



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 04:55 AM UTC

PDB ID : 6IJO / pdb_00006ijo
EMDB ID : EMD-9680
Title : Photosystem I of Chlamydomonas reinhardtii
Authors : Pan, X.; Ma, J.; Su, X.; Liu, Z.; Zhang, X.; Li, M.
Deposited on : 2018-10-10
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

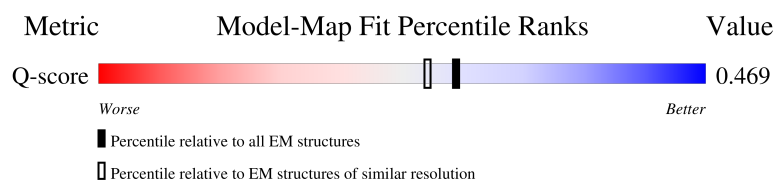
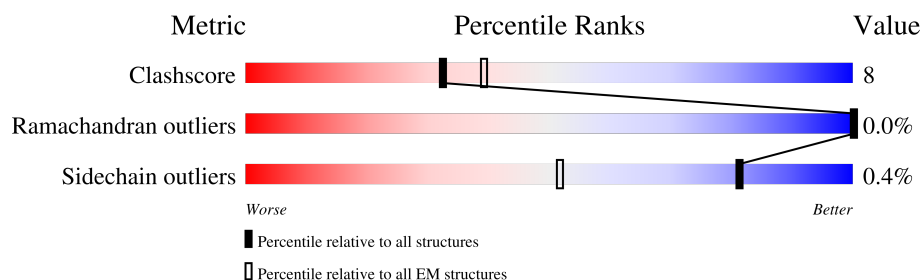
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	 83% 15%
2	B	735	 84% 16%
3	C	81	 79% 20%
4	D	247	 46% 12% 42%

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Mol	Chain	Length	Quality of chain
5	E	143	
6	F	227	
7	G	159	
8	H	155	
9	I	106	
10	J	41	
11	K	160	
12	L	258	
13	1	248	
13	a	248	
14	3	298	
15	4	290	
16	5	274	
17	6	318	
18	7	241	
19	8	272	
20	2	227	
21	9	213	
22	X	26	

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
23	CLA	1	601	X	-	-	-
23	CLA	1	602	X	-	-	-
23	CLA	1	603	X	-	-	-
23	CLA	1	604	X	-	-	-
23	CLA	1	606	X	-	-	-

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	804	X	-	-	-
23	CLA	A	805	X	-	-	-
23	CLA	A	806	X	-	-	-
23	CLA	A	807	X	-	-	-
23	CLA	A	808	X	-	-	-
23	CLA	A	809	X	-	-	-
23	CLA	A	810	X	-	-	-
23	CLA	A	811	X	-	-	-
23	CLA	A	812	X	-	-	-
23	CLA	A	813	X	-	-	-
23	CLA	A	814	X	-	-	-
23	CLA	A	815	X	-	-	-
23	CLA	A	816	X	-	-	-
23	CLA	A	817	X	-	-	-
23	CLA	A	818	X	-	-	-
23	CLA	A	819	X	-	-	-
23	CLA	A	820	X	-	-	-
23	CLA	A	821	X	-	-	-
23	CLA	A	822	X	-	-	-
23	CLA	A	823	X	-	-	-
23	CLA	A	824	X	-	-	-
23	CLA	A	825	X	-	-	-
23	CLA	A	826	X	-	-	-
23	CLA	A	827	X	-	-	-
23	CLA	A	828	X	-	-	-
23	CLA	A	829	X	-	-	-
23	CLA	A	830	X	-	-	-
23	CLA	A	831	X	-	-	-
23	CLA	A	832	X	-	-	-
23	CLA	A	833	X	-	-	-
23	CLA	A	834	X	-	-	-
23	CLA	A	835	X	-	-	-
23	CLA	A	836	X	-	-	-
23	CLA	A	837	X	-	-	-
23	CLA	A	838	X	-	-	-
23	CLA	A	839	X	-	-	-
23	CLA	A	840	X	-	-	-
23	CLA	A	841	X	-	-	-
23	CLA	A	842	X	-	-	-
23	CLA	A	843	X	-	-	-
23	CLA	A	845	X	-	-	-
23	CLA	A	854	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	802	X	-	-	-
23	CLA	B	803	X	-	-	-
23	CLA	B	804	X	-	-	-
23	CLA	B	805	X	-	-	-
23	CLA	B	806	X	-	-	-
23	CLA	B	807	X	-	-	-
23	CLA	B	808	X	-	-	-
23	CLA	B	809	X	-	-	-
23	CLA	B	810	X	-	-	-
23	CLA	B	811	X	-	-	-
23	CLA	B	812	X	-	-	-
23	CLA	B	813	X	-	-	-
23	CLA	B	814	X	-	-	-
23	CLA	B	815	X	-	-	-
23	CLA	B	816	X	-	-	-
23	CLA	B	817	X	-	-	-
23	CLA	B	818	X	-	-	-
23	CLA	B	819	X	-	-	-
23	CLA	B	820	X	-	-	-
23	CLA	B	821	X	-	-	-
23	CLA	B	823	X	-	-	-
23	CLA	B	824	X	-	-	-
23	CLA	B	825	X	-	-	-
23	CLA	B	826	X	-	-	-
23	CLA	B	827	X	-	-	-
23	CLA	B	828	X	-	-	-
23	CLA	B	829	X	-	-	-
23	CLA	B	830	X	-	-	-
23	CLA	B	831	X	-	-	-
23	CLA	B	832	X	-	-	-
23	CLA	B	833	X	-	-	-
23	CLA	B	834	X	-	-	-
23	CLA	B	835	X	-	-	-
23	CLA	B	837	X	-	-	-
23	CLA	B	838	X	-	-	-
23	CLA	B	839	X	-	-	-
23	CLA	B	840	X	-	-	-
23	CLA	B	841	X	-	-	-
23	CLA	F	301	X	-	-	-
23	CLA	F	303	X	-	-	-
23	CLA	F	304	X	-	-	-
23	CLA	G	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	G	204	X	-	-	-
23	CLA	J	101	X	-	-	-
23	CLA	K	201	X	-	-	-
23	CLA	K	203	X	-	-	-
23	CLA	K	204	X	-	-	-
23	CLA	K	206	X	-	-	-
23	CLA	L	302	X	-	-	-
23	CLA	L	303	X	-	-	-
23	CLA	L	304	X	-	-	-
23	CLA	a	601	X	-	-	-
23	CLA	a	602	X	-	-	-
23	CLA	a	603	X	-	-	-
23	CLA	a	604	X	-	-	-
23	CLA	a	606	X	-	-	-
23	CLA	a	607	X	-	-	-
23	CLA	a	608	X	-	-	-
23	CLA	a	609	X	-	-	-
23	CLA	a	610	X	-	-	-
23	CLA	a	611	X	-	-	-
23	CLA	a	612	X	-	-	-
23	CLA	a	613	X	-	-	-
23	CLA	a	614	X	-	-	-
23	CLA	a	616	X	-	-	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 49685 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 PsaA.

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 PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5812	3818	975	1001	18		

- Molecule 3 is a protein called PsaC.

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 PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1129	722	200	200	7		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	64	Total	C	N	O	0	0
			505	322	89	94		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	164	Total	C	N	O	S	0	0
			1254	811	209	231	3		

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	70	Total	C	N	O	0	0
			514	334	89	91		

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	51	Total	C	N	O	0	0
			357	223	66	68		

- Molecule 9 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	32	Total	C	N	O	S	0	0
			242	166	34	41	1		

- Molecule 10 is a protein called PsaJ.

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 PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	85	Total	C	N	O	S	0	0
			578	368	99	109	2		

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	106	Total	C	N	O	S	0	0
			768	507	123	136	2		

- Molecule 13 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	193	Total	C	N	O	S	0	0
			1433	932	239	259	3		
13	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

- Molecule 14 is a protein called Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	221	Total	C	N	O	S	0	0
			1683	1099	271	305	8		

- Molecule 15 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4	210	Total	C	N	O	S	0	0
			1631	1071	263	292	5		

- Molecule 16 is a protein called Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	5	226	Total	C	N	O	S	0	0
			1765	1149	295	313	8		

- Molecule 17 is a protein called Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	230	Total	C	N	O	S	0	0
			1771	1167	293	305	6		

- Molecule 18 is a protein called Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	7	213	Total	C	N	O	S	0	0
			1649	1072	274	297	6		

- Molecule 19 is a protein called Lhca8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	8	215	Total	C	N	O	S	0	0
			1630	1058	278	290	4		

- Molecule 20 is a protein called Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	173	Total	C	N	O	S	0	0
			1346	874	223	241	8		

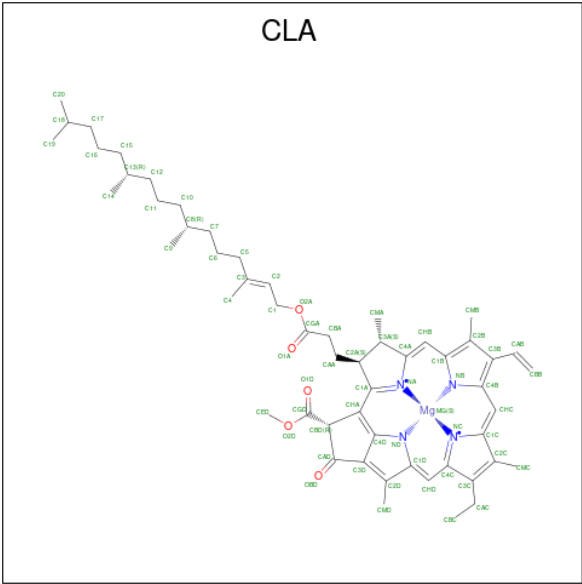
- Molecule 21 is a protein called Lhca9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	9	172	Total	C	N	O	S	0	0
			1302	840	220	235	7		

- Molecule 22 is a protein called ChainX.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	26	Total	C	N	O	0	0
			130	78	26	26		

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	A	1	Total 44	C 35	Mg 1	N 4	O 4	0
23	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 64	C 55	Mg 1	N 4	O 4	0
23	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	A	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
23	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	B	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
23	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
23	F	1	Total 57	C 47	Mg 1	N 4	O 5	0
23	F	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	K	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
23	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	1	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	1	1	Total 53	C 44	Mg 1	N 4	O 4	0
23	1	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	1	1	Total 39	C 32	Mg 1	N 4	O 2	0
23	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
23	1	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	1	1	Total 40	C 32	Mg 1	N 4	O 3	0
23	1	1	Total 39	C 31	Mg 1	N 4	O 3	0
23	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	1	1	Total 37	C 29	Mg 1	N 4	O 3	0
23	1	1	Total 43	C 33	Mg 1	N 4	O 5	0
23	a	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	a	1	Total 61	C 51	Mg 1	N 4	O 5	0
23	a	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
23	a	1	Total 44	C 35	Mg 1	N 4	O 4	0
23	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	a	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	a	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	a	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	a	1	Total 38	C 30	Mg 1	N 4	O 3	0
23	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	3	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
23	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	3	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
23	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
23	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
23	3	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
23	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
23	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
23	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	5	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
23	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
23	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
23	5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
23	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
23	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	6	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	6	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	6	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	6	1	Total 40	C 32	Mg 1	N 4	O 3	0
23	6	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
23	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	7	1	Total 44	C 35	Mg 1	N 4	O 4	0

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Mol	Chain	Residues	Atoms					AltConf
23	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	7	1	Total 59	C 49	Mg 1	N 4	O 5	0
23	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	7	1	Total 42	C 33	Mg 1	N 4	O 4	0
23	7	1	Total 43	C 33	Mg 1	N 4	O 5	0
23	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	8	1	Total 44	C 34	Mg 1	N 4	O 5	0
23	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
23	8	1	Total 64	C 54	Mg 1	N 4	O 5	0
23	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	8	1	Total 51	C 41	Mg 1	N 4	O 5	0
23	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
23	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
23	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
23	8	1	Total 41	C 33	Mg 1	N 4	O 3	0
23	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
23	8	1	Total 56	C 46	Mg 1	N 4	O 5	0
23	8	1	Total 43	C 33	Mg 1	N 4	O 5	0

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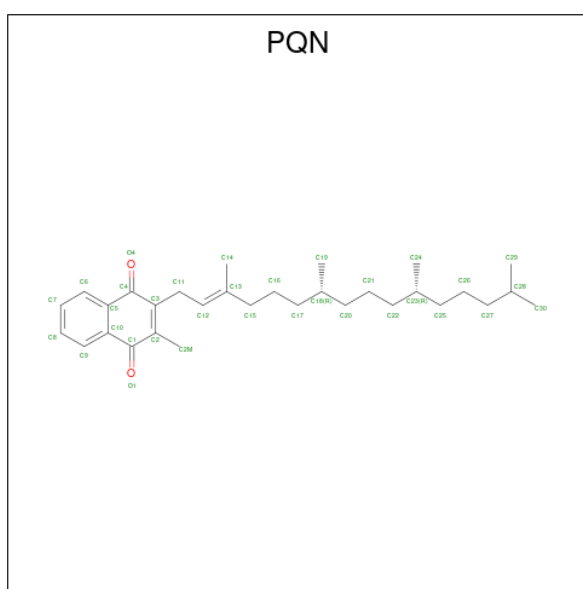
Mol	Chain	Residues	Atoms				AltConf
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 26	C 21	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	9	1	Total 27	C 22	Mg 1	N 4	0
23	9	1	Total 27	C 22	Mg 1	N 4	0
23	9	1	Total 27	C 22	Mg 1	N 4	0
23	9	1	Total 27	C 22	Mg 1	N 4	0
23	9	1	Total 27	C 22	Mg 1	N 4	0
23	9	1	Total 27	C 22	Mg 1	N 4	0
23	9	1	Total 27	C 22	Mg 1	N 4	0
23	9	1	Total 27	C 22	Mg 1	N 4	0

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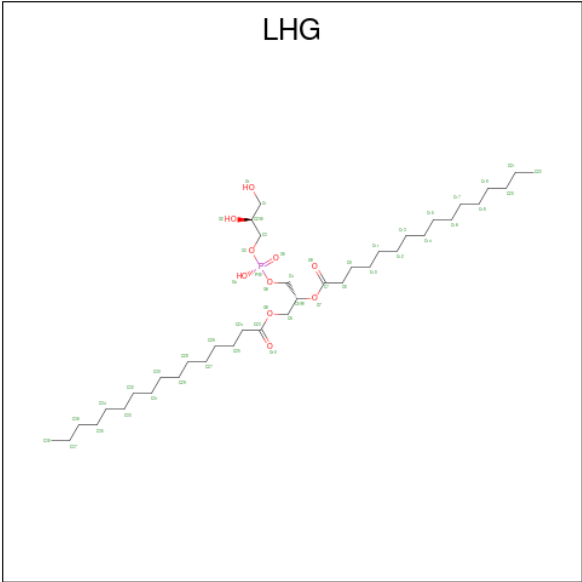
Mol	Chain	Residues	Atoms				AltConf
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	

- Molecule 24 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



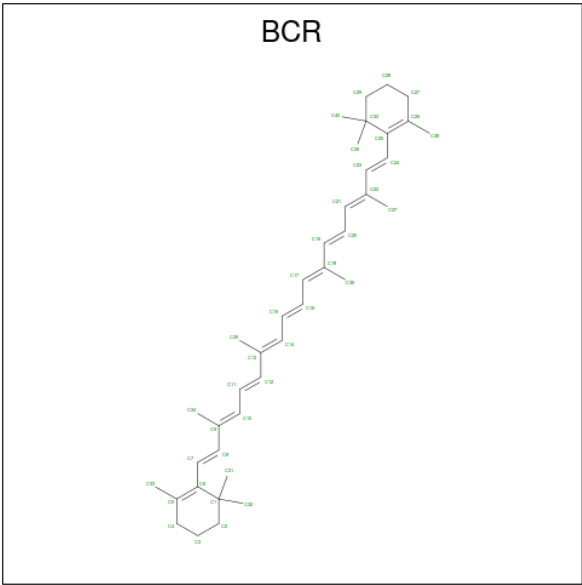
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			30	19	10	1	
25	B	1	Total	C	O	P	0
			38	27	10	1	
25	1	1	Total	C	O	P	0
			49	38	10	1	
25	a	1	Total	C	O	P	0
			49	38	10	1	
25	3	1	Total	C	O	P	0
			45	34	10	1	
25	3	1	Total	C	O	P	0
			49	38	10	1	
25	4	1	Total	C	O	P	0
			49	38	10	1	
25	5	1	Total	C	O	P	0
			49	38	10	1	
25	5	1	Total	C	O	P	0
			49	38	10	1	
25	6	1	Total	C	O	P	0
			48	37	10	1	
25	7	1	Total	C	O	P	0
			37	26	10	1	
25	8	1	Total	C	O	P	0
			49	38	10	1	
25	8	1	Total	C	O	P	0
			47	36	10	1	

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Mol	Chain	Residues	Atoms				AltConf
25	2	1	Total	C	O	P	0
			37	26	10	1	
25	9	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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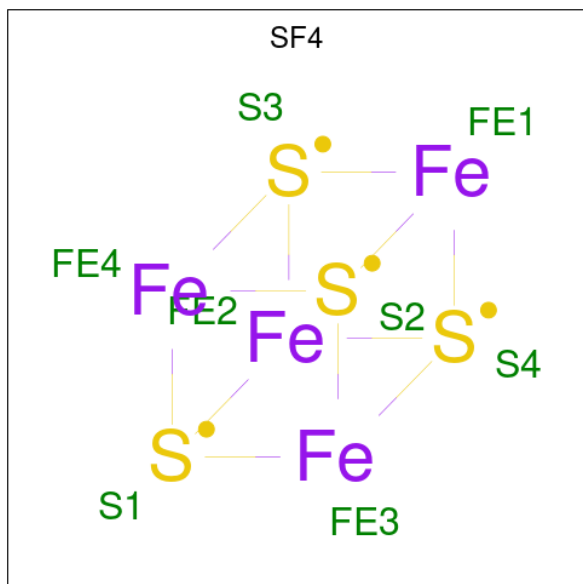
Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	F	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	J	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	1	1	Total C 40 40	0
26	a	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	4	1	Total C 40 40	0
26	5	1	Total C 40 40	0
26	6	1	Total C 40 40	0
26	7	1	Total C 40 40	0
26	7	1	Total C 40 40	0

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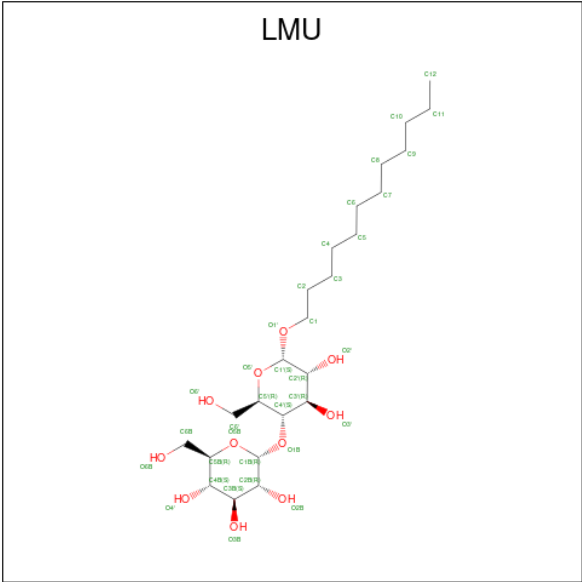
Mol	Chain	Residues	Atoms		AltConf
26	8	1	Total	C	0
			40	40	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



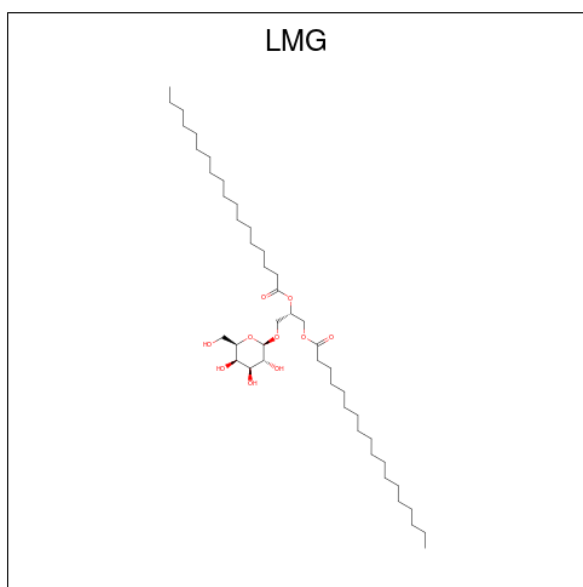
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 28 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



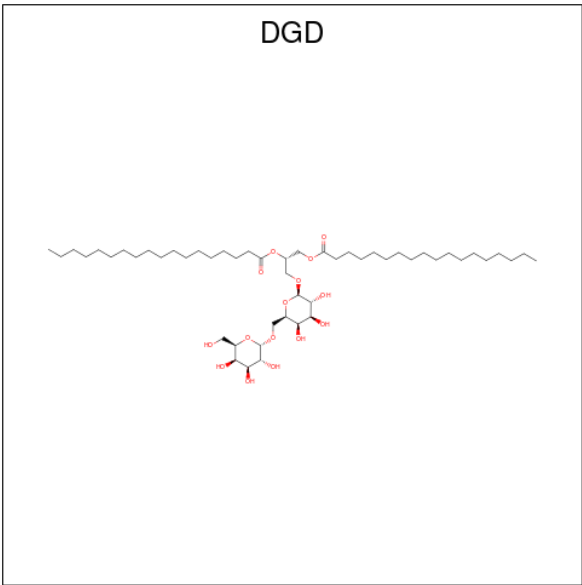
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			35	24	11	
28	A	1	Total	C	O	0
			34	24	10	
28	A	1	Total	C	O	0
			34	24	10	
28	K	1	Total	C	O	0
			35	24	11	
28	5	1	Total	C	O	0
			33	22	11	
28	8	1	Total	C	O	0
			35	24	11	
28	8	1	Total	C	O	0
			35	24	11	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



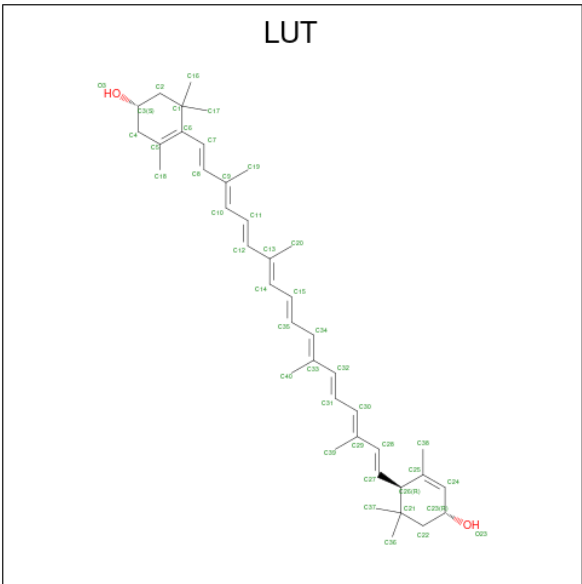
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			40	30	10	
29	J	1	Total	C	O	0
			40	30	10	
29	4	1	Total	C	O	0
			40	30	10	
29	4	1	Total	C	O	0
			40	30	10	
29	5	1	Total	C	O	0
			40	30	10	
29	5	1	Total	C	O	0
			40	30	10	
29	7	1	Total	C	O	0
			44	34	10	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			62	47	15	
30	J	1	Total	C	O	0
			58	43	15	

- Molecule 31 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



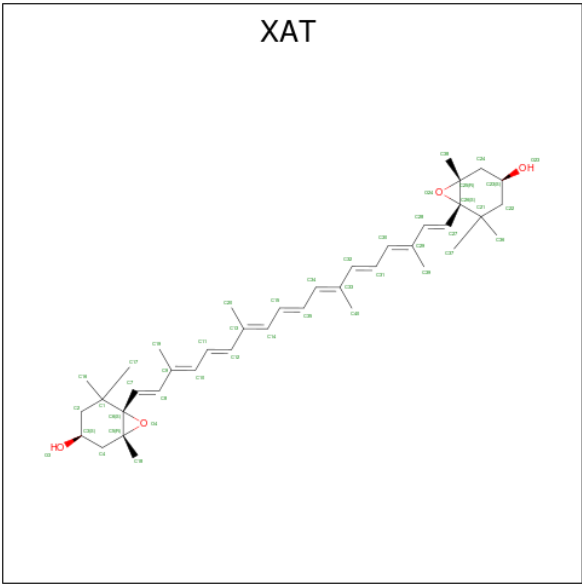
Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	a	1	42	40	2	0
31	3	1	42	40	2	0
31	4	1	42	40	2	0
31	5	1	42	40	2	0
31	6	1	42	40	2	0
31	7	1	42	40	2	0
31	8	1	42	40	2	0
31	2	1	42	40	2	0
31	9	1	42	40	2	0

- Molecule 32 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).



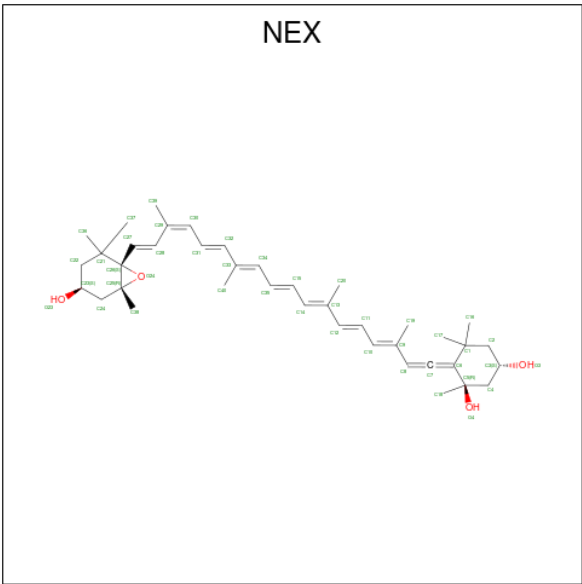
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	1	1	44	40	4	0
32	a	1	44	40	4	0

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Mol	Chain	Residues	Atoms			AltConf
32	3	1	Total	C	O	0
			44	40	4	
32	4	1	Total	C	O	0
			44	40	4	
32	5	1	Total	C	O	0
			44	40	4	
32	6	1	Total	C	O	0
			44	40	4	
32	7	1	Total	C	O	0
			44	40	4	
32	8	1	Total	C	O	0
			44	40	4	
32	2	1	Total	C	O	0
			44	40	4	
32	9	1	Total	C	O	0
			44	40	4	

- Molecule 33 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-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).

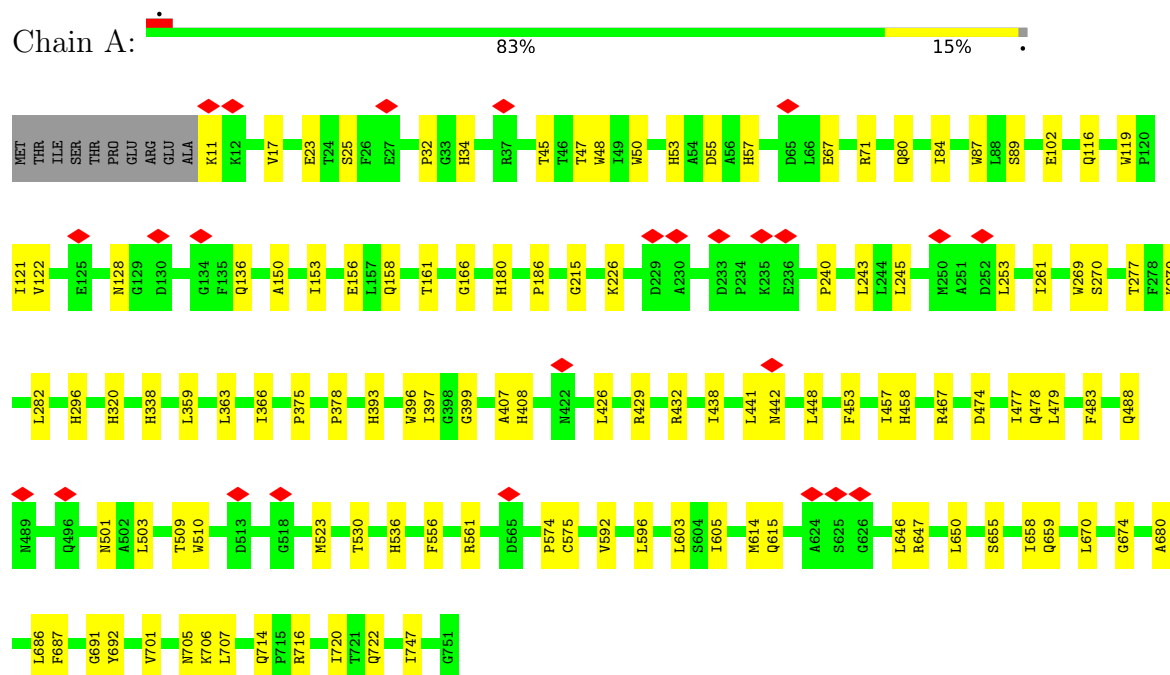


Mol	Chain	Residues	Atoms			AltConf
33	5	1	Total	C	O	0
			44	40	4	
33	6	1	Total	C	O	0
			44	40	4	

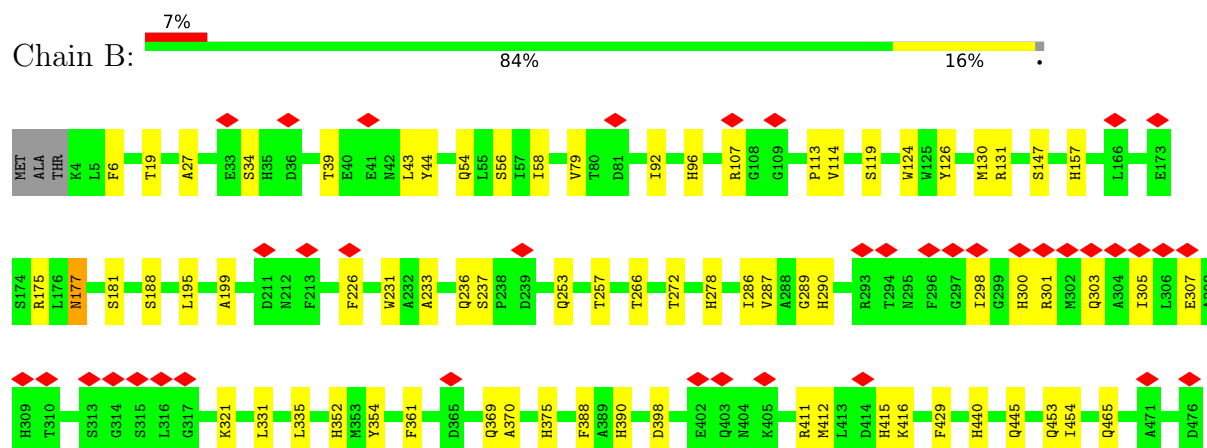
3 Residue-property plots [i](#)

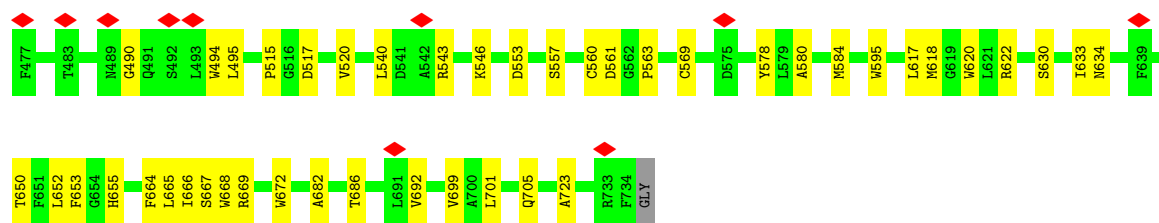
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: PsaA

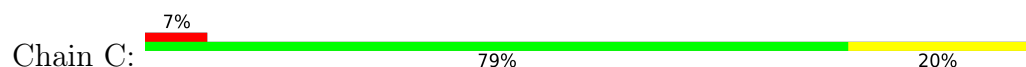


• Molecule 2: PsaB

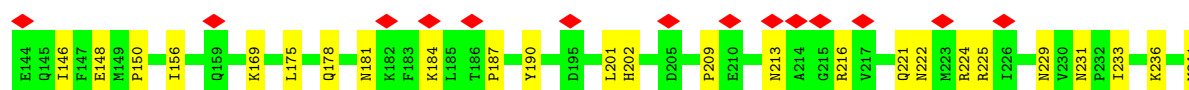
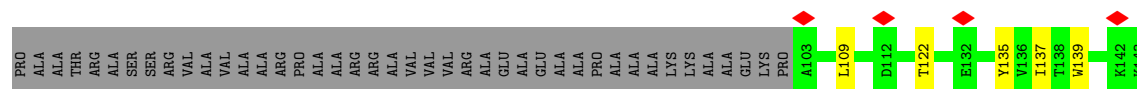
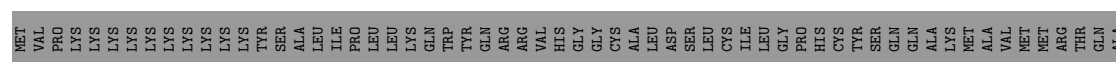




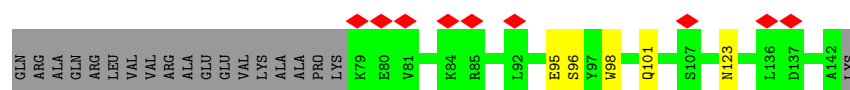
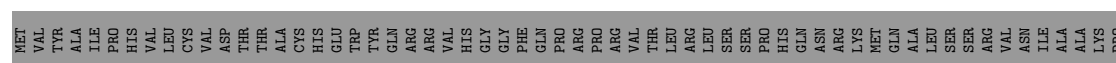
• Molecule 3: PsaC



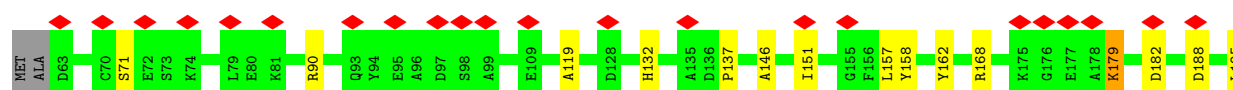
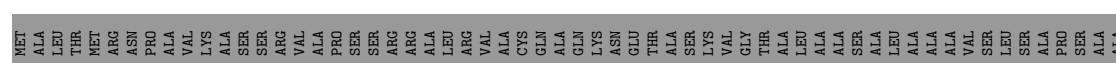
• Molecule 4: PsaD



• Molecule 5: PsaE

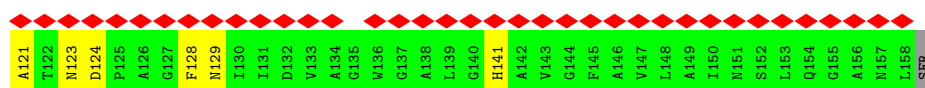
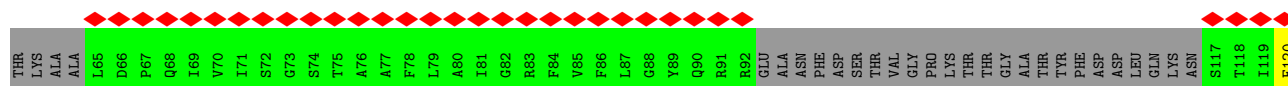


• Molecule 6: PsaF

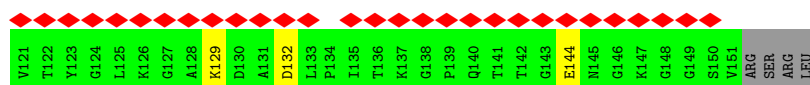
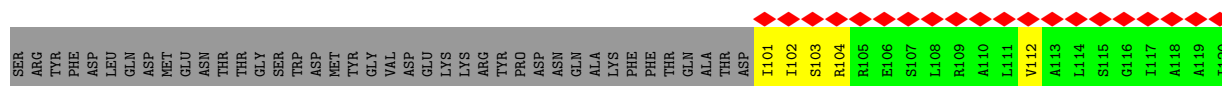




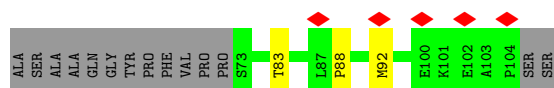
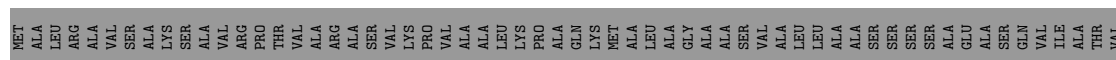
• Molecule 7: PsaG



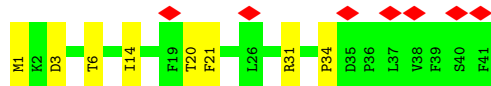
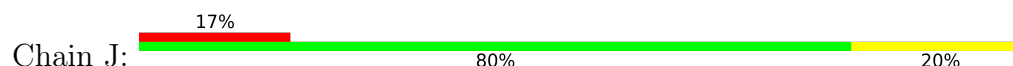
• Molecule 8: PsaH



• Molecule 9: PsaI



• Molecule 10: PsaJ



• Molecule 11: PsaK

- Molecule 12: PsaL

[illegible]

- Molecule 13: Lhca1

Chain 1:

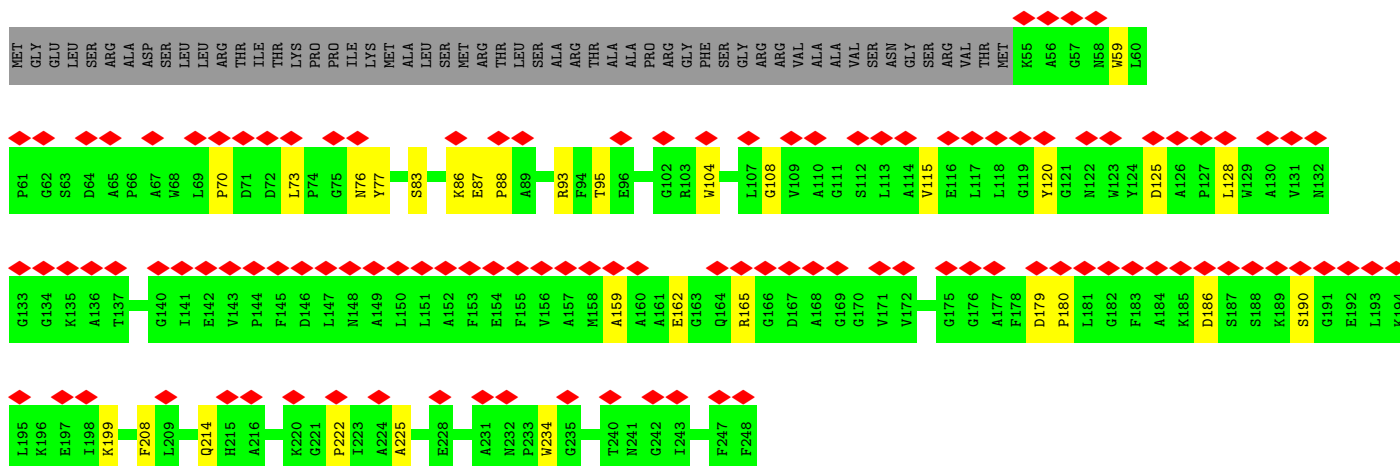
40% 64% 14% 22%

Sequence logo for Chain 1. The y-axis represents frequency in bits (0.00 to 0.15). The x-axis shows positions 1 to 200. A bar chart at the top indicates the percentage of positions with significant enrichment: 40% (red), 64% (green), 14% (yellow), and 22% (grey).

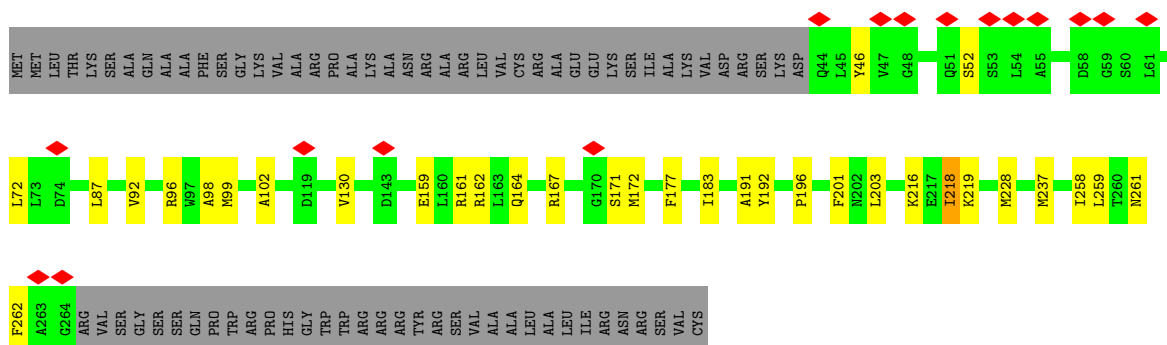
Key residues (positions and amino acids):

- 1: MET
- 2: GLY
- 3: LEU
- 4: SER
- 5: ARG
- 6: ALA
- 7: ASP
- 8: SER
- 9: LEU
- 10: LEU
- 11: ARG
- 12: THR
- 13: THR
- 14: LYS
- 15: PRO
- 16: PRO
- 17: ILE
- 18: LYS
- 19: MET
- 20: ALA
- 21: LEU
- 22: SER
- 23: MET
- 24: ARG
- 25: THR
- 26: LEU
- 27: SER
- 28: ALA
- 29: ARG
- 30: THR
- 31: ALA
- 32: ALA
- 33: PRO
- 34: ARG
- 35: GLY
- 36: PHE
- 37: SER
- 38: GLY
- 39: ARG
- 40: ARG
- 41: VAL
- 42: ALA
- 43: ALA
- 44: VAL
- 45: SER
- 46: ASN
- 47: GLY
- 48: SER
- 49: ARG
- 50: VAL
- 51: THR
- 52: MET
- 53: K55
- 54: A56
- 55: G57
- 56: M58
- 57: W59

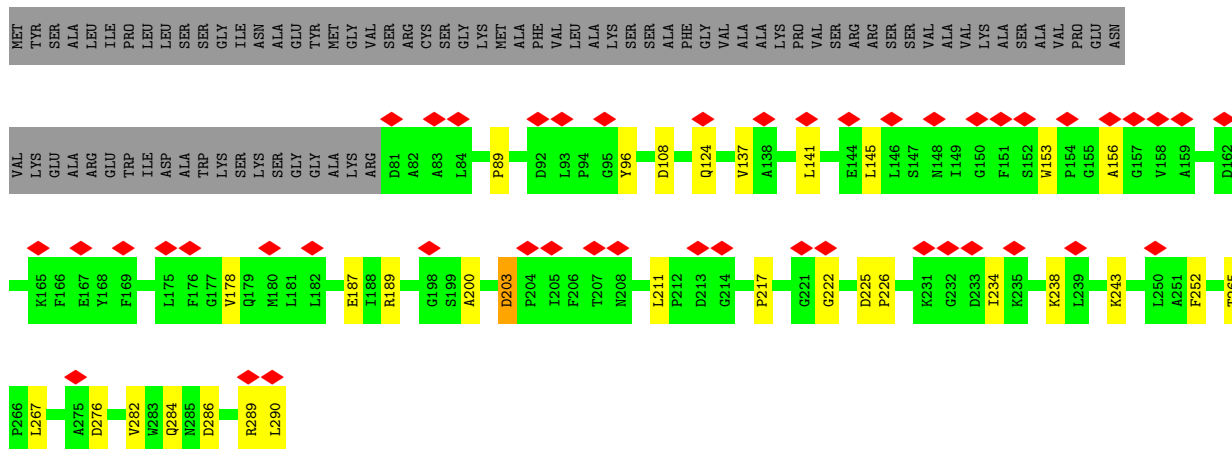




• Molecule 14: Lhca3

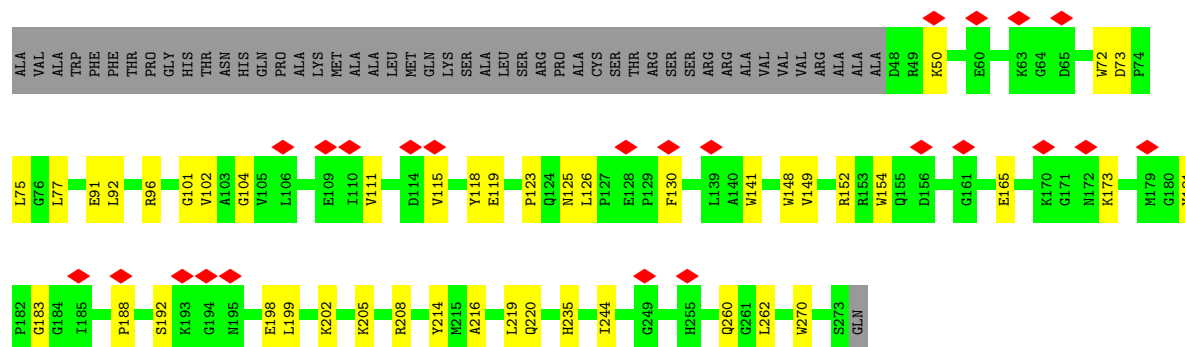


• Molecule 15: Lhca4

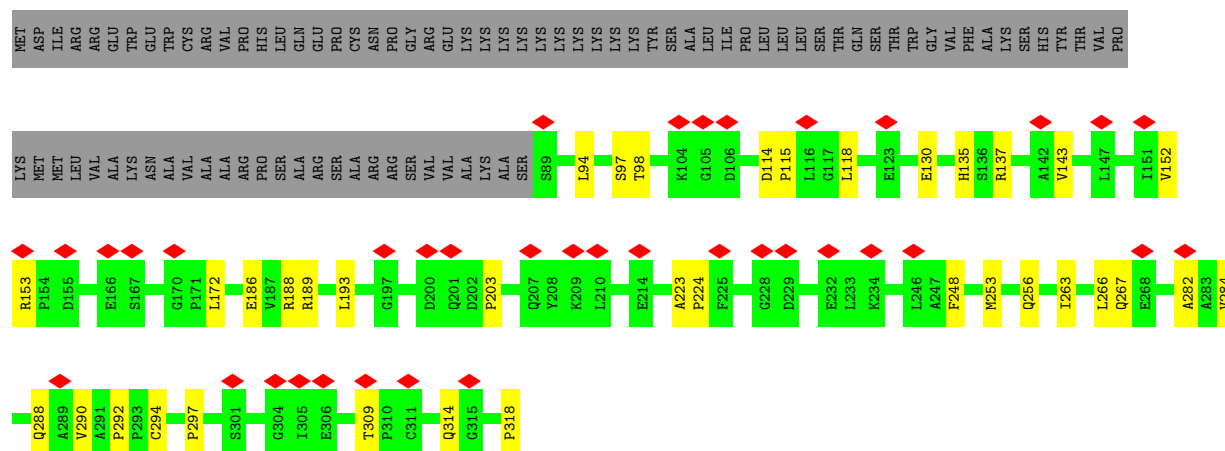


• Molecule 16: Lhca5

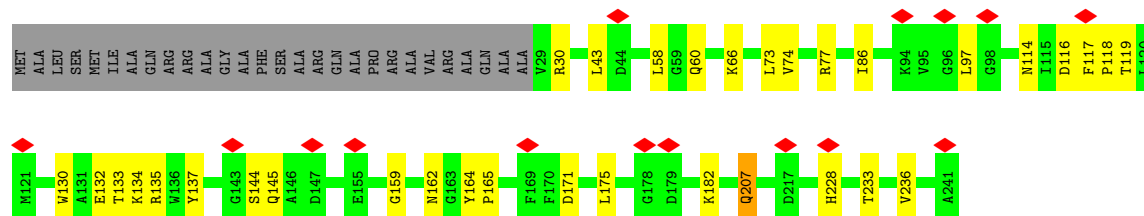
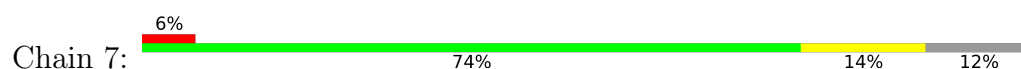




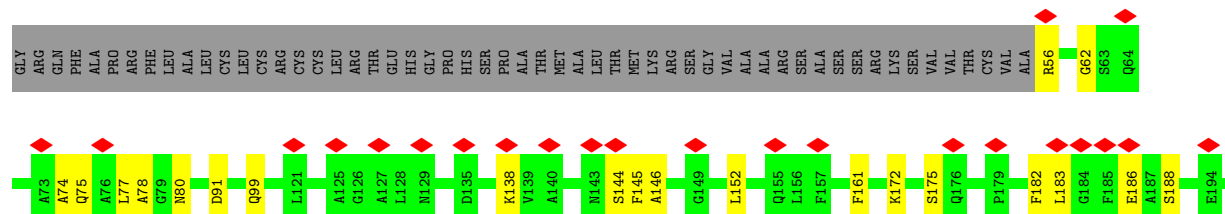
• Molecule 17: Lhca6

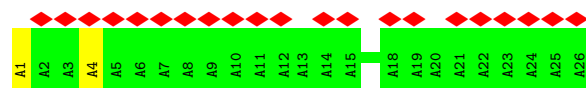


• Molecule 18: Lhca7



• Molecule 19: Lhca8





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17420	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.0	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	0.400	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/6015	0.54	0/8201
2	B	0.44	0/6024	0.56	2/8225 (0.0%)
3	C	0.43	0/610	0.71	2/826 (0.2%)
4	D	0.36	0/1157	0.62	0/1563
5	E	0.33	0/515	0.52	0/700
6	F	0.34	0/1280	0.54	0/1733
7	G	0.31	0/524	0.69	1/711 (0.1%)
8	H	0.25	0/359	0.56	0/483
9	I	0.37	0/250	0.61	0/345
10	J	0.34	0/349	0.56	0/478
11	K	0.27	0/583	0.64	2/790 (0.3%)
12	L	0.28	0/787	0.54	0/1074
13	1	0.33	0/1478	0.51	0/2012
13	a	0.33	0/1490	0.51	0/2028
14	3	0.43	0/1731	0.65	0/2349
15	4	0.29	0/1686	0.51	0/2300
16	5	0.36	0/1820	0.58	0/2480
17	6	0.32	0/1833	0.56	0/2505
18	7	0.41	0/1701	0.61	1/2310 (0.0%)
19	8	0.38	0/1680	0.62	1/2288 (0.0%)
20	2	0.22	0/1382	0.57	2/1870 (0.1%)
21	9	0.27	0/1337	0.67	0/1814
22	X	0.12	0/129	0.25	0/179
All	All	0.38	0/34720	0.57	11/47264 (0.0%)

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	124	ASP	N-CA-C	-7.14	101.75	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	7	236	VAL	N-CA-C	-6.41	106.55	112.96
3	C	62	PHE	CA-C-N	5.63	129.70	121.31
3	C	62	PHE	C-N-CA	5.63	129.70	121.31
19	8	238	GLN	CB-CG-CD	5.44	121.86	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5819	0	5672	92	0
2	B	5812	0	5569	88	0
3	C	600	0	589	9	0
4	D	1129	0	1144	23	0
5	E	505	0	504	5	0
6	F	1254	0	1288	15	0
7	G	514	0	509	6	0
8	H	357	0	382	6	0
9	I	242	0	252	2	0
10	J	337	0	336	9	0
11	K	578	0	617	8	0
12	L	768	0	776	20	0
13	1	1433	0	1387	23	0
13	a	1444	0	1396	22	0
14	3	1683	0	1641	26	0
15	4	1631	0	1587	26	0
16	5	1765	0	1738	41	0
17	6	1771	0	1770	31	0
18	7	1649	0	1589	29	0
19	8	1630	0	1609	28	0
20	2	1346	0	1330	18	0
21	9	1302	0	1275	30	0
22	X	130	0	132	3	0
23	1	674	0	541	15	0
23	2	350	0	39	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	3	724	0	628	18	0
23	4	782	0	686	24	0
23	5	878	0	758	35	0
23	6	912	0	845	35	0
23	7	760	0	643	19	0
23	8	727	0	635	15	0
23	9	324	0	36	12	0
23	A	2625	0	2614	115	0
23	B	2270	0	2210	80	0
23	F	140	0	113	6	0
23	G	87	0	64	4	0
23	J	42	0	31	2	0
23	K	201	0	171	2	0
23	L	135	0	99	5	0
23	a	709	0	597	12	0
24	A	33	0	46	4	0
24	B	33	0	46	6	0
25	1	49	0	74	6	0
25	2	37	0	44	1	0
25	3	94	0	137	3	0
25	4	49	0	74	6	0
25	5	98	0	148	7	0
25	6	48	0	69	3	0
25	7	37	0	44	2	0
25	8	96	0	141	5	0
25	9	49	0	74	5	0
25	A	79	0	104	3	0
25	B	38	0	46	2	0
25	a	49	0	74	4	0
26	1	40	0	56	2	0
26	3	120	0	168	9	0
26	4	40	0	56	2	0
26	5	40	0	56	3	0
26	6	40	0	56	4	0
26	7	80	0	112	3	0
26	8	40	0	56	3	0
26	A	240	0	336	26	0
26	B	280	0	392	13	0
26	F	40	0	56	4	0
26	G	40	0	56	5	0
26	J	40	0	56	5	0
26	K	80	0	112	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	L	80	0	112	6	0
26	a	40	0	56	4	0
27	A	8	0	0	0	0
27	C	16	0	0	0	0
28	5	33	0	39	3	0
28	8	70	0	92	3	0
28	A	103	0	134	3	0
28	K	35	0	46	0	0
29	4	80	0	100	1	0
29	5	80	0	100	4	0
29	7	44	0	61	1	0
29	A	40	0	50	2	0
29	J	40	0	50	1	0
30	B	62	0	84	5	0
30	J	58	0	77	1	0
31	1	42	0	56	3	0
31	2	42	0	56	3	0
31	3	42	0	56	1	0
31	4	42	0	56	5	0
31	5	42	0	56	5	0
31	6	42	0	56	4	0
31	7	42	0	56	5	0
31	8	42	0	56	6	0
31	9	42	0	56	1	0
31	a	42	0	56	5	0
32	1	44	0	56	4	0
32	2	44	0	56	3	0
32	3	44	0	56	3	0
32	4	44	0	56	3	0
32	5	44	0	56	9	0
32	6	44	0	56	1	0
32	7	44	0	56	1	0
32	8	44	0	56	1	0
32	9	44	0	56	3	0
32	a	44	0	56	3	0
33	5	44	0	56	3	0
33	6	44	0	56	4	0
All	All	49685	0	48724	835	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 835 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:9:182:GLN:CB	21:9:183:PRO:HD2	1.85	1.05
1:A:11:LYS:N	14:3:52:SER:HG	1.56	1.02
12:L:223:LEU:HD12	12:L:223:LEU:O	1.78	0.82
23:9:611:CLA:NB	25:9:622:LHG:O4	2.20	0.75
23:A:830:CLA:H2	26:A:849:BCR:HC7	1.68	0.74

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	708 (96%)	31 (4%)	0	100	100
2	B	729/735 (99%)	694 (95%)	35 (5%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	D	142/247 (58%)	131 (92%)	11 (8%)	0	100	100
5	E	62/143 (43%)	56 (90%)	6 (10%)	0	100	100
6	F	162/227 (71%)	149 (92%)	13 (8%)	0	100	100
7	G	66/159 (42%)	59 (89%)	7 (11%)	0	100	100
8	H	49/155 (32%)	41 (84%)	8 (16%)	0	100	100
9	I	30/106 (28%)	28 (93%)	2 (7%)	0	100	100
10	J	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
11	K	83/160 (52%)	74 (89%)	9 (11%)	0	100	100
12	L	102/258 (40%)	94 (92%)	8 (8%)	0	100	100
13	1	191/248 (77%)	177 (93%)	14 (7%)	0	100	100
13	a	192/248 (77%)	177 (92%)	15 (8%)	0	100	100
14	3	219/298 (74%)	199 (91%)	20 (9%)	0	100	100
15	4	208/290 (72%)	195 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	5	224/274 (82%)	198 (88%)	26 (12%)	0	100	100
17	6	228/318 (72%)	209 (92%)	19 (8%)	0	100	100
18	7	211/241 (88%)	192 (91%)	19 (9%)	0	100	100
19	8	213/272 (78%)	198 (93%)	15 (7%)	0	100	100
20	2	171/227 (75%)	145 (85%)	26 (15%)	0	100	100
21	9	168/213 (79%)	143 (85%)	23 (14%)	2 (1%)	10	37
22	X	24/26 (92%)	23 (96%)	1 (4%)	0	100	100
All	All	4330/5718 (76%)	3999 (92%)	329 (8%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	9	184	ILE
21	9	183	PRO

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	595/597 (100%)	593 (100%)	2 (0%)	86	86
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	120/197 (61%)	120 (100%)	0	100	100
5	E	55/123 (45%)	55 (100%)	0	100	100
6	F	126/169 (75%)	125 (99%)	1 (1%)	73	79
7	G	50/121 (41%)	50 (100%)	0	100	100
8	H	36/126 (29%)	36 (100%)	0	100	100
9	I	26/76 (34%)	26 (100%)	0	100	100
10	J	37/37 (100%)	37 (100%)	0	100	100
11	K	59/123 (48%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	75/198 (38%)	74 (99%)	1 (1%)	61	74
13	1	136/180 (76%)	136 (100%)	0	100	100
13	a	137/180 (76%)	137 (100%)	0	100	100
14	3	167/230 (73%)	166 (99%)	1 (1%)	78	81
15	4	165/226 (73%)	164 (99%)	1 (1%)	78	81
16	5	183/219 (84%)	182 (100%)	1 (0%)	81	83
17	6	184/260 (71%)	184 (100%)	0	100	100
18	7	164/181 (91%)	162 (99%)	2 (1%)	63	75
19	8	161/207 (78%)	160 (99%)	1 (1%)	78	81
20	2	134/183 (73%)	133 (99%)	1 (1%)	76	80
21	9	127/159 (80%)	124 (98%)	3 (2%)	43	65
All	All	3407/4472 (76%)	3393 (100%)	14 (0%)	81	84

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	7	86	ILE
18	7	207	GLN
21	9	184	ILE
21	9	131	LYS
21	9	177	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	154	GLN
16	5	260	GLN
13	1	214	GLN
15	4	284	GLN
17	6	240	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

333 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	$\# Z > 2$
23	CLA	5	612	16	44,49,73	1.39	11 (25%)	50,84,113	1.54	7 (14%)
31	LUT	3	618	-	42,43,43	0.79	0	51,60,60	1.85	16 (31%)
23	CLA	5	614	-	48,52,73	1.38	9 (18%)	53,87,113	1.45	5 (9%)
23	CLA	1	604	-	53,57,73	1.31	8 (15%)	61,93,113	1.51	4 (6%)
23	CLA	8	606	-	68,72,73	1.18	10 (14%)	81,112,113	1.35	8 (9%)
26	BCR	B	846	-	41,41,41	0.81	1 (2%)	56,56,56	2.20	26 (46%)
23	CLA	7	608	-	54,58,73	1.30	10 (18%)	64,95,113	1.41	4 (6%)
23	CLA	2	607	-	27,35,73	1.85	7 (25%)	32,60,113	1.64	4 (12%)
23	CLA	5	608	-	54,58,73	1.31	12 (22%)	63,95,113	1.42	5 (7%)
26	BCR	B	847	-	41,41,41	0.83	2 (4%)	56,56,56	2.03	19 (33%)
31	LUT	9	619	-	42,43,43	0.75	0	51,60,60	1.78	13 (25%)
23	CLA	a	610	13	63,67,73	1.23	9 (14%)	75,106,113	1.30	6 (8%)
23	CLA	2	614	-	27,35,73	1.84	7 (25%)	32,60,113	1.62	5 (15%)
33	NEX	5	624	-	40,46,46	1.06	2 (5%)	50,70,70	2.46	22 (44%)
24	PQN	A	844	-	34,34,34	2.91	11 (32%)	43,45,45	2.05	6 (13%)
26	BCR	B	843	-	41,41,41	0.77	1 (2%)	56,56,56	1.96	15 (26%)
23	CLA	4	602	15	64,68,73	1.19	10 (15%)	76,107,113	1.43	7 (9%)
23	CLA	9	610	21	27,35,73	1.83	7 (25%)	32,60,113	1.54	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	A	860	-	40,40,55	0.95	3 (7%)	48,48,63	1.32	5 (10%)
32	XAT	8	620	-	41,47,47	0.97	2 (4%)	54,74,74	2.61	19 (35%)
26	BCR	L	305	-	41,41,41	0.74	0	56,56,56	1.90	13 (23%)
23	CLA	A	833	-	49,53,73	1.35	10 (20%)	58,89,113	1.53	7 (12%)
23	CLA	A	841	-	69,73,73	1.14	9 (13%)	82,113,113	1.46	7 (8%)
23	CLA	B	815	-	47,51,73	1.36	9 (19%)	55,86,113	1.56	5 (9%)
23	CLA	K	204	-	50,54,73	1.35	9 (18%)	59,90,113	1.45	6 (10%)
23	CLA	2	612	20	27,35,73	1.84	6 (22%)	32,60,113	1.58	4 (12%)
23	CLA	1	603	-	56,61,73	1.27	10 (17%)	65,98,113	1.53	6 (9%)
25	LHG	9	622	23	48,48,48	0.63	1 (2%)	51,54,54	1.25	6 (11%)
23	CLA	6	610	17	69,73,73	1.12	9 (13%)	82,113,113	1.32	8 (9%)
26	BCR	6	622	-	41,41,41	0.65	0	56,56,56	1.96	17 (30%)
23	CLA	a	607	-	49,53,73	1.37	8 (16%)	58,89,113	1.48	5 (8%)
23	CLA	1	611	25	69,73,73	1.12	9 (13%)	82,113,113	1.29	6 (7%)
23	CLA	A	838	-	54,58,73	1.27	7 (12%)	64,95,113	1.60	13 (20%)
23	CLA	7	615	-	44,50,73	1.52	9 (20%)	57,85,113	1.58	8 (14%)
23	CLA	a	608	-	47,52,73	1.38	8 (17%)	55,88,113	1.48	4 (7%)
23	CLA	B	808	-	69,73,73	1.16	9 (13%)	82,113,113	1.56	9 (10%)
28	LMU	5	628	-	34,34,36	1.24	3 (8%)	45,45,47	1.52	8 (17%)
26	BCR	A	850	-	41,41,41	0.80	1 (2%)	56,56,56	2.04	20 (35%)
32	XAT	7	620	-	41,47,47	0.98	2 (4%)	54,74,74	2.52	20 (37%)
23	CLA	B	819	-	59,63,73	1.27	8 (13%)	70,101,113	1.40	4 (5%)
23	CLA	6	602	17	69,73,73	1.16	7 (10%)	82,113,113	1.36	5 (6%)
23	CLA	A	839	-	59,63,73	1.25	8 (13%)	70,101,113	1.41	5 (7%)
23	CLA	B	805	-	69,73,73	1.15	9 (13%)	82,113,113	1.48	8 (9%)
26	BCR	B	848	-	41,41,41	0.82	0	56,56,56	1.81	11 (19%)
23	CLA	G	204	7	49,53,73	1.41	8 (16%)	58,89,113	1.59	8 (13%)
23	CLA	A	826	-	68,72,73	1.18	10 (14%)	80,111,113	1.41	10 (12%)
23	CLA	B	814	-	68,72,73	1.15	9 (13%)	80,111,113	1.37	7 (8%)
23	CLA	9	614	-	27,35,73	1.84	7 (25%)	32,60,113	1.68	5 (15%)
28	LMU	K	208	-	36,36,36	1.19	2 (5%)	47,47,47	1.30	5 (10%)
26	BCR	A	848	-	41,41,41	0.86	2 (4%)	56,56,56	2.10	17 (30%)
23	CLA	a	611	25	41,46,73	1.52	10 (24%)	51,81,113	1.61	8 (15%)
32	XAT	2	620	-	41,47,47	0.94	2 (4%)	54,74,74	2.42	14 (25%)
26	BCR	F	305	-	41,41,41	0.77	1 (2%)	56,56,56	2.27	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	828	-	69,73,73	1.19	10 (14%)	82,113,113	1.35	8 (9%)
23	CLA	a	603	-	46,50,73	1.37	10 (21%)	53,85,113	1.65	6 (11%)
25	LHG	7	622	23	36,36,48	0.72	0	39,42,54	1.26	4 (10%)
23	CLA	1	601	13	57,62,73	1.26	9 (15%)	67,100,113	1.35	6 (8%)
23	CLA	8	613	19	69,73,73	1.13	8 (11%)	82,113,113	1.52	8 (9%)
26	BCR	B	844	-	41,41,41	0.80	1 (2%)	56,56,56	1.96	15 (26%)
23	CLA	5	616	16	44,50,73	1.55	10 (22%)	57,85,113	1.48	8 (14%)
23	CLA	9	603	21	27,35,73	1.86	6 (22%)	32,60,113	1.53	4 (12%)
23	CLA	4	606	-	43,48,73	1.45	9 (20%)	49,83,113	1.45	5 (10%)
23	CLA	8	601	19	69,73,73	1.16	9 (13%)	82,113,113	1.41	11 (13%)
25	LHG	A	846	-	48,48,48	0.75	1 (2%)	51,54,54	1.34	7 (13%)
23	CLA	a	609	13	67,72,73	1.17	7 (10%)	79,112,113	1.28	6 (7%)
32	XAT	3	619	-	41,47,47	1.01	2 (4%)	54,74,74	2.56	22 (40%)
23	CLA	2	610	20	27,35,73	1.81	6 (22%)	32,60,113	1.66	5 (15%)
23	CLA	K	206	11	49,53,73	1.35	9 (18%)	58,89,113	1.50	4 (6%)
23	CLA	B	810	-	68,72,73	1.16	9 (13%)	80,111,113	1.33	7 (8%)
26	BCR	a	619	-	41,41,41	0.69	0	56,56,56	2.01	16 (28%)
31	LUT	6	619	-	42,43,43	0.72	0	51,60,60	1.87	14 (27%)
23	CLA	B	839	-	69,73,73	1.16	10 (14%)	82,113,113	1.39	9 (10%)
23	CLA	3	612	14	47,51,73	1.39	9 (19%)	55,86,113	1.51	6 (10%)
32	XAT	6	621	-	41,47,47	0.93	2 (4%)	54,74,74	2.56	20 (37%)
29	LMG	5	627	-	40,40,55	0.91	2 (5%)	48,48,63	1.21	4 (8%)
23	CLA	9	611	25	27,35,73	1.86	7 (25%)	32,60,113	1.64	5 (15%)
23	CLA	A	825	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	7 (8%)
23	CLA	6	606	-	43,48,73	1.44	10 (23%)	49,83,113	1.48	6 (12%)
23	CLA	7	610	18	69,73,73	1.14	9 (13%)	82,113,113	1.34	6 (7%)
23	CLA	A	821	-	57,61,73	1.26	9 (15%)	67,98,113	1.47	5 (7%)
23	CLA	A	801	-	69,73,73	1.21	9 (13%)	82,113,113	1.35	6 (7%)
26	BCR	3	621	-	41,41,41	0.72	0	56,56,56	2.23	18 (32%)
23	CLA	5	602	16	69,73,73	1.18	9 (13%)	82,113,113	1.40	7 (8%)
26	BCR	K	202	-	41,41,41	0.73	0	56,56,56	2.29	21 (37%)
23	CLA	B	811	-	56,61,73	1.36	10 (17%)	68,99,113	1.39	8 (11%)
23	CLA	8	607	-	45,49,73	1.50	11 (24%)	54,84,113	1.53	5 (9%)
23	CLA	6	613	-	67,72,73	1.17	10 (14%)	79,112,113	1.34	7 (8%)
23	CLA	B	829	-	69,73,73	1.26	8 (11%)	82,113,113	1.54	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	802	-	69,73,73	1.18	10 (14%)	82,113,113	1.55	10 (12%)
23	CLA	B	822	-	46,50,73	1.36	8 (17%)	53,85,113	1.44	6 (11%)
23	CLA	7	606	-	45,49,73	1.45	11 (24%)	52,84,113	1.48	7 (13%)
23	CLA	5	606	-	43,48,73	1.43	8 (18%)	49,83,113	1.47	4 (8%)
23	CLA	A	805	-	56,60,73	1.28	10 (17%)	65,97,113	1.49	7 (10%)
26	BCR	J	102	-	41,41,41	0.71	0	56,56,56	2.17	18 (32%)
23	CLA	9	609	21	27,35,73	1.82	6 (22%)	32,60,113	1.67	4 (12%)
23	CLA	L	303	-	49,53,73	1.32	10 (20%)	58,89,113	1.52	4 (6%)
23	CLA	4	601	15	69,73,73	1.13	9 (13%)	82,113,113	1.39	7 (8%)
23	CLA	B	803	-	69,73,73	1.16	10 (14%)	82,113,113	1.66	13 (15%)
23	CLA	B	834	-	64,68,73	1.18	8 (12%)	76,107,113	1.33	5 (6%)
23	CLA	7	604	-	58,62,73	1.27	11 (18%)	69,100,113	1.50	9 (13%)
23	CLA	4	618	15	43,48,73	1.55	11 (25%)	51,83,113	1.48	6 (11%)
23	CLA	B	807	-	56,60,73	1.26	9 (16%)	65,97,113	1.40	5 (7%)
23	CLA	9	601	21	27,35,73	1.81	7 (25%)	32,60,113	1.59	4 (12%)
23	CLA	1	612	13	49,53,73	1.35	9 (18%)	58,89,113	1.48	8 (13%)
23	CLA	1	602	13	65,69,73	1.17	9 (13%)	77,108,113	1.37	7 (9%)
23	CLA	3	613	14	56,61,73	1.27	9 (16%)	65,98,113	1.41	4 (6%)
23	CLA	F	301	-	61,65,73	1.23	8 (13%)	72,103,113	1.42	6 (8%)
23	CLA	a	613	-	69,73,73	1.16	9 (13%)	82,113,113	1.43	7 (8%)
23	CLA	3	606	-	57,62,73	1.28	7 (12%)	67,100,113	1.36	5 (7%)
23	CLA	5	603	-	58,62,73	1.38	11 (18%)	71,100,113	1.46	8 (11%)
28	LMU	A	858	-	35,35,36	1.38	3 (8%)	44,45,47	1.54	7 (15%)
28	LMU	A	857	-	36,36,36	1.20	3 (8%)	47,47,47	1.35	4 (8%)
30	DGD	J	103	-	59,59,67	0.99	3 (5%)	73,73,81	1.49	8 (10%)
23	CLA	1	613	-	69,73,73	1.15	9 (13%)	82,113,113	1.43	7 (8%)
26	BCR	A	851	-	41,41,41	0.81	1 (2%)	56,56,56	1.99	17 (30%)
23	CLA	4	604	-	58,62,73	1.35	11 (18%)	71,100,113	1.34	6 (8%)
23	CLA	A	823	-	46,50,73	1.36	8 (17%)	53,85,113	1.66	5 (9%)
23	CLA	1	606	13	41,47,73	1.47	8 (19%)	50,80,113	1.59	6 (12%)
23	CLA	B	830	-	47,51,73	1.38	8 (17%)	55,86,113	1.56	4 (7%)
23	CLA	7	609	18	46,52,73	1.33	7 (15%)	57,87,113	1.65	7 (12%)
23	CLA	A	828	-	69,73,73	1.19	8 (11%)	82,113,113	1.33	6 (7%)
31	LUT	7	619	-	42,43,43	0.85	1 (2%)	51,60,60	1.99	17 (33%)
27	SF4	C	101	-	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	832	-	64,68,73	1.18	10 (15%)	76,107,113	1.42	11 (14%)
23	CLA	6	601	17	69,73,73	1.15	10 (14%)	82,113,113	1.39	9 (10%)
25	LHG	3	624	23	48,48,48	0.67	1 (2%)	51,54,54	1.26	5 (9%)
26	BCR	7	621	-	41,41,41	0.73	0	56,56,56	2.08	22 (39%)
26	BCR	8	621	-	41,41,41	0.68	0	56,56,56	2.01	18 (32%)
23	CLA	2	606	20	27,35,73	1.86	6 (22%)	32,60,113	1.50	3 (9%)
23	CLA	B	802	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	8 (9%)
31	LUT	8	619	-	42,43,43	0.77	1 (2%)	51,60,60	2.00	16 (31%)
24	PQN	B	842	-	34,34,34	2.92	10 (29%)	43,45,45	1.95	5 (11%)
23	CLA	a	604	-	53,57,73	1.31	8 (15%)	61,93,113	1.51	4 (6%)
23	CLA	5	618	16	43,48,73	1.52	10 (23%)	51,83,113	1.51	7 (13%)
23	CLA	B	806	2	69,73,73	1.18	11 (15%)	82,113,113	1.29	4 (4%)
28	LMU	8	625	-	36,36,36	1.16	2 (5%)	47,47,47	1.42	7 (14%)
23	CLA	2	602	20	27,35,73	1.83	6 (22%)	32,60,113	1.58	4 (12%)
23	CLA	A	810	1	54,58,73	1.30	10 (18%)	64,95,113	1.48	5 (7%)
23	CLA	A	854	-	69,73,73	1.18	10 (14%)	82,113,113	1.38	13 (15%)
23	CLA	3	610	14	69,73,73	1.13	9 (13%)	82,113,113	1.43	10 (12%)
23	CLA	A	842	-	69,73,73	1.14	8 (11%)	82,113,113	1.35	5 (6%)
23	CLA	8	609	19	49,53,73	1.32	9 (18%)	58,89,113	1.50	8 (13%)
23	CLA	7	613	18	69,73,73	1.17	7 (10%)	82,113,113	1.31	7 (8%)
23	CLA	a	602	13	65,69,73	1.18	9 (13%)	77,108,113	1.37	7 (9%)
26	BCR	A	852	-	41,41,41	0.70	0	56,56,56	1.92	12 (21%)
23	CLA	A	822	-	69,73,73	1.15	10 (14%)	82,113,113	1.36	9 (10%)
26	BCR	A	856	-	41,41,41	0.66	0	56,56,56	2.02	20 (35%)
23	CLA	A	806	-	69,73,73	1.19	11 (15%)	82,113,113	1.56	9 (10%)
23	CLA	B	837	-	69,73,73	1.16	10 (14%)	82,113,113	1.35	5 (6%)
23	CLA	7	601	18	64,68,73	1.20	11 (17%)	76,107,113	1.42	6 (7%)
23	CLA	8	604	-	54,58,73	1.29	9 (16%)	64,95,113	1.44	7 (10%)
23	CLA	2	603	20	27,35,73	1.84	7 (25%)	32,60,113	1.65	5 (15%)
23	CLA	9	602	21	27,35,73	1.82	7 (25%)	32,60,113	1.65	5 (15%)
23	CLA	B	816	-	58,62,73	1.23	9 (15%)	68,99,113	1.49	6 (8%)
23	CLA	7	614	-	46,50,73	1.35	9 (19%)	53,85,113	1.46	5 (9%)
23	CLA	2	611	25	28,33,73	3.10	8 (28%)	27,56,113	1.01	2 (7%)
23	CLA	B	804	-	45,49,73	1.41	11 (24%)	54,84,113	1.64	9 (16%)
23	CLA	9	607	-	27,35,73	1.81	7 (25%)	32,60,113	1.67	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	3	623	-	44,44,48	0.68	2 (4%)	47,50,54	1.28	6 (12%)
23	CLA	6	604	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	5 (6%)
26	BCR	4	621	-	41,41,41	0.68	0	56,56,56	2.12	22 (39%)
23	CLA	A	811	-	69,73,73	1.13	10 (14%)	82,113,113	1.37	9 (10%)
23	CLA	B	827	-	66,70,73	1.19	10 (15%)	78,109,113	1.34	8 (10%)
23	CLA	3	604	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
25	LHG	B	851	23	37,37,48	0.64	0	40,43,54	1.25	4 (10%)
30	DGD	B	850	-	63,63,67	1.07	4 (6%)	77,77,81	1.53	10 (12%)
23	CLA	A	835	-	65,69,73	1.19	7 (10%)	77,108,113	1.46	6 (7%)
25	LHG	A	847	23	29,29,48	0.98	1 (3%)	32,35,54	1.41	3 (9%)
33	NEX	6	624	-	40,46,46	1.13	3 (7%)	50,70,70	2.26	16 (32%)
23	CLA	a	614	-	58,62,73	1.26	9 (15%)	65,99,113	1.33	5 (7%)
26	BCR	G	205	-	41,41,41	0.70	0	56,56,56	2.08	21 (37%)
23	CLA	B	812	-	47,51,73	1.35	8 (17%)	55,86,113	1.54	5 (9%)
31	LUT	2	619	-	42,43,43	0.72	0	51,60,60	1.86	14 (27%)
23	CLA	4	613	15	69,73,73	1.17	9 (13%)	82,113,113	1.34	5 (6%)
23	CLA	2	613	20	27,35,73	1.85	7 (25%)	32,60,113	1.56	4 (12%)
25	LHG	8	623	-	46,46,48	0.67	1 (2%)	49,52,54	1.26	5 (10%)
23	CLA	1	616	13	47,51,73	1.50	10 (21%)	58,87,113	1.44	5 (8%)
23	CLA	6	603	-	58,62,73	1.36	11 (18%)	71,100,113	1.39	7 (9%)
29	LMG	5	626	-	40,40,55	0.95	3 (7%)	48,48,63	1.34	6 (12%)
23	CLA	2	601	20	27,35,73	1.82	6 (22%)	32,60,113	1.64	5 (15%)
23	CLA	A	816	-	46,52,73	1.39	9 (19%)	57,87,113	1.61	6 (10%)
23	CLA	3	603	-	59,63,73	1.28	11 (18%)	70,101,113	1.57	10 (14%)
23	CLA	9	604	-	27,35,73	1.83	6 (22%)	32,60,113	1.64	4 (12%)
23	CLA	A	809	1	69,73,73	1.15	11 (15%)	82,113,113	1.37	8 (9%)
23	CLA	8	616	19	47,51,73	1.51	9 (19%)	58,87,113	1.69	10 (17%)
25	LHG	5	623	23	48,48,48	0.64	1 (2%)	51,54,54	1.23	5 (9%)
23	CLA	L	302	12	49,53,73	1.38	6 (12%)	58,89,113	1.47	5 (8%)
29	LMG	4	624	-	40,40,55	1.01	4 (10%)	48,48,63	1.29	6 (12%)
26	BCR	7	623	-	41,41,41	0.69	0	56,56,56	1.82	10 (17%)
23	CLA	6	617	-	49,53,73	1.35	9 (18%)	58,89,113	1.35	4 (6%)
23	CLA	3	609	14	64,68,73	1.21	7 (10%)	76,107,113	1.42	8 (10%)
23	CLA	7	602	18	69,73,73	1.16	10 (14%)	82,113,113	1.29	7 (8%)
23	CLA	2	616	-	27,35,73	1.83	7 (25%)	32,60,113	1.66	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	815	-	54,58,73	1.29	9 (16%)	64,95,113	1.50	10 (15%)
23	CLA	1	614	-	40,45,73	1.60	10 (25%)	47,79,113	1.58	5 (10%)
23	CLA	6	611	25	46,50,73	1.35	9 (19%)	53,85,113	1.39	5 (9%)
26	BCR	B	845	-	41,41,41	0.77	0	56,56,56	2.06	18 (32%)
23	CLA	B	840	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	5 (6%)
23	CLA	B	831	-	69,73,73	1.11	8 (11%)	82,113,113	1.43	6 (7%)
23	CLA	A	837	1	49,53,73	1.38	9 (18%)	58,89,113	1.50	5 (8%)
23	CLA	5	609	16	69,73,73	1.16	9 (13%)	82,113,113	1.29	8 (9%)
23	CLA	8	608	-	55,59,73	1.26	9 (16%)	64,96,113	1.50	5 (7%)
23	CLA	B	835	-	49,53,73	1.39	10 (20%)	58,89,113	1.59	8 (13%)
31	LUT	1	617	-	42,43,43	0.71	0	51,60,60	1.79	15 (29%)
25	LHG	8	622	23	48,48,48	0.65	1 (2%)	51,54,54	1.29	6 (11%)
23	CLA	A	808	-	54,58,73	1.28	10 (18%)	64,95,113	1.50	9 (14%)
29	LMG	4	623	-	40,40,55	0.90	1 (2%)	48,48,63	1.29	5 (10%)
25	LHG	1	620	23	48,48,48	0.62	1 (2%)	51,54,54	1.28	6 (11%)
23	CLA	A	804	-	69,73,73	1.15	8 (11%)	82,113,113	1.51	8 (9%)
23	CLA	8	603	-	48,52,73	1.51	10 (20%)	59,88,113	1.50	9 (15%)
23	CLA	5	604	-	67,71,73	1.26	11 (16%)	82,111,113	1.33	8 (9%)
23	CLA	A	814	-	69,73,73	1.18	9 (13%)	82,113,113	1.44	10 (12%)
23	CLA	1	610	13	43,47,73	1.45	9 (20%)	50,81,113	1.58	6 (12%)
23	CLA	3	617	14	43,48,73	1.41	10 (23%)	51,83,113	1.60	6 (11%)
26	BCR	K	207	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
23	CLA	8	612	19	44,49,73	1.38	10 (22%)	50,84,113	1.57	7 (14%)
23	CLA	4	616	15	47,51,73	1.49	11 (23%)	58,87,113	1.48	7 (12%)
23	CLA	B	820	-	54,58,73	1.27	8 (14%)	64,95,113	1.45	5 (7%)
23	CLA	8	614	-	60,64,73	1.22	10 (16%)	71,102,113	1.38	8 (11%)
23	CLA	8	602	19	64,68,73	1.21	9 (14%)	76,107,113	1.44	11 (14%)
23	CLA	A	820	-	69,73,73	1.22	9 (13%)	82,113,113	1.51	16 (19%)
23	CLA	B	817	-	63,67,73	1.22	8 (12%)	74,105,113	1.46	9 (12%)
23	CLA	A	812	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	9 (10%)
23	CLA	3	611	25	41,46,73	1.55	11 (26%)	51,81,113	1.61	8 (15%)
23	CLA	6	609	17	49,53,73	1.38	9 (18%)	58,89,113	1.54	8 (13%)
23	CLA	K	201	11	49,53,73	1.39	7 (14%)	58,89,113	1.64	8 (13%)
23	CLA	3	615	-	43,48,73	1.41	9 (20%)	49,83,113	1.50	4 (8%)
26	BCR	A	849	-	41,41,41	0.80	1 (2%)	56,56,56	2.05	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	7	603	-	47,52,73	1.40	10 (21%)	55,88,113	1.50	5 (9%)
23	CLA	B	836	-	54,58,73	1.31	10 (18%)	64,95,113	1.53	12 (18%)
23	CLA	4	607	-	49,53,73	1.37	9 (18%)	58,89,113	1.46	4 (6%)
23	CLA	L	304	-	49,53,73	1.36	6 (12%)	58,89,113	1.48	6 (10%)
32	XAT	5	621	-	41,47,47	0.98	2 (4%)	54,74,74	2.73	24 (44%)
23	CLA	F	303	-	46,50,73	1.41	10 (21%)	53,85,113	1.48	6 (11%)
23	CLA	a	606	13	46,52,73	1.39	8 (17%)	57,87,113	1.46	5 (8%)
23	CLA	7	611	25	63,67,73	1.16	8 (12%)	74,105,113	1.38	7 (9%)
23	CLA	7	607	-	46,50,73	1.37	10 (21%)	53,85,113	1.60	7 (13%)
25	LHG	6	623	23	47,47,48	0.66	1 (2%)	50,53,54	1.26	5 (10%)
23	CLA	6	618	17	43,48,73	1.52	11 (25%)	51,83,113	1.55	7 (13%)
23	CLA	5	617	-	54,58,73	1.32	9 (16%)	64,95,113	1.46	6 (9%)
26	BCR	1	619	-	41,41,41	0.69	0	56,56,56	2.01	16 (28%)
31	LUT	a	617	-	42,43,43	0.71	0	51,60,60	1.79	15 (29%)
23	CLA	A	818	-	64,68,73	1.18	9 (14%)	76,107,113	1.42	7 (9%)
23	CLA	3	608	-	59,63,73	1.31	10 (16%)	70,101,113	1.50	8 (11%)
23	CLA	4	608	-	69,73,73	1.15	9 (13%)	82,113,113	1.40	7 (8%)
25	LHG	5	625	-	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
23	CLA	5	619	-	47,51,73	1.50	11 (23%)	58,87,113	1.82	11 (18%)
23	CLA	B	809	2	69,73,73	1.16	9 (13%)	82,113,113	1.42	8 (9%)
23	CLA	B	825	-	66,70,73	1.18	9 (13%)	78,109,113	1.33	11 (14%)
23	CLA	B	821	-	47,51,73	1.45	9 (19%)	54,86,113	1.63	7 (12%)
23	CLA	1	609	13	44,48,73	1.49	8 (18%)	55,83,113	1.64	10 (18%)
23	CLA	5	613	16	68,72,73	1.16	9 (13%)	80,111,113	1.41	5 (6%)
23	CLA	4	603	15	48,52,73	1.48	11 (22%)	59,88,113	1.51	7 (11%)
27	SF4	A	853	-	0,12,12	-	-	-	-	-
23	CLA	8	611	25	46,50,73	1.37	10 (21%)	53,85,113	1.46	5 (9%)
23	CLA	4	612	15	44,49,73	1.41	9 (20%)	50,84,113	1.54	6 (12%)
23	CLA	A	832	-	54,58,73	1.31	9 (16%)	64,95,113	1.51	7 (10%)
23	CLA	5	601	16	60,64,73	1.27	8 (13%)	71,102,113	1.31	6 (8%)
23	CLA	A	831	-	69,73,73	1.28	9 (13%)	82,113,113	1.57	15 (18%)
23	CLA	4	614	-	60,64,73	1.25	8 (13%)	71,102,113	1.31	5 (7%)
23	CLA	G	203	-	46,50,73	1.39	7 (15%)	53,85,113	1.52	3 (5%)
23	CLA	B	813	-	69,73,73	1.16	10 (14%)	82,113,113	1.33	7 (8%)
23	CLA	3	602	14	64,68,73	1.20	9 (14%)	76,107,113	1.38	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	F	304	-	45,49,73	1.38	8 (17%)	54,84,113	1.54	7 (12%)
23	CLA	8	610	19	64,68,73	1.16	9 (14%)	76,107,113	1.35	8 (10%)
23	CLA	K	203	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	7 (8%)
23	CLA	A	819	-	63,67,73	1.26	9 (14%)	74,105,113	1.41	9 (12%)
23	CLA	6	608	-	55,59,73	1.30	8 (14%)	64,96,113	1.50	7 (10%)
29	LMG	7	624	-	44,44,55	0.83	1 (2%)	52,52,63	1.26	6 (11%)
26	BCR	3	622	-	41,41,41	0.76	0	56,56,56	2.63	22 (39%)
23	CLA	B	841	25	47,51,73	1.41	9 (19%)	55,86,113	1.57	6 (10%)
31	LUT	4	619	-	42,43,43	0.71	0	51,60,60	1.93	13 (25%)
23	CLA	2	604	-	27,35,73	1.83	6 (22%)	32,60,113	1.69	5 (15%)
23	CLA	A	807	1	69,73,73	1.21	10 (14%)	82,113,113	1.33	8 (9%)
23	CLA	6	616	17	69,73,73	1.16	9 (13%)	82,113,113	1.51	14 (17%)
31	LUT	5	620	-	42,43,43	0.74	0	51,60,60	1.88	13 (25%)
23	CLA	6	620	-	68,72,73	1.13	10 (14%)	80,111,113	1.35	7 (8%)
32	XAT	4	620	-	41,47,47	0.91	2 (4%)	54,74,74	2.54	20 (37%)
23	CLA	B	818	-	64,68,73	1.19	9 (14%)	76,107,113	1.46	7 (9%)
26	BCR	5	622	-	41,41,41	0.66	0	56,56,56	2.20	20 (35%)
23	CLA	A	840	-	56,60,73	1.29	9 (16%)	65,97,113	1.54	10 (15%)
23	CLA	A	829	-	69,73,73	1.14	9 (13%)	82,113,113	1.39	9 (10%)
23	CLA	6	607	-	45,49,73	1.49	11 (24%)	54,84,113	1.59	8 (14%)
23	CLA	A	827	-	63,67,73	1.25	11 (17%)	74,105,113	1.41	8 (10%)
23	CLA	6	614	-	64,68,73	1.18	9 (14%)	76,107,113	1.33	4 (5%)
23	CLA	3	607	14	60,64,73	1.29	11 (18%)	73,102,113	1.40	9 (12%)
23	CLA	4	609	15	65,69,73	1.20	7 (10%)	77,108,113	1.39	5 (6%)
23	CLA	B	824	-	69,73,73	1.17	11 (15%)	82,113,113	1.45	10 (12%)
23	CLA	A	830	-	69,73,73	1.16	8 (11%)	82,113,113	1.46	9 (10%)
23	CLA	9	612	21	27,35,73	1.84	7 (25%)	32,60,113	1.56	5 (15%)
23	CLA	2	609	20	27,35,73	1.86	6 (22%)	32,60,113	1.63	5 (15%)
25	LHG	a	620	23	48,48,48	0.62	1 (2%)	51,54,54	1.28	6 (11%)
23	CLA	1	608	-	47,52,73	1.37	8 (17%)	55,88,113	1.49	4 (7%)
23	CLA	a	601	13	57,62,73	1.27	9 (15%)	67,100,113	1.35	5 (7%)
23	CLA	4	611	25	46,50,73	1.37	9 (19%)	53,85,113	1.44	4 (7%)
23	CLA	9	613	21	27,35,73	1.83	6 (22%)	32,60,113	1.62	4 (12%)
25	LHG	4	622	23	48,48,48	0.62	1 (2%)	51,54,54	1.32	6 (11%)
23	CLA	A	803	-	69,73,73	1.22	9 (13%)	82,113,113	1.35	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	XAT	9	620	-	41,47,47	0.95	2 (4%)	54,74,74	2.47	17 (31%)
28	LMU	8	624	-	36,36,36	1.19	2 (5%)	47,47,47	0.93	1 (2%)
23	CLA	9	606	21	27,35,73	1.86	6 (22%)	32,60,113	1.61	4 (12%)
23	CLA	a	612	13	49,53,73	1.35	9 (18%)	58,89,113	1.48	8 (13%)
23	CLA	A	843	-	68,72,73	1.20	8 (11%)	80,111,113	1.37	6 (7%)
23	CLA	A	824	-	45,49,73	1.40	7 (15%)	54,84,113	1.60	7 (12%)
27	SF4	C	102	-	0,12,12	-	-	-	-	-
28	LMU	A	859	-	35,35,36	1.31	2 (5%)	44,45,47	1.28	6 (13%)
29	LMG	J	104	-	40,40,55	0.89	1 (2%)	48,48,63	1.26	4 (8%)
23	CLA	A	834	-	69,73,73	1.14	8 (11%)	82,113,113	1.38	6 (7%)
23	CLA	A	836	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	7 (8%)
26	BCR	B	801	-	41,41,41	0.76	0	56,56,56	2.06	14 (25%)
23	CLA	6	612	17	44,49,73	1.43	10 (22%)	50,84,113	1.53	6 (12%)
23	CLA	B	833	-	69,73,73	1.16	9 (13%)	82,113,113	1.43	7 (8%)
23	CLA	A	817	-	49,53,73	1.39	10 (20%)	58,89,113	1.58	7 (12%)
23	CLA	7	612	18	48,52,73	1.41	10 (20%)	57,88,113	1.50	8 (14%)
23	CLA	B	826	-	59,63,73	1.27	10 (16%)	70,101,113	1.40	8 (11%)
23	CLA	a	616	13	49,53,73	1.38	9 (18%)	58,89,113	1.40	4 (6%)
23	CLA	3	614	-	43,48,73	1.42	7 (16%)	51,83,113	1.48	6 (11%)
23	CLA	5	607	-	69,73,73	1.17	10 (14%)	82,113,113	1.46	8 (9%)
23	CLA	J	101	10	46,50,73	1.36	8 (17%)	53,85,113	1.54	4 (7%)
23	CLA	1	607	-	43,48,73	1.42	8 (18%)	51,83,113	1.52	5 (9%)
23	CLA	5	610	16	58,62,73	1.27	10 (17%)	68,99,113	1.42	9 (13%)
23	CLA	A	813	-	58,62,73	1.25	11 (18%)	68,99,113	1.47	7 (10%)
23	CLA	B	838	-	51,55,73	1.28	8 (15%)	60,91,113	1.61	5 (8%)
23	CLA	7	616	18	47,51,73	1.49	10 (21%)	58,87,113	1.53	9 (15%)
32	XAT	1	618	-	41,47,47	0.92	2 (4%)	54,74,74	2.50	18 (33%)
23	CLA	A	845	25	54,58,73	1.28	9 (16%)	64,95,113	1.51	5 (7%)
26	BCR	3	620	-	41,41,41	0.80	1 (2%)	56,56,56	2.19	18 (32%)
23	CLA	4	610	15	65,69,73	1.18	8 (12%)	77,108,113	1.32	6 (7%)
23	CLA	5	611	25	46,50,73	1.37	10 (21%)	53,85,113	1.45	5 (9%)
26	BCR	L	301	-	41,41,41	0.77	0	56,56,56	1.79	15 (26%)
25	LHG	2	622	23	36,36,48	0.79	2 (5%)	39,42,54	1.32	5 (12%)
23	CLA	B	823	-	49,53,73	1.37	9 (18%)	58,89,113	1.53	8 (13%)
32	XAT	a	618	-	41,47,47	0.92	2 (4%)	54,74,74	2.49	18 (33%)

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
23	CLA	5	612	16	1/1/10/20	3/10/86/115	-
31	LUT	3	618	-	-	3/29/67/67	0/2/2/2
23	CLA	5	614	-	1/1/10/20	7/15/87/115	-
23	CLA	1	604	-	1/1/11/20	10/20/96/115	-
23	CLA	8	606	-	1/1/15/20	16/37/113/115	-
26	BCR	B	846	-	-	4/29/63/63	0/2/2/2
23	CLA	7	608	-	1/1/12/20	6/21/97/115	-
23	CLA	2	607	-	1/1/5/20	-	-
23	CLA	5	608	-	1/1/12/20	8/21/97/115	-
26	BCR	B	847	-	-	0/29/63/63	0/2/2/2
31	LUT	9	619	-	-	1/29/67/67	0/2/2/2
23	CLA	a	610	13	1/1/14/20	6/31/107/115	-
23	CLA	2	614	-	1/1/5/20	-	-
33	NEX	5	624	-	-	2/27/83/83	0/3/3/3
24	PQN	A	844	-	-	6/23/43/43	0/2/2/2
26	BCR	B	843	-	-	8/29/63/63	0/2/2/2
23	CLA	4	602	15	1/1/14/20	7/33/109/115	-
23	CLA	9	610	21	1/1/5/20	-	-
29	LMG	A	860	-	-	18/35/55/70	0/1/1/1
32	XAT	8	620	-	-	2/31/93/93	0/4/4/4
26	BCR	L	305	-	-	10/29/63/63	0/2/2/2
23	CLA	A	833	-	1/1/11/20	2/15/91/115	-
23	CLA	A	841	-	1/1/15/20	17/39/115/115	-
23	CLA	B	815	-	1/1/10/20	4/13/89/115	-
23	CLA	K	204	-	1/1/11/20	8/17/93/115	-
23	CLA	2	612	20	1/1/5/20	-	-
23	CLA	1	603	-	1/1/12/20	13/23/99/115	-
25	LHG	9	622	23	-	22/53/53/53	-
23	CLA	6	610	17	1/1/15/20	8/39/115/115	-
26	BCR	6	622	-	-	7/29/63/63	0/2/2/2
23	CLA	a	607	-	1/1/11/20	6/15/91/115	-
23	CLA	1	611	25	1/1/15/20	11/39/115/115	-
23	CLA	A	838	-	1/1/12/20	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	7	615	-	1/1/10/20	4/8/84/115	-
23	CLA	a	608	-	1/1/11/20	6/13/89/115	-
23	CLA	B	808	-	1/1/15/20	14/39/115/115	-
28	LMU	5	628	-	-	11/19/59/61	0/2/2/2
26	BCR	A	850	-	-	1/29/63/63	0/2/2/2
32	XAT	7	620	-	-	1/31/93/93	0/4/4/4
23	CLA	B	819	-	1/1/13/20	10/27/103/115	-
23	CLA	6	602	17	1/1/15/20	9/39/115/115	-
23	CLA	A	839	-	1/1/13/20	7/27/103/115	-
23	CLA	B	805	-	1/1/15/20	15/39/115/115	-
26	BCR	B	848	-	-	4/29/63/63	0/2/2/2
23	CLA	G	204	7	1/1/11/20	8/15/91/115	-
23	CLA	A	826	-	1/1/14/20	10/37/113/115	-
23	CLA	B	814	-	1/1/14/20	12/38/114/115	-
23	CLA	9	614	-	1/1/5/20	-	-
28	LMU	K	208	-	-	10/21/61/61	0/2/2/2
26	BCR	A	848	-	-	2/29/63/63	0/2/2/2
23	CLA	a	611	25	1/1/10/20	0/4/80/115	-
32	XAT	2	620	-	-	0/31/93/93	0/4/4/4
26	BCR	F	305	-	-	2/29/63/63	0/2/2/2
23	CLA	B	828	-	1/1/15/20	16/39/115/115	-
23	CLA	a	603	-	1/1/10/20	6/12/88/115	-
25	LHG	7	622	23	-	22/41/41/53	-
23	CLA	1	601	13	1/1/13/20	6/25/101/115	-
23	CLA	8	613	19	1/1/15/20	17/39/115/115	-
26	BCR	B	844	-	-	7/29/63/63	0/2/2/2
23	CLA	5	616	16	1/1/10/20	4/8/84/115	-
23	CLA	9	603	21	1/1/5/20	-	-
23	CLA	4	606	-	1/1/10/20	5/8/84/115	-
23	CLA	8	601	19	1/1/15/20	18/39/115/115	-
25	LHG	A	846	-	-	24/53/53/53	-
23	CLA	a	609	13	1/1/15/20	21/37/113/115	-
32	XAT	3	619	-	-	1/31/93/93	0/4/4/4
23	CLA	2	610	20	1/1/5/20	-	-
23	CLA	K	206	11	1/1/11/20	5/15/91/115	-
23	CLA	B	810	-	1/1/14/20	18/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	a	619	-	-	3/29/63/63	0/2/2/2
31	LUT	6	619	-	-	2/29/67/67	0/2/2/2
23	CLA	B	839	-	1/1/15/20	14/39/115/115	-
23	CLA	3	612	14	1/1/10/20	3/13/89/115	-
32	XAT	6	621	-	-	2/31/93/93	0/4/4/4
29	LMG	5	627	-	-	13/35/55/70	0/1/1/1
23	CLA	9	611	25	1/1/5/20	-	-
23	CLA	A	825	-	1/1/15/20	19/39/115/115	-
23	CLA	6	606	-	1/1/10/20	0/8/84/115	-
23	CLA	7	610	18	1/1/15/20	7/39/115/115	-
23	CLA	A	821	-	1/1/12/20	14/25/101/115	-
23	CLA	A	801	-	1/1/15/20	12/39/115/115	-
26	BCR	3	621	-	-	6/29/63/63	0/2/2/2
23	CLA	5	602	16	1/1/15/20	9/39/115/115	-
26	BCR	K	202	-	-	4/29/63/63	0/2/2/2
23	CLA	B	811	-	1/1/13/20	8/23/99/115	-
23	CLA	8	607	-	1/1/10/20	3/10/86/115	-
23	CLA	6	613	-	1/1/15/20	14/37/113/115	-
23	CLA	B	829	-	1/1/15/20	8/39/115/115	-
23	CLA	A	802	-	1/1/15/20	6/39/115/115	-
23	CLA	B	822	-	-	6/12/88/115	-
23	CLA	7	606	-	1/1/10/20	4/10/86/115	-
23	CLA	5	606	-	1/1/10/20	4/8/84/115	-
23	CLA	A	805	-	1/1/12/20	6/24/100/115	-
26	BCR	J	102	-	-	5/29/63/63	0/2/2/2
23	CLA	9	609	21	1/1/5/20	-	-
23	CLA	L	303	-	1/1/11/20	5/15/91/115	-
23	CLA	4	601	15	1/1/15/20	16/39/115/115	-
23	CLA	B	803	-	1/1/15/20	16/39/115/115	-
23	CLA	B	834	-	1/1/14/20	14/33/109/115	-
23	CLA	7	604	-	1/1/13/20	8/25/101/115	-
23	CLA	4	618	15	1/1/10/20	0/8/84/115	-
23	CLA	B	807	-	1/1/12/20	5/24/100/115	-
23	CLA	9	601	21	1/1/5/20	-	-
23	CLA	1	612	13	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	1	602	13	1/1/14/20	7/35/111/115	-
23	CLA	3	613	14	1/1/12/20	7/23/99/115	-
23	CLA	F	301	-	1/1/13/20	10/30/106/115	-
23	CLA	a	613	-	1/1/15/20	13/39/115/115	-
23	CLA	3	606	-	1/1/13/20	11/25/101/115	-
23	CLA	5	603	-	1/1/13/20	10/25/101/115	-
28	LMU	A	858	-	-	6/21/57/61	0/2/2/2
28	LMU	A	857	-	-	11/21/61/61	0/2/2/2
30	DGD	J	103	-	-	25/47/87/95	0/2/2/2
23	CLA	1	613	-	1/1/15/20	13/39/115/115	-
26	BCR	A	851	-	-	4/29/63/63	0/2/2/2
23	CLA	4	604	-	1/1/13/20	5/25/101/115	-
23	CLA	A	823	-	1/1/10/20	7/12/88/115	-
23	CLA	1	606	13	1/1/8/20	3/7/79/115	-
23	CLA	B	830	-	1/1/10/20	4/13/89/115	-
23	CLA	7	609	18	1/1/10/20	3/12/88/115	-
23	CLA	A	828	-	1/1/15/20	10/39/115/115	-
31	LUT	7	619	-	-	5/29/67/67	0/2/2/2
27	SF4	C	101	-	-	-	0/6/5/5
23	CLA	B	832	-	1/1/14/20	7/33/109/115	-
23	CLA	6	601	17	1/1/15/20	13/39/115/115	-
25	LHG	3	624	23	-	26/53/53/53	-
26	BCR	7	621	-	-	4/29/63/63	0/2/2/2
26	BCR	8	621	-	-	6/29/63/63	0/2/2/2
23	CLA	2	606	20	1/1/5/20	-	-
23	CLA	B	802	-	1/1/15/20	18/39/115/115	-
31	LUT	8	619	-	-	2/29/67/67	0/2/2/2
24	PQN	B	842	-	-	7/23/43/43	0/2/2/2
23	CLA	a	604	-	1/1/11/20	10/20/96/115	-
23	CLA	5	618	16	1/1/10/20	2/8/84/115	-
23	CLA	B	806	2	1/1/15/20	12/39/115/115	-
28	LMU	8	625	-	-	10/21/61/61	0/2/2/2
23	CLA	2	602	20	1/1/5/20	-	-
23	CLA	A	810	1	1/1/12/20	7/21/97/115	-
23	CLA	A	854	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	3	610	14	1/1/15/20	17/39/115/115	-
23	CLA	A	842	-	1/1/15/20	11/39/115/115	-
23	CLA	8	609	19	1/1/11/20	4/15/91/115	-
23	CLA	7	613	18	1/1/15/20	17/39/115/115	-
23	CLA	a	602	13	1/1/14/20	8/35/111/115	-
26	BCR	A	852	-	-	11/29/63/63	0/2/2/2
23	CLA	A	822	-	1/1/15/20	9/39/115/115	-
26	BCR	A	856	-	-	8/29/63/63	0/2/2/2
23	CLA	A	806	-	1/1/15/20	13/39/115/115	-
23	CLA	B	837	-	1/1/15/20	15/39/115/115	-
23	CLA	7	601	18	1/1/14/20	13/33/109/115	-
23	CLA	8	604	-	1/1/12/20	5/21/97/115	-
23	CLA	2	603	20	1/1/5/20	-	-
23	CLA	9	602	21	1/1/5/20	-	-
23	CLA	B	816	-	1/1/12/20	9/25/101/115	-
23	CLA	7	614	-	1/1/10/20	5/12/88/115	-
23	CLA	2	611	25	1/1/4/20	-	-
23	CLA	B	804	-	1/1/10/20	2/10/86/115	-
23	CLA	9	607	-	1/1/5/20	-	-
25	LHG	3	623	-	-	24/49/49/53	-
23	CLA	6	604	-	1/1/15/20	21/39/115/115	-
26	BCR	4	621	-	-	0/29/63/63	0/2/2/2
23	CLA	A	811	-	1/1/15/20	15/39/115/115	-
23	CLA	B	827	-	1/1/14/20	12/36/112/115	-
23	CLA	3	604	-	1/1/15/20	13/39/115/115	-
25	LHG	B	851	23	-	21/42/42/53	-
30	DGD	B	850	-	-	22/51/91/95	0/2/2/2
23	CLA	A	835	-	1/1/14/20	15/35/111/115	-
25	LHG	A	847	23	-	11/34/34/53	-
33	NEX	6	624	-	-	4/27/83/83	0/3/3/3
23	CLA	a	614	-	1/1/12/20	9/27/99/115	-
26	BCR	G	205	-	-	0/29/63/63	0/2/2/2
23	CLA	B	812	-	1/1/10/20	8/13/89/115	-
31	LUT	2	619	-	-	2/29/67/67	0/2/2/2
23	CLA	4	613	15	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	2	613	20	1/1/5/20	-	-
25	LHG	8	623	-	-	23/51/51/53	-
23	CLA	1	616	13	1/1/11/20	4/11/87/115	-
23	CLA	6	603	-	1/1/13/20	4/25/101/115	-
29	LMG	5	626	-	-	22/35/55/70	0/1/1/1
23	CLA	2	601	20	1/1/5/20	-	-
23	CLA	A	816	-	1/1/10/20	2/12/88/115	-
23	CLA	3	603	-	1/1/13/20	10/27/103/115	-
23	CLA	9	604	-	1/1/5/20	-	-
23	CLA	A	809	1	1/1/15/20	14/39/115/115	-
23	CLA	8	616	19	-	7/11/87/115	-
25	LHG	5	623	23	-	22/53/53/53	-
23	CLA	L	302	12	1/1/11/20	5/15/91/115	-
29	LMG	4	624	-	-	14/35/55/70	0/1/1/1
26	BCR	7	623	-	-	0/29/63/63	0/2/2/2
23	CLA	6	617	-	1/1/11/20	9/15/91/115	-
23	CLA	3	609	14	1/1/14/20	16/33/109/115	-
23	CLA	7	602	18	1/1/15/20	16/39/115/115	-
23	CLA	2	616	-	1/1/5/20	-	-
23	CLA	A	815	-	1/1/12/20	6/21/97/115	-
23	CLA	1	614	-	1/1/9/20	0/4/76/115	-
23	CLA	6	611	25	1/1/10/20	4/12/88/115	-
26	BCR	B	845	-	-	5/29/63/63	0/2/2/2
23	CLA	B	840	-	1/1/15/20	10/39/115/115	-
23	CLA	B	831	-	1/1/15/20	13/39/115/115	-
23	CLA	A	837	1	1/1/11/20	7/15/91/115	-
23	CLA	5	609	16	1/1/15/20	15/39/115/115	-
23	CLA	8	608	-	1/1/12/20	5/23/99/115	-
23	CLA	B	835	-	1/1/11/20	9/15/91/115	-
31	LUT	1	617	-	-	1/29/67/67	0/2/2/2
25	LHG	8	622	23	-	26/53/53/53	-
23	CLA	A	808	-	1/1/12/20	2/21/97/115	-
29	LMG	4	623	-	-	11/35/55/70	0/1/1/1
25	LHG	1	620	23	-	24/53/53/53	-
23	CLA	A	804	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	8	603	-	1/1/11/20	7/13/89/115	-
23	CLA	5	604	-	1/1/15/20	11/35/111/115	-
23	CLA	A	814	-	1/1/15/20	20/39/115/115	-
23	CLA	1	610	13	1/1/9/20	2/8/80/115	-
23	CLA	3	617	14	1/1/10/20	2/8/84/115	-
26	BCR	K	207	-	-	1/29/63/63	0/2/2/2
23	CLA	8	612	19	1/1/10/20	2/10/86/115	-
23	CLA	4	616	15	1/1/11/20	5/11/87/115	-
23	CLA	B	820	-	1/1/12/20	6/21/97/115	-
23	CLA	8	614	-	1/1/13/20	10/29/105/115	-
23	CLA	8	602	19	1/1/14/20	9/33/109/115	-
23	CLA	A	820	-	1/1/15/20	14/39/115/115	-
23	CLA	B	817	-	1/1/13/20	11/32/108/115	-
23	CLA	A	812	-	1/1/15/20	13/39/115/115	-
23	CLA	3	611	25	1/1/10/20	2/4/80/115	-
23	CLA	6	609	17	1/1/11/20	6/15/91/115	-
23	CLA	K	201	11	1/1/11/20	7/15/91/115	-
23	CLA	3	615	-	1/1/10/20	3/8/84/115	-
26	BCR	A	849	-	-	5/29/63/63	0/2/2/2
23	CLA	7	603	-	1/1/11/20	4/13/89/115	-
23	CLA	B	836	-	-	5/21/97/115	-
23	CLA	4	607	-	1/1/11/20	7/15/91/115	-
23	CLA	L	304	-	1/1/11/20	9/15/91/115	-
32	XAT	5	621	-	-	2/31/93/93	0/4/4/4
23	CLA	F	303	-	1/1/10/20	6/12/88/115	-
23	CLA	a	606	13	1/1/10/20	5/12/88/115	-
23	CLA	7	611	25	1/1/13/20	10/31/107/115	-
23	CLA	7	607	-	1/1/10/20	4/12/88/115	-
25	LHG	6	623	23	-	22/52/52/53	-
23	CLA	6	618	17	1/1/10/20	2/8/84/115	-
23	CLA	5	617	-	1/1/12/20	8/21/97/115	-
26	BCR	1	619	-	-	3/29/63/63	0/2/2/2
31	LUT	a	617	-	-	1/29/67/67	0/2/2/2
23	CLA	A	818	-	1/1/14/20	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	3	608	-	1/1/13/20	11/27/103/115	-
23	CLA	4	608	-	1/1/15/20	9/39/115/115	-
25	LHG	5	625	-	-	22/53/53/53	-
23	CLA	5	619	-	1/1/11/20	7/11/87/115	-
23	CLA	B	809	2	1/1/15/20	15/39/115/115	-
23	CLA	B	825	-	1/1/14/20	10/36/112/115	-
23	CLA	B	821	-	1/1/11/20	5/13/89/115	-
23	CLA	1	609	13	1/1/10/20	2/8/84/115	-
23	CLA	5	613	16	1/1/14/20	19/37/113/115	-
23	CLA	4	603	15	1/1/11/20	7/13/89/115	-
27	SF4	A	853	-	-	-	0/6/5/5
23	CLA	8	611	25	1/1/10/20	6/12/88/115	-
23	CLA	4	612	15	-	2/10/86/115	-
23	CLA	A	832	-	1/1/12/20	8/21/97/115	-
23	CLA	5	601	16	1/1/13/20	7/29/105/115	-
23	CLA	A	831	-	1/1/15/20	13/39/115/115	-
23	CLA	4	614	-	1/1/13/20	9/29/105/115	-
23	CLA	G	203	-	1/1/10/20	4/12/88/115	-
23	CLA	B	813	-	1/1/15/20	20/39/115/115	-
23	CLA	3	602	14	1/1/14/20	11/33/109/115	-
23	CLA	F	304	-	1/1/10/20	2/10/86/115	-
23	CLA	8	610	19	1/1/14/20	7/33/109/115	-
23	CLA	K	203	-	1/1/15/20	12/39/115/115	-
23	CLA	A	819	-	1/1/13/20	10/32/108/115	-
23	CLA	6	608	-	1/1/12/20	10/23/99/115	-
29	LMG	7	624	-	-	19/39/59/70	0/1/1/1
26	BCR	3	622	-	-	8/29/63/63	0/2/2/2
23	CLA	B	841	25	1/1/10/20	2/13/89/115	-
31	LUT	4	619	-	-	4/29/67/67	0/2/2/2
23	CLA	2	604	-	1/1/5/20	-	-
23	CLA	A	807	1	1/1/15/20	16/39/115/115	-
23	CLA	6	616	17	1/1/15/20	16/39/115/115	-
31	LUT	5	620	-	-	2/29/67/67	0/2/2/2
23	CLA	6	620	-	1/1/14/20	17/37/113/115	-
32	XAT	4	620	-	-	1/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	818	-	1/1/14/20	16/33/109/115	-
26	BCR	5	622	-	-	1/29/63/63	0/2/2/2
23	CLA	A	840	-	1/1/12/20	3/24/100/115	-
23	CLA	A	829	-	1/1/15/20	11/39/115/115	-
23	CLA	6	607	-	1/1/10/20	4/10/86/115	-
23	CLA	A	827	-	1/1/13/20	4/32/108/115	-
23	CLA	6	614	-	1/1/14/20	8/33/109/115	-
23	CLA	3	607	14	1/1/13/20	9/28/104/115	-
23	CLA	4	609	15	1/1/14/20	11/35/111/115	-
23	CLA	B	824	-	1/1/15/20	9/39/115/115	-
23	CLA	A	830	-	1/1/15/20	14/39/115/115	-
23	CLA	9	612	21	1/1/5/20	-	-
23	CLA	2	609	20	1/1/5/20	-	-
25	LHG	a	620	23	-	24/53/53/53	-
23	CLA	1	608	-	1/1/11/20	6/13/89/115	-
23	CLA	a	601	13	1/1/13/20	6/25/101/115	-
23	CLA	4	611	25	1/1/10/20	6/12/88/115	-
23	CLA	9	613	21	1/1/5/20	-	-
25	LHG	4	622	23	-	19/53/53/53	-
23	CLA	A	803	-	1/1/15/20	9/39/115/115	-
32	XAT	9	620	-	-	0/31/93/93	0/4/4/4
28	LMU	8	624	-	-	6/21/61/61	0/2/2/2
23	CLA	9	606	21	1/1/5/20	-	-
23	CLA	a	612	13	1/1/11/20	6/15/91/115	-
23	CLA	A	843	-	1/1/14/20	18/37/113/115	-
23	CLA	A	824	-	1/1/10/20	2/10/86/115	-
27	SF4	C	102	-	-	-	0/6/5/5
28	LMU	A	859	-	-	13/21/57/61	0/2/2/2
29	LMG	J	104	-	-	19/35/55/70	0/1/1/1
23	CLA	A	834	-	1/1/15/20	20/39/115/115	-
23	CLA	A	836	-	1/1/15/20	12/39/115/115	-
26	BCR	B	801	-	-	4/29/63/63	0/2/2/2
23	CLA	6	612	17	1/1/10/20	3/10/86/115	-
23	CLA	B	833	-	1/1/15/20	19/39/115/115	-
23	CLA	A	817	-	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	7	612	18	-	4/13/89/115	-
23	CLA	B	826	-	1/1/13/20	6/27/103/115	-
23	CLA	a	616	13	1/1/11/20	6/15/91/115	-
23	CLA	3	614	-	1/1/10/20	2/8/84/115	-
23	CLA	5	607	-	1/1/15/20	15/39/115/115	-
23	CLA	J	101	10	1/1/10/20	5/12/88/115	-
23	CLA	1	607	-	1/1/10/20	5/8/84/115	-
23	CLA	5	610	16	1/1/12/20	6/26/102/115	-
23	CLA	A	813	-	1/1/12/20	6/26/102/115	-
23	CLA	B	838	-	1/1/11/20	6/18/94/115	-
23	CLA	7	616	18	1/1/11/20	7/11/87/115	-
32	XAT	1	618	-	-	1/31/93/93	0/4/4/4
23	CLA	A	845	25	1/1/12/20	10/21/97/115	-
26	BCR	3	620	-	-	4/29/63/63	0/2/2/2
23	CLA	4	610	15	1/1/14/20	14/35/111/115	-
23	CLA	5	611	25	1/1/10/20	4/12/88/115	-
26	BCR	L	301	-	-	6/29/63/63	0/2/2/2
25	LHG	2	622	23	-	16/41/41/53	-
23	CLA	B	823	-	1/1/11/20	4/15/91/115	-
32	XAT	a	618	-	-	1/31/93/93	0/4/4/4

The worst 5 of 2276 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	611	CLA	C1A-NA	13.27	1.40	1.29
24	A	844	PQN	C12-C13	8.94	1.53	1.33
24	B	842	PQN	C12-C13	8.87	1.53	1.33
24	A	844	PQN	O1-C1	8.02	1.40	1.23
24	B	842	PQN	O1-C1	7.73	1.39	1.23

The worst 5 of 2742 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	803	CLA	C4A-NA-C1A	8.97	110.77	106.68
23	8	613	CLA	C4A-NA-C1A	8.92	110.75	106.68
32	5	621	XAT	O24-C25-C24	8.66	121.61	113.49
23	B	808	CLA	C4A-NA-C1A	8.61	110.61	106.68
32	2	620	XAT	O24-C25-C24	8.60	121.55	113.49

5 of 238 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	801	CLA	ND
23	A	802	CLA	ND
23	A	803	CLA	ND
23	A	804	CLA	ND
23	A	805	CLA	ND

5 of 2667 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	801	CLA	C2B-C3B-CAB-CBB
23	A	801	CLA	C4B-C3B-CAB-CBB
23	A	801	CLA	CBD-CGD-O2D-CED
23	A	804	CLA	C1A-C2A-CAA-CBA
23	A	804	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

264 monomers are involved in 558 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	3	618	LUT	1	0
26	B	846	BCR	1	0
23	7	608	CLA	4	0
23	5	608	CLA	2	0
26	B	847	BCR	2	0
31	9	619	LUT	1	0
23	a	610	CLA	2	0
23	2	614	CLA	1	0
33	5	624	NEX	3	0
24	A	844	PQN	4	0
26	B	843	BCR	1	0
23	4	602	CLA	1	0
29	A	860	LMG	2	0
32	8	620	XAT	1	0
26	L	305	BCR	4	0
23	A	841	CLA	5	0
23	B	815	CLA	1	0
23	K	204	CLA	1	0
23	1	603	CLA	1	0
25	9	622	LHG	5	0
23	6	610	CLA	4	0
26	6	622	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	607	CLA	1	0
23	1	611	CLA	5	0
23	A	838	CLA	2	0
23	a	608	CLA	1	0
23	B	808	CLA	2	0
28	5	628	LMU	3	0
26	A	850	BCR	3	0
32	7	620	XAT	1	0
23	B	819	CLA	1	0
23	6	602	CLA	6	0
23	A	839	CLA	2	0
23	B	805	CLA	4	0
26	B	848	BCR	1	0
23	G	204	CLA	2	0
23	A	826	CLA	1	0
23	B	814	CLA	3	0
23	9	614	CLA	1	0
26	A	848	BCR	5	0
32	2	620	XAT	3	0
26	F	305	BCR	4	0
23	B	828	CLA	1	0
23	a	603	CLA	1	0
25	7	622	LHG	2	0
23	1	601	CLA	5	0
23	8	613	CLA	1	0
26	B	844	BCR	3	0
23	5	616	CLA	1	0
23	8	601	CLA	4	0
25	A	846	LHG	2	0
23	a	609	CLA	2	0
32	3	619	XAT	3	0
23	2	610	CLA	1	0
23	B	810	CLA	3	0
26	a	619	BCR	4	0
31	6	619	LUT	4	0
23	B	839	CLA	3	0
23	3	612	CLA	1	0
32	6	621	XAT	1	0
29	5	627	LMG	3	0
23	9	611	CLA	7	0
23	A	825	CLA	5	0
23	6	606	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	7	610	CLA	5	0
23	A	821	CLA	1	0
23	A	801	CLA	4	0
26	3	621	BCR	2	0
23	5	602	CLA	5	0
26	K	202	BCR	3	0
23	B	811	CLA	2	0
23	8	607	CLA	2	0
23	6	613	CLA	4	0
23	B	829	CLA	7	0
23	A	802	CLA	7	0
23	B	822	CLA	1	0
23	5	606	CLA	4	0
23	A	805	CLA	4	0
26	J	102	BCR	5	0
23	9	609	CLA	1	0
23	L	303	CLA	2	0
23	4	601	CLA	6	0
23	B	803	CLA	3	0
23	B	834	CLA	2	0
23	4	618	CLA	1	0
23	B	807	CLA	2	0
23	9	601	CLA	1	0
23	1	612	CLA	1	0
23	F	301	CLA	3	0
23	a	613	CLA	3	0
23	3	606	CLA	1	0
28	A	857	LMU	1	0
30	J	103	DGD	1	0
26	A	851	BCR	3	0
23	4	604	CLA	1	0
23	A	823	CLA	1	0
23	1	606	CLA	1	0
23	B	830	CLA	5	0
23	A	828	CLA	1	0
31	7	619	LUT	5	0
23	B	832	CLA	4	0
23	6	601	CLA	5	0
25	3	624	LHG	2	0
26	7	621	BCR	3	0
26	8	621	BCR	3	0
23	B	802	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	8	619	LUT	6	0
24	B	842	PQN	6	0
23	B	806	CLA	1	0
23	A	810	CLA	1	0
23	A	854	CLA	5	0
23	3	610	CLA	3	0
23	A	842	CLA	5	0
23	8	609	CLA	1	0
23	7	613	CLA	3	0
26	A	852	BCR	5	0
23	A	822	CLA	3	0
26	A	856	BCR	7	0
23	A	806	CLA	3	0
23	B	837	CLA	3	0
23	7	601	CLA	4	0
25	3	623	LHG	1	0
23	6	604	CLA	3	0
26	4	621	BCR	2	0
23	A	811	CLA	5	0
23	B	827	CLA	6	0
23	3	604	CLA	1	0
25	B	851	LHG	2	0
30	B	850	DGD	5	0
23	A	835	CLA	4	0
25	A	847	LHG	1	0
33	6	624	NEX	4	0
26	G	205	BCR	5	0
31	2	619	LUT	3	0
23	4	613	CLA	5	0
23	2	613	CLA	1	0
25	8	623	LHG	3	0
23	6	603	CLA	1	0
29	5	626	LMG	1	0
23	A	816	CLA	1	0
23	3	603	CLA	2	0
23	A	809	CLA	4	0
23	8	616	CLA	1	0
25	5	623	LHG	2	0
23	L	302	CLA	1	0
29	4	624	LMG	1	0
23	3	609	CLA	6	0
23	7	602	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	845	BCR	2	0
23	B	840	CLA	2	0
23	B	831	CLA	2	0
23	A	837	CLA	2	0
23	5	609	CLA	4	0
23	8	608	CLA	3	0
23	B	835	CLA	1	0
31	1	617	LUT	3	0
25	8	622	LHG	2	0
23	A	808	CLA	1	0
25	1	620	LHG	6	0
23	A	804	CLA	2	0
23	8	603	CLA	1	0
23	5	604	CLA	5	0
23	A	814	CLA	4	0
23	3	617	CLA	2	0
26	K	207	BCR	3	0
23	4	616	CLA	1	0
23	B	820	CLA	1	0
23	8	614	CLA	1	0
23	A	820	CLA	4	0
23	B	817	CLA	2	0
23	A	812	CLA	3	0
23	6	609	CLA	1	0
23	K	201	CLA	1	0
26	A	849	BCR	4	0
23	7	603	CLA	1	0
23	B	836	CLA	1	0
23	L	304	CLA	2	0
32	5	621	XAT	9	0
23	F	303	CLA	2	0
23	a	606	CLA	2	0
23	7	611	CLA	2	0
23	7	607	CLA	2	0
25	6	623	LHG	3	0
26	1	619	BCR	2	0
31	a	617	LUT	5	0
23	A	818	CLA	4	0
23	3	608	CLA	2	0
23	4	608	CLA	3	0
25	5	625	LHG	5	0
23	5	619	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	809	CLA	1	0
23	B	825	CLA	4	0
23	B	821	CLA	2	0
23	1	609	CLA	1	0
23	5	613	CLA	5	0
23	4	603	CLA	1	0
23	4	612	CLA	1	0
23	A	832	CLA	1	0
23	5	601	CLA	1	0
23	A	831	CLA	4	0
23	4	614	CLA	1	0
23	G	203	CLA	2	0
23	B	813	CLA	5	0
23	3	602	CLA	1	0
23	F	304	CLA	1	0
23	8	610	CLA	2	0
23	A	819	CLA	2	0
23	6	608	CLA	2	0
29	7	624	LMG	1	0
26	3	622	BCR	4	0
23	B	841	CLA	3	0
31	4	619	LUT	5	0
23	A	807	CLA	1	0
23	6	616	CLA	4	0
31	5	620	LUT	5	0
23	6	620	CLA	5	0
32	4	620	XAT	3	0
23	B	818	CLA	2	0
26	5	622	BCR	3	0
23	A	840	CLA	2	0
23	A	829	CLA	9	0
23	A	827	CLA	2	0
23	6	614	CLA	4	0
23	3	607	CLA	1	0
23	4	609	CLA	4	0
23	B	824	CLA	3	0
23	A	830	CLA	6	0
23	2	609	CLA	1	0
25	a	620	LHG	4	0
23	1	608	CLA	1	0
23	a	601	CLA	1	0
23	9	613	CLA	1	0

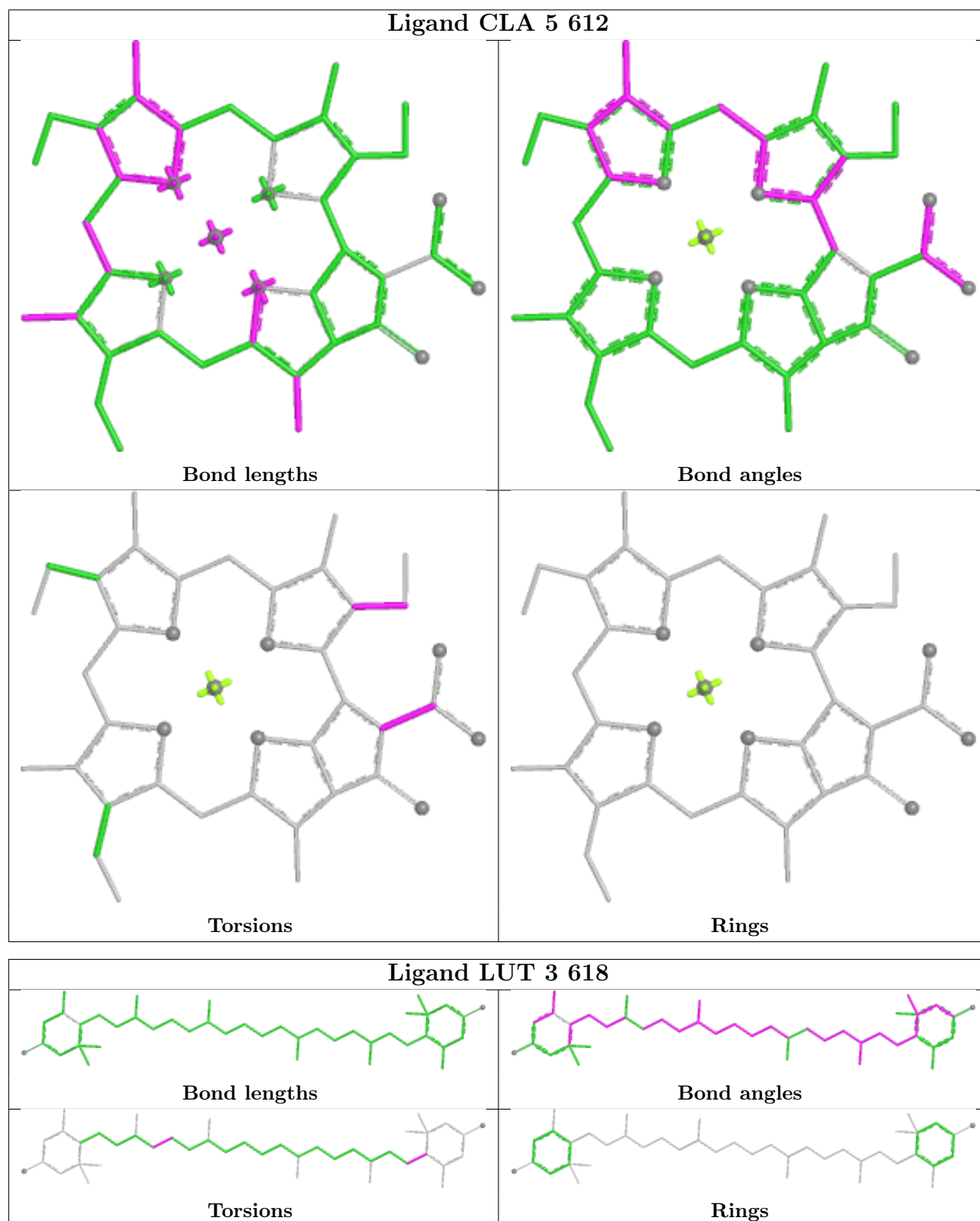
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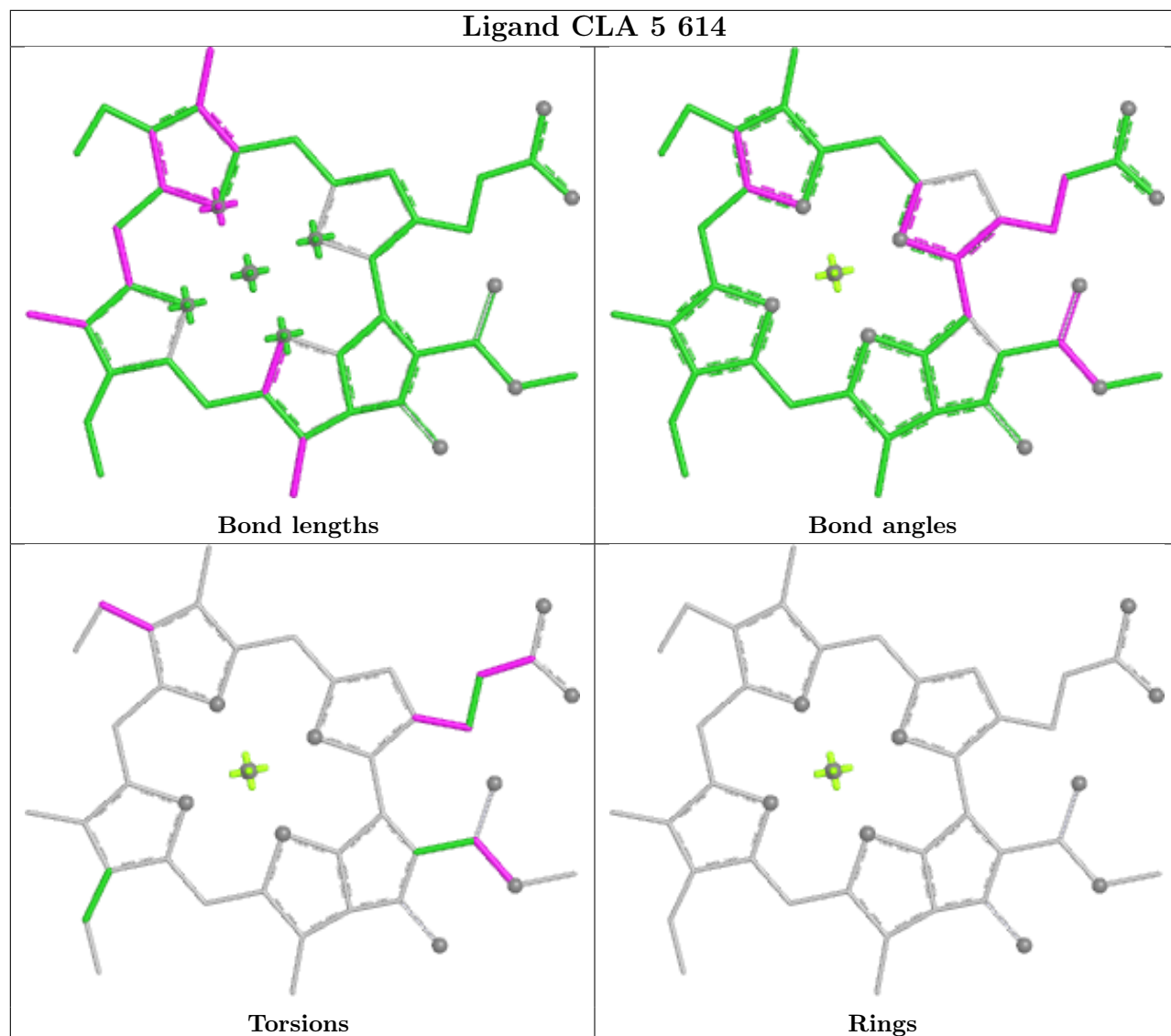
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	4	622	LHG	6	0
23	A	803	CLA	5	0
32	9	620	XAT	3	0
28	8	624	LMU	3	0
23	9	606	CLA	1	0
23	A	843	CLA	4	0
23	A	824	CLA	1	0
28	A	859	LMU	2	0
29	J	104	LMG	1	0
23	A	834	CLA	4	0
23	A	836	CLA	4	0
26	B	801	BCR	4	0
23	6	612	CLA	1	0
23	B	833	CLA	2	0
23	A	817	CLA	1	0
23	B	826	CLA	2	0
23	5	607	CLA	5	0
23	J	101	CLA	2	0
23	1	607	CLA	1	0
23	5	610	CLA	5	0
23	A	813	CLA	2	0
23	B	838	CLA	3	0
23	7	616	CLA	1	0
32	1	618	XAT	4	0
23	A	845	CLA	1	0
26	3	620	BCR	3	0
23	4	610	CLA	2	0
23	5	611	CLA	1	0
26	L	301	BCR	2	0
25	2	622	LHG	1	0
23	B	823	CLA	1	0
32	a	618	XAT	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

