



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 10:17 AM UTC

PDB ID : 7DZ7 / pdb_00007dz7
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

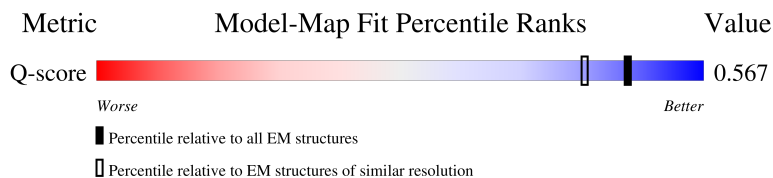
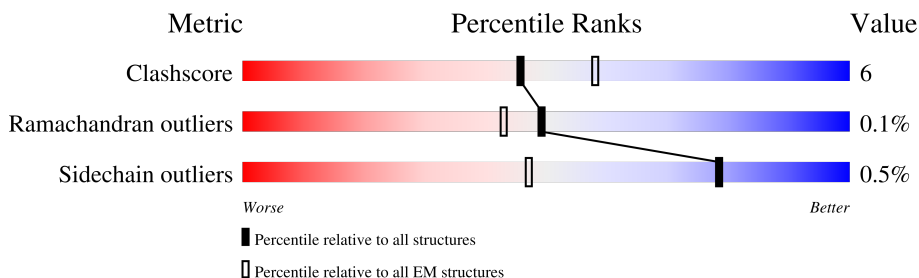
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 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.



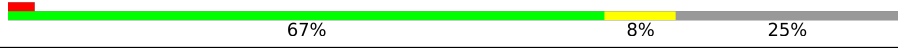
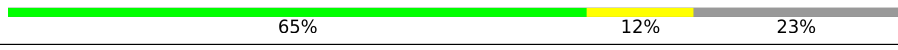
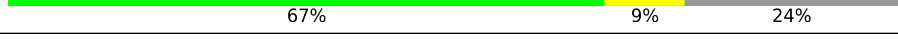
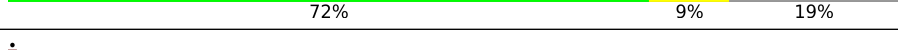
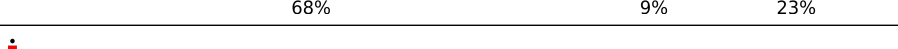
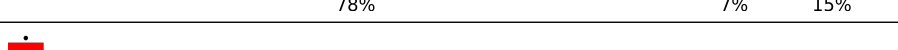
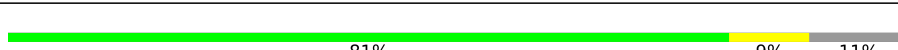
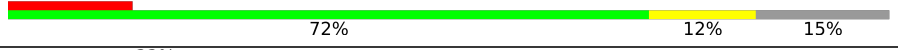
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11884 (2.34 - 3.34)

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	

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Mol	Chain	Length	Quality of chain
5	E	97	
6	F	227	
7	G	126	
8	H	130	
9	I	106	
10	J	41	
11	K	113	
12	L	196	
13	O	126	
14	1	228	
14	a	228	
15	2	246	
16	3	298	
17	4	264	
18	5	257	
19	6	257	
20	7	241	
21	8	243	
22	9	213	
23	W	249	
23	X	249	
24	U	257	
24	Y	257	
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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		

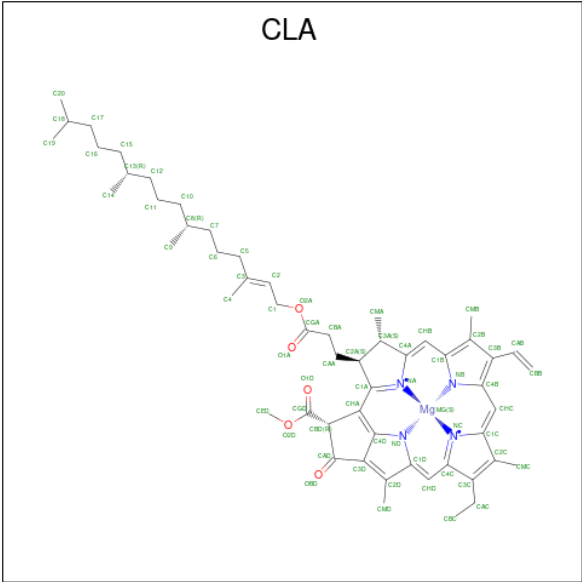
- Molecule 25 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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 (CCD ID: 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 65	C 55	Mg 1	N 4	O 5	0
27	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
27	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	8	1	Total 64	C 54	Mg 1	N 4	O 5	0
27	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	8	1	Total 51	C 41	Mg 1	N 4	O 5	0
27	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	8	1	Total 53	C 43	Mg 1	N 4	O 5	0
27	8	1	Total 43	C 33	Mg 1	N 4	O 5	0
27	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	9	1	Total 44	C 34	Mg 1	N 4	O 5	0
27	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
27	9	1	Total 40	C 32	Mg 1	N 4	O 3	0
27	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	9	1	Total 61	C 51	Mg 1	N 4	O 5	0

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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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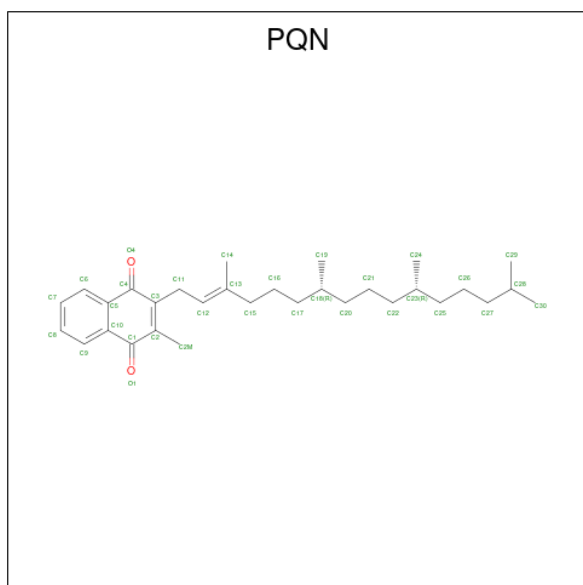
Mol	Chain	Residues	Atoms					AltConf
27	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Z	1	Total 57	C 47	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
27	Z	1	Total 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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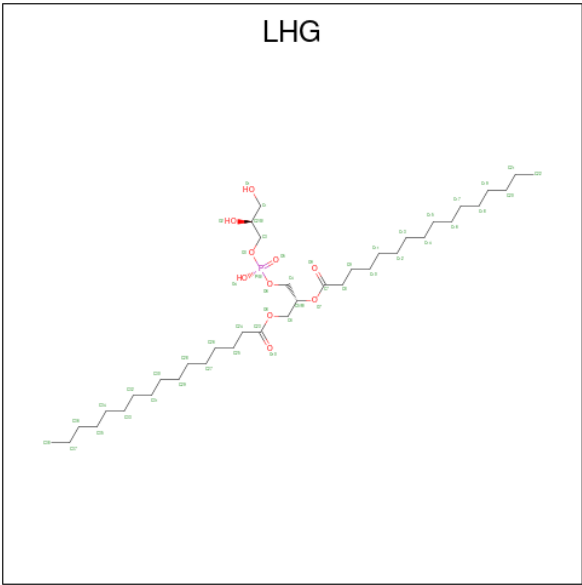
Mol	Chain	Residues	Atoms					AltConf
27	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	V	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	W	1	Total	C	Mg	N	O	0
			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 (CCD ID: 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 (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



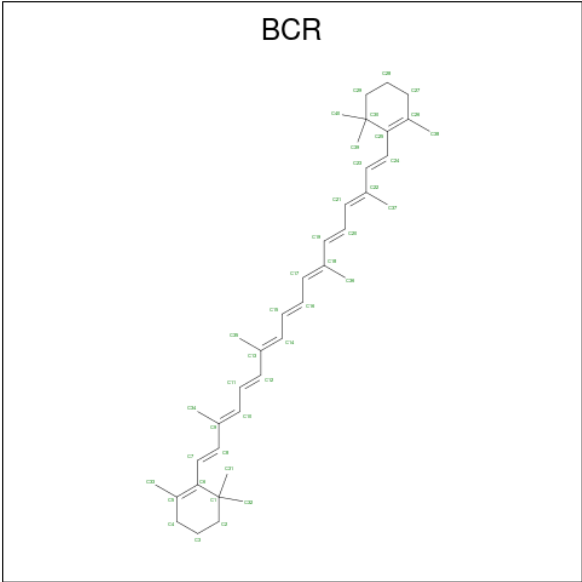
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	P	0
			49	38	10	1	
29	A	1	Total	C	O	P	0
			30	19	10	1	
29	B	1	Total	C	O	P	0
			38	27	10	1	
29	B	1	Total	C	O	P	0
			49	38	10	1	
29	H	1	Total	C	O	P	0
			49	38	10	1	
29	O	1	Total	C	O	P	0
			36	25	10	1	
29	a	1	Total	C	O	P	0
			43	32	10	1	
29	1	1	Total	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 (CCD ID: 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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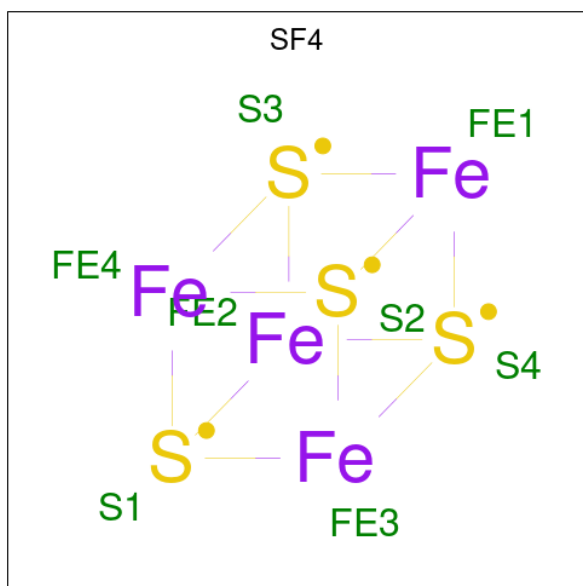
Mol	Chain	Residues	Atoms	AltConf
30	B	1	Total C 40 40	0
30	B	1	Total C 40 40	0
30	F	1	Total C 40 40	0
30	G	1	Total C 40 40	0
30	J	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	K	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	L	1	Total C 40 40	0
30	O	1	Total C 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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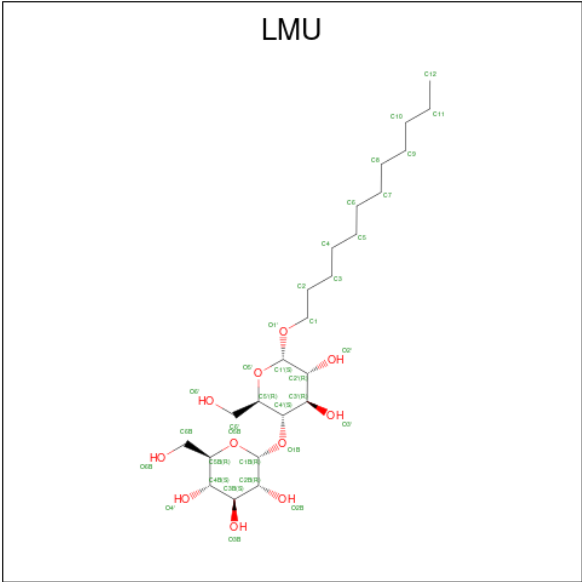
Mol	Chain	Residues	Atoms	AltConf
30	6	1	Total C 40 40	0
30	7	1	Total C 40 40	0
30	7	1	Total C 40 40	0
30	8	1	Total C 40 40	0
30	9	1	Total C 40 40	0

- Molecule 31 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



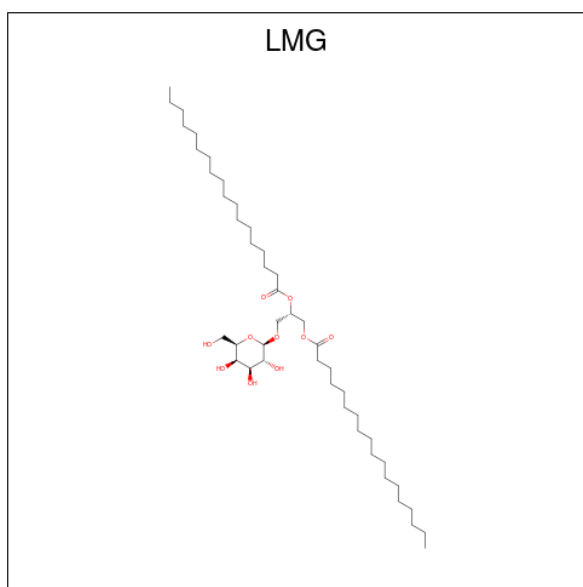
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total Fe S 8 4 4	0
31	C	1	Total Fe S 8 4 4	0
31	C	1	Total Fe S 8 4 4	0

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



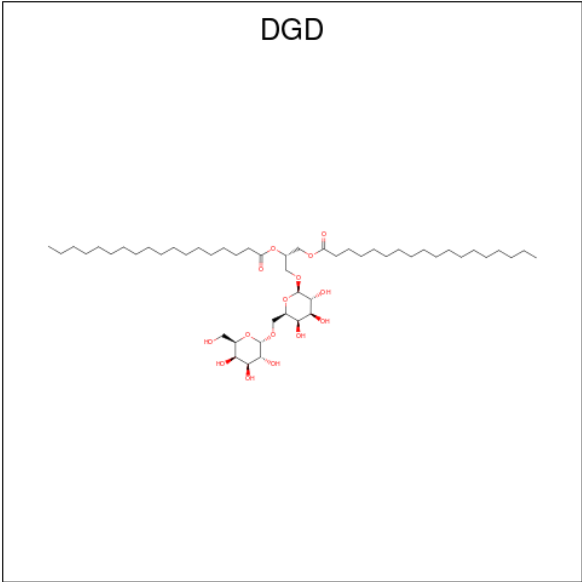
Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			35	24	11	
32	A	1	Total	C	O	0
			34	24	10	
32	K	1	Total	C	O	0
			35	24	11	
32	1	1	Total	C	O	0
			35	24	11	
32	5	1	Total	C	O	0
			33	22	11	
32	5	1	Total	C	O	0
			32	21	11	
32	8	1	Total	C	O	0
			35	24	11	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



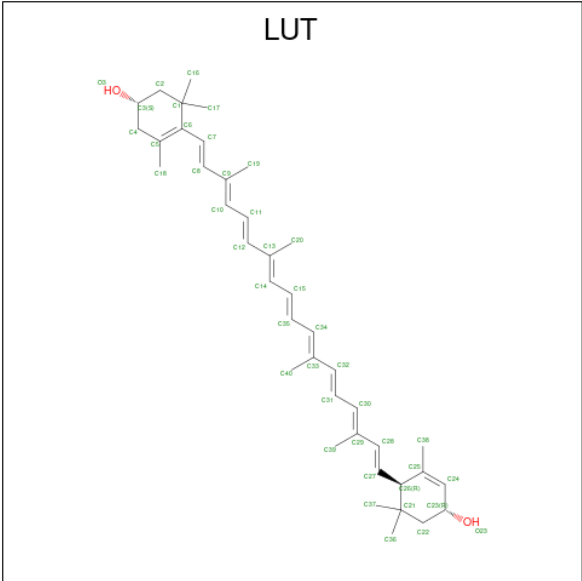
Mol	Chain	Residues	Atoms			AltConf
33	A	1	Total	C	O	0
			40	30	10	
33	H	1	Total	C	O	0
			55	45	10	
33	J	1	Total	C	O	0
			42	32	10	
33	J	1	Total	C	O	0
			40	30	10	
33	L	1	Total	C	O	0
			37	27	10	
33	4	1	Total	C	O	0
			40	30	10	
33	4	1	Total	C	O	0
			40	30	10	
33	5	1	Total	C	O	0
			40	30	10	
33	8	1	Total	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) (CCD ID: 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 (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



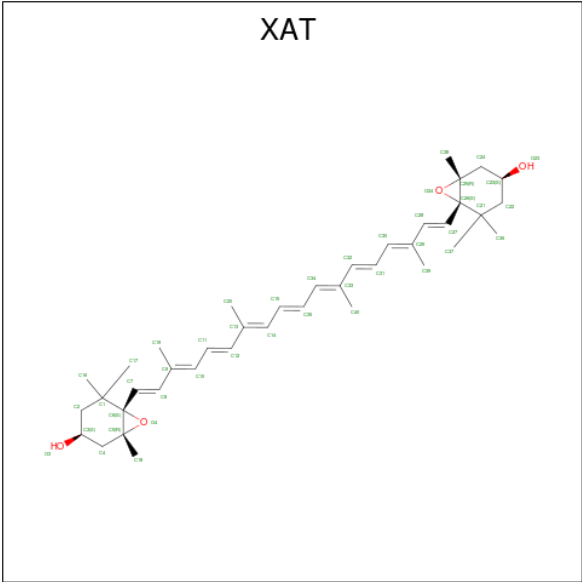
Mol	Chain	Residues	Atoms			AltConf
35	a	1	Total	C	O	0
			42	40	2	
35	1	1	Total	C	O	0
			42	40	2	

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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 (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



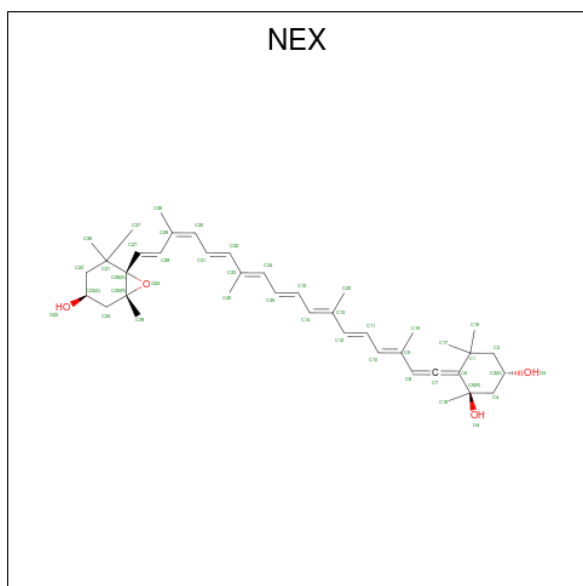
Mol	Chain	Residues	Atoms			AltConf
36	a	1	Total	C	O	0
			44	40	4	
36	1	1	Total	C	O	0
			44	40	4	
36	2	1	Total	C	O	0
			44	40	4	
36	3	1	Total	C	O	0
			44	40	4	
36	4	1	Total	C	O	0
			44	40	4	
36	5	1	Total	C	O	0
			44	40	4	
36	6	1	Total	C	O	0
			44	40	4	
36	7	1	Total	C	O	0
			44	40	4	
36	8	1	Total	C	O	0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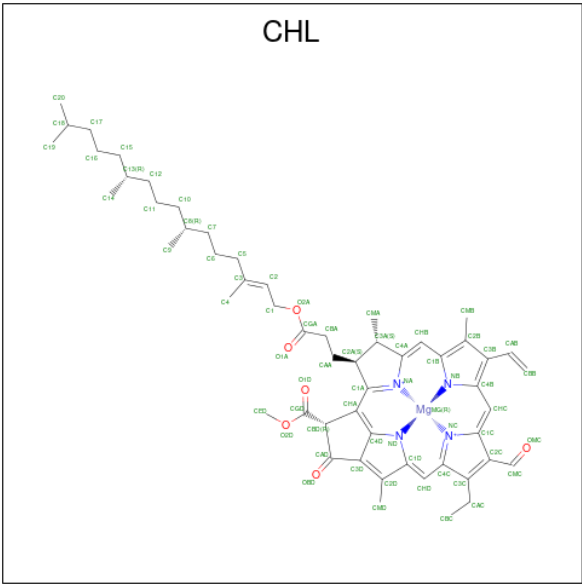
Mol	Chain	Residues	Atoms			AltConf
36	V	1	Total	C	O	0
			44	40	4	
36	W	1	Total	C	O	0
			44	40	4	

- 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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
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 (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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

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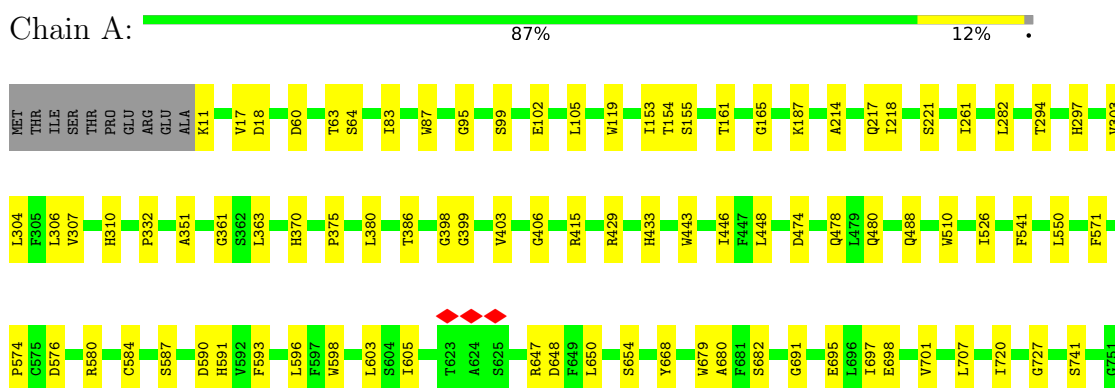
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Mol	Chain	Residues	Atoms					AltConf
38	W	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
38	W	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
38	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

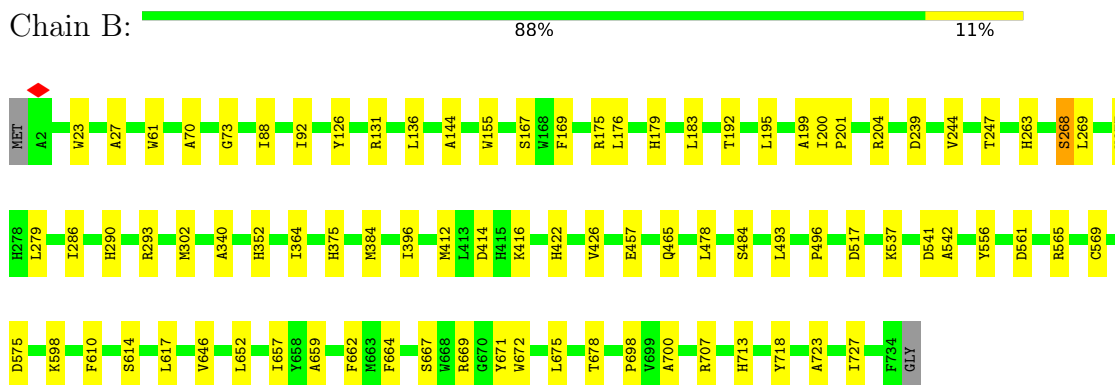
3 Residue-property plots

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

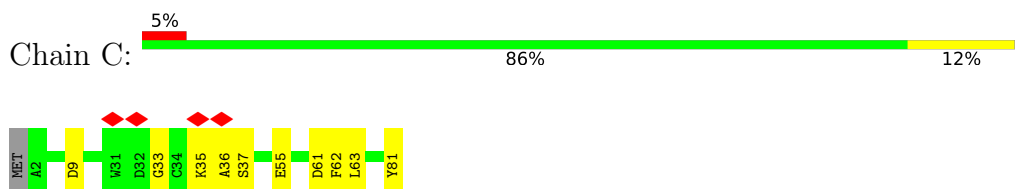
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

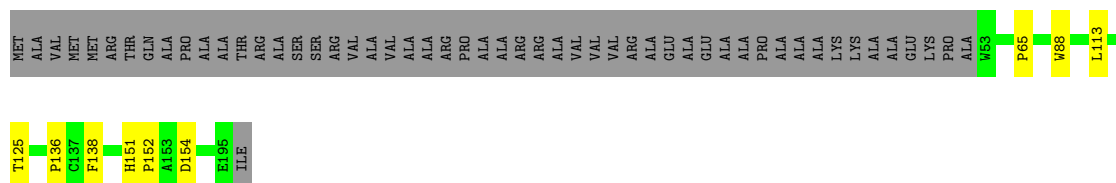


- Molecule 3: Photosystem I iron-sulfur center



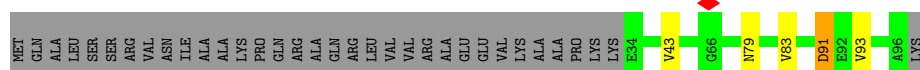
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:  68% 5% 27%



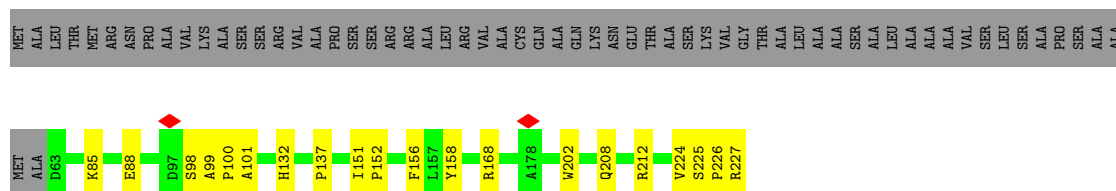
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:  60% 35%



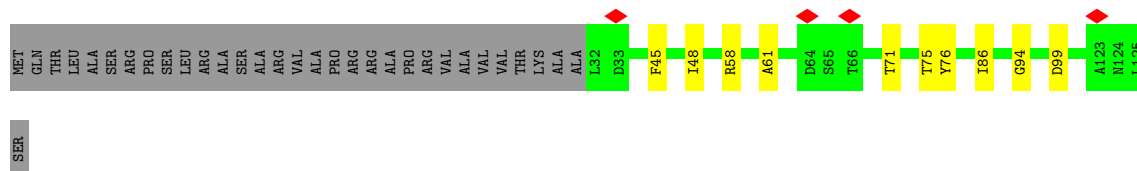
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:  64% 9% 27%



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

Chain G:  67% 8% 25%



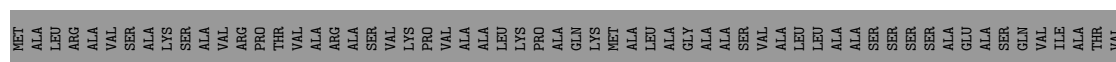
- Molecule 8: Photosystem I reaction center subunit VI, chloroplastic

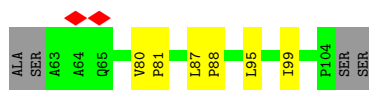
Chain H:  65% 12% 23%



- Molecule 9: Photosystem I reaction center subunit VIII

Chain I:  34% 6% 60%





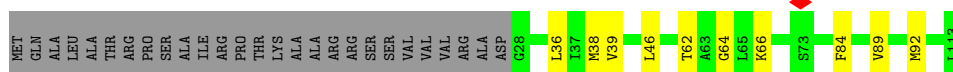
- Molecule 10: Photosystem I reaction center subunit IX

Chain J: 83% 17%



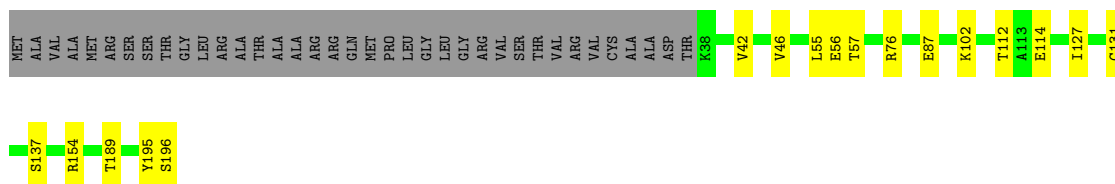
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K: 67% 9% 24%



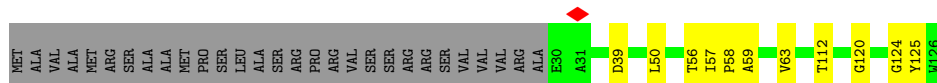
- Molecule 12: PSI subunit V

Chain L: 72% 9% 19%



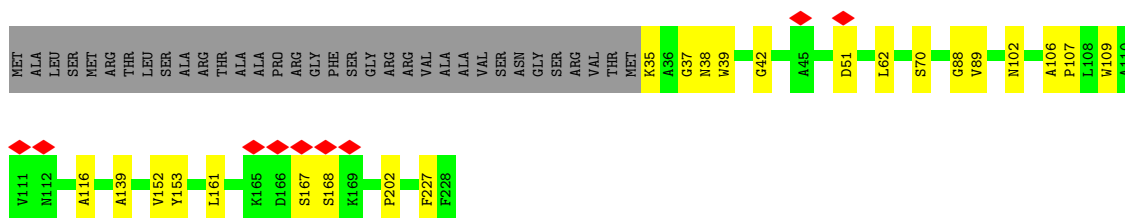
- Molecule 13: Photosystem I subunit O

Chain O: 68% 9% 23%



- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain a: 75% 10% 15%

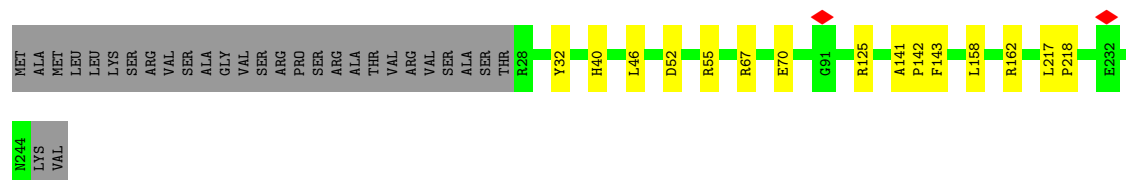
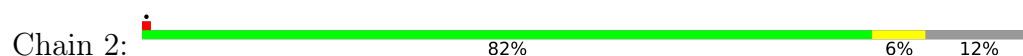


- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

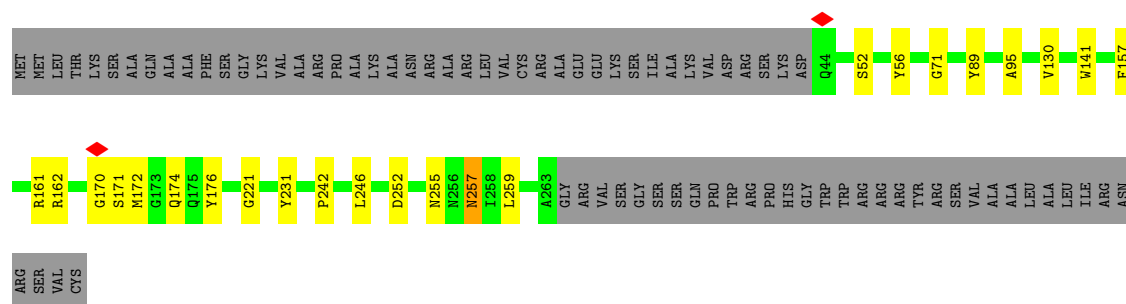
Chain 1: 78% 7% 15%



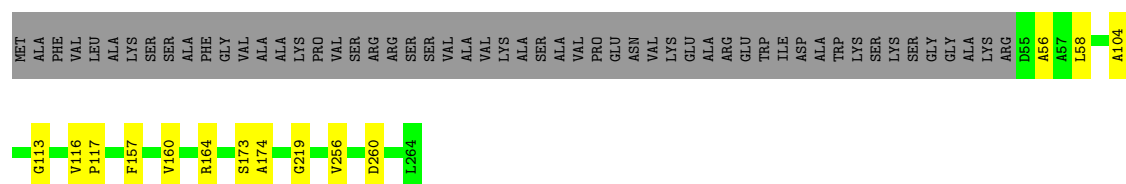
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



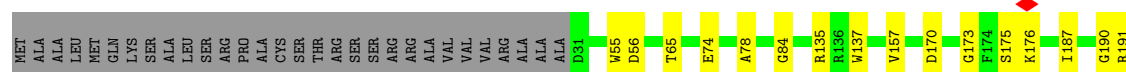
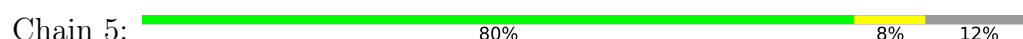
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

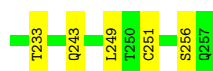


- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



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





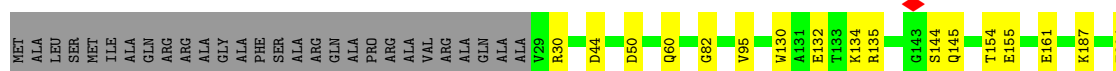
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 6: 81% 9% 11%



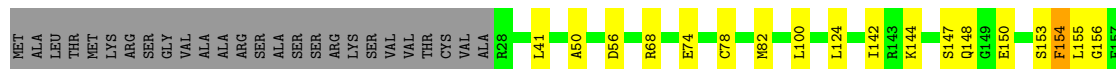
- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 7: 80% 8% 12%



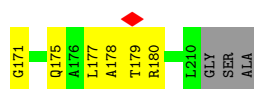
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 77% 12% 11%



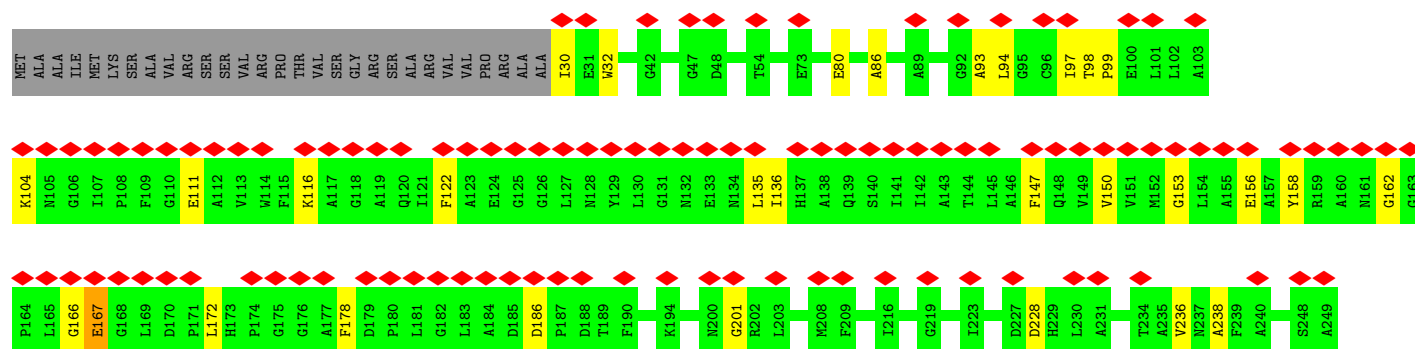
- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

Chain 9: 76% 10% 14%

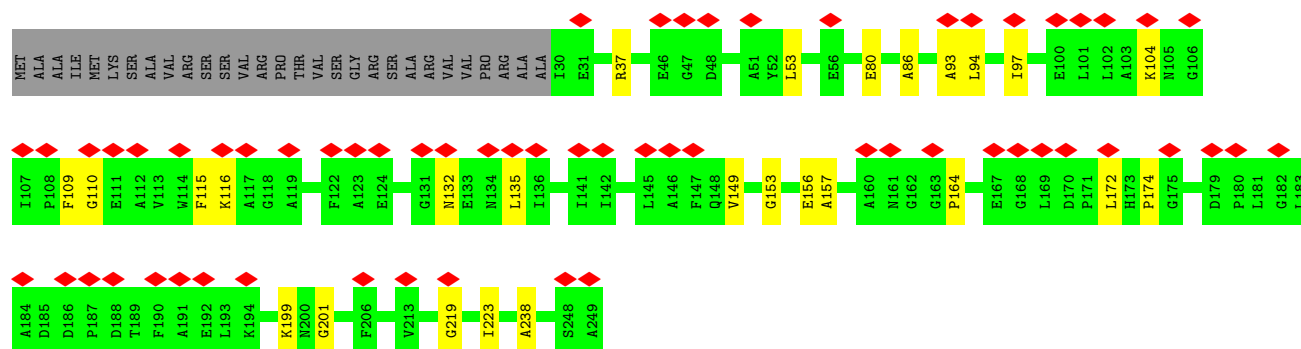
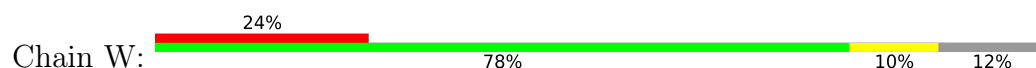


- Molecule 23: Chlorophyll a-b binding protein, chloroplastic

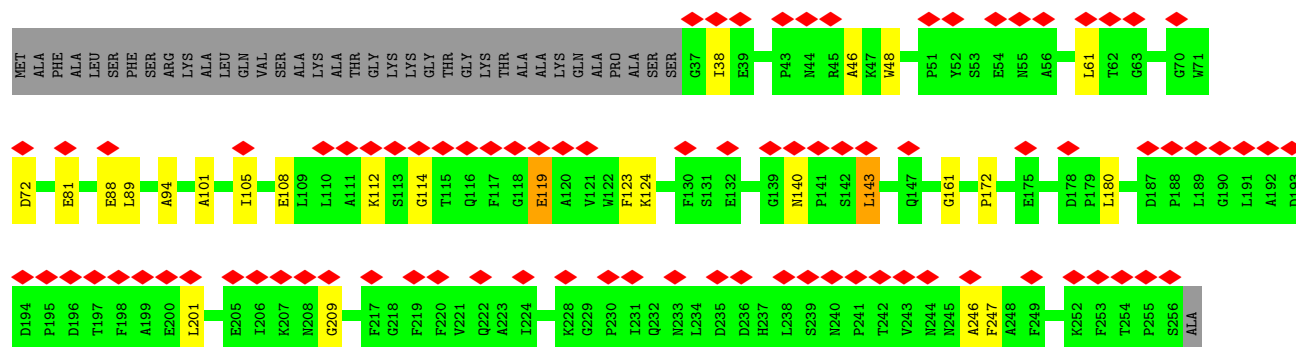
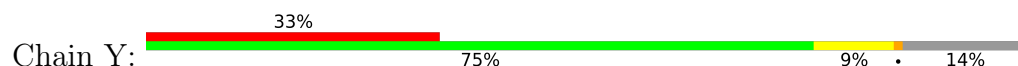
Chain X: 44% 76% 12% 12%



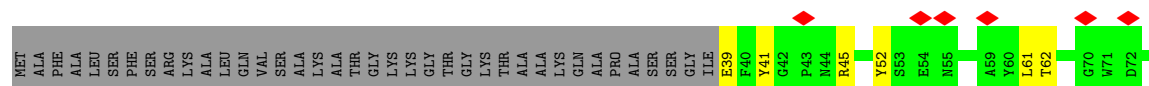
- Molecule 23: Chlorophyll a-b binding protein, chloroplastic

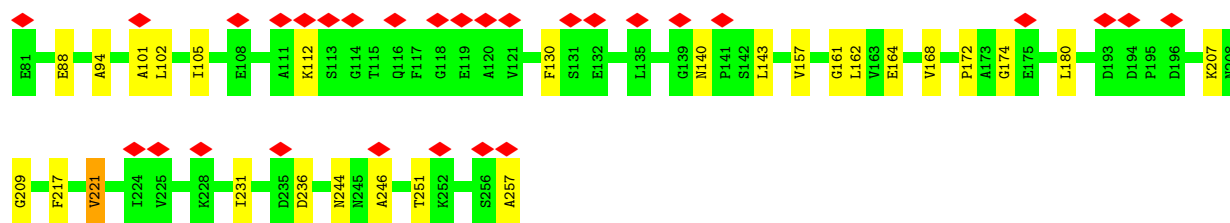


- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

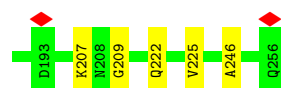
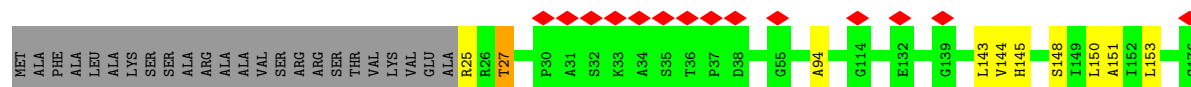
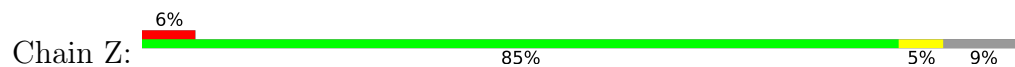


- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

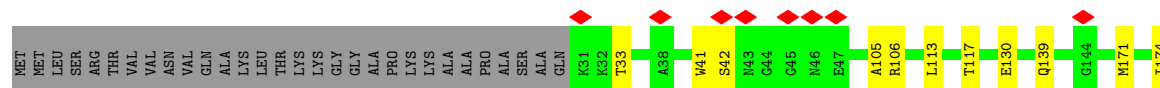
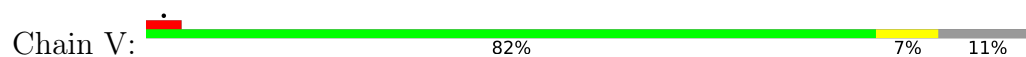




- Molecule 25: Chlorophyll a-b binding protein, chloroplastic



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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/6015	0.32	0/8201
2	B	0.29	0/6036	0.34	0/8242
3	C	0.24	0/610	0.37	0/826
4	D	0.24	0/1152	0.36	0/1556
5	E	0.21	0/506	0.30	0/689
6	F	0.23	0/1291	0.33	0/1747
7	G	0.20	0/714	0.33	0/972
8	H	0.23	0/788	0.32	0/1059
9	I	0.28	0/329	0.35	0/456
10	J	0.27	0/349	0.30	0/478
11	K	0.24	0/587	0.38	0/795
12	L	0.27	0/1190	0.36	0/1628
13	O	0.25	0/784	0.35	0/1069
14	1	0.29	0/1490	0.41	0/2028
14	a	0.32	0/1490	0.44	0/2028
15	2	0.22	0/1730	0.35	0/2353
16	3	0.26	0/1726	0.34	0/2342
17	4	0.22	0/1686	0.33	0/2300
18	5	0.24	0/1829	0.36	0/2492
19	6	0.29	0/1833	0.42	0/2505
20	7	0.27	0/1701	0.34	0/2310
21	8	0.27	0/1700	0.35	0/2315
22	9	0.23	0/1444	0.39	0/1964
23	W	0.39	0/1721	0.43	0/2341
23	X	0.24	0/1725	0.47	1/2348 (0.0%)
24	U	0.42	0/1718	0.48	0/2338
24	Y	0.25	0/1727	0.46	0/2350
25	Z	0.13	0/1822	0.30	0/2474
26	V	0.40	0/1856	0.40	0/2518
All	All	0.28	0/47549	0.37	1/64724 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	166	GLY	CA-C-O	-6.01	118.31	122.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5819	0	5670	68	0
2	B	5824	0	5579	72	0
3	C	600	0	581	6	0
4	D	1124	0	1139	6	0
5	E	496	0	491	4	0
6	F	1265	0	1301	16	0
7	G	699	0	681	9	0
8	H	776	0	765	17	0
9	I	316	0	321	3	0
10	J	337	0	336	5	0
11	K	582	0	620	13	0
12	L	1161	0	1184	16	0
13	O	758	0	740	10	0
14	1	1444	0	1396	12	0
14	a	1444	0	1396	20	0
15	2	1682	0	1665	15	0
16	3	1678	0	1637	19	0
17	4	1631	0	1587	11	0
18	5	1774	0	1746	18	0
19	6	1771	0	1770	19	0
20	7	1649	0	1589	15	0
21	8	1649	0	1629	32	0
22	9	1403	0	1381	21	0
23	W	1671	0	1604	28	0
23	X	1675	0	1617	27	0
24	U	1670	0	1604	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	Y	1679	0	1620	26	0
25	Z	1780	0	1723	14	0
26	V	1815	0	1765	32	0
27	1	666	0	522	1	0
27	2	641	0	533	9	0
27	3	724	0	628	9	0
27	4	778	0	678	8	0
27	5	878	0	758	9	0
27	6	903	0	831	6	0
27	7	756	0	635	5	0
27	8	724	0	629	4	0
27	9	595	0	491	5	0
27	A	2669	0	2693	40	0
27	B	2282	0	2232	40	0
27	F	140	0	113	1	0
27	G	87	0	64	0	0
27	H	104	0	93	1	0
27	J	42	0	31	0	0
27	K	191	0	150	7	0
27	L	235	0	184	4	0
27	O	116	0	61	0	0
27	U	401	0	344	4	0
27	V	415	0	365	4	0
27	W	426	0	377	5	0
27	X	436	0	415	5	0
27	Y	429	0	389	6	0
27	Z	496	0	520	2	0
27	a	710	0	591	2	0
28	A	33	0	46	0	0
28	B	33	0	46	2	0
29	1	49	0	74	0	0
29	2	36	0	42	0	0
29	3	94	0	137	1	0
29	4	49	0	74	0	0
29	5	98	0	148	1	0
29	6	48	0	69	0	0
29	7	37	0	44	1	0
29	8	89	0	124	0	0
29	9	128	0	178	2	0
29	A	79	0	104	0	0
29	B	87	0	120	1	0
29	H	49	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	O	36	0	42	0	0
29	U	49	0	74	0	0
29	V	48	0	69	2	0
29	W	44	0	61	0	0
29	X	49	0	74	0	0
29	Y	49	0	74	0	0
29	Z	49	0	74	2	0
29	a	43	0	59	0	0
30	1	40	0	56	2	0
30	2	40	0	56	9	0
30	3	120	0	168	15	0
30	4	40	0	56	3	0
30	5	40	0	56	3	0
30	6	40	0	56	3	0
30	7	80	0	112	10	0
30	8	40	0	56	3	0
30	9	40	0	56	5	0
30	A	240	0	336	38	0
30	B	400	0	560	50	0
30	F	40	0	56	8	0
30	G	40	0	56	2	0
30	J	40	0	56	10	0
30	K	80	0	112	17	0
30	L	160	0	224	20	0
30	O	80	0	112	11	0
30	a	40	0	56	2	0
31	A	8	0	0	0	0
31	C	16	0	0	0	0
32	1	35	0	46	0	0
32	5	65	0	76	0	0
32	8	35	0	46	0	0
32	A	69	0	90	1	0
32	K	35	0	46	1	0
33	4	80	0	100	0	0
33	5	40	0	50	1	0
33	8	46	0	65	0	0
33	9	55	0	86	0	0
33	A	40	0	50	1	0
33	H	55	0	86	0	0
33	J	82	0	107	0	0
33	L	37	0	44	1	0
33	V	41	0	52	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B	62	0	85	3	0
35	1	42	0	56	3	0
35	2	42	0	56	2	0
35	3	42	0	56	3	0
35	4	42	0	56	4	0
35	5	42	0	56	0	0
35	6	42	0	56	3	0
35	7	42	0	56	2	0
35	8	42	0	56	3	0
35	9	42	0	56	2	0
35	U	84	0	112	2	0
35	V	84	0	112	2	0
35	W	84	0	112	2	0
35	X	84	0	112	5	0
35	Y	84	0	112	3	0
35	Z	84	0	112	4	0
35	a	42	0	56	4	0
36	1	44	0	56	1	0
36	2	44	0	56	0	0
36	3	44	0	56	1	0
36	4	44	0	56	0	0
36	5	44	0	56	3	0
36	6	44	0	56	1	0
36	7	44	0	56	2	0
36	8	44	0	56	0	0
36	9	44	0	56	0	0
36	U	44	0	56	3	0
36	V	44	0	56	0	0
36	W	44	0	56	1	0
36	X	44	0	56	0	0
36	Y	44	0	56	1	0
36	Z	44	0	56	1	0
36	a	44	0	56	1	0
37	5	44	0	56	2	0
37	6	44	0	56	1	0
37	U	44	0	56	0	0
37	V	44	0	56	1	0
37	W	44	0	56	2	0
37	X	44	0	56	2	0
37	Y	43	0	55	2	0
37	Z	44	0	56	4	0
38	U	303	0	248	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	V	309	0	253	28	0
38	W	336	0	298	19	0
38	X	354	0	342	16	0
38	Y	335	0	302	19	0
38	Z	338	0	309	17	0
All	All	69647	0	68867	860	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 860 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:140:ASN:CB	24:U:143:LEU:HD13	1.49	1.42
12:L:114:GLU:HG2	12:L:189:THR:CG2	1.67	1.24
22:9:133:THR:HG22	22:9:135:THR:CG2	1.71	1.20
22:9:133:THR:CG2	22:9:135:THR:HG22	1.74	1.18
12:L:114:GLU:CG	12:L:189:THR:HG21	1.75	1.16

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	24	43
24	U	217/257 (84%)	197 (91%)	19 (9%)	1 (0%)	24	43
24	Y	218/257 (85%)	202 (93%)	15 (7%)	1 (0%)	24	43
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%)	49	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%)	601 (100%)	0	100	100
2	B	596/597 (100%)	594 (100%)	2 (0%)	86	94
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	120/152 (79%)	119 (99%)	1 (1%)	73	86
5	E	54/81 (67%)	53 (98%)	1 (2%)	50	73
6	F	127/169 (75%)	127 (100%)	0	100	100
7	G	70/94 (74%)	70 (100%)	0	100	100
8	H	81/102 (79%)	80 (99%)	1 (1%)	63	80
9	I	33/76 (43%)	33 (100%)	0	100	100
10	J	37/37 (100%)	37 (100%)	0	100	100
11	K	59/80 (74%)	59 (100%)	0	100	100
12	L	121/148 (82%)	120 (99%)	1 (1%)	73	86
13	O	78/101 (77%)	78 (100%)	0	100	100
14	1	137/162 (85%)	136 (99%)	1 (1%)	76	88
14	a	137/162 (85%)	137 (100%)	0	100	100
15	2	173/198 (87%)	173 (100%)	0	100	100
16	3	167/230 (73%)	166 (99%)	1 (1%)	78	89
17	4	165/205 (80%)	165 (100%)	0	100	100
18	5	184/206 (89%)	181 (98%)	3 (2%)	55	76
19	6	184/203 (91%)	182 (99%)	2 (1%)	65	81
20	7	164/181 (91%)	163 (99%)	1 (1%)	78	89
21	8	163/183 (89%)	162 (99%)	1 (1%)	78	89
22	9	140/159 (88%)	140 (100%)	0	100	100
23	W	163/187 (87%)	163 (100%)	0	100	100
23	X	165/187 (88%)	163 (99%)	2 (1%)	63	80
24	U	168/194 (87%)	166 (99%)	2 (1%)	63	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Y	170/194 (88%)	167 (98%)	3 (2%)	51	74
25	Z	178/195 (91%)	178 (100%)	0	100	100
26	V	178/201 (89%)	178 (100%)	0	100	100
All	All	4682/5364 (87%)	4660 (100%)	22 (0%)	78	90

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	8	154	PHE
24	Y	81	GLU
23	X	186	ASP
24	Y	119	GLU
14	1	225	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
15	2	240	ASN
20	7	113	ASN
26	V	158	GLN
16	3	256	ASN
18	5	138	GLN

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
25	TPO	Z	27	25	8,10,11	1.12	0	10,14,16	1.81	1 (10%)
26	TPO	V	33	26	8,10,11	1.60	1 (12%)	10,14,16	1.95	2 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	TPO	Z	27	25	-	1/9/11/13	-
26	TPO	V	33	26	-	5/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	33	TPO	P-O1P	3.31	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	-5.16	109.31	123.33
25	Z	27	TPO	P-OG1-CB	-5.12	109.42	123.33
26	V	33	TPO	CG2-CB-CA	-2.34	108.70	113.26

There are no chirality outliers.

5 of 6 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
25	Z	27	TPO	C-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	27	TPO	1	0

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	3	613	16	56,61,73	1.29	8 (14%)	65,98,113	1.17	5 (7%)
27	CLA	J	101	10	46,50,73	1.40	8 (17%)	53,85,113	1.26	5 (9%)
27	CLA	A	812	-	69,73,73	1.15	7 (10%)	82,113,113	1.12	4 (4%)
27	CLA	2	602	15	67,72,73	1.17	9 (13%)	79,112,113	1.15	4 (5%)
27	CLA	A	819	-	63,67,73	1.21	8 (12%)	74,105,113	1.27	6 (8%)
27	CLA	B	807	-	56,60,73	1.28	7 (12%)	65,97,113	1.30	7 (10%)
35	LUT	X	1621	-	42,43,43	0.81	1 (2%)	51,60,60	1.86	16 (31%)
27	CLA	B	803	-	69,73,73	1.15	8 (11%)	82,113,113	1.12	4 (4%)
38	CHL	Z	601	25	60,74,74	3.40	20 (33%)	58,114,114	2.41	15 (25%)
27	CLA	2	603	15	47,52,73	1.43	8 (17%)	55,88,113	1.29	5 (9%)
35	LUT	5	620	-	42,43,43	0.84	1 (2%)	51,60,60	2.16	12 (23%)
27	CLA	B	836	-	54,58,73	1.31	9 (16%)	64,95,113	1.32	6 (9%)
27	CLA	1	607	-	43,48,73	1.40	7 (16%)	51,83,113	1.27	5 (9%)
36	XAT	W	1622	-	41,47,47	0.97	3 (7%)	54,74,74	3.86	25 (46%)
27	CLA	Y	602	24	62,66,73	1.25	7 (11%)	73,104,113	1.14	4 (5%)
27	CLA	L	302	12	49,53,73	1.36	7 (14%)	58,89,113	1.26	5 (8%)
27	CLA	2	612	15	48,52,73	1.40	7 (14%)	57,88,113	1.28	4 (7%)
30	BCR	K	202	-	41,41,41	0.80	0	56,56,56	2.18	18 (32%)
32	LMU	A	857	-	36,36,36	1.14	2 (5%)	47,47,47	0.99	1 (2%)
33	LMG	8	626	-	46,46,55	0.97	2 (4%)	54,54,63	1.11	4 (7%)
38	CHL	W	606	-	40,54,74	3.96	19 (47%)	34,90,114	5.43	19 (55%)
37	NEX	Z	1623	-	40,46,46	1.27	4 (10%)	50,70,70	2.24	16 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	A	802	-	69,73,73	1.15	8 (11%)	82,113,113	1.21	6 (7%)
27	CLA	8	609	21	49,53,73	1.36	7 (14%)	58,89,113	1.24	4 (6%)
27	CLA	7	613	20	69,73,73	1.16	7 (10%)	82,113,113	1.08	6 (7%)
27	CLA	H	203	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	5 (6%)
27	CLA	A	823	-	46,50,73	1.39	7 (15%)	53,85,113	1.23	4 (7%)
27	CLA	A	831	-	69,73,73	1.16	6 (8%)	82,113,113	1.09	6 (7%)
38	CHL	W	605	23	40,54,74	4.03	19 (47%)	34,90,114	3.22	17 (50%)
27	CLA	4	609	17	61,65,73	1.22	7 (11%)	72,103,113	1.20	6 (8%)
27	CLA	9	613	22	69,73,73	1.17	7 (10%)	82,113,113	1.13	5 (6%)
38	CHL	U	607	-	40,54,74	3.95	19 (47%)	34,90,114	3.00	15 (44%)
27	CLA	B	810	-	68,72,73	1.17	9 (13%)	80,111,113	1.15	4 (5%)
27	CLA	9	601	22	49,53,73	1.38	7 (14%)	58,89,113	1.26	4 (6%)
27	CLA	A	821	-	57,61,73	1.28	7 (12%)	67,98,113	1.27	5 (7%)
27	CLA	Z	614	-	58,62,73	1.28	6 (10%)	68,99,113	1.15	4 (5%)
36	XAT	6	621	-	41,47,47	0.88	2 (4%)	54,74,74	2.36	20 (37%)
38	CHL	V	609	26	55,69,74	3.59	19 (34%)	52,108,114	2.21	15 (28%)
38	CHL	Z	608	-	44,58,74	4.00	19 (43%)	37,94,114	2.93	18 (48%)
27	CLA	B	821	-	47,51,73	1.45	9 (19%)	54,86,113	1.28	5 (9%)
27	CLA	8	616	-	47,51,73	1.50	9 (19%)	58,87,113	1.31	6 (10%)
27	CLA	V	611	29	47,51,73	1.35	7 (14%)	55,86,113	1.33	4 (7%)
38	CHL	U	609	24	54,68,74	3.58	20 (37%)	50,106,114	2.47	15 (30%)
31	SF4	C	101	3	0,12,12	-	-	-	-	-
27	CLA	2	604	-	46,50,73	1.40	8 (17%)	54,85,113	1.22	4 (7%)
38	CHL	Y	606	-	40,54,74	4.15	18 (45%)	34,90,114	3.10	15 (44%)
27	CLA	Y	614	-	52,56,73	1.36	7 (13%)	61,92,113	1.20	5 (8%)
27	CLA	W	613	23	69,73,73	1.16	6 (8%)	82,113,113	1.17	5 (6%)
27	CLA	a	609	14	67,72,73	1.18	7 (10%)	79,112,113	1.11	4 (5%)
30	BCR	B	852	-	41,41,41	0.78	0	56,56,56	3.62	24 (42%)
30	BCR	7	621	-	41,41,41	0.76	1 (2%)	56,56,56	2.37	22 (39%)
27	CLA	Y	604	-	54,58,73	1.33	7 (12%)	64,95,113	1.17	6 (9%)
27	CLA	8	608	-	55,59,73	1.31	8 (14%)	64,96,113	1.30	5 (7%)
27	CLA	L	307	-	43,48,73	1.45	7 (16%)	49,83,113	1.32	4 (8%)
27	CLA	A	808	-	54,58,73	1.30	7 (12%)	64,95,113	1.25	6 (9%)
27	CLA	7	608	-	54,58,73	1.29	7 (12%)	64,95,113	1.22	4 (6%)
27	CLA	4	604	-	58,62,73	1.34	8 (13%)	71,100,113	1.22	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	U	603	-	56,60,73	1.29	8 (14%)	65,97,113	1.34	6 (9%)
27	CLA	7	616	20	47,51,73	1.50	8 (17%)	58,87,113	1.28	6 (10%)
27	CLA	A	801	-	69,73,73	1.18	6 (8%)	82,113,113	1.19	8 (9%)
27	CLA	4	613	17	69,73,73	1.16	8 (11%)	82,113,113	1.11	5 (6%)
27	CLA	6	610	19	69,73,73	1.17	8 (11%)	82,113,113	1.08	5 (6%)
27	CLA	Z	610	25	69,73,73	1.17	6 (8%)	82,113,113	1.15	7 (8%)
27	CLA	G	204	7	49,53,73	1.38	8 (16%)	58,89,113	1.33	5 (8%)
27	CLA	3	609	16	64,68,73	1.20	6 (9%)	76,107,113	1.32	7 (9%)
27	CLA	Y	603	-	59,63,73	1.29	7 (11%)	70,101,113	1.23	5 (7%)
35	LUT	V	1621	-	42,43,43	0.98	2 (4%)	51,60,60	1.82	12 (23%)
36	XAT	Y	1622	-	41,47,47	0.91	1 (2%)	54,74,74	3.78	26 (48%)
27	CLA	2	601	15	69,73,73	1.16	8 (11%)	82,113,113	1.36	9 (10%)
33	LMG	A	860	-	40,40,55	1.04	2 (5%)	48,48,63	1.10	4 (8%)
27	CLA	6	602	19	69,73,73	1.17	8 (11%)	82,113,113	1.14	7 (8%)
32	LMU	A	858	-	35,35,36	1.22	3 (8%)	44,45,47	0.92	1 (2%)
27	CLA	2	610	15	59,63,73	1.24	8 (13%)	70,101,113	1.29	8 (11%)
32	LMU	8	625	-	36,36,36	1.15	2 (5%)	47,47,47	1.03	3 (6%)
27	CLA	B	818	-	64,68,73	1.19	7 (10%)	76,107,113	1.33	6 (7%)
27	CLA	B	812	-	47,51,73	1.37	8 (17%)	55,86,113	1.28	6 (10%)
35	LUT	2	619	-	42,43,43	0.82	2 (4%)	51,60,60	2.02	12 (23%)
27	CLA	4	616	17	47,51,73	1.51	9 (19%)	58,87,113	1.28	6 (10%)
27	CLA	Y	611	29	47,51,73	1.40	7 (14%)	55,86,113	1.27	4 (7%)
27	CLA	6	608	-	49,53,73	1.37	8 (16%)	58,89,113	1.27	5 (8%)
27	CLA	A	804	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	5 (6%)
30	BCR	A	856	-	41,41,41	0.75	0	56,56,56	2.17	18 (32%)
27	CLA	B	835	-	49,53,73	1.37	7 (14%)	58,89,113	1.21	4 (6%)
27	CLA	O	2001	-	41,46,73	1.48	8 (19%)	47,80,113	1.34	4 (8%)
27	CLA	4	608	-	69,73,73	1.17	7 (10%)	82,113,113	1.15	5 (6%)
27	CLA	a	610	14	63,67,73	1.20	7 (11%)	75,106,113	1.19	6 (8%)
27	CLA	A	817	-	49,53,73	1.36	7 (14%)	58,89,113	1.40	6 (10%)
27	CLA	A	827	-	62,66,73	1.22	8 (12%)	73,104,113	1.20	5 (6%)
29	LHG	A	847	27	29,29,48	1.18	2 (6%)	32,35,54	1.05	2 (6%)
37	NEX	5	624	-	40,46,46	1.23	3 (7%)	50,70,70	2.14	15 (30%)
30	BCR	3	621	-	41,41,41	0.82	2 (4%)	56,56,56	1.81	14 (25%)
33	LMG	J	104	-	40,40,55	1.06	2 (5%)	48,48,63	1.18	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	5	606	-	43,48,73	1.45	8 (18%)	49,83,113	1.21	3 (6%)
33	LMG	L	2631	-	37,37,55	1.10	2 (5%)	45,45,63	1.12	3 (6%)
35	LUT	U	1620	-	42,43,43	0.89	1 (2%)	51,60,60	1.89	10 (19%)
27	CLA	B	824	-	69,73,73	1.17	8 (11%)	82,113,113	1.15	4 (4%)
27	CLA	5	604	-	67,71,73	1.26	8 (11%)	82,111,113	1.17	7 (8%)
29	LHG	9	624	-	48,48,48	0.95	2 (4%)	51,54,54	1.01	2 (3%)
27	CLA	U	604	-	52,56,73	1.43	8 (15%)	61,91,113	1.26	6 (9%)
27	CLA	5	614	-	48,52,73	1.39	8 (16%)	53,87,113	1.27	4 (7%)
27	CLA	A	822	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	8 (9%)
30	BCR	a	619	-	41,41,41	0.72	0	56,56,56	2.44	21 (37%)
36	XAT	7	620	-	41,47,47	0.90	2 (4%)	54,74,74	2.35	23 (42%)
29	LHG	2	622	27	35,35,48	1.08	2 (5%)	38,41,54	0.99	2 (5%)
30	BCR	7	623	-	41,41,41	0.67	0	56,56,56	2.24	25 (44%)
38	CHL	Y	609	24	60,74,74	3.41	20 (33%)	58,114,114	2.16	16 (27%)
27	CLA	5	616	18	44,50,73	1.52	8 (18%)	57,85,113	1.23	6 (10%)
35	LUT	Y	1621	-	42,43,43	0.79	0	51,60,60	1.86	16 (31%)
27	CLA	5	607	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	4 (4%)
29	LHG	1	620	27	48,48,48	0.92	2 (4%)	51,54,54	0.98	4 (7%)
27	CLA	6	613	-	67,72,73	1.18	8 (11%)	79,112,113	1.08	4 (5%)
27	CLA	B	813	-	69,73,73	1.18	9 (13%)	82,113,113	1.20	6 (7%)
30	BCR	4	621	-	41,41,41	0.78	1 (2%)	56,56,56	2.50	23 (41%)
29	LHG	9	623	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	3 (5%)
27	CLA	A	828	-	69,73,73	1.16	9 (13%)	82,113,113	1.17	6 (7%)
27	CLA	B	825	-	53,57,73	1.29	7 (13%)	61,93,113	1.22	6 (9%)
27	CLA	L	304	-	49,53,73	1.35	7 (14%)	58,89,113	1.20	4 (6%)
30	BCR	G	205	-	41,41,41	0.81	1 (2%)	56,56,56	1.97	15 (26%)
30	BCR	3	622	-	41,41,41	0.74	0	56,56,56	2.32	19 (33%)
38	CHL	X	609	23	60,74,74	3.41	19 (31%)	58,114,114	2.30	17 (29%)
27	CLA	V	603	-	49,53,73	1.38	7 (14%)	58,89,113	1.38	3 (5%)
29	LHG	4	622	27	48,48,48	0.93	2 (4%)	51,54,54	0.90	2 (3%)
27	CLA	A	806	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
27	CLA	1	610	14	43,47,73	1.42	7 (16%)	50,81,113	1.51	7 (14%)
27	CLA	2	609	15	49,53,73	1.37	8 (16%)	58,89,113	1.25	4 (6%)
27	CLA	X	610	23	69,73,73	1.19	7 (10%)	82,113,113	1.11	6 (7%)
27	CLA	3	602	16	64,68,73	1.19	8 (12%)	76,107,113	1.12	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	4	607	-	49,53,73	1.35	7 (14%)	58,89,113	1.29	4 (6%)
27	CLA	A	820	-	69,73,73	1.16	7 (10%)	82,113,113	1.21	6 (7%)
27	CLA	W	611	29	61,65,73	1.22	8 (13%)	72,103,113	1.22	5 (6%)
27	CLA	9	611	29	46,50,73	1.39	8 (17%)	53,85,113	1.23	4 (7%)
30	BCR	B	849	-	41,41,41	0.73	0	56,56,56	2.52	24 (42%)
27	CLA	G	203	-	46,50,73	1.38	8 (17%)	53,85,113	1.30	4 (7%)
38	CHL	Z	607	-	60,74,74	3.39	19 (31%)	58,114,114	2.49	18 (31%)
27	CLA	B	811	-	56,60,73	1.45	10 (17%)	70,97,113	1.22	6 (8%)
27	CLA	3	612	16	47,51,73	1.40	7 (14%)	55,86,113	1.30	5 (9%)
27	CLA	A	841	-	69,73,73	1.14	9 (13%)	82,113,113	1.16	4 (4%)
27	CLA	B	809	2	69,73,73	1.18	7 (10%)	82,113,113	1.20	5 (6%)
27	CLA	1	611	29	61,65,73	1.24	7 (11%)	72,103,113	1.16	4 (5%)
27	CLA	A	854	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	7 (8%)
27	CLA	3	604	-	69,73,73	1.15	7 (10%)	82,113,113	1.17	5 (6%)
27	CLA	1	616	14	47,51,73	1.49	7 (14%)	58,87,113	1.36	7 (12%)
27	CLA	A	845	29	54,58,73	1.30	7 (12%)	64,95,113	1.19	4 (6%)
27	CLA	7	609	20	46,52,73	1.38	7 (15%)	57,87,113	1.21	5 (8%)
38	CHL	X	601	23	60,74,74	3.39	20 (33%)	58,114,114	2.46	15 (25%)
27	CLA	7	615	-	44,50,73	1.54	8 (18%)	57,85,113	1.28	5 (8%)
27	CLA	6	607	-	45,49,73	1.48	9 (20%)	54,84,113	1.33	5 (9%)
27	CLA	1	604	-	53,57,73	1.30	7 (13%)	61,93,113	1.18	3 (4%)
29	LHG	A	846	-	48,48,48	0.92	2 (4%)	51,54,54	0.91	2 (3%)
27	CLA	X	614	-	46,50,73	1.41	7 (15%)	53,85,113	1.24	4 (7%)
27	CLA	B	805	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	6 (7%)
27	CLA	9	603	22	48,52,73	1.49	9 (18%)	59,88,113	1.30	5 (8%)
29	LHG	Z	2630	27	48,48,48	0.94	2 (4%)	51,54,54	0.86	2 (3%)
29	LHG	O	2631	-	35,35,48	1.09	2 (5%)	38,41,54	1.09	3 (7%)
35	LUT	U	1621	-	42,43,43	0.96	2 (4%)	51,60,60	1.82	14 (27%)
27	CLA	9	606	-	43,48,73	1.46	8 (18%)	49,83,113	1.28	4 (8%)
38	CHL	Y	607	-	60,74,74	3.45	19 (31%)	58,114,114	2.14	18 (31%)
35	LUT	V	1620	-	42,43,43	0.90	2 (4%)	51,60,60	1.79	13 (25%)
27	CLA	V	602	26	64,68,73	1.21	9 (14%)	76,107,113	1.23	7 (9%)
32	LMU	K	208	-	36,36,36	1.14	2 (5%)	47,47,47	0.98	2 (4%)
27	CLA	A	810	1	54,58,73	1.33	9 (16%)	64,95,113	1.33	6 (9%)
27	CLA	4	603	17	48,52,73	1.49	8 (16%)	59,88,113	1.39	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	5	611	29	46,50,73	1.37	7 (15%)	53,85,113	1.23	4 (7%)
27	CLA	W	604	-	51,55,73	1.34	7 (13%)	60,91,113	1.22	4 (6%)
33	LMG	J	103	-	42,42,55	1.02	2 (4%)	50,50,63	1.09	3 (6%)
35	LUT	W	1621	-	42,43,43	0.97	2 (4%)	51,60,60	1.82	14 (27%)
38	CHL	X	608	-	60,74,74	3.44	18 (30%)	58,114,114	2.01	15 (25%)
27	CLA	Z	602	25	64,68,73	1.22	6 (9%)	76,107,113	1.13	6 (7%)
27	CLA	3	608	-	59,63,73	1.30	8 (13%)	70,101,113	1.18	5 (7%)
38	CHL	Z	606	-	40,54,74	4.17	19 (47%)	34,90,114	3.08	16 (47%)
27	CLA	4	606	-	43,48,73	1.44	8 (18%)	49,83,113	1.27	4 (8%)
27	CLA	A	833	-	49,53,73	1.36	8 (16%)	58,89,113	1.32	5 (8%)
27	CLA	8	611	29	46,50,73	1.37	8 (17%)	53,85,113	1.22	4 (7%)
29	LHG	V	2630	27	47,47,48	0.90	2 (4%)	50,53,54	1.13	3 (6%)
27	CLA	6	601	19	69,73,73	1.17	7 (10%)	82,113,113	1.19	6 (7%)
30	BCR	O	2005	-	41,41,41	0.83	1 (2%)	56,56,56	3.07	25 (44%)
27	CLA	B	833	-	69,73,73	1.15	8 (11%)	82,113,113	1.14	9 (10%)
27	CLA	Y	612	24	49,53,73	1.40	7 (14%)	58,89,113	1.29	4 (6%)
30	BCR	F	305	-	41,41,41	0.80	0	56,56,56	2.27	27 (48%)
38	CHL	U	608	-	38,52,74	4.01	18 (47%)	31,87,114	3.05	14 (45%)
36	XAT	9	620	-	41,47,47	0.90	3 (7%)	54,74,74	2.33	21 (38%)
38	CHL	Z	605	25	38,52,74	4.26	17 (44%)	31,87,114	3.17	18 (58%)
27	CLA	Z	604	-	61,65,73	1.25	6 (9%)	72,103,113	1.17	4 (5%)
32	LMU	5	629	-	33,33,36	1.17	2 (6%)	44,44,47	1.10	3 (6%)
33	LMG	4	623	-	40,40,55	1.05	2 (5%)	48,48,63	1.15	4 (8%)
27	CLA	B	815	-	47,51,73	1.37	6 (12%)	55,86,113	1.24	3 (5%)
30	BCR	L	301	-	41,41,41	0.71	0	56,56,56	2.27	27 (48%)
27	CLA	A	840	-	56,60,73	1.29	8 (14%)	65,97,113	1.32	6 (9%)
37	NEX	Y	1623	-	41,45,46	1.03	3 (7%)	50,67,70	2.35	18 (36%)
33	LMG	5	627	-	40,40,55	1.05	2 (5%)	48,48,63	1.02	2 (4%)
27	CLA	V	604	-	54,58,73	1.32	6 (11%)	64,95,113	1.25	5 (7%)
33	LMG	V	2631	-	41,41,55	1.02	3 (7%)	49,49,63	1.17	4 (8%)
27	CLA	2	613	15	69,73,73	1.14	7 (10%)	82,113,113	1.09	5 (6%)
37	NEX	6	624	-	40,46,46	1.39	3 (7%)	50,70,70	2.02	15 (30%)
27	CLA	V	610	26	66,70,73	1.19	7 (10%)	78,109,113	1.14	6 (7%)
27	CLA	A	807	1	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
27	CLA	9	612	22	44,49,73	1.42	7 (15%)	50,84,113	1.28	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	A	814	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
30	BCR	2	623	-	41,41,41	0.80	0	56,56,56	2.34	22 (39%)
29	LHG	5	623	27	48,48,48	0.92	2 (4%)	51,54,54	0.84	2 (3%)
27	CLA	U	610	24	60,64,73	1.26	8 (13%)	71,102,113	1.16	6 (8%)
27	CLA	7	611	29	63,67,73	1.19	7 (11%)	74,105,113	1.12	5 (6%)
36	XAT	1	618	-	41,47,47	0.89	2 (4%)	54,74,74	2.42	23 (42%)
27	CLA	Z	613	25	69,73,73	1.17	8 (11%)	82,113,113	1.12	5 (6%)
27	CLA	1	612	14	49,53,73	1.37	7 (14%)	58,89,113	1.26	3 (5%)
35	LUT	Y	1620	-	42,43,43	0.80	1 (2%)	51,60,60	2.04	12 (23%)
38	CHL	V	601	26	60,74,74	3.37	19 (31%)	58,114,114	2.40	14 (24%)
27	CLA	A	803	-	69,73,73	1.16	7 (10%)	82,113,113	1.14	2 (2%)
27	CLA	B	816	-	58,62,73	1.24	7 (12%)	68,99,113	1.22	5 (7%)
27	CLA	F	304	6	45,49,73	1.39	8 (17%)	54,84,113	1.29	4 (7%)
27	CLA	4	618	17	43,48,73	1.52	7 (16%)	51,83,113	1.39	5 (9%)
35	LUT	9	619	-	42,43,43	0.72	0	51,60,60	1.88	14 (27%)
27	CLA	3	607	16	60,64,73	1.31	8 (13%)	73,102,113	1.28	8 (10%)
27	CLA	B	839	-	69,73,73	1.15	7 (10%)	82,113,113	1.08	4 (4%)
27	CLA	B	841	29	69,73,73	1.16	9 (13%)	82,113,113	1.19	5 (6%)
30	BCR	6	622	-	41,41,41	0.73	1 (2%)	56,56,56	3.56	27 (48%)
27	CLA	a	601	14	57,62,73	1.27	7 (12%)	67,100,113	1.18	5 (7%)
27	CLA	A	811	-	69,73,73	1.15	7 (10%)	82,113,113	1.11	6 (7%)
27	CLA	B	808	-	69,73,73	1.13	7 (10%)	82,113,113	1.15	7 (8%)
29	LHG	8	622	27	48,48,48	0.93	2 (4%)	51,54,54	0.86	2 (3%)
30	BCR	B	848	-	41,41,41	0.74	0	56,56,56	2.23	20 (35%)
27	CLA	7	612	20	48,52,73	1.40	7 (14%)	57,88,113	1.32	3 (5%)
27	CLA	5	603	-	58,62,73	1.36	9 (15%)	71,100,113	1.28	7 (9%)
36	XAT	8	620	-	41,47,47	0.89	2 (4%)	54,74,74	2.46	26 (48%)
30	BCR	B	846	-	41,41,41	0.76	1 (2%)	56,56,56	2.26	20 (35%)
27	CLA	W	602	23	64,68,73	1.21	8 (12%)	76,107,113	1.23	4 (5%)
29	LHG	3	624	27	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
27	CLA	B	834	-	64,68,73	1.19	7 (10%)	76,107,113	1.19	5 (6%)
27	CLA	1	603	-	56,61,73	1.28	8 (14%)	65,98,113	1.30	5 (7%)
29	LHG	U	2630	27	48,48,48	0.92	2 (4%)	51,54,54	0.93	2 (3%)
27	CLA	A	843	-	68,72,73	1.17	8 (11%)	80,111,113	1.13	6 (7%)
27	CLA	A	815	-	54,58,73	1.31	8 (14%)	64,95,113	1.29	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	V	613	26	69,73,73	1.18	6 (8%)	82,113,113	1.16	5 (6%)
38	CHL	U	605	24	37,51,74	4.11	18 (48%)	30,86,114	3.38	16 (53%)
27	CLA	O	2002	-	41,46,73	1.58	8 (19%)	51,81,113	1.28	5 (9%)
27	CLA	U	612	24	47,51,73	1.38	8 (17%)	55,86,113	1.30	4 (7%)
29	LHG	B	851	27	37,37,48	1.08	2 (5%)	40,43,54	1.15	3 (7%)
30	BCR	J	102	-	41,41,41	0.74	0	56,56,56	2.20	22 (39%)
27	CLA	1	602	14	65,69,73	1.20	8 (12%)	77,108,113	1.18	6 (7%)
31	SF4	A	853	2,1	0,12,12	-	-	-		
27	CLA	6	604	-	69,73,73	1.16	7 (10%)	82,113,113	1.10	6 (7%)
38	CHL	U	601	24	60,74,74	3.40	19 (31%)	58,114,114	2.46	16 (27%)
27	CLA	5	610	18	58,62,73	1.24	8 (13%)	68,99,113	1.21	6 (8%)
27	CLA	9	607	-	49,53,73	1.38	7 (14%)	58,89,113	1.28	4 (6%)
36	XAT	Z	1622	-	41,47,47	0.93	1 (2%)	54,74,74	3.72	25 (46%)
27	CLA	L	306	-	43,48,73	1.42	7 (16%)	49,83,113	1.30	3 (6%)
27	CLA	Z	612	25	69,73,73	1.18	6 (8%)	82,113,113	1.11	3 (3%)
29	LHG	9	622	27	29,29,48	1.19	2 (6%)	32,35,54	1.05	2 (6%)
35	LUT	3	618	-	42,43,43	0.82	2 (4%)	51,60,60	1.83	12 (23%)
27	CLA	H	202	8	42,47,73	1.46	7 (16%)	50,82,113	1.22	3 (6%)
27	CLA	B	830	-	47,51,73	1.37	7 (14%)	55,86,113	1.21	6 (10%)
38	CHL	V	608	-	42,56,74	3.80	19 (45%)	36,92,114	2.93	14 (38%)
27	CLA	4	611	29	46,50,73	1.38	7 (15%)	53,85,113	1.25	4 (7%)
27	CLA	B	802	-	69,73,73	1.16	7 (10%)	82,113,113	1.08	5 (6%)
27	CLA	1	613	-	69,73,73	1.16	7 (10%)	82,113,113	1.10	6 (7%)
36	XAT	3	619	-	41,47,47	0.87	2 (4%)	54,74,74	2.46	23 (42%)
27	CLA	U	602	24	63,67,73	1.21	7 (11%)	74,105,113	1.24	4 (5%)
29	LHG	7	622	27	36,36,48	1.05	2 (5%)	39,42,54	0.86	2 (5%)
38	CHL	W	601	23	60,74,74	3.39	19 (31%)	58,114,114	2.46	17 (29%)
27	CLA	Z	611	29	69,73,73	1.16	5 (7%)	82,113,113	1.12	4 (4%)
35	LUT	8	619	-	42,43,43	0.80	1 (2%)	51,60,60	1.78	14 (27%)
27	CLA	7	607	-	46,50,73	1.37	7 (15%)	53,85,113	1.24	4 (7%)
27	CLA	U	613	24	63,67,73	1.20	6 (9%)	74,105,113	1.21	5 (6%)
27	CLA	K	204	-	49,53,73	1.37	8 (16%)	58,89,113	1.37	5 (8%)
27	CLA	8	602	21	64,68,73	1.20	9 (14%)	76,107,113	1.18	5 (6%)
27	CLA	B	840	-	69,73,73	1.17	7 (10%)	82,113,113	1.19	3 (3%)
36	XAT	V	1622	-	41,47,47	0.94	4 (9%)	54,74,74	2.47	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	V	612	26	49,53,73	1.37	8 (16%)	58,89,113	1.33	6 (10%)
27	CLA	8	603	-	48,52,73	1.49	9 (18%)	59,88,113	1.43	5 (8%)
27	CLA	A	826	-	68,72,73	1.17	9 (13%)	80,111,113	1.24	6 (7%)
27	CLA	6	618	19	43,48,73	1.52	10 (23%)	51,83,113	1.38	5 (9%)
29	LHG	a	620	27	42,42,48	0.98	2 (4%)	45,48,54	1.03	4 (8%)
35	LUT	a	617	-	42,43,43	0.81	1 (2%)	51,60,60	1.92	15 (29%)
27	CLA	A	825	-	69,73,73	1.15	6 (8%)	82,113,113	1.14	6 (7%)
33	LMG	4	624	-	40,40,55	1.05	2 (5%)	48,48,63	1.21	7 (14%)
38	CHL	X	607	-	60,74,74	3.41	19 (31%)	58,114,114	2.38	19 (32%)
27	CLA	1	608	-	47,52,73	1.40	7 (14%)	55,88,113	1.23	4 (7%)
27	CLA	8	606	-	68,72,73	1.17	8 (11%)	81,112,113	1.13	5 (6%)
27	CLA	8	612	21	44,49,73	1.42	7 (15%)	50,84,113	1.30	3 (6%)
27	CLA	8	601	21	69,73,73	1.16	7 (10%)	82,113,113	1.18	6 (7%)
27	CLA	a	611	29	41,46,73	1.57	9 (21%)	51,81,113	1.33	6 (11%)
27	CLA	F	301	-	61,65,73	1.25	9 (14%)	72,103,113	1.14	4 (5%)
27	CLA	O	2003	-	43,48,73	1.46	8 (18%)	49,83,113	1.22	3 (6%)
27	CLA	8	610	21	64,68,73	1.18	8 (12%)	76,107,113	1.28	7 (9%)
30	BCR	B	843	-	41,41,41	0.73	0	56,56,56	1.83	16 (28%)
38	CHL	W	607	-	59,73,74	3.23	19 (32%)	59,113,114	2.15	17 (28%)
35	LUT	6	619	-	42,43,43	0.80	2 (4%)	51,60,60	1.98	16 (31%)
27	CLA	6	603	-	55,59,73	1.39	7 (12%)	66,96,113	1.29	5 (7%)
38	CHL	U	606	-	38,52,74	3.97	18 (47%)	31,87,114	3.21	16 (51%)
30	BCR	A	852	-	41,41,41	0.80	1 (2%)	56,56,56	2.46	25 (44%)
27	CLA	a	613	-	58,62,73	1.25	7 (12%)	68,99,113	1.16	5 (7%)
27	CLA	3	615	-	43,48,73	1.45	7 (16%)	49,83,113	1.39	5 (10%)
35	LUT	7	619	-	42,43,43	0.86	2 (4%)	51,60,60	1.99	13 (25%)
27	CLA	A	837	1	49,53,73	1.36	8 (16%)	58,89,113	1.33	4 (6%)
27	CLA	A	824	-	69,73,73	1.14	7 (10%)	82,113,113	1.19	7 (8%)
27	CLA	3	606	-	57,62,73	1.27	7 (12%)	67,100,113	1.18	5 (7%)
27	CLA	A	809	1	69,73,73	1.13	6 (8%)	82,113,113	1.21	5 (6%)
34	DGD	B	850	-	63,63,67	0.85	2 (3%)	77,77,81	1.04	4 (5%)
27	CLA	7	610	20	69,73,73	1.14	7 (10%)	82,113,113	1.16	7 (8%)
27	CLA	Z	603	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	4 (4%)
30	BCR	A	850	-	41,41,41	0.77	1 (2%)	56,56,56	2.19	22 (39%)
27	CLA	6	617	-	49,53,73	1.36	7 (14%)	58,89,113	1.23	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	6	616	19	69,73,73	1.16	8 (11%)	82,113,113	1.26	8 (9%)
27	CLA	9	604	-	54,58,73	1.40	9 (16%)	65,95,113	1.24	6 (9%)
27	CLA	2	607	-	49,53,73	1.37	9 (18%)	58,89,113	1.33	4 (6%)
27	CLA	7	603	-	47,52,73	1.40	8 (17%)	55,88,113	1.40	4 (7%)
38	CHL	X	605	23	40,54,74	4.21	19 (47%)	34,90,114	3.23	16 (47%)
27	CLA	B	832	-	64,68,73	1.20	7 (10%)	76,107,113	1.20	6 (7%)
27	CLA	W	610	23	59,63,73	1.26	8 (13%)	70,101,113	1.16	6 (8%)
29	LHG	5	625	-	48,48,48	0.93	2 (4%)	51,54,54	1.07	3 (5%)
27	CLA	B	837	-	69,73,73	1.17	8 (11%)	82,113,113	1.21	8 (9%)
27	CLA	5	618	18	43,48,73	1.53	8 (18%)	51,83,113	1.36	6 (11%)
27	CLA	7	606	-	45,49,73	1.42	8 (17%)	52,84,113	1.28	3 (5%)
35	LUT	Z	1621	-	42,43,43	0.77	1 (2%)	51,60,60	1.89	16 (31%)
38	CHL	W	609	23	60,74,74	3.40	20 (33%)	58,114,114	2.34	16 (27%)
30	BCR	B	801	-	41,41,41	0.76	0	56,56,56	2.13	21 (37%)
27	CLA	A	829	-	69,73,73	1.15	9 (13%)	82,113,113	1.14	6 (7%)
27	CLA	2	606	-	49,53,73	1.38	8 (16%)	58,89,113	1.34	4 (6%)
27	CLA	a	608	-	47,52,73	1.39	7 (14%)	55,88,113	1.22	4 (7%)
27	CLA	8	607	-	45,49,73	1.50	8 (17%)	54,84,113	1.34	5 (9%)
27	CLA	8	613	21	69,73,73	1.17	8 (11%)	82,113,113	1.12	5 (6%)
27	CLA	W	603	-	56,60,73	1.29	9 (16%)	65,97,113	1.35	6 (9%)
29	LHG	6	623	27	47,47,48	0.93	2 (4%)	50,53,54	0.91	3 (6%)
27	CLA	X	602	23	69,73,73	1.19	7 (10%)	82,113,113	1.11	4 (4%)
27	CLA	7	604	-	54,58,73	1.32	8 (14%)	63,95,113	1.21	6 (9%)
32	LMU	5	628	-	34,34,36	1.15	2 (5%)	45,45,47	1.17	6 (13%)
27	CLA	6	609	19	49,53,73	1.37	8 (16%)	58,89,113	1.27	4 (6%)
30	BCR	B	847	-	41,41,41	0.83	1 (2%)	56,56,56	2.10	15 (26%)
27	CLA	4	610	17	65,69,73	1.18	7 (10%)	77,108,113	1.17	7 (9%)
36	XAT	U	1622	-	41,47,47	0.98	3 (7%)	54,74,74	3.86	25 (46%)
27	CLA	7	614	-	46,50,73	1.37	9 (19%)	53,85,113	1.24	5 (9%)
27	CLA	2	616	-	47,51,73	1.49	9 (19%)	58,87,113	1.28	5 (8%)
27	CLA	A	835	-	65,69,73	1.20	7 (10%)	77,108,113	1.19	5 (6%)
30	BCR	B	844	-	41,41,41	0.79	1 (2%)	56,56,56	2.13	20 (35%)
35	LUT	X	1620	-	42,43,43	0.80	1 (2%)	51,60,60	2.03	11 (21%)
37	NEX	W	1623	-	40,46,46	1.00	2 (5%)	50,70,70	2.35	17 (34%)
27	CLA	2	614	-	45,50,73	1.40	7 (15%)	52,85,113	1.19	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	B	823	-	49,53,73	1.38	8 (16%)	58,89,113	1.19	4 (6%)
27	CLA	5	617	-	54,58,73	1.30	6 (11%)	64,95,113	1.21	5 (7%)
38	CHL	X	606	-	38,52,74	4.20	17 (44%)	31,87,114	3.23	15 (48%)
27	CLA	a	607	-	49,53,73	1.37	7 (14%)	58,89,113	1.23	5 (8%)
27	CLA	X	613	23	69,73,73	1.18	8 (11%)	82,113,113	1.14	6 (7%)
30	BCR	B	845	-	41,41,41	0.78	1 (2%)	56,56,56	2.08	22 (39%)
27	CLA	9	614	-	49,53,73	1.37	7 (14%)	58,89,113	1.30	5 (8%)
35	LUT	4	619	-	42,43,43	0.71	1 (2%)	51,60,60	1.90	15 (29%)
27	CLA	9	602	22	64,68,73	1.19	9 (14%)	76,107,113	1.22	7 (9%)
27	CLA	B	827	-	66,70,73	1.17	8 (12%)	78,109,113	1.19	5 (6%)
32	LMU	1	621	-	36,36,36	1.17	2 (5%)	47,47,47	0.97	1 (2%)
29	LHG	H	204	-	48,48,48	0.90	2 (4%)	51,54,54	0.91	1 (1%)
27	CLA	A	813	-	58,62,73	1.26	7 (12%)	68,99,113	1.27	7 (10%)
27	CLA	3	611	29	41,46,73	1.57	8 (19%)	51,81,113	1.30	6 (11%)
27	CLA	1	609	14	44,48,73	1.52	8 (18%)	55,83,113	1.37	6 (10%)
27	CLA	W	614	-	49,53,73	1.37	8 (16%)	58,89,113	1.31	4 (6%)
27	CLA	a	616	14	49,53,73	1.38	8 (16%)	58,89,113	1.26	5 (8%)
30	BCR	L	309	-	41,41,41	0.65	0	56,56,56	1.99	18 (32%)
27	CLA	3	617	16	43,48,73	1.42	7 (16%)	51,83,113	1.35	5 (9%)
27	CLA	K	206	11	49,53,73	1.39	7 (14%)	58,89,113	1.30	3 (5%)
37	NEX	V	1623	-	40,46,46	0.96	3 (7%)	50,70,70	2.10	13 (26%)
27	CLA	4	614	-	60,64,73	1.25	8 (13%)	71,102,113	1.21	7 (9%)
33	LMG	9	625	-	55,55,55	0.89	2 (3%)	63,63,63	0.95	2 (3%)
30	BCR	L	305	-	41,41,41	0.70	0	56,56,56	2.10	23 (41%)
38	CHL	W	608	-	41,55,74	3.94	19 (46%)	35,91,114	2.93	15 (42%)
38	CHL	Y	601	24	60,74,74	3.39	19 (31%)	58,114,114	2.45	16 (27%)
30	BCR	8	621	-	41,41,41	0.86	1 (2%)	56,56,56	2.56	18 (32%)
30	BCR	A	849	-	41,41,41	0.75	0	56,56,56	2.26	20 (35%)
29	LHG	X	2630	27	48,48,48	0.96	2 (4%)	51,54,54	0.98	2 (3%)
27	CLA	B	804	-	45,49,73	1.38	7 (15%)	54,84,113	1.24	4 (7%)
27	CLA	V	614	-	49,53,73	1.38	8 (16%)	58,89,113	1.26	4 (6%)
27	CLA	6	606	-	43,48,73	1.45	8 (18%)	49,83,113	1.21	4 (8%)
27	CLA	1	601	14	57,62,73	1.27	9 (15%)	67,100,113	1.17	5 (7%)
30	BCR	9	621	-	41,41,41	0.77	0	56,56,56	2.08	18 (32%)
27	CLA	B	828	-	69,73,73	1.16	8 (11%)	82,113,113	1.12	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	A	832	-	54,58,73	1.33	7 (12%)	64,95,113	1.21	8 (12%)
27	CLA	A	836	-	69,73,73	1.15	7 (10%)	82,113,113	1.15	6 (7%)
27	CLA	6	614	-	64,68,73	1.22	7 (10%)	76,107,113	1.14	5 (6%)
27	CLA	F	303	-	46,50,73	1.41	9 (19%)	53,85,113	1.33	4 (7%)
27	CLA	8	604	-	54,58,73	1.28	7 (12%)	64,95,113	1.27	6 (9%)
27	CLA	1	606	-	41,47,73	1.44	8 (19%)	50,80,113	1.42	6 (12%)
36	XAT	a	618	-	41,47,47	0.89	1 (2%)	54,74,74	2.42	23 (42%)
27	CLA	a	612	14	49,53,73	1.37	7 (14%)	58,89,113	1.26	3 (5%)
27	CLA	A	842	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	7 (8%)
27	CLA	8	614	-	57,61,73	1.27	9 (15%)	67,98,113	1.25	6 (8%)
37	NEX	U	1623	-	40,46,46	1.02	3 (7%)	50,70,70	2.35	17 (34%)
27	CLA	Y	613	24	69,73,73	1.18	8 (11%)	82,113,113	1.14	6 (7%)
27	CLA	a	602	14	65,69,73	1.19	8 (12%)	77,108,113	1.17	6 (7%)
27	CLA	4	602	17	64,68,73	1.20	8 (12%)	76,107,113	1.24	7 (9%)
38	CHL	V	605	26	38,52,74	4.05	18 (47%)	31,87,114	3.09	13 (41%)
27	CLA	B	820	-	54,58,73	1.29	8 (14%)	64,95,113	1.29	6 (9%)
27	CLA	L	303	-	69,73,73	1.15	6 (8%)	82,113,113	1.19	7 (8%)
38	CHL	Y	605	24	36,50,74	4.37	18 (50%)	29,85,114	3.18	15 (51%)
27	CLA	9	610	22	61,65,73	1.24	8 (13%)	72,103,113	1.18	7 (9%)
27	CLA	B	831	-	69,73,73	1.15	8 (11%)	82,113,113	1.25	7 (8%)
27	CLA	B	838	-	50,54,73	1.32	8 (16%)	59,90,113	1.33	5 (8%)
27	CLA	A	834	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
27	CLA	U	614	-	46,50,73	1.39	8 (17%)	53,85,113	1.29	4 (7%)
35	LUT	Z	1620	-	42,43,43	0.75	1 (2%)	51,60,60	1.87	12 (23%)
27	CLA	B	822	-	46,50,73	1.37	7 (15%)	53,85,113	1.23	5 (9%)
27	CLA	B	819	-	59,63,73	1.27	7 (11%)	70,101,113	1.22	6 (8%)
27	CLA	5	609	18	69,73,73	1.17	7 (10%)	82,113,113	1.15	5 (6%)
27	CLA	a	603	-	58,62,73	1.27	8 (13%)	68,99,113	1.31	5 (7%)
27	CLA	A	818	-	64,68,73	1.18	7 (10%)	76,107,113	1.20	7 (9%)
27	CLA	W	612	23	49,53,73	1.38	8 (16%)	58,89,113	1.30	4 (6%)
27	CLA	6	620	-	68,72,73	1.15	8 (11%)	80,111,113	1.10	5 (6%)
36	XAT	X	1622	-	41,47,47	0.92	2 (4%)	54,74,74	3.78	26 (48%)
27	CLA	2	611	29	46,50,73	1.38	8 (17%)	53,85,113	1.27	4 (7%)
27	CLA	X	612	23	47,51,73	1.40	7 (14%)	55,86,113	1.28	4 (7%)
35	LUT	1	617	-	42,43,43	0.82	1 (2%)	51,60,60	1.92	15 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	1	619	-	41,41,41	0.71	0	56,56,56	2.44	21 (37%)
27	CLA	a	606	-	46,52,73	1.40	8 (17%)	57,87,113	1.26	4 (7%)
30	BCR	3	620	-	41,41,41	0.86	0	56,56,56	4.43	32 (57%)
29	LHG	Y	2630	27	48,48,48	0.95	2 (4%)	51,54,54	0.98	2 (3%)
38	CHL	V	606	-	38,52,74	3.97	19 (50%)	31,87,114	3.18	13 (41%)
36	XAT	5	621	-	41,47,47	0.90	3 (7%)	54,74,74	2.39	22 (40%)
27	CLA	Y	610	24	69,73,73	1.20	7 (10%)	82,113,113	1.11	6 (7%)
36	XAT	4	620	-	41,47,47	0.87	2 (4%)	54,74,74	2.42	23 (42%)
27	CLA	5	612	18	44,49,73	1.41	7 (15%)	50,84,113	1.25	3 (6%)
27	CLA	B	806	2	69,73,73	1.18	8 (11%)	82,113,113	1.20	4 (4%)
30	BCR	L	308	-	41,41,41	0.82	2 (4%)	56,56,56	2.34	26 (46%)
27	CLA	B	826	-	66,70,73	1.19	9 (13%)	78,109,113	1.27	7 (8%)
31	SF4	C	102	3	0,12,12	-	-	-	-	-
27	CLA	3	610	16	69,73,73	1.15	8 (11%)	82,113,113	1.12	7 (8%)
27	CLA	5	613	18	68,72,73	1.16	7 (10%)	80,111,113	1.11	5 (6%)
30	BCR	5	622	-	41,41,41	0.75	0	56,56,56	2.37	20 (35%)
28	PQN	B	842	-	34,34,34	3.48	10 (29%)	43,45,45	1.54	6 (13%)
29	LHG	8	623	-	39,39,48	1.03	2 (5%)	42,45,54	1.10	3 (7%)
27	CLA	5	602	18	69,73,73	1.15	9 (13%)	82,113,113	1.15	5 (6%)
30	BCR	A	851	-	41,41,41	0.80	1 (2%)	56,56,56	2.12	23 (41%)
27	CLA	B	817	-	63,67,73	1.21	8 (12%)	74,105,113	1.30	7 (9%)
27	CLA	7	601	20	64,68,73	1.18	8 (12%)	76,107,113	1.29	7 (9%)
27	CLA	3	614	-	43,48,73	1.44	9 (20%)	51,83,113	1.28	4 (7%)
29	LHG	3	623	-	44,44,48	0.96	2 (4%)	47,50,54	1.07	3 (6%)
27	CLA	6	611	29	46,50,73	1.38	8 (17%)	53,85,113	1.25	4 (7%)
27	CLA	A	839	-	59,63,73	1.25	8 (13%)	70,101,113	1.21	5 (7%)
27	CLA	1	614	-	40,45,73	1.61	9 (22%)	47,79,113	1.43	6 (12%)
35	LUT	W	1620	-	42,43,43	0.89	1 (2%)	51,60,60	1.89	9 (17%)
30	BCR	A	848	-	41,41,41	0.85	1 (2%)	56,56,56	1.98	14 (25%)
36	XAT	2	620	-	41,47,47	0.90	2 (4%)	54,74,74	2.43	21 (38%)
27	CLA	5	619	-	47,51,73	1.52	8 (17%)	58,87,113	1.35	8 (13%)
27	CLA	X	611	29	49,53,73	1.40	7 (14%)	58,89,113	1.30	6 (10%)
38	CHL	Y	608	-	43,57,74	4.06	18 (41%)	37,93,114	2.89	16 (43%)
30	BCR	O	2004	-	41,41,41	0.78	1 (2%)	56,56,56	2.44	19 (33%)
27	CLA	A	838	-	54,58,73	1.28	8 (14%)	64,95,113	1.36	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	B	814	-	66,70,73	1.16	8 (12%)	78,109,113	1.11	6 (7%)
27	CLA	K	201	11	49,53,73	1.37	7 (14%)	58,89,113	1.16	3 (5%)
27	CLA	3	603	-	59,63,73	1.26	8 (13%)	70,101,113	1.39	7 (10%)
27	CLA	4	612	17	44,49,73	1.42	7 (15%)	50,84,113	1.28	3 (6%)
30	BCR	B	853	-	41,41,41	0.75	1 (2%)	56,56,56	1.71	14 (25%)
29	LHG	B	854	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
27	CLA	9	609	22	65,69,73	1.20	7 (10%)	77,108,113	1.14	4 (5%)
30	BCR	K	207	-	41,41,41	0.76	1 (2%)	56,56,56	3.01	24 (42%)
27	CLA	X	604	-	53,57,73	1.33	7 (13%)	61,93,113	1.17	5 (8%)
27	CLA	U	611	29	46,50,73	1.36	8 (17%)	53,85,113	1.32	4 (7%)
27	CLA	B	829	-	69,73,73	1.15	6 (8%)	82,113,113	1.13	5 (6%)
27	CLA	K	203	-	60,64,73	1.26	8 (13%)	71,102,113	1.31	8 (11%)
27	CLA	5	608	-	54,58,73	1.31	8 (14%)	63,95,113	1.19	5 (7%)
27	CLA	6	612	19	44,49,73	1.41	7 (15%)	50,84,113	1.26	3 (6%)
27	CLA	A	830	-	69,73,73	1.17	7 (10%)	82,113,113	1.22	5 (6%)
27	CLA	a	604	-	53,57,73	1.31	7 (13%)	61,93,113	1.18	3 (4%)
27	CLA	X	603	-	66,70,73	1.22	7 (10%)	78,109,113	1.19	5 (6%)
27	CLA	a	614	-	58,62,73	1.27	8 (13%)	65,99,113	1.24	6 (9%)
27	CLA	A	805	-	56,60,73	1.27	7 (12%)	65,97,113	1.36	6 (9%)
28	PQN	A	844	-	34,34,34	3.54	10 (29%)	43,45,45	1.54	4 (9%)
27	CLA	A	816	-	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
37	NEX	X	1623	-	40,46,46	1.03	3 (7%)	50,70,70	2.33	17 (34%)
27	CLA	5	601	18	60,64,73	1.24	7 (11%)	71,102,113	1.32	7 (9%)
29	LHG	W	2630	27	43,43,48	0.96	2 (4%)	46,49,54	0.97	2 (4%)
38	CHL	Z	609	25	60,74,74	3.47	20 (33%)	58,114,114	2.02	16 (27%)
38	CHL	V	607	-	40,54,74	3.94	19 (47%)	34,90,114	2.93	14 (41%)
27	CLA	7	602	20	69,73,73	1.15	9 (13%)	82,113,113	1.13	4 (4%)
27	CLA	4	601	17	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)
33	LMG	H	205	-	55,55,55	0.89	2 (3%)	63,63,63	1.12	7 (11%)

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	3	613	16	1/1/12/20	9/23/99/115	-
27	CLA	J	101	10	1/1/10/20	5/12/88/115	-
27	CLA	A	812	-	1/1/15/20	4/39/115/115	-
27	CLA	2	602	15	1/1/15/20	8/37/113/115	-
27	CLA	A	819	-	1/1/13/20	5/32/108/115	-
27	CLA	B	807	-	-	3/24/100/115	-
35	LUT	X	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	B	803	-	1/1/15/20	11/39/115/115	-
38	CHL	Z	601	25	3/3/20/26	19/39/137/137	-
27	CLA	2	603	15	1/1/11/20	3/13/89/115	-
35	LUT	5	620	-	-	1/29/67/67	0/2/2/2
27	CLA	B	836	-	1/1/12/20	2/21/97/115	-
27	CLA	1	607	-	1/1/10/20	2/8/84/115	-
36	XAT	W	1622	-	-	1/31/93/93	0/4/4/4
27	CLA	Y	602	24	1/1/13/20	6/31/107/115	-
27	CLA	L	302	12	1/1/11/20	4/15/91/115	-
27	CLA	2	612	15	1/1/11/20	7/13/89/115	-
30	BCR	K	202	-	-	4/29/63/63	0/2/2/2
32	LMU	A	857	-	-	3/21/61/61	0/2/2/2
33	LMG	8	626	-	-	16/41/61/70	0/1/1/1
38	CHL	W	606	-	3/3/16/26	2/15/113/137	-
37	NEX	Z	1623	-	-	3/27/83/83	0/3/3/3
27	CLA	A	802	-	1/1/15/20	10/39/115/115	-
27	CLA	8	609	21	1/1/11/20	6/15/91/115	-
27	CLA	7	613	20	1/1/15/20	10/39/115/115	-
27	CLA	H	203	-	-	12/39/115/115	-
27	CLA	A	823	-	1/1/10/20	4/12/88/115	-
27	CLA	A	831	-	1/1/15/20	11/39/115/115	-
38	CHL	W	605	23	3/3/16/26	3/15/113/137	-
27	CLA	4	609	17	1/1/13/20	4/30/106/115	-
27	CLA	9	613	22	1/1/15/20	6/39/115/115	-
38	CHL	U	607	-	3/3/16/26	4/15/113/137	-
27	CLA	B	810	-	1/1/14/20	15/37/113/115	-
27	CLA	9	601	22	1/1/11/20	4/15/91/115	-
27	CLA	A	821	-	1/1/12/20	15/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	Z	614	-	1/1/12/20	7/26/102/115	-
36	XAT	6	621	-	-	0/31/93/93	0/4/4/4
38	CHL	V	609	26	3/3/19/26	17/33/131/137	-
38	CHL	Z	608	-	3/3/16/26	5/20/118/137	-
27	CLA	B	821	-	1/1/11/20	4/13/89/115	-
27	CLA	8	616	-	1/1/11/20	5/11/87/115	-
27	CLA	V	611	29	1/1/10/20	4/13/89/115	-
38	CHL	U	609	24	3/3/18/26	12/32/130/137	-
31	SF4	C	101	3	-	-	0/6/5/5
27	CLA	2	604	-	1/1/10/20	4/11/87/115	-
38	CHL	Y	606	-	3/3/16/26	2/15/113/137	-
27	CLA	Y	614	-	1/1/11/20	8/19/95/115	-
27	CLA	W	613	23	1/1/15/20	12/39/115/115	-
27	CLA	a	609	14	1/1/15/20	13/37/113/115	-
30	BCR	B	852	-	-	6/29/63/63	0/2/2/2
30	BCR	7	621	-	-	5/29/63/63	0/2/2/2
27	CLA	Y	604	-	1/1/12/20	4/21/97/115	-
27	CLA	8	608	-	1/1/12/20	8/23/99/115	-
27	CLA	L	307	-	1/1/10/20	2/8/84/115	-
27	CLA	A	808	-	-	4/21/97/115	-
27	CLA	7	608	-	1/1/12/20	3/21/97/115	-
27	CLA	4	604	-	1/1/13/20	8/25/101/115	-
27	CLA	U	603	-	1/1/12/20	11/24/100/115	-
27	CLA	7	616	20	1/1/11/20	2/11/87/115	-
27	CLA	A	801	-	1/1/15/20	9/39/115/115	-
27	CLA	4	613	17	1/1/15/20	12/39/115/115	-
27	CLA	6	610	19	1/1/15/20	8/39/115/115	-
27	CLA	Z	610	25	1/1/15/20	10/39/115/115	-
27	CLA	G	204	7	1/1/11/20	4/15/91/115	-
27	CLA	3	609	16	1/1/14/20	15/33/109/115	-
27	CLA	Y	603	-	1/1/13/20	11/27/103/115	-
35	LUT	V	1621	-	-	2/29/67/67	0/2/2/2
36	XAT	Y	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	2	601	15	1/1/15/20	13/39/115/115	-
33	LMG	A	860	-	-	10/35/55/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	6	602	19	1/1/15/20	9/39/115/115	-
32	LMU	A	858	-	-	12/21/57/61	0/2/2/2
27	CLA	2	610	15	1/1/13/20	9/27/103/115	-
32	LMU	8	625	-	-	8/21/61/61	0/2/2/2
27	CLA	B	818	-	-	14/33/109/115	-
27	CLA	B	812	-	1/1/10/20	2/13/89/115	-
35	LUT	2	619	-	-	1/29/67/67	0/2/2/2
27	CLA	4	616	17	1/1/11/20	7/11/87/115	-
27	CLA	Y	611	29	1/1/10/20	6/13/89/115	-
27	CLA	6	608	-	1/1/11/20	6/15/91/115	-
27	CLA	A	804	-	1/1/15/20	16/39/115/115	-
30	BCR	A	856	-	-	2/29/63/63	0/2/2/2
27	CLA	B	835	-	1/1/11/20	4/15/91/115	-
27	CLA	O	2001	-	1/1/9/20	1/6/78/115	-
27	CLA	4	608	-	1/1/15/20	10/39/115/115	-
27	CLA	a	610	14	1/1/14/20	2/31/107/115	-
27	CLA	A	827	-	1/1/13/20	6/31/107/115	-
27	CLA	A	817	-	-	2/15/91/115	-
29	LHG	A	847	27	-	4/34/34/53	-
37	NEX	5	624	-	-	2/27/83/83	0/3/3/3
30	BCR	3	621	-	-	0/29/63/63	0/2/2/2
33	LMG	J	104	-	-	13/35/55/70	0/1/1/1
27	CLA	5	606	-	-	3/8/84/115	-
33	LMG	L	2631	-	-	8/32/52/70	0/1/1/1
35	LUT	U	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	B	824	-	1/1/15/20	12/39/115/115	-
27	CLA	5	604	-	1/1/15/20	15/35/111/115	-
29	LHG	9	624	-	-	19/53/53/53	-
27	CLA	U	604	-	1/1/10/20	6/20/92/115	-
27	CLA	5	614	-	1/1/10/20	10/15/87/115	-
27	CLA	A	822	-	1/1/15/20	7/39/115/115	-
30	BCR	a	619	-	-	4/29/63/63	0/2/2/2
36	XAT	7	620	-	-	0/31/93/93	0/4/4/4
29	LHG	2	622	27	-	13/40/40/53	-
30	BCR	7	623	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	Y	609	24	3/3/20/26	14/39/137/137	-
27	CLA	5	616	18	1/1/10/20	2/8/84/115	-
35	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	5	607	-	1/1/15/20	12/39/115/115	-
29	LHG	1	620	27	-	9/53/53/53	-
27	CLA	6	613	-	1/1/15/20	13/37/113/115	-
27	CLA	B	813	-	1/1/15/20	18/39/115/115	-
30	BCR	4	621	-	-	4/29/63/63	0/2/2/2
29	LHG	9	623	-	-	16/53/53/53	-
27	CLA	A	828	-	1/1/15/20	9/39/115/115	-
27	CLA	B	825	-	-	4/20/96/115	-
27	CLA	L	304	-	1/1/11/20	0/15/91/115	-
30	BCR	G	205	-	-	0/29/63/63	0/2/2/2
30	BCR	3	622	-	-	2/29/63/63	0/2/2/2
38	CHL	X	609	23	3/3/20/26	17/39/137/137	-
27	CLA	V	603	-	1/1/11/20	4/15/91/115	-
29	LHG	4	622	27	-	10/53/53/53	-
27	CLA	A	806	-	1/1/15/20	14/39/115/115	-
27	CLA	1	610	14	1/1/9/20	1/8/80/115	-
27	CLA	2	609	15	1/1/11/20	2/15/91/115	-
27	CLA	X	610	23	1/1/15/20	9/39/115/115	-
27	CLA	3	602	16	1/1/14/20	3/33/109/115	-
27	CLA	4	607	-	1/1/11/20	6/15/91/115	-
27	CLA	A	820	-	1/1/15/20	10/39/115/115	-
27	CLA	W	611	29	1/1/13/20	12/30/106/115	-
27	CLA	9	611	29	1/1/10/20	3/12/88/115	-
30	BCR	B	849	-	-	3/29/63/63	0/2/2/2
27	CLA	G	203	-	1/1/10/20	4/12/88/115	-
38	CHL	Z	607	-	3/3/20/26	19/39/137/137	-
27	CLA	B	811	-	1/1/12/20	8/23/95/115	-
27	CLA	3	612	16	1/1/10/20	1/13/89/115	-
27	CLA	A	841	-	1/1/15/20	17/39/115/115	-
27	CLA	B	809	2	1/1/15/20	15/39/115/115	-
27	CLA	1	611	29	1/1/13/20	7/30/106/115	-
27	CLA	A	854	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	3	604	-	1/1/15/20	8/39/115/115	-
27	CLA	1	616	14	1/1/11/20	5/11/87/115	-
27	CLA	A	845	29	1/1/12/20	3/21/97/115	-
27	CLA	7	609	20	1/1/10/20	4/12/88/115	-
38	CHL	X	601	23	3/3/20/26	21/39/137/137	-
27	CLA	7	615	-	1/1/10/20	6/8/84/115	-
27	CLA	6	607	-	1/1/10/20	2/10/86/115	-
27	CLA	1	604	-	1/1/11/20	10/20/96/115	-
29	LHG	A	846	-	-	12/53/53/53	-
27	CLA	X	614	-	1/1/10/20	5/12/88/115	-
27	CLA	B	805	-	1/1/15/20	14/39/115/115	-
27	CLA	9	603	22	1/1/11/20	2/13/89/115	-
29	LHG	Z	2630	27	-	17/53/53/53	-
29	LHG	O	2631	-	-	15/40/40/53	-
35	LUT	U	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	9	606	-	1/1/10/20	4/8/84/115	-
38	CHL	Y	607	-	3/3/20/26	21/39/137/137	-
35	LUT	V	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	V	602	26	1/1/14/20	5/33/109/115	-
32	LMU	K	208	-	-	14/21/61/61	0/2/2/2
27	CLA	A	810	1	1/1/12/20	10/21/97/115	-
27	CLA	4	603	17	1/1/11/20	2/13/89/115	-
27	CLA	5	611	29	1/1/10/20	5/12/88/115	-
27	CLA	W	604	-	1/1/11/20	2/18/94/115	-
33	LMG	J	103	-	-	5/37/57/70	0/1/1/1
35	LUT	W	1621	-	-	1/29/67/67	0/2/2/2
38	CHL	X	608	-	3/3/20/26	21/39/137/137	-
27	CLA	Z	602	25	1/1/14/20	3/33/109/115	-
27	CLA	3	608	-	1/1/13/20	4/27/103/115	-
38	CHL	Z	606	-	3/3/16/26	4/15/113/137	-
27	CLA	4	606	-	1/1/10/20	4/8/84/115	-
27	CLA	A	833	-	1/1/11/20	5/15/91/115	-
27	CLA	8	611	29	1/1/10/20	4/12/88/115	-
29	LHG	V	2630	27	-	7/52/52/53	-
27	CLA	6	601	19	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	O	2005	-	-	4/29/63/63	0/2/2/2
27	CLA	B	833	-	1/1/15/20	11/39/115/115	-
27	CLA	Y	612	24	1/1/11/20	6/15/91/115	-
38	CHL	U	608	-	3/3/15/26	3/13/111/137	-
30	BCR	F	305	-	-	6/29/63/63	0/2/2/2
36	XAT	9	620	-	-	0/31/93/93	0/4/4/4
38	CHL	Z	605	25	3/3/15/26	1/13/111/137	-
27	CLA	Z	604	-	1/1/13/20	6/30/106/115	-
32	LMU	5	629	-	-	11/18/58/61	0/2/2/2
33	LMG	4	623	-	-	5/35/55/70	0/1/1/1
27	CLA	B	815	-	1/1/10/20	2/13/89/115	-
30	BCR	L	301	-	-	4/29/63/63	0/2/2/2
27	CLA	A	840	-	-	4/24/100/115	-
37	NEX	Y	1623	-	-	3/27/80/83	0/3/3/3
33	LMG	5	627	-	-	12/35/55/70	0/1/1/1
27	CLA	V	604	-	1/1/12/20	5/21/97/115	-
33	LMG	V	2631	-	-	9/36/56/70	0/1/1/1
27	CLA	2	613	15	1/1/15/20	6/39/115/115	-
37	NEX	6	624	-	-	2/27/83/83	0/3/3/3
27	CLA	V	610	26	1/1/14/20	6/36/112/115	-
27	CLA	A	807	1	1/1/15/20	19/39/115/115	-
27	CLA	9	612	22	1/1/10/20	2/10/86/115	-
27	CLA	A	814	-	1/1/15/20	14/39/115/115	-
30	BCR	2	623	-	-	4/29/63/63	0/2/2/2
29	LHG	5	623	27	-	14/53/53/53	-
27	CLA	U	610	24	1/1/13/20	8/29/105/115	-
27	CLA	7	611	29	1/1/13/20	6/31/107/115	-
36	XAT	1	618	-	-	0/31/93/93	0/4/4/4
27	CLA	Z	613	25	1/1/15/20	16/39/115/115	-
27	CLA	1	612	14	1/1/11/20	5/15/91/115	-
35	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
38	CHL	V	601	26	3/3/20/26	13/39/137/137	-
27	CLA	A	803	-	1/1/15/20	3/39/115/115	-
27	CLA	B	816	-	1/1/12/20	11/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	F	304	6	-	4/10/86/115	-
27	CLA	4	618	17	1/1/10/20	2/8/84/115	-
35	LUT	9	619	-	-	0/29/67/67	0/2/2/2
27	CLA	3	607	16	1/1/13/20	10/28/104/115	-
27	CLA	B	839	-	1/1/15/20	14/39/115/115	-
27	CLA	B	841	29	1/1/15/20	9/39/115/115	-
30	BCR	6	622	-	-	5/29/63/63	0/2/2/2
27	CLA	a	601	14	-	4/25/101/115	-
27	CLA	A	811	-	1/1/15/20	10/39/115/115	-
27	CLA	B	808	-	1/1/15/20	14/39/115/115	-
29	LHG	8	622	27	-	8/53/53/53	-
30	BCR	B	848	-	-	3/29/63/63	0/2/2/2
27	CLA	7	612	20	1/1/11/20	4/13/89/115	-
27	CLA	5	603	-	1/1/13/20	6/25/101/115	-
36	XAT	8	620	-	-	0/31/93/93	0/4/4/4
30	BCR	B	846	-	-	2/29/63/63	0/2/2/2
27	CLA	W	602	23	1/1/14/20	6/33/109/115	-
29	LHG	3	624	27	-	22/53/53/53	-
27	CLA	B	834	-	1/1/14/20	7/33/109/115	-
27	CLA	1	603	-	1/1/12/20	3/23/99/115	-
29	LHG	U	2630	27	-	12/53/53/53	-
27	CLA	A	843	-	1/1/14/20	12/37/113/115	-
27	CLA	A	815	-	1/1/12/20	8/21/97/115	-
27	CLA	V	613	26	1/1/15/20	16/39/115/115	-
38	CHL	U	605	24	3/3/15/26	0/12/110/137	-
27	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
27	CLA	U	612	24	1/1/10/20	4/13/89/115	-
29	LHG	B	851	27	-	11/42/42/53	-
30	BCR	J	102	-	-	2/29/63/63	0/2/2/2
27	CLA	1	602	14	1/1/14/20	3/35/111/115	-
31	SF4	A	853	2,1	-	-	0/6/5/5
27	CLA	6	604	-	-	13/39/115/115	-
38	CHL	U	601	24	3/3/20/26	20/39/137/137	-
27	CLA	5	610	18	1/1/12/20	3/26/102/115	-
27	CLA	9	607	-	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	XAT	Z	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	L	306	-	1/1/10/20	0/8/84/115	-
27	CLA	Z	612	25	1/1/15/20	6/39/115/115	-
29	LHG	9	622	27	-	11/34/34/53	-
35	LUT	3	618	-	-	0/29/67/67	0/2/2/2
27	CLA	H	202	8	1/1/10/20	2/6/82/115	-
27	CLA	B	830	-	1/1/10/20	4/13/89/115	-
38	CHL	V	608	-	3/3/16/26	5/18/116/137	-
27	CLA	4	611	29	1/1/10/20	4/12/88/115	-
27	CLA	B	802	-	1/1/15/20	19/39/115/115	-
27	CLA	1	613	-	1/1/15/20	12/39/115/115	-
36	XAT	3	619	-	-	0/31/93/93	0/4/4/4
27	CLA	U	602	24	1/1/13/20	6/32/108/115	-
29	LHG	7	622	27	-	21/41/41/53	-
38	CHL	W	601	23	3/3/20/26	20/39/137/137	-
27	CLA	Z	611	29	1/1/15/20	5/39/115/115	-
35	LUT	8	619	-	-	1/29/67/67	0/2/2/2
27	CLA	7	607	-	1/1/10/20	3/12/88/115	-
27	CLA	U	613	24	1/1/13/20	10/32/108/115	-
27	CLA	K	204	-	1/1/11/20	4/15/91/115	-
27	CLA	8	602	21	1/1/14/20	7/33/109/115	-
27	CLA	B	840	-	1/1/15/20	5/39/115/115	-
36	XAT	V	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	V	612	26	1/1/11/20	4/15/91/115	-
27	CLA	8	603	-	1/1/11/20	5/13/89/115	-
27	CLA	A	826	-	1/1/14/20	12/37/113/115	-
27	CLA	6	618	19	1/1/10/20	0/8/84/115	-
29	LHG	a	620	27	-	9/47/47/53	-
35	LUT	a	617	-	-	0/29/67/67	0/2/2/2
27	CLA	A	825	-	1/1/15/20	20/39/115/115	-
38	CHL	X	607	-	3/3/20/26	17/39/137/137	-
33	LMG	4	624	-	-	8/35/55/70	0/1/1/1
27	CLA	1	608	-	1/1/11/20	5/13/89/115	-
27	CLA	8	606	-	1/1/15/20	8/37/113/115	-
27	CLA	8	612	21	1/1/10/20	2/10/86/115	-
27	CLA	8	601	21	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	611	29	1/1/10/20	2/4/80/115	-
27	CLA	F	301	-	1/1/13/20	10/30/106/115	-
27	CLA	O	2003	-	1/1/10/20	2/8/84/115	-
27	CLA	8	610	21	1/1/14/20	8/33/109/115	-
30	BCR	B	843	-	-	4/29/63/63	0/2/2/2
38	CHL	W	607	-	3/3/20/26	25/37/135/137	-
35	LUT	6	619	-	-	0/29/67/67	0/2/2/2
27	CLA	6	603	-	1/1/12/20	3/22/98/115	-
38	CHL	U	606	-	3/3/15/26	0/13/111/137	-
30	BCR	A	852	-	-	8/29/63/63	0/2/2/2
27	CLA	a	613	-	1/1/12/20	8/26/102/115	-
27	CLA	3	615	-	1/1/10/20	2/8/84/115	-
35	LUT	7	619	-	-	1/29/67/67	0/2/2/2
27	CLA	A	837	1	-	9/15/91/115	-
27	CLA	A	824	-	1/1/15/20	9/39/115/115	-
27	CLA	3	606	-	1/1/13/20	6/25/101/115	-
27	CLA	A	809	1	1/1/15/20	10/39/115/115	-
34	DGD	B	850	-	-	16/51/91/95	0/2/2/2
27	CLA	7	610	20	1/1/15/20	2/39/115/115	-
27	CLA	Z	603	-	1/1/15/20	20/39/115/115	-
30	BCR	A	850	-	-	2/29/63/63	0/2/2/2
27	CLA	6	617	-	1/1/11/20	8/15/91/115	-
27	CLA	6	616	19	1/1/15/20	20/39/115/115	-
27	CLA	9	604	-	1/1/12/20	2/20/96/115	-
27	CLA	2	607	-	1/1/11/20	4/15/91/115	-
27	CLA	7	603	-	1/1/11/20	3/13/89/115	-
38	CHL	X	605	23	3/3/16/26	1/15/113/137	-
27	CLA	B	832	-	-	9/33/109/115	-
27	CLA	W	610	23	1/1/13/20	8/27/103/115	-
29	LHG	5	625	-	-	15/53/53/53	-
27	CLA	B	837	-	-	12/39/115/115	-
27	CLA	5	618	18	1/1/10/20	0/8/84/115	-
27	CLA	7	606	-	-	2/10/86/115	-
35	LUT	Z	1621	-	-	2/29/67/67	0/2/2/2
38	CHL	W	609	23	3/3/20/26	15/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	B	801	-	-	3/29/63/63	0/2/2/2
27	CLA	A	829	-	1/1/15/20	13/39/115/115	-
27	CLA	2	606	-	1/1/11/20	4/15/91/115	-
27	CLA	a	608	-	1/1/11/20	5/13/89/115	-
27	CLA	8	607	-	1/1/10/20	4/10/86/115	-
27	CLA	8	613	21	1/1/15/20	11/39/115/115	-
27	CLA	W	603	-	1/1/12/20	11/24/100/115	-
29	LHG	6	623	27	-	24/52/52/53	-
27	CLA	X	602	23	1/1/15/20	9/39/115/115	-
27	CLA	7	604	-	1/1/12/20	9/21/97/115	-
32	LMU	5	628	-	-	9/19/59/61	0/2/2/2
27	CLA	6	609	19	1/1/11/20	2/15/91/115	-
30	BCR	B	847	-	-	2/29/63/63	0/2/2/2
27	CLA	4	610	17	1/1/14/20	7/35/111/115	-
36	XAT	U	1622	-	-	1/31/93/93	0/4/4/4
27	CLA	7	614	-	1/1/10/20	3/12/88/115	-
27	CLA	2	616	-	1/1/11/20	4/11/87/115	-
27	CLA	A	835	-	-	11/35/111/115	-
30	BCR	B	844	-	-	2/29/63/63	0/2/2/2
35	LUT	X	1620	-	-	2/29/67/67	0/2/2/2
37	NEX	W	1623	-	-	4/27/83/83	0/3/3/3
27	CLA	2	614	-	1/1/10/20	1/11/87/115	-
27	CLA	B	823	-	1/1/11/20	6/15/91/115	-
27	CLA	5	617	-	1/1/12/20	8/21/97/115	-
38	CHL	X	606	-	3/3/15/26	0/13/111/137	-
27	CLA	a	607	-	1/1/11/20	3/15/91/115	-
27	CLA	X	613	23	1/1/15/20	14/39/115/115	-
30	BCR	B	845	-	-	9/29/63/63	0/2/2/2
27	CLA	9	614	-	1/1/11/20	7/15/91/115	-
35	LUT	4	619	-	-	4/29/67/67	0/2/2/2
27	CLA	9	602	22	-	7/33/109/115	-
27	CLA	B	827	-	1/1/14/20	15/36/112/115	-
32	LMU	1	621	-	-	7/21/61/61	0/2/2/2
29	LHG	H	204	-	-	16/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	813	-	1/1/12/20	5/26/102/115	-
27	CLA	3	611	29	1/1/10/20	2/4/80/115	-
27	CLA	1	609	14	1/1/10/20	2/8/84/115	-
27	CLA	W	614	-	1/1/11/20	4/15/91/115	-
27	CLA	a	616	14	1/1/11/20	5/15/91/115	-
30	BCR	L	309	-	-	1/29/63/63	0/2/2/2
27	CLA	3	617	16	1/1/10/20	2/8/84/115	-
27	CLA	K	206	11	1/1/11/20	4/15/91/115	-
37	NEX	V	1623	-	-	4/27/83/83	0/3/3/3
27	CLA	4	614	-	1/1/13/20	11/29/105/115	-
33	LMG	9	625	-	-	16/50/70/70	0/1/1/1
30	BCR	L	305	-	-	2/29/63/63	0/2/2/2
38	CHL	W	608	-	3/3/16/26	5/17/115/137	-
38	CHL	Y	601	24	3/3/20/26	21/39/137/137	-
30	BCR	8	621	-	-	4/29/63/63	0/2/2/2
30	BCR	A	849	-	-	5/29/63/63	0/2/2/2
29	LHG	X	2630	27	-	11/53/53/53	-
27	CLA	B	804	-	1/1/10/20	0/10/86/115	-
27	CLA	V	614	-	1/1/11/20	5/15/91/115	-
27	CLA	6	606	-	1/1/10/20	0/8/84/115	-
27	CLA	1	601	14	-	4/25/101/115	-
30	BCR	9	621	-	-	4/29/63/63	0/2/2/2
27	CLA	B	828	-	1/1/15/20	13/39/115/115	-
27	CLA	A	832	-	1/1/12/20	7/21/97/115	-
27	CLA	A	836	-	1/1/15/20	5/39/115/115	-
27	CLA	6	614	-	1/1/14/20	10/33/109/115	-
27	CLA	F	303	-	-	6/12/88/115	-
27	CLA	8	604	-	1/1/12/20	3/21/97/115	-
27	CLA	1	606	-	1/1/8/20	3/7/79/115	-
36	XAT	a	618	-	-	0/31/93/93	0/4/4/4
27	CLA	a	612	14	1/1/11/20	5/15/91/115	-
27	CLA	A	842	-	1/1/15/20	17/39/115/115	-
27	CLA	8	614	-	1/1/12/20	9/25/101/115	-
37	NEX	U	1623	-	-	5/27/83/83	0/3/3/3
27	CLA	Y	613	24	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	602	14	1/1/14/20	3/35/111/115	-
27	CLA	4	602	17	1/1/14/20	5/33/109/115	-
38	CHL	V	605	26	3/3/15/26	0/13/111/137	-
27	CLA	B	820	-	1/1/12/20	3/21/97/115	-
38	CHL	Y	605	24	3/3/15/26	0/10/108/137	-
27	CLA	L	303	-	-	12/39/115/115	-
27	CLA	9	610	22	1/1/13/20	3/30/106/115	-
27	CLA	B	831	-	1/1/15/20	13/39/115/115	-
27	CLA	B	838	-	-	2/17/93/115	-
27	CLA	A	834	-	1/1/15/20	15/39/115/115	-
27	CLA	U	614	-	1/1/10/20	5/12/88/115	-
35	LUT	Z	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	B	822	-	-	4/12/88/115	-
27	CLA	B	819	-	1/1/13/20	9/27/103/115	-
27	CLA	5	609	18	1/1/15/20	13/39/115/115	-
27	CLA	a	603	-	1/1/12/20	2/25/101/115	-
27	CLA	A	818	-	-	12/33/109/115	-
27	CLA	W	612	23	1/1/11/20	6/15/91/115	-
27	CLA	6	620	-	1/1/14/20	10/37/113/115	-
36	XAT	X	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	2	611	29	1/1/10/20	5/12/88/115	-
27	CLA	X	612	23	1/1/10/20	4/13/89/115	-
35	LUT	1	617	-	-	0/29/67/67	0/2/2/2
30	BCR	1	619	-	-	4/29/63/63	0/2/2/2
27	CLA	a	606	-	1/1/10/20	5/12/88/115	-
30	BCR	3	620	-	-	4/29/63/63	0/2/2/2
29	LHG	Y	2630	27	-	11/53/53/53	-
38	CHL	V	606	-	3/3/15/26	2/13/111/137	-
36	XAT	5	621	-	-	0/31/93/93	0/4/4/4
27	CLA	Y	610	24	1/1/15/20	9/39/115/115	-
36	XAT	4	620	-	-	0/31/93/93	0/4/4/4
27	CLA	5	612	18	1/1/10/20	4/10/86/115	-
27	CLA	B	806	2	1/1/15/20	16/39/115/115	-
30	BCR	L	308	-	-	2/29/63/63	0/2/2/2
27	CLA	B	826	-	1/1/14/20	7/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	SF4	C	102	3	-	-	0/6/5/5
27	CLA	3	610	16	1/1/15/20	12/39/115/115	-
27	CLA	5	613	18	1/1/14/20	15/37/113/115	-
30	BCR	5	622	-	-	3/29/63/63	0/2/2/2
28	PQN	B	842	-	-	5/23/43/43	0/2/2/2
29	LHG	8	623	-	-	10/44/44/53	-
27	CLA	5	602	18	-	12/39/115/115	-
30	BCR	A	851	-	-	2/29/63/63	0/2/2/2
27	CLA	B	817	-	1/1/13/20	10/32/108/115	-
27	CLA	7	601	20	1/1/14/20	10/33/109/115	-
27	CLA	3	614	-	1/1/10/20	3/8/84/115	-
29	LHG	3	623	-	-	19/49/49/53	-
27	CLA	6	611	29	1/1/10/20	4/12/88/115	-
27	CLA	A	839	-	1/1/13/20	6/27/103/115	-
27	CLA	1	614	-	1/1/9/20	4/4/76/115	-
35	LUT	W	1620	-	-	2/29/67/67	0/2/2/2
30	BCR	A	848	-	-	0/29/63/63	0/2/2/2
36	XAT	2	620	-	-	0/31/93/93	0/4/4/4
27	CLA	5	619	-	1/1/11/20	6/11/87/115	-
27	CLA	X	611	29	1/1/11/20	8/15/91/115	-
38	CHL	Y	608	-	3/3/16/26	6/19/117/137	-
30	BCR	O	2004	-	-	3/29/63/63	0/2/2/2
27	CLA	A	838	-	1/1/12/20	7/21/97/115	-
27	CLA	B	814	-	1/1/14/20	9/36/112/115	-
27	CLA	K	201	11	1/1/11/20	7/15/91/115	-
27	CLA	3	603	-	1/1/13/20	6/27/103/115	-
27	CLA	4	612	17	1/1/10/20	2/10/86/115	-
30	BCR	B	853	-	-	4/29/63/63	0/2/2/2
29	LHG	B	854	-	-	16/53/53/53	-
27	CLA	9	609	22	1/1/14/20	7/35/111/115	-
30	BCR	K	207	-	-	0/29/63/63	0/2/2/2
27	CLA	X	604	-	1/1/11/20	6/20/96/115	-
27	CLA	U	611	29	1/1/10/20	6/12/88/115	-
27	CLA	B	829	-	1/1/15/20	11/39/115/115	-
27	CLA	K	203	-	-	8/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	5	608	-	1/1/12/20	6/21/97/115	-
27	CLA	6	612	19	1/1/10/20	2/10/86/115	-
27	CLA	A	830	-	1/1/15/20	11/39/115/115	-
27	CLA	a	604	-	1/1/11/20	10/20/96/115	-
27	CLA	X	603	-	1/1/14/20	11/36/112/115	-
27	CLA	a	614	-	1/1/12/20	5/27/99/115	-
27	CLA	A	805	-	-	5/24/100/115	-
28	PQN	A	844	-	-	10/23/43/43	0/2/2/2
27	CLA	A	816	-	1/1/15/20	9/39/115/115	-
37	NEX	X	1623	-	-	3/27/83/83	0/3/3/3
27	CLA	5	601	18	1/1/13/20	4/29/105/115	-
29	LHG	W	2630	27	-	10/48/48/53	-
38	CHL	Z	609	25	3/3/20/26	20/39/137/137	-
38	CHL	V	607	-	3/3/16/26	2/15/113/137	-
27	CLA	7	602	20	1/1/15/20	13/39/115/115	-
27	CLA	4	601	17	1/1/15/20	14/39/115/115	-
33	LMG	H	205	-	-	8/50/70/70	0/1/1/1

The worst 5 of 3162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	Y	608	CHL	C2C-C3C	11.50	1.47	1.36
38	Z	606	CHL	C2C-C3C	11.35	1.47	1.36
38	X	606	CHL	C2C-C3C	11.14	1.47	1.36
38	Y	606	CHL	C2C-C3C	11.12	1.47	1.36
38	Z	609	CHL	C2C-C3C	11.10	1.47	1.36

The worst 5 of 3890 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	W	606	CHL	O2A-CGA-O1A	-17.09	79.39	123.33
30	B	852	BCR	C32-C1-C6	-15.22	86.38	110.24
38	W	606	CHL	O2A-CGA-CBA	14.67	160.37	114.00
30	6	622	BCR	C40-C30-C25	-14.46	87.56	110.24
36	U	1622	XAT	C37-C21-C36	-14.22	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 3213 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
27	A	804	CLA	C1A-C2A-CAA-CBA
27	A	804	CLA	C3A-C2A-CAA-CBA
27	A	804	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

232 monomers are involved in 515 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	812	CLA	1	0
27	A	819	CLA	1	0
35	X	1621	LUT	2	0
27	B	803	CLA	4	0
38	Z	601	CHL	7	0
27	2	603	CLA	2	0
27	B	836	CLA	1	0
36	W	1622	XAT	1	0
30	K	202	BCR	8	0
32	A	857	LMU	1	0
38	W	606	CHL	3	0
37	Z	1623	NEX	4	0
27	A	802	CLA	2	0
27	7	613	CLA	3	0
27	H	203	CLA	1	0
38	W	605	CHL	3	0
27	4	609	CLA	1	0
27	9	613	CLA	1	0
38	U	607	CHL	2	0
36	6	621	XAT	1	0
38	V	609	CHL	4	0
38	Z	608	CHL	1	0
27	B	821	CLA	2	0
27	V	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	U	609	CHL	7	0
38	Y	606	CHL	3	0
27	W	613	CLA	2	0
30	B	852	BCR	5	0
30	7	621	BCR	3	0
27	L	307	CLA	2	0
27	A	808	CLA	2	0
27	7	608	CLA	1	0
27	A	801	CLA	2	0
27	4	613	CLA	1	0
27	3	609	CLA	1	0
36	Y	1622	XAT	1	0
27	2	601	CLA	5	0
33	A	860	LMG	1	0
27	2	610	CLA	1	0
27	B	818	CLA	3	0
35	2	619	LUT	2	0
27	4	616	CLA	1	0
27	Y	611	CLA	3	0
30	A	856	BCR	10	0
27	B	835	CLA	1	0
27	4	608	CLA	1	0
27	A	817	CLA	1	0
37	5	624	NEX	2	0
30	3	621	BCR	9	0
33	L	2631	LMG	1	0
35	U	1620	LUT	2	0
29	9	624	LHG	1	0
27	U	604	CLA	1	0
30	a	619	BCR	2	0
36	7	620	XAT	2	0
30	7	623	BCR	7	0
38	Y	609	CHL	6	0
27	5	607	CLA	1	0
27	6	613	CLA	1	0
27	B	813	CLA	1	0
30	4	621	BCR	3	0
29	9	623	LHG	2	0
27	B	825	CLA	1	0
30	G	205	BCR	2	0
30	3	622	BCR	4	0
38	X	609	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	3	602	CLA	1	0
27	A	820	CLA	3	0
27	W	611	CLA	1	0
30	B	849	BCR	4	0
38	Z	607	CHL	2	0
27	3	612	CLA	1	0
27	A	841	CLA	1	0
27	B	809	CLA	1	0
27	1	611	CLA	1	0
27	A	854	CLA	7	0
38	X	601	CHL	3	0
29	Z	2630	LHG	2	0
38	Y	607	CHL	6	0
35	V	1620	LUT	2	0
27	V	602	CLA	1	0
32	K	208	LMU	1	0
27	W	604	CLA	1	0
38	X	608	CHL	5	0
27	3	608	CLA	1	0
38	Z	606	CHL	3	0
27	8	611	CLA	1	0
29	V	2630	LHG	2	0
27	6	601	CLA	1	0
30	O	2005	BCR	8	0
27	B	833	CLA	2	0
30	F	305	BCR	8	0
38	U	608	CHL	1	0
38	Z	605	CHL	1	0
30	L	301	BCR	7	0
37	Y	1623	NEX	2	0
33	5	627	LMG	1	0
33	V	2631	LMG	3	0
27	2	613	CLA	1	0
37	6	624	NEX	1	0
27	V	610	CLA	1	0
30	2	623	BCR	9	0
36	1	618	XAT	1	0
27	Z	613	CLA	2	0
35	Y	1620	LUT	3	0
38	V	601	CHL	5	0
27	A	803	CLA	5	0
35	9	619	LUT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	839	CLA	1	0
30	6	622	BCR	3	0
27	A	811	CLA	1	0
27	B	808	CLA	6	0
30	B	848	BCR	8	0
27	5	603	CLA	1	0
30	B	846	BCR	4	0
27	B	834	CLA	1	0
27	A	843	CLA	1	0
27	V	613	CLA	1	0
38	U	605	CHL	3	0
29	B	851	LHG	1	0
30	J	102	BCR	10	0
38	U	601	CHL	3	0
36	Z	1622	XAT	1	0
35	3	618	LUT	3	0
27	B	830	CLA	1	0
38	V	608	CHL	12	0
27	B	802	CLA	2	0
36	3	619	XAT	1	0
29	7	622	LHG	1	0
38	W	601	CHL	3	0
35	8	619	LUT	3	0
27	U	613	CLA	2	0
27	K	204	CLA	1	0
27	B	840	CLA	3	0
27	6	618	CLA	1	0
35	a	617	LUT	4	0
27	A	825	CLA	1	0
38	X	607	CHL	4	0
27	8	606	CLA	1	0
27	a	611	CLA	1	0
30	B	843	BCR	7	0
38	W	607	CHL	7	0
35	6	619	LUT	3	0
38	U	606	CHL	2	0
30	A	852	BCR	11	0
35	7	619	LUT	2	0
27	3	606	CLA	2	0
27	A	809	CLA	2	0
34	B	850	DGD	3	0
30	A	850	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	6	616	CLA	1	0
38	X	605	CHL	1	0
27	B	832	CLA	2	0
27	W	610	CLA	1	0
29	5	625	LHG	1	0
27	B	837	CLA	1	0
35	Z	1621	LUT	1	0
38	W	609	CHL	4	0
30	B	801	BCR	9	0
27	A	829	CLA	4	0
27	8	613	CLA	2	0
30	B	847	BCR	5	0
27	4	610	CLA	2	0
36	U	1622	XAT	3	0
30	B	844	BCR	4	0
35	X	1620	LUT	3	0
37	W	1623	NEX	2	0
27	5	617	CLA	1	0
38	X	606	CHL	1	0
27	X	613	CLA	2	0
30	B	845	BCR	3	0
27	9	614	CLA	1	0
35	4	619	LUT	4	0
27	B	827	CLA	1	0
30	L	309	BCR	7	0
27	3	617	CLA	3	0
37	V	1623	NEX	1	0
27	4	614	CLA	1	0
30	L	305	BCR	6	0
38	W	608	CHL	1	0
38	Y	601	CHL	3	0
30	8	621	BCR	3	0
30	A	849	BCR	4	0
27	B	804	CLA	1	0
27	6	606	CLA	1	0
30	9	621	BCR	5	0
27	B	828	CLA	1	0
27	F	303	CLA	1	0
27	8	604	CLA	1	0
36	a	618	XAT	1	0
27	Y	613	CLA	2	0
38	V	605	CHL	4	0

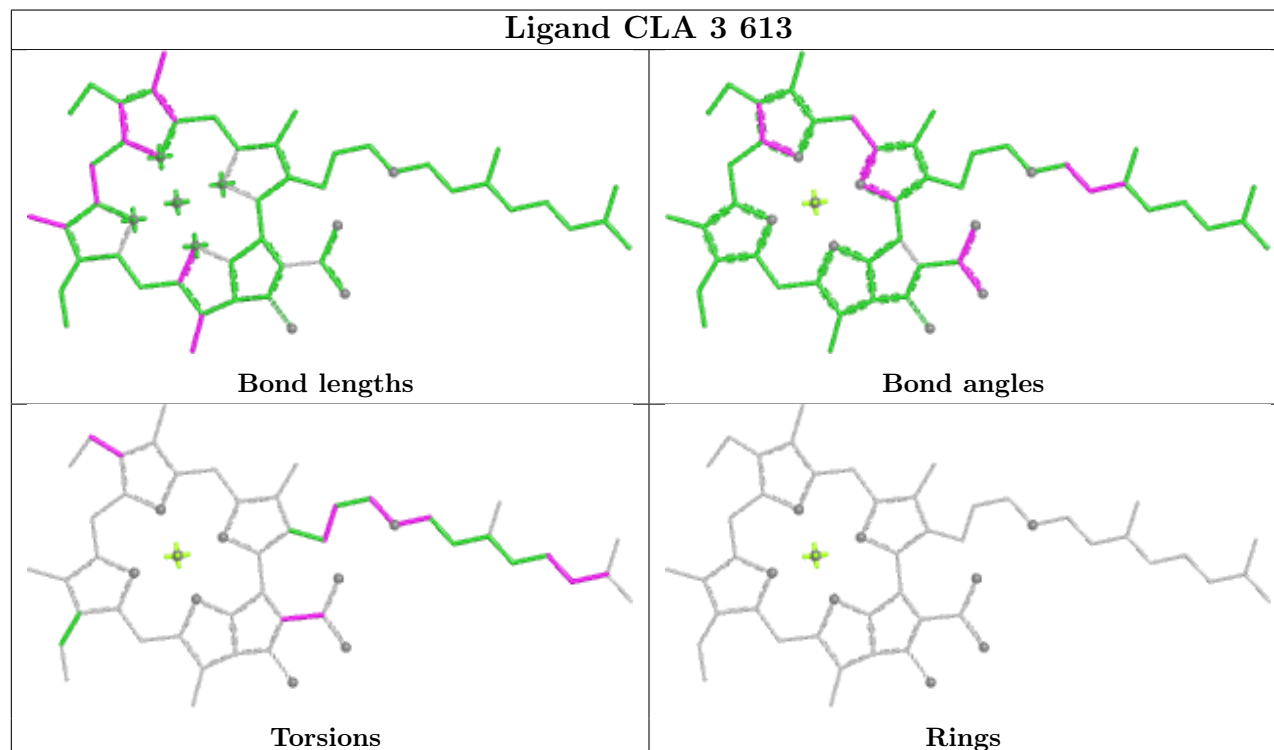
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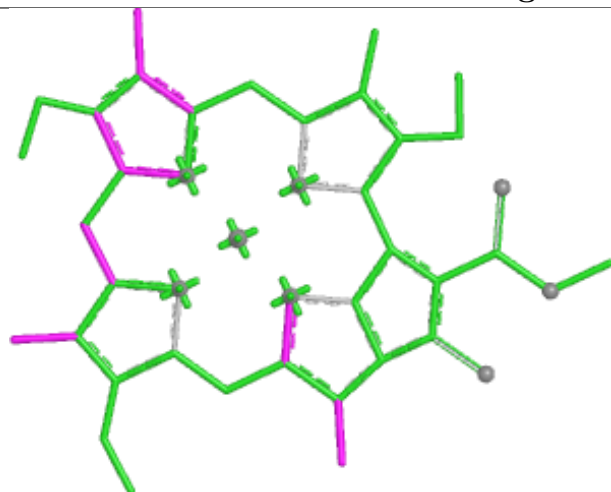
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	L	303	CLA	2	0
38	Y	605	CHL	1	0
27	9	610	CLA	3	0
27	A	834	CLA	3	0
35	Z	1620	LUT	3	0
27	B	819	CLA	2	0
27	a	603	CLA	1	0
27	A	818	CLA	1	0
35	1	617	LUT	3	0
30	1	619	BCR	2	0
30	3	620	BCR	2	0
38	V	606	CHL	3	0
36	5	621	XAT	3	0
27	Y	610	CLA	1	0
27	B	826	CLA	2	0
30	5	622	BCR	3	0
28	B	842	PQN	2	0
27	5	602	CLA	1	0
30	A	851	BCR	4	0
27	B	817	CLA	1	0
27	7	601	CLA	1	0
29	3	623	LHG	1	0
27	6	611	CLA	1	0
35	W	1620	LUT	2	0
30	A	848	BCR	4	0
27	5	619	CLA	5	0
27	X	611	CLA	3	0
38	Y	608	CHL	2	0
30	O	2004	BCR	3	0
27	K	201	CLA	6	0
27	3	603	CLA	1	0
30	B	853	BCR	2	0
27	9	609	CLA	1	0
30	K	207	BCR	9	0
27	U	611	CLA	1	0
27	A	816	CLA	4	0
37	X	1623	NEX	2	0
38	Z	609	CHL	5	0
38	V	607	CHL	5	0
27	4	601	CLA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

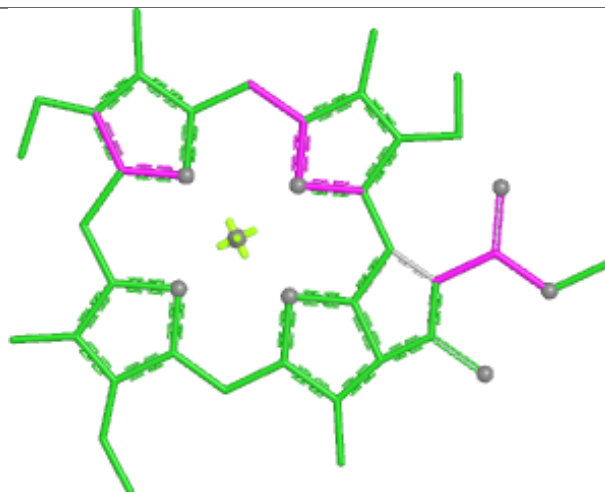
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



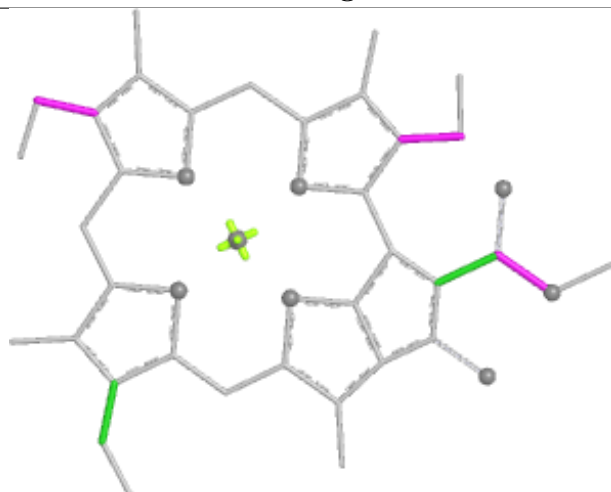
Ligand CLA J 101



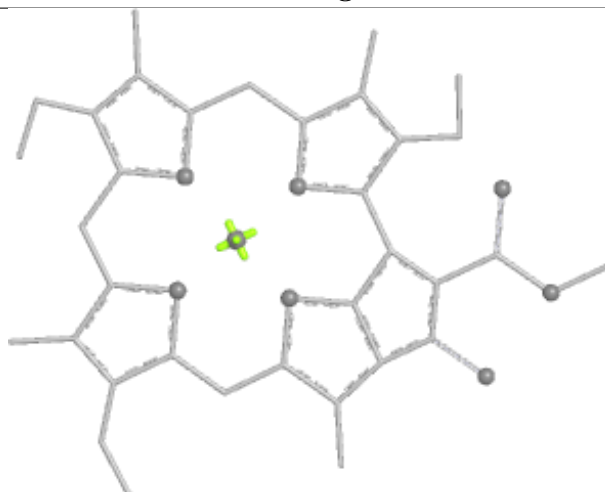
Bond lengths



Bond angles

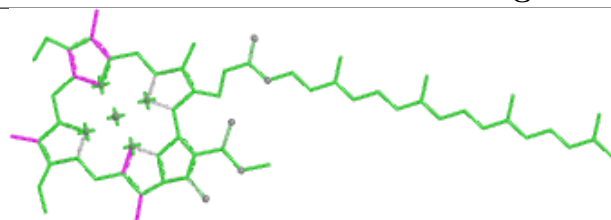


Torsions

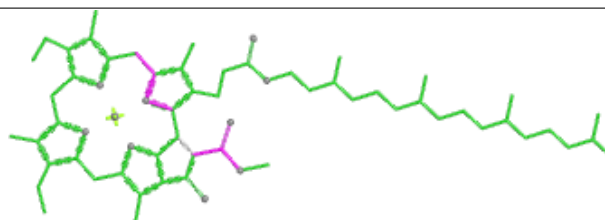


Rings

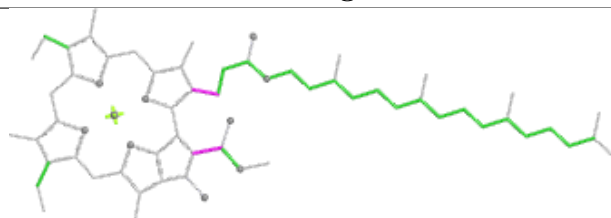
Ligand CLA A 812



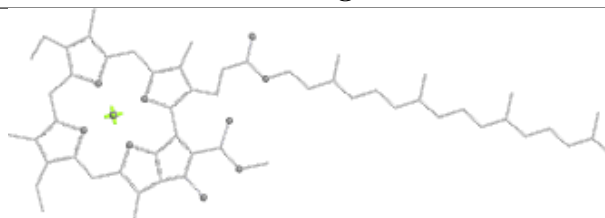
Bond lengths



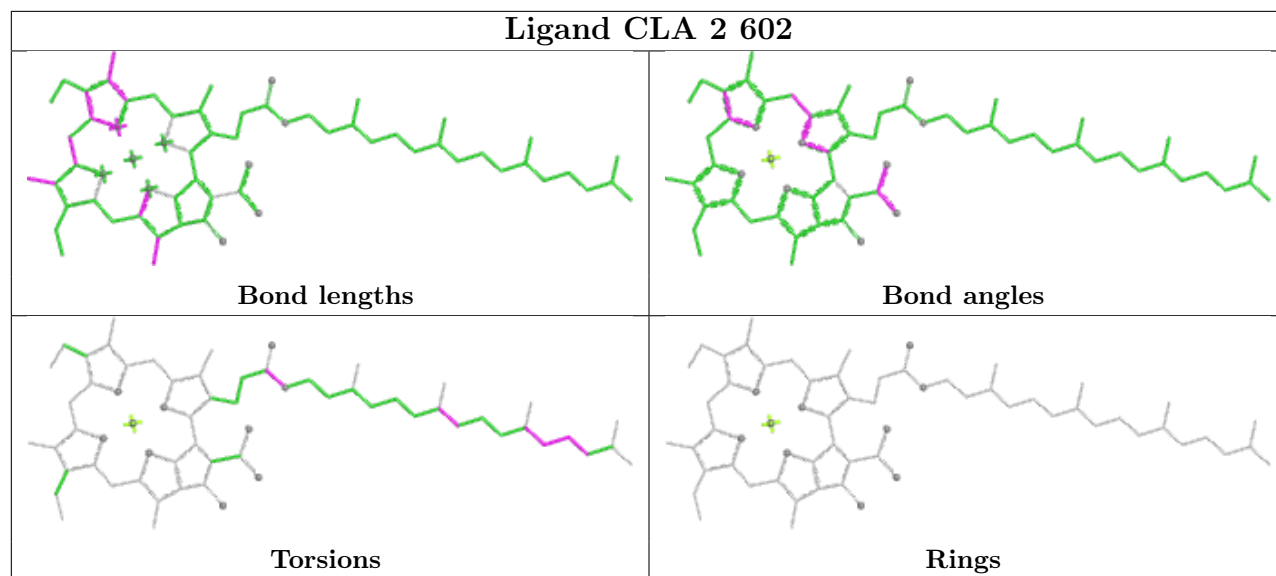
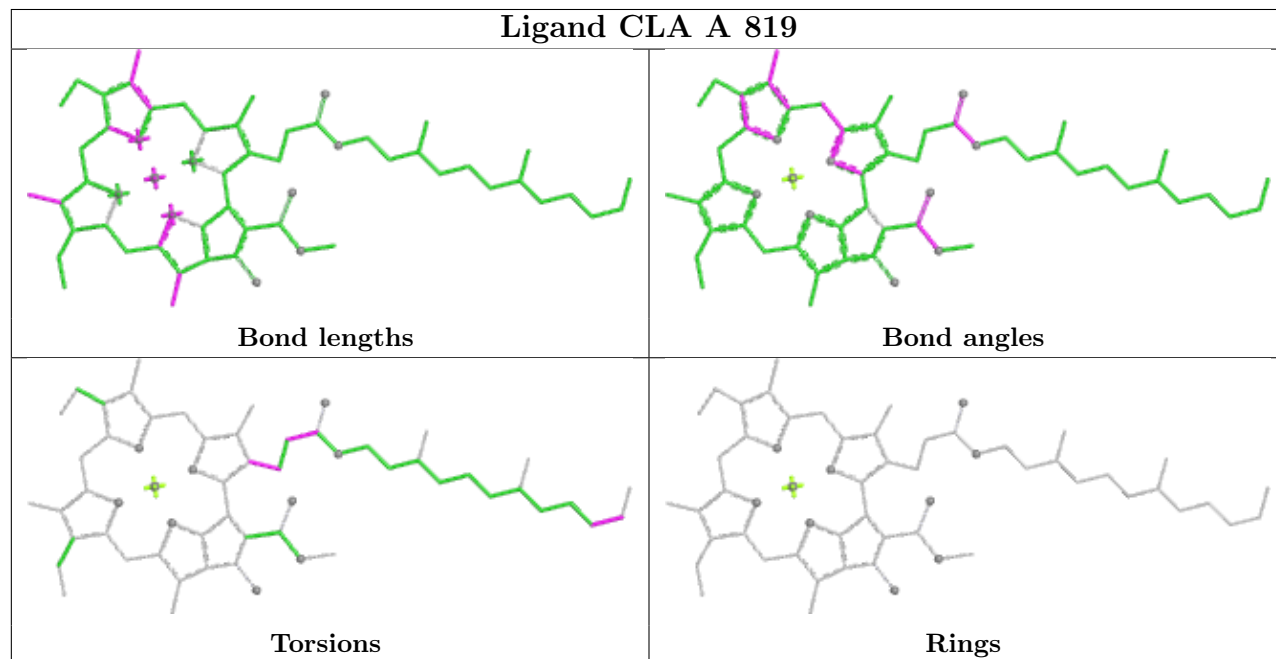
Bond angles

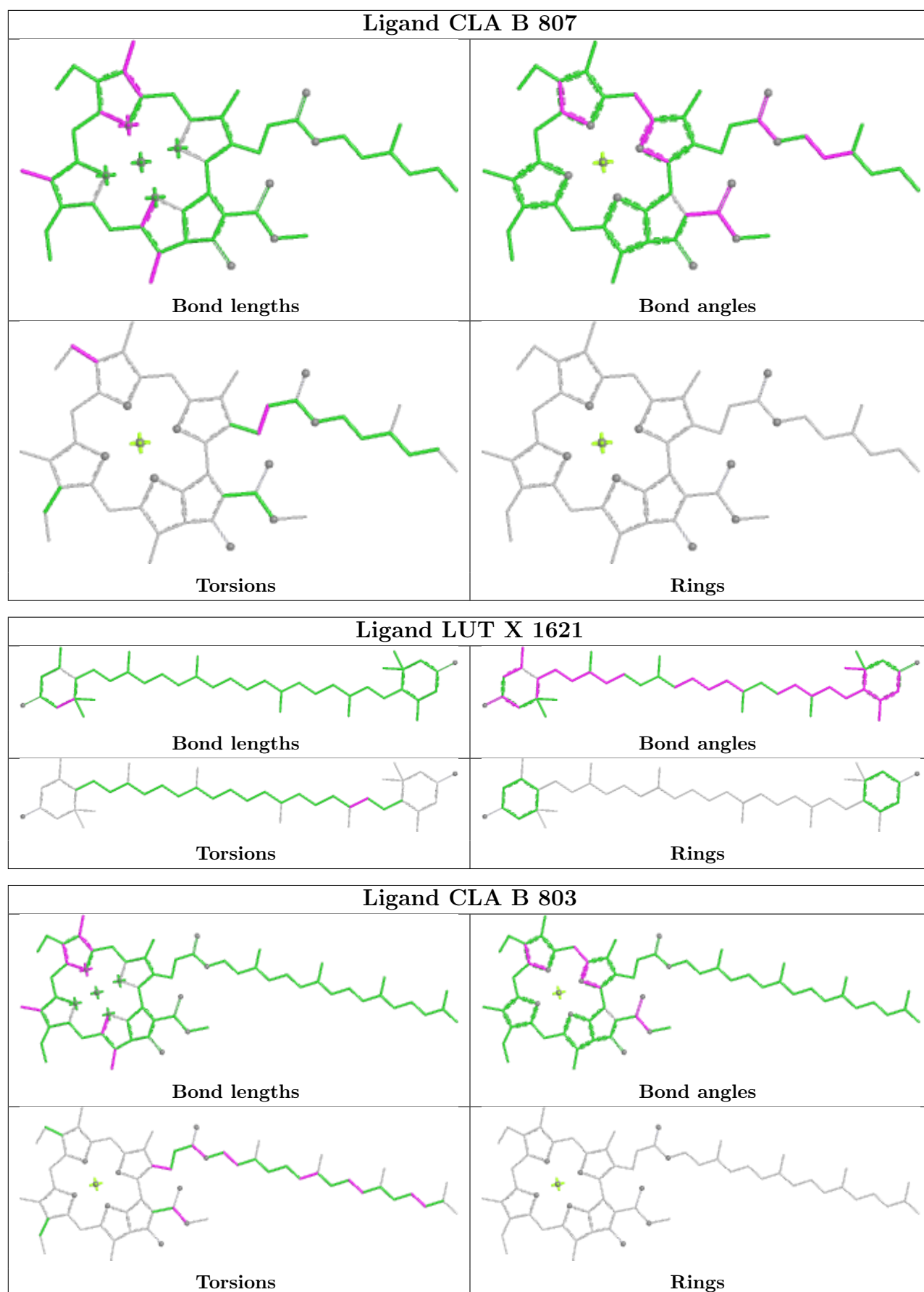


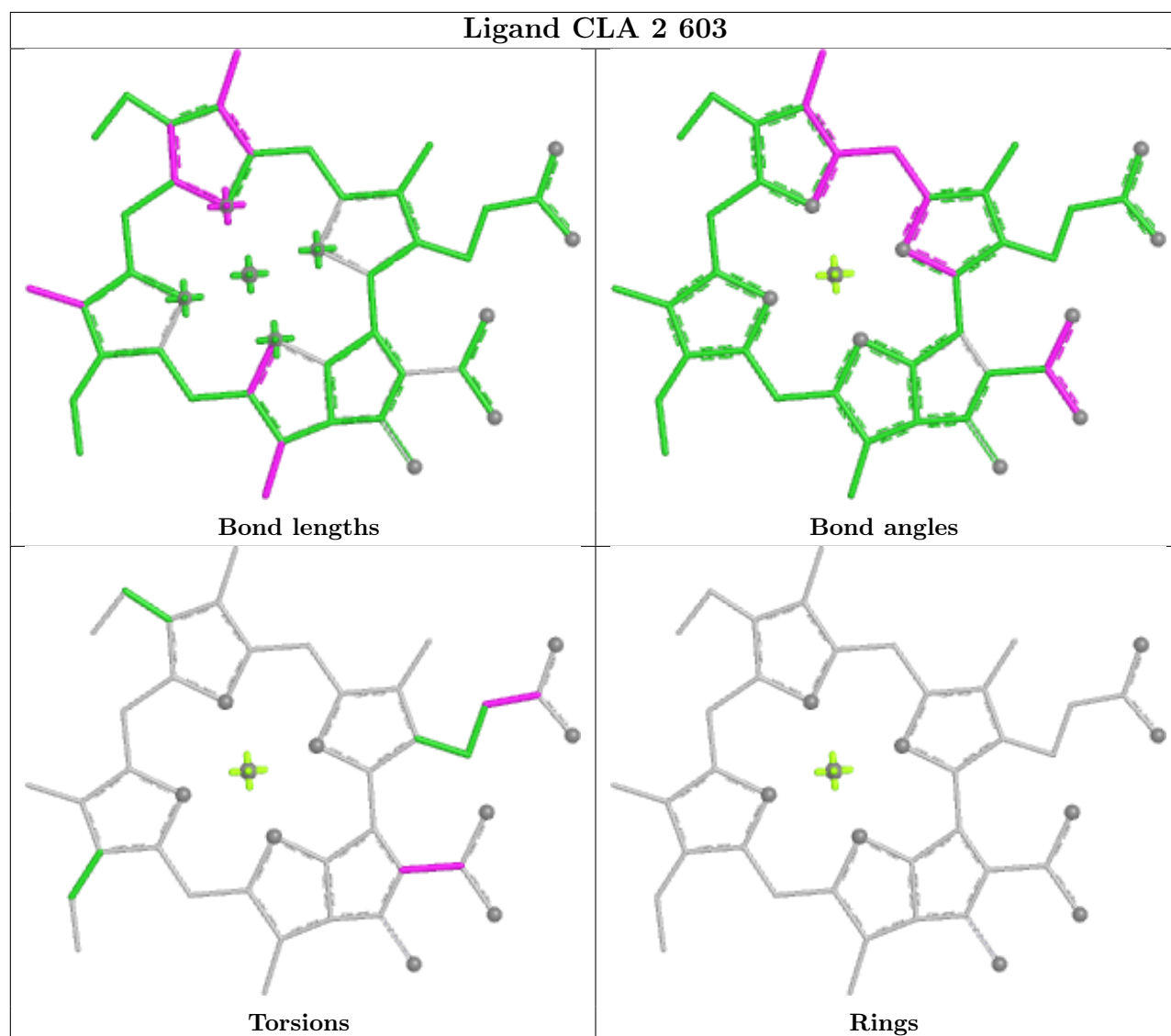
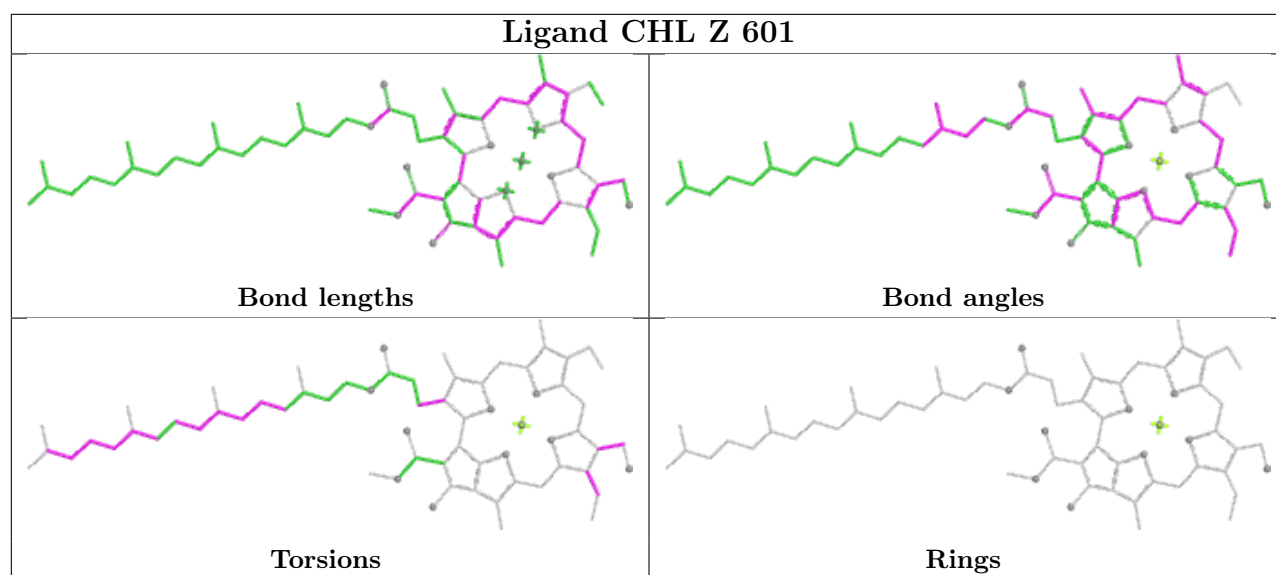
Torsions

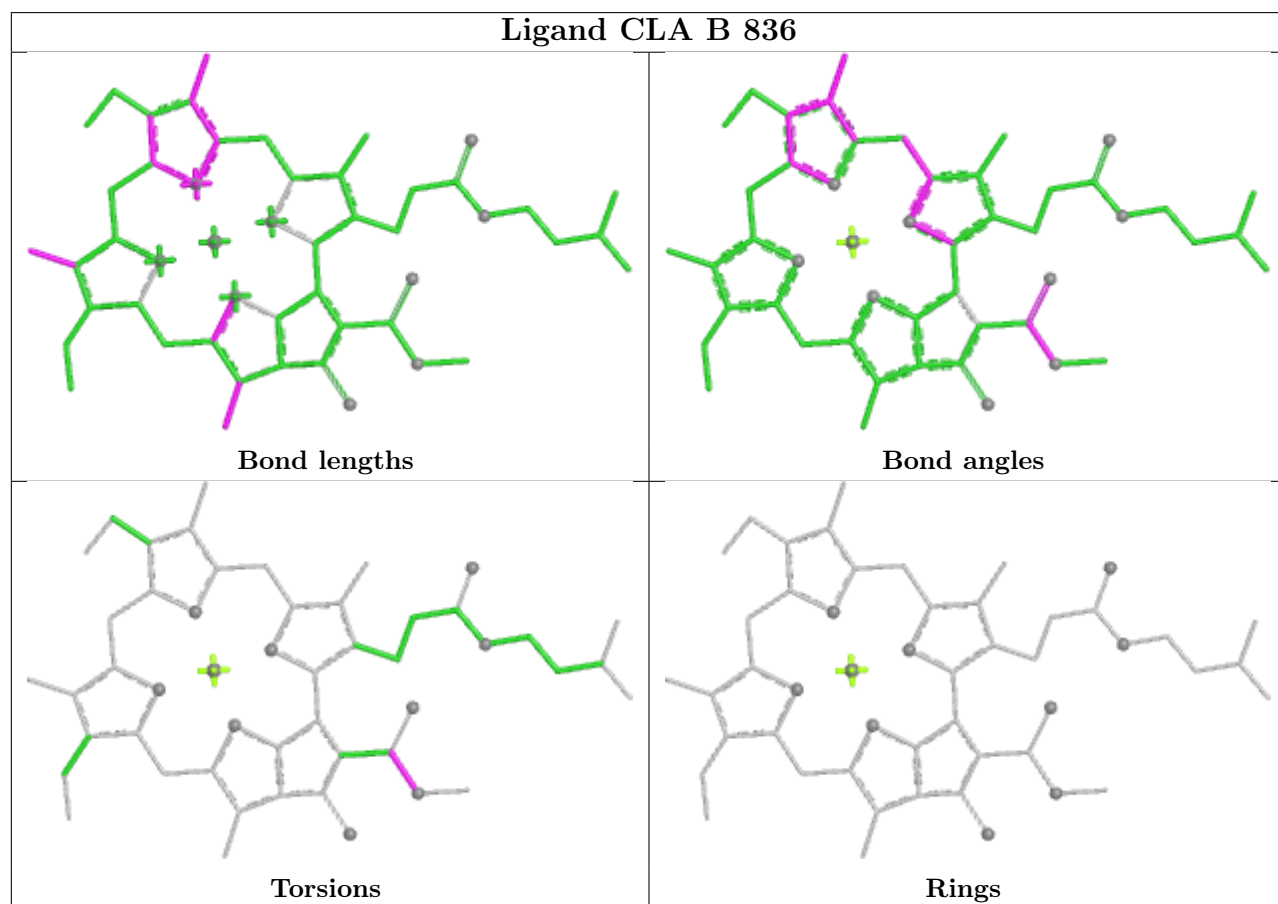
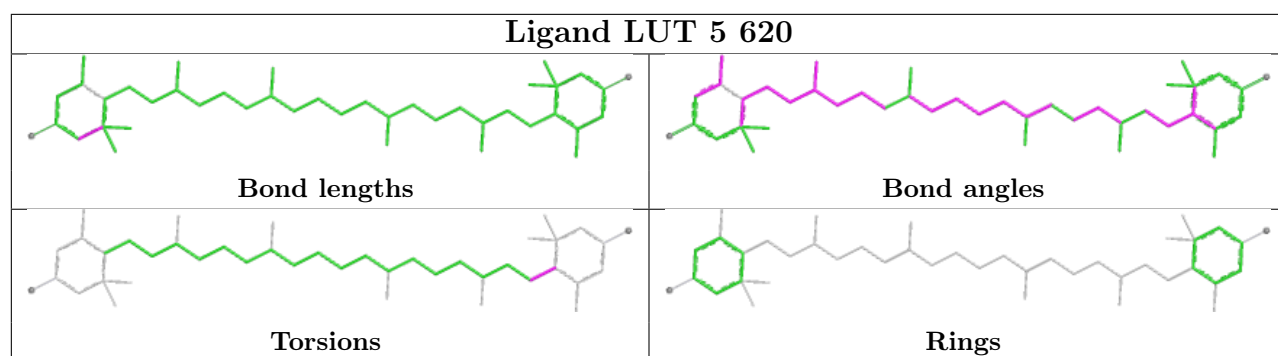


