



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 10:30 AM JST

PDB ID : 6IJO
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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

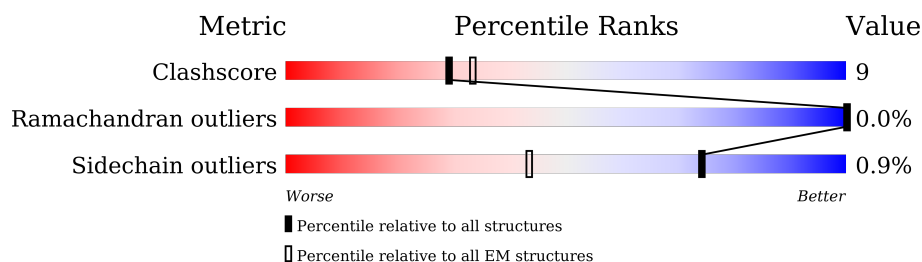
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




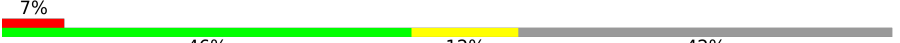
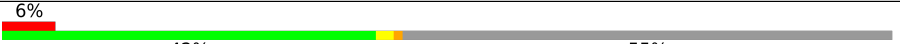
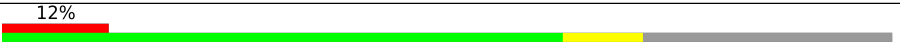

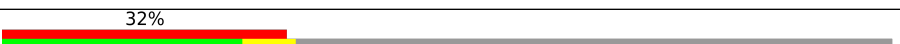
The reported resolution of this entry is 3.30 Å.

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	751	 83% 15% .
2	B	735	 7% 83% 16% ..
3	C	81	 7% 79% 20% .
4	D	247	 7% 46% 12% 42%
5	E	143	 6% 42% .. 55%
6	F	227	 12% 63% 9% 28%
7	G	159	 43% 39% 5% 56%
8	H	155	 32% 27% 6% 67%

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Mol	Chain	Length	Quality of chain
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	-	-	-
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	-	-	-

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

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

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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		

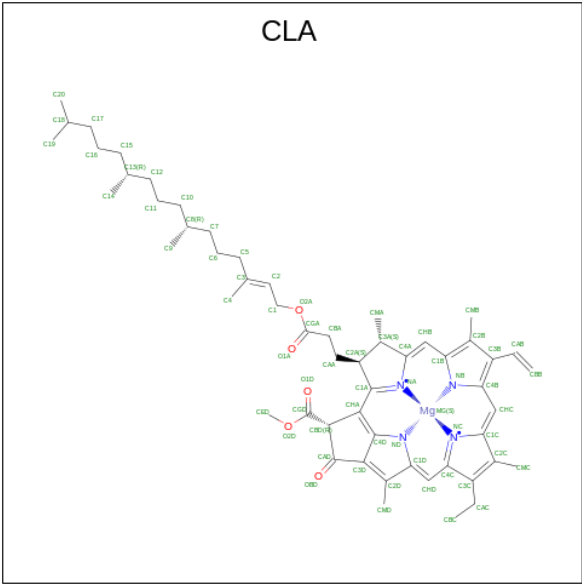
- Molecule 21 is a protein called Lhca9.

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 (three-letter code: 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	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			50	40	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
			54	44	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	
23	A	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
23	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			59	49	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
			53	43	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
			42	34	1	4	3	
23	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
23	A	1	Total	C	Mg	N	O	0
			59	49	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	

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

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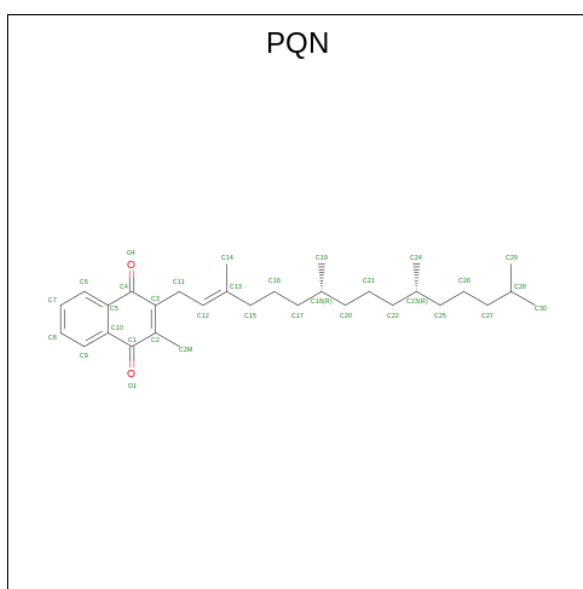
Mol	Chain	Residues	Atoms				AltConf
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total 27	C 22	Mg 1	N 4	0
23	2	1	Total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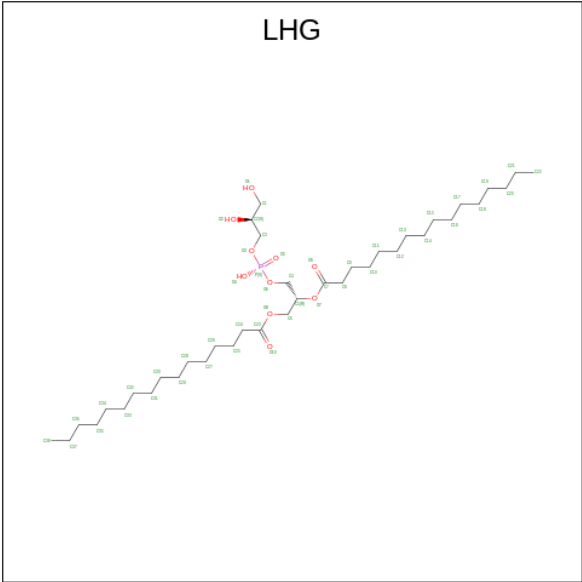
Mol	Chain	Residues	Atoms				AltConf
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	
23	9	1	Total	C	Mg	N	0
			27	22	1	4	

- Molecule 24 is PHYLLOQUINONE (three-letter code: 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 (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



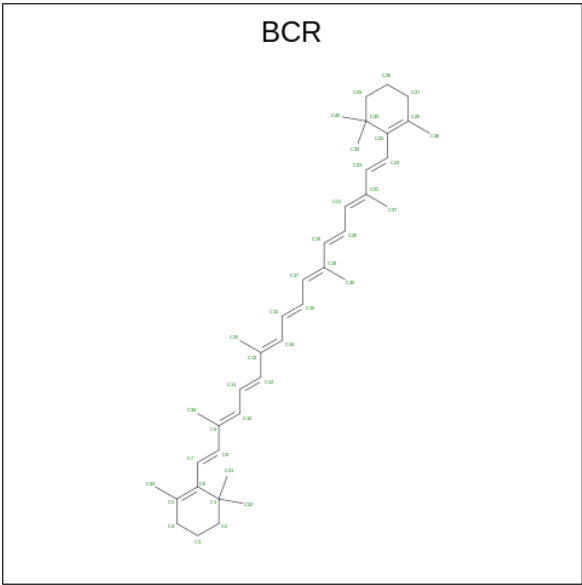
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			30	19	10	1	
25	B	1	Total	C	O	P	0
			38	27	10	1	
25	1	1	Total	C	O	P	0
			49	38	10	1	
25	a	1	Total	C	O	P	0
			49	38	10	1	
25	3	1	Total	C	O	P	0
			45	34	10	1	
25	3	1	Total	C	O	P	0
			49	38	10	1	
25	4	1	Total	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 (three-letter code: 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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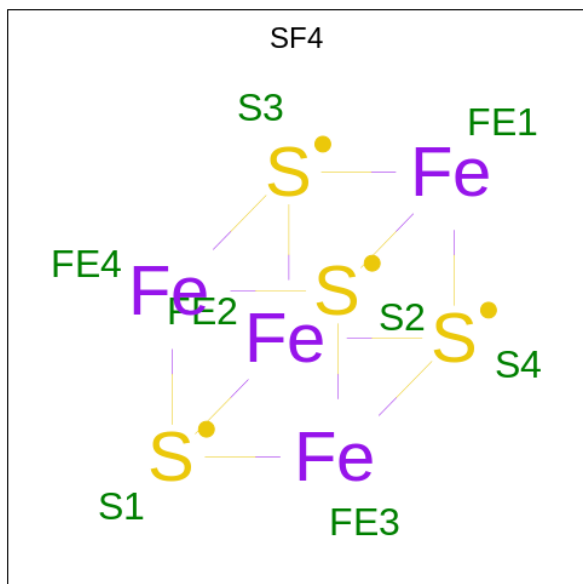
Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	F	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	J	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	L	1	Total C 40 40	0
26	1	1	Total C 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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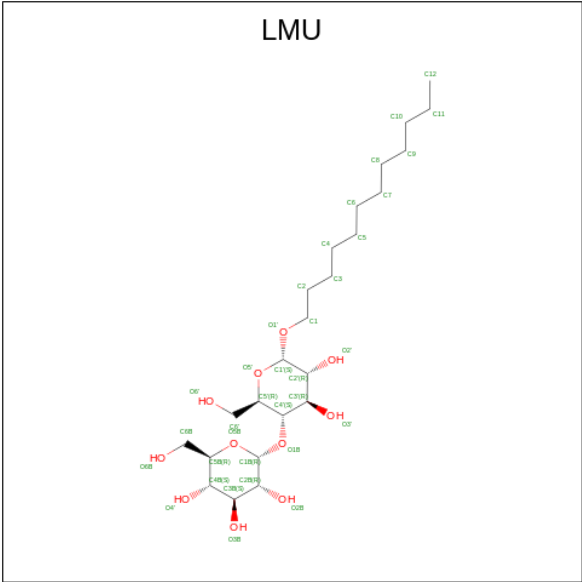
Mol	Chain	Residues	Atoms	AltConf
26	8	1	Total C 40 40	0

- Molecule 27 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



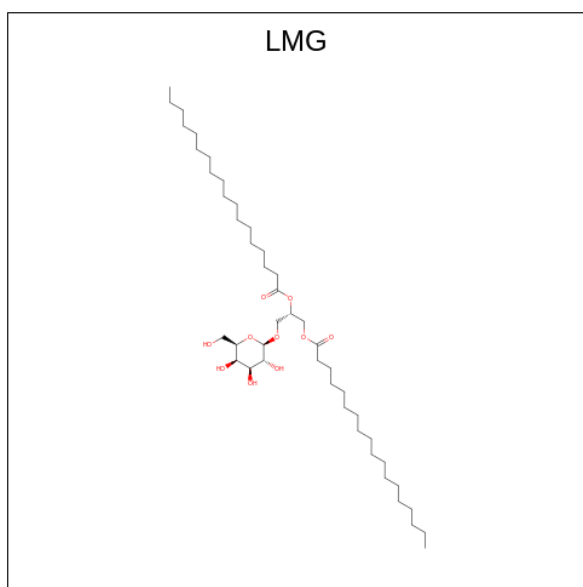
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total Fe S 8 4 4	0
27	C	1	Total Fe S 8 4 4	0
27	C	1	Total Fe S 8 4 4	0

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



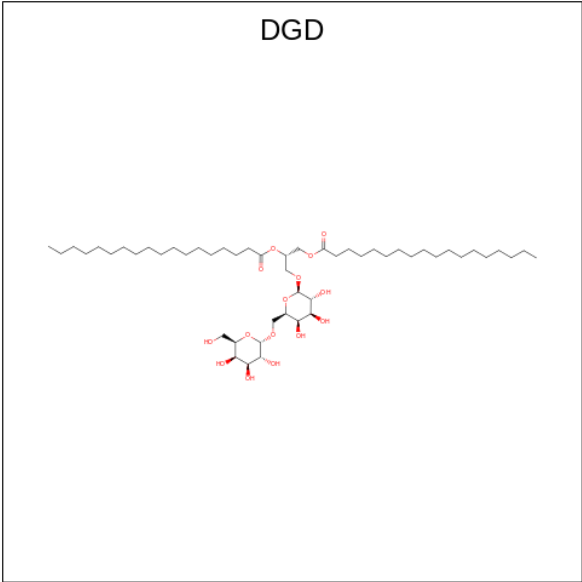
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			35	24	11	
28	A	1	Total	C	O	0
			34	24	10	
28	A	1	Total	C	O	0
			34	24	10	
28	K	1	Total	C	O	0
			35	24	11	
28	5	1	Total	C	O	0
			33	22	11	
28	8	1	Total	C	O	0
			35	24	11	
28	8	1	Total	C	O	0
			35	24	11	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



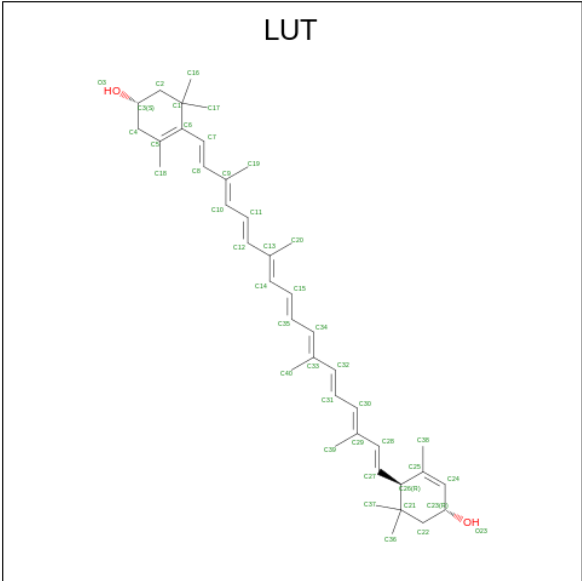
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			40	30	10	
29	J	1	Total	C	O	0
			40	30	10	
29	4	1	Total	C	O	0
			40	30	10	
29	4	1	Total	C	O	0
			40	30	10	
29	5	1	Total	C	O	0
			40	30	10	
29	5	1	Total	C	O	0
			40	30	10	
29	7	1	Total	C	O	0
			44	34	10	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: 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 (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



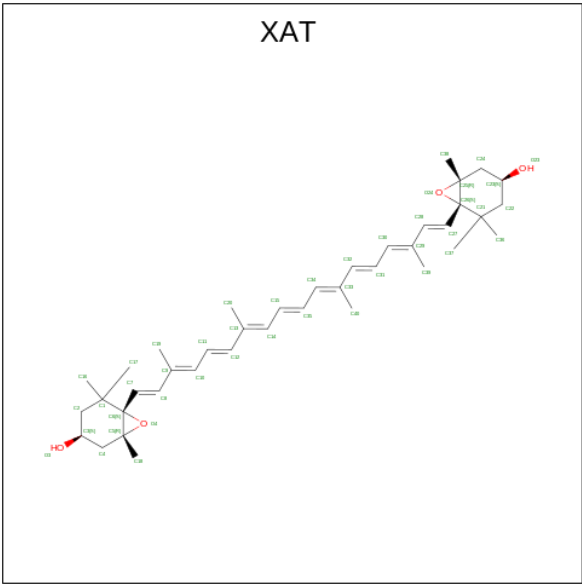
Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			42	40	2	

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

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



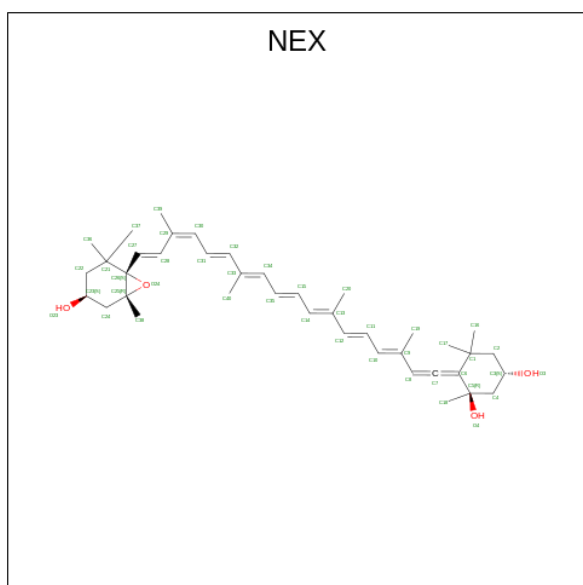
Mol	Chain	Residues	Atoms			AltConf
32	1	1	Total	C	O	0
			44	40	4	
32	a	1	Total	C	O	0
			44	40	4	

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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 (three-letter code: NEX) (formula: C₄₀H₅₆O₄).

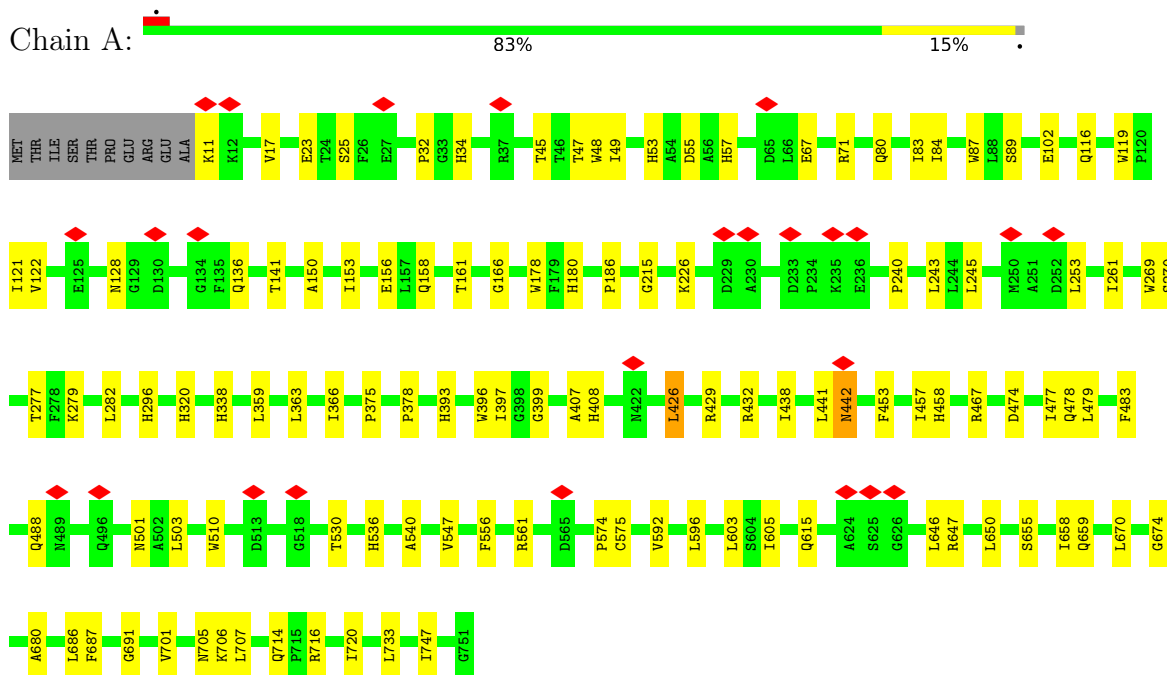


Mol	Chain	Residues	Atoms			AltConf
33	5	1	Total	C	O	0
			44	40	4	
33	6	1	Total	C	O	0
			44	40	4	

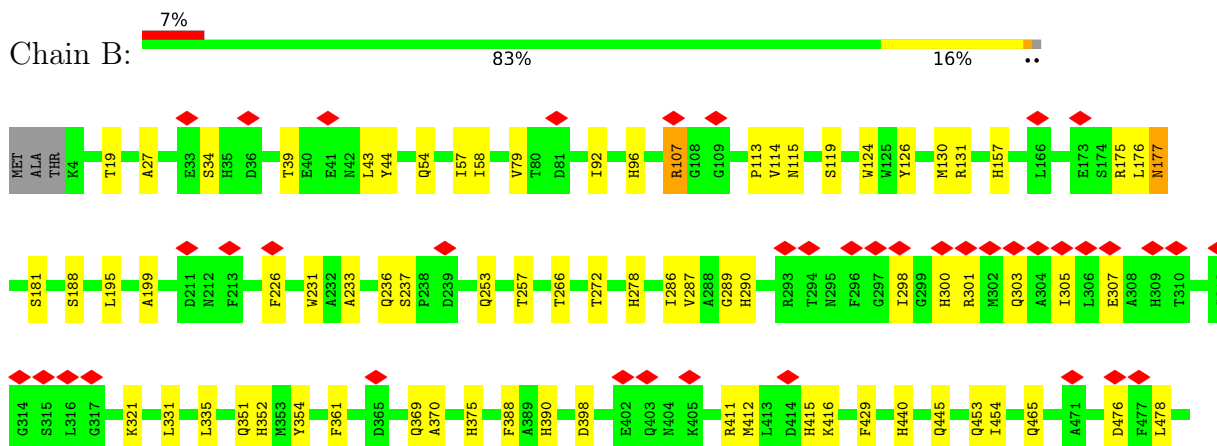
3 Residue-property plots [i](#)

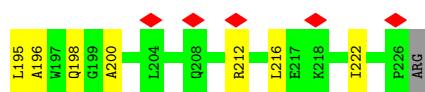
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

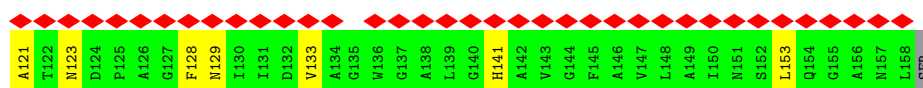
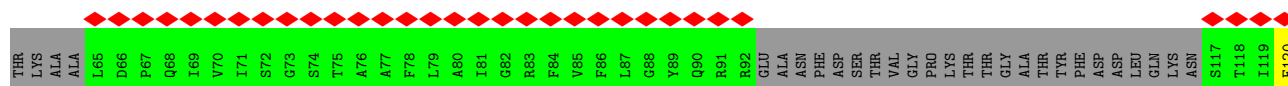
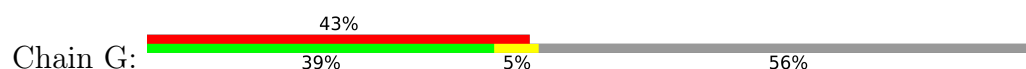


• Molecule 2: PsaB

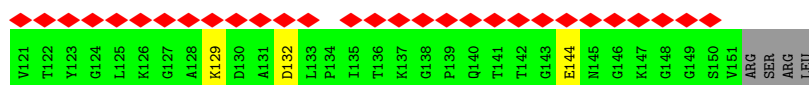
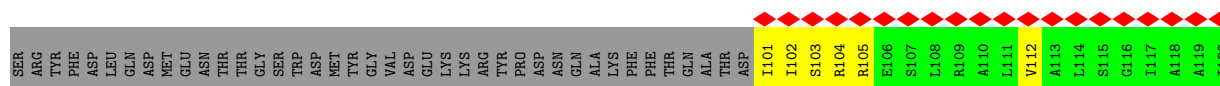




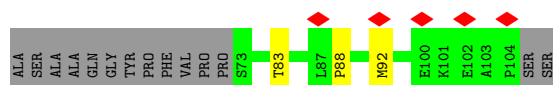
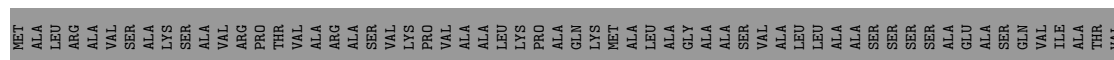
• Molecule 7: PsaG



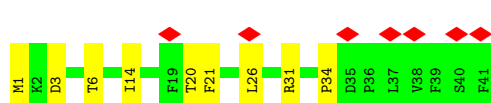
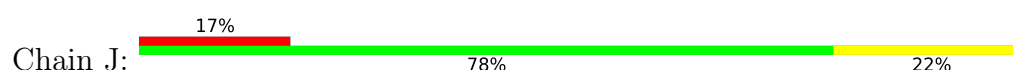
• Molecule 8: PsaH



• Molecule 9: PsaI



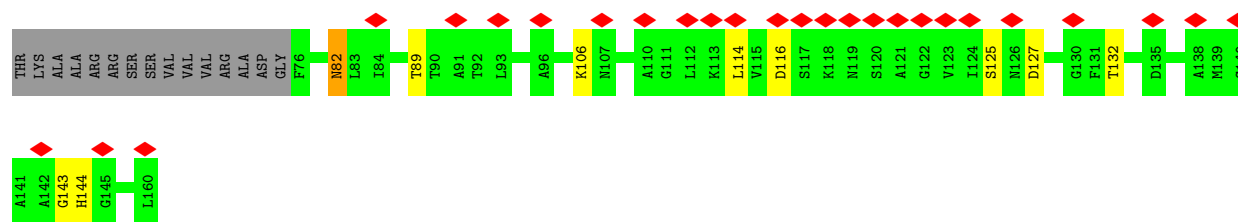
• Molecule 10: PsaJ



• Molecule 11: PsaK



PRO ARG CYS ILE ALA CYS ARG LYS MET THR ALA ARG GLN VAL SER ARG ILE SER HIS CYS PRO LEU ARG ALA PHE ARG ALA THR CYS THR ASN VAL LEU HIS THR CYS PRO ARG LEU SER SER ILE THR ILE SER TYR GLN PRO ALA THR MET GLN ALA LEU THR ARG PRO SER ALA ARG PRO

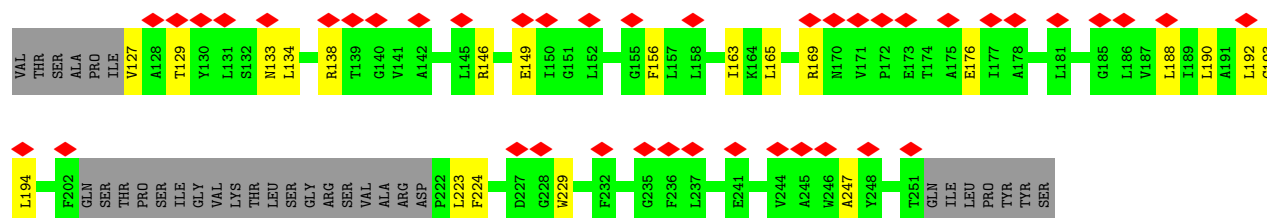


• Molecule 12: PsaL

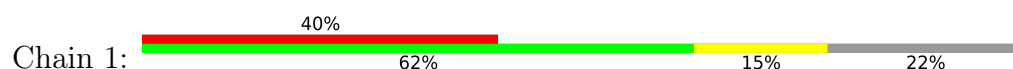


MET PRO THR LYS VAL GLY SER PRO LEU THR THR GLY LEU THR THR ILE THR TRP PHE LEU VAL SER ARG ALA ALA GLN MET THR ARG THR GLY THR VAL ASP THR ARG PRO ARG THR CYS ILE TRP ARG ARG ALA VAL ARG GLN ARG ARG VAL THR VAL LYS LYS GLN ARG PRO ARG VAL ILE VAL ASN ILE ASP THR PHE GLY SER LEU ALA HIS THR TYR

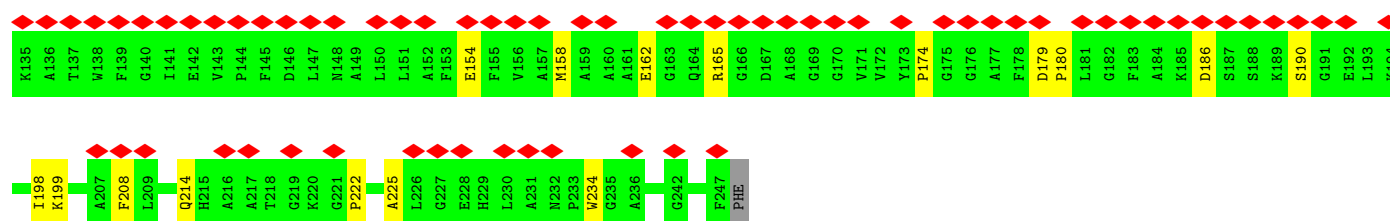
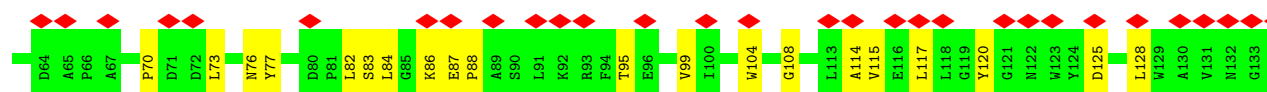
HIS LYS MET ALA VAL MET ARG SER THR THR GLY LEU ARG ALA ALA ARG ALA GLN MET THR ARG THR GLY LEU GLY VAL THR VAL ARG CYS VAL ALA ASP THR LYS LYS VAL GLN VAL ILE SER VAL PRO VAL ASN ASP THR PHE GLY SER LEU ALA HIS THR TYR



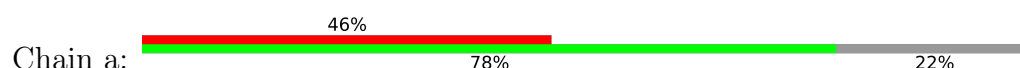
• Molecule 13: Lhca1

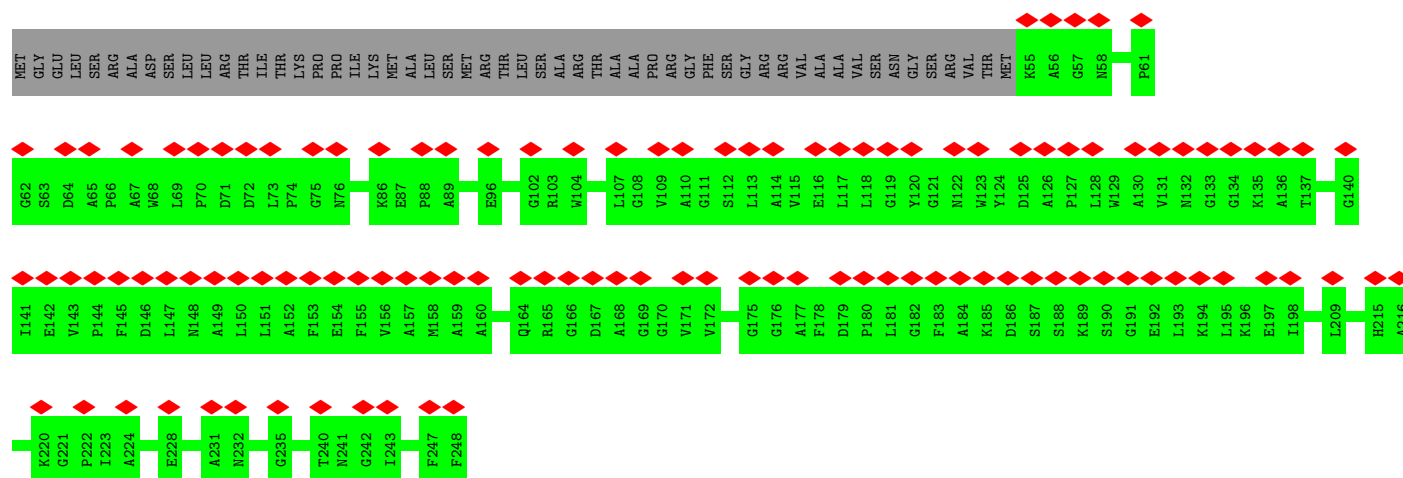


MET GLY LEU LEU SER ARG ALA ASP SER LEU LEU ARG THR LYS PRO PRO THR ILE LYS MET MET ALA LEU SER MET ARG THR ALA ALA PRO ARG GLY PHE SER GLY ARG VAL ALA ALA VAL SER ASN GLY SER ARG VAL THR MET K55 A56 G57 N58 W59 L60

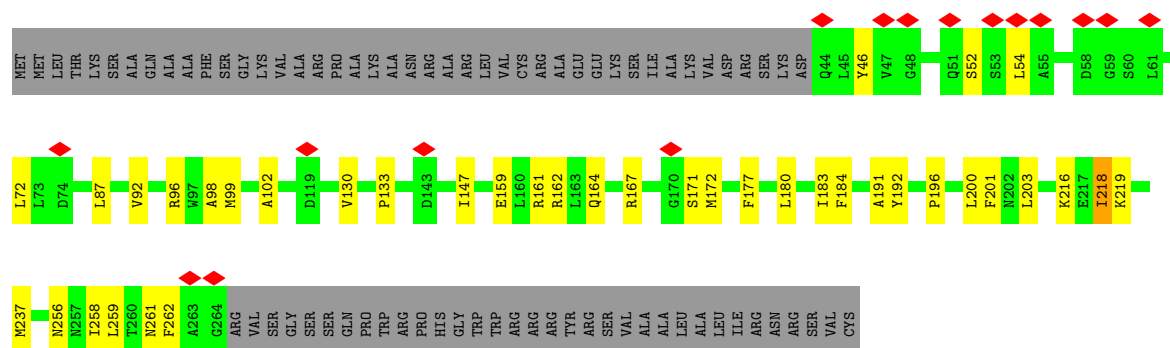


• Molecule 13: Lhca1

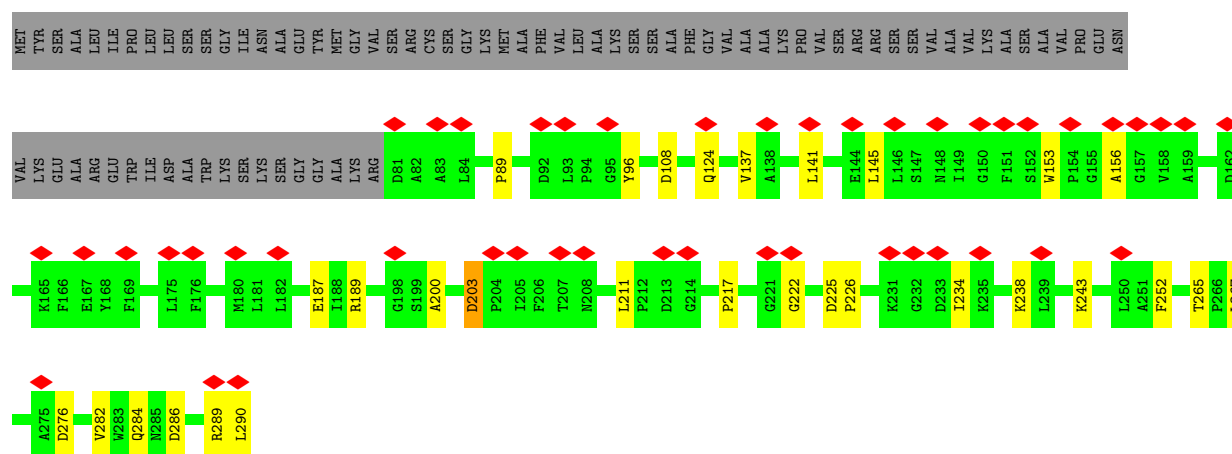




- Molecule 14: Lhca3

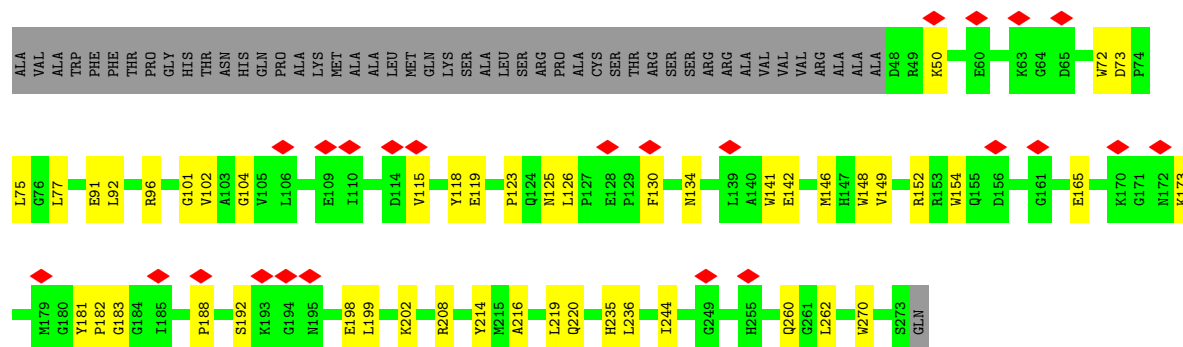


- Molecule 15: Lhca4

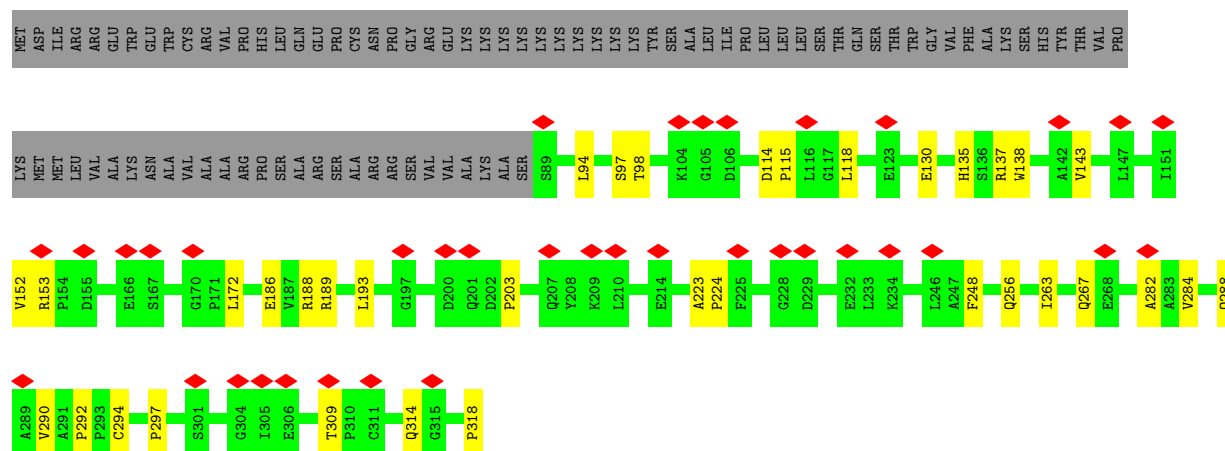


- Molecule 16: Lhca5

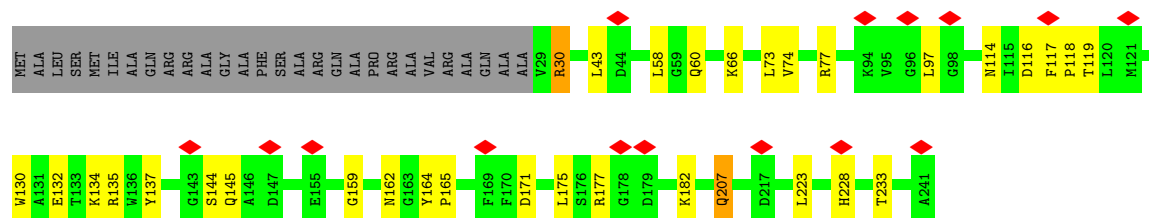
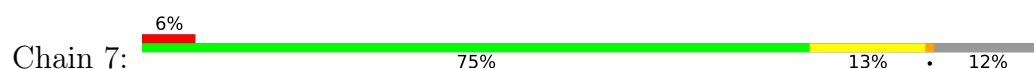




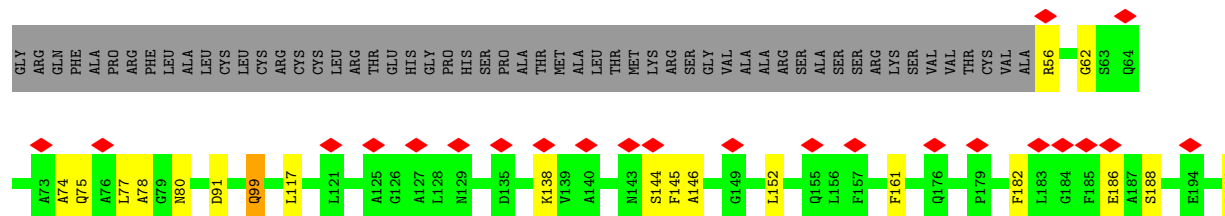
• Molecule 17: Lhca6



• 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

5.1 Standard geometry

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

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	0.51	0/6015	0.57	1/8201 (0.0%)
2	B	0.49	0/6024	0.59	3/8225 (0.0%)
3	C	0.51	0/610	0.66	0/826
4	D	0.43	0/1157	0.61	0/1563
5	E	0.46	0/515	0.54	0/700
6	F	0.41	0/1280	0.55	0/1733
7	G	0.31	0/524	0.66	1/711 (0.1%)
8	H	0.31	0/359	0.61	0/483
9	I	0.43	0/250	0.63	0/345
10	J	0.43	0/349	0.58	0/478
11	K	0.32	0/583	0.69	1/790 (0.1%)
12	L	0.36	0/787	0.63	0/1074
13	1	0.38	0/1478	0.55	0/2012
13	a	0.39	0/1490	0.55	0/2028
14	3	0.49	0/1731	0.67	3/2349 (0.1%)
15	4	0.37	0/1686	0.53	0/2300
16	5	0.43	0/1820	0.62	0/2480
17	6	0.40	0/1833	0.58	0/2505
18	7	0.48	0/1701	0.61	0/2310
19	8	0.43	0/1680	0.63	1/2288 (0.0%)
20	2	0.29	0/1382	0.56	0/1870
21	9	0.32	0/1337	0.65	1/1814 (0.1%)
22	X	0.24	0/129	0.33	0/179
All	All	0.44	0/34720	0.59	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(°)
14	3	180	LEU	CA-CB-CG	6.59	130.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	3	200	LEU	CA-CB-CG	6.43	130.10	115.30
7	G	153	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	426	LEU	CA-CB-CG	6.20	129.56	115.30
11	K	114	LEU	CA-CB-CG	6.05	129.21	115.30

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	96	0
2	B	5812	0	5569	94	0
3	C	600	0	589	10	0
4	D	1129	0	1144	23	0
5	E	505	0	504	4	0
6	F	1254	0	1288	14	0
7	G	514	0	509	7	0
8	H	357	0	382	6	0
9	I	242	0	252	2	0
10	J	337	0	336	10	0
11	K	578	0	617	7	0
12	L	768	0	776	20	0
13	1	1433	0	1387	29	0
13	a	1444	0	1396	0	0
14	3	1683	0	1641	28	0
15	4	1631	0	1587	26	0
16	5	1765	0	1738	45	0
17	6	1771	0	1770	30	0
18	7	1649	0	1589	30	0
19	8	1630	0	1609	26	0
20	2	1346	0	1330	17	0
21	9	1302	0	1275	30	0
22	X	130	0	132	2	0
23	1	674	0	541	19	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	22	0
23	4	782	0	686	24	0
23	5	878	0	758	45	0
23	6	912	0	845	37	0
23	7	760	0	643	26	0
23	8	727	0	635	16	0
23	9	324	0	36	12	0
23	A	2625	0	2614	129	0
23	B	2270	0	2210	101	0
23	F	140	0	113	8	0
23	G	87	0	64	6	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	0	0
24	A	33	0	46	5	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	4	0
25	9	49	0	74	5	0
25	A	79	0	104	4	0
25	B	38	0	46	2	0
25	a	49	0	74	0	0
26	1	40	0	56	2	0
26	3	120	0	168	11	0
26	4	40	0	56	2	0
26	5	40	0	56	4	0
26	6	40	0	56	4	0
26	7	80	0	112	3	0
26	8	40	0	56	4	0
26	A	240	0	336	28	0
26	B	280	0	392	15	0
26	F	40	0	56	4	0
26	G	40	0	56	6	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	5	0
26	a	40	0	56	0	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	6	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	0	0
32	1	44	0	56	4	0
32	2	44	0	56	3	0
32	3	44	0	56	2	0
32	4	44	0	56	3	0
32	5	44	0	56	10	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	0	0
33	5	44	0	56	3	0
33	6	44	0	56	4	0
All	All	49685	0	48724	855	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 9.

The worst 5 of 855 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	1.04
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%)	11	38
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%)	600 (100%)	1 (0%)	92	95
2	B	595/597 (100%)	588 (99%)	7 (1%)	67	80
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	120/197 (61%)	119 (99%)	1 (1%)	79	87
5	E	55/123 (45%)	54 (98%)	1 (2%)	54	74
6	F	126/169 (75%)	125 (99%)	1 (1%)	79	87
7	G	50/121 (41%)	50 (100%)	0	100	100
8	H	36/126 (29%)	35 (97%)	1 (3%)	38	64
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%)	58 (98%)	1 (2%)	56	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	75/198 (38%)	74 (99%)	1 (1%)	65	79
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%)	165 (99%)	2 (1%)	67	80
15	4	165/226 (73%)	164 (99%)	1 (1%)	84	90
16	5	183/219 (84%)	181 (99%)	2 (1%)	70	82
17	6	184/260 (71%)	184 (100%)	0	100	100
18	7	164/181 (91%)	161 (98%)	3 (2%)	54	74
19	8	161/207 (78%)	159 (99%)	2 (1%)	67	80
20	2	134/183 (73%)	132 (98%)	2 (2%)	60	77
21	9	127/159 (80%)	124 (98%)	3 (2%)	44	68
All	All	3407/4472 (76%)	3378 (99%)	29 (1%)	74	85

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	3	218	ILE
21	9	149	MET
16	5	75	LEU
20	2	9	ARG
15	4	203	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	132	HIS
14	3	164	GLN
21	9	49	ASN
10	J	30	ASN
15	4	284	GLN

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	B	818	-	60,68,73	1.49	10 (16%)	70,107,113	1.59	10 (14%)
29	LMG	A	860	-	40,40,55	0.95	3 (7%)	48,48,63	1.32	5 (10%)
23	CLA	5	606	-	39,48,73	1.88	10 (25%)	44,83,113	1.60	7 (15%)
31	LUT	8	619	-	42,43,43	0.87	1 (2%)	51,60,60	1.82	14 (27%)
23	CLA	2	601	20	29,35,73	2.72	9 (31%)	28,60,113	1.75	6 (21%)
23	CLA	K	201	11	45,53,73	1.77	7 (15%)	52,89,113	1.79	10 (19%)
23	CLA	a	610	13	59,67,73	1.57	9 (15%)	69,106,113	1.42	7 (10%)
23	CLA	6	601	17	65,73,73	1.42	9 (13%)	76,113,113	1.52	9 (11%)
32	XAT	a	618	-	39,47,47	0.94	2 (5%)	54,74,74	2.57	18 (33%)
23	CLA	6	617	-	45,53,73	1.73	9 (20%)	52,89,113	1.49	7 (13%)
23	CLA	5	614	-	45,52,73	1.86	8 (17%)	48,87,113	1.65	7 (14%)
23	CLA	a	602	13	61,69,73	1.47	8 (13%)	71,108,113	1.51	7 (9%)
23	CLA	5	616	16	41,50,73	1.89	9 (21%)	50,85,113	1.61	9 (18%)
23	CLA	a	616	13	45,53,73	1.76	9 (20%)	52,89,113	1.56	6 (11%)
23	CLA	7	609	18	43,52,73	1.71	7 (16%)	48,87,113	1.87	6 (12%)
23	CLA	7	610	18	65,73,73	1.44	10 (15%)	76,113,113	1.43	8 (10%)
23	CLA	A	809	1	65,73,73	1.43	10 (15%)	76,113,113	1.50	8 (10%)
27	SF4	C	101	-	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMU	8	625	-	36,36,36	1.16	2 (5%)	47,47,47	1.41	7 (14%)
26	BCR	F	305	-	41,41,41	0.83	1 (2%)	56,56,56	2.26	23 (41%)
28	LMU	A	857	-	36,36,36	1.20	3 (8%)	47,47,47	1.33	4 (8%)
23	CLA	6	613	-	63,72,73	1.45	10 (15%)	73,112,113	1.43	9 (12%)
26	BCR	A	851	-	41,41,41	0.88	2 (4%)	56,56,56	1.97	16 (28%)
29	LMG	5	626	-	40,40,55	0.94	1 (2%)	48,48,63	1.33	5 (10%)
25	LHG	1	620	23	48,48,48	0.60	1 (2%)	51,54,54	1.26	6 (11%)
23	CLA	7	616	18	43,51,73	1.80	9 (20%)	54,87,113	1.70	10 (18%)
23	CLA	a	613	-	65,73,73	1.46	9 (13%)	76,113,113	1.52	9 (11%)
23	CLA	8	610	19	60,68,73	1.41	8 (13%)	70,107,113	1.53	8 (11%)
25	LHG	3	623	-	44,44,48	0.66	2 (4%)	47,50,54	1.26	6 (12%)
23	CLA	L	303	-	45,53,73	1.71	8 (17%)	52,89,113	1.67	6 (11%)
23	CLA	a	601	13	53,62,73	1.60	9 (16%)	61,100,113	1.48	7 (11%)
23	CLA	5	610	16	54,62,73	1.59	10 (18%)	62,99,113	1.57	9 (14%)
23	CLA	4	609	15	61,69,73	1.57	7 (11%)	71,108,113	1.49	7 (9%)
26	BCR	B	848	-	41,41,41	0.87	0	56,56,56	1.79	12 (21%)
28	LMU	5	628	-	34,34,36	1.24	3 (8%)	45,45,47	1.50	8 (17%)
23	CLA	B	810	-	64,72,73	1.44	10 (15%)	74,111,113	1.41	8 (10%)
26	BCR	A	849	-	41,41,41	0.89	1 (2%)	56,56,56	2.03	17 (30%)
26	BCR	4	621	-	41,41,41	0.73	0	56,56,56	2.10	22 (39%)
31	LUT	a	617	-	42,43,43	0.79	0	51,60,60	1.56	12 (23%)
23	CLA	2	614	-	29,35,73	2.64	9 (31%)	28,60,113	1.72	5 (17%)
23	CLA	3	602	14	60,68,73	1.47	10 (16%)	70,107,113	1.48	8 (11%)
23	CLA	4	616	15	43,51,73	1.84	9 (20%)	54,87,113	1.66	9 (16%)
23	CLA	7	614	-	42,50,73	1.71	10 (23%)	48,85,113	1.65	8 (16%)
23	CLA	A	843	-	64,72,73	1.50	11 (17%)	74,111,113	1.46	7 (9%)
23	CLA	8	612	19	40,49,73	1.78	8 (20%)	45,84,113	1.82	8 (17%)
28	LMU	K	208	-	36,36,36	1.19	3 (8%)	47,47,47	1.30	5 (10%)
23	CLA	G	203	-	42,50,73	1.82	6 (14%)	48,85,113	1.74	7 (14%)
23	CLA	8	608	-	51,59,73	1.60	10 (19%)	59,96,113	1.62	7 (11%)
23	CLA	2	616	-	29,35,73	2.65	9 (31%)	28,60,113	1.78	6 (21%)
23	CLA	5	601	16	56,64,73	1.55	8 (14%)	65,102,113	1.42	8 (12%)
26	BCR	B	847	-	41,41,41	0.89	1 (2%)	56,56,56	2.01	19 (33%)
26	BCR	5	622	-	41,41,41	0.71	0	56,56,56	2.17	19 (33%)
30	DGD	J	103	-	59,59,67	0.99	3 (5%)	73,73,81	1.48	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	XAT	4	620	-	39,47,47	0.91	1 (2%)	54,74,74	2.59	20 (37%)
23	CLA	B	831	-	65,73,73	1.38	7 (10%)	76,113,113	1.61	6 (7%)
23	CLA	9	606	21	29,35,73	2.74	8 (27%)	28,60,113	1.68	4 (14%)
23	CLA	8	603	-	44,52,73	1.87	9 (20%)	55,88,113	1.65	12 (21%)
23	CLA	2	607	-	29,35,73	2.63	9 (31%)	28,60,113	1.72	4 (14%)
23	CLA	B	819	-	55,63,73	1.63	9 (16%)	64,101,113	1.51	6 (9%)
23	CLA	B	813	-	65,73,73	1.43	9 (13%)	76,113,113	1.46	10 (13%)
23	CLA	3	603	-	55,63,73	1.60	12 (21%)	64,101,113	1.71	10 (15%)
23	CLA	4	614	-	56,64,73	1.59	8 (14%)	65,102,113	1.46	9 (13%)
23	CLA	9	610	21	29,35,73	2.63	10 (34%)	28,60,113	1.70	5 (17%)
23	CLA	A	839	-	55,63,73	1.61	9 (16%)	64,101,113	1.50	7 (10%)
23	CLA	A	831	-	65,73,73	1.56	11 (16%)	76,113,113	1.70	12 (15%)
23	CLA	8	604	-	50,58,73	1.64	7 (14%)	58,95,113	1.63	8 (13%)
23	CLA	A	822	-	65,73,73	1.45	10 (15%)	76,113,113	1.49	8 (10%)
23	CLA	5	607	-	65,73,73	1.47	10 (15%)	76,113,113	1.58	8 (10%)
23	CLA	8	611	25	42,50,73	1.72	9 (21%)	48,85,113	1.69	9 (18%)
26	BCR	L	305	-	41,41,41	0.80	0	56,56,56	1.88	14 (25%)
23	CLA	5	603	-	54,62,73	1.70	10 (18%)	67,100,113	1.59	10 (14%)
23	CLA	A	825	-	65,73,73	1.45	10 (15%)	76,113,113	1.47	11 (14%)
25	LHG	A	847	23	29,29,48	0.95	1 (3%)	32,35,54	1.37	3 (9%)
23	CLA	B	824	-	65,73,73	1.46	7 (10%)	76,113,113	1.61	11 (14%)
23	CLA	9	609	21	29,35,73	2.62	8 (27%)	28,60,113	1.76	4 (14%)
23	CLA	B	816	-	54,62,73	1.55	7 (12%)	62,99,113	1.65	6 (9%)
26	BCR	B	801	-	41,41,41	0.77	0	56,56,56	2.05	13 (23%)
25	LHG	B	851	23	37,37,48	0.63	0	40,43,54	1.22	4 (10%)
23	CLA	A	837	1	45,53,73	1.76	9 (20%)	52,89,113	1.65	7 (13%)
23	CLA	a	612	13	45,53,73	1.73	8 (17%)	52,89,113	1.69	9 (17%)
23	CLA	B	841	25	43,51,73	1.83	7 (16%)	49,86,113	1.72	7 (14%)
23	CLA	a	608	-	43,52,73	1.77	6 (13%)	49,88,113	1.66	7 (14%)
26	BCR	a	619	-	41,41,41	0.69	0	56,56,56	2.01	16 (28%)
23	CLA	6	610	17	65,73,73	1.40	7 (10%)	76,113,113	1.45	9 (11%)
26	BCR	B	844	-	41,41,41	0.79	1 (2%)	56,56,56	1.95	15 (26%)
23	CLA	9	611	25	29,35,73	2.73	9 (31%)	28,60,113	1.75	6 (21%)
23	CLA	7	606	-	41,49,73	1.81	10 (24%)	47,84,113	1.74	9 (19%)
24	PQN	B	842	-	34,34,34	2.91	11 (32%)	42,45,45	2.04	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	3	609	14	60,68,73	1.53	7 (11%)	70,107,113	1.55	9 (12%)
23	CLA	A	854	-	65,73,73	1.42	9 (13%)	76,113,113	1.56	13 (17%)
23	CLA	B	838	-	47,55,73	1.63	10 (21%)	54,91,113	1.80	8 (14%)
23	CLA	2	610	20	29,35,73	2.61	8 (27%)	28,60,113	1.79	5 (17%)
25	LHG	A	846	-	48,48,48	0.72	1 (2%)	51,54,54	1.32	6 (11%)
24	PQN	A	844	-	34,34,34	2.89	11 (32%)	42,45,45	2.11	5 (11%)
23	CLA	B	834	-	60,68,73	1.51	8 (13%)	70,107,113	1.47	8 (11%)
23	CLA	A	806	-	65,73,73	1.47	13 (20%)	76,113,113	1.69	12 (15%)
26	BCR	J	102	-	41,41,41	0.84	1 (2%)	56,56,56	2.15	16 (28%)
23	CLA	7	603	-	43,52,73	1.79	9 (20%)	49,88,113	1.66	8 (16%)
23	CLA	5	617	-	50,58,73	1.67	10 (20%)	58,95,113	1.58	8 (13%)
23	CLA	8	609	19	45,53,73	1.68	8 (17%)	52,89,113	1.74	8 (15%)
23	CLA	9	614	-	29,35,73	2.65	9 (31%)	28,60,113	1.76	5 (17%)
23	CLA	5	609	16	65,73,73	1.47	10 (15%)	76,113,113	1.38	10 (13%)
23	CLA	A	805	-	52,60,73	1.66	10 (19%)	60,97,113	1.66	7 (11%)
23	CLA	1	601	13	53,62,73	1.60	10 (18%)	61,100,113	1.47	7 (11%)
26	BCR	8	621	-	41,41,41	0.74	0	56,56,56	1.98	18 (32%)
23	CLA	5	608	-	50,58,73	1.66	11 (22%)	58,95,113	1.54	7 (12%)
23	CLA	1	612	13	45,53,73	1.73	8 (17%)	52,89,113	1.69	9 (17%)
26	BCR	K	207	-	41,41,41	0.75	0	56,56,56	1.86	16 (28%)
25	LHG	8	622	23	48,48,48	0.63	1 (2%)	51,54,54	1.27	6 (11%)
23	CLA	3	615	-	39,48,73	1.81	8 (20%)	44,83,113	1.72	7 (15%)
23	CLA	4	607	-	45,53,73	1.77	9 (20%)	52,89,113	1.60	6 (11%)
23	CLA	4	603	15	44,52,73	1.83	9 (20%)	55,88,113	1.69	10 (18%)
23	CLA	K	206	11	45,53,73	1.73	7 (15%)	52,89,113	1.66	7 (13%)
25	LHG	4	622	23	48,48,48	0.60	0	51,54,54	1.29	6 (11%)
23	CLA	6	604	-	65,73,73	1.42	10 (15%)	76,113,113	1.42	8 (10%)
32	XAT	3	619	-	39,47,47	1.02	2 (5%)	54,74,74	2.60	22 (40%)
23	CLA	B	833	-	65,73,73	1.46	10 (15%)	76,113,113	1.54	10 (13%)
26	BCR	A	850	-	41,41,41	0.82	1 (2%)	56,56,56	2.02	18 (32%)
23	CLA	a	604	-	49,57,73	1.67	7 (14%)	55,93,113	1.67	6 (10%)
23	CLA	A	833	-	45,53,73	1.72	9 (20%)	52,89,113	1.73	6 (11%)
23	CLA	6	611	25	42,50,73	1.72	8 (19%)	48,85,113	1.62	7 (14%)
23	CLA	A	803	-	65,73,73	1.52	10 (15%)	76,113,113	1.54	6 (7%)
23	CLA	8	614	-	56,64,73	1.54	9 (16%)	65,102,113	1.53	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	824	-	41,49,73	1.75	8 (19%)	47,84,113	1.77	9 (19%)
27	SF4	A	853	-	0,12,12	-	-	-		
23	CLA	G	204	7	45,53,73	1.83	5 (11%)	52,89,113	1.78	12 (23%)
23	CLA	B	822	-	42,50,73	1.81	7 (16%)	48,85,113	1.66	7 (14%)
26	BCR	B	845	-	41,41,41	0.84	0	56,56,56	2.06	19 (33%)
23	CLA	7	601	18	60,68,73	1.53	11 (18%)	70,107,113	1.51	9 (12%)
23	CLA	4	610	15	61,69,73	1.47	9 (14%)	71,108,113	1.44	7 (9%)
23	CLA	A	807	1	65,73,73	1.49	10 (15%)	76,113,113	1.42	9 (11%)
23	CLA	6	606	-	39,48,73	1.84	8 (20%)	44,83,113	1.72	7 (15%)
31	LUT	4	619	-	42,43,43	0.82	0	51,60,60	1.70	11 (21%)
23	CLA	B	835	-	45,53,73	1.79	8 (17%)	52,89,113	1.74	11 (21%)
31	LUT	6	619	-	42,43,43	0.81	0	51,60,60	1.69	13 (25%)
23	CLA	1	614	-	37,45,73	2.12	10 (27%)	44,79,113	1.80	8 (18%)
23	CLA	5	604	-	63,71,73	1.54	9 (14%)	78,111,113	1.45	9 (11%)
26	BCR	K	202	-	41,41,41	0.79	0	56,56,56	2.26	20 (35%)
23	CLA	2	613	20	29,35,73	2.70	9 (31%)	28,60,113	1.66	5 (17%)
23	CLA	7	607	-	42,50,73	1.78	8 (19%)	48,85,113	1.86	9 (18%)
23	CLA	B	840	-	65,73,73	1.48	10 (15%)	76,113,113	1.46	7 (9%)
31	LUT	3	618	-	42,43,43	0.88	0	51,60,60	1.73	13 (25%)
25	LHG	7	622	23	36,36,48	0.70	0	39,42,54	1.23	4 (10%)
23	CLA	4	608	-	65,73,73	1.42	7 (10%)	76,113,113	1.56	8 (10%)
26	BCR	G	205	-	41,41,41	0.75	0	56,56,56	2.06	21 (37%)
23	CLA	1	608	-	43,52,73	1.77	5 (11%)	49,88,113	1.67	7 (14%)
23	CLA	2	609	20	29,35,73	2.76	9 (31%)	28,60,113	1.75	6 (21%)
25	LHG	6	623	23	47,47,48	0.64	1 (2%)	50,53,54	1.24	5 (10%)
23	CLA	B	809	2	65,73,73	1.43	11 (16%)	76,113,113	1.55	7 (9%)
23	CLA	6	608	-	51,59,73	1.67	11 (21%)	59,96,113	1.65	9 (15%)
23	CLA	a	614	-	55,62,73	1.72	9 (16%)	60,99,113	1.47	7 (11%)
23	CLA	B	829	-	65,73,73	1.55	10 (15%)	76,113,113	1.69	10 (13%)
23	CLA	A	830	-	65,73,73	1.46	11 (16%)	76,113,113	1.59	11 (14%)
23	CLA	B	806	2	65,73,73	1.47	11 (16%)	76,113,113	1.39	6 (7%)
23	CLA	3	606	-	53,62,73	1.62	9 (16%)	61,100,113	1.45	7 (11%)
28	LMU	A	859	-	35,35,36	1.33	3 (8%)	43,45,47	1.27	6 (13%)
23	CLA	6	603	-	54,62,73	1.67	9 (16%)	67,100,113	1.54	8 (11%)
23	CLA	2	606	20	29,35,73	2.72	8 (27%)	28,60,113	1.61	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	803	-	65,73,73	1.43	9 (13%)	76,113,113	1.80	13 (17%)
23	CLA	4	604	-	54,62,73	1.63	9 (16%)	67,100,113	1.46	7 (10%)
23	CLA	B	805	-	65,73,73	1.42	8 (12%)	76,113,113	1.66	9 (11%)
25	LHG	5	625	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
32	XAT	6	621	-	39,47,47	0.93	2 (5%)	54,74,74	2.61	20 (37%)
23	CLA	4	613	15	65,73,73	1.45	10 (15%)	76,113,113	1.45	7 (9%)
23	CLA	A	811	-	65,73,73	1.43	10 (15%)	76,113,113	1.52	10 (13%)
23	CLA	B	836	-	50,58,73	1.61	8 (16%)	58,95,113	1.73	11 (18%)
23	CLA	5	611	25	42,50,73	1.76	9 (21%)	48,85,113	1.62	8 (16%)
23	CLA	4	611	25	42,50,73	1.76	7 (16%)	48,85,113	1.64	7 (14%)
23	CLA	A	812	-	65,73,73	1.44	10 (15%)	76,113,113	1.52	10 (13%)
23	CLA	A	817	-	45,53,73	1.73	9 (20%)	52,89,113	1.75	9 (17%)
23	CLA	A	804	-	65,73,73	1.40	9 (13%)	76,113,113	1.62	11 (14%)
23	CLA	9	601	21	29,35,73	2.64	9 (31%)	28,60,113	1.68	4 (14%)
26	BCR	A	852	-	41,41,41	0.73	0	56,56,56	1.90	12 (21%)
23	CLA	A	838	-	50,58,73	1.56	8 (16%)	58,95,113	1.77	12 (20%)
23	CLA	A	829	-	65,73,73	1.42	10 (15%)	76,113,113	1.55	9 (11%)
28	LMU	8	624	-	36,36,36	1.19	2 (5%)	47,47,47	0.93	1 (2%)
23	CLA	A	823	-	42,50,73	1.77	9 (21%)	48,85,113	1.84	9 (18%)
23	CLA	3	610	14	65,73,73	1.41	9 (13%)	76,113,113	1.57	10 (13%)
23	CLA	6	602	17	65,73,73	1.43	9 (13%)	76,113,113	1.46	6 (7%)
23	CLA	1	610	13	38,47,73	1.90	9 (23%)	44,81,113	1.76	8 (18%)
23	CLA	A	832	-	50,58,73	1.65	11 (22%)	58,95,113	1.66	9 (15%)
23	CLA	B	802	-	65,73,73	1.47	10 (15%)	76,113,113	1.34	7 (9%)
23	CLA	1	604	-	49,57,73	1.68	7 (14%)	55,93,113	1.67	6 (10%)
32	XAT	5	621	-	39,47,47	1.02	2 (5%)	54,74,74	2.89	23 (42%)
31	LUT	2	619	-	42,43,43	0.75	0	51,60,60	1.77	13 (25%)
23	CLA	A	808	-	50,58,73	1.63	10 (20%)	58,95,113	1.65	9 (15%)
23	CLA	A	821	-	53,61,73	1.57	10 (18%)	61,98,113	1.61	7 (11%)
23	CLA	B	823	-	45,53,73	1.73	7 (15%)	52,89,113	1.76	8 (15%)
23	CLA	B	817	-	59,67,73	1.54	10 (16%)	68,105,113	1.57	9 (13%)
23	CLA	A	828	-	65,73,73	1.43	10 (15%)	76,113,113	1.44	8 (10%)
23	CLA	8	602	19	60,68,73	1.52	9 (15%)	70,107,113	1.58	10 (14%)
23	CLA	B	839	-	65,73,73	1.44	10 (15%)	76,113,113	1.51	9 (11%)
30	DGD	B	850	-	63,63,67	1.06	5 (7%)	77,77,81	1.55	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	XAT	7	620	-	39,47,47	1.04	2 (5%)	54,74,74	2.59	18 (33%)
23	CLA	a	606	13	43,52,73	1.78	7 (16%)	48,87,113	1.60	6 (12%)
23	CLA	6	616	17	65,73,73	1.42	7 (10%)	76,113,113	1.68	13 (17%)
23	CLA	F	301	-	57,65,73	1.57	10 (17%)	66,103,113	1.44	5 (7%)
33	NEX	6	624	-	38,46,46	1.01	2 (5%)	50,70,70	2.27	17 (34%)
32	XAT	1	618	-	39,47,47	0.93	2 (5%)	54,74,74	2.58	18 (33%)
23	CLA	A	802	-	65,73,73	1.48	10 (15%)	76,113,113	1.71	10 (13%)
28	LMU	A	858	-	34,35,36	1.29	2 (5%)	42,45,47	1.28	6 (14%)
26	BCR	7	623	-	41,41,41	0.68	0	56,56,56	1.81	13 (23%)
26	BCR	B	846	-	41,41,41	0.88	2 (4%)	56,56,56	2.17	25 (44%)
23	CLA	B	811	-	52,61,73	1.67	9 (17%)	64,99,113	1.56	10 (15%)
29	LMG	4	623	-	40,40,55	0.90	1 (2%)	48,48,63	1.28	5 (10%)
23	CLA	8	601	19	65,73,73	1.44	9 (13%)	76,113,113	1.52	10 (13%)
26	BCR	3	621	-	41,41,41	0.72	0	56,56,56	2.28	19 (33%)
23	CLA	A	826	-	64,72,73	1.43	8 (12%)	74,111,113	1.58	10 (13%)
23	CLA	8	606	-	64,72,73	1.45	9 (14%)	75,112,113	1.48	8 (10%)
23	CLA	2	603	20	29,35,73	2.70	9 (31%)	28,60,113	1.77	6 (21%)
32	XAT	2	620	-	39,47,47	0.89	0	54,74,74	2.65	14 (25%)
23	CLA	F	303	-	42,50,73	1.83	8 (19%)	48,85,113	1.71	10 (20%)
23	CLA	B	828	-	65,73,73	1.48	10 (15%)	76,113,113	1.48	9 (11%)
23	CLA	9	602	21	29,35,73	2.64	9 (31%)	28,60,113	1.76	4 (14%)
23	CLA	B	825	-	62,70,73	1.42	10 (16%)	72,109,113	1.46	11 (15%)
23	CLA	A	845	25	50,58,73	1.63	10 (20%)	58,95,113	1.67	7 (12%)
23	CLA	1	609	13	40,48,73	1.83	7 (17%)	50,83,113	1.84	12 (24%)
26	BCR	1	619	-	41,41,41	0.68	0	56,56,56	2.01	16 (28%)
23	CLA	B	804	-	41,49,73	1.81	10 (24%)	47,84,113	1.85	8 (17%)
31	LUT	1	617	-	42,43,43	0.79	0	51,60,60	1.56	12 (23%)
23	CLA	A	816	-	43,52,73	1.76	7 (16%)	48,87,113	1.82	6 (12%)
23	CLA	A	814	-	65,73,73	1.44	10 (15%)	76,113,113	1.56	12 (15%)
23	CLA	2	602	20	29,35,73	2.65	9 (31%)	28,60,113	1.69	3 (10%)
26	BCR	6	622	-	41,41,41	0.69	0	56,56,56	1.94	17 (30%)
23	CLA	1	616	13	43,51,73	1.85	9 (20%)	54,87,113	1.61	8 (14%)
25	LHG	8	623	-	46,46,48	0.66	1 (2%)	49,52,54	1.24	5 (10%)
23	CLA	1	606	13	37,47,73	1.90	6 (16%)	41,80,113	1.77	7 (17%)
23	CLA	4	618	15	39,48,73	1.93	9 (23%)	48,83,113	1.67	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	7	602	18	65,73,73	1.48	9 (13%)	76,113,113	1.40	7 (9%)
32	XAT	9	620	-	39,47,47	0.92	0	54,74,74	2.63	16 (29%)
23	CLA	7	613	18	65,73,73	1.46	9 (13%)	76,113,113	1.42	8 (10%)
23	CLA	1	613	-	65,73,73	1.46	9 (13%)	76,113,113	1.52	9 (11%)
23	CLA	B	821	-	43,51,73	1.86	9 (20%)	48,86,113	1.78	9 (18%)
29	LMG	J	104	-	40,40,55	0.89	2 (5%)	48,48,63	1.26	5 (10%)
33	NEX	5	624	-	38,46,46	0.93	0	50,70,70	2.49	19 (38%)
23	CLA	3	608	-	55,63,73	1.62	10 (18%)	64,101,113	1.62	9 (14%)
23	CLA	F	304	-	41,49,73	1.78	7 (17%)	47,84,113	1.78	7 (14%)
23	CLA	A	841	-	65,73,73	1.42	10 (15%)	76,113,113	1.57	9 (11%)
23	CLA	4	602	15	60,68,73	1.46	7 (11%)	70,107,113	1.62	8 (11%)
23	CLA	A	835	-	61,69,73	1.51	10 (16%)	71,108,113	1.57	8 (11%)
23	CLA	1	602	13	61,69,73	1.46	8 (13%)	71,108,113	1.51	7 (9%)
23	CLA	A	827	-	59,67,73	1.51	8 (13%)	68,105,113	1.59	10 (14%)
23	CLA	B	837	-	65,73,73	1.48	10 (15%)	76,113,113	1.46	7 (9%)
23	CLA	a	611	25	37,46,73	1.88	9 (24%)	46,81,113	1.87	10 (21%)
23	CLA	3	613	14	52,61,73	1.61	9 (17%)	59,98,113	1.55	7 (11%)
23	CLA	6	612	17	40,49,73	1.83	7 (17%)	45,84,113	1.78	9 (20%)
29	LMG	5	627	-	40,40,55	0.91	2 (5%)	48,48,63	1.20	4 (8%)
26	BCR	A	848	-	41,41,41	0.92	1 (2%)	56,56,56	2.07	17 (30%)
23	CLA	3	612	14	43,51,73	1.83	9 (20%)	49,86,113	1.65	8 (16%)
23	CLA	3	614	-	39,48,73	1.85	9 (23%)	44,83,113	1.66	8 (18%)
25	LHG	a	620	23	48,48,48	0.60	1 (2%)	51,54,54	1.26	6 (11%)
23	CLA	5	619	-	43,51,73	1.81	10 (23%)	54,87,113	2.04	12 (22%)
23	CLA	B	814	-	64,72,73	1.43	9 (14%)	74,111,113	1.52	8 (10%)
23	CLA	a	609	13	63,72,73	1.45	7 (11%)	73,112,113	1.39	8 (10%)
23	CLA	L	302	12	45,53,73	1.79	5 (11%)	52,89,113	1.67	8 (15%)
23	CLA	A	819	-	59,67,73	1.57	10 (16%)	68,105,113	1.52	8 (11%)
32	XAT	8	620	-	39,47,47	1.00	2 (5%)	54,74,74	2.70	19 (35%)
23	CLA	9	613	21	29,35,73	2.70	8 (27%)	28,60,113	1.72	4 (14%)
23	CLA	7	615	-	41,50,73	1.90	7 (17%)	50,85,113	1.76	9 (18%)
23	CLA	9	604	-	29,35,73	2.63	9 (31%)	28,60,113	1.73	5 (17%)
23	CLA	A	810	1	50,58,73	1.63	10 (20%)	58,95,113	1.58	7 (12%)
23	CLA	K	204	-	46,54,73	1.72	7 (15%)	53,90,113	1.60	8 (15%)
23	CLA	3	607	14	56,64,73	1.58	9 (16%)	69,102,113	1.54	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	820	-	65,73,73	1.52	11 (16%)	76,113,113	1.68	15 (19%)
25	LHG	2	622	23	36,36,48	0.78	1 (2%)	39,42,54	1.29	5 (12%)
23	CLA	B	807	-	52,60,73	1.61	10 (19%)	60,97,113	1.53	7 (11%)
23	CLA	3	604	-	65,73,73	1.47	10 (15%)	76,113,113	1.44	7 (9%)
23	CLA	6	618	17	39,48,73	1.89	9 (23%)	48,83,113	1.75	10 (20%)
25	LHG	3	624	23	48,48,48	0.66	0	51,54,54	1.24	5 (9%)
23	CLA	5	612	16	40,49,73	1.77	8 (20%)	45,84,113	1.81	8 (17%)
23	CLA	B	830	-	43,51,73	1.78	11 (25%)	49,86,113	1.71	6 (12%)
23	CLA	B	827	-	62,70,73	1.48	8 (12%)	72,109,113	1.51	8 (11%)
23	CLA	7	608	-	50,58,73	1.63	10 (20%)	58,95,113	1.53	7 (12%)
23	CLA	2	612	20	29,35,73	2.72	8 (27%)	28,60,113	1.68	3 (10%)
23	CLA	B	826	-	55,63,73	1.58	8 (14%)	64,101,113	1.56	8 (12%)
23	CLA	A	818	-	60,68,73	1.45	8 (13%)	70,107,113	1.60	7 (10%)
23	CLA	a	607	-	45,53,73	1.74	7 (15%)	52,89,113	1.64	7 (13%)
23	CLA	J	101	10	42,50,73	1.80	7 (16%)	48,85,113	1.71	8 (16%)
25	LHG	5	623	23	48,48,48	0.62	1 (2%)	51,54,54	1.21	5 (9%)
23	CLA	A	842	-	65,73,73	1.45	10 (15%)	76,113,113	1.43	7 (9%)
23	CLA	K	203	-	65,73,73	1.47	8 (12%)	76,113,113	1.43	7 (9%)
26	BCR	A	856	-	41,41,41	0.70	0	56,56,56	1.99	19 (33%)
31	LUT	7	619	-	42,43,43	0.95	2 (4%)	51,60,60	1.79	16 (31%)
23	CLA	4	601	15	65,73,73	1.44	8 (12%)	76,113,113	1.49	8 (10%)
23	CLA	1	603	-	52,61,73	1.63	9 (17%)	59,98,113	1.68	9 (15%)
23	CLA	6	609	17	45,53,73	1.78	9 (20%)	52,89,113	1.69	8 (15%)
23	CLA	9	612	21	29,35,73	2.71	9 (31%)	28,60,113	1.67	4 (14%)
23	CLA	A	815	-	50,58,73	1.64	9 (18%)	58,95,113	1.69	11 (18%)
23	CLA	5	602	16	65,73,73	1.44	7 (10%)	76,113,113	1.57	8 (10%)
23	CLA	7	612	18	44,52,73	1.83	9 (20%)	51,88,113	1.63	9 (17%)
29	LMG	7	624	-	44,44,55	0.83	1 (2%)	52,52,63	1.26	6 (11%)
23	CLA	1	611	25	65,73,73	1.40	9 (13%)	76,113,113	1.45	8 (10%)
23	CLA	3	617	14	39,48,73	1.86	9 (23%)	44,83,113	1.78	8 (18%)
23	CLA	9	607	-	29,35,73	2.60	9 (31%)	28,60,113	1.79	6 (21%)
23	CLA	A	840	-	52,60,73	1.62	10 (19%)	60,97,113	1.69	10 (16%)
27	SF4	C	102	-	0,12,12	-	-	-	-	-
23	CLA	9	603	21	29,35,73	2.66	9 (31%)	28,60,113	1.63	4 (14%)
23	CLA	L	304	-	45,53,73	1.76	5 (11%)	52,89,113	1.66	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	9	622	23	48,48,48	0.62	0	51,54,54	1.23	6 (11%)
23	CLA	5	618	16	39,48,73	1.91	8 (20%)	48,83,113	1.74	9 (18%)
23	CLA	6	607	-	41,49,73	1.84	9 (21%)	51,84,113	1.78	12 (23%)
31	LUT	5	620	-	42,43,43	0.80	0	51,60,60	1.70	13 (25%)
23	CLA	A	834	-	65,73,73	1.45	10 (15%)	76,113,113	1.47	7 (9%)
26	BCR	L	301	-	41,41,41	0.84	0	56,56,56	1.78	16 (28%)
23	CLA	7	604	-	54,62,73	1.56	8 (14%)	63,100,113	1.66	10 (15%)
23	CLA	6	620	-	64,72,73	1.43	10 (15%)	74,111,113	1.49	7 (9%)
23	CLA	4	612	15	40,49,73	1.80	7 (17%)	45,84,113	1.78	8 (17%)
23	CLA	2	611	25	30,33,73	3.40	10 (33%)	24,56,113	1.05	2 (8%)
29	LMG	4	624	-	40,40,55	1.01	4 (10%)	48,48,63	1.29	6 (12%)
23	CLA	A	801	-	65,73,73	1.48	10 (15%)	76,113,113	1.41	7 (9%)
23	CLA	8	607	-	41,49,73	1.83	9 (21%)	51,84,113	1.75	9 (17%)
23	CLA	A	836	-	65,73,73	1.44	10 (15%)	76,113,113	1.53	7 (9%)
26	BCR	3	622	-	41,41,41	0.79	0	56,56,56	2.67	21 (37%)
31	LUT	9	619	-	42,43,43	0.76	0	51,60,60	1.67	11 (21%)
23	CLA	8	616	19	43,51,73	1.89	7 (16%)	54,87,113	1.85	12 (22%)
23	CLA	B	832	-	60,68,73	1.48	10 (16%)	70,107,113	1.57	10 (14%)
23	CLA	6	614	-	60,68,73	1.50	7 (11%)	70,107,113	1.47	6 (8%)
23	CLA	B	820	-	50,58,73	1.62	7 (14%)	58,95,113	1.62	7 (12%)
23	CLA	4	606	-	39,48,73	1.84	8 (20%)	44,83,113	1.70	8 (18%)
23	CLA	8	613	19	65,73,73	1.48	9 (13%)	76,113,113	1.64	10 (13%)
23	CLA	B	812	-	43,51,73	1.78	7 (16%)	49,86,113	1.72	7 (14%)
23	CLA	5	613	16	64,72,73	1.56	9 (14%)	74,111,113	1.54	7 (9%)
26	BCR	3	620	-	41,41,41	0.83	0	56,56,56	2.17	20 (35%)
23	CLA	3	611	25	37,46,73	1.94	8 (21%)	46,81,113	1.82	10 (21%)
26	BCR	7	621	-	41,41,41	0.80	0	56,56,56	2.04	18 (32%)
23	CLA	1	607	-	39,48,73	1.85	7 (17%)	44,83,113	1.72	7 (15%)
23	CLA	A	813	-	54,62,73	1.55	9 (16%)	62,99,113	1.64	7 (11%)
23	CLA	a	603	-	42,50,73	1.77	9 (21%)	48,85,113	1.86	9 (18%)
23	CLA	B	808	-	65,73,73	1.46	10 (15%)	76,113,113	1.66	11 (14%)
23	CLA	2	604	-	29,35,73	2.68	8 (27%)	28,60,113	1.80	6 (21%)
26	BCR	B	843	-	41,41,41	0.79	0	56,56,56	1.92	14 (25%)
23	CLA	7	611	25	59,67,73	1.47	9 (15%)	68,105,113	1.56	8 (11%)
23	CLA	B	815	-	43,51,73	1.70	10 (23%)	49,86,113	1.74	7 (14%)

