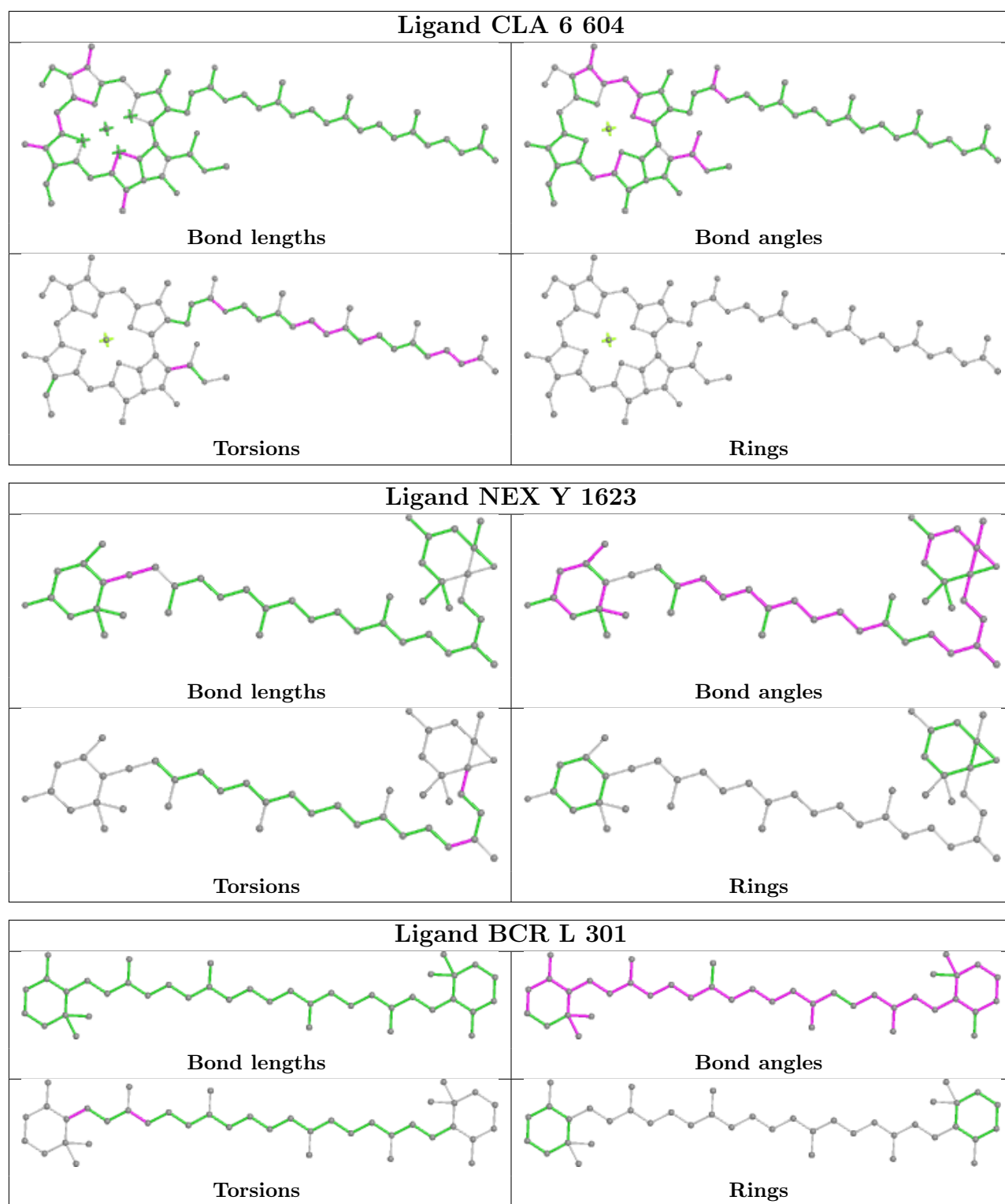


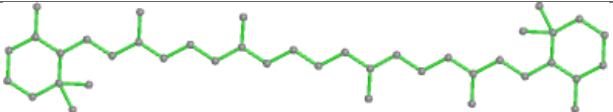
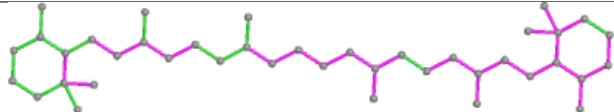
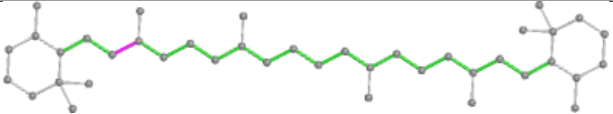
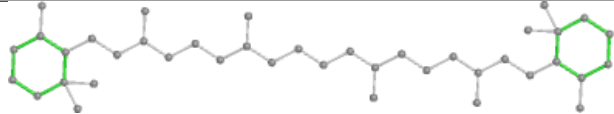
Ligand CLA 1 608

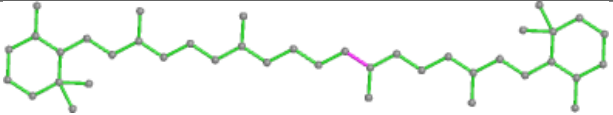
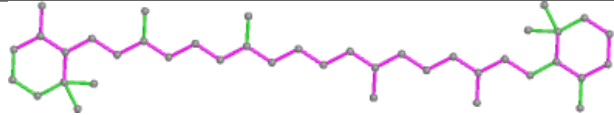
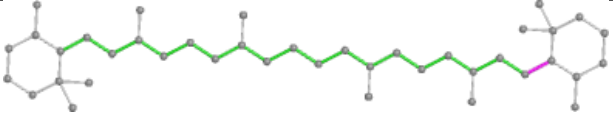
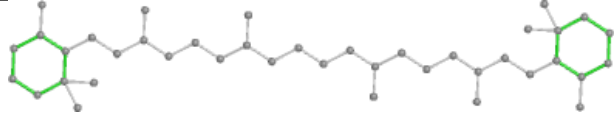


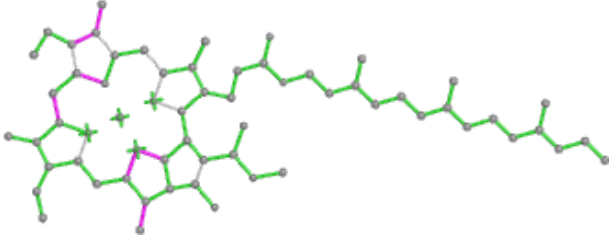
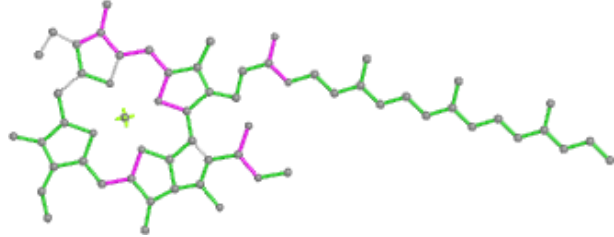
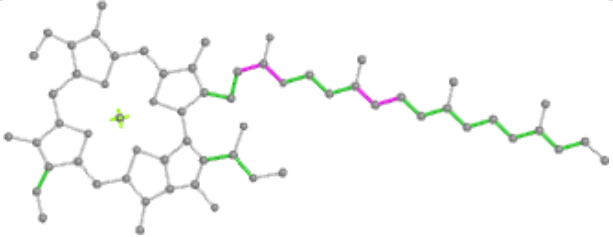
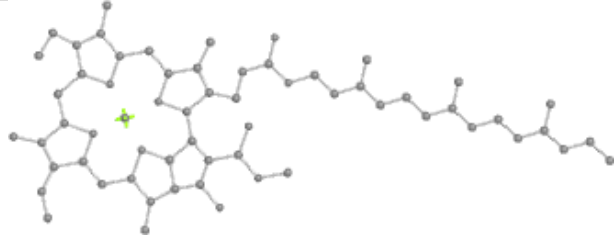
Ligand CLA 5 602

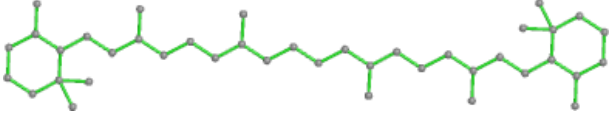
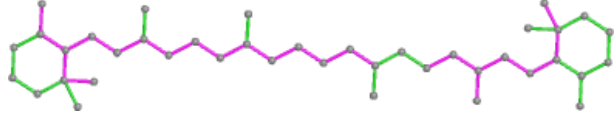
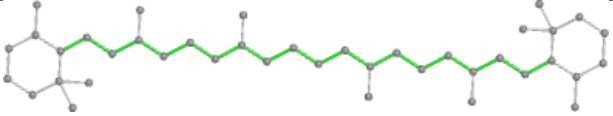
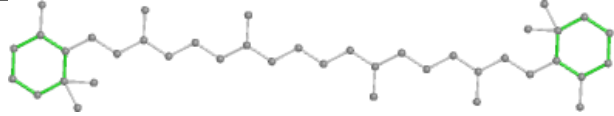




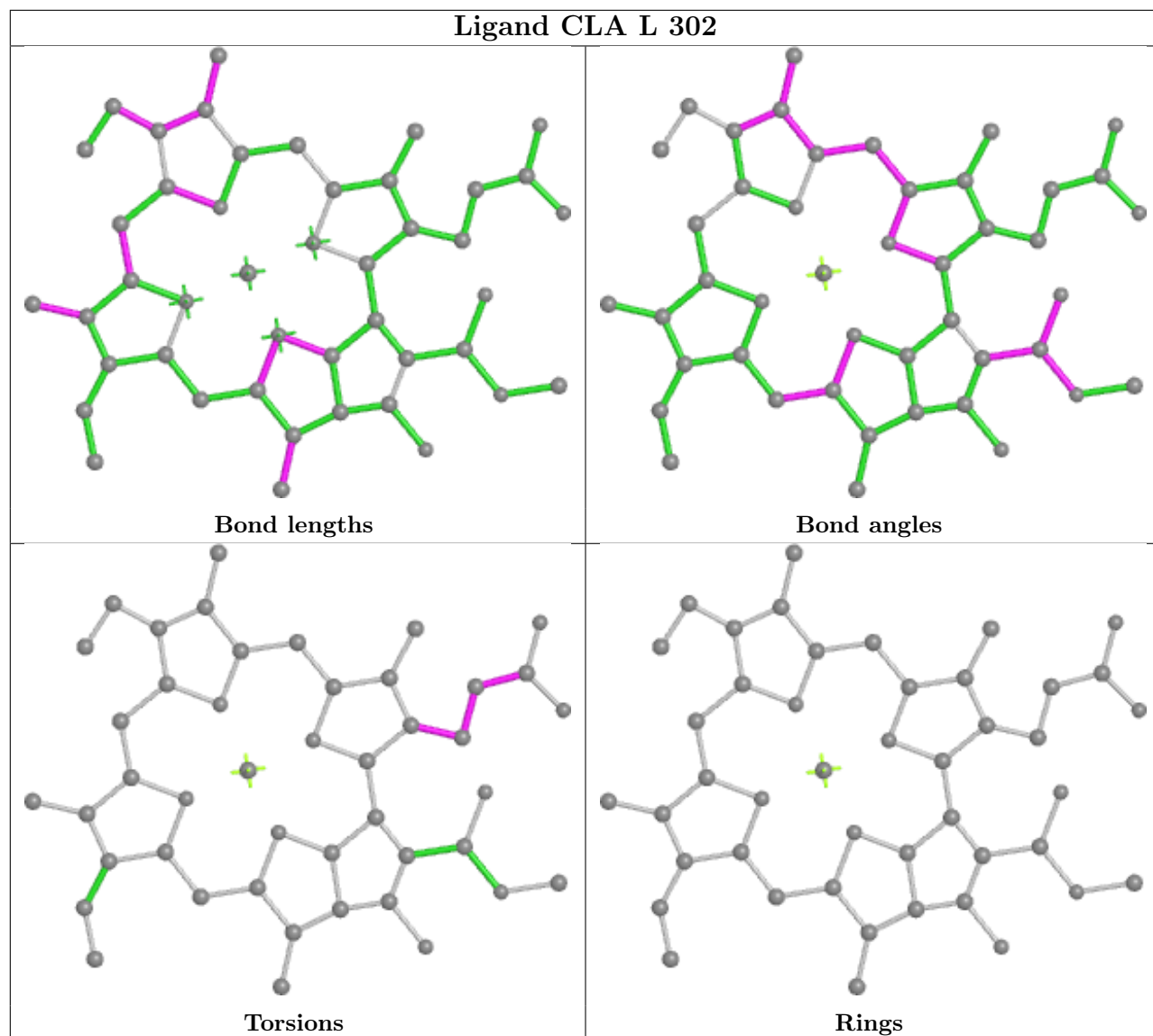
Ligand BCR K 207	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

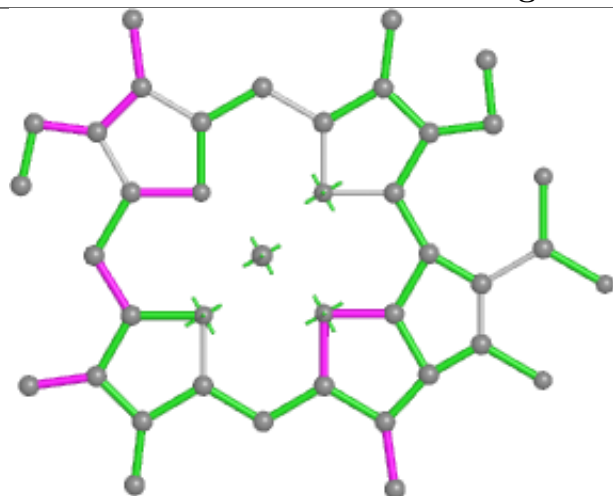
Ligand CLA X 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 3 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

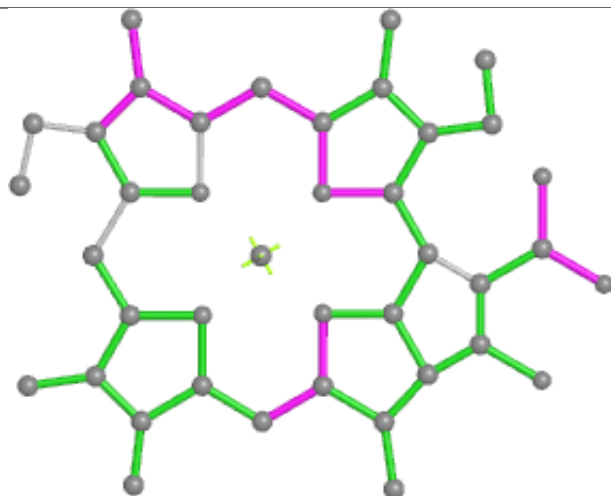
Ligand CLA L 302



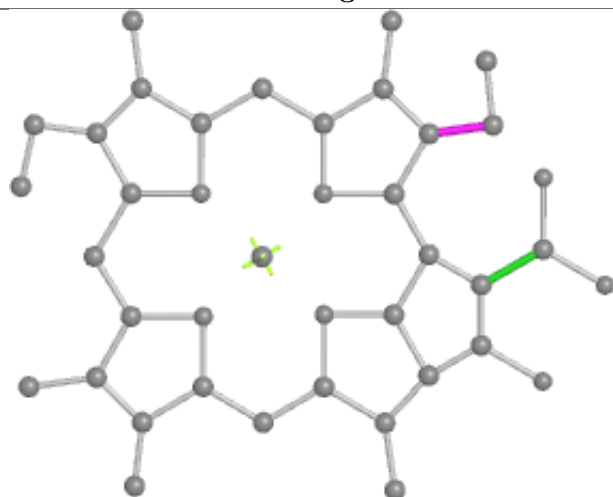
Ligand CLA 5 606



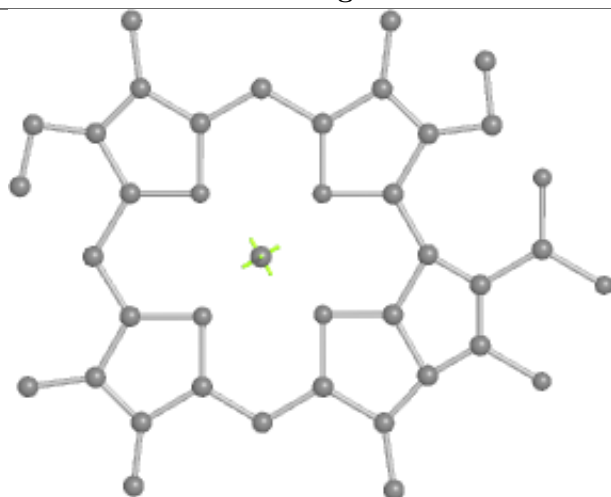
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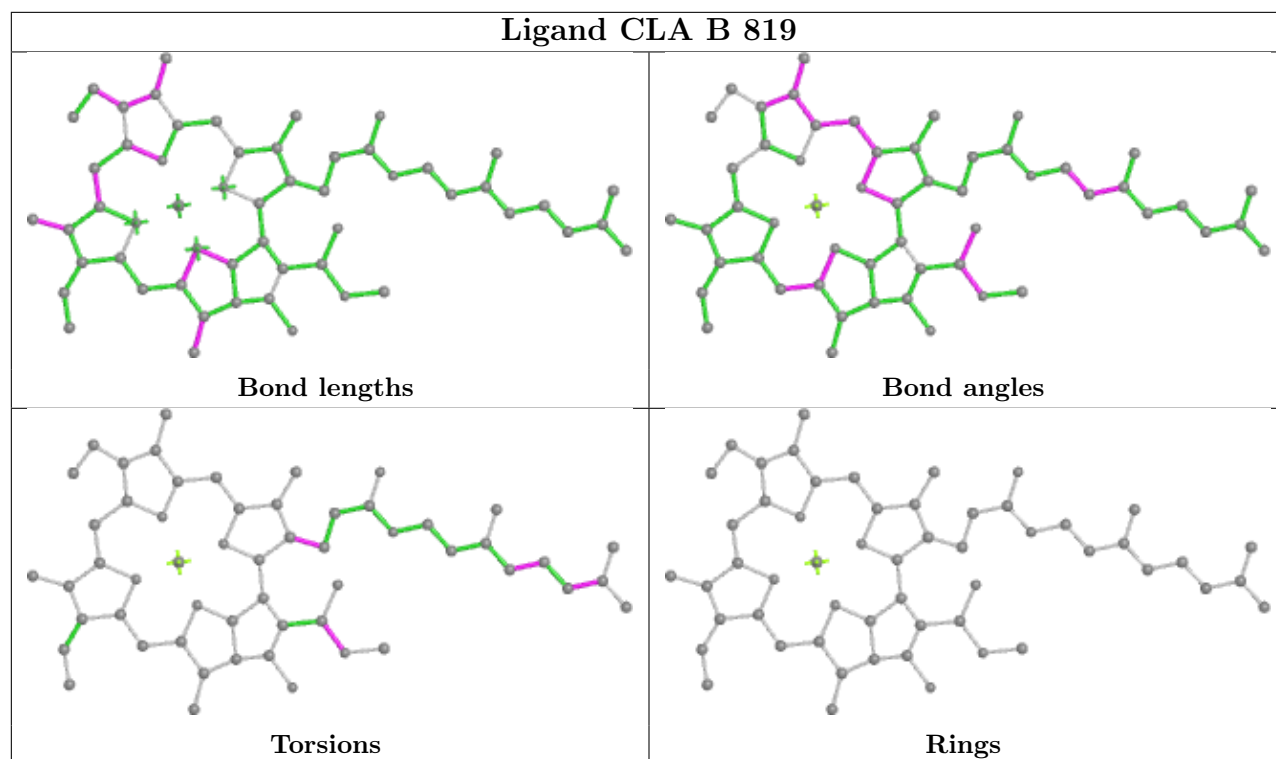
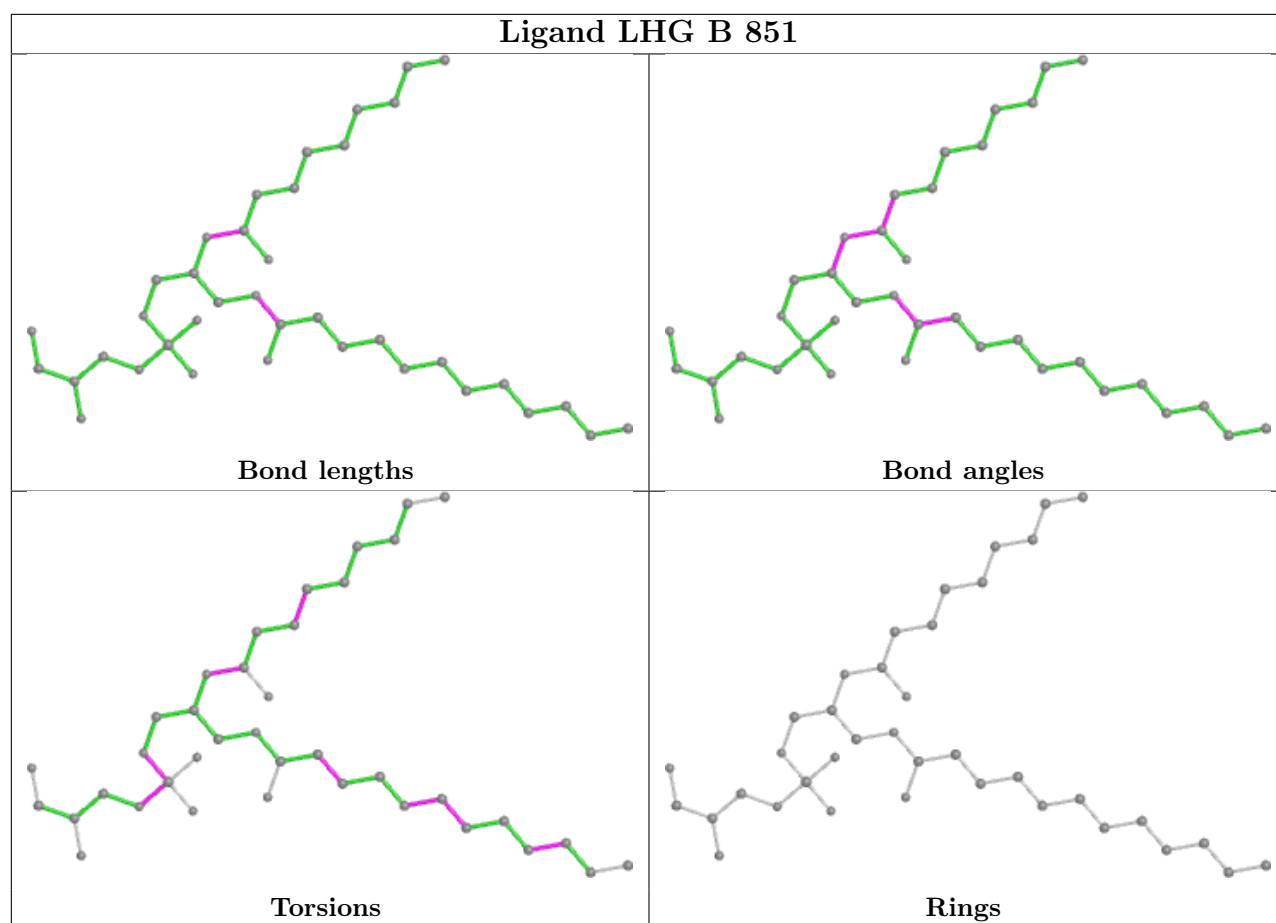
Bond angles



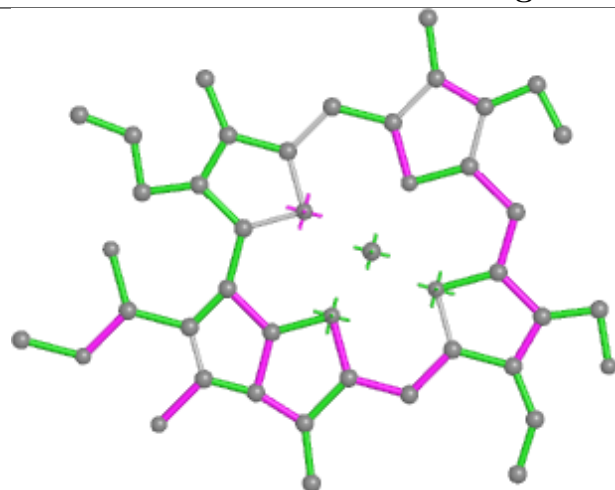
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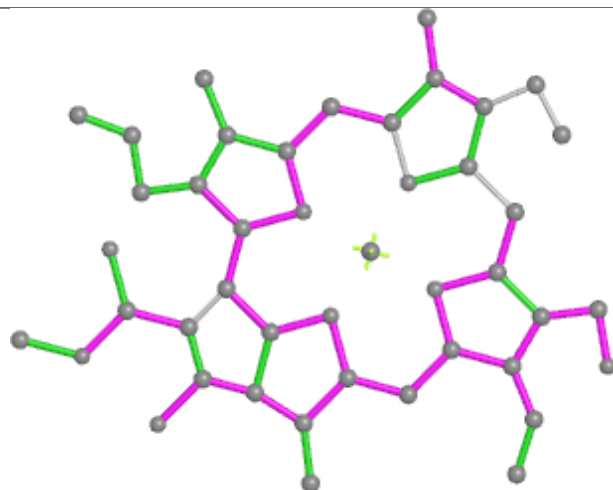
Rings



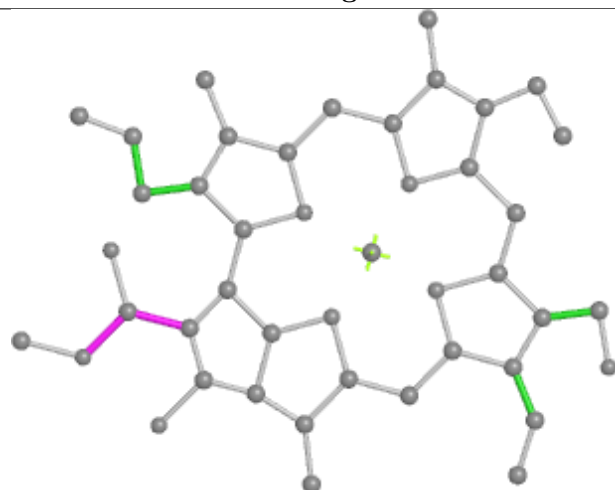
Ligand CHL V 606



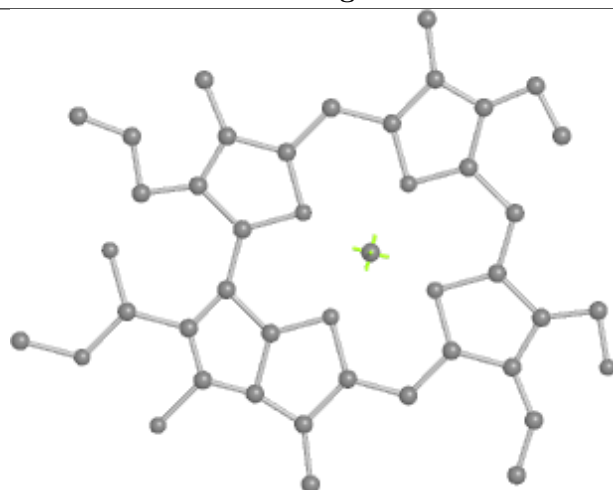
Bond lengths



Bond angles

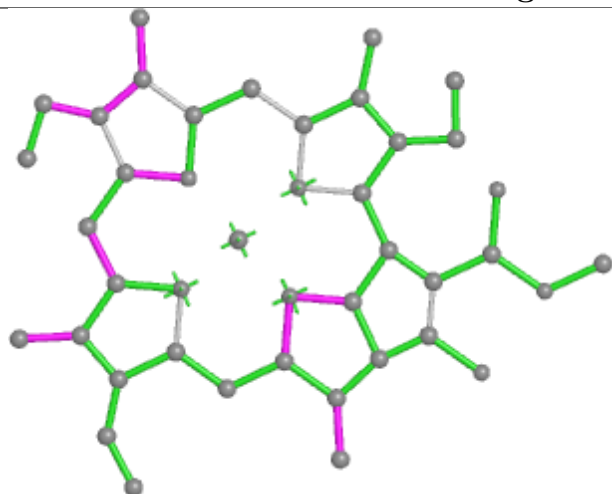


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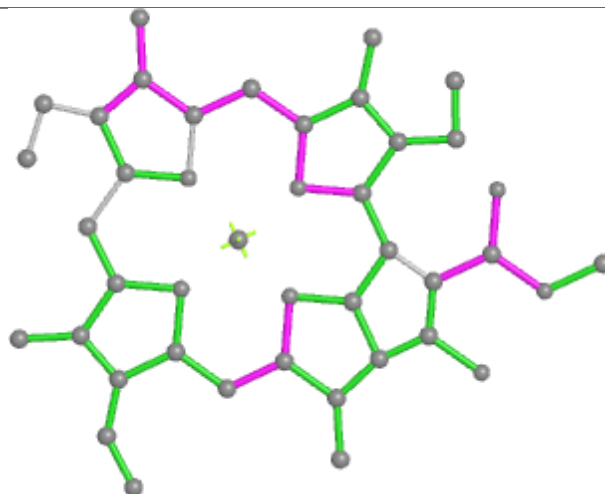


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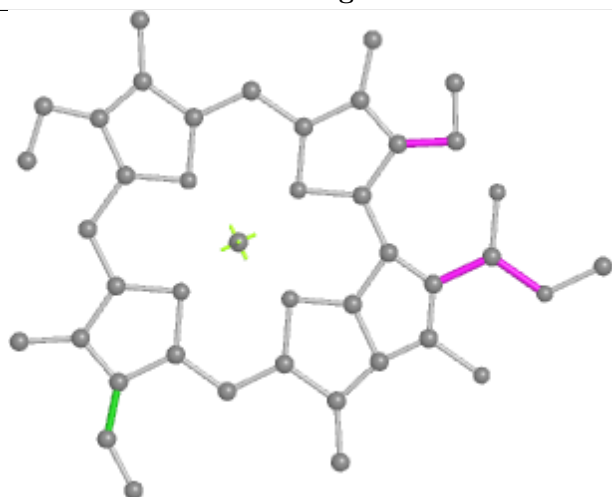
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Bond lengths



Bond angles

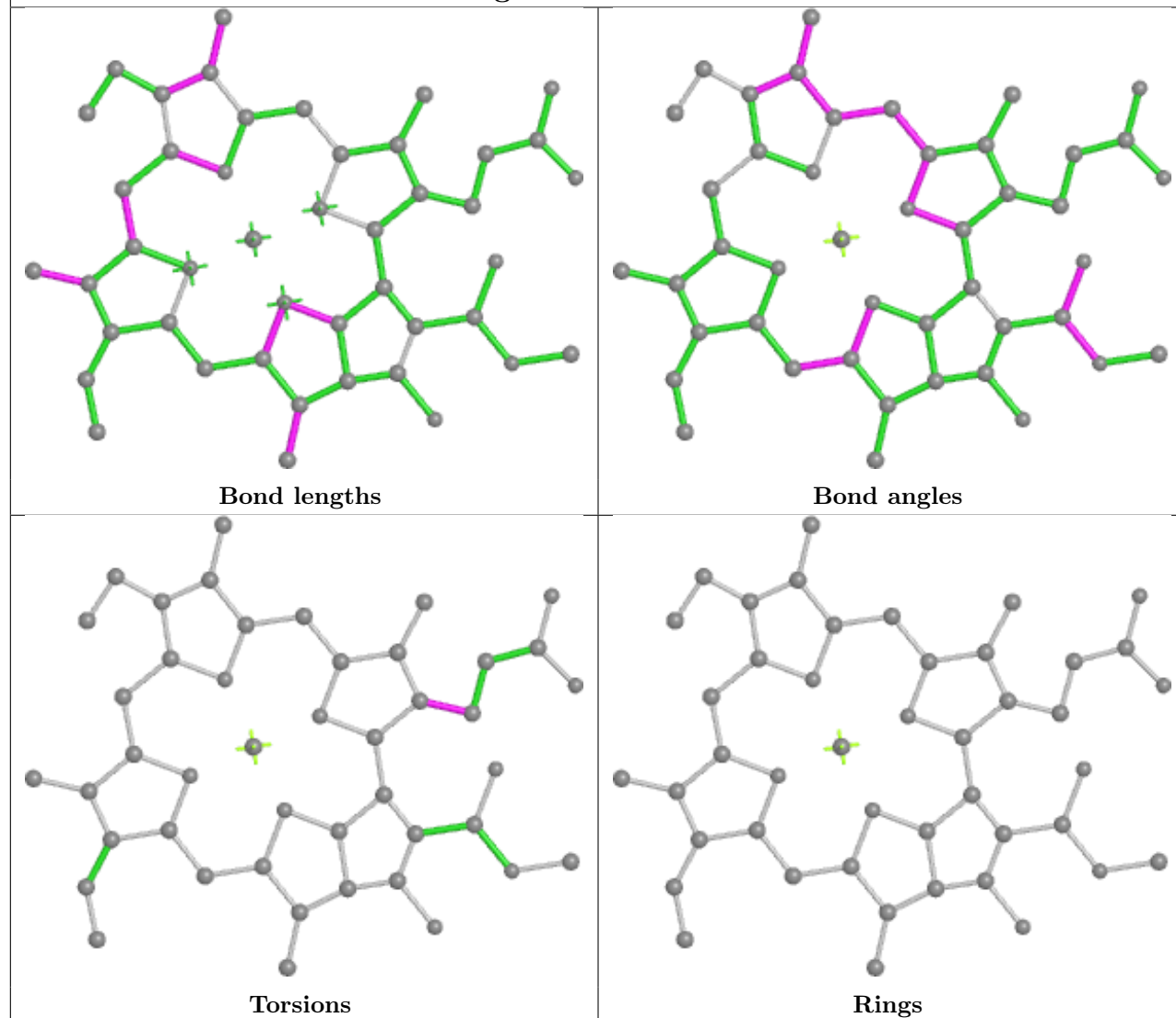


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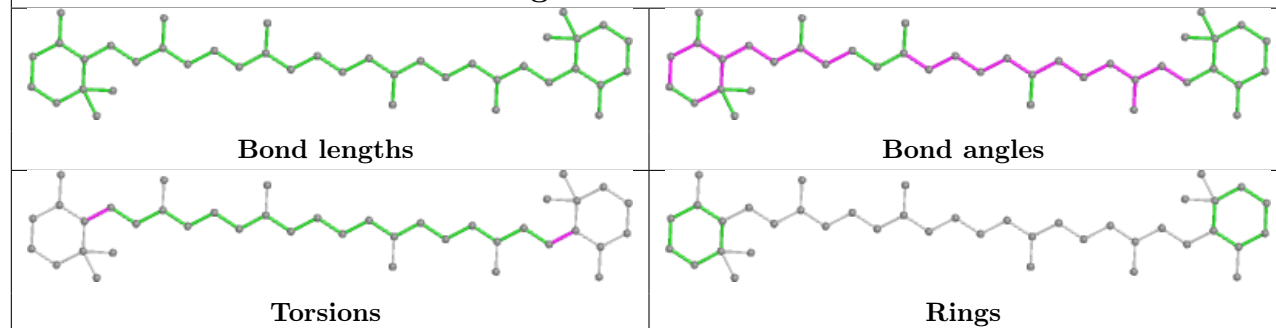


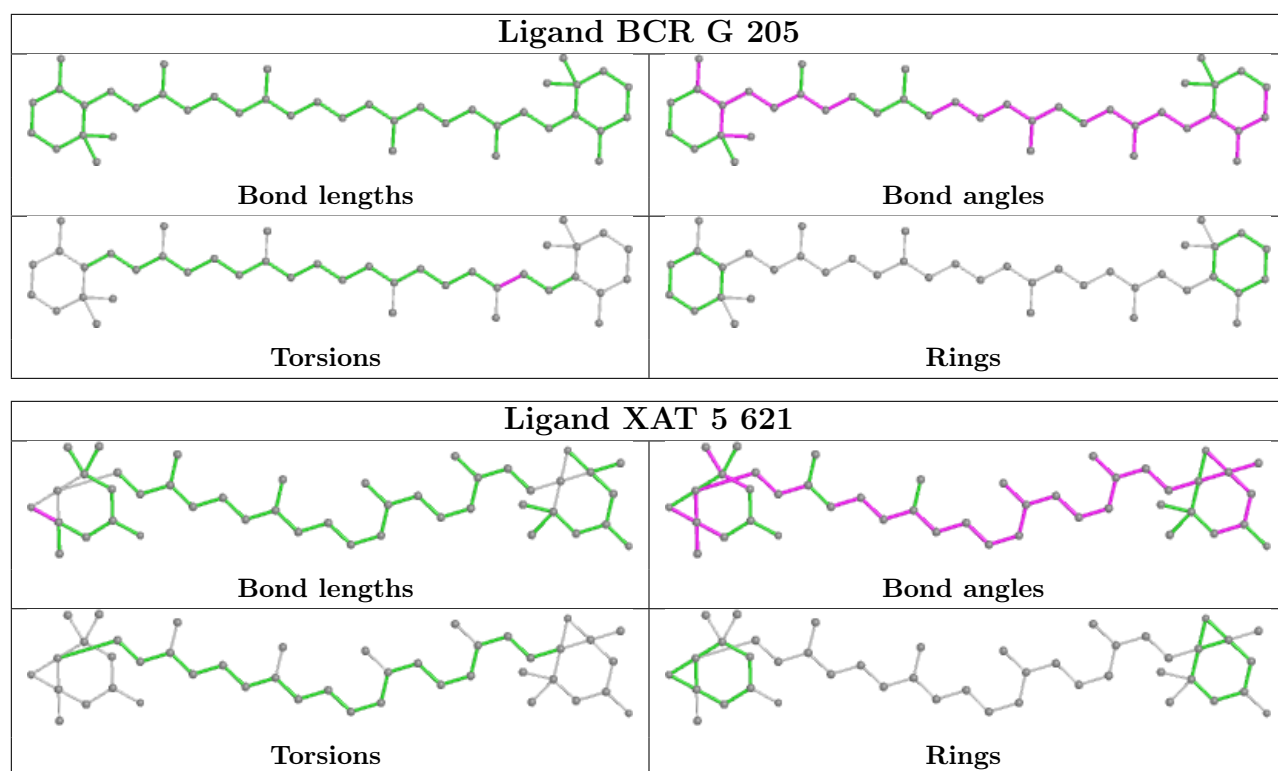
Rings

Ligand CLA 2 609

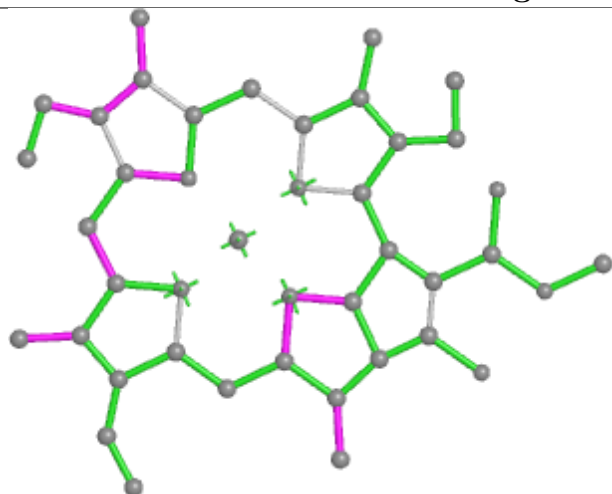


Ligand BCR B 843

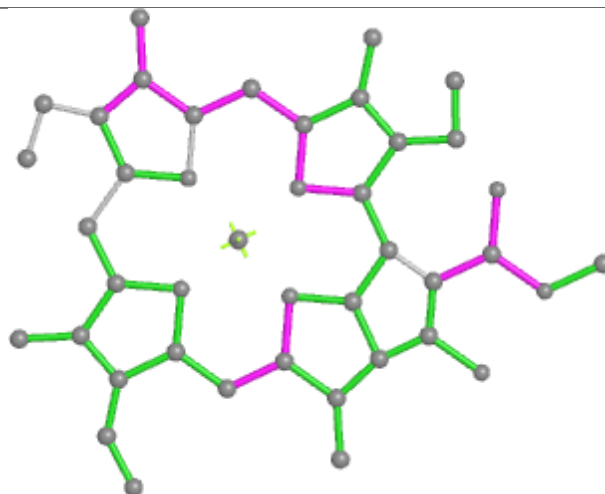




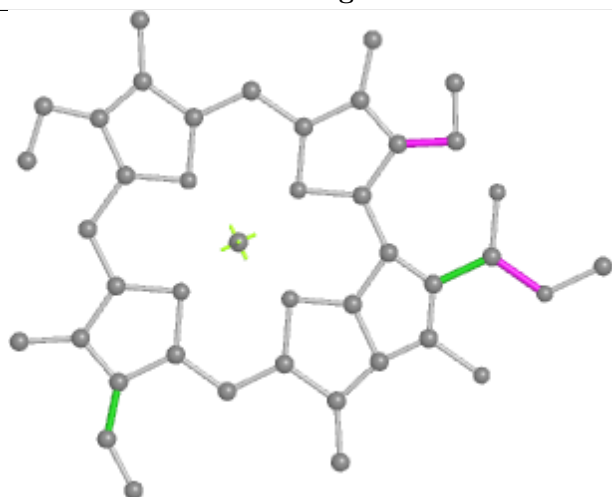
Ligand CLA B 822



Bond lengths



Bond angles

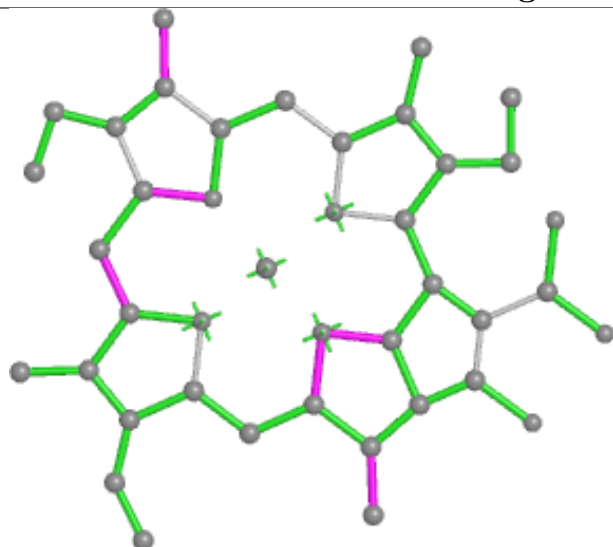


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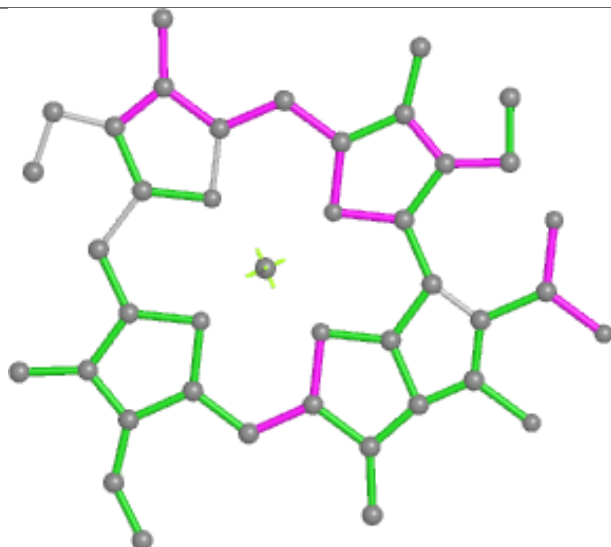


Rings

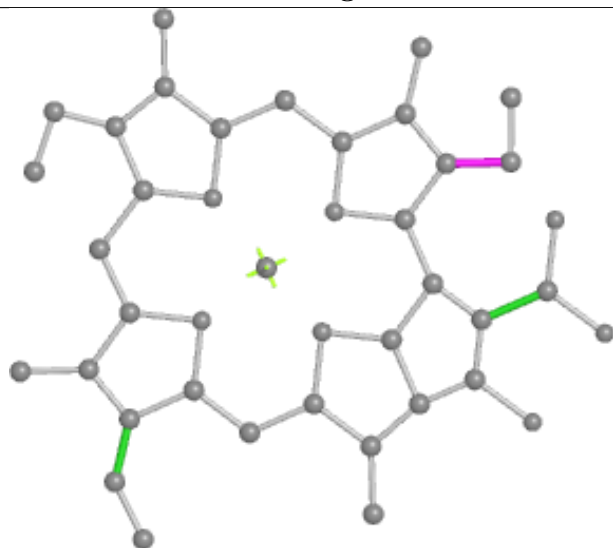
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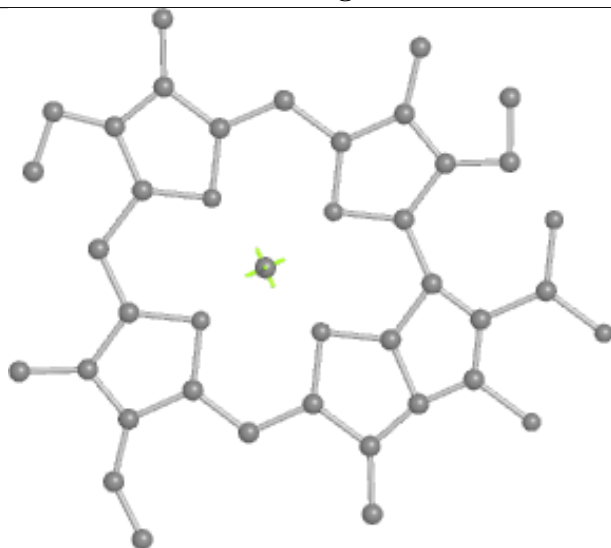
Bond lengths