Rings

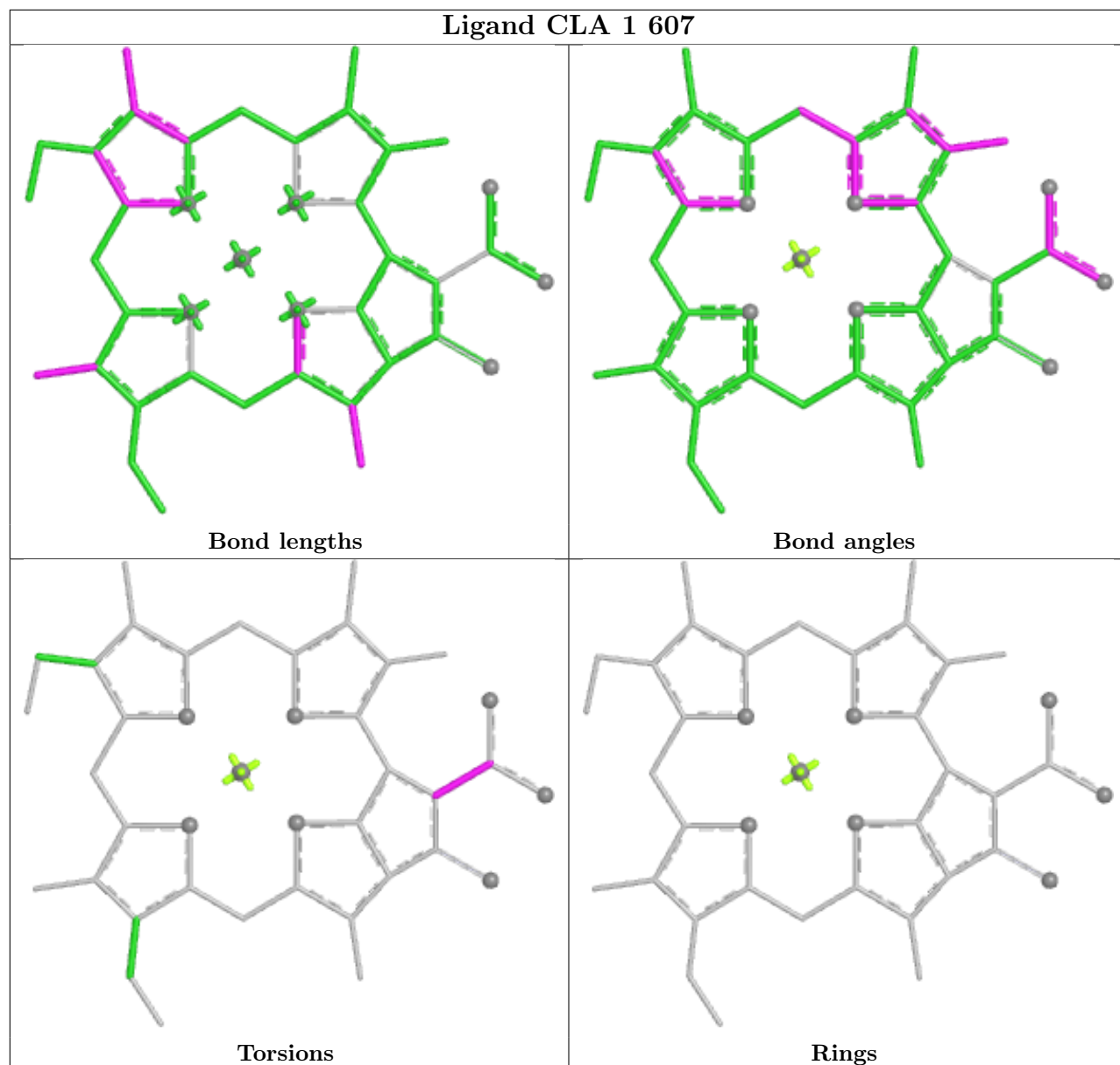
Ligand CLA 2 602**Ligand CLA A 819**



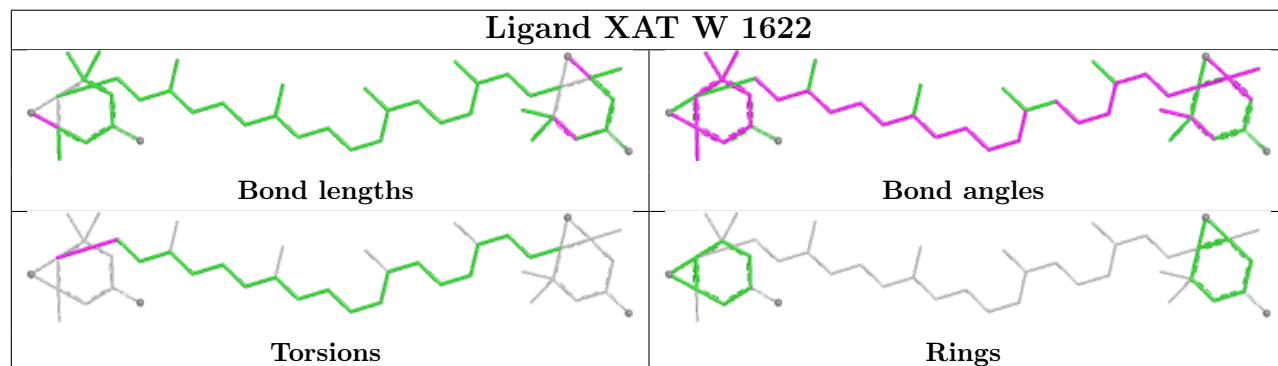




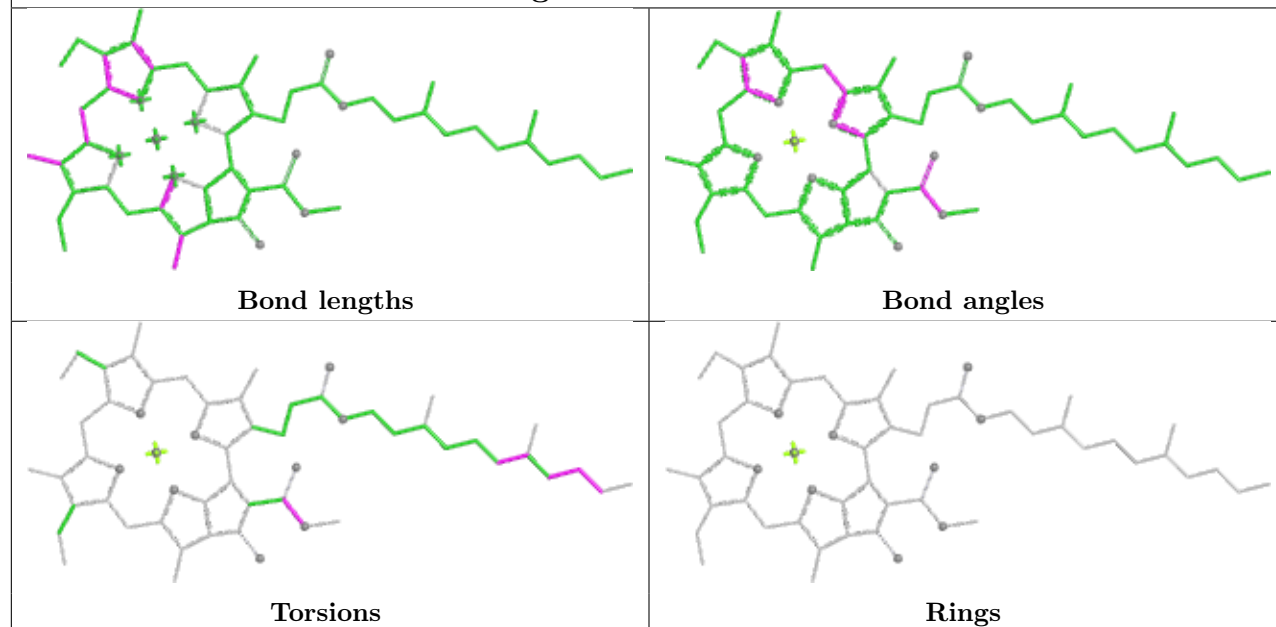
Ligand CLA 1 607



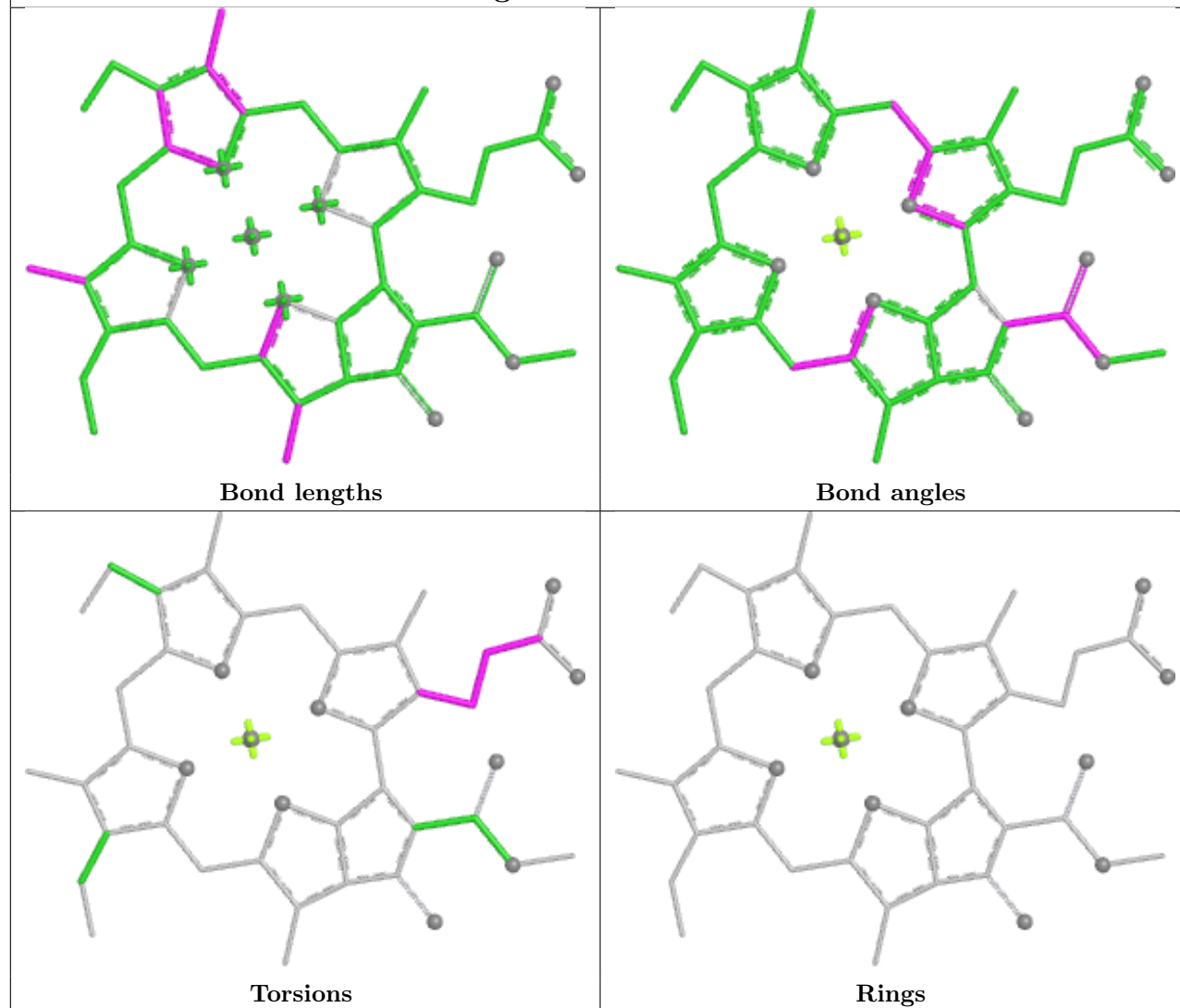
Ligand XAT W 1622



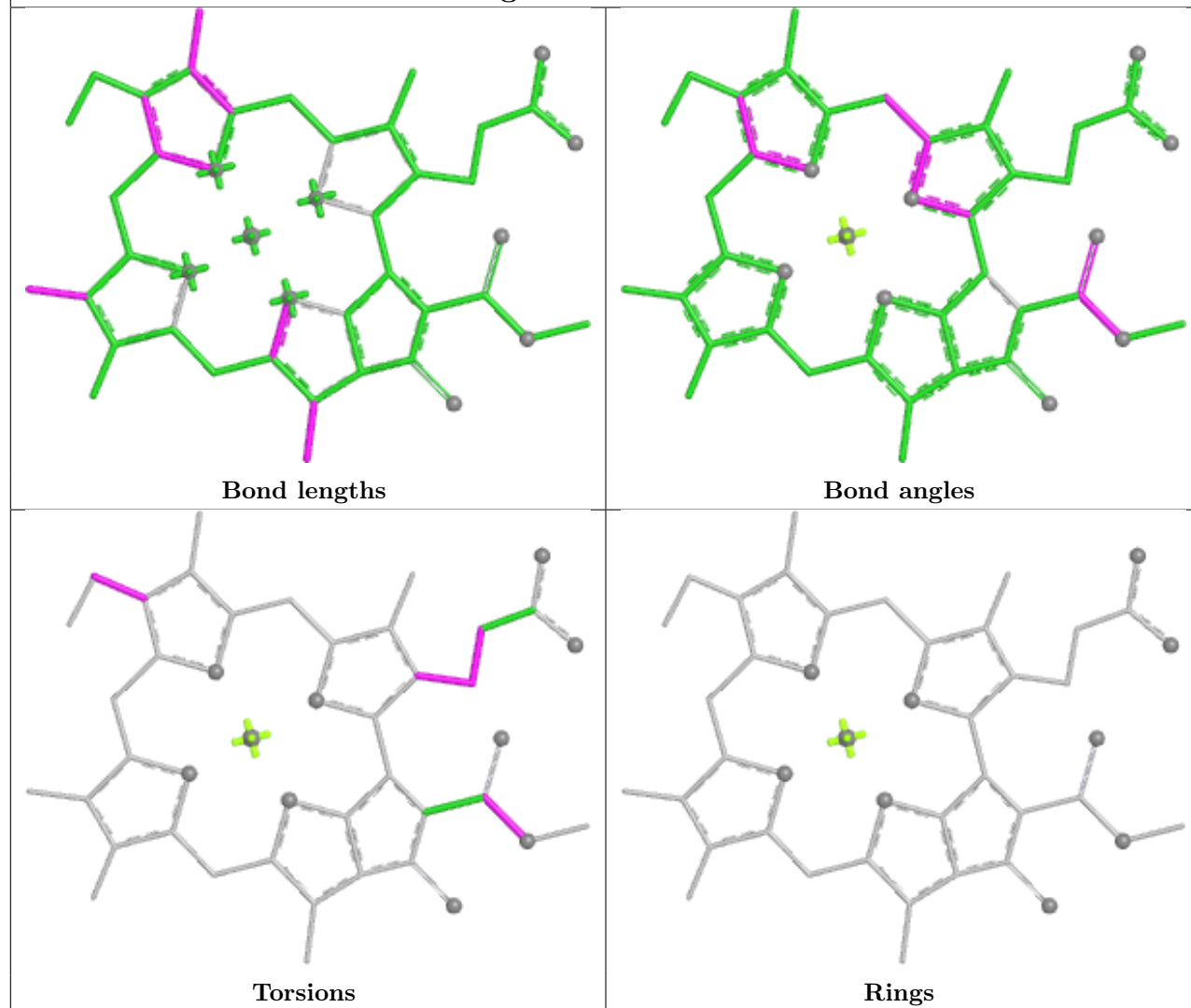
Ligand CLA Y 602



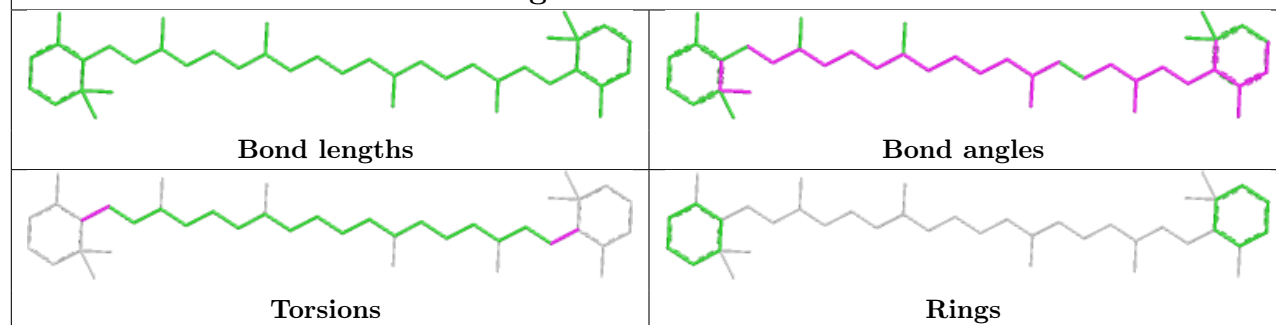
Ligand CLA L 302

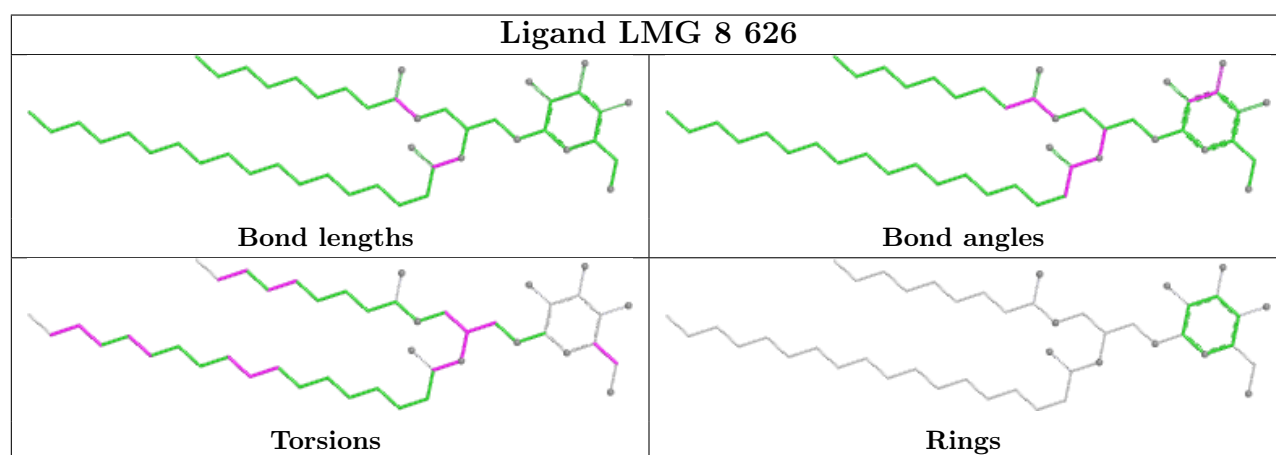
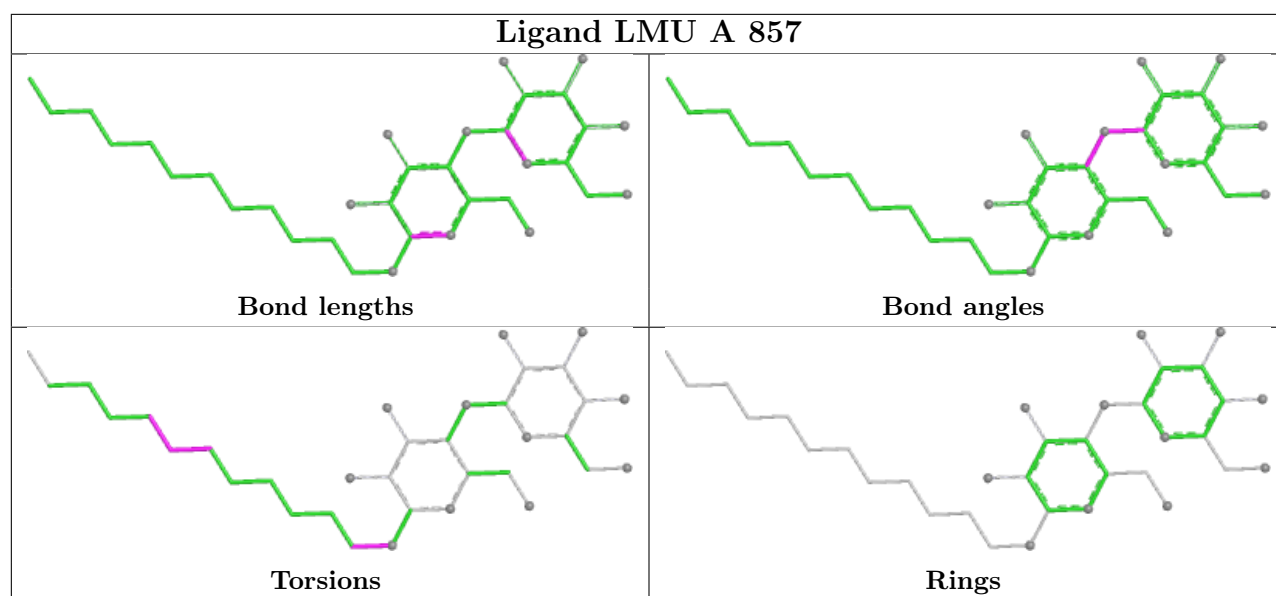


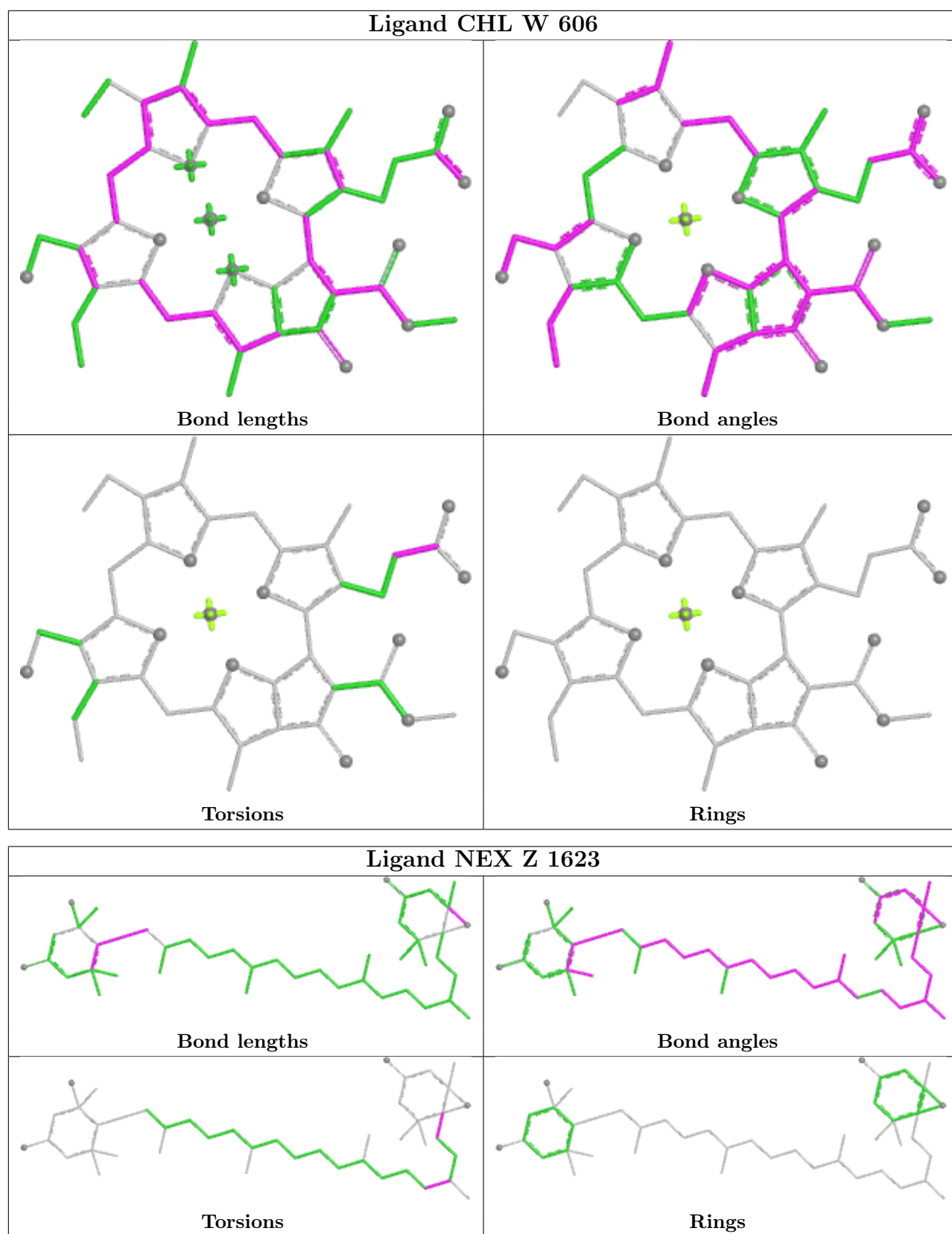
Ligand CLA 2 612

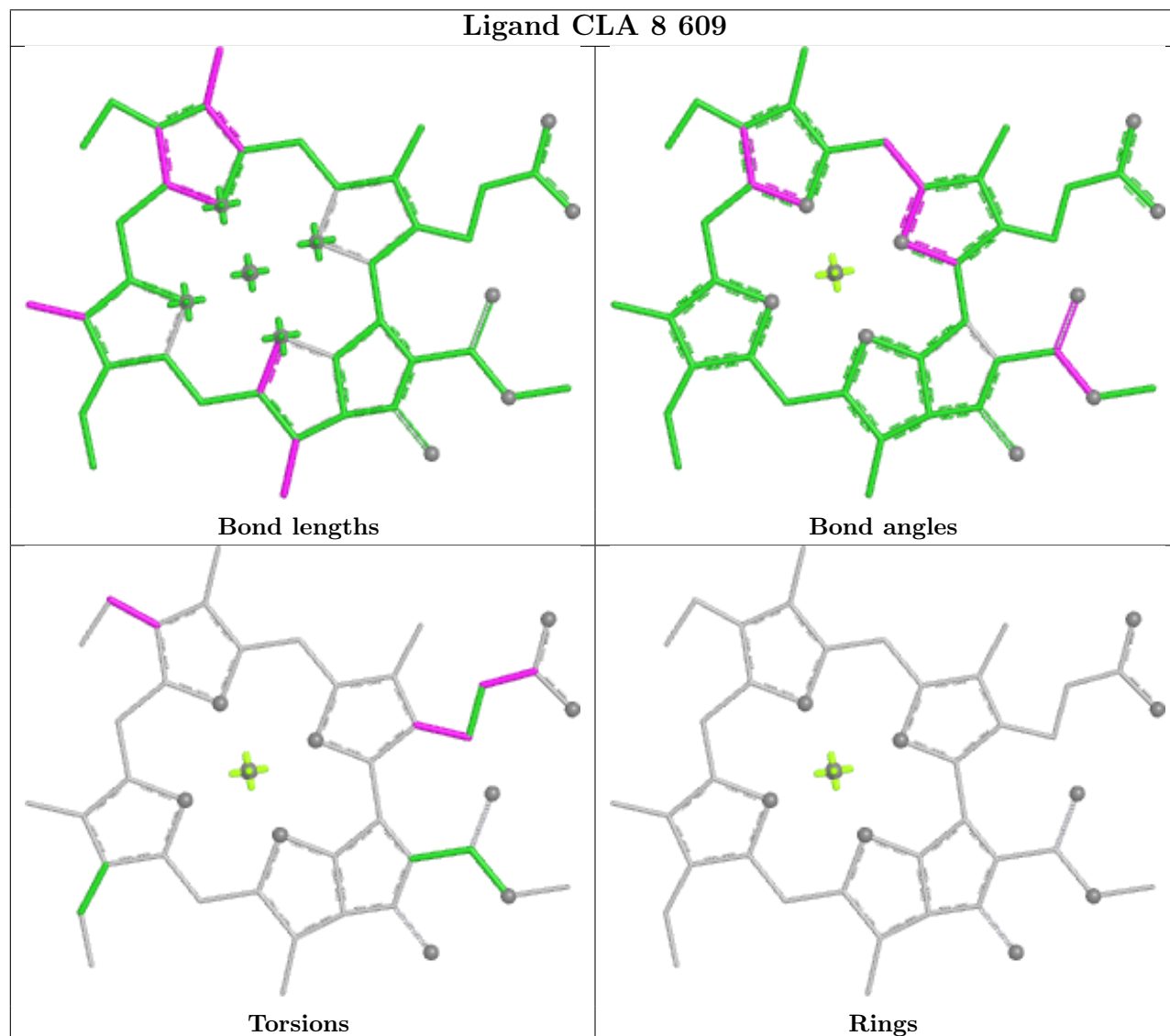
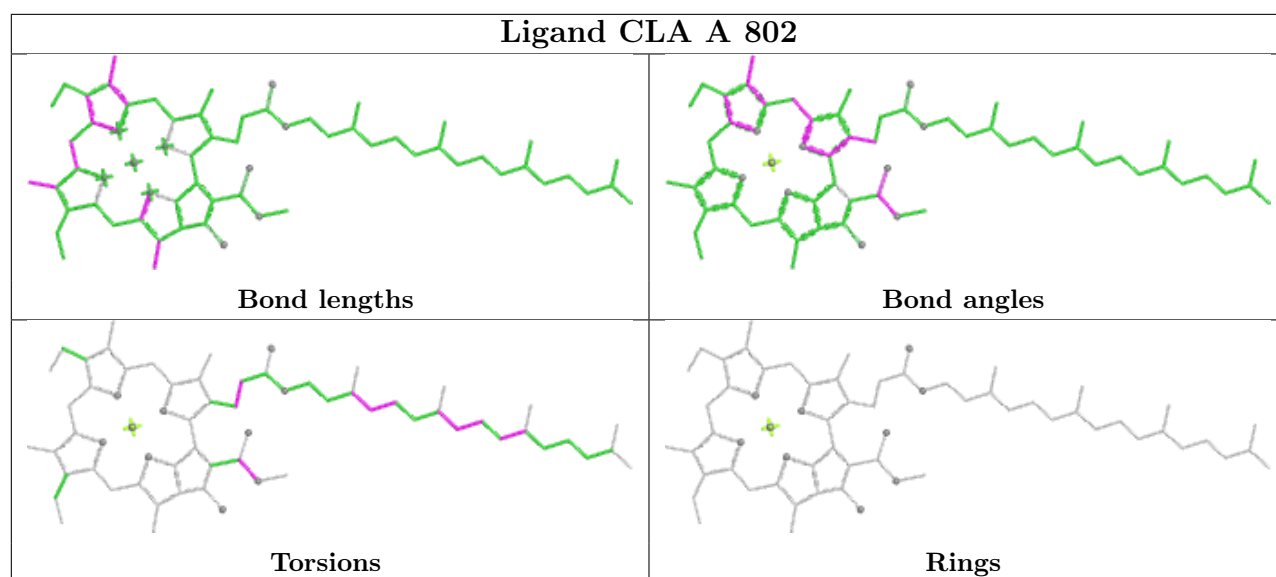


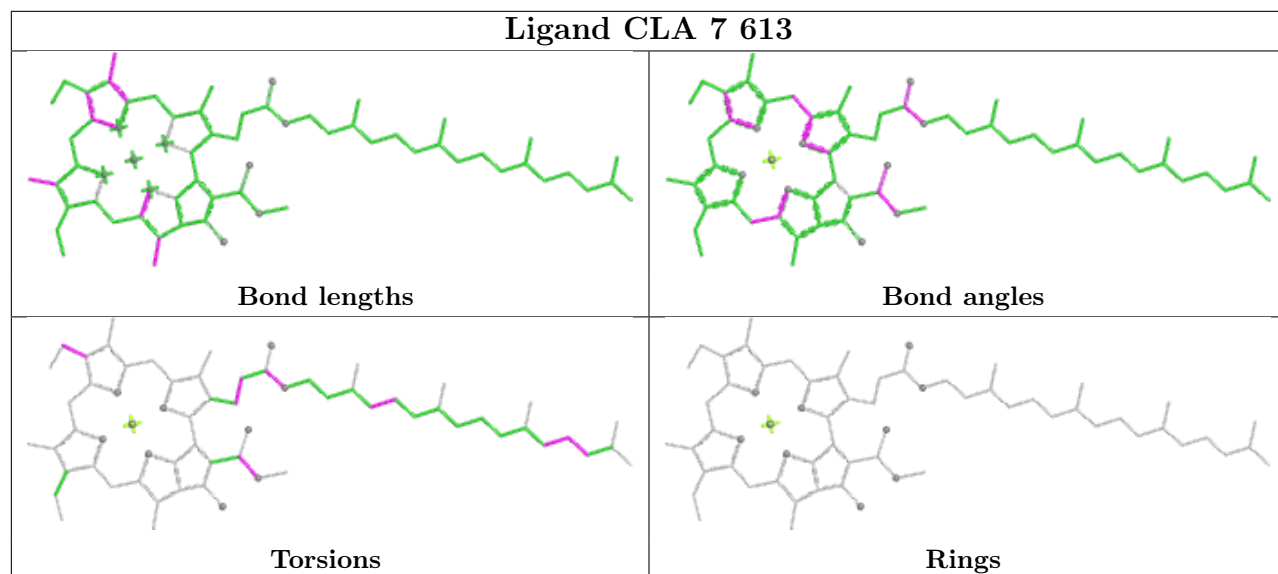
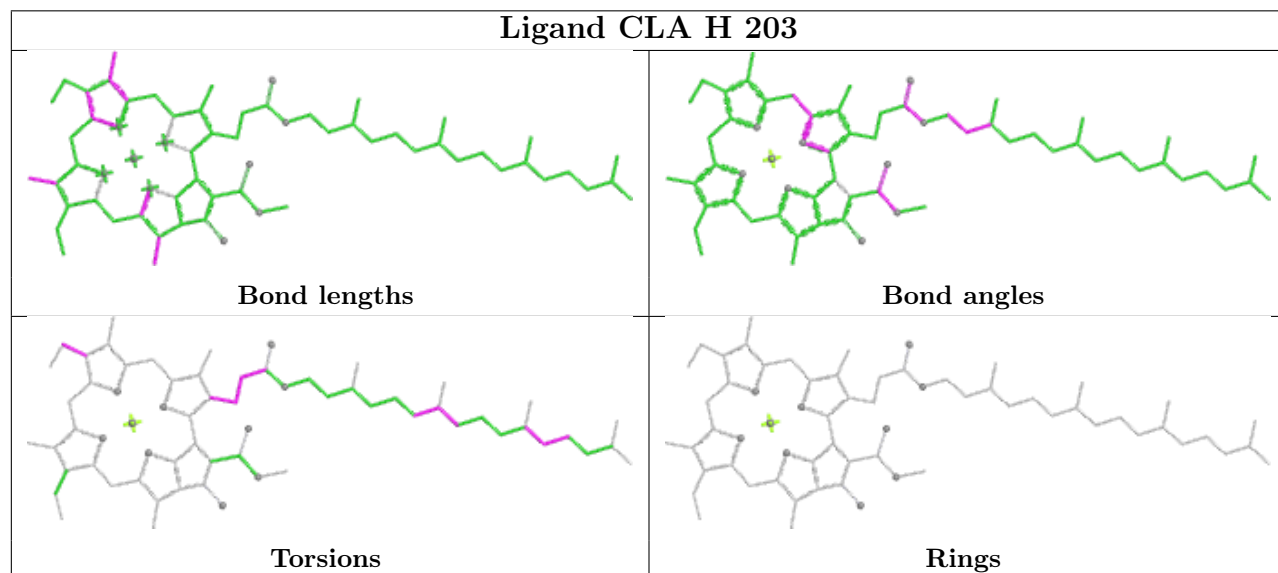
Ligand BCR K 202



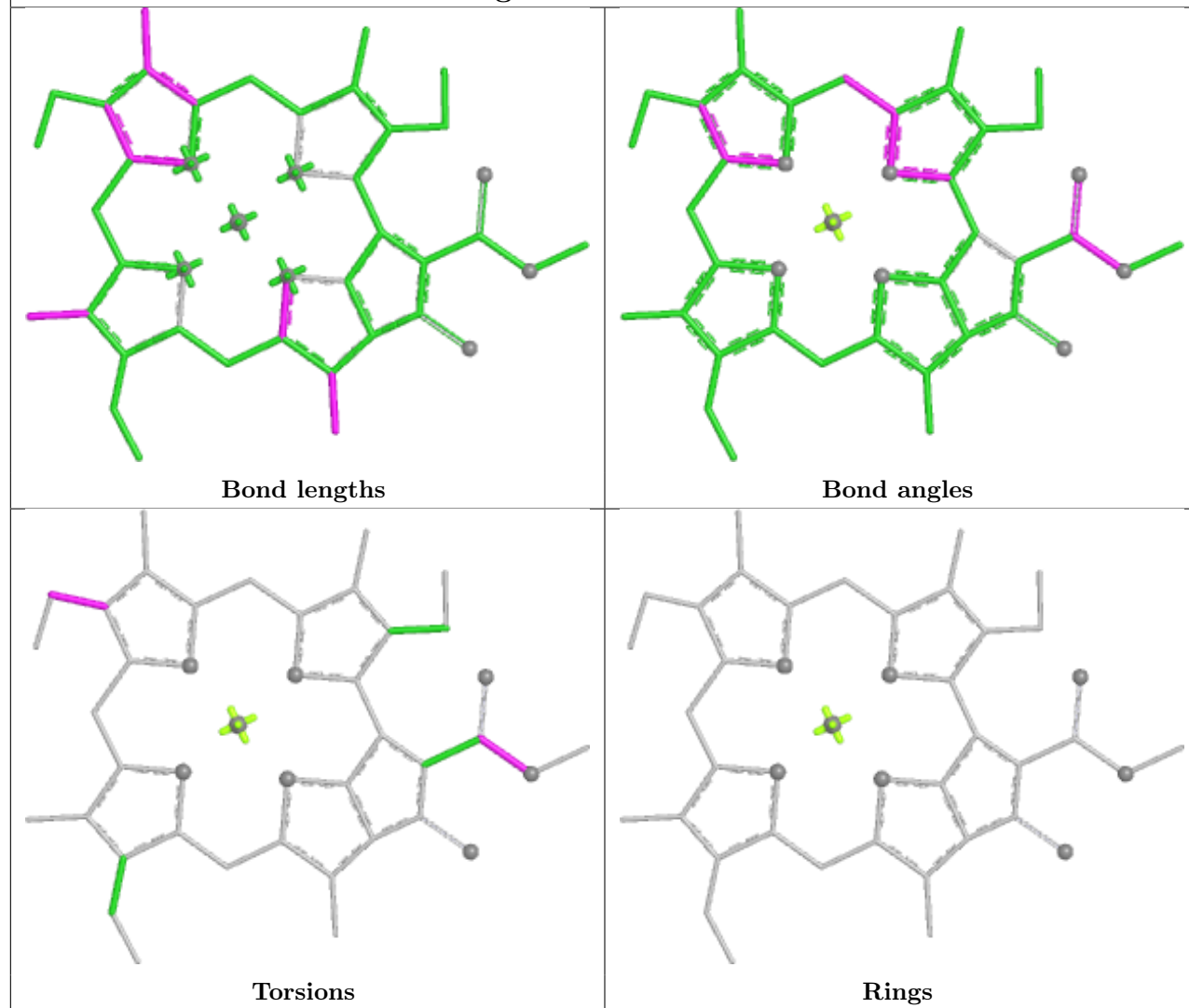




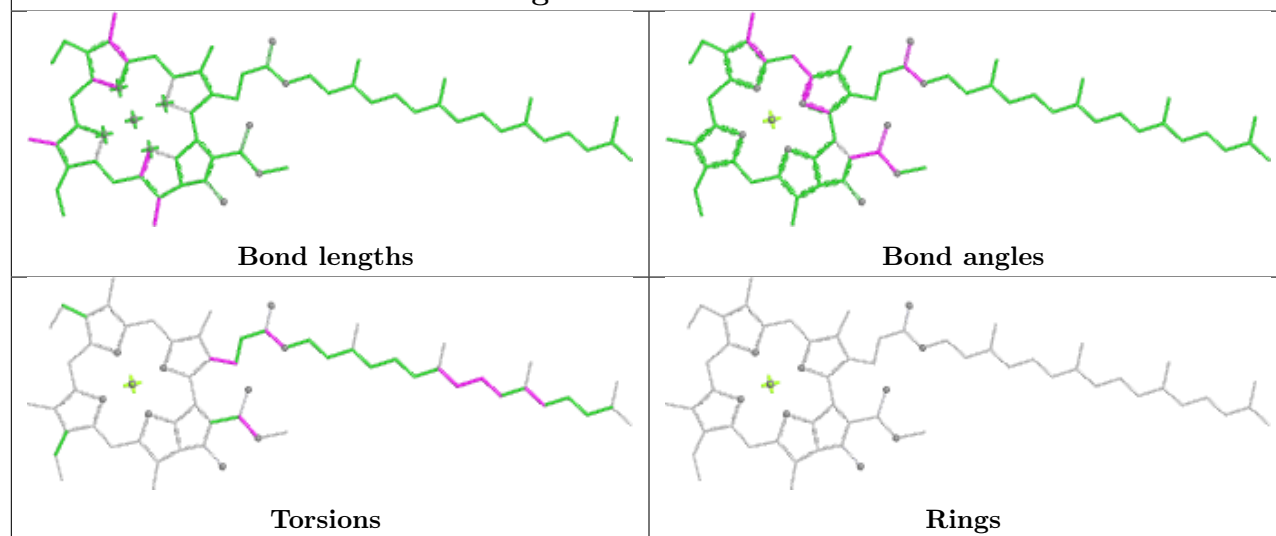


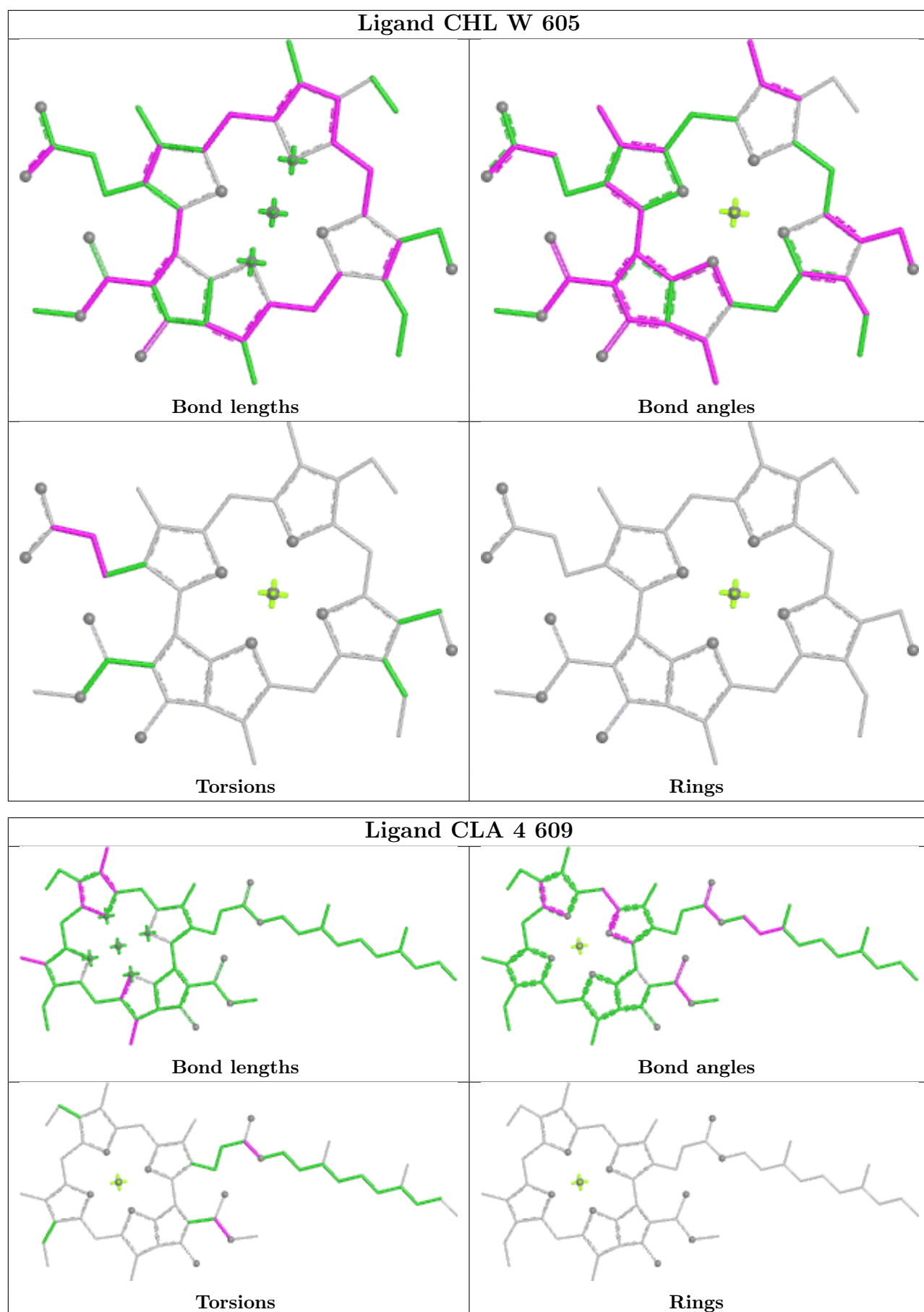
Ligand CLA 7 613**Ligand CLA H 203**

Ligand CLA A 823

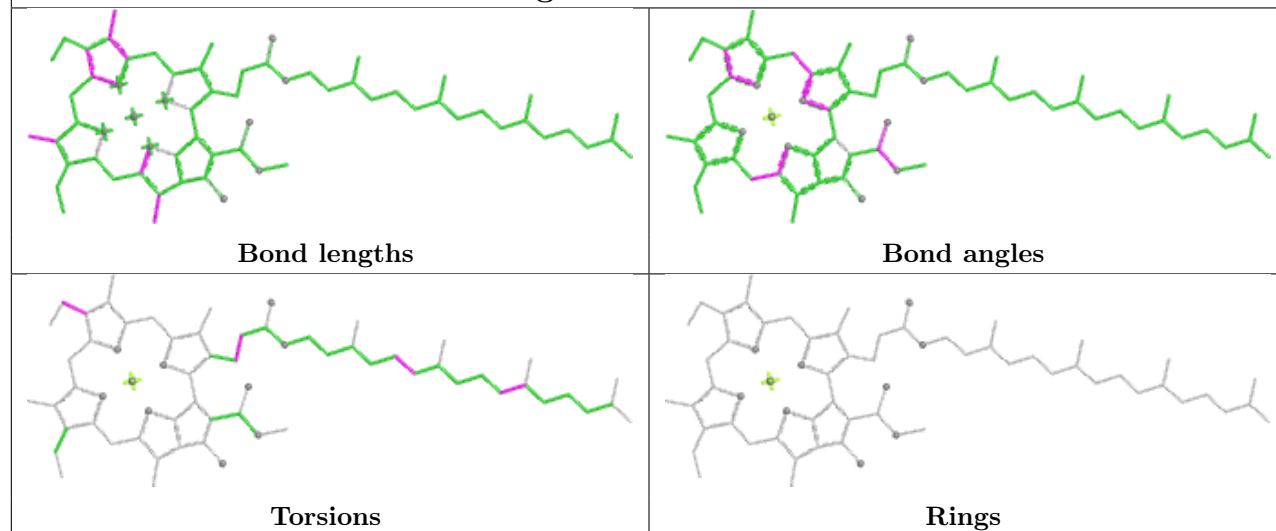


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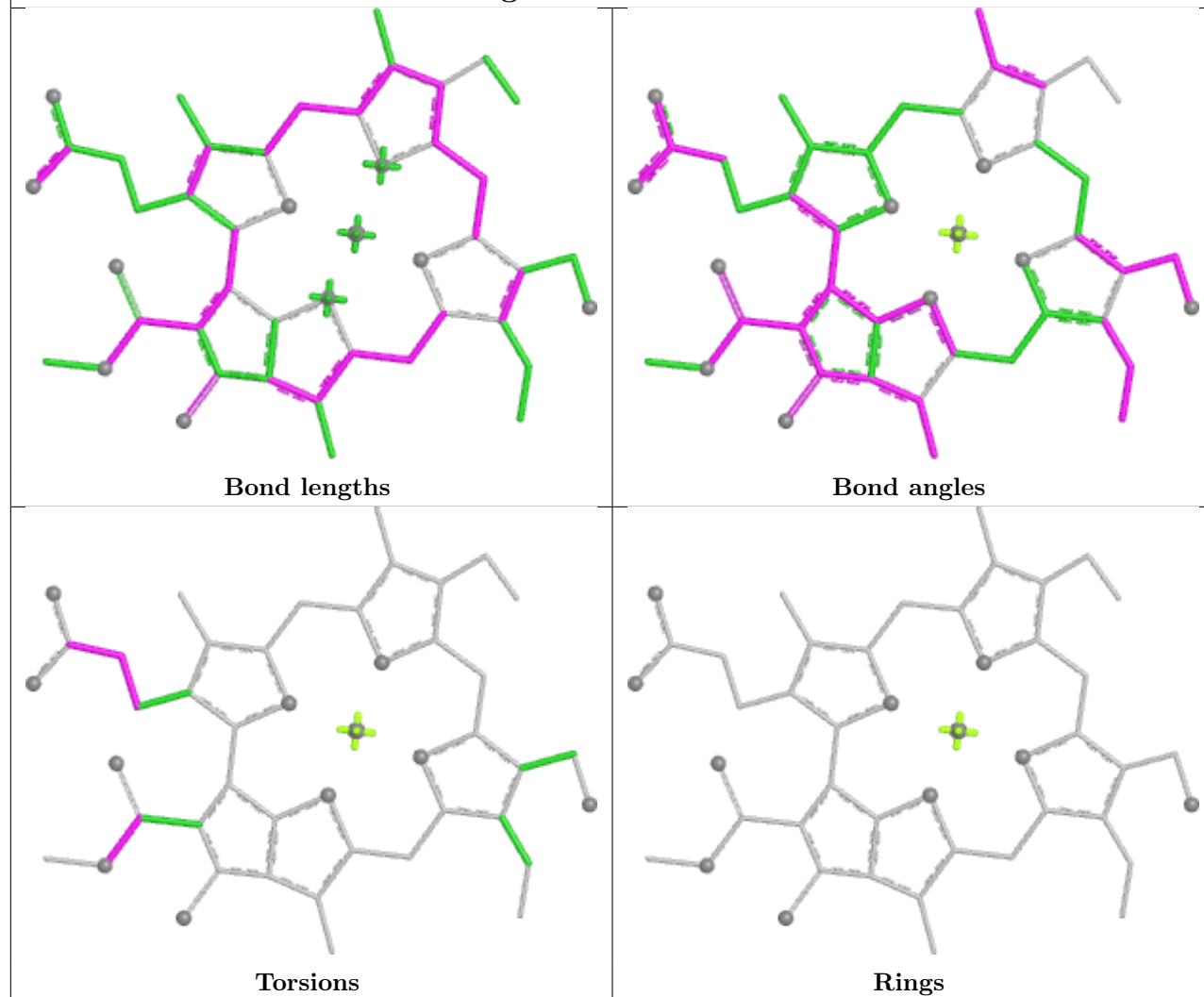


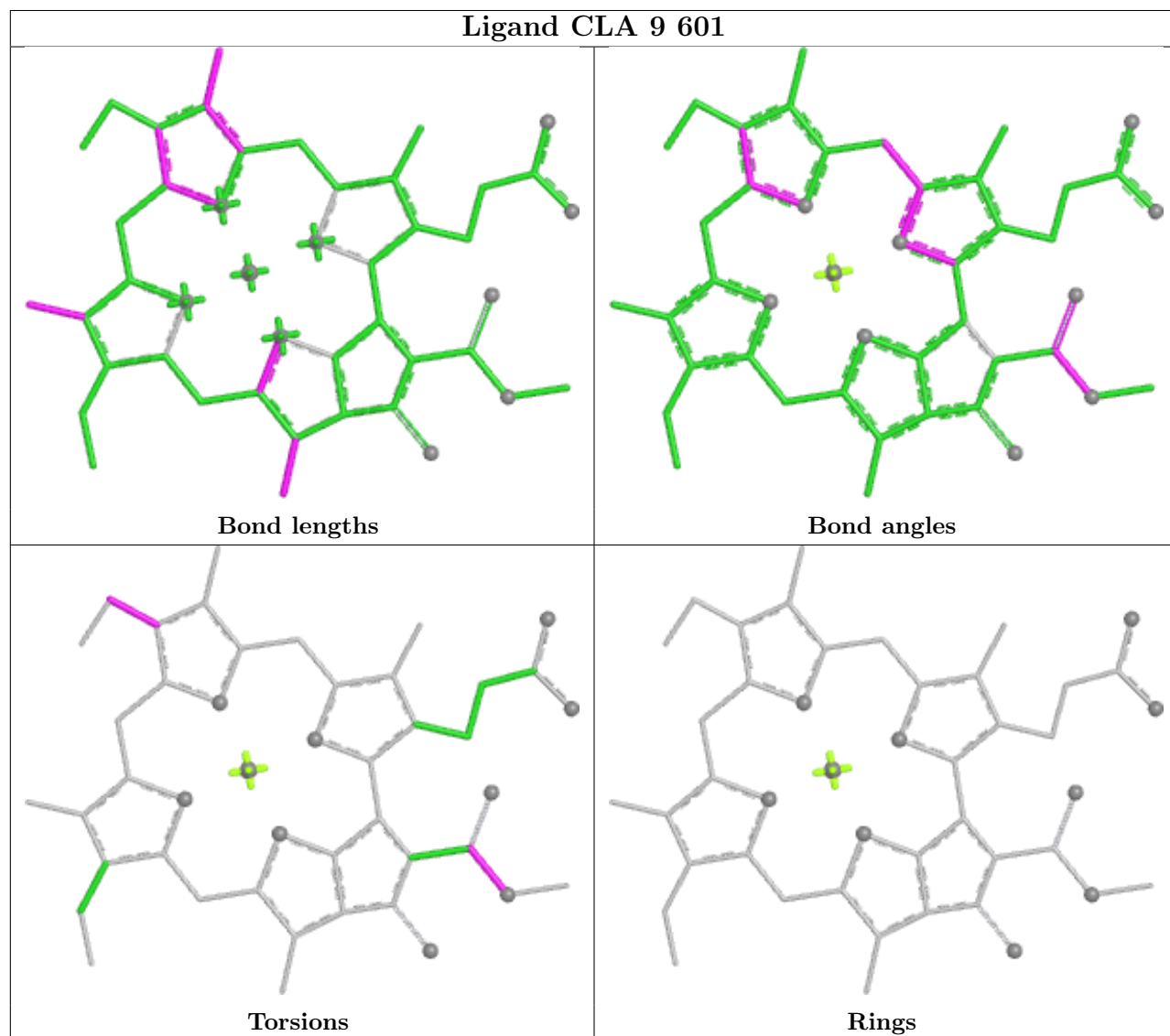
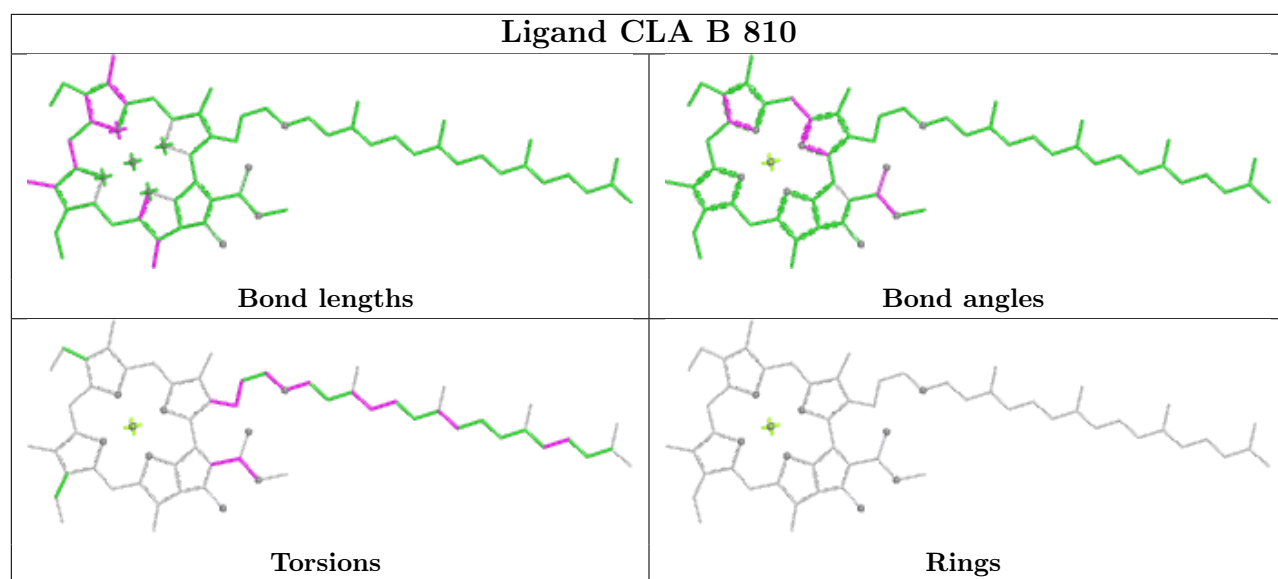


Ligand CLA 9 613

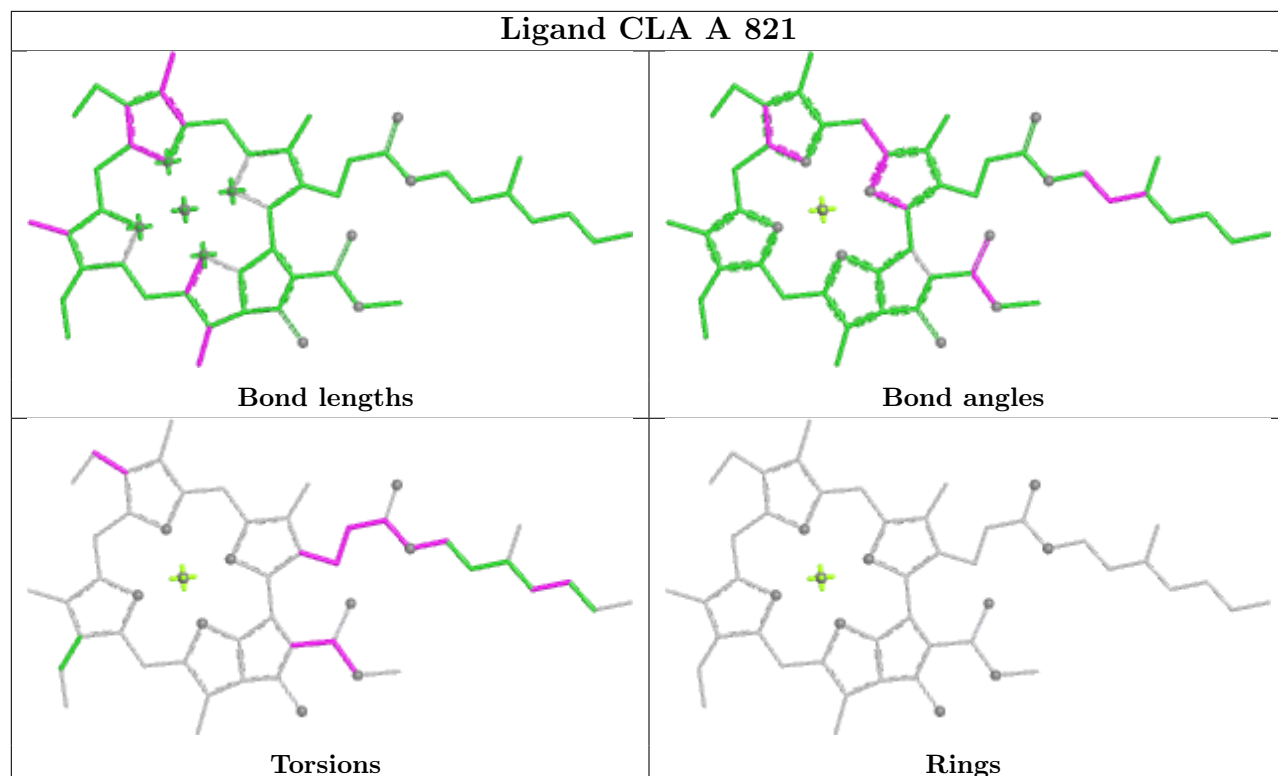


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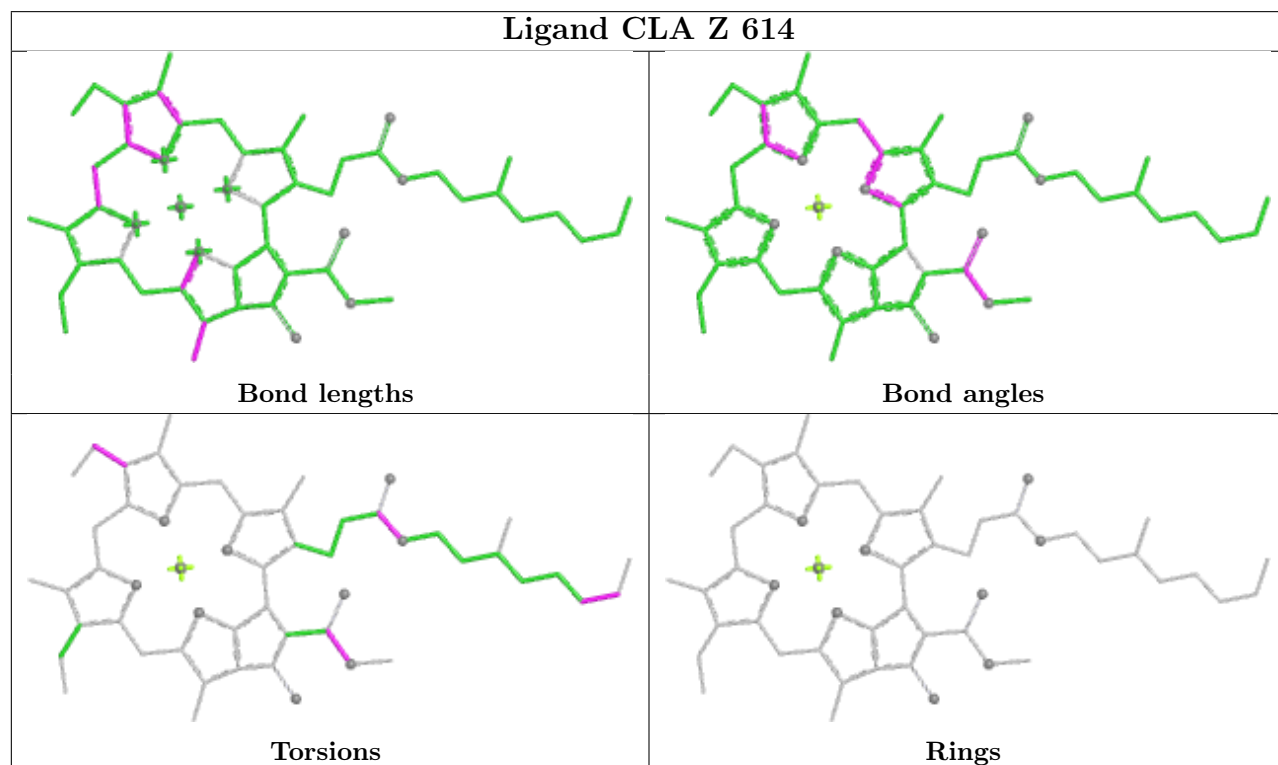


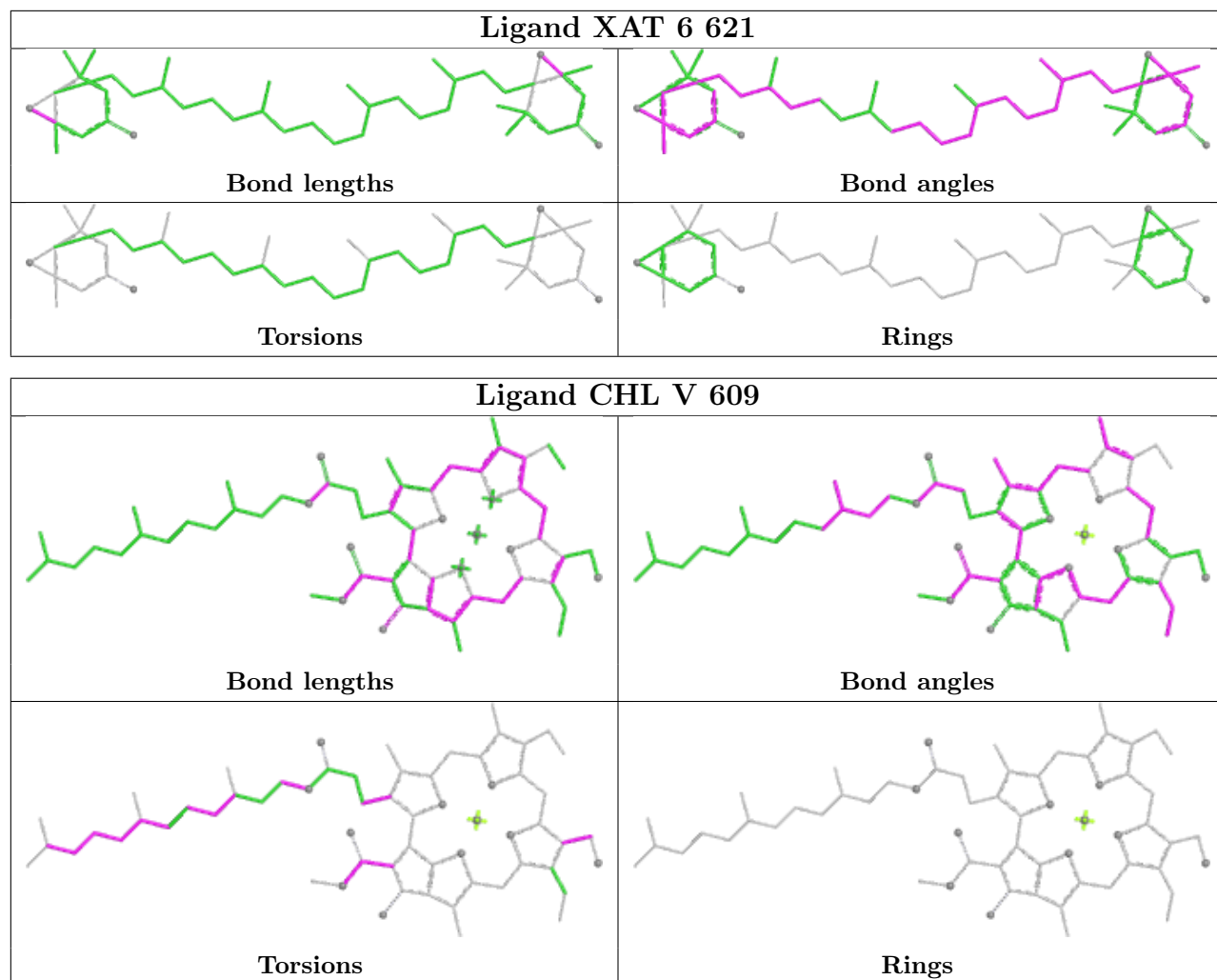


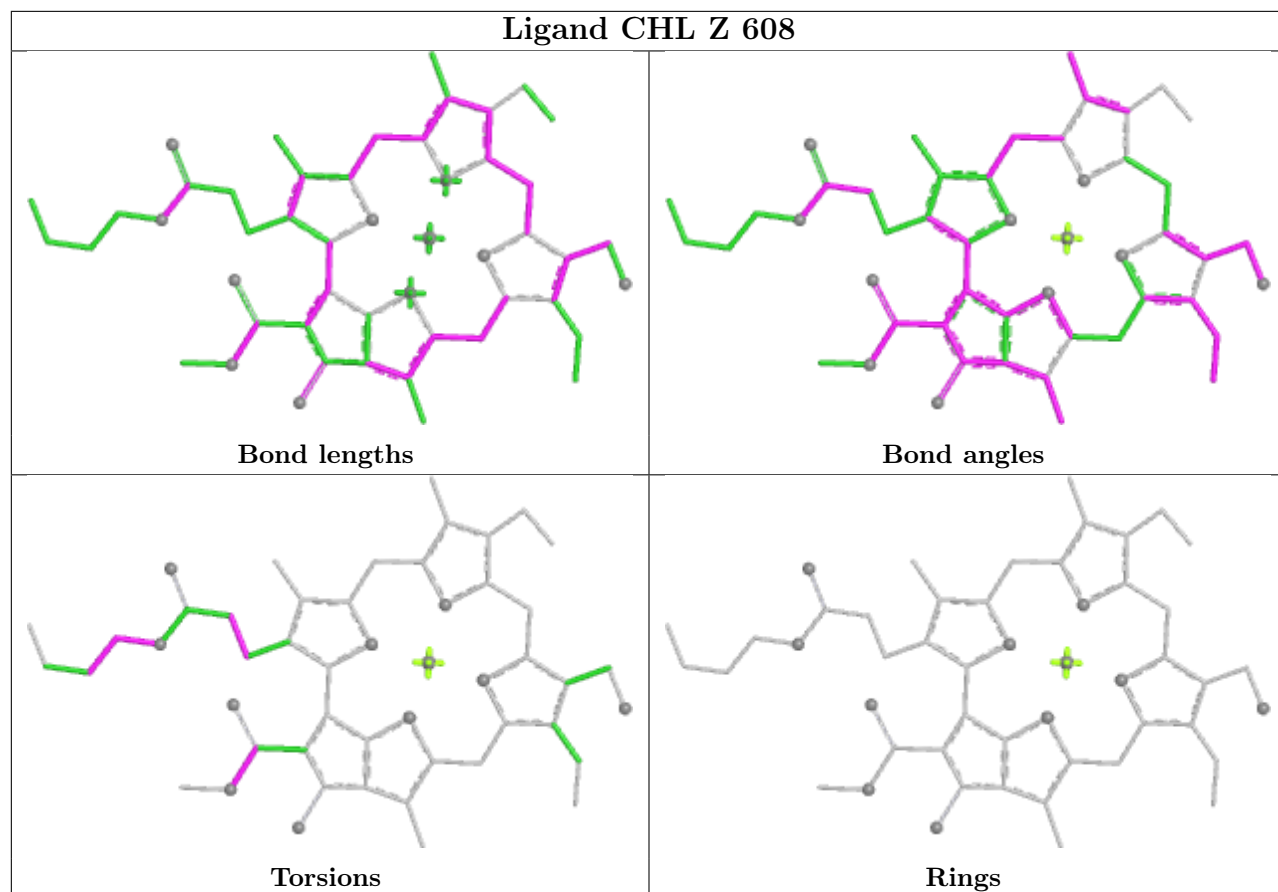
Ligand CLA A 821



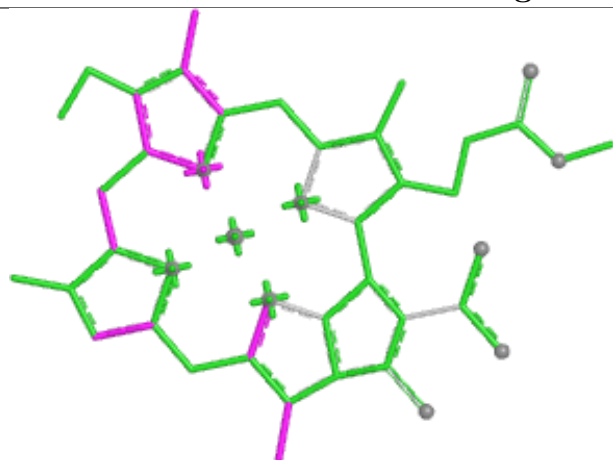
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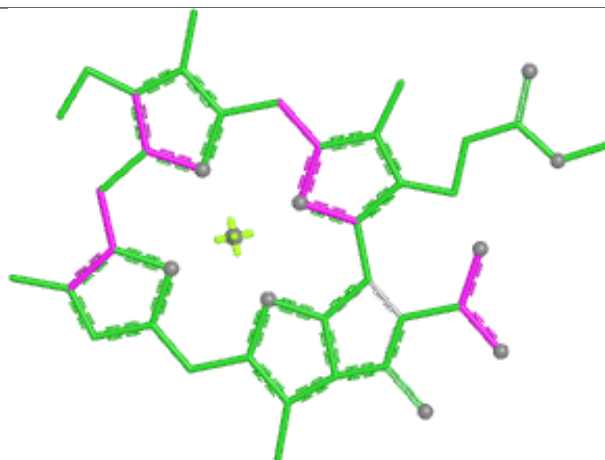




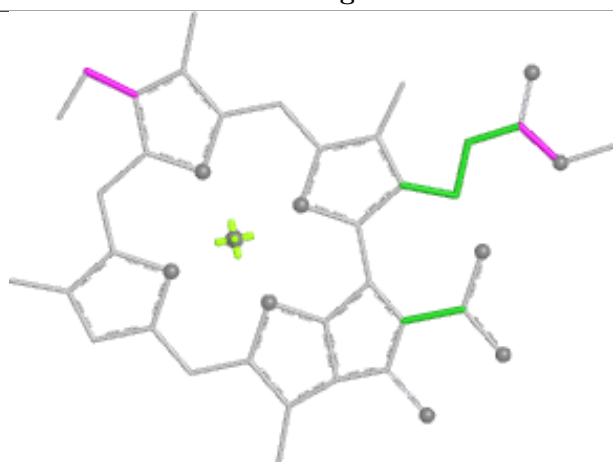
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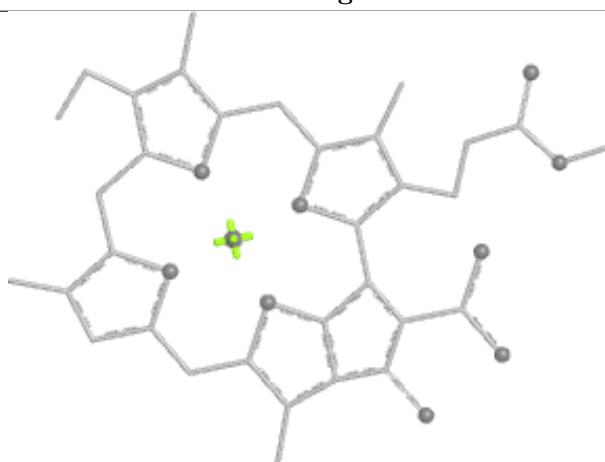
Bond lengths



Bond angles

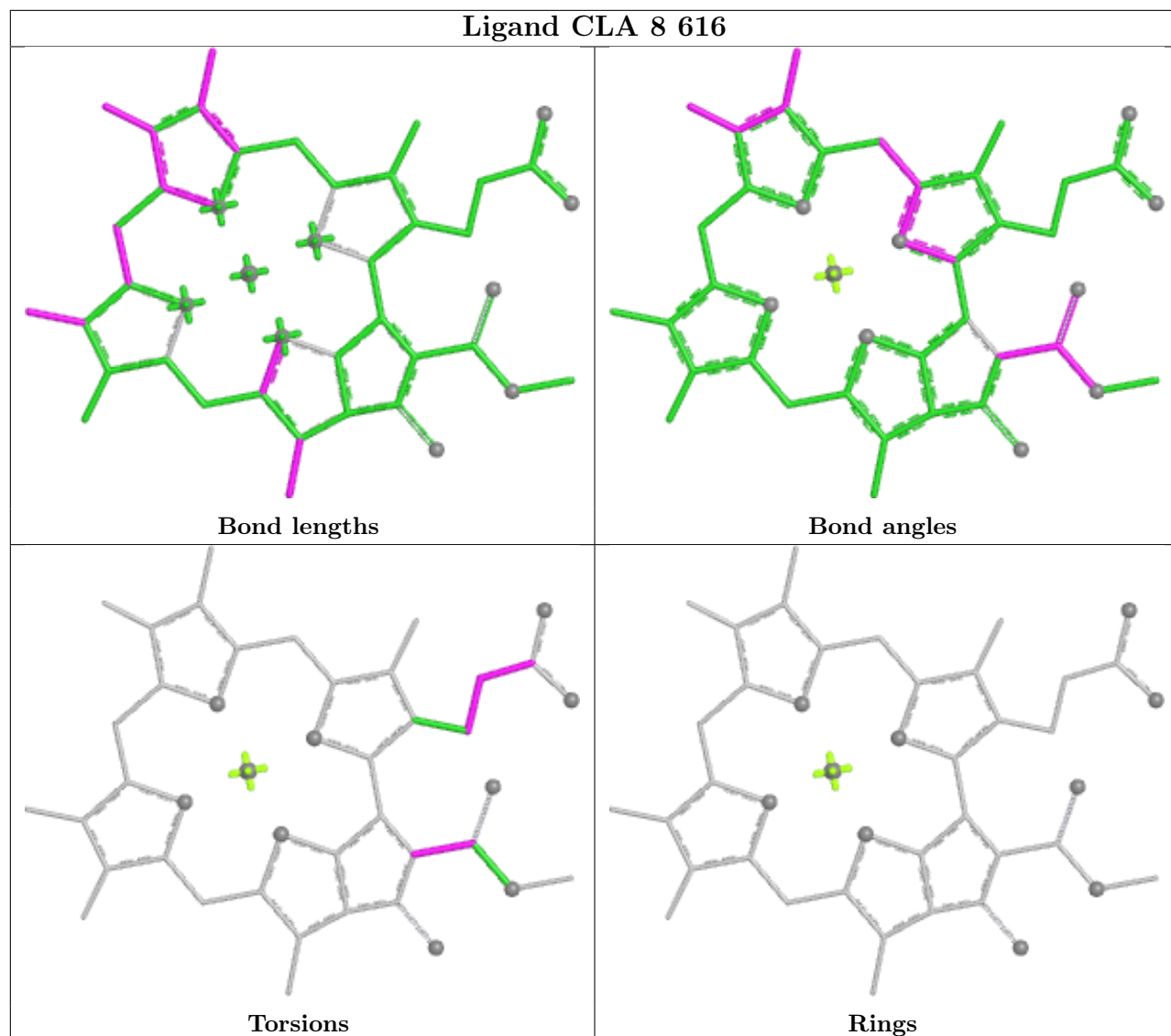


Torsions

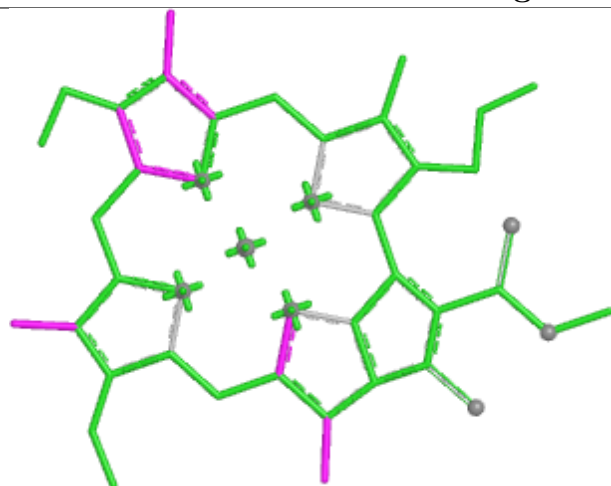


Rings

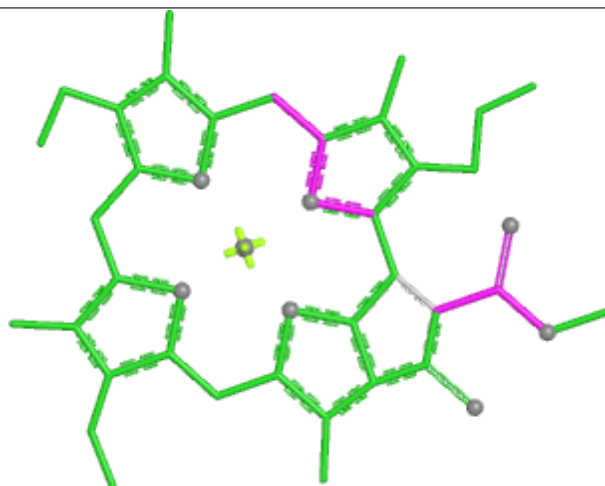
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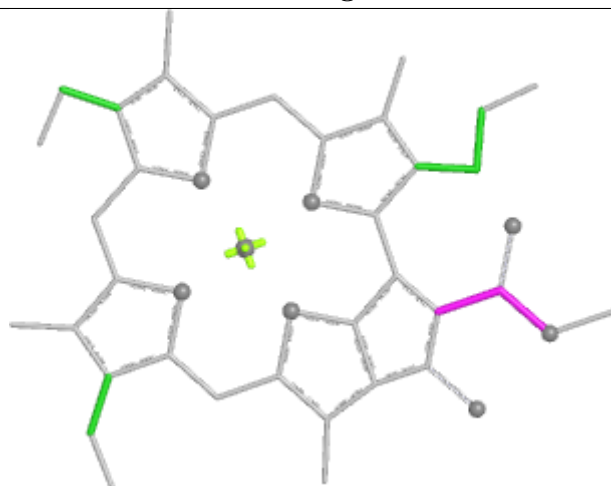
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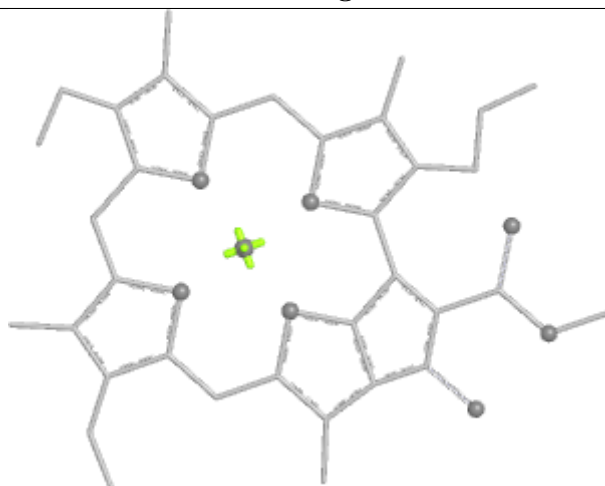
Bond lengths



Bond angles

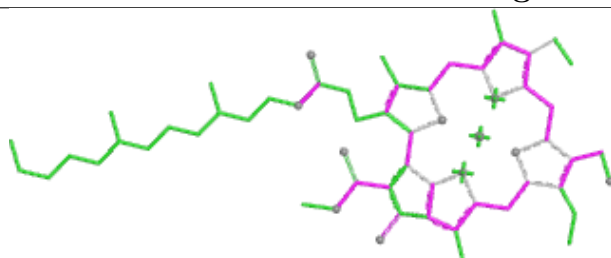


Torsions

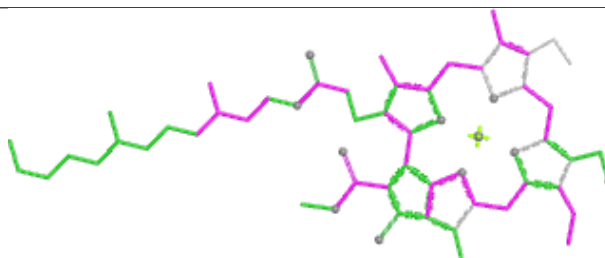


Rings

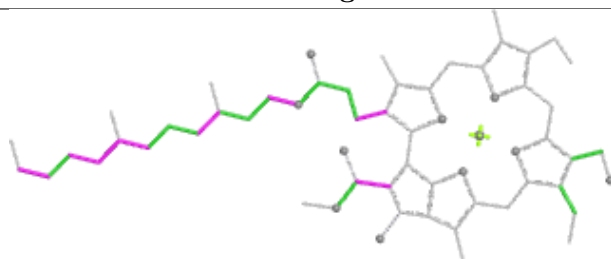
Ligand CHL U 609



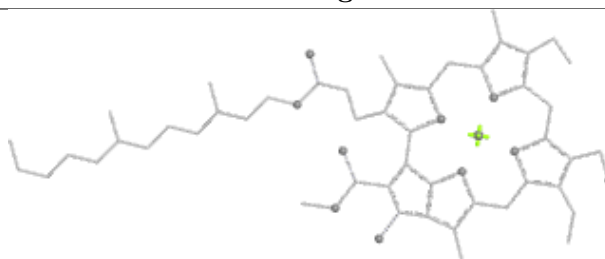
Bond lengths



Bond angles

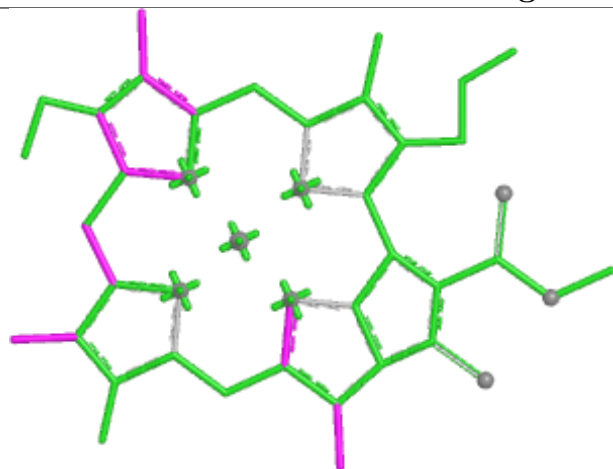


Torsions

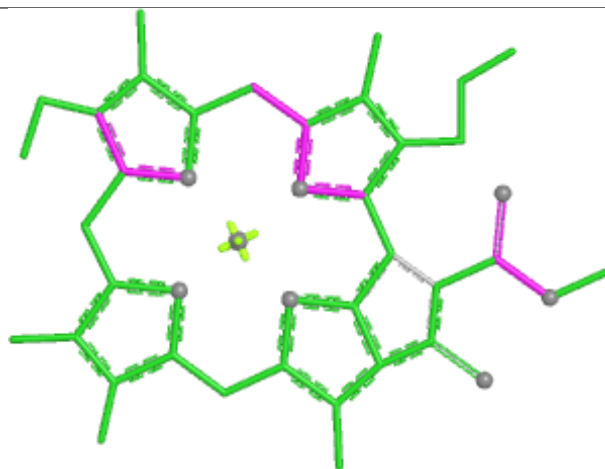


Rings

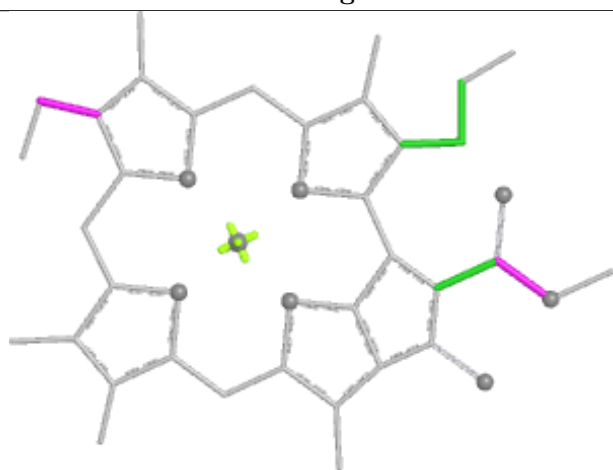
Ligand CLA 2 604



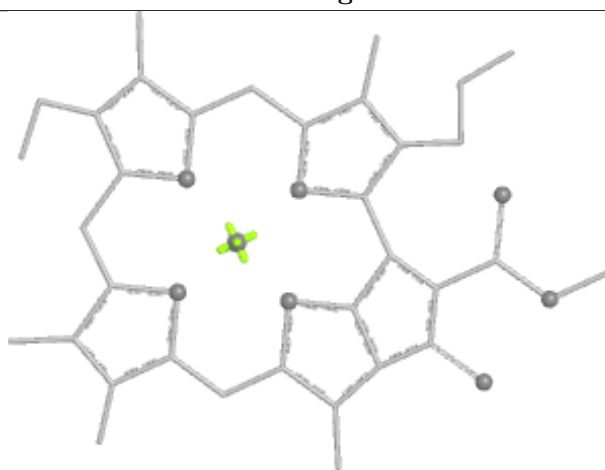
Bond lengths



Bond angles

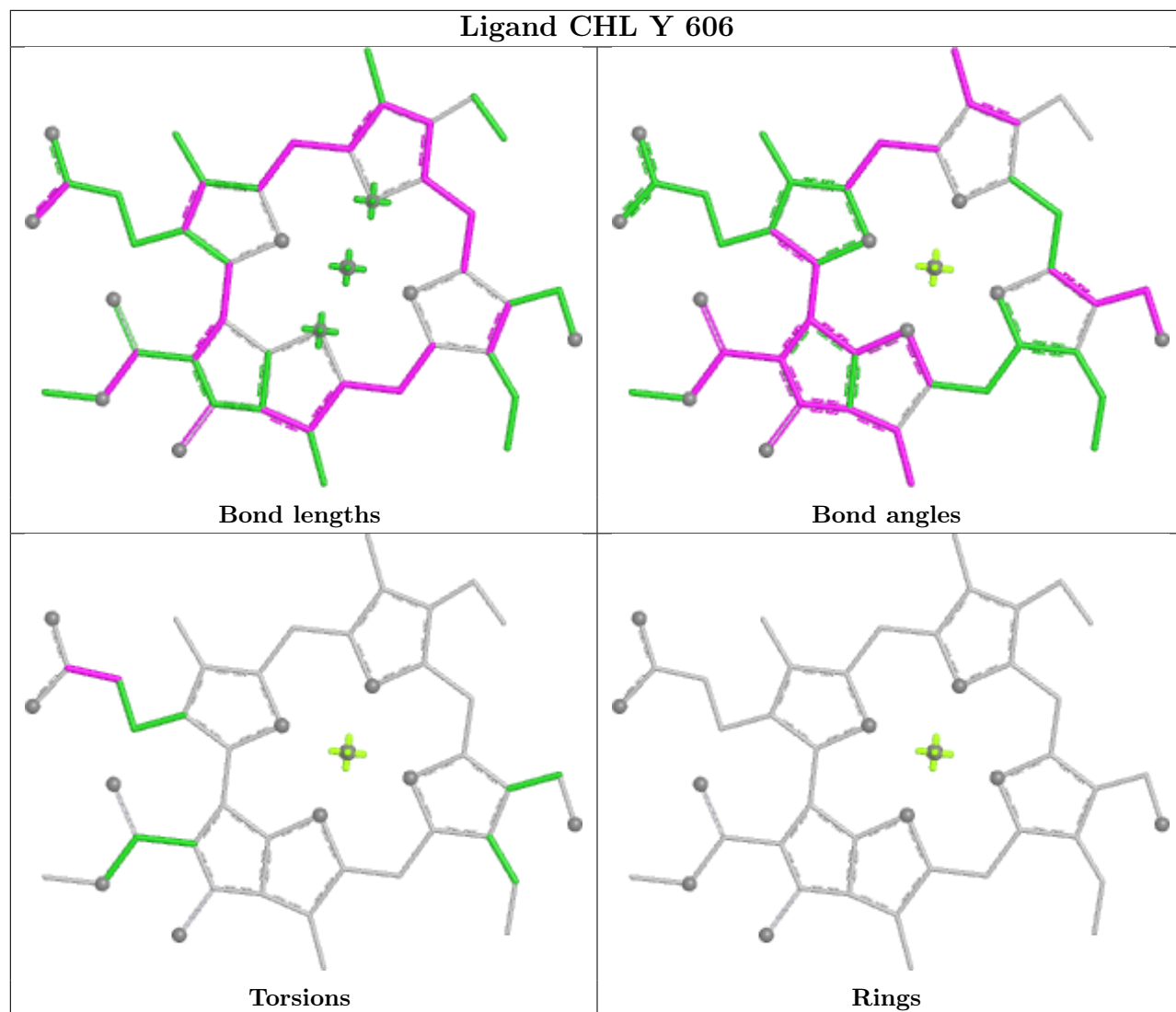


Torsions

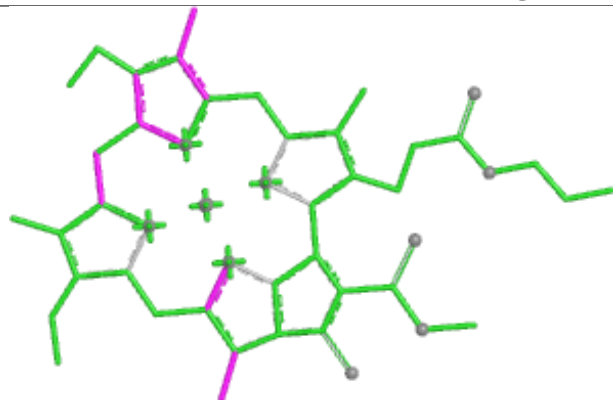


Rings

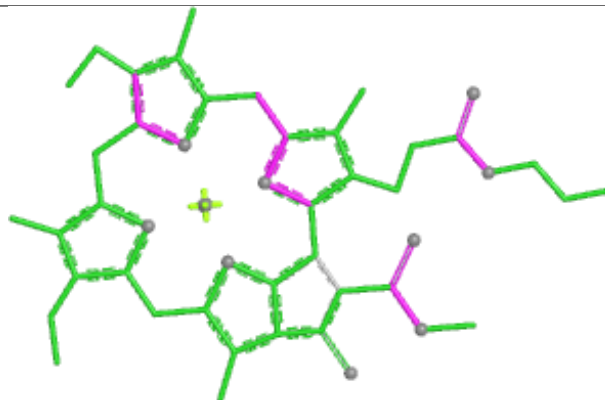
Ligand CHL Y 606



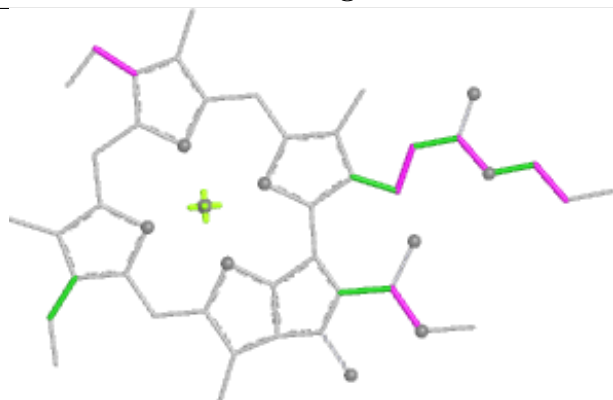
Ligand CLA Y 614



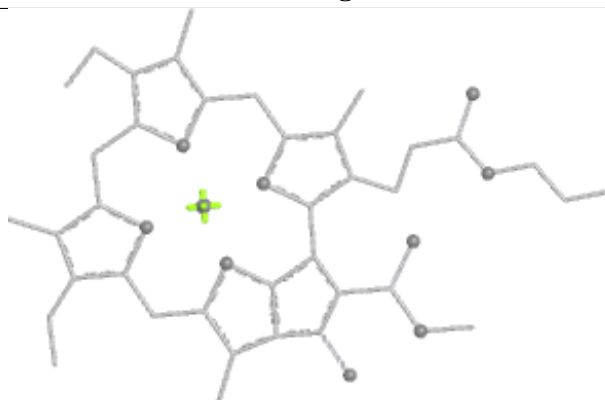
Bond lengths



Bond angles

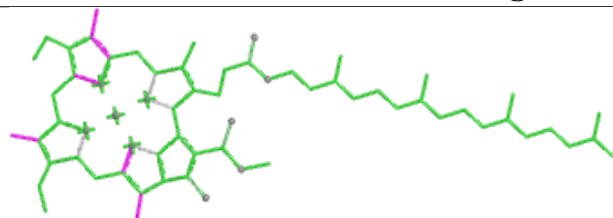


Torsions

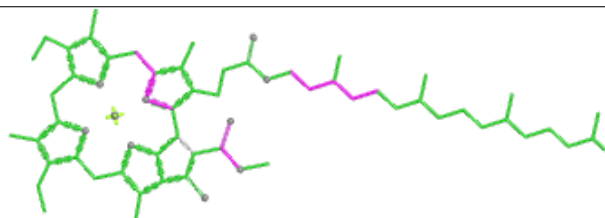


Rings

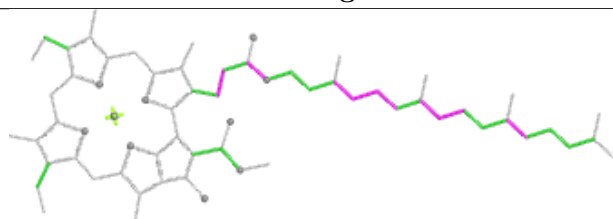
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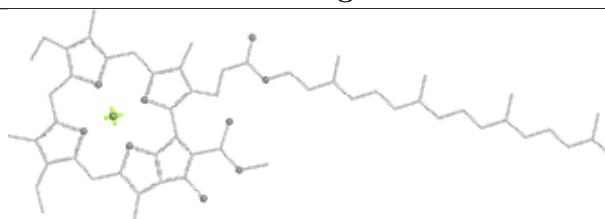
Bond lengths



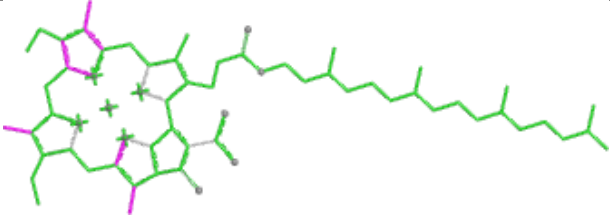
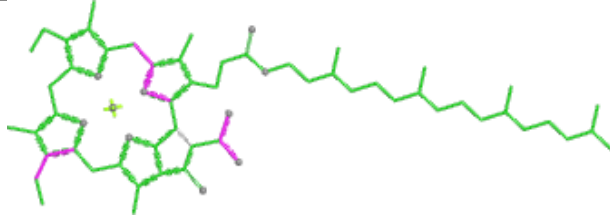
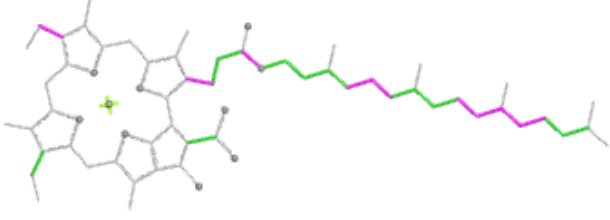
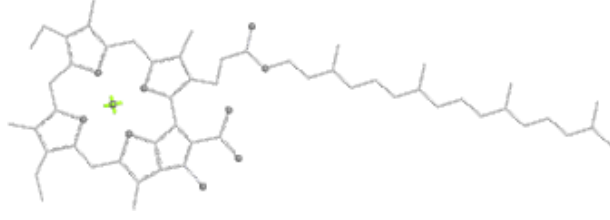
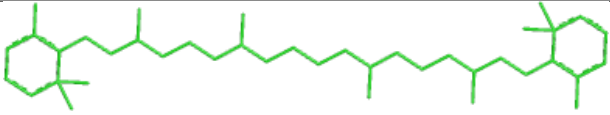
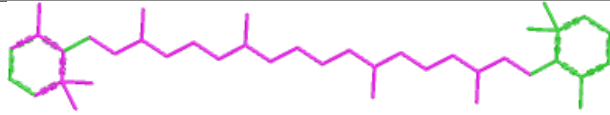
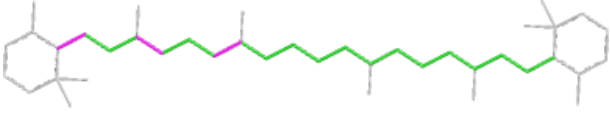
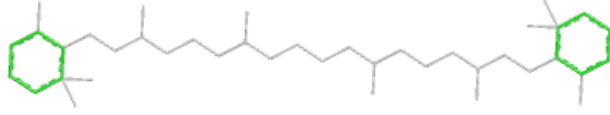
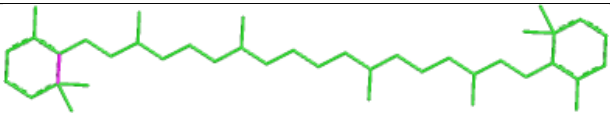
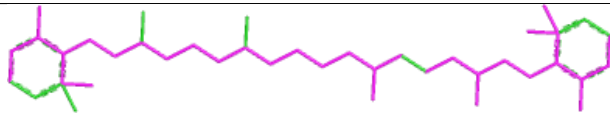
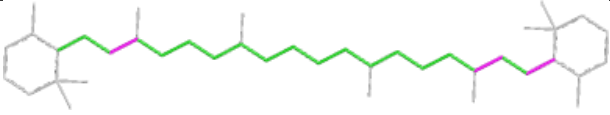
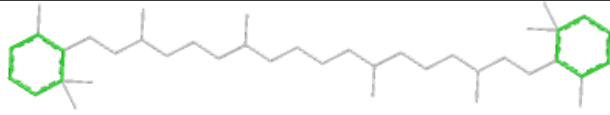
Bond angles



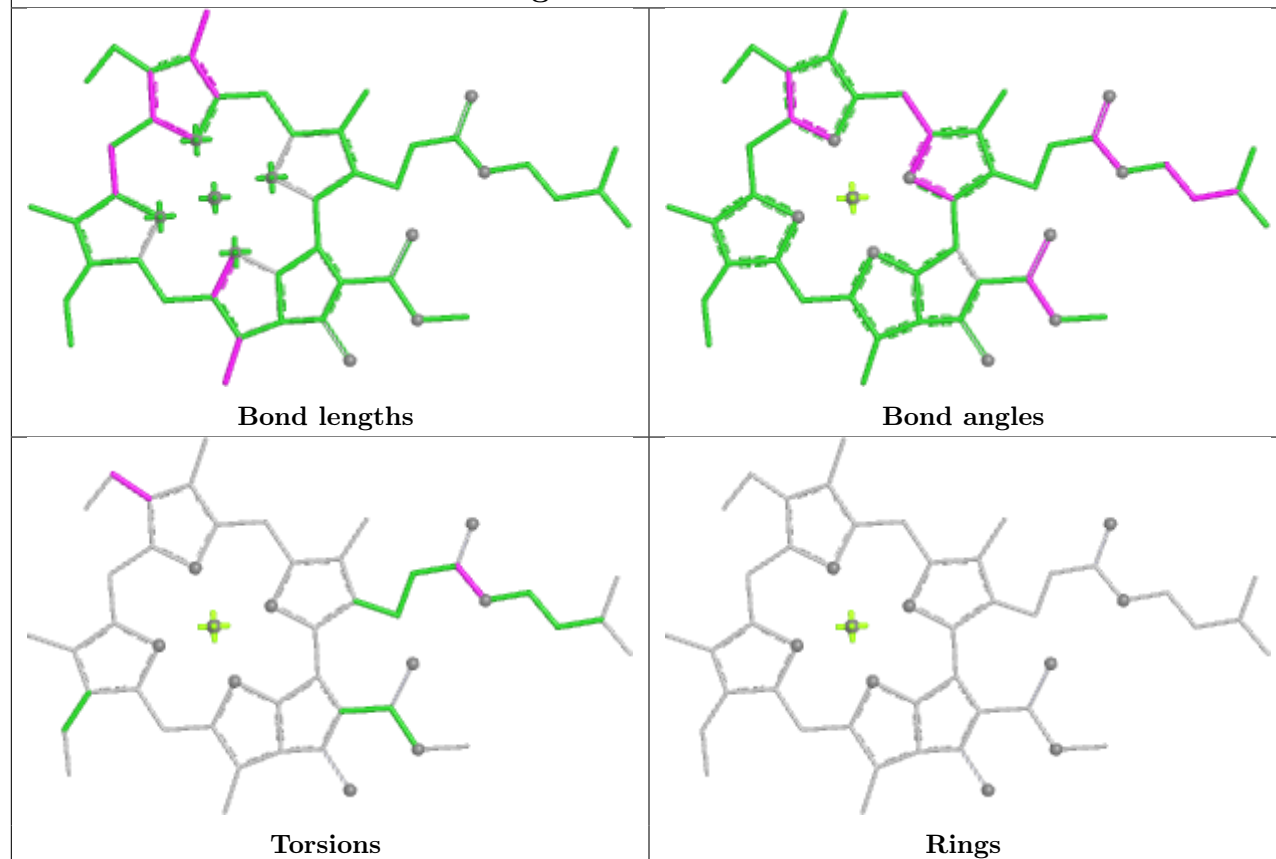
Torsions



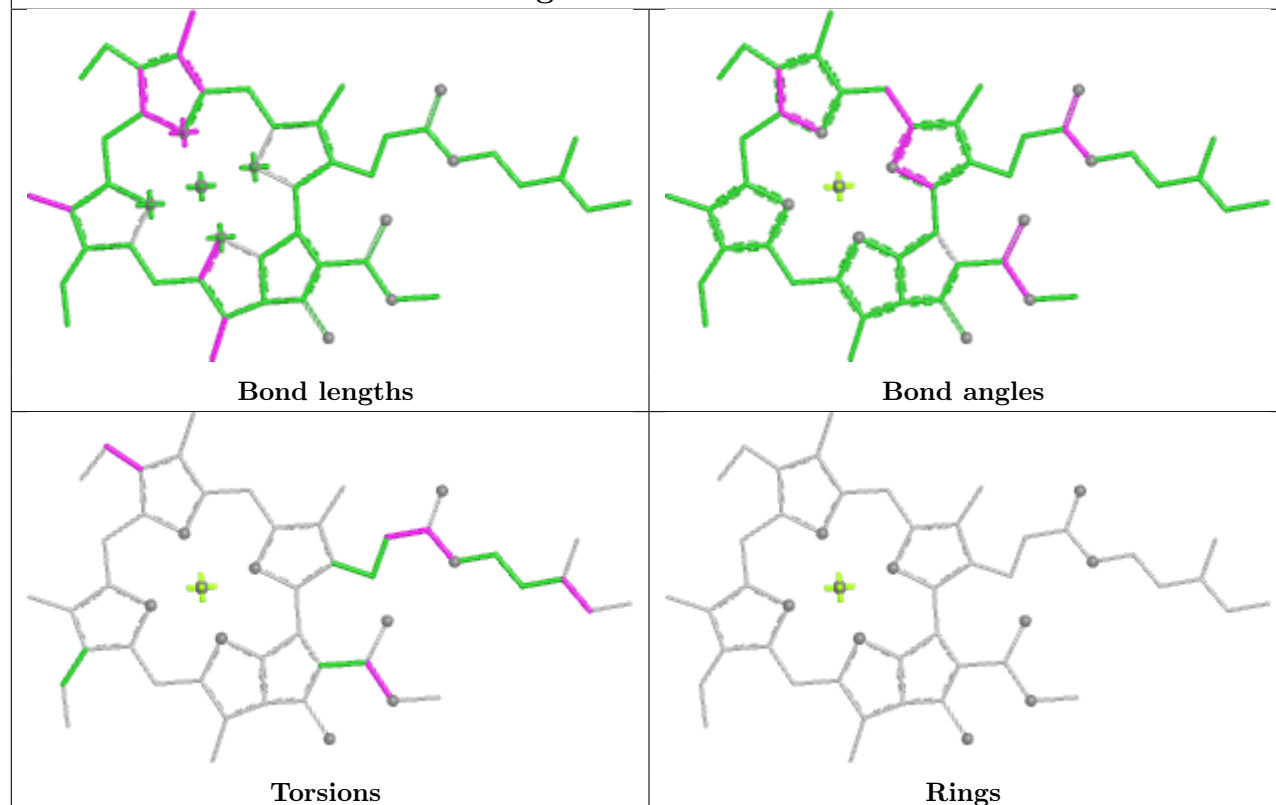
Rings

Ligand CLA a 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 852	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 7 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

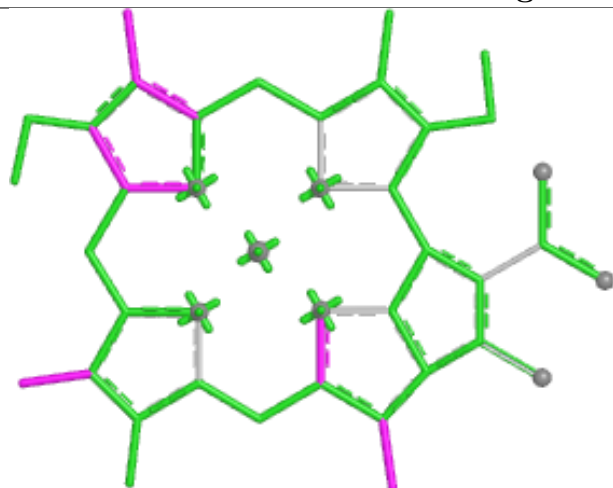
Ligand CLA Y 604



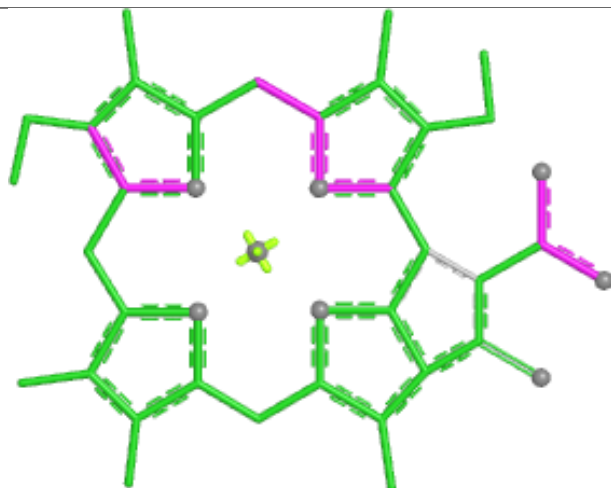
Ligand CLA 8 608



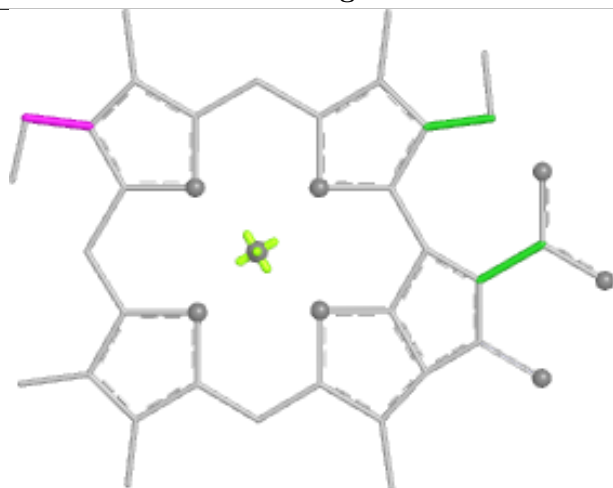
Ligand CLA L 307



Bond lengths



Bond angles

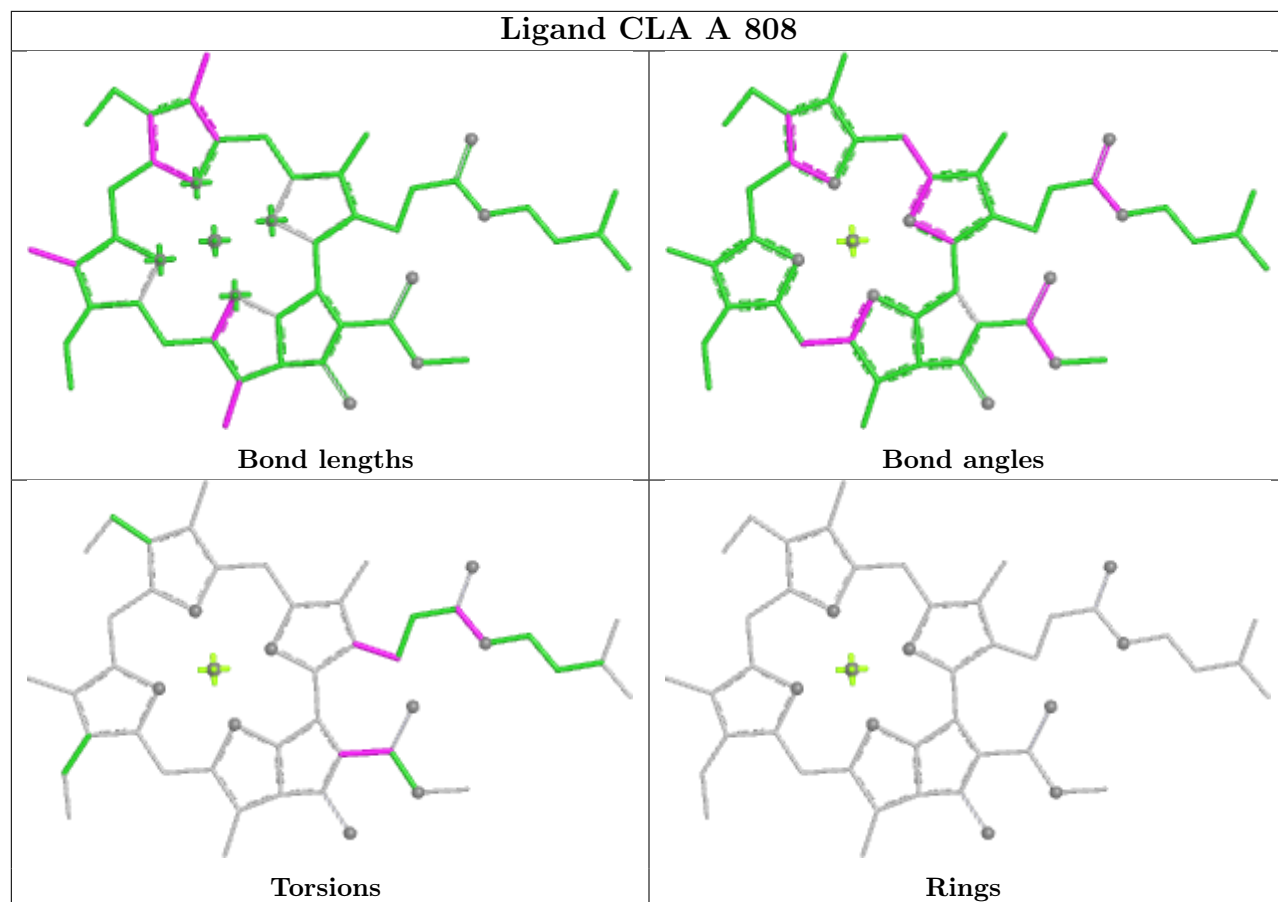


Torsions

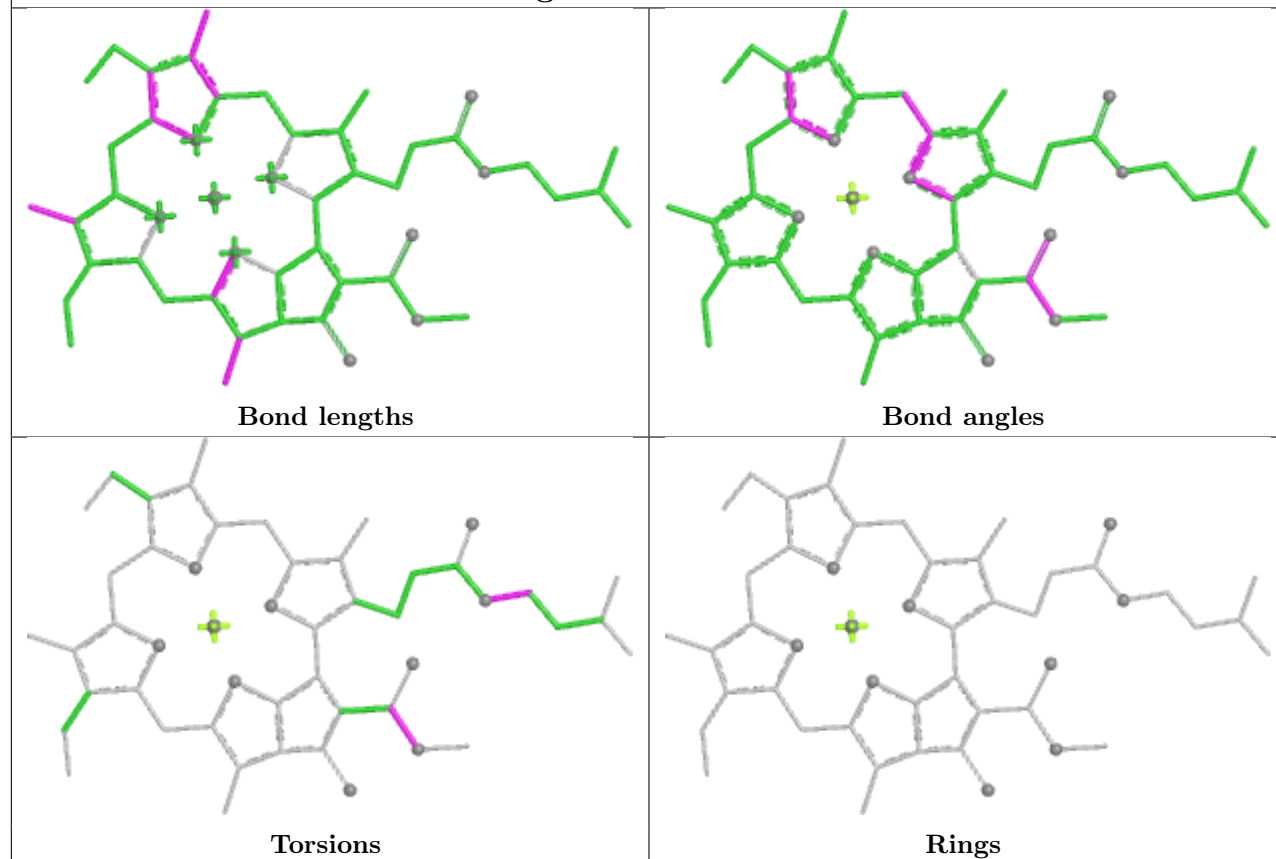


Rings

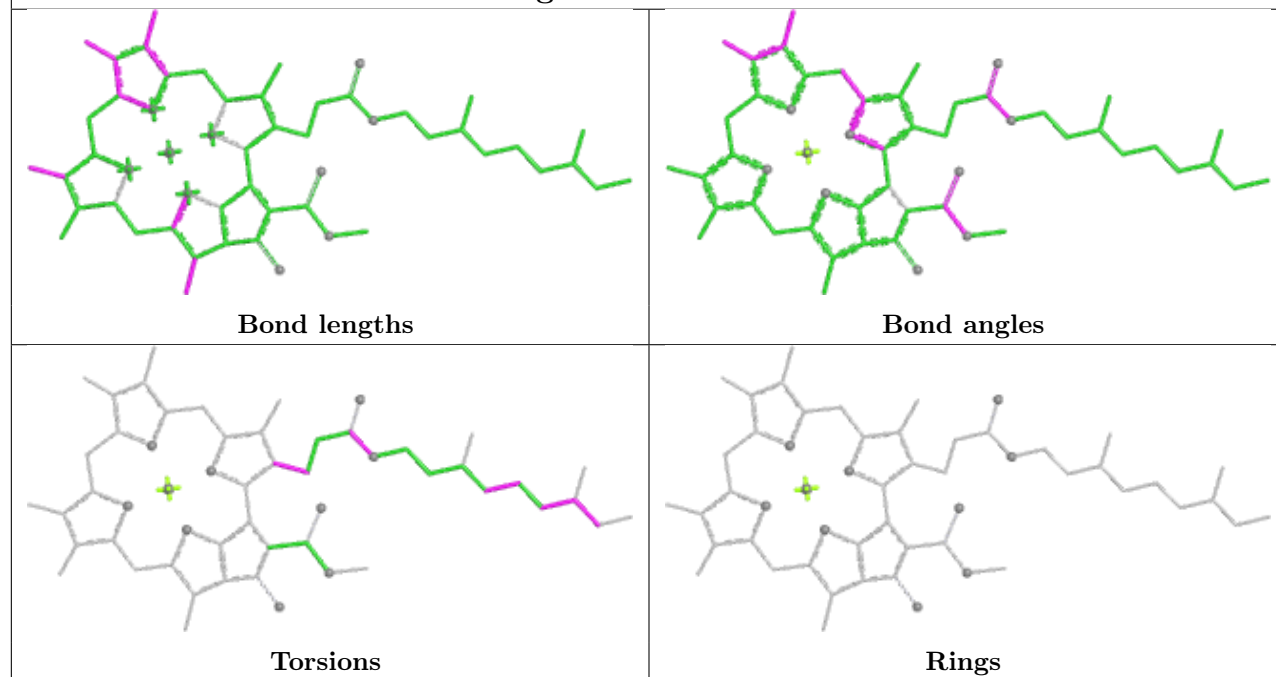
Ligand CLA A 808

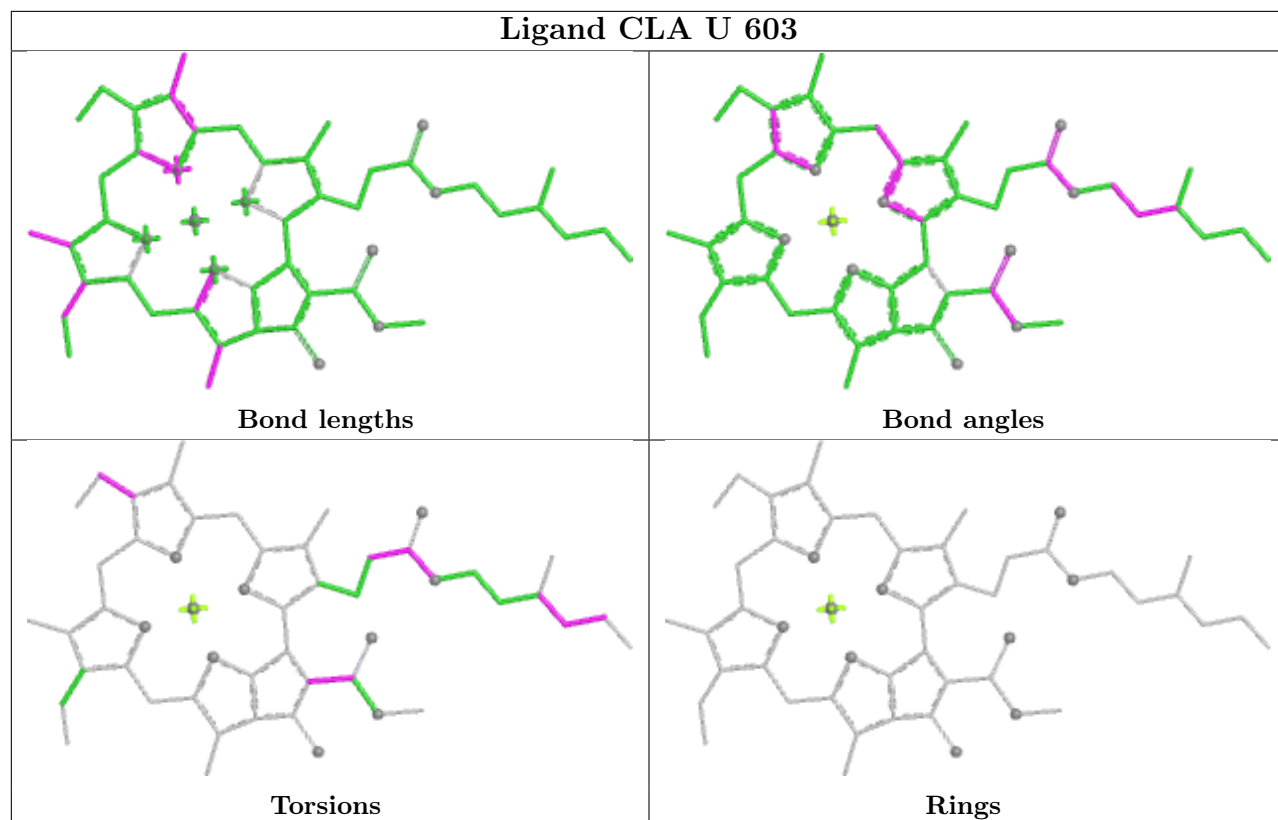


Ligand CLA 7 608

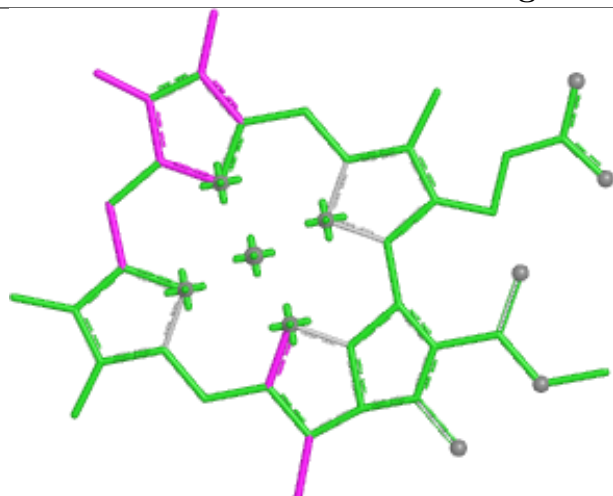


Ligand CLA 4 604

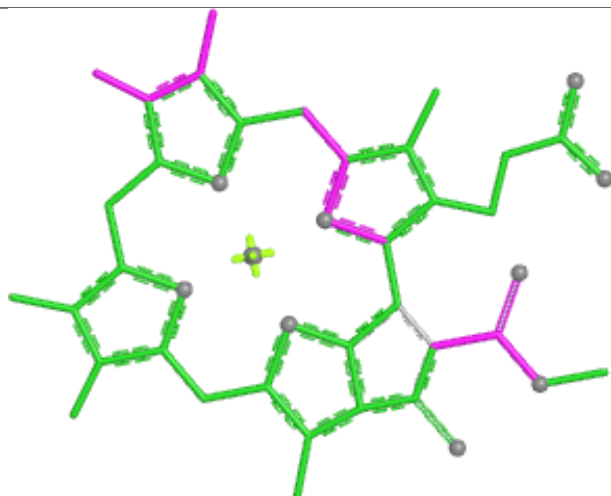




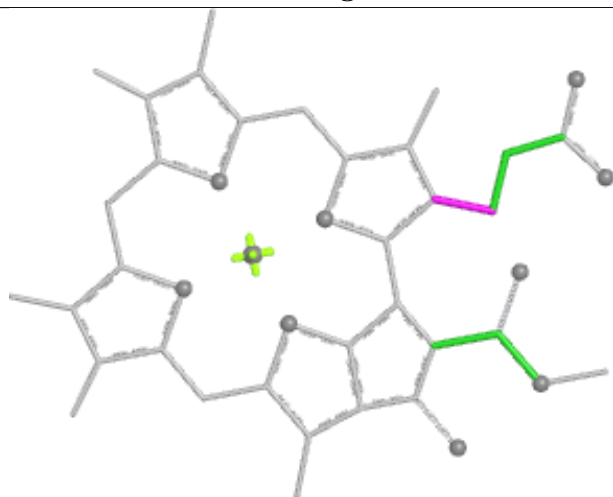
Ligand CLA 7 616



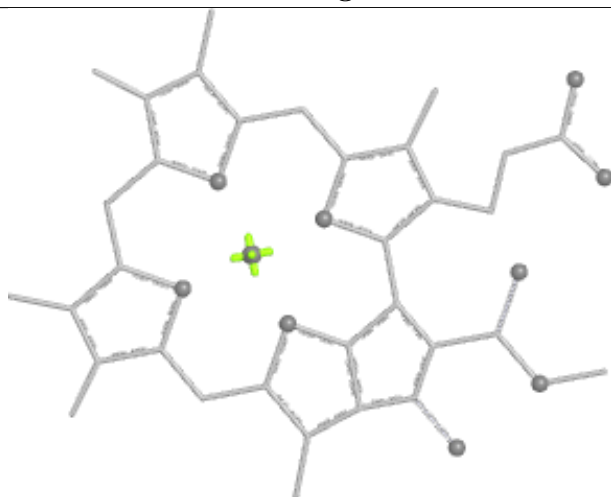
Bond lengths



Bond angles

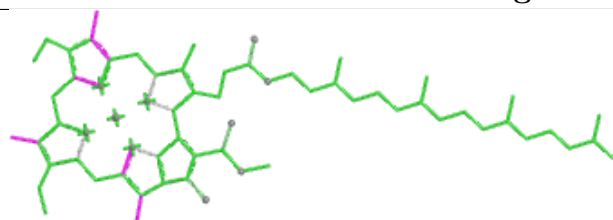


Torsions

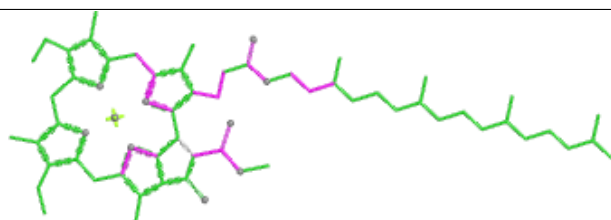


Rings

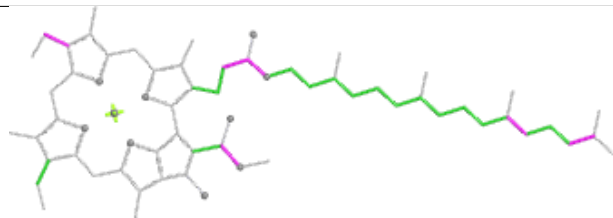
Ligand CLA A 801



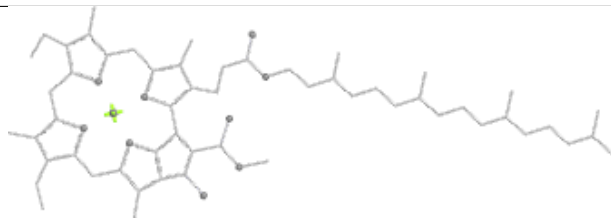
Bond lengths



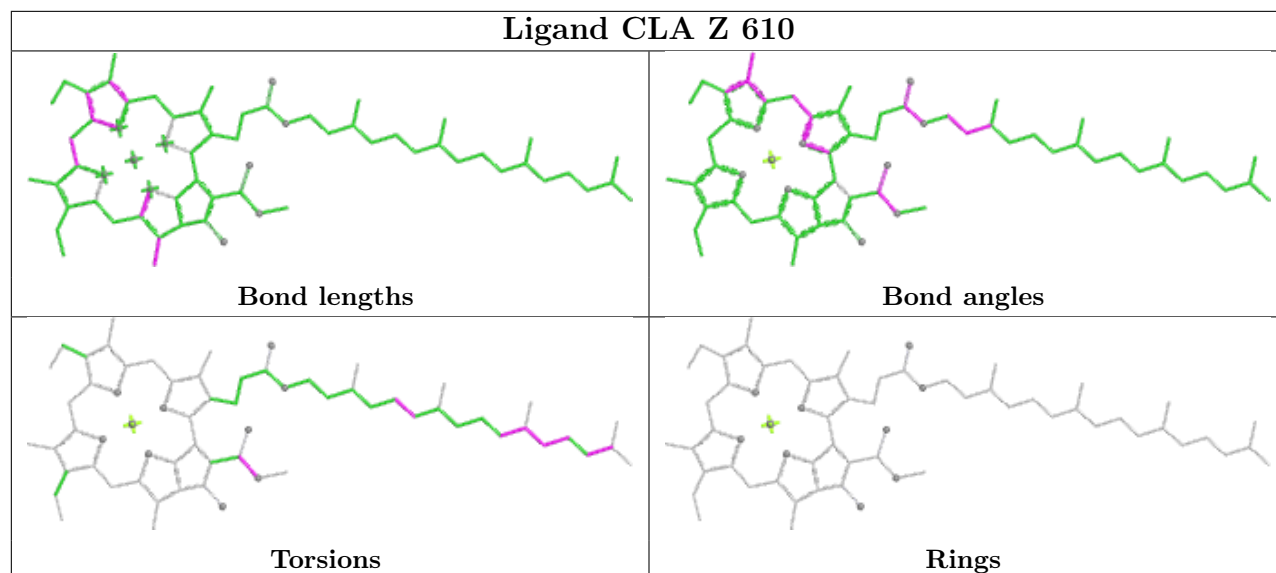
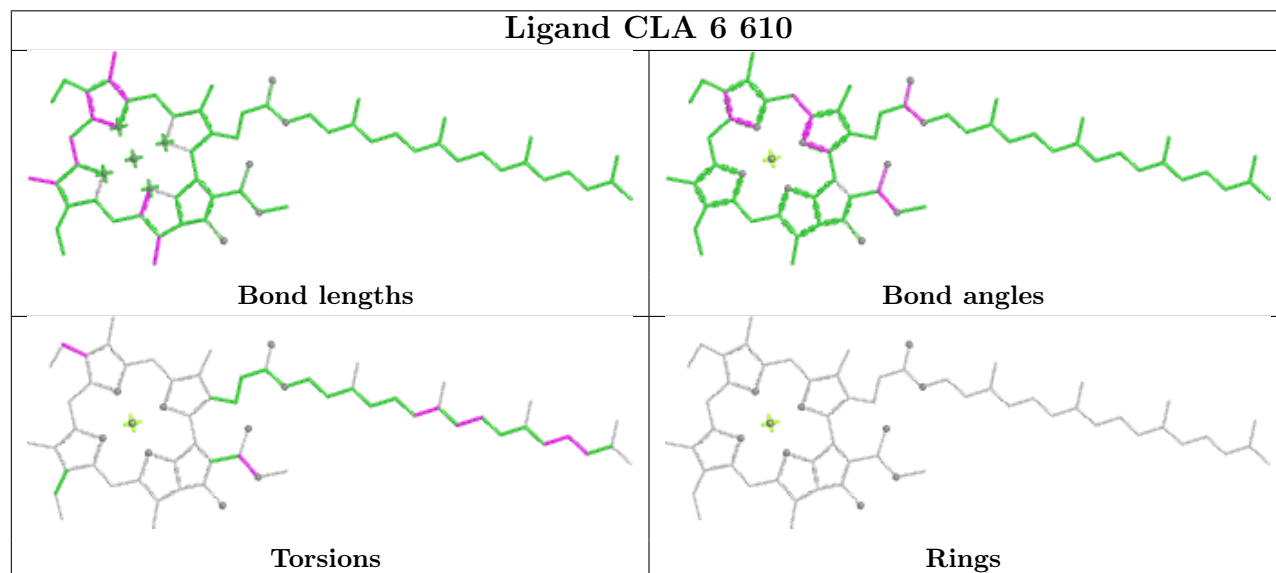
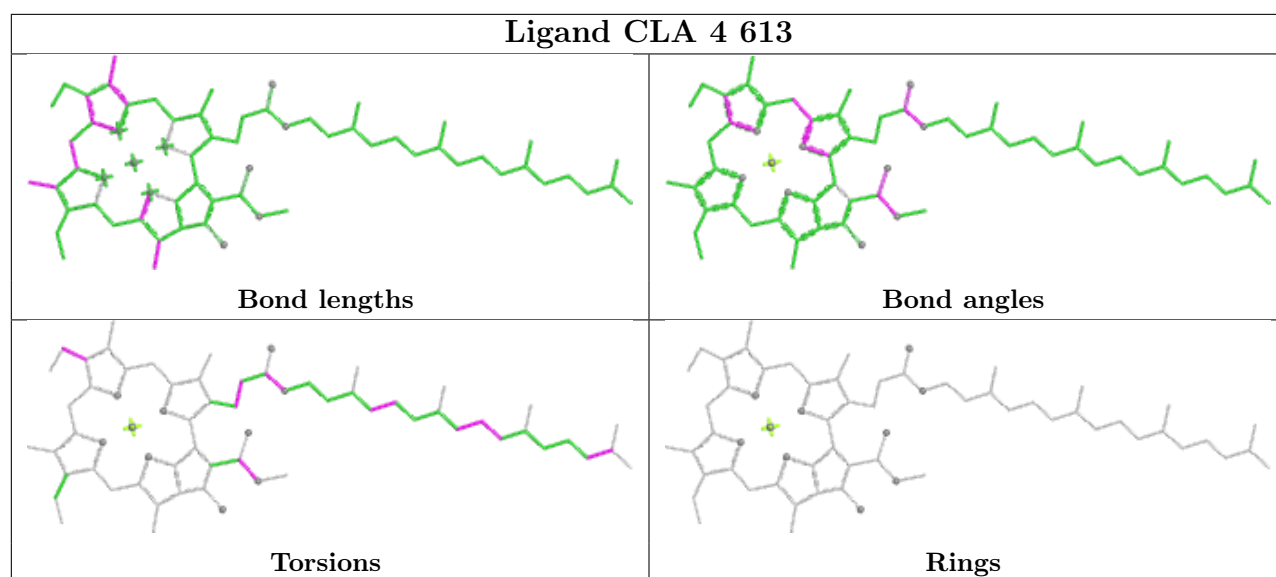
Bond angles



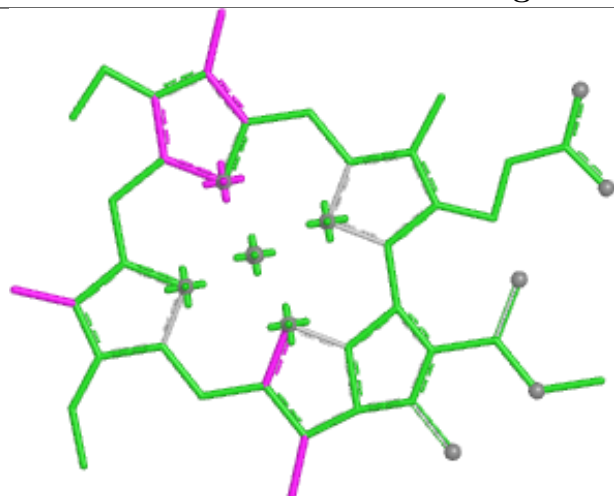
Torsions



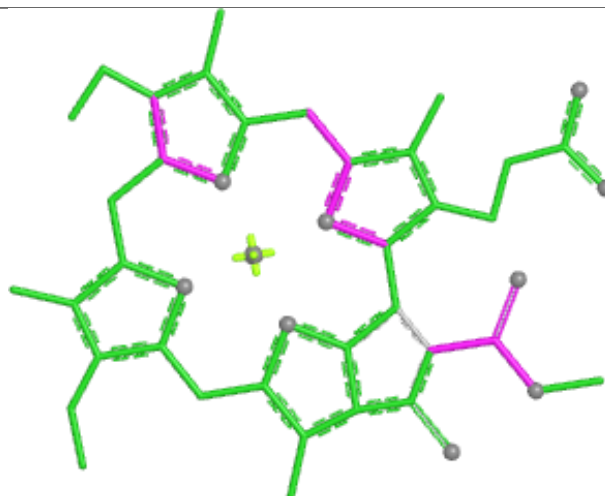
Rings



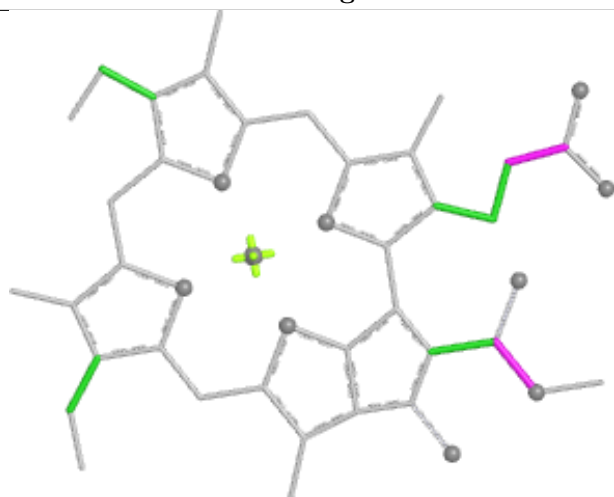
Ligand CLA G 204



Bond lengths



Bond angles

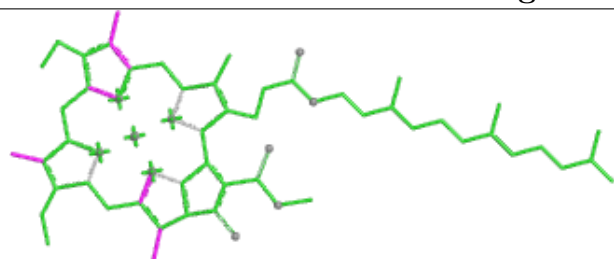


Torsions

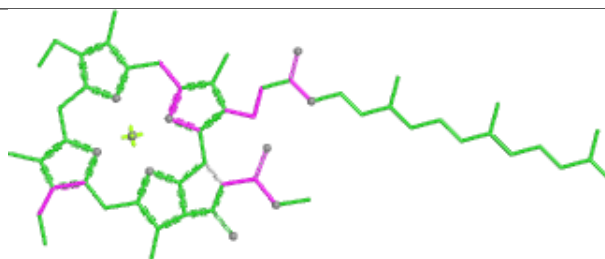


Rings

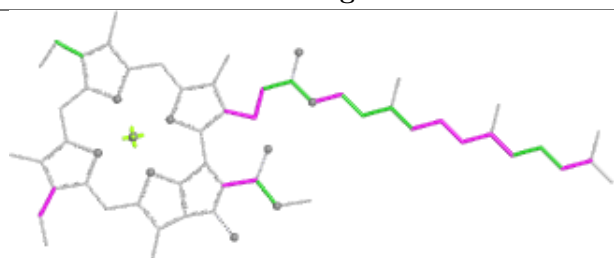
Ligand CLA 3 609



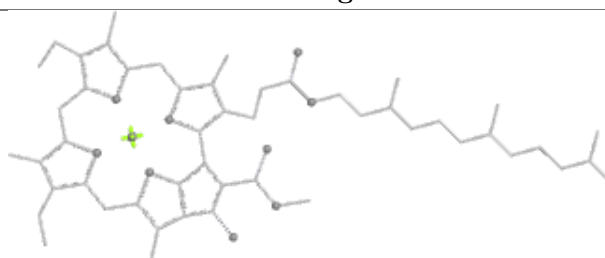
Bond lengths



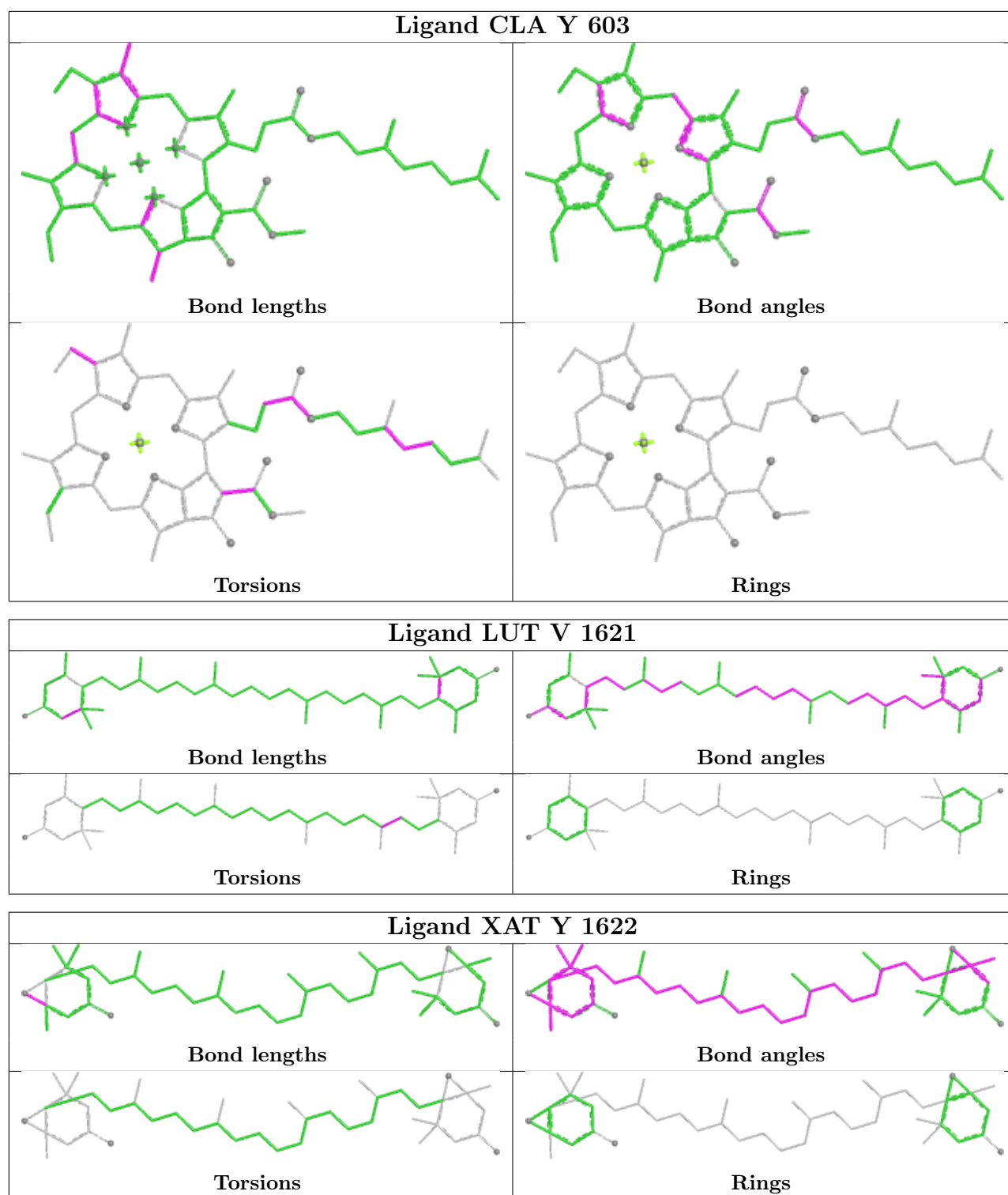
Bond angles



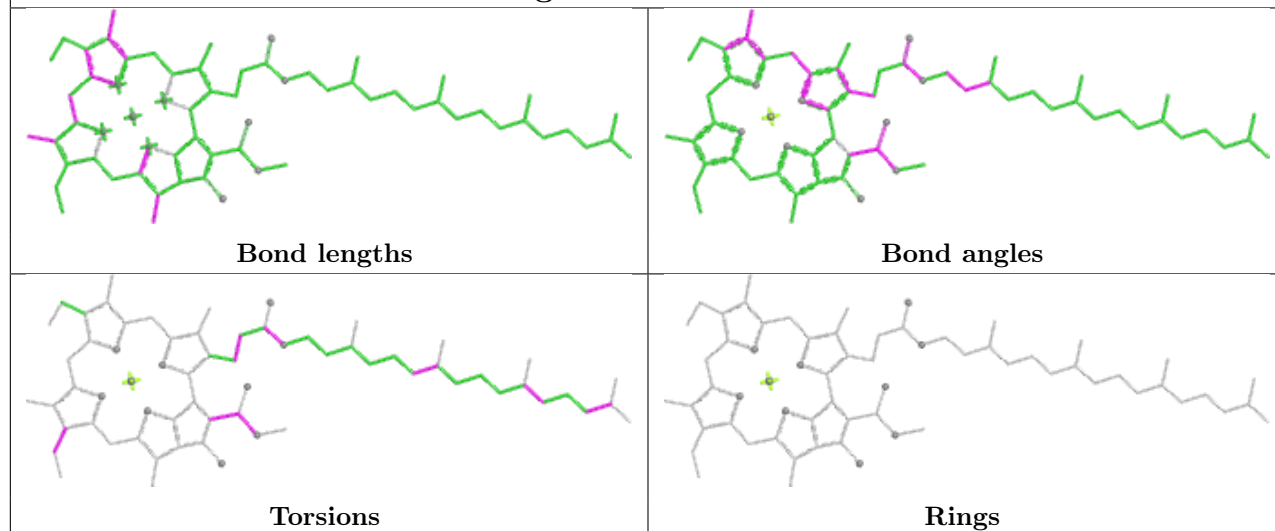
Torsions



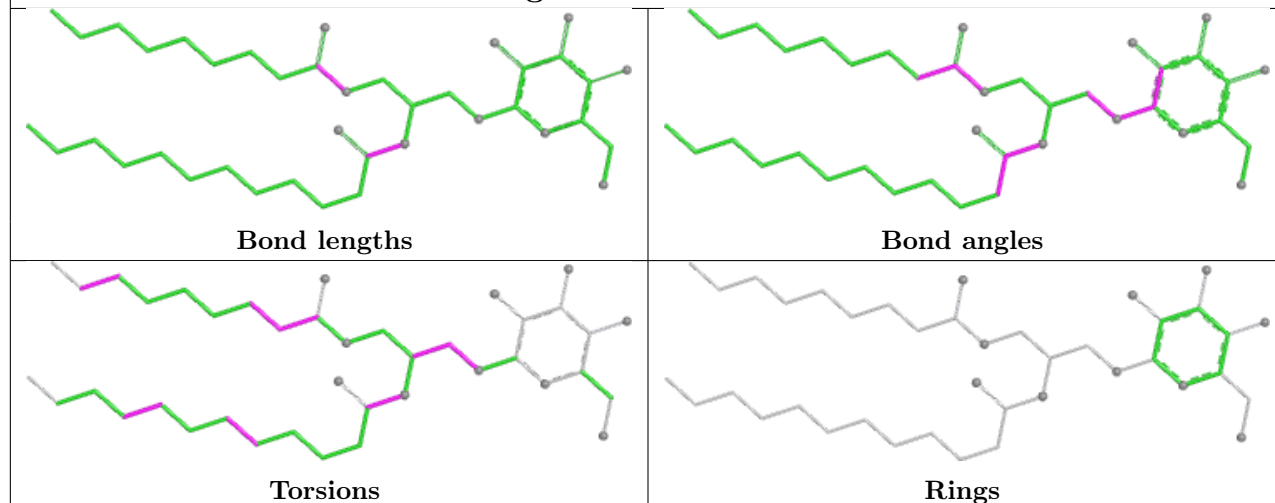
Rings



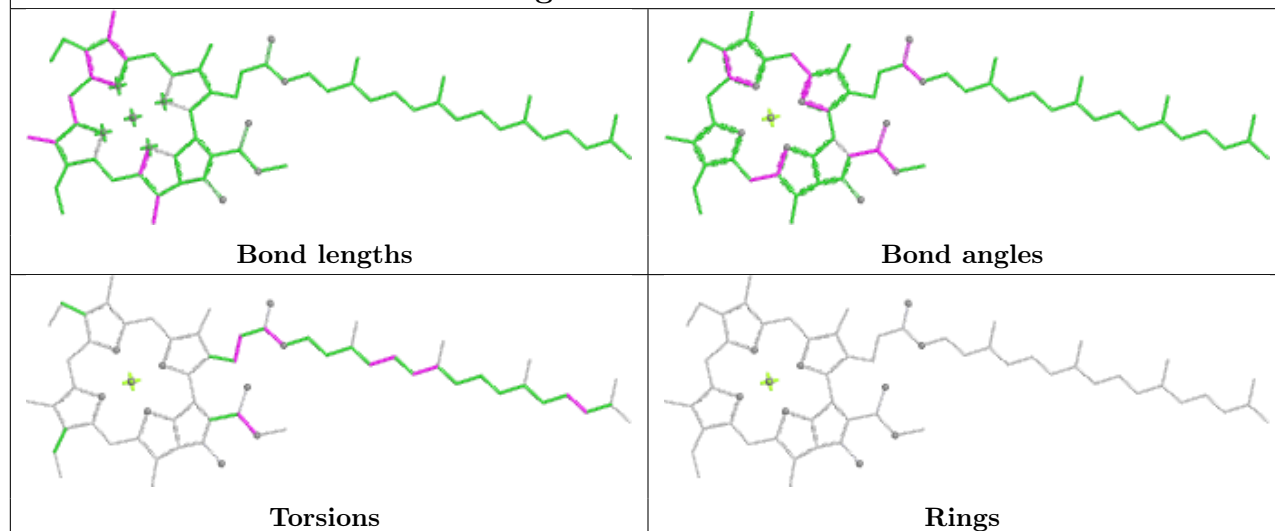
Ligand CLA 2 601

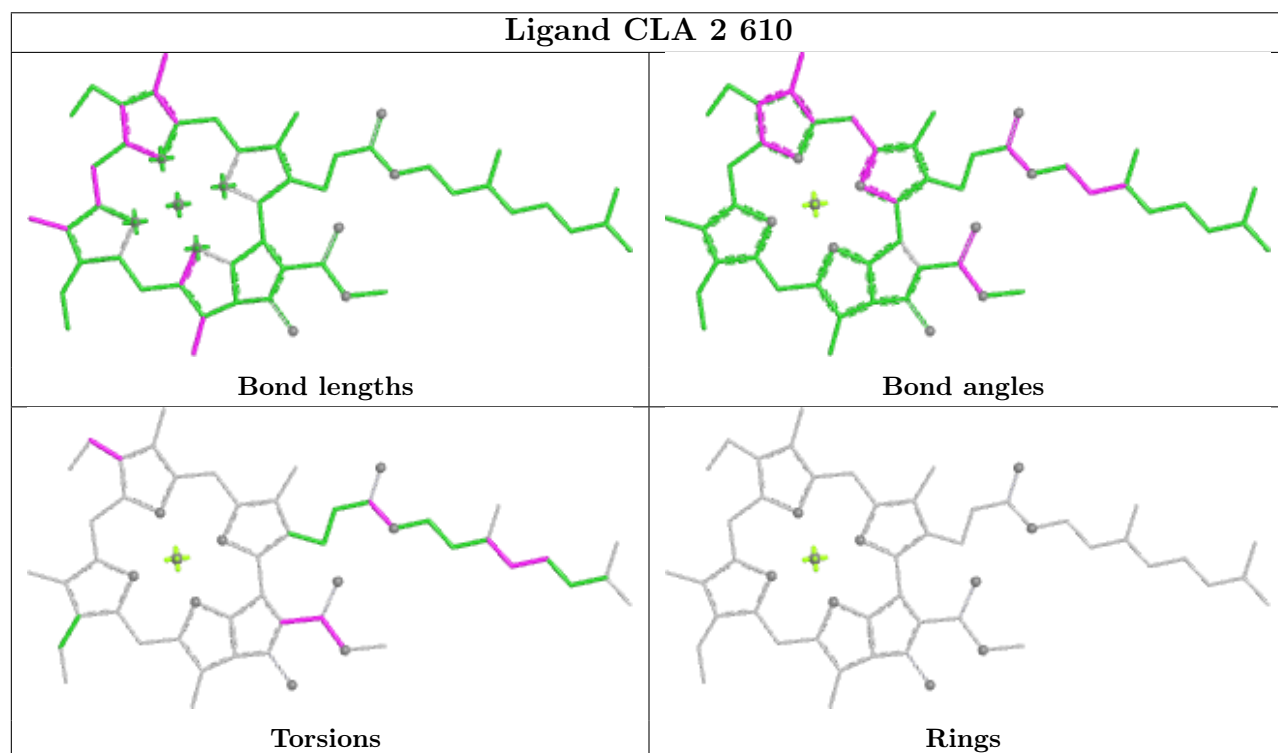
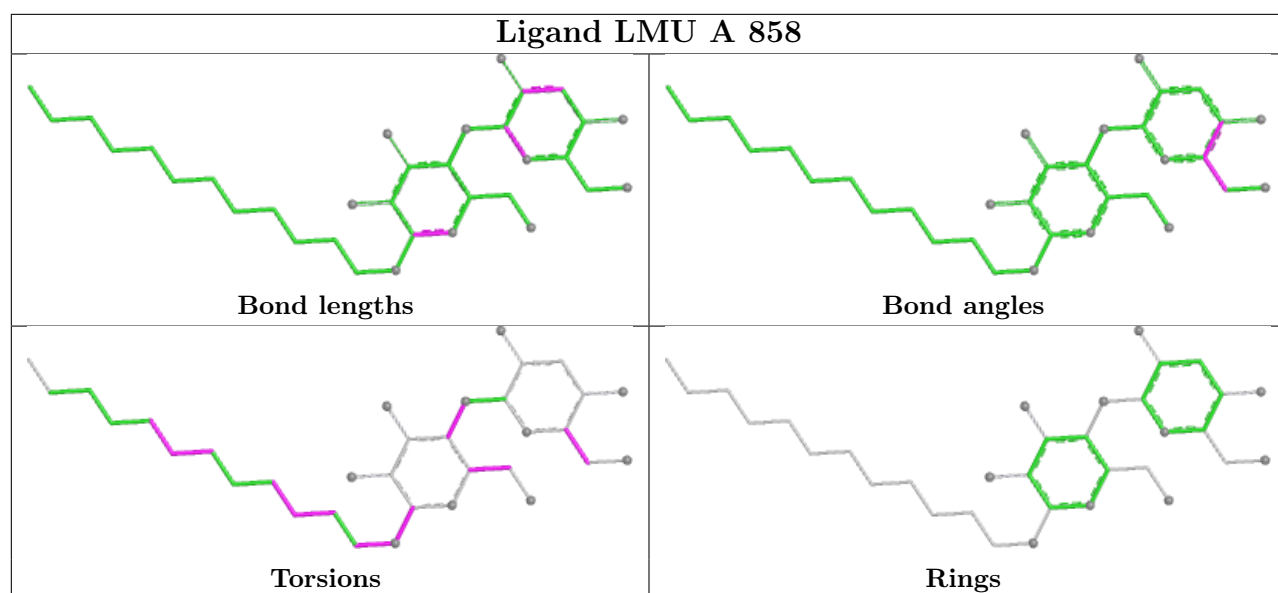


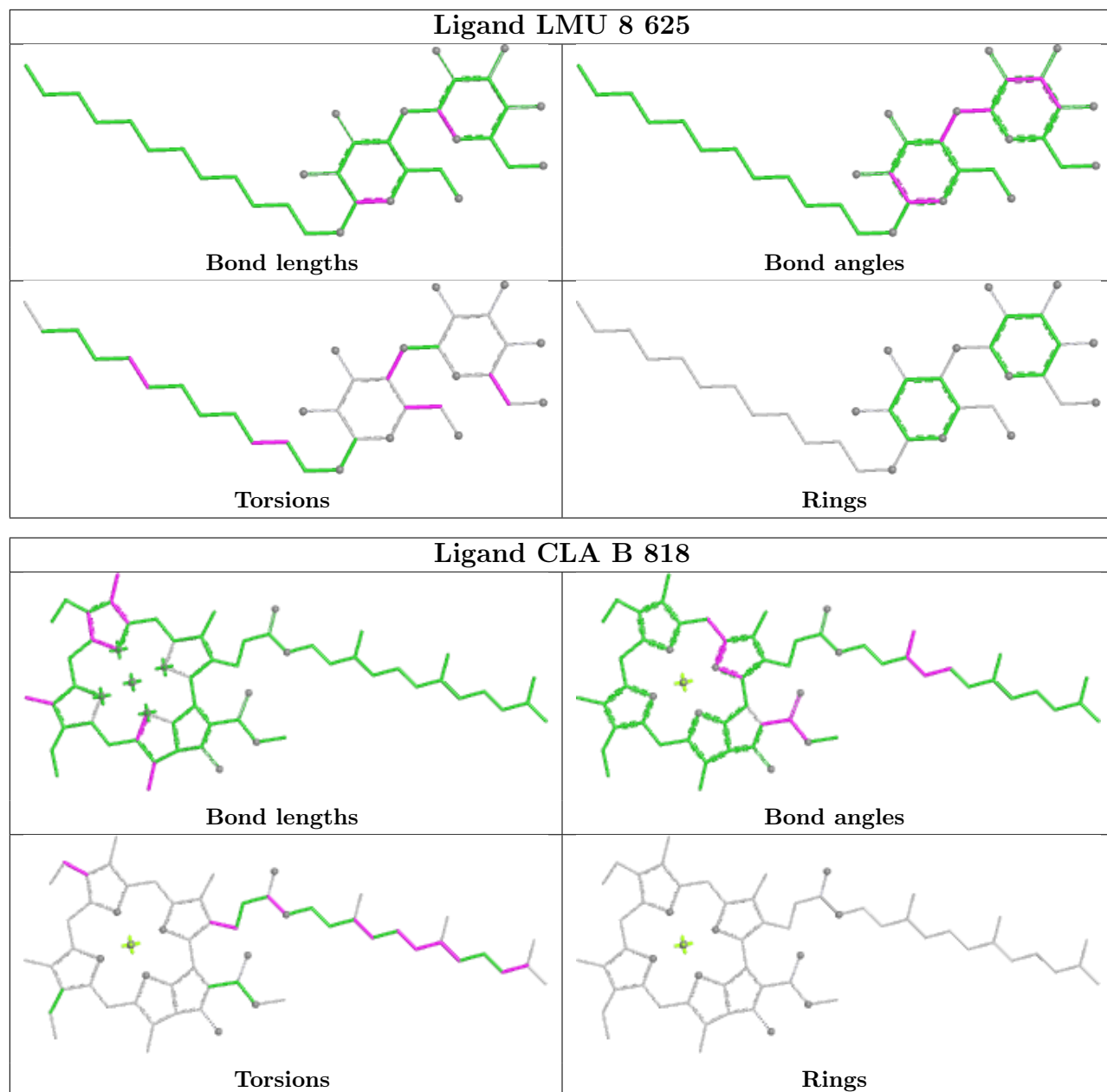
Ligand LMG A 860



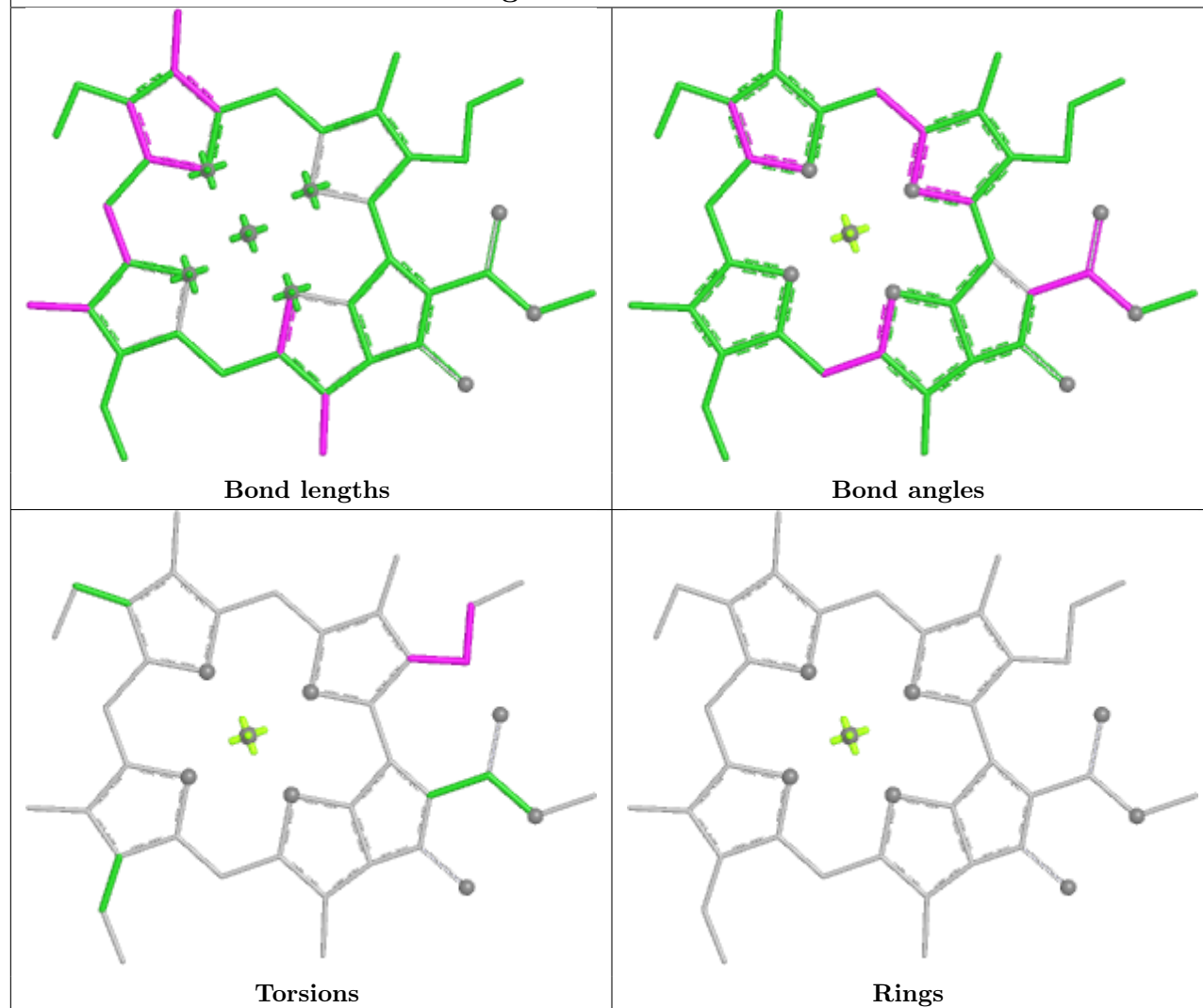
Ligand CLA 6 602



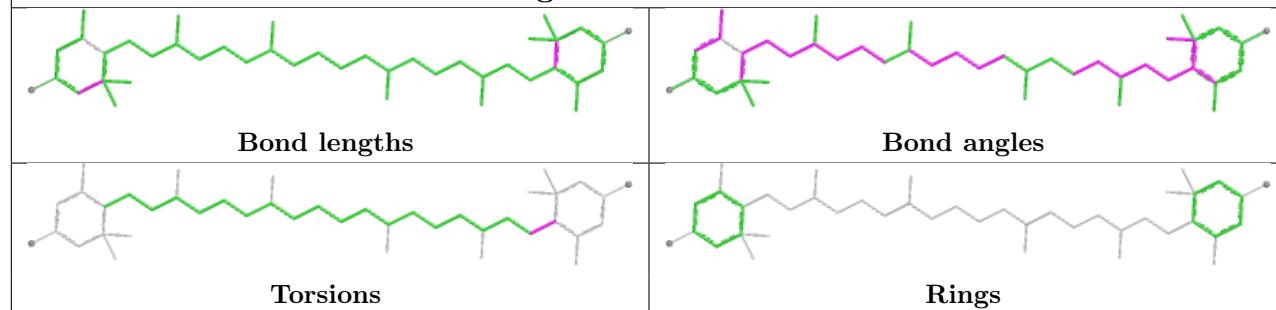




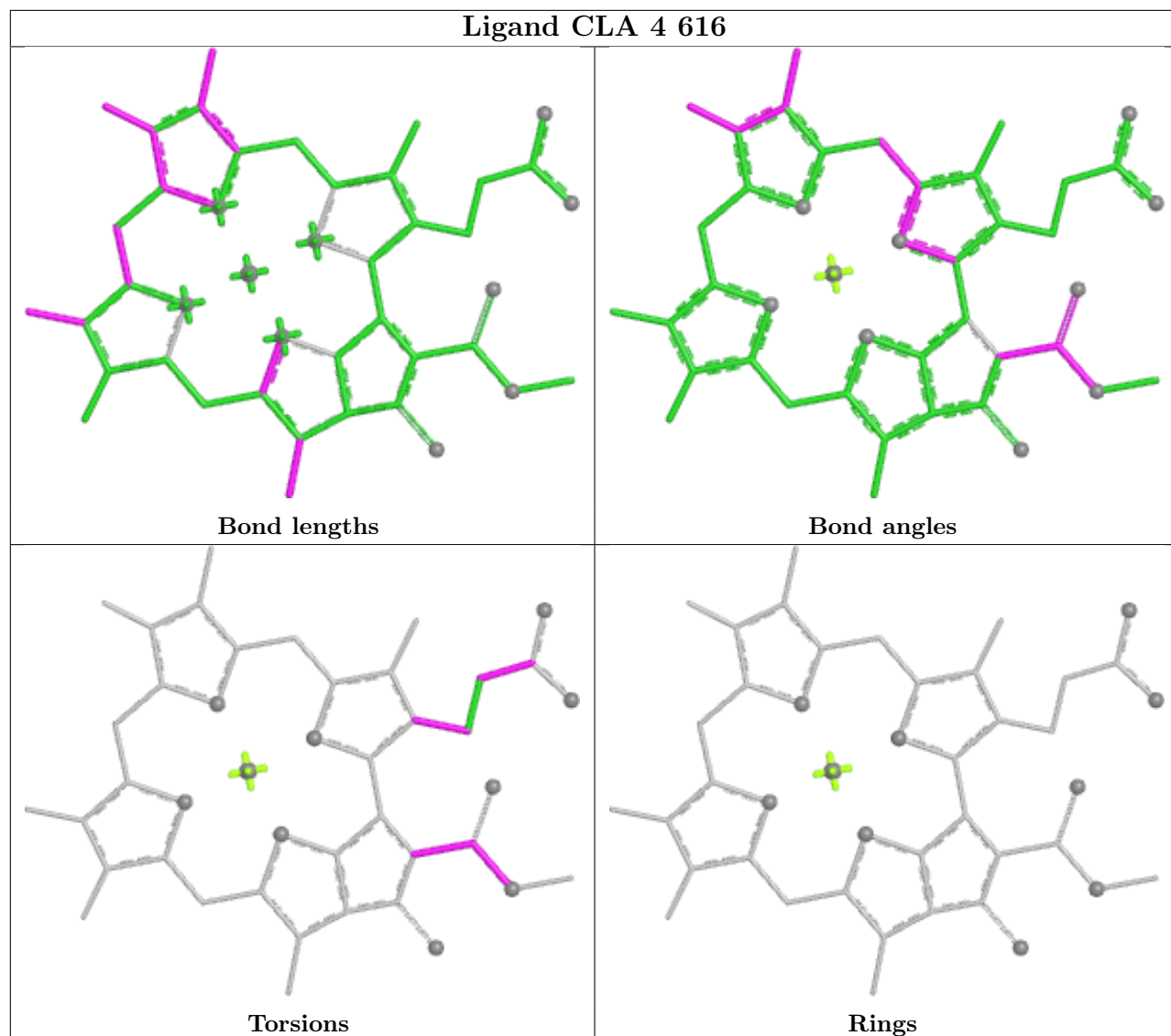
Ligand CLA B 812



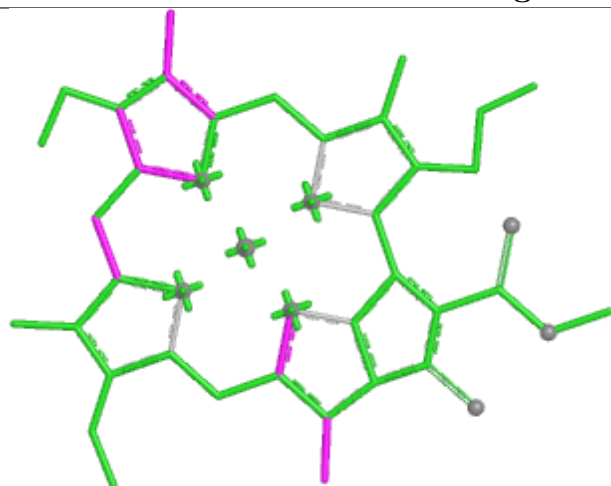
Ligand LUT 2 619



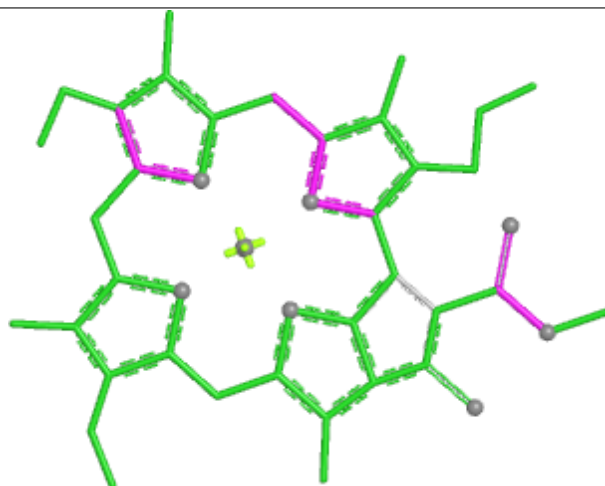
Ligand CLA 4 616



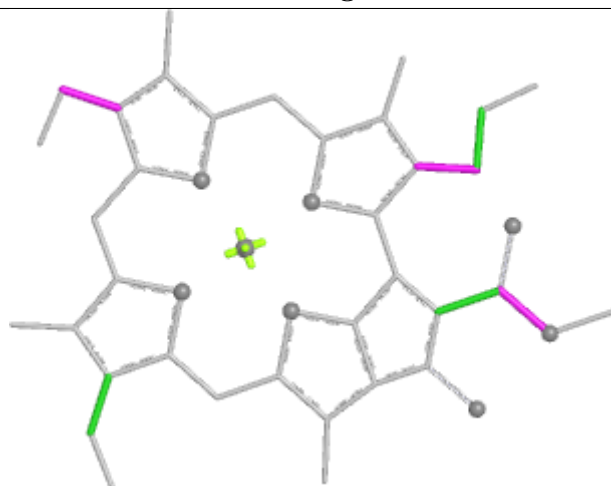
Ligand CLA Y 611



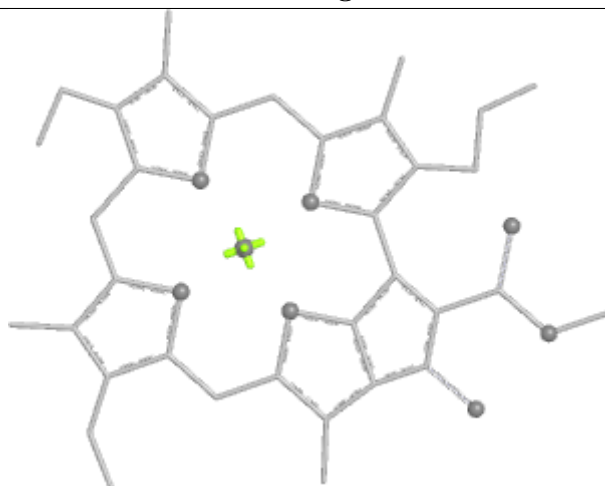
Bond lengths



Bond angles

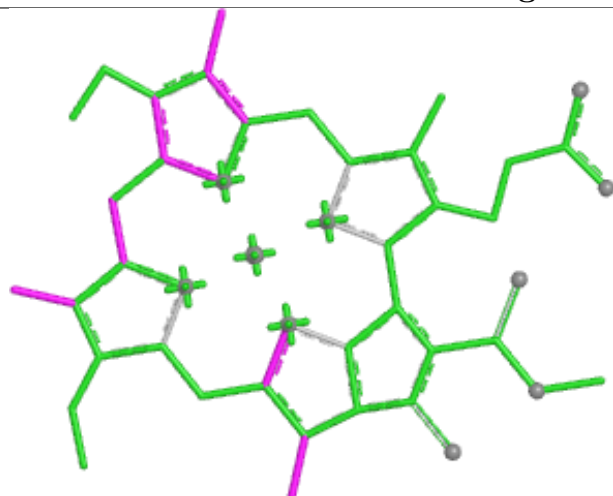


Torsions

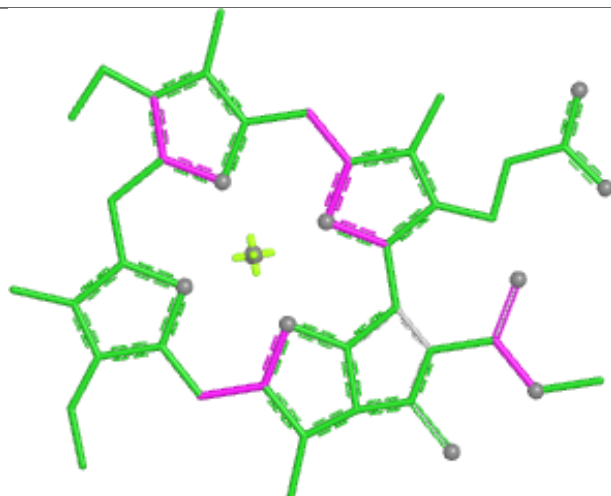


Rings

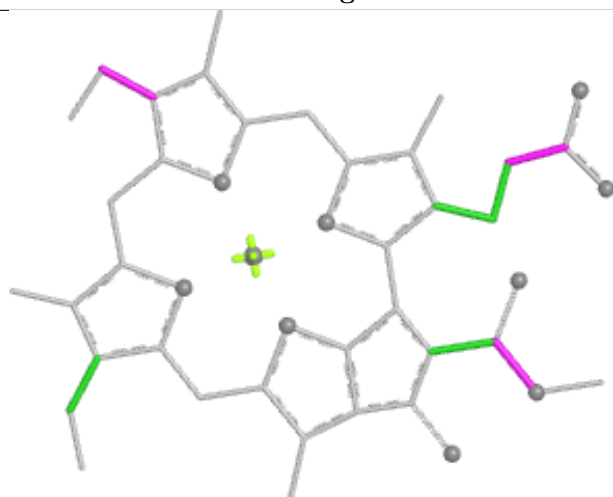
Ligand CLA 6 608



Bond lengths



Bond angles

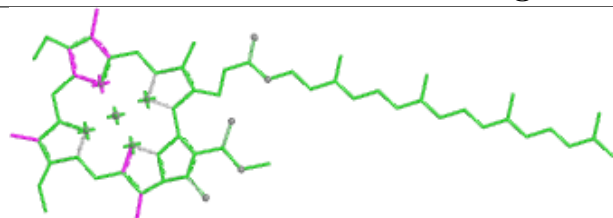


Torsions

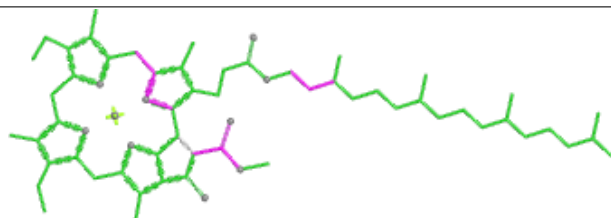


Rings

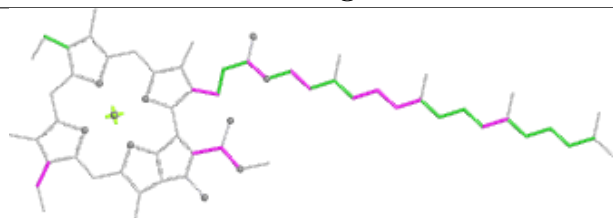
Ligand CLA A 804



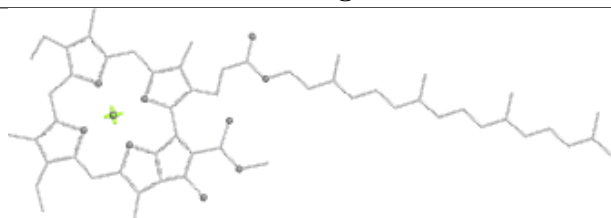
Bond lengths



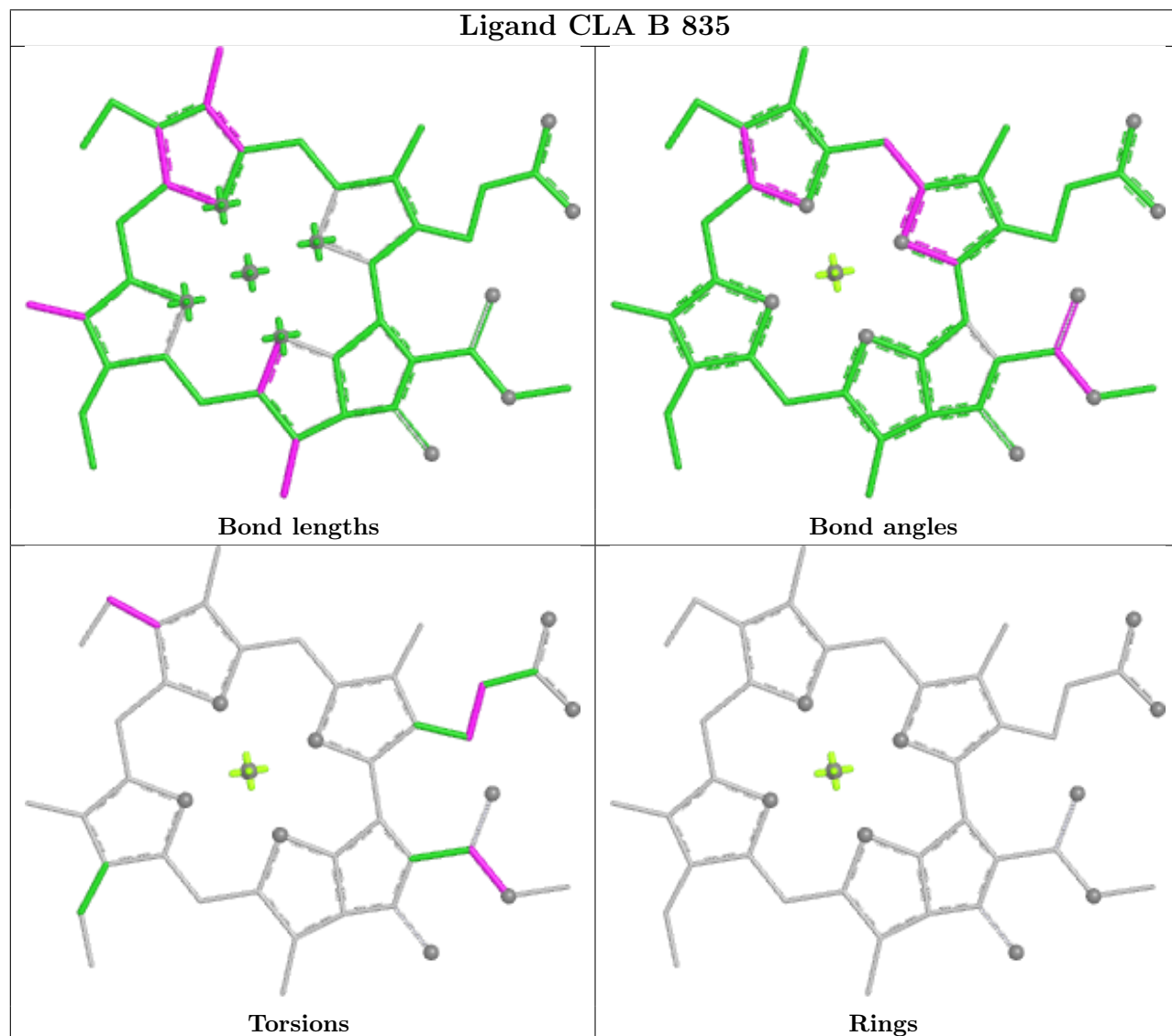
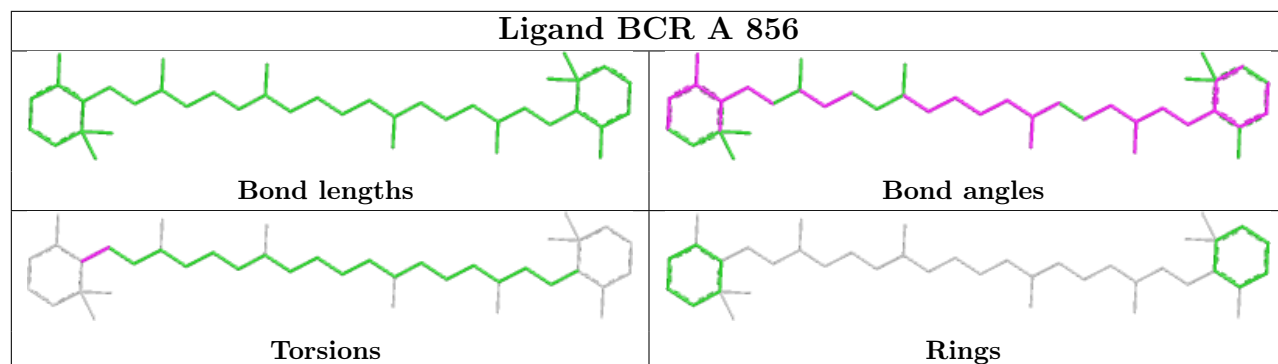
Bond angles