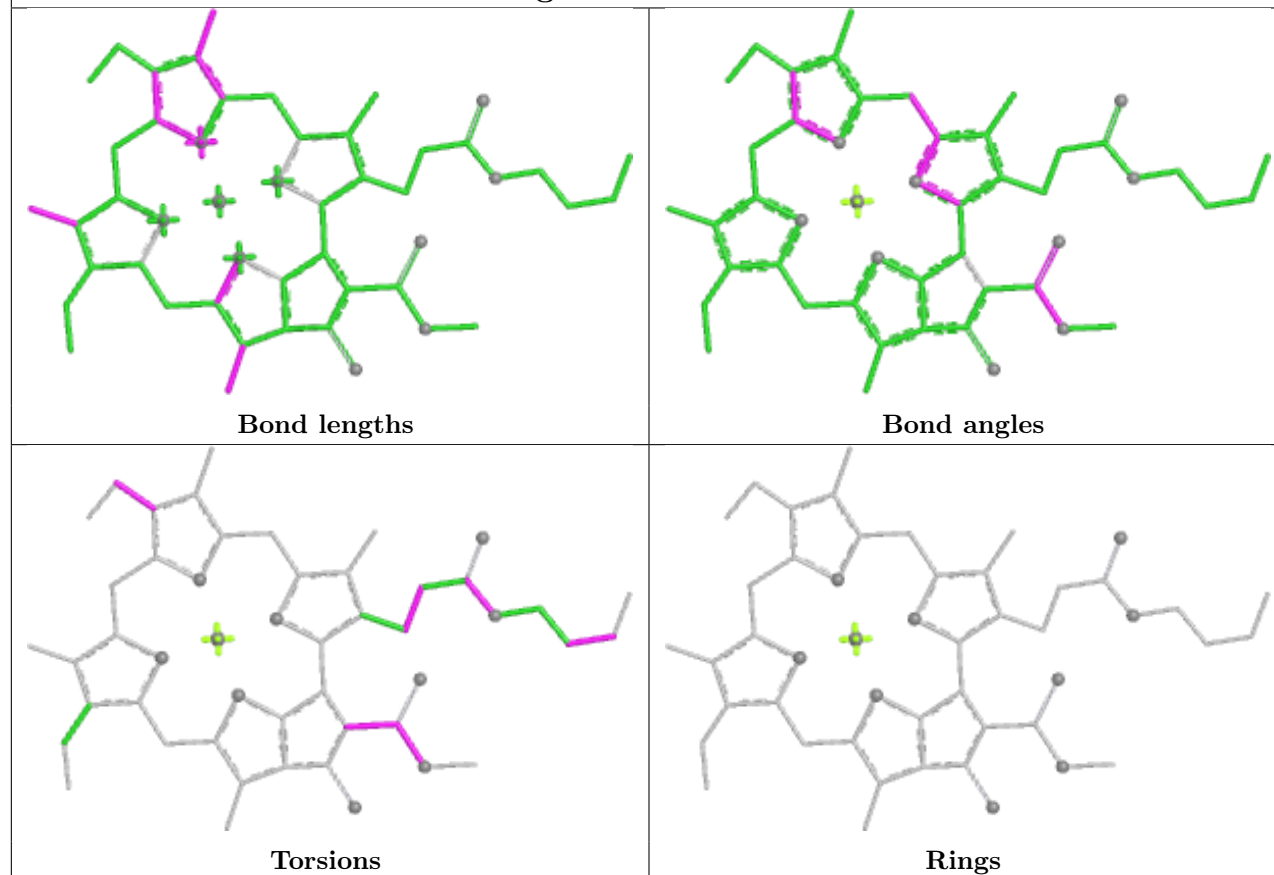
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



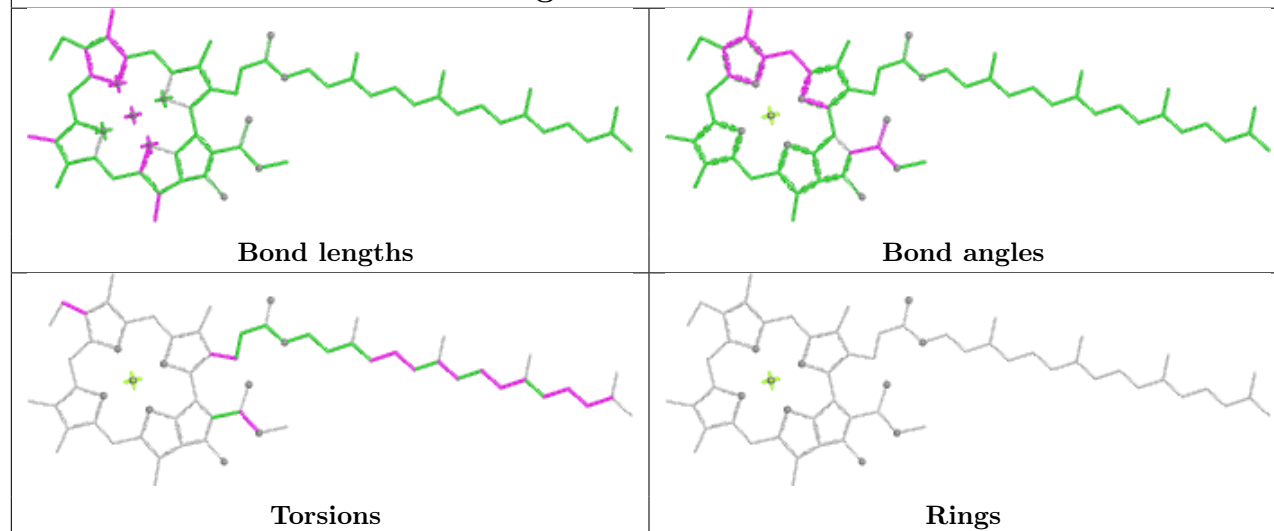
Ligand CLA 5 614

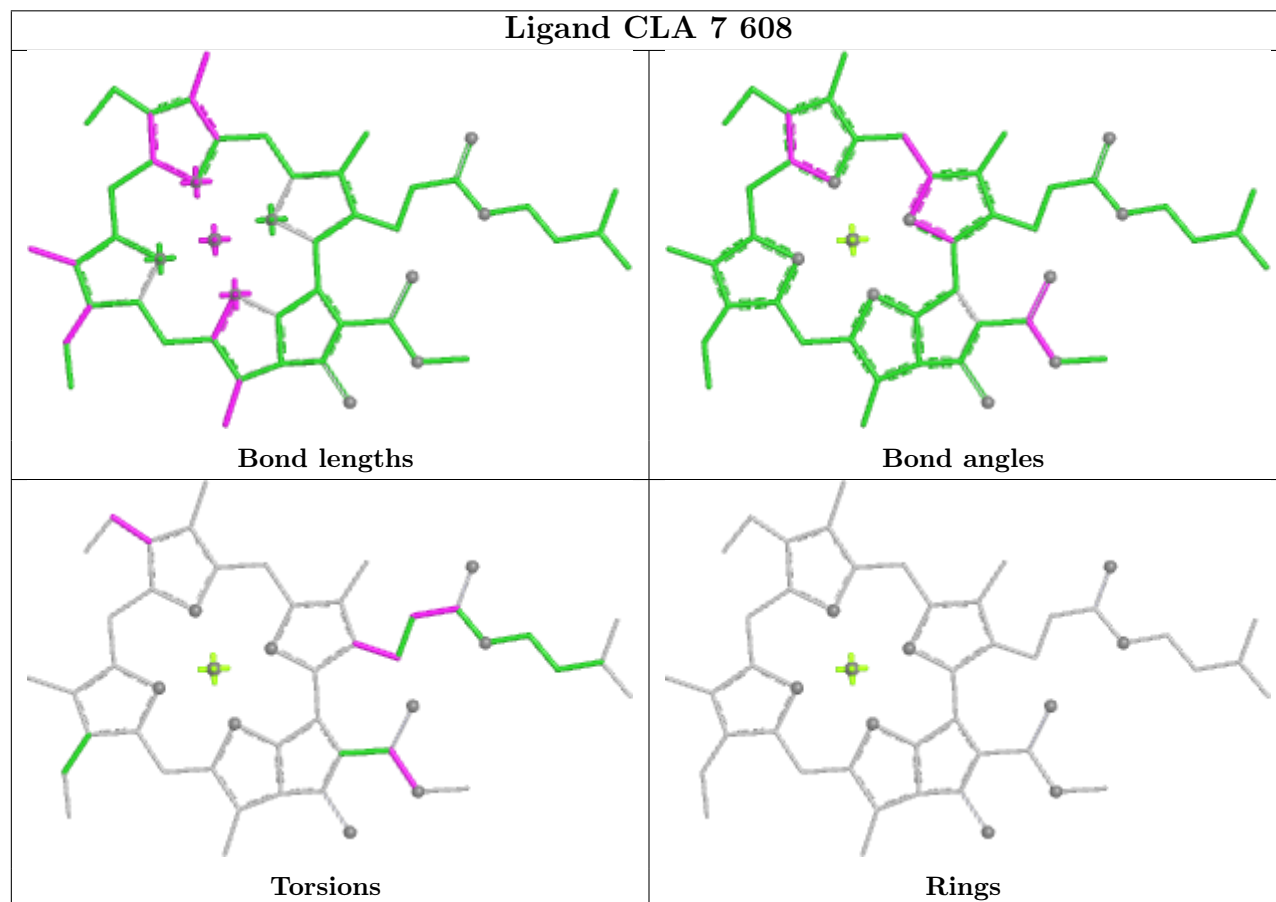
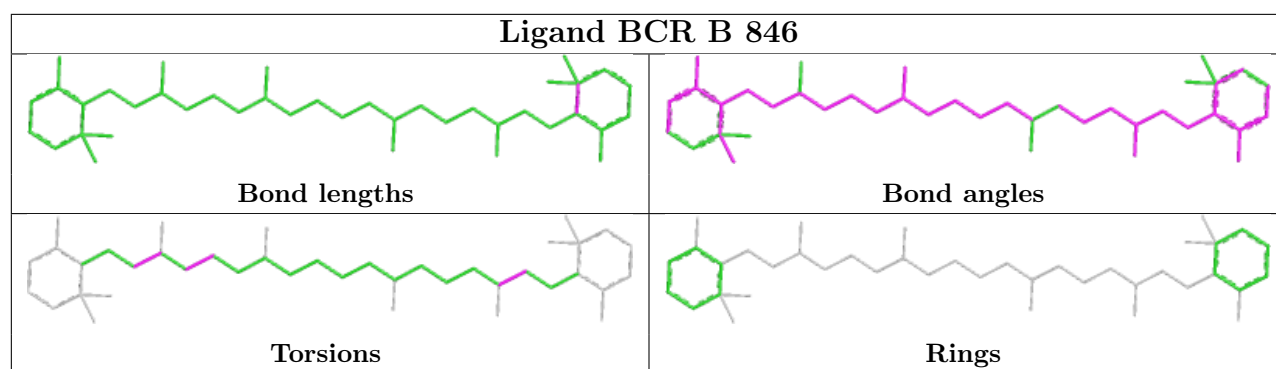


Ligand CLA 1 604

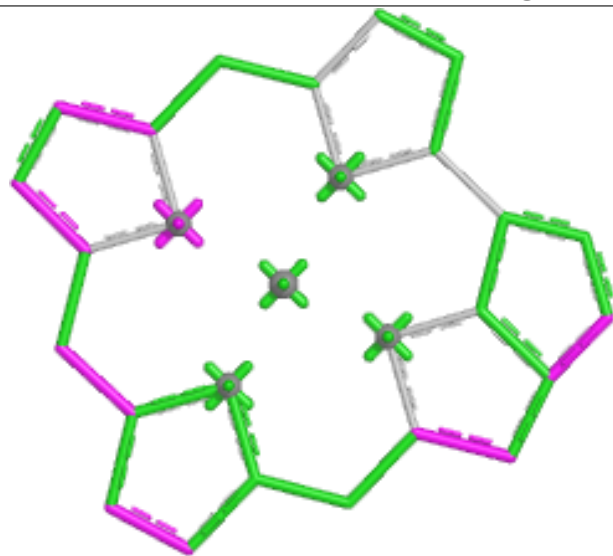


Ligand CLA 8 606

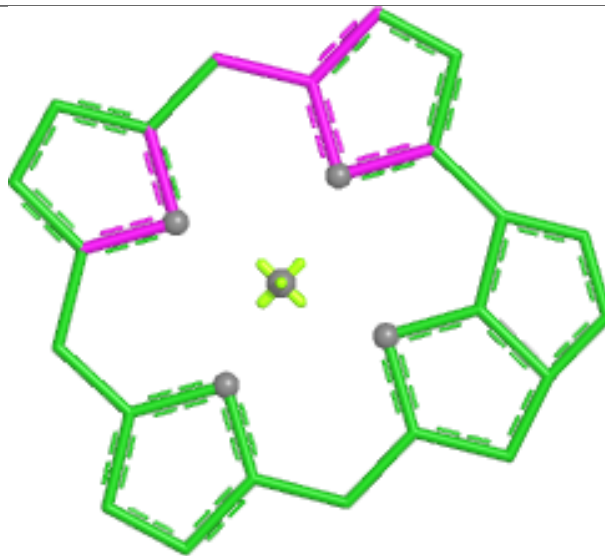




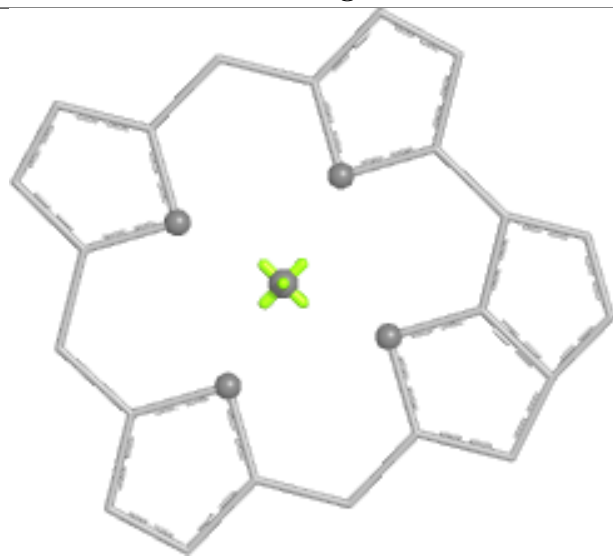
Ligand CLA 2 607



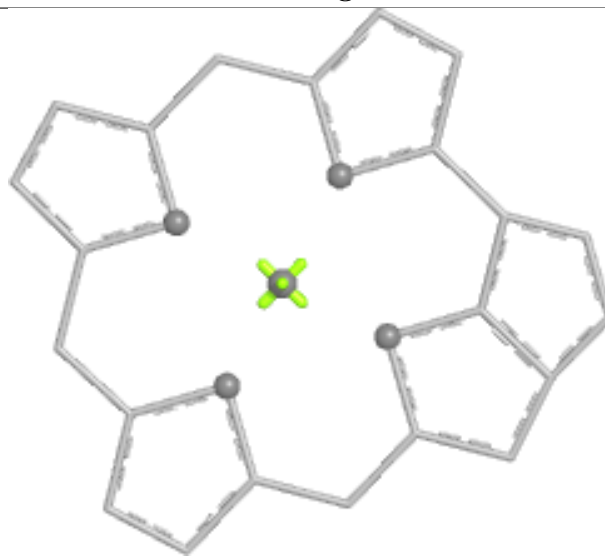
Bond lengths



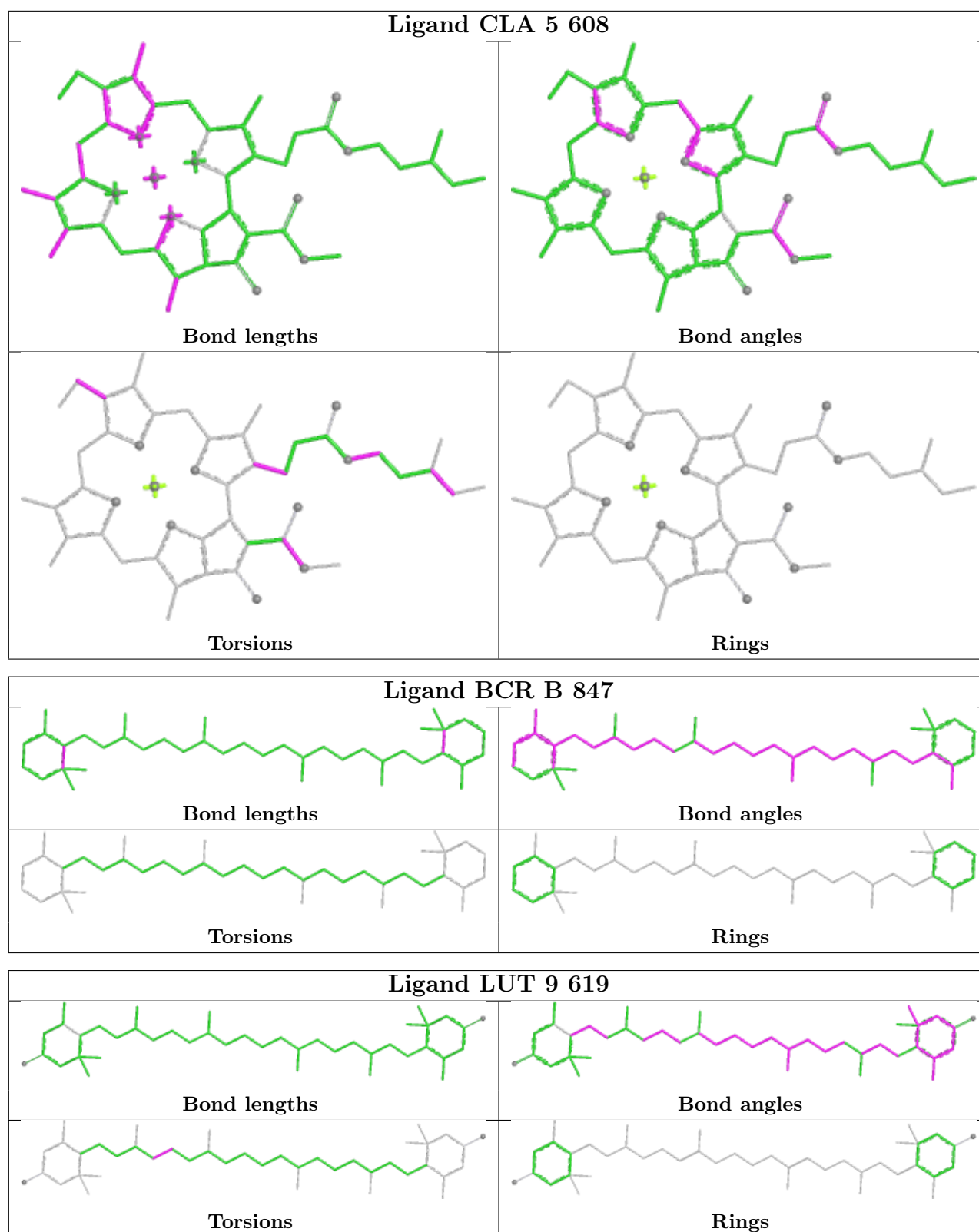
Bond angles

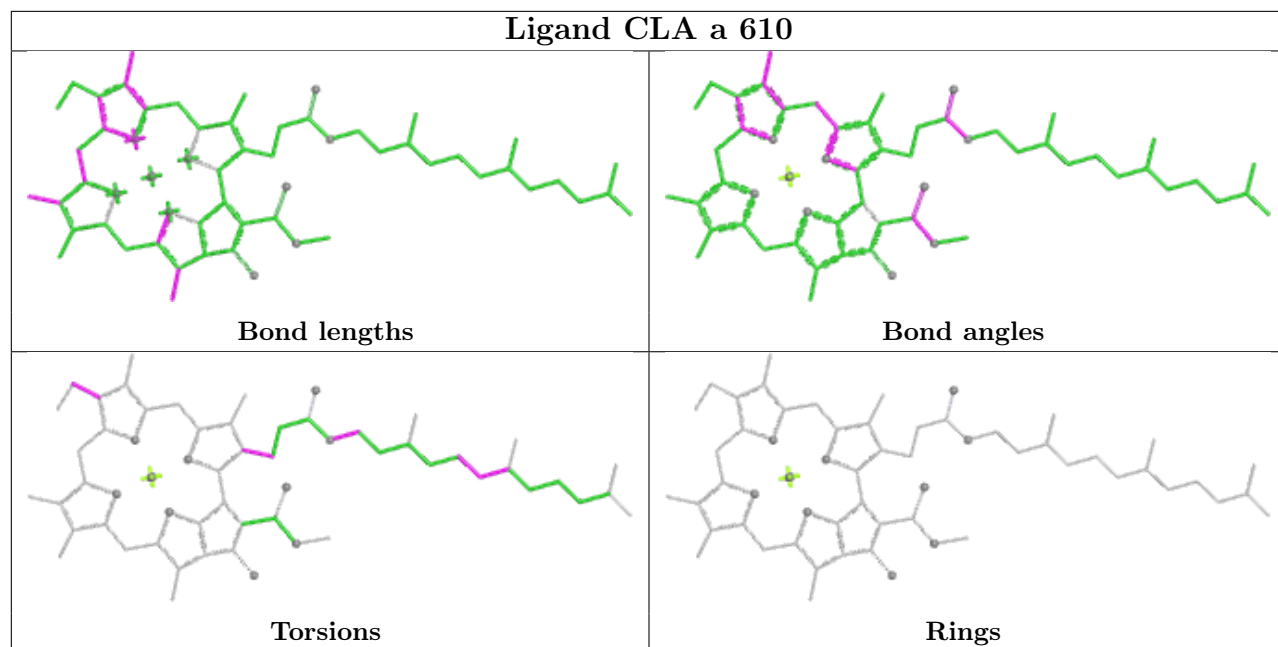


Torsions

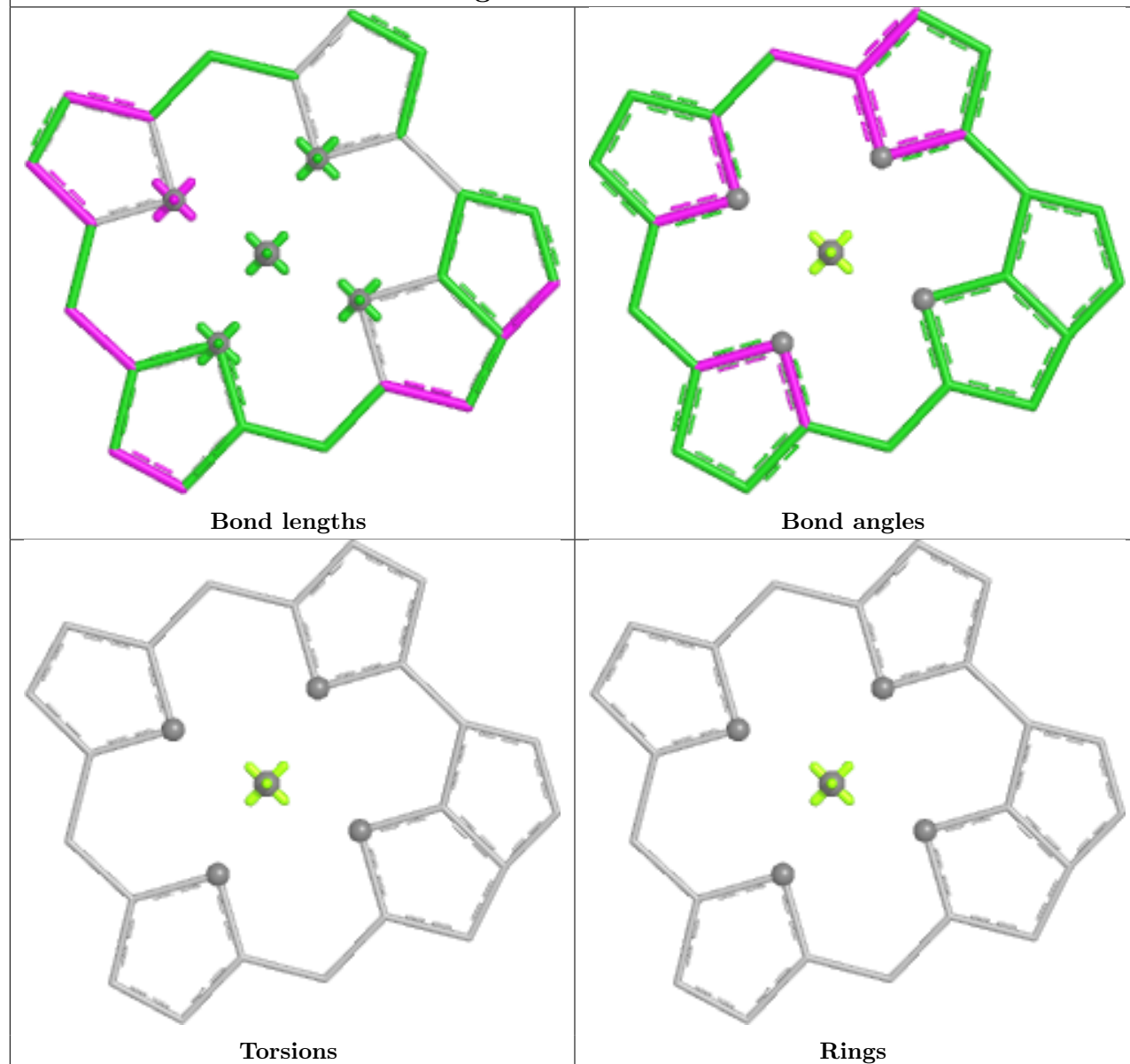


Rings

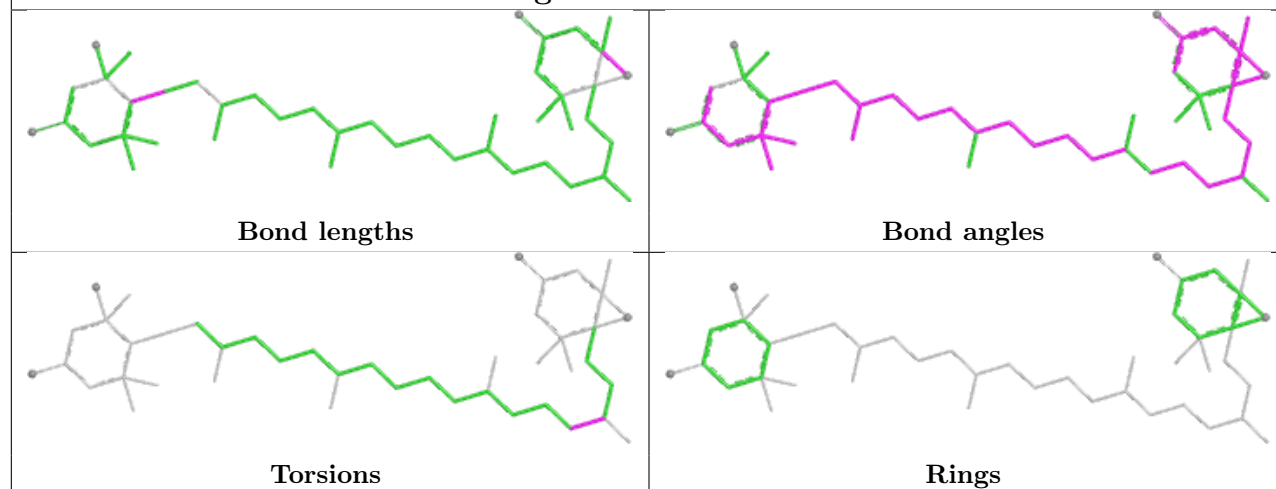


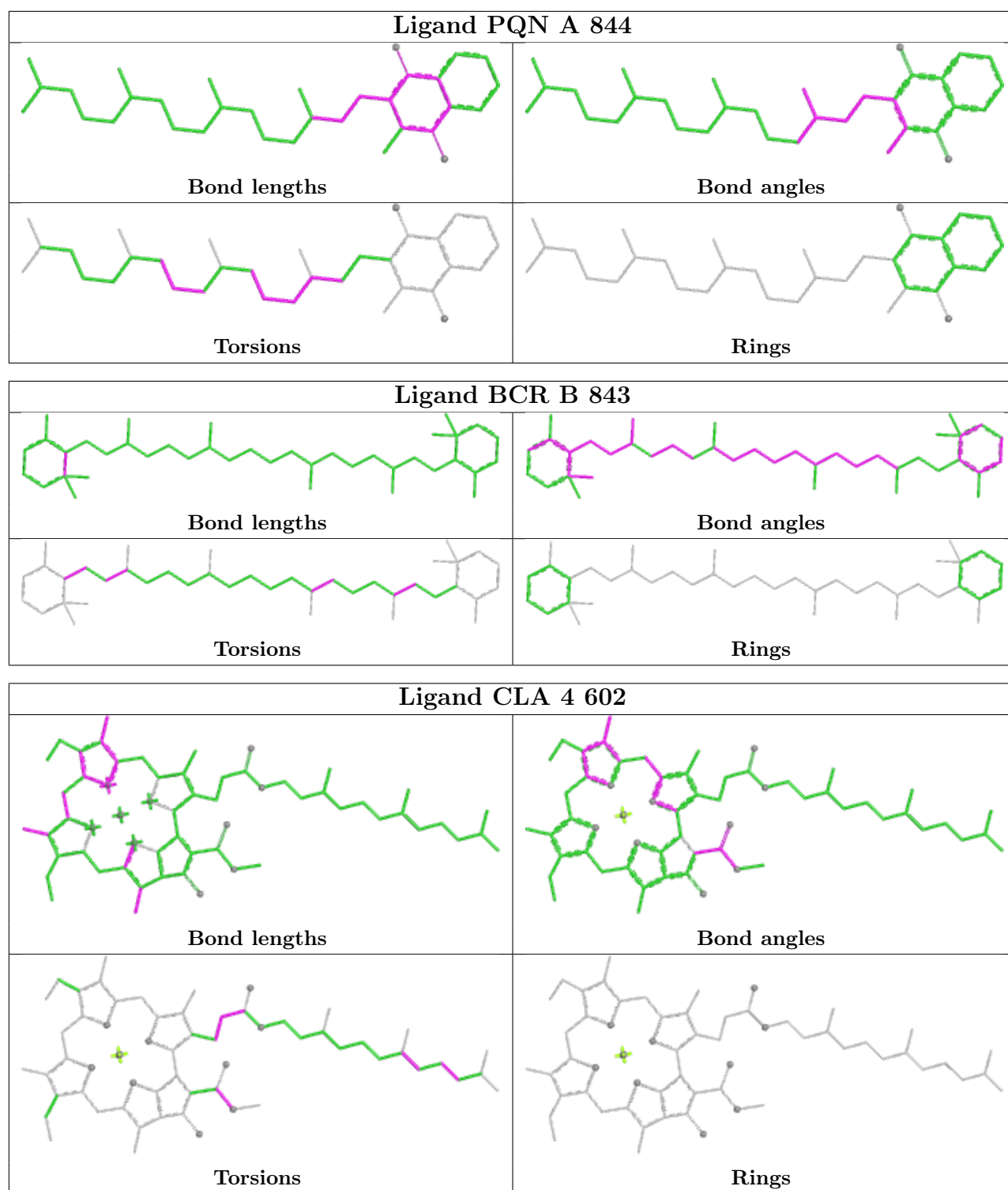


Ligand CLA 2 614

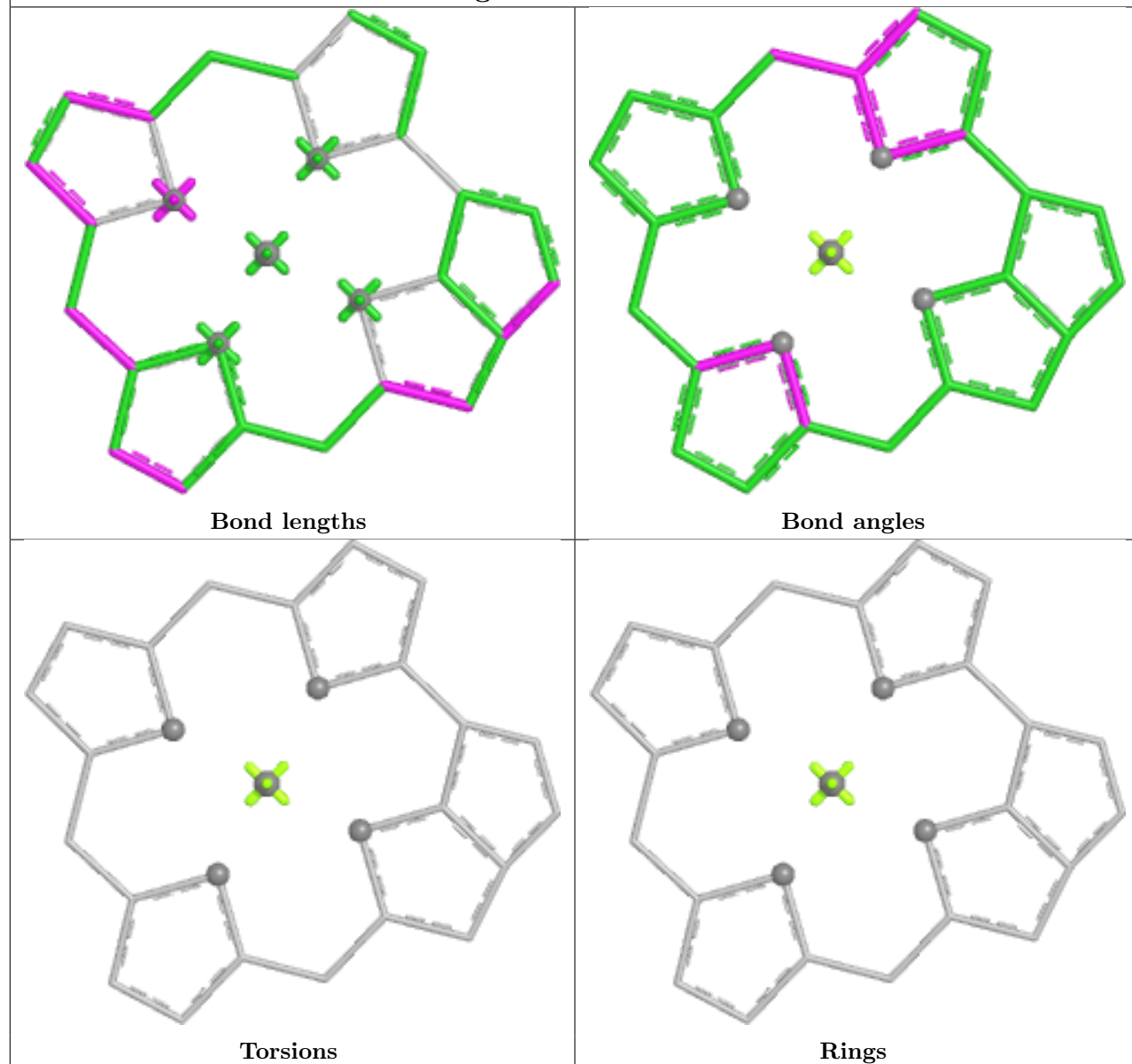


Ligand NEX 5 624

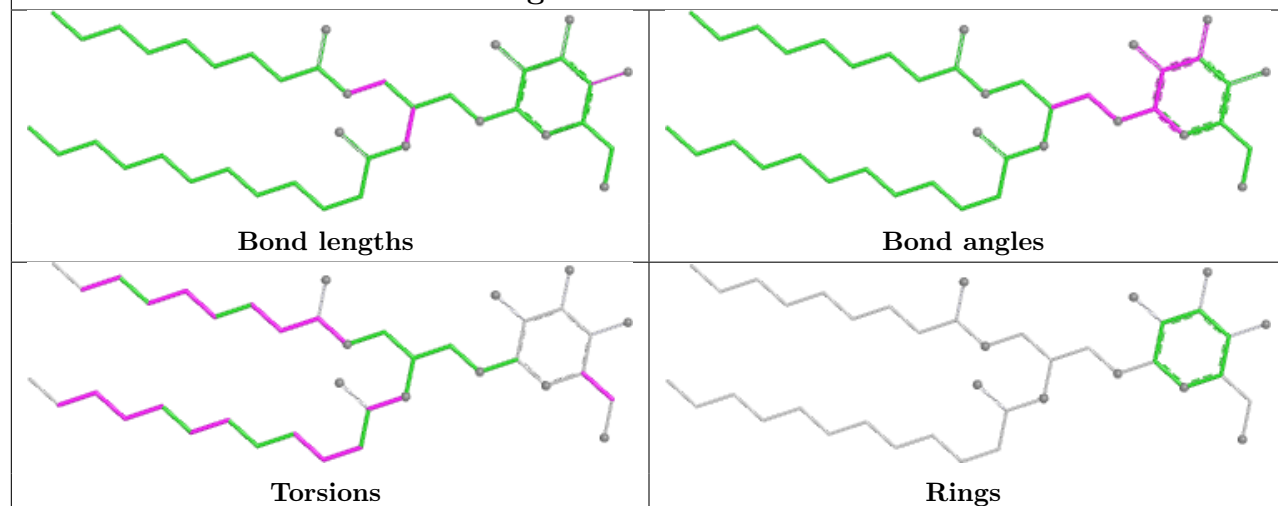


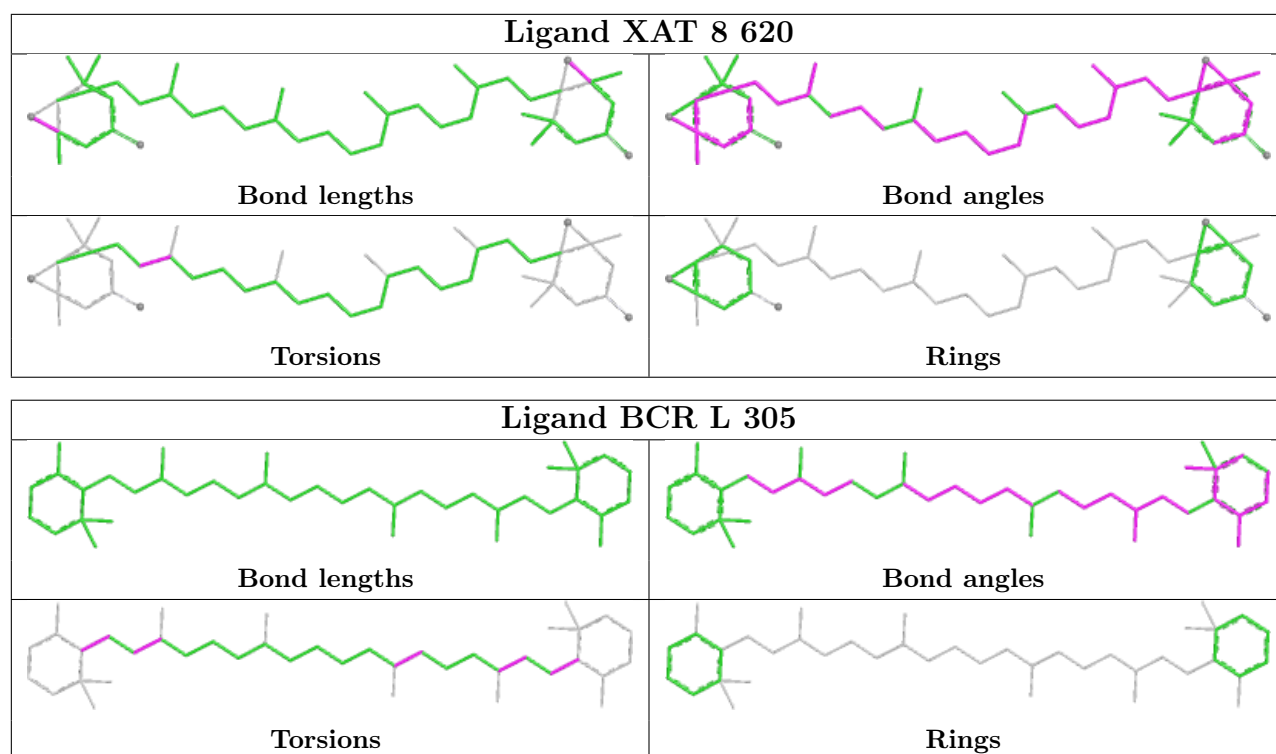


Ligand CLA 9 610

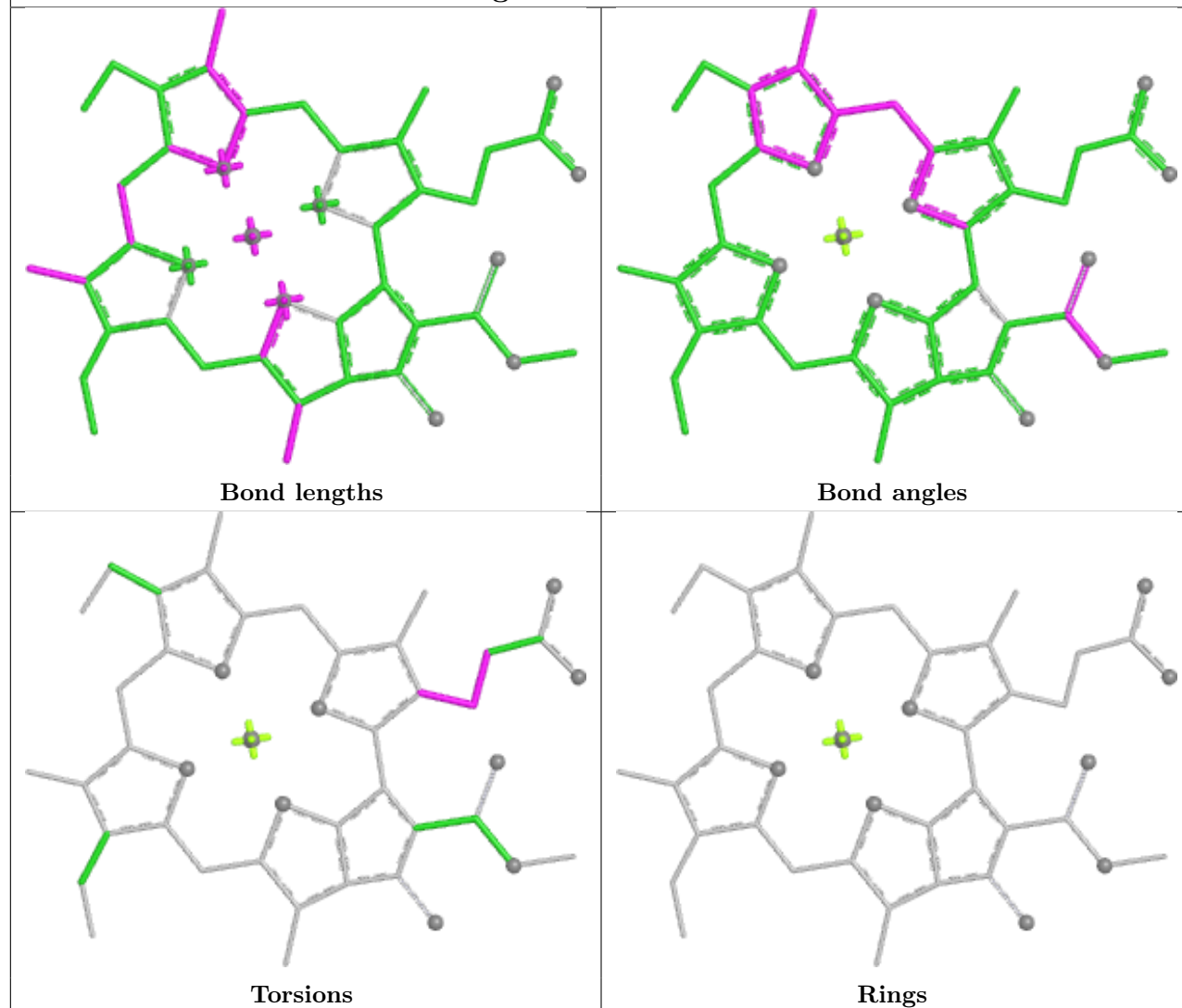


Ligand LMG A 860

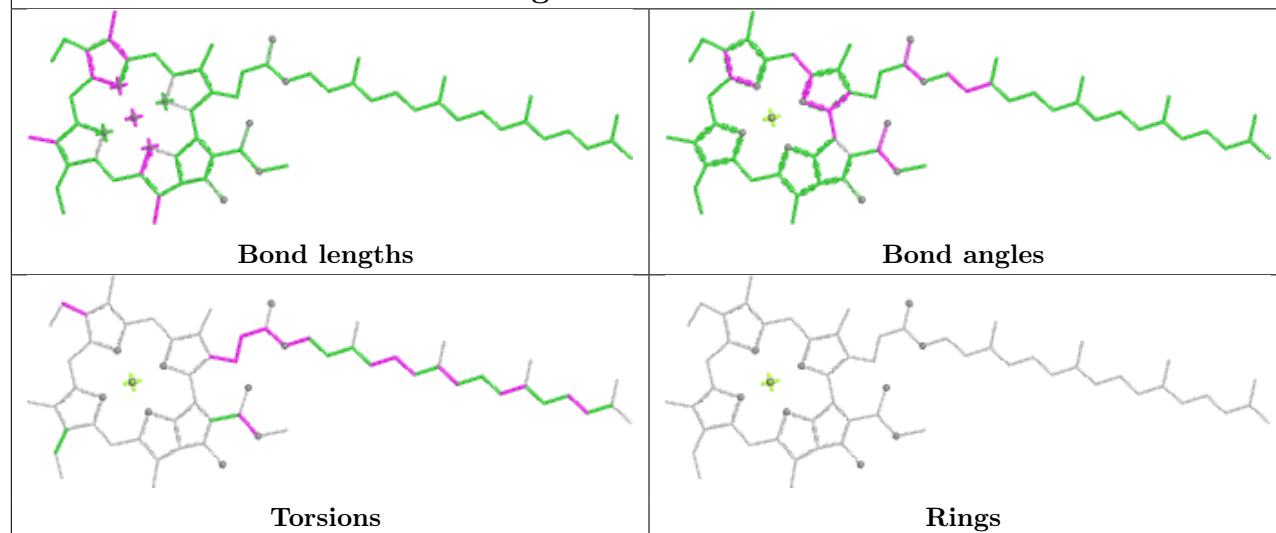




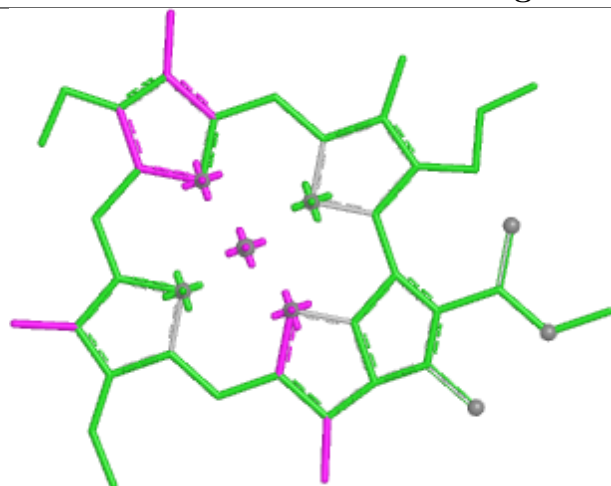
Ligand CLA A 833



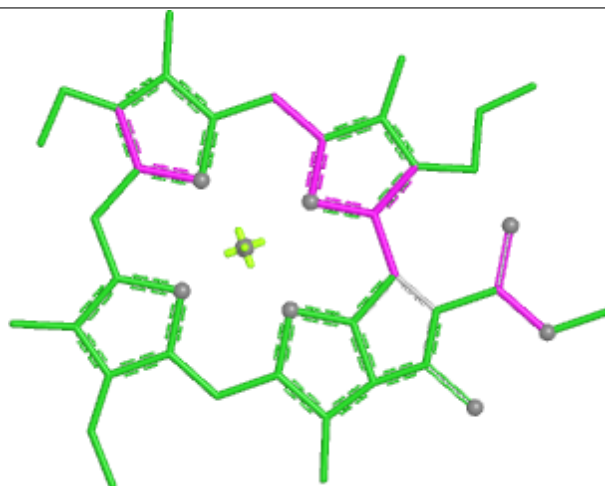
Ligand CLA A 841



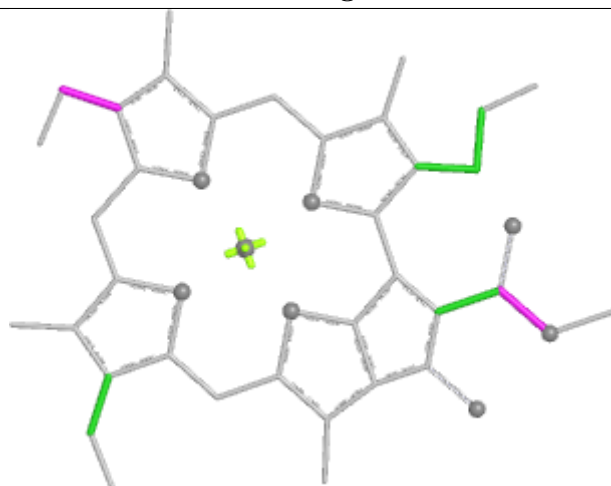
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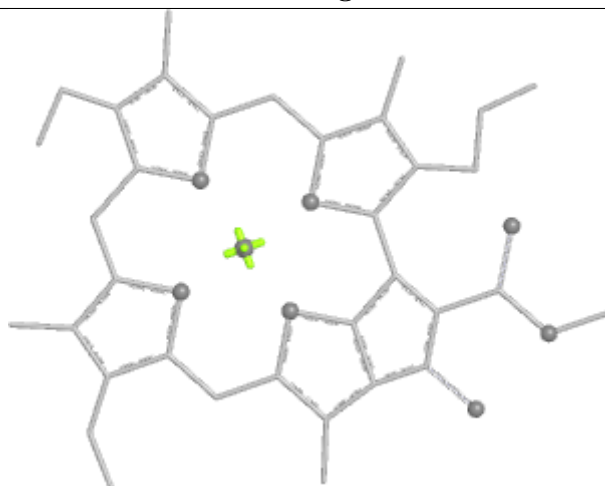
Bond lengths



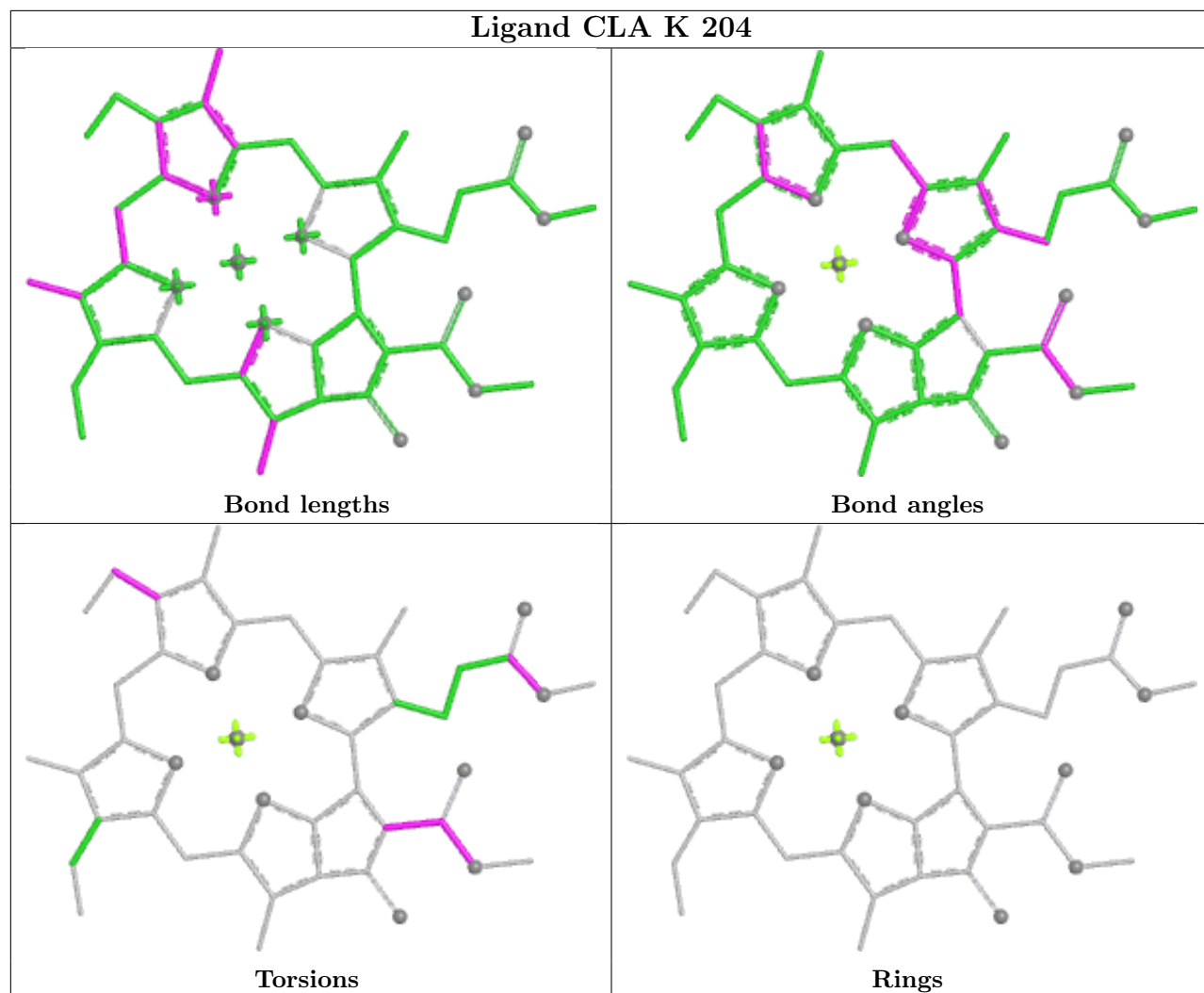
Bond angles



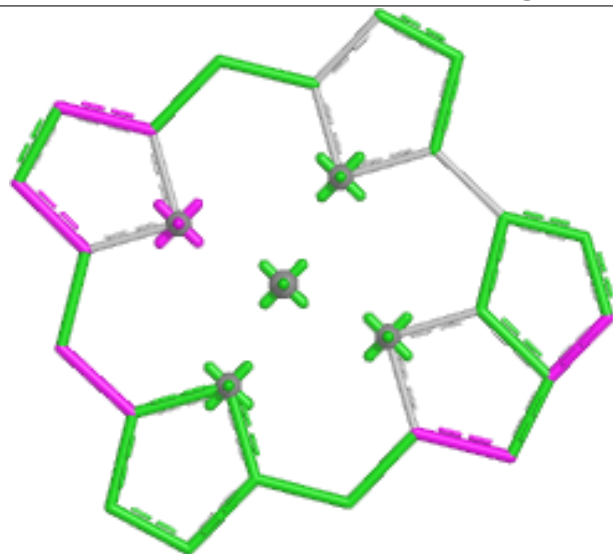
Torsions



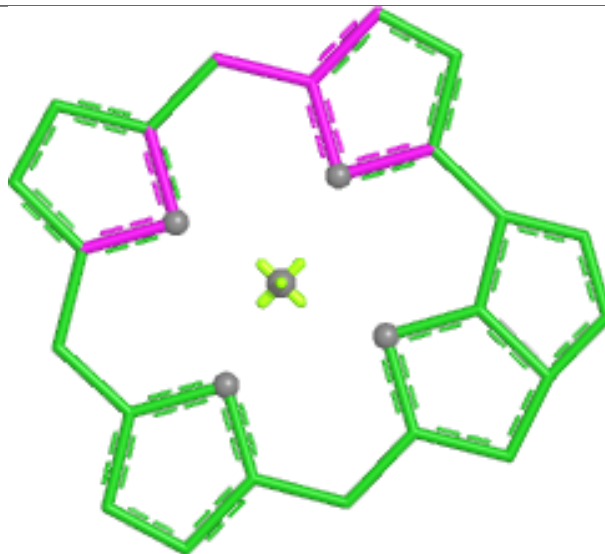
Rings



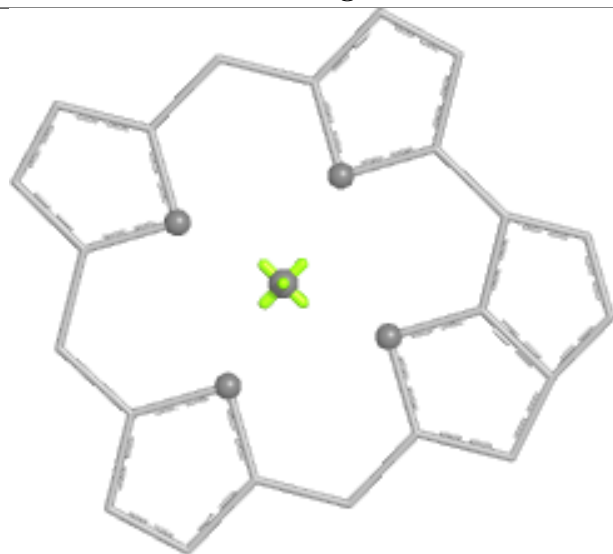
Ligand CLA 2 612



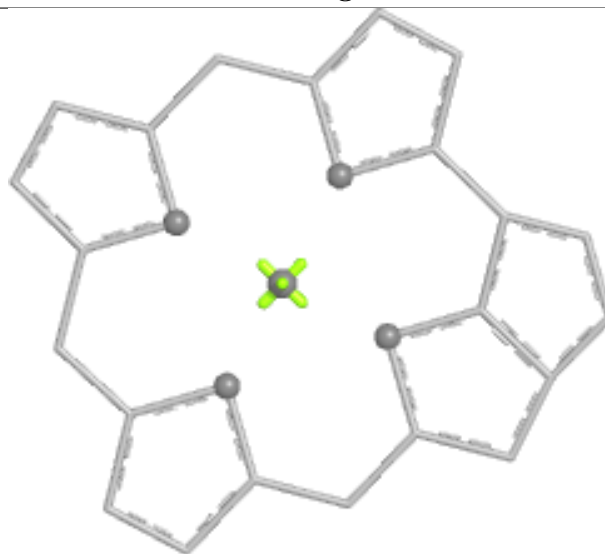
Bond lengths



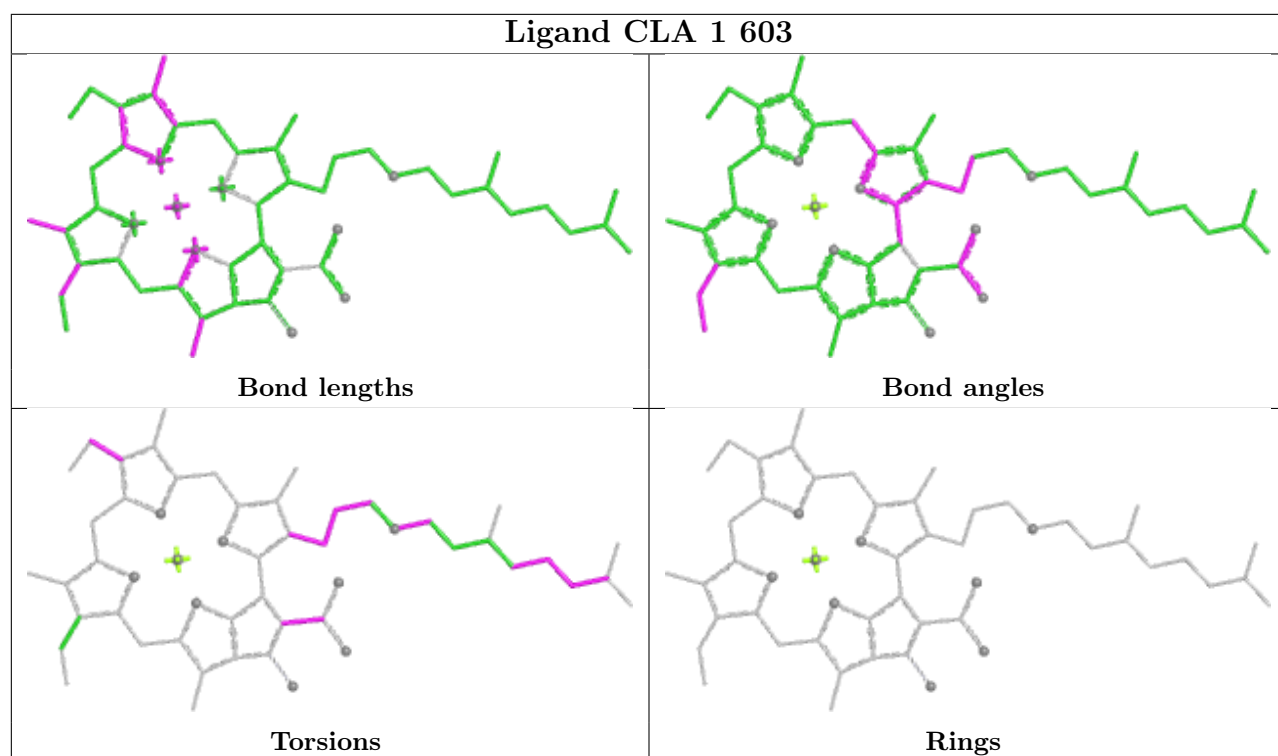
Bond angles

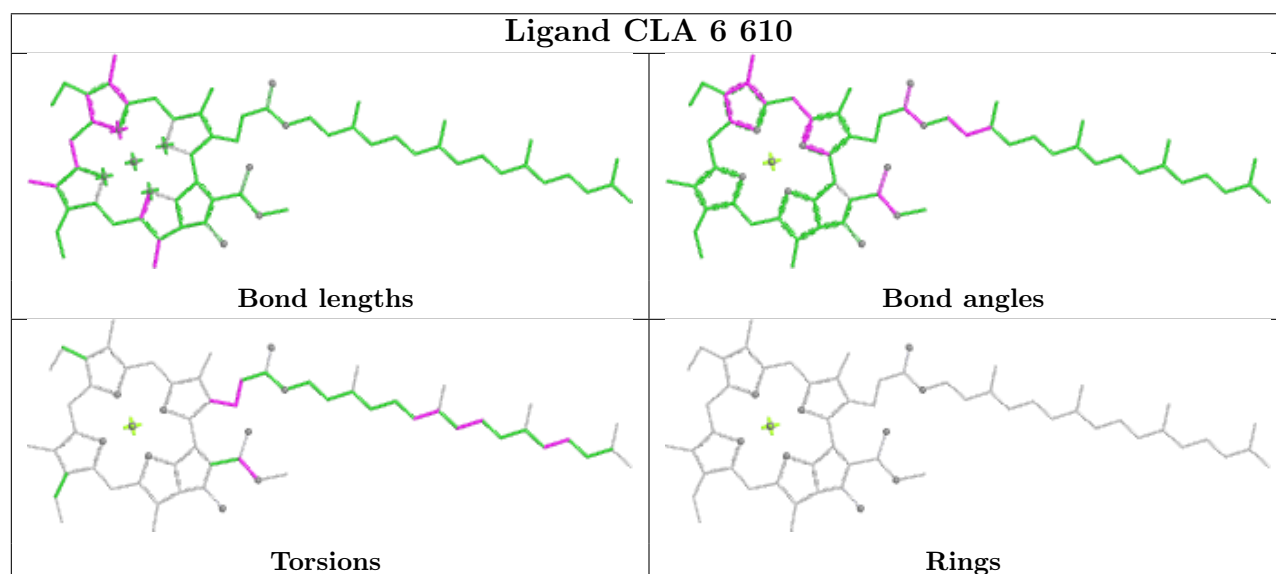
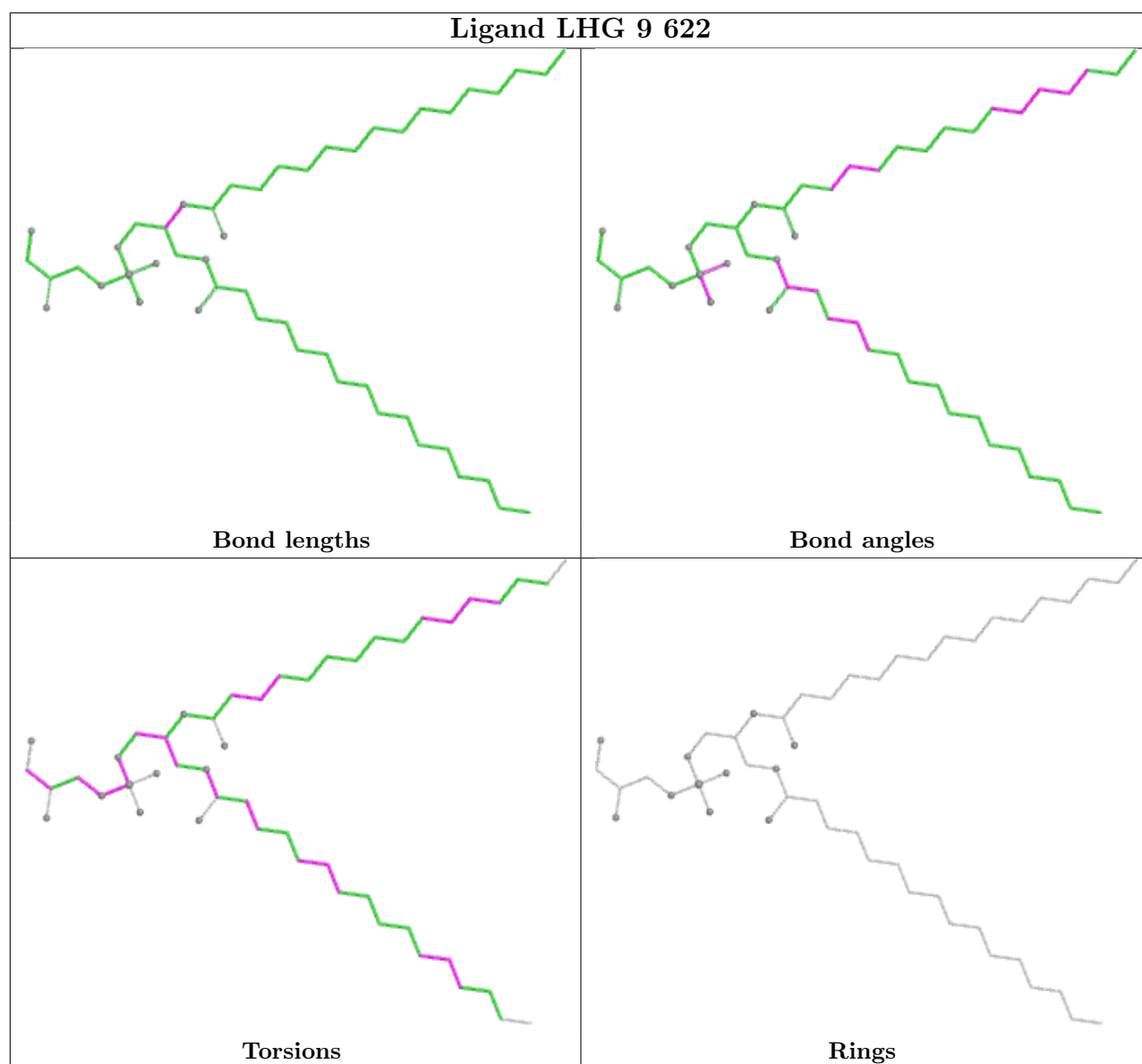


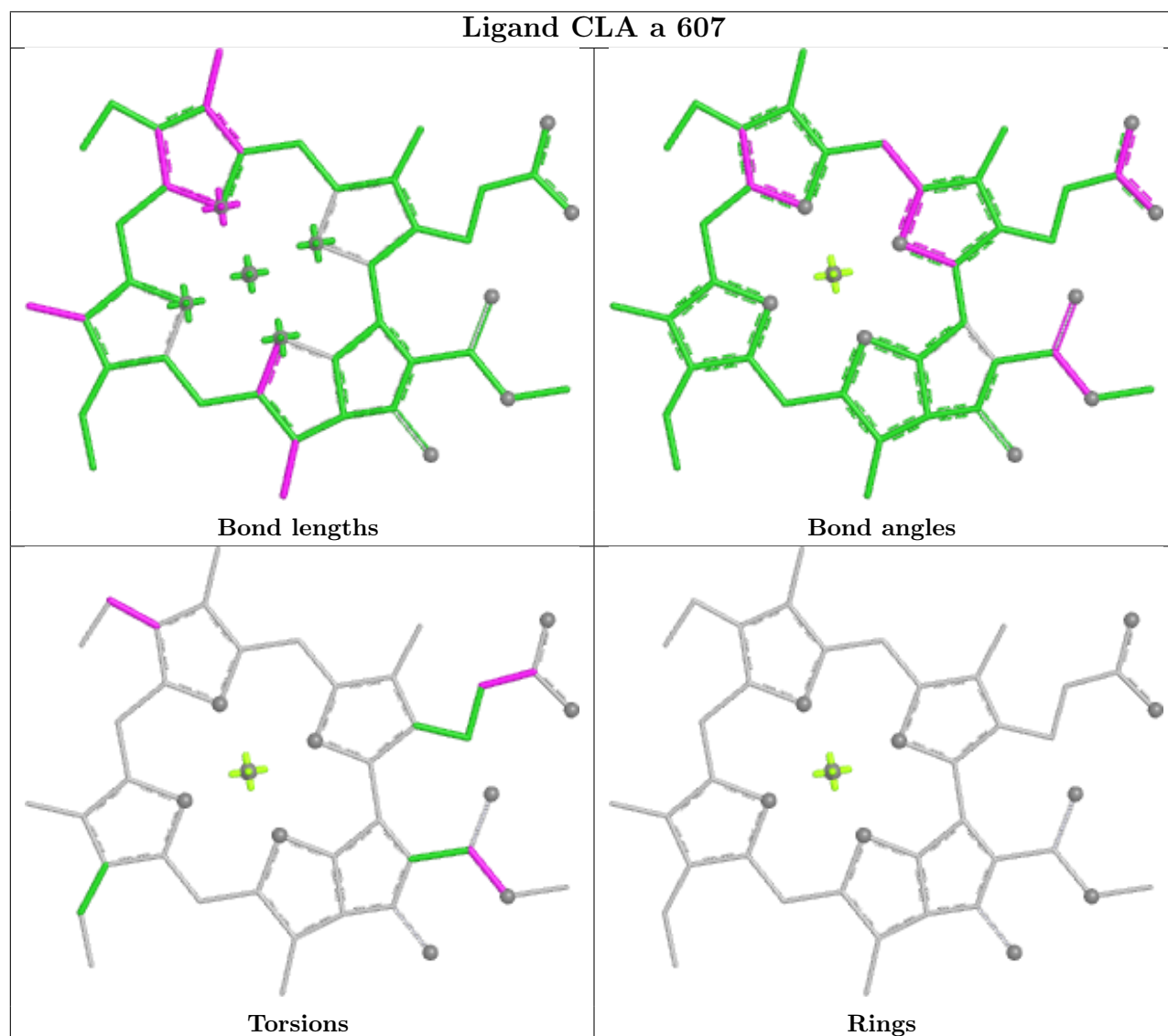
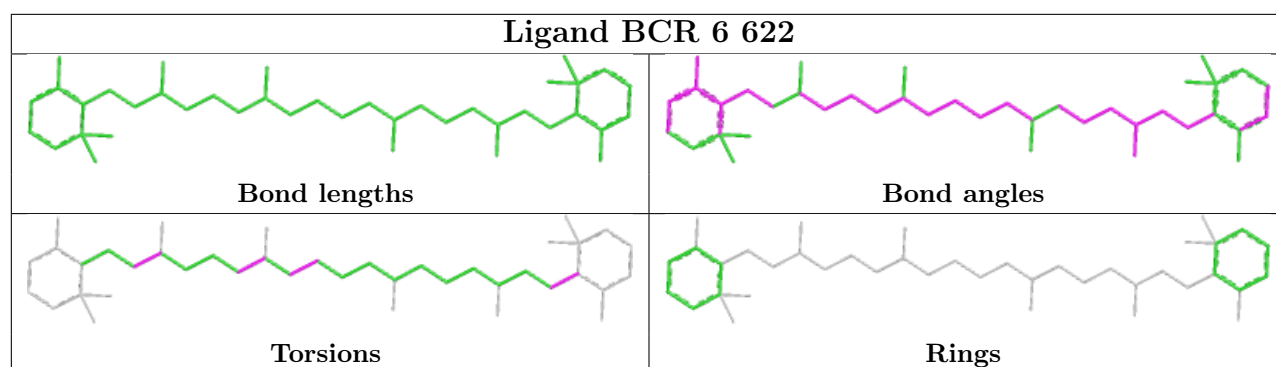
Torsions



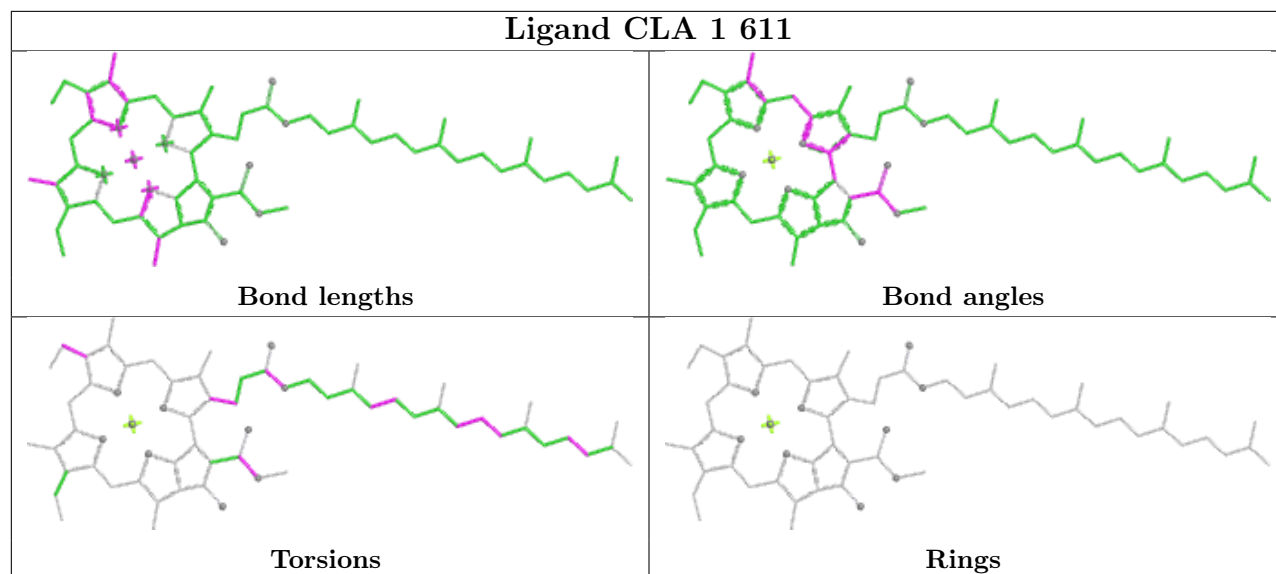
Rings



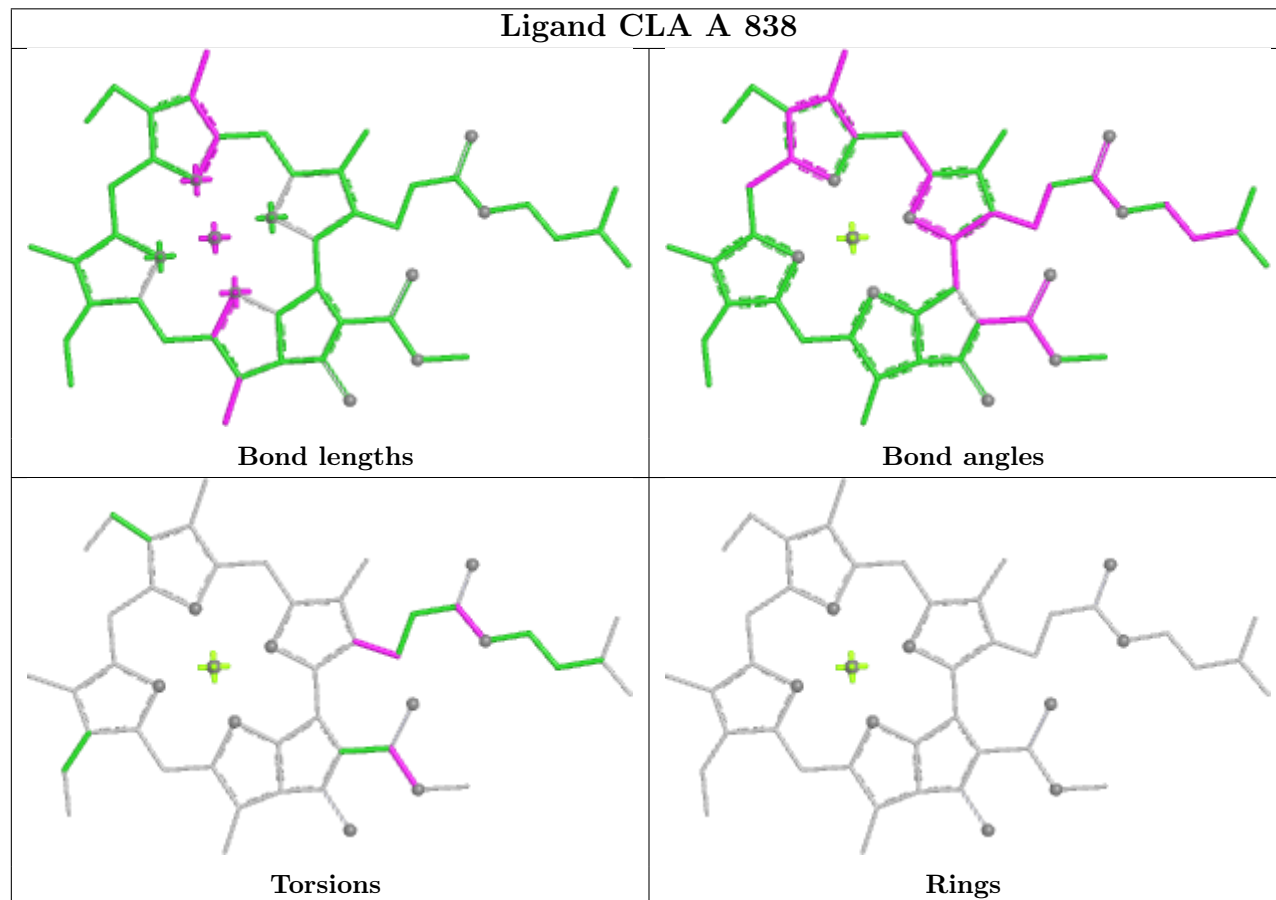




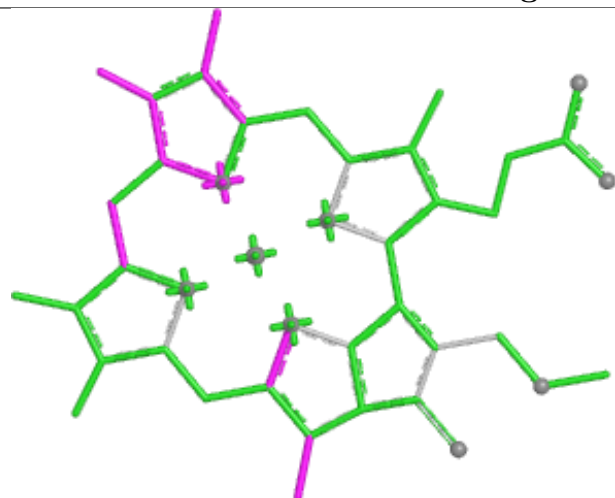
Ligand CLA 1 611



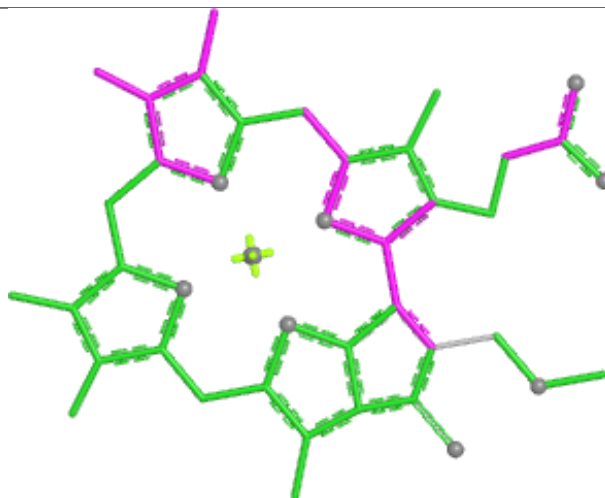
Ligand CLA A 838



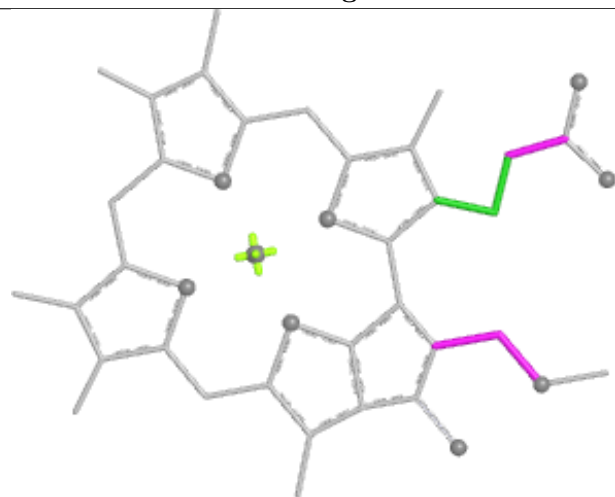
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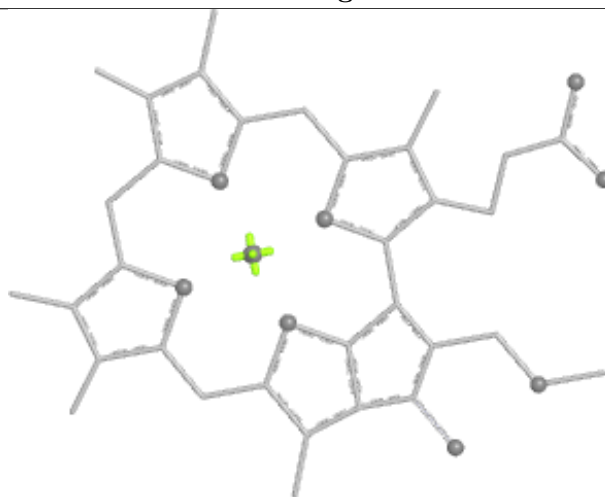
Bond lengths



Bond angles

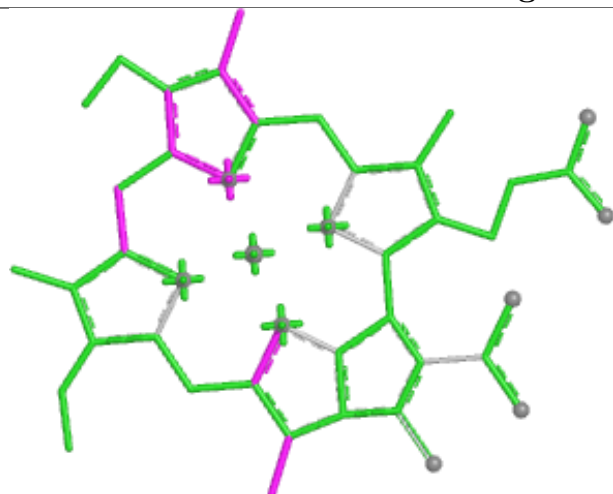


Torsions

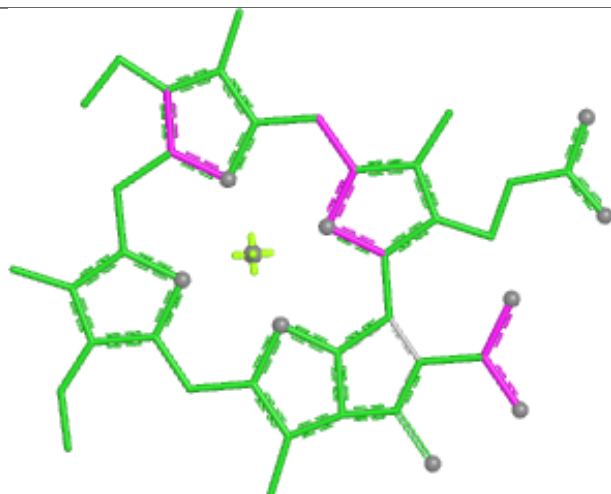


Rings

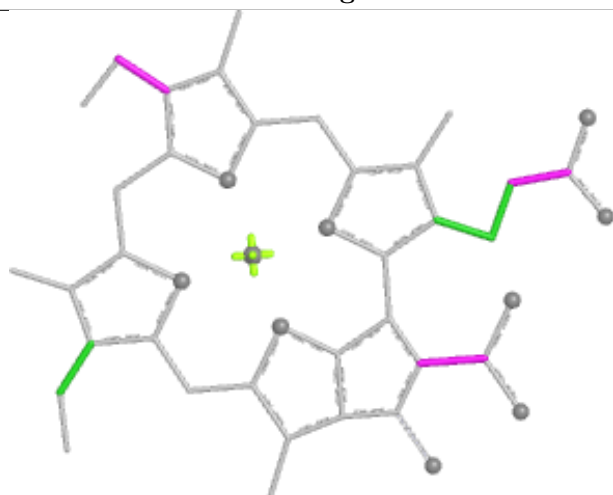
Ligand CLA a 608



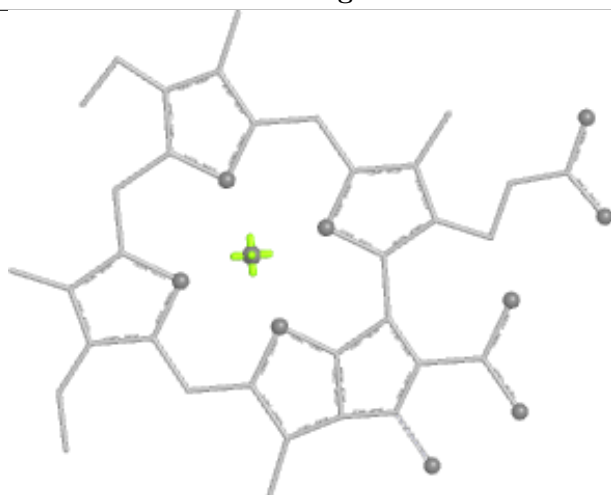
Bond lengths



Bond angles

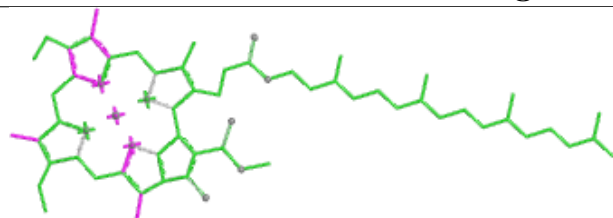


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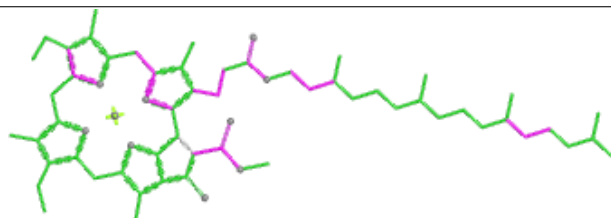


Rings

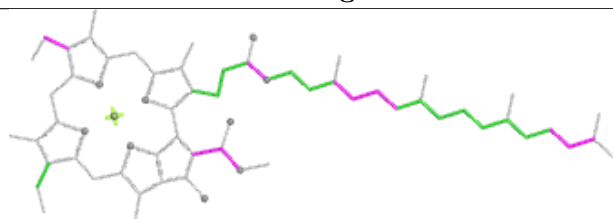
Ligand CLA B 808



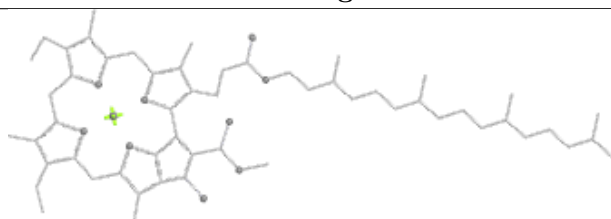
Bond lengths



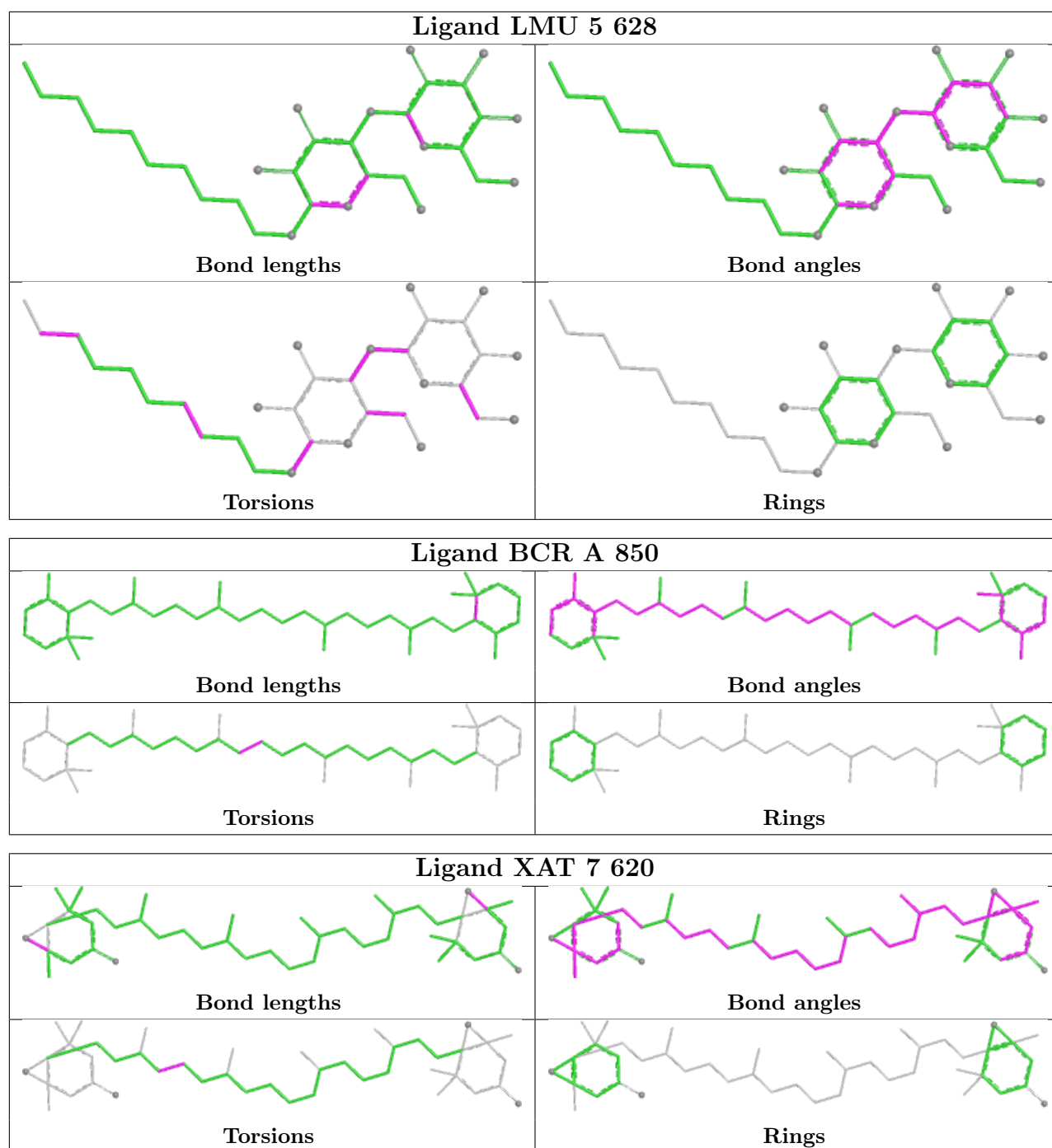
Bond angles

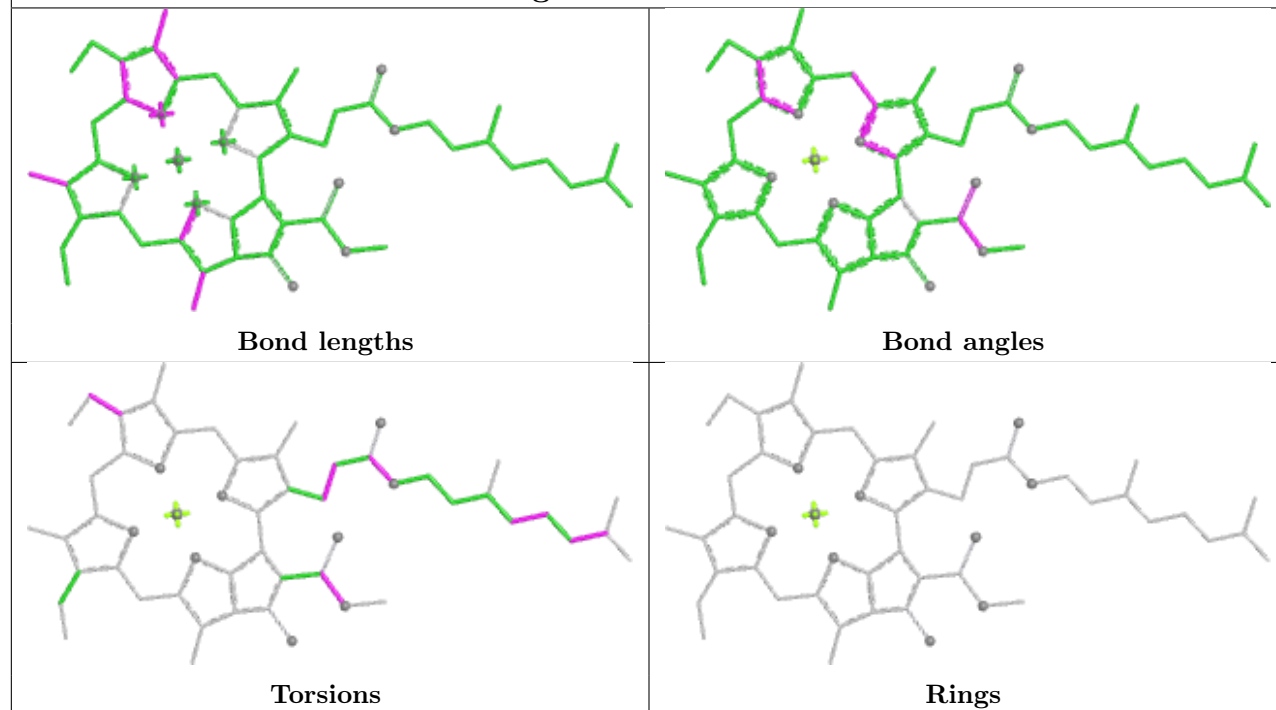
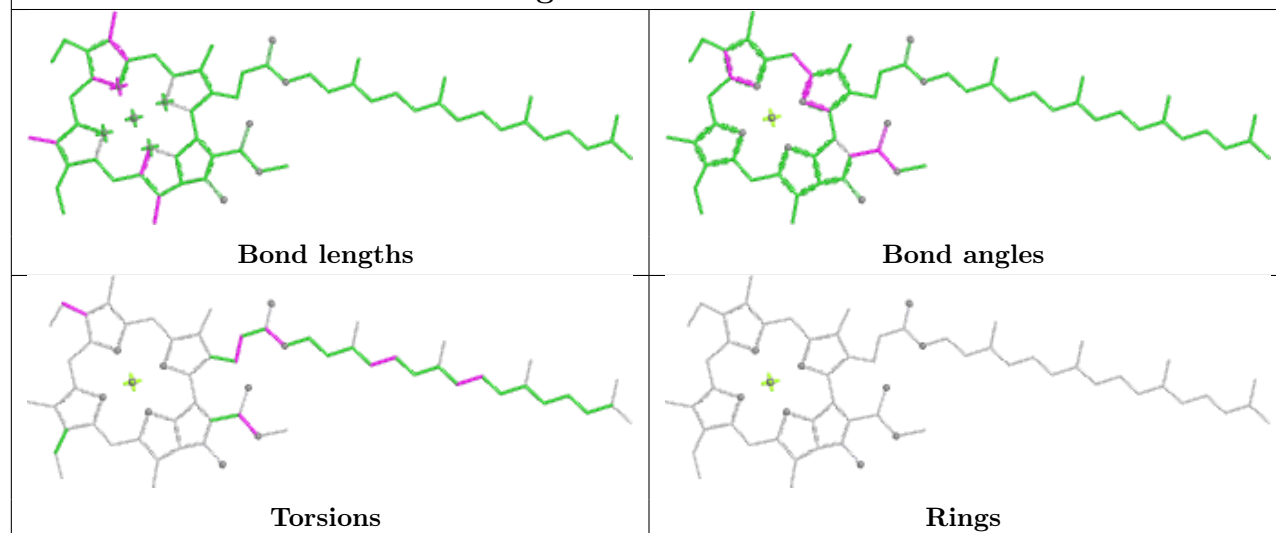


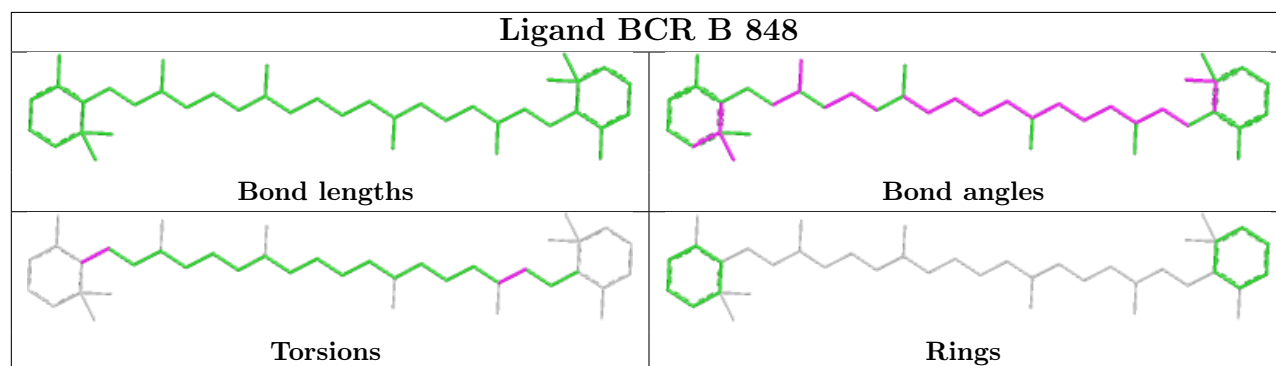
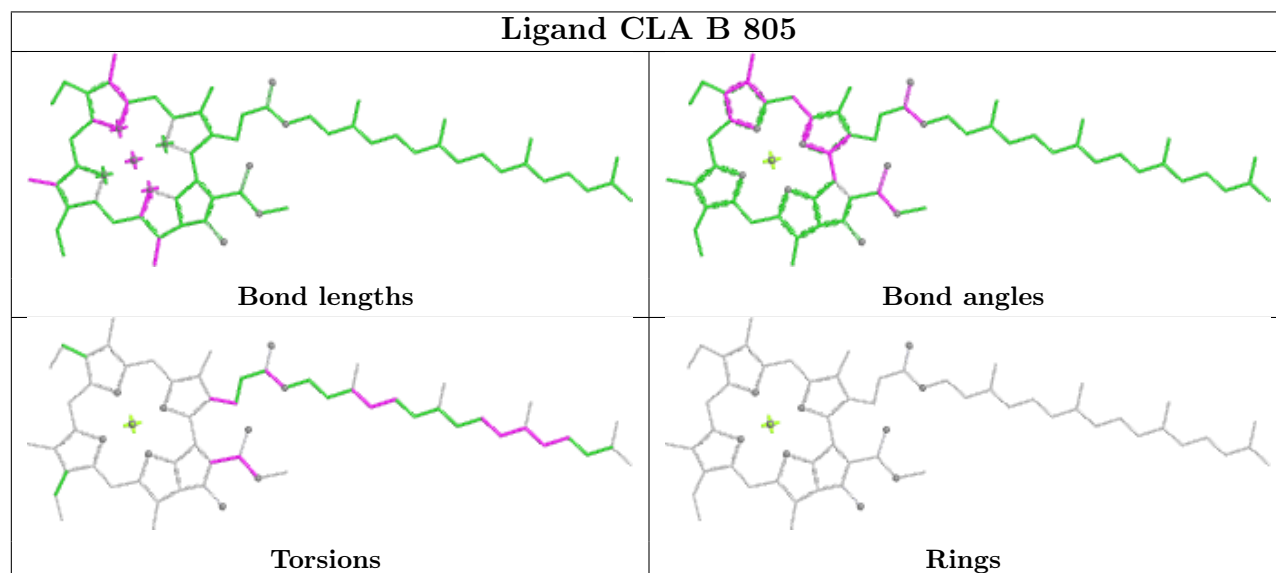
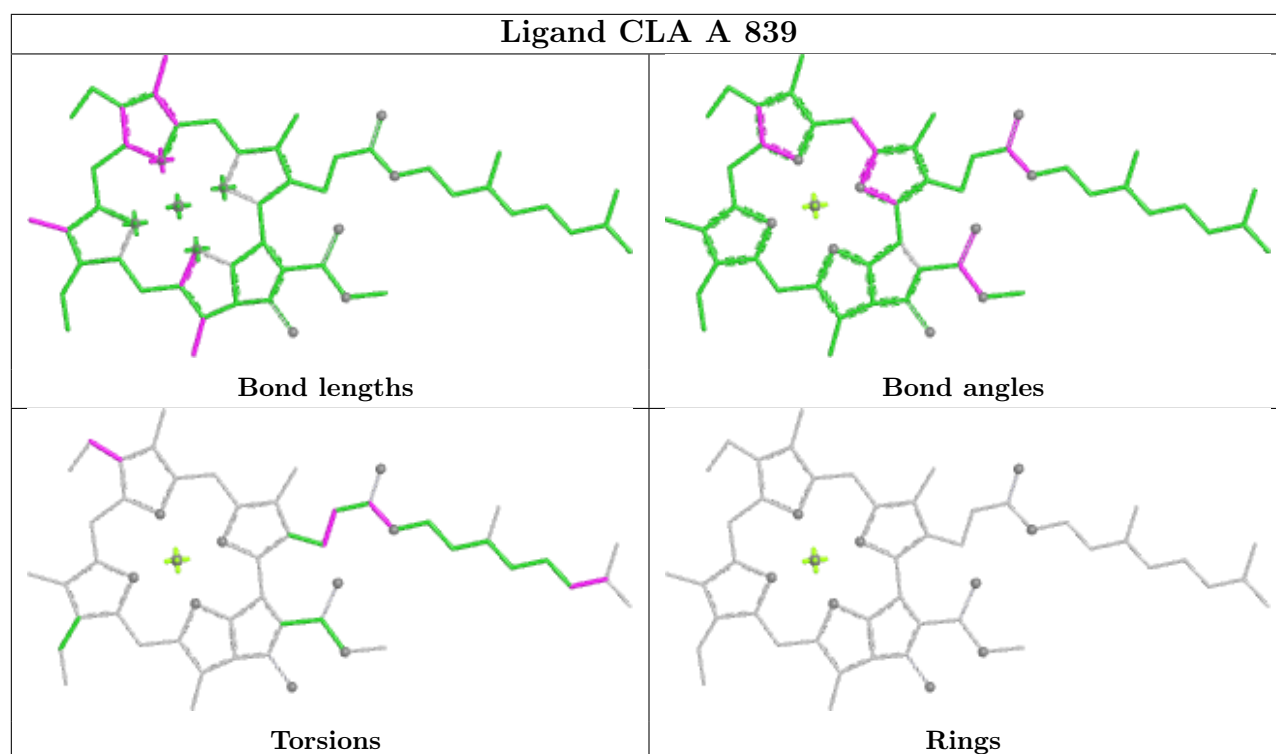
Torsions



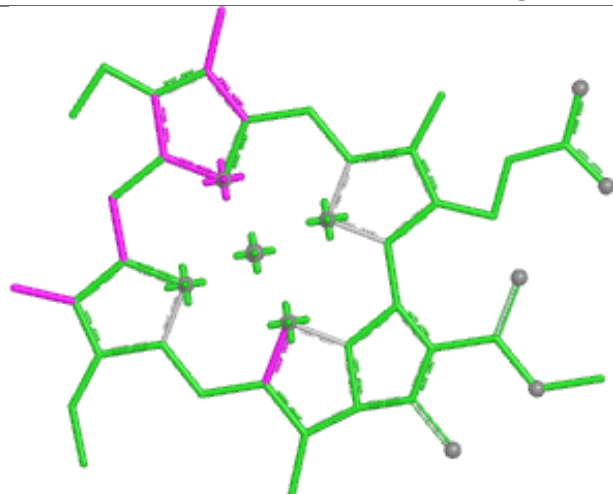
Rings



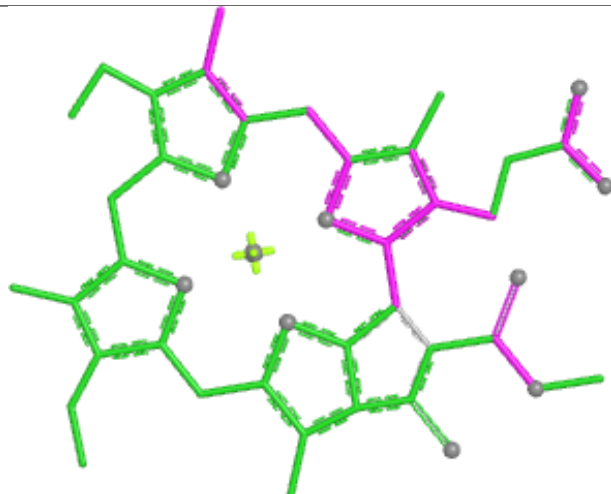
Ligand CLA B 819**Ligand CLA 6 602**



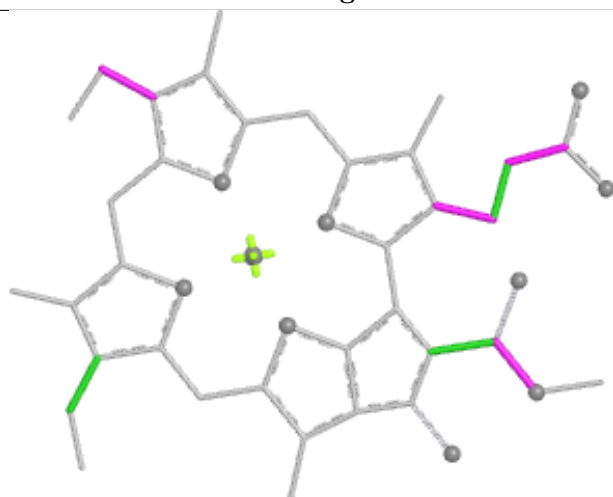
Ligand CLA G 204



Bond lengths



Bond angles

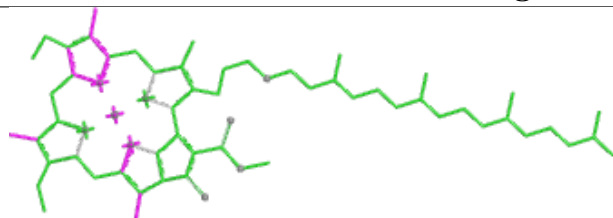


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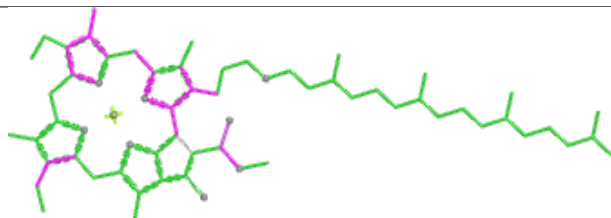


Rings

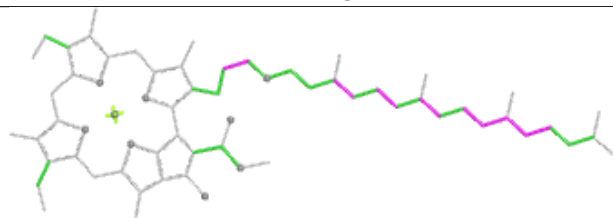
Ligand CLA A 826



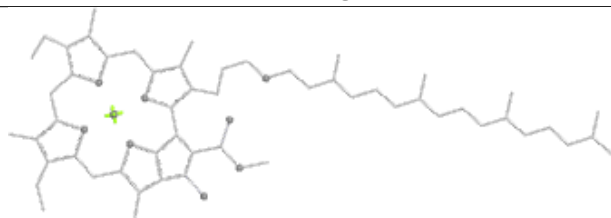
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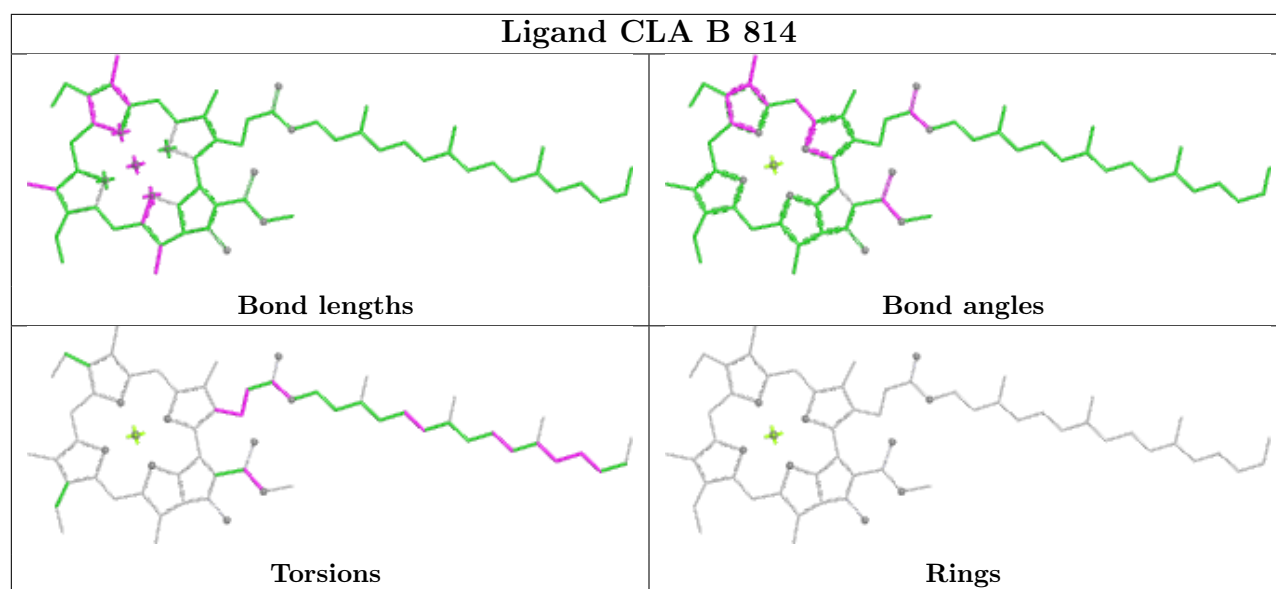
Bond angles



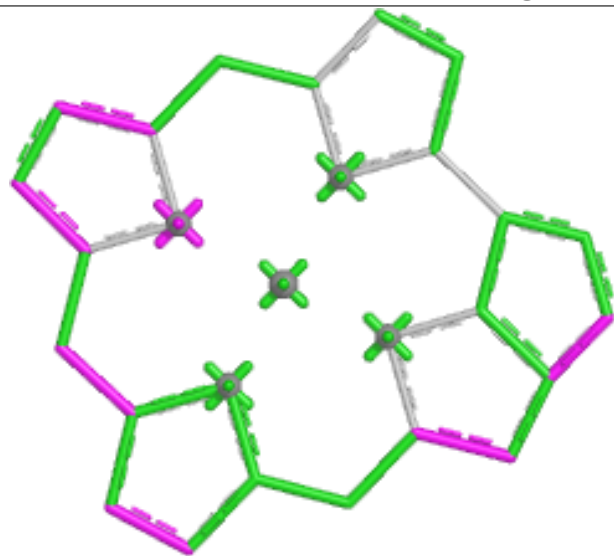
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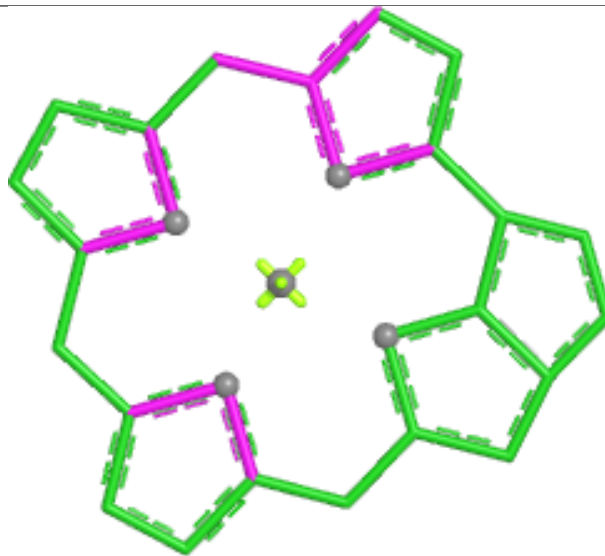
Rings



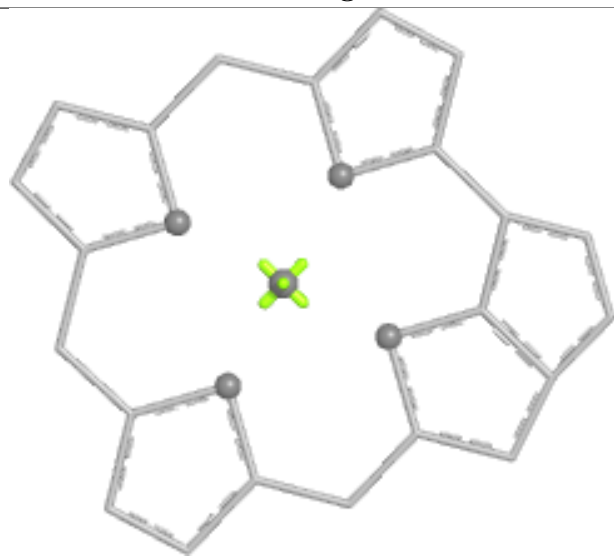
Ligand CLA 9 614



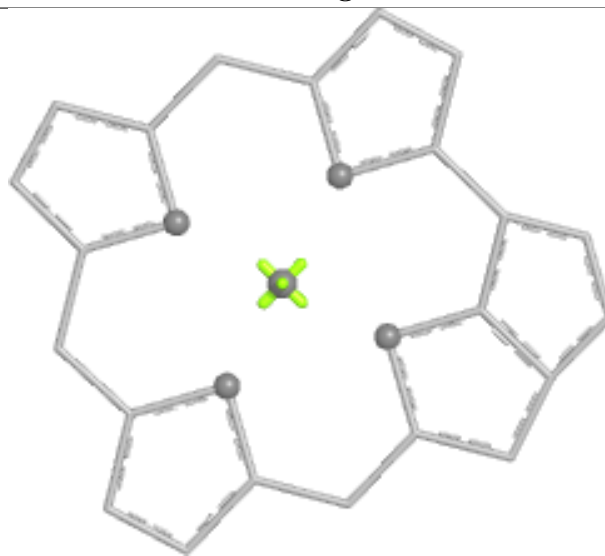
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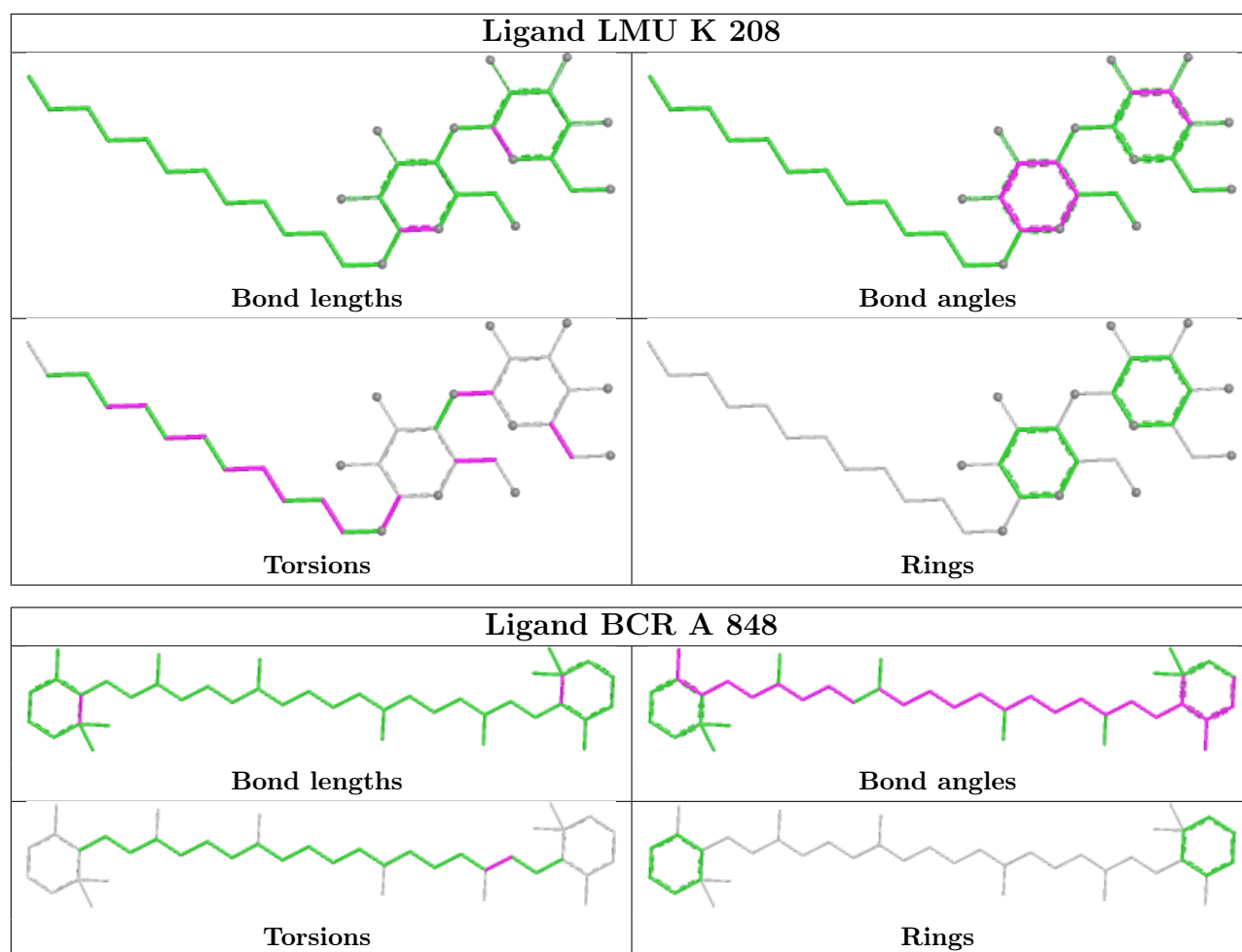
Bond angles



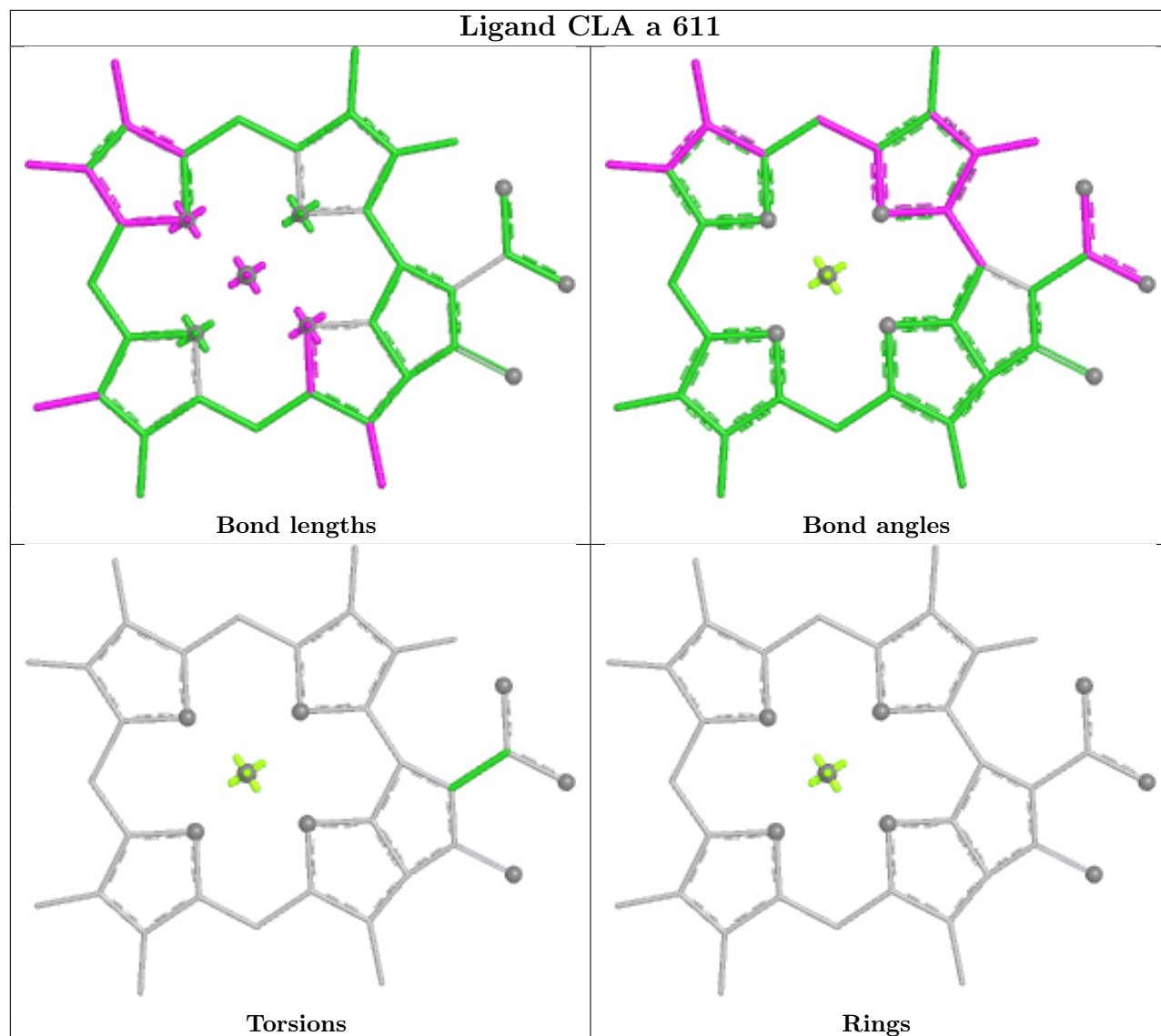
Torsions



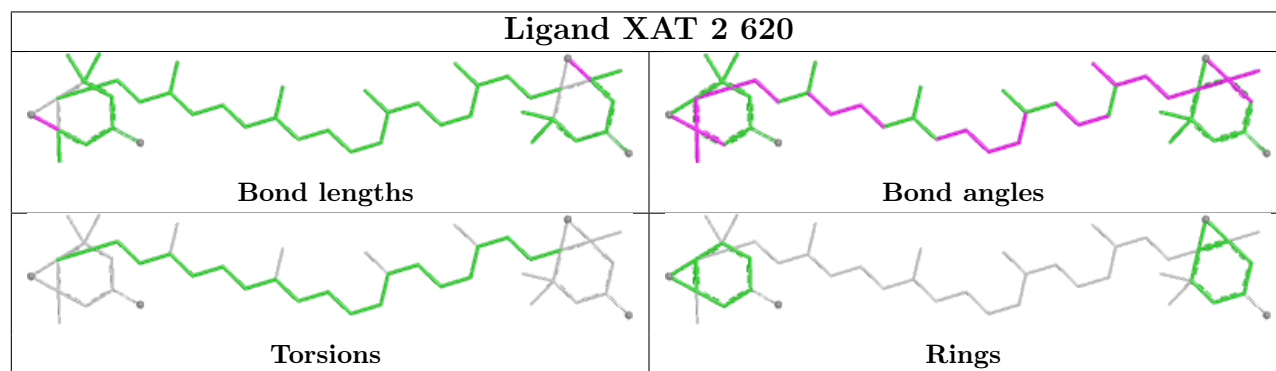
Rings

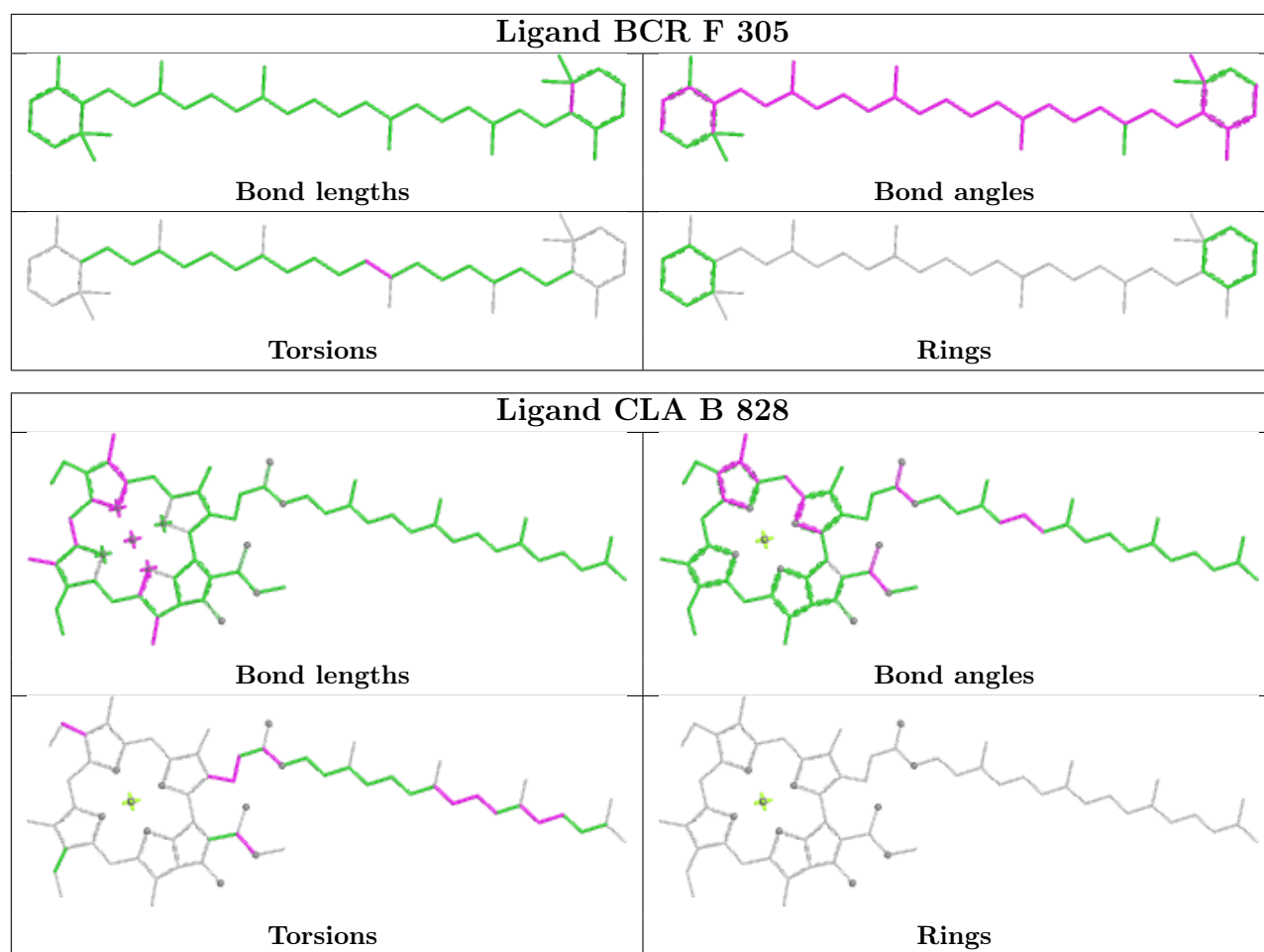


Ligand CLA a 611

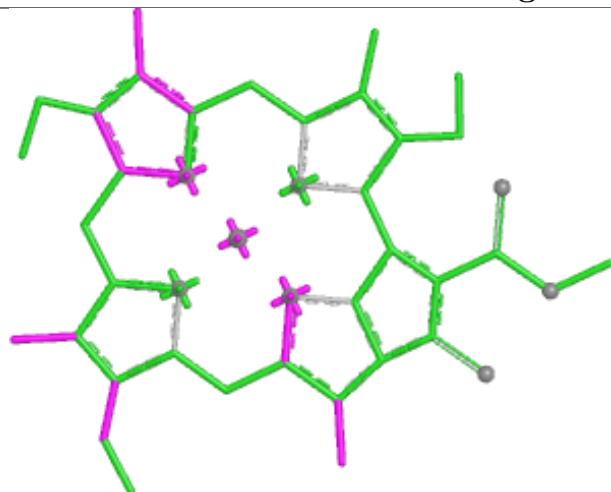


Ligand XAT 2 620





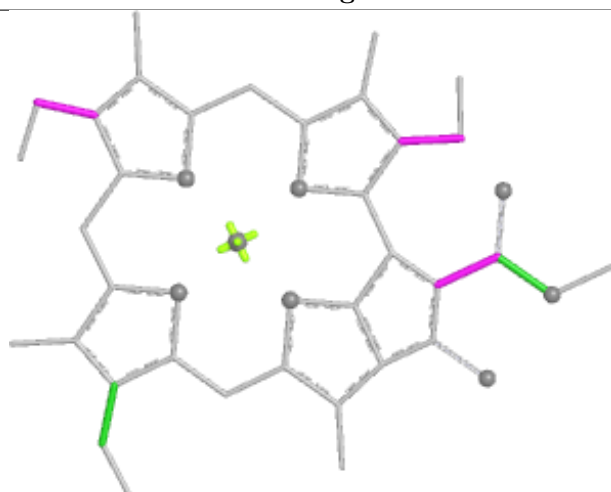
Ligand CLA a 603



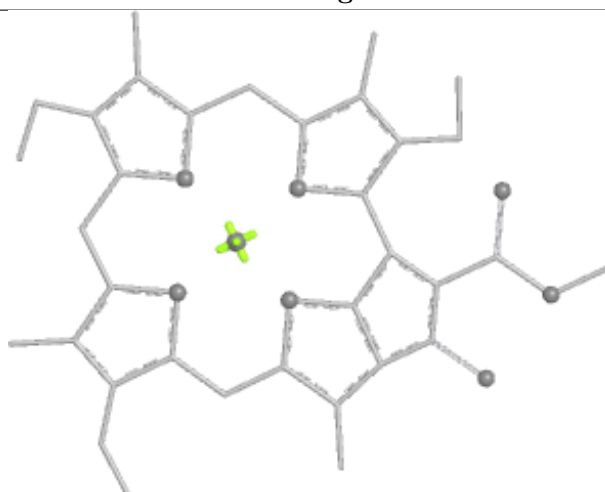
Bond lengths



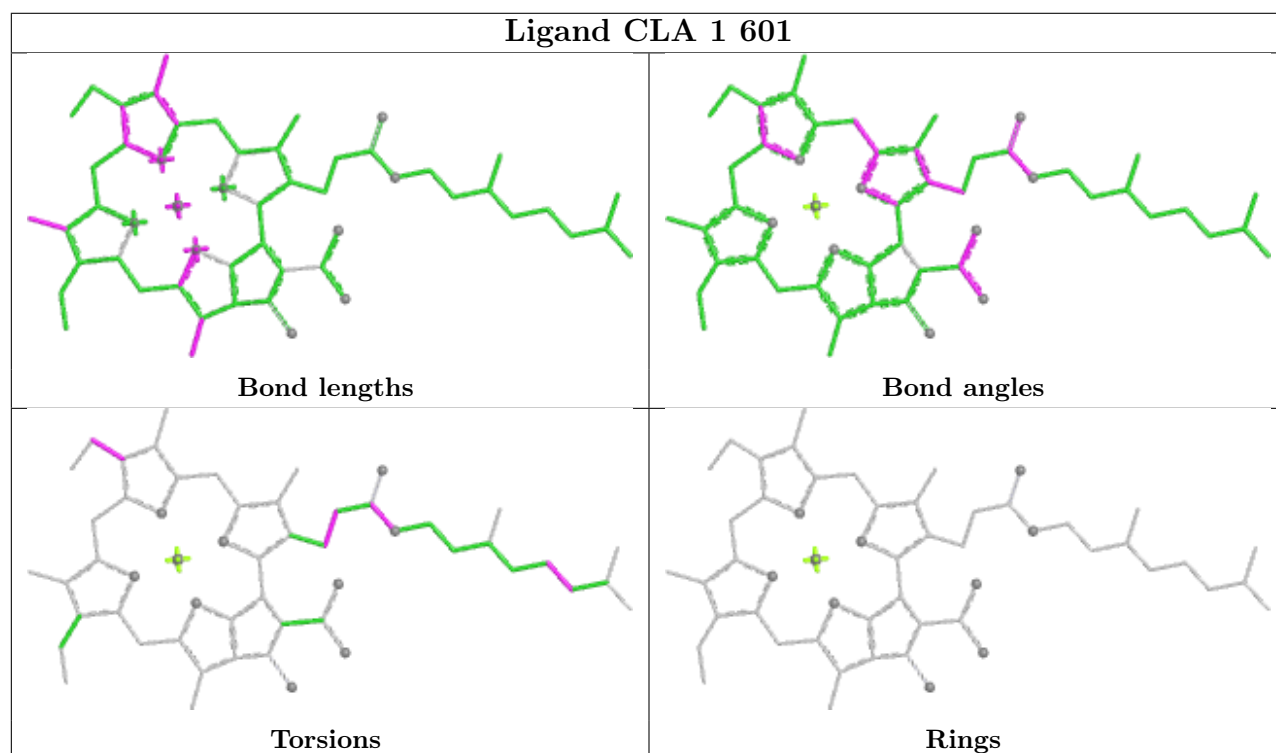
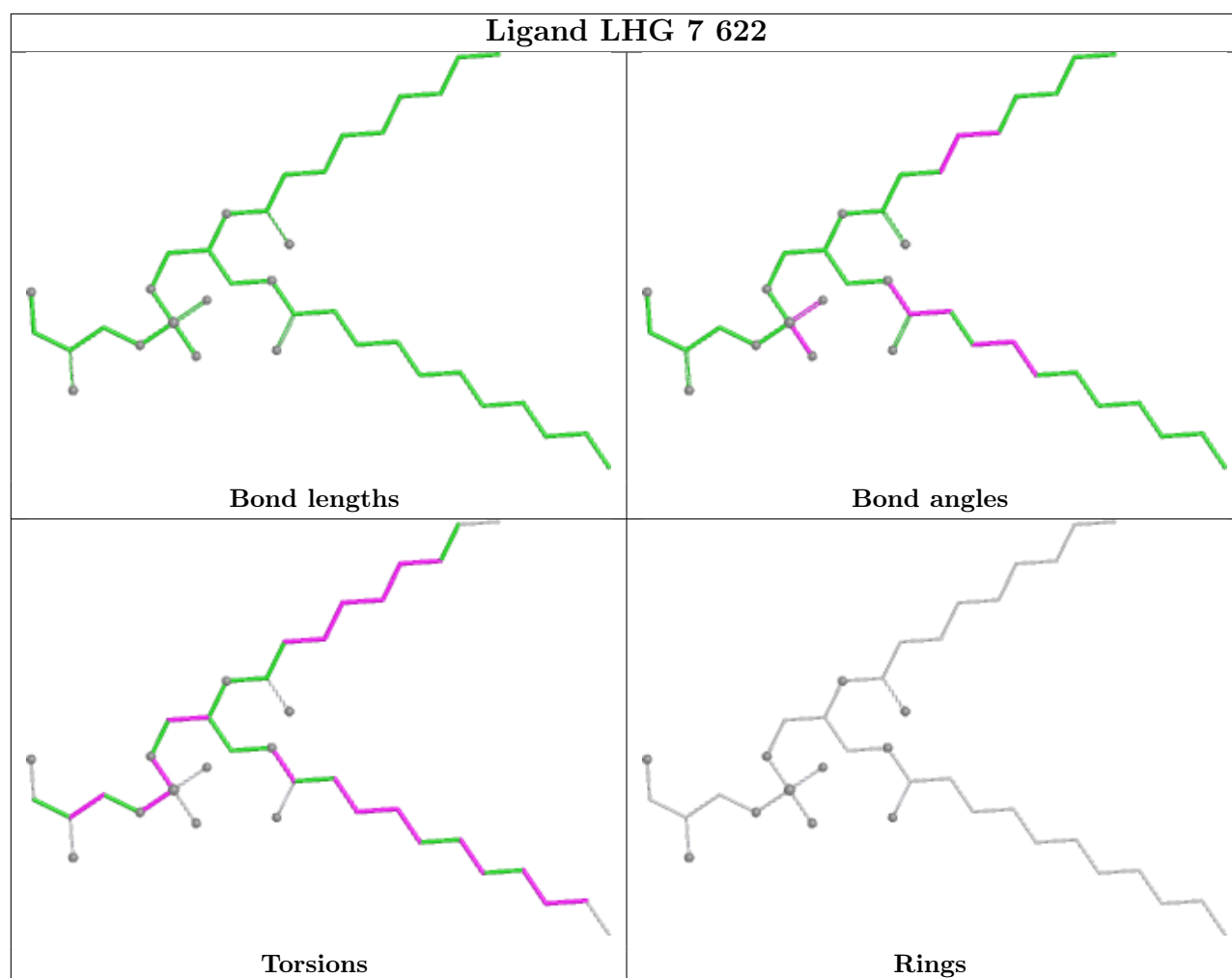
Bond angles