Bond angles

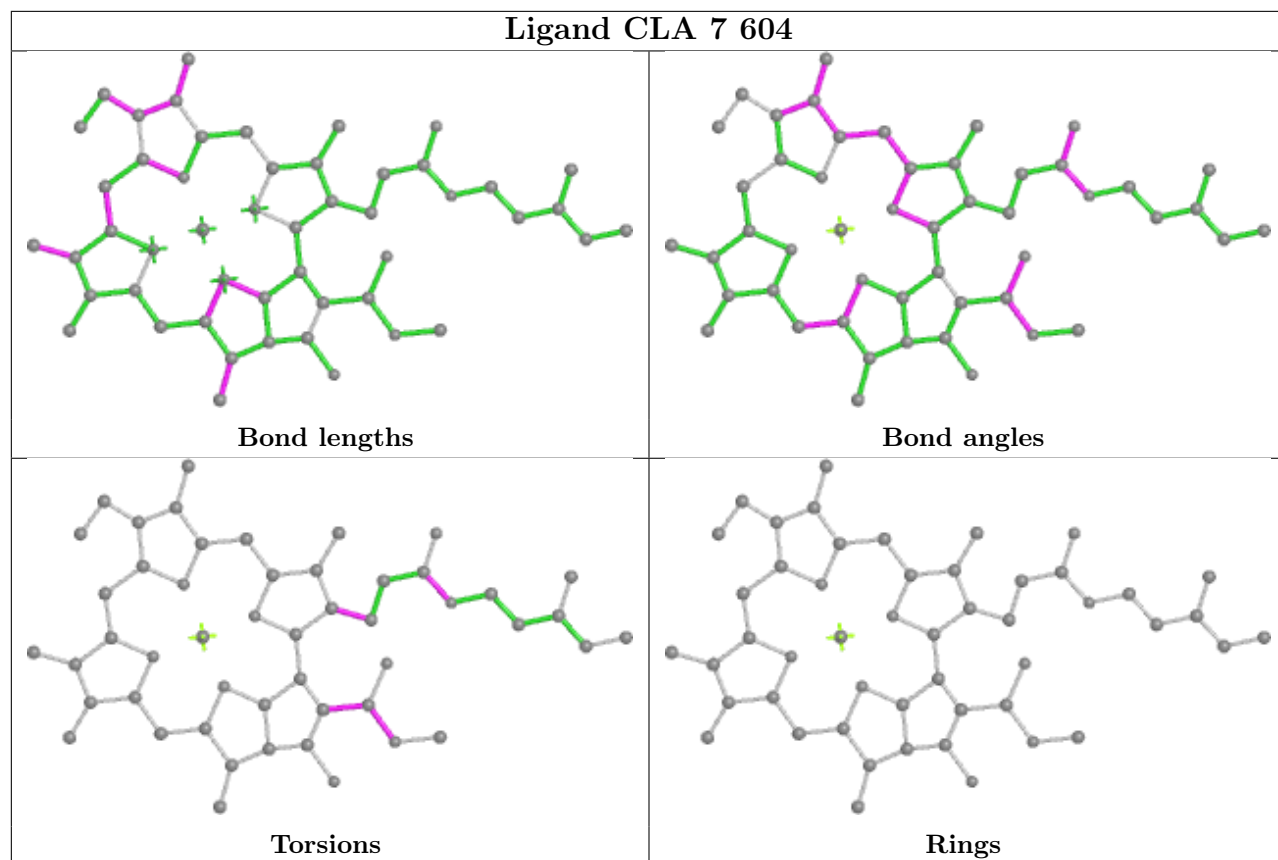


Torsions

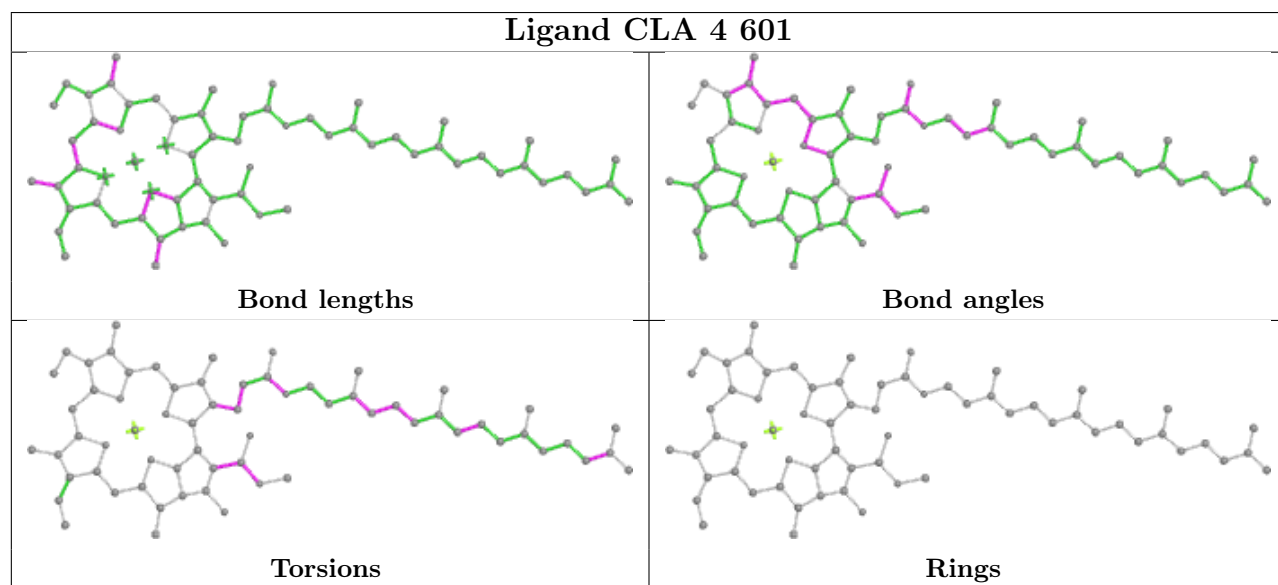


Rings

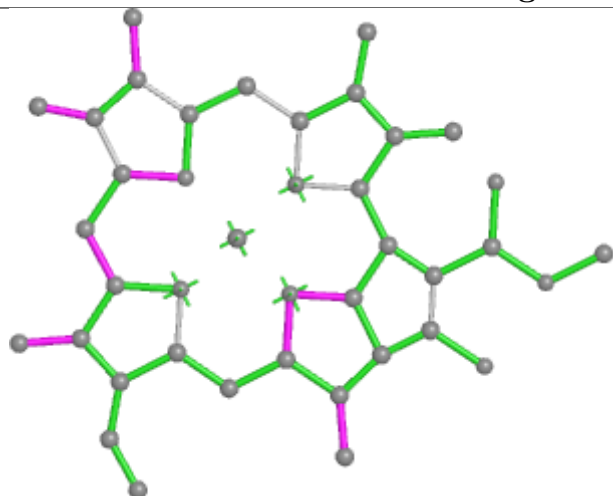
Ligand CLA 7 604



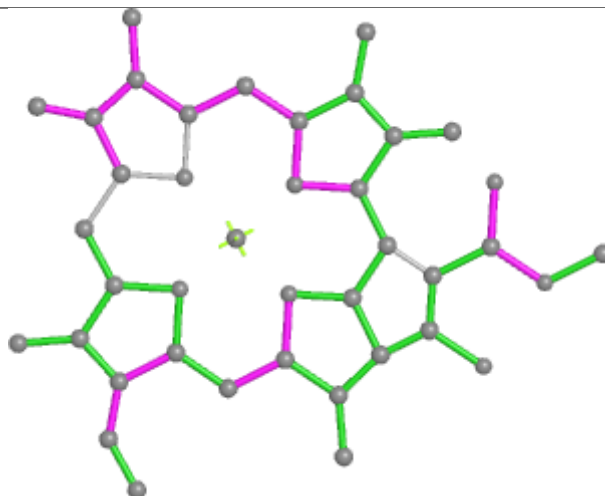
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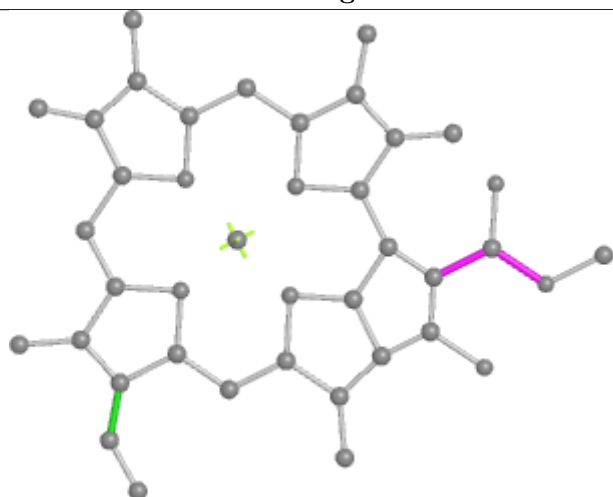
Ligand CLA 1 609



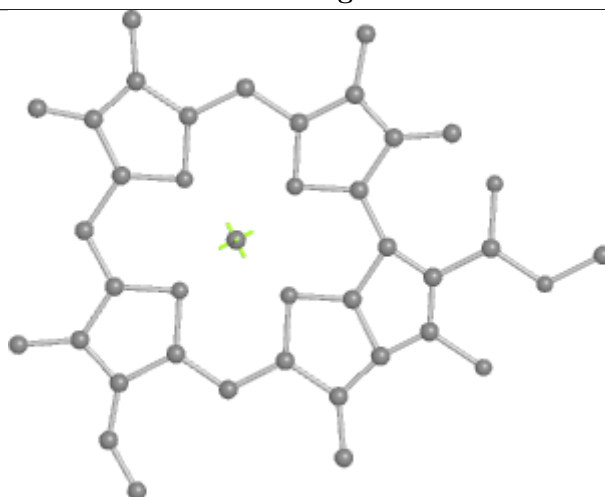
Bond lengths



Bond angles

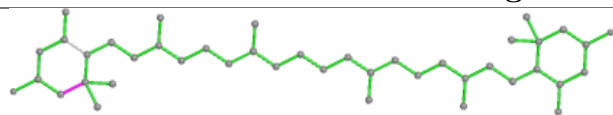


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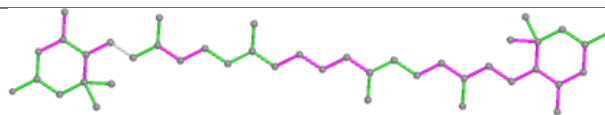


Rings

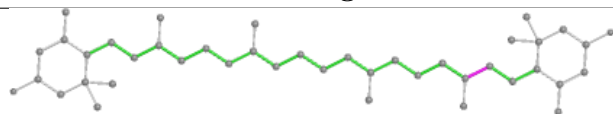
Ligand LUT X 1621



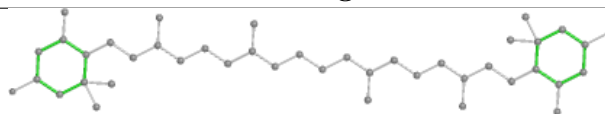
Bond lengths



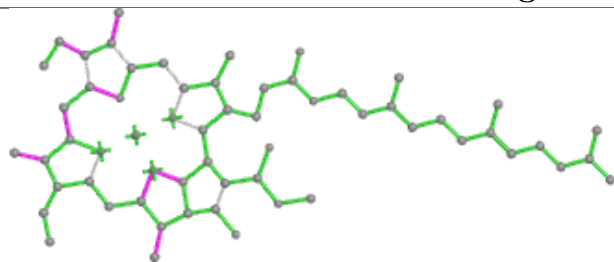
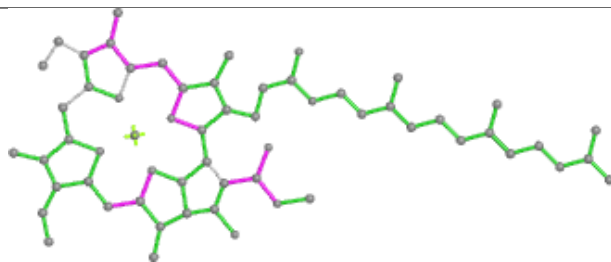
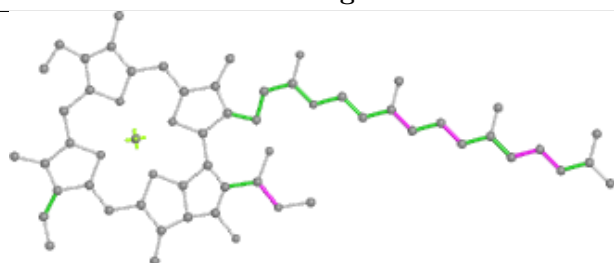
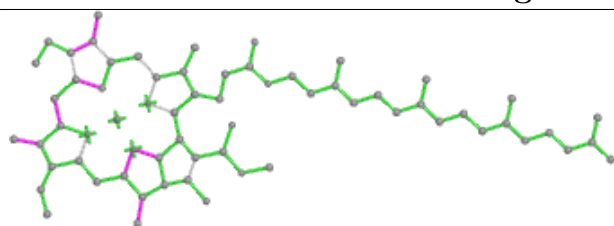
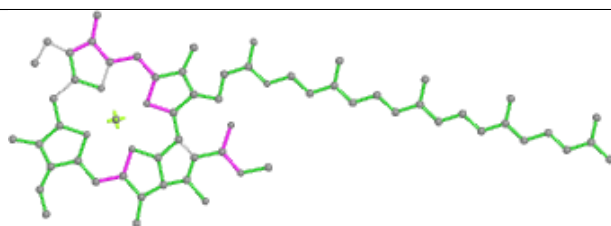
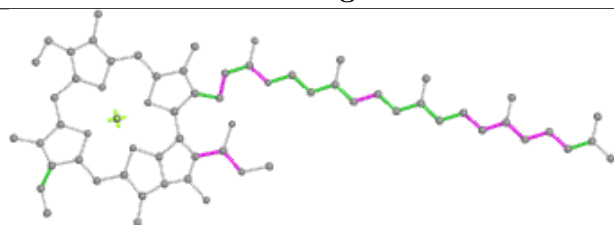
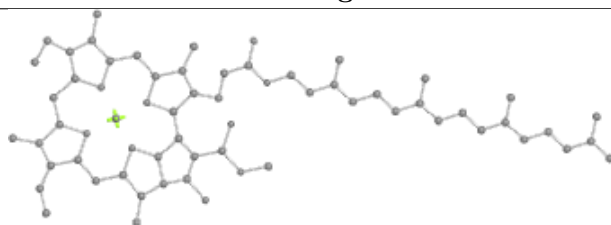
Bond angles



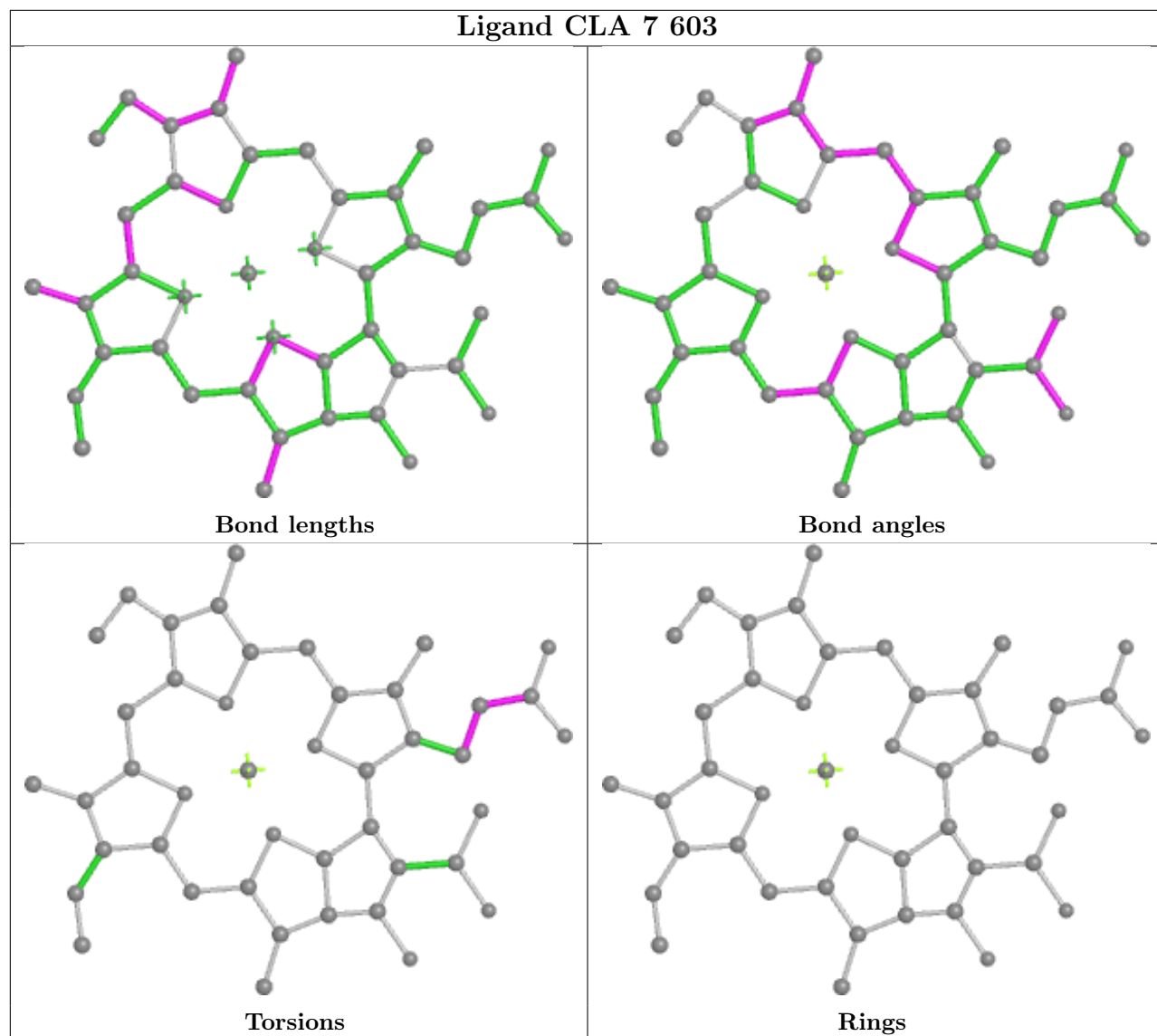
Torsions



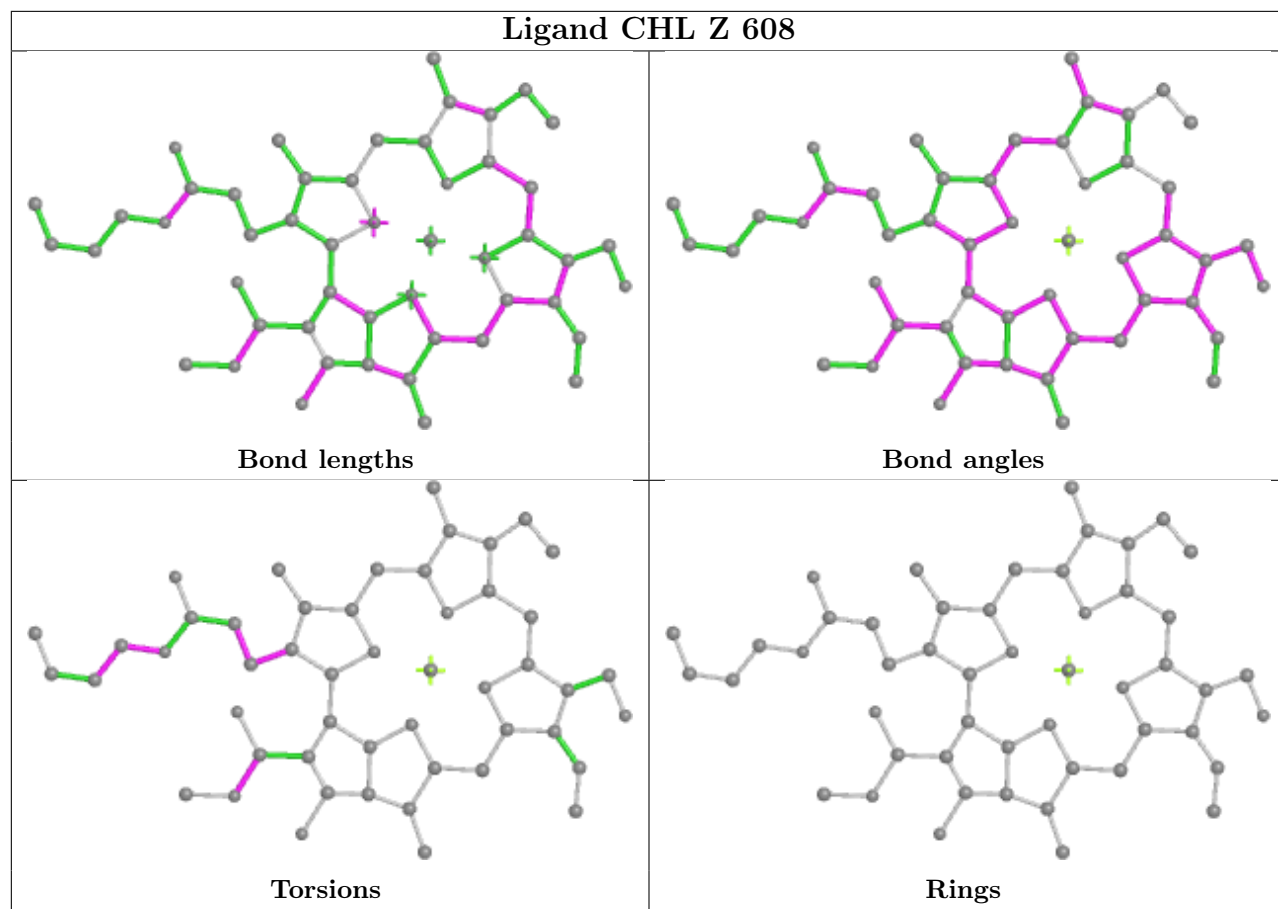
Rings

Ligand CLA 9 602**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 839****Bond lengths****Bond angles****Torsions****Rings**

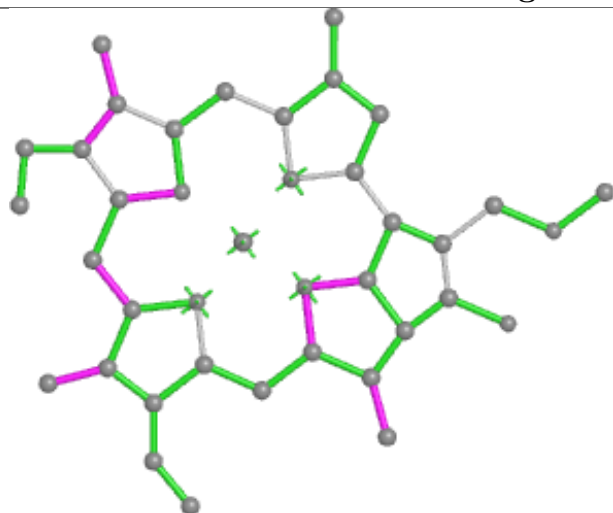
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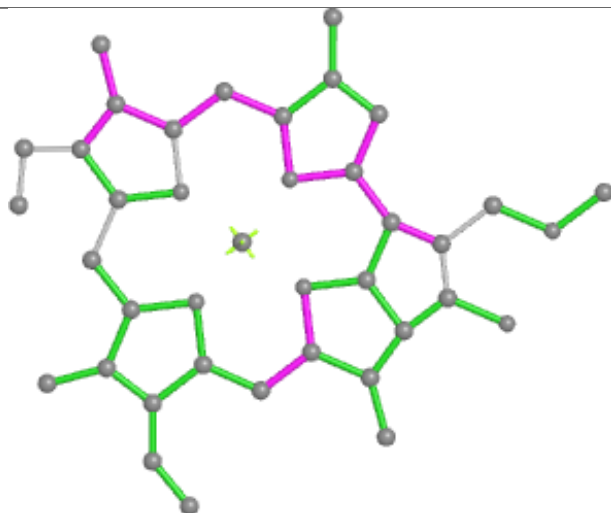
Ligand CHL Z 608



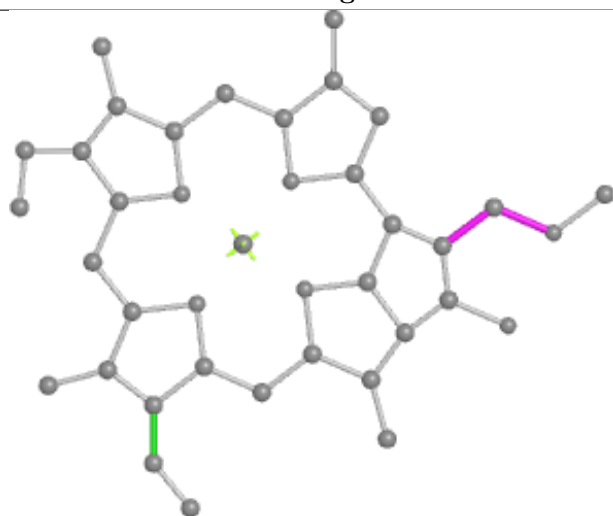
Ligand CLA 1 606



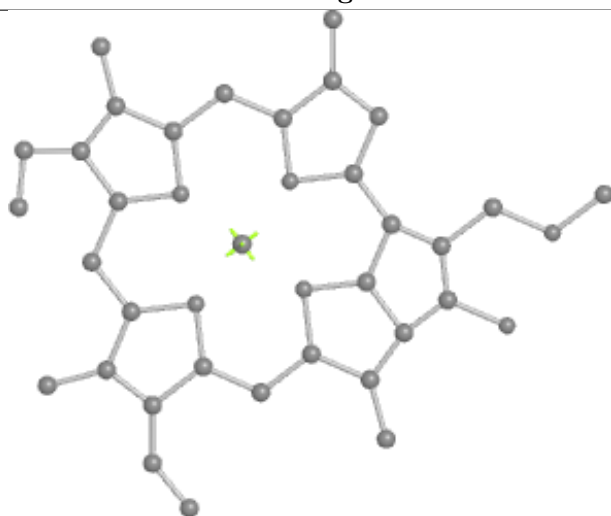
Bond lengths



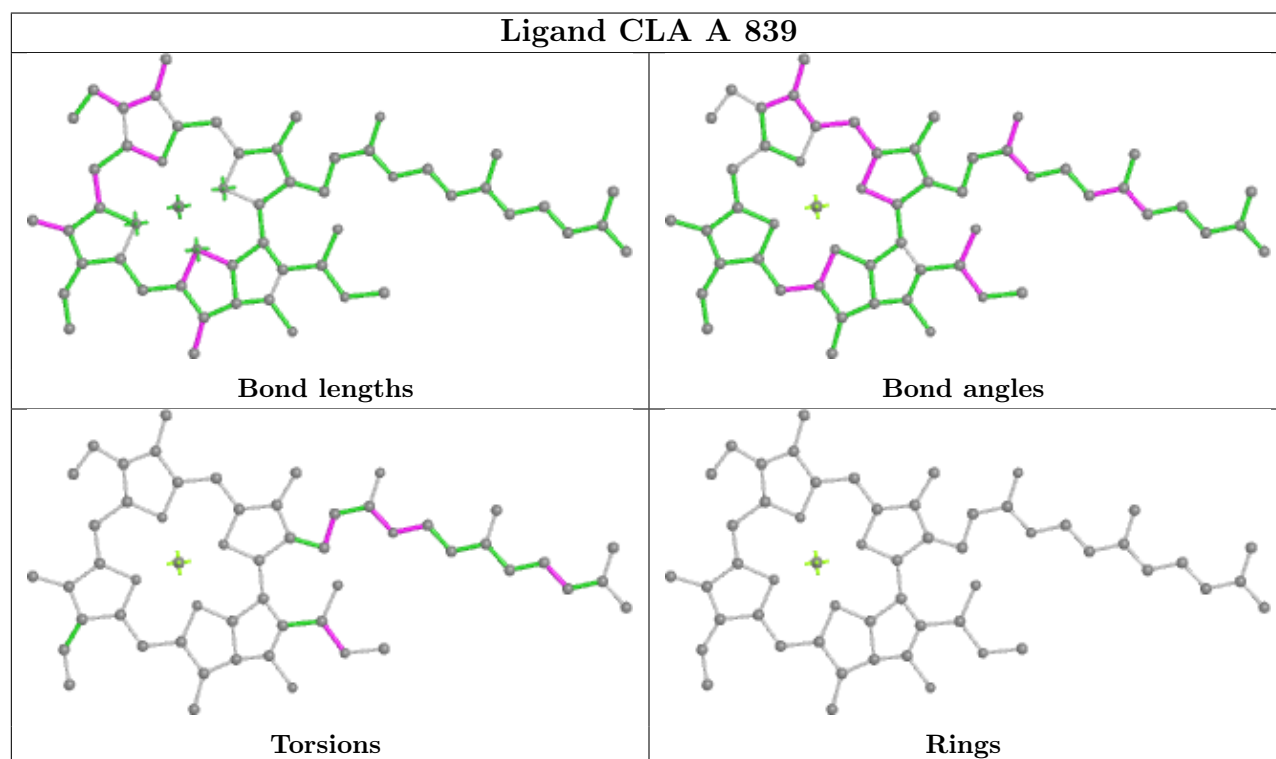
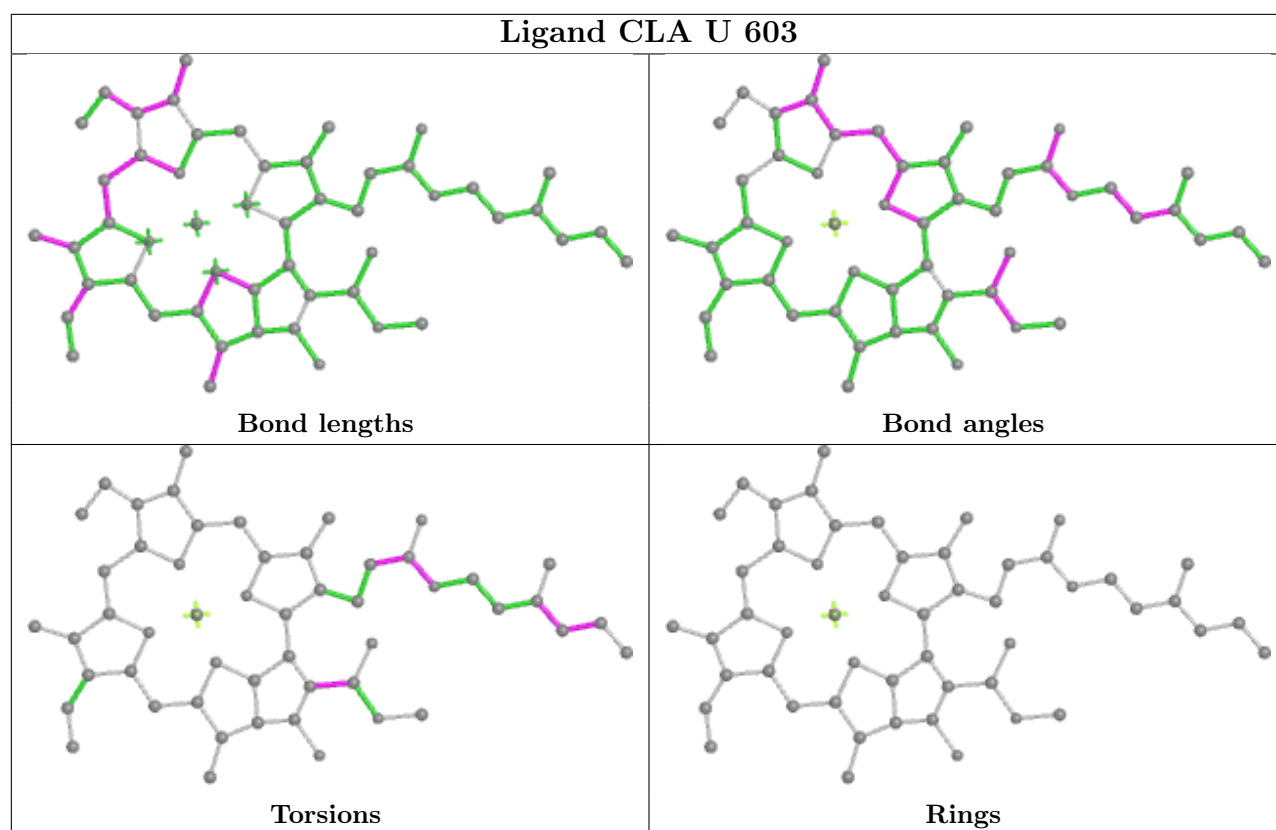
Bond angles

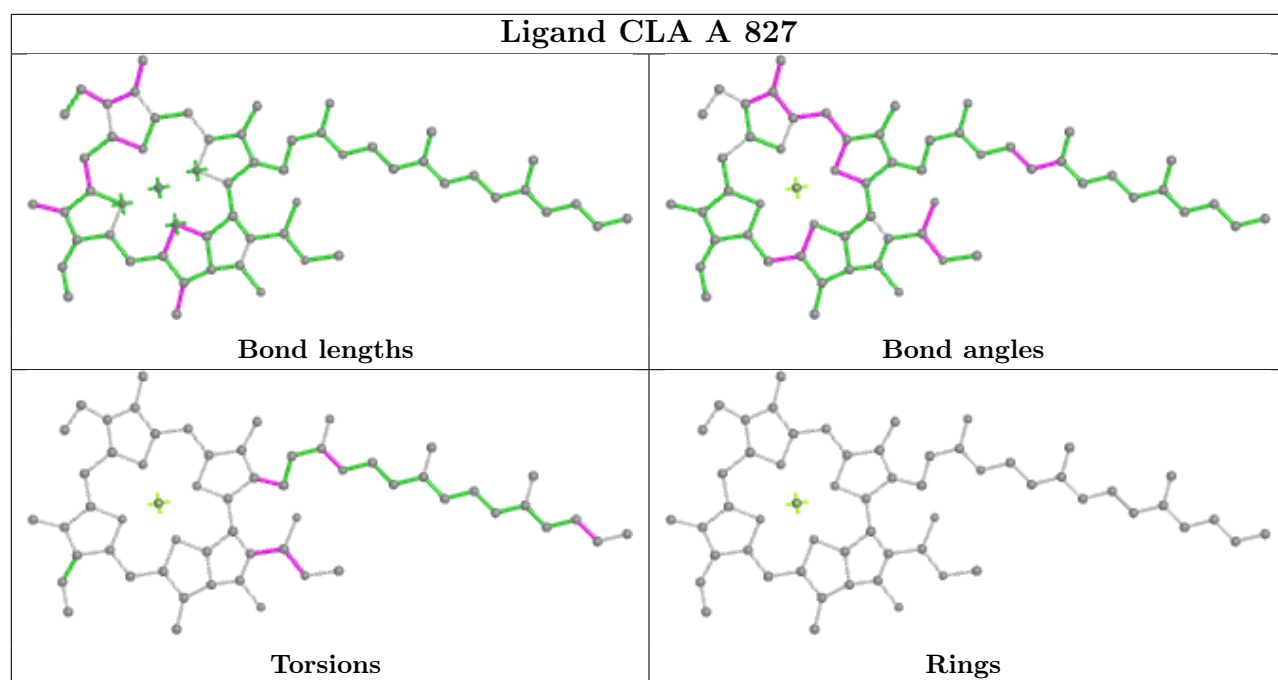


Torsions

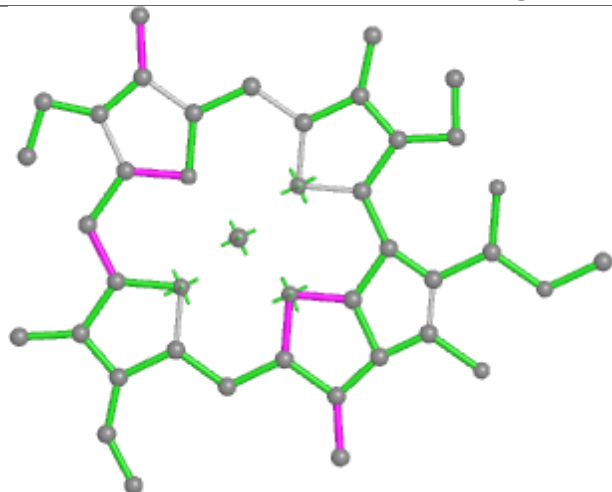


Rings

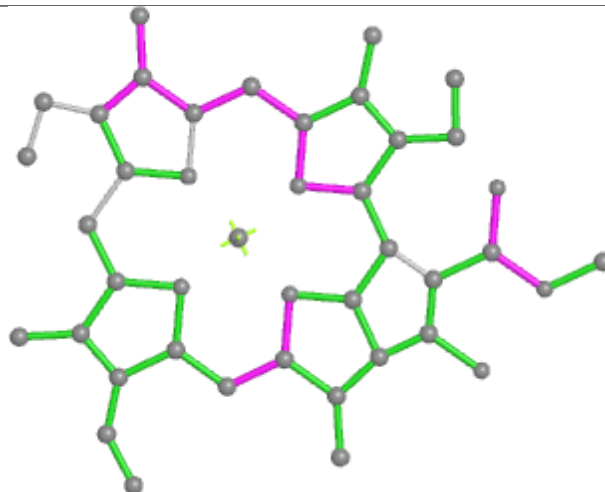




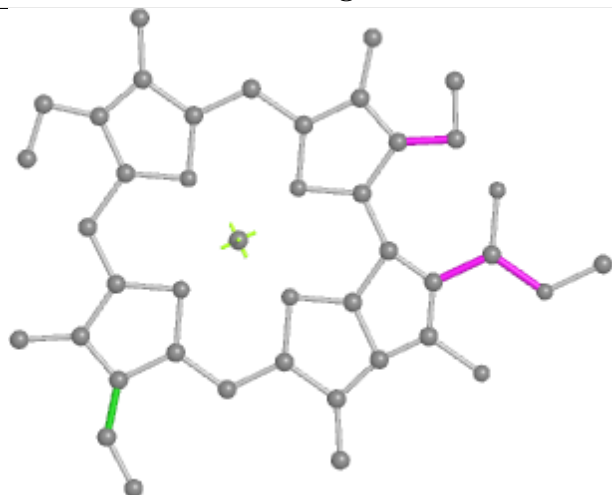
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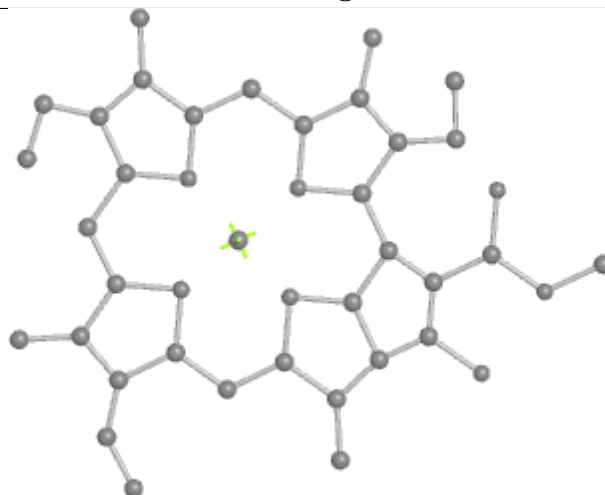
Bond lengths



Bond angles

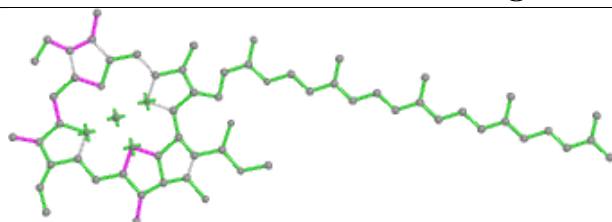


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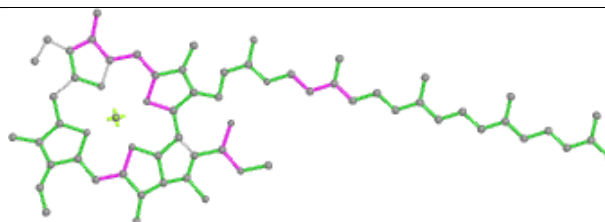


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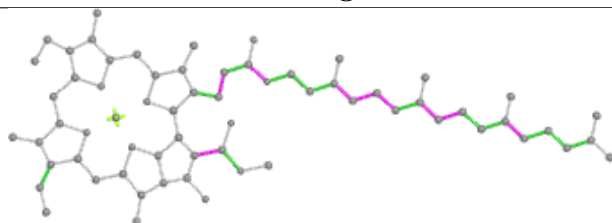
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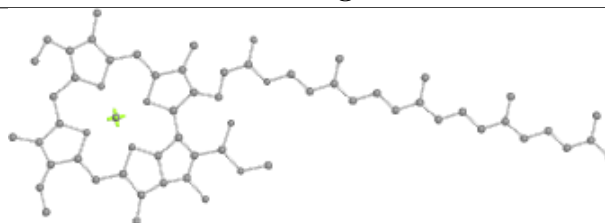
Bond lengths



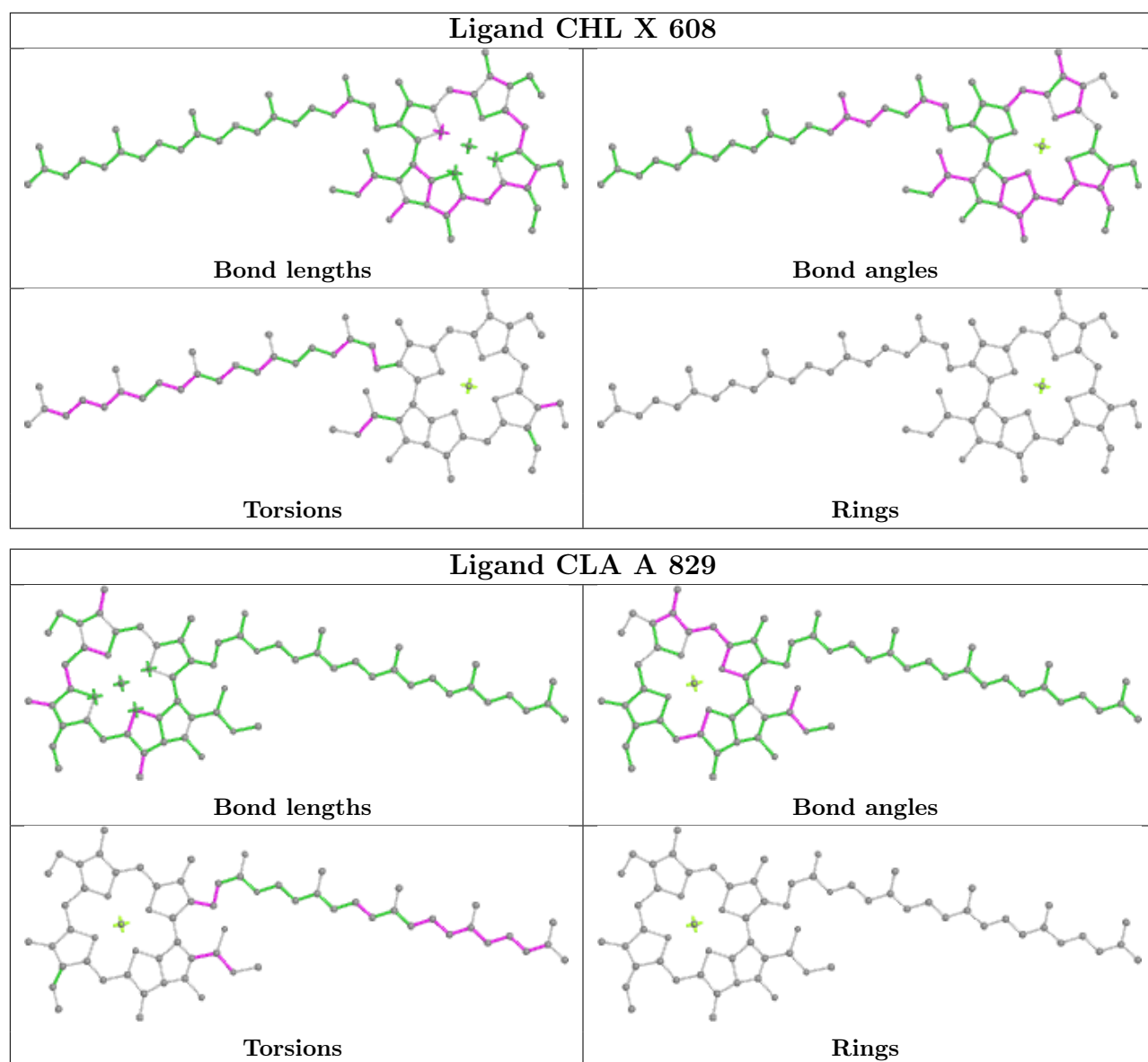
Bond angles



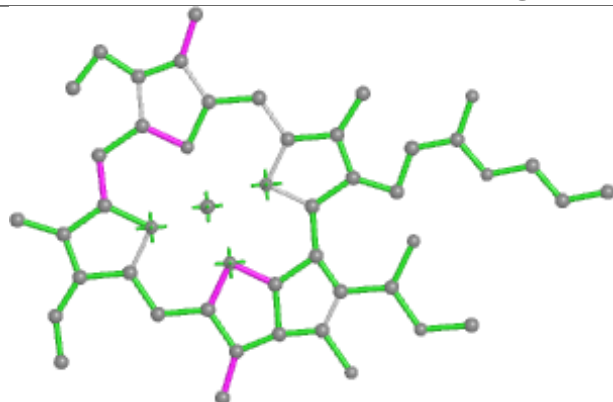
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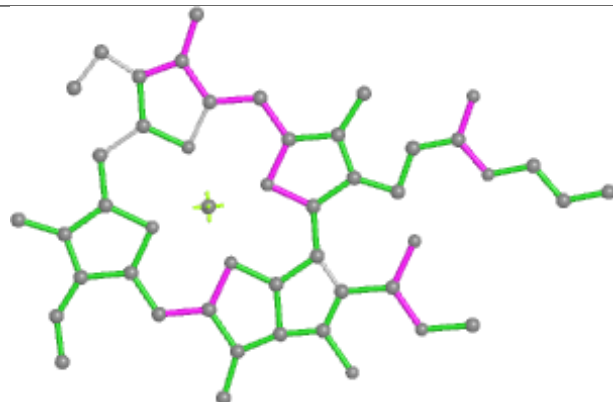
Rings



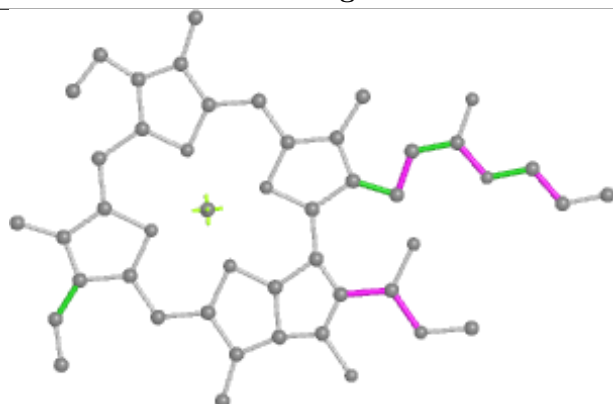
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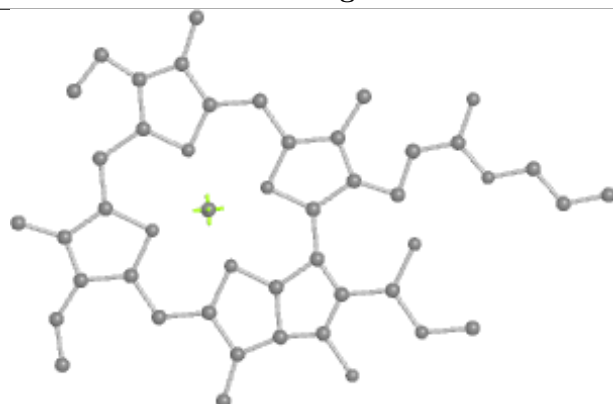
Bond lengths



Bond angles

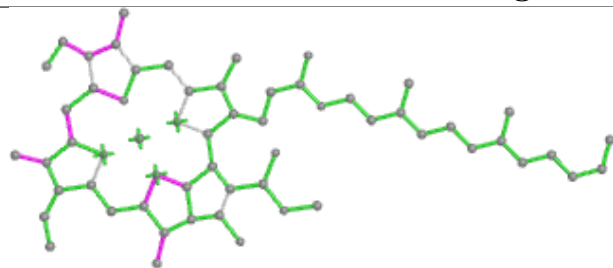


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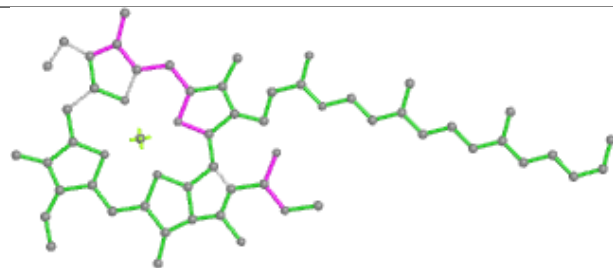


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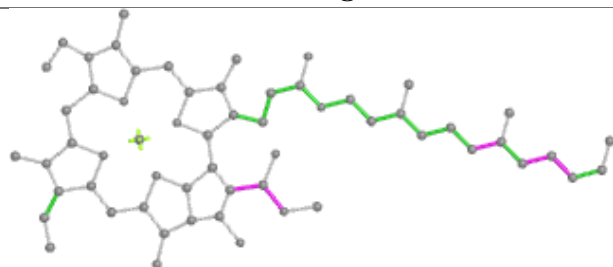
Ligand CLA U 602