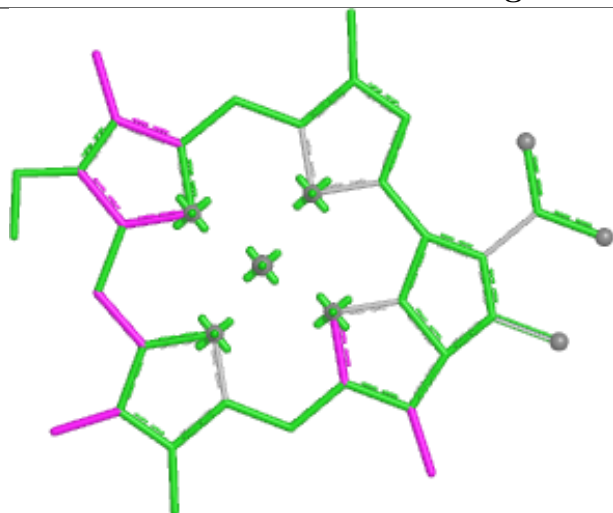
Torsions



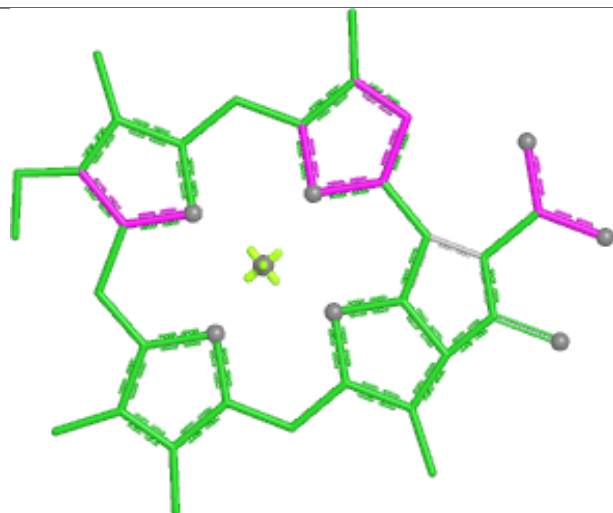
Rings



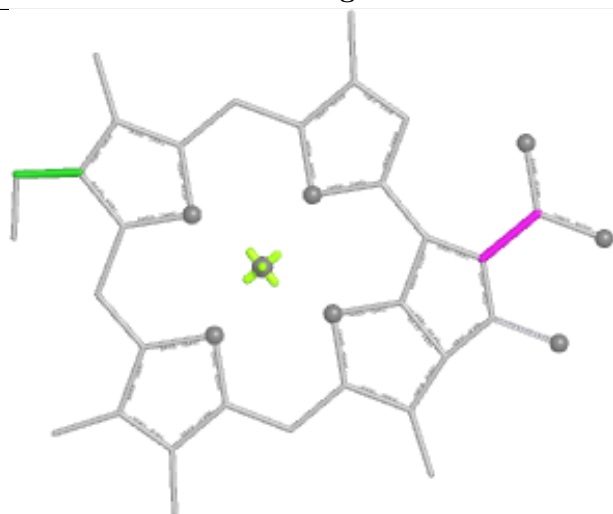
Ligand CLA O 2001



Bond lengths



Bond angles

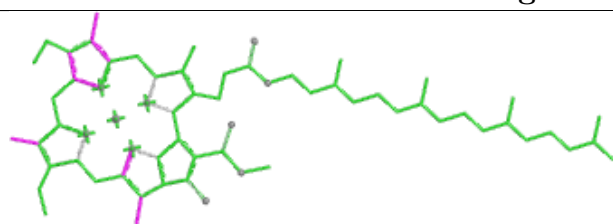


Torsions

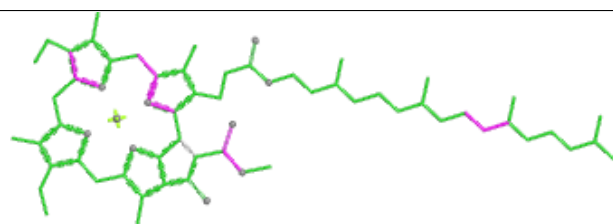


Rings

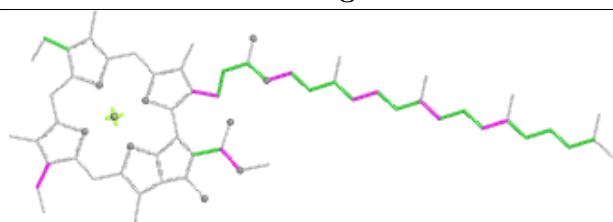
Ligand CLA 4 608



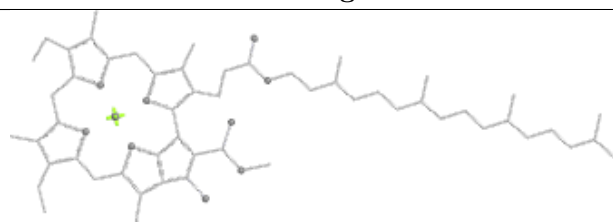
Bond lengths



Bond angles

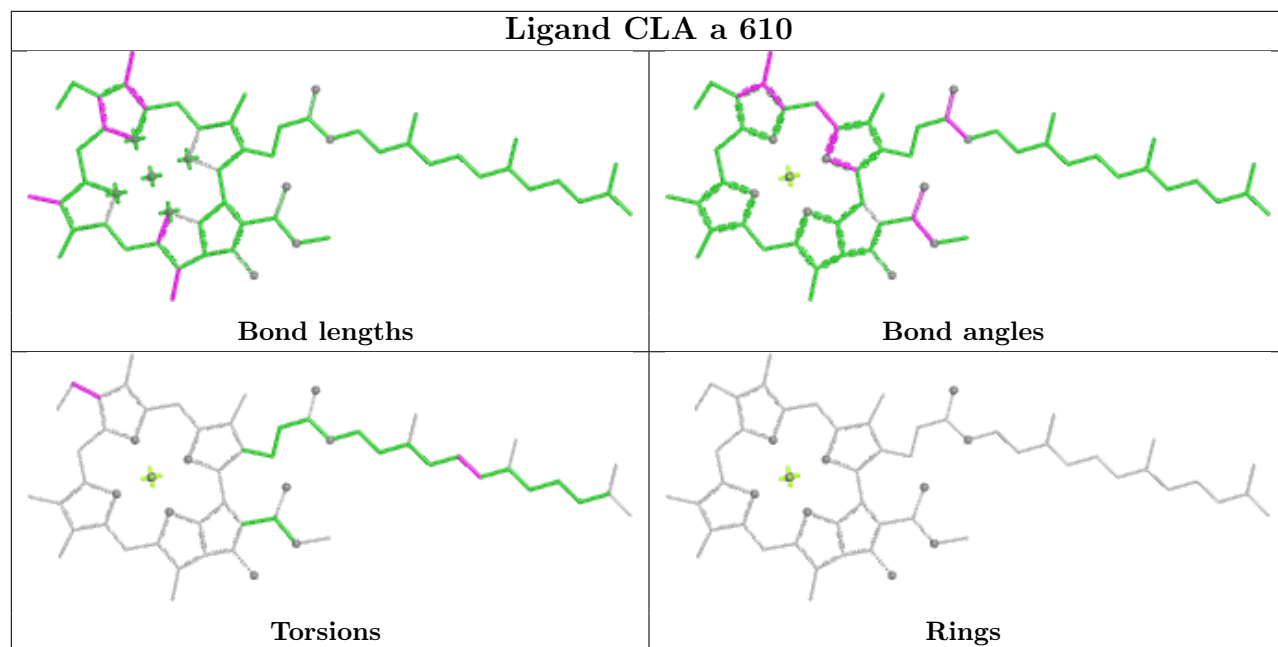


Torsions

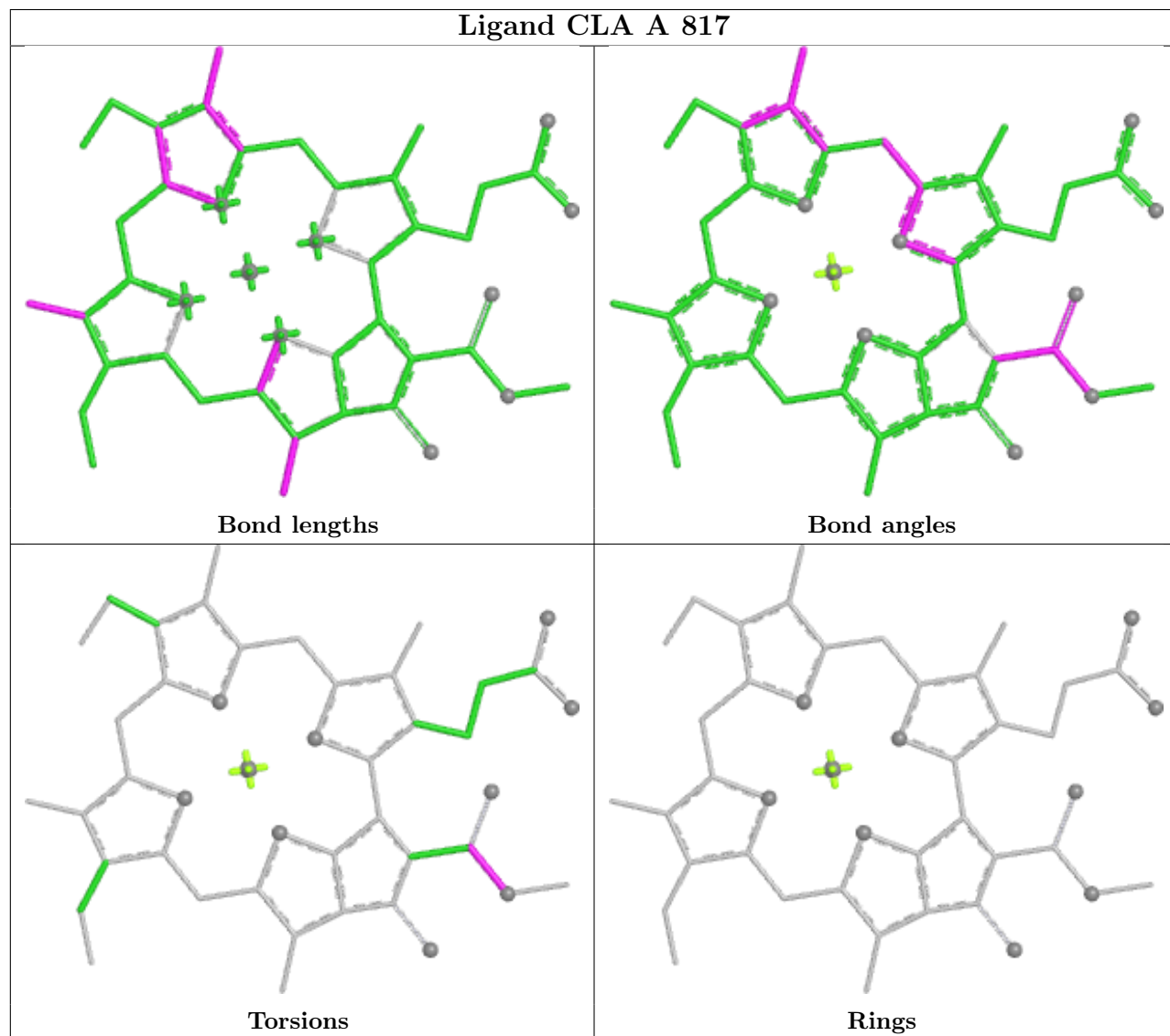


Rings

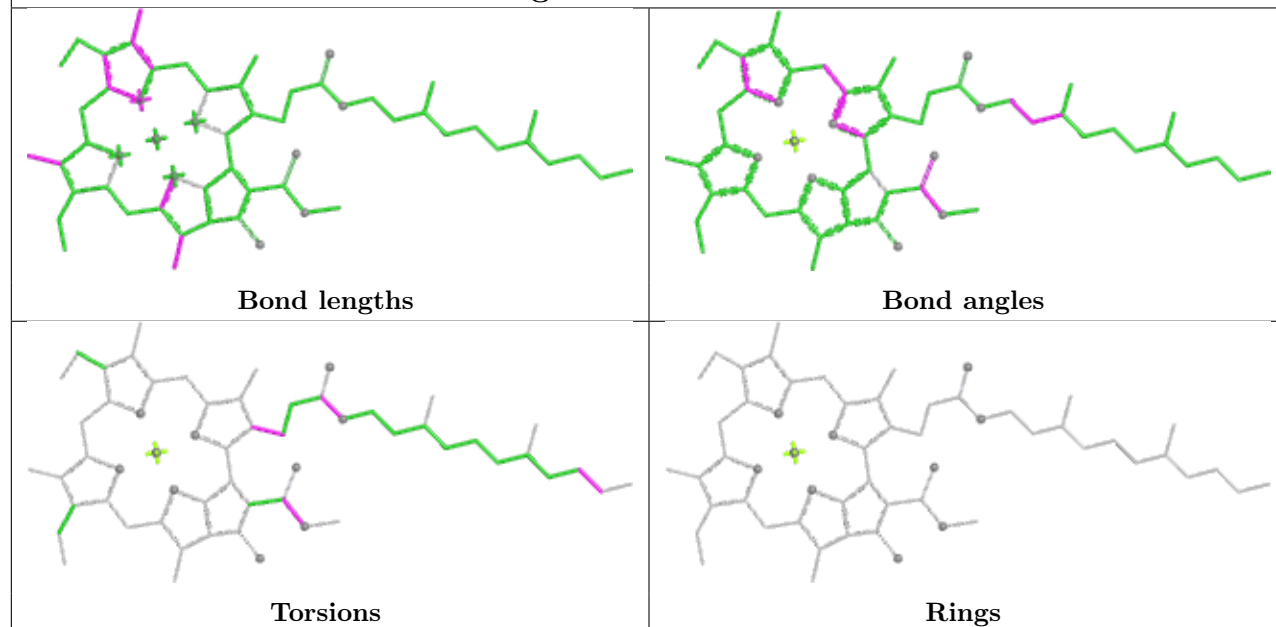
Ligand CLA a 610



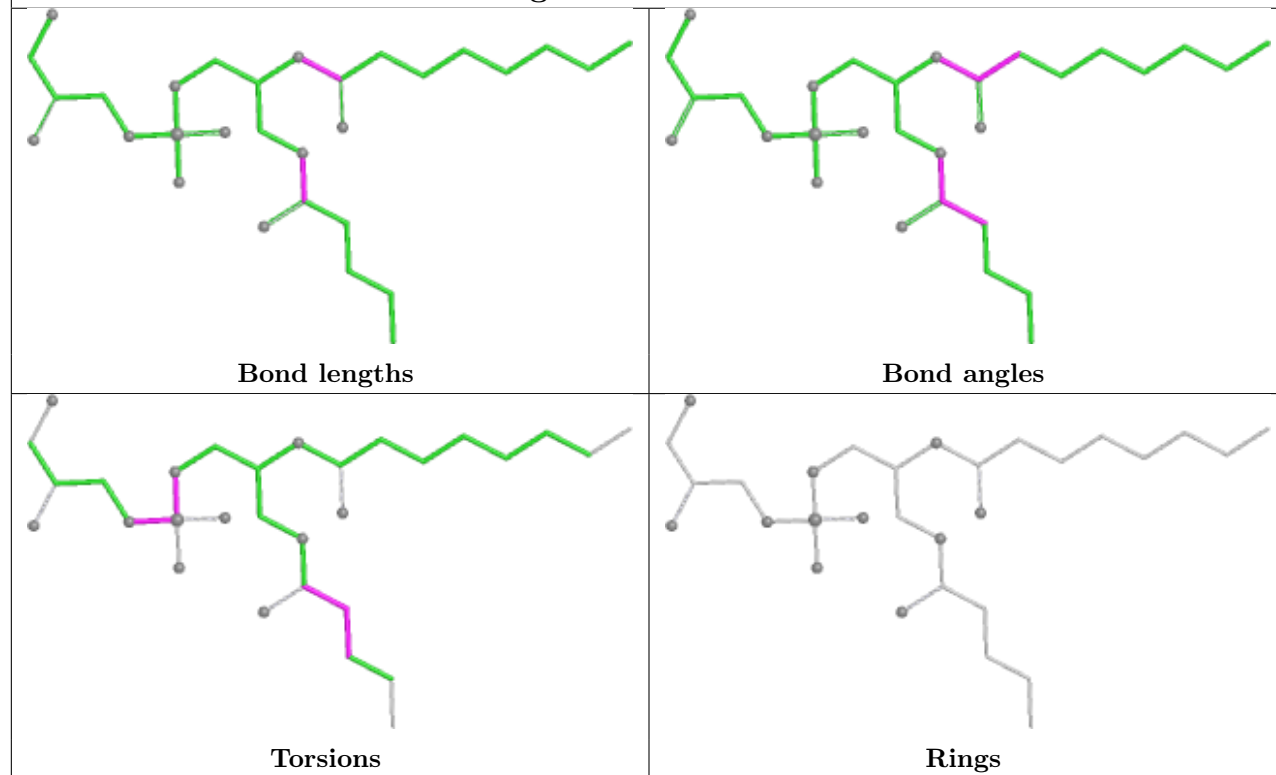
Ligand CLA A 817

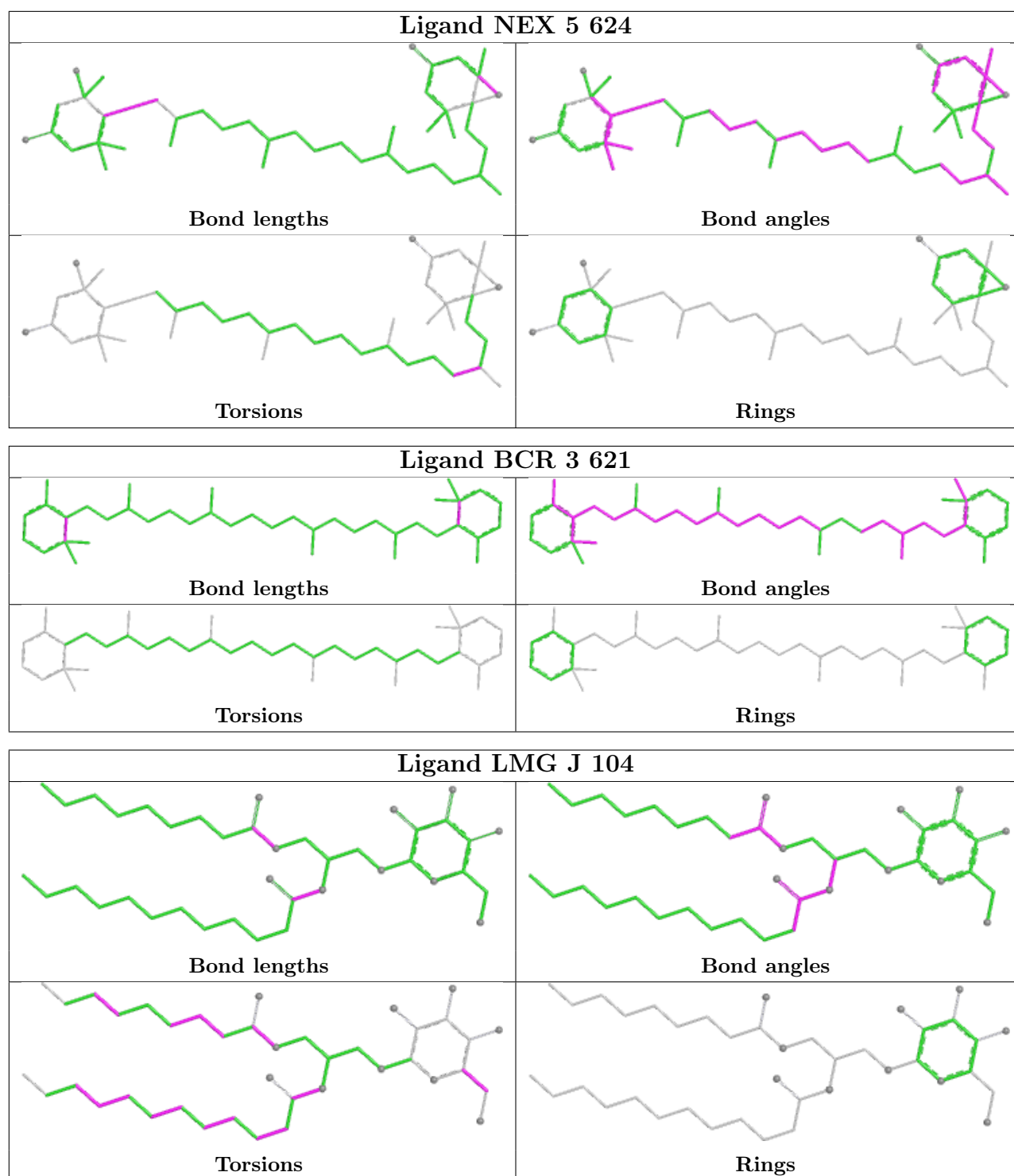


Ligand CLA A 827

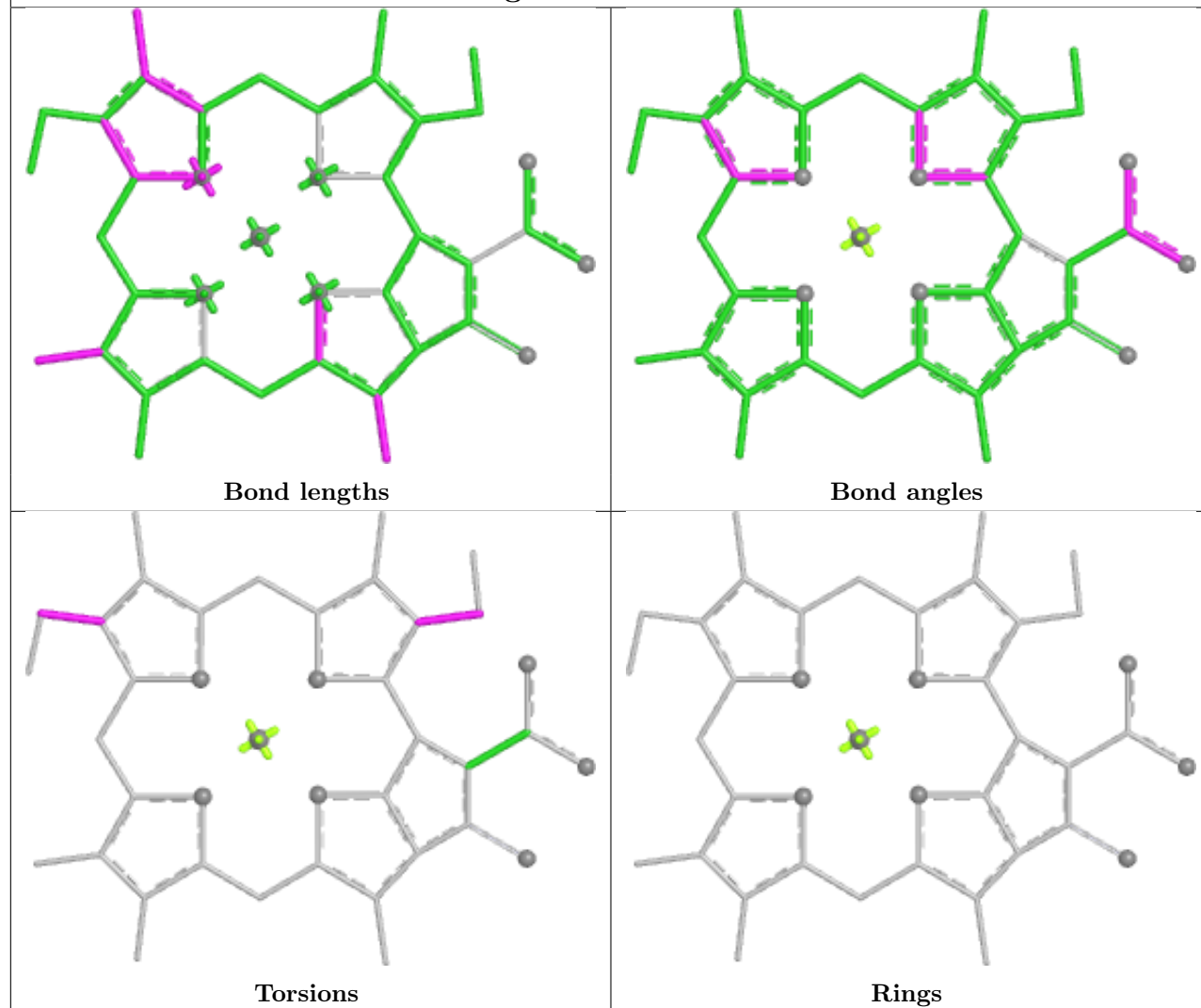


Ligand LHG A 847

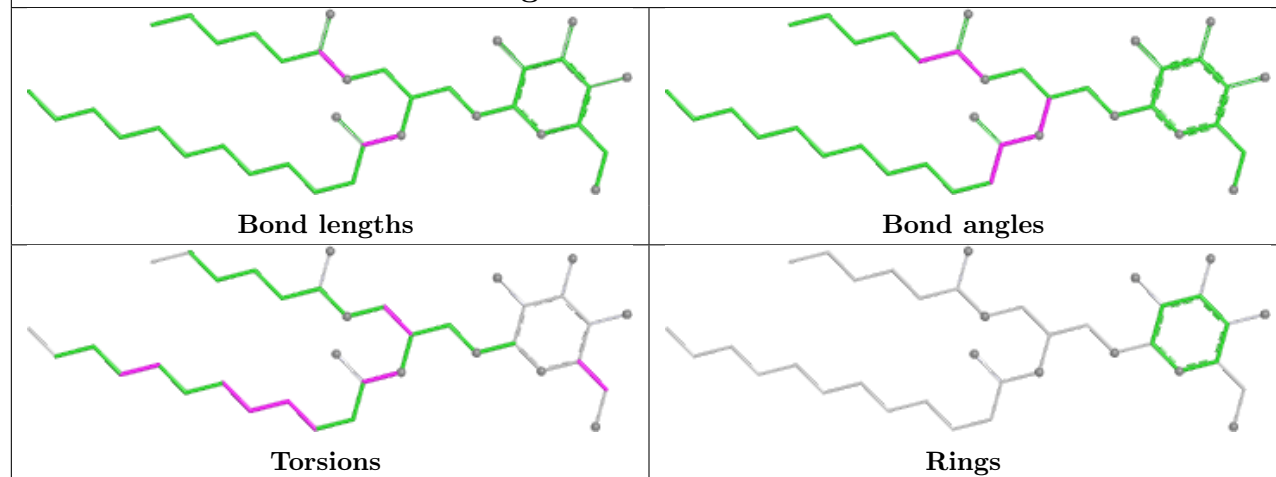


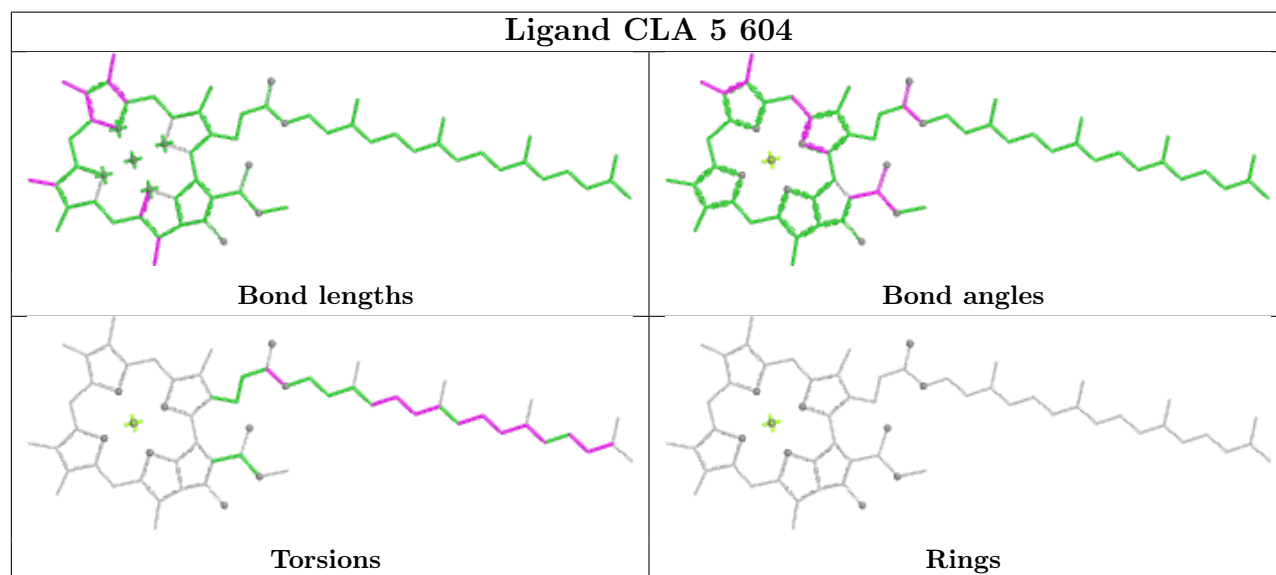
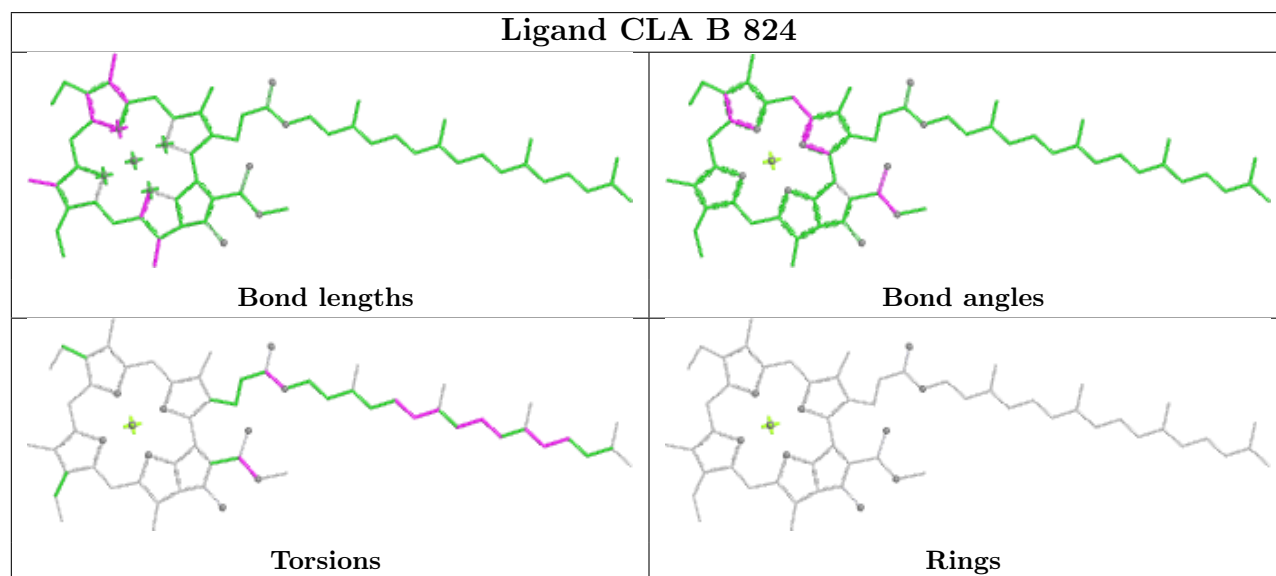
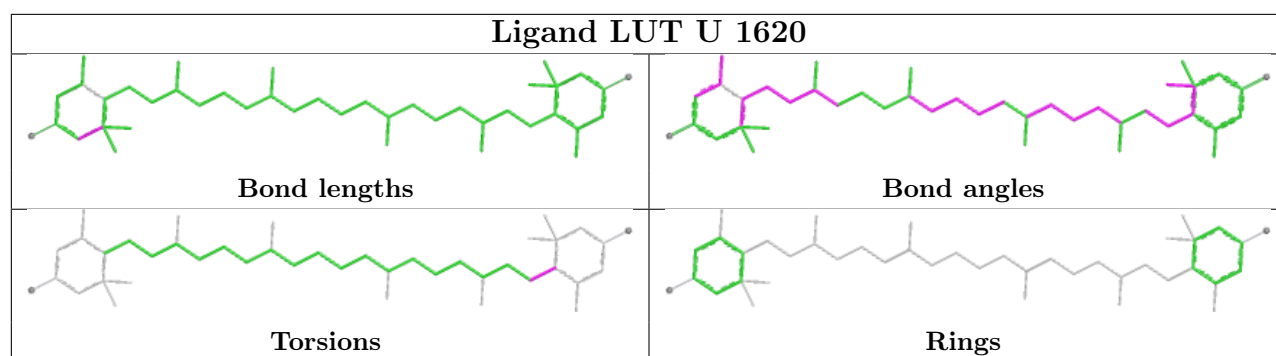


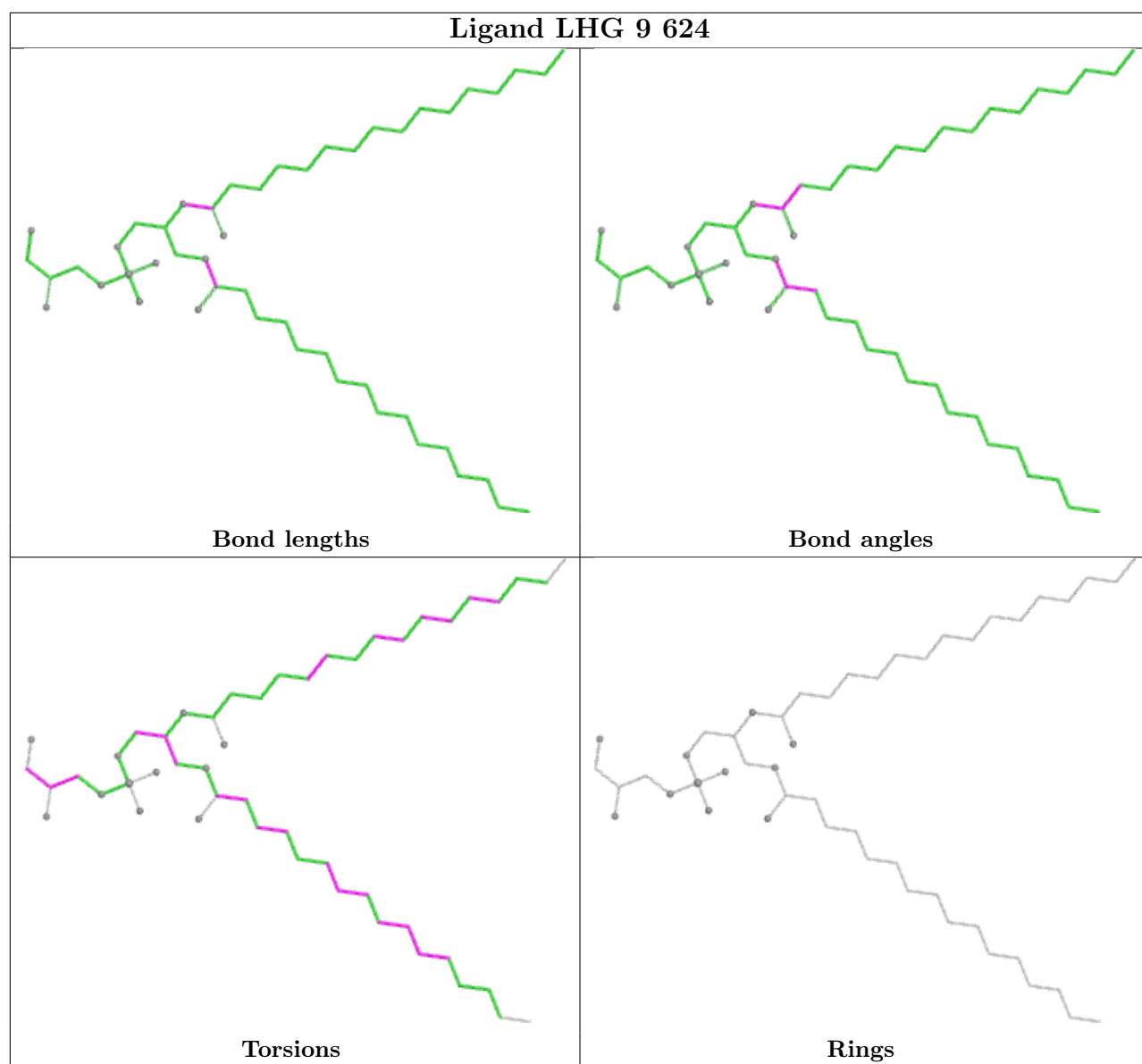
Ligand CLA 5 606

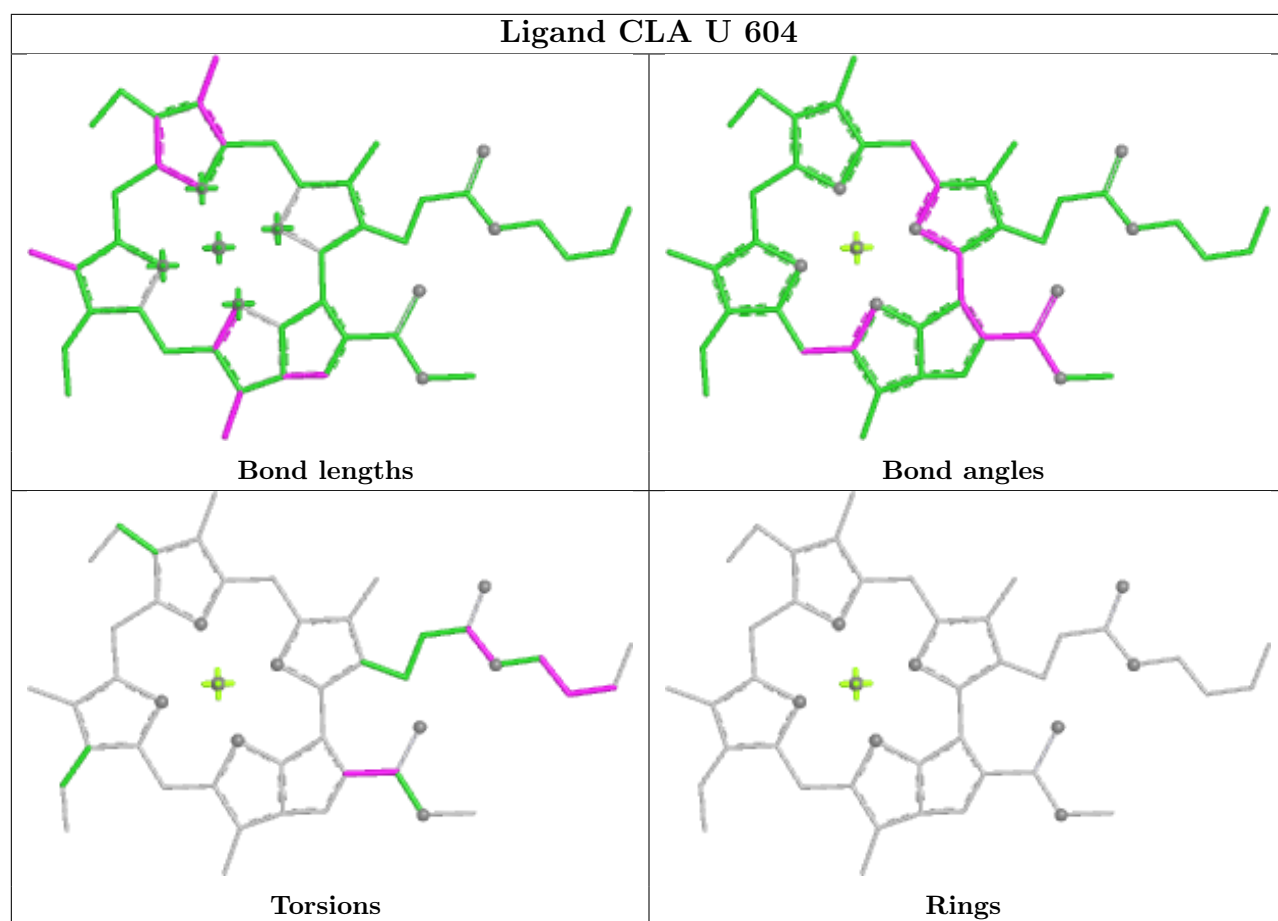


Ligand LMG L 2631

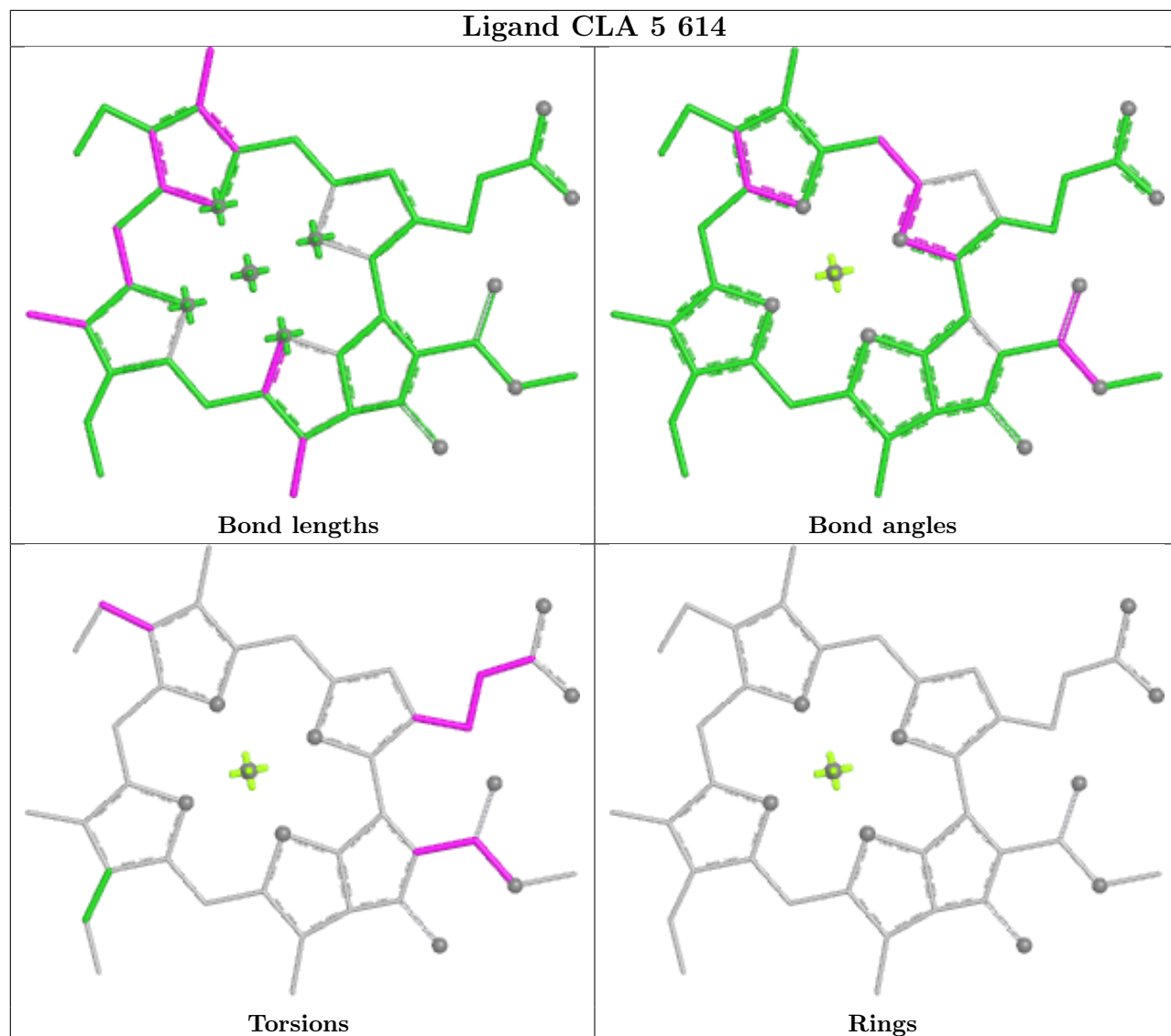




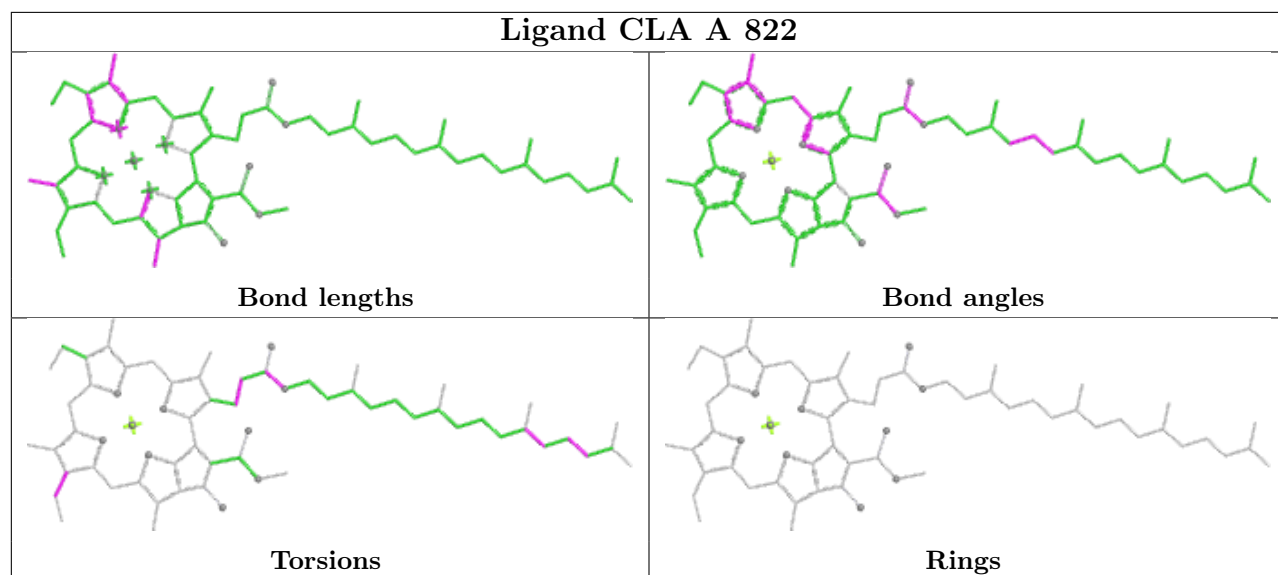


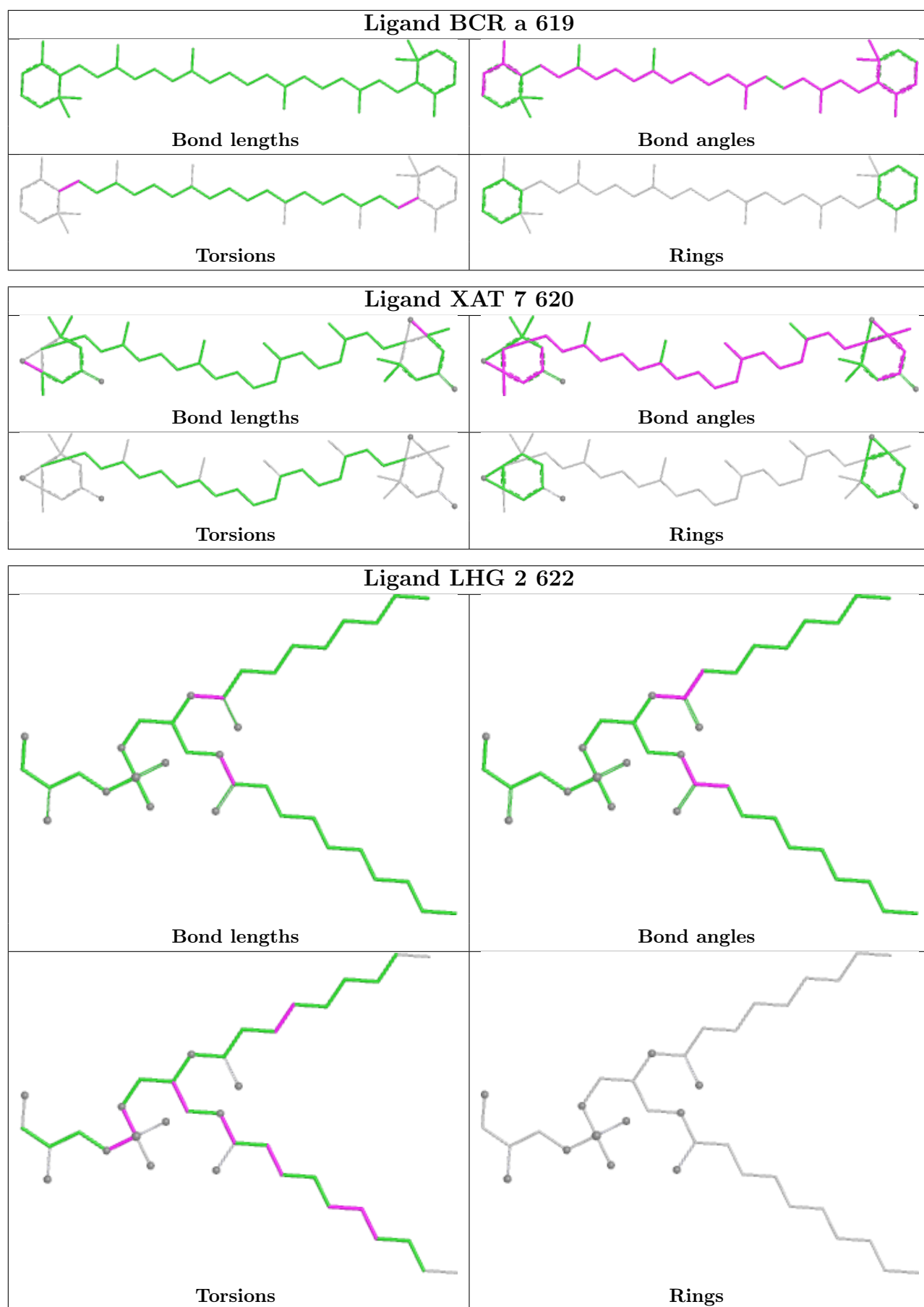


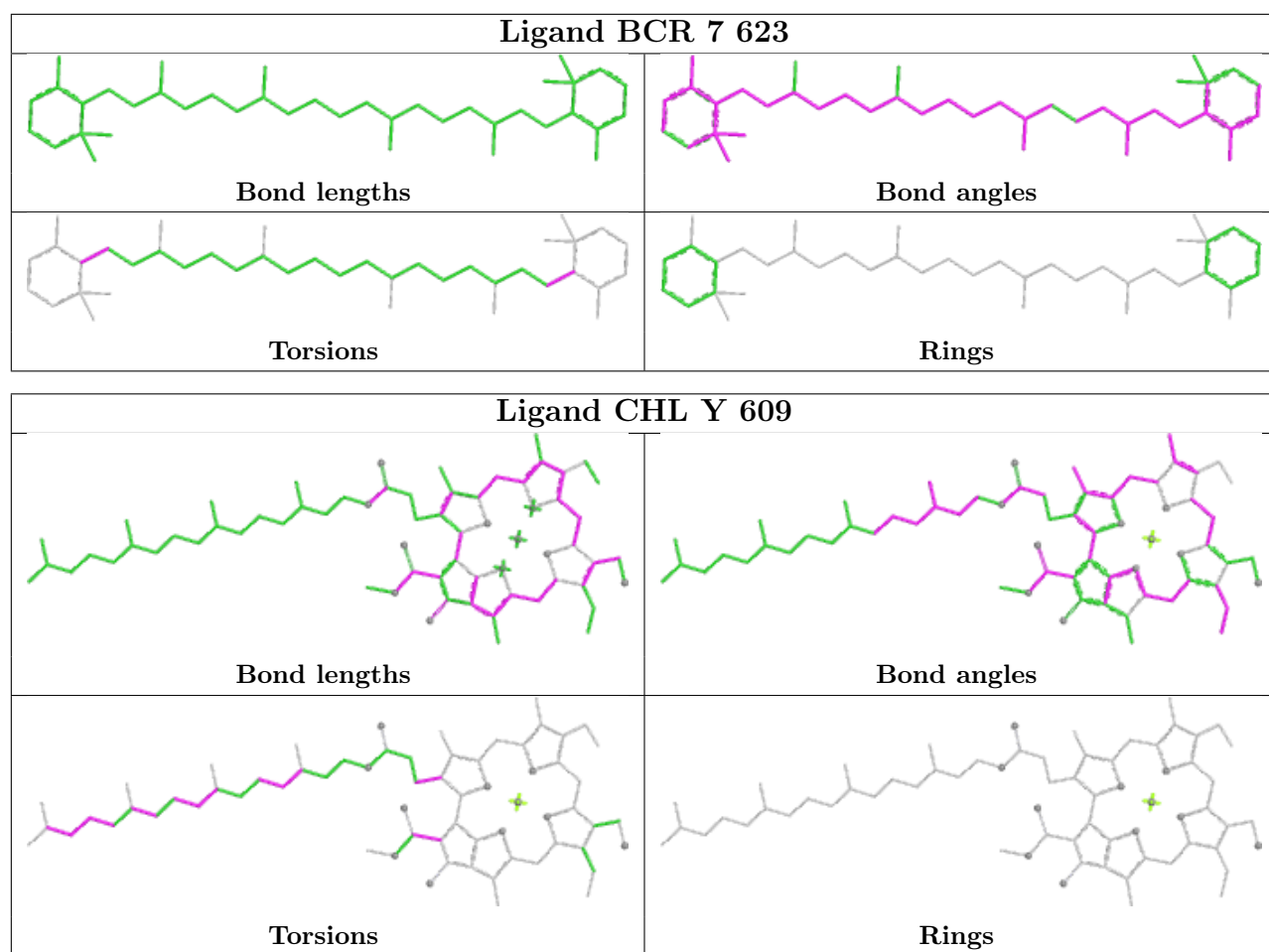
Ligand CLA 5 614



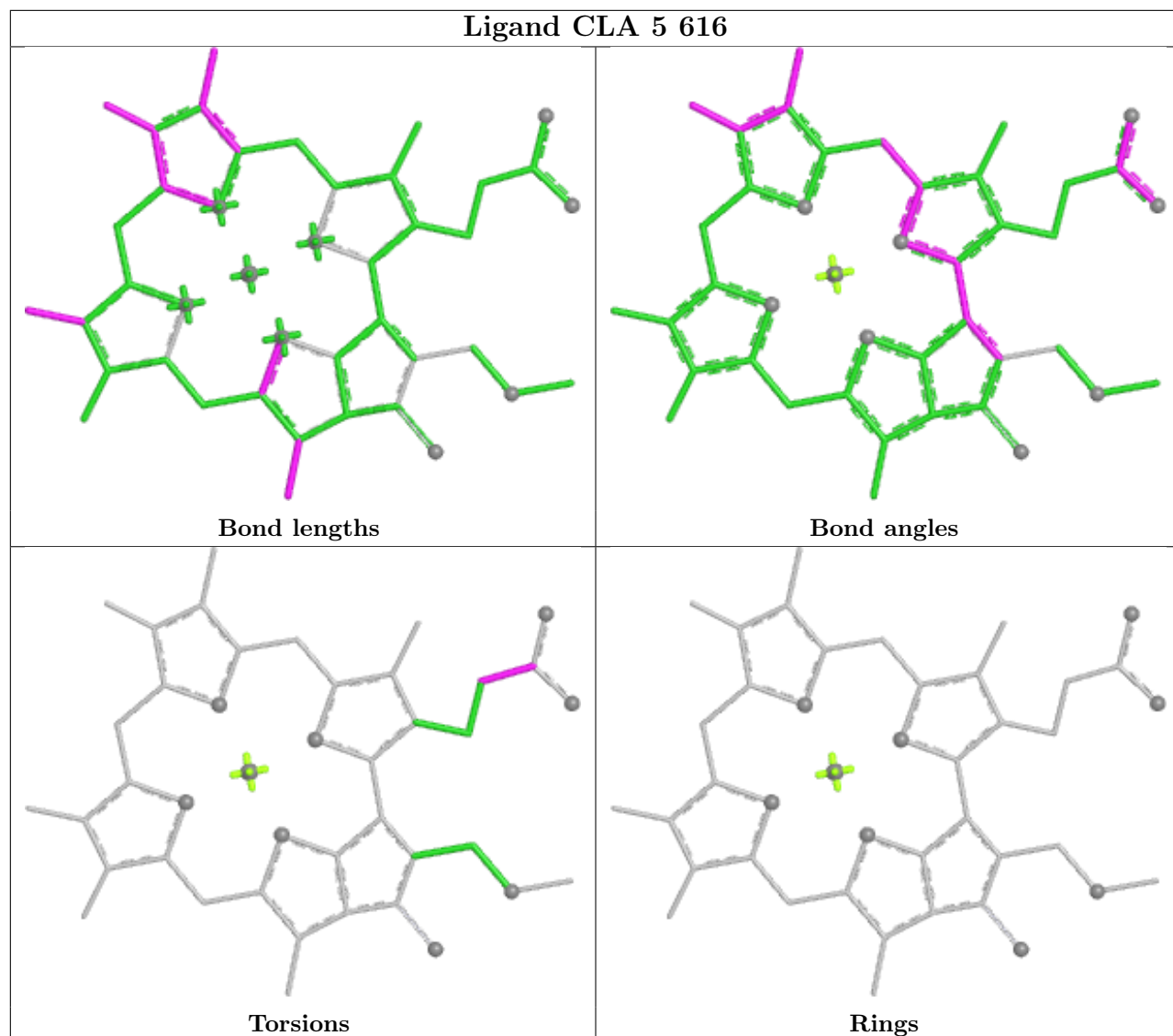
Ligand CLA A 822



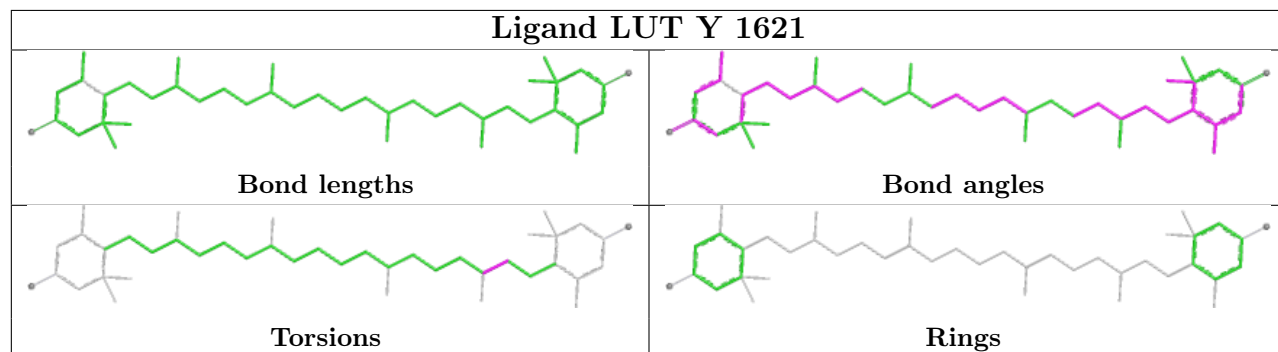


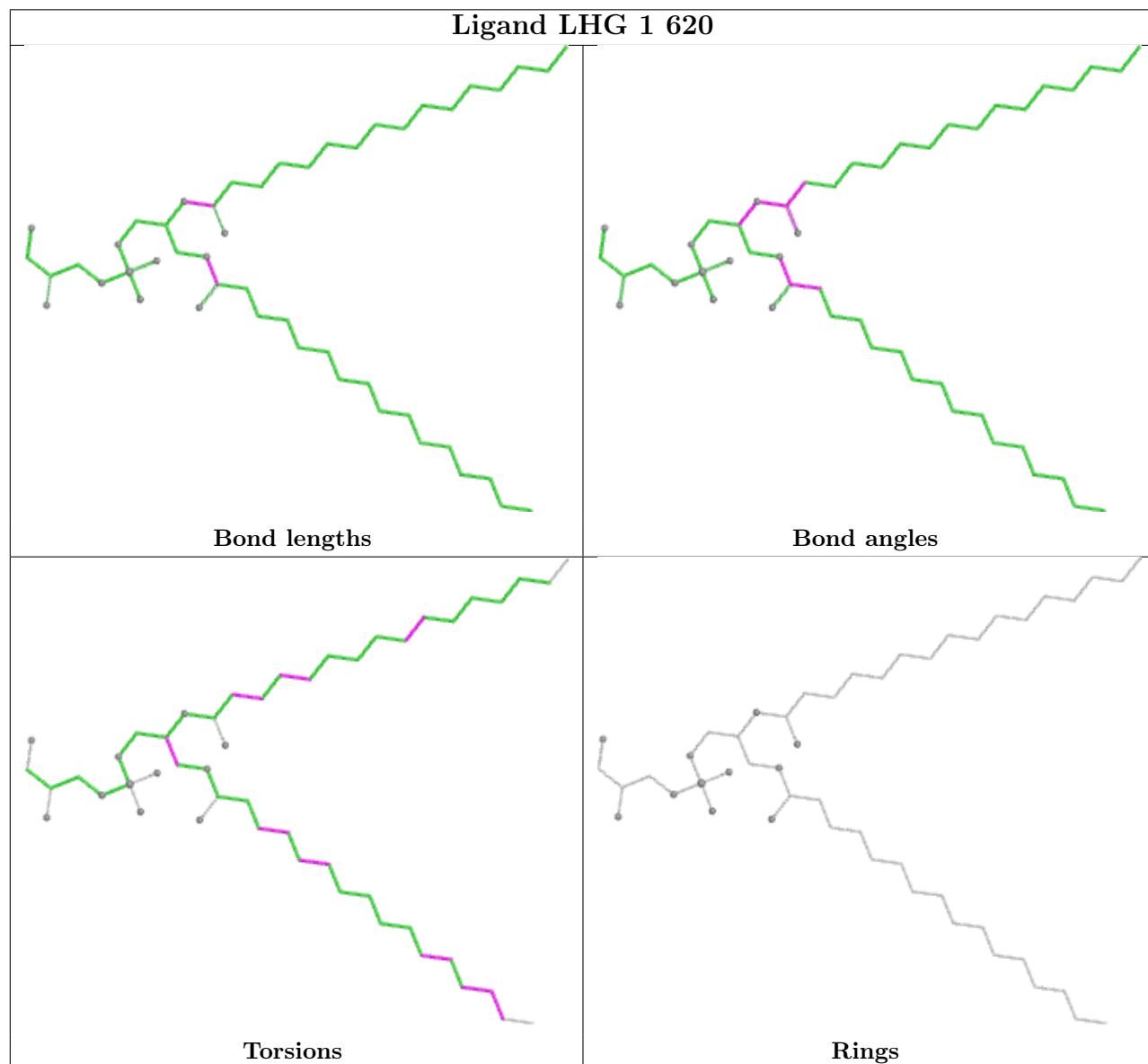
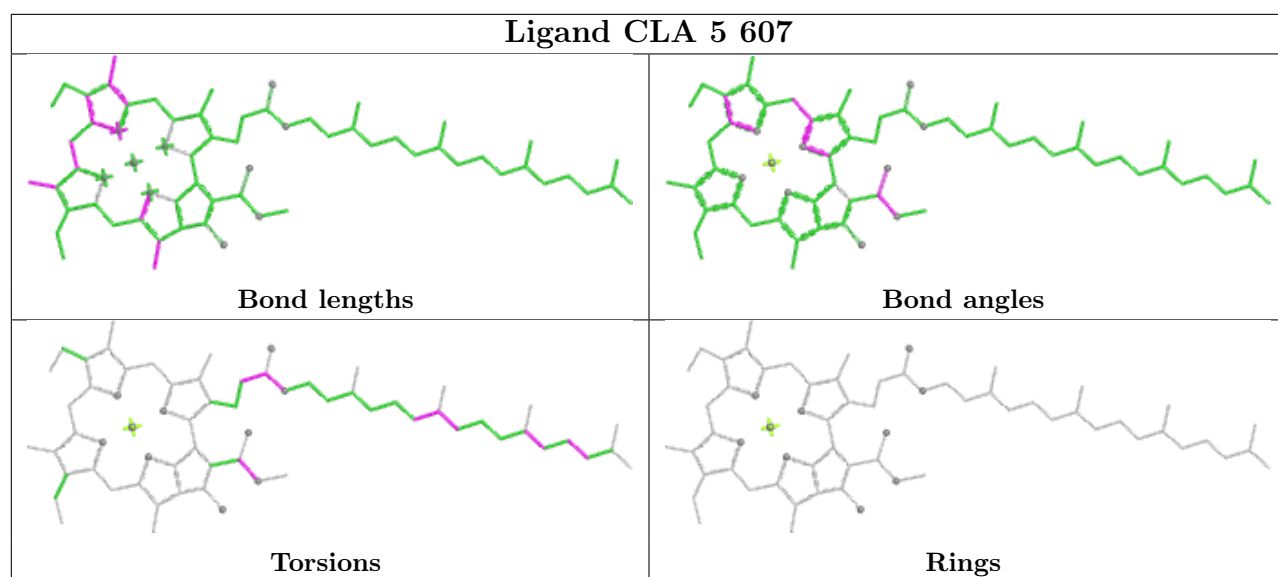


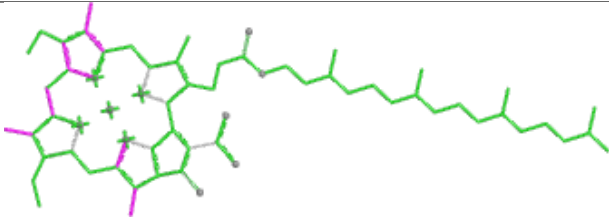
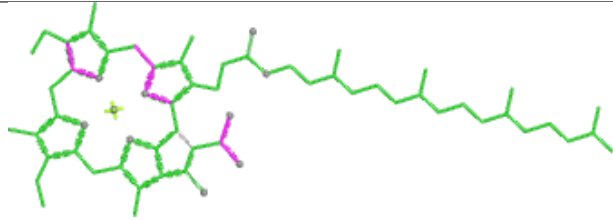
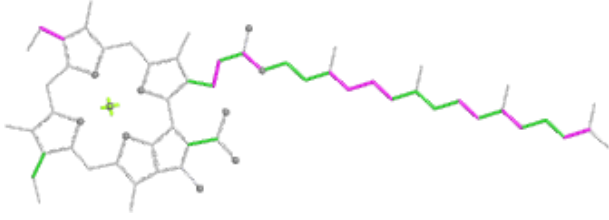
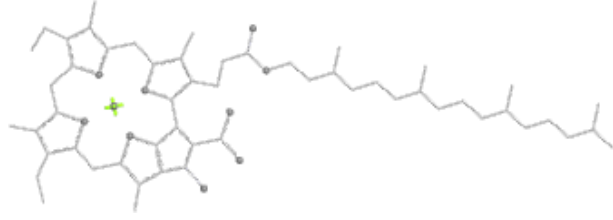
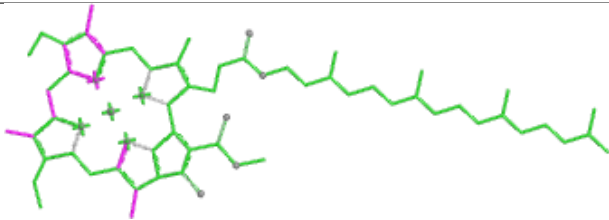
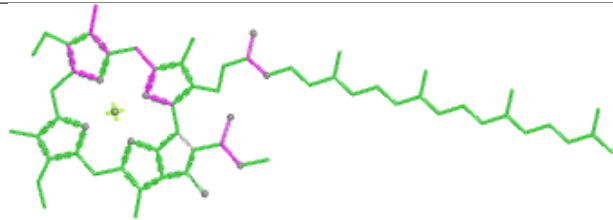
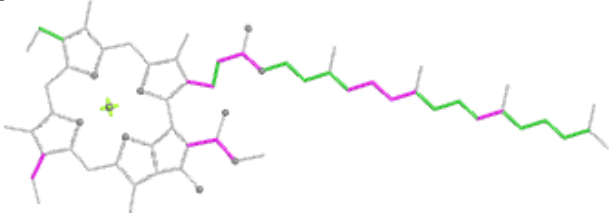
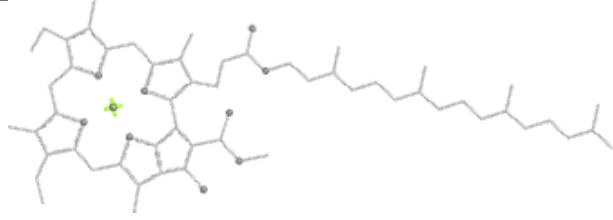
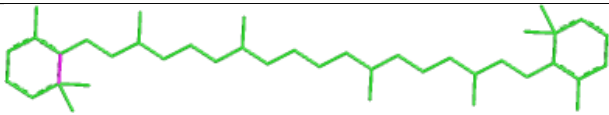
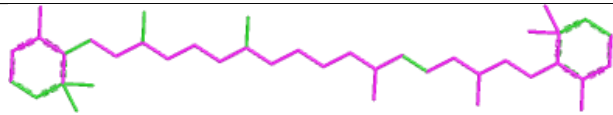
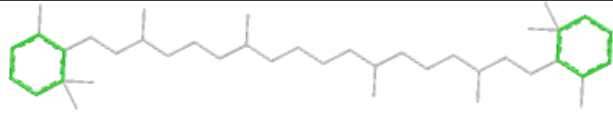
Ligand CLA 5 616



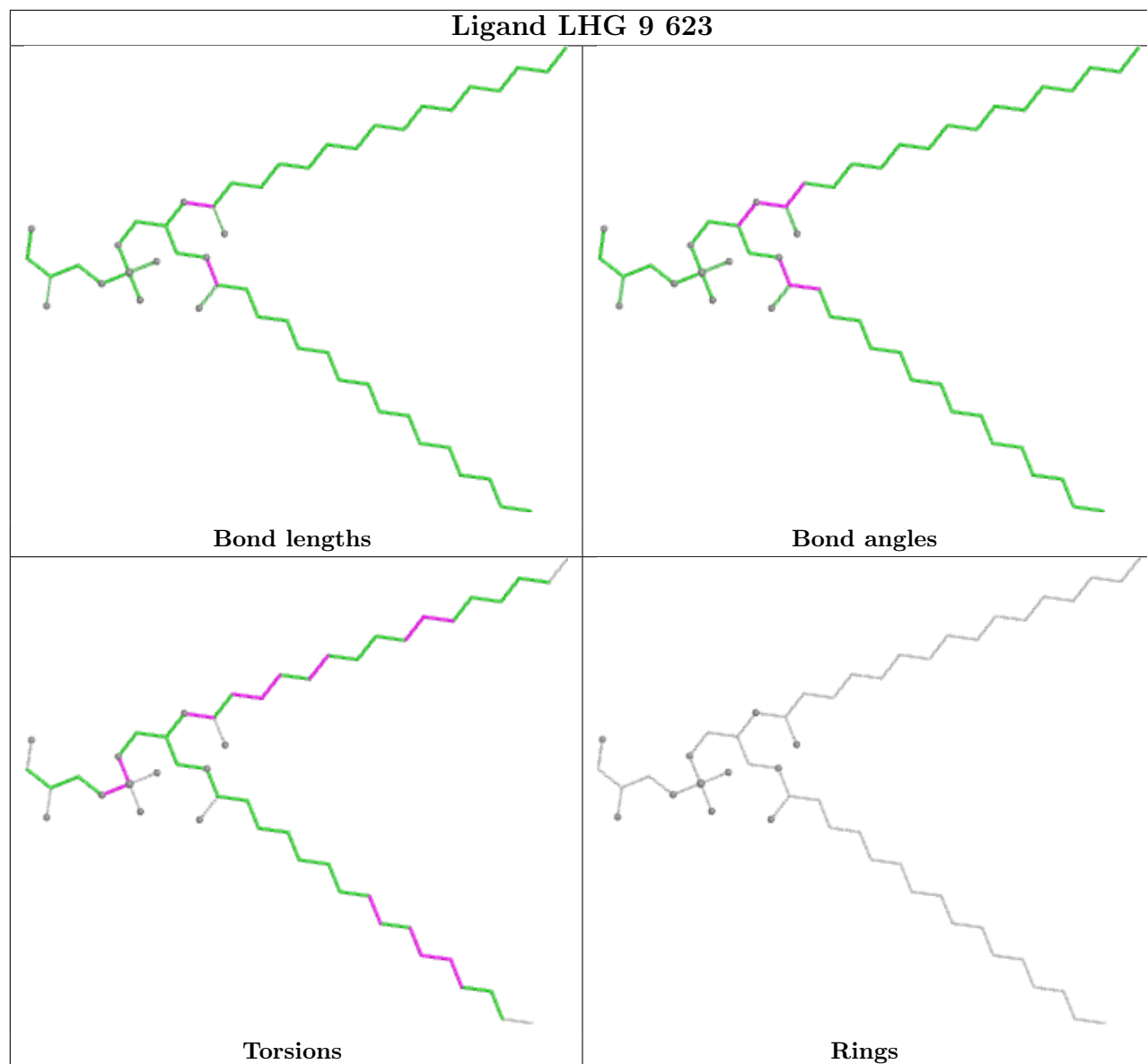
Ligand LUT Y 1621



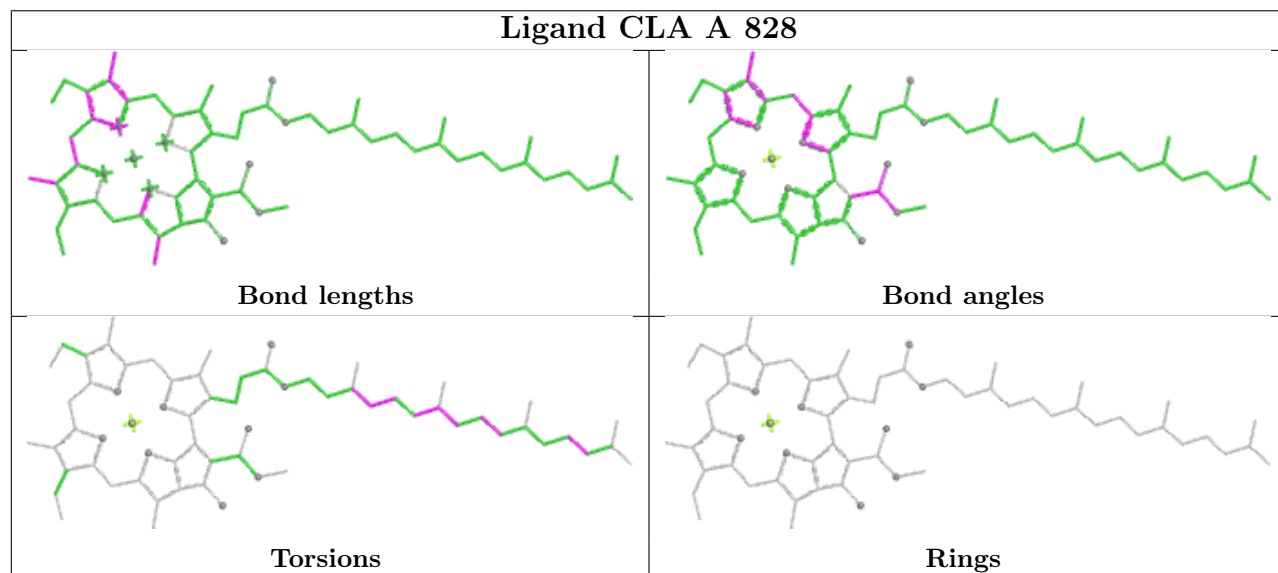


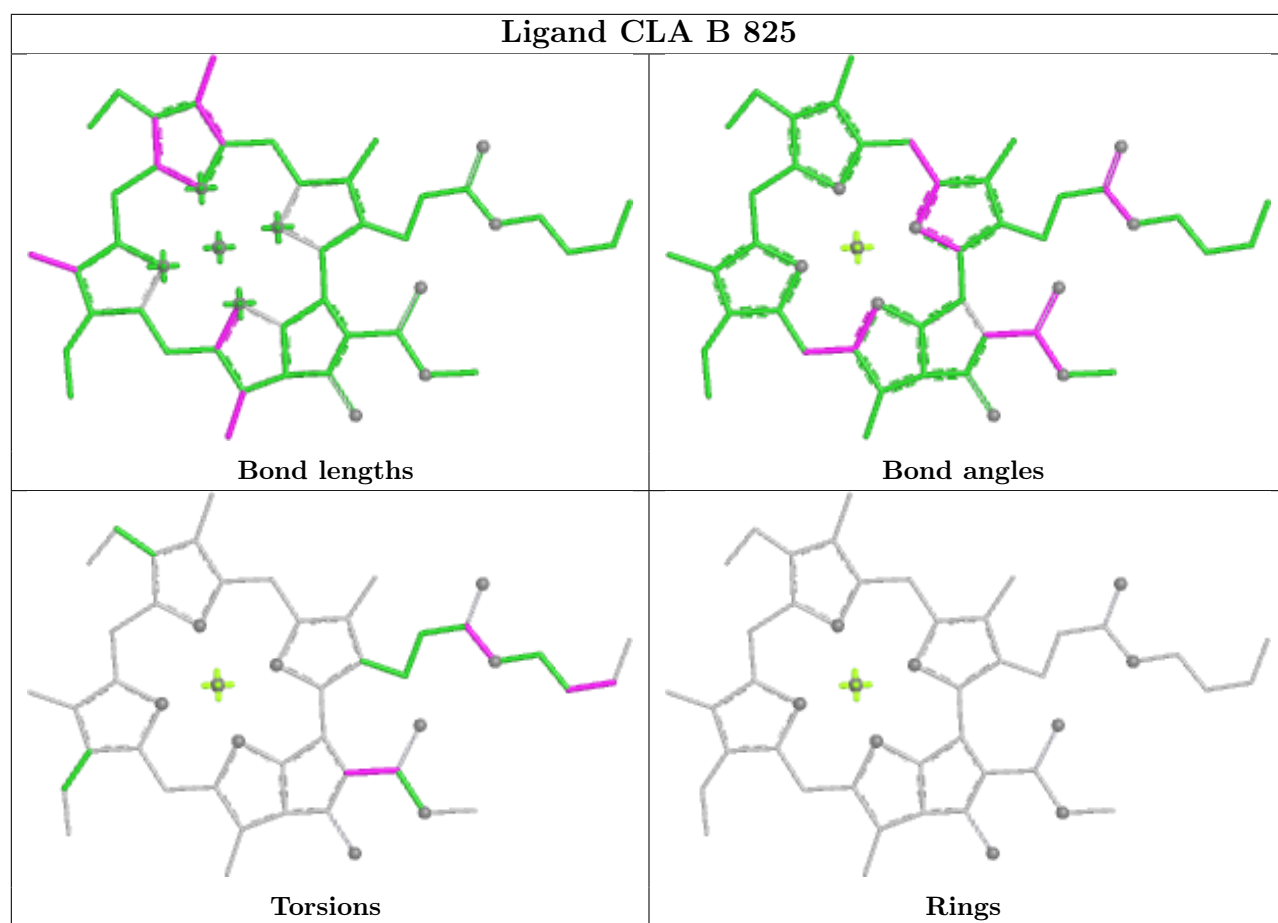
Ligand CLA 6 613	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings
Ligand CLA B 813	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings
Ligand BCR 4 621	
	
Bond lengths	
	Bond angles
	
Torsions	
	Rings

Ligand LHG 9 623

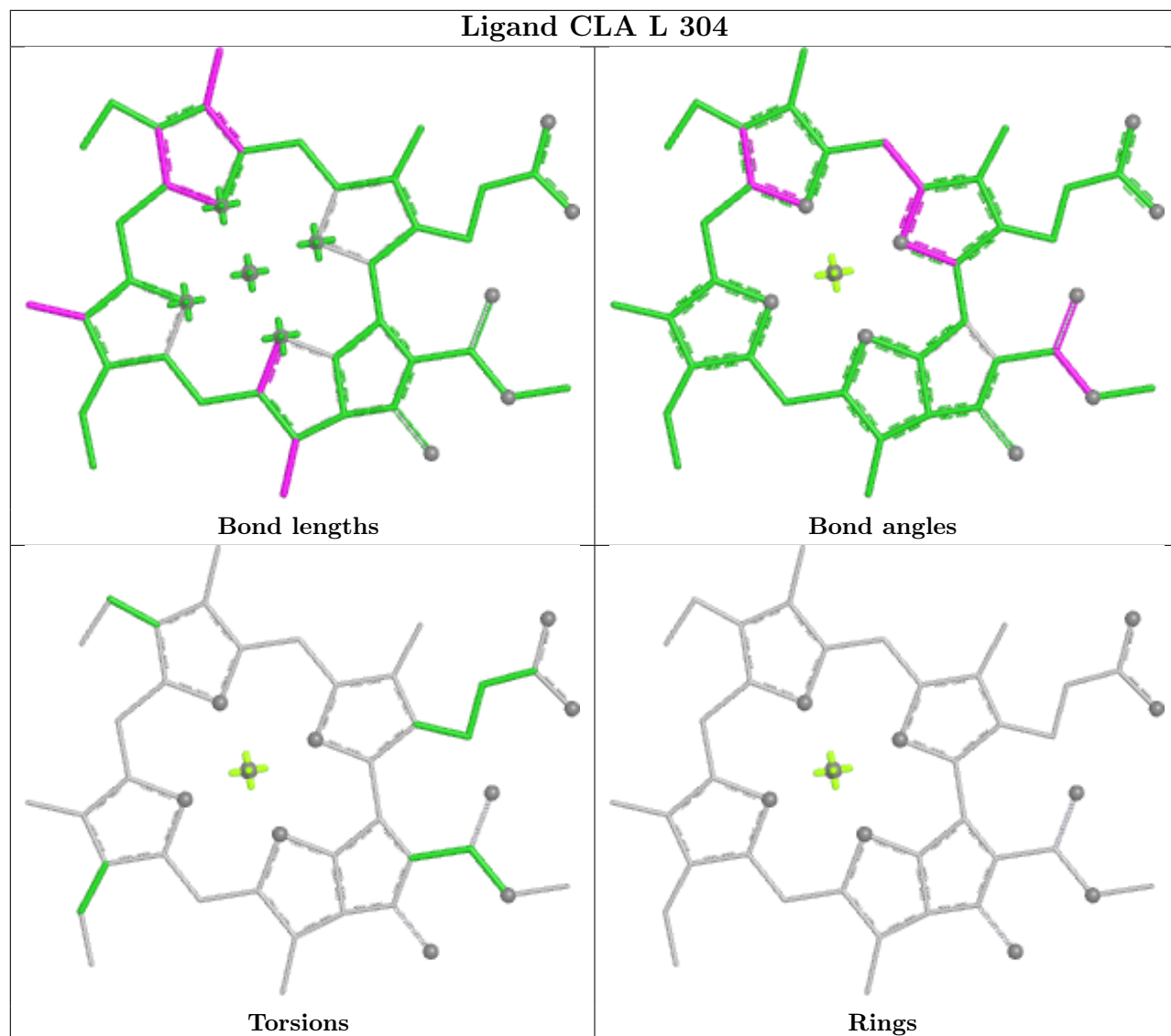


Ligand CLA A 828

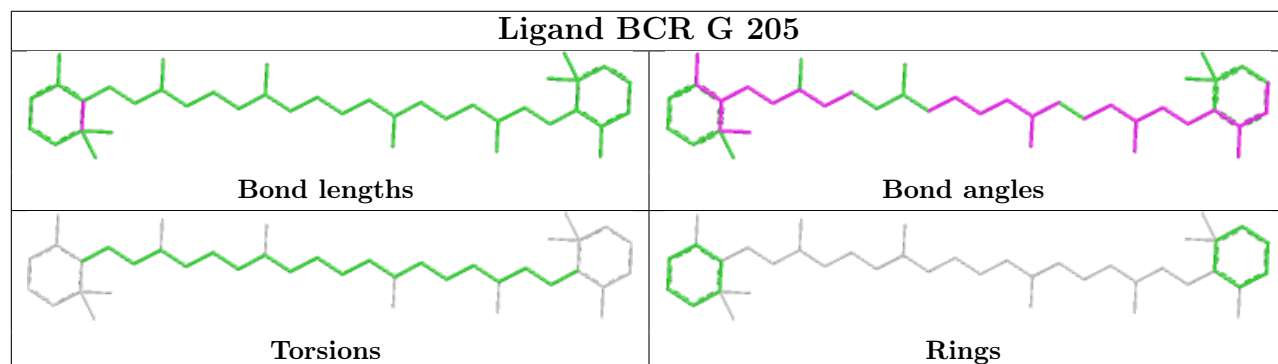


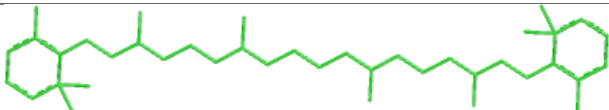
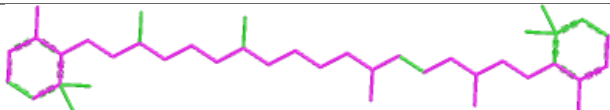
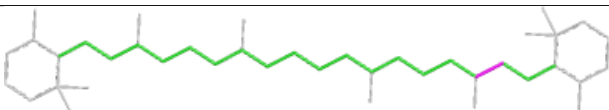
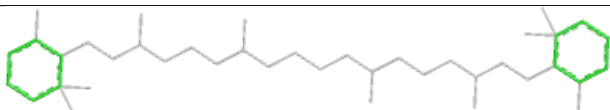


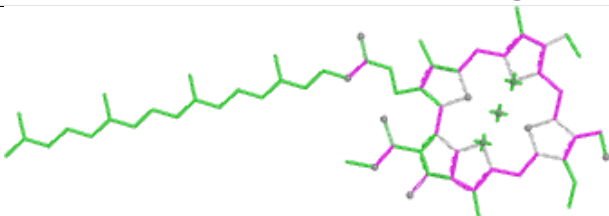
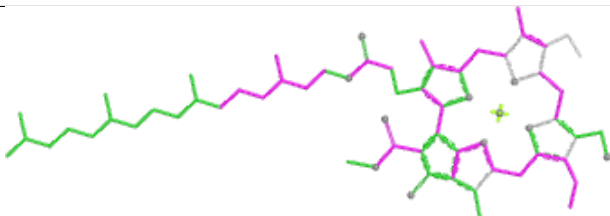
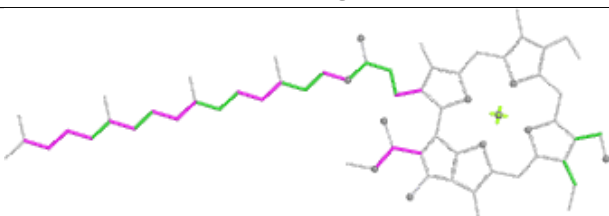
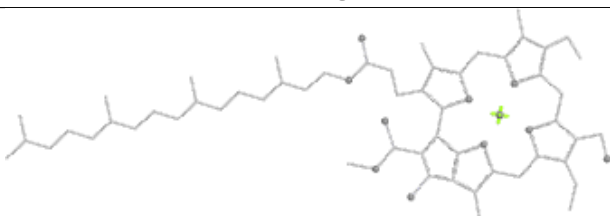
Ligand CLA L 304



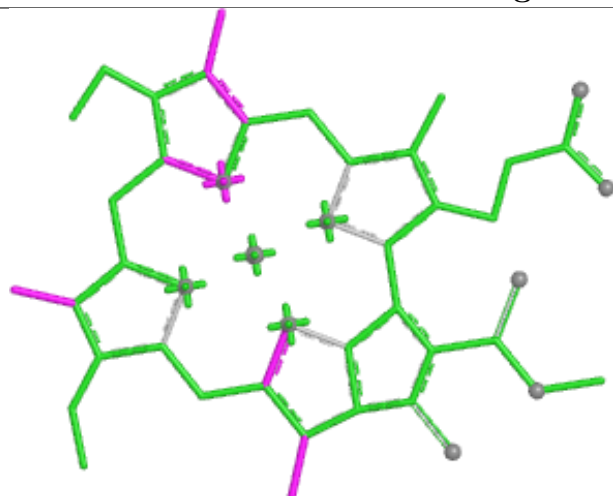
Ligand BCR G 205



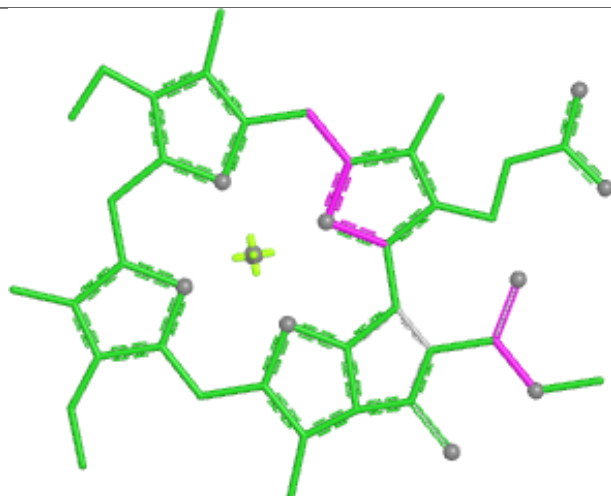
Ligand BCR 3 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL X 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

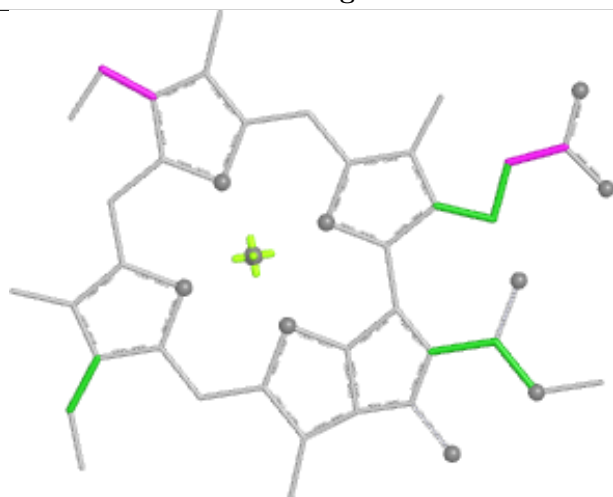
Ligand CLA V 603



Bond lengths



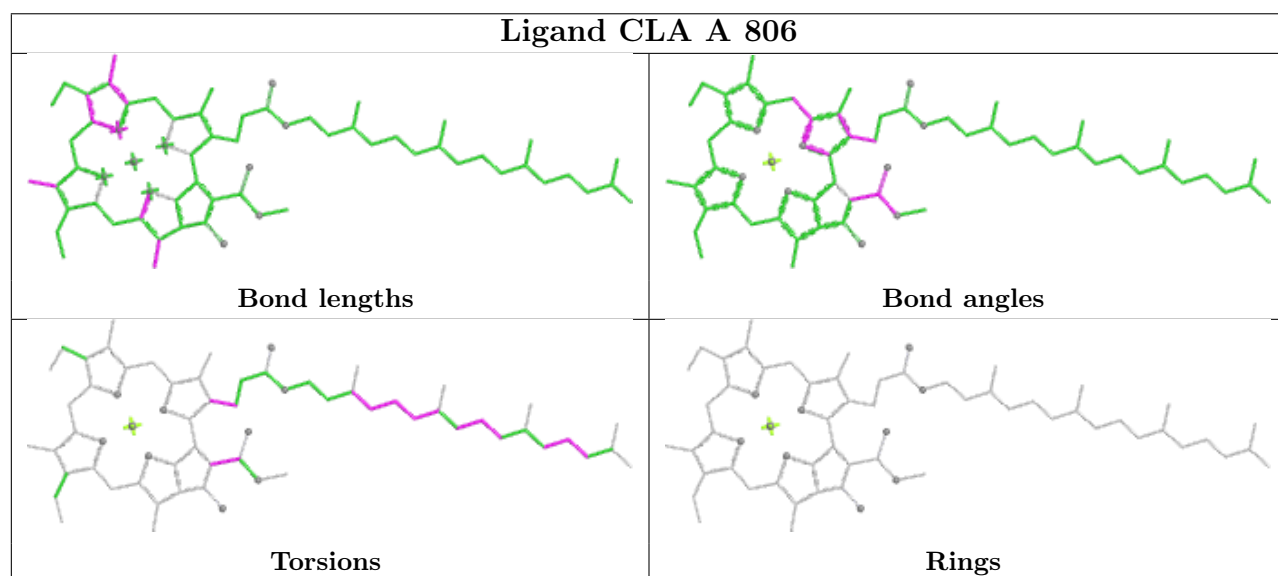
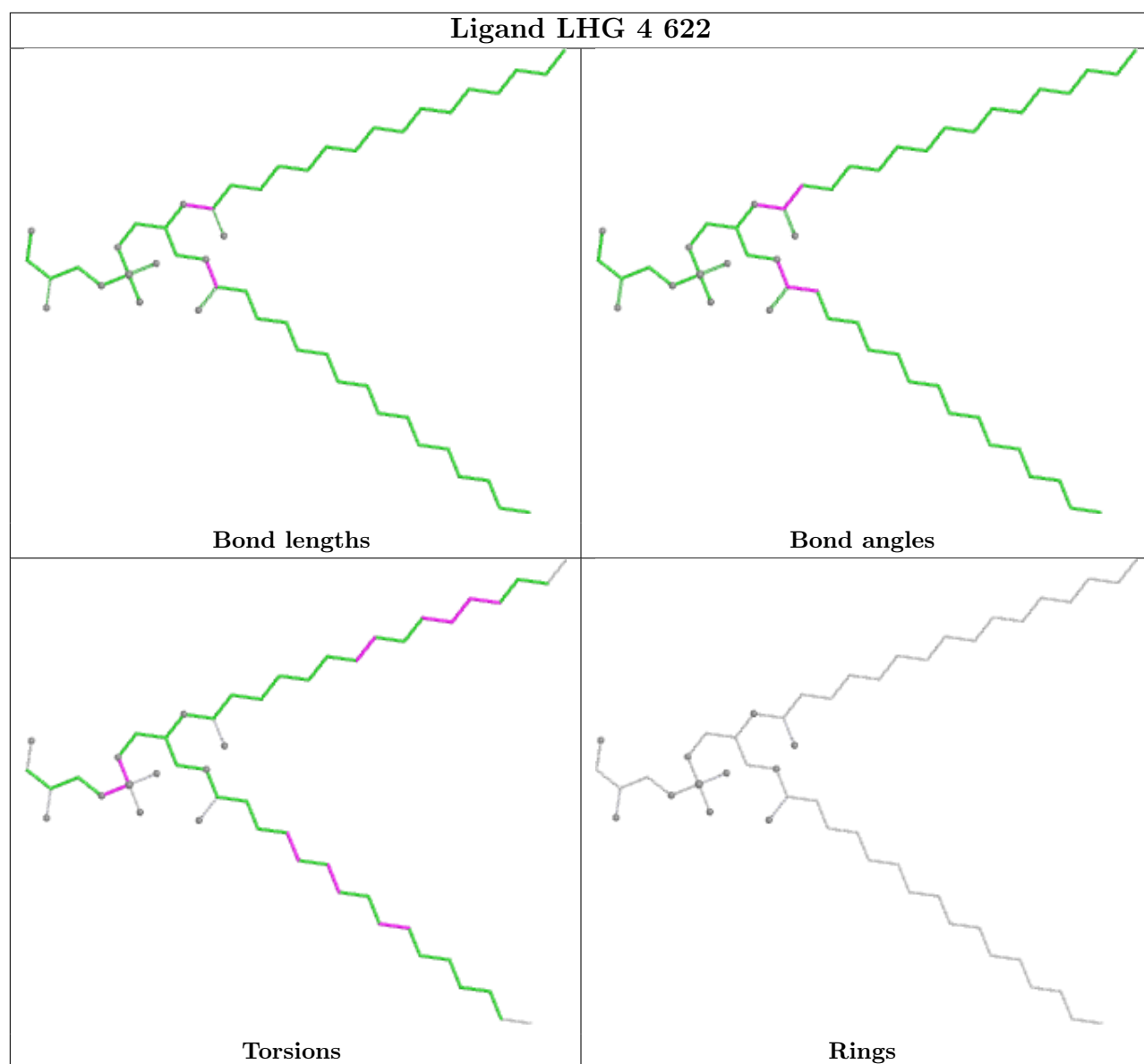
Bond angles



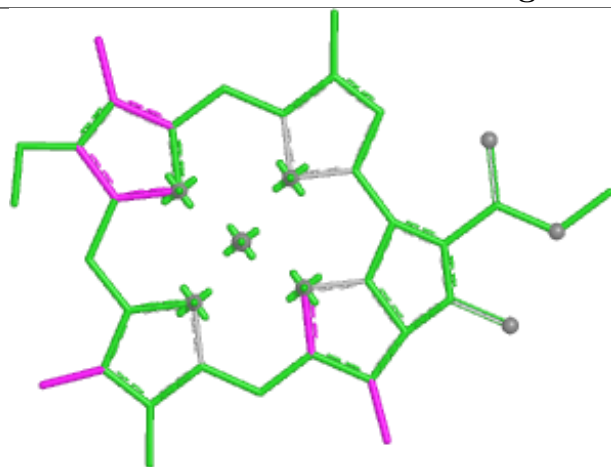
Torsions



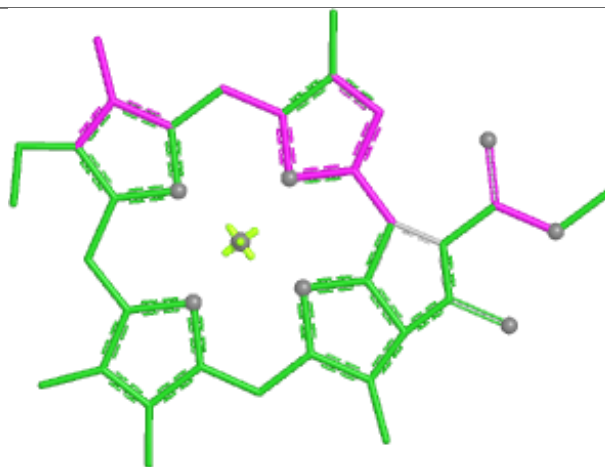
Rings



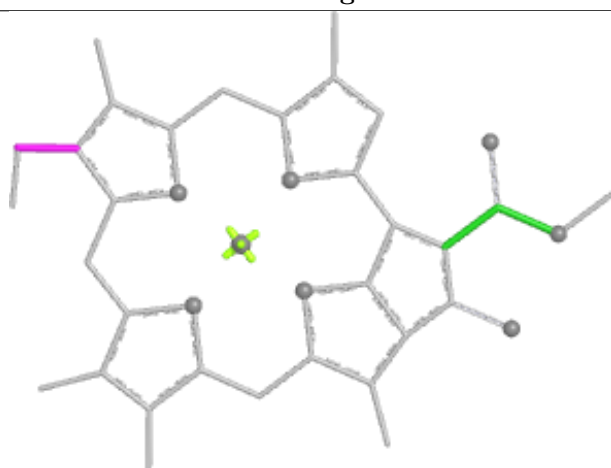
Ligand CLA 1 610



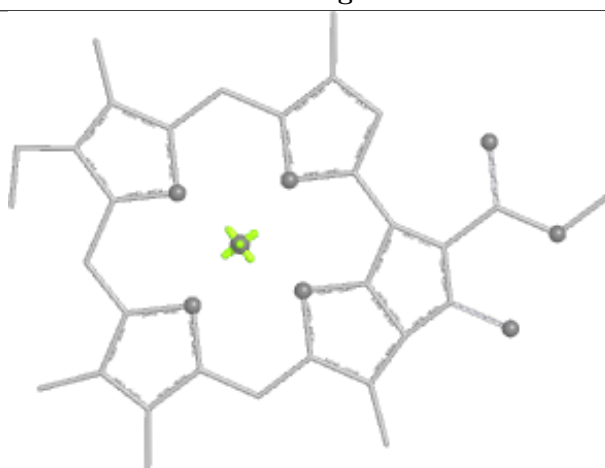
Bond lengths



Bond angles

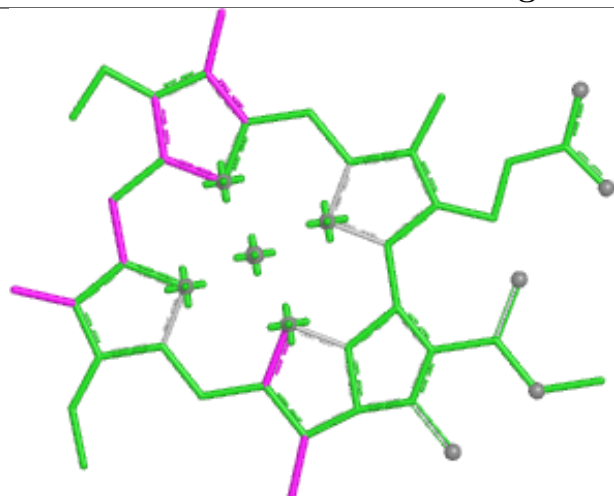


Torsions

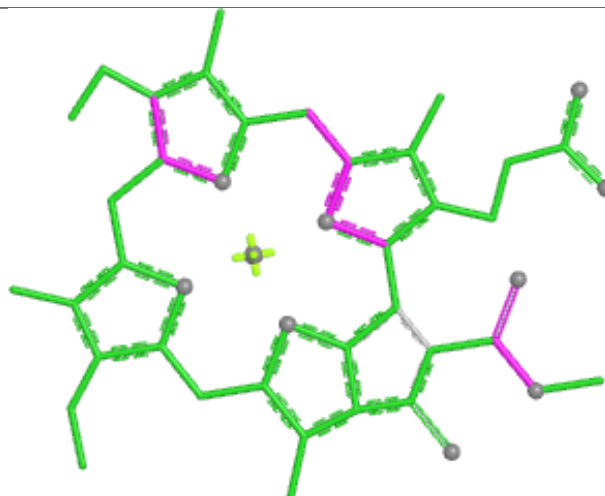


Rings

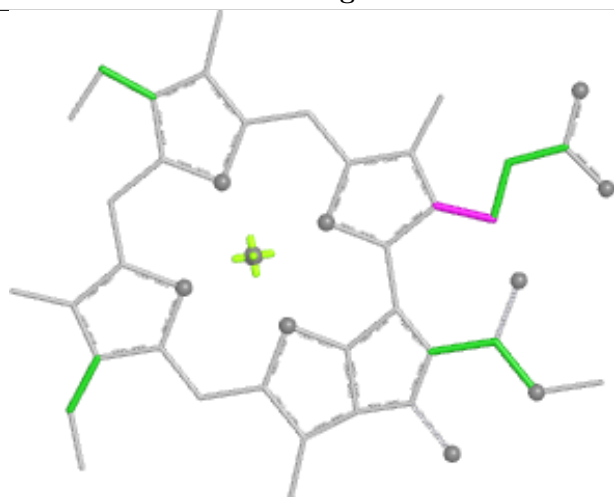
Ligand CLA 2 609



Bond lengths



Bond angles

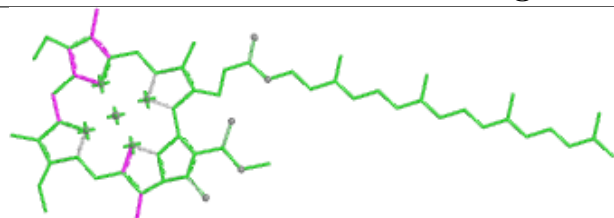


Torsions

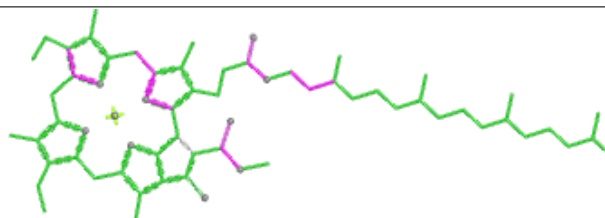


Rings

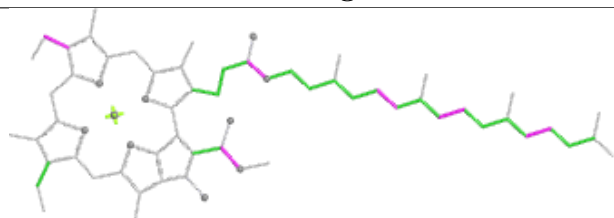
Ligand CLA X 610



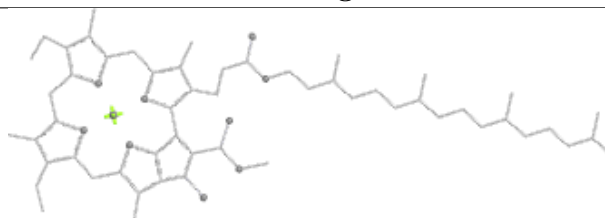
Bond lengths



Bond angles

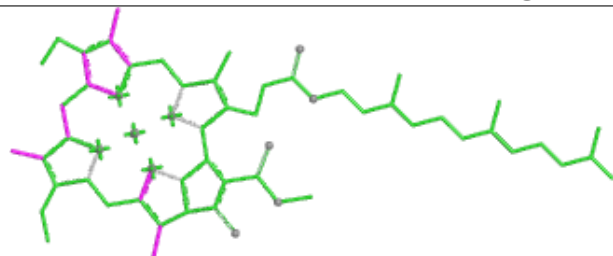


Torsions

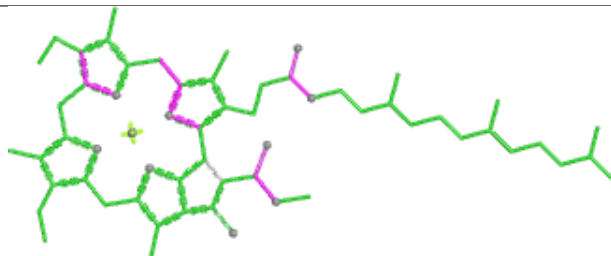


Rings

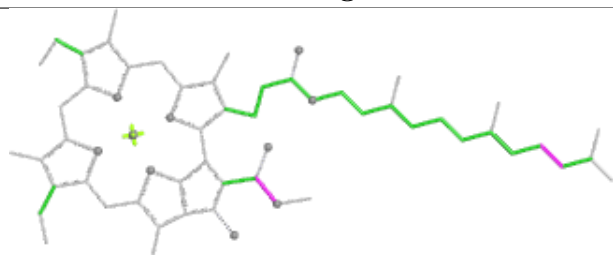
Ligand CLA 3 602



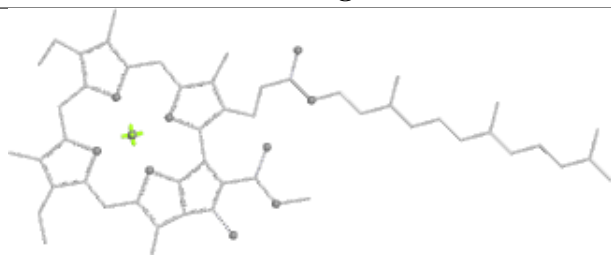
Bond lengths



Bond angles

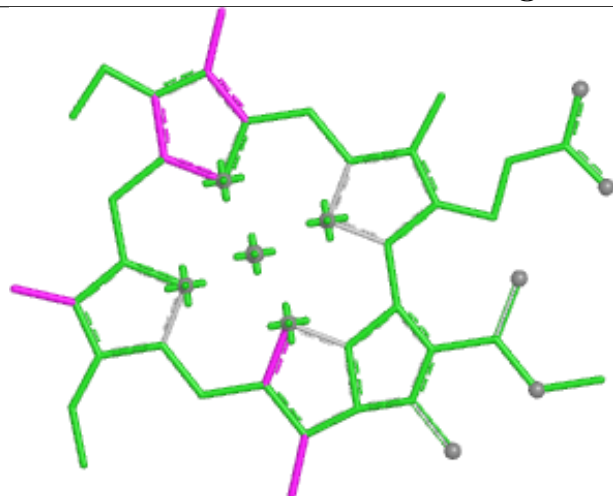


Torsions

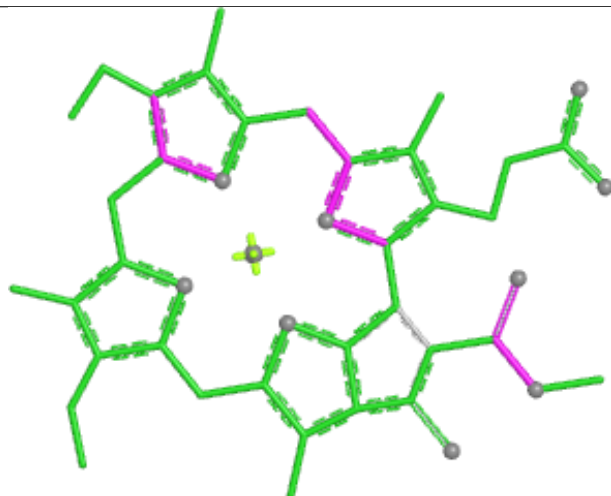


Rings

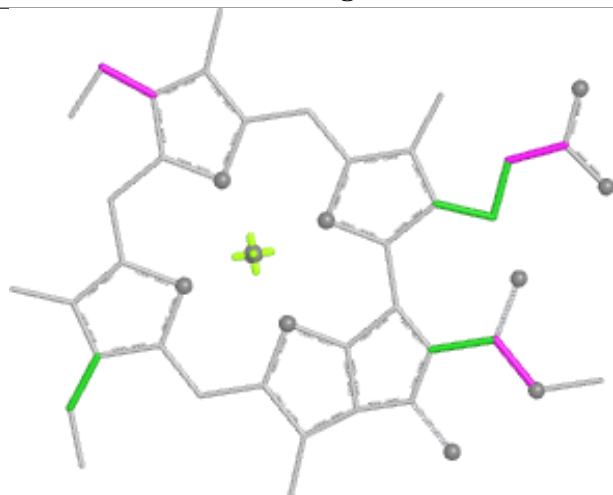
Ligand CLA 4 607



Bond lengths



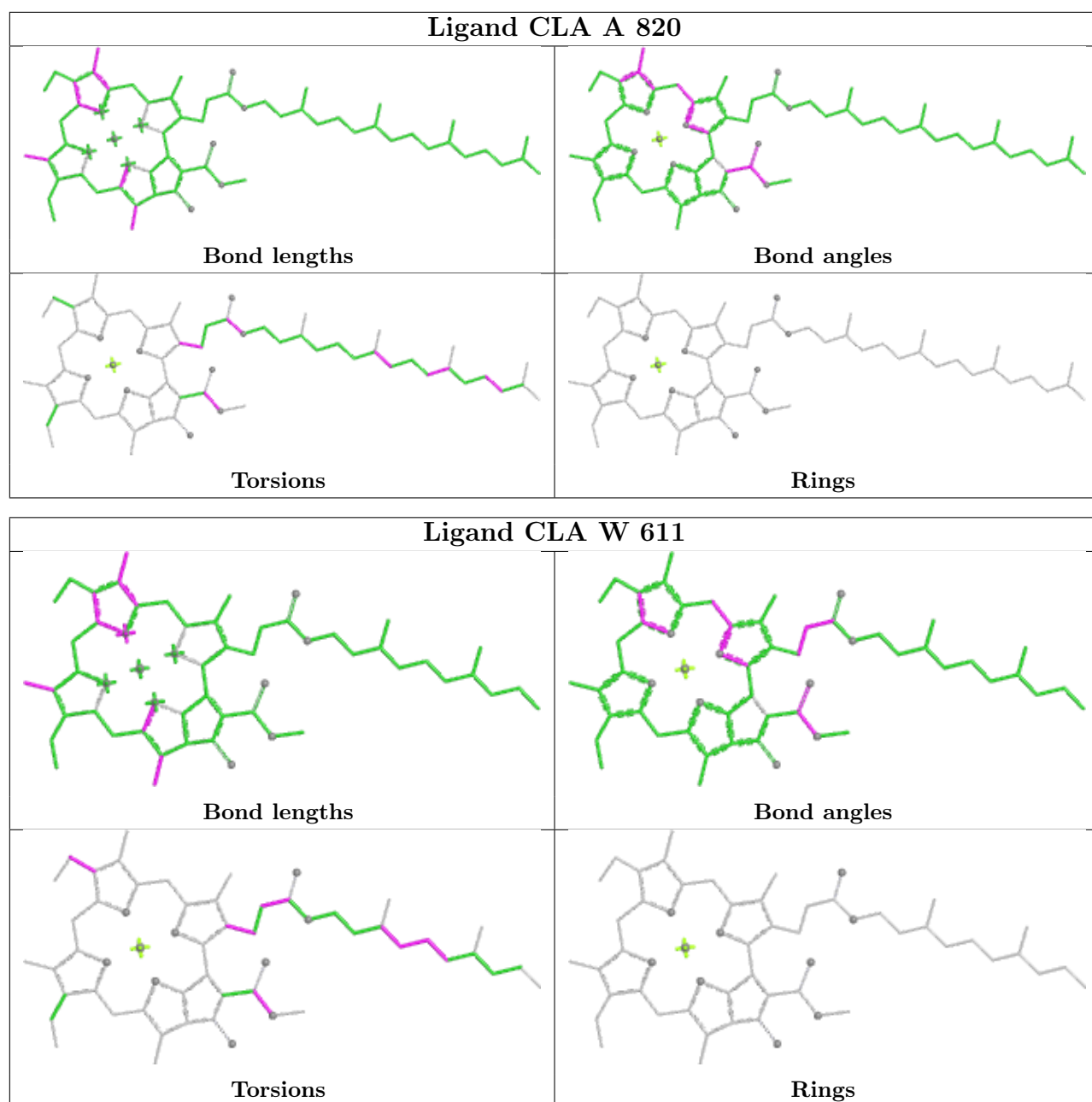
Bond angles



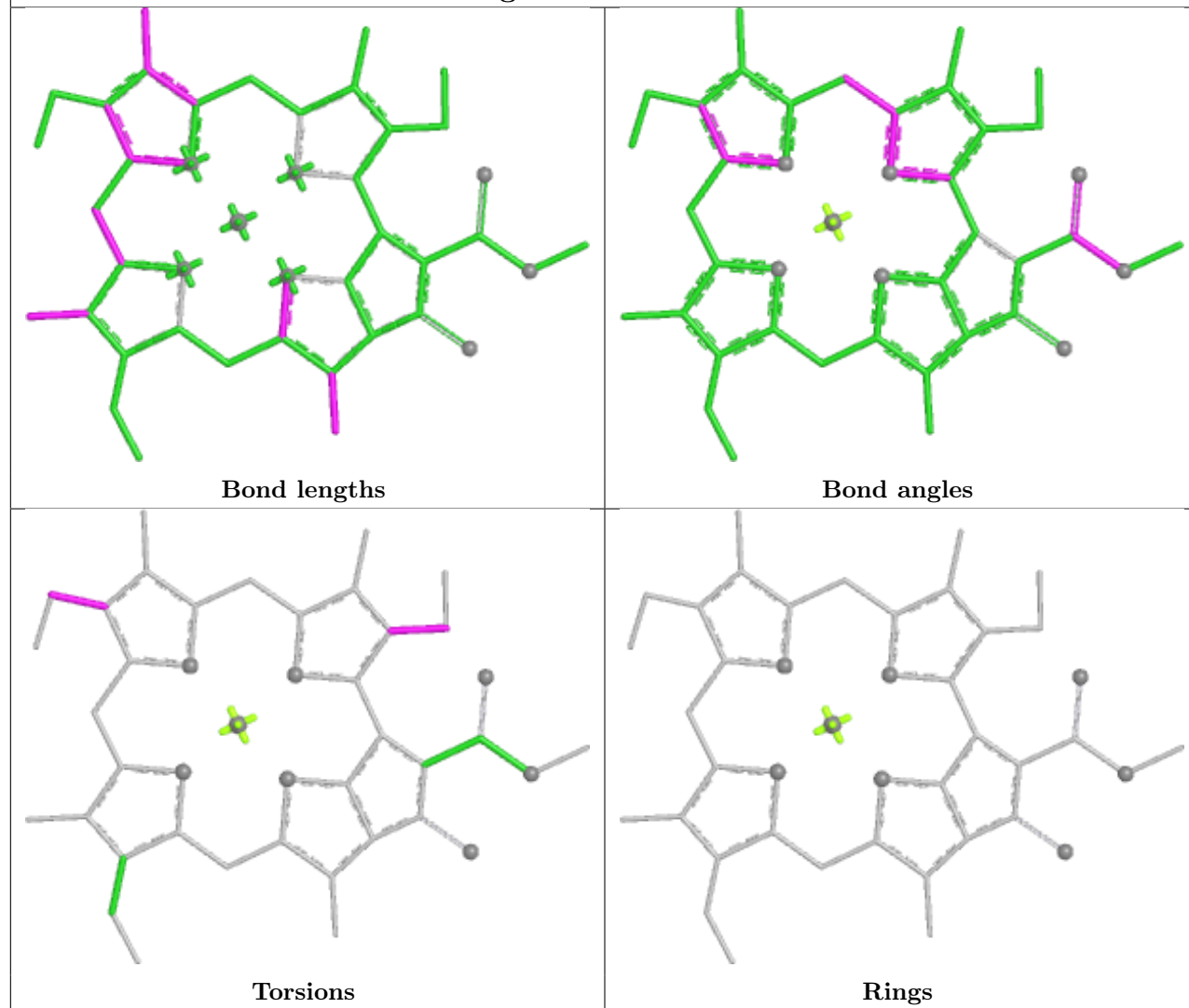
Torsions



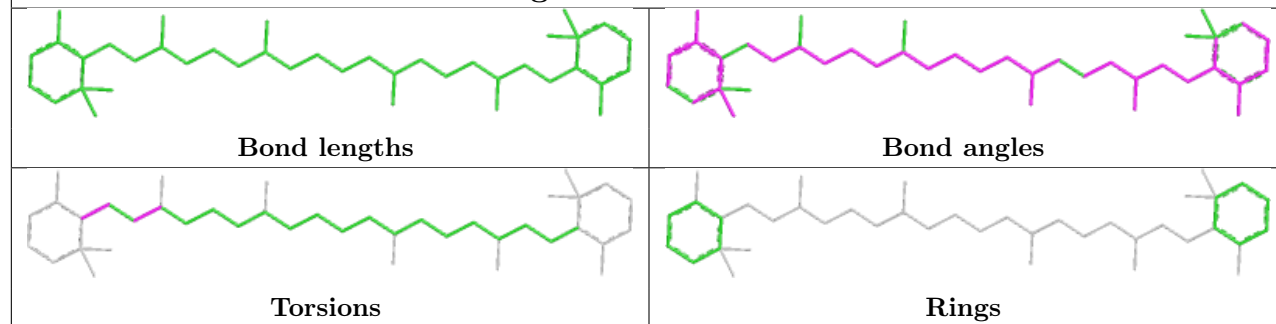
Rings



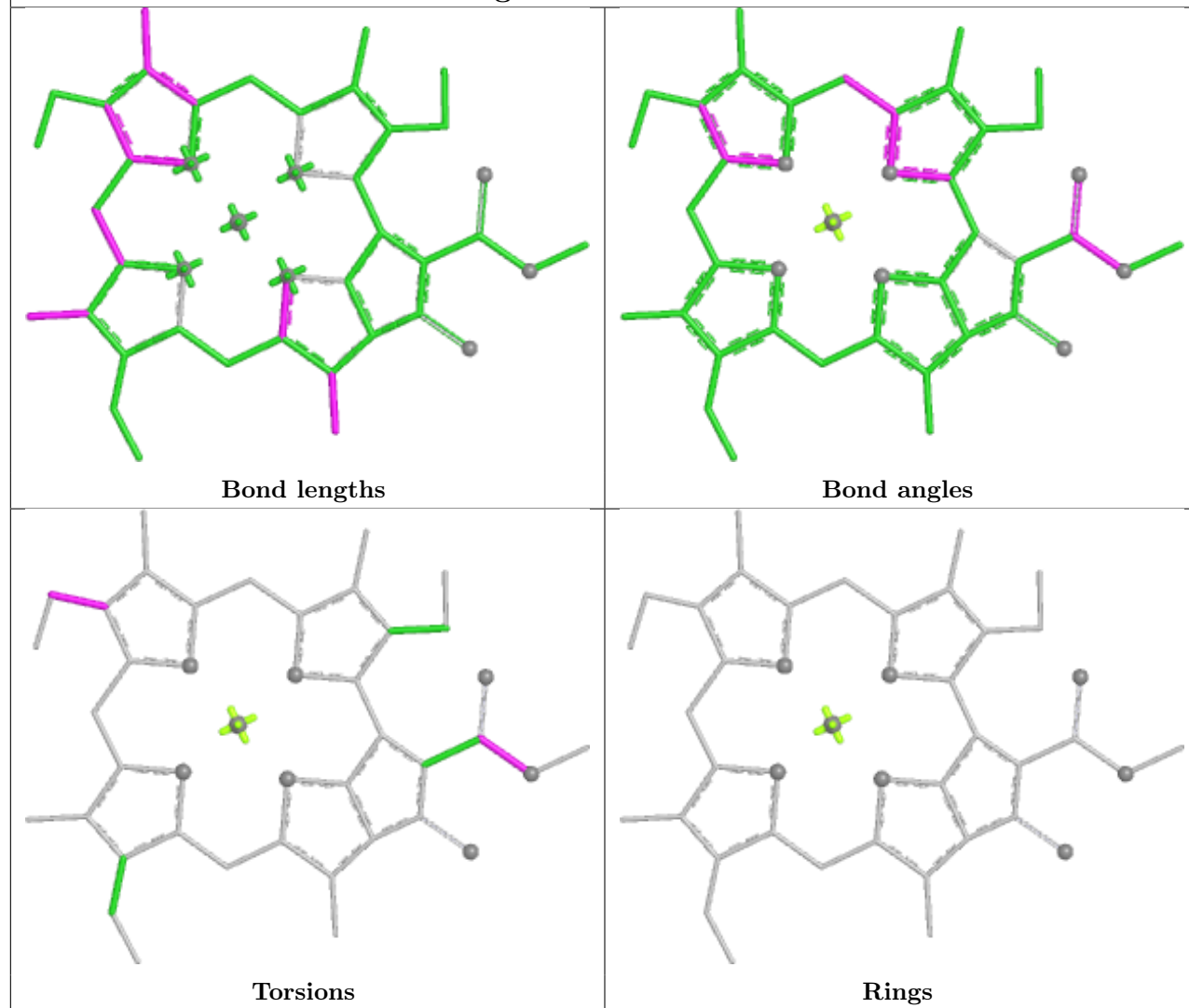
Ligand CLA 9 611



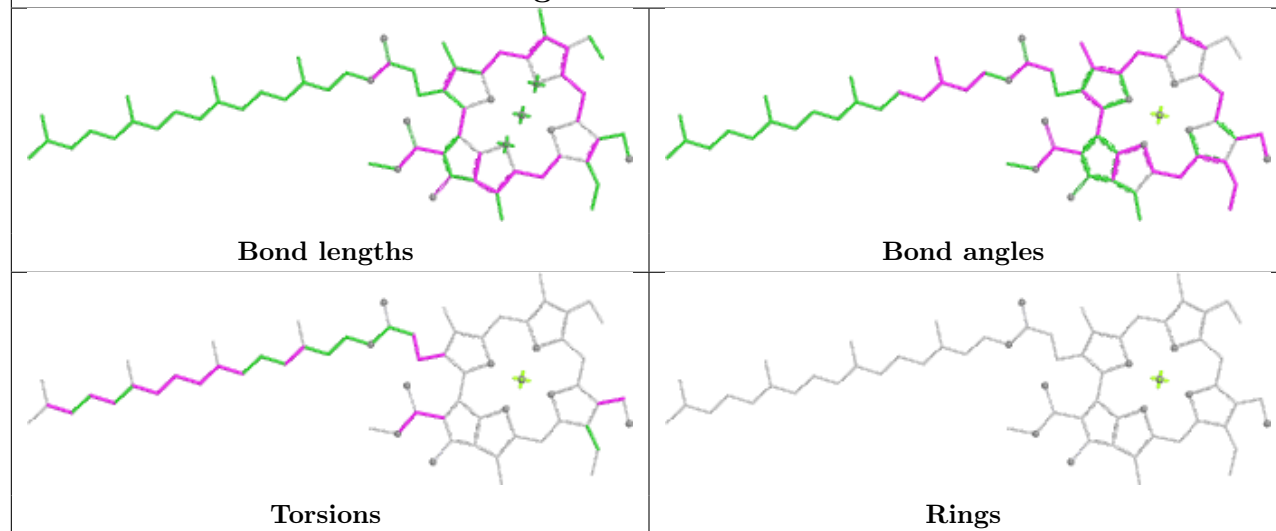
Ligand BCR B 849

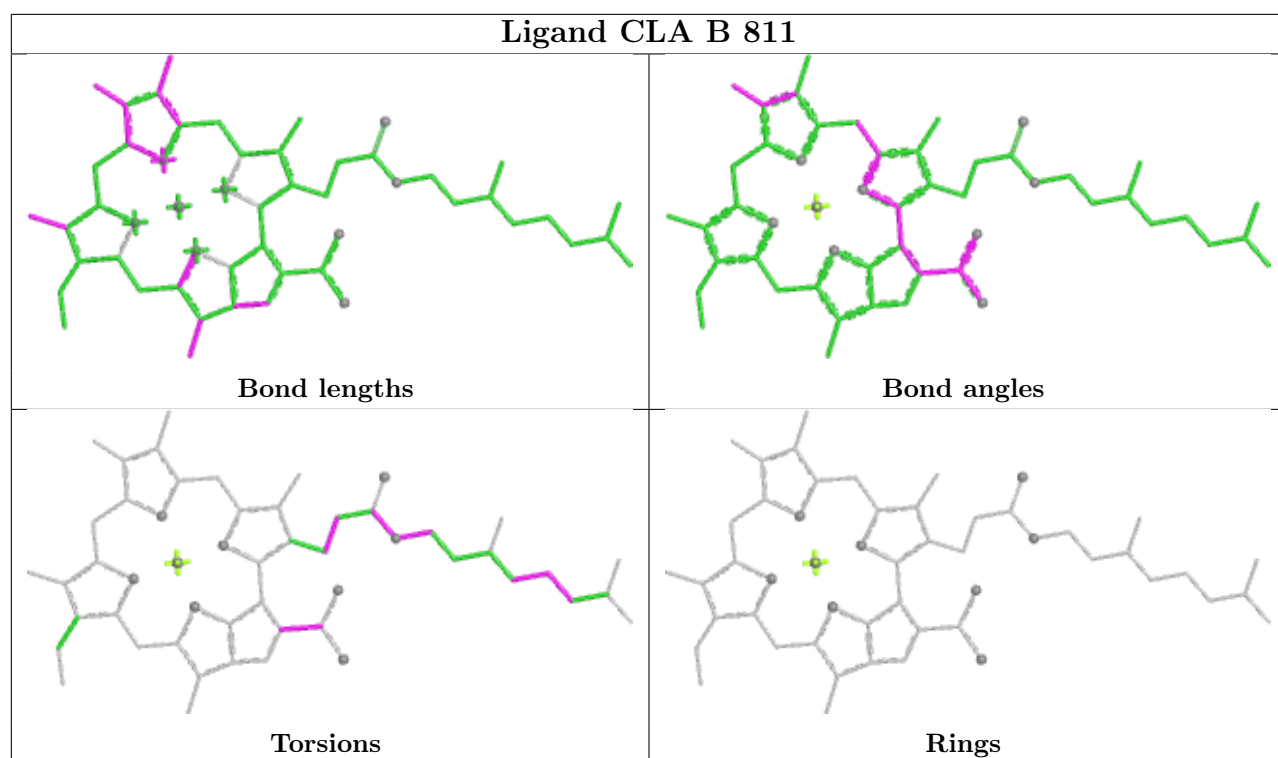


Ligand CLA G 203

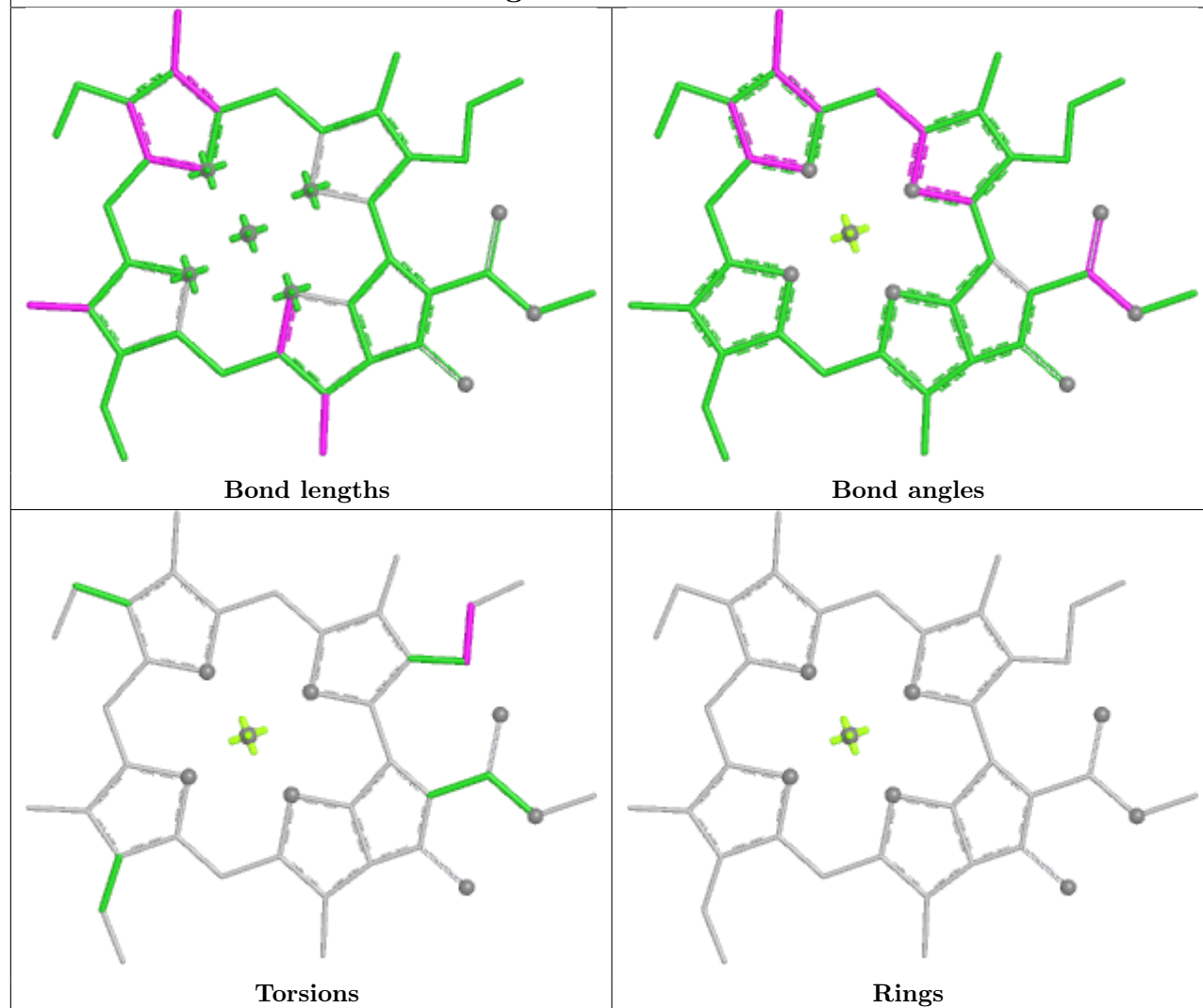


Ligand CHL Z 607

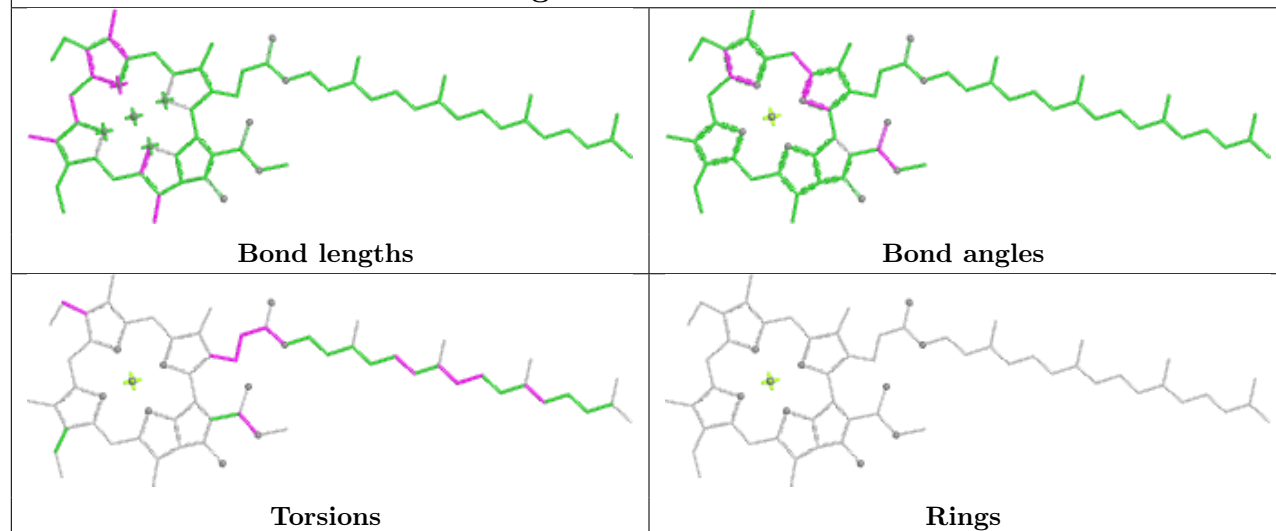


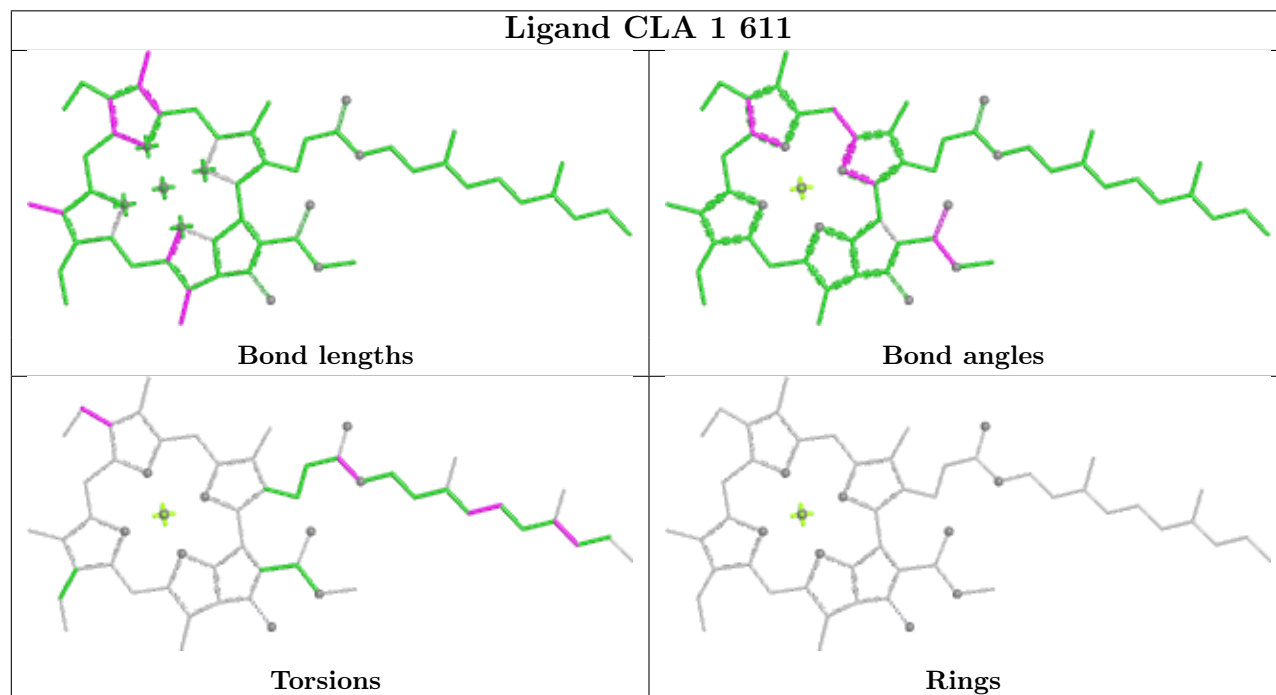
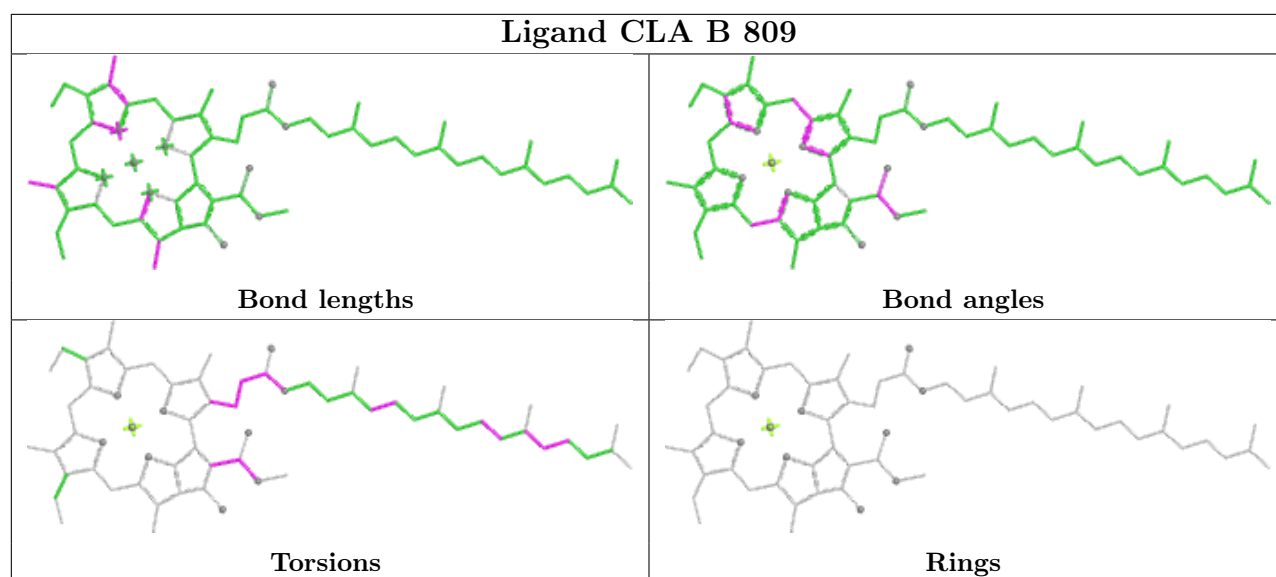


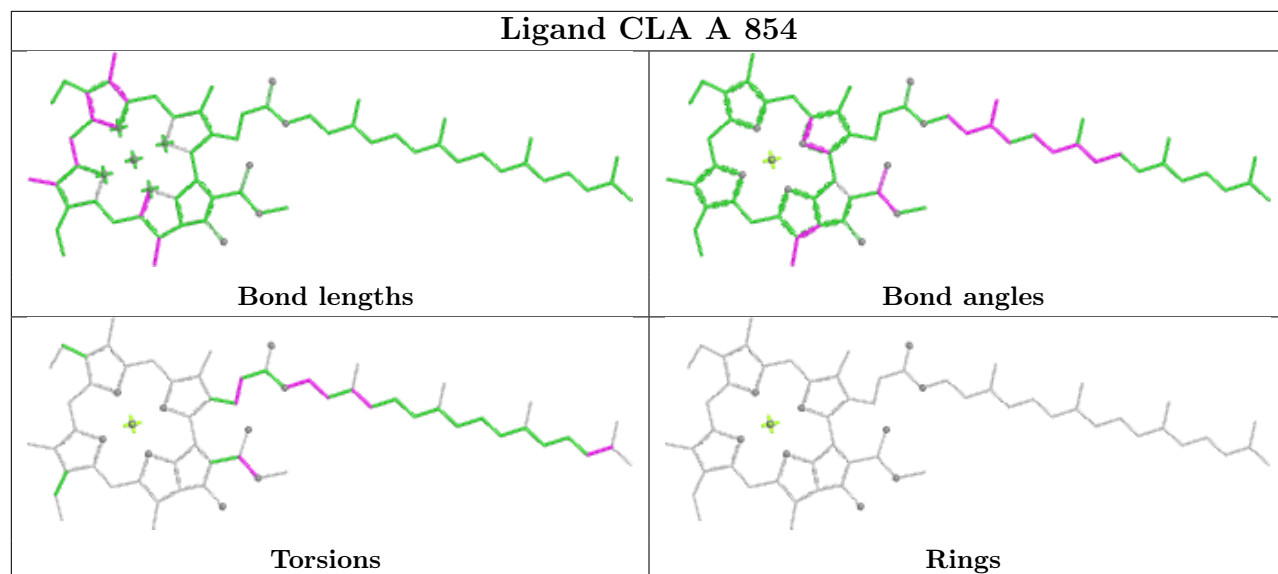
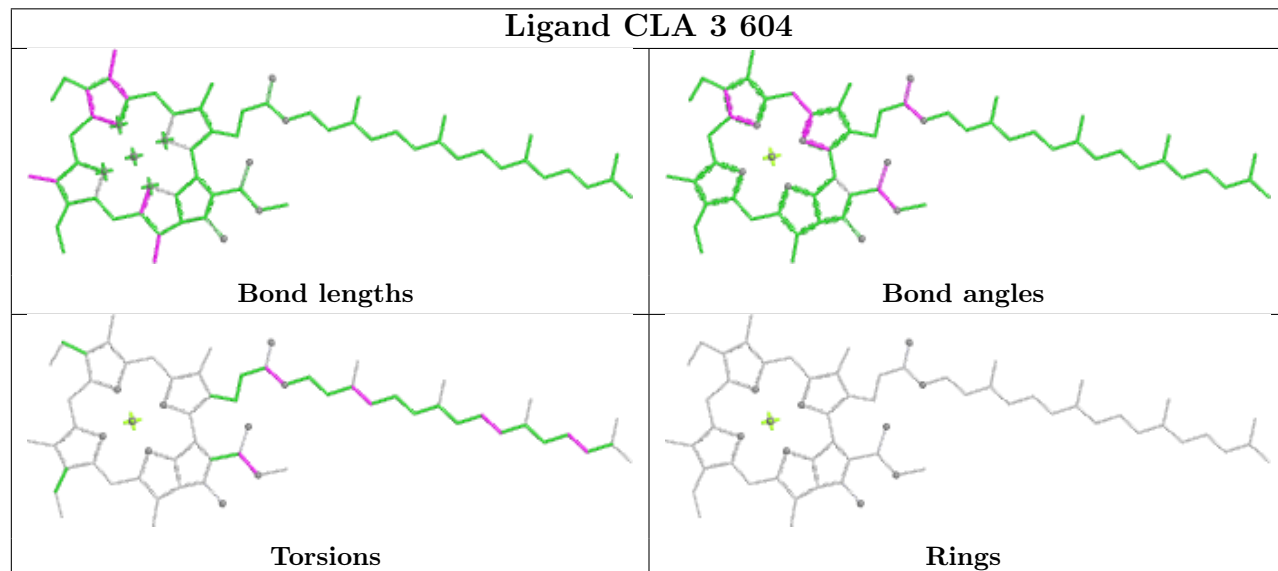
Ligand CLA 3 612