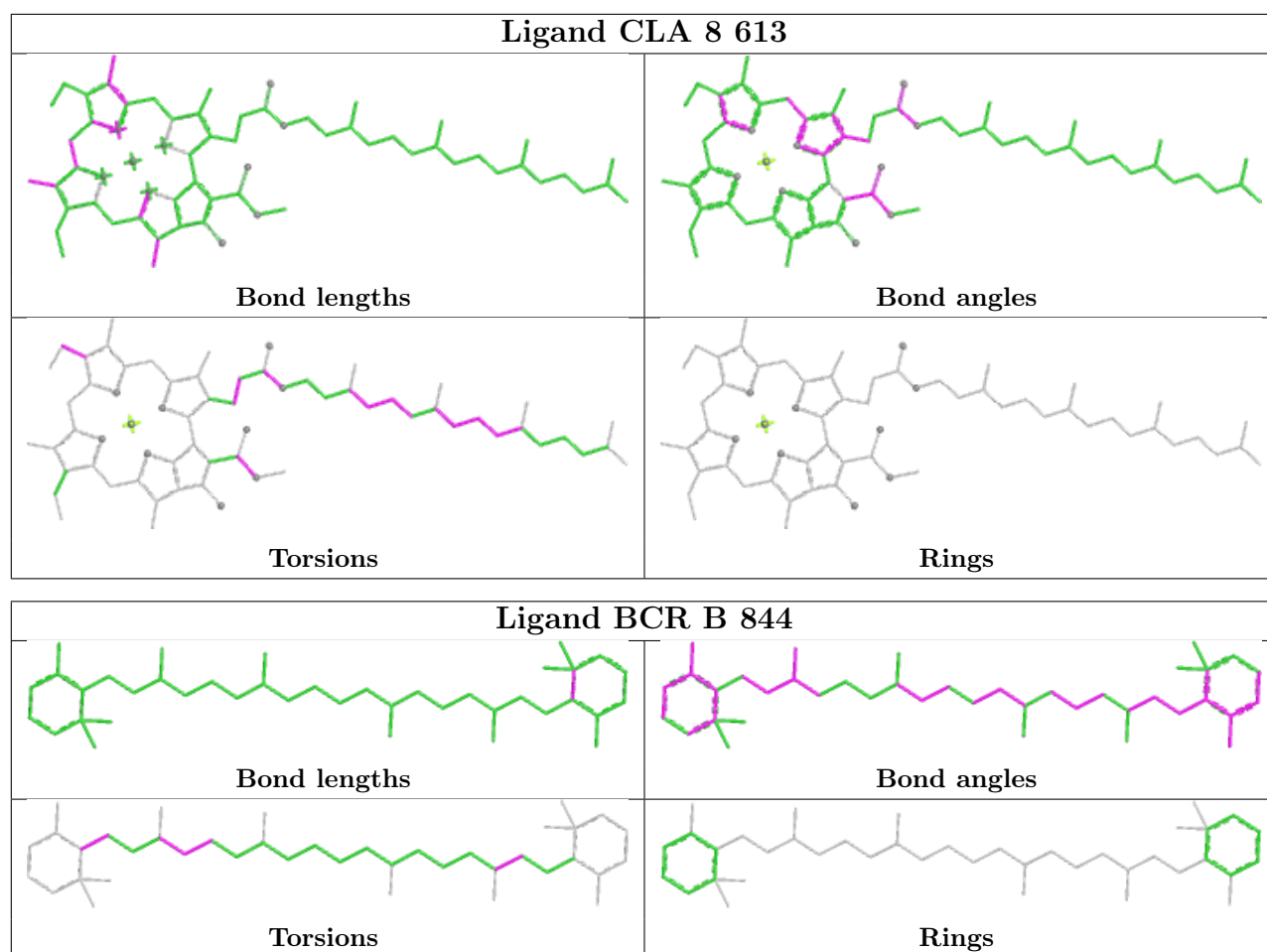


Torsions

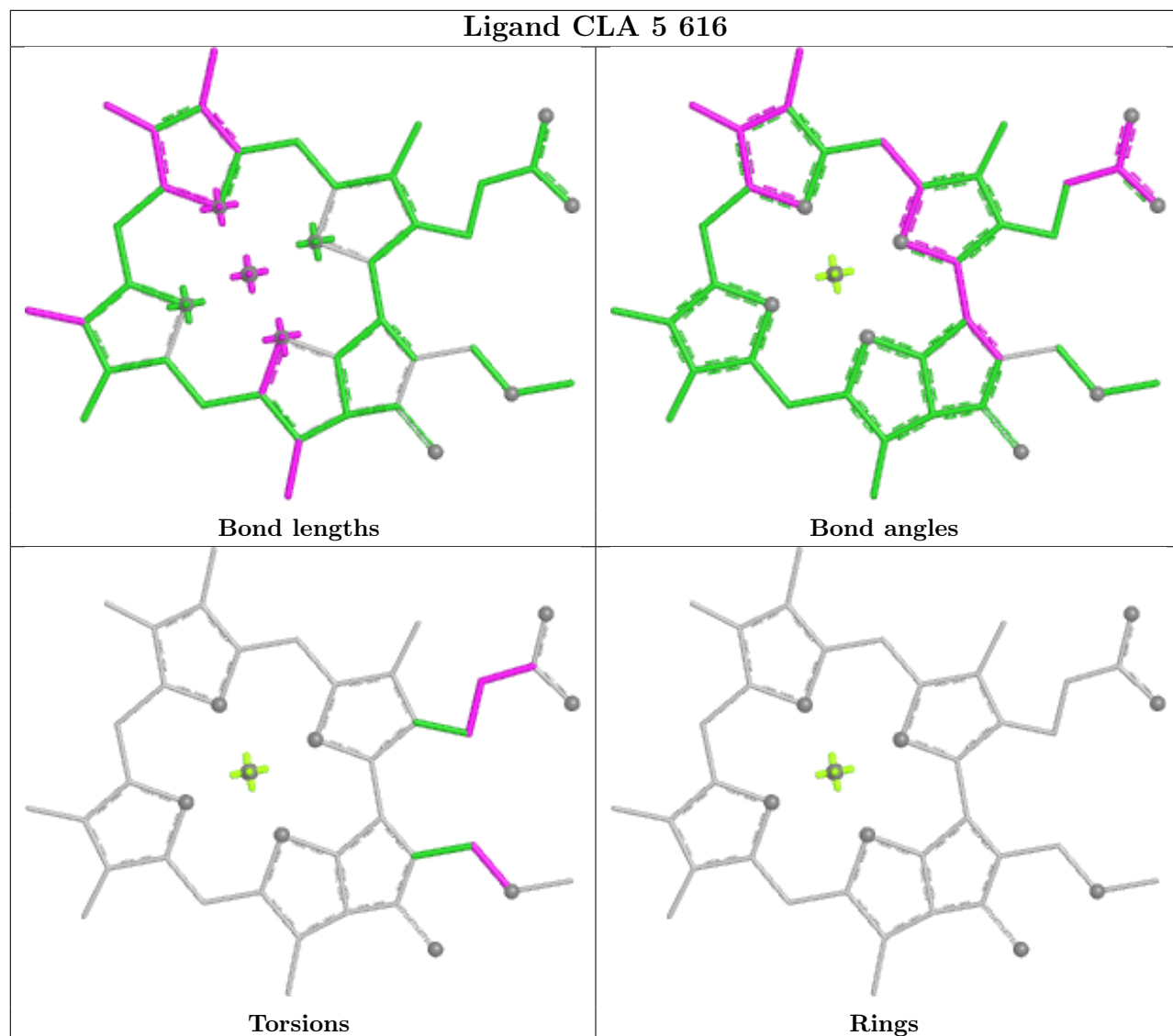


Rings

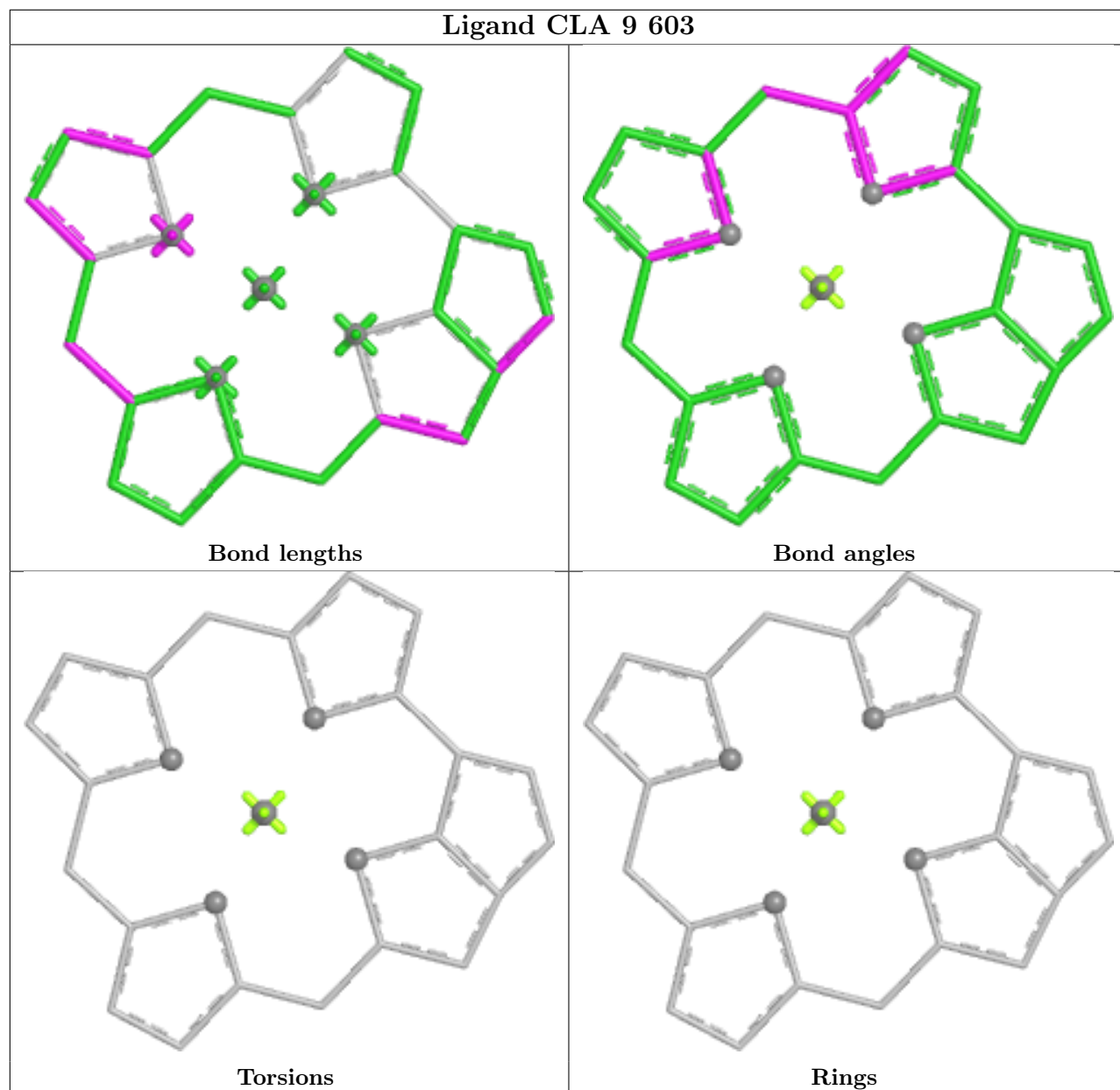




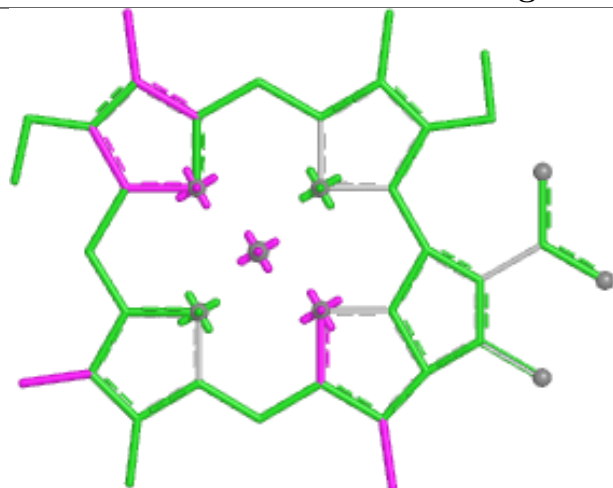
Ligand CLA 5 616



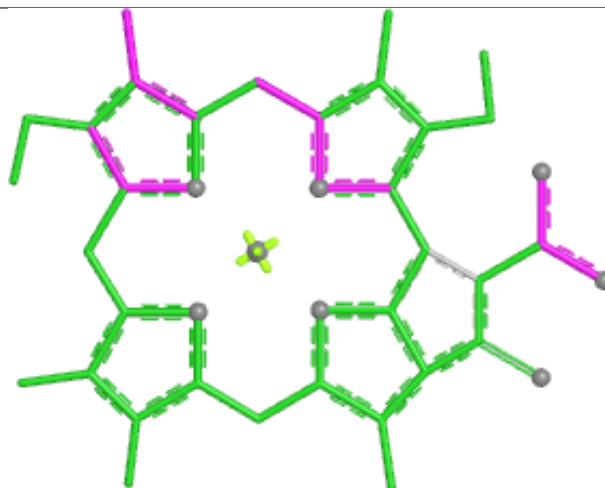
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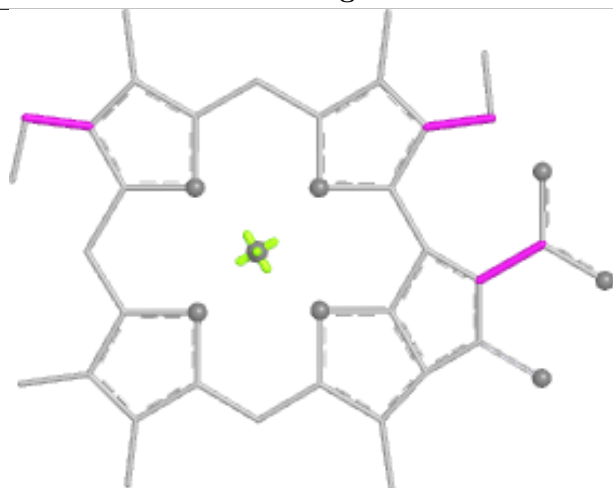
Ligand CLA 4 606



Bond lengths



Bond angles

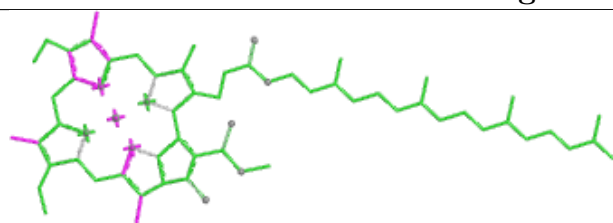


Torsions

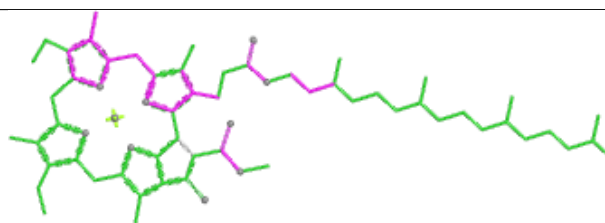


Rings

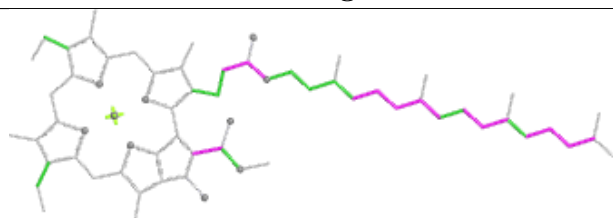
Ligand CLA 8 601



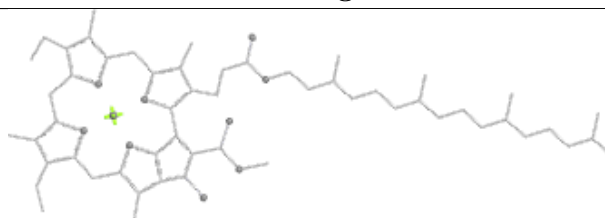
Bond lengths



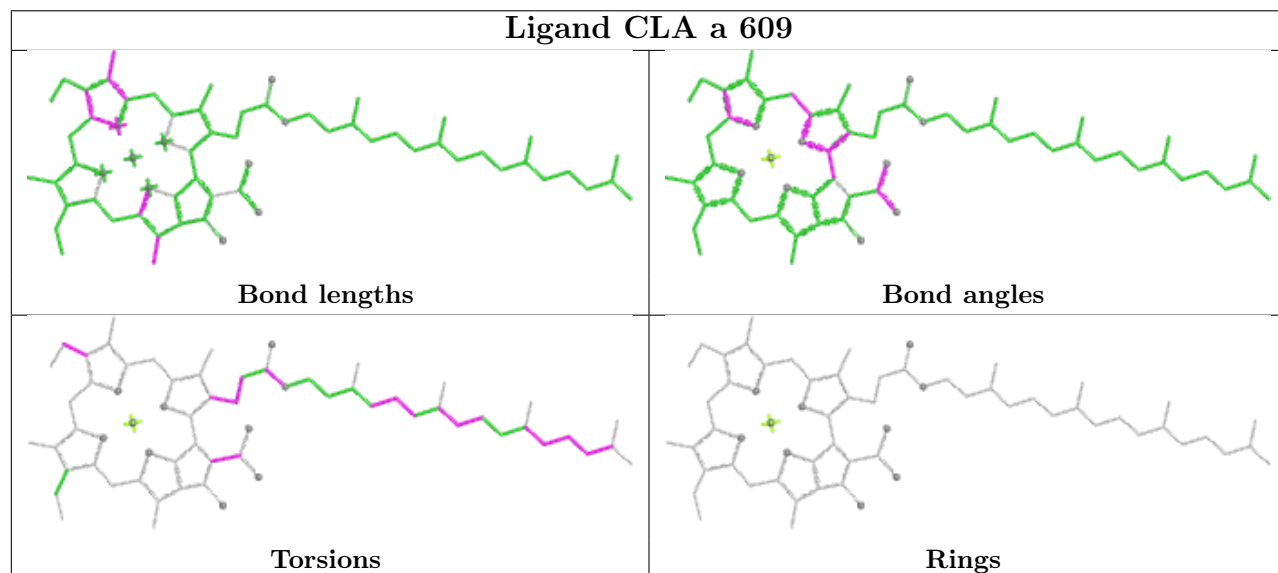
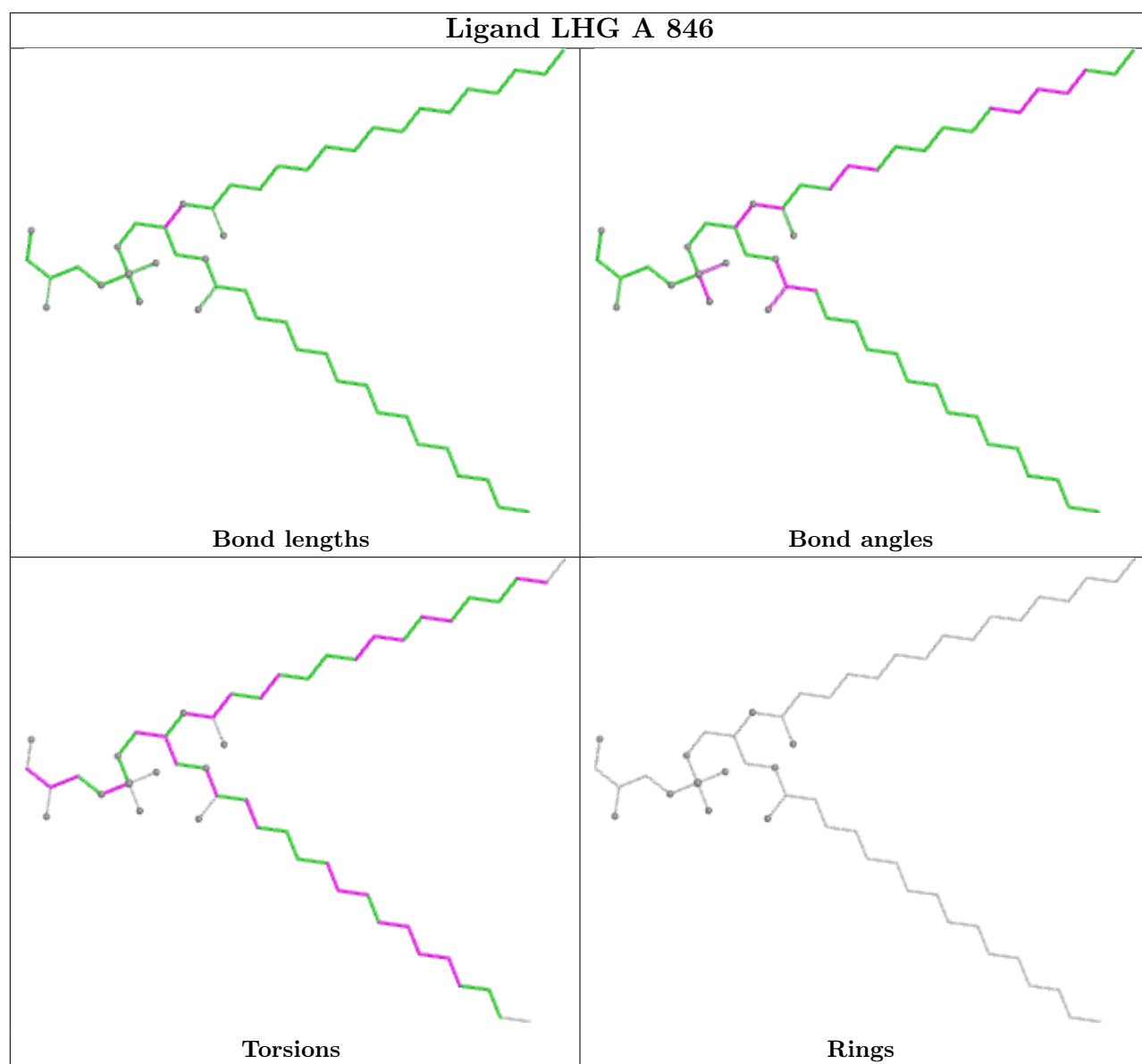
Bond angles

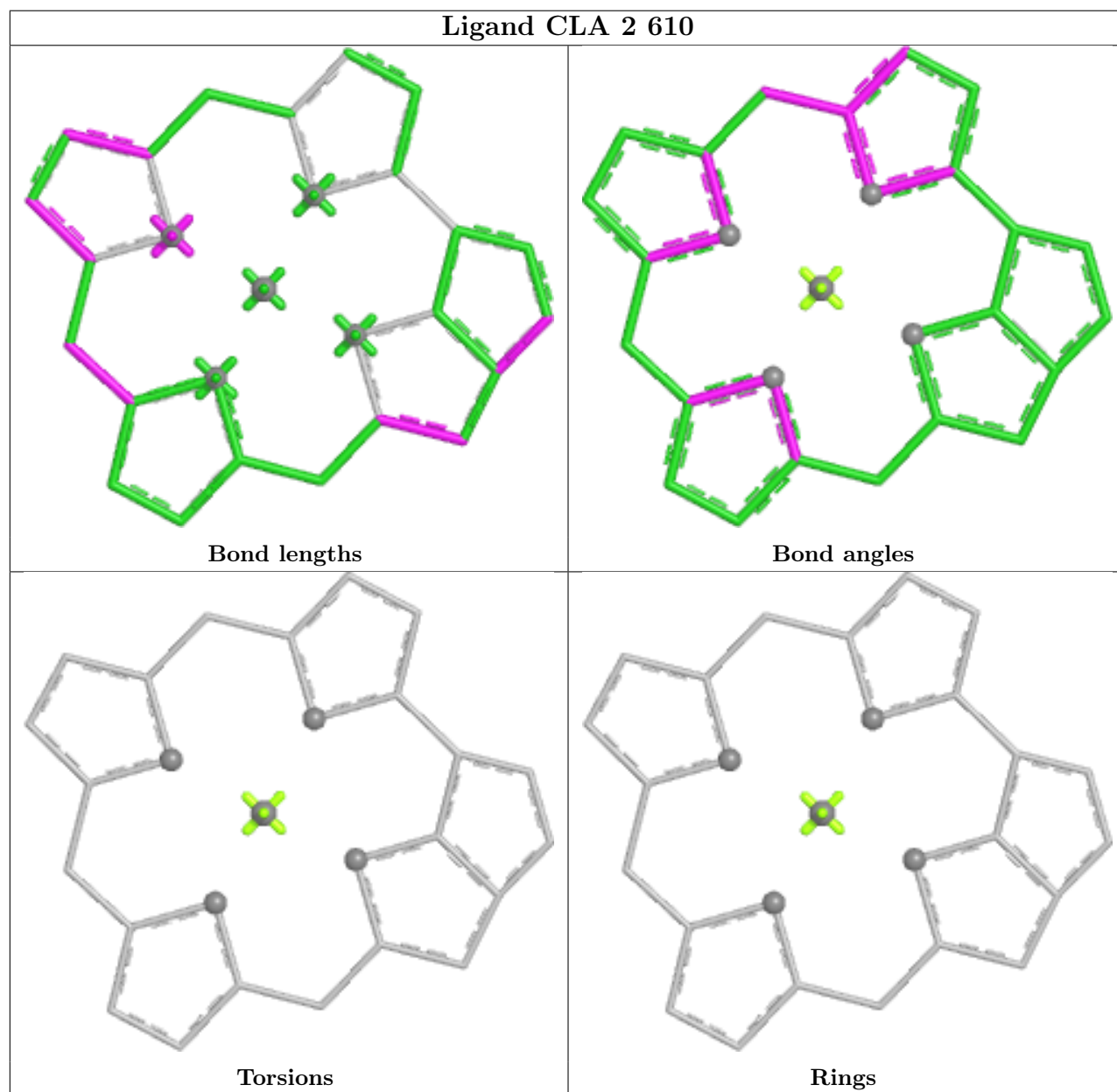
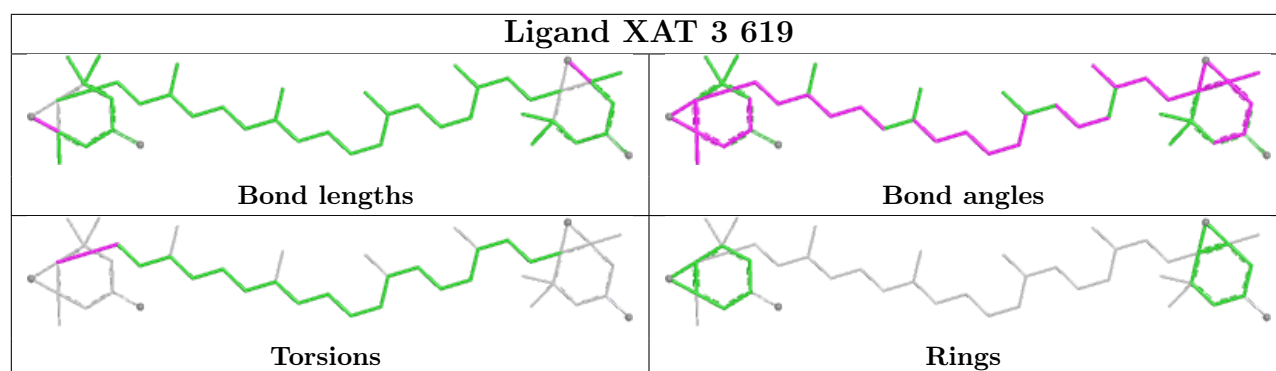


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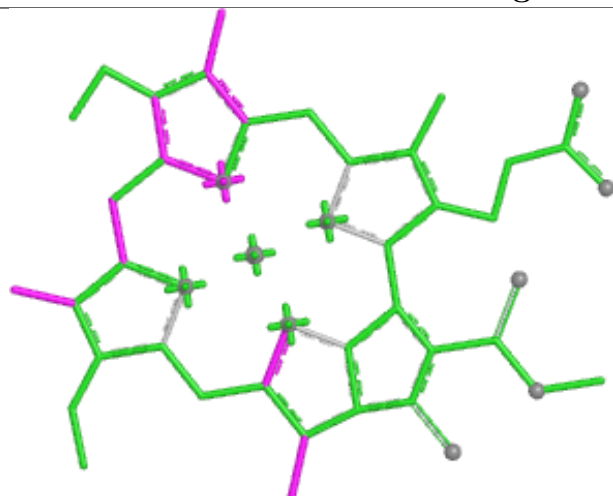


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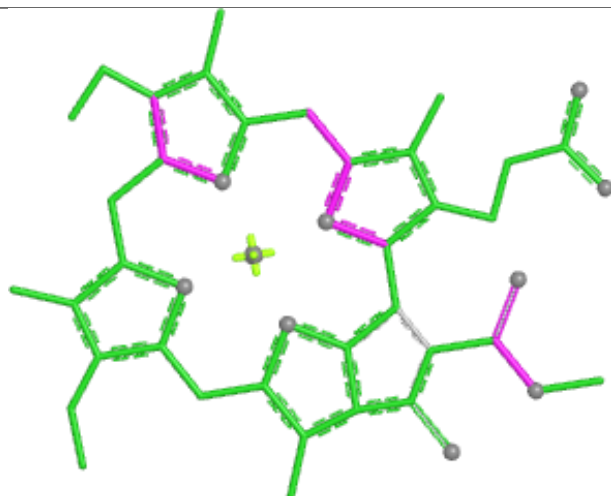




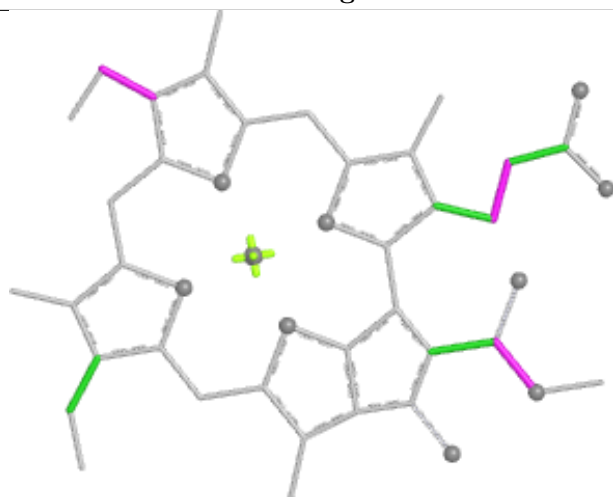
Ligand CLA K 206



Bond lengths



Bond angles

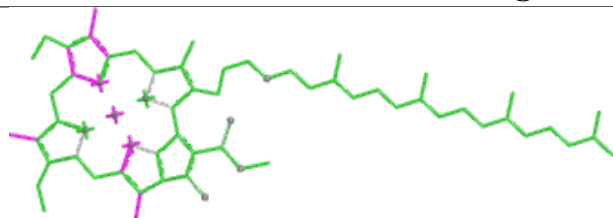


Torsions

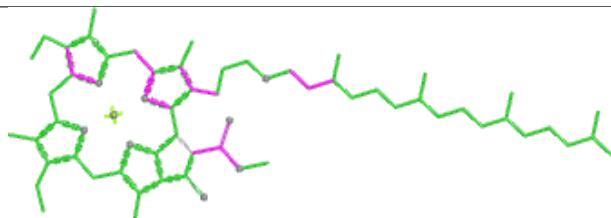


Rings

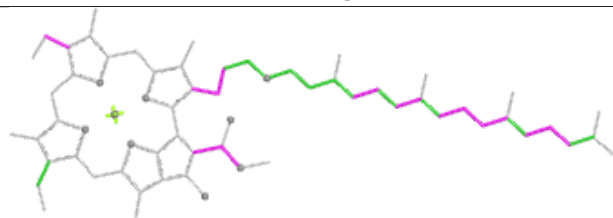
Ligand CLA B 810



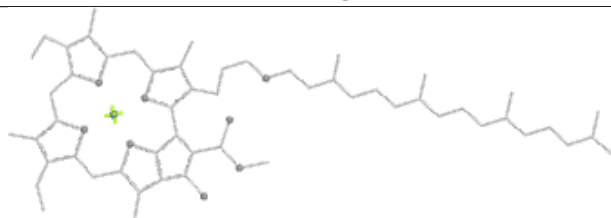
Bond lengths



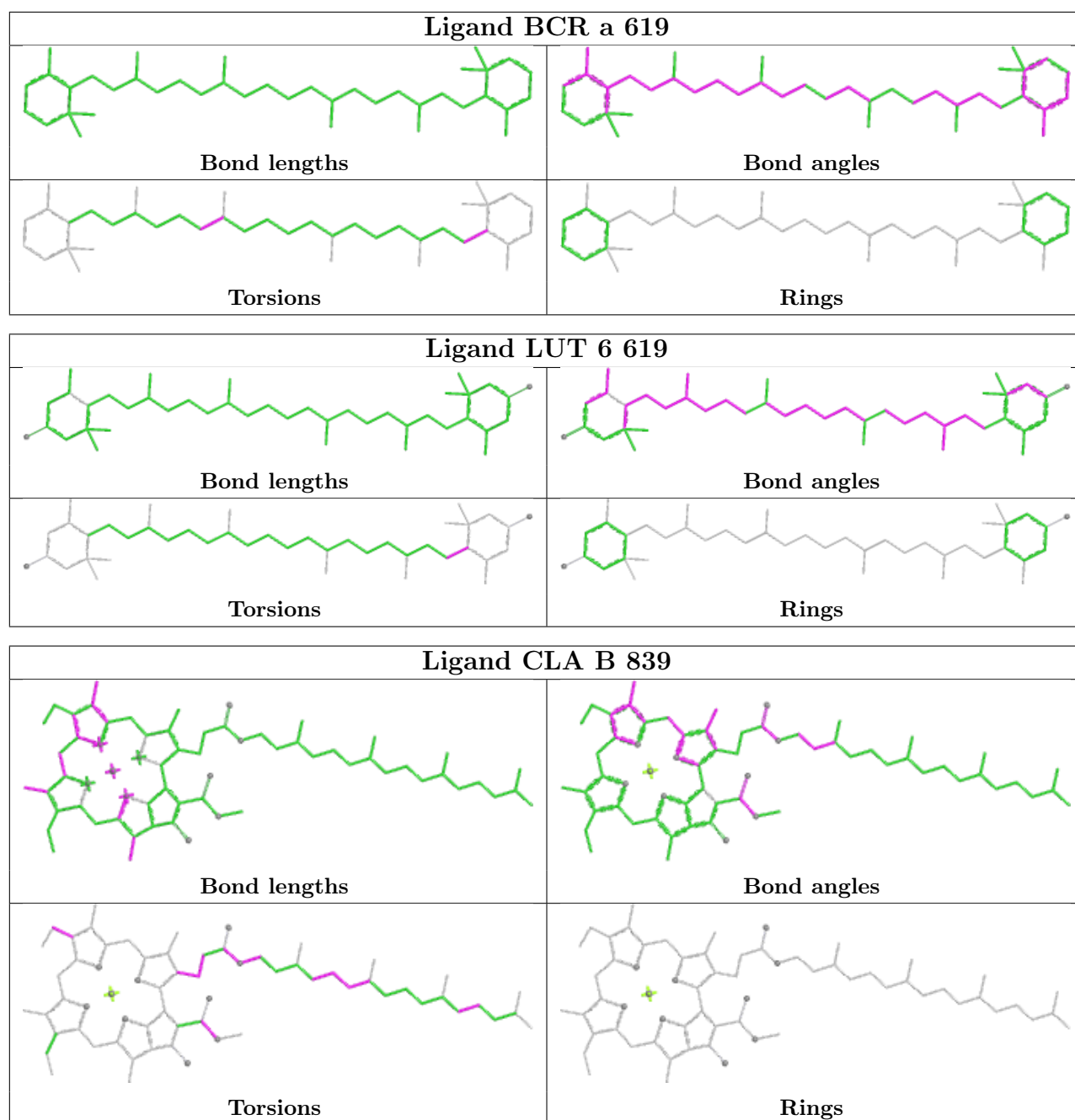
Bond angles



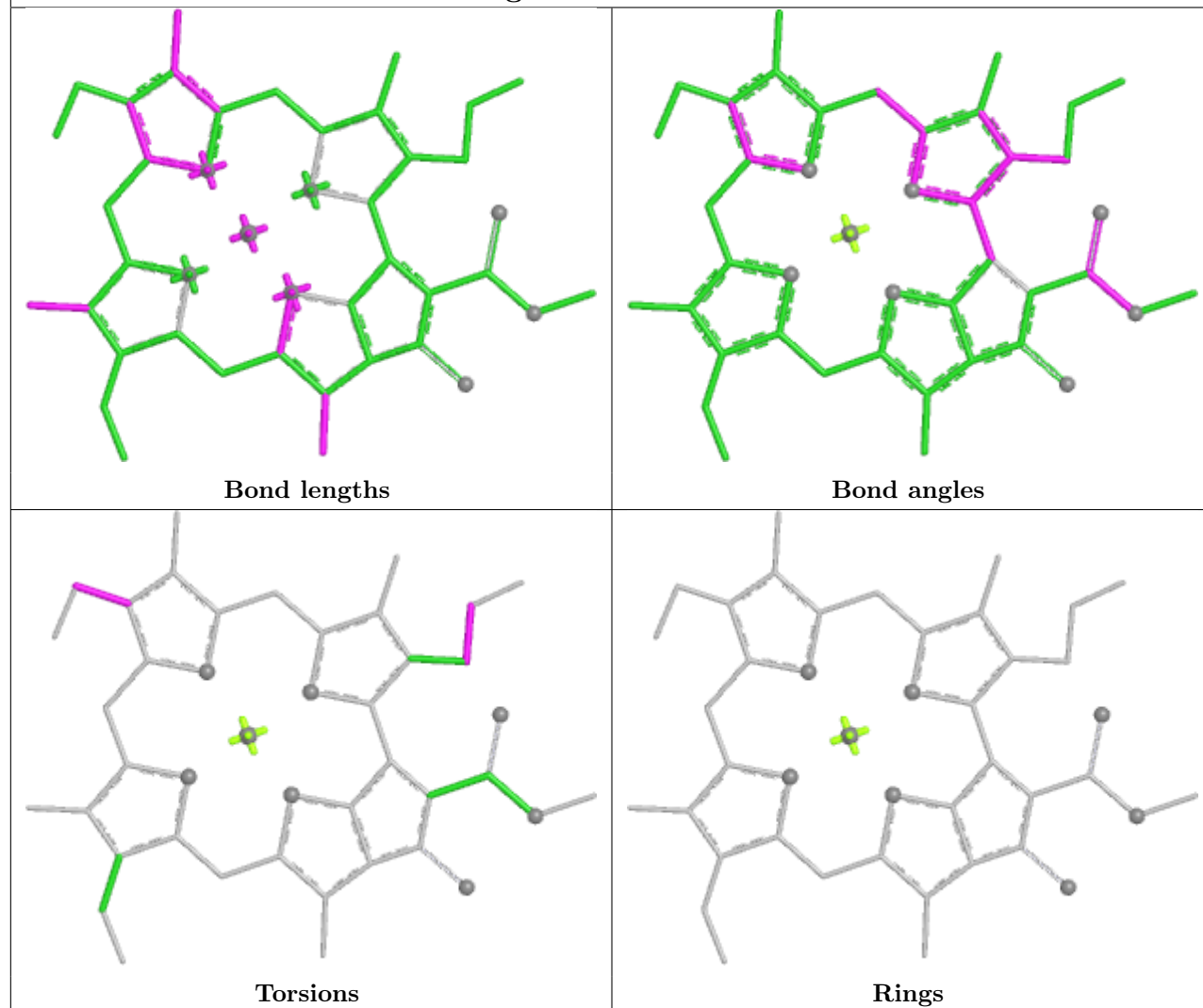
Torsions



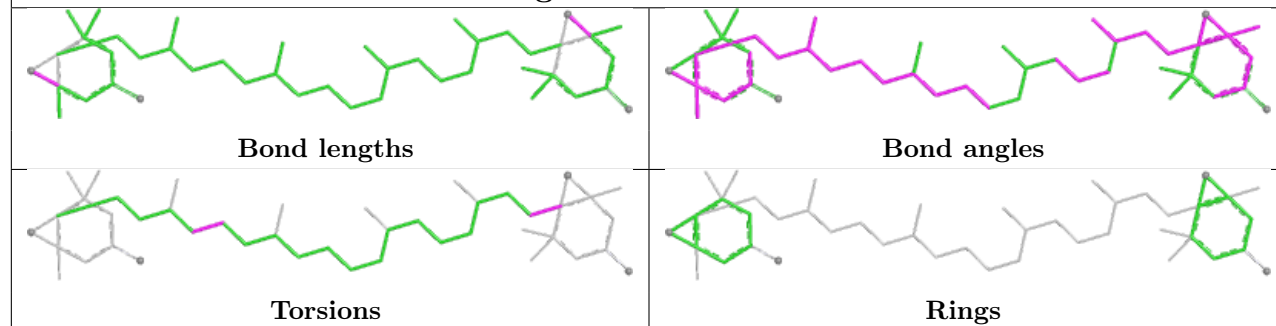
Rings

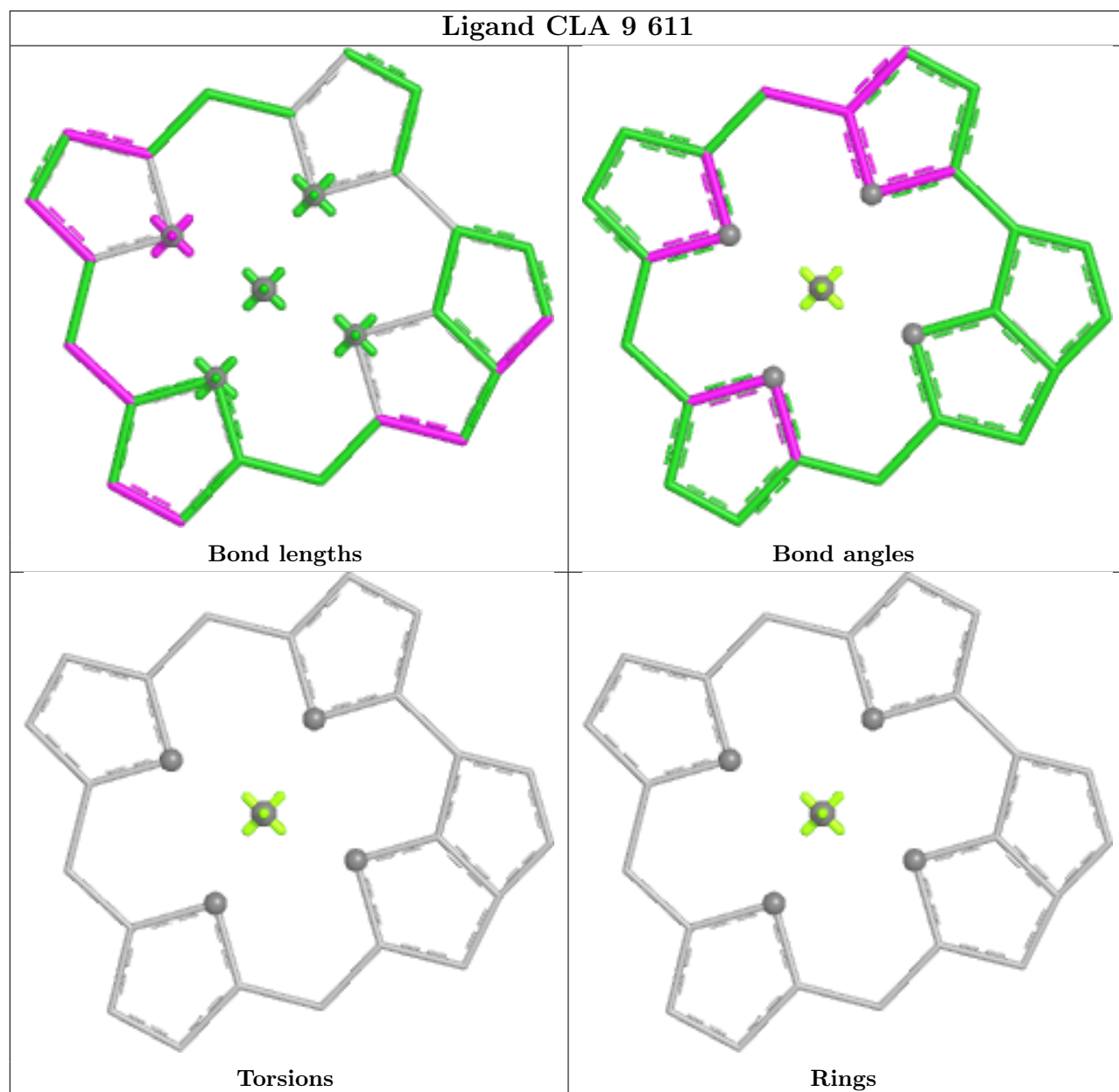
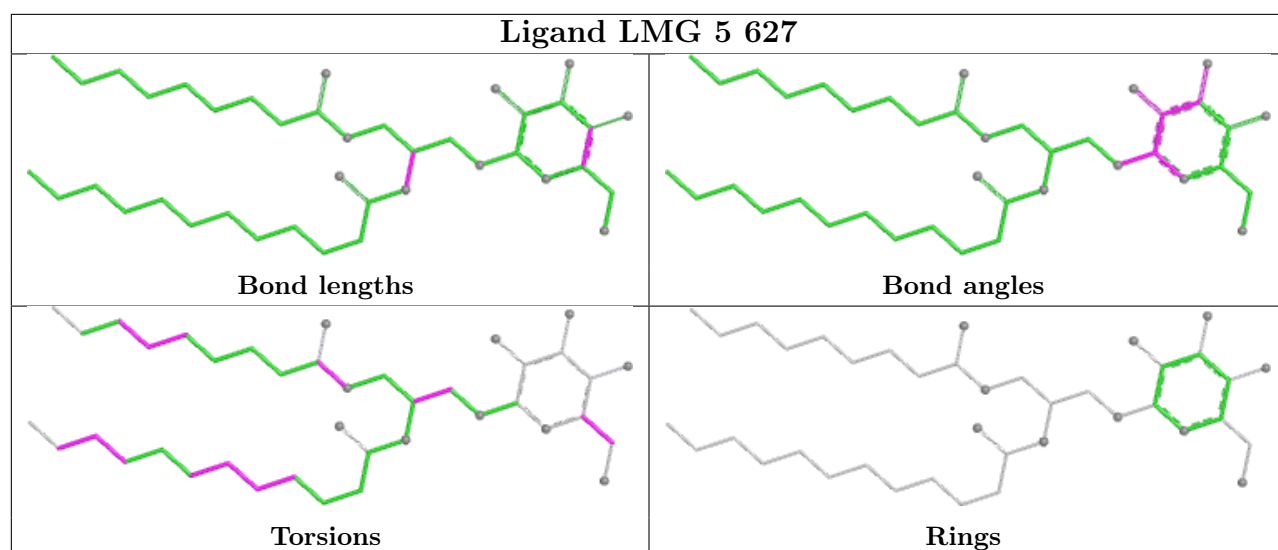


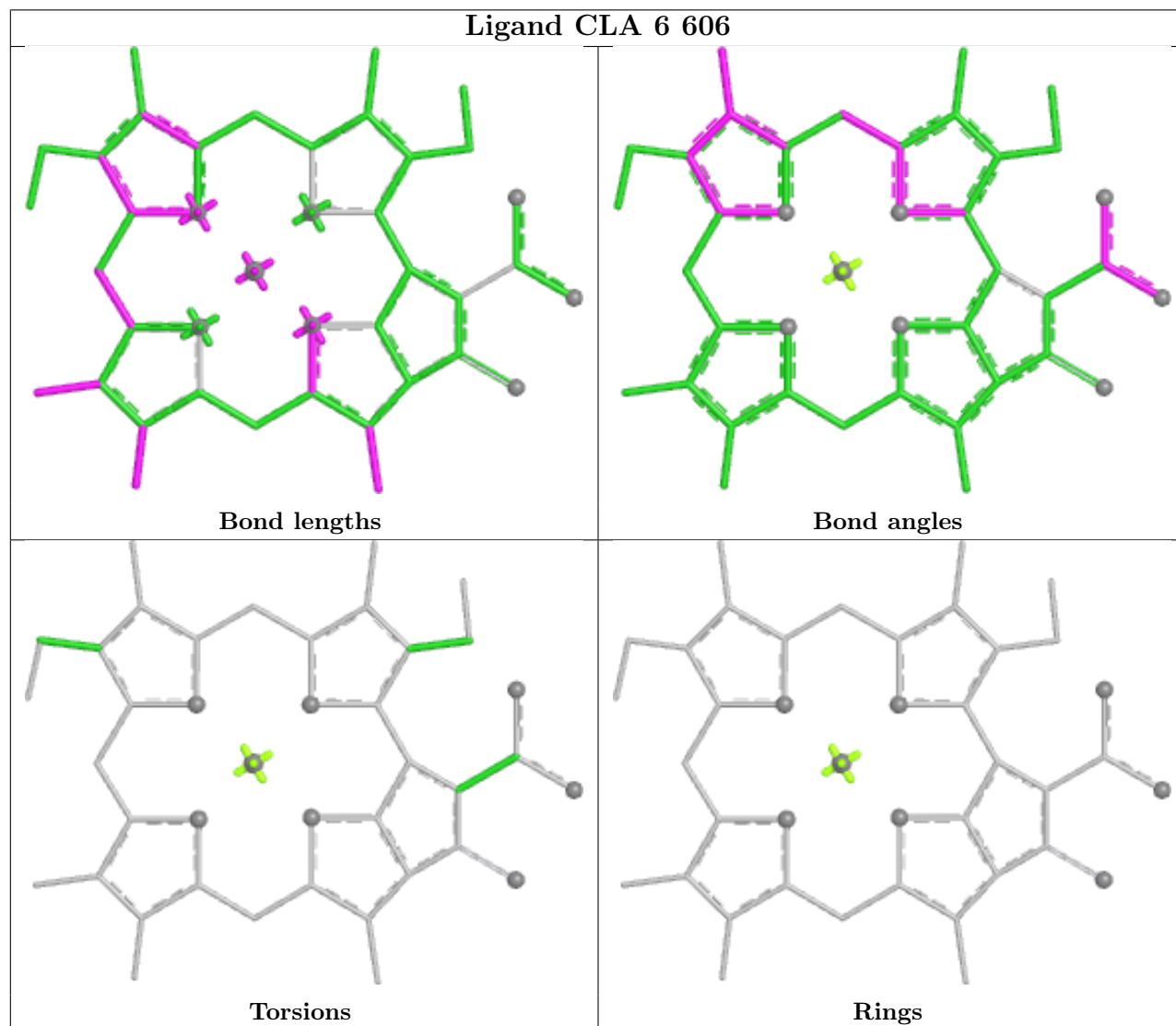
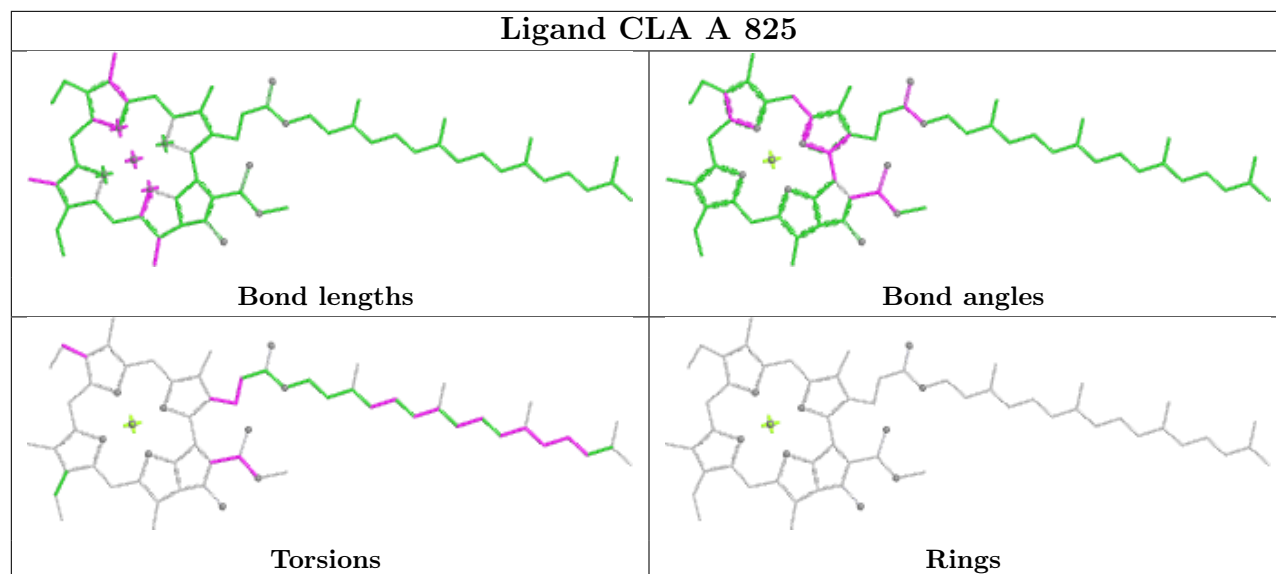
Ligand CLA 3 612



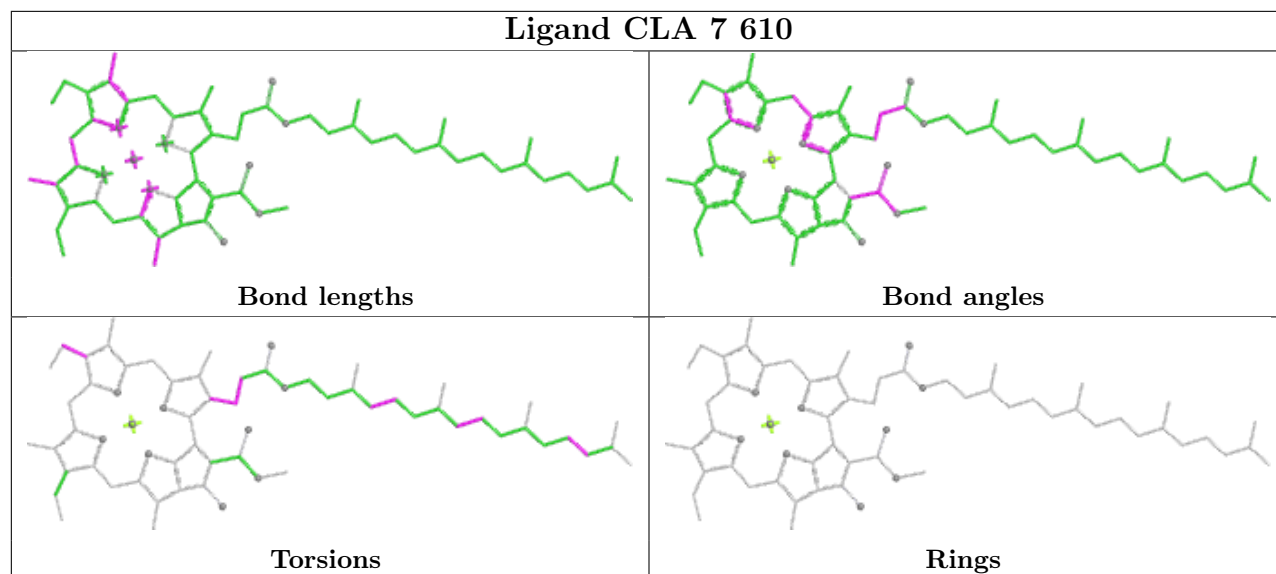
Ligand XAT 6 621



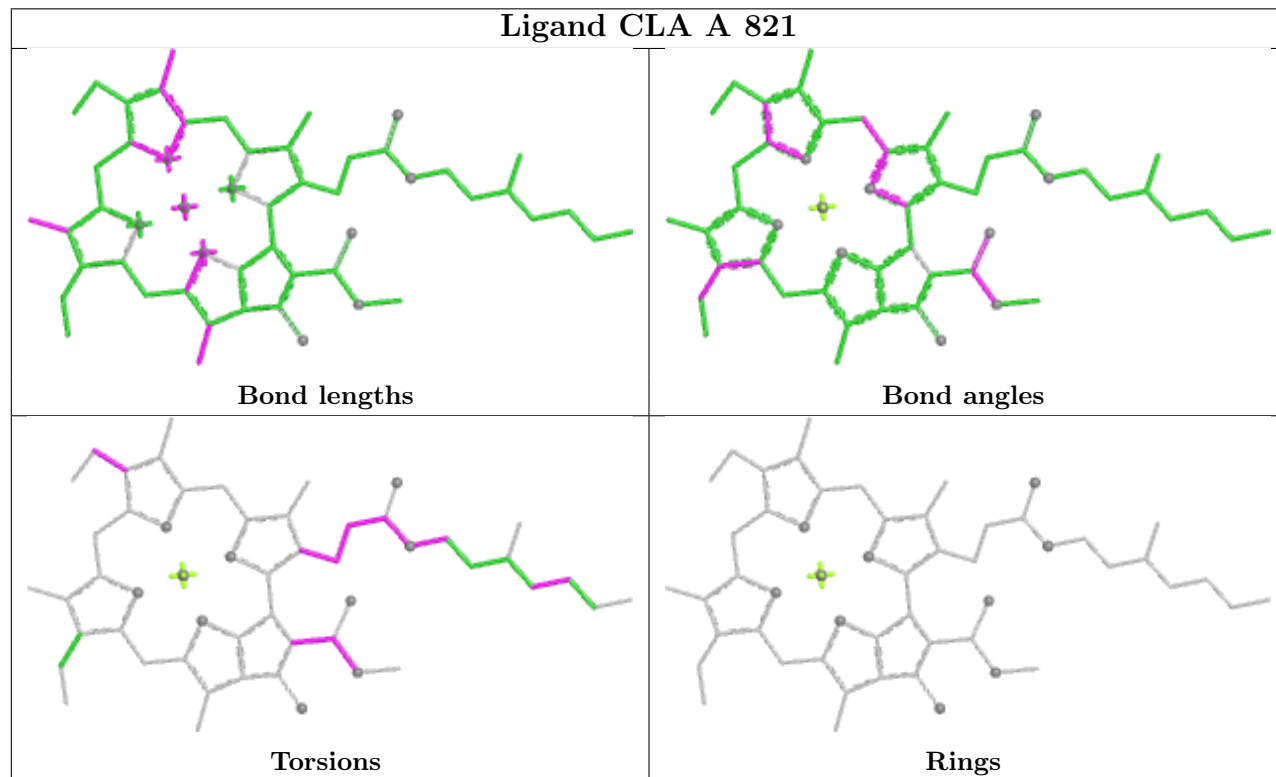


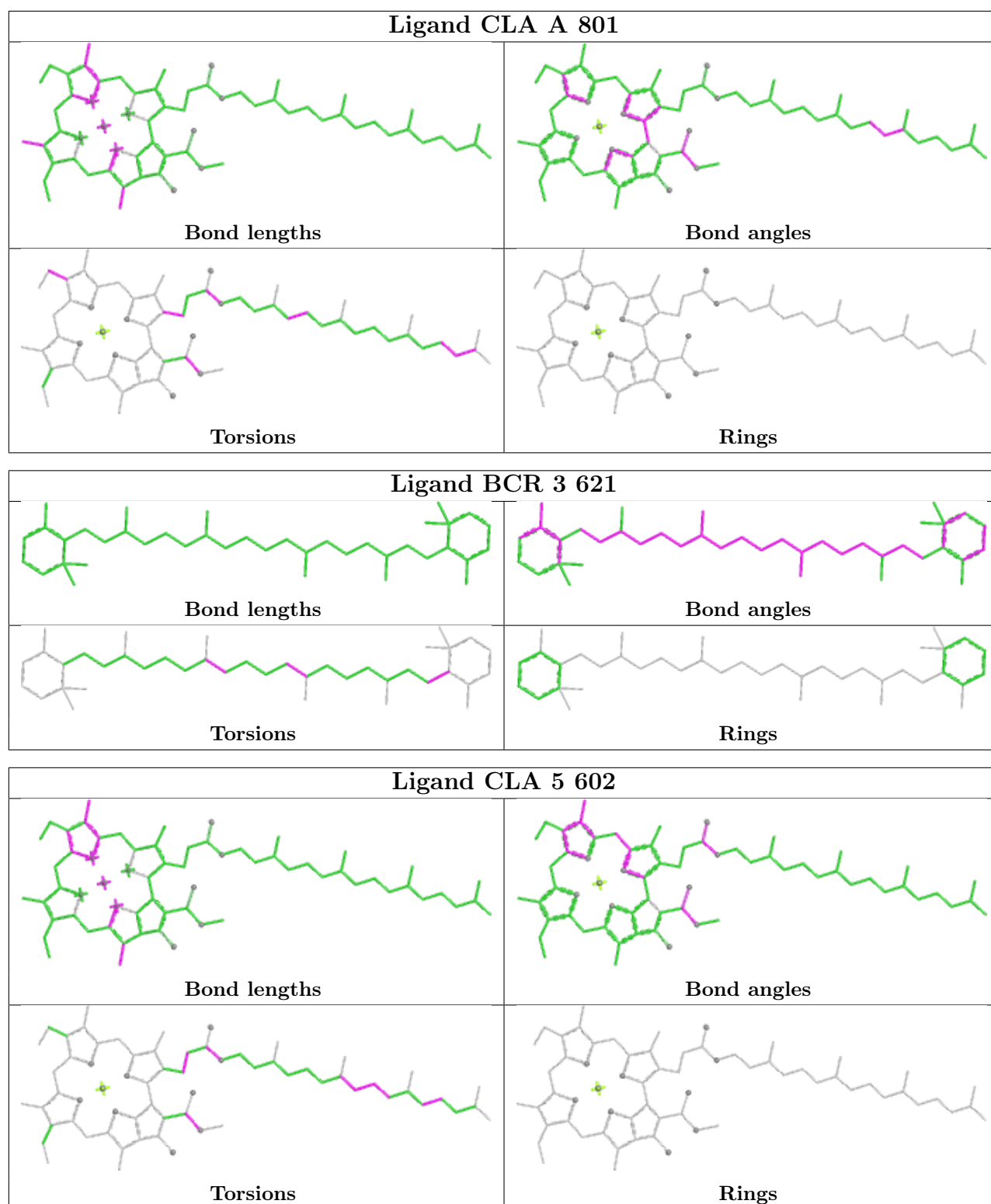


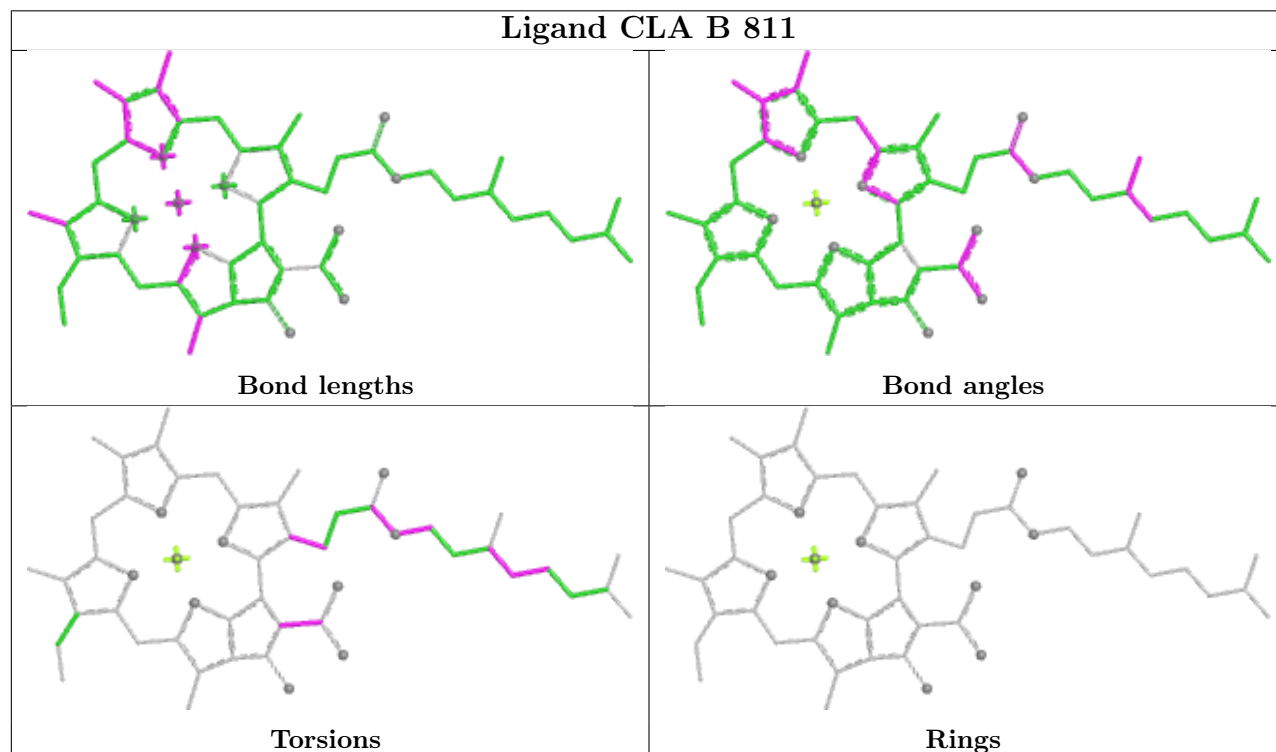
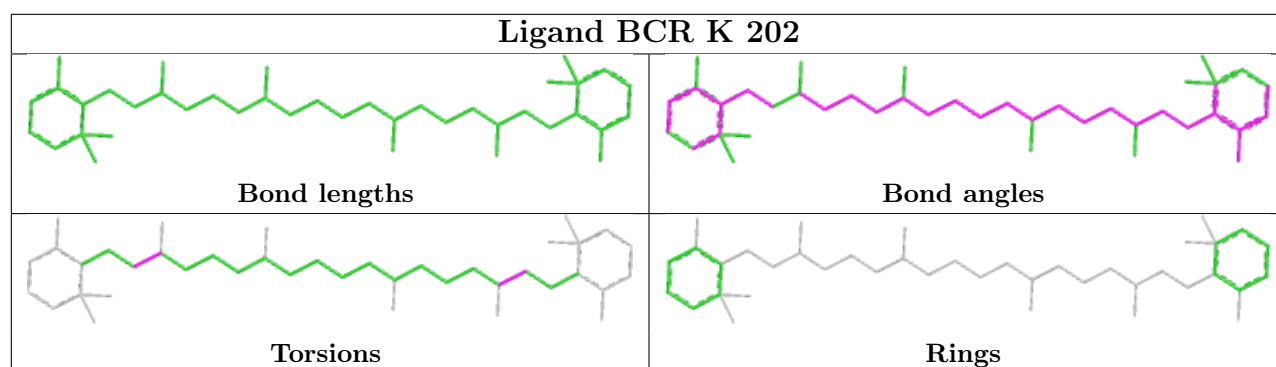
Ligand CLA 7 610



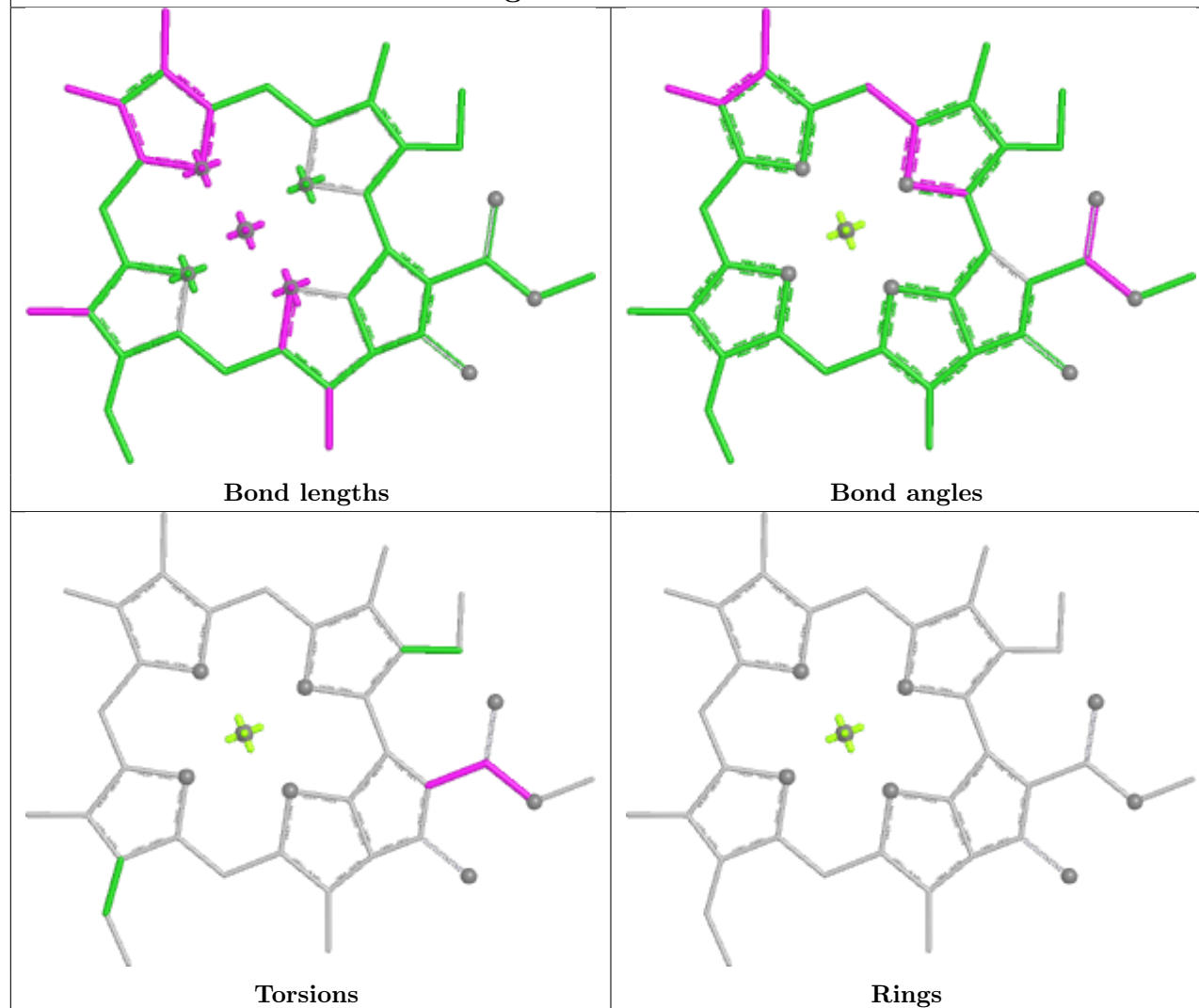
Ligand CLA A 821



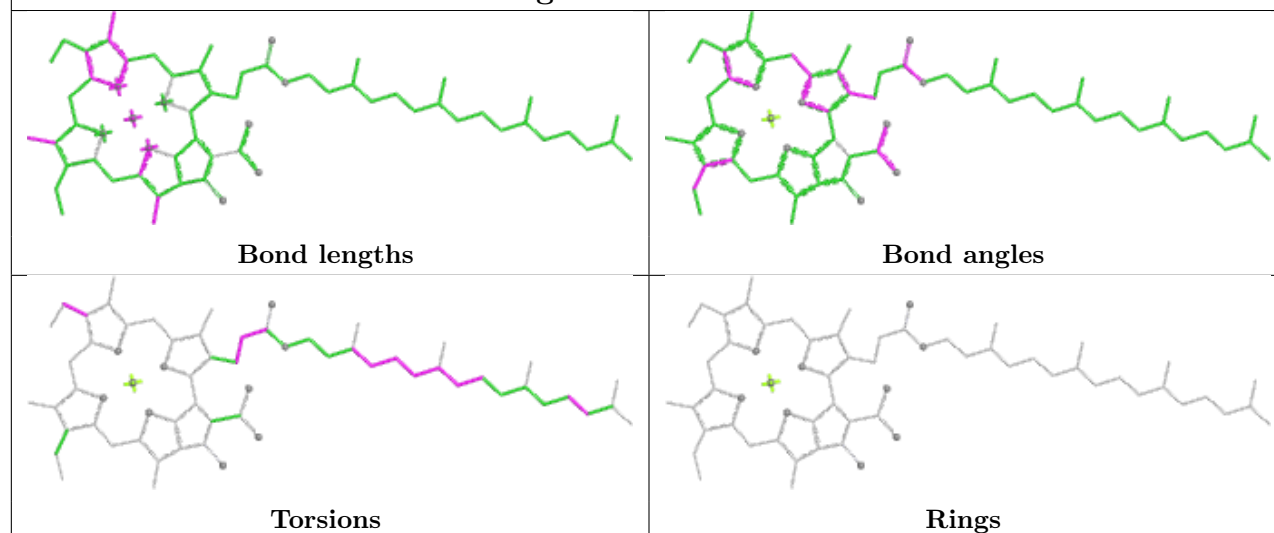


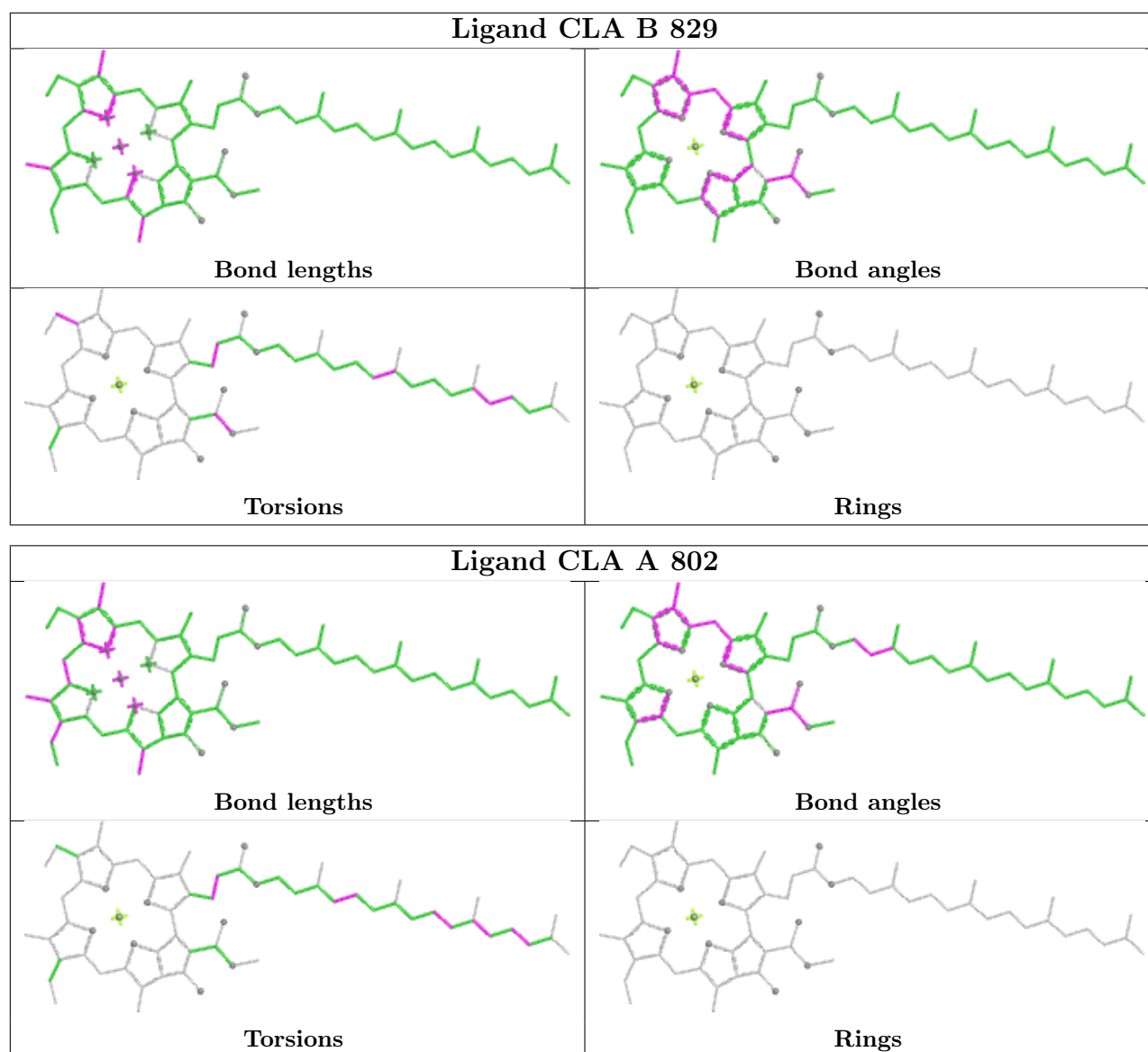


Ligand CLA 8 607

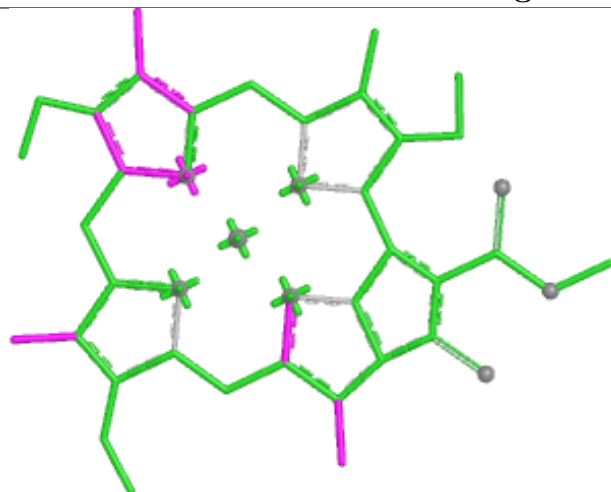


Ligand CLA 6 613





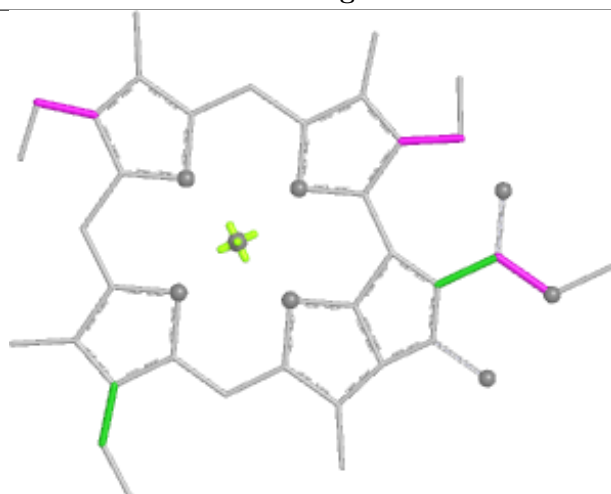
Ligand CLA B 822



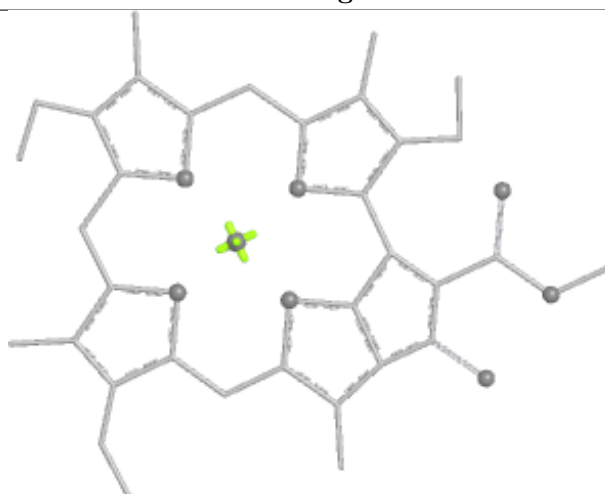
Bond lengths



Bond angles

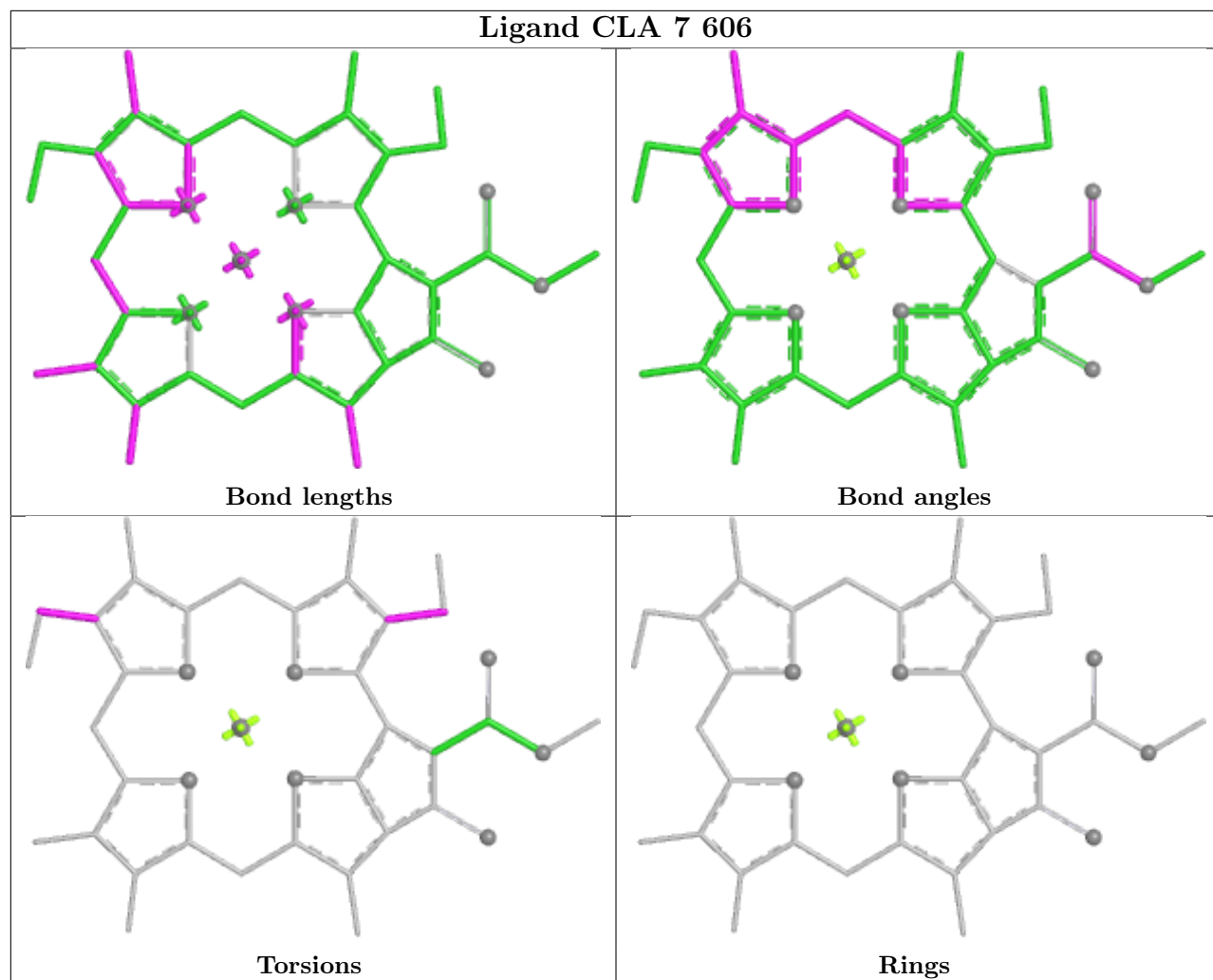


Torsions

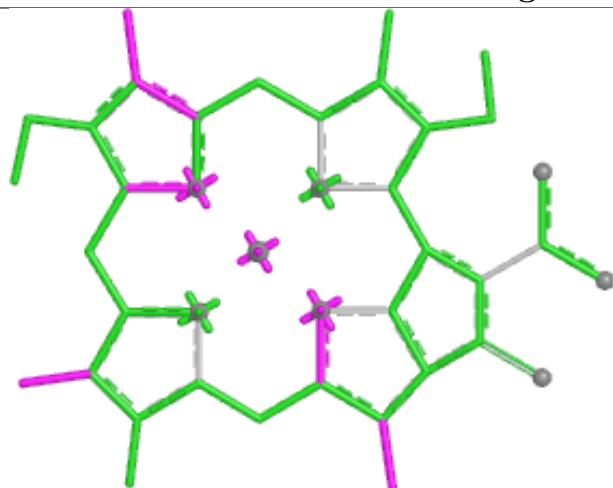


Rings

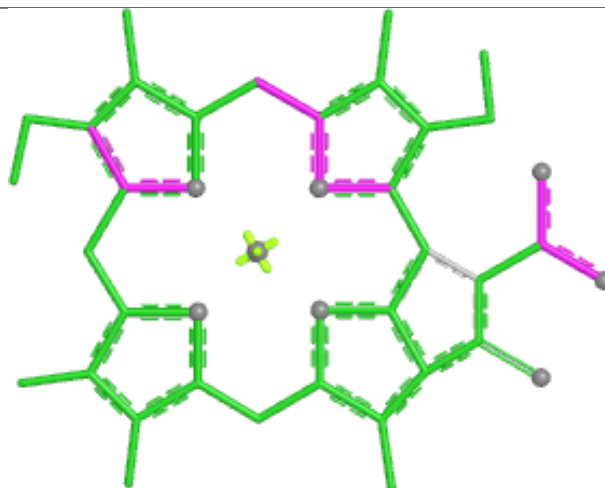
Ligand CLA 7 606



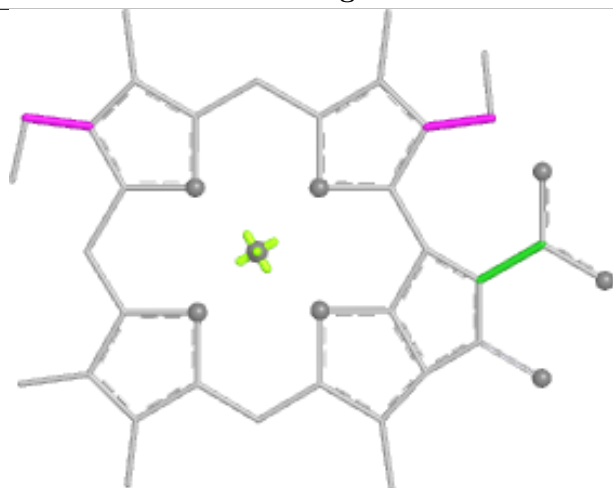
Ligand CLA 5 606



Bond lengths



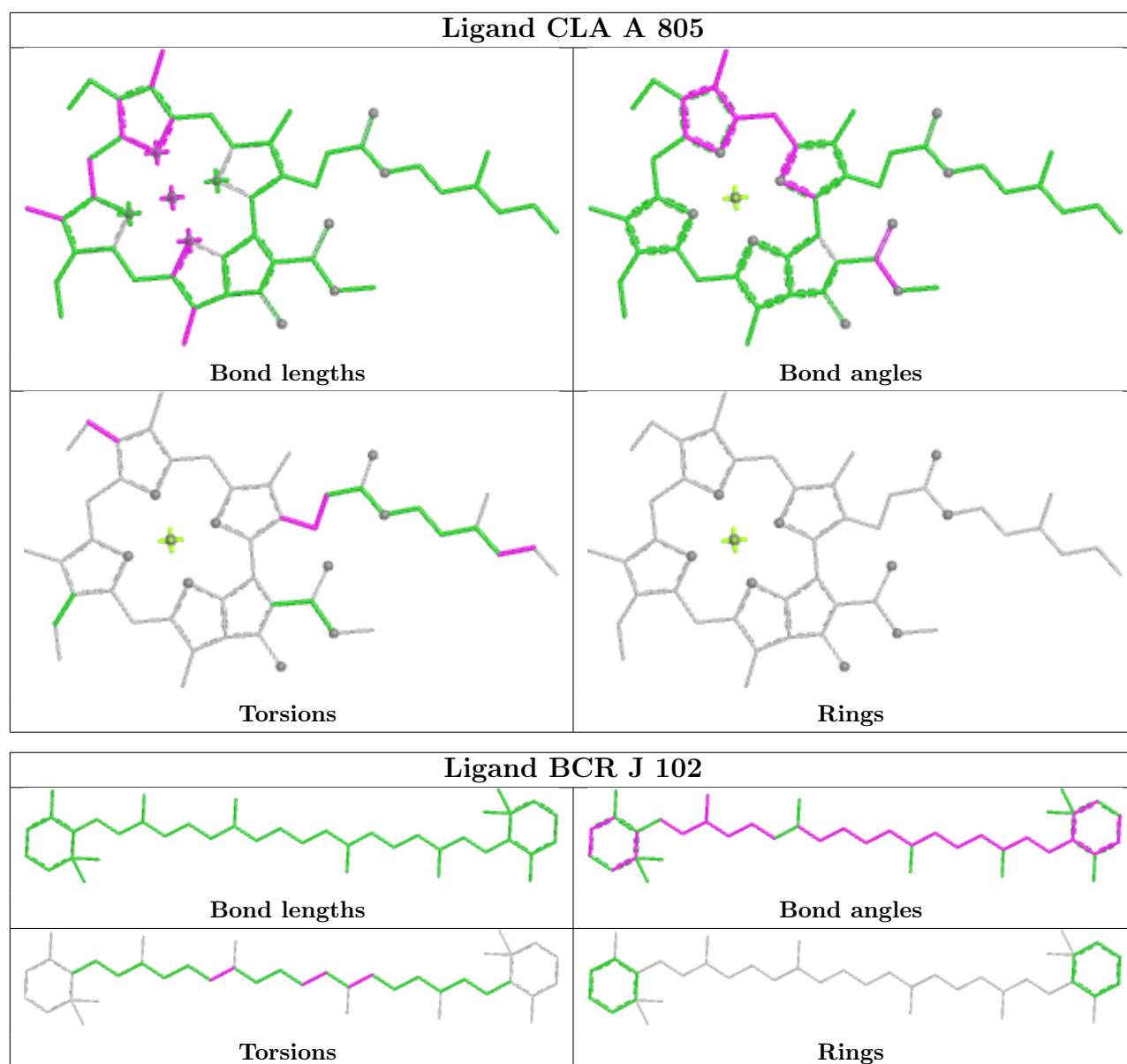
Bond angles



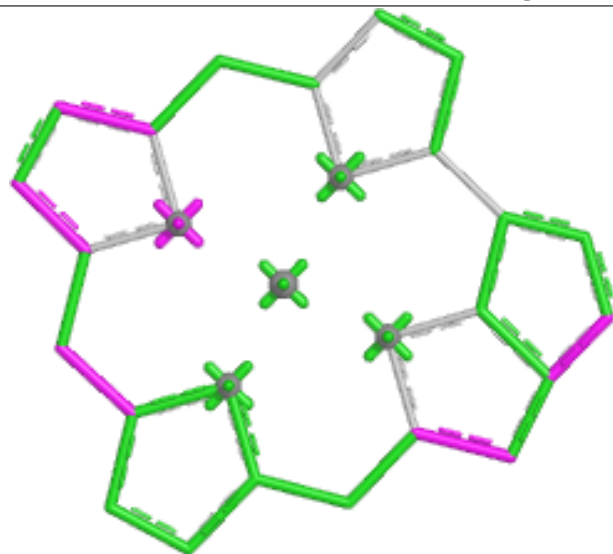
Torsions



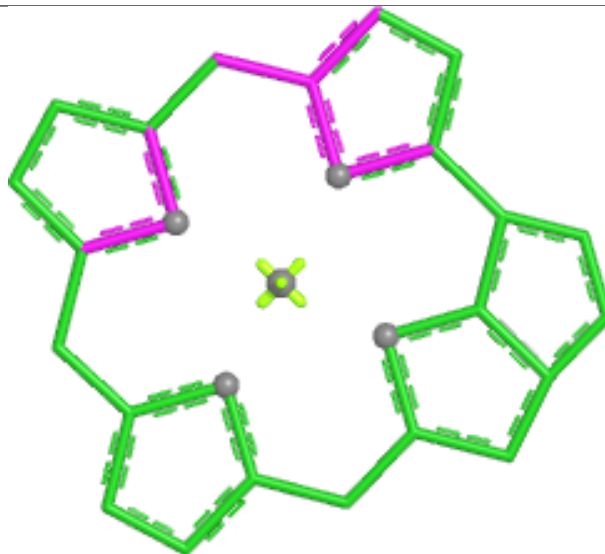
Rings



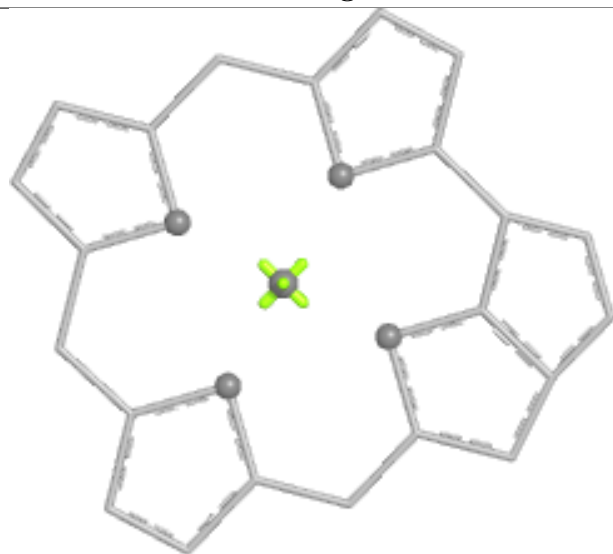
Ligand CLA 9 609



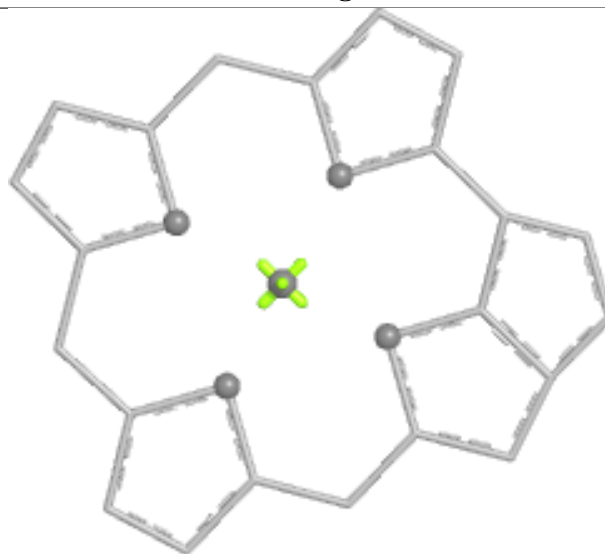
Bond lengths



Bond angles

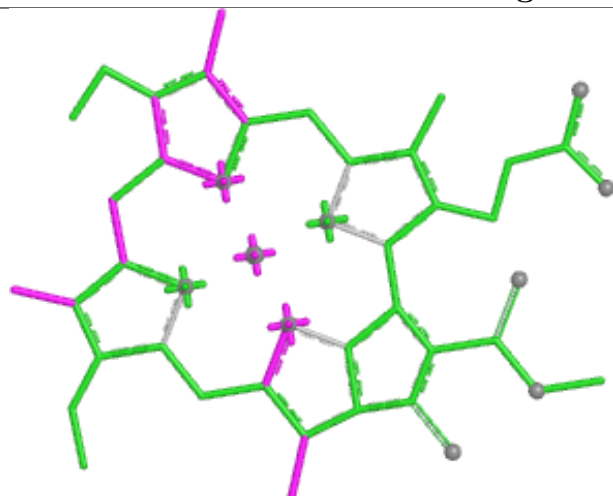


Torsions

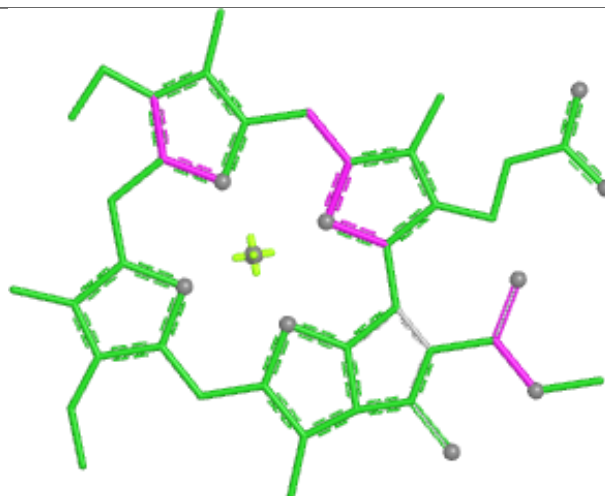


Rings

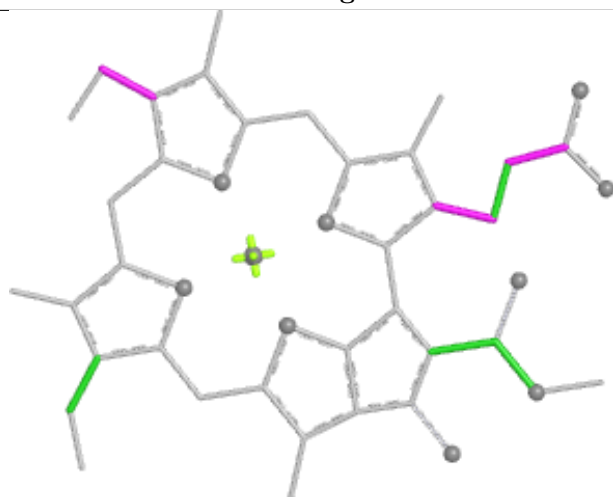
Ligand CLA L 303



Bond lengths



Bond angles

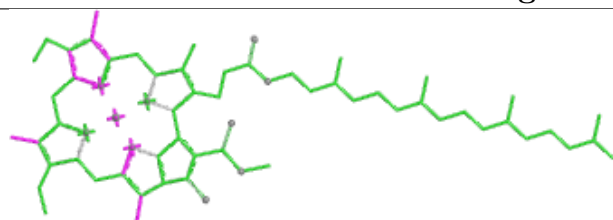


Torsions

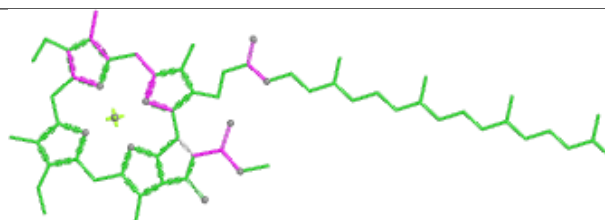


Rings

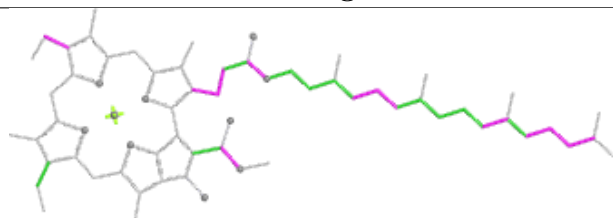
Ligand CLA 4 601



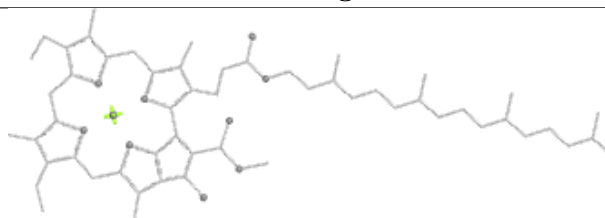
Bond lengths



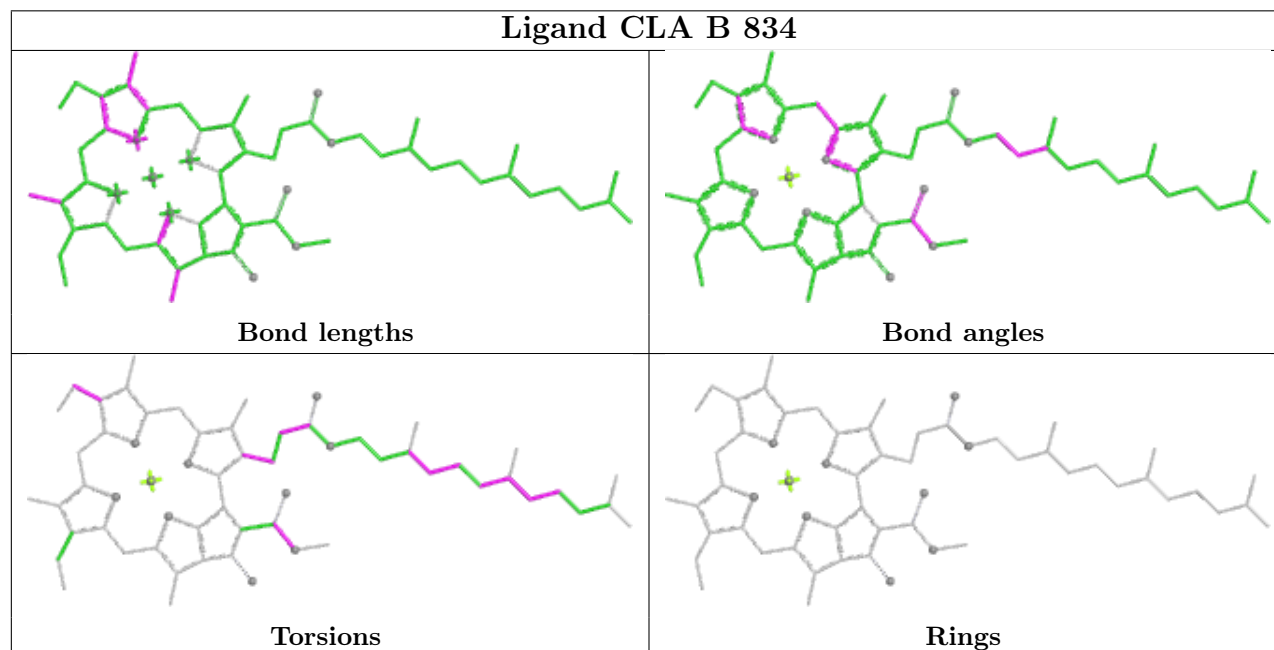
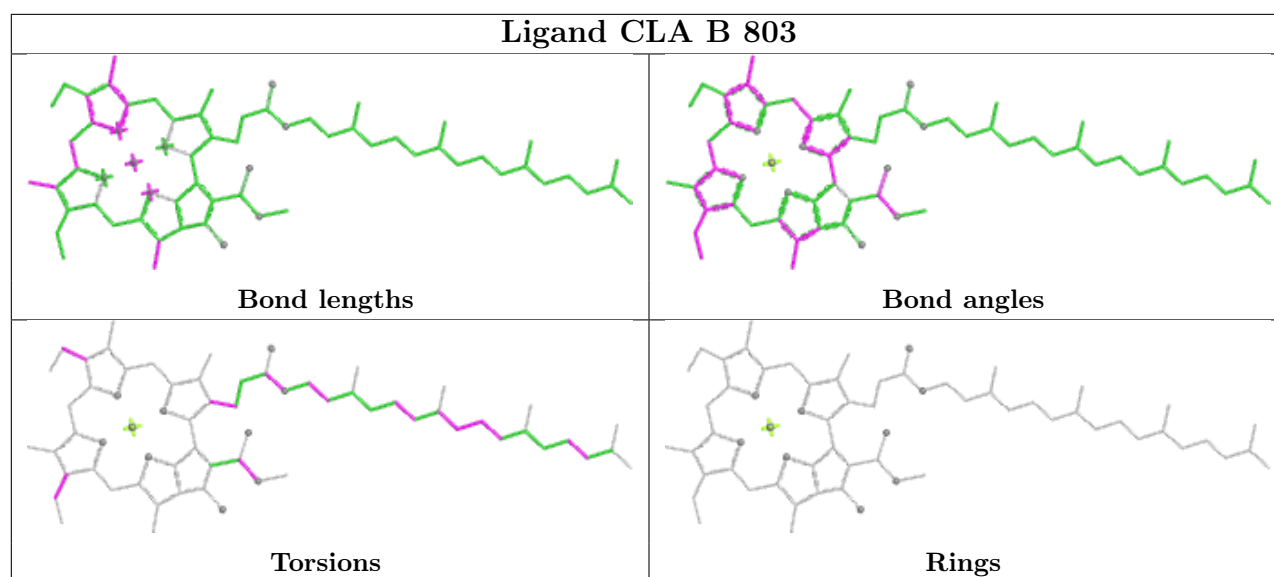
Bond angles

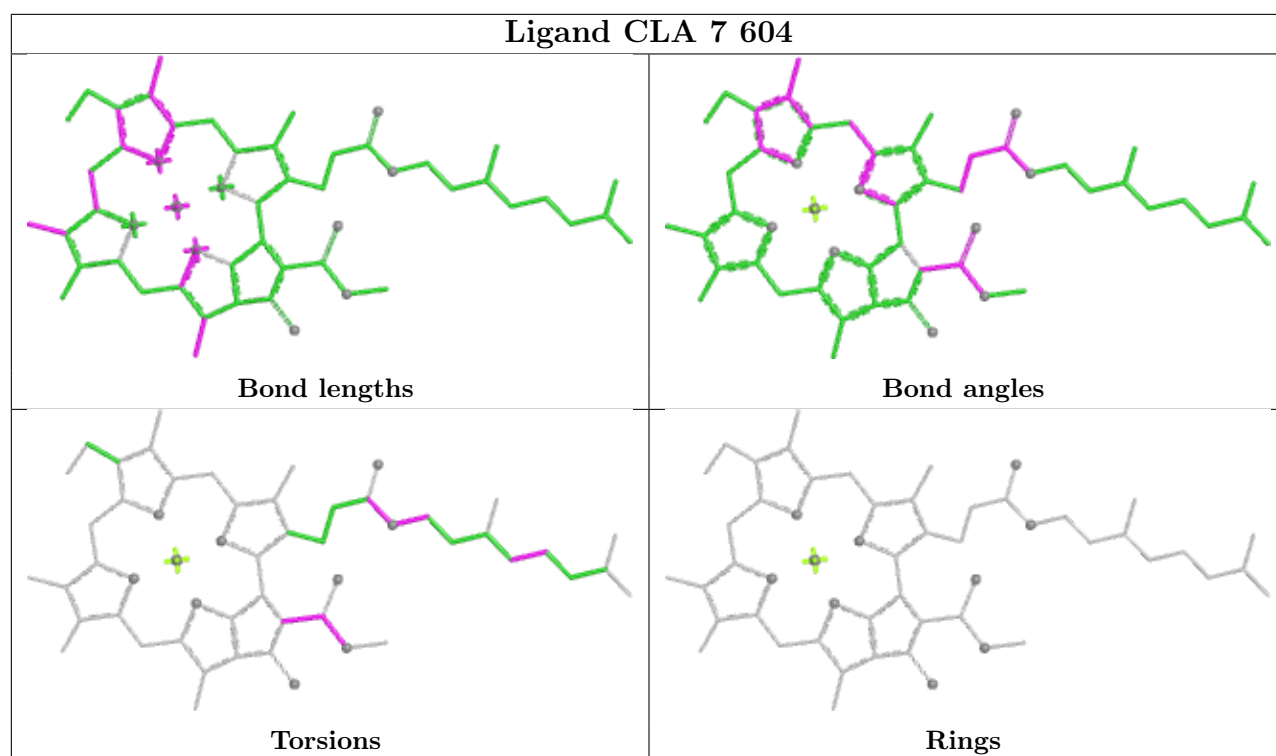


Torsions

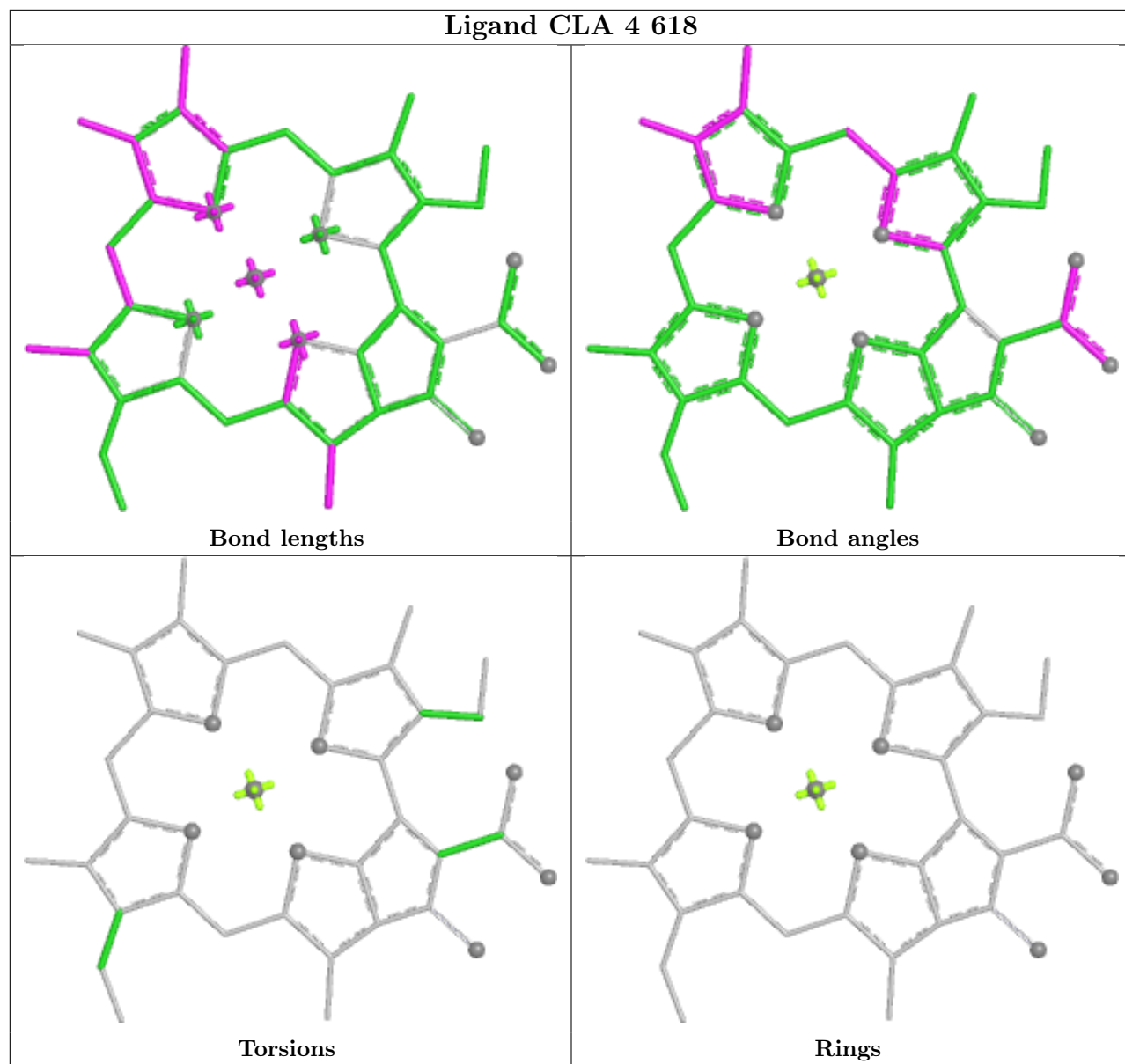


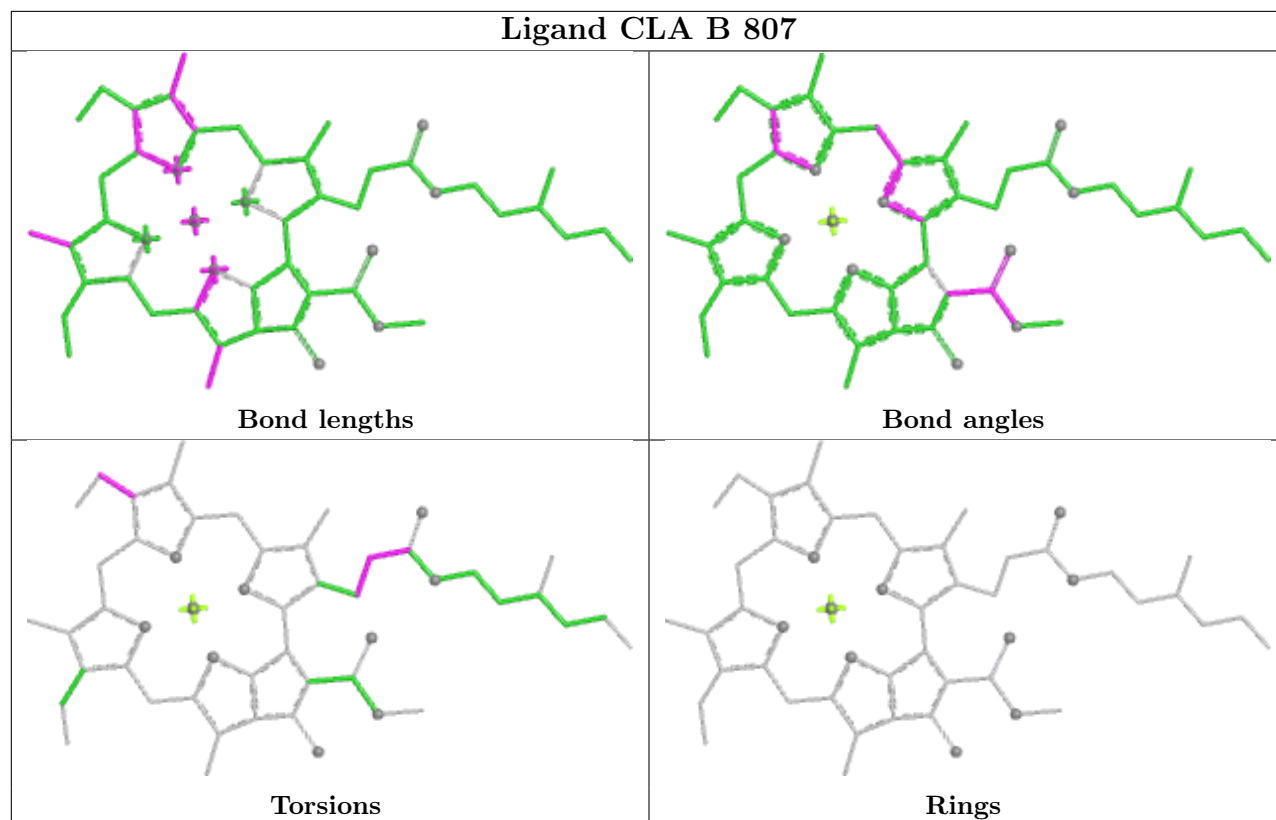
Rings



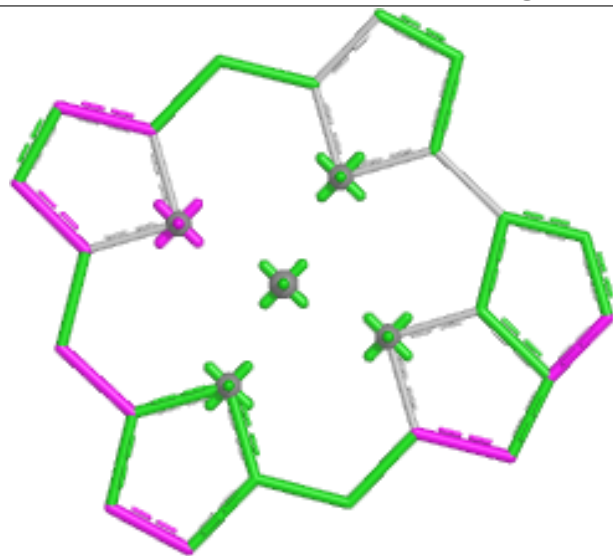


Ligand CLA 4 618

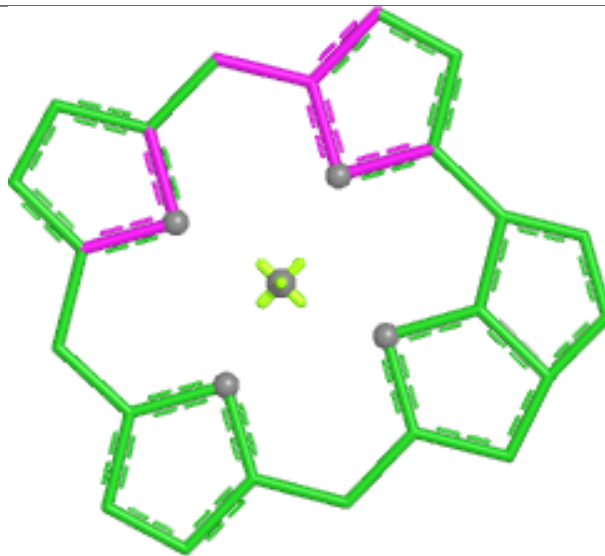




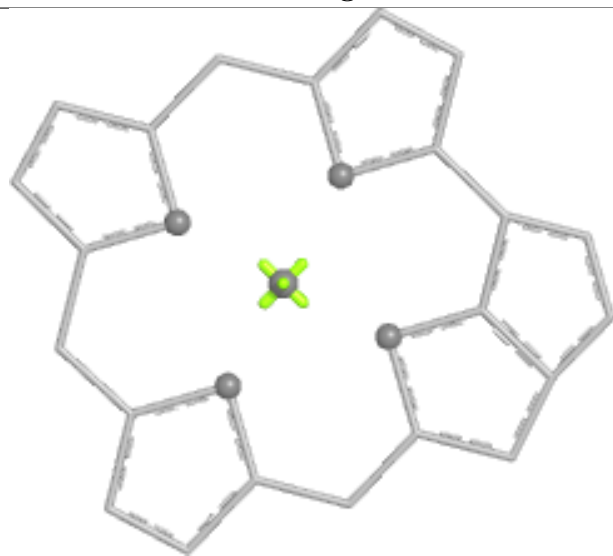
Ligand CLA 9 601



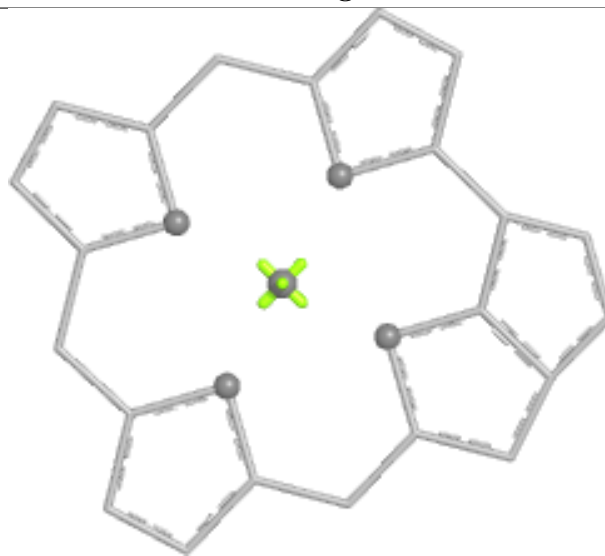
Bond lengths



Bond angles

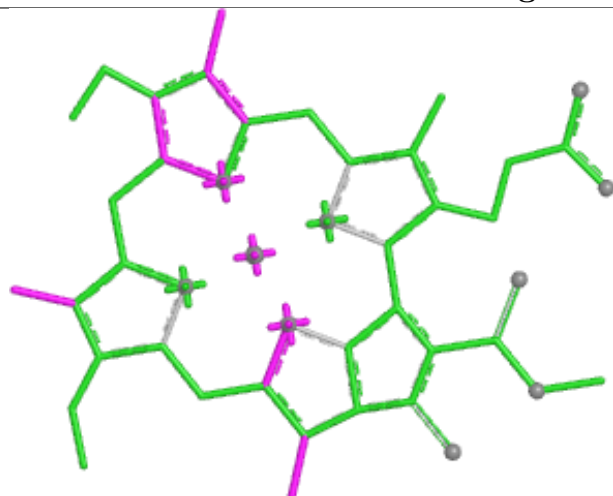


Torsions

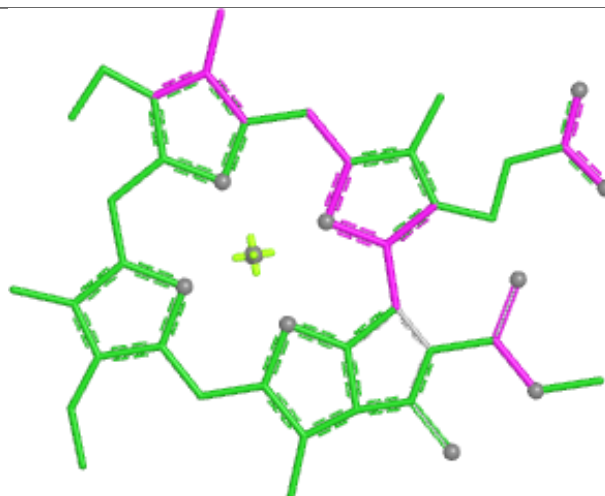


Rings

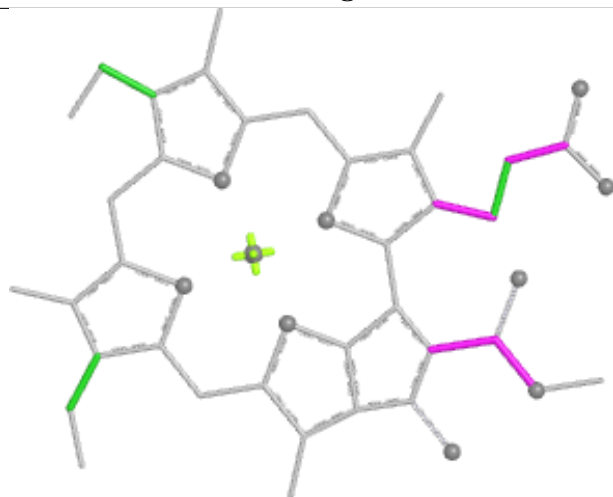
Ligand CLA 1 612



Bond lengths



Bond angles

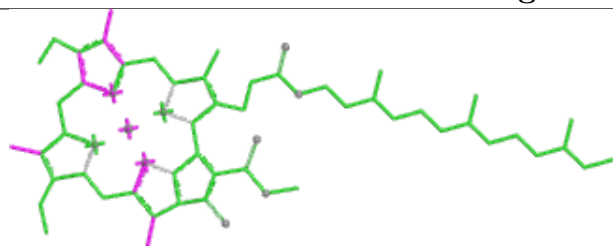


Torsions

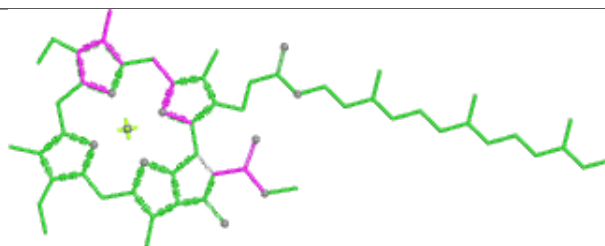


Rings

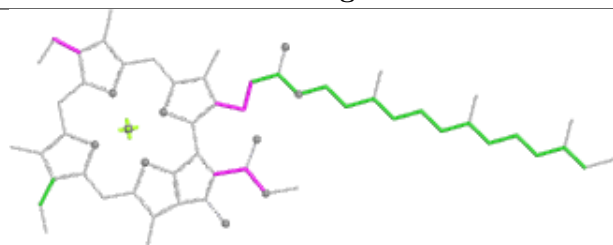
Ligand CLA 1 602



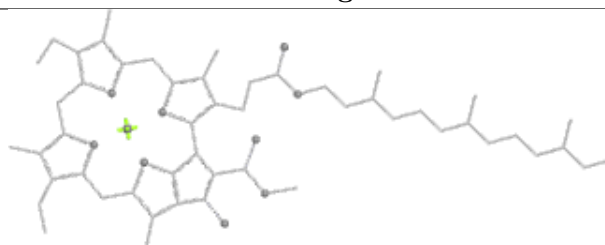
Bond lengths



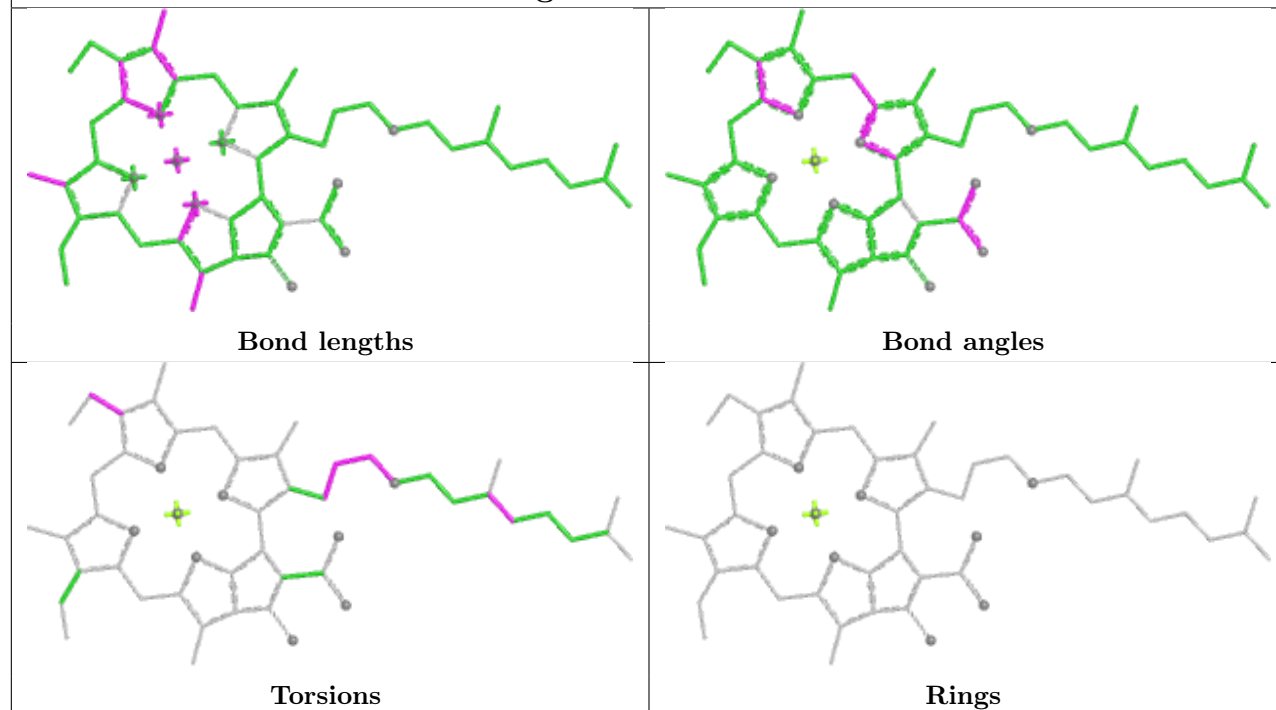
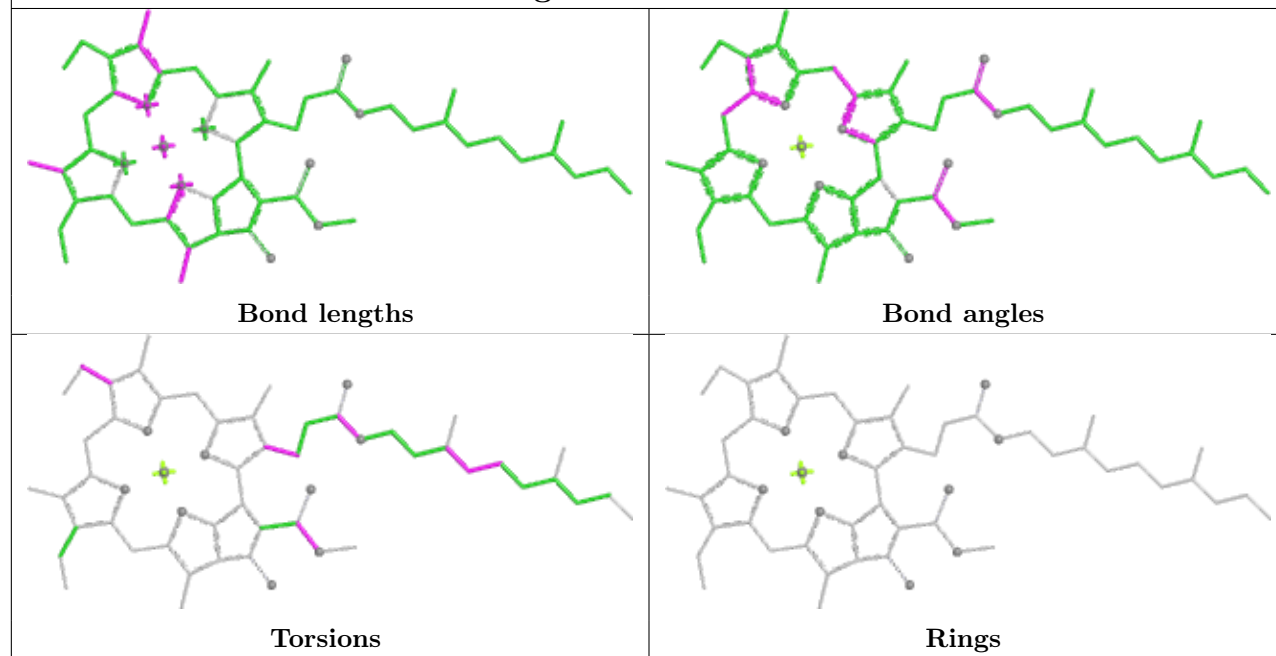
Bond angles