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	B	818	-	1/1/14/20	14/31/109/115	-
29	LMG	A	860	-	-	18/35/55/70	0/1/1/1
23	CLA	5	606	-	1/1/10/20	2/6/84/115	-
31	LUT	8	619	-	-	2/29/67/67	0/2/2/2
23	CLA	2	601	20	1/1/5/20	-	-
23	CLA	K	201	11	1/1/11/20	6/13/91/115	-
23	CLA	a	610	13	1/1/14/20	5/29/107/115	-
23	CLA	6	601	17	1/1/15/20	14/37/115/115	-
32	XAT	a	618	-	-	1/31/93/93	0/4/4/4
23	CLA	6	617	-	1/1/11/20	7/13/91/115	-
23	CLA	5	614	-	1/1/10/20	7/13/87/115	-
23	CLA	a	602	13	1/1/14/20	6/33/111/115	-
23	CLA	5	616	16	1/1/10/20	4/8/84/115	-
23	CLA	a	616	13	1/1/11/20	4/13/91/115	-
23	CLA	7	609	18	1/1/10/20	4/10/88/115	-
23	CLA	7	610	18	1/1/15/20	6/37/115/115	-
23	CLA	A	809	1	1/1/15/20	12/37/115/115	-
27	SF4	C	101	-	-	-	0/6/5/5
28	LMU	8	625	-	-	10/21/61/61	0/2/2/2
26	BCR	F	305	-	-	2/29/63/63	0/2/2/2
28	LMU	A	857	-	-	11/21/61/61	0/2/2/2
23	CLA	6	613	-	1/1/15/20	13/35/113/115	-
26	BCR	A	851	-	-	4/29/63/63	0/2/2/2
29	LMG	5	626	-	-	23/35/55/70	0/1/1/1
25	LHG	1	620	23	-	24/53/53/53	-
23	CLA	7	616	18	1/1/11/20	7/11/87/115	-
23	CLA	a	613	-	1/1/15/20	12/37/115/115	-
23	CLA	8	610	19	1/1/14/20	7/31/109/115	-
25	LHG	3	623	-	-	26/49/49/53	-
23	CLA	L	303	-	1/1/11/20	5/13/91/115	-
23	CLA	a	601	13	1/1/13/20	5/23/101/115	-
23	CLA	5	610	16	1/1/12/20	5/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	4	609	15	1/1/14/20	13/33/111/115	-
26	BCR	B	848	-	-	4/29/63/63	0/2/2/2
28	LMU	5	628	-	-	11/19/59/61	0/2/2/2
23	CLA	B	810	-	1/1/14/20	15/35/113/115	-
26	BCR	A	849	-	-	5/29/63/63	0/2/2/2
26	BCR	4	621	-	-	1/29/63/63	0/2/2/2
31	LUT	a	617	-	-	2/29/67/67	0/2/2/2
23	CLA	2	614	-	1/1/5/20	-	-
23	CLA	3	602	14	1/1/14/20	8/31/109/115	-
23	CLA	4	616	15	1/1/11/20	6/11/87/115	-
23	CLA	7	614	-	1/1/10/20	3/10/88/115	-
23	CLA	A	843	-	1/1/14/20	16/35/113/115	-
23	CLA	8	612	19	1/1/10/20	2/8/86/115	-
28	LMU	K	208	-	-	10/21/61/61	0/2/2/2
23	CLA	G	203	-	1/1/10/20	3/10/88/115	-
23	CLA	8	608	-	1/1/12/20	4/21/99/115	-
23	CLA	2	616	-	1/1/5/20	-	-
23	CLA	5	601	16	1/1/13/20	6/27/105/115	-
26	BCR	B	847	-	-	1/29/63/63	0/2/2/2
26	BCR	5	622	-	-	3/29/63/63	0/2/2/2
30	DGD	J	103	-	-	25/47/87/95	0/2/2/2
32	XAT	4	620	-	-	1/31/93/93	0/4/4/4
23	CLA	B	831	-	1/1/15/20	12/37/115/115	-
23	CLA	9	606	21	1/1/5/20	-	-
23	CLA	8	603	-	1/1/11/20	8/13/89/115	-
23	CLA	2	607	-	1/1/5/20	-	-
23	CLA	B	819	-	1/1/13/20	11/25/103/115	-
23	CLA	B	813	-	1/1/15/20	20/37/115/115	-
23	CLA	3	603	-	1/1/13/20	11/25/103/115	-
23	CLA	4	614	-	1/1/13/20	7/27/105/115	-
23	CLA	9	610	21	1/1/5/20	-	-
23	CLA	A	839	-	1/1/13/20	5/25/103/115	-
23	CLA	A	831	-	1/1/15/20	14/37/115/115	-
23	CLA	8	604	-	1/1/12/20	5/19/97/115	-
23	CLA	A	822	-	1/1/15/20	13/37/115/115	-
23	CLA	5	607	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	8	611	25	1/1/10/20	4/10/88/115	-
26	BCR	L	305	-	-	10/29/63/63	0/2/2/2
23	CLA	5	603	-	1/1/13/20	10/25/101/115	-
23	CLA	A	825	-	1/1/15/20	18/37/115/115	-
25	LHG	A	847	23	-	11/34/34/53	-
23	CLA	B	824	-	1/1/15/20	9/37/115/115	-
23	CLA	9	609	21	1/1/5/20	-	-
23	CLA	B	816	-	1/1/12/20	10/23/101/115	-
26	BCR	B	801	-	-	4/29/63/63	0/2/2/2
25	LHG	B	851	23	-	22/42/42/53	-
23	CLA	A	837	1	1/1/11/20	7/13/91/115	-
23	CLA	a	612	13	1/1/11/20	6/13/91/115	-
23	CLA	B	841	25	1/1/10/20	1/11/89/115	-
23	CLA	a	608	-	1/1/11/20	4/11/89/115	-
26	BCR	a	619	-	-	4/29/63/63	0/2/2/2
23	CLA	6	610	17	1/1/15/20	10/37/115/115	-
26	BCR	B	844	-	-	9/29/63/63	0/2/2/2
23	CLA	9	611	25	1/1/5/20	-	-
23	CLA	7	606	-	1/1/10/20	2/8/86/115	-
24	PQN	B	842	-	-	7/23/43/43	0/2/2/2
23	CLA	3	609	14	1/1/14/20	16/31/109/115	-
23	CLA	A	854	-	1/1/15/20	13/37/115/115	-
23	CLA	B	838	-	1/1/11/20	5/16/94/115	-
23	CLA	2	610	20	1/1/5/20	-	-
25	LHG	A	846	-	-	25/53/53/53	-
24	PQN	A	844	-	-	8/23/43/43	0/2/2/2
23	CLA	B	834	-	1/1/14/20	13/31/109/115	-
23	CLA	A	806	-	1/1/15/20	15/37/115/115	-
26	BCR	J	102	-	-	5/29/63/63	0/2/2/2
23	CLA	7	603	-	1/1/11/20	2/11/89/115	-
23	CLA	5	617	-	1/1/12/20	6/19/97/115	-
23	CLA	8	609	19	1/1/11/20	4/13/91/115	-
23	CLA	9	614	-	1/1/5/20	-	-
23	CLA	5	609	16	1/1/15/20	13/37/115/115	-
23	CLA	A	805	-	1/1/12/20	5/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	1	601	13	1/1/13/20	5/23/101/115	-
26	BCR	8	621	-	-	6/29/63/63	0/2/2/2
23	CLA	5	608	-	1/1/12/20	7/19/97/115	-
23	CLA	1	612	13	1/1/11/20	6/13/91/115	-
26	BCR	K	207	-	-	3/29/63/63	0/2/2/2
25	LHG	8	622	23	-	26/53/53/53	-
23	CLA	3	615	-	1/1/10/20	1/6/84/115	-
23	CLA	4	607	-	1/1/11/20	5/13/91/115	-
23	CLA	4	603	15	1/1/11/20	7/13/89/115	-
23	CLA	K	206	11	1/1/11/20	5/13/91/115	-
25	LHG	4	622	23	-	21/53/53/53	-
23	CLA	6	604	-	1/1/15/20	22/37/115/115	-
32	XAT	3	619	-	-	1/31/93/93	0/4/4/4
23	CLA	B	833	-	1/1/15/20	19/37/115/115	-
26	BCR	A	850	-	-	1/29/63/63	0/2/2/2
23	CLA	a	604	-	1/1/11/20	10/18/96/115	-
23	CLA	A	833	-	1/1/11/20	2/13/91/115	-
23	CLA	6	611	25	1/1/10/20	3/10/88/115	-
23	CLA	A	803	-	1/1/15/20	9/37/115/115	-
23	CLA	8	614	-	1/1/13/20	10/27/105/115	-
23	CLA	A	824	-	1/1/10/20	0/8/86/115	-
27	SF4	A	853	-	-	-	0/6/5/5
23	CLA	G	204	7	1/1/11/20	6/13/91/115	-
23	CLA	B	822	-	-	4/10/88/115	-
26	BCR	B	845	-	-	5/29/63/63	0/2/2/2
23	CLA	7	601	18	1/1/14/20	13/31/109/115	-
23	CLA	4	610	15	1/1/14/20	12/33/111/115	-
23	CLA	A	807	1	1/1/15/20	13/37/115/115	-
23	CLA	6	606	-	1/1/10/20	0/6/84/115	-
31	LUT	4	619	-	-	4/29/67/67	0/2/2/2
23	CLA	B	835	-	1/1/11/20	8/13/91/115	-
31	LUT	6	619	-	-	2/29/67/67	0/2/2/2
23	CLA	1	614	-	1/1/9/20	0/4/76/115	-
23	CLA	5	604	-	1/1/15/20	13/35/111/115	-
26	BCR	K	202	-	-	4/29/63/63	0/2/2/2
23	CLA	2	613	20	1/1/5/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	7	607	-	1/1/10/20	6/10/88/115	-
23	CLA	B	840	-	1/1/15/20	9/37/115/115	-
31	LUT	3	618	-	-	2/29/67/67	0/2/2/2
25	LHG	7	622	23	-	24/41/41/53	-
23	CLA	4	608	-	1/1/15/20	11/37/115/115	-
26	BCR	G	205	-	-	0/29/63/63	0/2/2/2
23	CLA	1	608	-	1/1/11/20	4/11/89/115	-
23	CLA	2	609	20	1/1/5/20	-	-
25	LHG	6	623	23	-	23/52/52/53	-
23	CLA	B	809	2	1/1/15/20	15/37/115/115	-
23	CLA	6	608	-	1/1/12/20	8/21/99/115	-
23	CLA	a	614	-	1/1/12/20	10/25/99/115	-
23	CLA	B	829	-	1/1/15/20	7/37/115/115	-
23	CLA	A	830	-	1/1/15/20	14/37/115/115	-
23	CLA	B	806	2	1/1/15/20	13/37/115/115	-
23	CLA	3	606	-	1/1/13/20	10/23/101/115	-
28	LMU	A	859	-	-	13/21/57/61	0/2/2/2
23	CLA	6	603	-	1/1/13/20	4/25/101/115	-
23	CLA	2	606	20	1/1/5/20	-	-
23	CLA	B	803	-	1/1/15/20	15/37/115/115	-
23	CLA	4	604	-	1/1/13/20	6/25/101/115	-
23	CLA	B	805	-	1/1/15/20	16/37/115/115	-
25	LHG	5	625	-	-	23/53/53/53	-
32	XAT	6	621	-	-	2/31/93/93	0/4/4/4
23	CLA	4	613	15	1/1/15/20	12/37/115/115	-
23	CLA	A	811	-	1/1/15/20	16/37/115/115	-
23	CLA	5	611	25	1/1/10/20	3/10/88/115	-
23	CLA	B	836	-	-	6/19/97/115	-
23	CLA	4	611	25	1/1/10/20	4/10/88/115	-
23	CLA	A	812	-	1/1/15/20	11/37/115/115	-
23	CLA	A	817	-	1/1/11/20	5/13/91/115	-
23	CLA	A	804	-	1/1/15/20	11/37/115/115	-
23	CLA	9	601	21	1/1/5/20	-	-
26	BCR	A	852	-	-	11/29/63/63	0/2/2/2
23	CLA	A	838	-	1/1/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	829	-	1/1/15/20	11/37/115/115	-
28	LMU	8	624	-	-	6/21/61/61	0/2/2/2
23	CLA	A	823	-	1/1/10/20	5/10/88/115	-
23	CLA	3	610	14	1/1/15/20	16/37/115/115	-
23	CLA	6	602	17	1/1/15/20	8/37/115/115	-
23	CLA	1	610	13	1/1/9/20	1/6/80/115	-
23	CLA	A	832	-	1/1/12/20	7/19/97/115	-
23	CLA	B	802	-	1/1/15/20	19/37/115/115	-
23	CLA	1	604	-	1/1/11/20	10/18/96/115	-
32	XAT	5	621	-	-	2/31/93/93	0/4/4/4
31	LUT	2	619	-	-	2/29/67/67	0/2/2/2
23	CLA	A	808	-	1/1/12/20	0/19/97/115	-
23	CLA	A	821	-	1/1/12/20	12/23/101/115	-
23	CLA	B	823	-	1/1/11/20	4/13/91/115	-
23	CLA	B	817	-	1/1/13/20	10/30/108/115	-
23	CLA	A	828	-	1/1/15/20	9/37/115/115	-
23	CLA	8	602	19	1/1/14/20	8/31/109/115	-
23	CLA	B	839	-	1/1/15/20	12/37/115/115	-
30	DGD	B	850	-	-	22/51/91/95	0/2/2/2
32	XAT	7	620	-	-	1/31/93/93	0/4/4/4
23	CLA	a	606	13	1/1/10/20	3/10/88/115	-
23	CLA	6	616	17	1/1/15/20	18/37/115/115	-
23	CLA	F	301	-	1/1/13/20	9/28/106/115	-
33	NEX	6	624	-	-	4/27/83/83	0/3/3/3
32	XAT	1	618	-	-	1/31/93/93	0/4/4/4
23	CLA	A	802	-	1/1/15/20	9/37/115/115	-
28	LMU	A	858	-	-	6/21/57/61	0/2/2/2
26	BCR	7	623	-	-	0/29/63/63	0/2/2/2
26	BCR	B	846	-	-	5/29/63/63	0/2/2/2
23	CLA	B	811	-	1/1/13/20	8/23/99/115	-
29	LMG	4	623	-	-	11/35/55/70	0/1/1/1
23	CLA	8	601	19	1/1/15/20	20/37/115/115	-
26	BCR	3	621	-	-	6/29/63/63	0/2/2/2
23	CLA	A	826	-	1/1/14/20	12/35/113/115	-
23	CLA	8	606	-	1/1/15/20	14/35/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	2	603	20	1/1/5/20	-	-
32	XAT	2	620	-	-	0/31/93/93	0/4/4/4
23	CLA	F	303	-	1/1/10/20	5/10/88/115	-
23	CLA	B	828	-	1/1/15/20	16/37/115/115	-
23	CLA	9	602	21	1/1/5/20	-	-
23	CLA	B	825	-	1/1/14/20	9/34/112/115	-
23	CLA	A	845	25	1/1/12/20	9/19/97/115	-
23	CLA	1	609	13	1/1/10/20	5/8/84/115	-
26	BCR	1	619	-	-	4/29/63/63	0/2/2/2
23	CLA	B	804	-	1/1/10/20	3/8/86/115	-
31	LUT	1	617	-	-	2/29/67/67	0/2/2/2
23	CLA	A	816	-	1/1/10/20	2/10/88/115	-
23	CLA	A	814	-	1/1/15/20	20/37/115/115	-
23	CLA	2	602	20	1/1/5/20	-	-
26	BCR	6	622	-	-	7/29/63/63	0/2/2/2
23	CLA	1	616	13	1/1/11/20	4/11/87/115	-
25	LHG	8	623	-	-	24/51/51/53	-
23	CLA	1	606	13	1/1/8/20	1/5/79/115	-
23	CLA	4	618	15	1/1/10/20	0/8/84/115	-
23	CLA	7	602	18	1/1/15/20	16/37/115/115	-
32	XAT	9	620	-	-	0/31/93/93	0/4/4/4
23	CLA	7	613	18	1/1/15/20	17/37/115/115	-
23	CLA	1	613	-	1/1/15/20	12/37/115/115	-
23	CLA	B	821	-	1/1/11/20	3/11/89/115	-
29	LMG	J	104	-	-	19/35/55/70	0/1/1/1
33	NEX	5	624	-	-	2/27/83/83	0/3/3/3
23	CLA	3	608	-	1/1/13/20	9/25/103/115	-
23	CLA	F	304	-	1/1/10/20	4/8/86/115	-
23	CLA	A	841	-	1/1/15/20	18/37/115/115	-
23	CLA	4	602	15	1/1/14/20	10/31/109/115	-
23	CLA	A	835	-	1/1/14/20	13/33/111/115	-
23	CLA	1	602	13	1/1/14/20	6/33/111/115	-
23	CLA	A	827	-	1/1/13/20	5/30/108/115	-
23	CLA	B	837	-	1/1/15/20	15/37/115/115	-
23	CLA	a	611	25	1/1/10/20	0/4/80/115	-
23	CLA	3	613	14	1/1/12/20	5/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	6	612	17	1/1/10/20	2/8/86/115	-
29	LMG	5	627	-	-	13/35/55/70	0/1/1/1
26	BCR	A	848	-	-	4/29/63/63	0/2/2/2
23	CLA	3	612	14	1/1/10/20	3/11/89/115	-
23	CLA	3	614	-	1/1/10/20	0/6/84/115	-
25	LHG	a	620	23	-	24/53/53/53	-
23	CLA	5	619	-	1/1/11/20	7/11/87/115	-
23	CLA	B	814	-	1/1/14/20	12/36/114/115	-
23	CLA	a	609	13	1/1/15/20	19/35/113/115	-
23	CLA	L	302	12	1/1/11/20	3/13/91/115	-
23	CLA	A	819	-	1/1/13/20	8/30/108/115	-
32	XAT	8	620	-	-	2/31/93/93	0/4/4/4
23	CLA	9	613	21	1/1/5/20	-	-
23	CLA	7	615	-	1/1/10/20	4/8/84/115	-
23	CLA	9	604	-	1/1/5/20	-	-
23	CLA	A	810	1	1/1/12/20	5/19/97/115	-
23	CLA	K	204	-	1/1/11/20	7/15/93/115	-
23	CLA	3	607	14	1/1/13/20	9/28/104/115	-
23	CLA	A	820	-	1/1/15/20	15/37/115/115	-
25	LHG	2	622	23	-	19/41/41/53	-
23	CLA	B	807	-	1/1/12/20	4/22/100/115	-
23	CLA	3	604	-	1/1/15/20	11/37/115/115	-
23	CLA	6	618	17	1/1/10/20	2/8/84/115	-
25	LHG	3	624	23	-	26/53/53/53	-
23	CLA	5	612	16	1/1/10/20	3/8/86/115	-
23	CLA	B	830	-	1/1/10/20	2/11/89/115	-
23	CLA	B	827	-	1/1/14/20	14/34/112/115	-
23	CLA	7	608	-	1/1/12/20	4/19/97/115	-
23	CLA	2	612	20	1/1/5/20	-	-
23	CLA	B	826	-	1/1/13/20	8/25/103/115	-
23	CLA	A	818	-	1/1/14/20	12/31/109/115	-
23	CLA	a	607	-	1/1/11/20	6/13/91/115	-
23	CLA	J	101	10	1/1/10/20	5/10/88/115	-
25	LHG	5	623	23	-	23/53/53/53	-
23	CLA	A	842	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	K	203	-	1/1/15/20	10/37/115/115	-
26	BCR	A	856	-	-	8/29/63/63	0/2/2/2
31	LUT	7	619	-	-	5/29/67/67	0/2/2/2
23	CLA	4	601	15	1/1/15/20	16/37/115/115	-
23	CLA	1	603	-	1/1/12/20	11/21/99/115	-
23	CLA	6	609	17	1/1/11/20	4/13/91/115	-
23	CLA	9	612	21	1/1/5/20	-	-
23	CLA	A	815	-	1/1/12/20	7/19/97/115	-
23	CLA	5	602	16	1/1/15/20	11/37/115/115	-
23	CLA	7	612	18	-	6/11/89/115	-
29	LMG	7	624	-	-	19/39/59/70	0/1/1/1
23	CLA	1	611	25	1/1/15/20	11/37/115/115	-
23	CLA	3	617	14	1/1/10/20	0/6/84/115	-
23	CLA	9	607	-	1/1/5/20	-	-
23	CLA	A	840	-	1/1/12/20	5/22/100/115	-
27	SF4	C	102	-	-	-	0/6/5/5
23	CLA	9	603	21	1/1/5/20	-	-
23	CLA	L	304	-	1/1/11/20	6/13/91/115	-
25	LHG	9	622	23	-	23/53/53/53	-
23	CLA	5	618	16	1/1/10/20	2/8/84/115	-
23	CLA	6	607	-	1/1/10/20	6/10/86/115	-
31	LUT	5	620	-	-	2/29/67/67	0/2/2/2
23	CLA	A	834	-	1/1/15/20	17/37/115/115	-
26	BCR	L	301	-	-	6/29/63/63	0/2/2/2
23	CLA	7	604	-	1/1/13/20	8/23/101/115	-
23	CLA	6	620	-	1/1/14/20	14/35/113/115	-
23	CLA	2	611	25	1/1/4/20	-	-
23	CLA	4	612	15	-	2/8/86/115	-
29	LMG	4	624	-	-	15/35/55/70	0/1/1/1
23	CLA	A	801	-	1/1/15/20	10/37/115/115	-
23	CLA	8	607	-	1/1/10/20	3/10/86/115	-
23	CLA	A	836	-	1/1/15/20	11/37/115/115	-
26	BCR	3	622	-	-	8/29/63/63	0/2/2/2
31	LUT	9	619	-	-	3/29/67/67	0/2/2/2
23	CLA	8	616	19	-	7/11/87/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	832	-	1/1/14/20	7/31/109/115	-
23	CLA	6	614	-	1/1/14/20	7/31/109/115	-
23	CLA	B	820	-	1/1/12/20	7/19/97/115	-
23	CLA	4	606	-	1/1/10/20	3/6/84/115	-
23	CLA	8	613	19	1/1/15/20	16/37/115/115	-
23	CLA	B	812	-	1/1/10/20	6/11/89/115	-
23	CLA	5	613	16	1/1/14/20	19/35/113/115	-
26	BCR	3	620	-	-	4/29/63/63	0/2/2/2
23	CLA	3	611	25	1/1/10/20	2/4/80/115	-
26	BCR	7	621	-	-	6/29/63/63	0/2/2/2
23	CLA	1	607	-	1/1/10/20	3/6/84/115	-
23	CLA	A	813	-	1/1/12/20	5/24/102/115	-
23	CLA	a	603	-	1/1/10/20	3/10/88/115	-
23	CLA	B	808	-	1/1/15/20	14/37/115/115	-
23	CLA	2	604	-	1/1/5/20	-	-
26	BCR	B	843	-	-	8/29/63/63	0/2/2/2
23	CLA	7	611	25	1/1/13/20	10/29/107/115	-
23	CLA	B	815	-	1/1/10/20	2/11/89/115	-

The worst 5 of 2248 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	611	CLA	C1A-NA	12.76	1.40	1.29
24	A	844	PQN	C12-C13	8.62	1.53	1.33
24	B	842	PQN	C12-C13	8.55	1.53	1.33
23	4	609	CLA	C4B-NB	8.10	1.42	1.35
23	5	613	CLA	C4B-NB	7.97	1.42	1.35

The worst 5 of 3030 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	621	XAT	O24-C25-C24	10.95	121.61	113.38
32	2	620	XAT	O24-C25-C24	10.87	121.55	113.38
32	9	620	XAT	O4-C5-C4	10.55	121.31	113.38
23	B	803	CLA	C4A-NA-C1A	9.04	110.77	106.71
23	8	613	CLA	C4A-NA-C1A	8.99	110.75	106.71

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 2598 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	801	CLA	CBD-CGD-O2D-CED
23	A	804	CLA	C1A-C2A-CAA-CBA
23	A	804	CLA	CHA-CBD-CGD-O1D
23	A	804	CLA	CHA-CBD-CGD-O2D
23	A	805	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

257 monomers are involved in 596 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	818	CLA	2	0
29	A	860	LMG	2	0
23	5	606	CLA	6	0
31	8	619	LUT	6	0
23	K	201	CLA	1	0
23	6	601	CLA	5	0
23	5	614	CLA	2	0
23	5	616	CLA	2	0
23	7	610	CLA	5	0
23	A	809	CLA	6	0
26	F	305	BCR	4	0
28	A	857	LMU	1	0
23	6	613	CLA	5	0
26	A	851	BCR	3	0
29	5	626	LMG	1	0
25	1	620	LHG	6	0
23	7	616	CLA	2	0
23	8	610	CLA	3	0
25	3	623	LHG	1	0
23	L	303	CLA	2	0
23	5	610	CLA	5	0
23	4	609	CLA	3	0
26	B	848	BCR	1	0
28	5	628	LMU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	810	CLA	3	0
26	A	849	BCR	4	0
26	4	621	BCR	2	0
23	2	614	CLA	1	0
23	3	602	CLA	1	0
23	4	616	CLA	1	0
23	7	614	CLA	2	0
23	A	843	CLA	5	0
23	8	612	CLA	1	0
23	G	203	CLA	3	0
23	8	608	CLA	3	0
23	5	601	CLA	1	0
26	B	847	BCR	2	0
26	5	622	BCR	4	0
30	J	103	DGD	1	0
32	4	620	XAT	3	0
23	B	831	CLA	3	0
23	9	606	CLA	1	0
23	8	603	CLA	1	0
23	B	819	CLA	2	0
23	B	813	CLA	5	0
23	3	603	CLA	2	0
23	4	614	CLA	1	0
23	A	839	CLA	3	0
23	A	831	CLA	4	0
23	A	822	CLA	4	0
23	5	607	CLA	5	0
26	L	305	BCR	4	0
23	5	603	CLA	1	0
23	A	825	CLA	5	0
25	A	847	LHG	1	0
23	B	824	CLA	5	0
23	9	609	CLA	1	0
26	B	801	BCR	5	0
25	B	851	LHG	2	0
23	A	837	CLA	2	0
23	B	841	CLA	3	0
23	6	610	CLA	4	0
26	B	844	BCR	3	0
23	9	611	CLA	7	0
24	B	842	PQN	6	0
23	3	609	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	854	CLA	5	0
23	B	838	CLA	4	0
23	2	610	CLA	1	0
25	A	846	LHG	3	0
24	A	844	PQN	5	0
23	B	834	CLA	3	0
23	A	806	CLA	3	0
26	J	102	BCR	5	0
23	7	603	CLA	2	0
23	8	609	CLA	1	0
23	9	614	CLA	1	0
23	5	609	CLA	6	0
23	A	805	CLA	4	0
23	1	601	CLA	6	0
26	8	621	BCR	4	0
23	5	608	CLA	4	0
23	1	612	CLA	1	0
26	K	207	BCR	3	0
25	8	622	LHG	1	0
23	4	607	CLA	1	0
25	4	622	LHG	6	0
23	6	604	CLA	3	0
32	3	619	XAT	2	0
23	B	833	CLA	4	0
26	A	850	BCR	3	0
23	A	803	CLA	5	0
23	8	614	CLA	2	0
23	A	824	CLA	1	0
23	G	204	CLA	3	0
23	B	822	CLA	1	0
26	B	845	BCR	2	0
23	7	601	CLA	5	0
23	4	610	CLA	1	0
23	A	807	CLA	2	0
23	6	606	CLA	1	0
31	4	619	LUT	5	0
23	B	835	CLA	2	0
31	6	619	LUT	4	0
23	5	604	CLA	5	0
26	K	202	BCR	3	0
23	2	613	CLA	1	0
23	7	607	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	840	CLA	3	0
31	3	618	LUT	1	0
25	7	622	LHG	2	0
23	4	608	CLA	4	0
26	G	205	BCR	6	0
23	1	608	CLA	2	0
23	2	609	CLA	1	0
25	6	623	LHG	3	0
23	B	809	CLA	3	0
23	6	608	CLA	2	0
23	B	829	CLA	9	0
23	A	830	CLA	5	0
23	B	806	CLA	3	0
23	3	606	CLA	2	0
28	A	859	LMU	2	0
23	6	603	CLA	1	0
23	B	803	CLA	3	0
23	4	604	CLA	1	0
23	B	805	CLA	4	0
25	5	625	LHG	5	0
32	6	621	XAT	1	0
23	4	613	CLA	5	0
23	A	811	CLA	5	0
23	B	836	CLA	2	0
23	A	812	CLA	4	0
23	A	817	CLA	2	0
23	A	804	CLA	3	0
23	9	601	CLA	1	0
26	A	852	BCR	7	0
23	A	838	CLA	1	0
23	A	829	CLA	10	0
28	8	624	LMU	3	0
23	A	823	CLA	2	0
23	3	610	CLA	3	0
23	6	602	CLA	6	0
23	A	832	CLA	2	0
23	B	802	CLA	2	0
32	5	621	XAT	10	0
31	2	619	LUT	3	0
23	A	808	CLA	1	0
23	A	821	CLA	1	0
23	B	823	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	817	CLA	2	0
23	A	828	CLA	1	0
23	B	839	CLA	4	0
30	B	850	DGD	5	0
32	7	620	XAT	1	0
23	6	616	CLA	6	0
23	F	301	CLA	4	0
33	6	624	NEX	4	0
32	1	618	XAT	4	0
23	A	802	CLA	7	0
26	B	846	BCR	1	0
23	B	811	CLA	2	0
23	8	601	CLA	3	0
26	3	621	BCR	2	0
23	A	826	CLA	1	0
32	2	620	XAT	3	0
23	F	303	CLA	3	0
23	B	828	CLA	1	0
23	B	825	CLA	4	0
23	A	845	CLA	1	0
23	1	609	CLA	2	0
26	1	619	BCR	2	0
31	1	617	LUT	3	0
23	A	816	CLA	1	0
23	A	814	CLA	4	0
26	6	622	BCR	4	0
25	8	623	LHG	3	0
23	1	606	CLA	2	0
23	4	618	CLA	1	0
23	7	602	CLA	2	0
32	9	620	XAT	3	0
23	7	613	CLA	4	0
23	B	821	CLA	3	0
29	J	104	LMG	1	0
33	5	624	NEX	3	0
23	3	608	CLA	3	0
23	F	304	CLA	1	0
23	A	841	CLA	6	0
23	4	602	CLA	1	0
23	A	835	CLA	3	0
23	A	827	CLA	2	0
23	B	837	CLA	5	0

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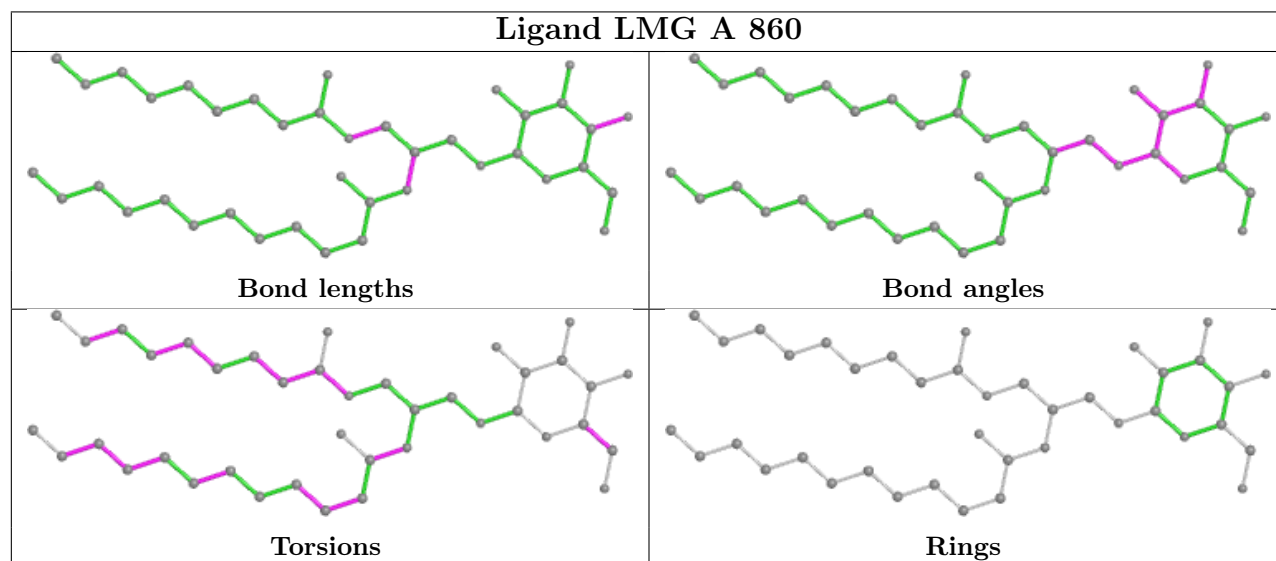
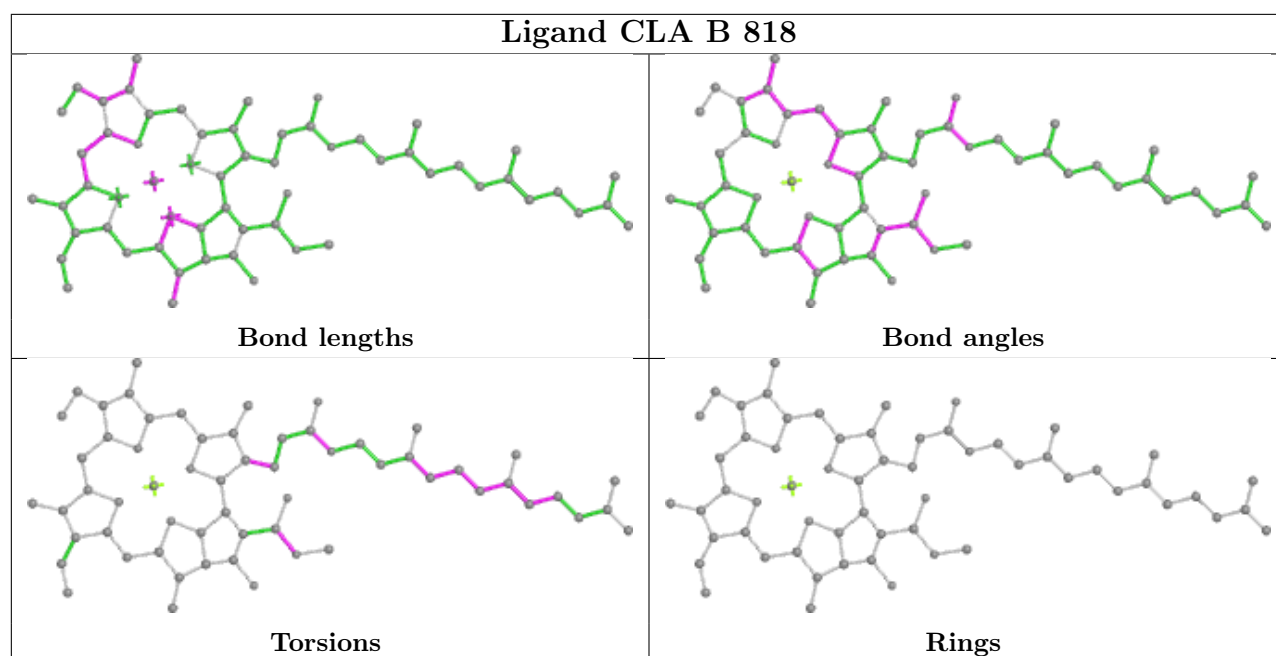
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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23	6	612	CLA	1	0
29	5	627	LMG	3	0
26	A	848	BCR	5	0
23	3	612	CLA	1	0
23	3	614	CLA	1	0
23	5	619	CLA	2	0
23	B	814	CLA	3	0
23	L	302	CLA	1	0
23	A	819	CLA	2	0
32	8	620	XAT	1	0
23	9	613	CLA	1	0
23	A	810	CLA	3	0
23	K	204	CLA	1	0
23	3	607	CLA	2	0
23	A	820	CLA	4	0
25	2	622	LHG	1	0
23	B	807	CLA	2	0
23	3	604	CLA	1	0
25	3	624	LHG	2	0
23	B	830	CLA	5	0
23	B	827	CLA	6	0
23	7	608	CLA	5	0
23	B	826	CLA	3	0
23	A	818	CLA	4	0
23	J	101	CLA	2	0
25	5	623	LHG	2	0
23	A	842	CLA	8	0
26	A	856	BCR	7	0
31	7	619	LUT	5	0
23	4	601	CLA	6	0
23	1	603	CLA	1	0
23	6	609	CLA	2	0
23	5	602	CLA	5	0
29	7	624	LMG	1	0
23	1	611	CLA	5	0
23	3	617	CLA	2	0
23	A	840	CLA	5	0
23	L	304	CLA	2	0
25	9	622	LHG	5	0
31	5	620	LUT	6	0
23	A	834	CLA	2	0

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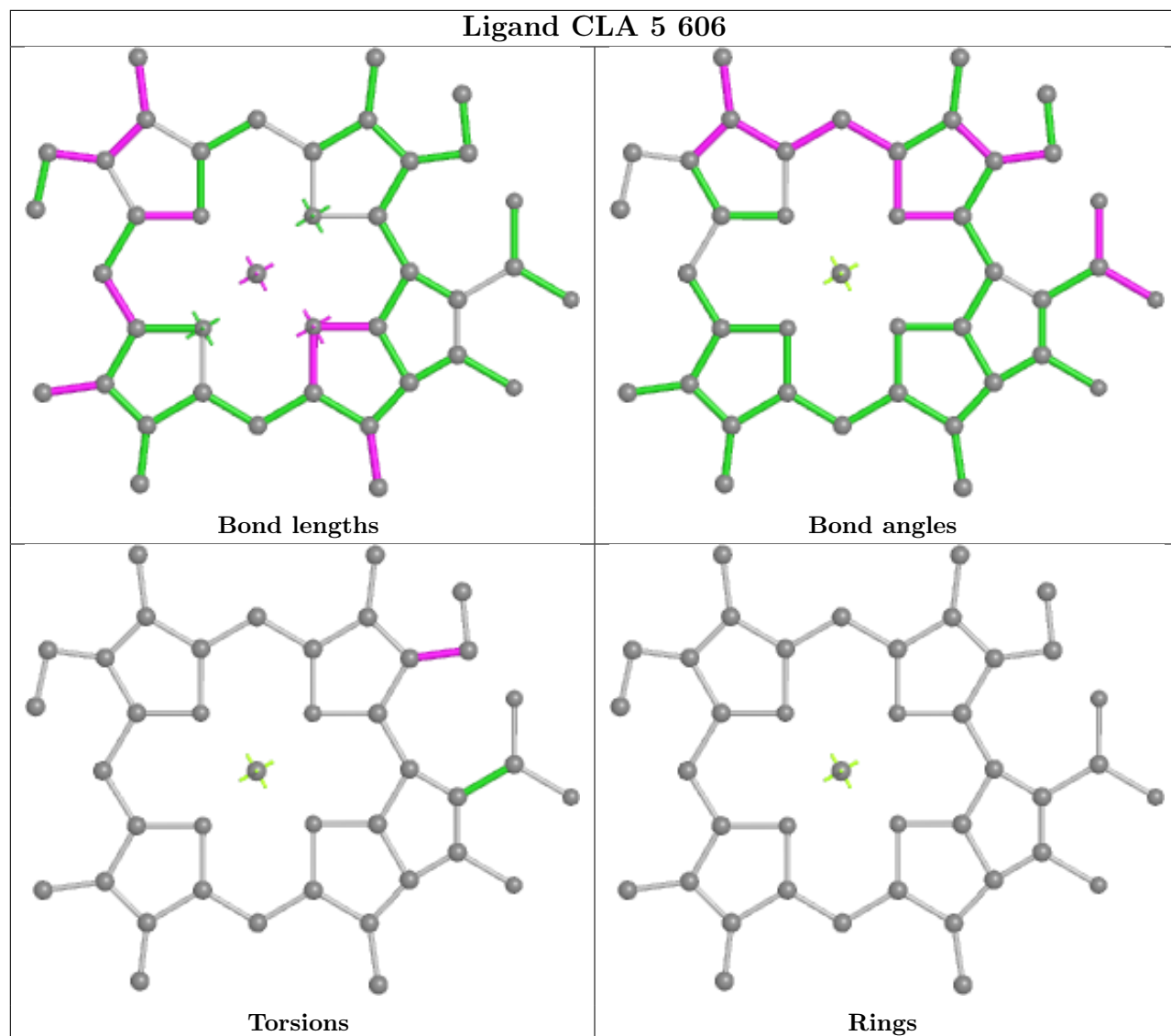
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	L	301	BCR	1	0
23	6	620	CLA	5	0
29	4	624	LMG	1	0
23	A	801	CLA	5	0
23	8	607	CLA	2	0
23	A	836	CLA	4	0
26	3	622	BCR	4	0
31	9	619	LUT	1	0
23	8	616	CLA	1	0
23	B	832	CLA	6	0
23	6	614	CLA	3	0
23	B	820	CLA	1	0
23	4	606	CLA	1	0
23	8	613	CLA	1	0
23	5	613	CLA	7	0
26	3	620	BCR	5	0
26	7	621	BCR	3	0
23	1	607	CLA	1	0
23	A	813	CLA	2	0
23	B	808	CLA	2	0
26	B	843	BCR	2	0
23	7	611	CLA	3	0
23	B	815	CLA	1	0

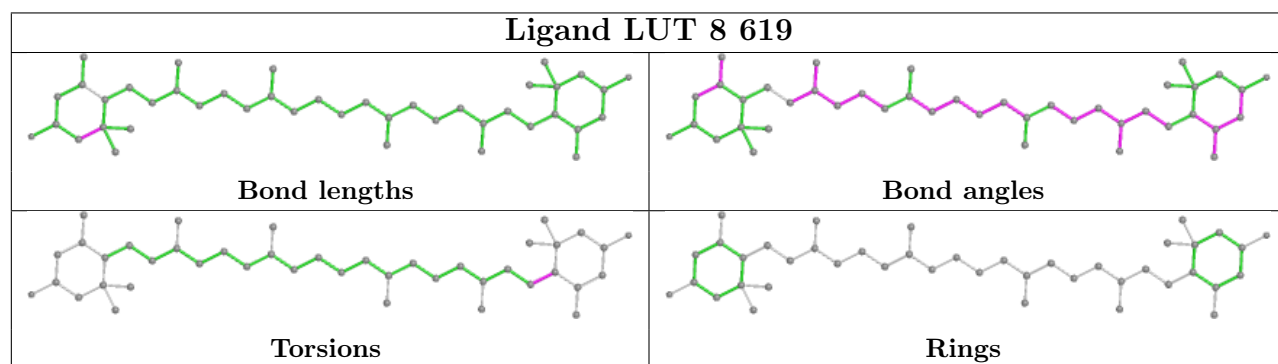
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



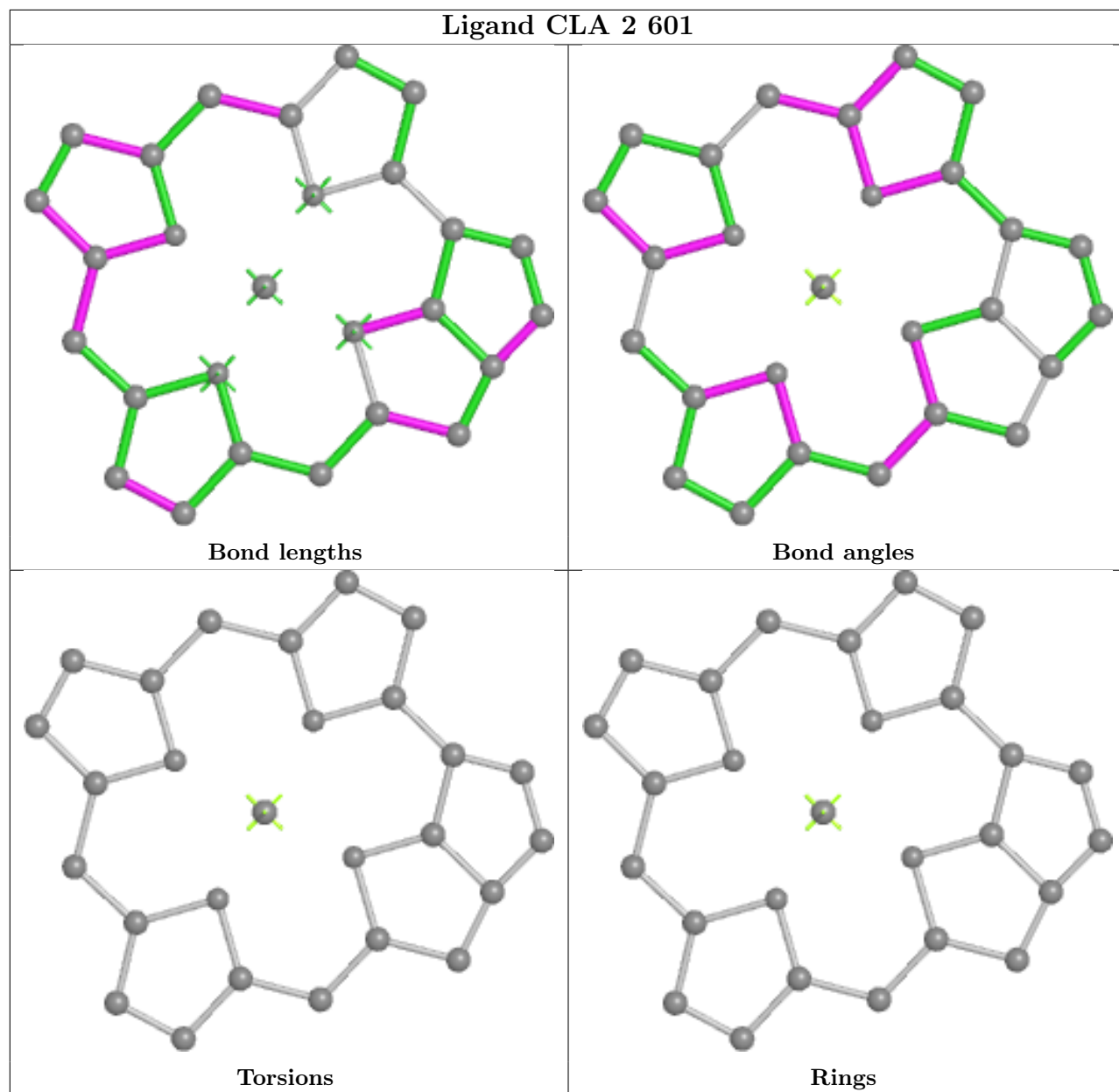
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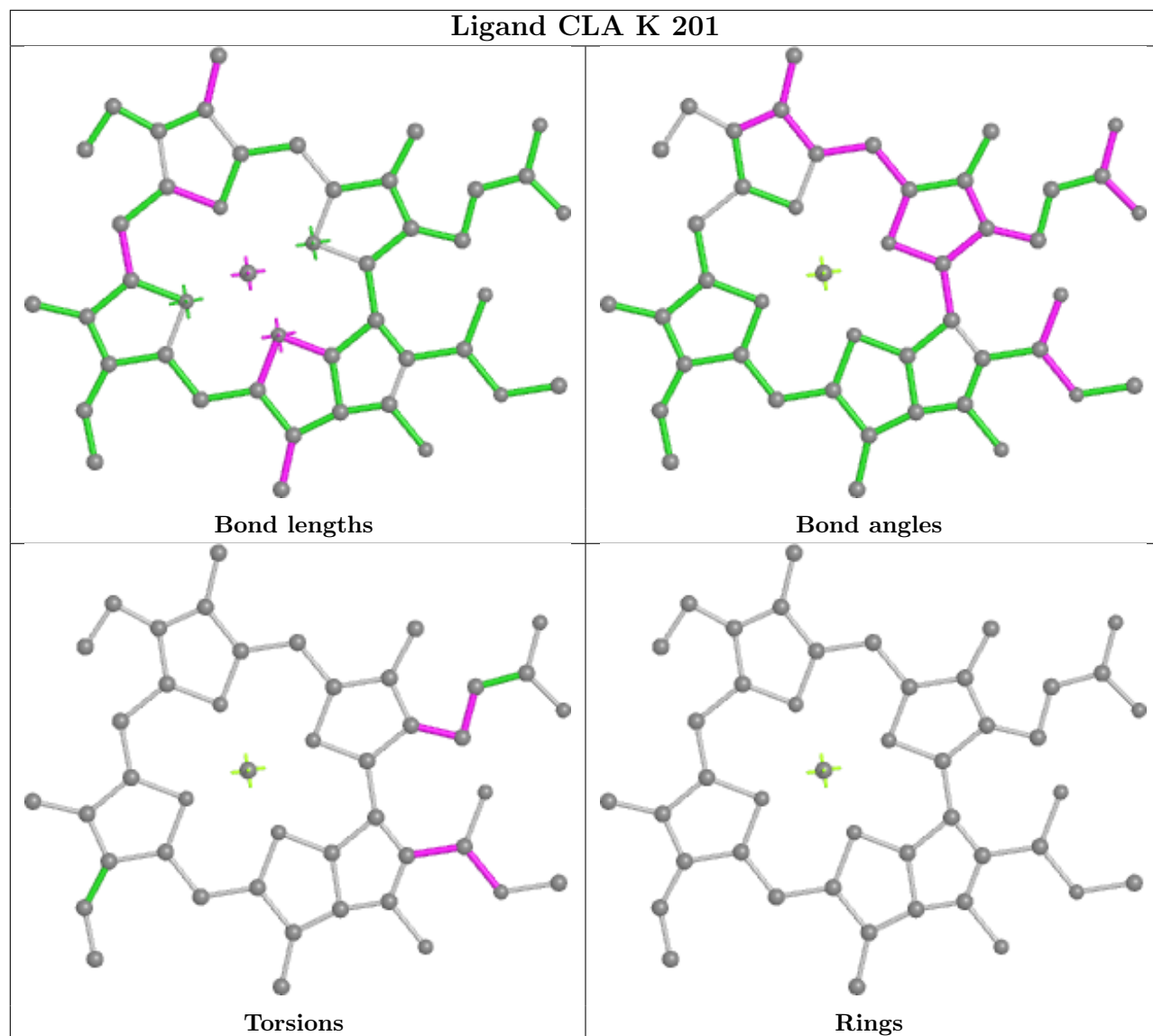


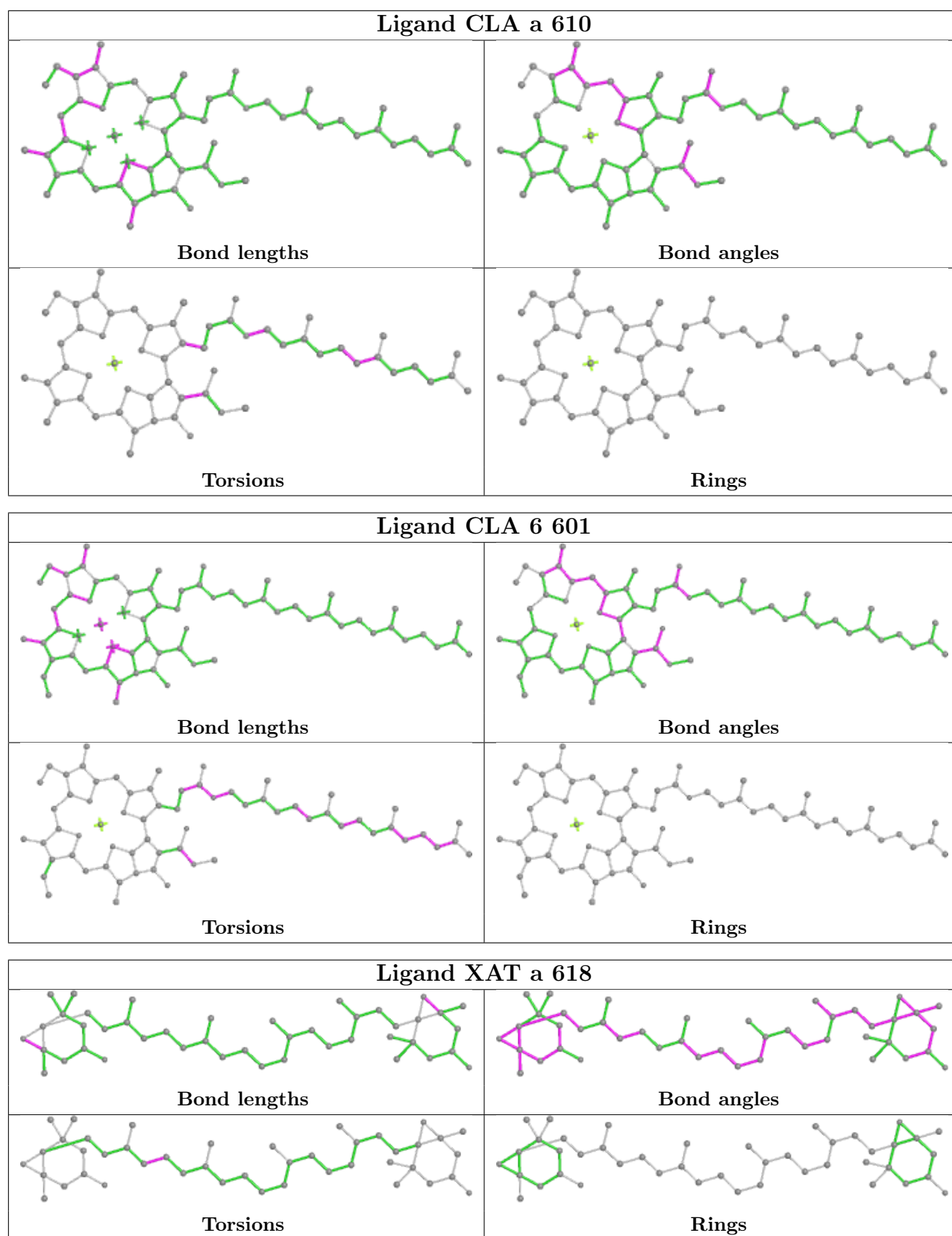
Ligand LUT 8 619



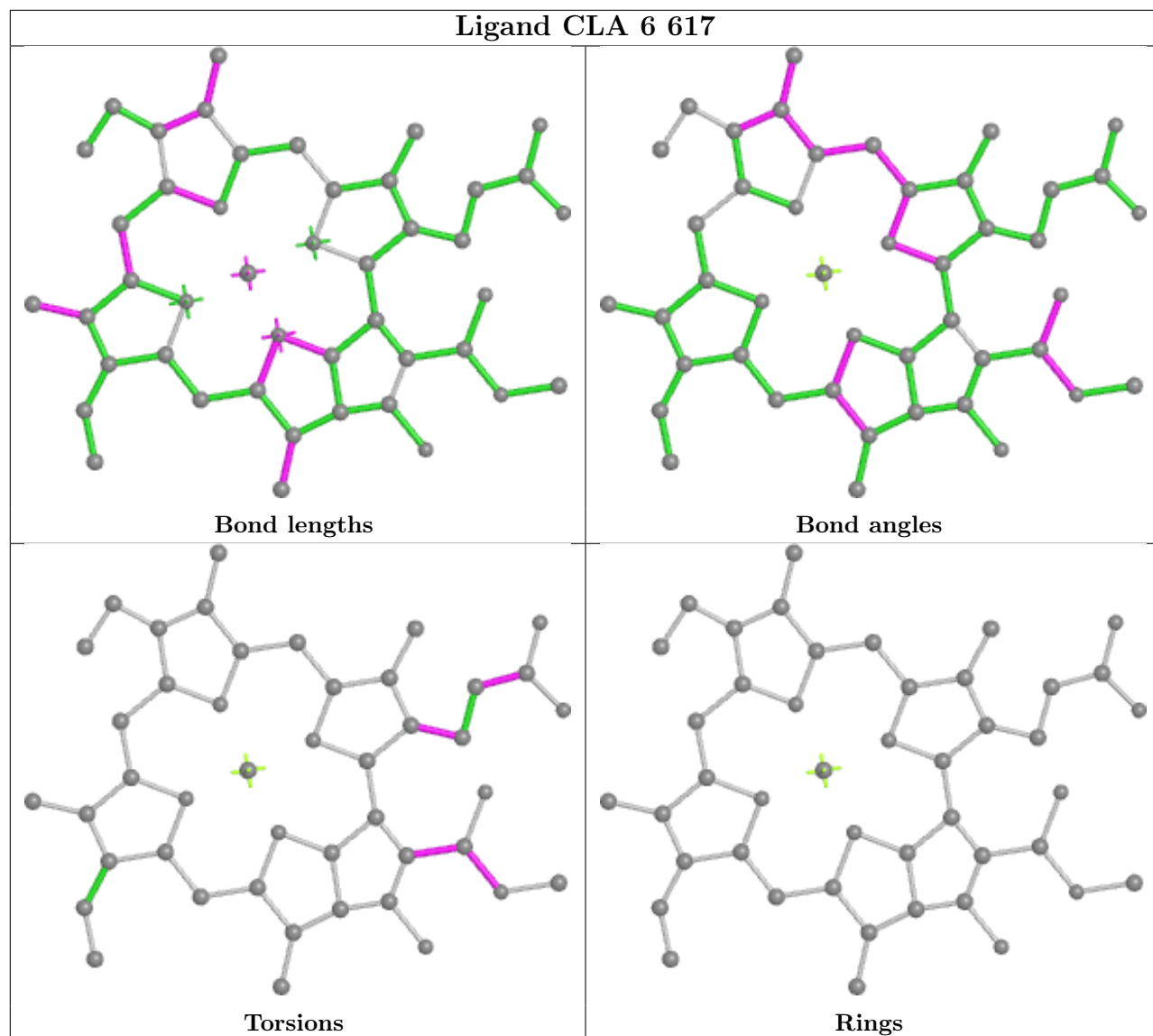
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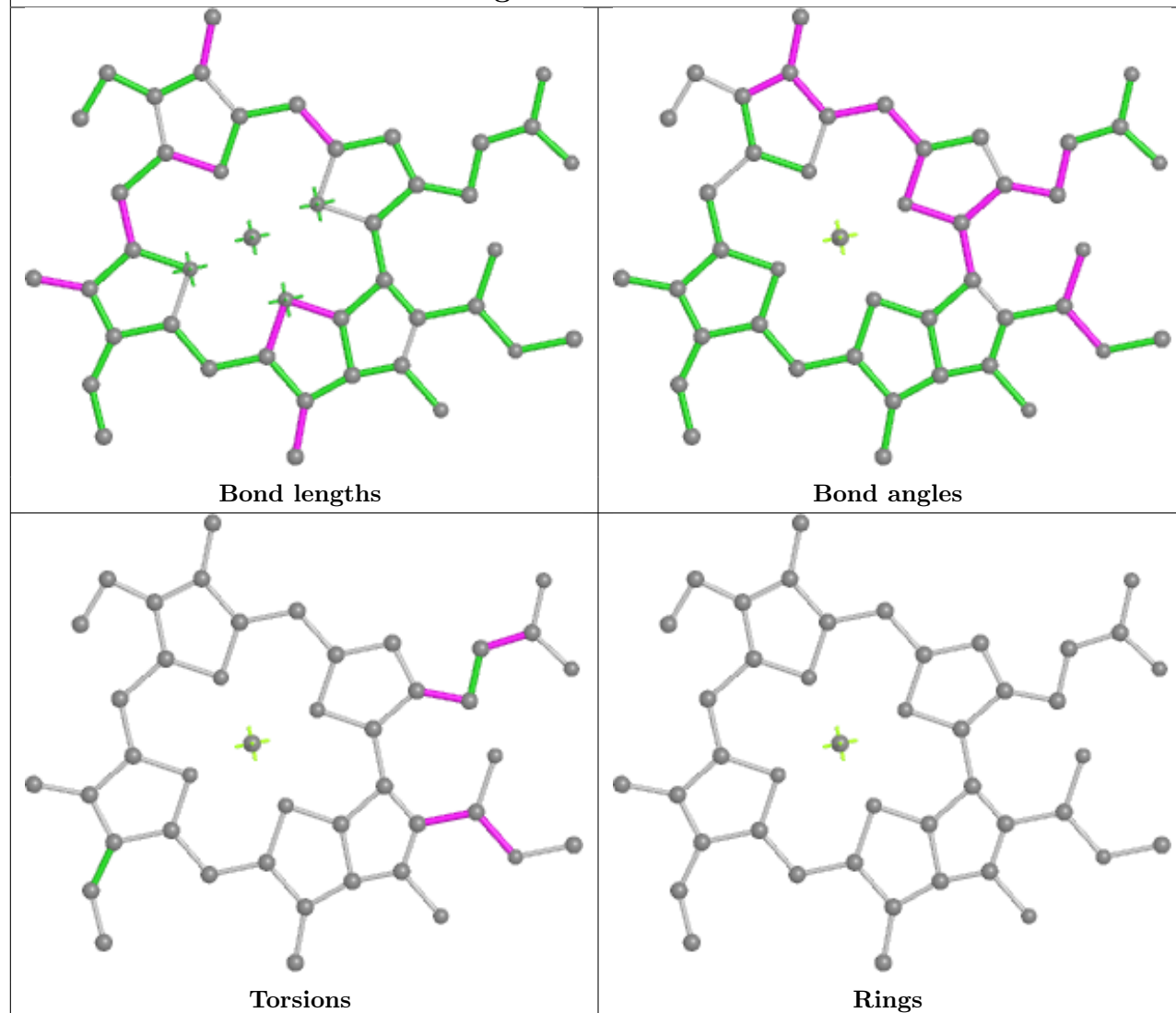




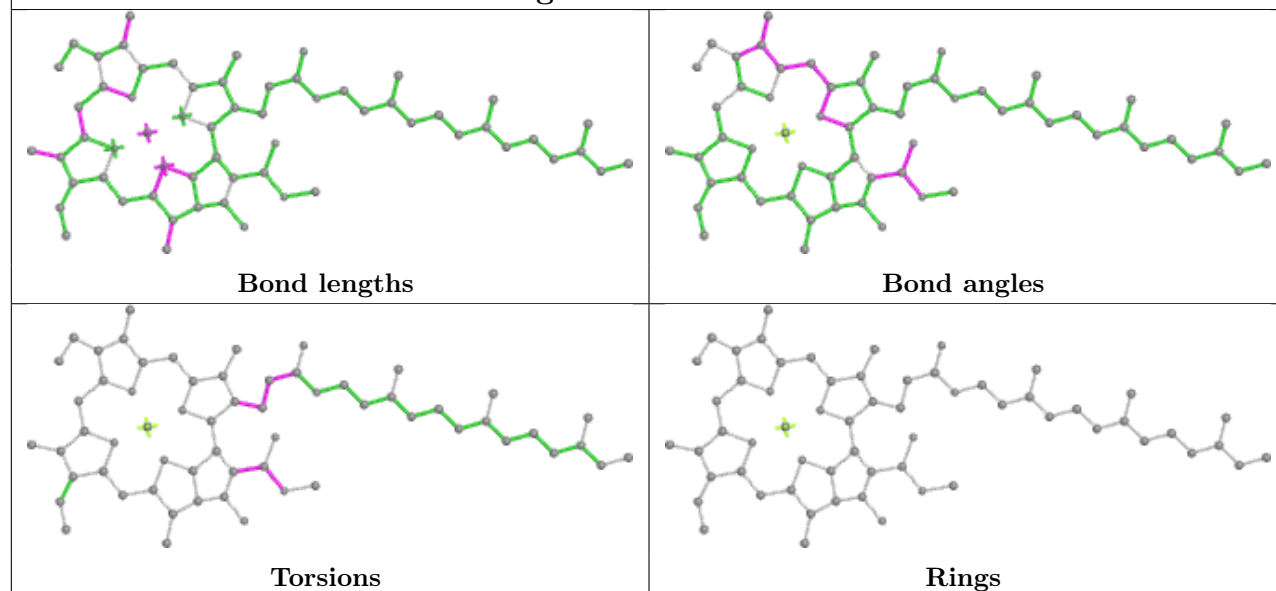
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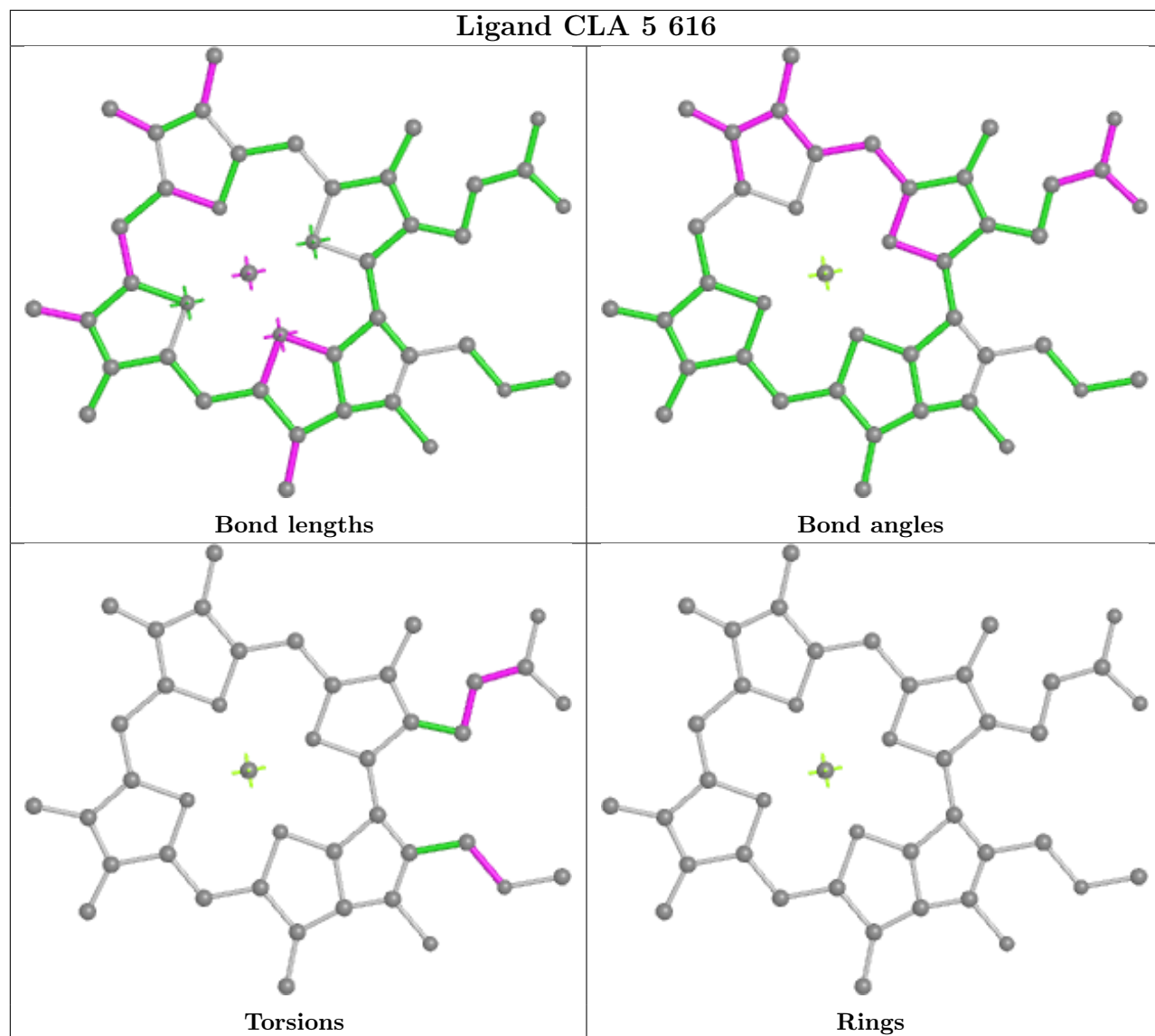
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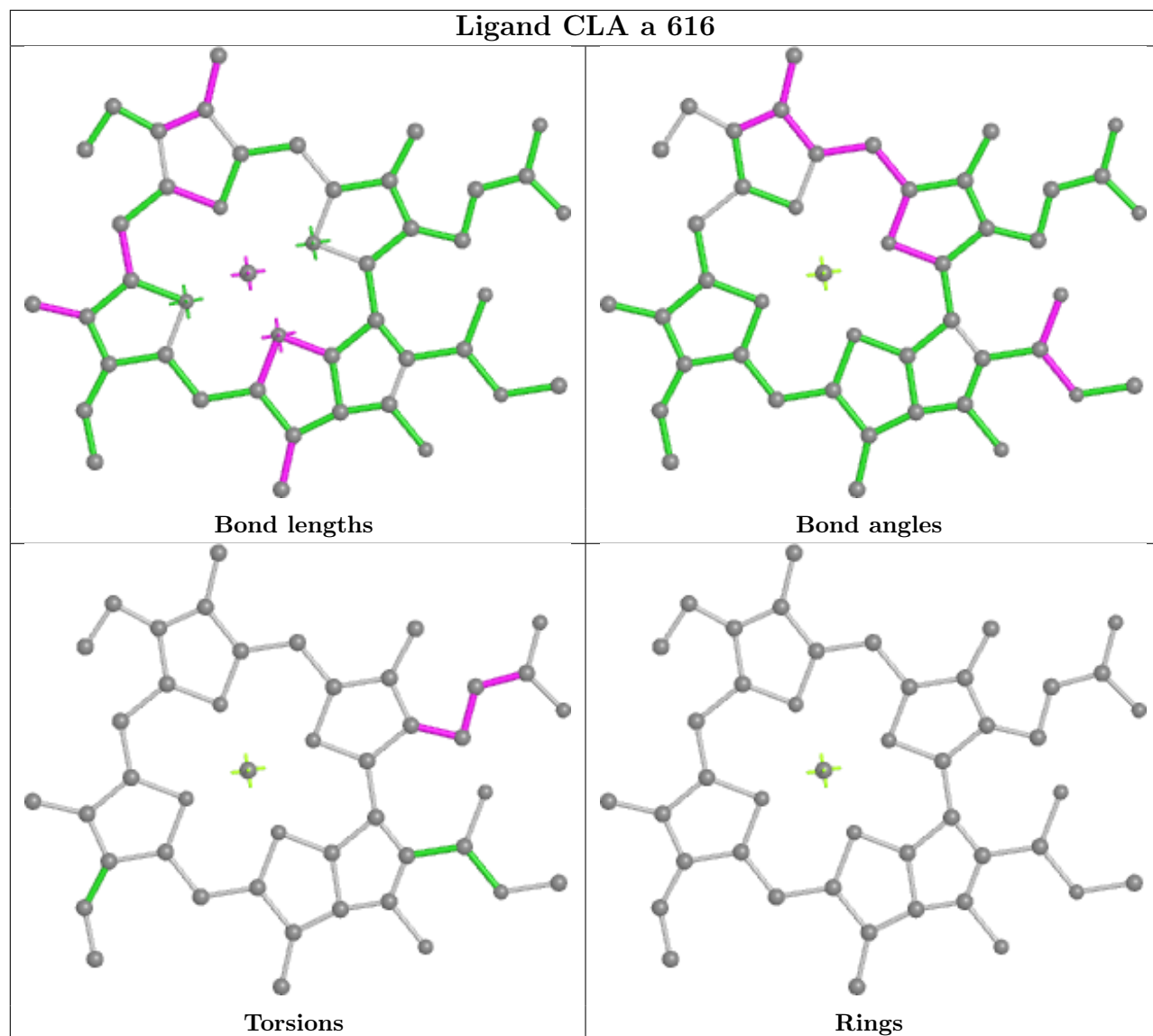
Ligand CLA a 602



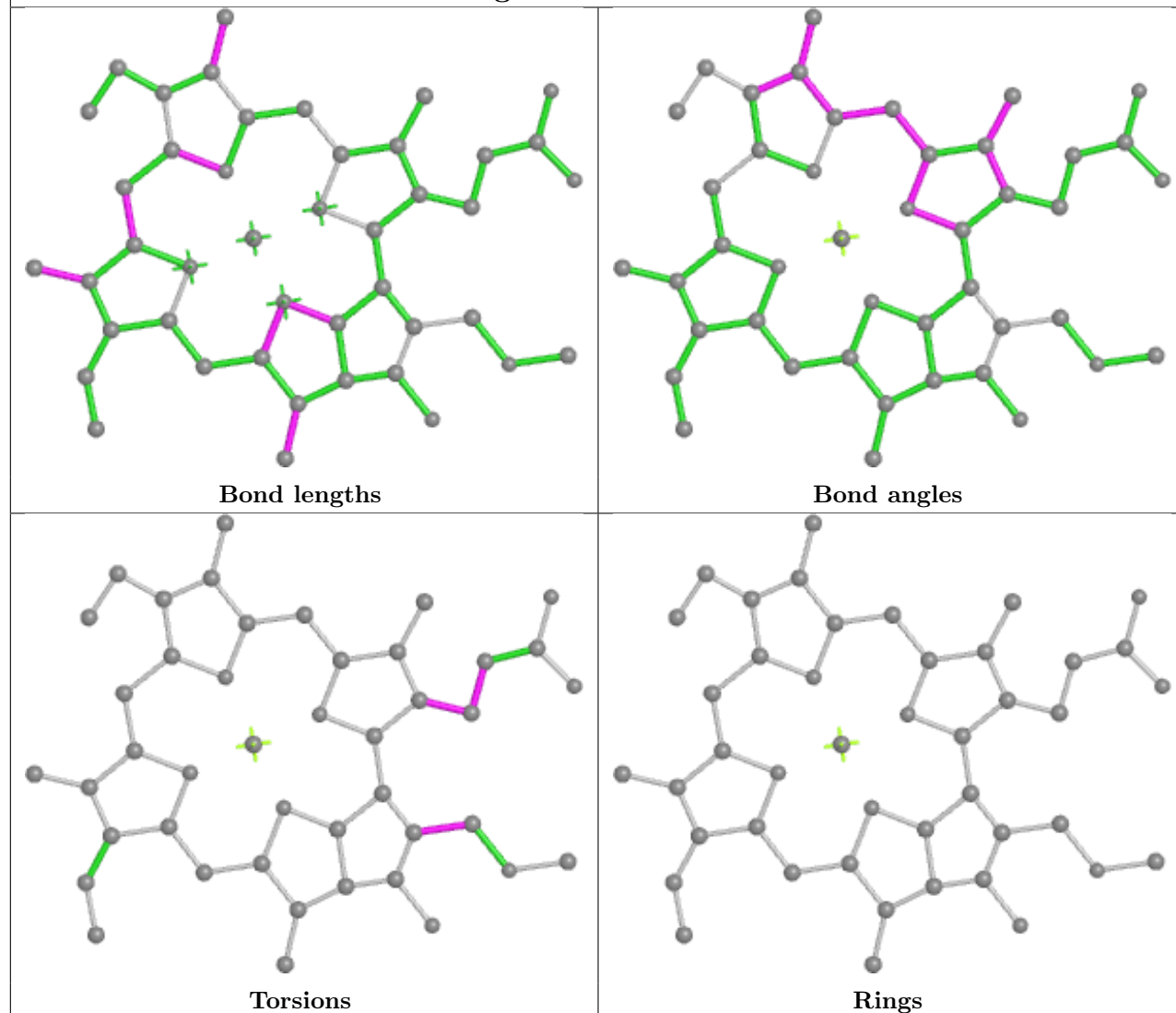
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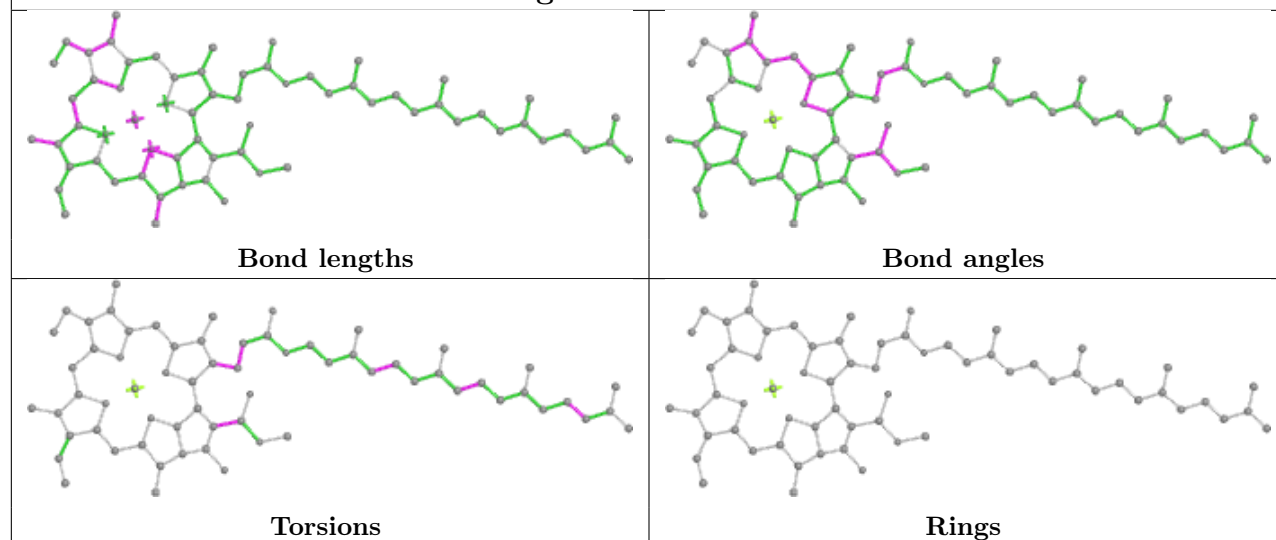
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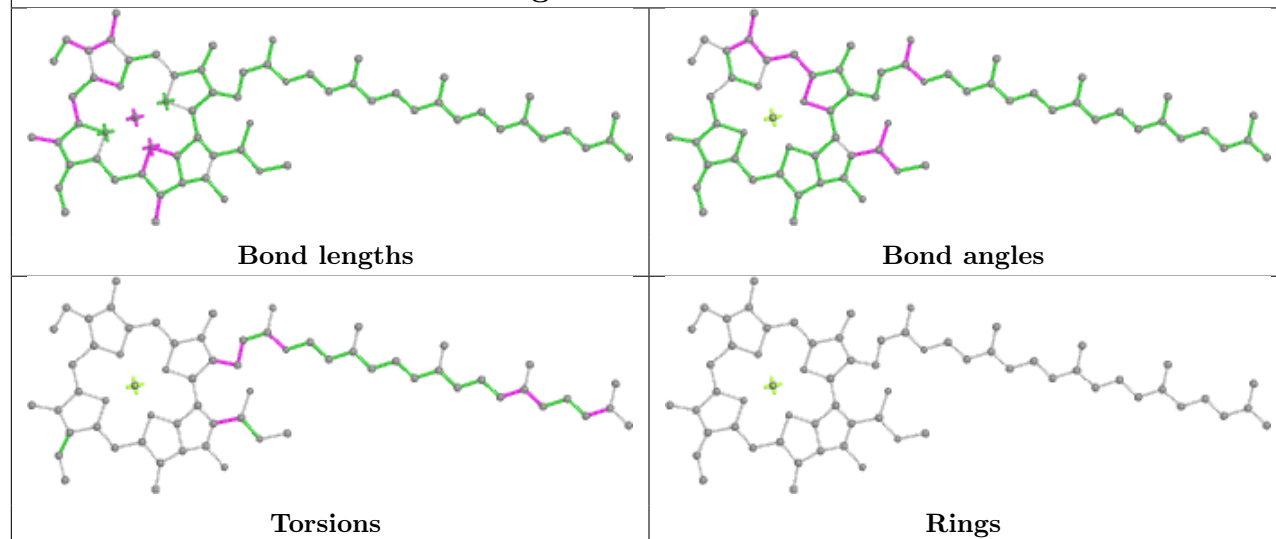
Ligand CLA 7 609