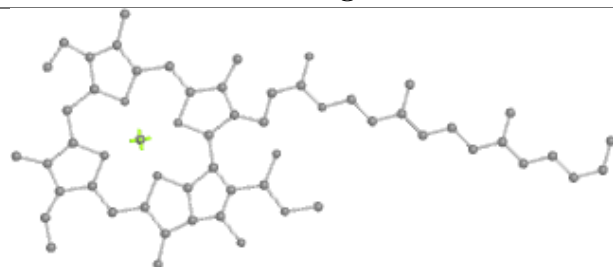
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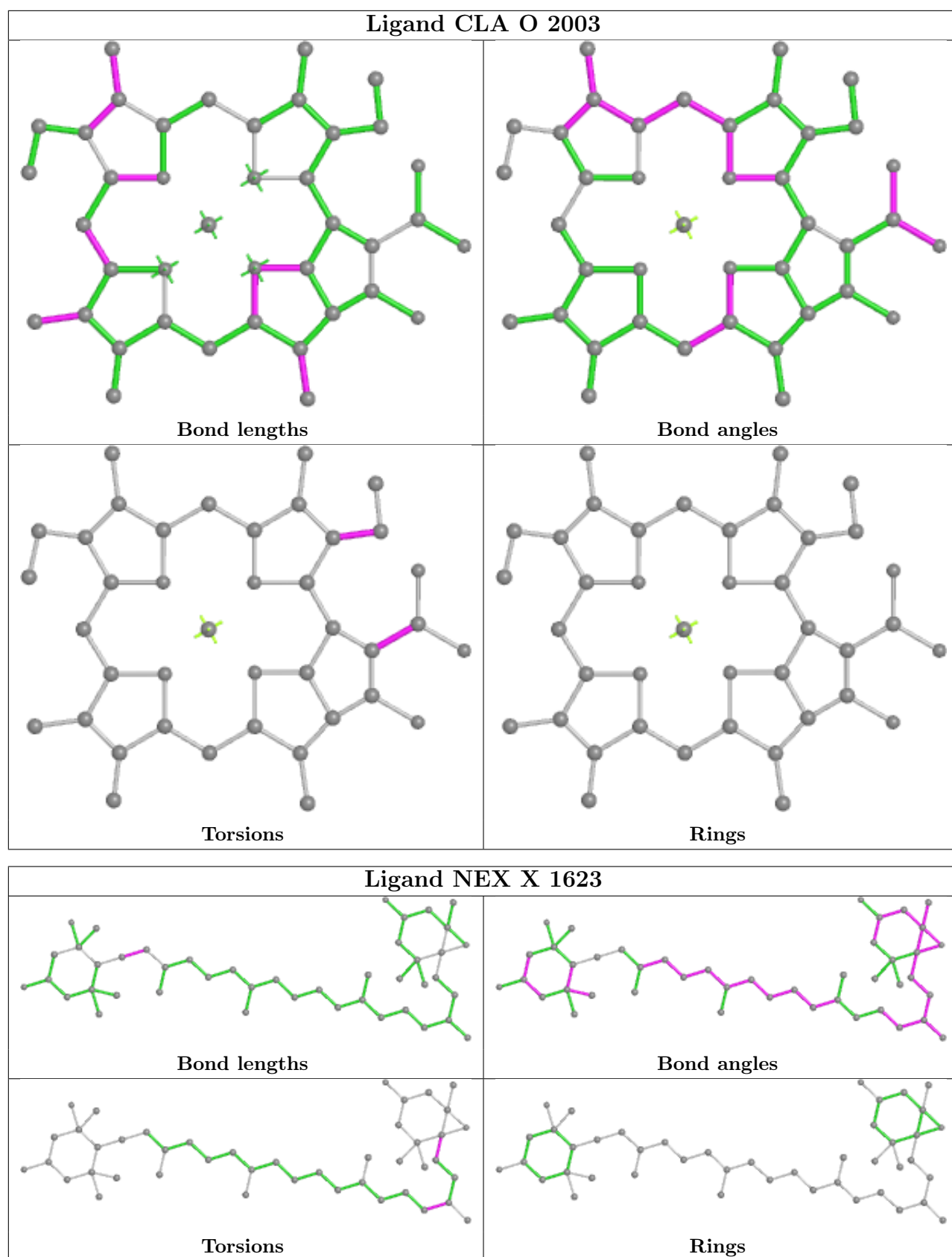
Bond angles

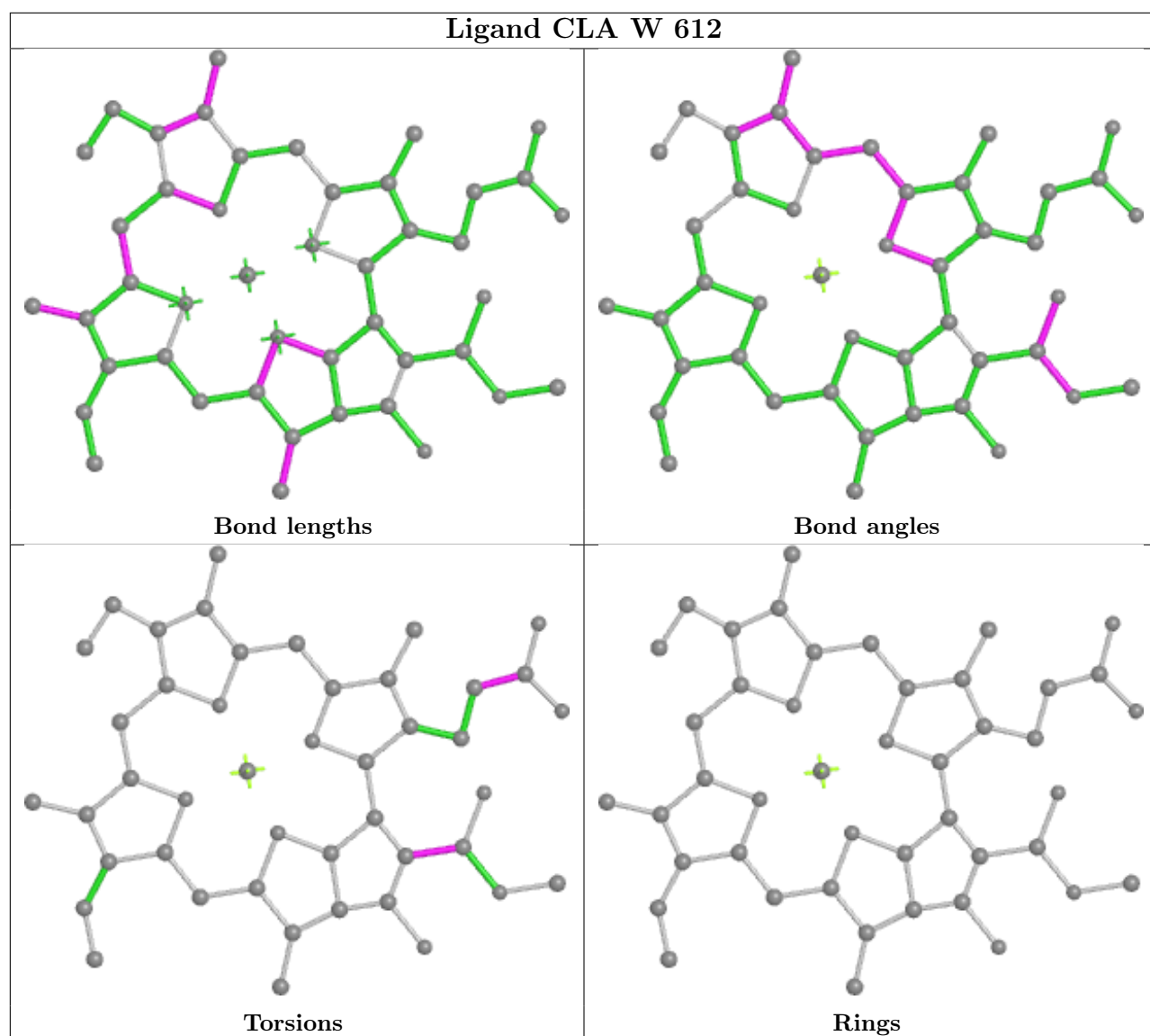


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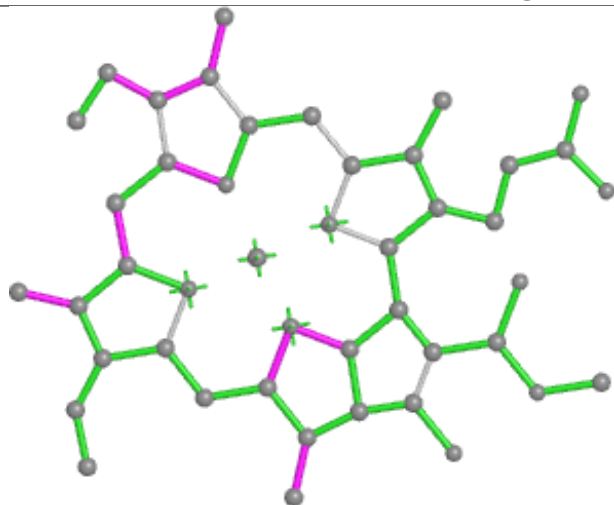


Rings

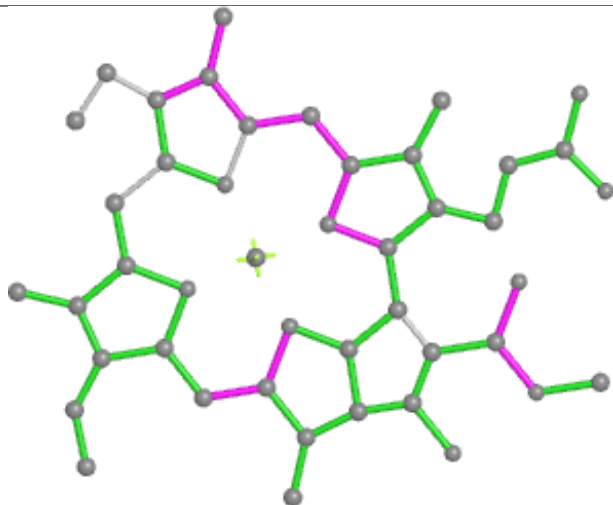




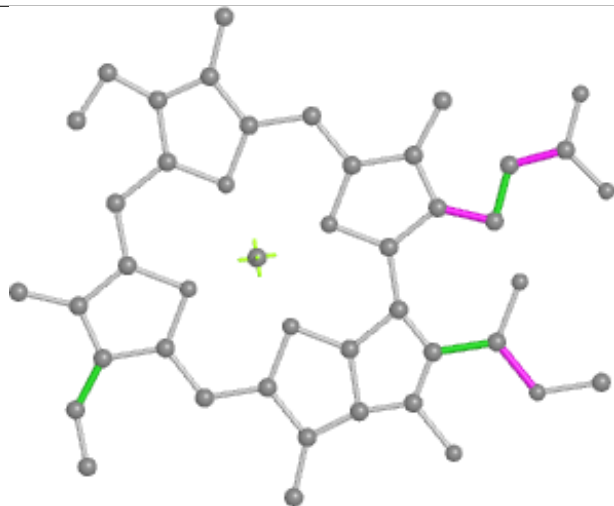
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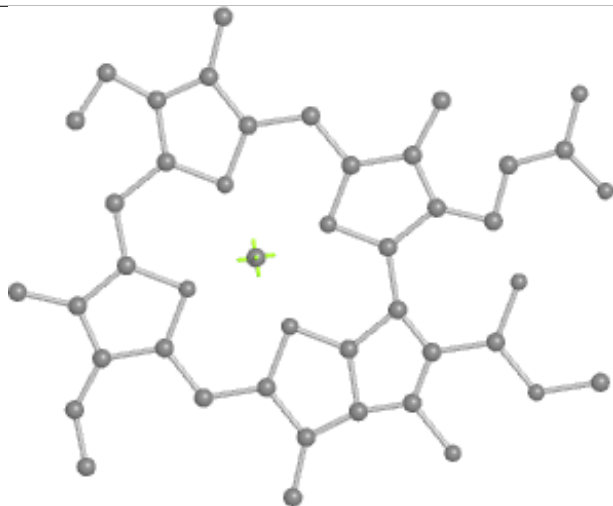
Bond lengths



Bond angles

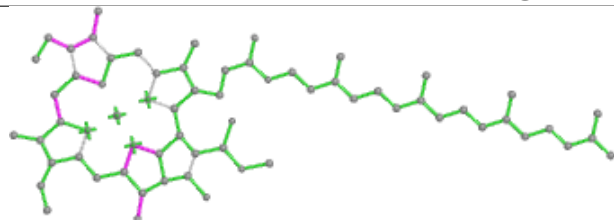


Torsions

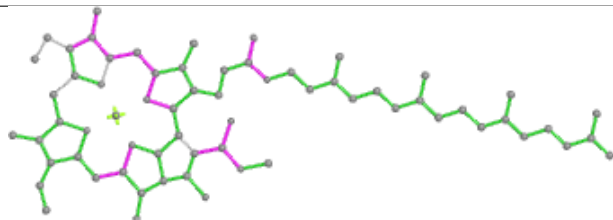


Rings

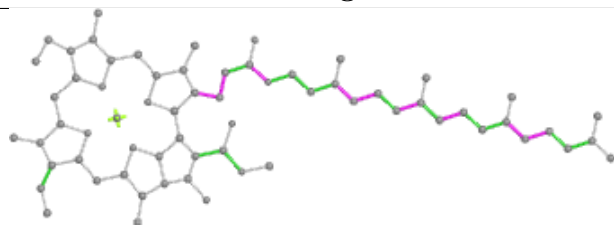
Ligand CLA L 303



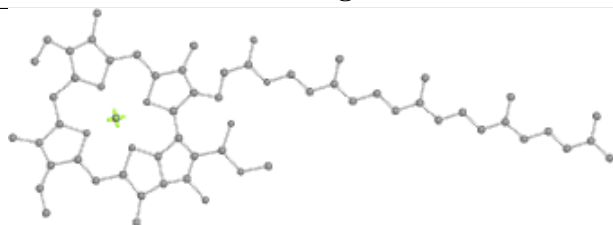
Bond lengths



Bond angles

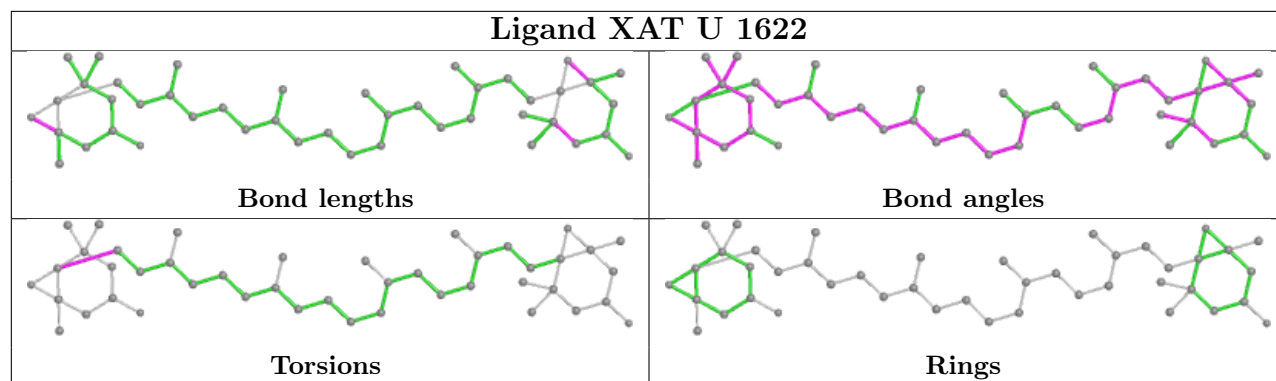


Torsions

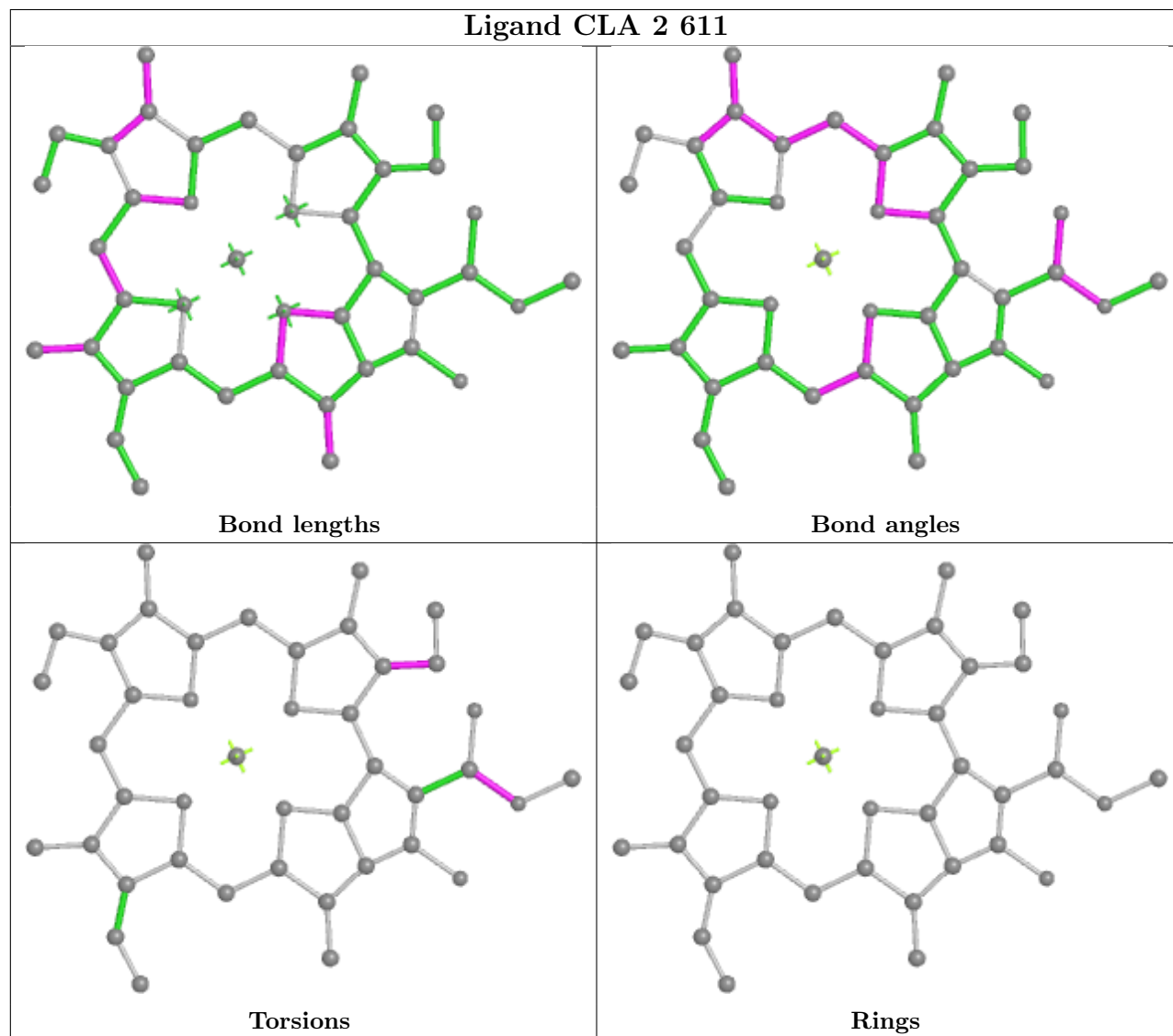


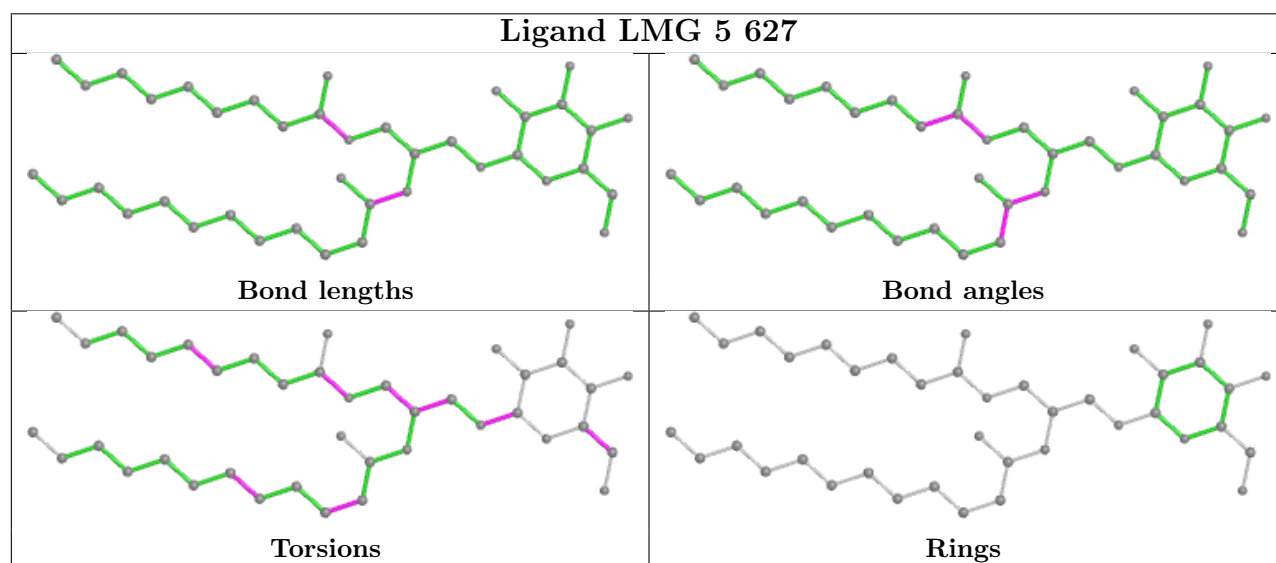
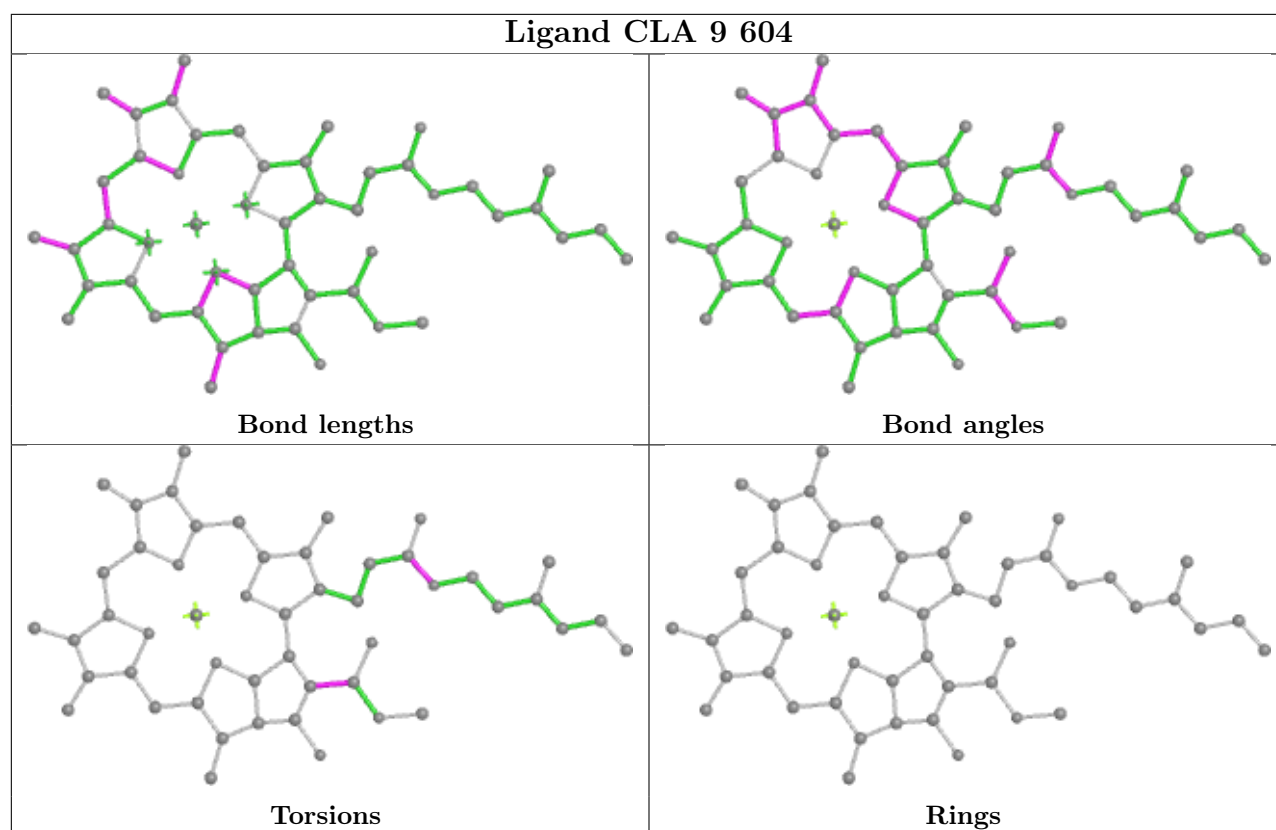
Rings

Ligand XAT U 1622

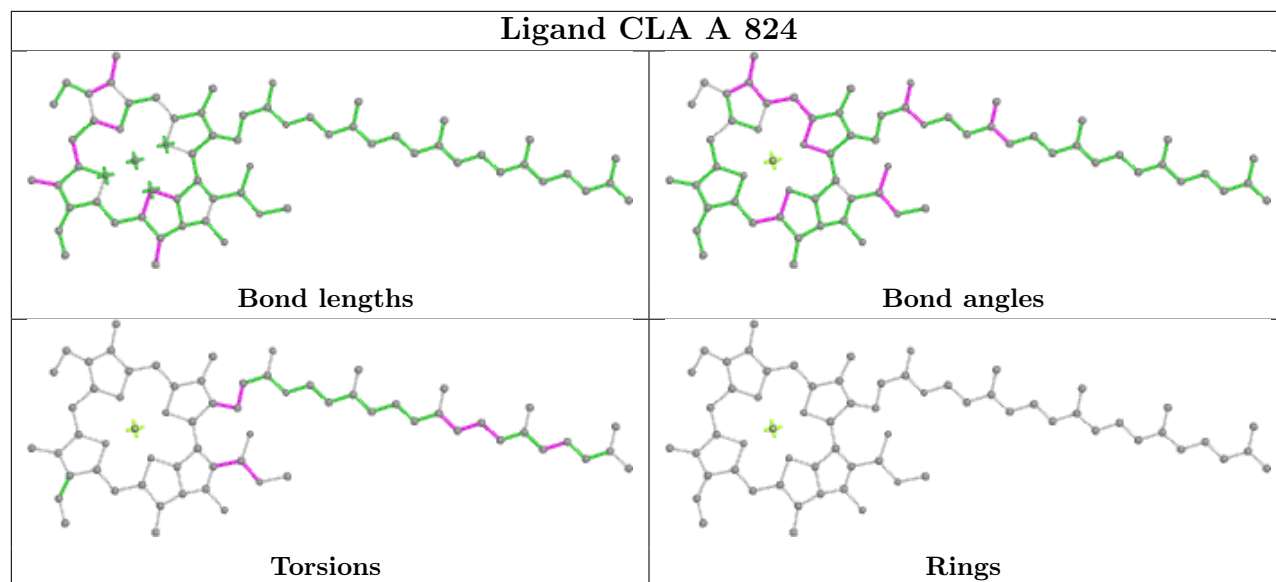


Ligand CLA 2 611

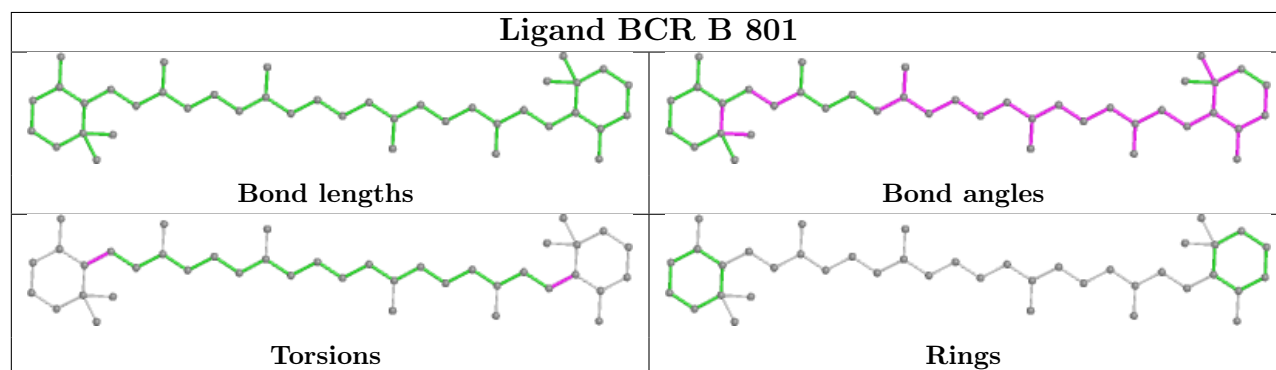




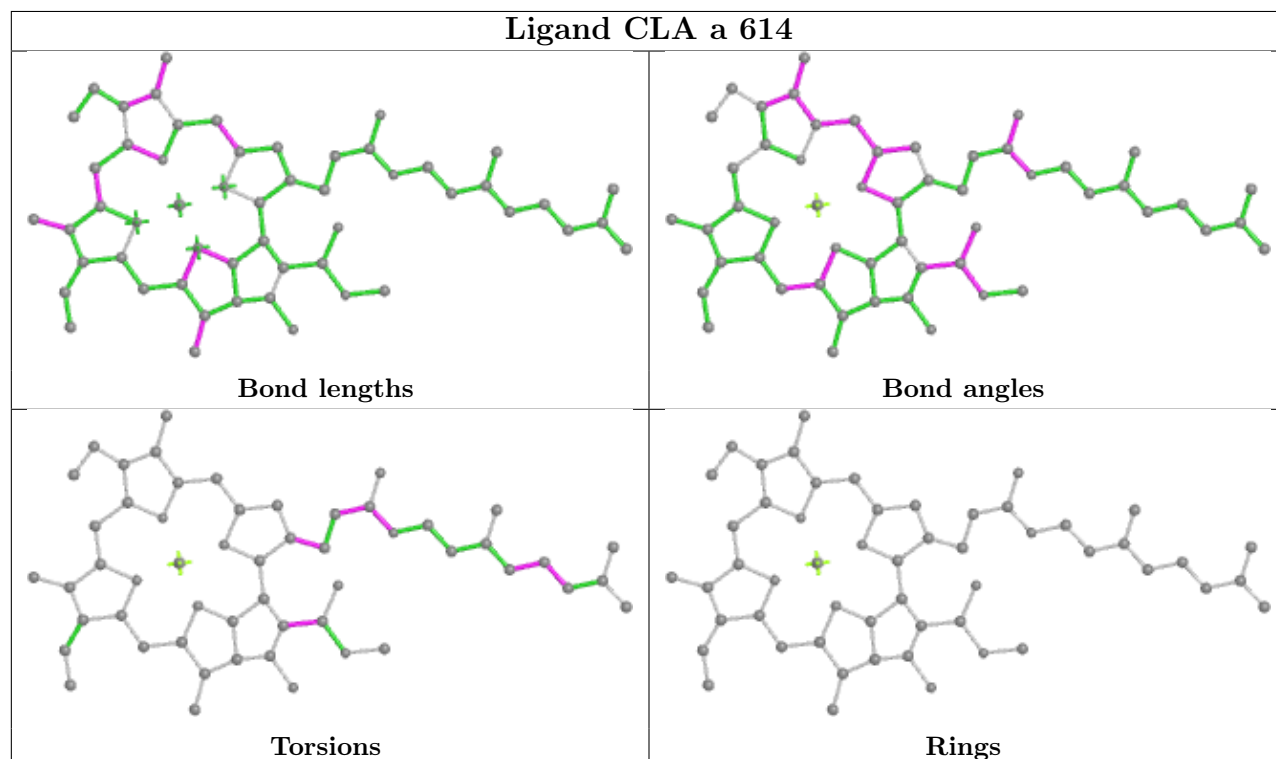
Ligand CLA A 824

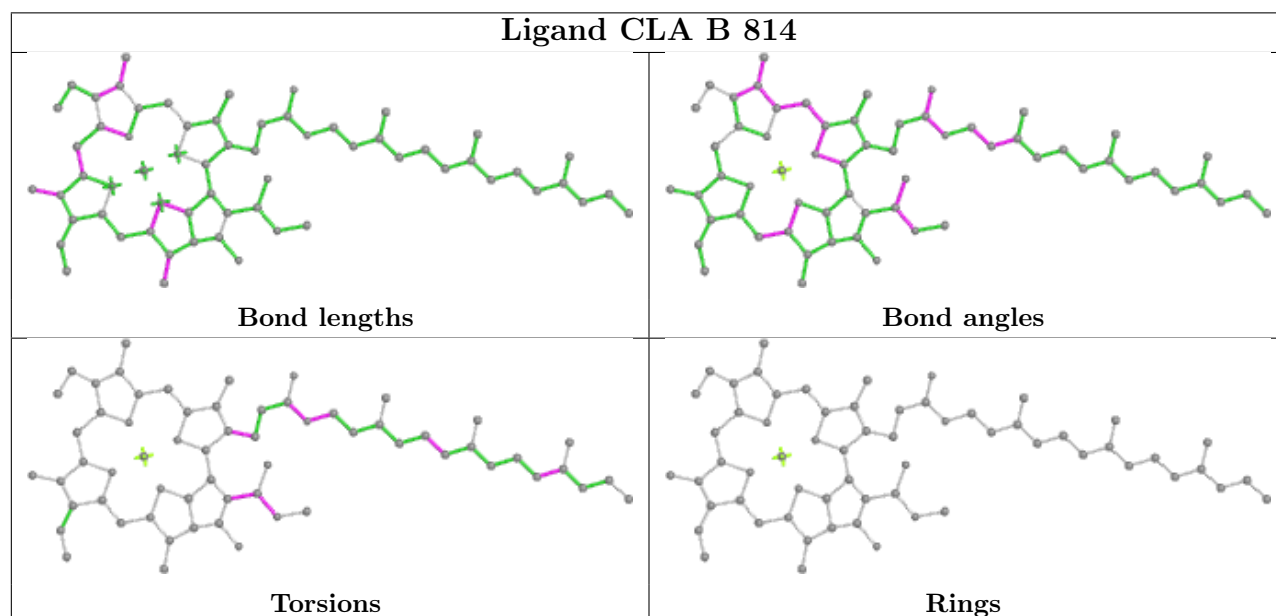
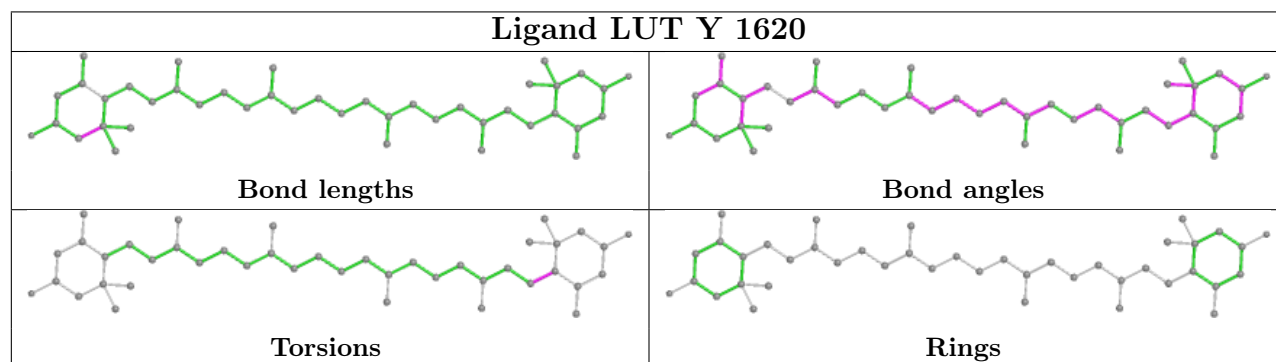
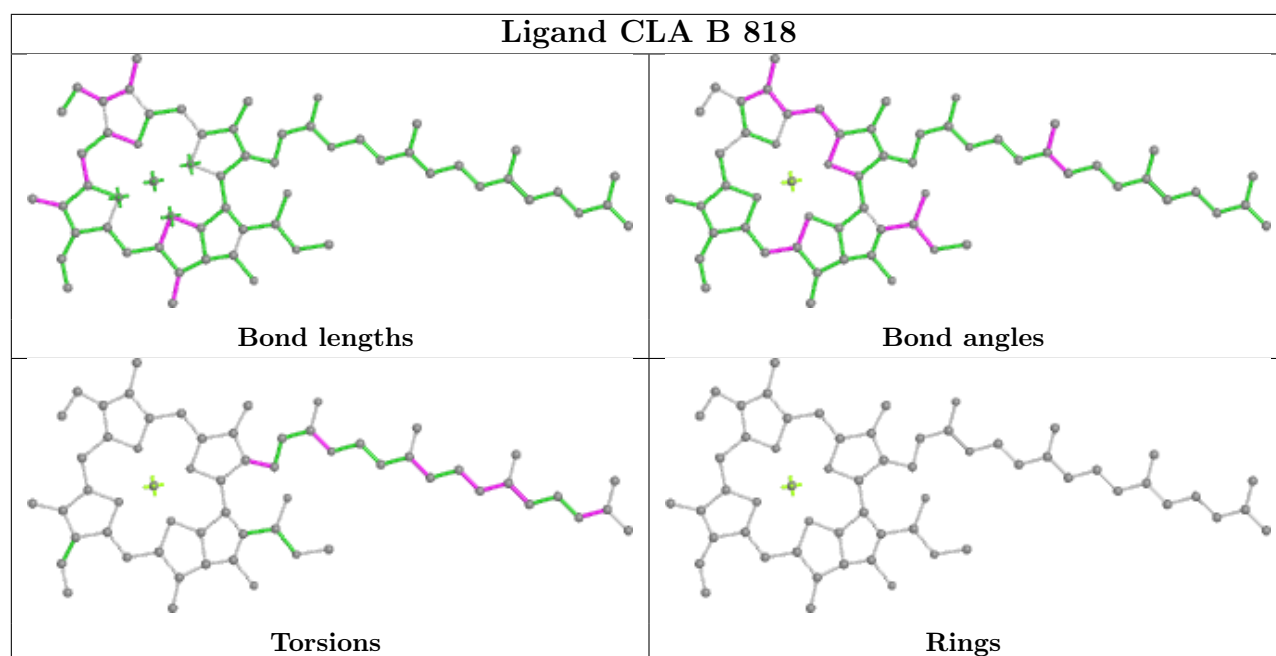


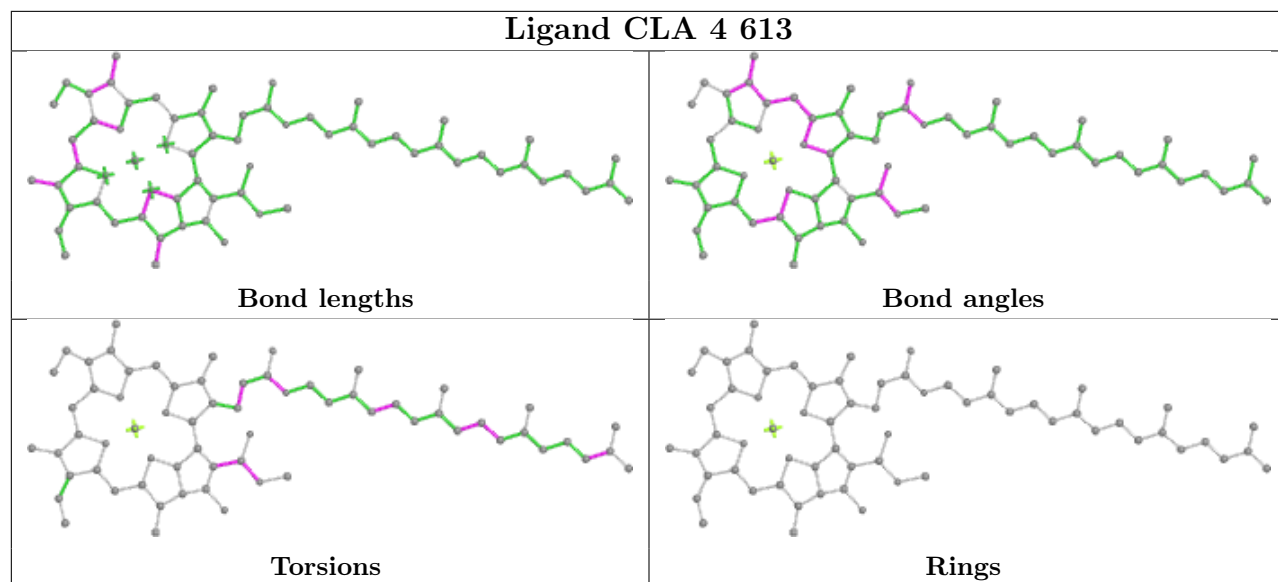
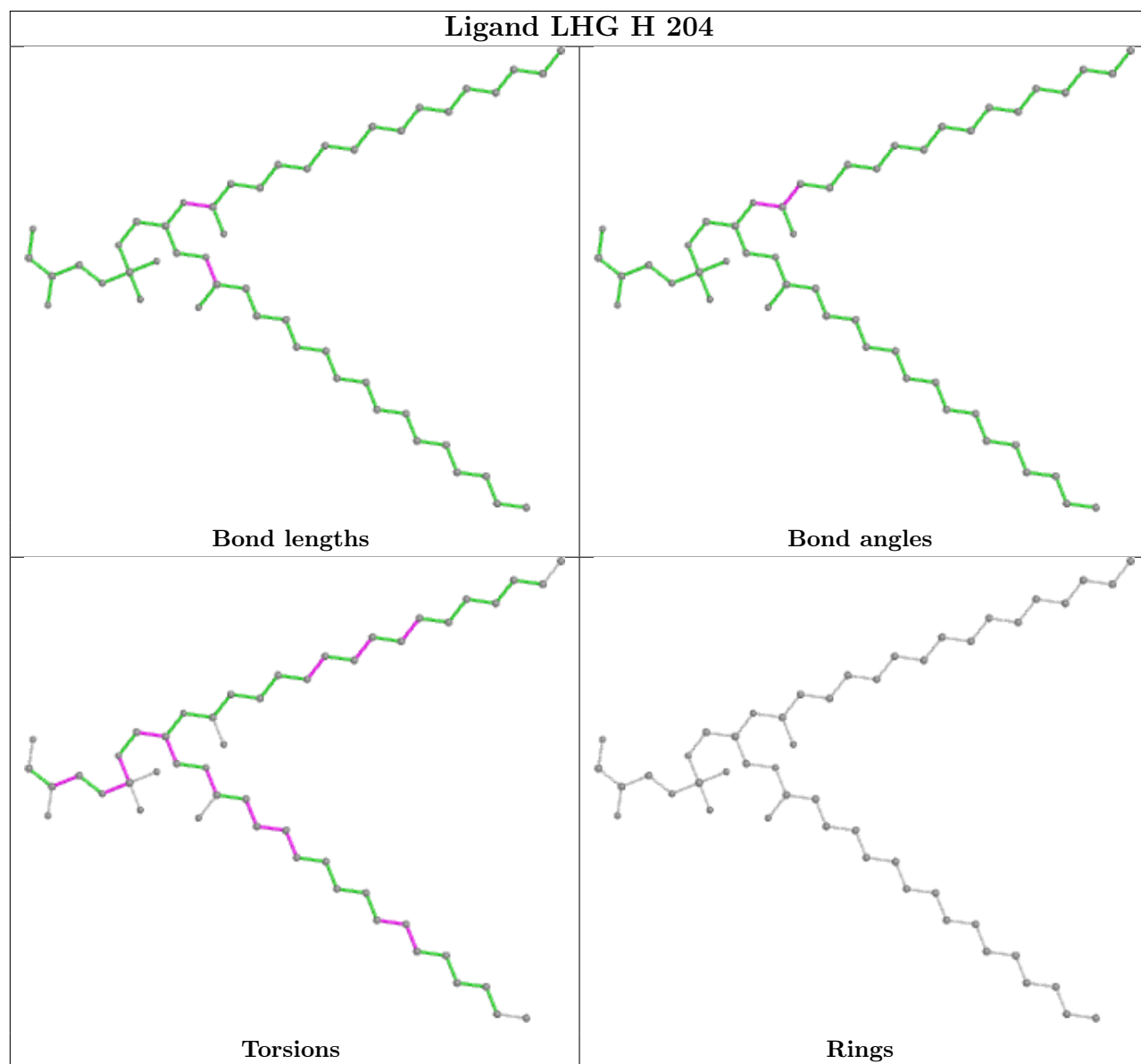
Ligand BCR B 801

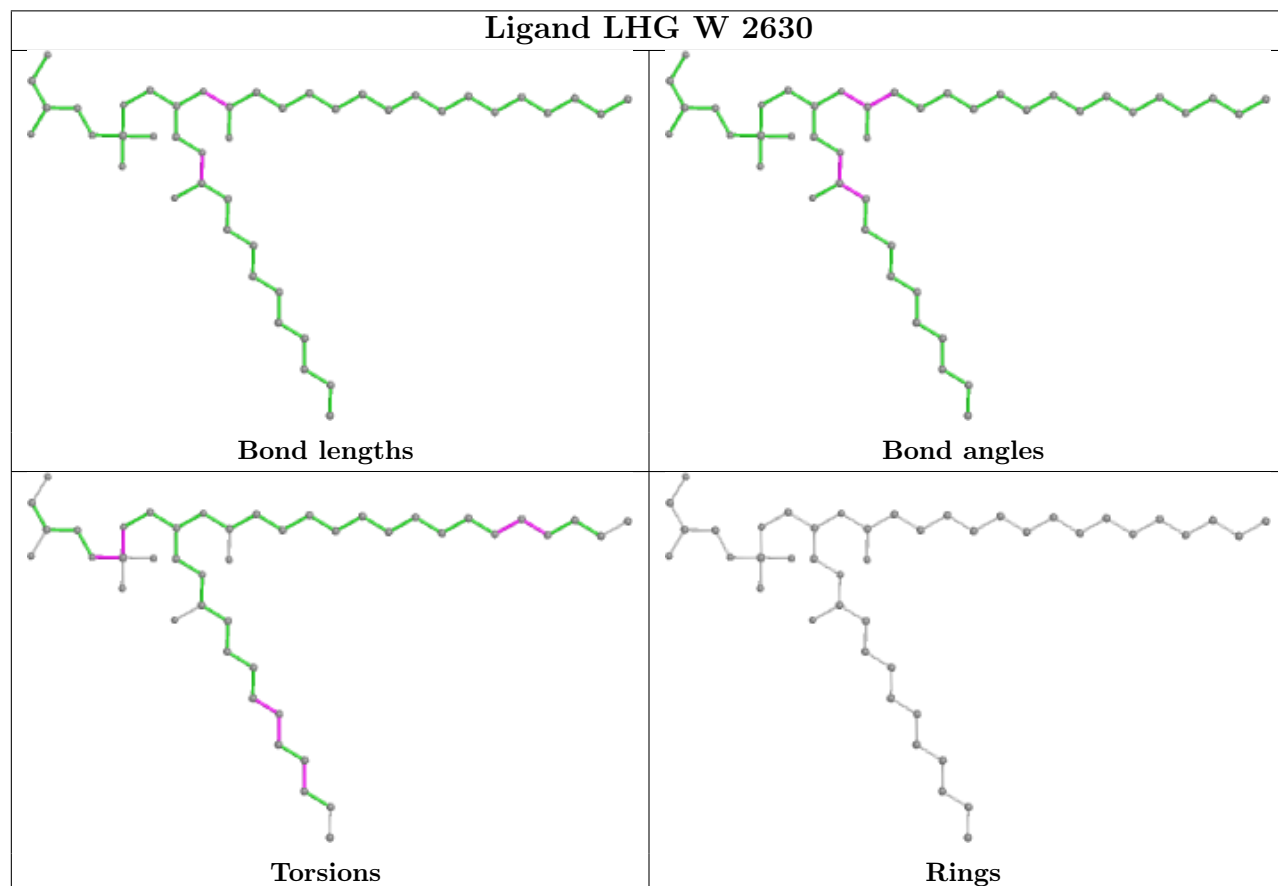
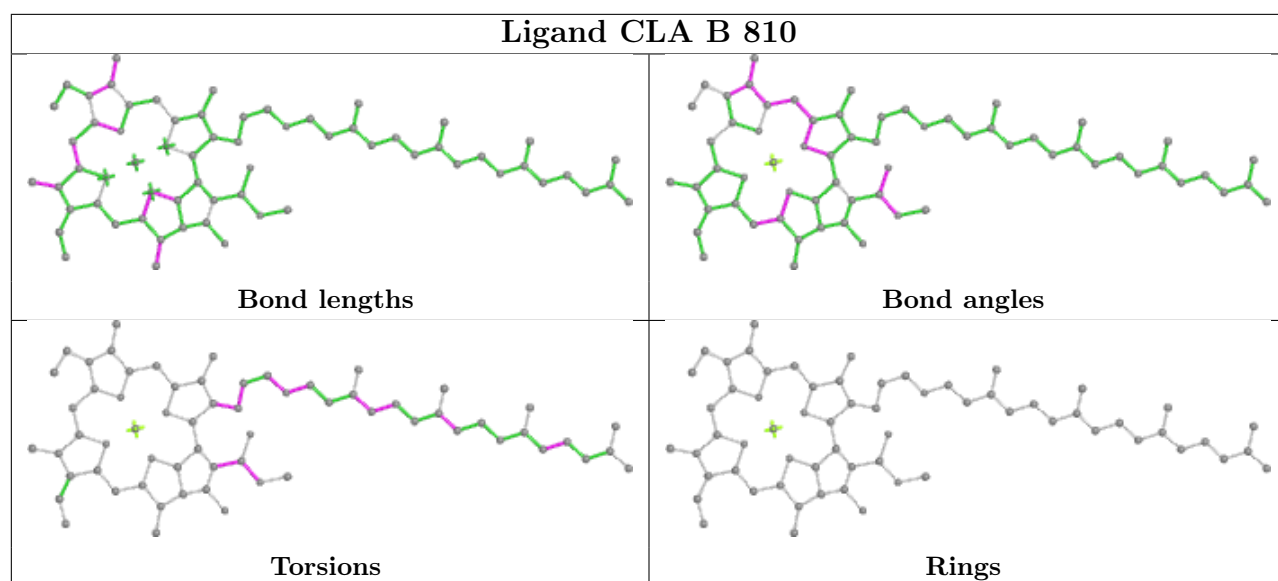