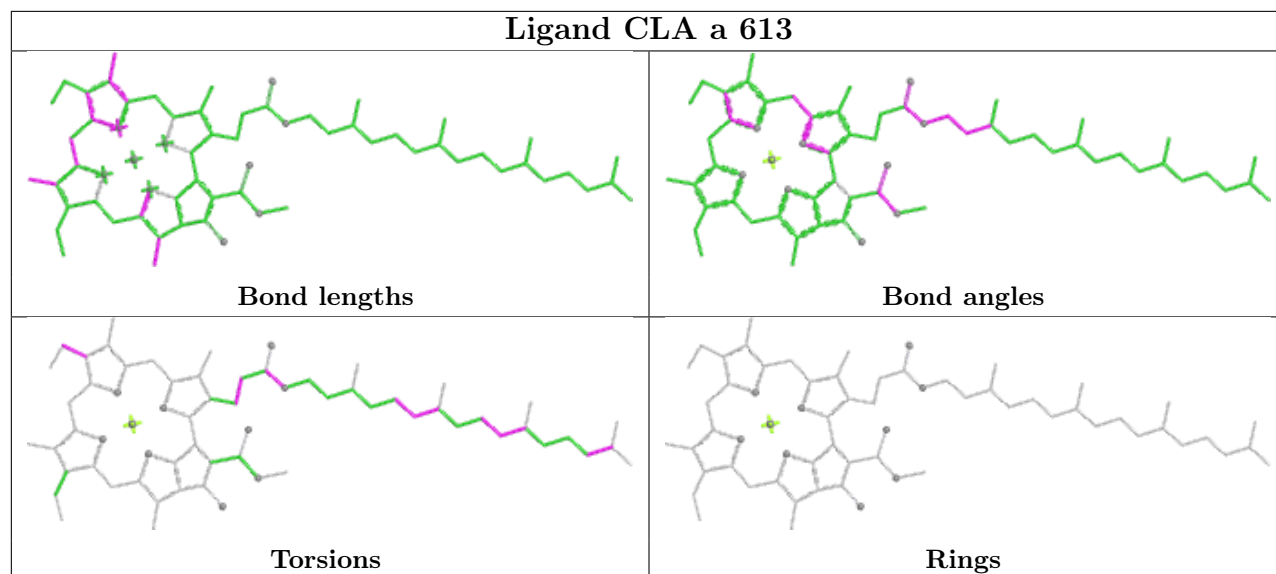
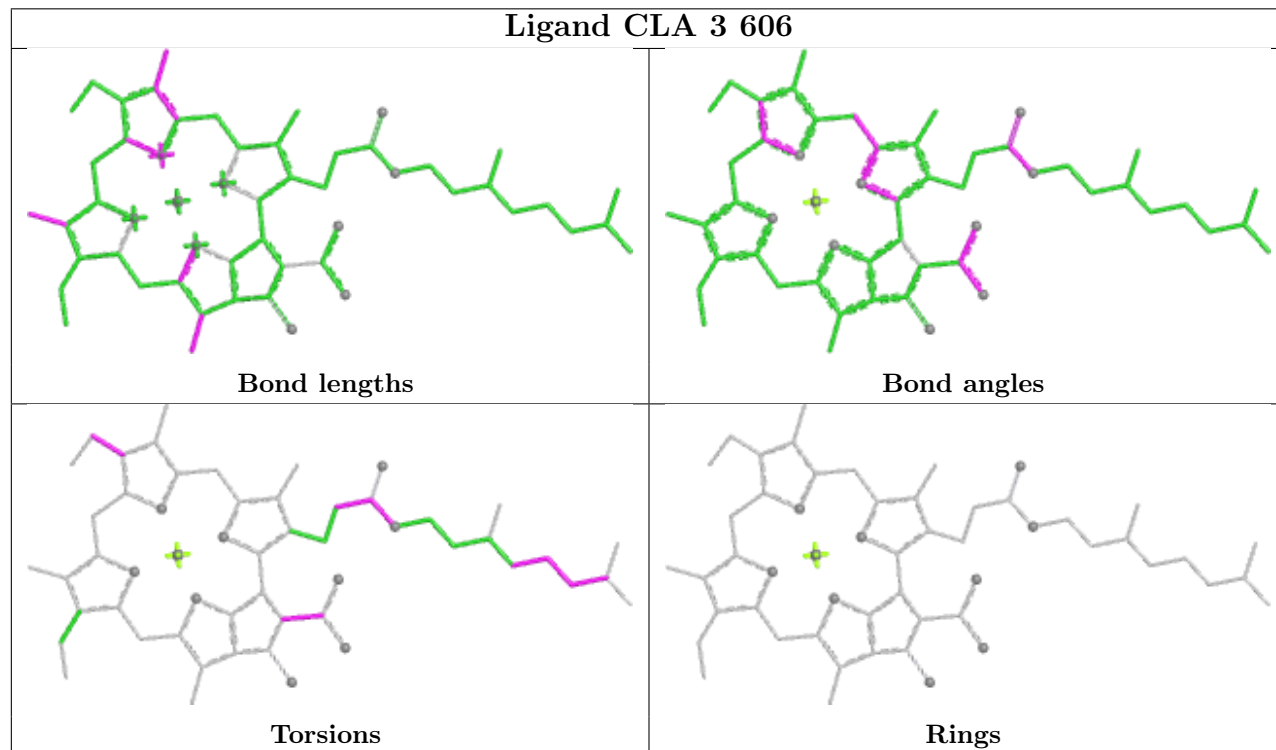


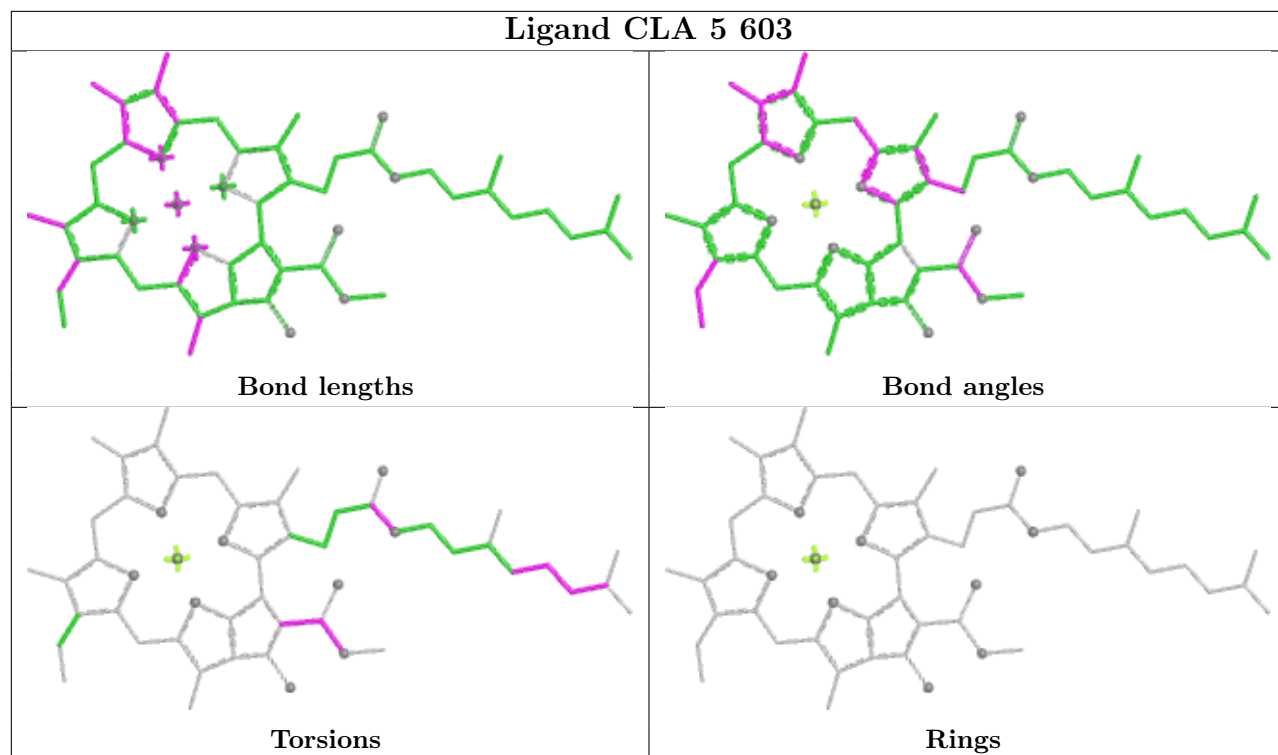
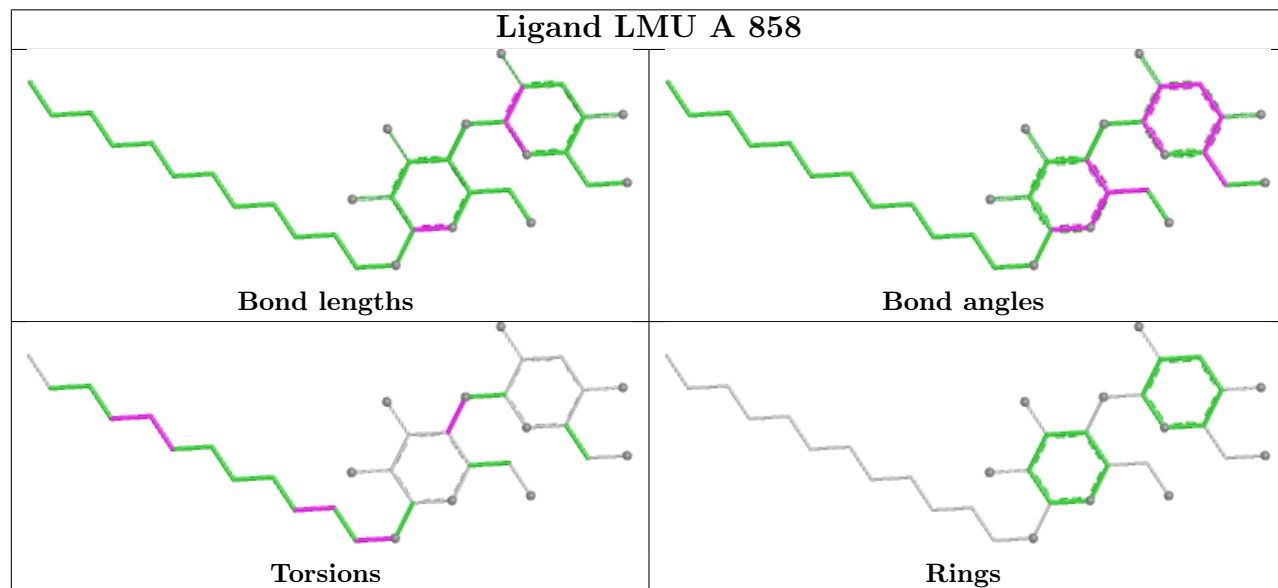
Torsions

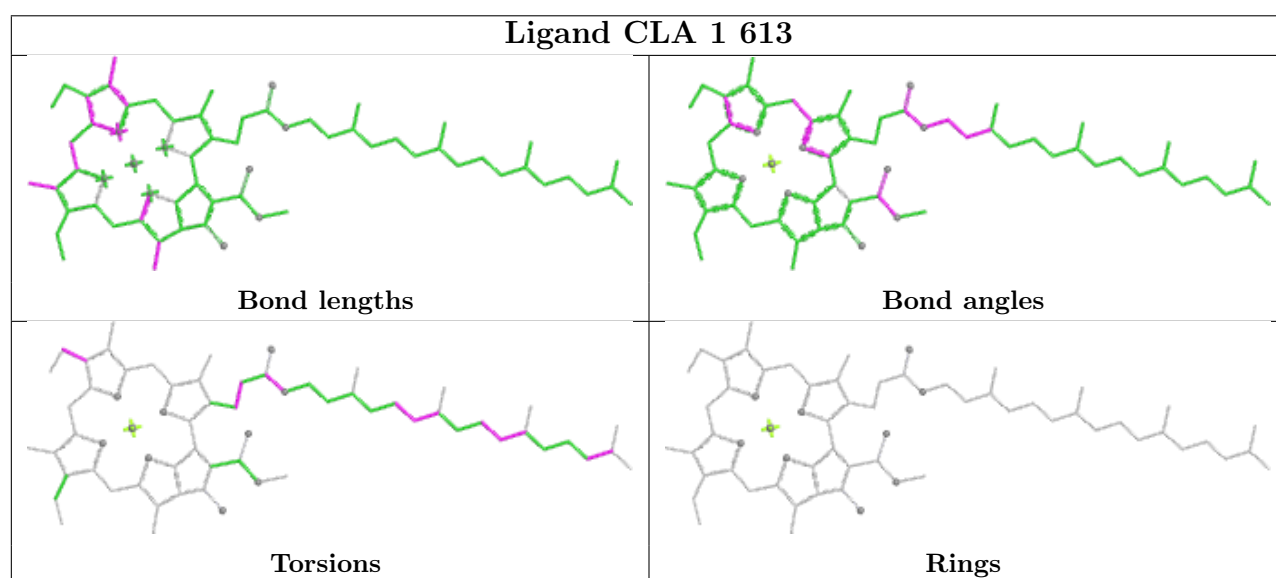
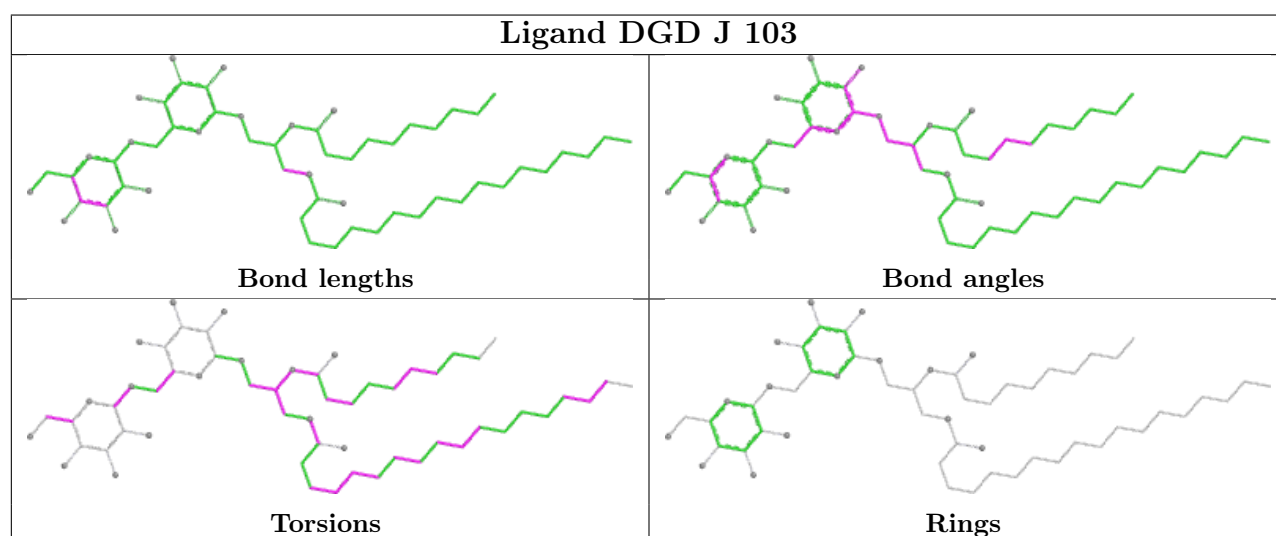
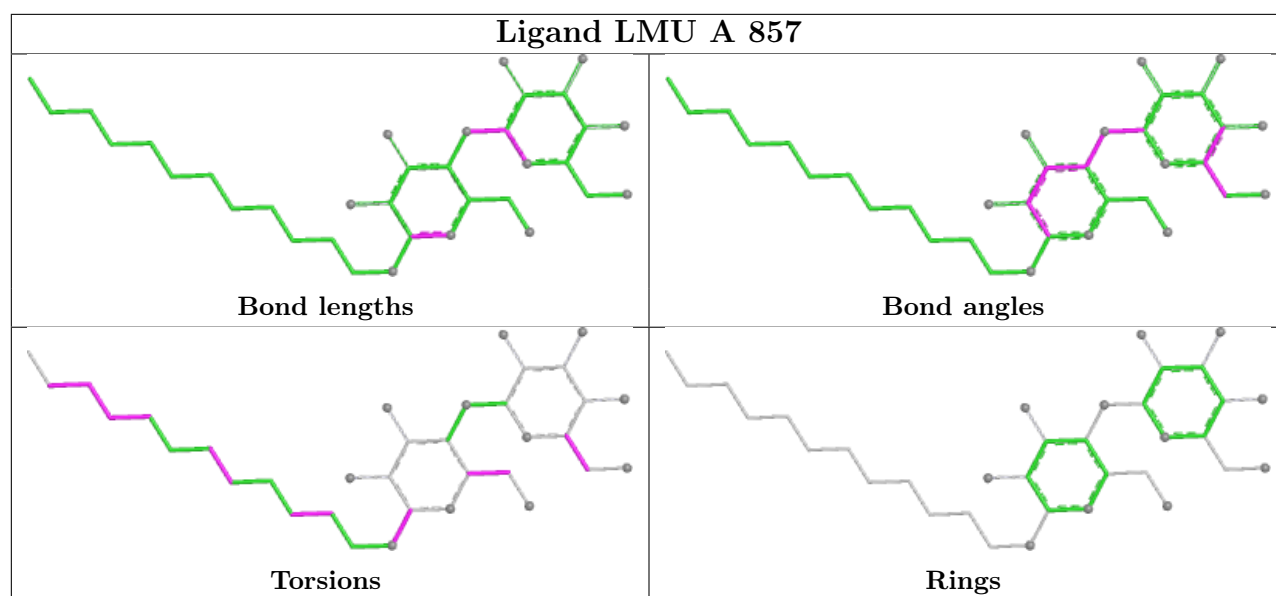


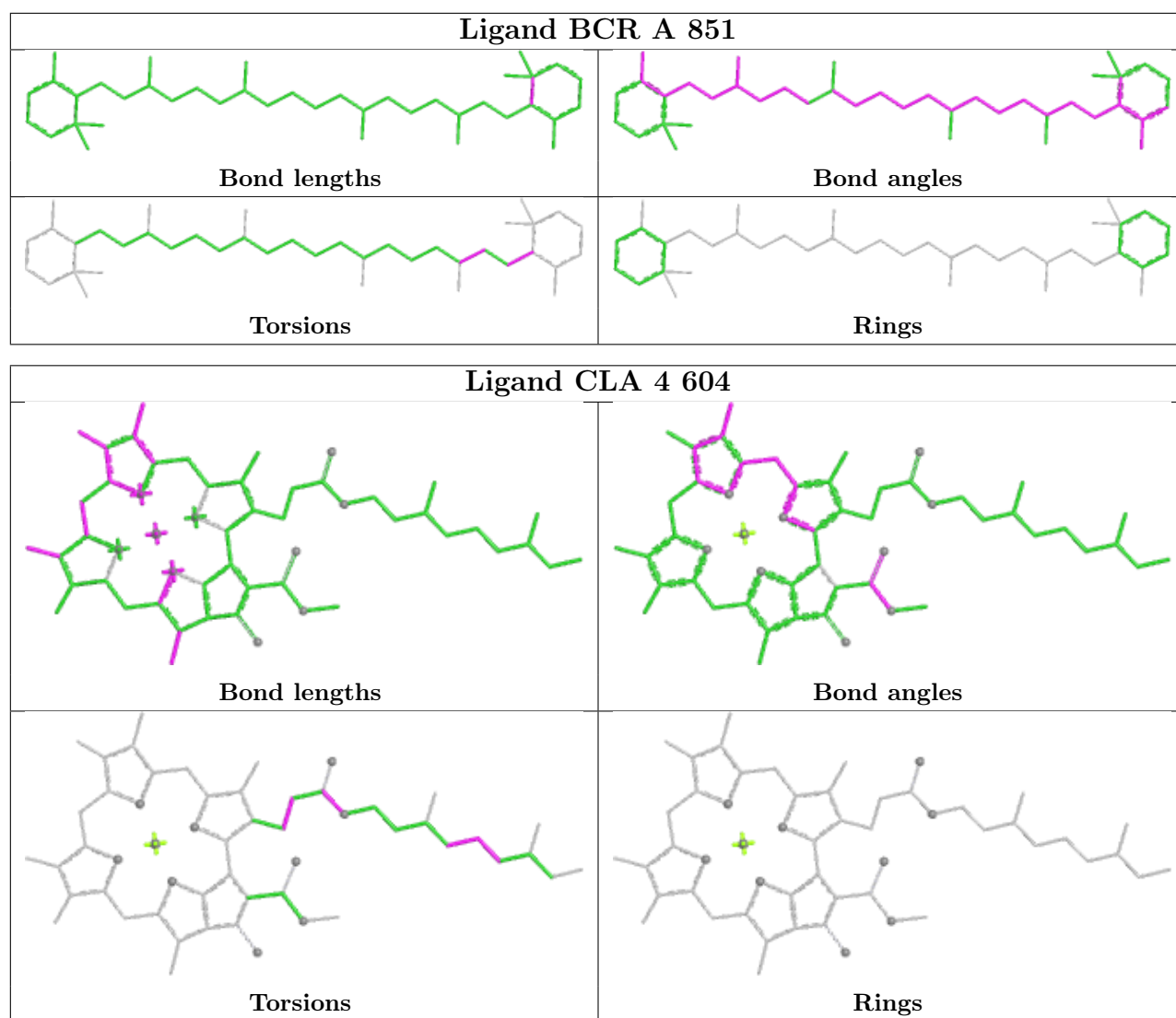
Rings

Ligand CLA 3 613**Ligand CLA F 301**

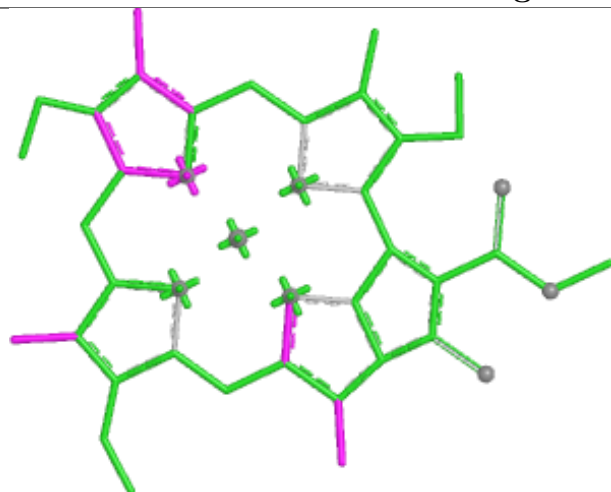
Ligand CLA a 613**Ligand CLA 3 606**

Ligand CLA 5 603**Ligand LMU A 858**

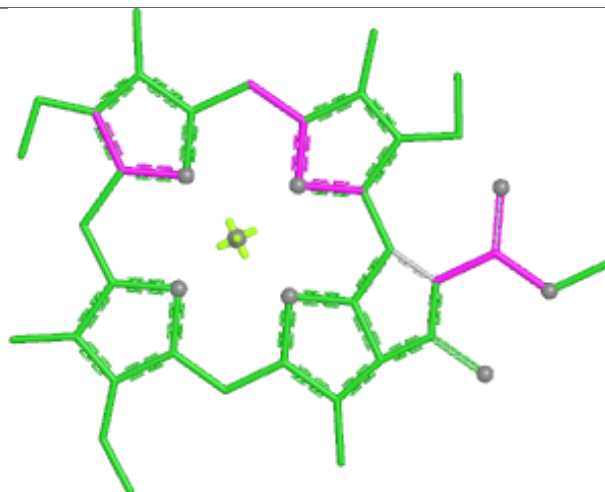




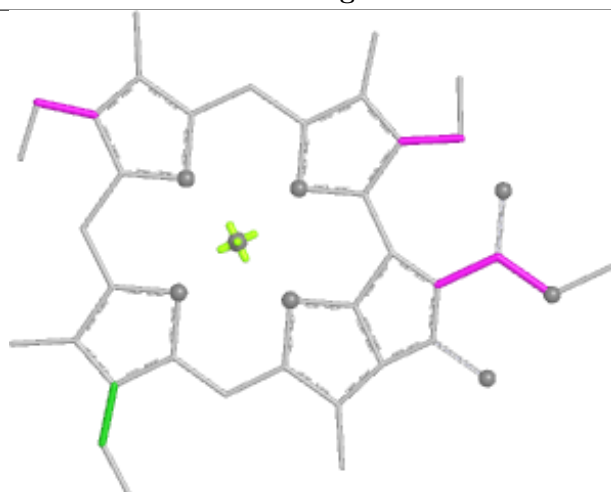
Ligand CLA A 823



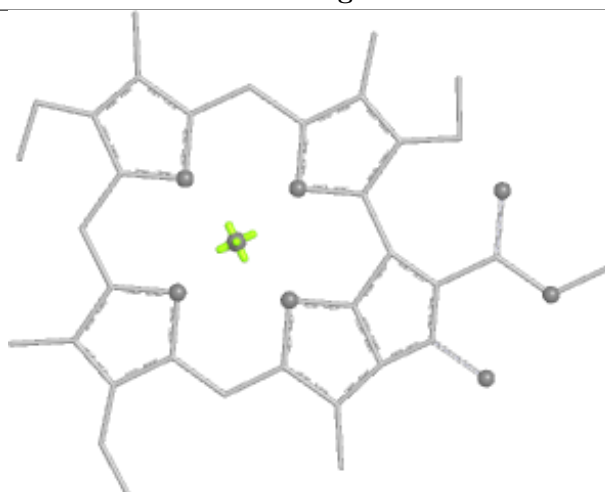
Bond lengths



Bond angles

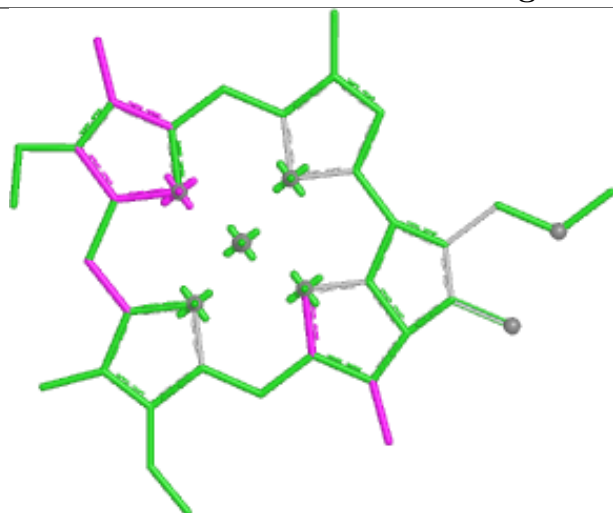


Torsions

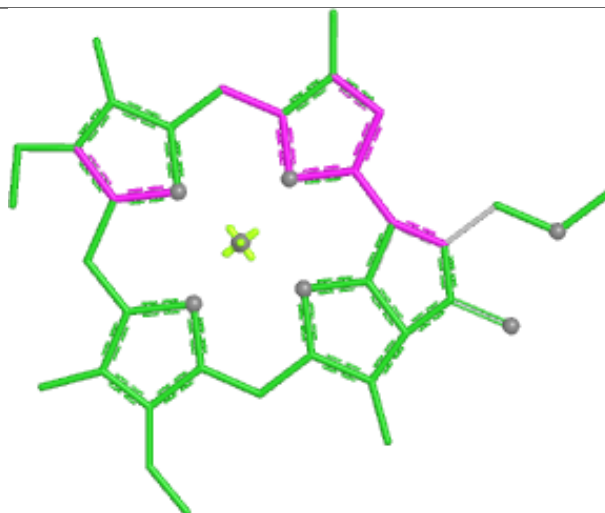


Rings

Ligand CLA 1 606



Bond lengths



Bond angles

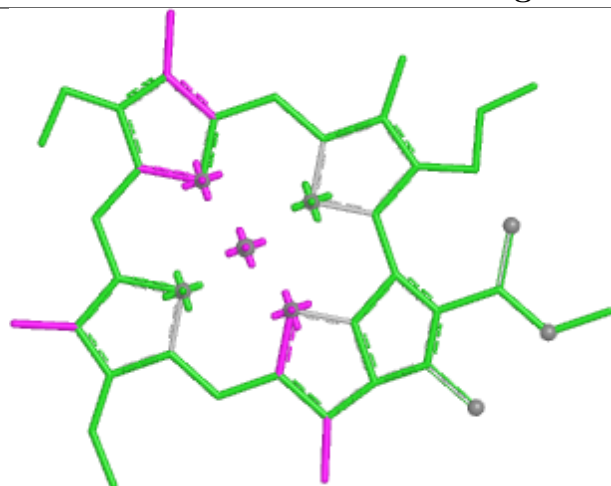


Torsions

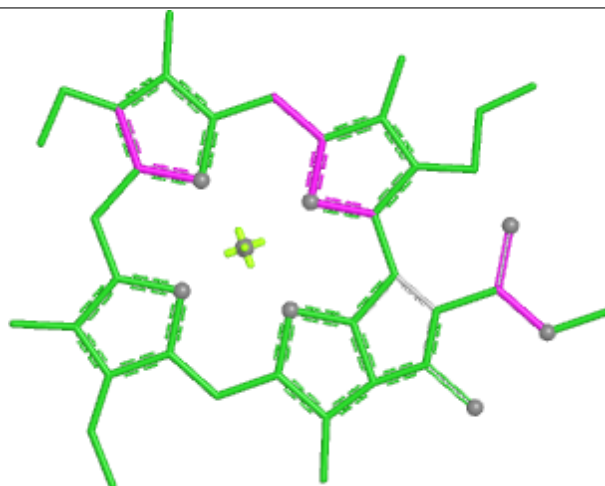


Rings

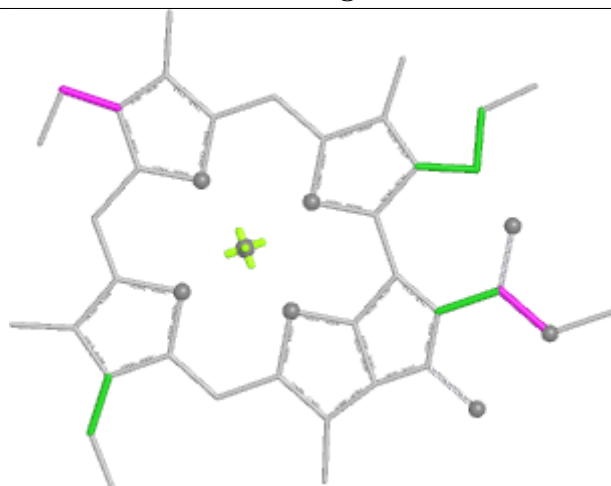
Ligand CLA B 830



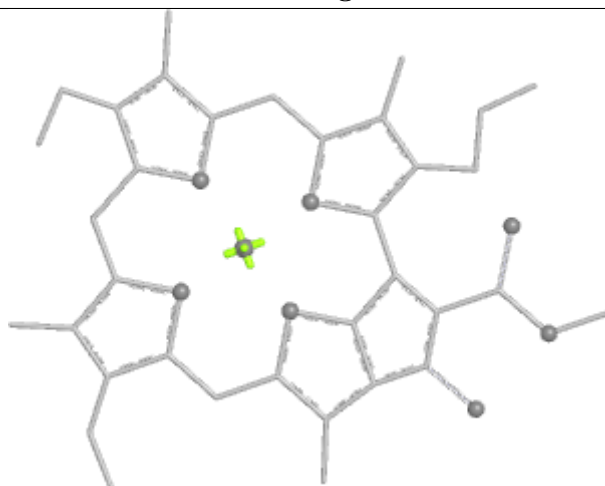
Bond lengths



Bond angles

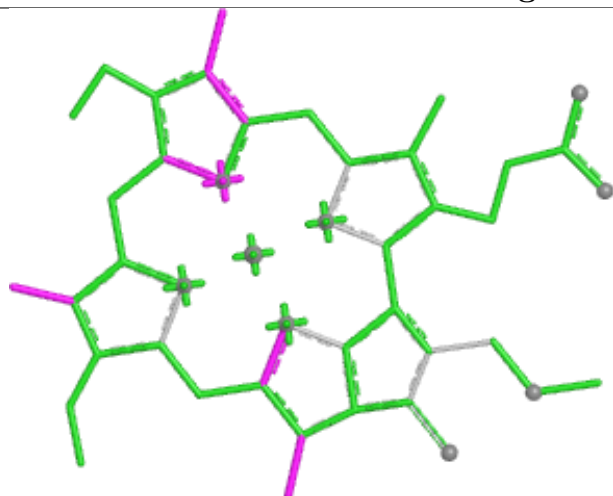


Torsions

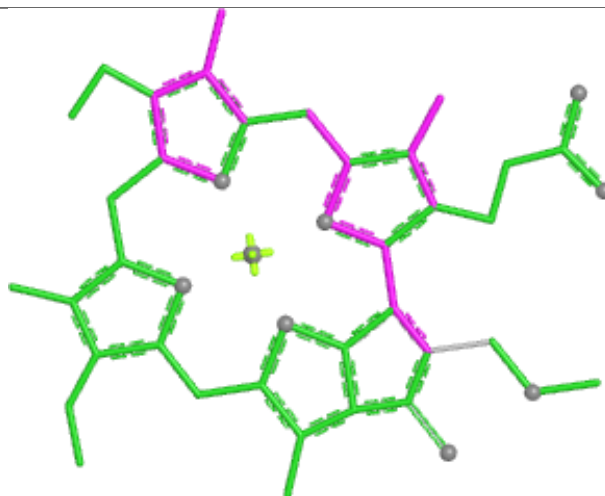


Rings

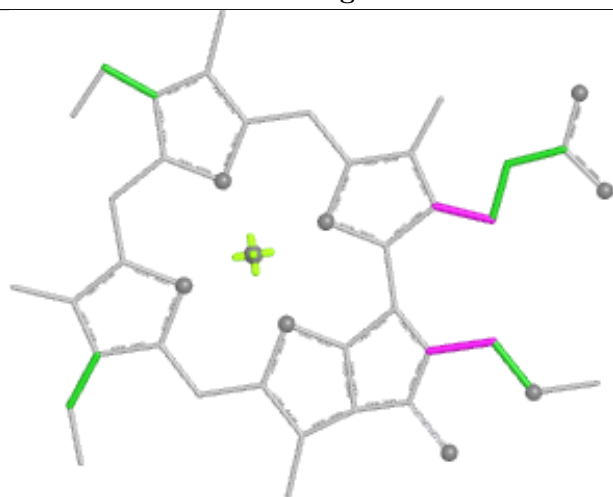
Ligand CLA 7 609



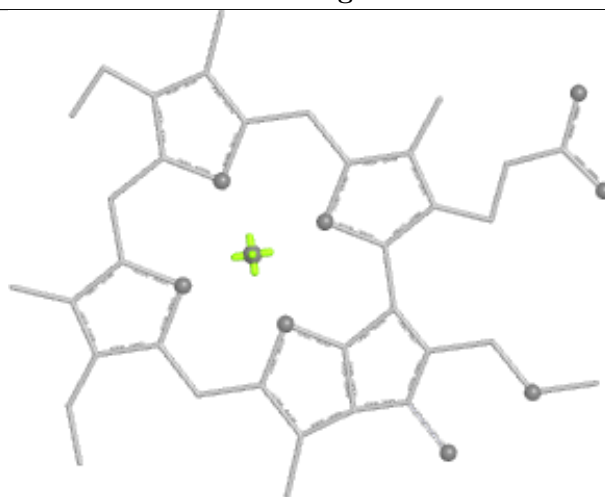
Bond lengths



Bond angles

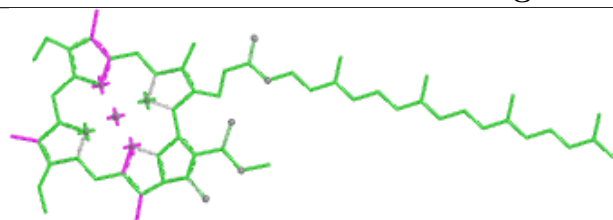


Torsions

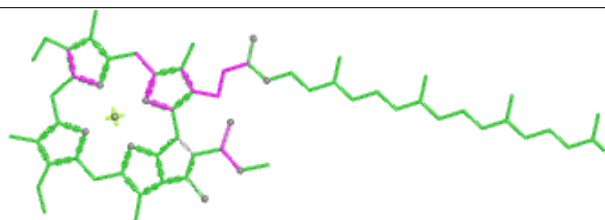


Rings

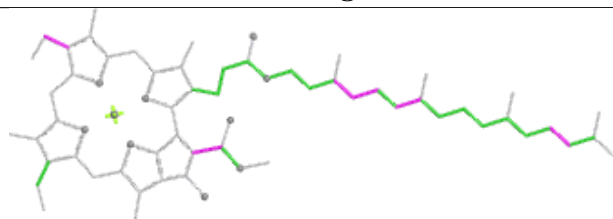
Ligand CLA A 828



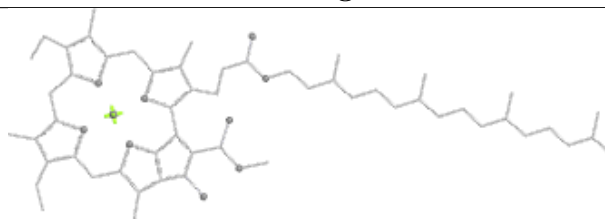
Bond lengths



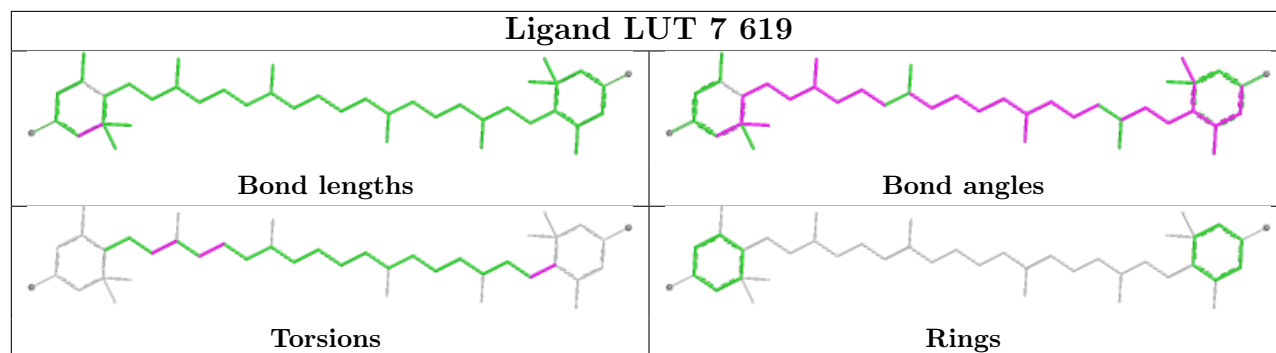
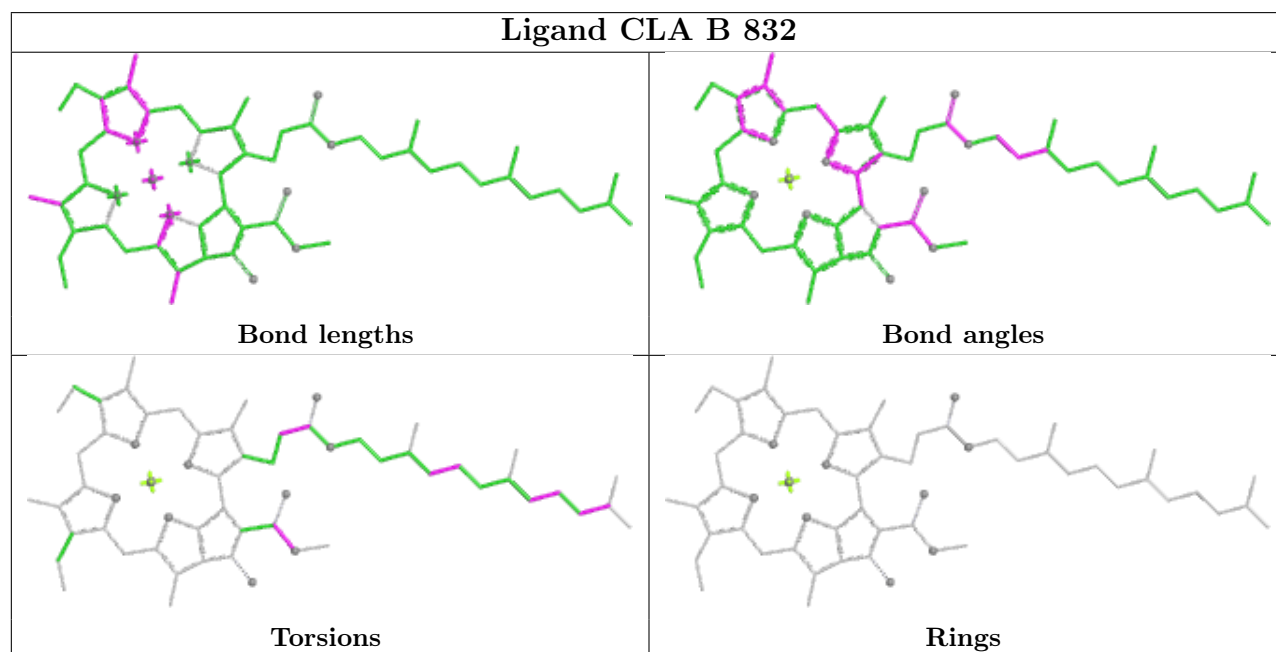
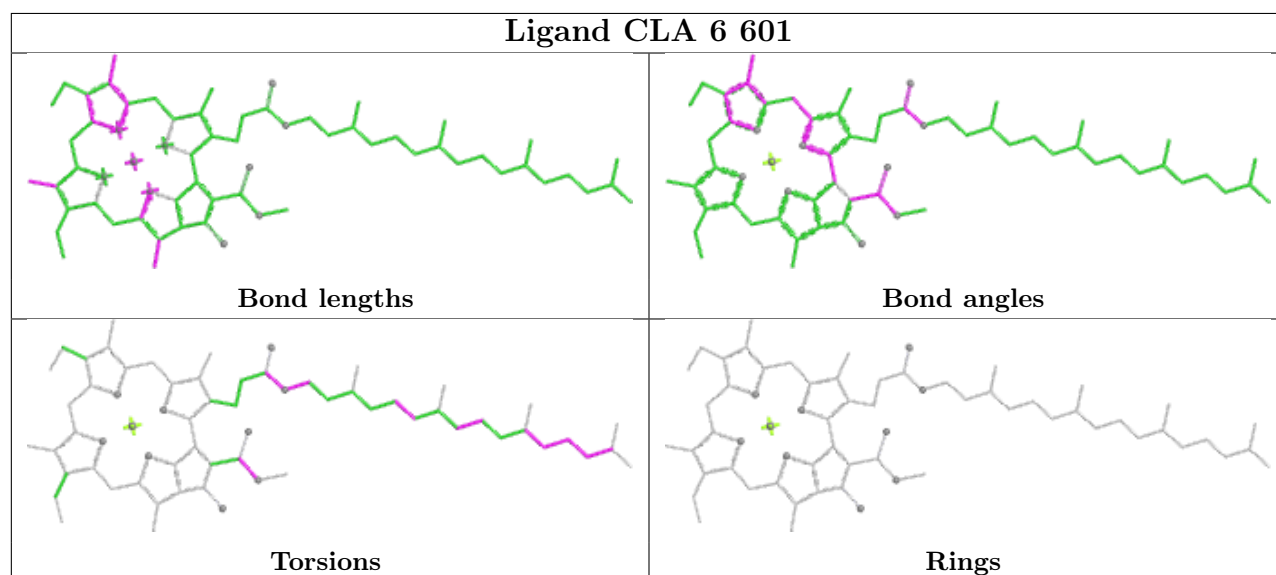
Bond angles

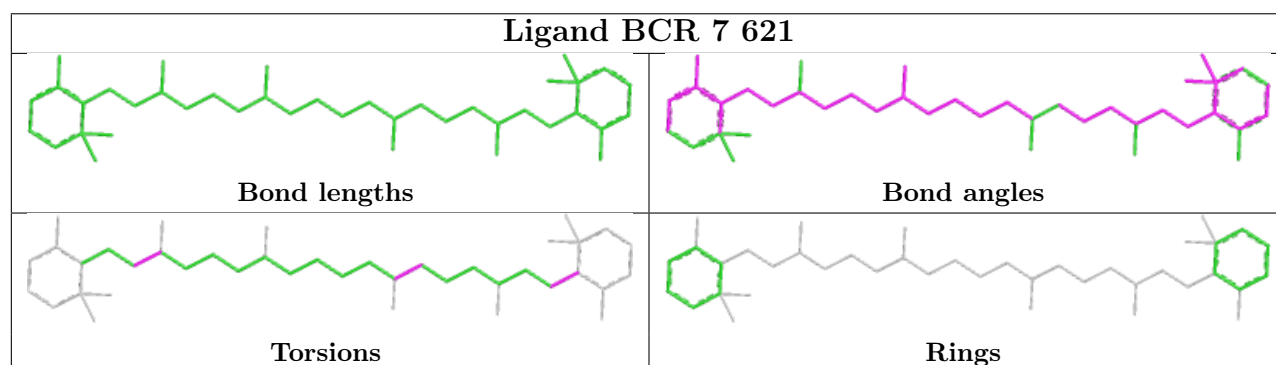
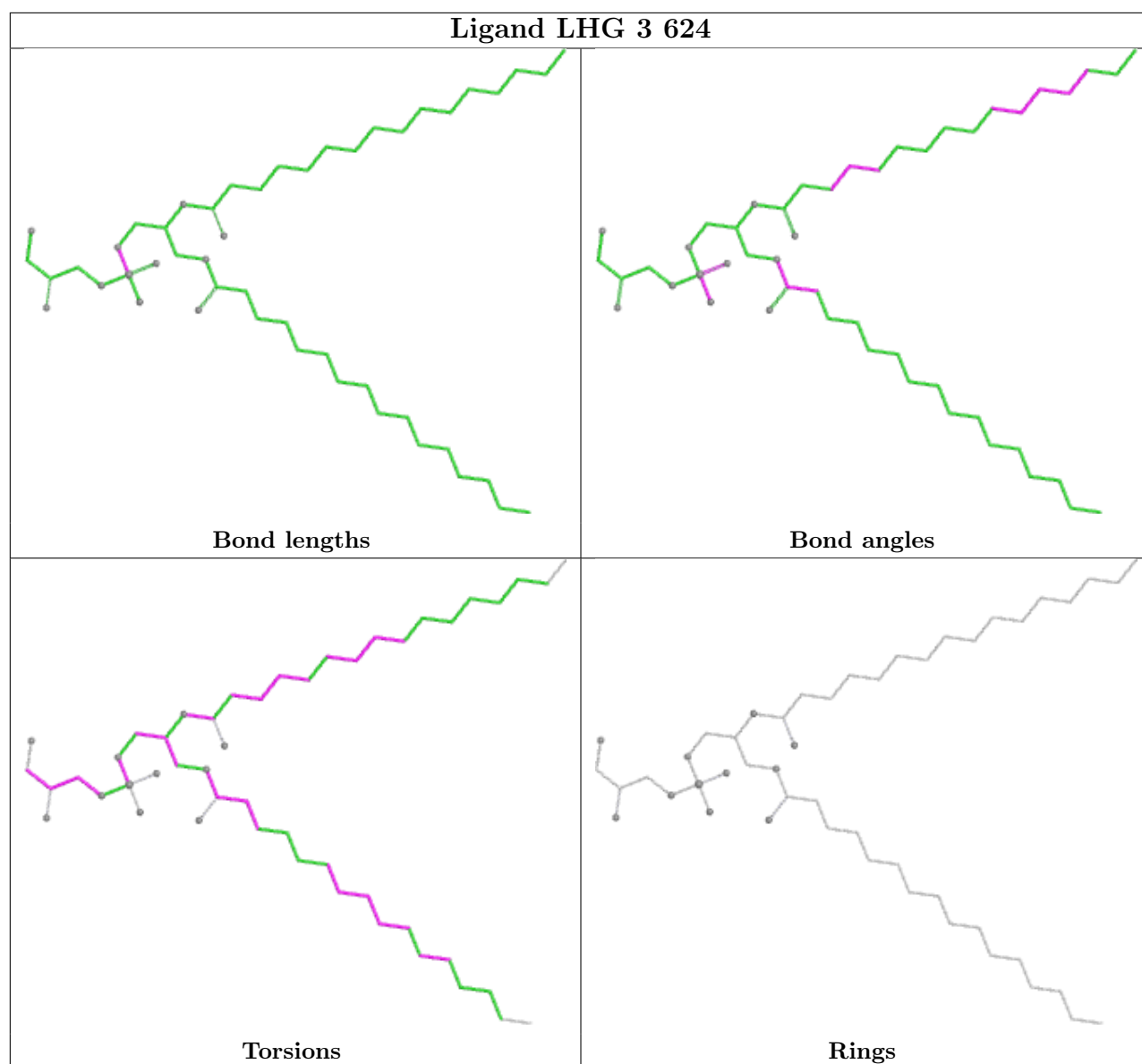


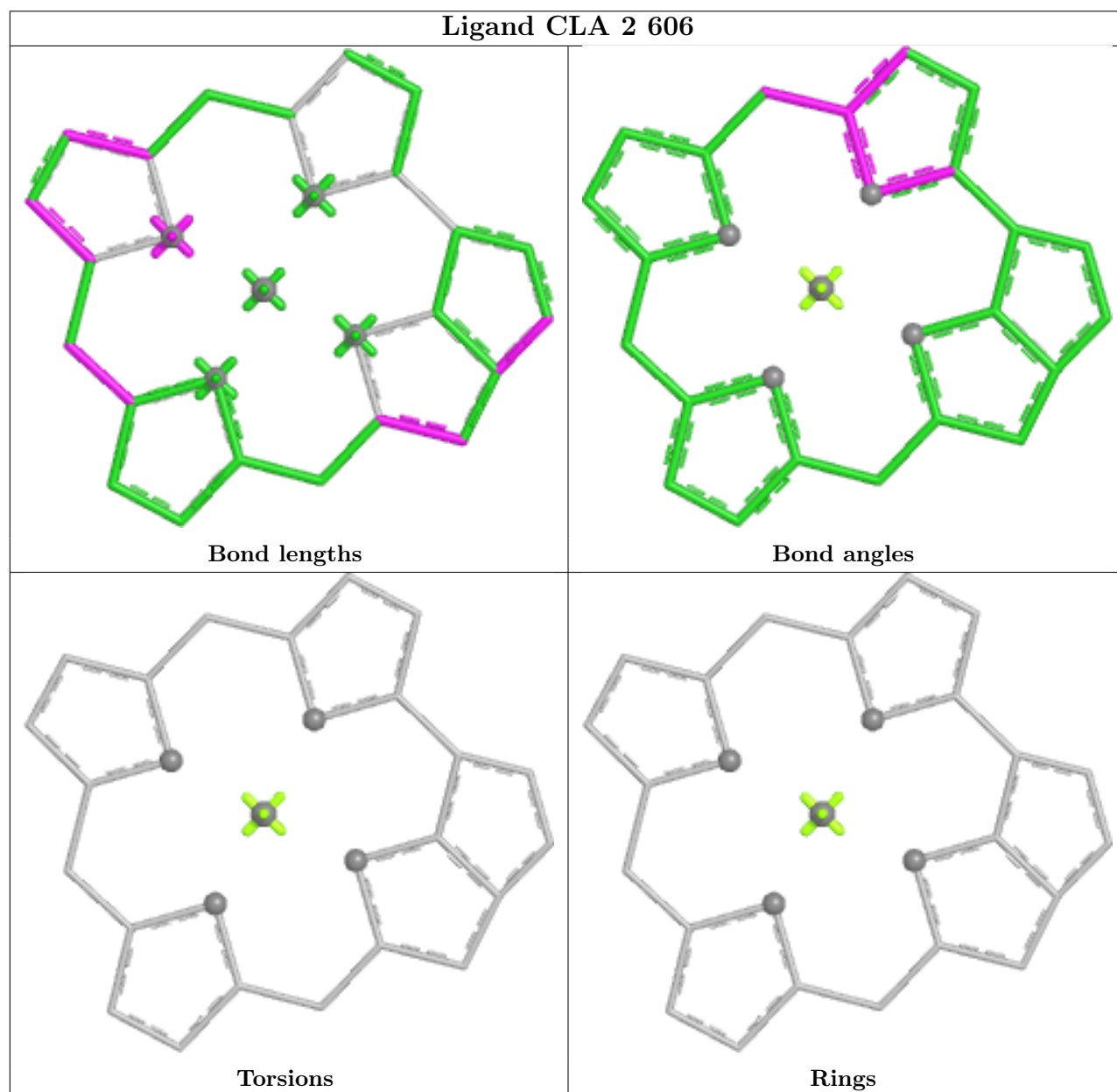
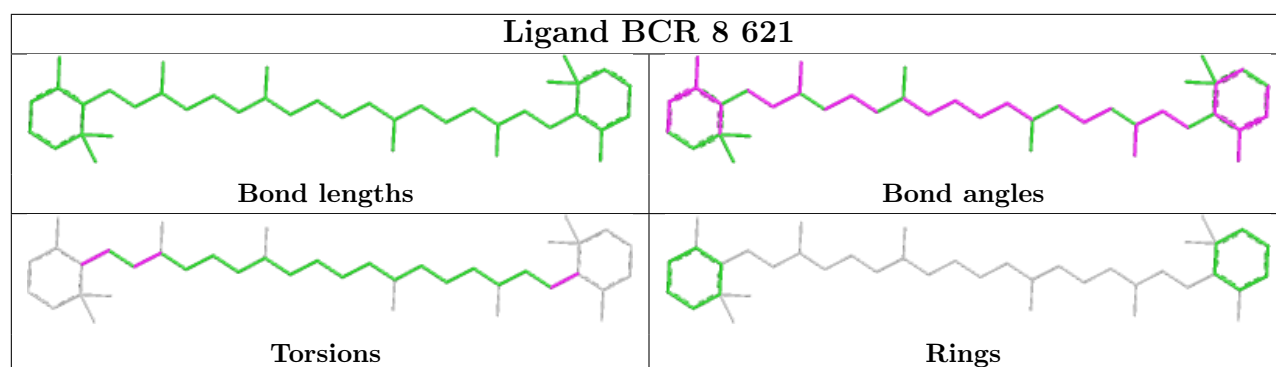
Torsions

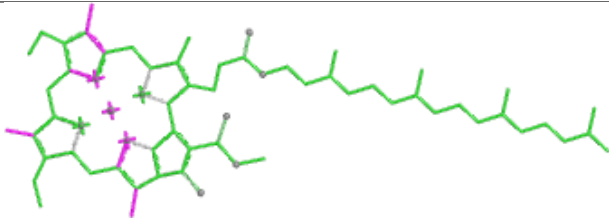
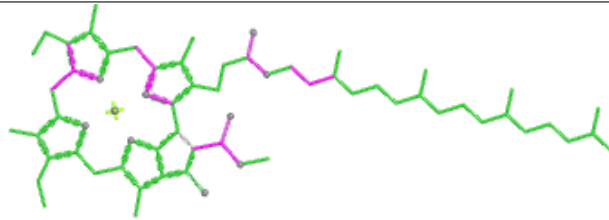
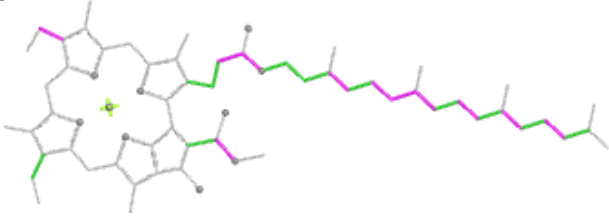
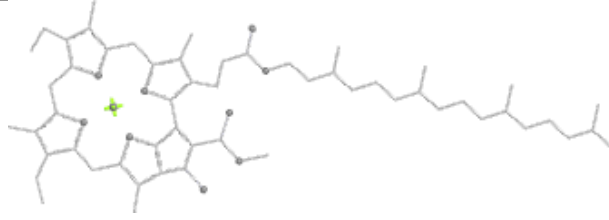


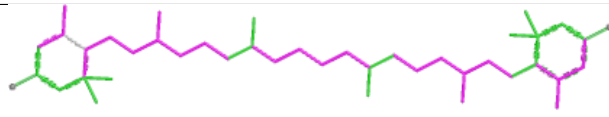
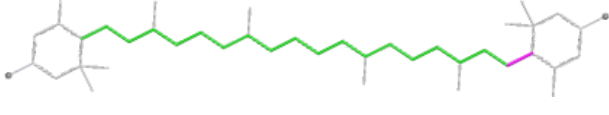
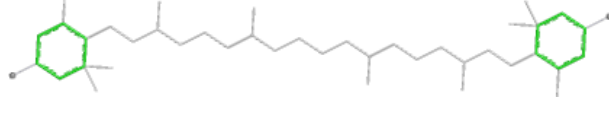
Rings

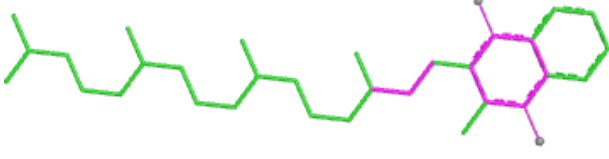
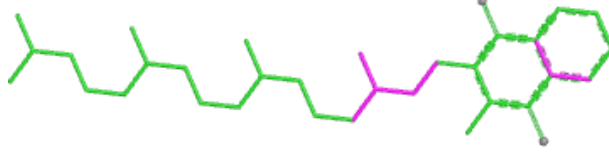
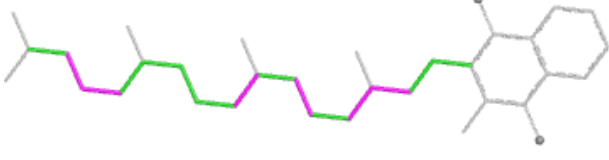
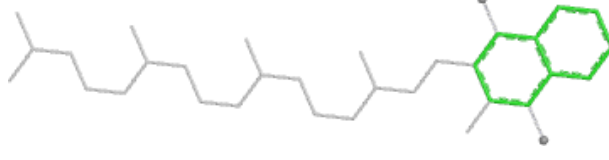
Ligand LUT 7 619**Ligand CLA B 832****Ligand CLA 6 601**



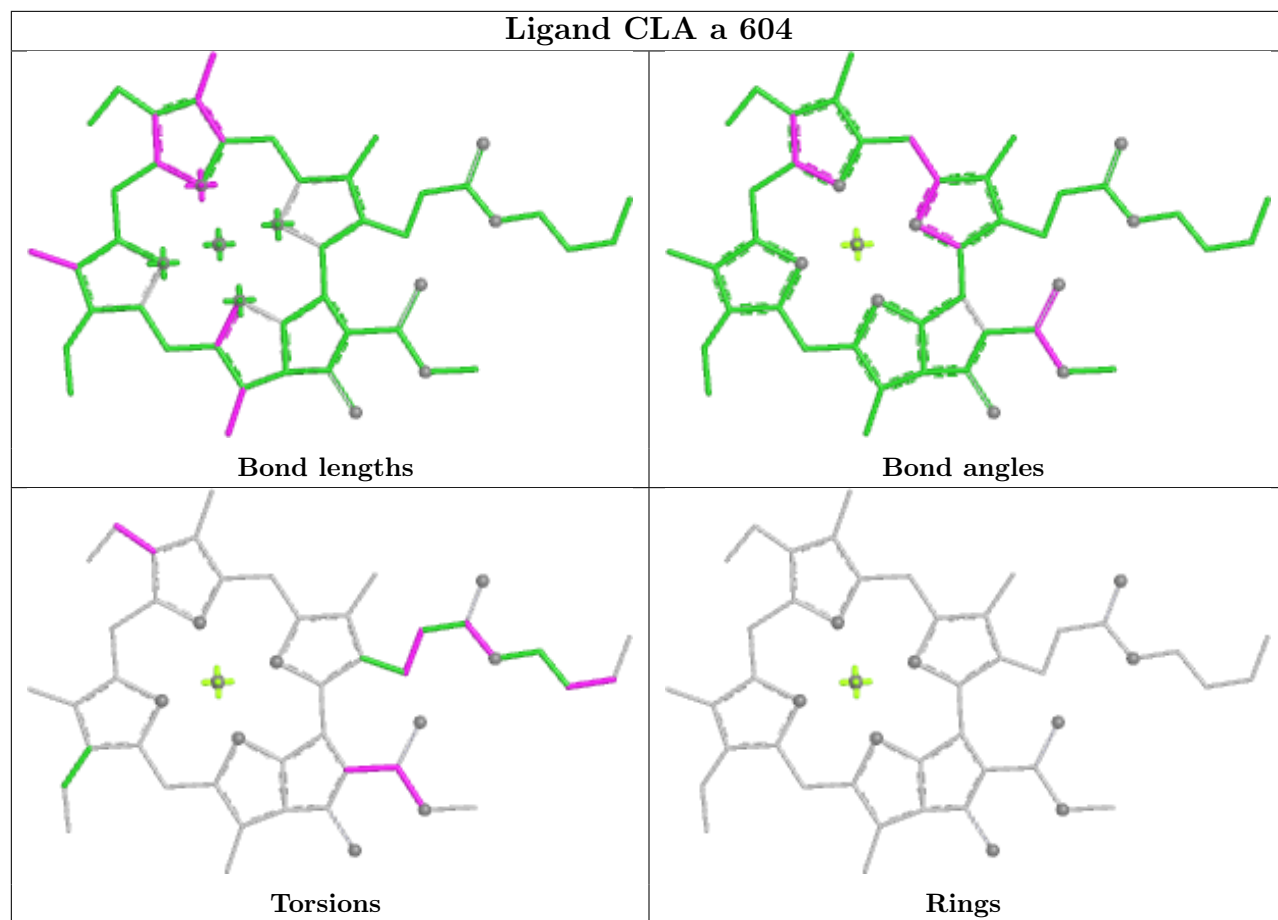


Ligand CLA B 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

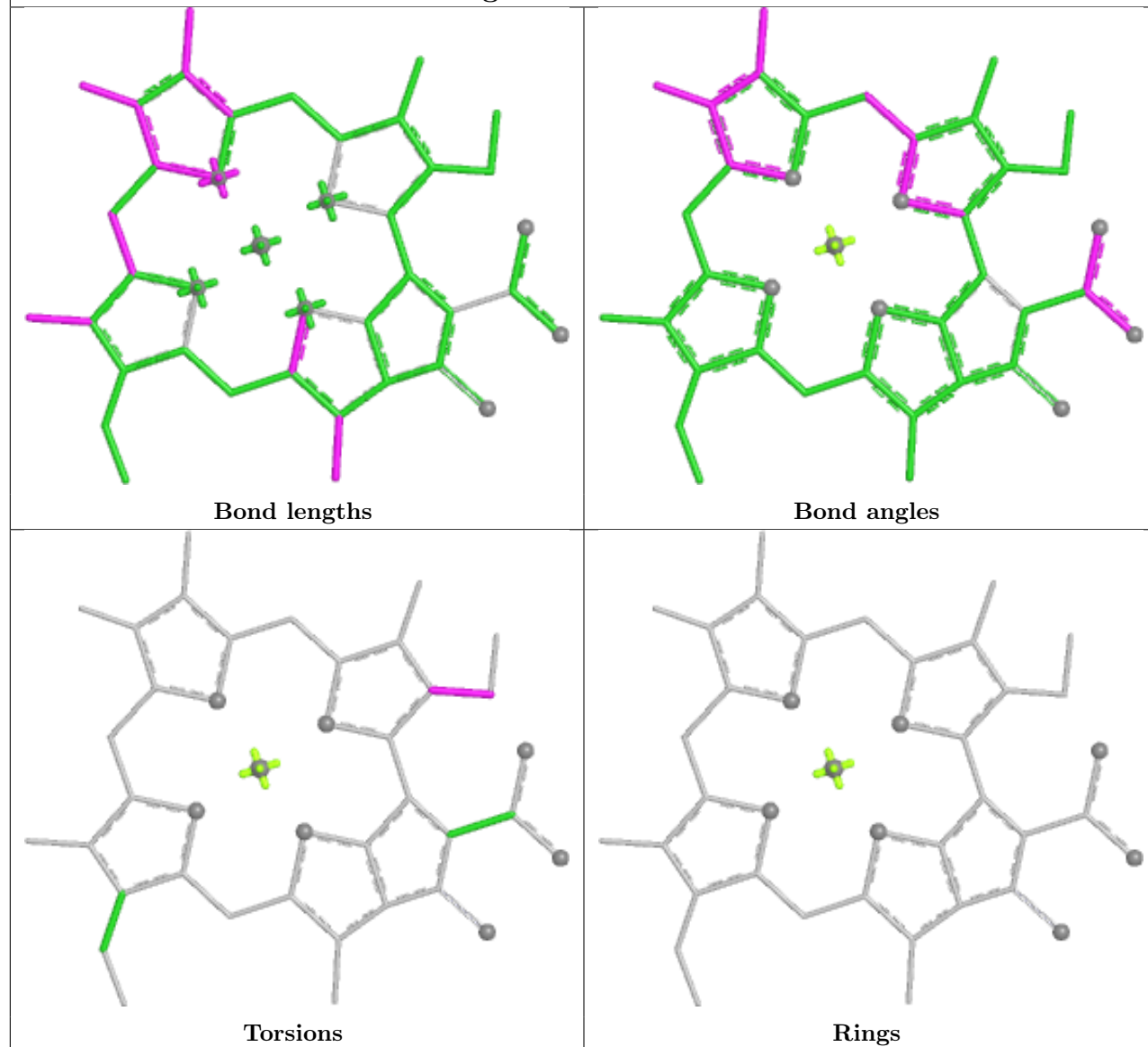
Ligand LUT 8 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PQN B 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

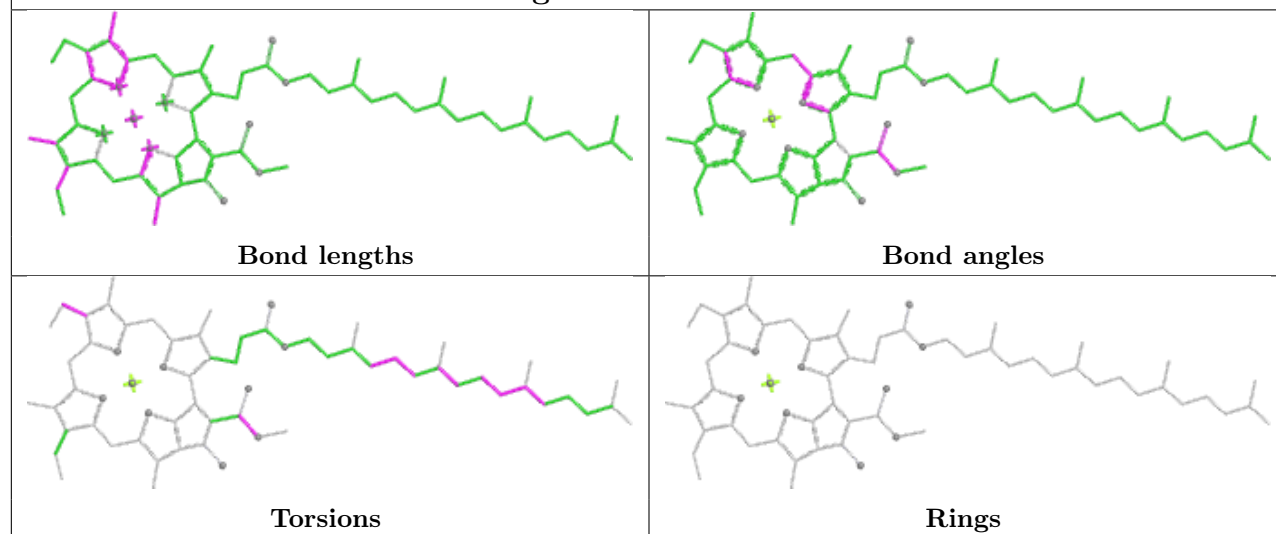
Ligand CLA a 604

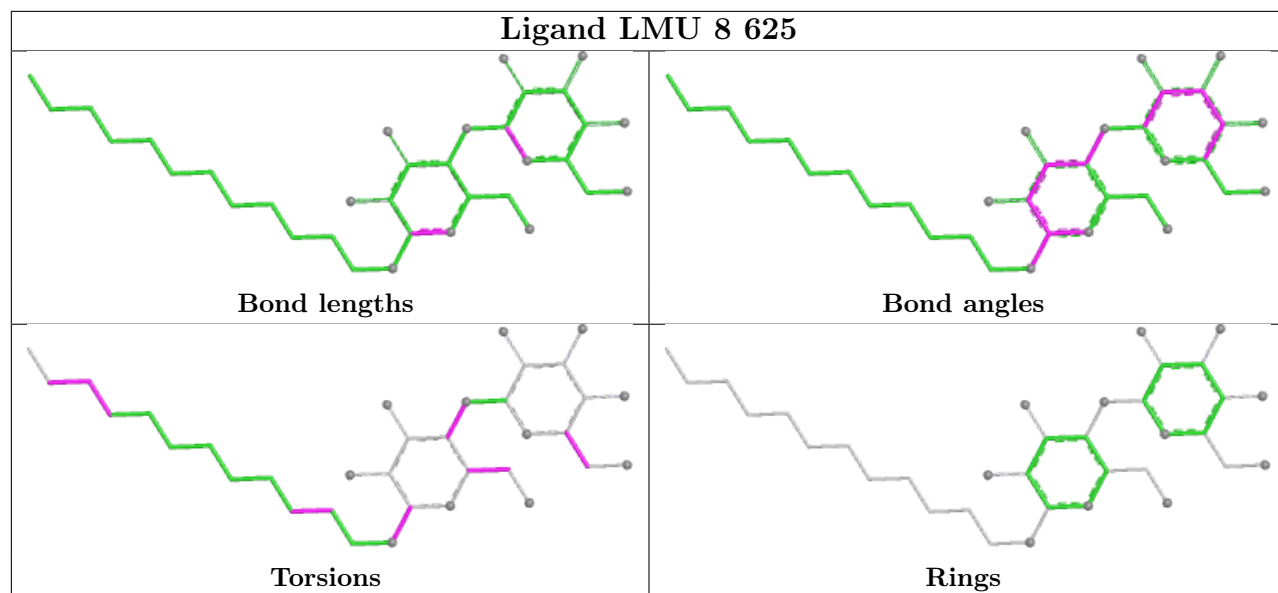


Ligand CLA 5 618

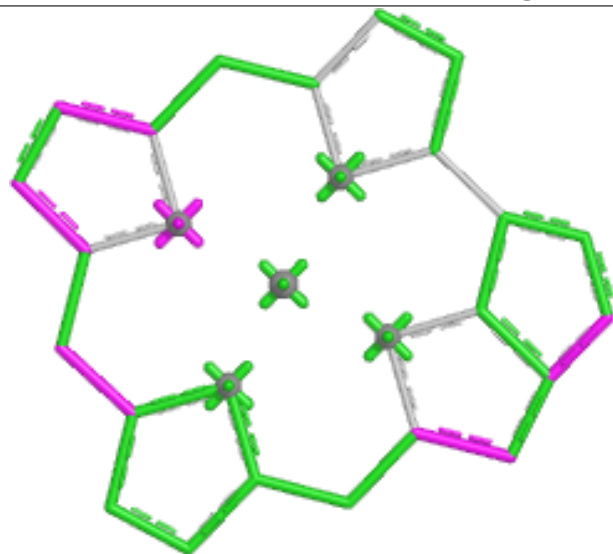


Ligand CLA B 806

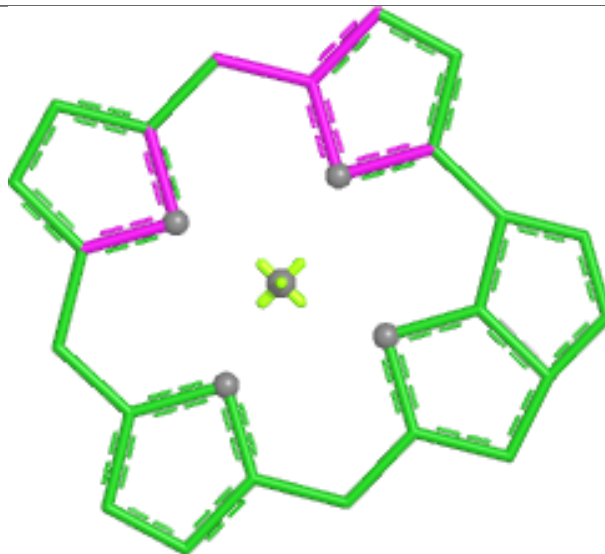




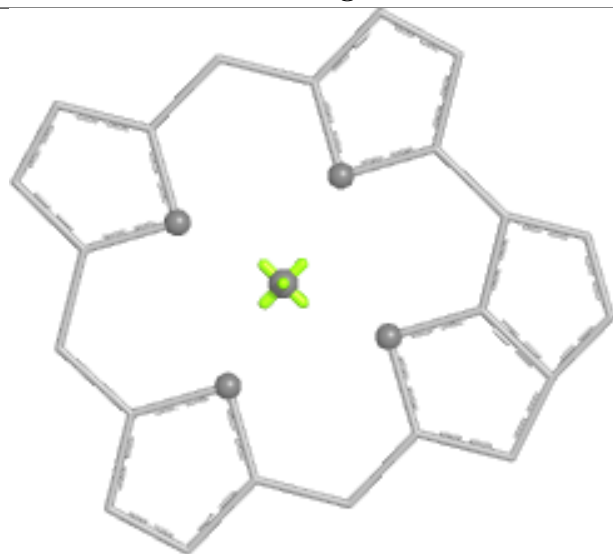
Ligand CLA 2 602



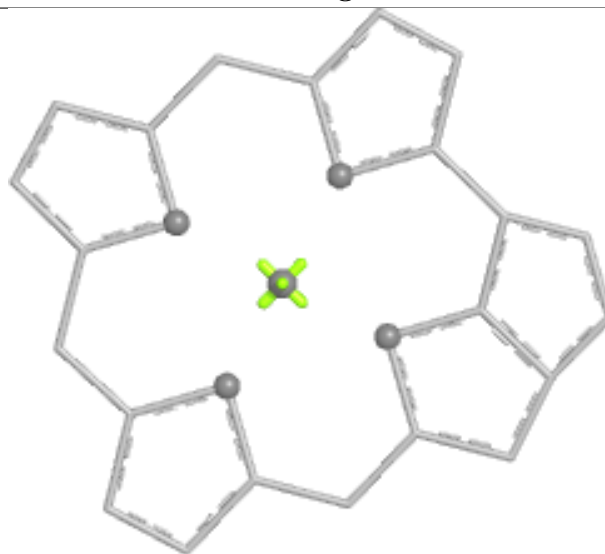
Bond lengths



Bond angles

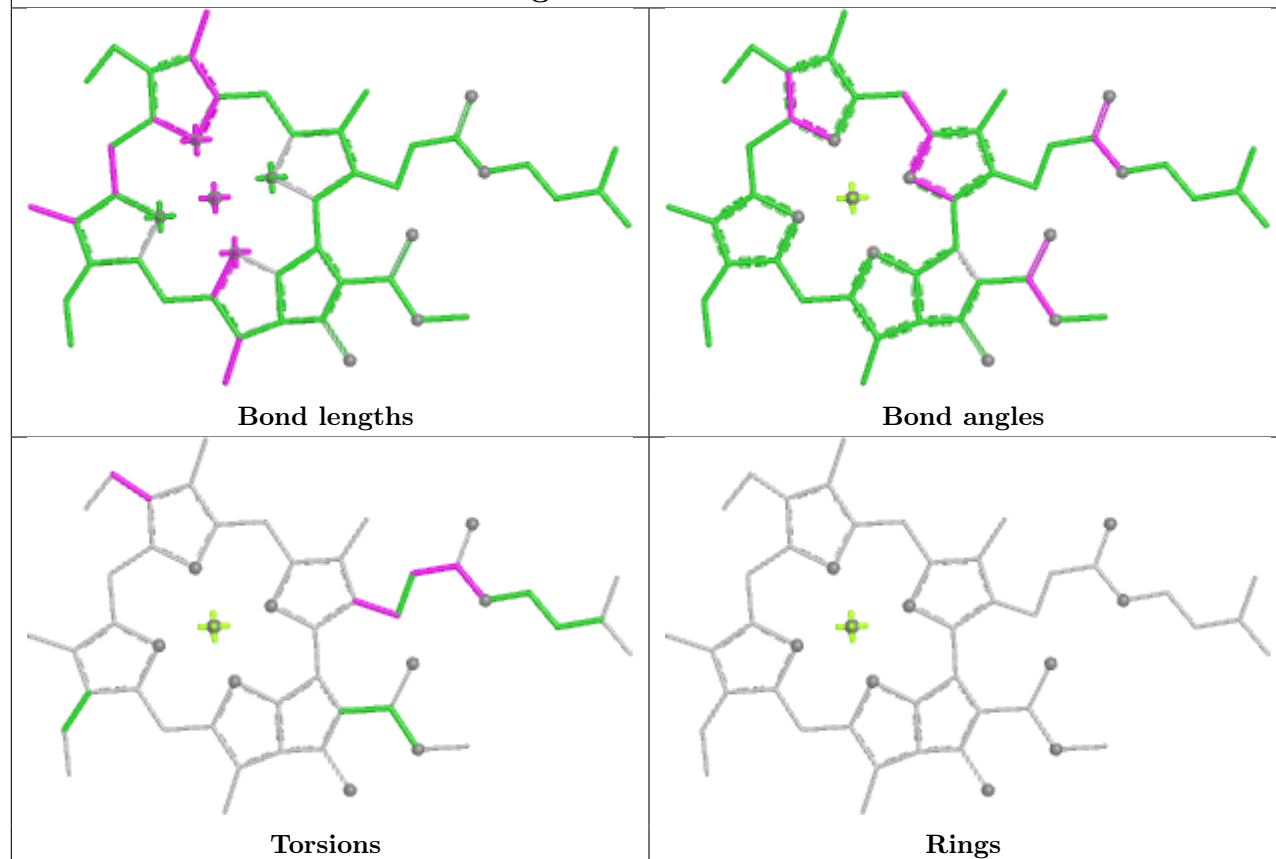


Torsions

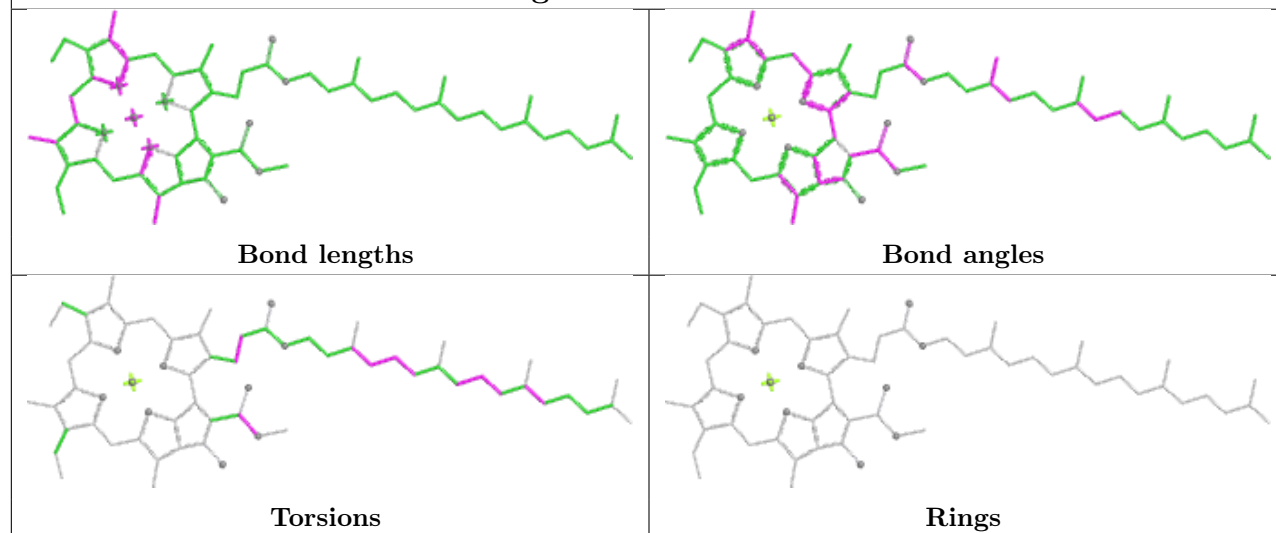


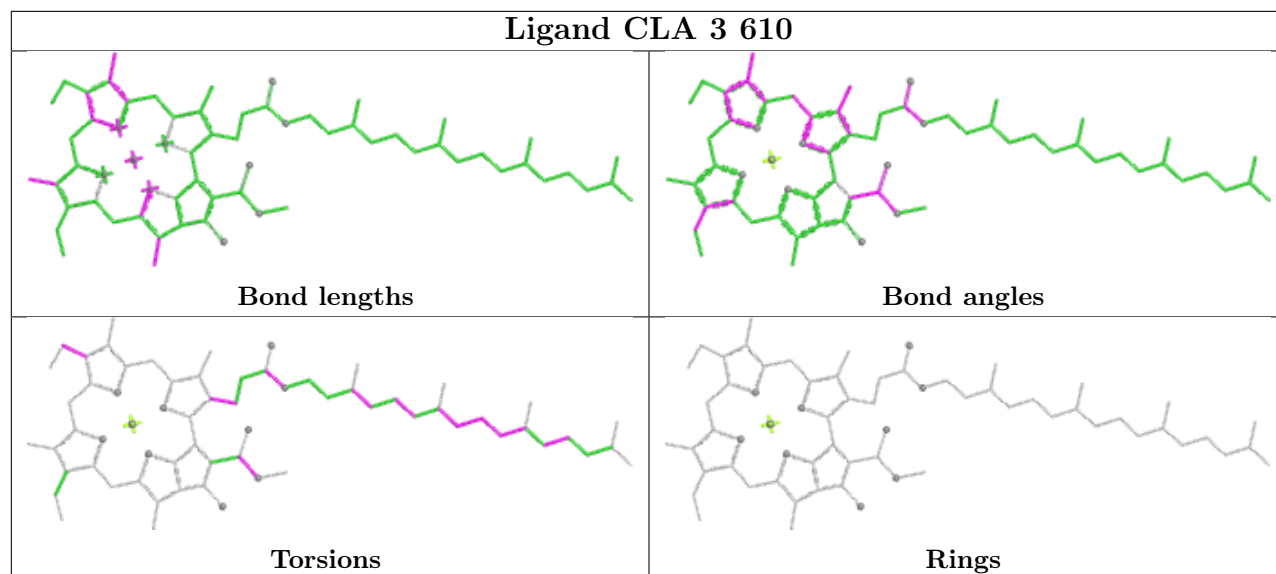
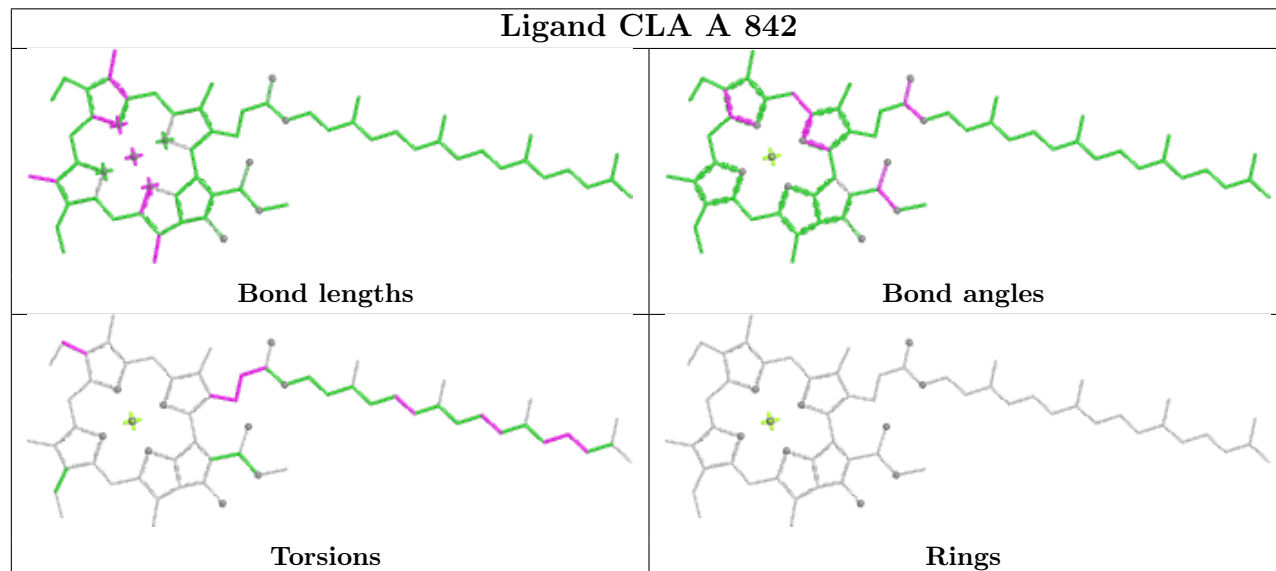
Rings

Ligand CLA A 810

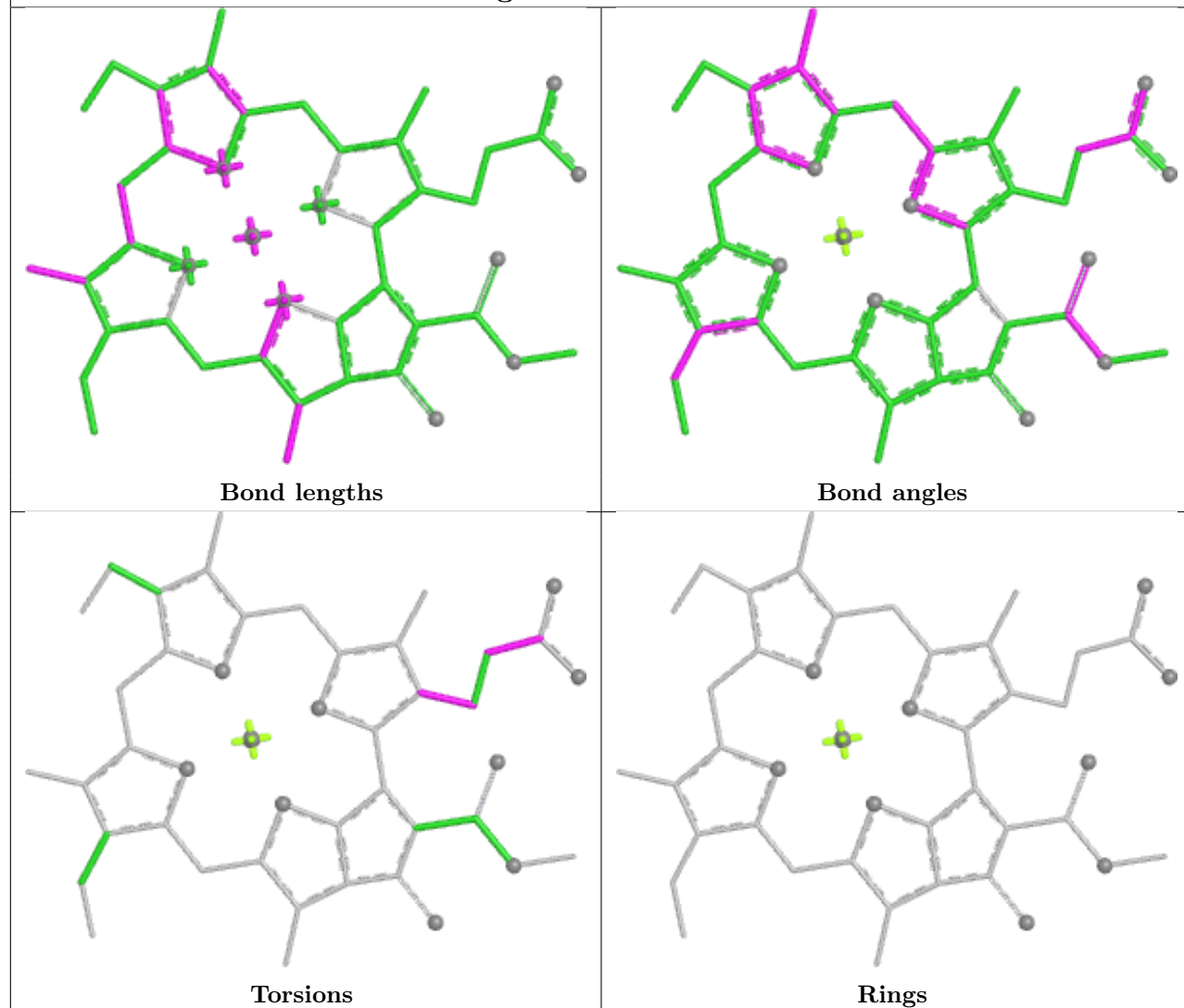


Ligand CLA A 854

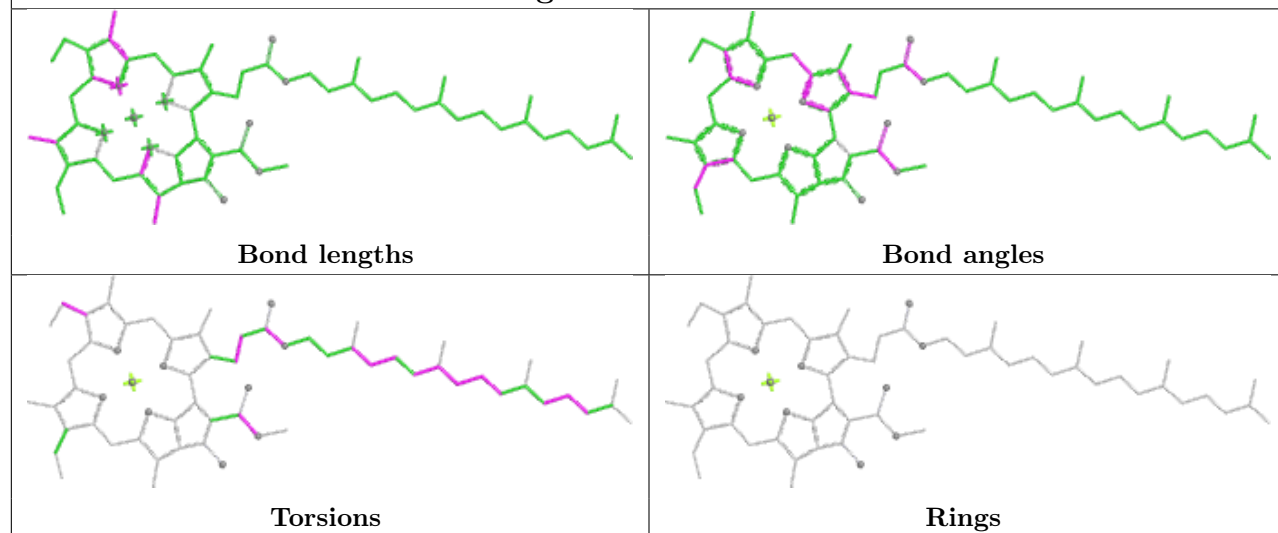


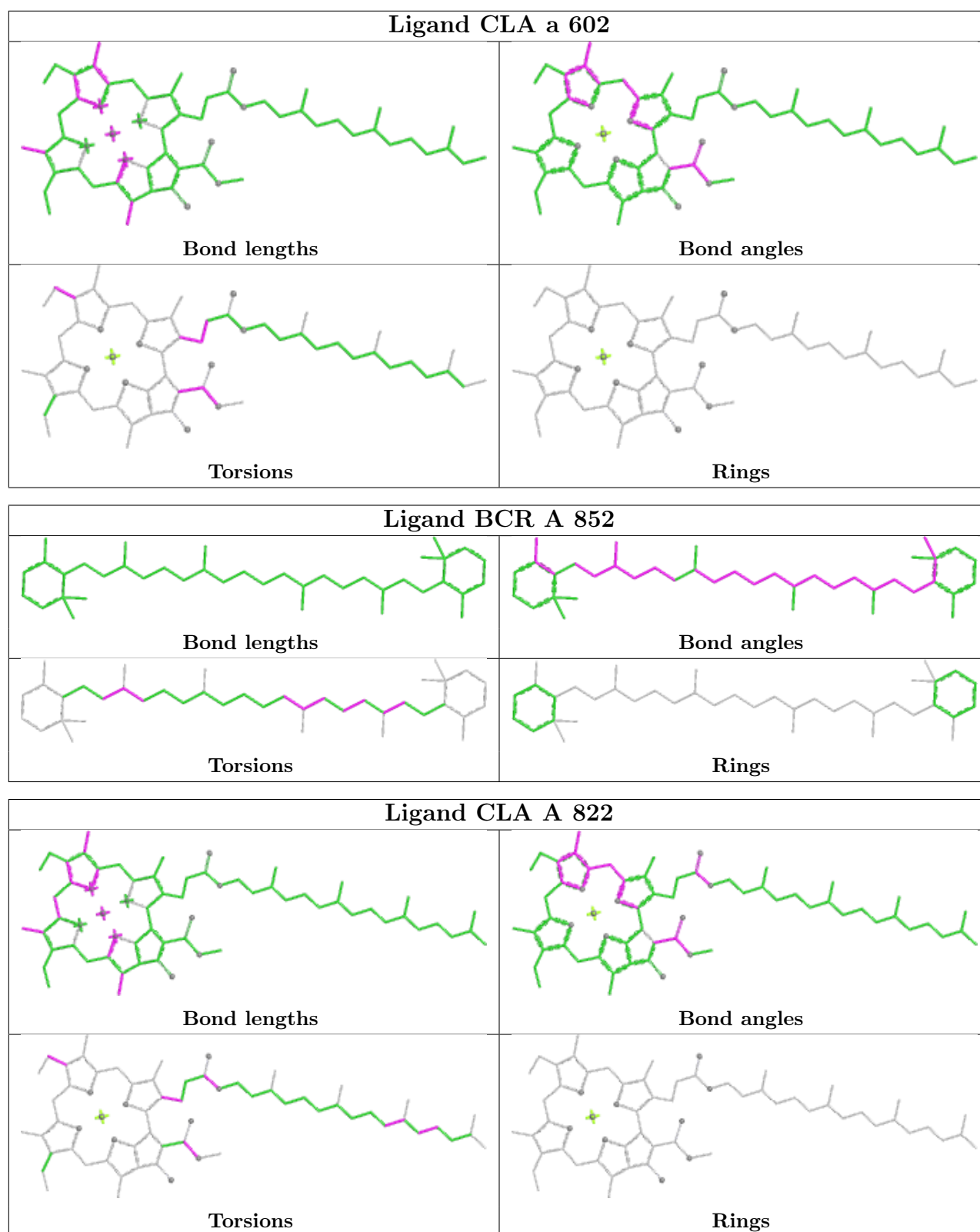
Ligand CLA 3 610**Ligand CLA A 842**

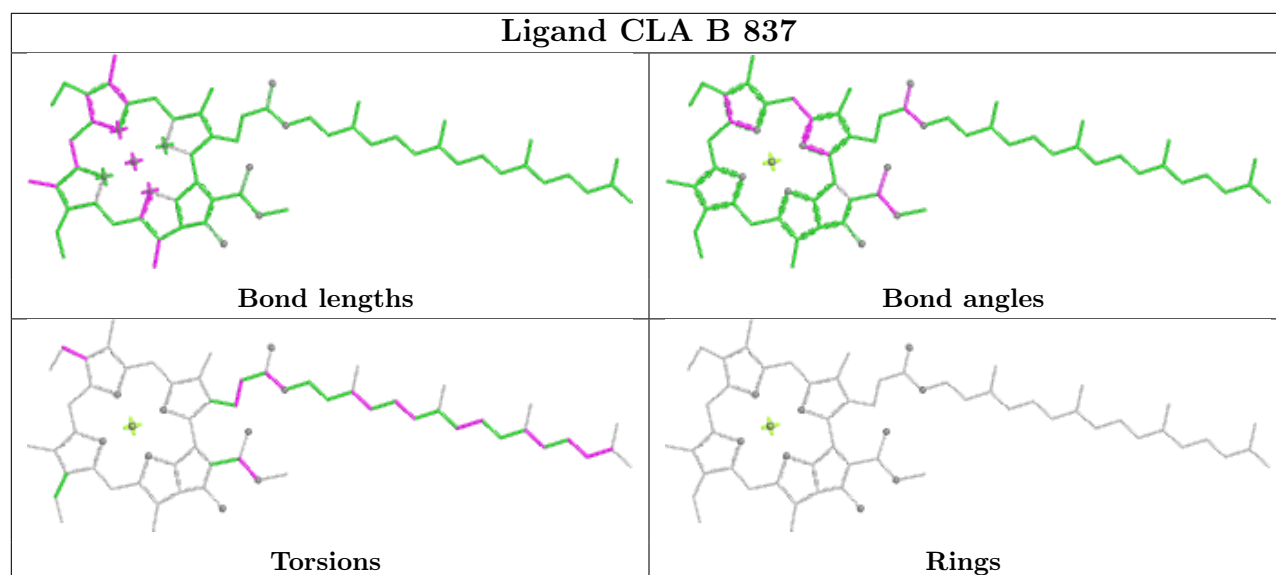
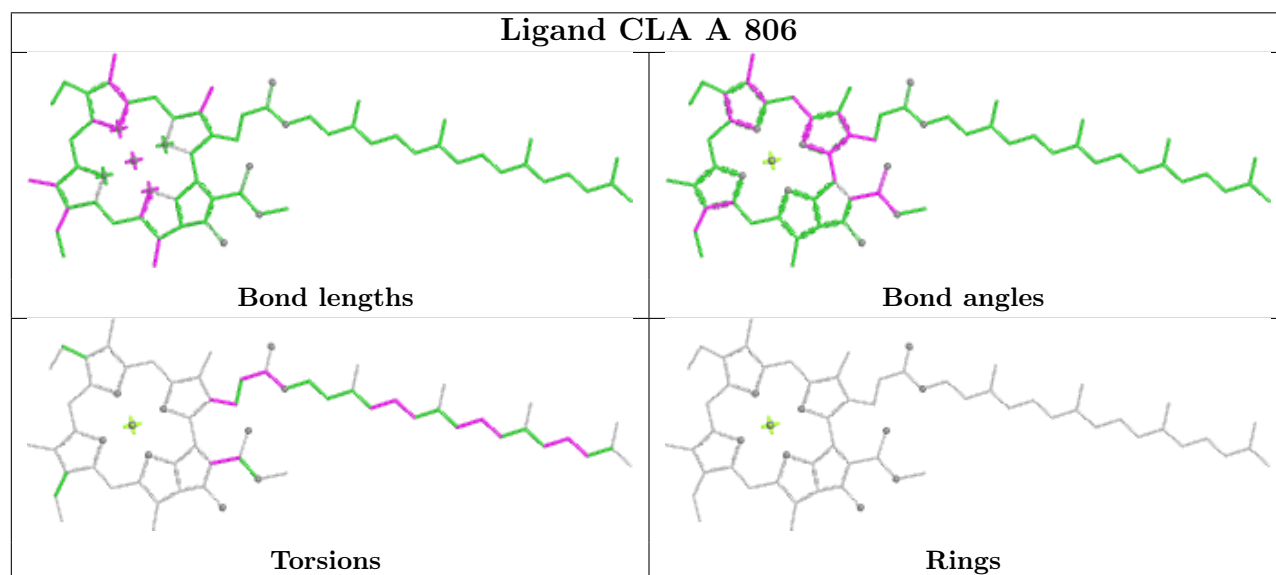
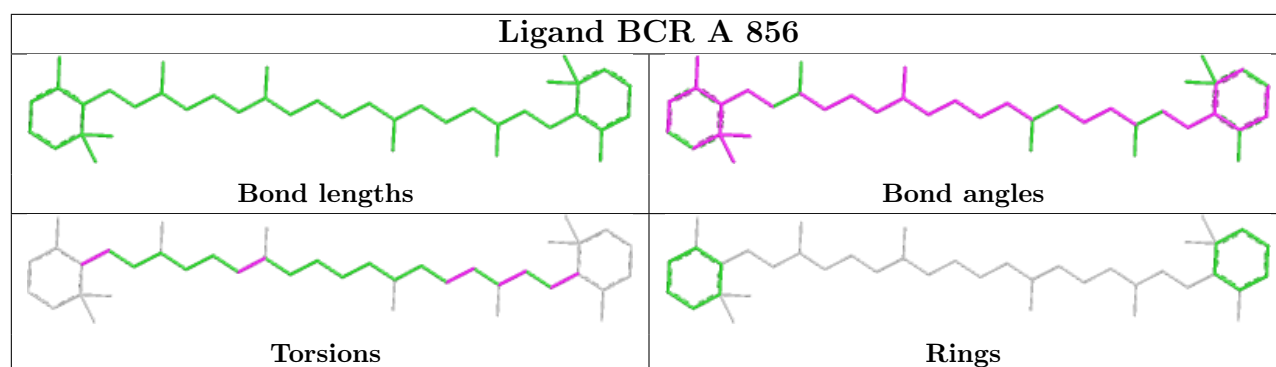
Ligand CLA 8 609



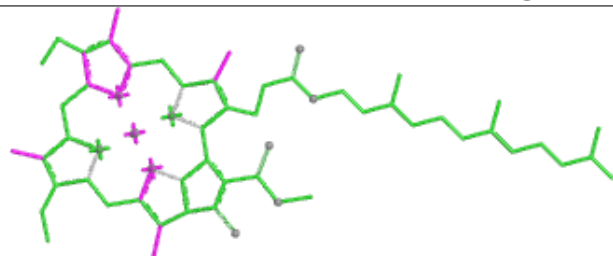
Ligand CLA 7 613



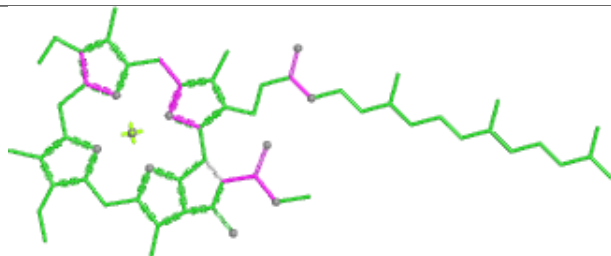




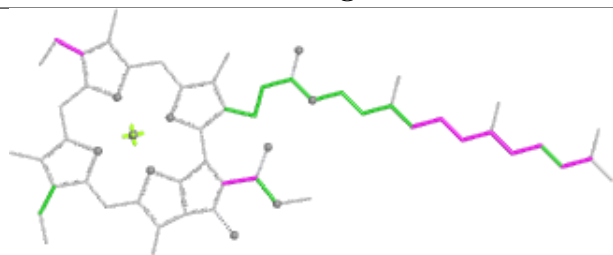
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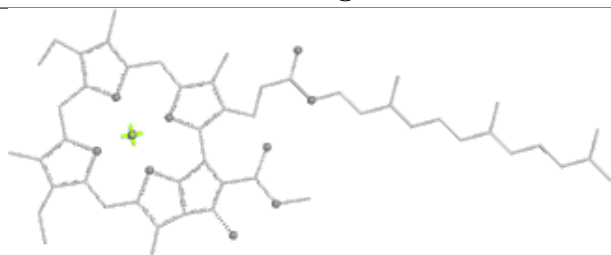
Bond lengths



Bond angles

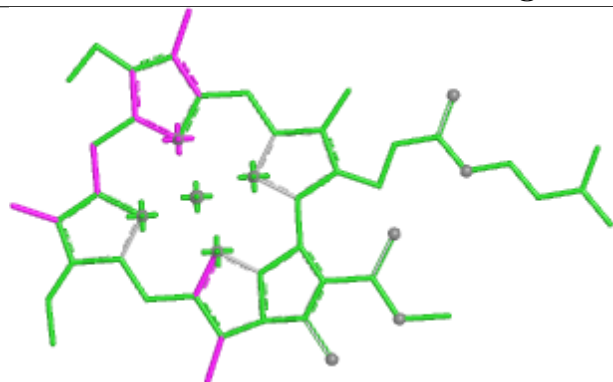


Torsions

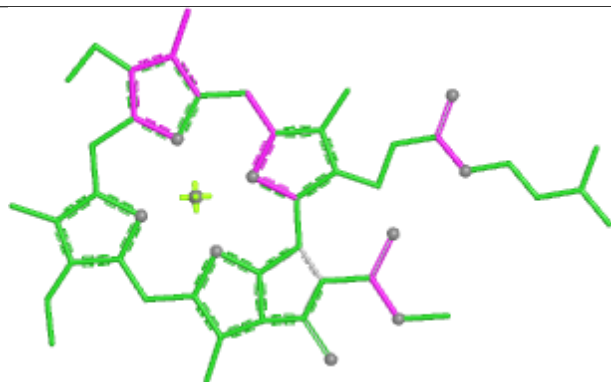


Rings

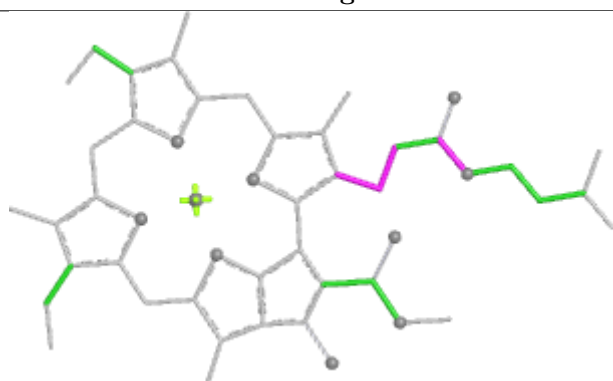
Ligand CLA 8 604



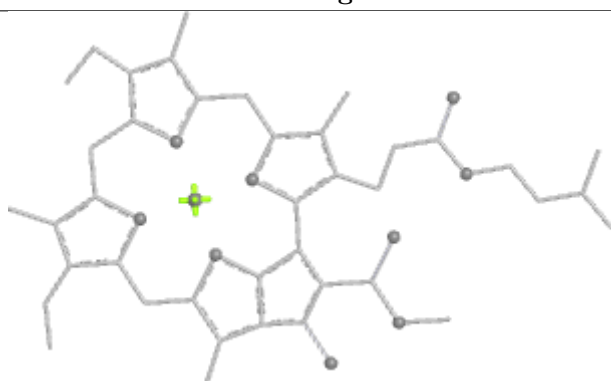
Bond lengths



Bond angles

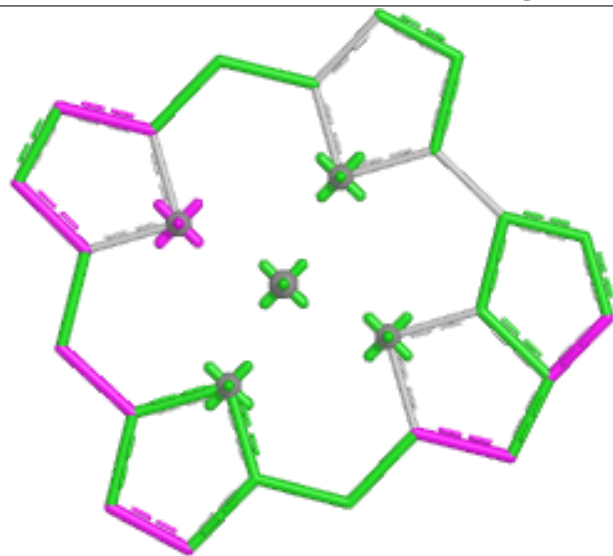


Torsions

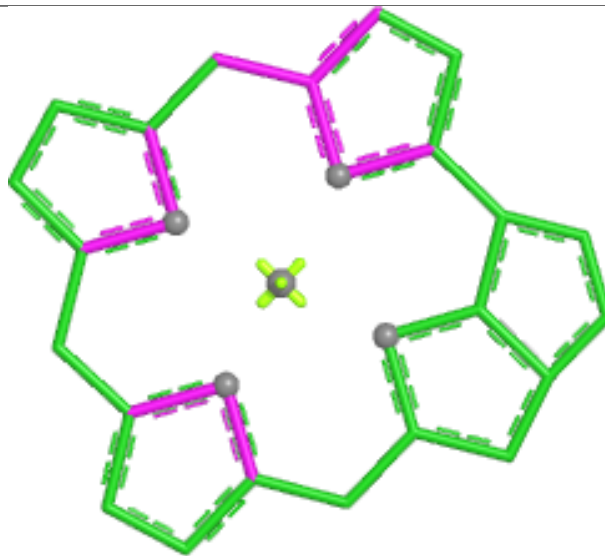


Rings

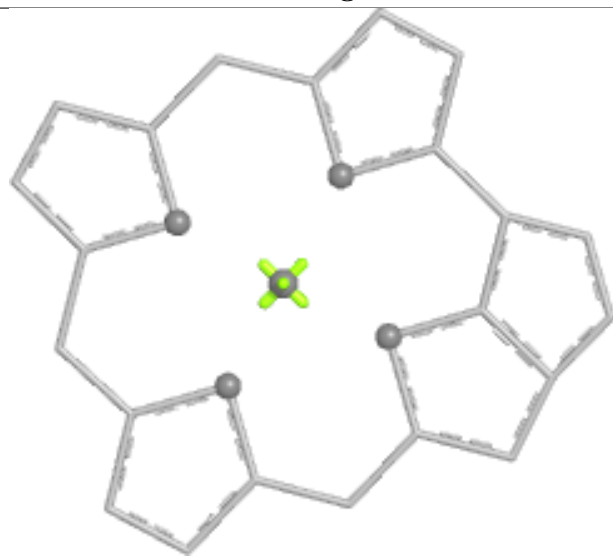
Ligand CLA 2 603



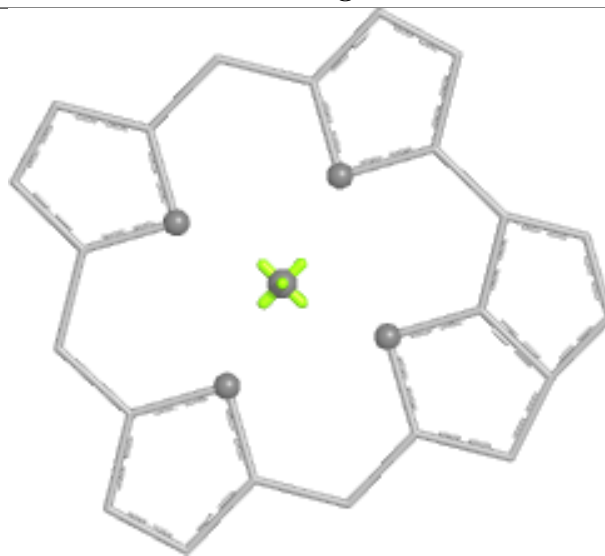
Bond lengths



Bond angles

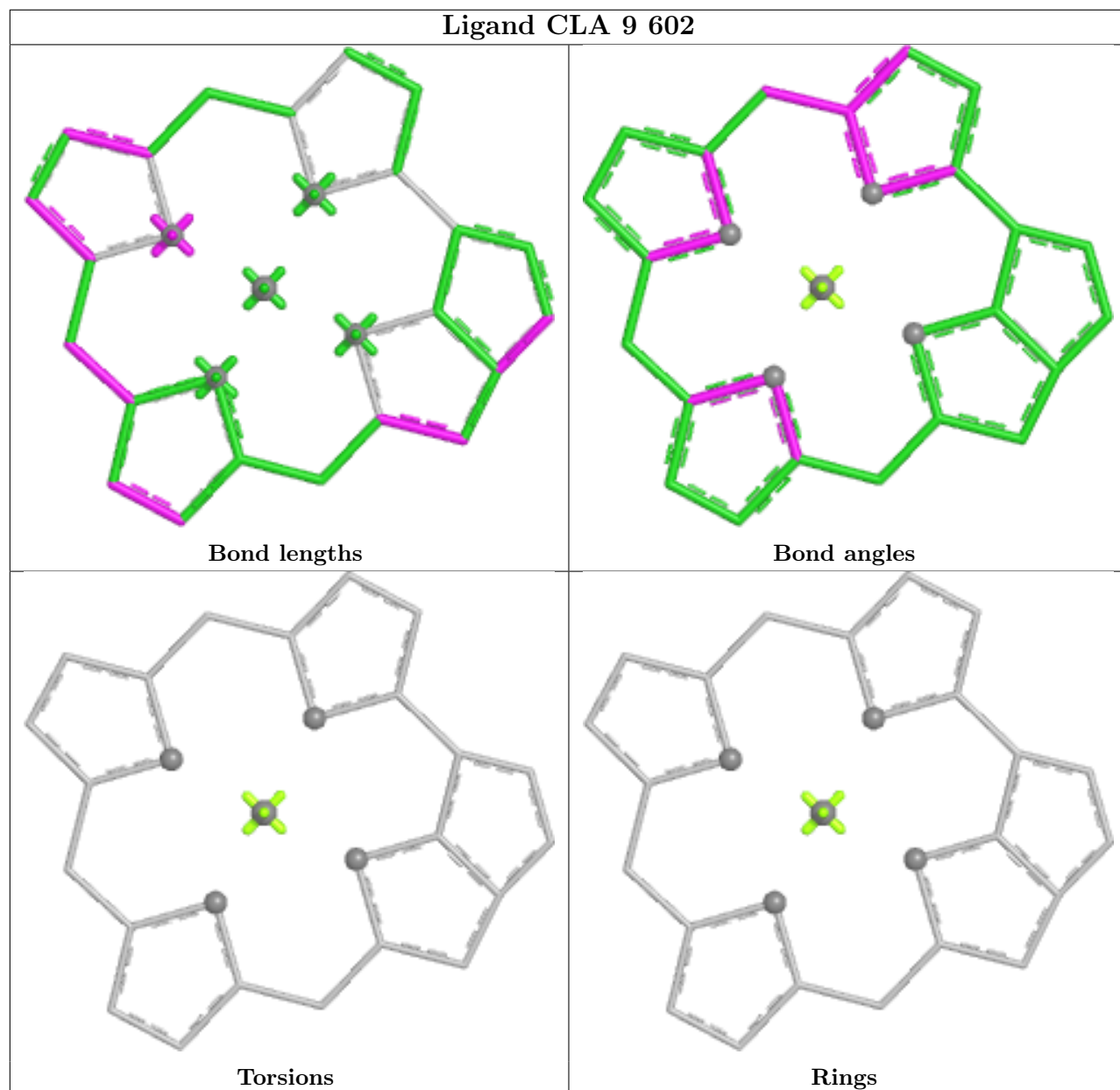


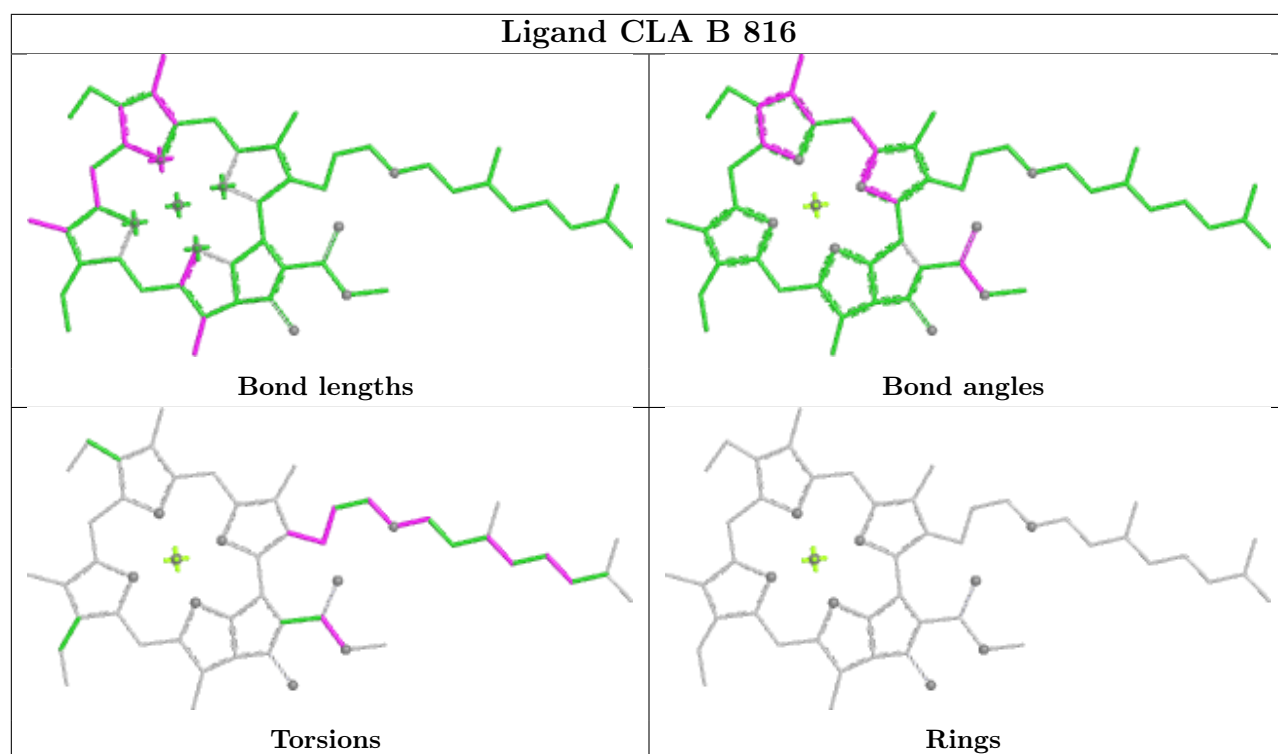
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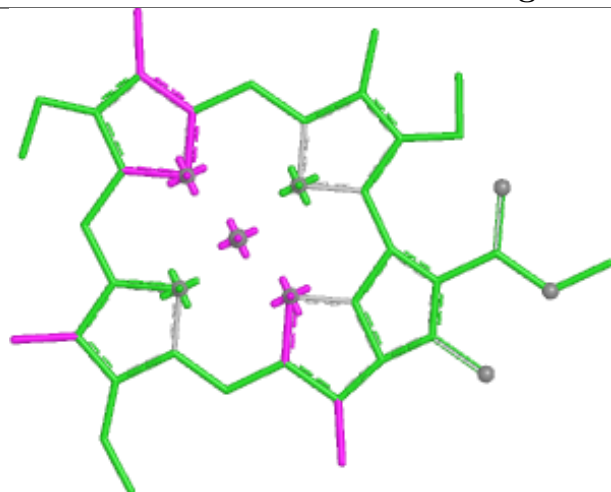
Rings

Ligand CLA 9 602

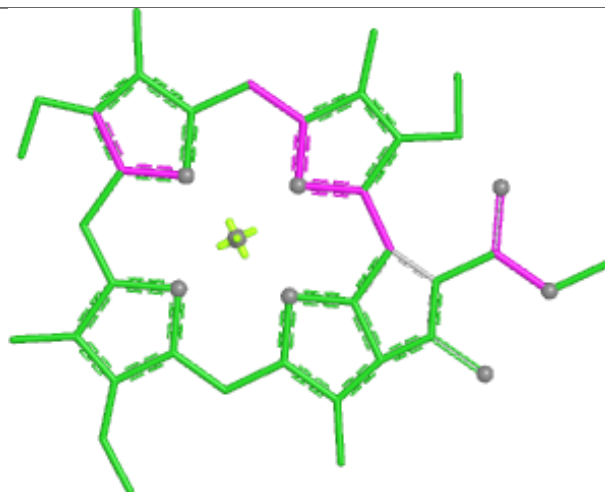




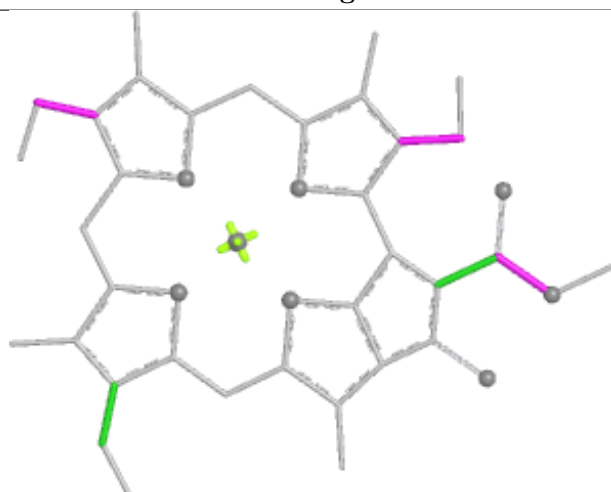
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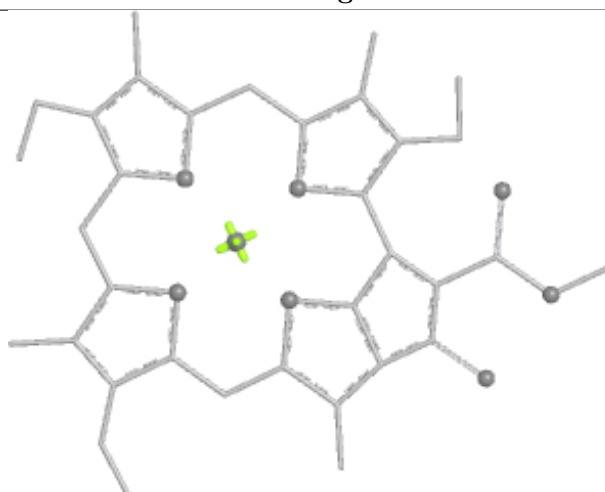
Bond lengths



Bond angles

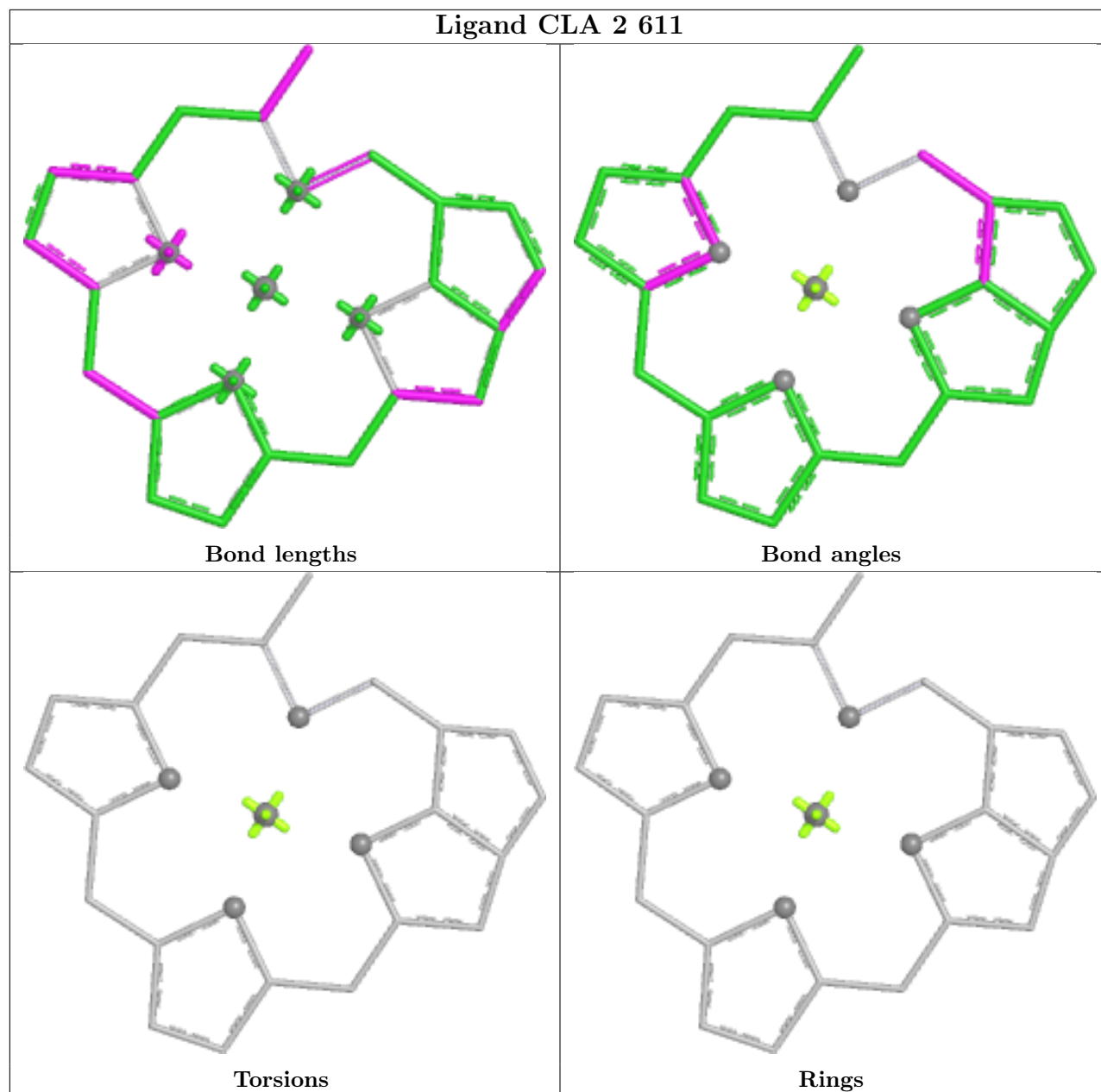


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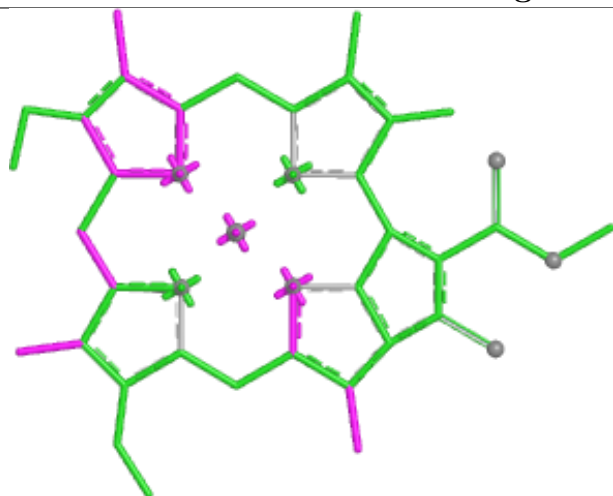