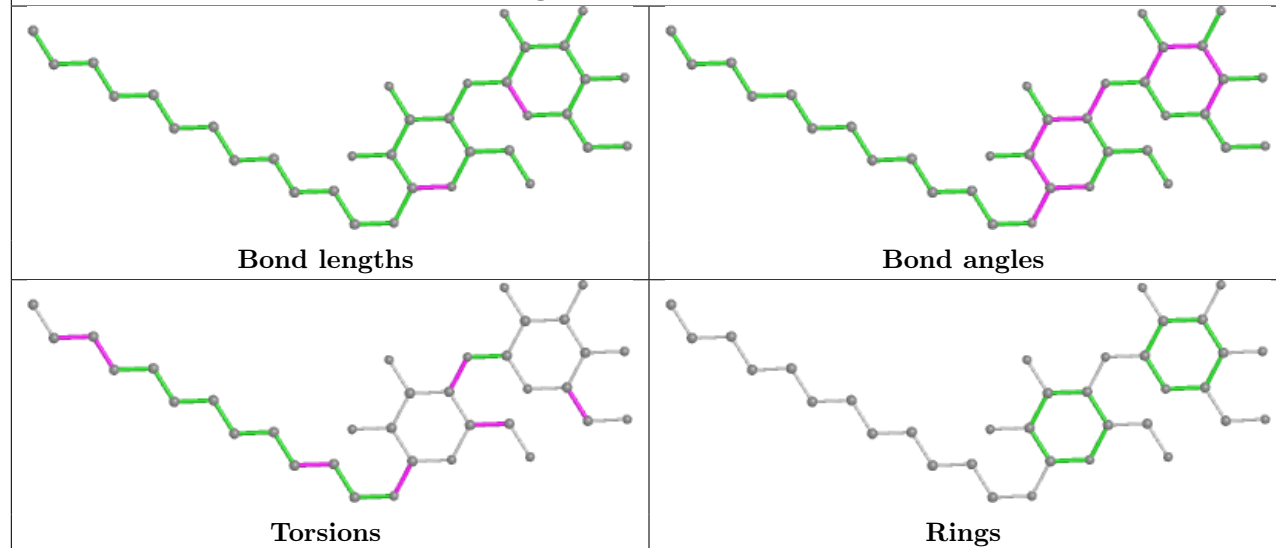
Ligand CLA 7 610



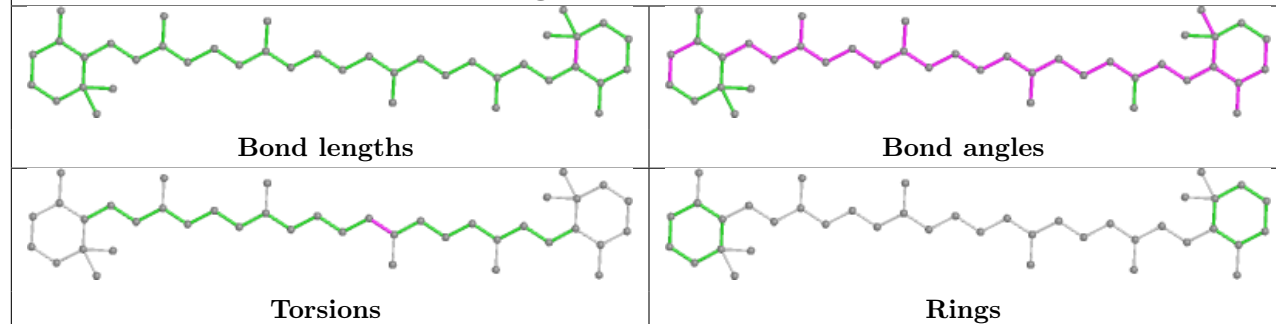
Ligand CLA A 809

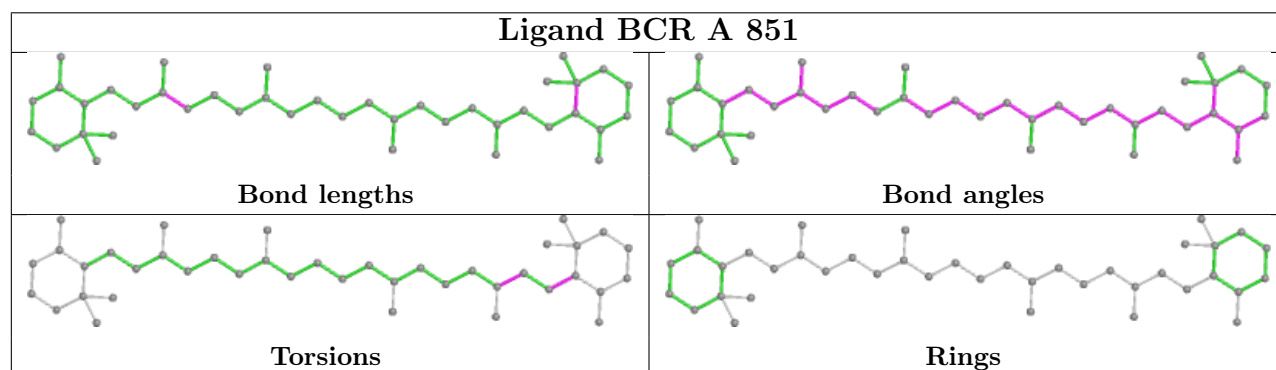
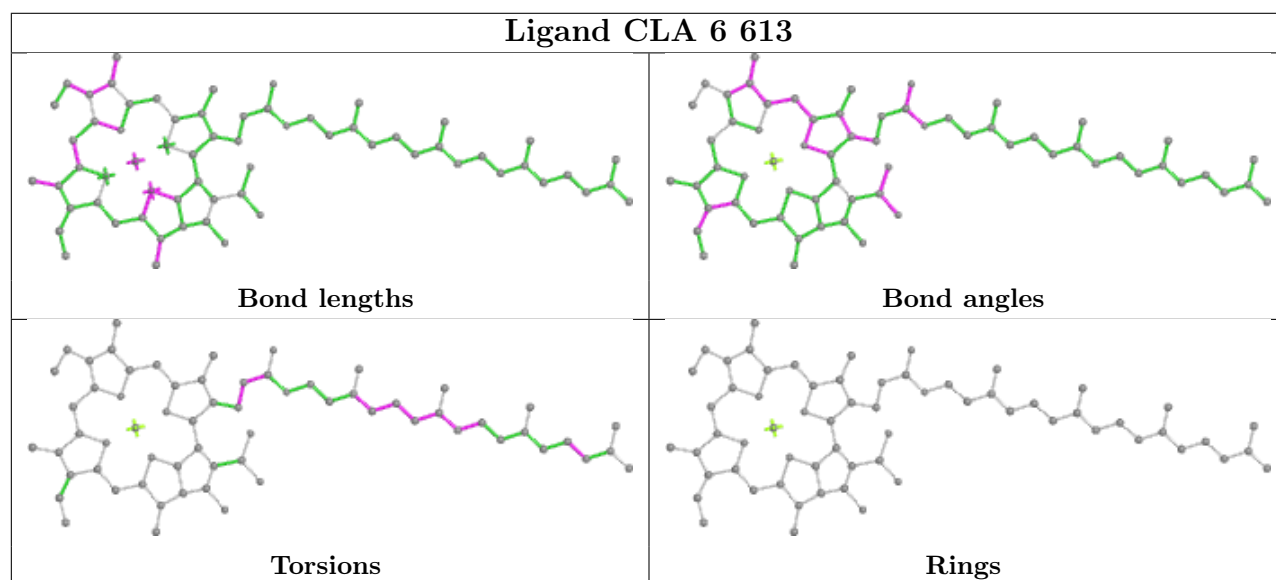
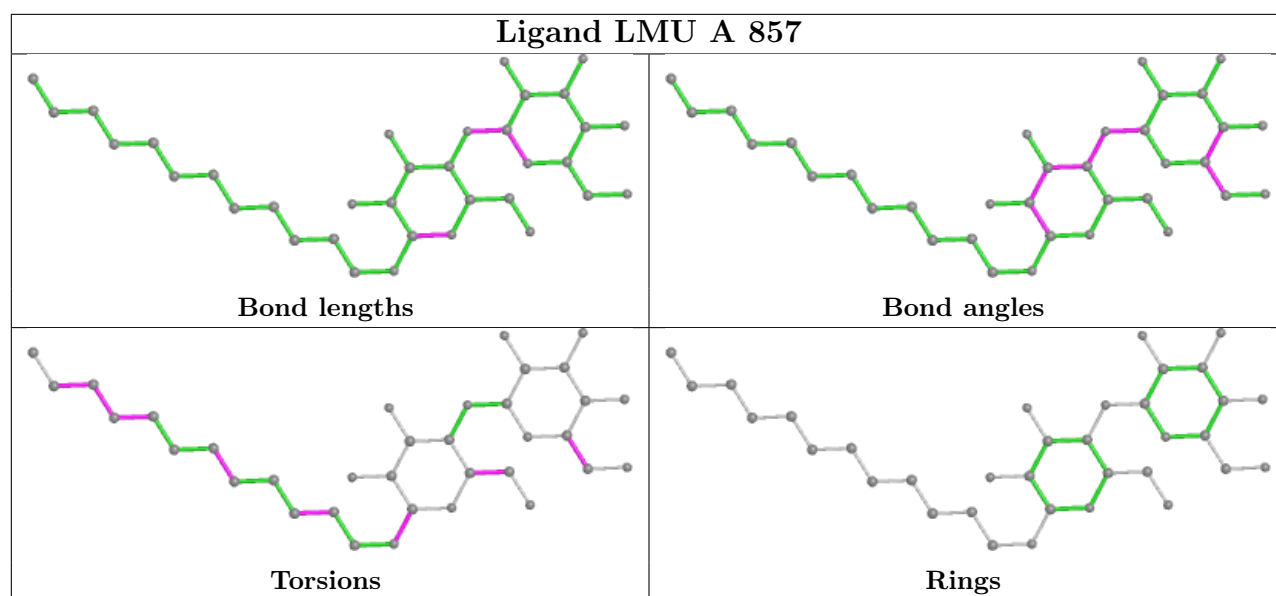


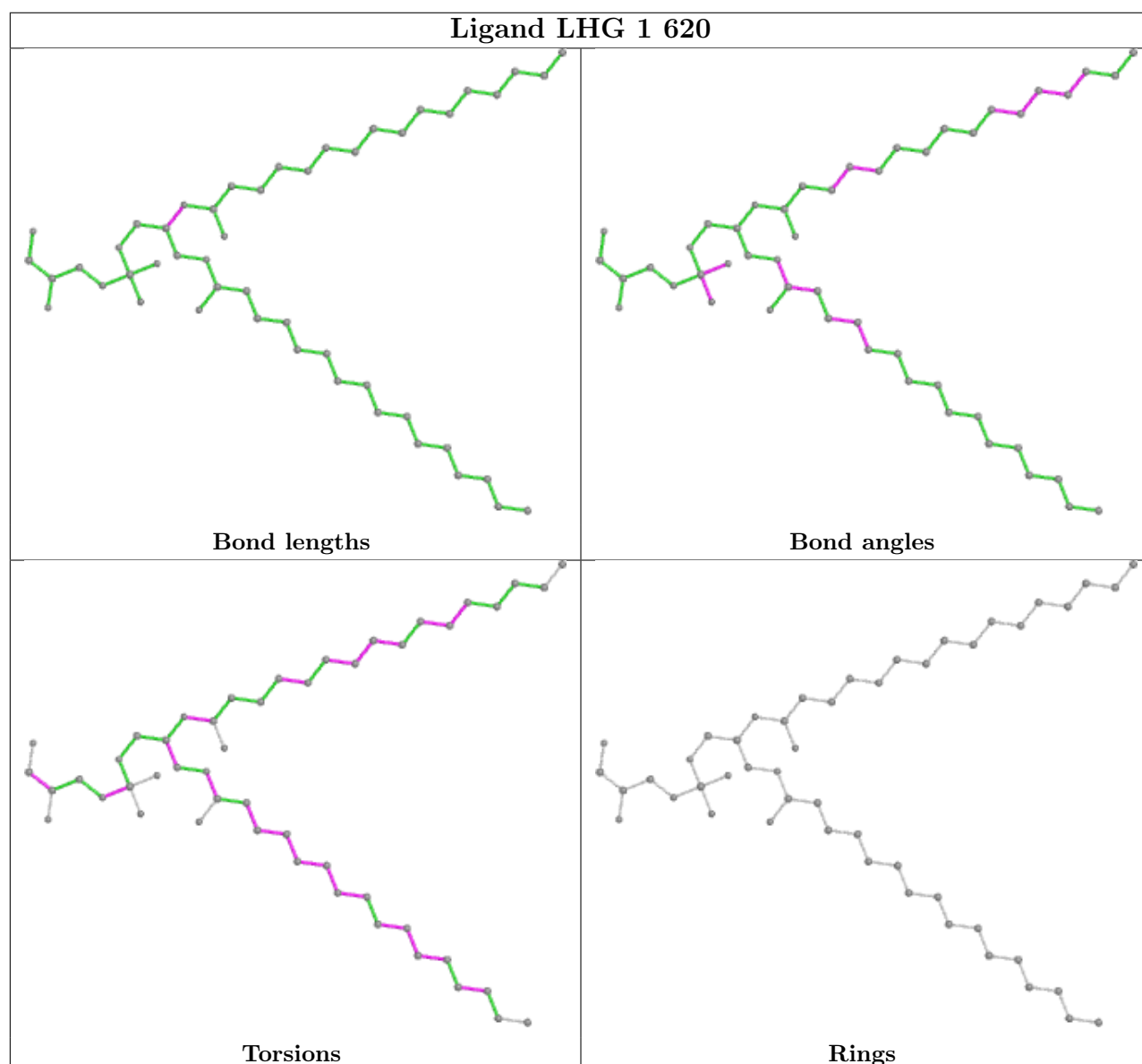
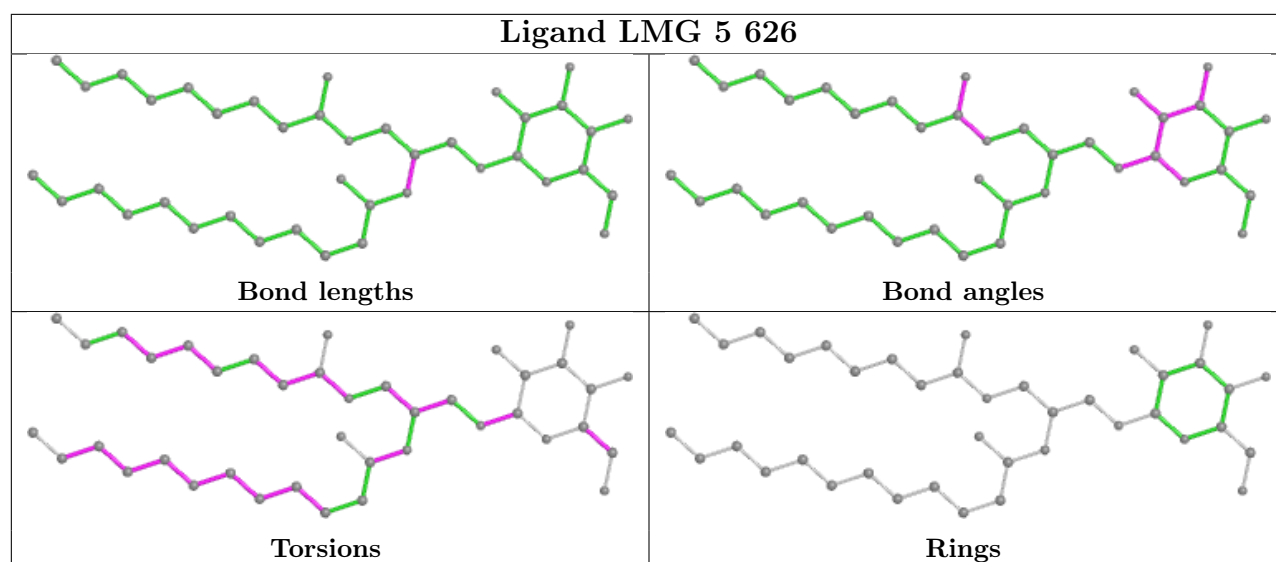
Ligand LMU 8 625



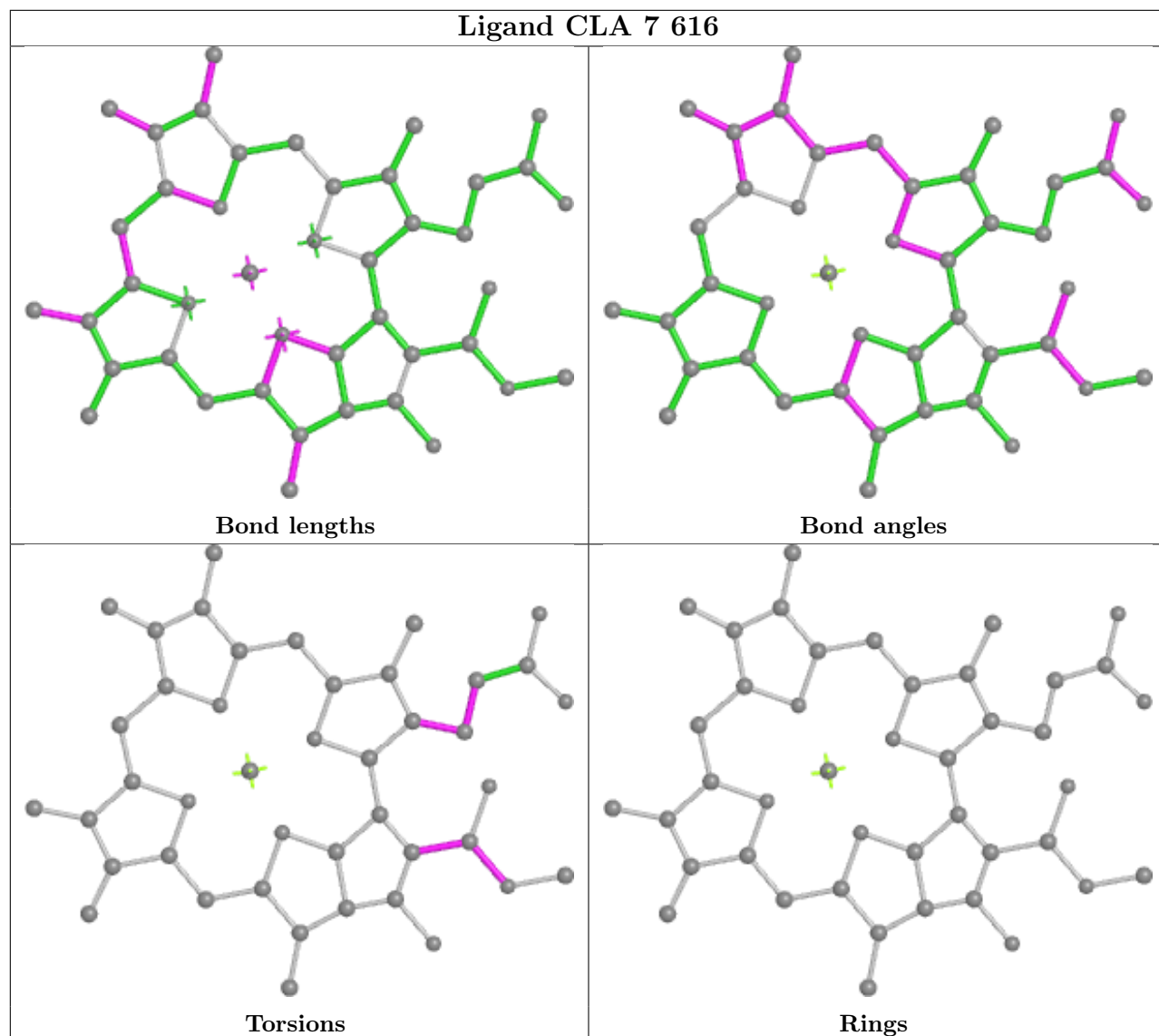
Ligand BCR F 305



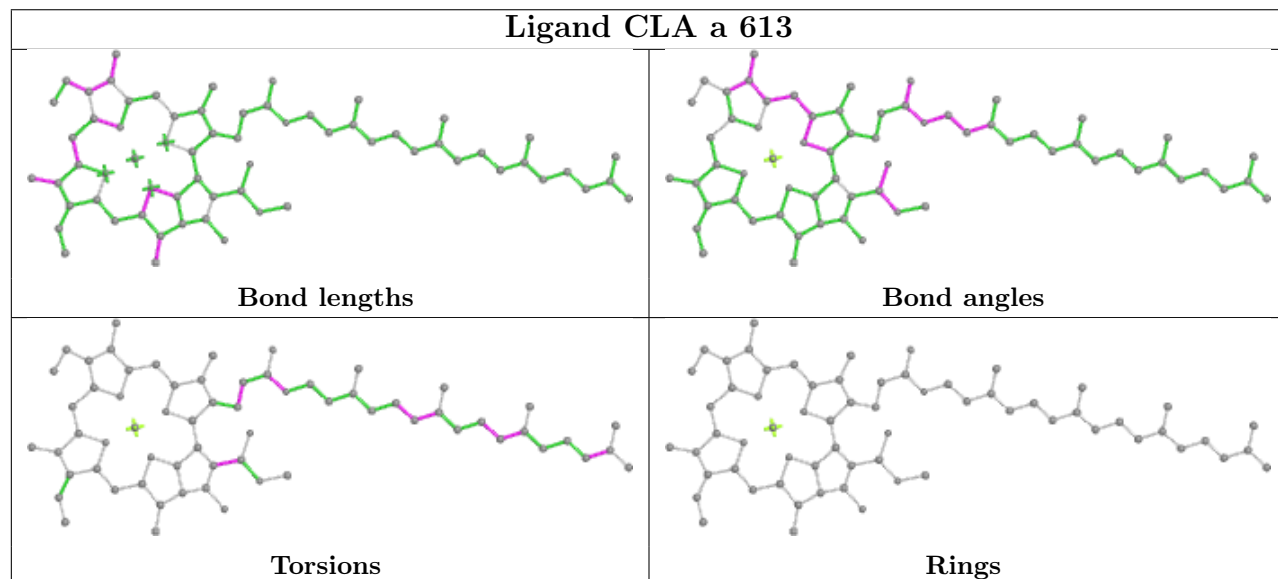


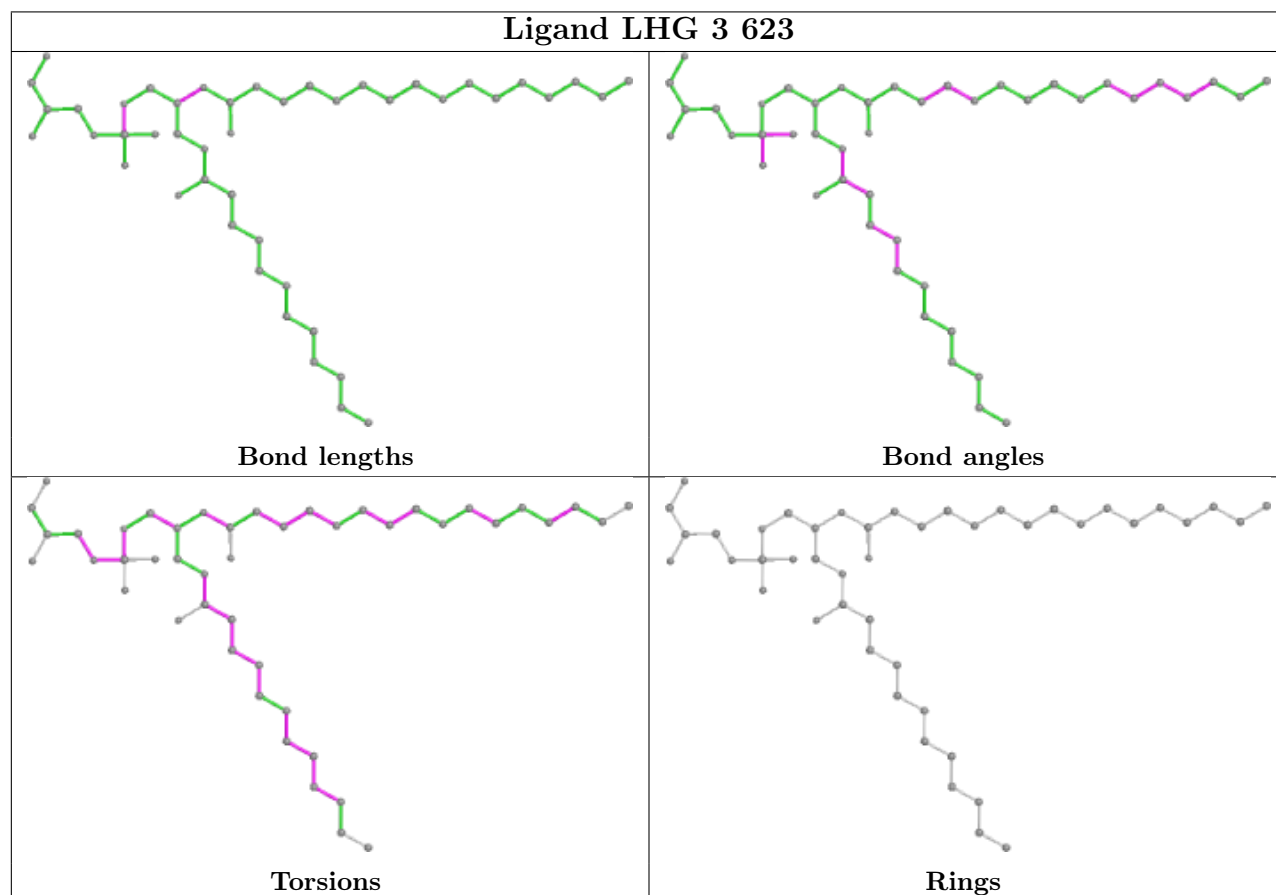
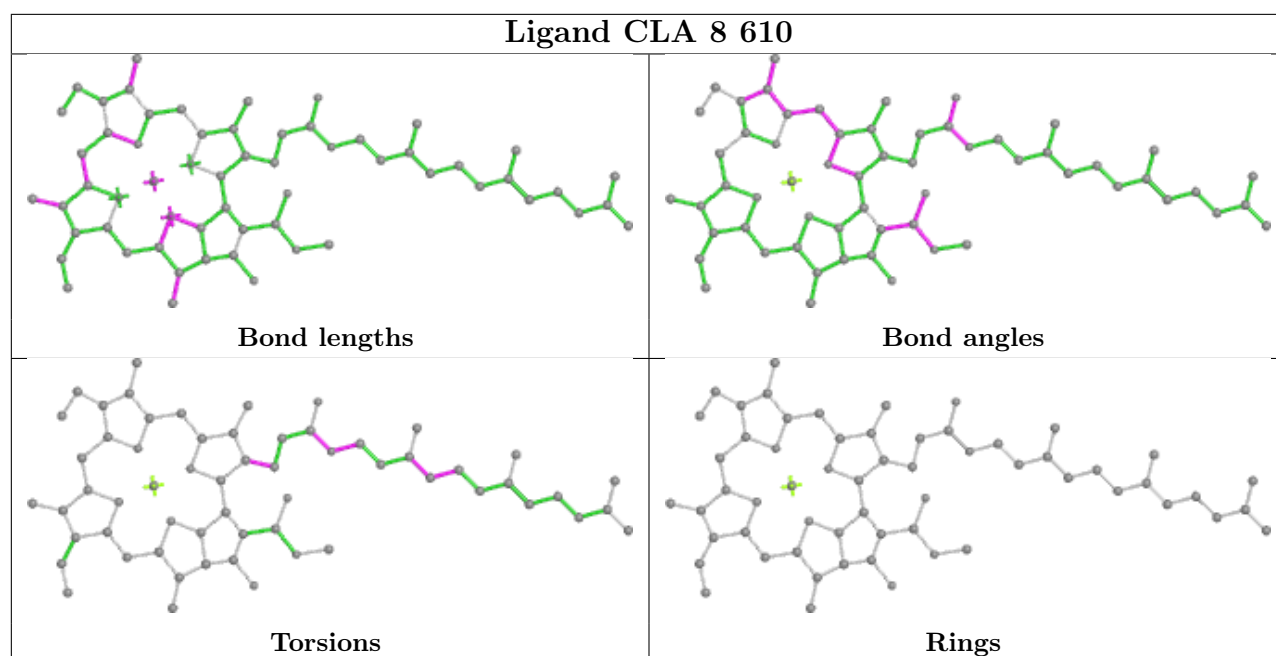


Ligand CLA 7 616

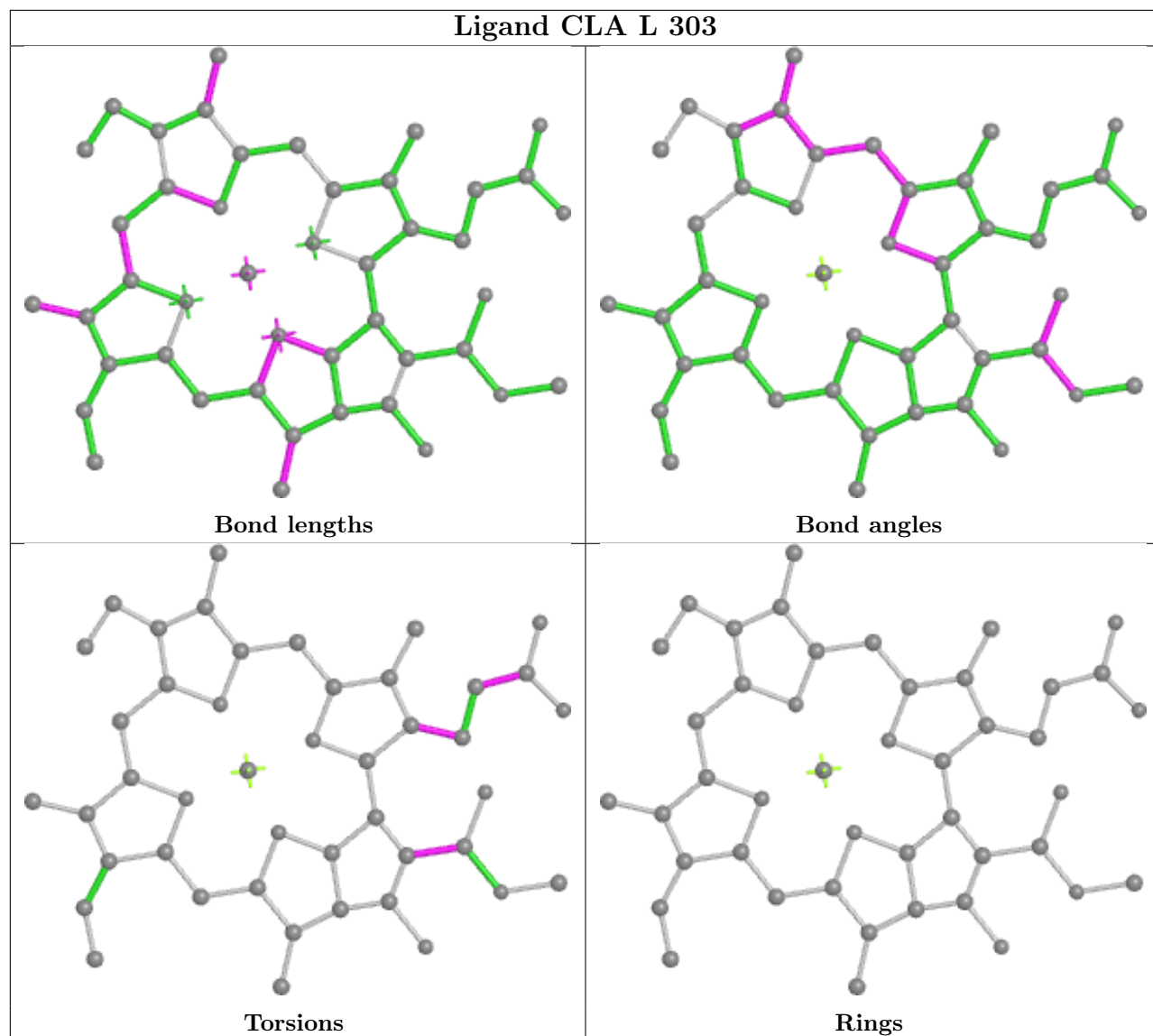


Ligand CLA a 613

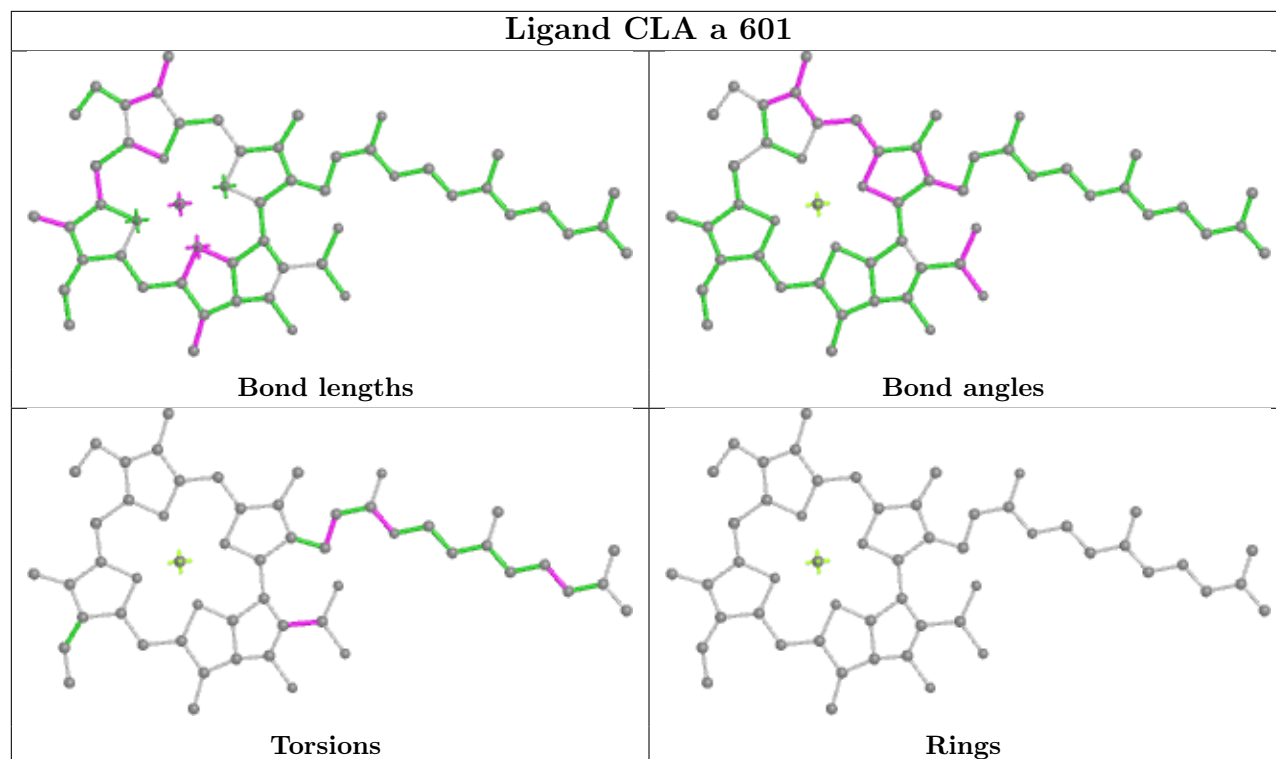




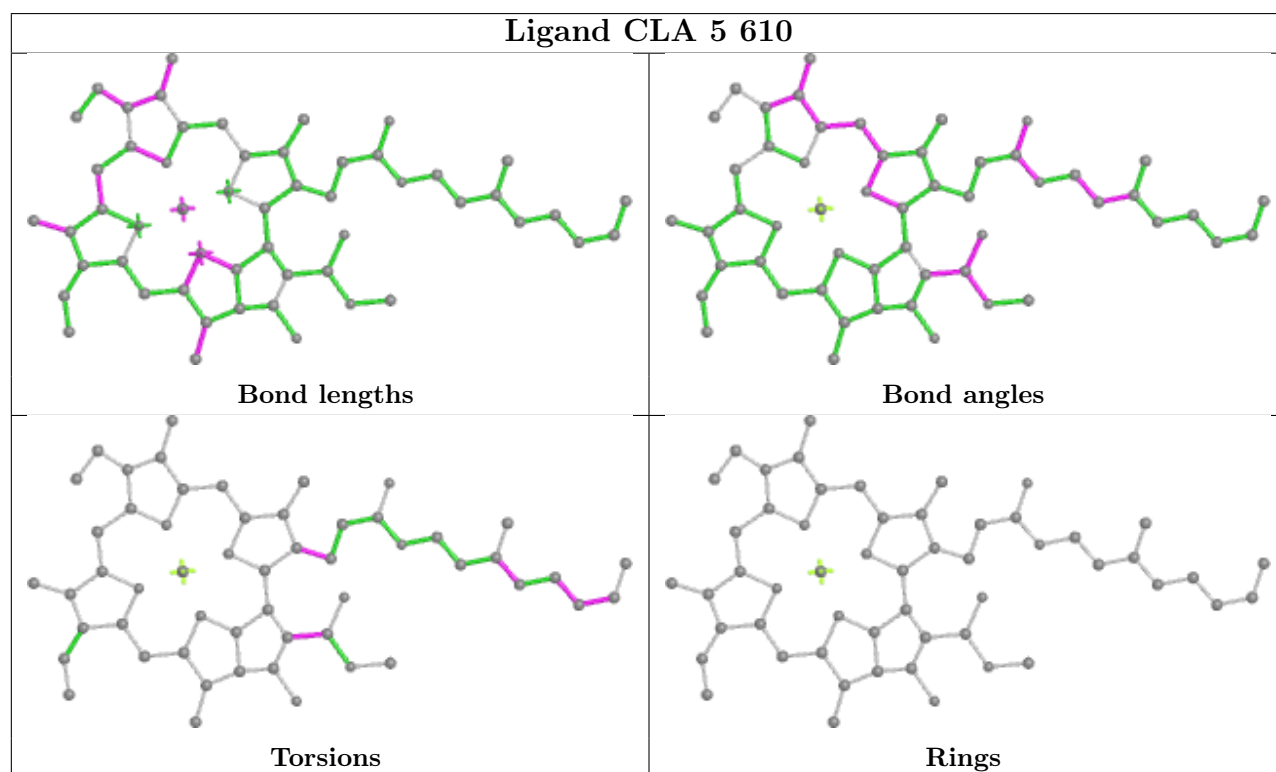
Ligand CLA L 303

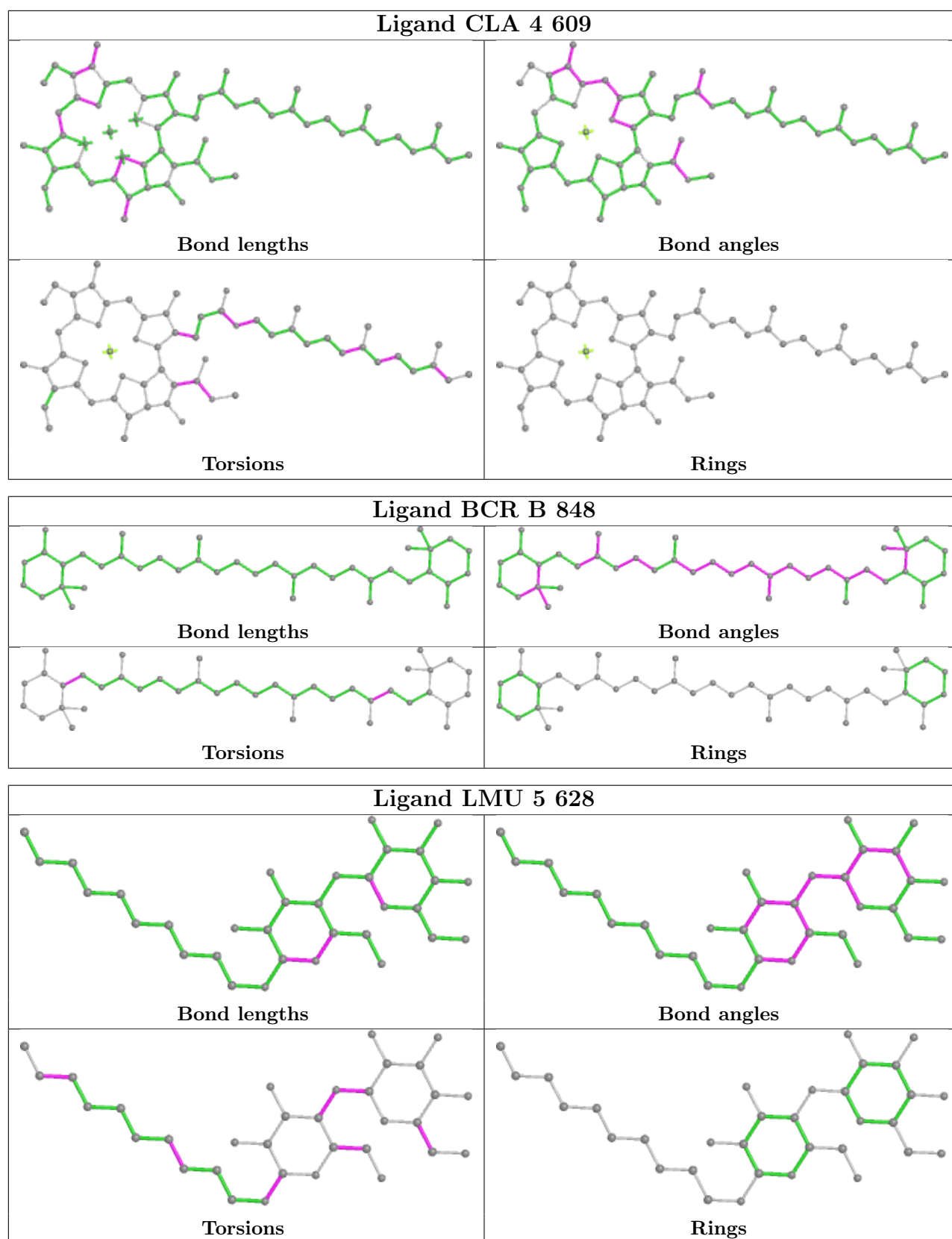


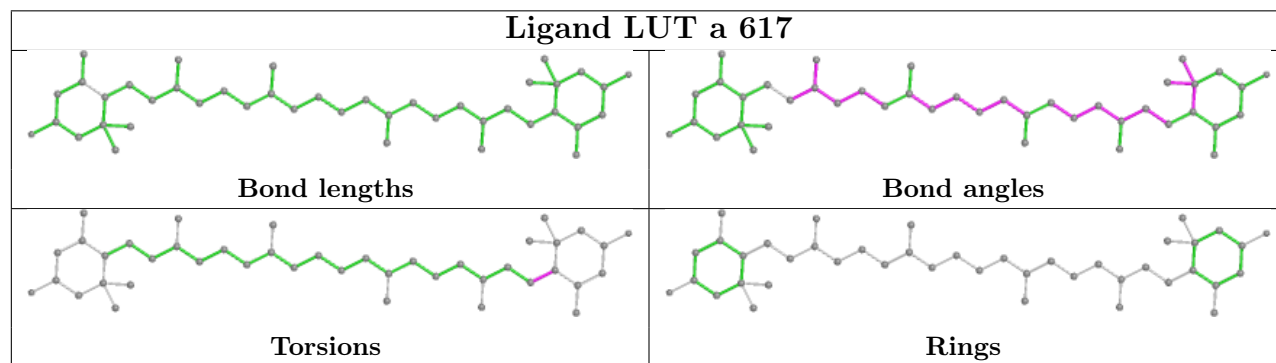
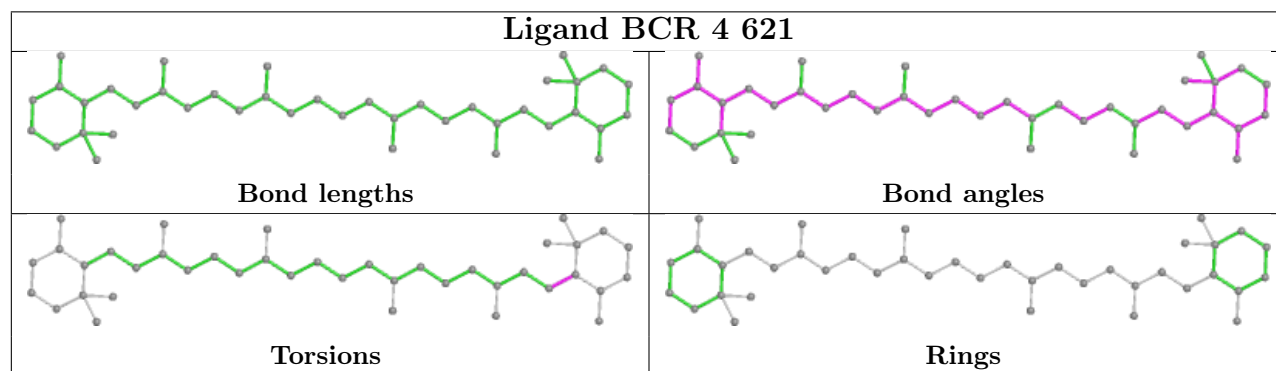
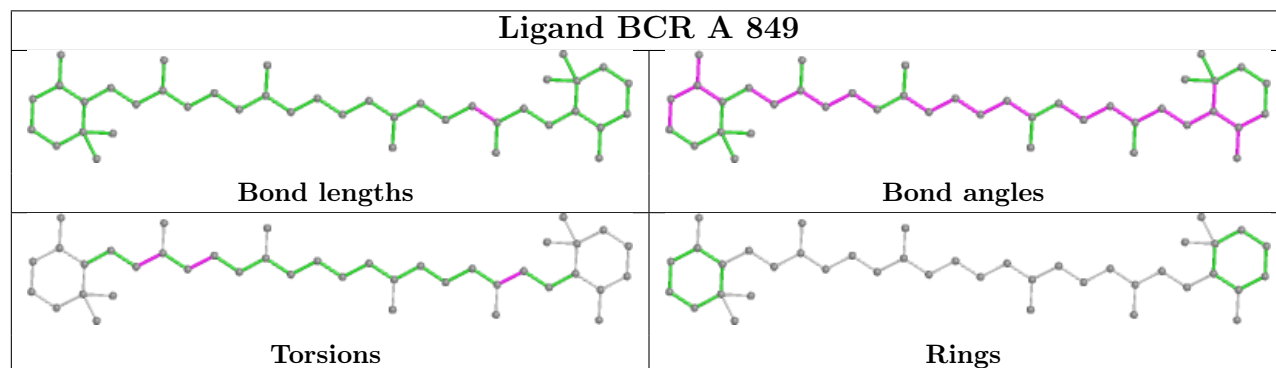
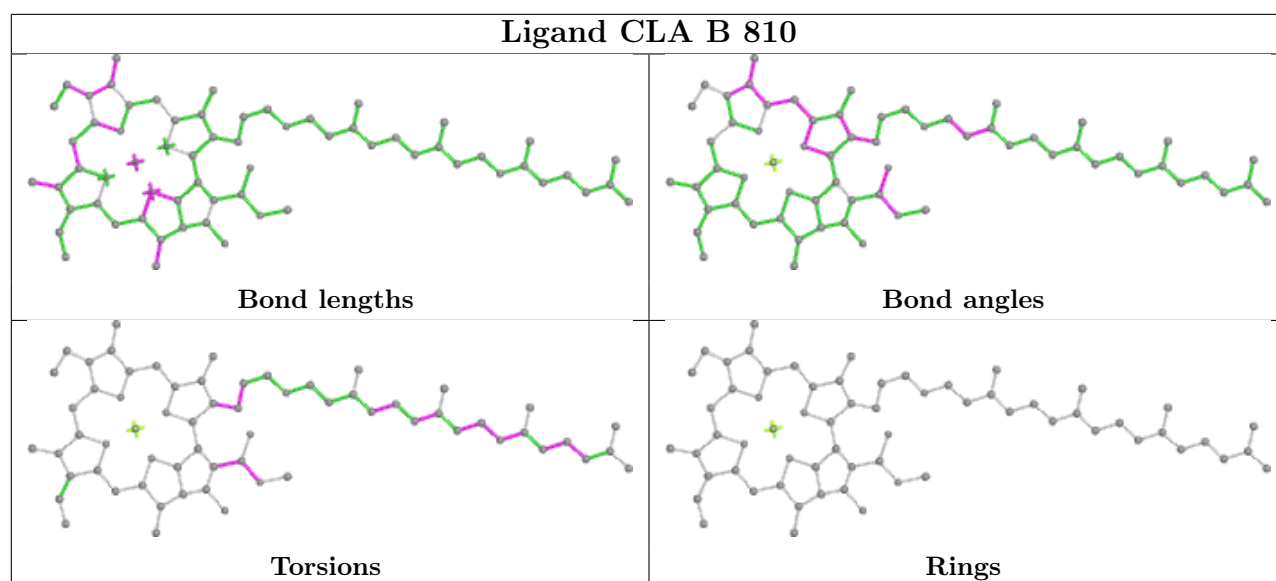
Ligand CLA a 601



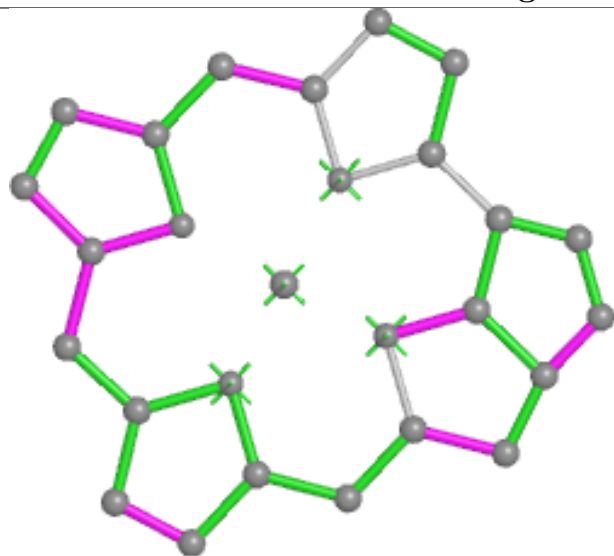
Ligand CLA 5 610



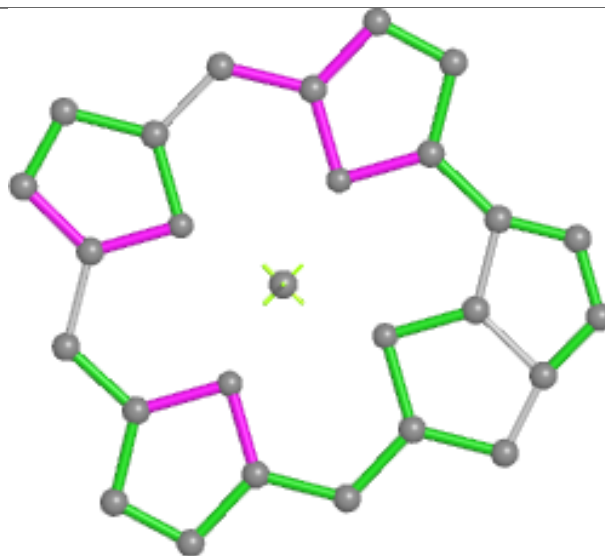




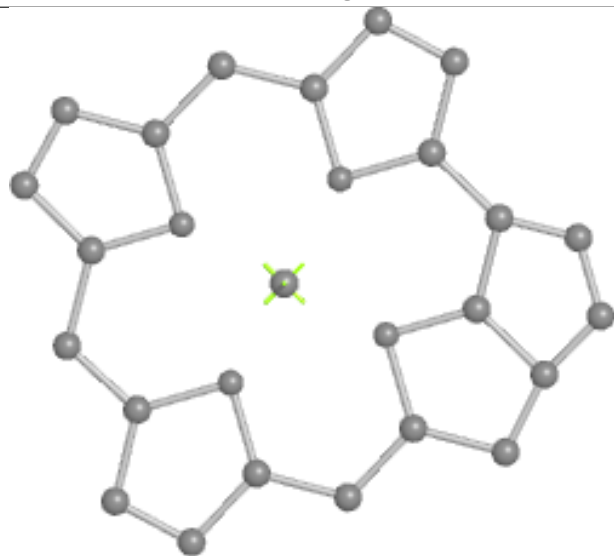
Ligand CLA 2 614



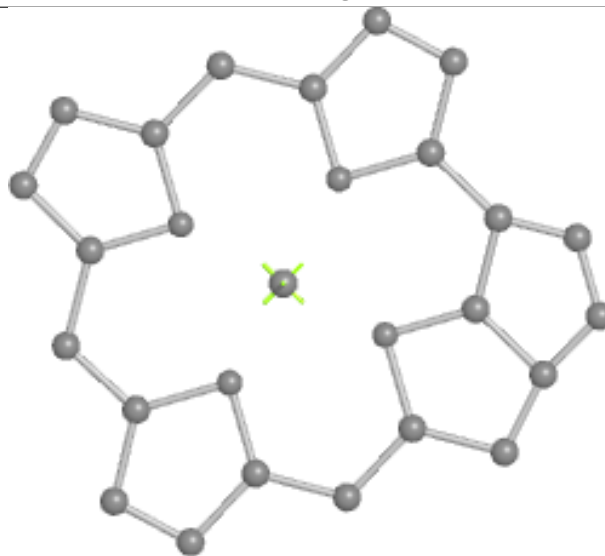
Bond lengths



Bond angles

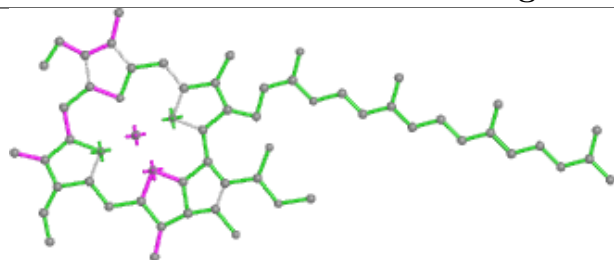


Torsions

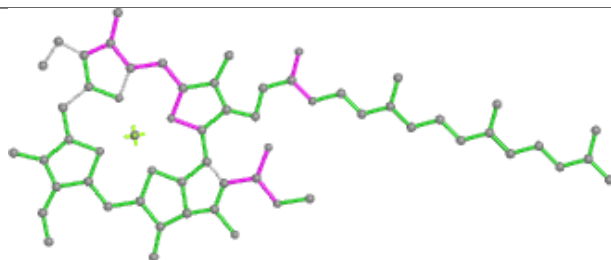


Rings

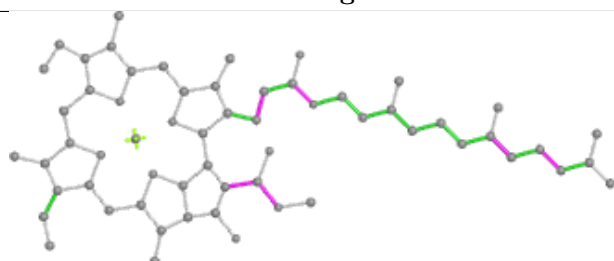
Ligand CLA 3 602



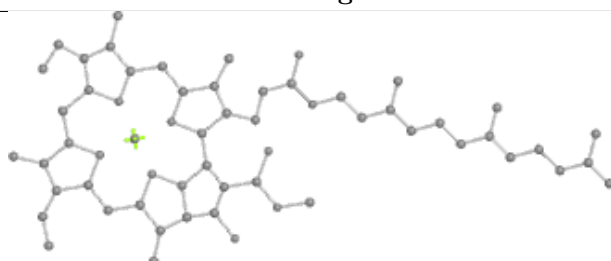
Bond lengths



Bond angles

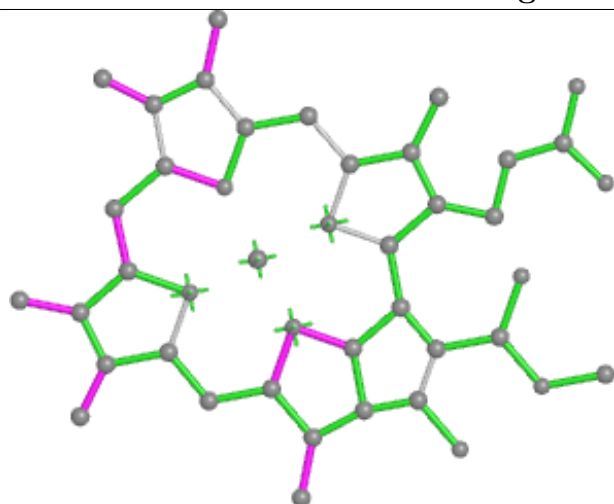


Torsions

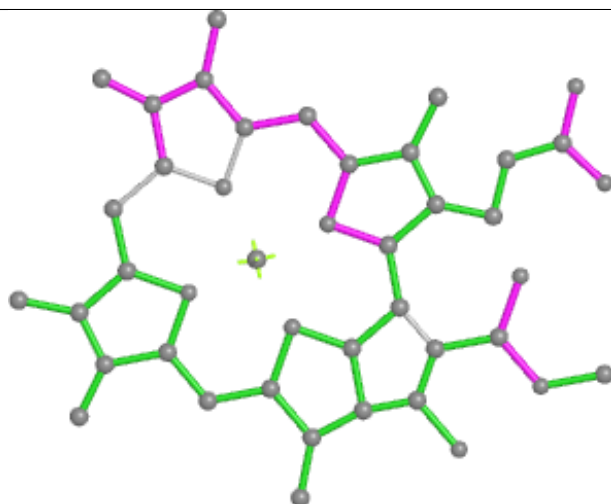


Rings

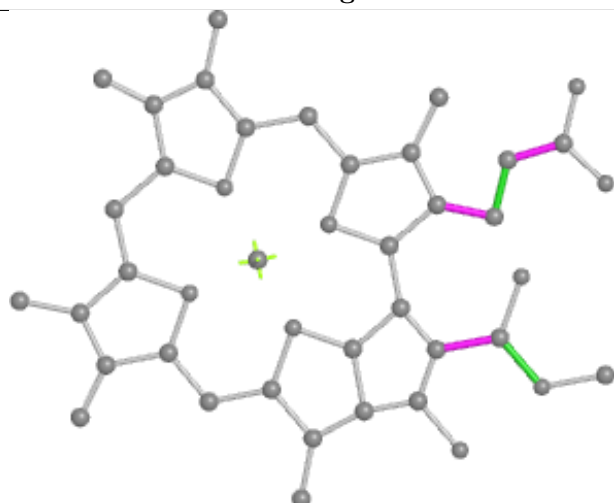
Ligand CLA 4 616



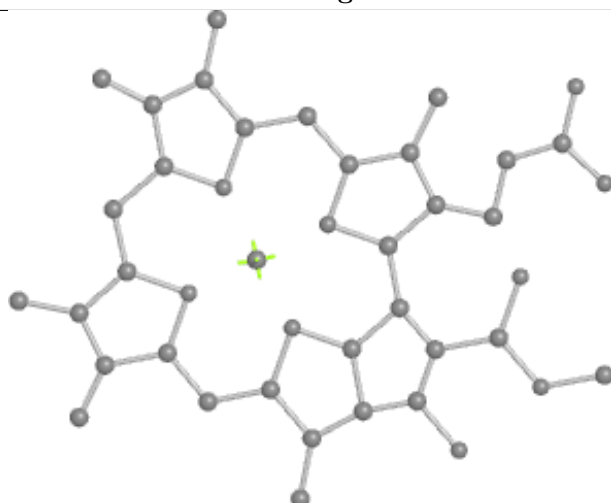
Bond lengths



Bond angles

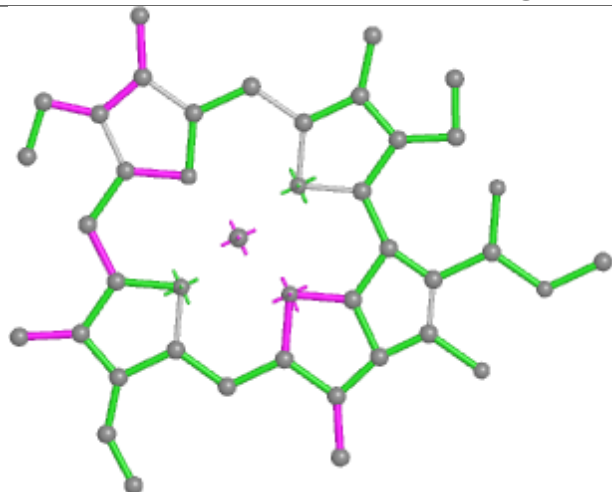


Torsions

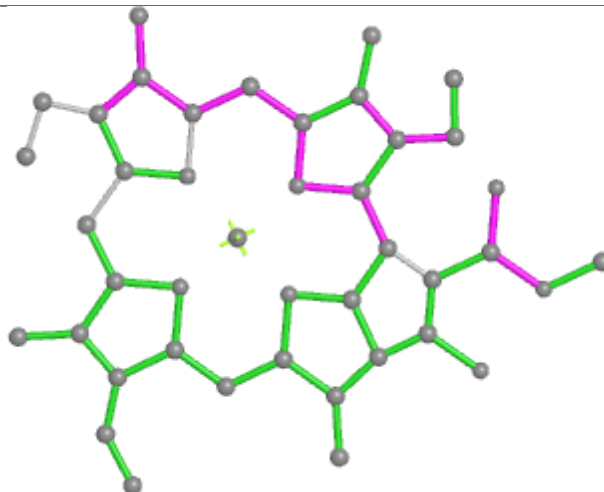


Rings

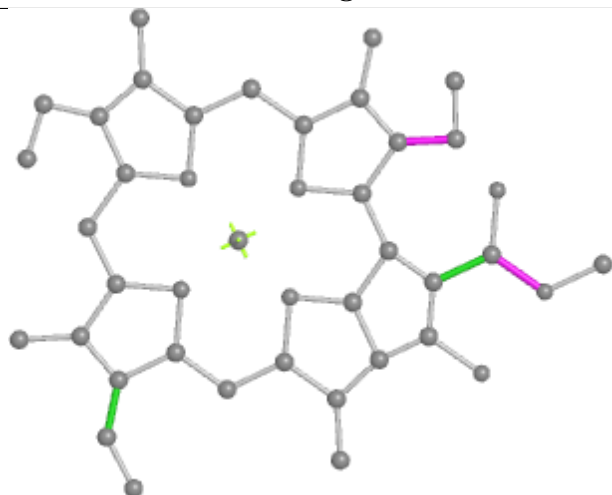
Ligand CLA 7 614



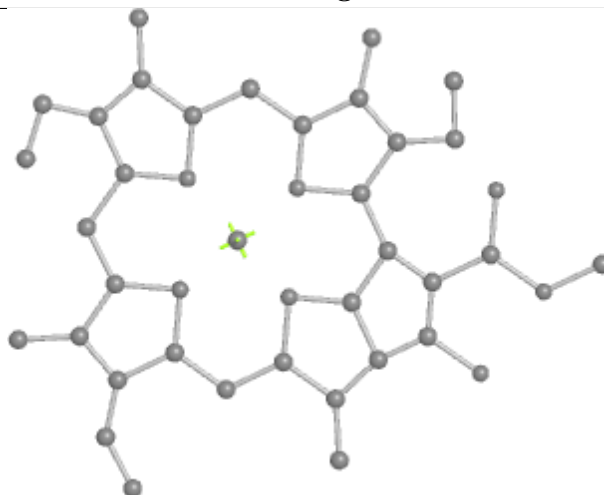
Bond lengths



Bond angles

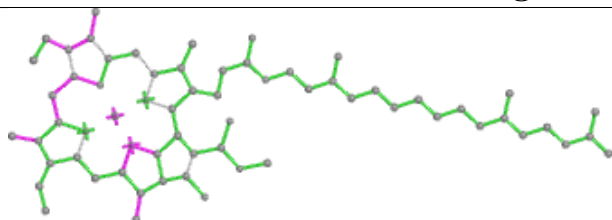


Torsions

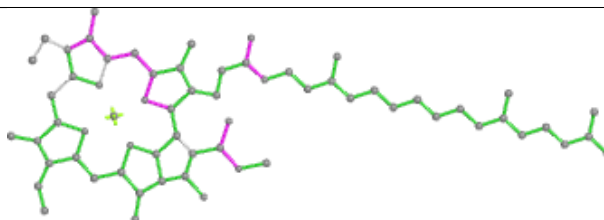


Rings

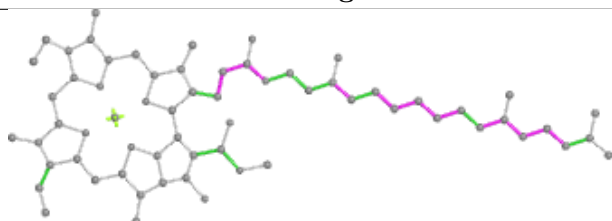
Ligand CLA A 843



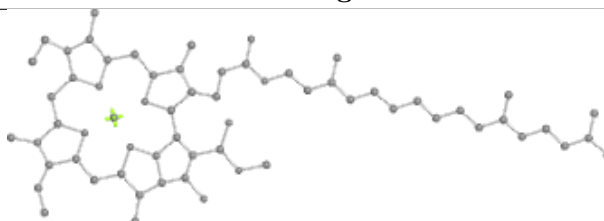
Bond lengths



Bond angles

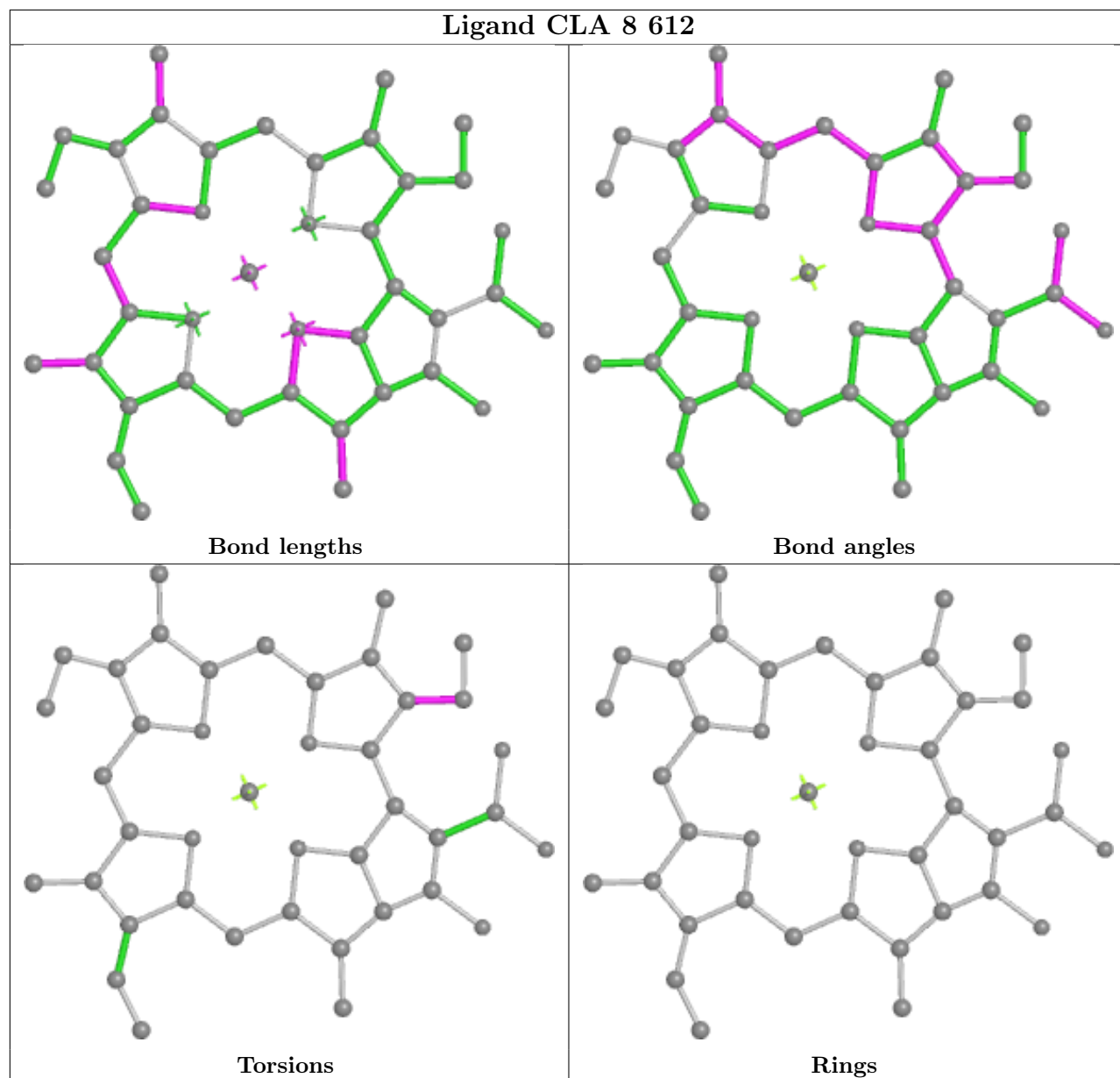


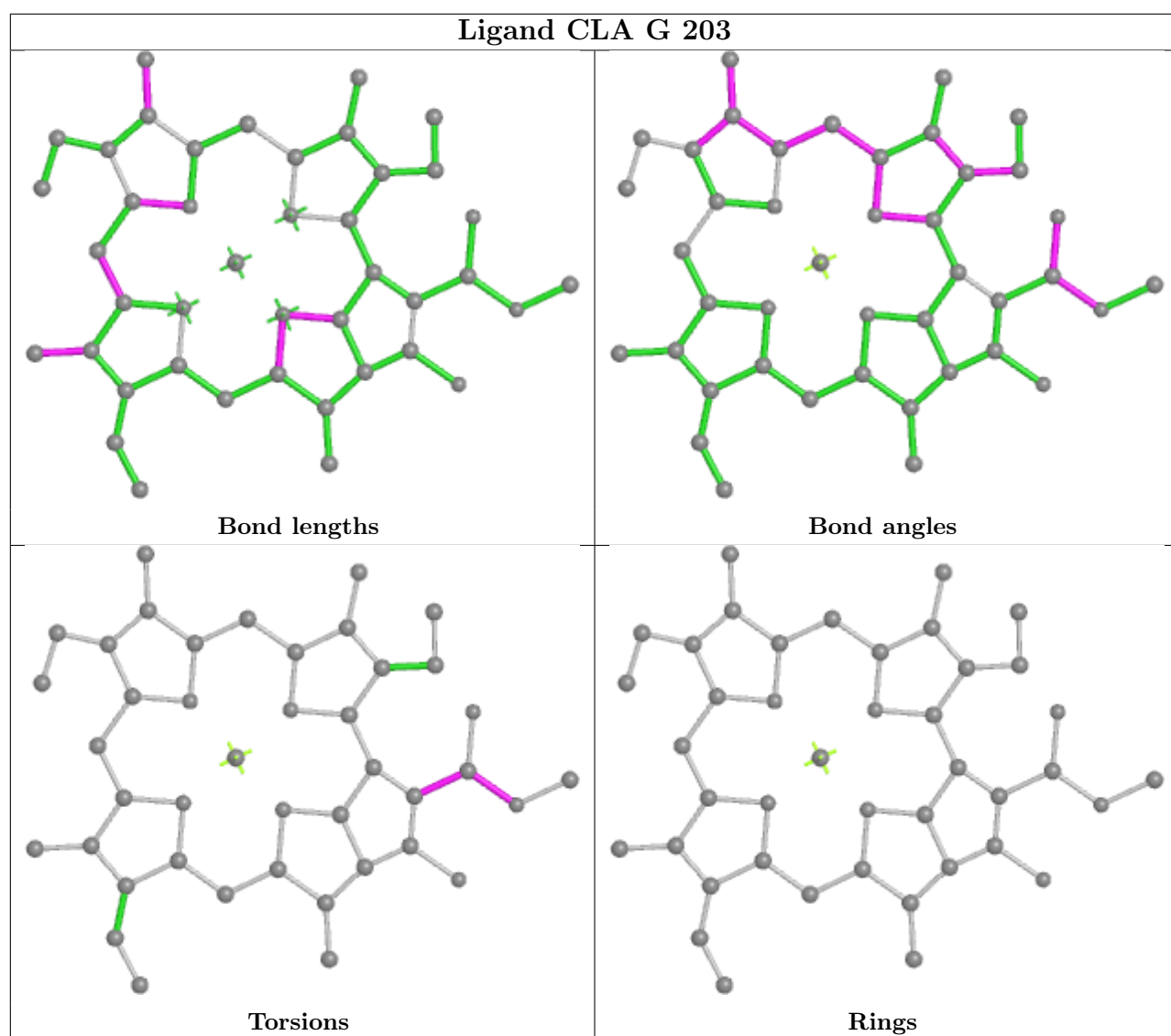
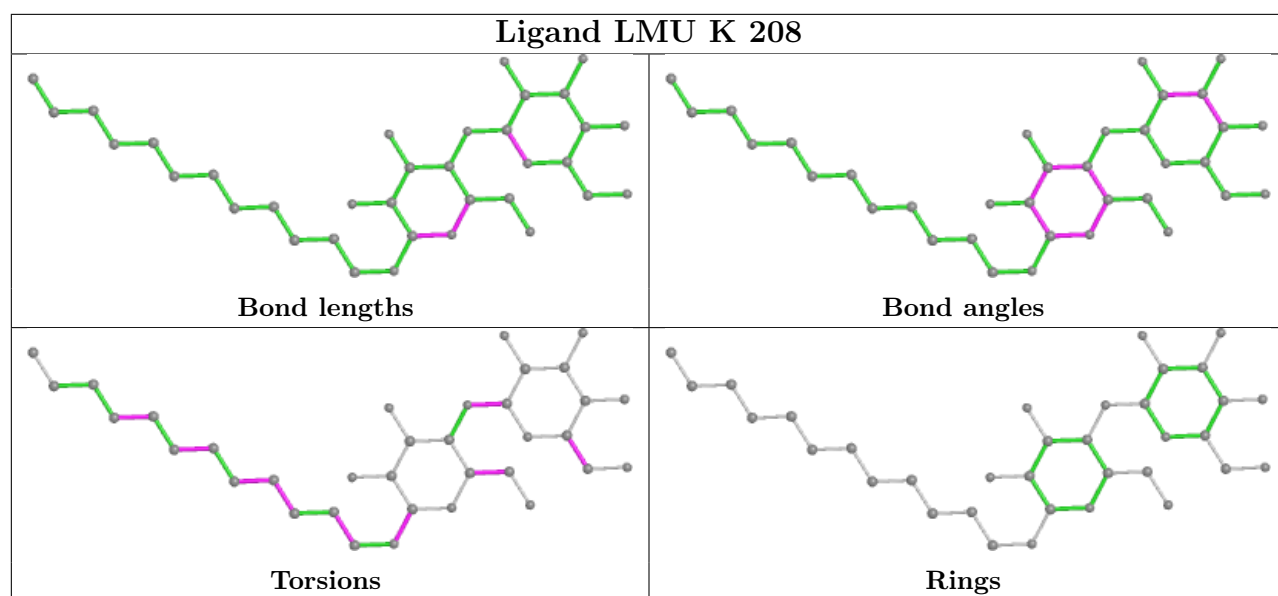
Torsions