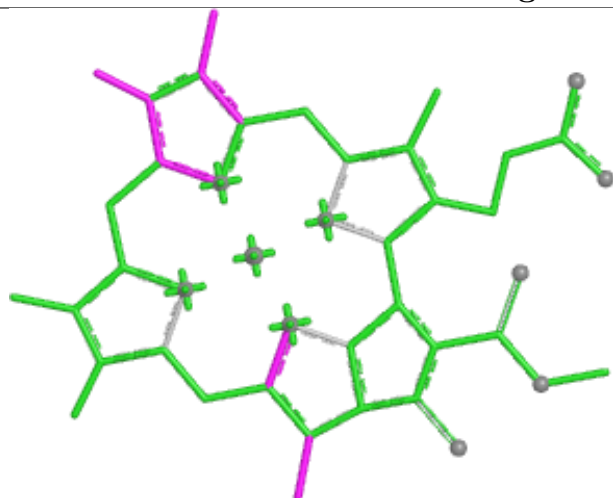
Ligand CLA A 841



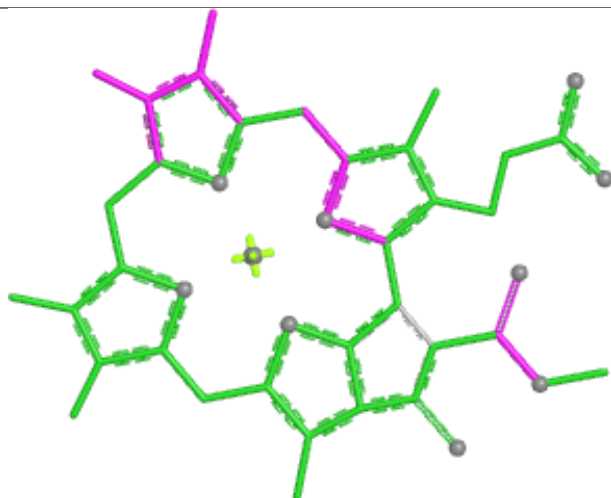


Ligand CLA A 854**Ligand CLA 3 604**

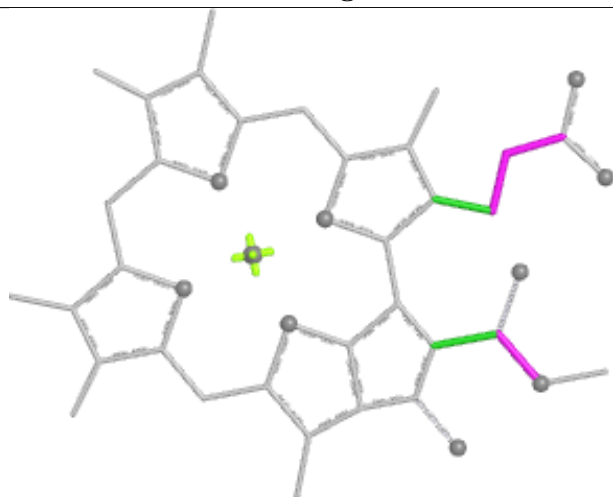
Ligand CLA 1 616



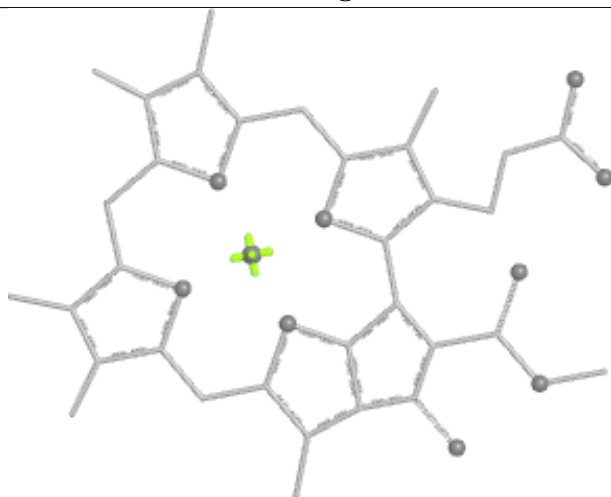
Bond lengths



Bond angles

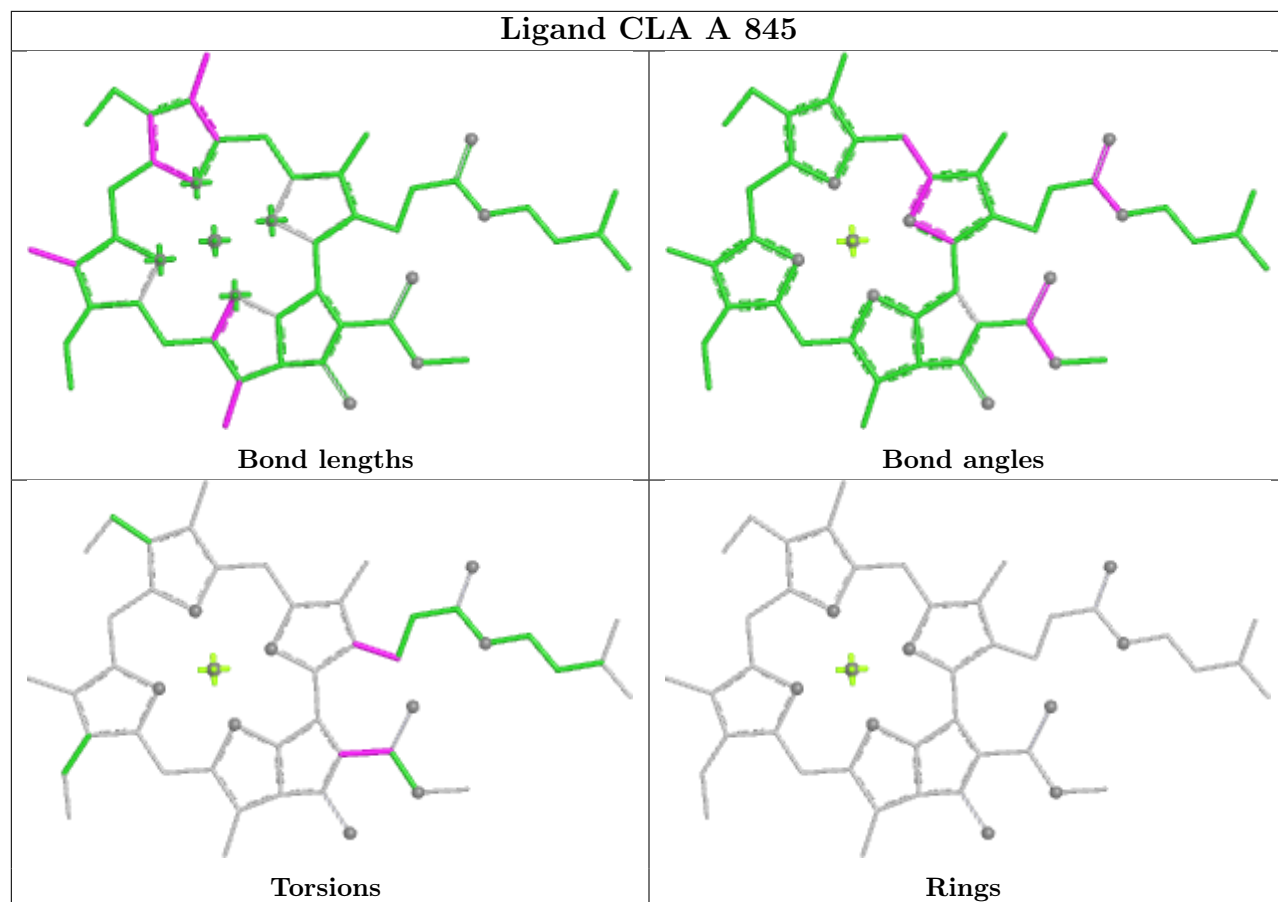


Torsions

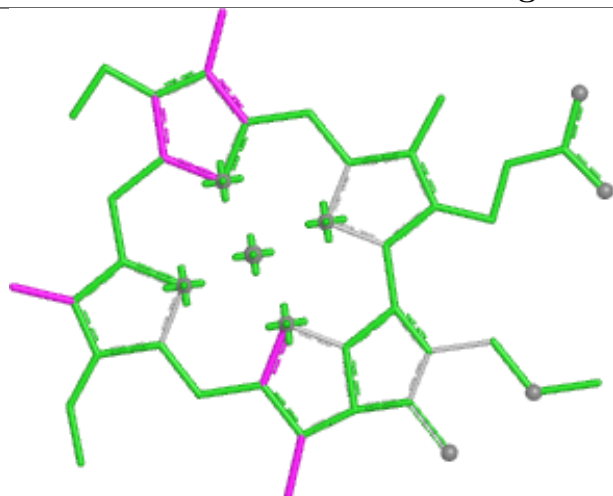


Rings

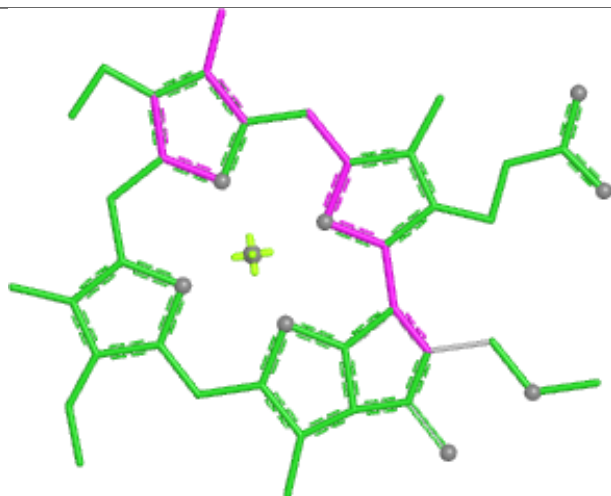
Ligand CLA A 845



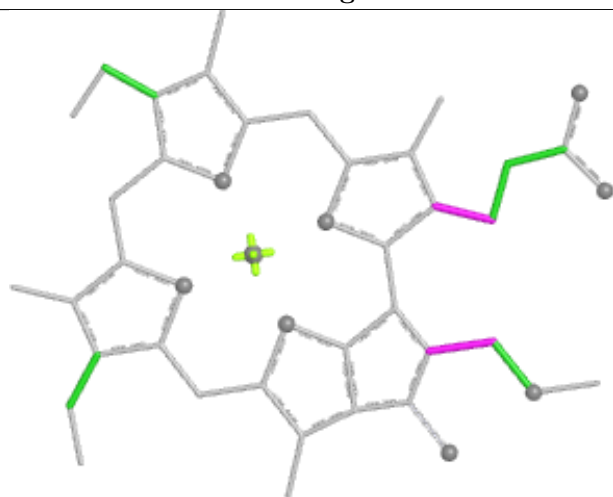
Ligand CLA 7 609



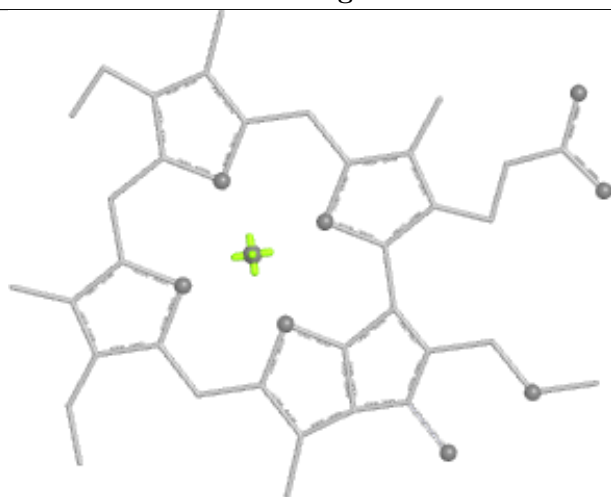
Bond lengths



Bond angles

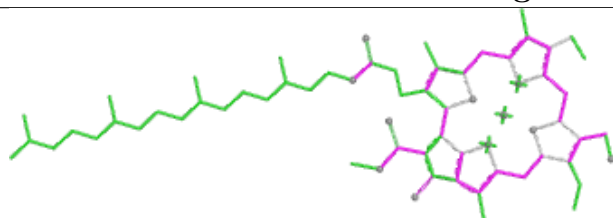


Torsions

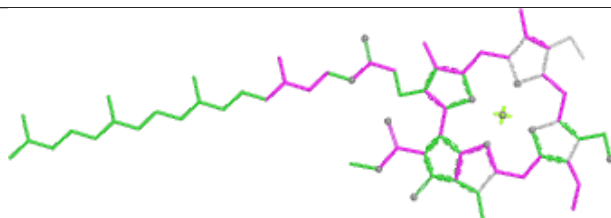


Rings

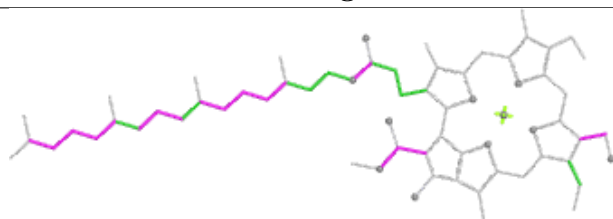
Ligand CHL X 601



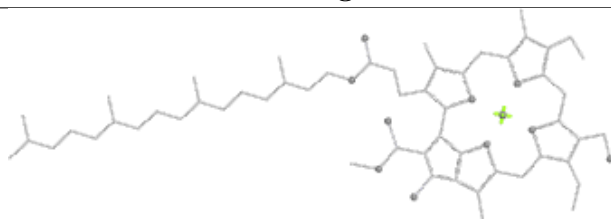
Bond lengths



Bond angles

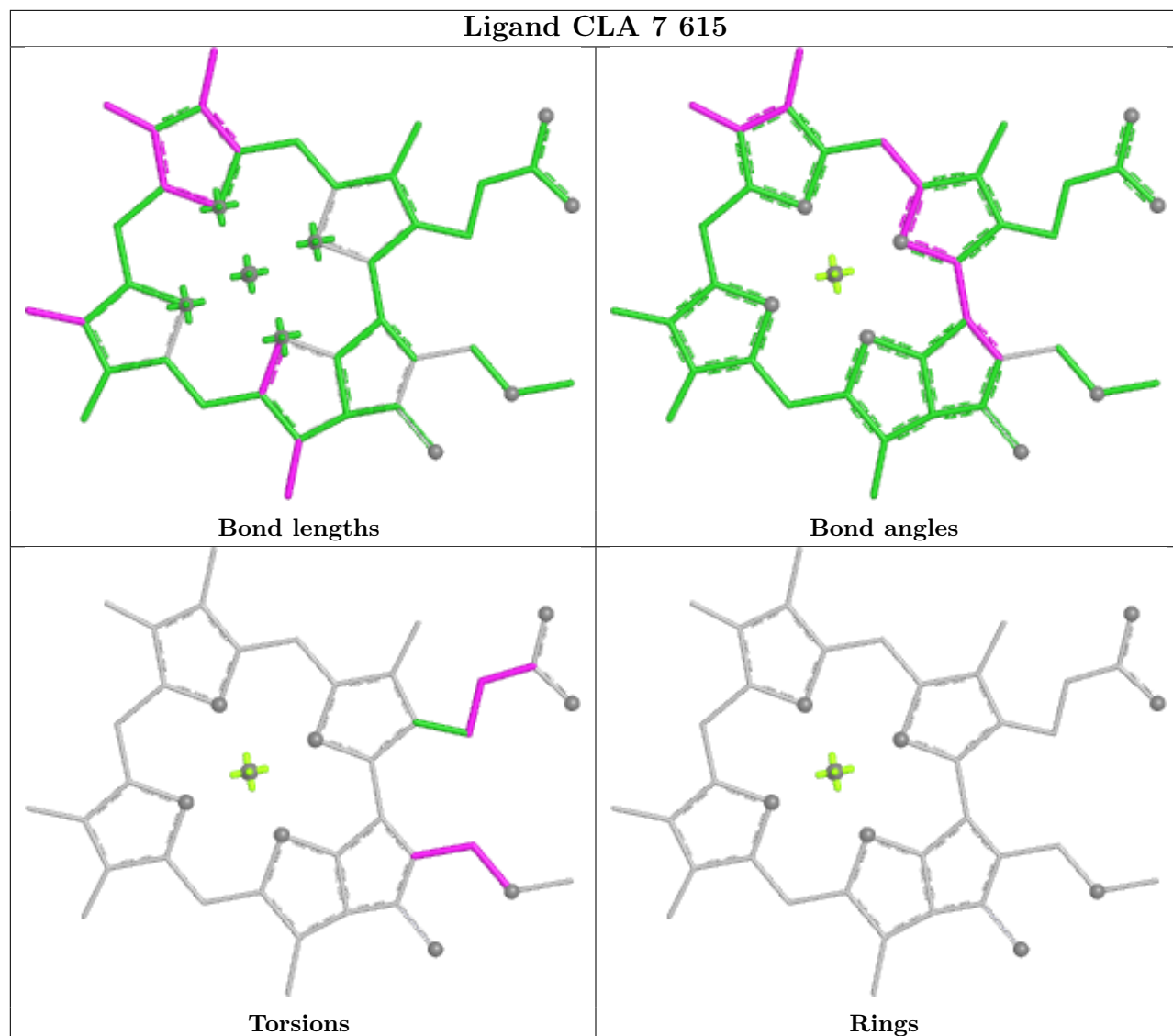


Torsions

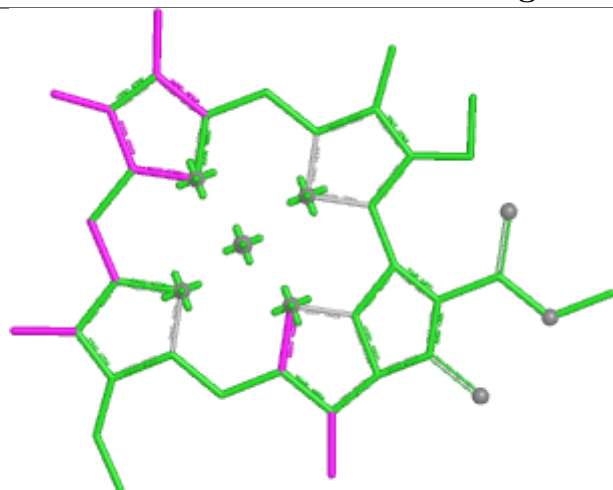


Rings

Ligand CLA 7 615



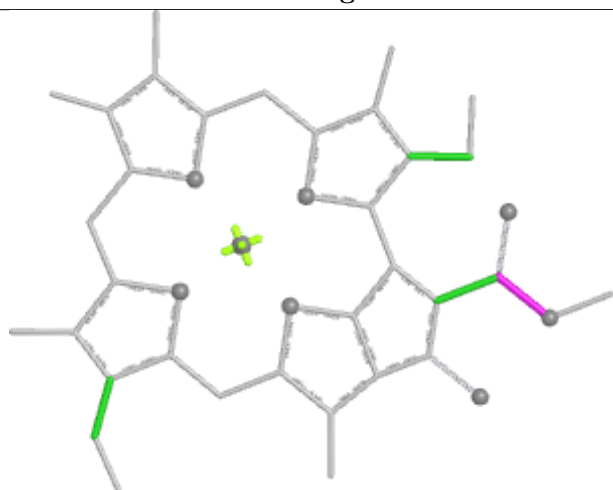
Ligand CLA 6 607



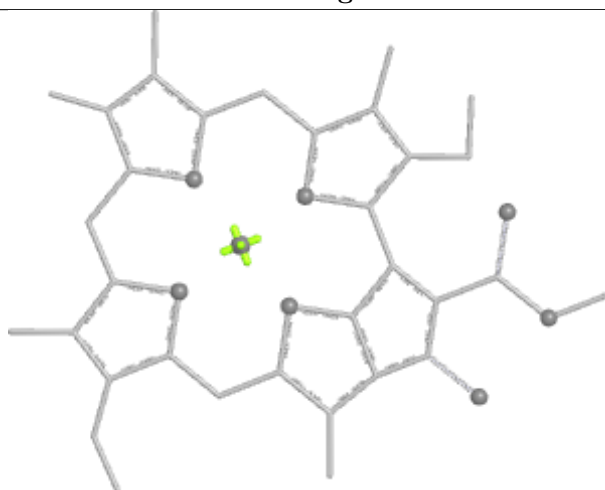
Bond lengths



Bond angles

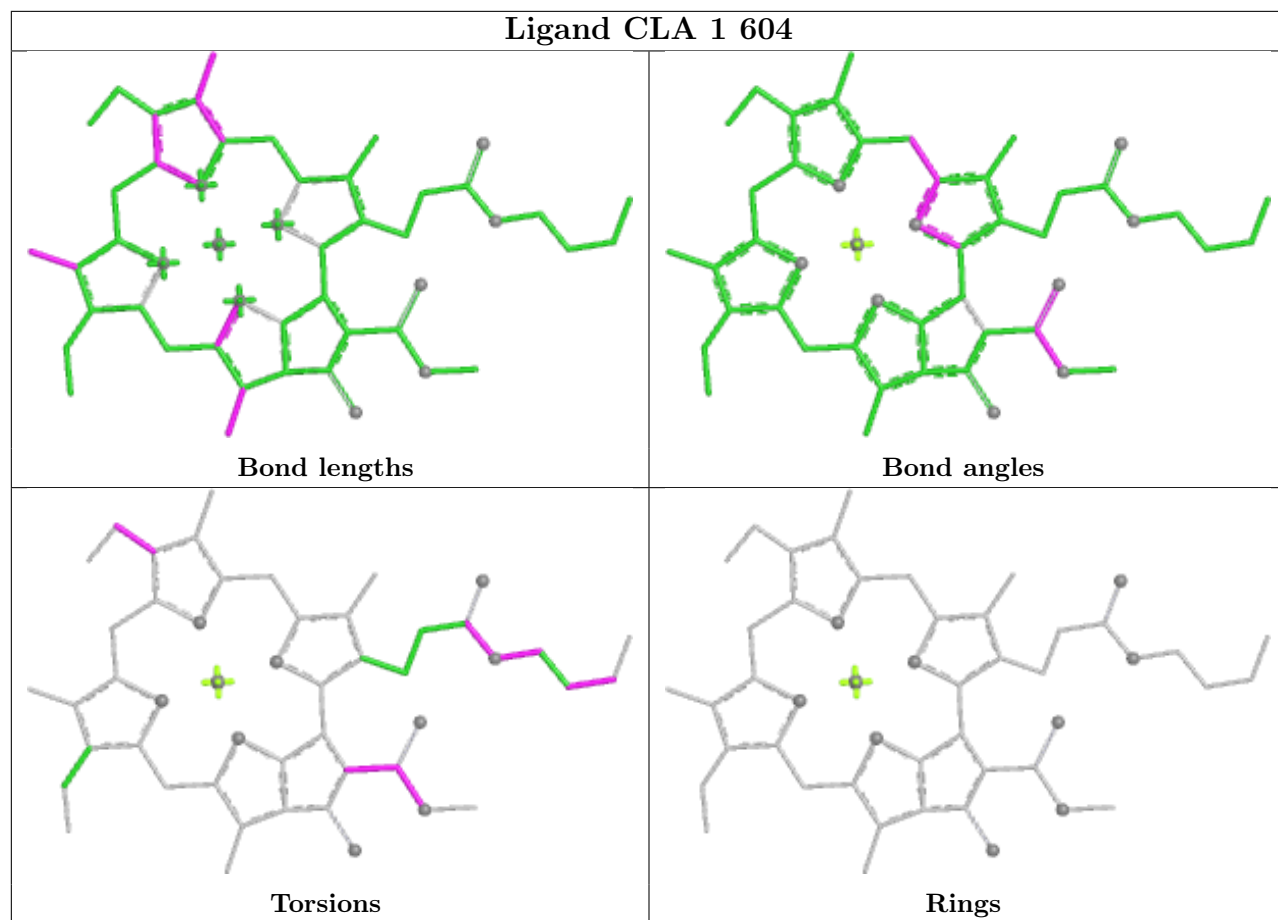


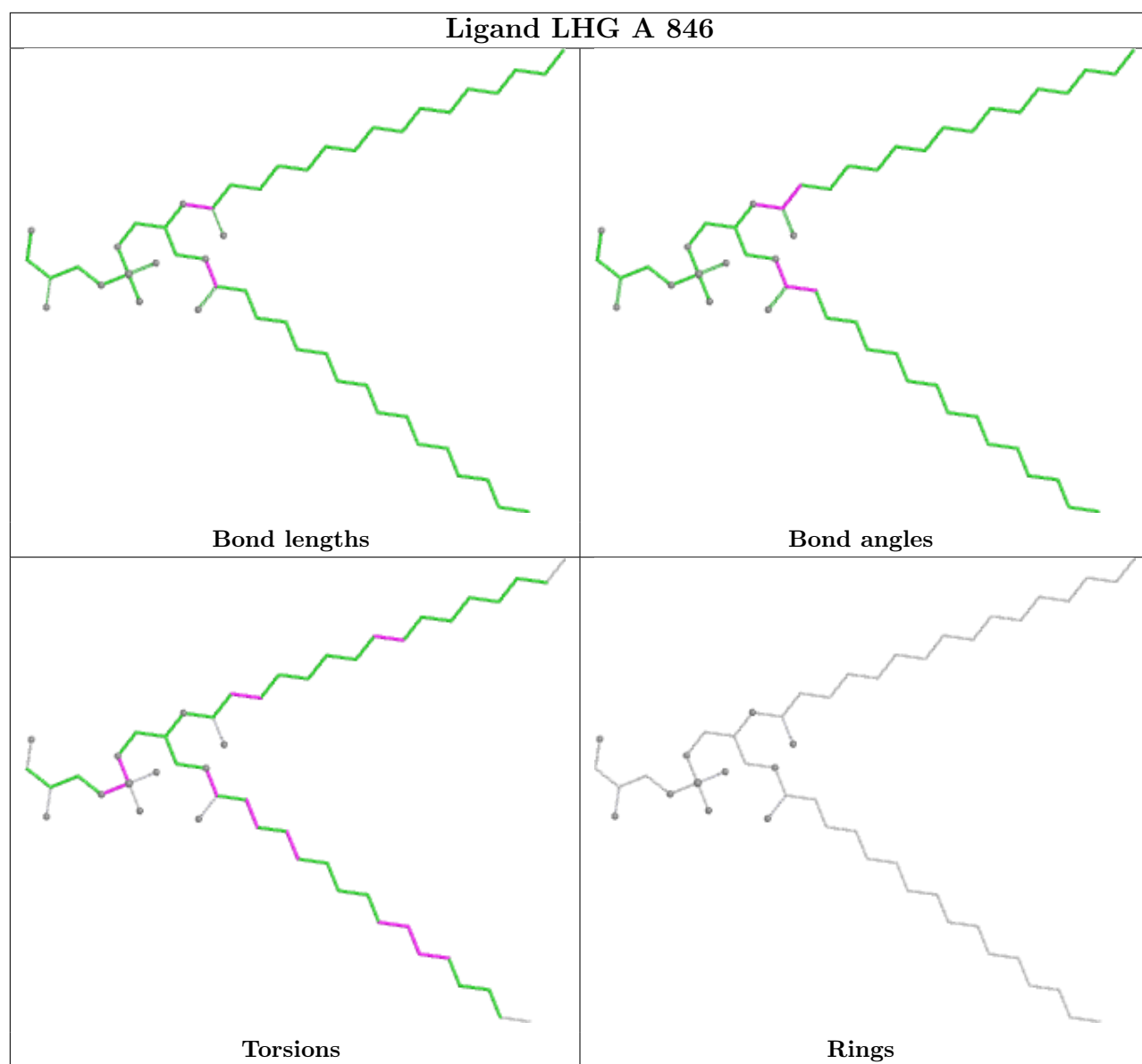
Torsions



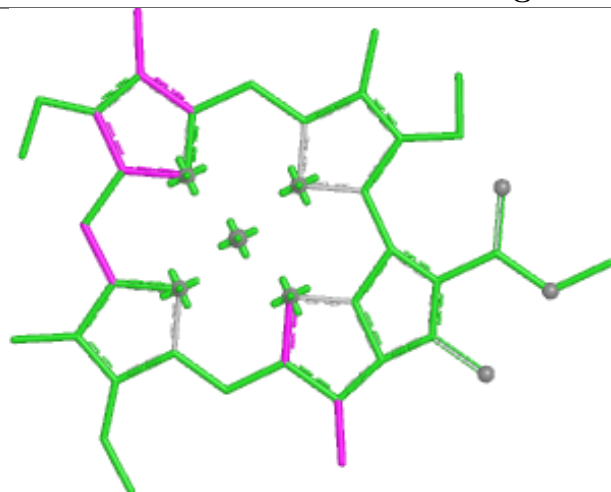
Rings

Ligand CLA 1 604

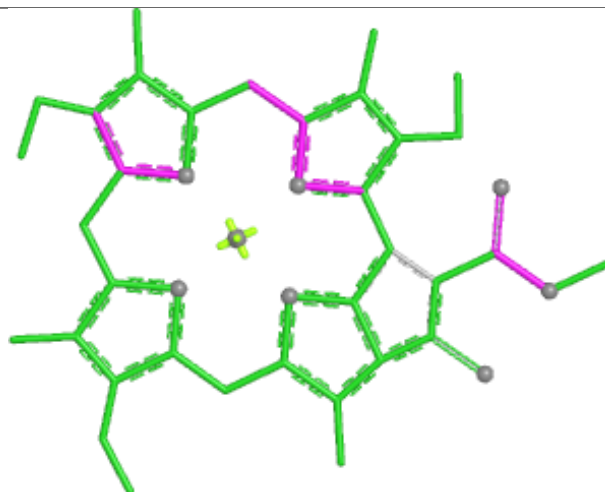




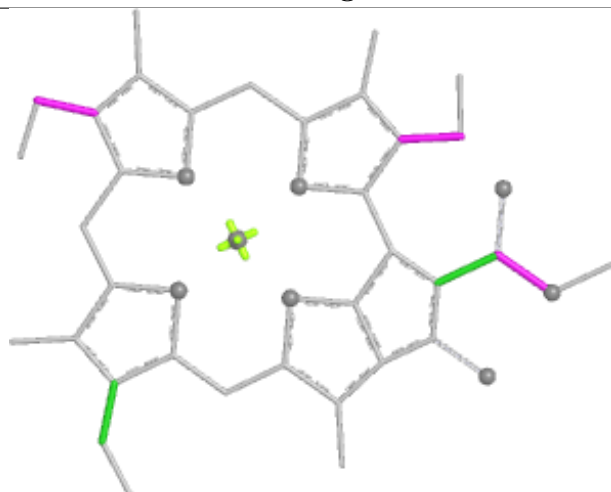
Ligand CLA X 614



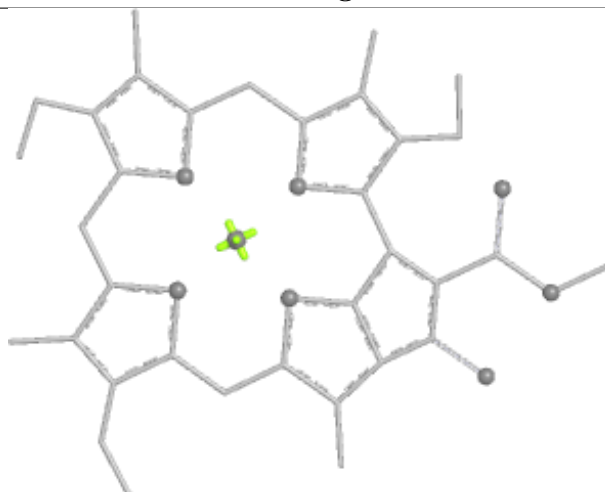
Bond lengths



Bond angles

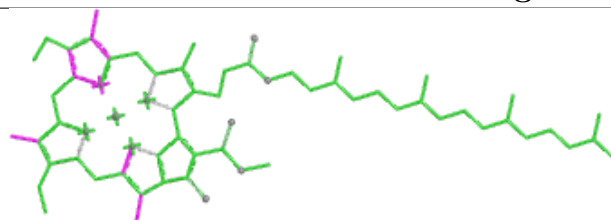


Torsions

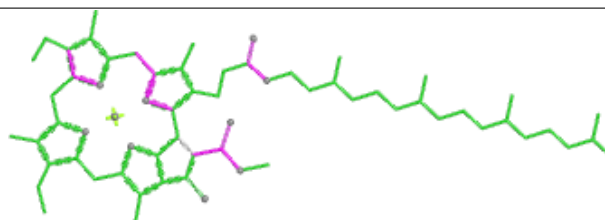


Rings

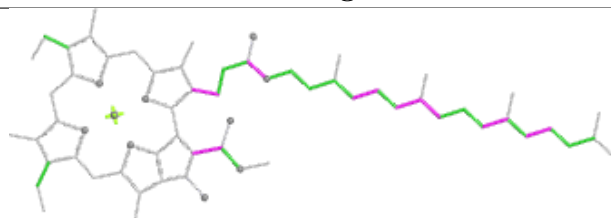
Ligand CLA B 805



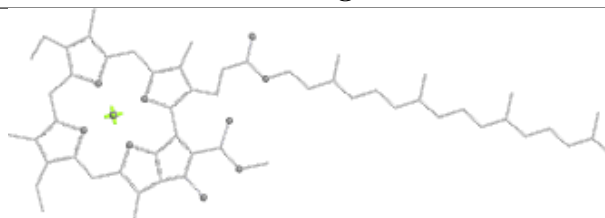
Bond lengths



Bond angles

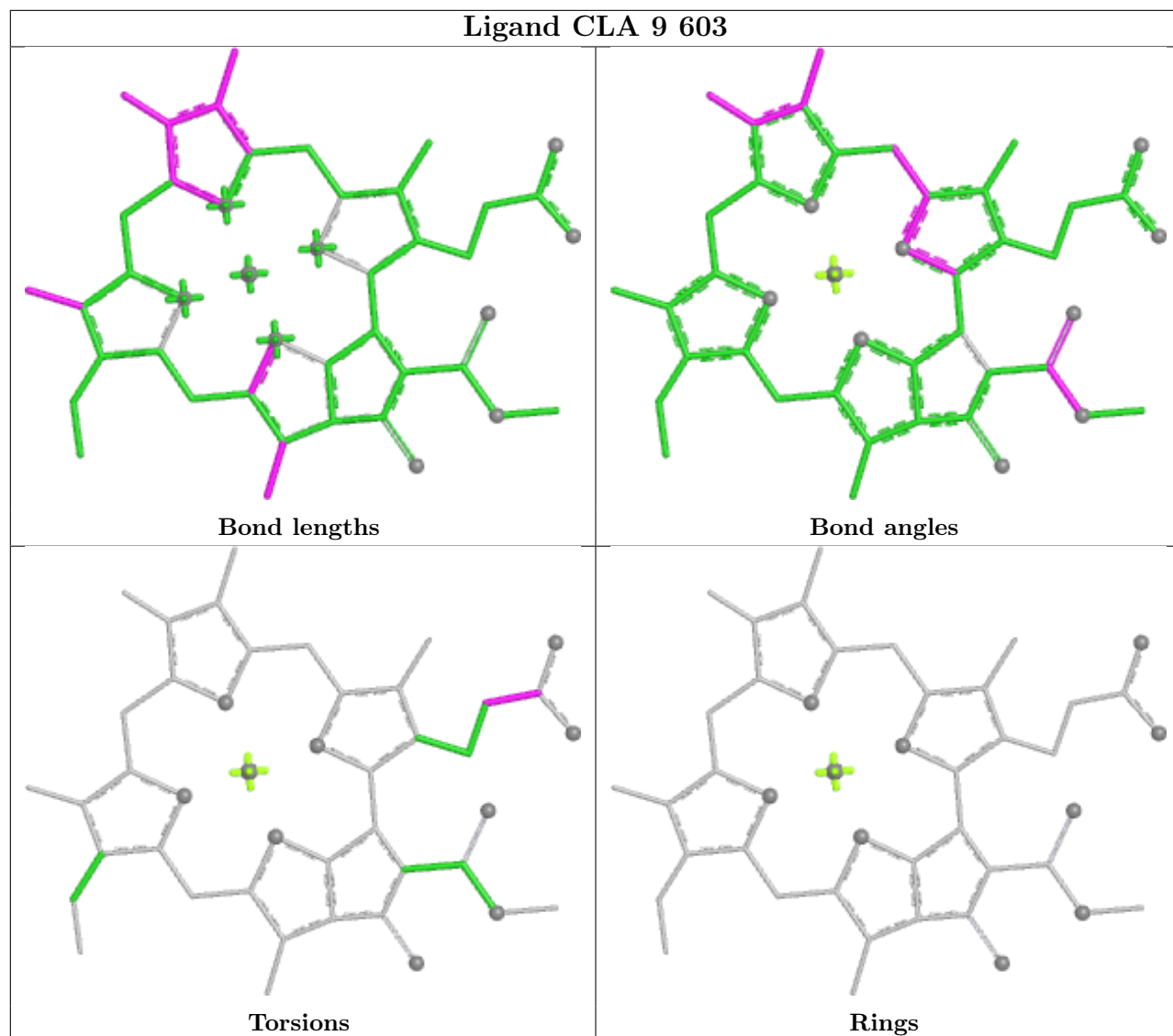


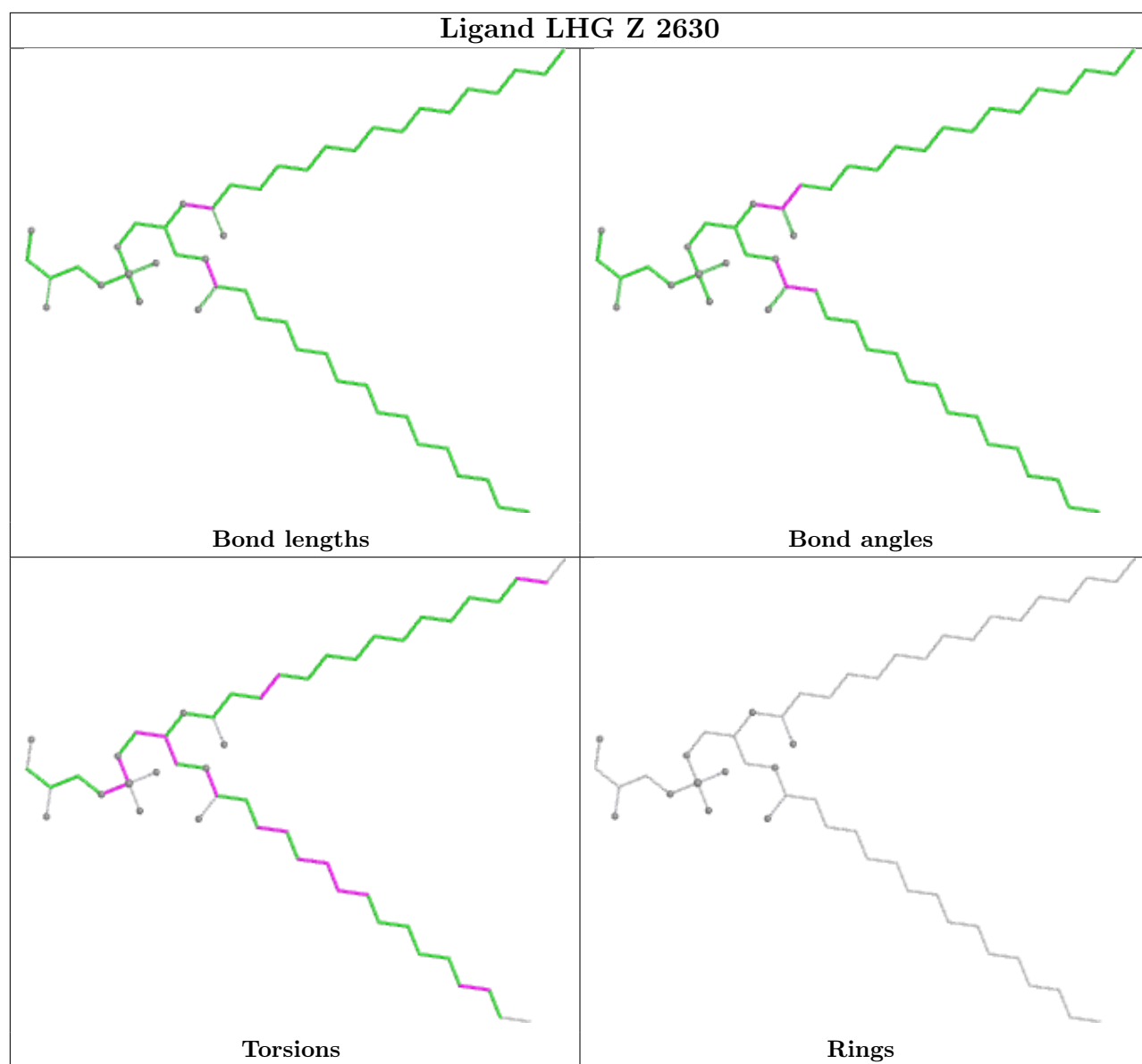
Torsions

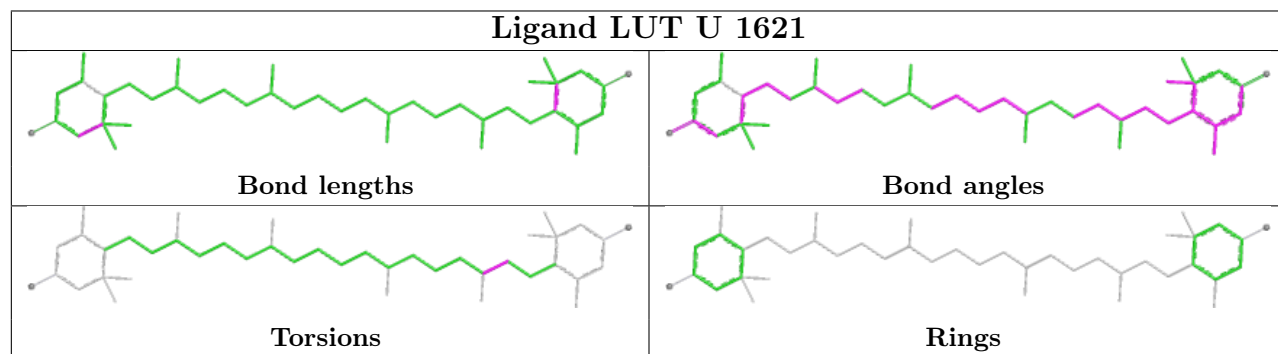
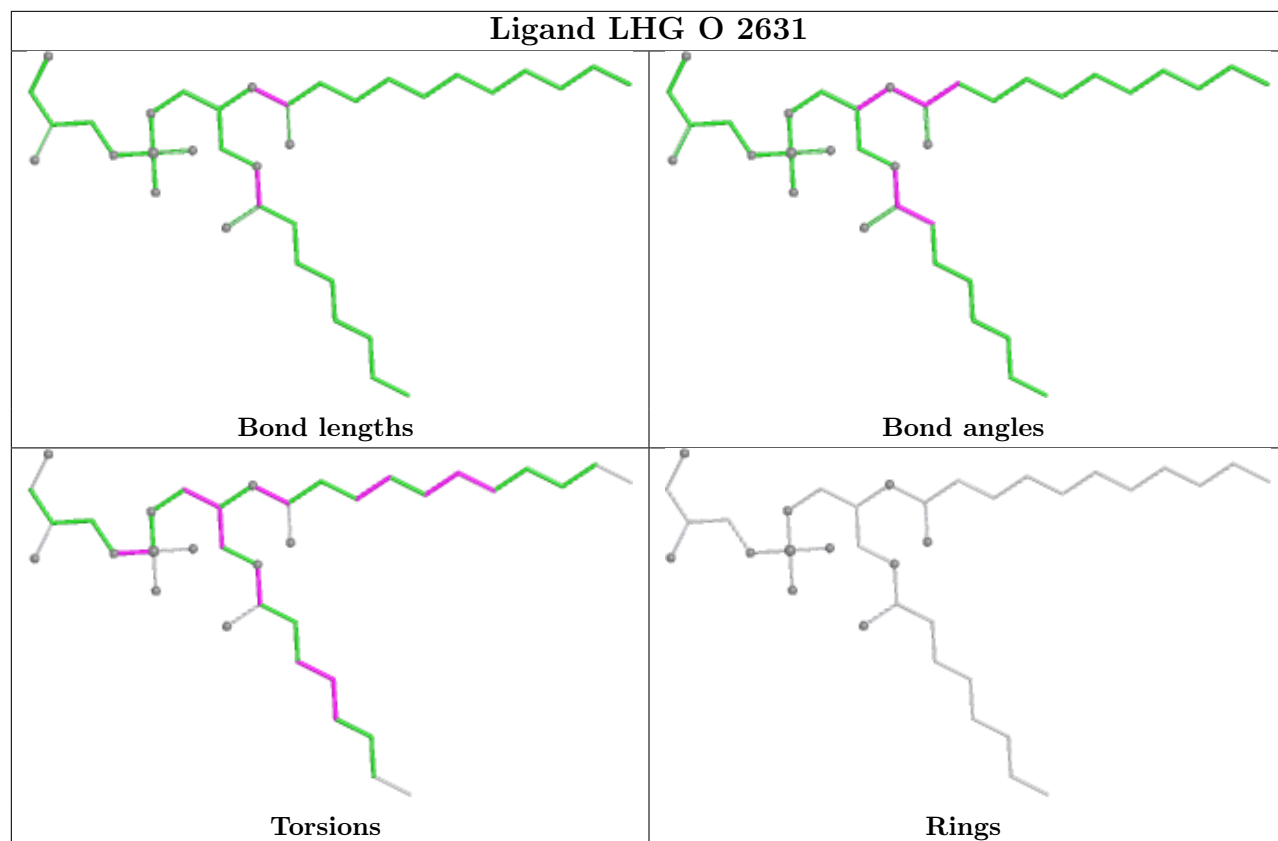


Rings

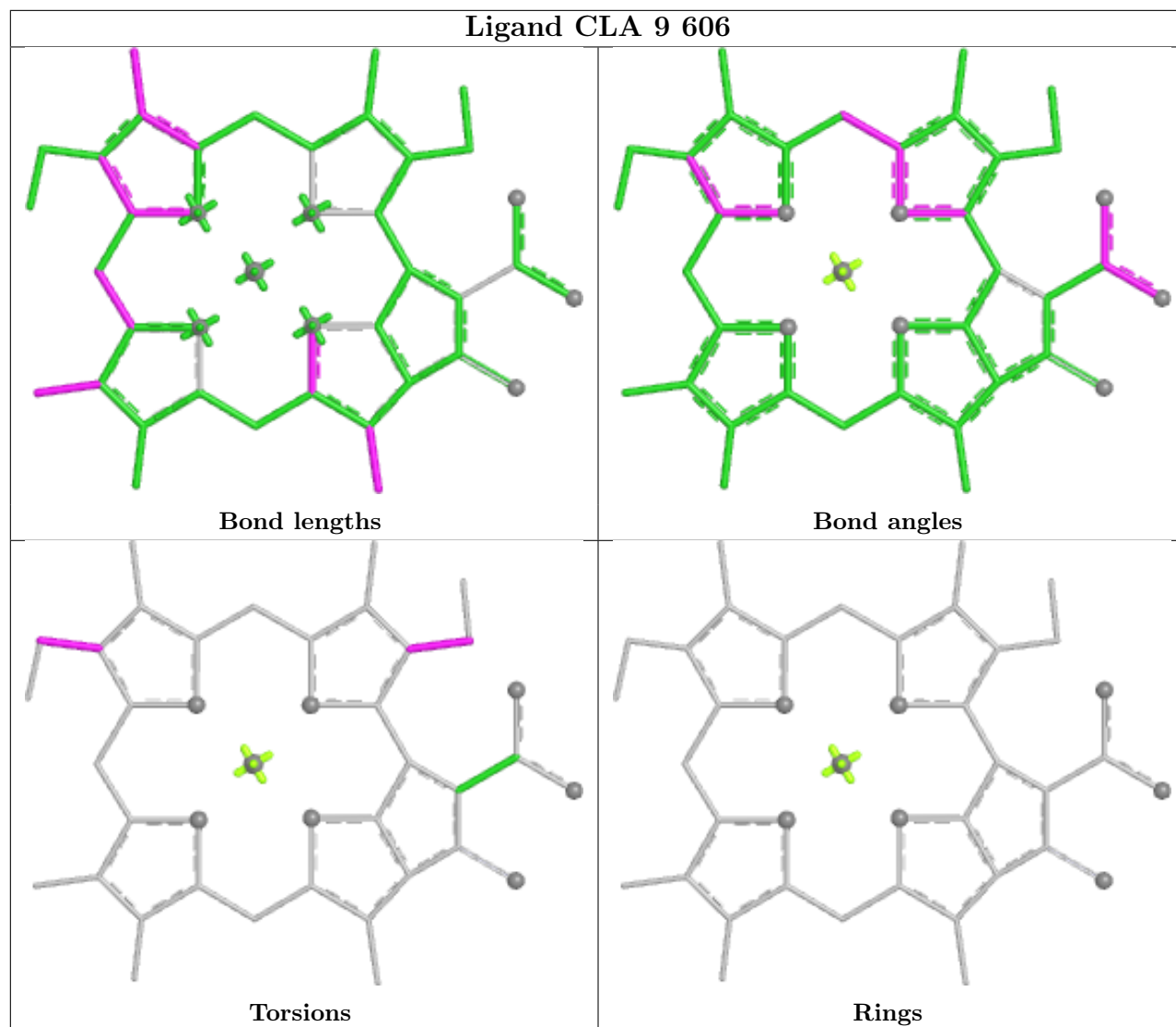
Ligand CLA 9 603



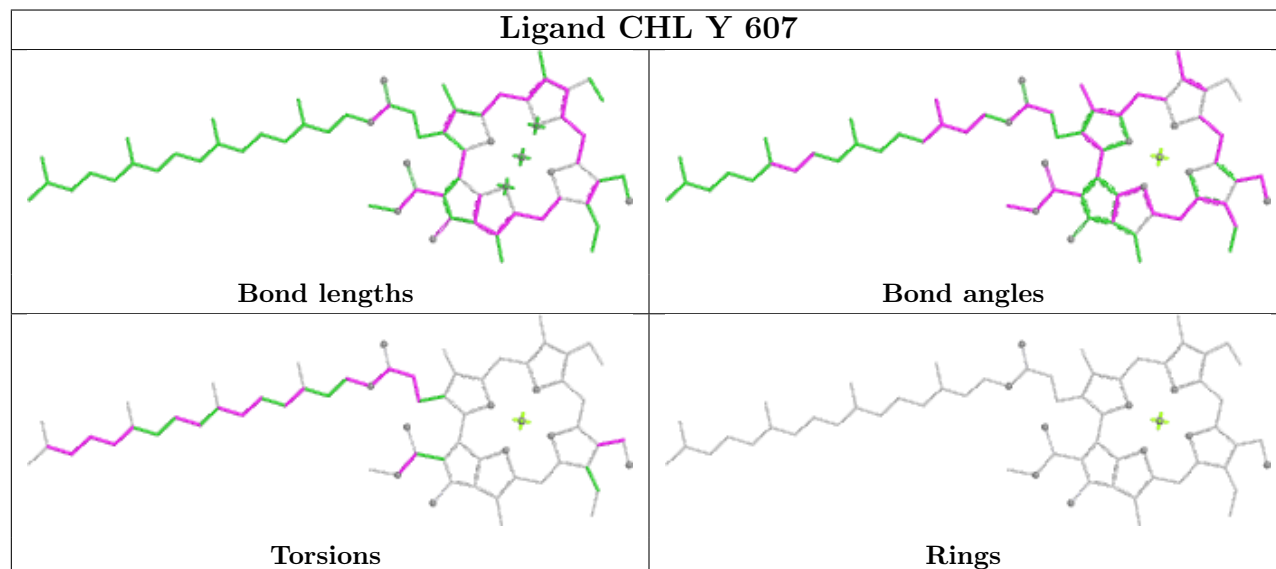


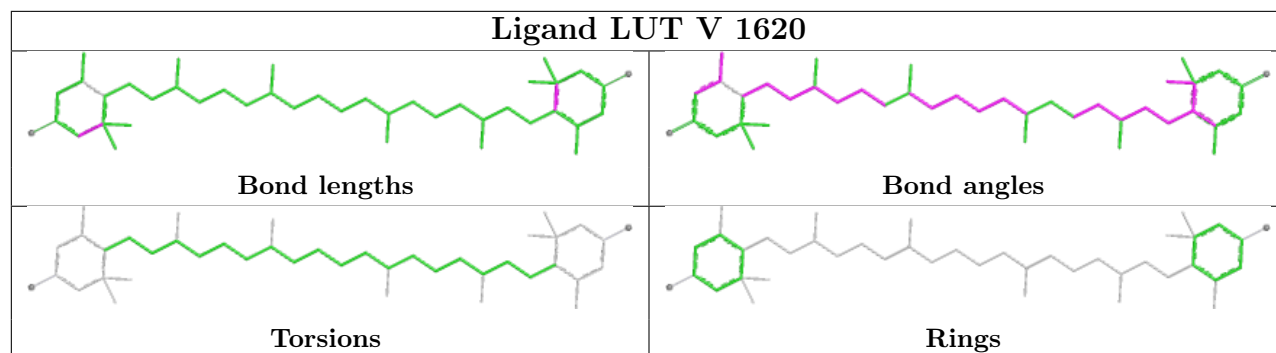
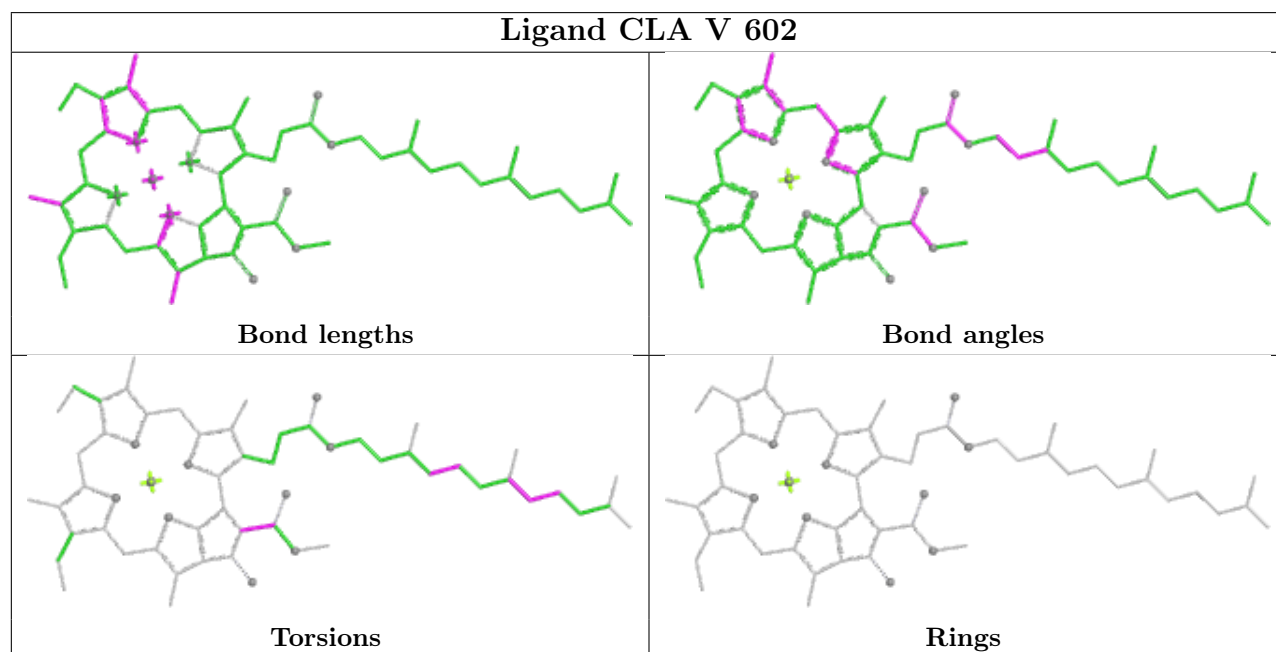
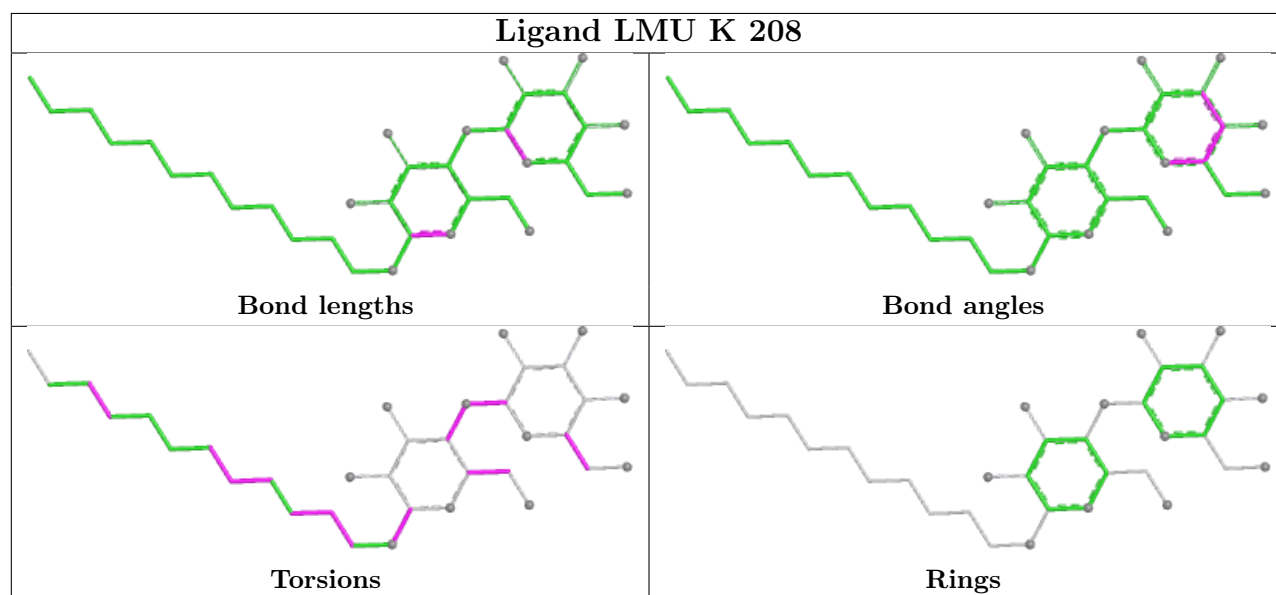


Ligand CLA 9 606

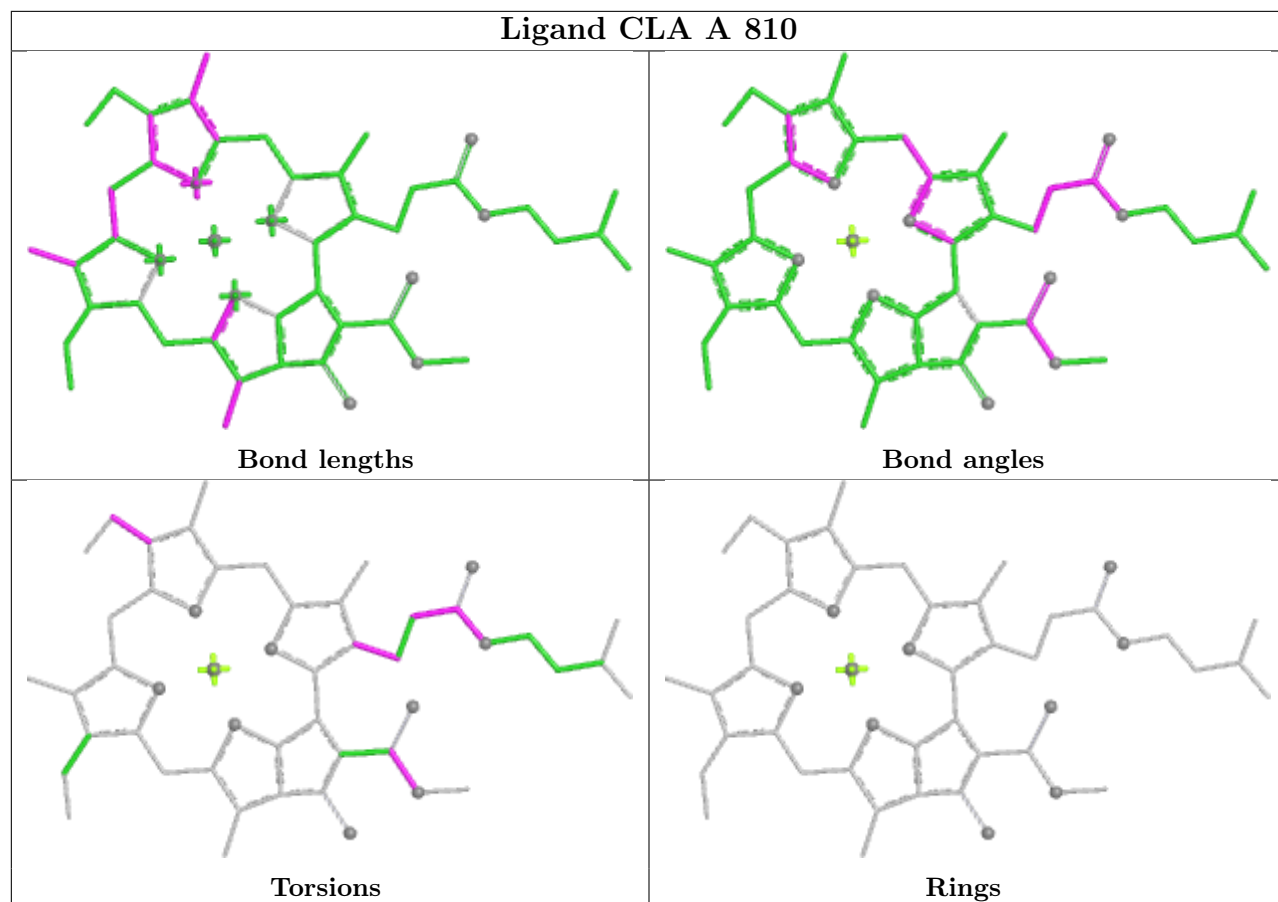


Ligand CHL Y 607

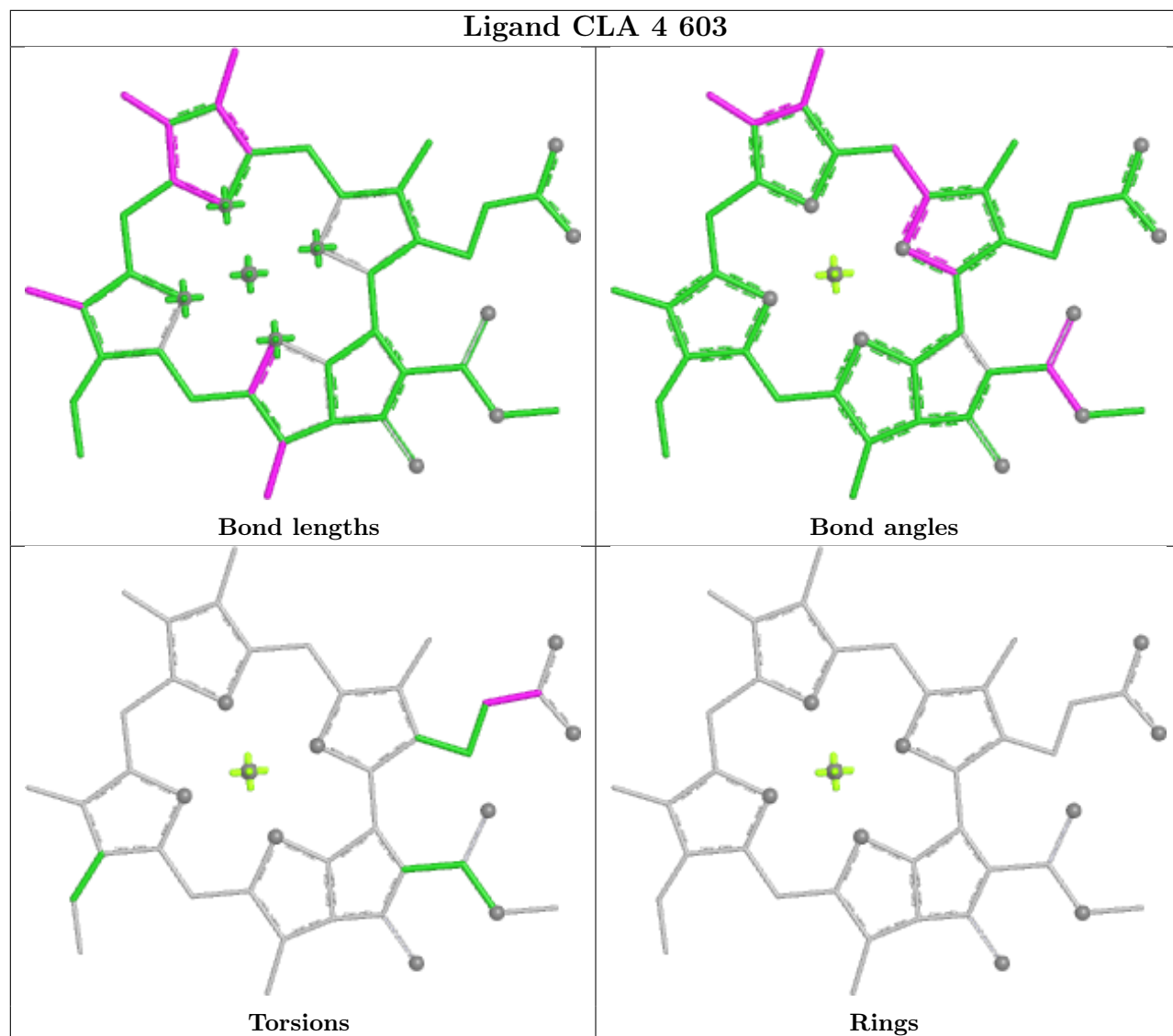


Ligand LUT V 1620**Ligand CLA V 602****Ligand LMU K 208**

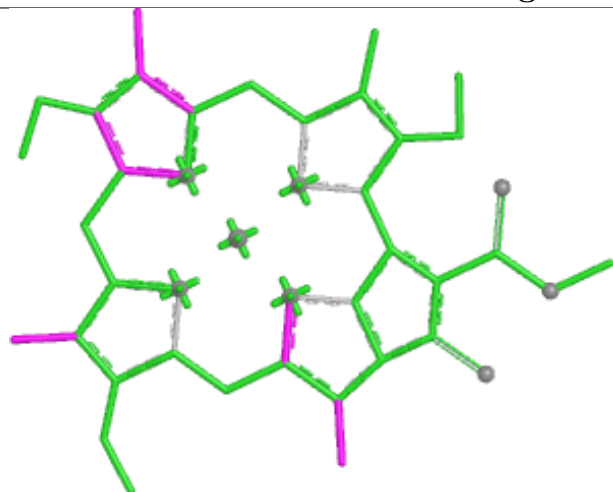
Ligand CLA A 810



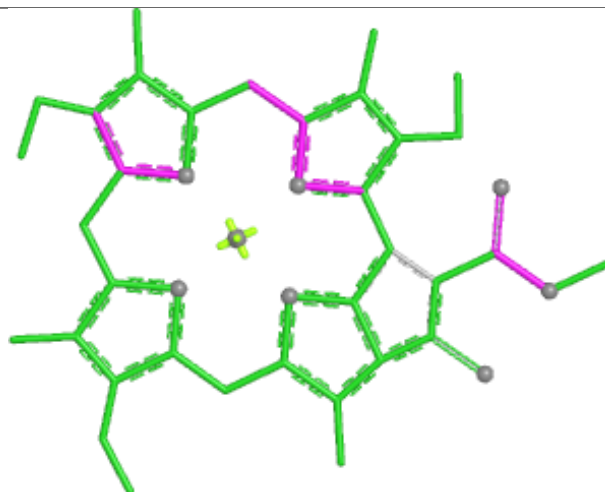
Ligand CLA 4 603



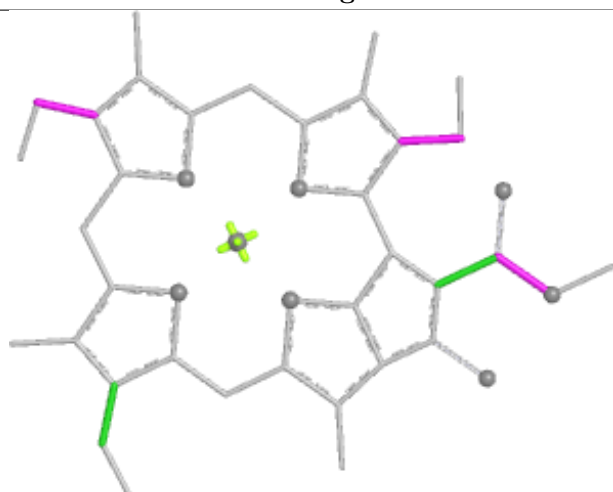
Ligand CLA 5 611



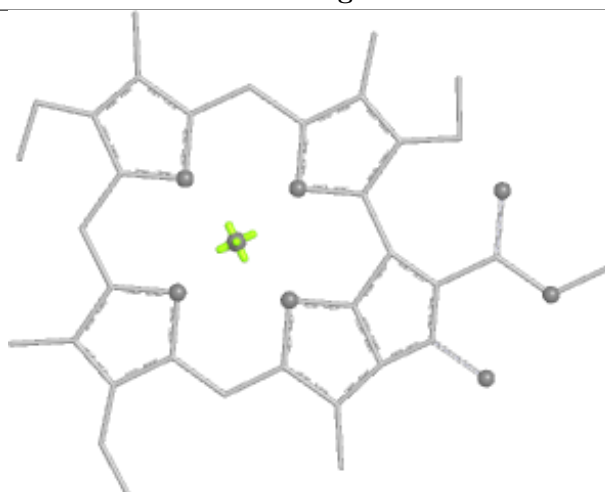
Bond lengths



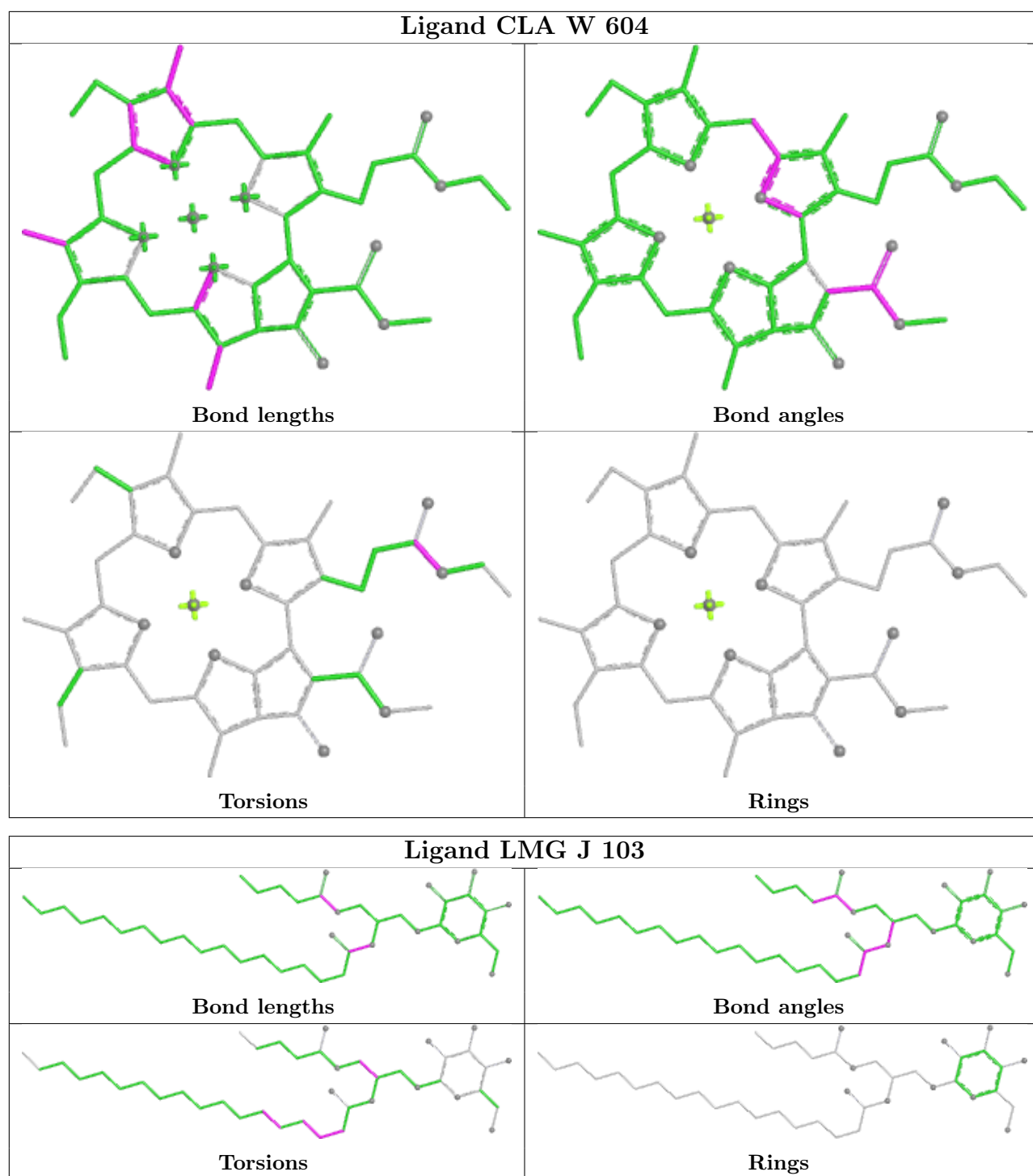
Bond angles

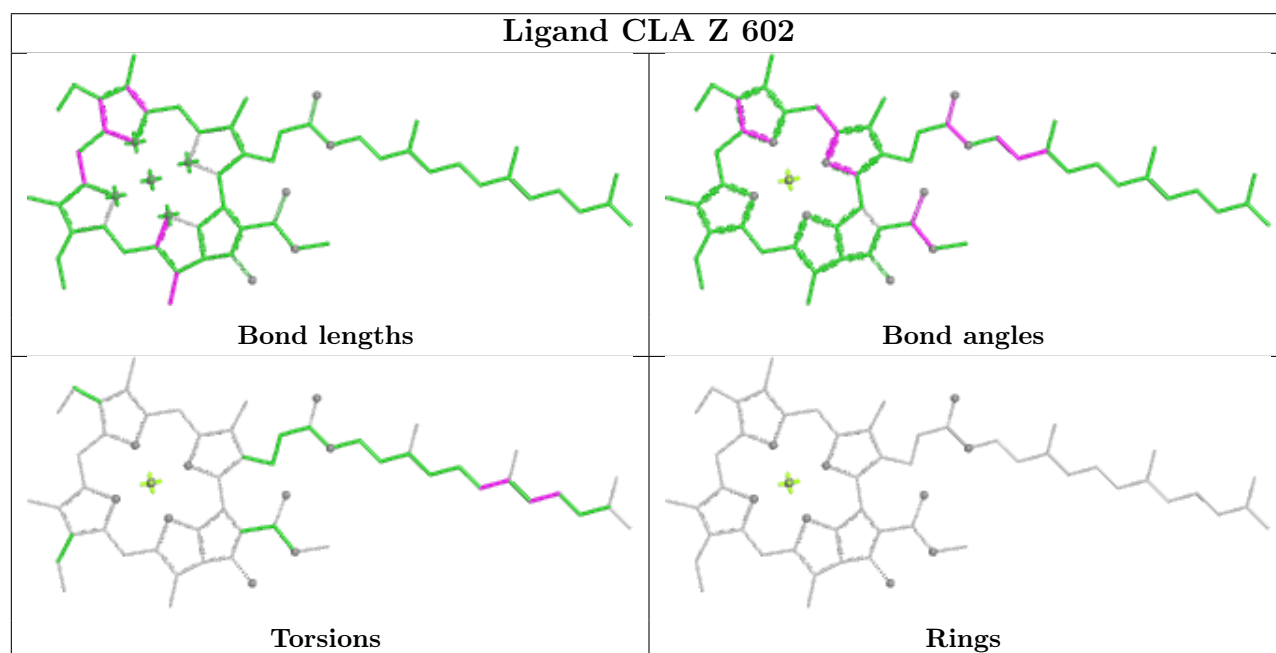
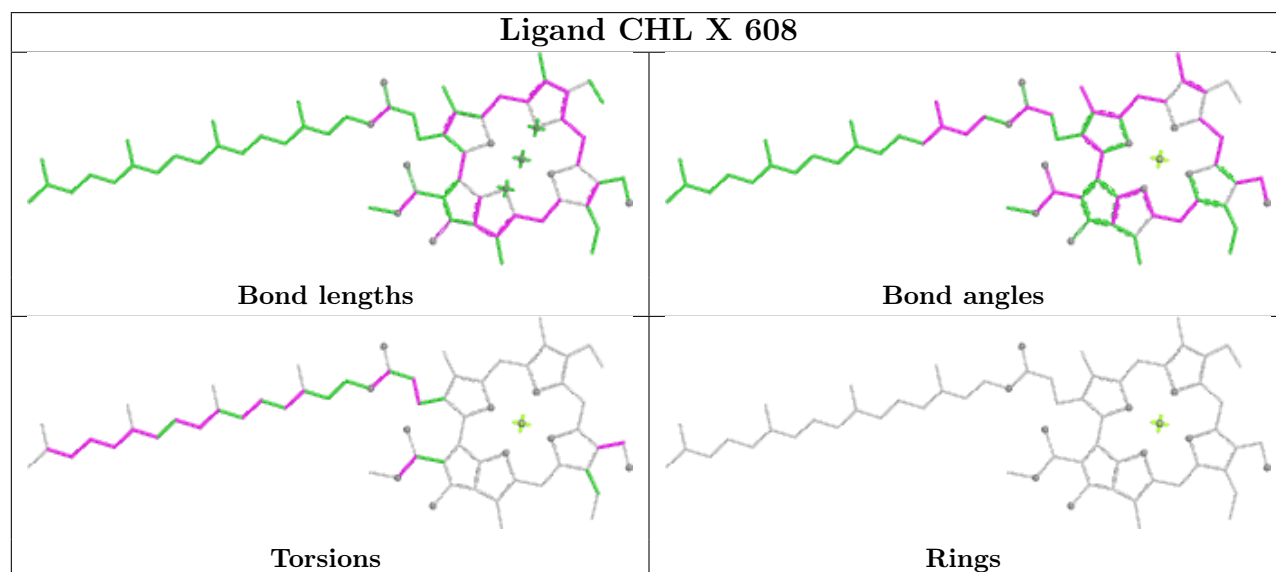
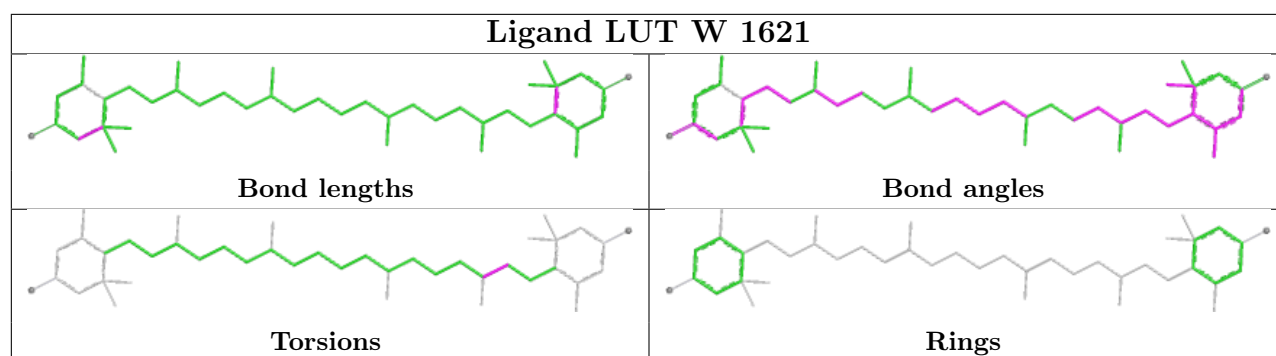


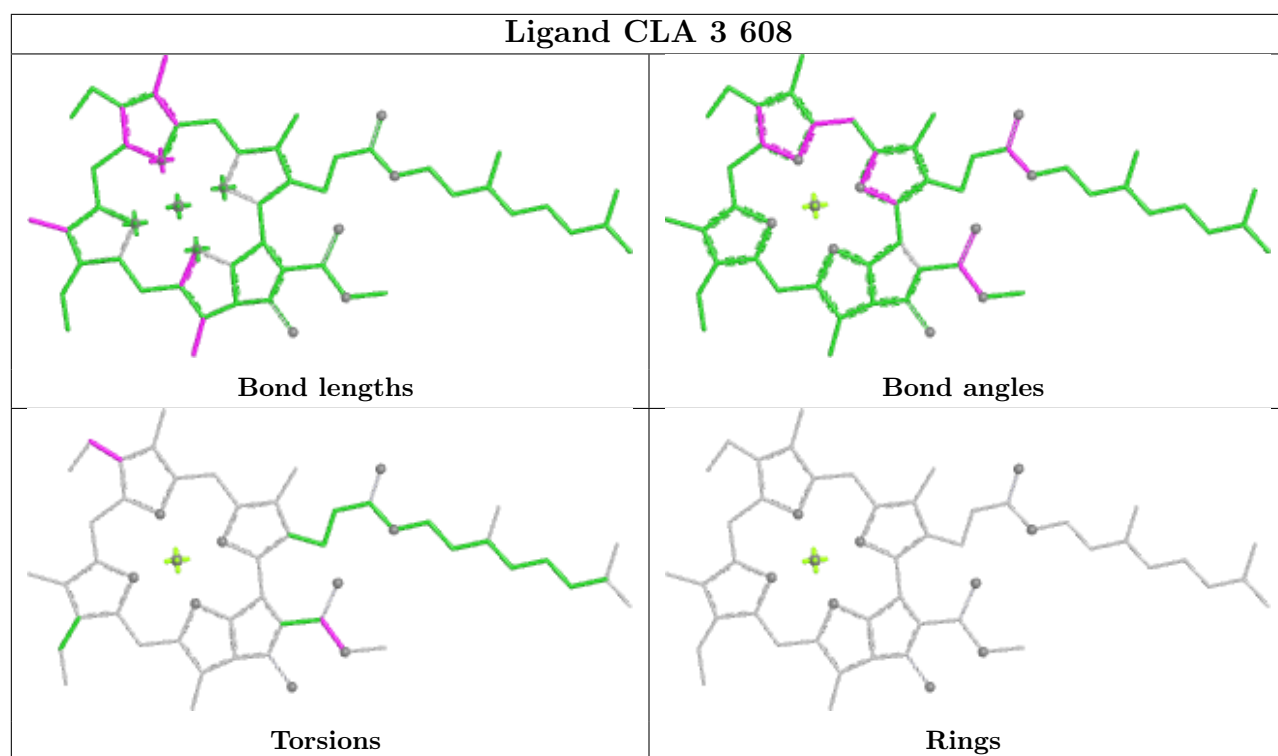
Torsions



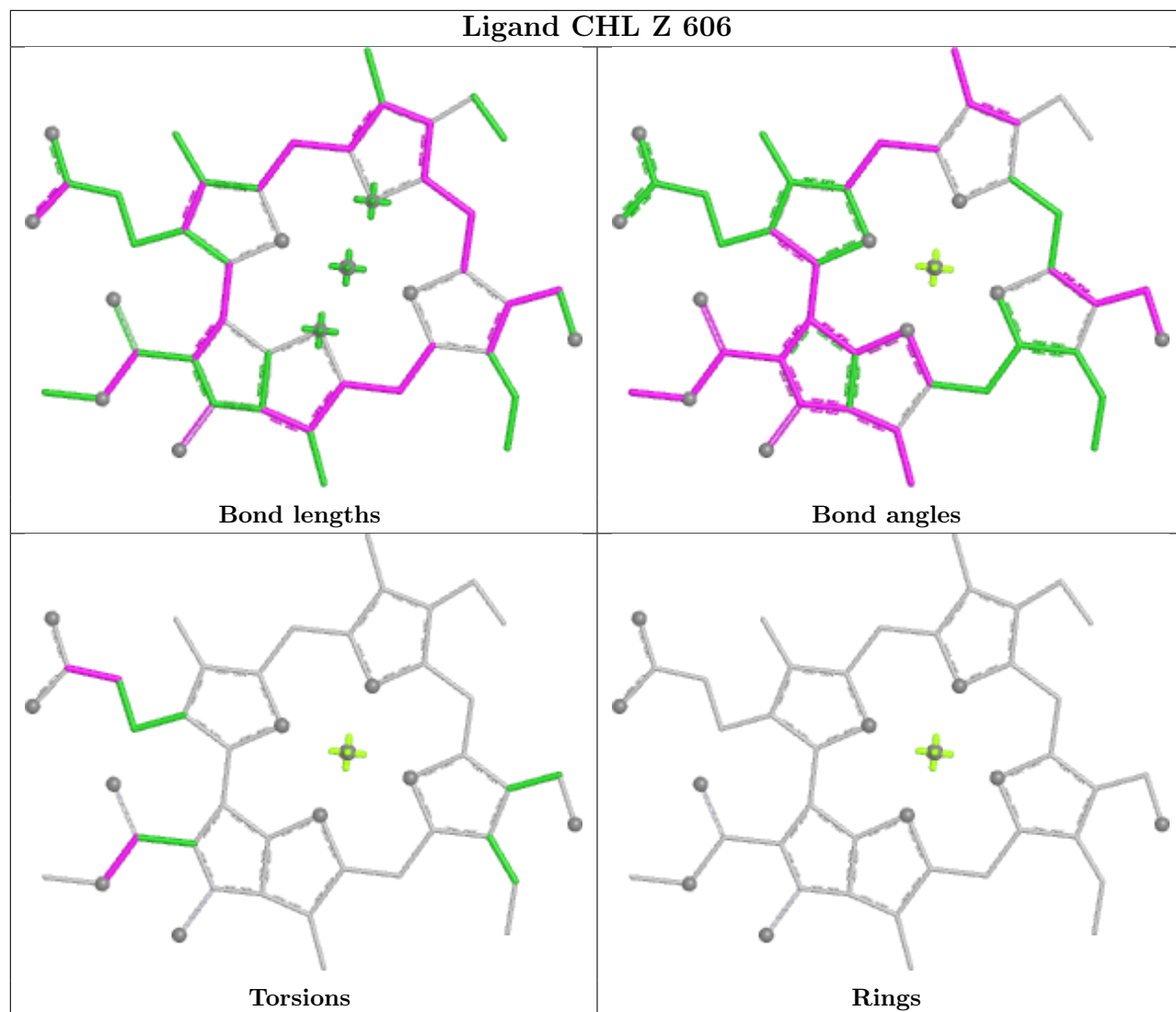
Rings



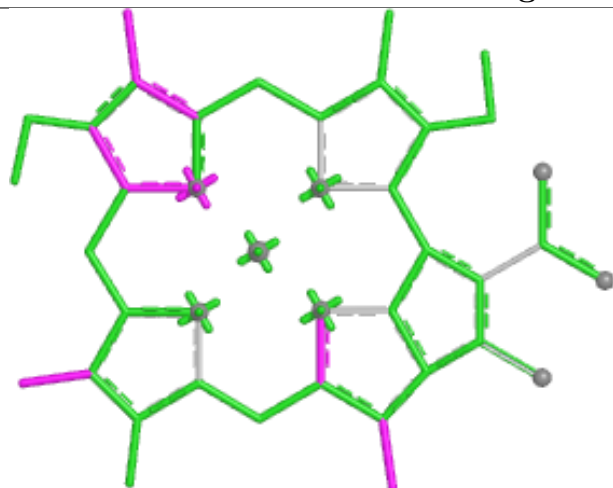




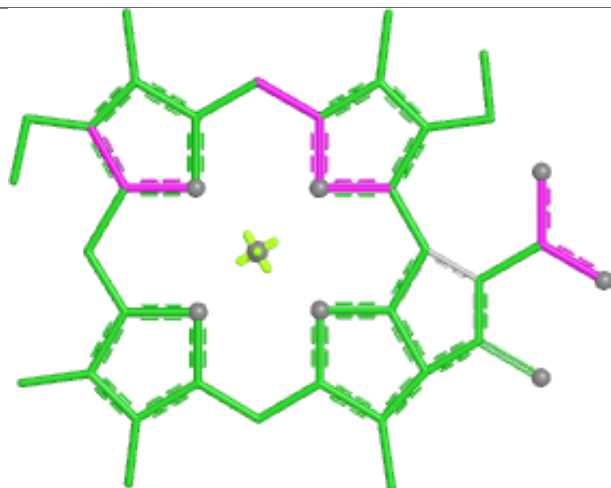
Ligand CHL Z 606



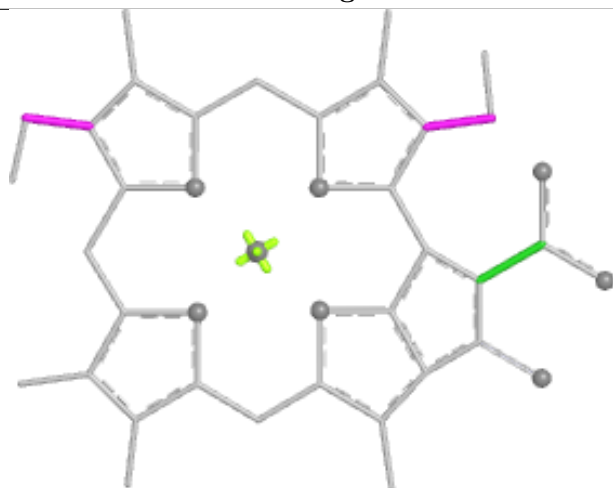
Ligand CLA 4 606



Bond lengths



Bond angles

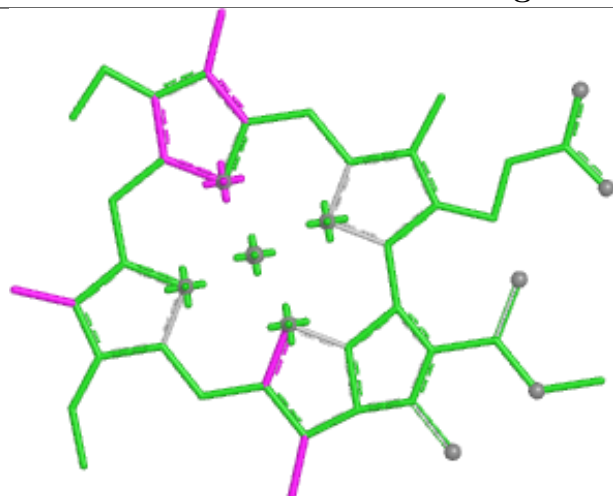


Torsions

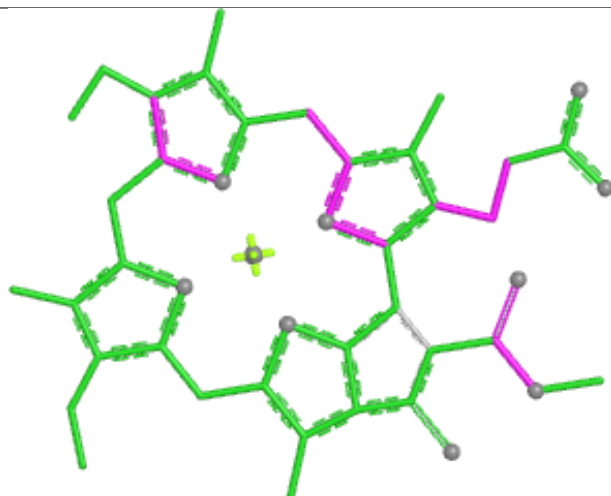


Rings

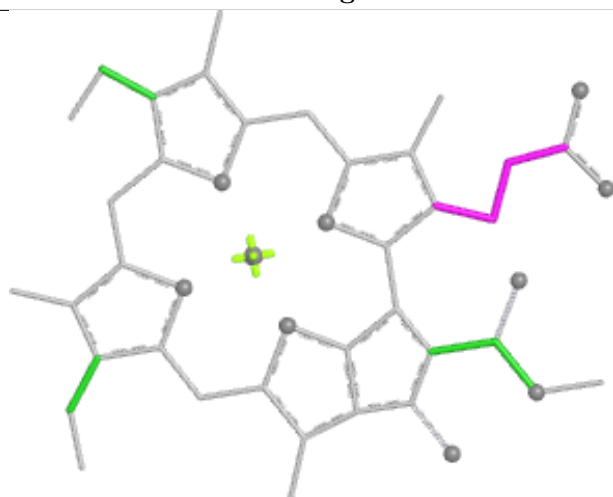
Ligand CLA A 833



Bond lengths



Bond angles

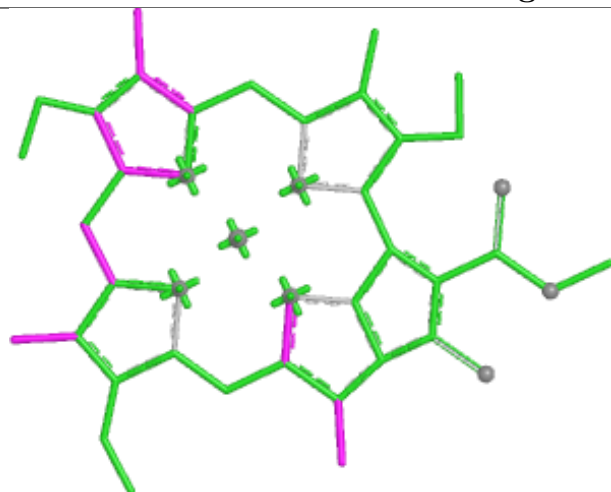


Torsions

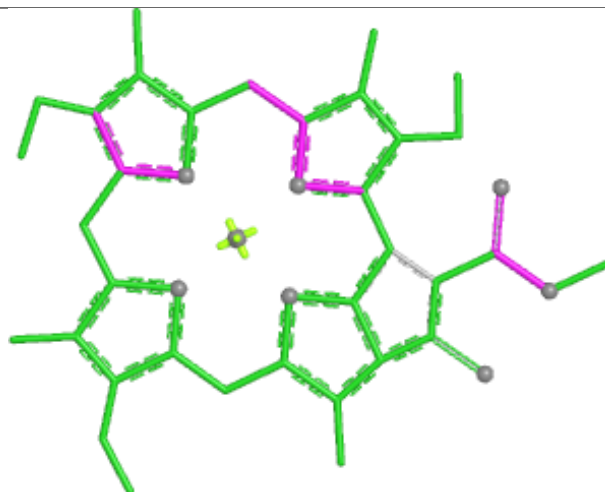


Rings

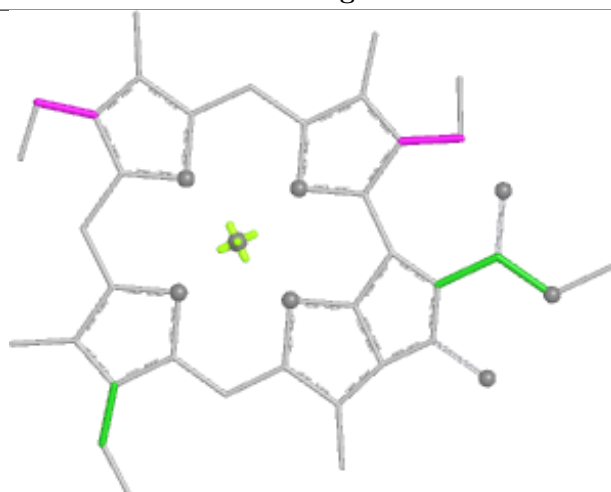
Ligand CLA 8 611



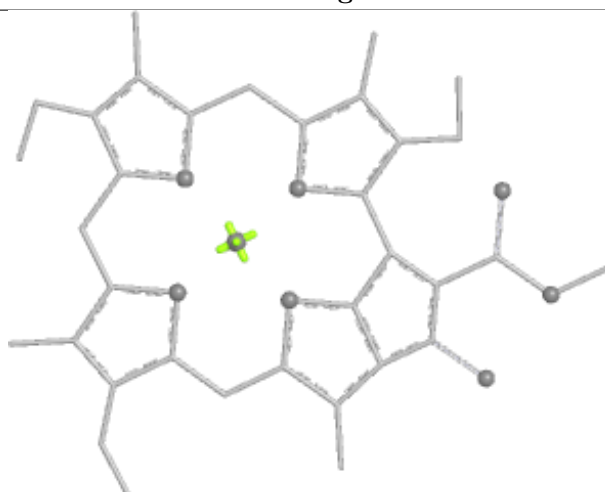
Bond lengths



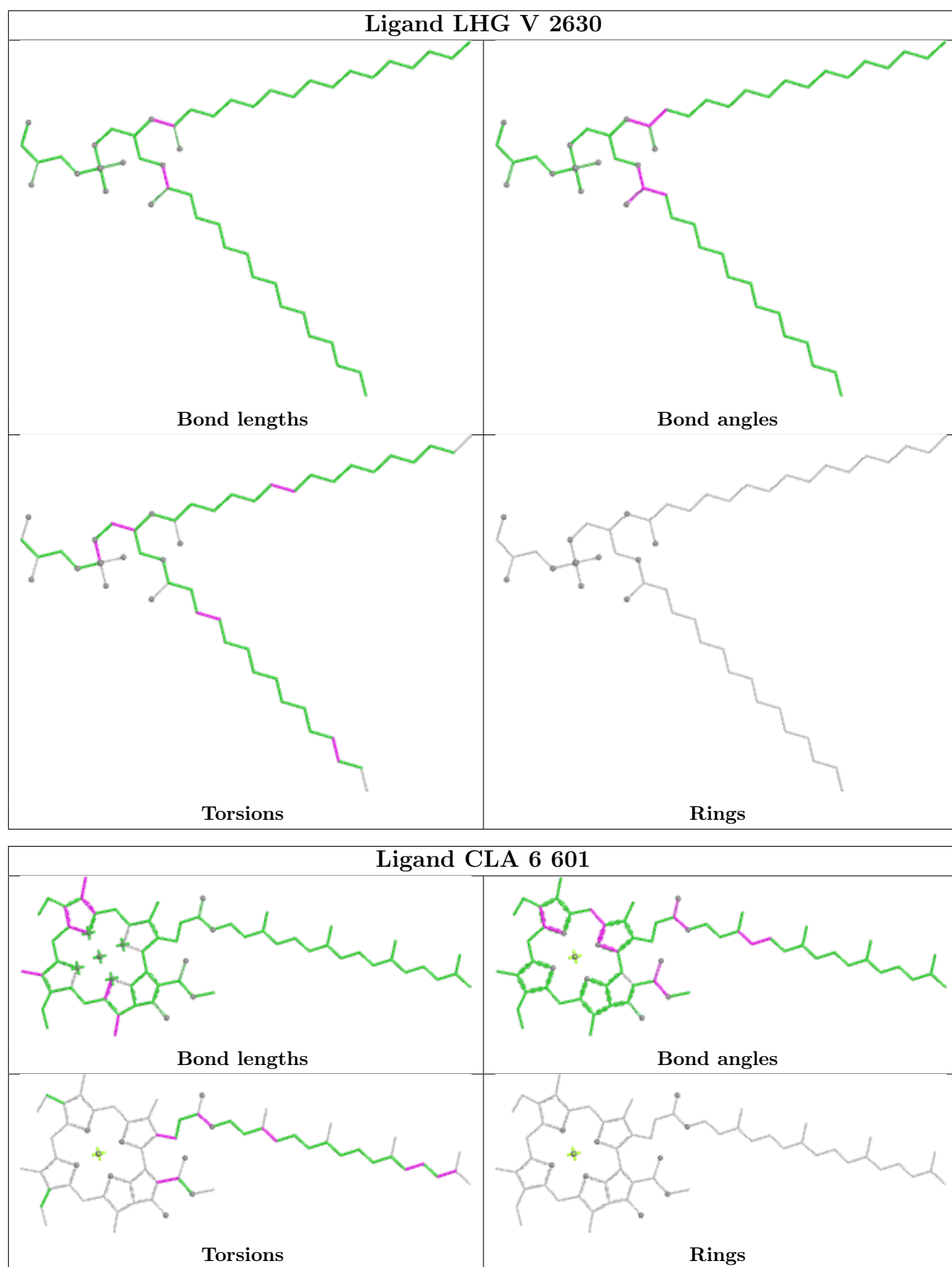
Bond angles

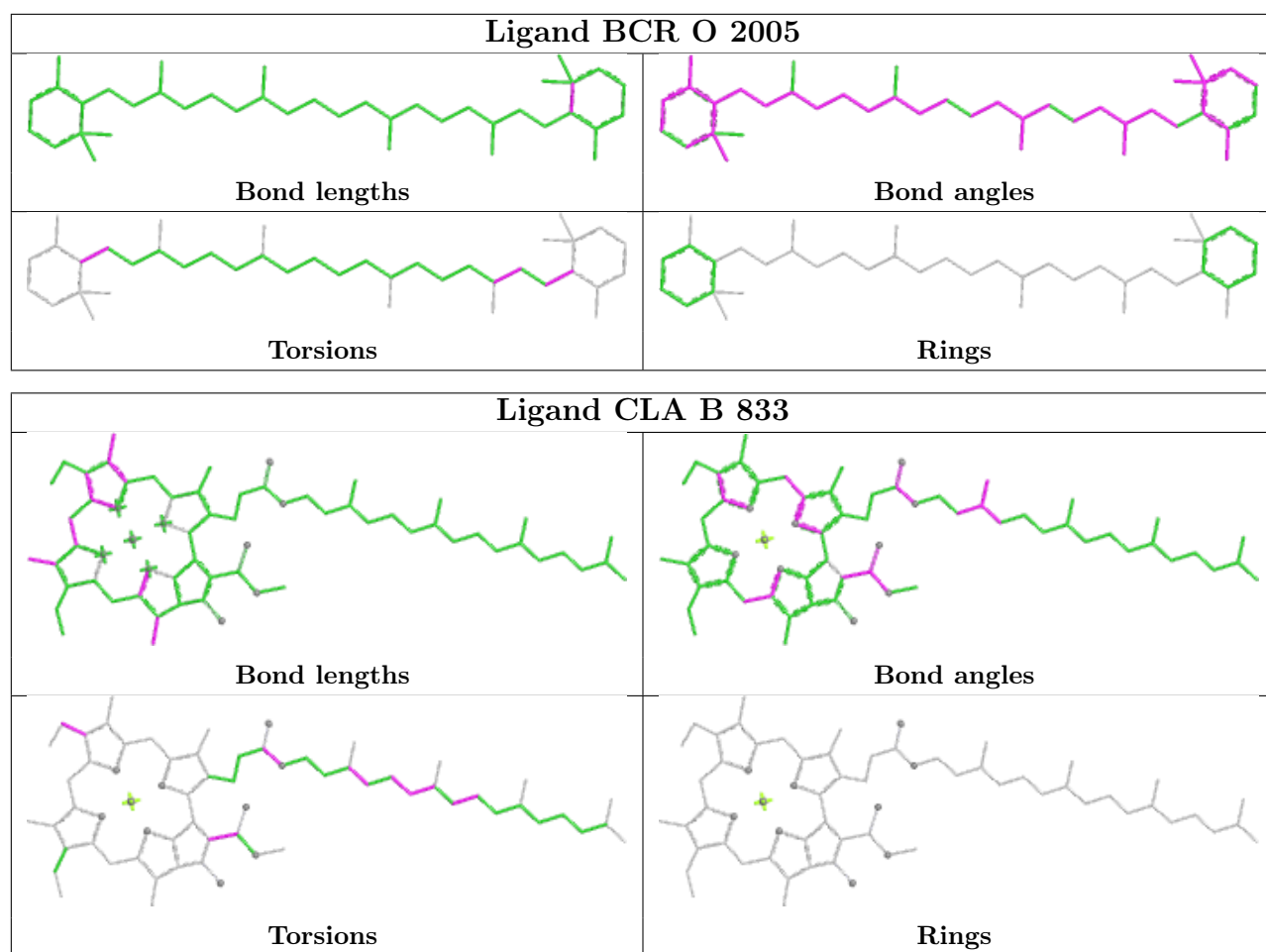


Torsions

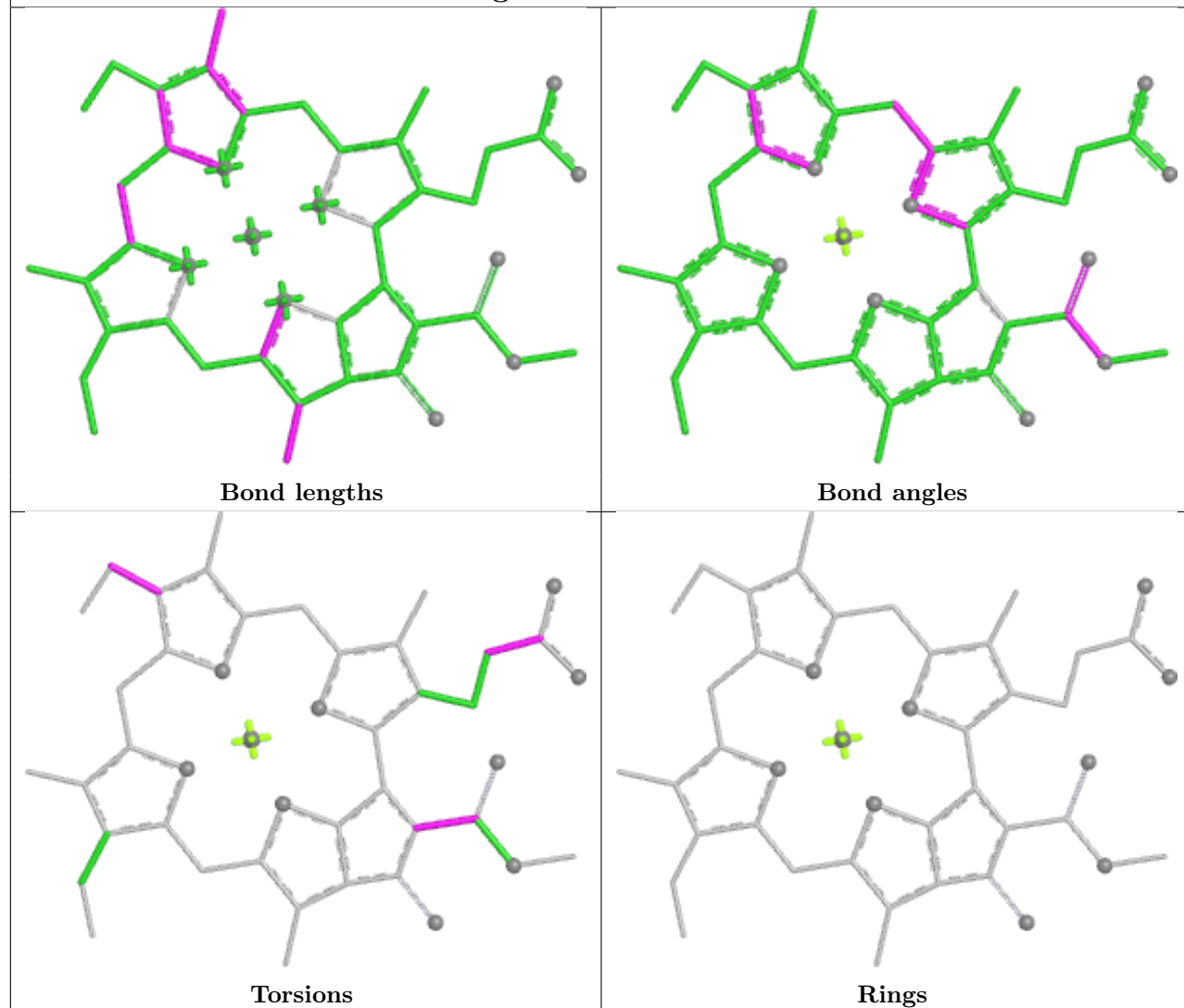


Rings

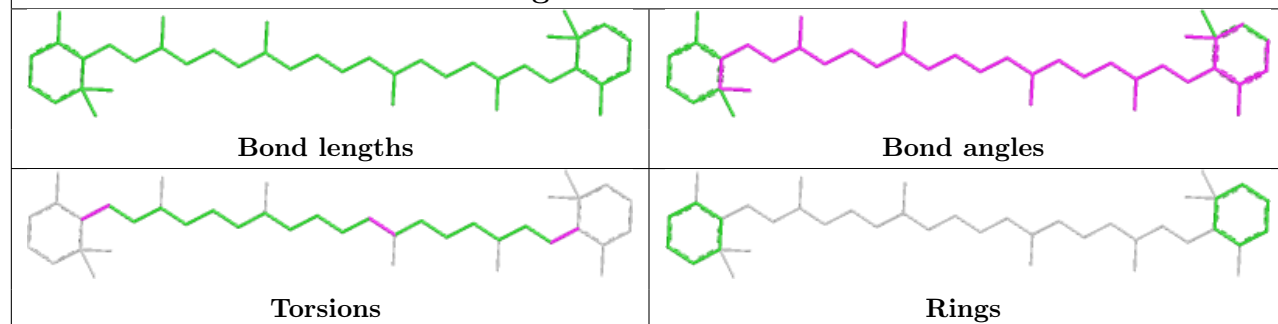


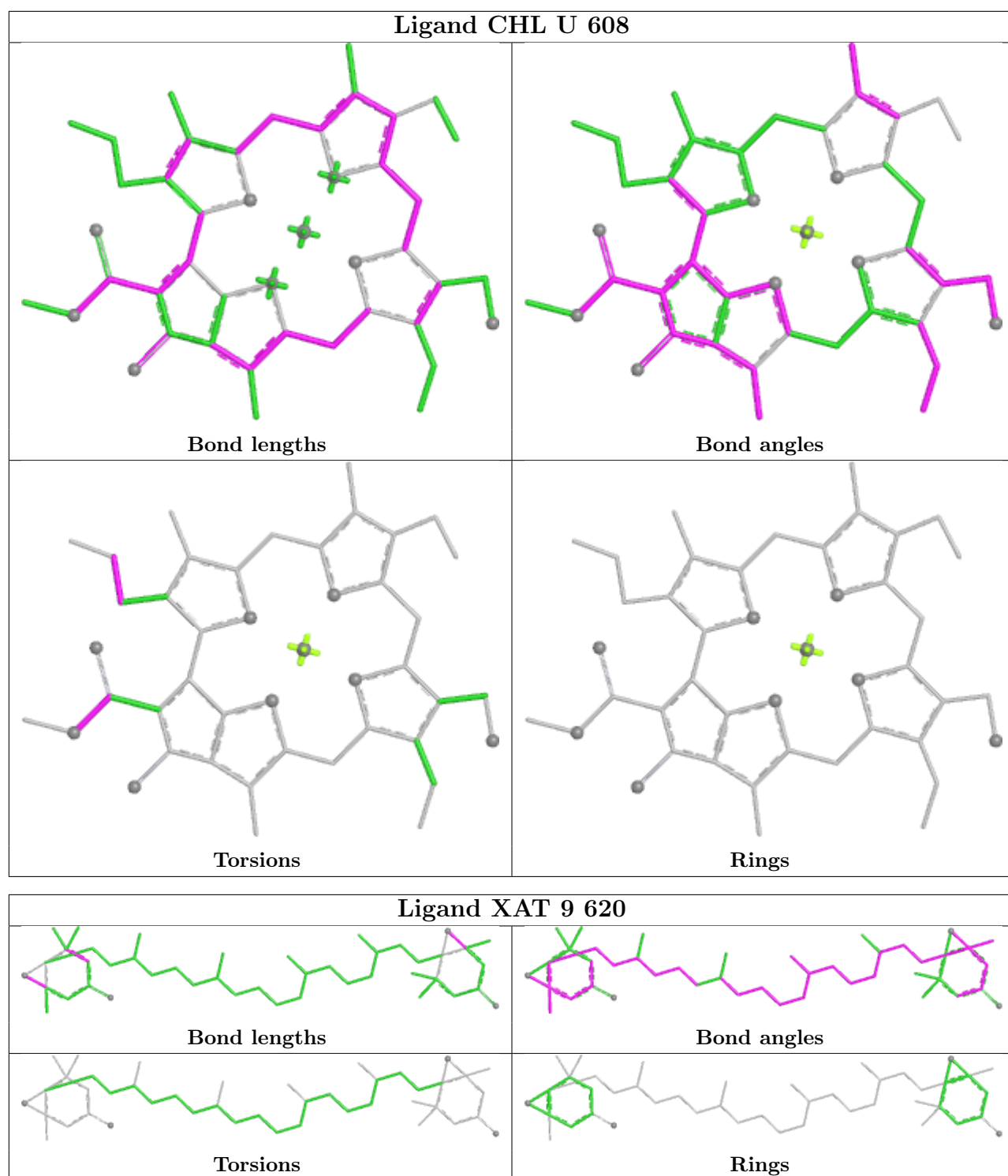


Ligand CLA Y 612

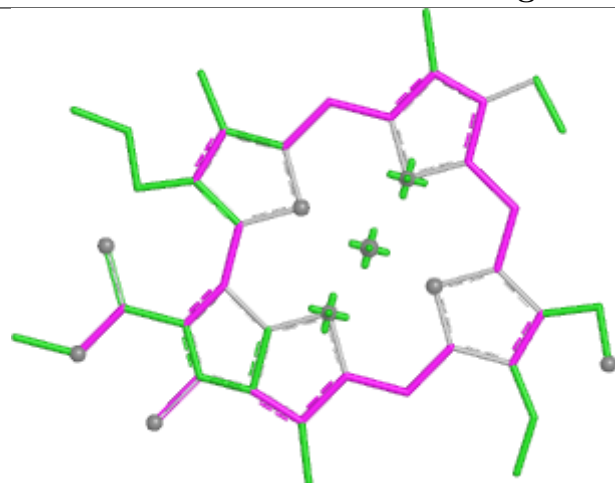


Ligand BCR F 305

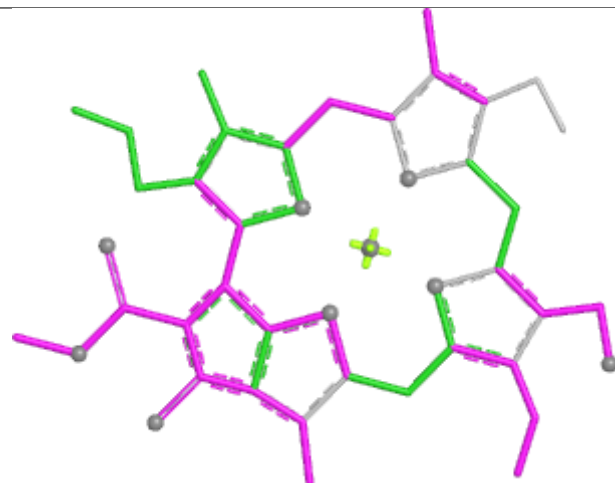




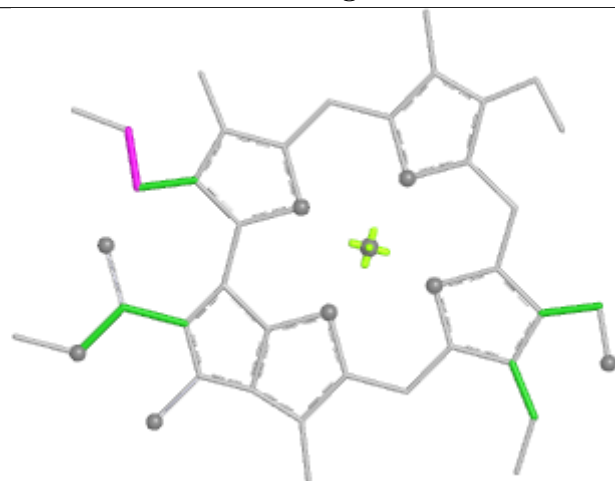
Ligand CHL Z 605



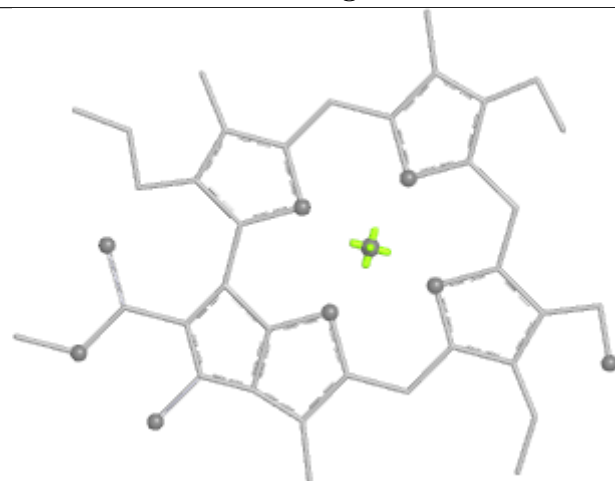
Bond lengths



Bond angles

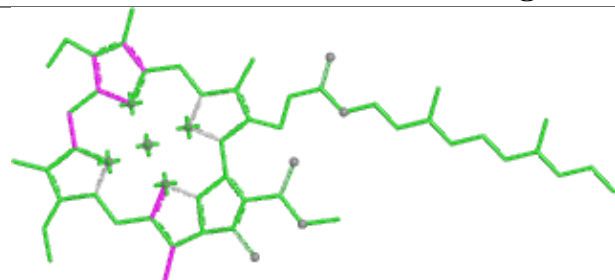


Torsions

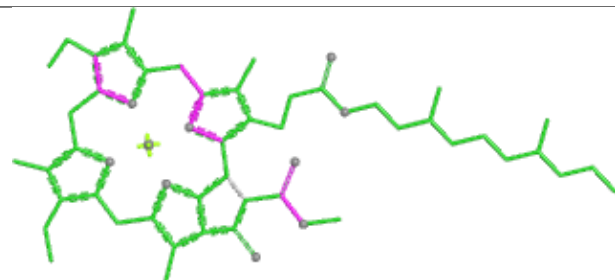


Rings

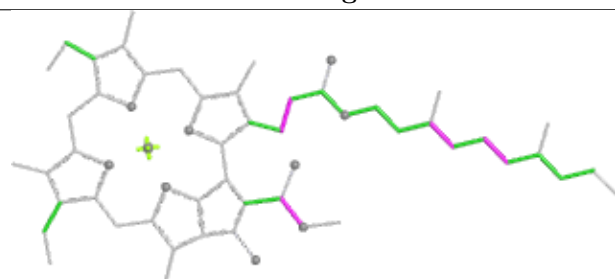
Ligand CLA Z 604



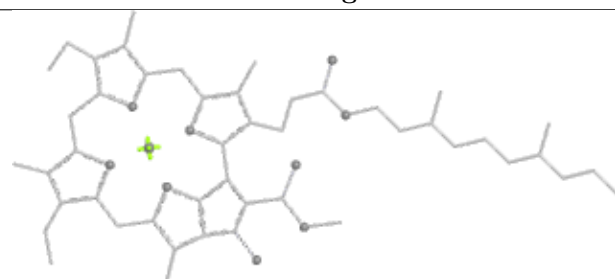
Bond lengths



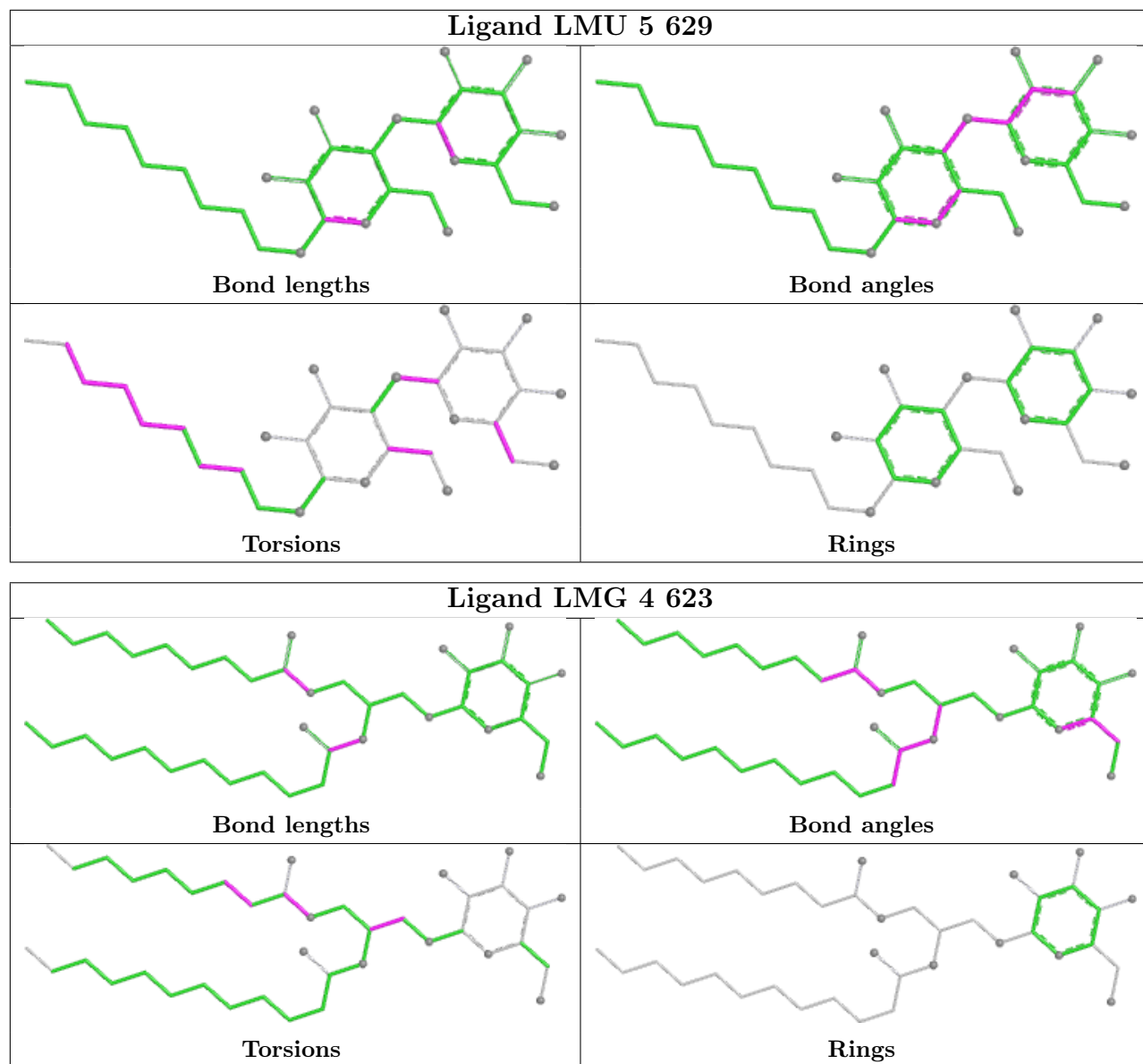
Bond angles

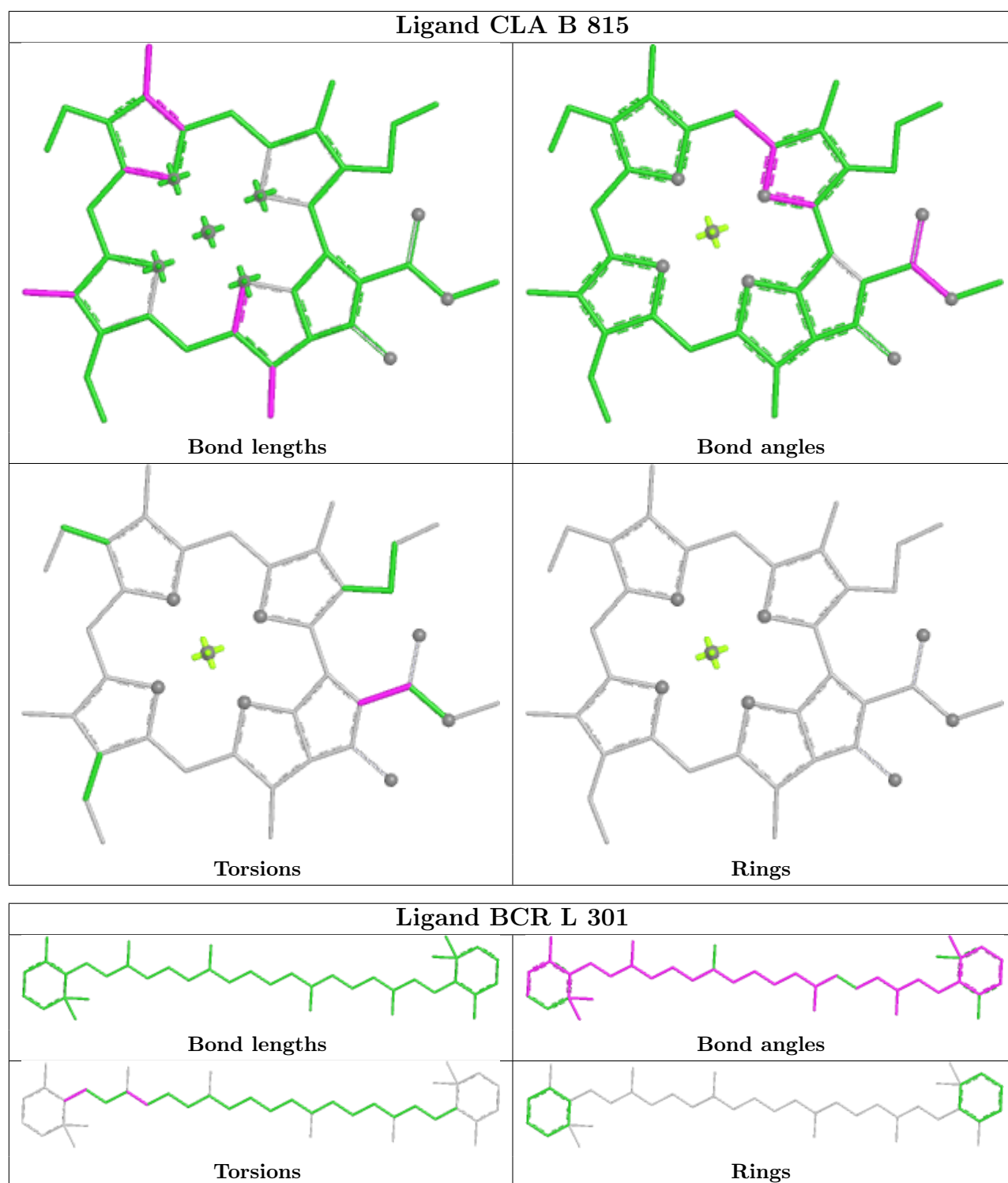


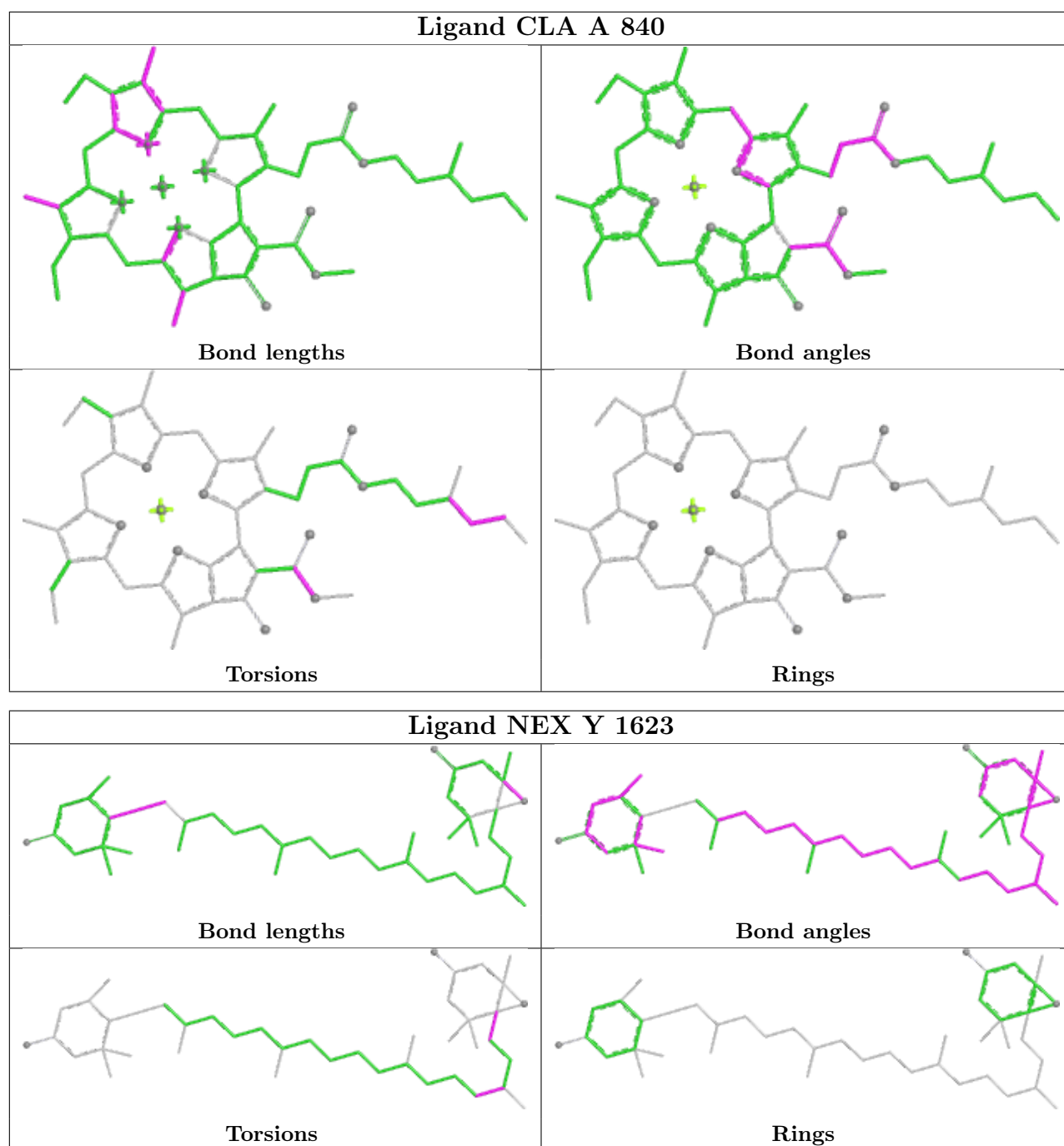
Torsions

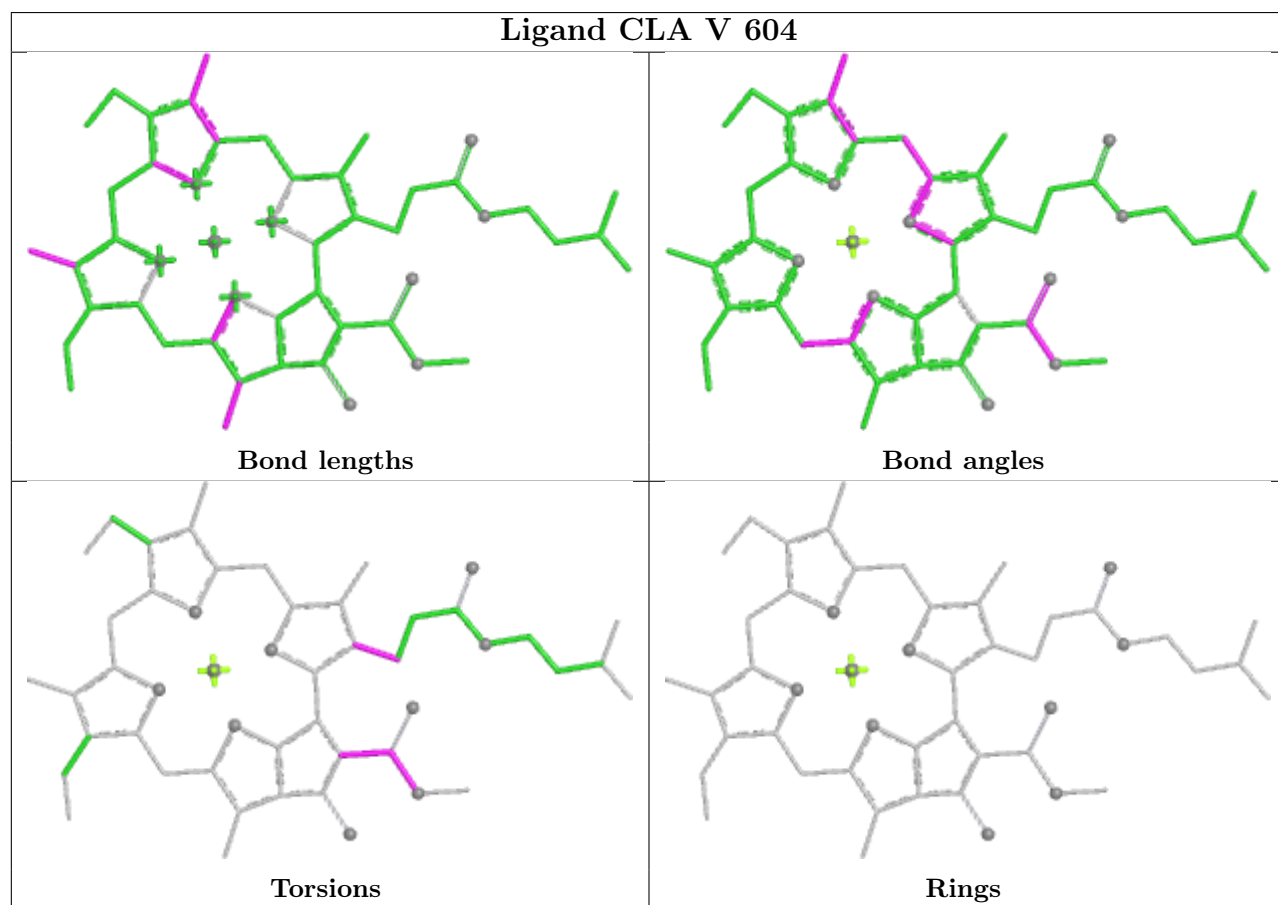
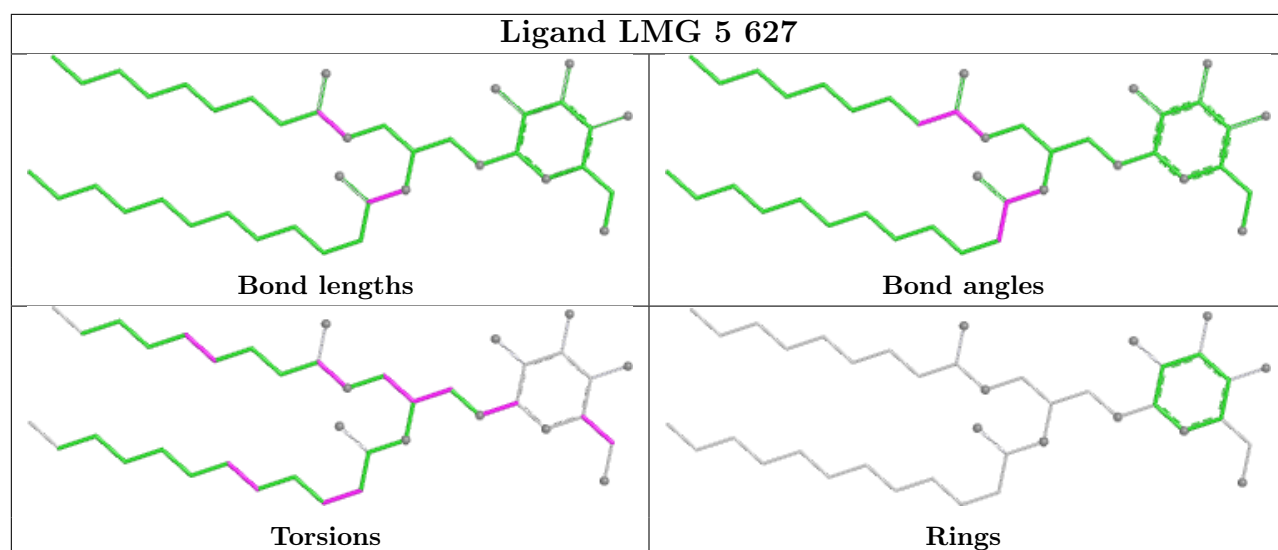


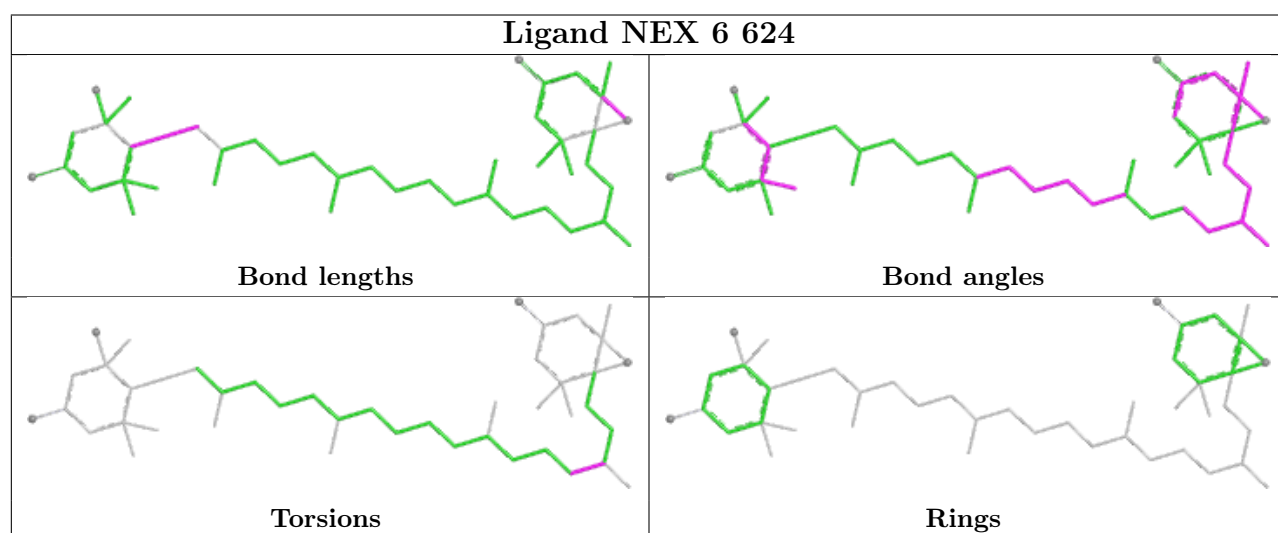
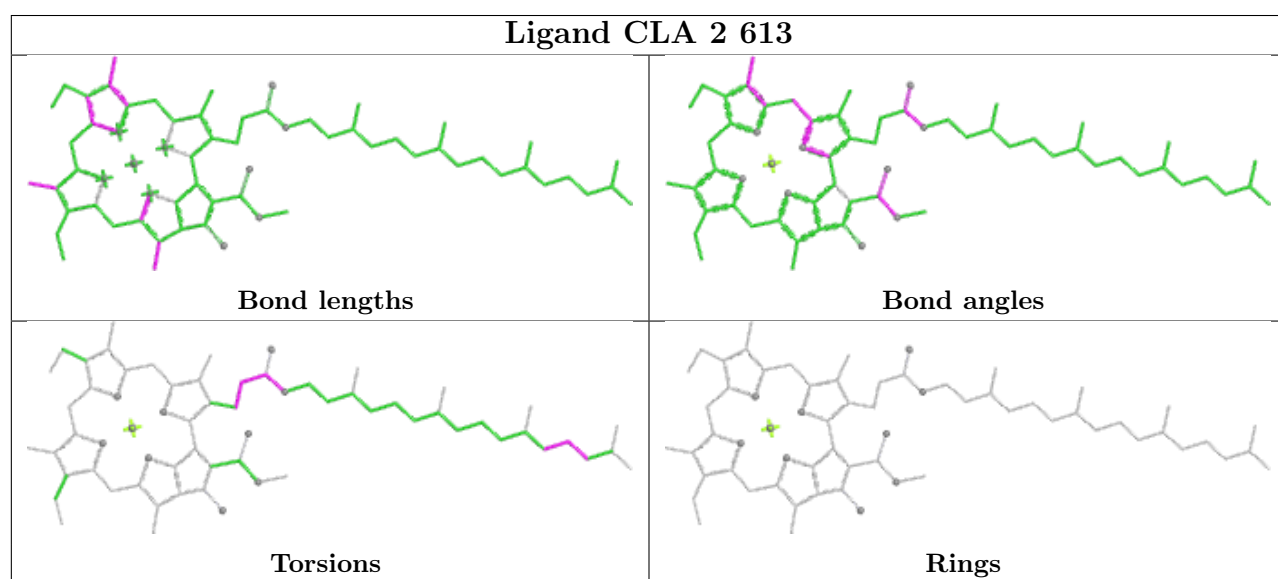
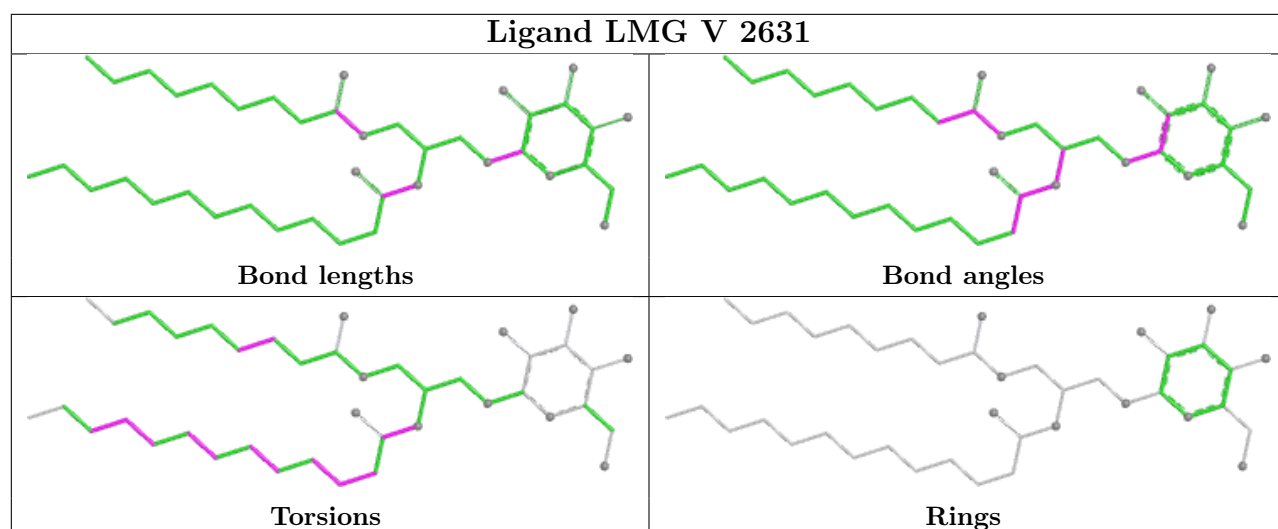
Rings

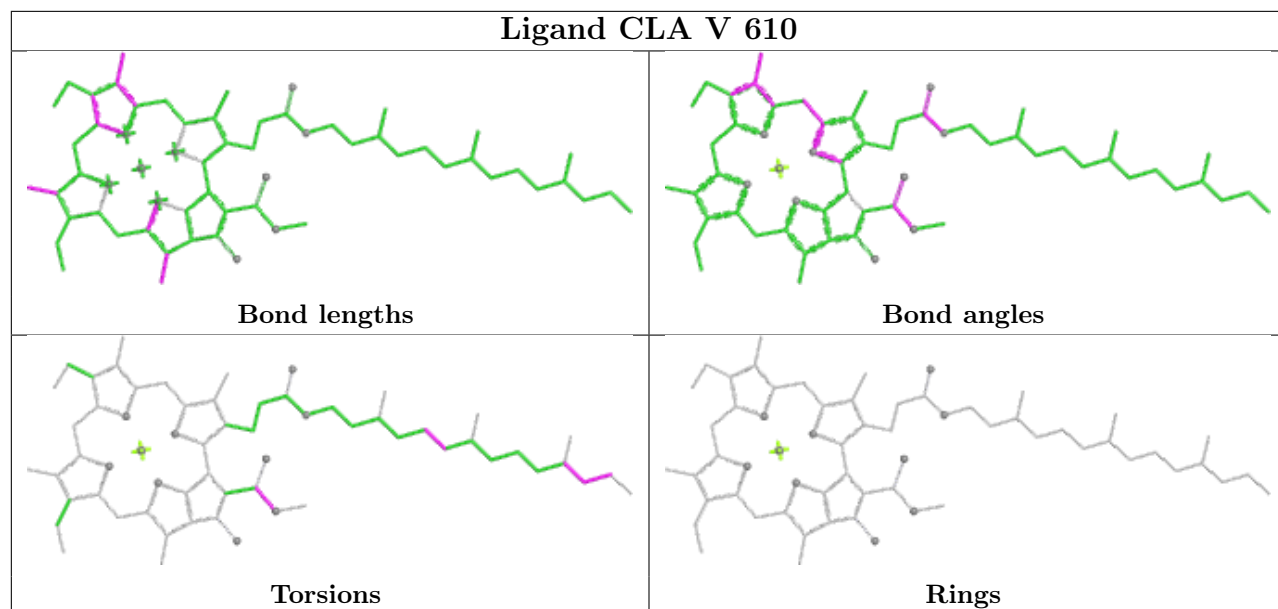
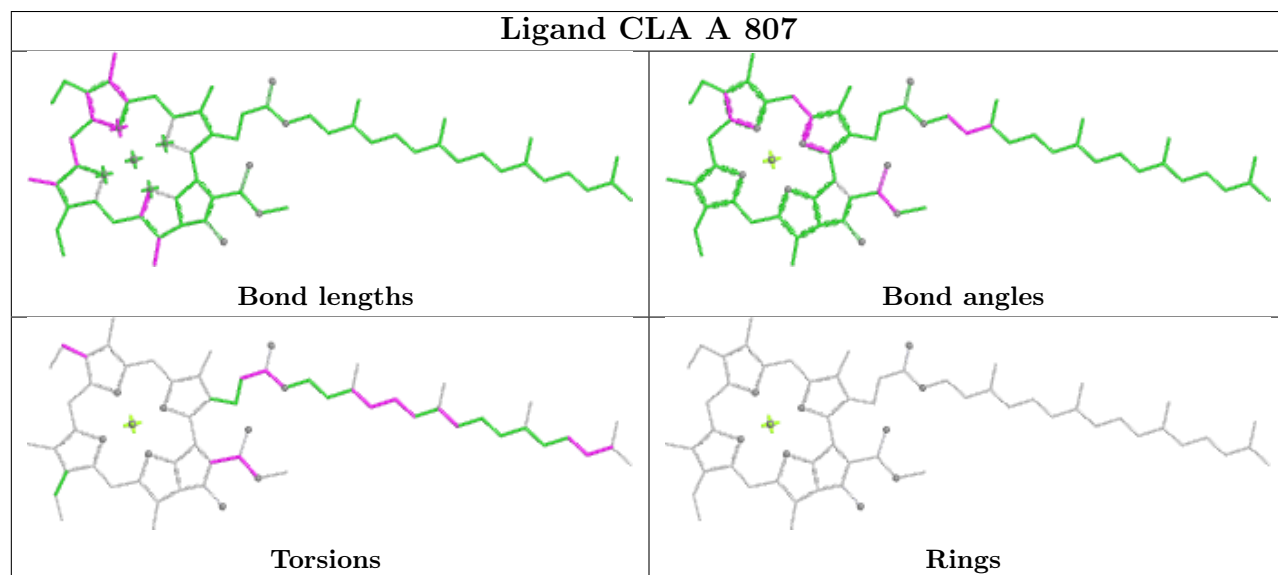




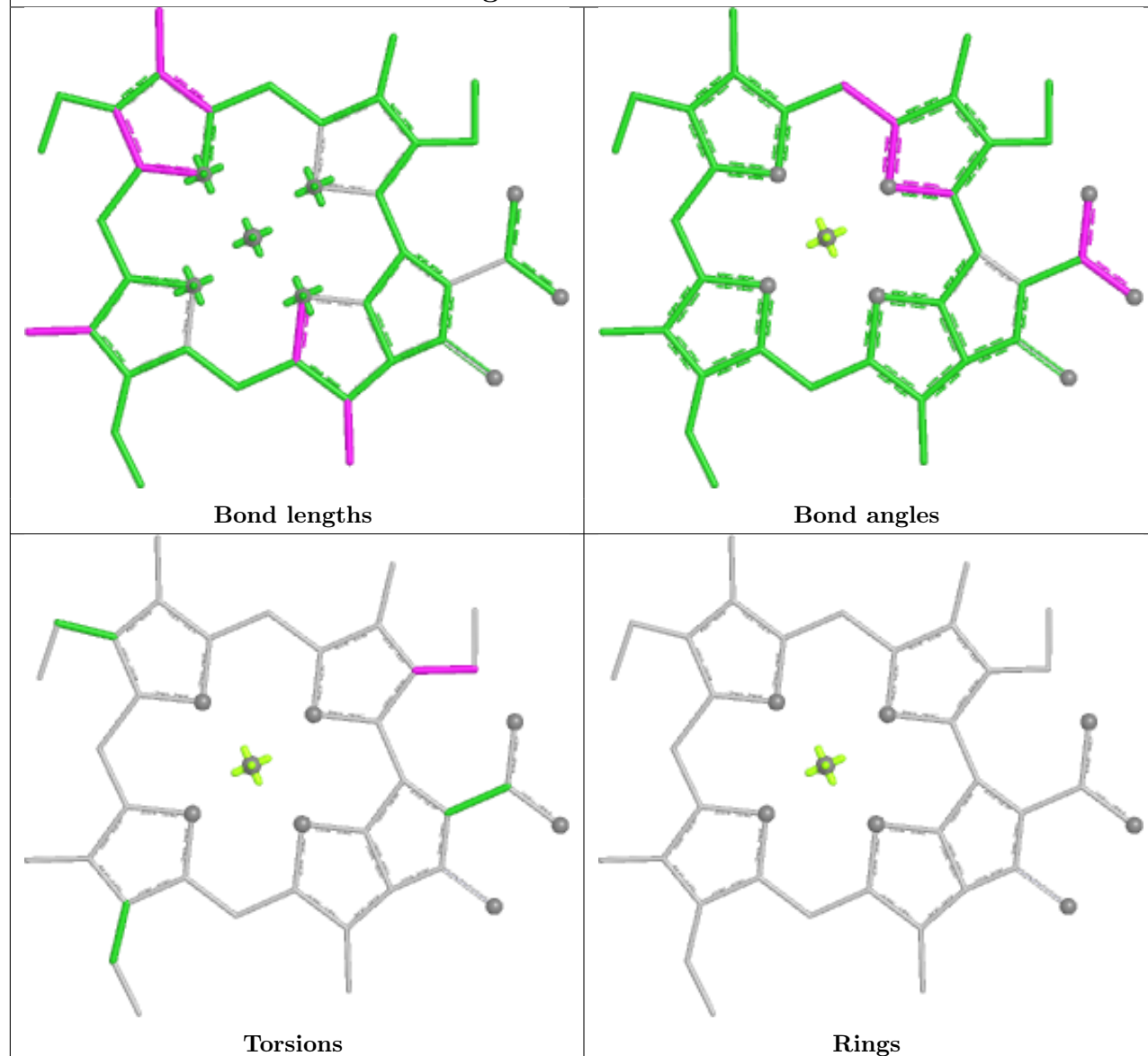




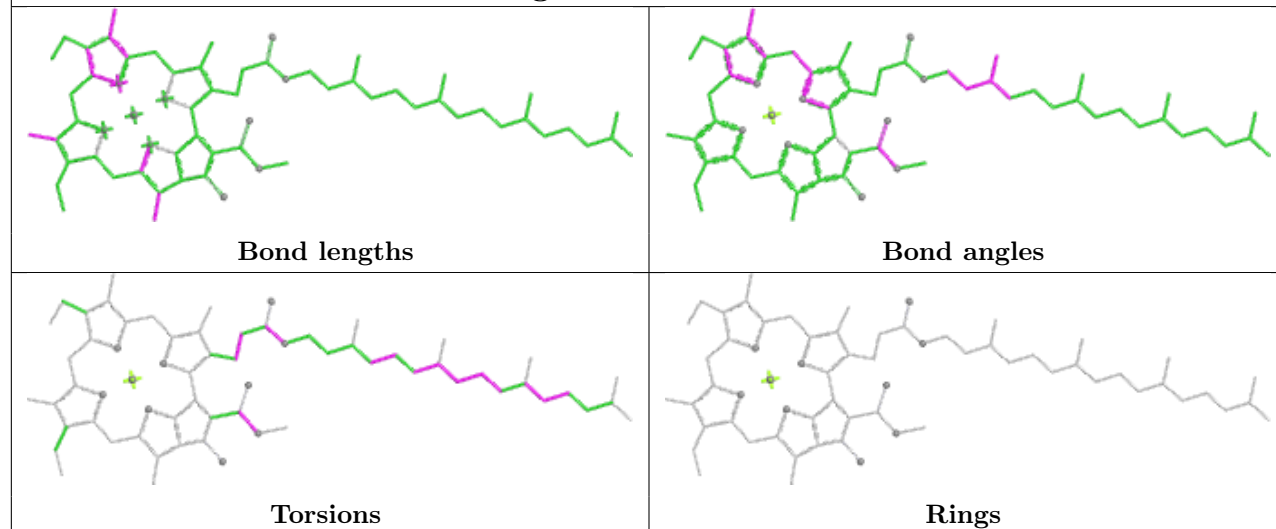


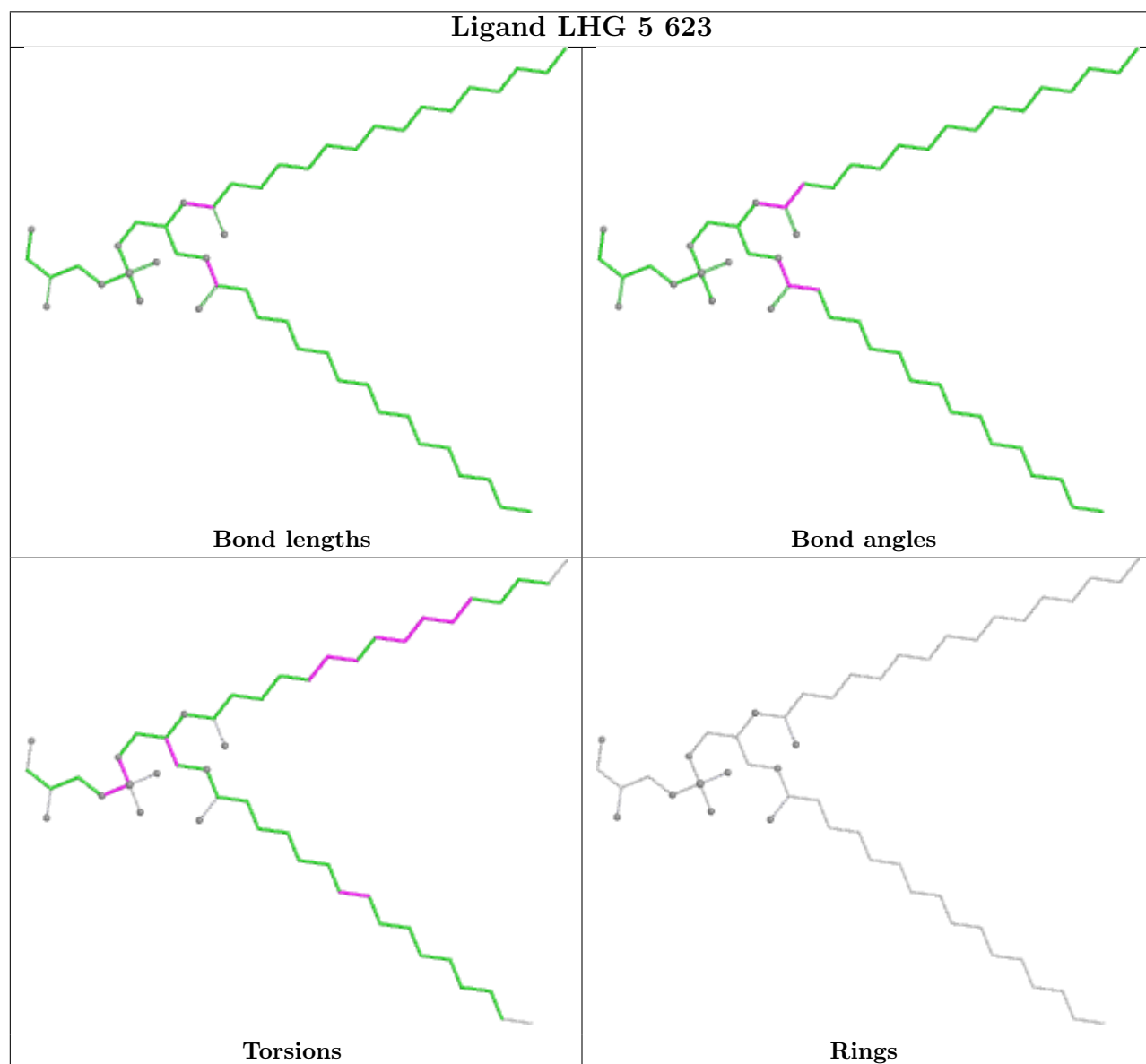
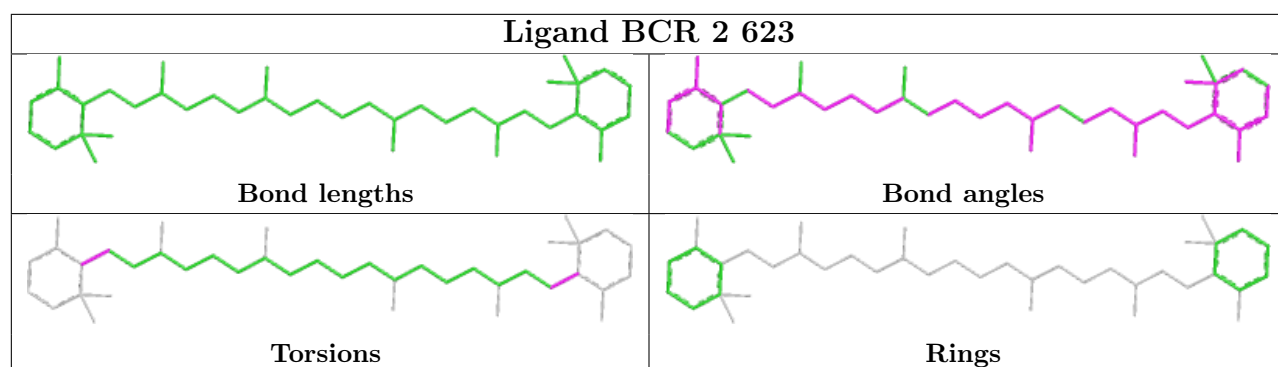
Ligand CLA V 610**Ligand CLA A 807**

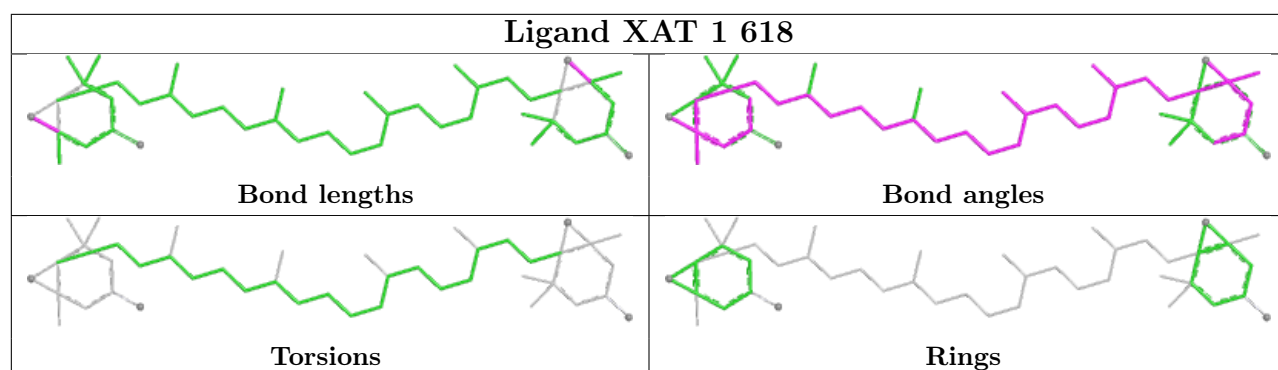
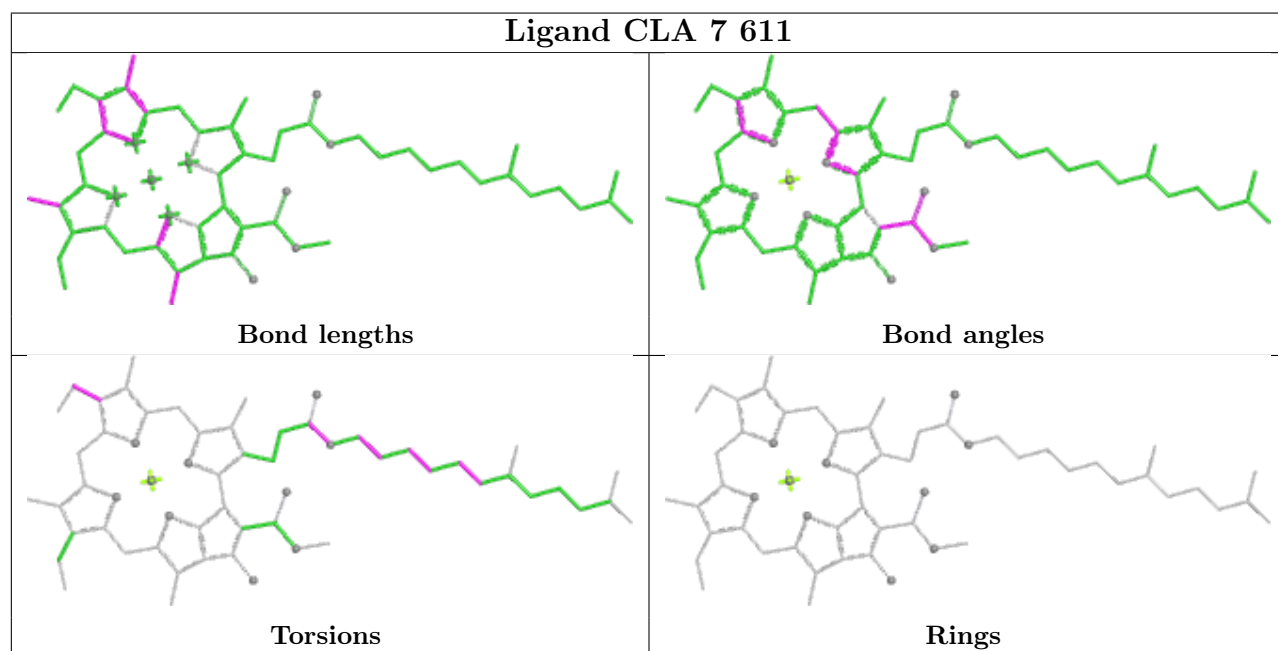
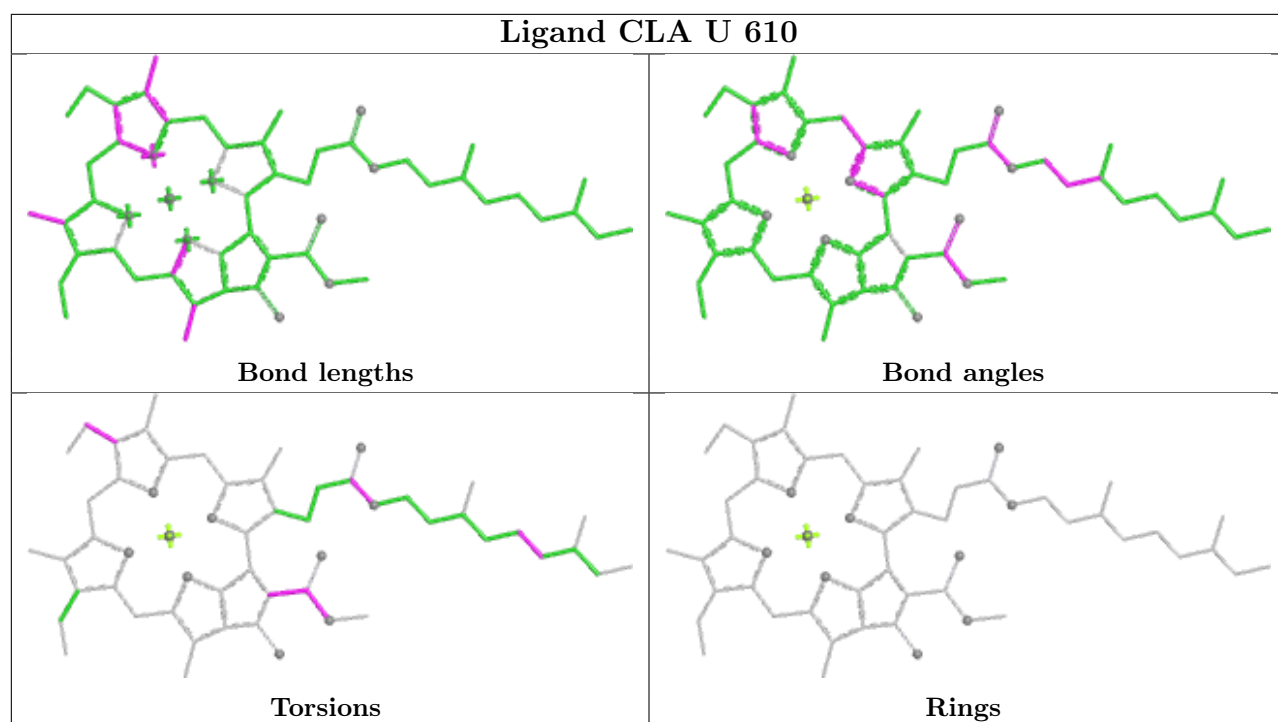
Ligand CLA 9 612



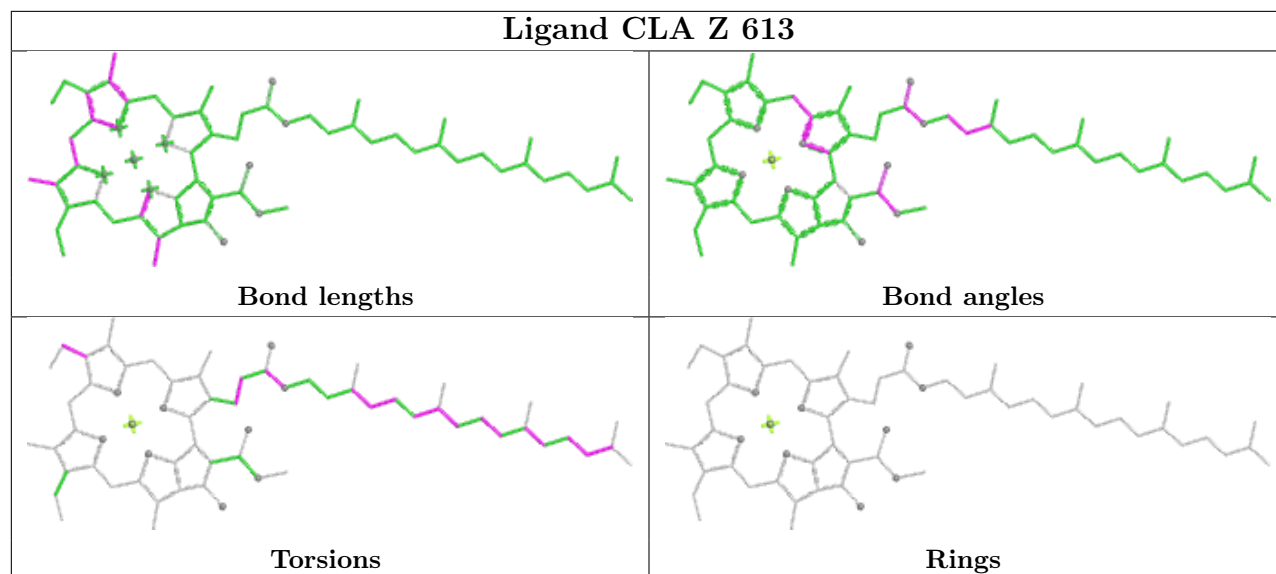
Ligand CLA A 814



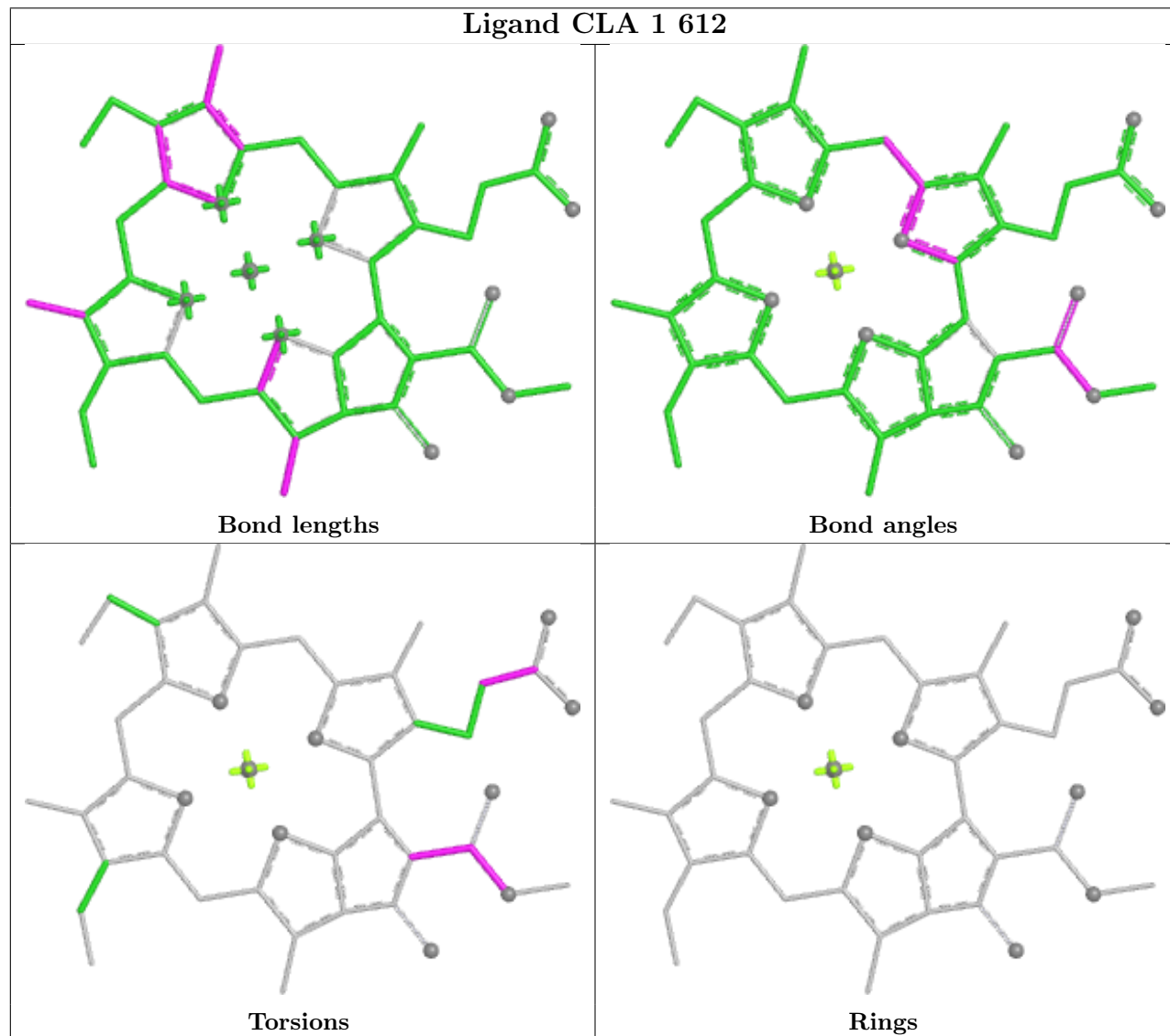


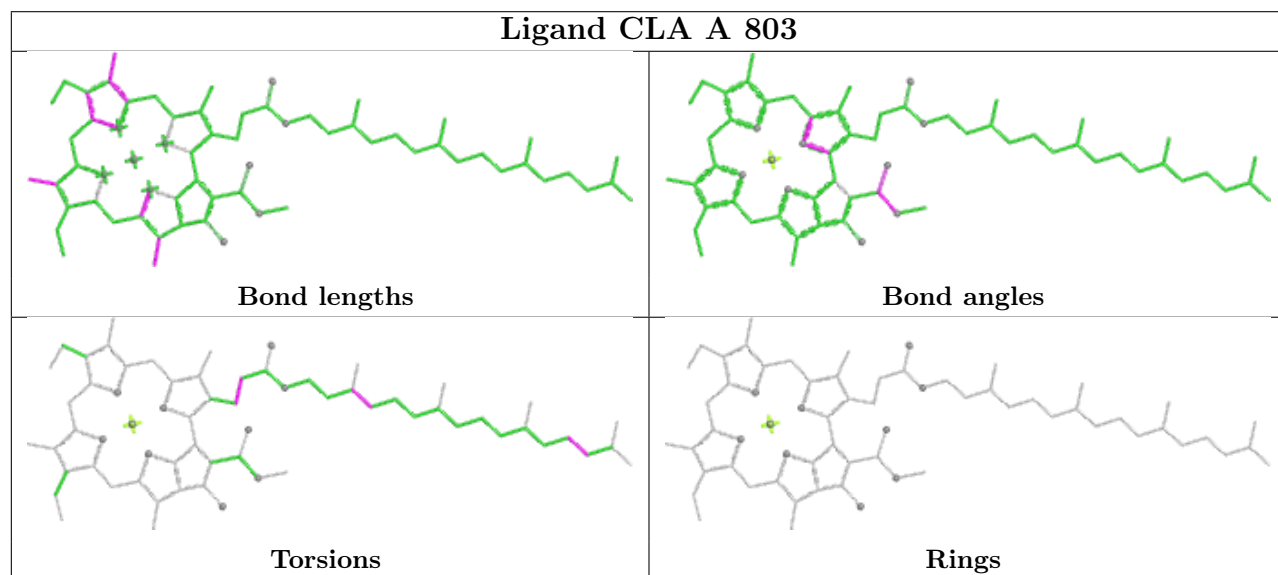
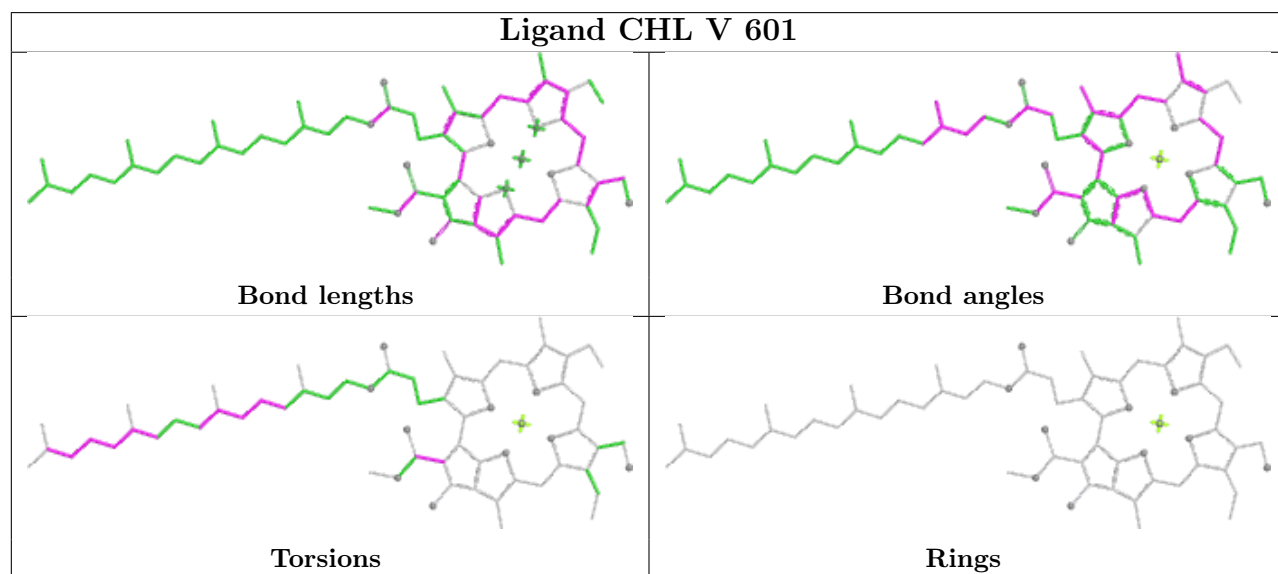
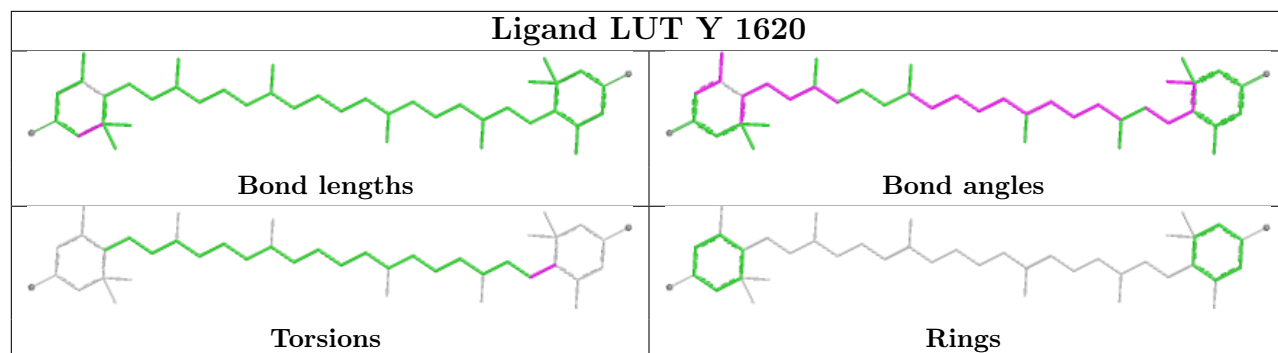


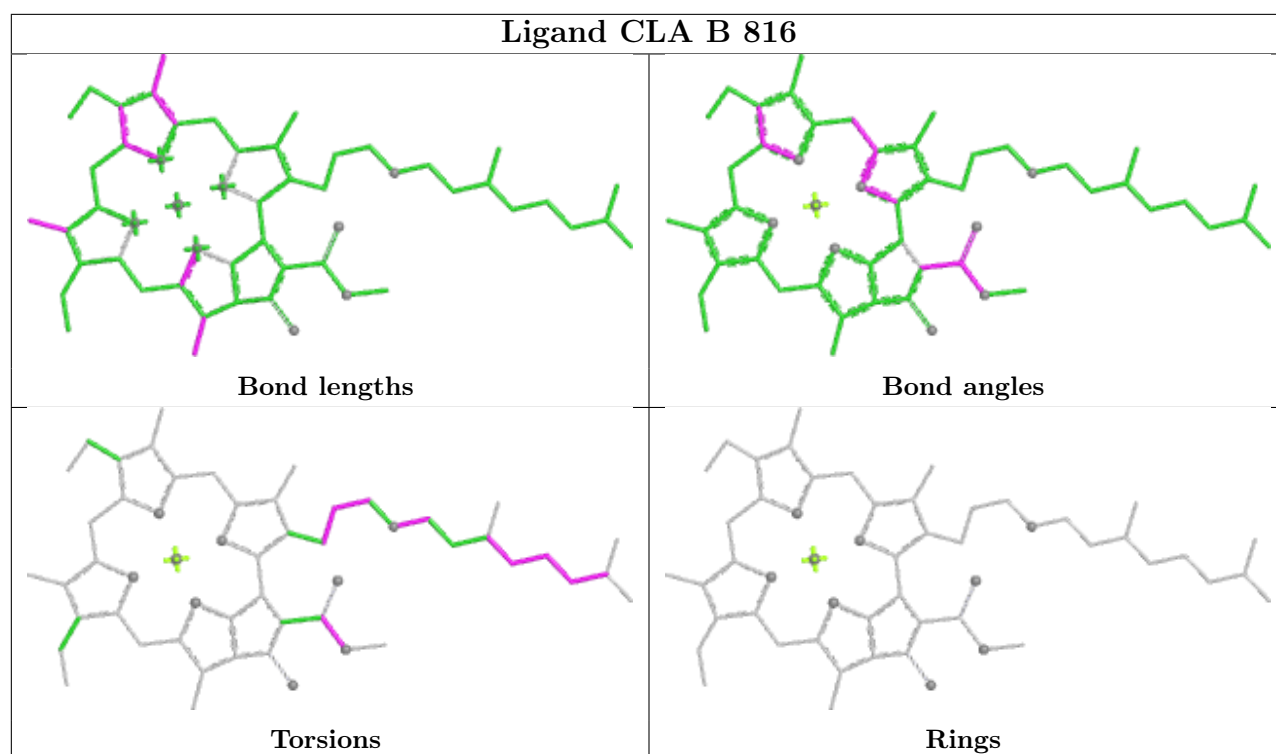
Ligand CLA Z 613



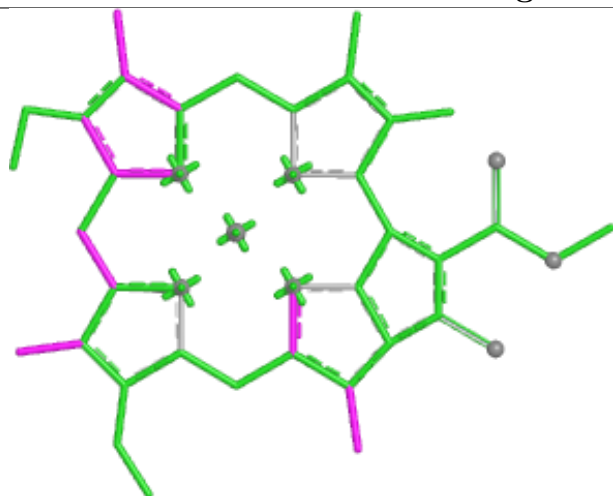
Ligand CLA 1 612



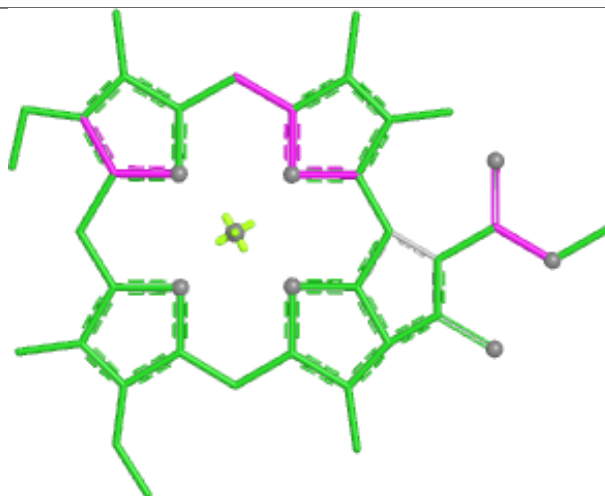




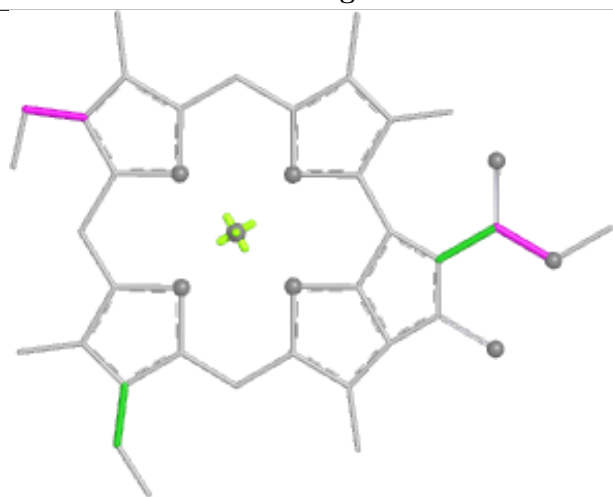
Ligand CLA F 304



Bond lengths



Bond angles

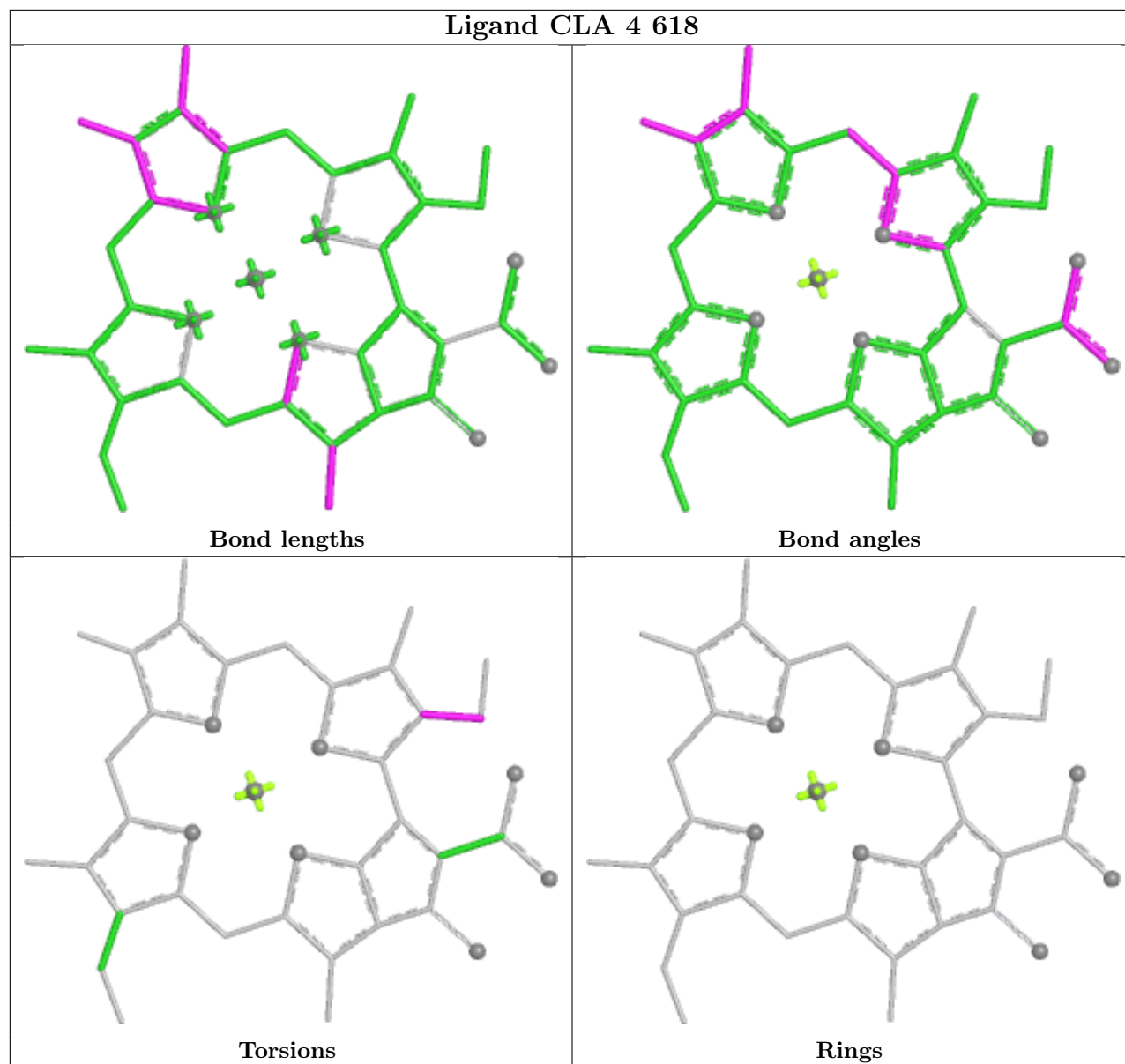


Torsions

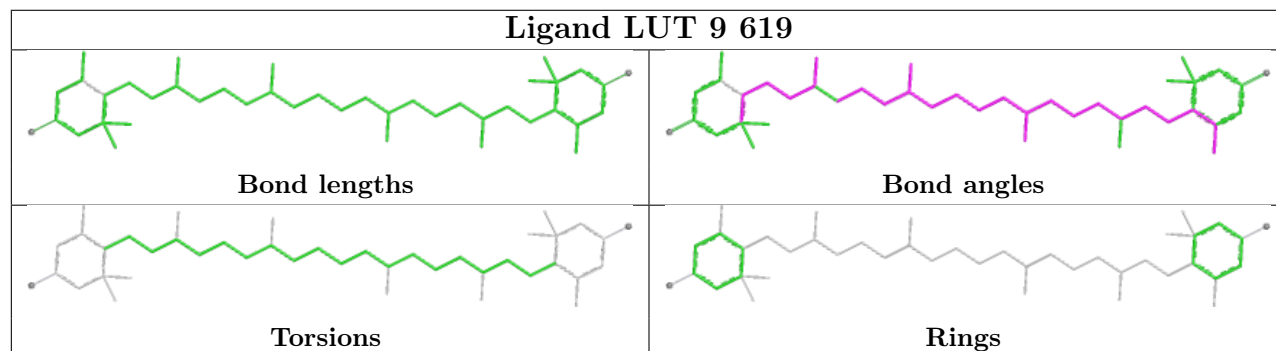


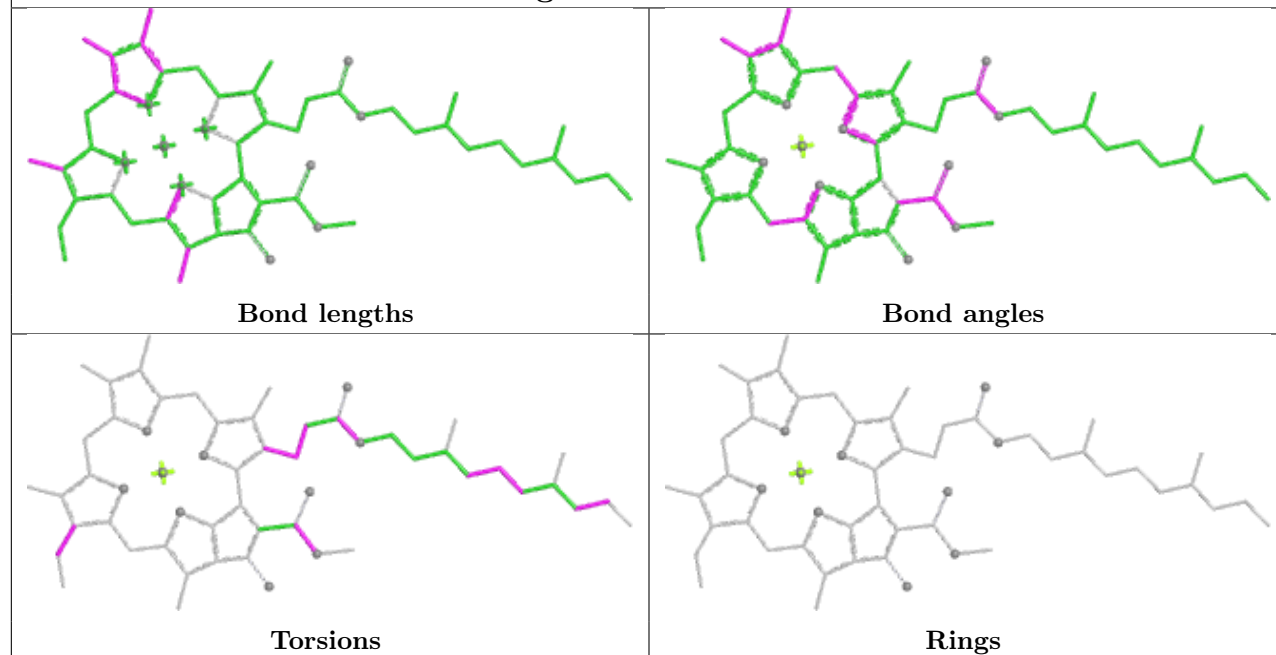
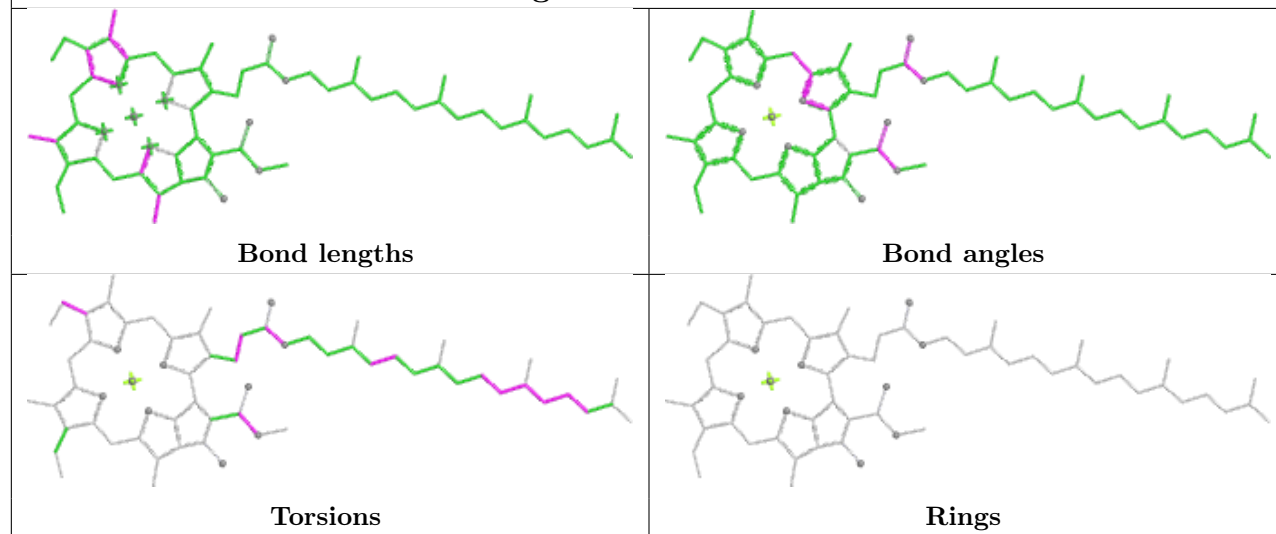
Rings