Rings

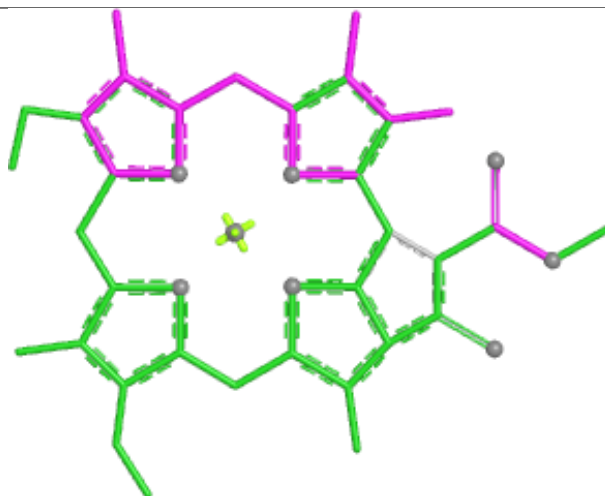
Ligand CLA 2 611



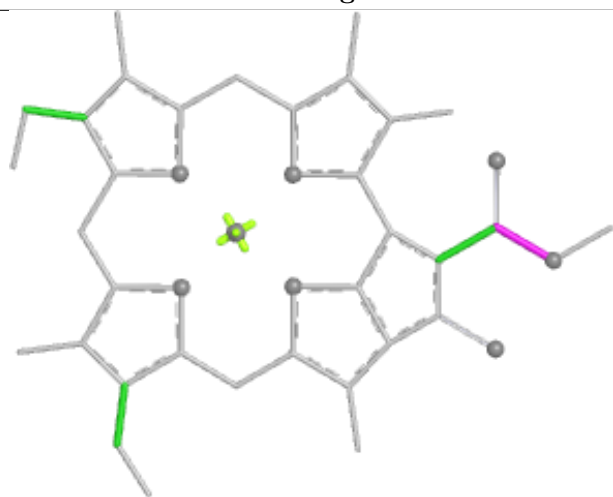
Ligand CLA B 804



Bond lengths



Bond angles

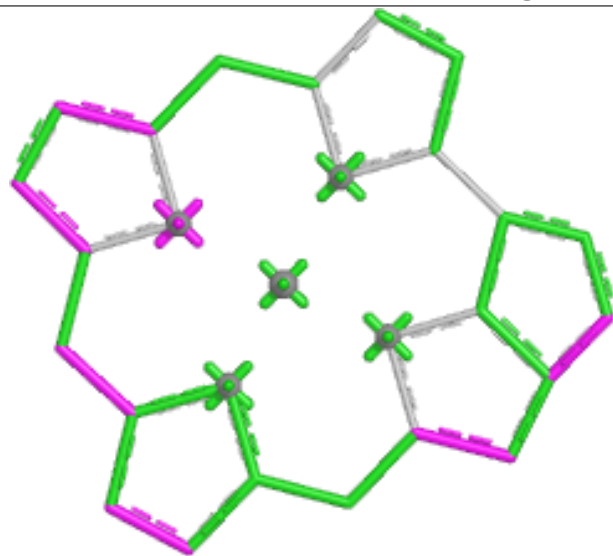


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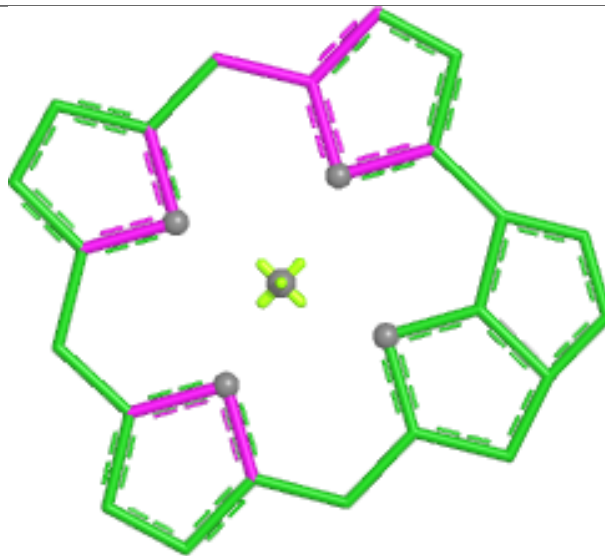


Rings

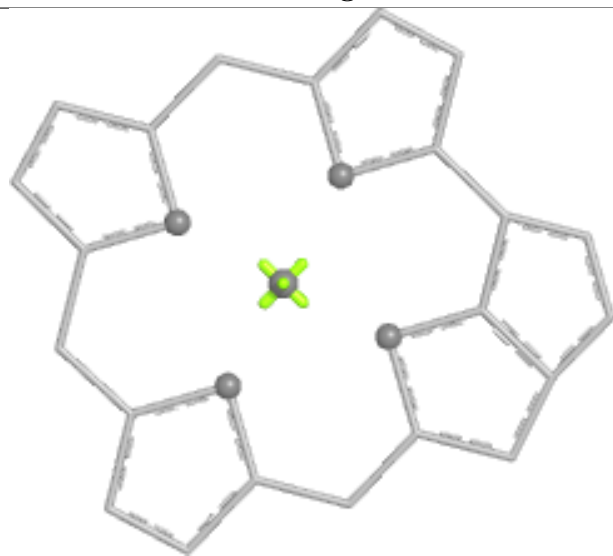
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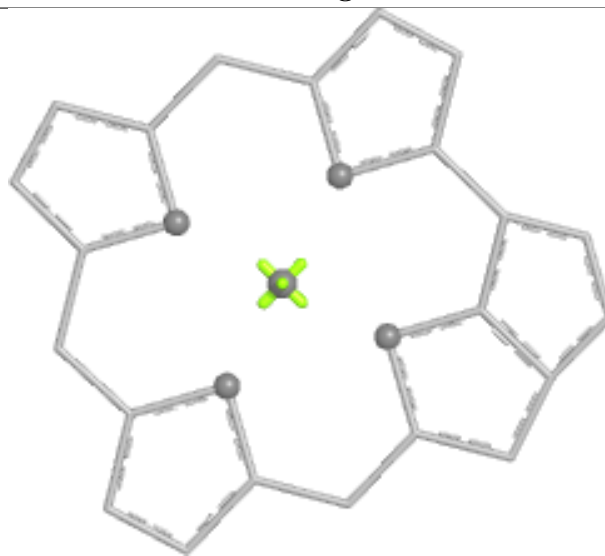
Bond lengths



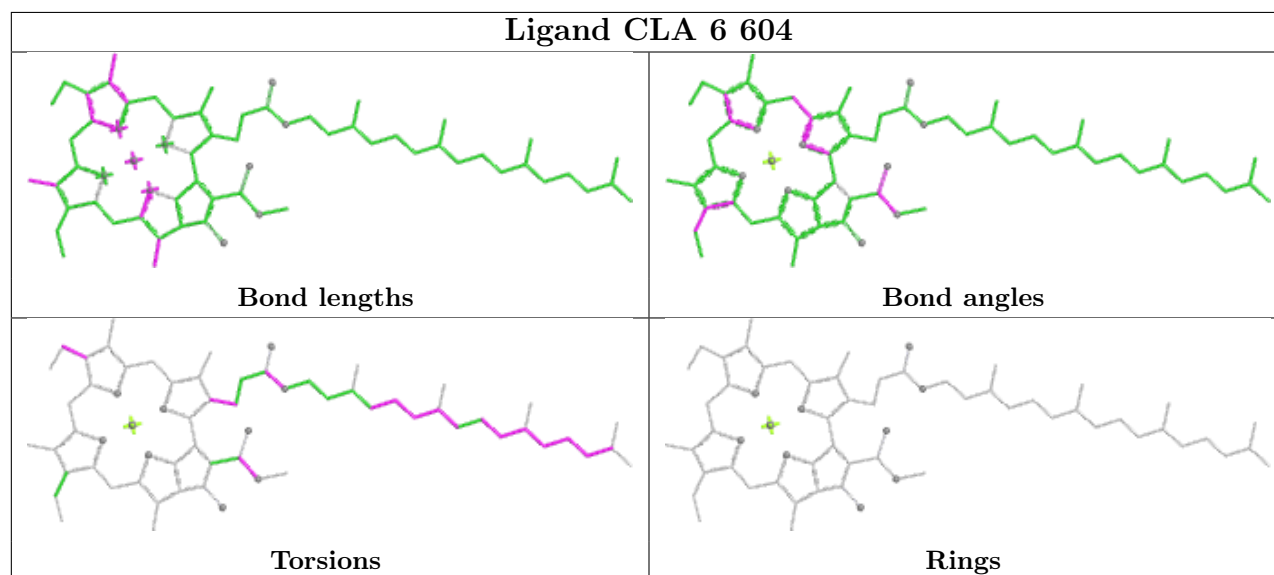
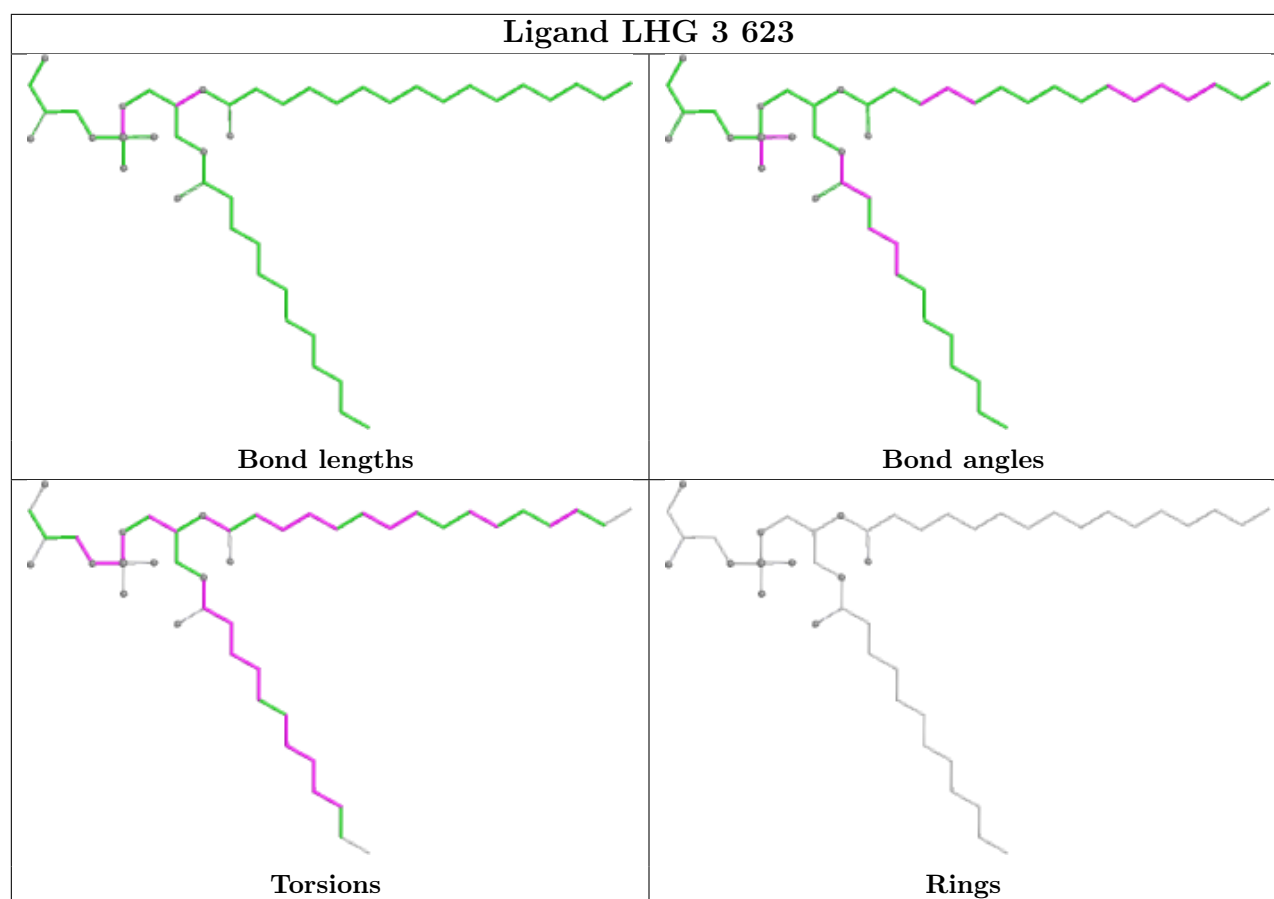
Bond angles

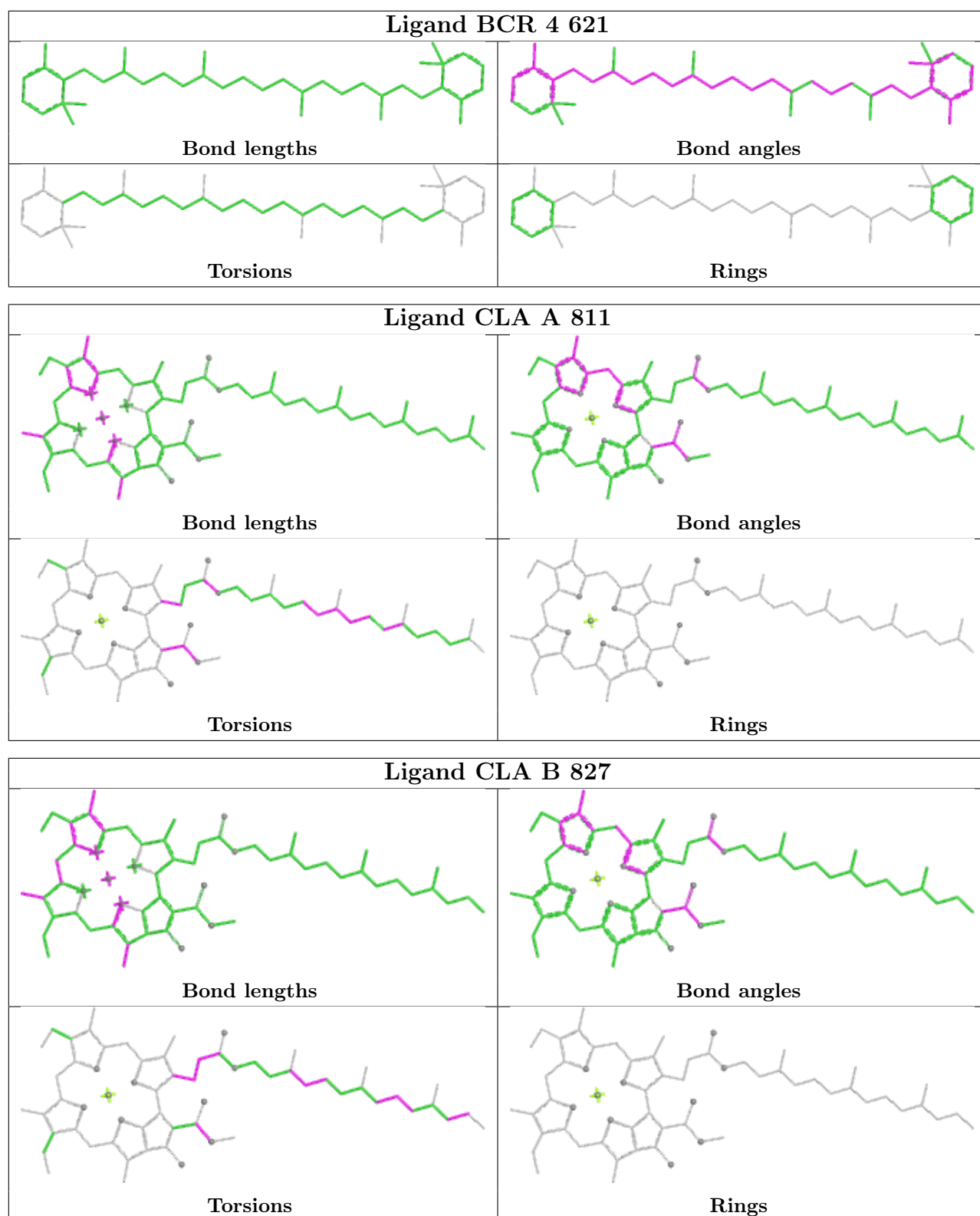


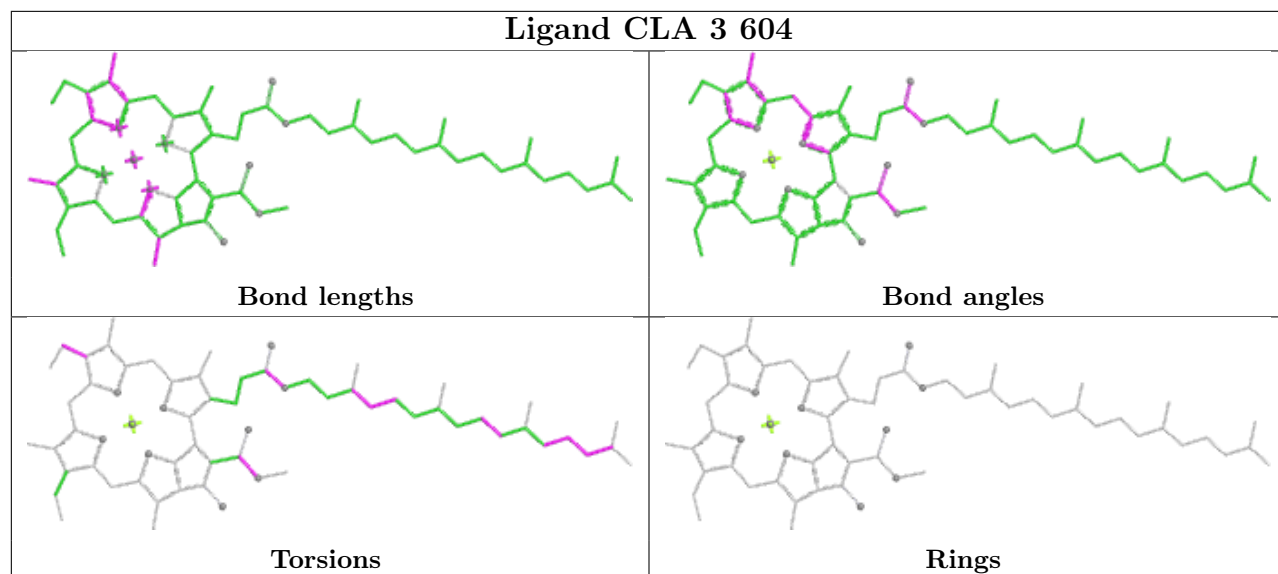
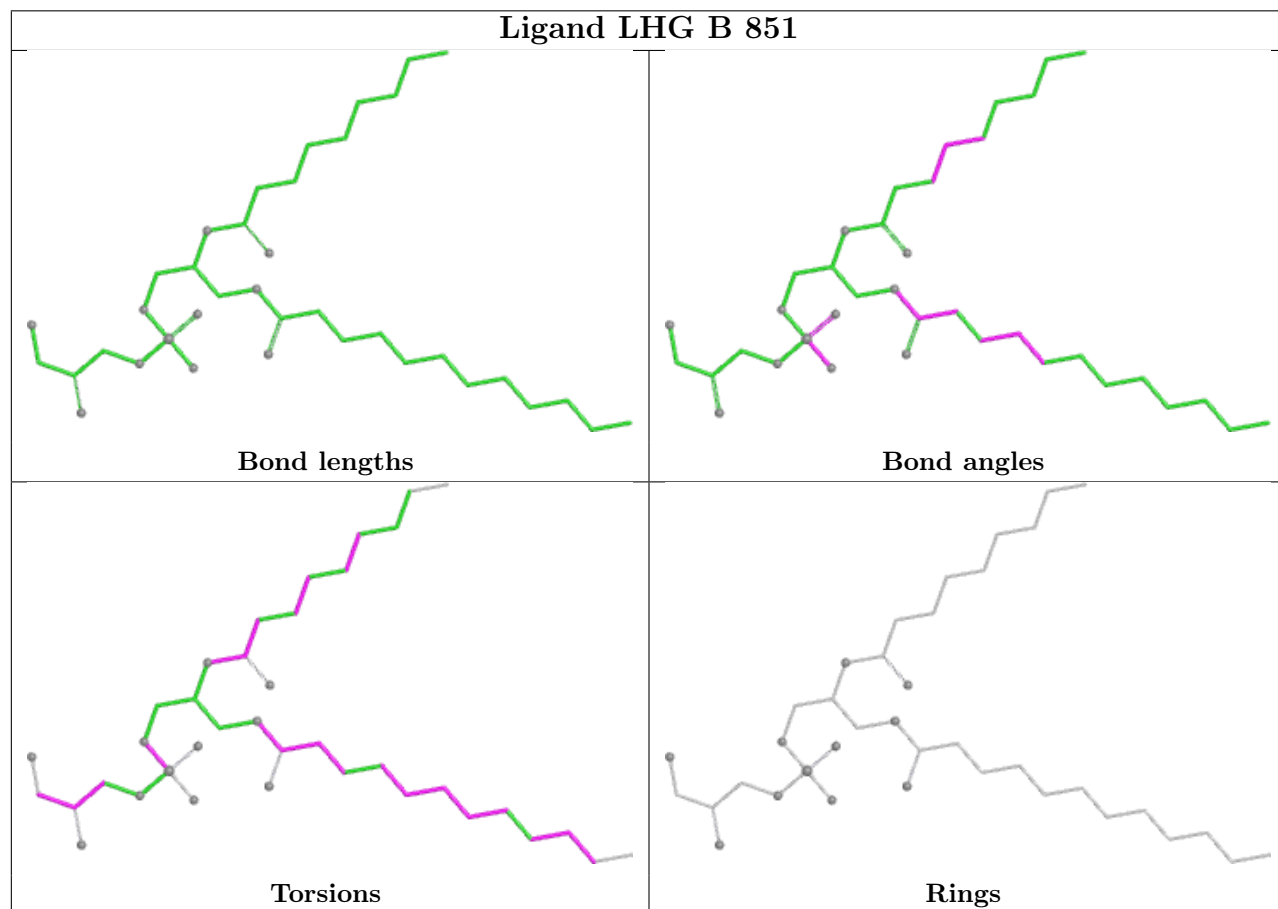
Torsions

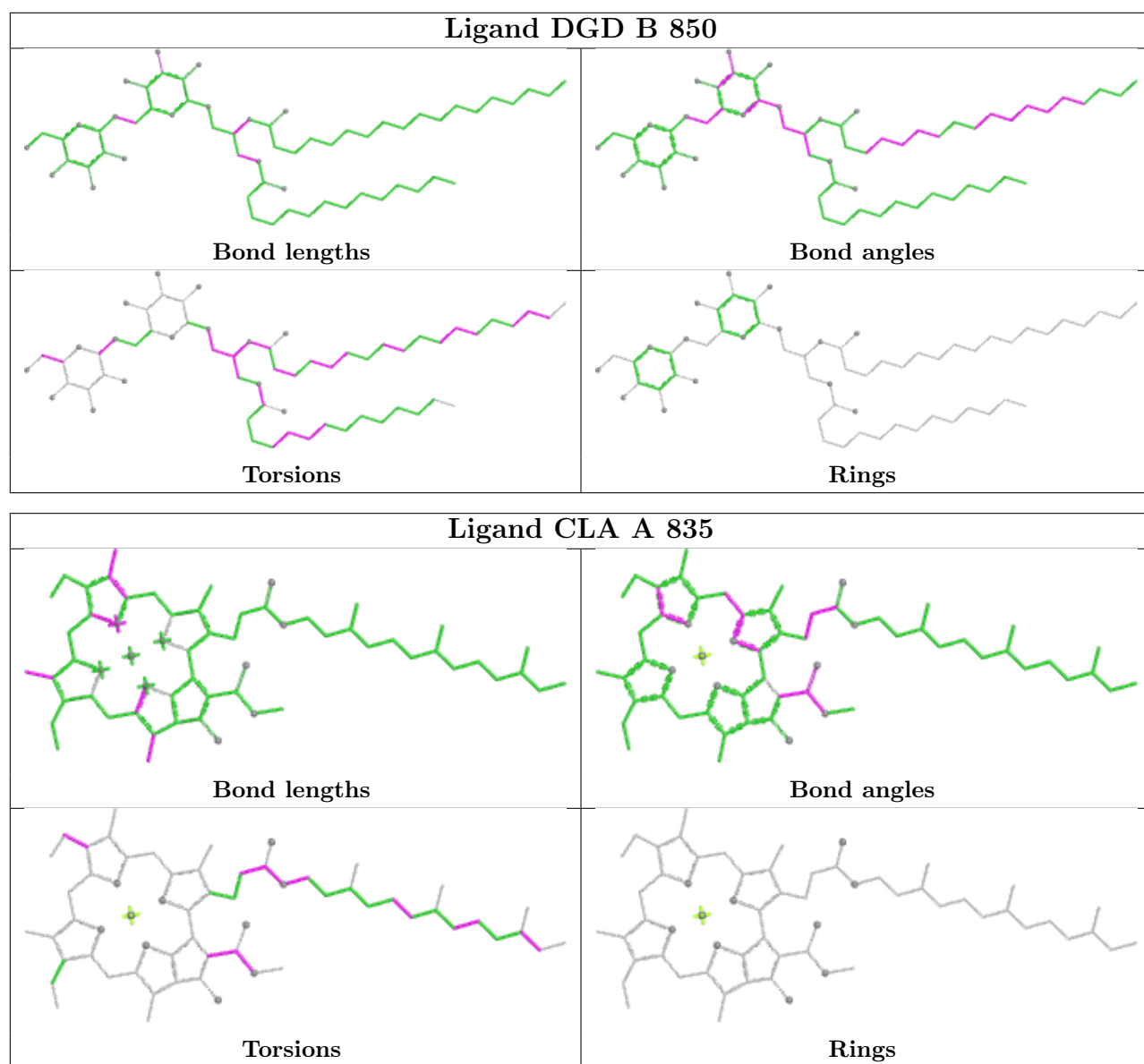


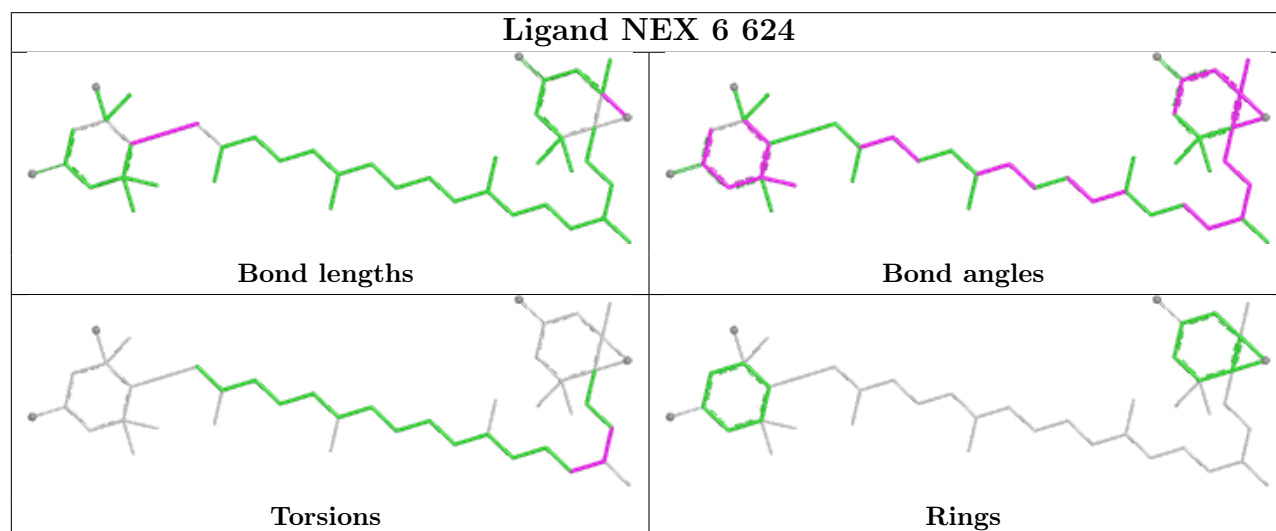
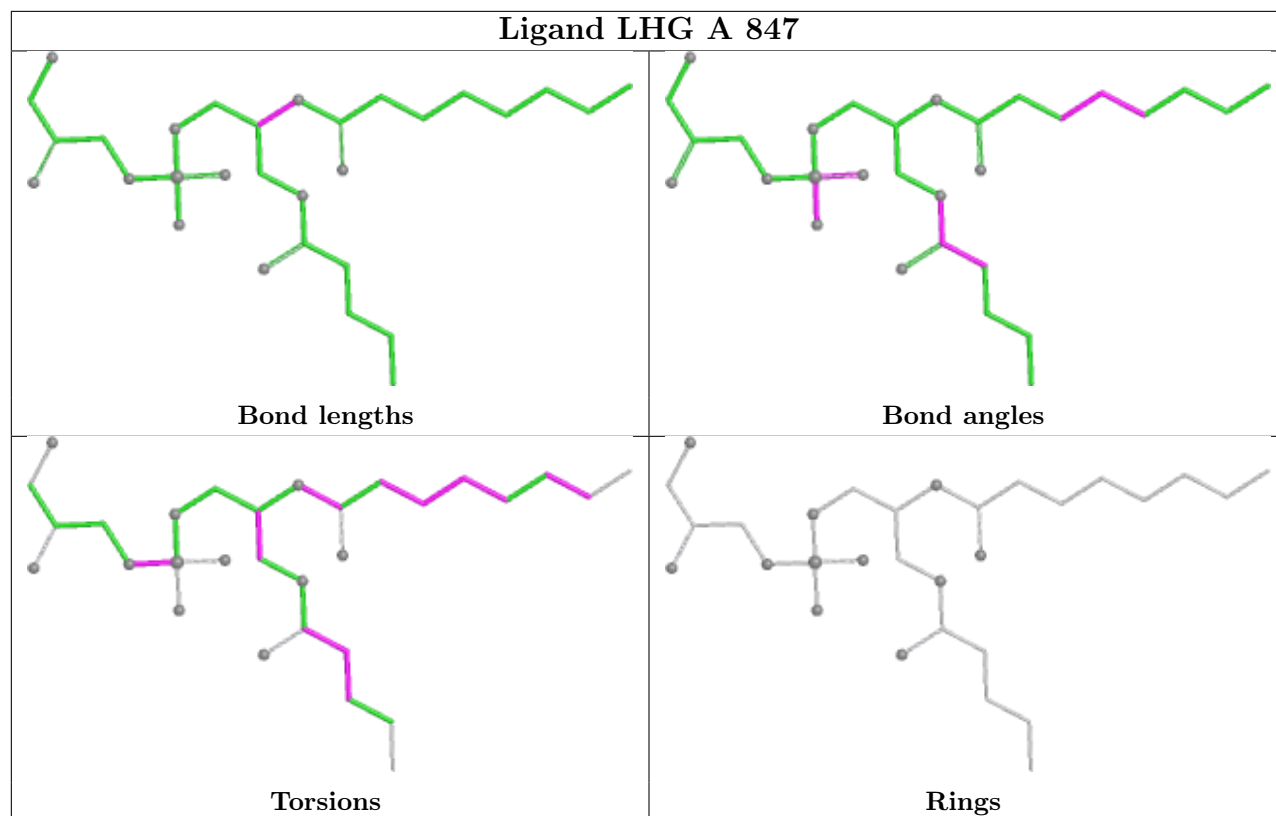
Rings

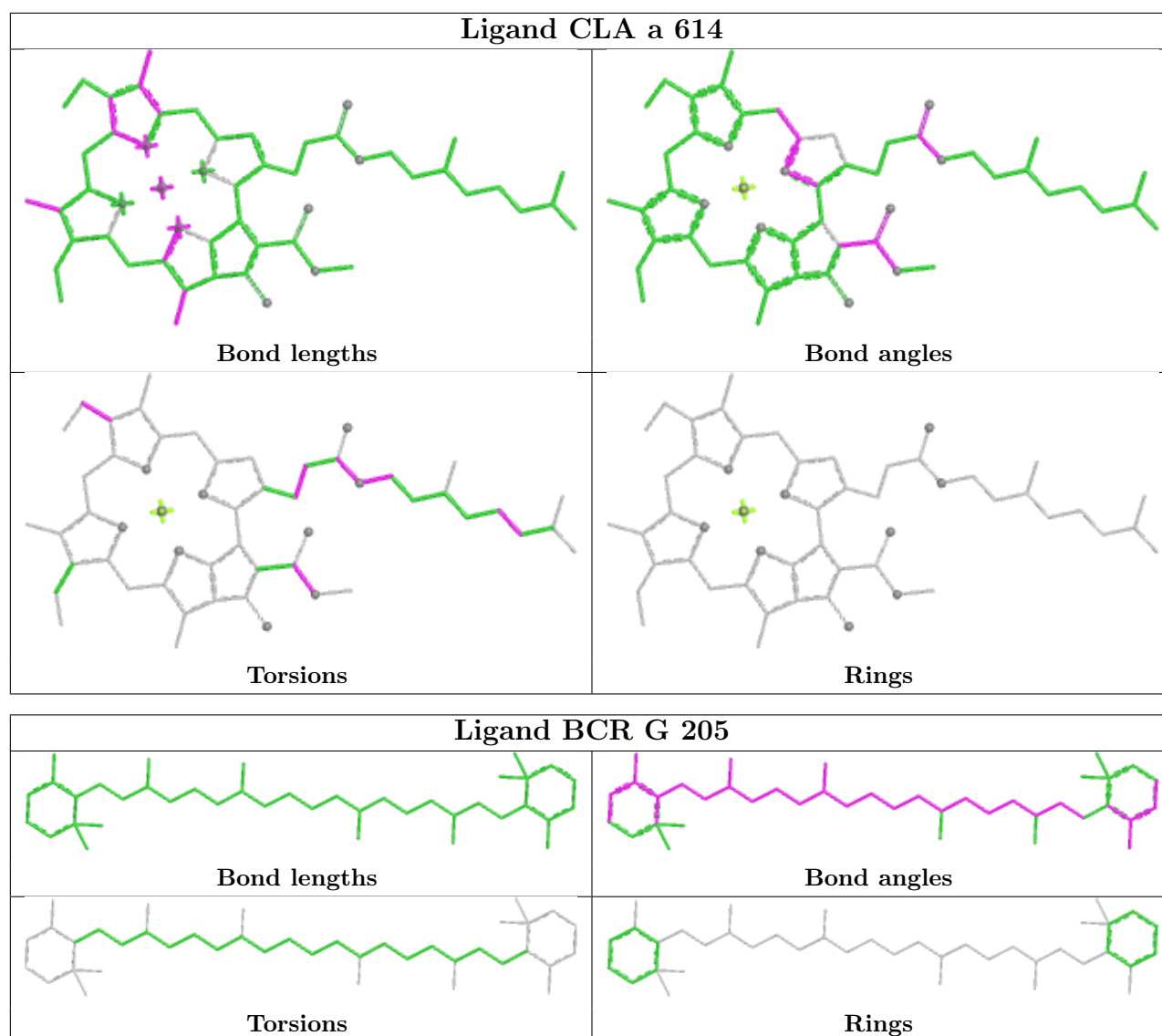




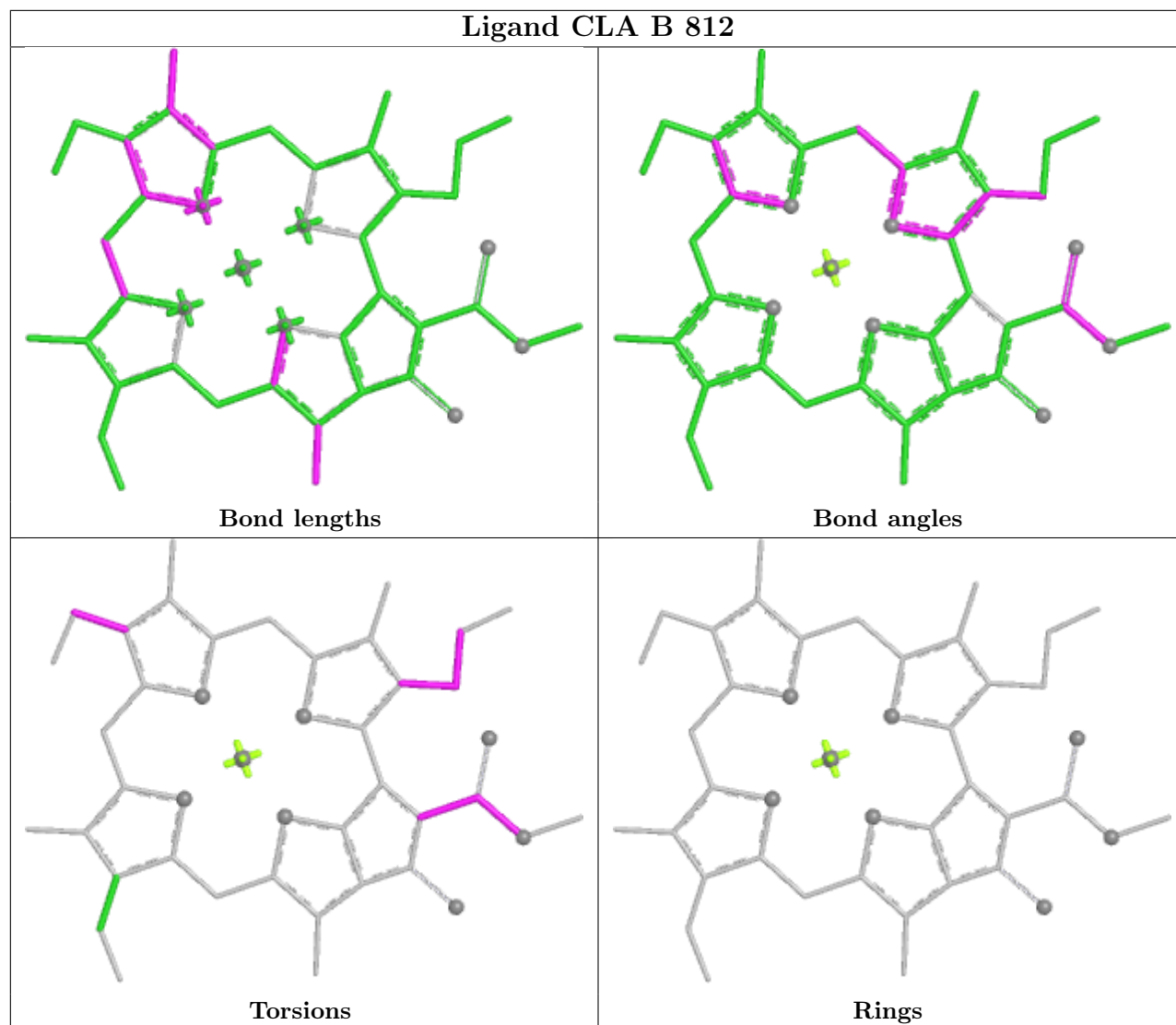
Ligand CLA 3 604**Ligand LHG B 851**



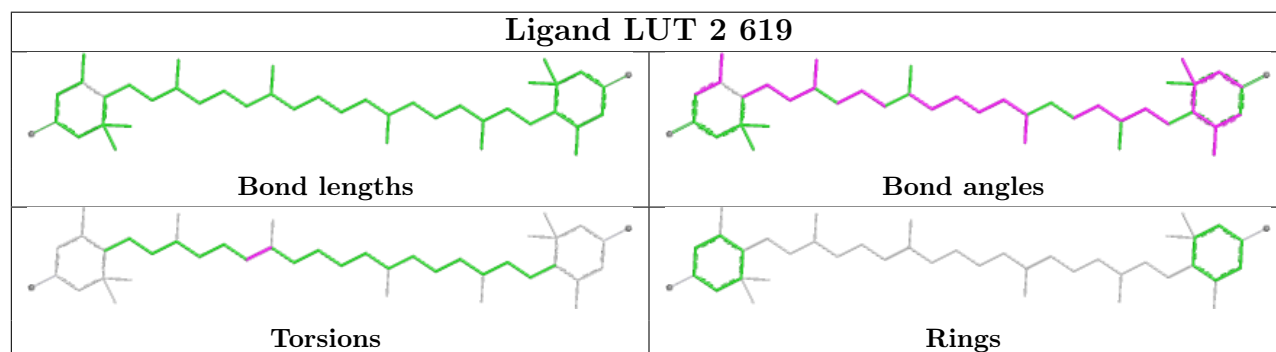


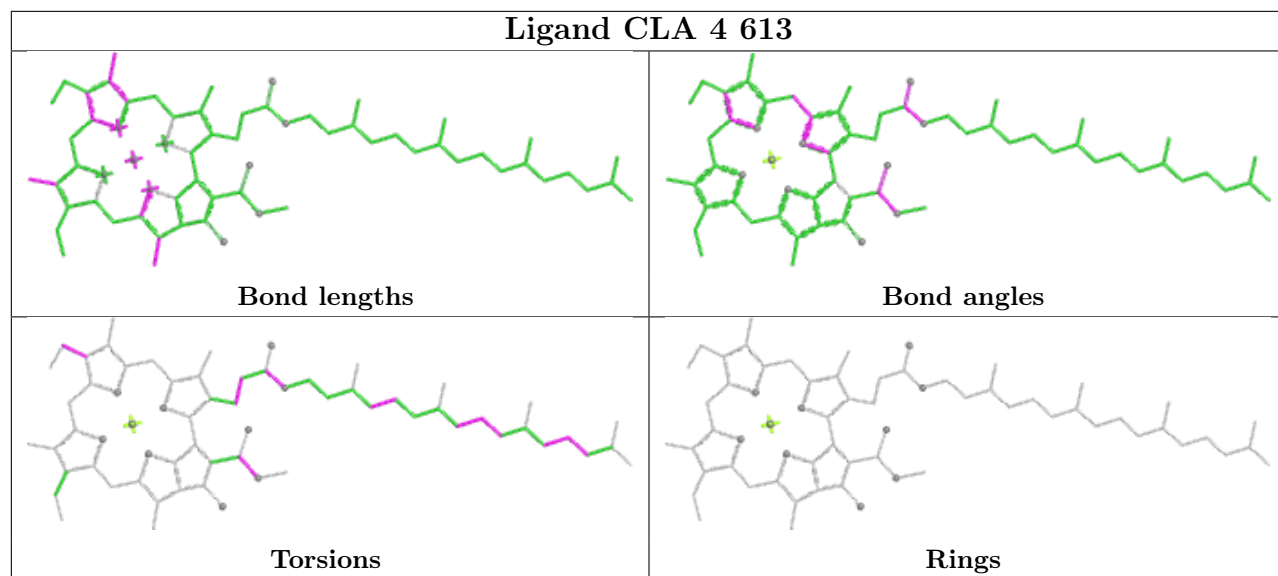


Ligand CLA B 812

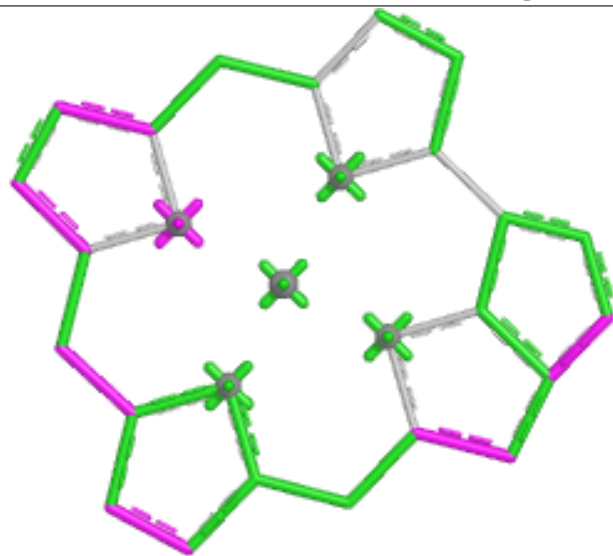


Ligand LUT 2 619

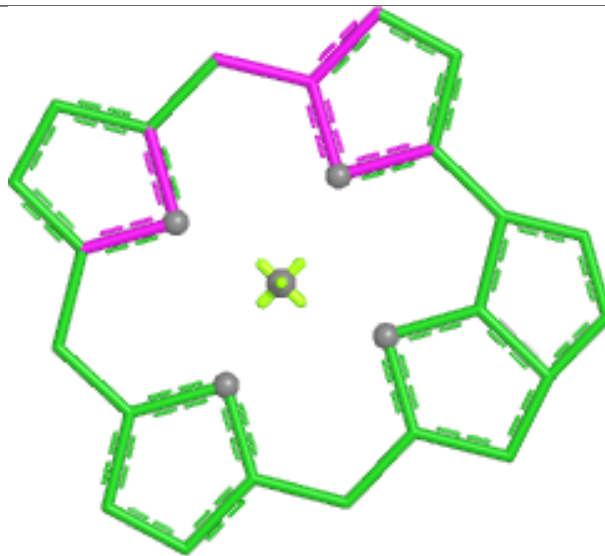




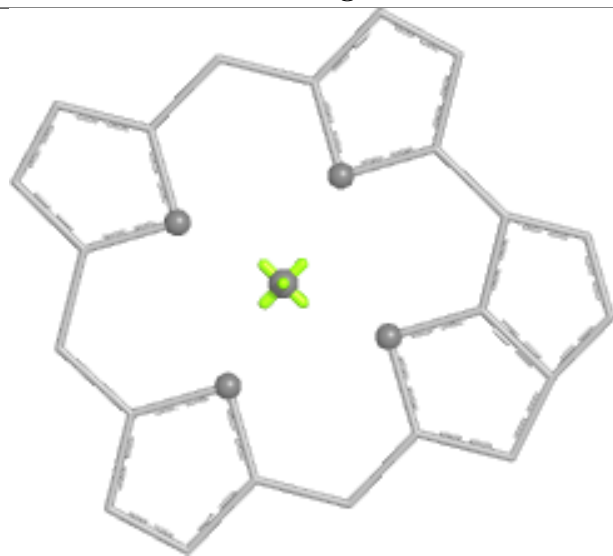
Ligand CLA 2 613



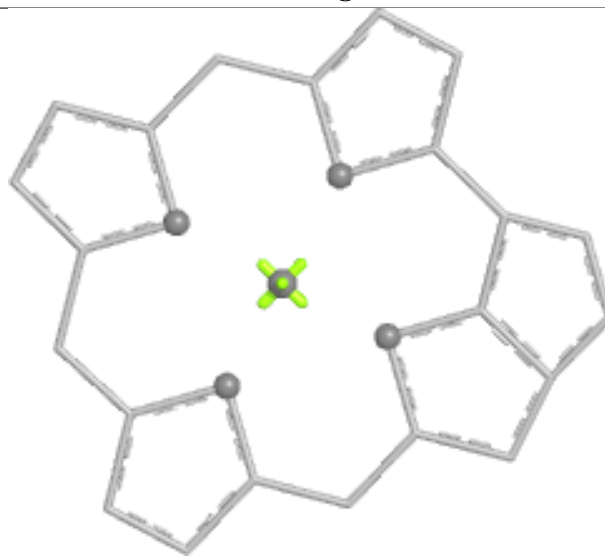
Bond lengths



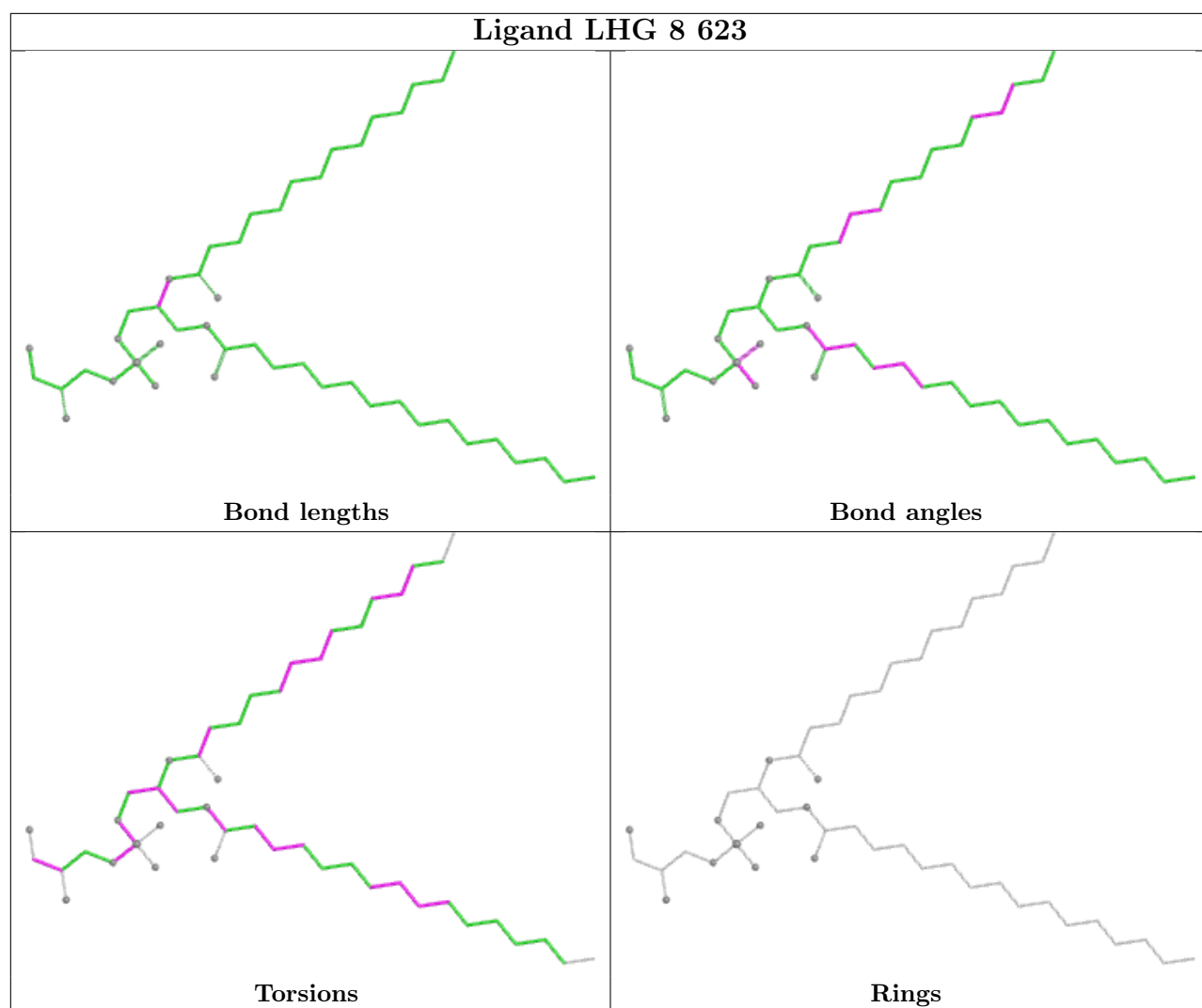
Bond angles



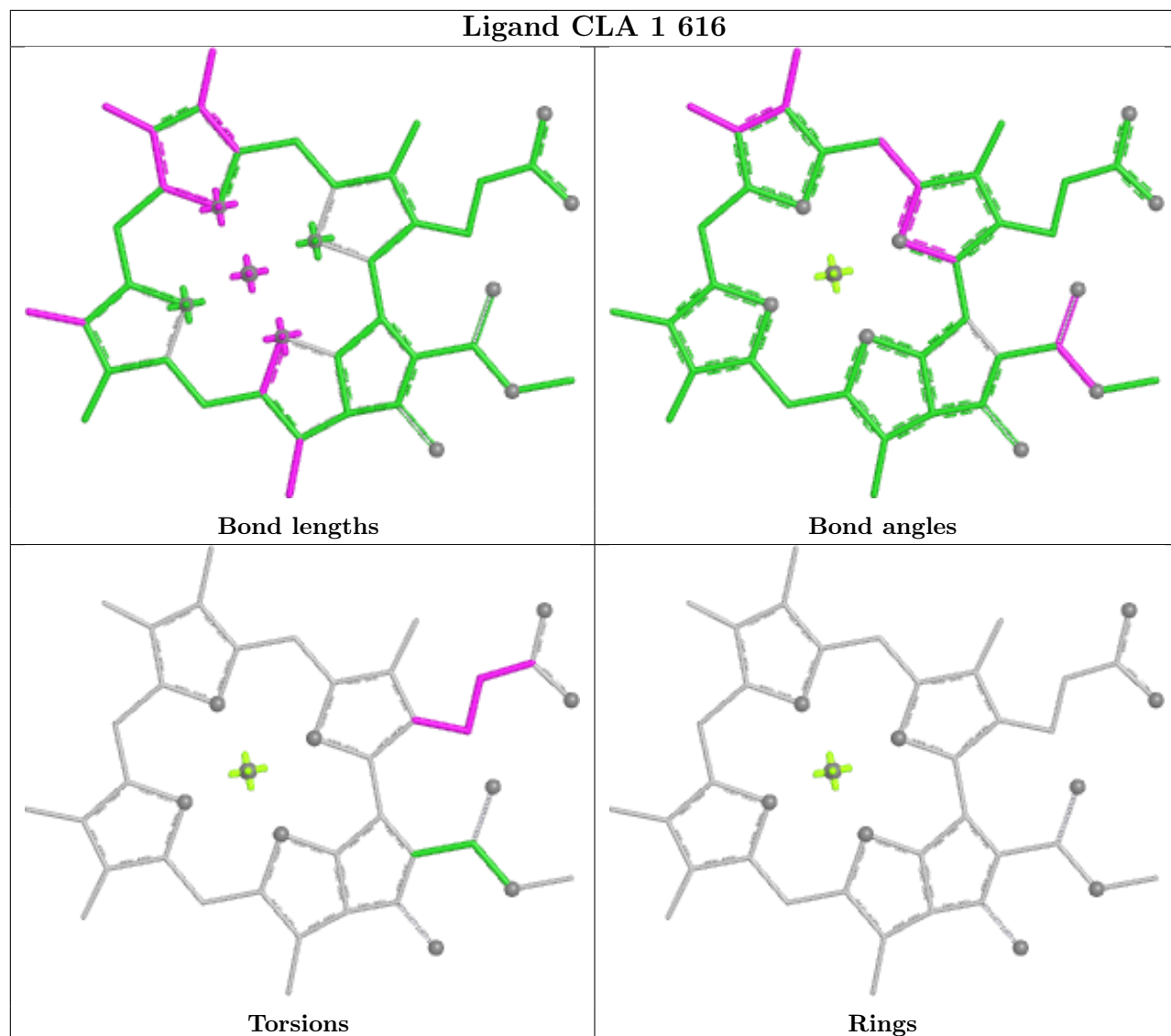
Torsions

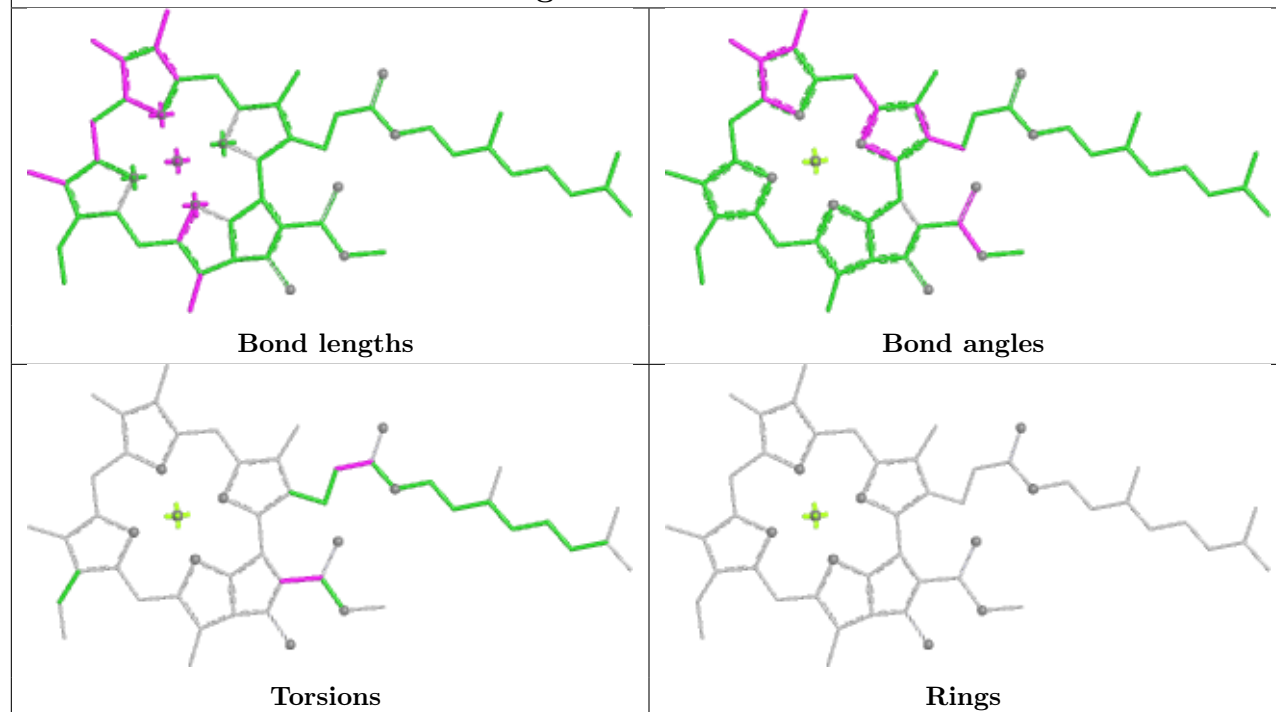
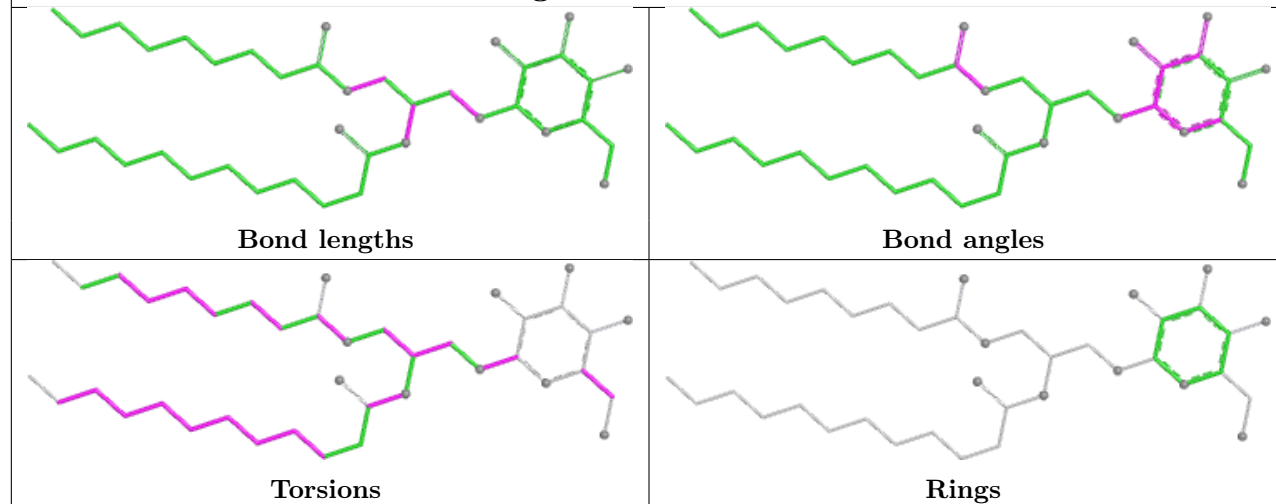


Rings

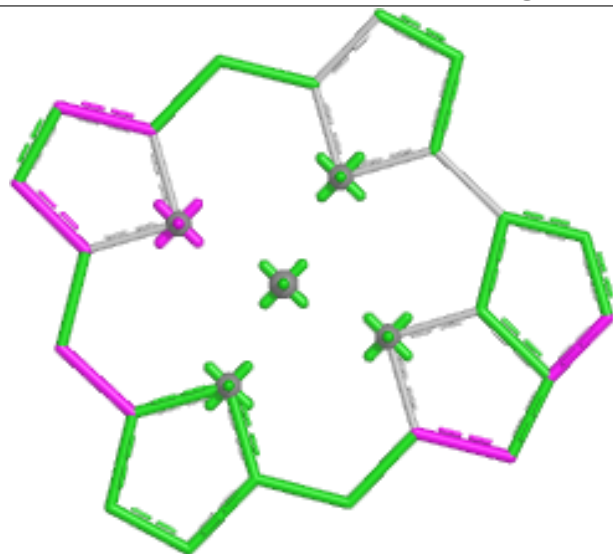


Ligand CLA 1 616

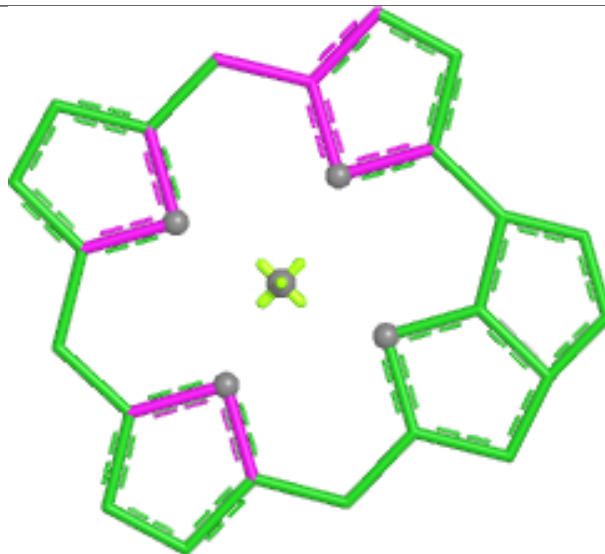


Ligand CLA 6 603**Ligand LMG 5 626**

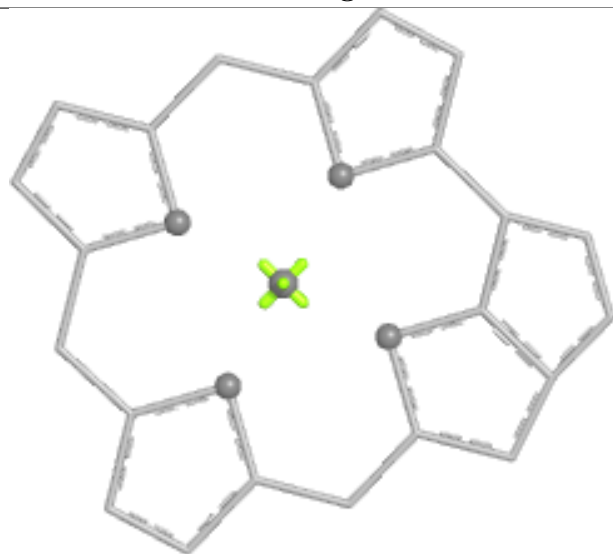
Ligand CLA 2 601



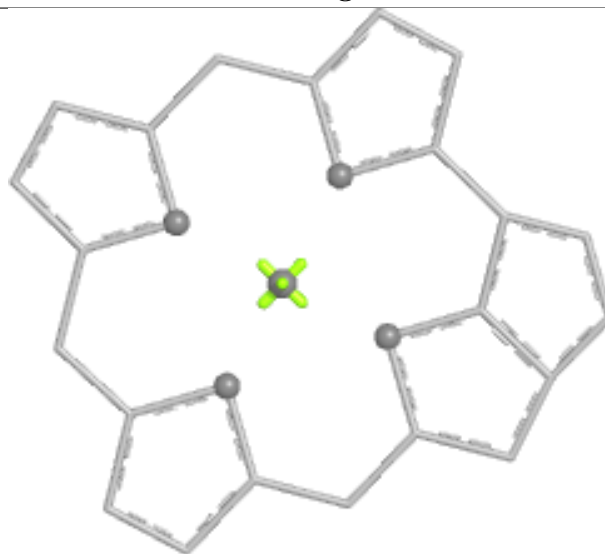
Bond lengths



Bond angles

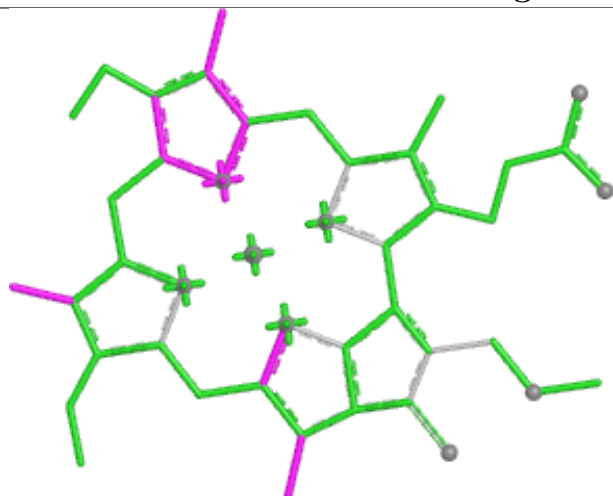


Torsions

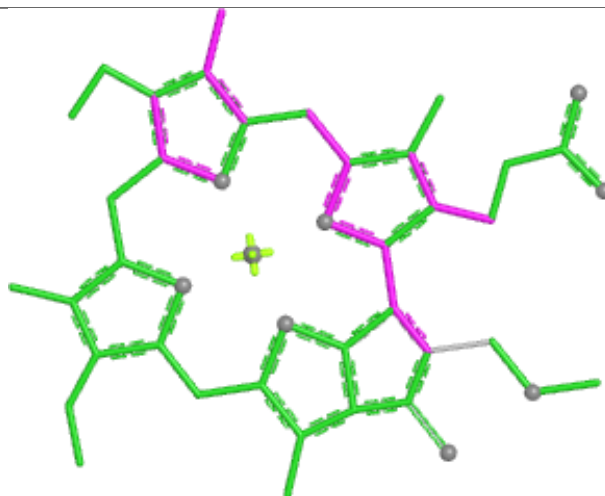


Rings

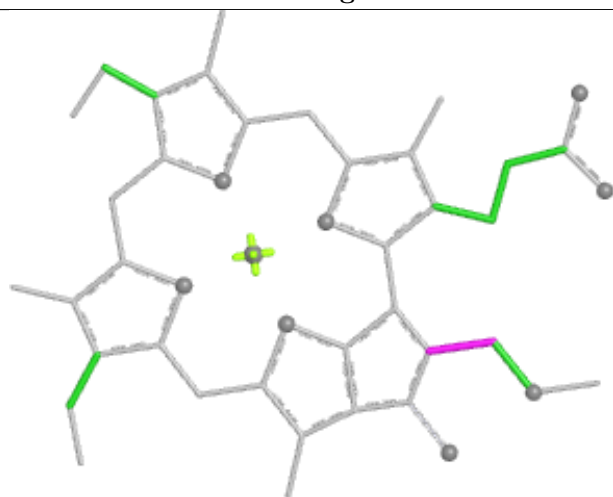
Ligand CLA A 816



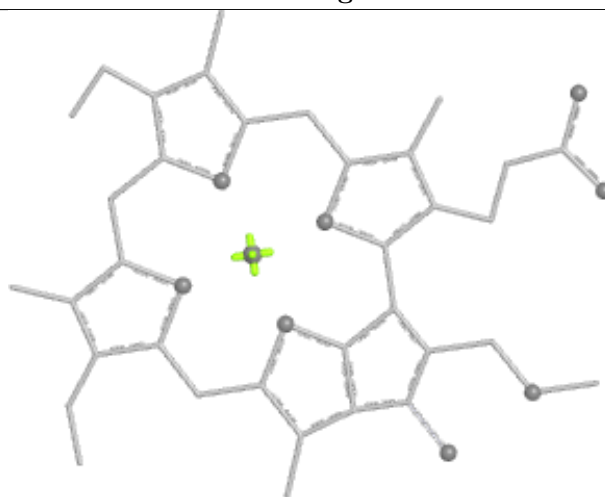
Bond lengths



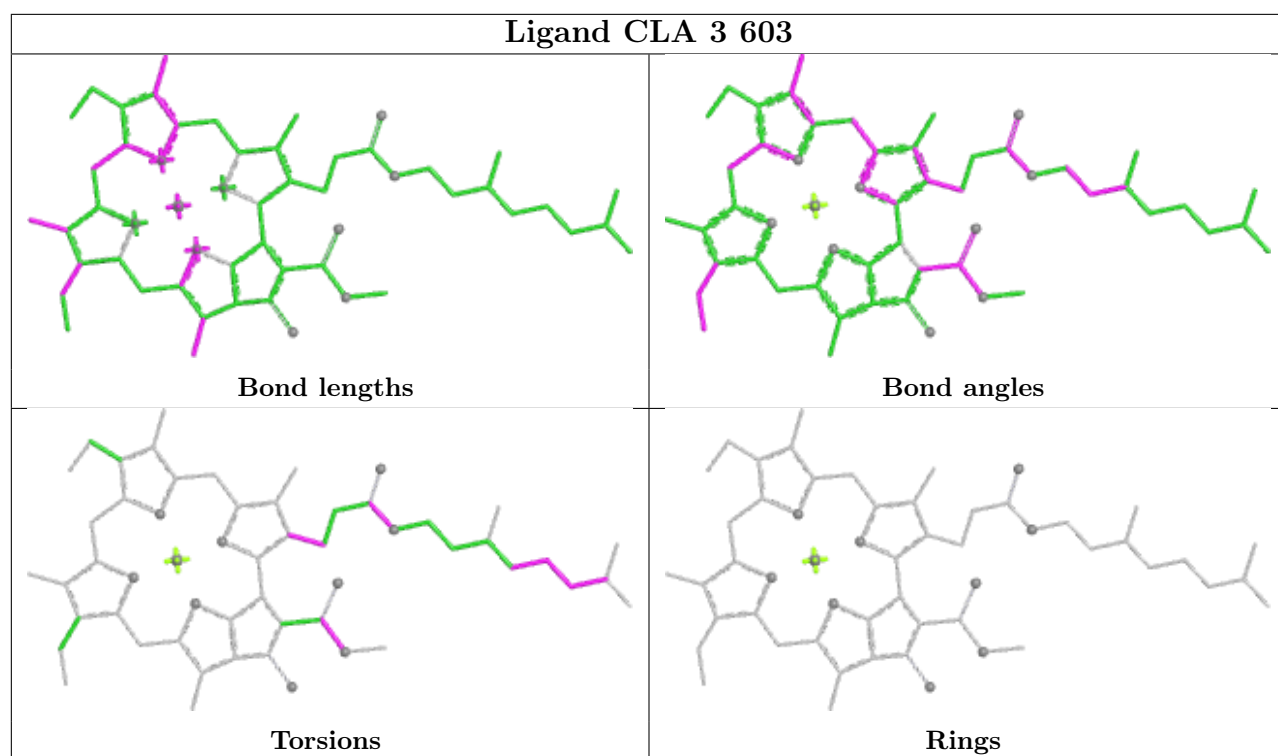
Bond angles



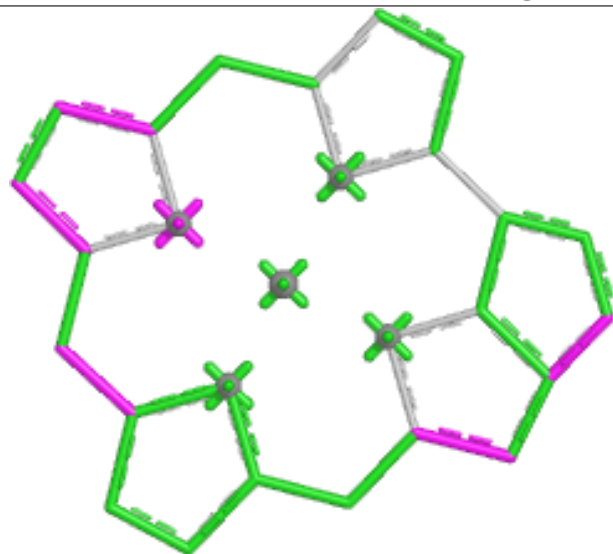
Torsions



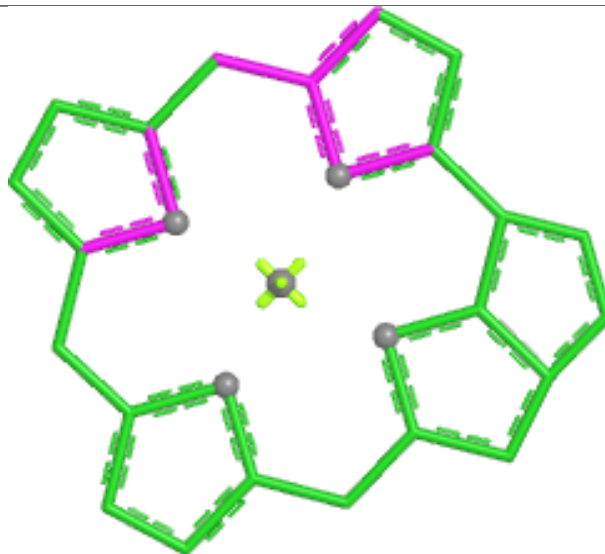
Rings



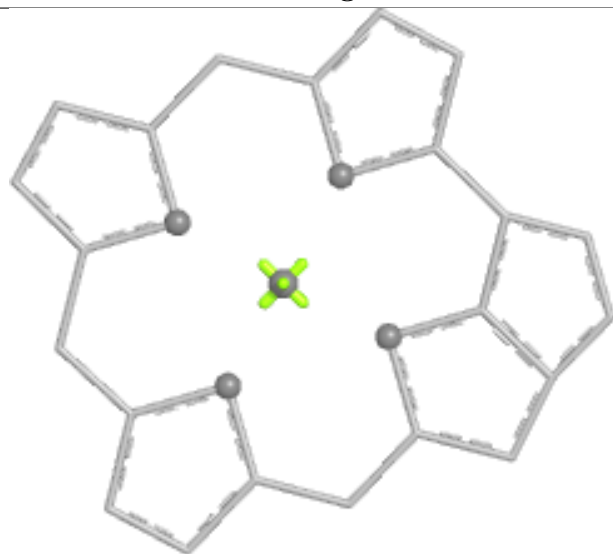
Ligand CLA 9 604



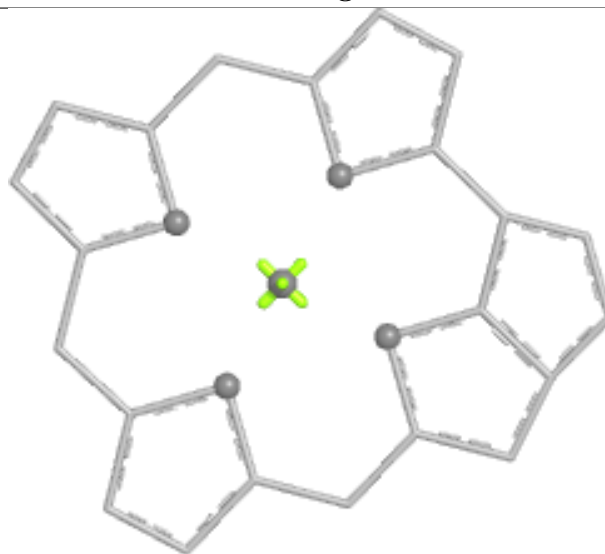
Bond lengths



Bond angles

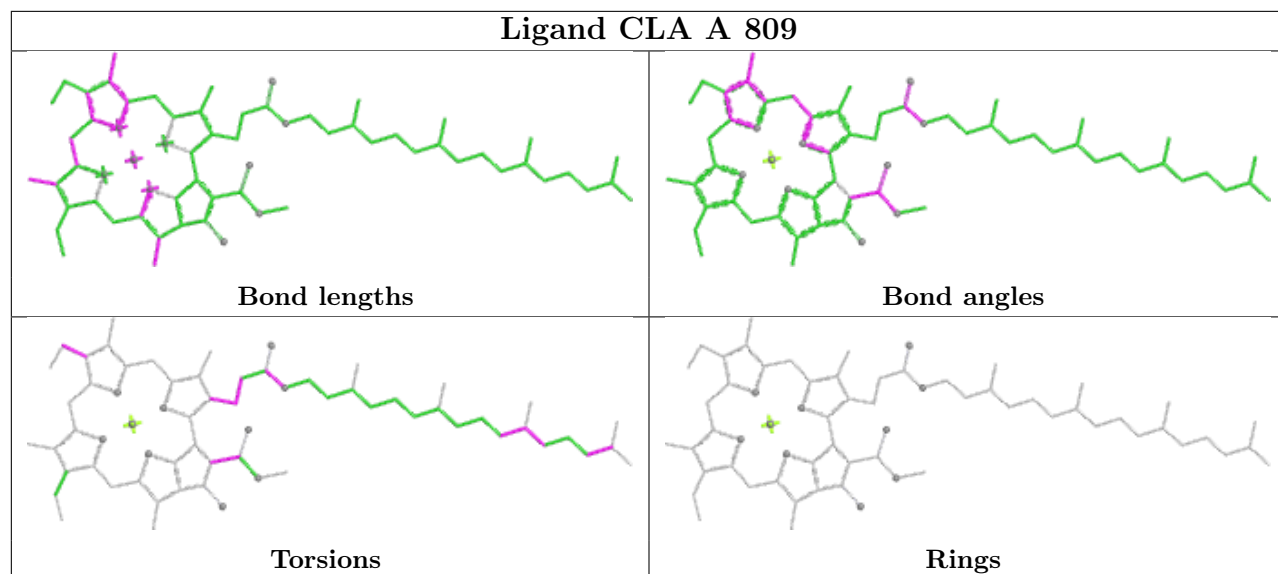


Torsions

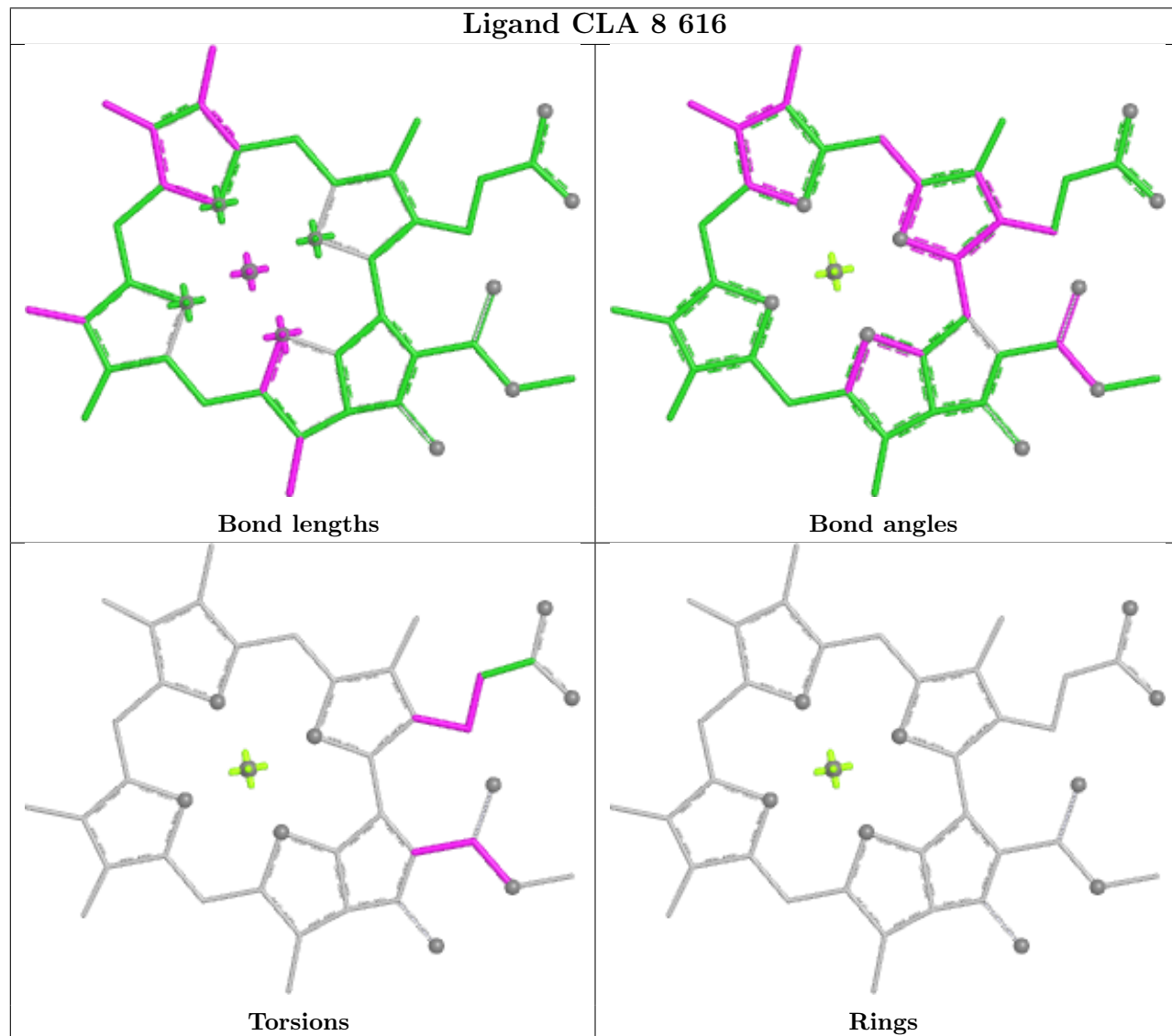


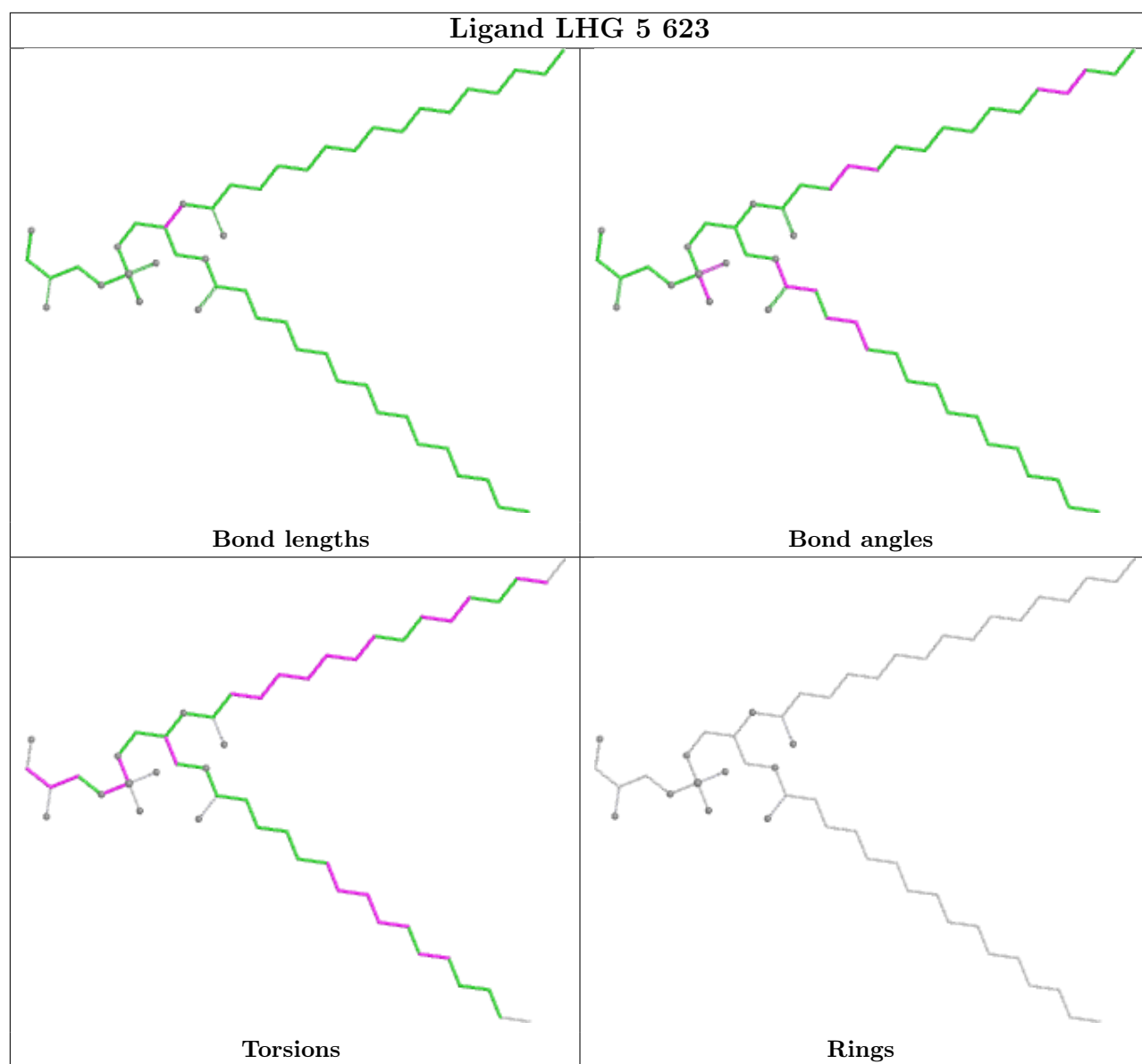
Rings

Ligand CLA A 809

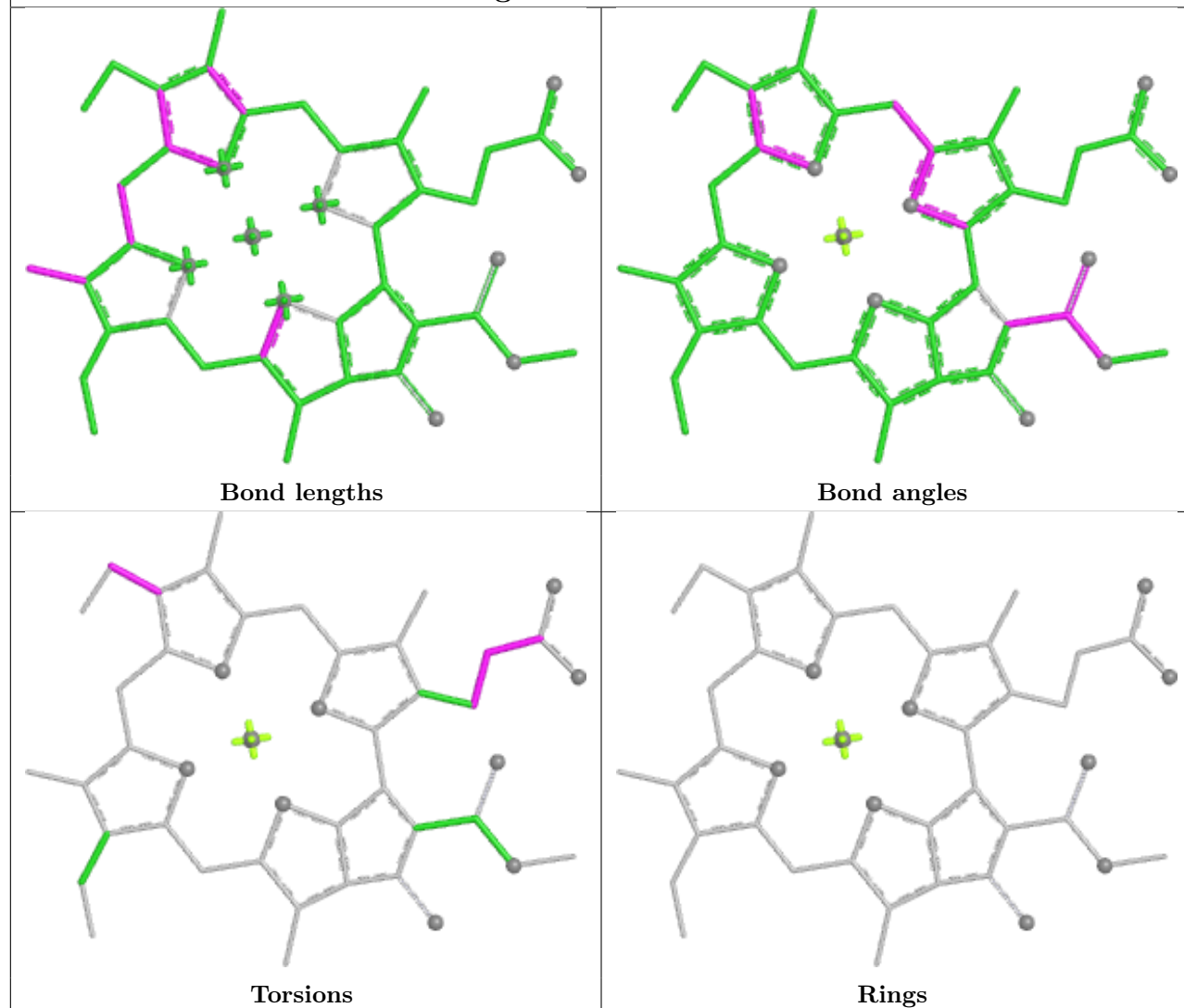


Ligand CLA 8 616

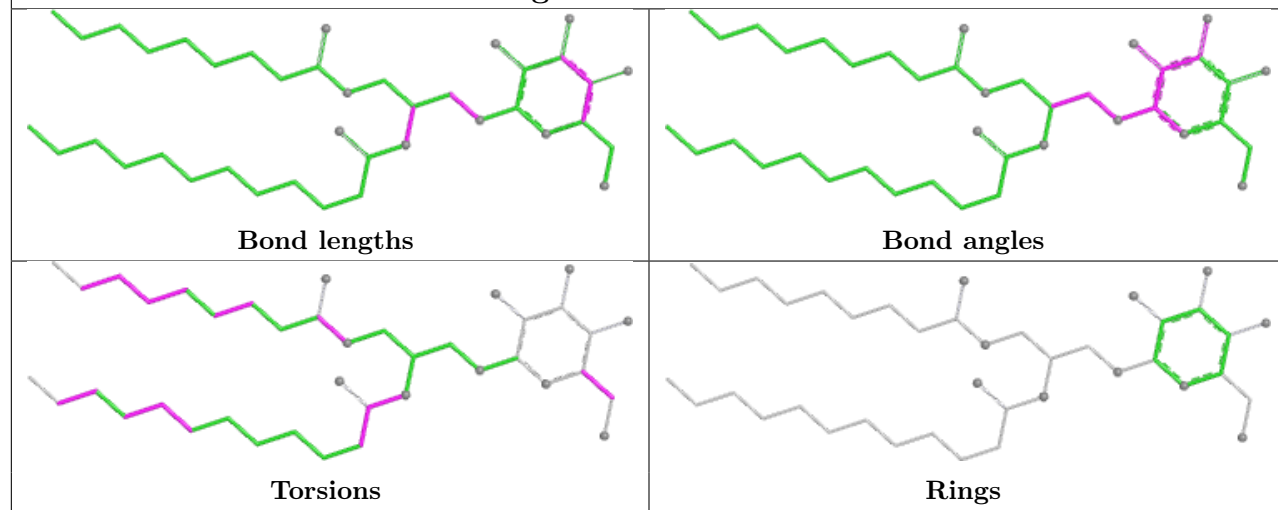


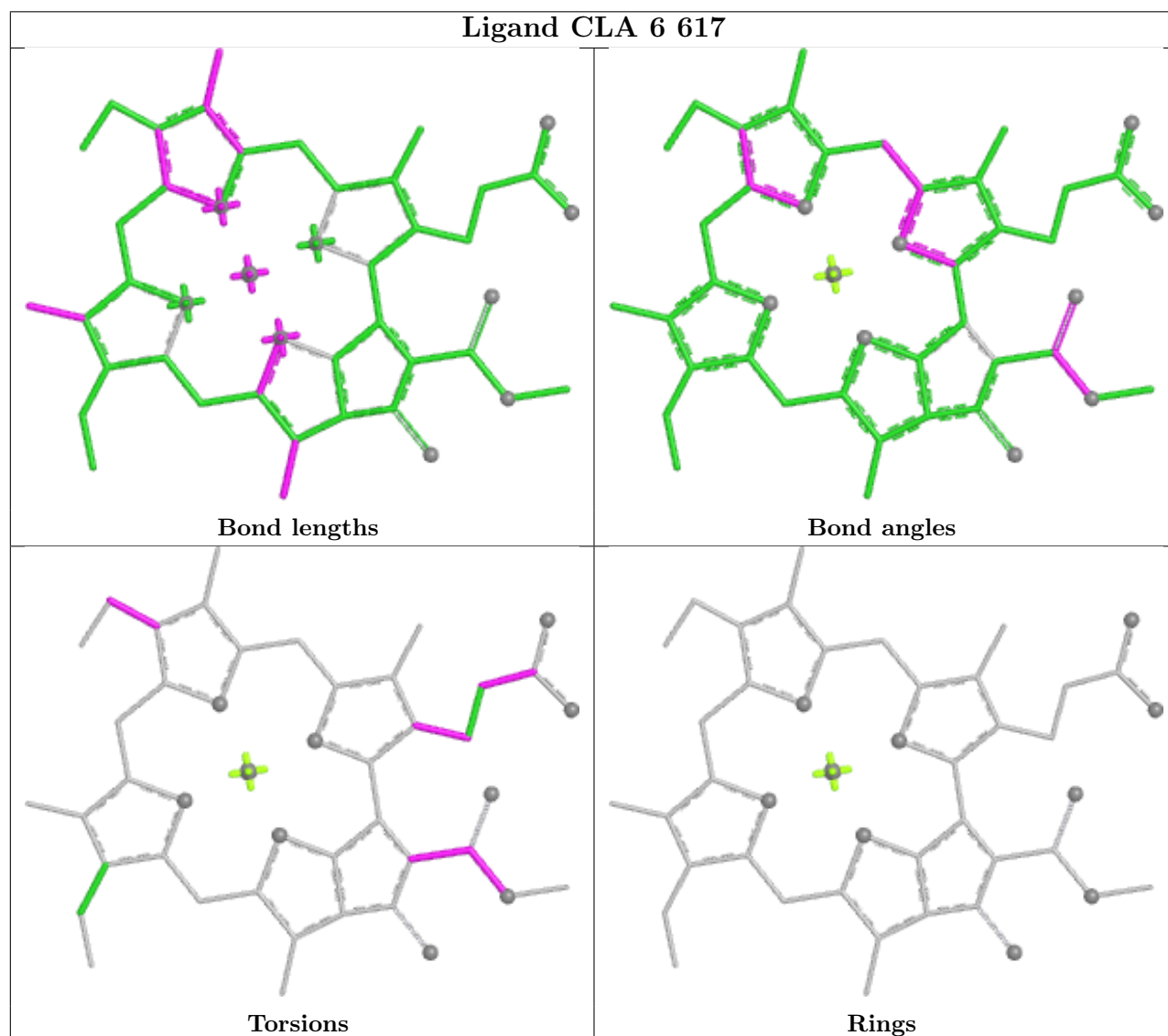
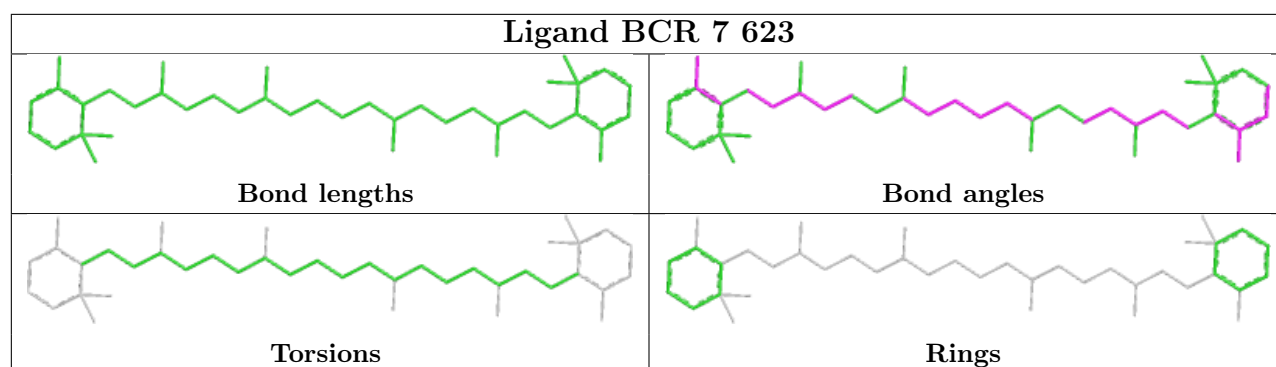


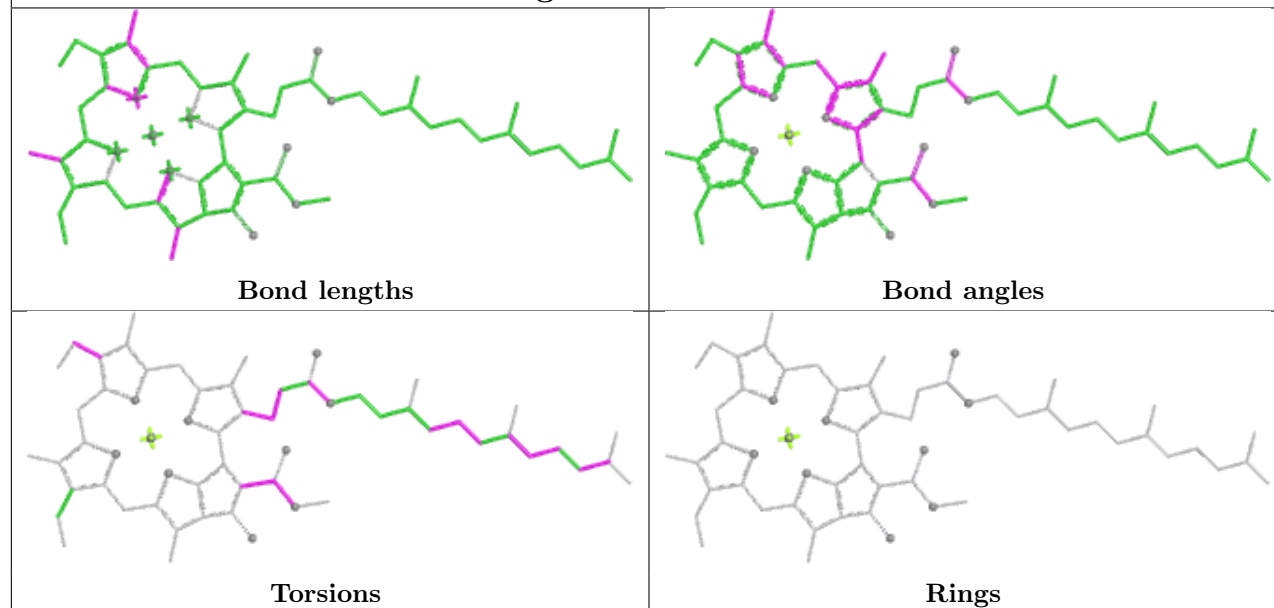
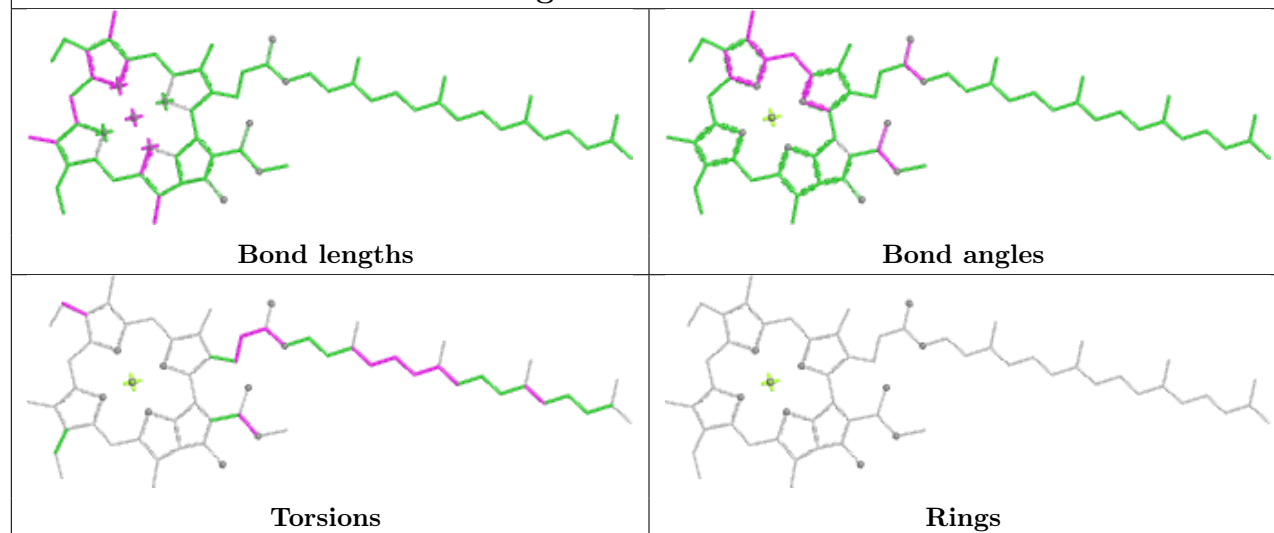
Ligand CLA L 302



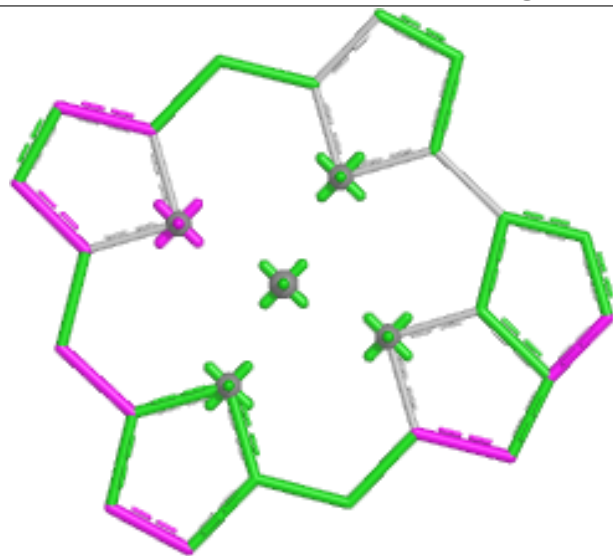
Ligand LMG 4 624



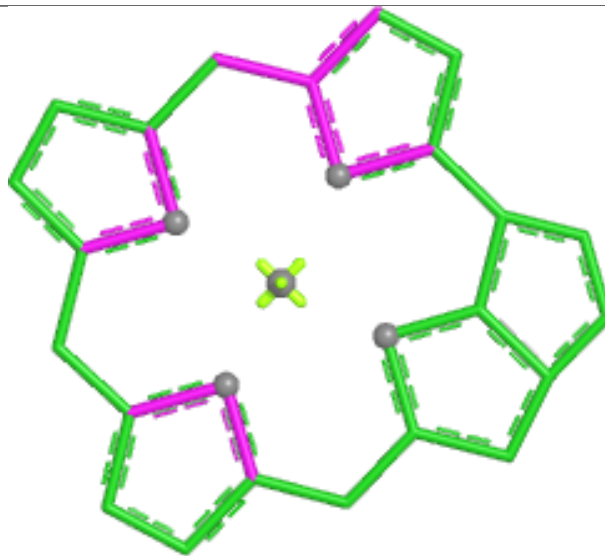


Ligand CLA 3 609**Ligand CLA 7 602**

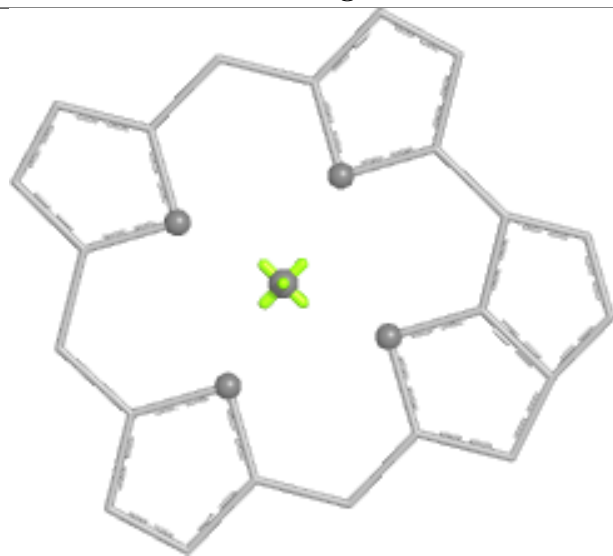
Ligand CLA 2 616



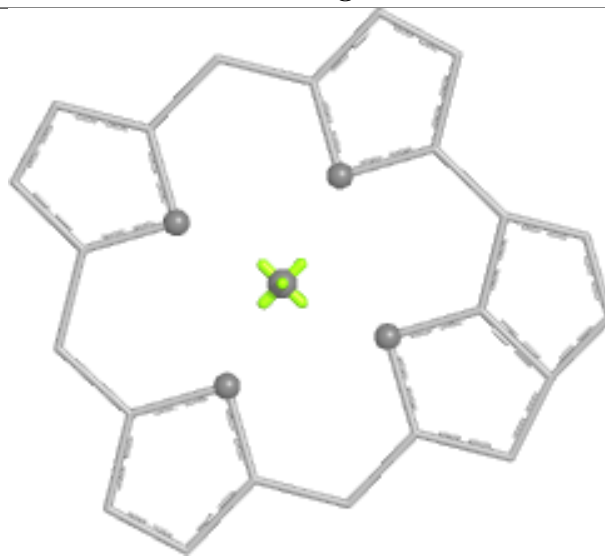
Bond lengths



Bond angles

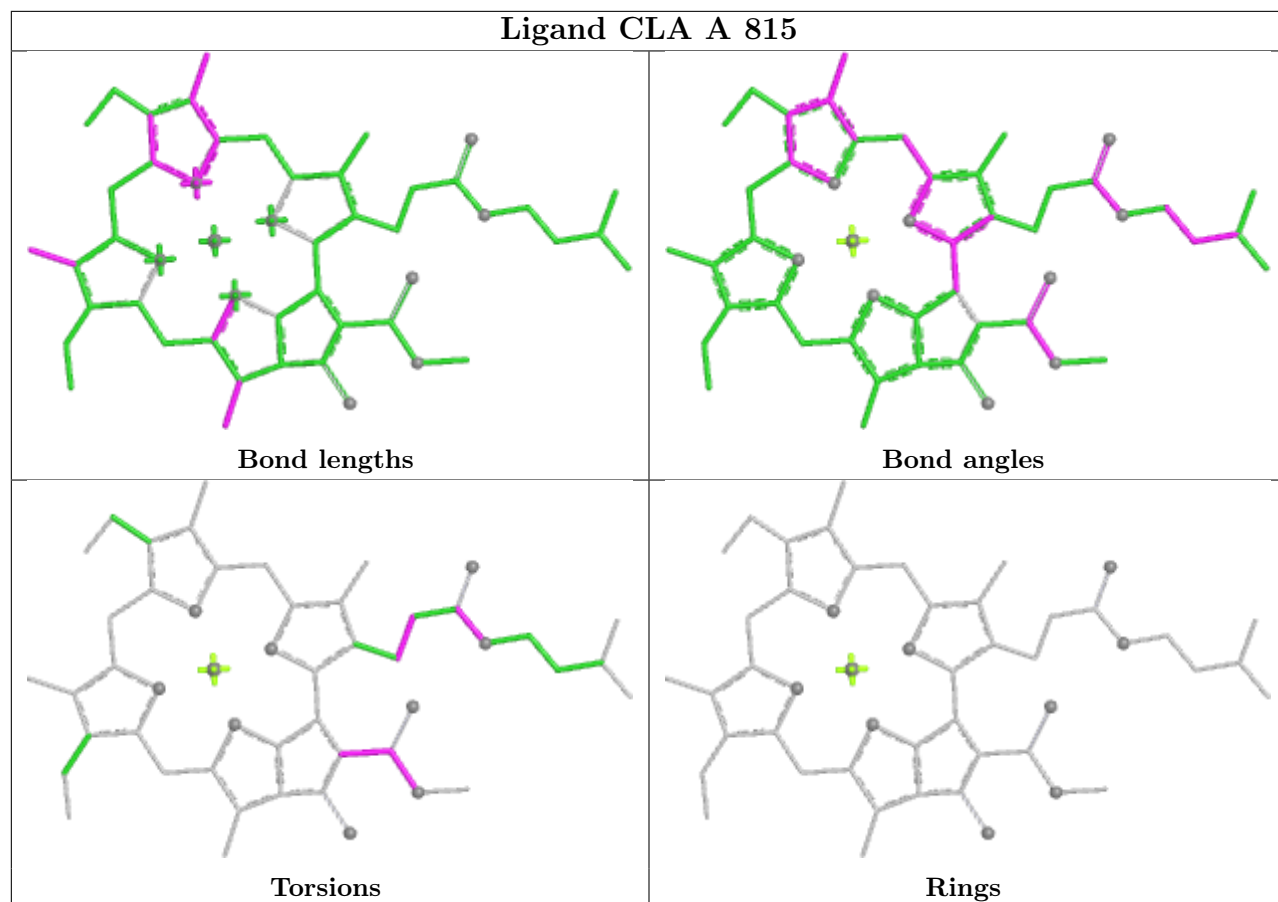


Torsions

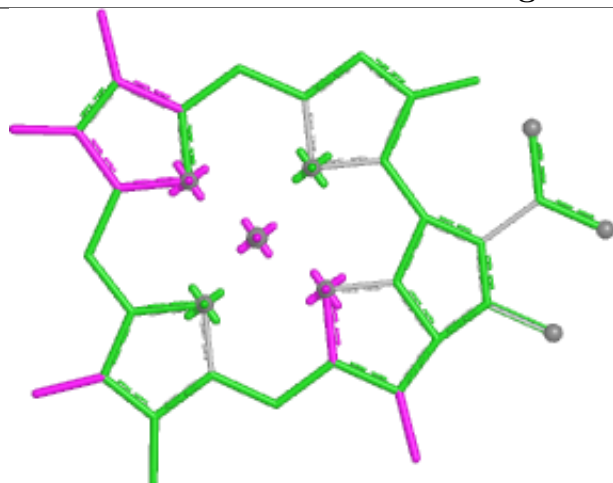


Rings

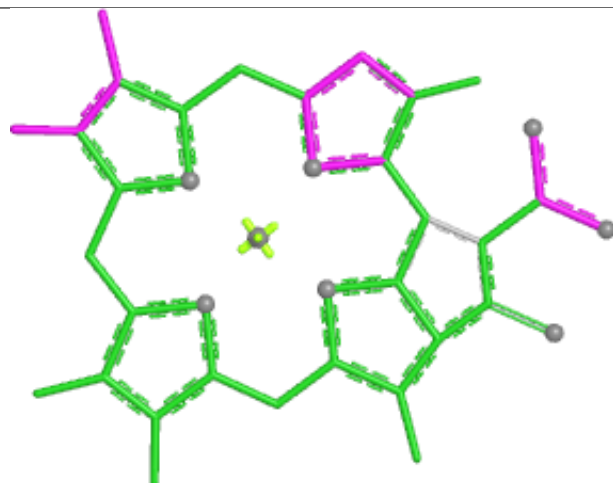
Ligand CLA A 815



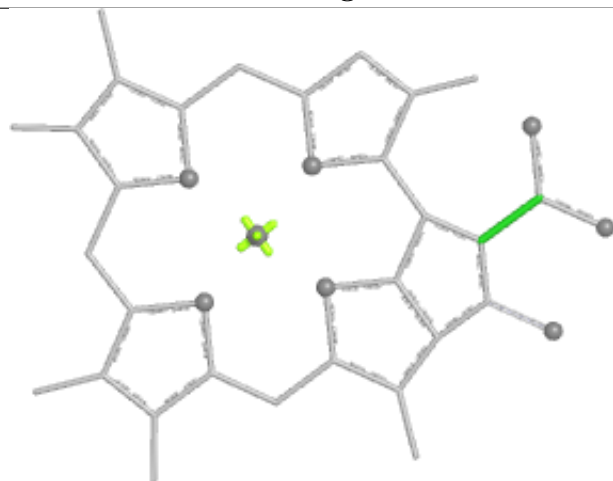
Ligand CLA 1 614



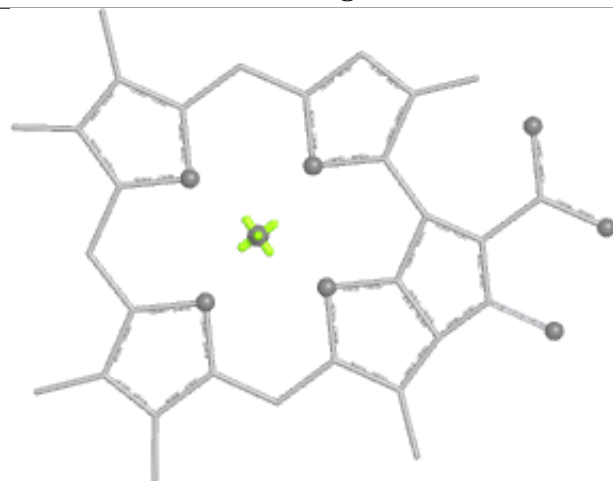
Bond lengths



Bond angles

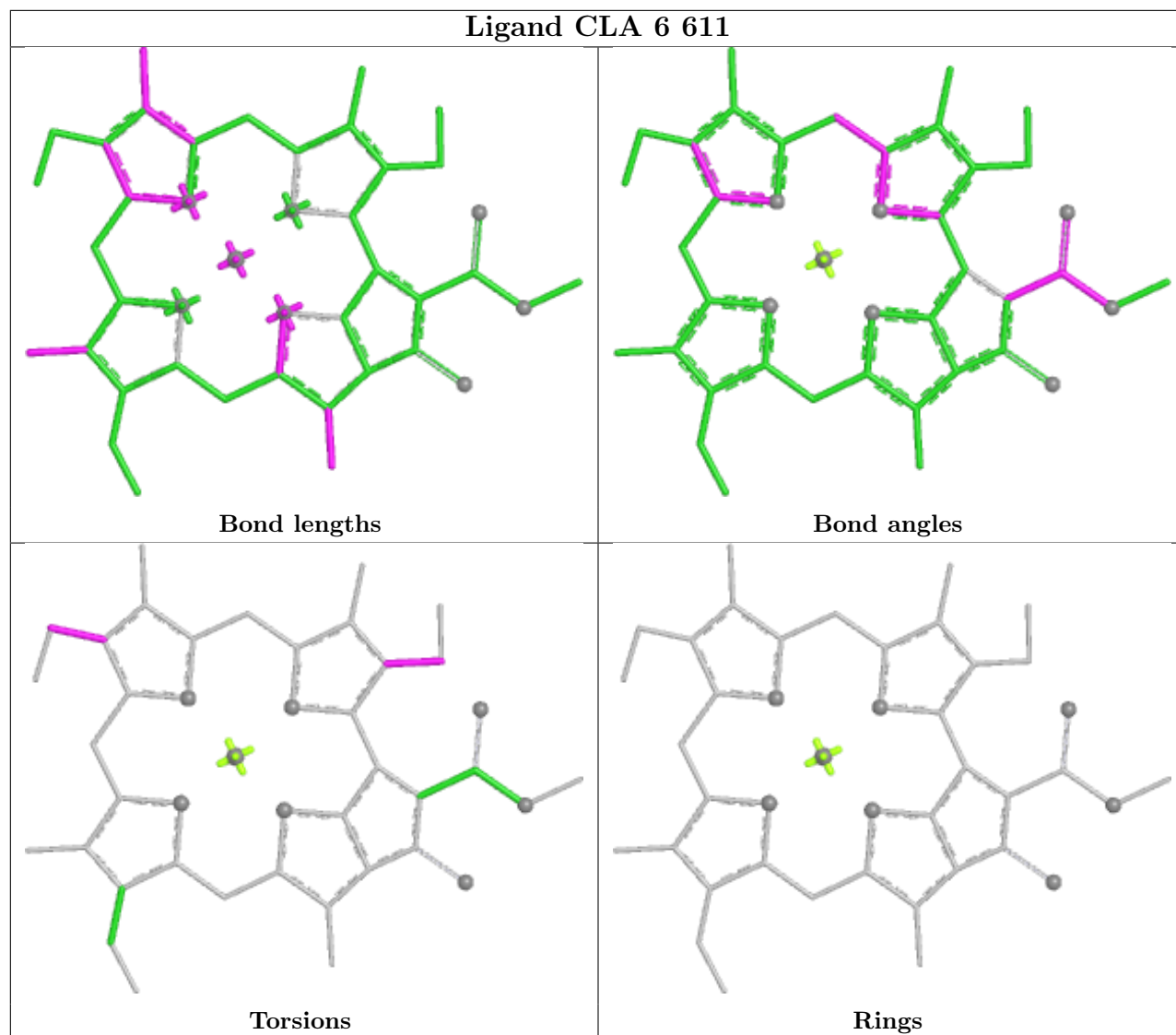


Torsions

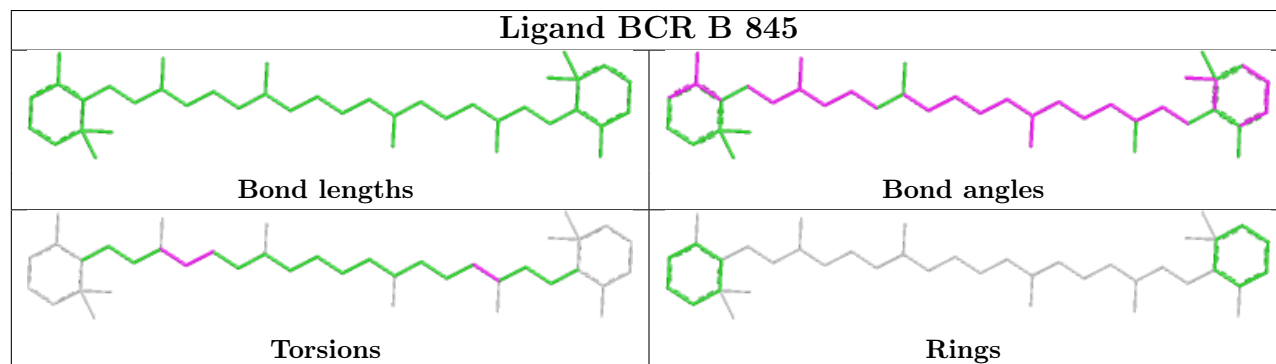


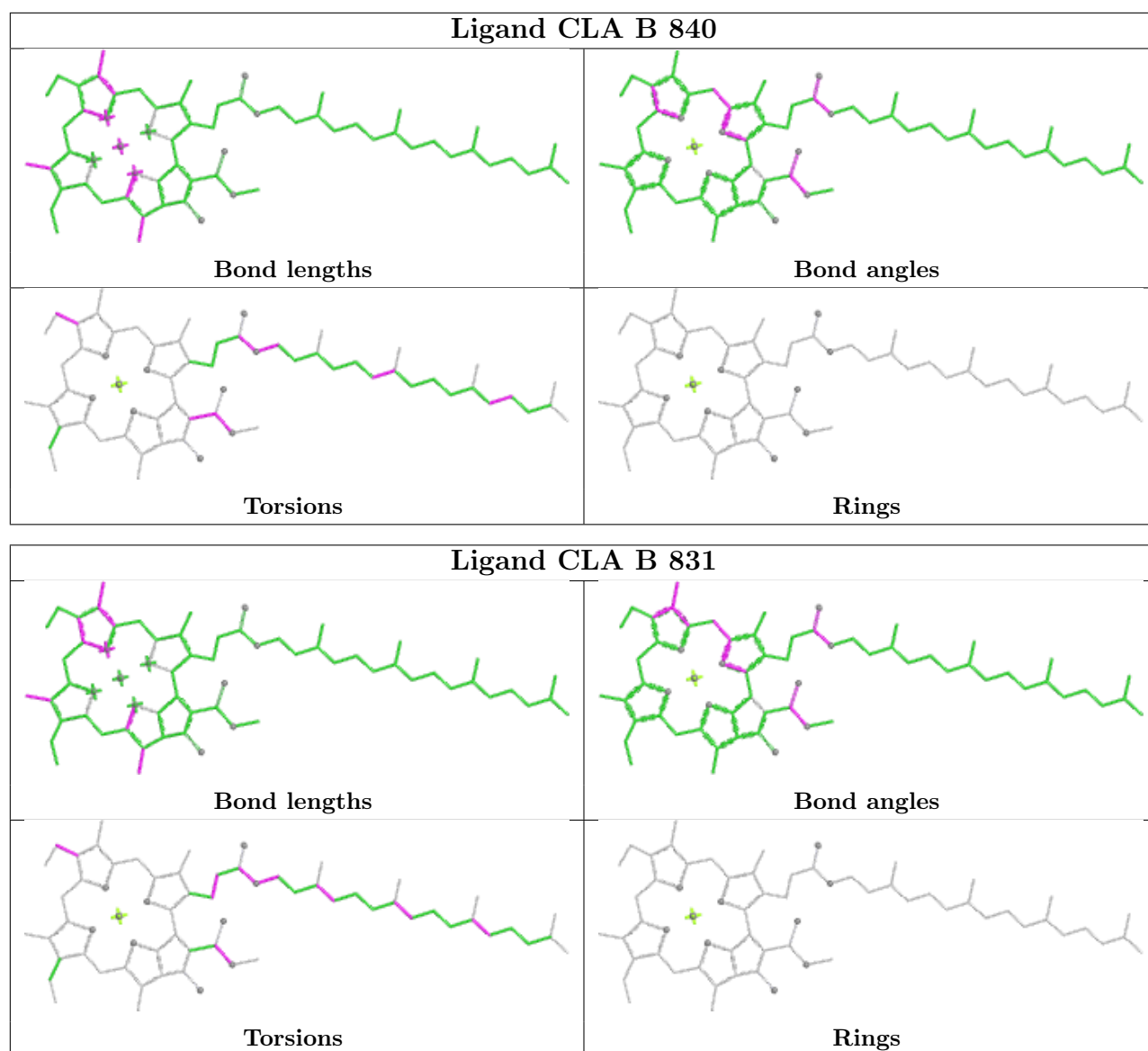
Rings

Ligand CLA 6 611

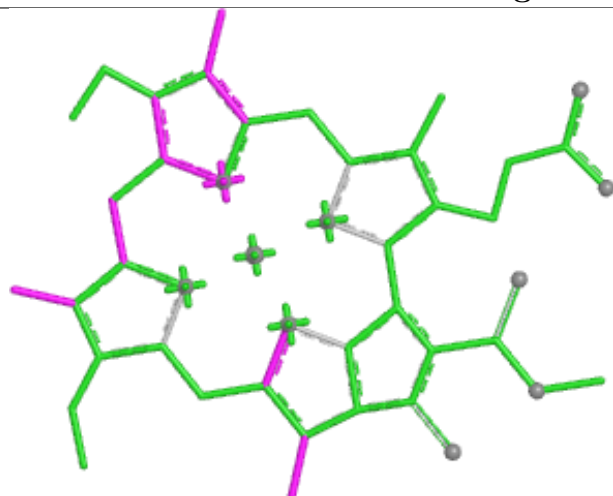


Ligand BCR B 845

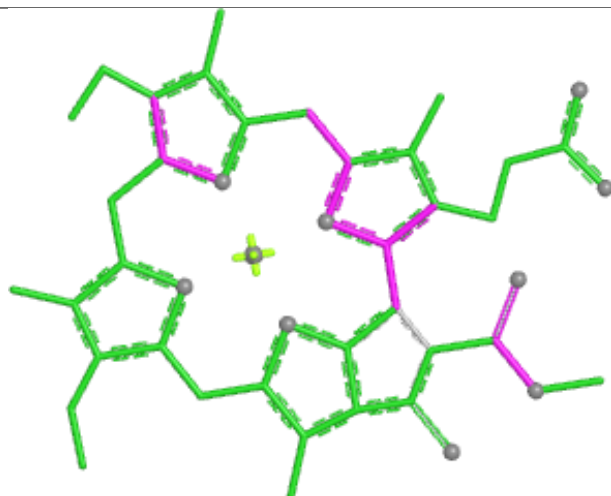




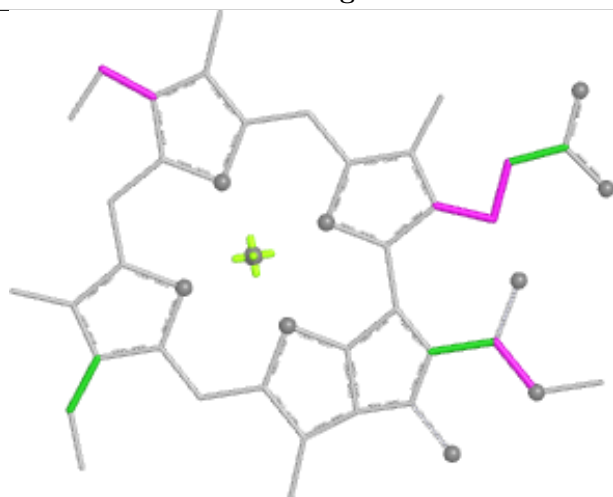
Ligand CLA A 837



Bond lengths



Bond angles

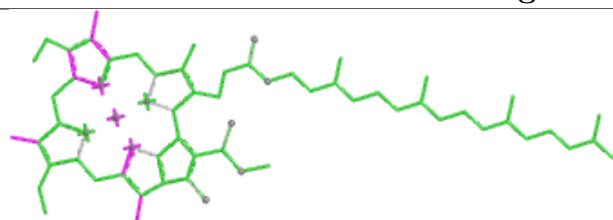


Torsions

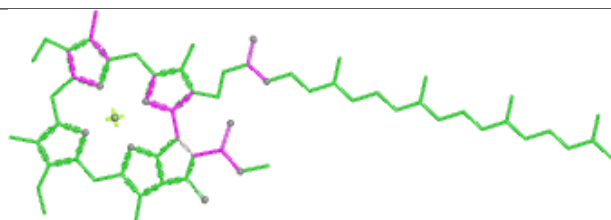


Rings

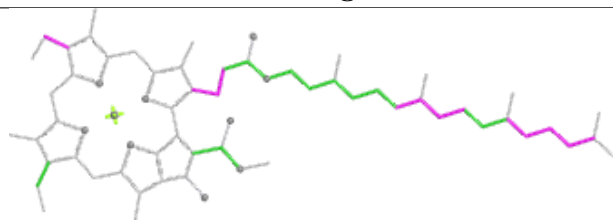
Ligand CLA 5 609



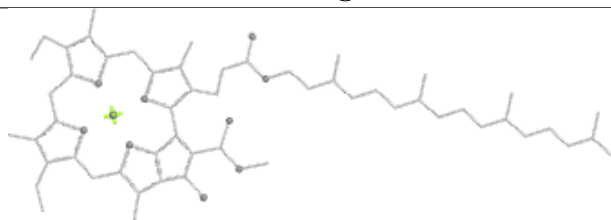
Bond lengths



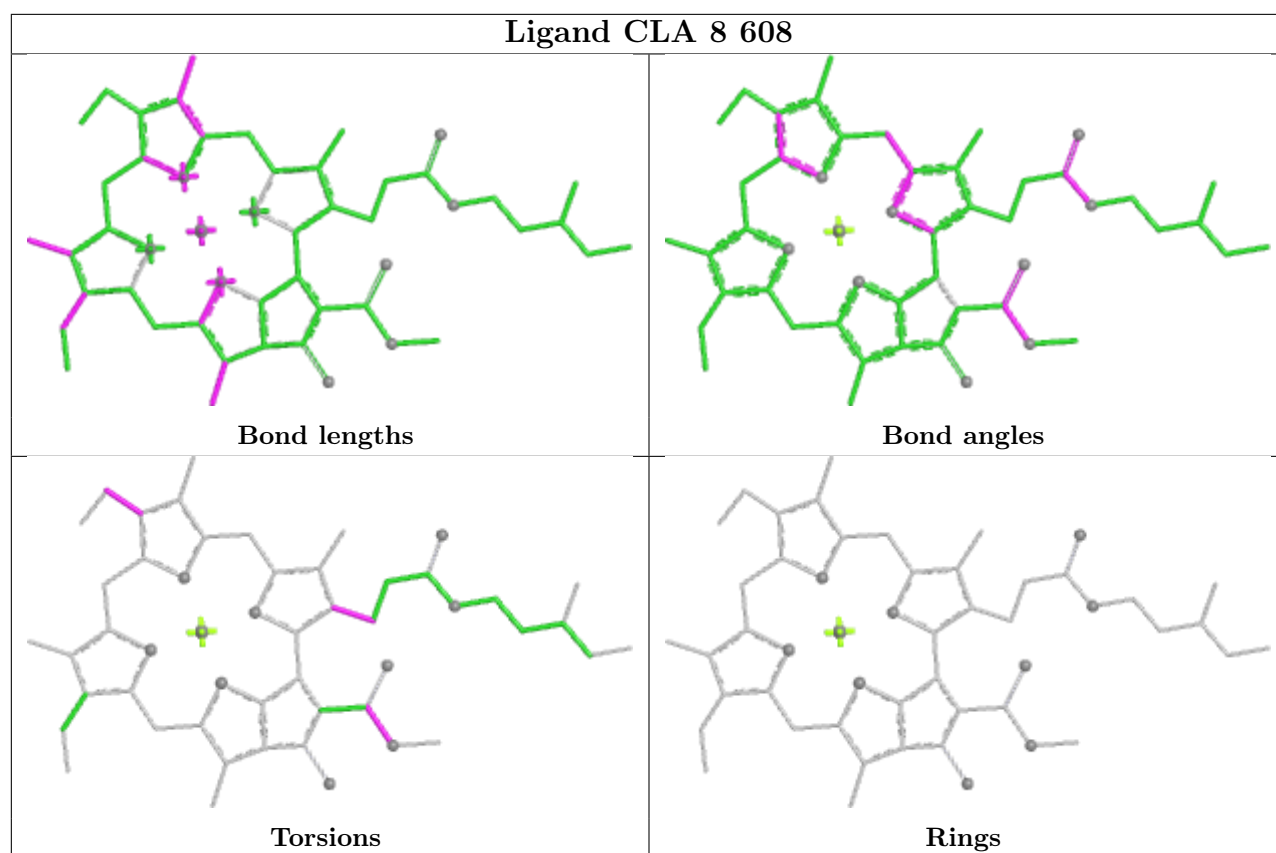
Bond angles



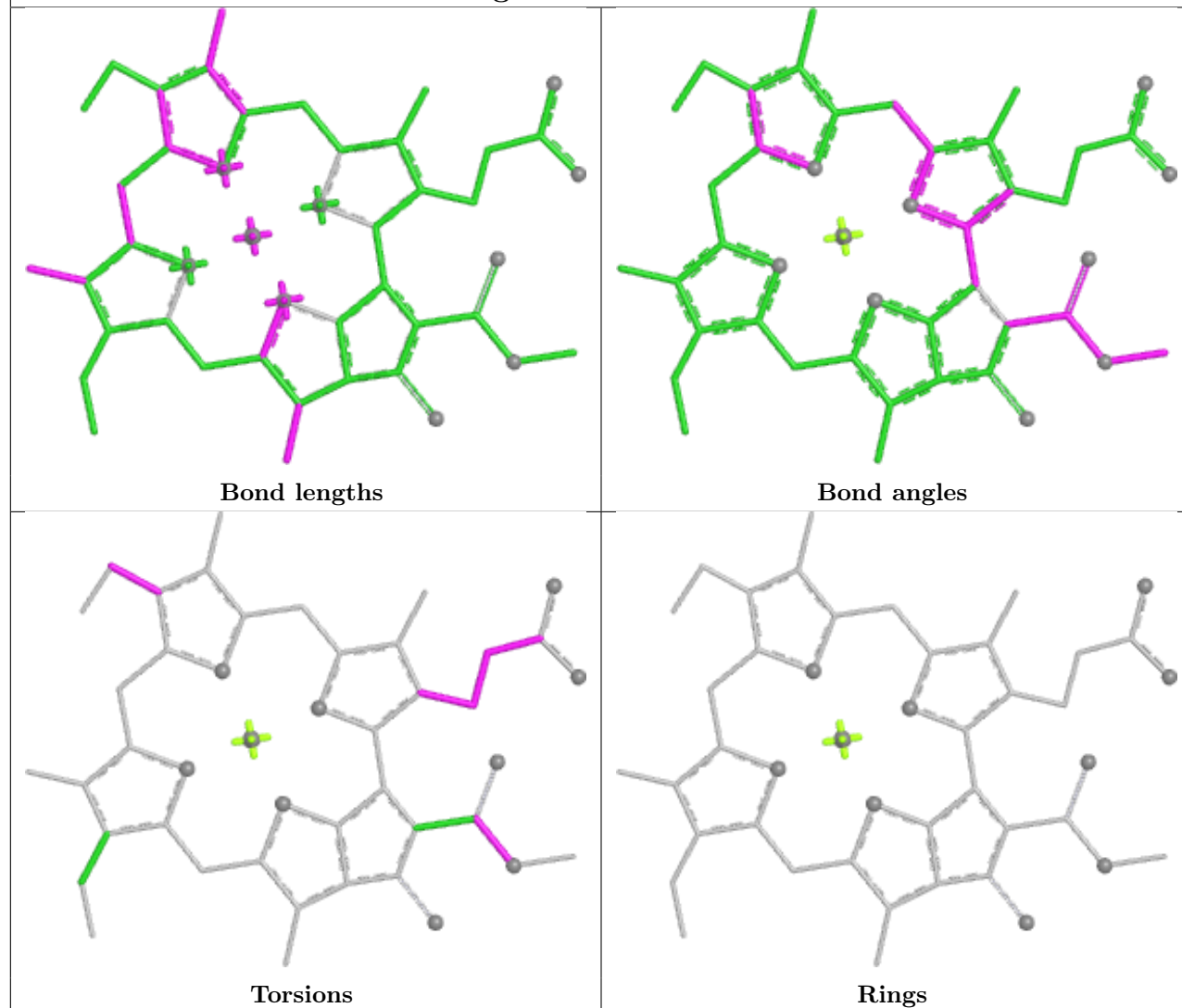
Torsions



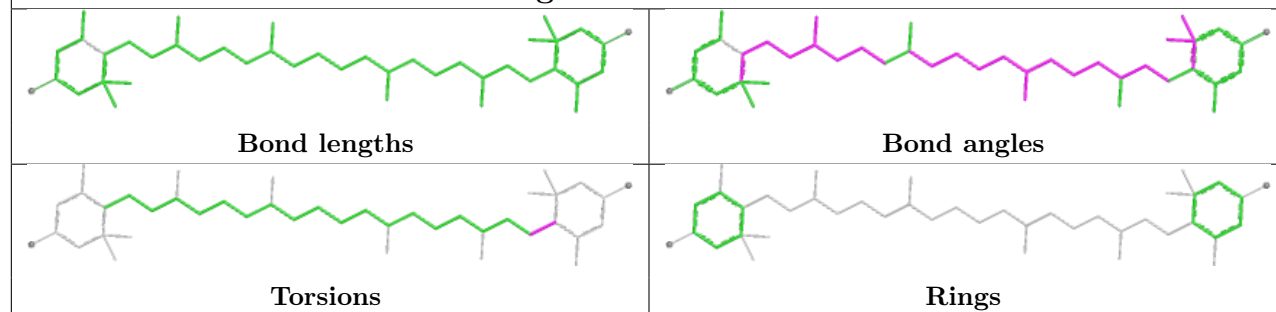
Rings

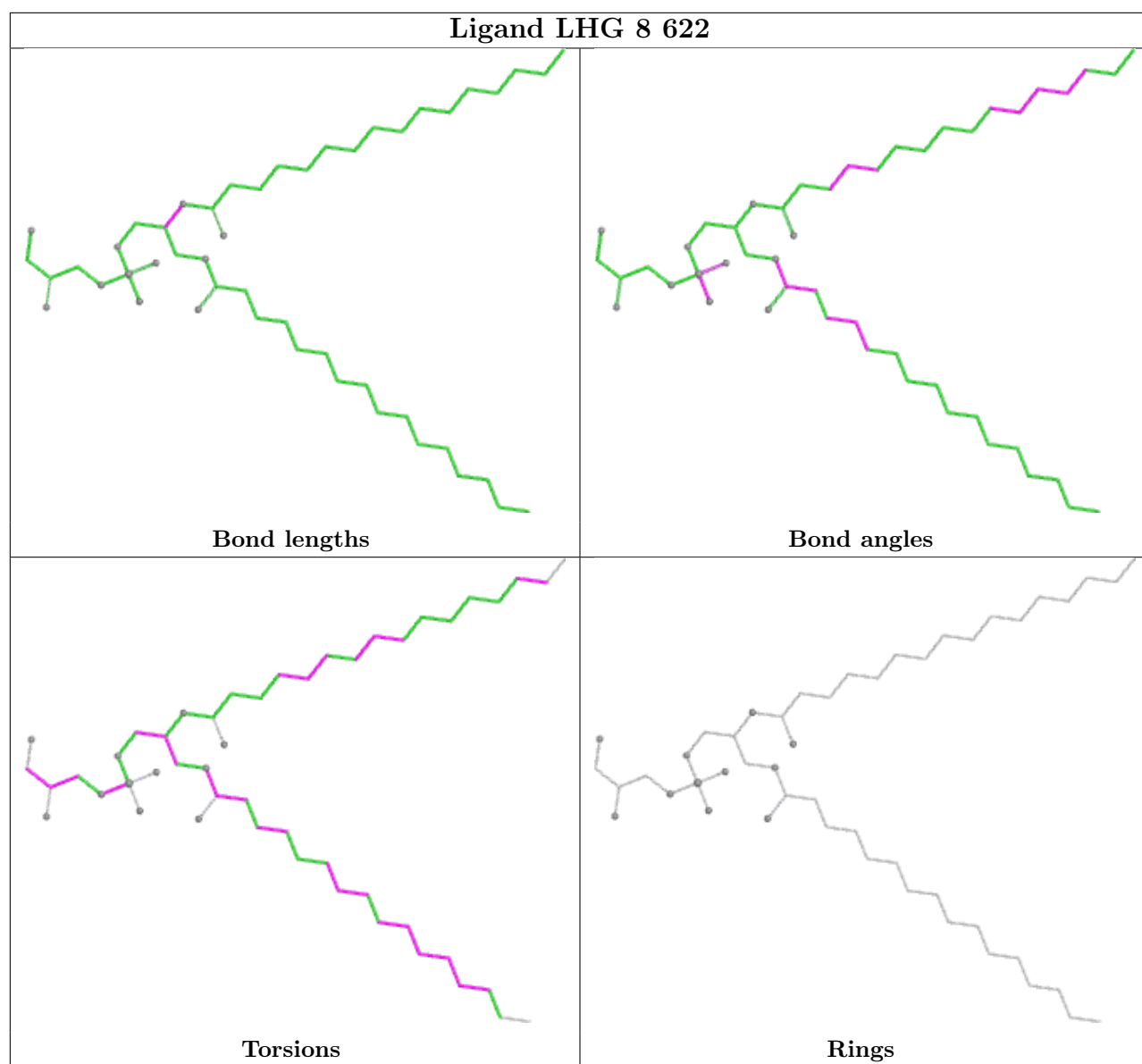


Ligand CLA B 835

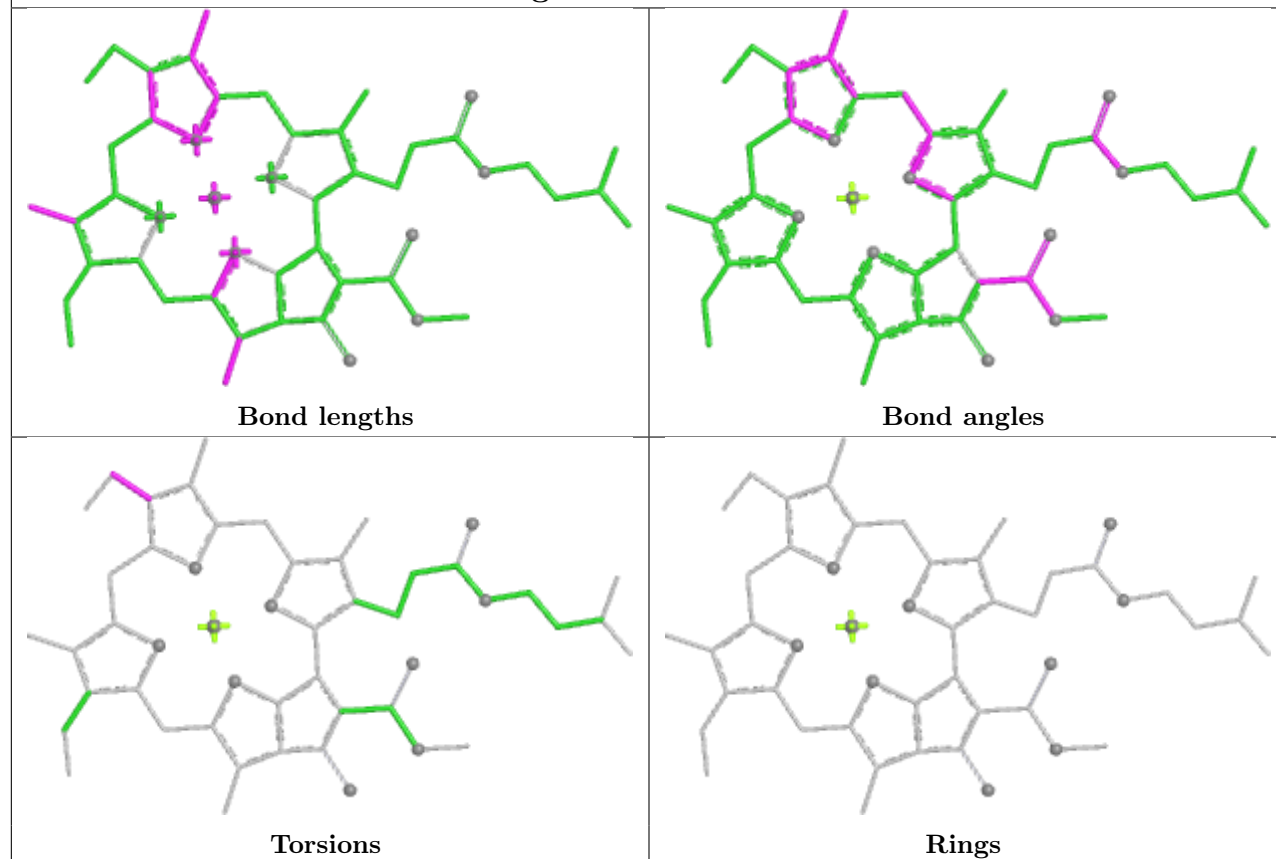


Ligand LUT 1 617

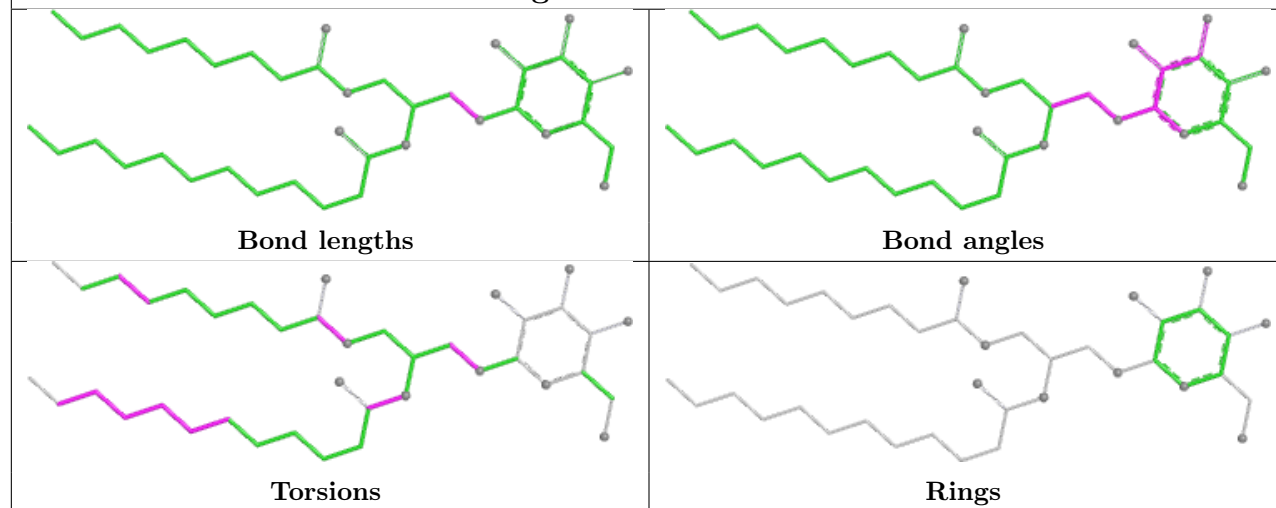


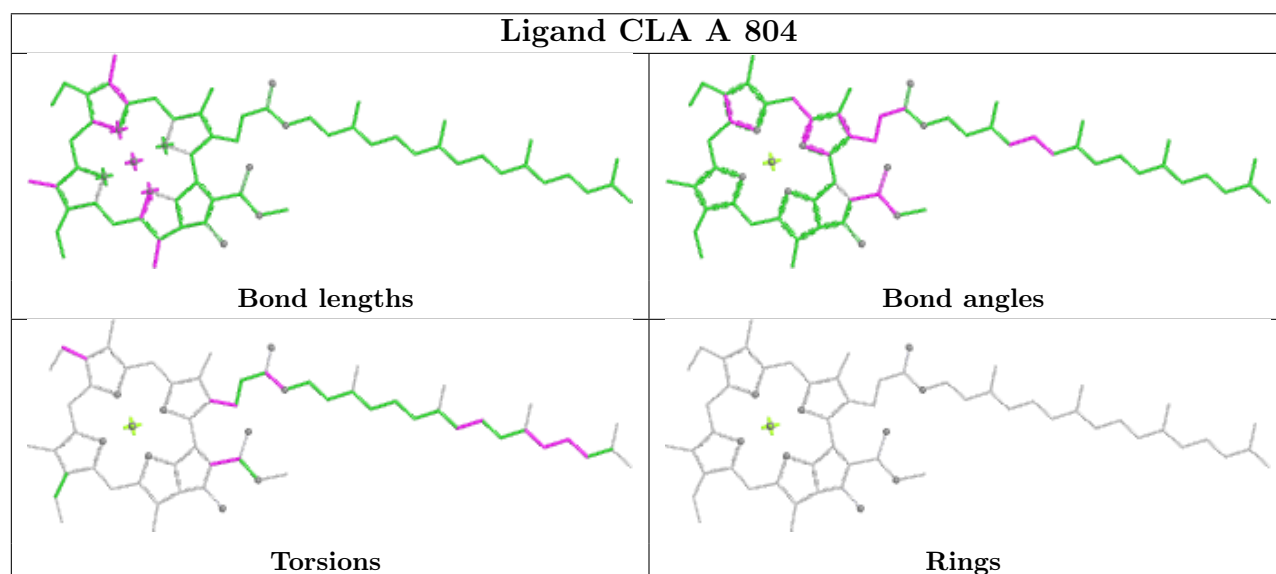
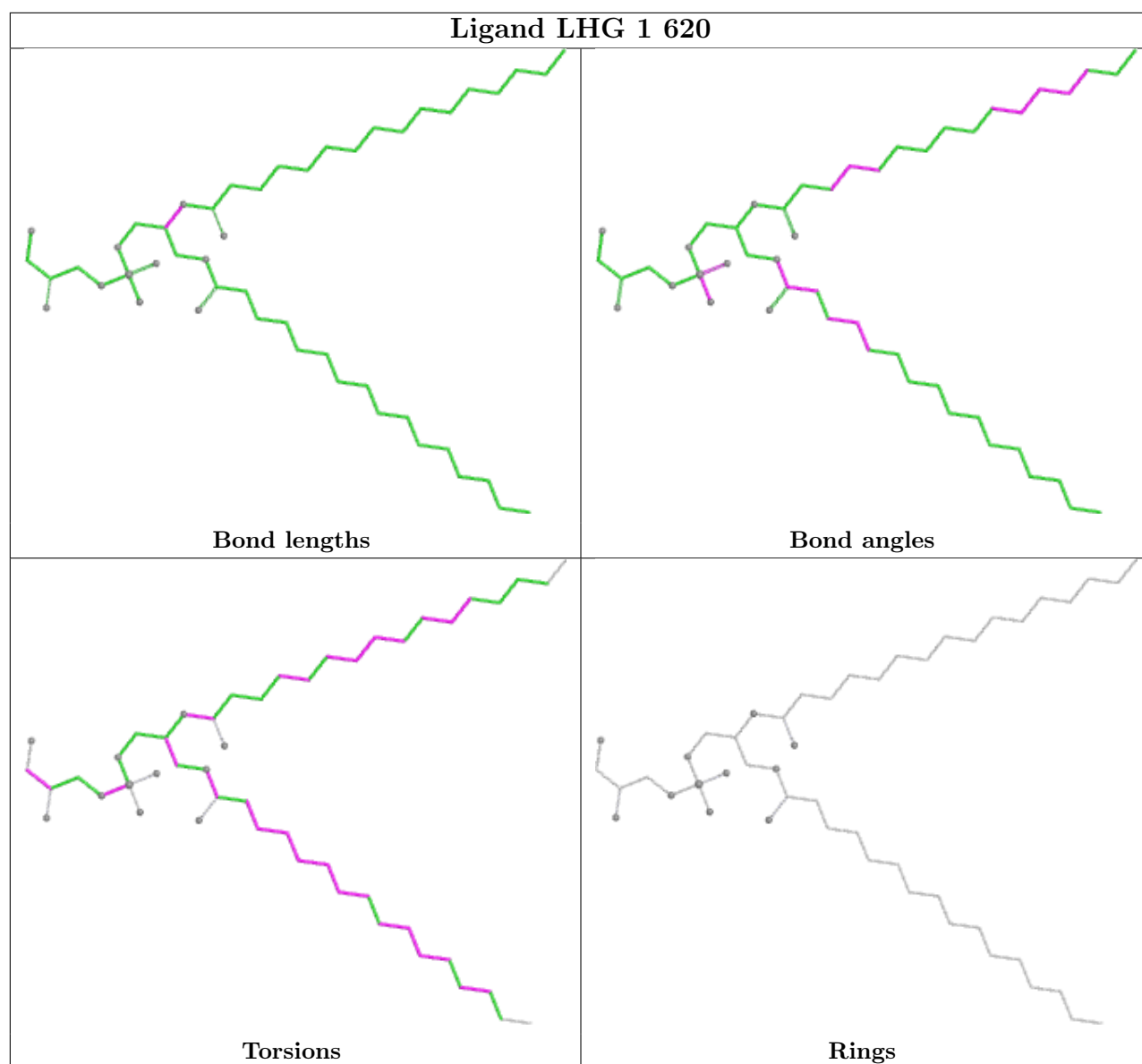