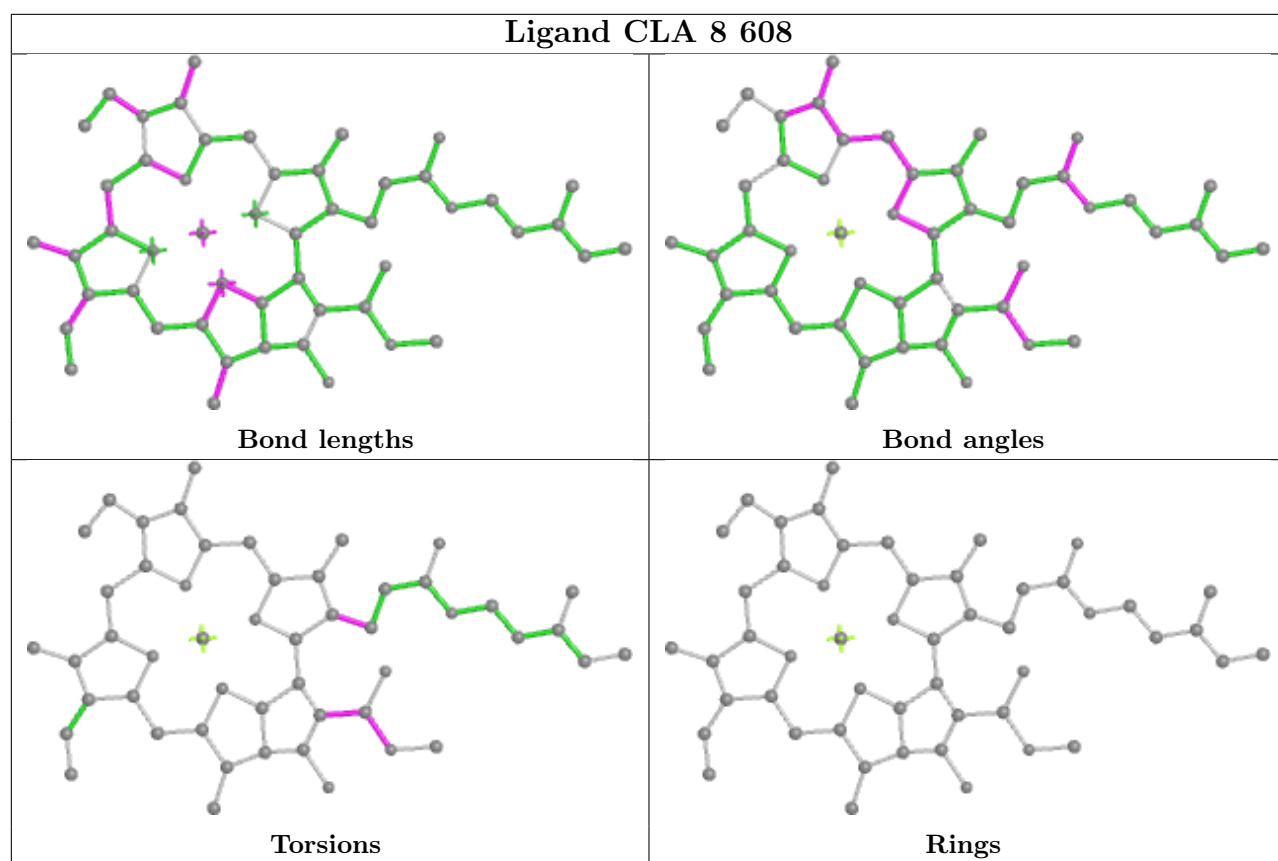


Rings

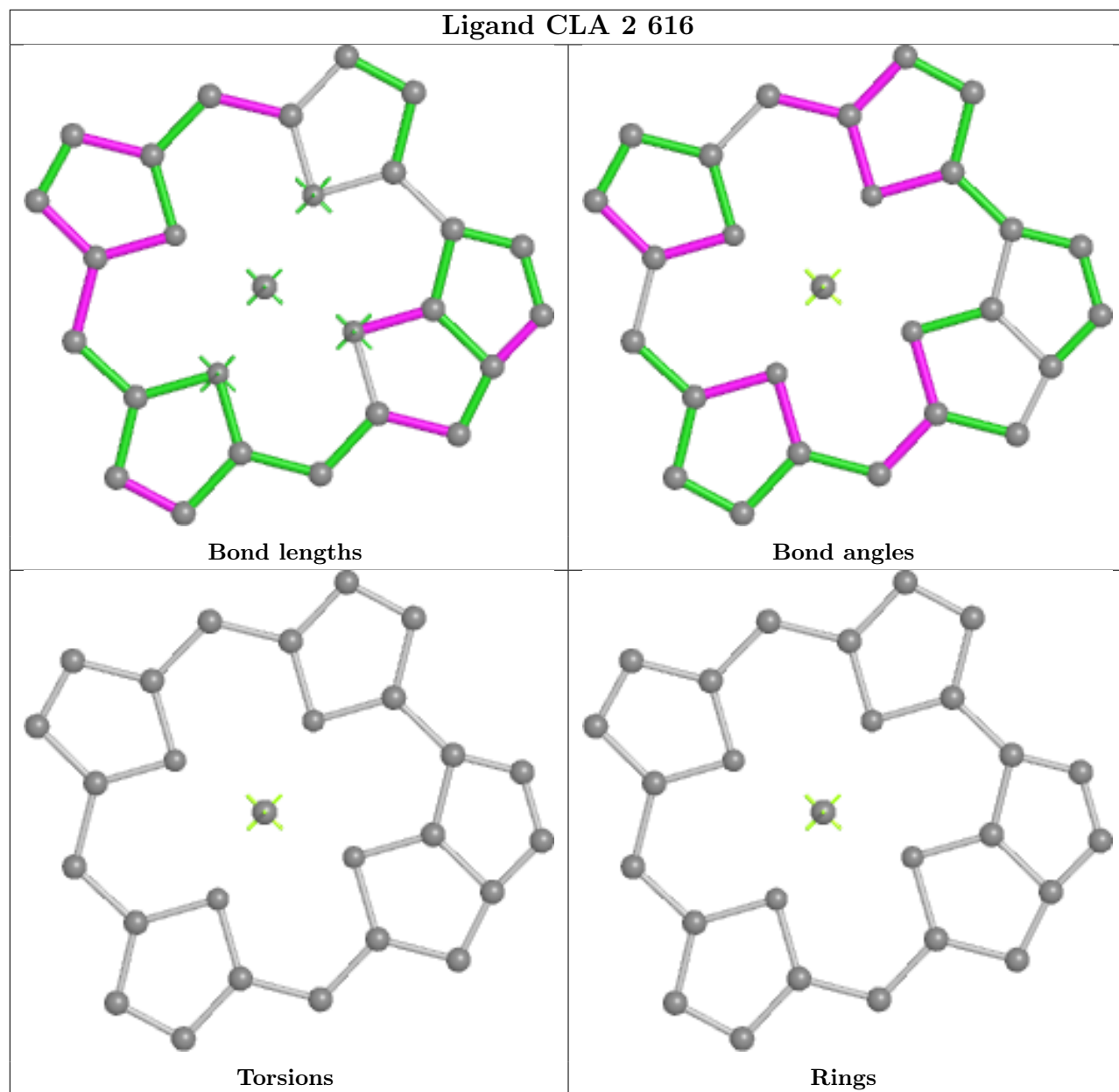
Ligand CLA 8 612

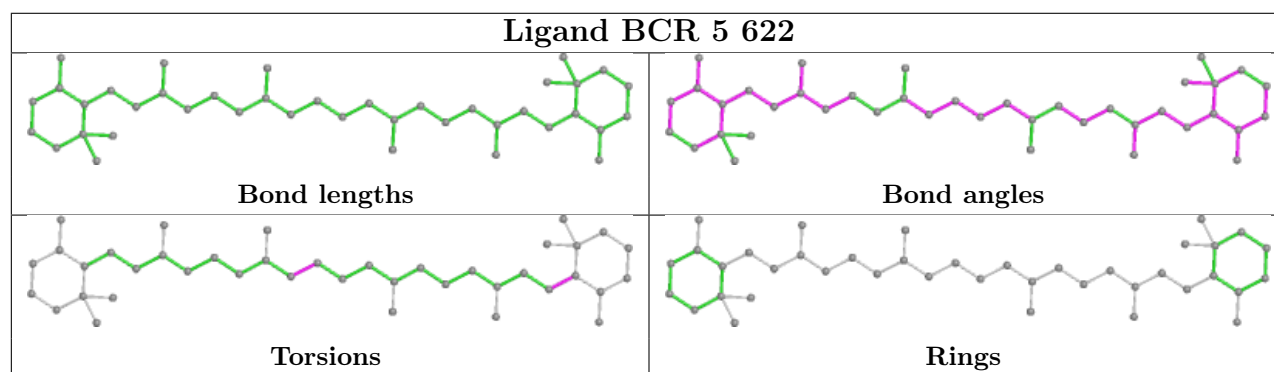
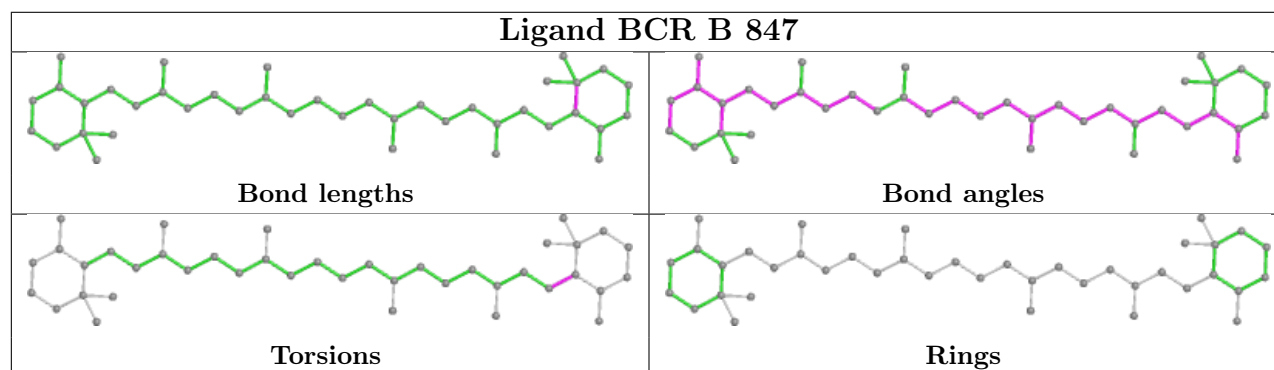
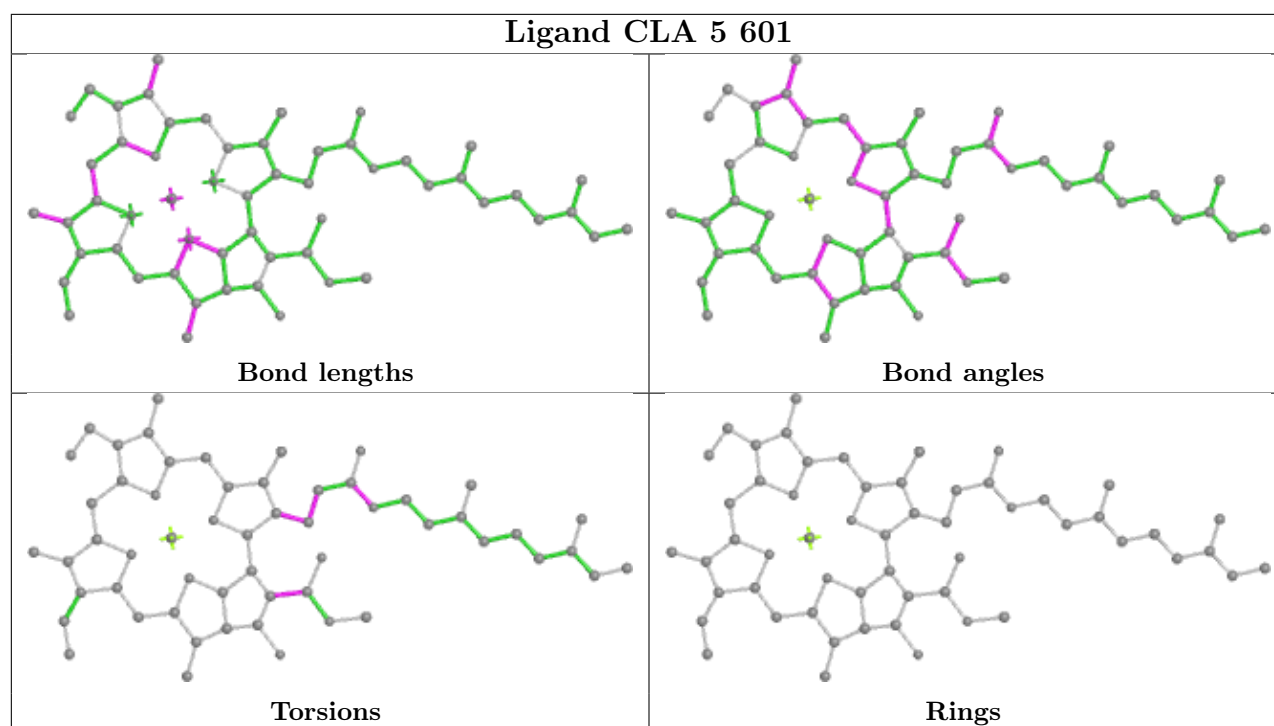


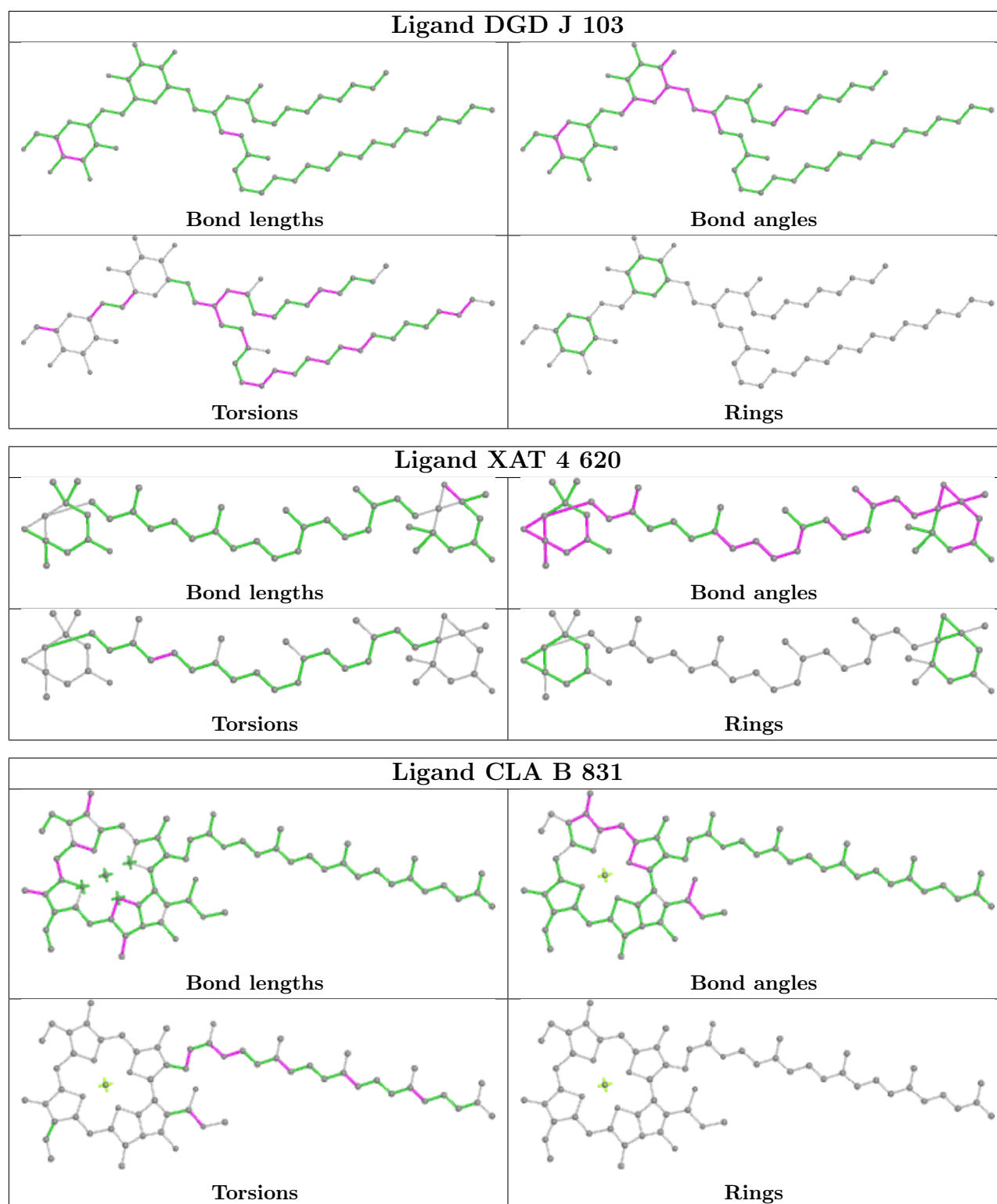




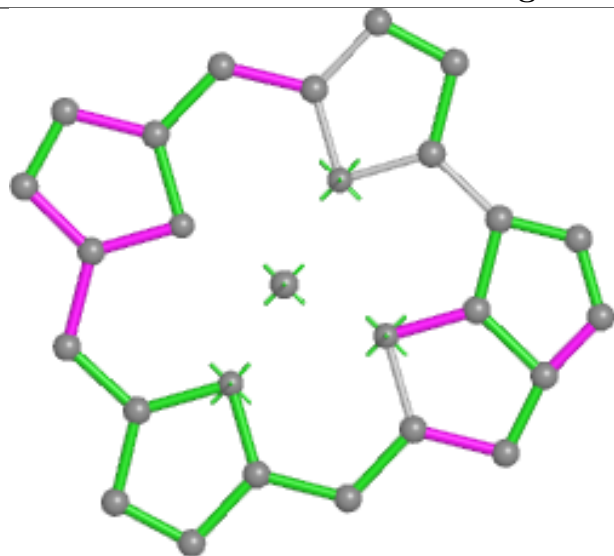
Ligand CLA 2 616



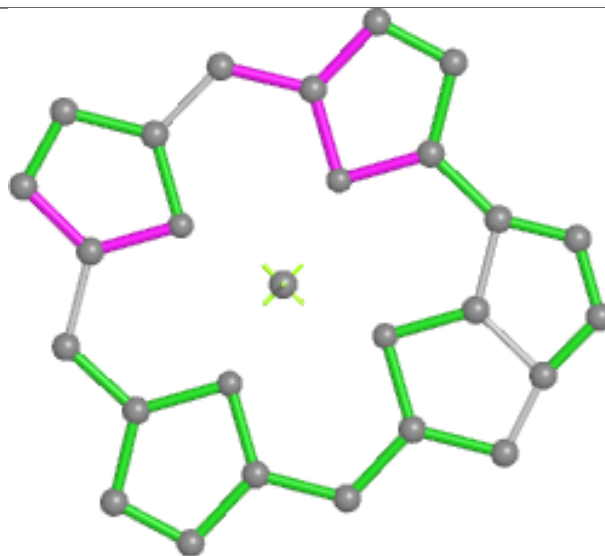




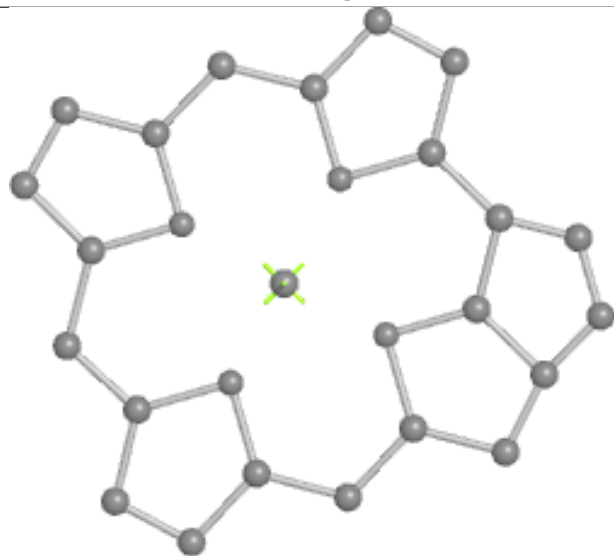
Ligand CLA 9 606



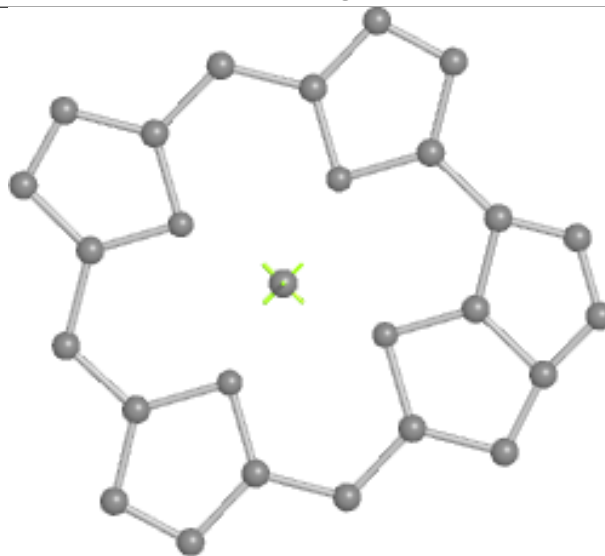
Bond lengths



Bond angles

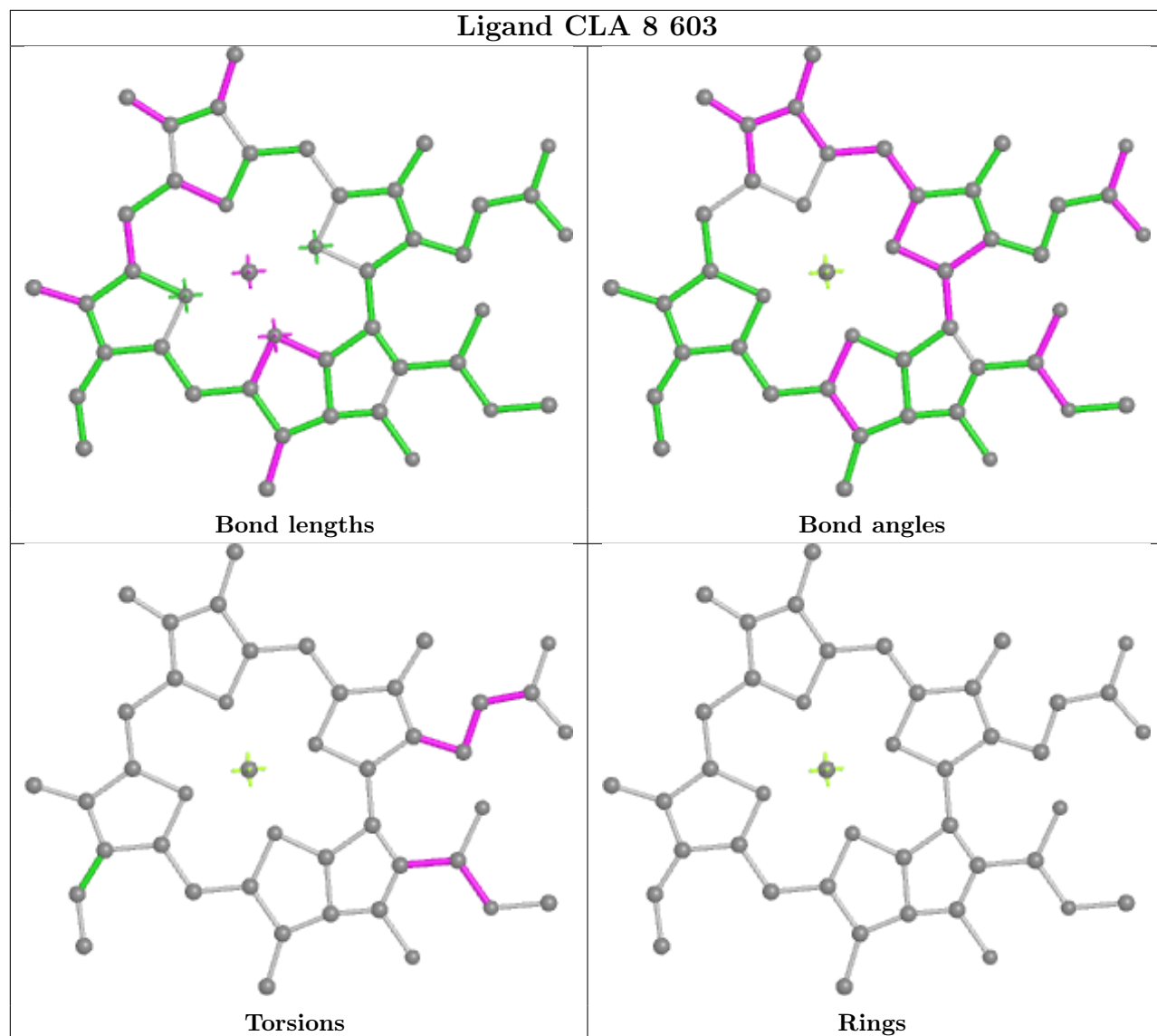


Torsions

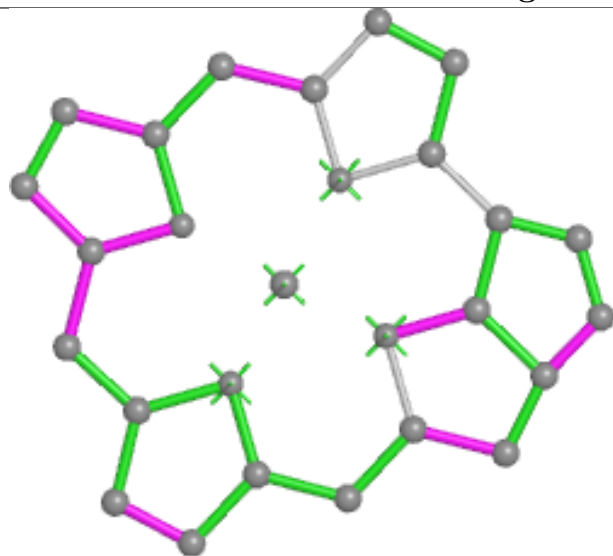


Rings

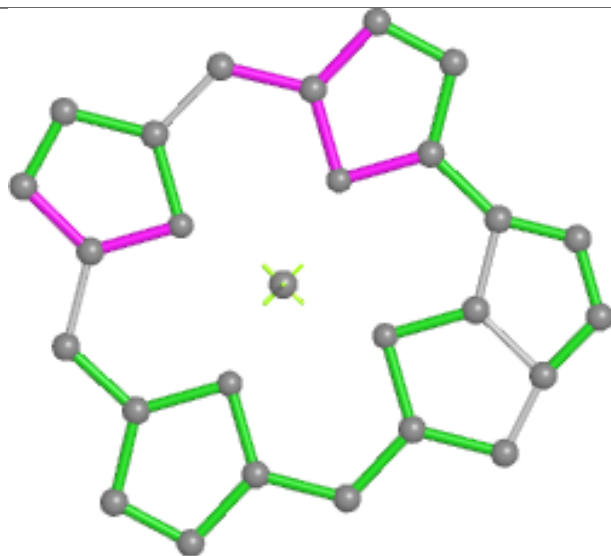
Ligand CLA 8 603



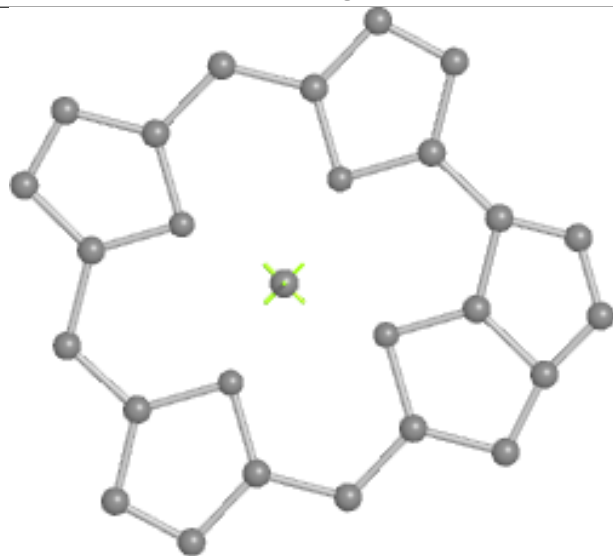
Ligand CLA 2 607



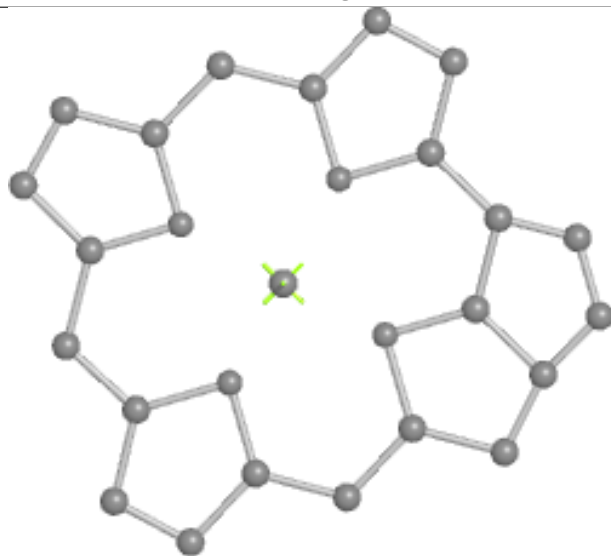
Bond lengths



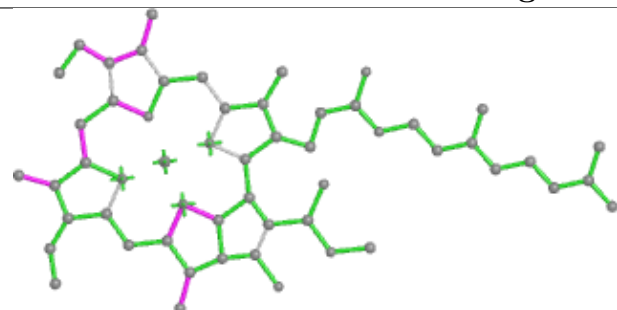
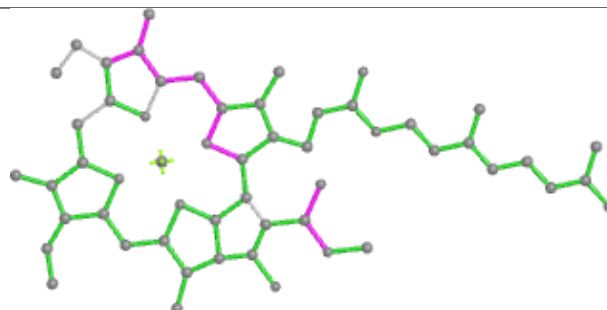
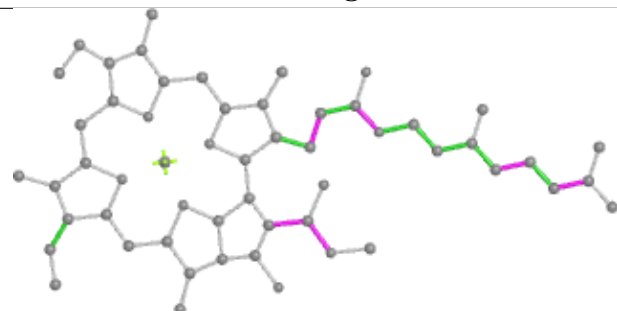
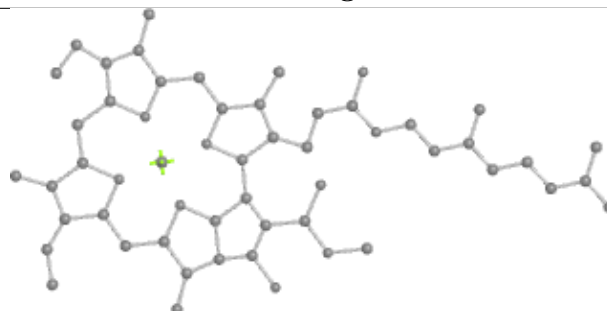
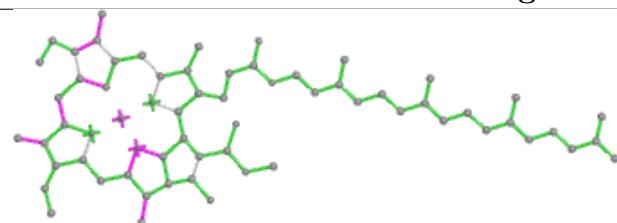
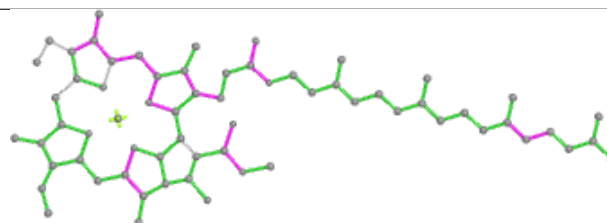
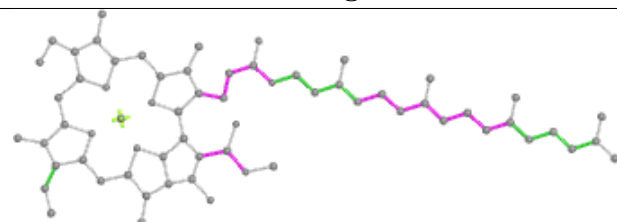
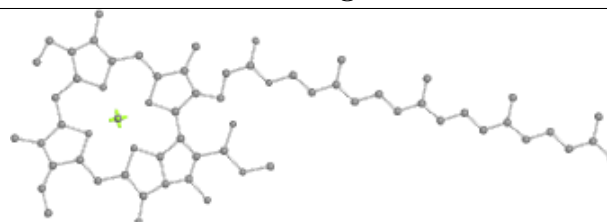
Bond angles

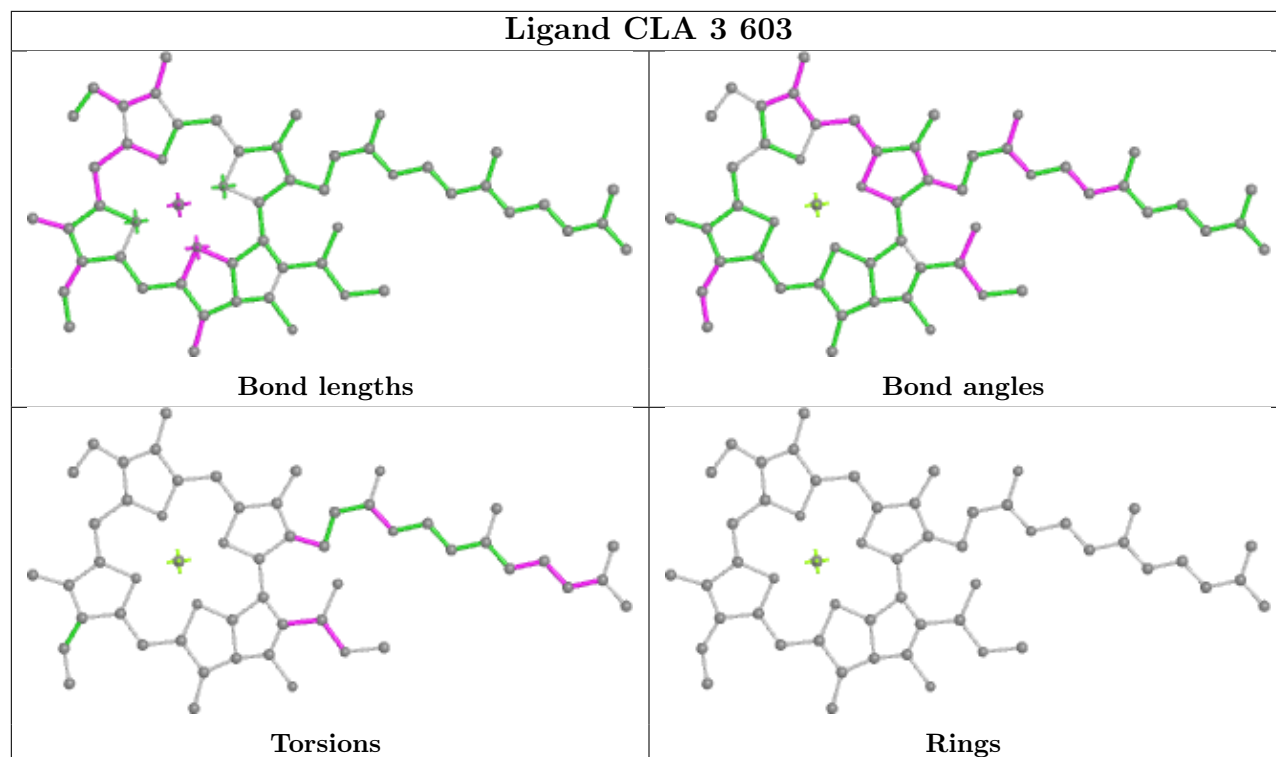
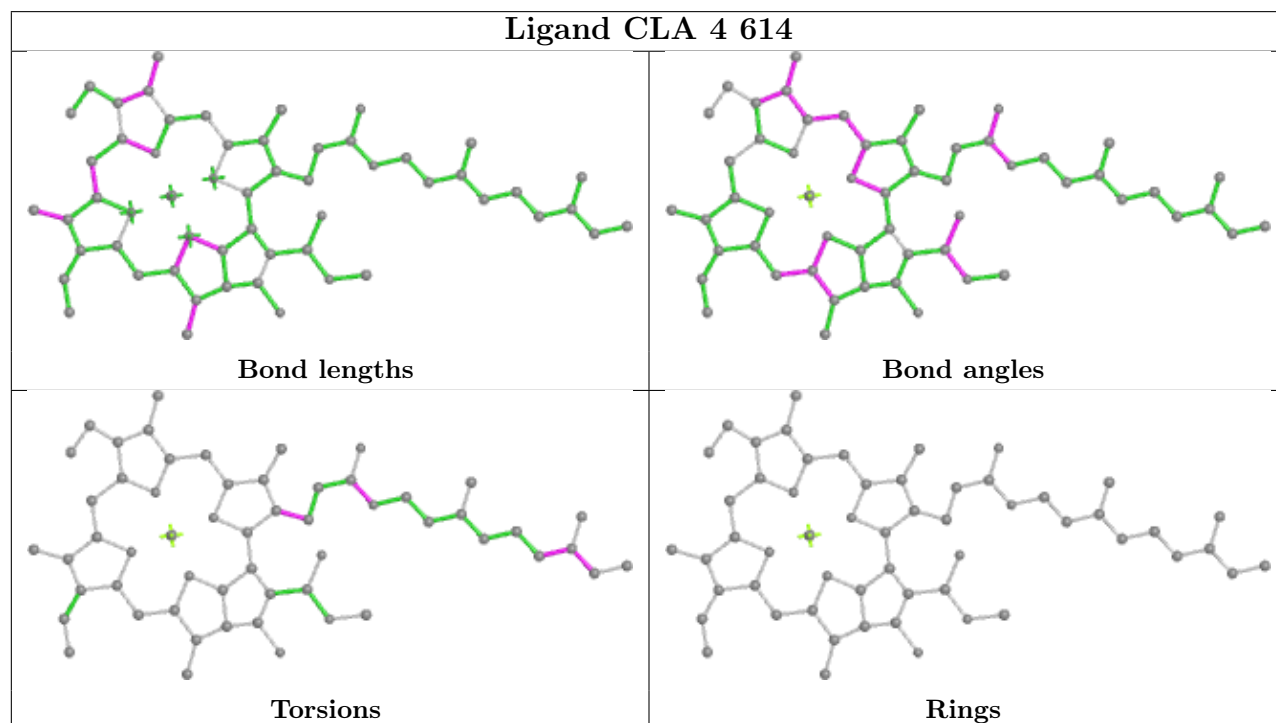


Torsions

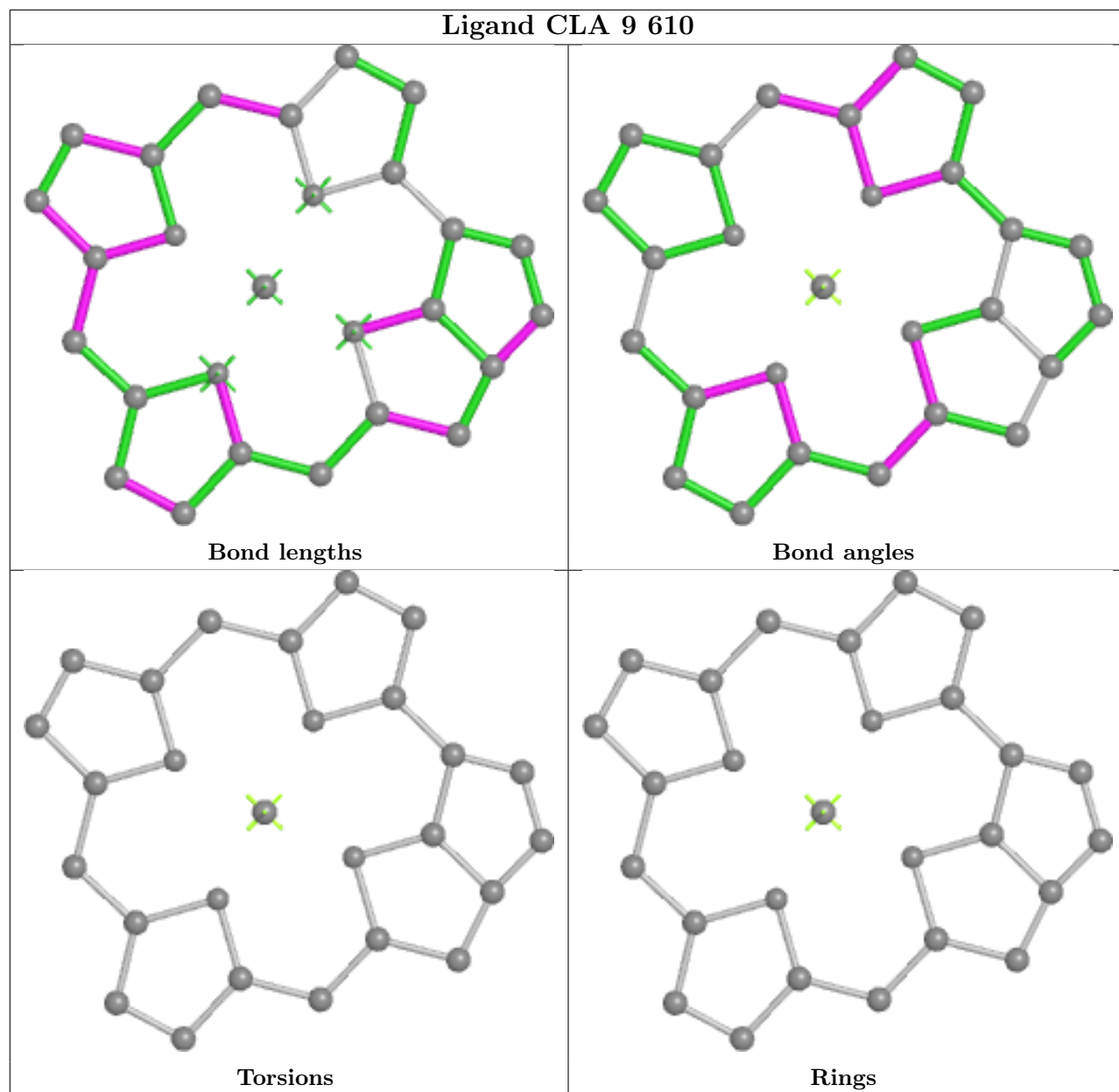


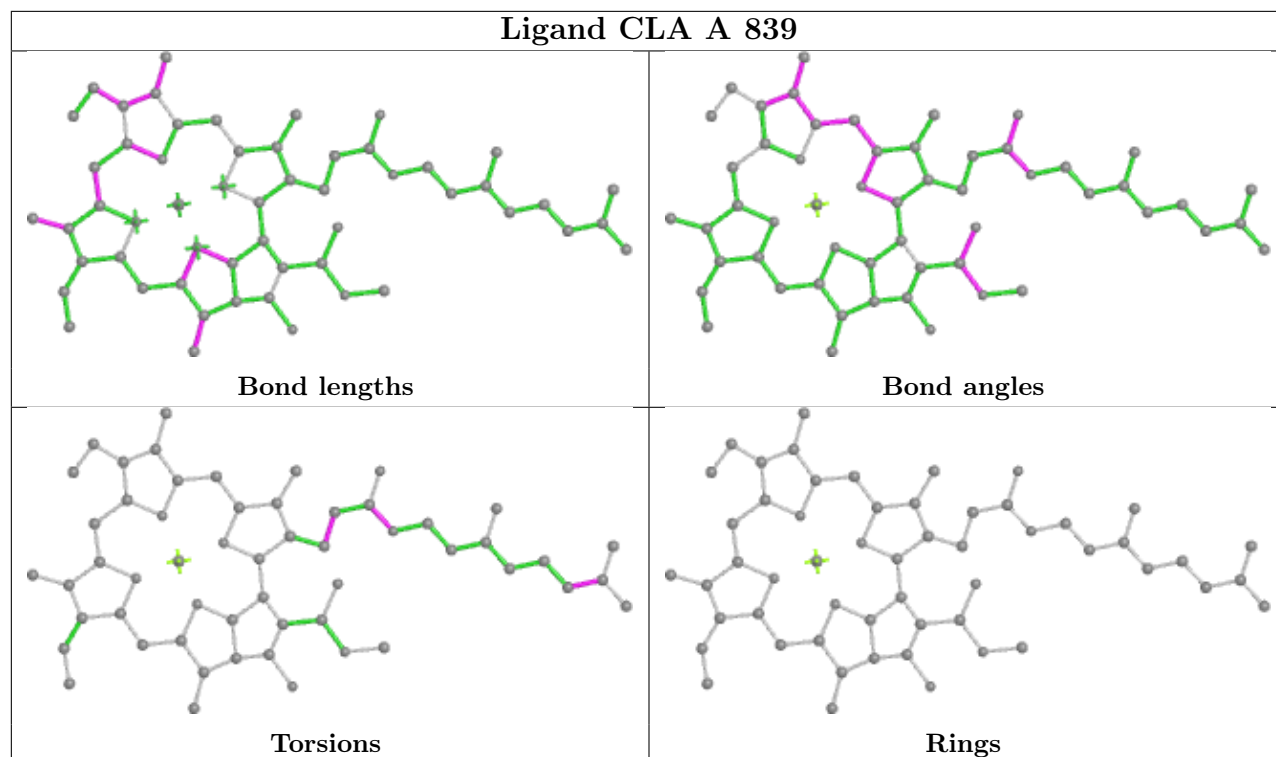
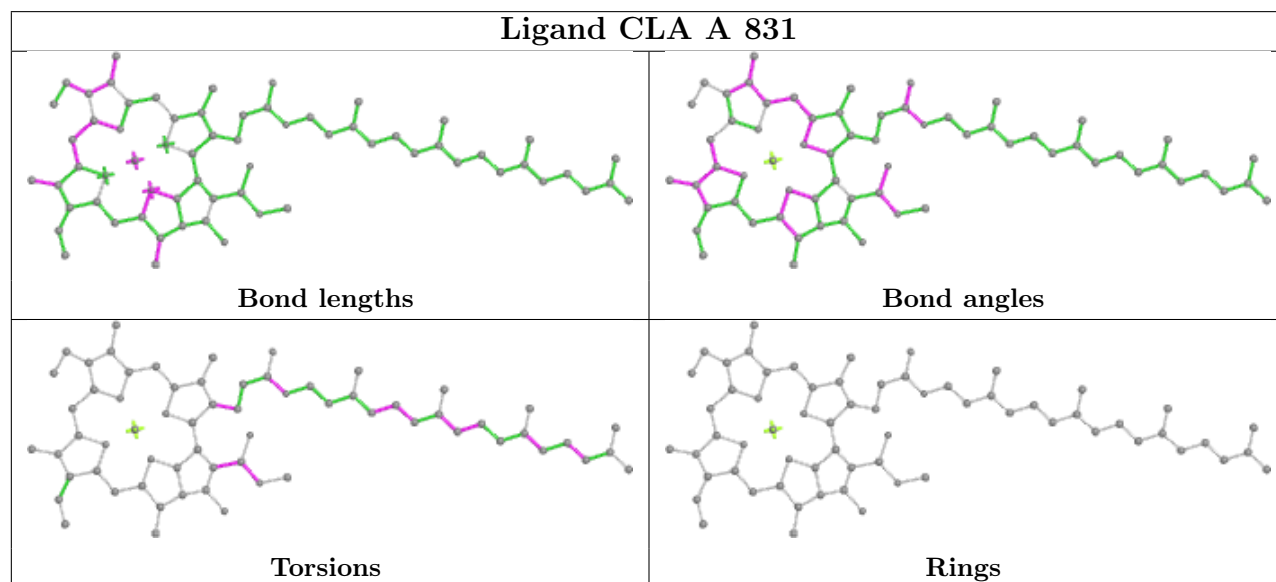
Rings

Ligand CLA B 819**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 813****Bond lengths****Bond angles****Torsions****Rings**

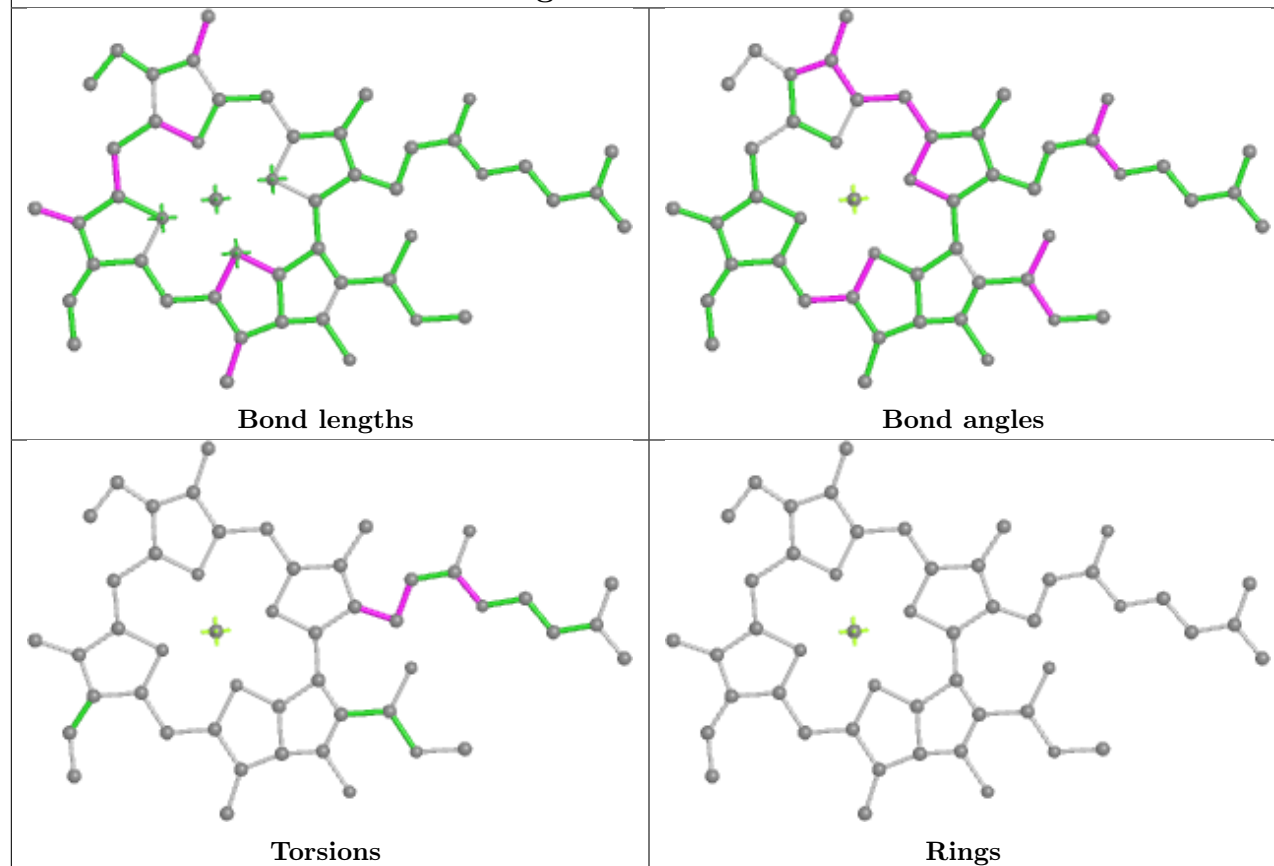
Ligand CLA 3 603**Ligand CLA 4 614**

Ligand CLA 9 610

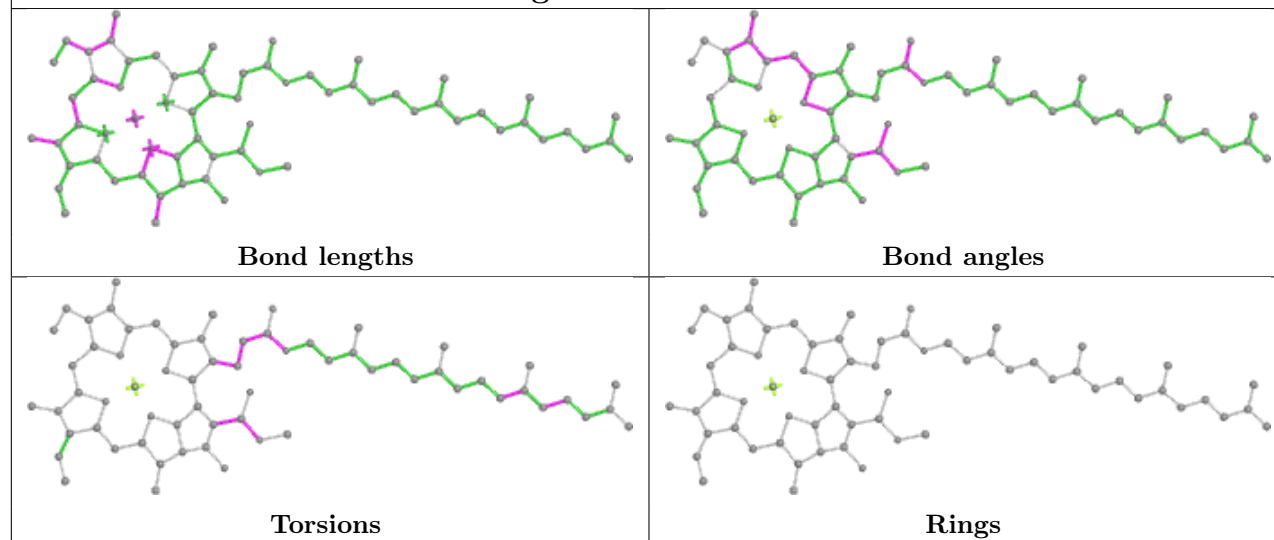


Ligand CLA A 839**Ligand CLA A 831**

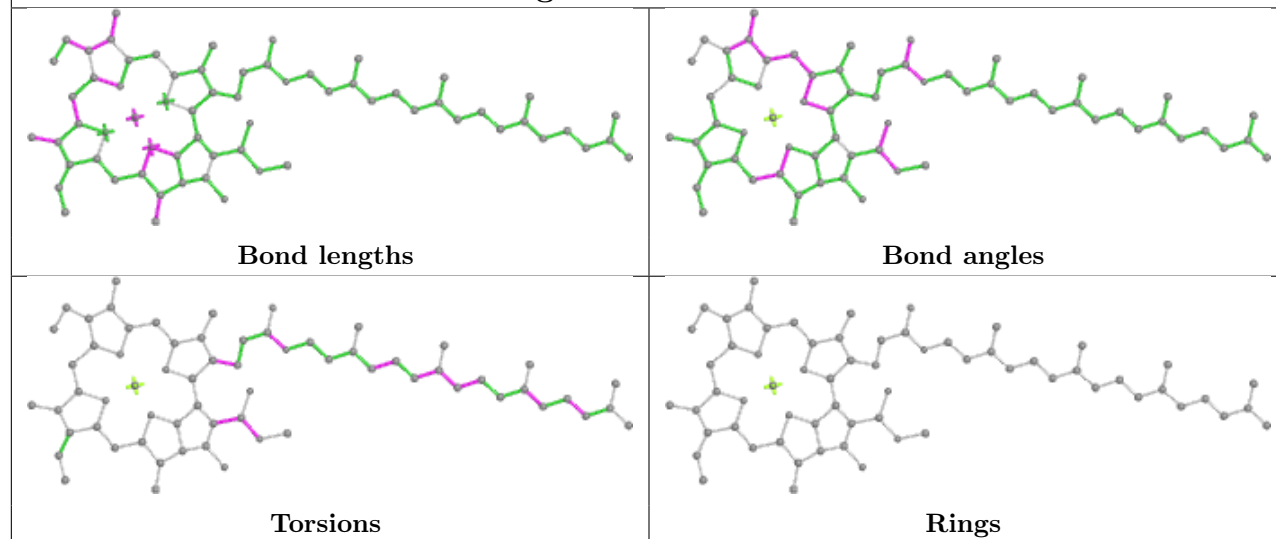
Ligand CLA 8 604



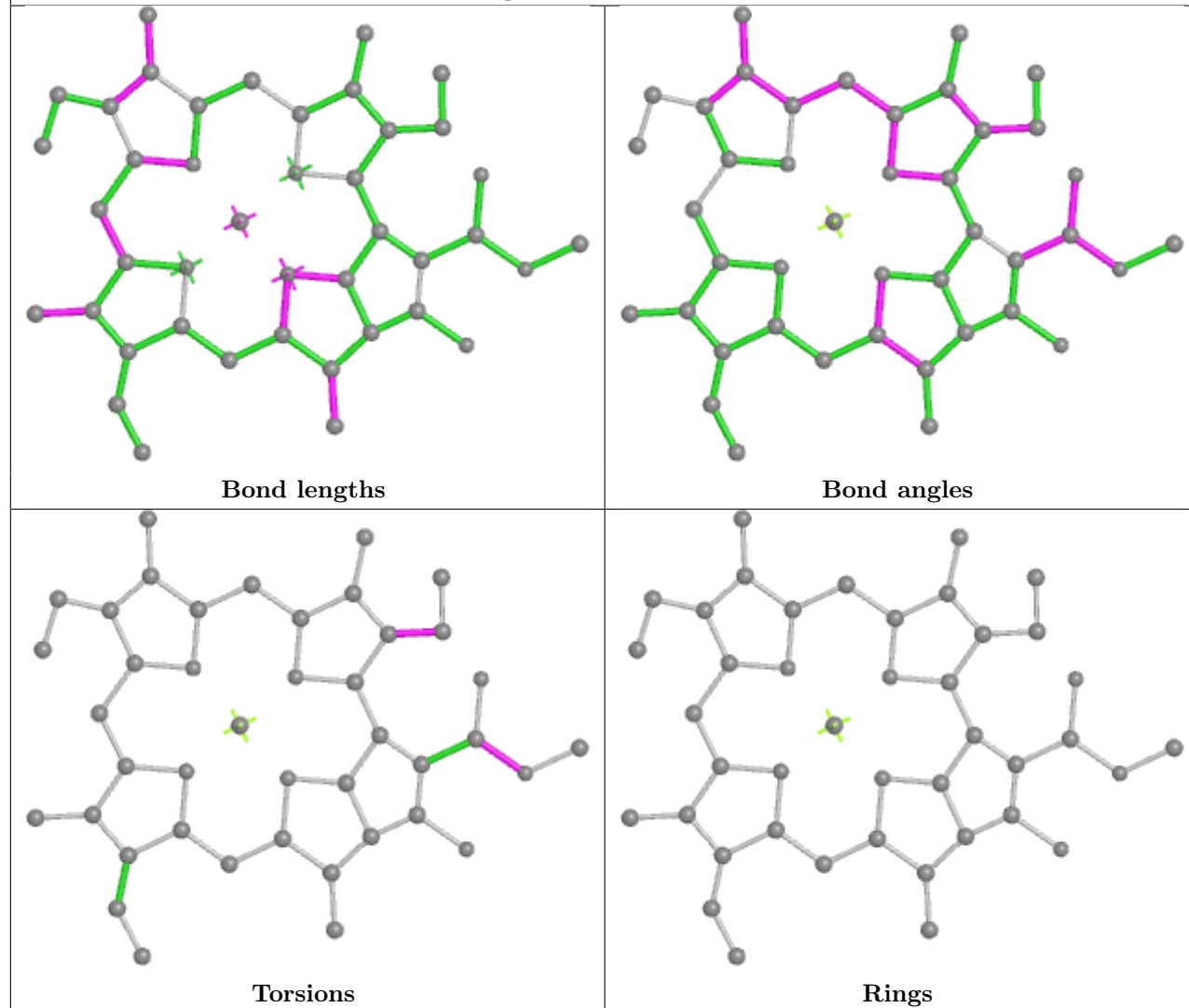
Ligand CLA A 822

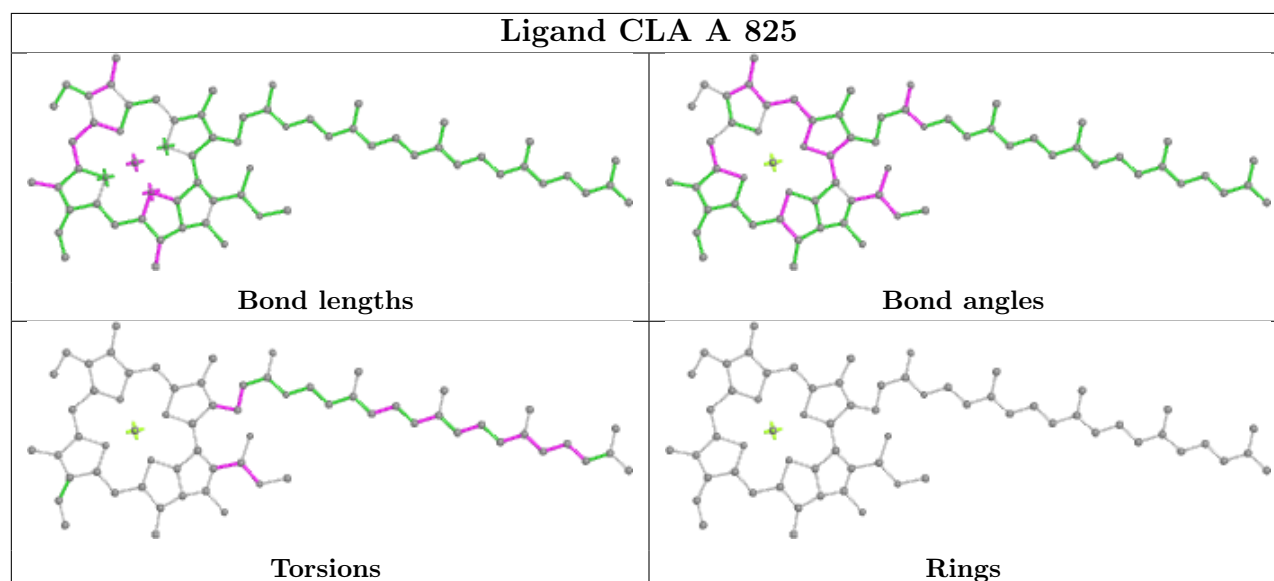
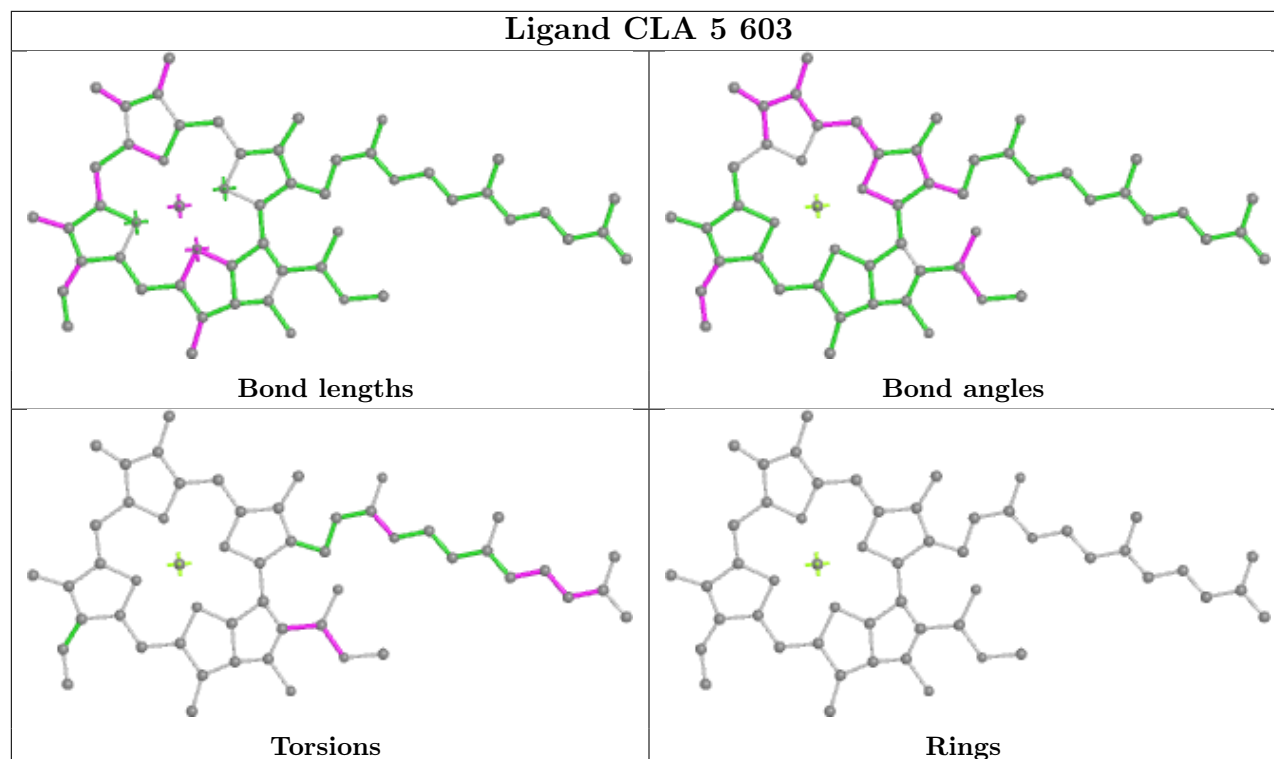
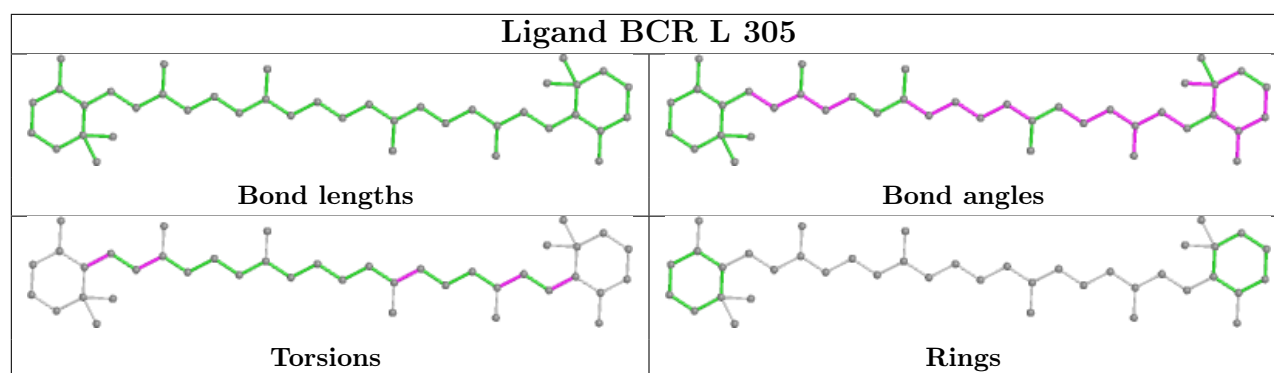


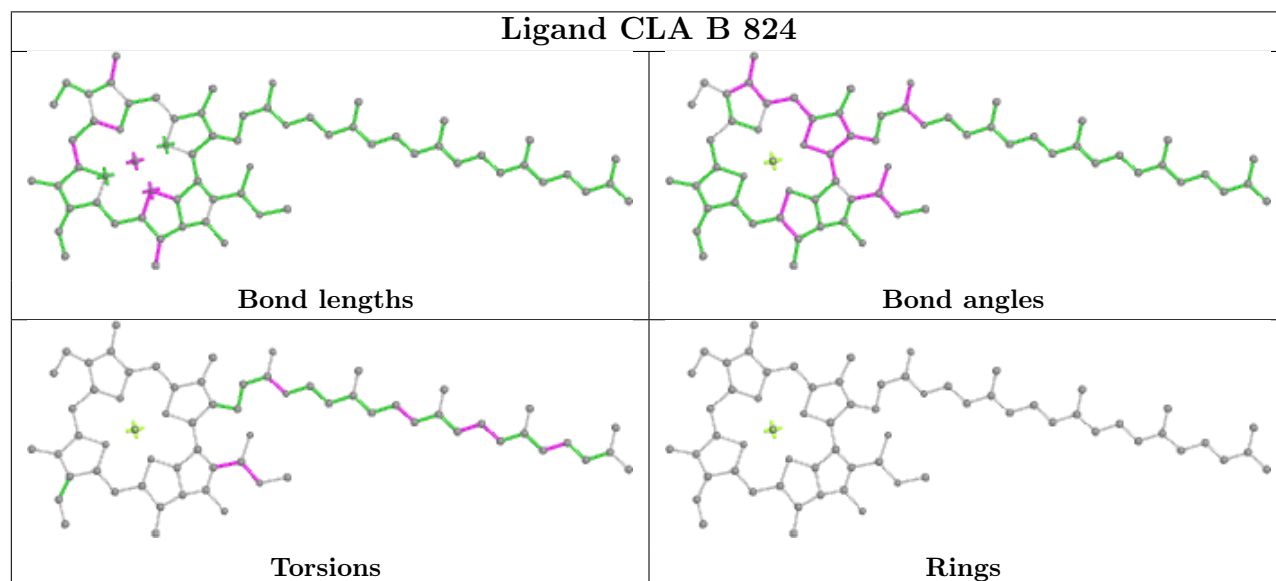
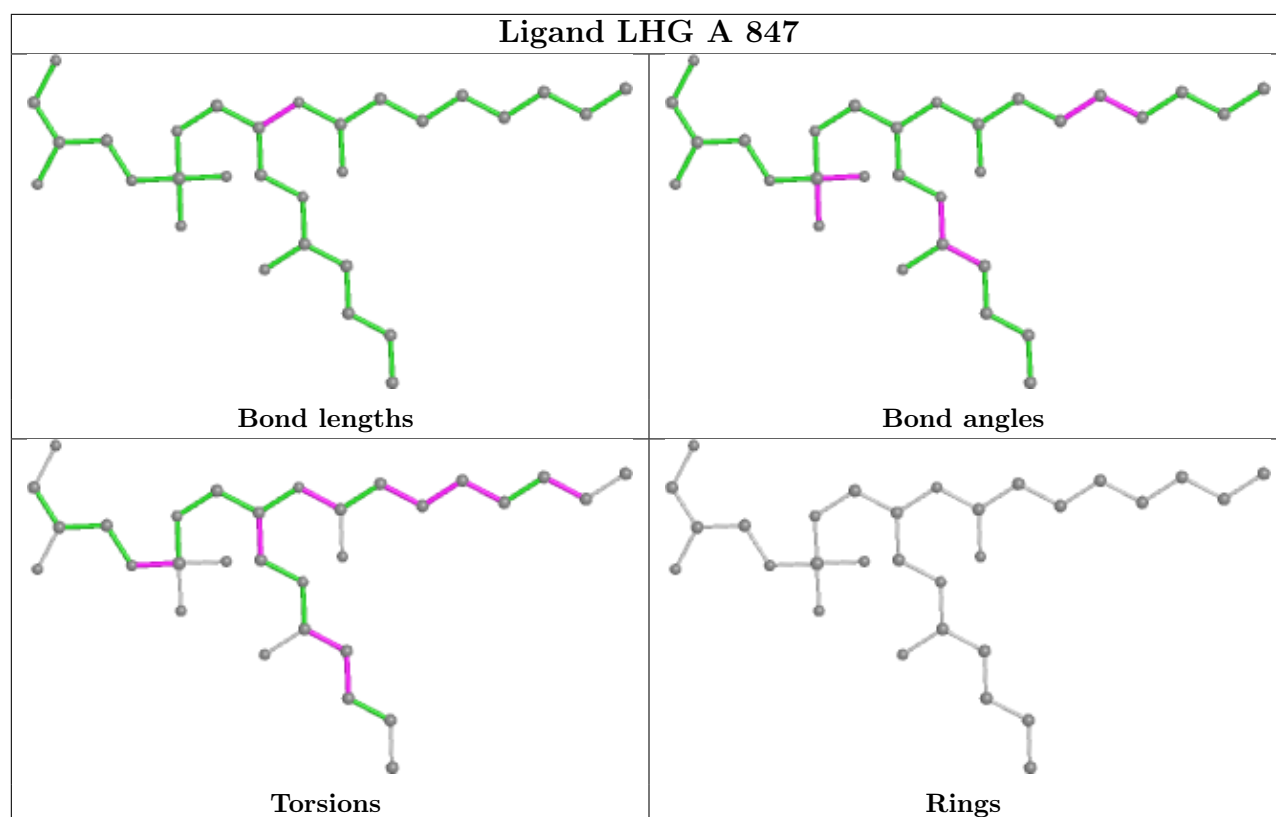
Ligand CLA 5 607