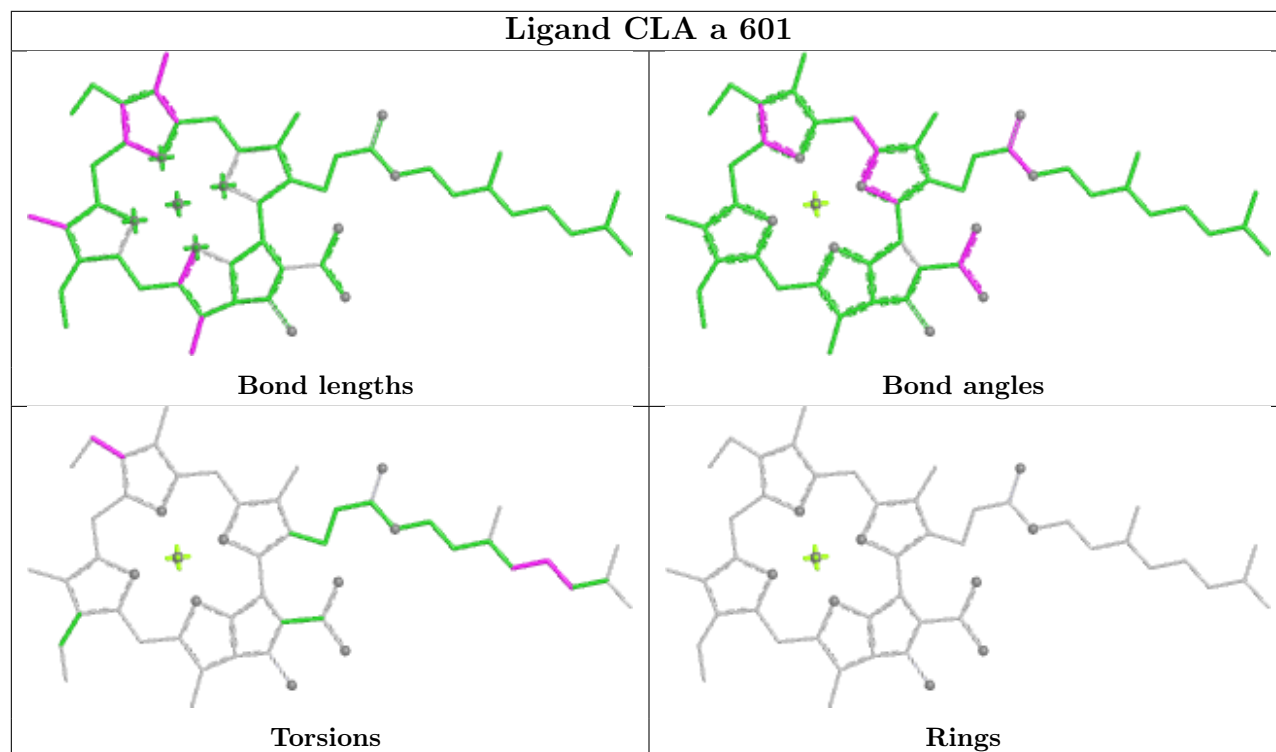
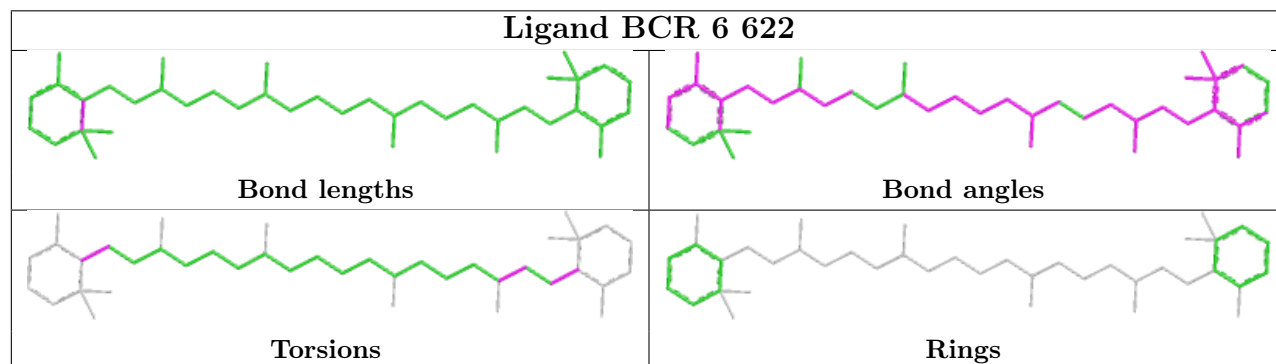
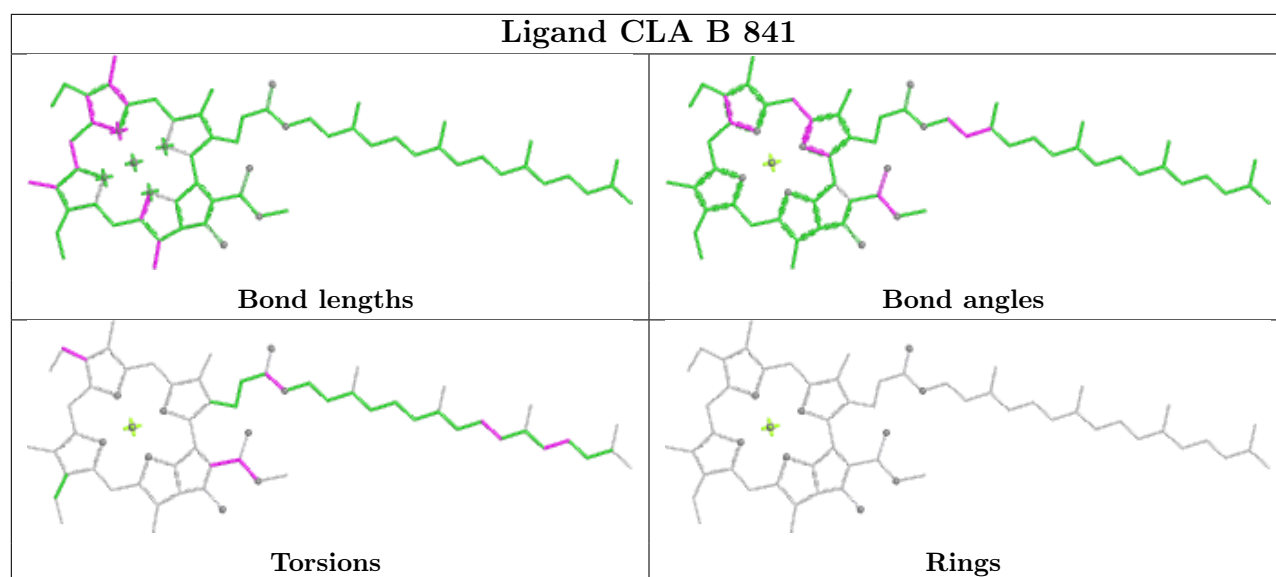
Ligand CLA 4 618

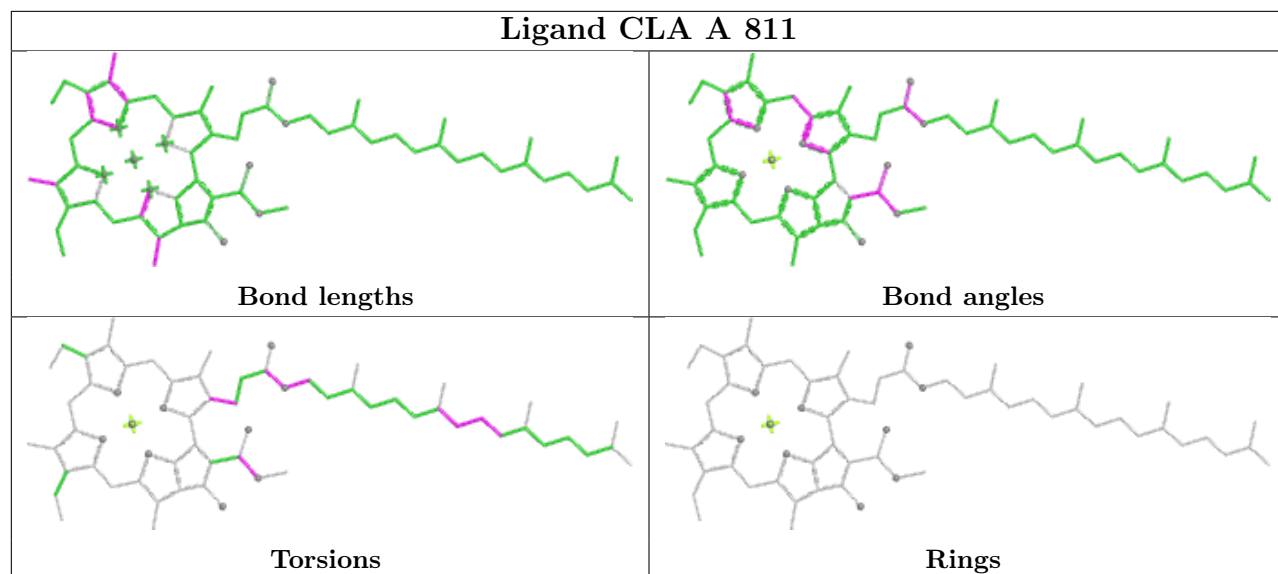
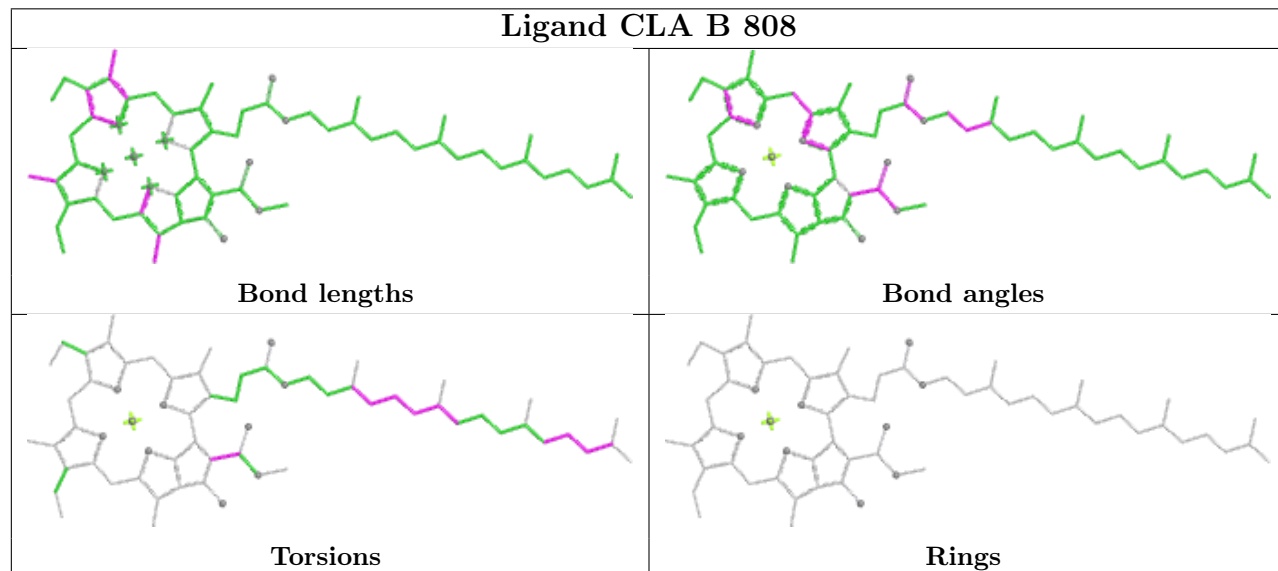


Ligand LUT 9 619

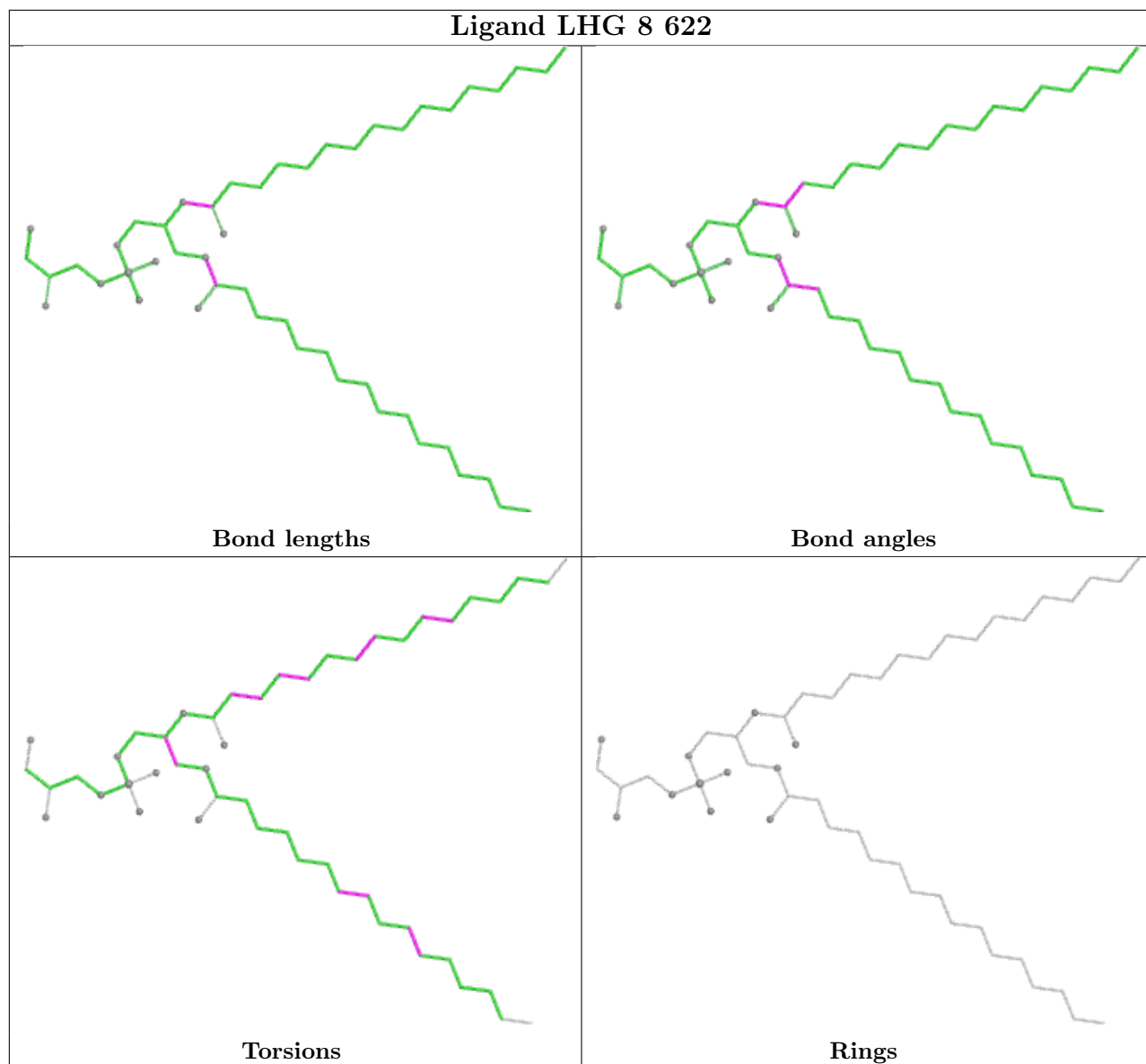


Ligand CLA 3 607**Ligand CLA B 839**

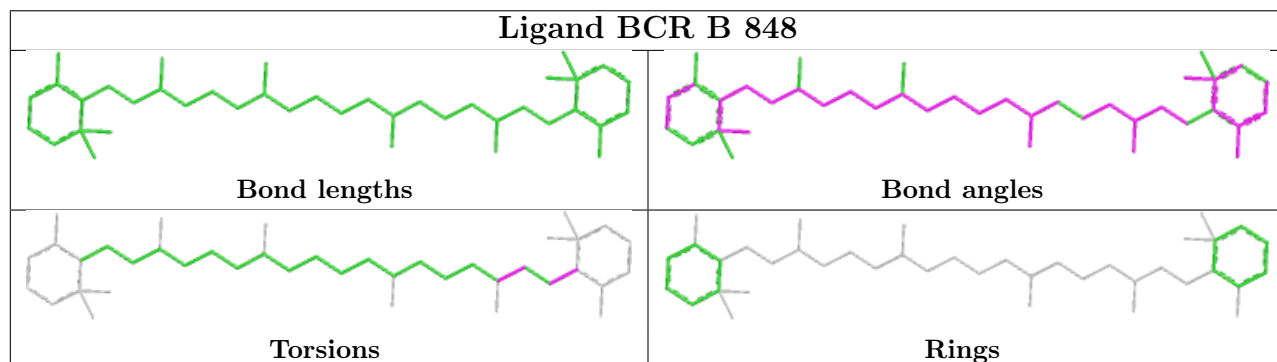


Ligand CLA A 811**Ligand CLA B 808**

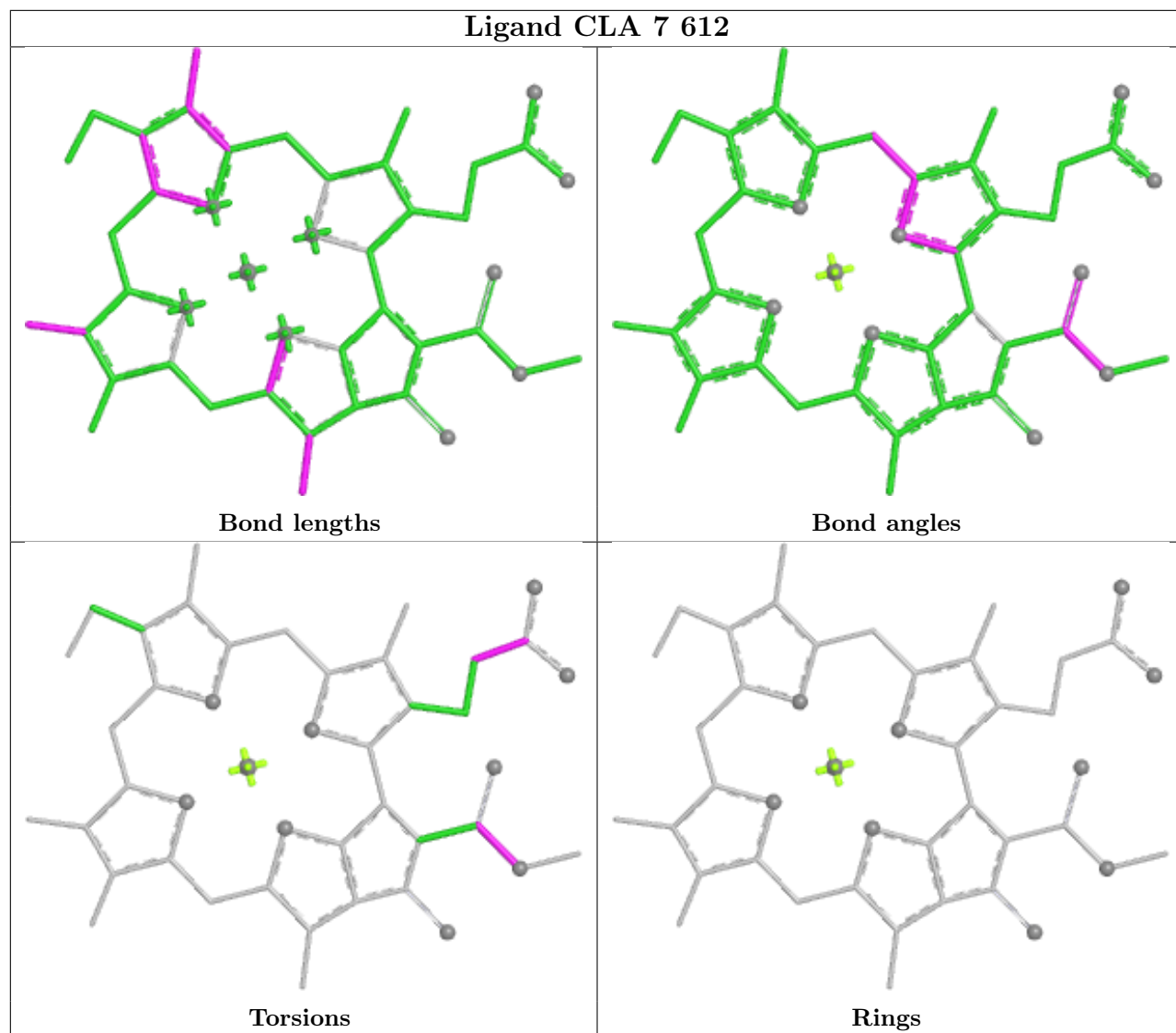
Ligand LHG 8 622

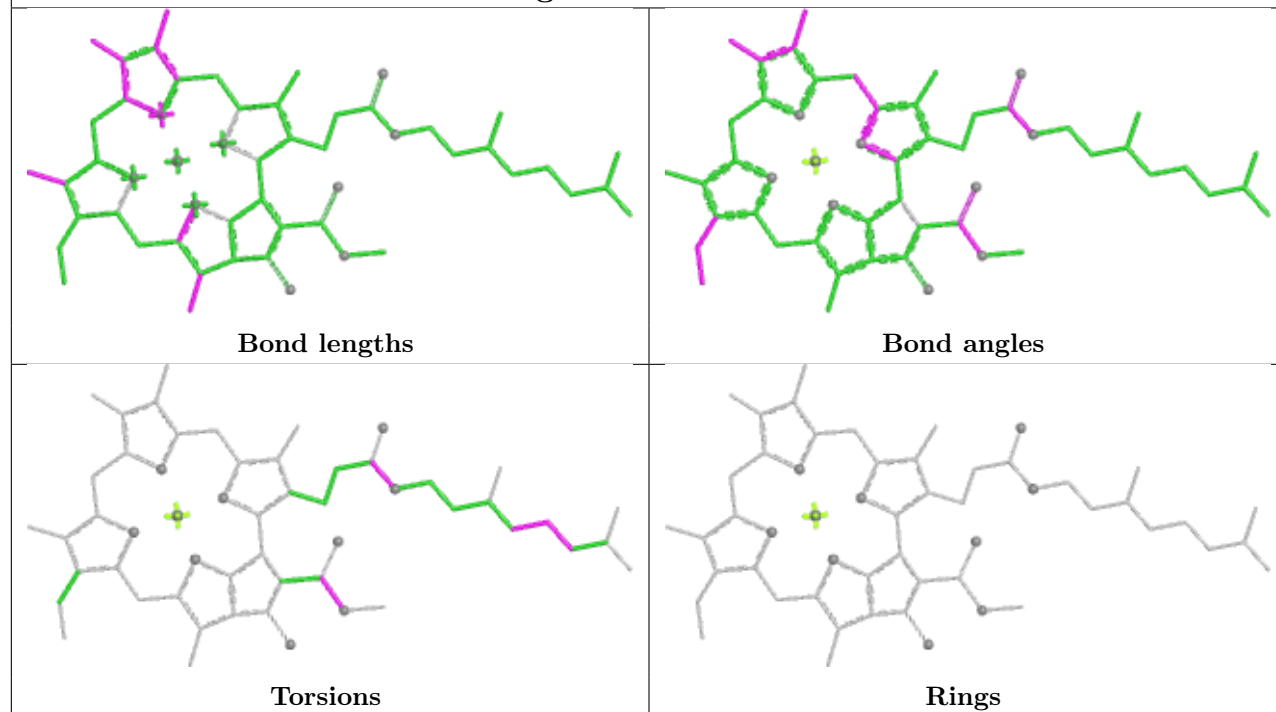
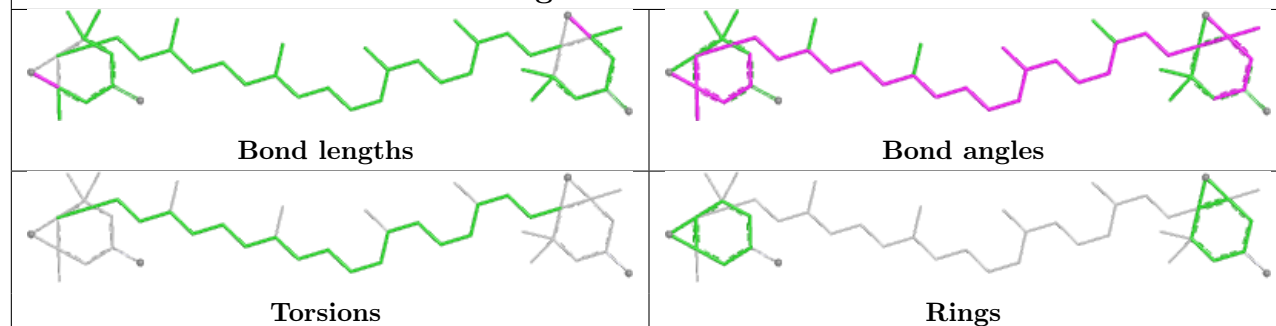
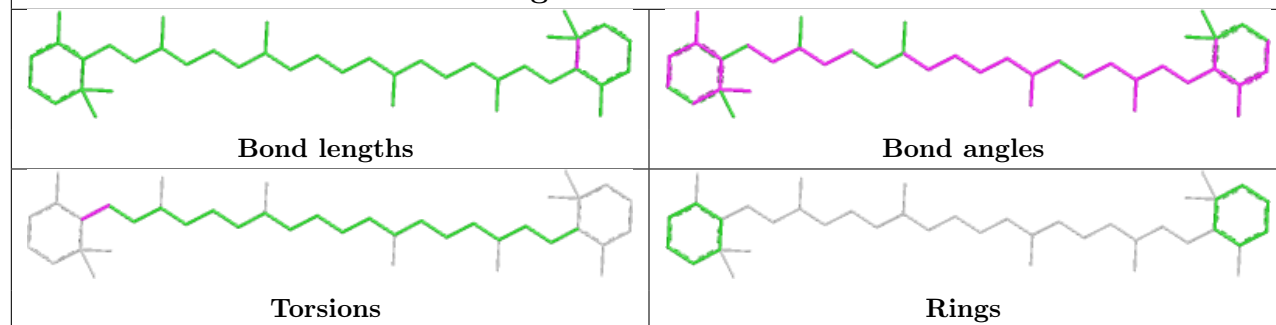


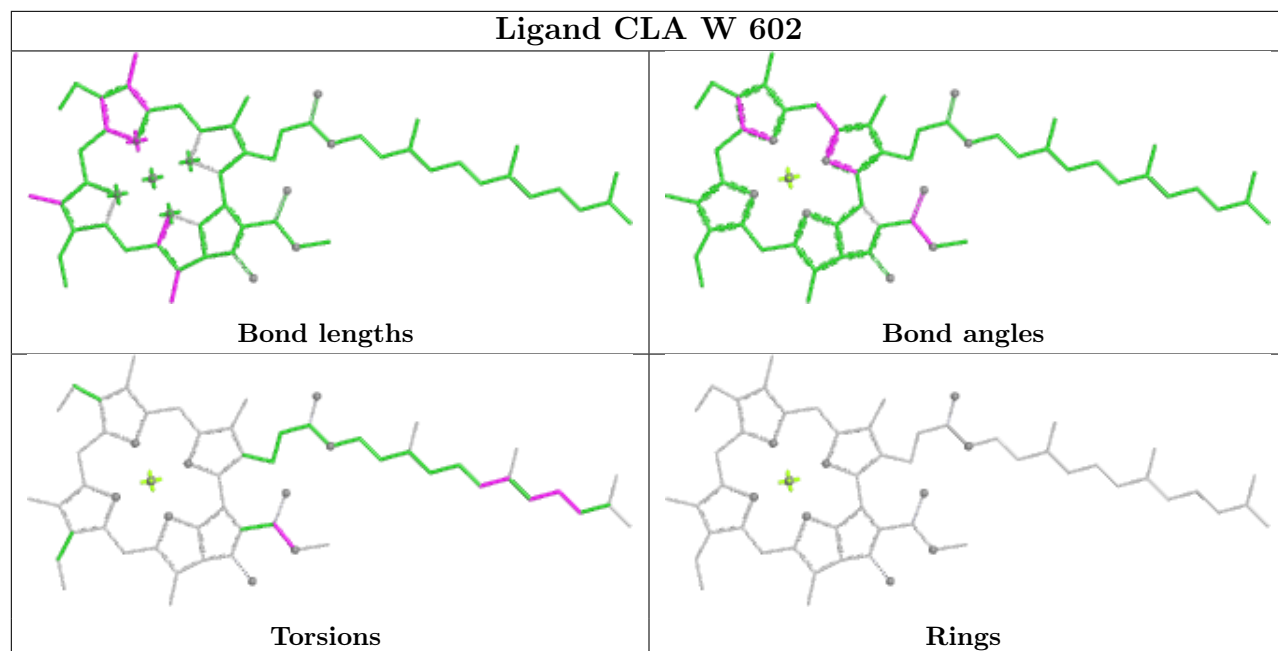
Ligand BCR B 848

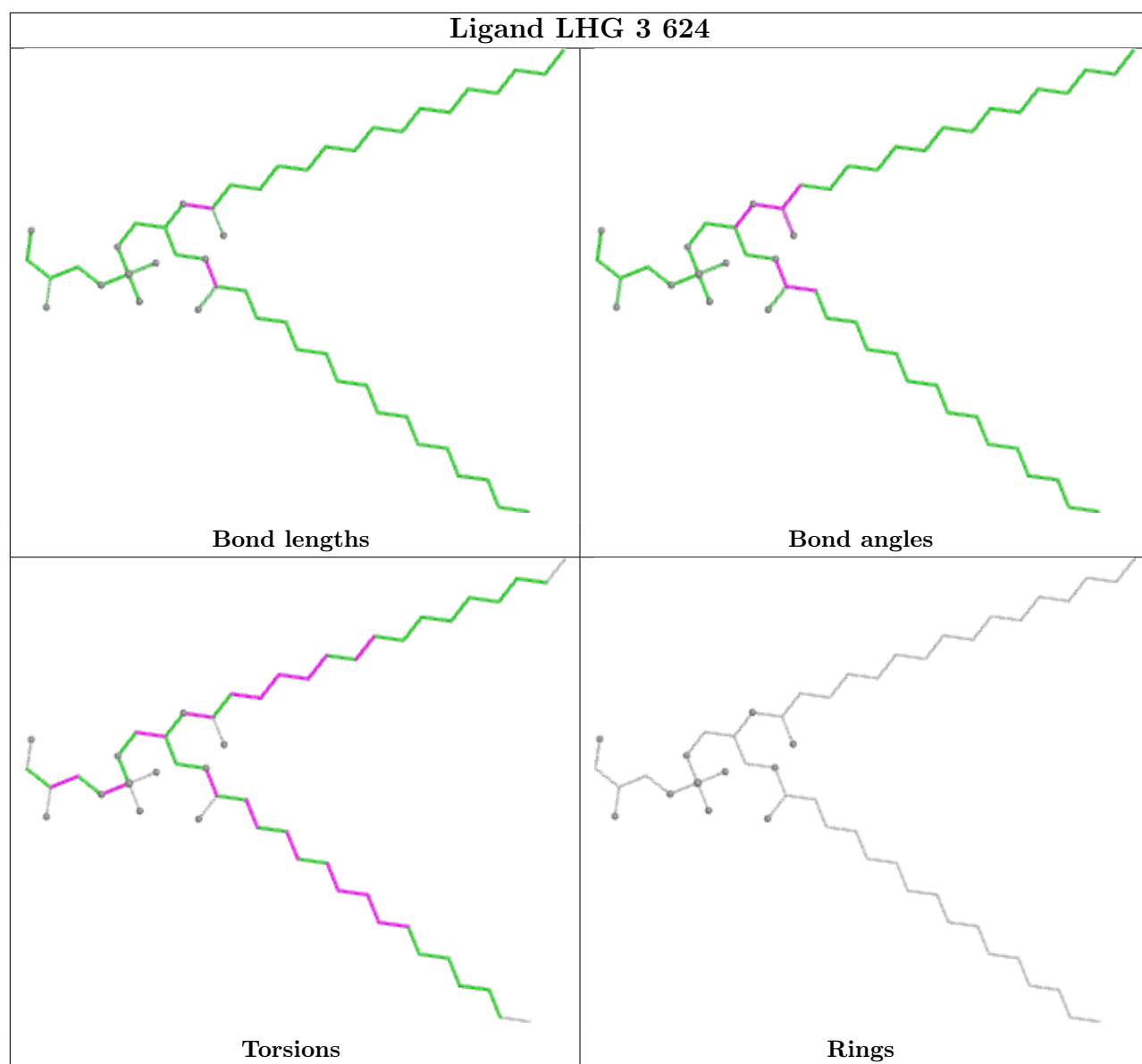


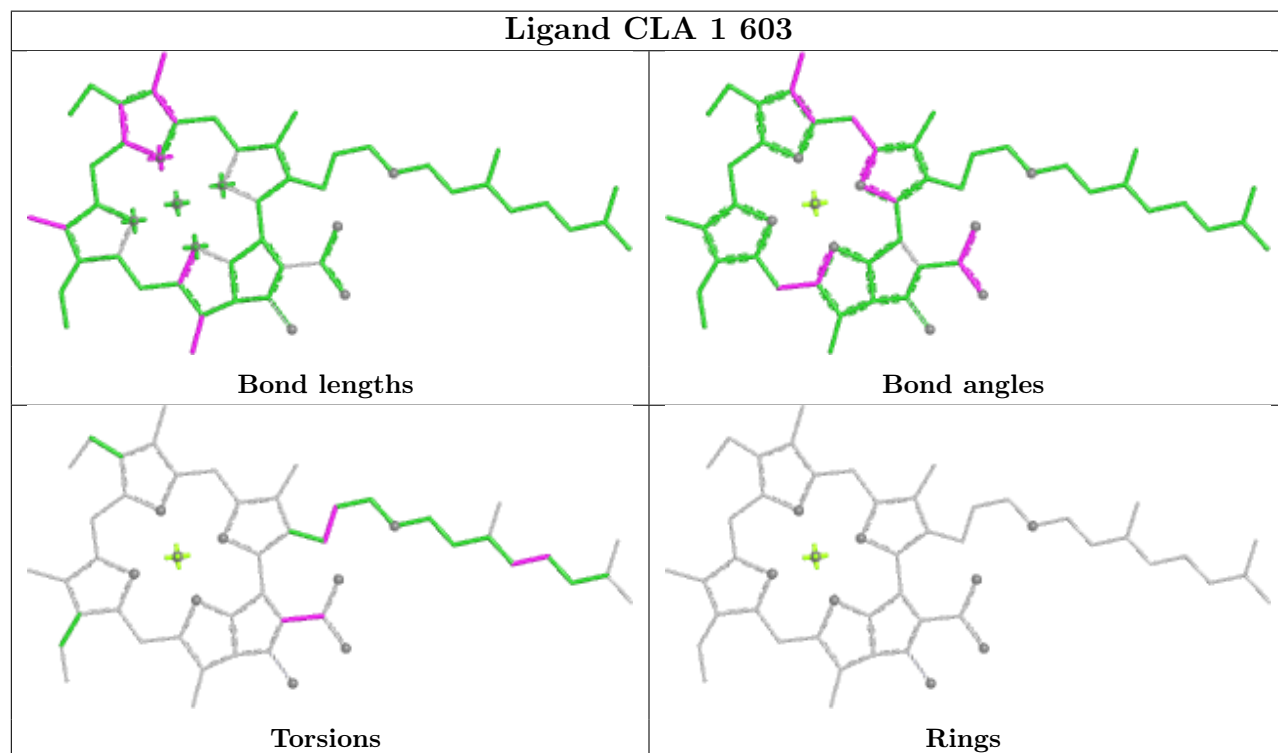
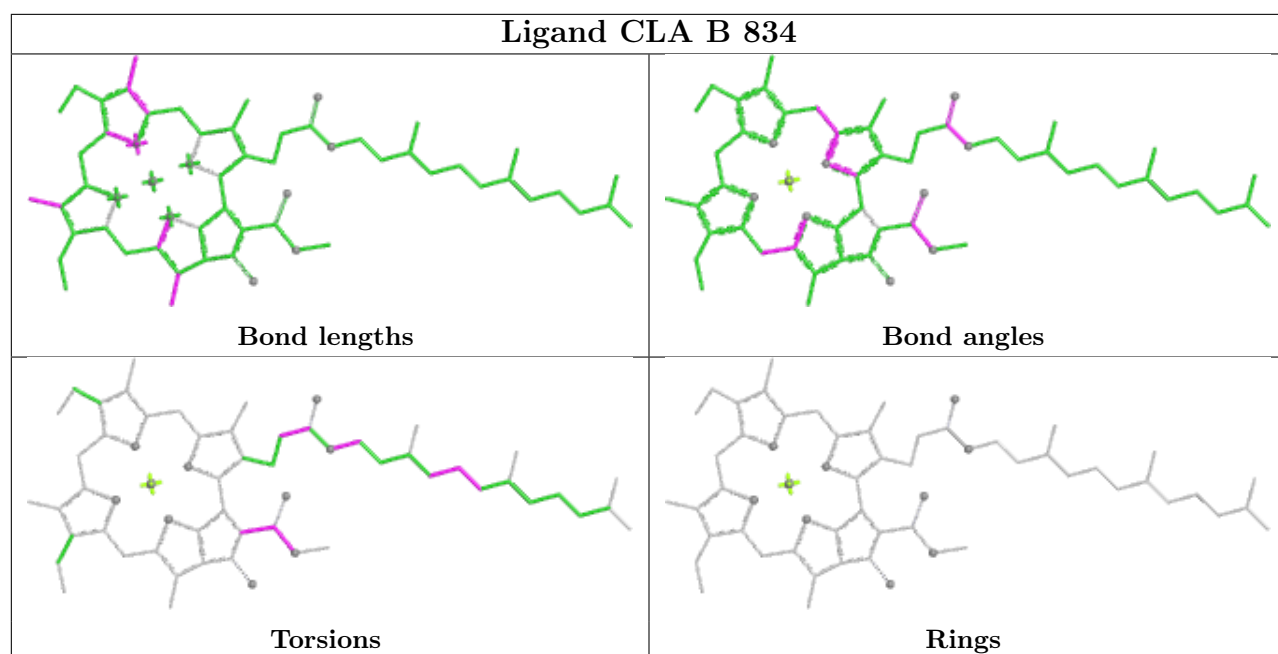
Ligand CLA 7 612

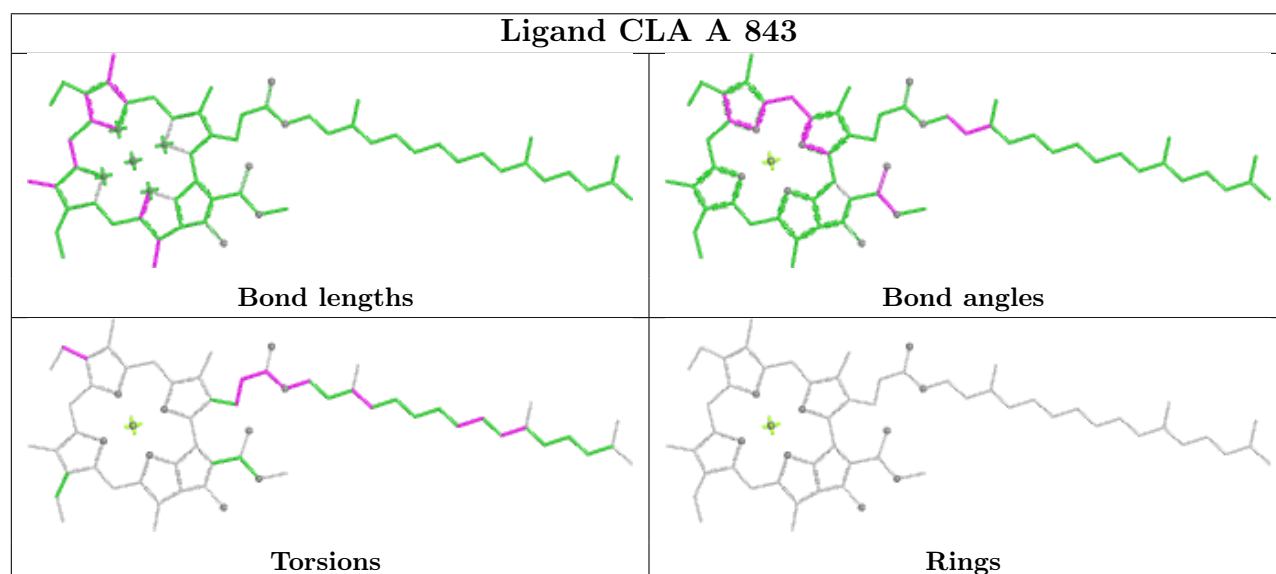
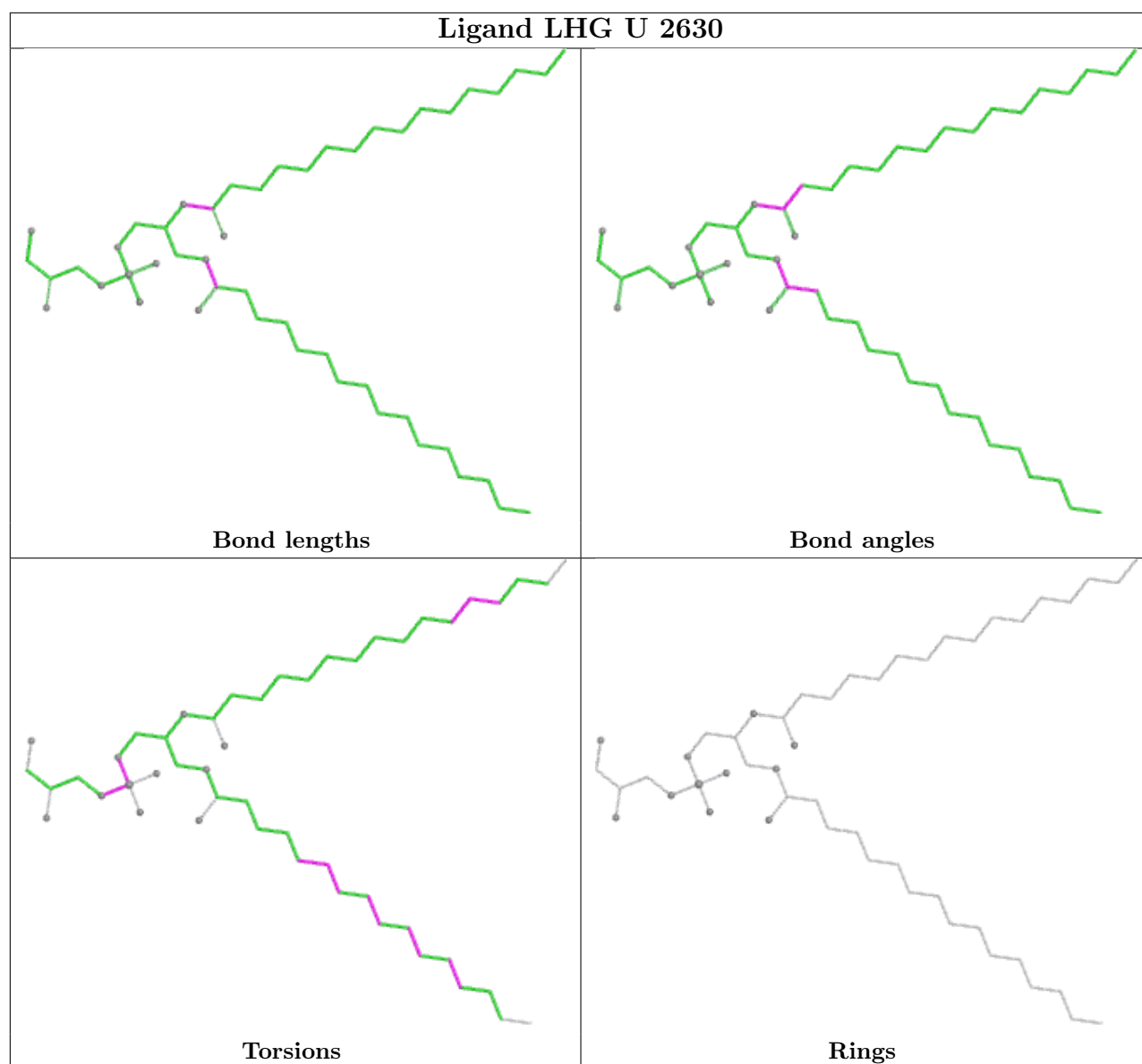


Ligand CLA 5 603**Ligand XAT 8 620****Ligand BCR B 846**

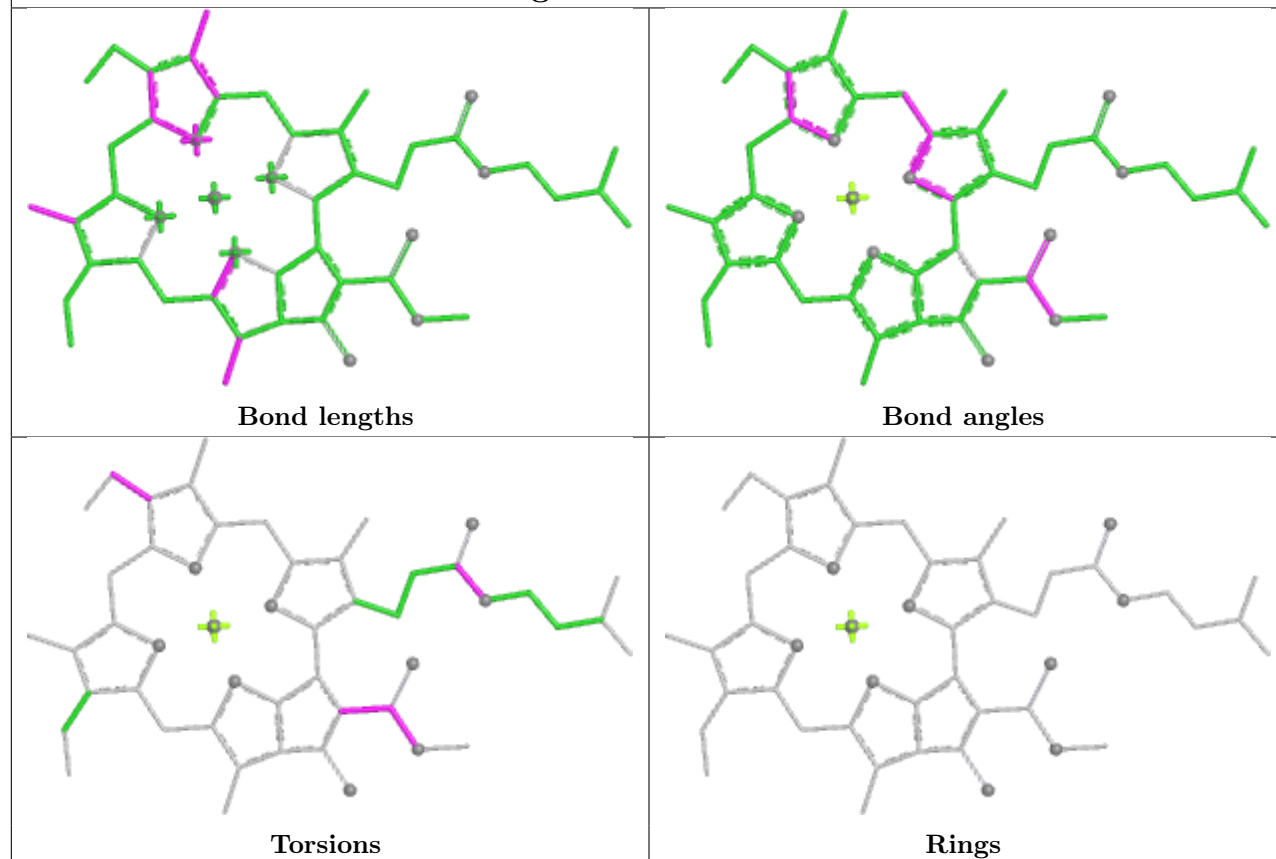




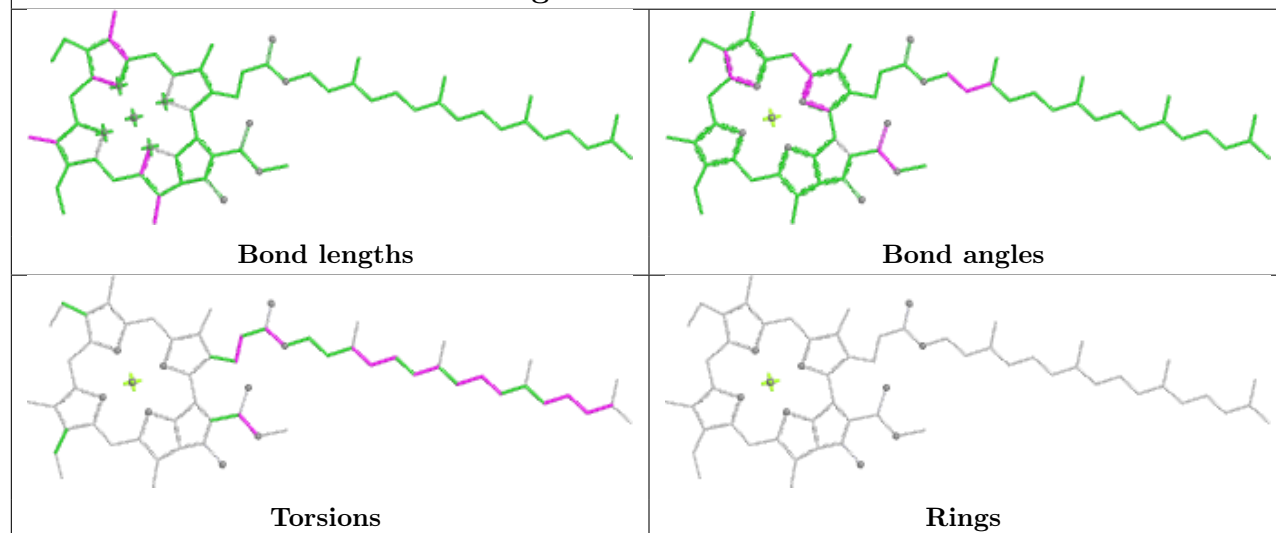




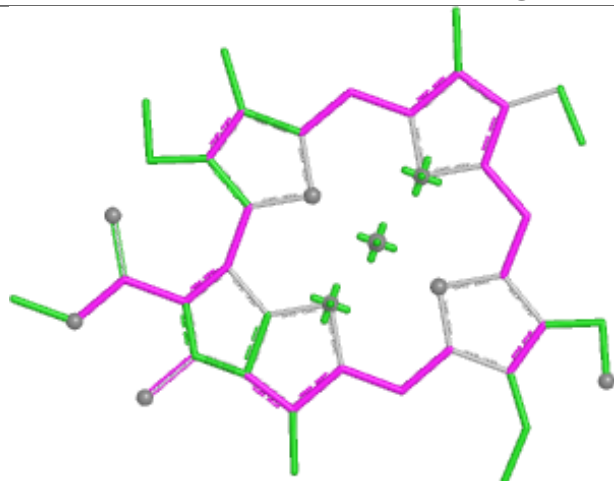
Ligand CLA A 815



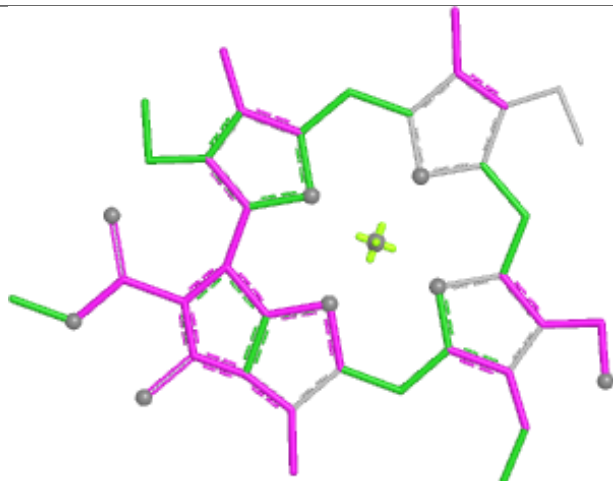
Ligand CLA V 613



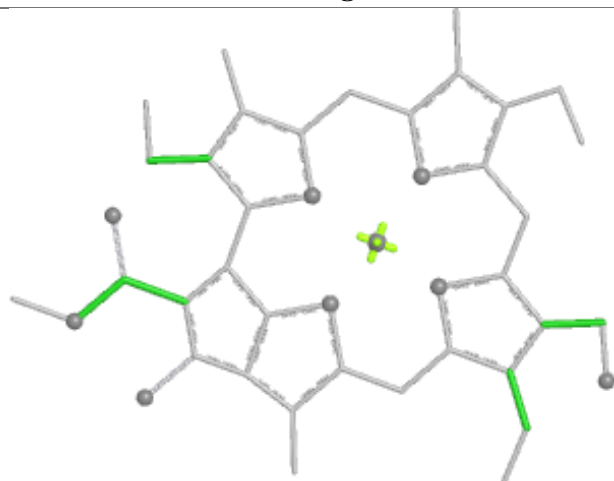
Ligand CHL U 605



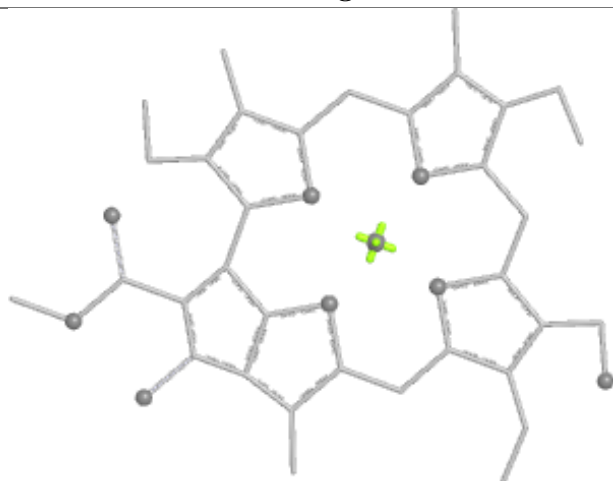
Bond lengths



Bond angles

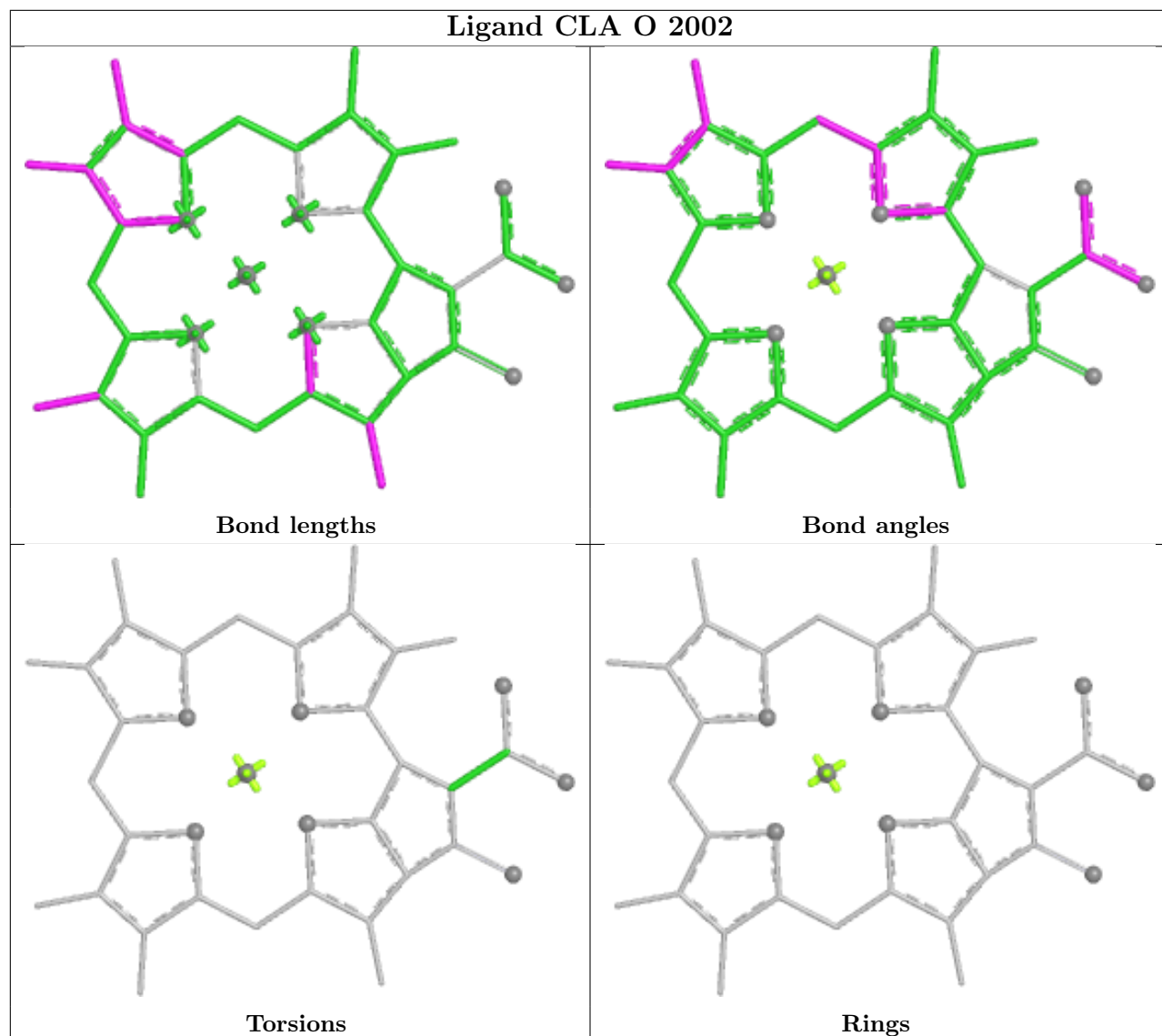


Torsions

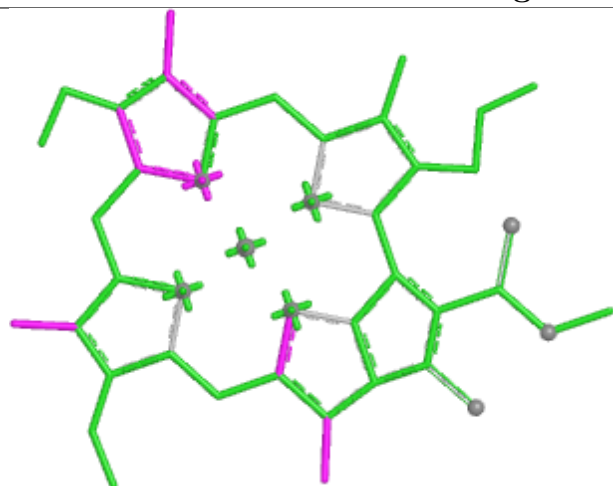


Rings

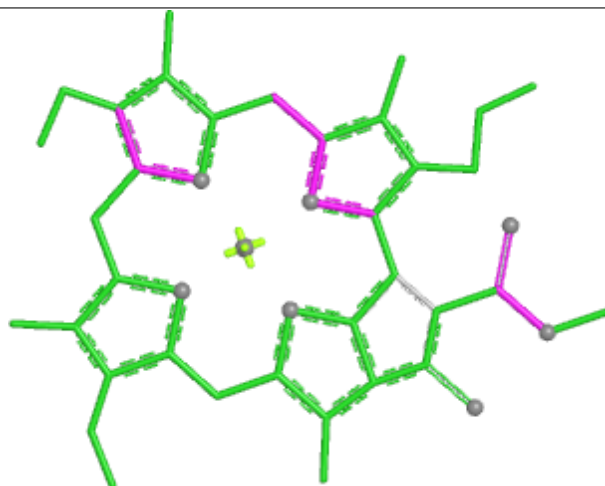
Ligand CLA O 2002



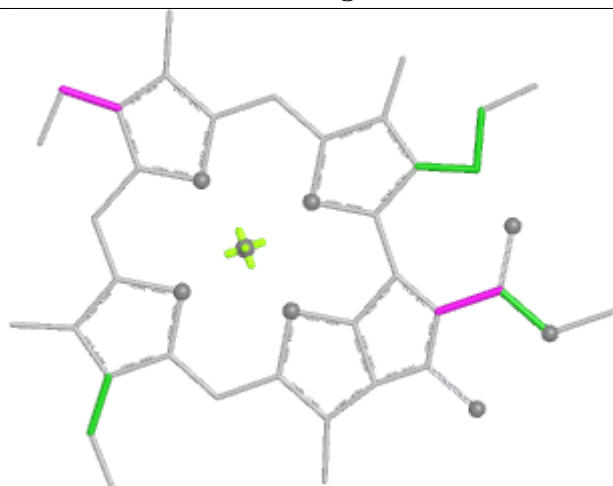
Ligand CLA U 612



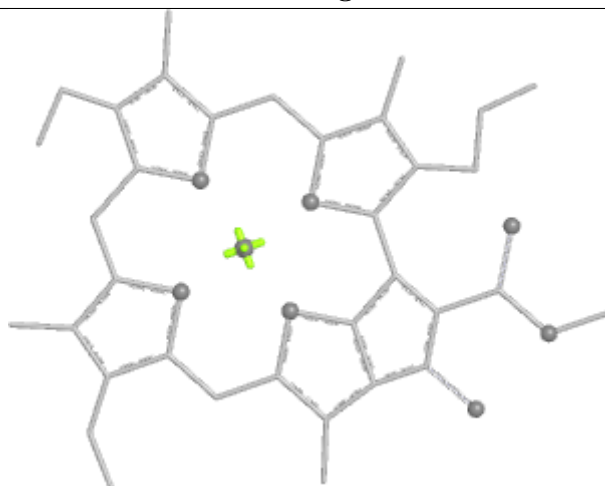
Bond lengths



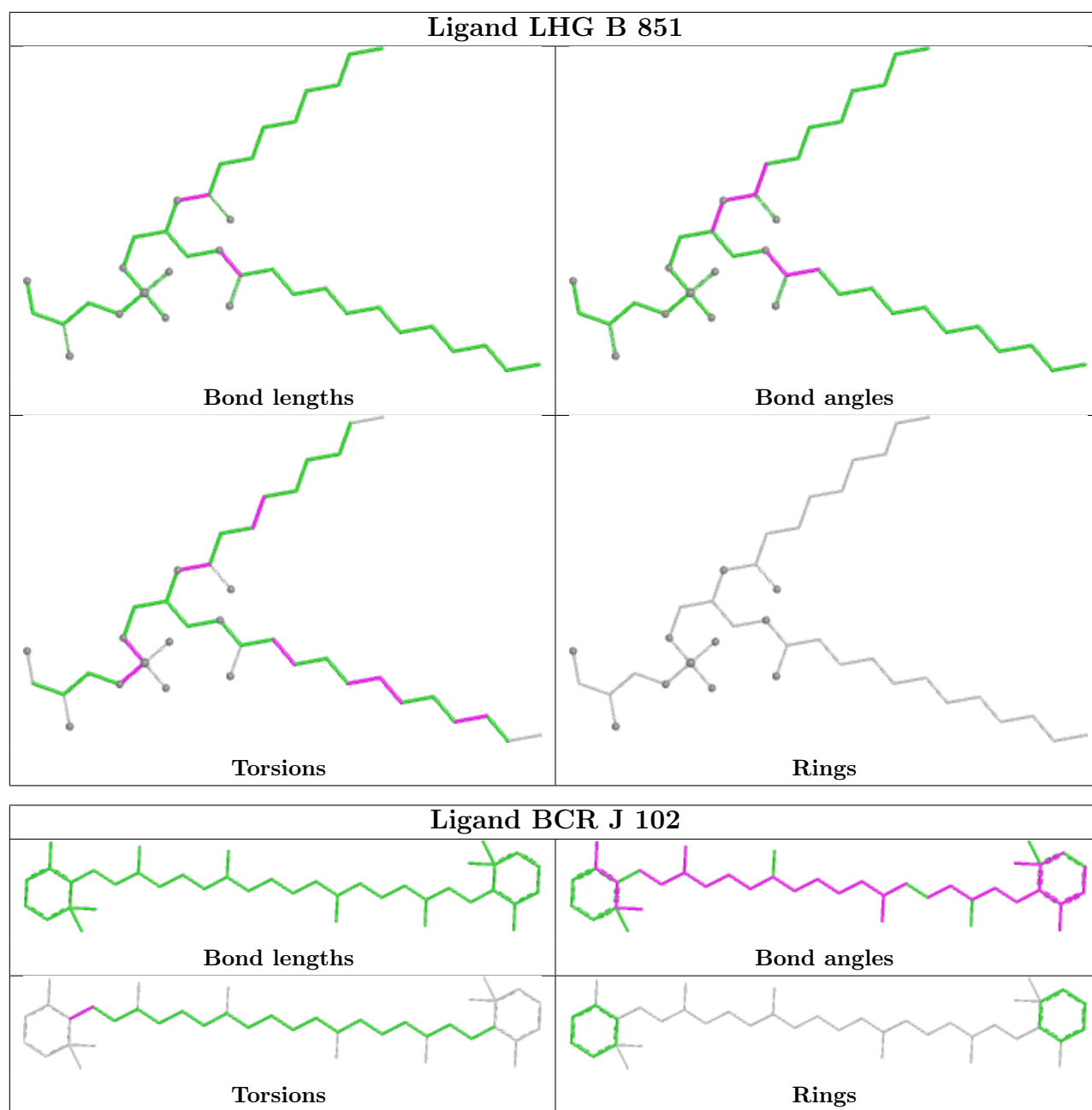
Bond angles

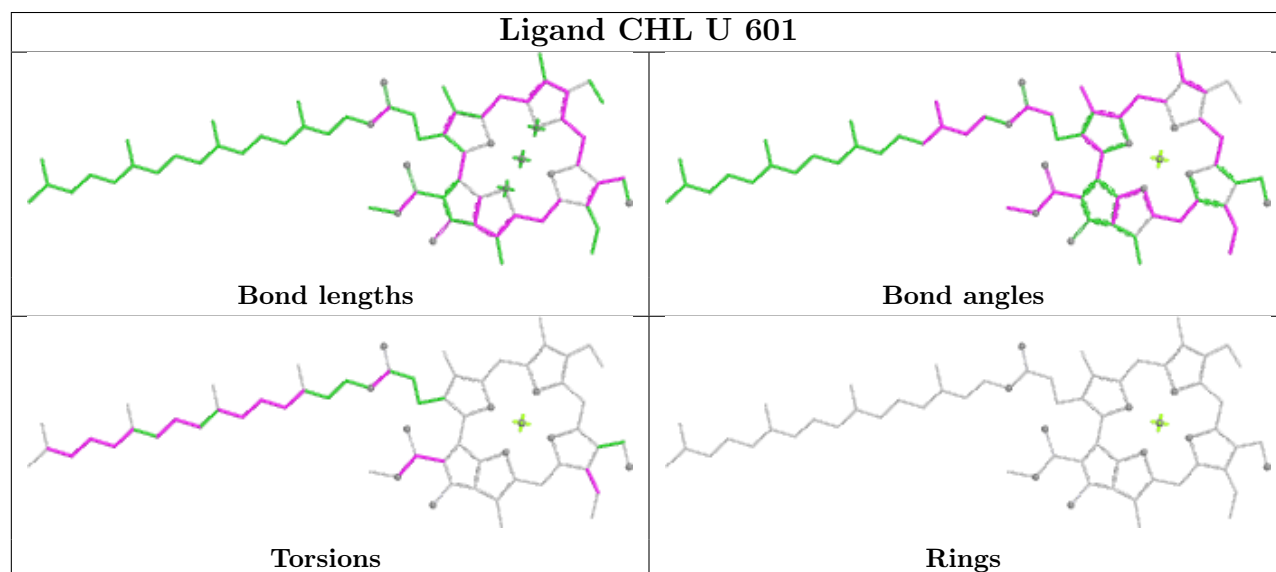
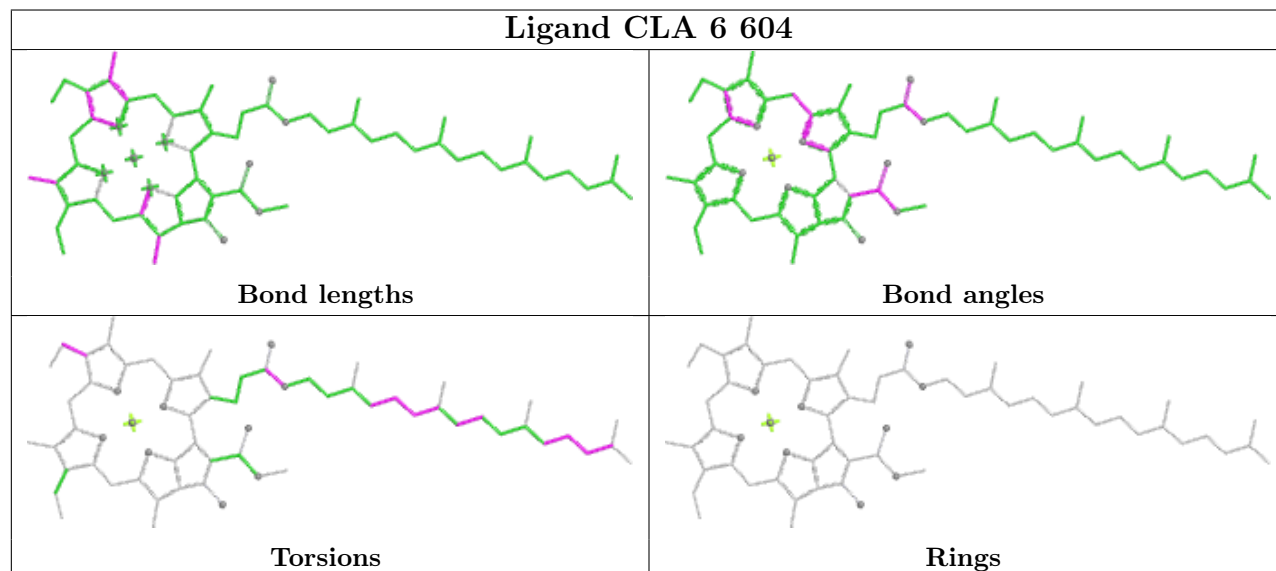
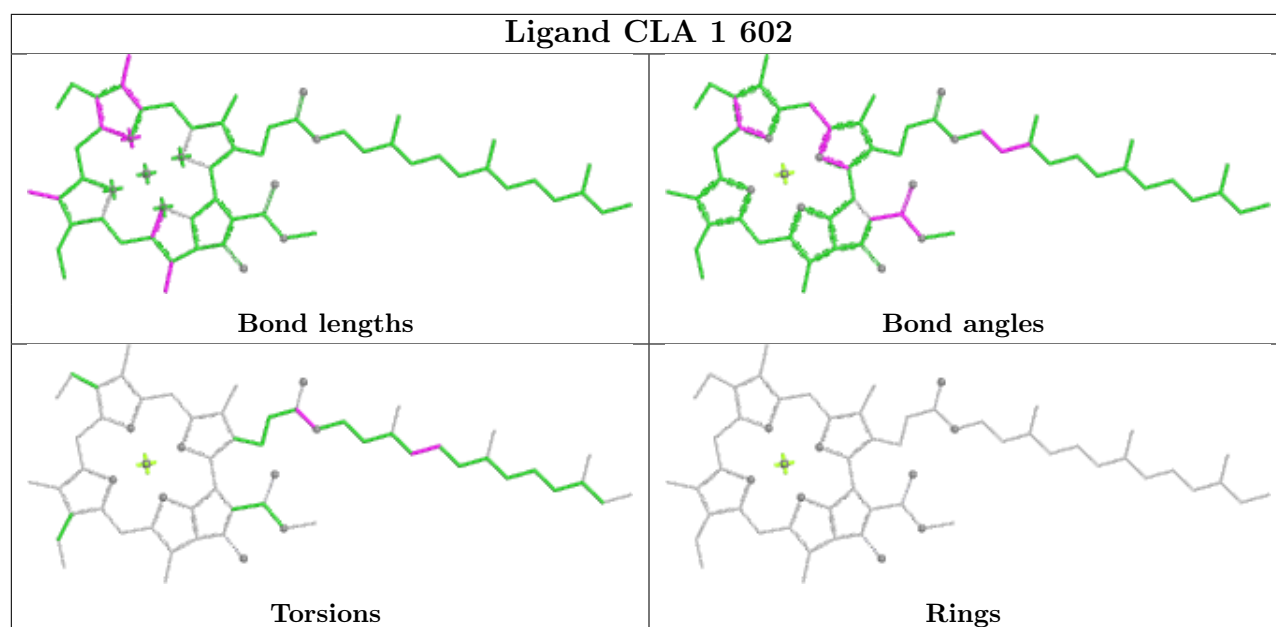


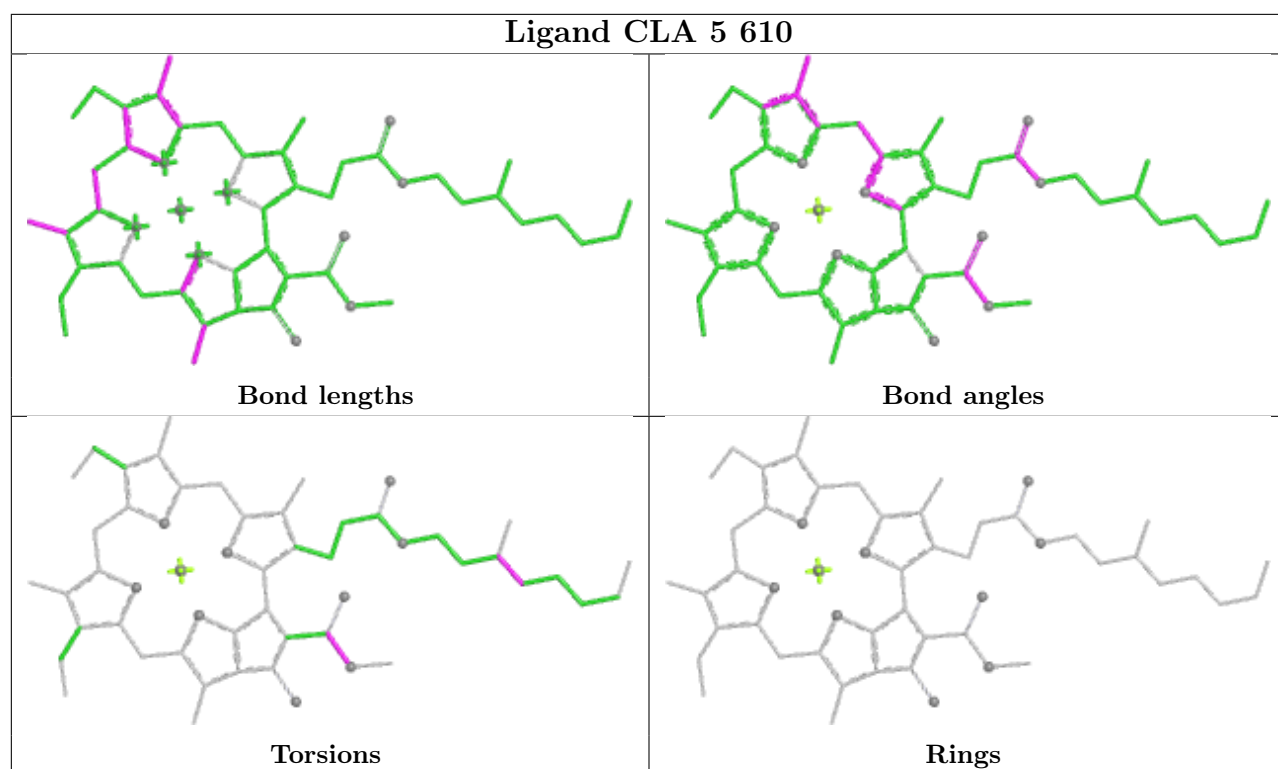
Torsions



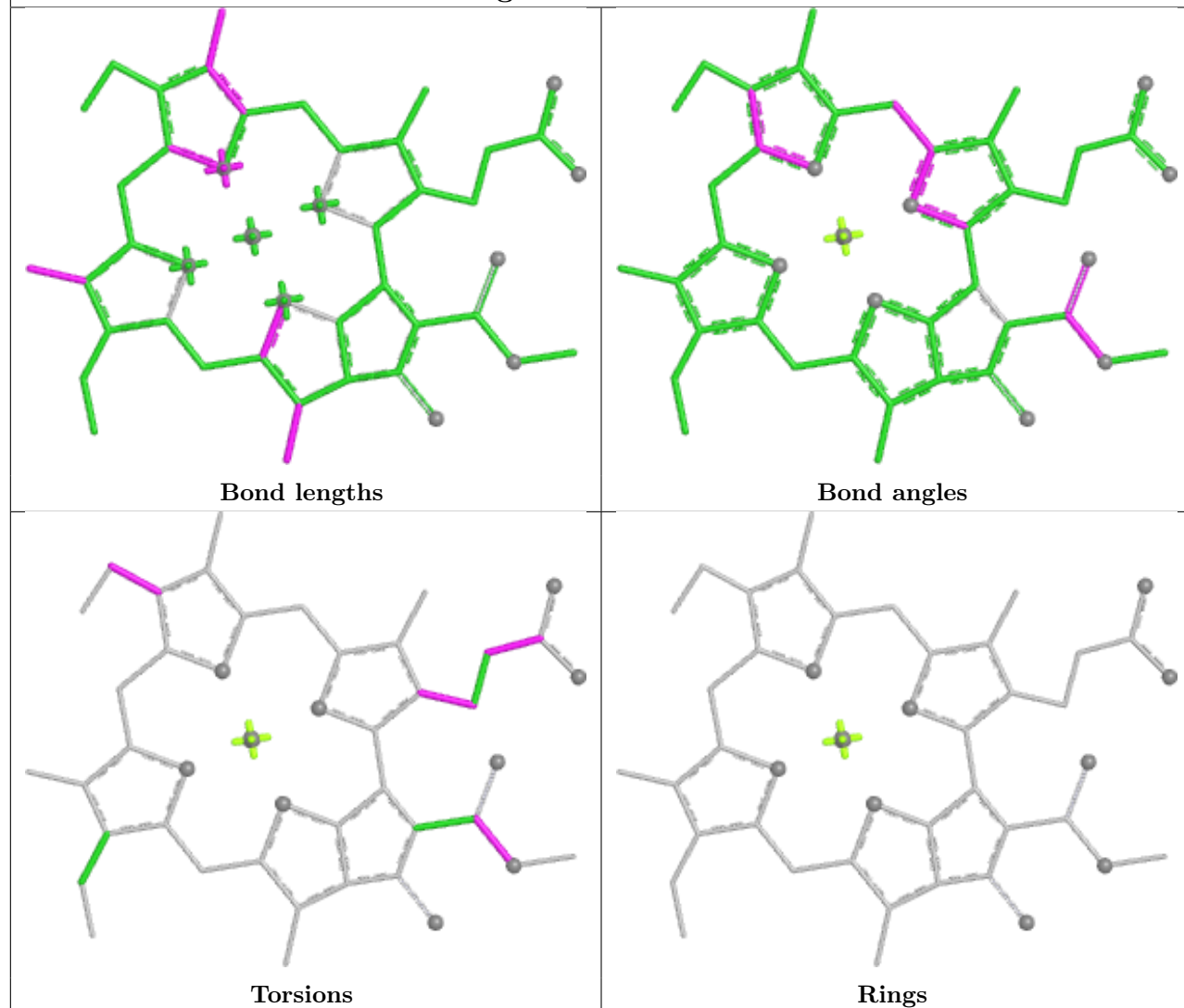
Rings



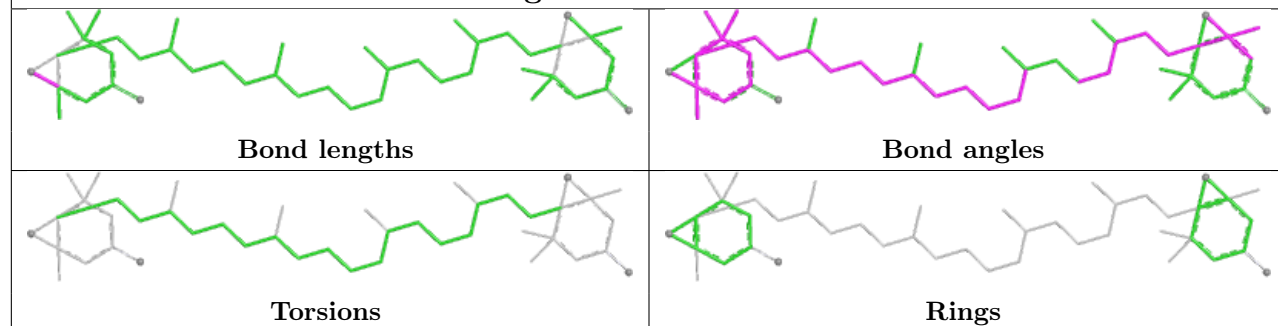




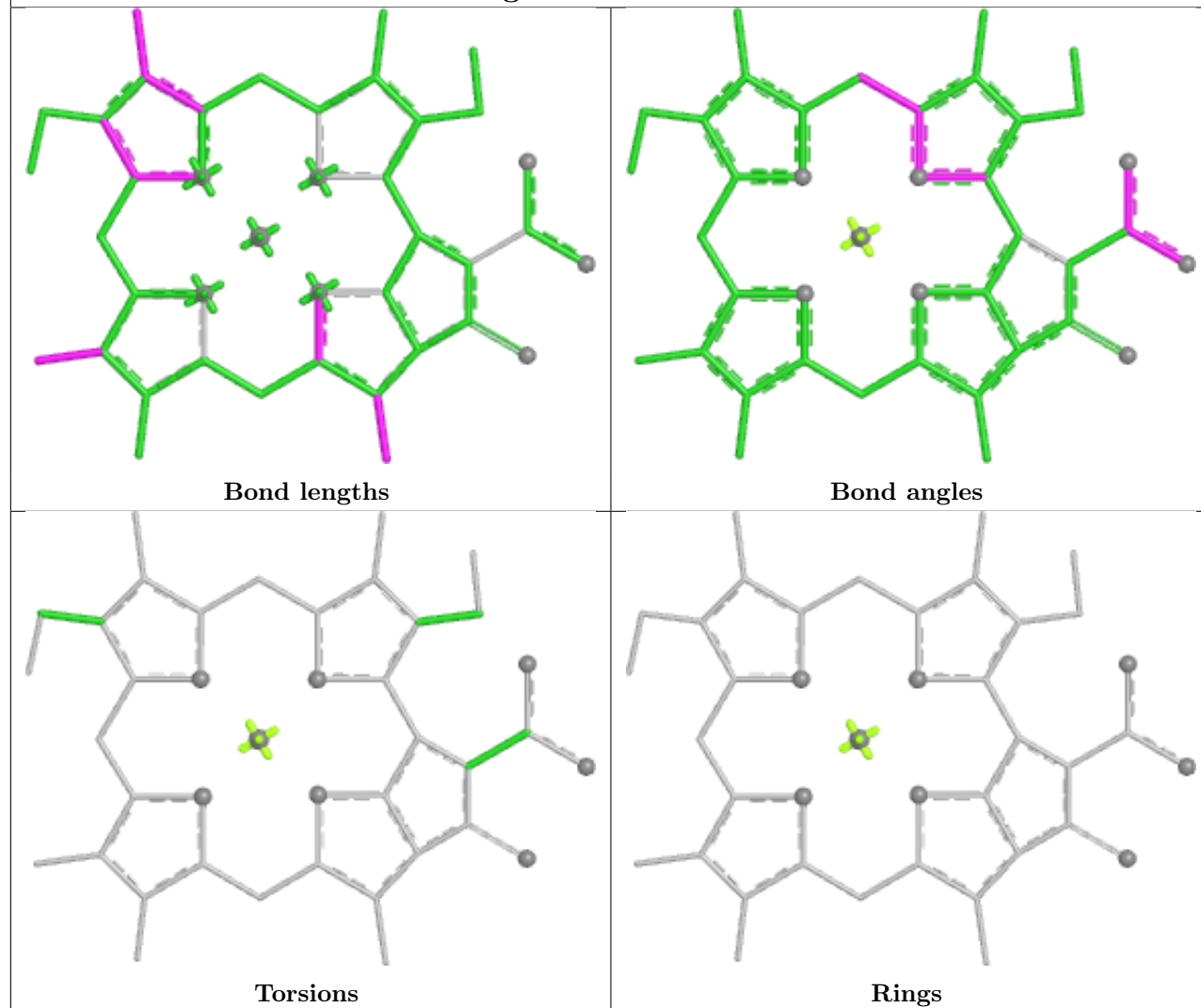
Ligand CLA 9 607



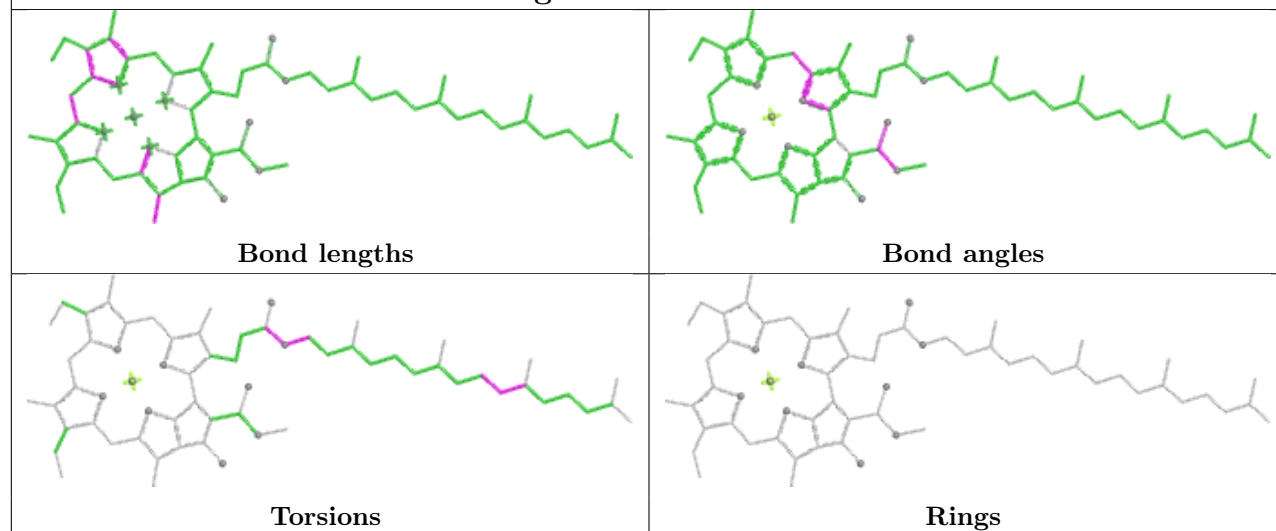
Ligand XAT Z 1622



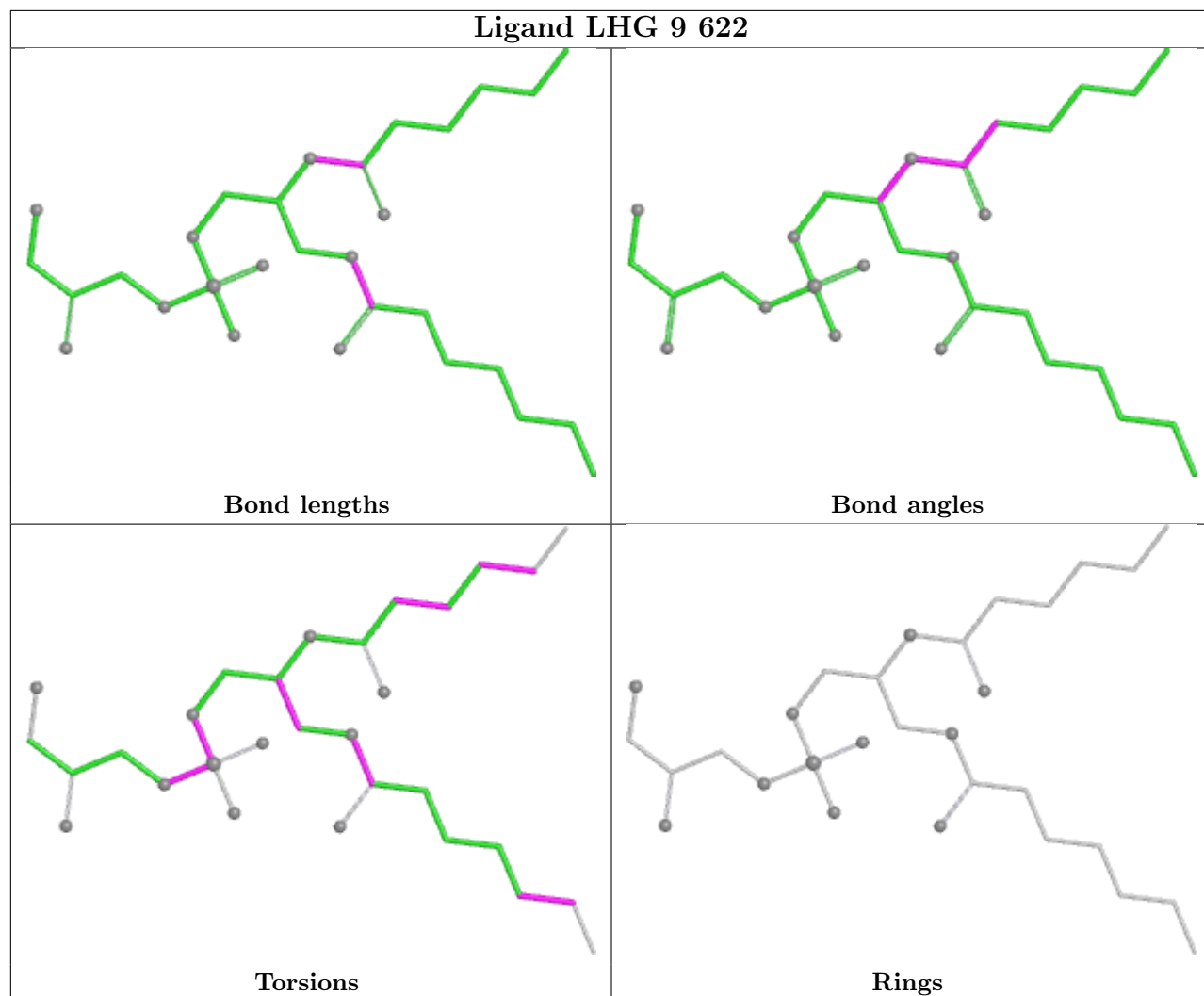
Ligand CLA L 306



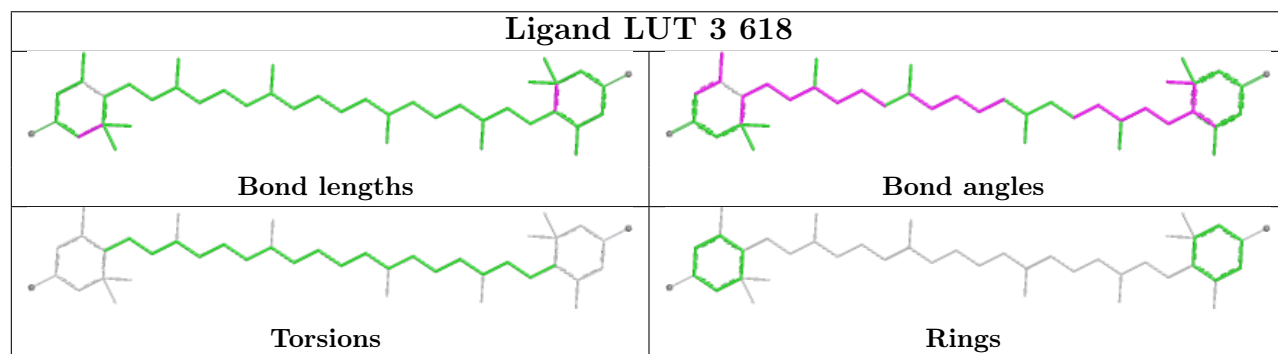
Ligand CLA Z 612



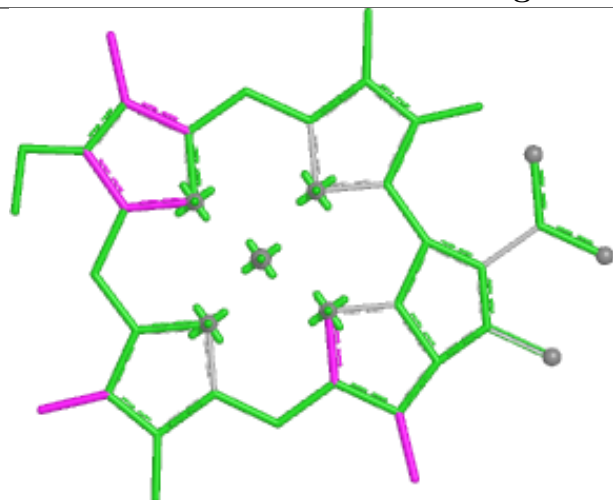
Ligand LHG 9 622



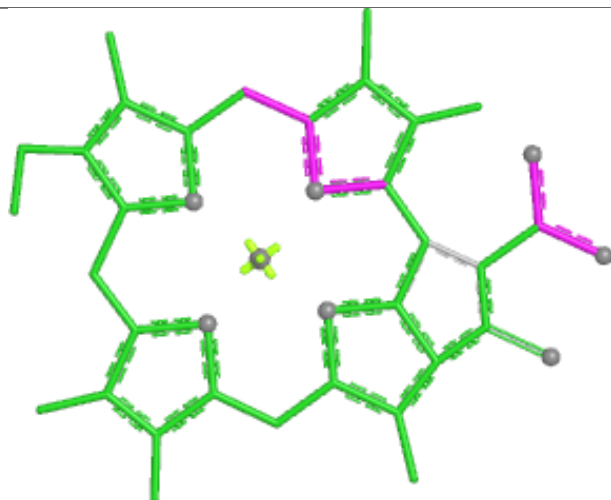
Ligand LUT 3 618



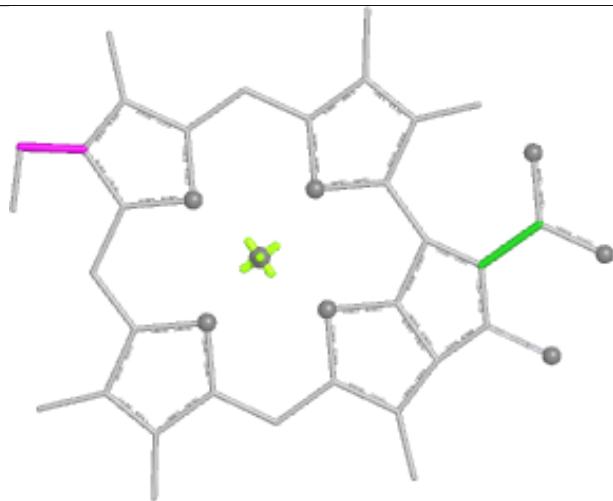
Ligand CLA H 202



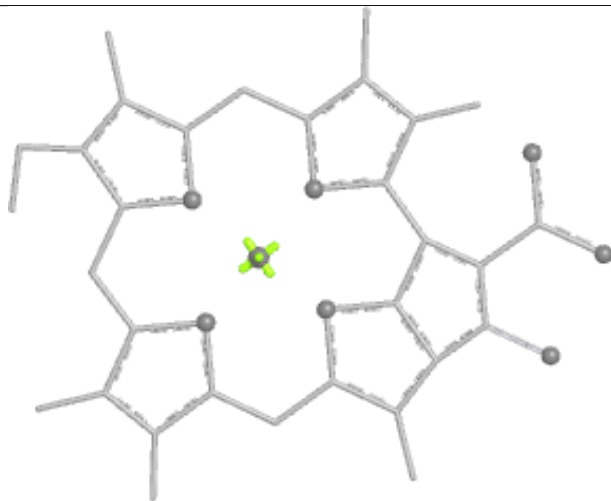
Bond lengths



Bond angles

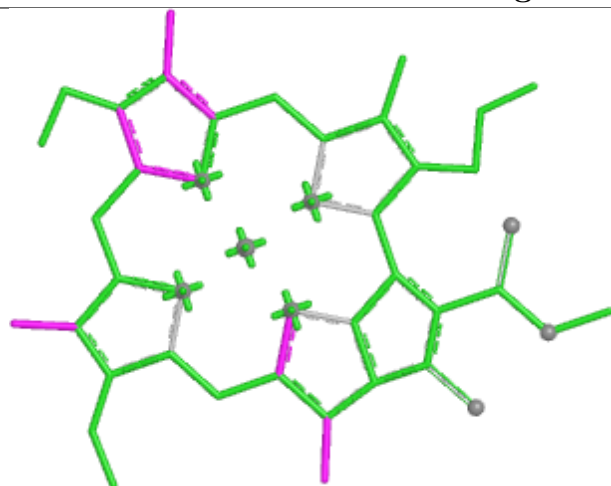


Torsions

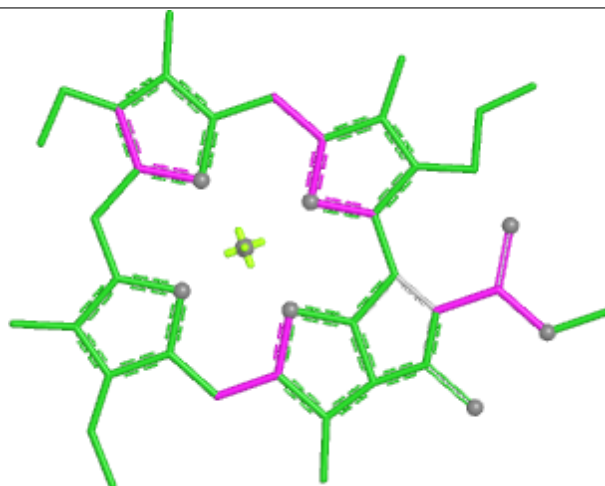


Rings

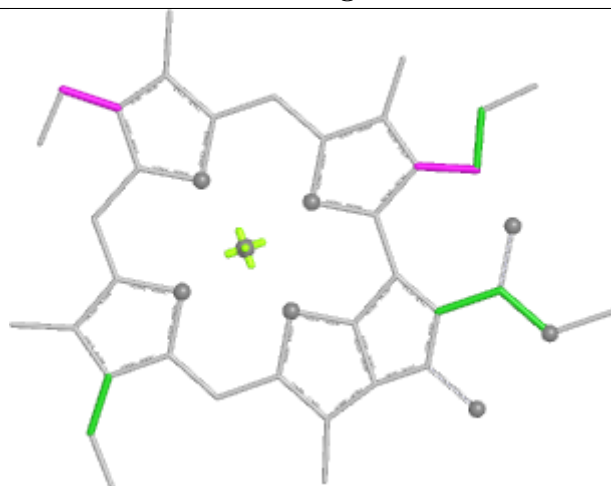
Ligand CLA B 830



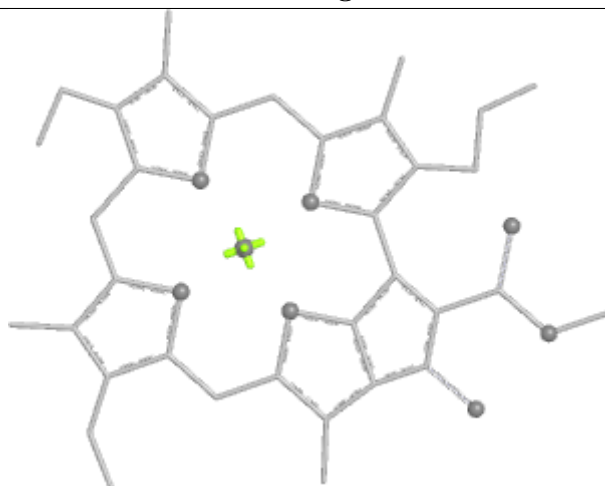
Bond lengths



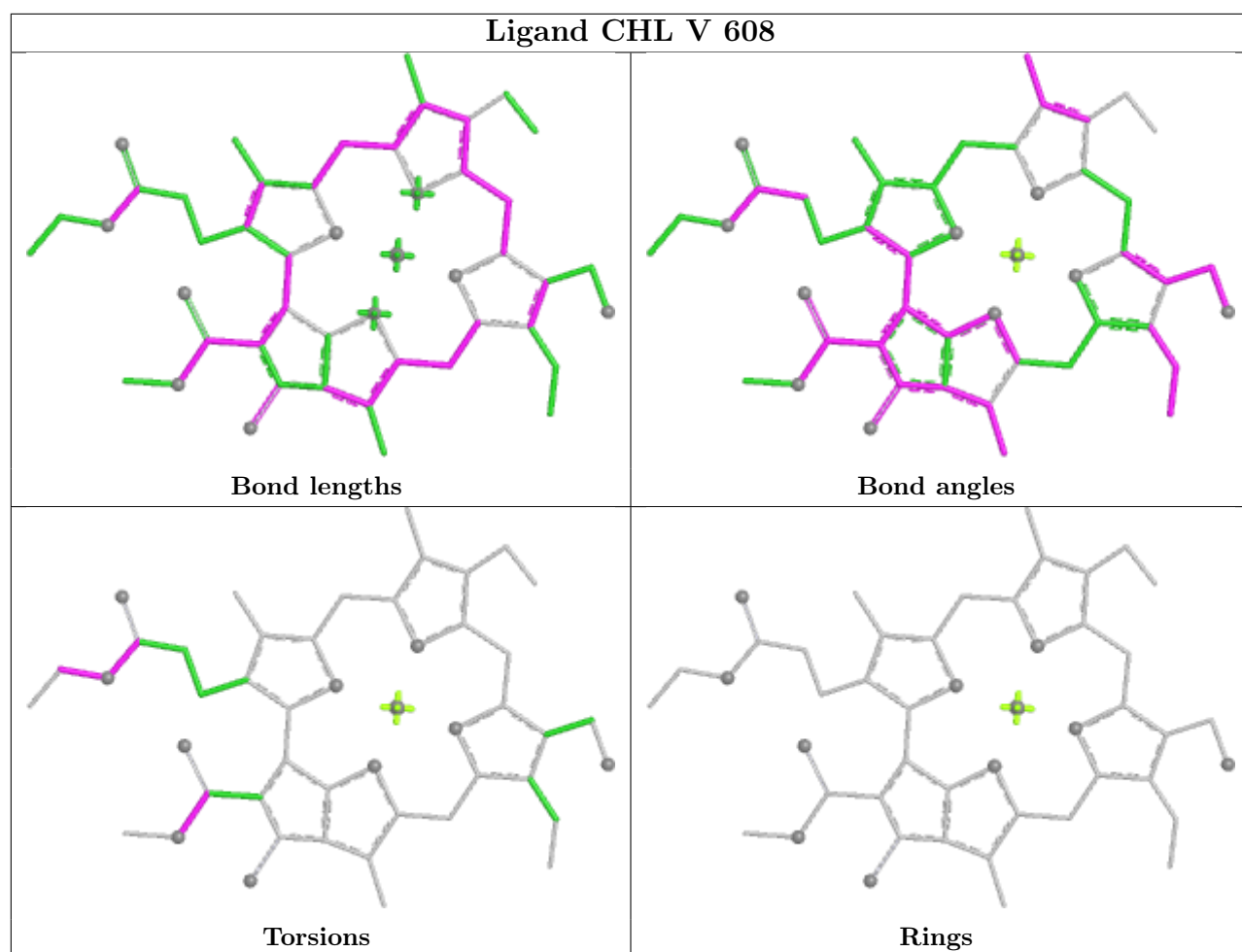
Bond angles



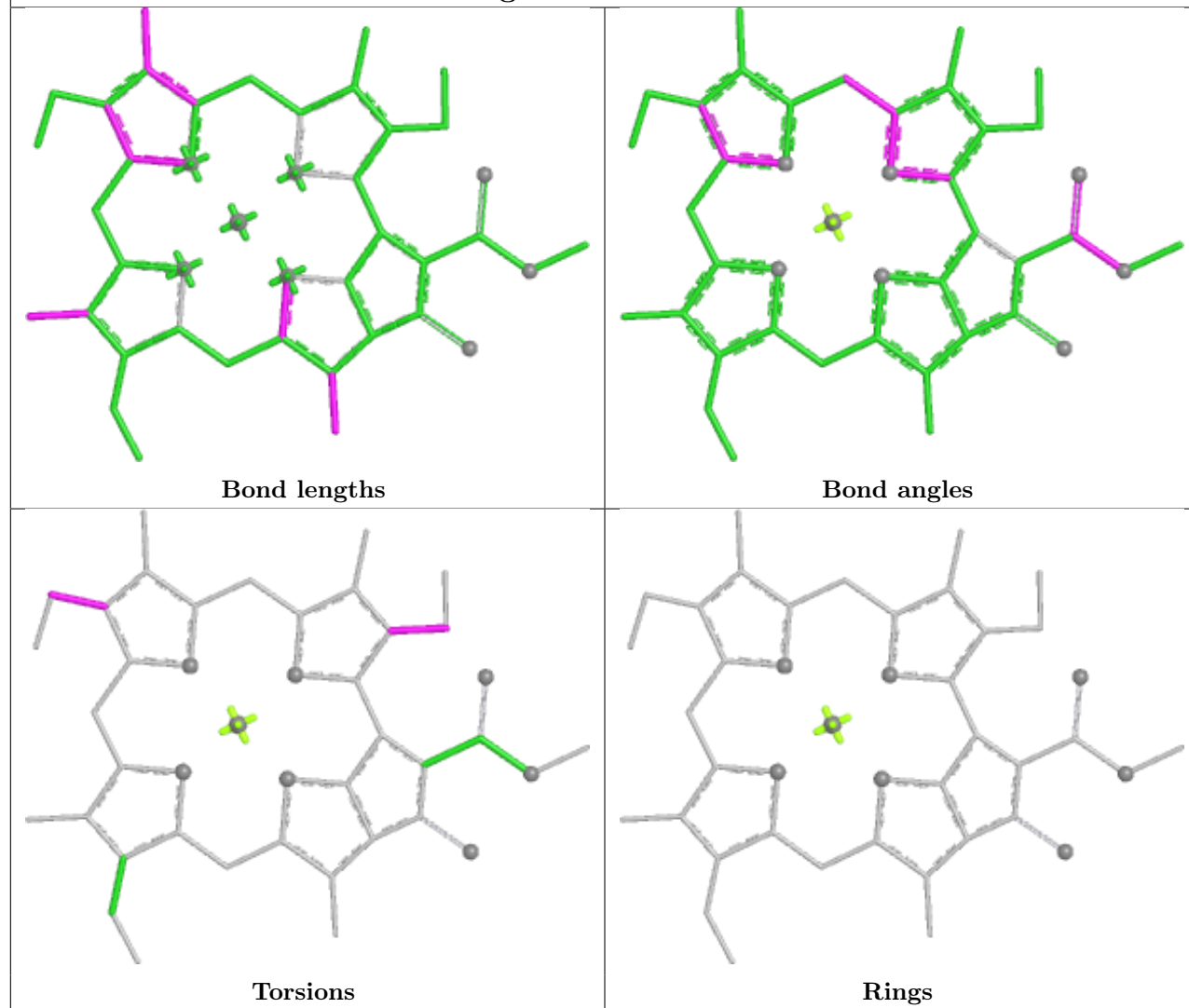
Torsions



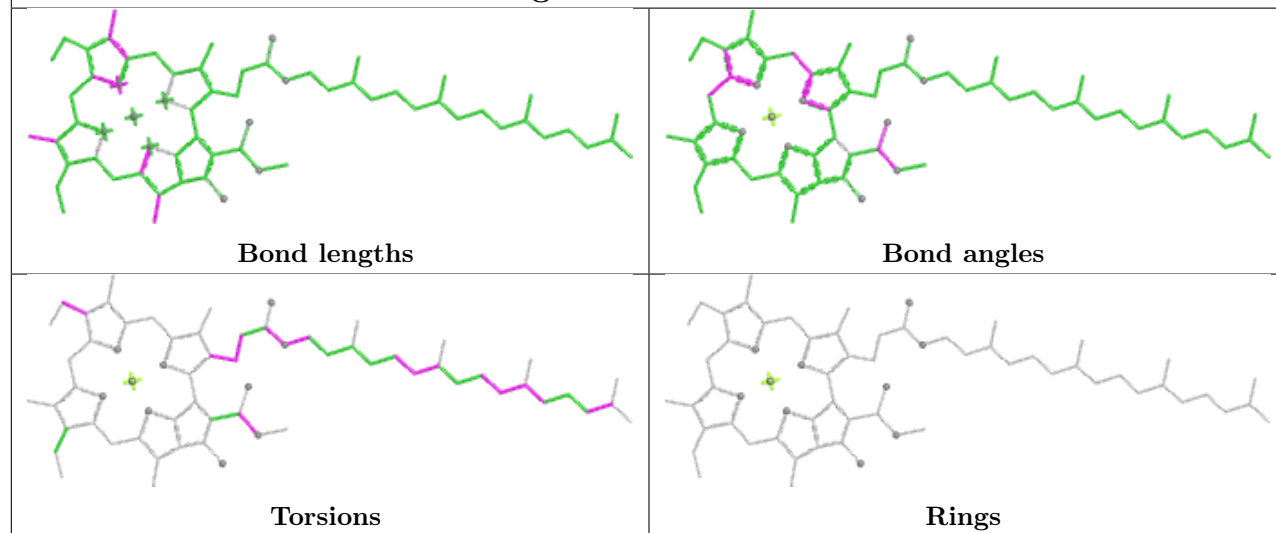
Rings

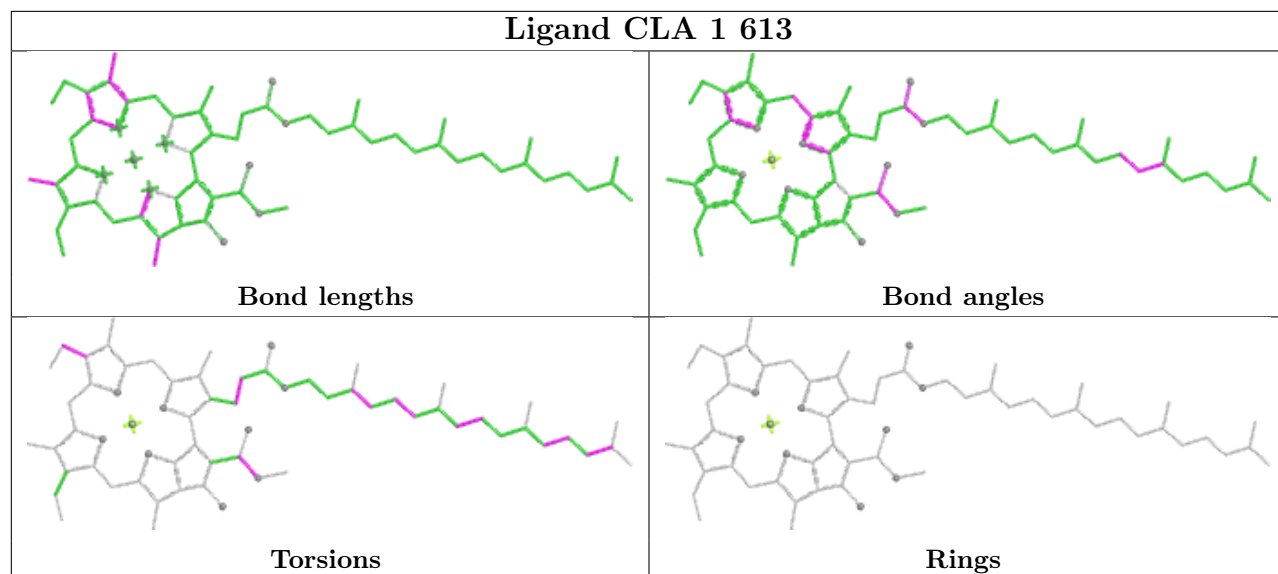
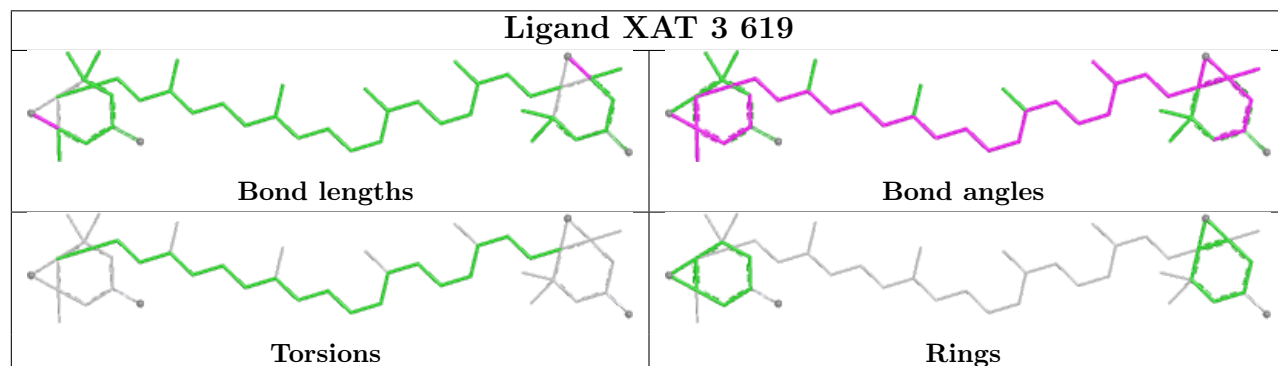
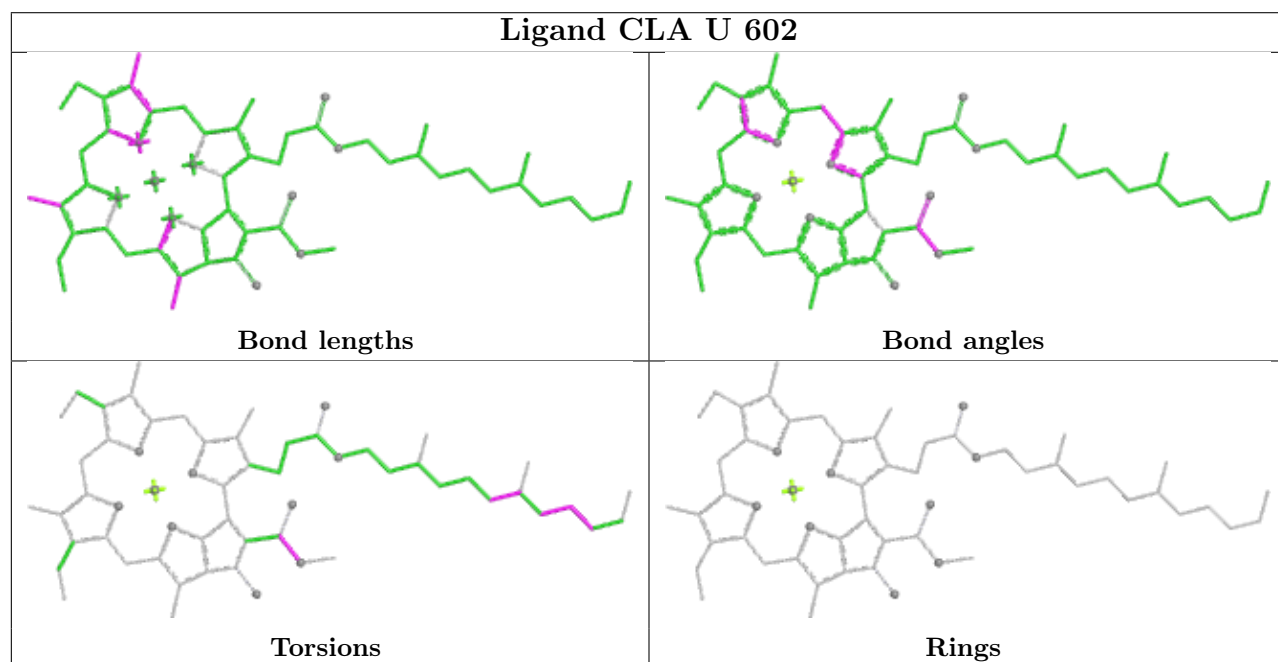


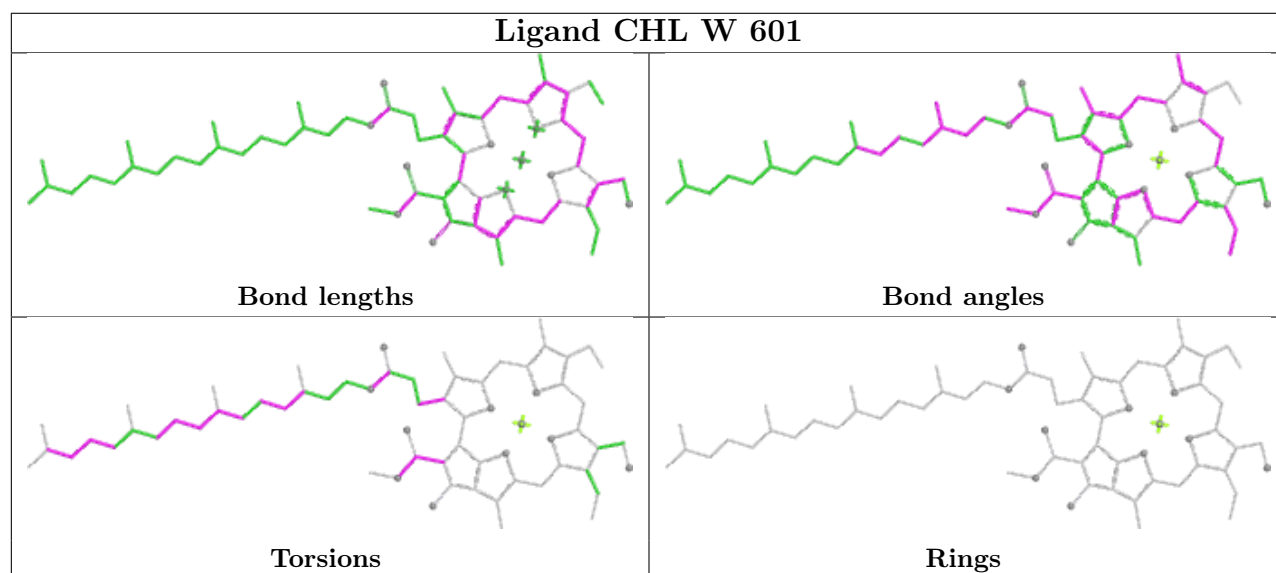
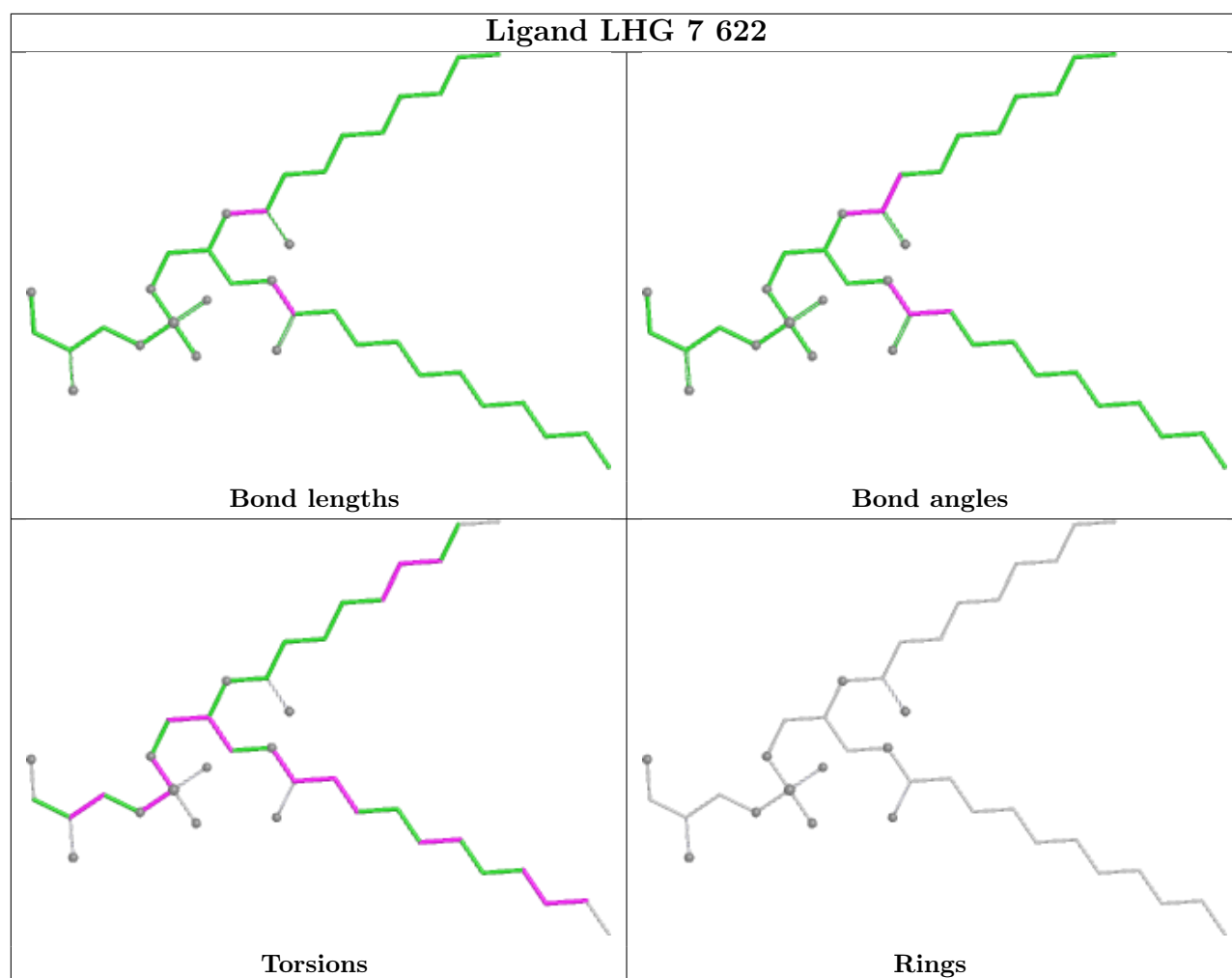
Ligand CLA 4 611

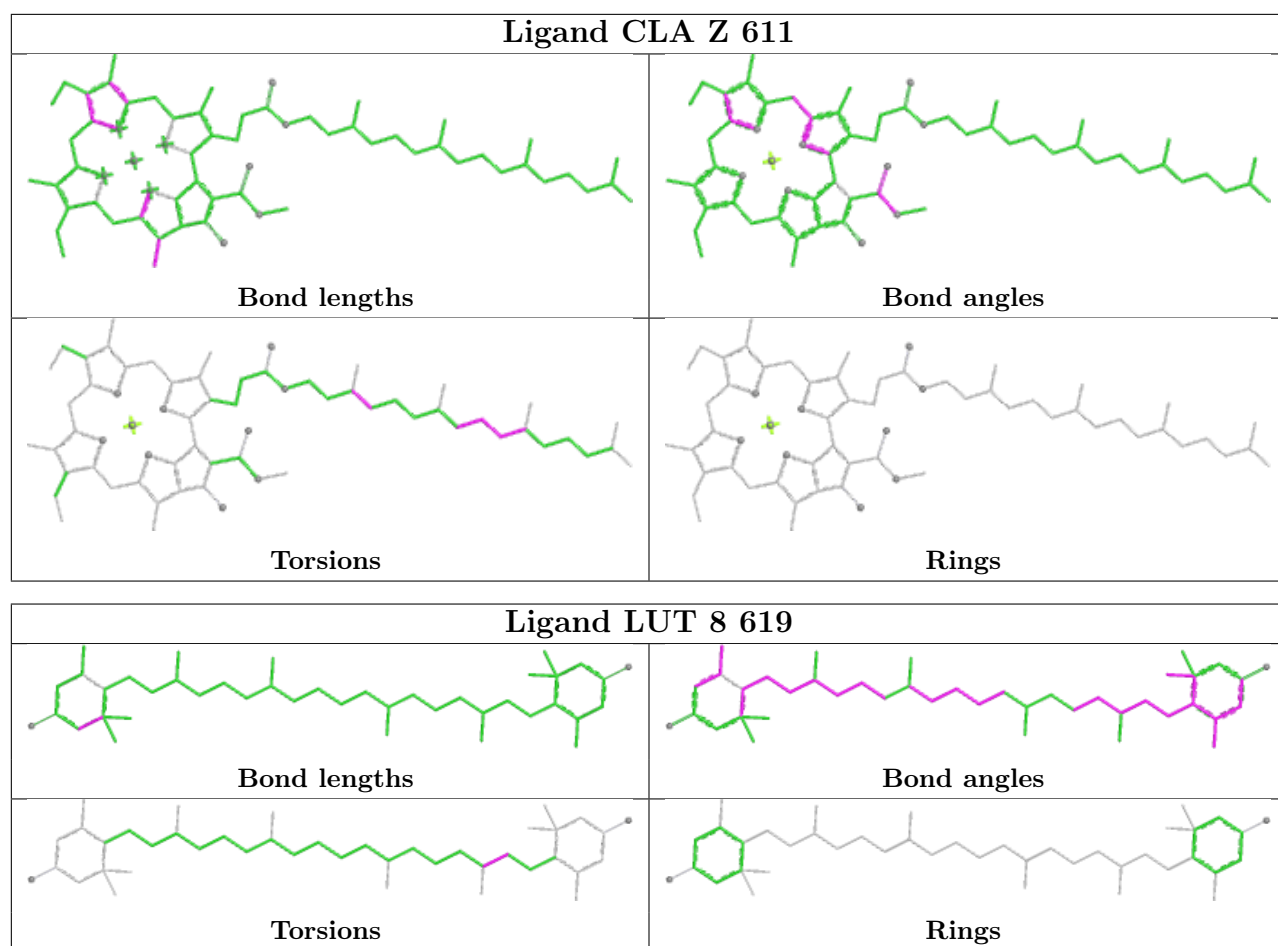


Ligand CLA B 802

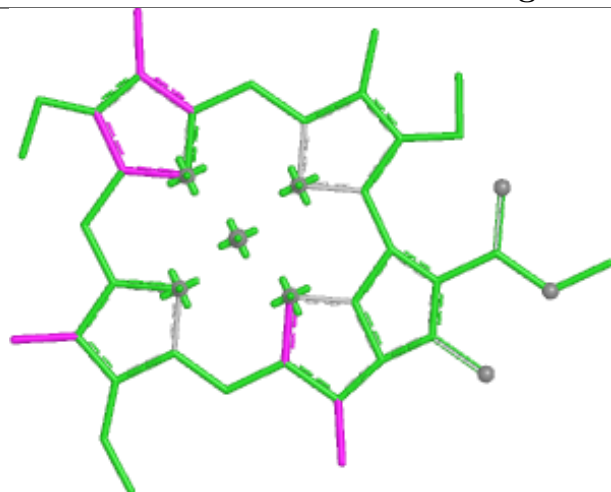


Ligand CLA 1 613**Ligand XAT 3 619****Ligand CLA U 602**

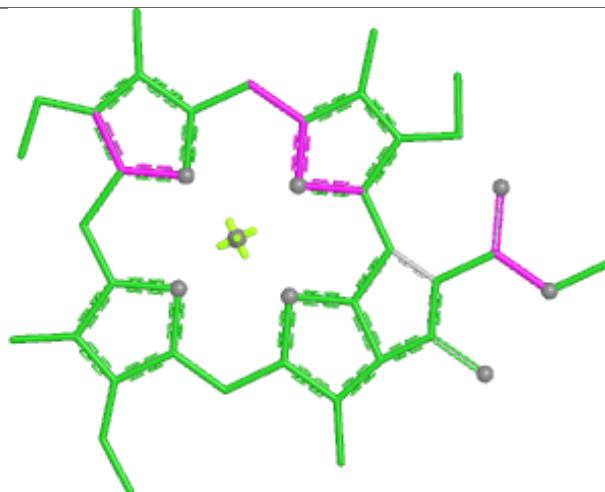




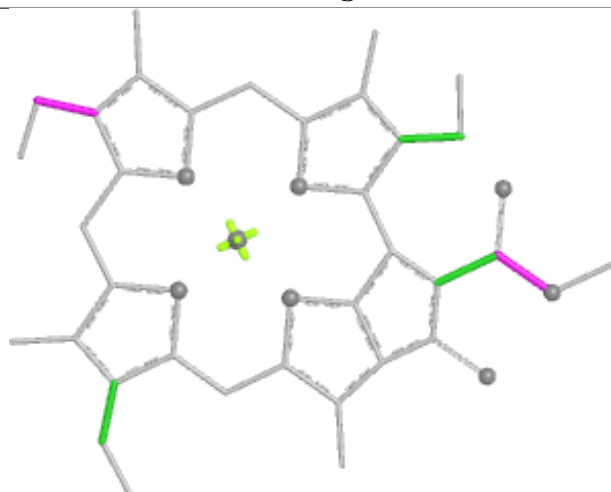
Ligand CLA 7 607



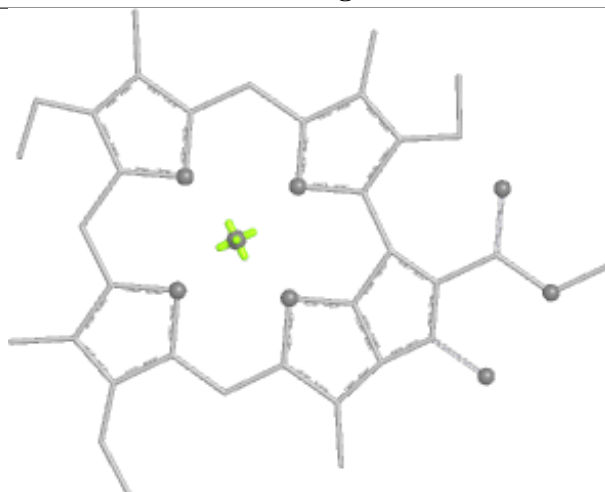
Bond lengths



Bond angles

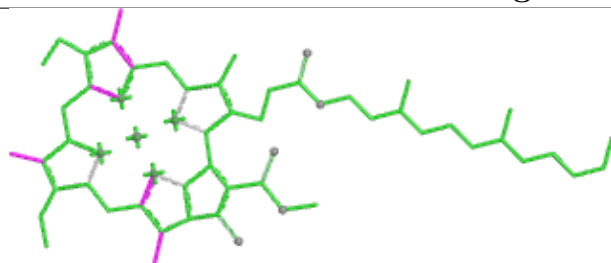


Torsions

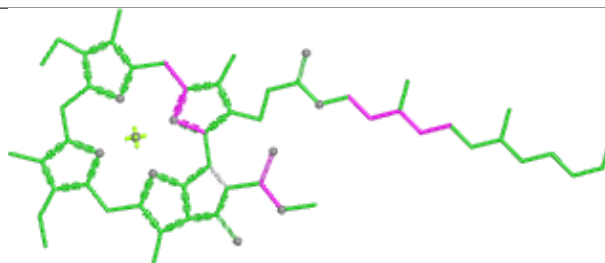


Rings

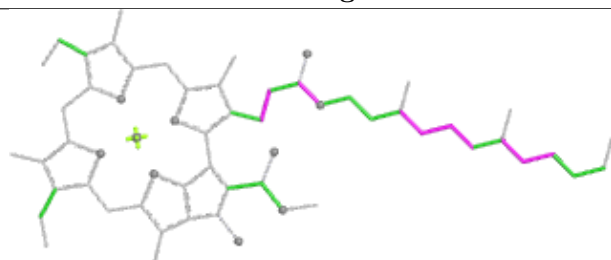
Ligand CLA U 613



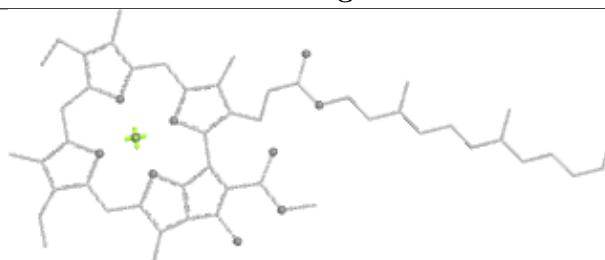
Bond lengths



Bond angles

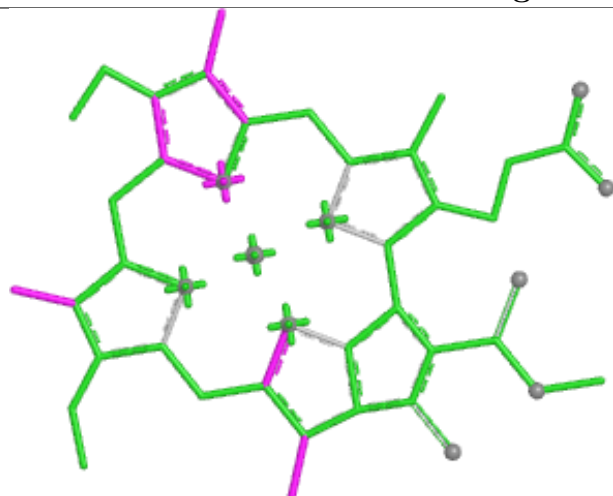


Torsions

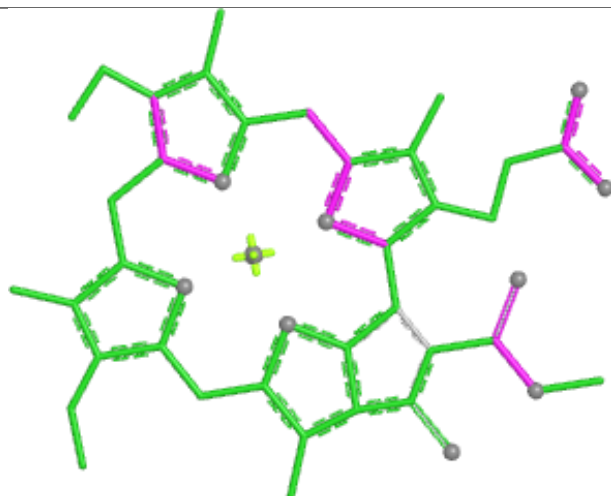


Rings

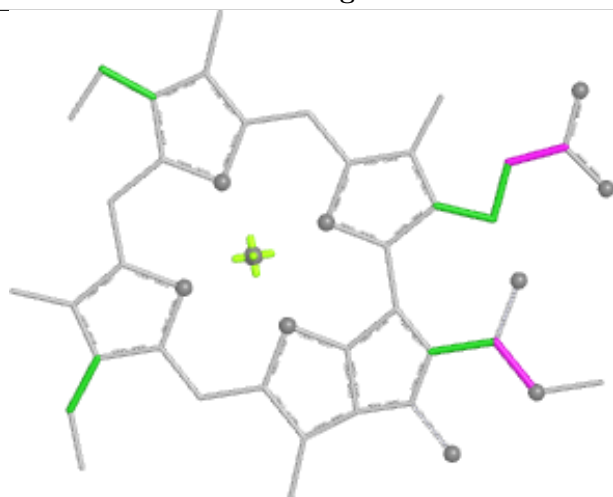
Ligand CLA K 204



Bond lengths



Bond angles

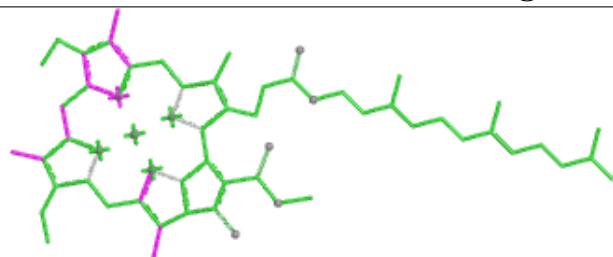


Torsions

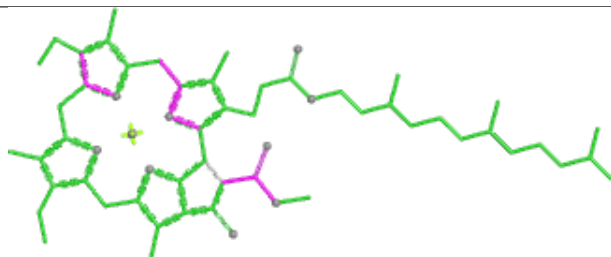


Rings

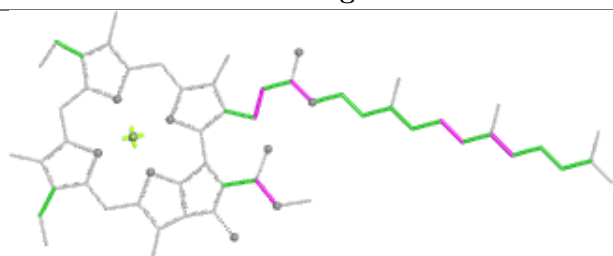
Ligand CLA 8 602



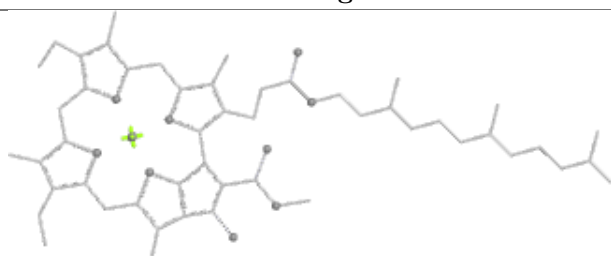
Bond lengths



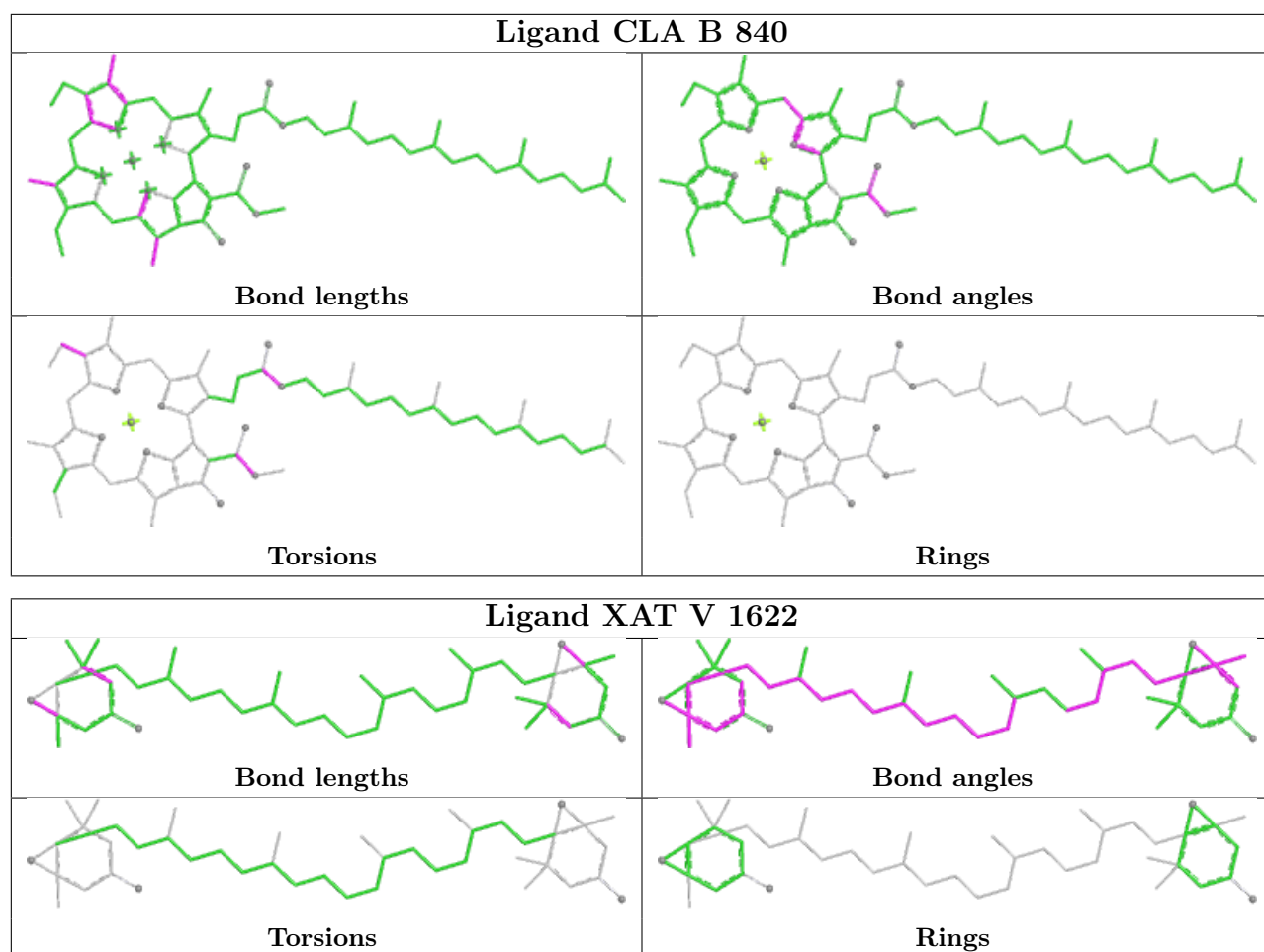
Bond angles



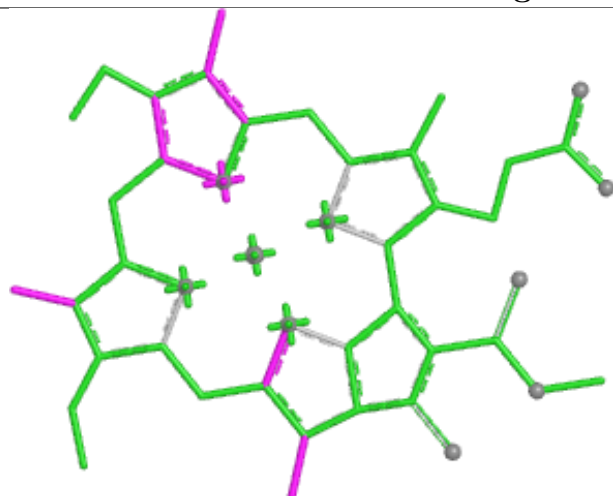
Torsions



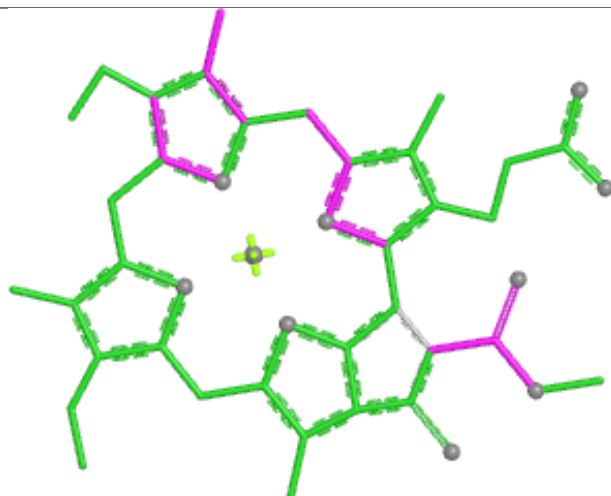
Rings



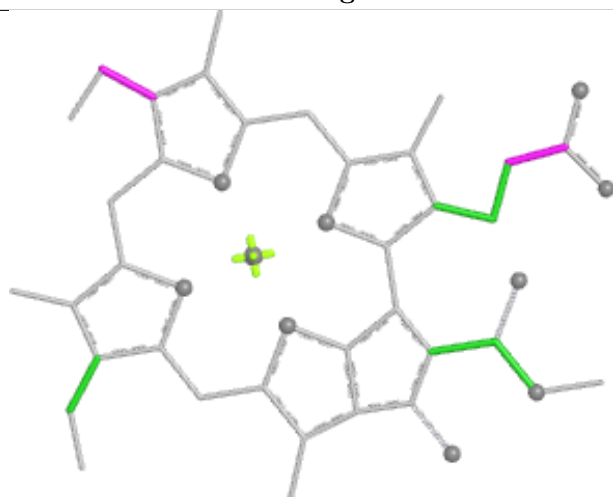
Ligand CLA V 612



Bond lengths



Bond angles

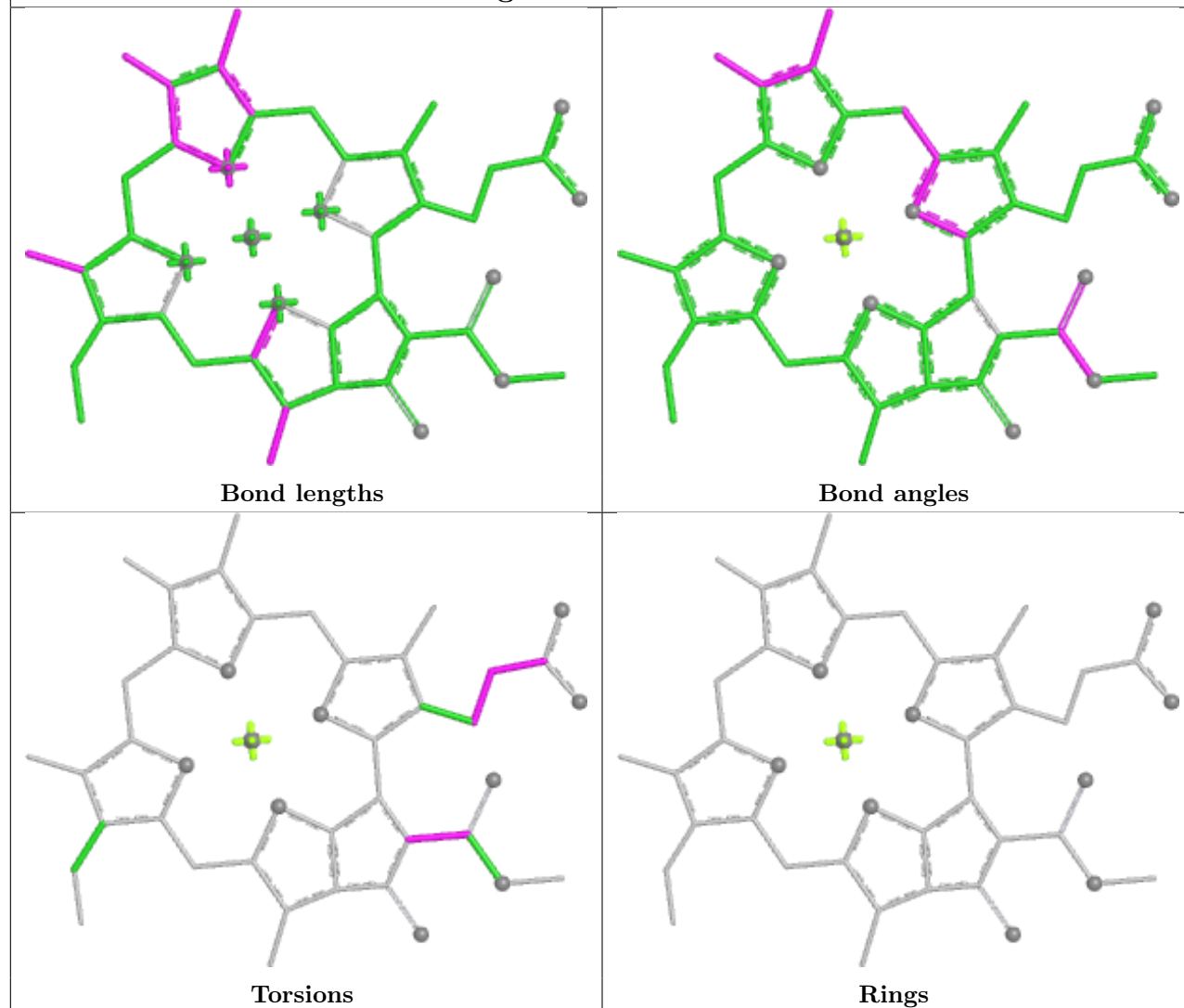


Torsions

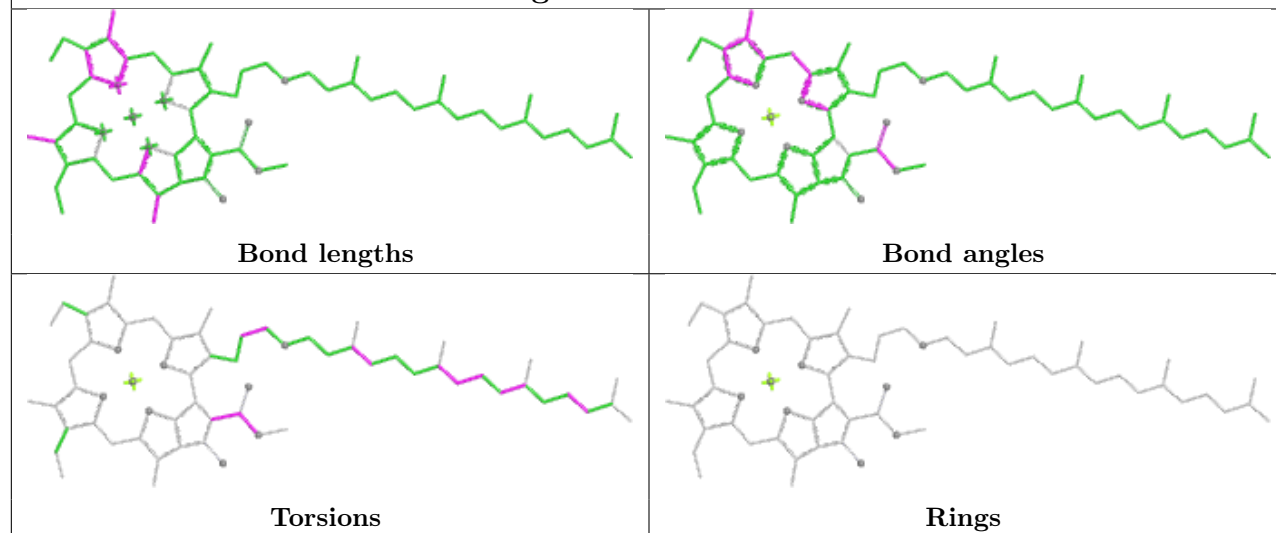


Rings

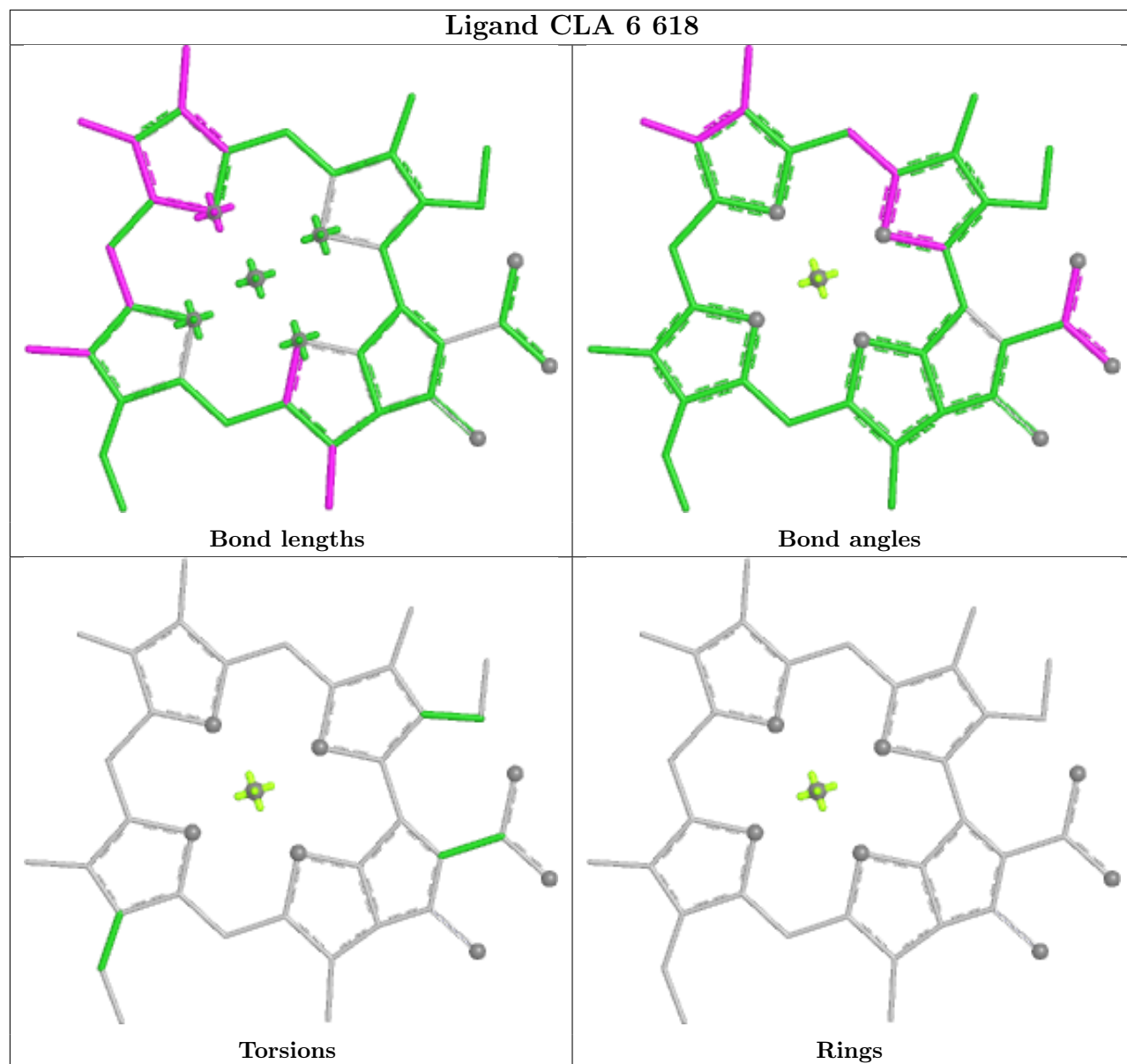
Ligand CLA 8 603

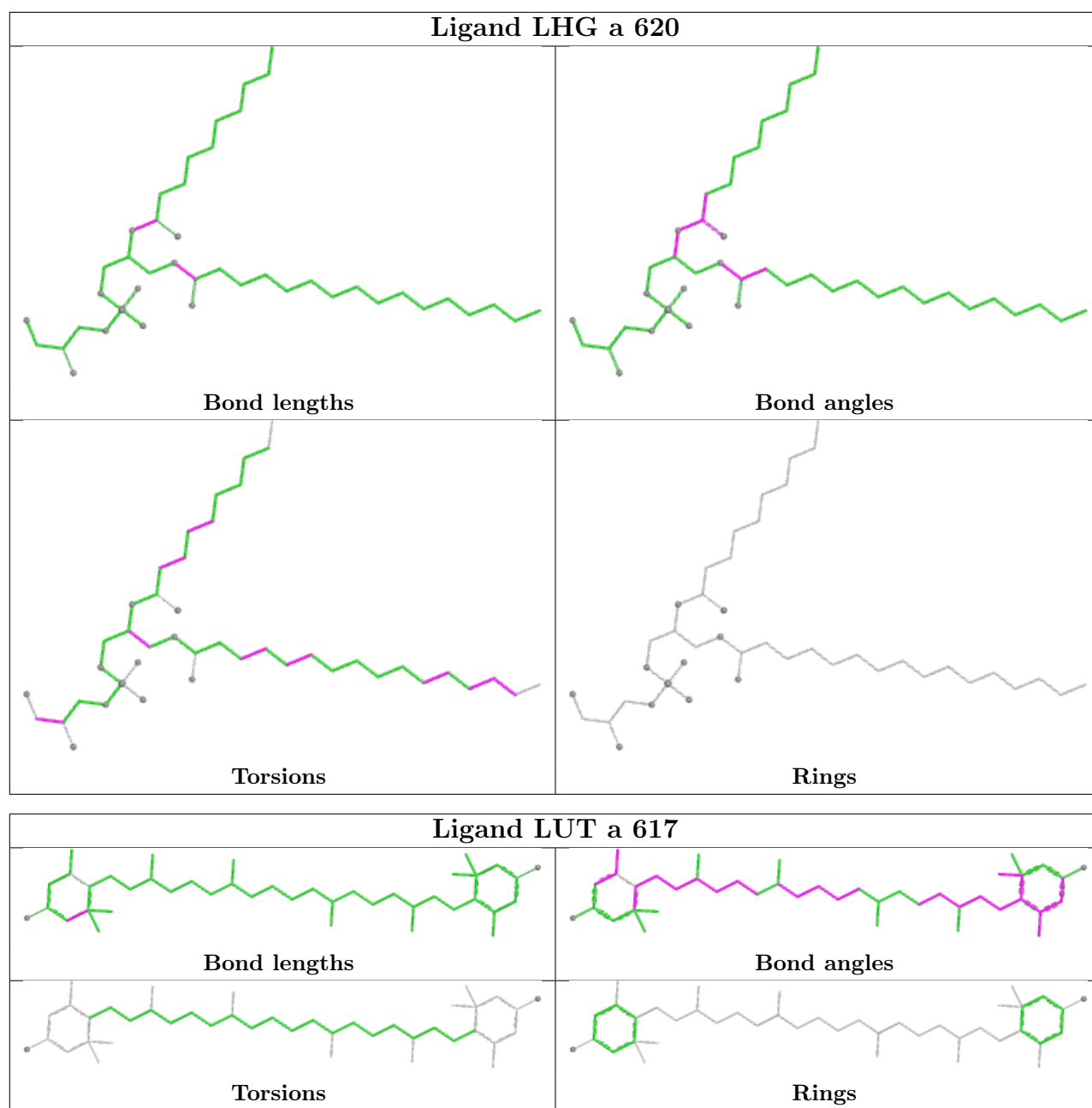


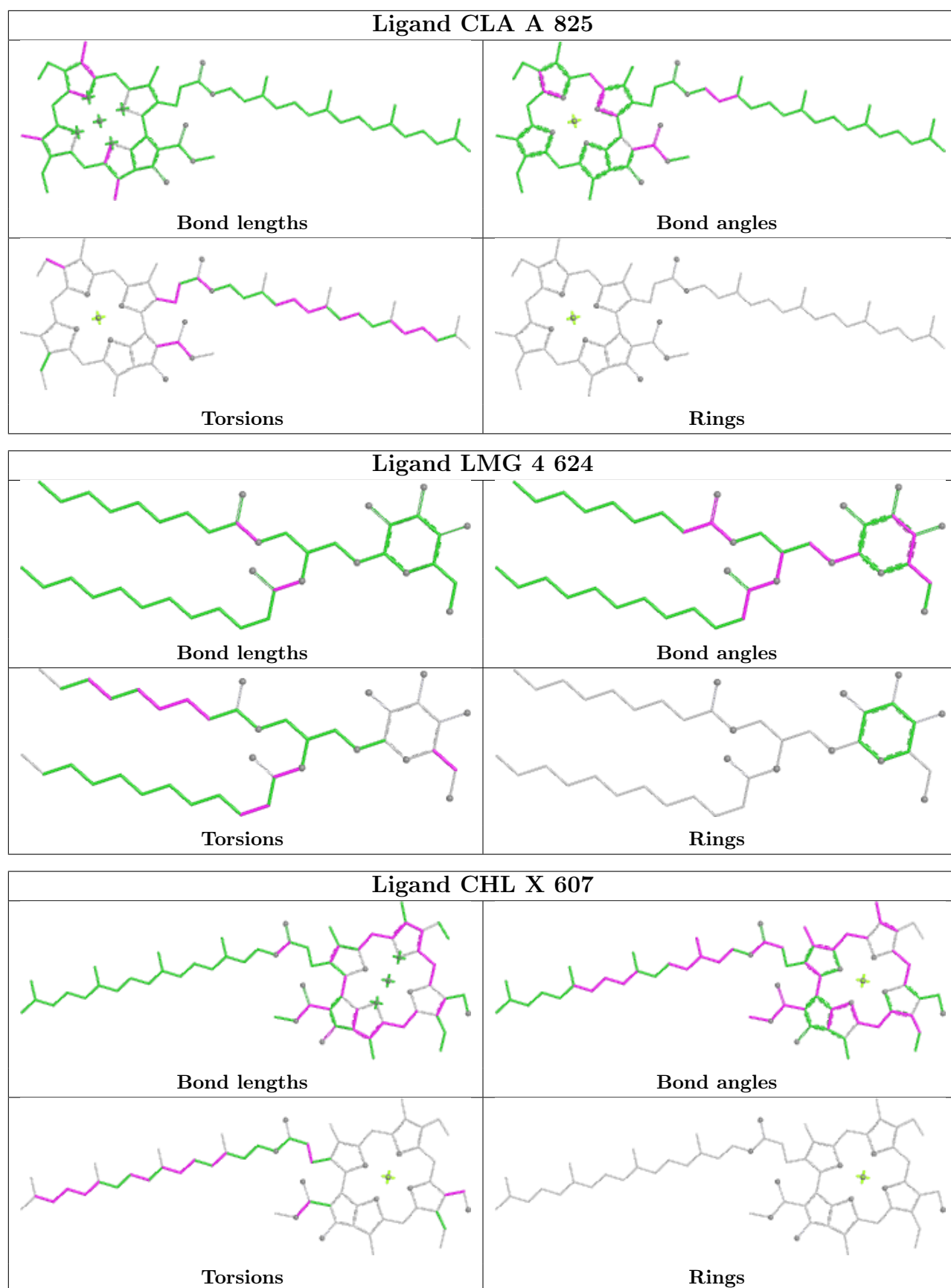
Ligand CLA A 826



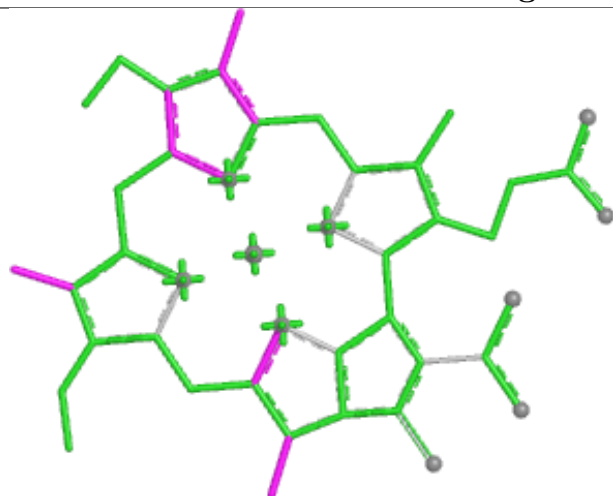
Ligand CLA 6 618



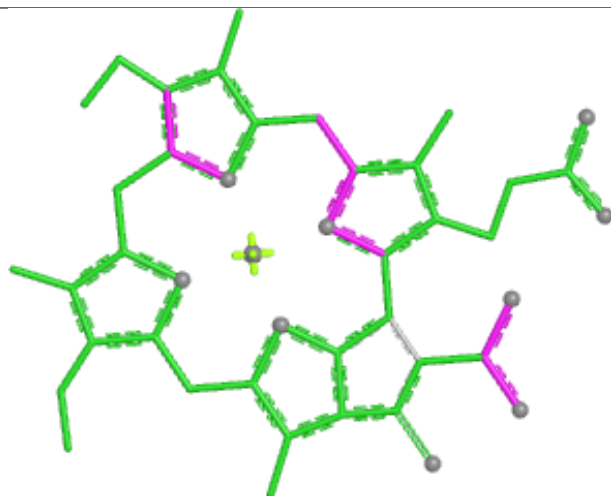




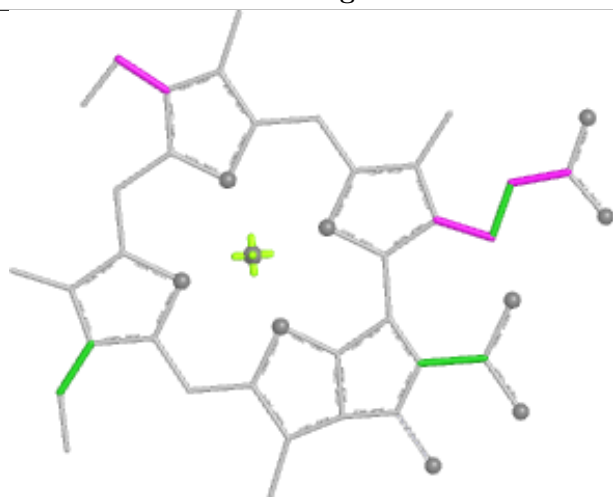
Ligand CLA 1 608



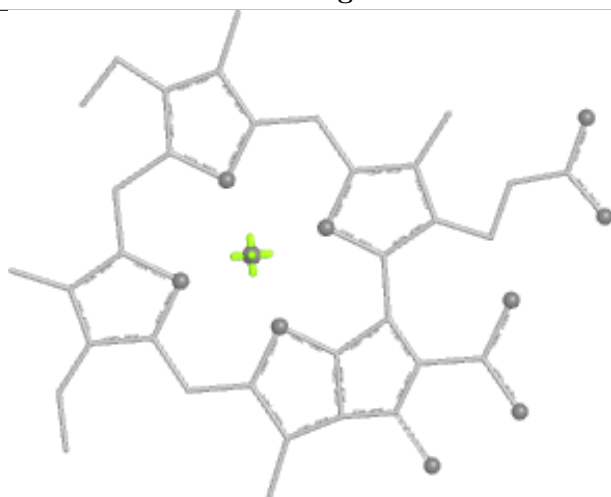
Bond lengths



Bond angles

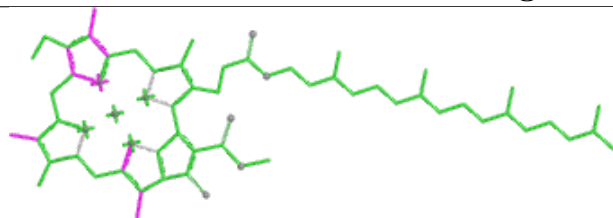


Torsions

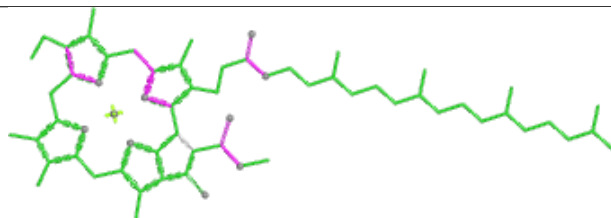


Rings

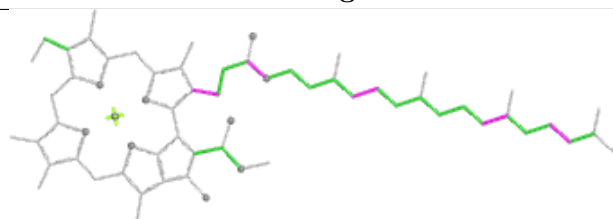
Ligand CLA 8 606



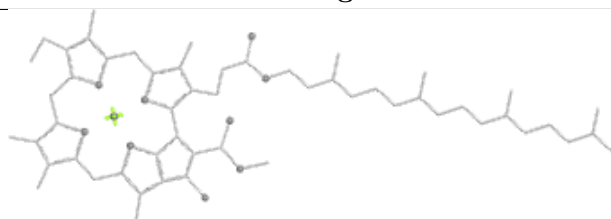
Bond lengths



Bond angles

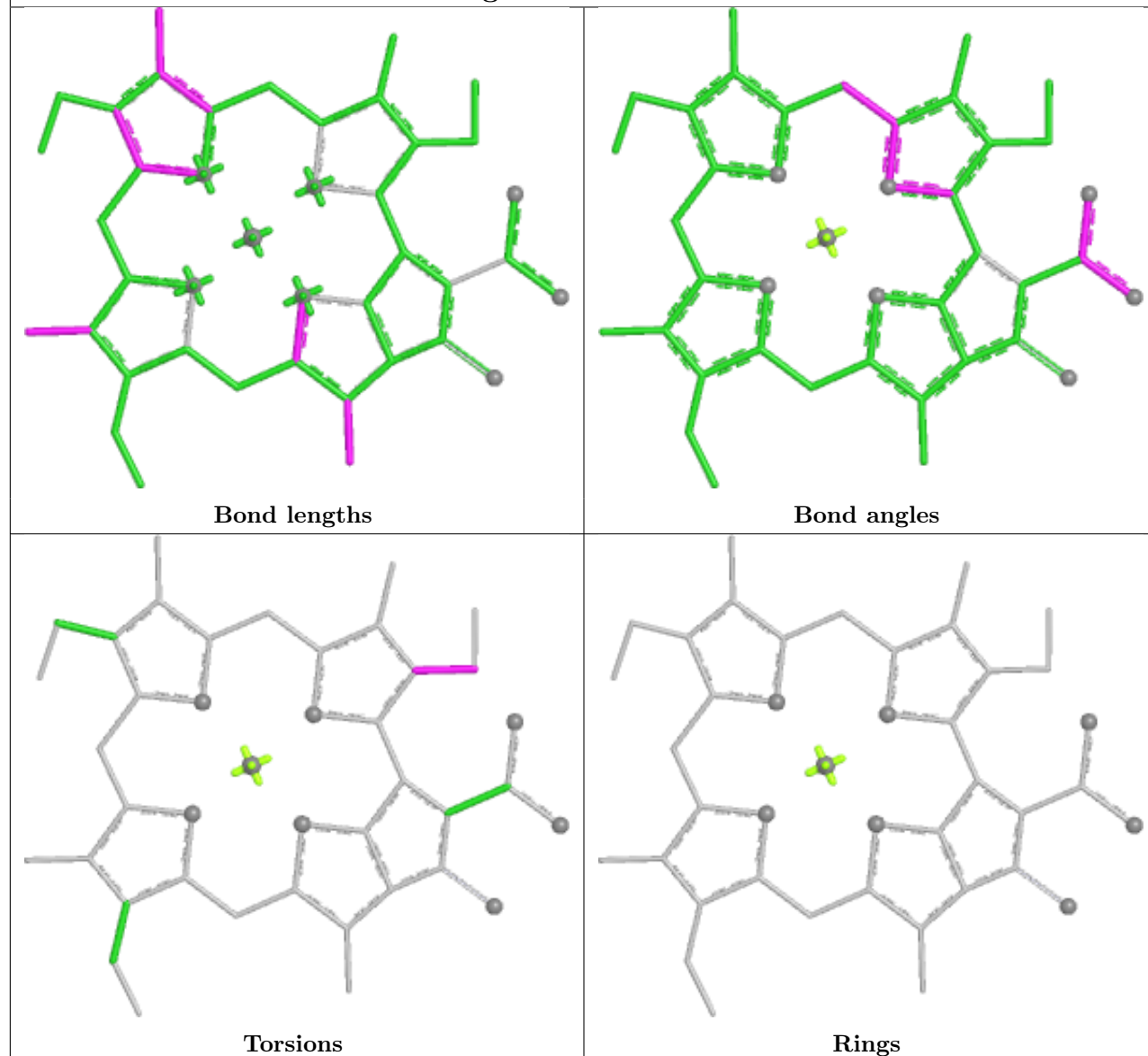


Torsions

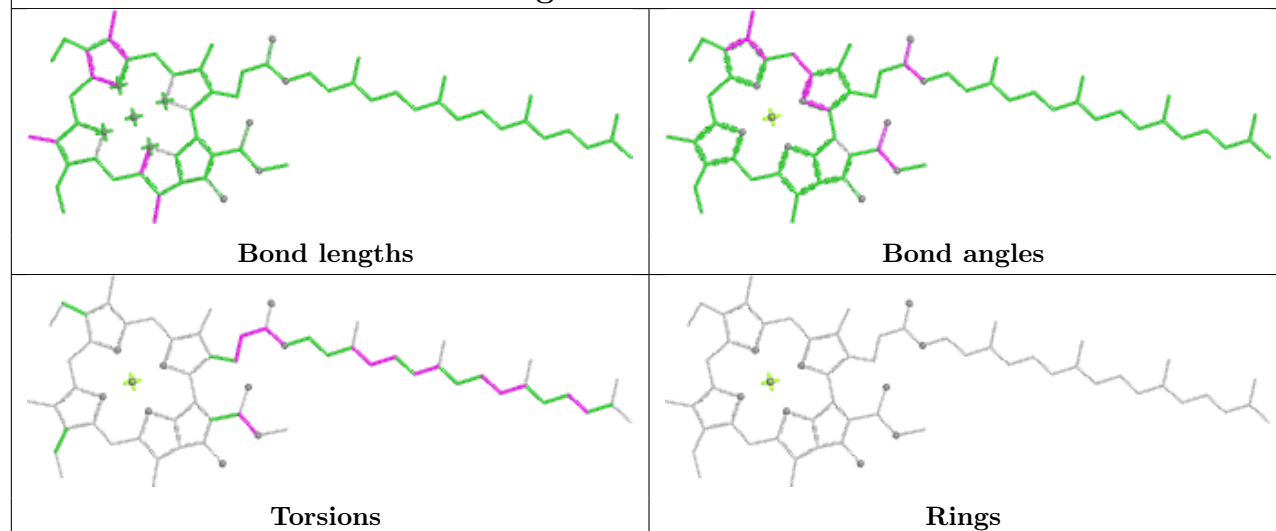


Rings

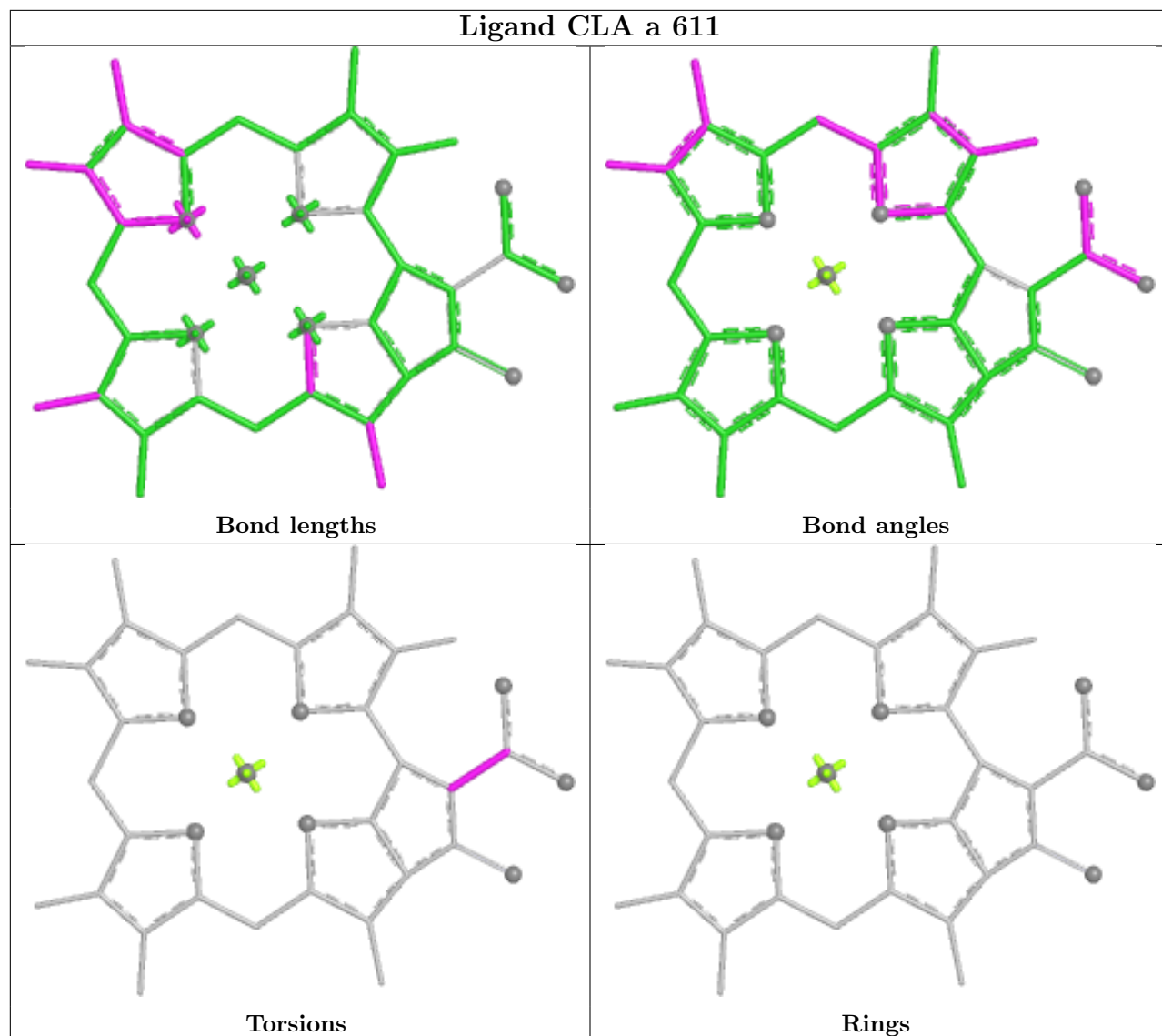
Ligand CLA 8 612

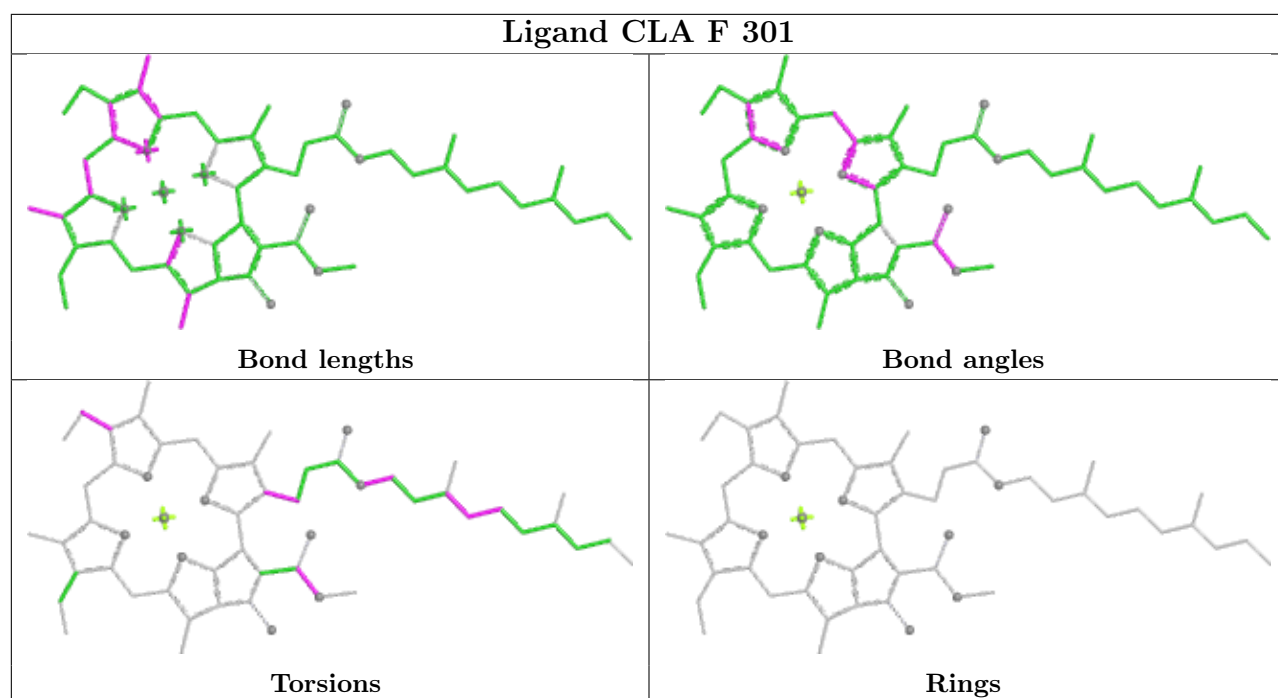


Ligand CLA 8 601

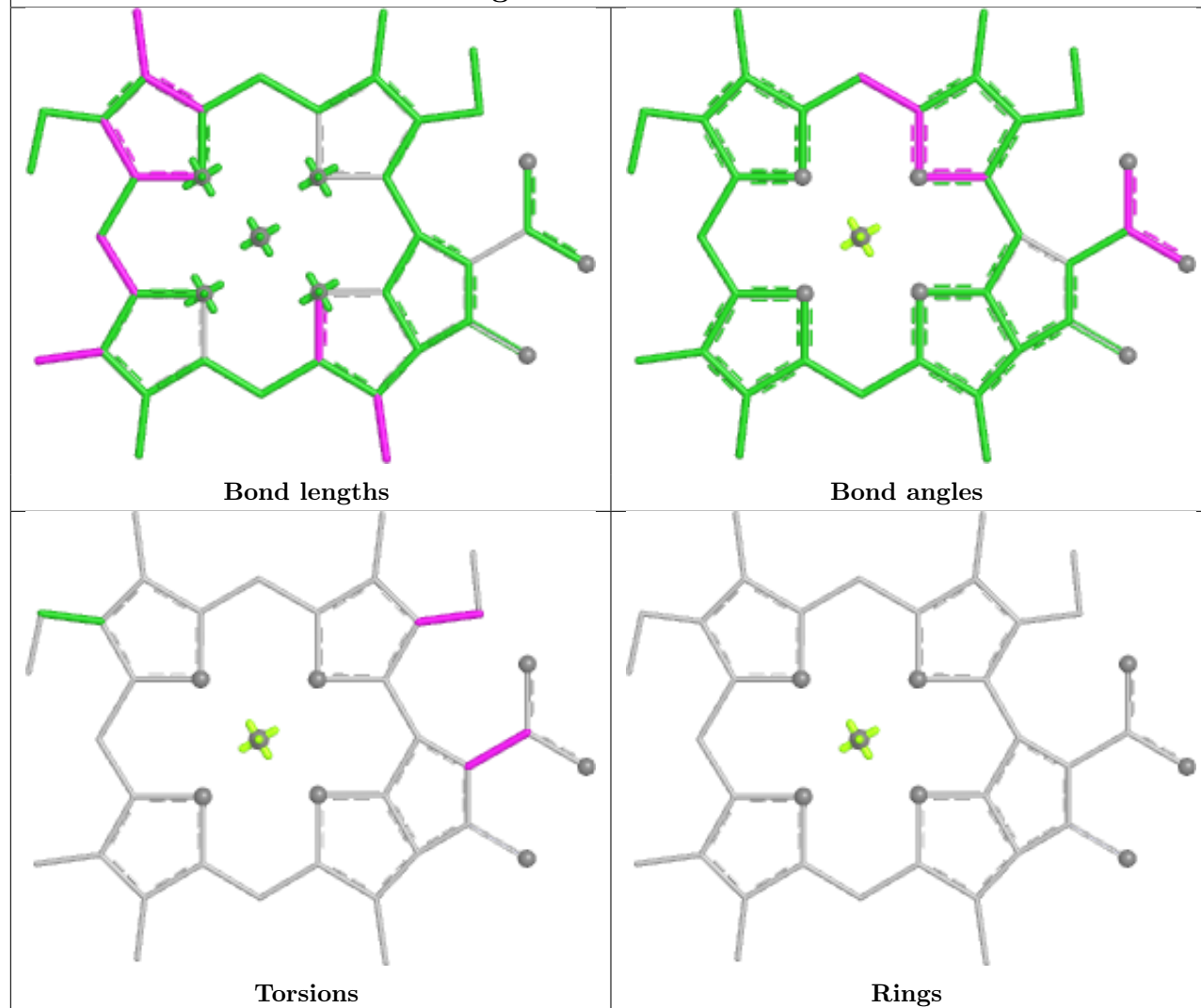


Ligand CLA a 611

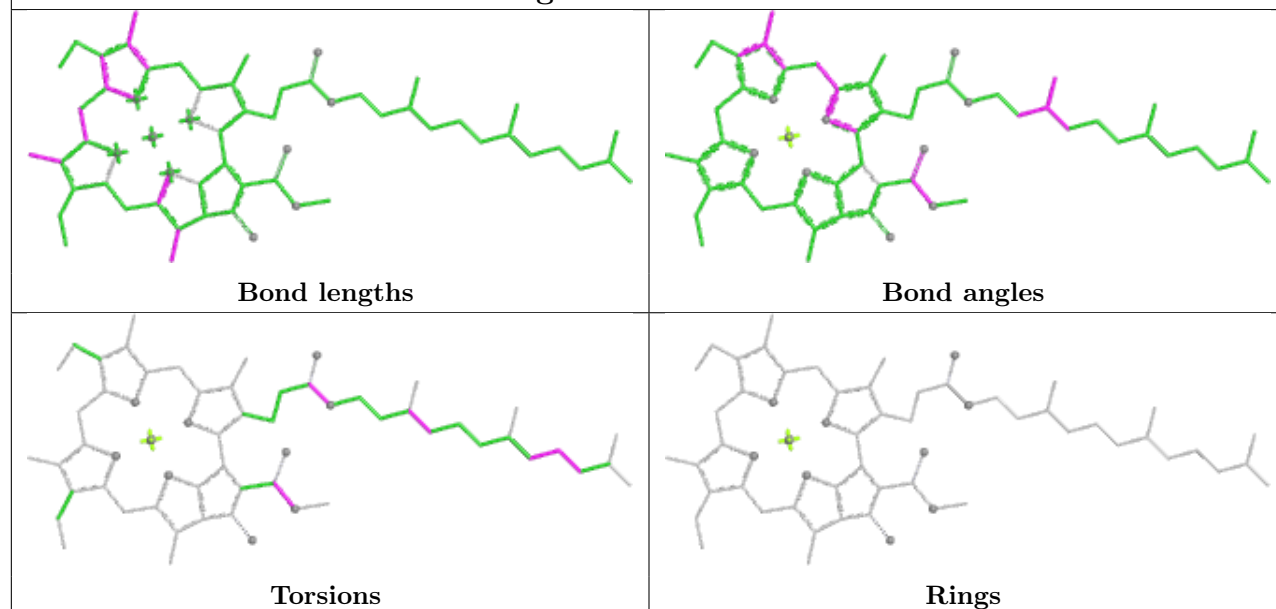


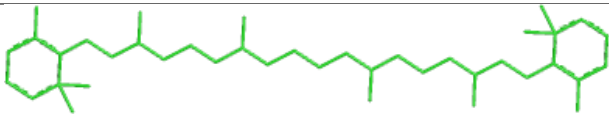
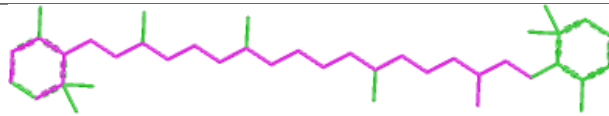
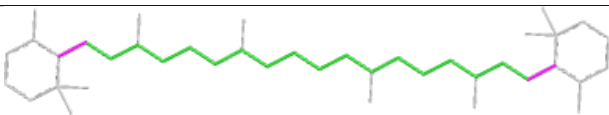
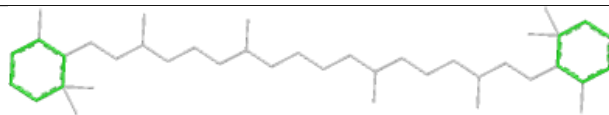