Ligand CLA A 808

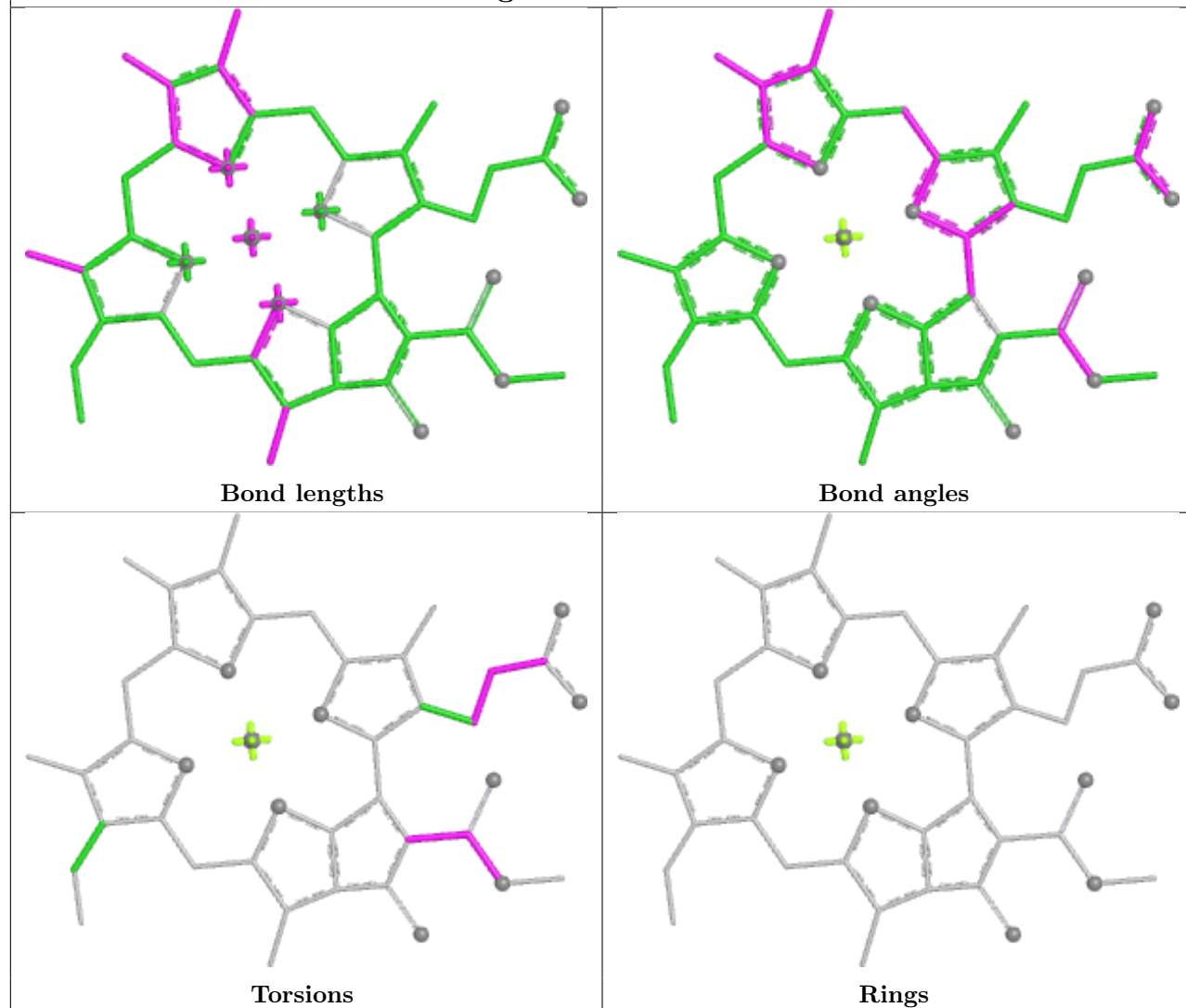


Ligand LMG 4 623

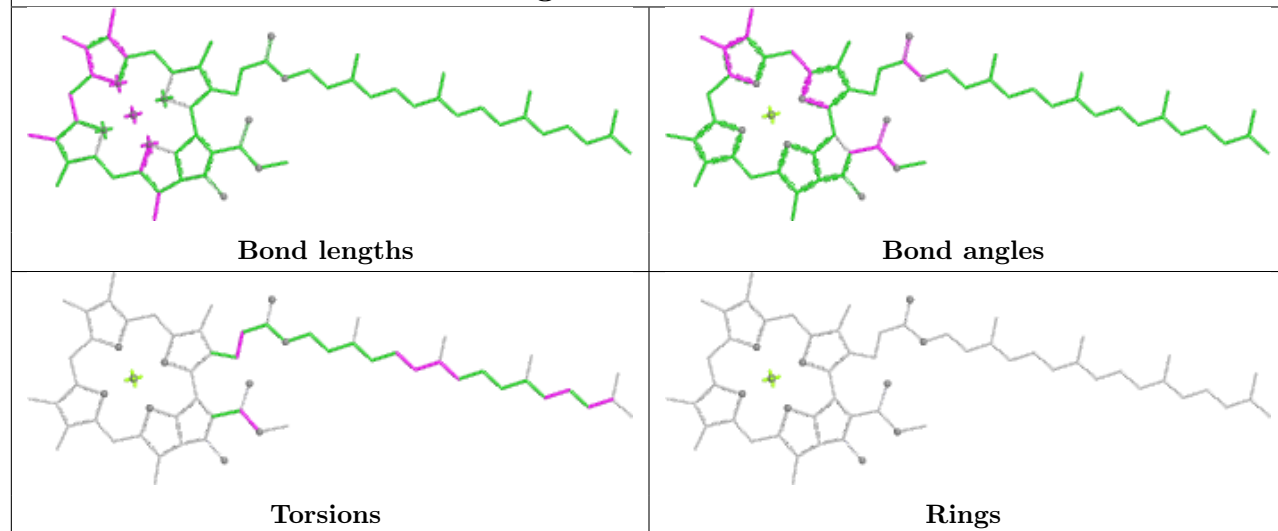


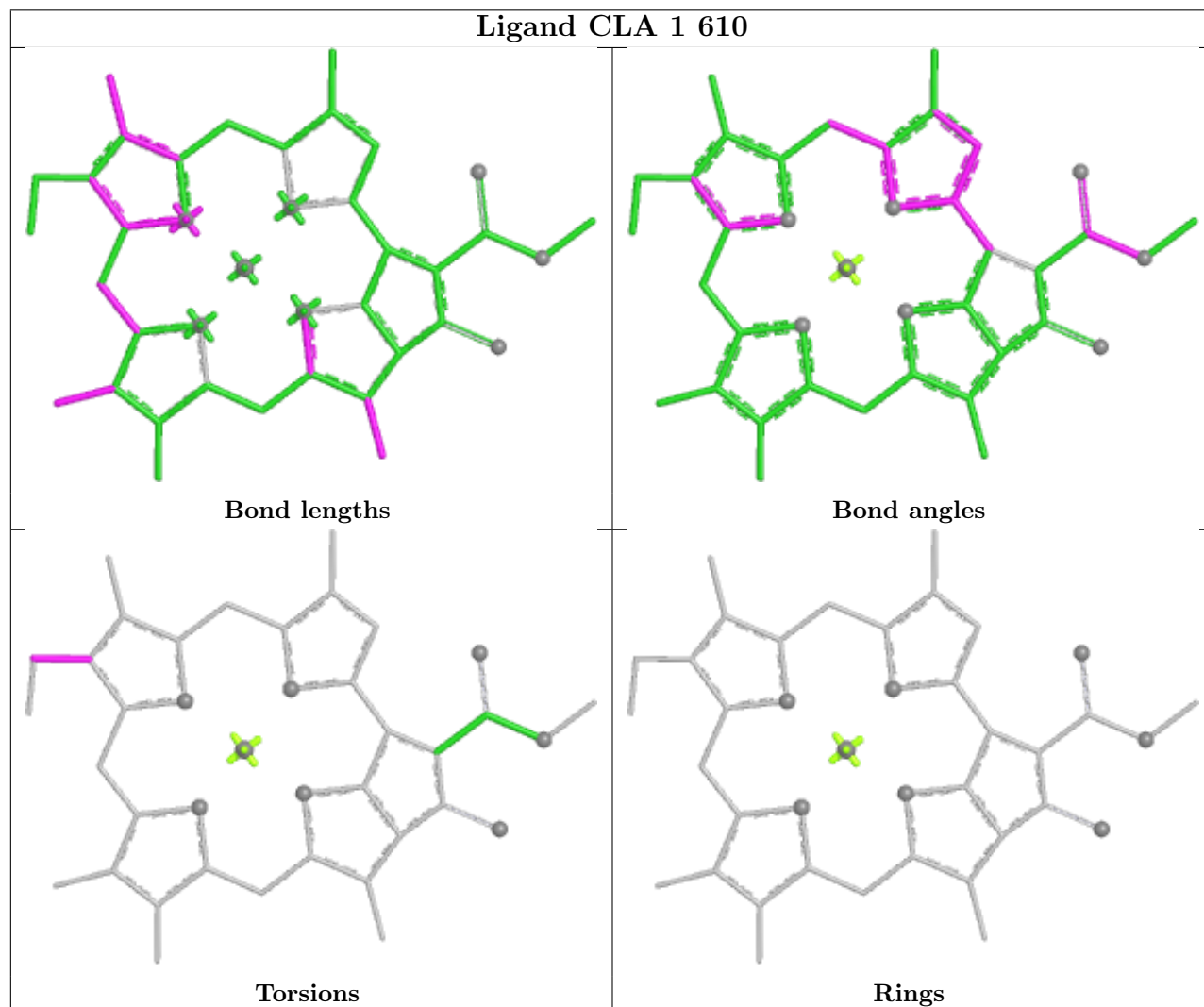
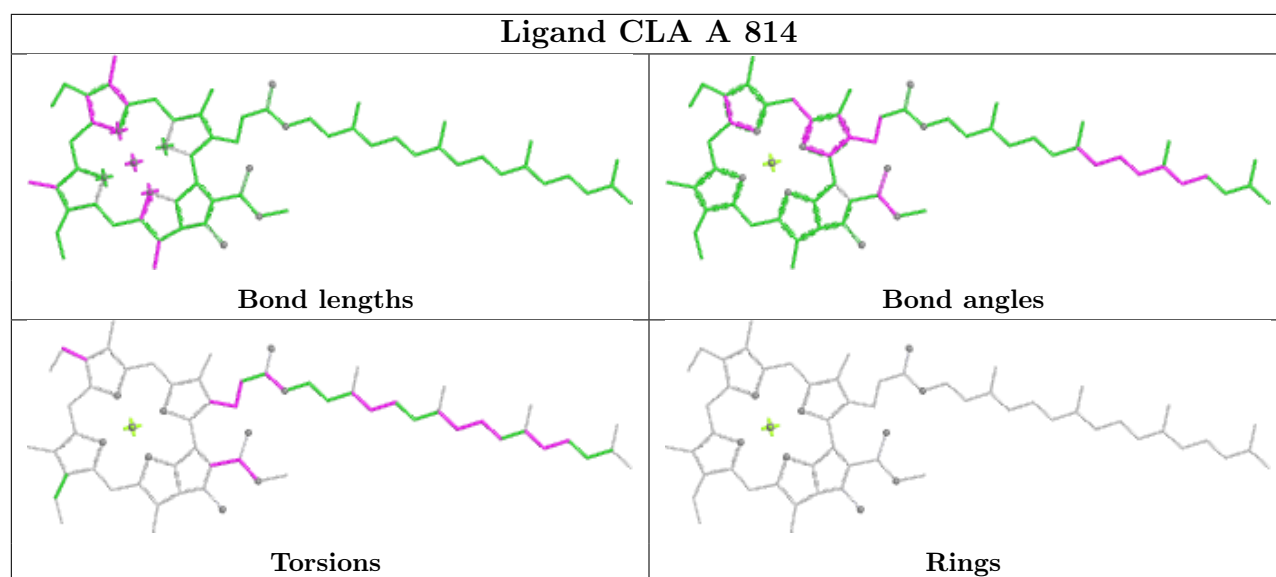


Ligand CLA 8 603

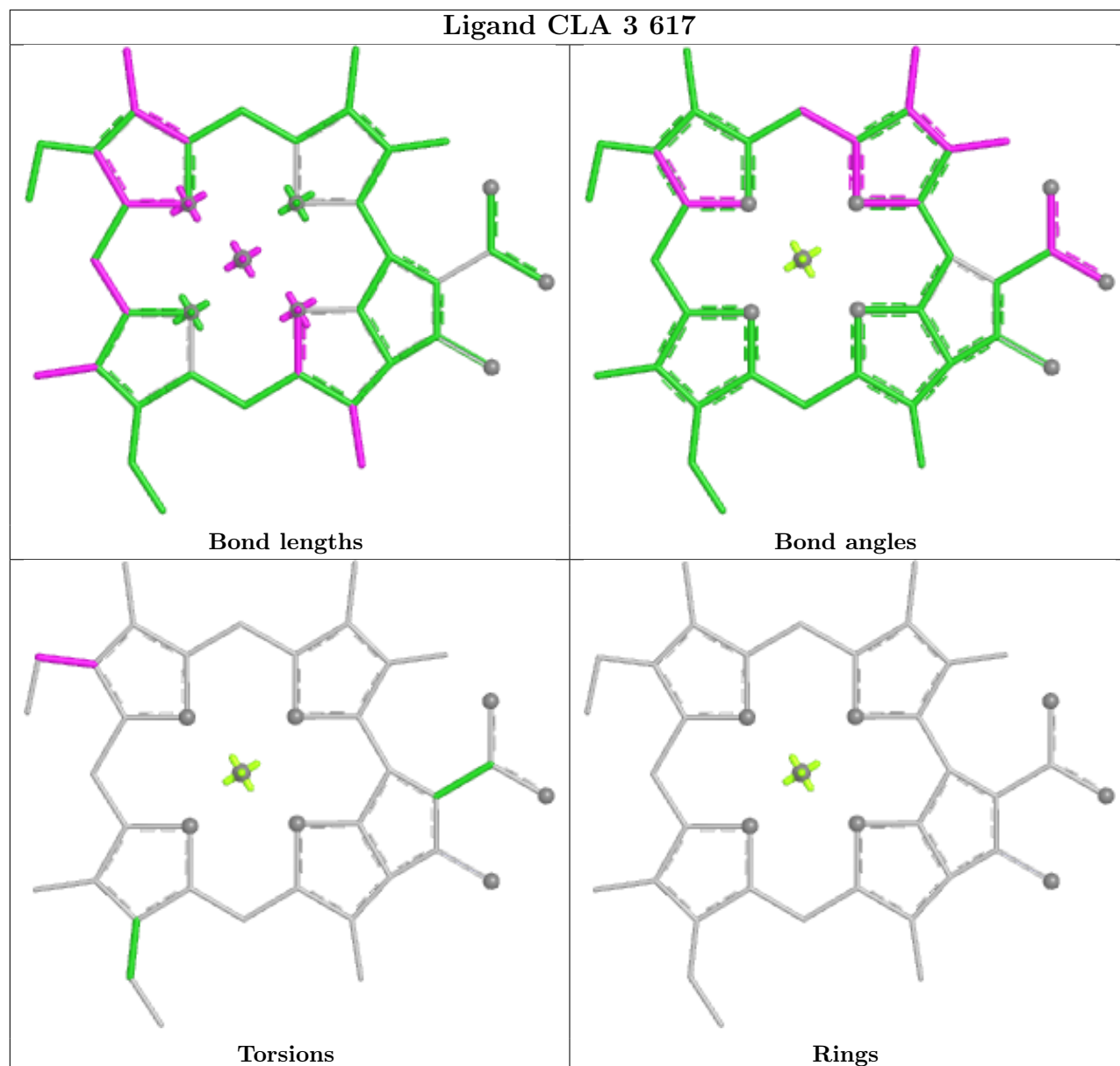


Ligand CLA 5 604

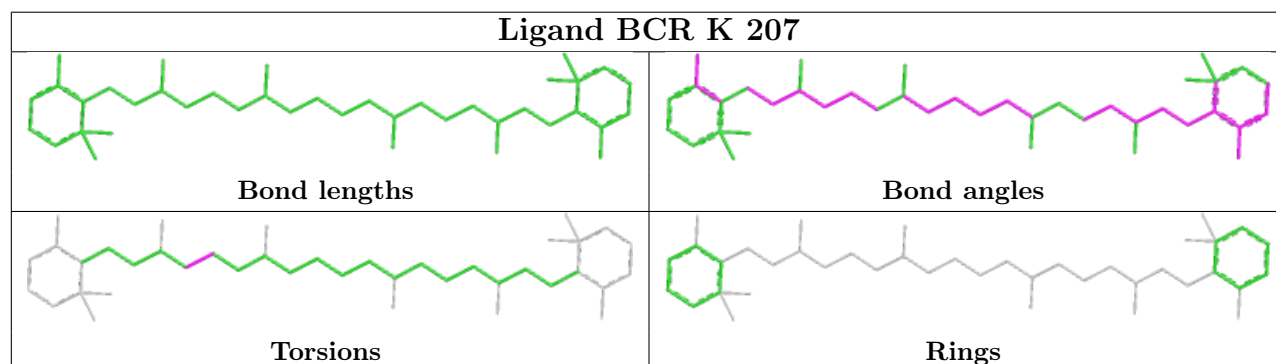




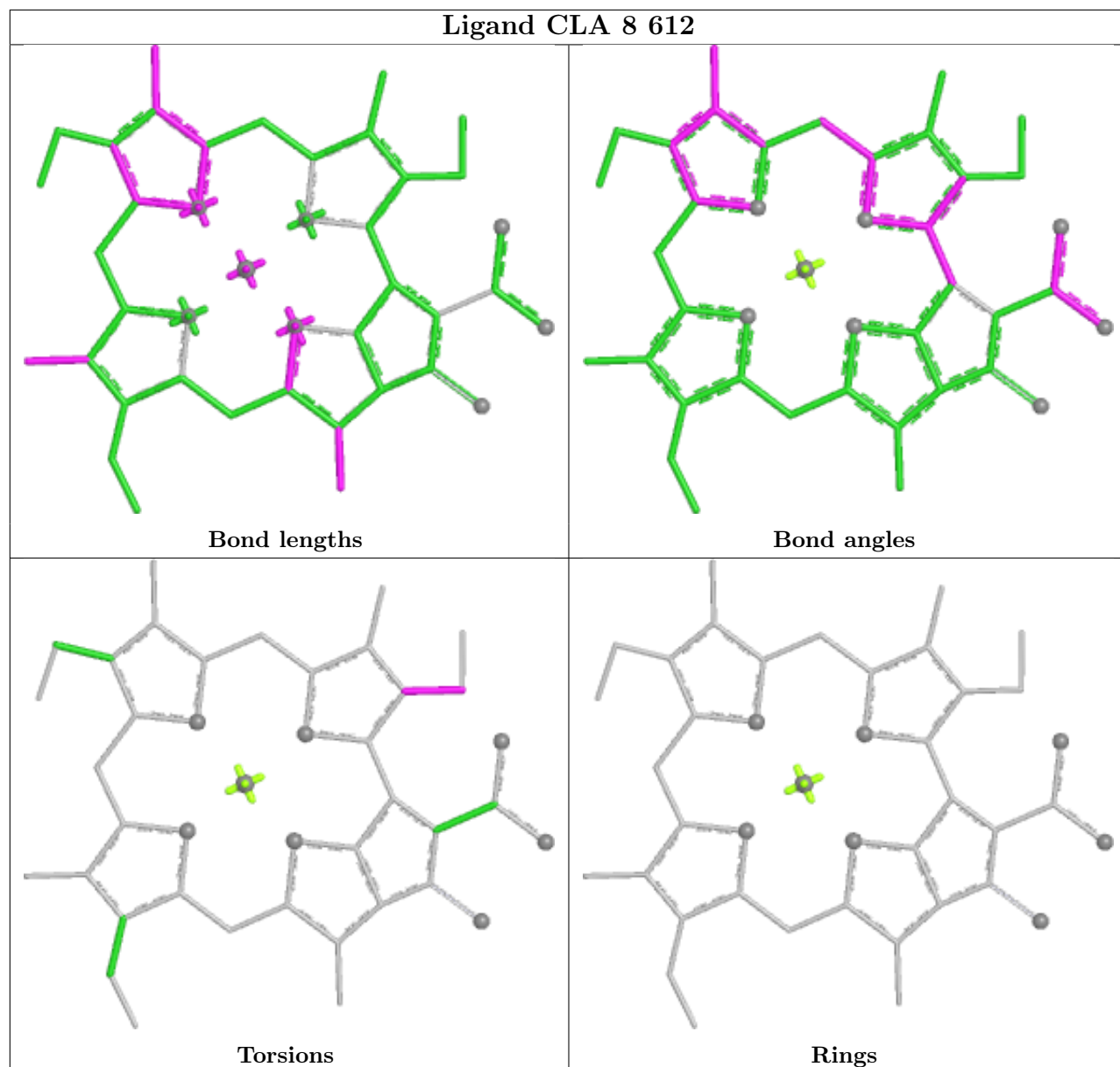
Ligand CLA 3 617



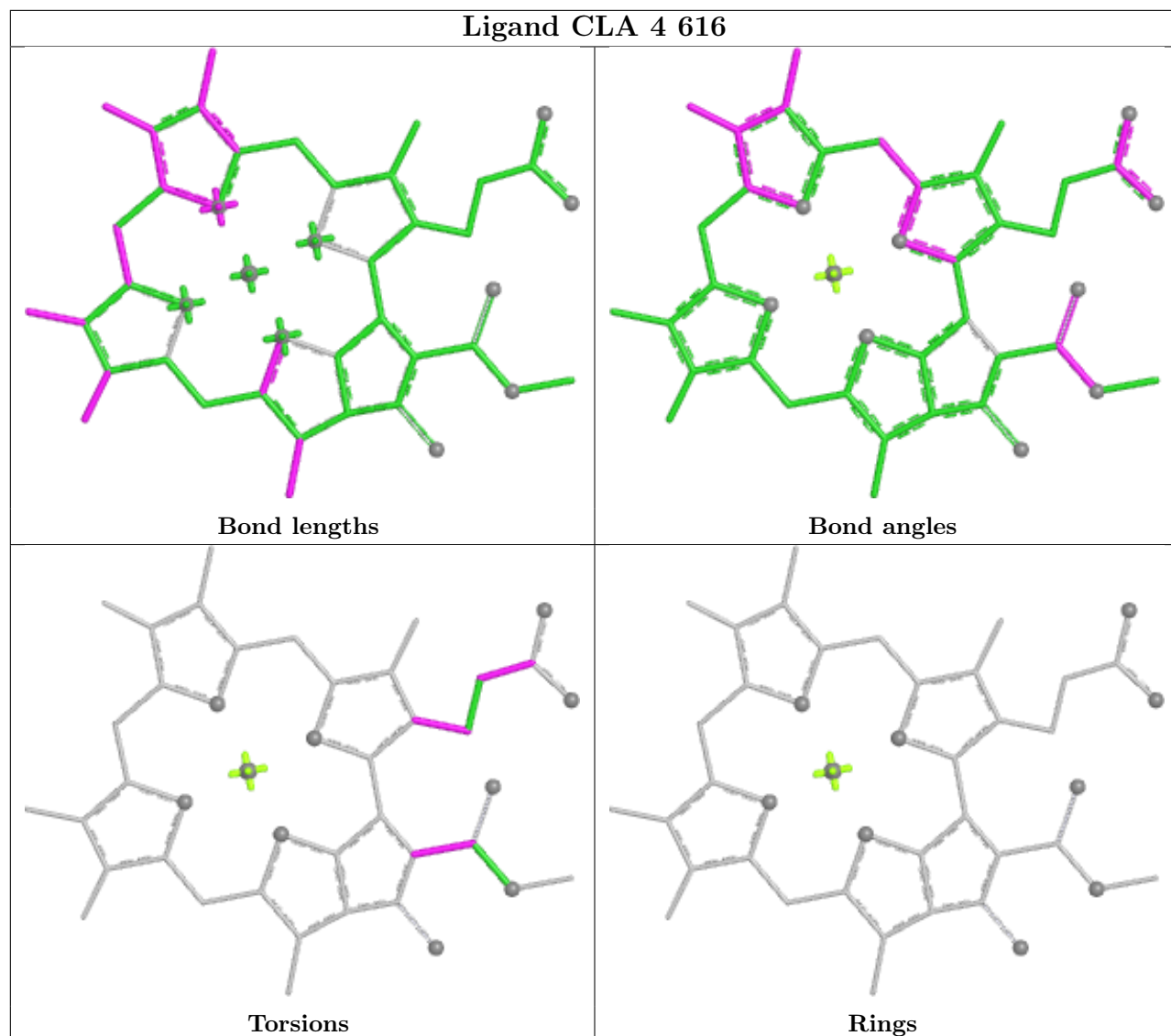
Ligand BCR K 207



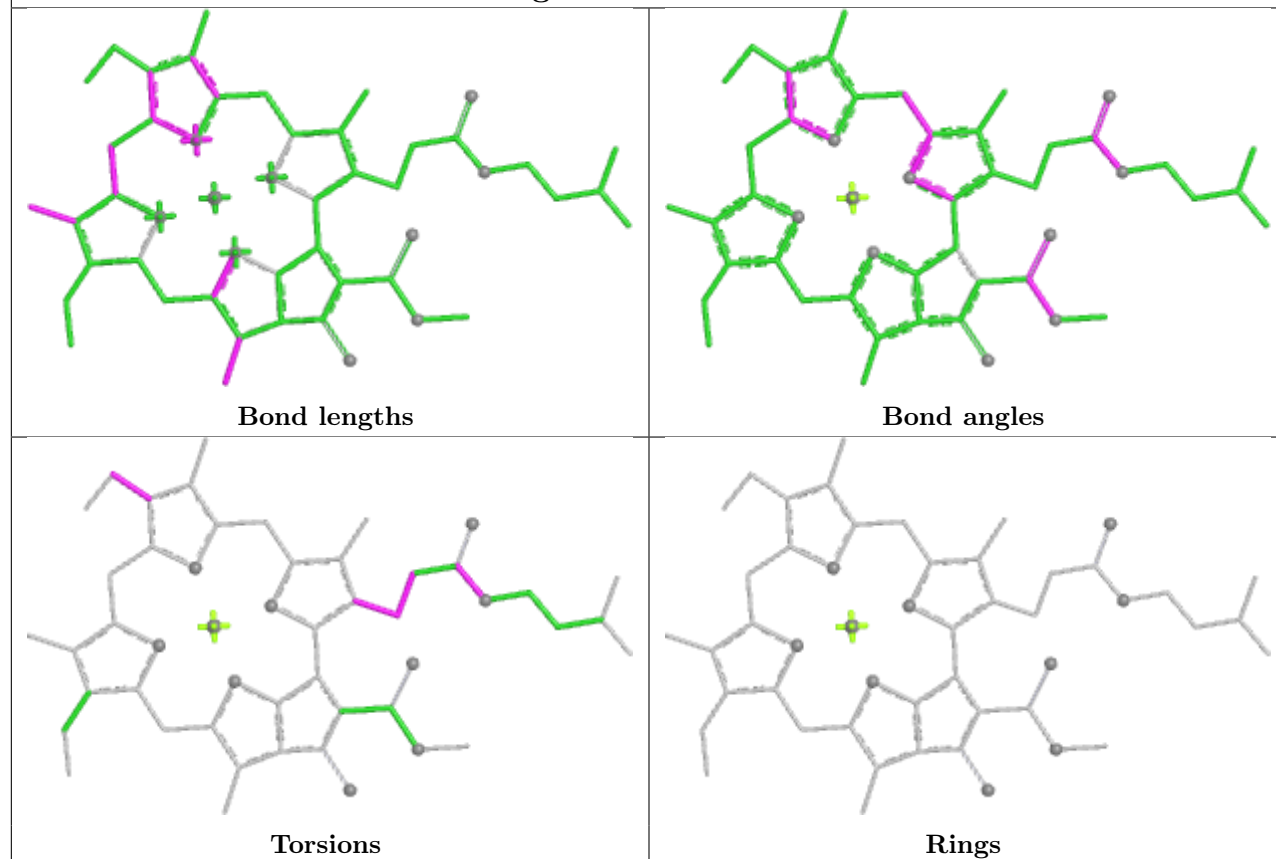
Ligand CLA 8 612



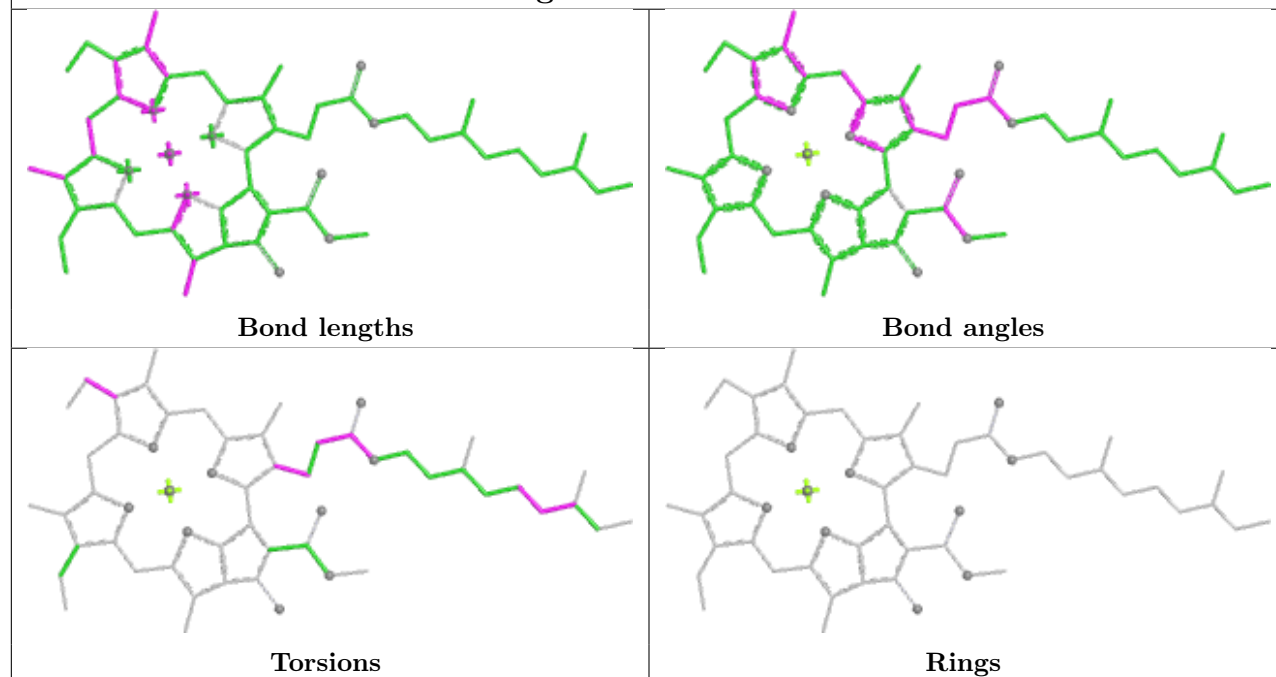
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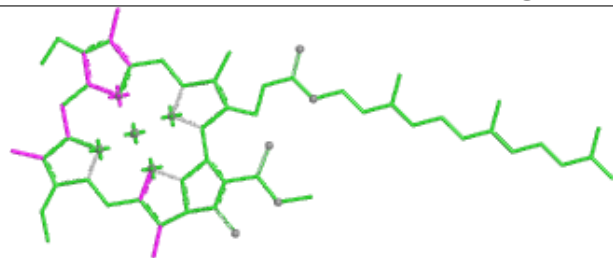
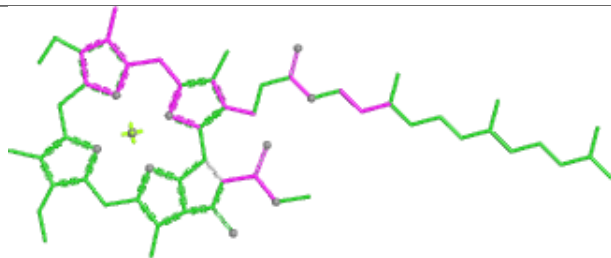
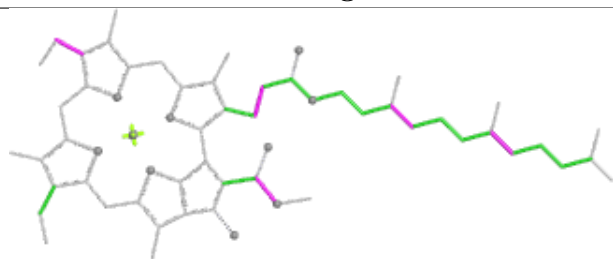
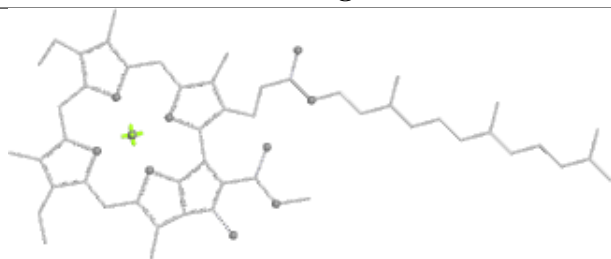
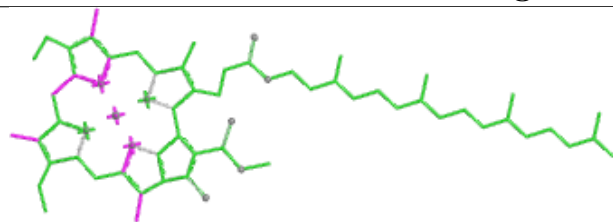
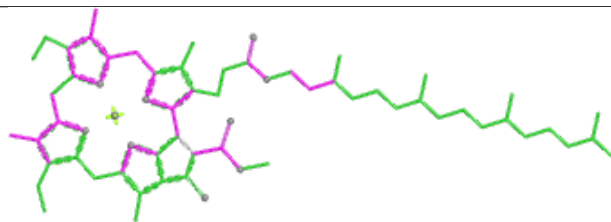
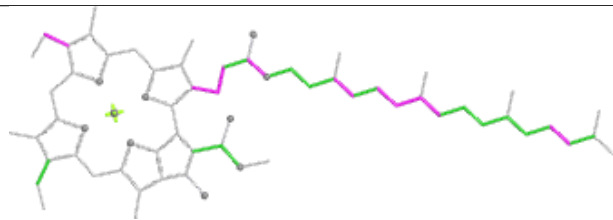
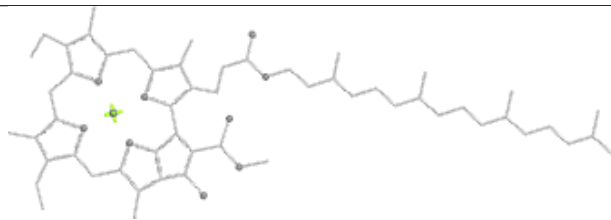


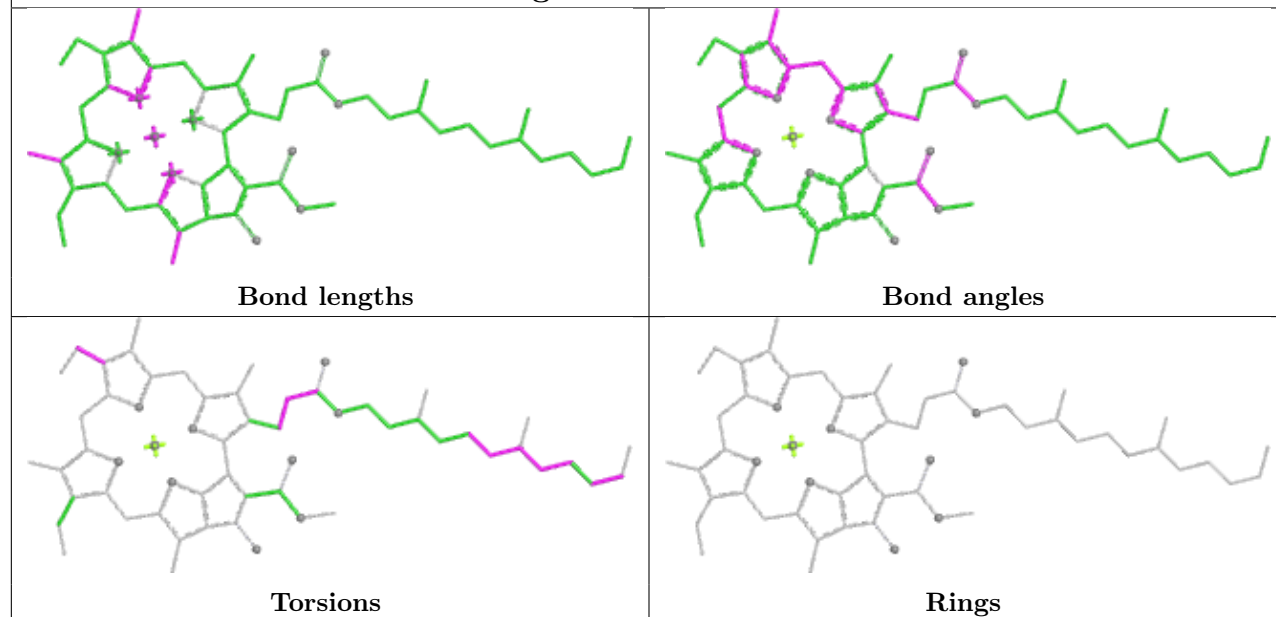
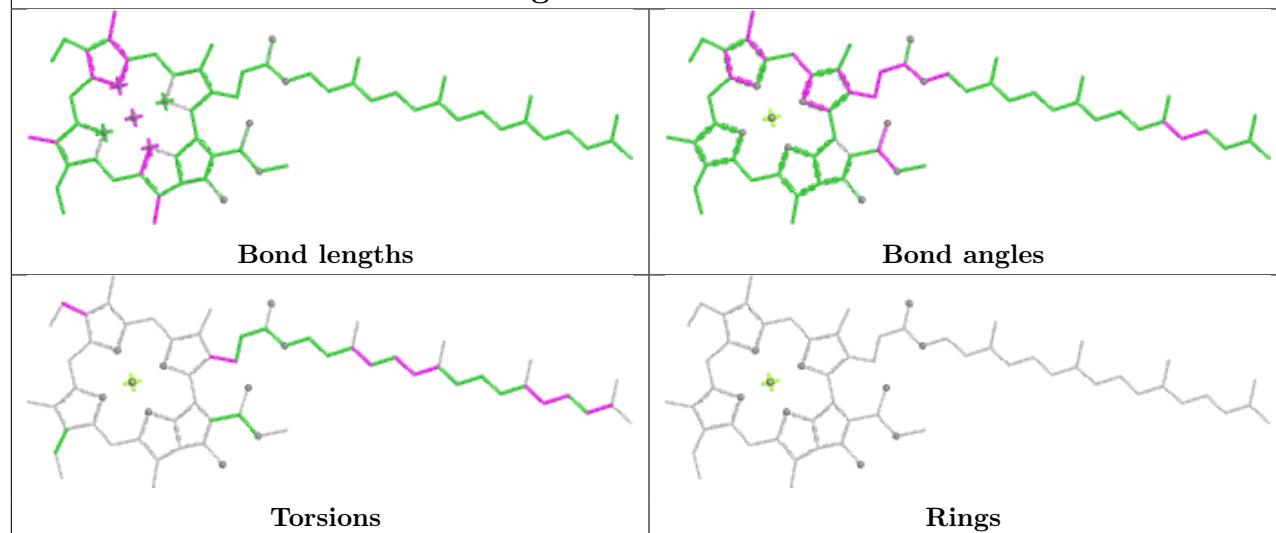
Ligand CLA B 820



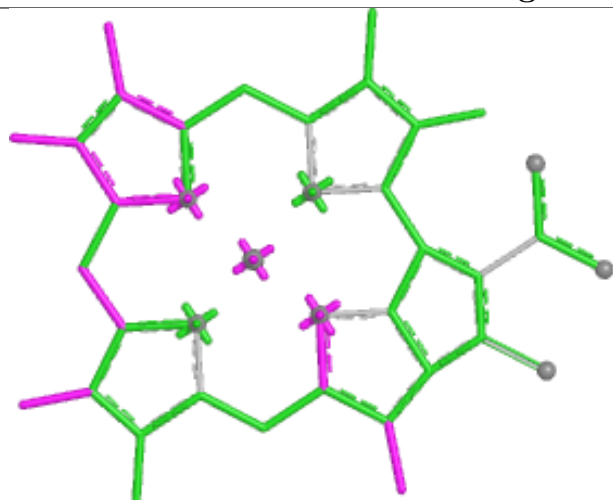
Ligand CLA 8 614



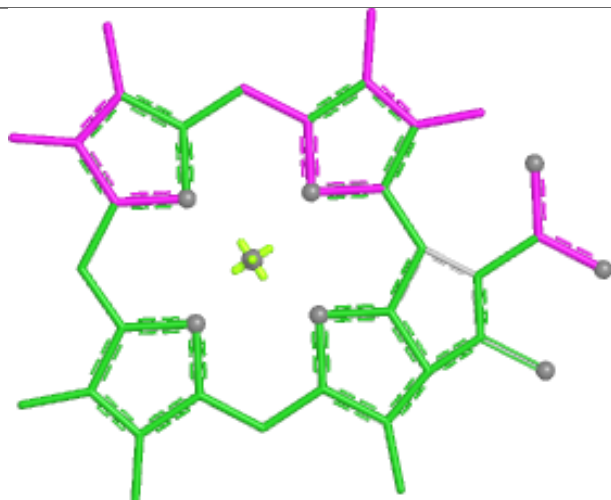
Ligand CLA 8 602**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 820****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA B 817**Ligand CLA A 812**

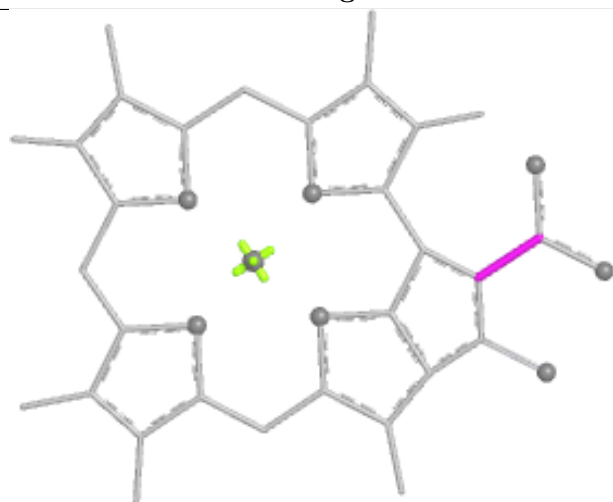
Ligand CLA 3 611



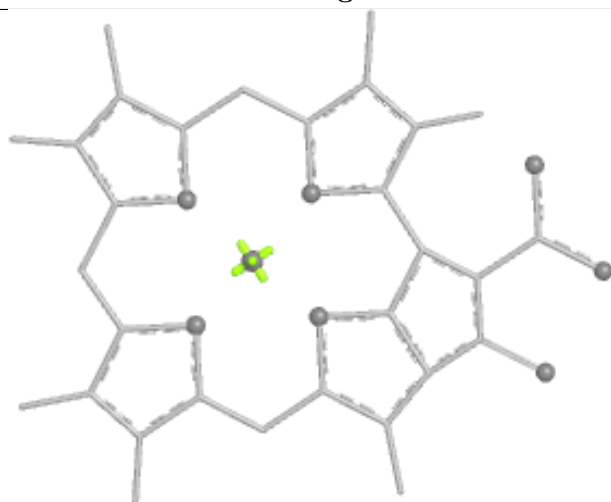
Bond lengths



Bond angles

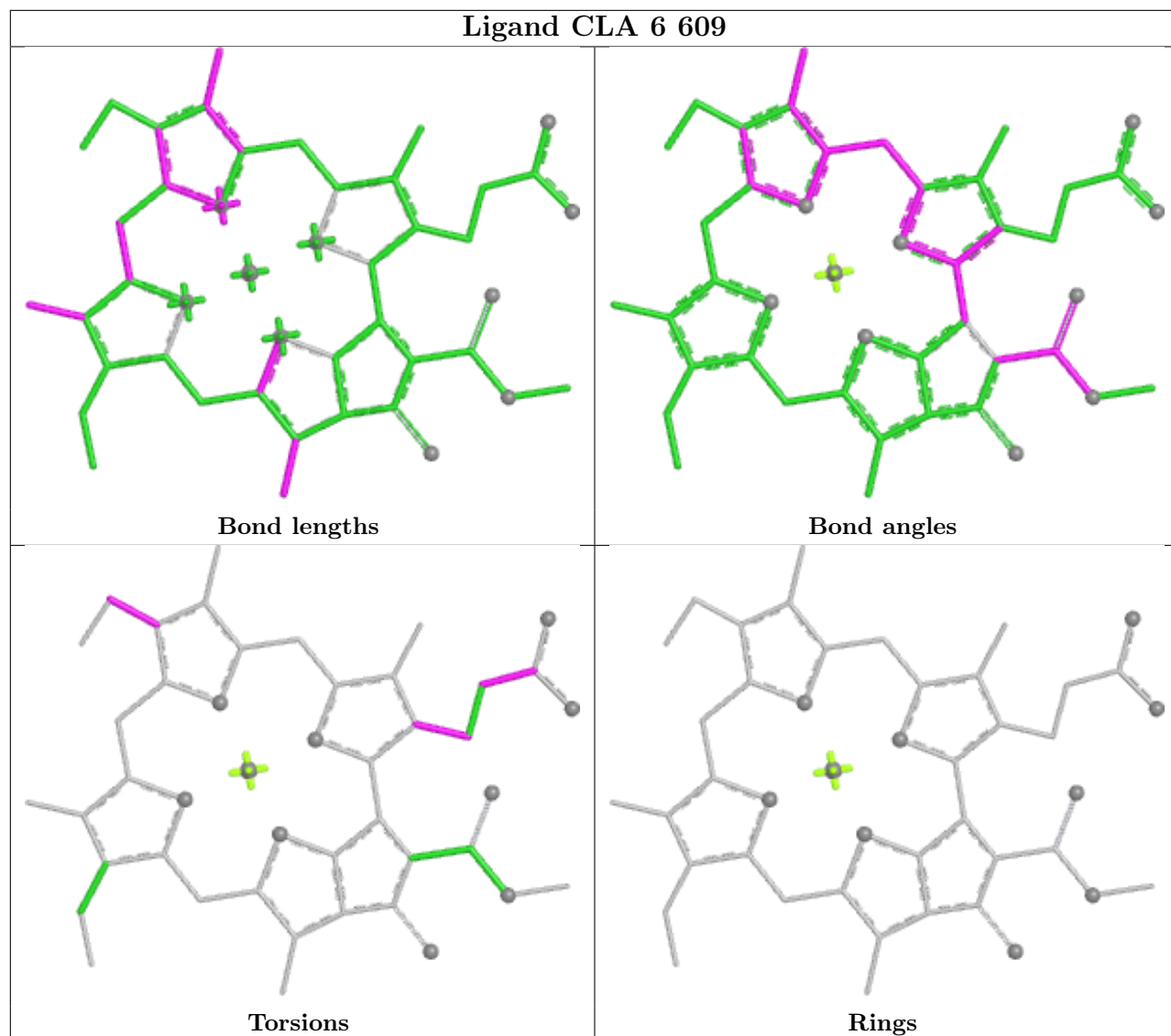


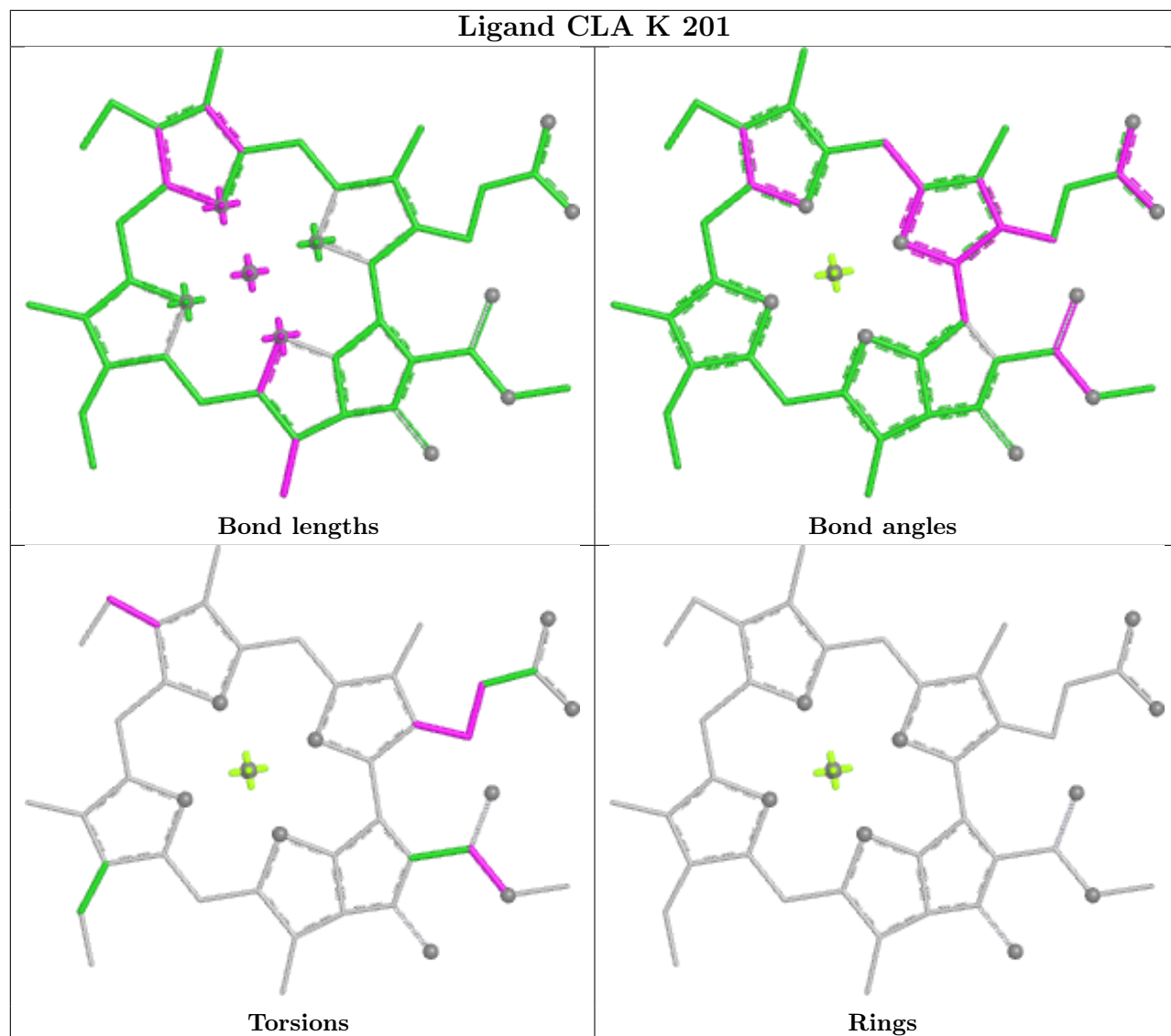
Torsions



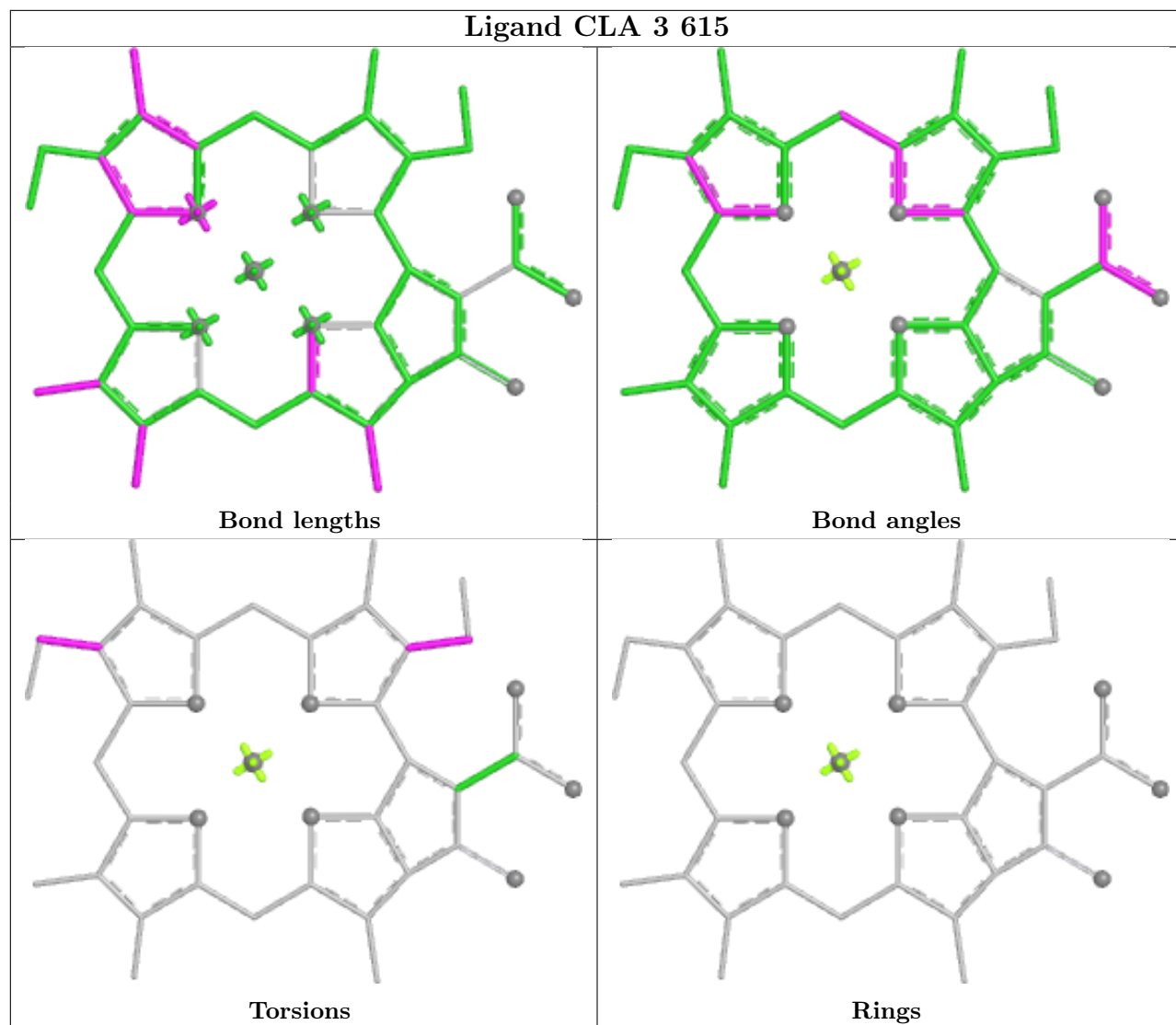
Rings

Ligand CLA 6 609

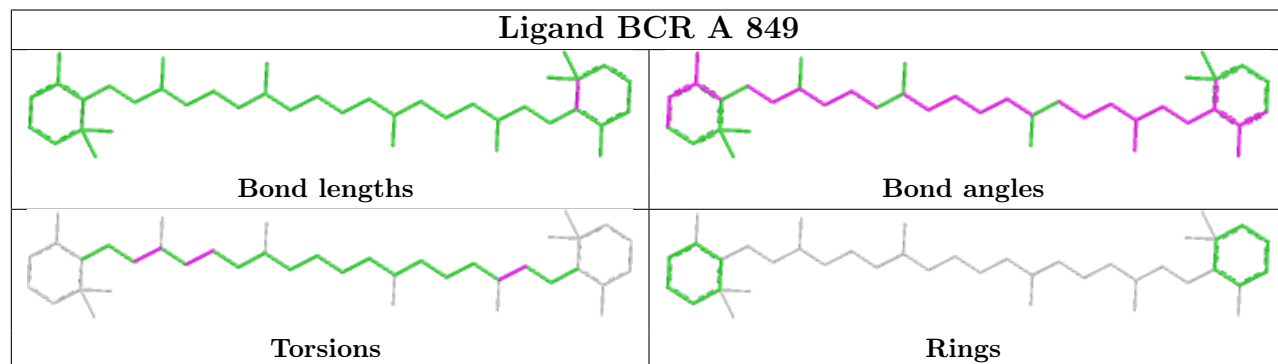




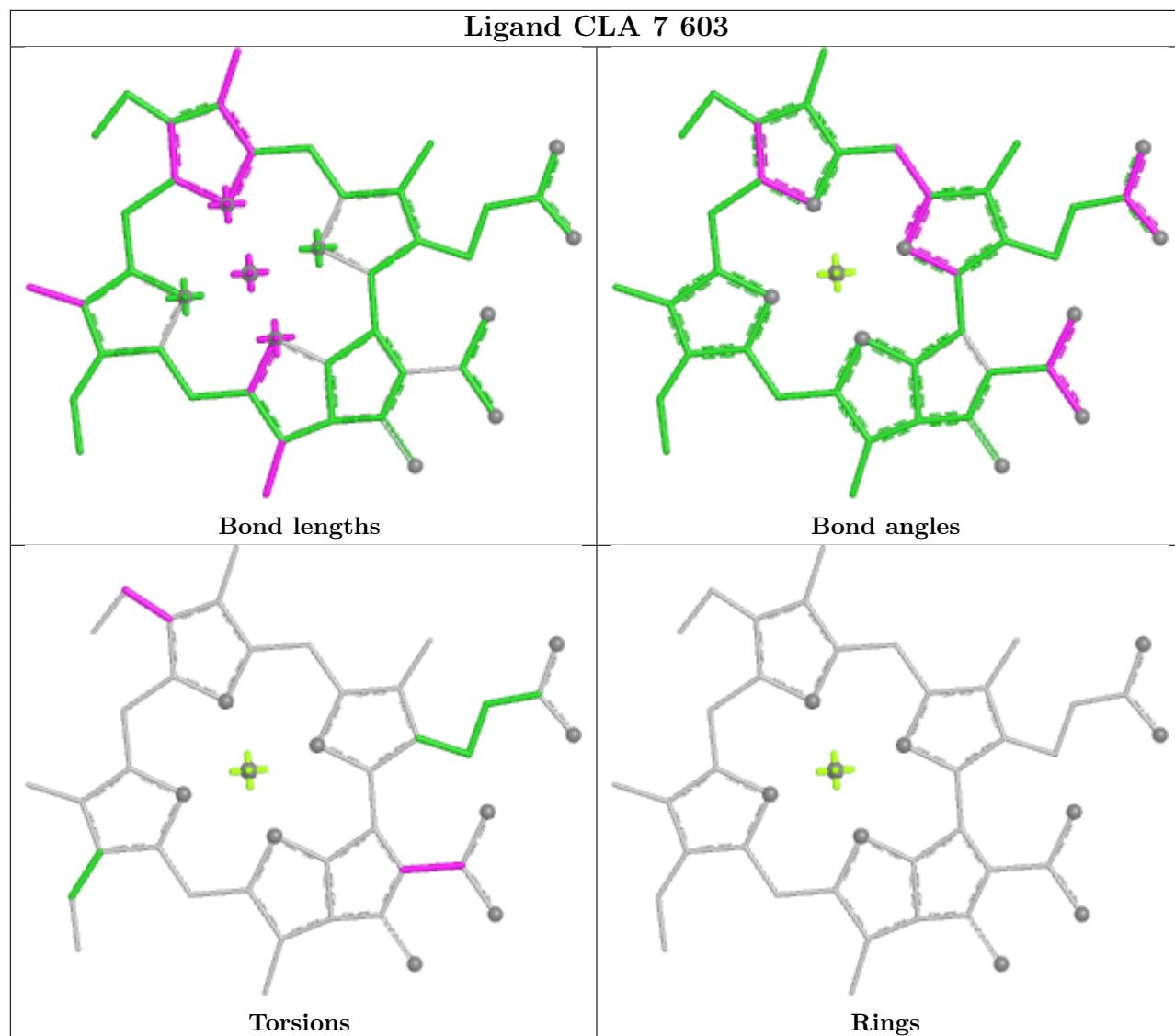
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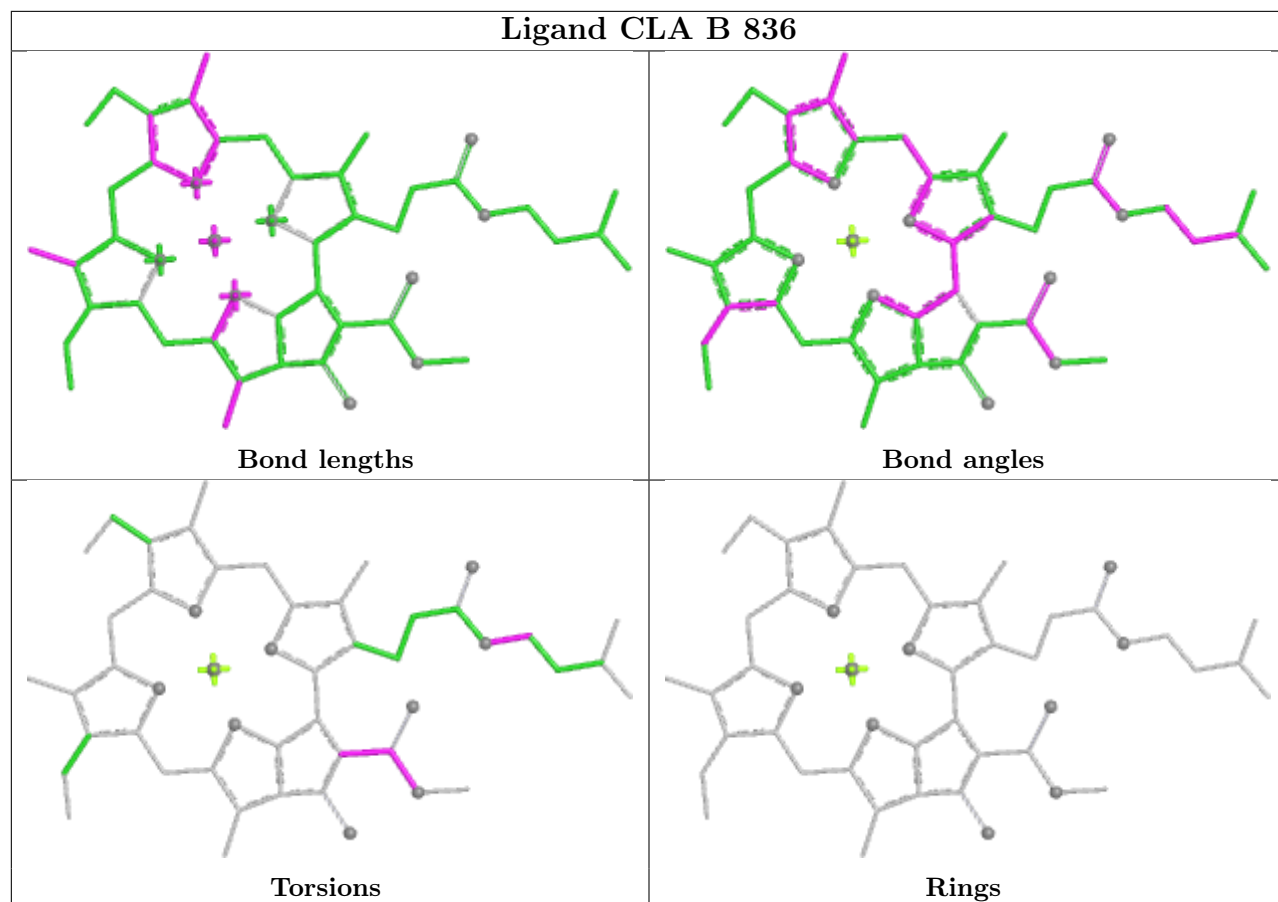
Ligand BCR A 849



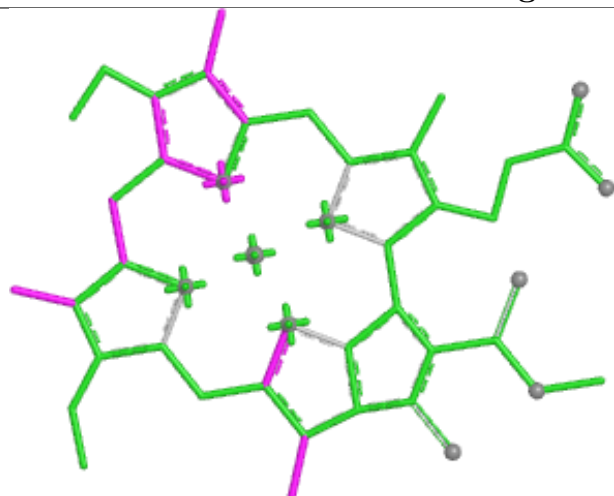
Ligand CLA 7 603



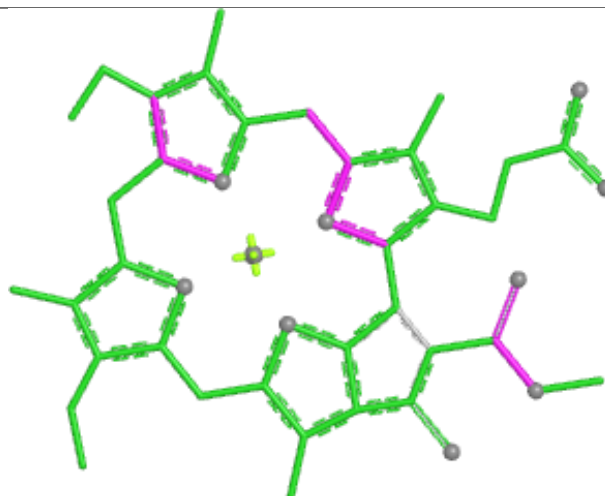
Ligand CLA B 836



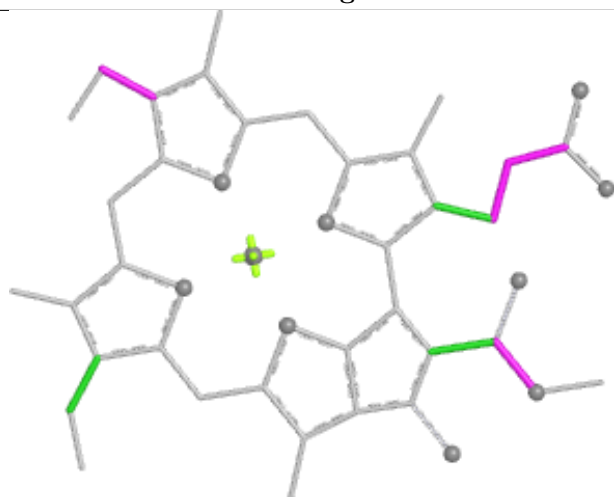
Ligand CLA 4 607



Bond lengths



Bond angles

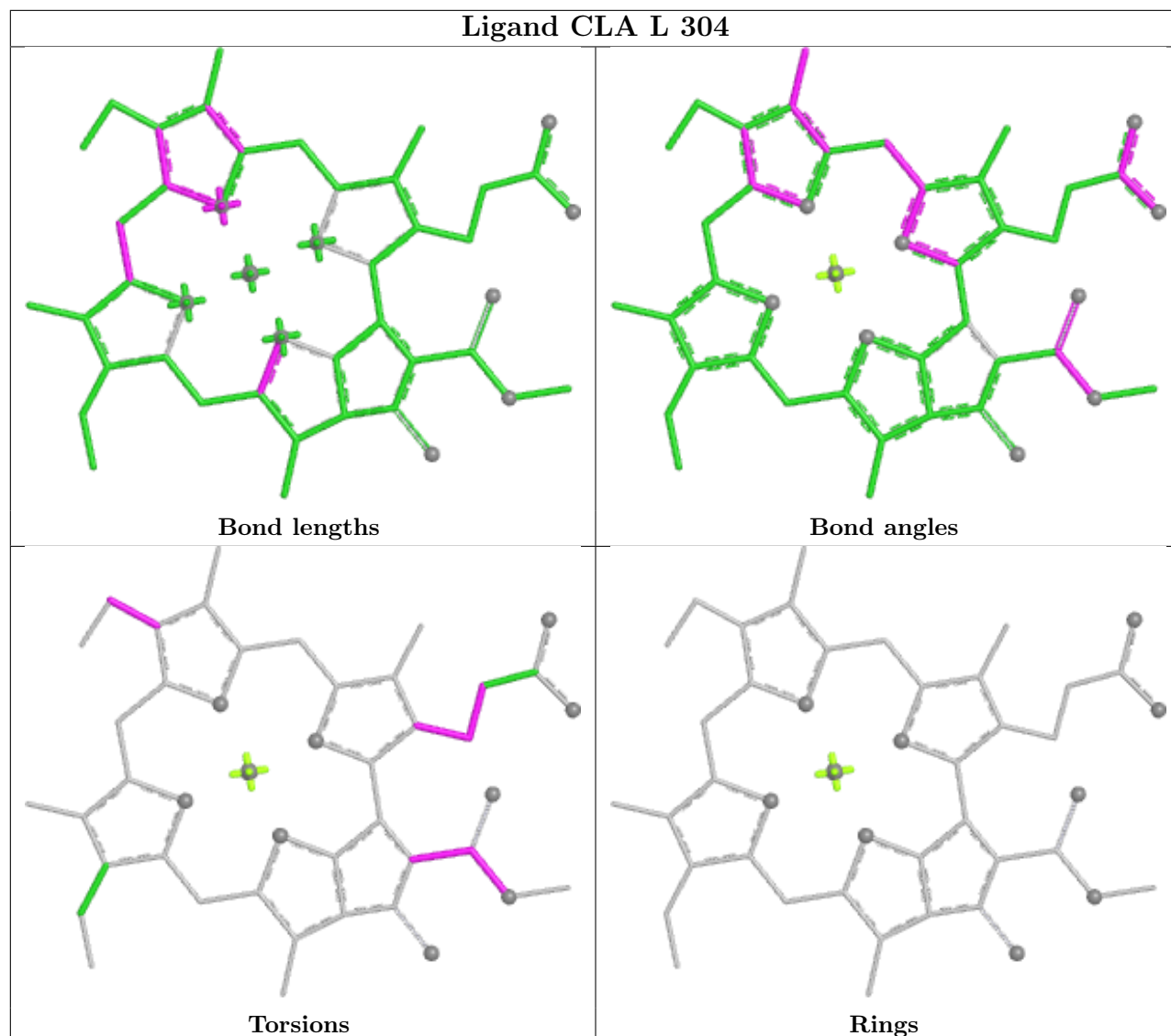


Torsions

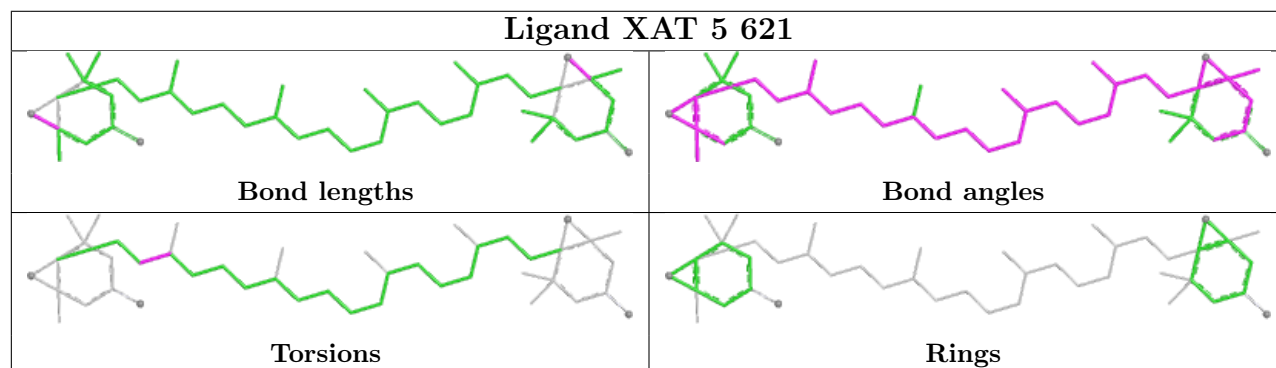


Rings

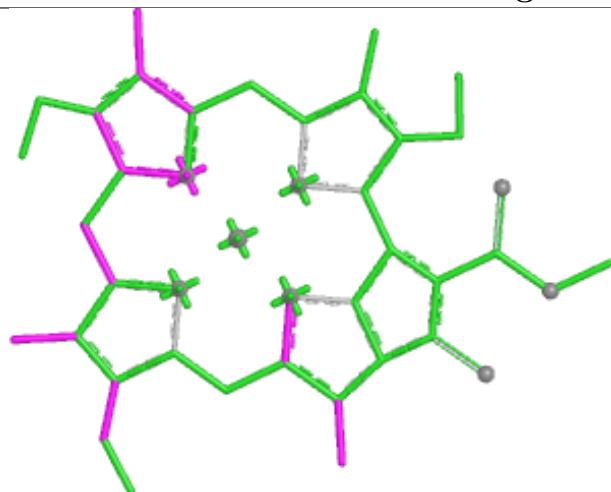
Ligand CLA L 304



Ligand XAT 5 621



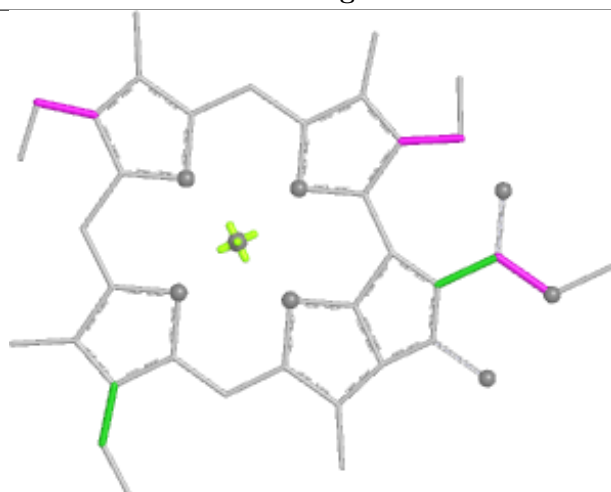
Ligand CLA F 303



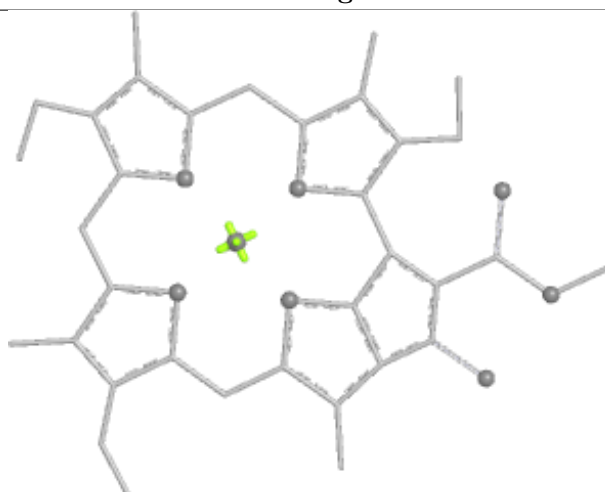
Bond lengths



Bond angles

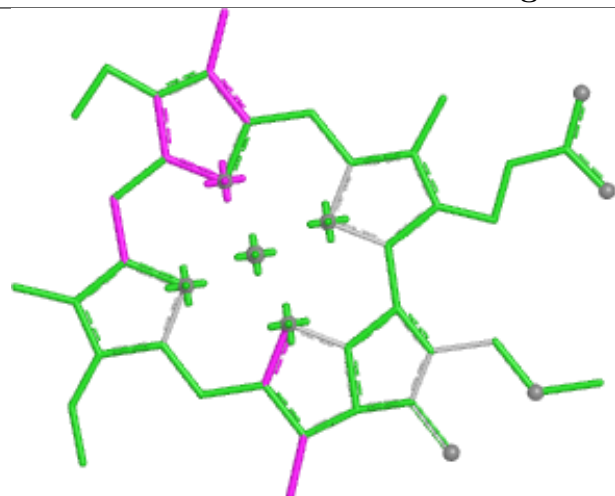


Torsions

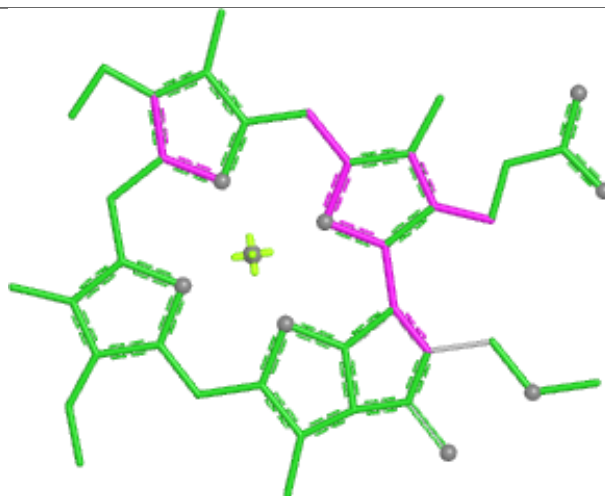


Rings

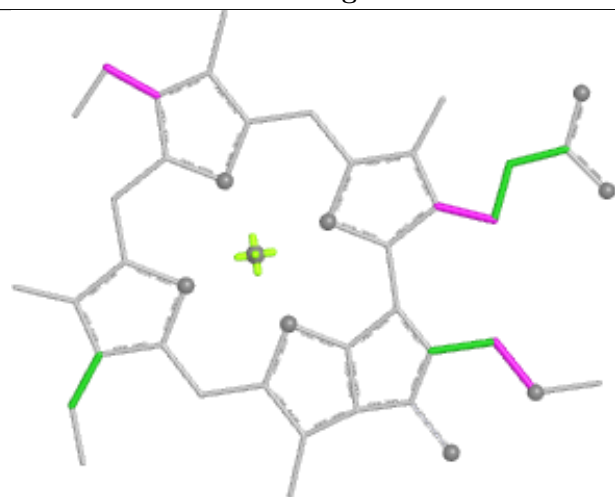
Ligand CLA a 606



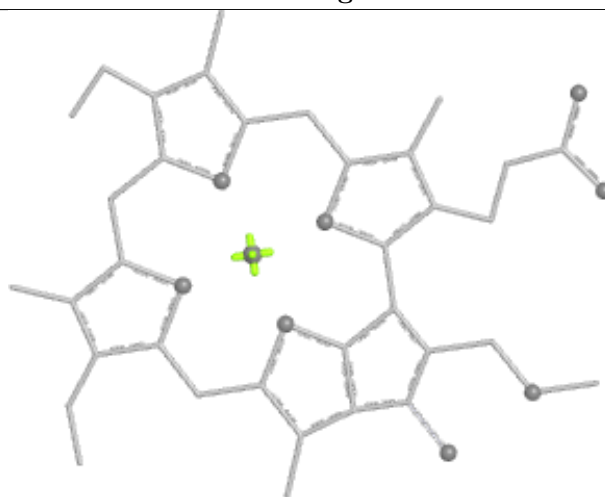
Bond lengths



Bond angles

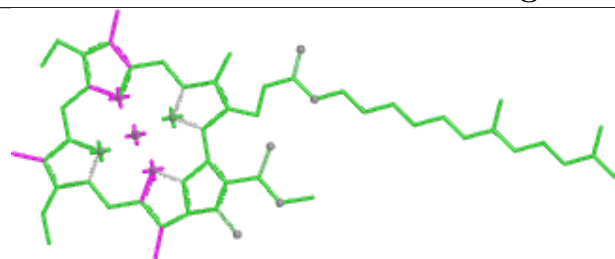


Torsions

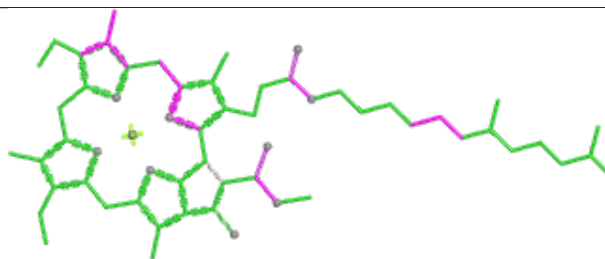


Rings

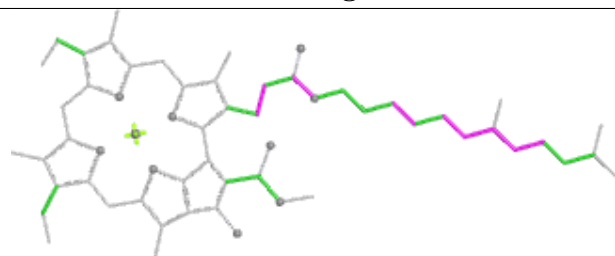
Ligand CLA 7 611



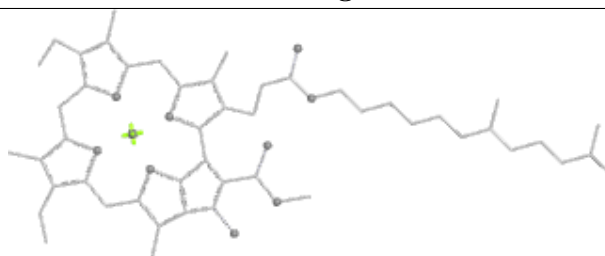
Bond lengths



Bond angles

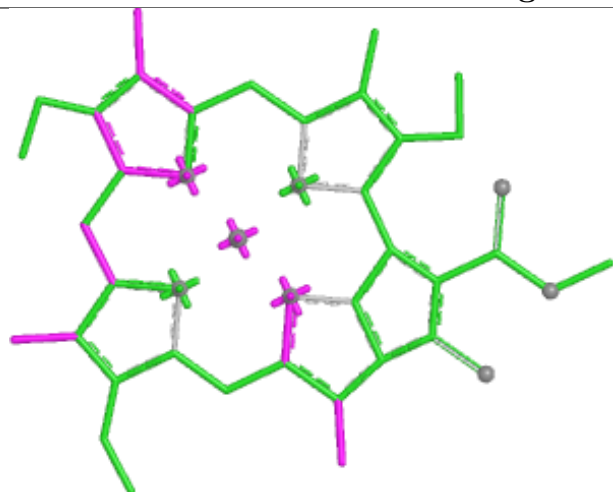


Torsions



Rings

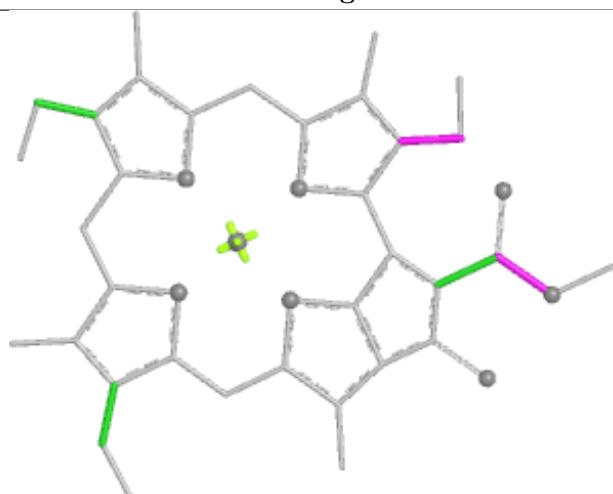
Ligand CLA 7 607



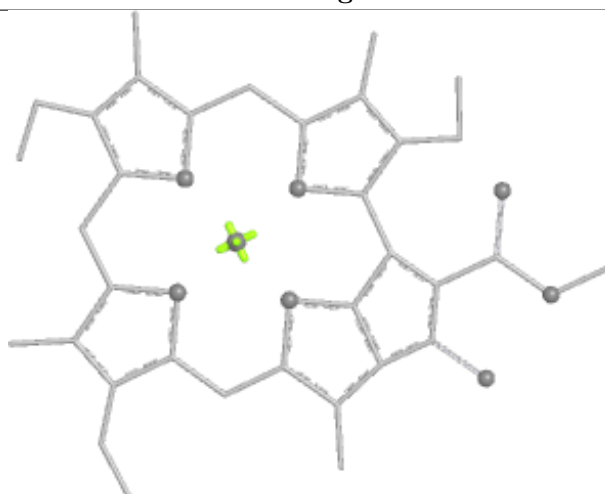
Bond lengths



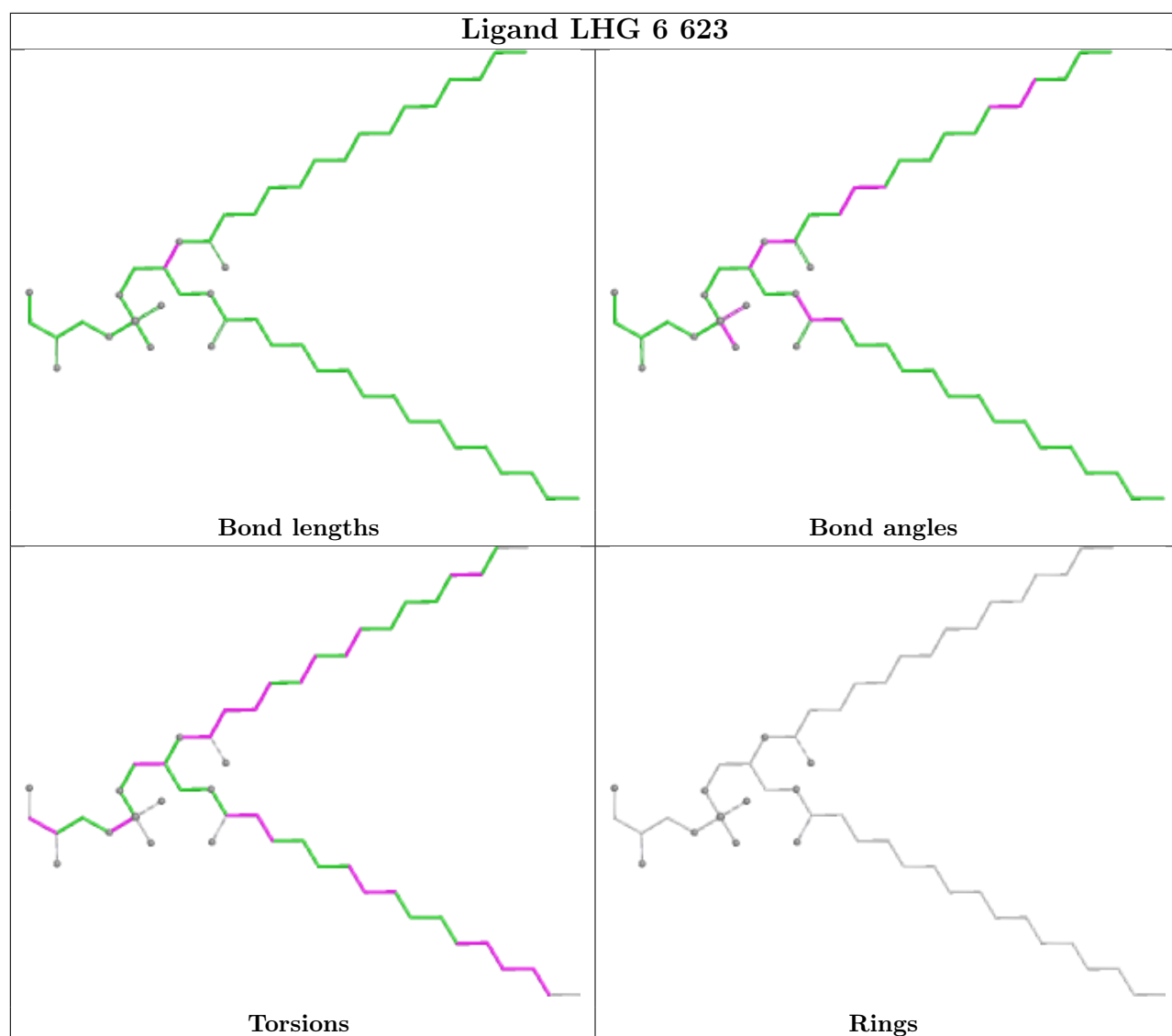
Bond angles



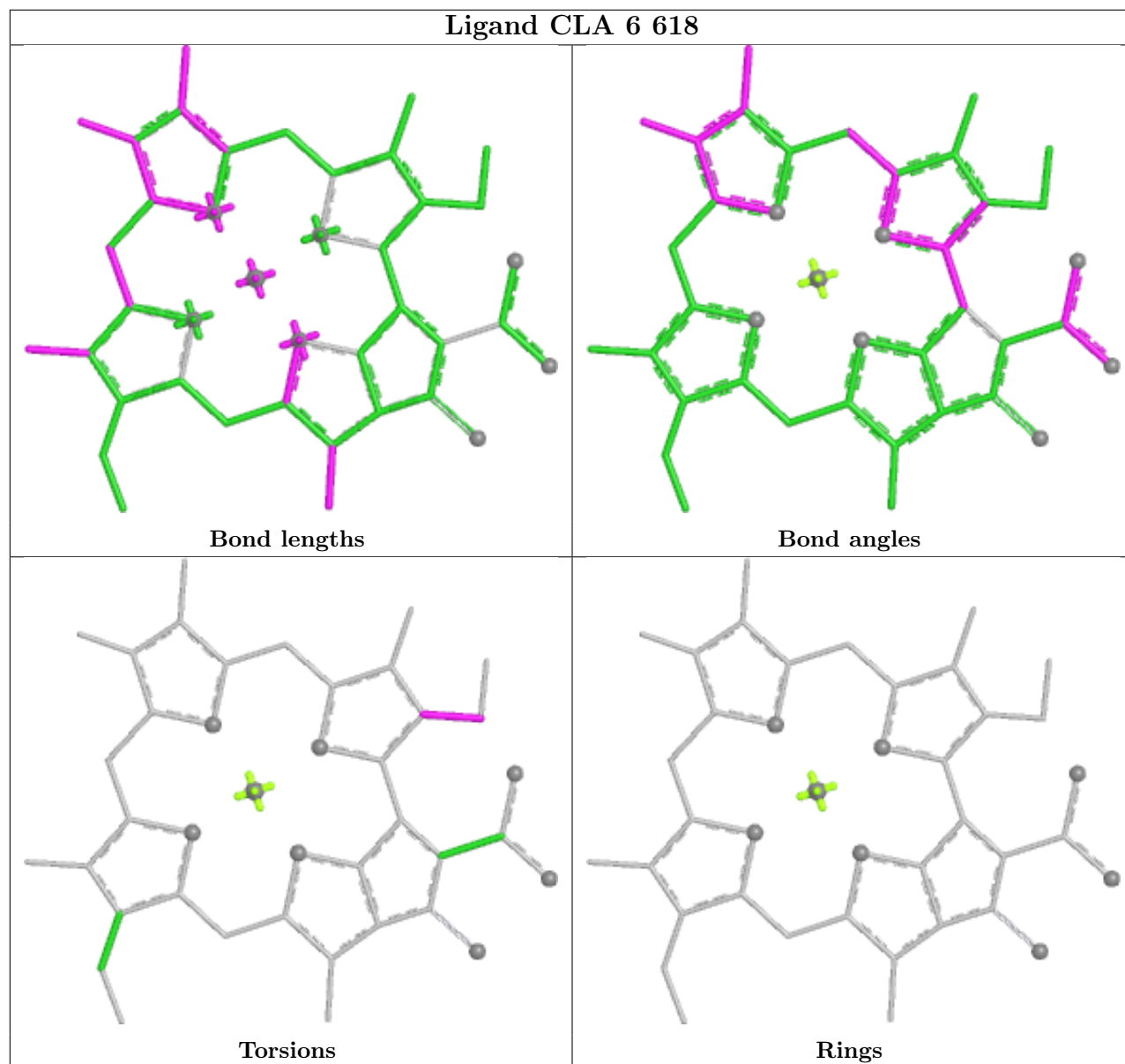
Torsions



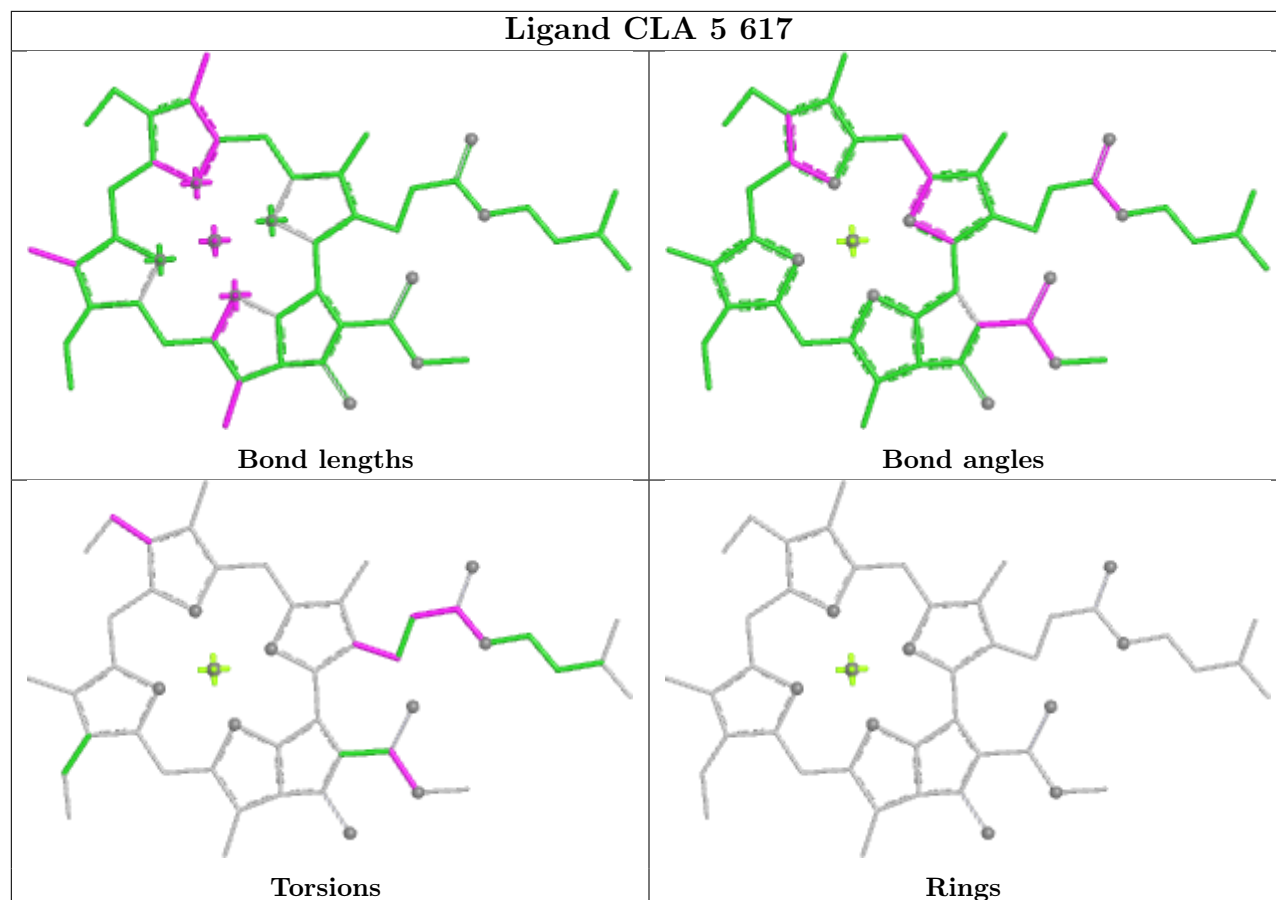
Rings



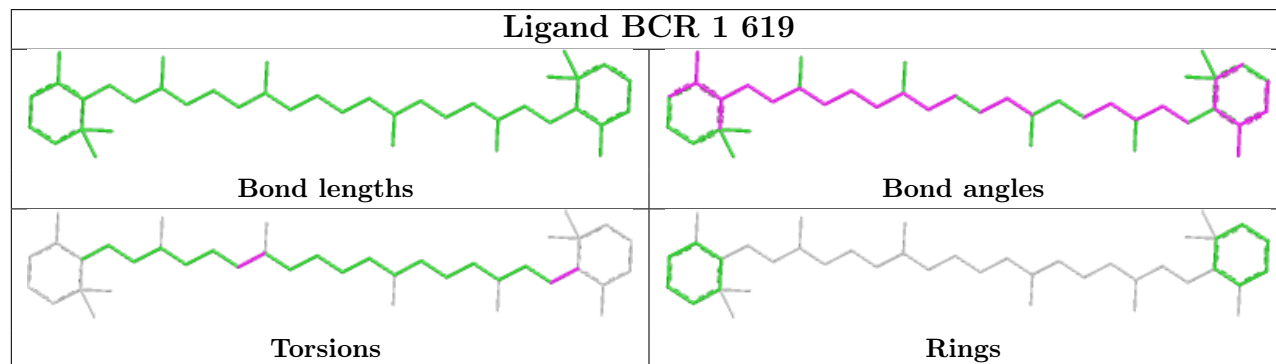
Ligand CLA 6 618



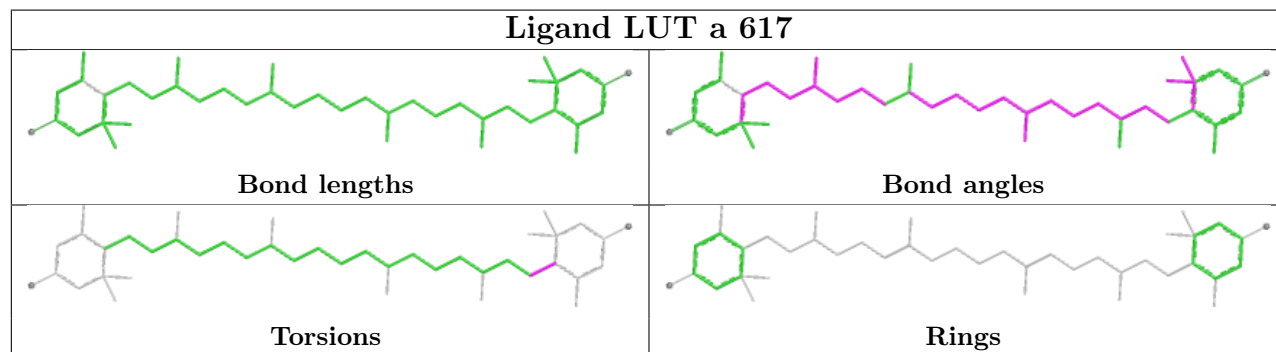
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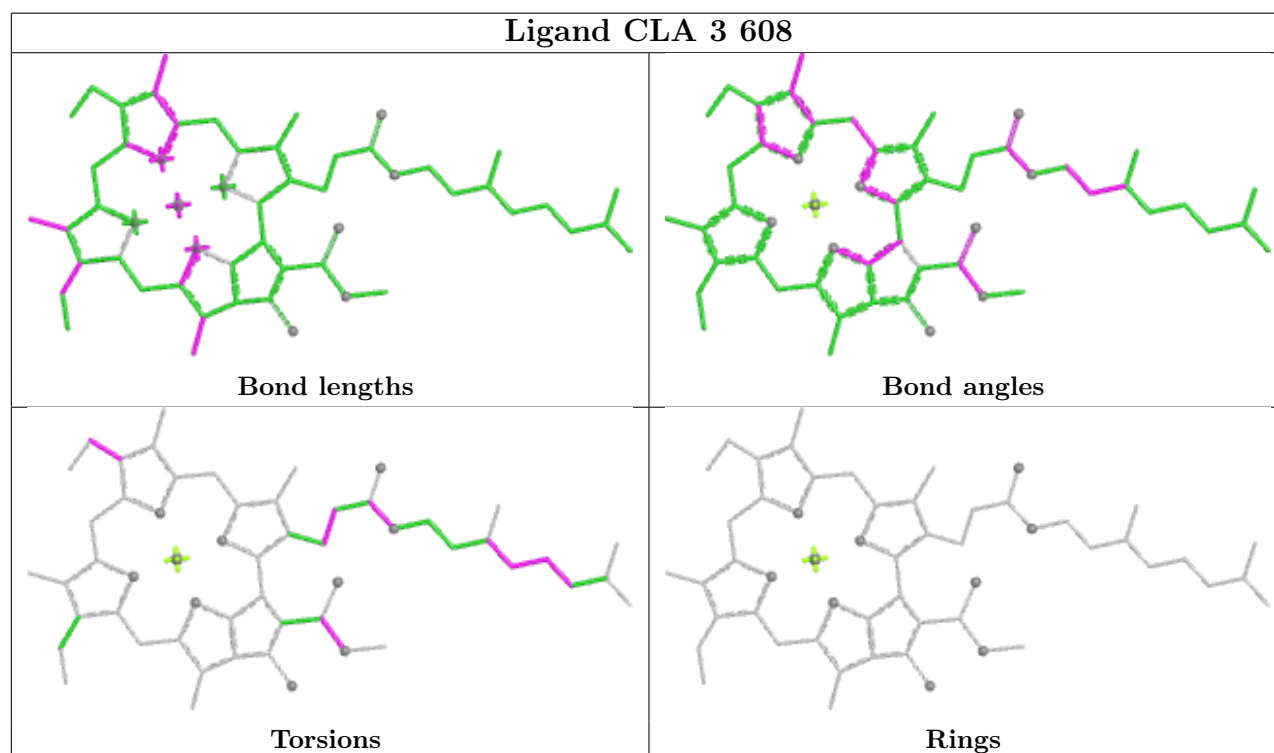
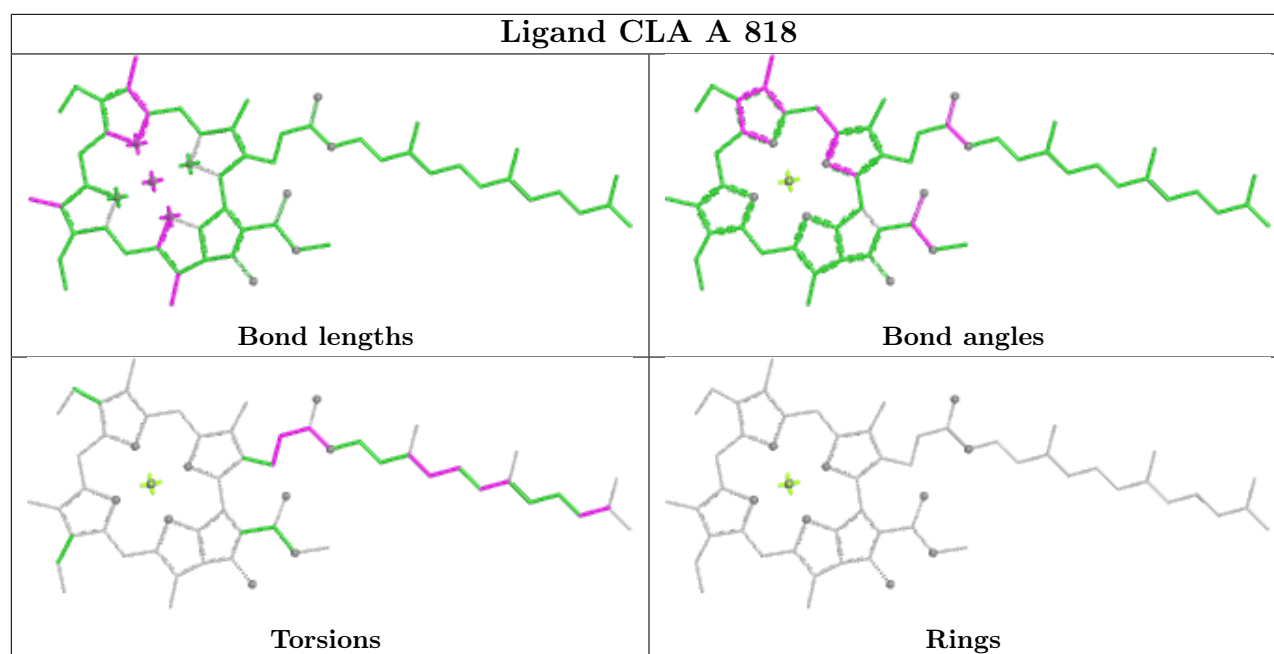


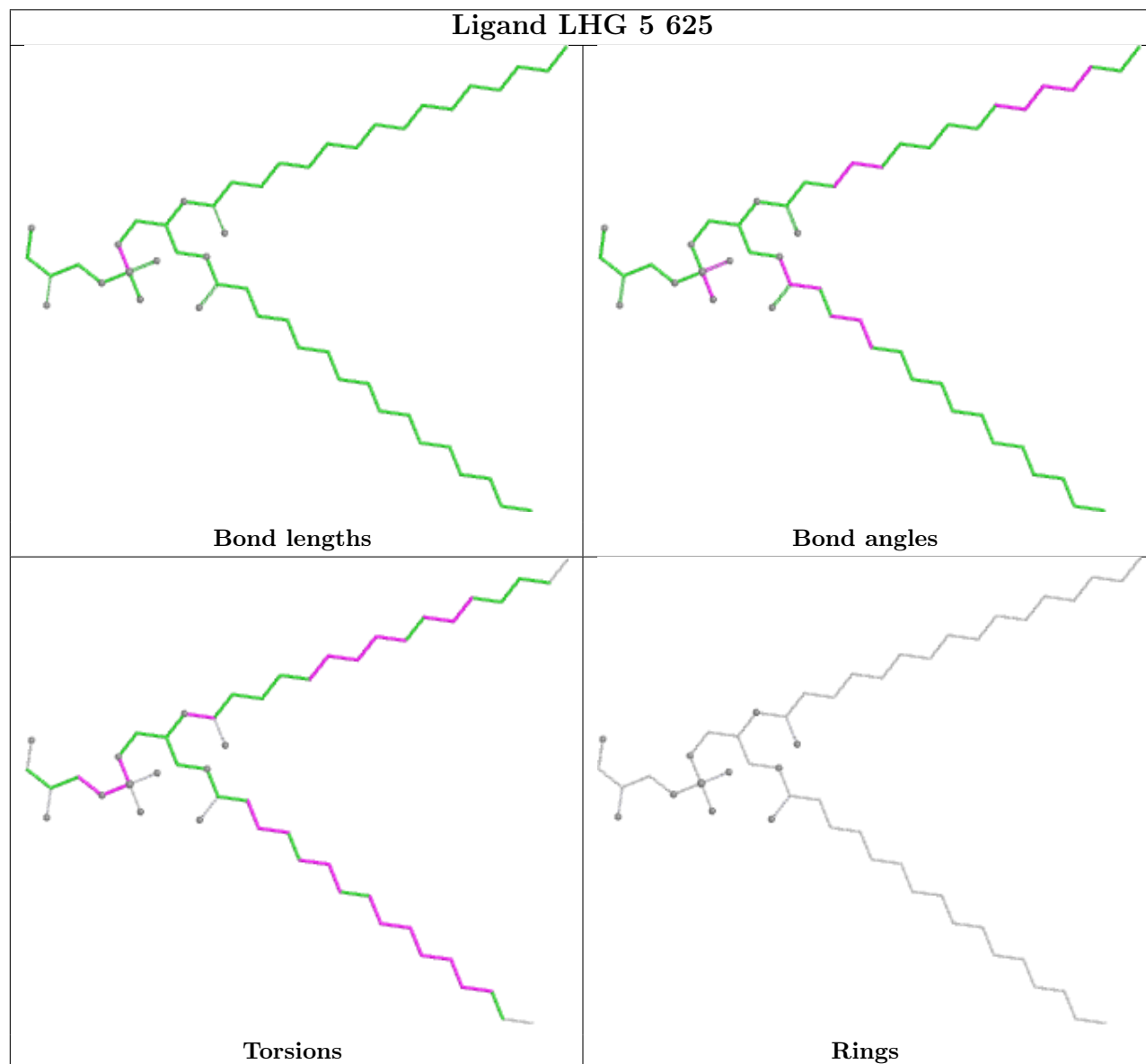
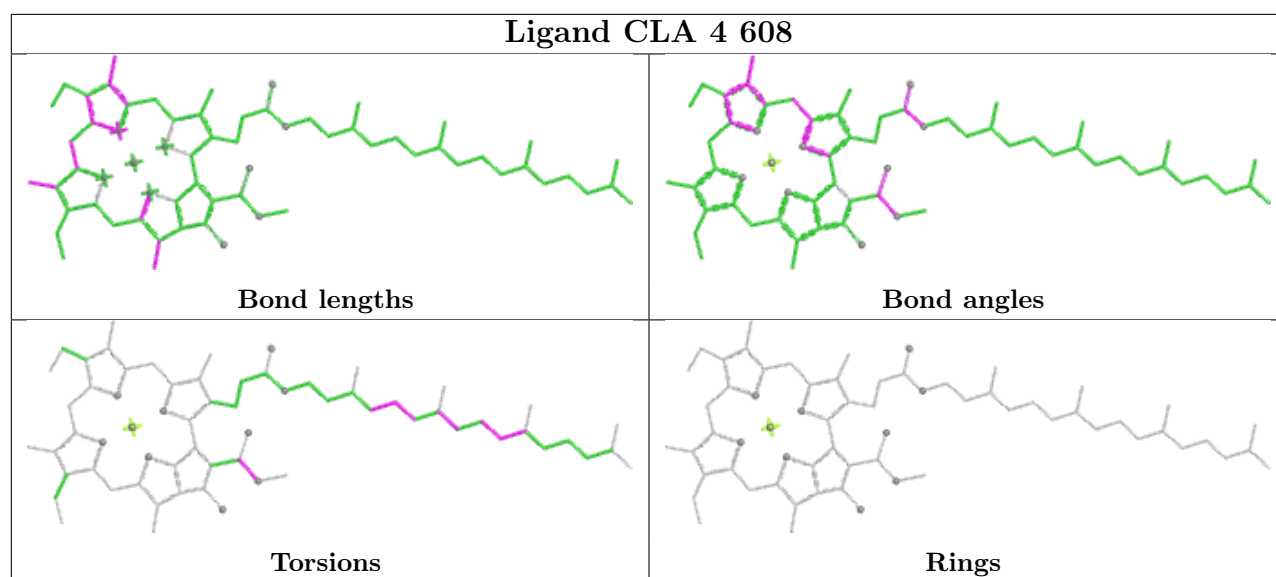
Ligand BCR 1 619