Ligand CLA a 614

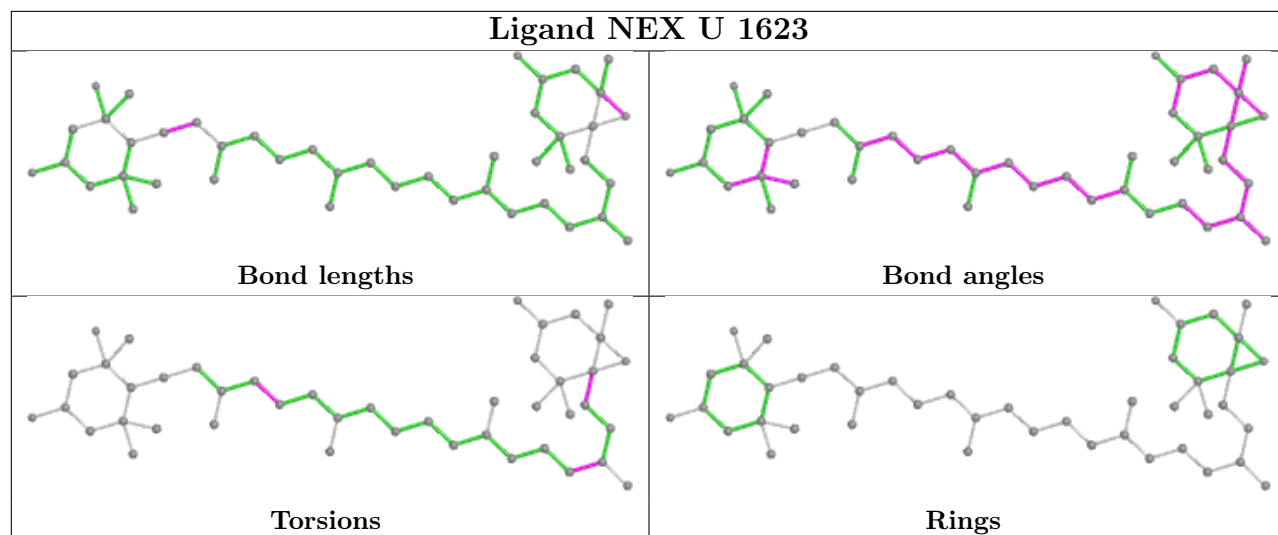




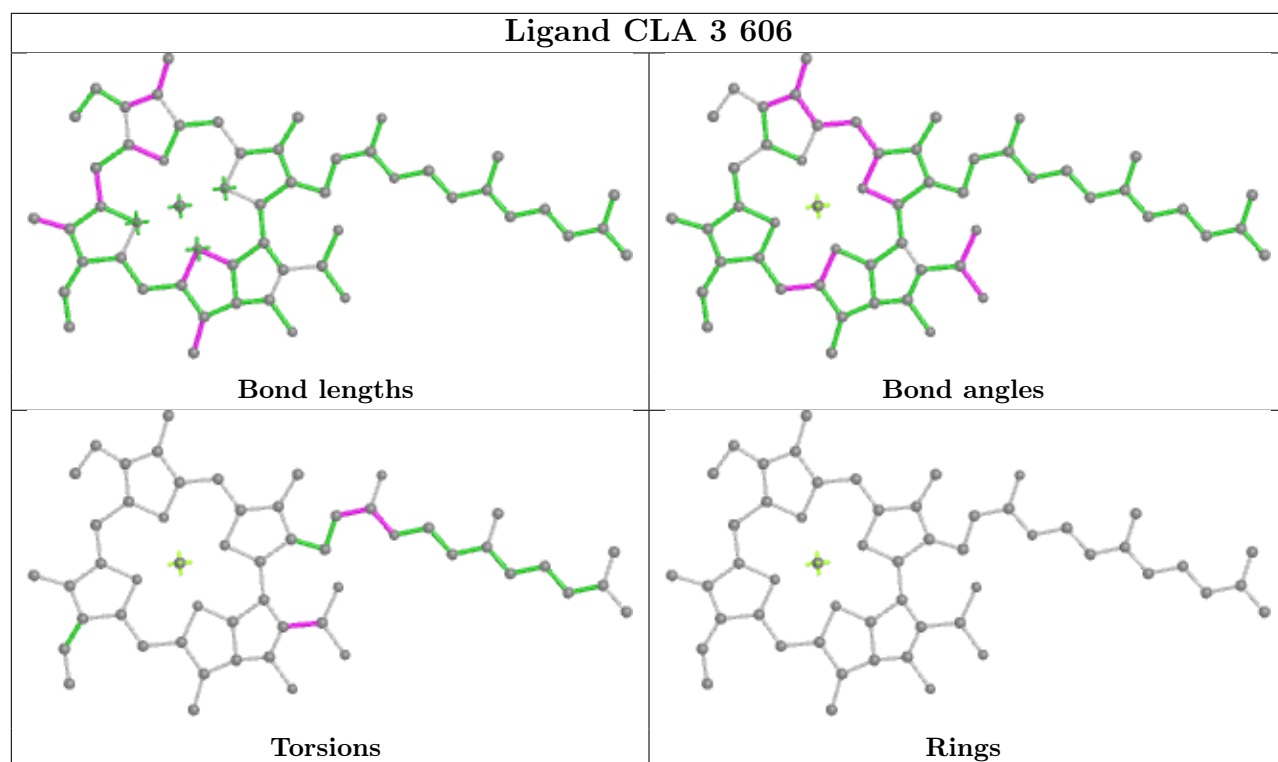
Ligand CLA 4 613**Ligand LHG H 204**



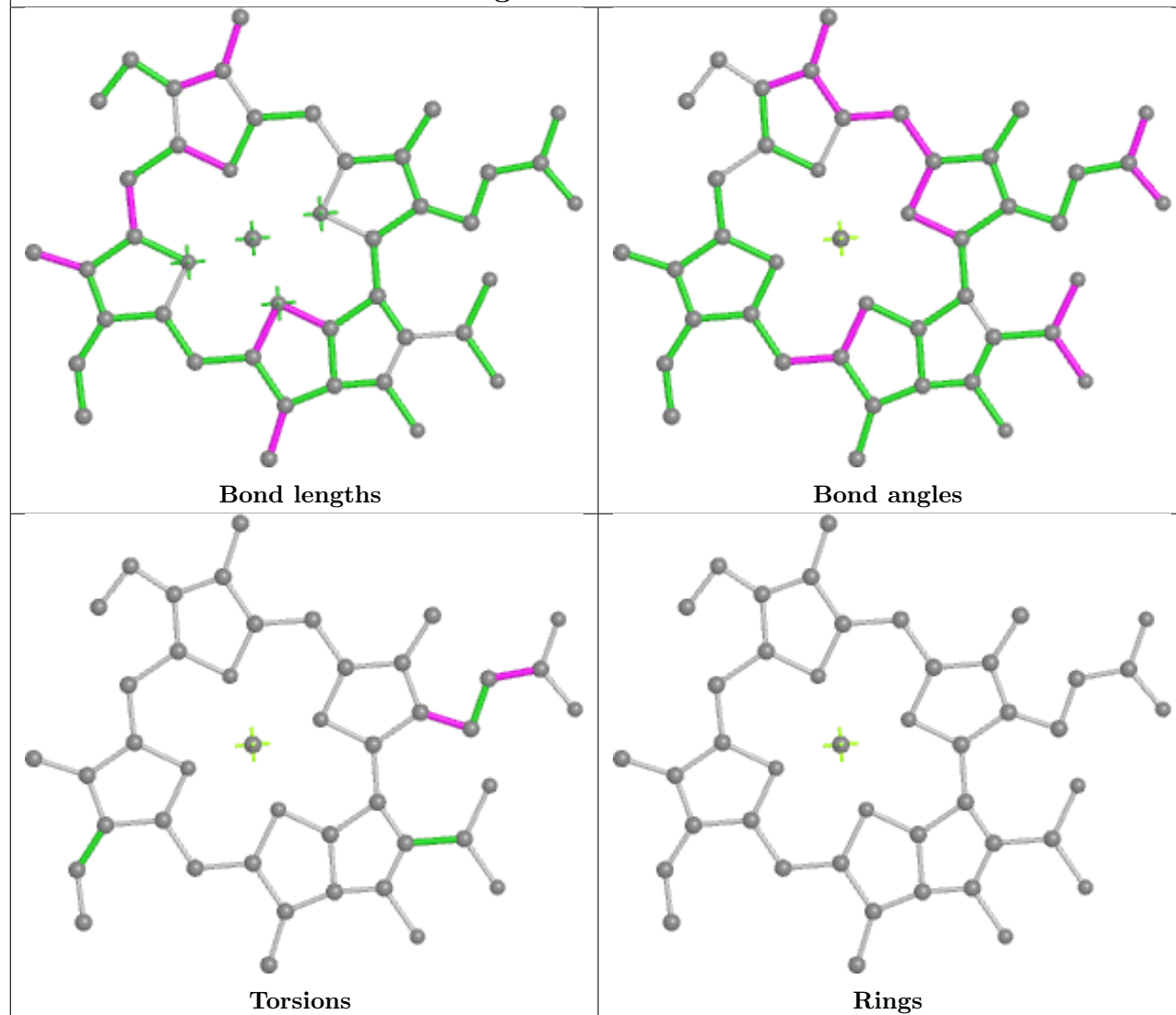
Ligand NEX U 1623



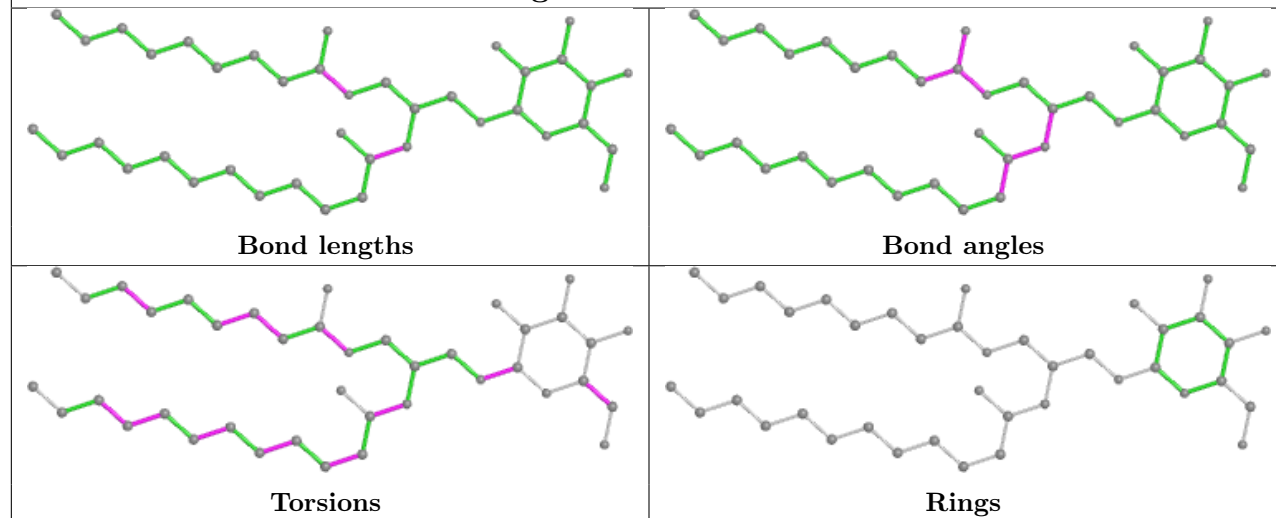
Ligand CLA 3 606

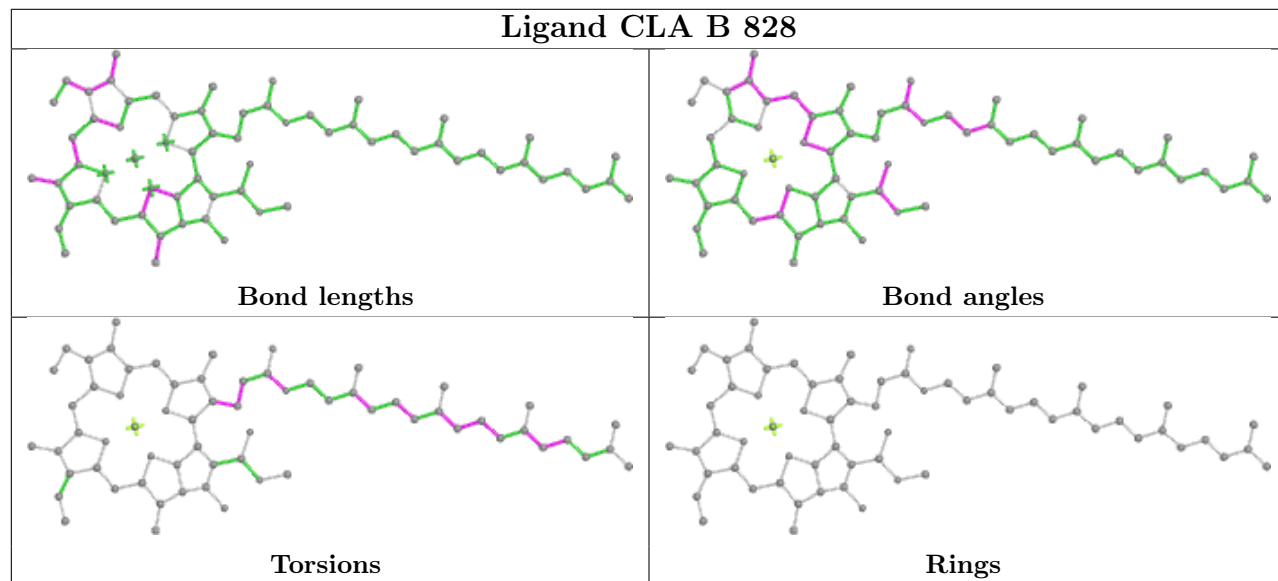
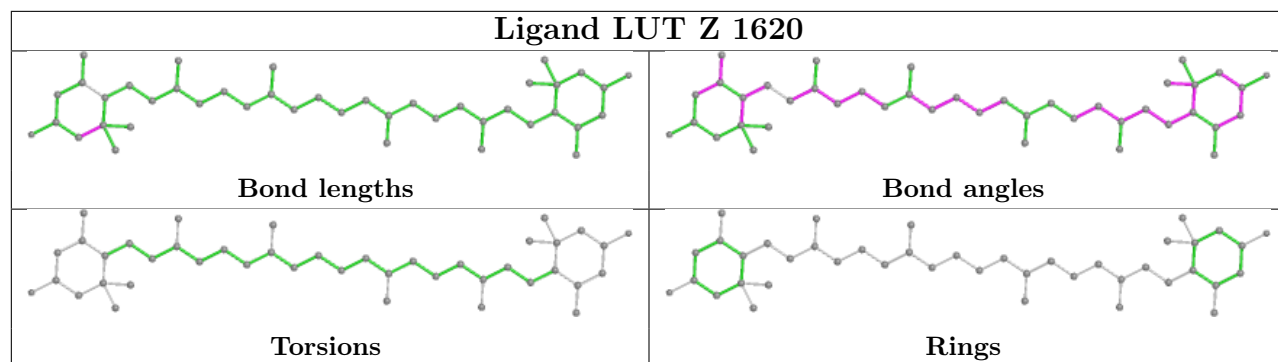