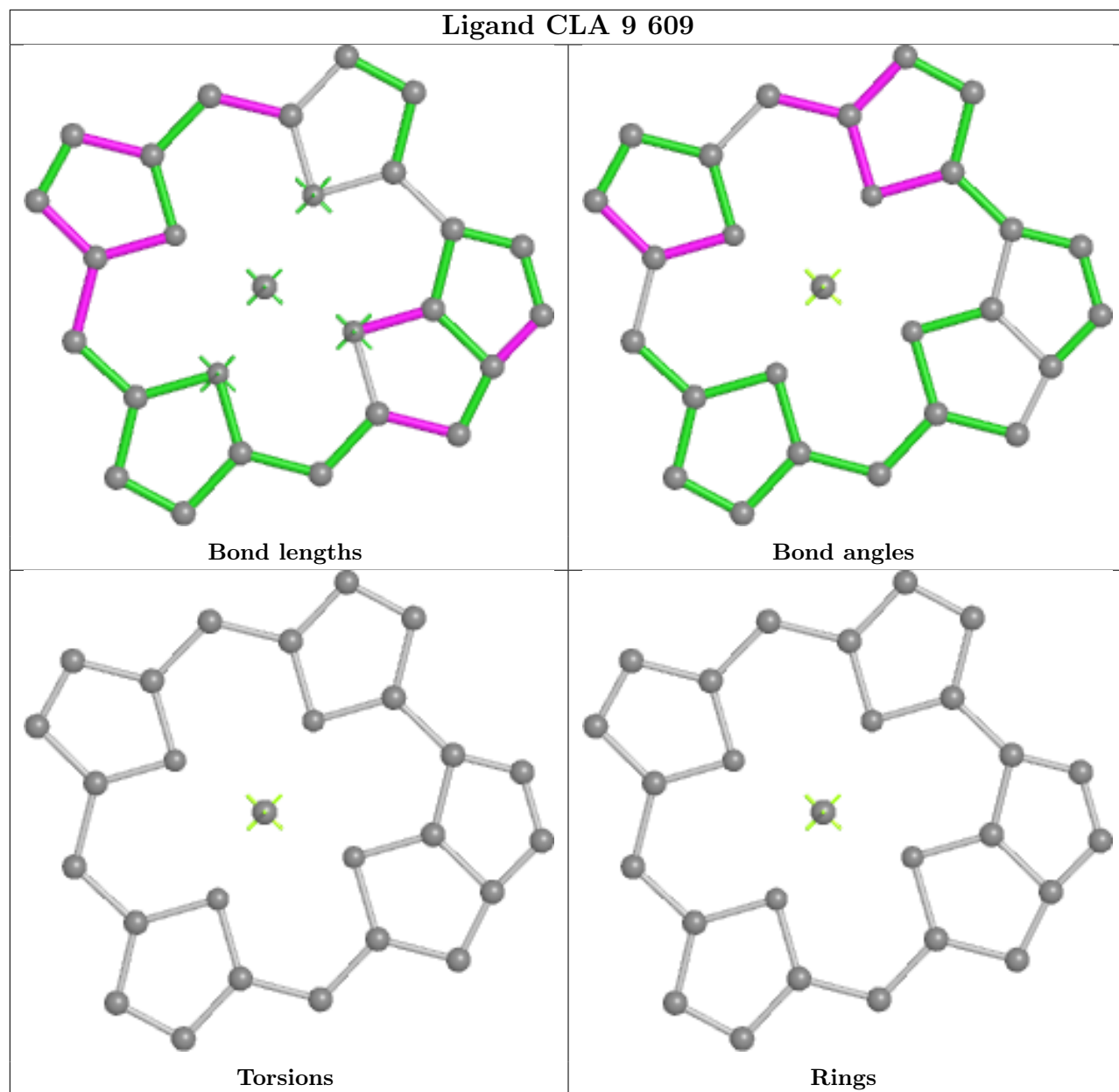
Ligand CLA 8 611

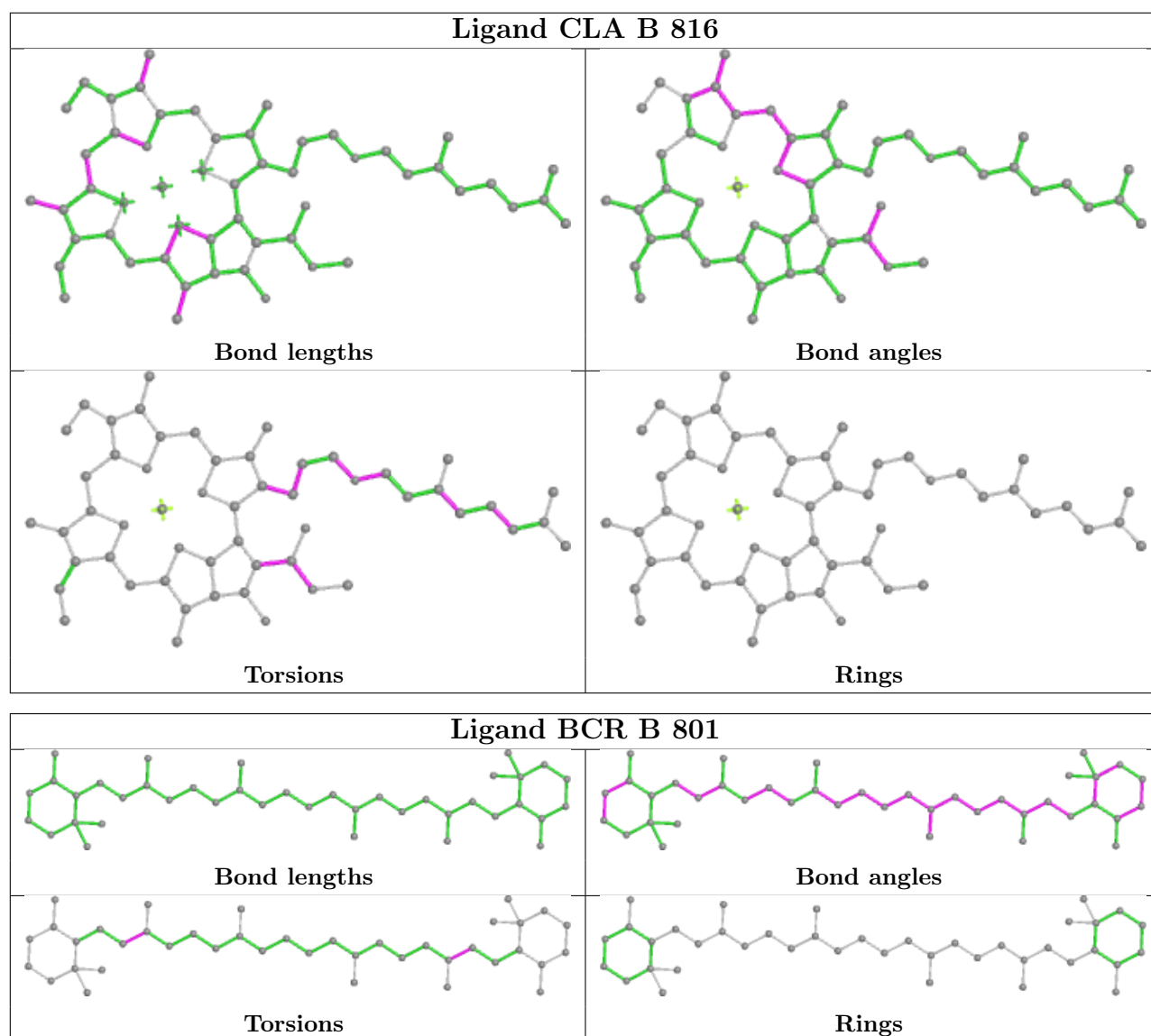


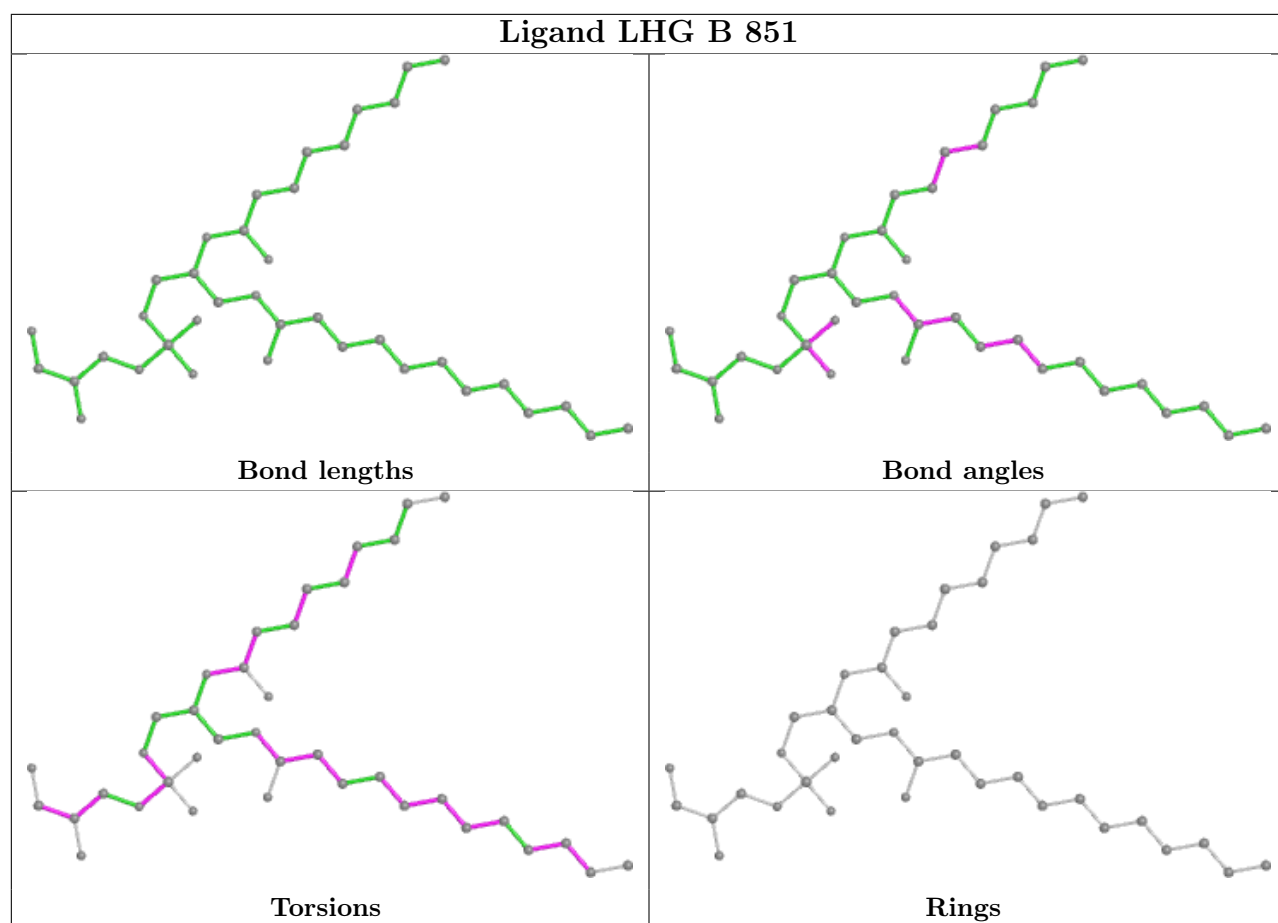




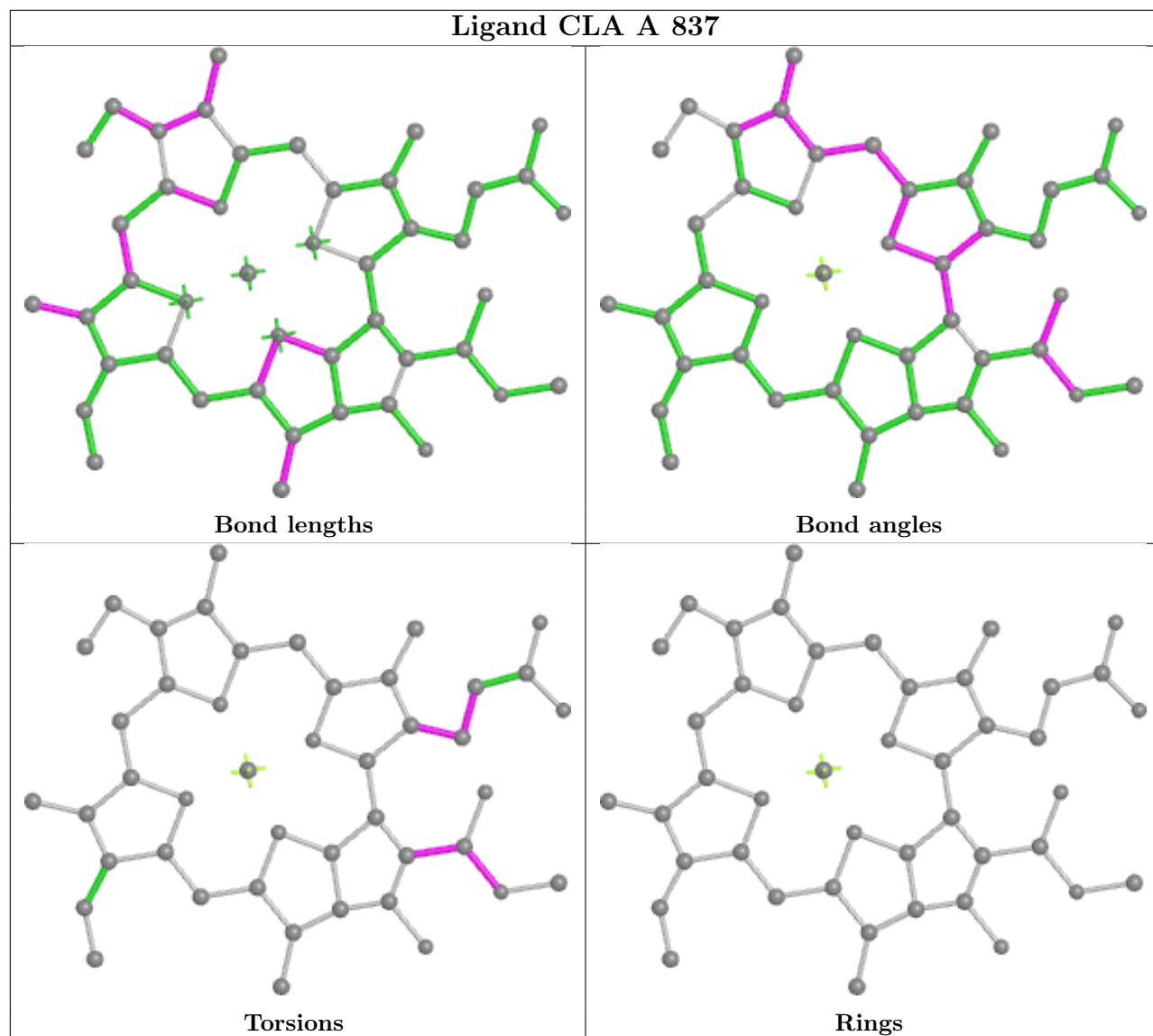
Ligand CLA 9 609



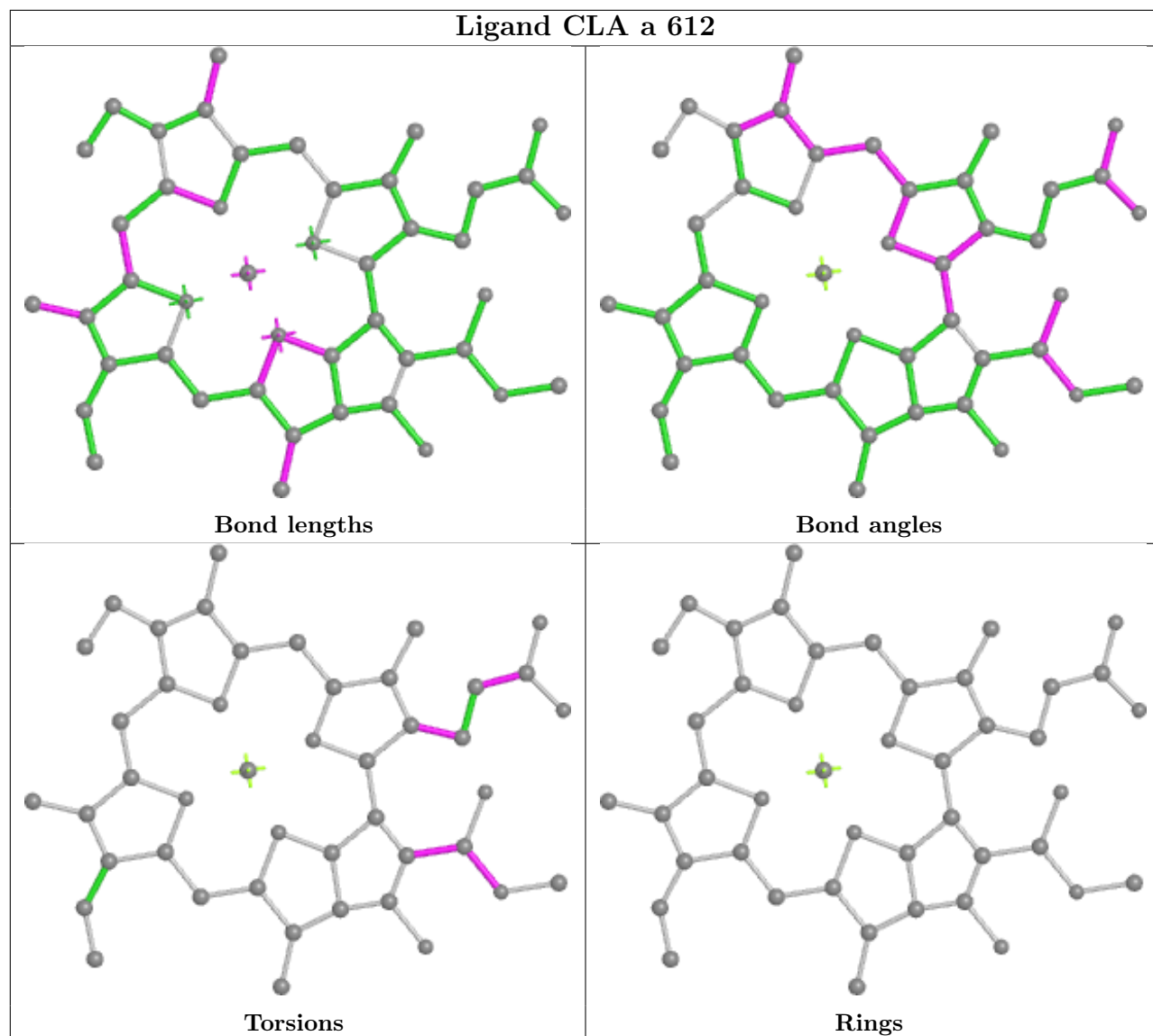




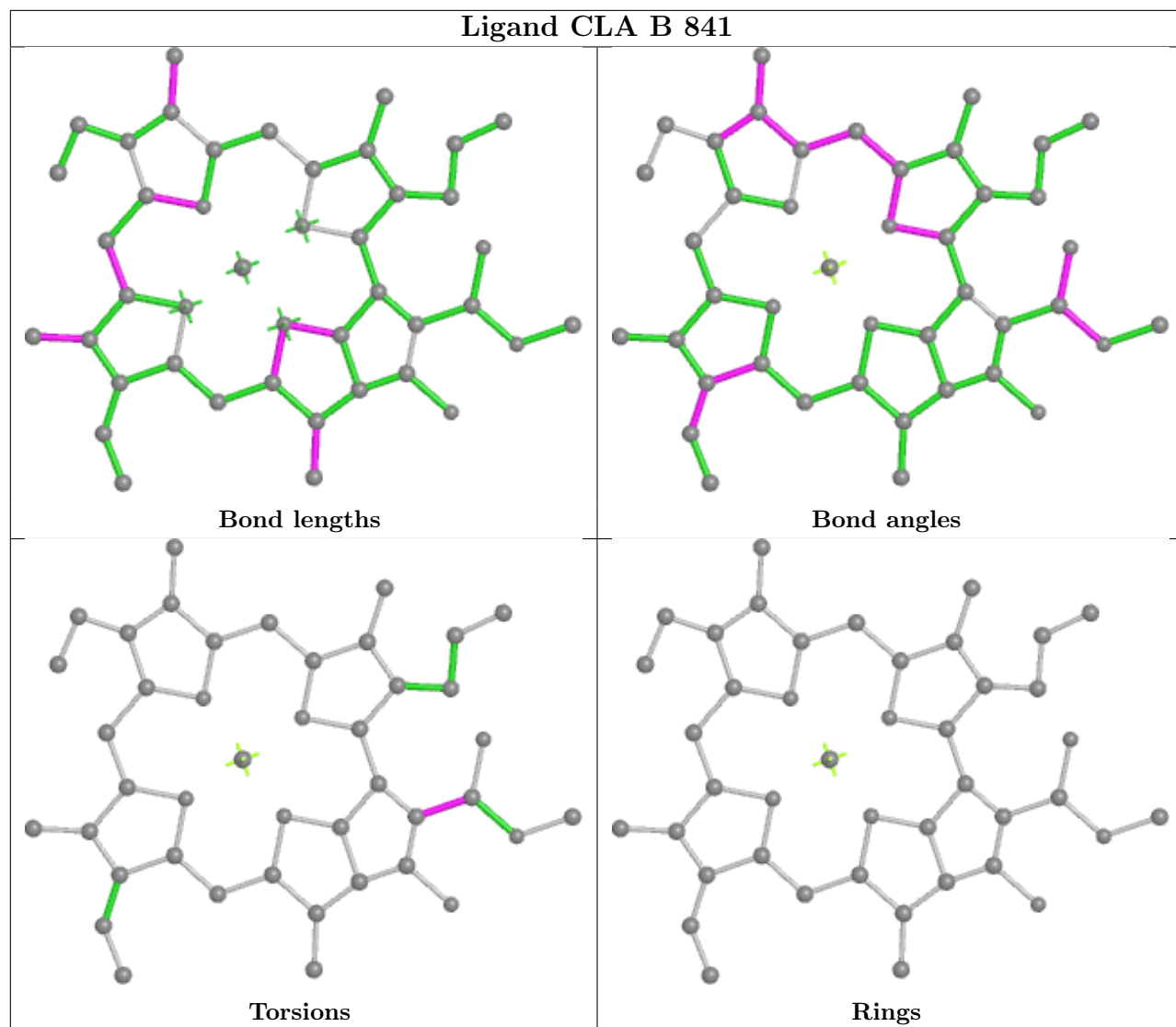
Ligand CLA A 837



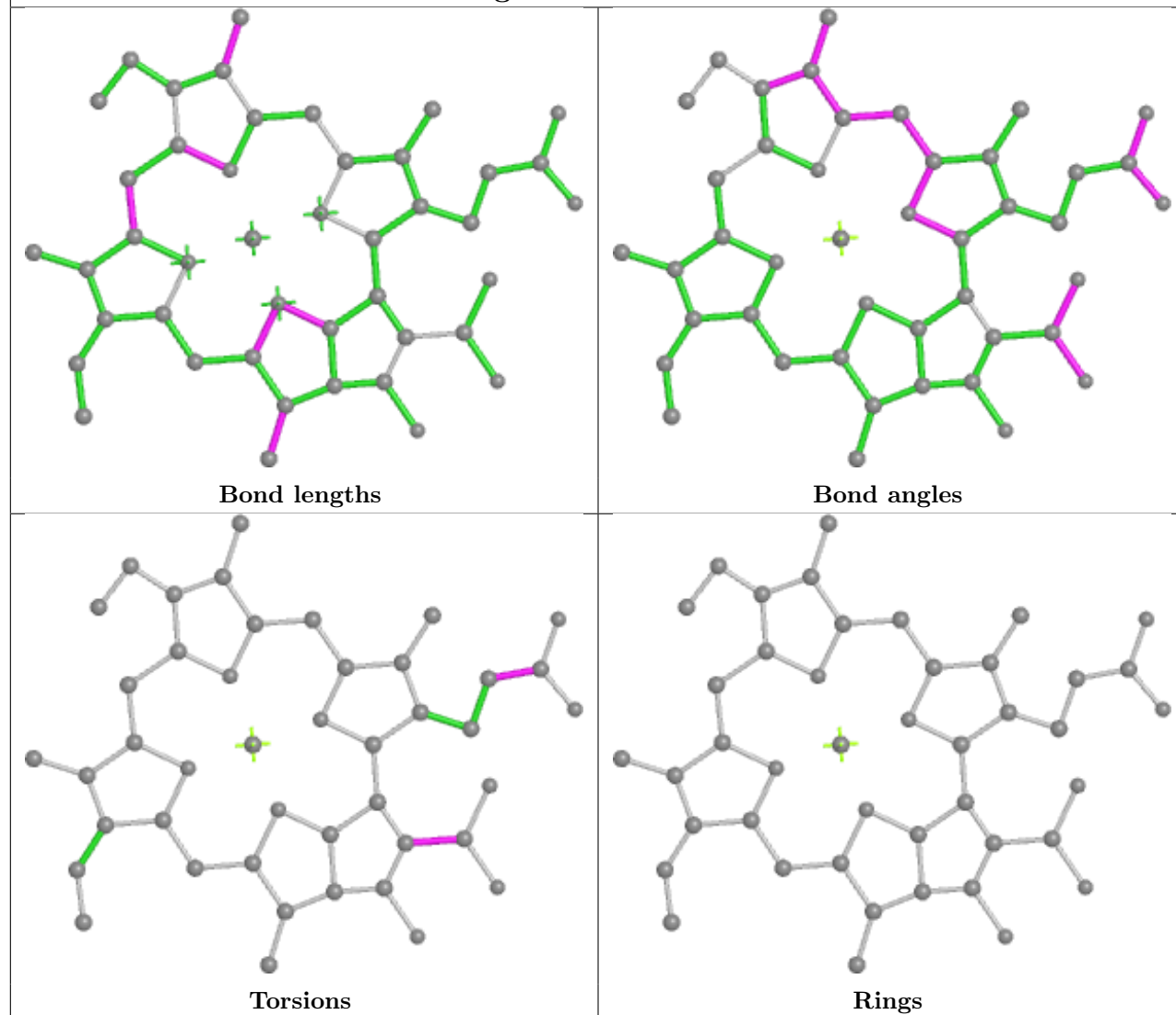
Ligand CLA a 612



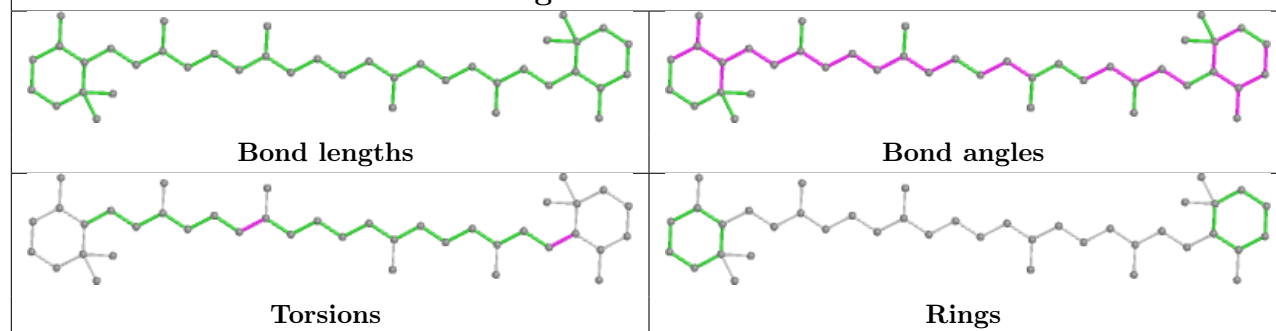
Ligand CLA B 841

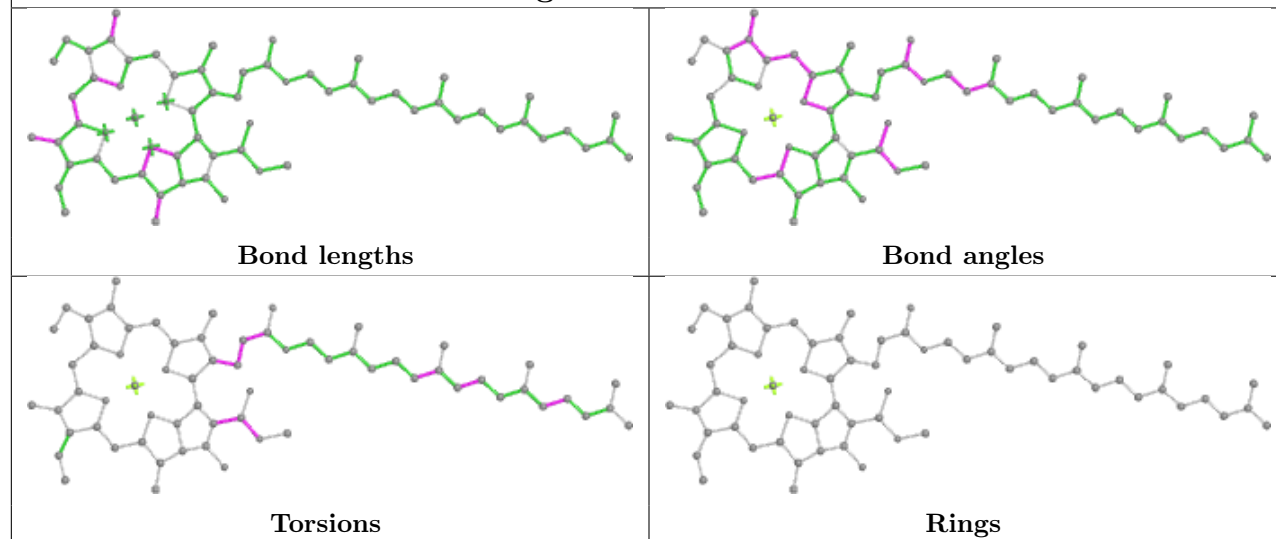


Ligand CLA a 608

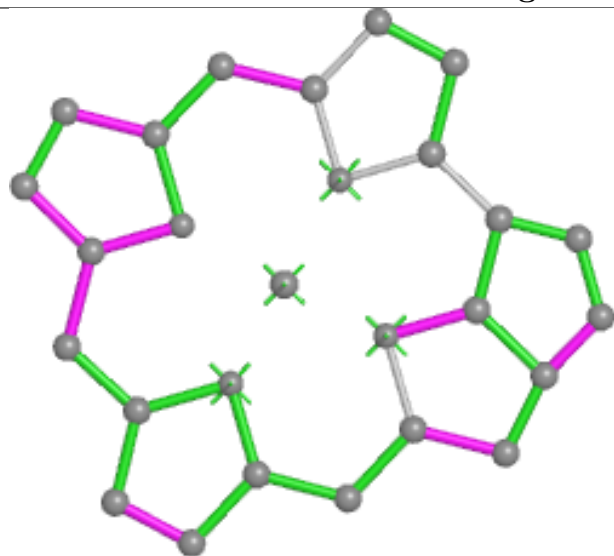


Ligand BCR a 619

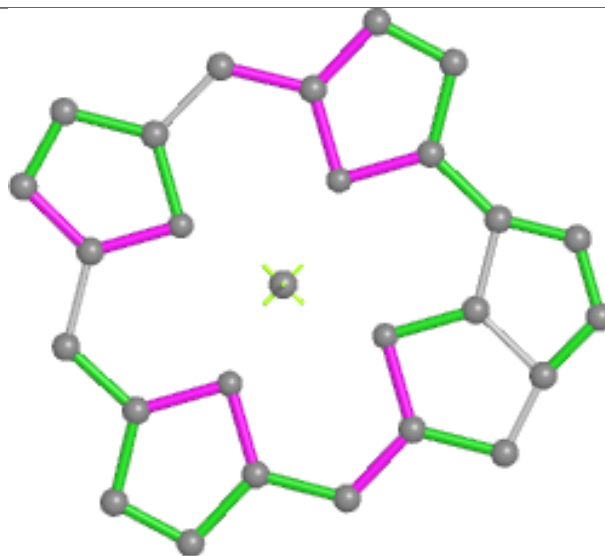


Ligand CLA 6 610**Ligand BCR B 844**

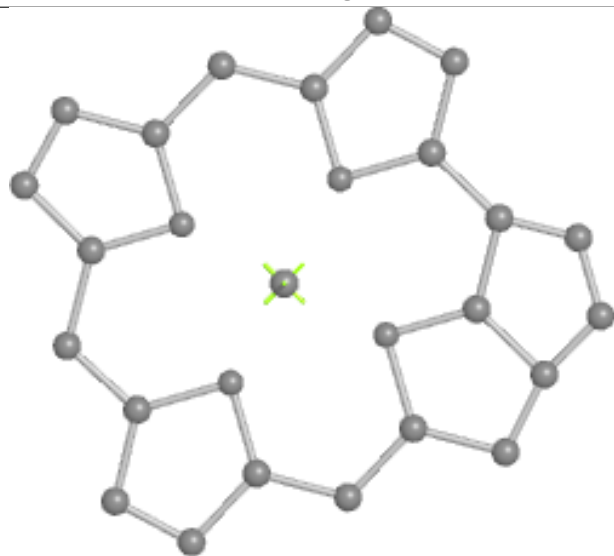
Ligand CLA 9 611



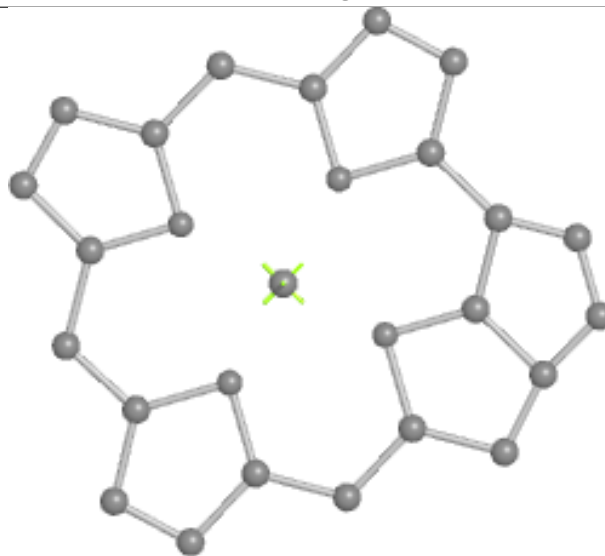
Bond lengths



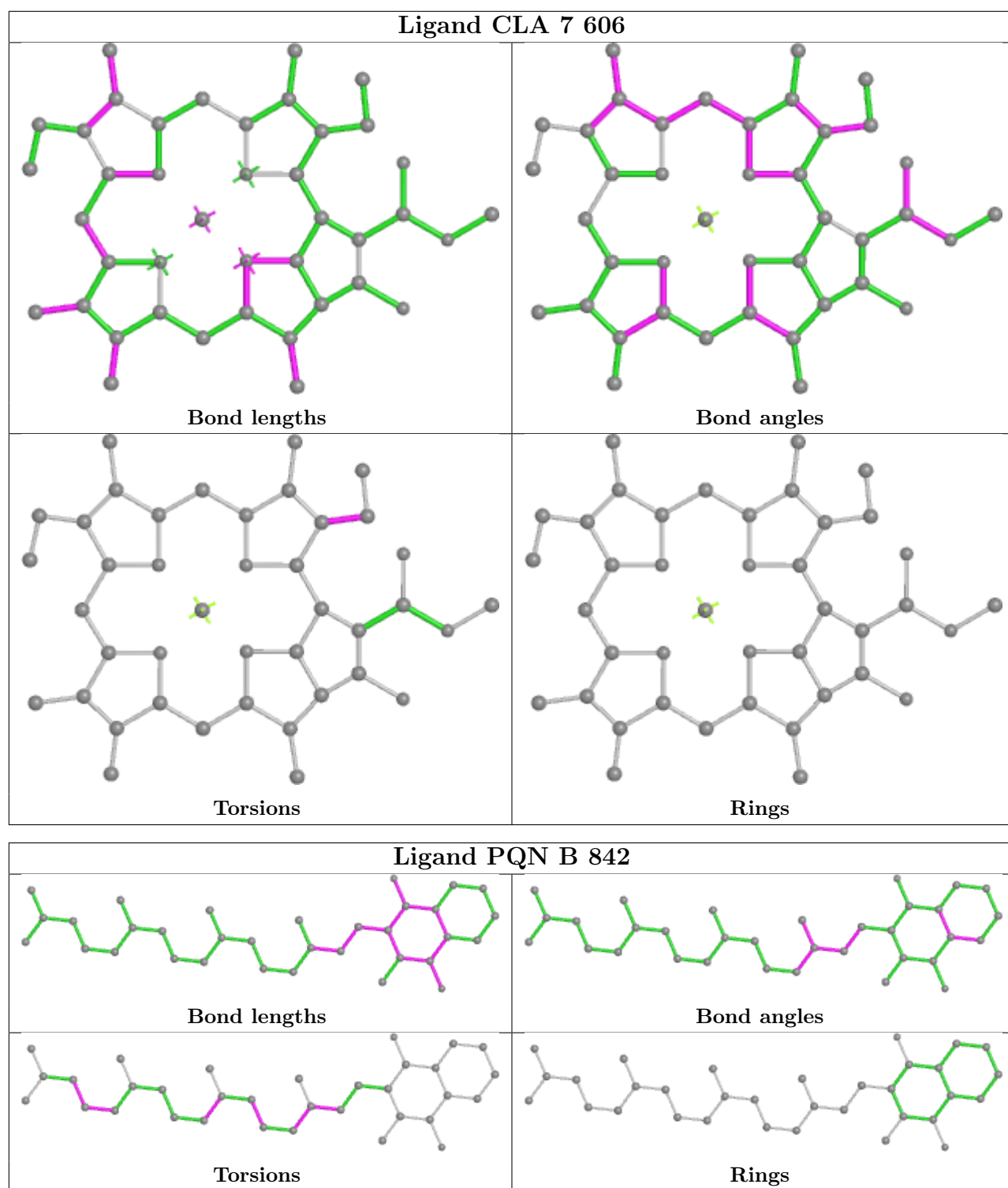
Bond angles

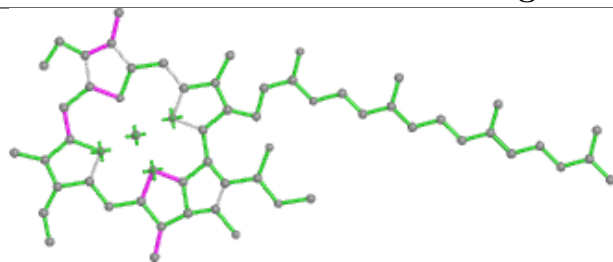
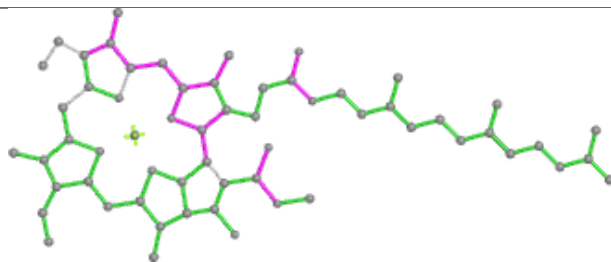
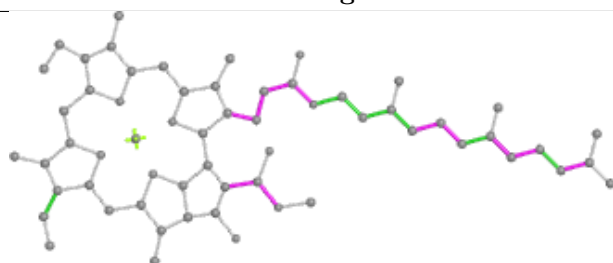
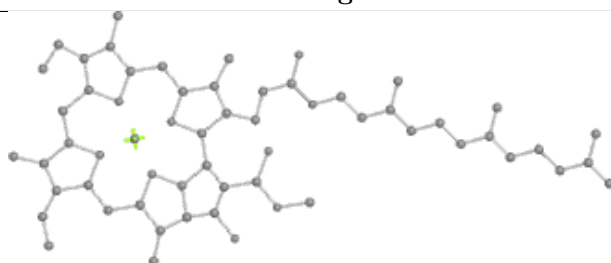
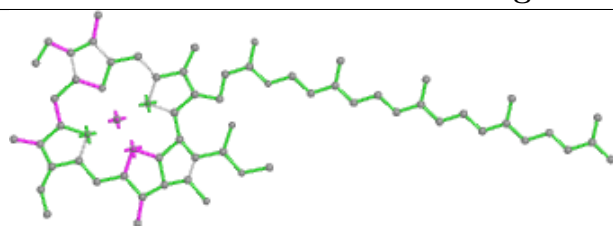
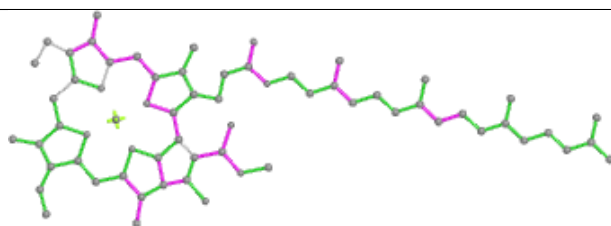
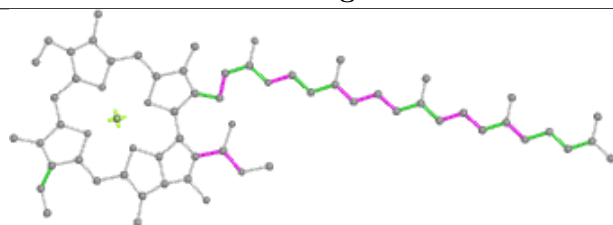
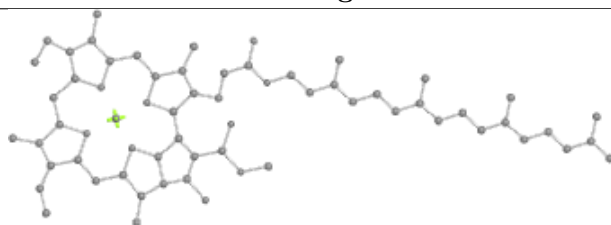


Torsions

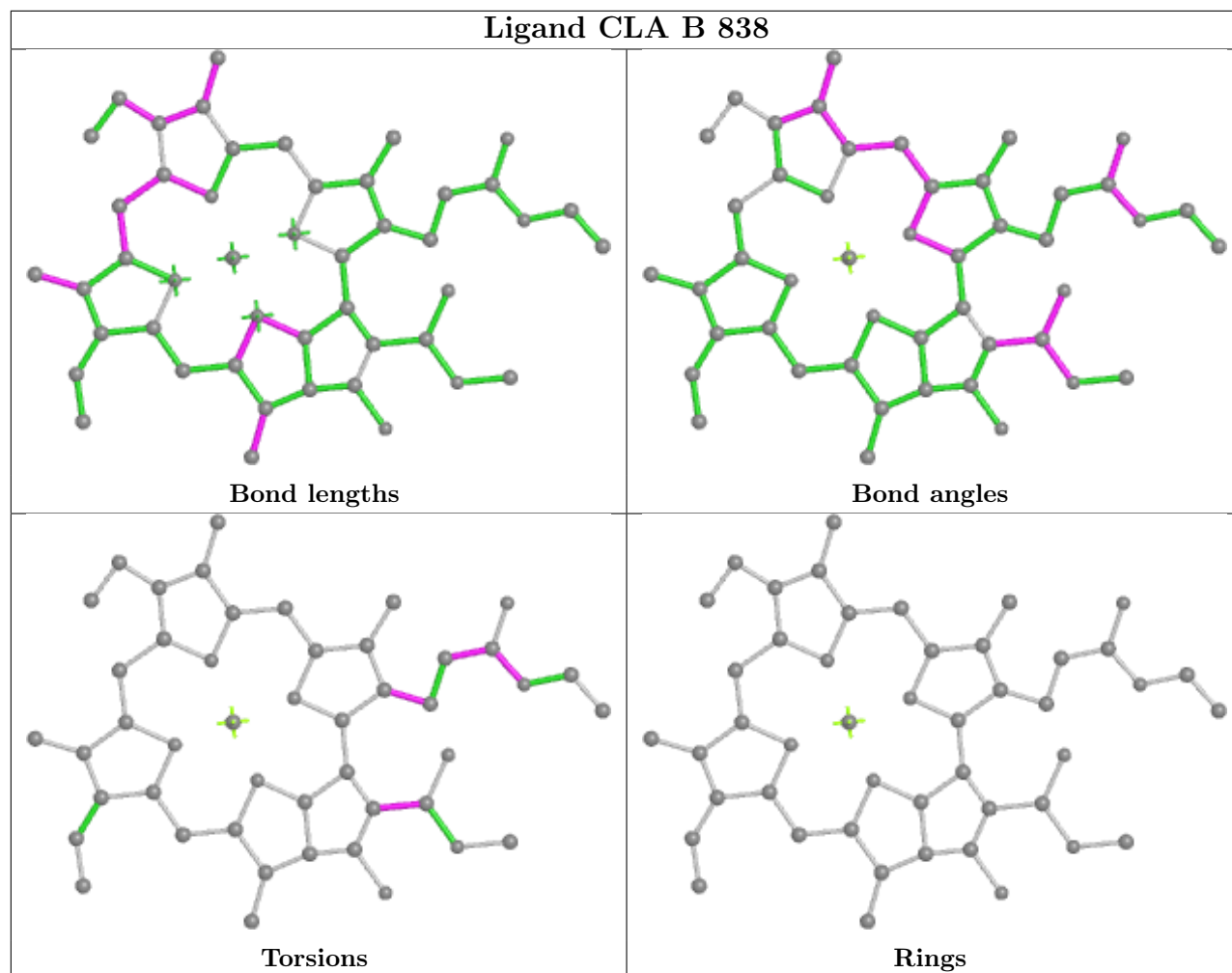


Rings

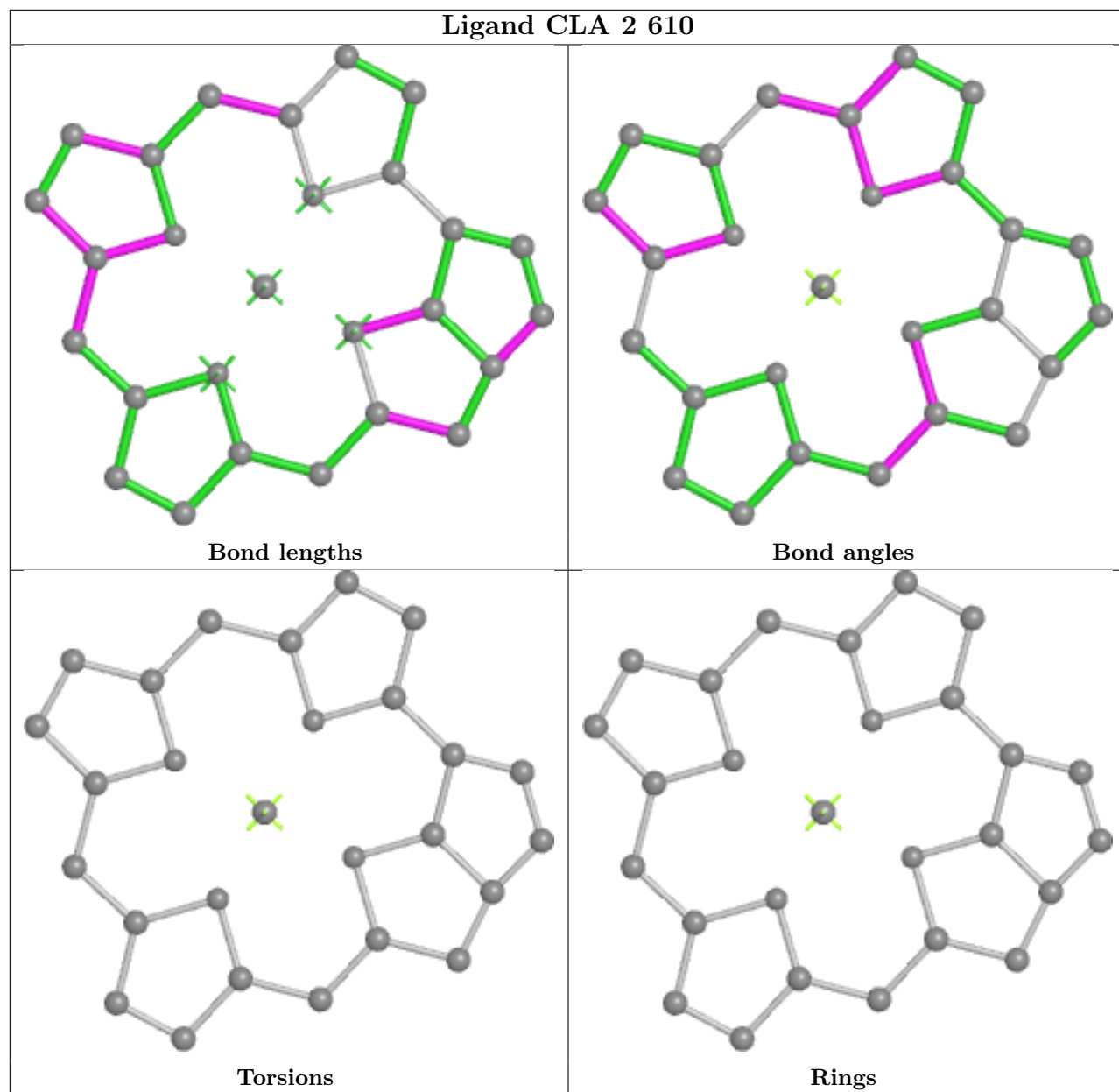


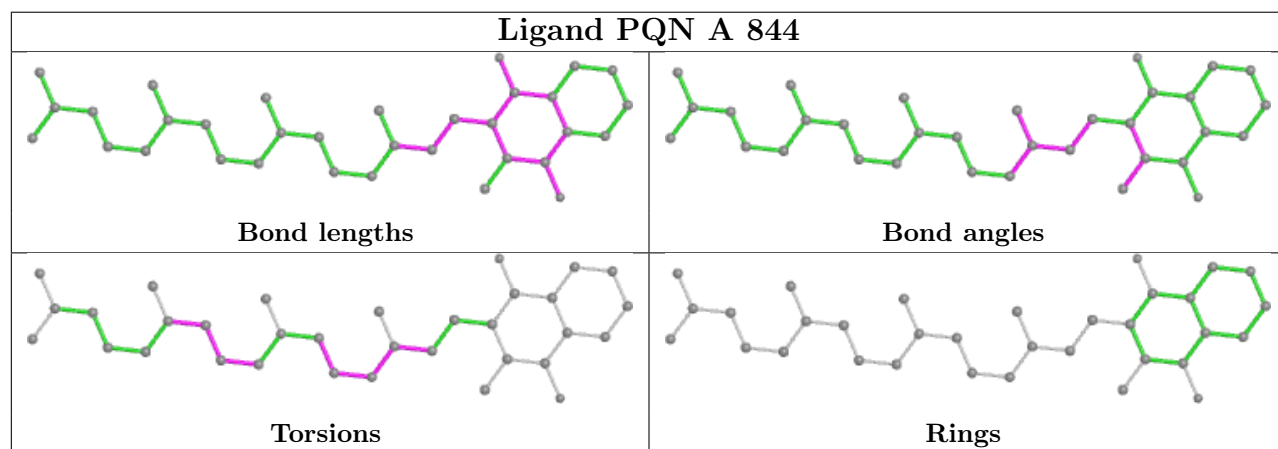
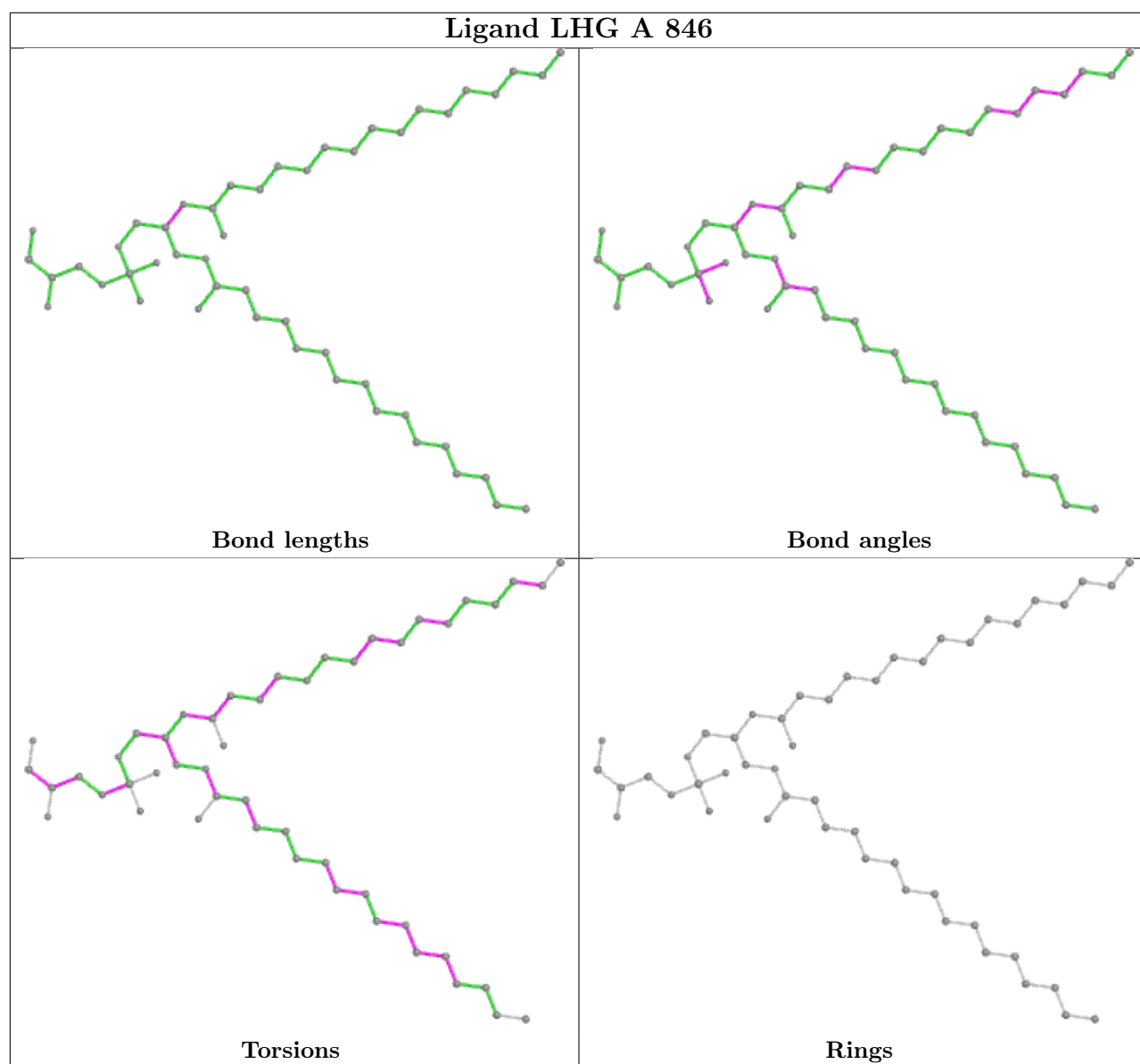
Ligand CLA 3 609**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 854****Bond lengths****Bond angles****Torsions****Rings**

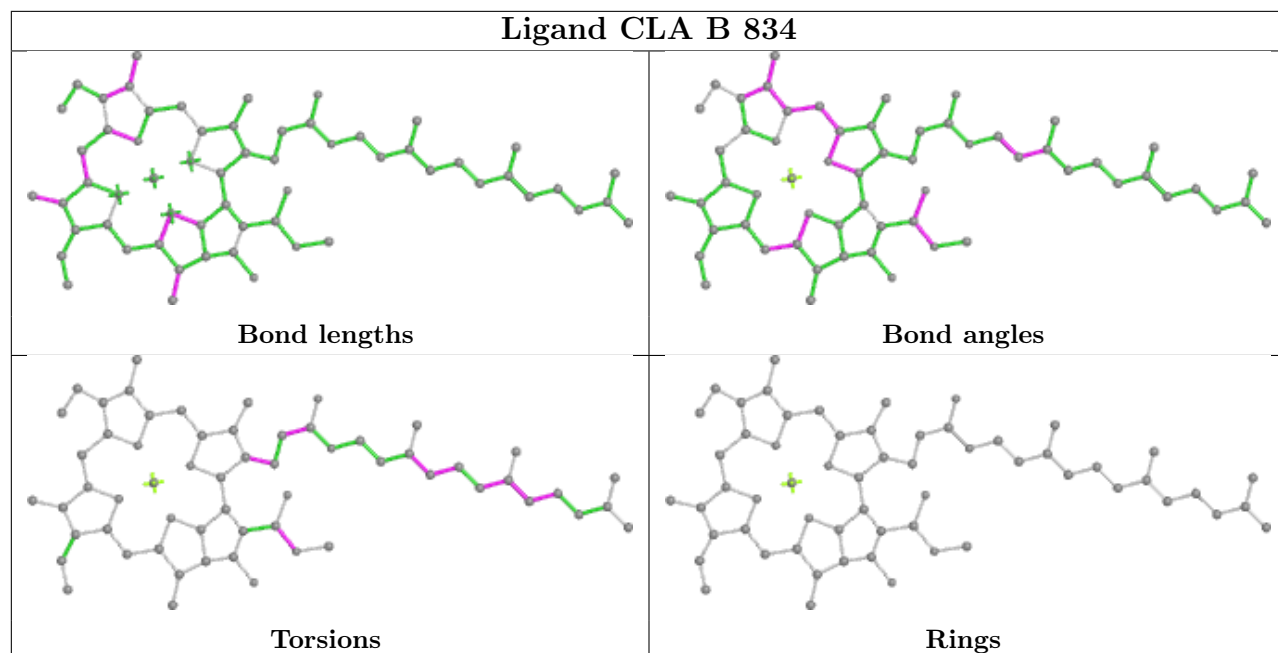
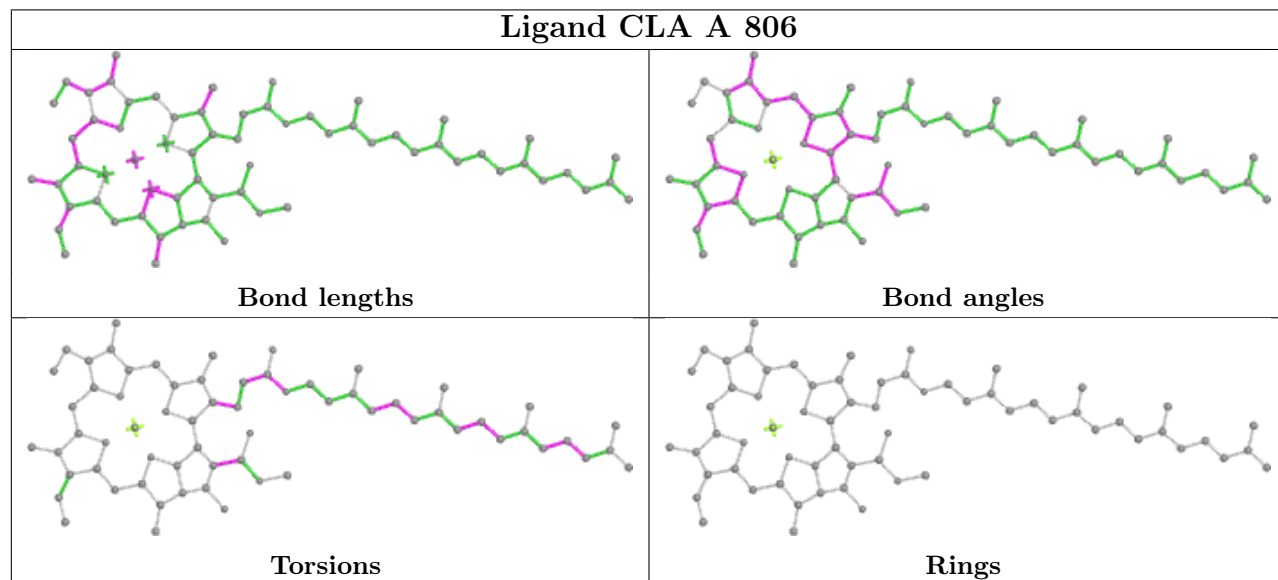
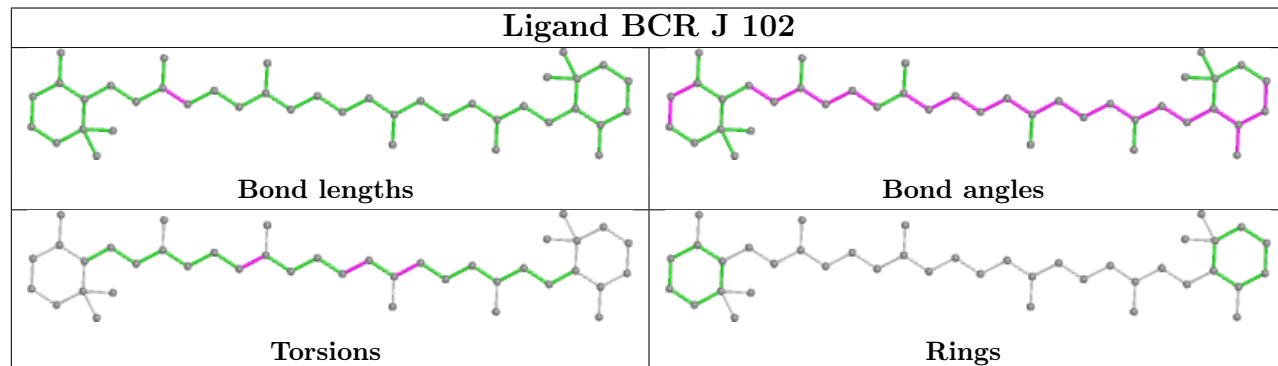
Ligand CLA B 838