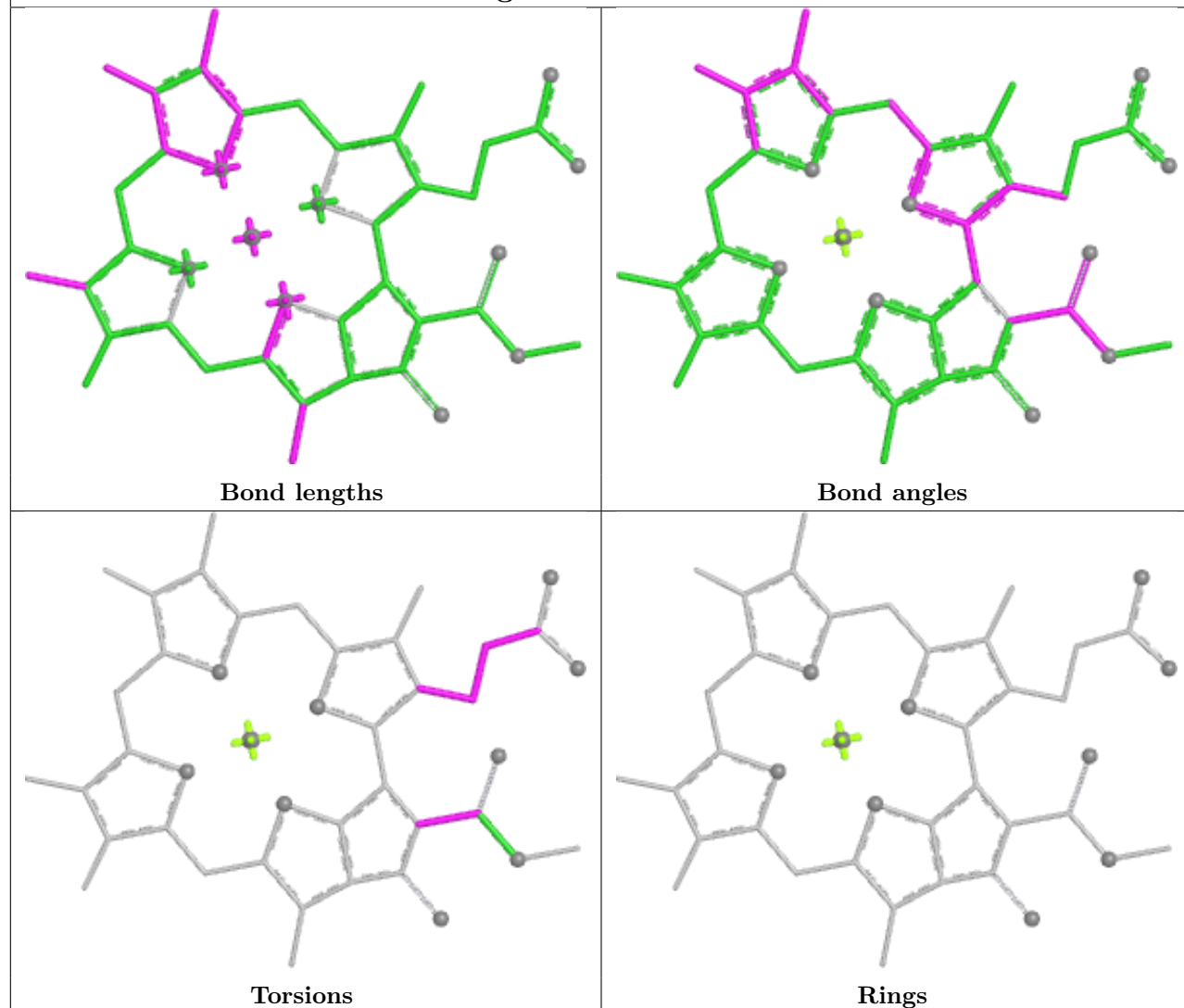
Ligand LUT a 617



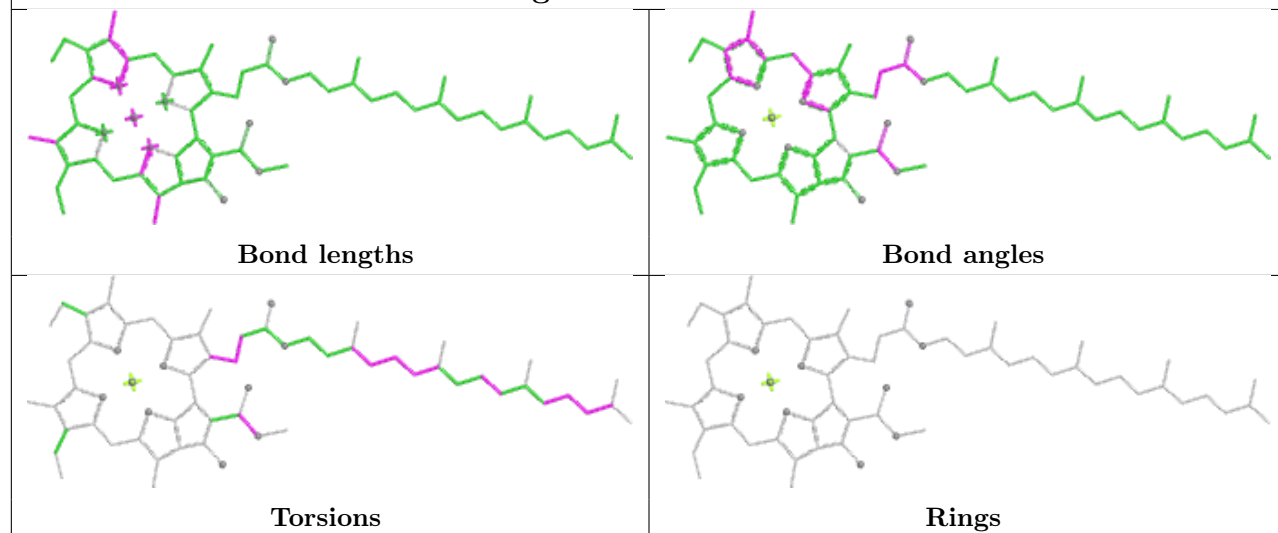




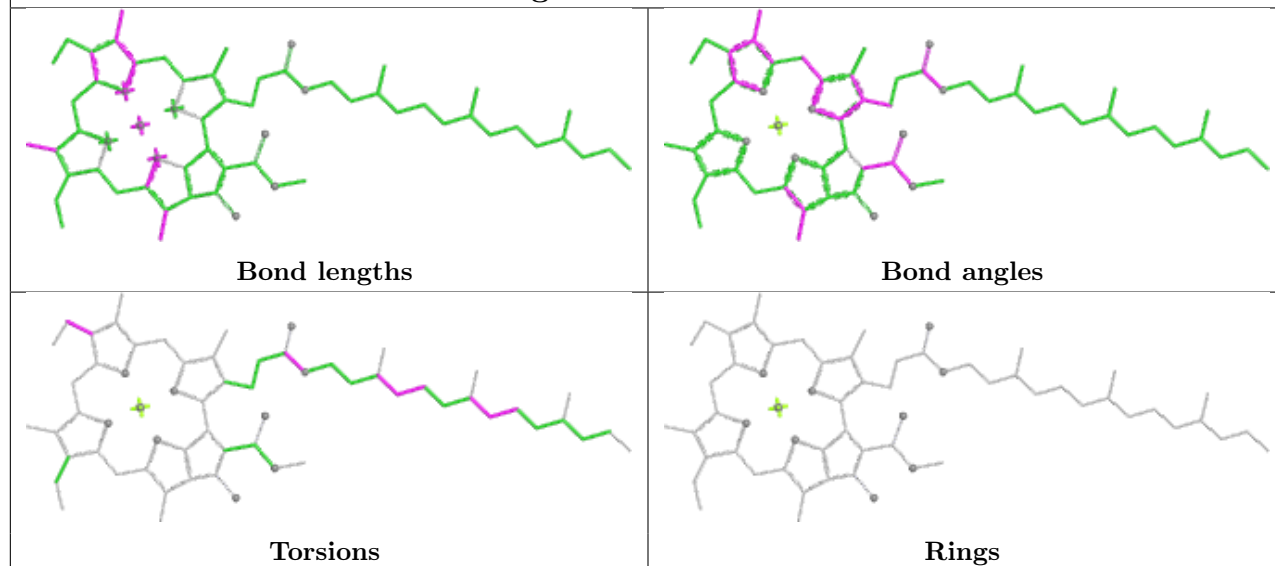
Ligand CLA 5 619



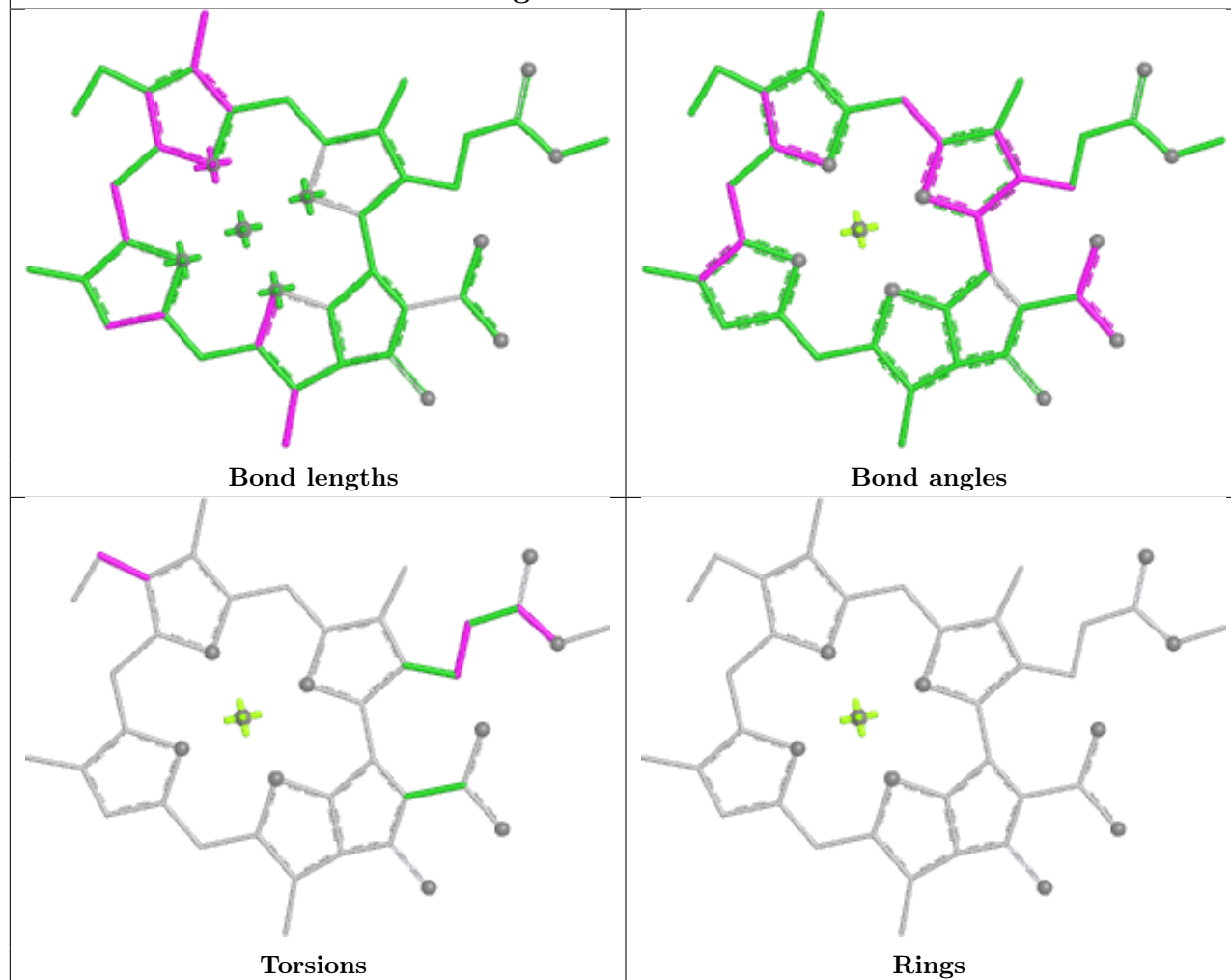
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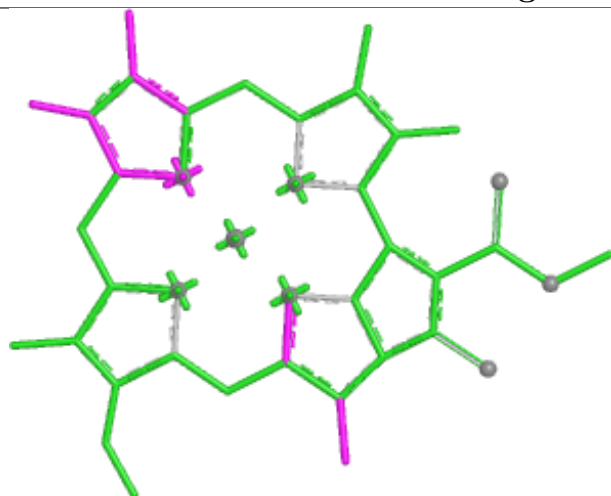
Ligand CLA B 825



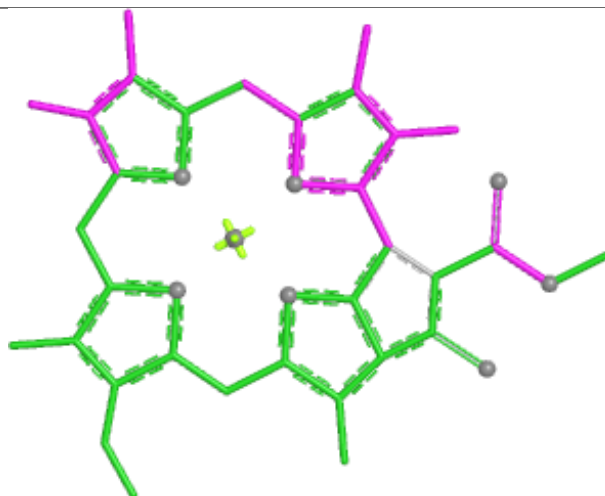
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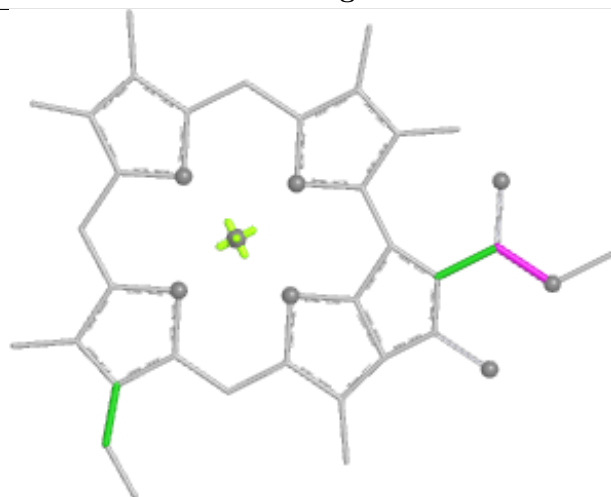
Ligand CLA 1 609



Bond lengths



Bond angles

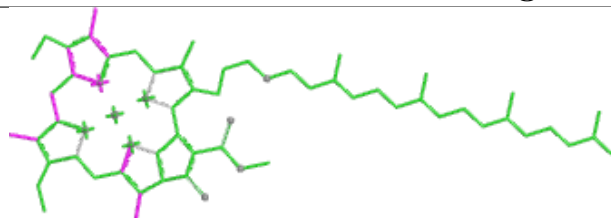


Torsions

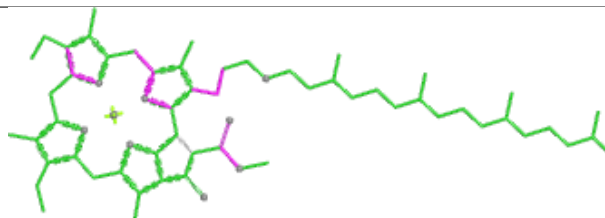


Rings

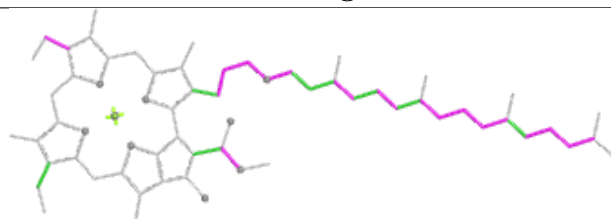
Ligand CLA 5 613



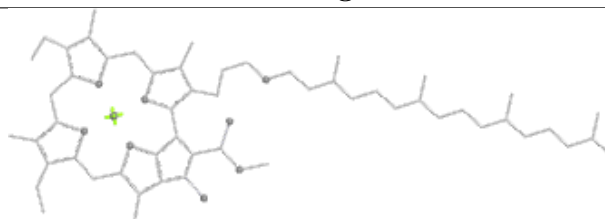
Bond lengths



Bond angles

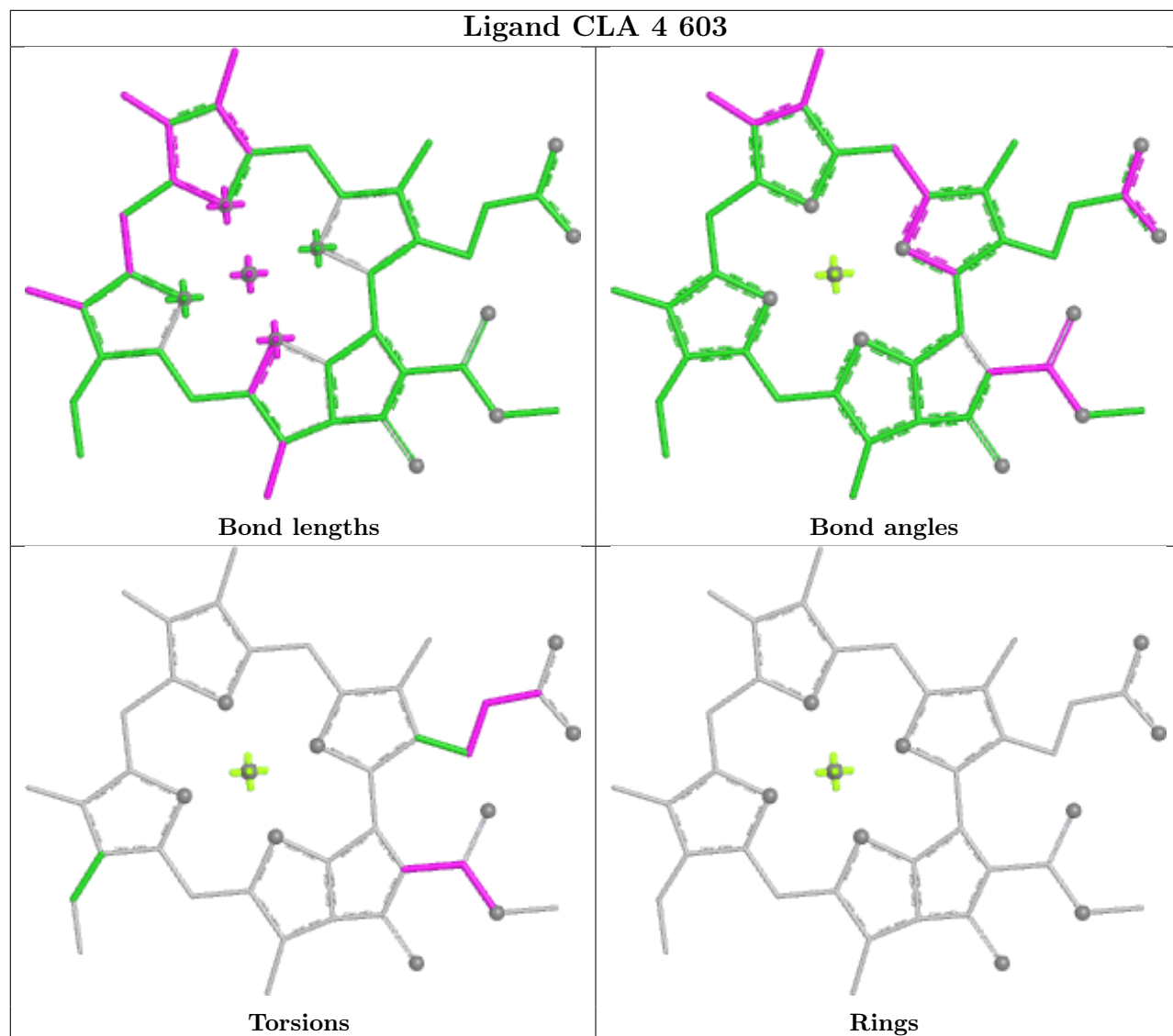


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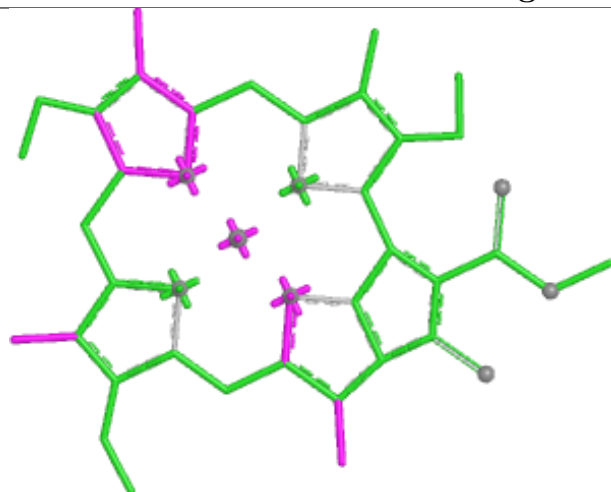


Rings

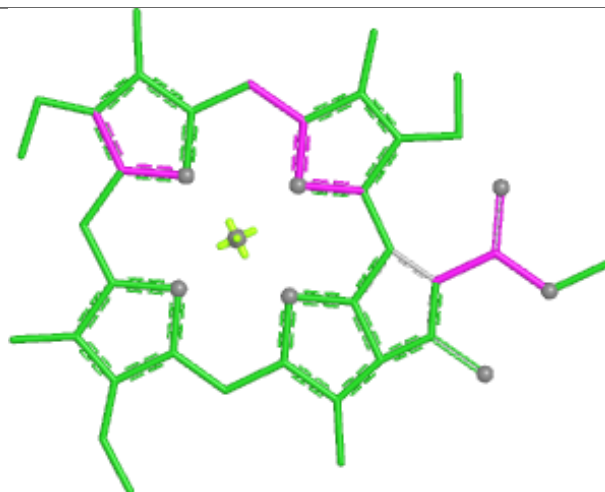
Ligand CLA 4 603



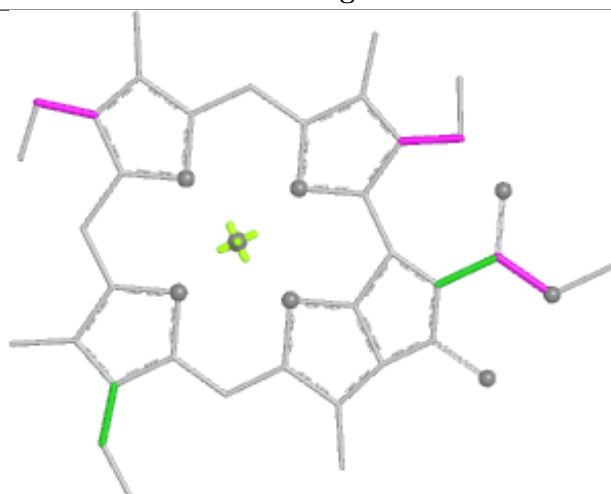
Ligand CLA 8 611



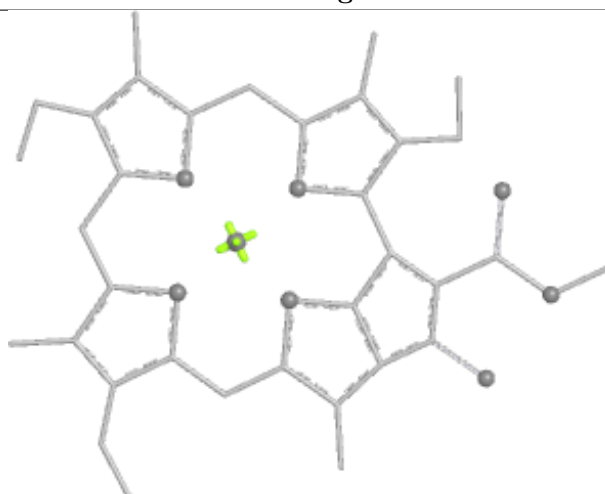
Bond lengths



Bond angles

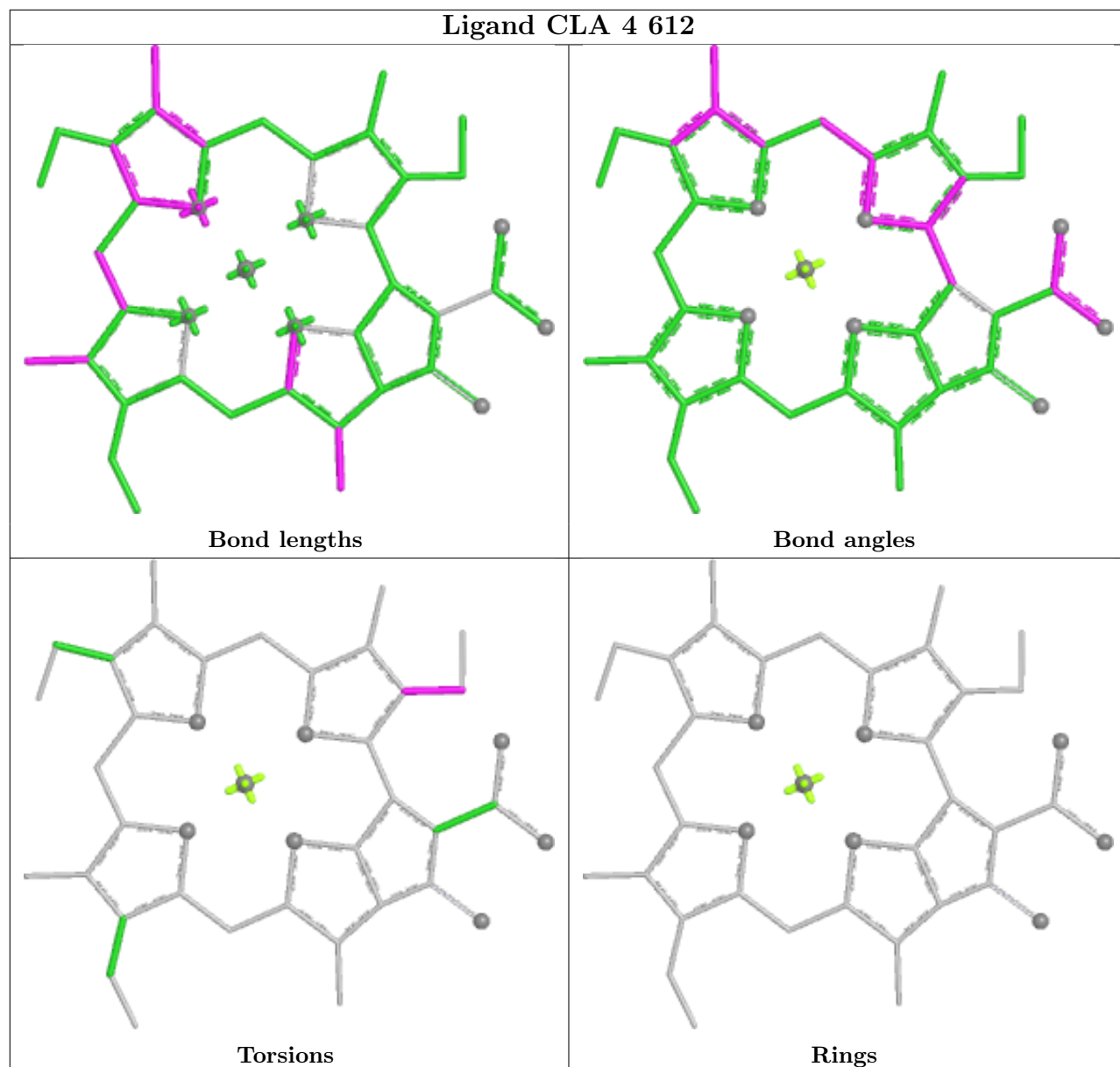


Torsions

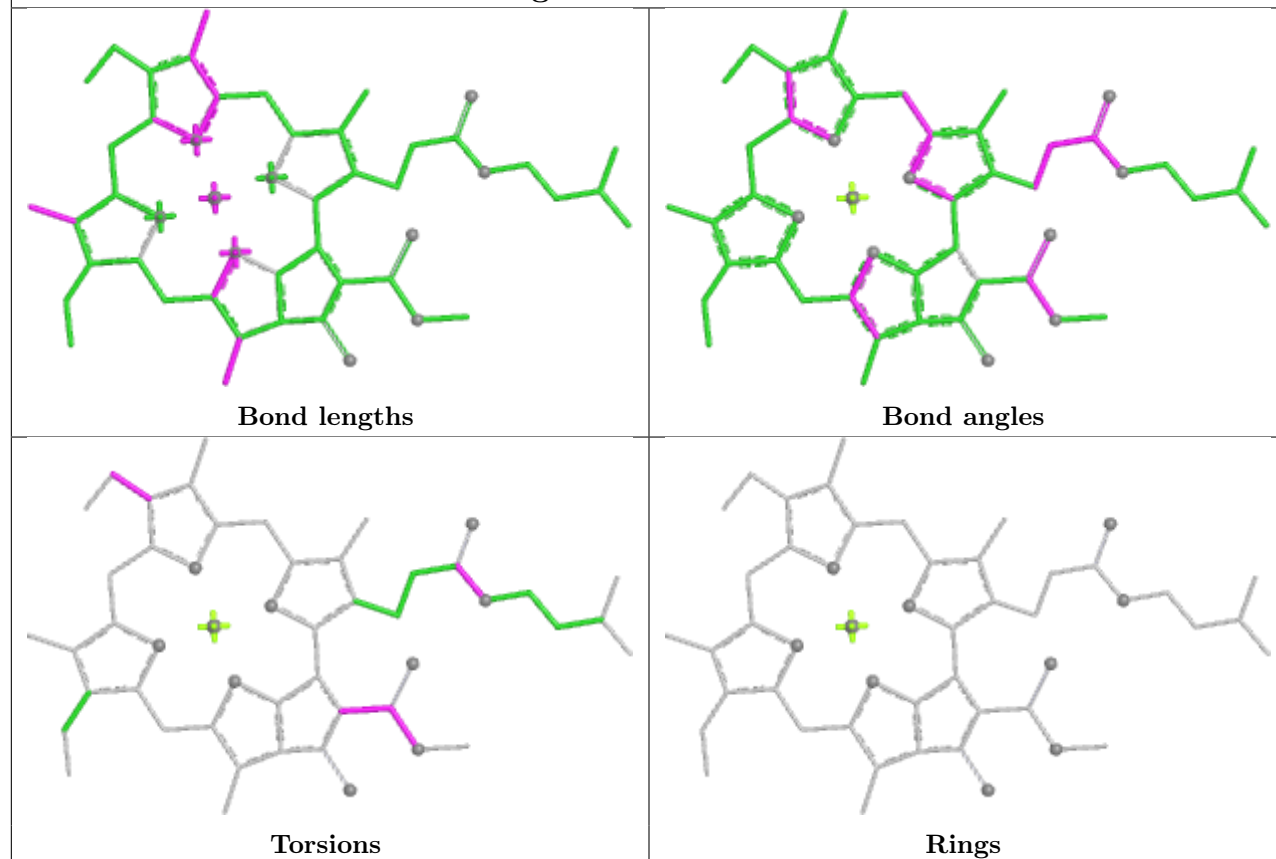


Rings

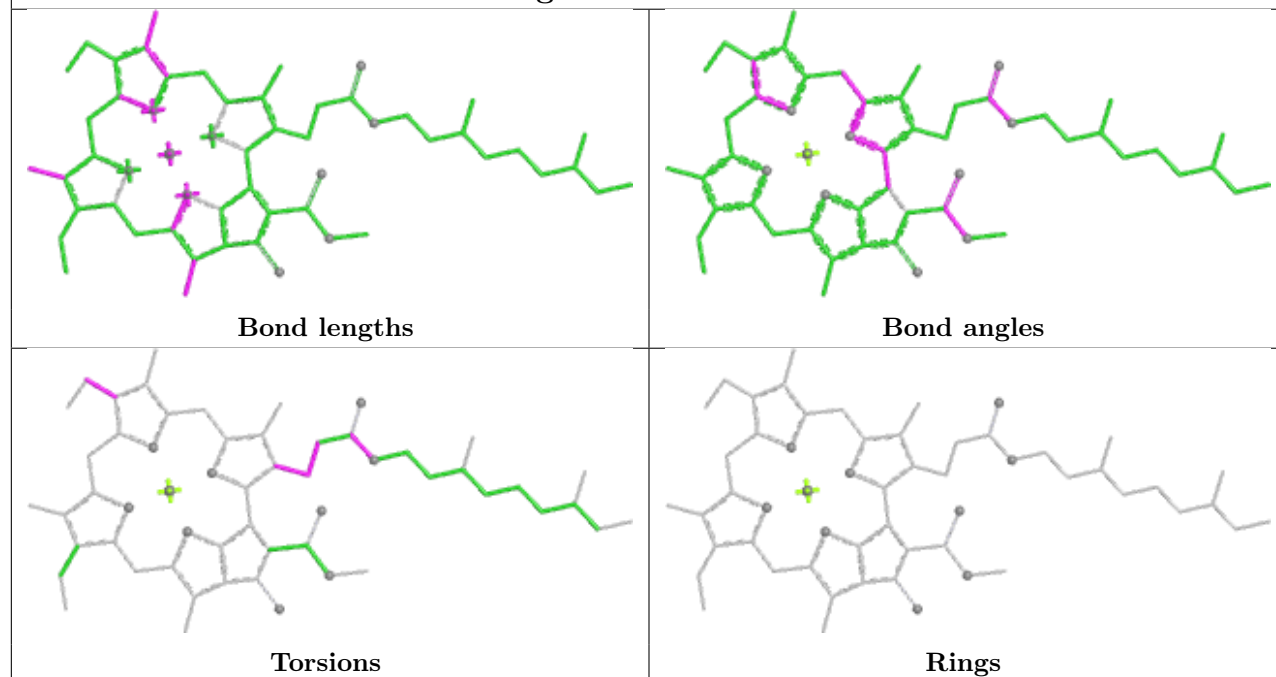
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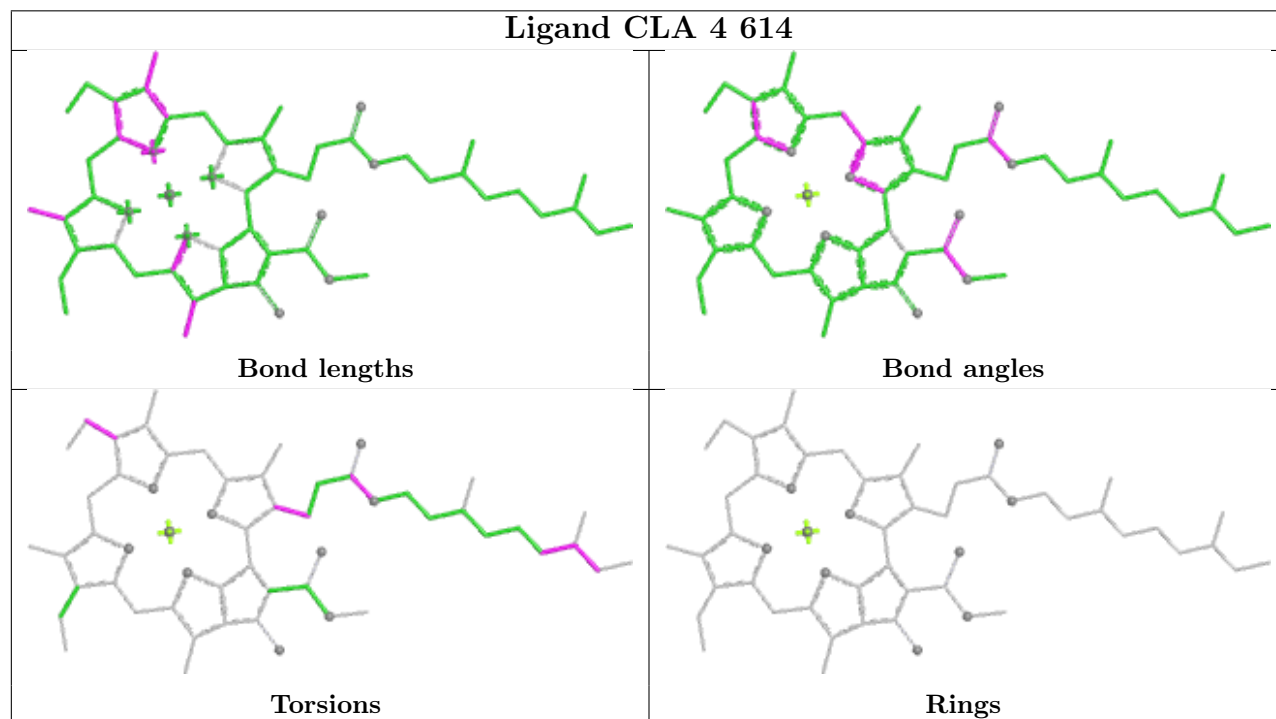
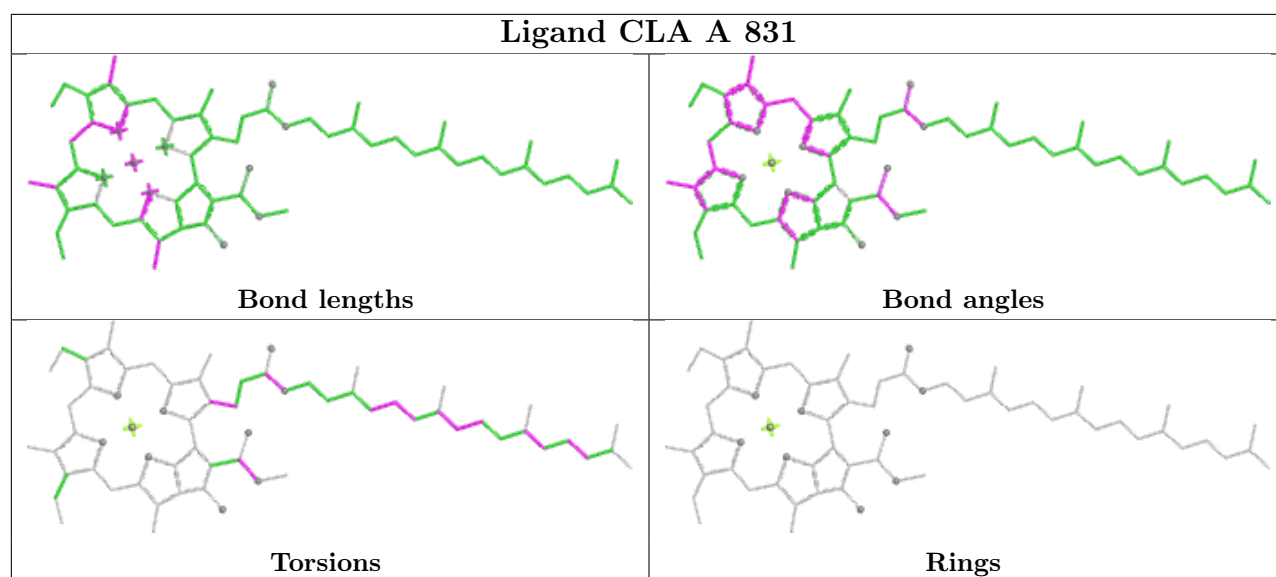


Ligand CLA A 832

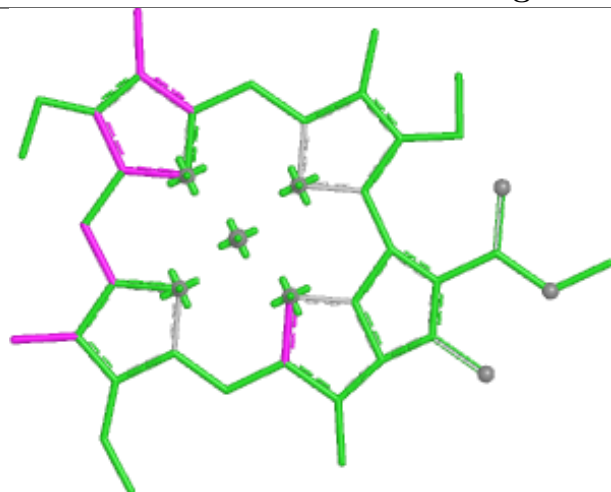


Ligand CLA 5 601

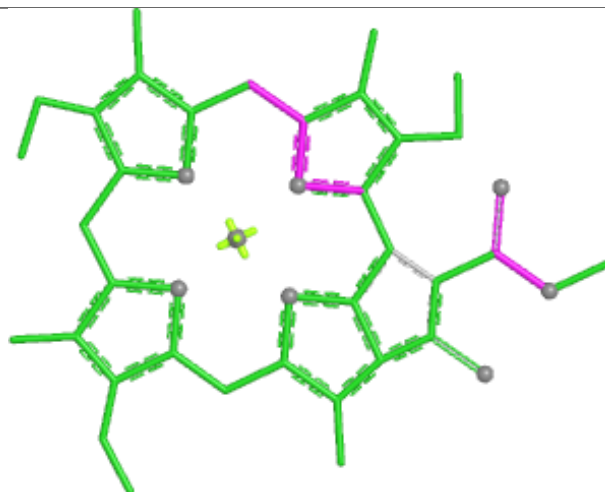




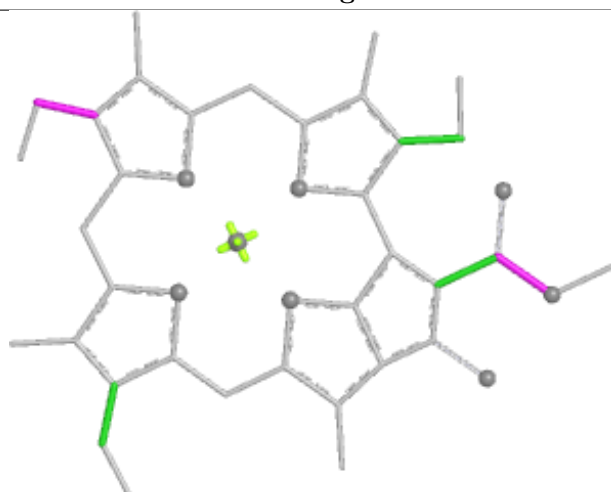
Ligand CLA G 203



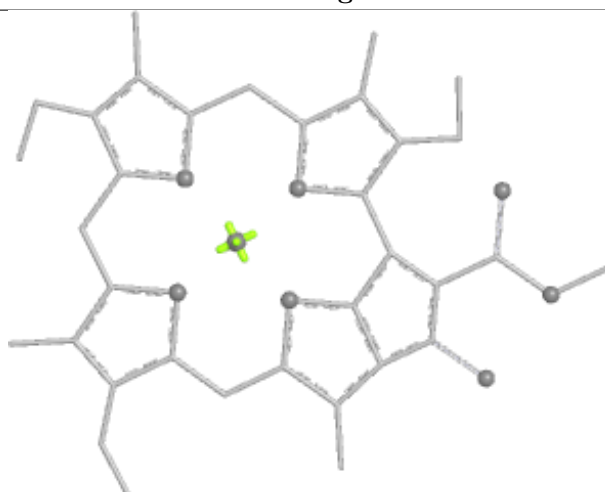
Bond lengths



Bond angles

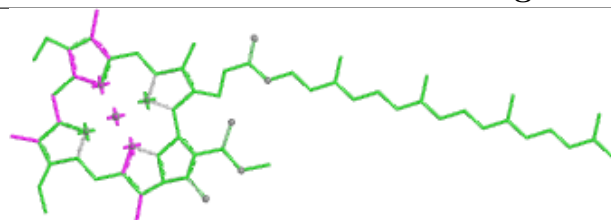


Torsions

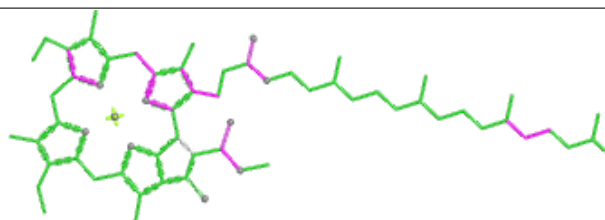


Rings

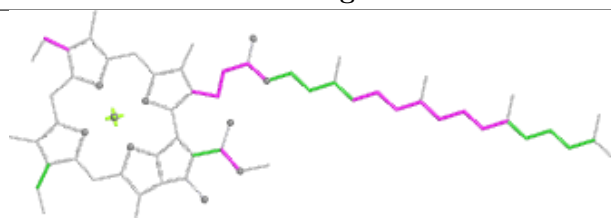
Ligand CLA B 813



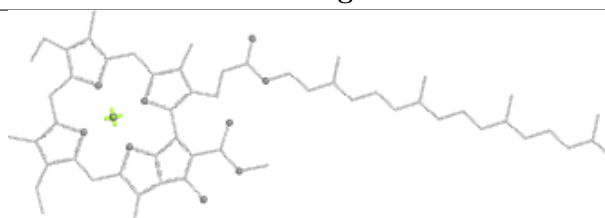
Bond lengths



Bond angles

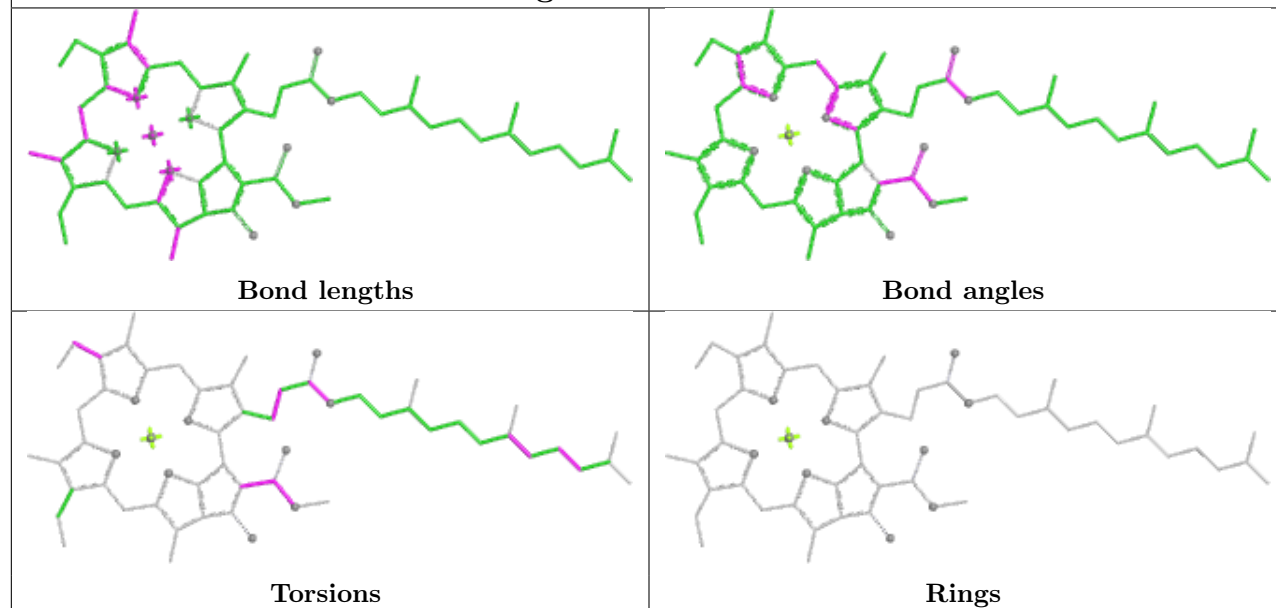


Torsions

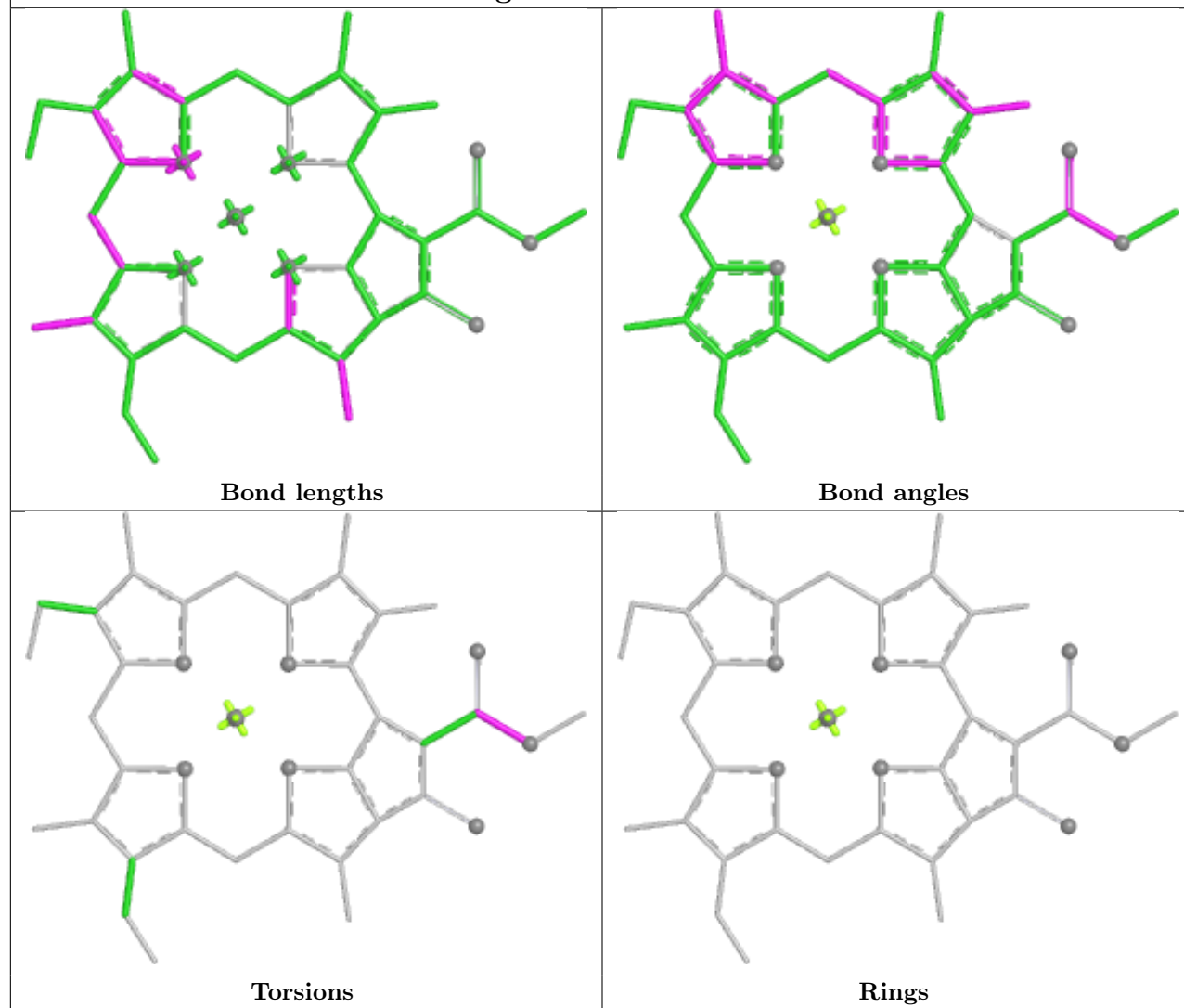


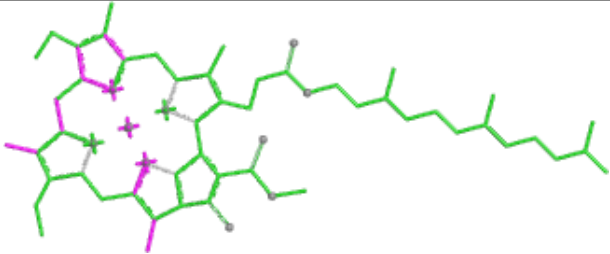
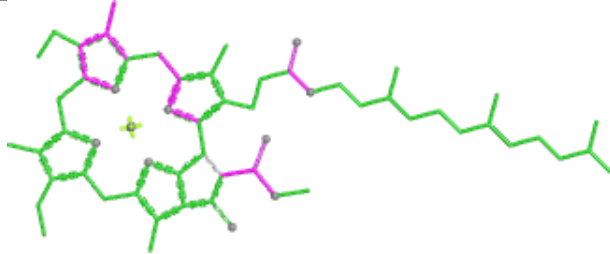
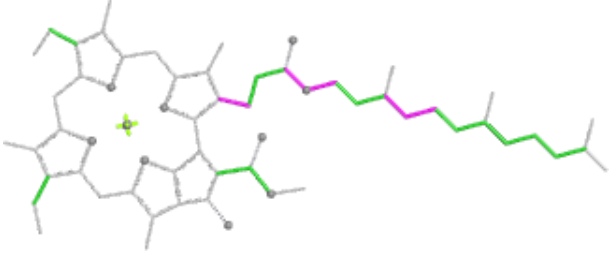
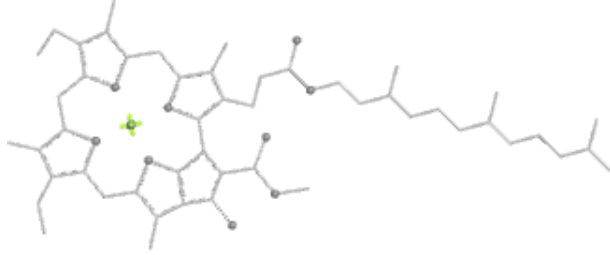
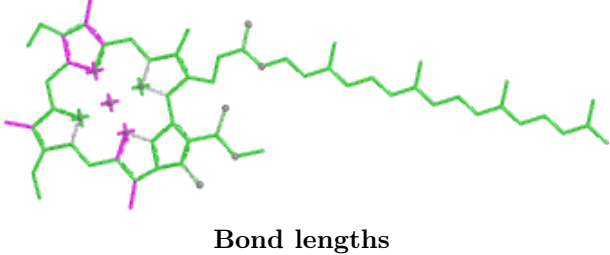
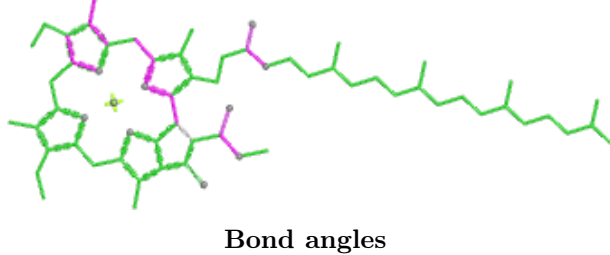
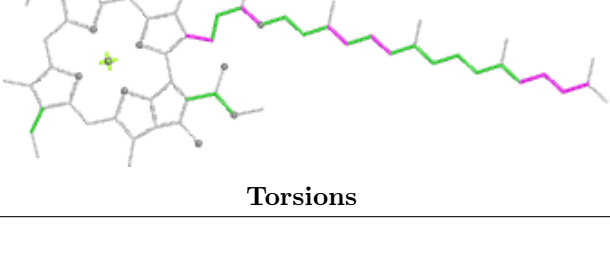
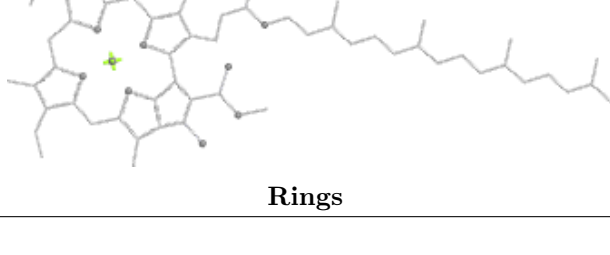
Rings

Ligand CLA 3 602

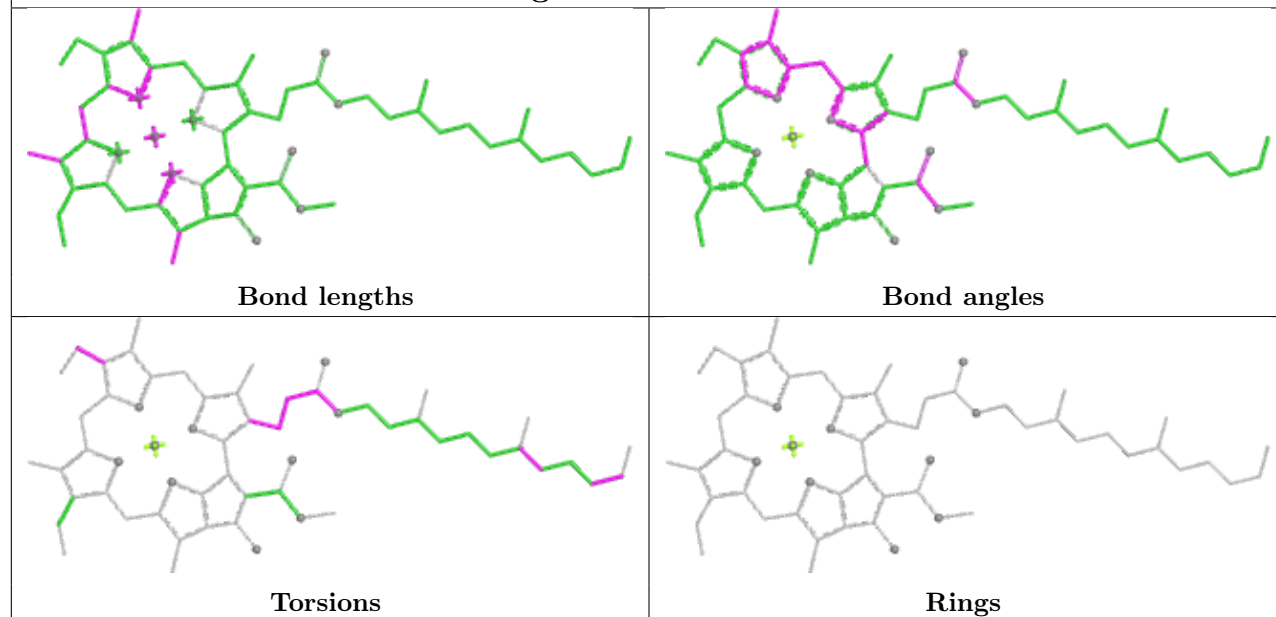


Ligand CLA F 304

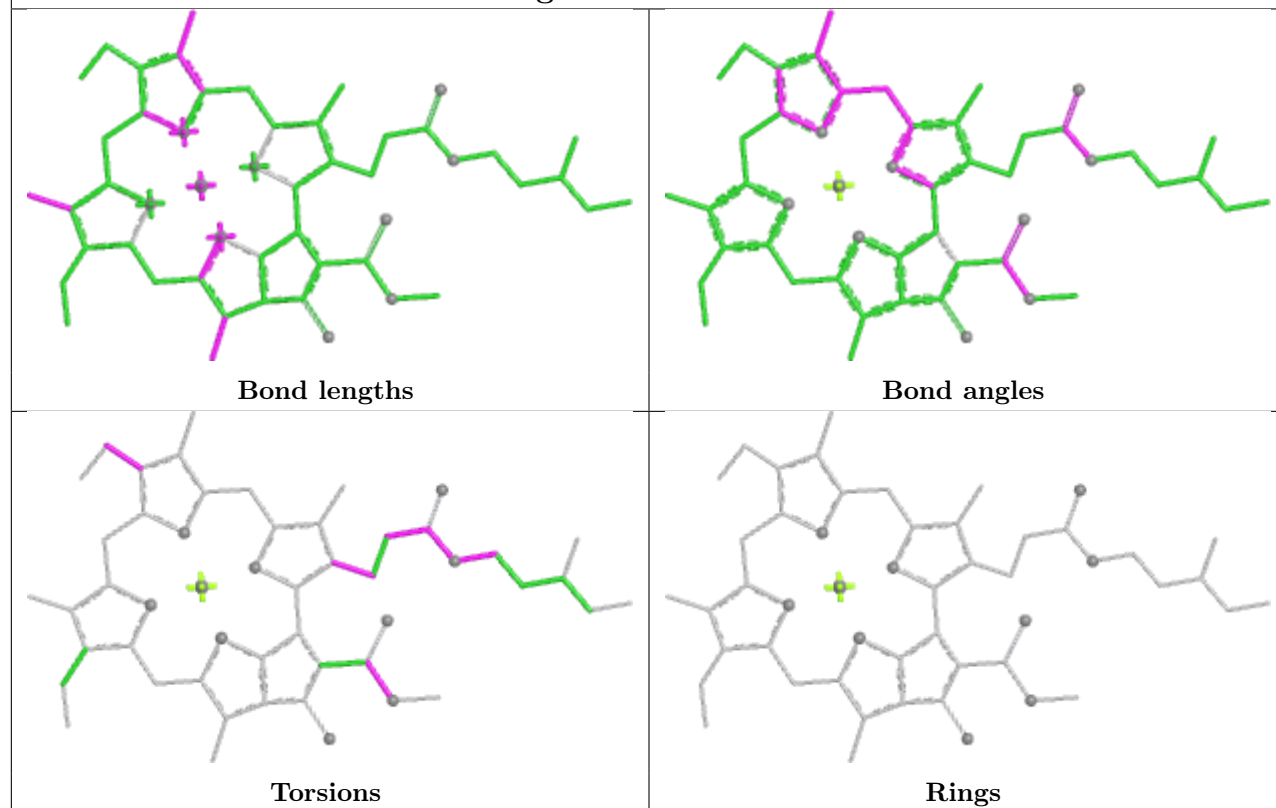


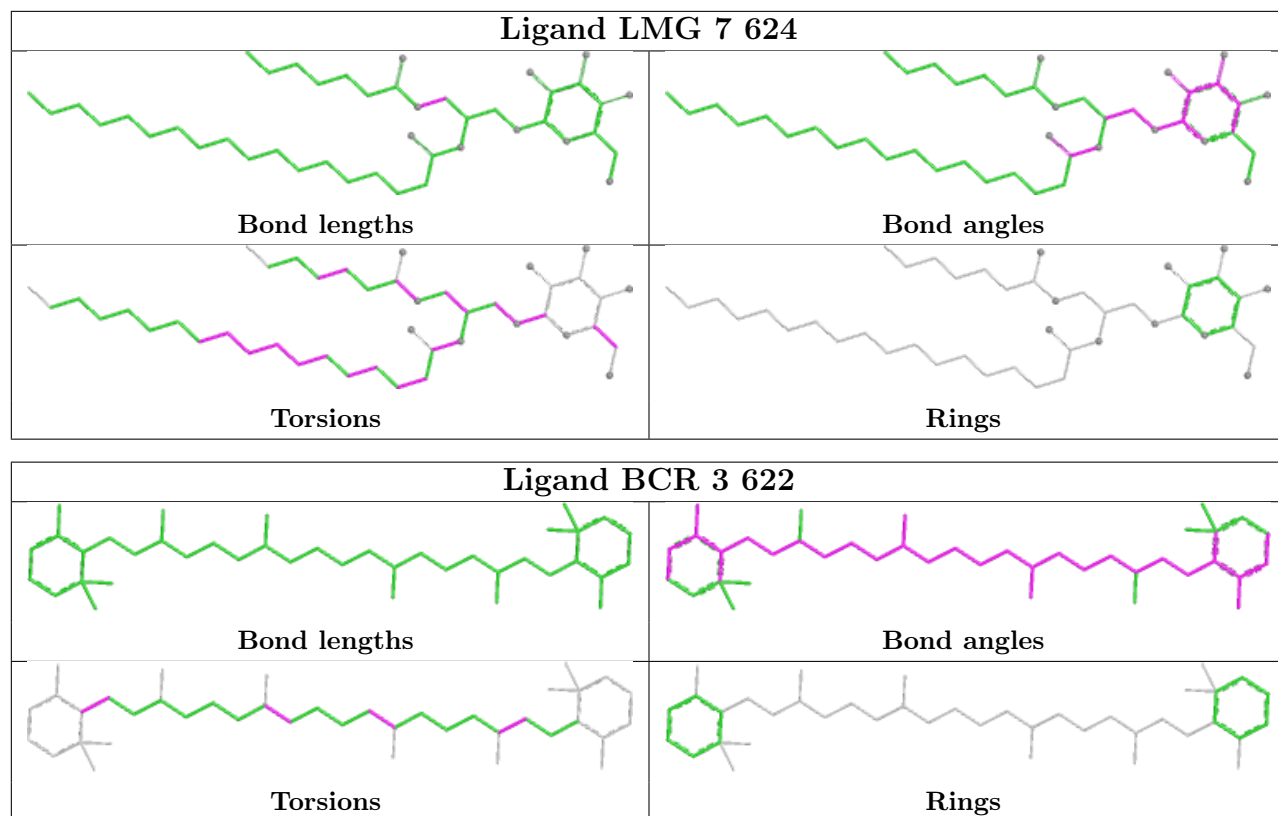
Ligand CLA 8 610	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA K 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 819

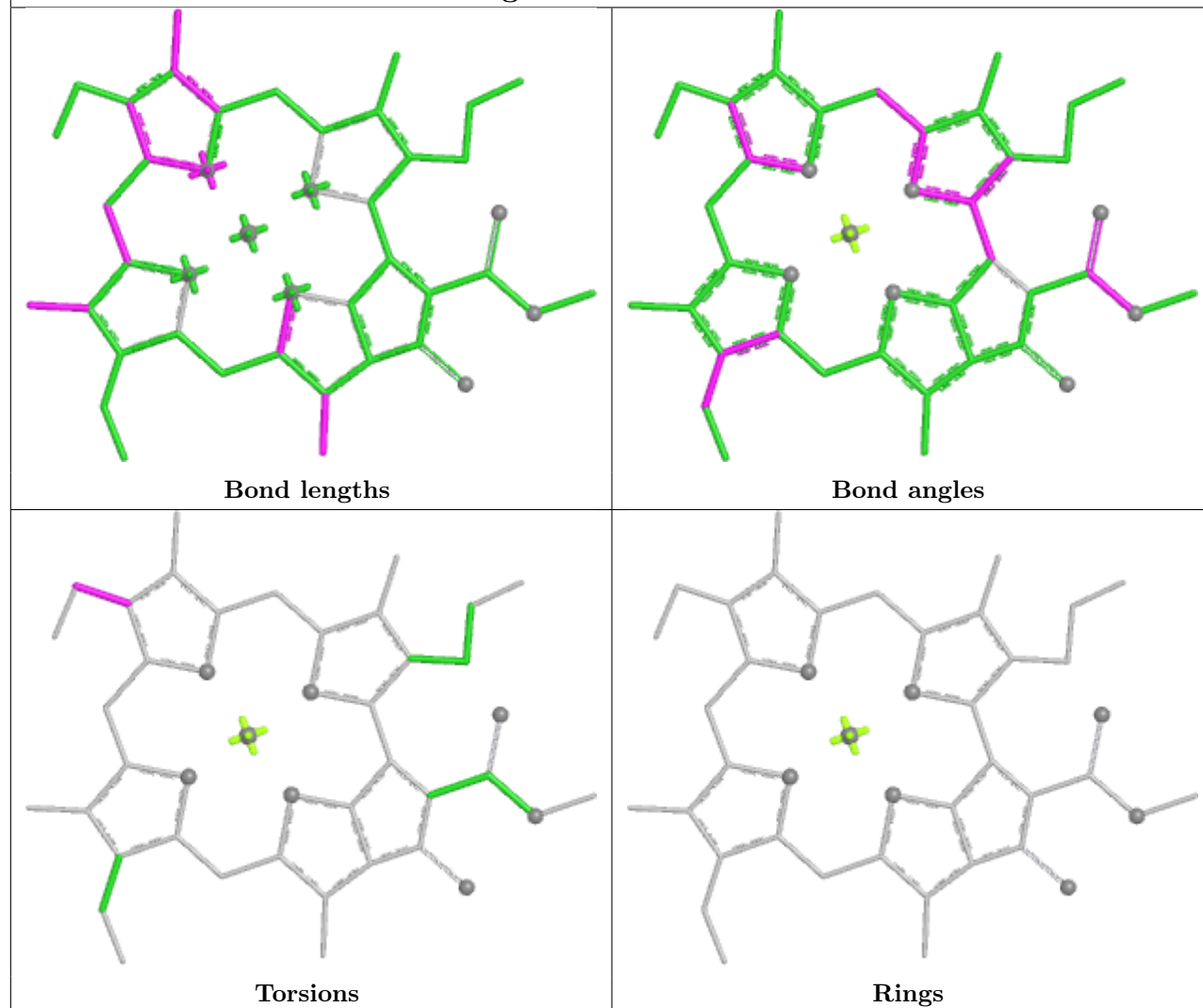


Ligand CLA 6 608

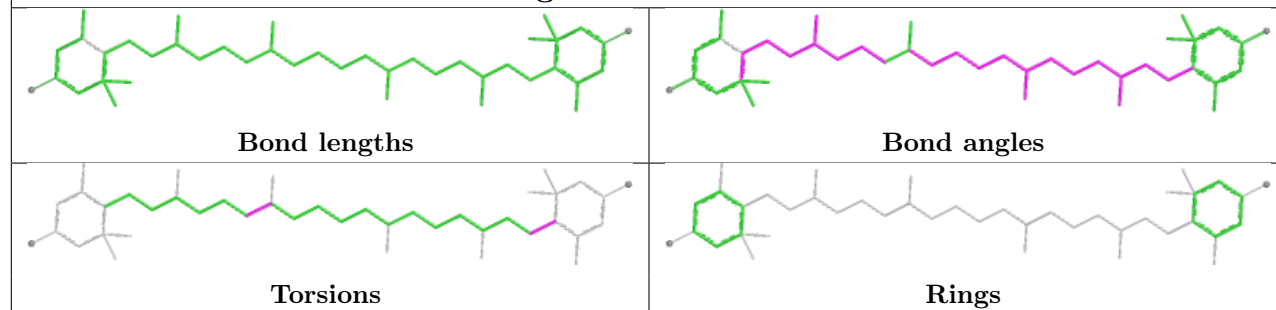




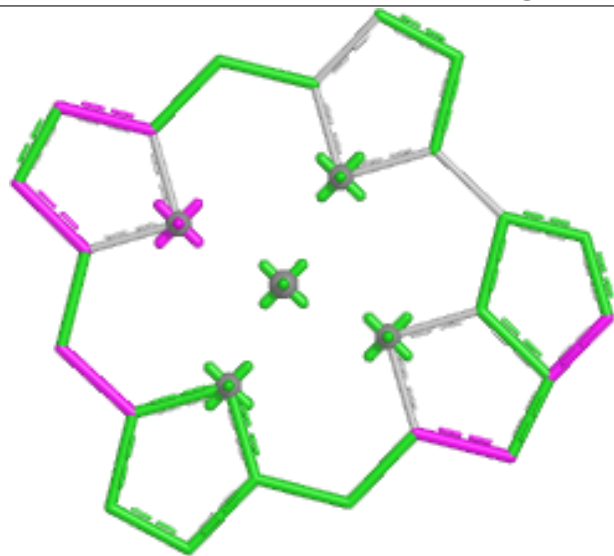
Ligand CLA B 841



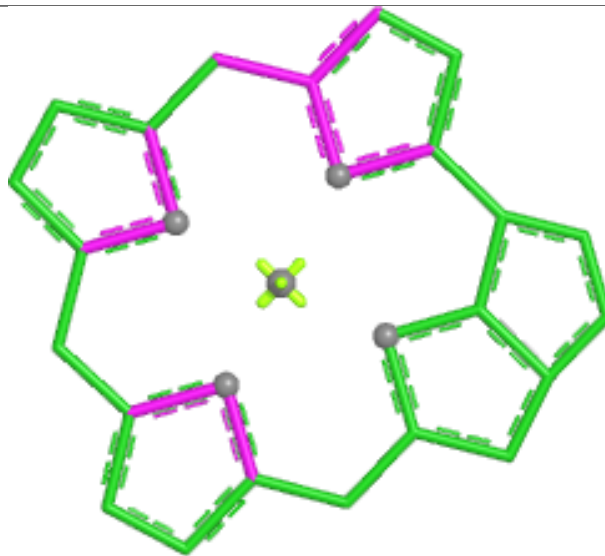
Ligand LUT 4 619



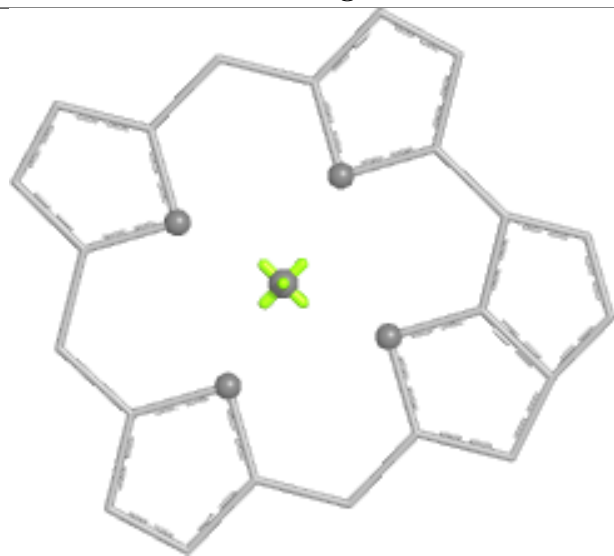
Ligand CLA 2 604



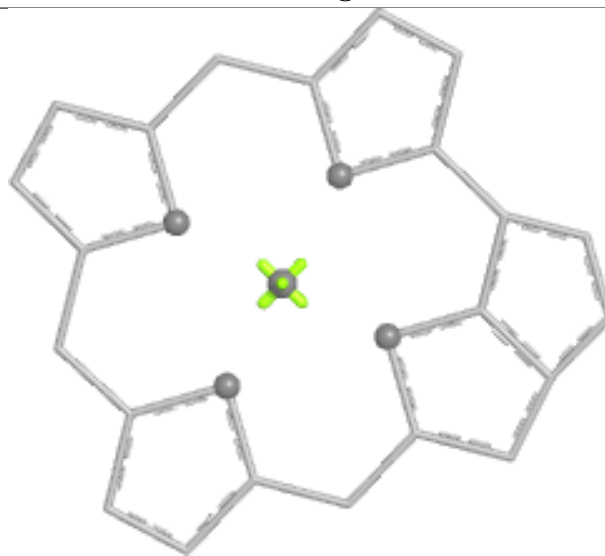
Bond lengths



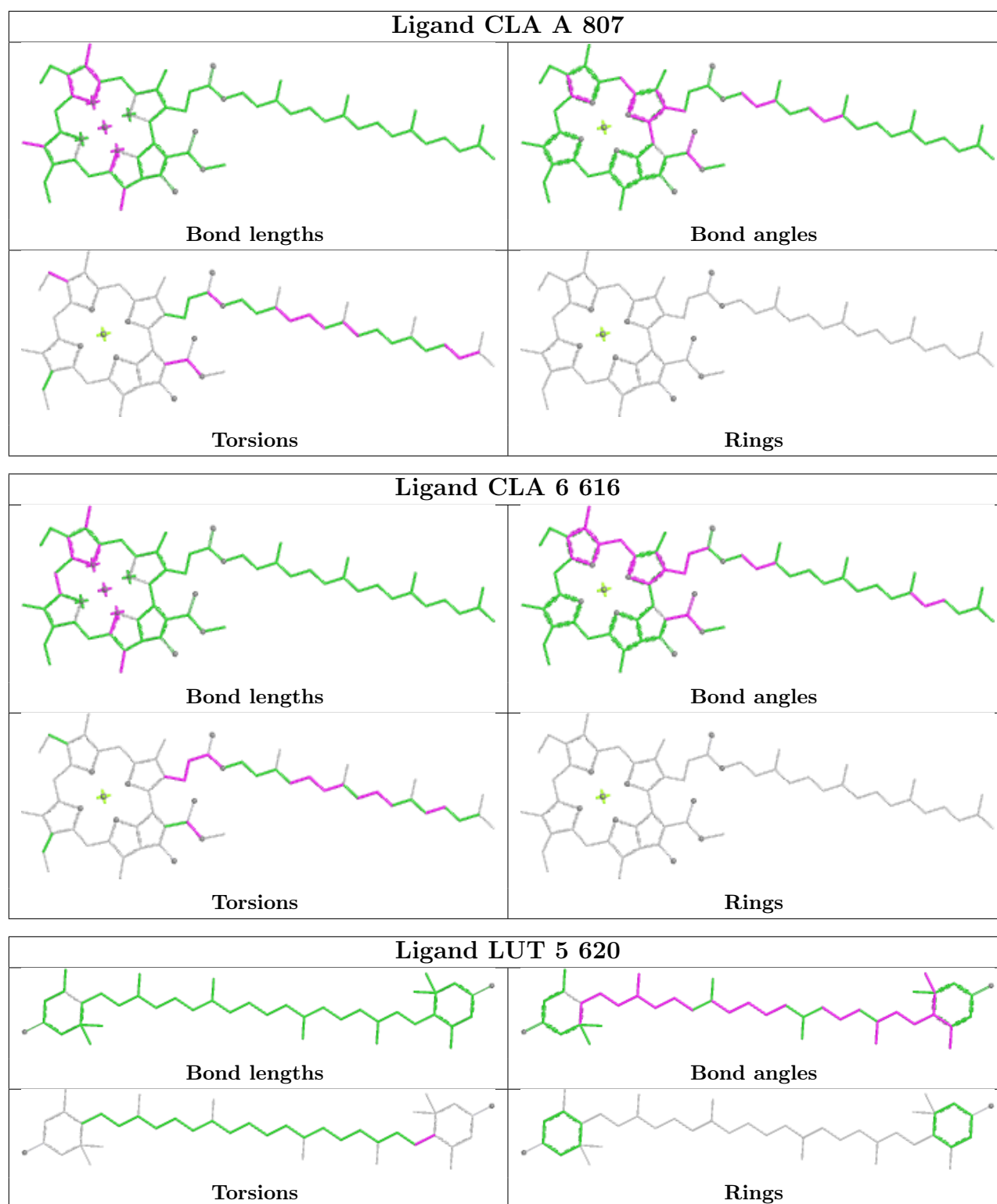
Bond angles

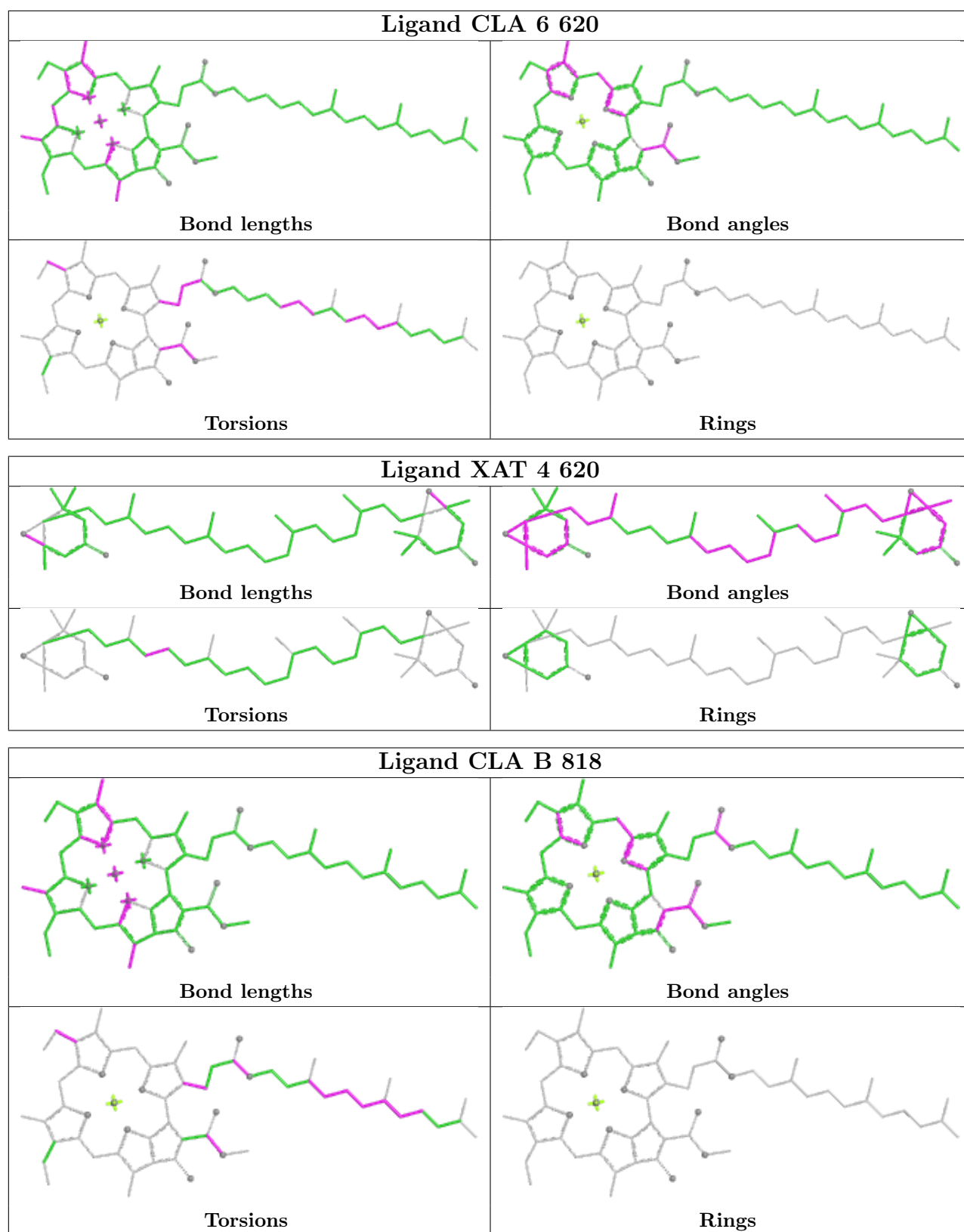


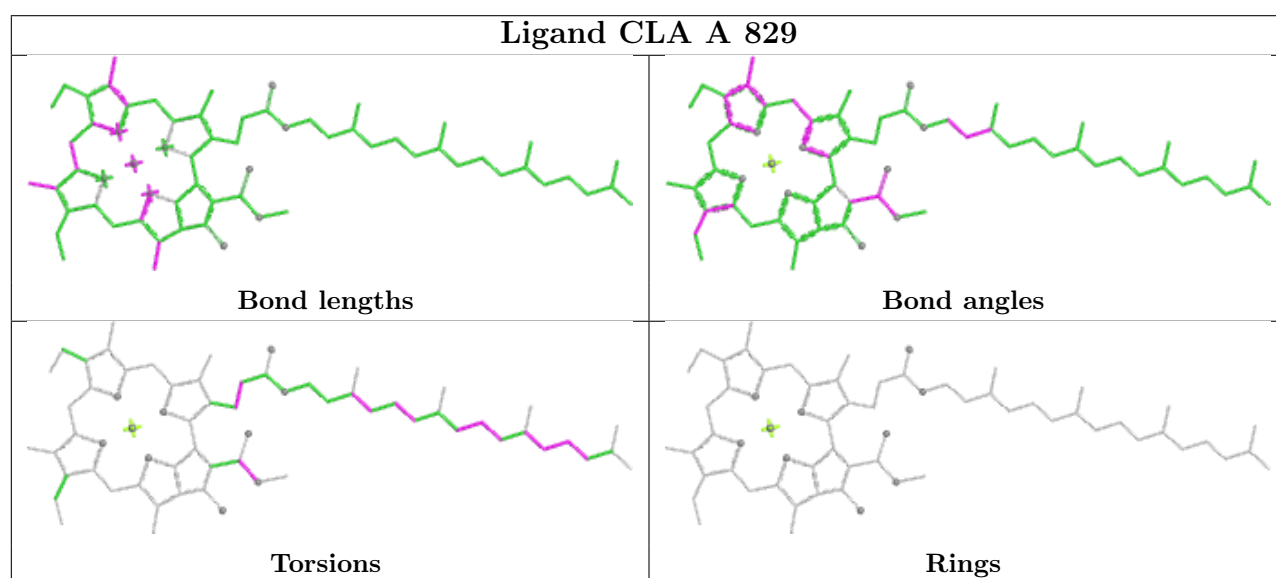
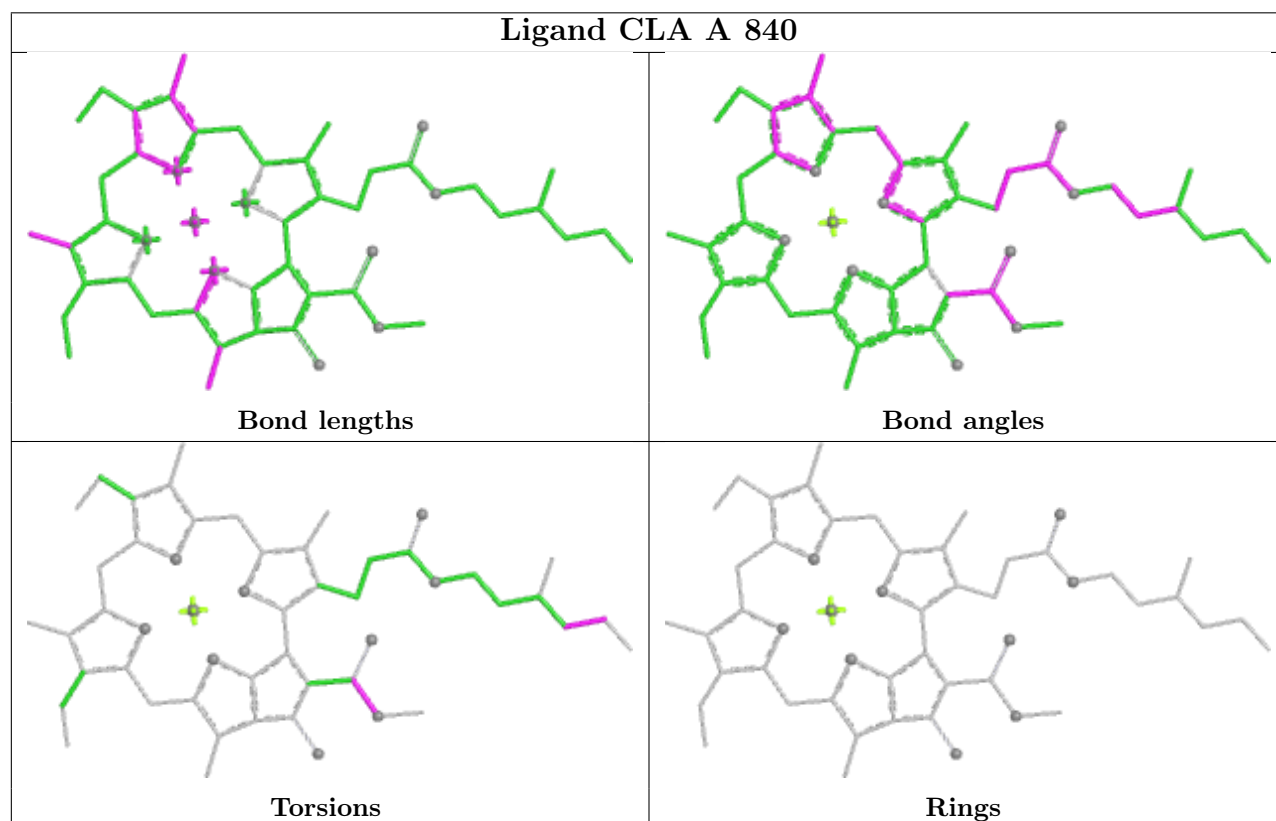
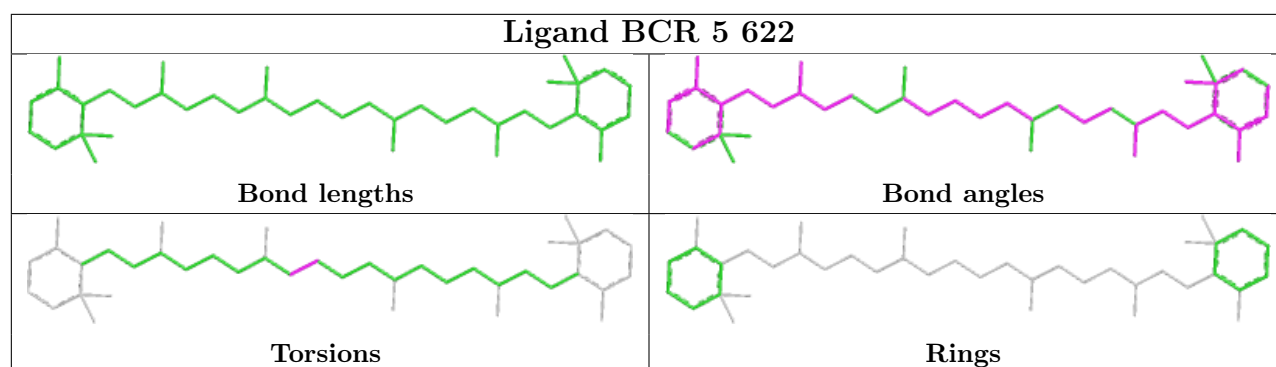
Torsions



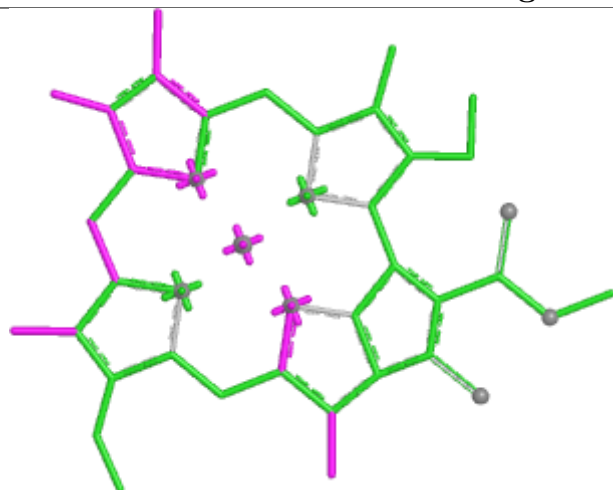
Rings



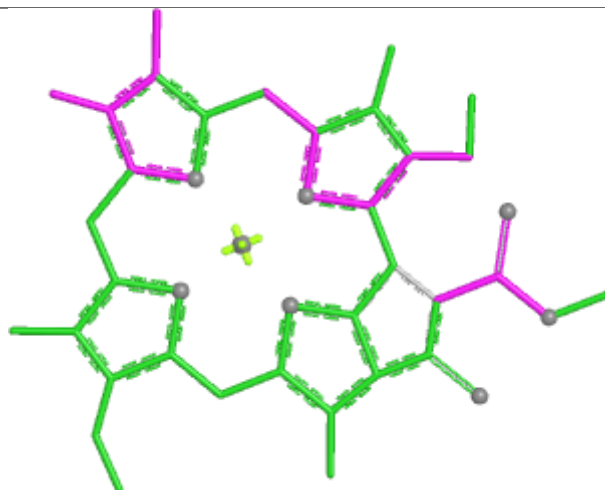




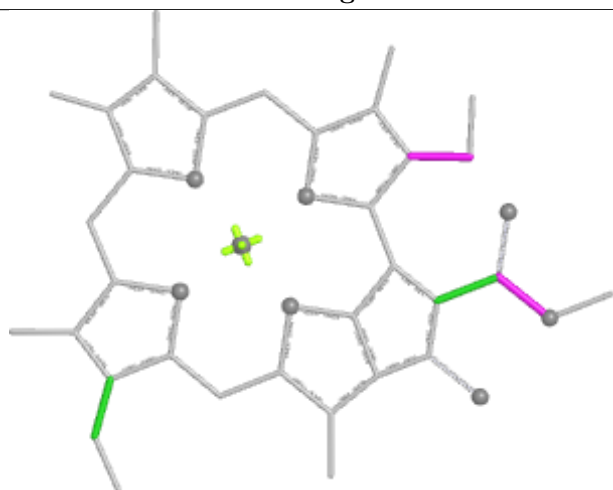
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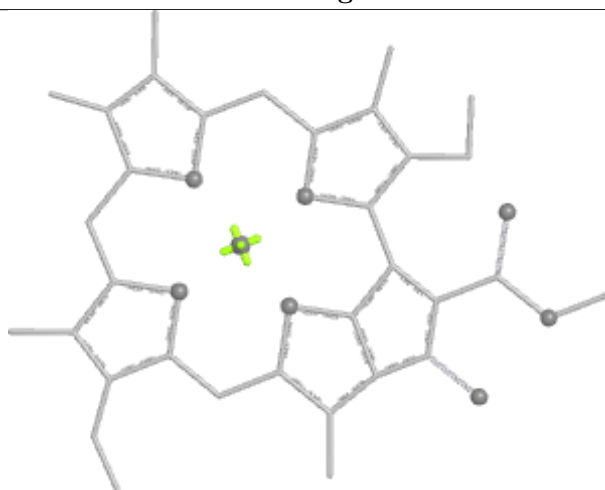
Bond lengths



Bond angles

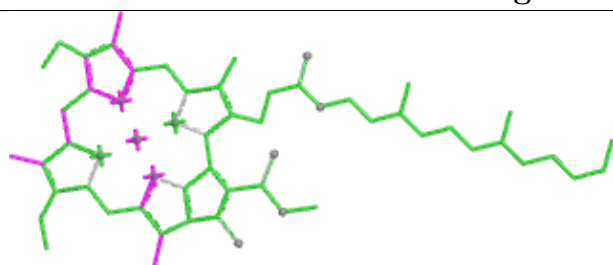


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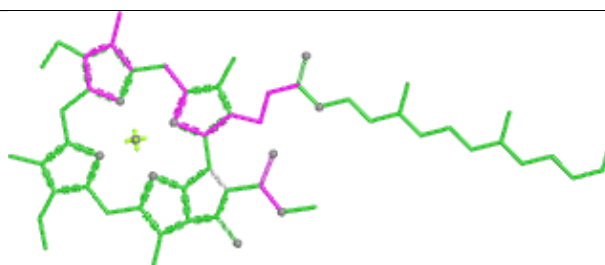


Rings

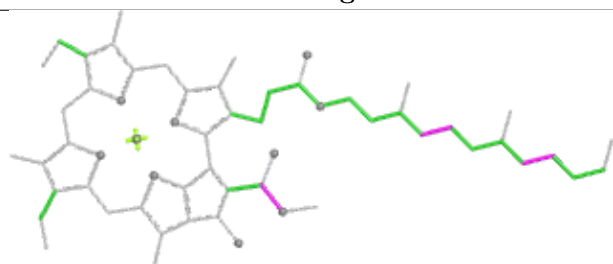
Ligand CLA A 827



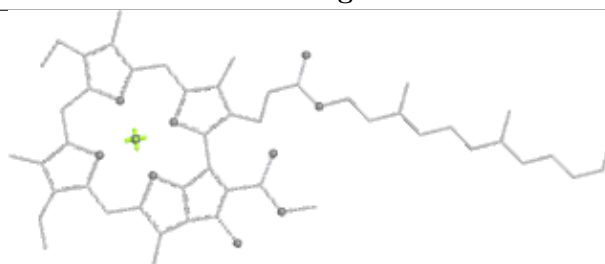
Bond lengths



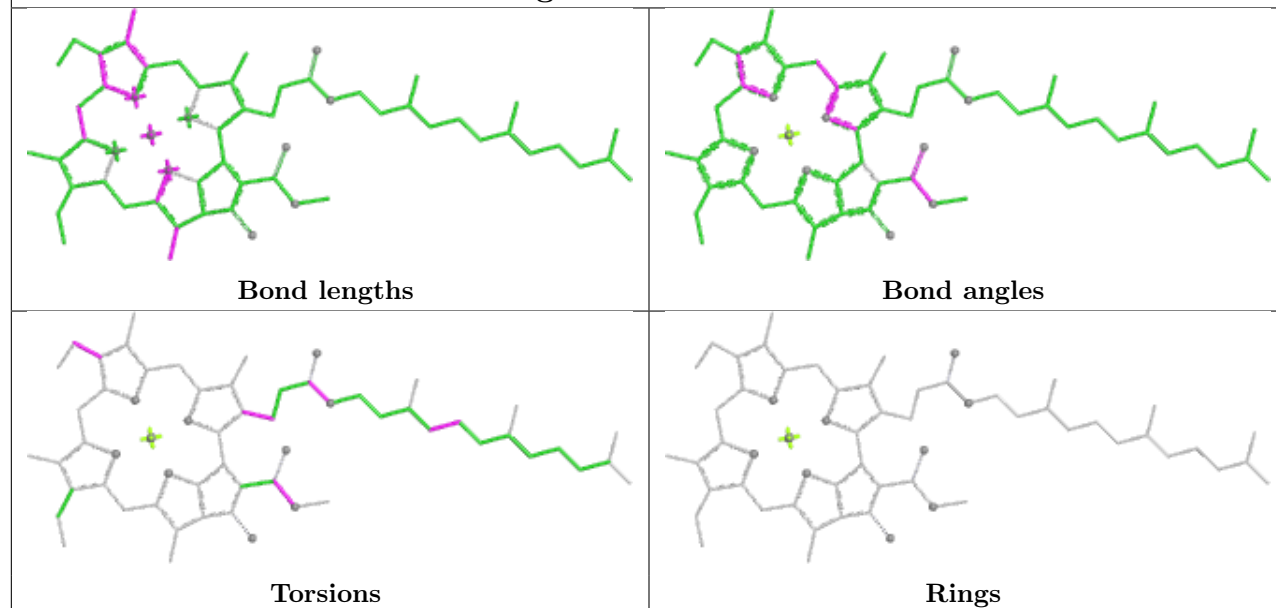
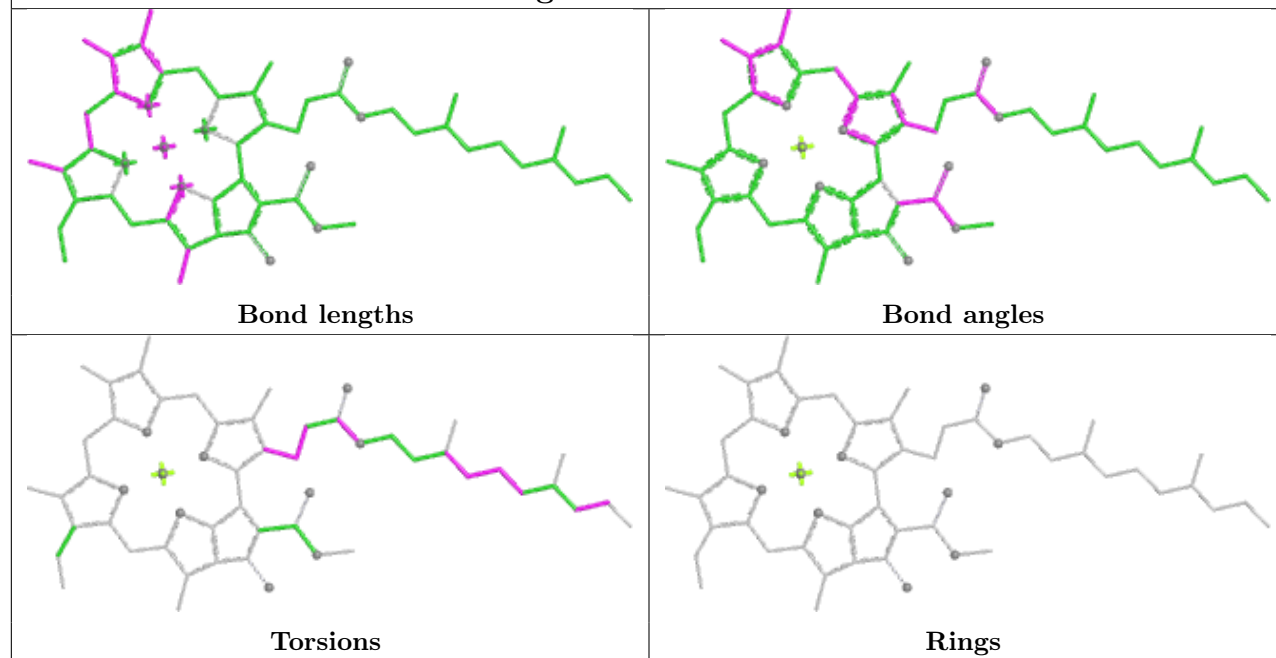
Bond angles

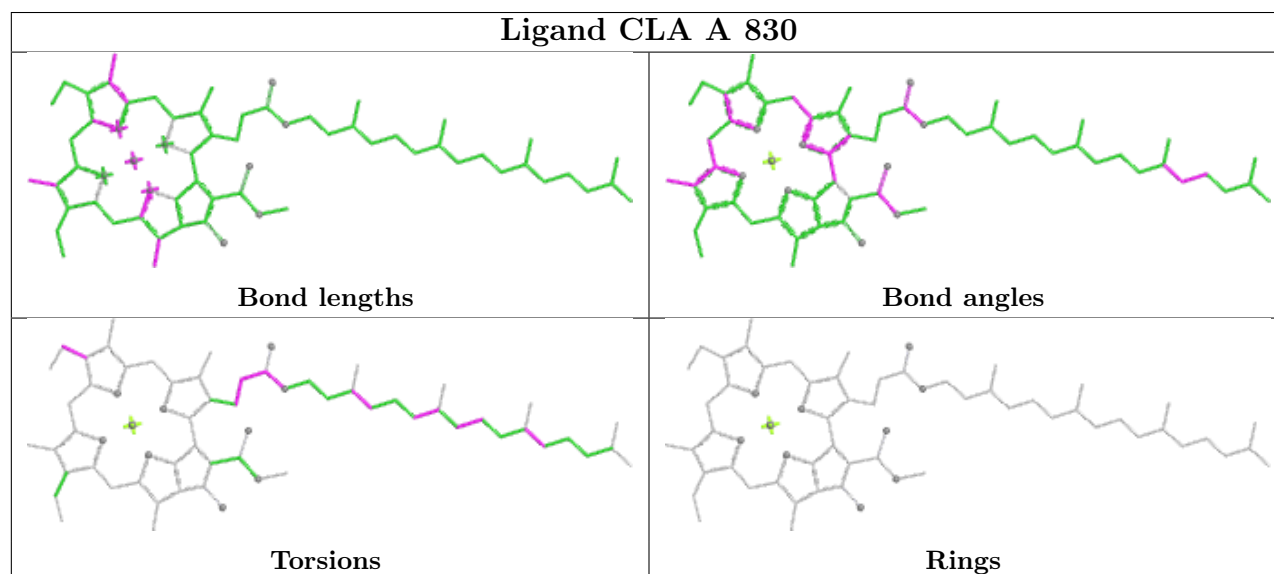
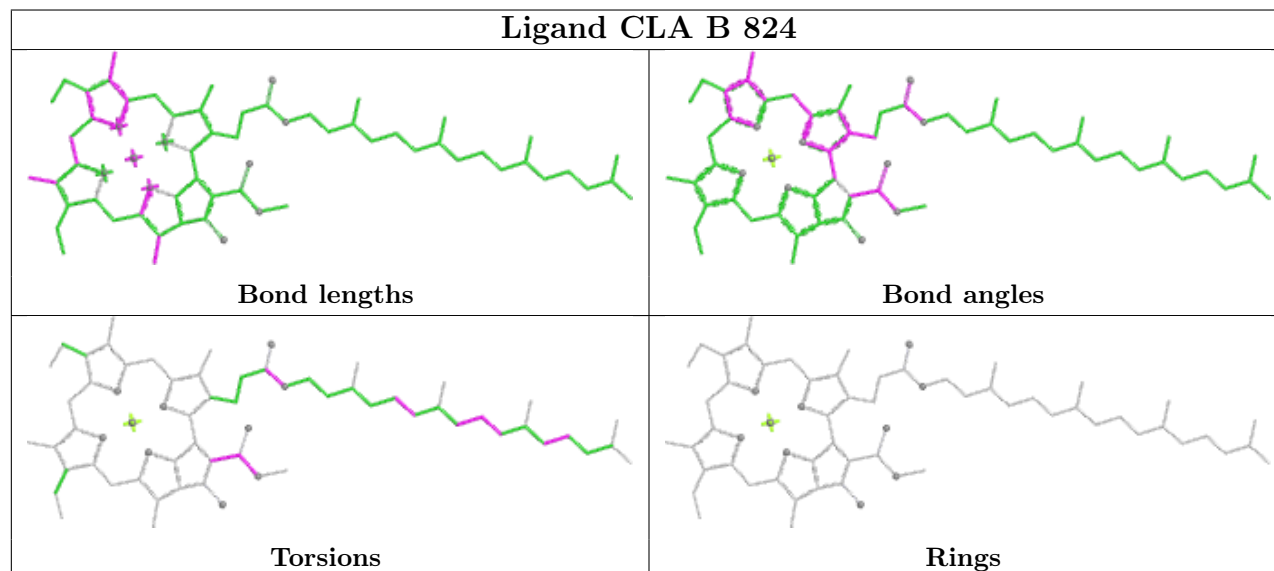
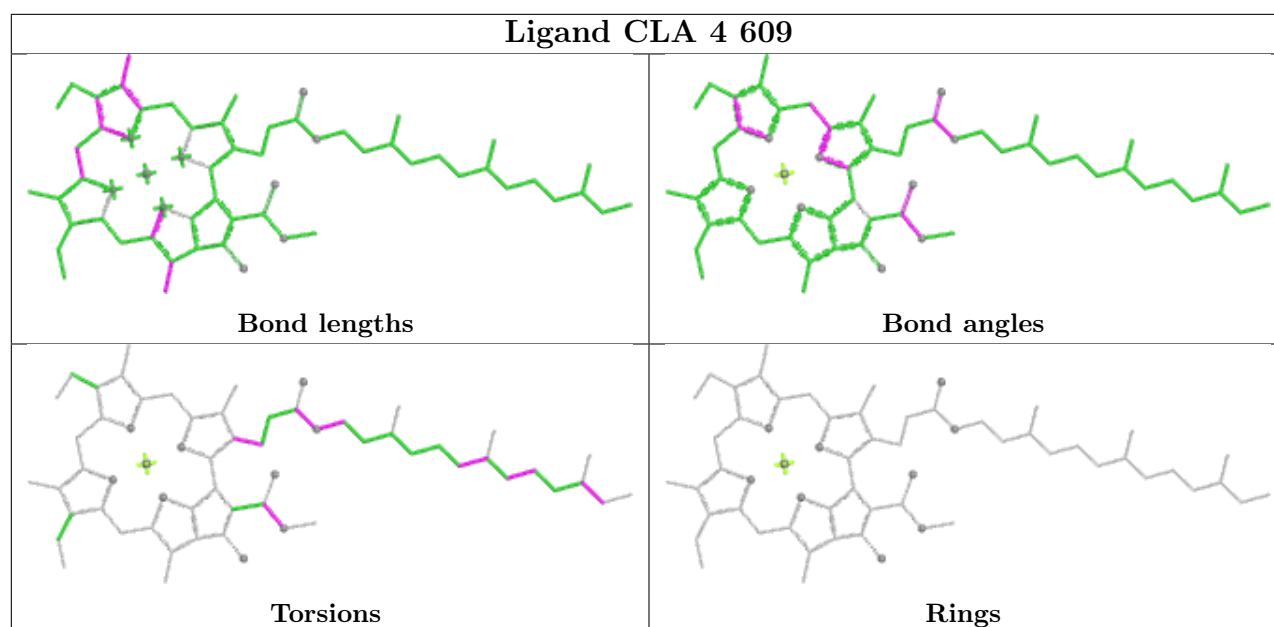


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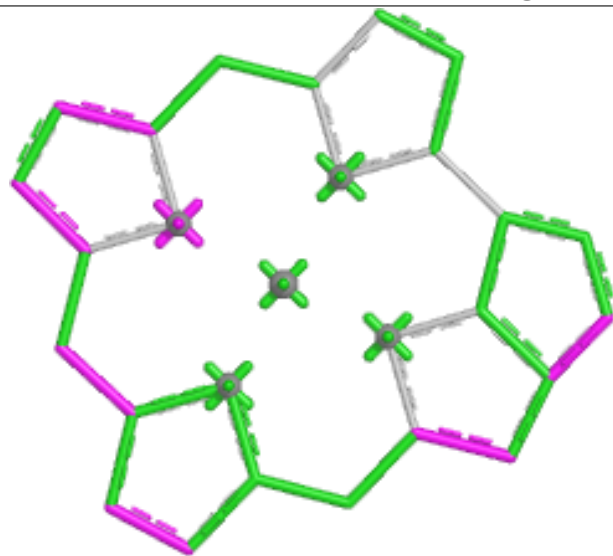


Rings

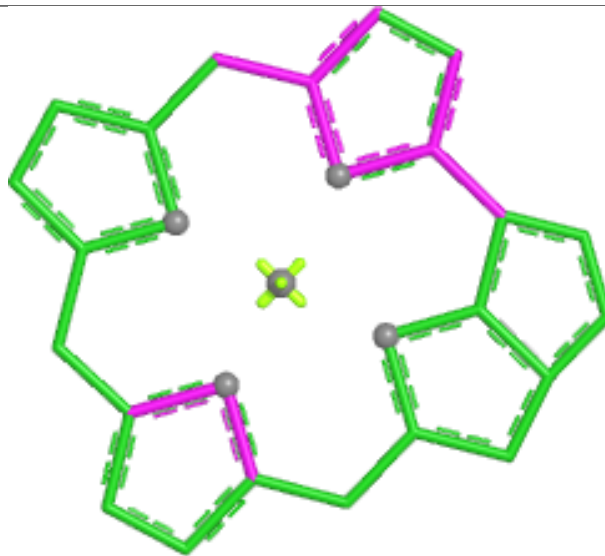
Ligand CLA 6 614**Ligand CLA 3 607**



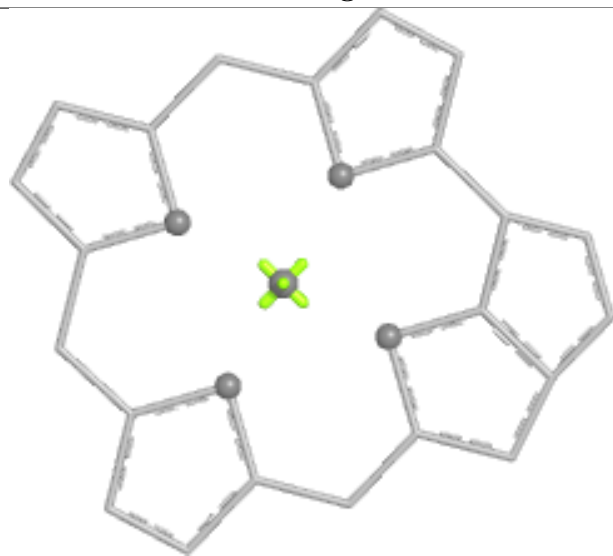
Ligand CLA 9 612



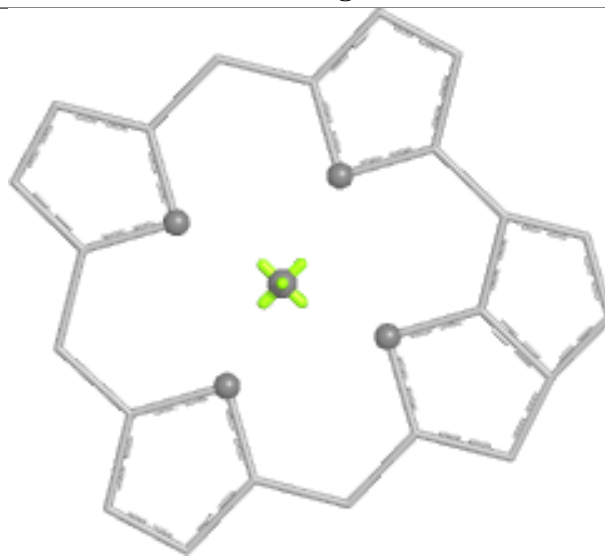
Bond lengths



Bond angles

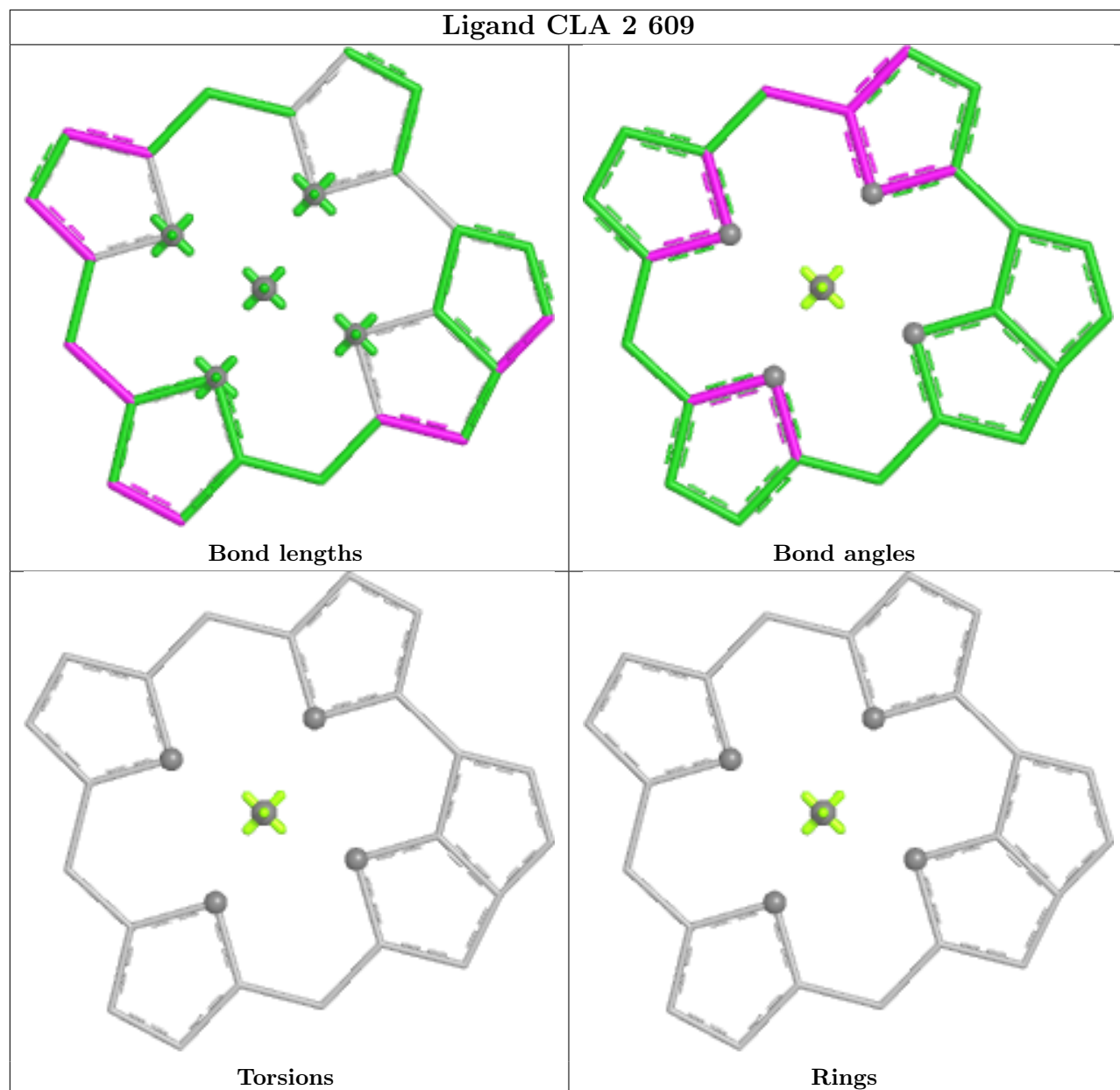


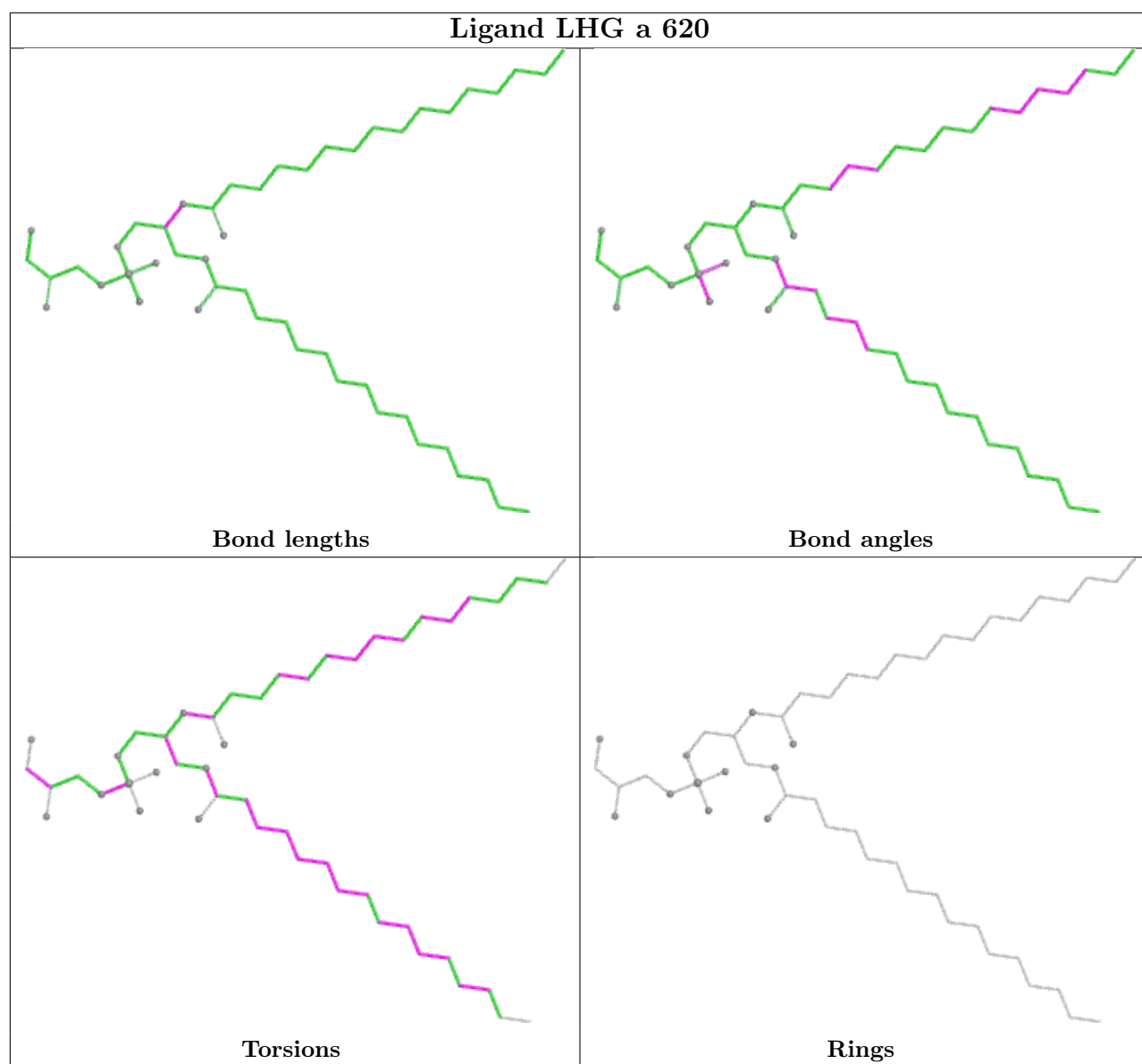
Torsions



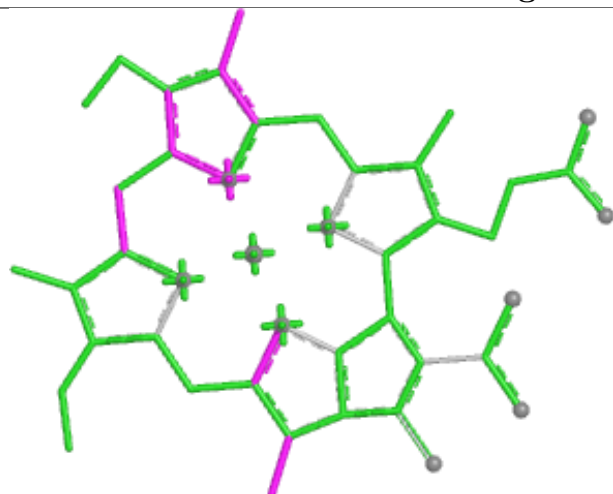
Rings

Ligand CLA 2 609

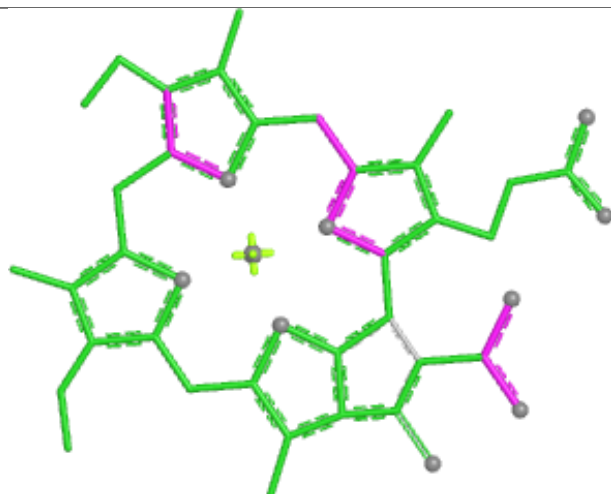




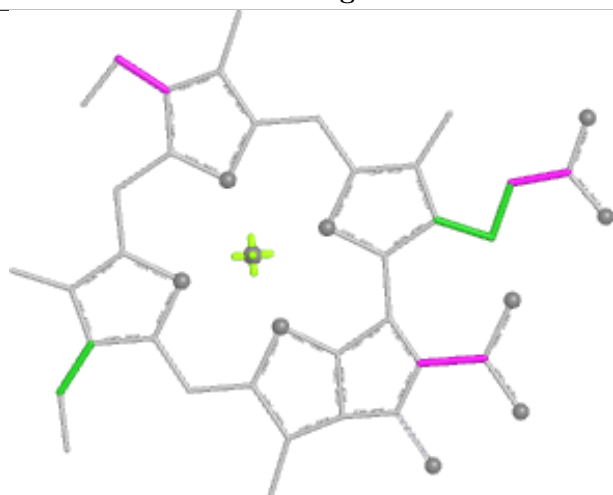
Ligand CLA 1 608



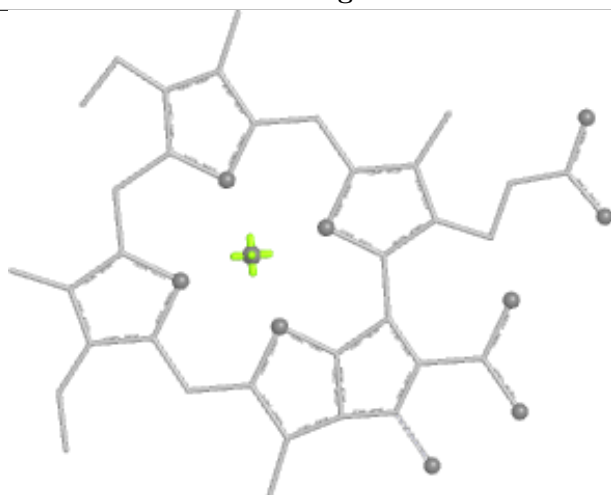
Bond lengths



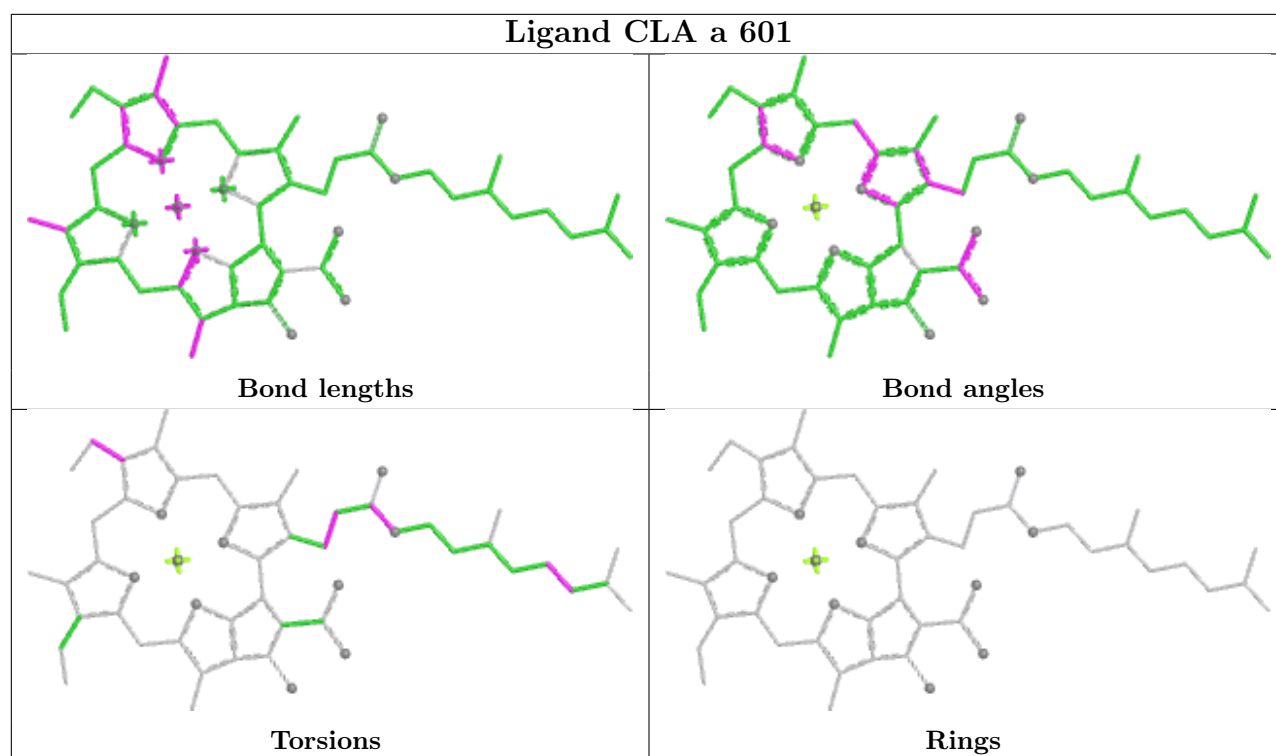
Bond angles



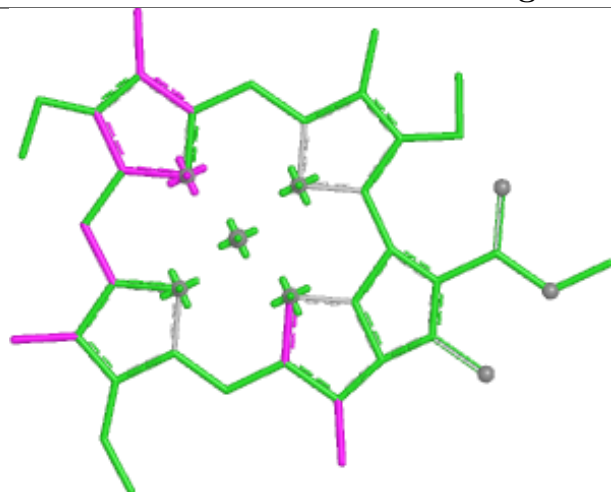
Torsions



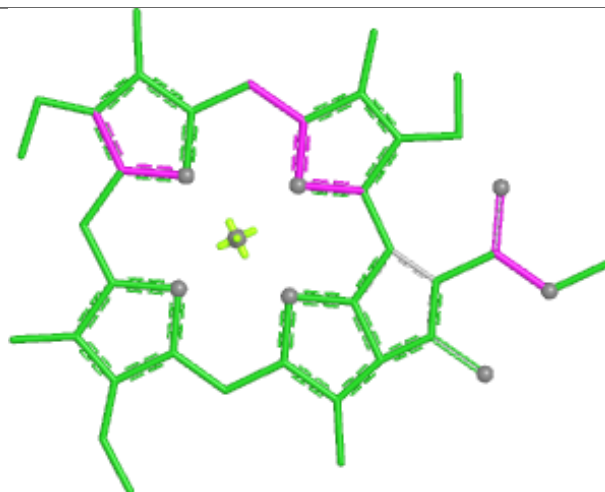
Rings



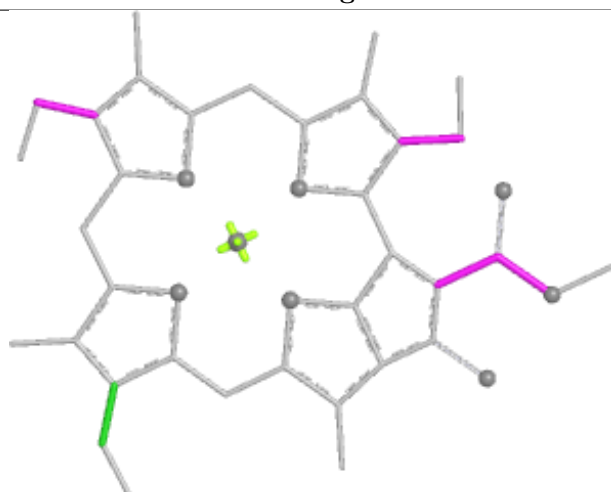
Ligand CLA 4 611



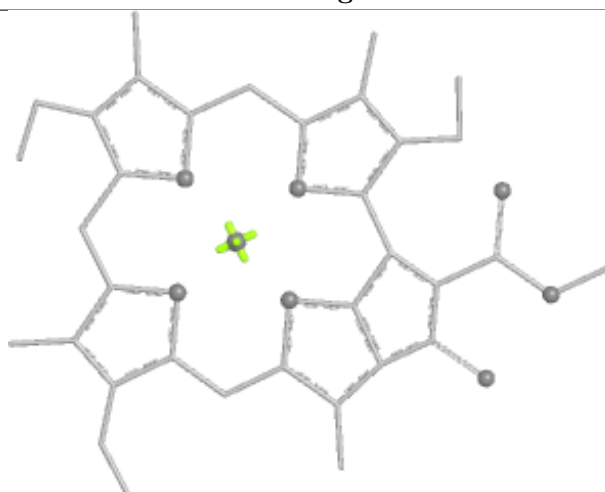
Bond lengths



Bond angles

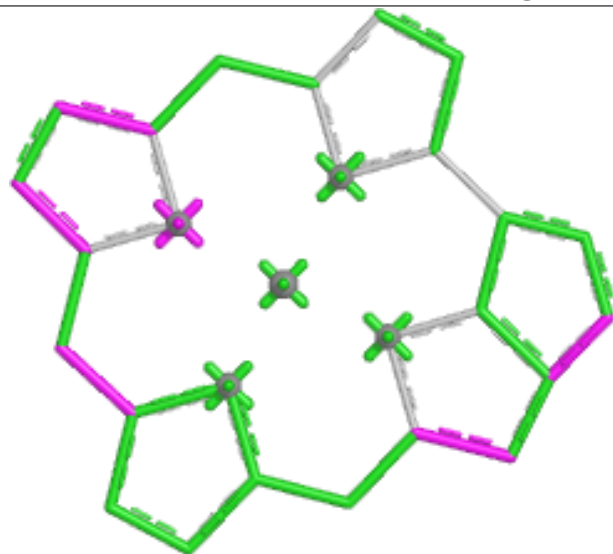


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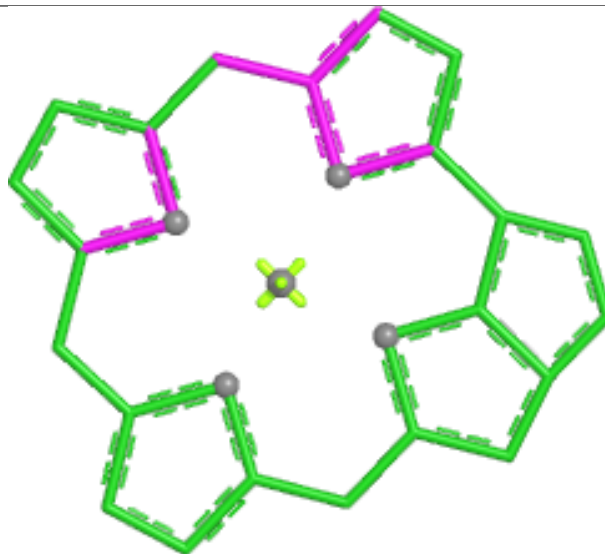