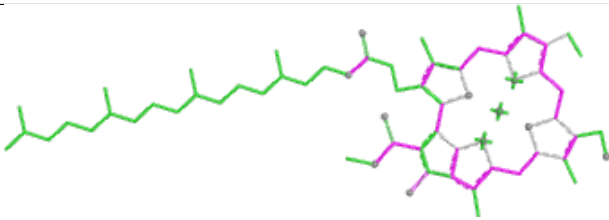
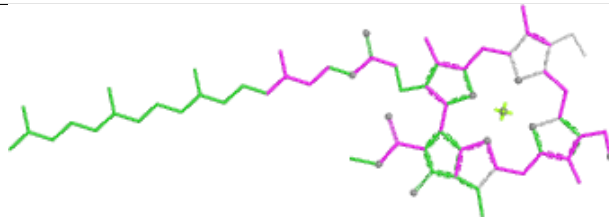
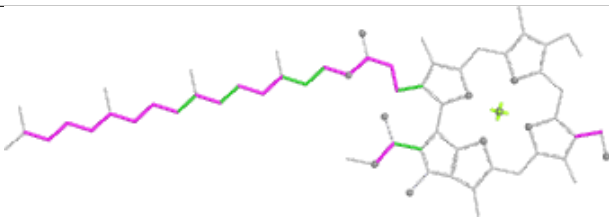
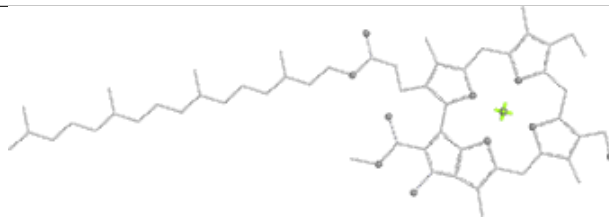
Ligand CLA O 2003

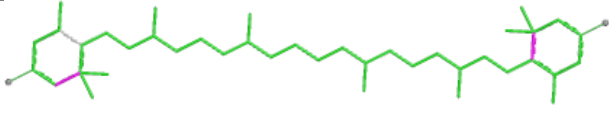
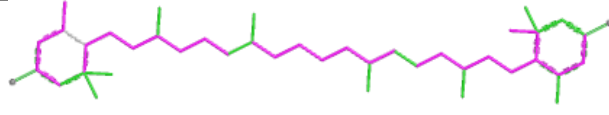
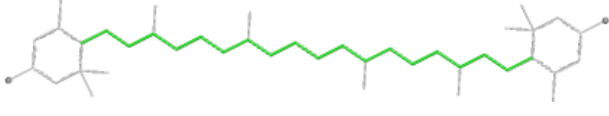
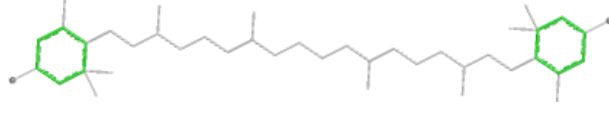


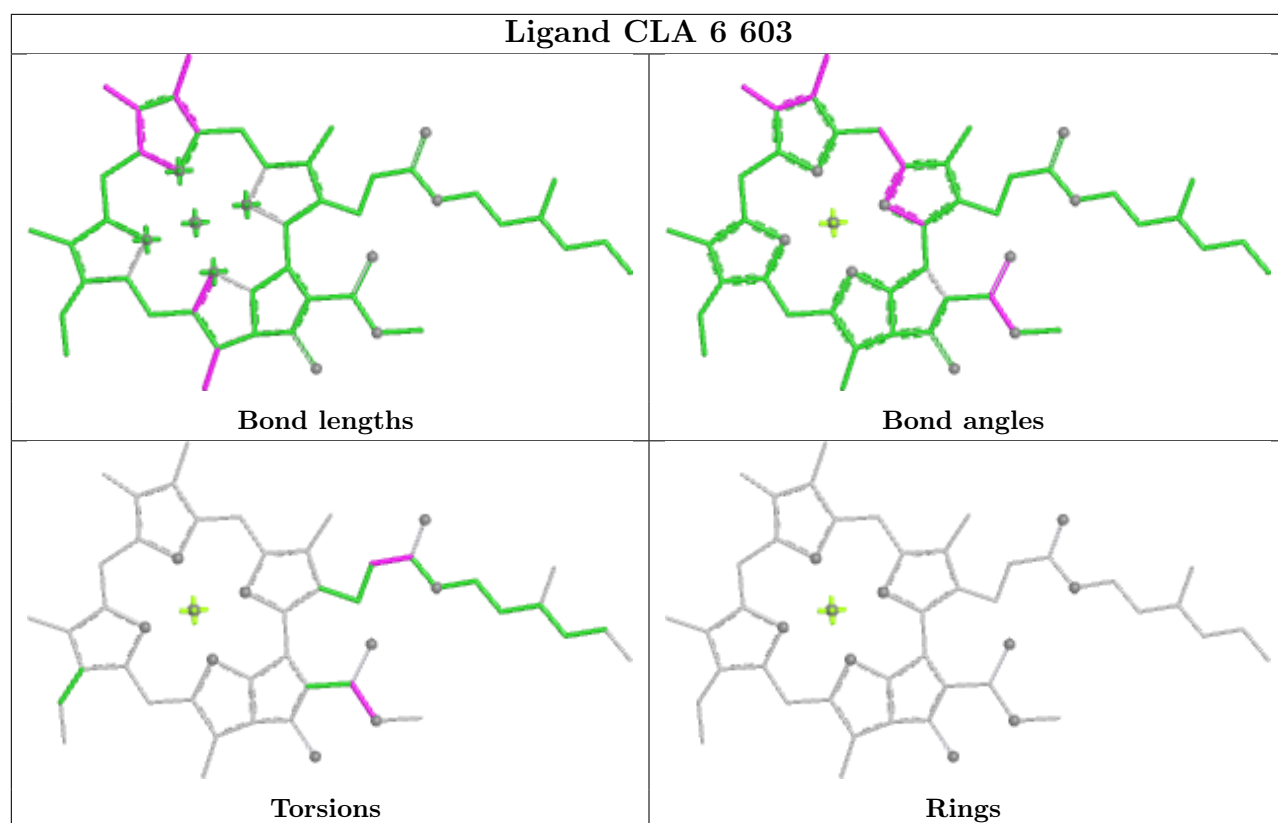
Ligand CLA 8 610

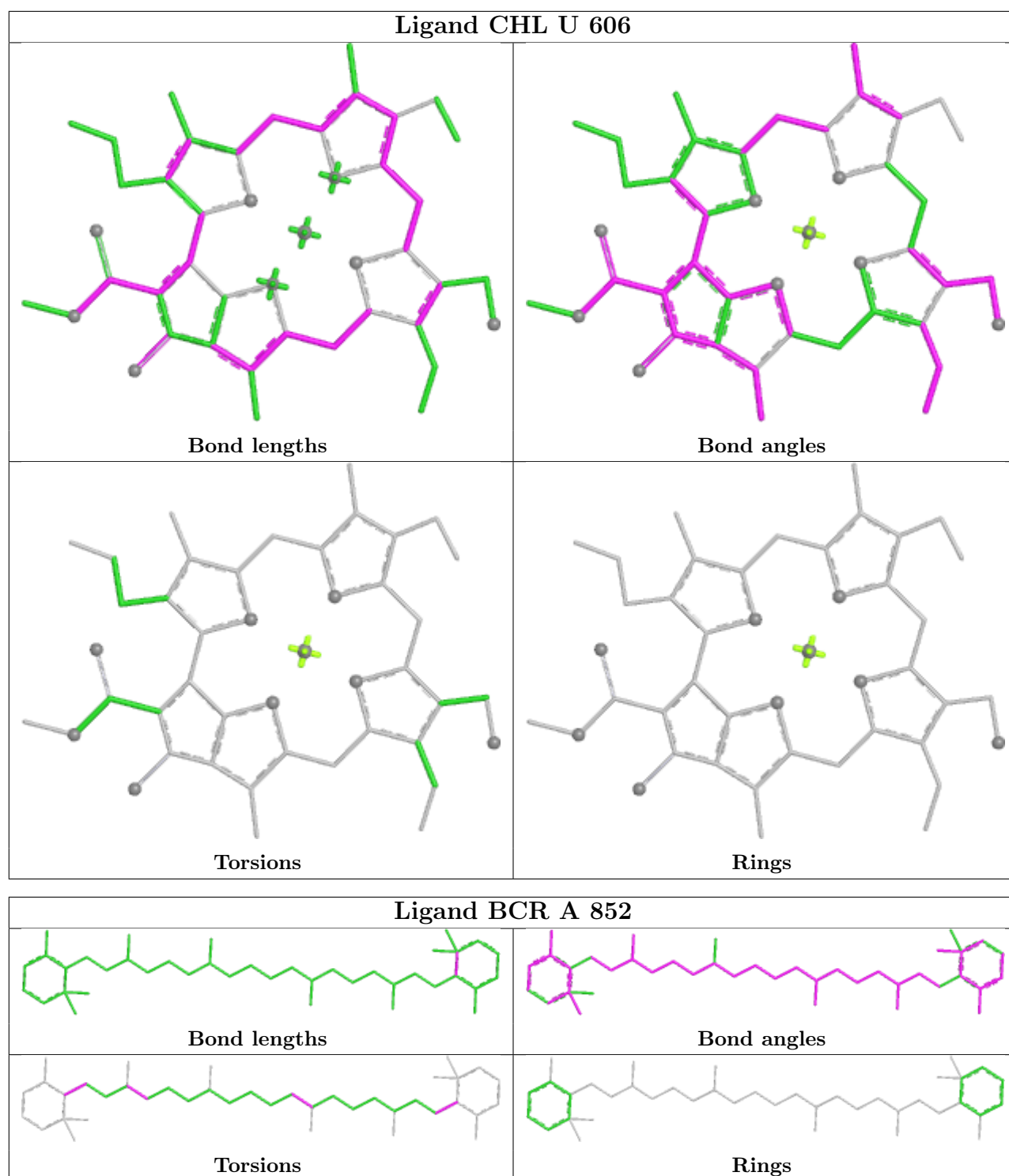


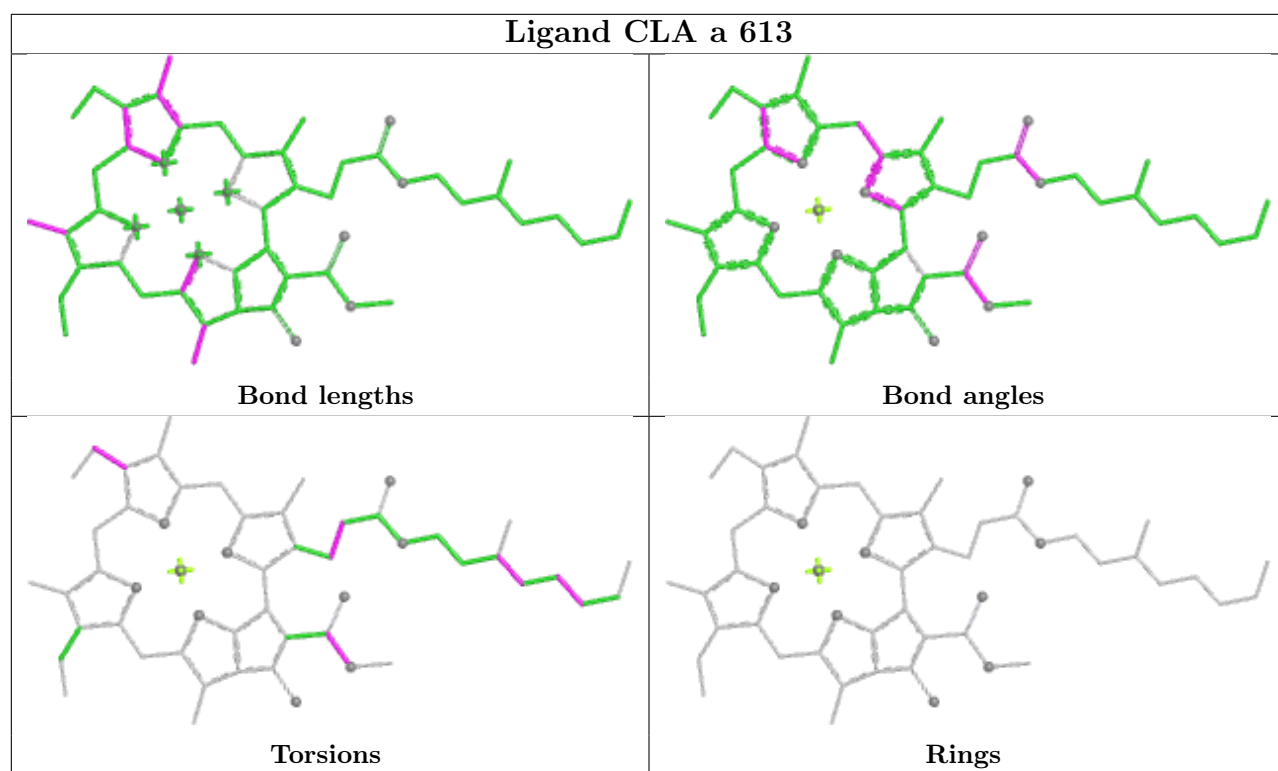
Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL W 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

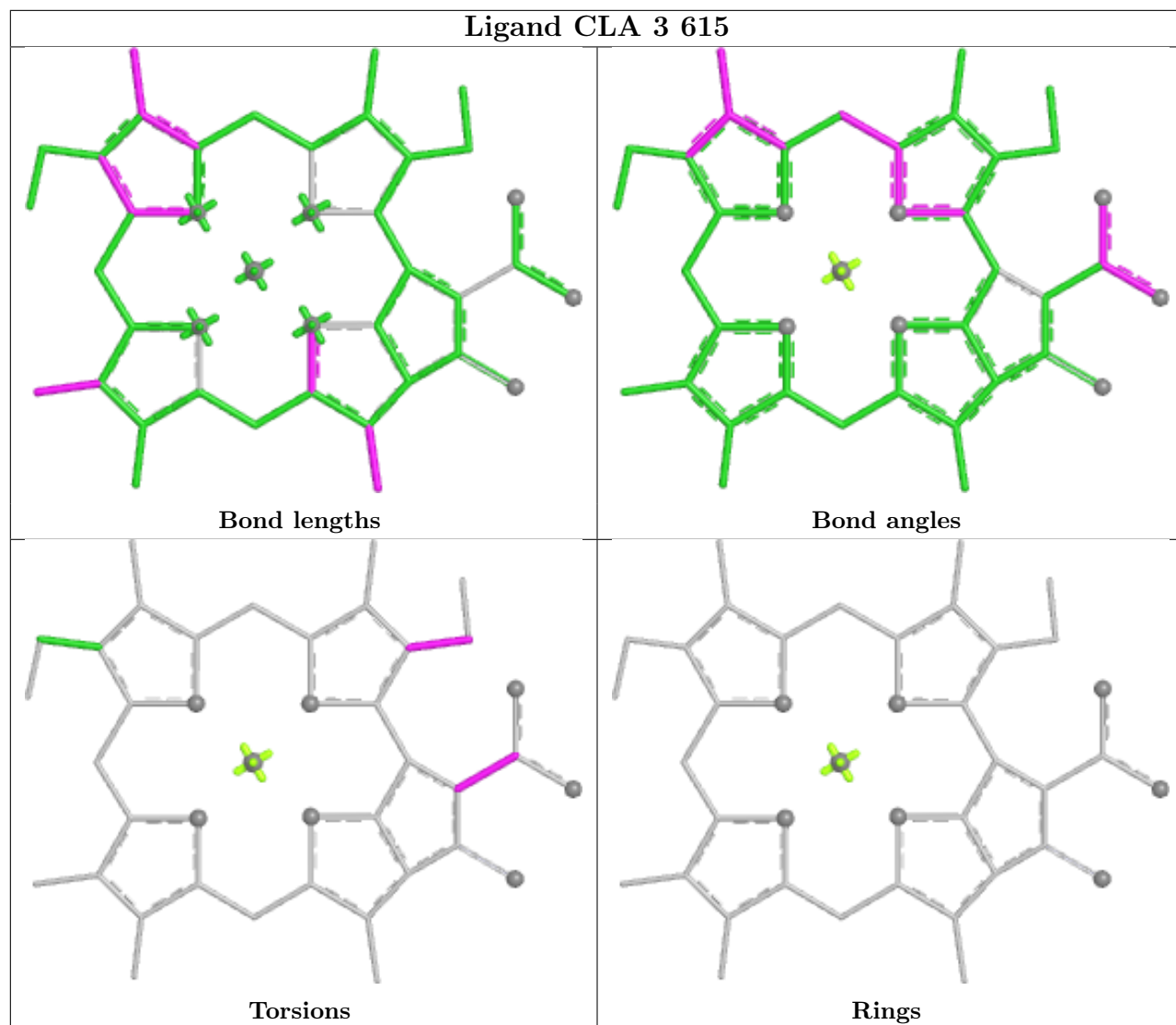
Ligand LUT 6 619	
	
Bond lengths	Bond angles
	
Torsions	Rings



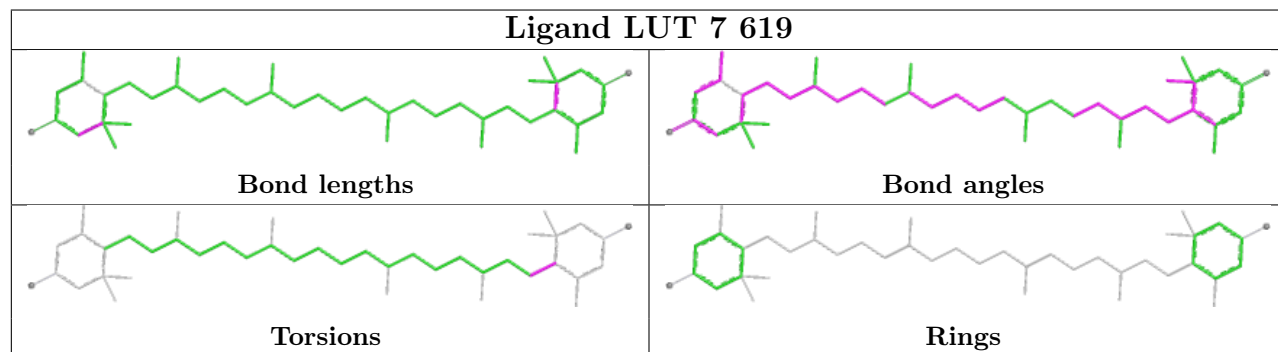




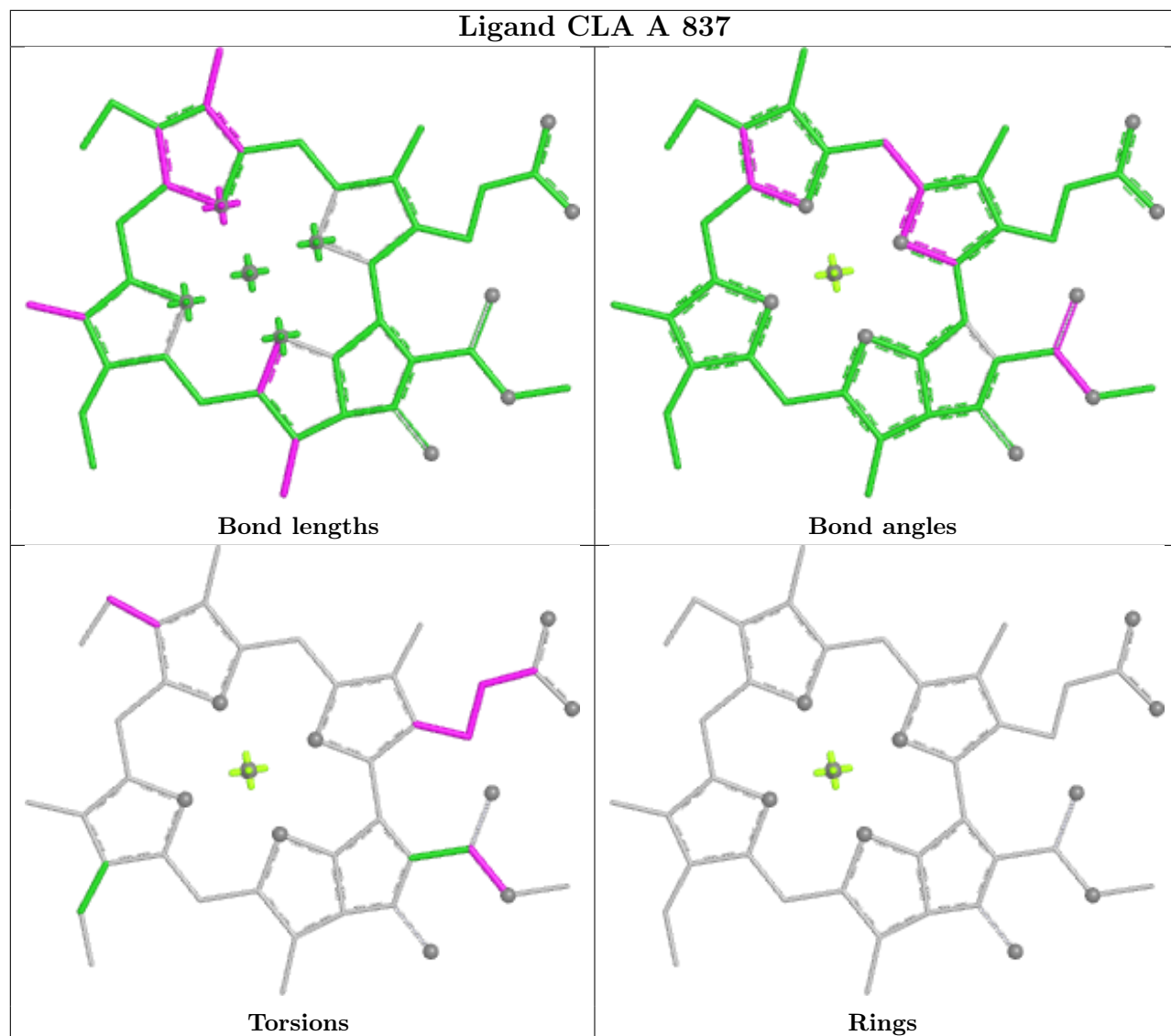
Ligand CLA 3 615



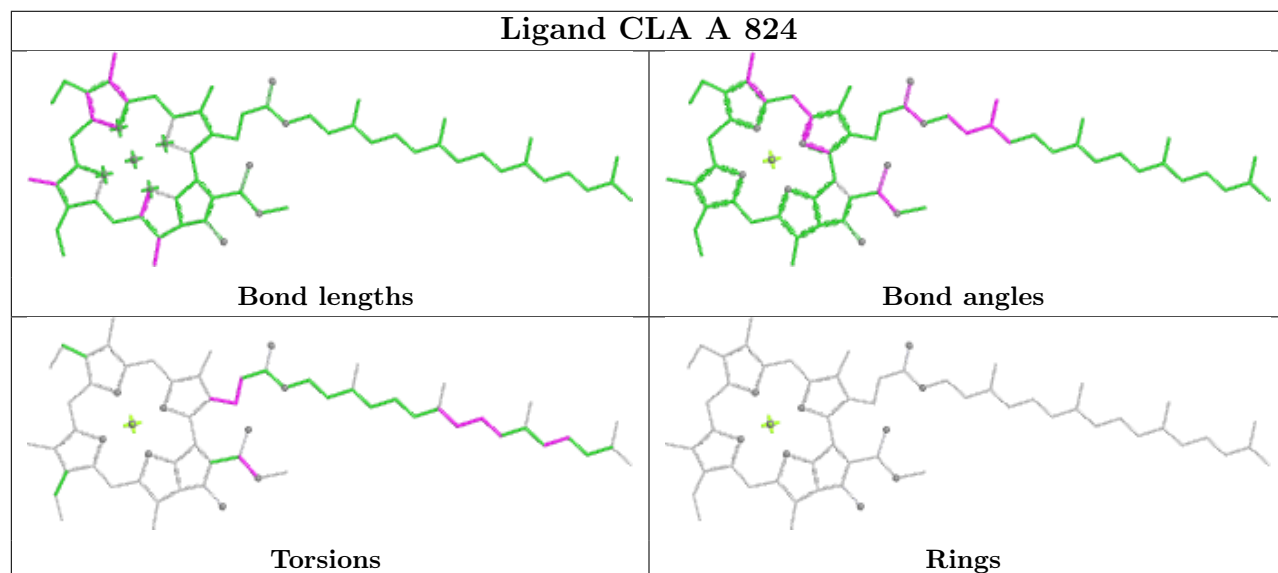
Ligand LUT 7 619

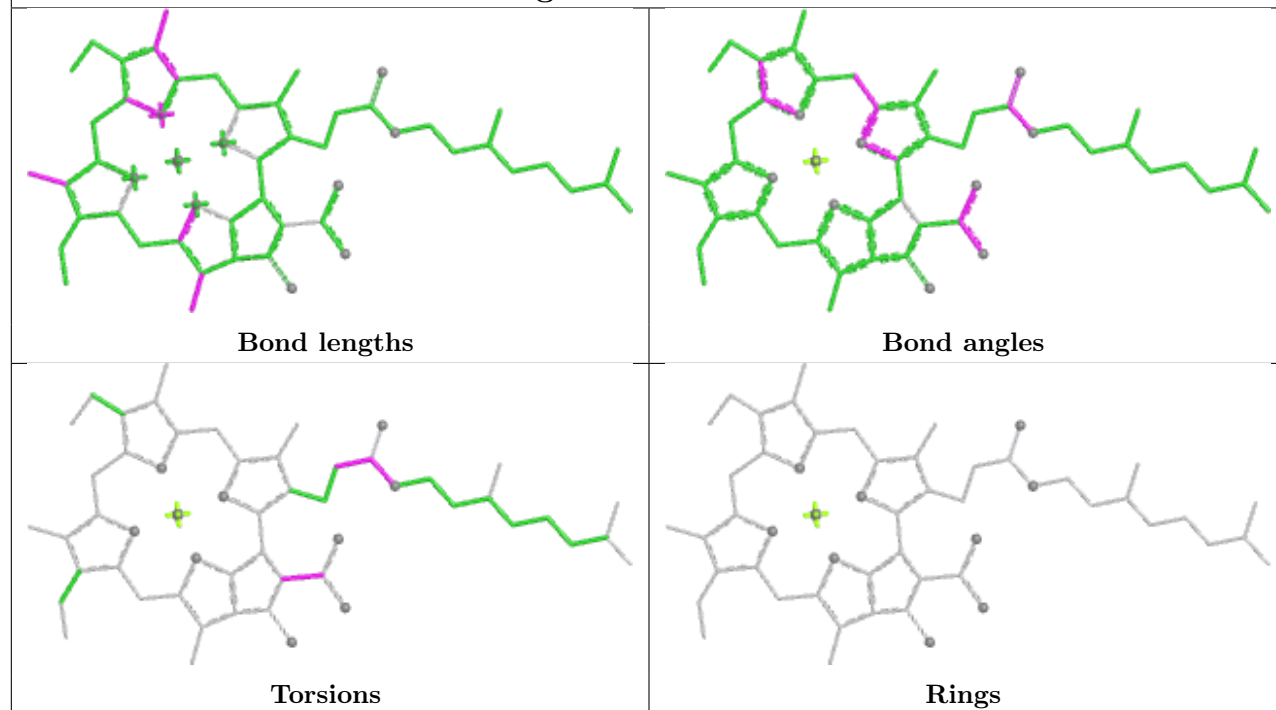
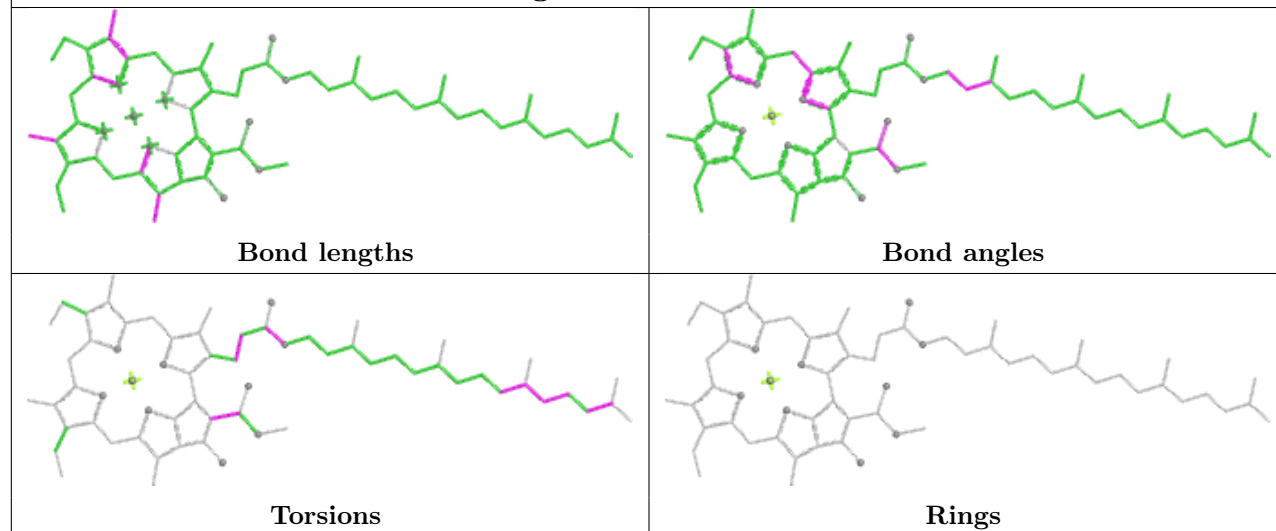


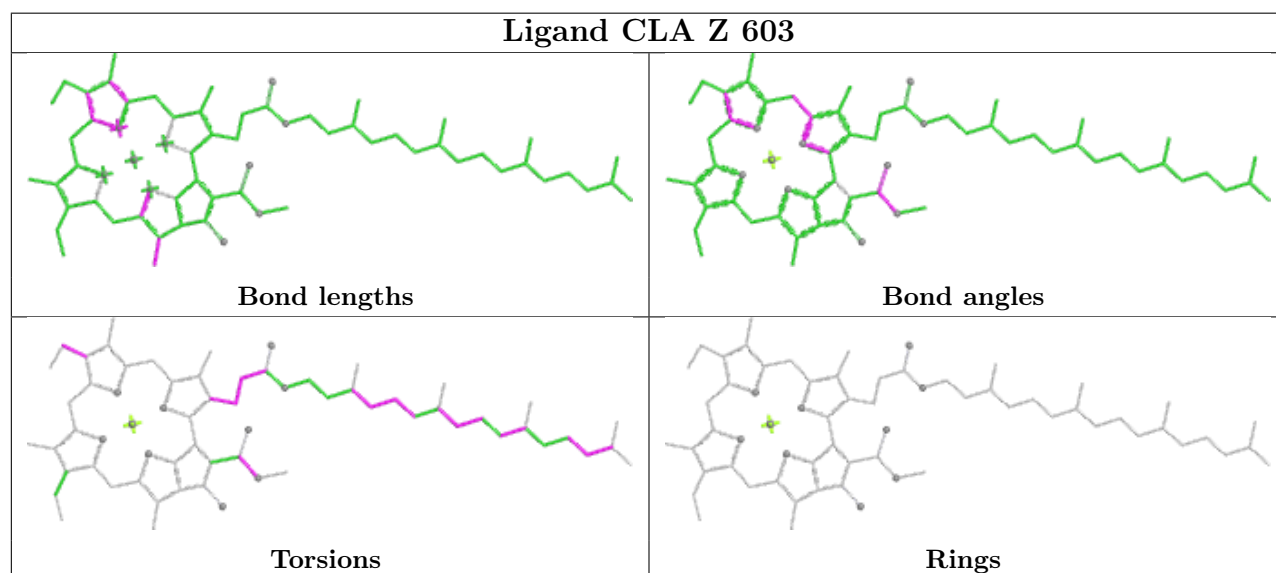
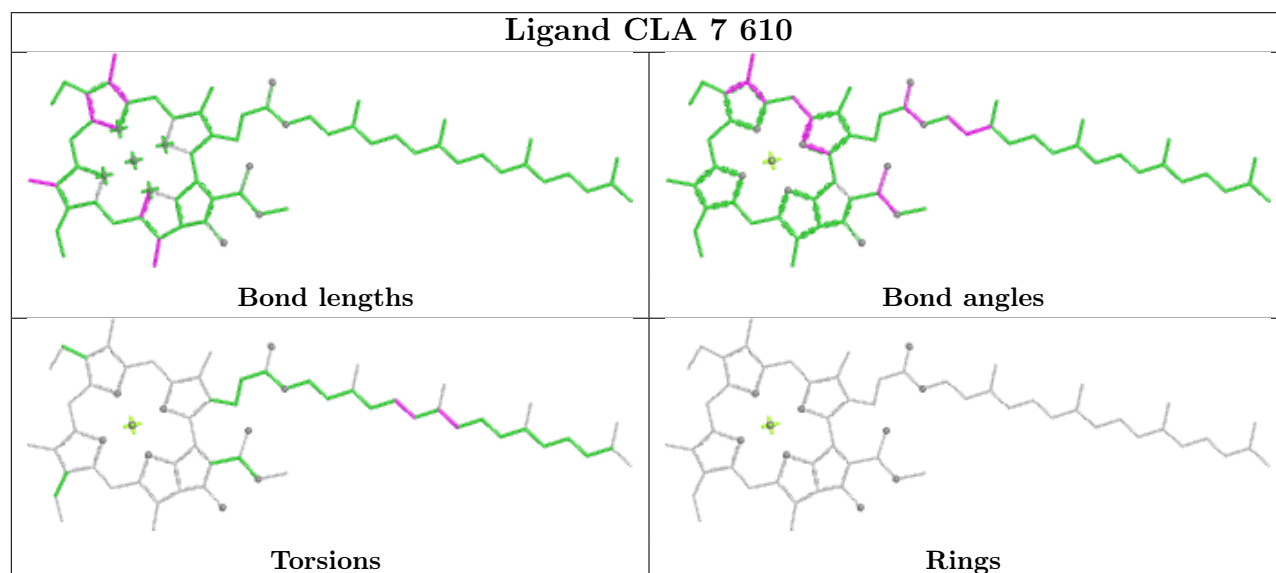
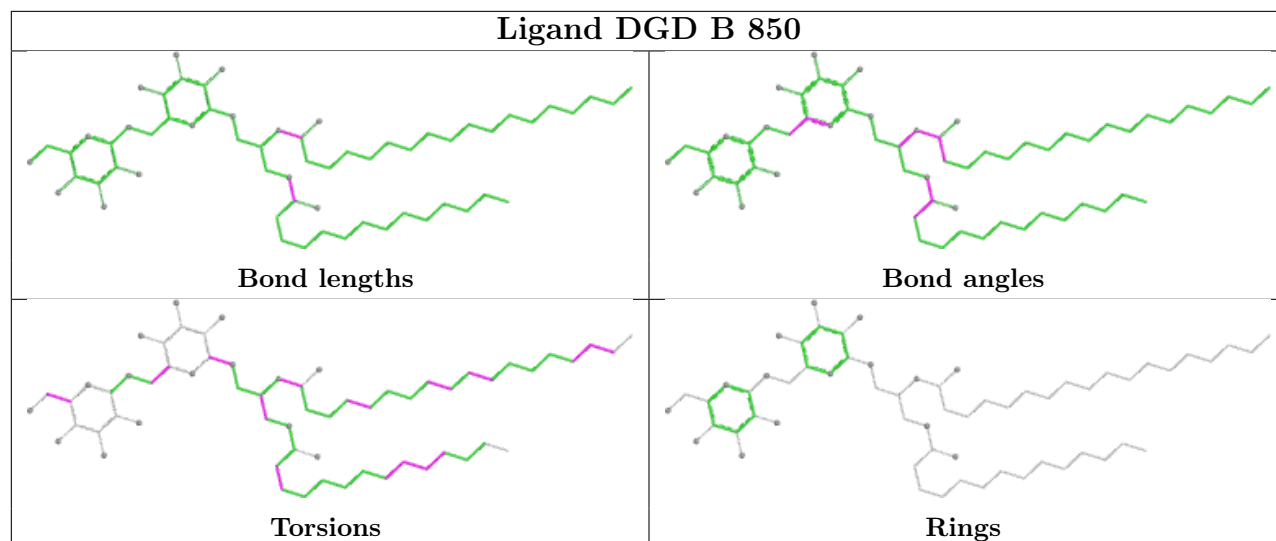
Ligand CLA A 837

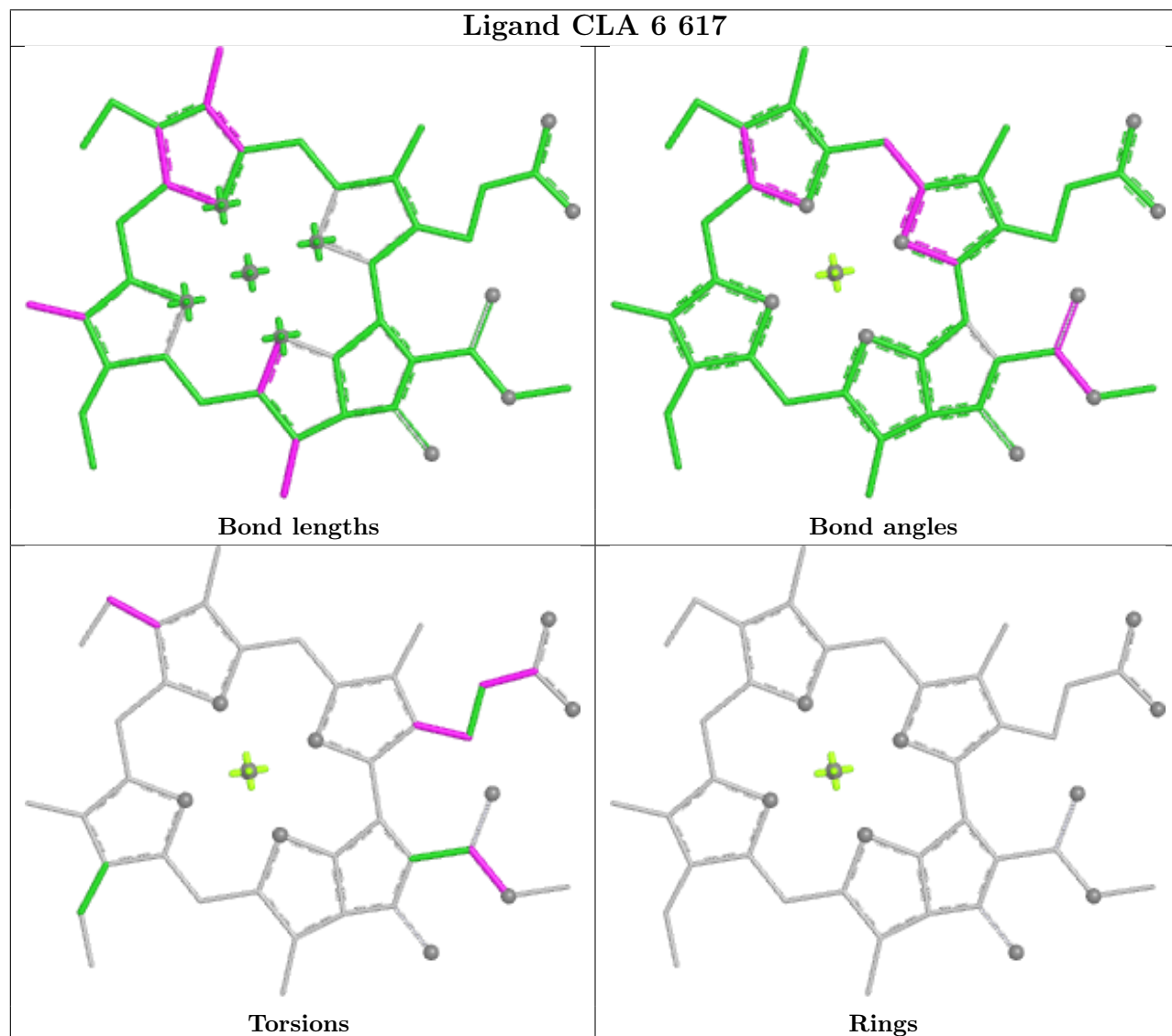
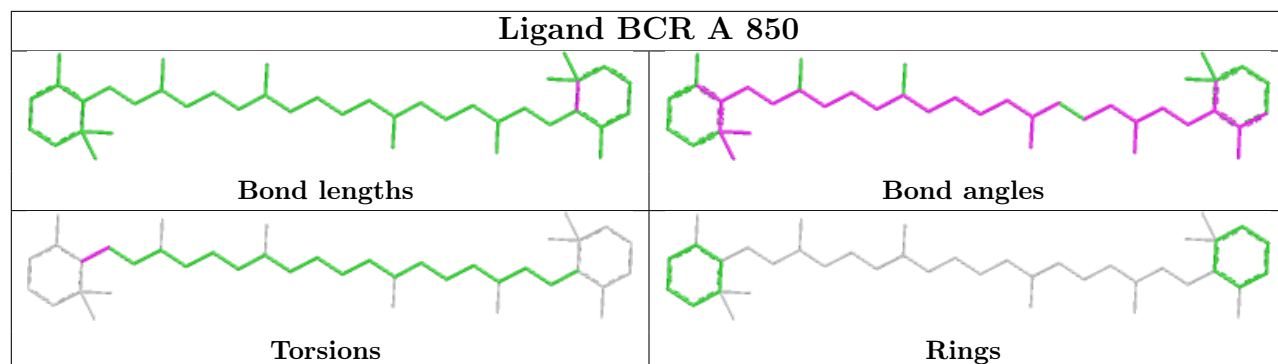


Ligand CLA A 824

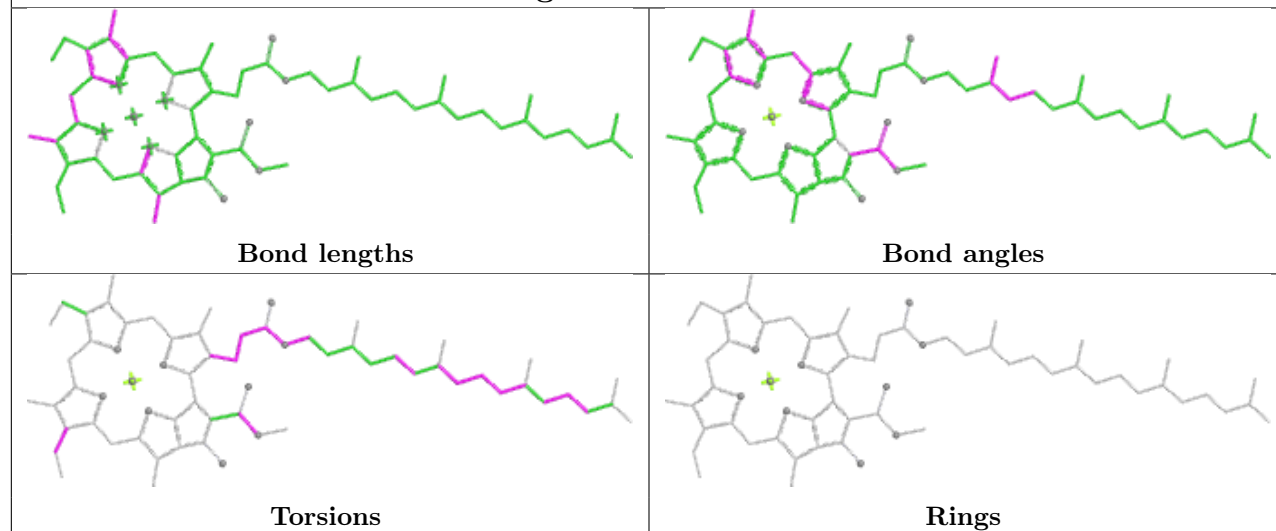


Ligand CLA 3 606**Ligand CLA A 809**

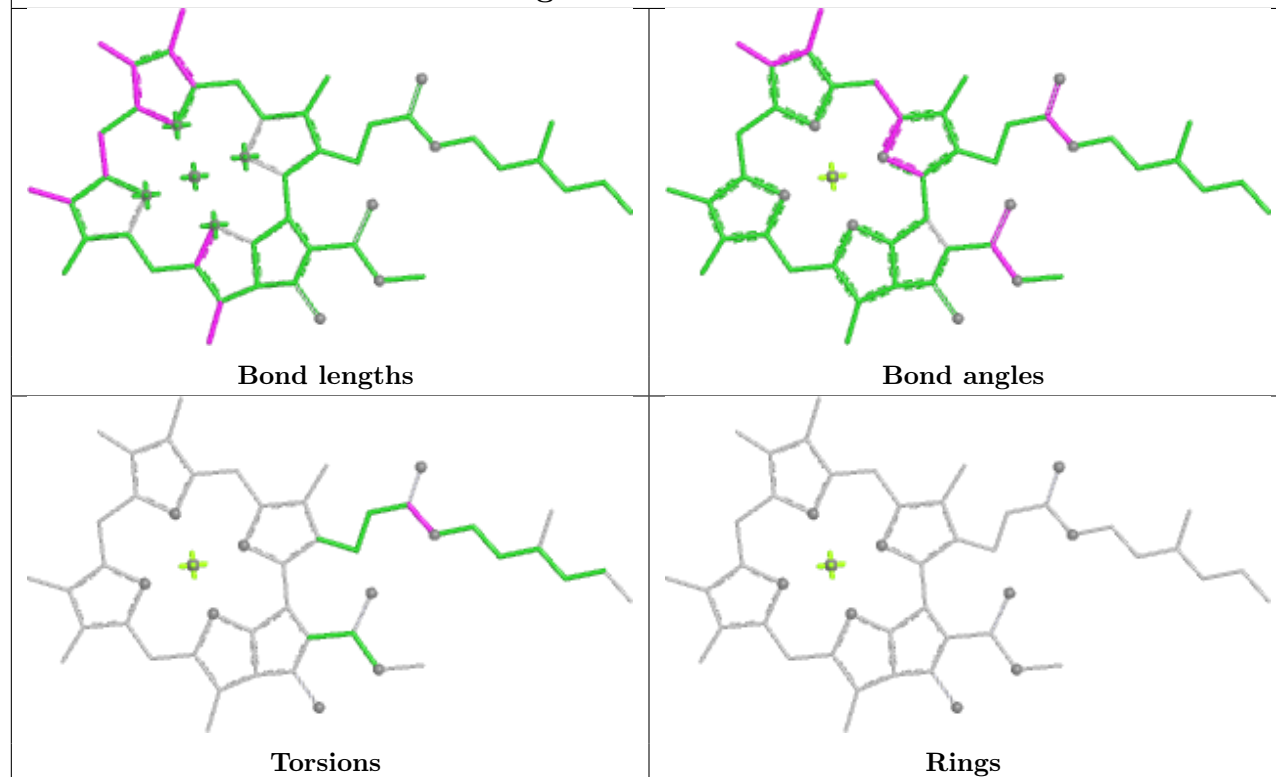




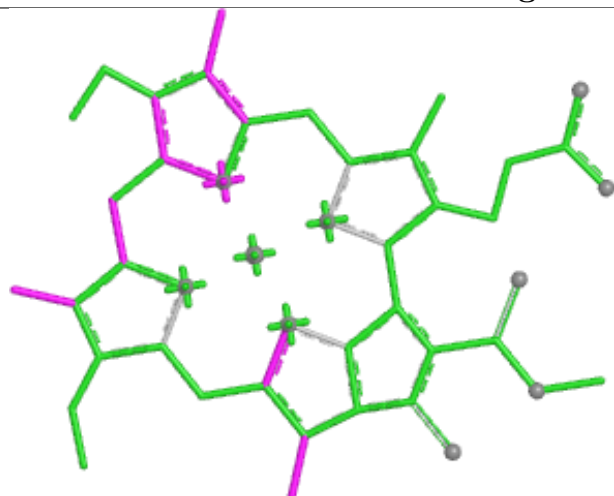
Ligand CLA 6 616



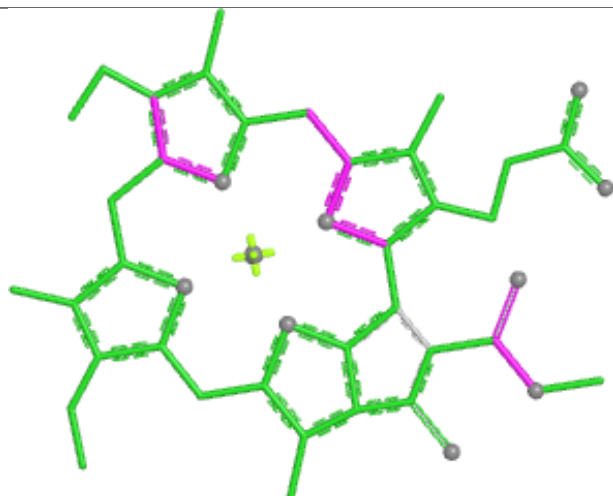
Ligand CLA 9 604



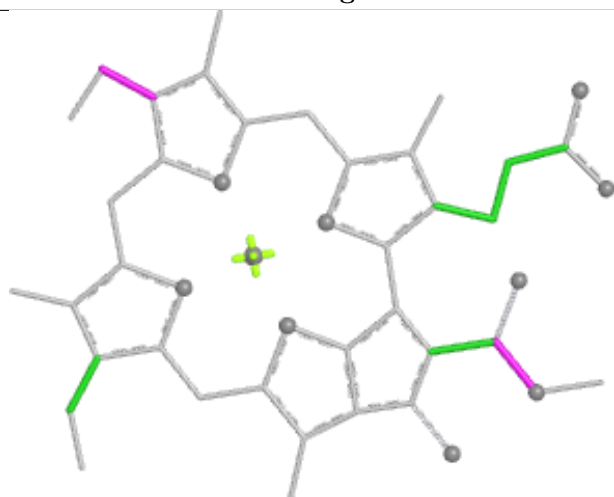
Ligand CLA 2 607



Bond lengths



Bond angles

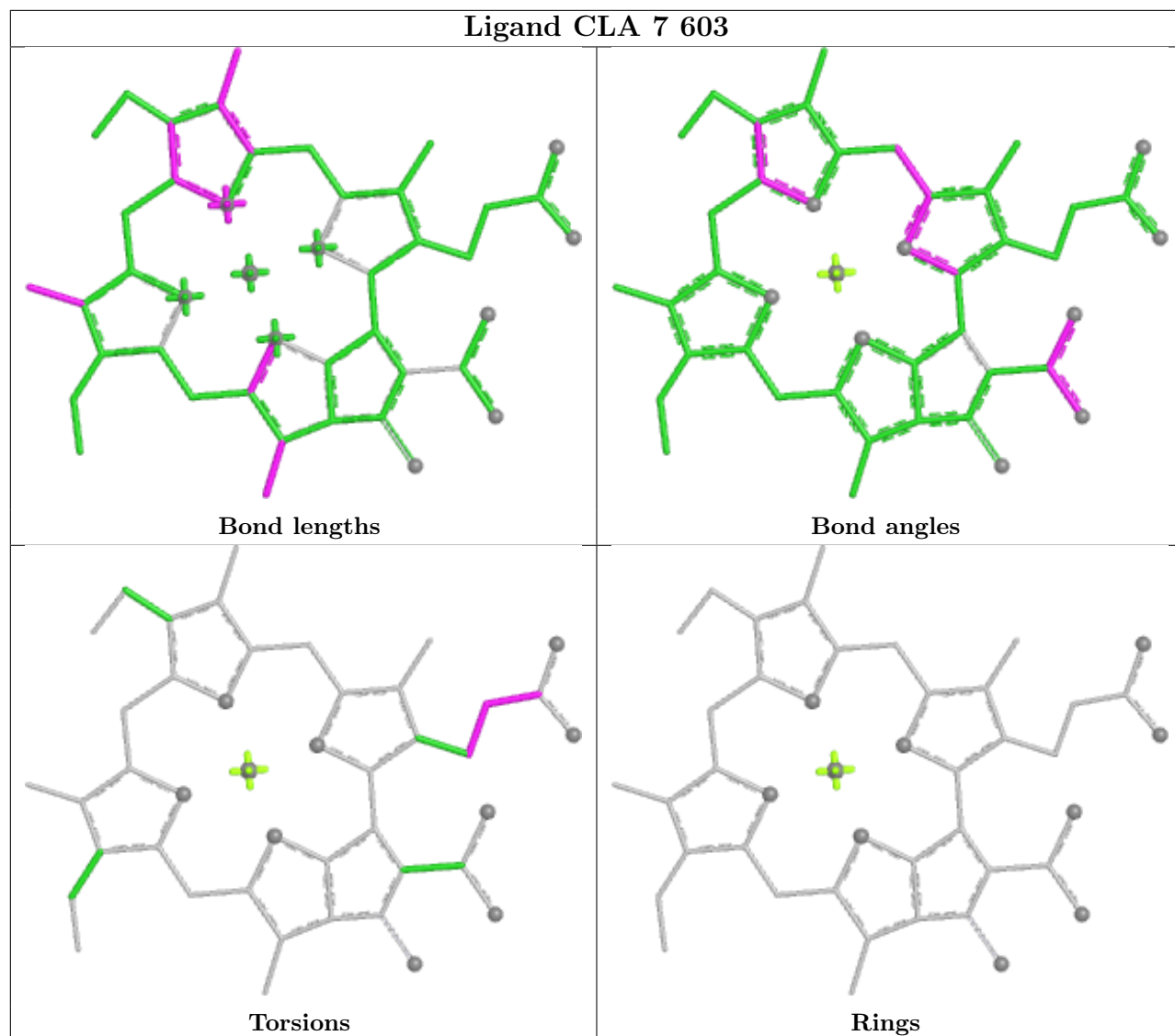


Torsions

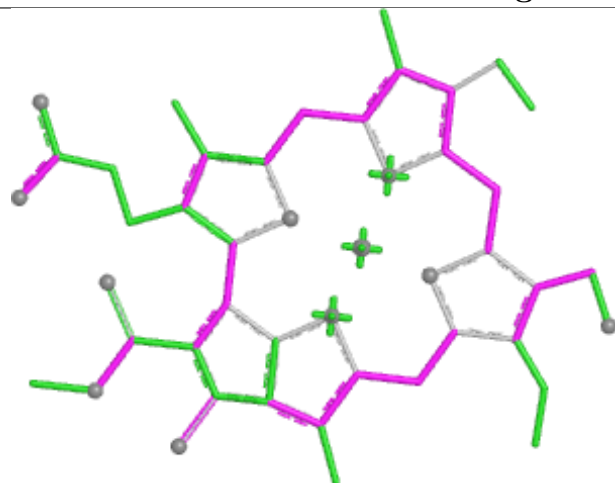


Rings

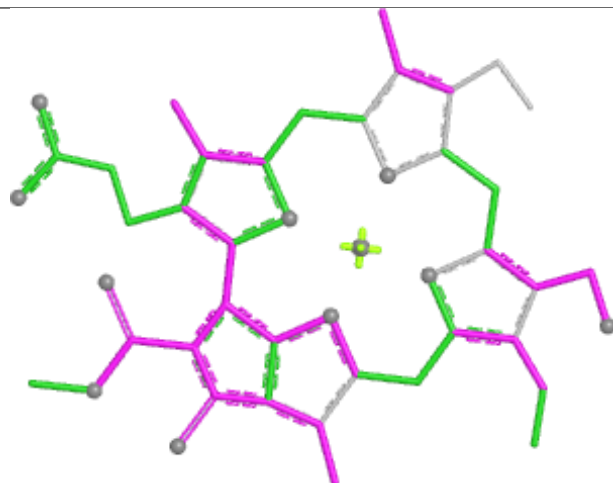
Ligand CLA 7 603



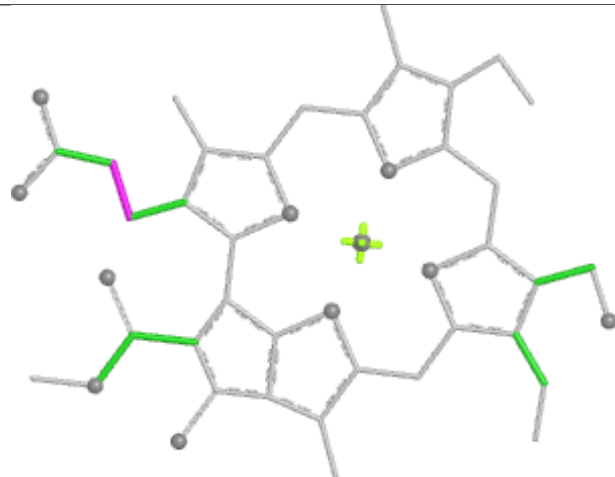
Ligand CHL X 605



Bond lengths



Bond angles

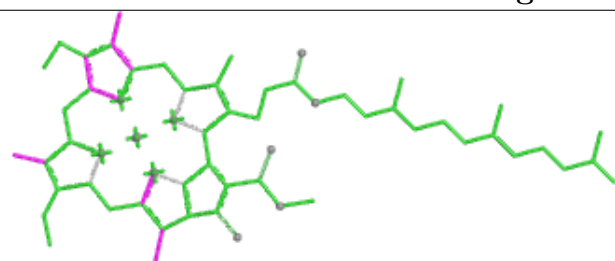


Torsions

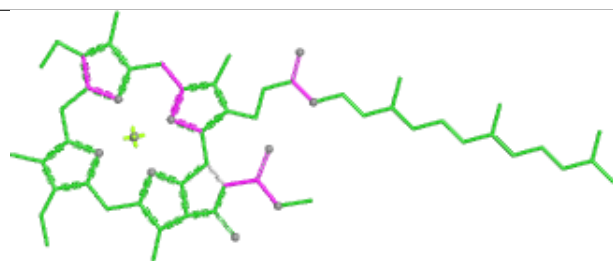


Rings

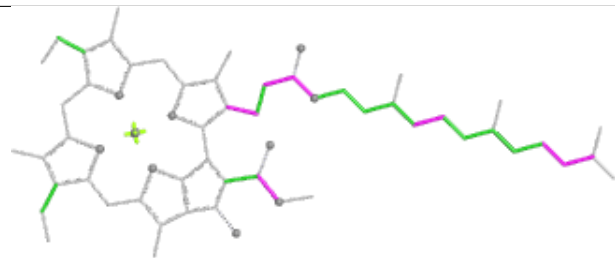
Ligand CLA B 832



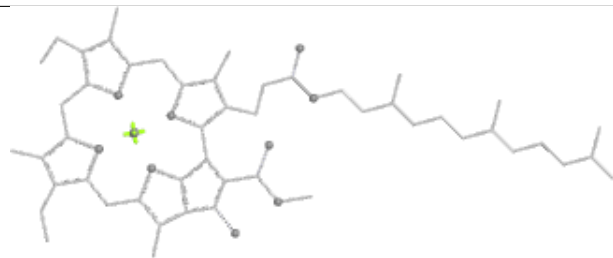
Bond lengths



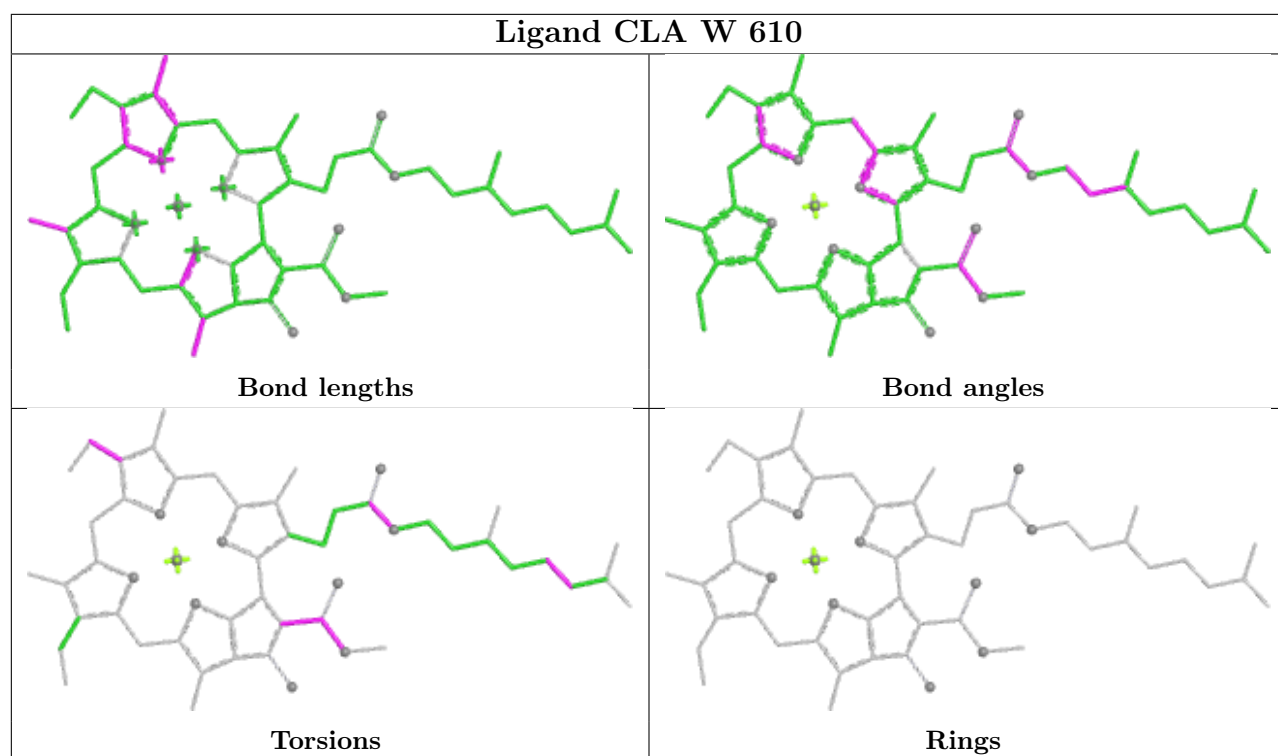
Bond angles

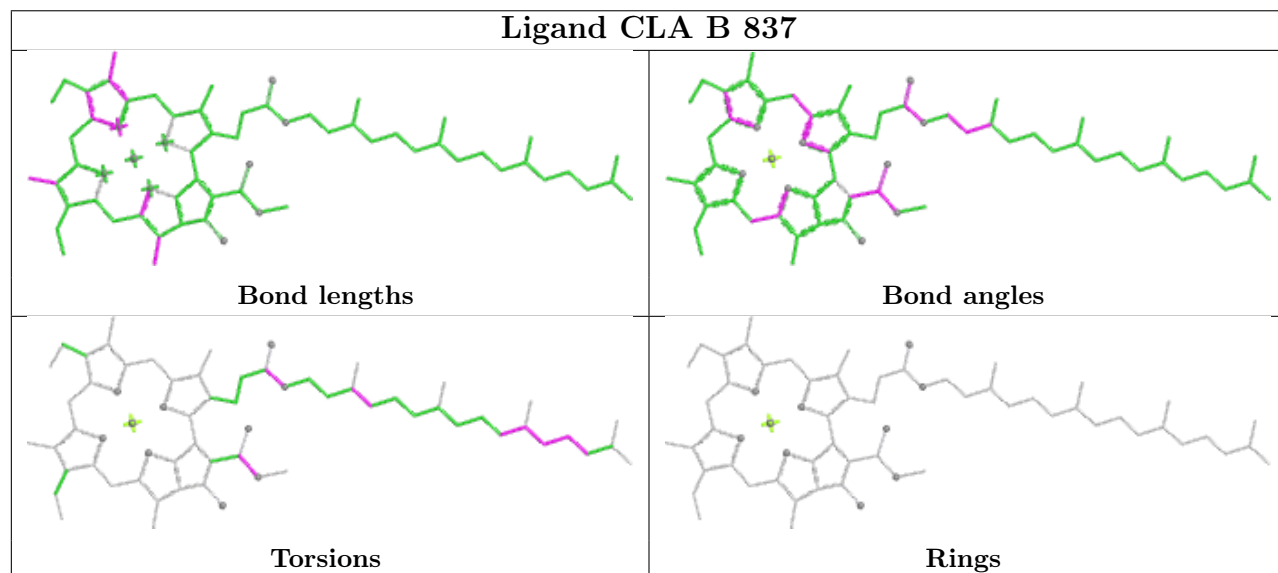
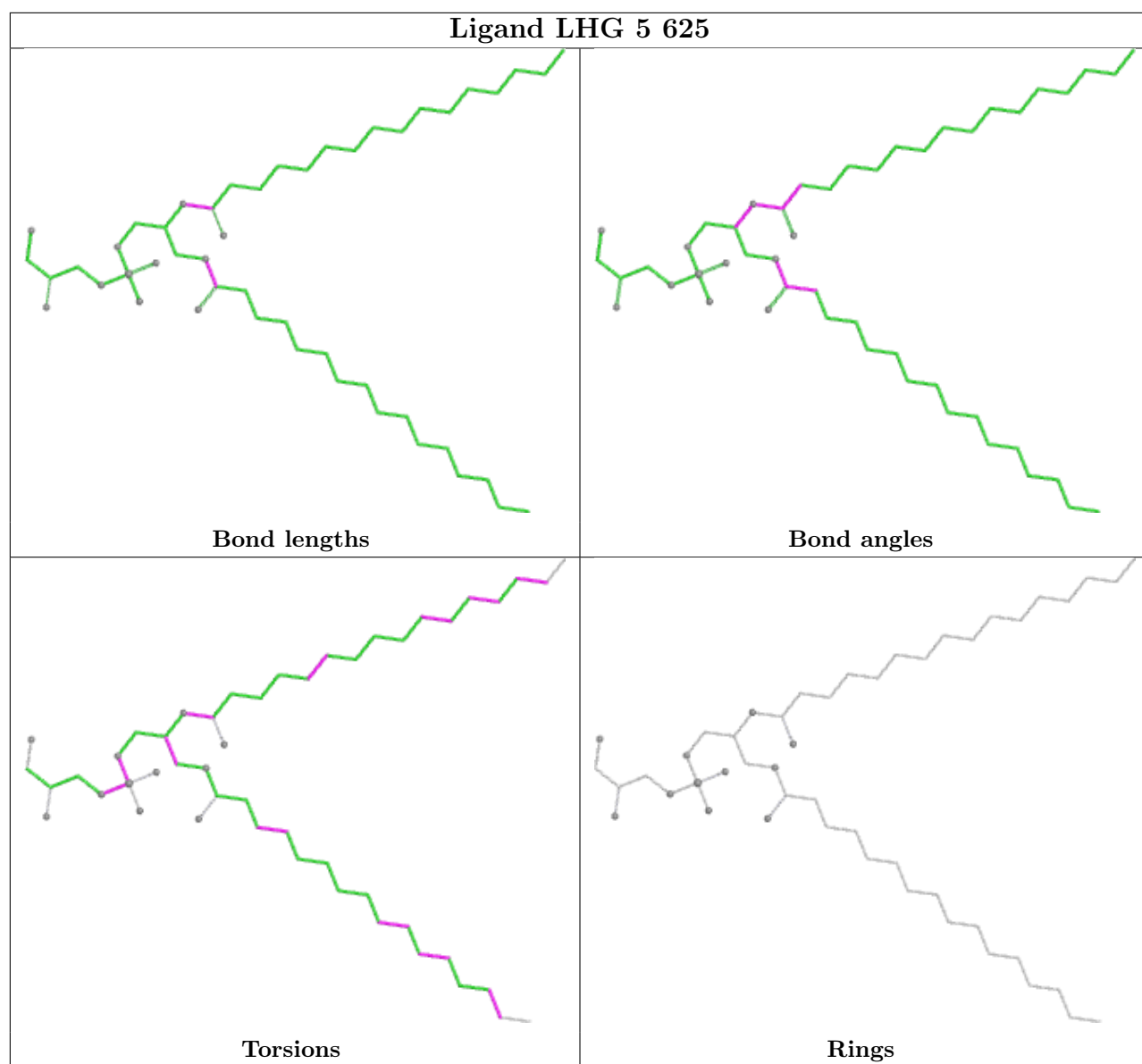


Torsions

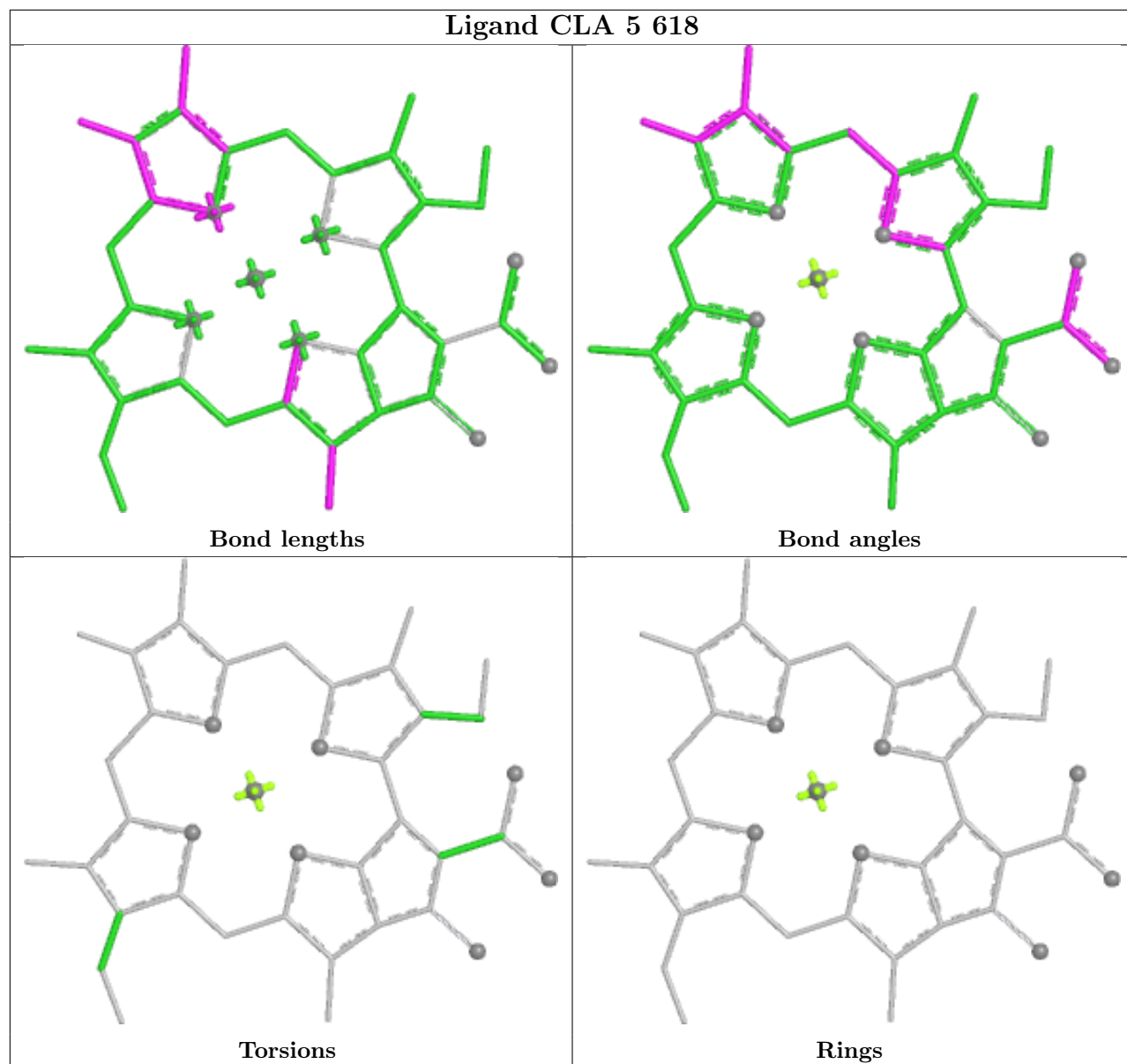


Rings

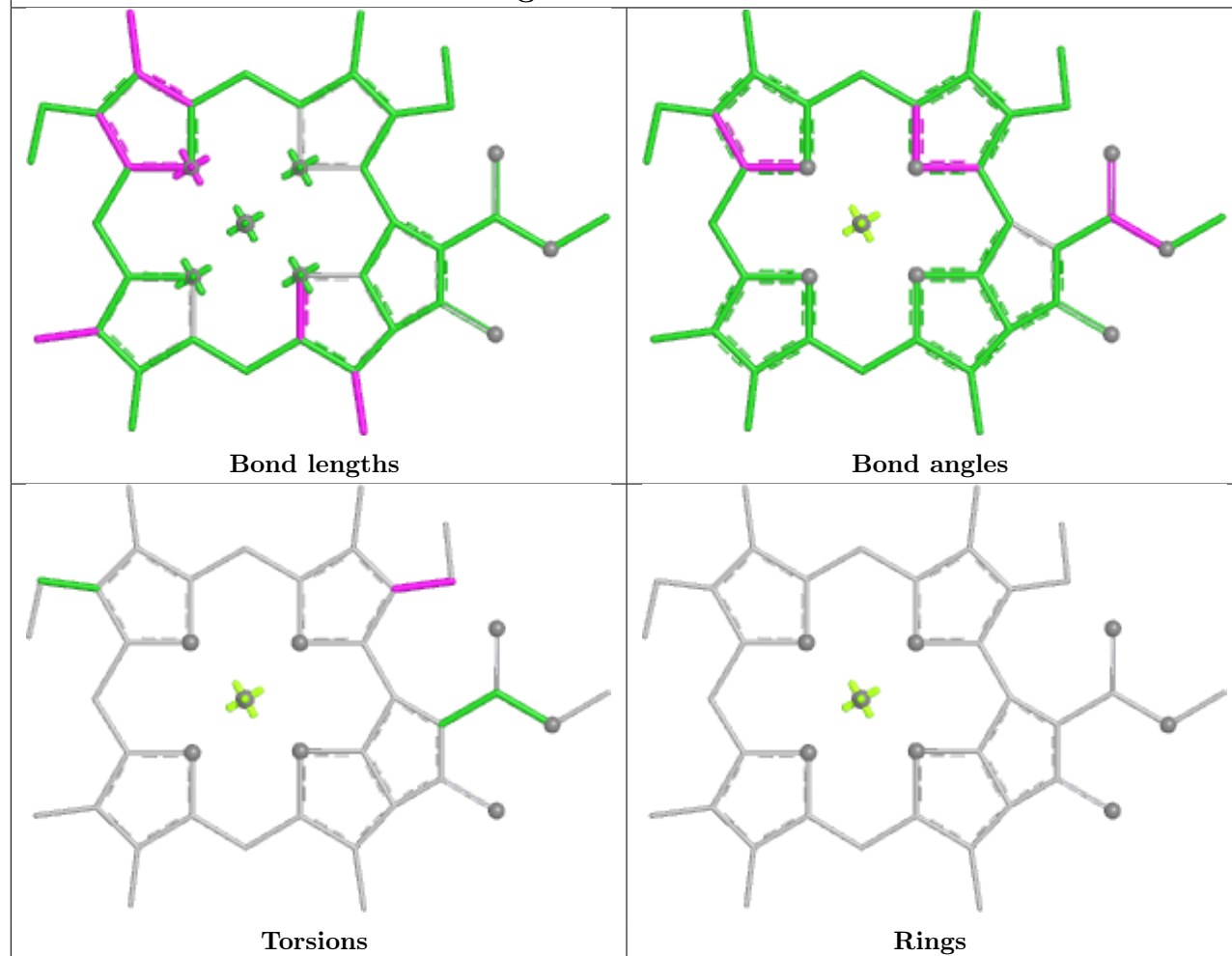




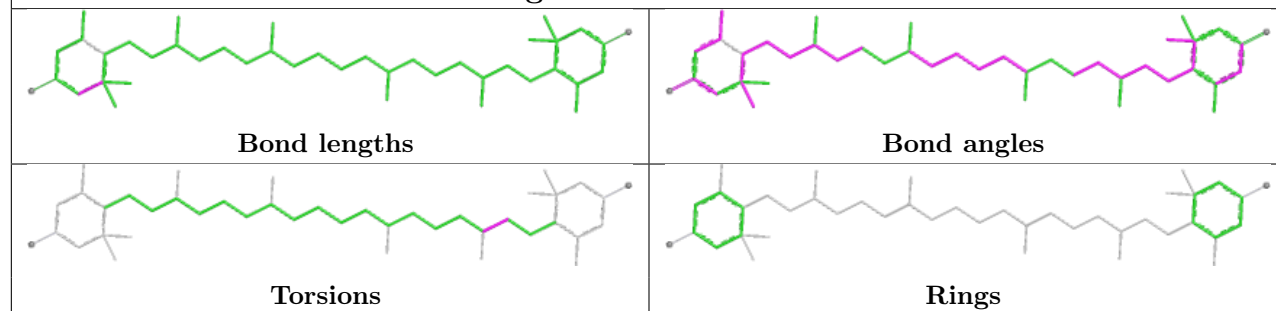
Ligand CLA 5 618

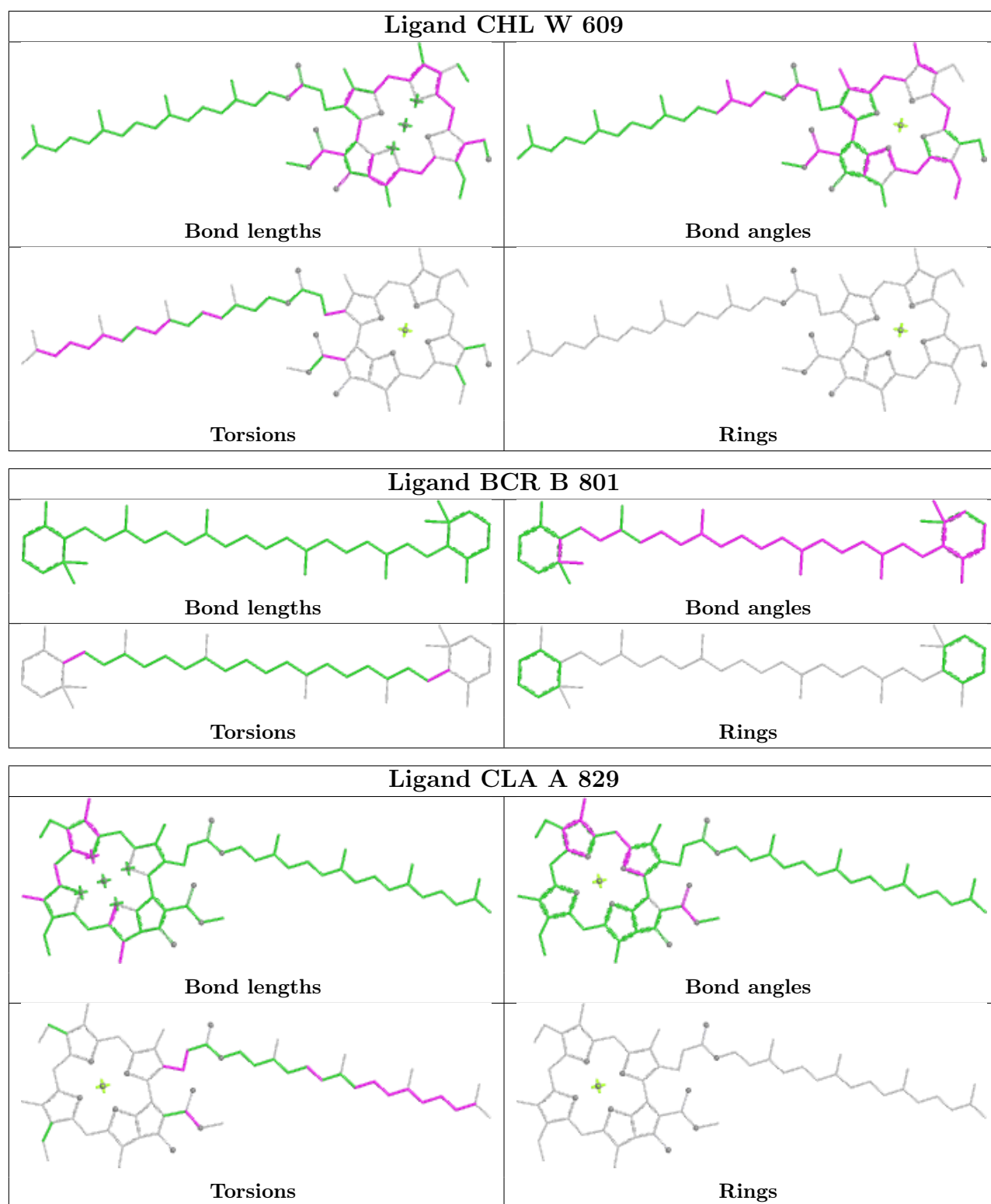


Ligand CLA 7 606

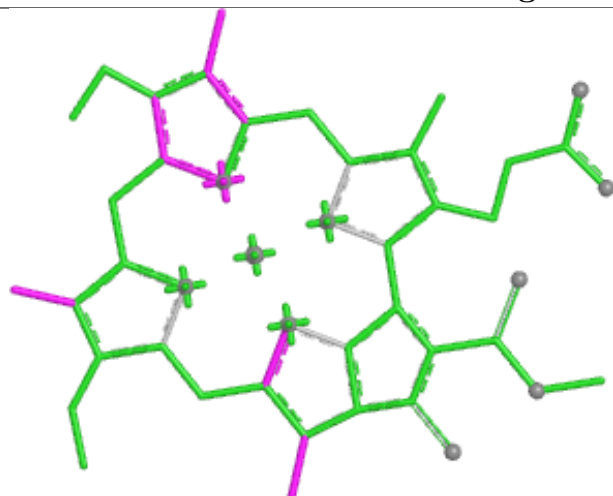


Ligand LUT Z 1621

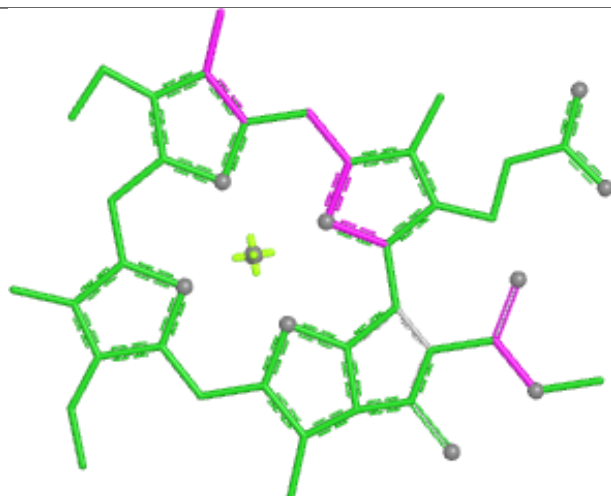




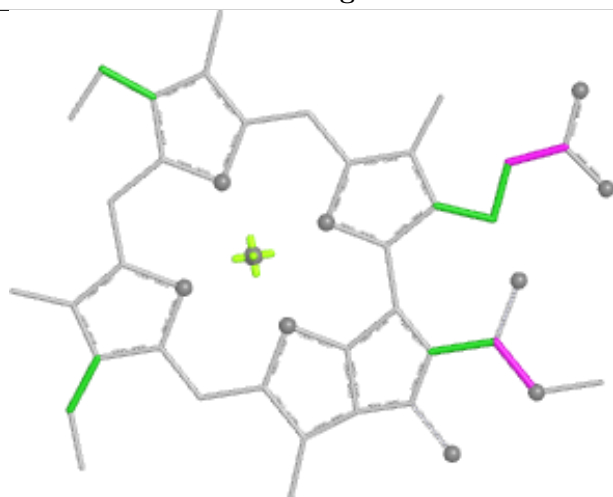
Ligand CLA 2 606



Bond lengths



Bond angles

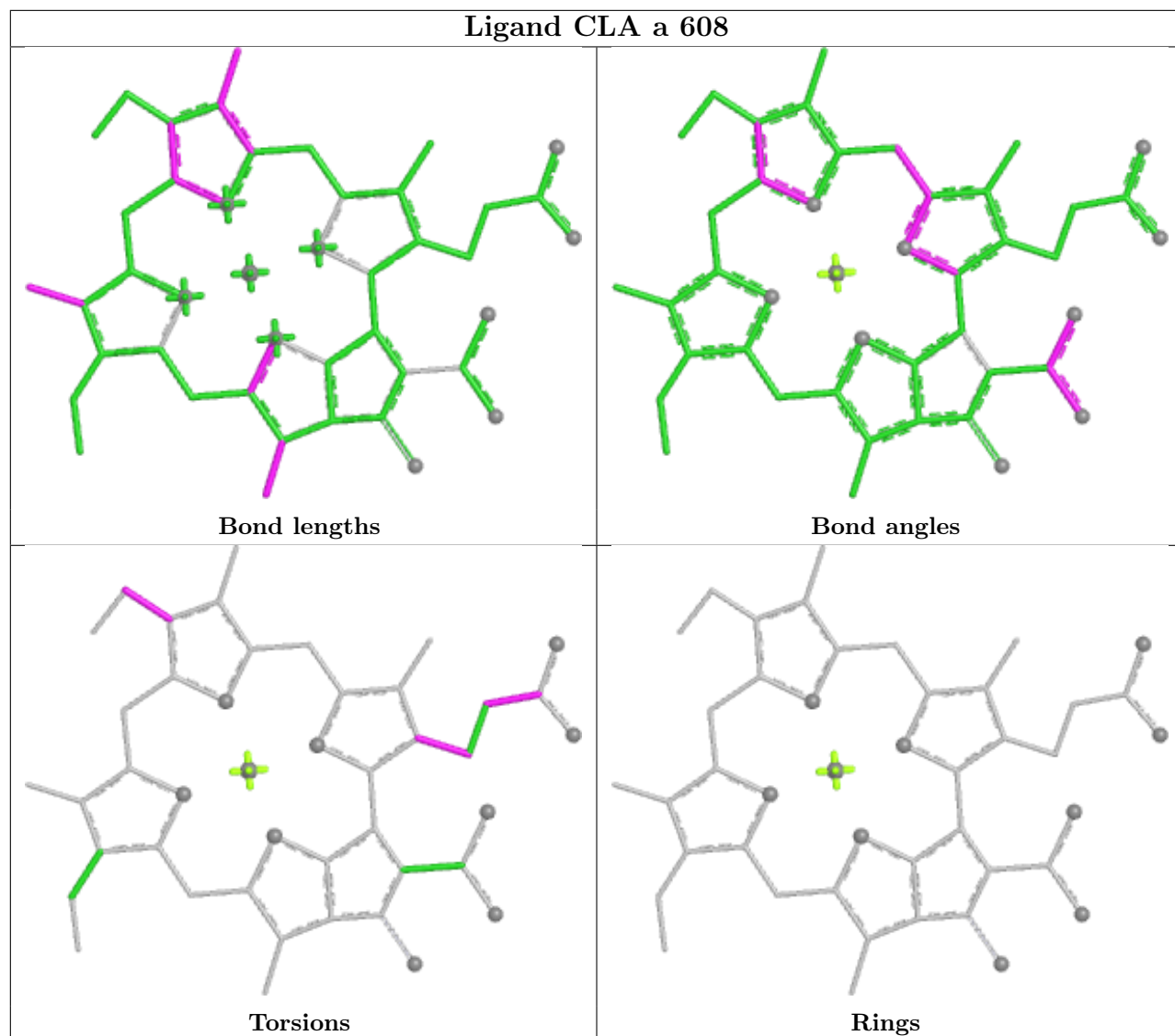


Torsions

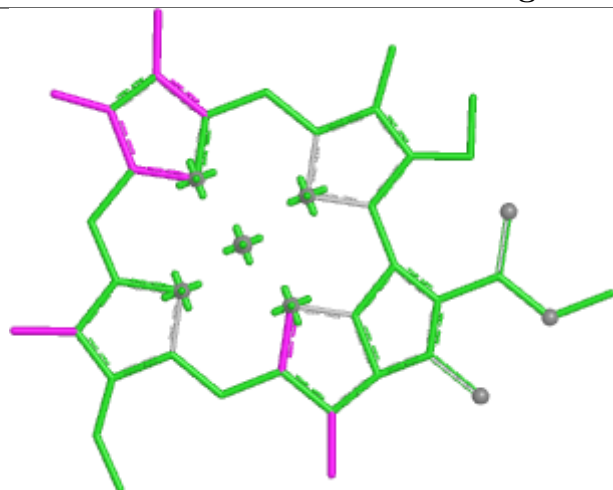


Rings

Ligand CLA a 608



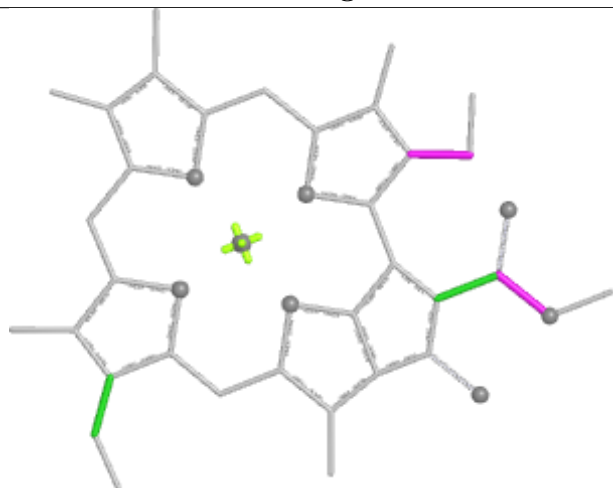
Ligand CLA 8 607



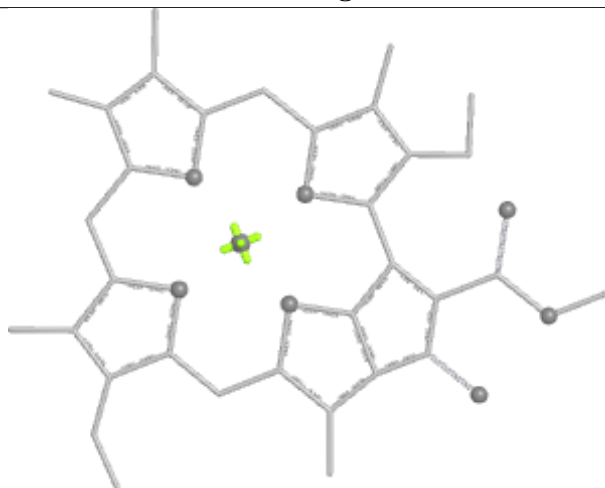
Bond lengths



Bond angles

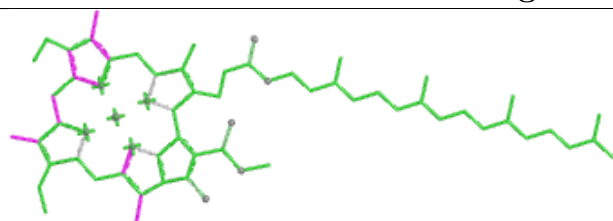


Torsions

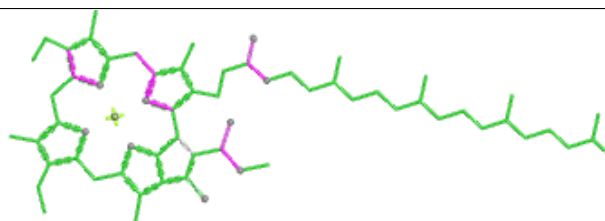


Rings

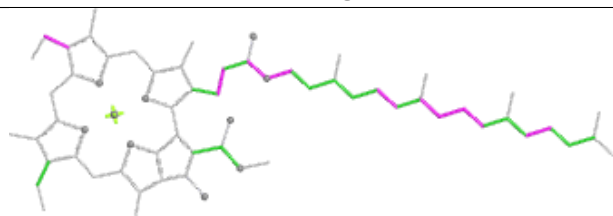
Ligand CLA 8 613



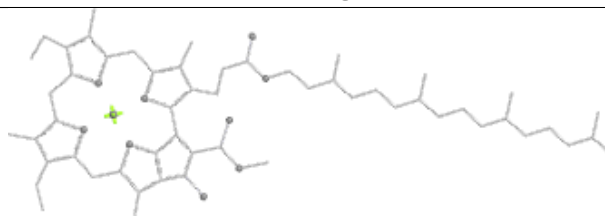
Bond lengths



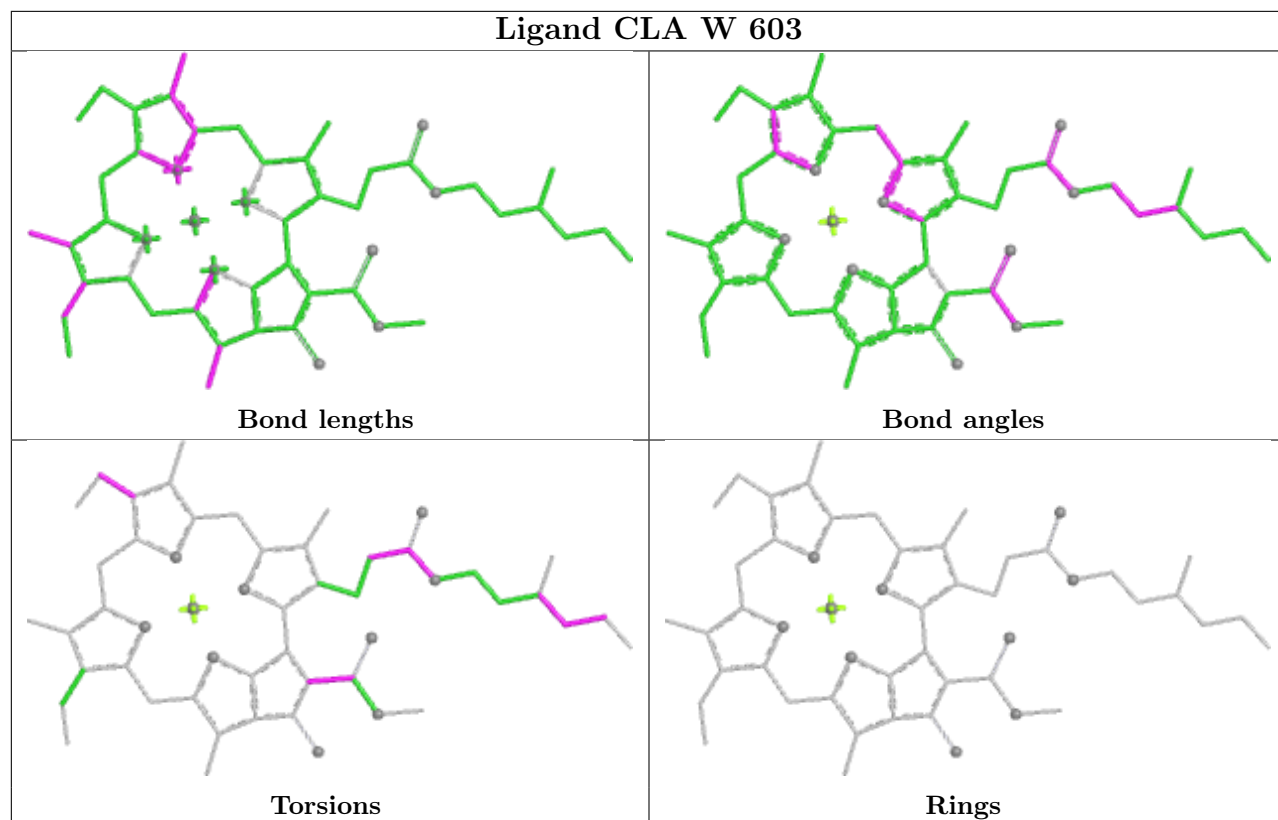
Bond angles

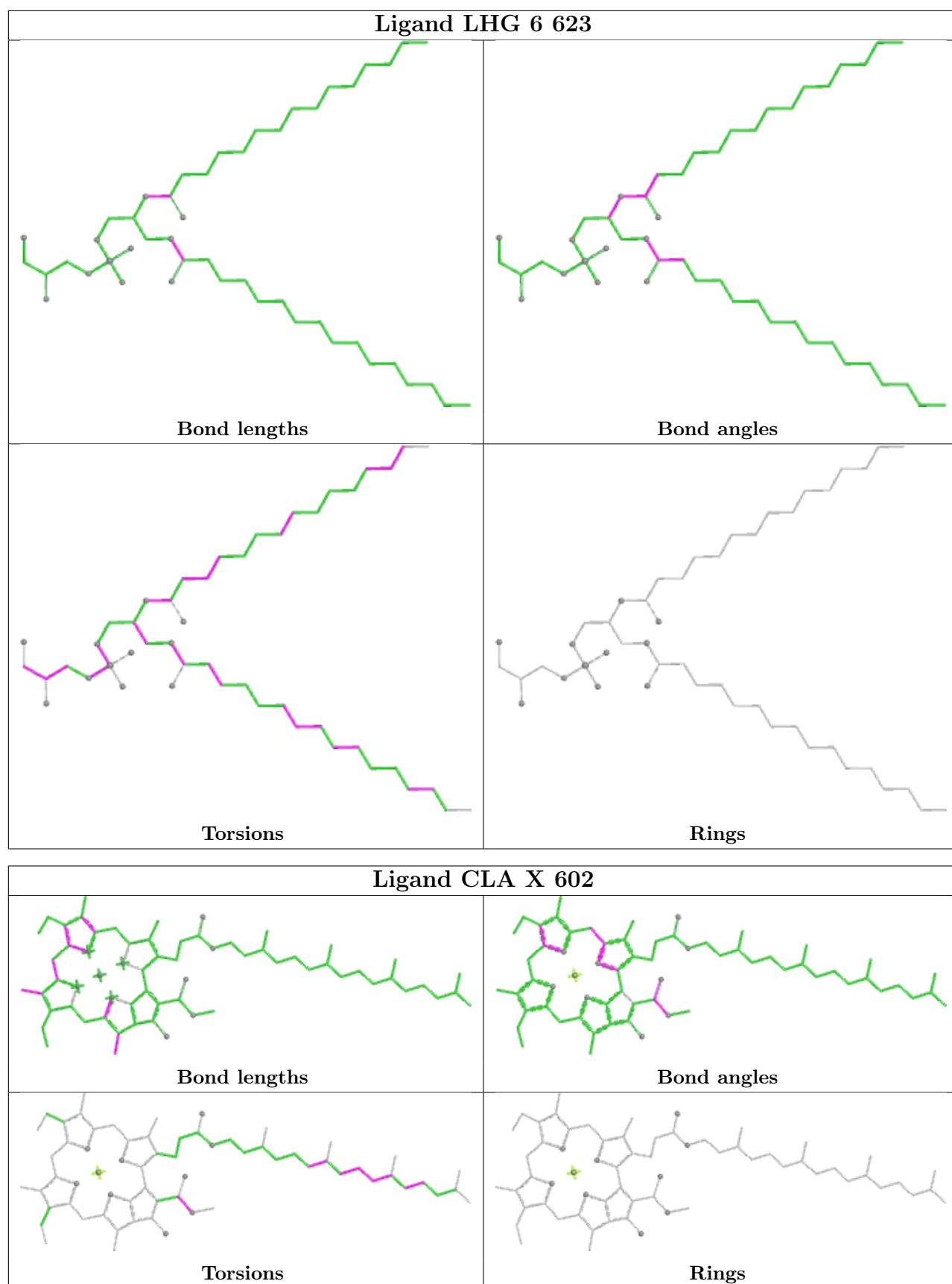


Torsions

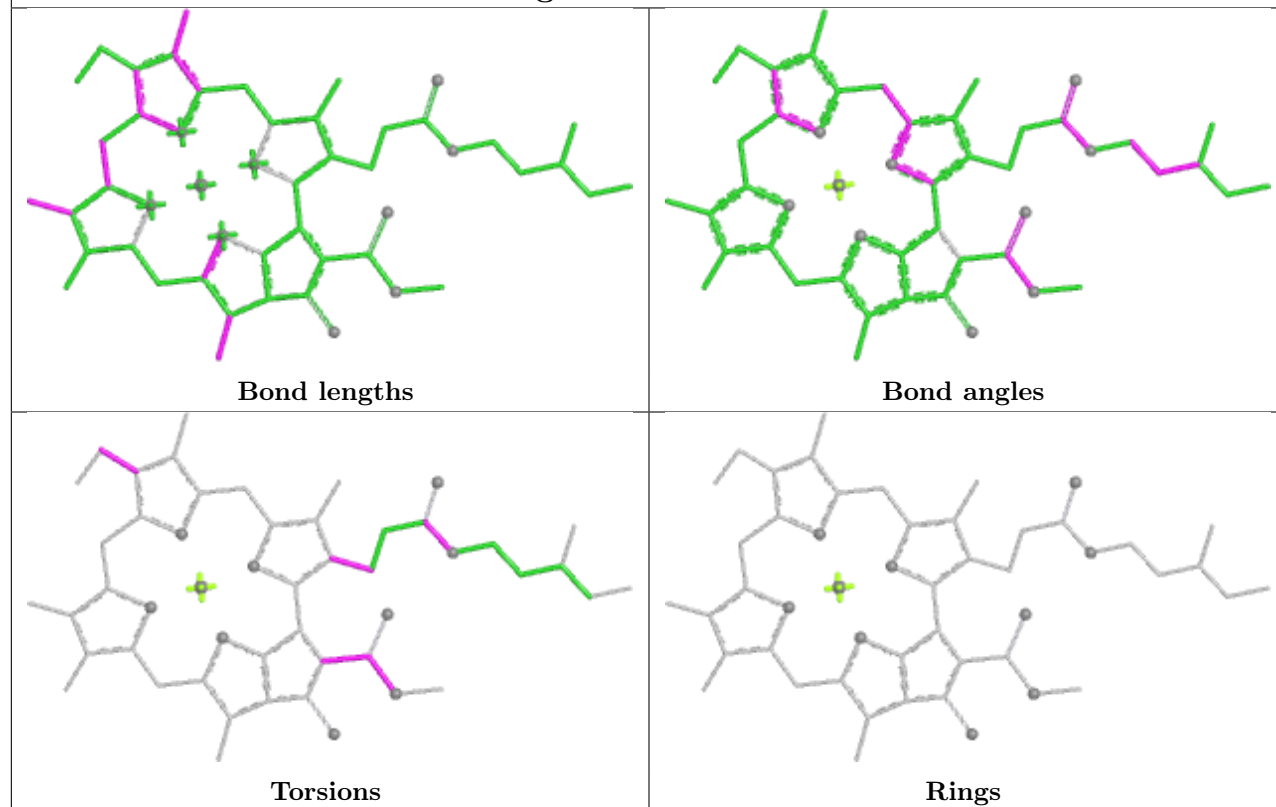


Rings

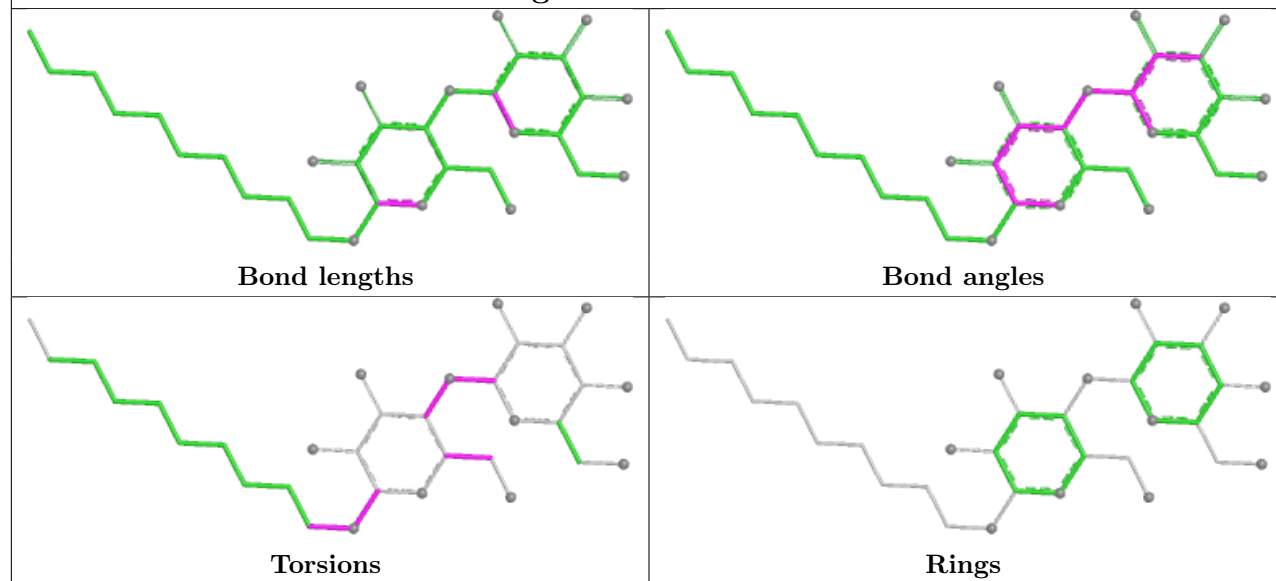




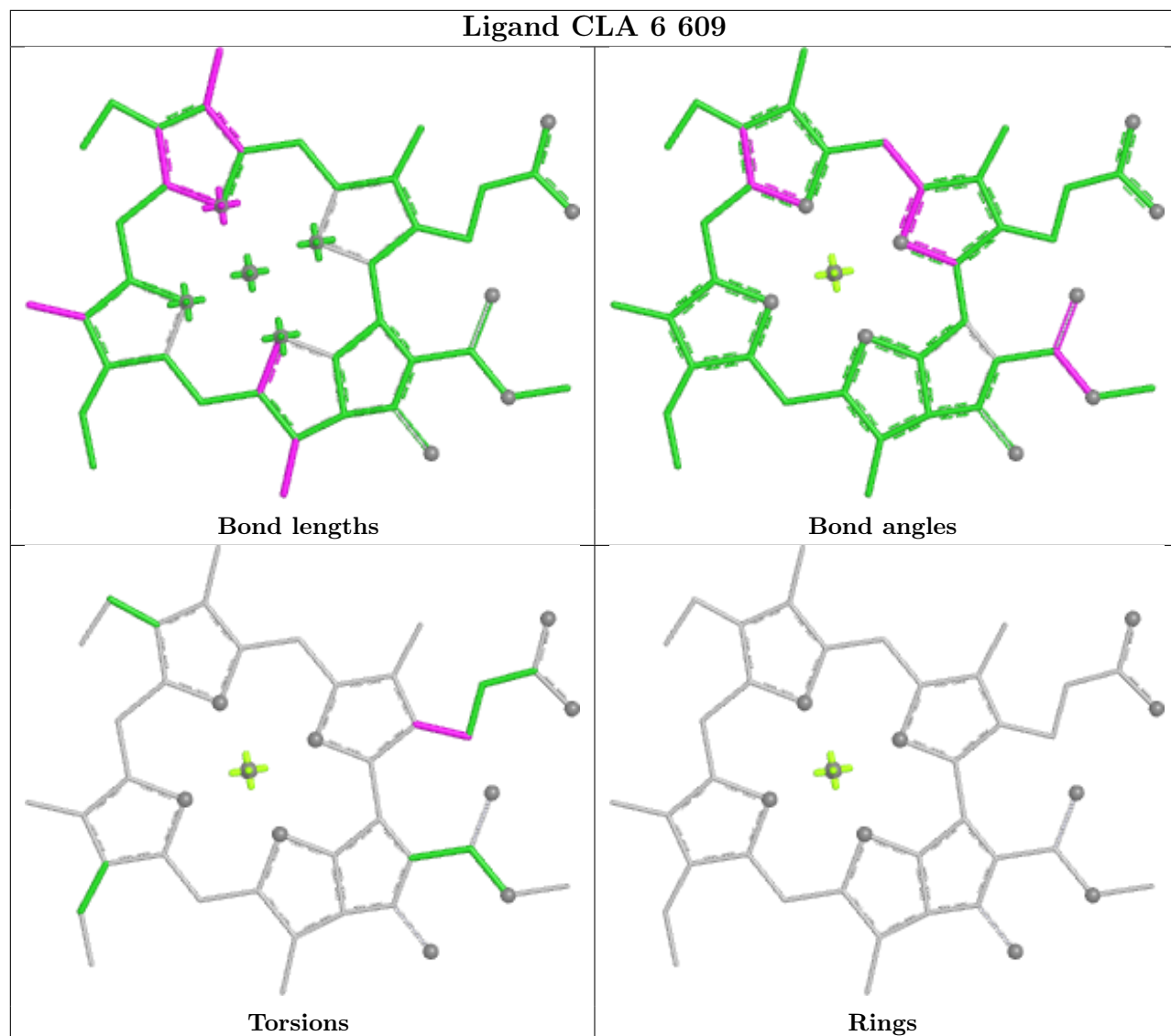
Ligand CLA 7 604



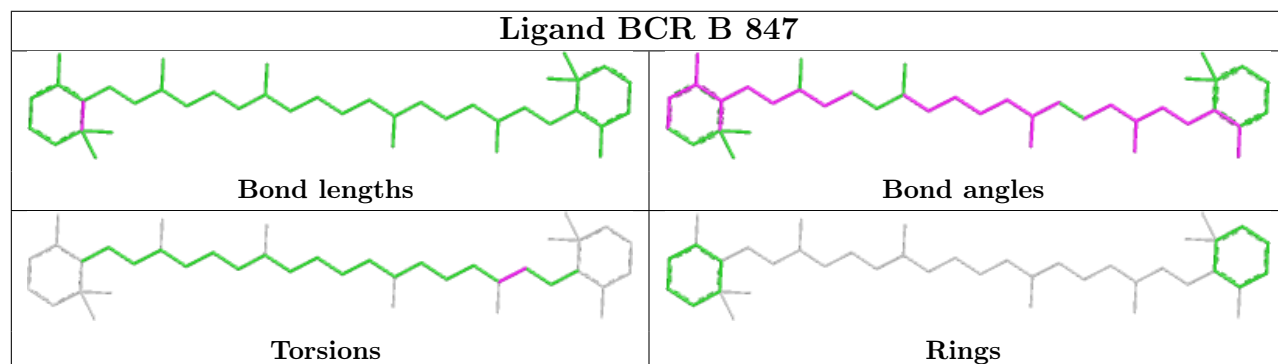
Ligand LMU 5 628

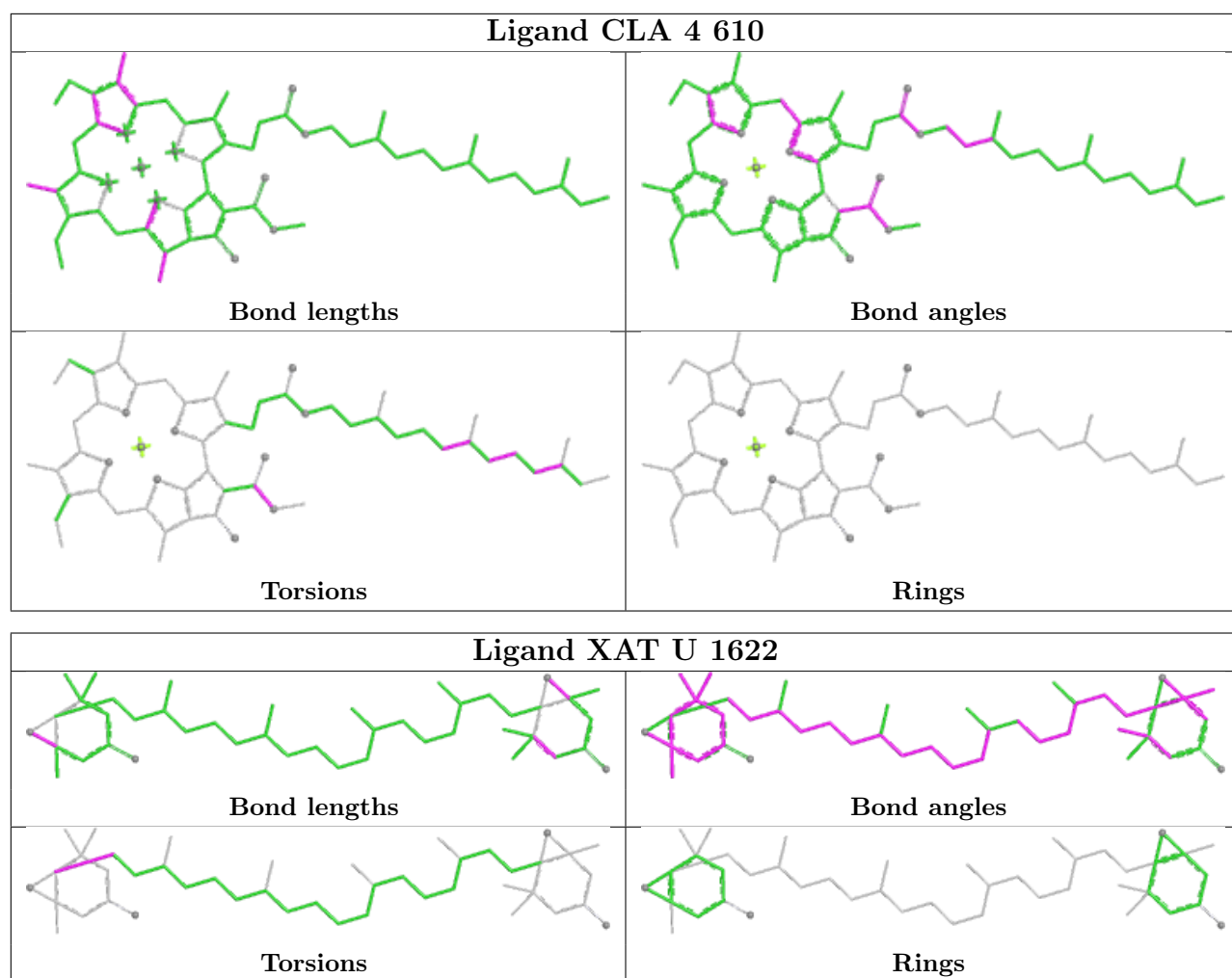


Ligand CLA 6 609

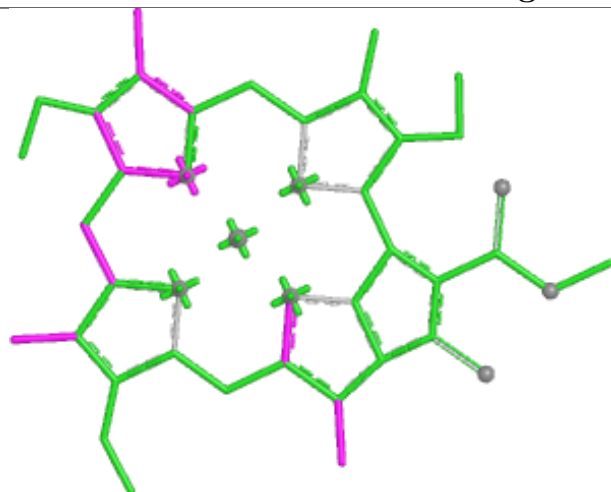


Ligand BCR B 847





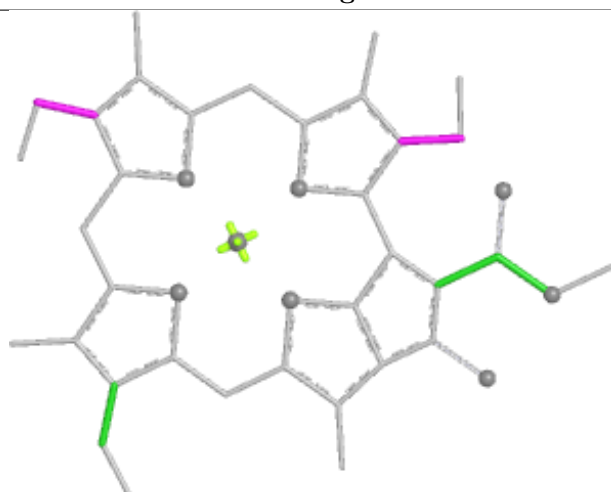
Ligand CLA 7 614



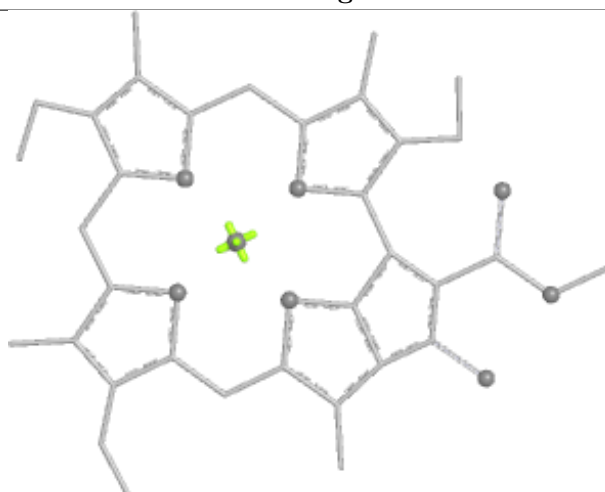
Bond lengths



Bond angles

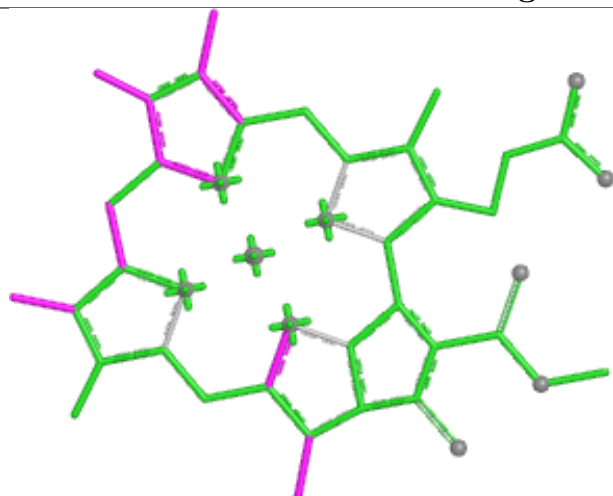


Torsions

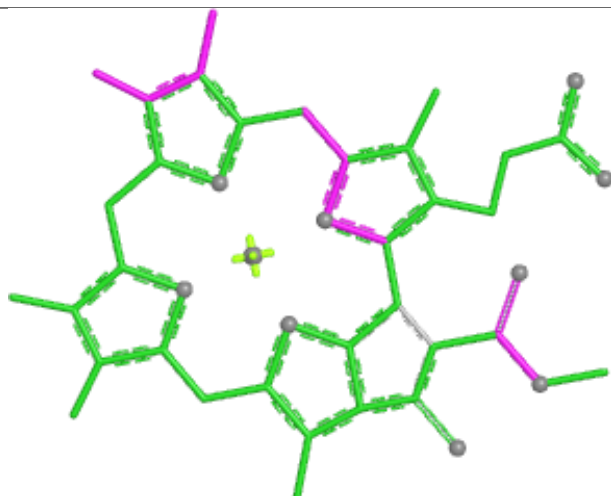


Rings

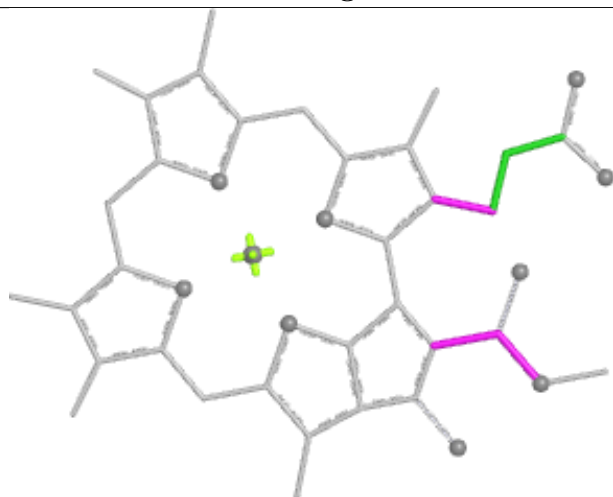
Ligand CLA 2 616



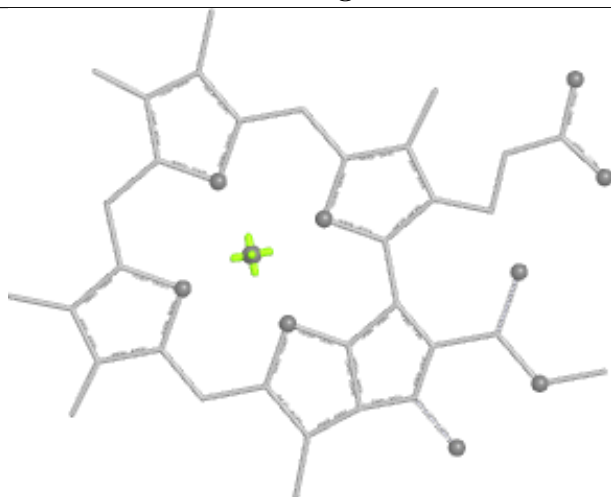
Bond lengths



Bond angles

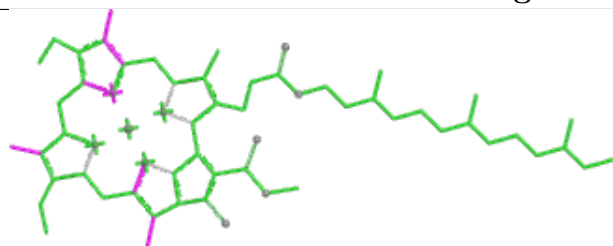


Torsions

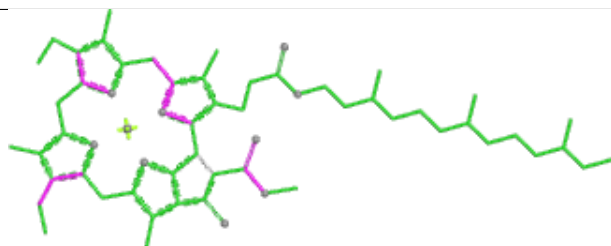


Rings

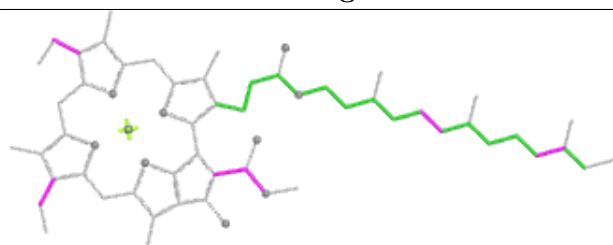
Ligand CLA A 835



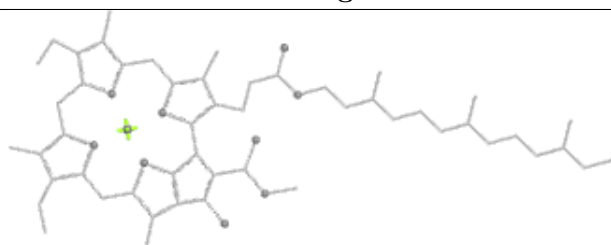
Bond lengths



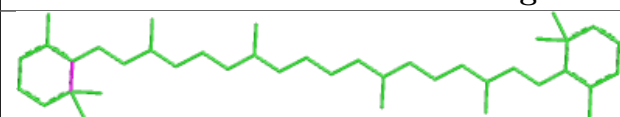
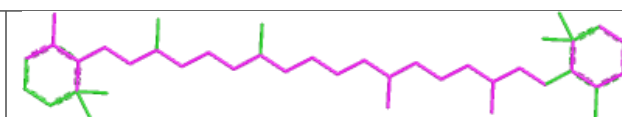
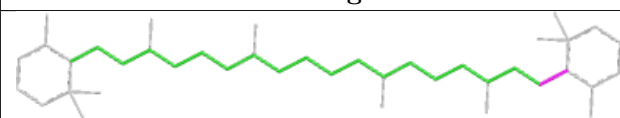
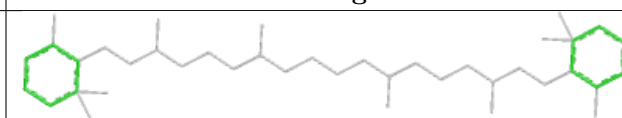
Bond angles

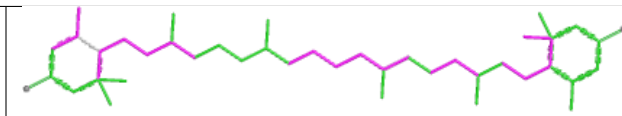
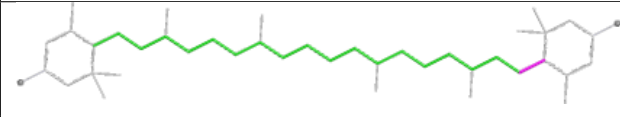
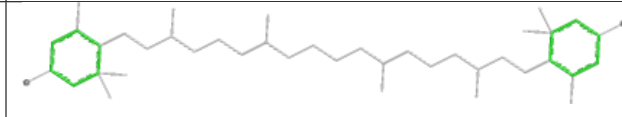


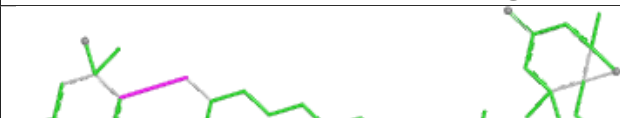
Torsions



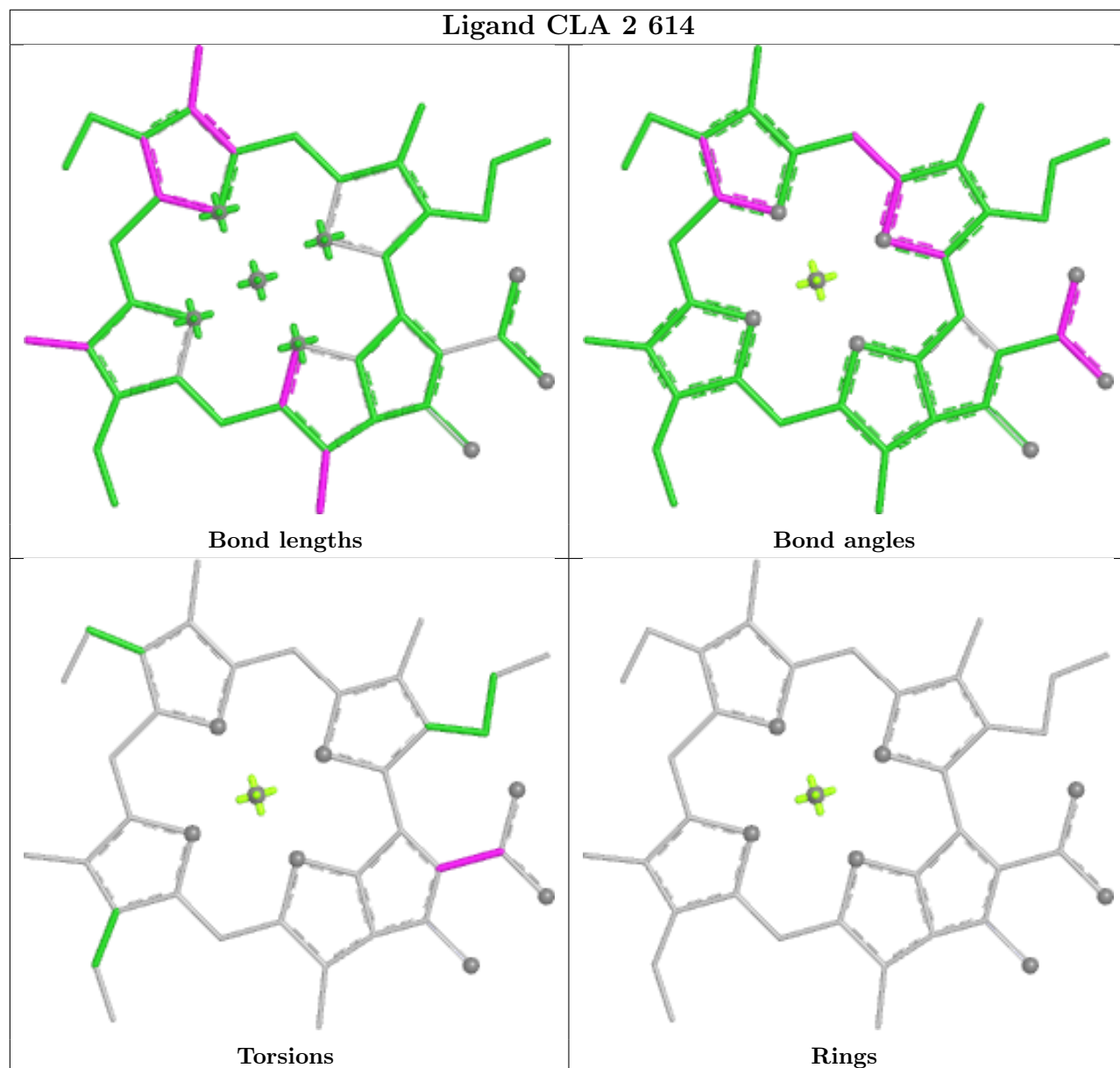
Rings

Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

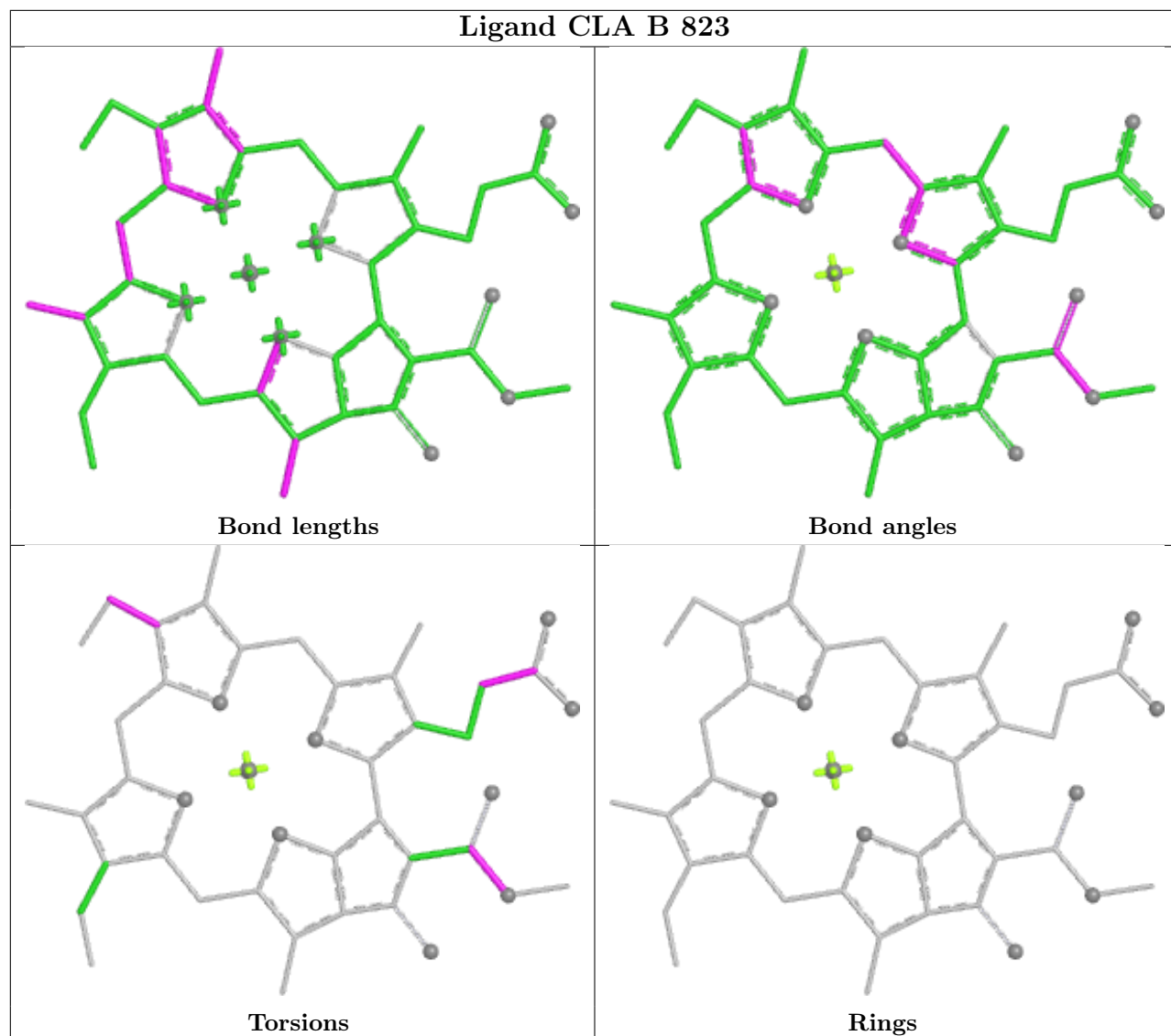
Ligand LUT X 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NEX W 1623	
	
Bond lengths	Bond angles
	
Torsions	Rings

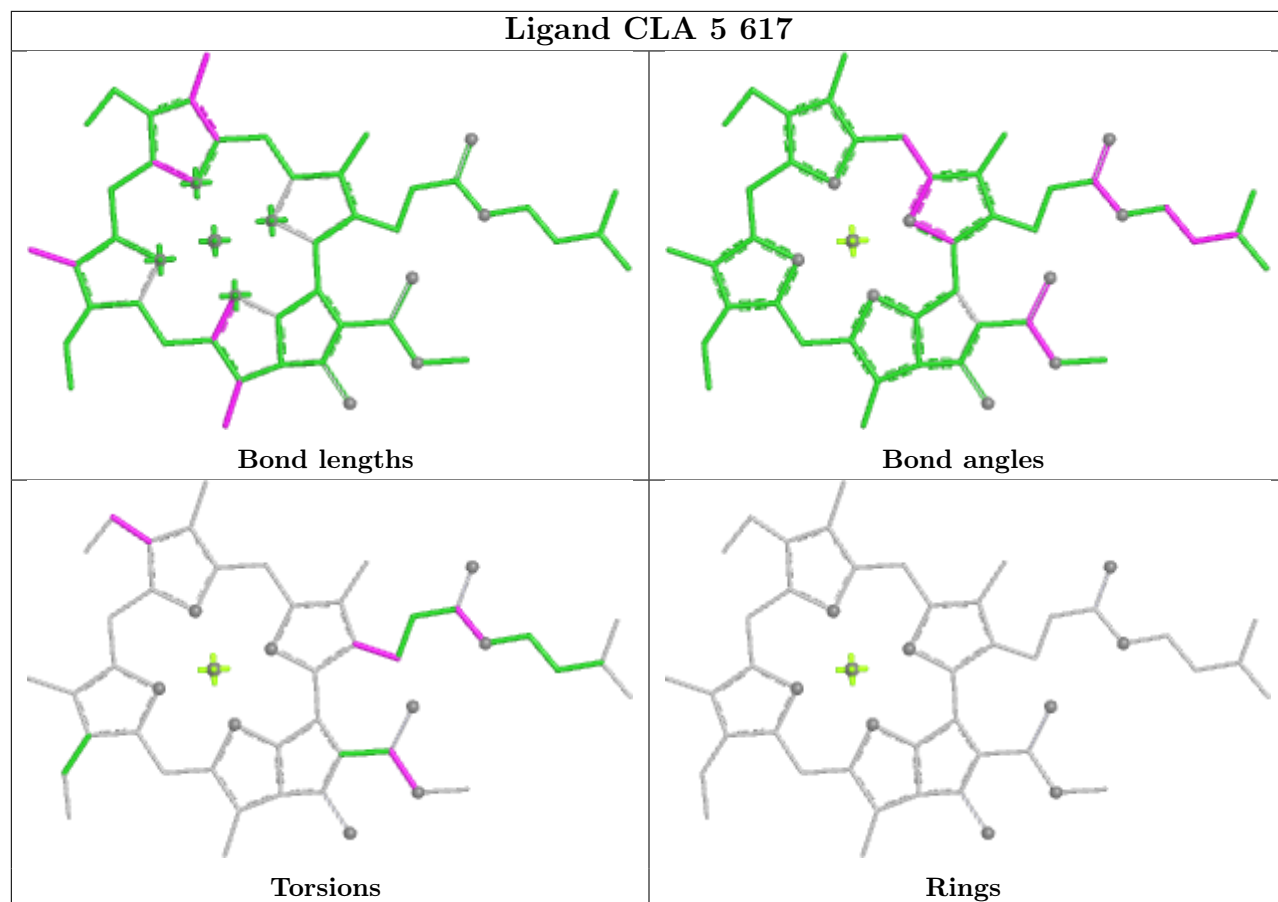
Ligand CLA 2 614



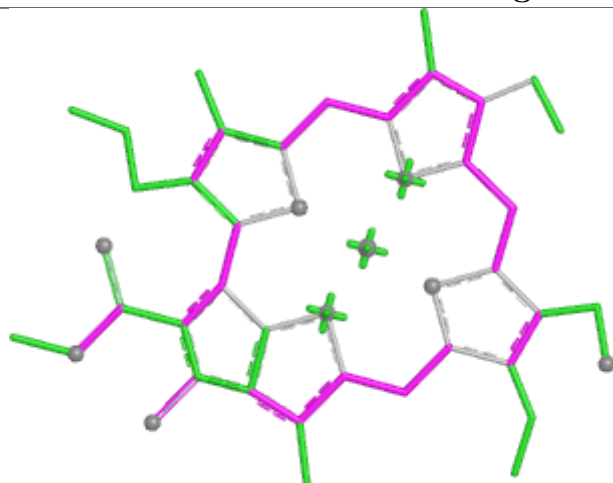
Ligand CLA B 823



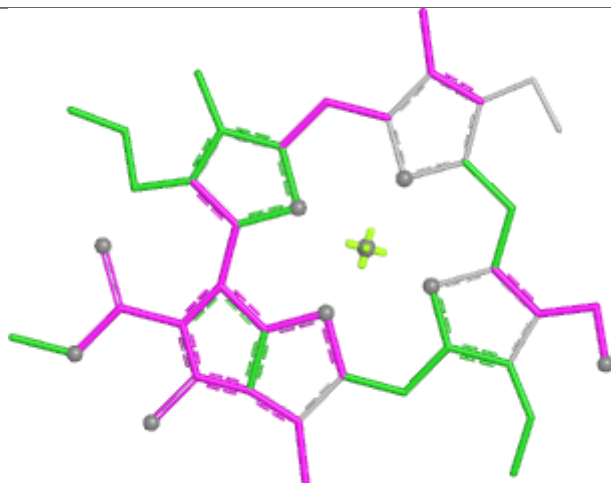
Ligand CLA 5 617



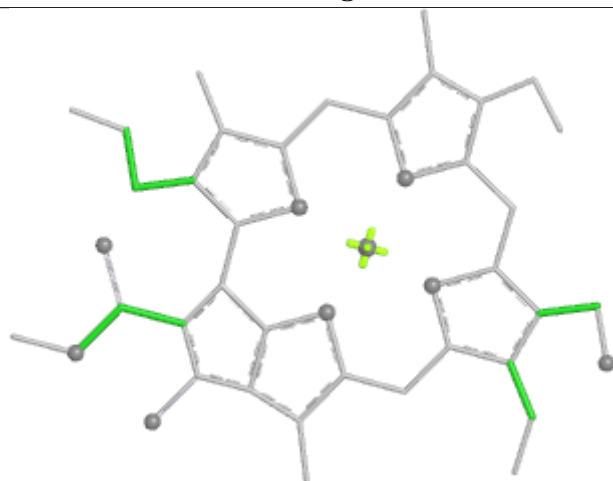
Ligand CHL X 606



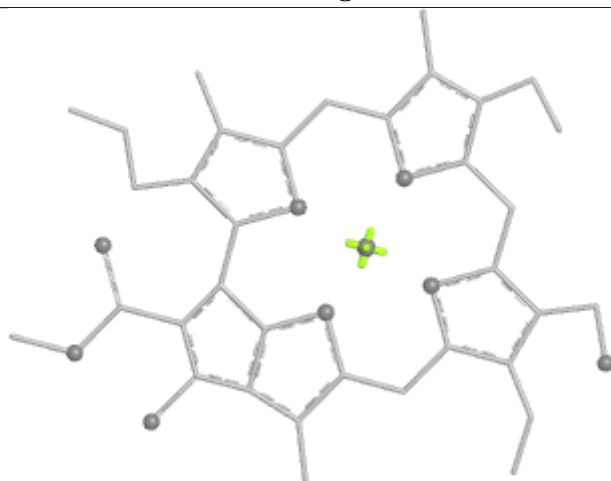
Bond lengths



Bond angles

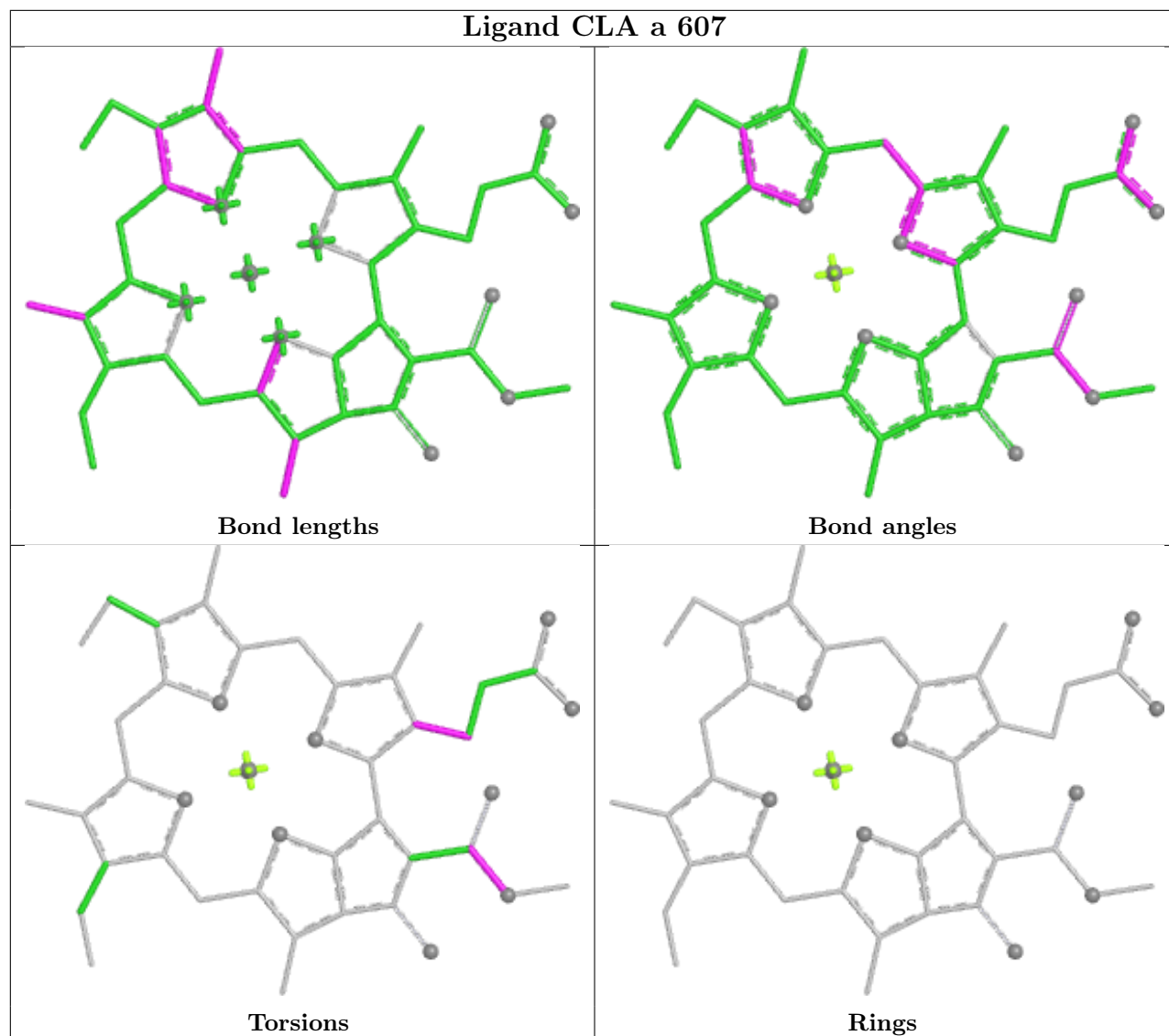


Torsions

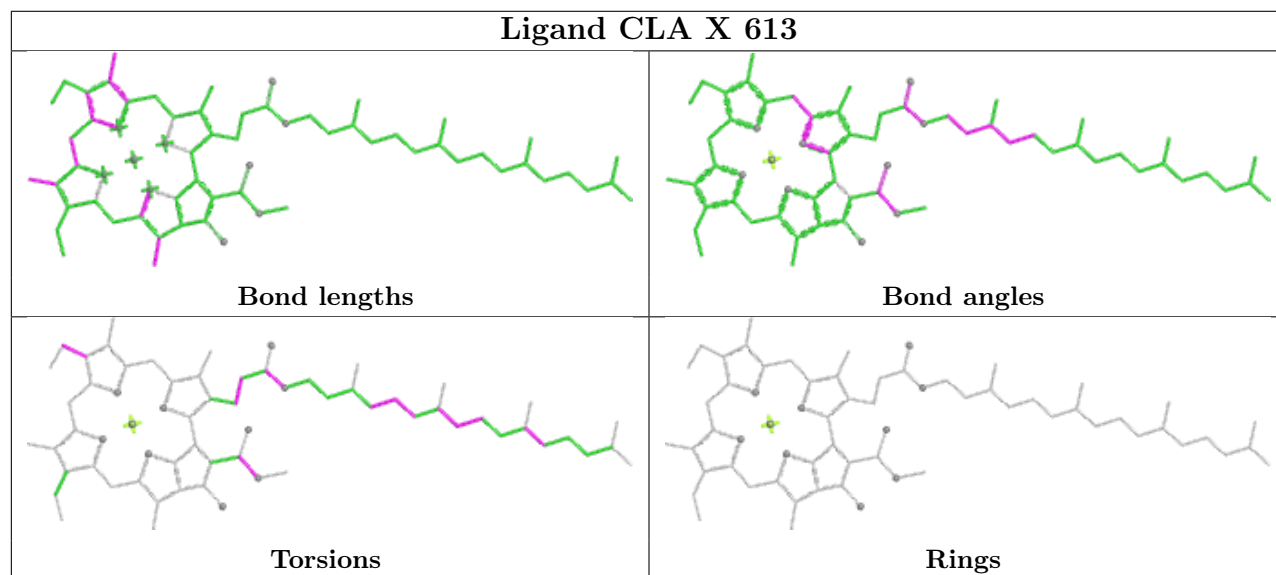


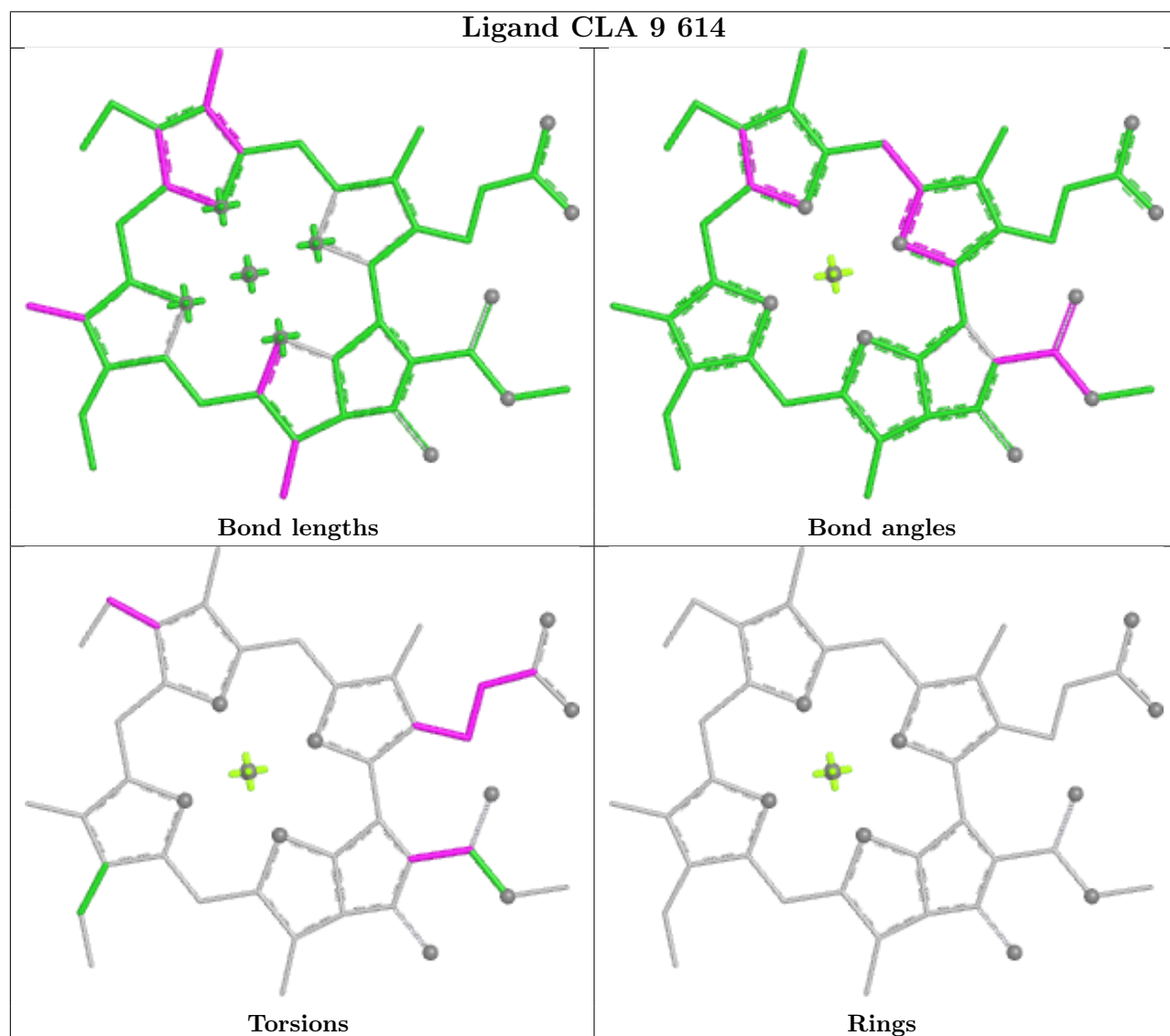
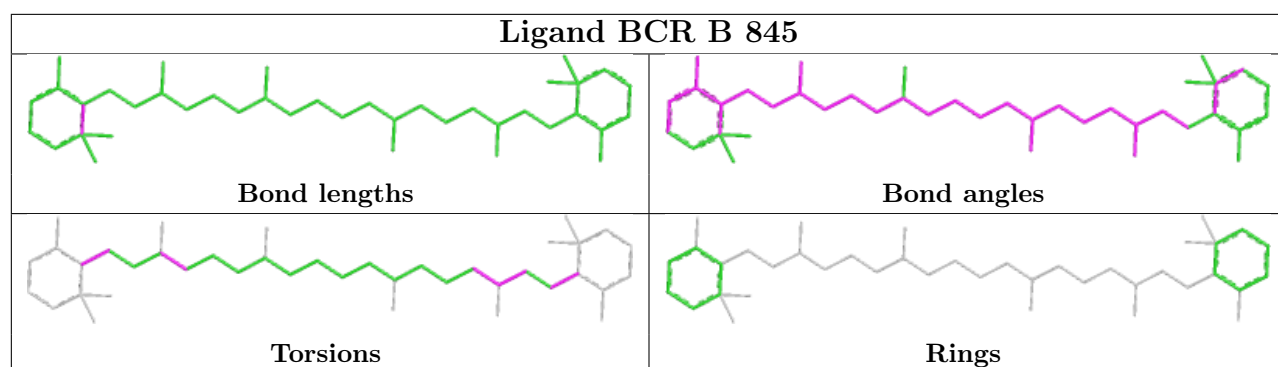
Rings

Ligand CLA a 607

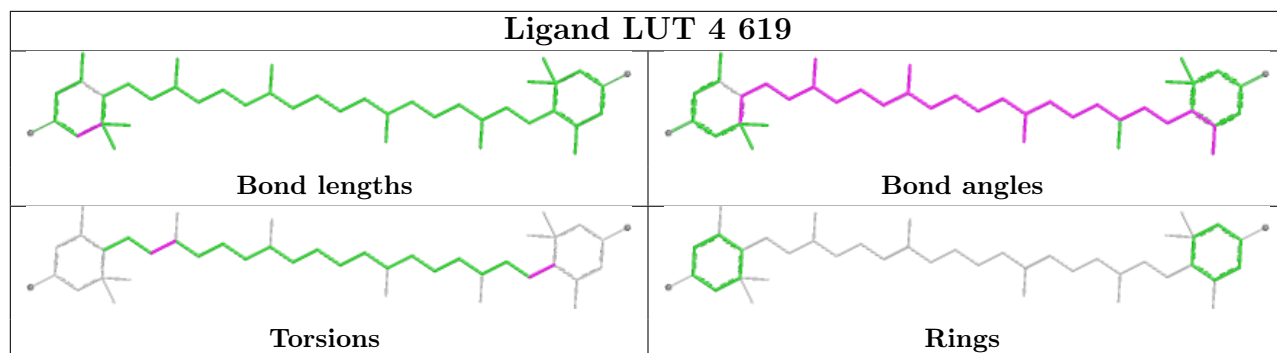


Ligand CLA X 613

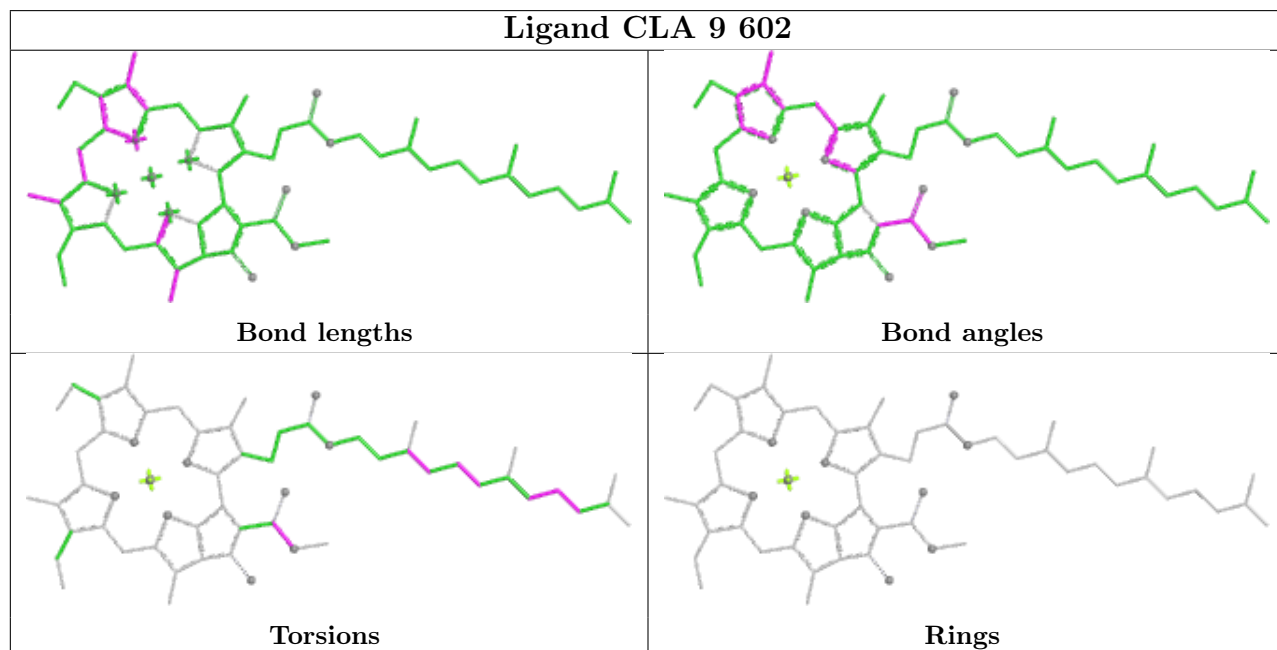




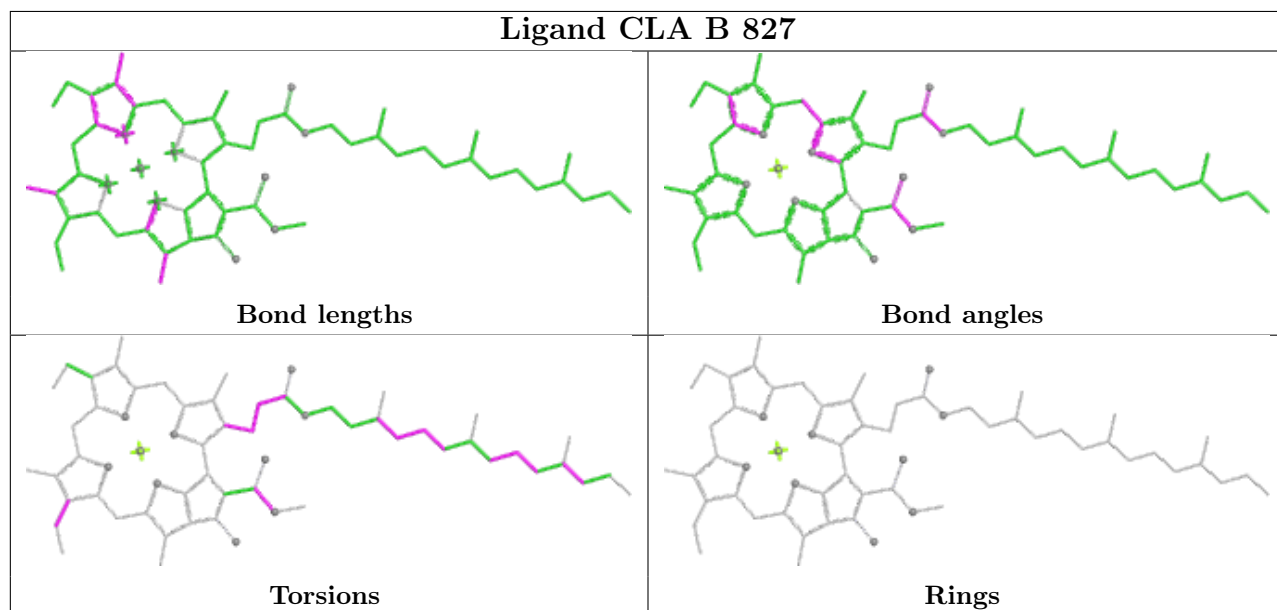
Ligand LUT 4 619

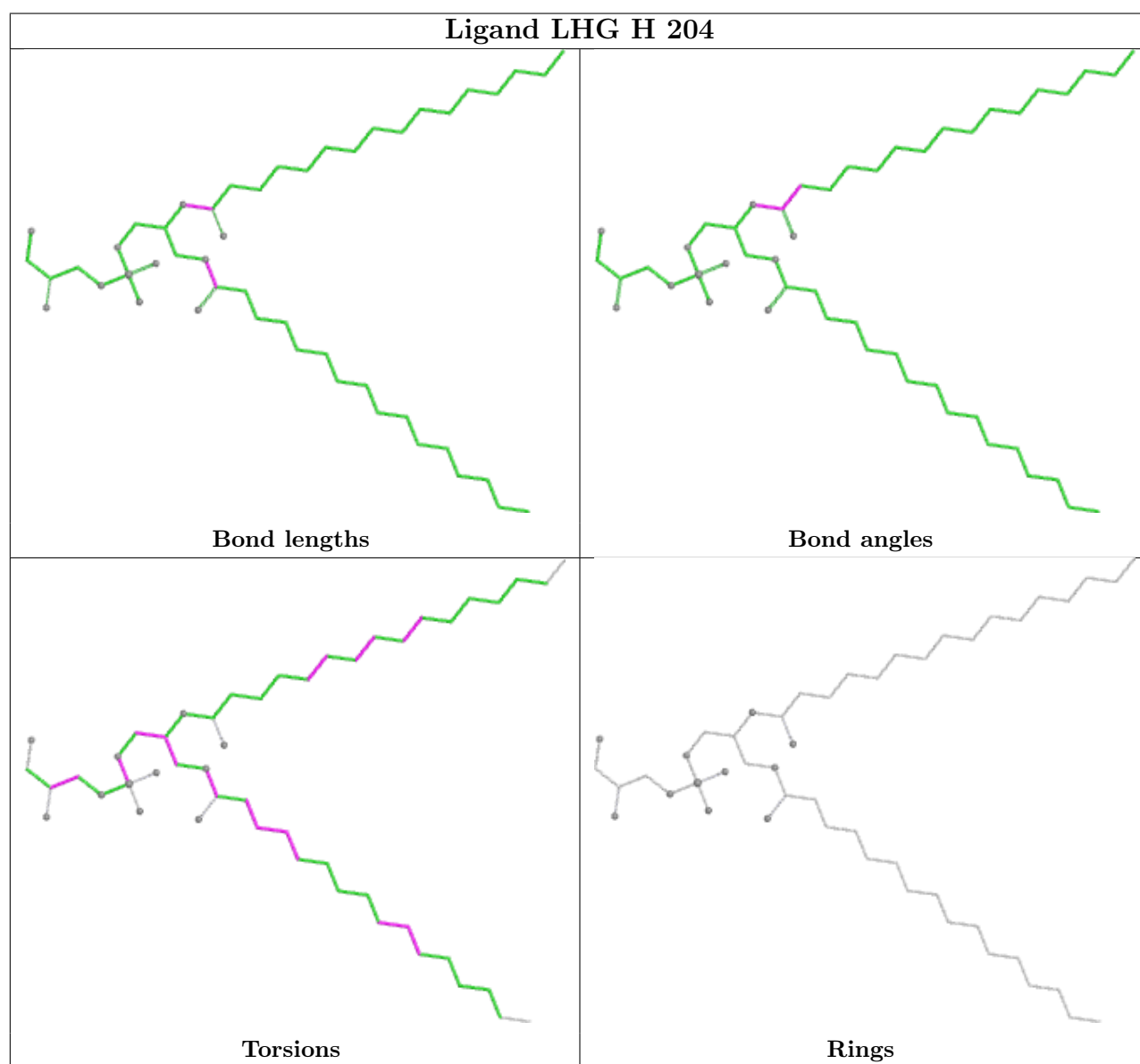
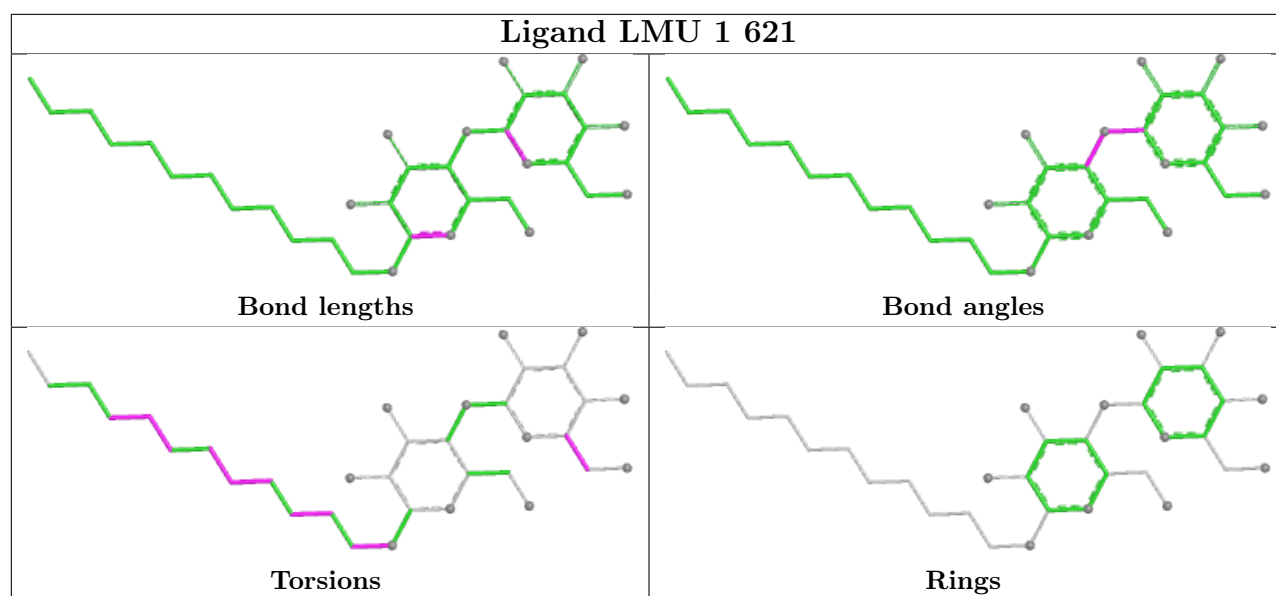