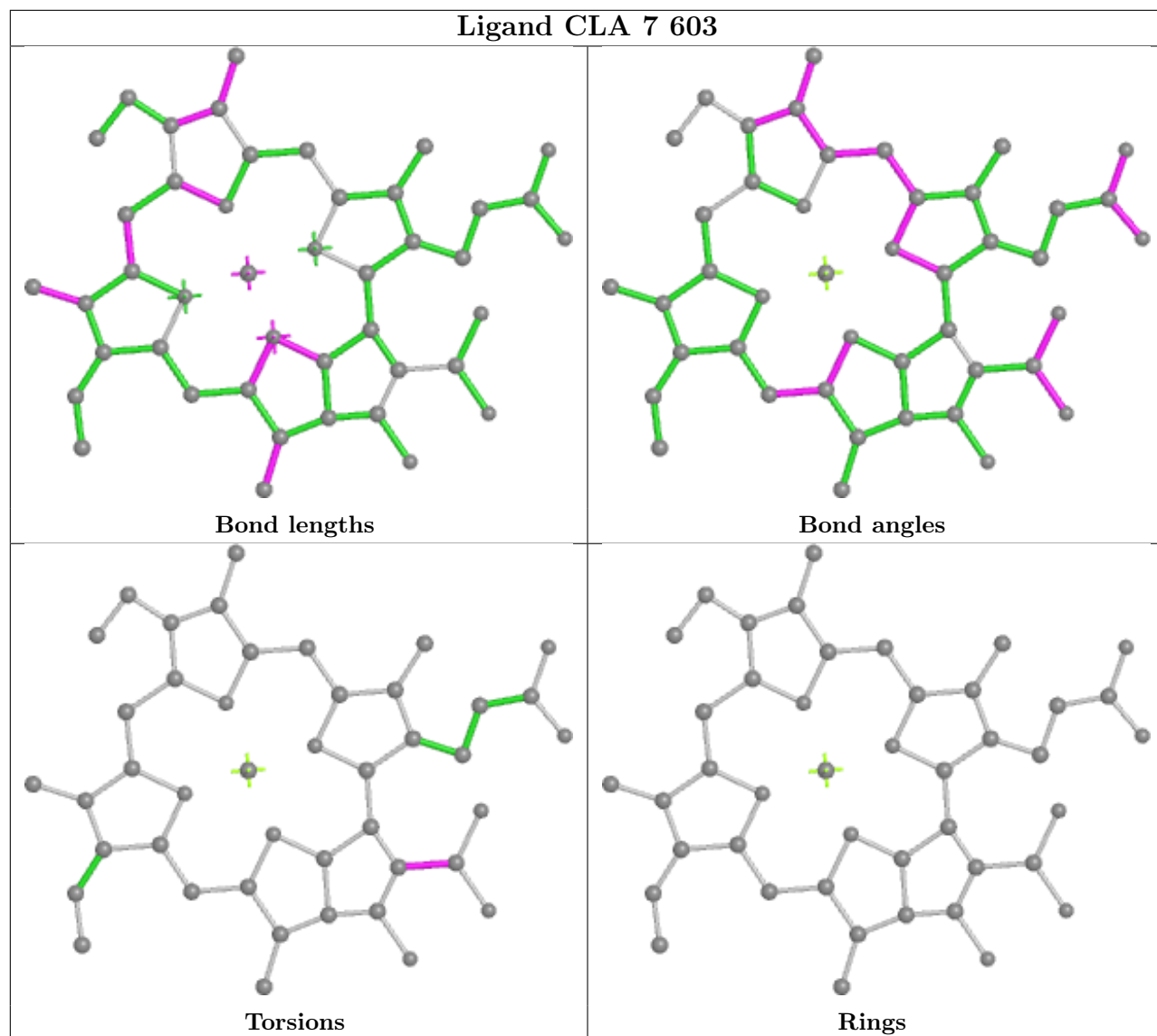
Ligand CLA 2 610



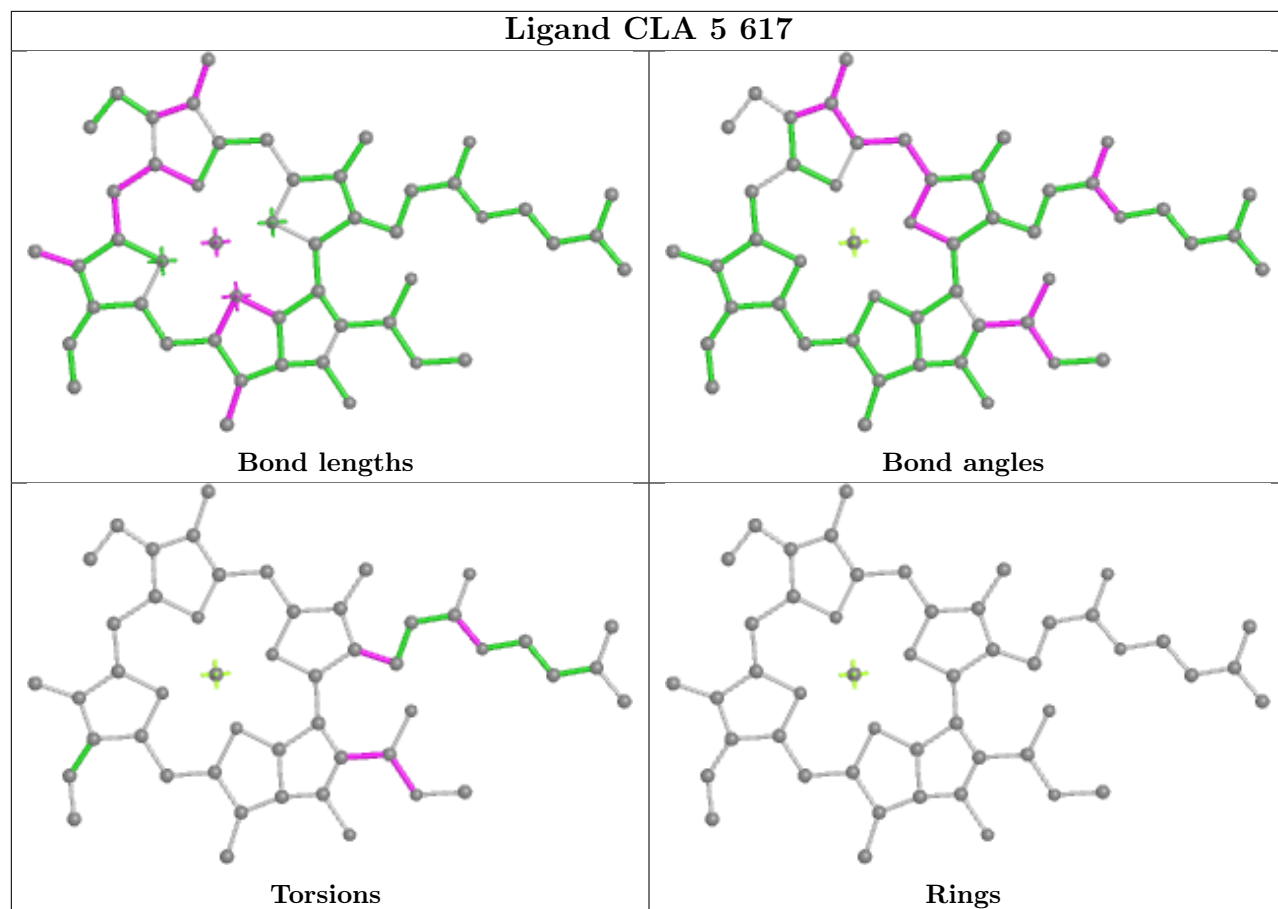


Ligand CLA B 834**Ligand CLA A 806****Ligand BCR J 102**

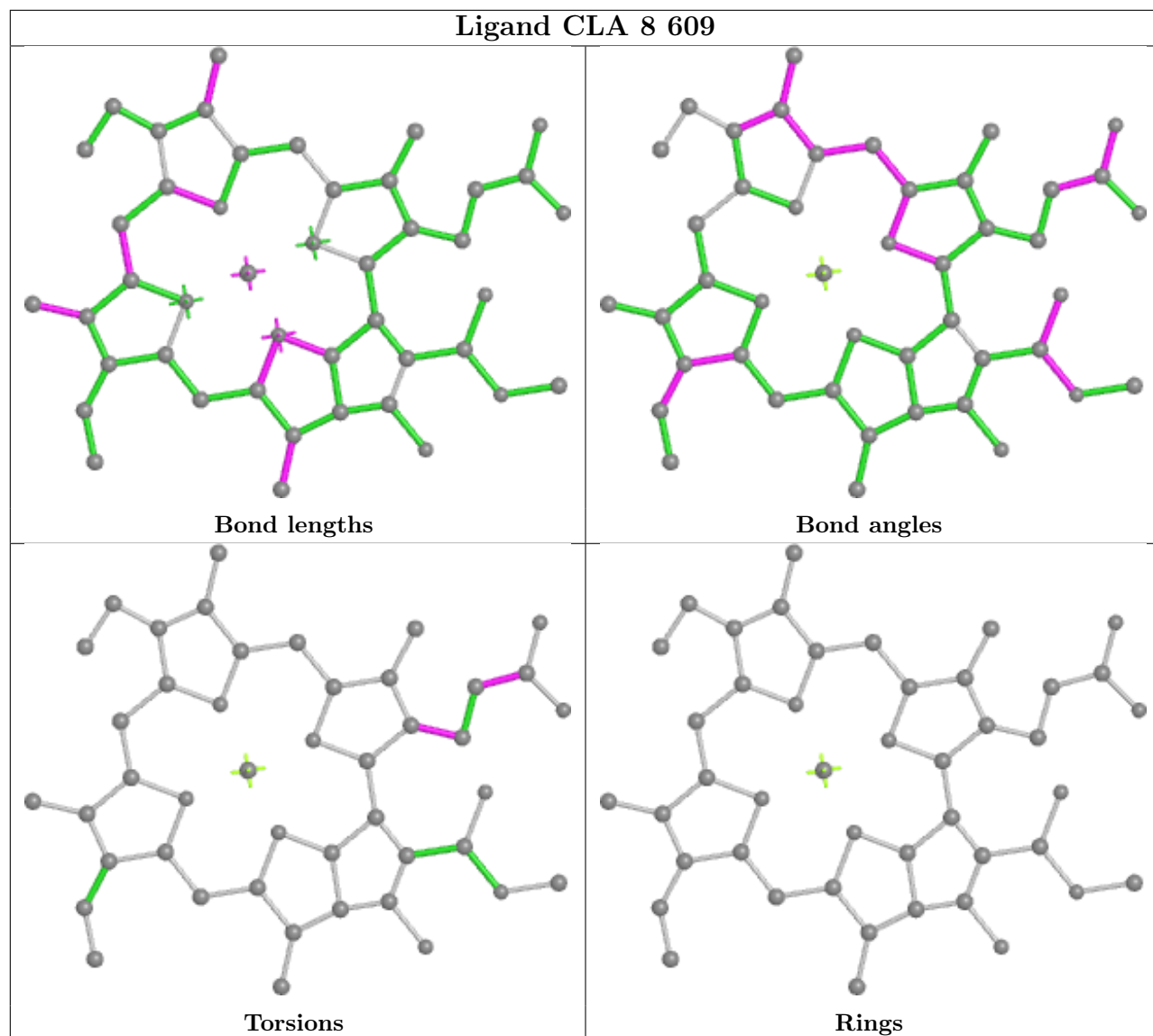
Ligand CLA 7 603



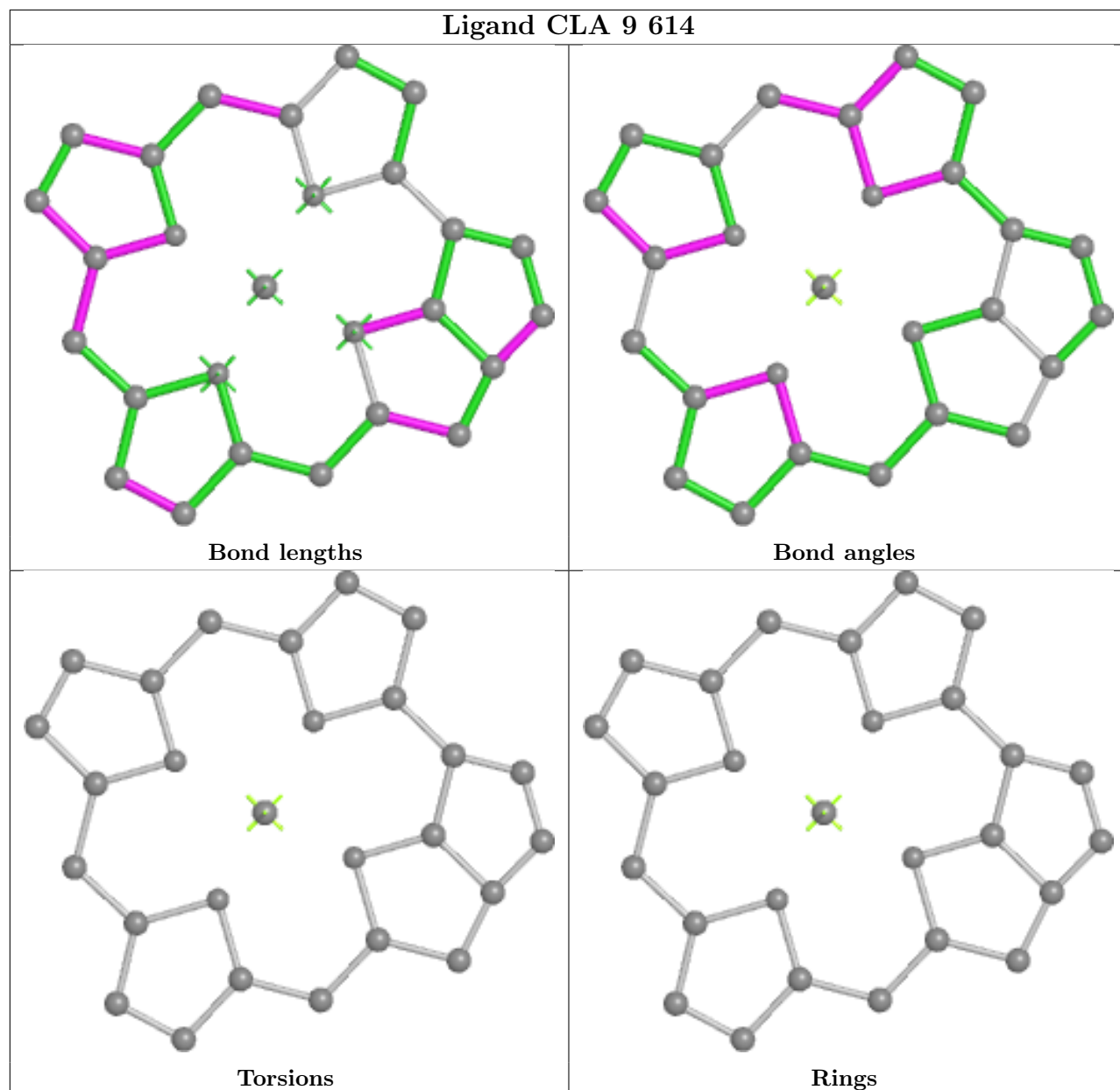
Ligand CLA 5 617



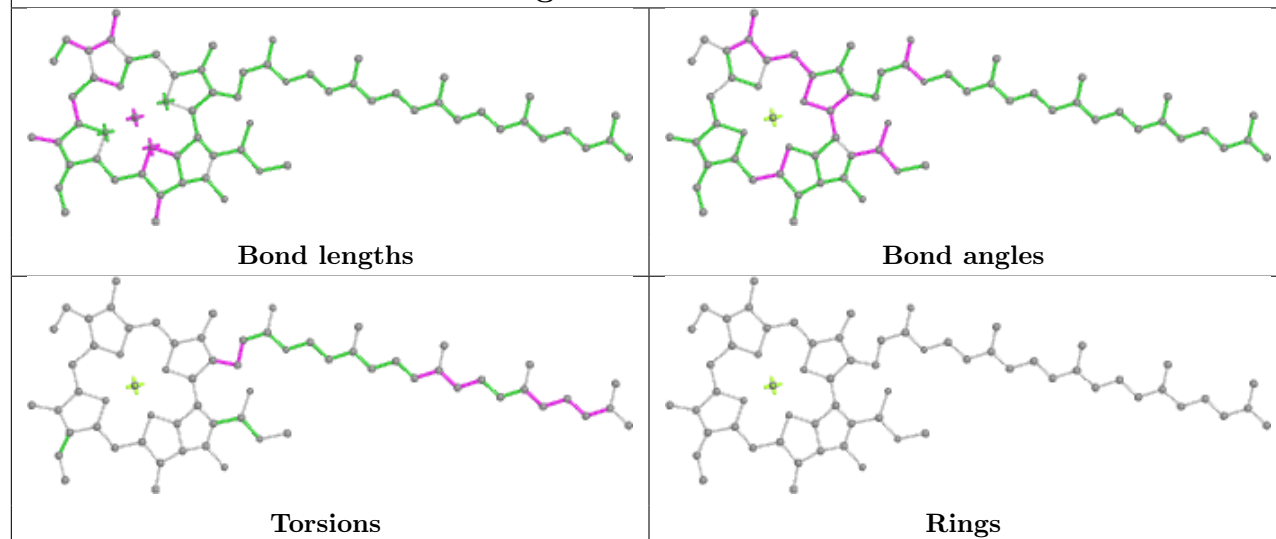
Ligand CLA 8 609



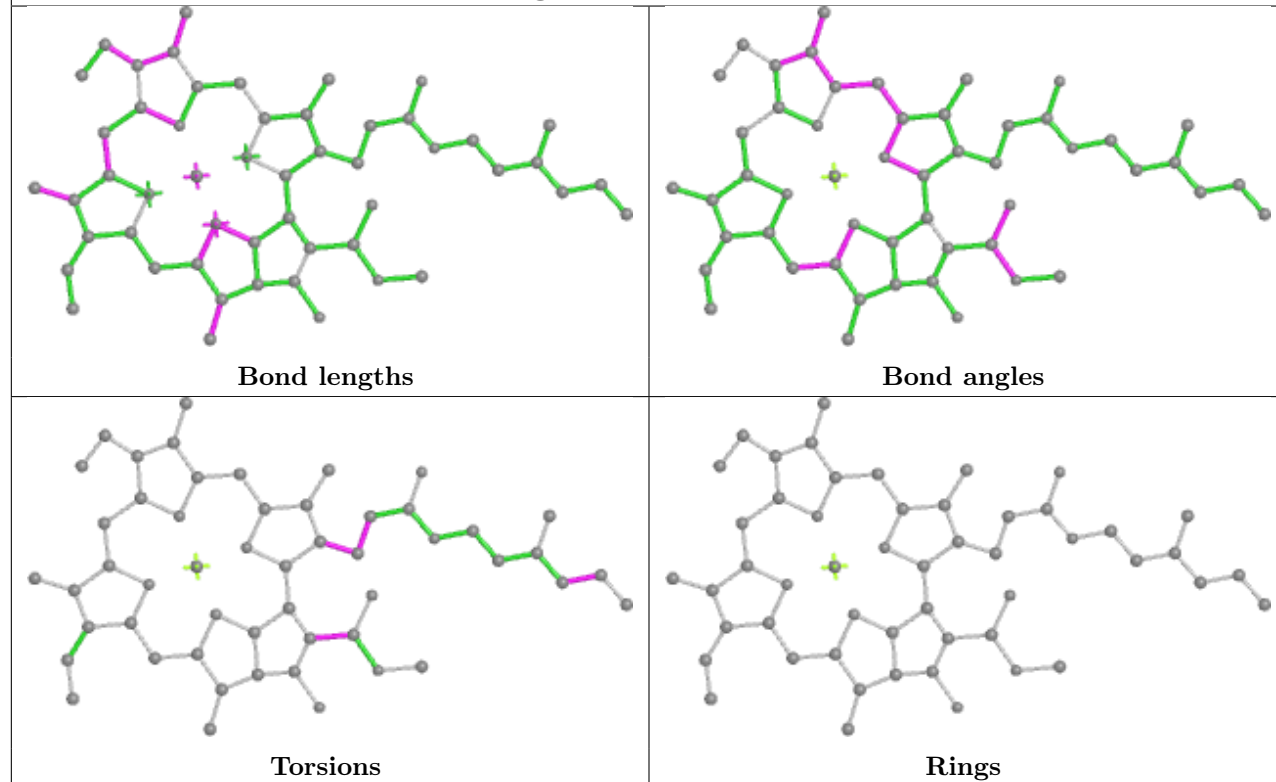
Ligand CLA 9 614

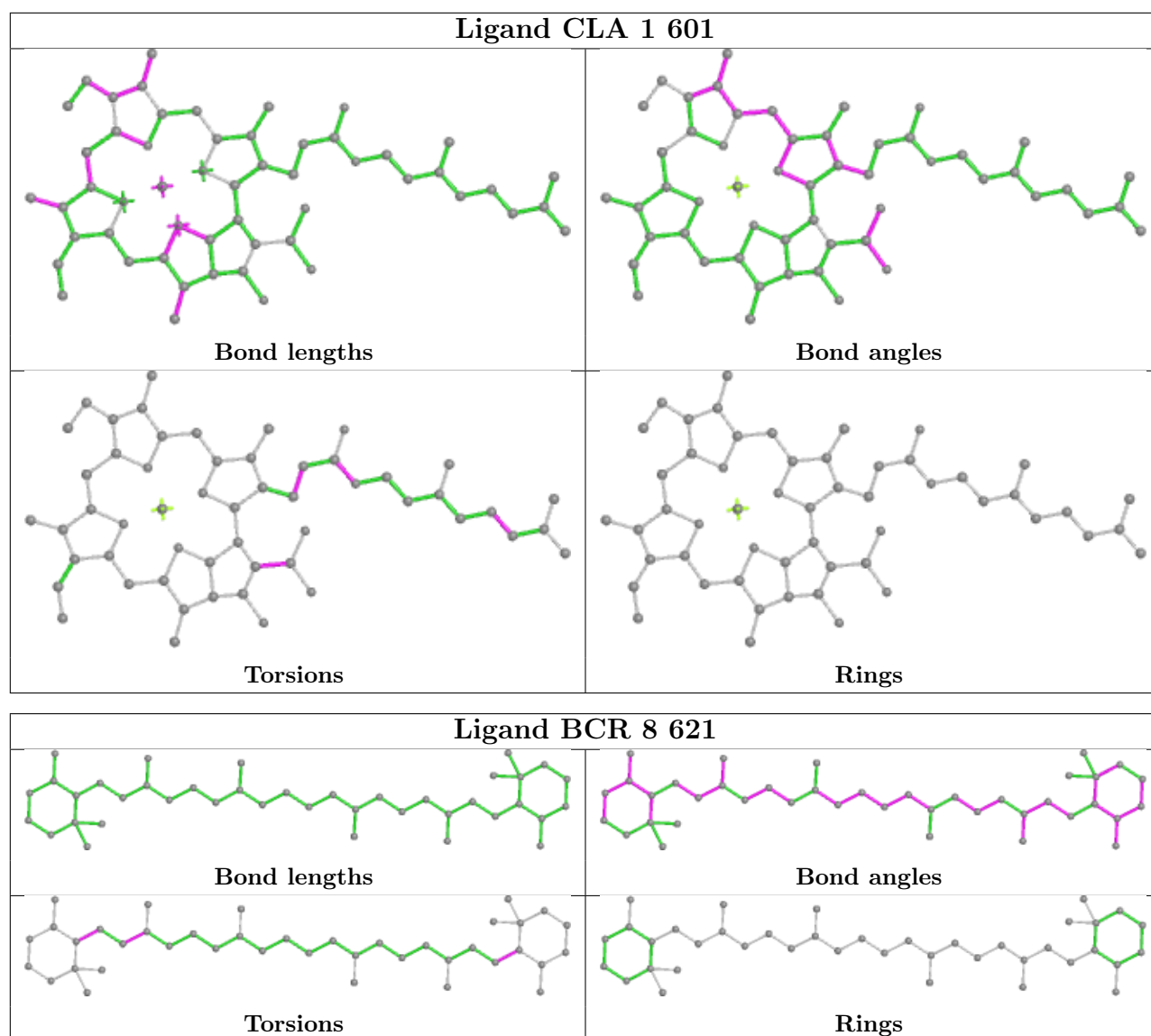


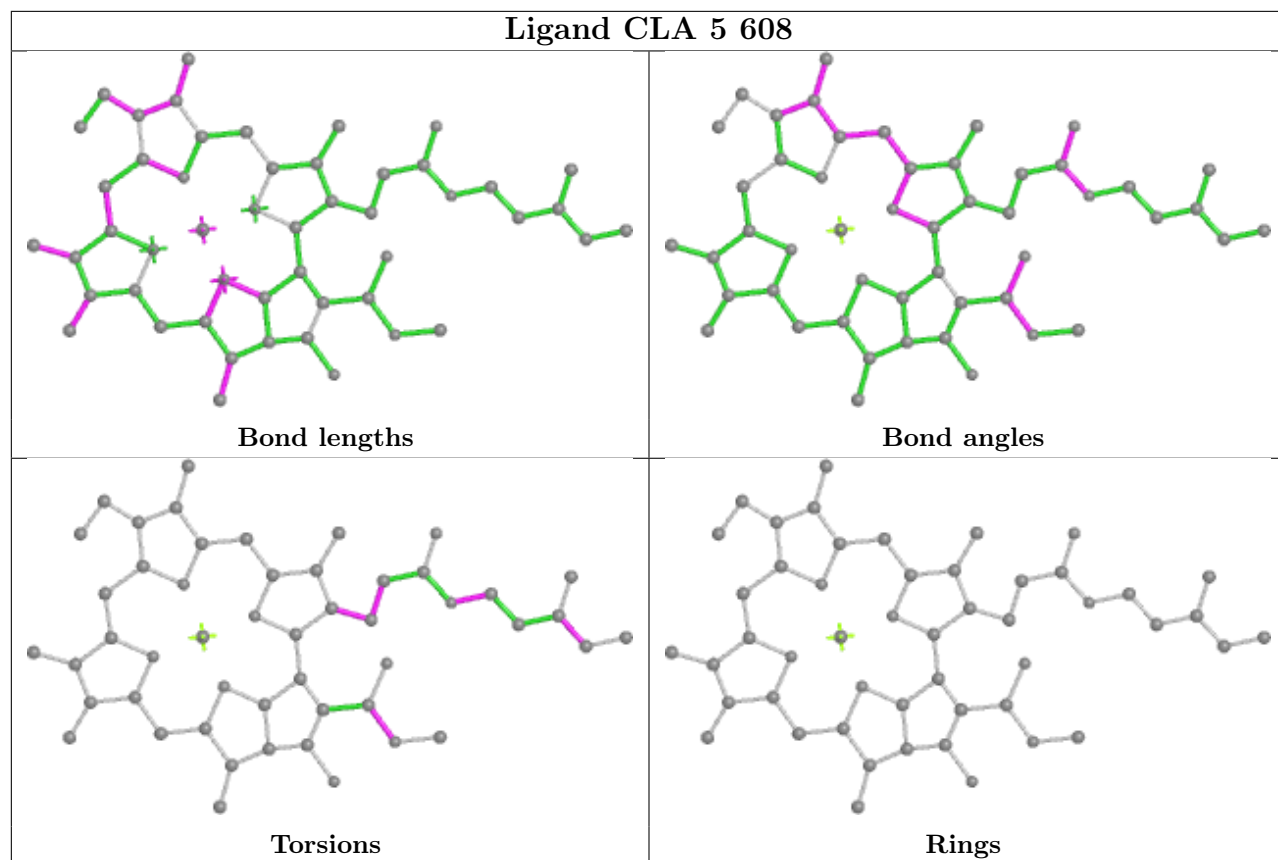
Ligand CLA 5 609



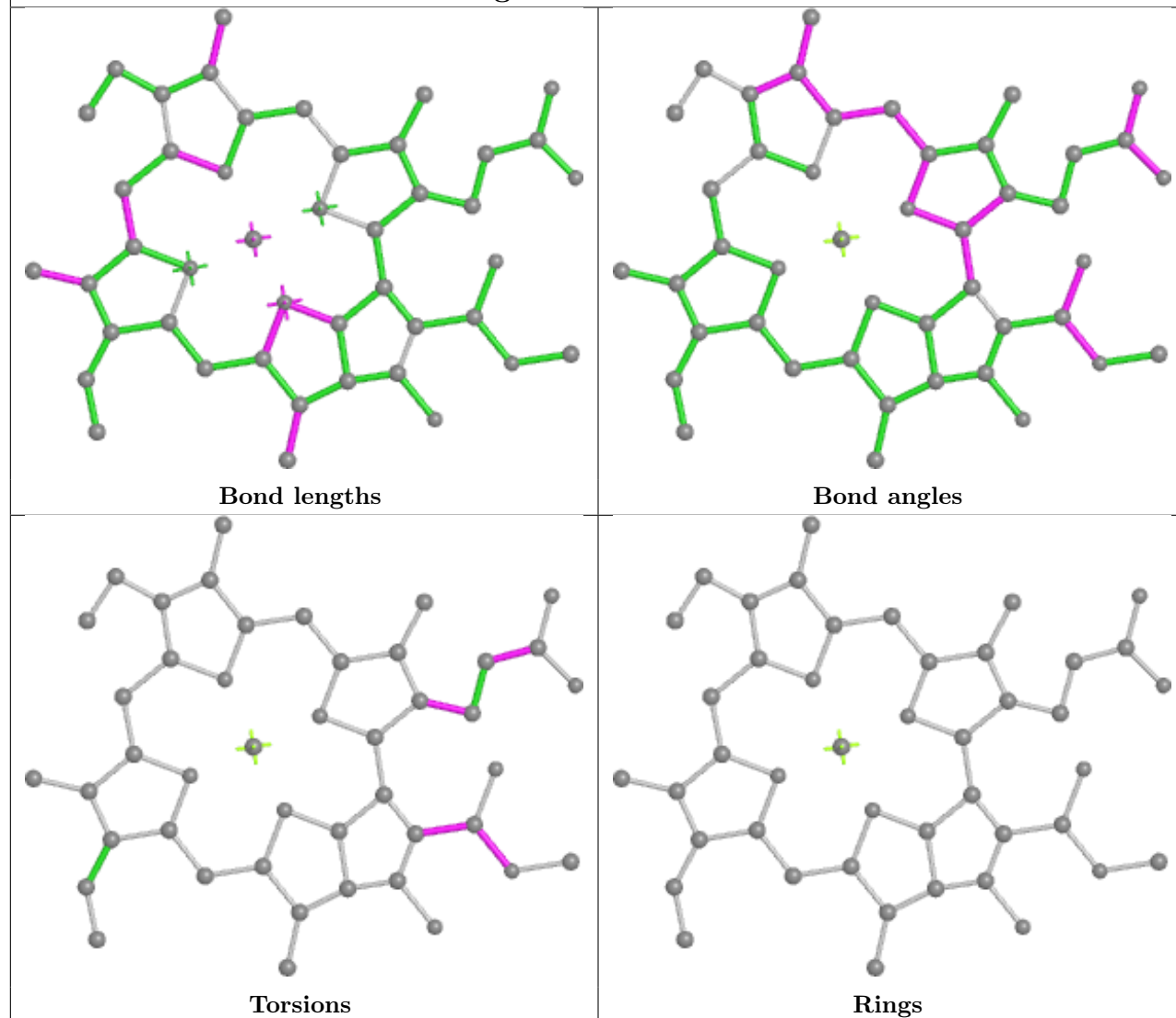
Ligand CLA A 805



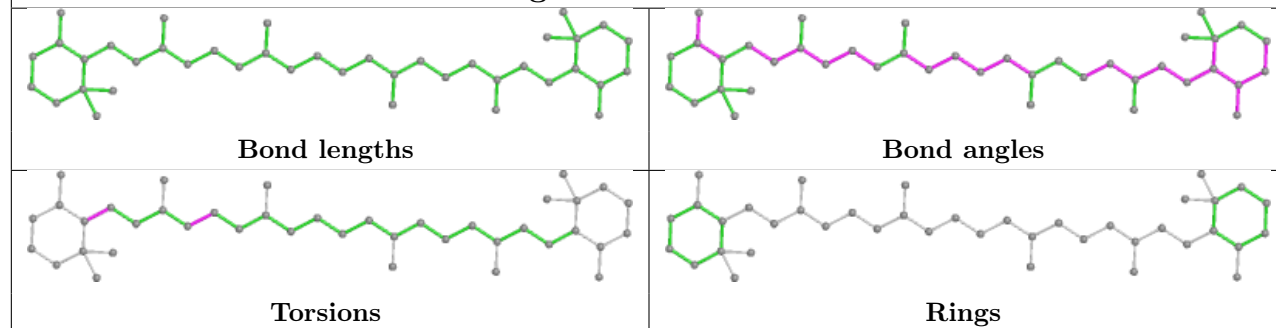


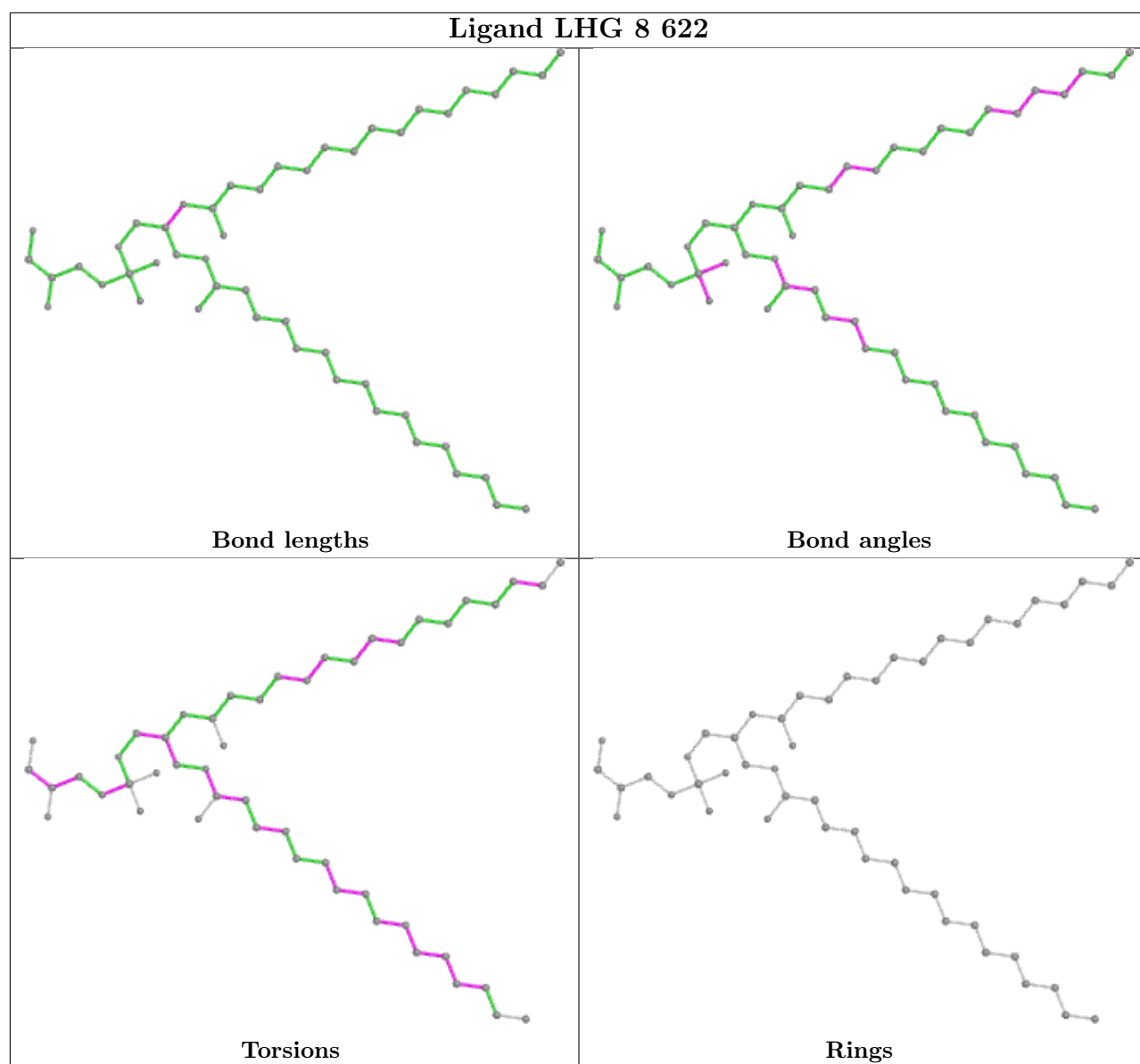


Ligand CLA 1 612

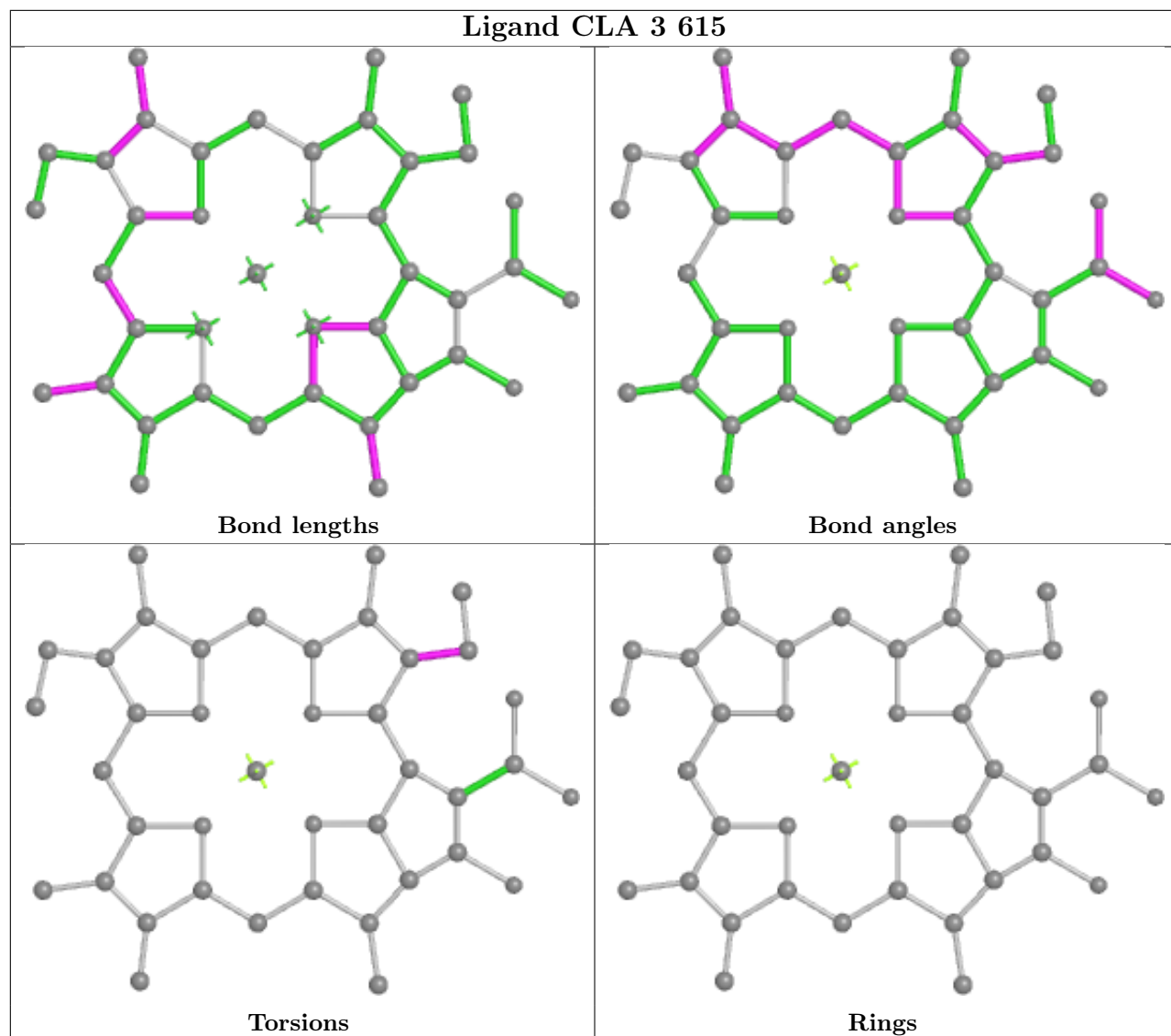


Ligand BCR K 207

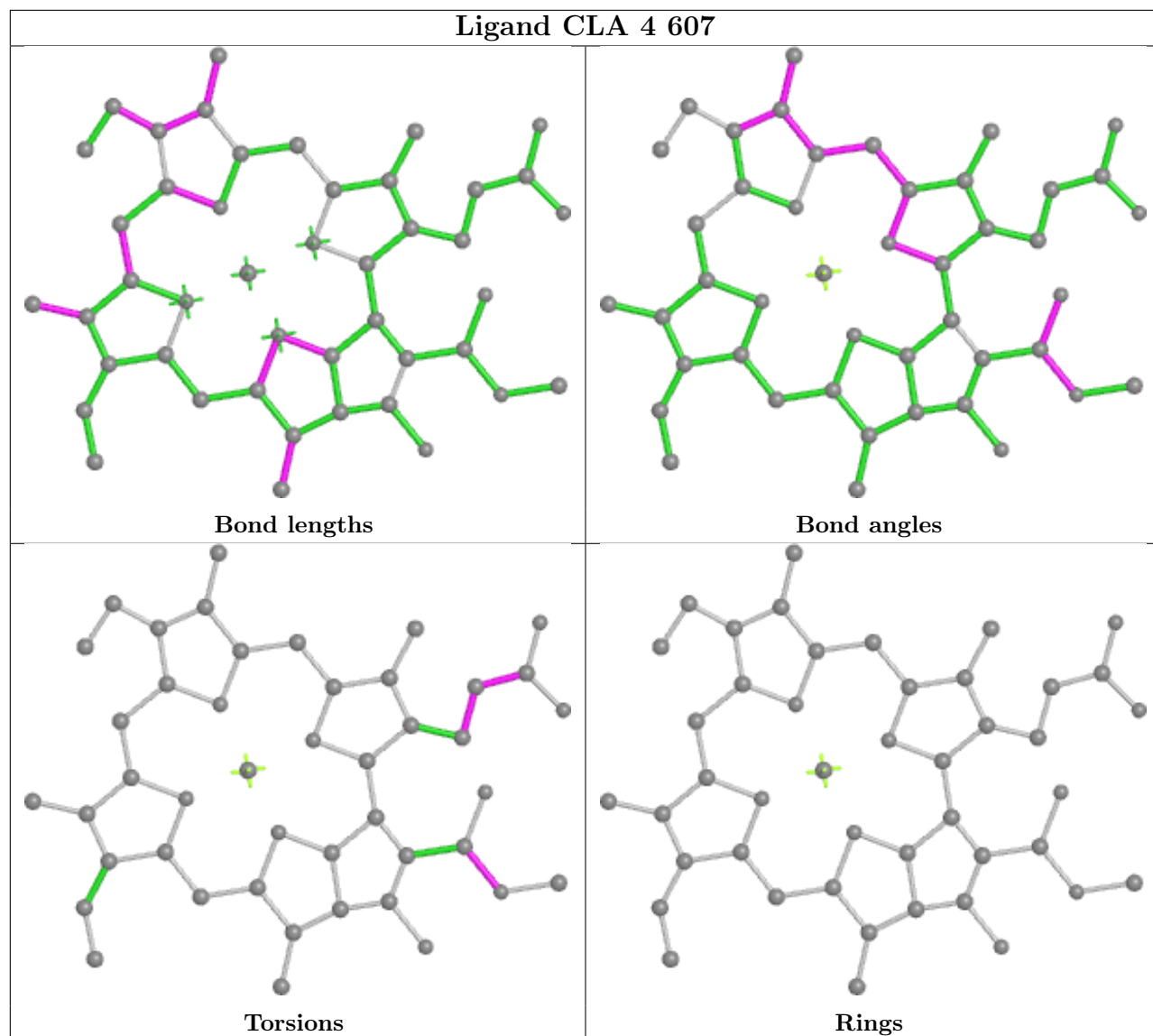




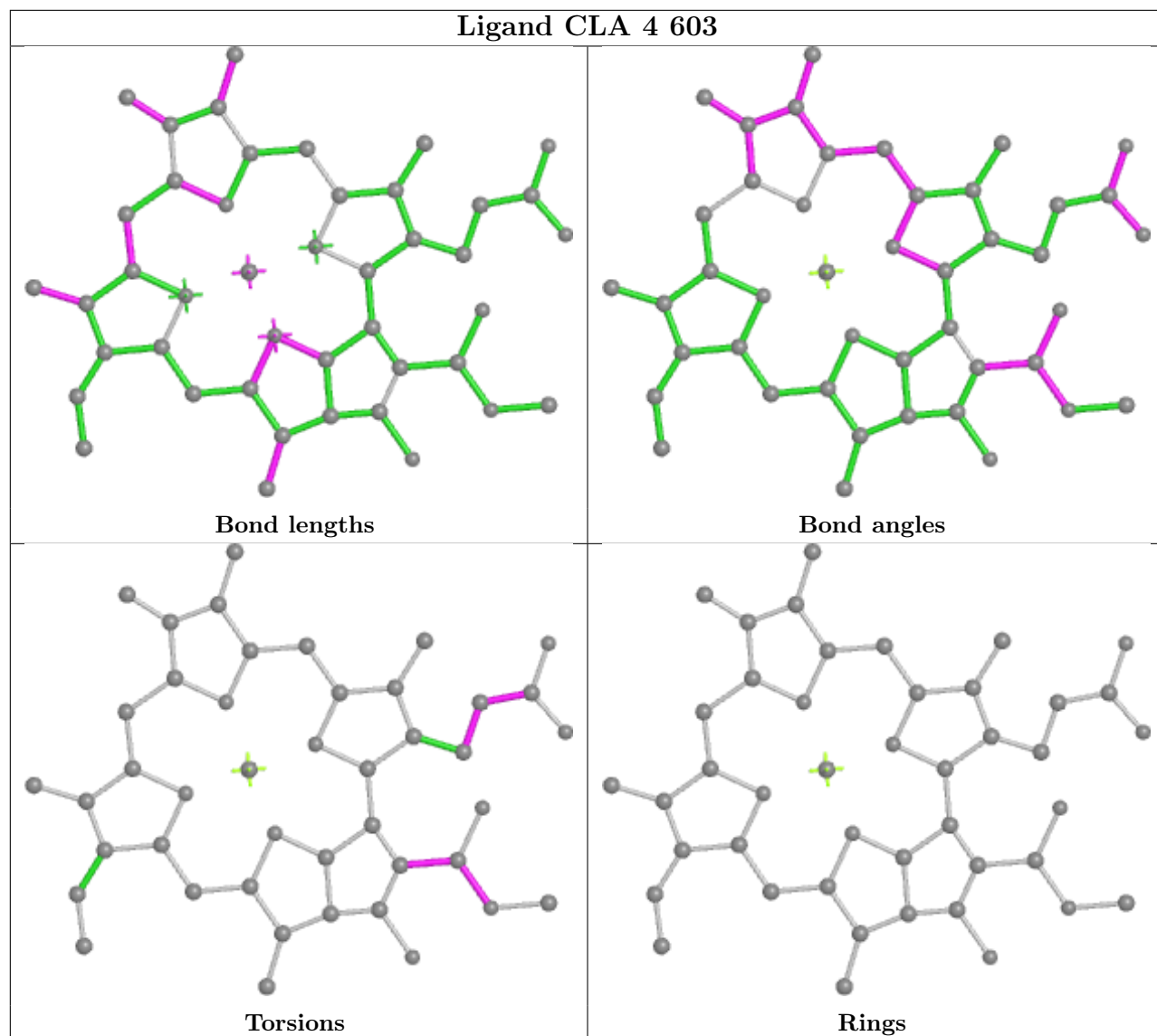
Ligand CLA 3 615



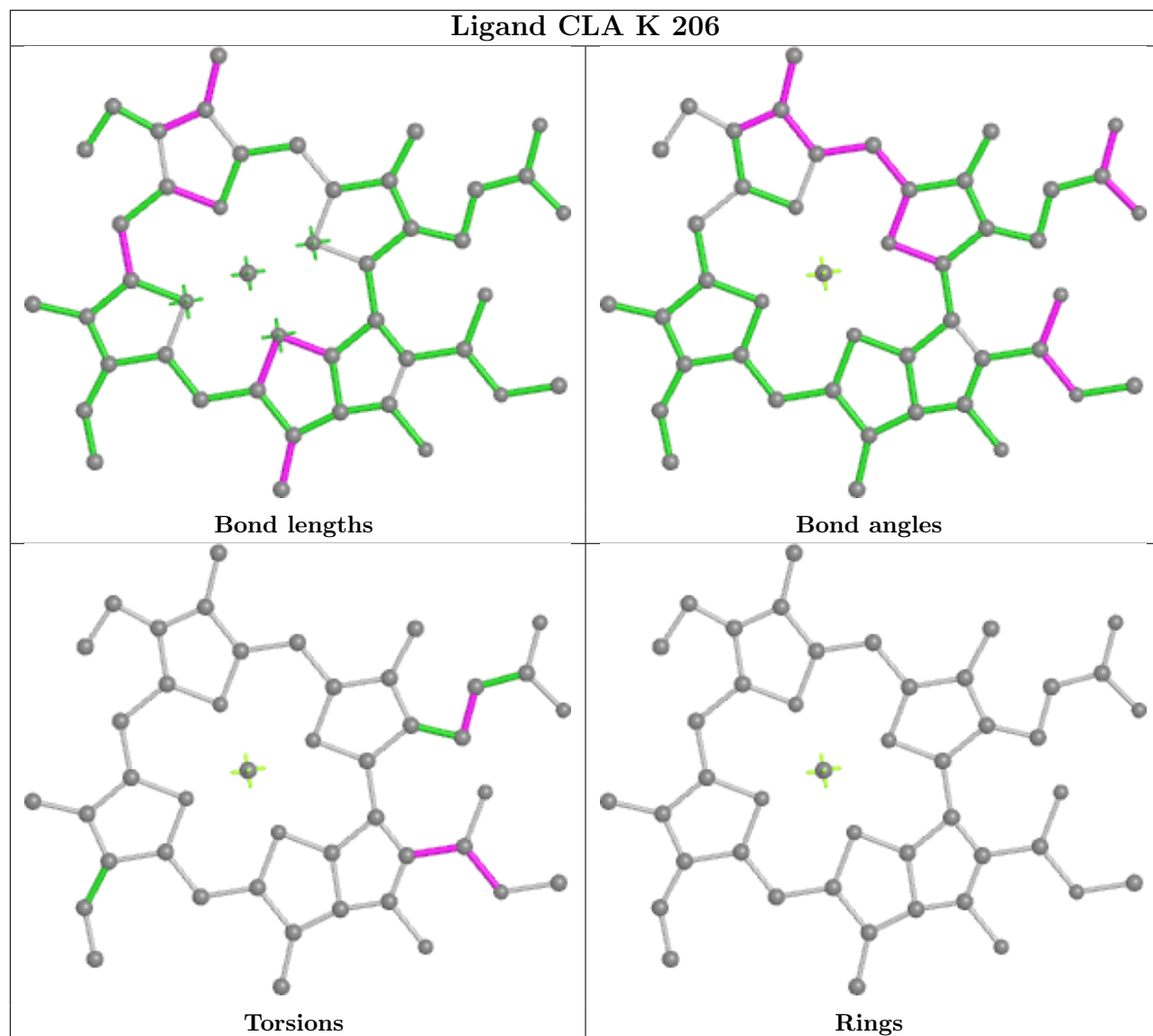
Ligand CLA 4 607

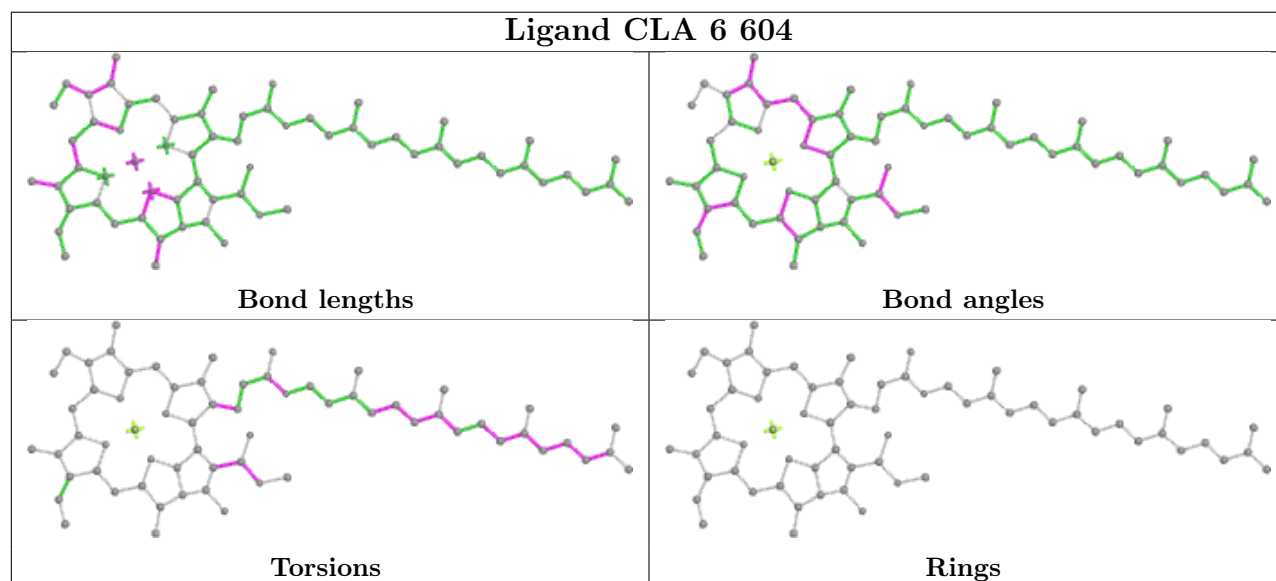
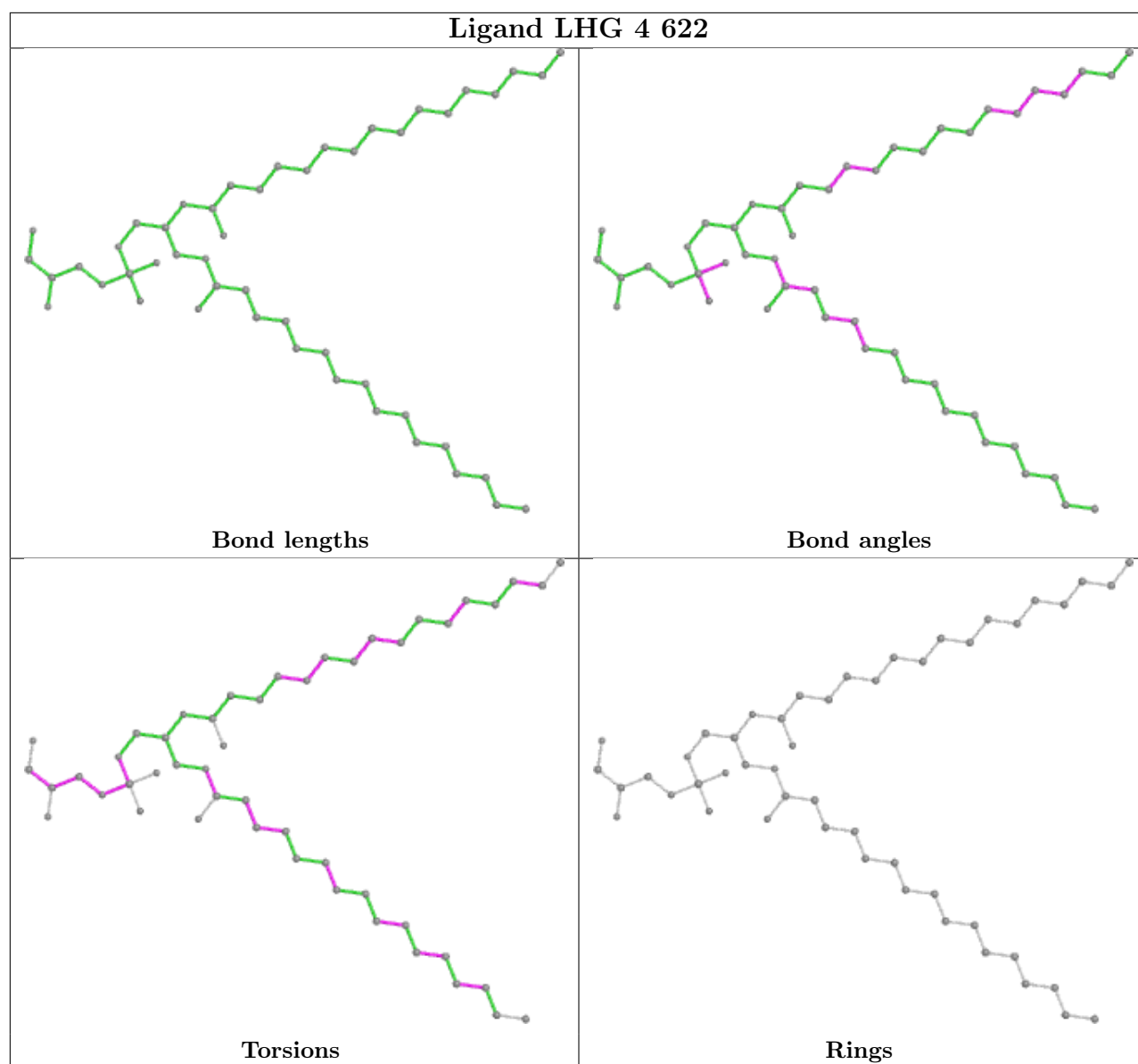


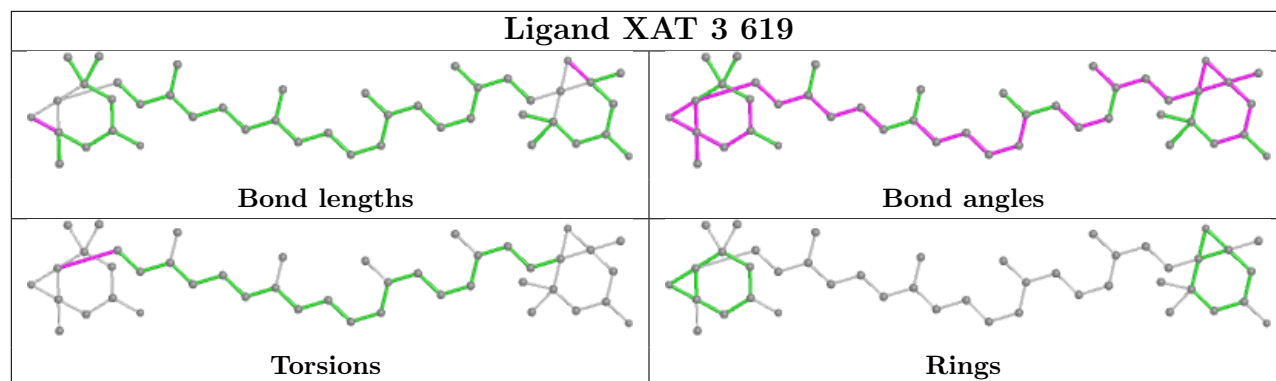
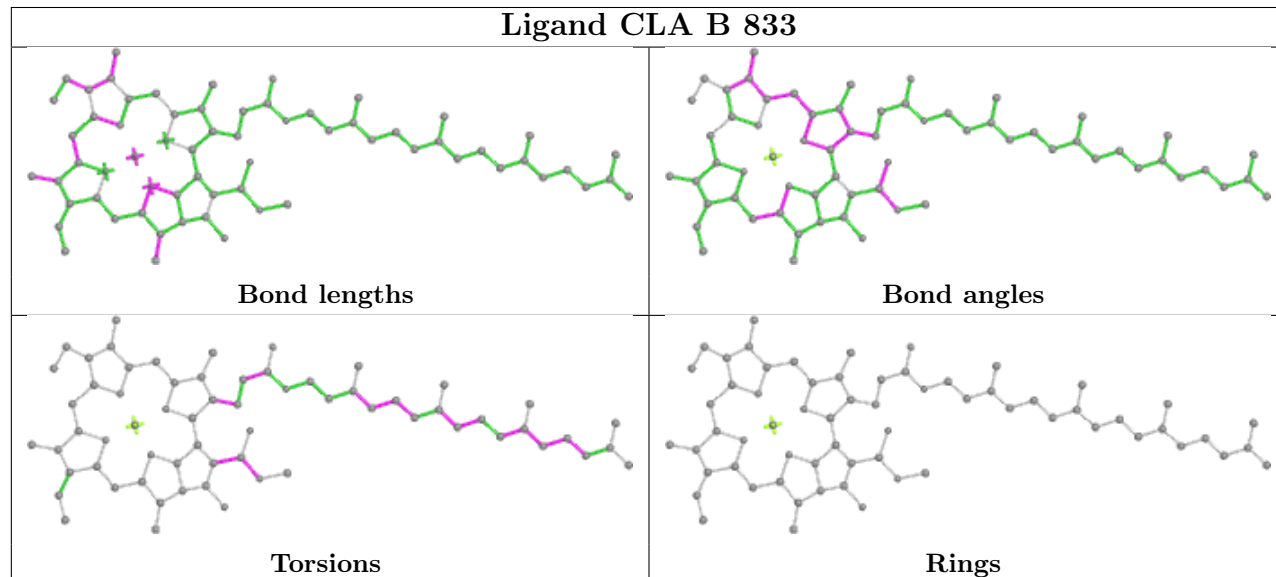
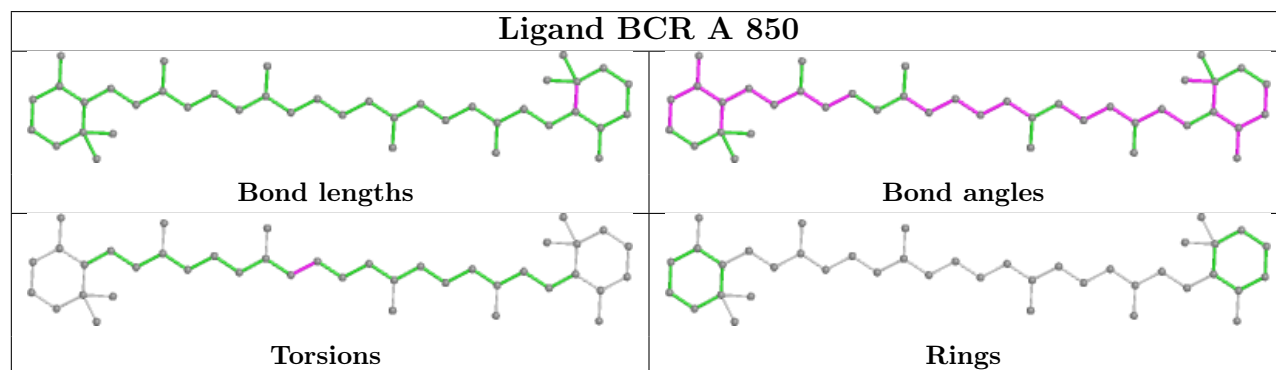
Ligand CLA 4 603

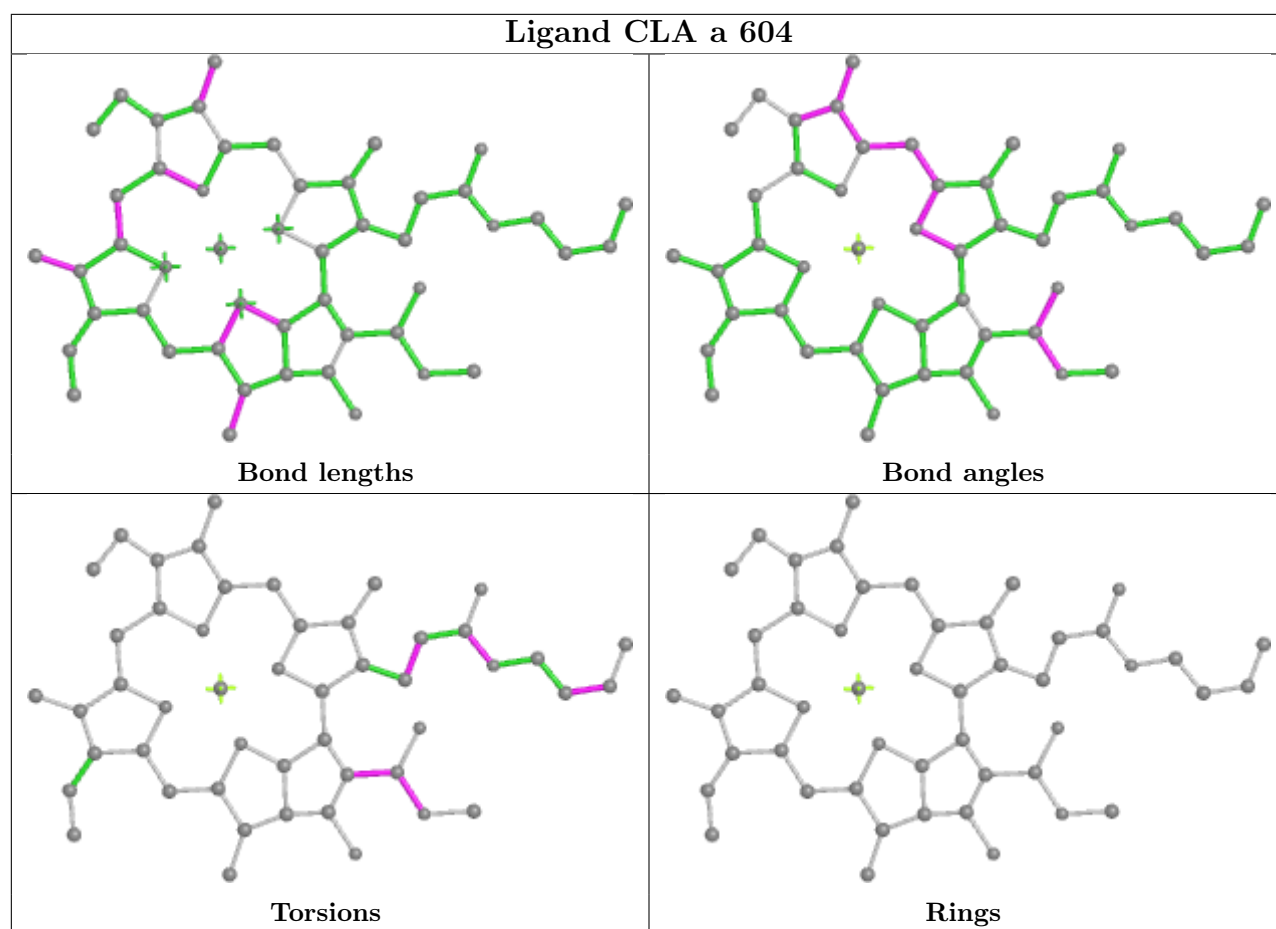


Ligand CLA K 206

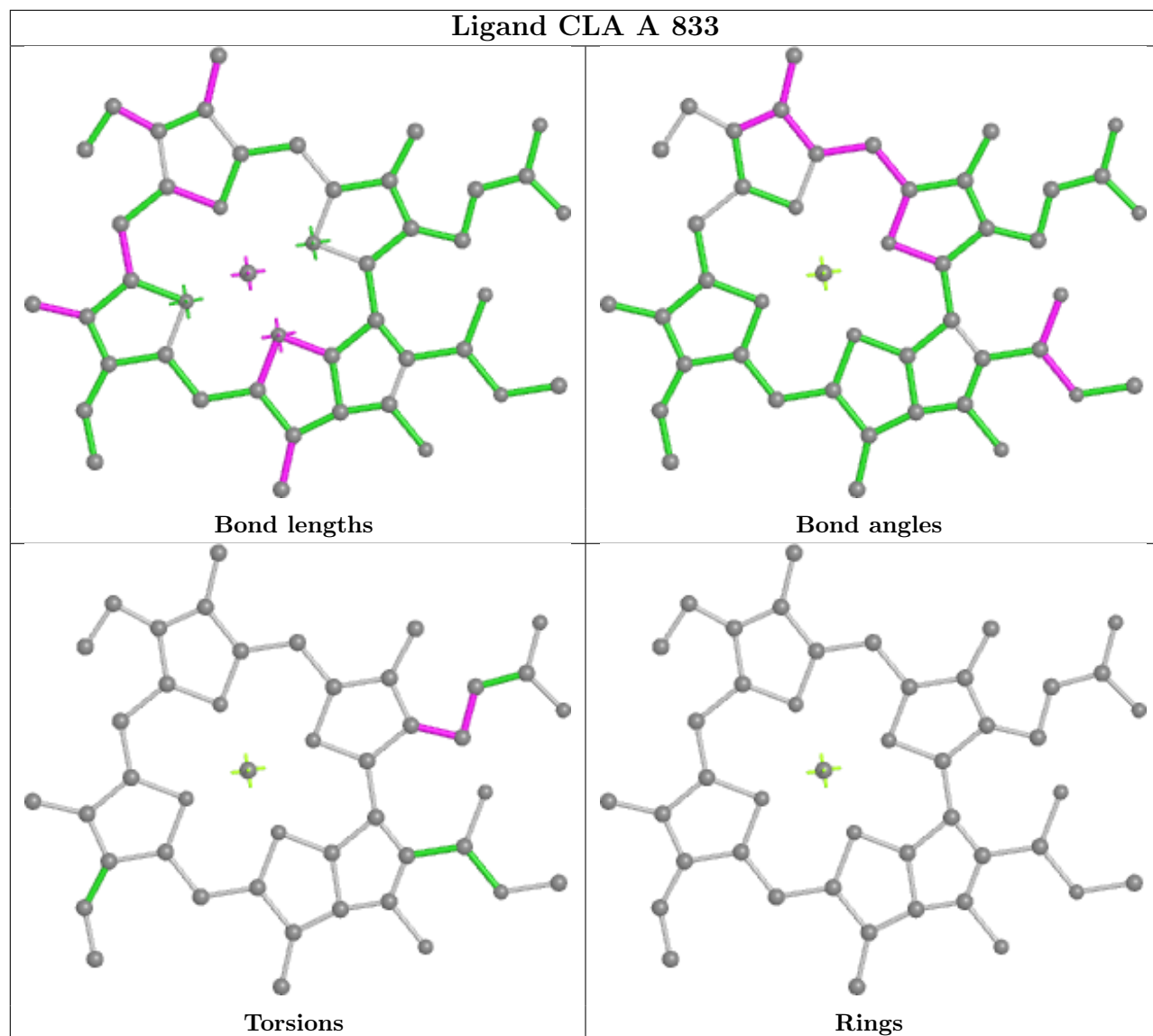




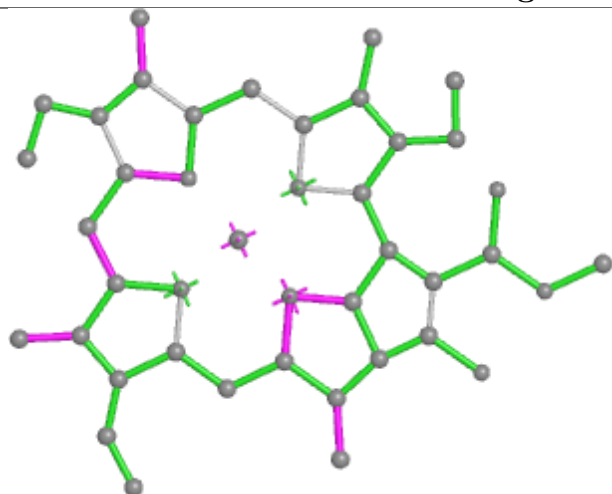
Ligand XAT 3 619**Ligand CLA B 833****Ligand BCR A 850**



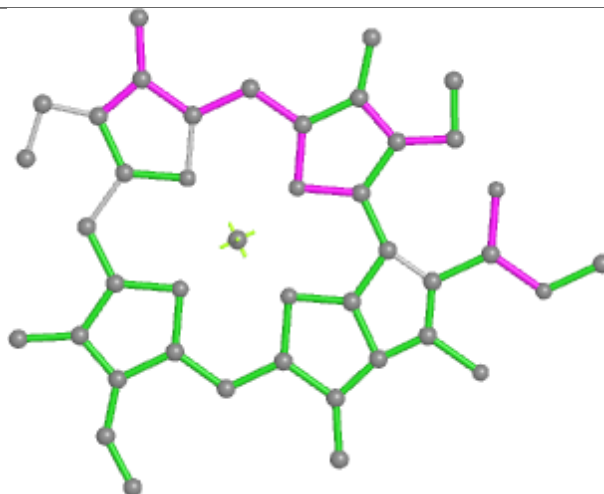
Ligand CLA A 833



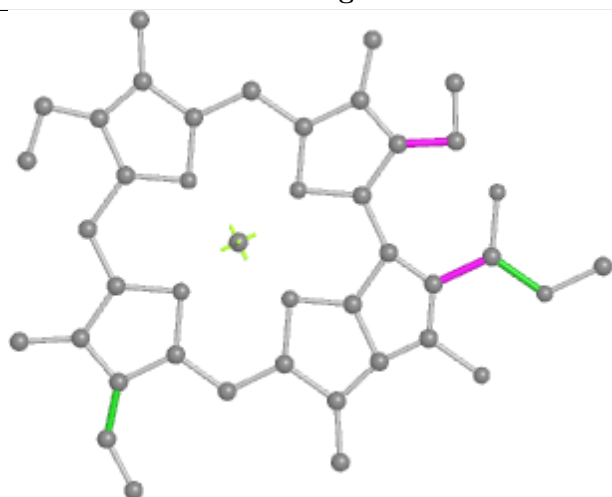
Ligand CLA 6 611



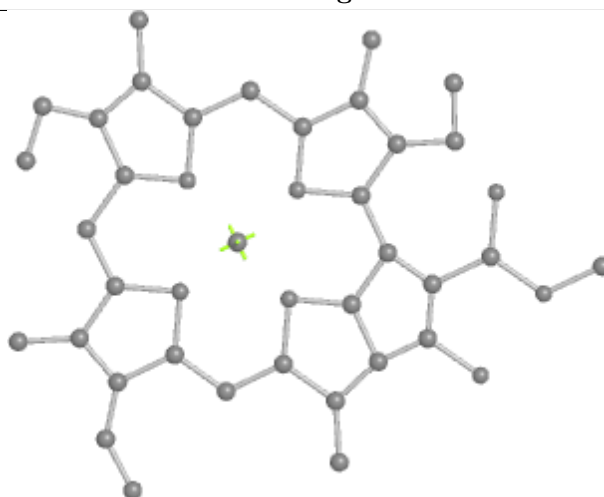
Bond lengths



Bond angles

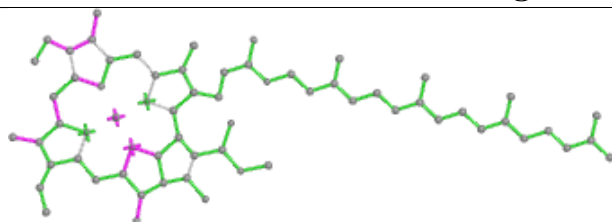


Torsions

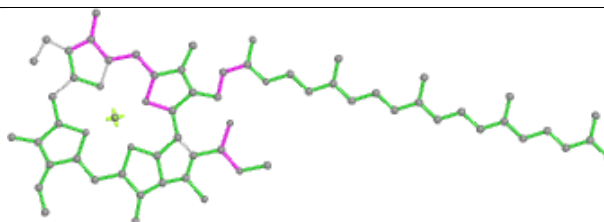


Rings

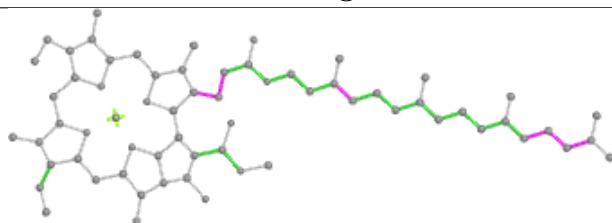
Ligand CLA A 803



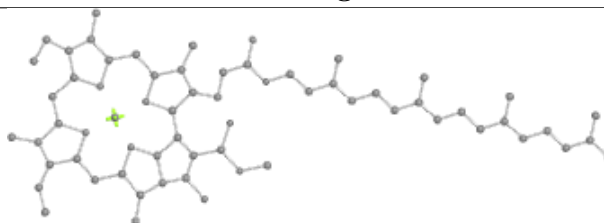
Bond lengths



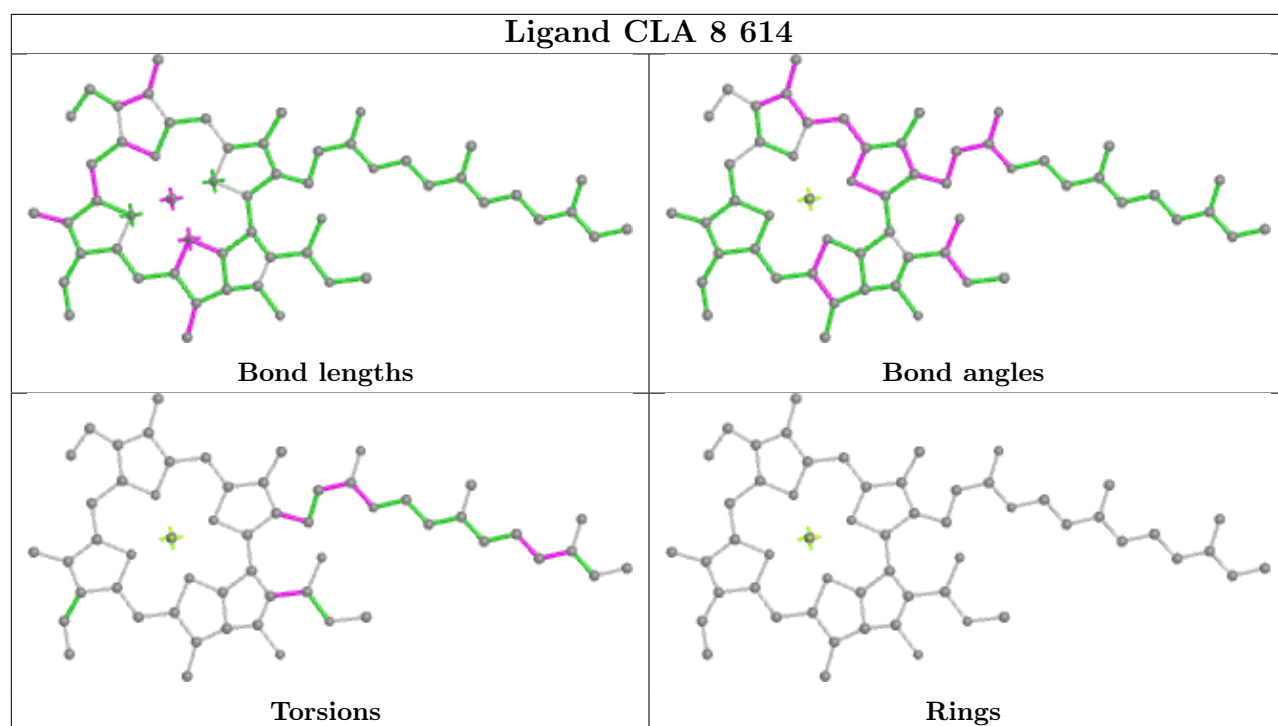
Bond angles



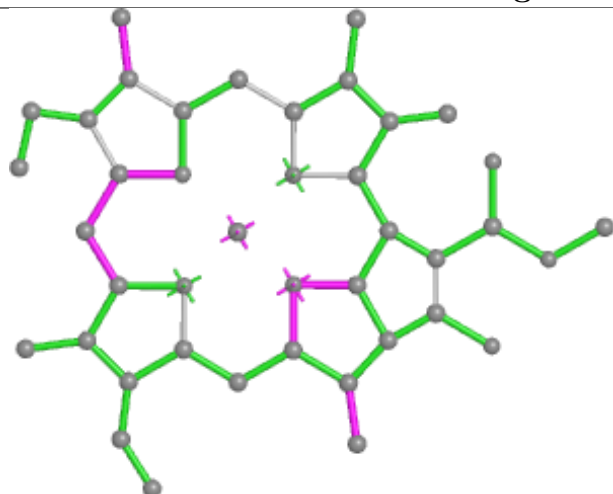
Torsions



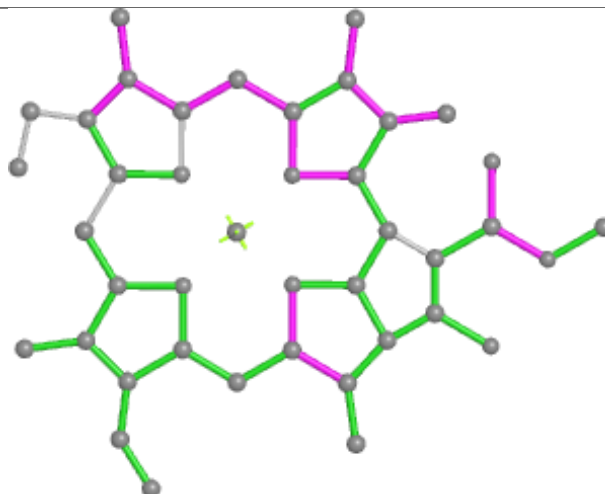
Rings



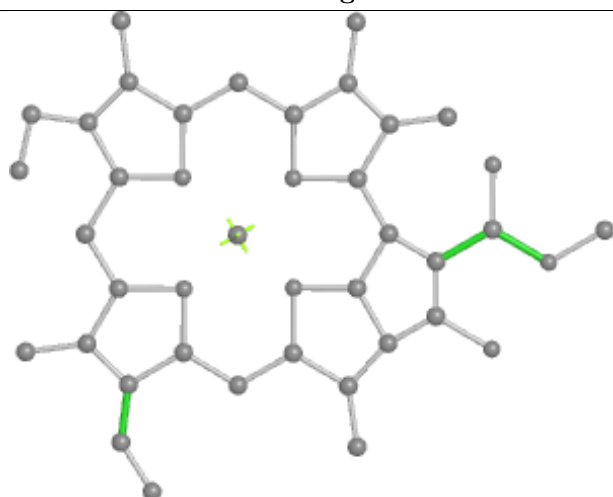
Ligand CLA A 824



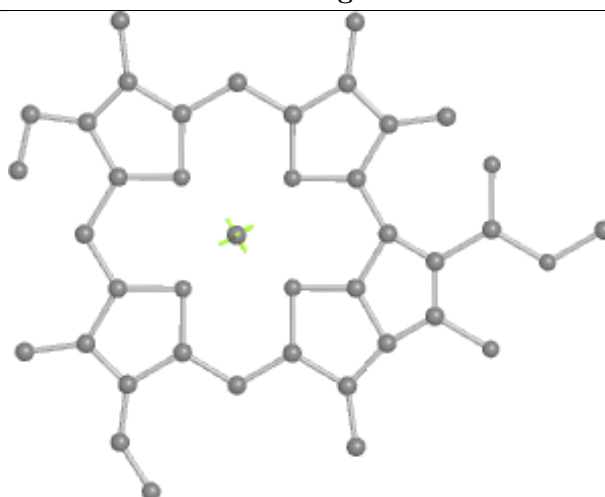
Bond lengths



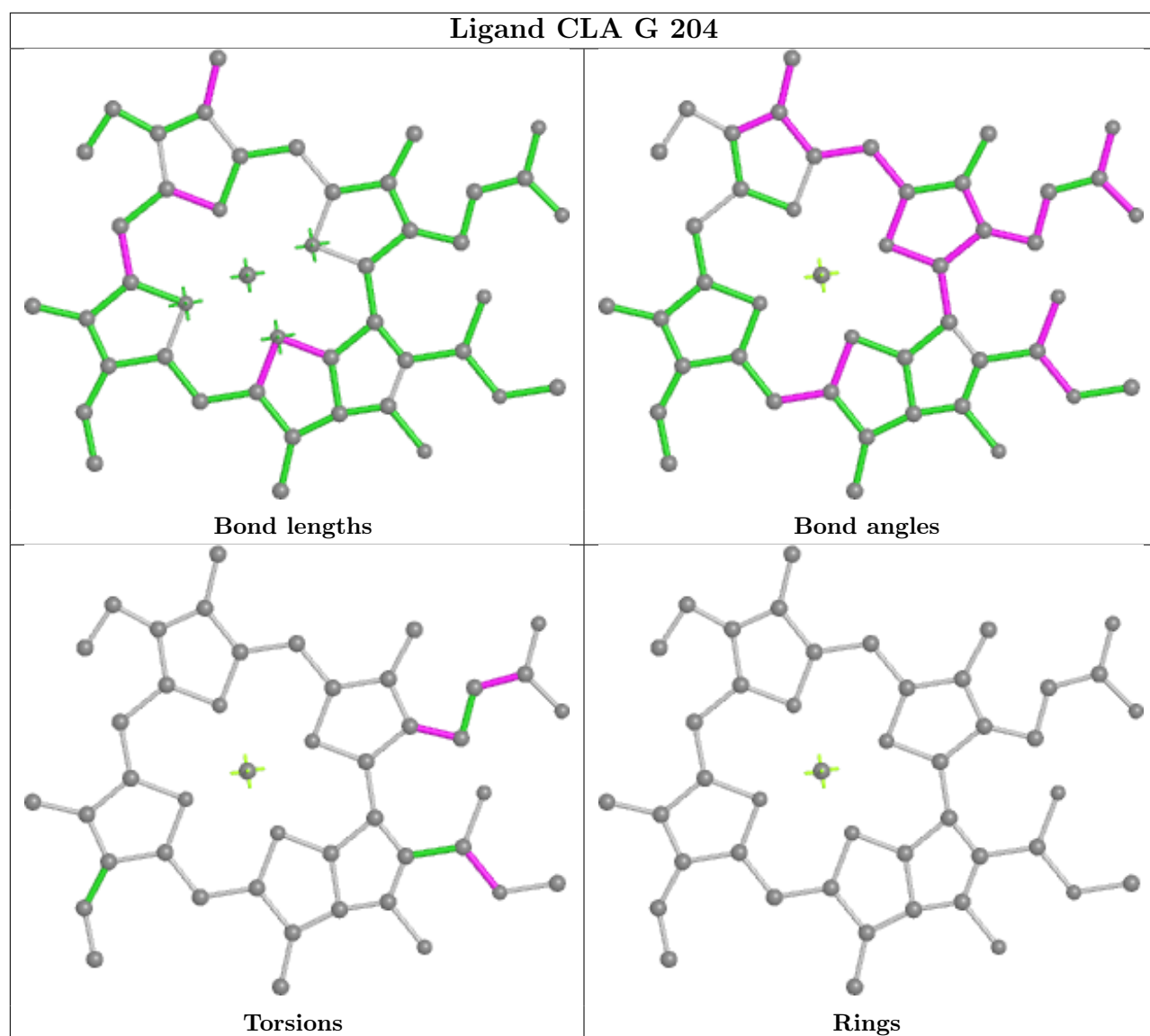
Bond angles



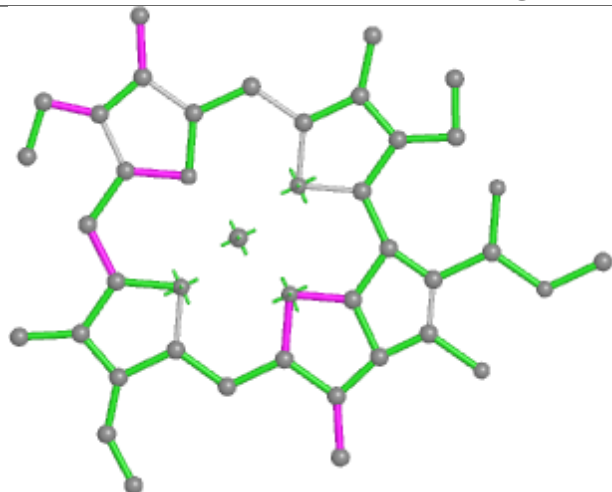
Torsions



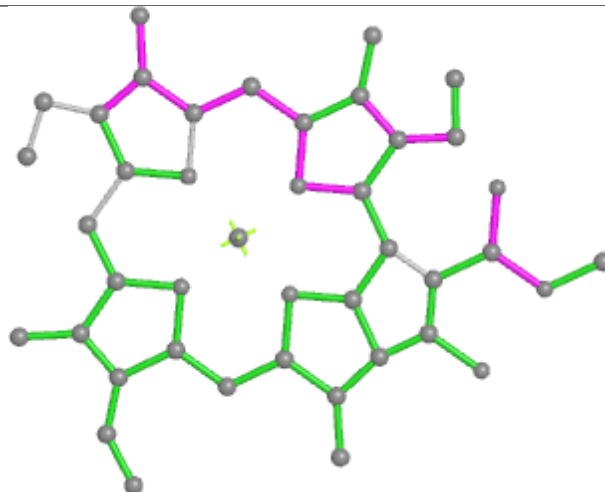
Rings



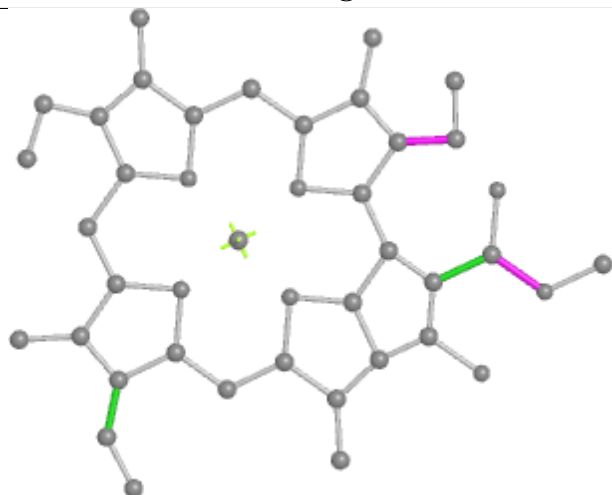
Ligand CLA B 822



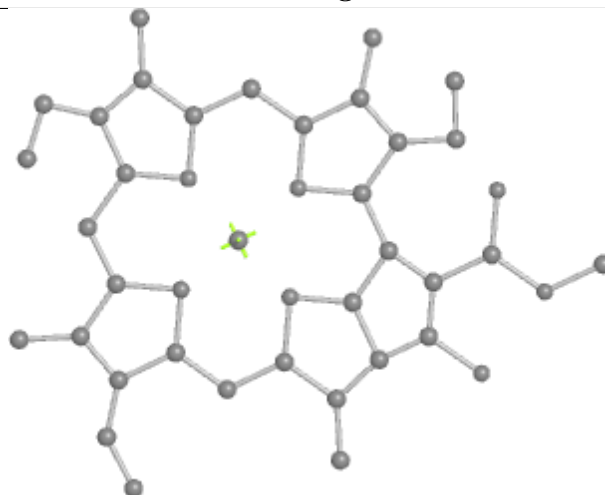
Bond lengths



Bond angles

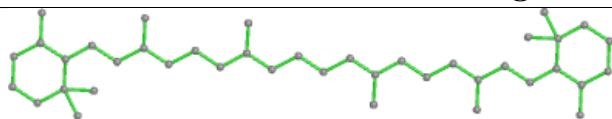


Torsions

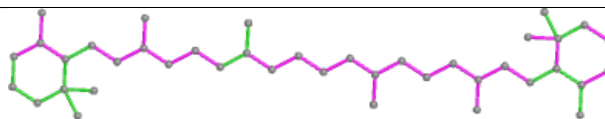


Rings

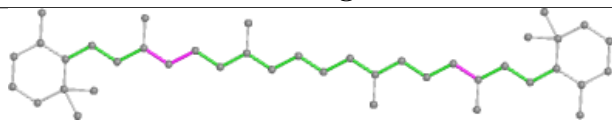
Ligand BCR B 845



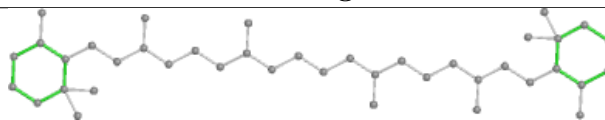
Bond lengths



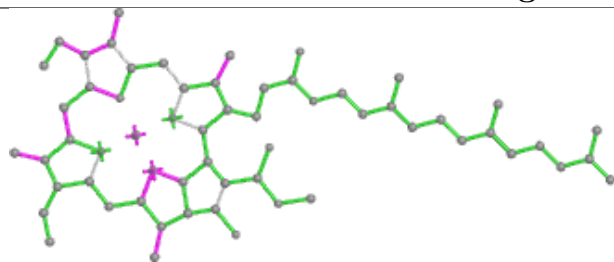
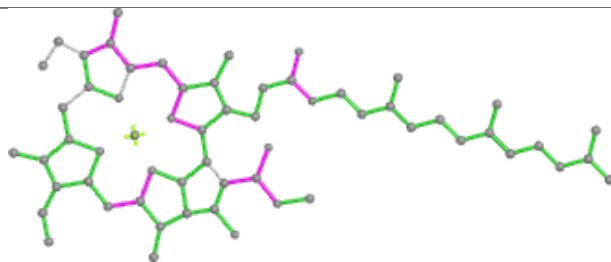
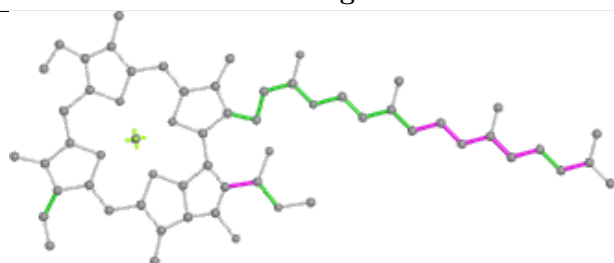
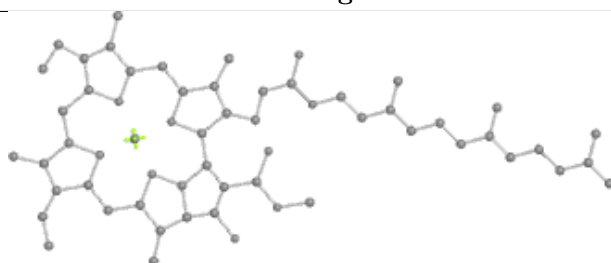
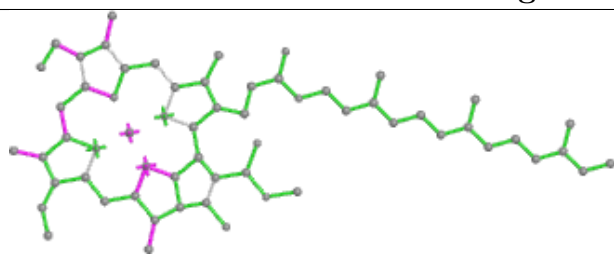
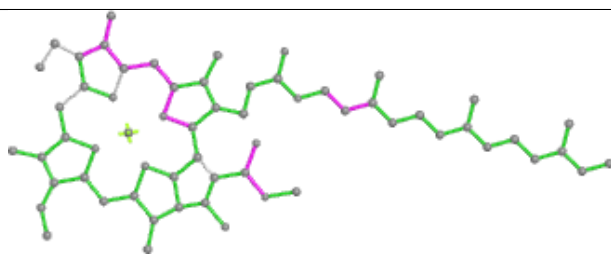
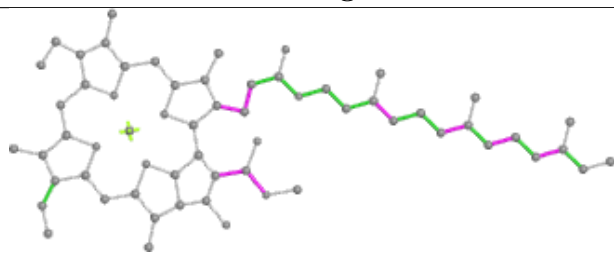
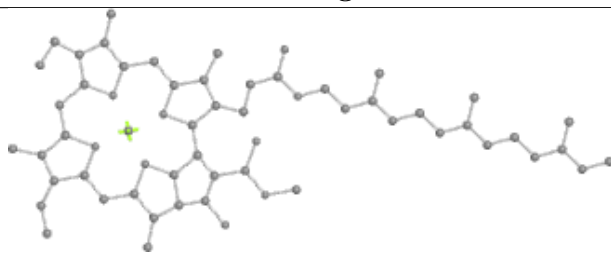
Bond angles



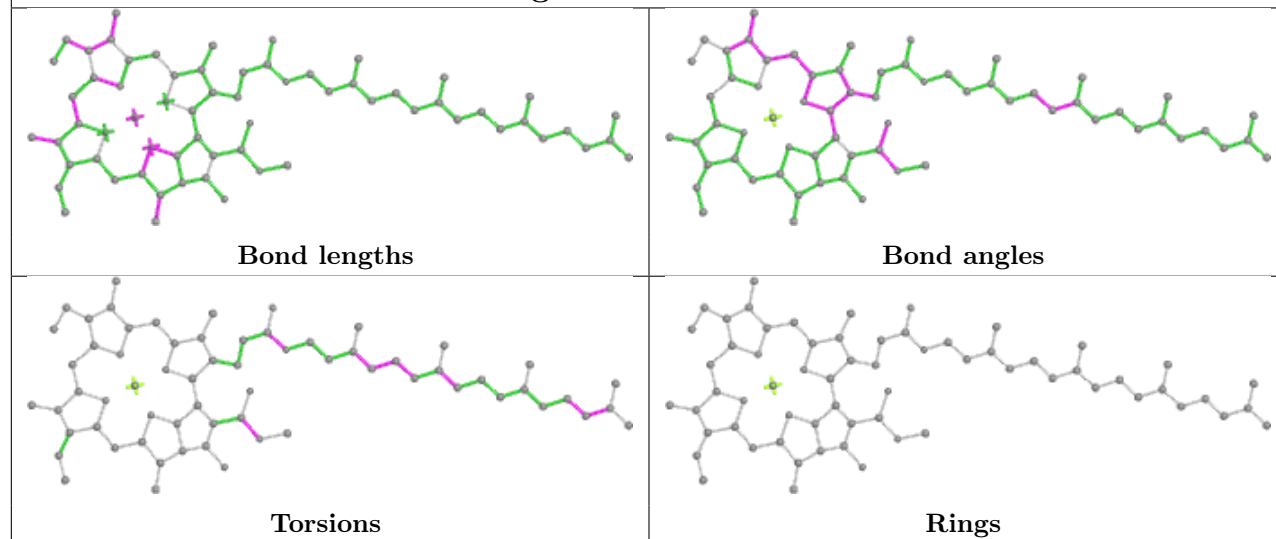
Torsions



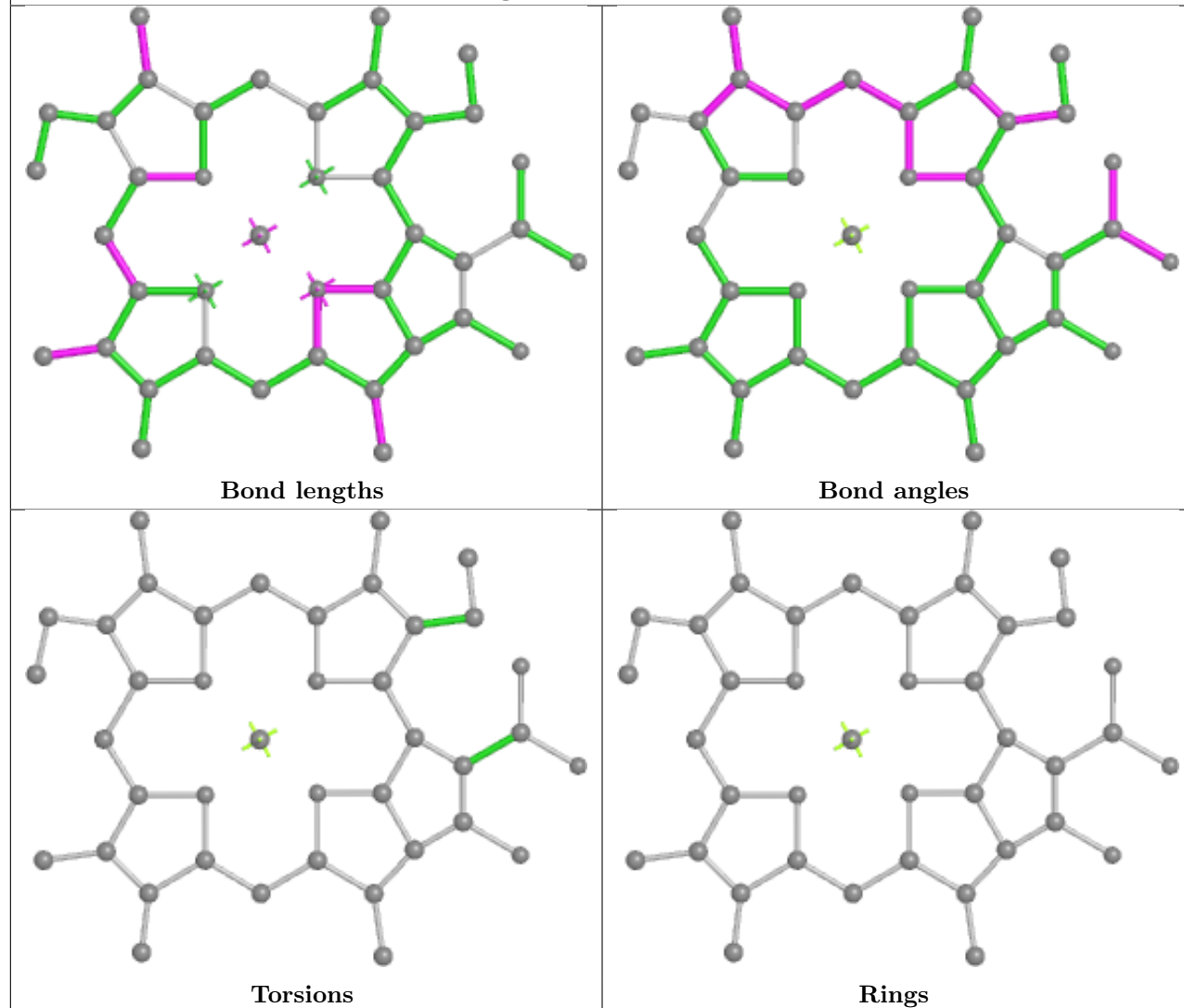
Rings

Ligand CLA 7 601**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 4 610****Bond lengths****Bond angles****Torsions****Rings**

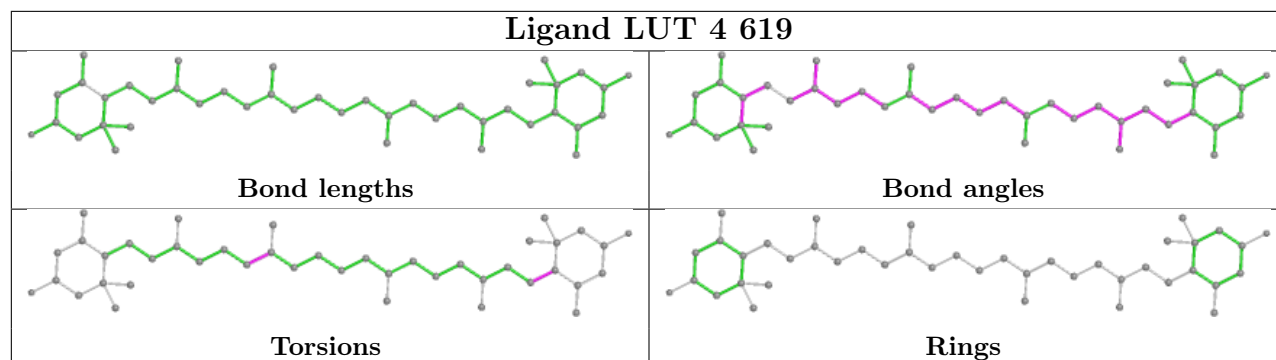
Ligand CLA A 807



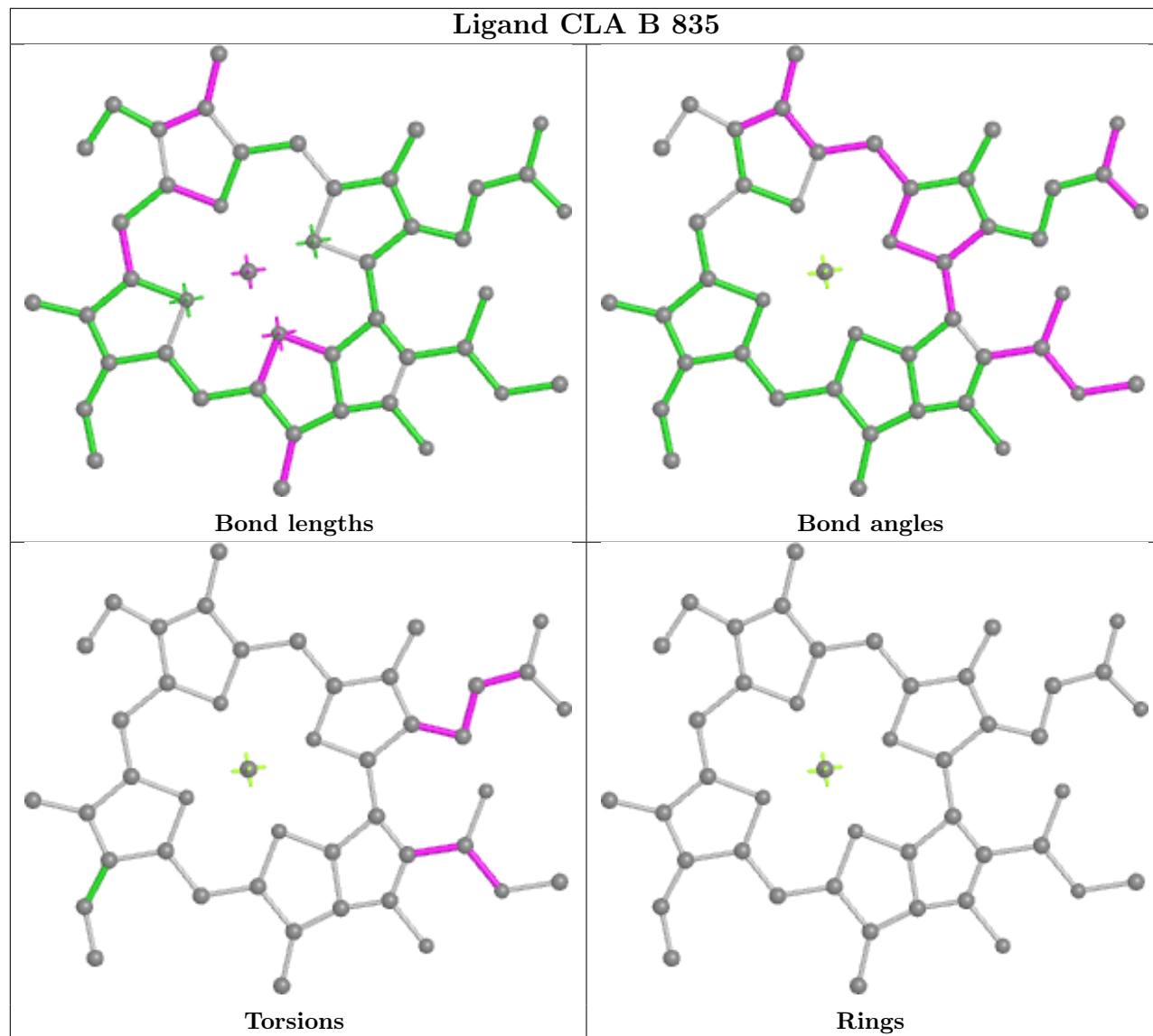
Ligand CLA 6 606

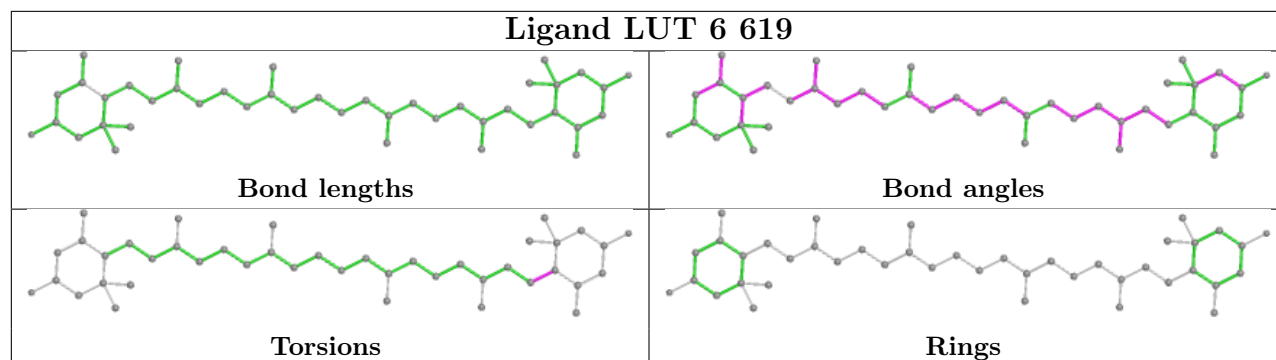
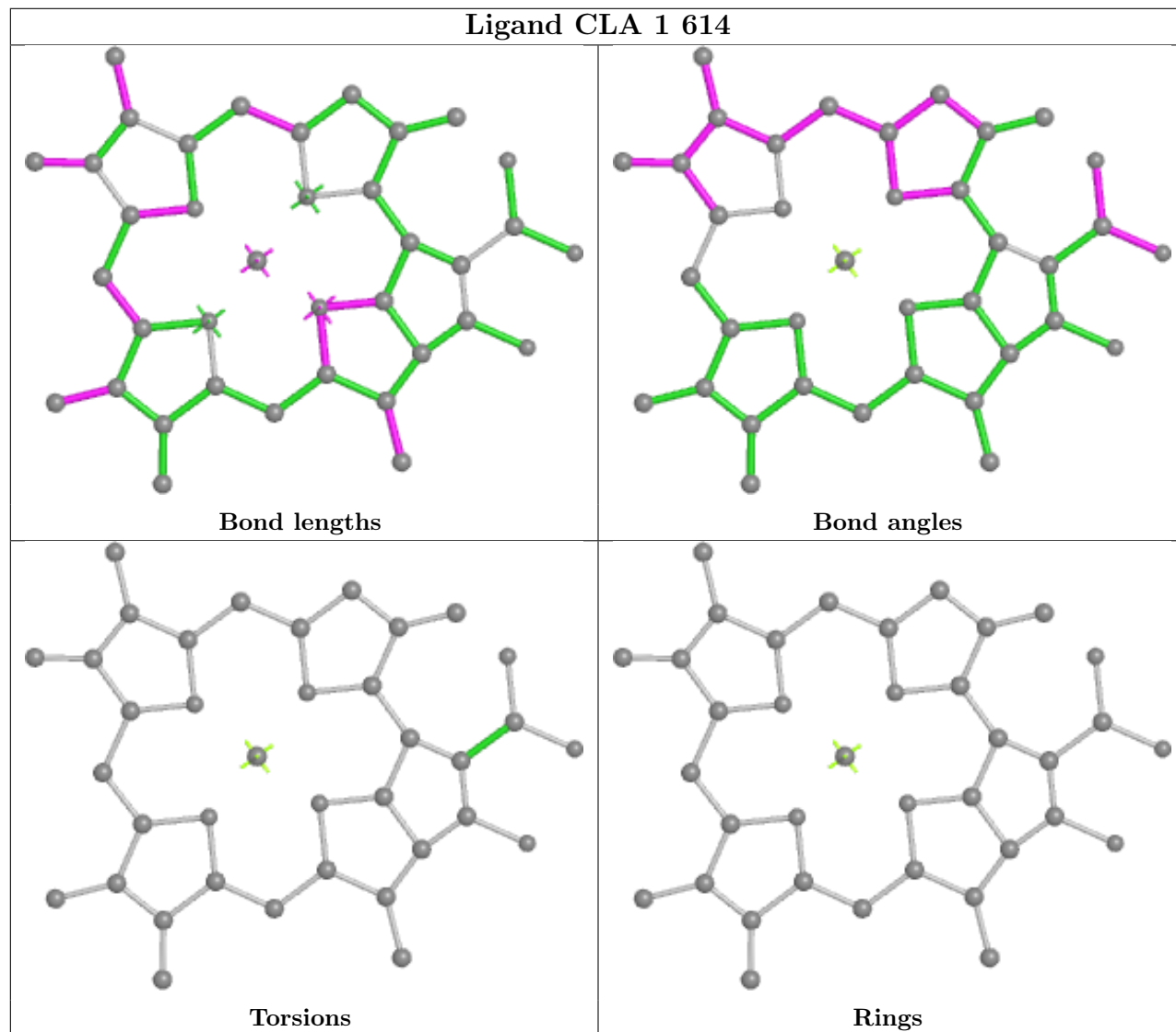