Ligand CLA a 608

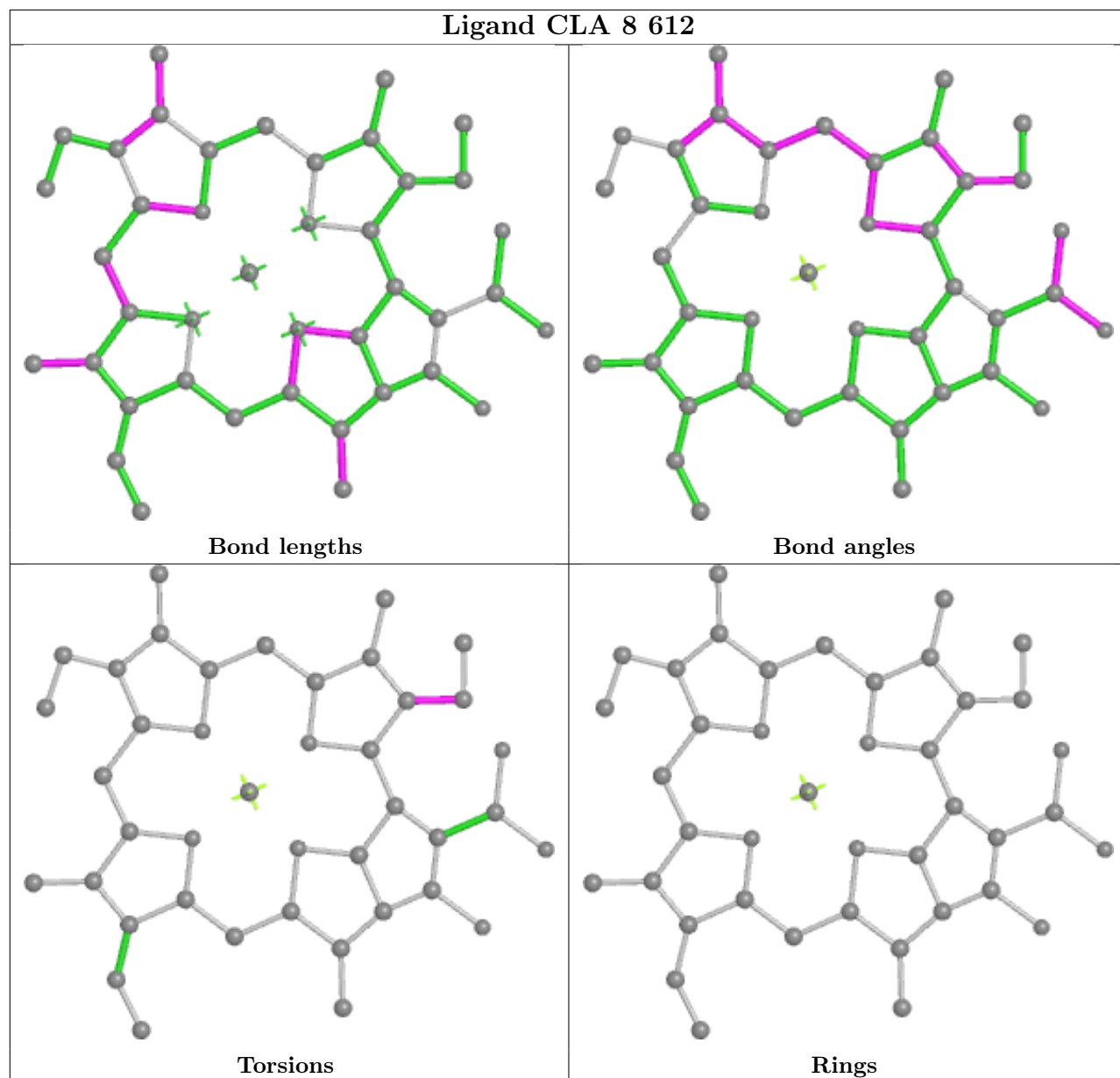


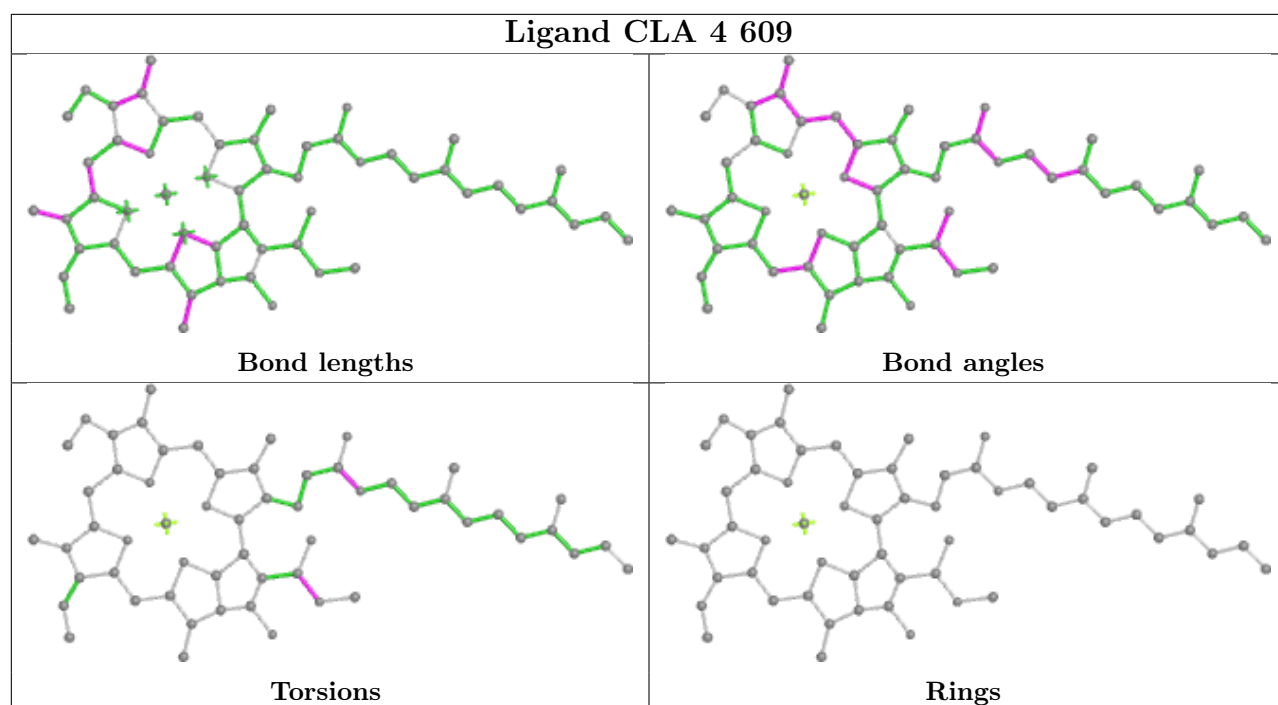
Ligand LMG J 104



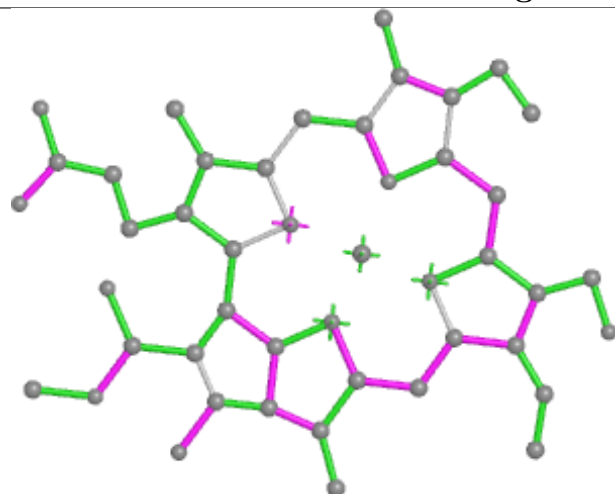


Ligand CLA 8 612

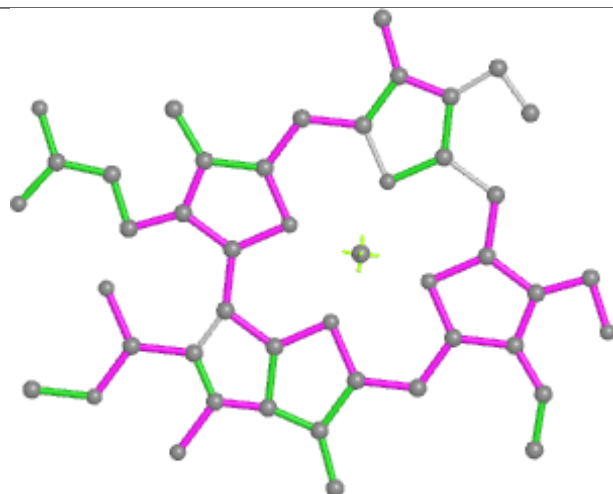




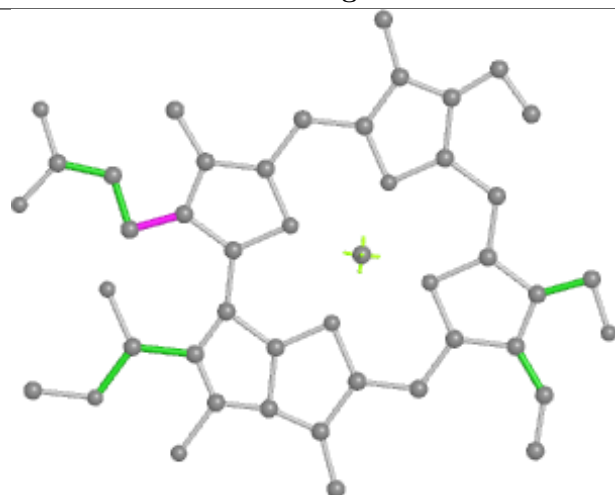
Ligand CHL V 607



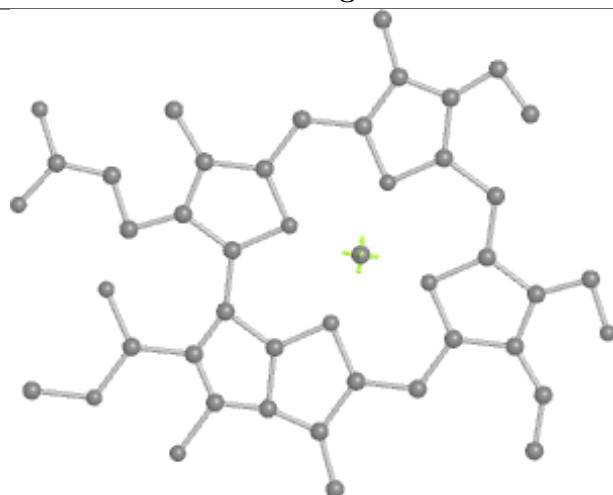
Bond lengths



Bond angles

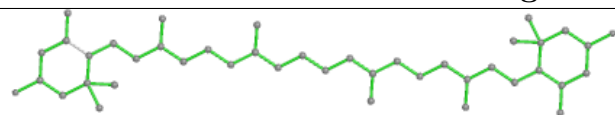


Torsions

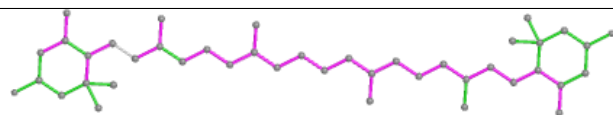


Rings

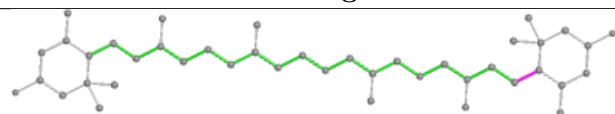
Ligand LUT 9 619



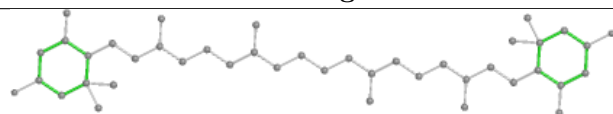
Bond lengths



Bond angles

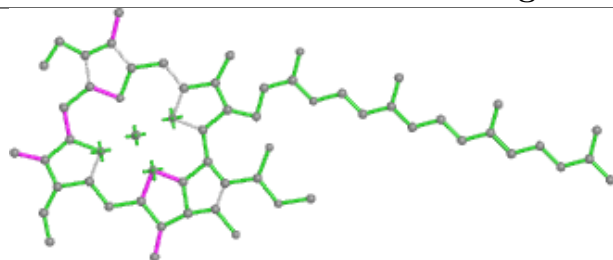


Torsions

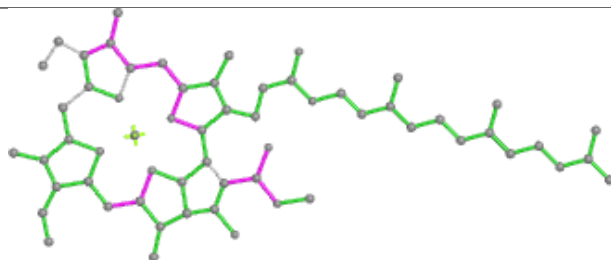


Rings

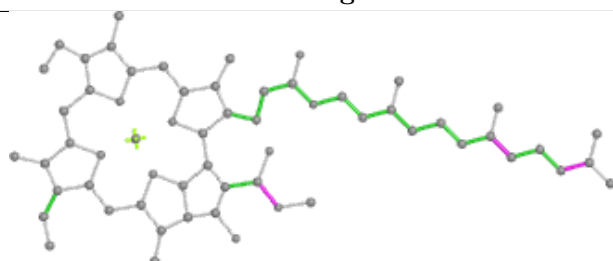
Ligand CLA 4 602



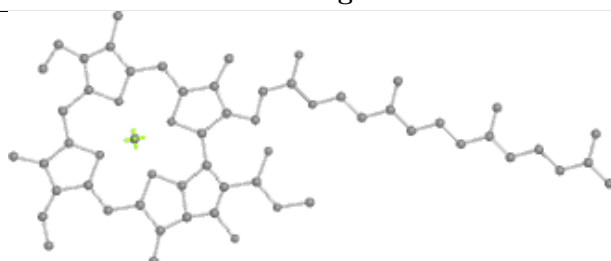
Bond lengths



Bond angles

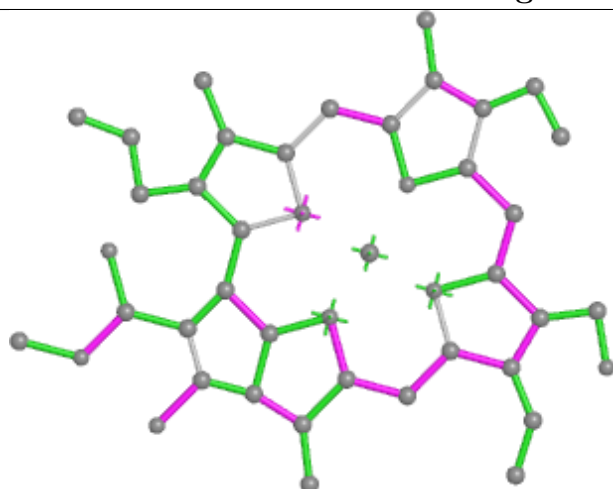


Torsions

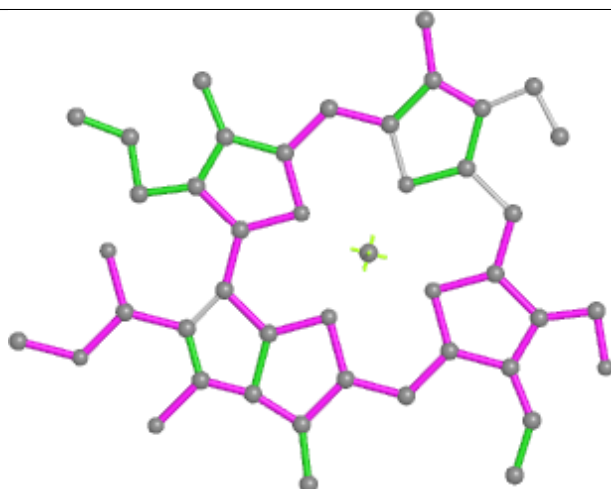


Rings

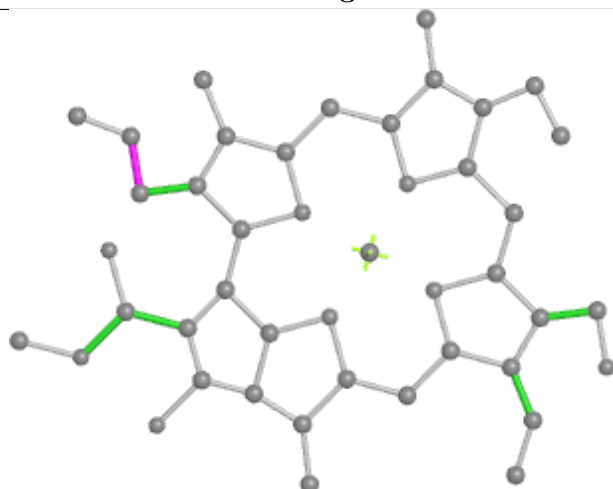
Ligand CHL Z 605



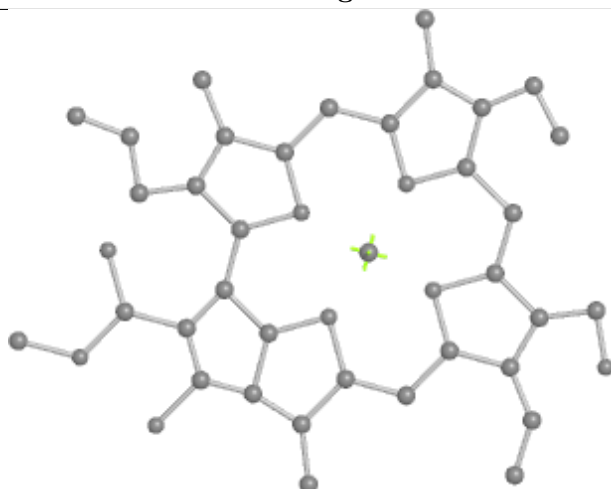
Bond lengths



Bond angles

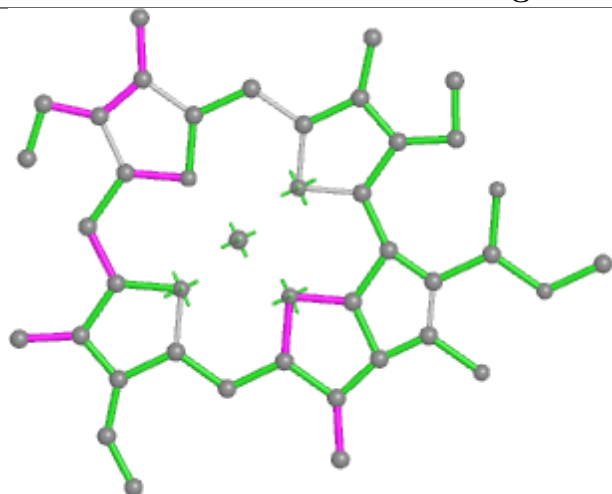


Torsions

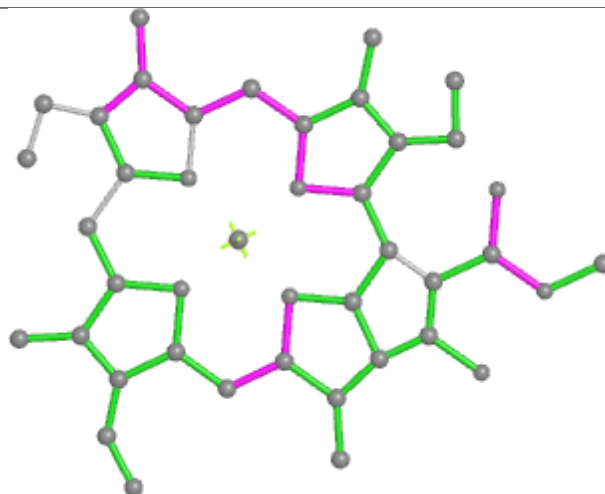


Rings

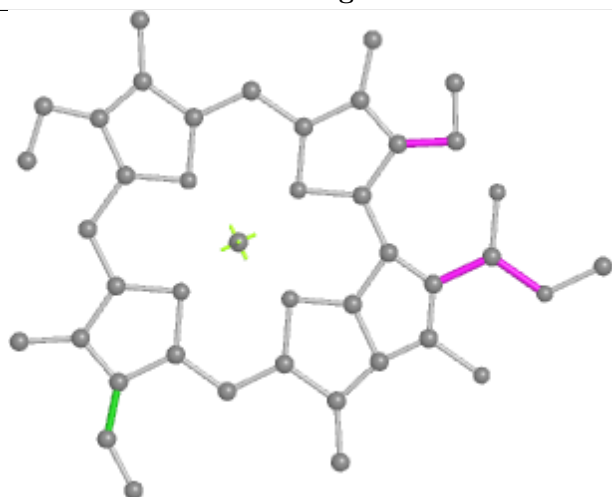
Ligand CLA U 611



Bond lengths



Bond angles

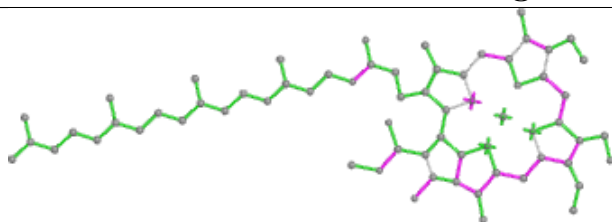


Torsions

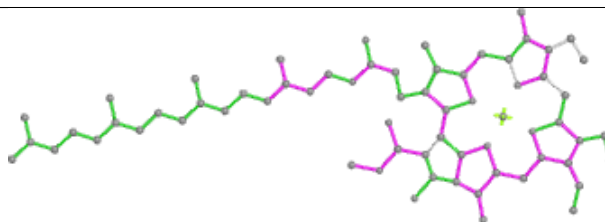


Rings

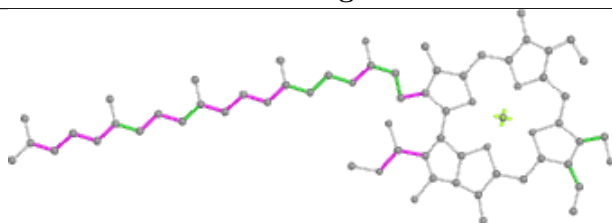
Ligand CHL Y 601



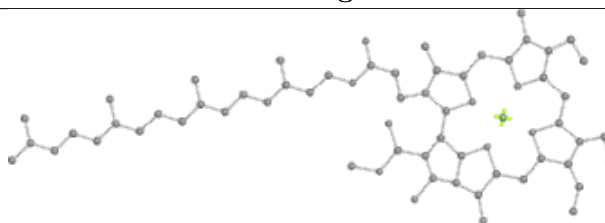
Bond lengths



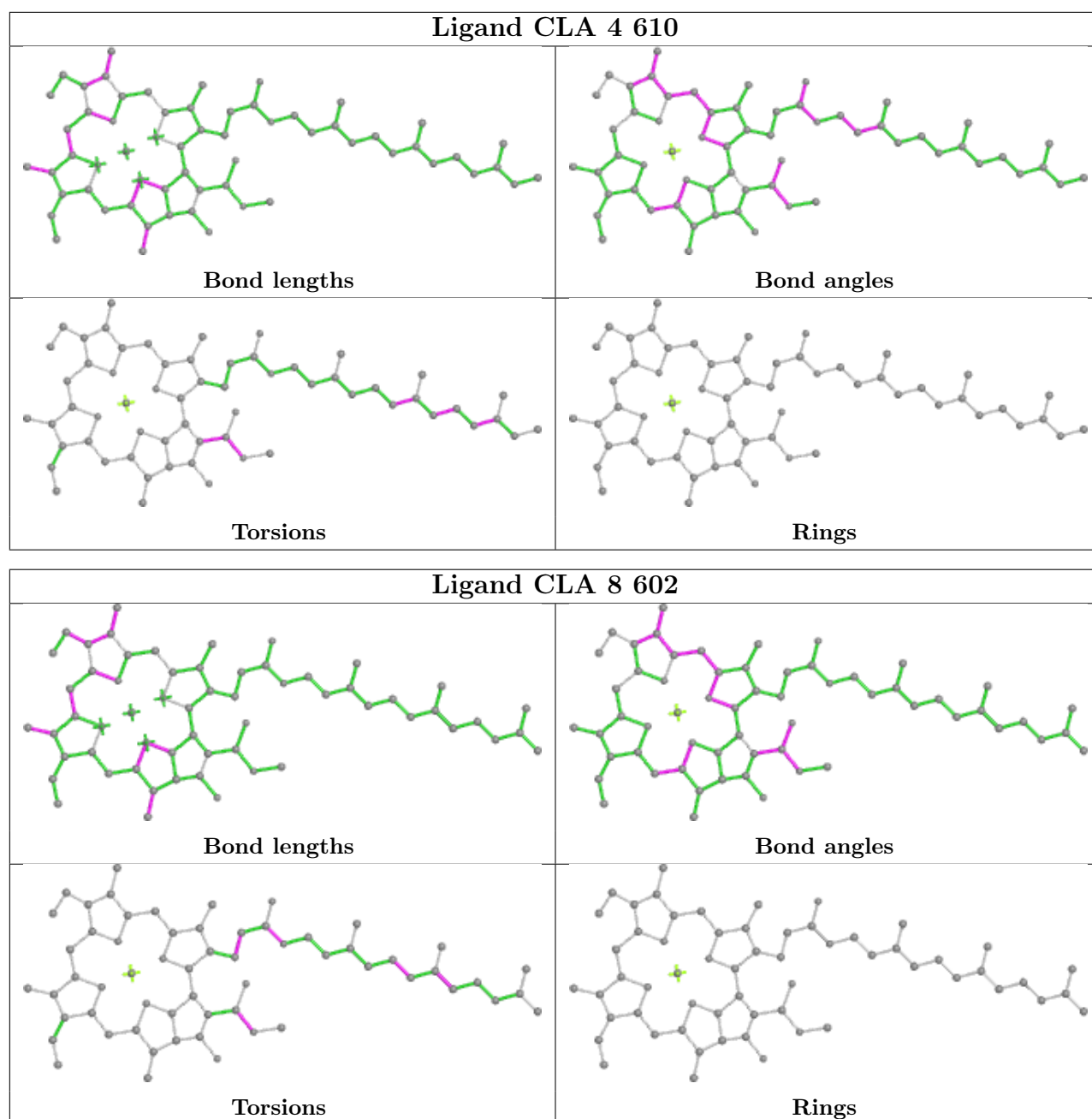
Bond angles

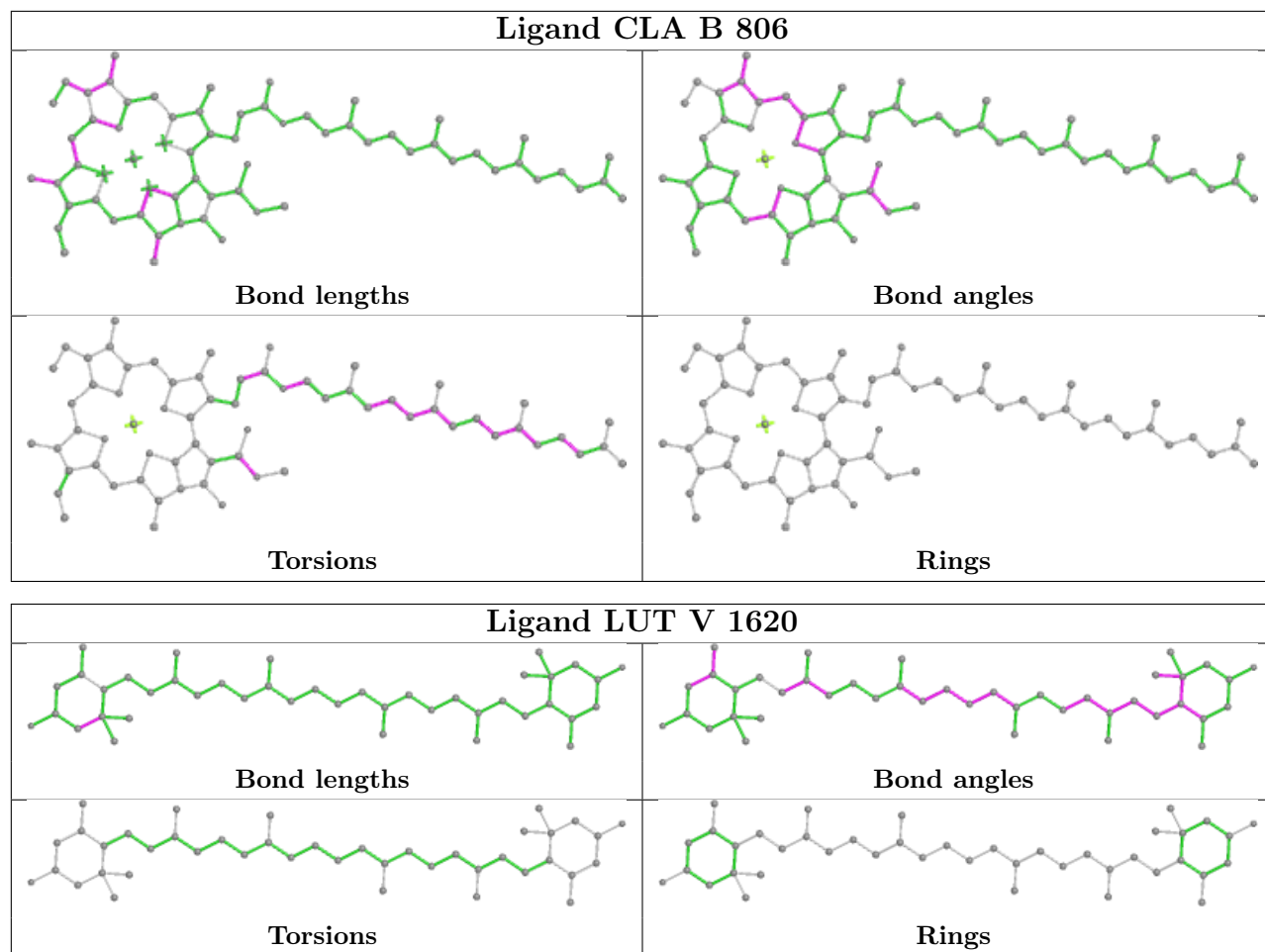


Torsions

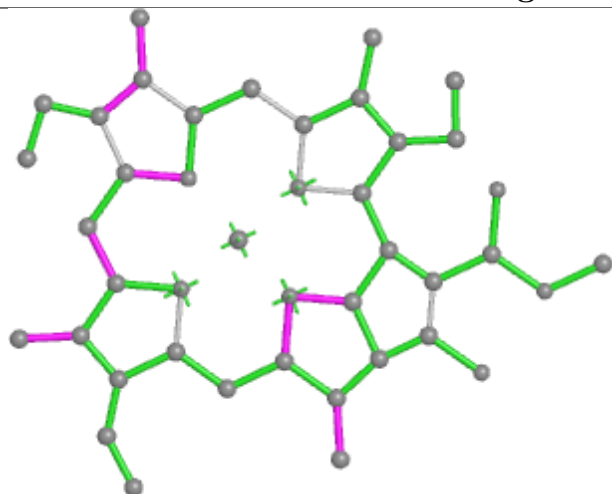


Rings

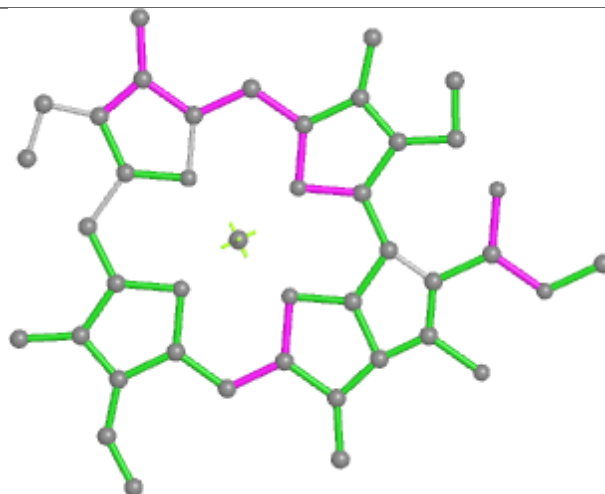




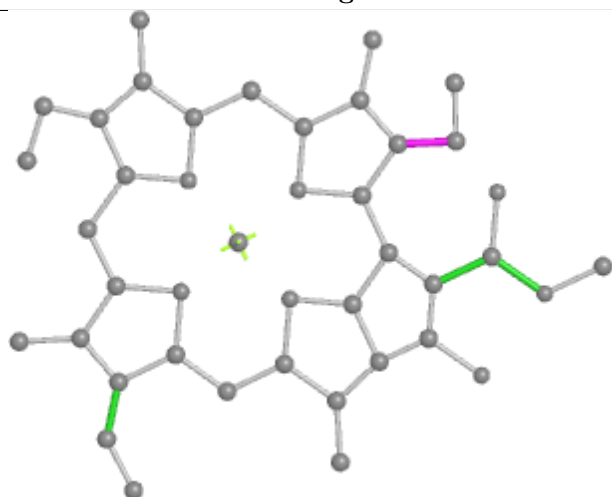
Ligand CLA 6 611



Bond lengths



Bond angles

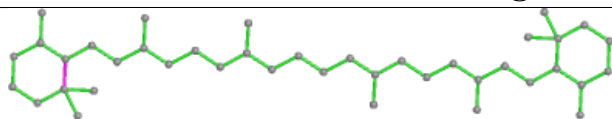


Torsions

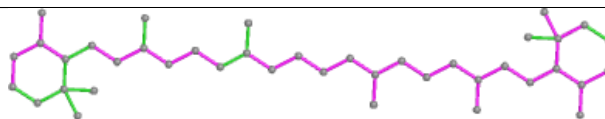


Rings

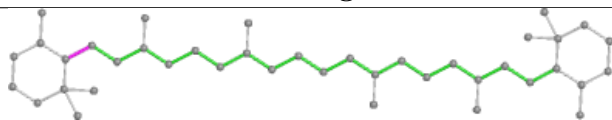
Ligand BCR A 851



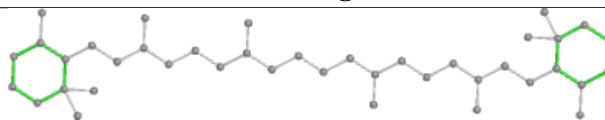
Bond lengths



Bond angles

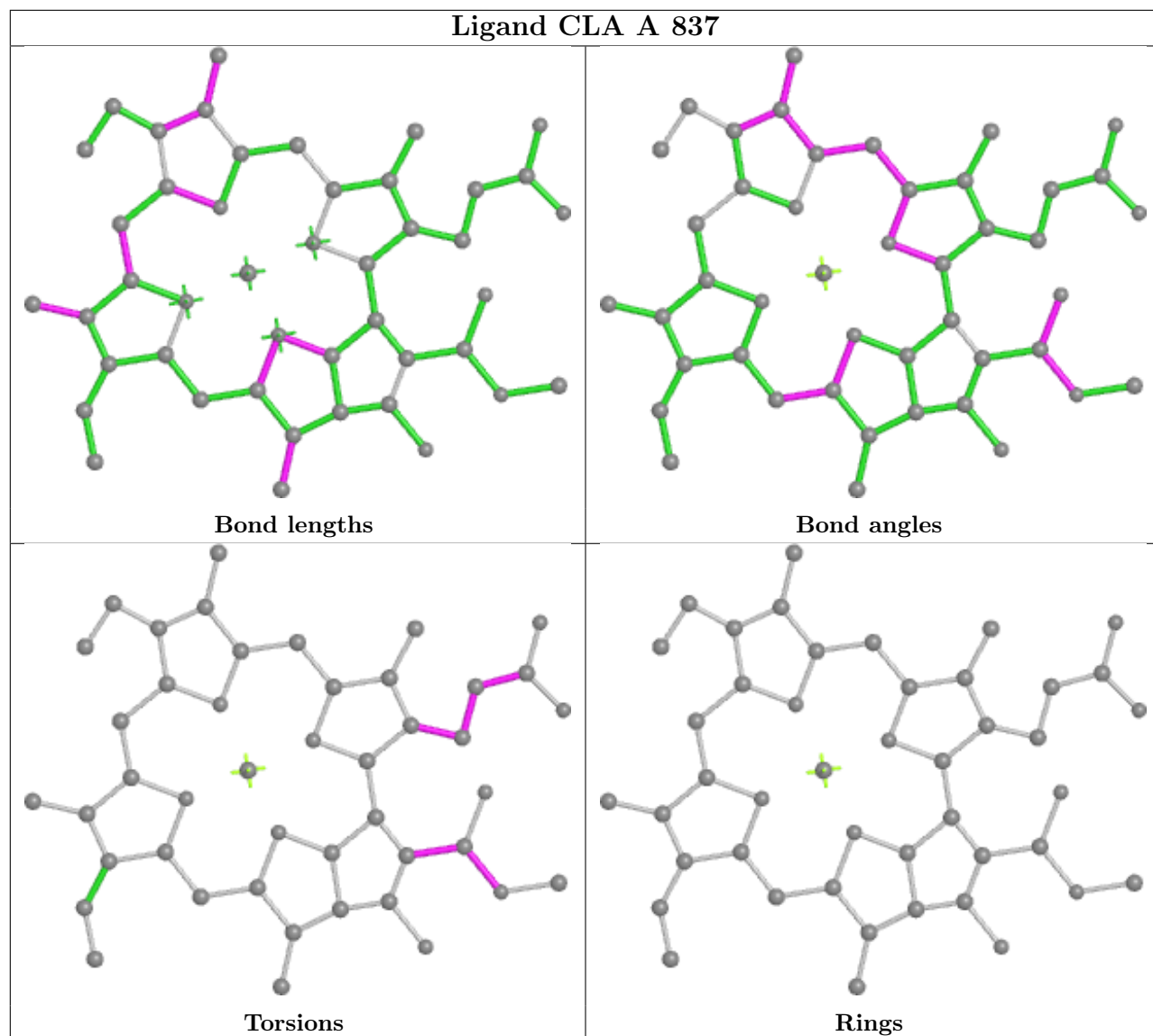


Torsions

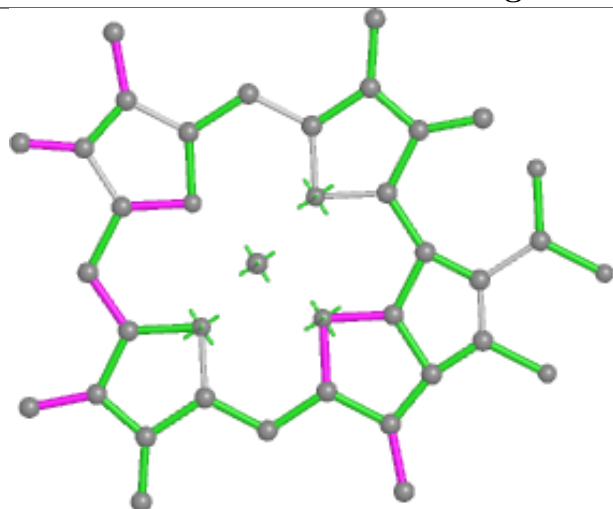


Rings

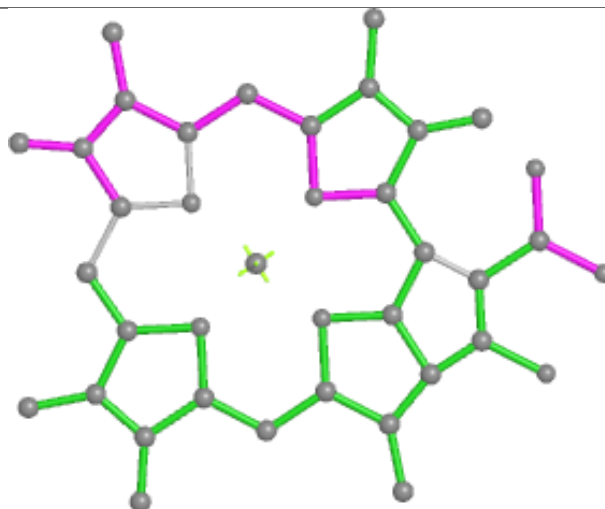
Ligand CLA A 837



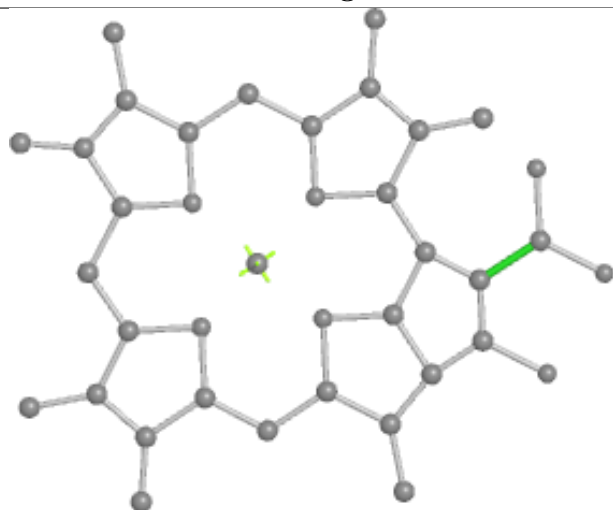
Ligand CLA O 2002



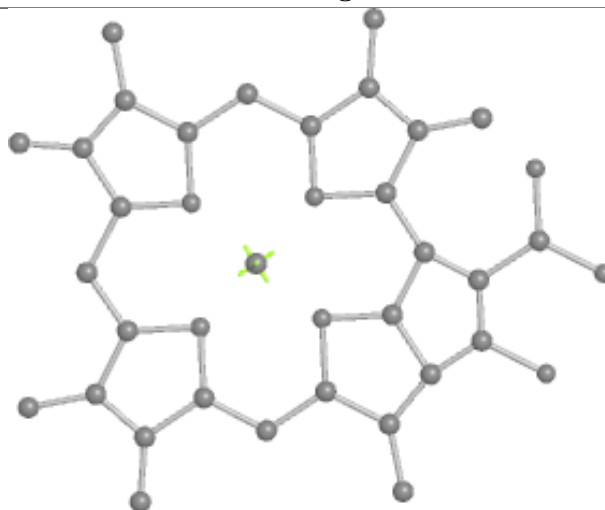
Bond lengths



Bond angles

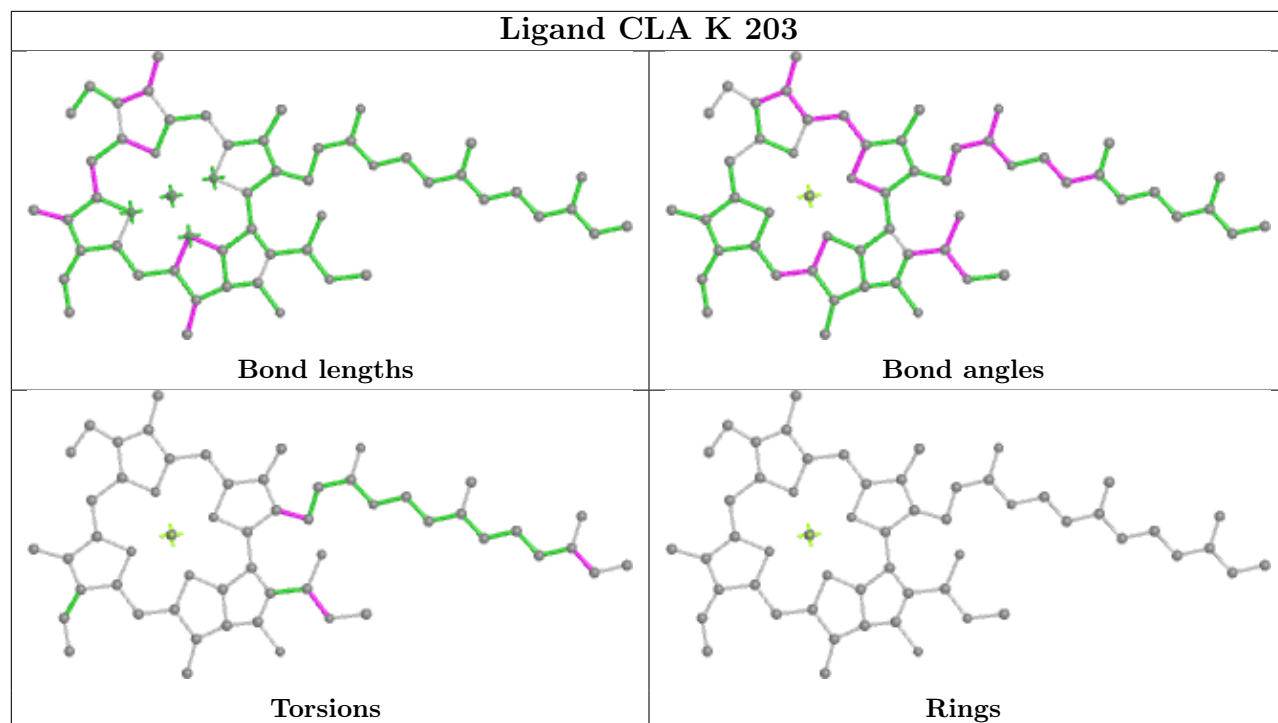


Torsions

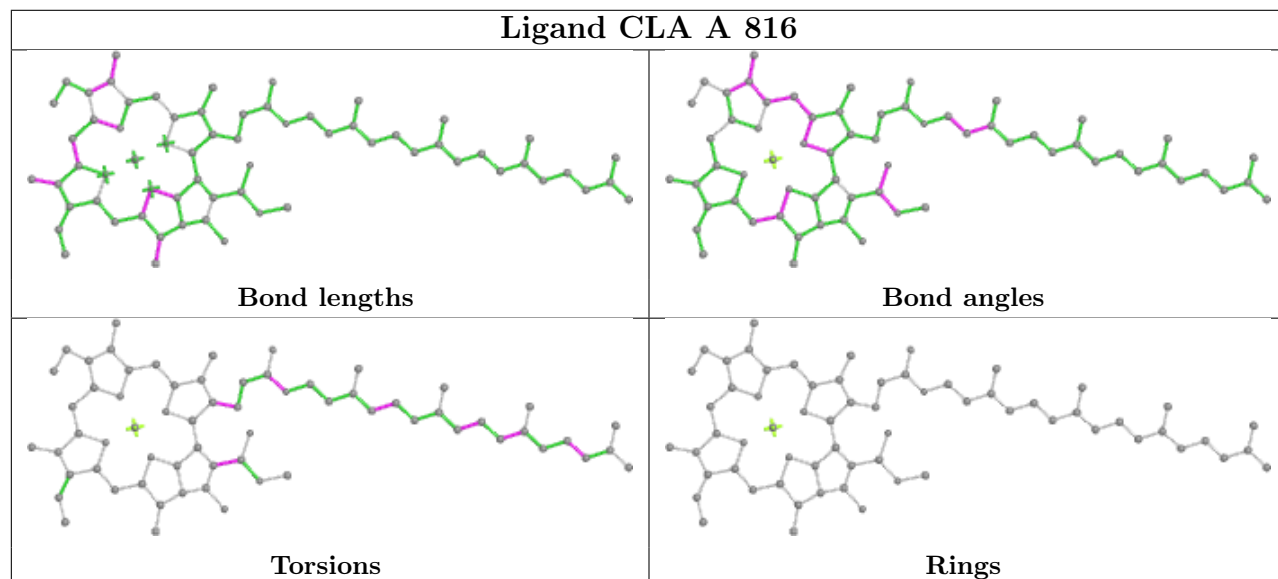


Rings

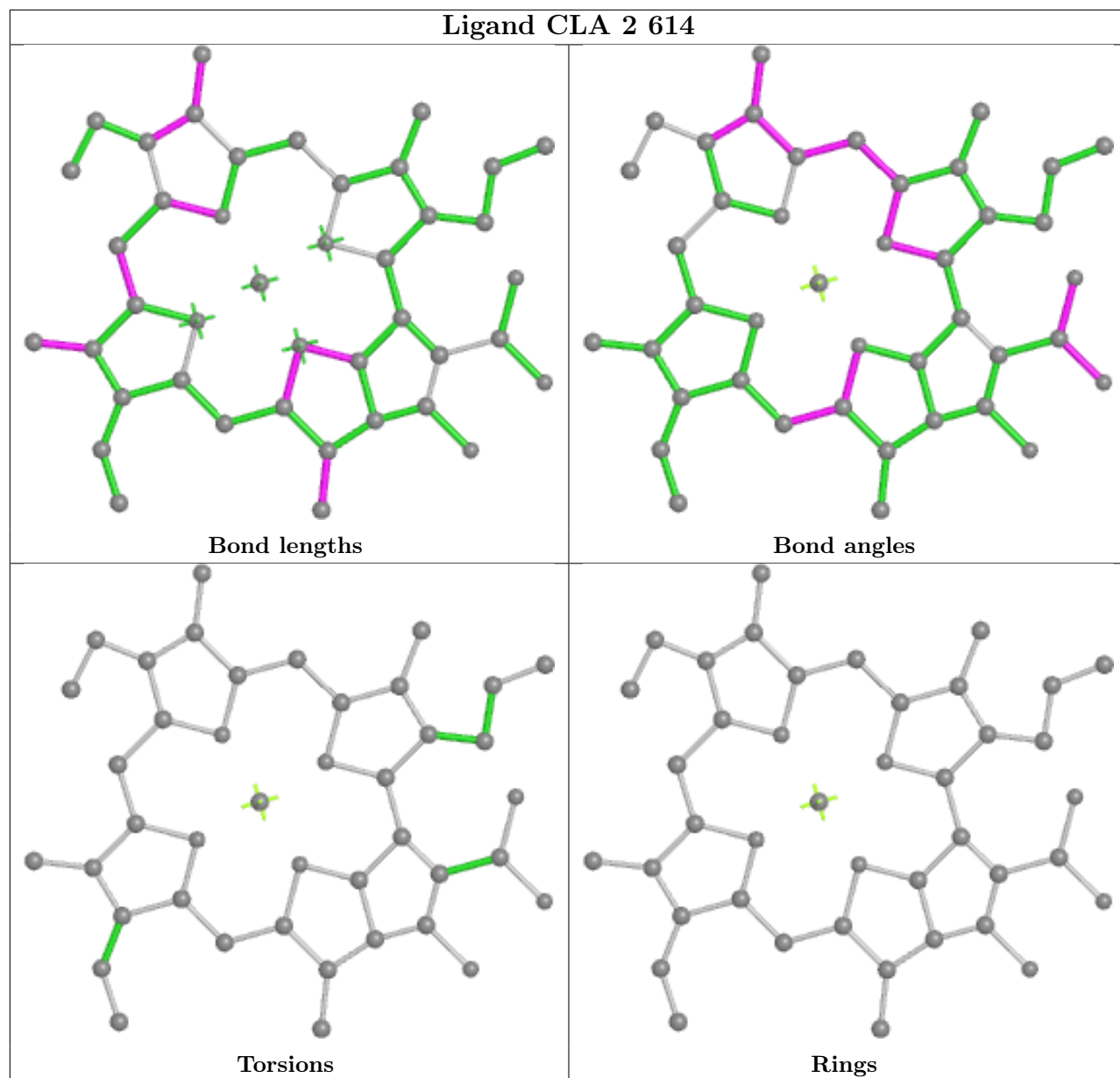
Ligand CLA K 203

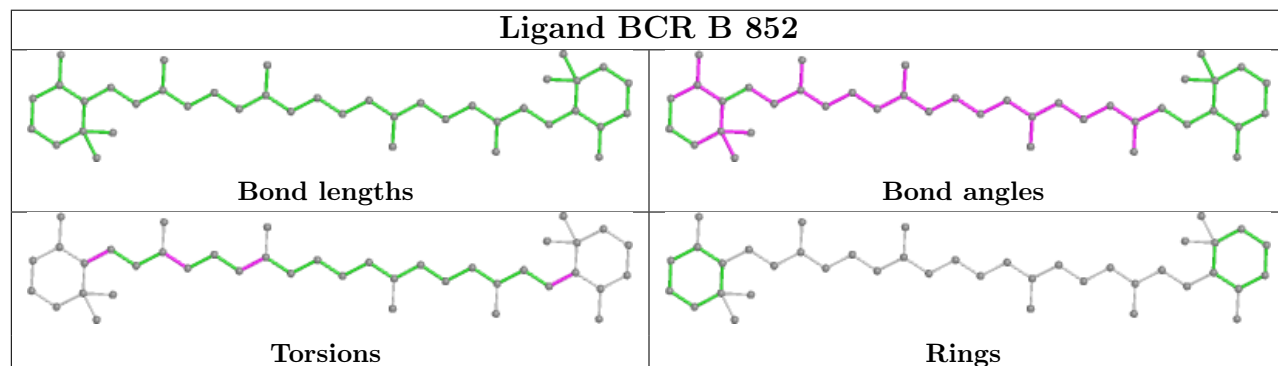
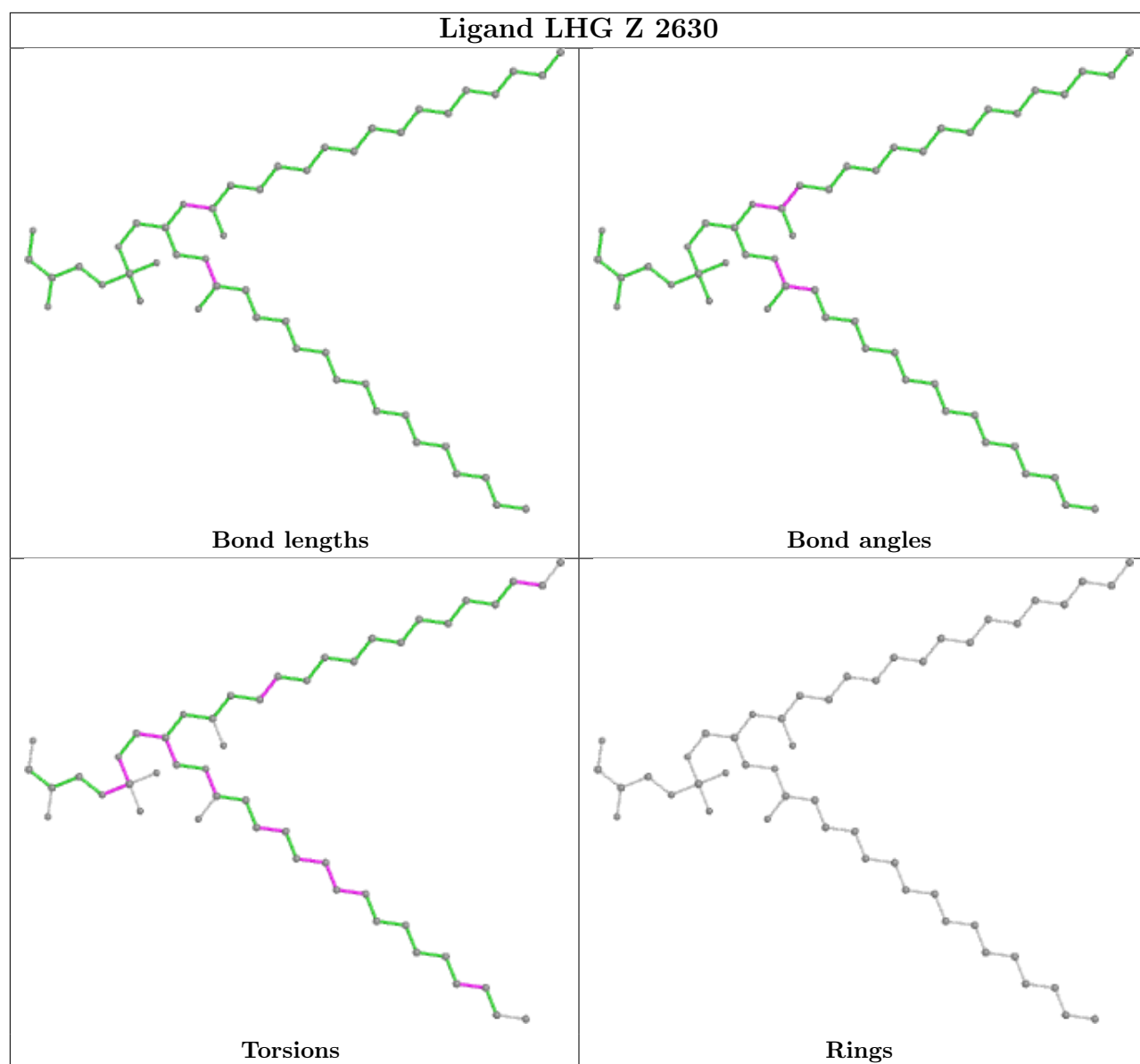


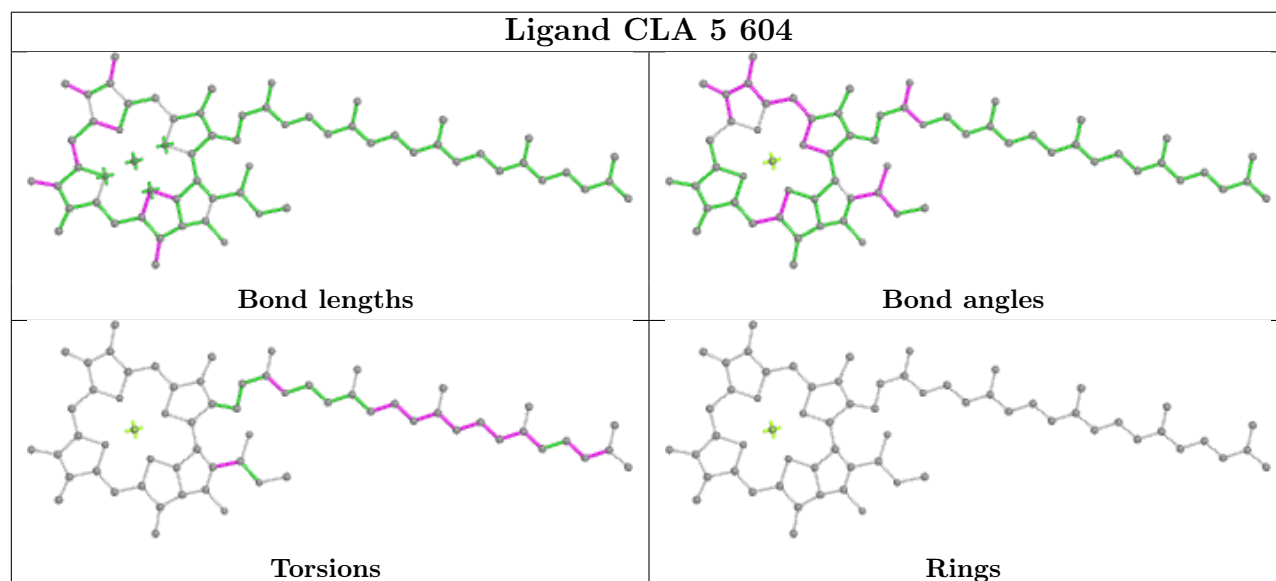
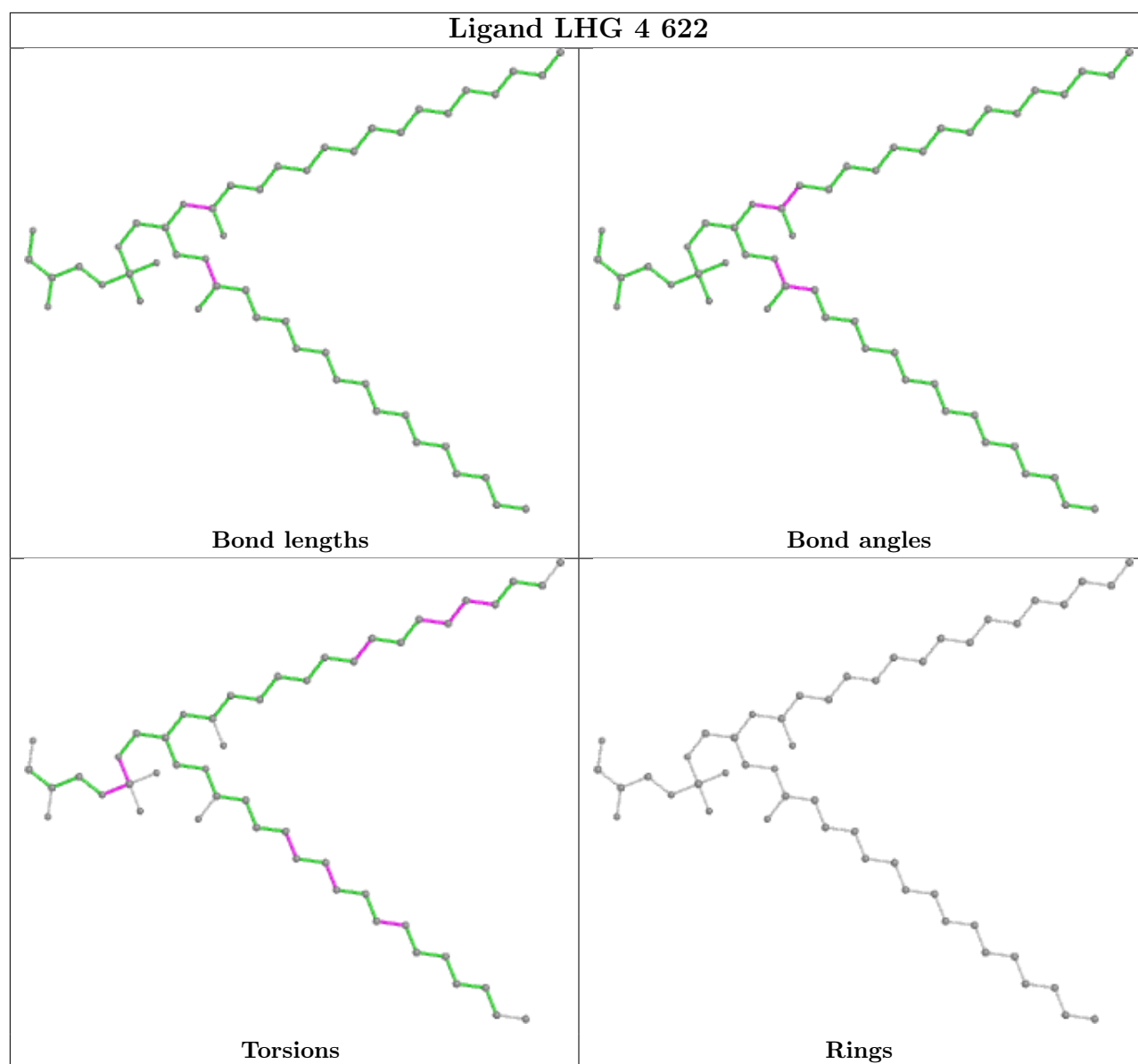
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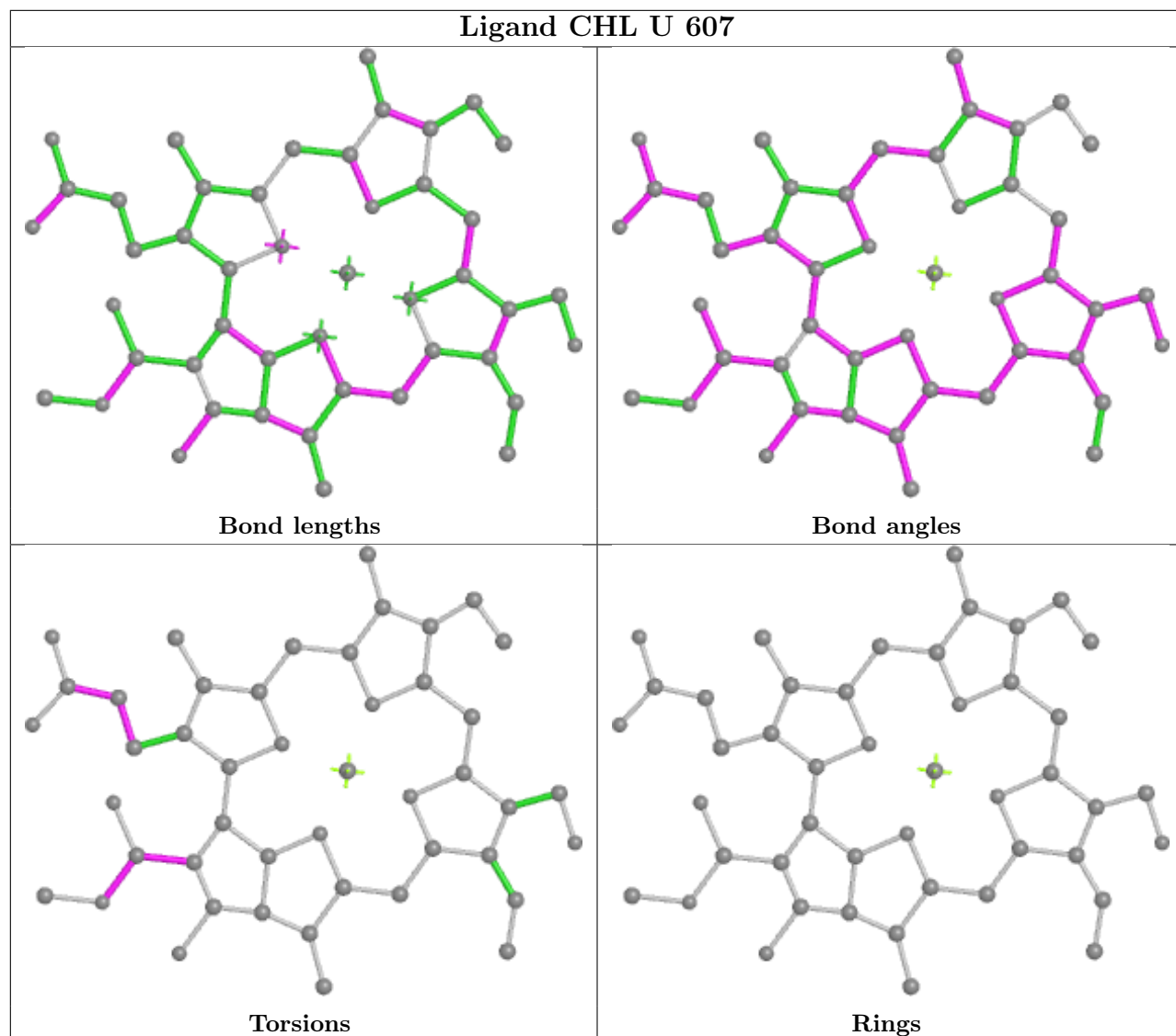
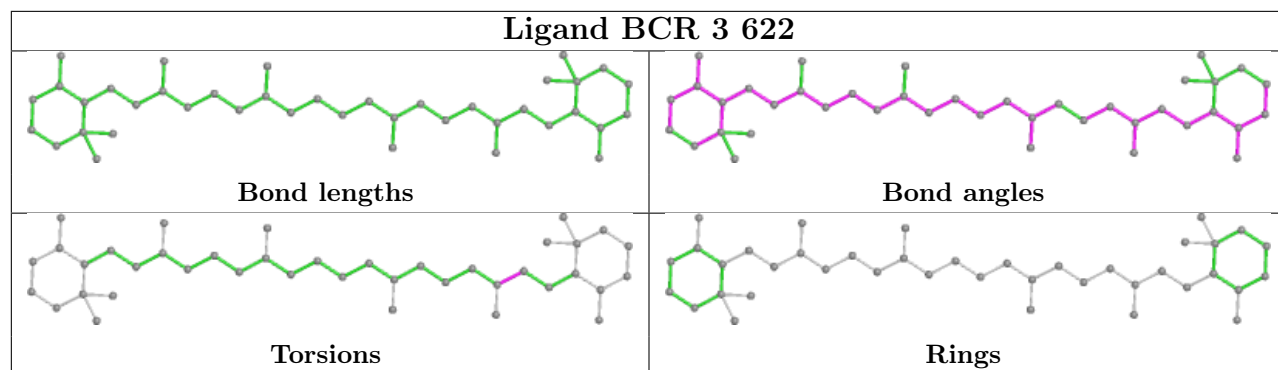


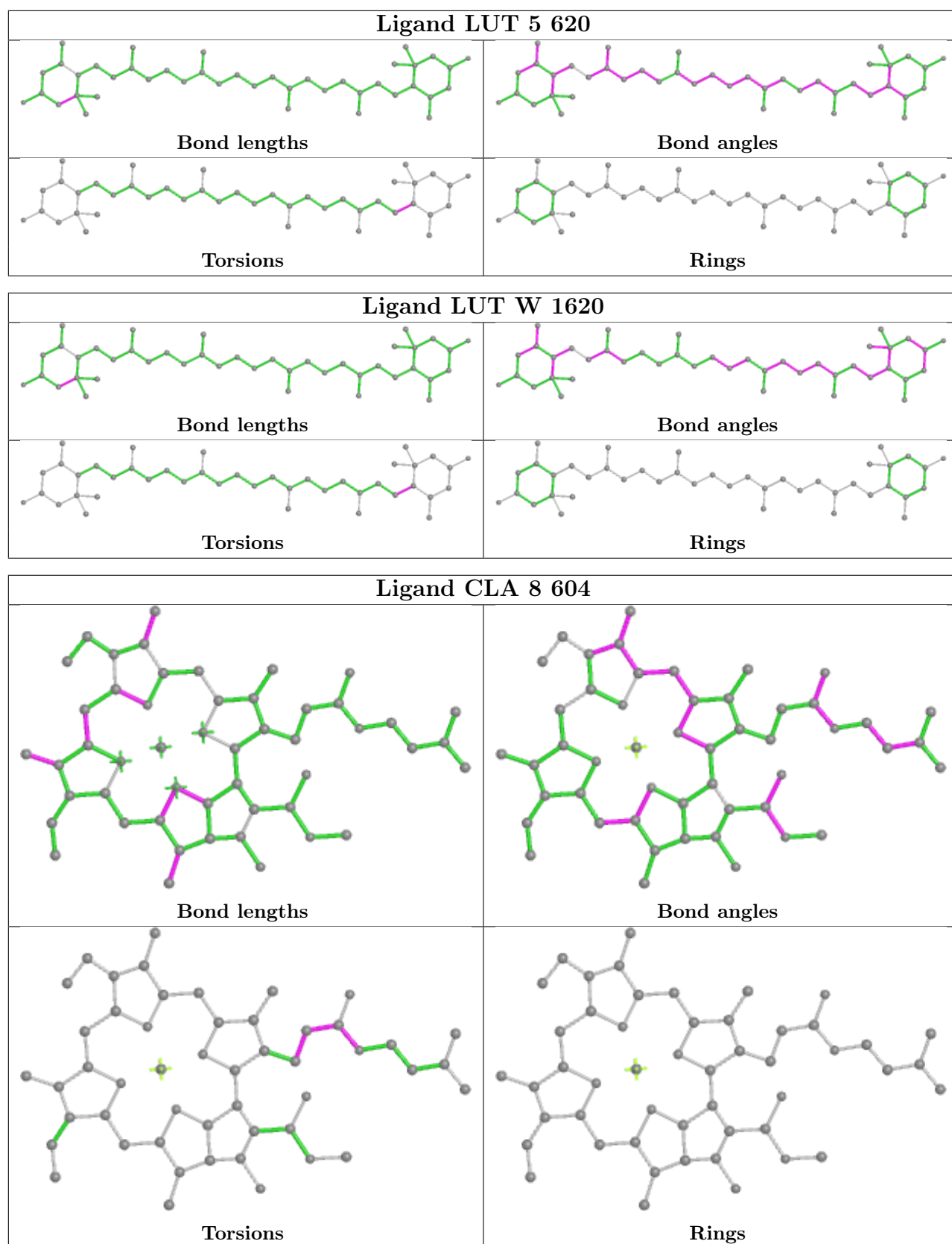
Ligand CLA 2 614

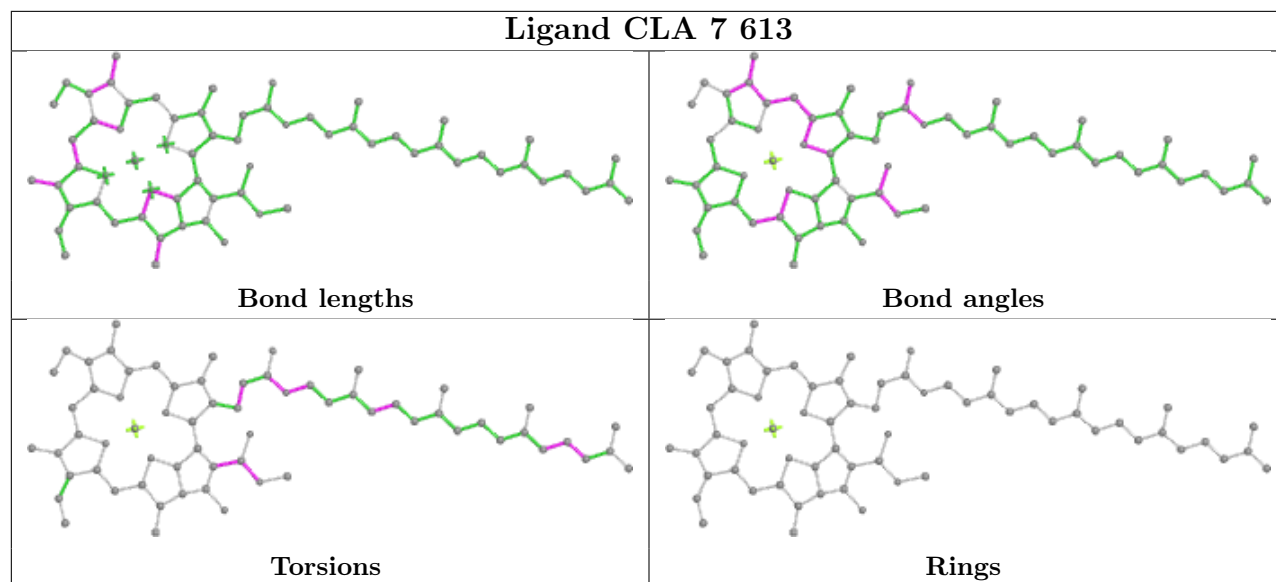
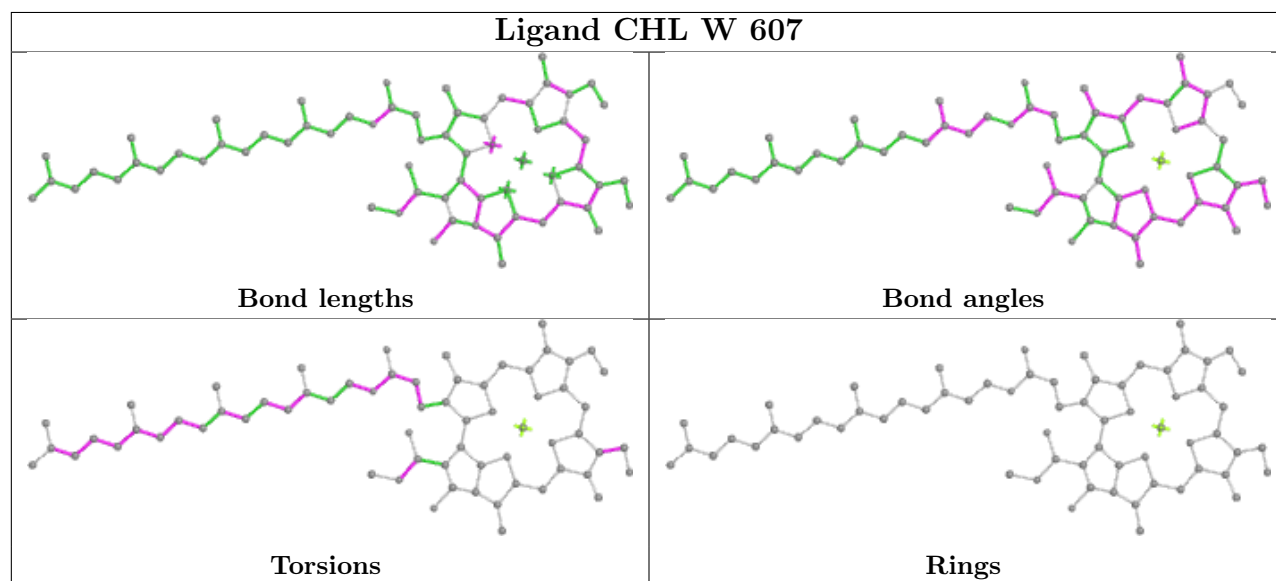