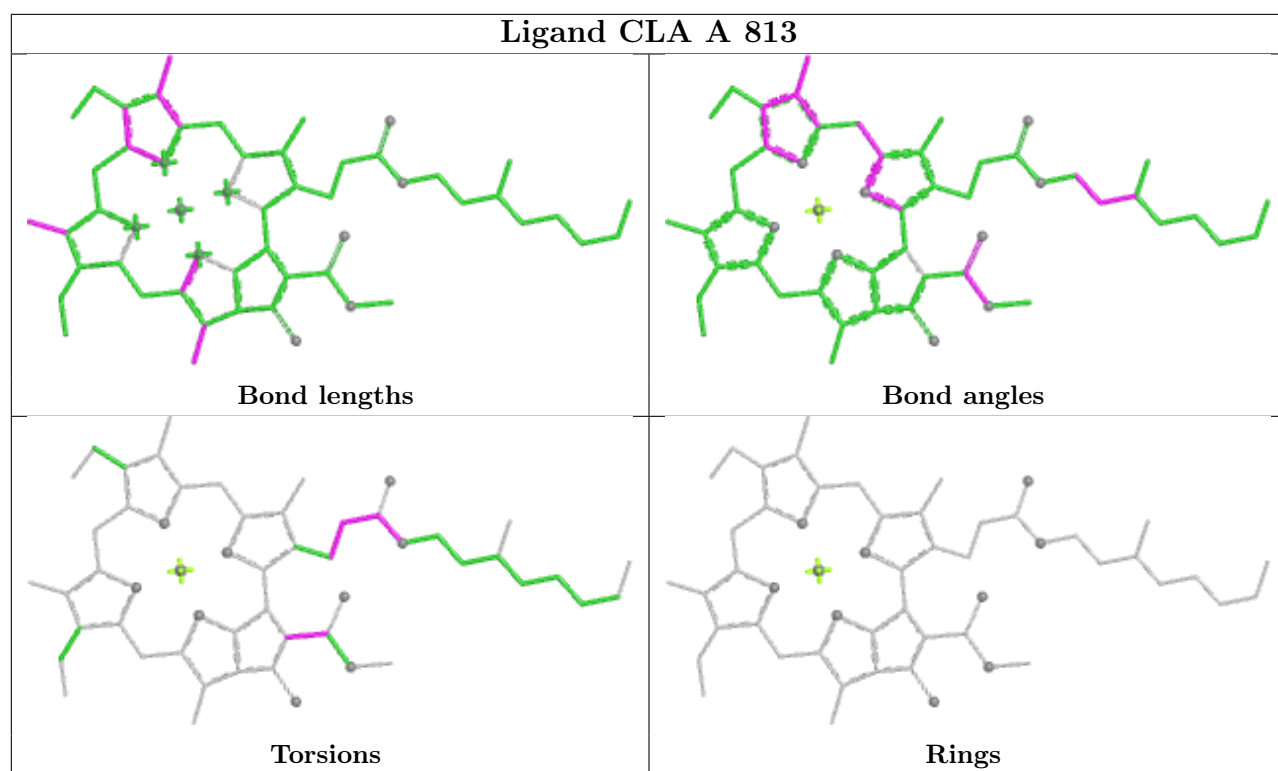
Ligand CLA 9 602



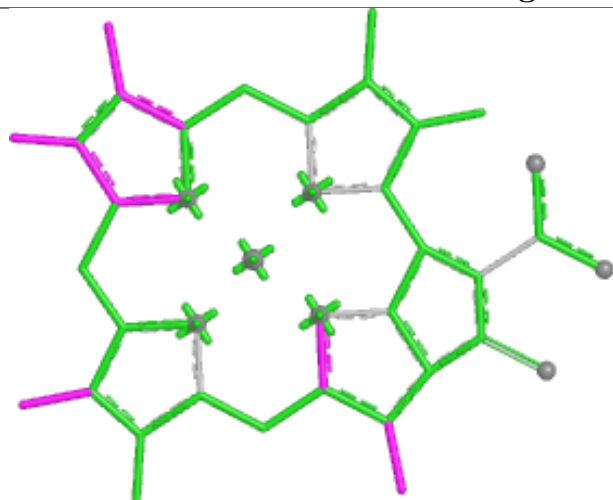
Ligand CLA B 827



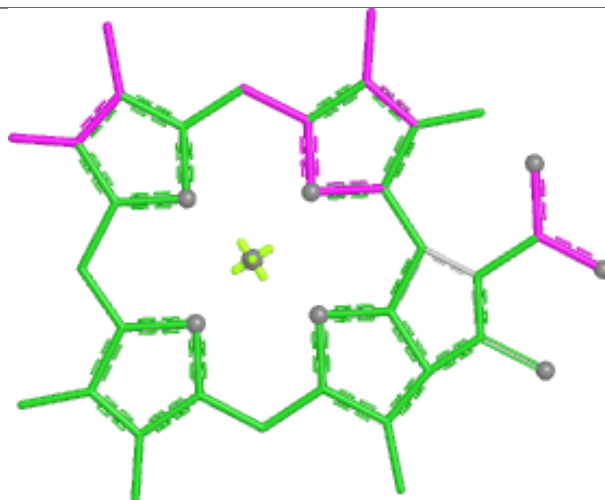




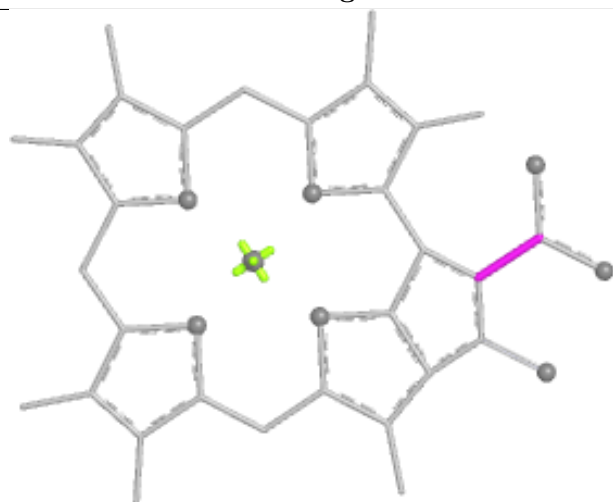
Ligand CLA 3 611



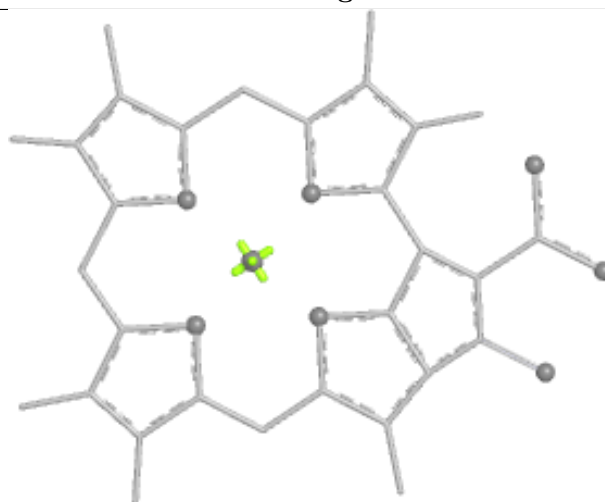
Bond lengths



Bond angles

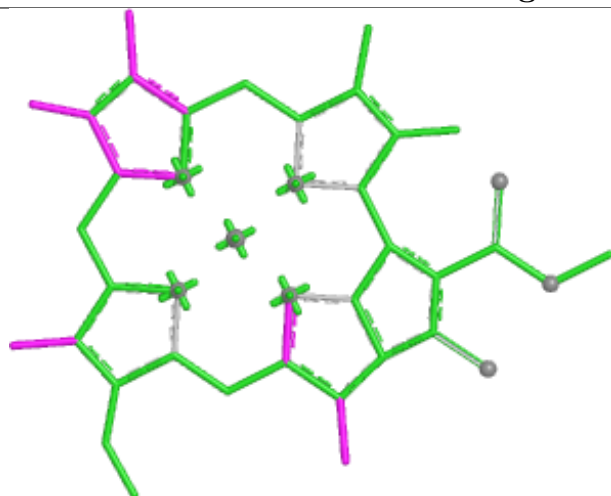


Torsions

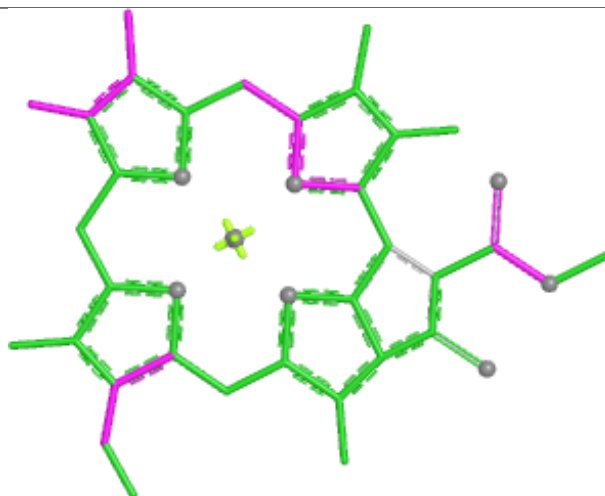


Rings

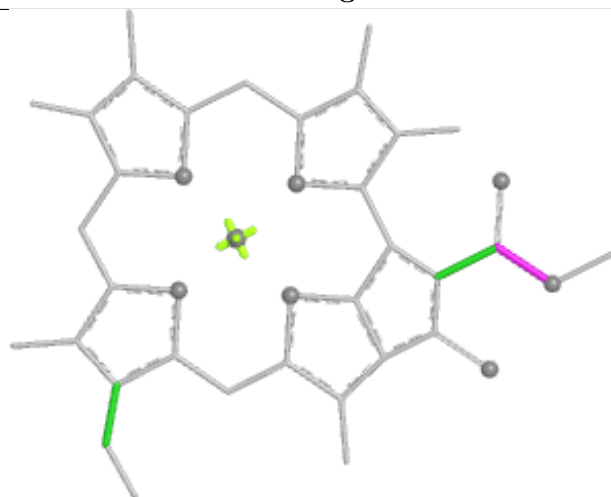
Ligand CLA 1 609



Bond lengths



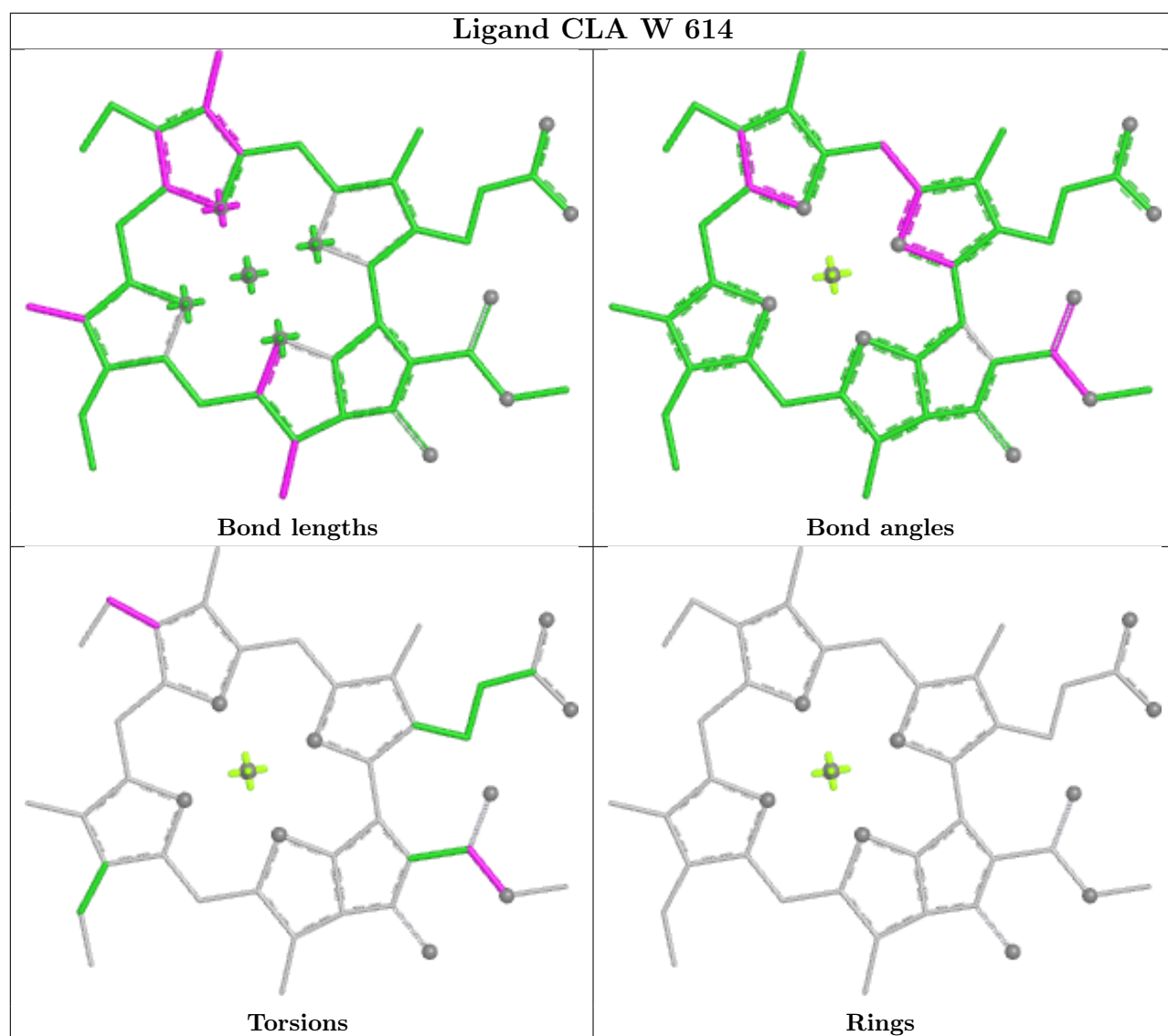
Bond angles



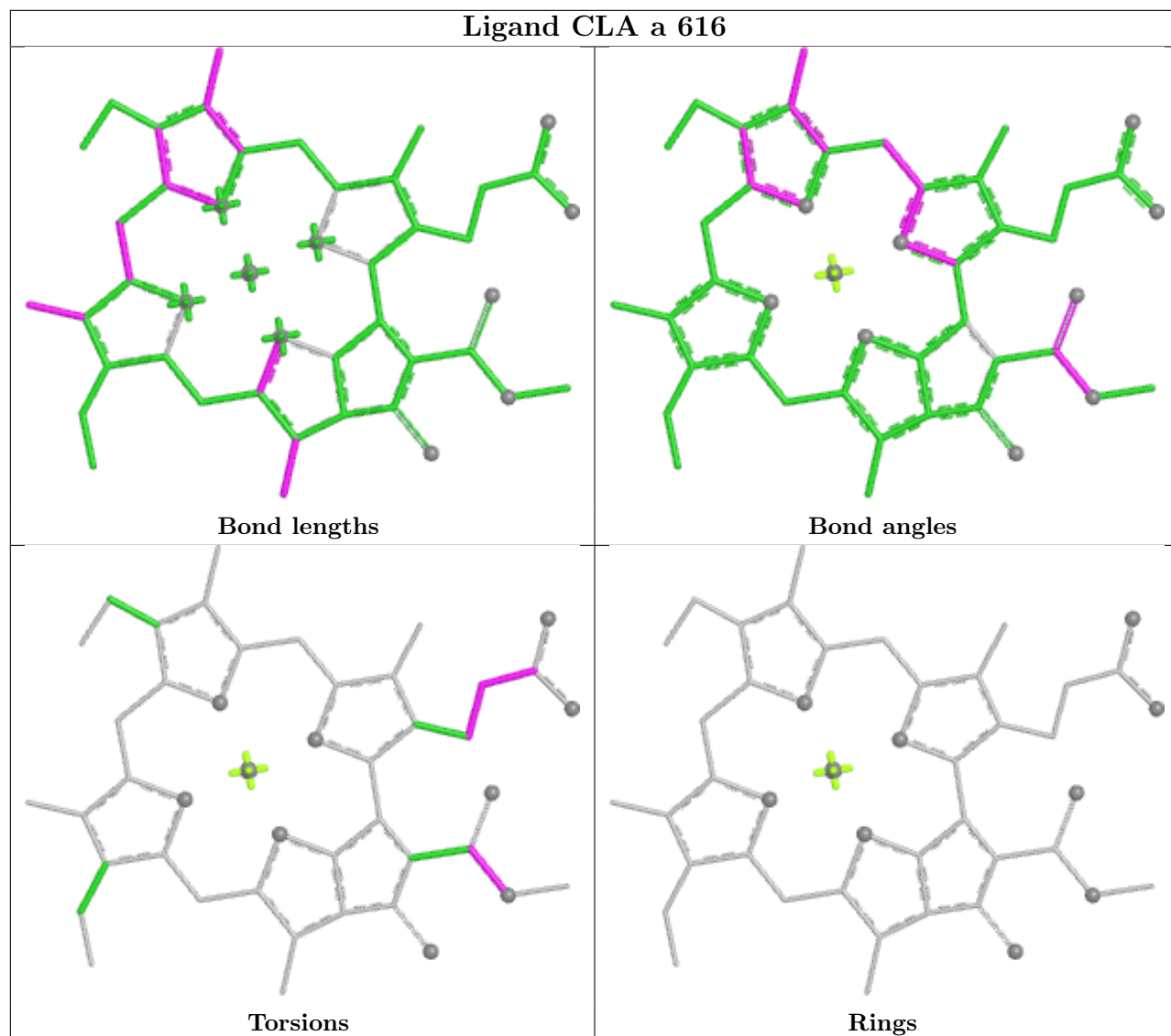
Torsions



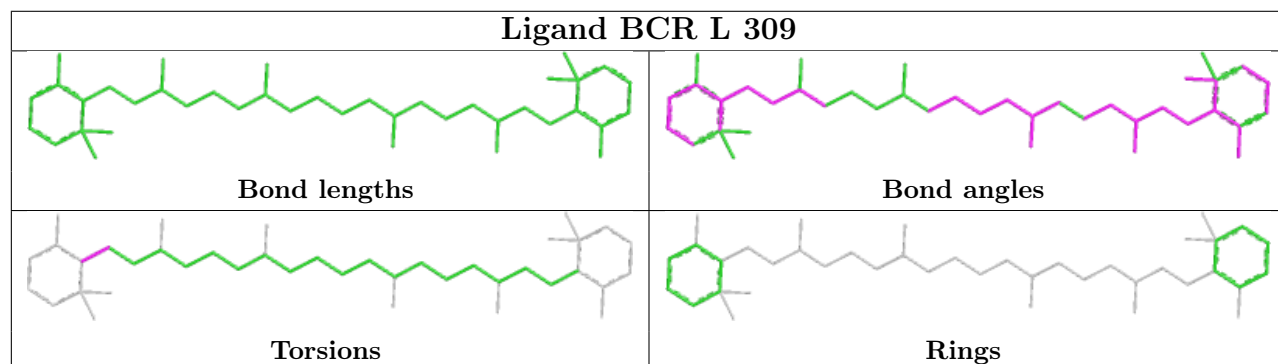
Rings



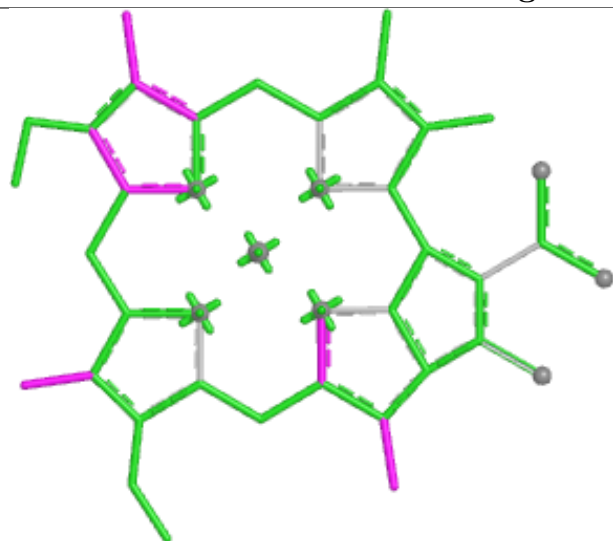
Ligand CLA a 616



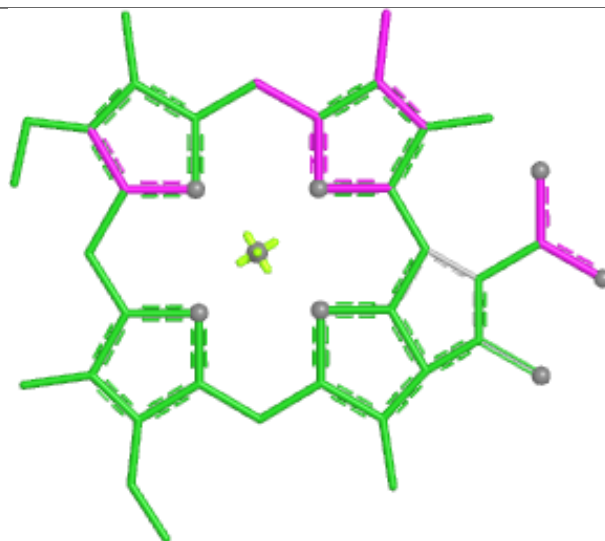
Ligand BCR L 309



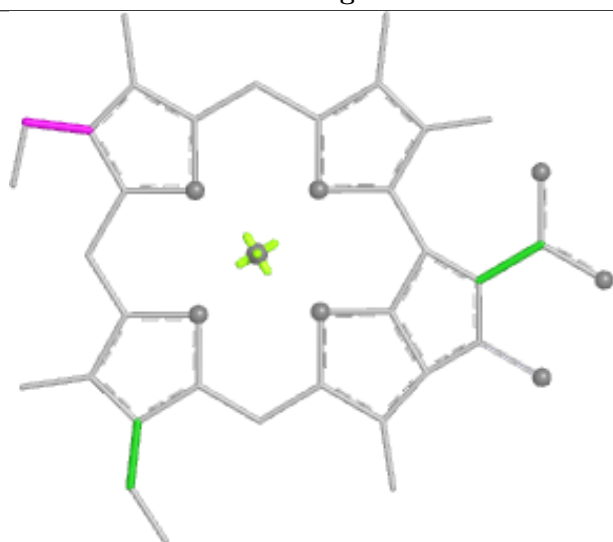
Ligand CLA 3 617



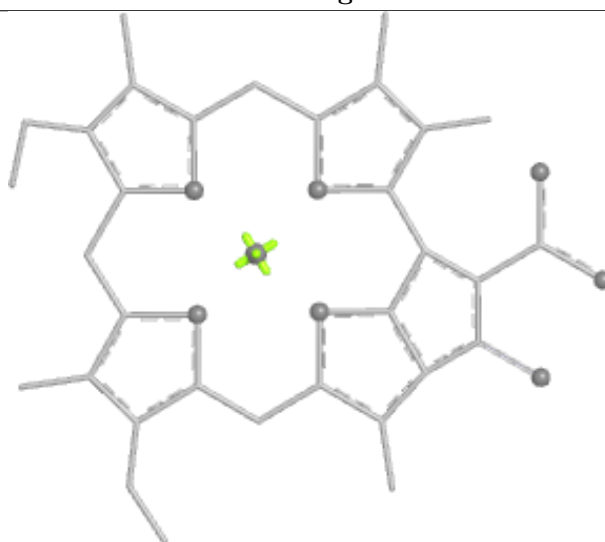
Bond lengths



Bond angles

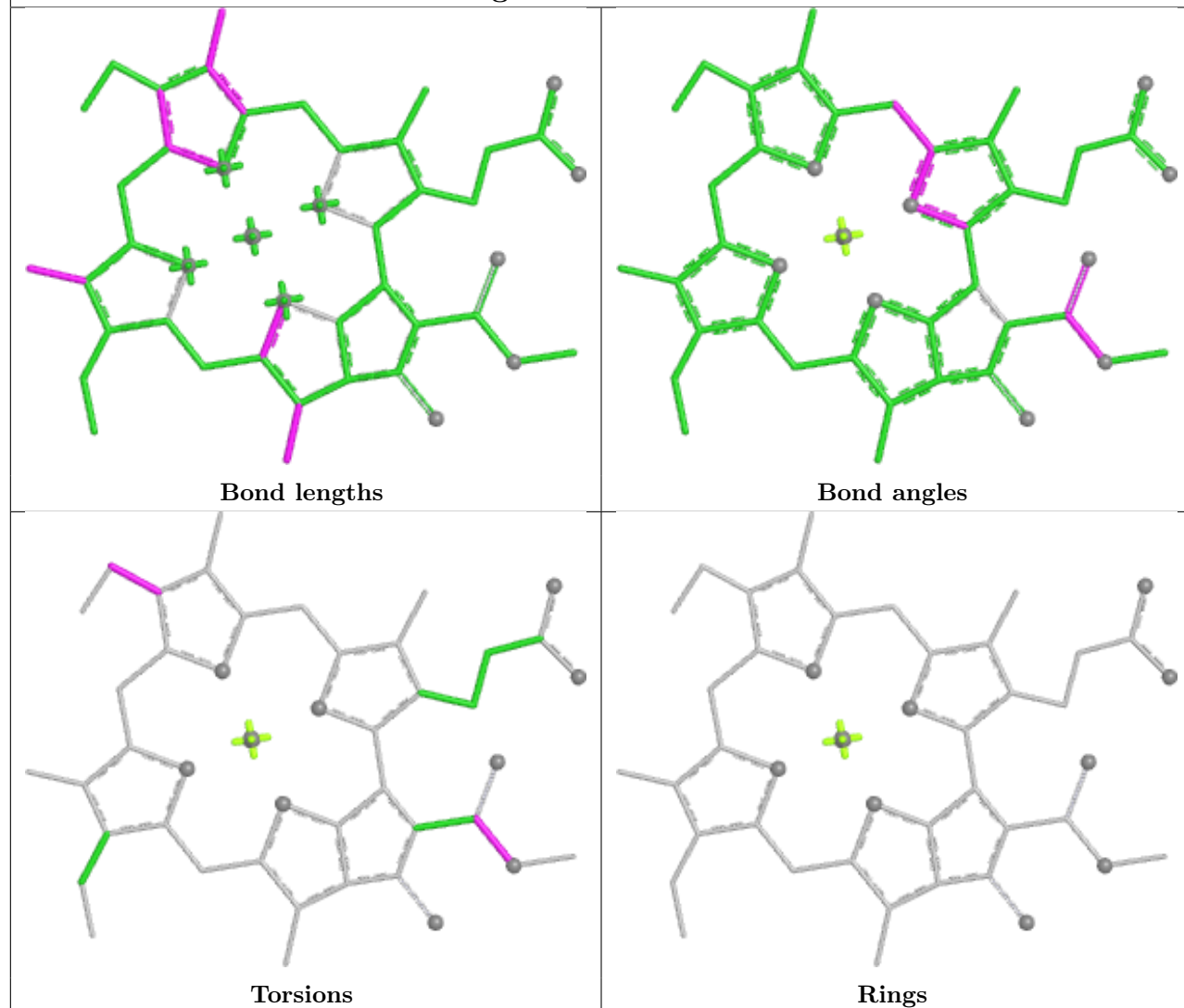


Torsions

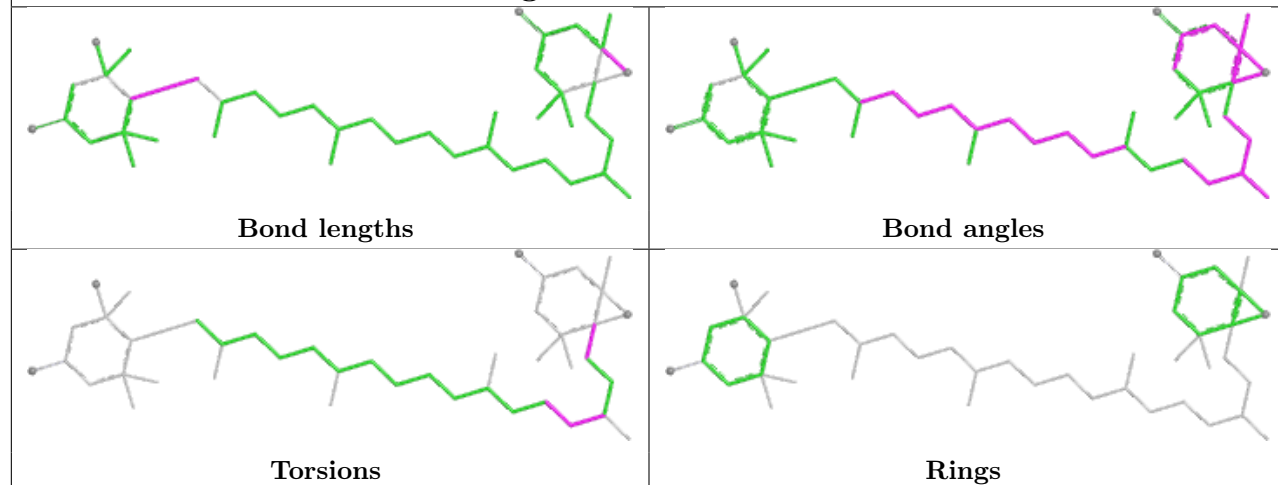


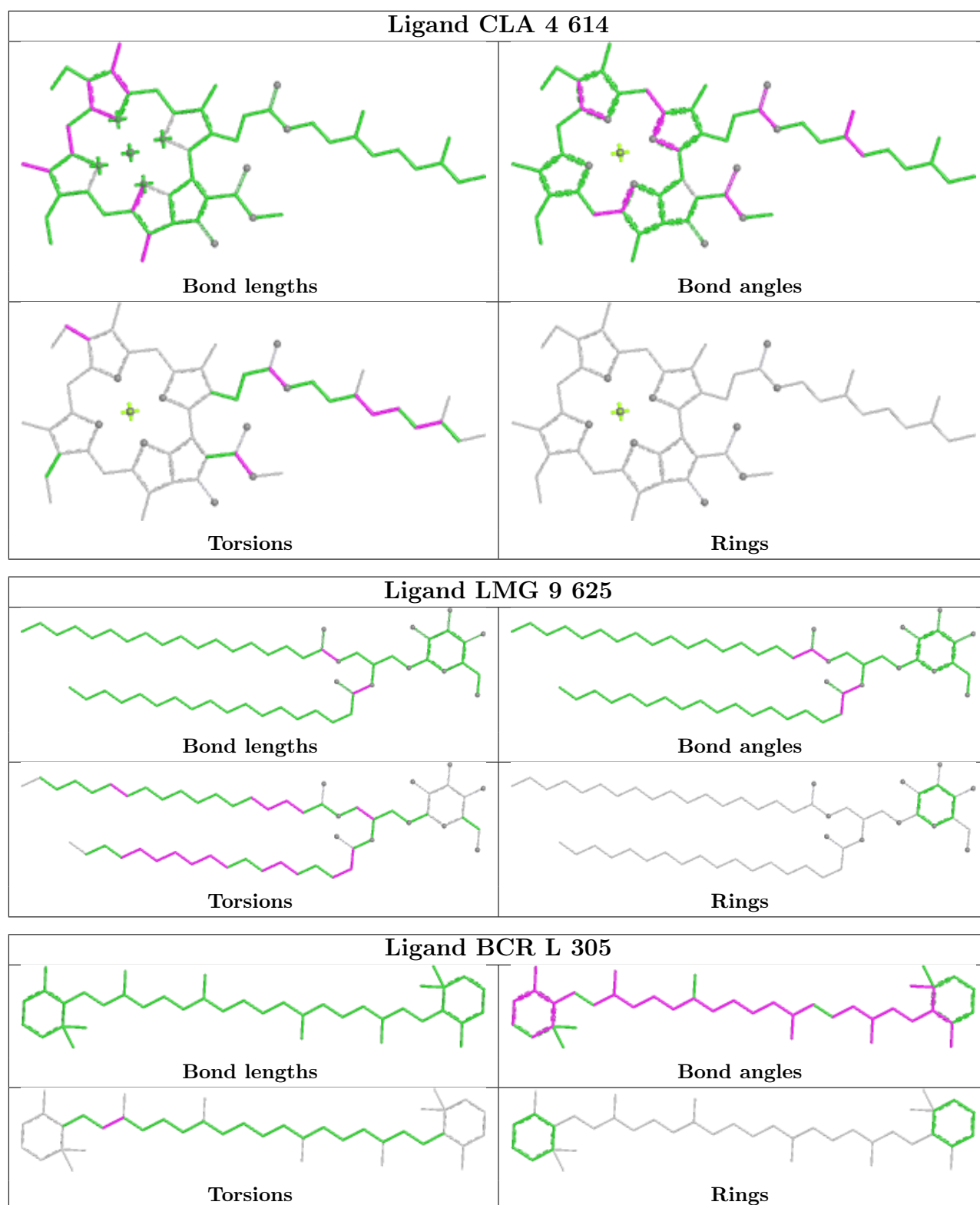
Rings

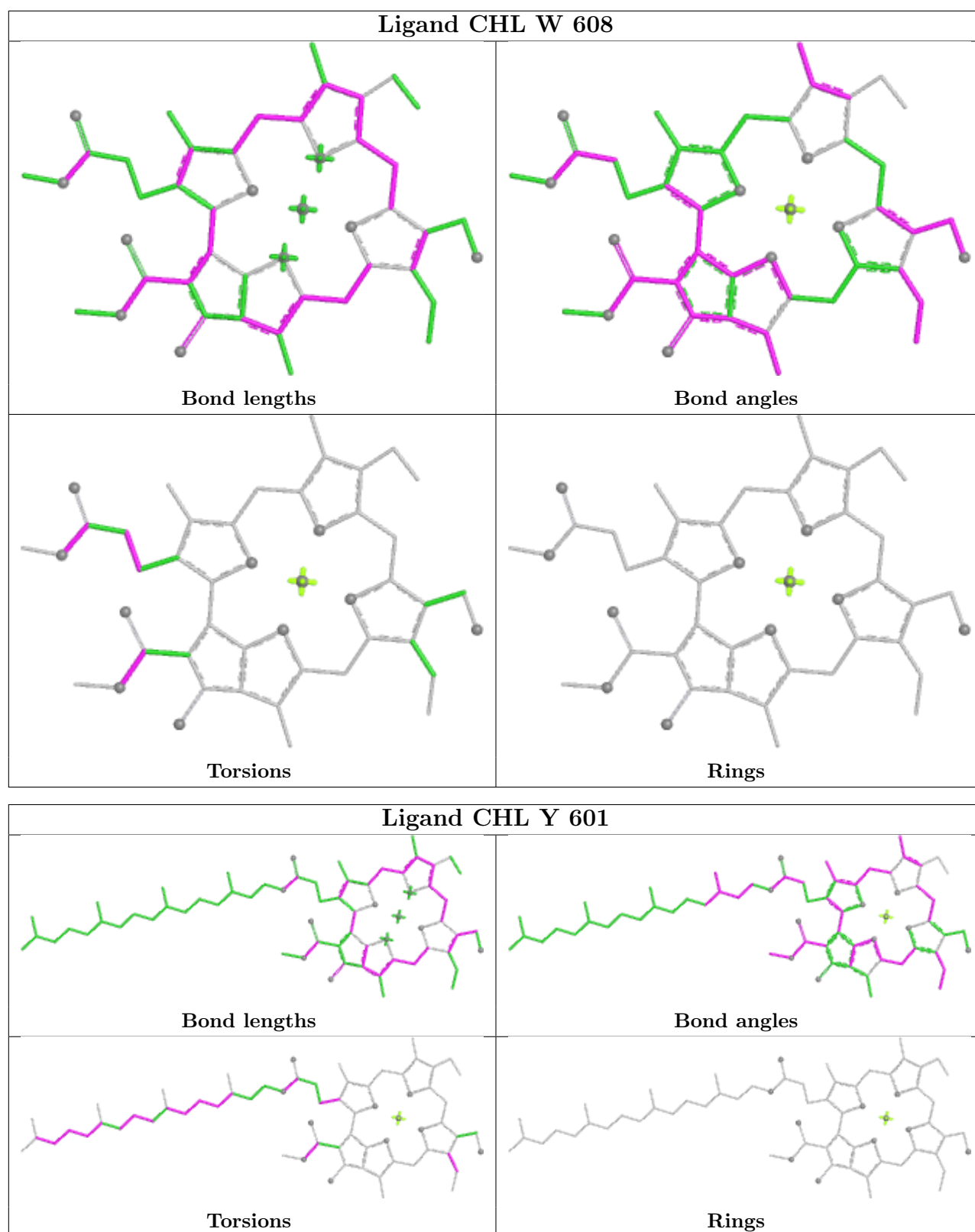
Ligand CLA K 206

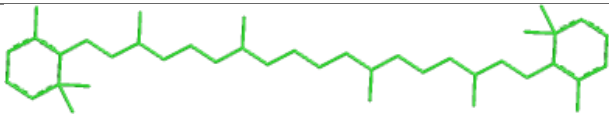
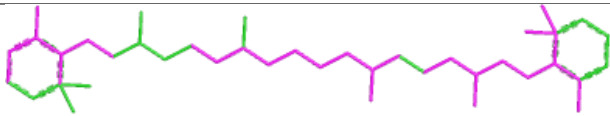
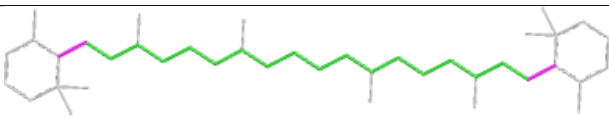
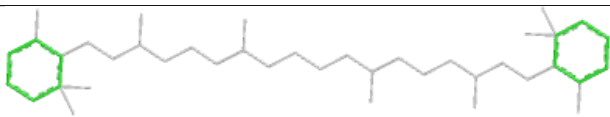


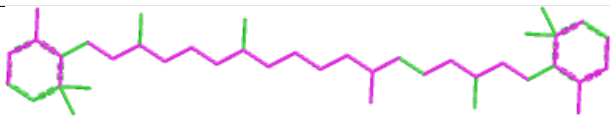
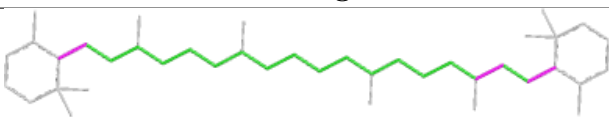
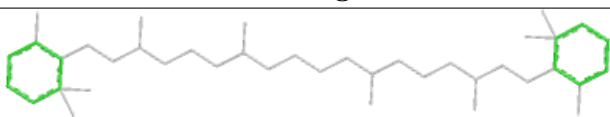
Ligand NEX V 1623

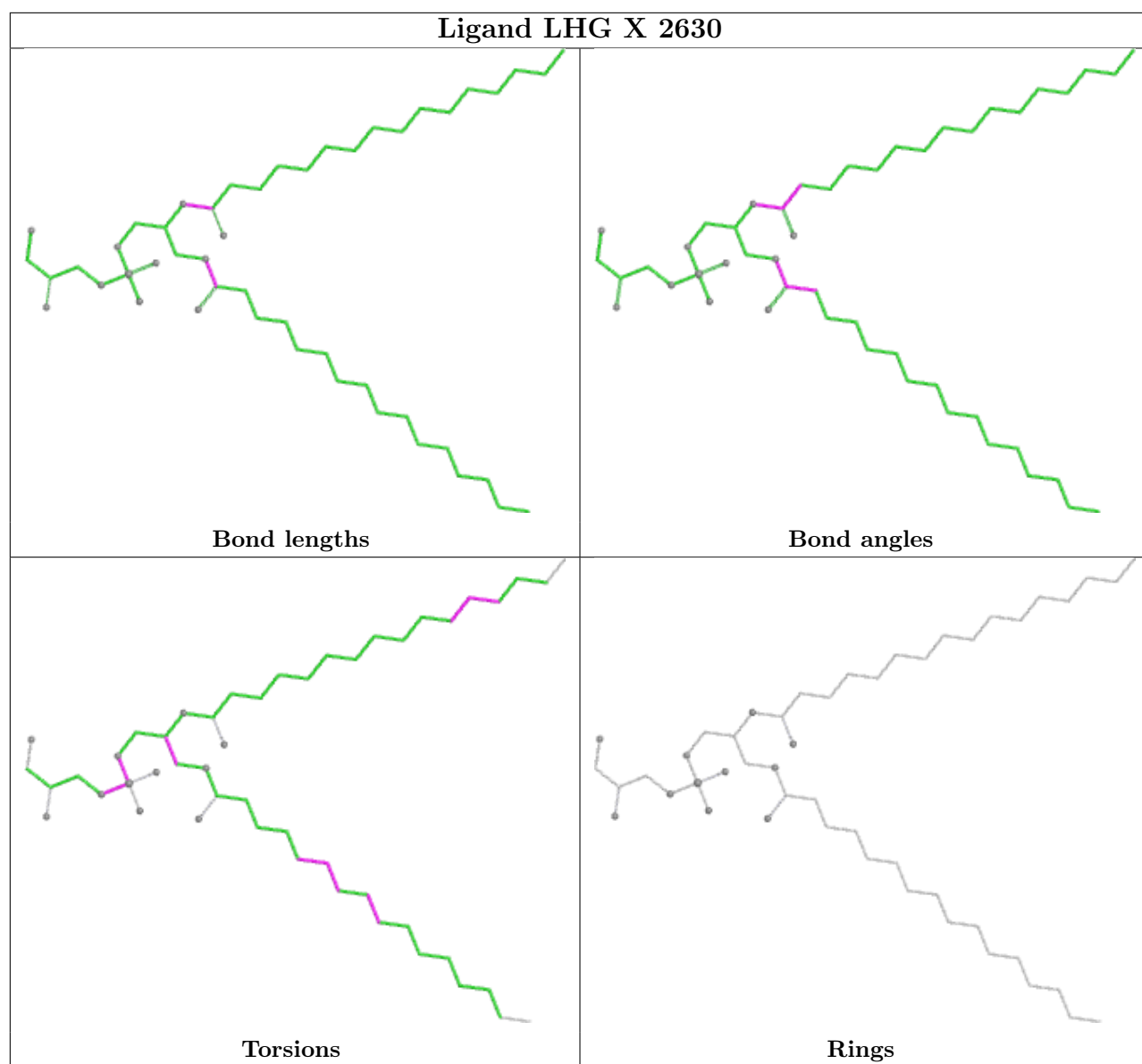




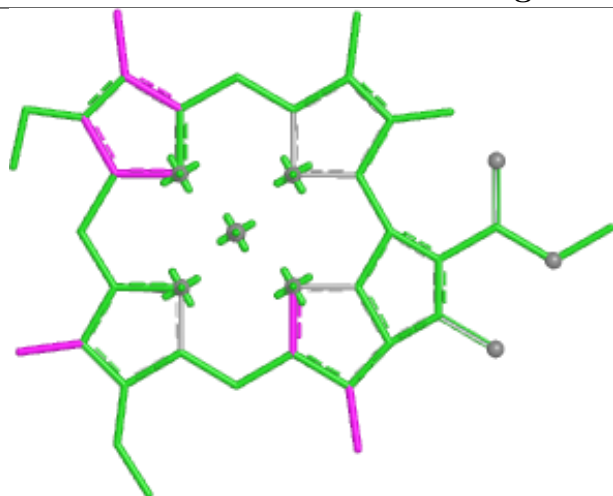


Ligand BCR 8 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

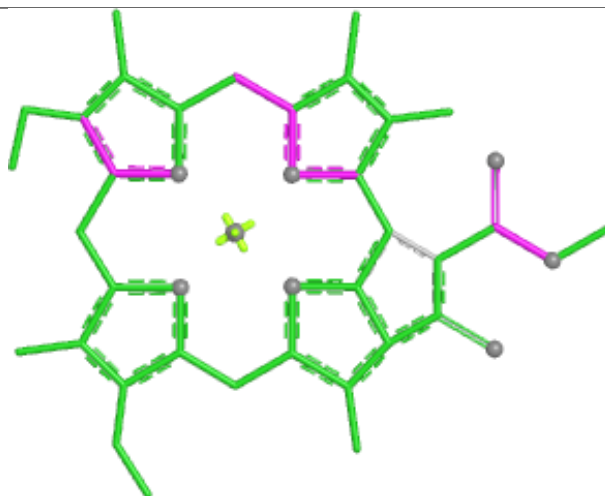
Ligand BCR A 849	
	
Bond lengths	Bond angles
	
Torsions	Rings



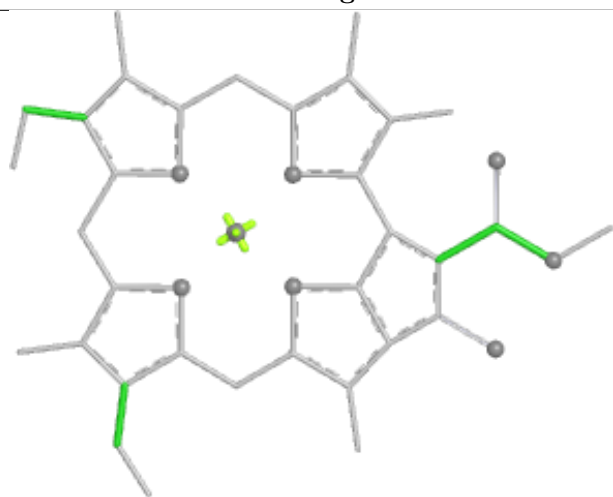
Ligand CLA B 804



Bond lengths



Bond angles

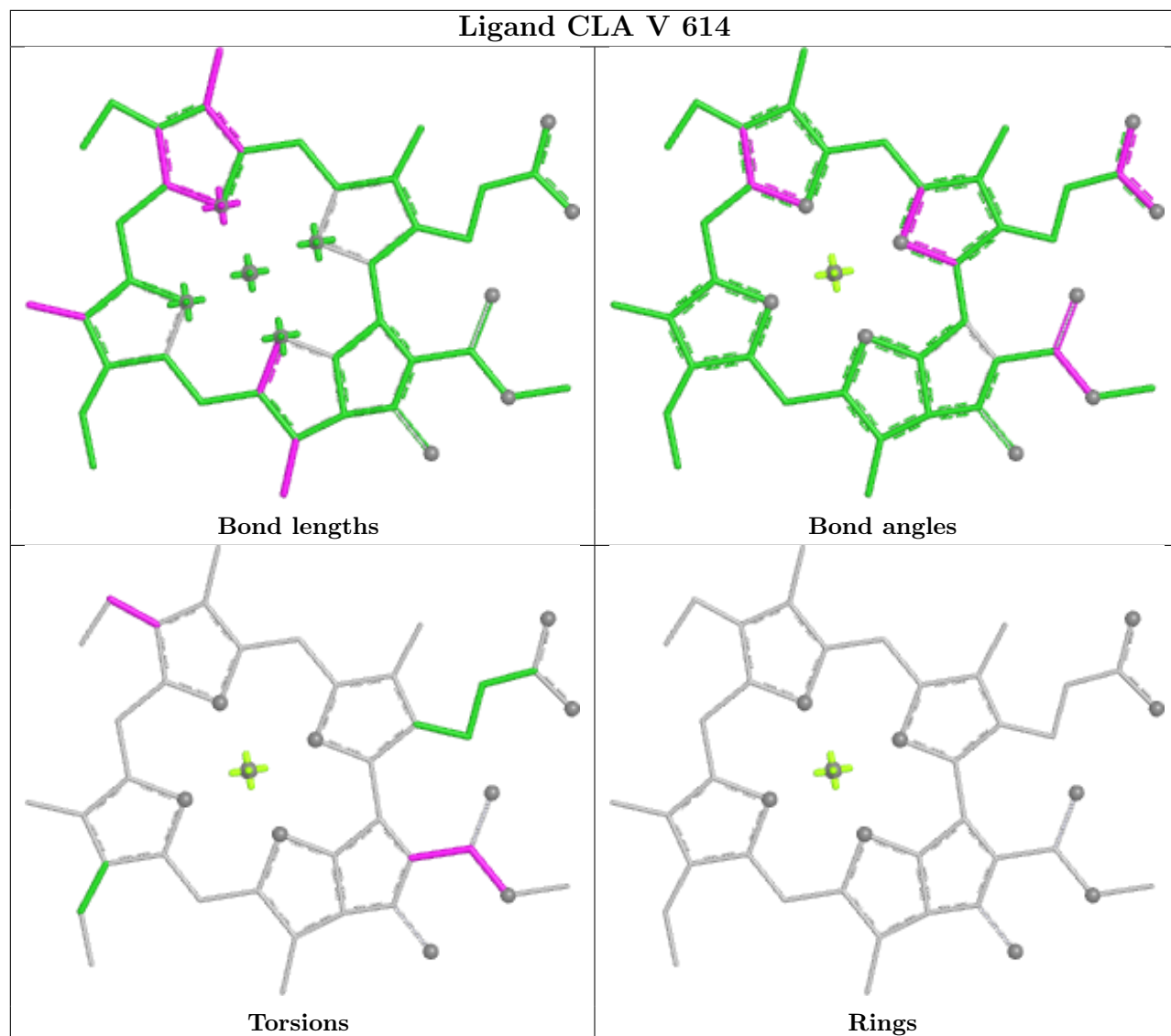


Torsions

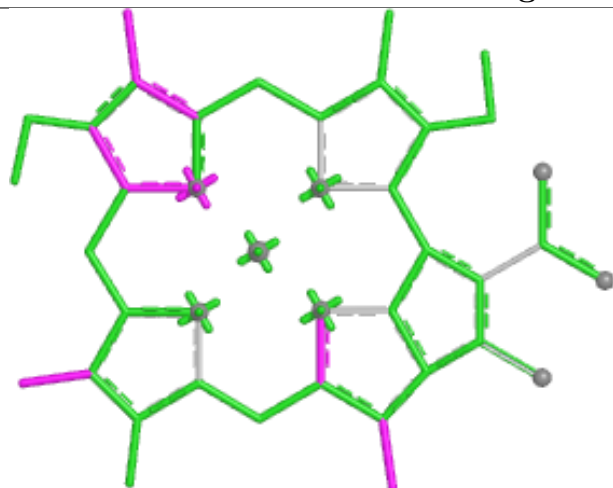


Rings

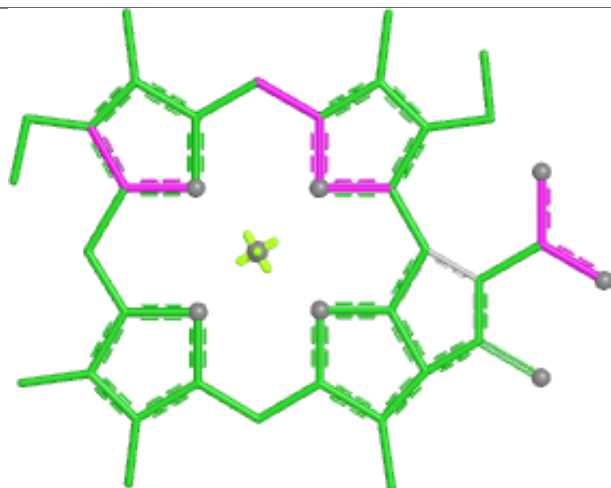
Ligand CLA V 614



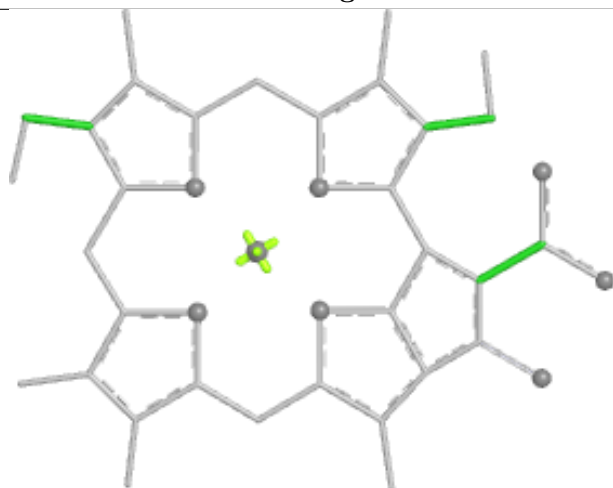
Ligand CLA 6 606



Bond lengths



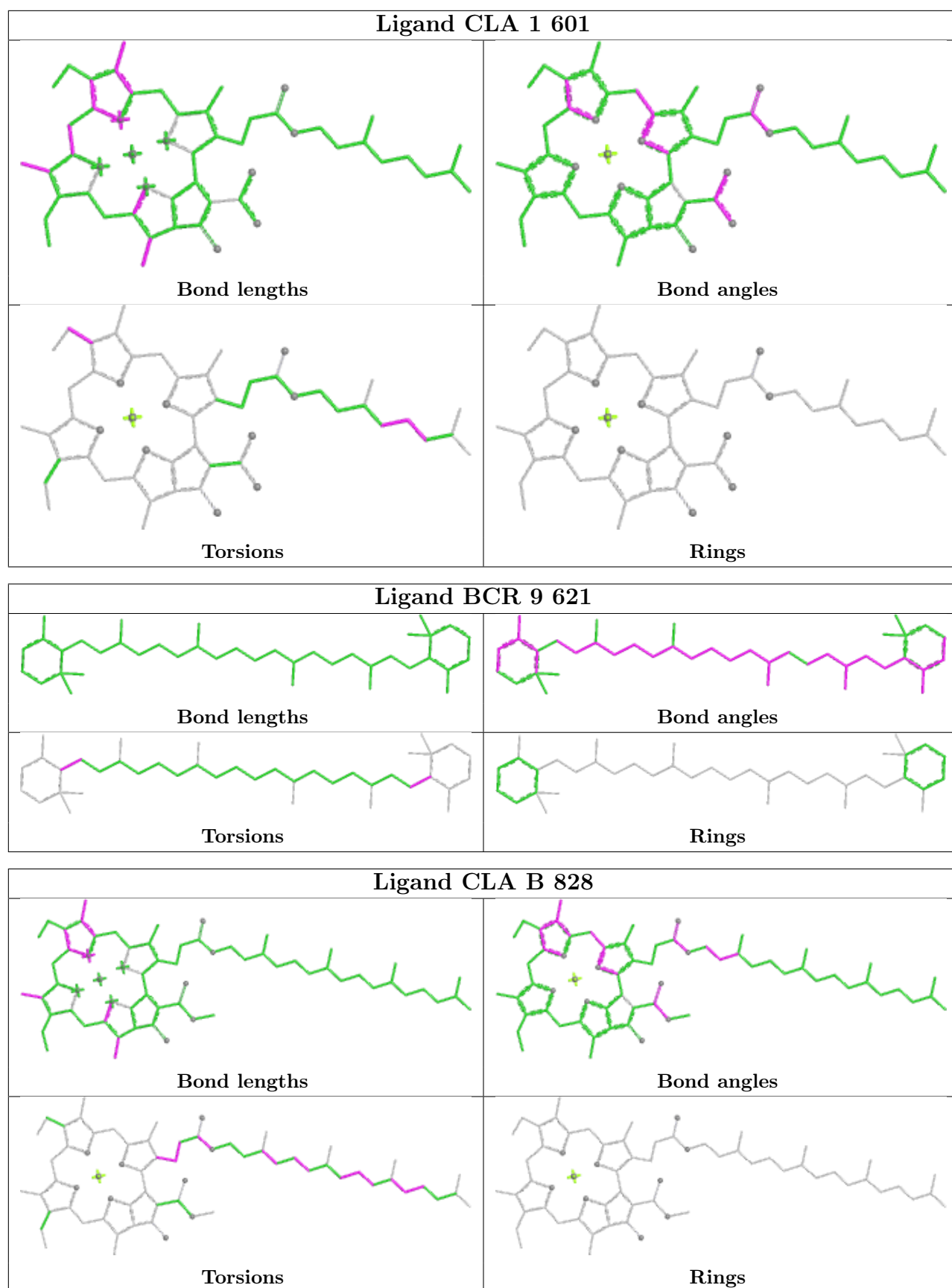
Bond angles



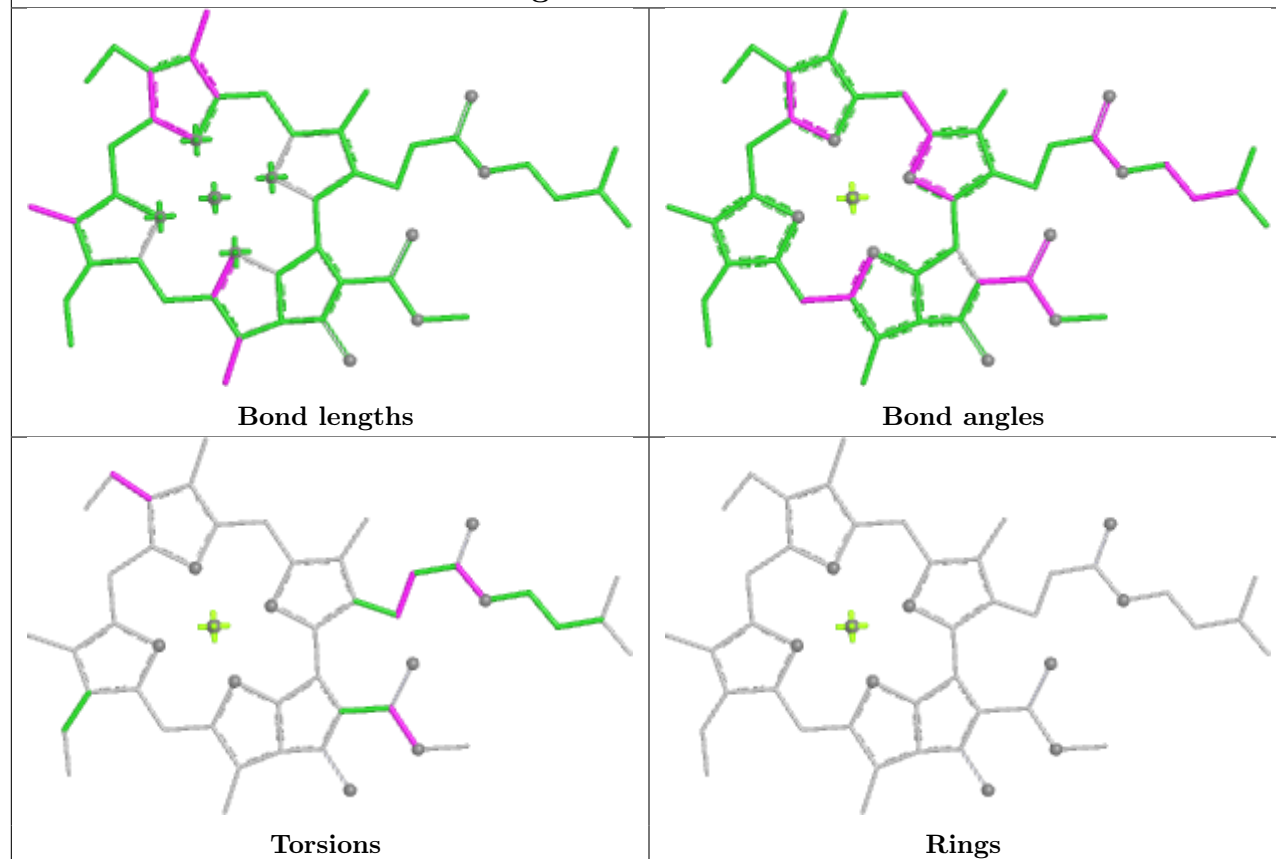
Torsions



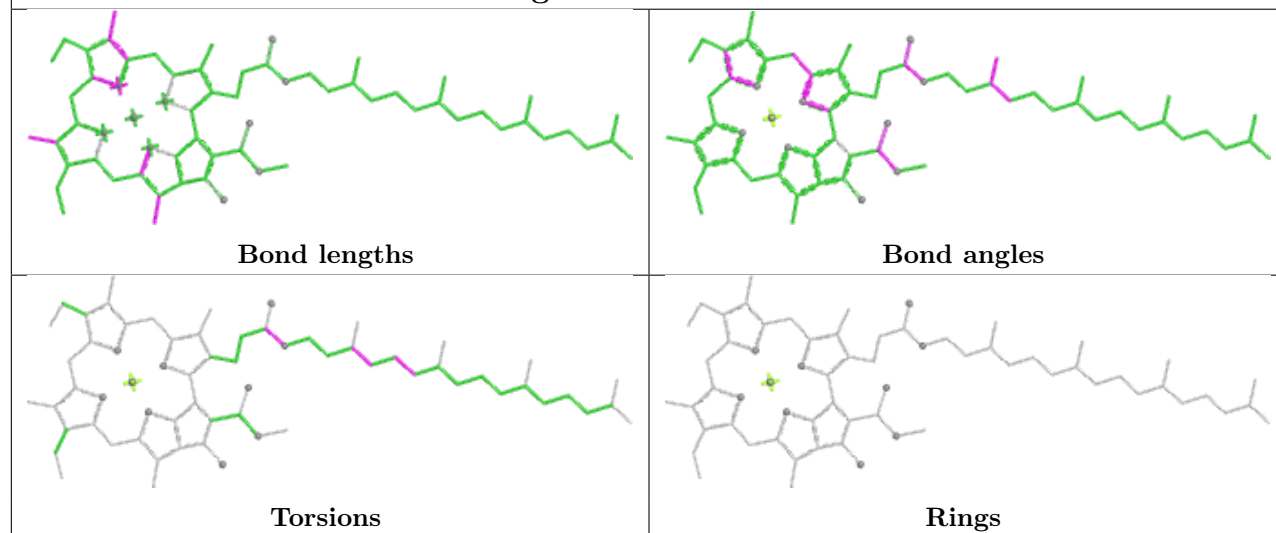
Rings



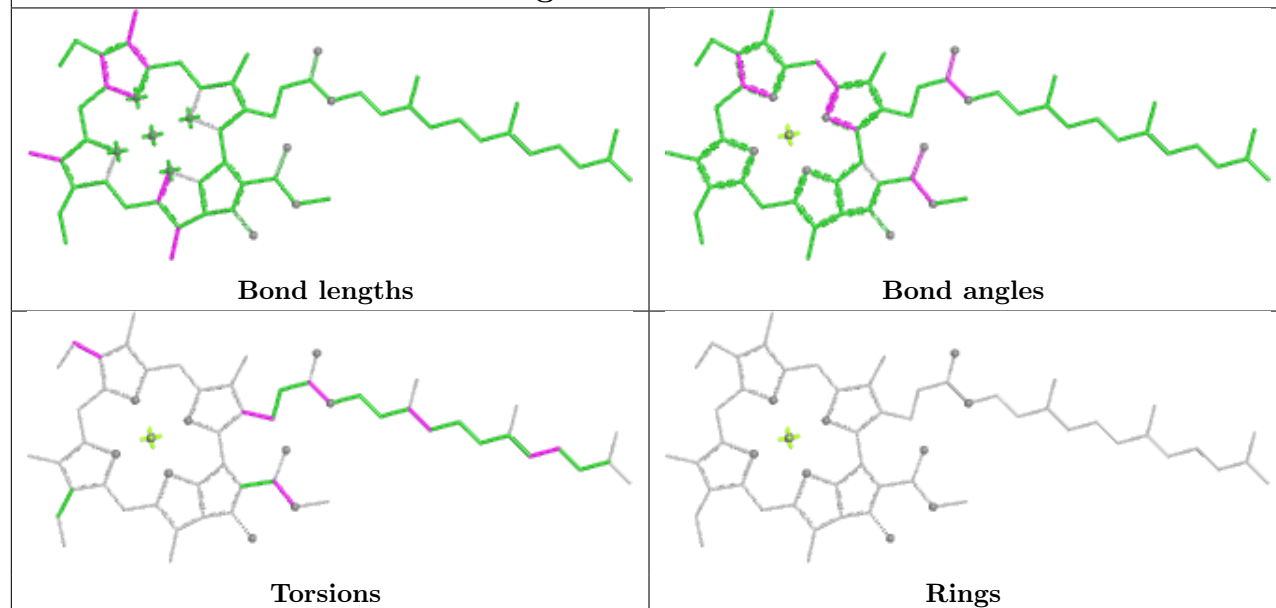
Ligand CLA A 832



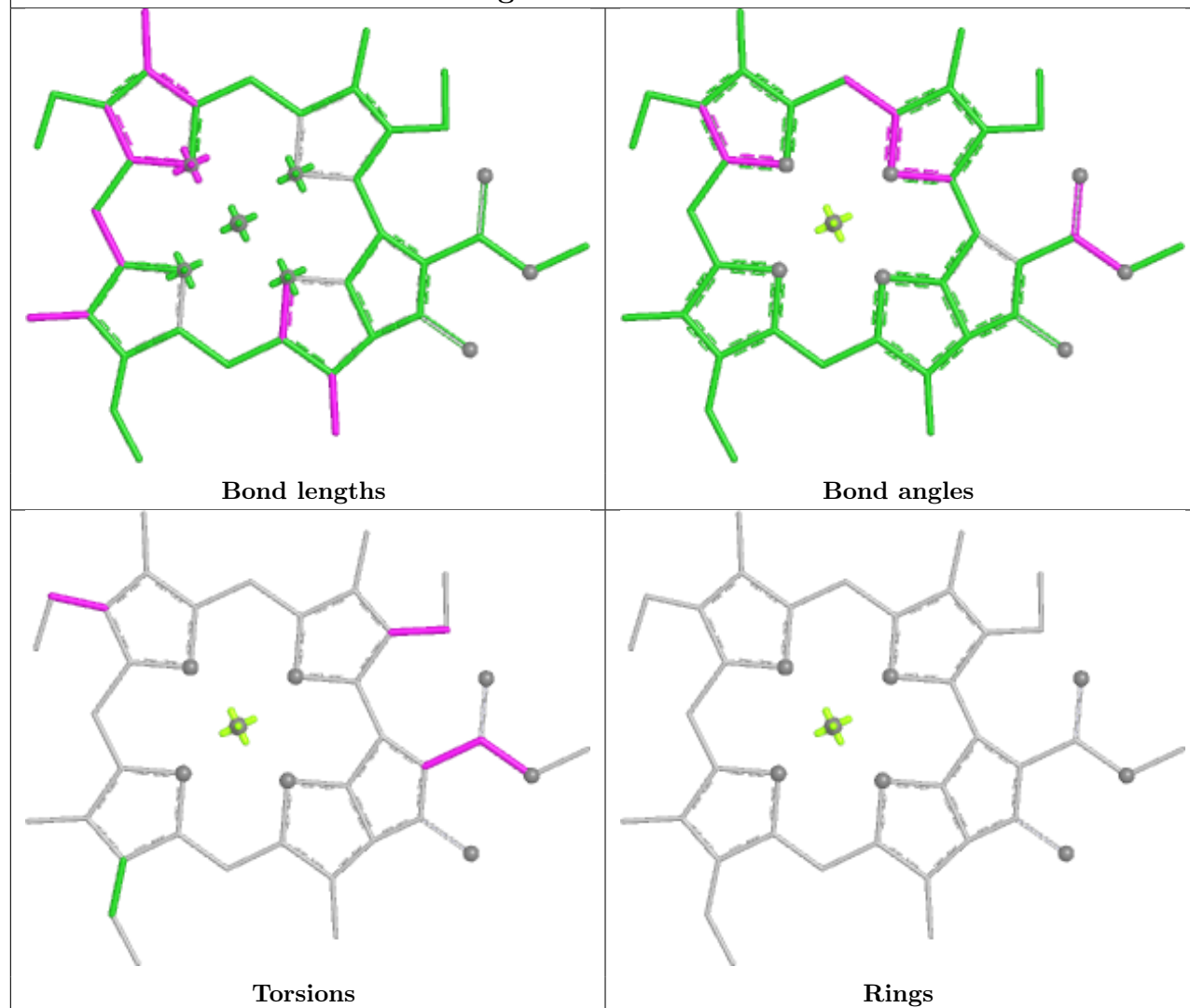
Ligand CLA A 836



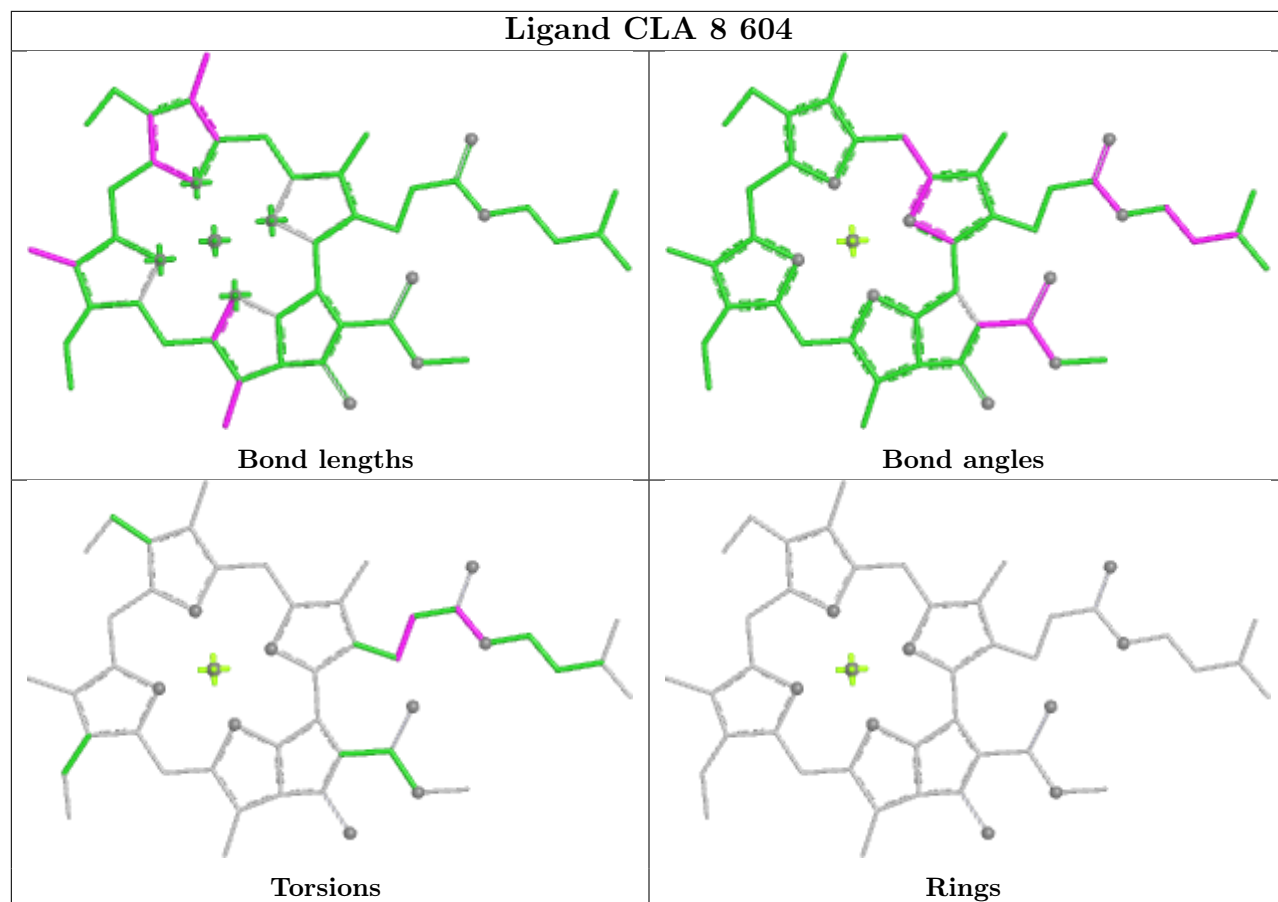
Ligand CLA 6 614



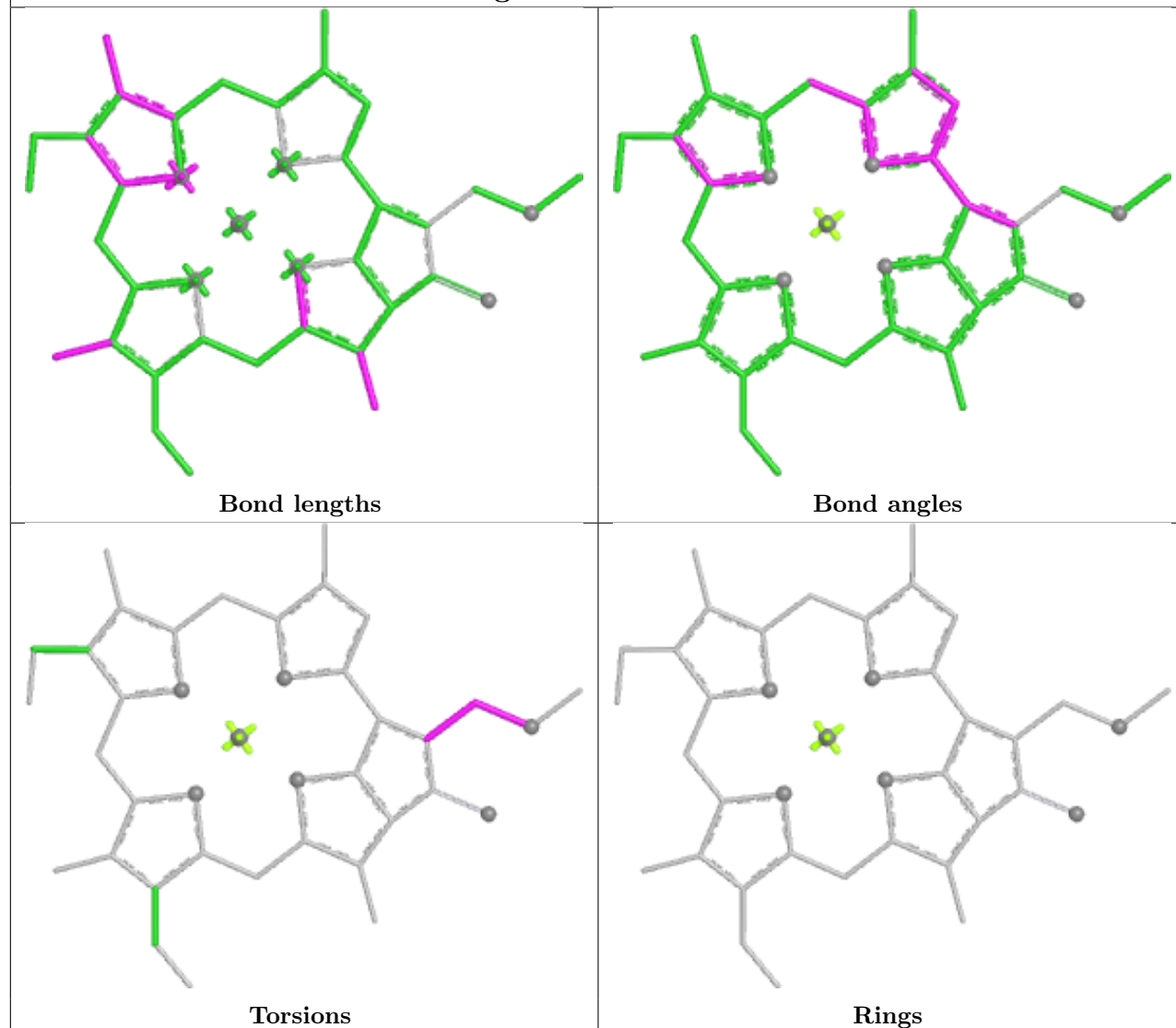
Ligand CLA F 303



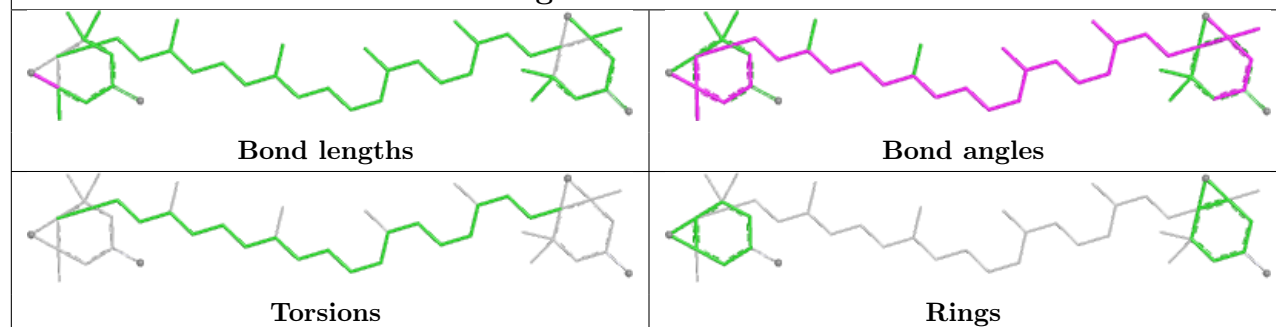
Ligand CLA 8 604



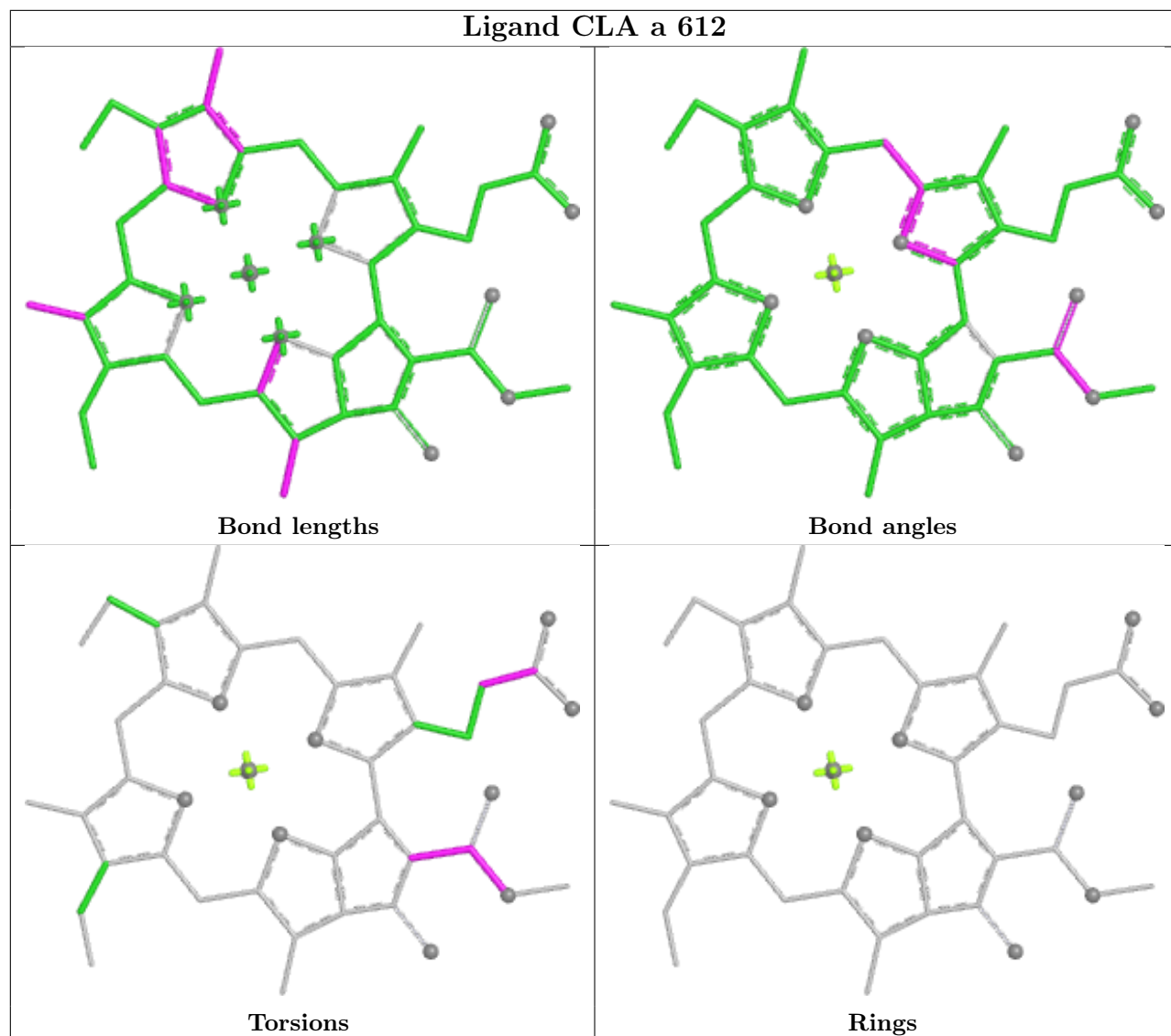
Ligand CLA 1 606



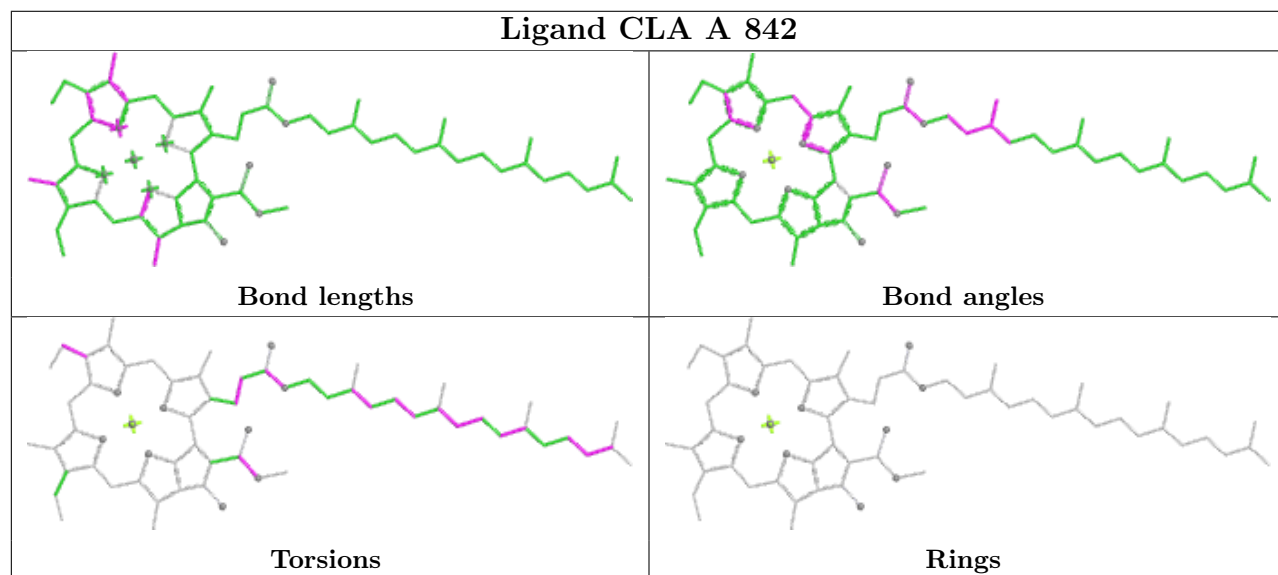
Ligand XAT a 618

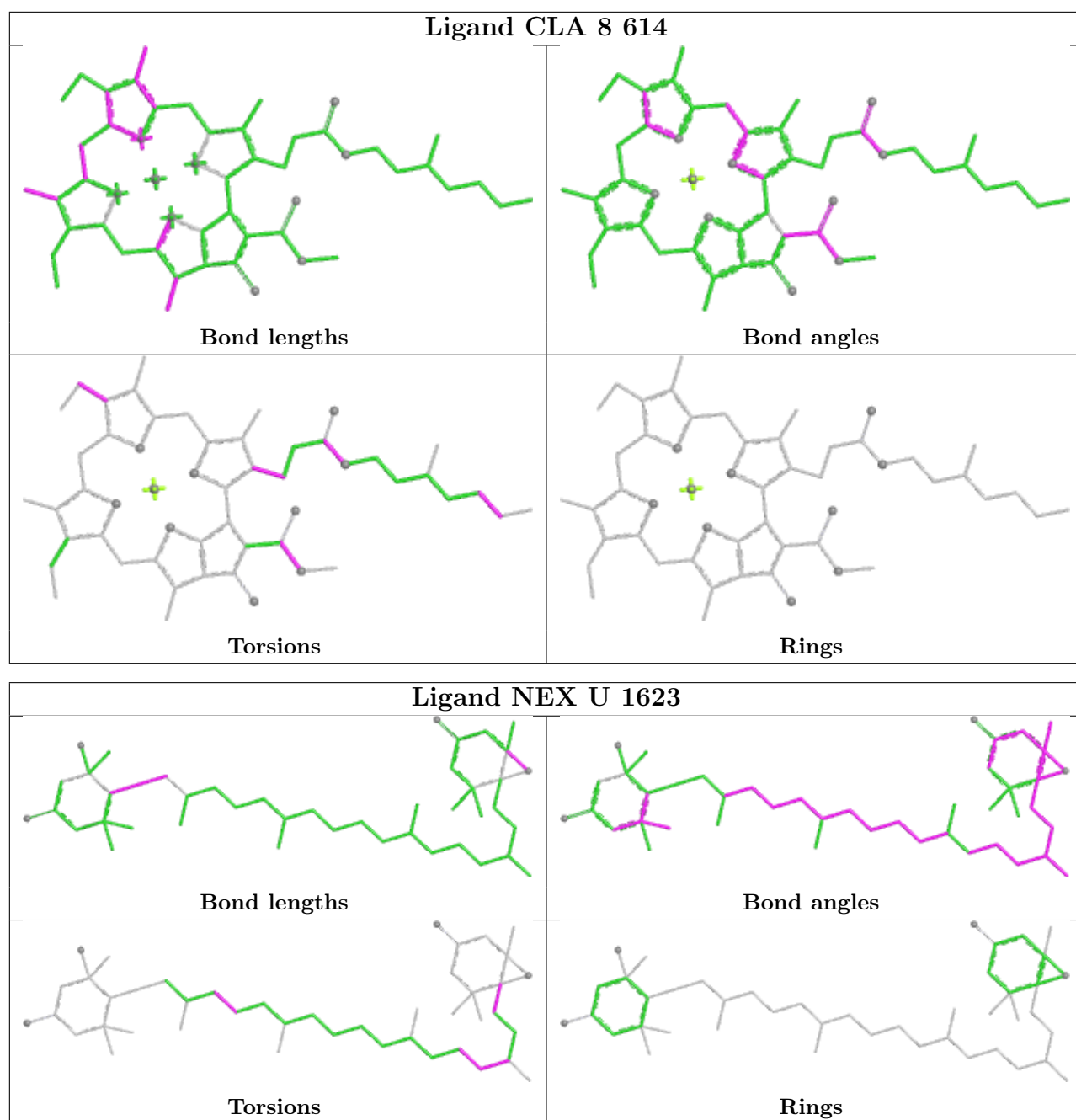


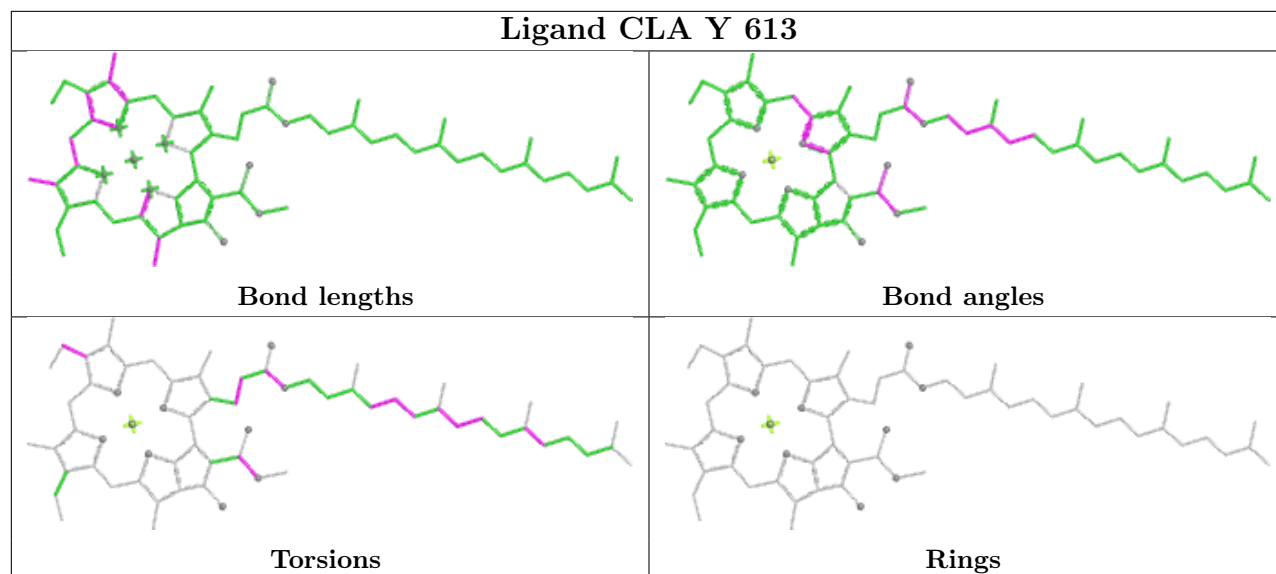
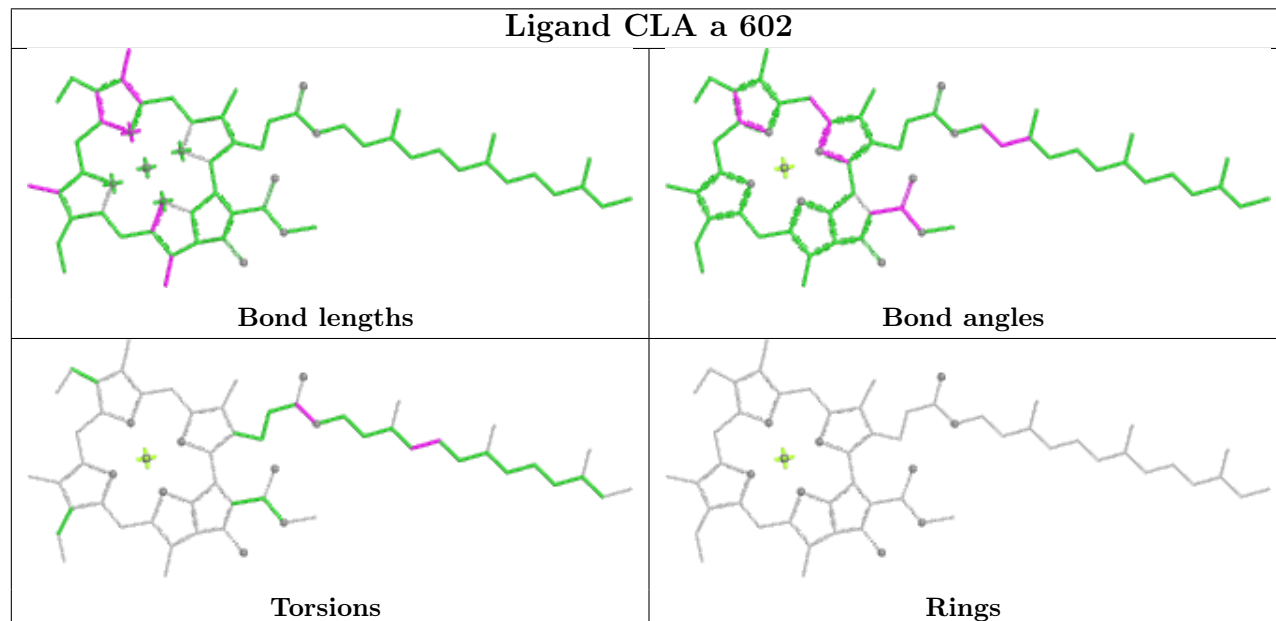
Ligand CLA a 612



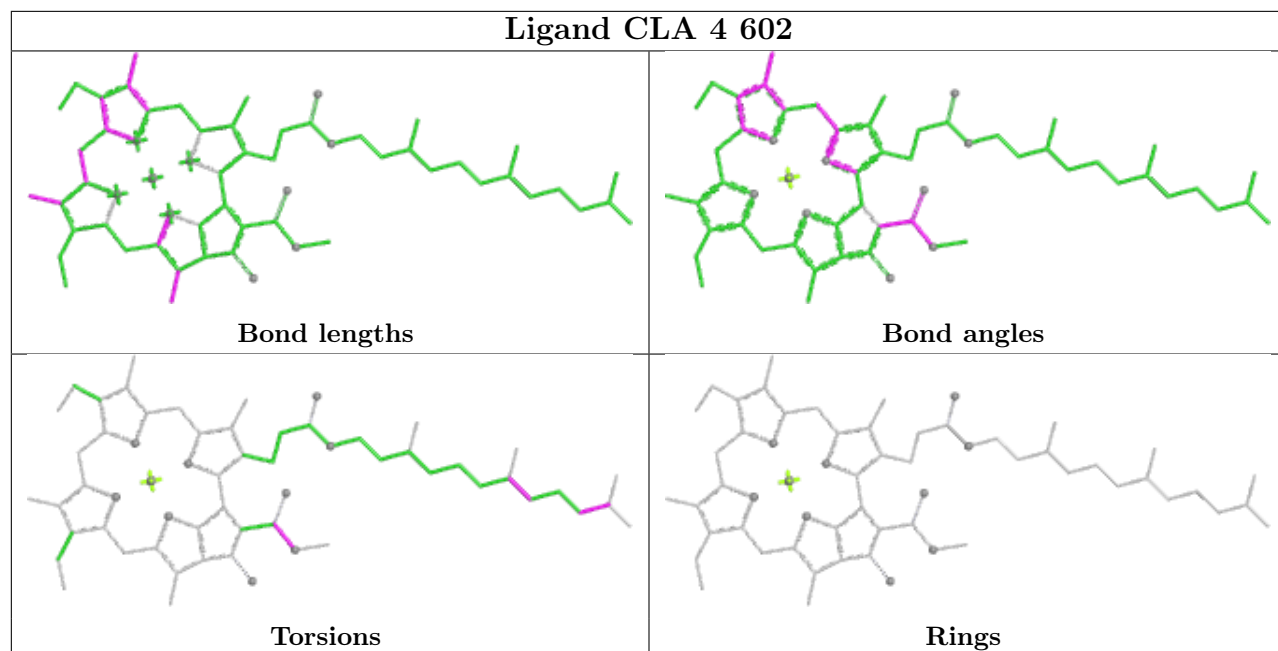
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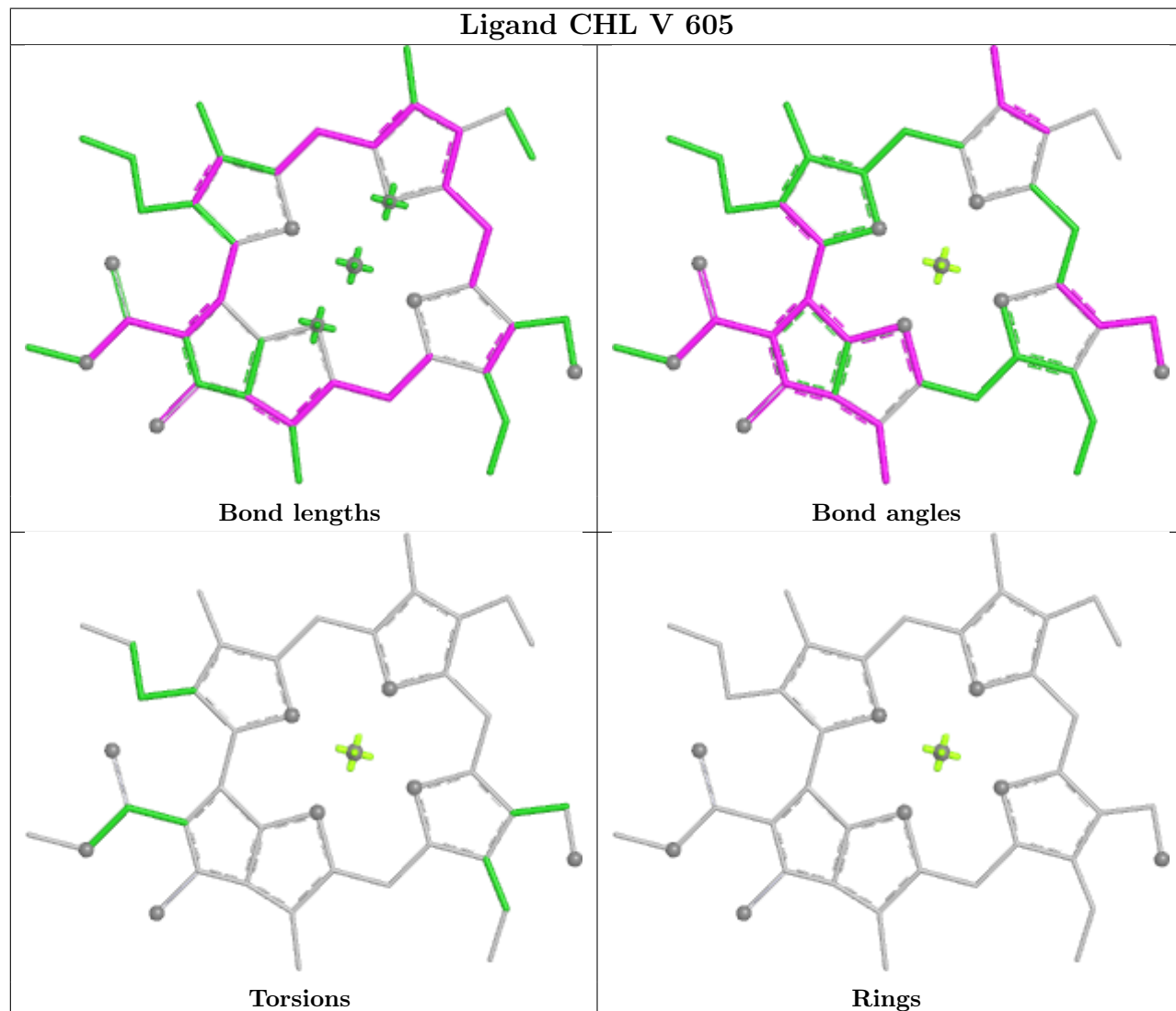


Ligand CLA Y 613**Ligand CLA a 602**

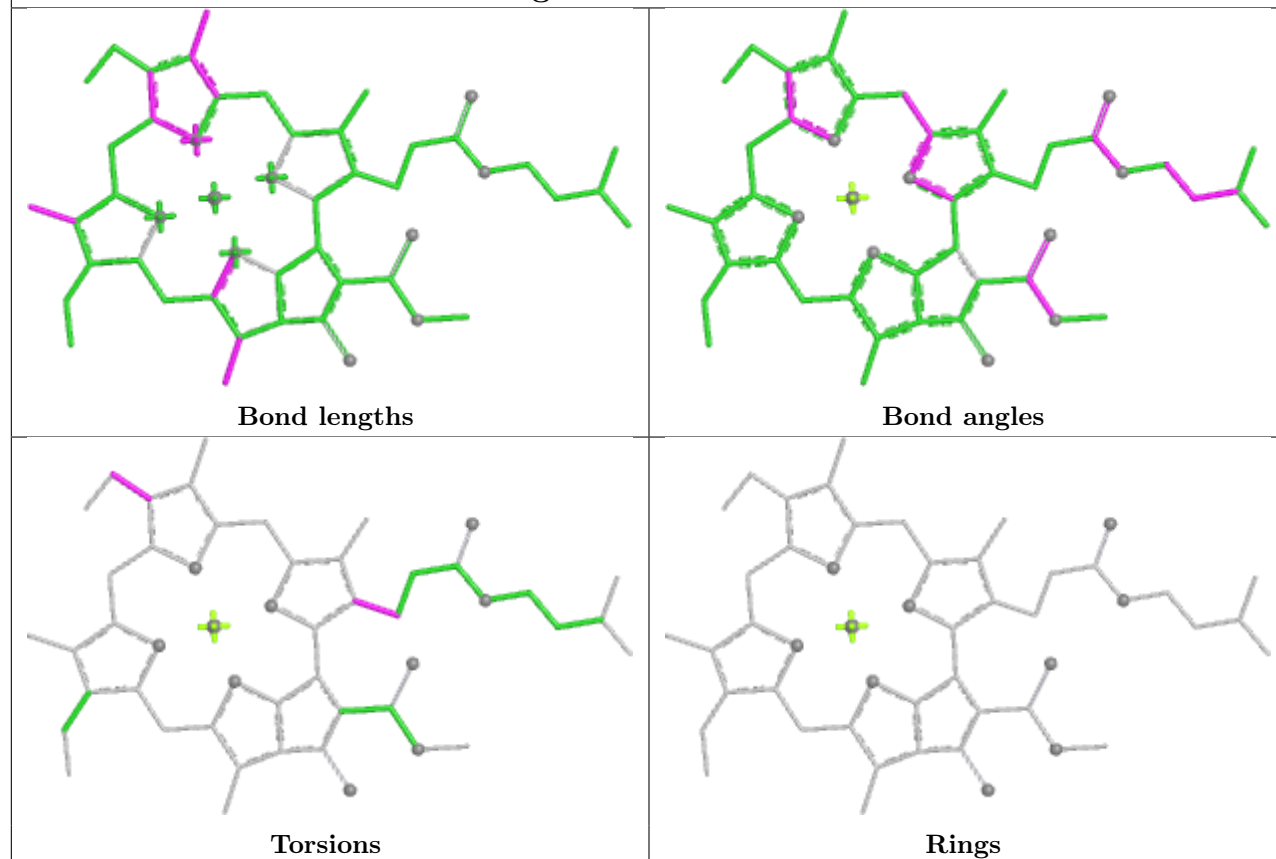
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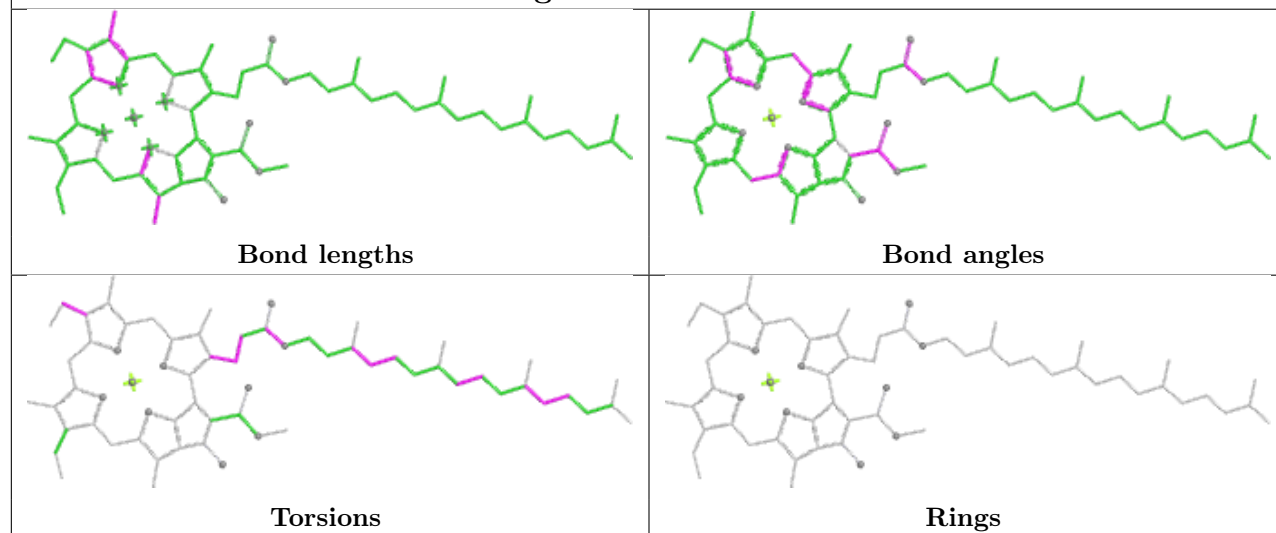
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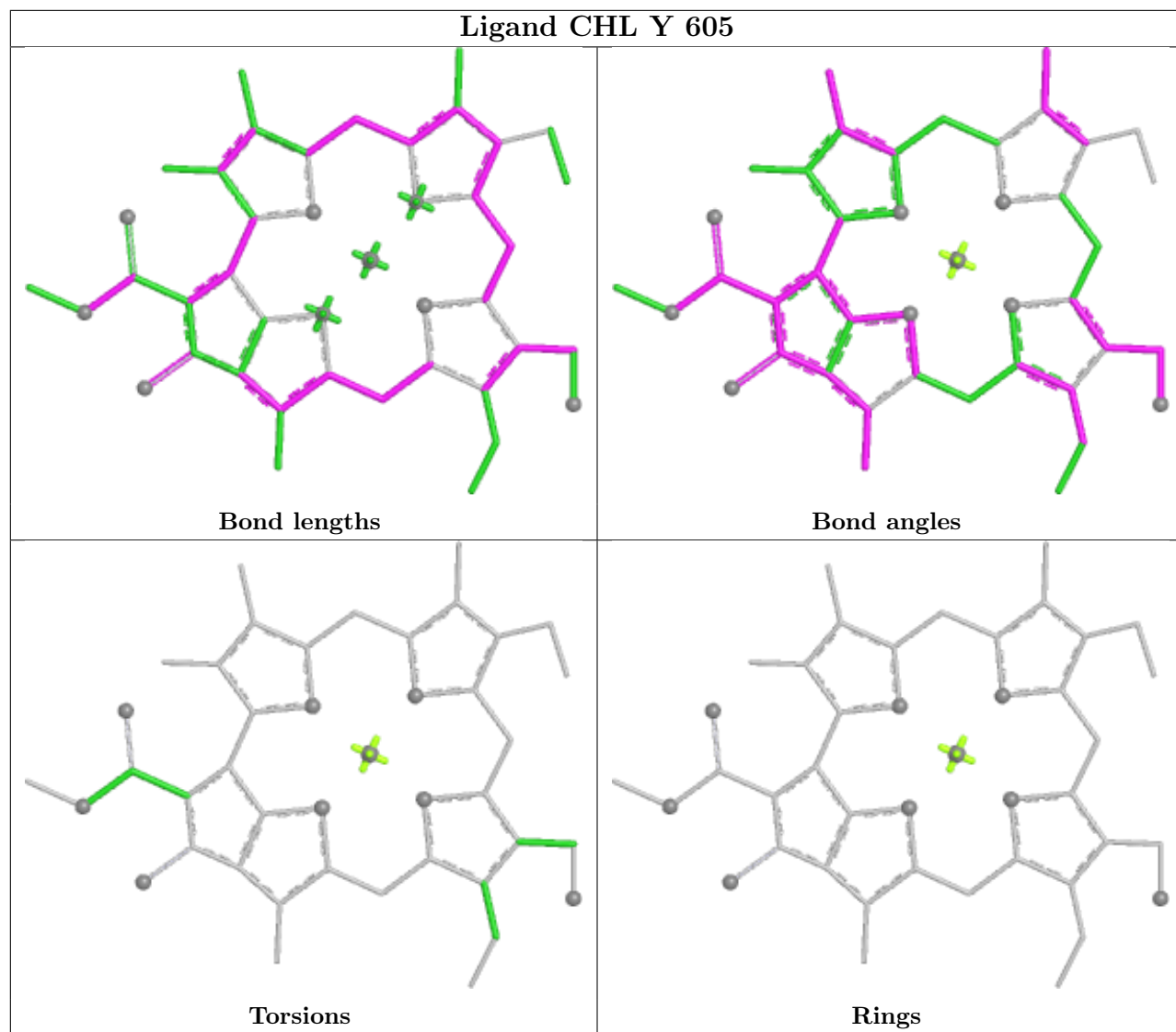


Ligand CLA B 820

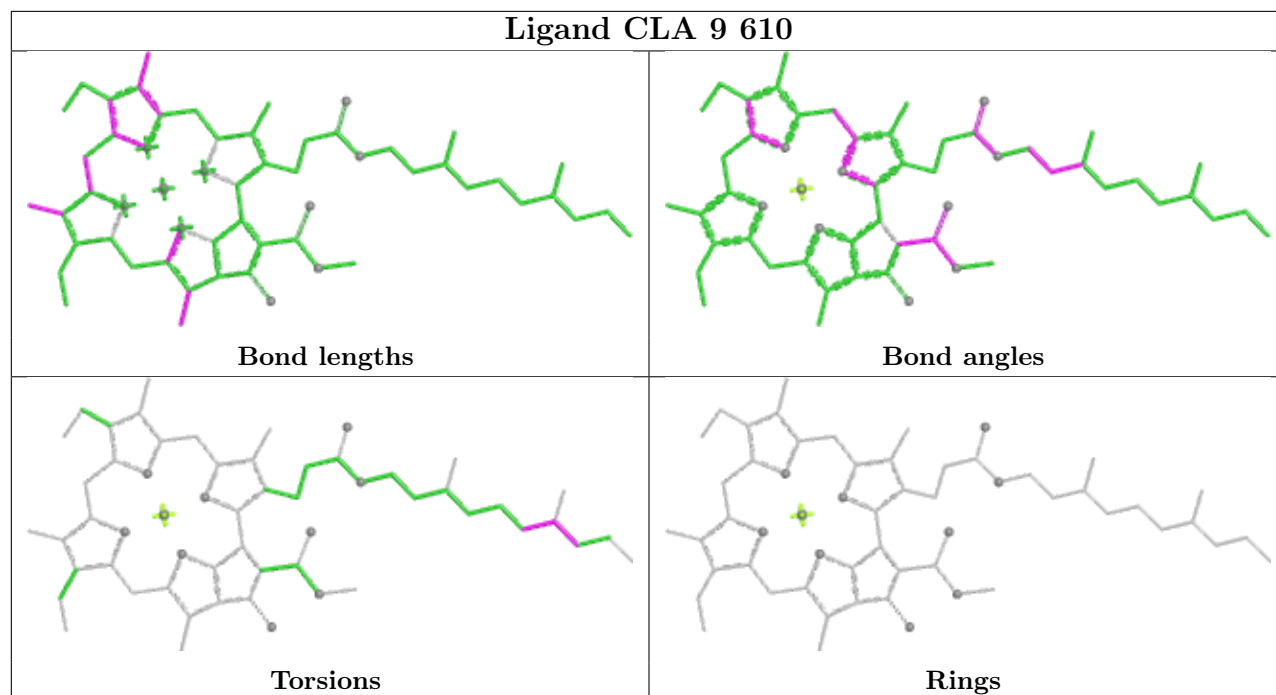


Ligand CLA L 303

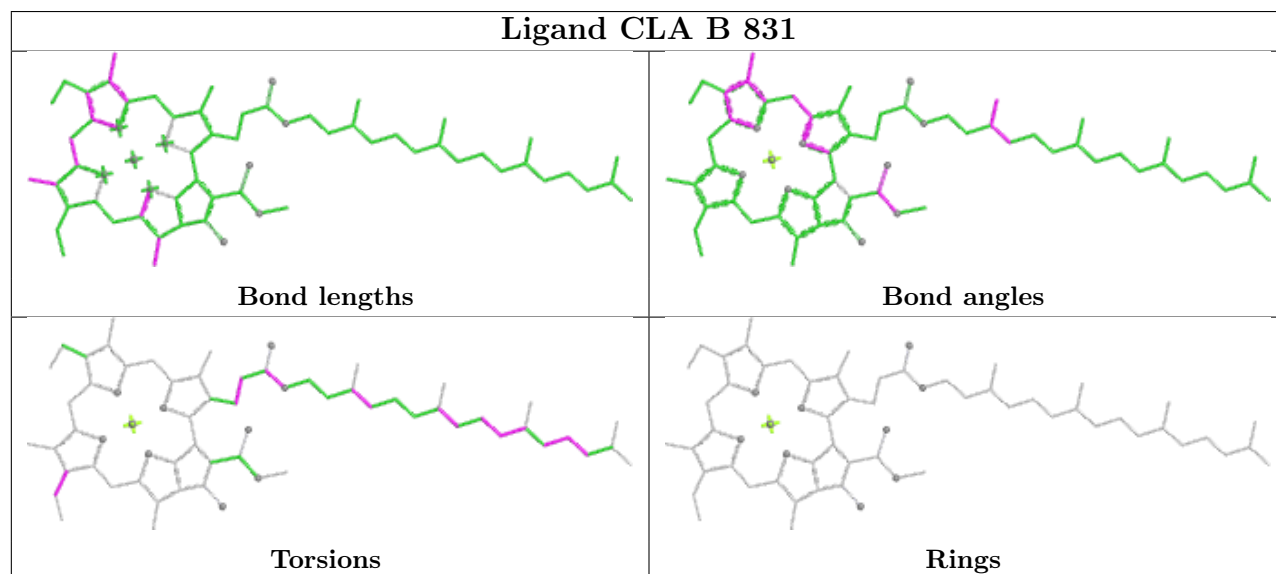




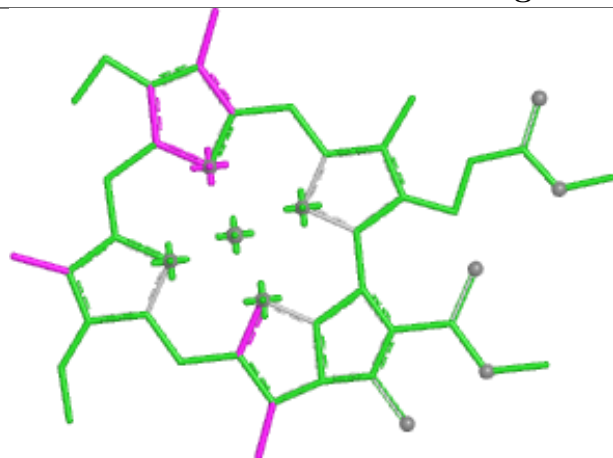
Ligand CLA 9 610



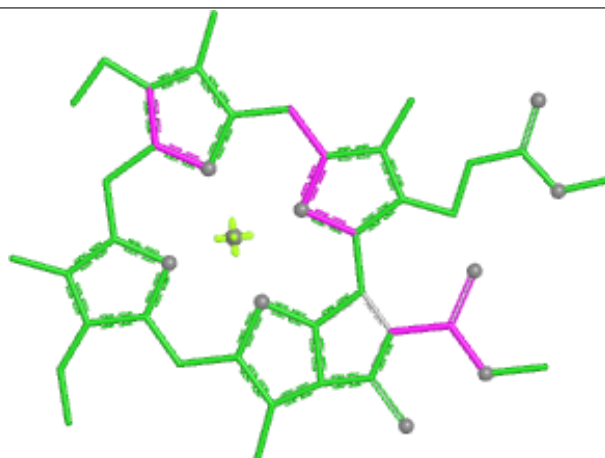
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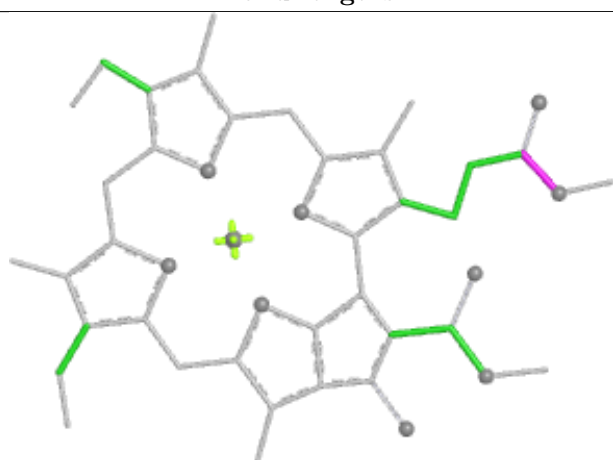
Ligand CLA B 838



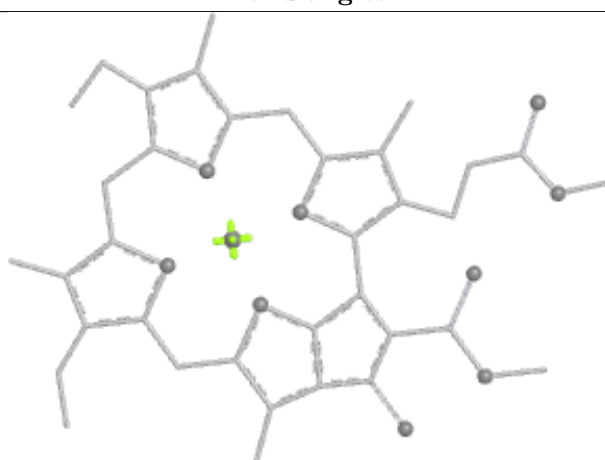
Bond lengths



Bond angles

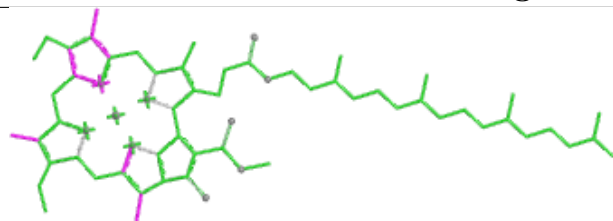


Torsions

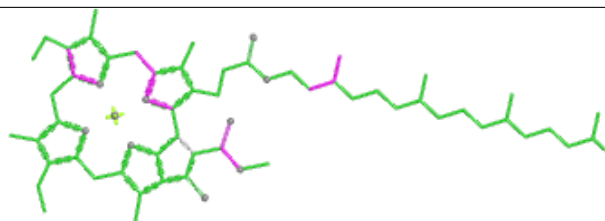


Rings

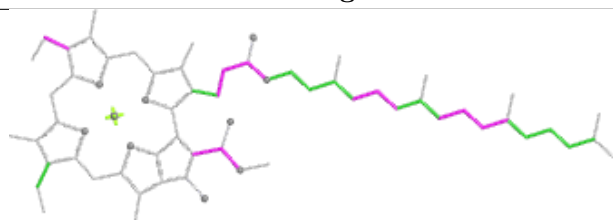
Ligand CLA A 834



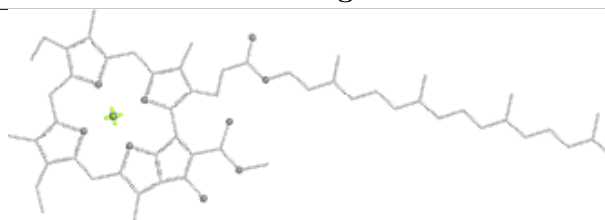
Bond lengths



Bond angles

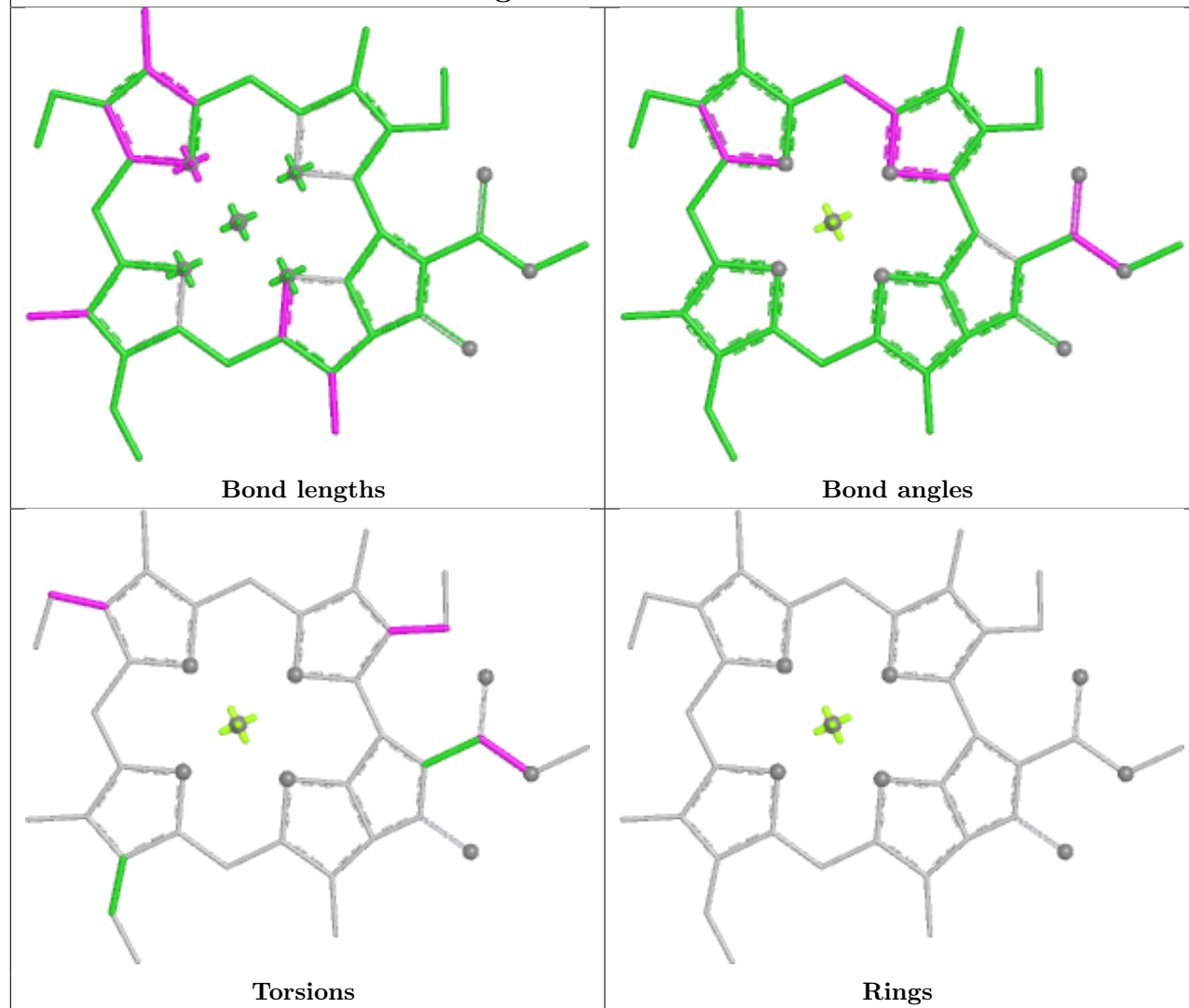


Torsions

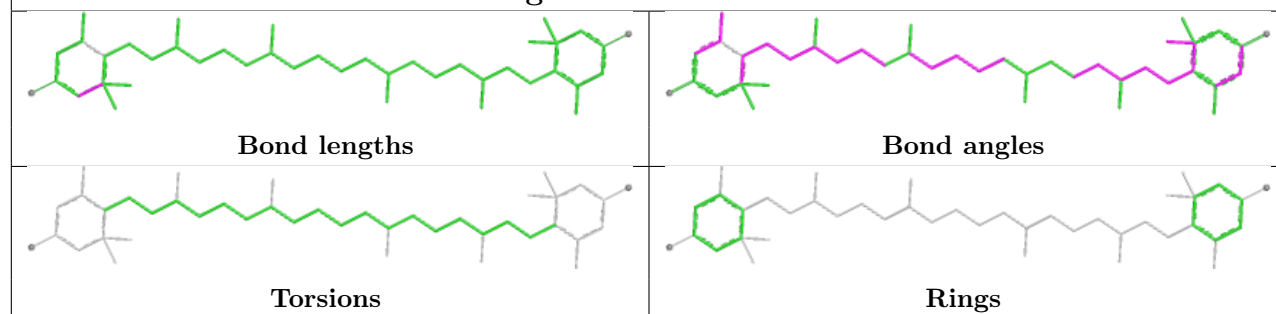


Rings

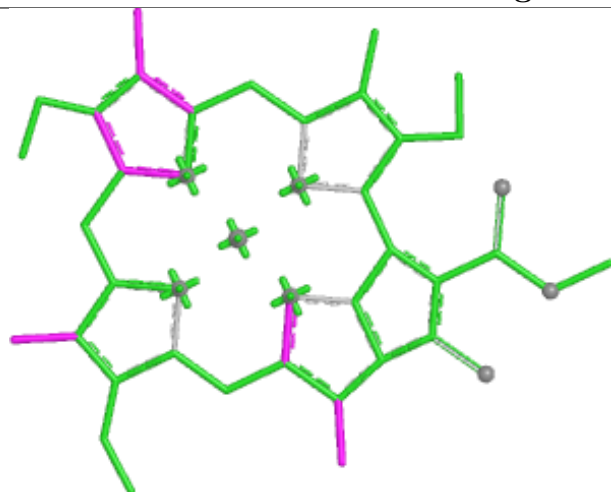
Ligand CLA U 614



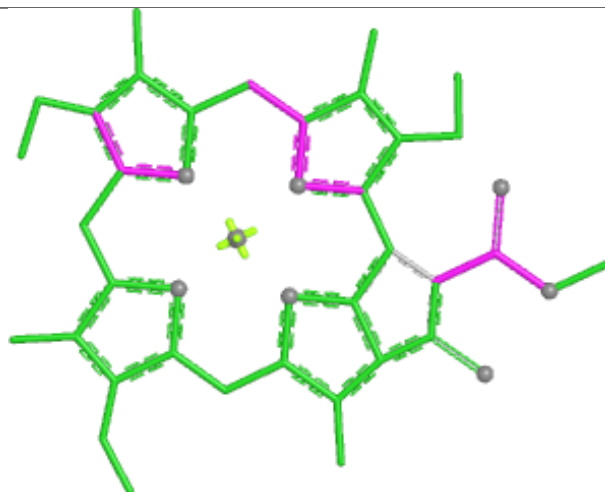
Ligand LUT Z 1620



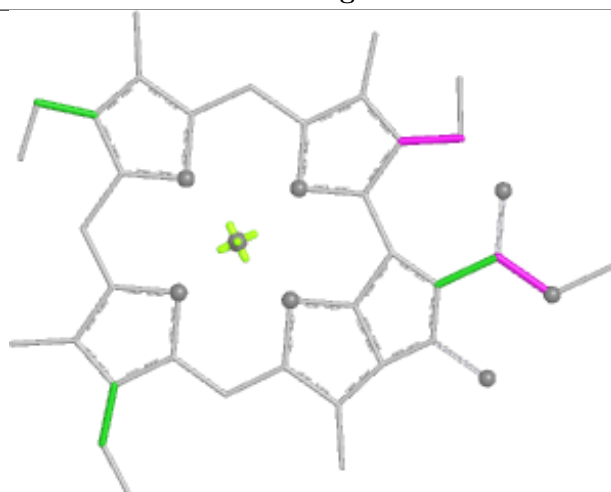
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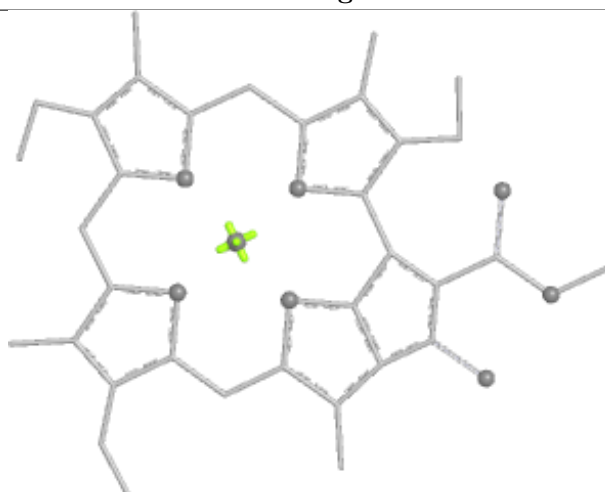
Bond lengths



Bond angles

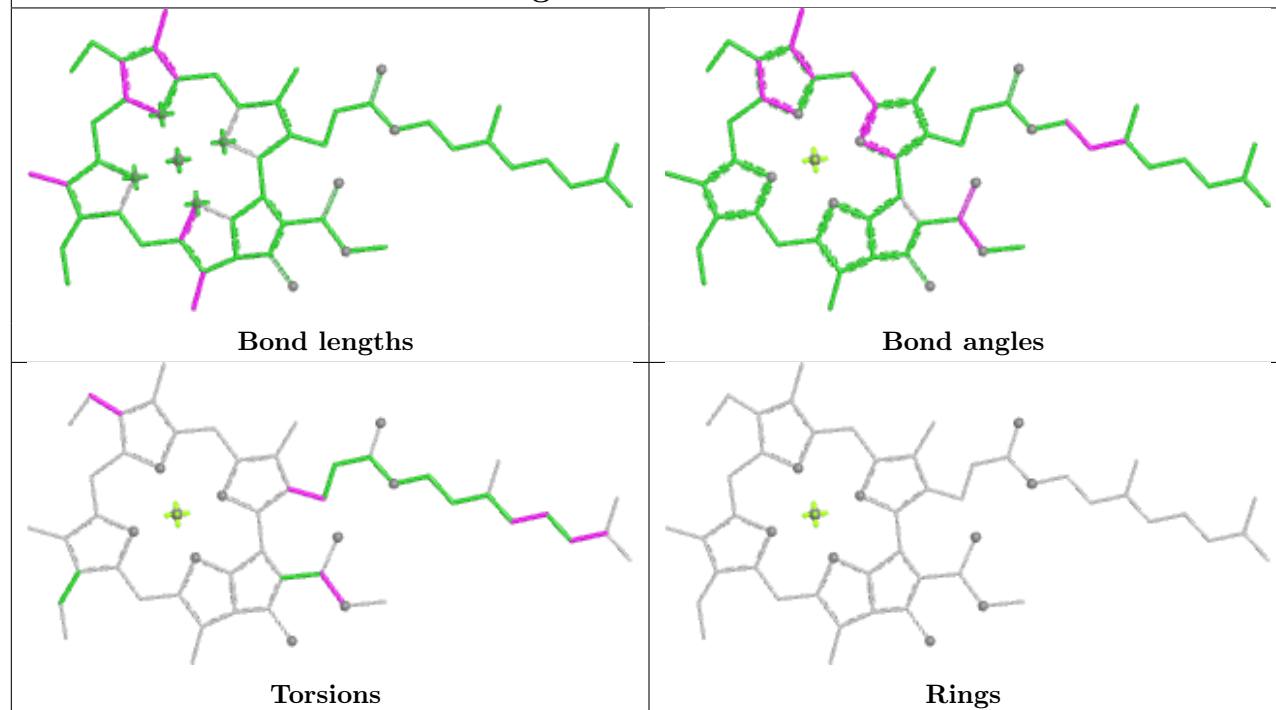


Torsions

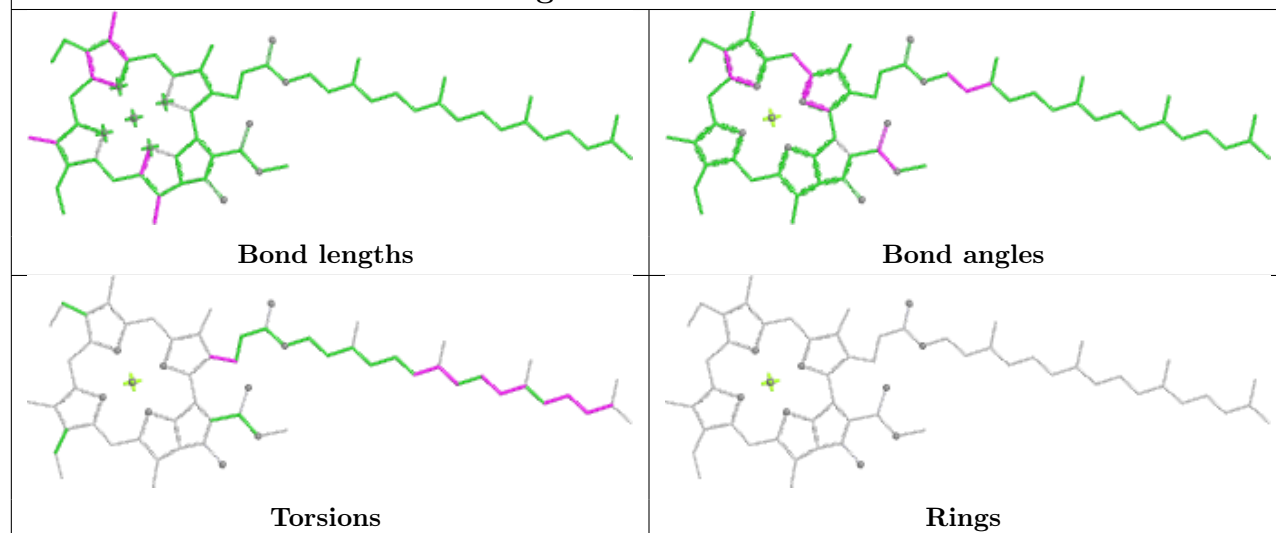


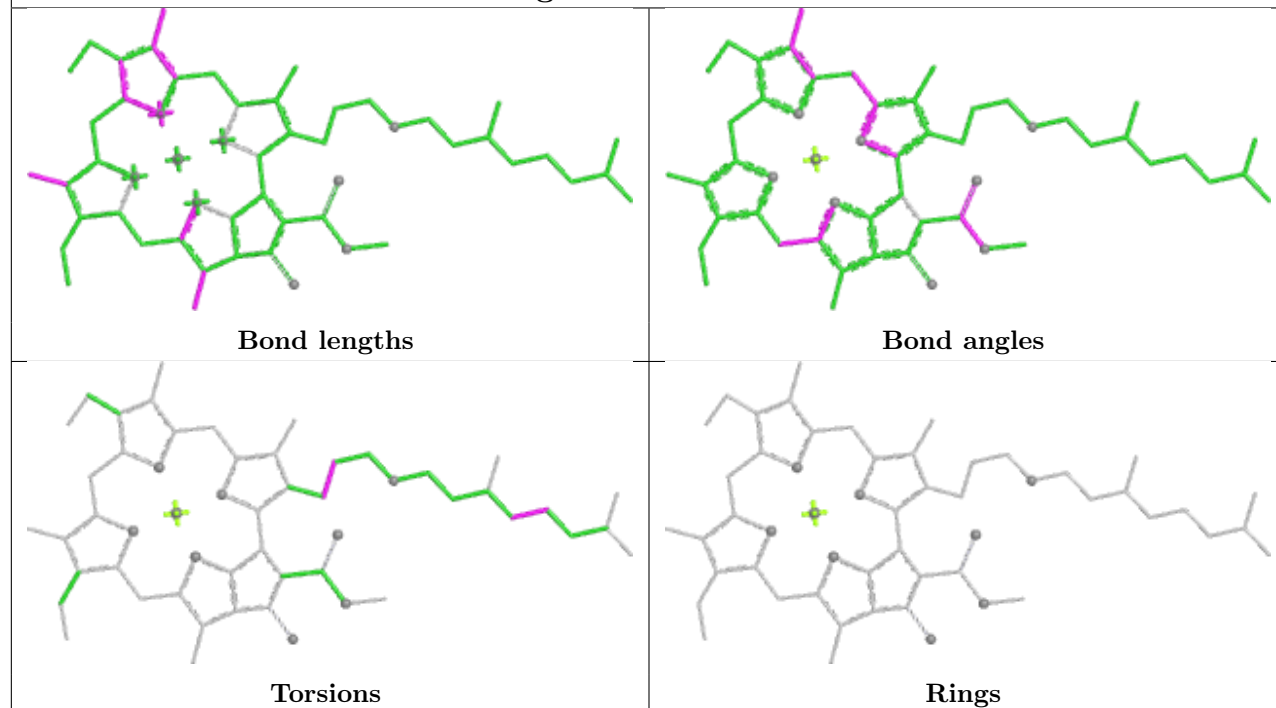
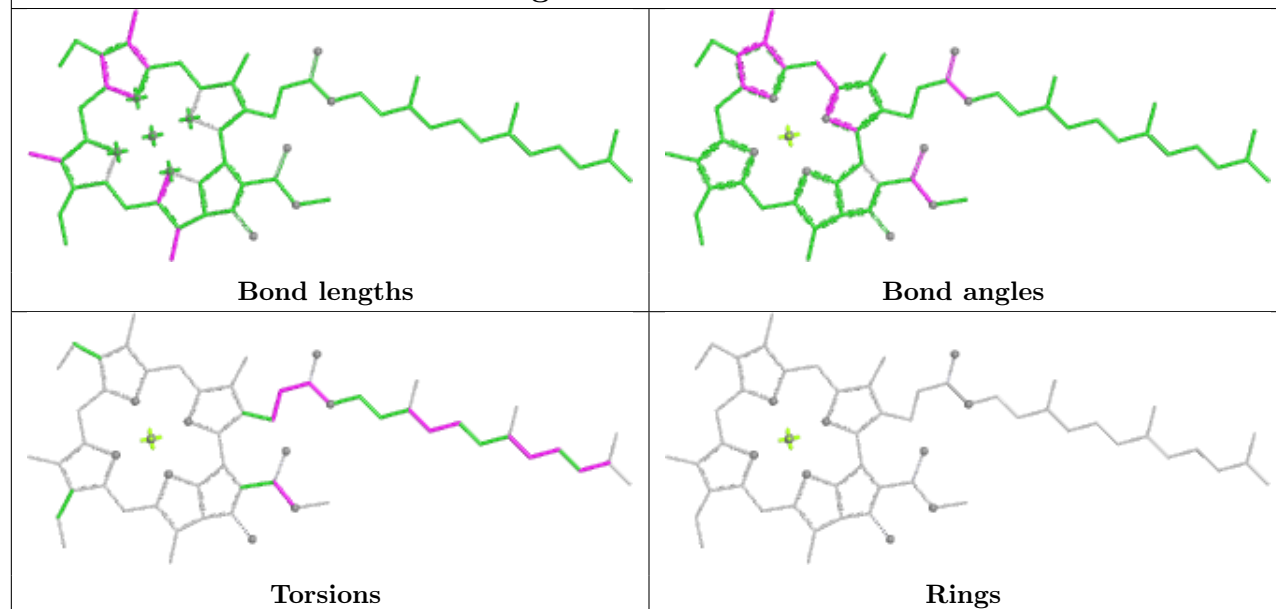
Rings

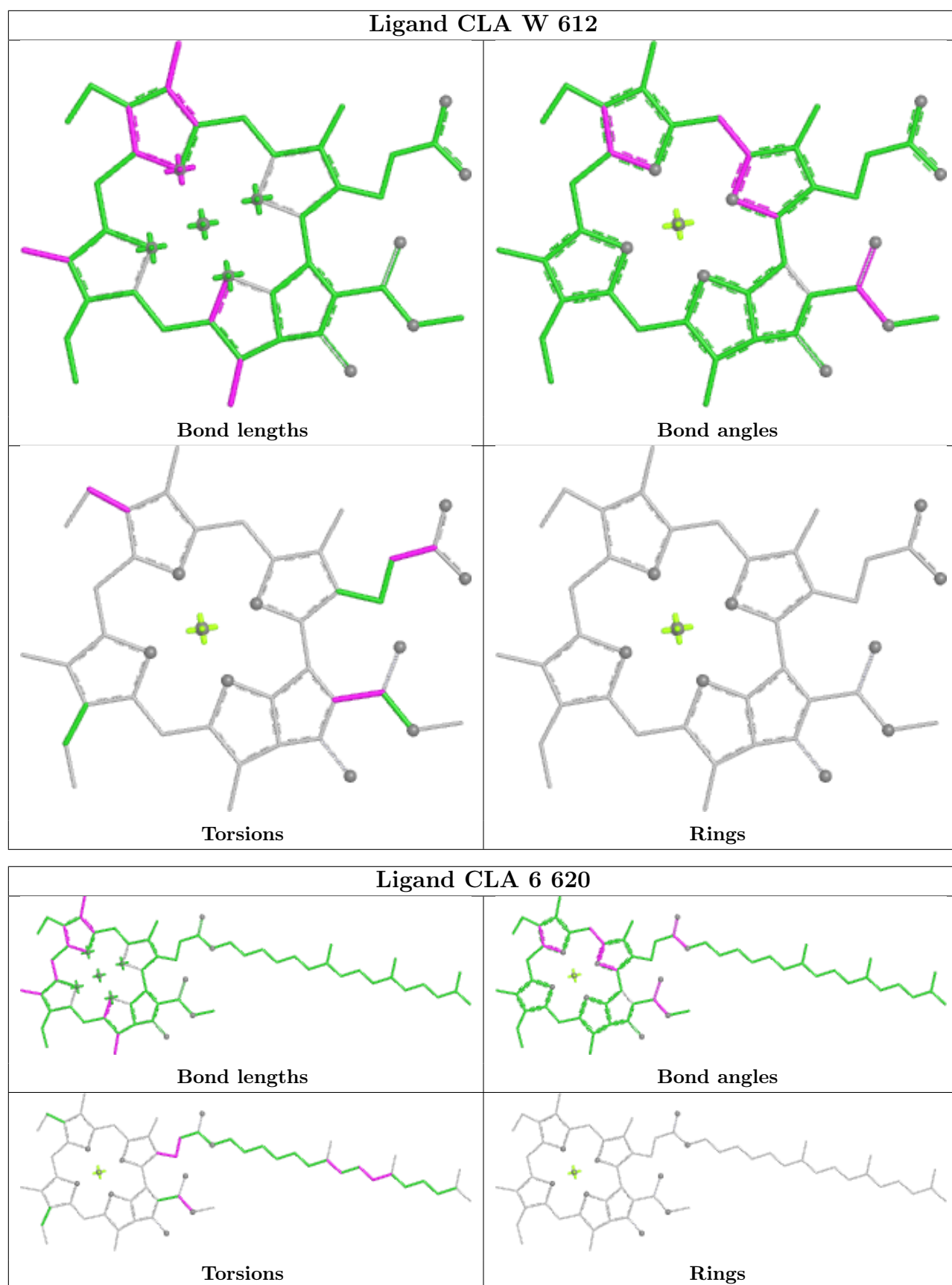
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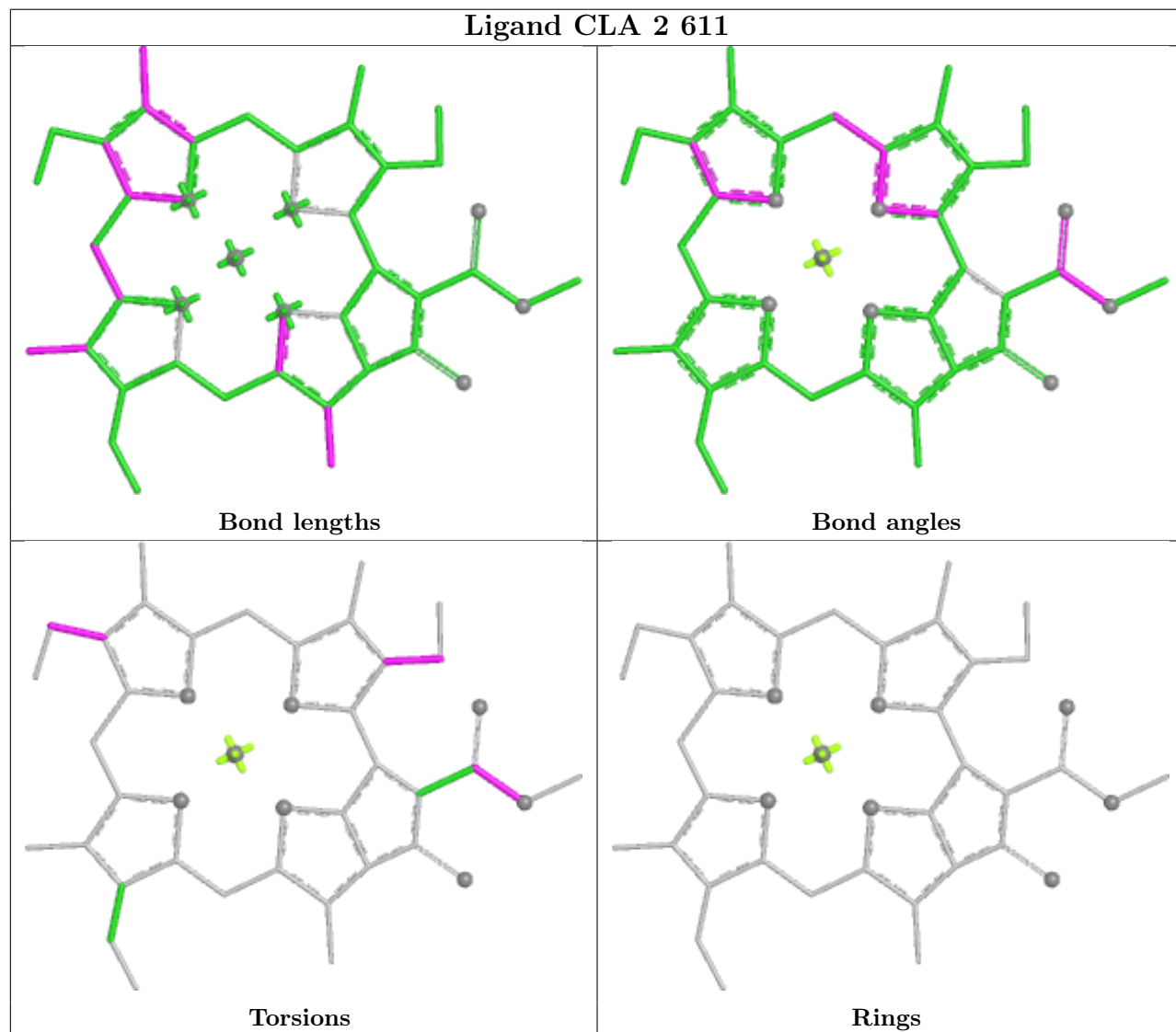
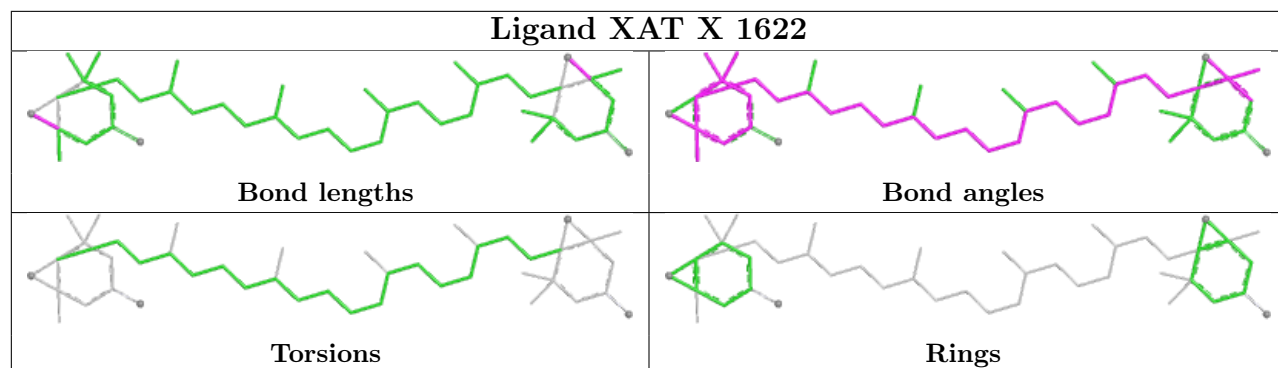


Ligand CLA 5 609

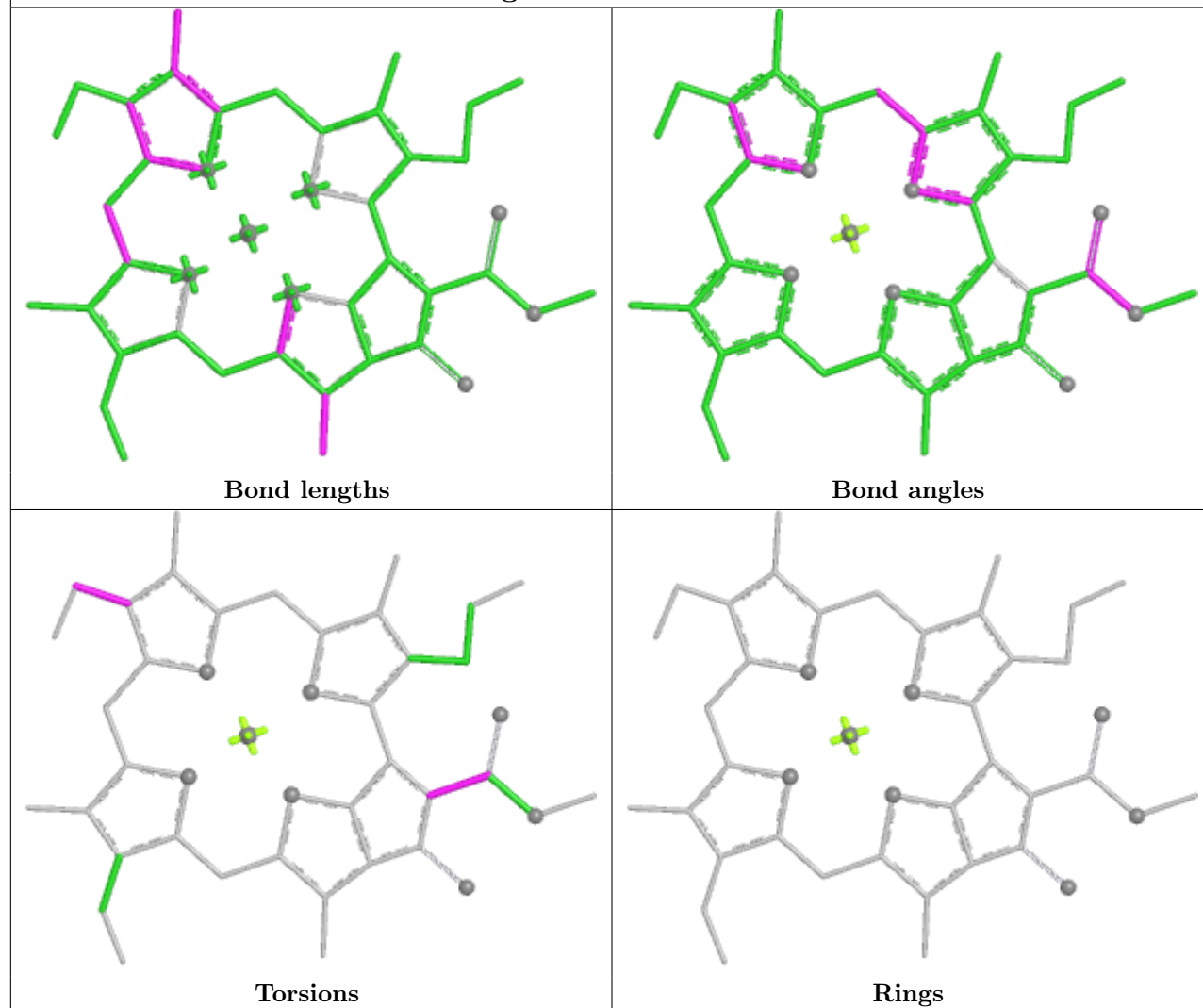


Ligand CLA a 603**Ligand CLA A 818**

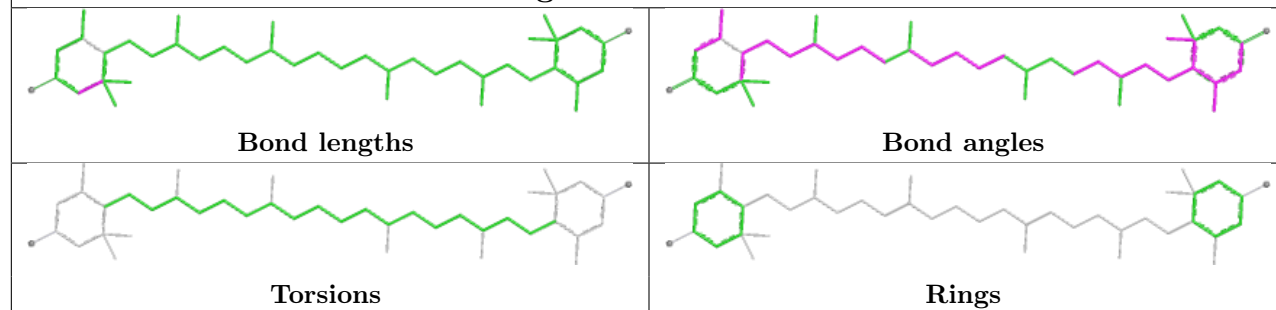


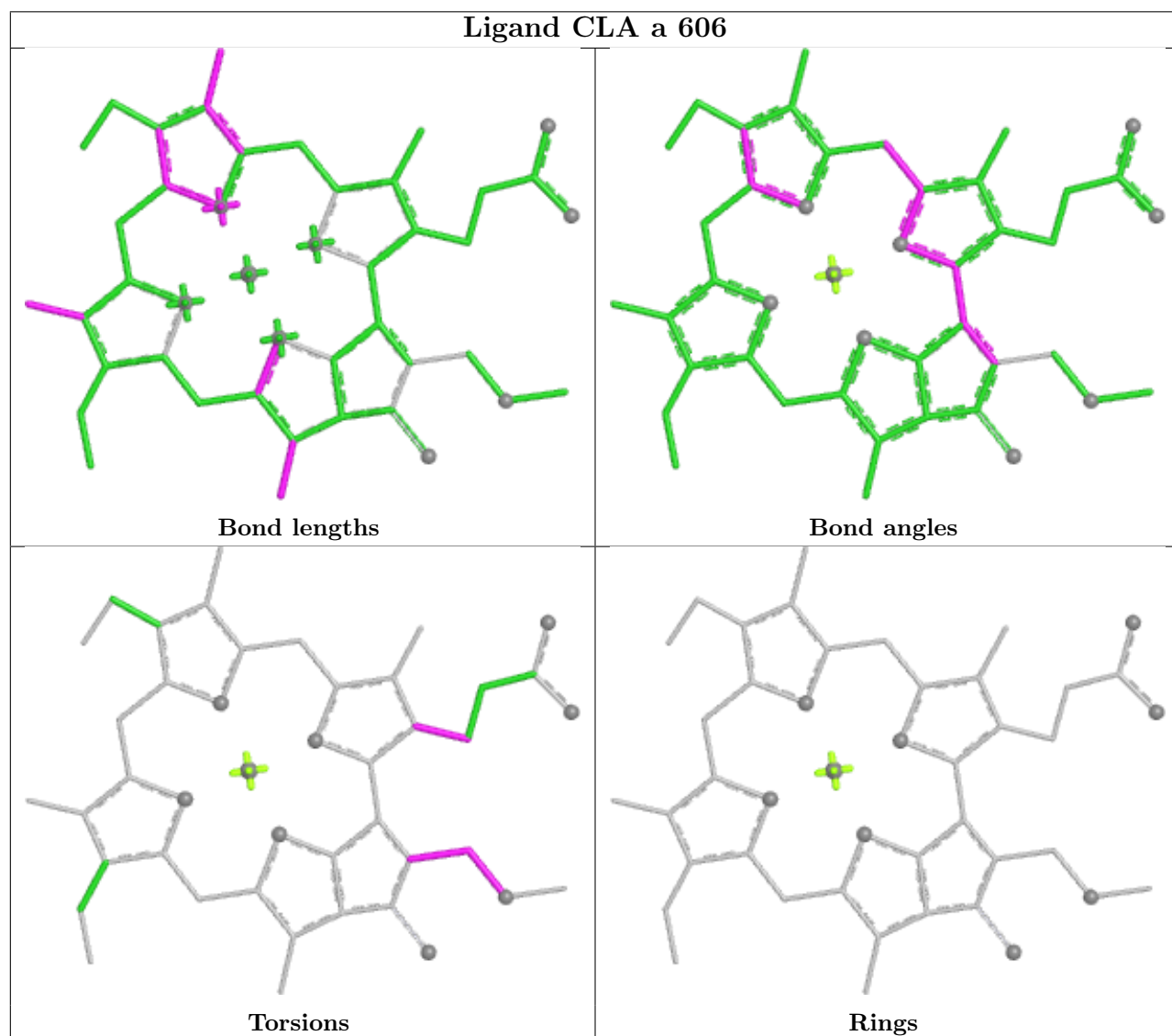
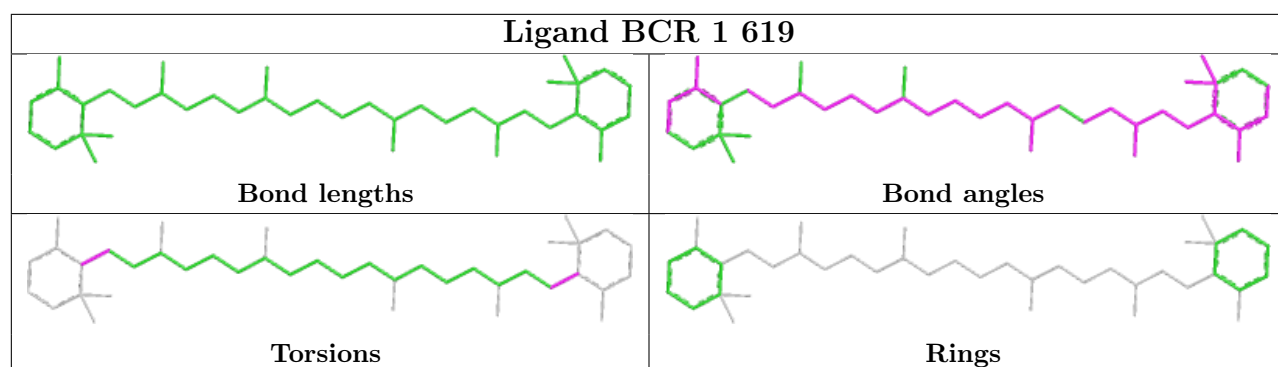


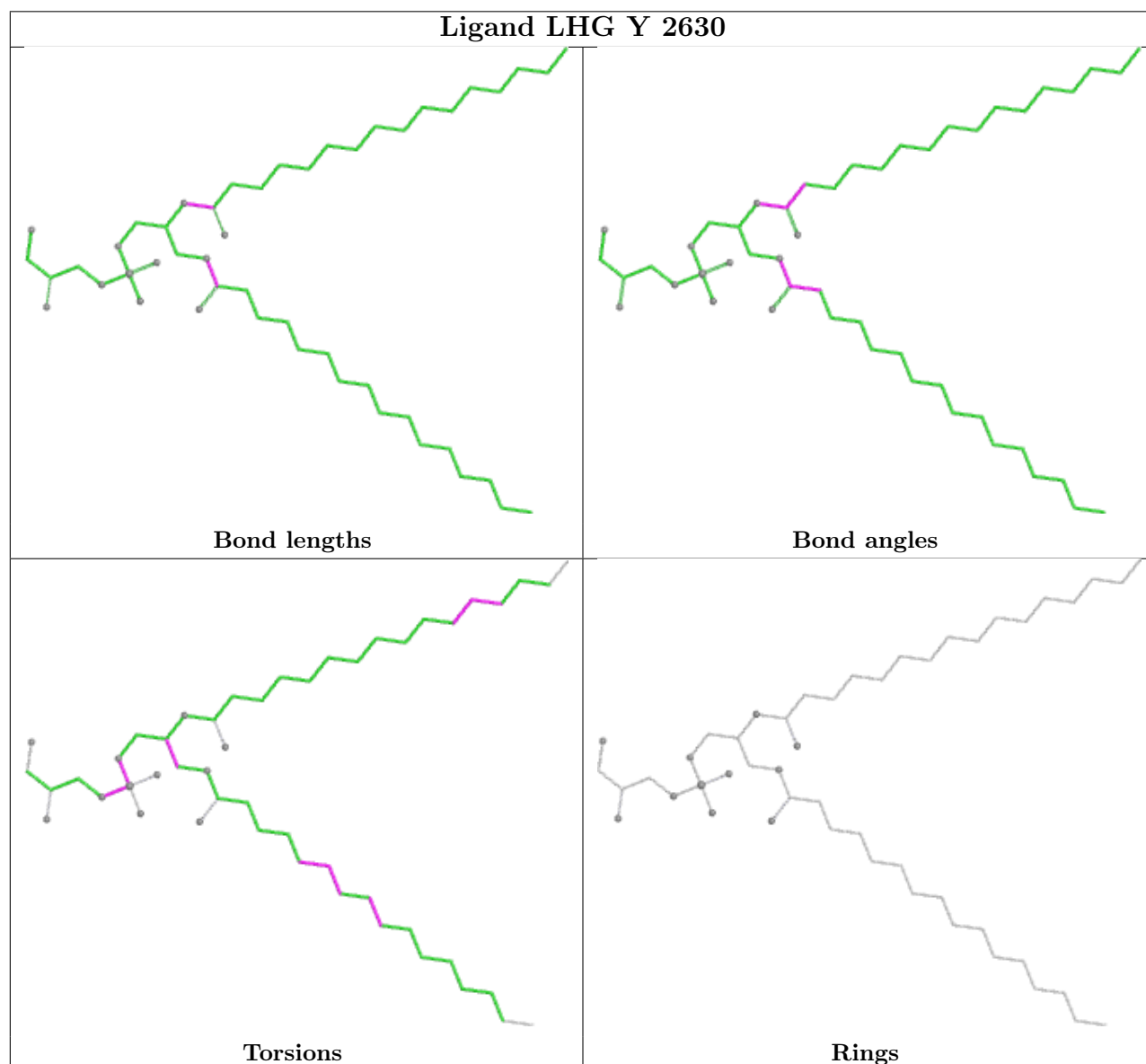
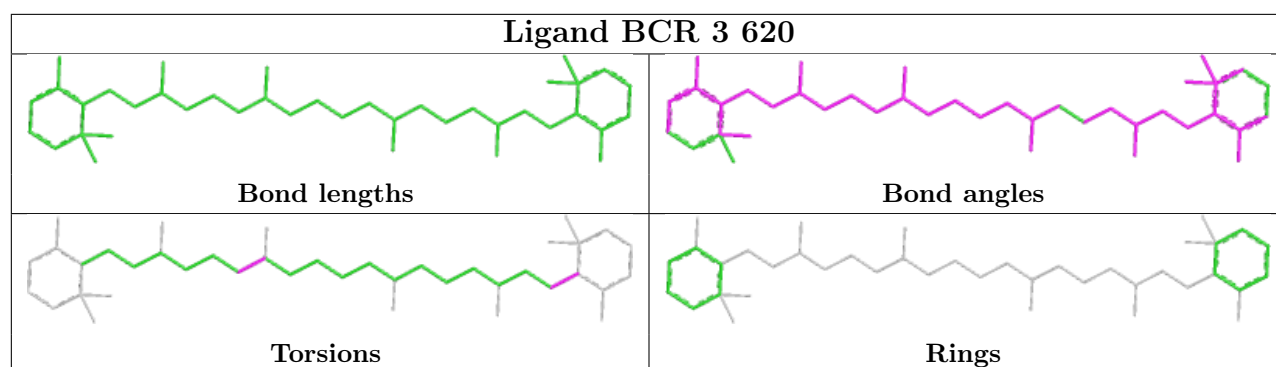
Ligand CLA X 612