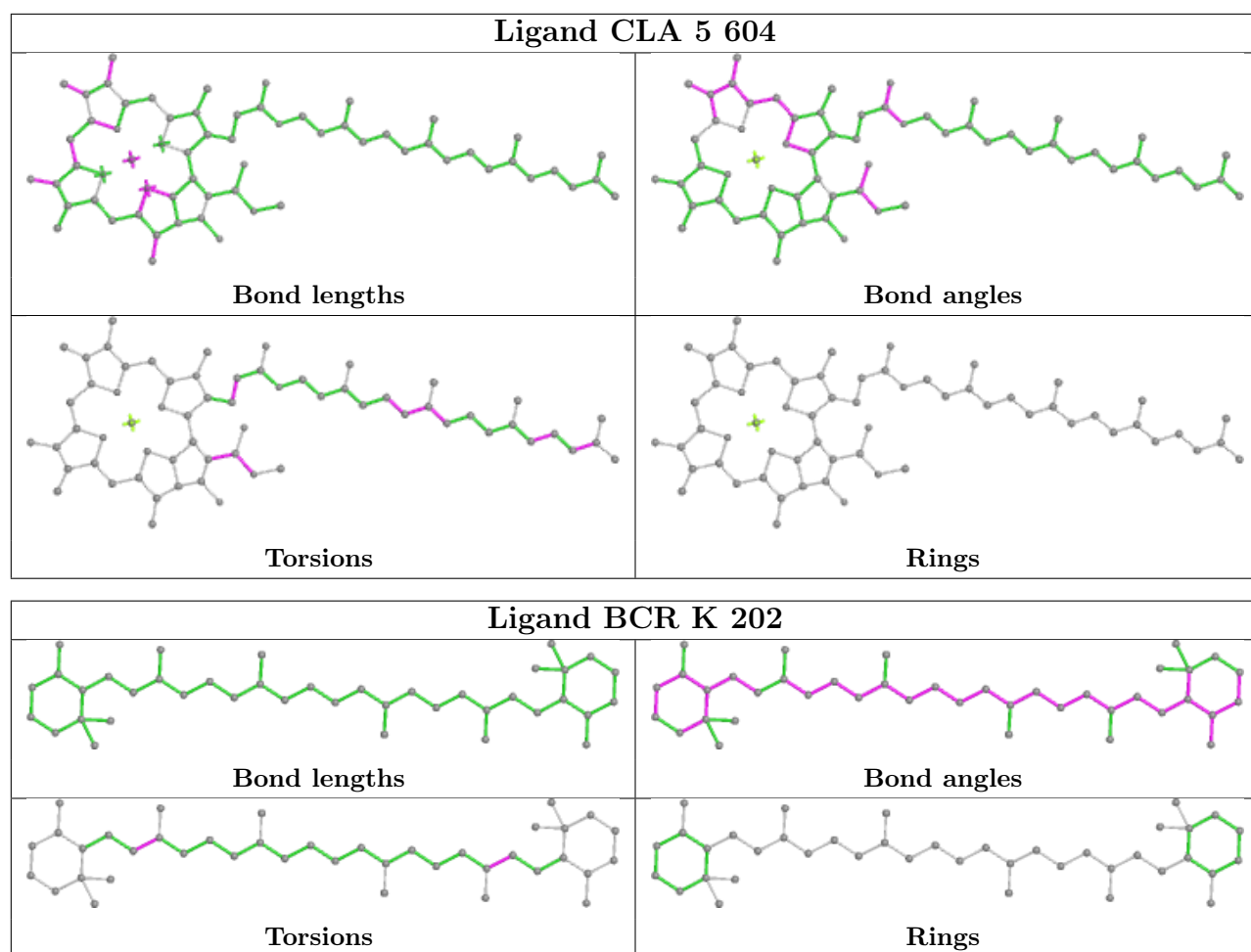
Ligand LUT 4 619



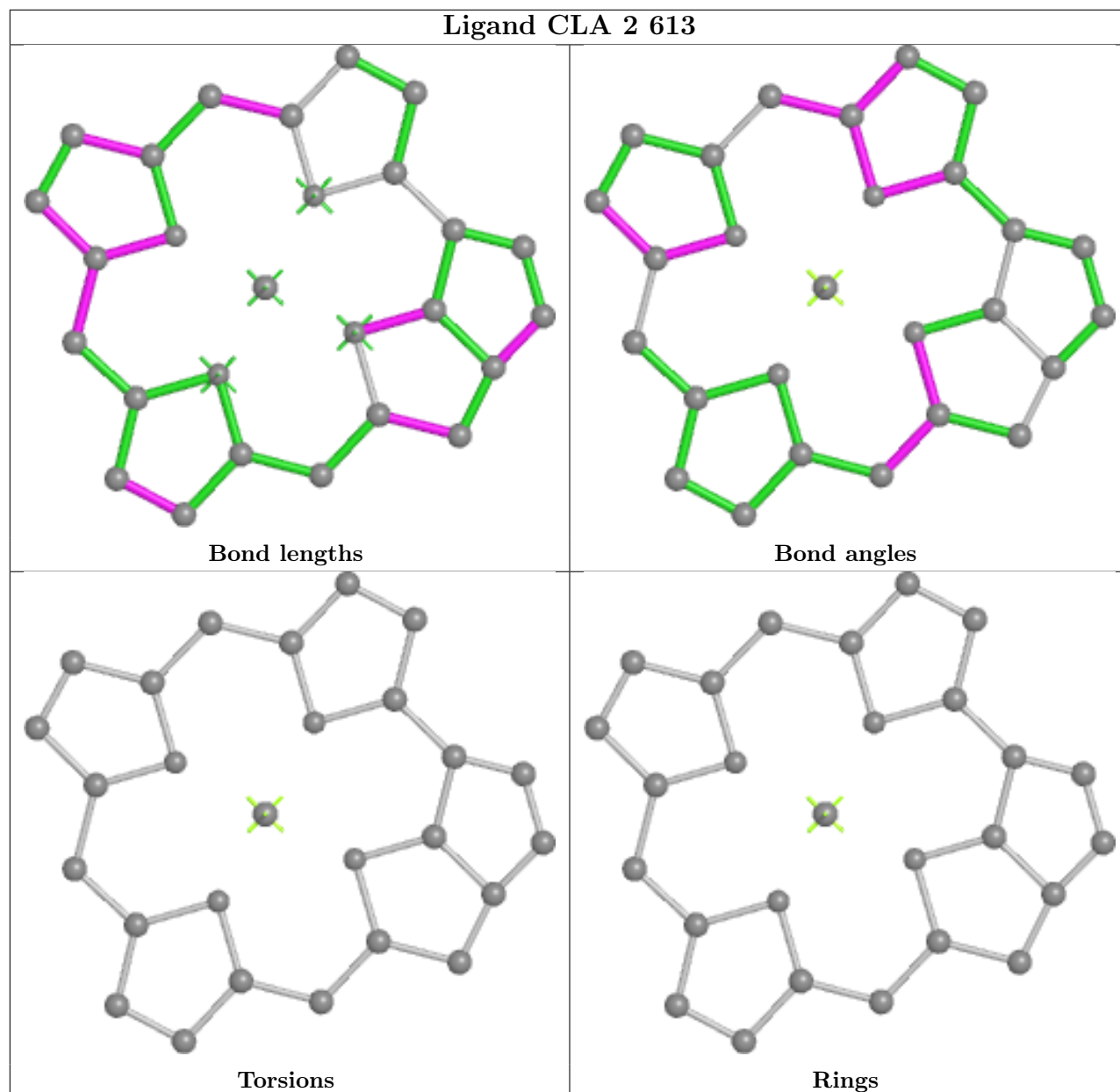
Ligand CLA B 835



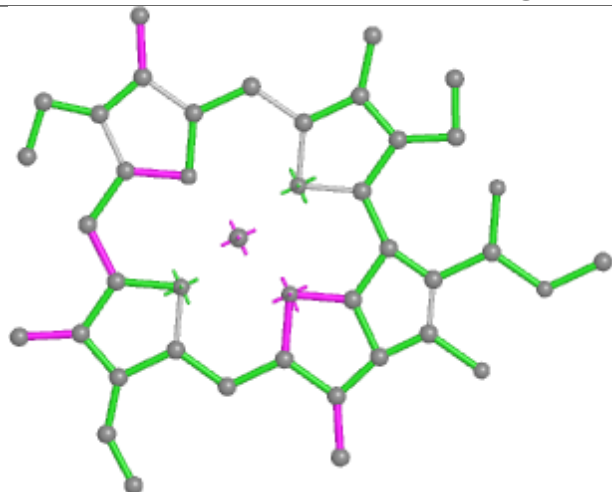
Ligand LUT 6 619**Ligand CLA 1 614**



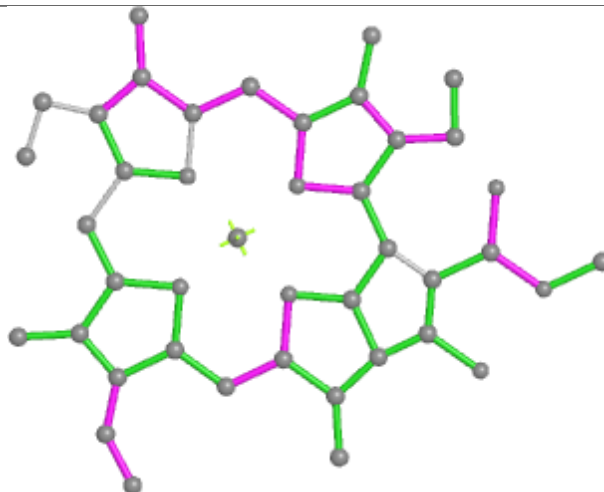
Ligand CLA 2 613



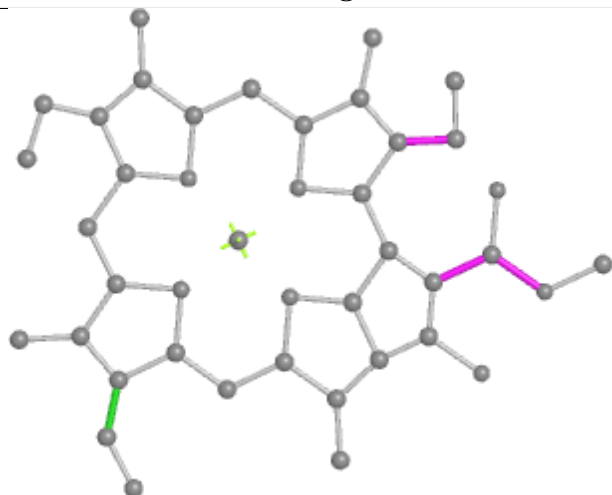
Ligand CLA 7 607



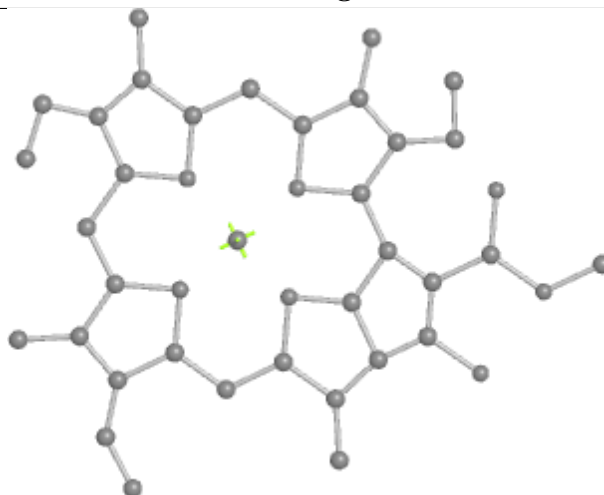
Bond lengths



Bond angles

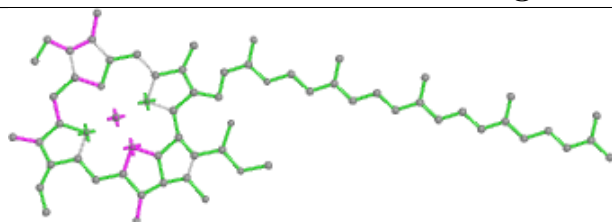


Torsions

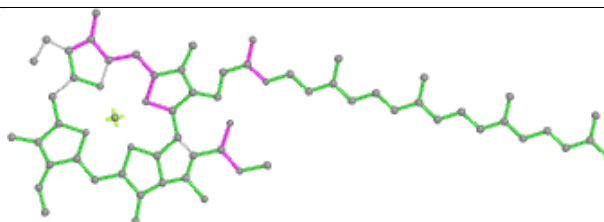


Rings

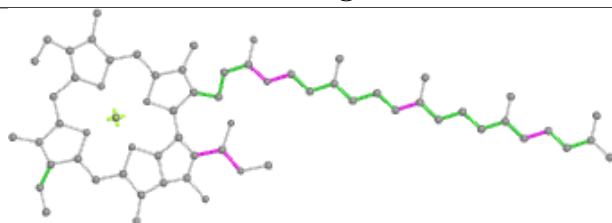
Ligand CLA B 840



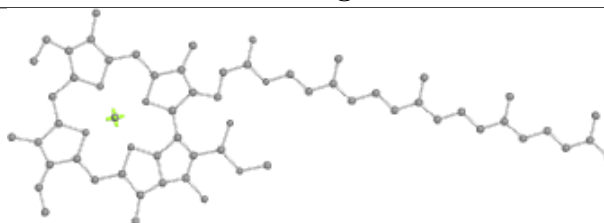
Bond lengths



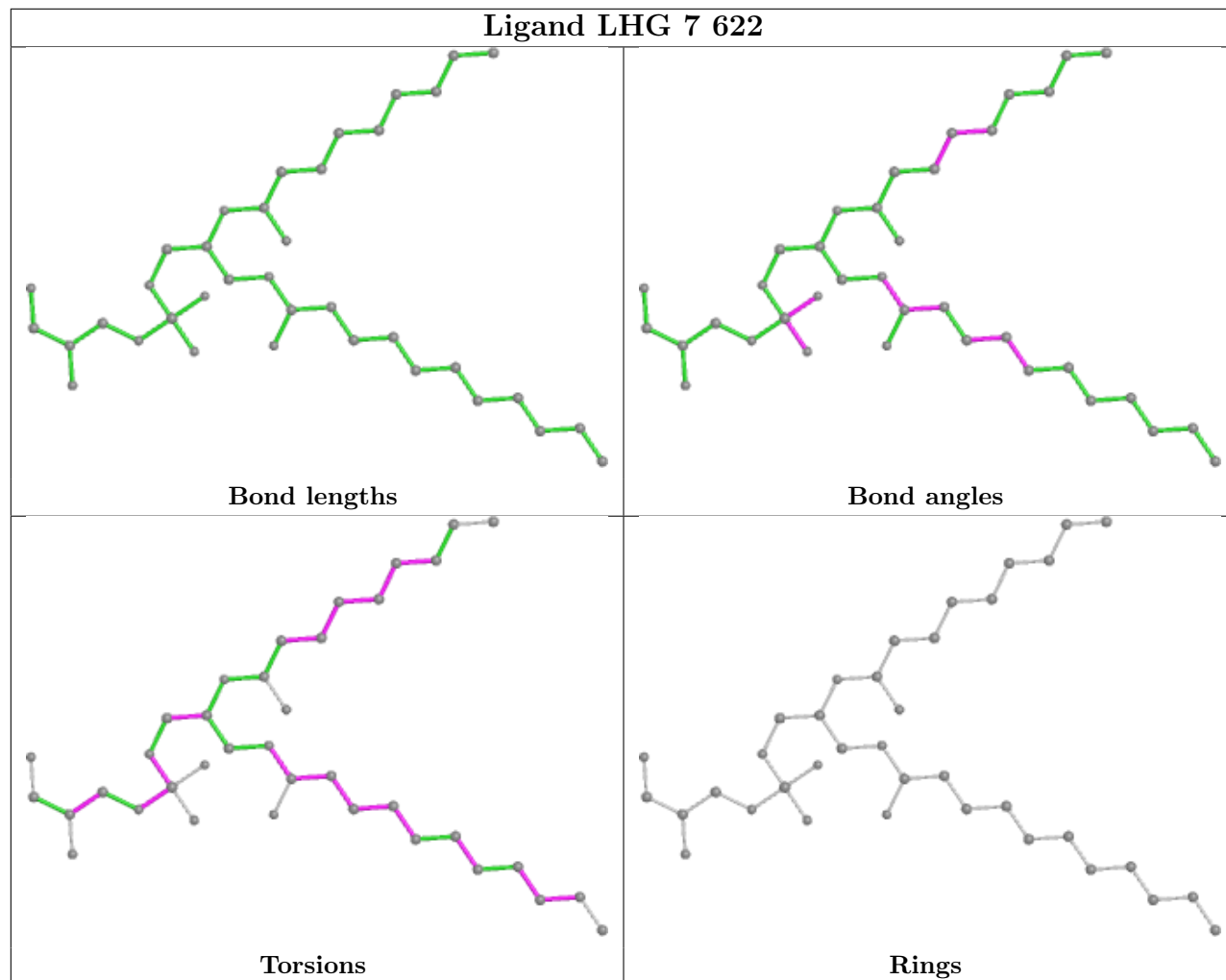
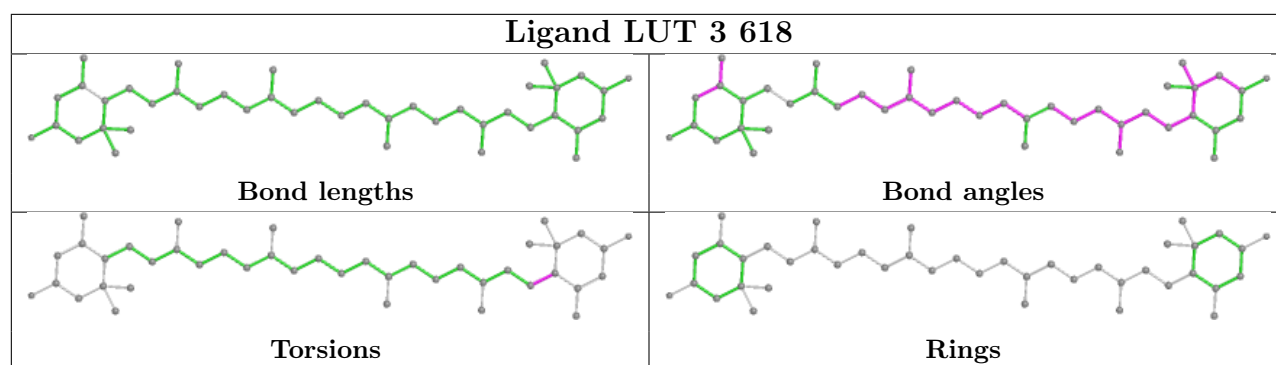
Bond angles

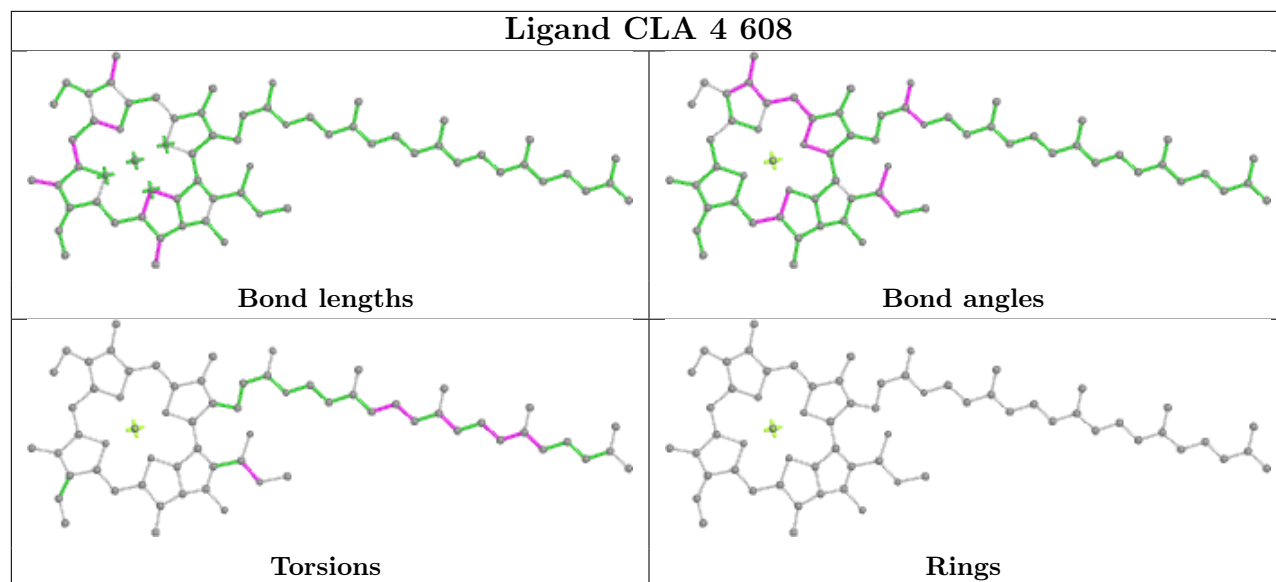
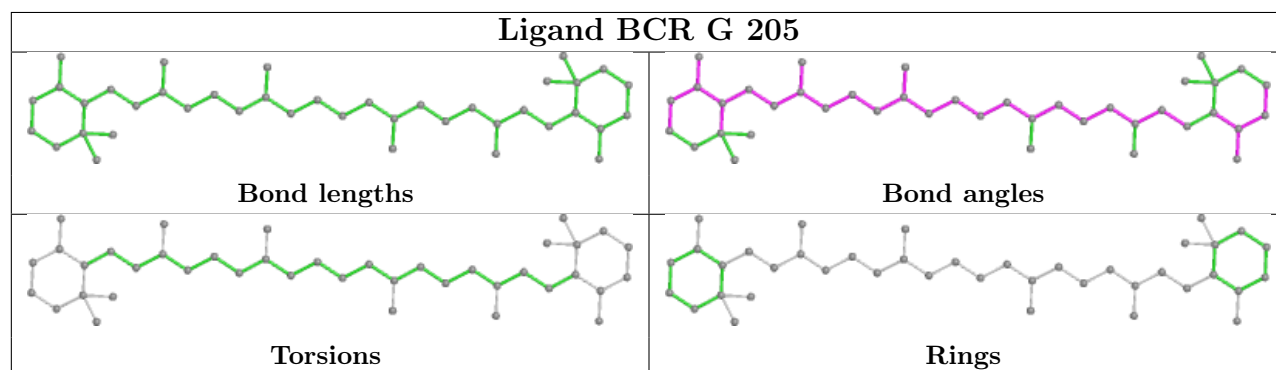


Torsions

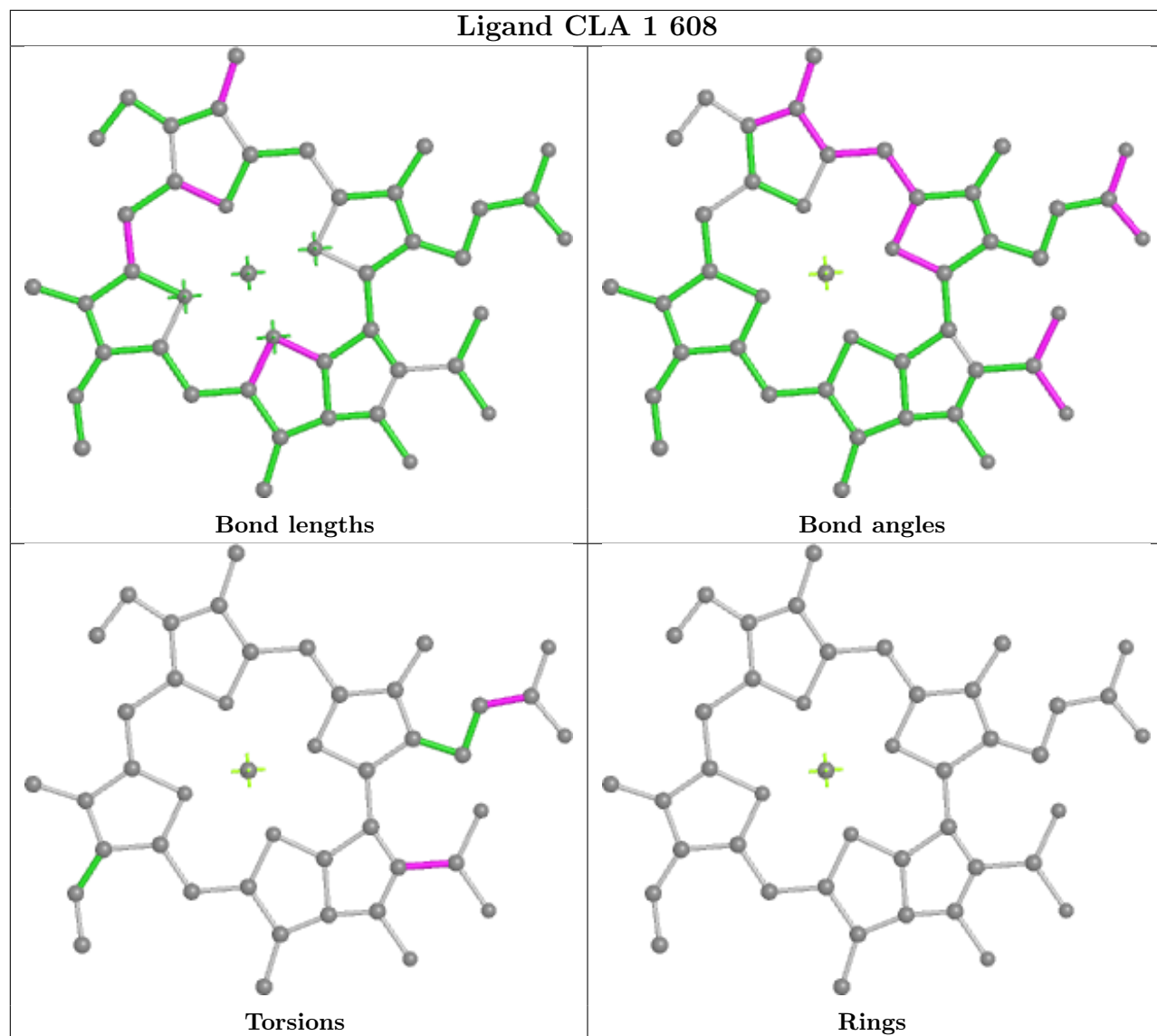


Rings

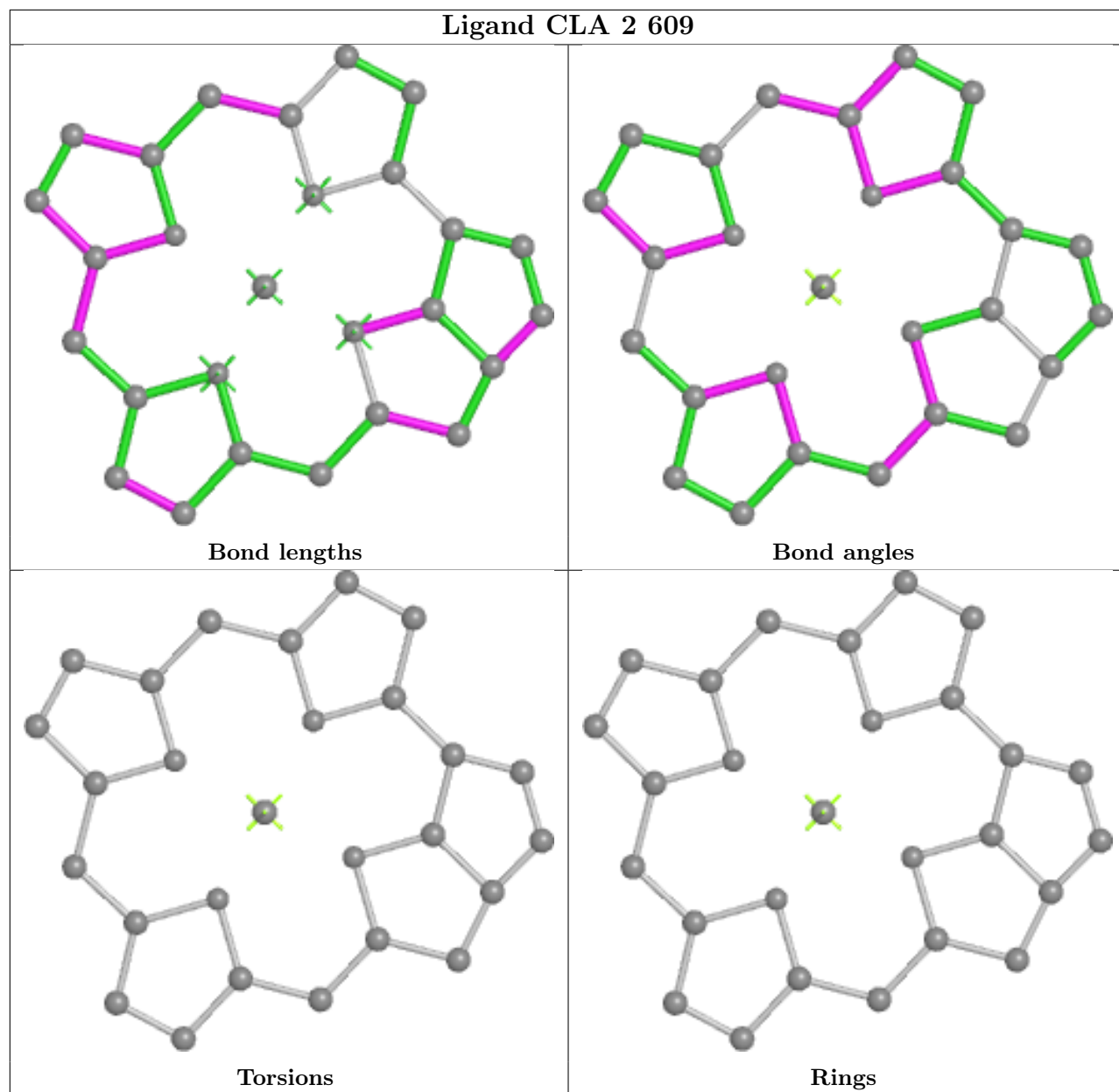


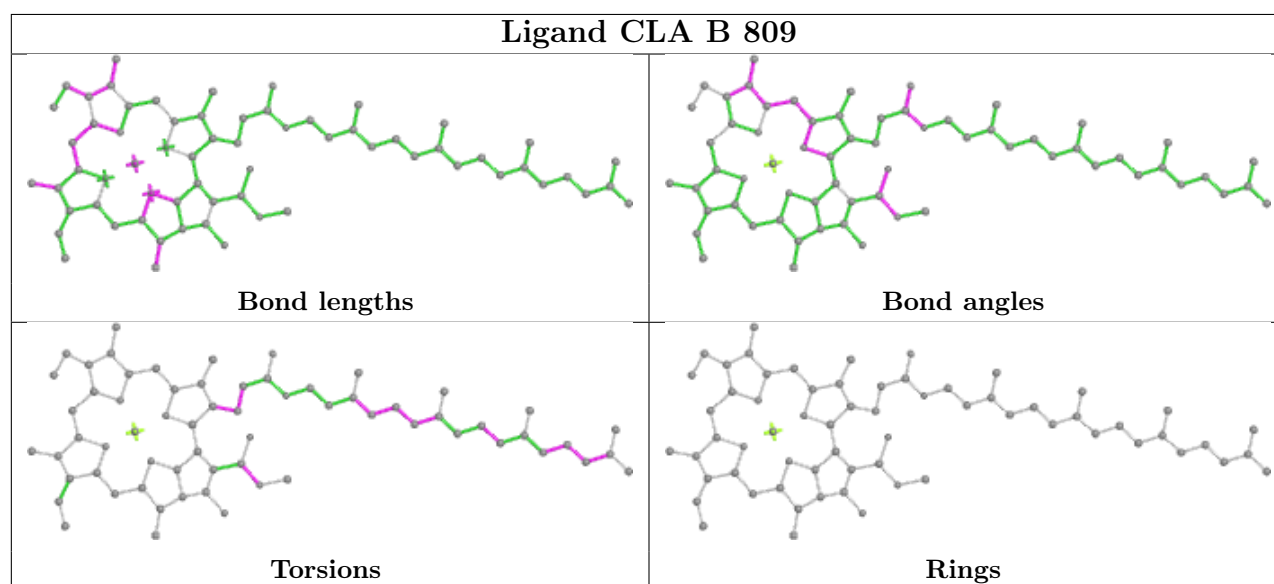
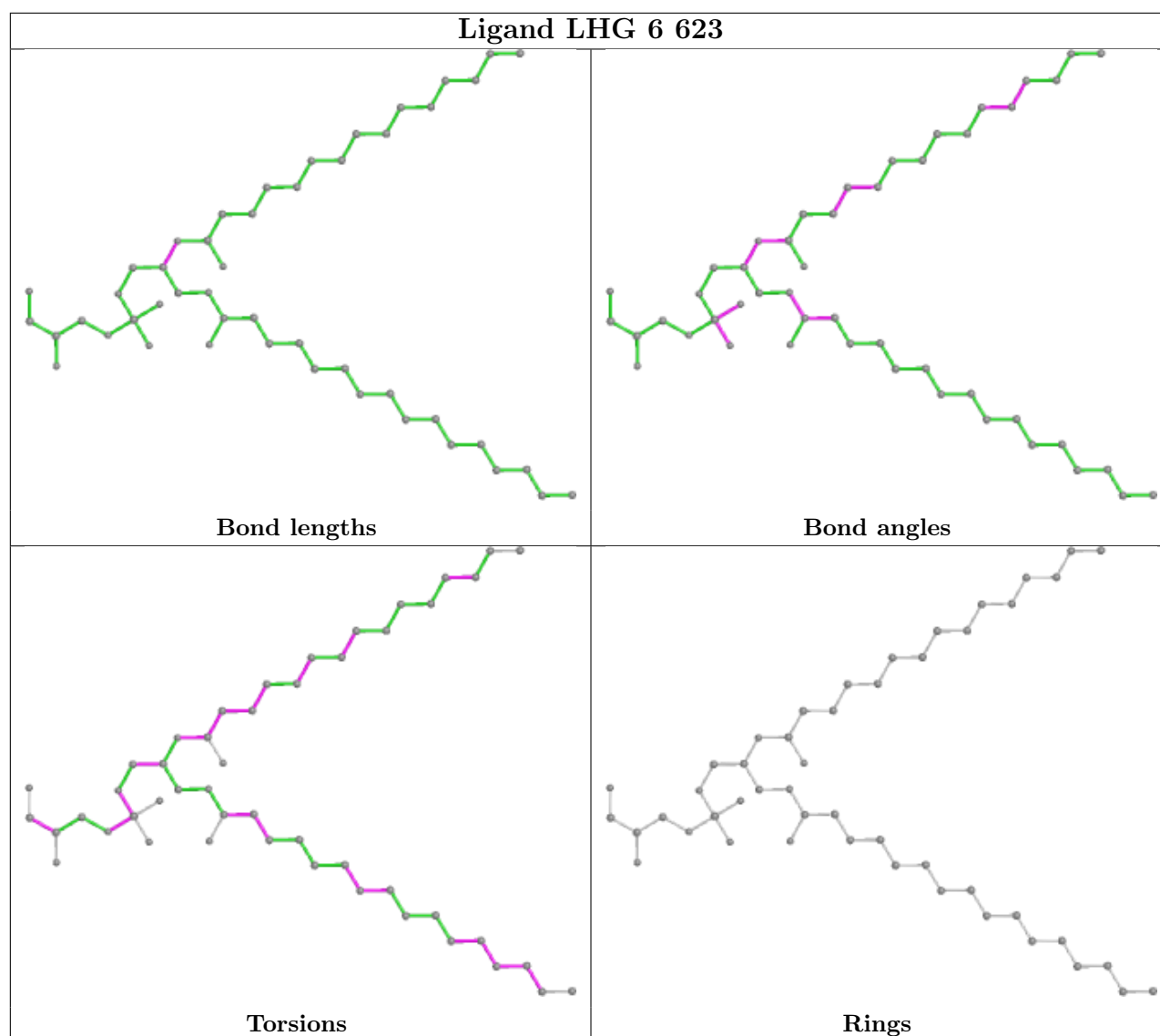
Ligand CLA 4 608**Ligand BCR G 205**

Ligand CLA 1 608

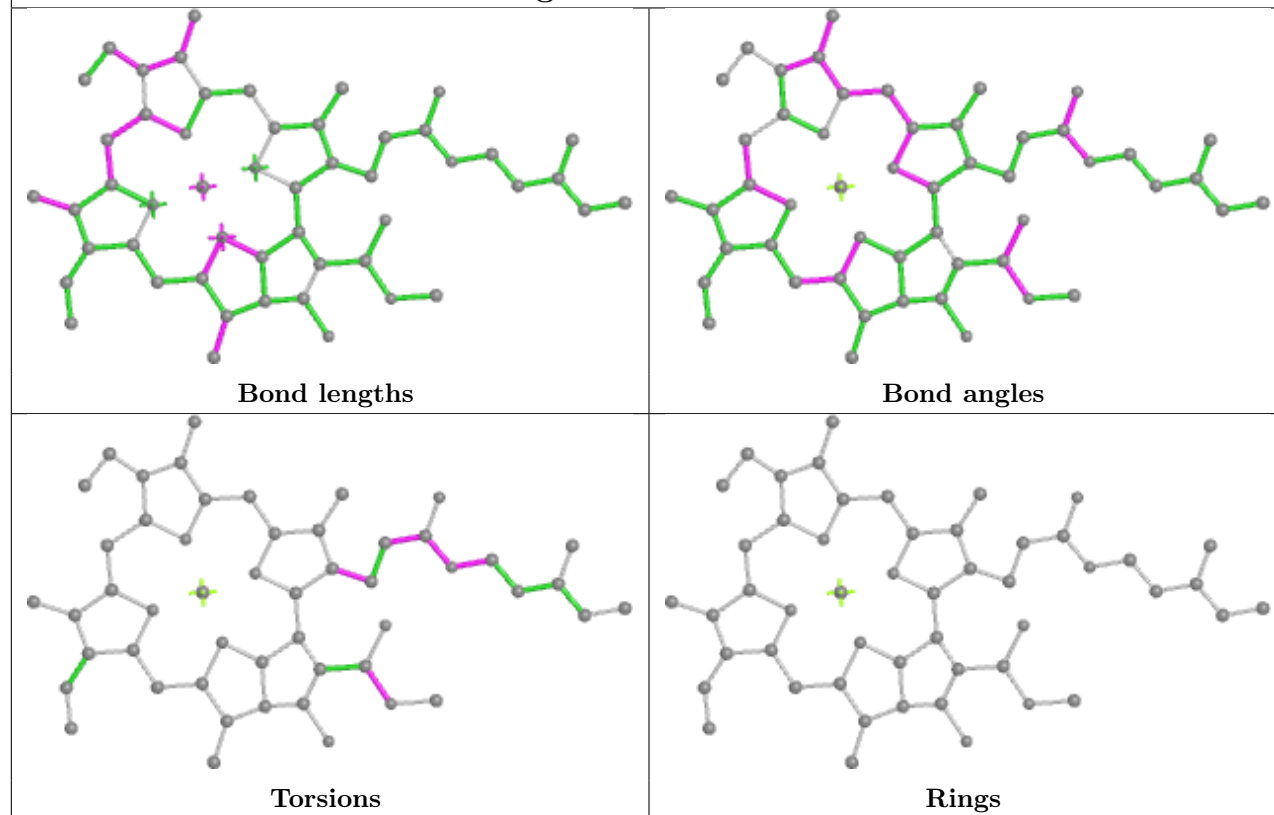


Ligand CLA 2 609

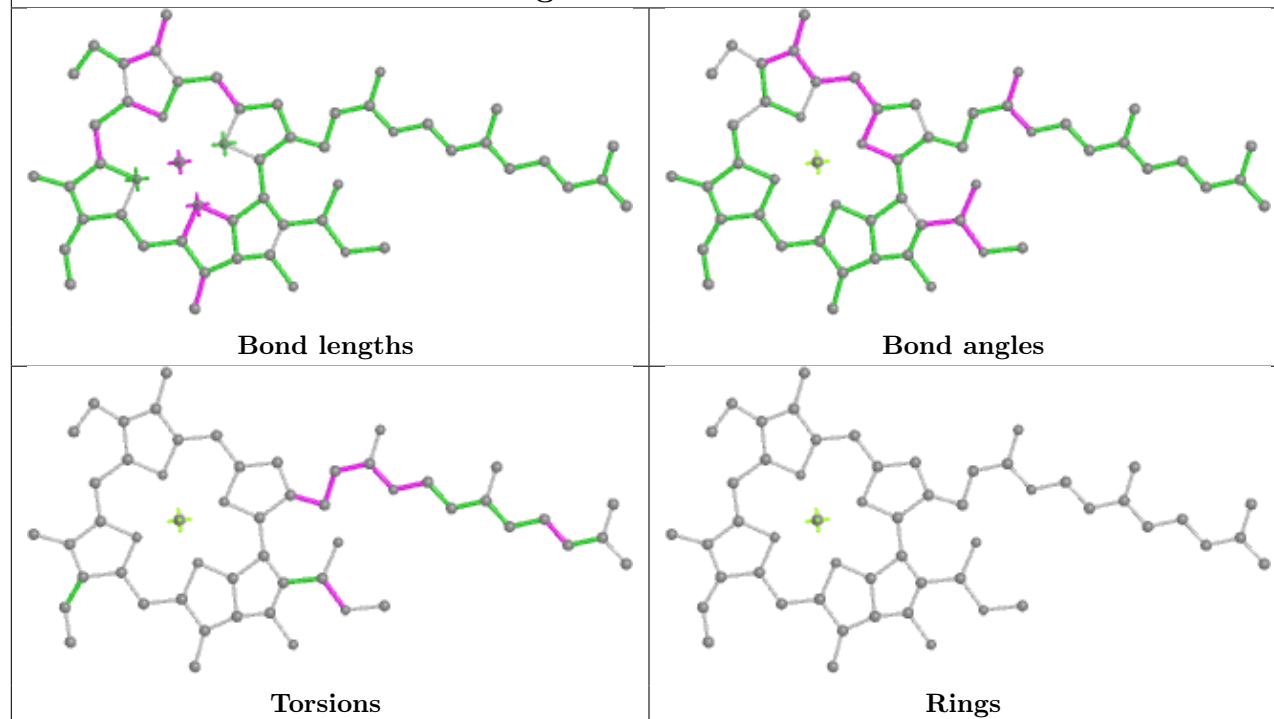


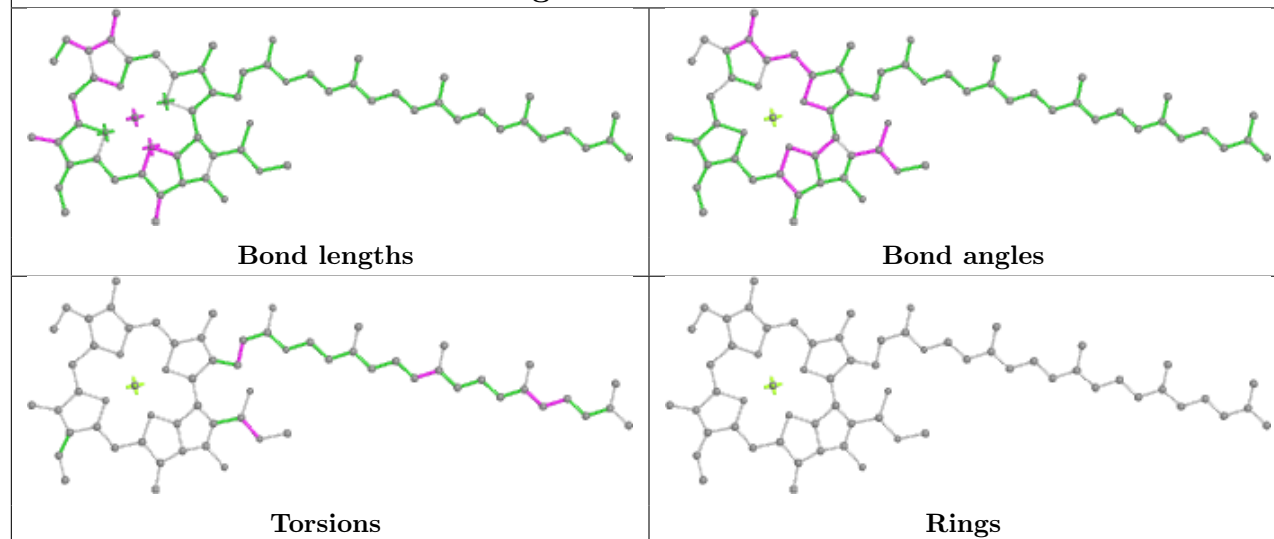
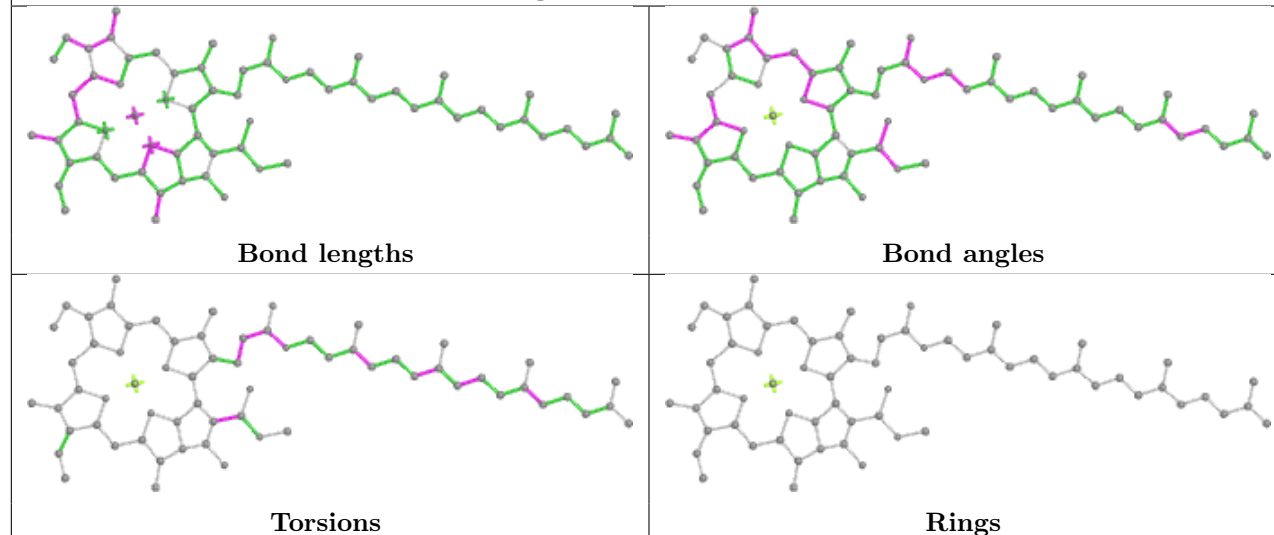
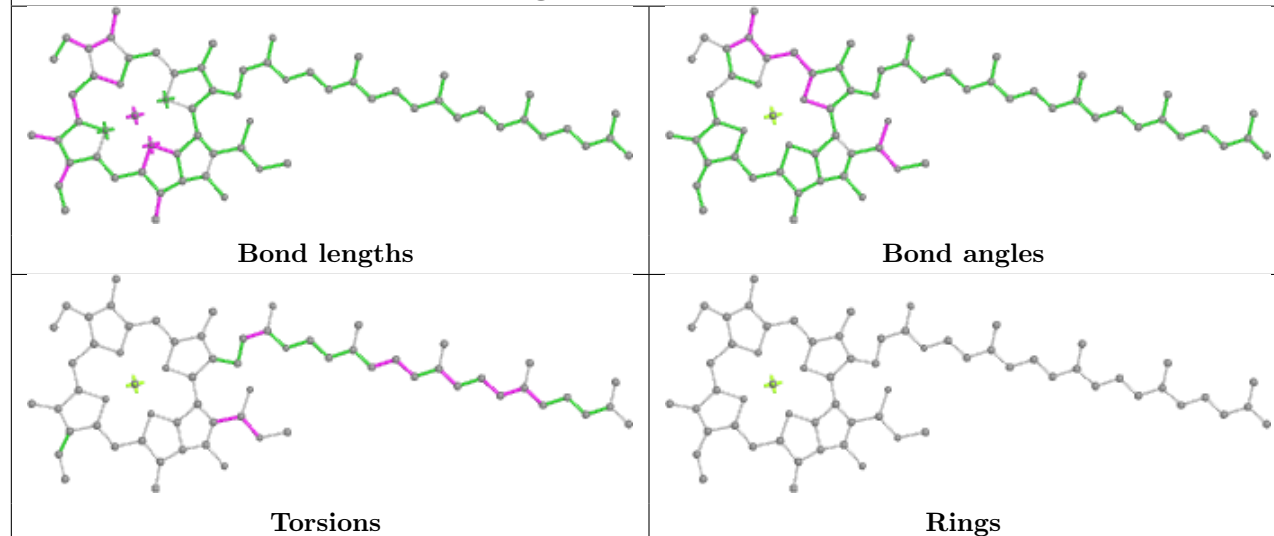


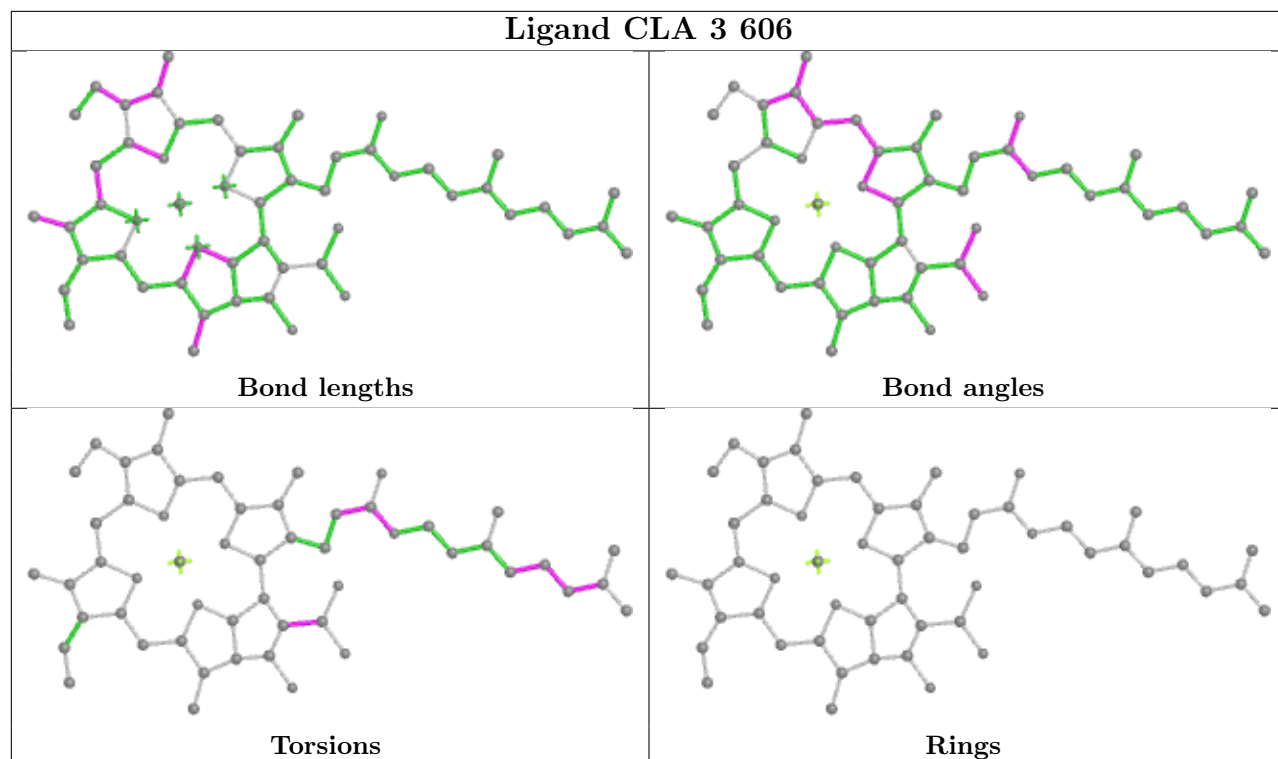
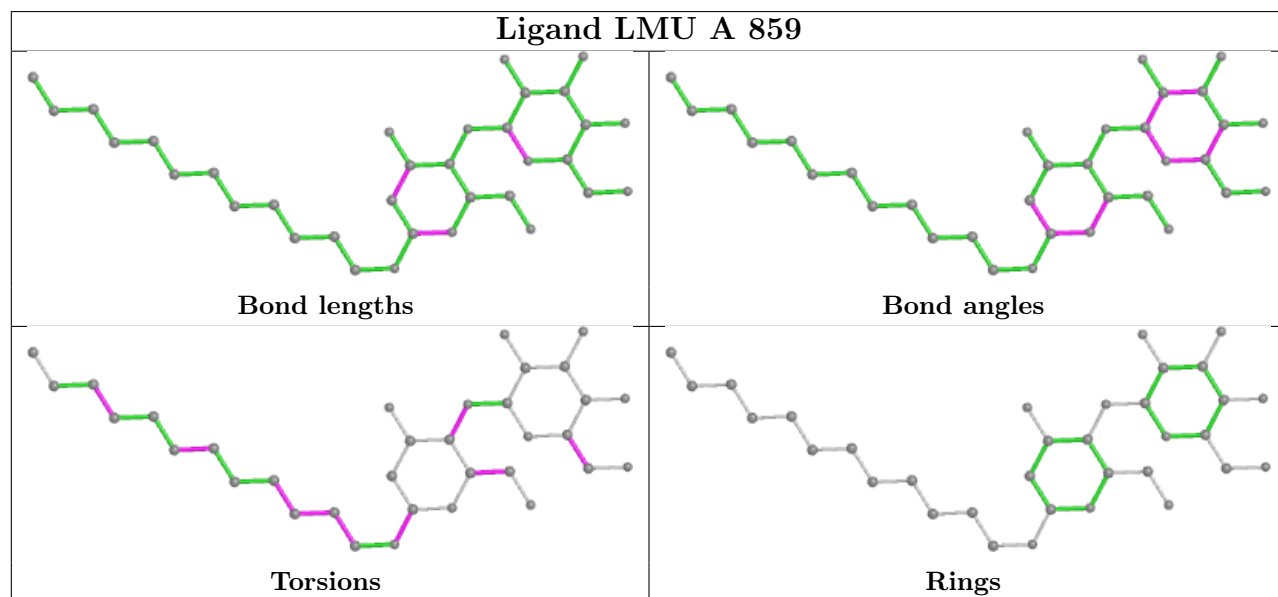
Ligand CLA 6 608

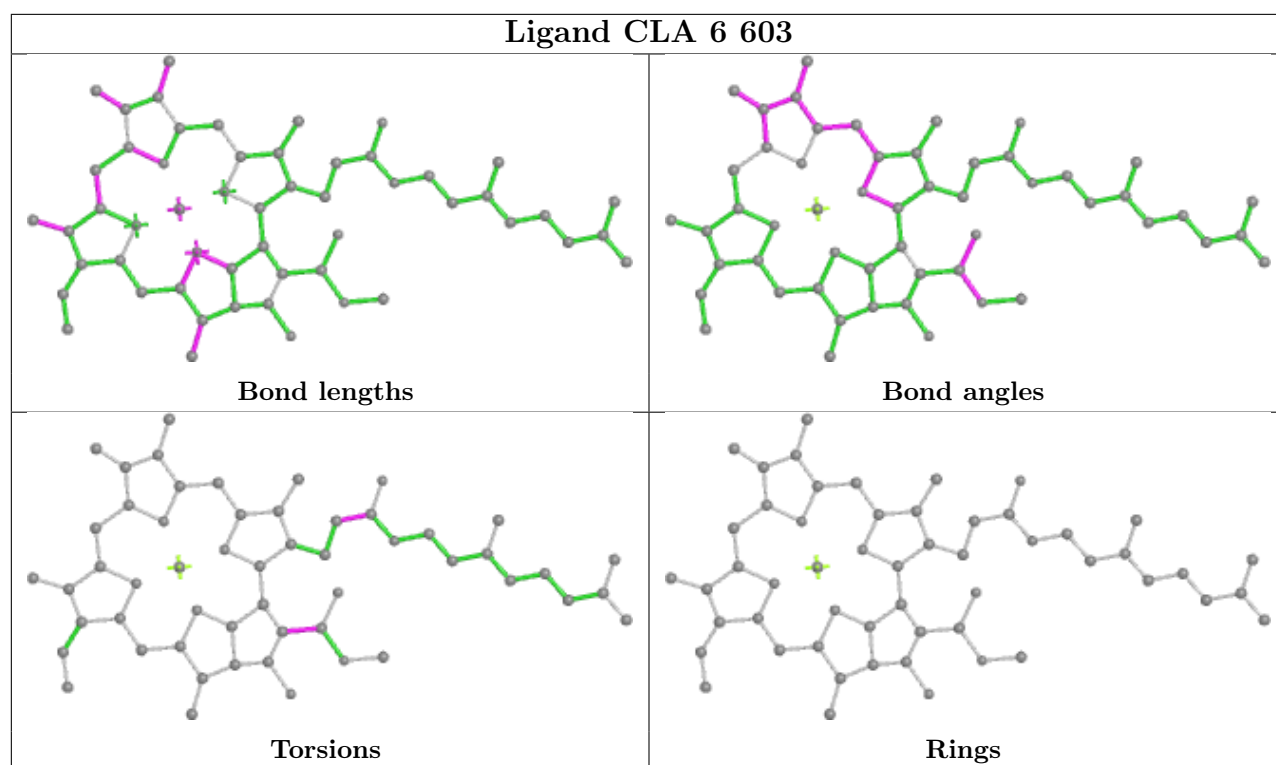


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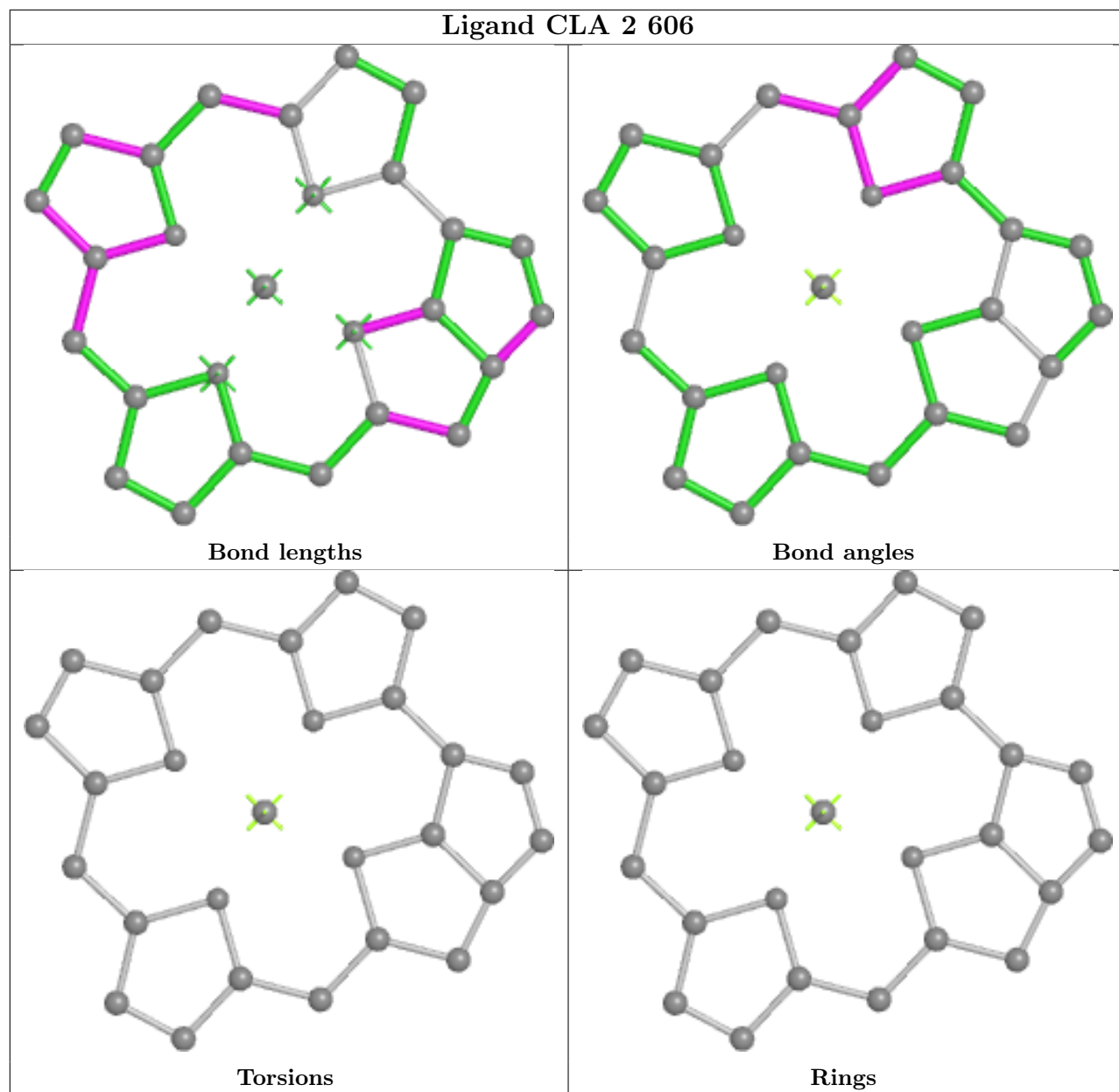


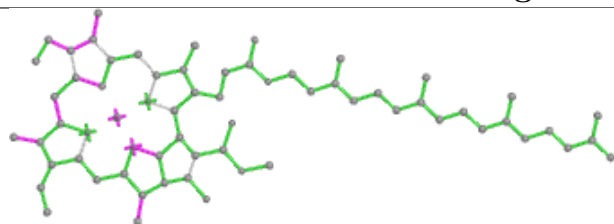
Ligand CLA B 829**Ligand CLA A 830****Ligand CLA B 806**

Ligand CLA 3 606**Ligand LMU A 859**

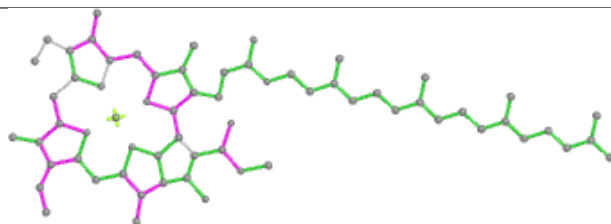


Ligand CLA 2 606

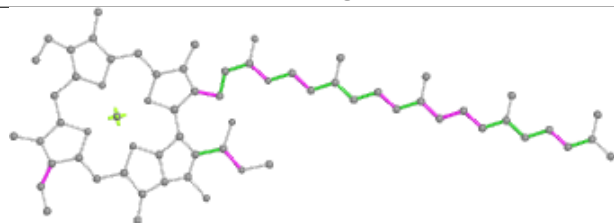


Ligand CLA B 803

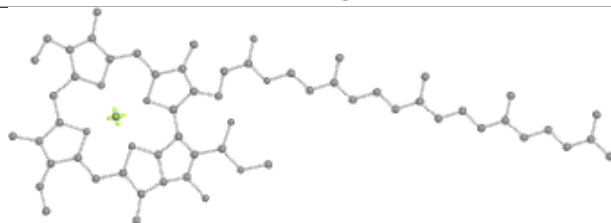
Bond lengths



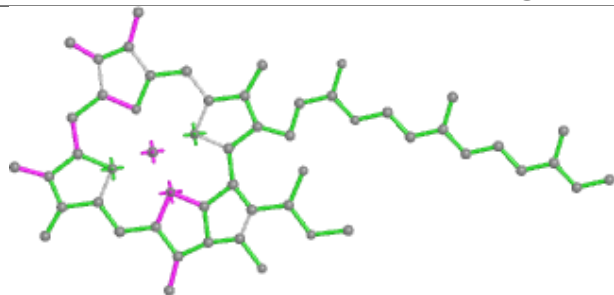
Bond angles



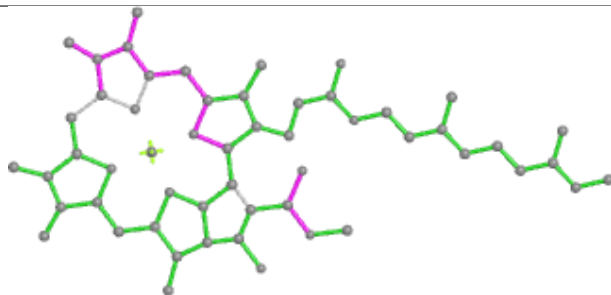
Torsions



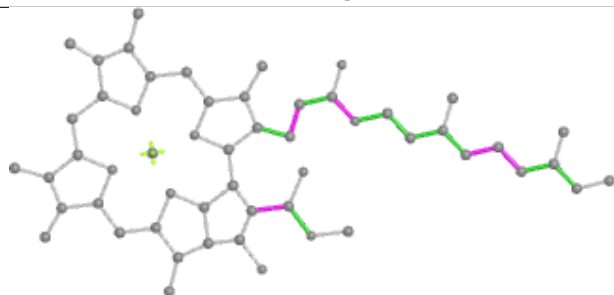
Rings

Ligand CLA 4 604

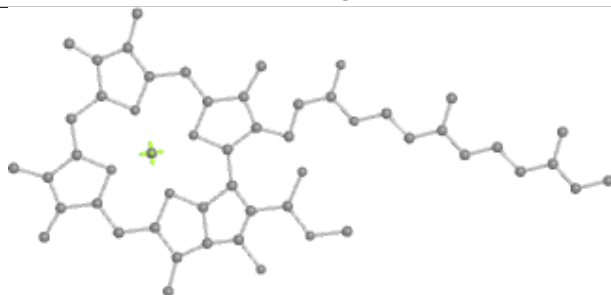
Bond lengths



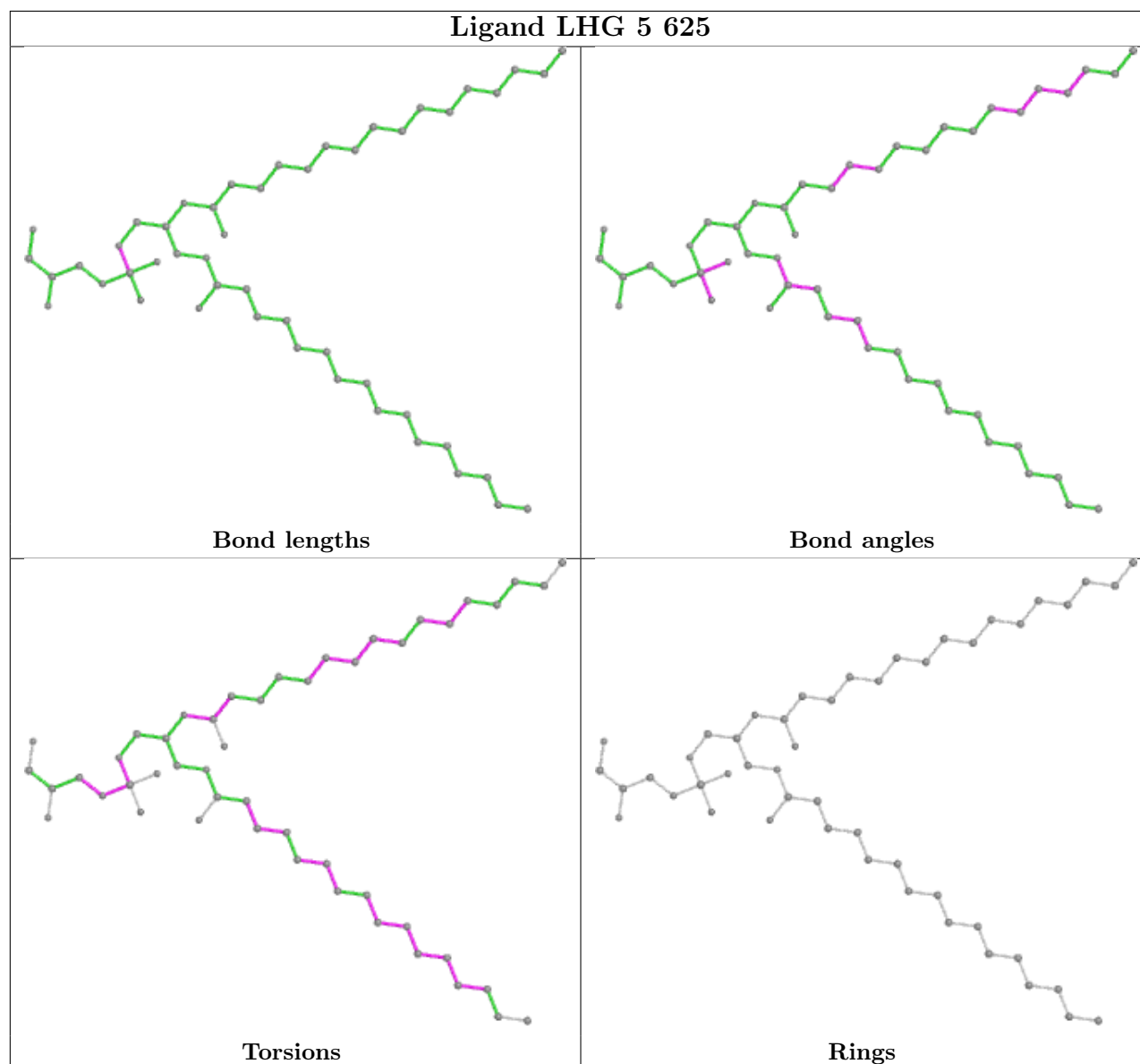
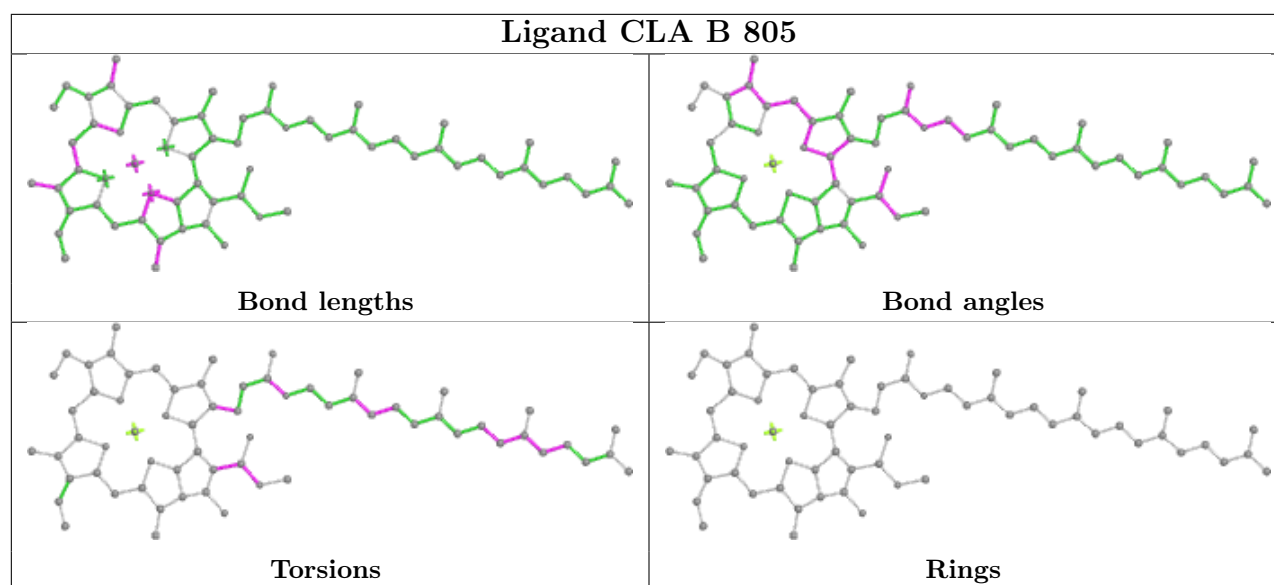
Bond angles

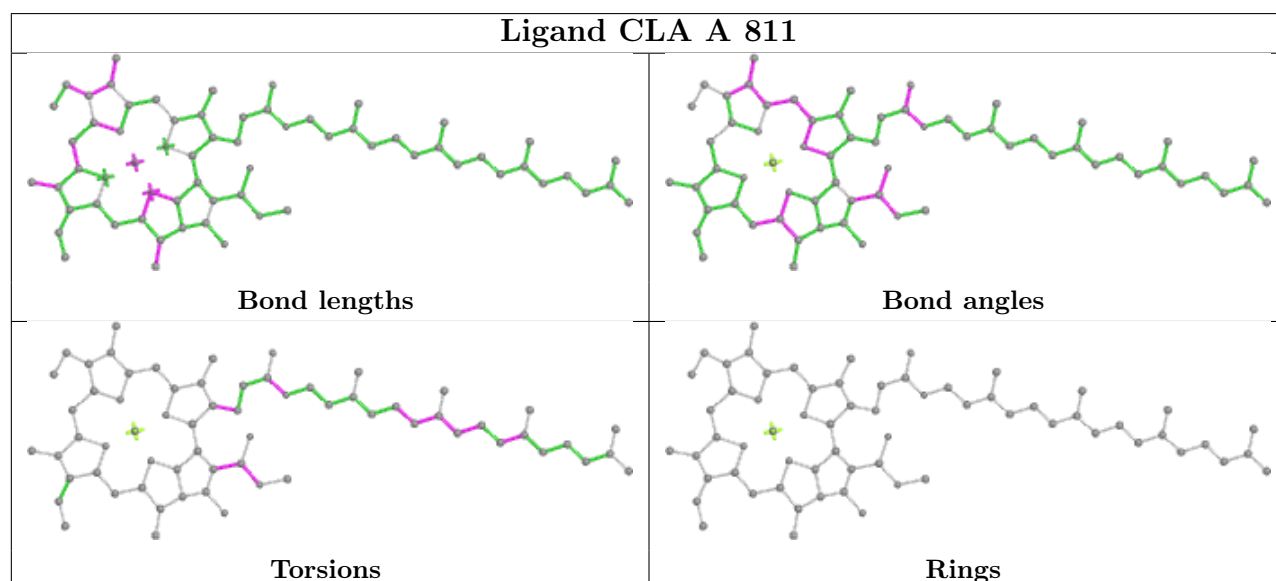
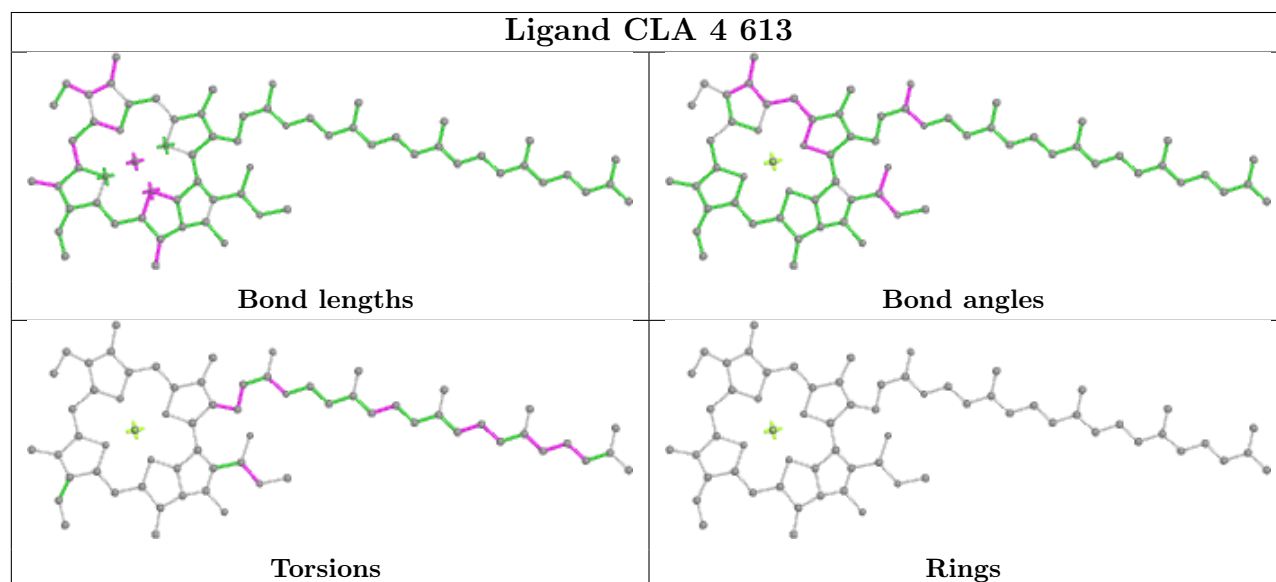
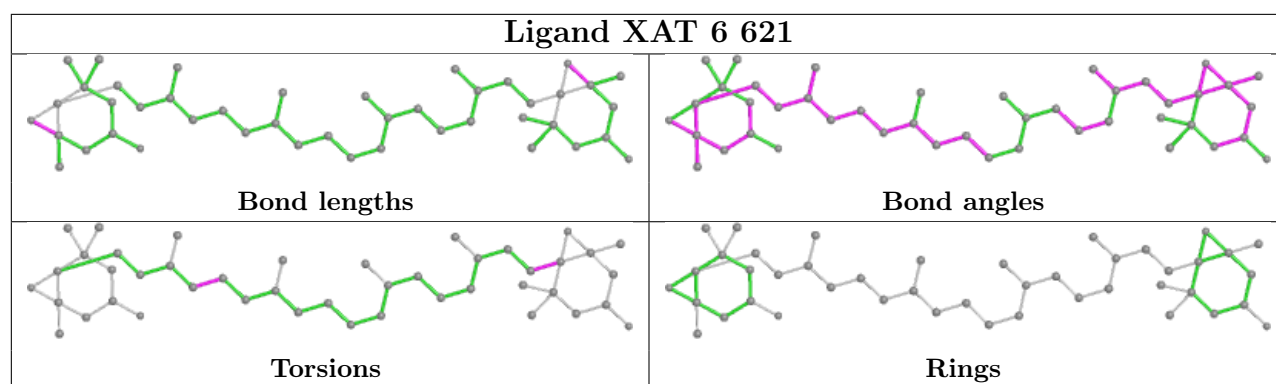