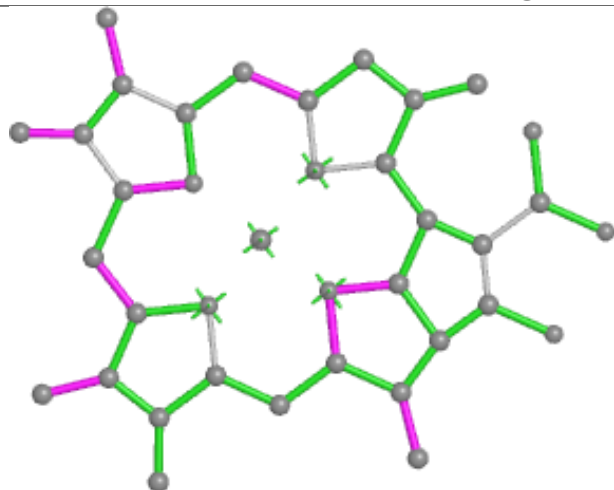




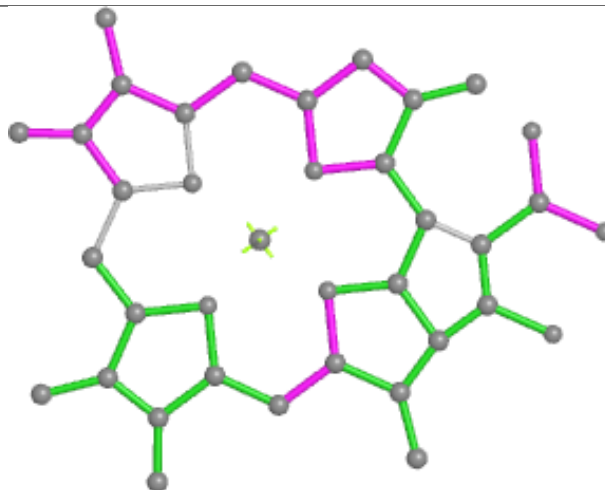


Ligand CLA 7 613**Ligand CHL W 607**

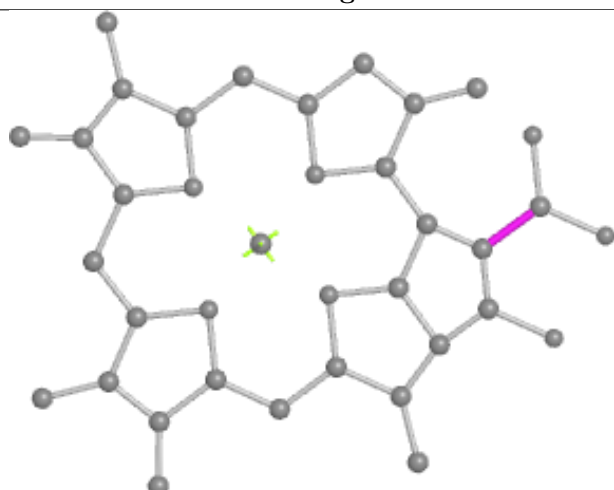
Ligand CLA 1 614



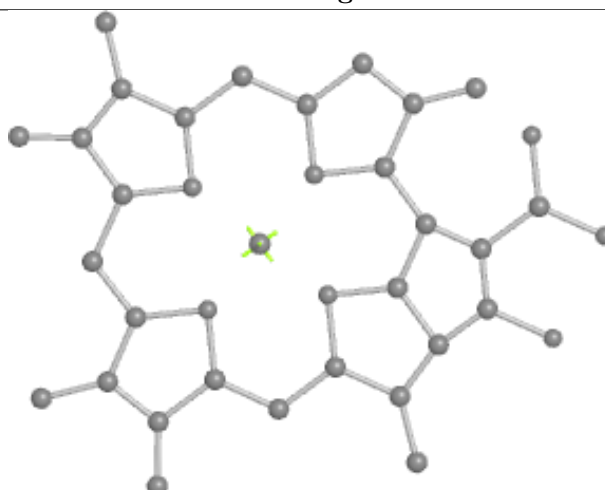
Bond lengths



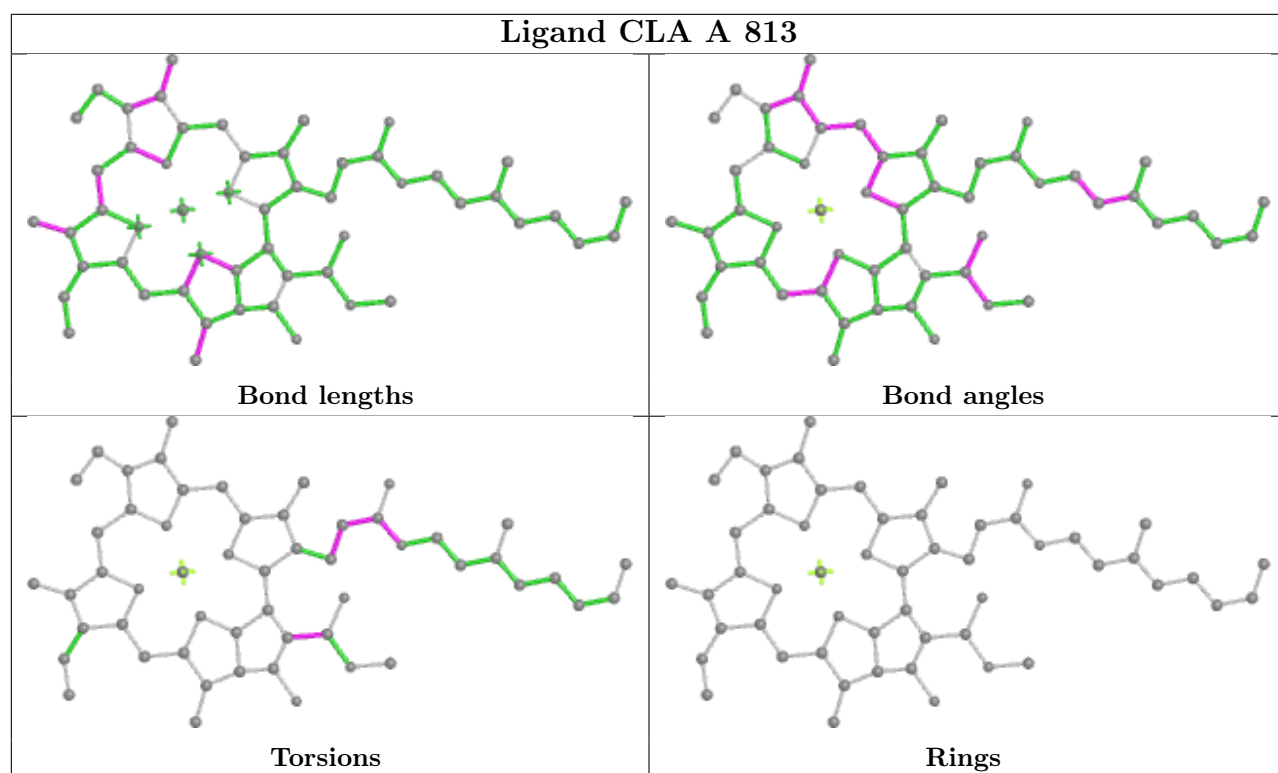
Bond angles

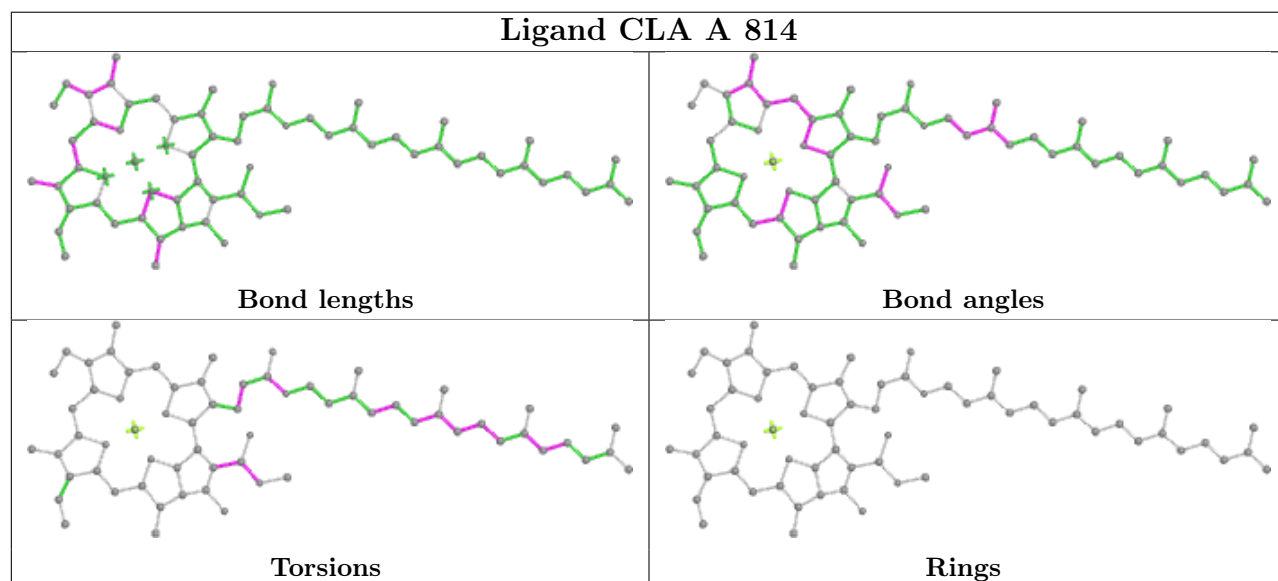
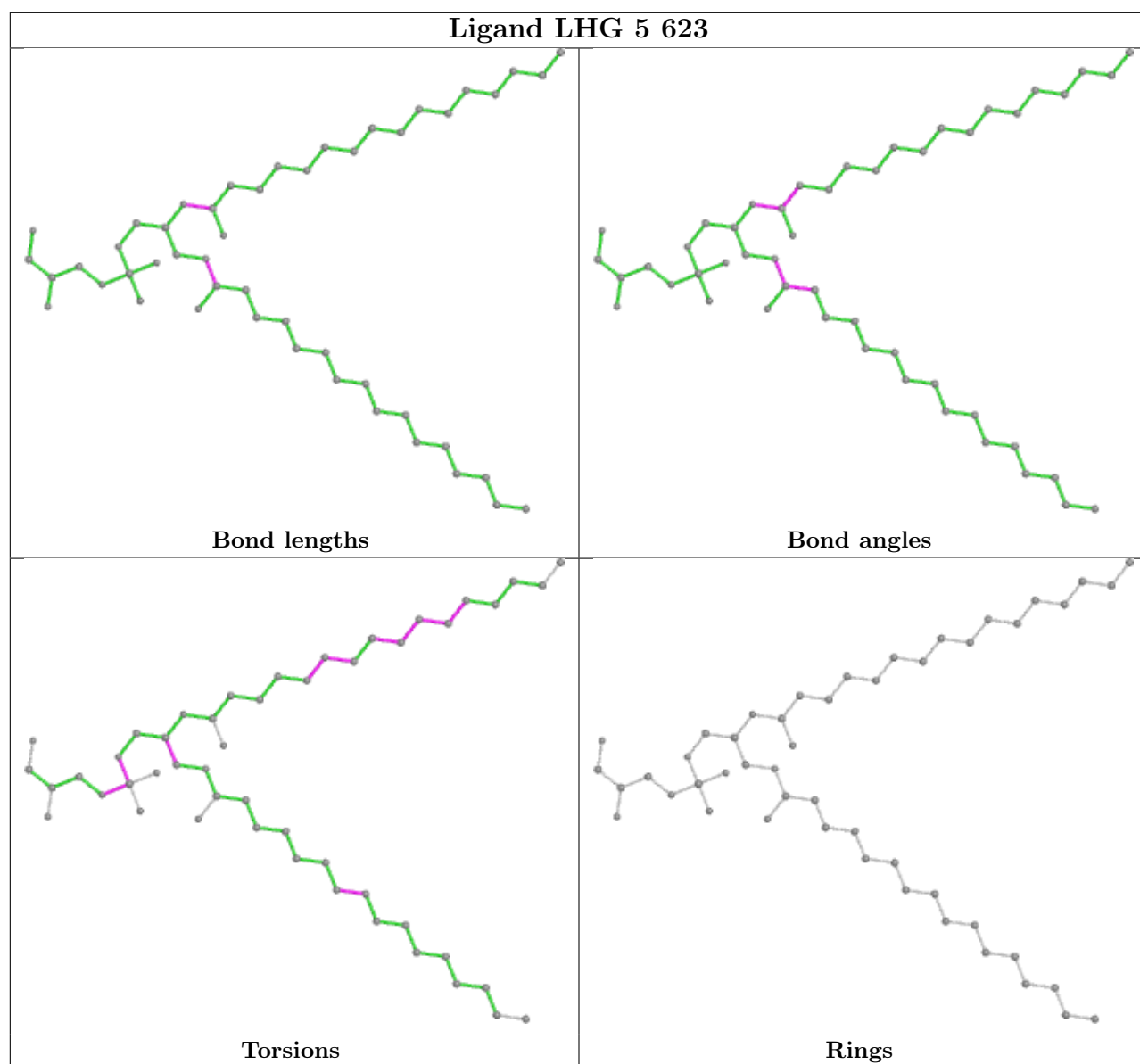


Torsions

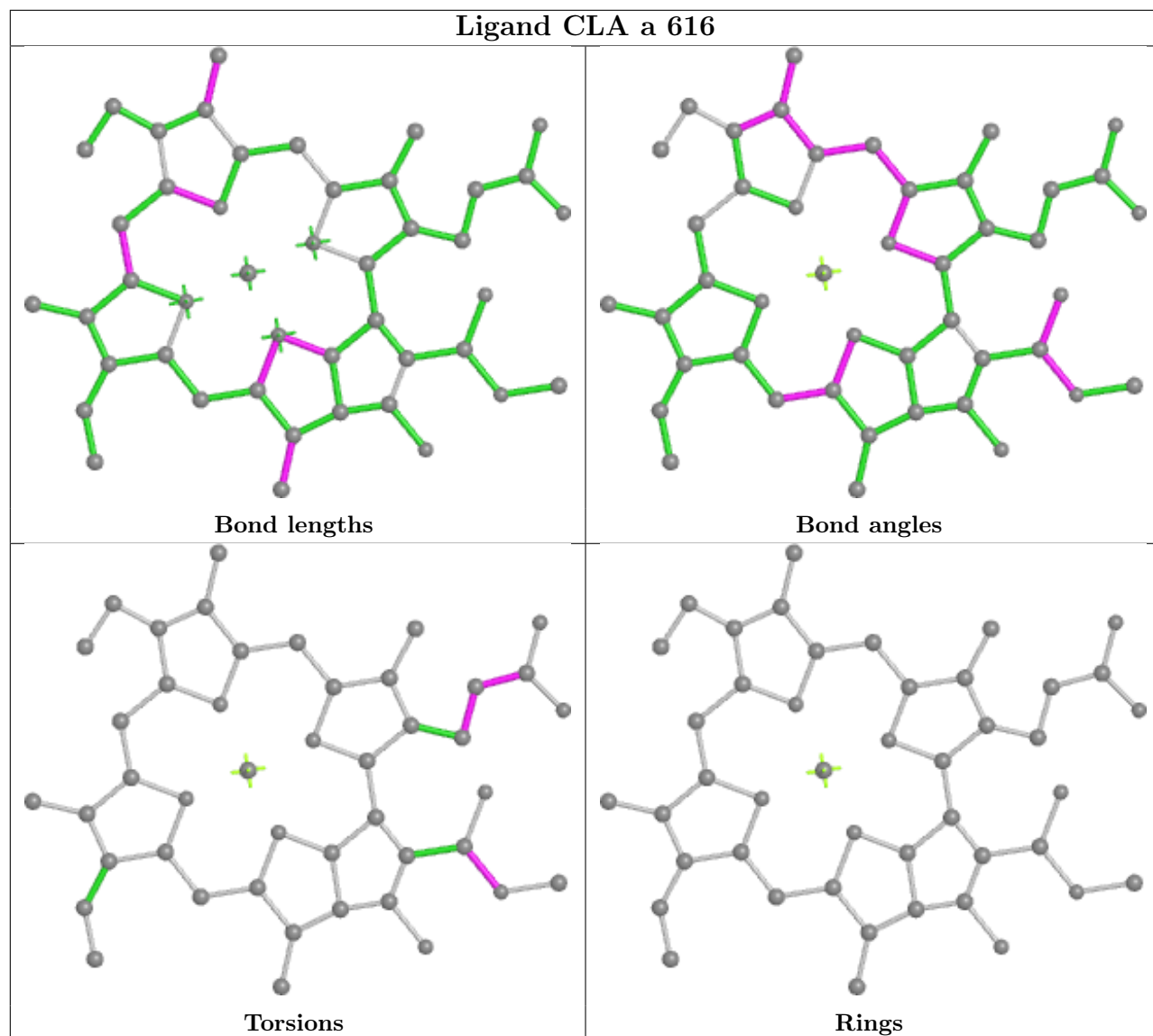


Rings

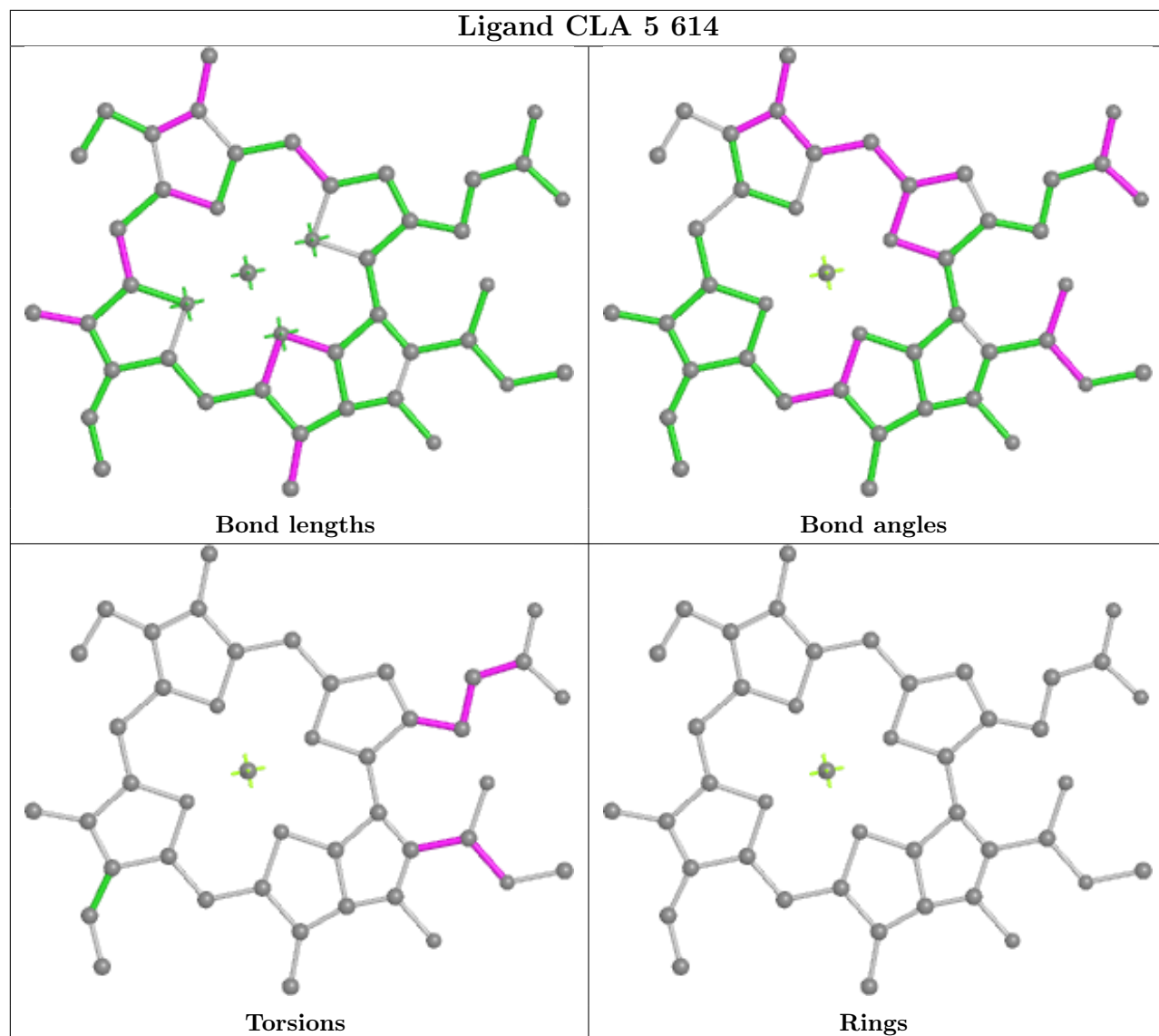




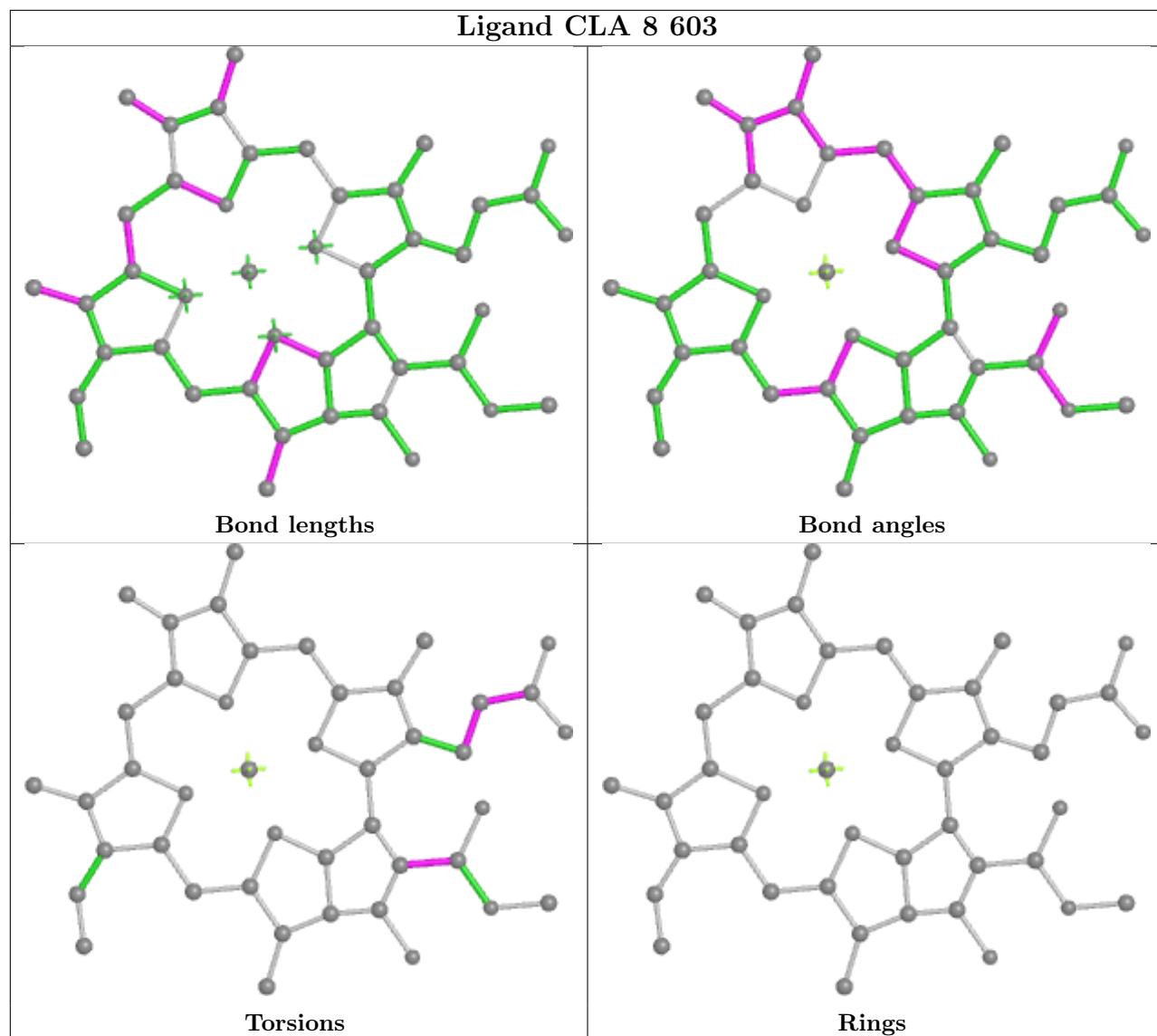
Ligand CLA a 616



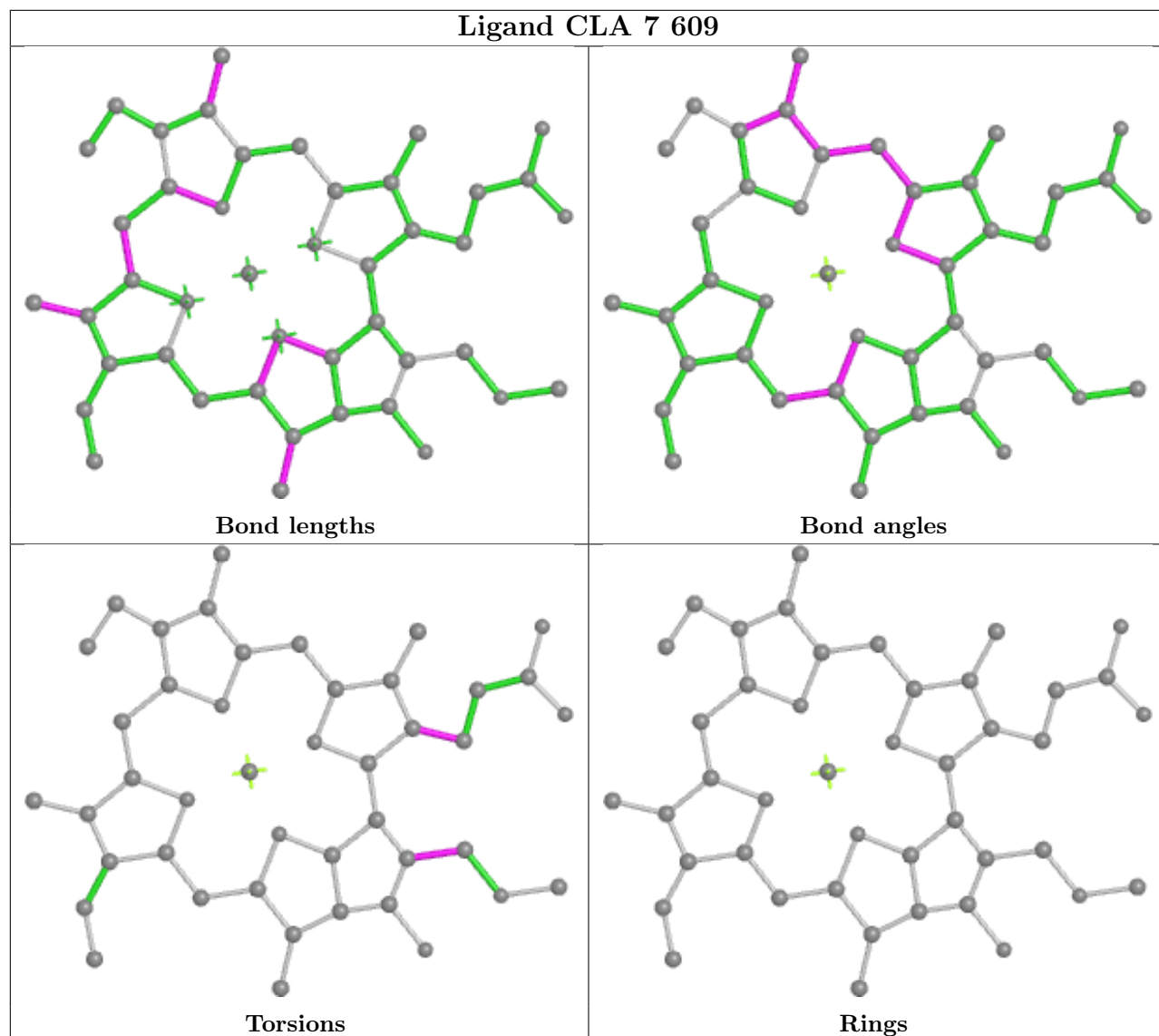
Ligand CLA 5 614



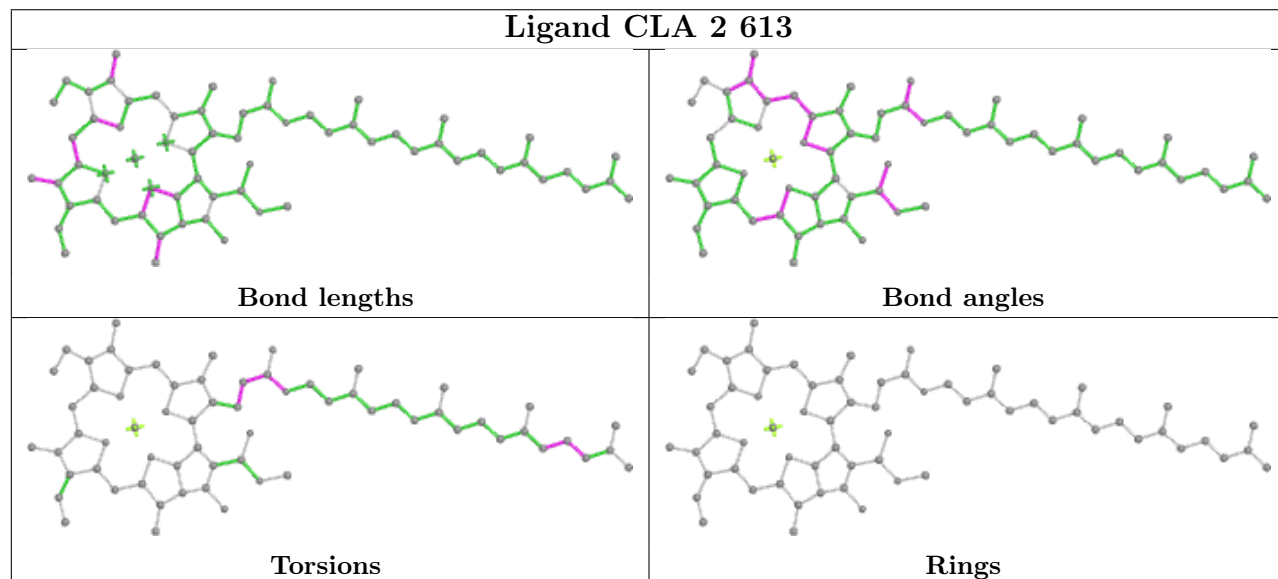
Ligand CLA 8 603

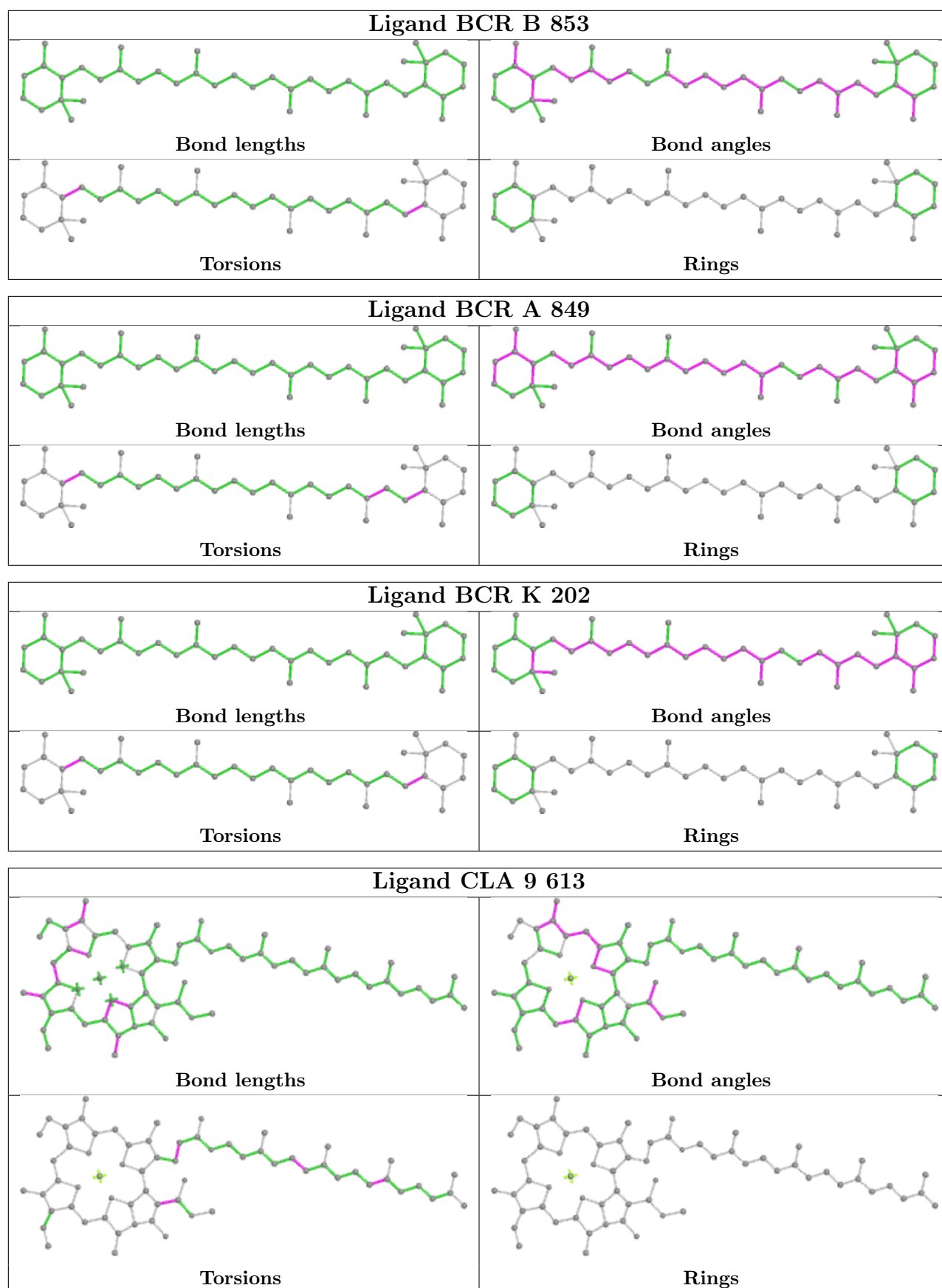


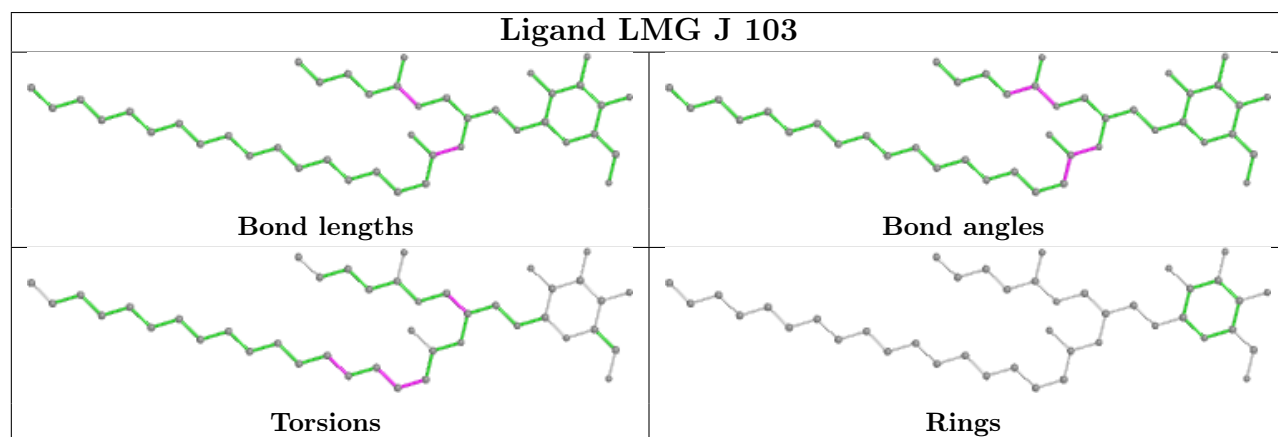
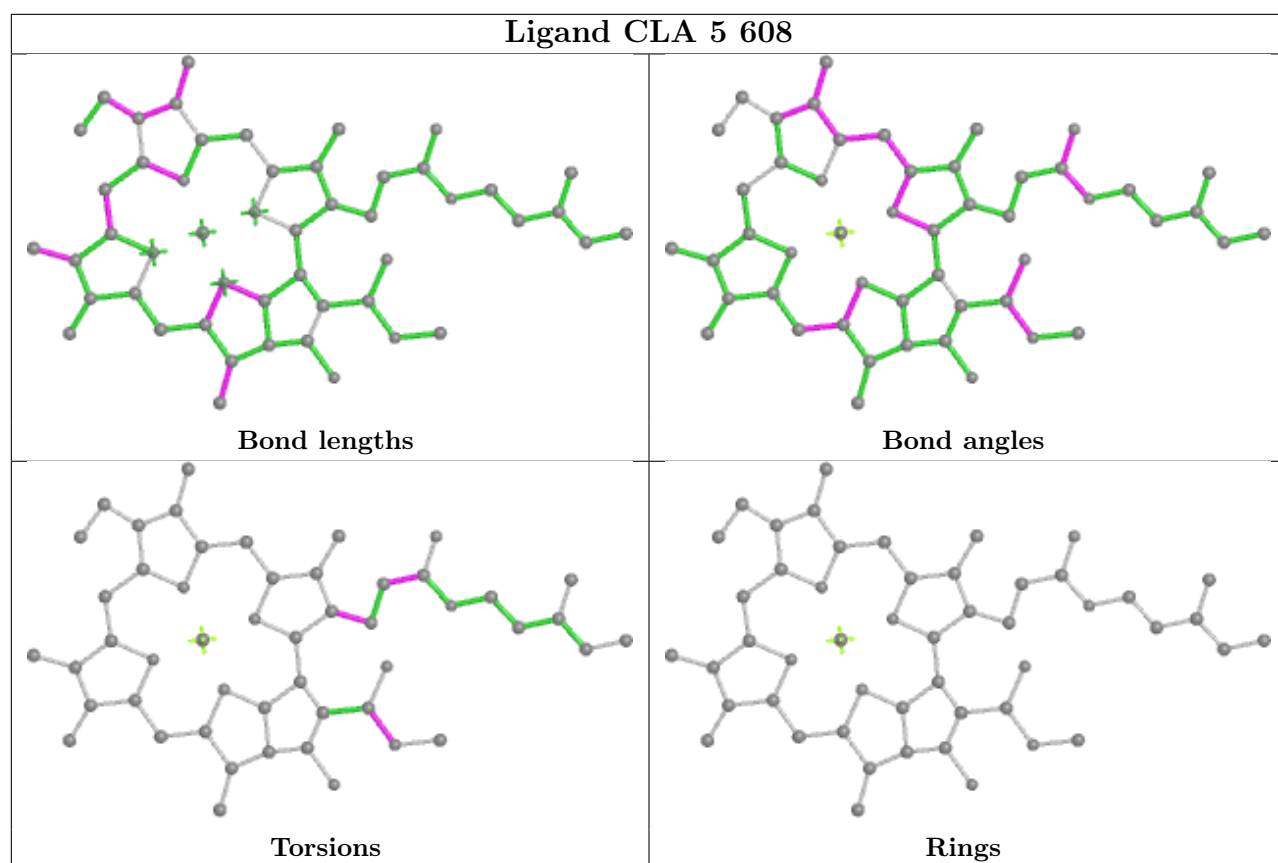
Ligand CLA 7 609

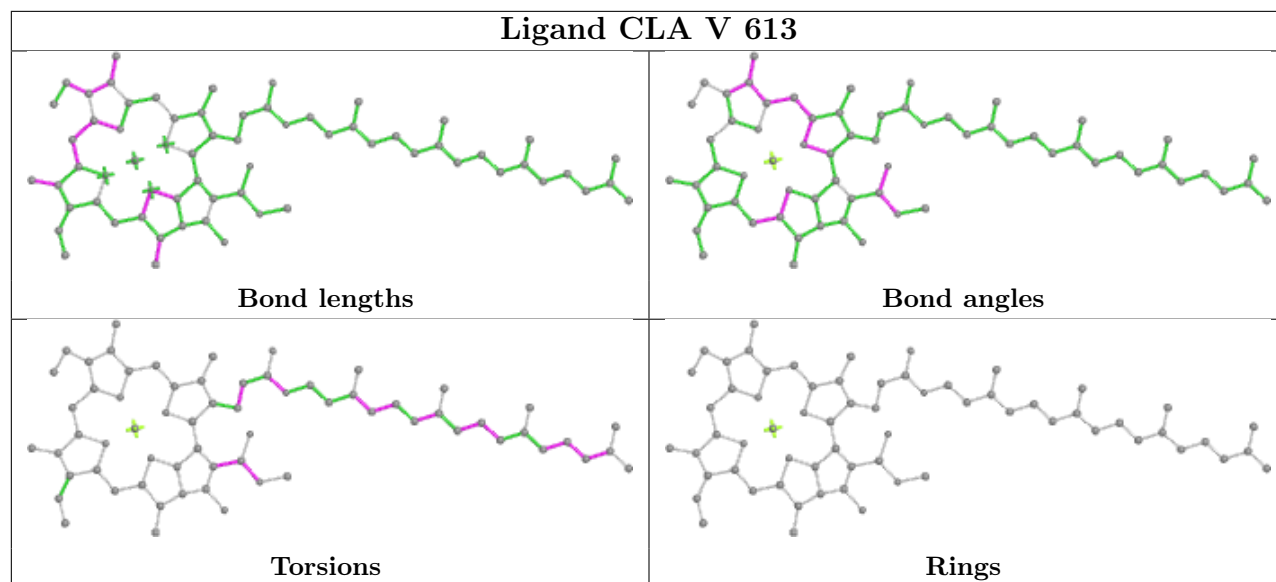
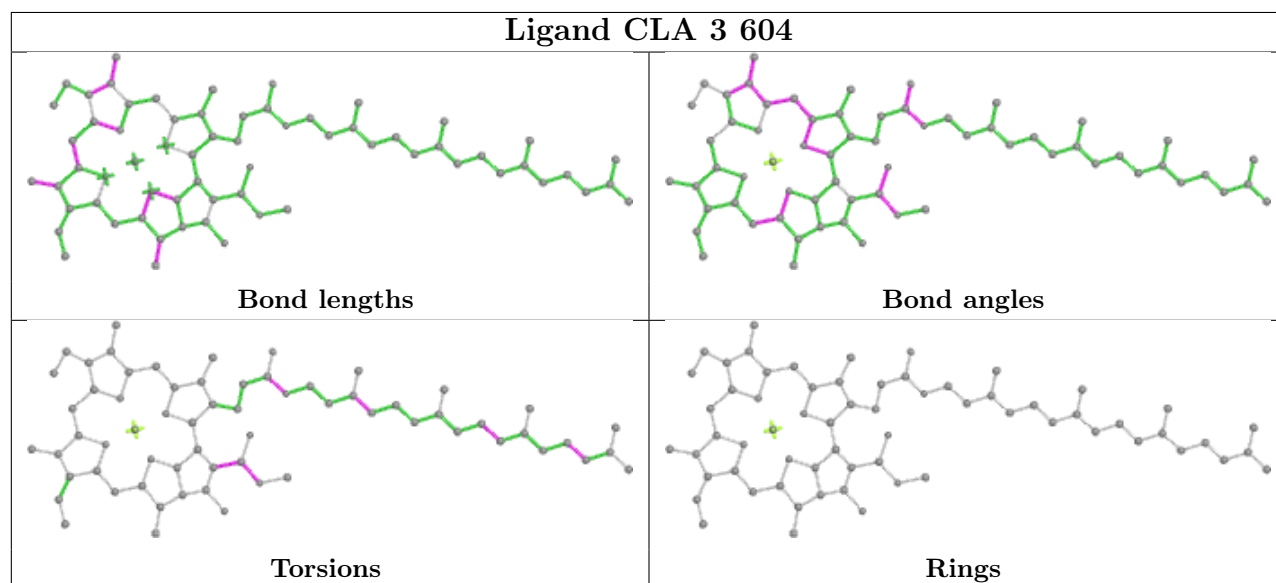