Rings

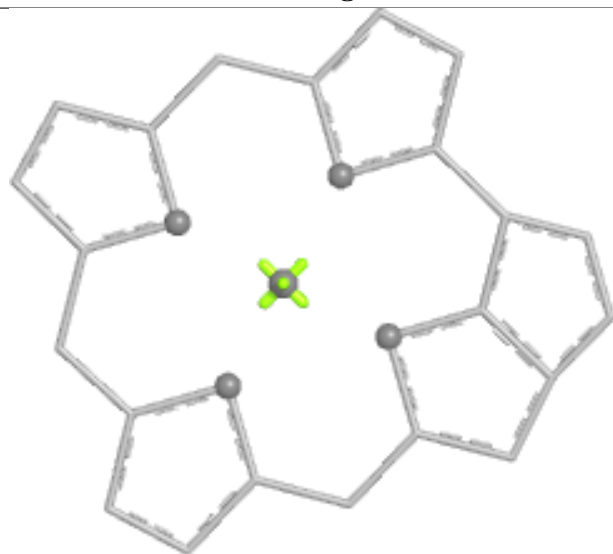
Ligand CLA 9 613



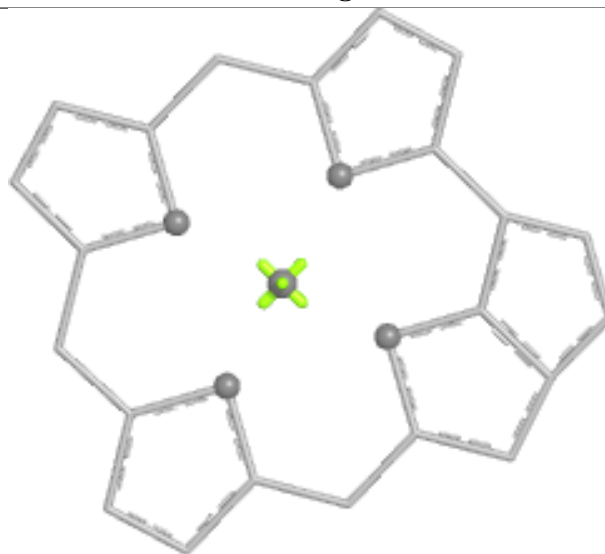
Bond lengths



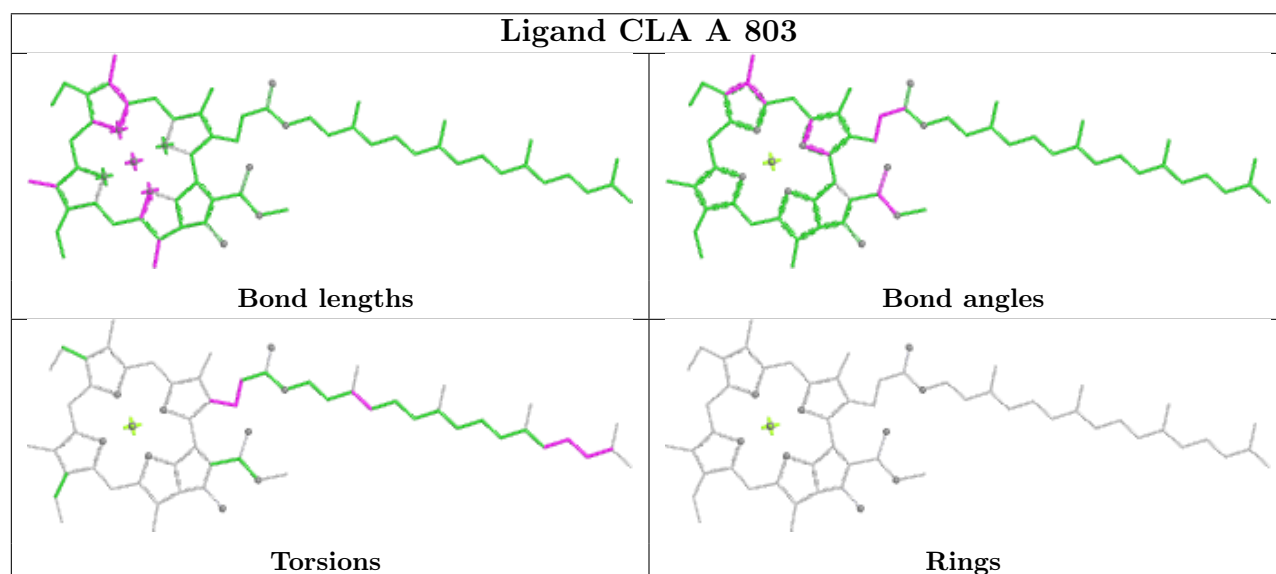
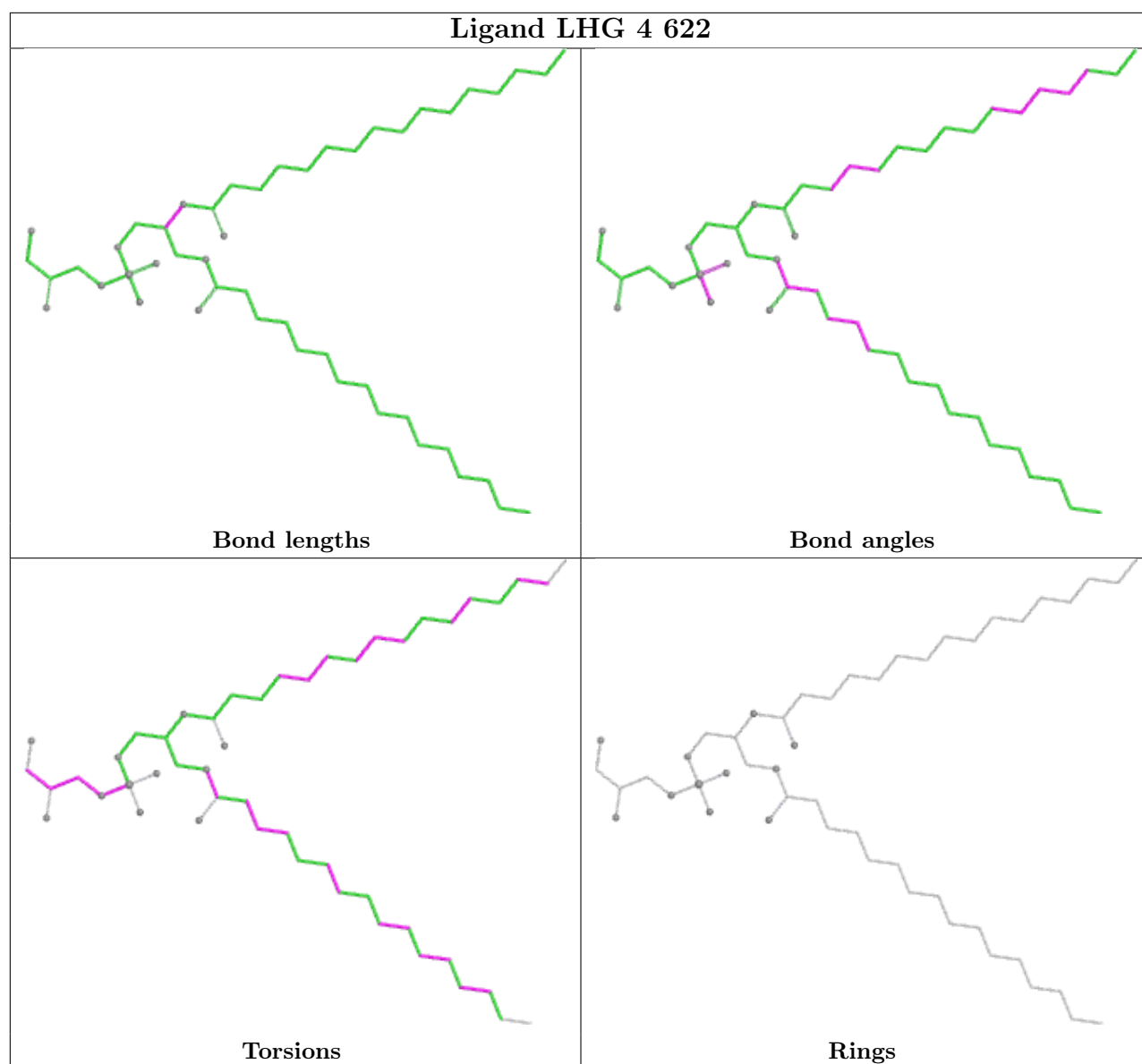
Bond angles

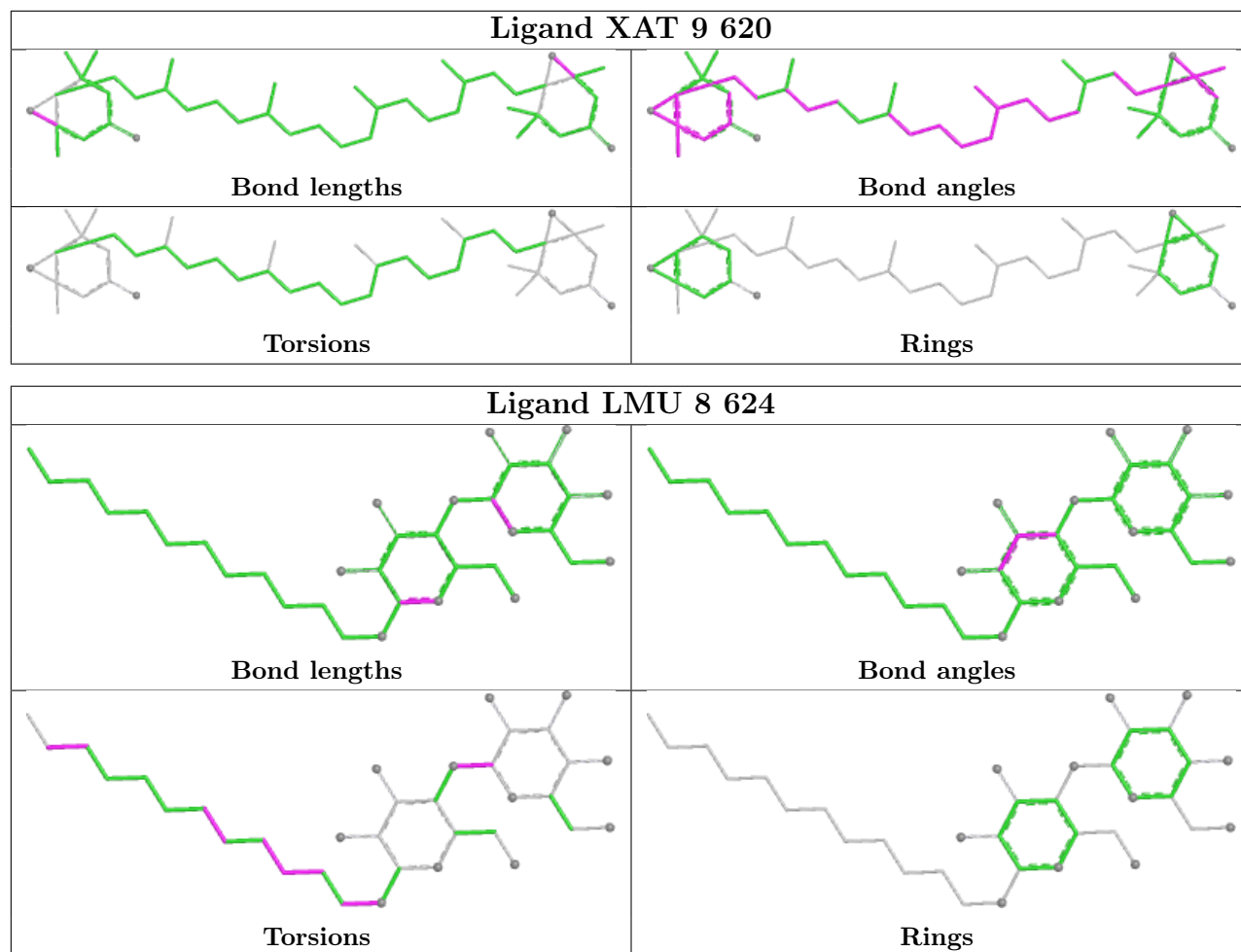


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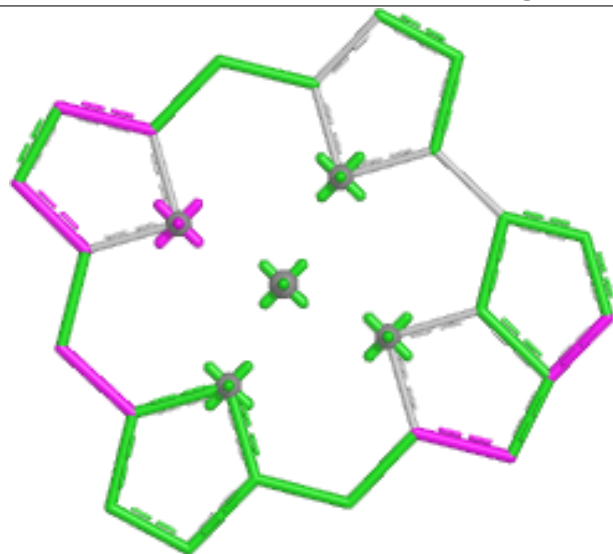


Rings

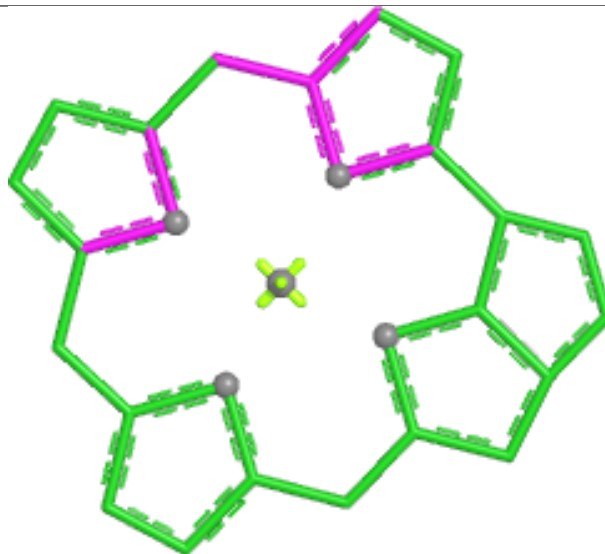




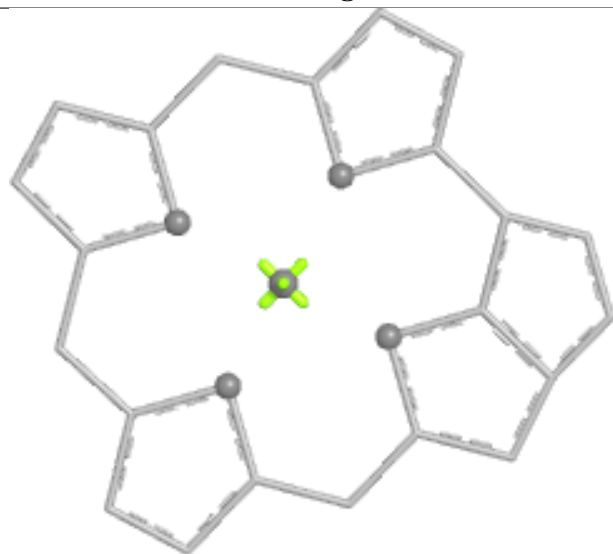
Ligand CLA 9 606



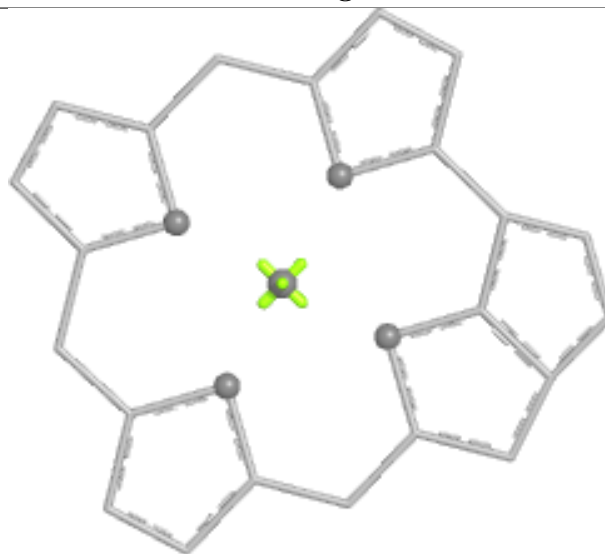
Bond lengths



Bond angles

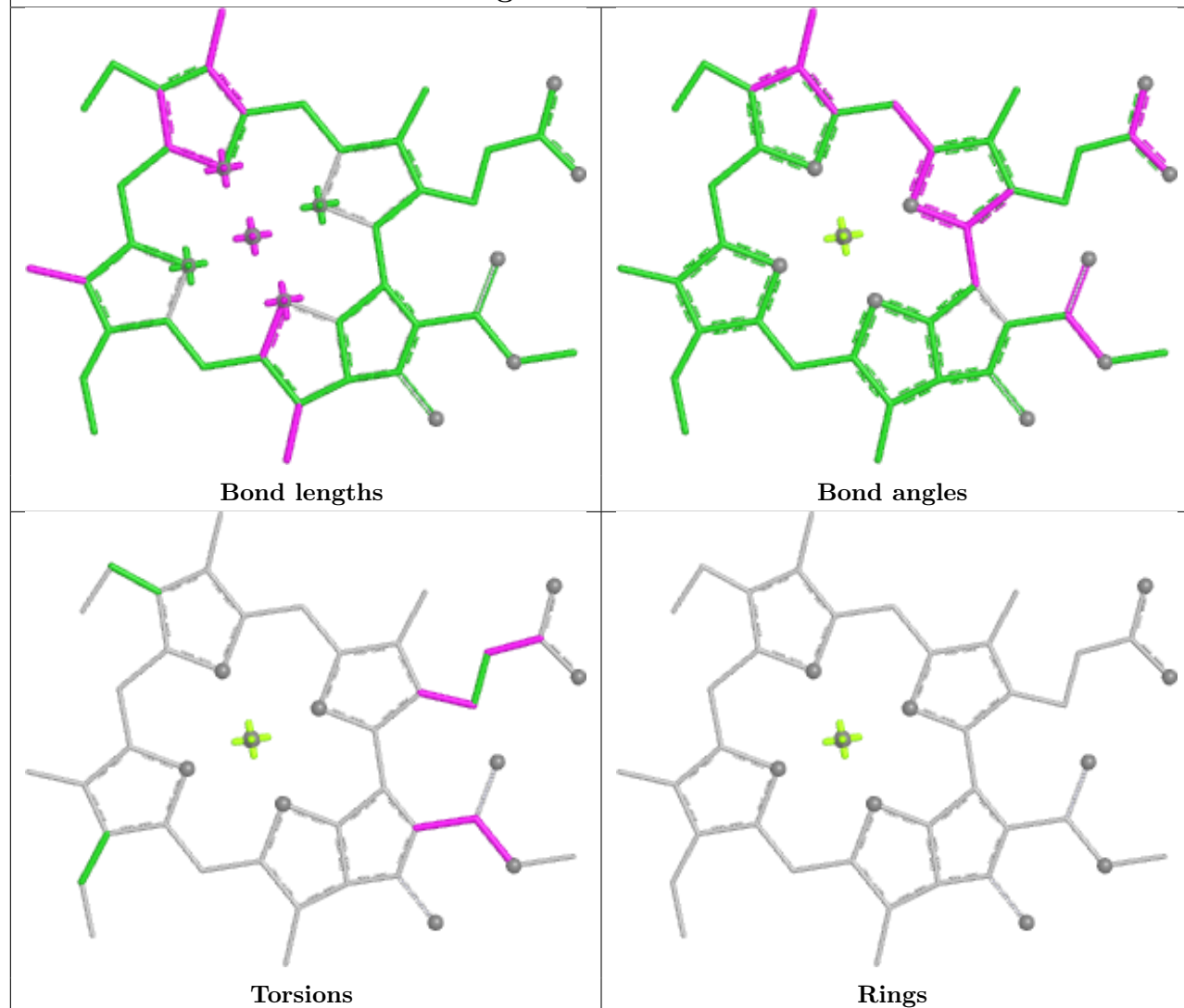


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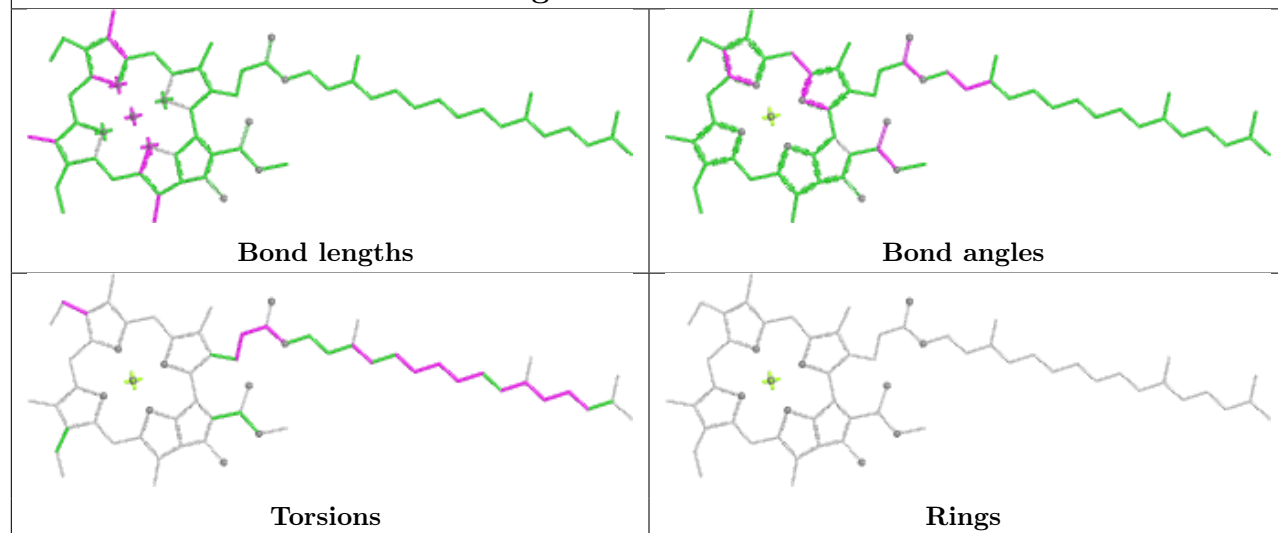


Rings

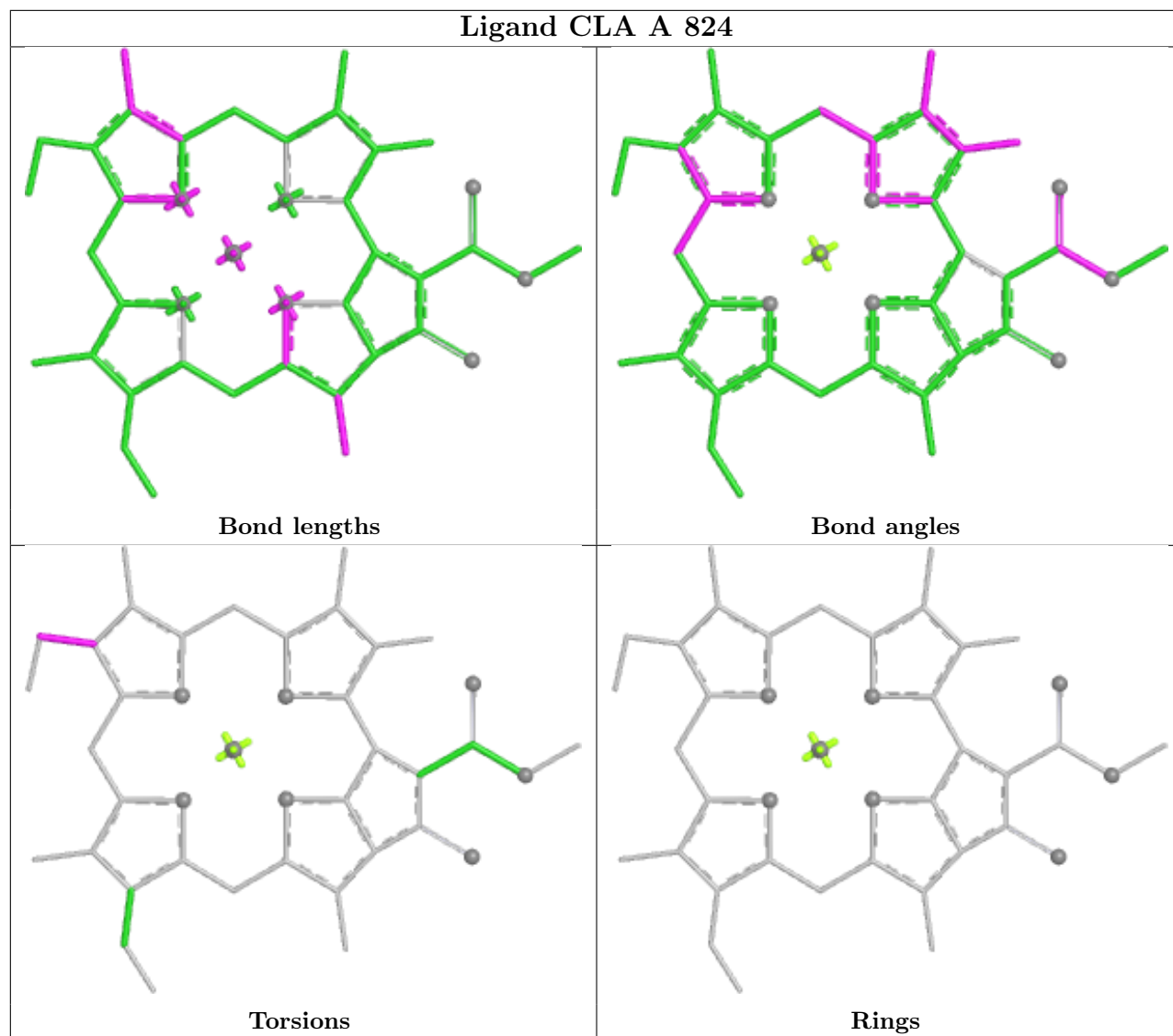
Ligand CLA a 612



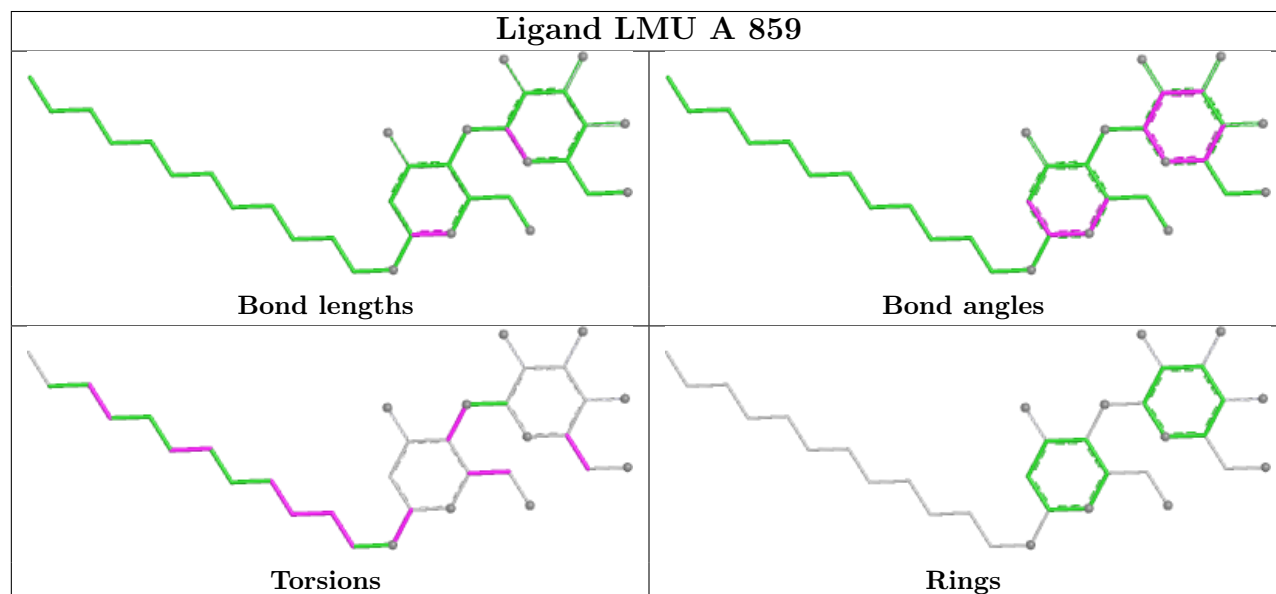
Ligand CLA A 843

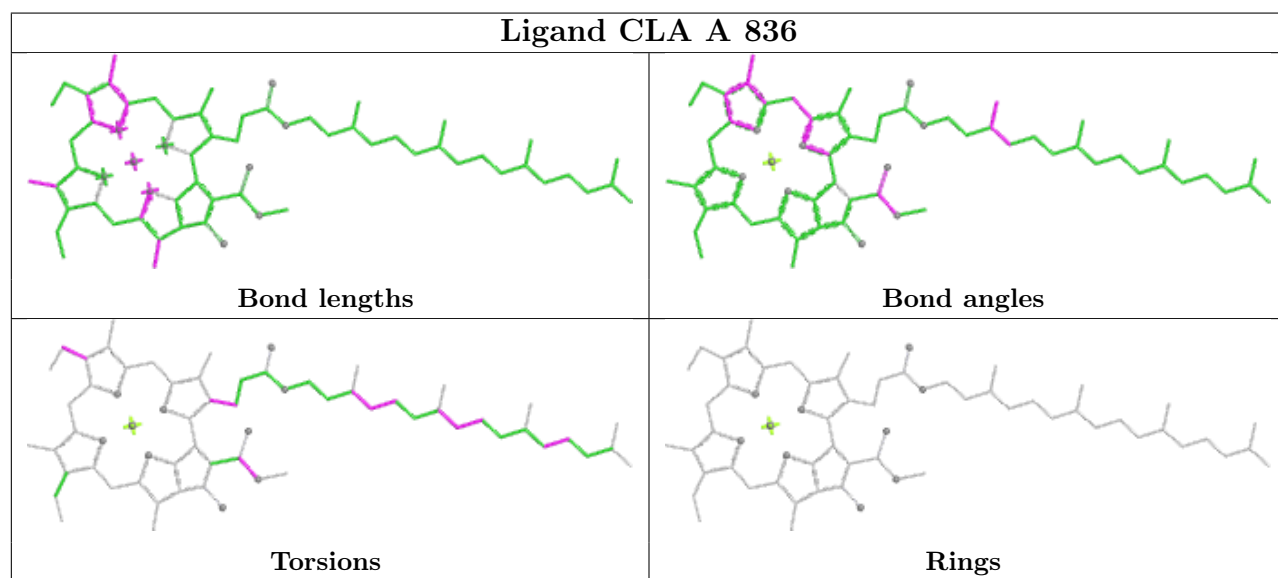
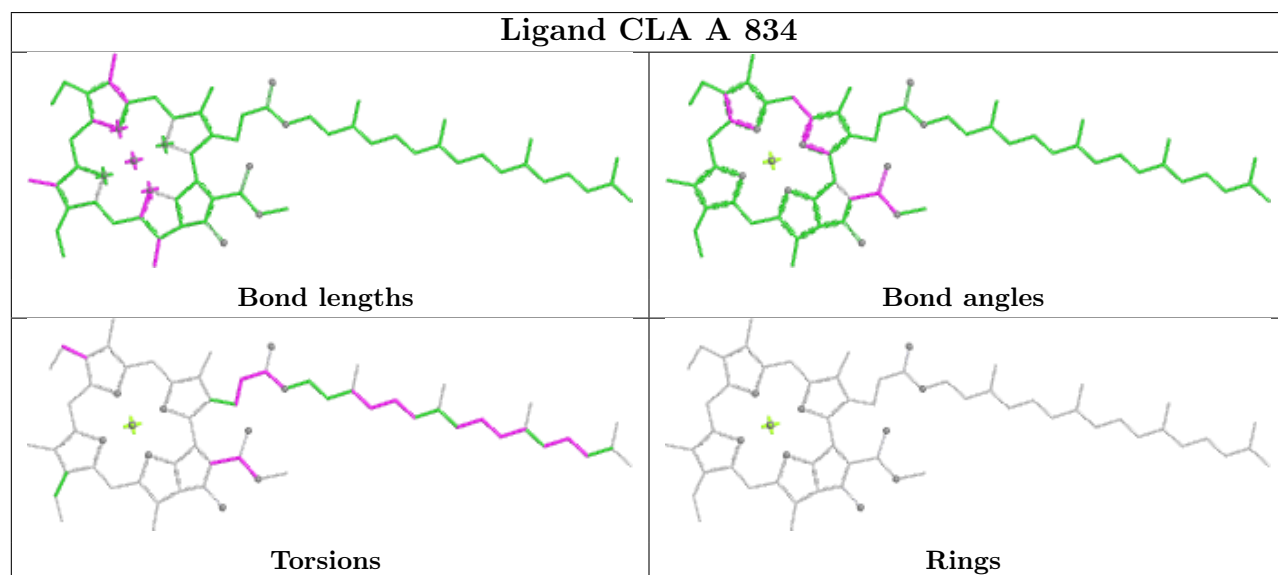
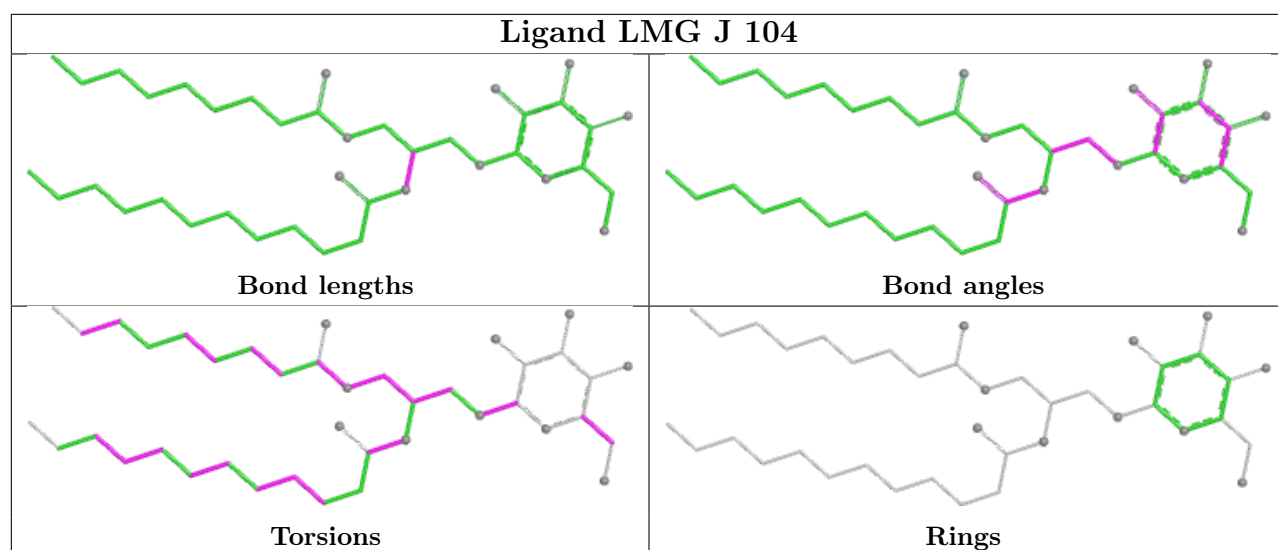


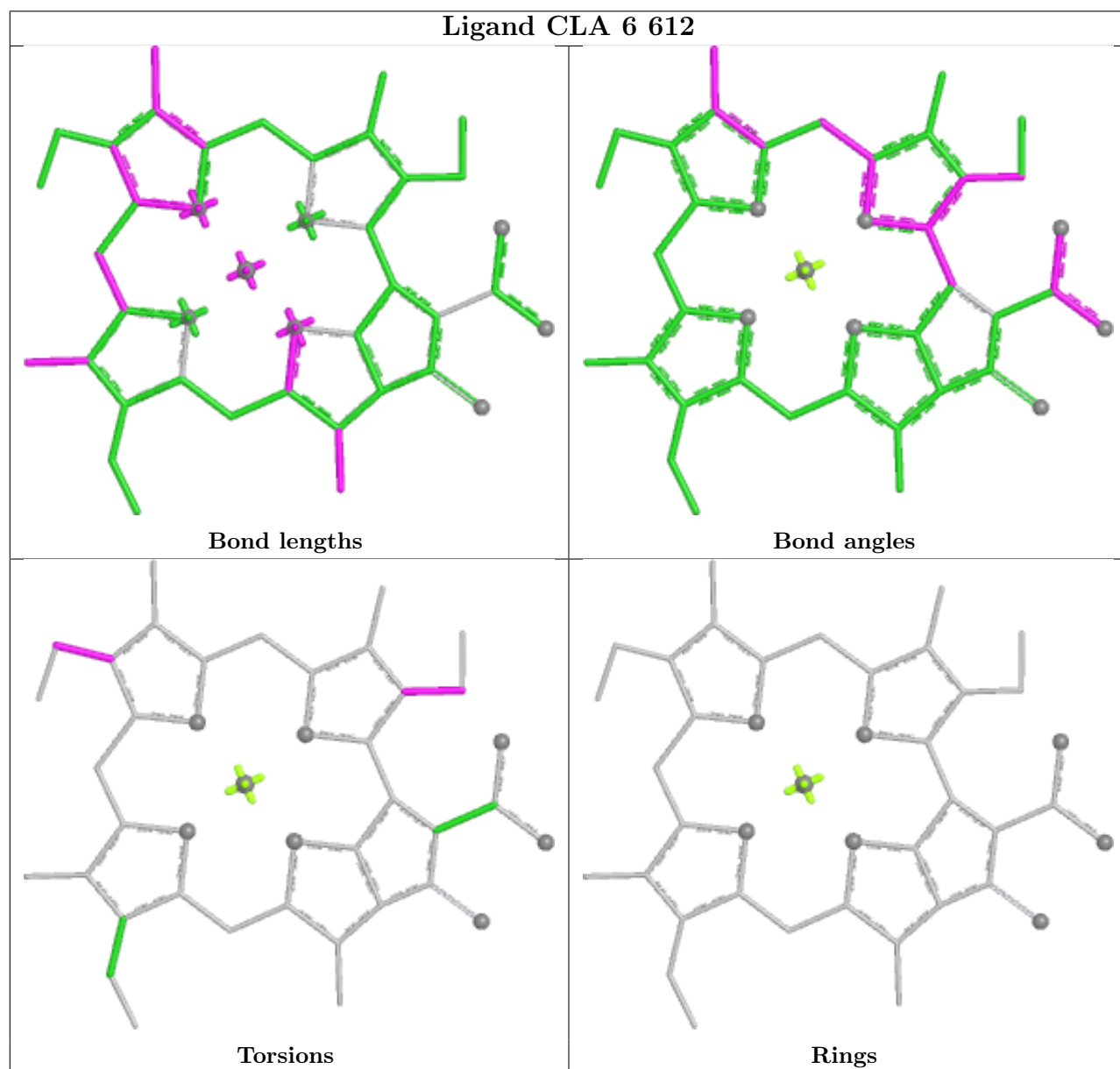
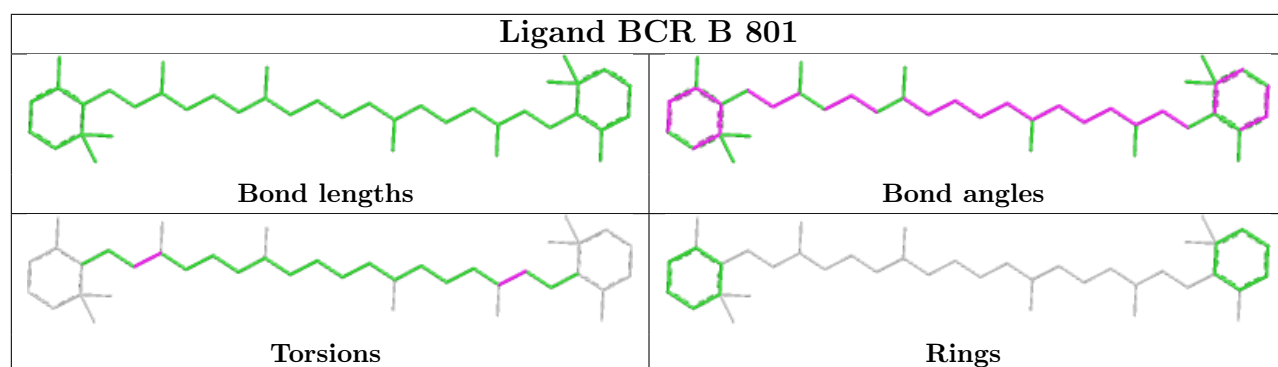
Ligand CLA A 824



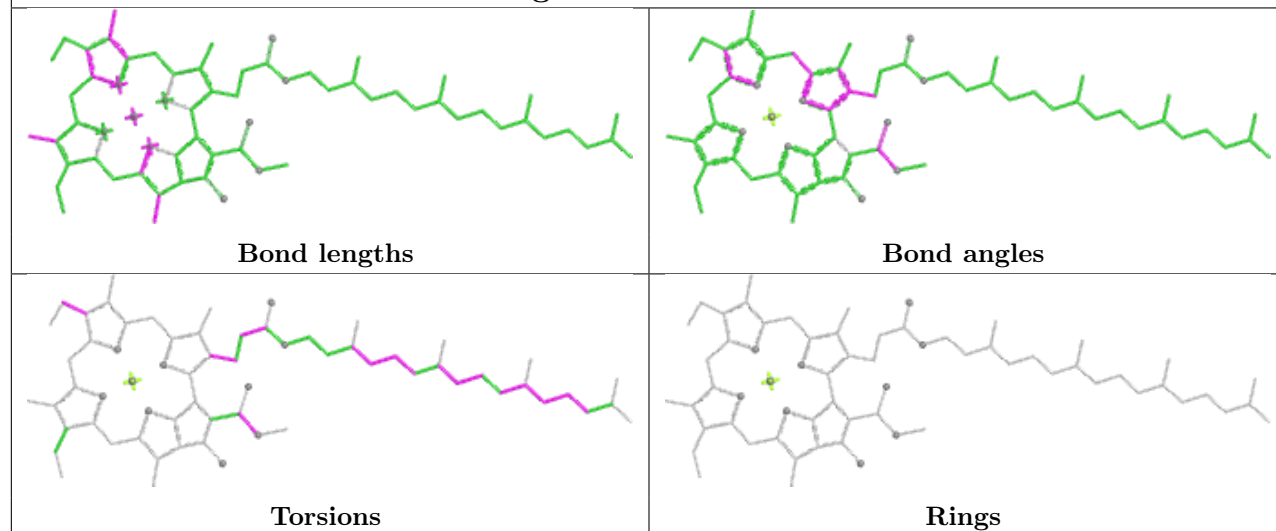
Ligand LMU A 859



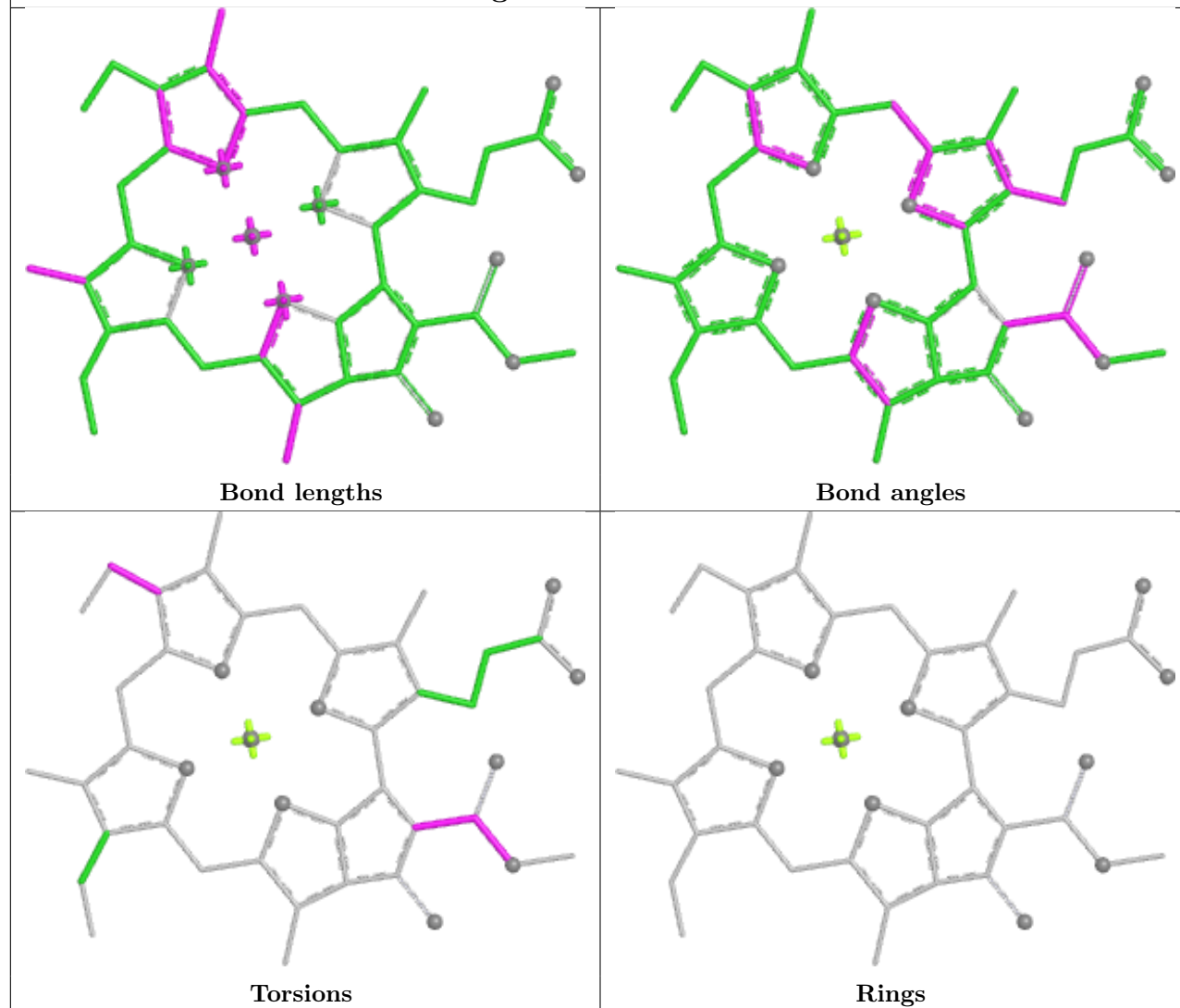




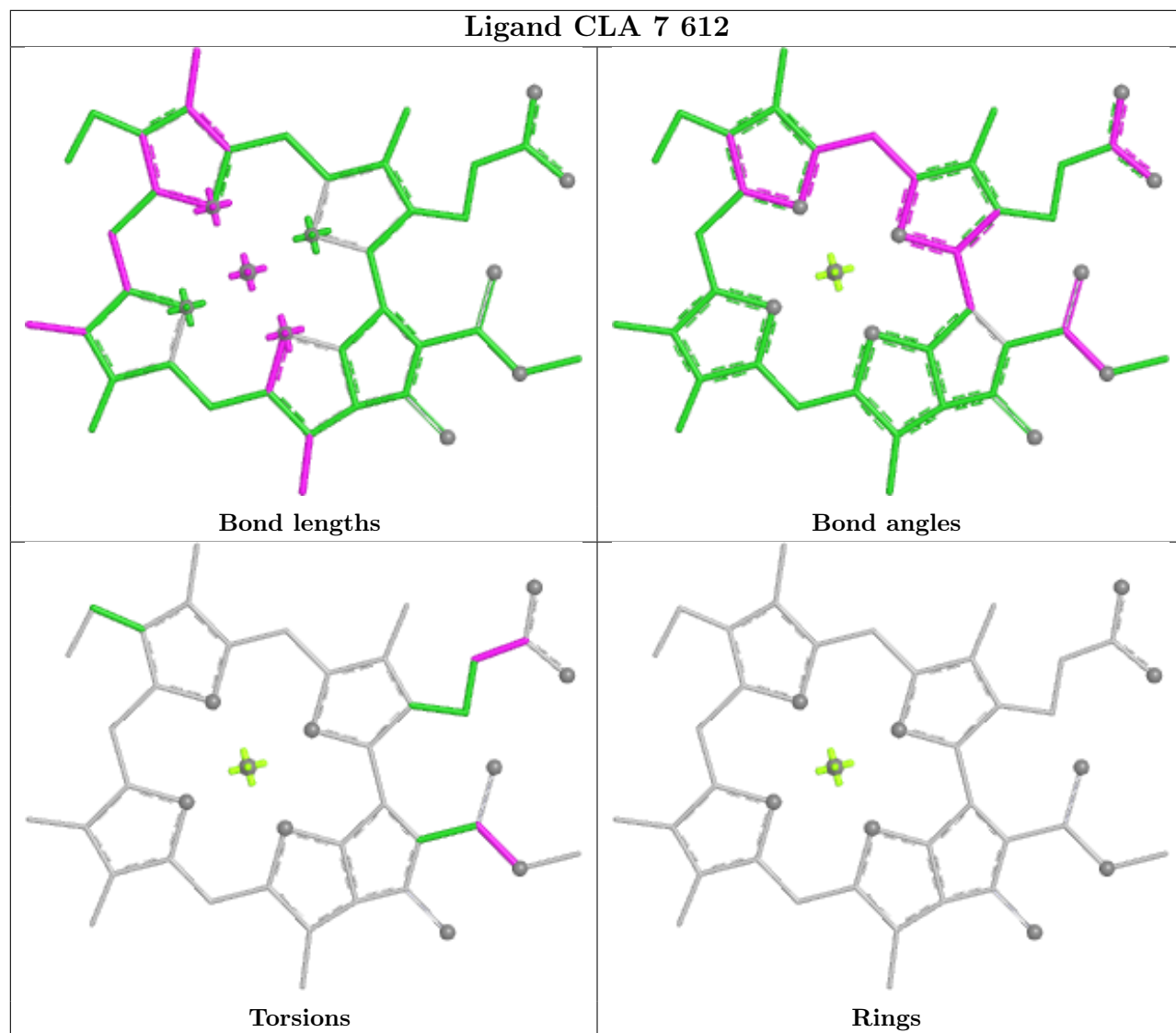
Ligand CLA B 833

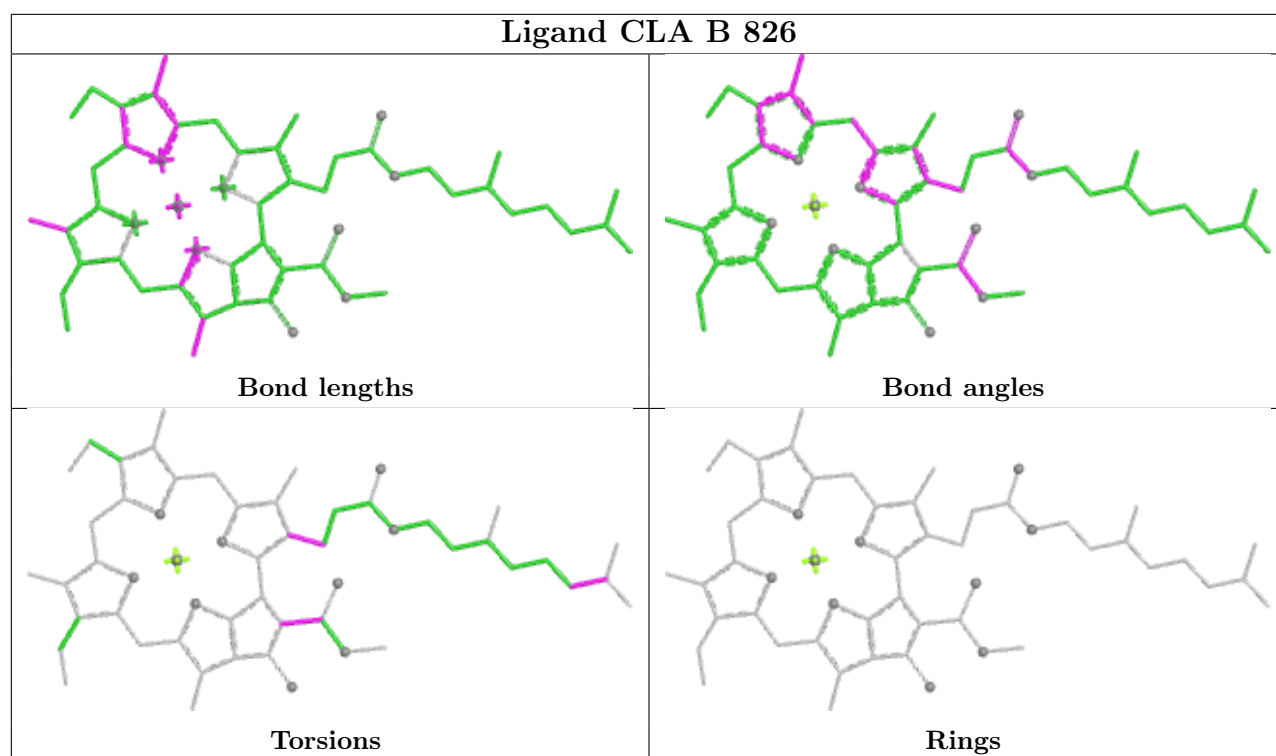


Ligand CLA A 817

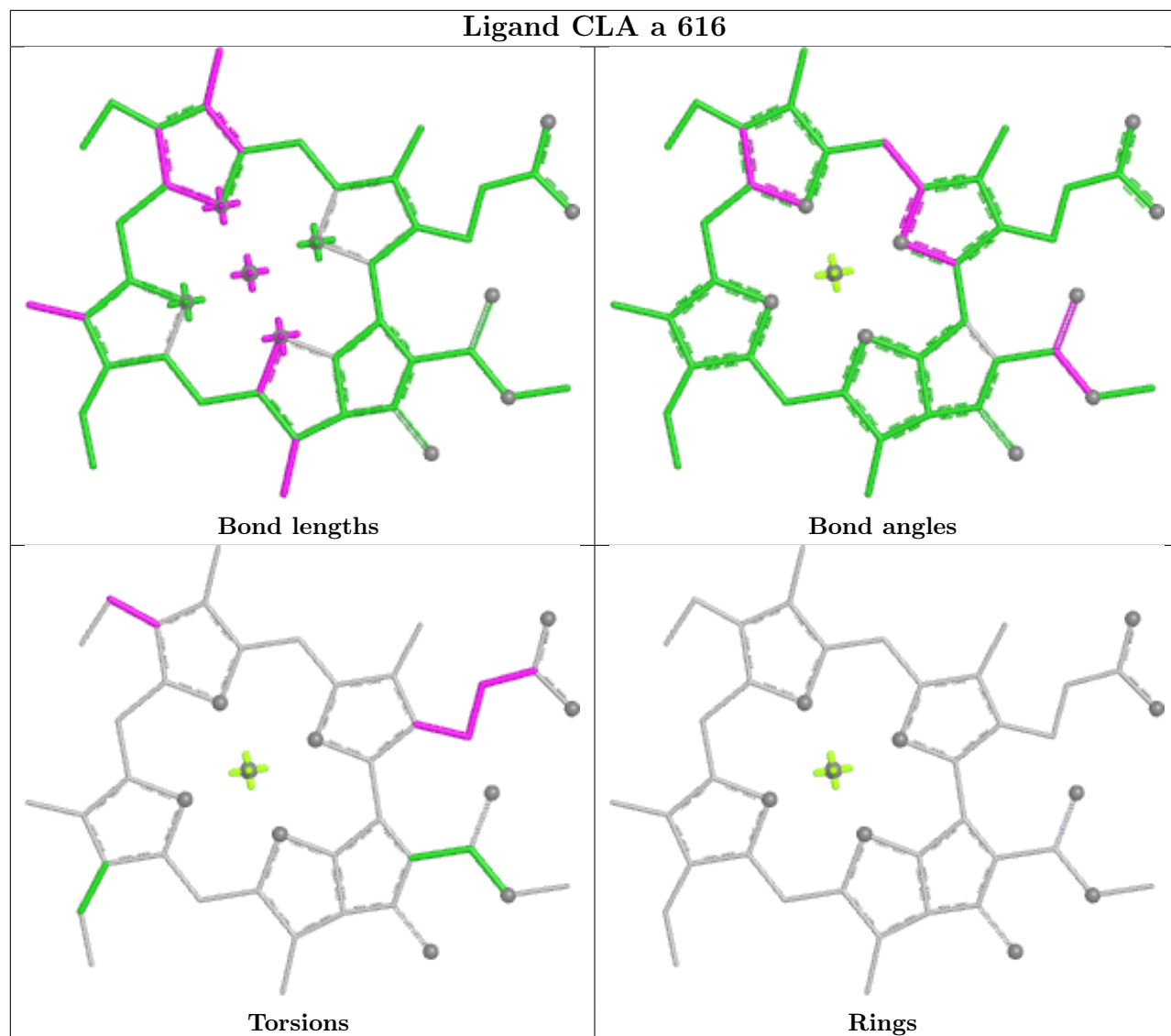


Ligand CLA 7 612

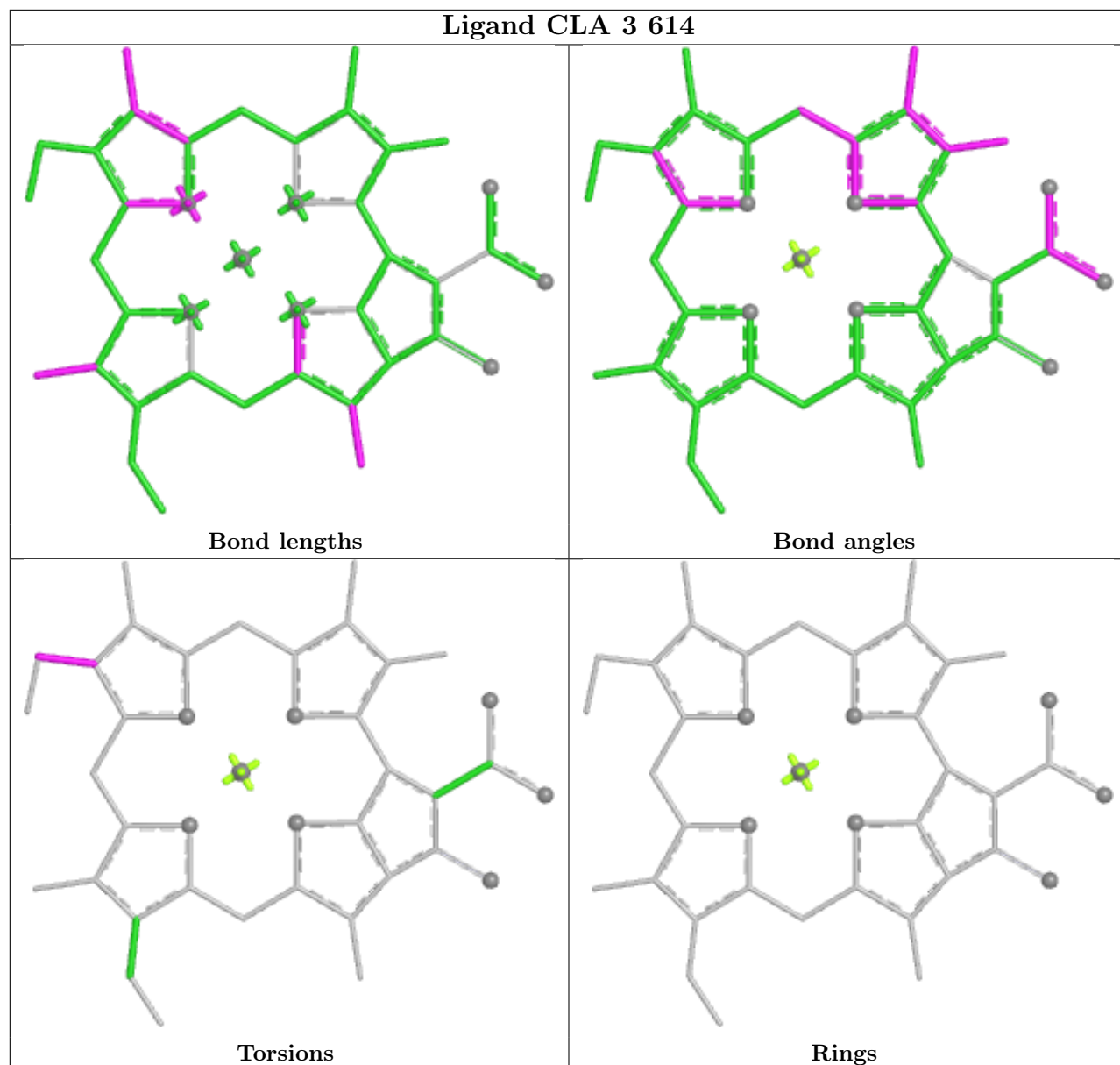




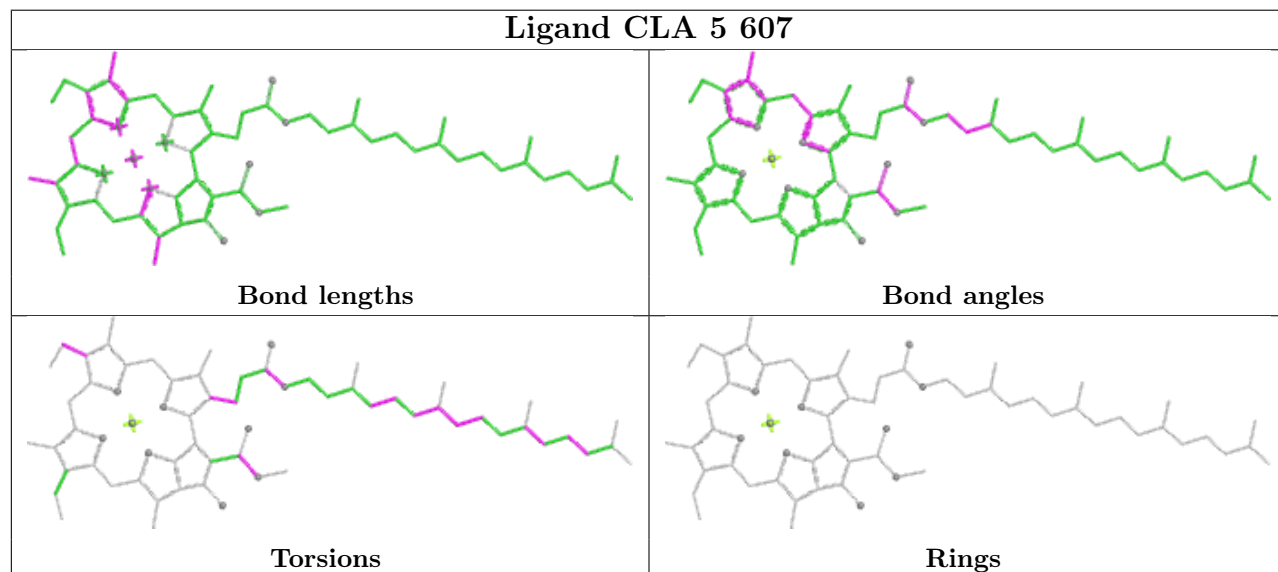
Ligand CLA a 616



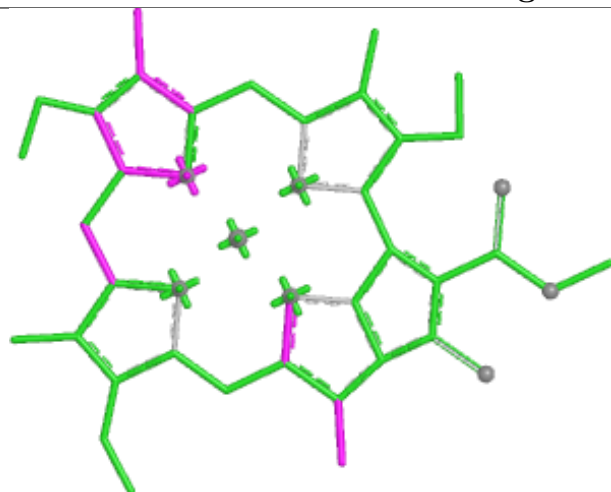
Ligand CLA 3 614



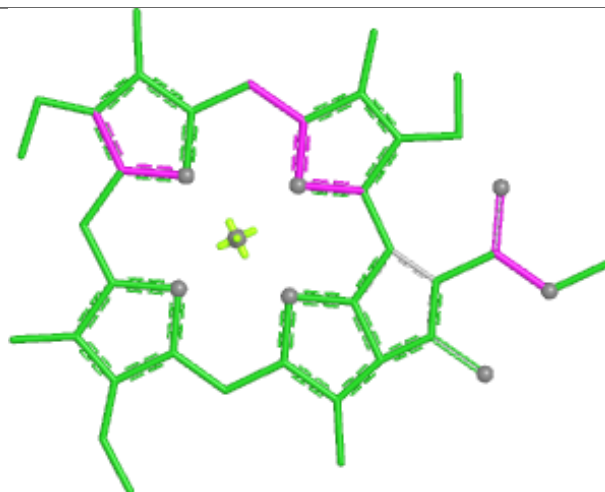
Ligand CLA 5 607



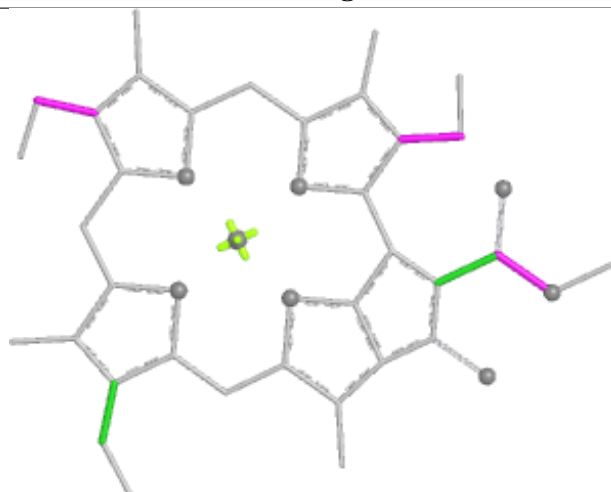
Ligand CLA J 101



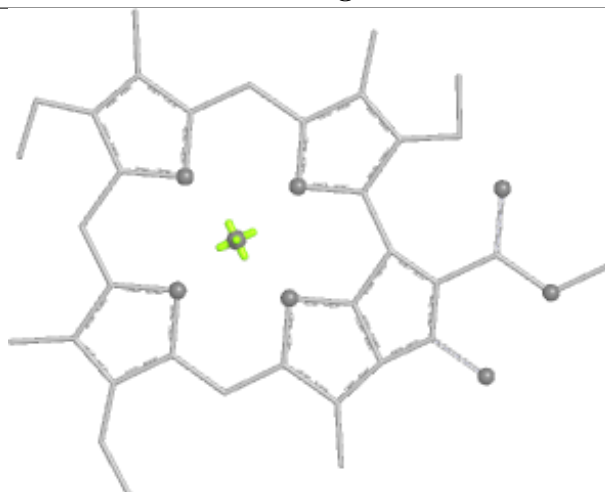
Bond lengths



Bond angles

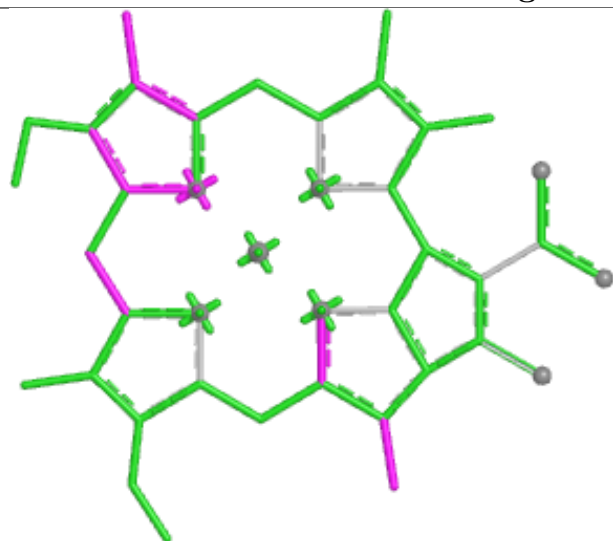


Torsions

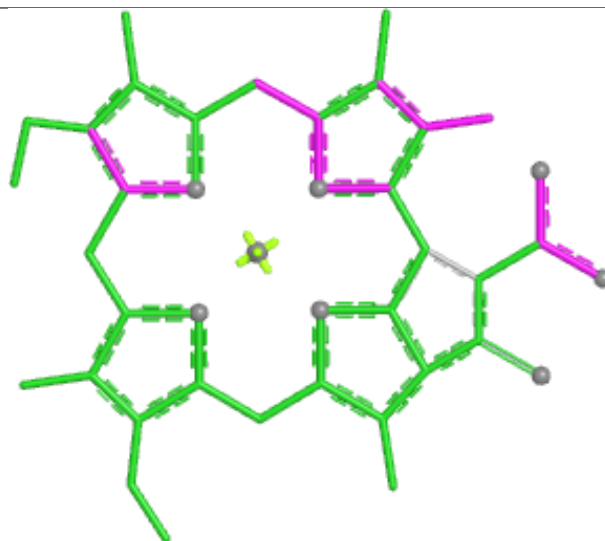


Rings

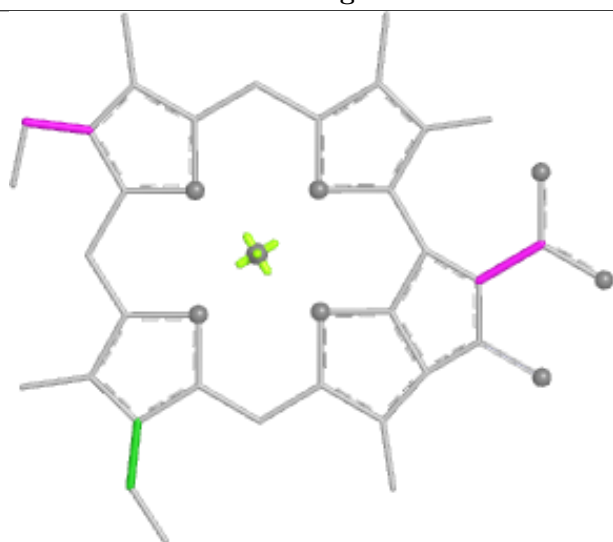
Ligand CLA 1 607



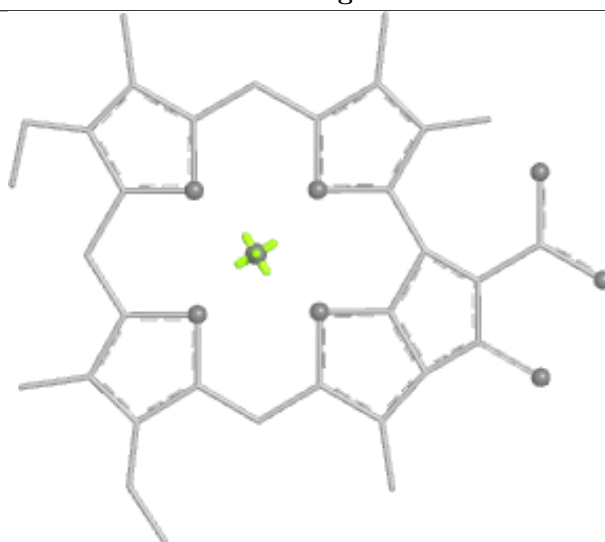
Bond lengths



Bond angles

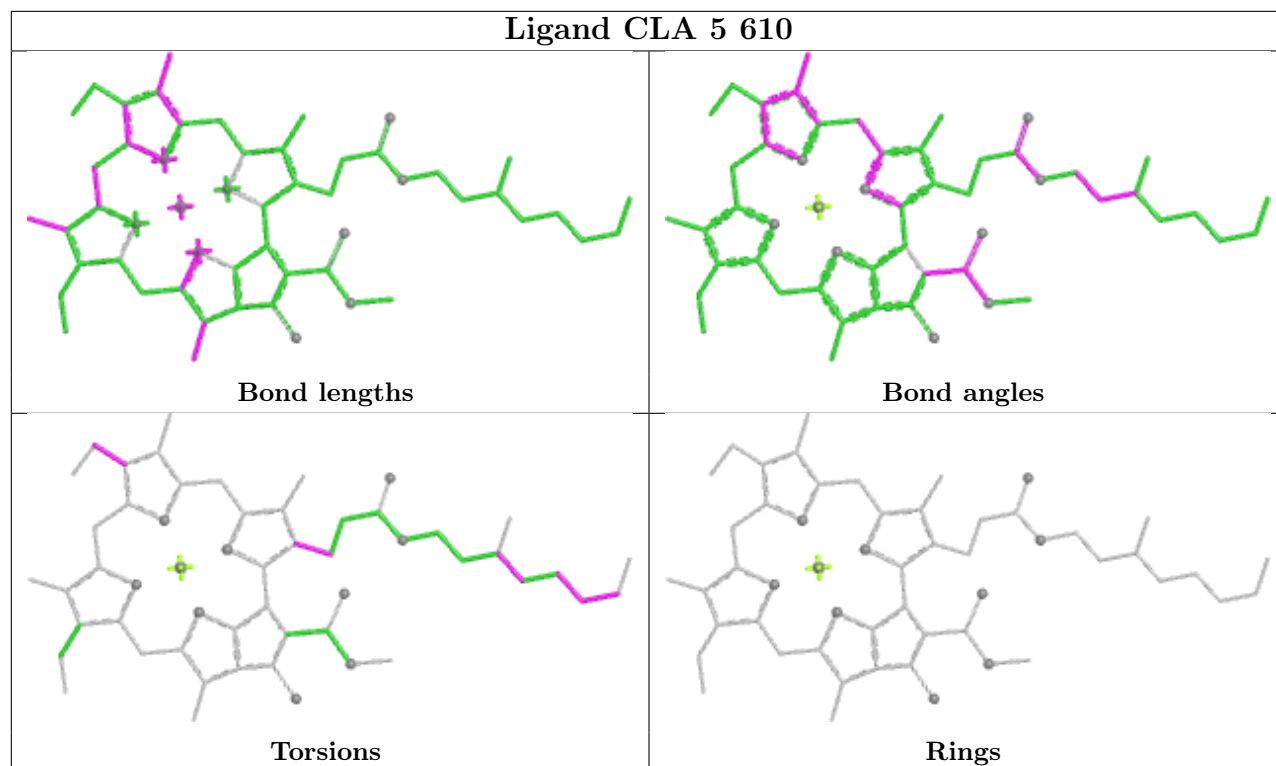


Torsions

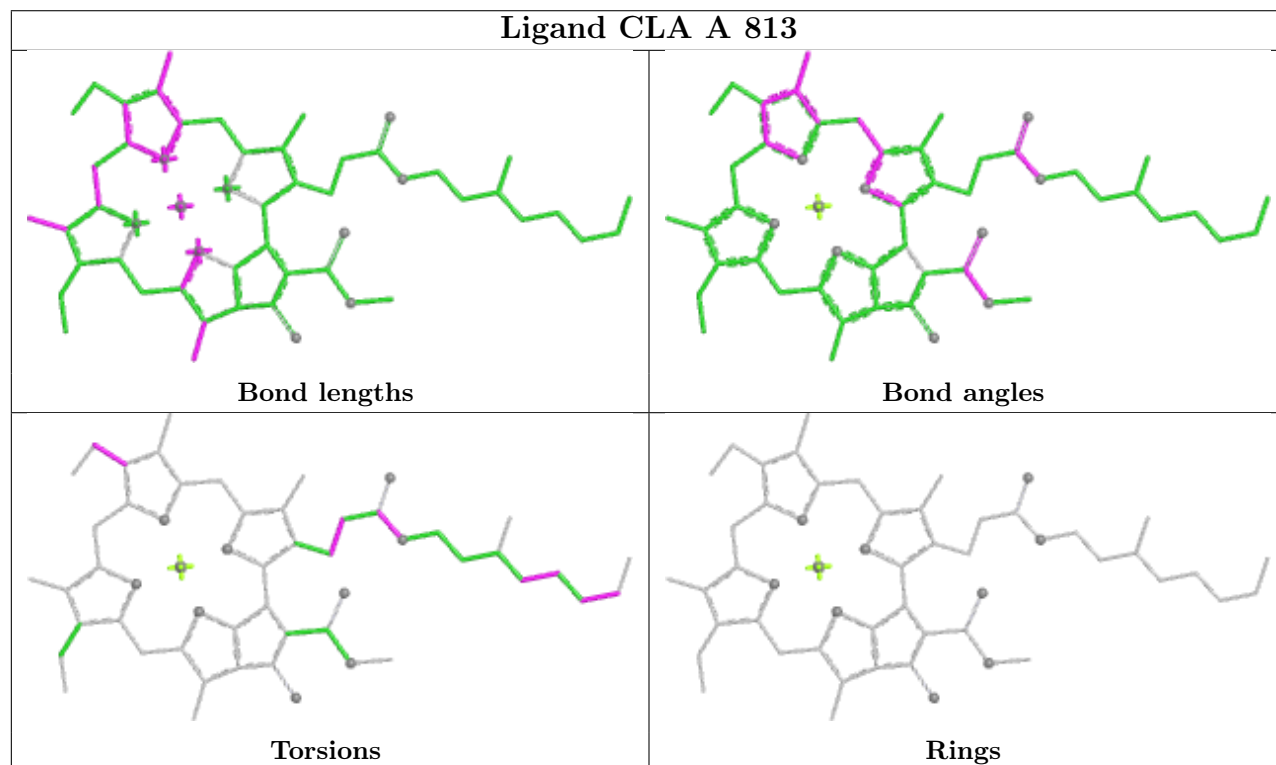


Rings

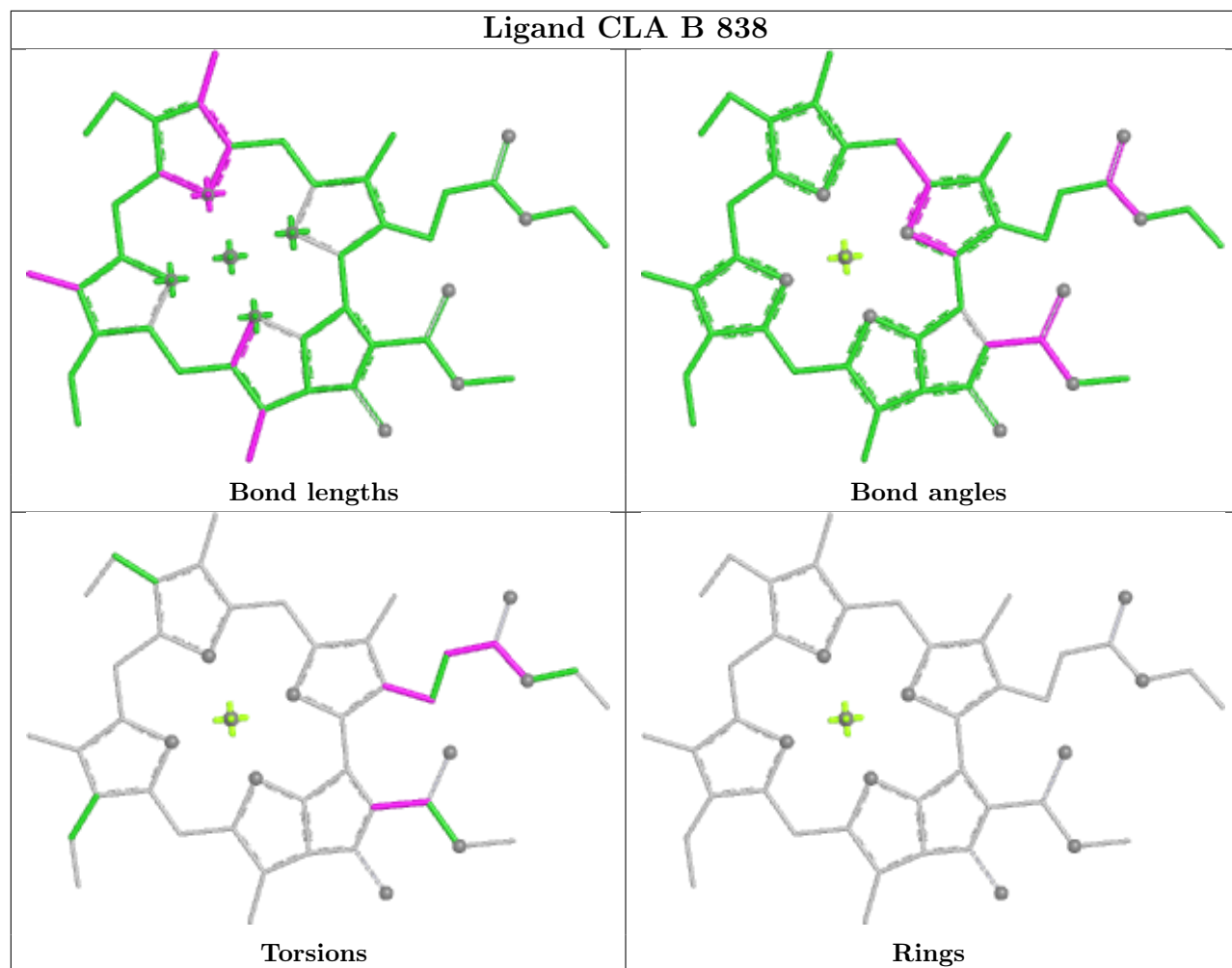
Ligand CLA 5 610



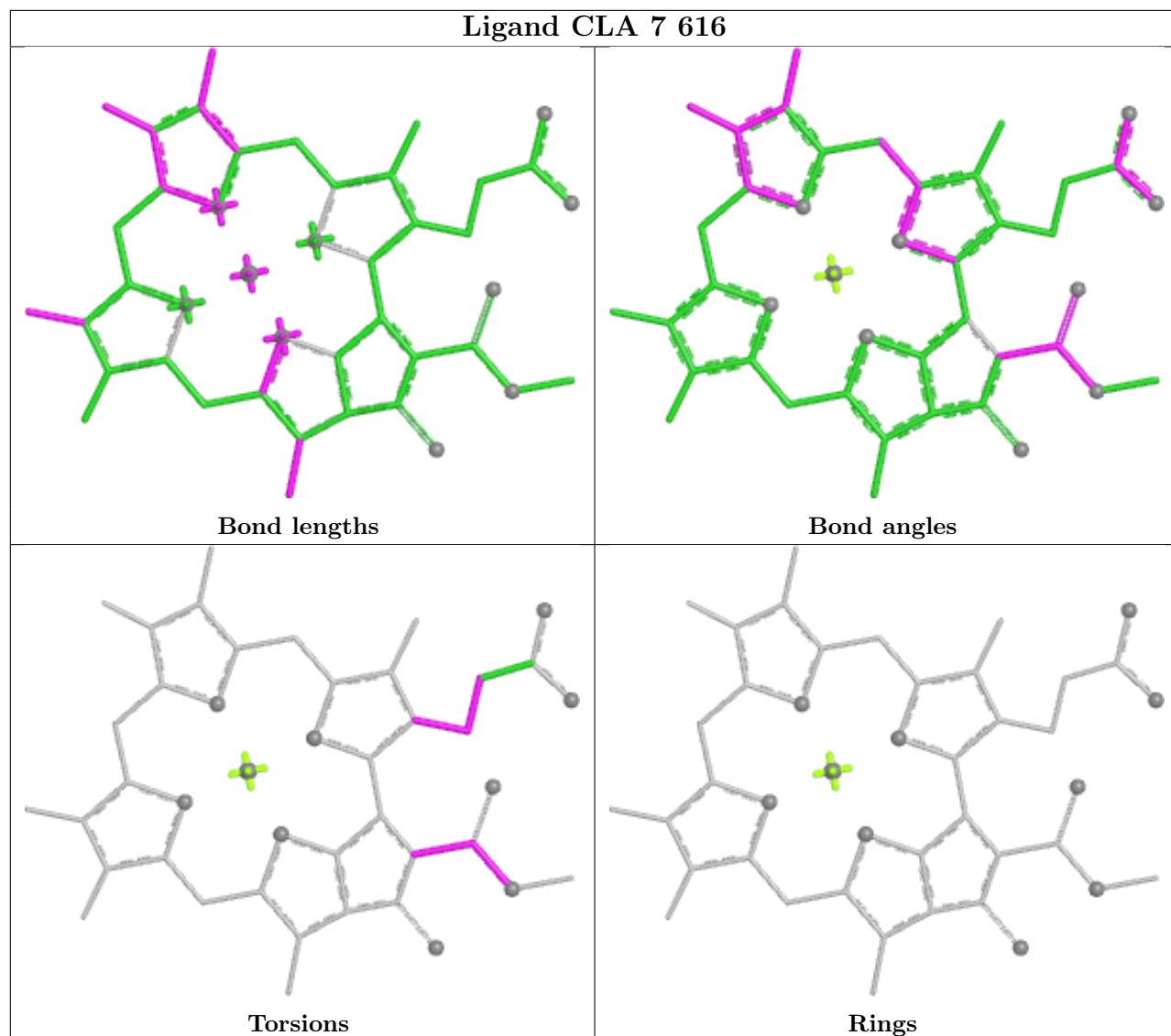
Ligand CLA A 813



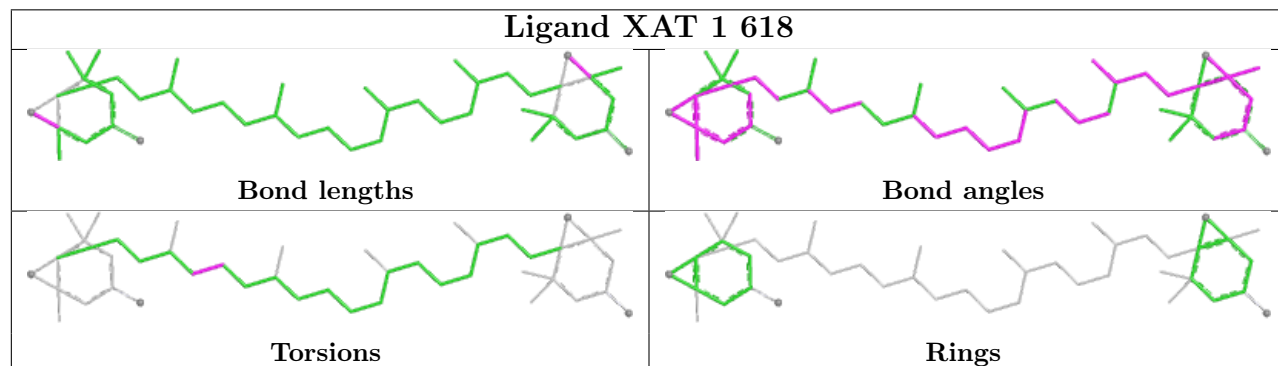
Ligand CLA B 838

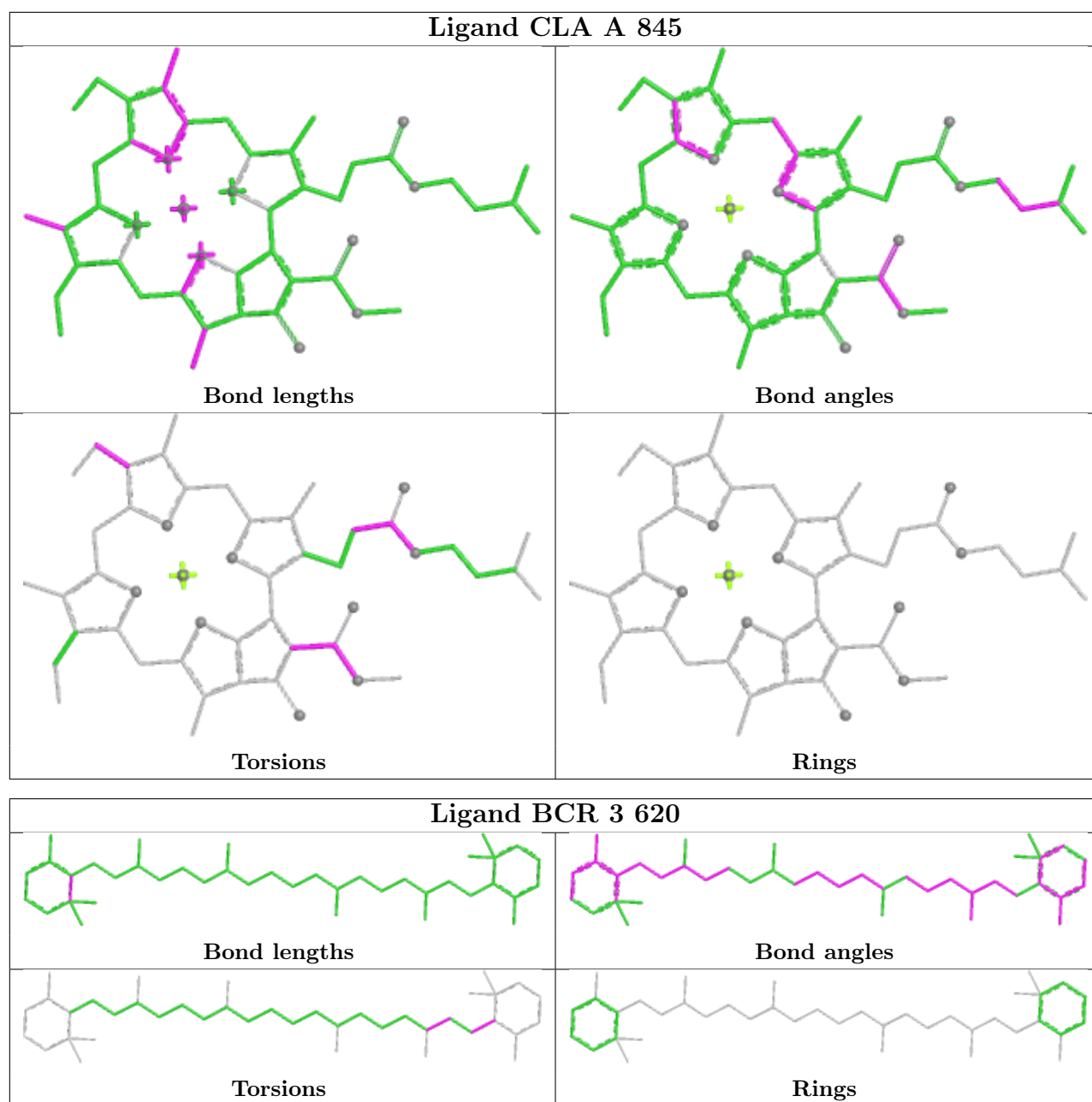


Ligand CLA 7 616

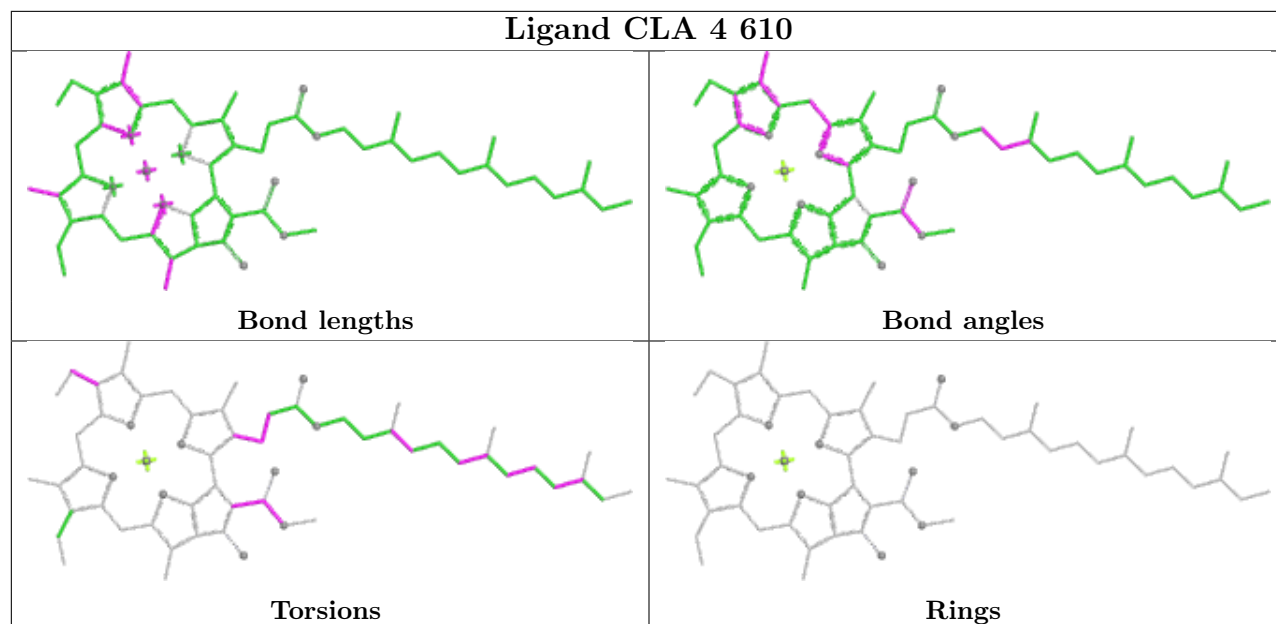


Ligand XAT 1 618

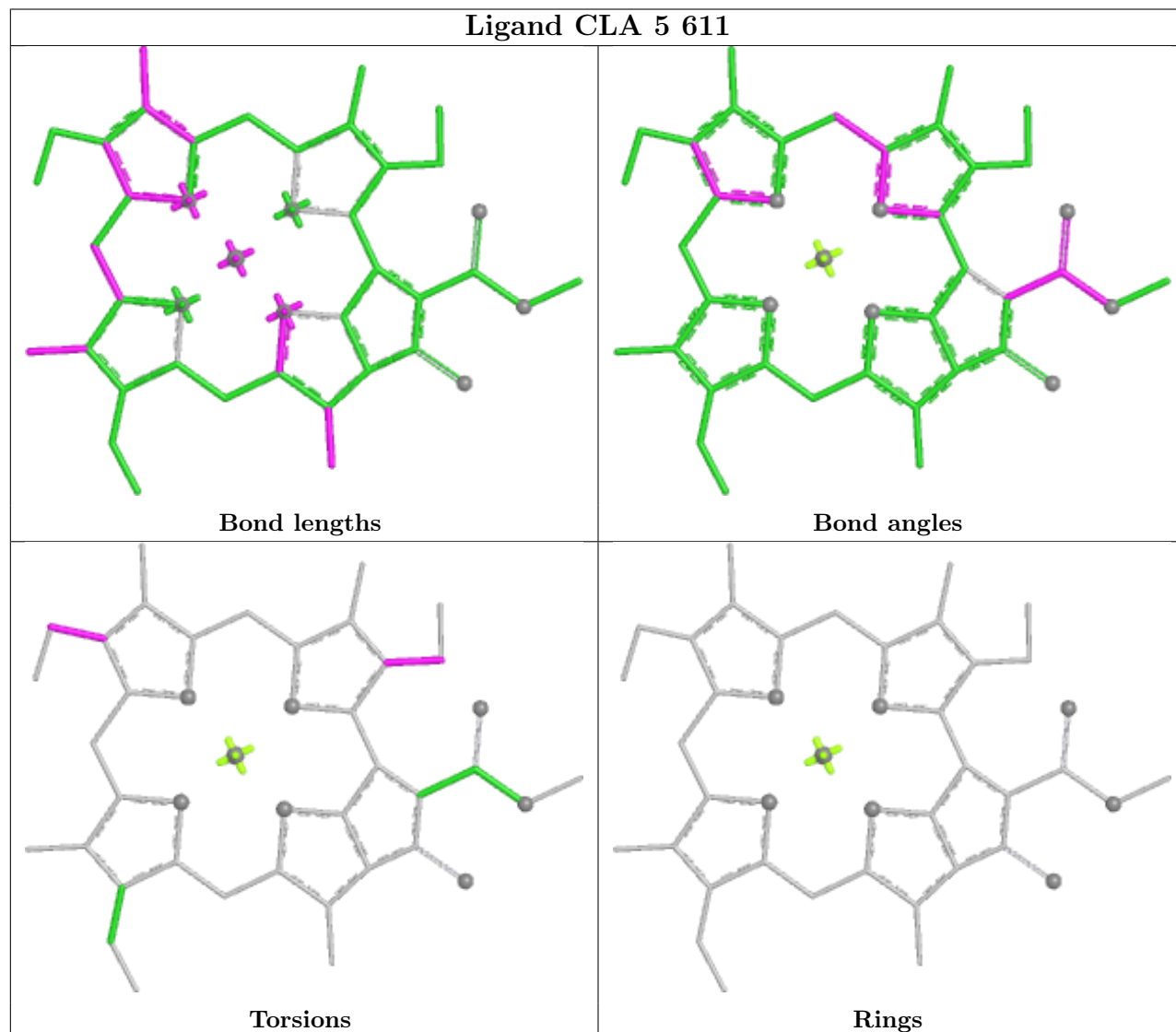


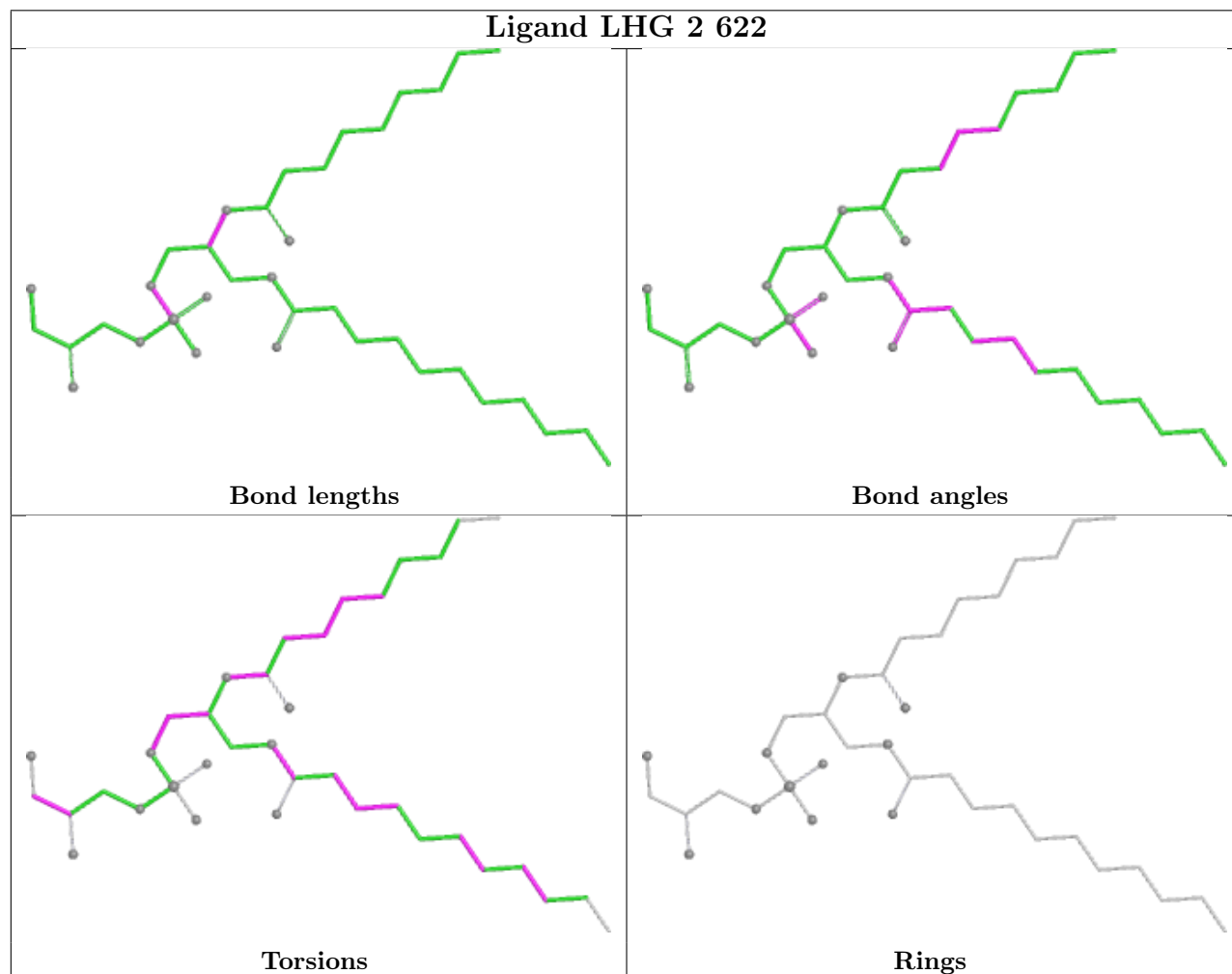
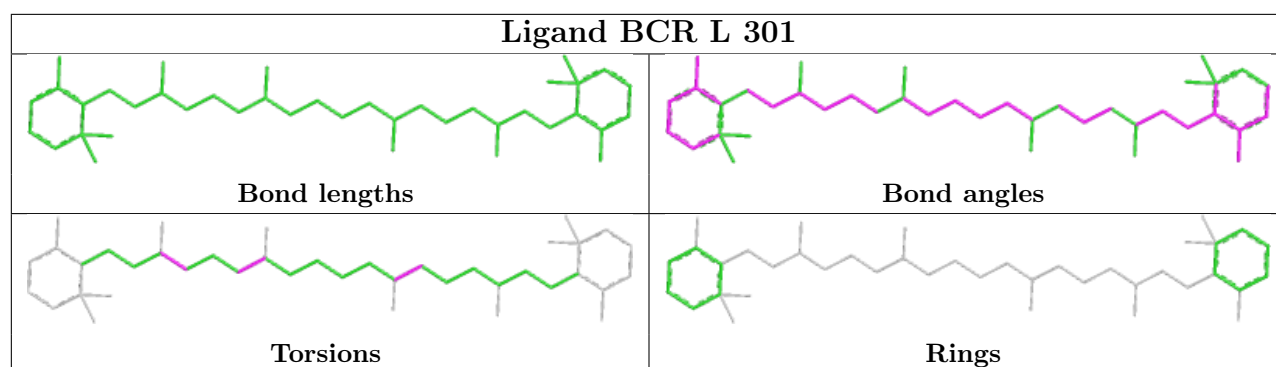


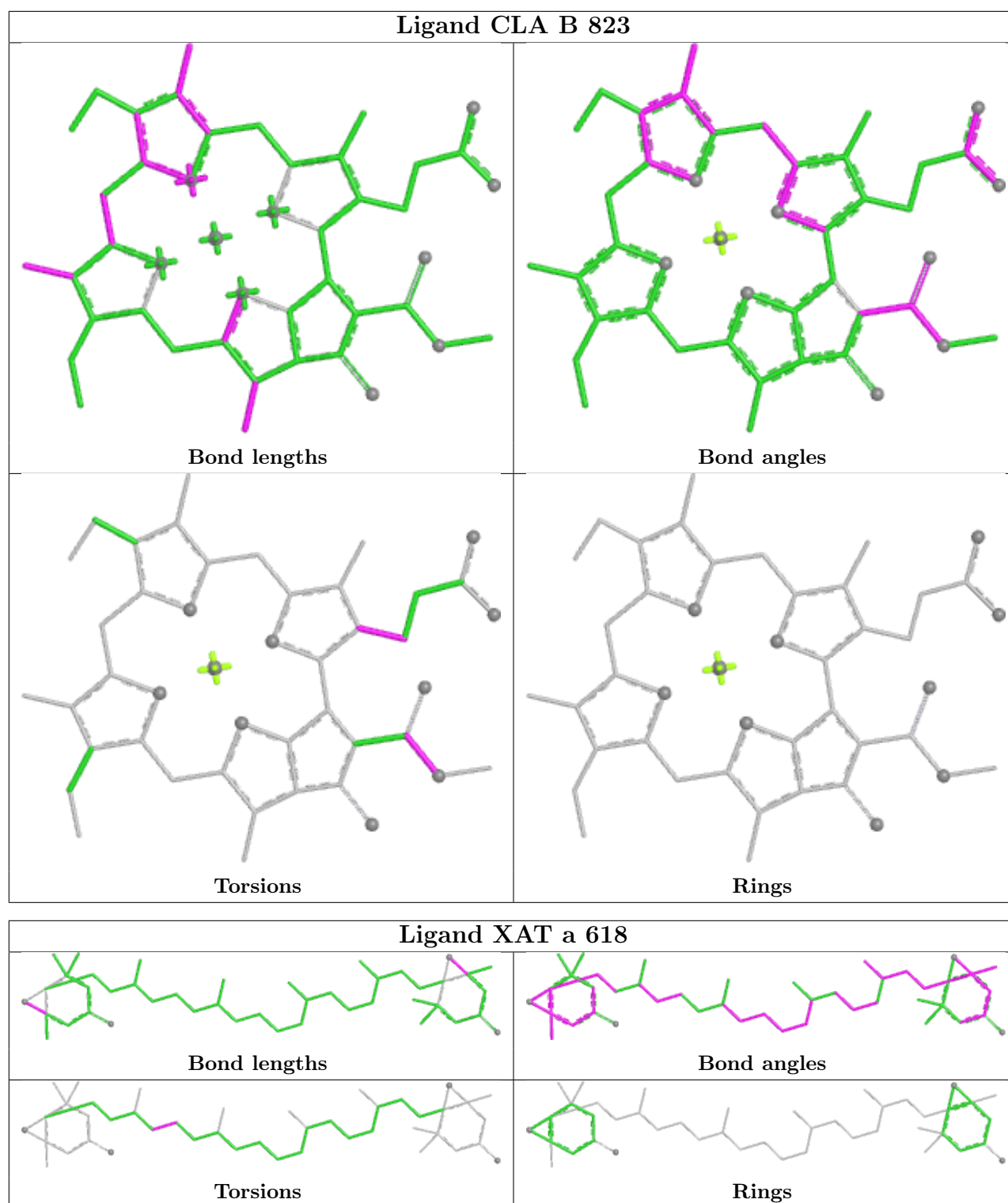
Ligand CLA 4 610



Ligand CLA 5 611







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

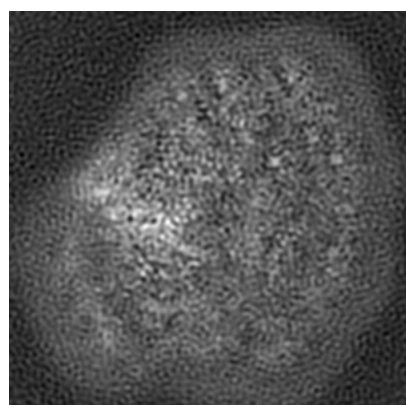
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9680. These allow visual inspection of the internal detail of the map and identification of artifacts.

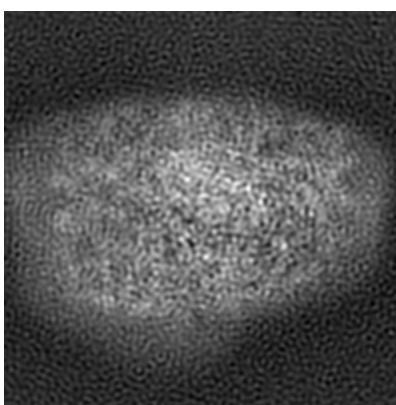
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

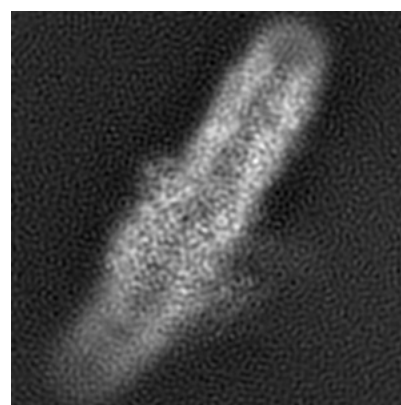
6.1.1 Primary map



X



Y

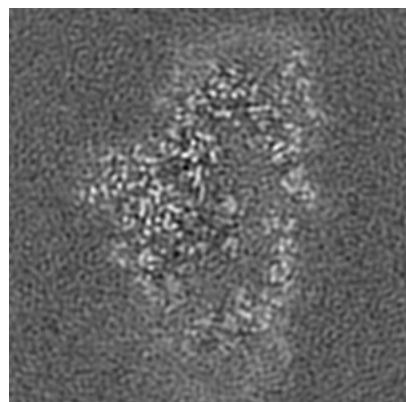


Z

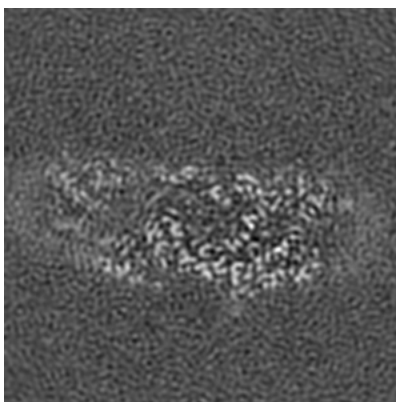
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

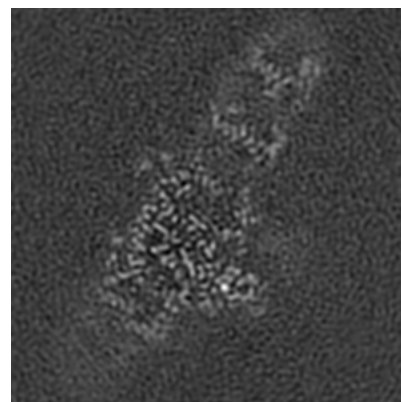
6.2.1 Primary map



X Index: 100



Y Index: 100

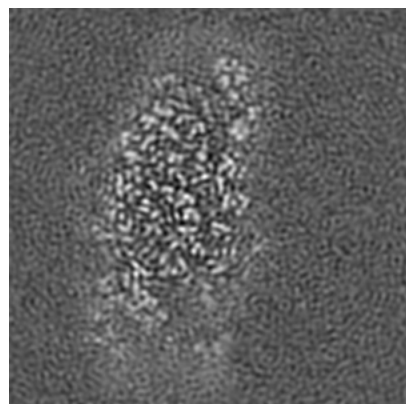


Z Index: 100

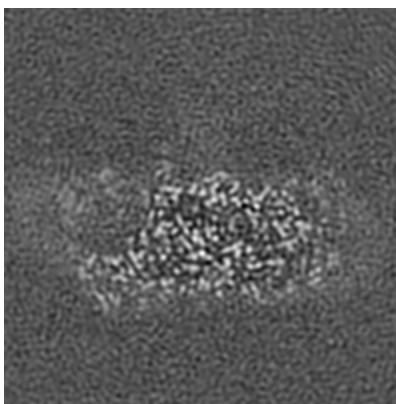
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

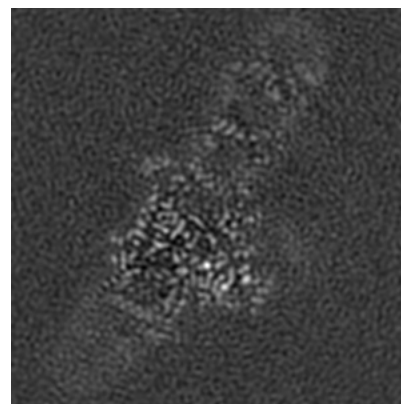
6.3.1 Primary map



X Index: 84



Y Index: 88

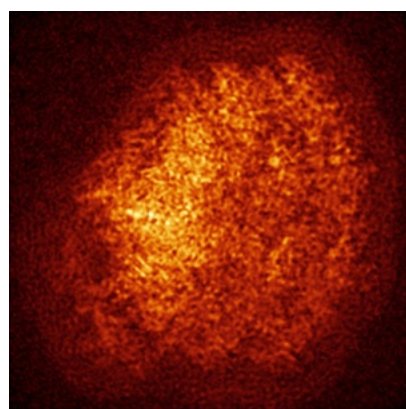


Z Index: 98

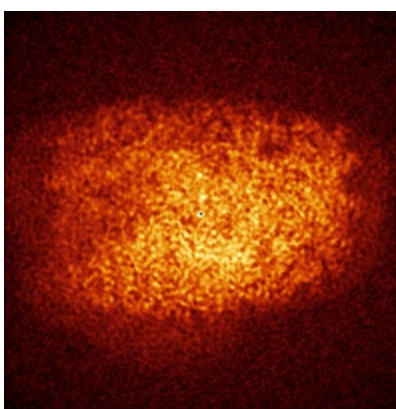
The images above show the largest variance slices of the map in three orthogonal directions.

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

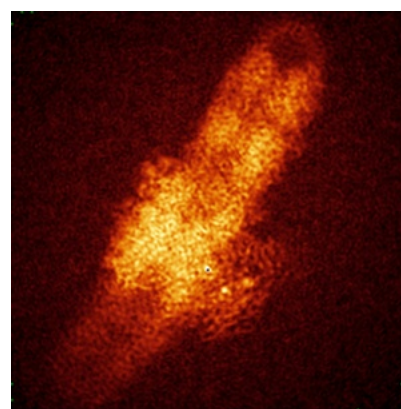
6.4.1 Primary map



X



Y

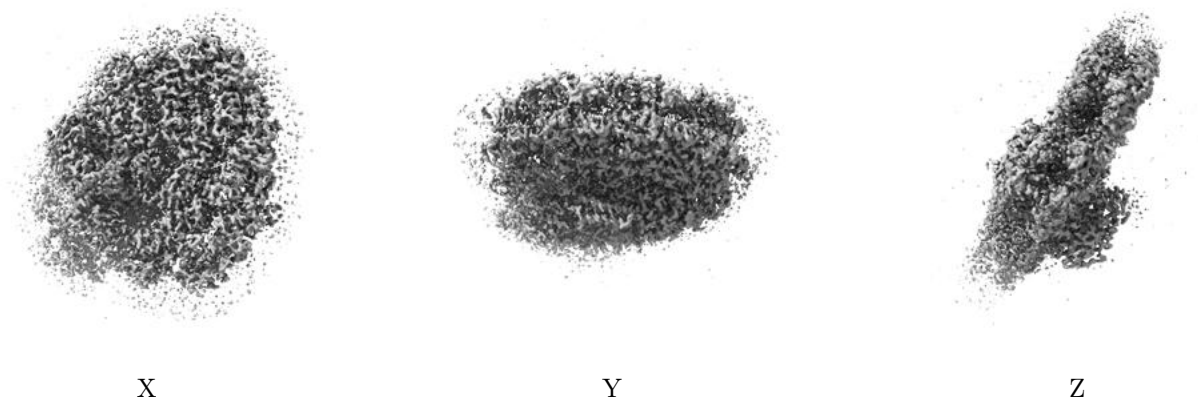


Z

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

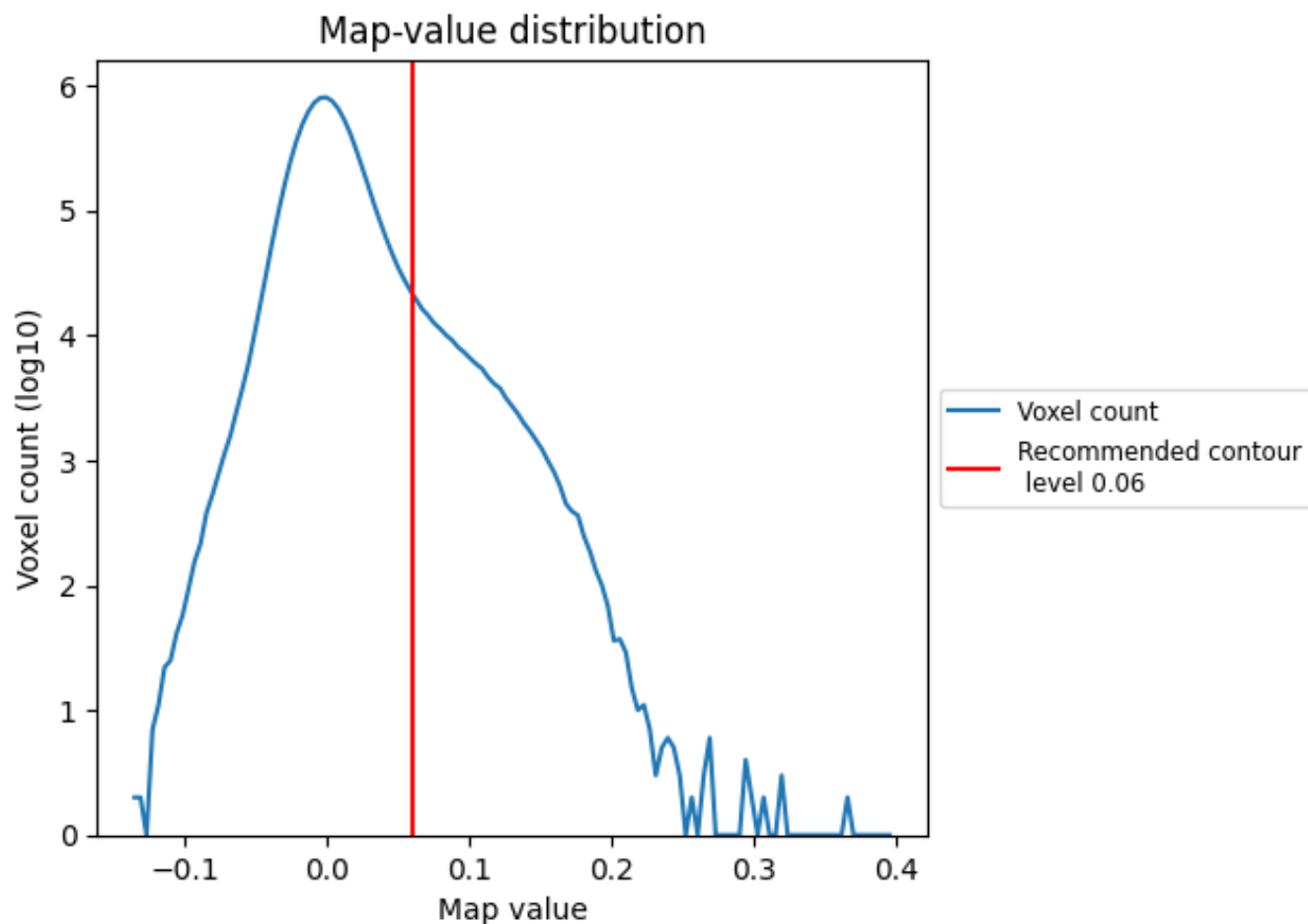
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

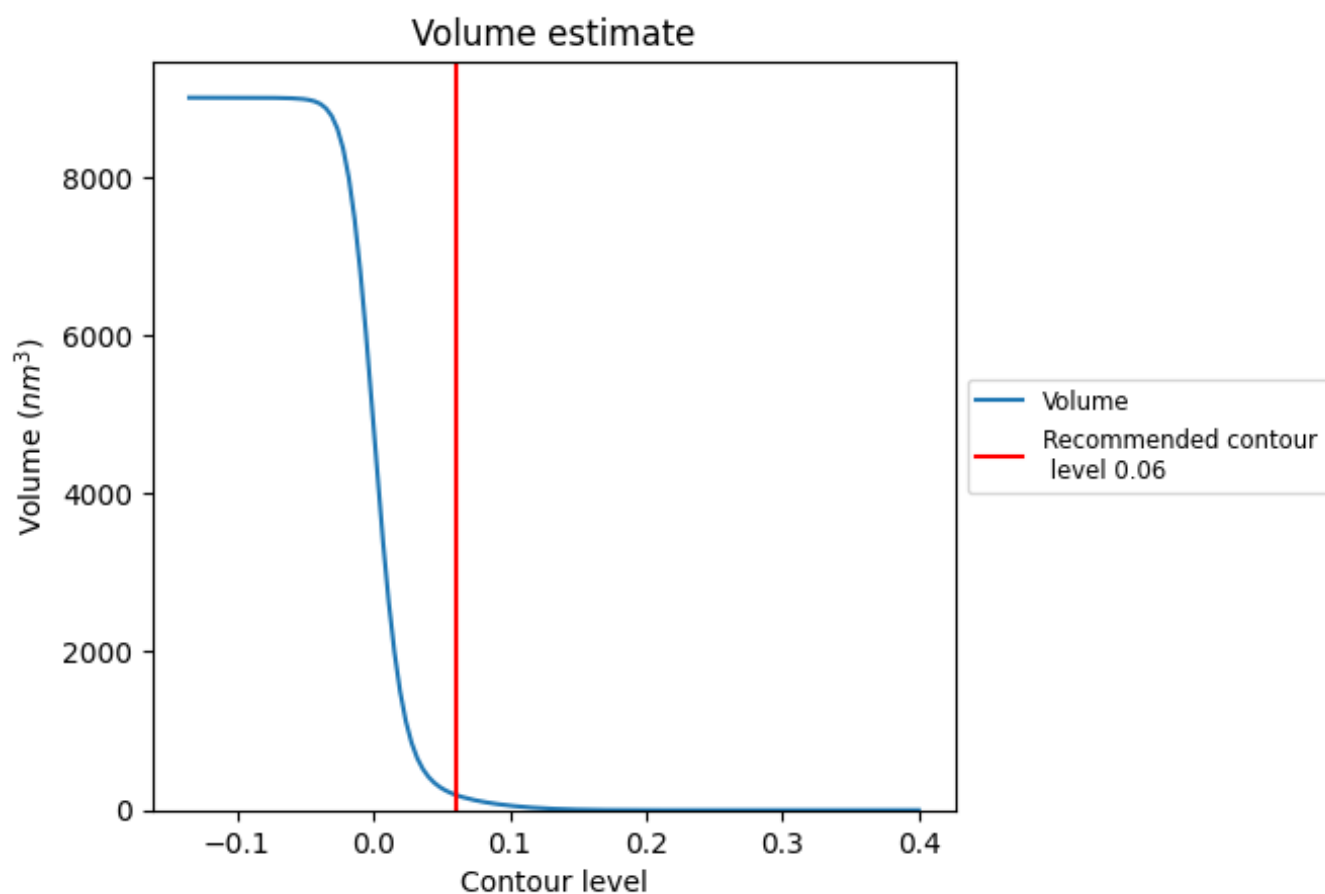
This section contains the results of statistical analysis of the map.

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.

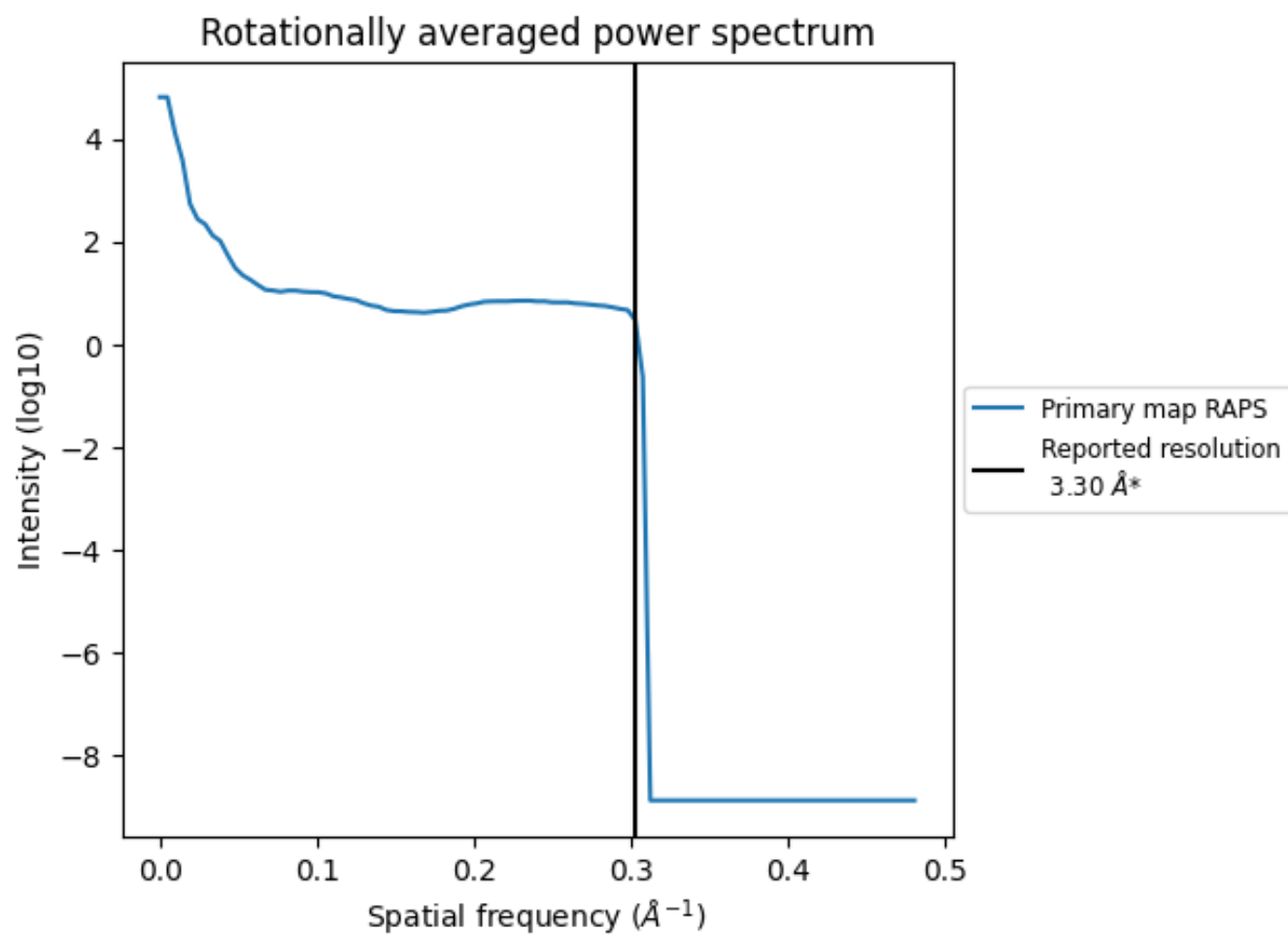
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196 nm³; this corresponds to an approximate mass of 177 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 0.303 Å⁻¹

8 Fourier-Shell correlation

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

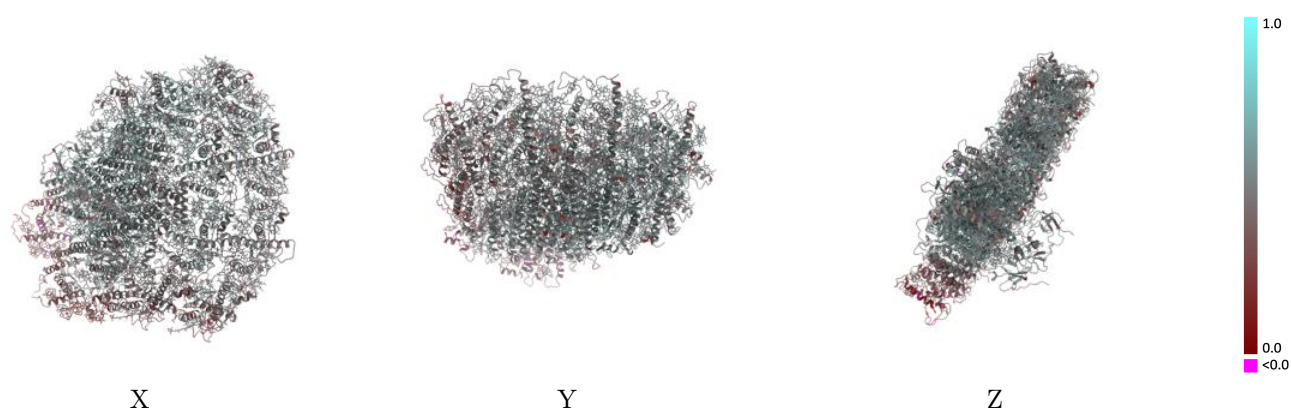
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9680 and PDB model 6IJO. Per-residue inclusion information can be found in section 3 on page 35.

9.1 Map-model overlay [i](#)

This section was not generated.

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

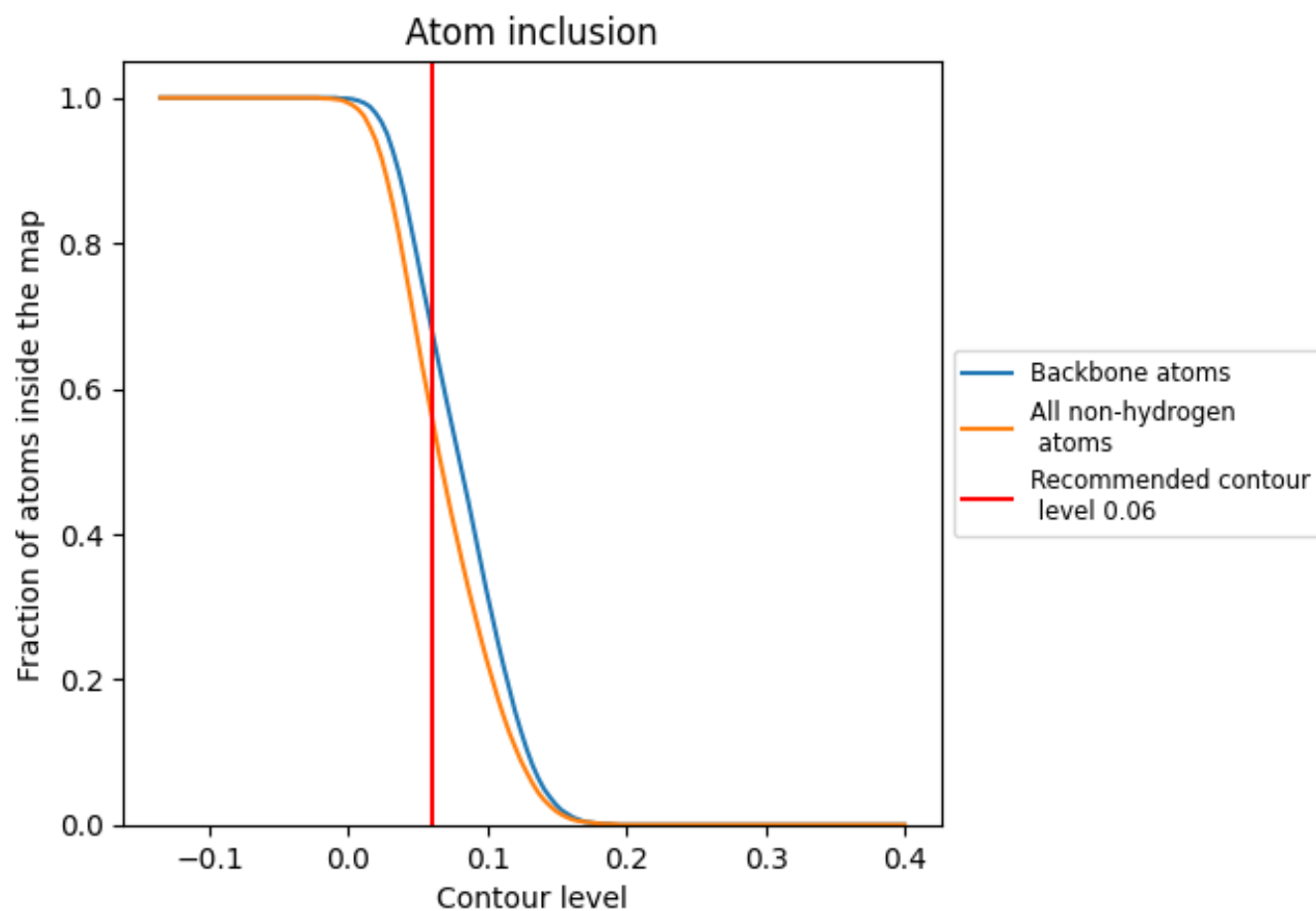


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 56% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5620	 0.4690
1	 0.4300	 0.3900
2	 0.0930	 0.2380
3	 0.6630	 0.5120
4	 0.5190	 0.4540
5	 0.5820	 0.4790
6	 0.5810	 0.4770
7	 0.6370	 0.4970
8	 0.5960	 0.4870
9	 0.2720	 0.2900
A	 0.7080	 0.5400
B	 0.6440	 0.5150
C	 0.7140	 0.4870
D	 0.6490	 0.4900
E	 0.6160	 0.4570
F	 0.5690	 0.4590
G	 0.0740	 0.3300
H	 0.0910	 0.3340
I	 0.5670	 0.4660
J	 0.4220	 0.4370
K	 0.4790	 0.4470
L	 0.4380	 0.4150
X	 0.2620	 0.2840
a	 0.4000	 0.4140