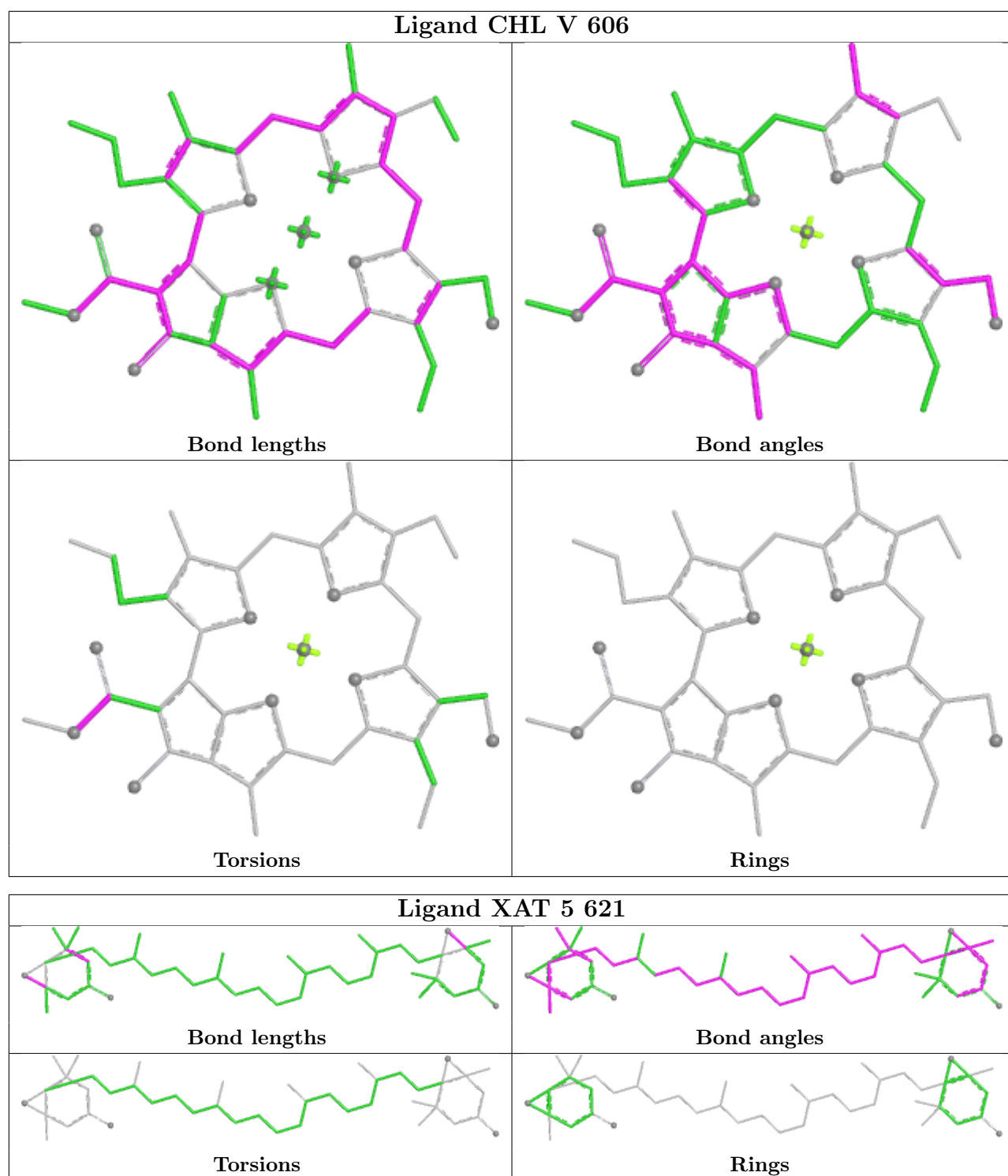


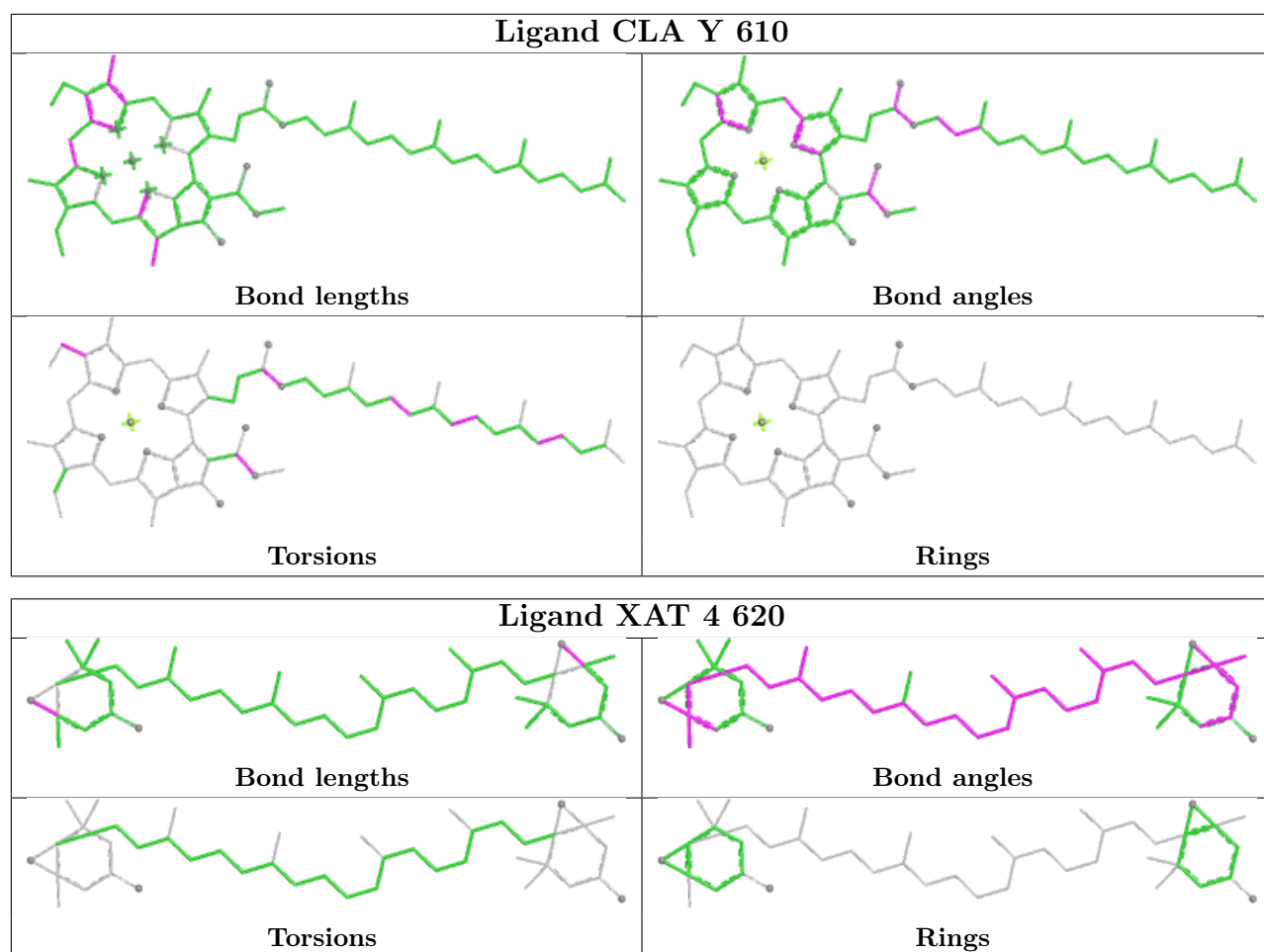
Ligand LUT 1 617



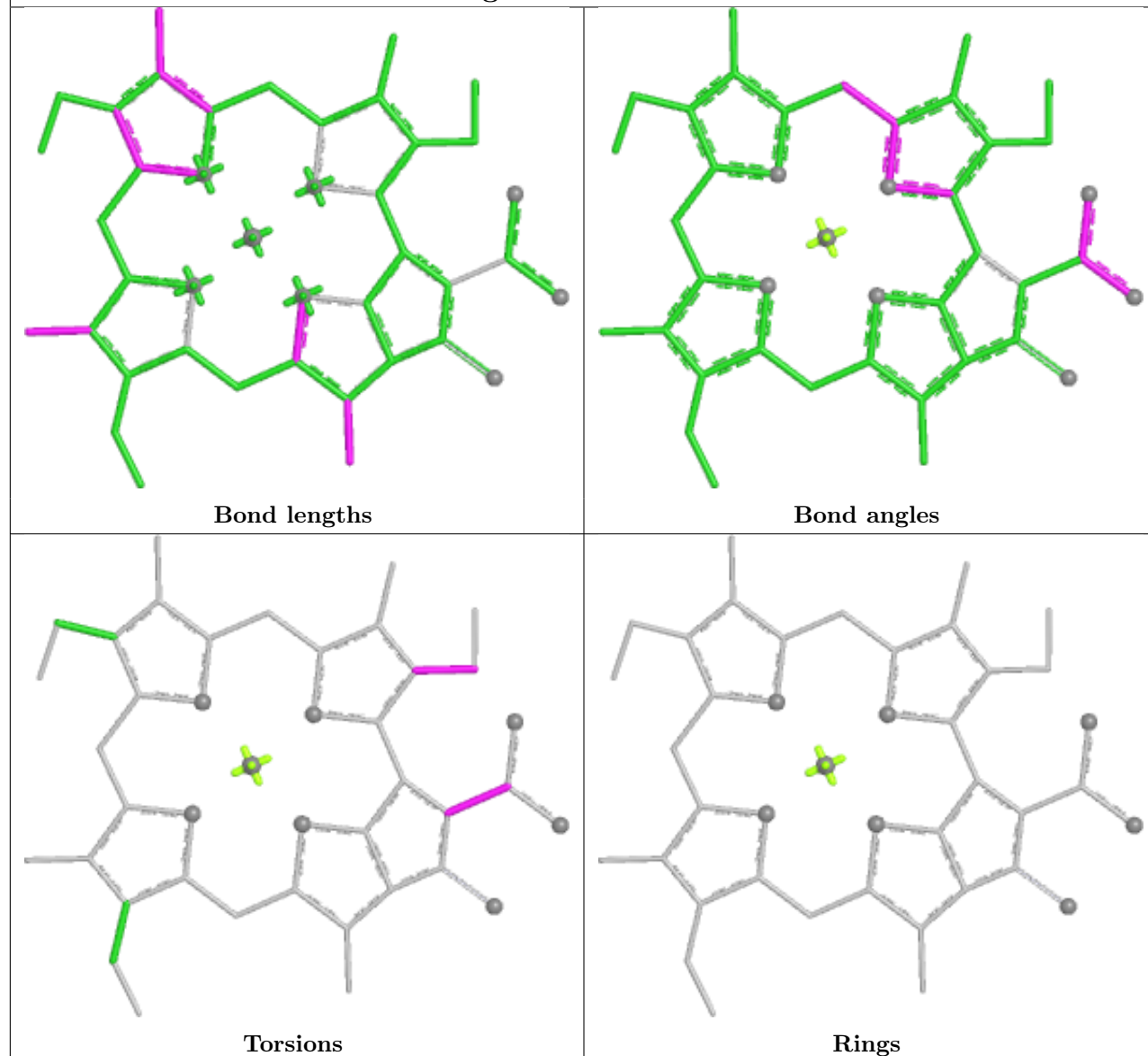




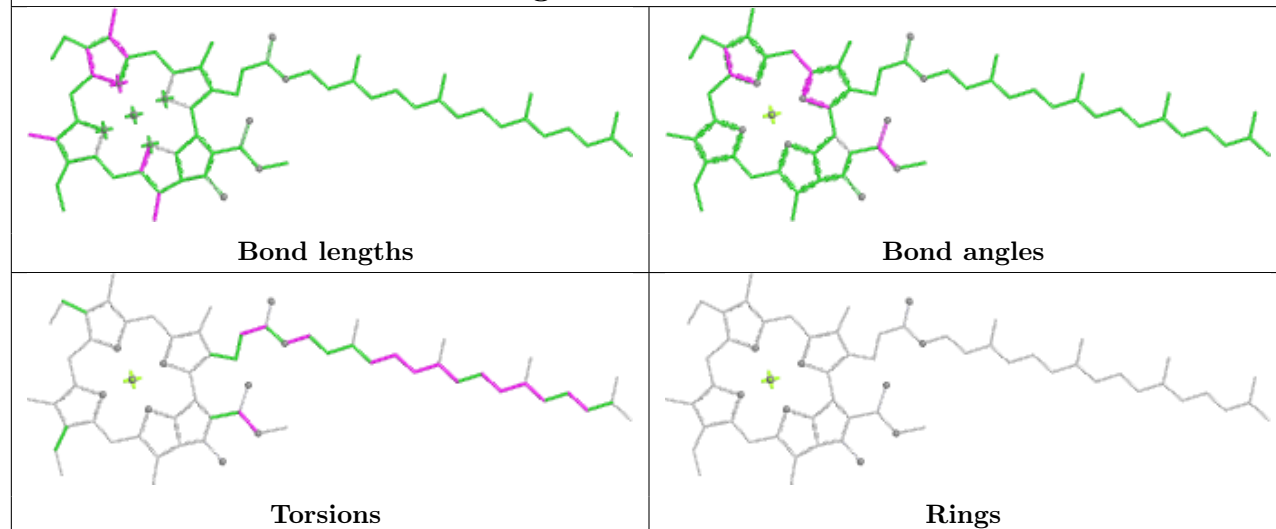


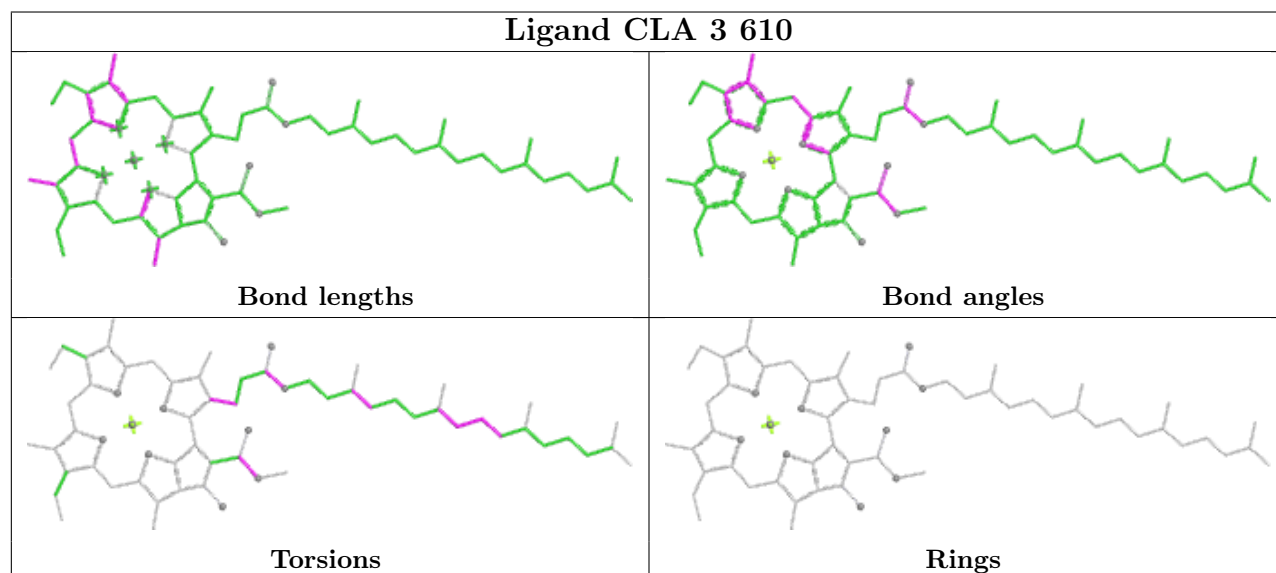
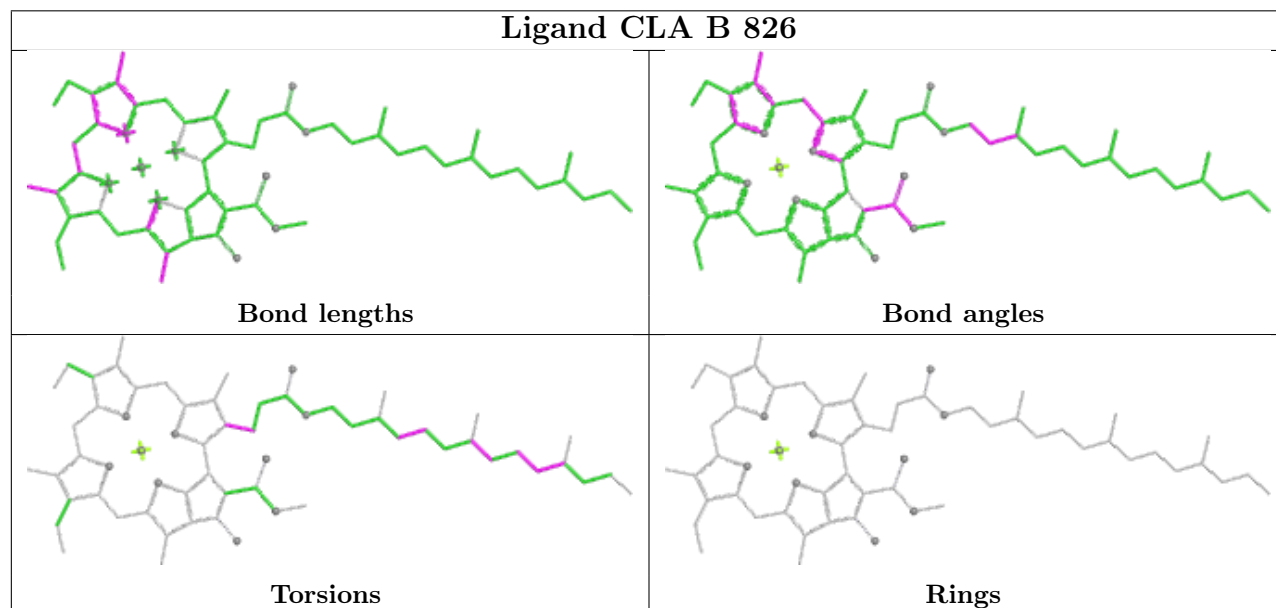
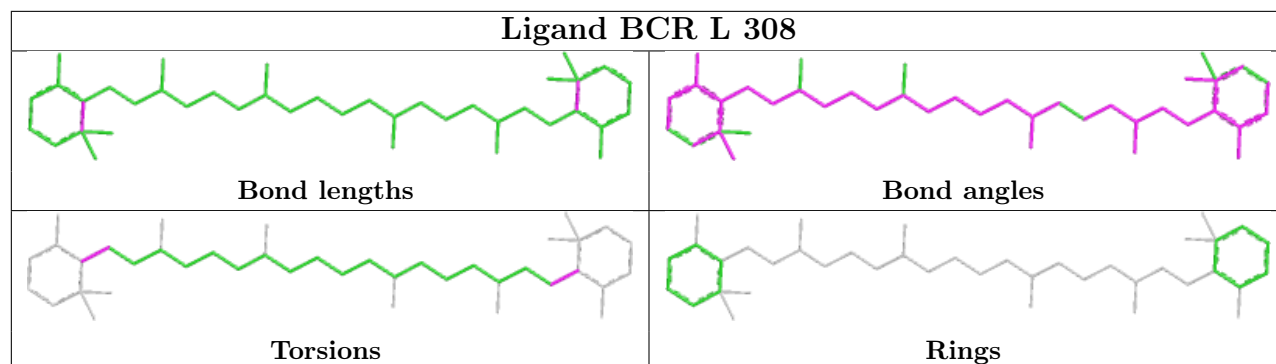


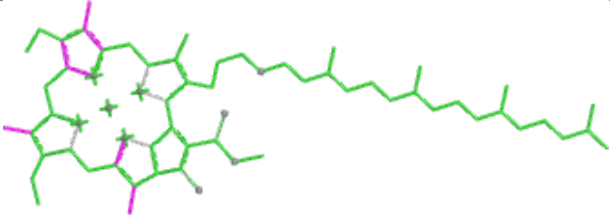
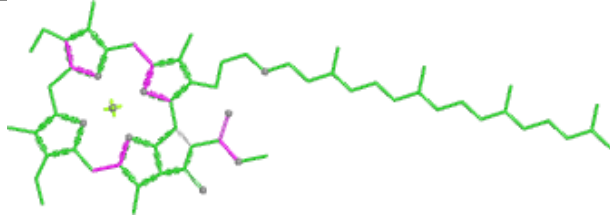
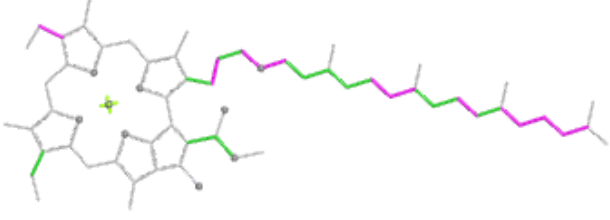
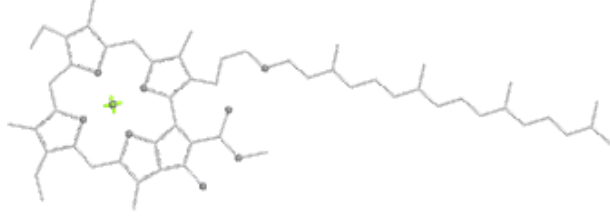
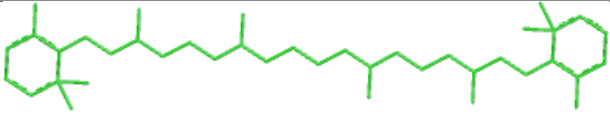
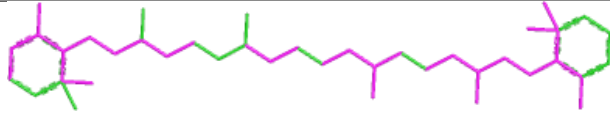
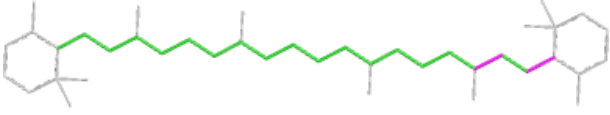
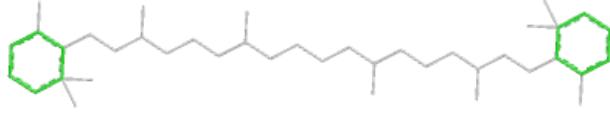
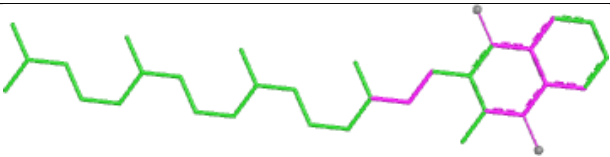
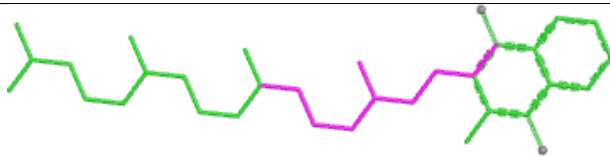
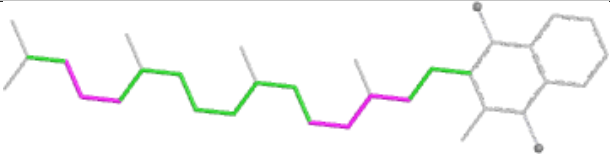
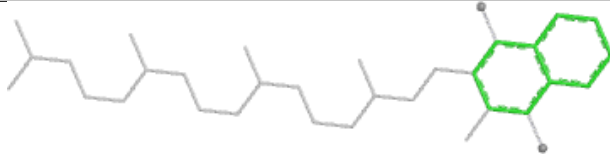
Ligand CLA 5 612

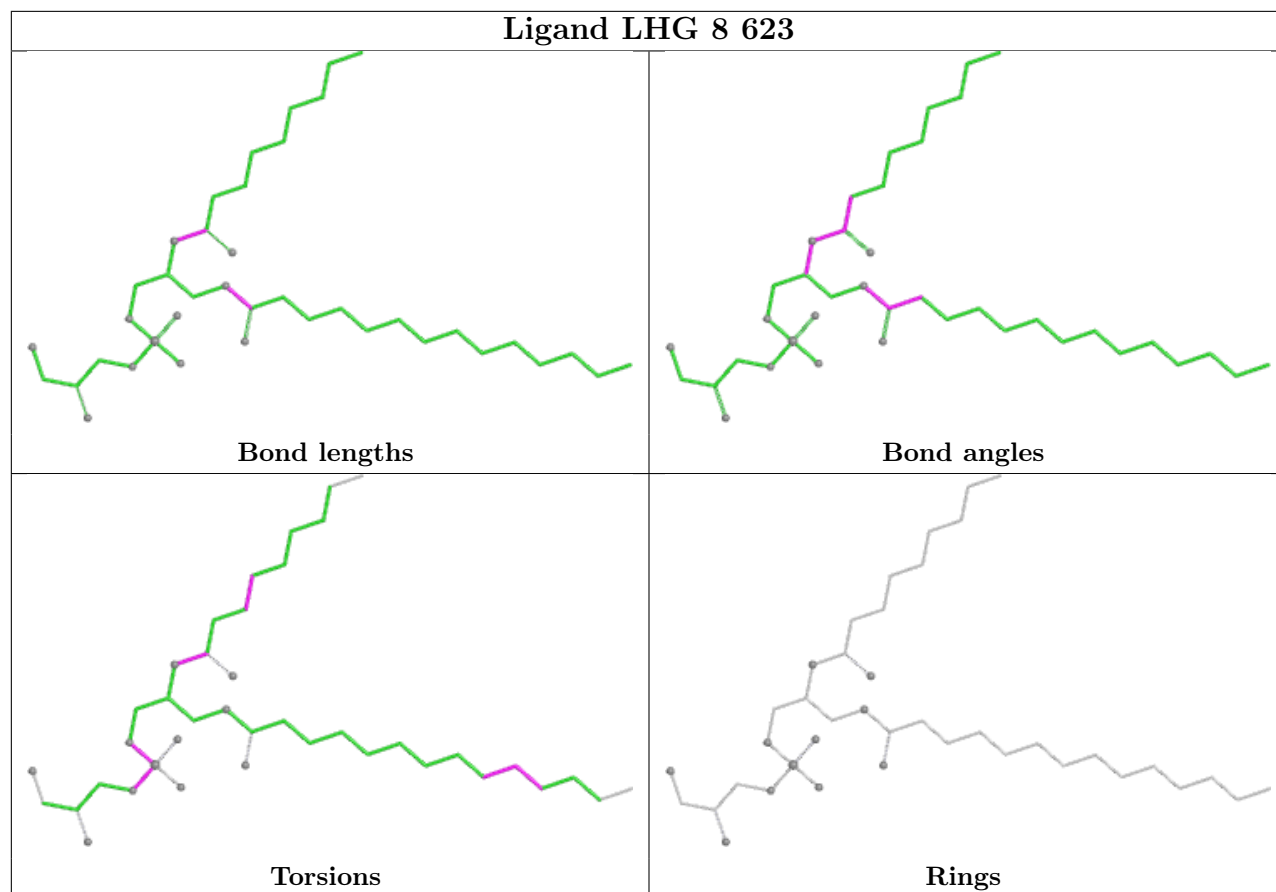
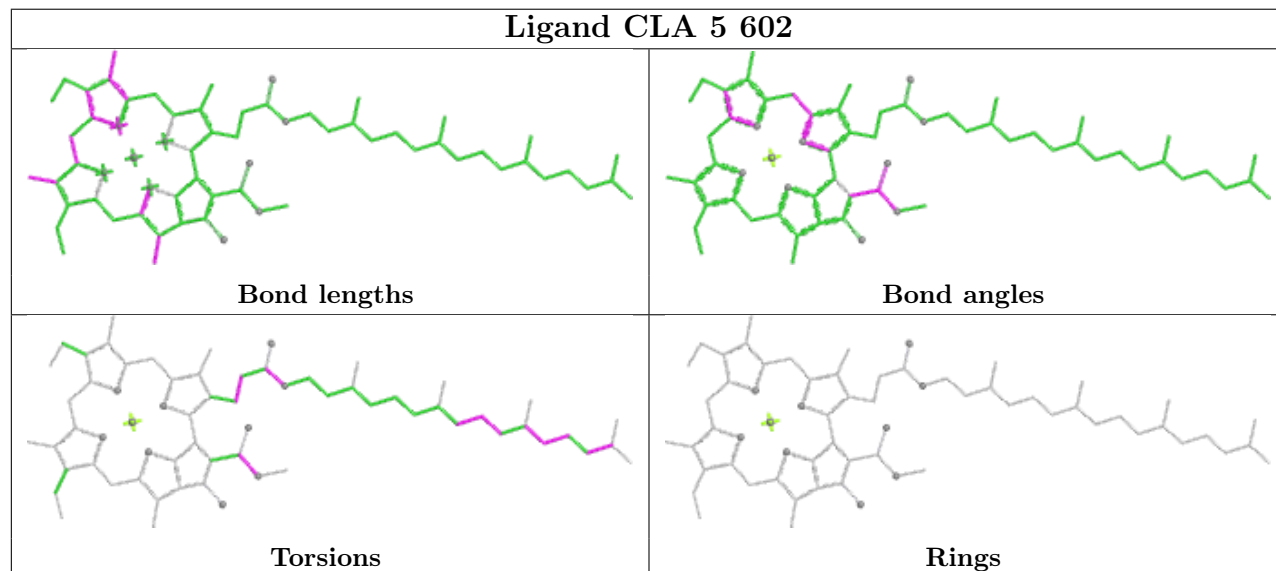


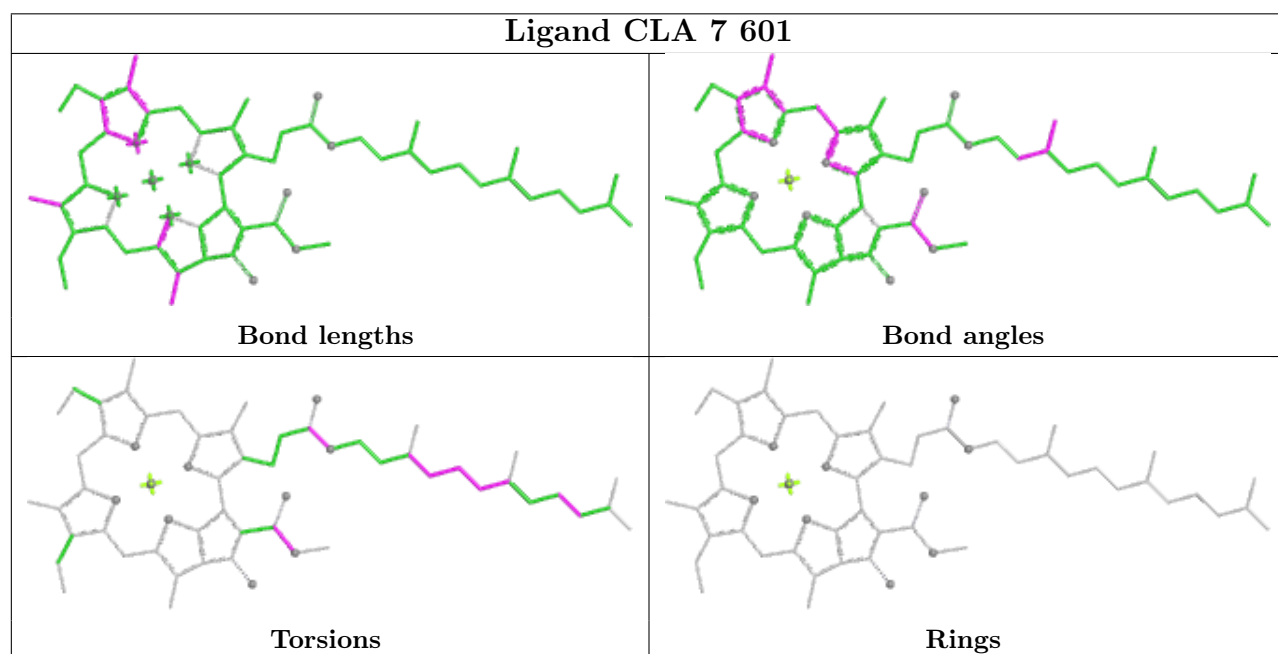
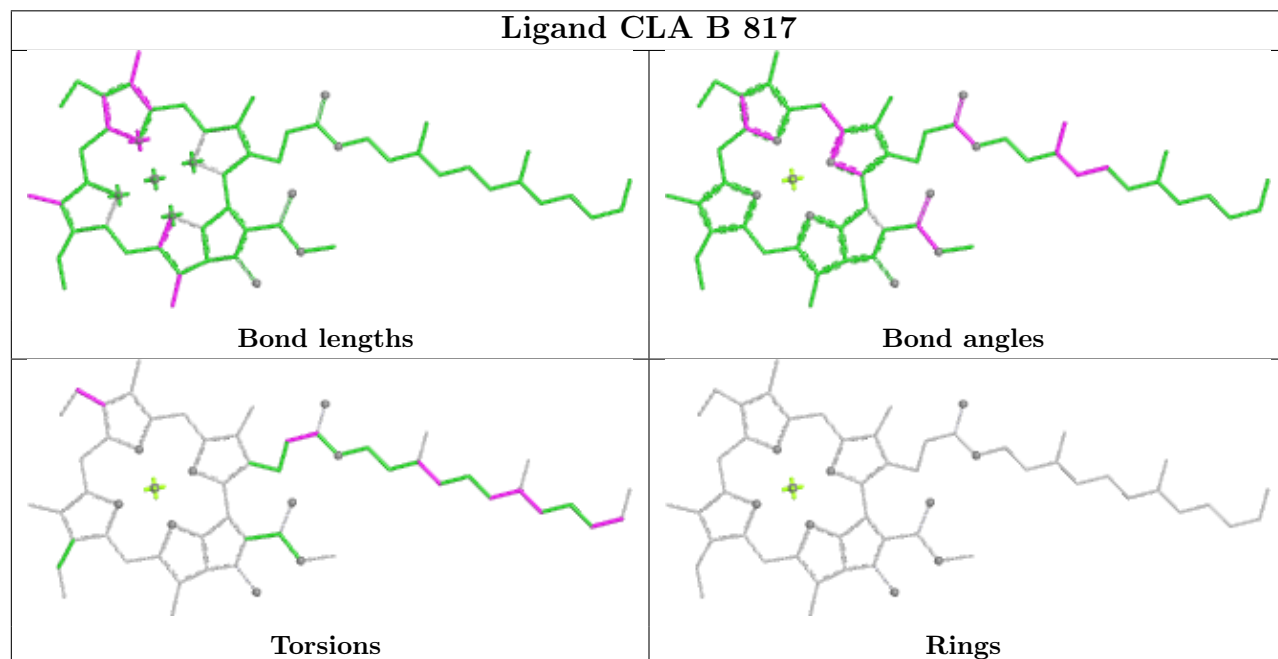
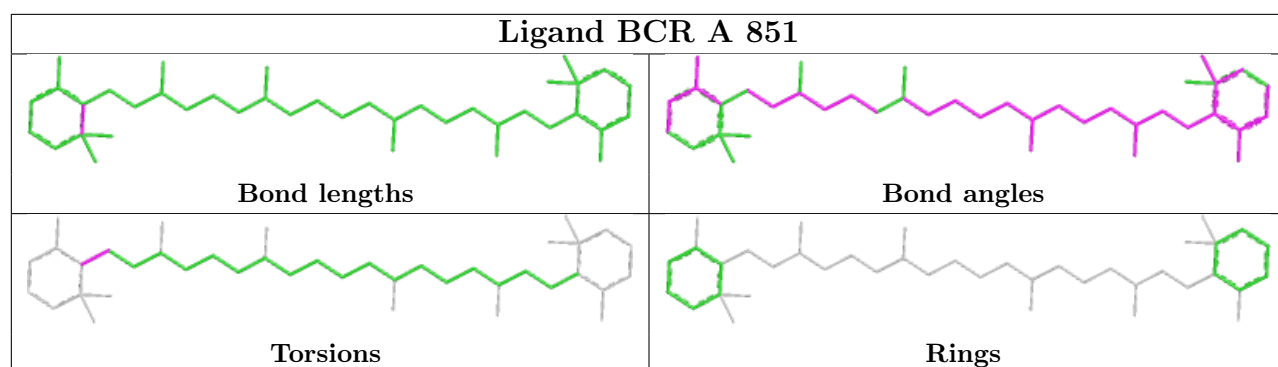
Ligand CLA B 806



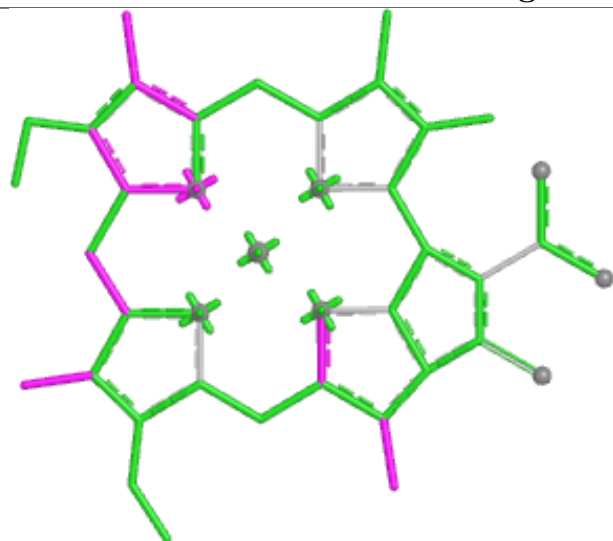


Ligand CLA 5 613	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 5 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PQN B 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

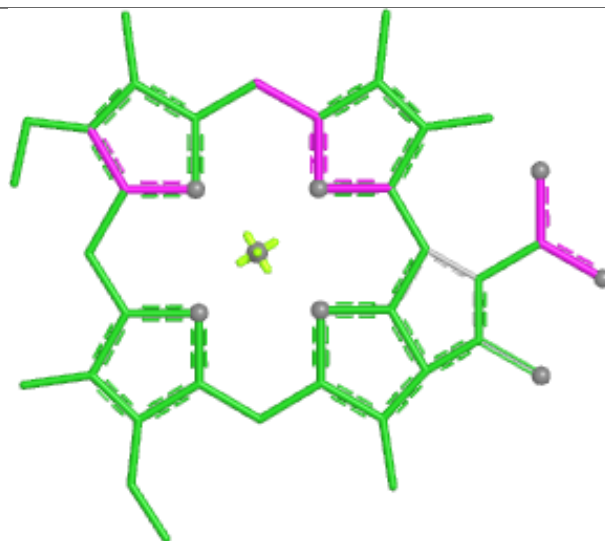
Ligand LHG 8 623**Ligand CLA 5 602**



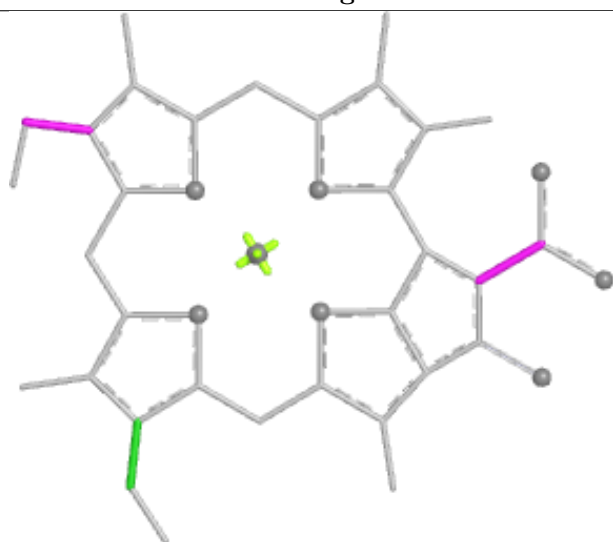
Ligand CLA 3 614



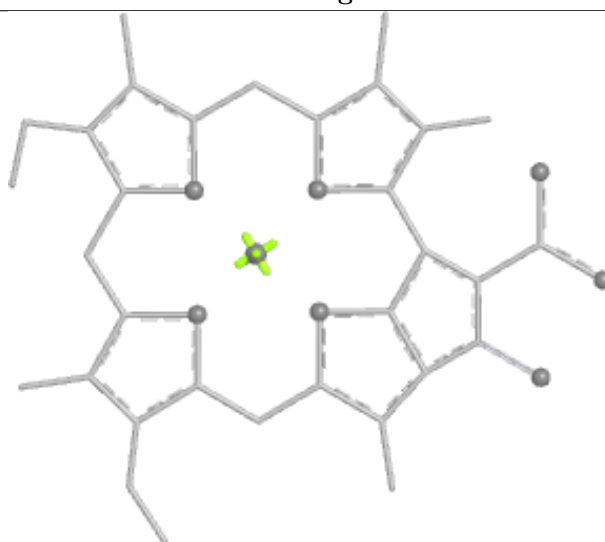
Bond lengths



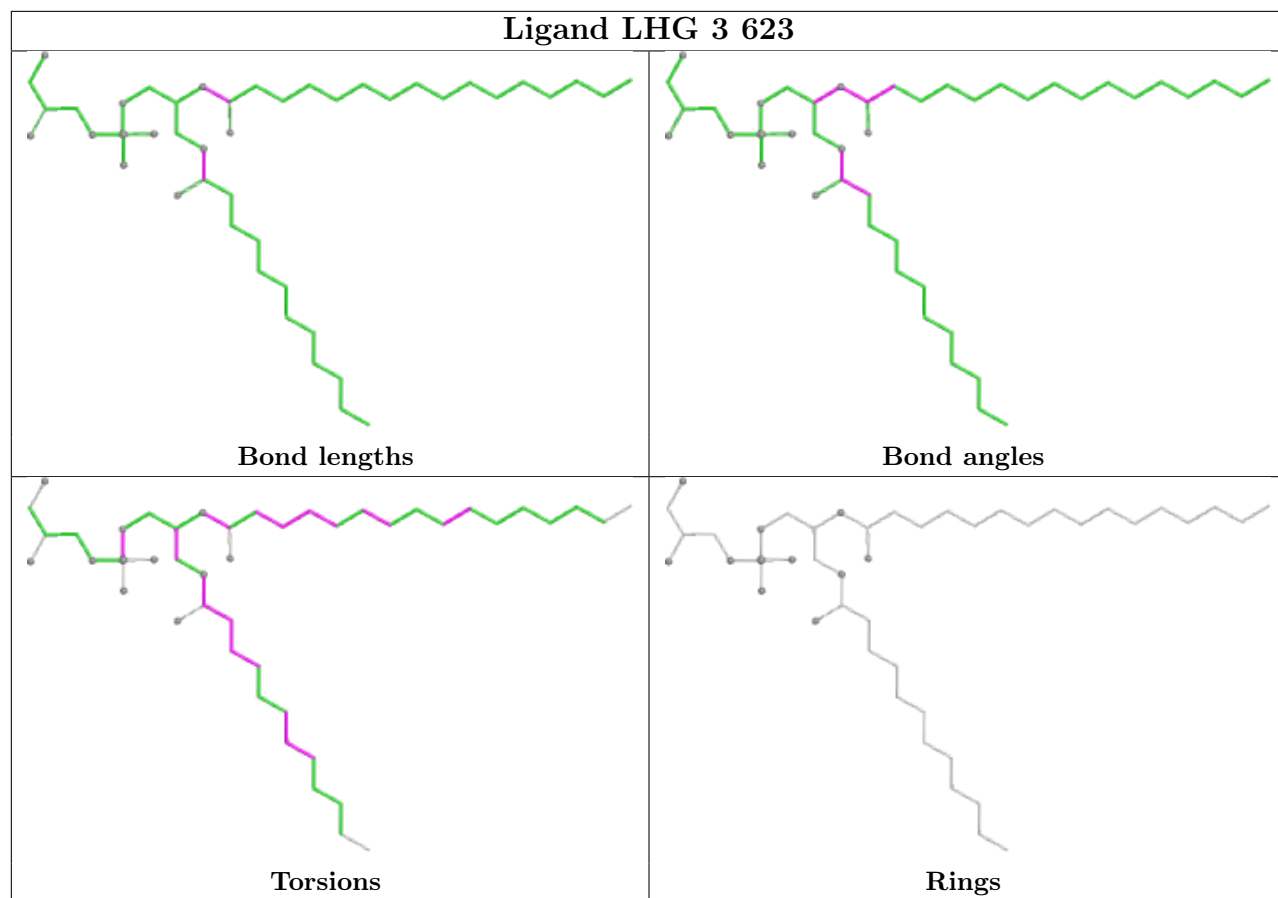
Bond angles



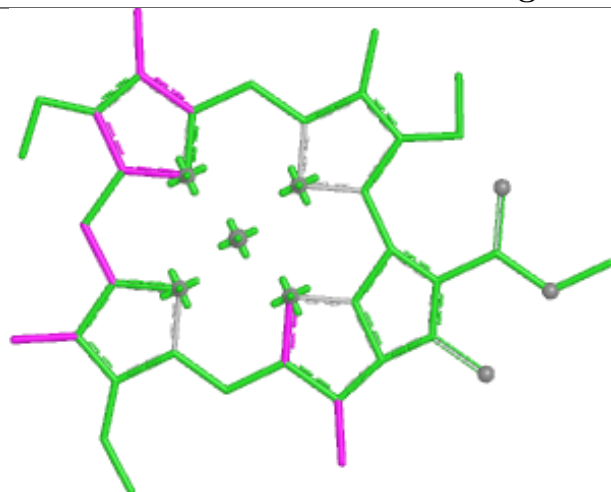
Torsions



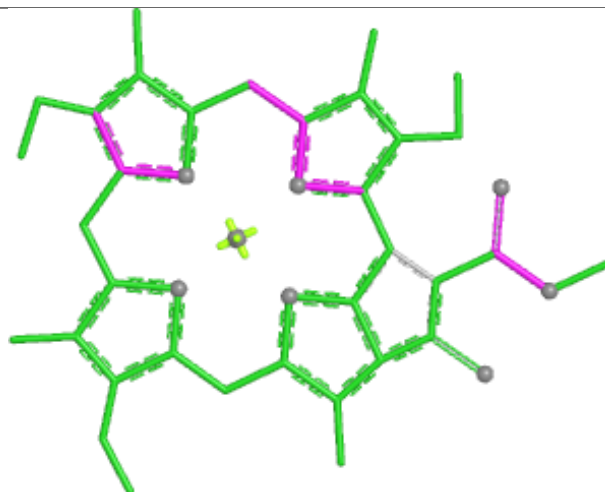
Rings



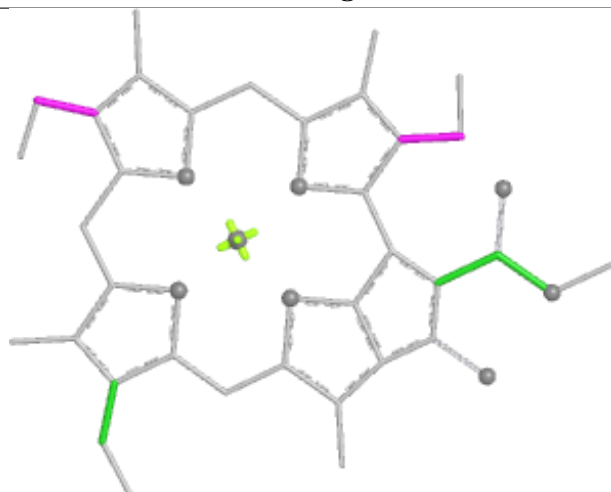
Ligand CLA 6 611



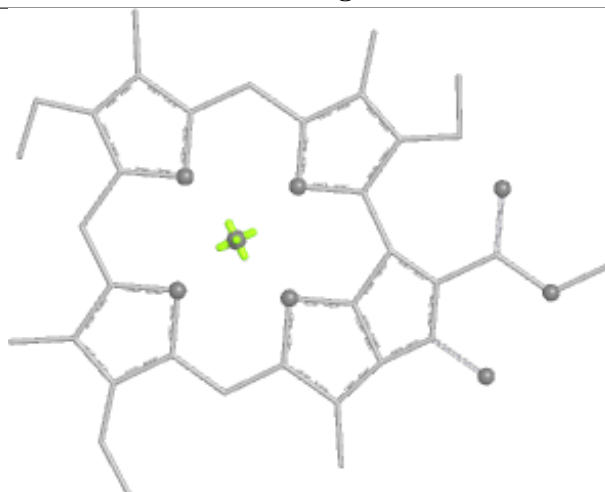
Bond lengths



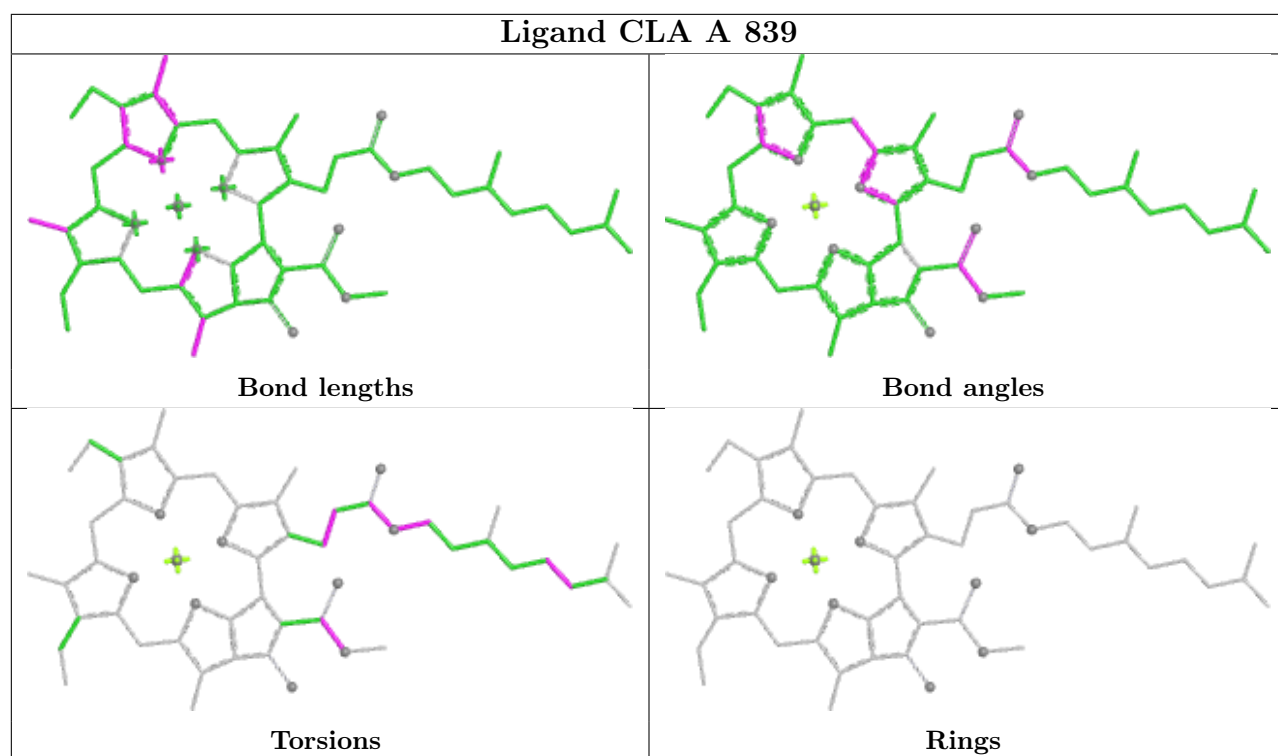
Bond angles



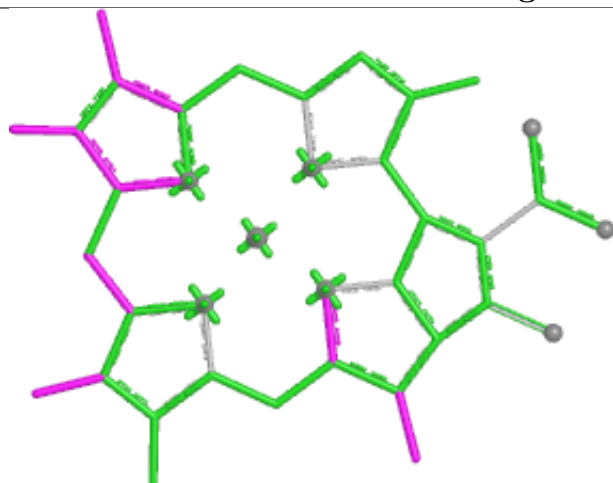
Torsions



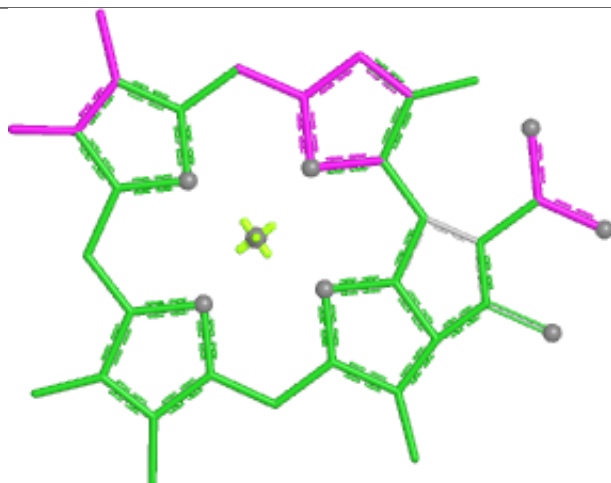
Rings



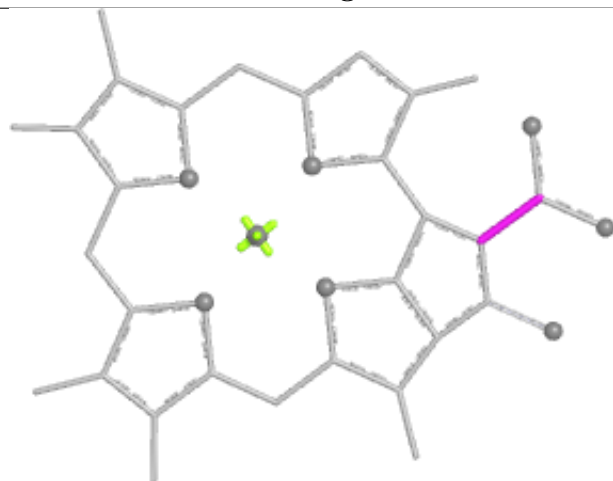
Ligand CLA 1 614



Bond lengths



Bond angles

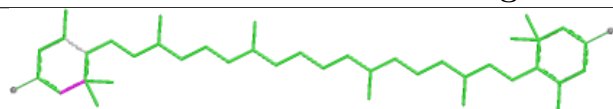


Torsions

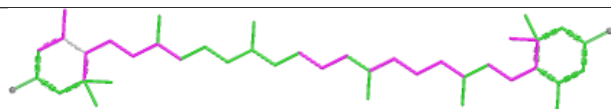


Rings

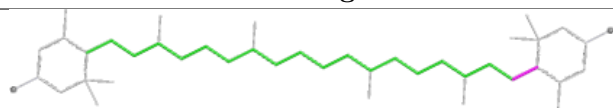
Ligand LUT W 1620



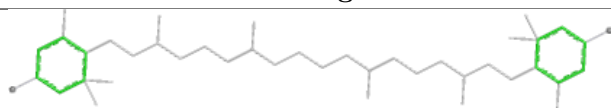
Bond lengths



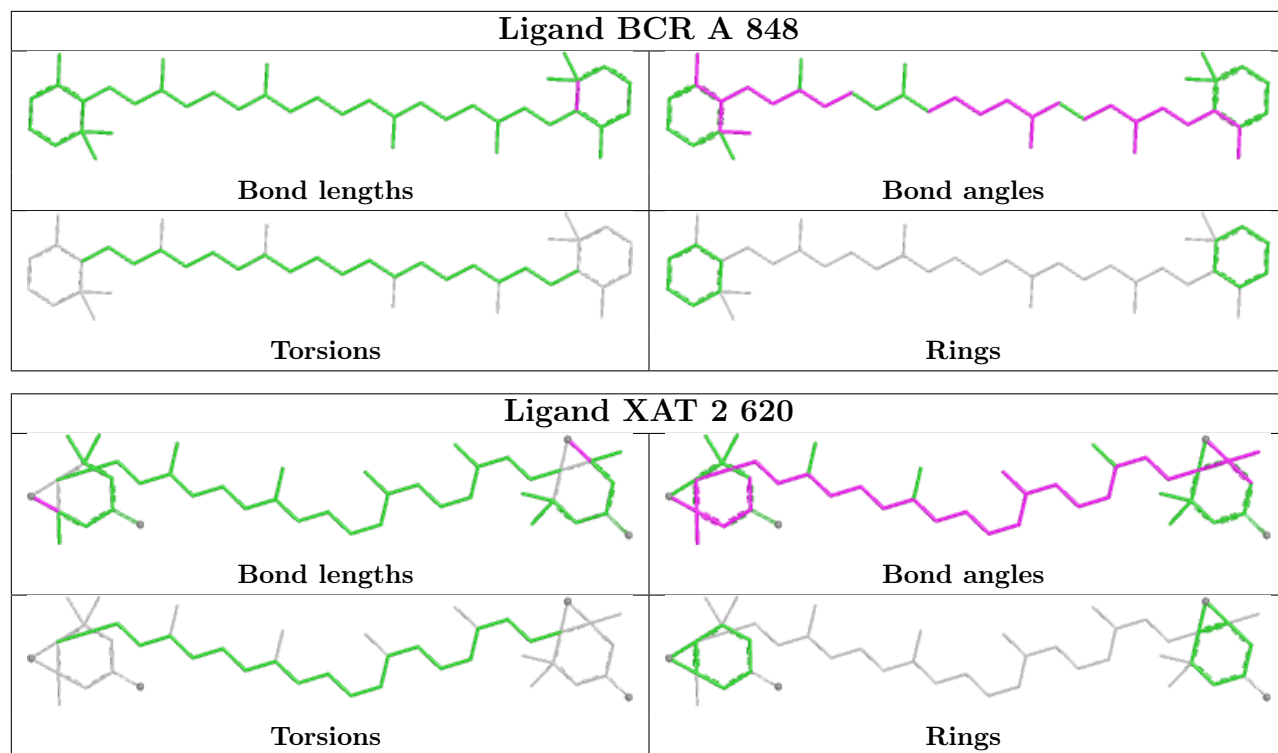
Bond angles



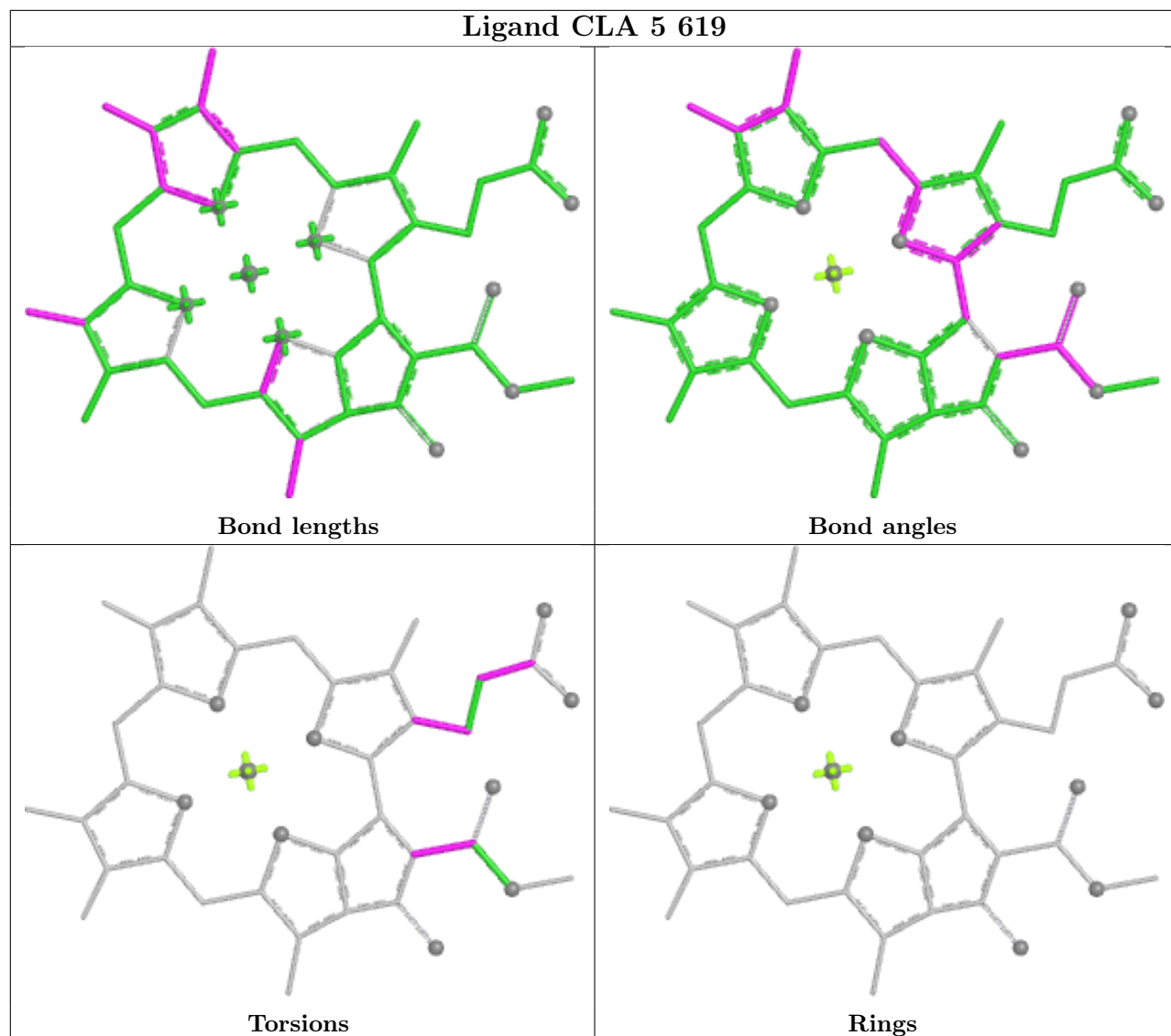
Torsions



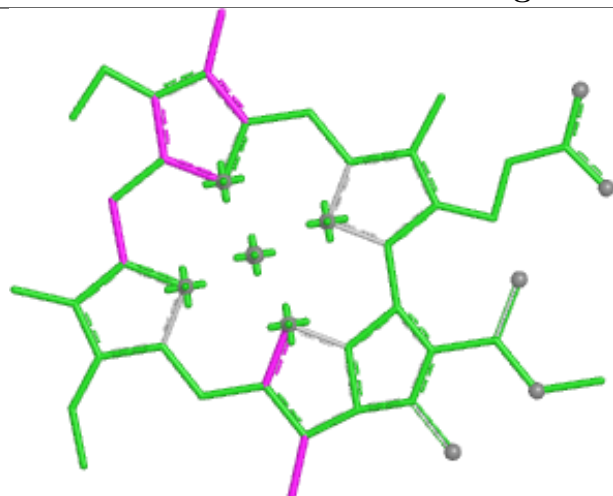
Rings



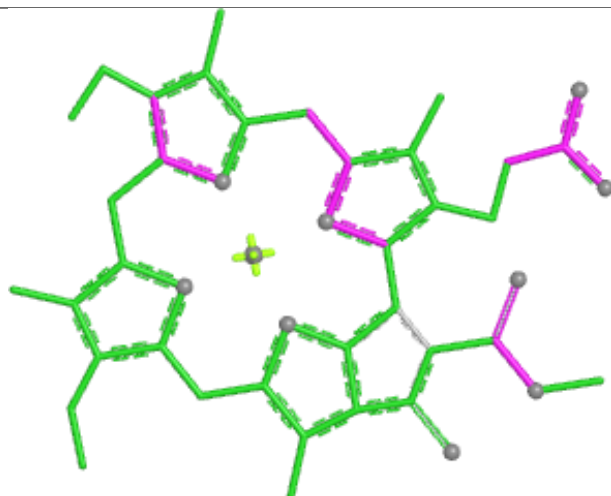
Ligand CLA 5 619



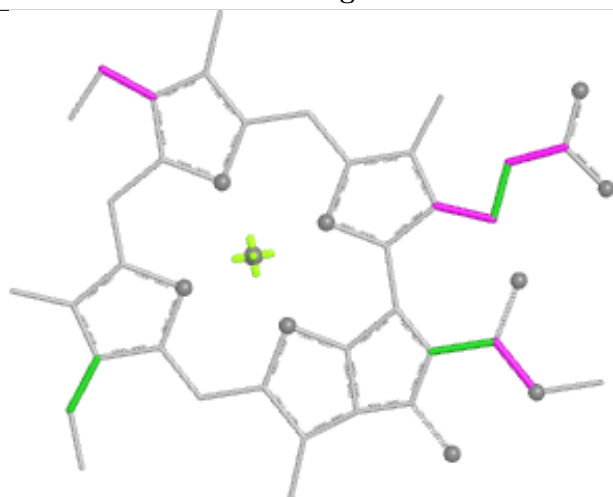
Ligand CLA X 611



Bond lengths



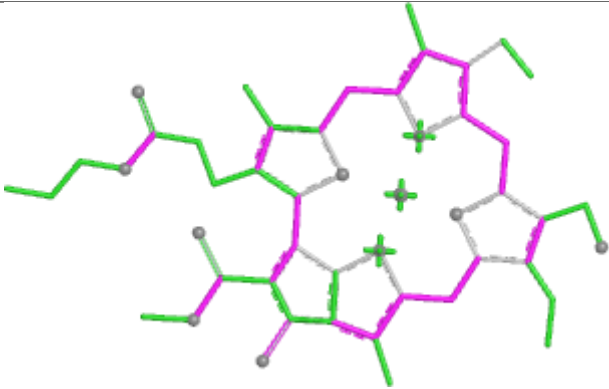
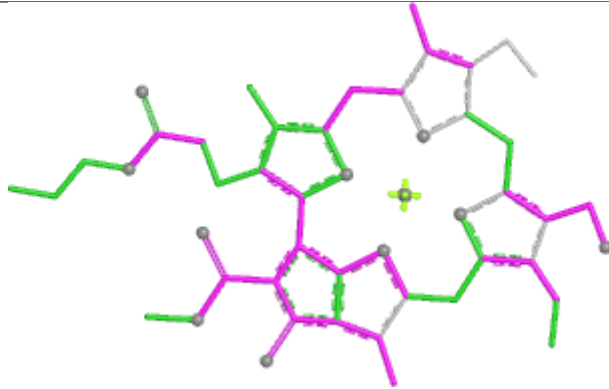
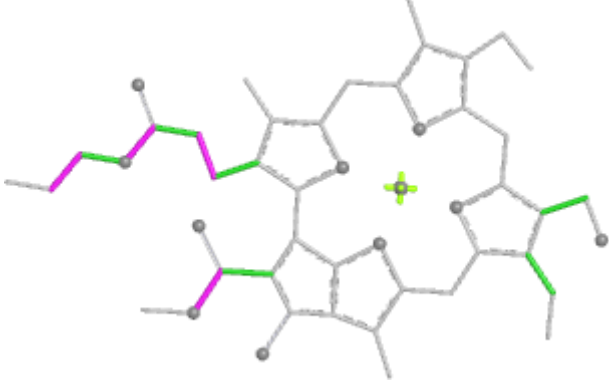
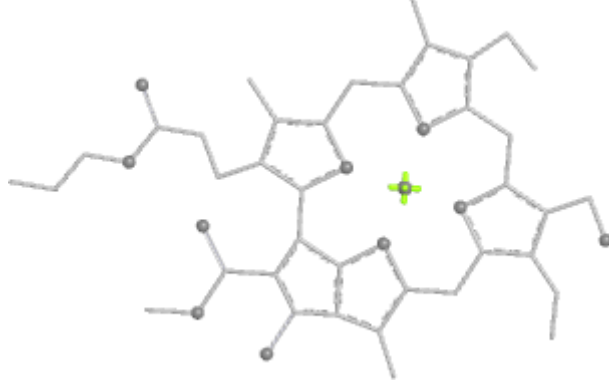
Bond angles

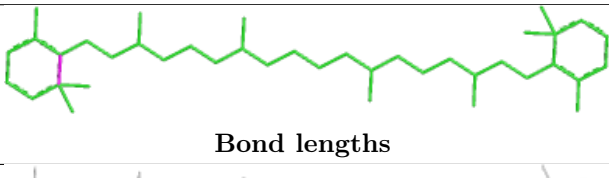
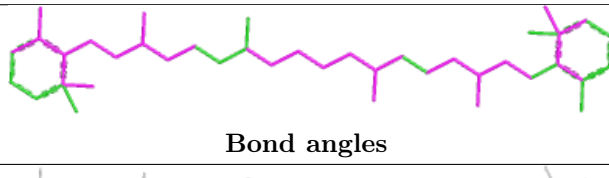
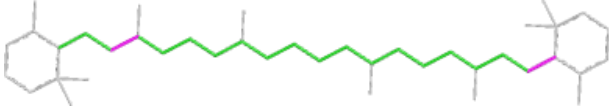
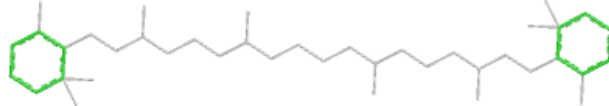


Torsions

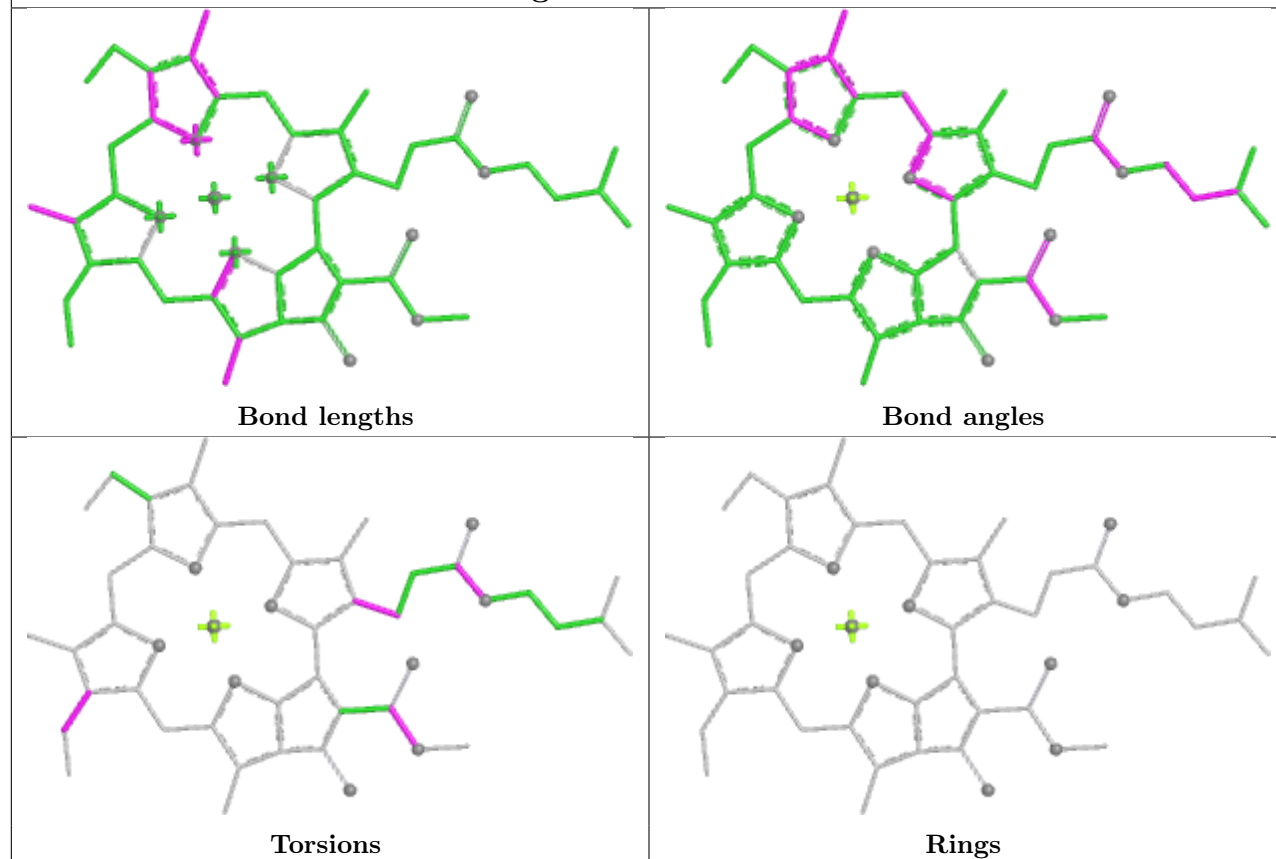


Rings

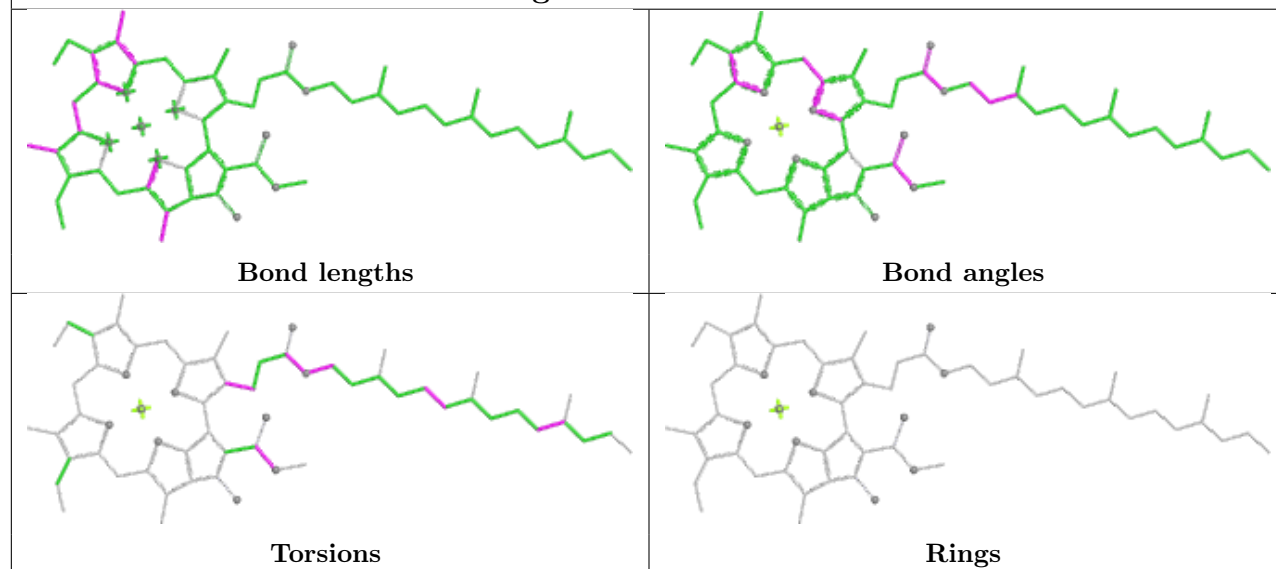
Ligand CHL Y 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR O 2004	
	
Bond lengths	Bond angles
	
Torsions	Rings

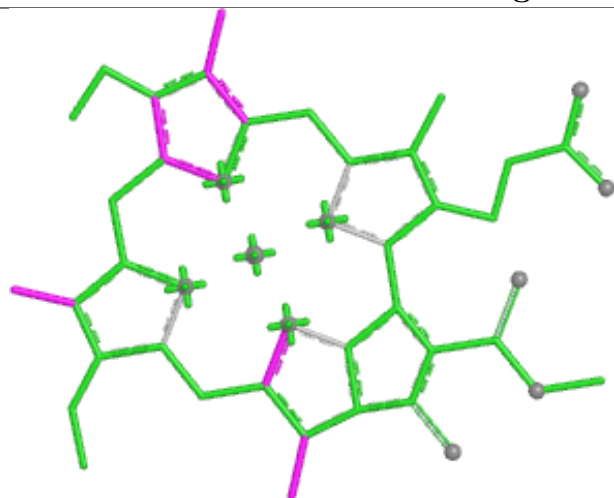
Ligand CLA A 838



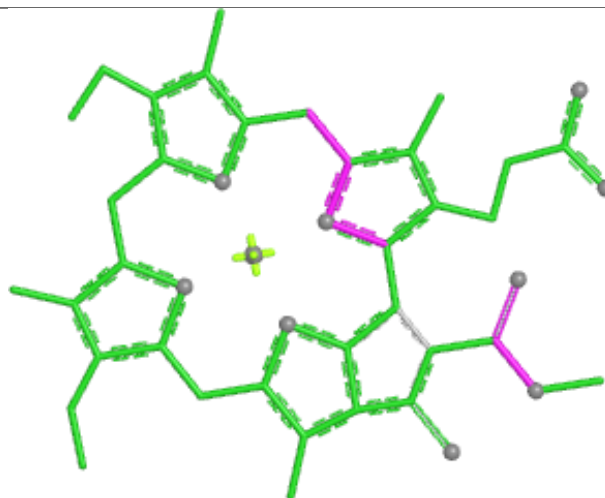
Ligand CLA B 814



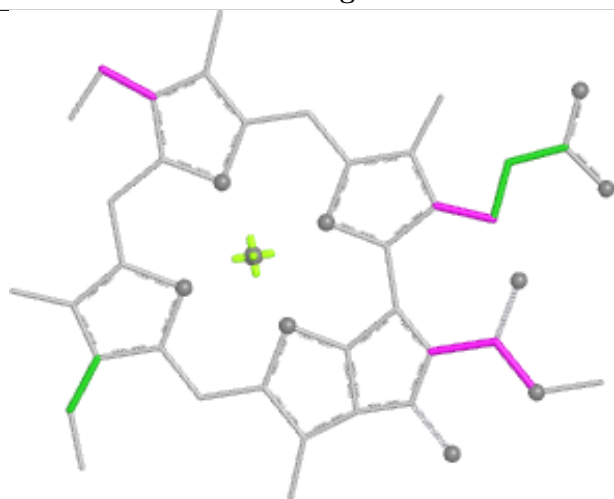
Ligand CLA K 201



Bond lengths



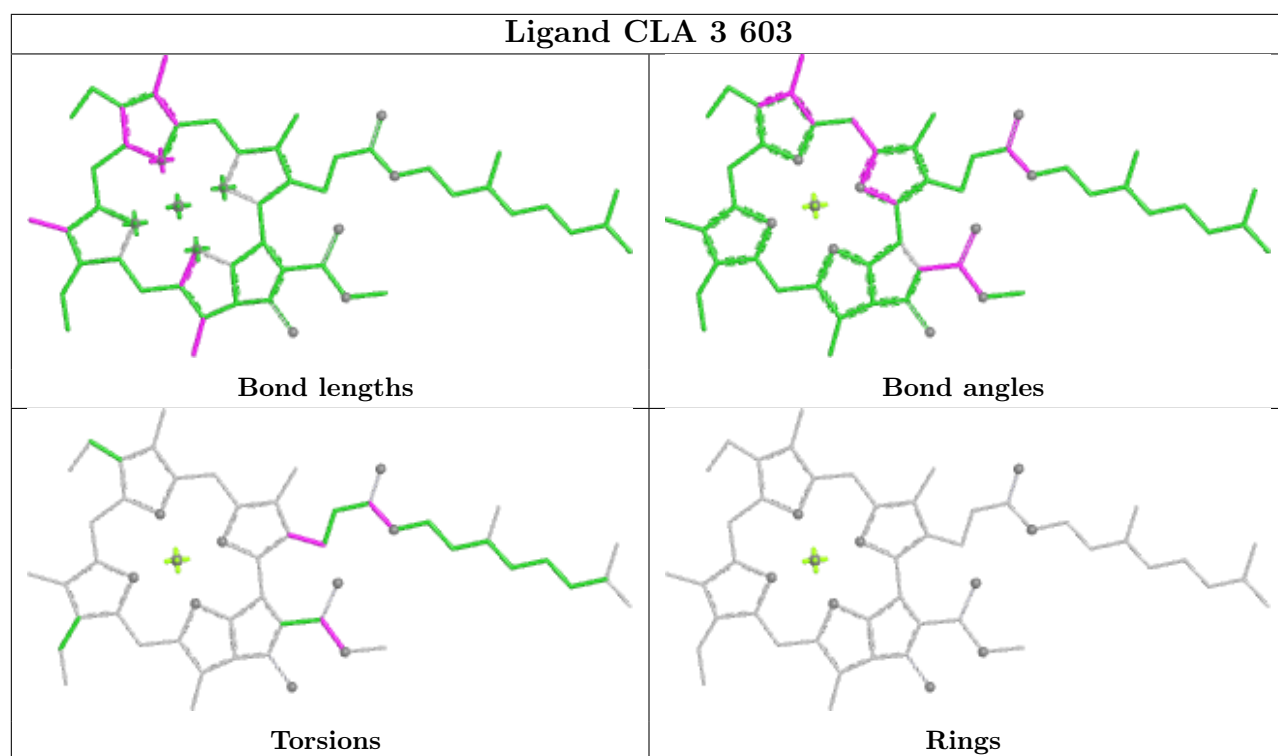
Bond angles



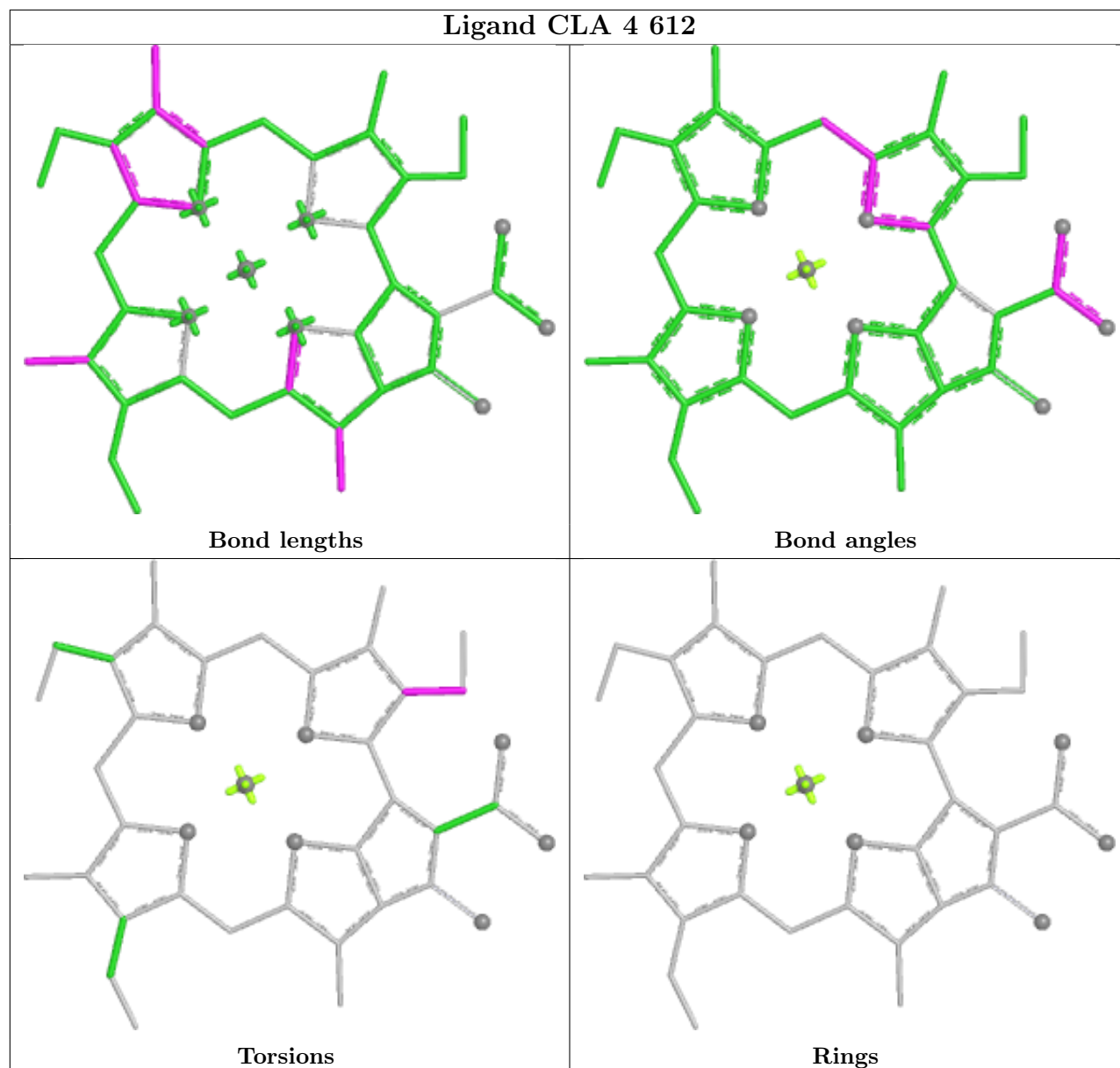
Torsions



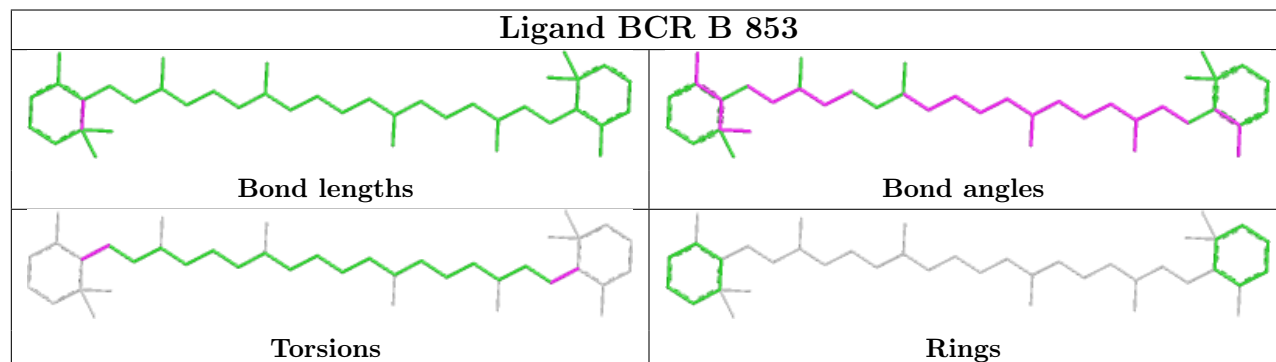
Rings

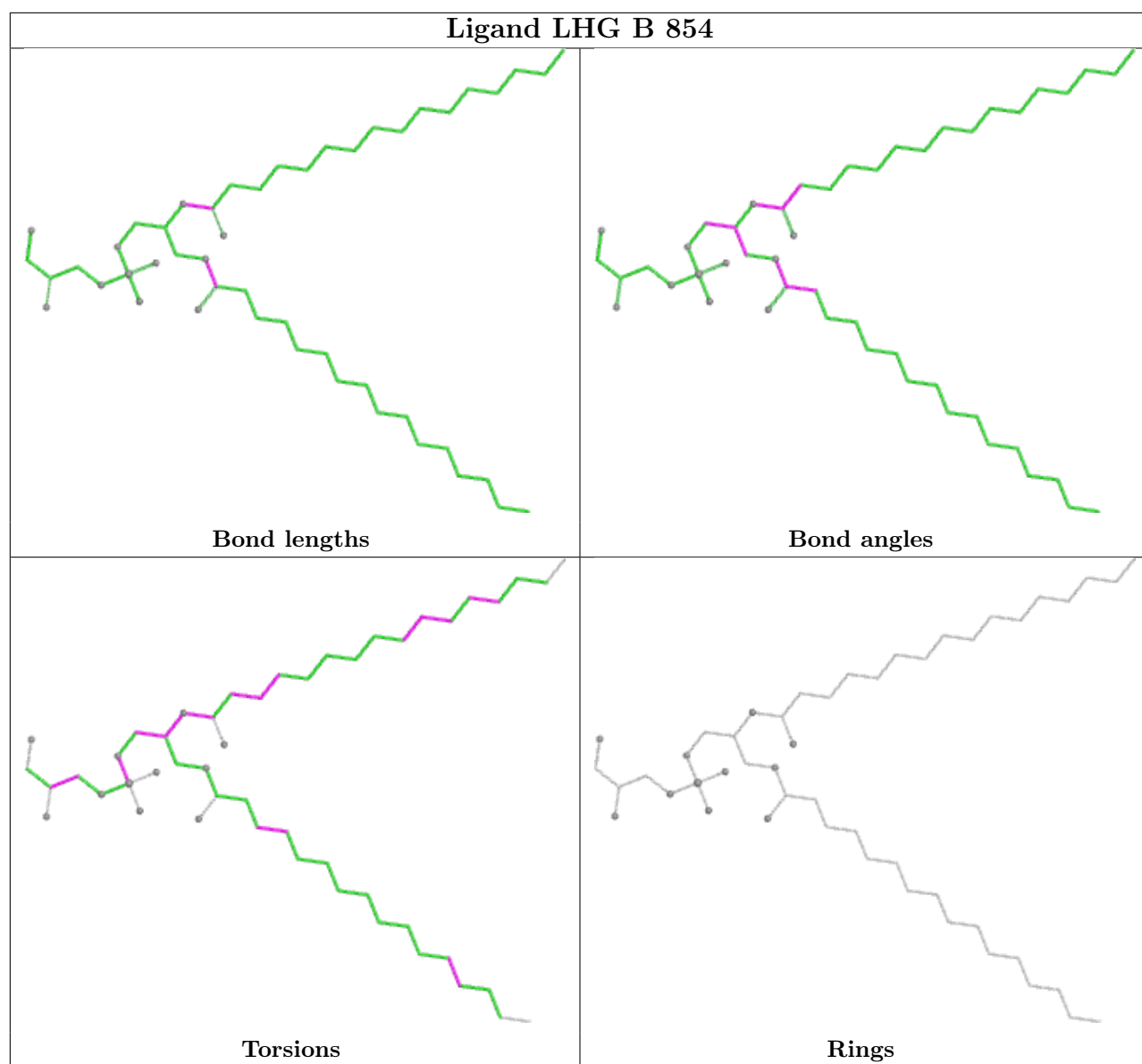


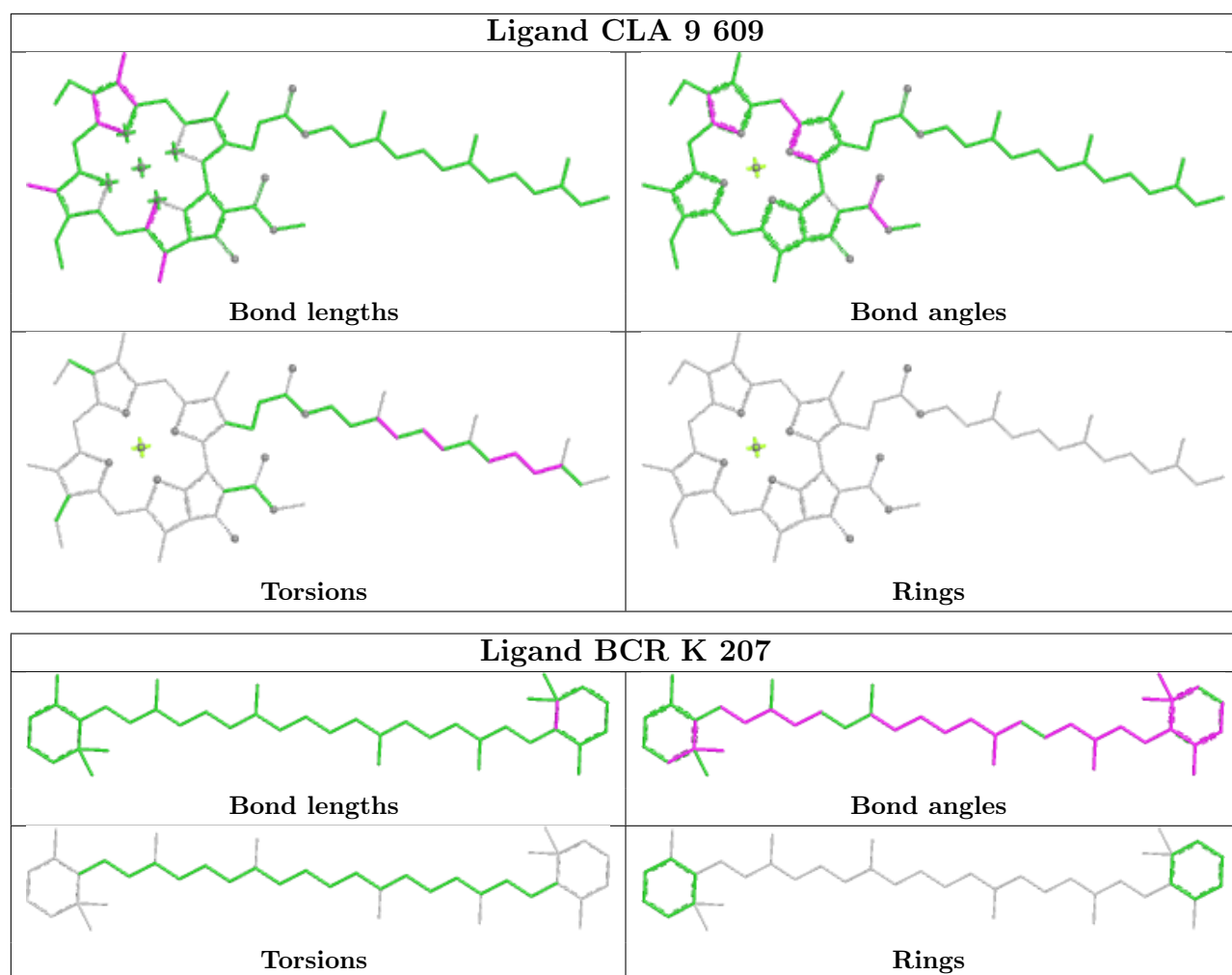
Ligand CLA 4 612



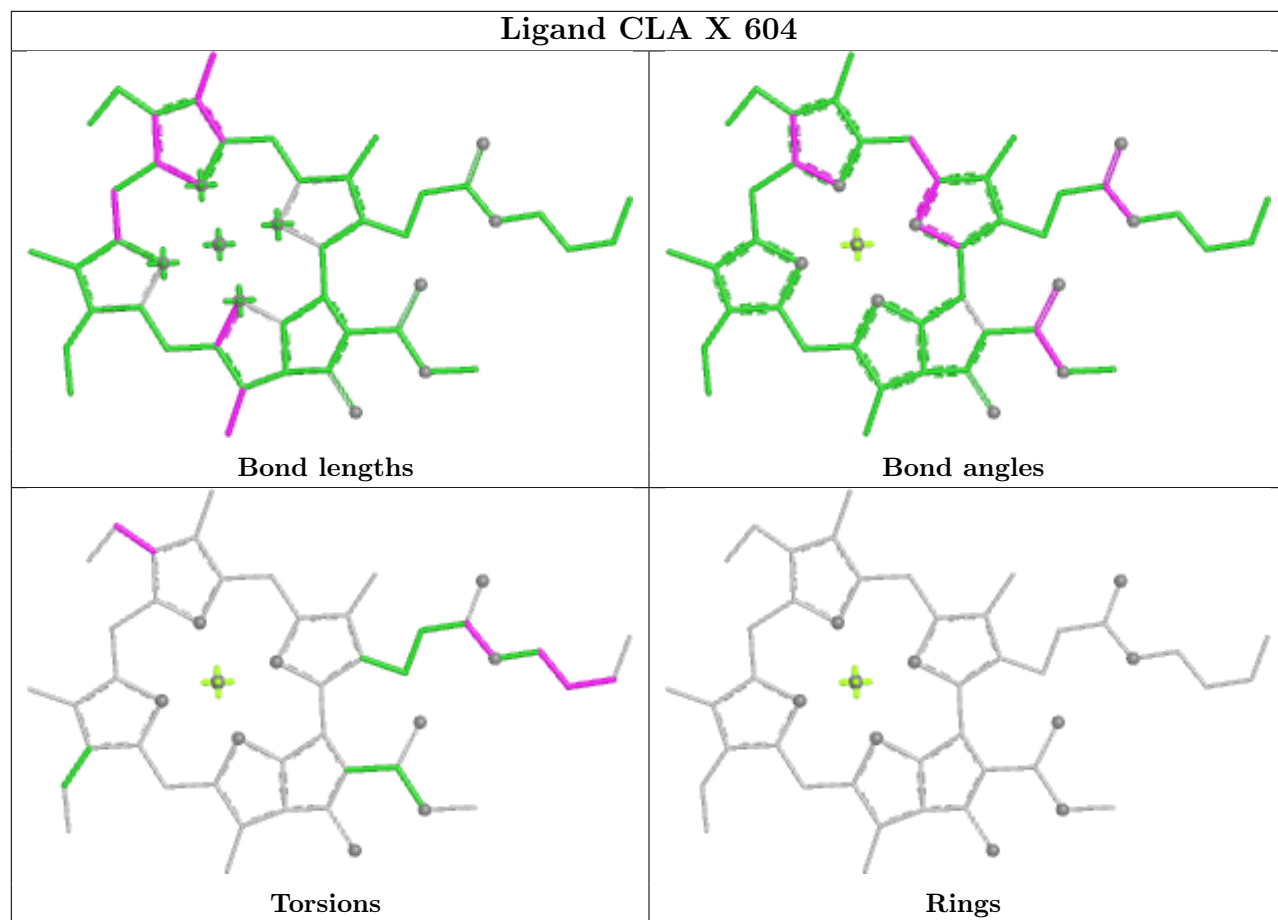
Ligand BCR B 853



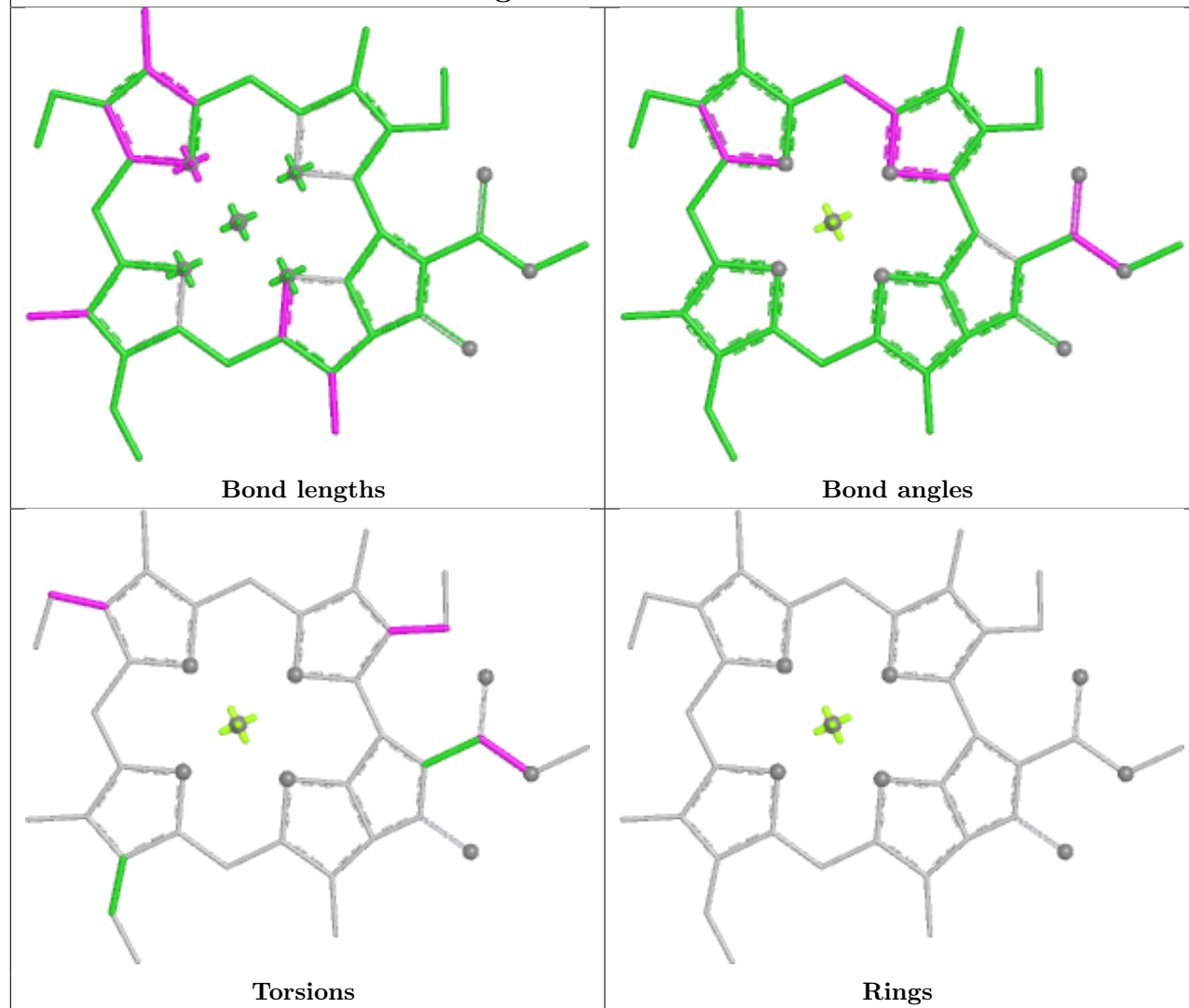




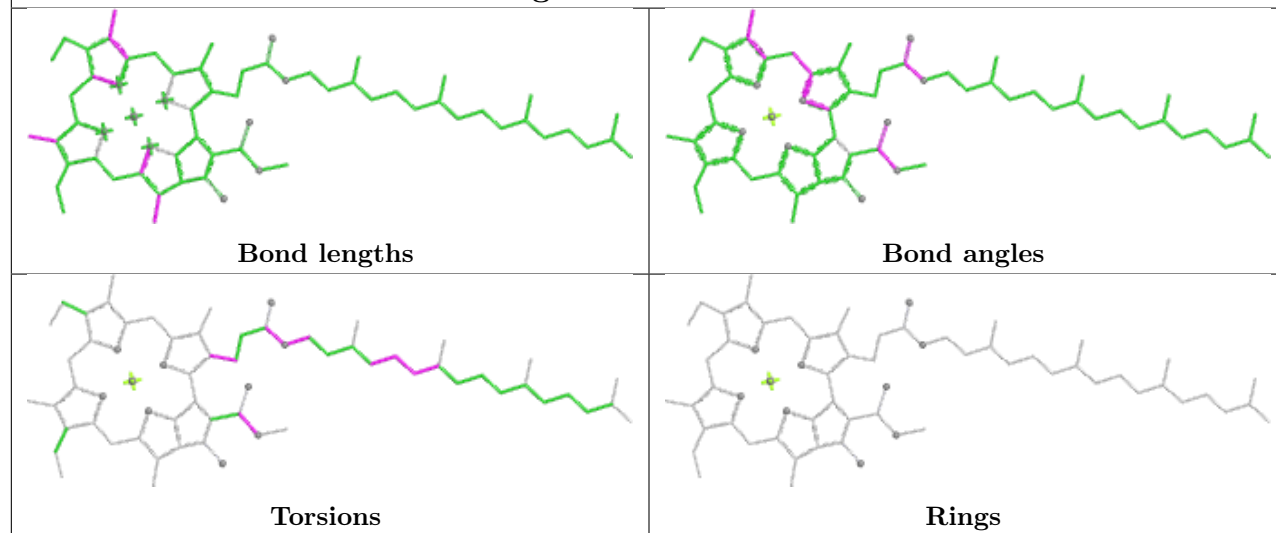
Ligand CLA X 604



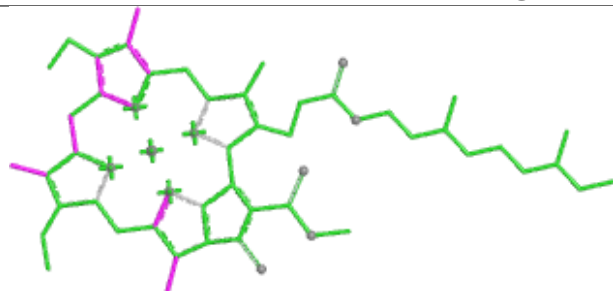
Ligand CLA U 611



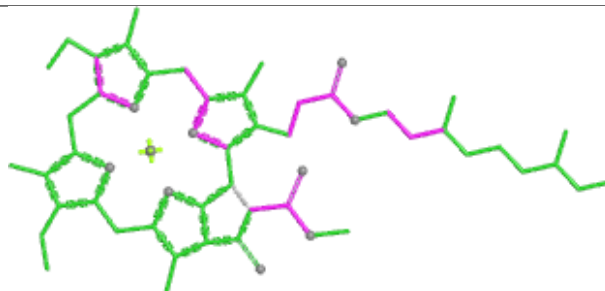
Ligand CLA B 829



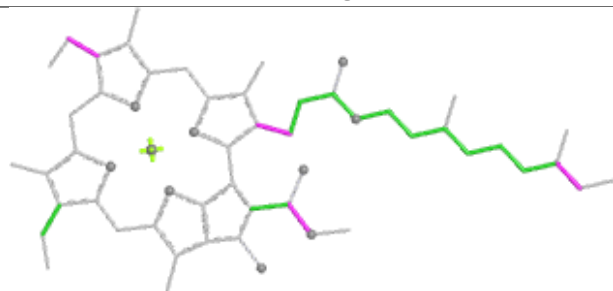
Ligand CLA K 203



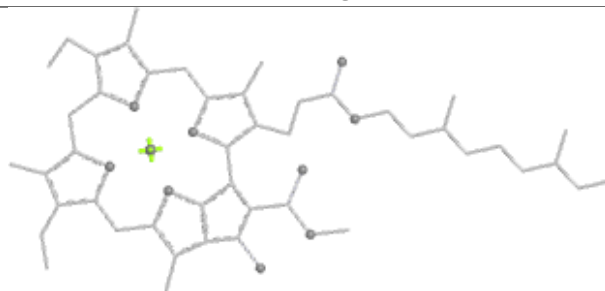
Bond lengths



Bond angles

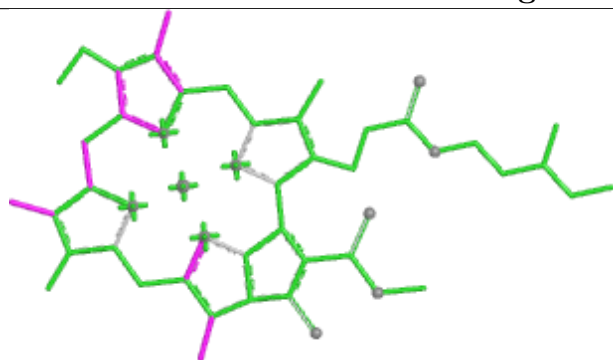


Torsions

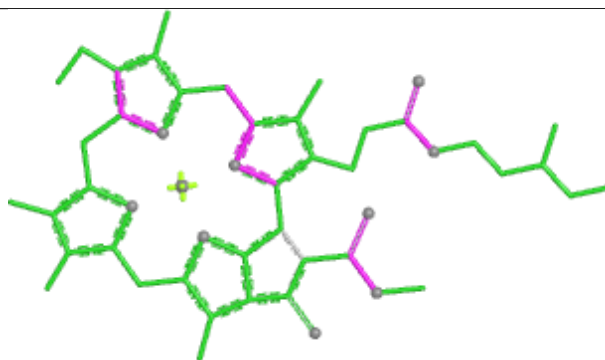


Rings

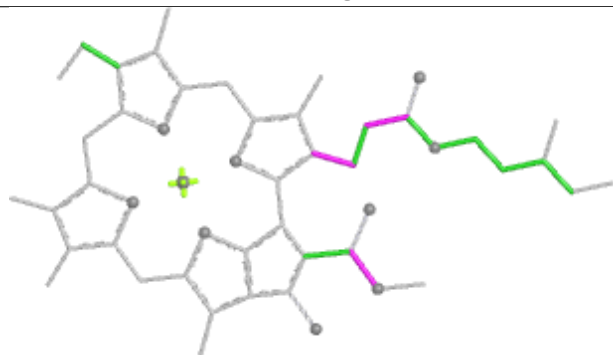
Ligand CLA 5 608



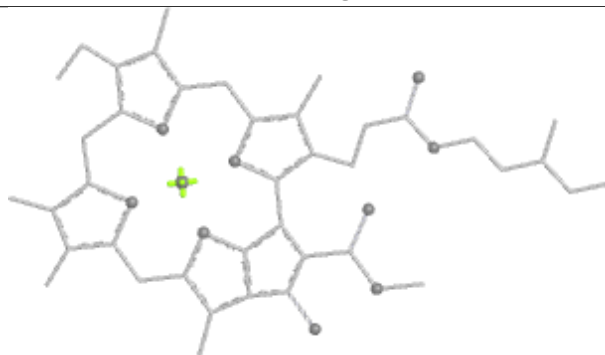
Bond lengths



Bond angles

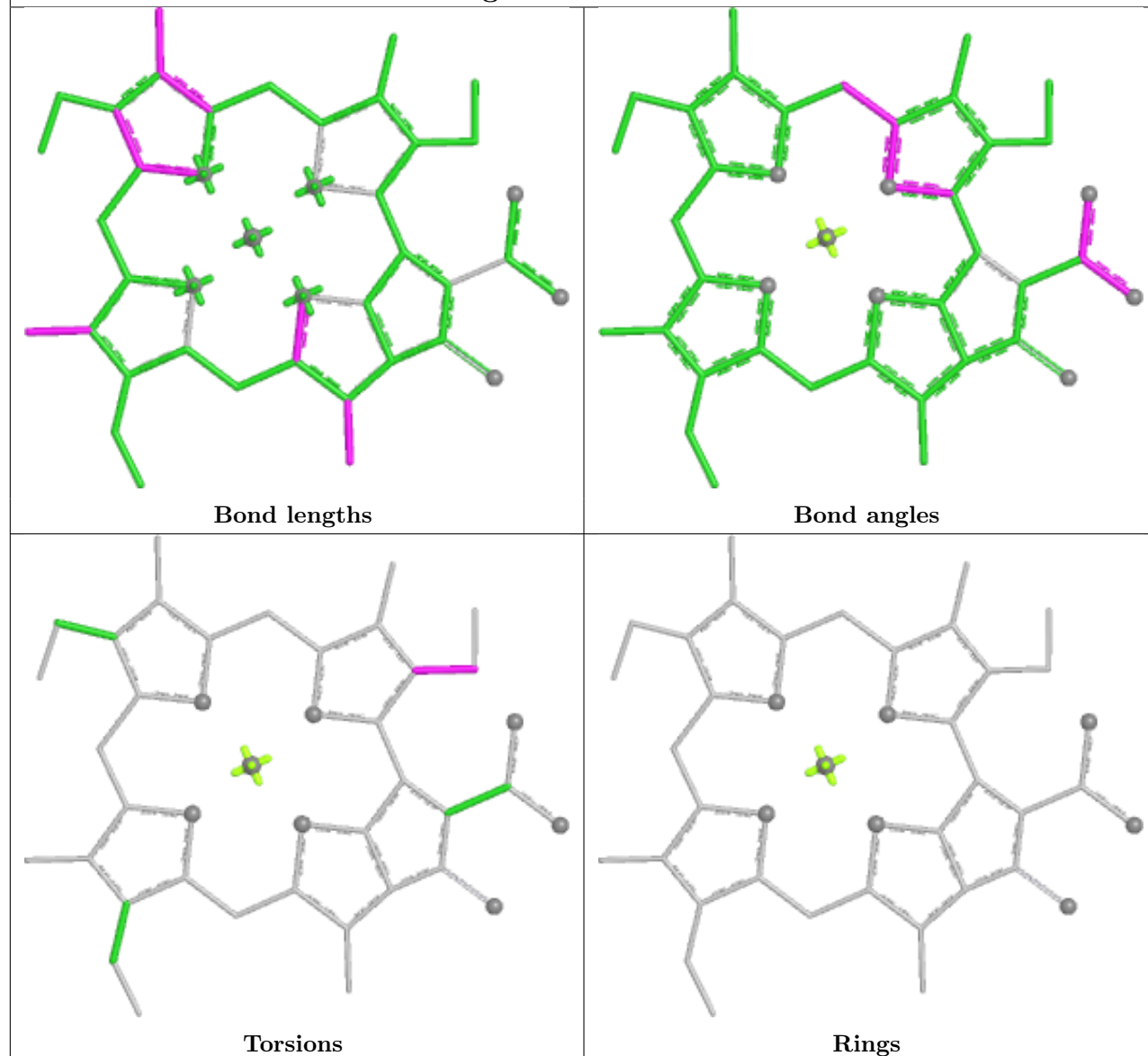


Torsions

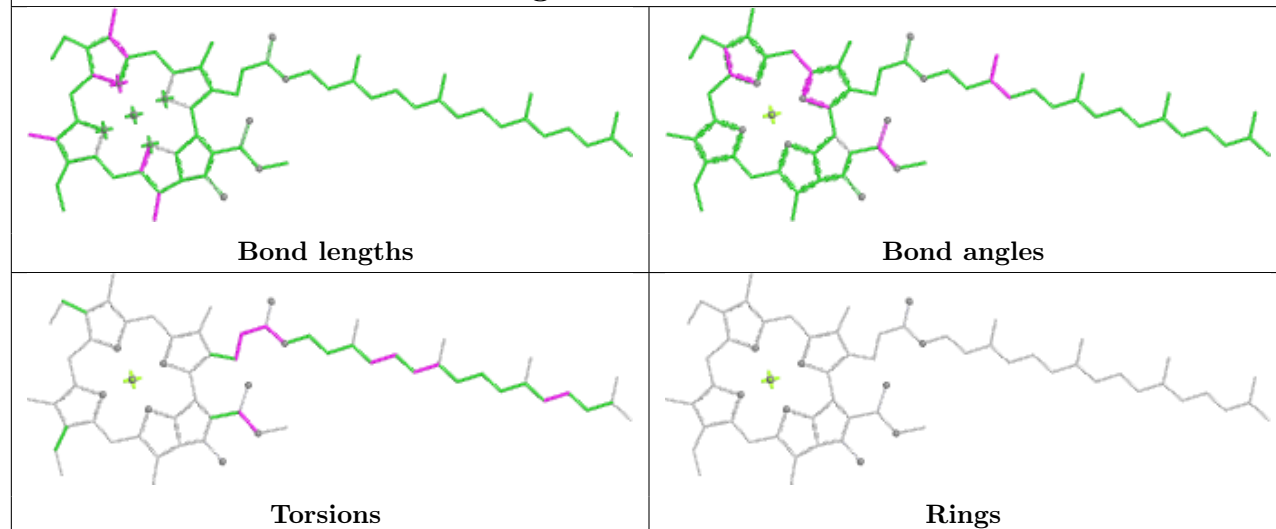


Rings

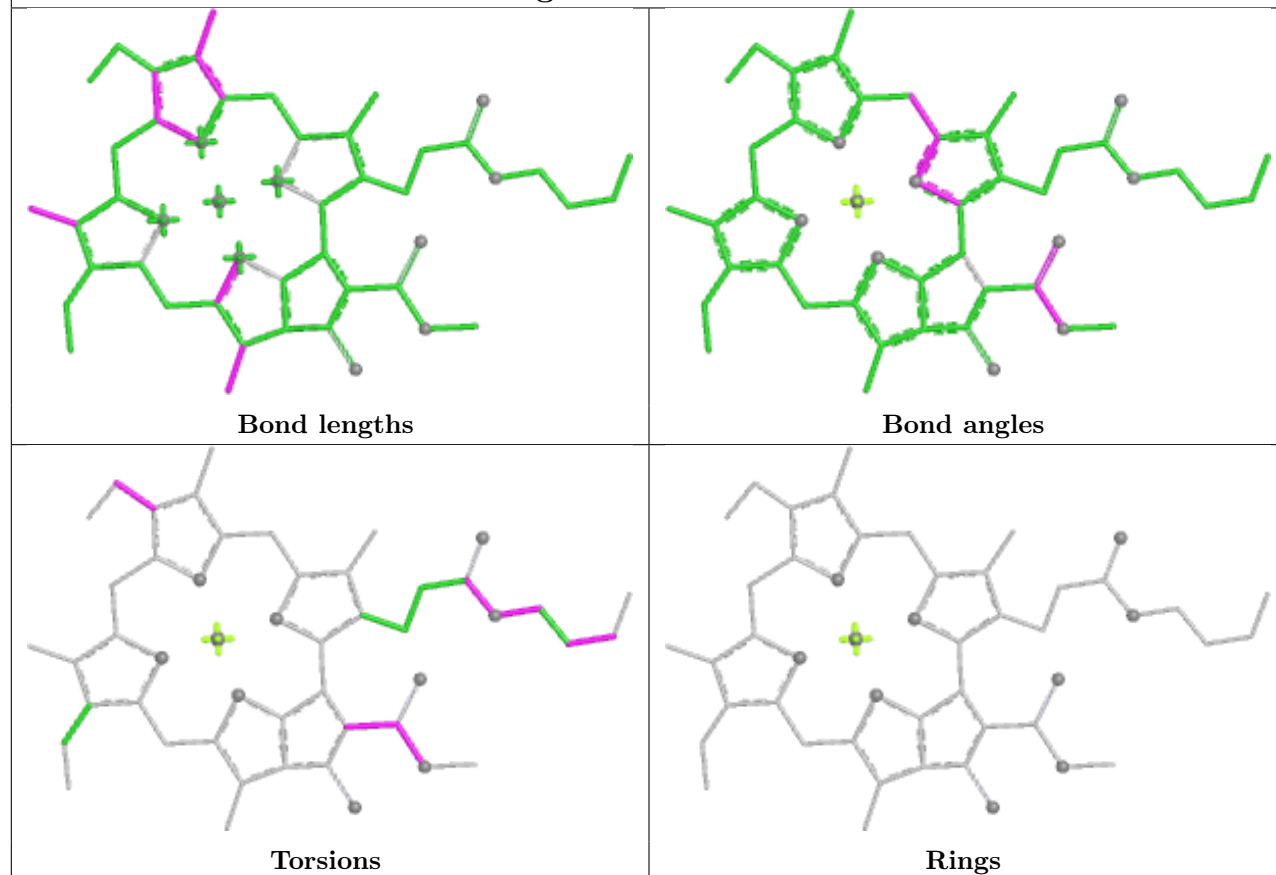
Ligand CLA 6 612



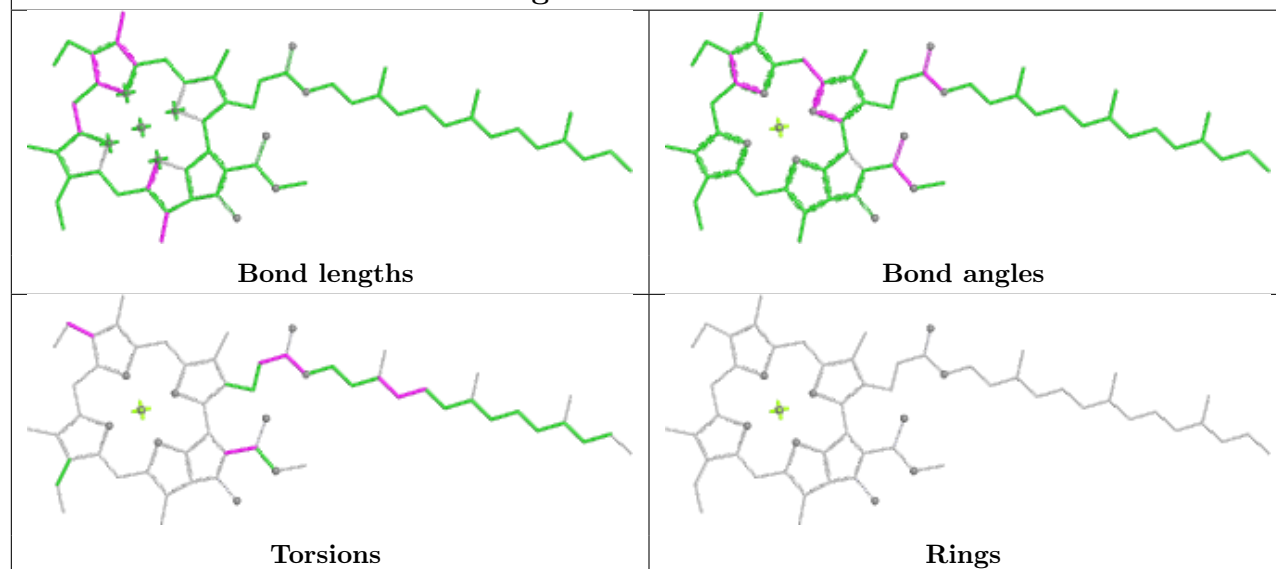
Ligand CLA A 830



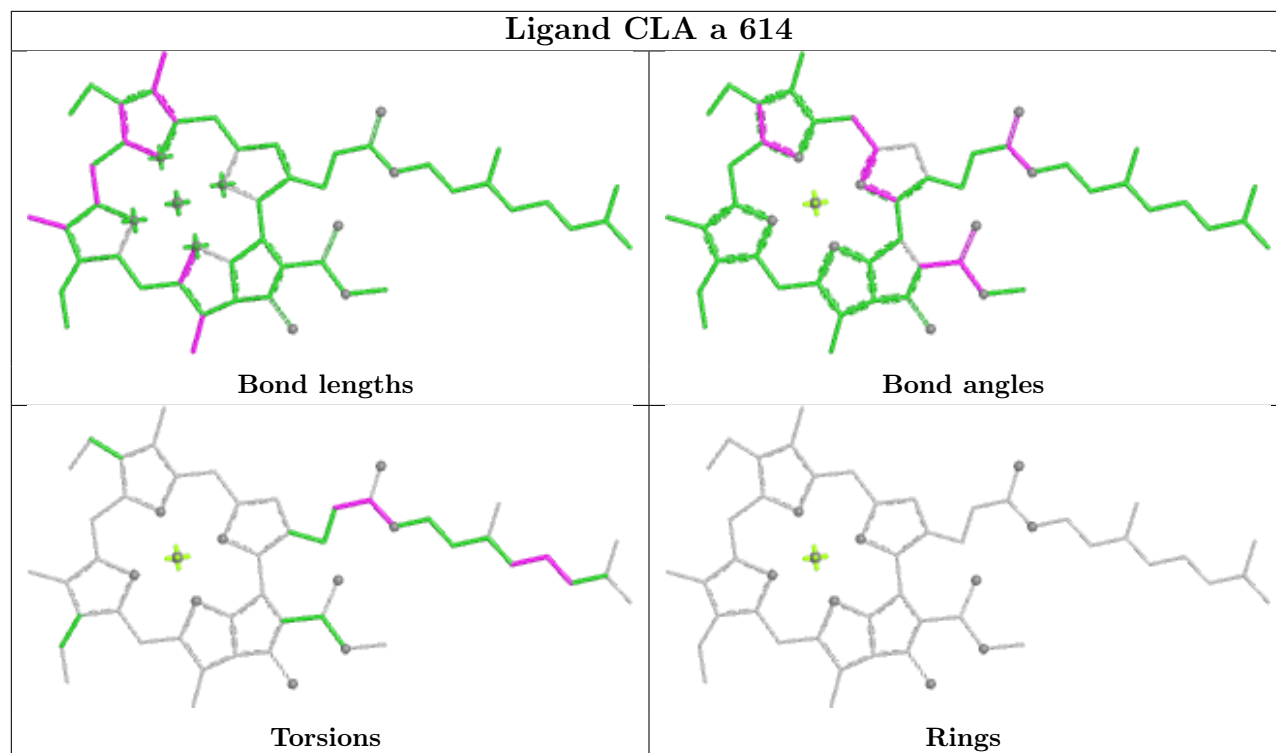
Ligand CLA a 604



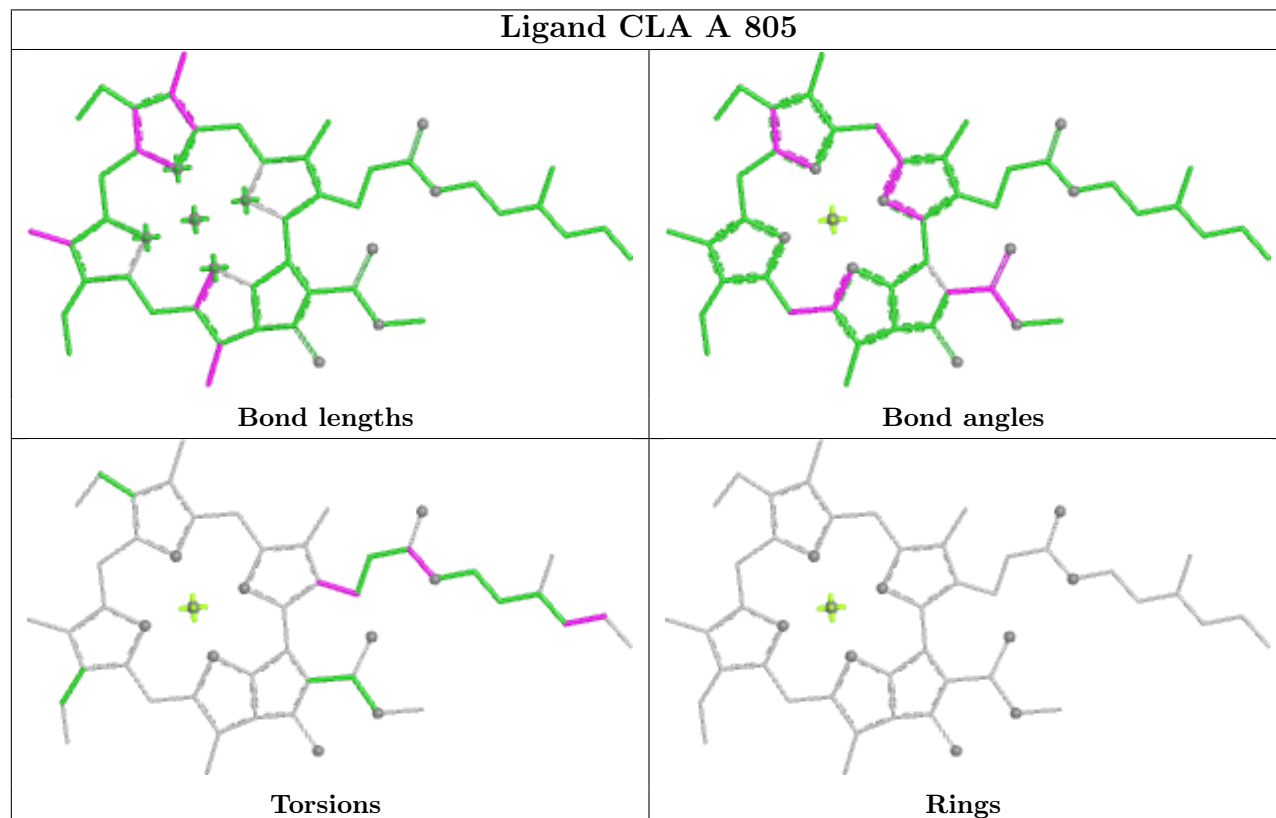
Ligand CLA X 603

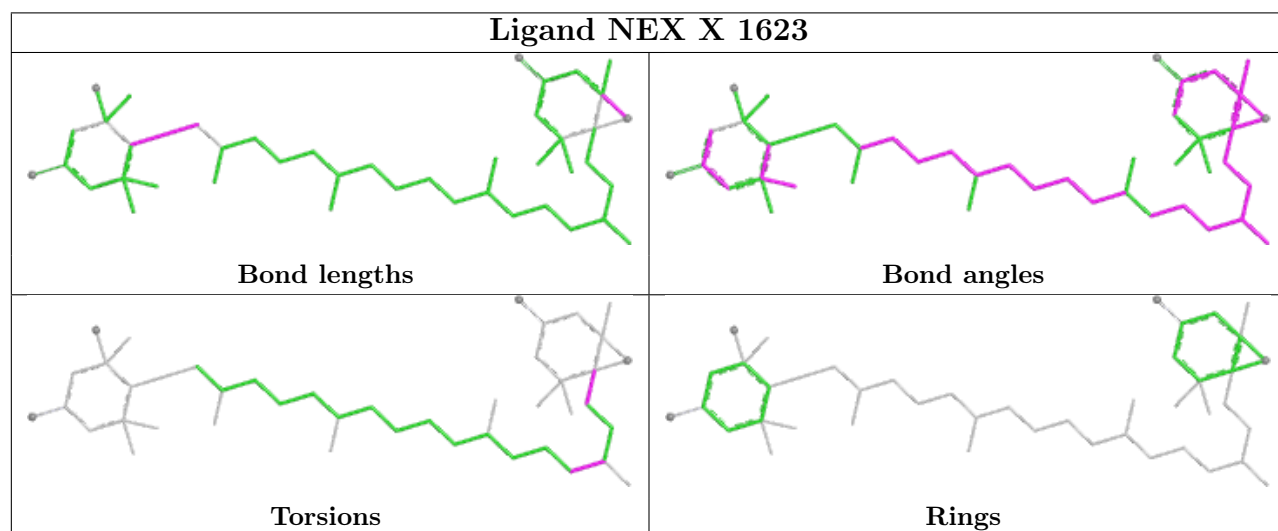
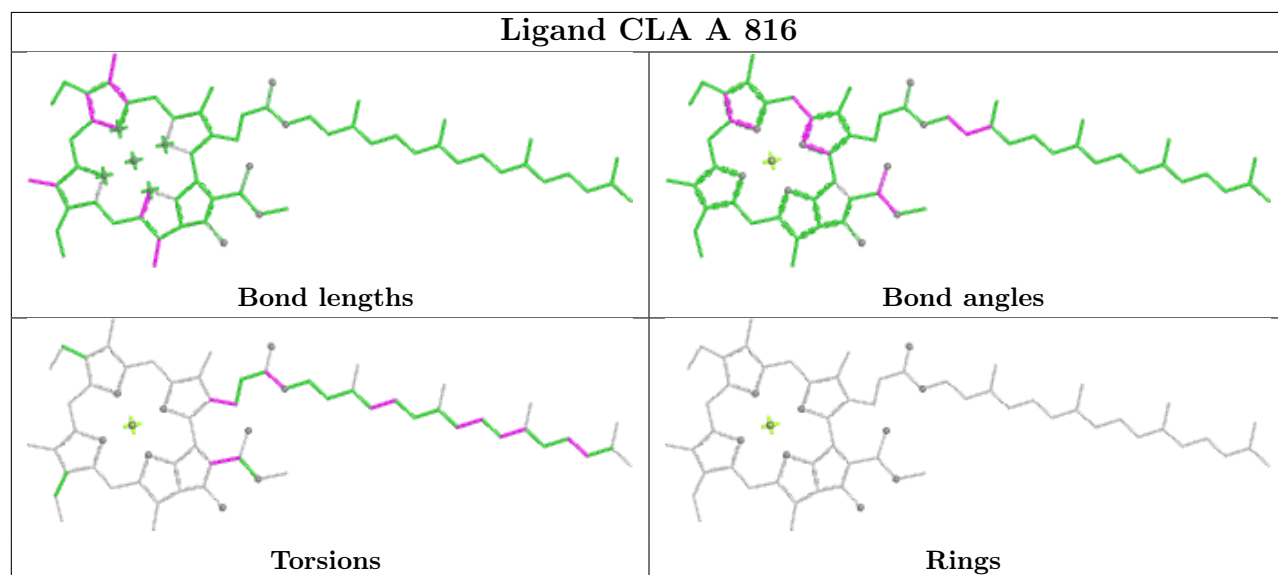
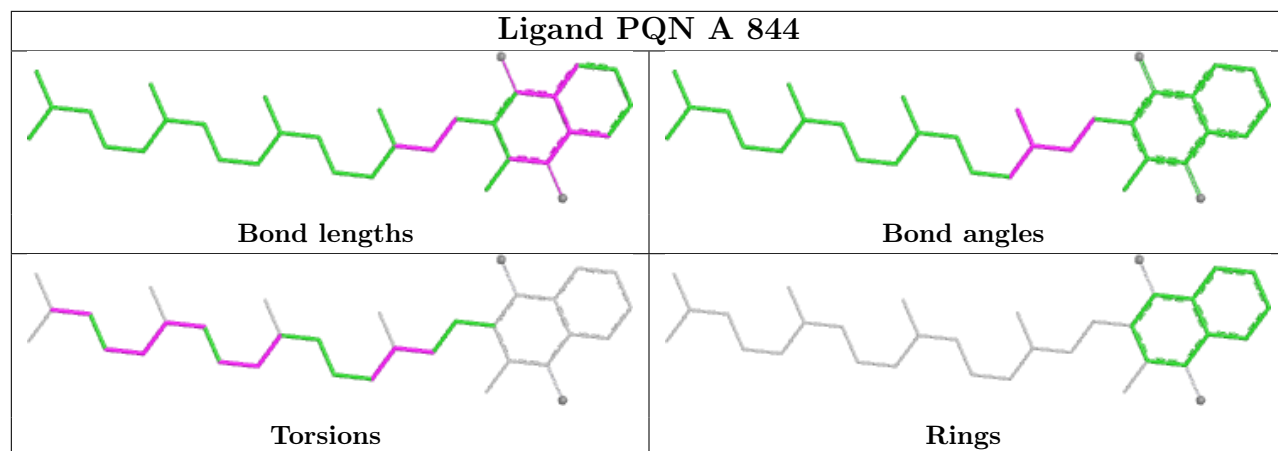


Ligand CLA a 614

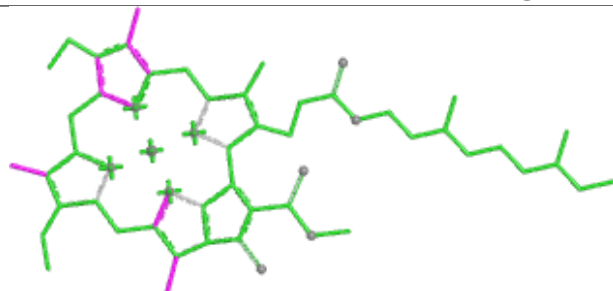


Ligand CLA A 805

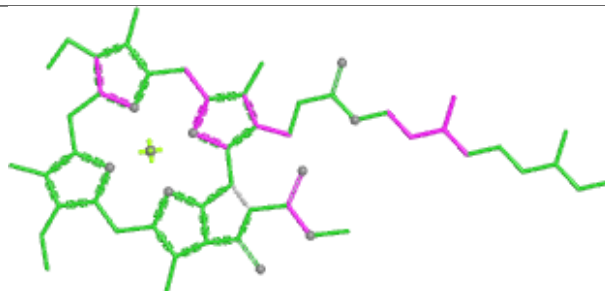




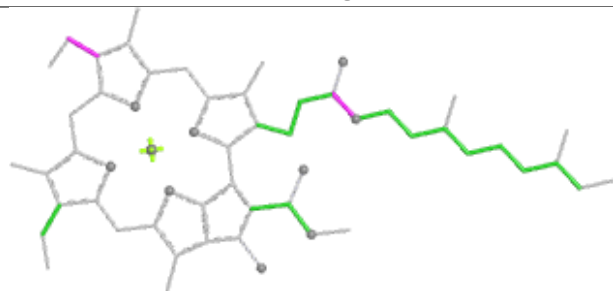
Ligand CLA 5 601



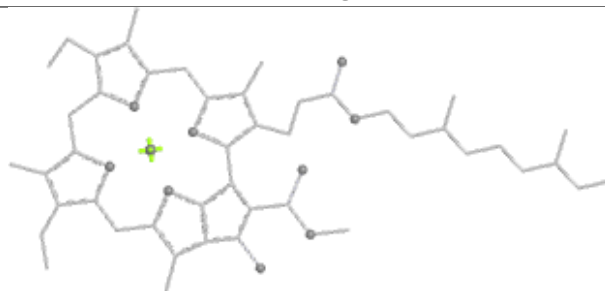
Bond lengths



Bond angles

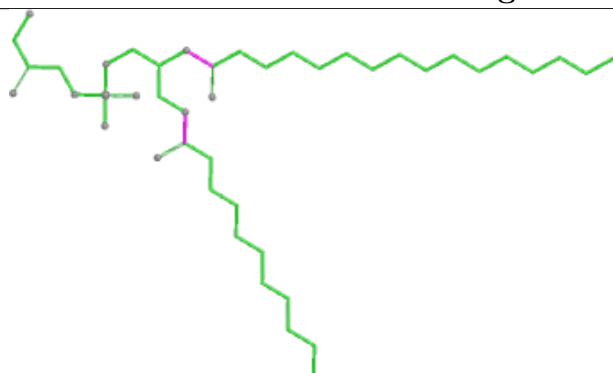


Torsions

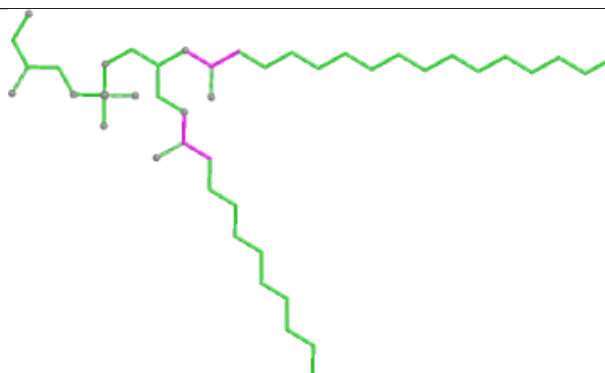


Rings

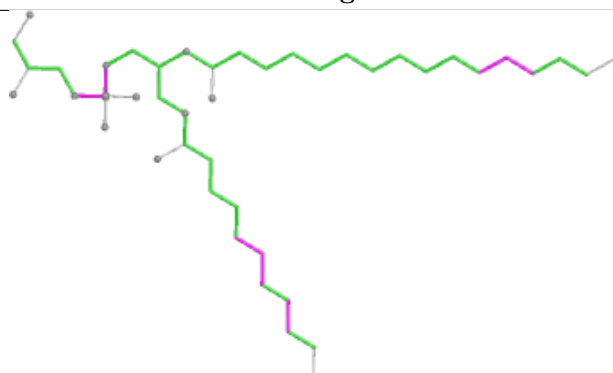
Ligand LHG W 2630



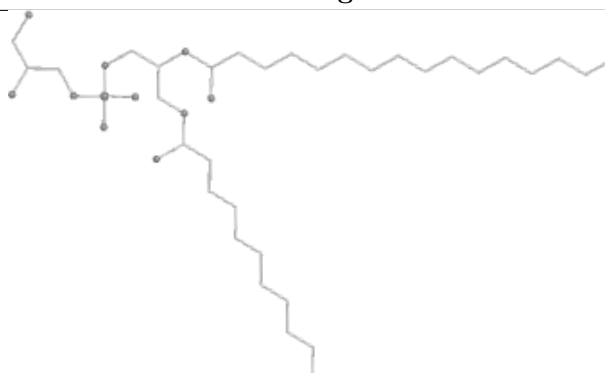
Bond lengths



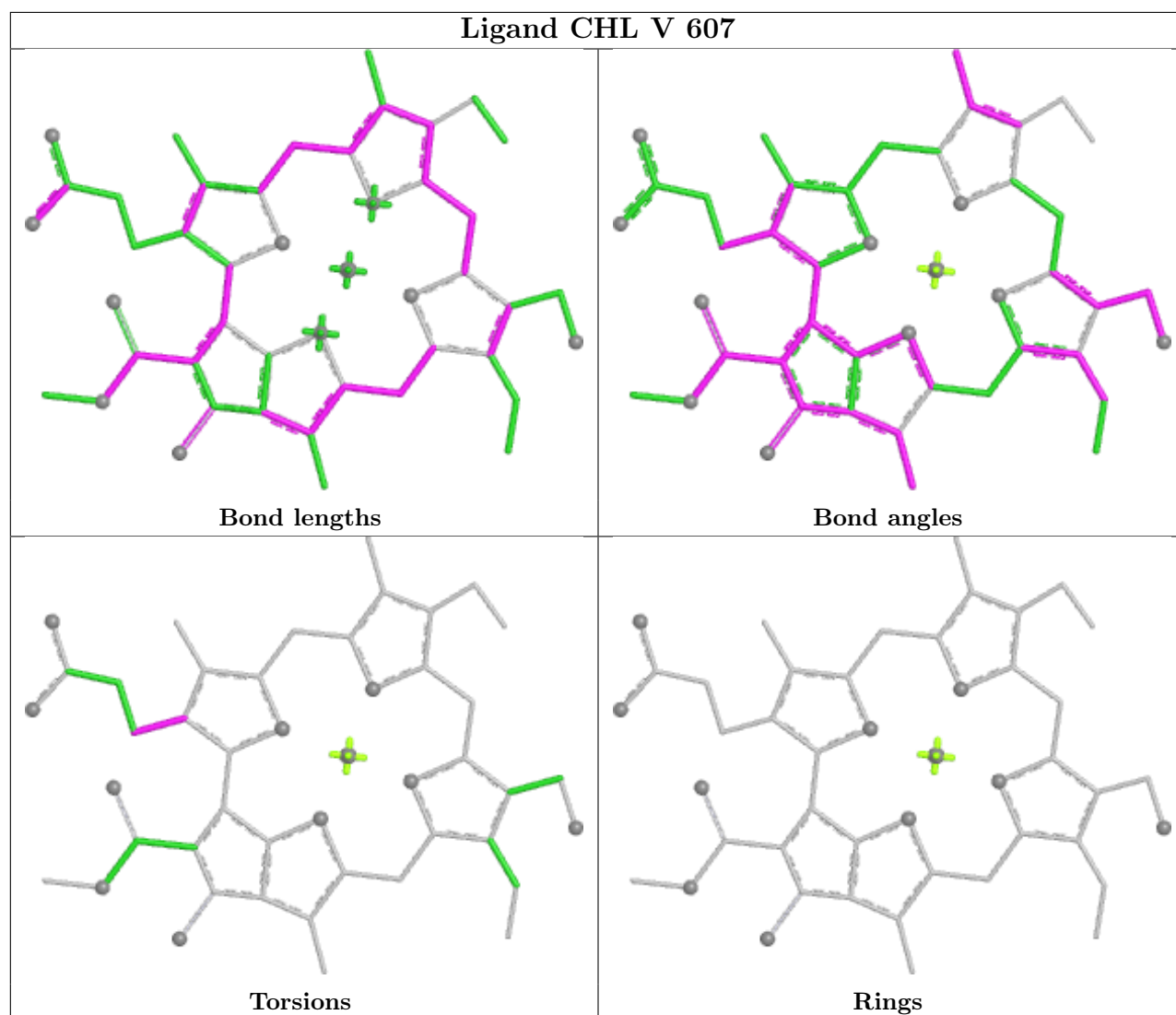
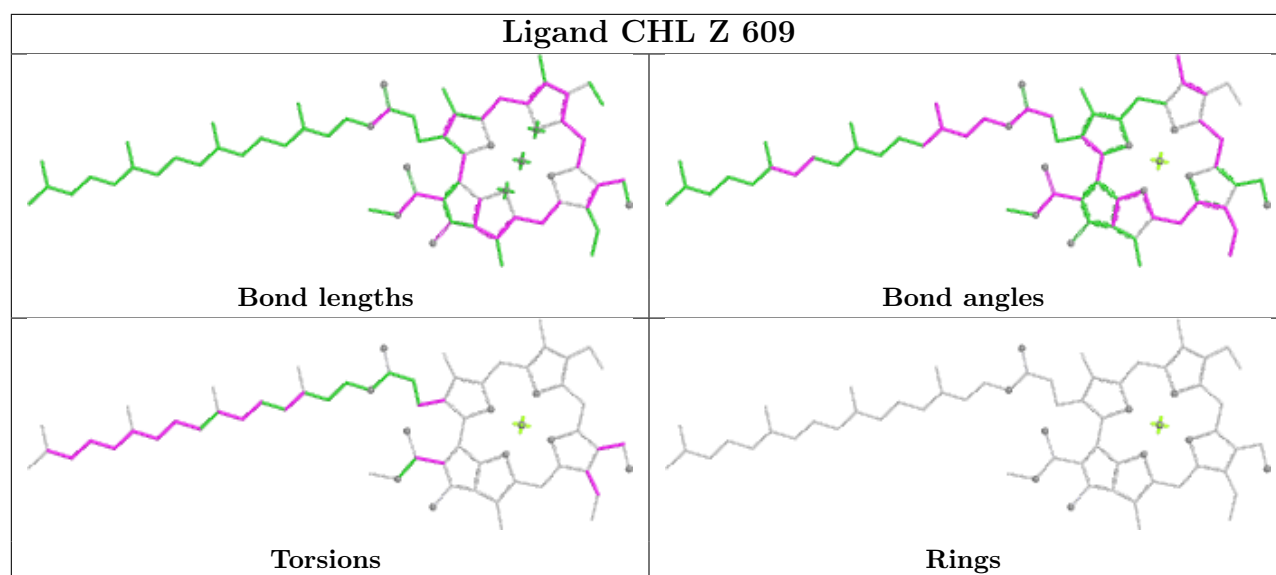
Bond angles

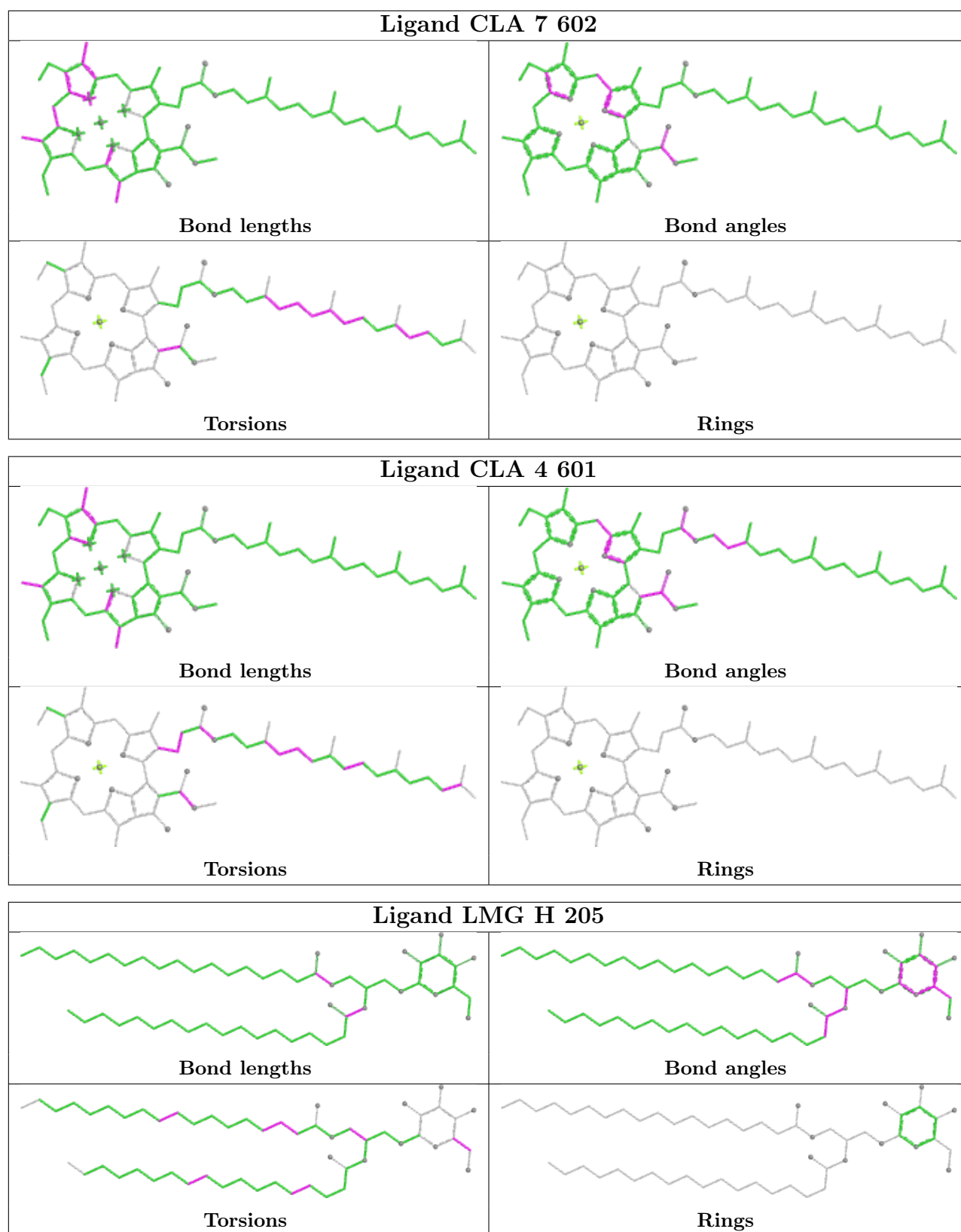


Torsions



Rings





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.

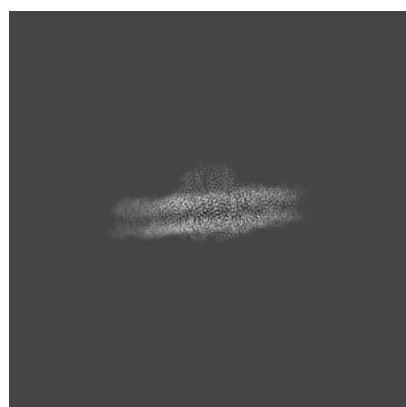
6 Map visualisation [i](#)

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.

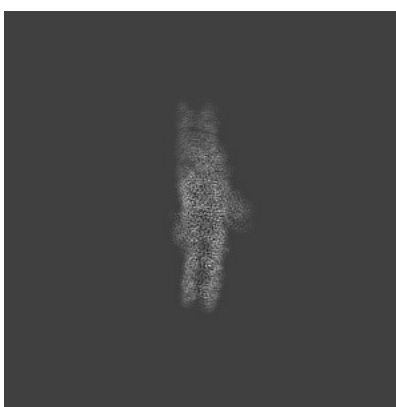
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

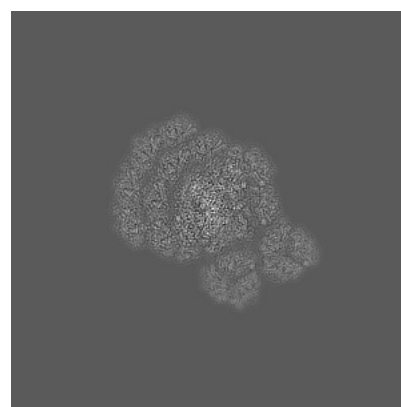
6.1.1 Primary map



X



Y

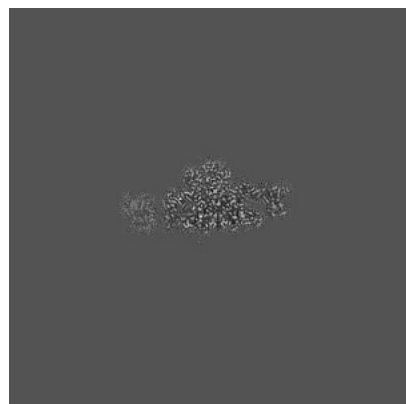


Z

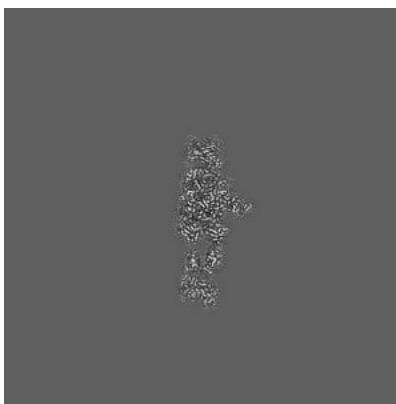
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

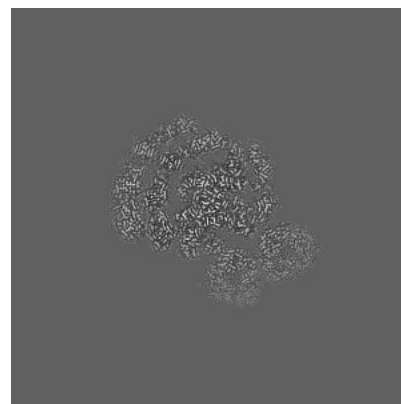
6.2.1 Primary map



X Index: 240



Y Index: 240

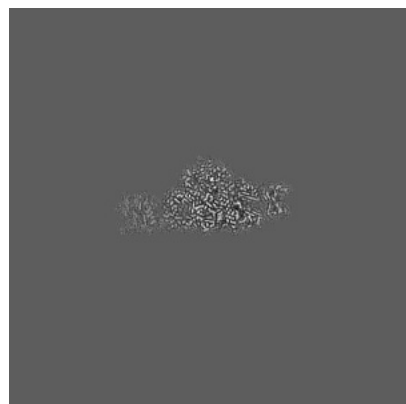


Z Index: 240

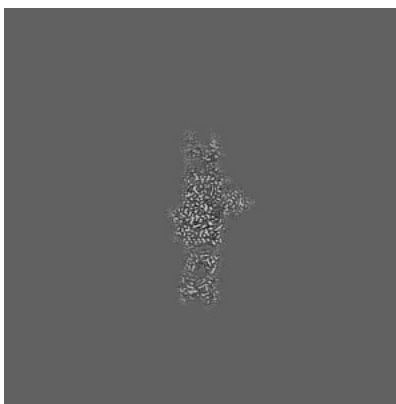
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

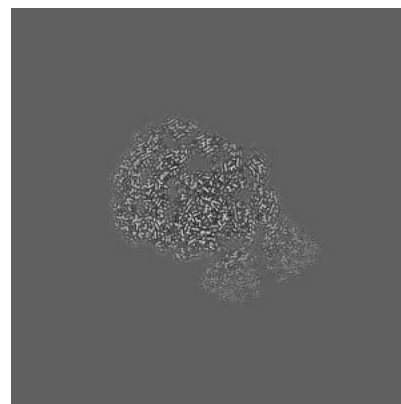
6.3.1 Primary map



X Index: 243



Y Index: 231

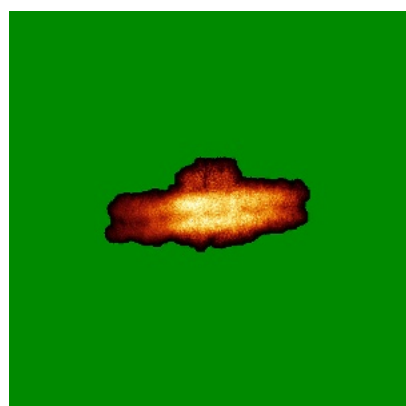


Z Index: 248

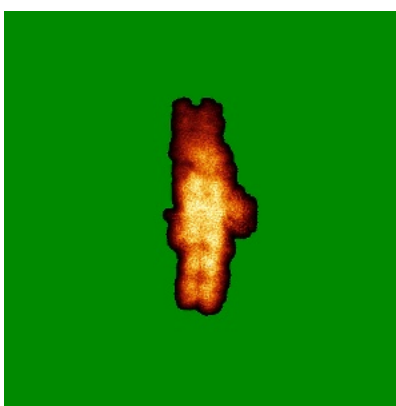
The images above show the largest variance slices of the map in three orthogonal directions.

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

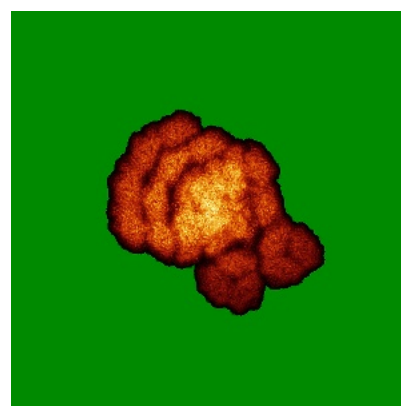
6.4.1 Primary map



X



Y

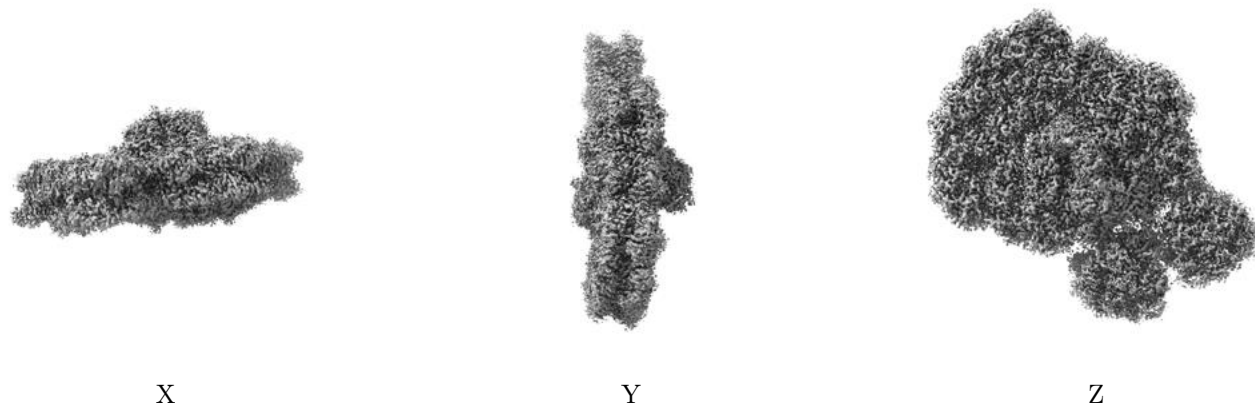


Z

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.

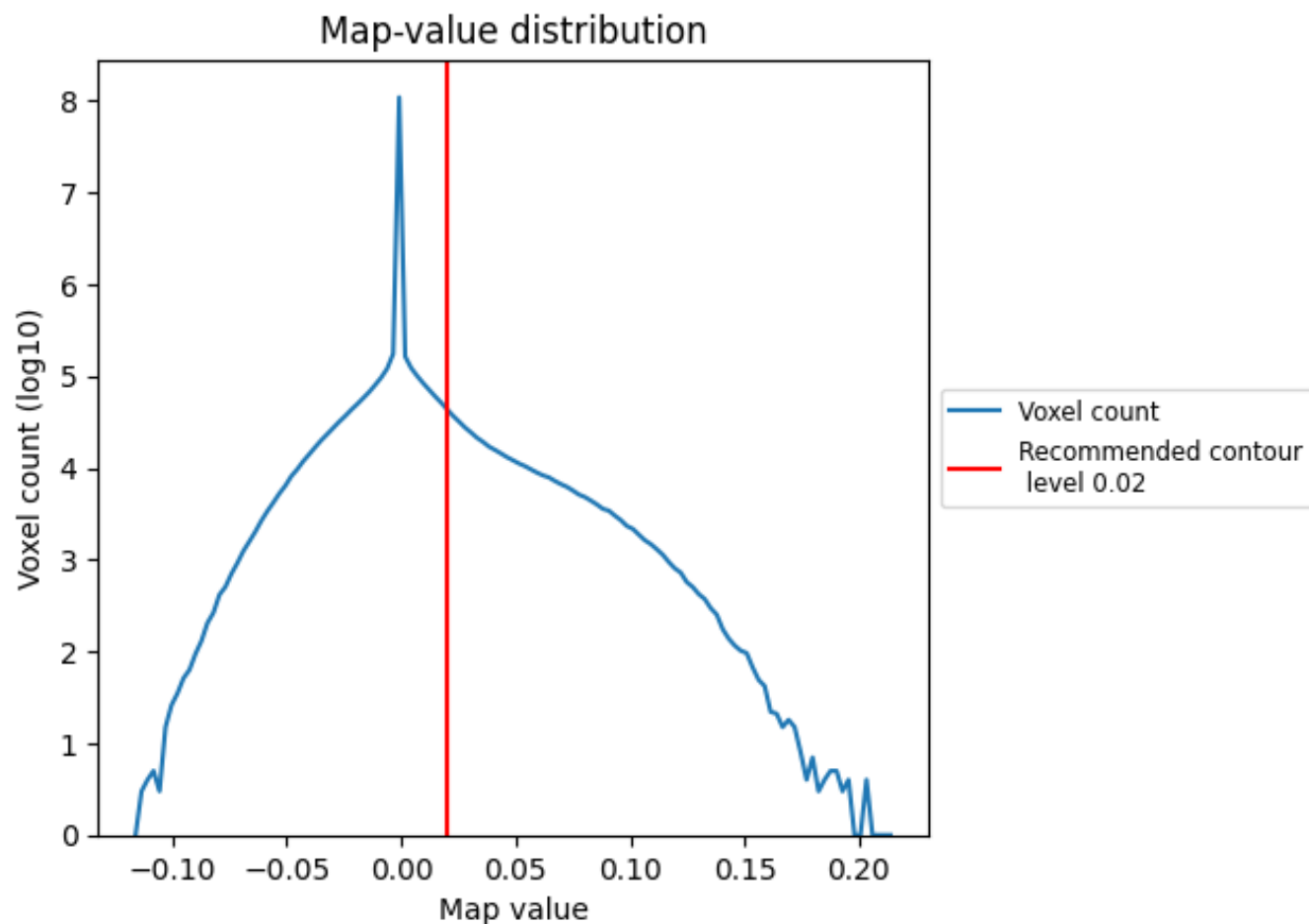
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

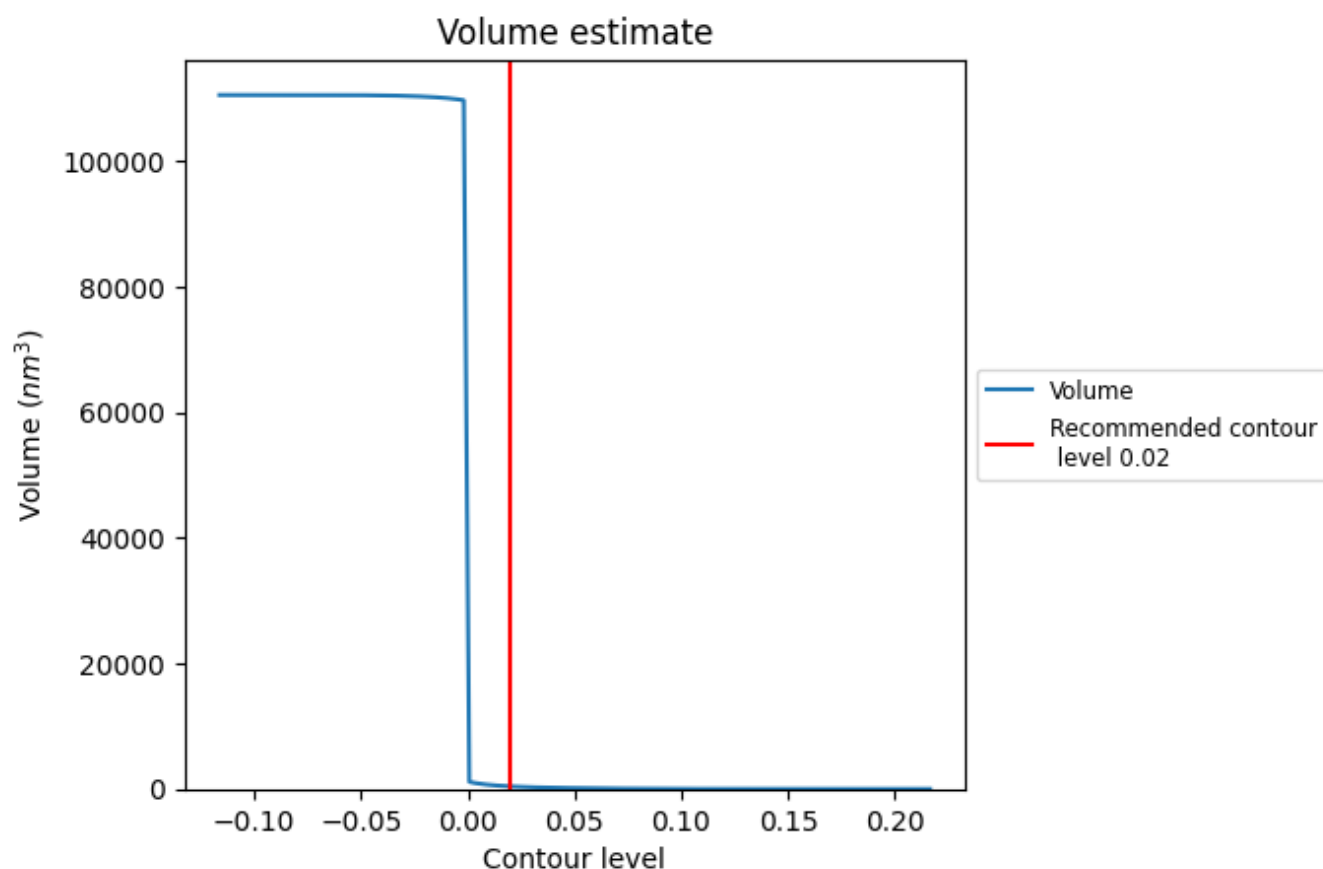
This section contains the results of statistical analysis of the map.

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.

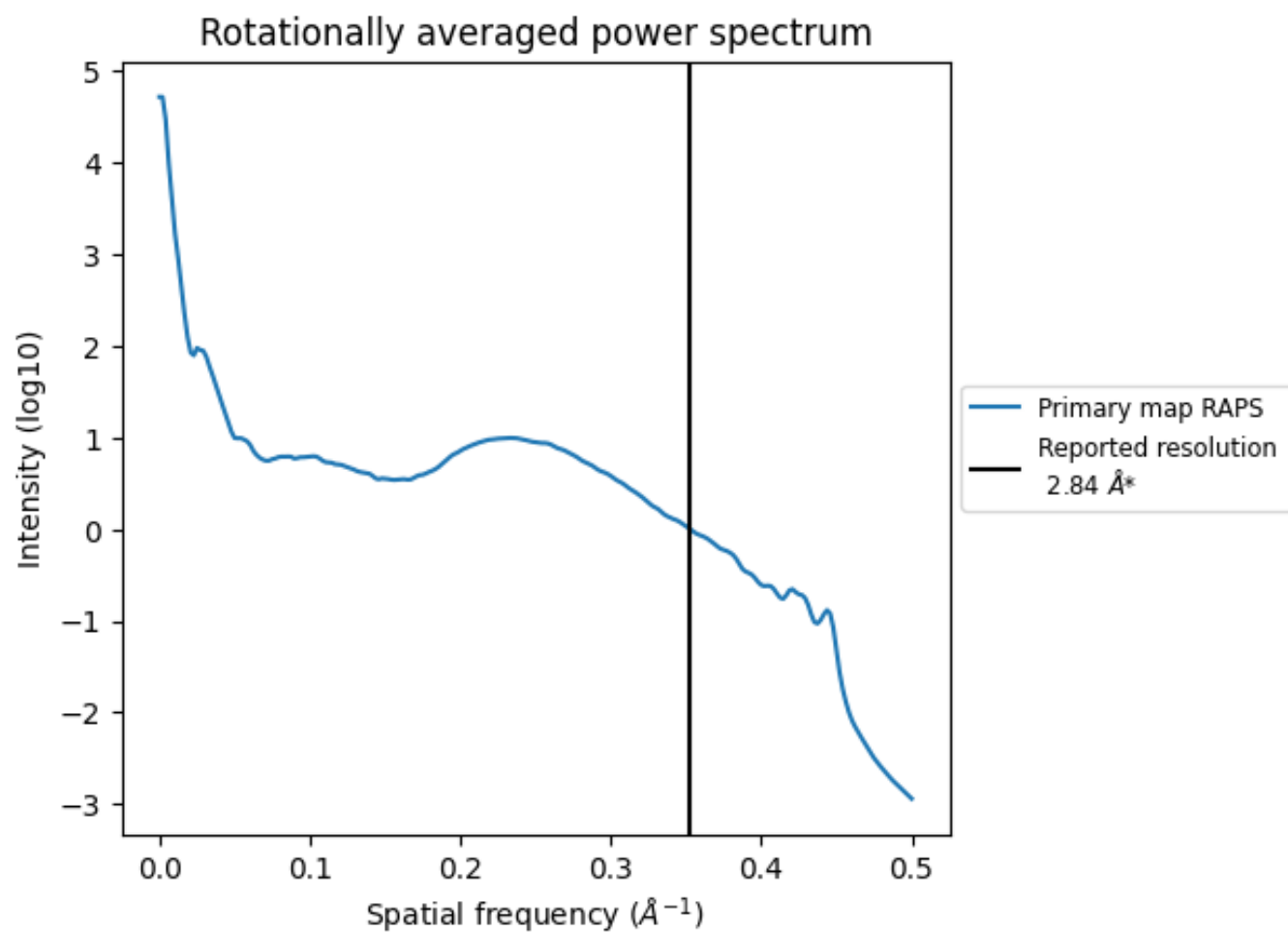
7.2 Volume estimate [i](#)



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

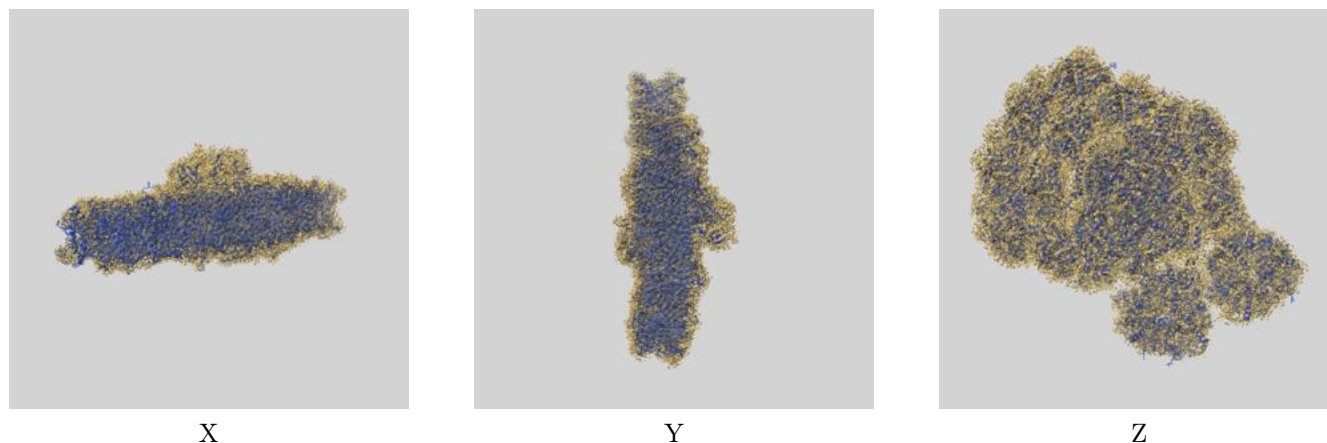
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

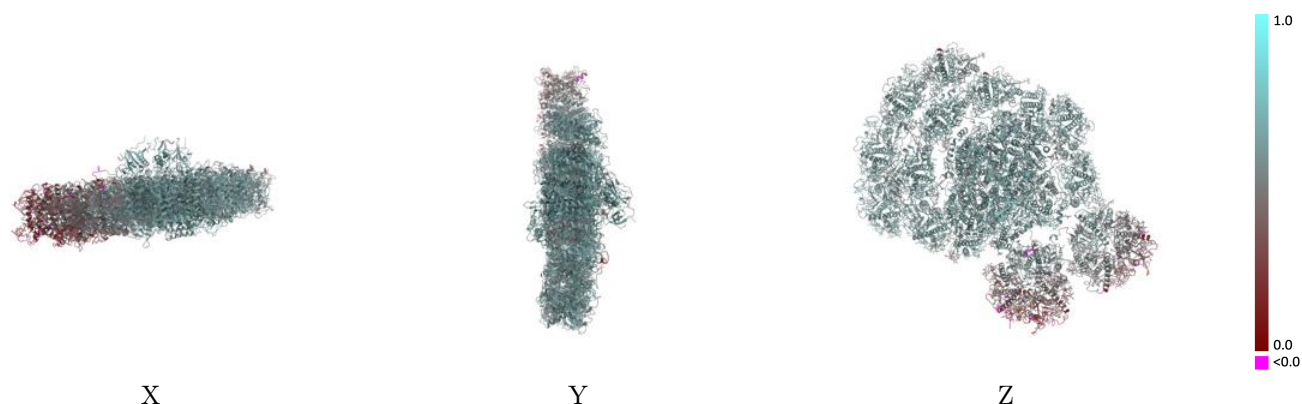
This section contains information regarding the fit between EMDB map EMD-30925 and PDB model 7DZ7. Per-residue inclusion information can be found in section [3](#) on page [45](#).

9.1 Map-model overlay [i](#)



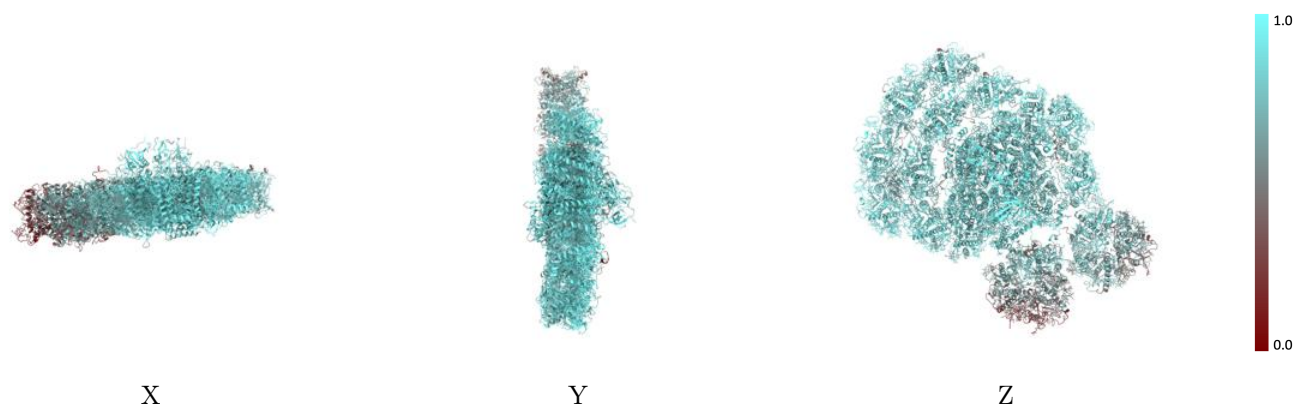
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



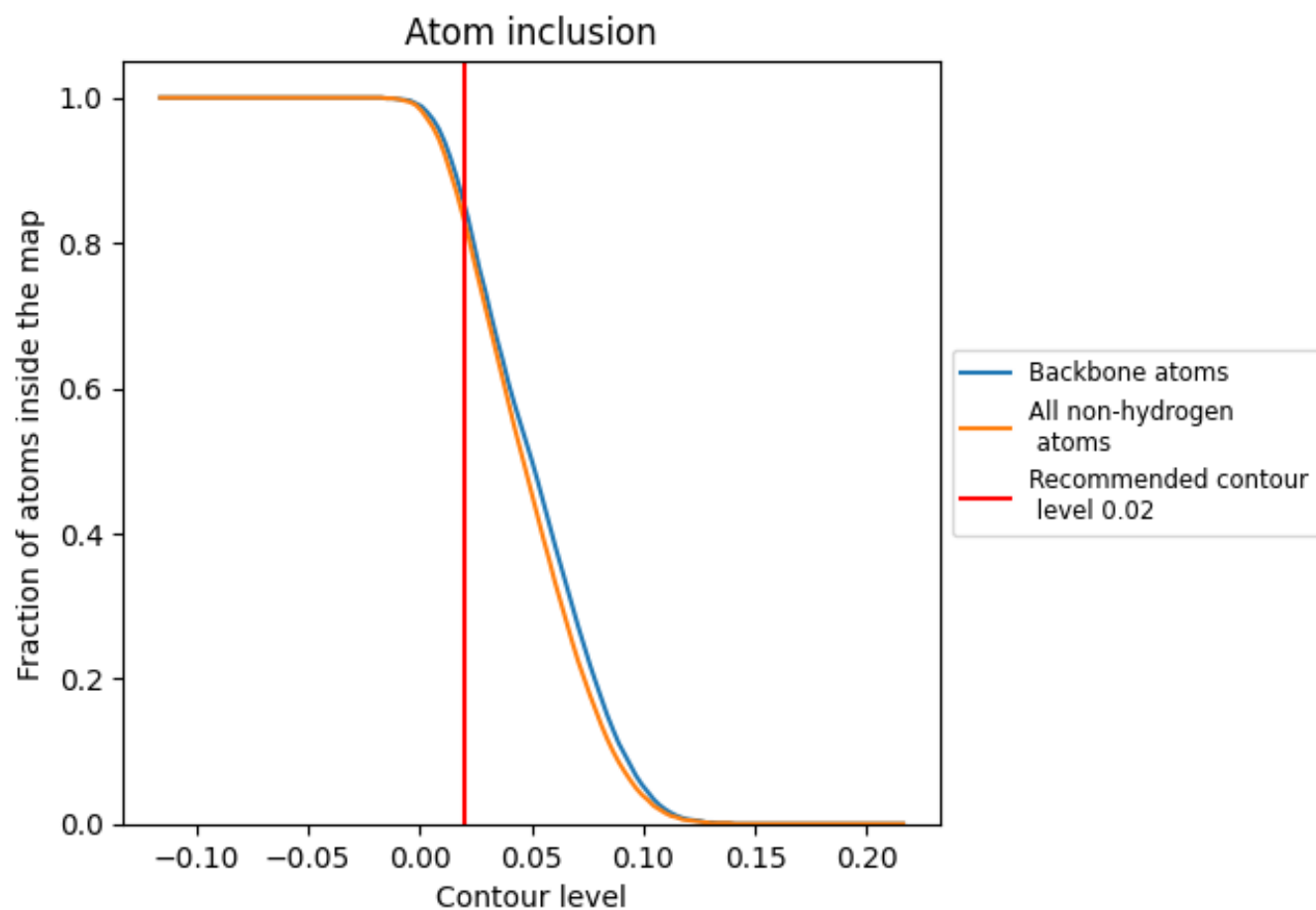
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