Ligand CLA 2 613

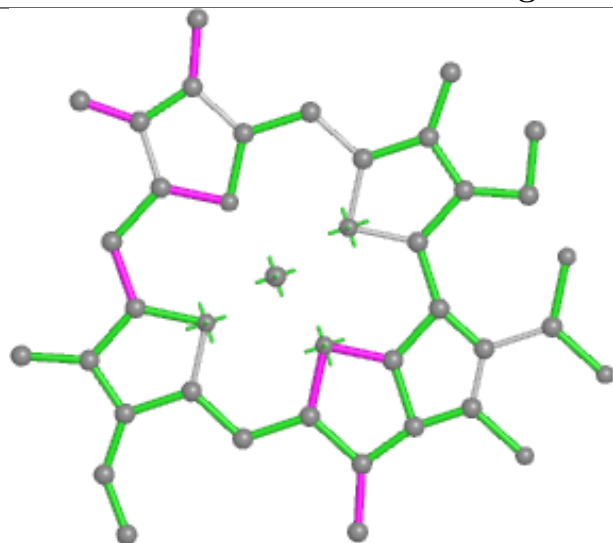




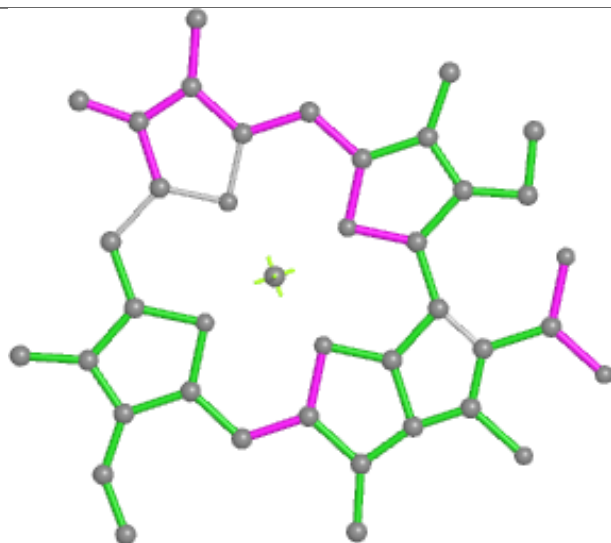


Ligand CLA V 613**Ligand CLA 3 604**

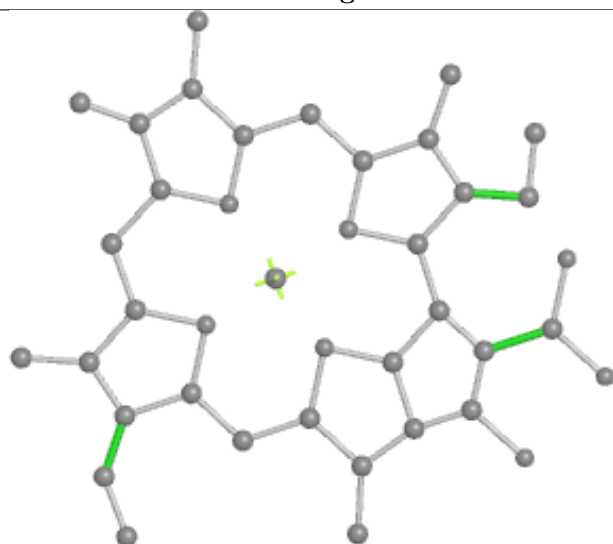
Ligand CLA 5 618



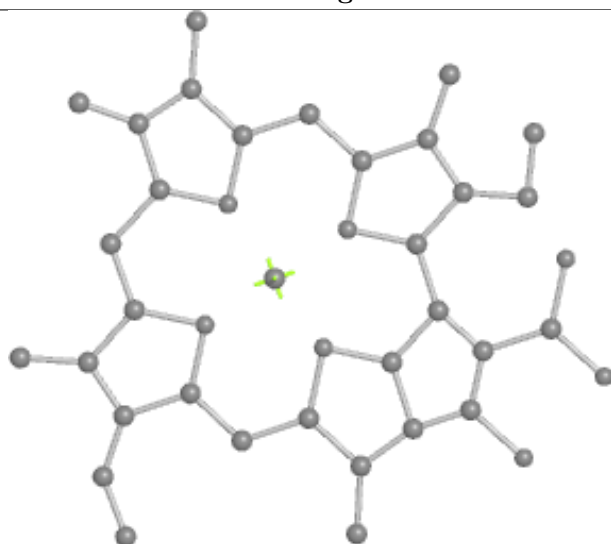
Bond lengths



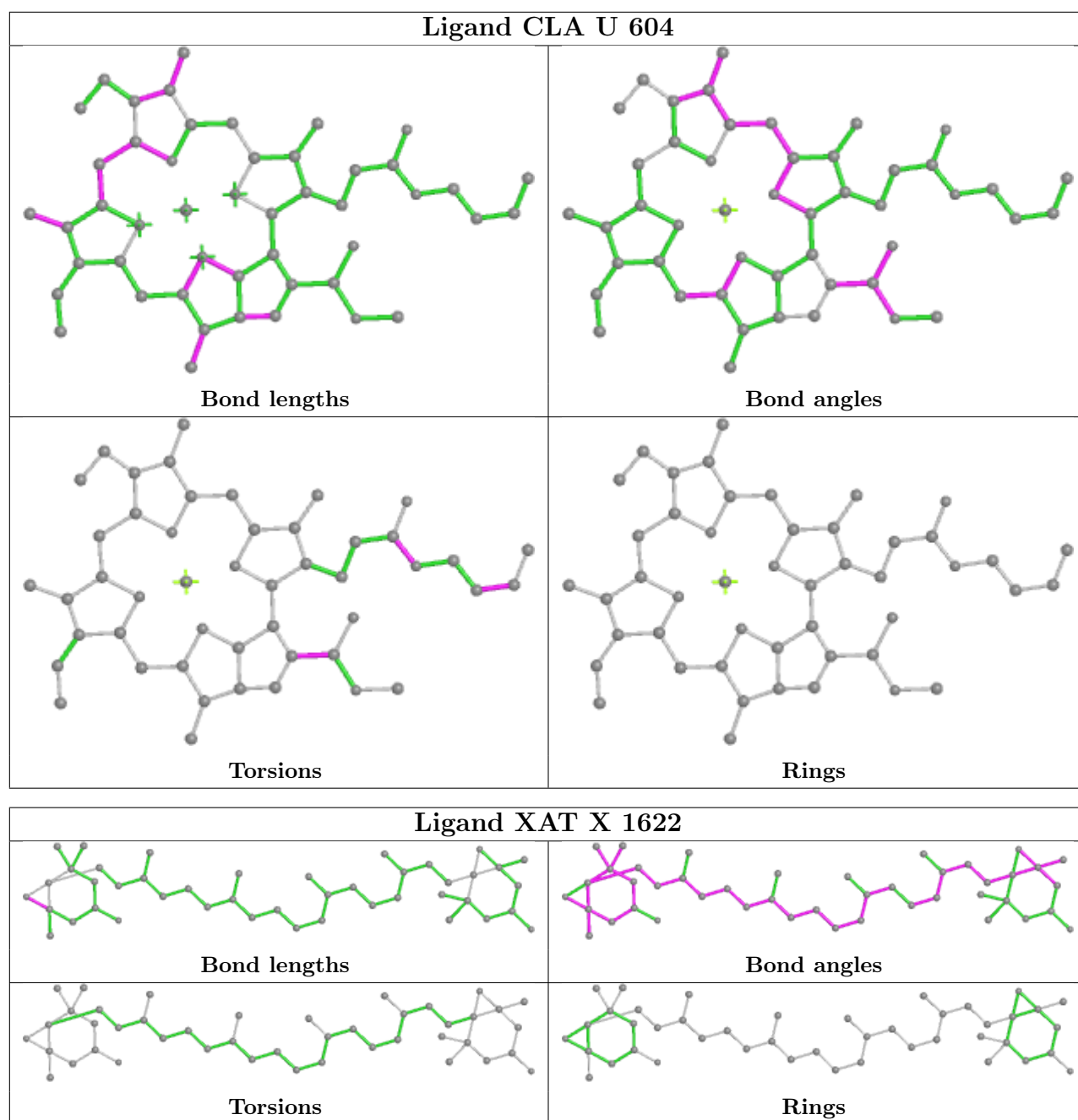
Bond angles



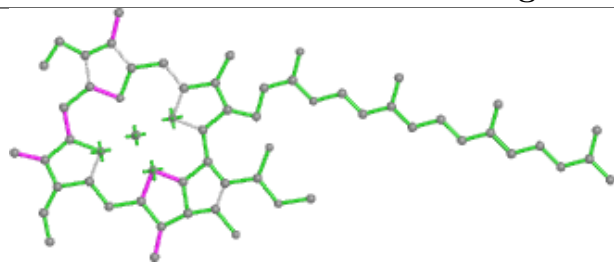
Torsions



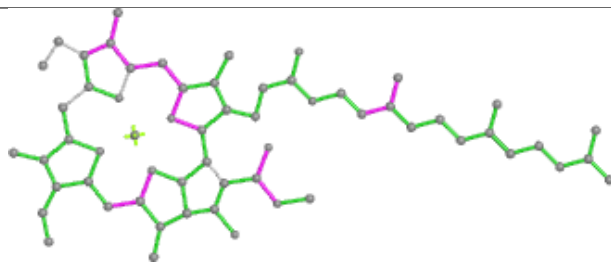
Rings



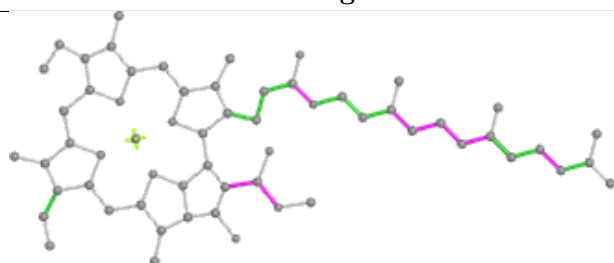
Ligand CLA 7 601



Bond lengths



Bond angles

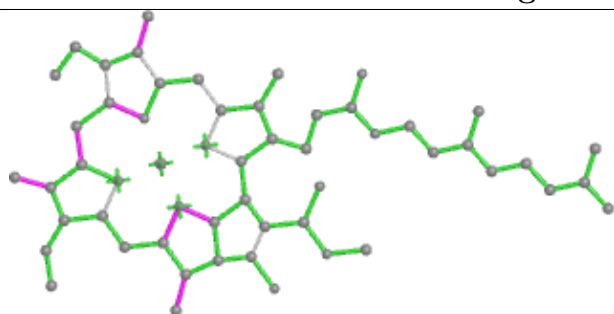


Torsions

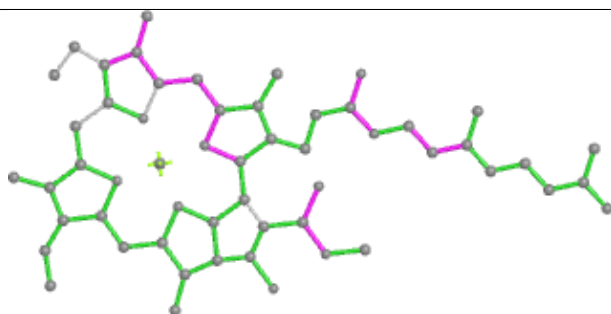


Rings

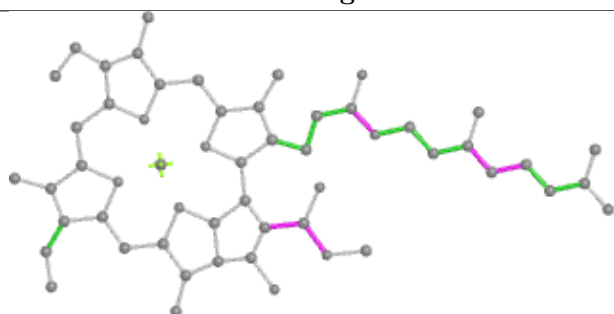
Ligand CLA 2 610



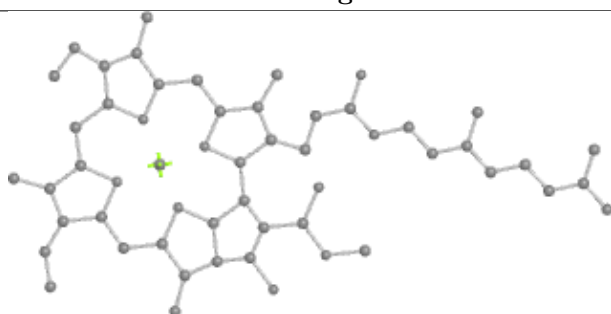
Bond lengths



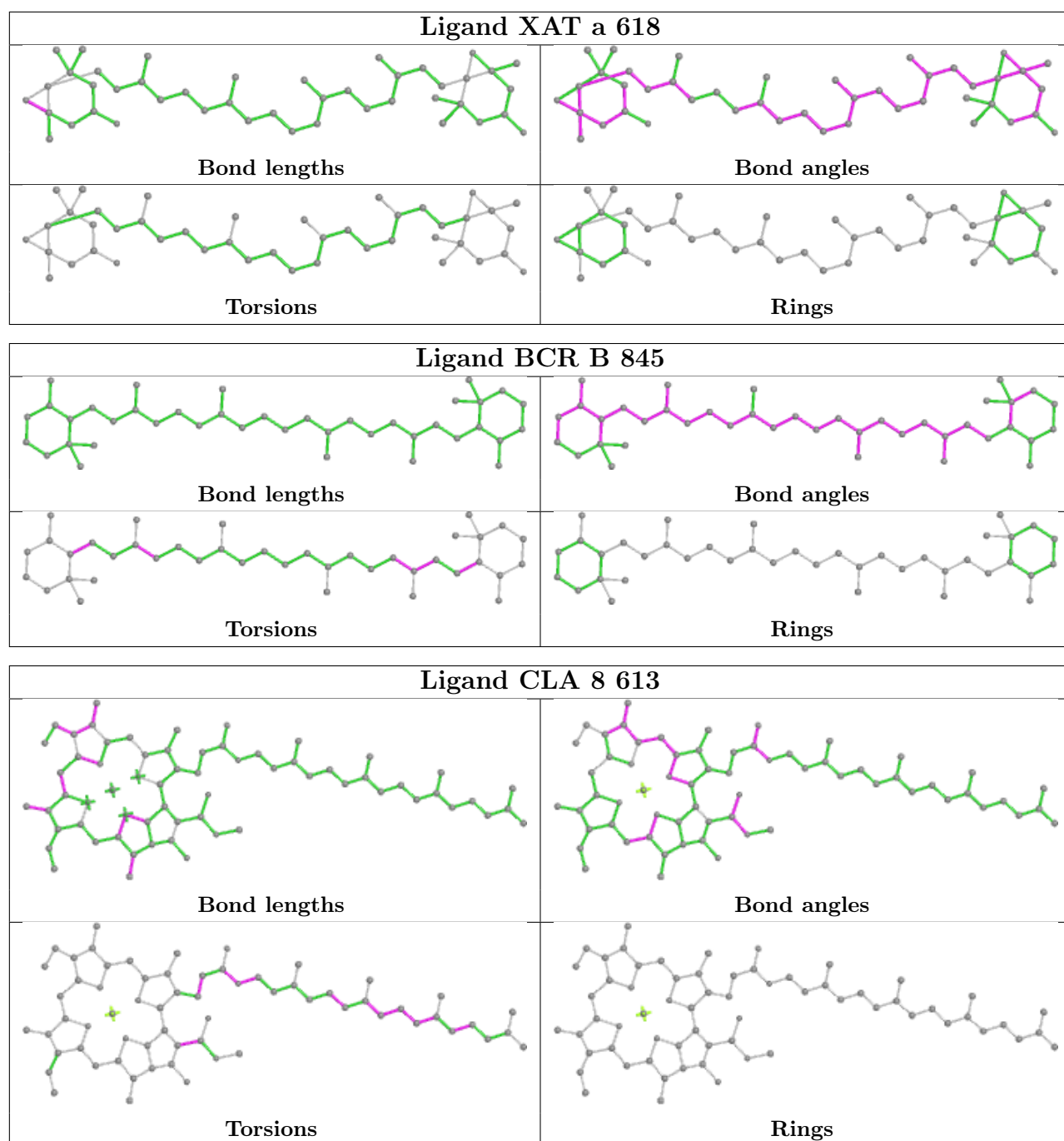
Bond angles

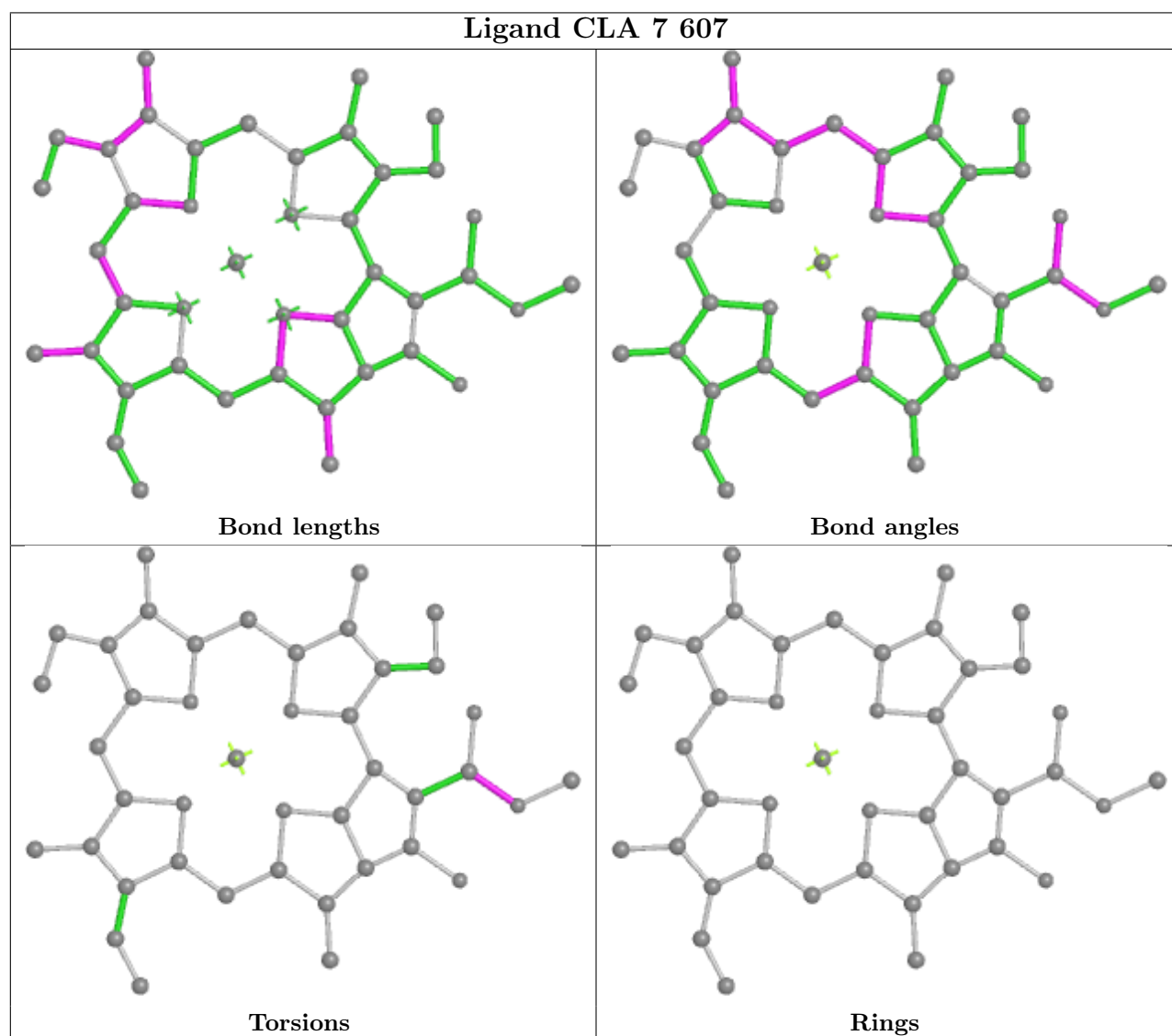
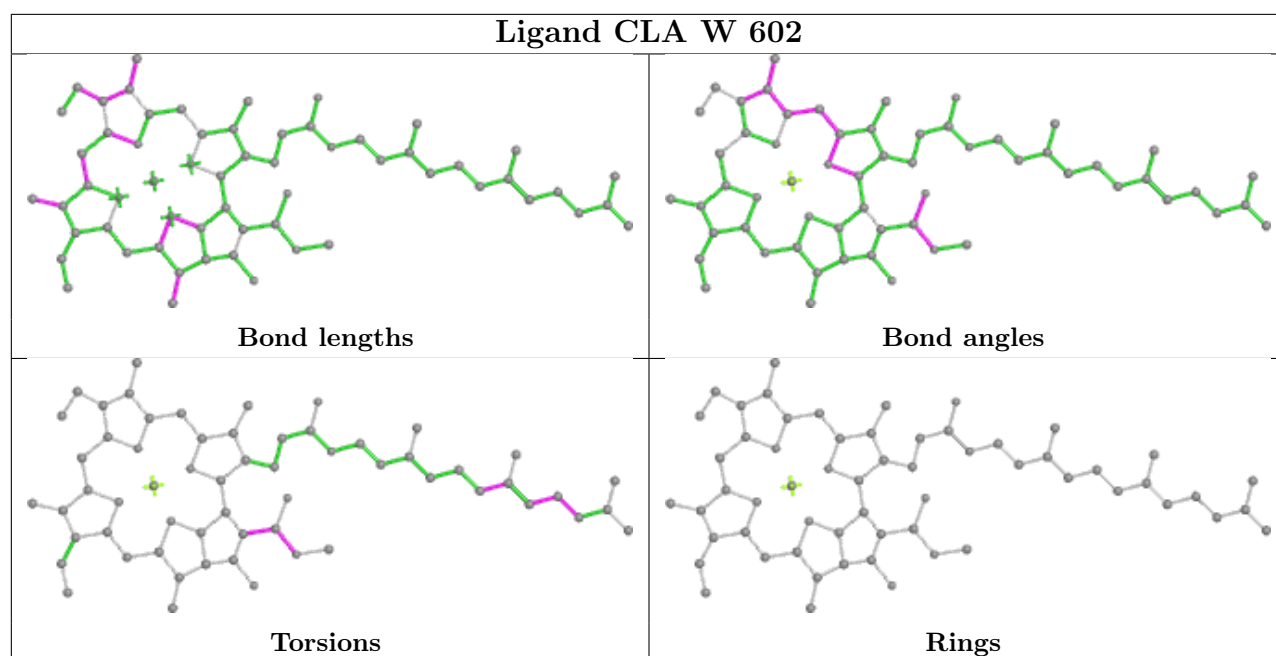


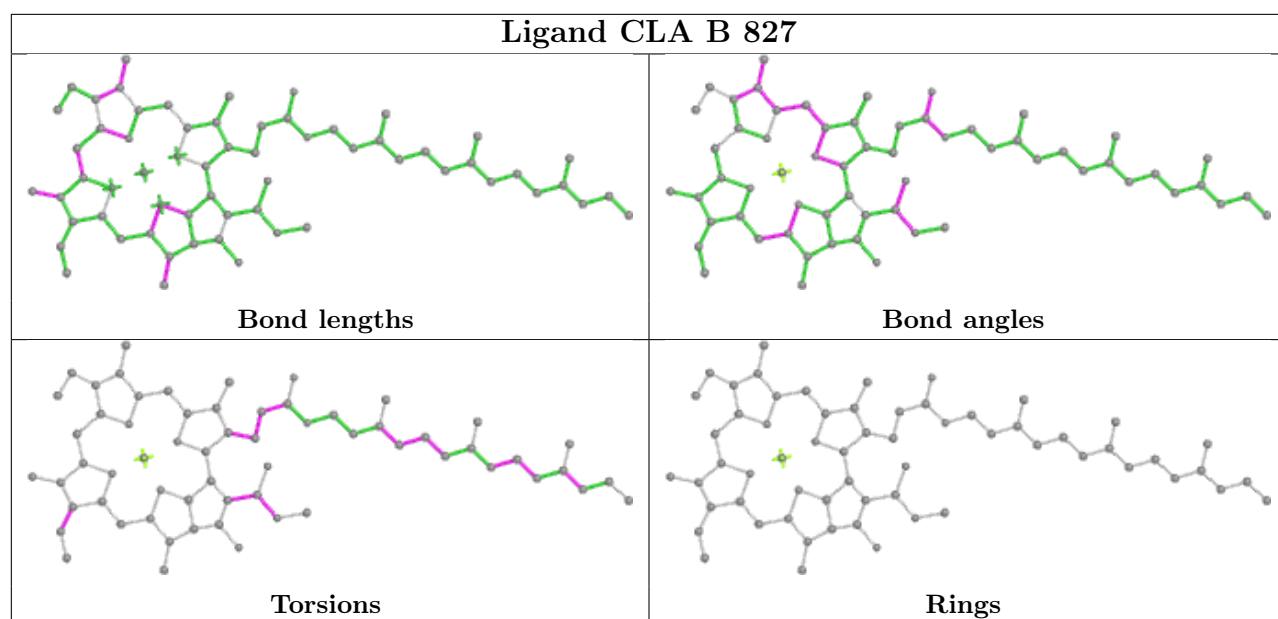
Torsions



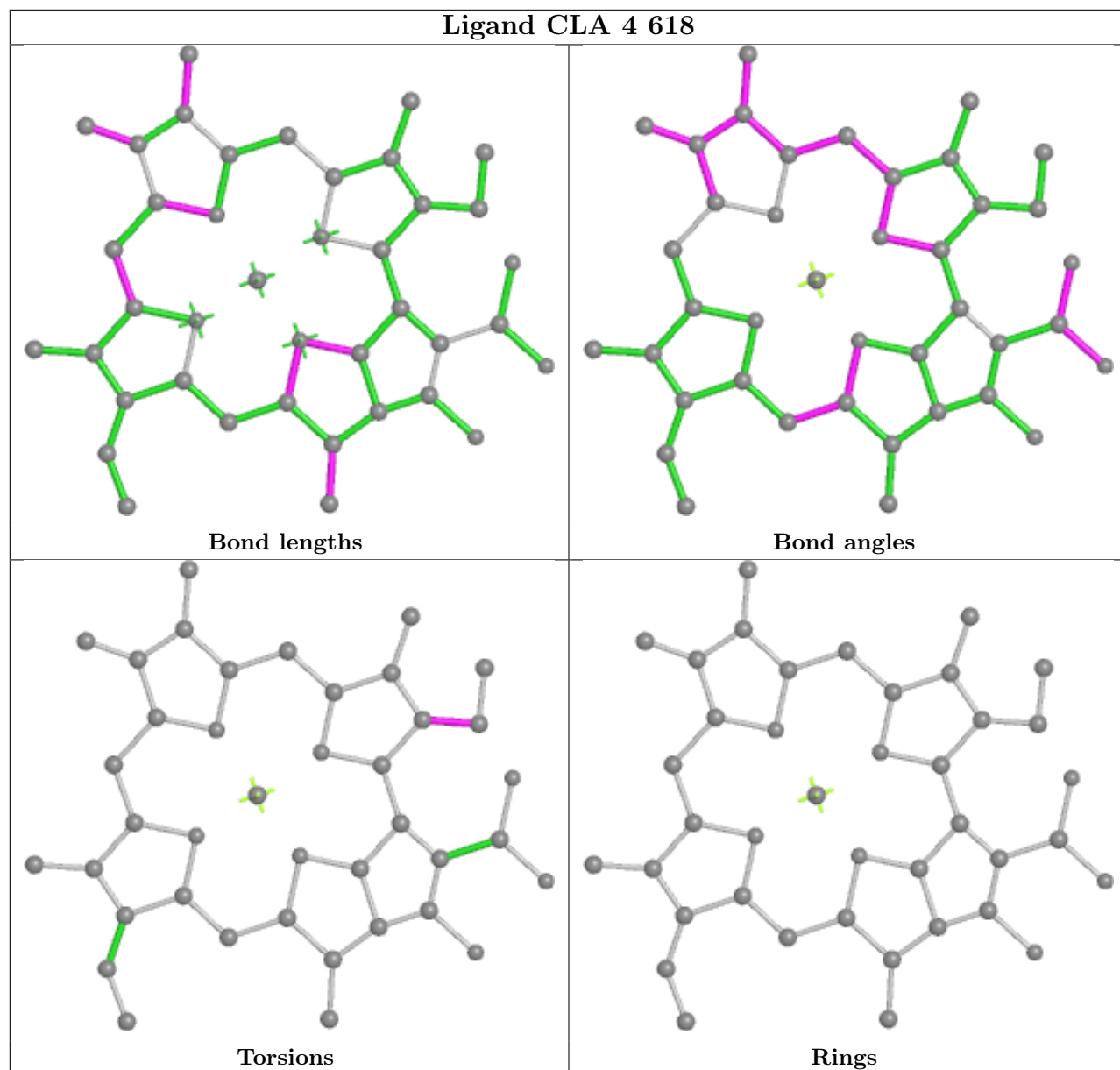
Rings



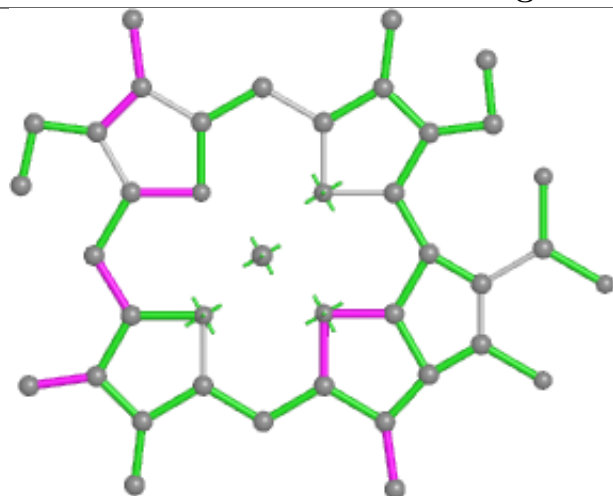




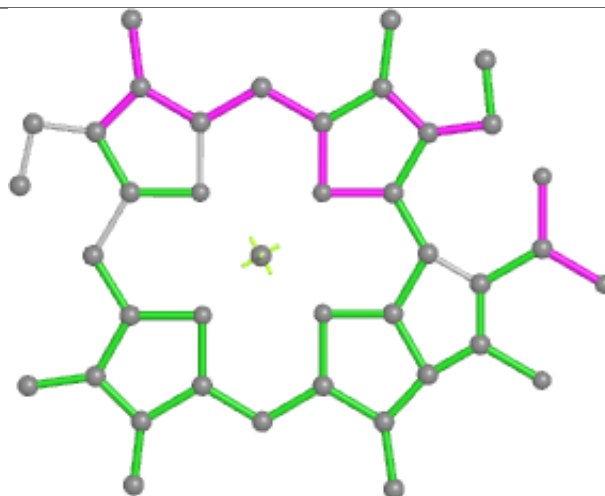
Ligand CLA 4 618



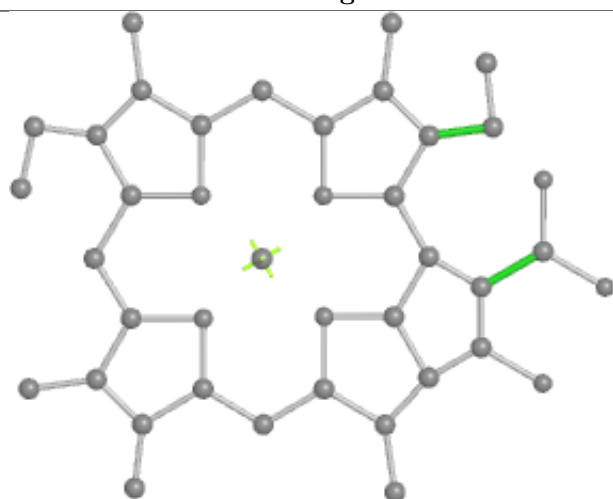
Ligand CLA L 306



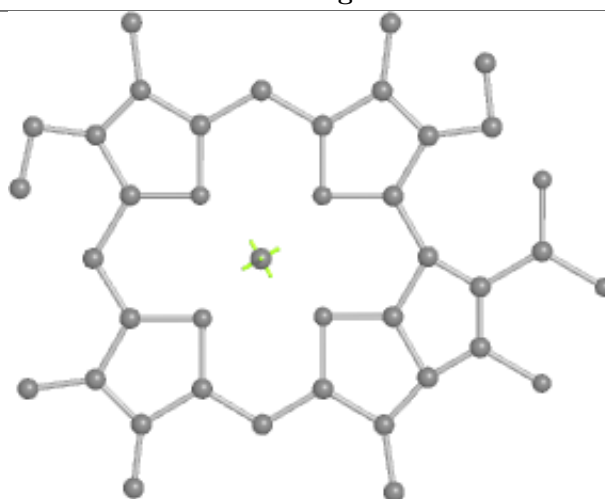
Bond lengths



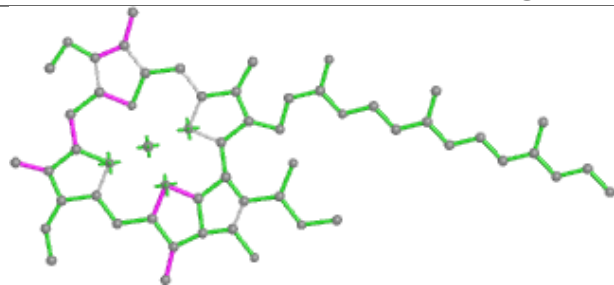
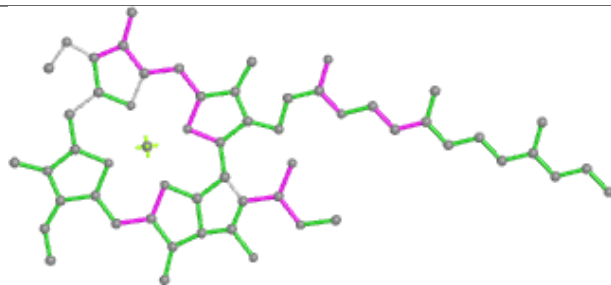
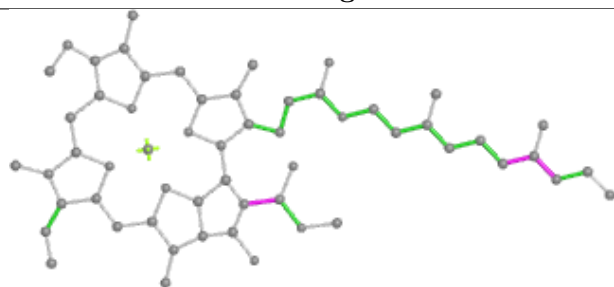
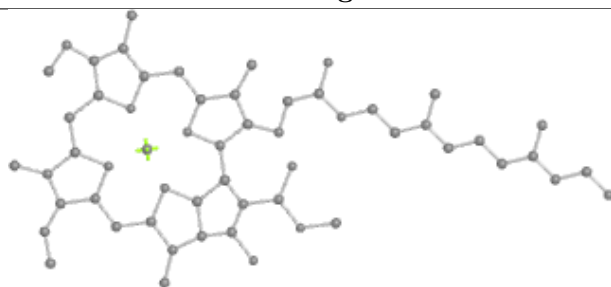
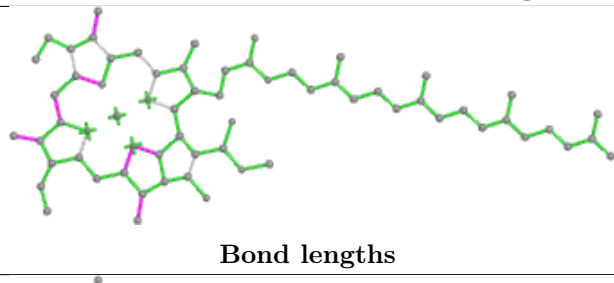
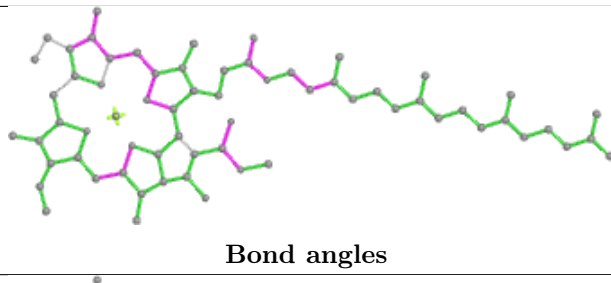
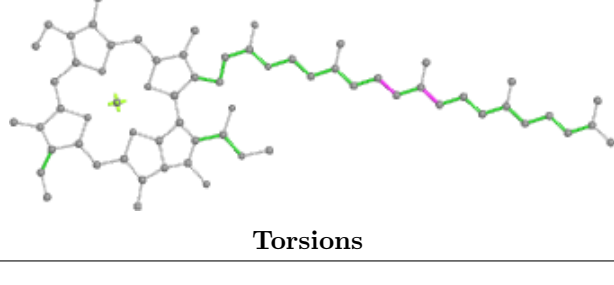
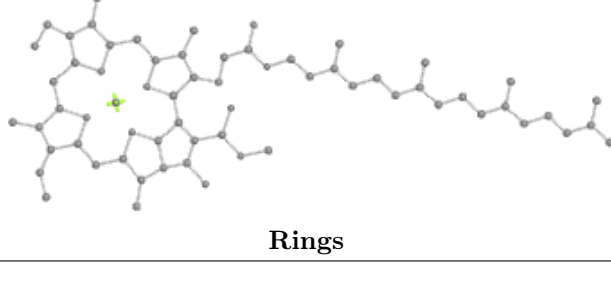
Bond angles



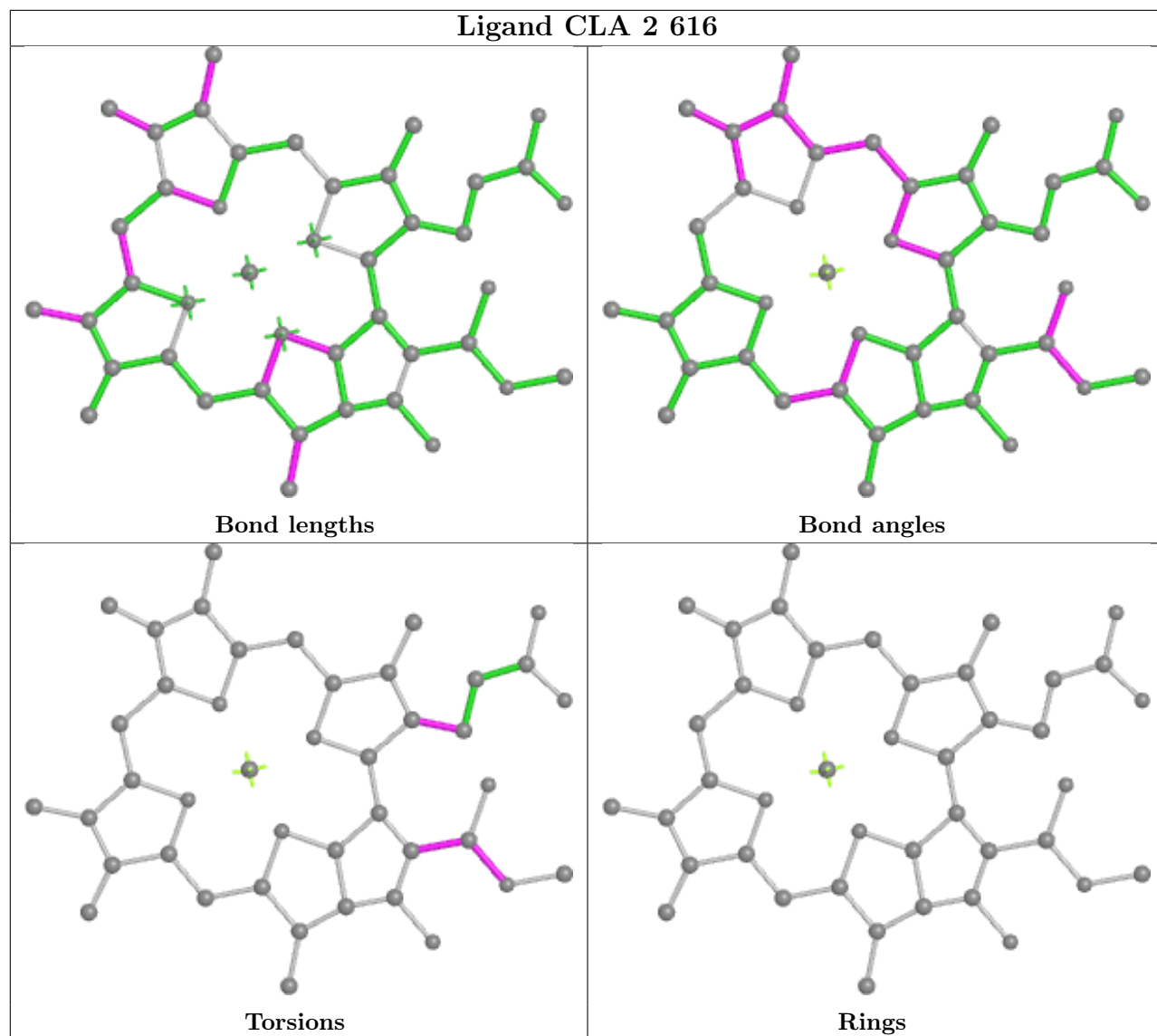
Torsions

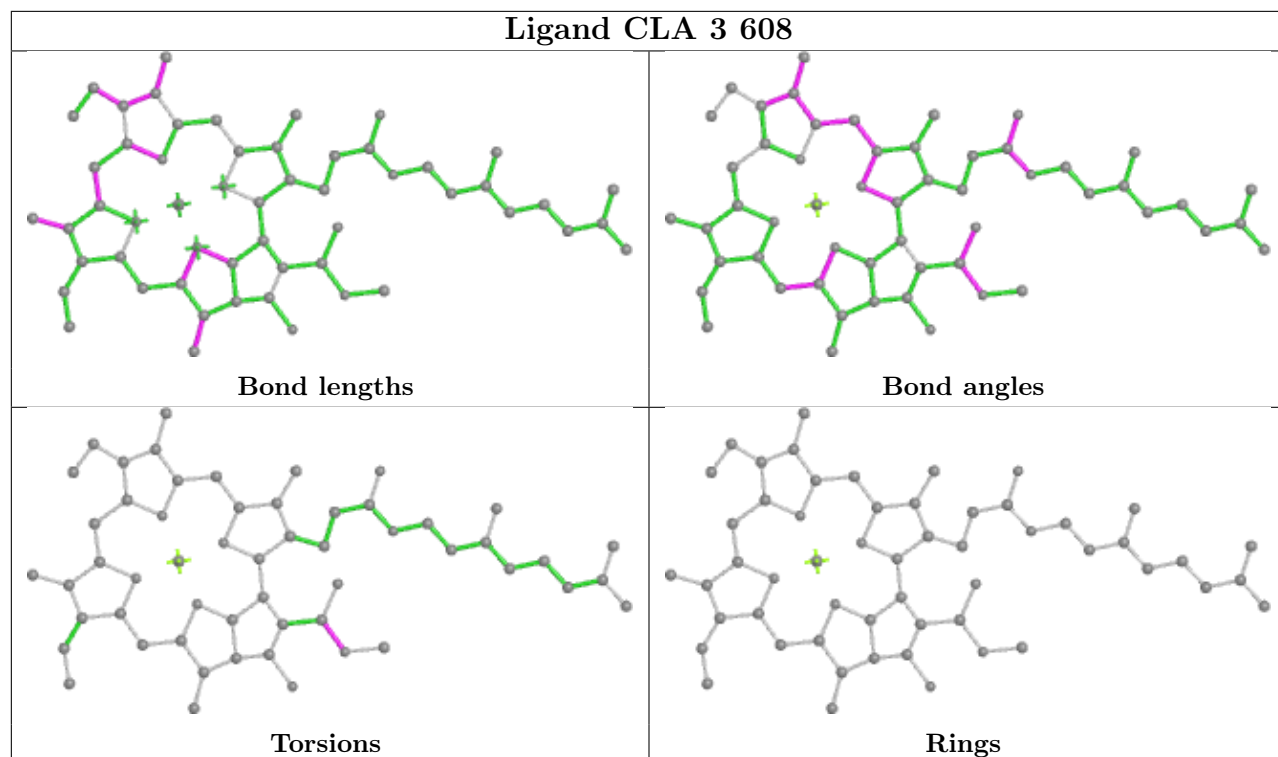
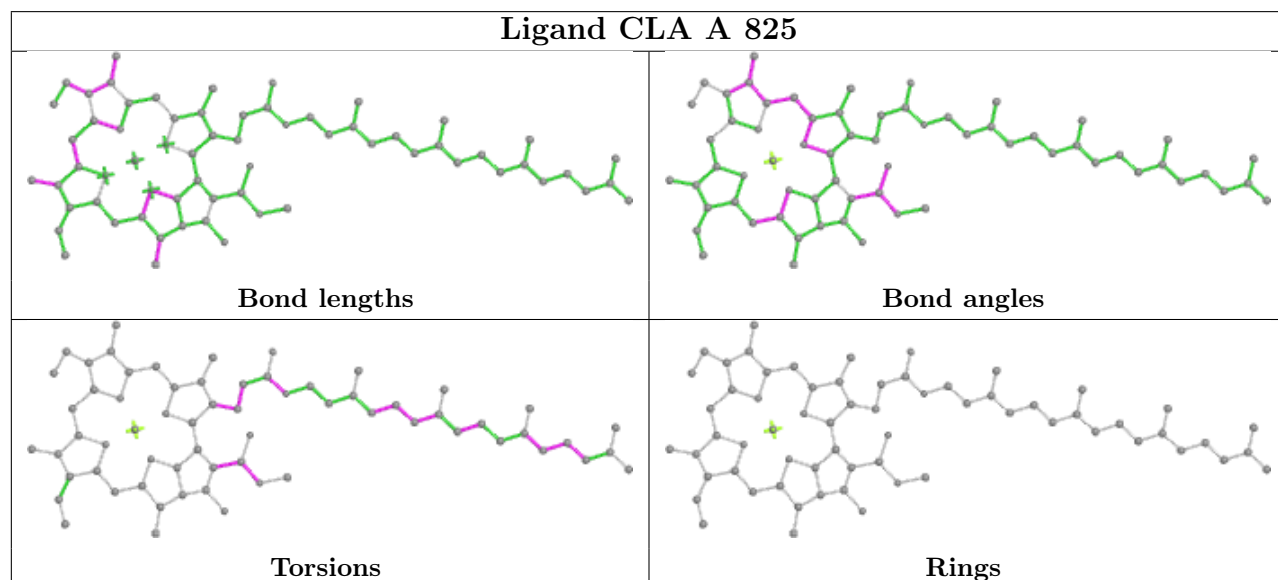
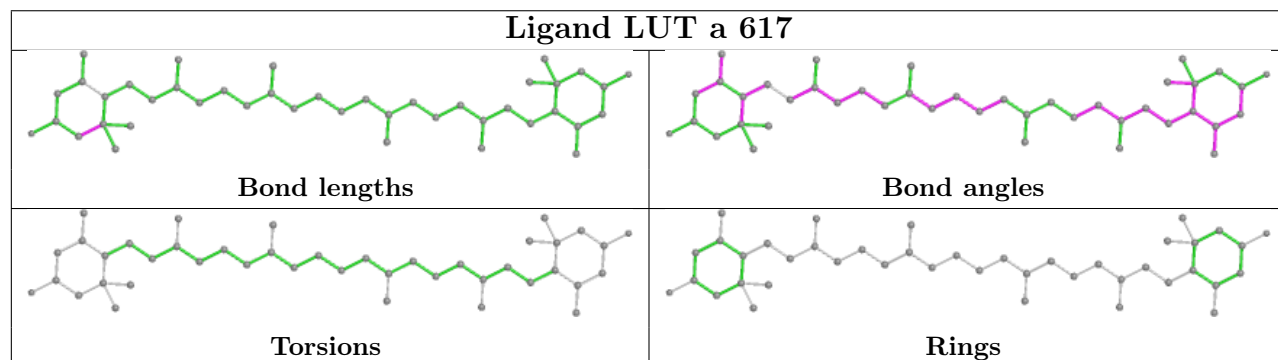


Rings

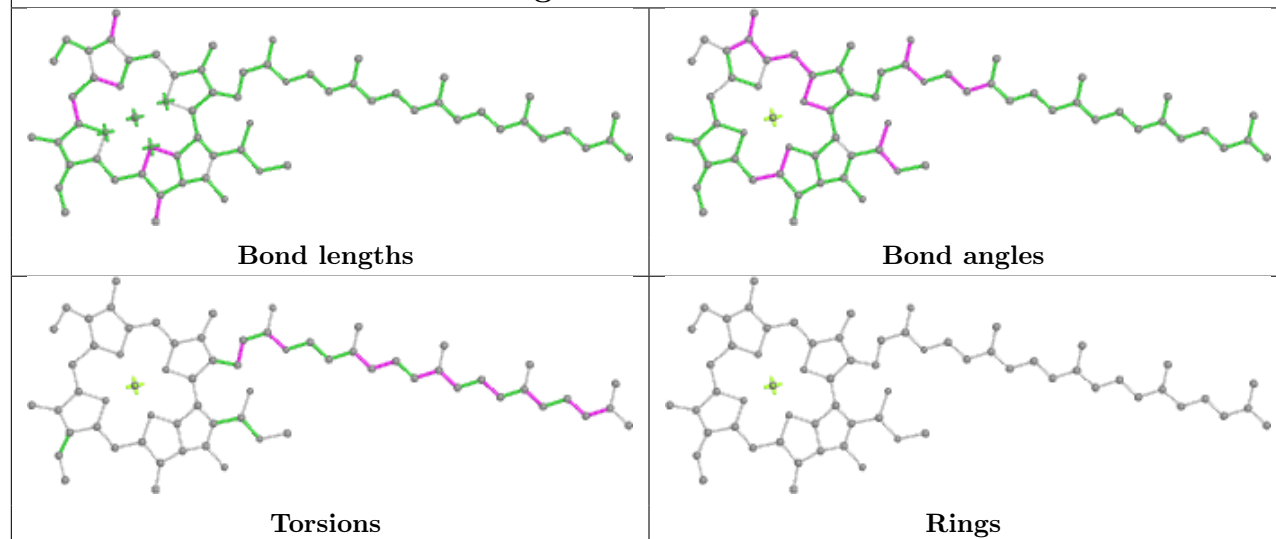
Ligand CLA 9 610**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 7 610****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA 2 616

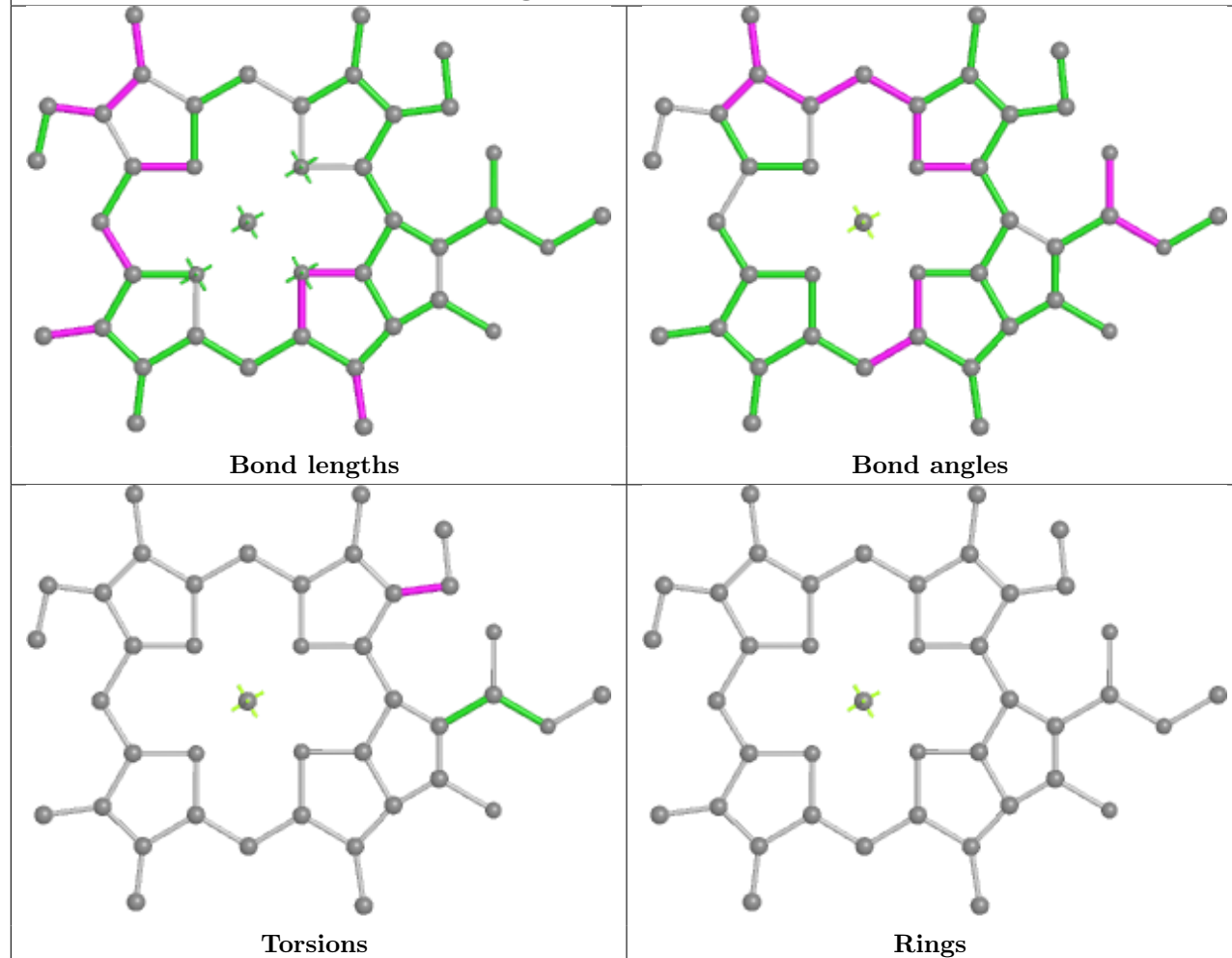


Ligand CLA 3 608**Ligand CLA A 825****Ligand LUT a 617**

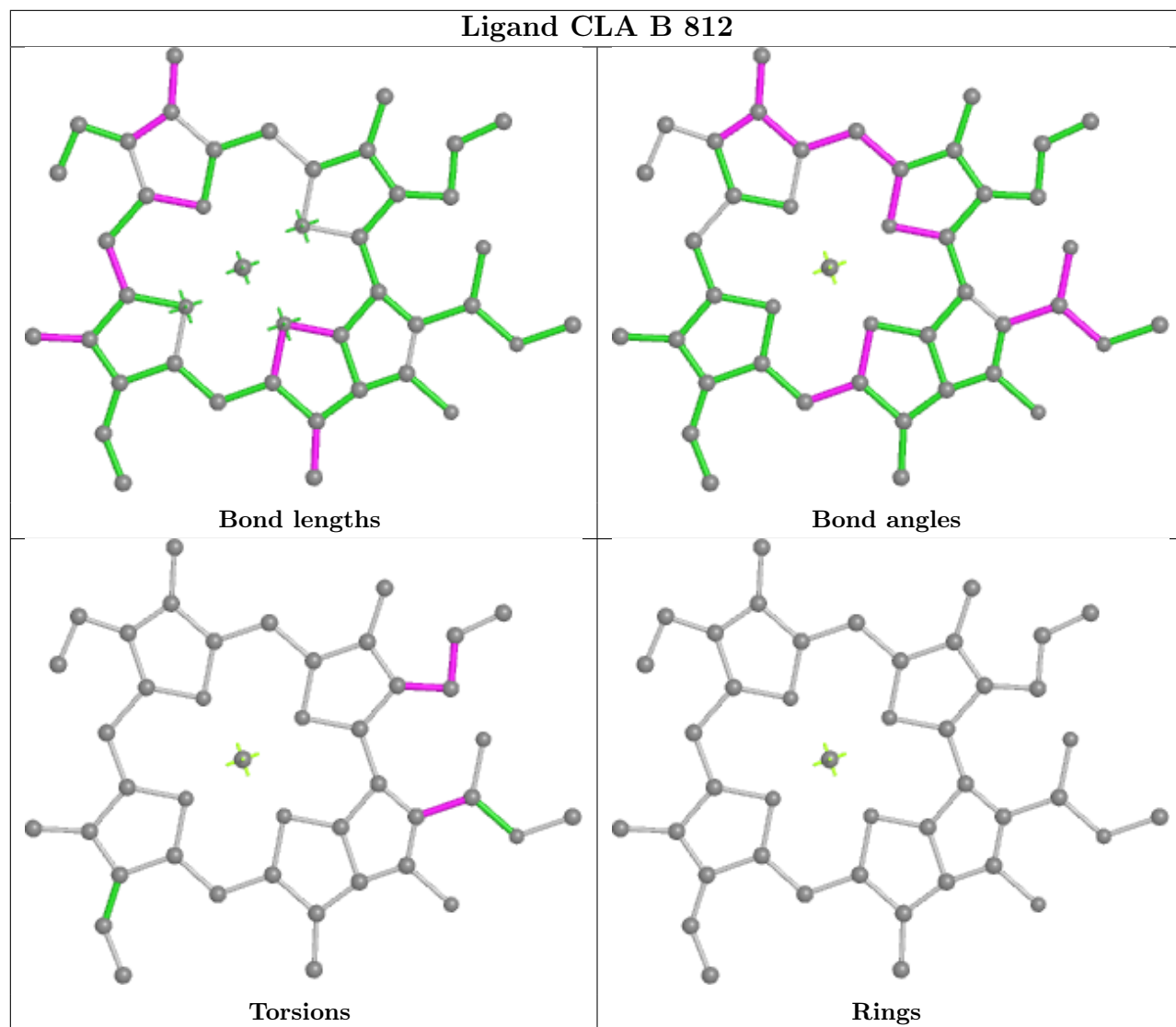
Ligand CLA Z 613



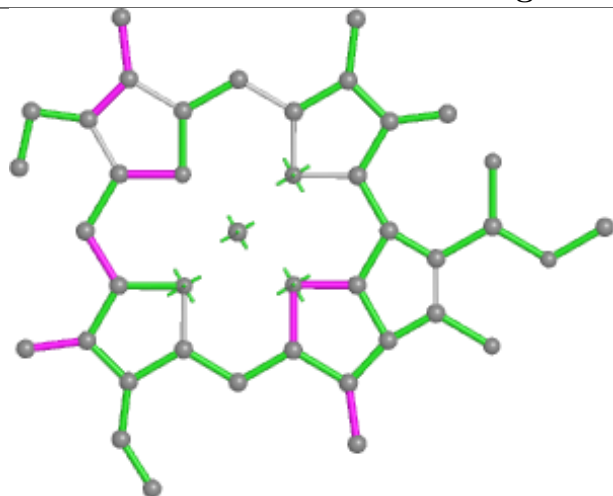
Ligand CLA 7 606



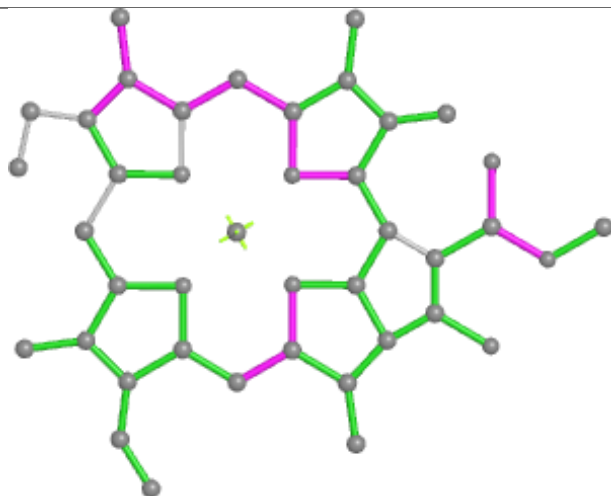
Ligand CLA B 812



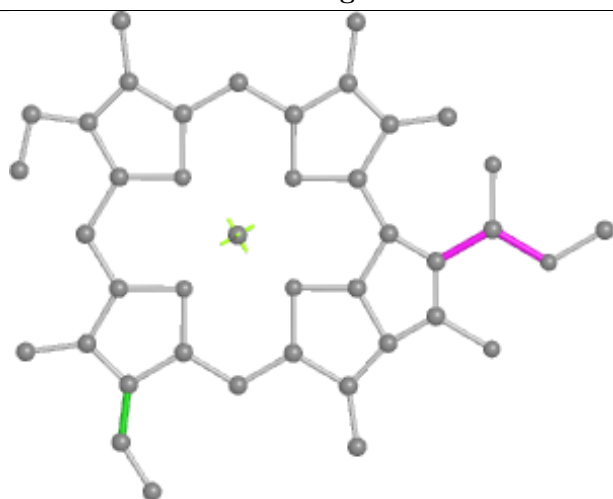
Ligand CLA F 304



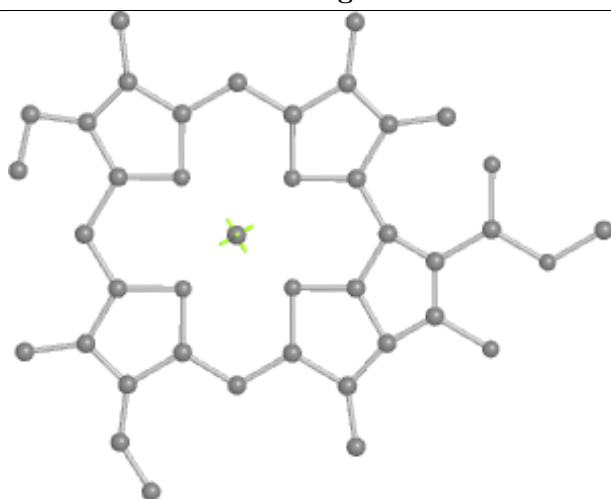
Bond lengths



Bond angles

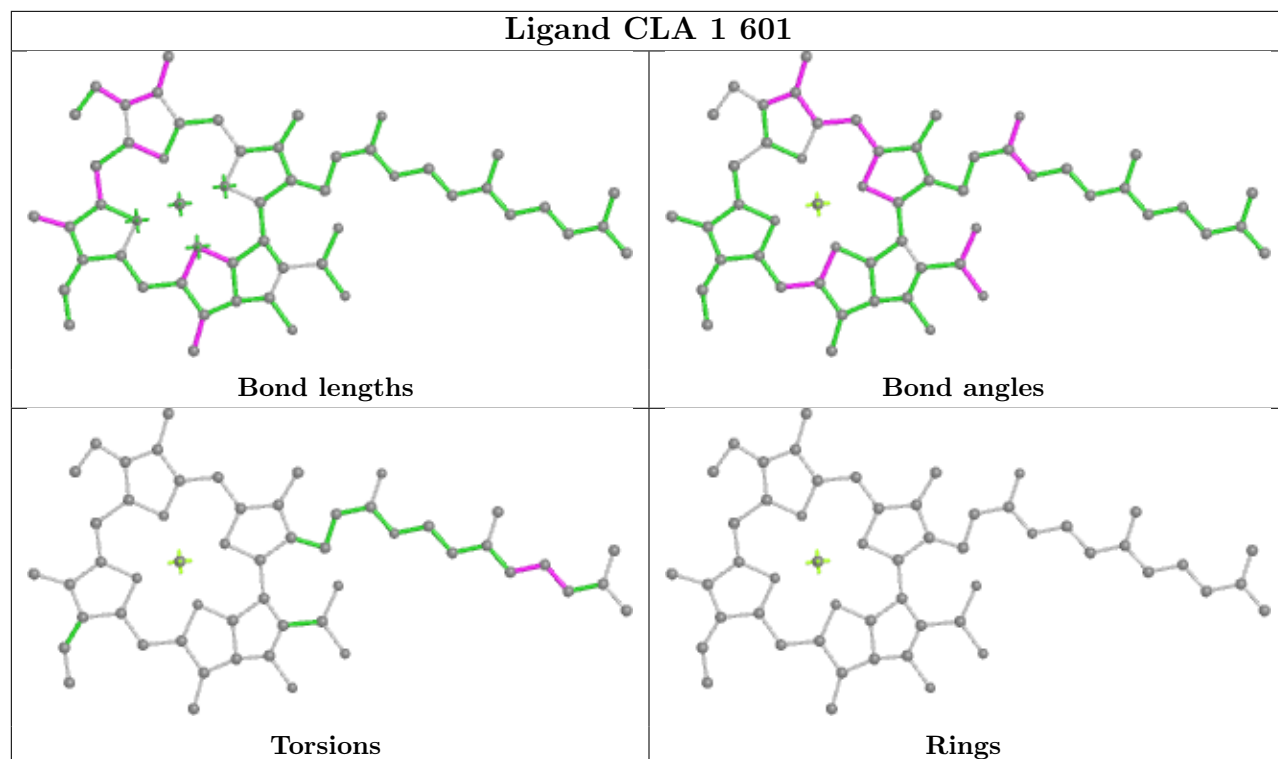


Torsions

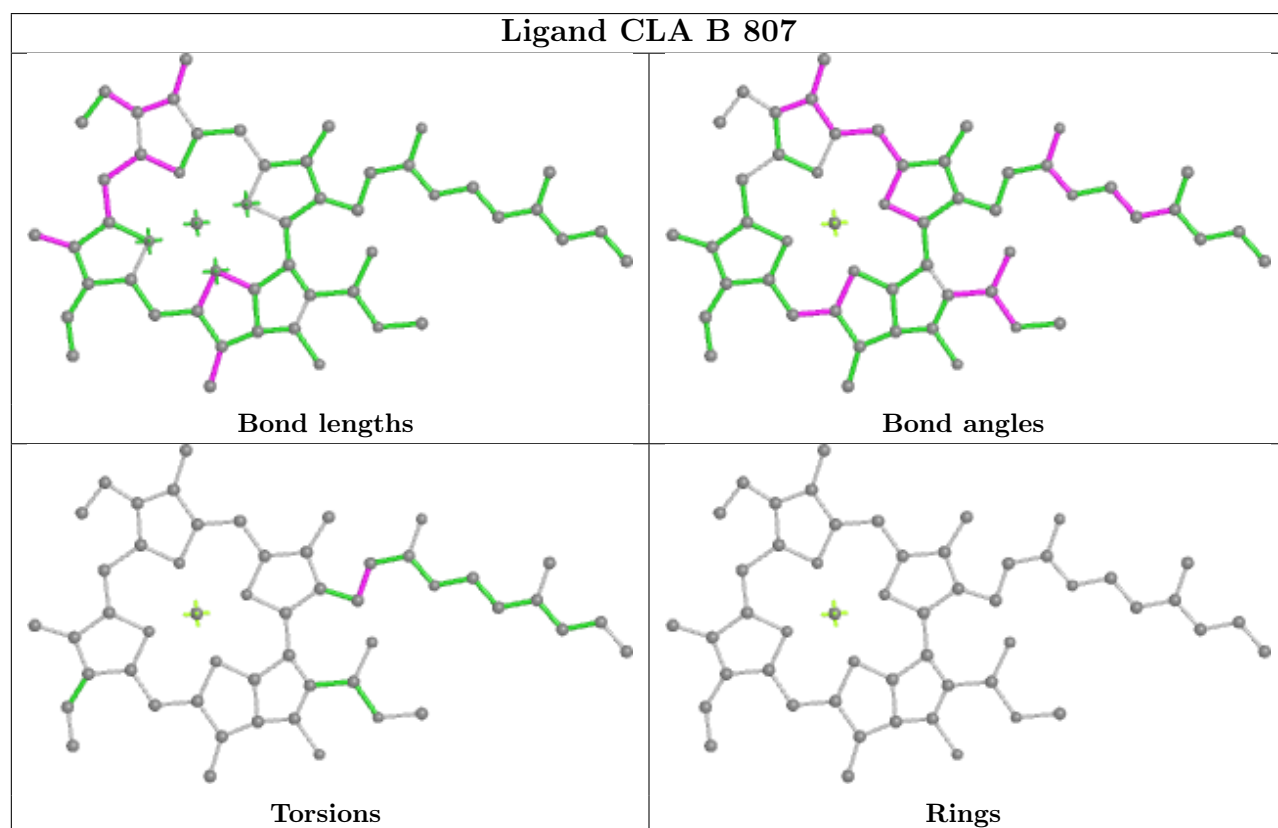


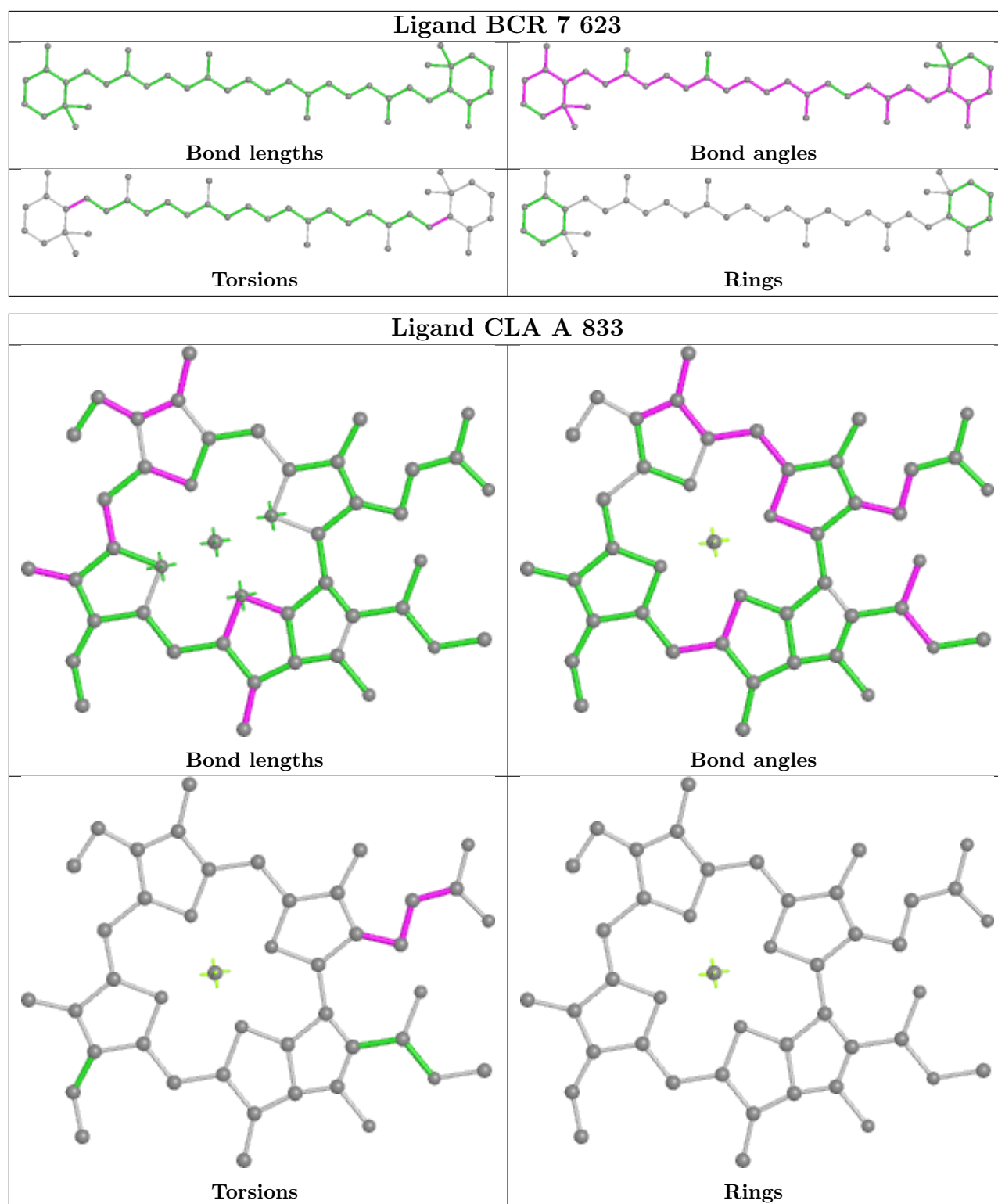
Rings

Ligand CLA 1 601



Ligand CLA B 807





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

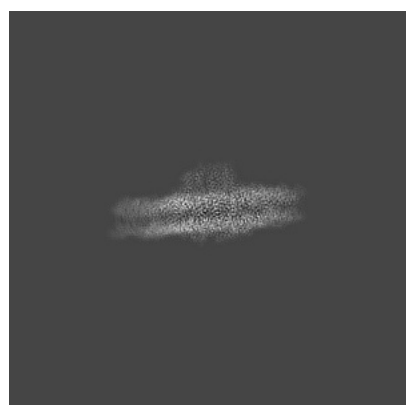
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30925. These allow visual inspection of the internal detail of the map and identification of artifacts.

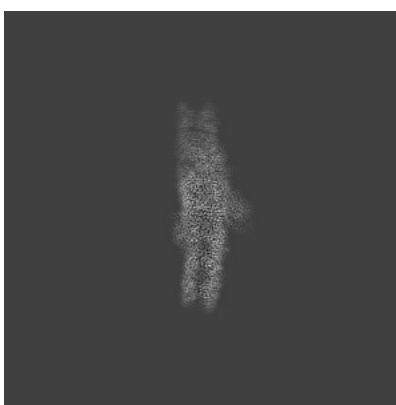
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

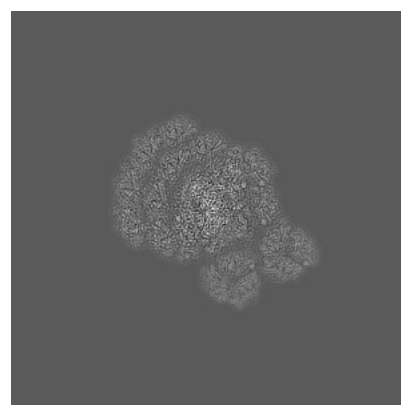
6.1.1 Primary map



X



Y



Z

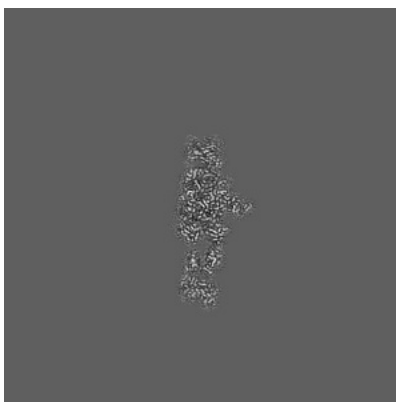
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

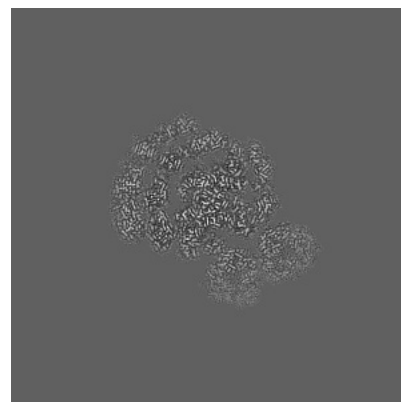
6.2.1 Primary map



X Index: 240



Y Index: 240

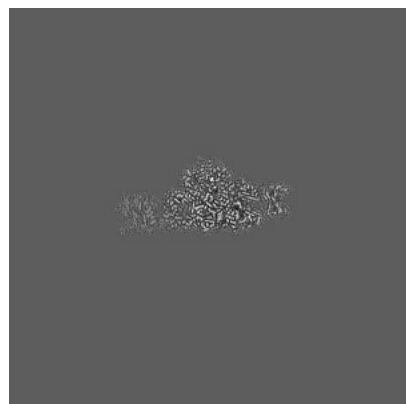


Z Index: 240

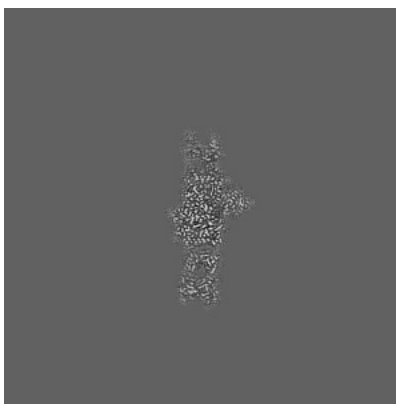
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

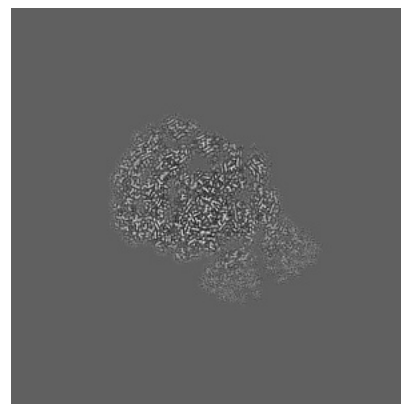
6.3.1 Primary map



X Index: 243



Y Index: 231

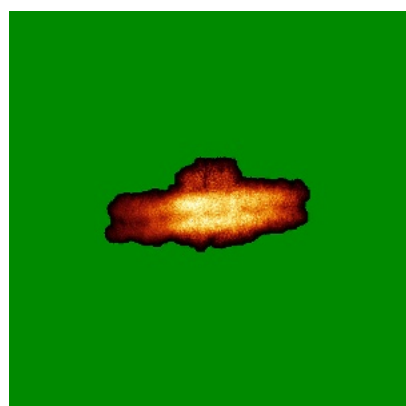


Z Index: 248

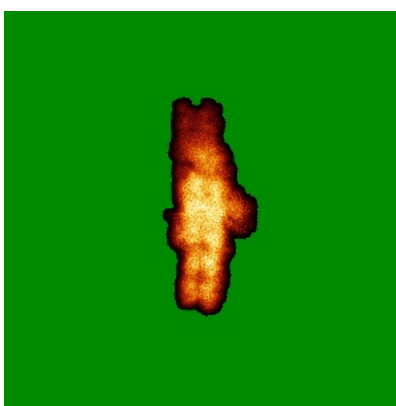
The images above show the largest variance slices of the map in three orthogonal directions.

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

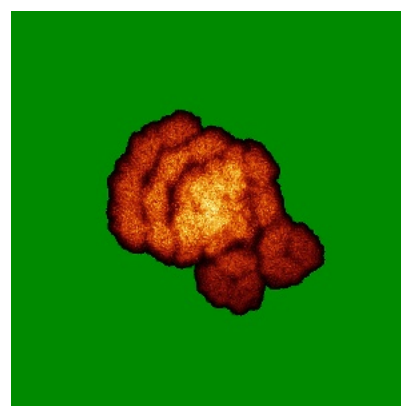
6.4.1 Primary map



X



Y

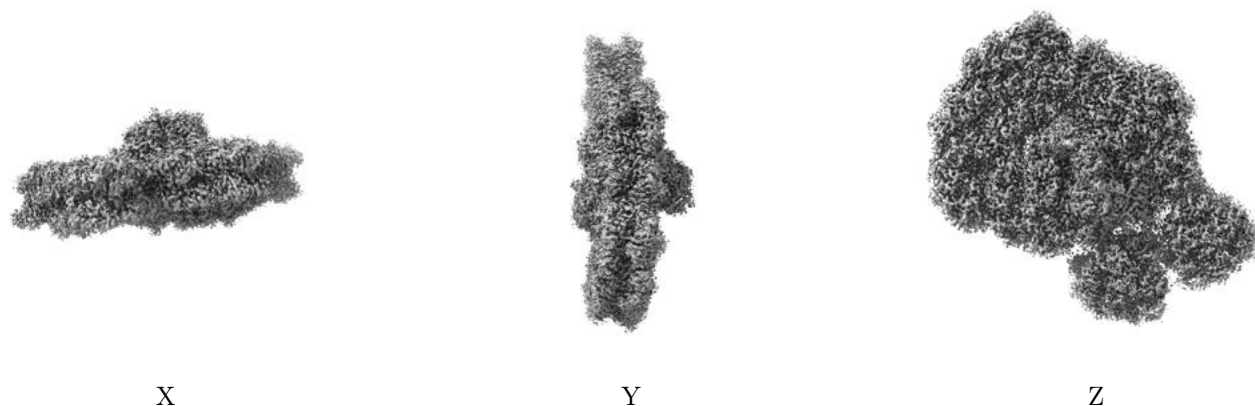


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

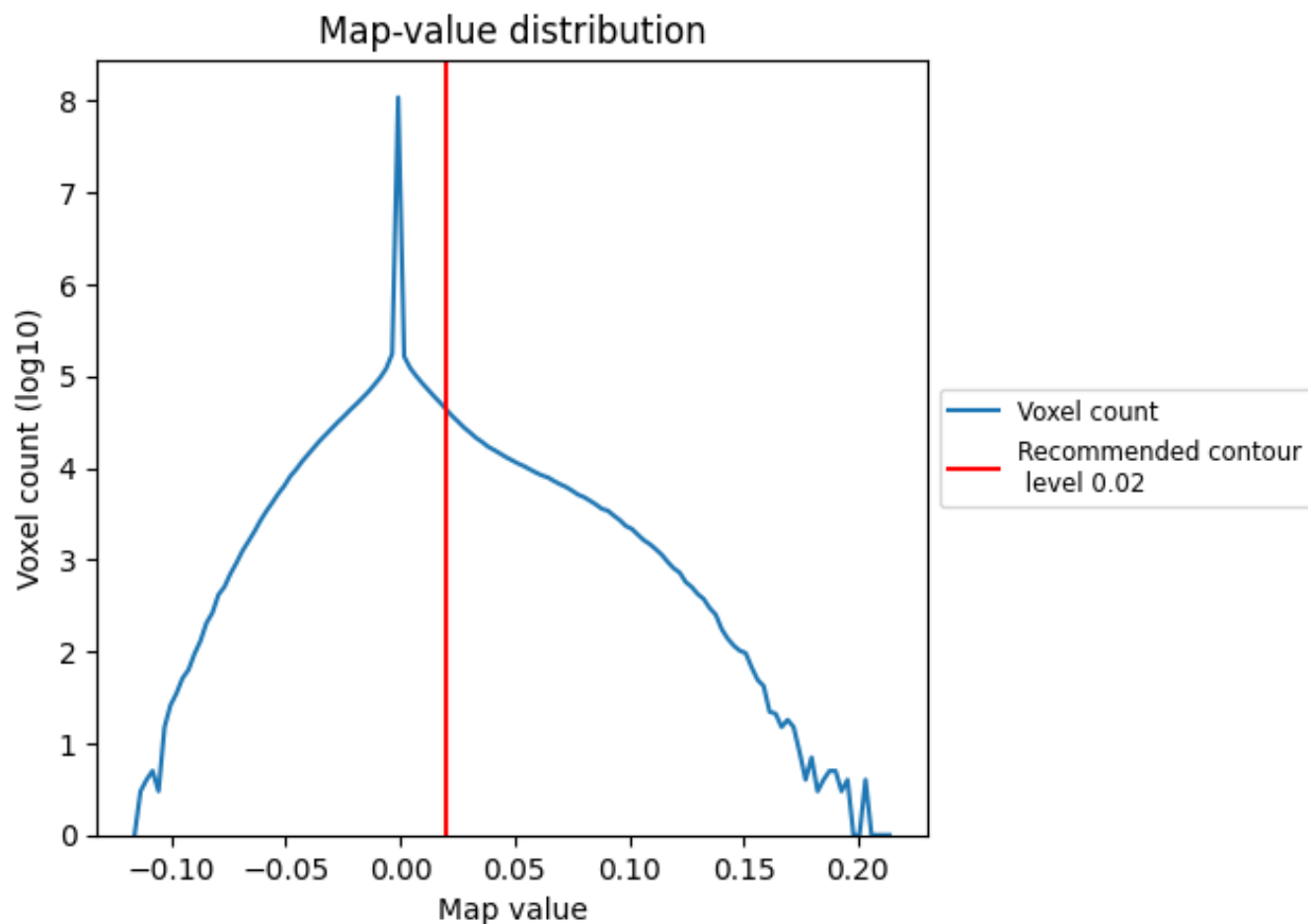
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

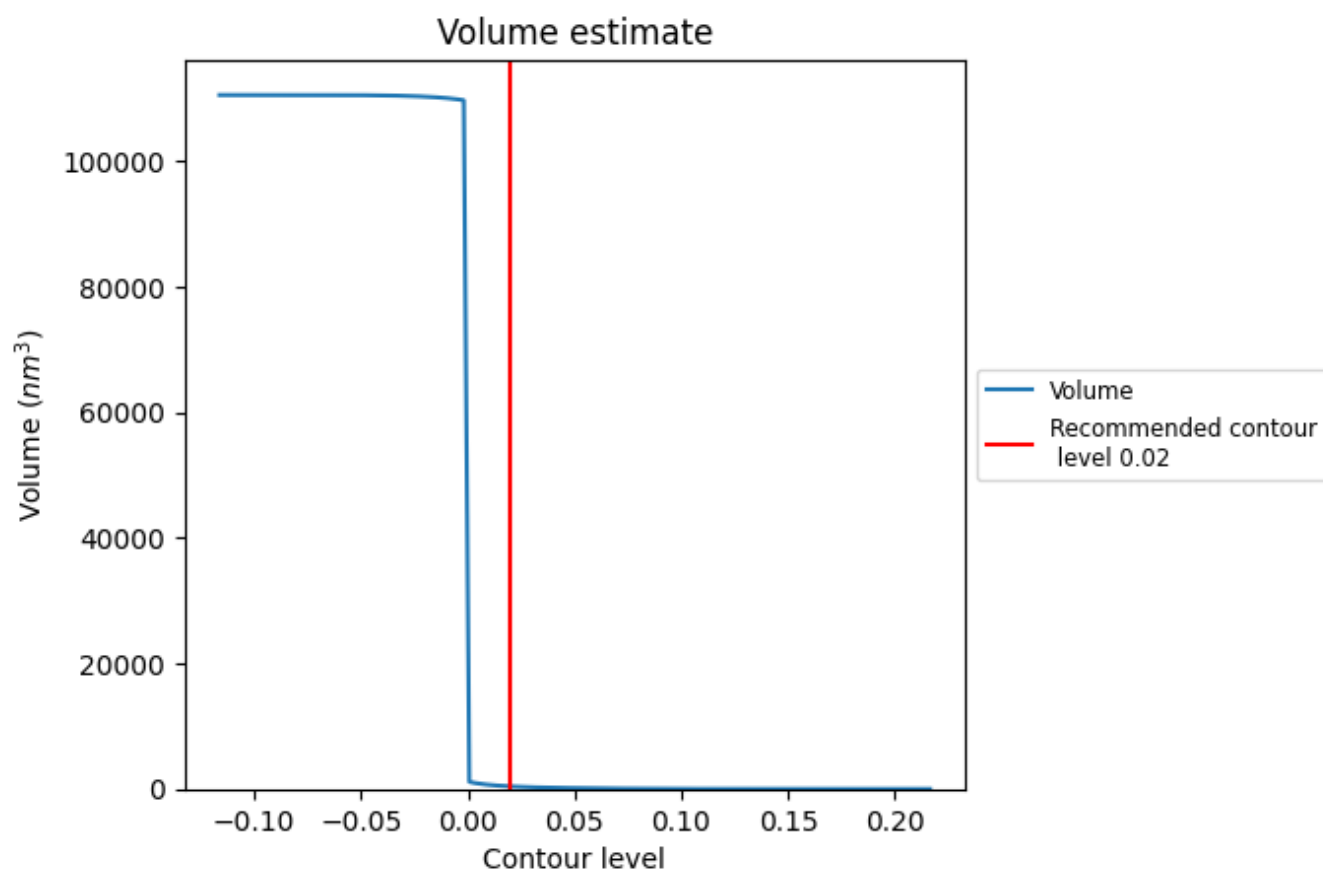
This section contains the results of statistical analysis of the map.

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.

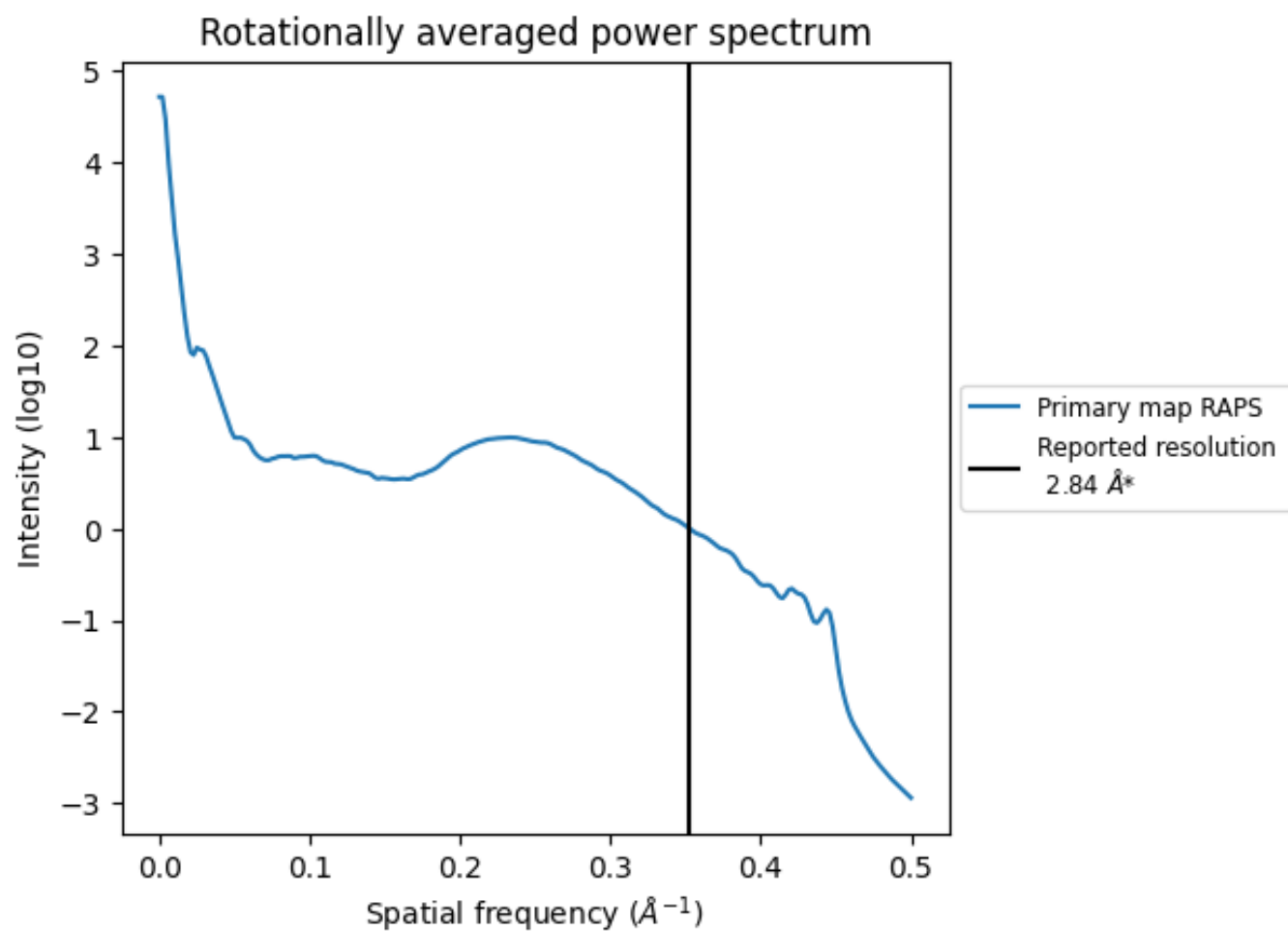
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 408 nm^3 ; this corresponds to an approximate mass of 369 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 0.352 Å⁻¹

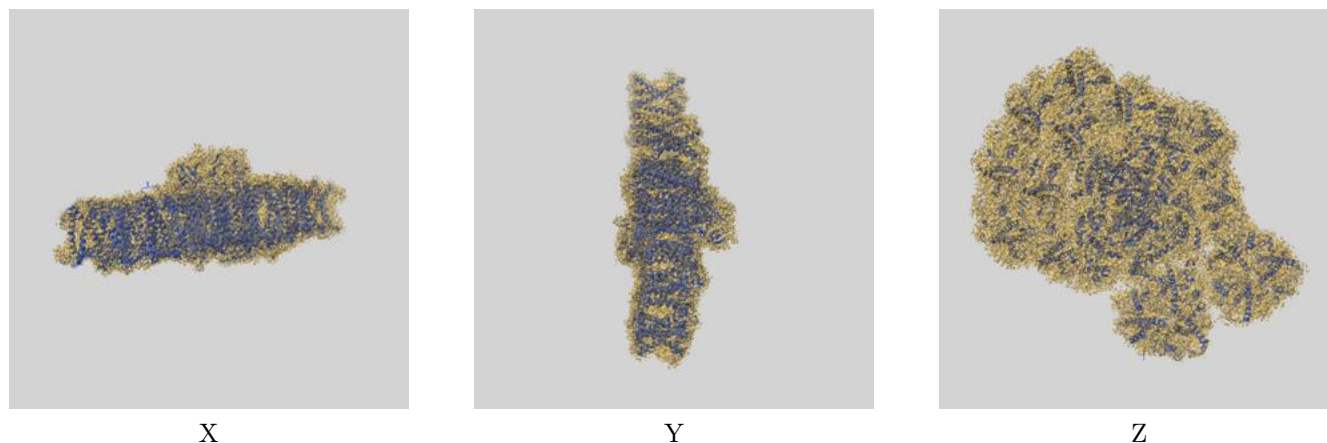
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

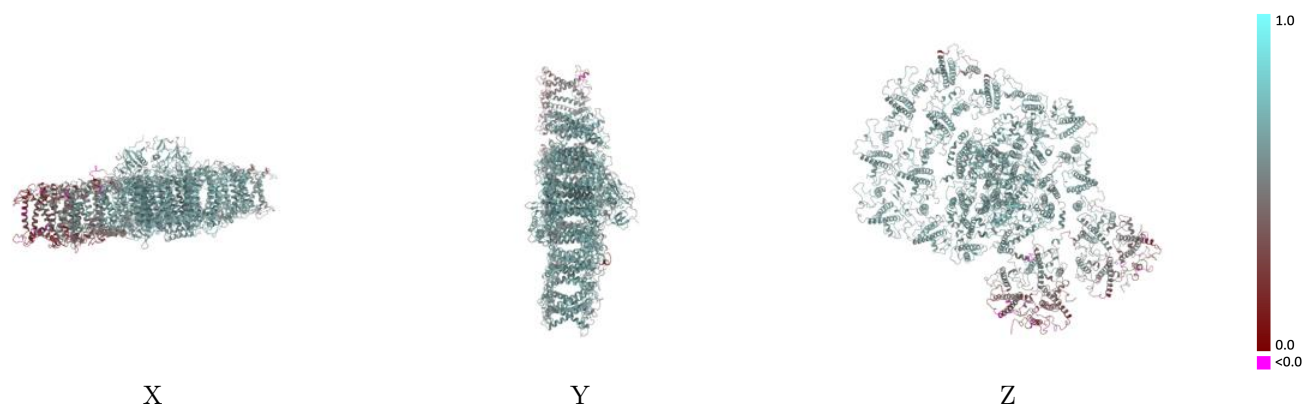
This section contains information regarding the fit between EMDB map EMD-30925 and PDB model 7DZ7. Per-residue inclusion information can be found in section [3](#) on page [45](#).

9.1 Map-model overlay [i](#)



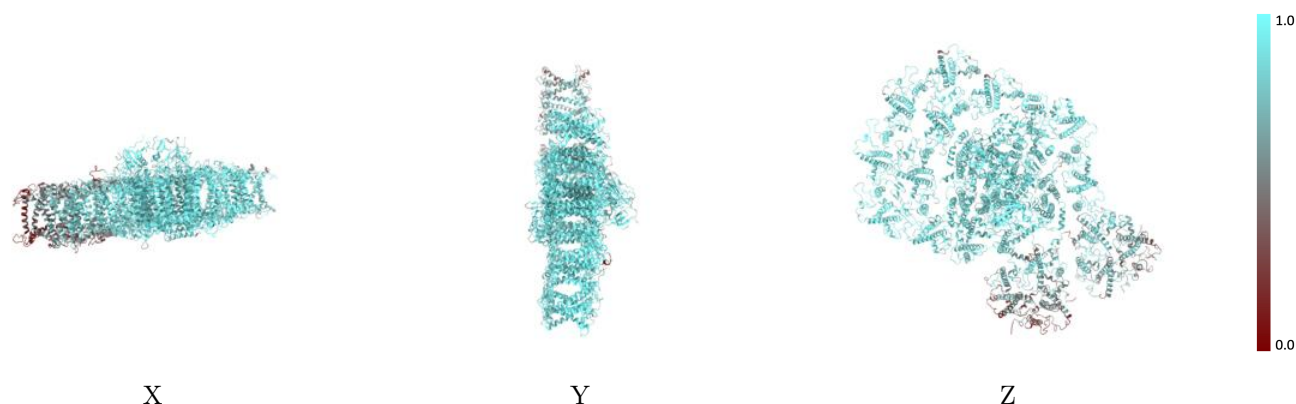
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



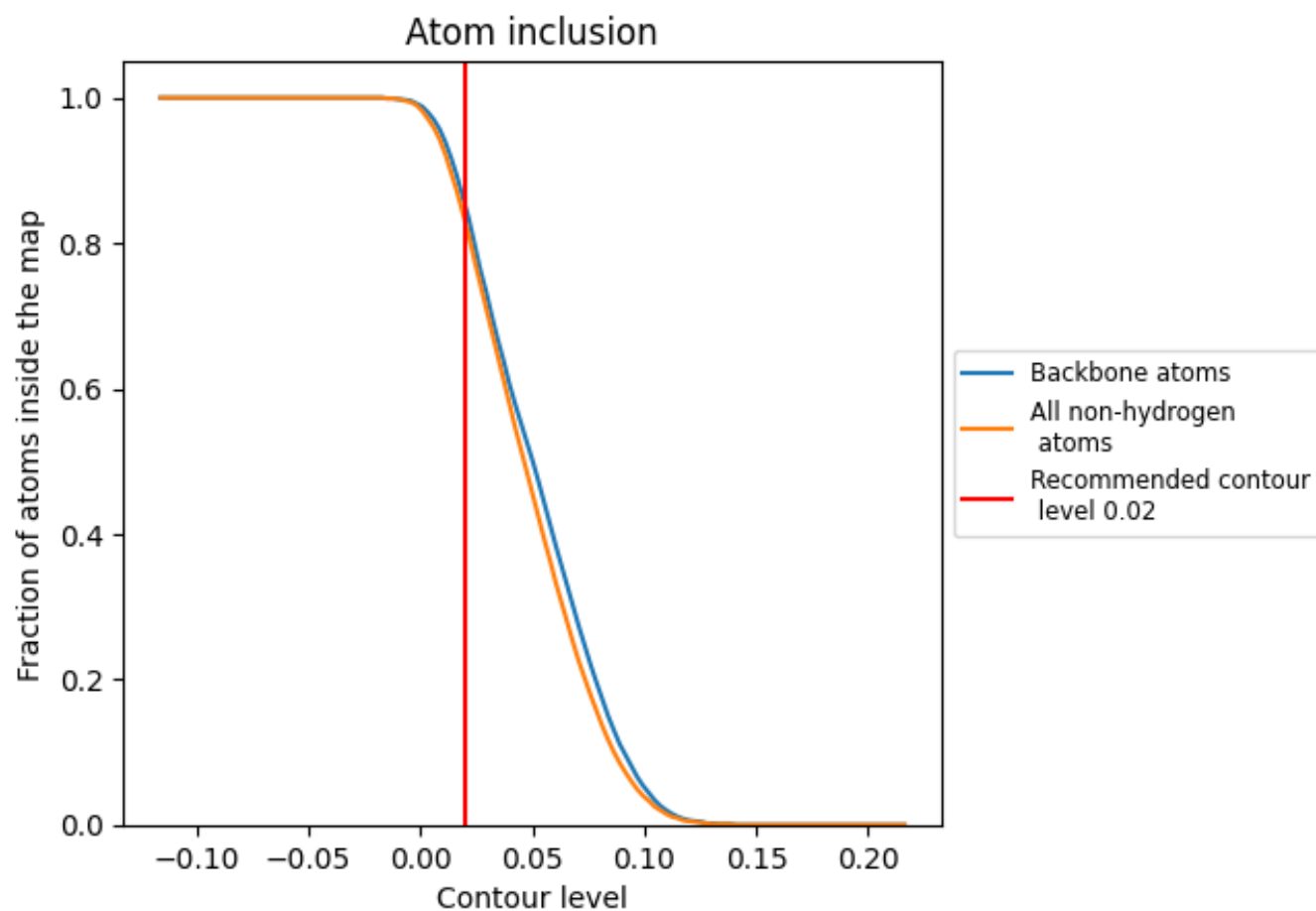
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8300	 0.5670
1	 0.8790	 0.5940
2	 0.8800	 0.5990
3	 0.9020	 0.6140
4	 0.8490	 0.5800
5	 0.8630	 0.5940
6	 0.8900	 0.5990
7	 0.9060	 0.6200
8	 0.8970	 0.6110
9	 0.8670	 0.5870
A	 0.9410	 0.6400
B	 0.9360	 0.6400
C	 0.9190	 0.6060
D	 0.9060	 0.6130
E	 0.9070	 0.6130
F	 0.8790	 0.6120
G	 0.8270	 0.5770
H	 0.8620	 0.5940
I	 0.8530	 0.5910
J	 0.8680	 0.6090
K	 0.8660	 0.5900
L	 0.9110	 0.6180
O	 0.8830	 0.5910
U	 0.6390	 0.4250
V	 0.7890	 0.5490
W	 0.5720	 0.3910
X	 0.4220	 0.2990
Y	 0.4770	 0.3310
Z	 0.7410	 0.5250
a	 0.8060	 0.5410