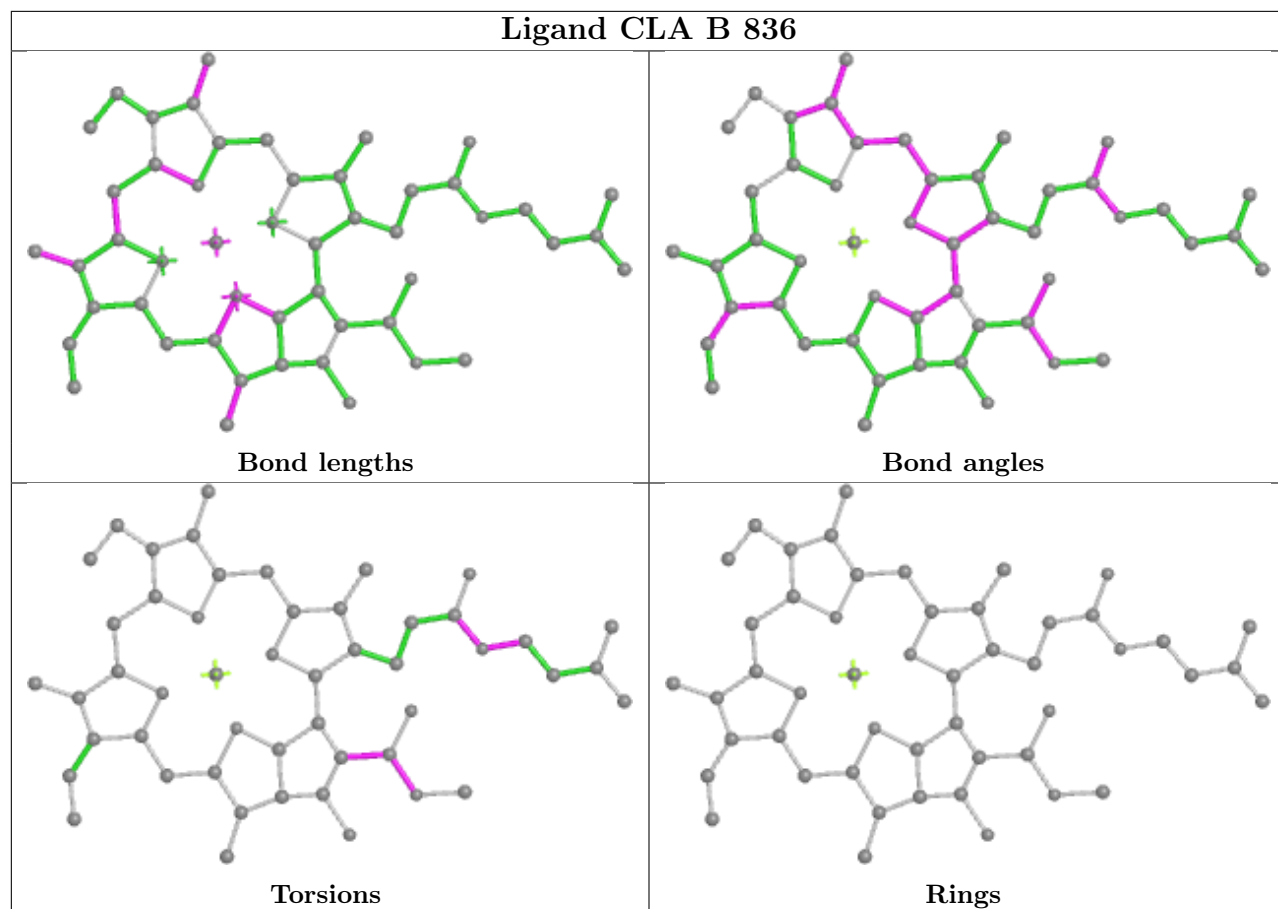
Torsions



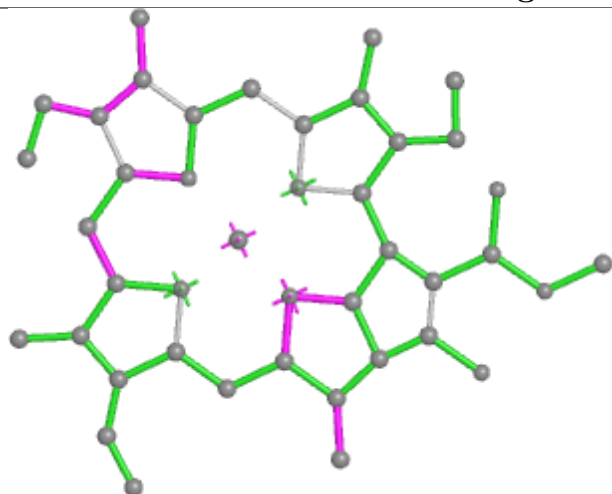
Rings



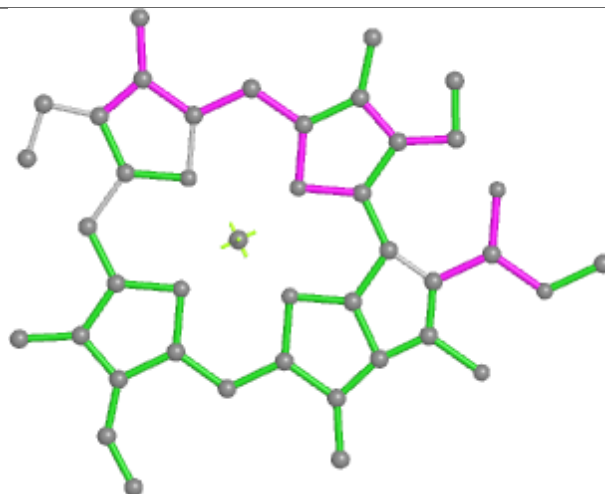




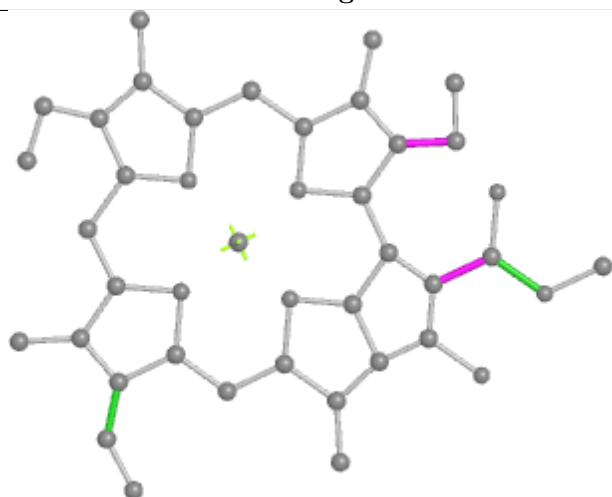
Ligand CLA 5 611



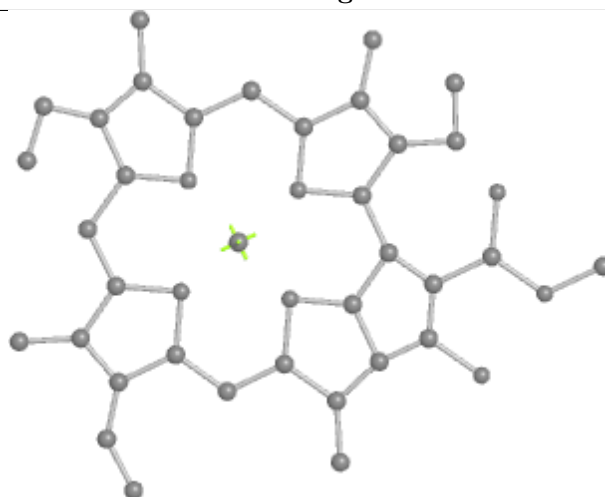
Bond lengths



Bond angles

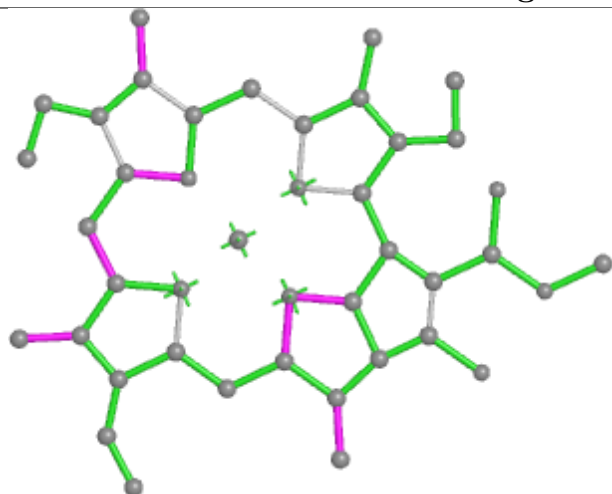


Torsions

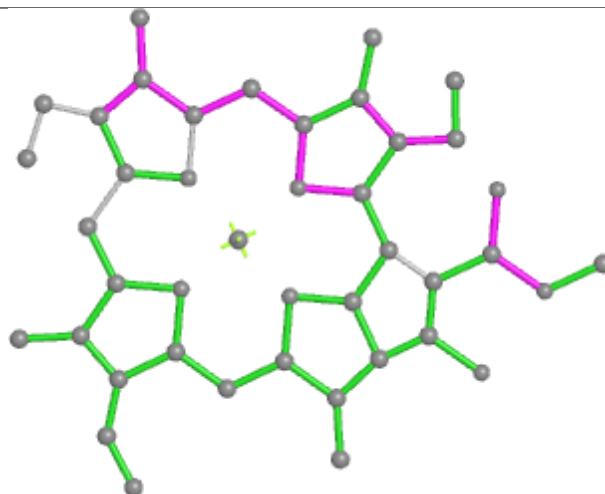


Rings

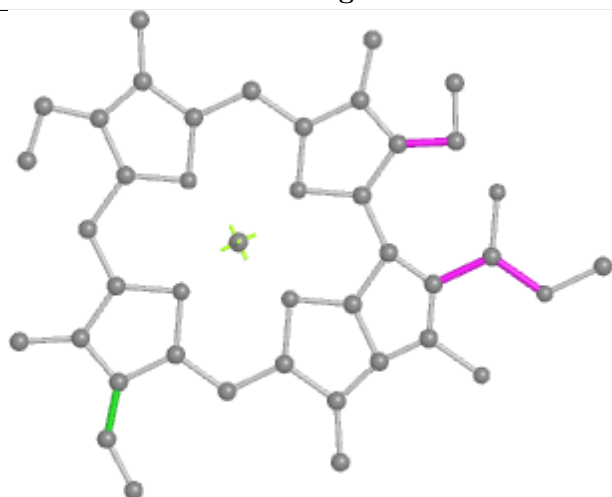
Ligand CLA 4 611



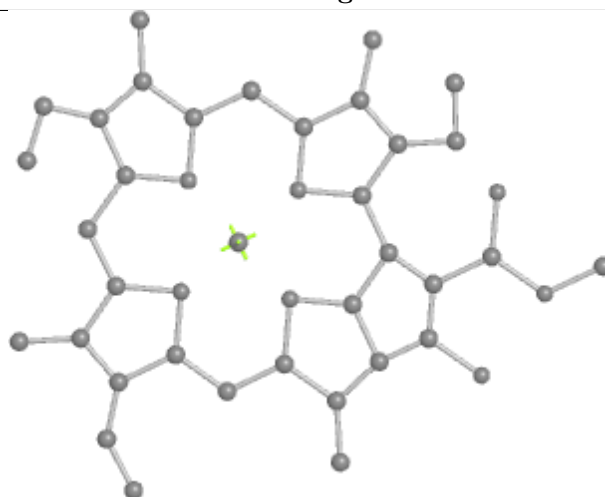
Bond lengths



Bond angles

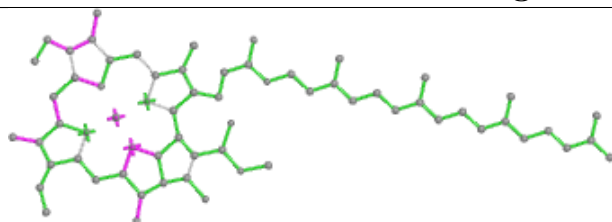


Torsions

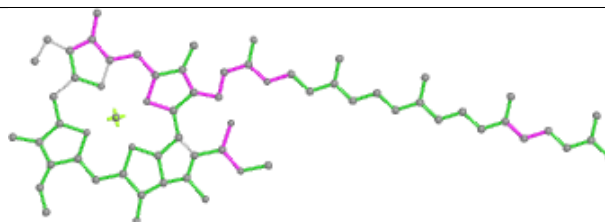


Rings

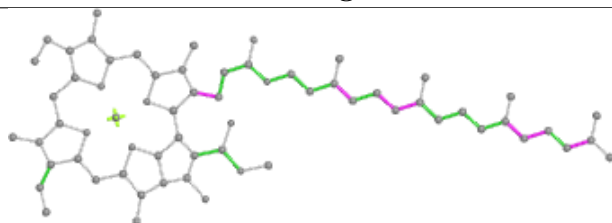
Ligand CLA A 812



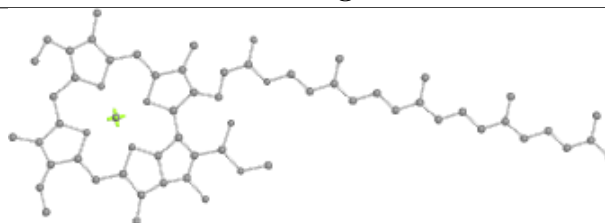
Bond lengths



Bond angles

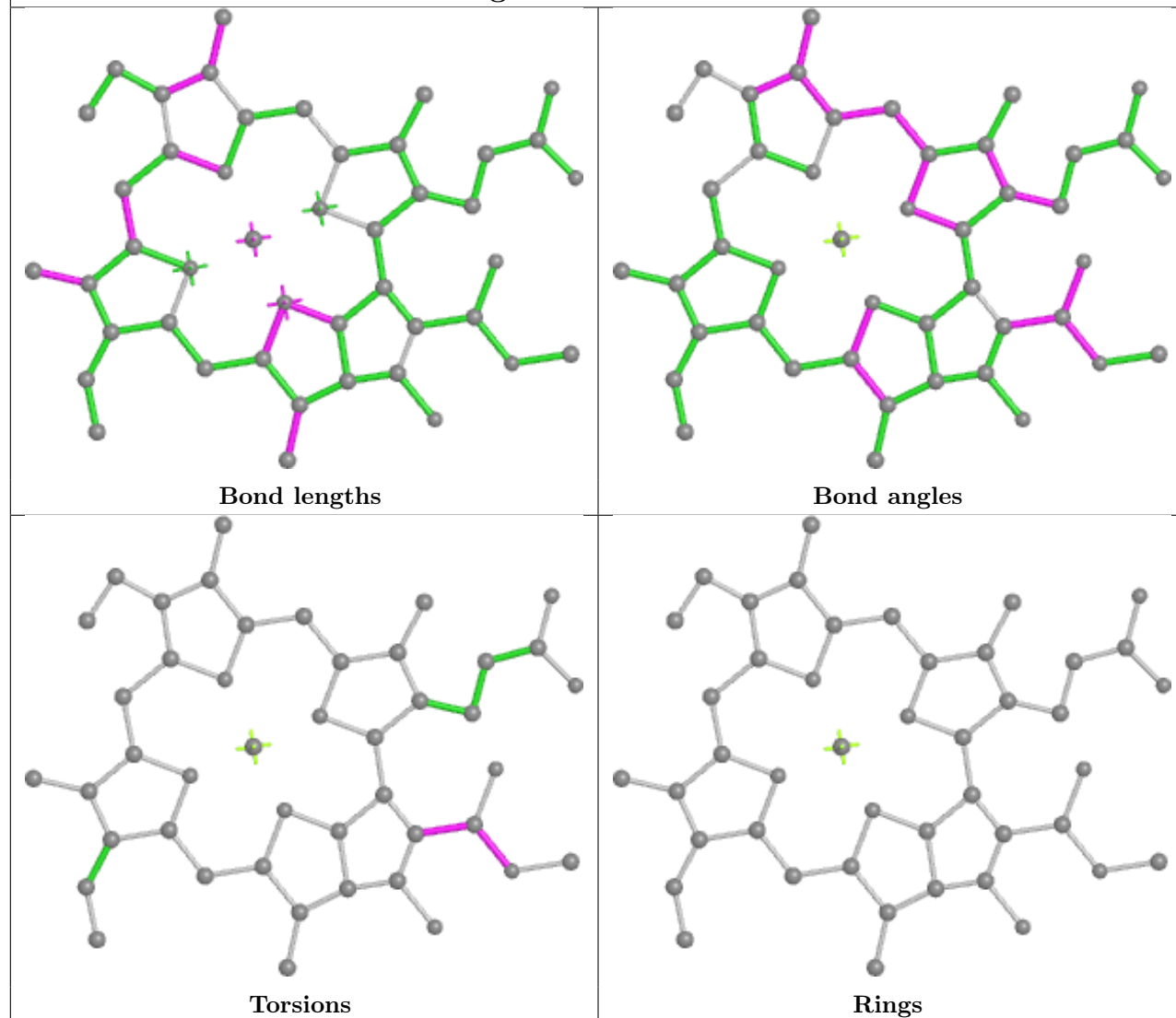


Torsions

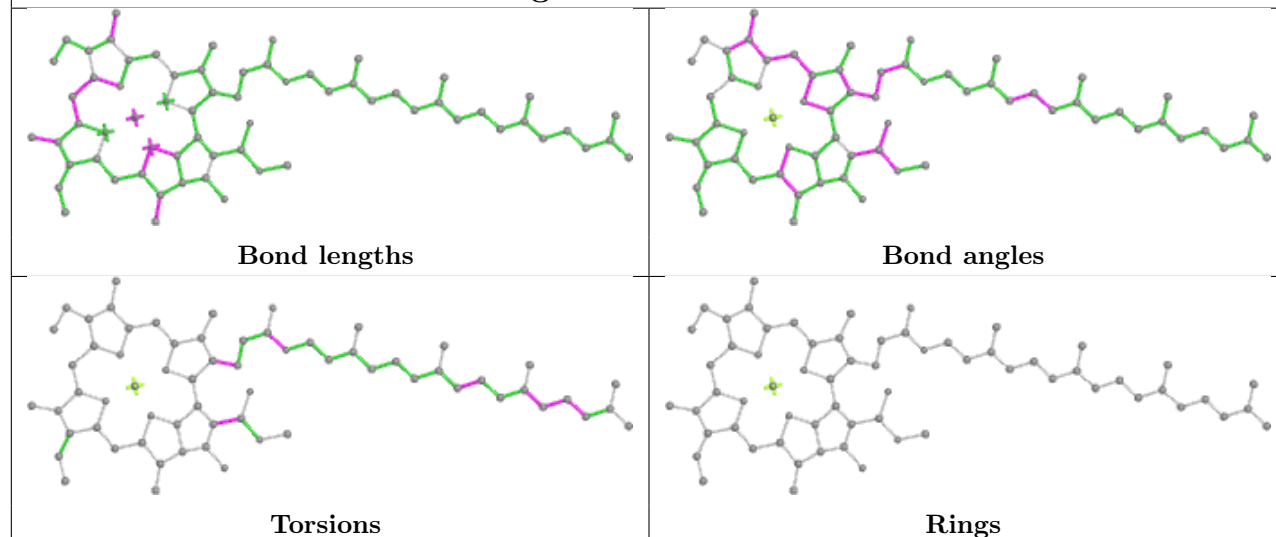


Rings

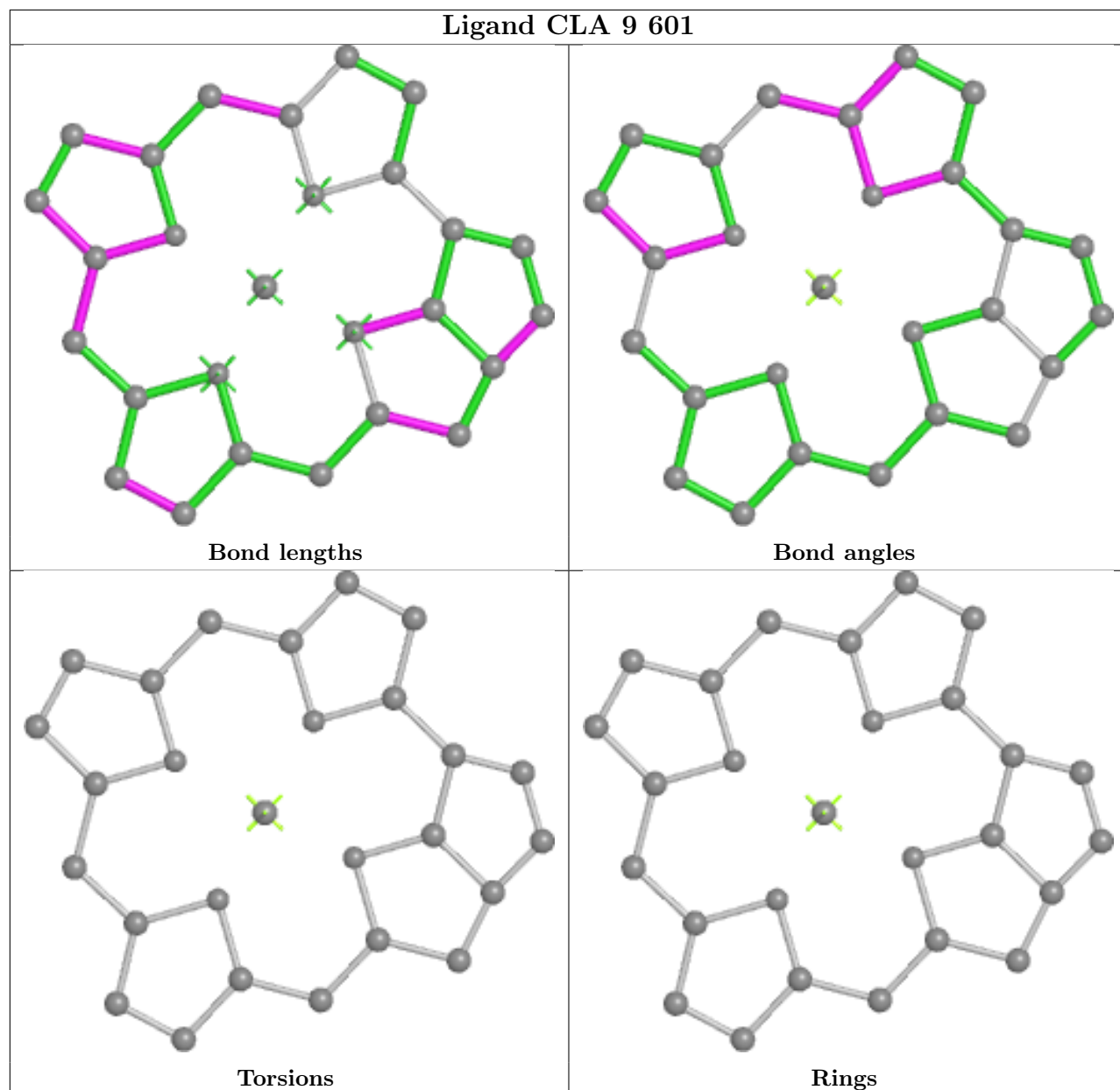
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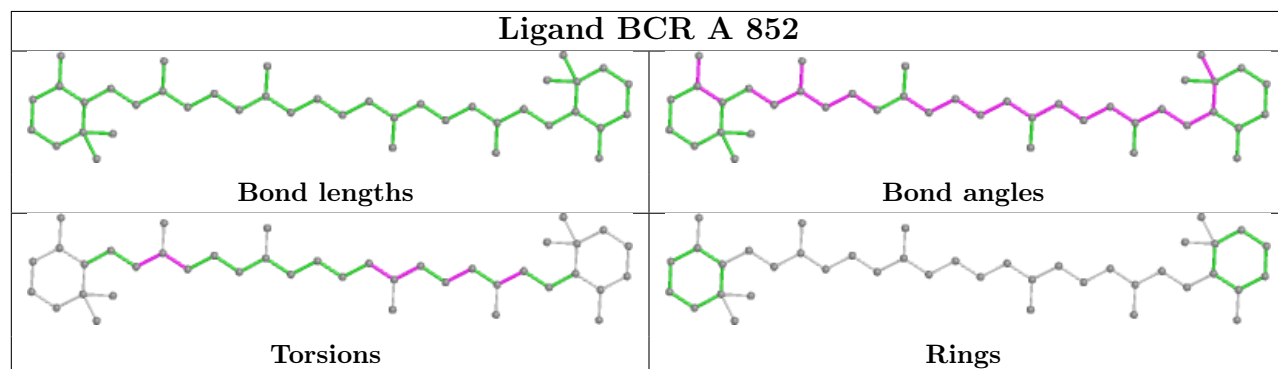
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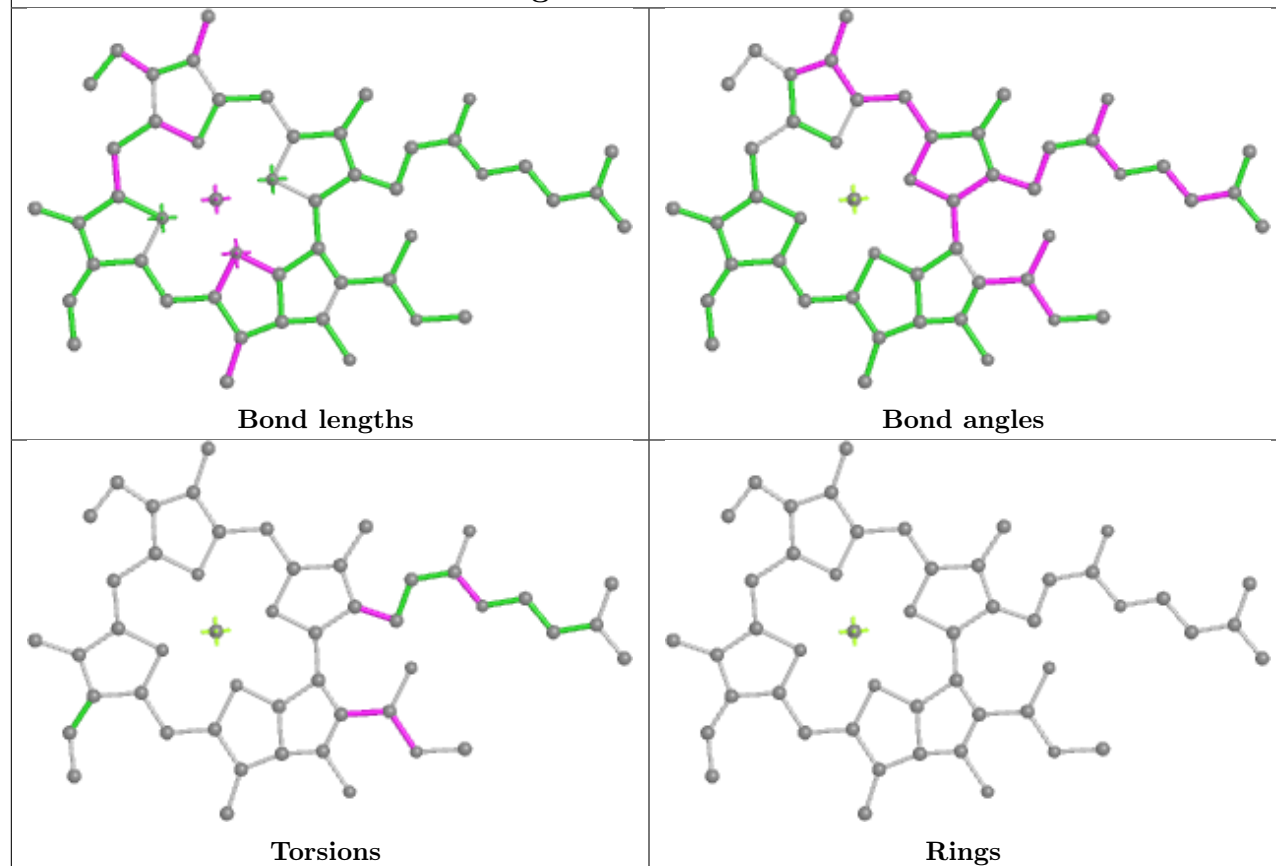
Ligand CLA 9 601



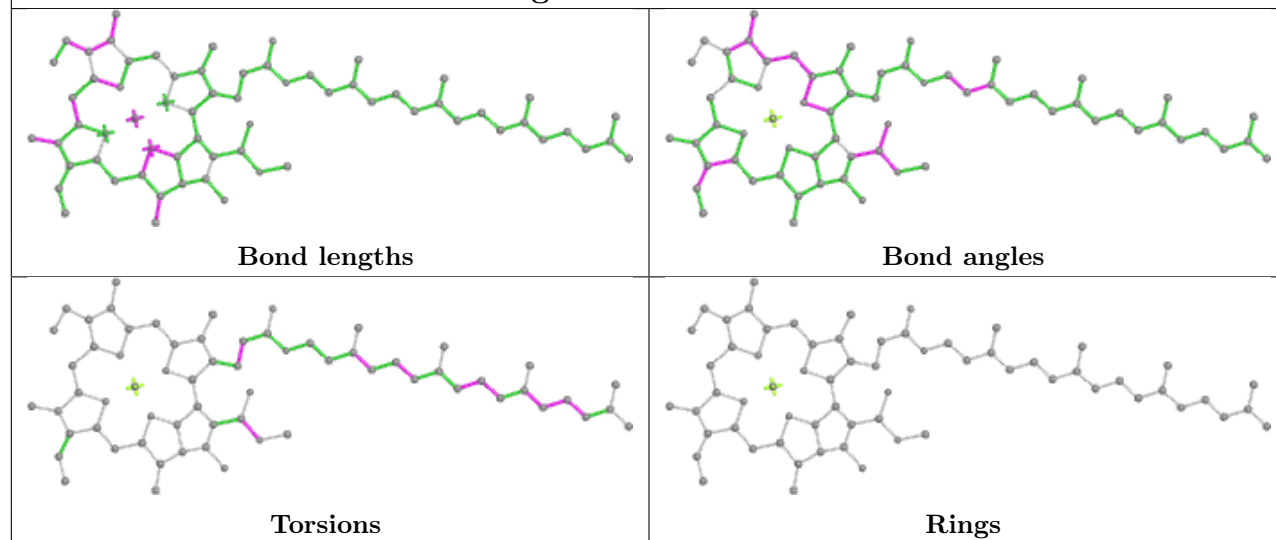
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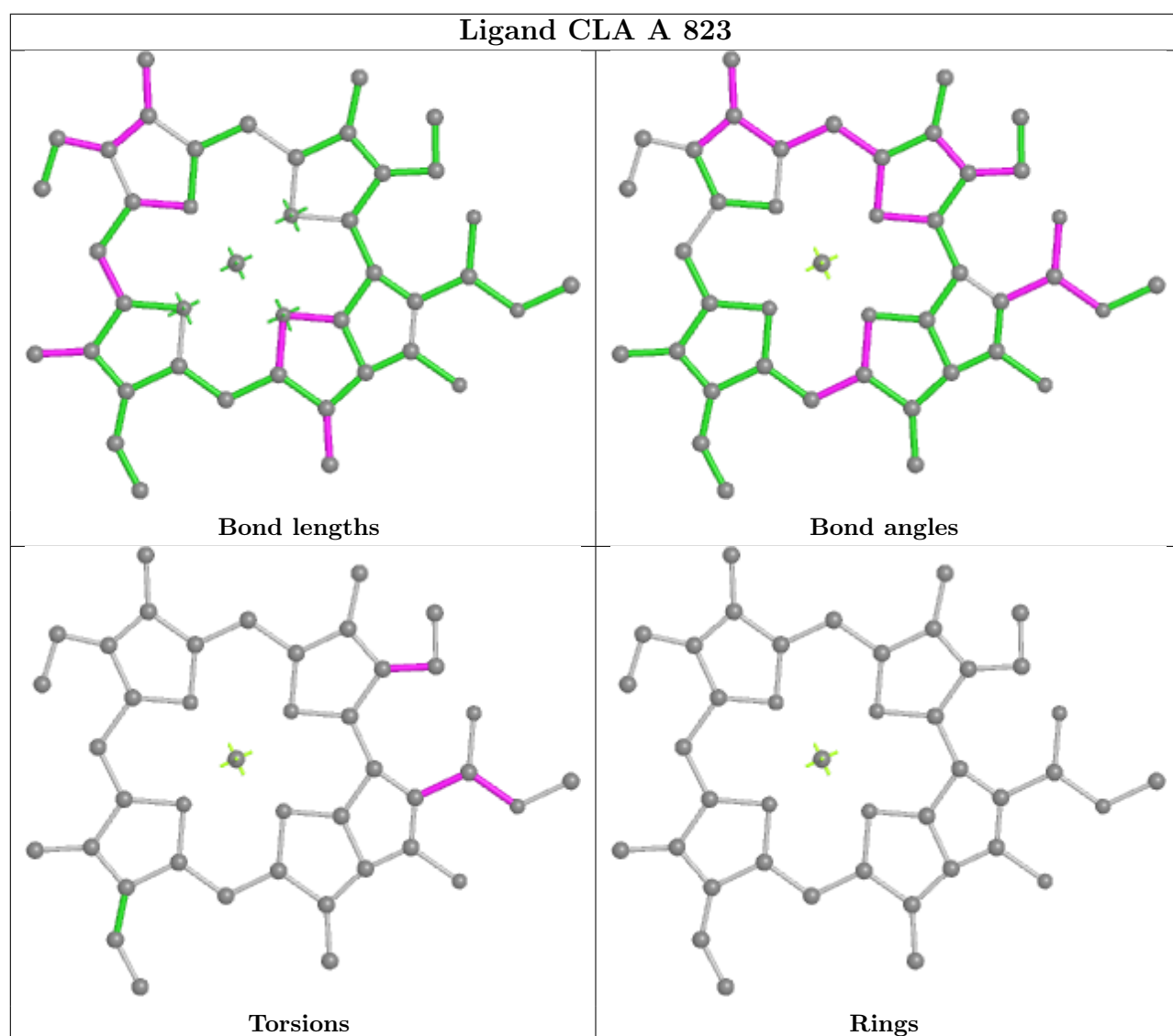
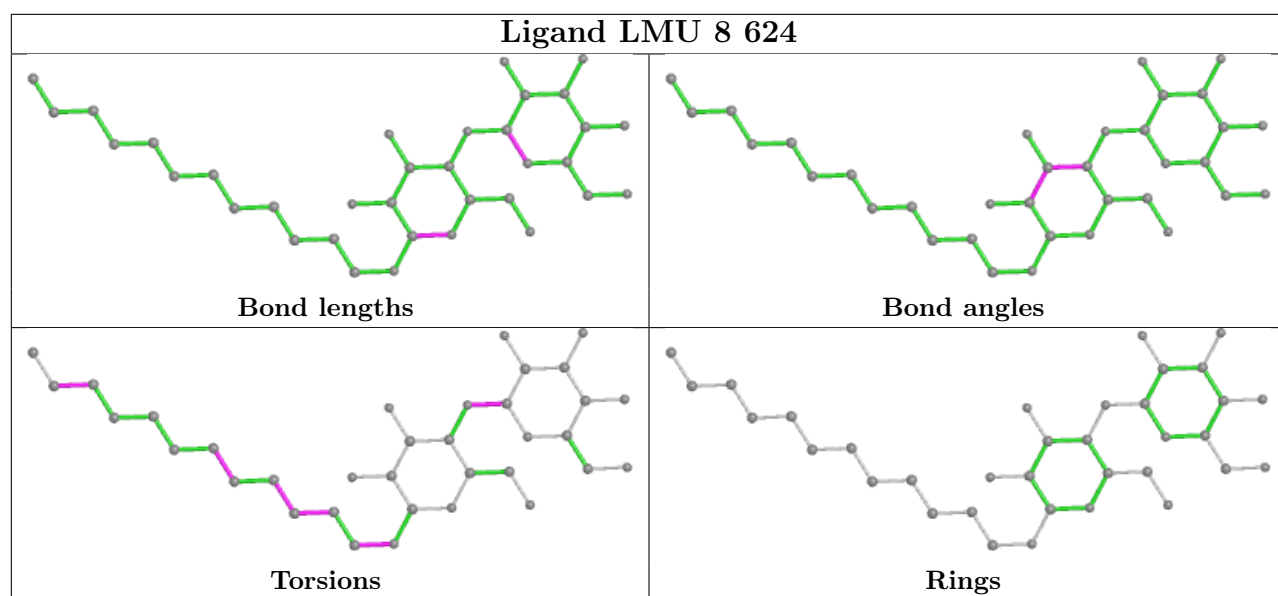


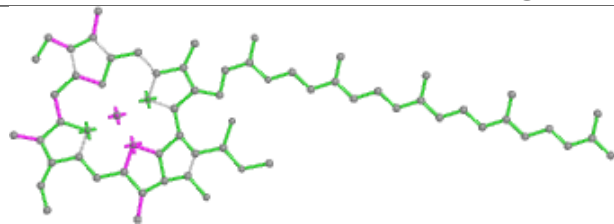
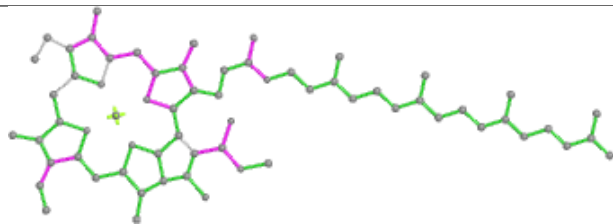
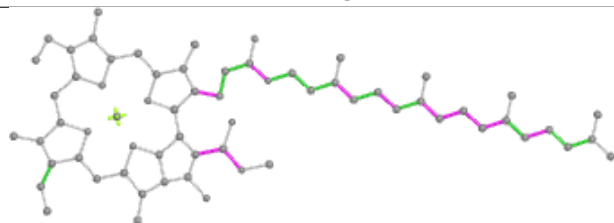
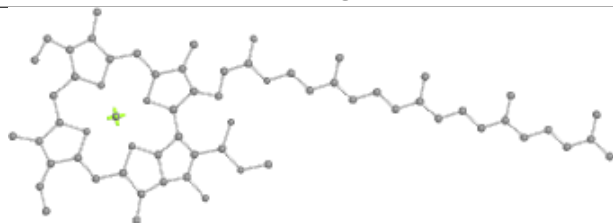
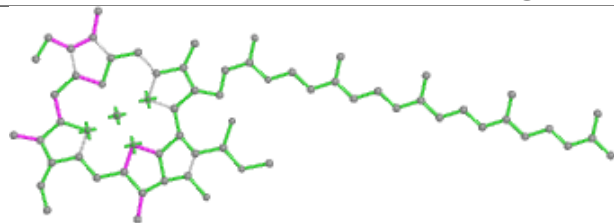
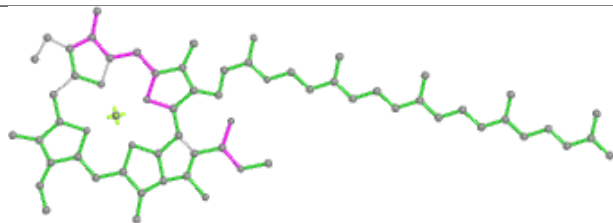
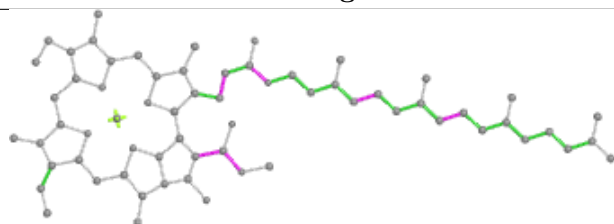
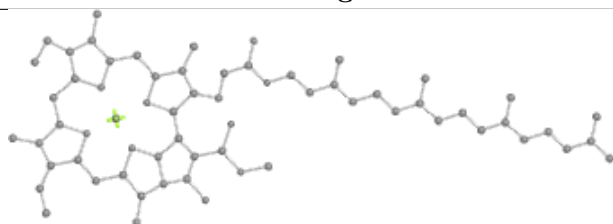
Ligand CLA A 838



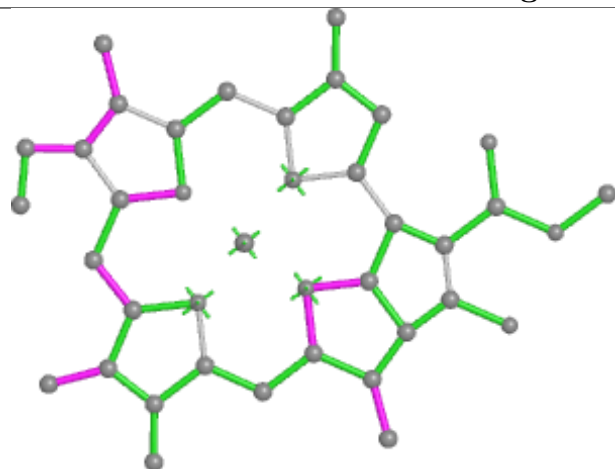
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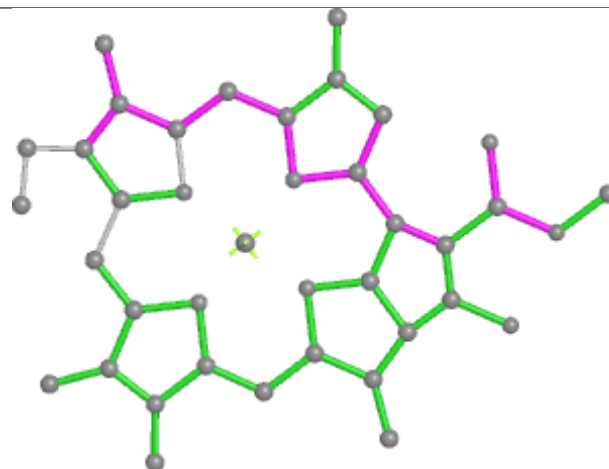


Ligand CLA 3 610**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 6 602****Bond lengths****Bond angles****Torsions****Rings**

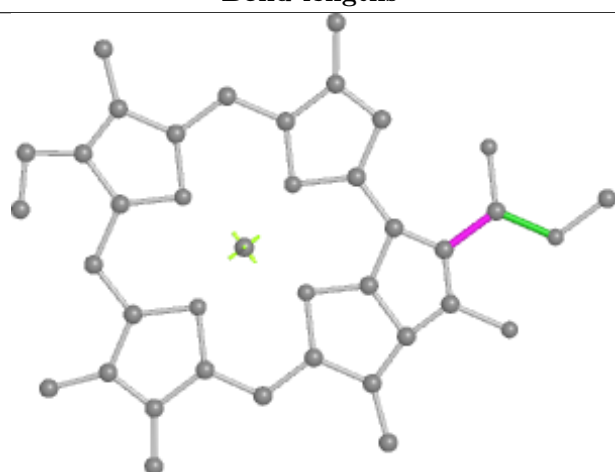
Ligand CLA 1 610



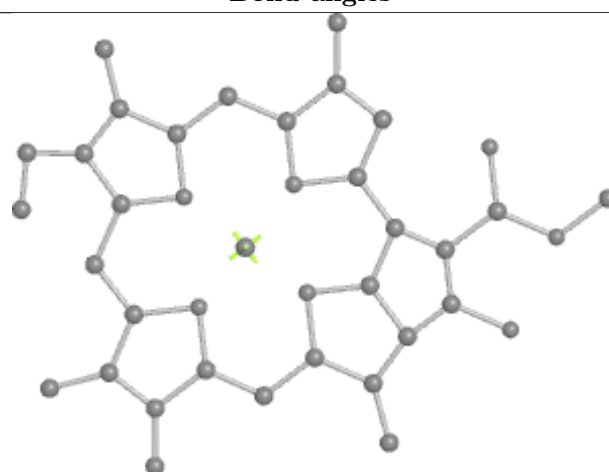
Bond lengths



Bond angles

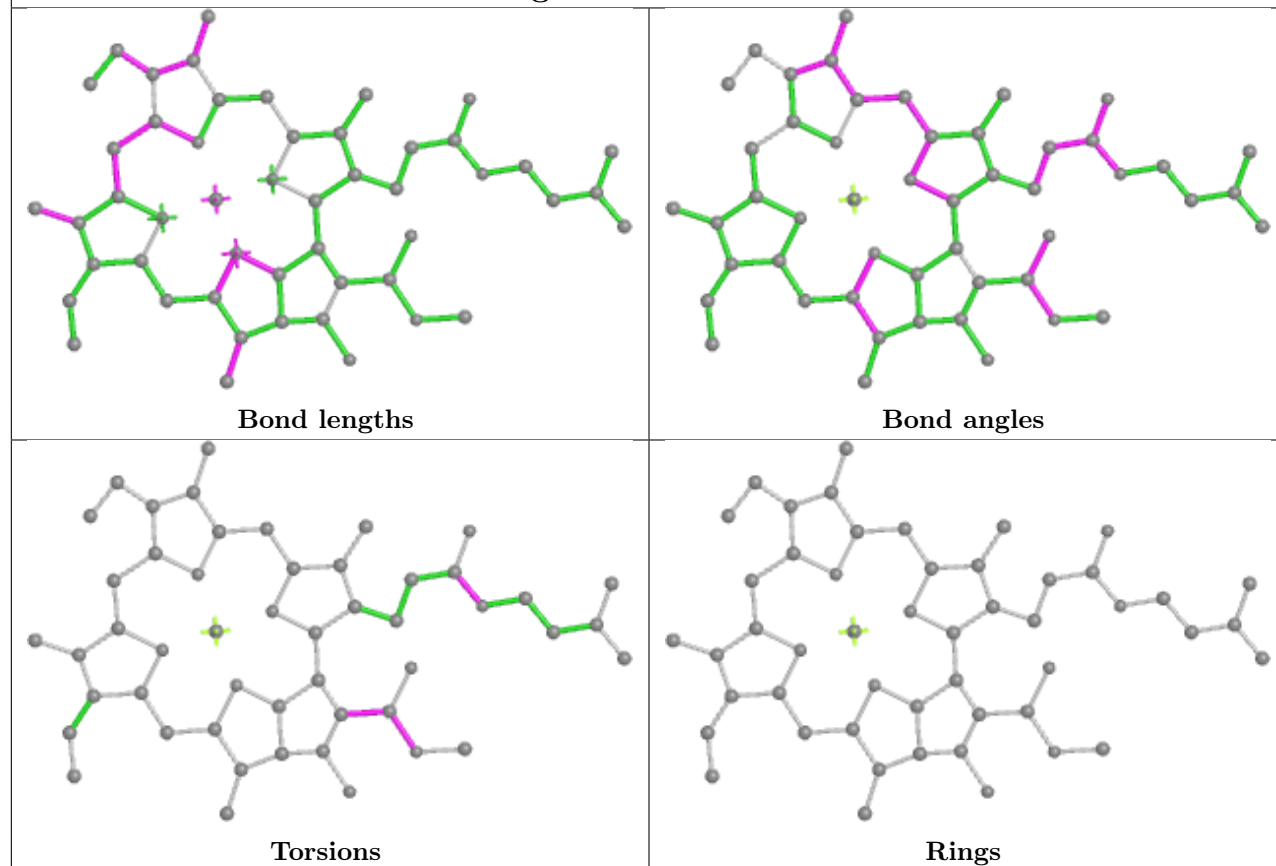


Torsions

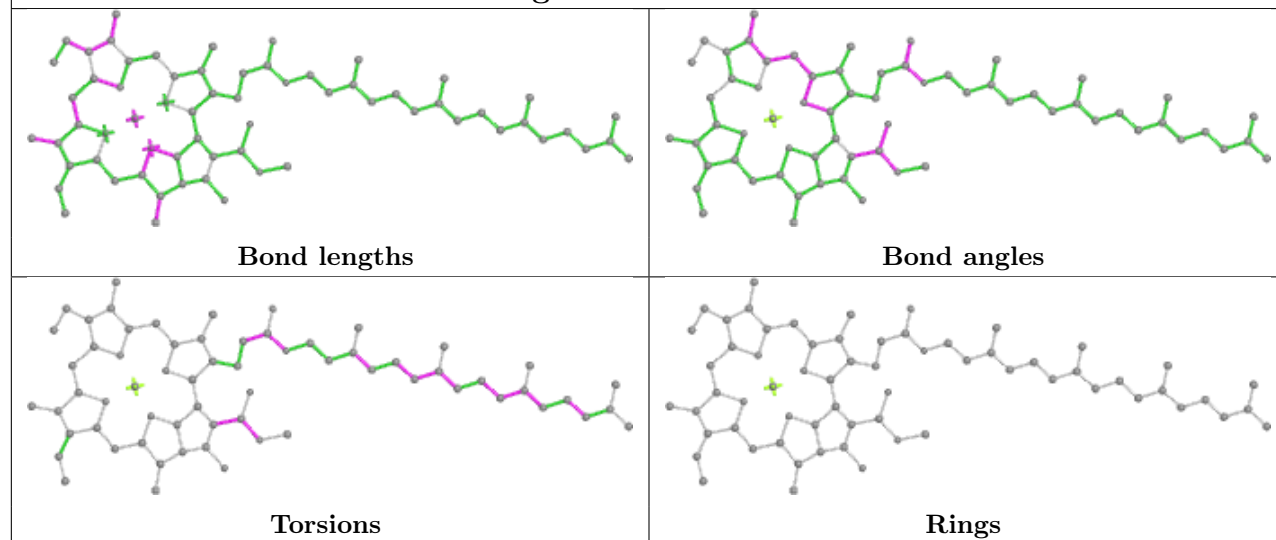


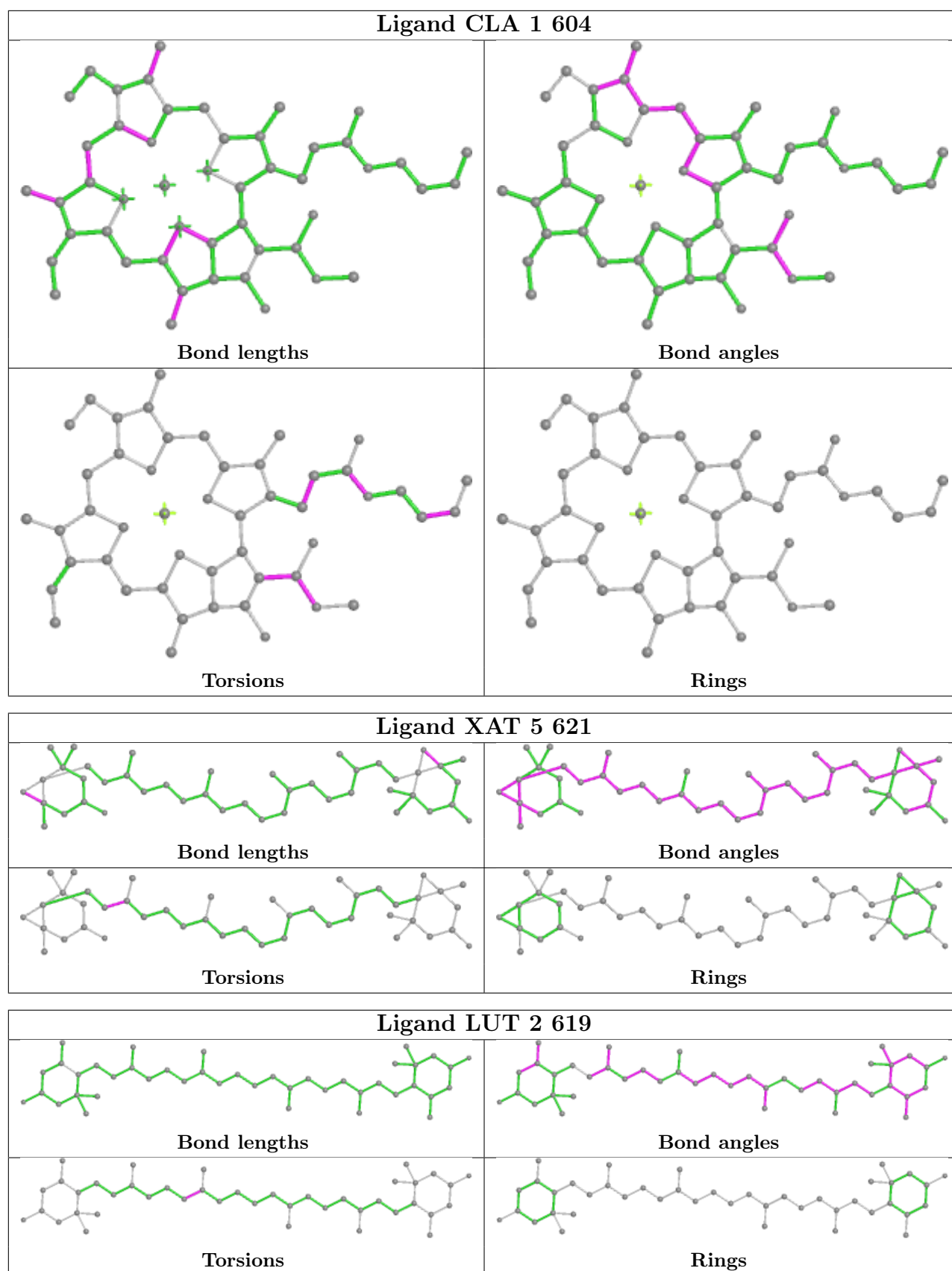
Rings

Ligand CLA A 832

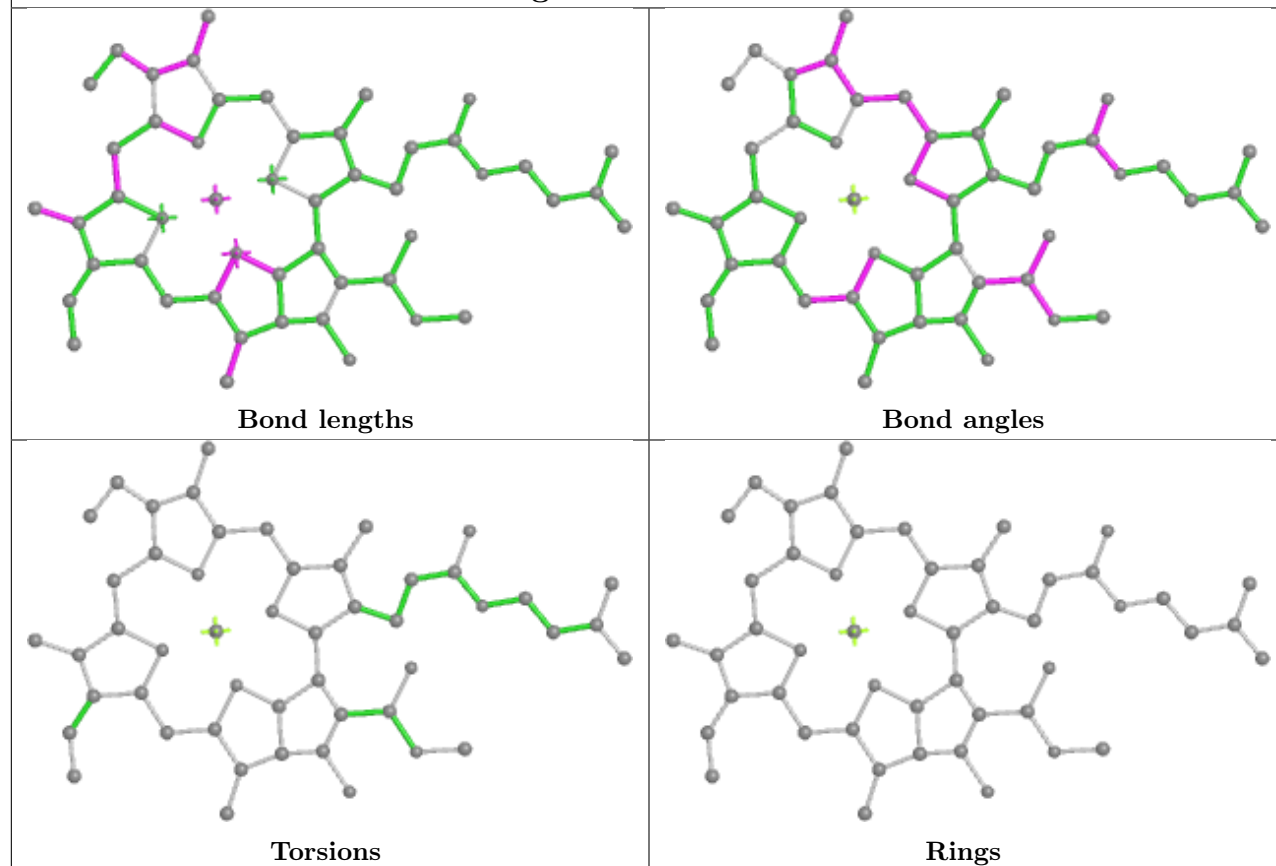


Ligand CLA B 802

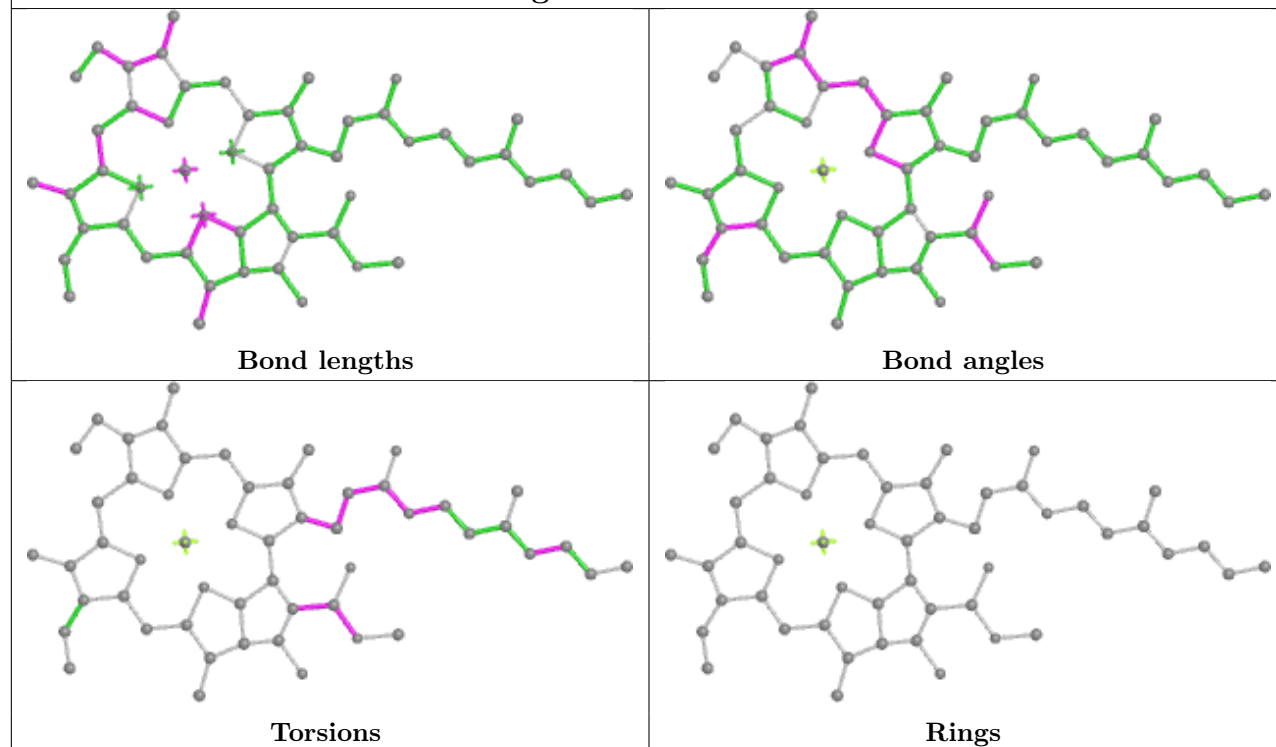




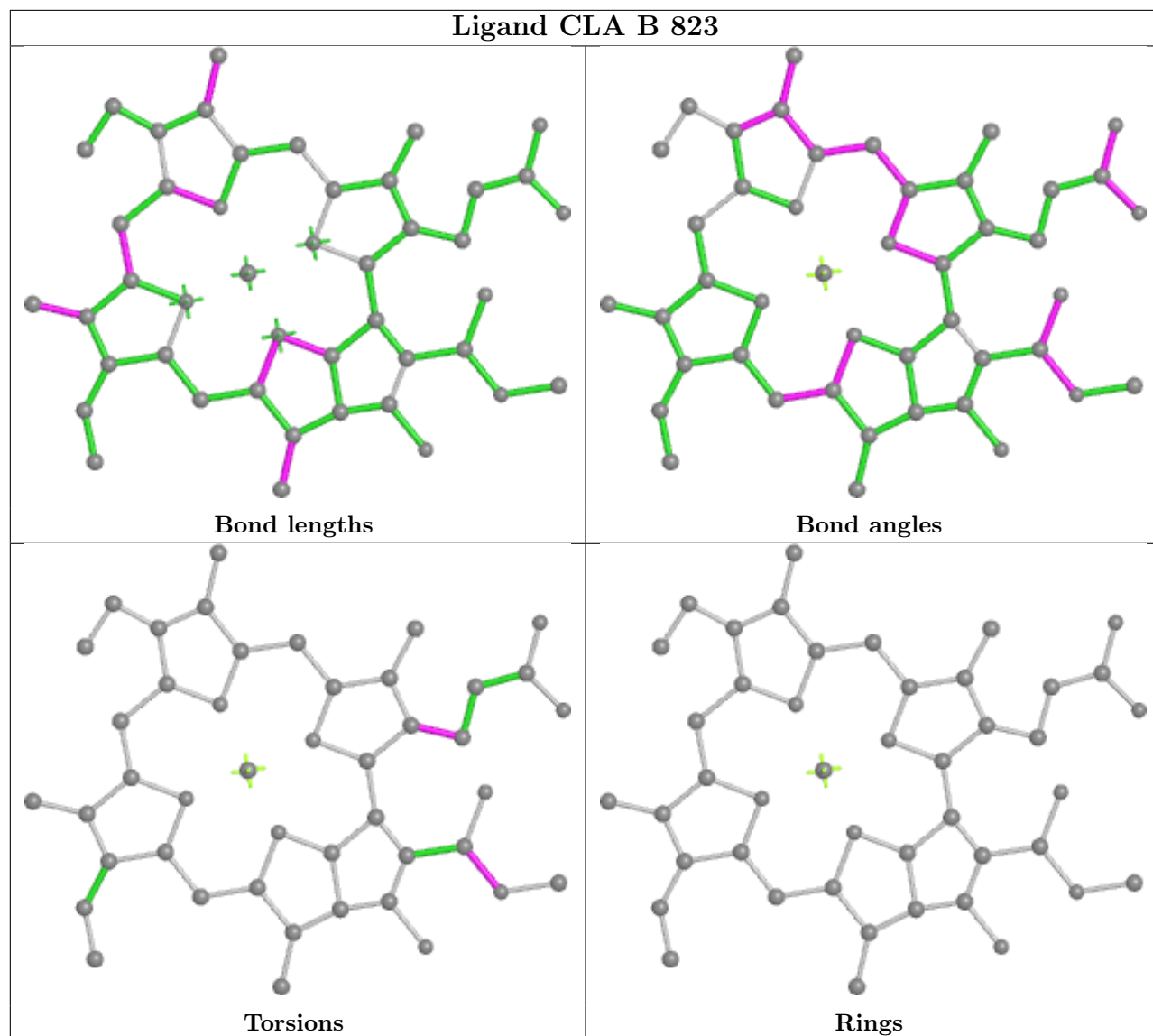
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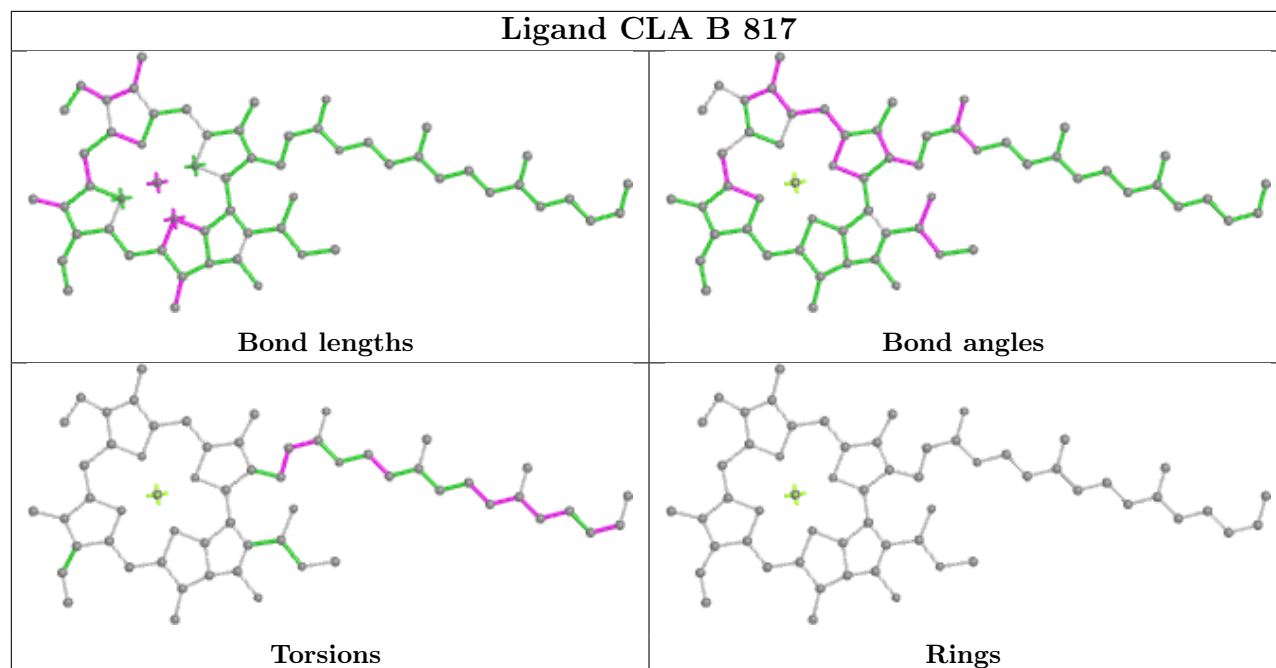
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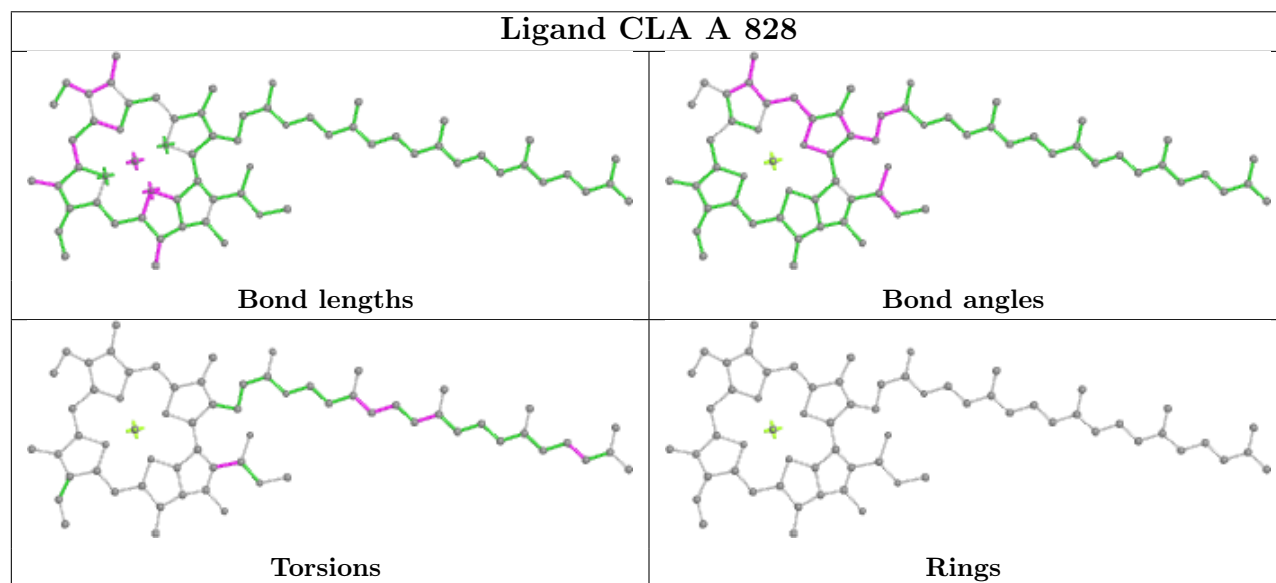
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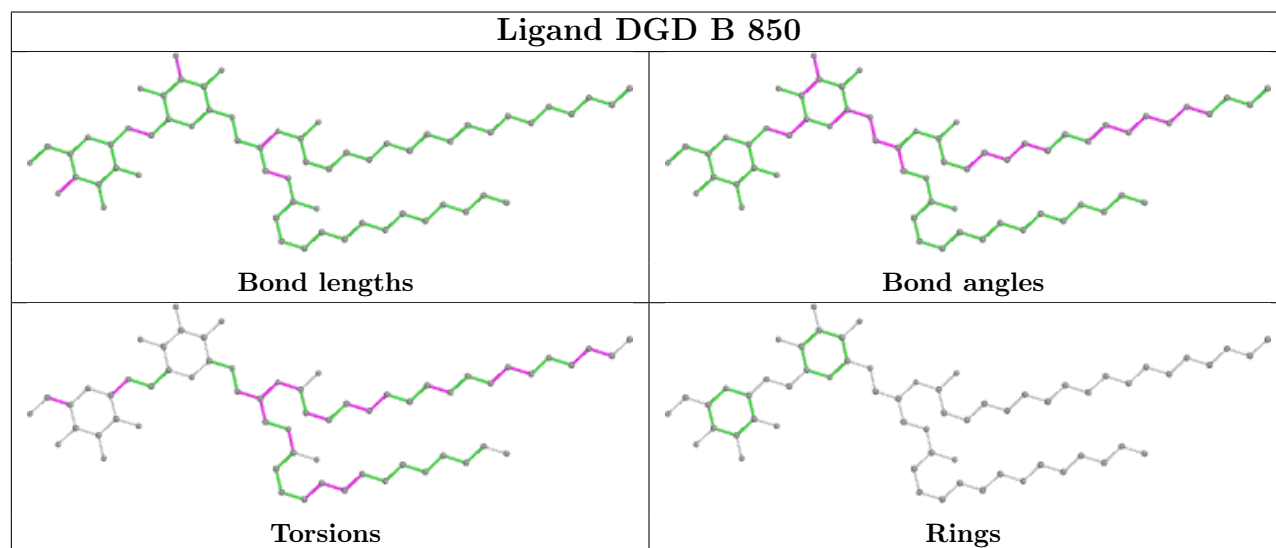
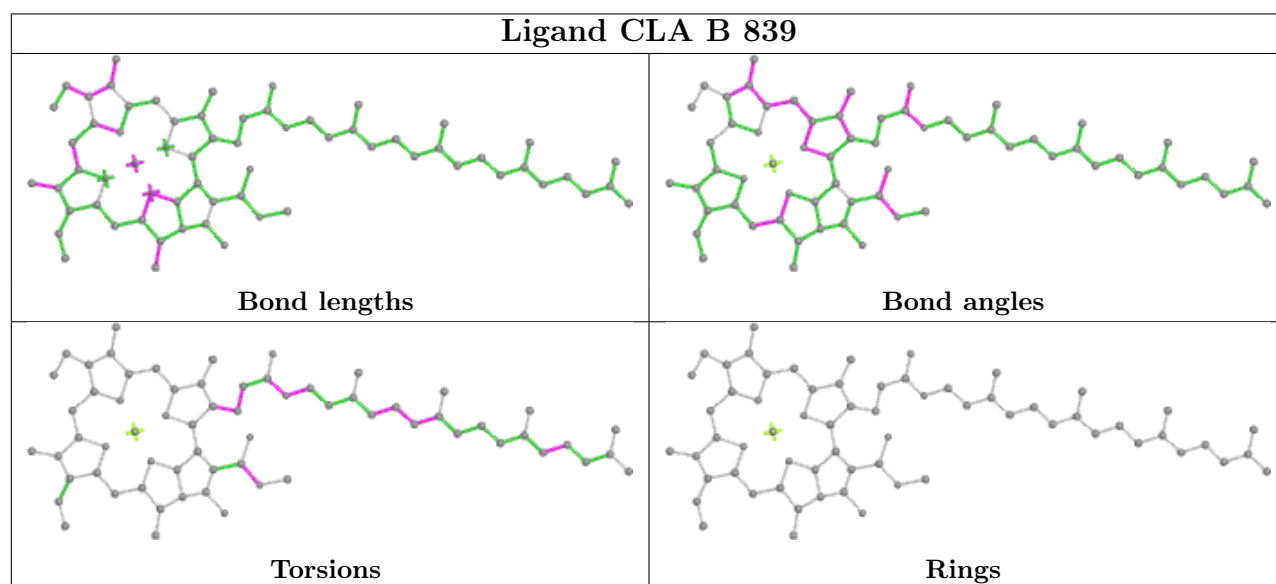
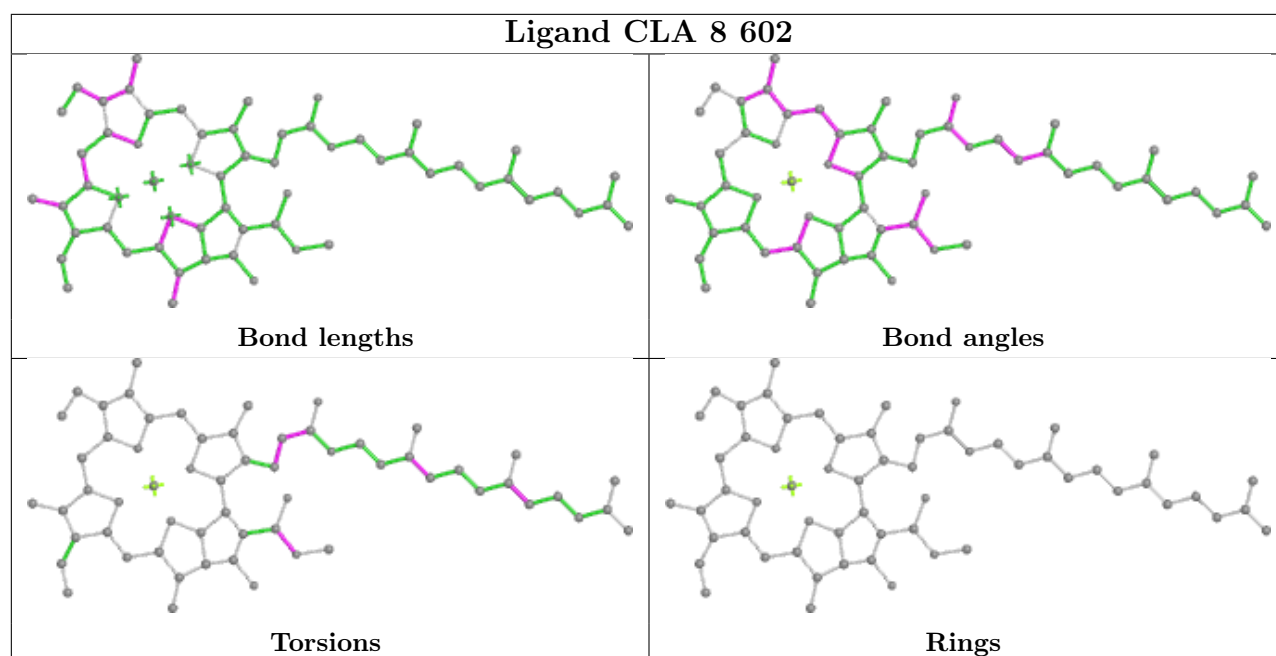


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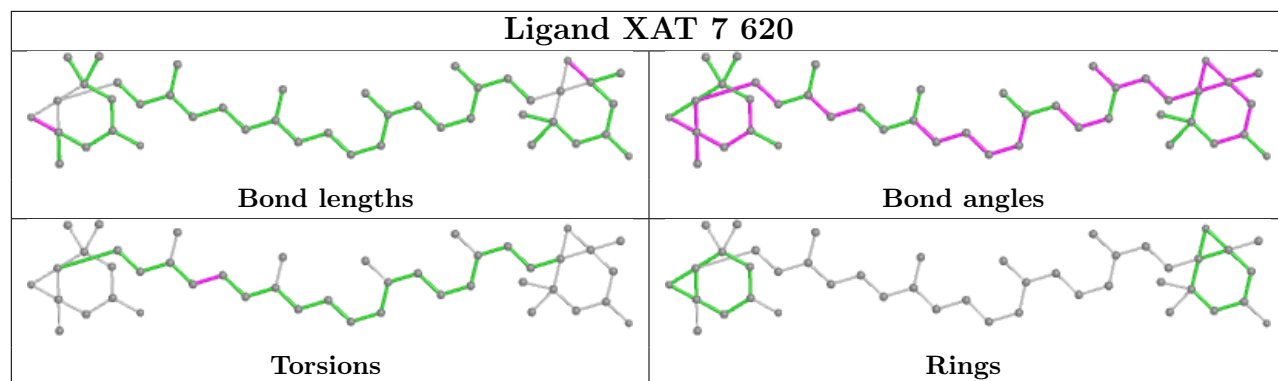


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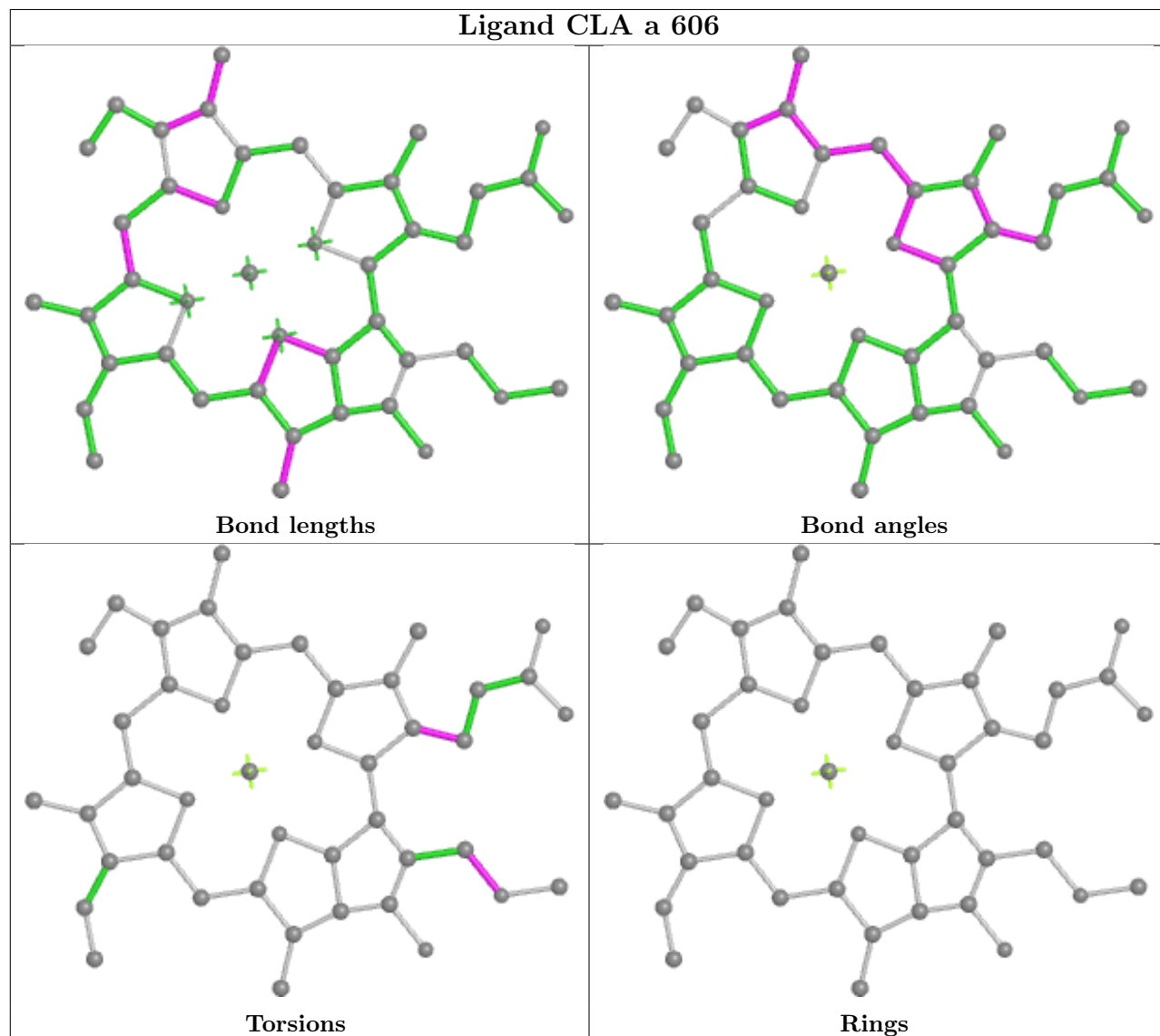


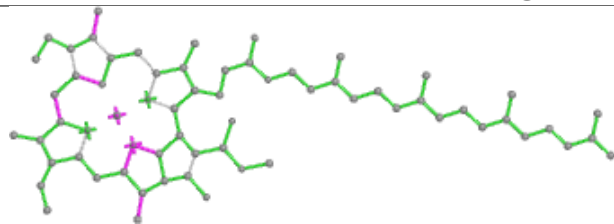
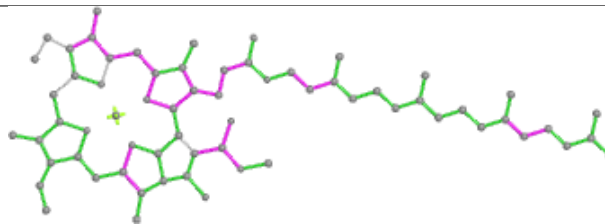
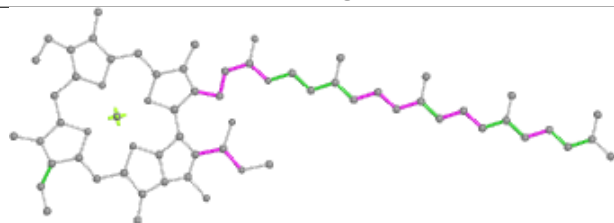
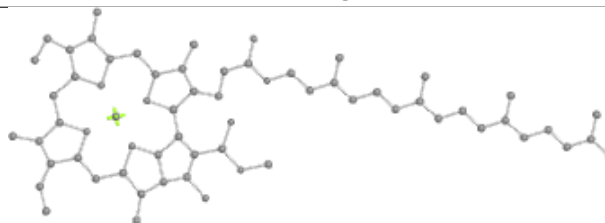
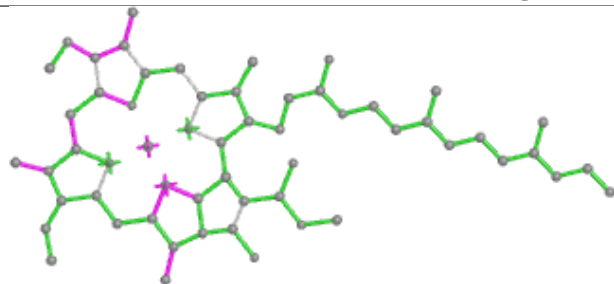
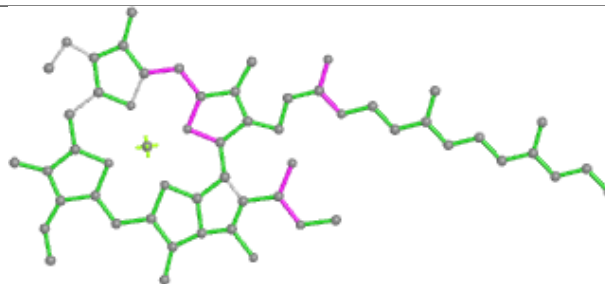
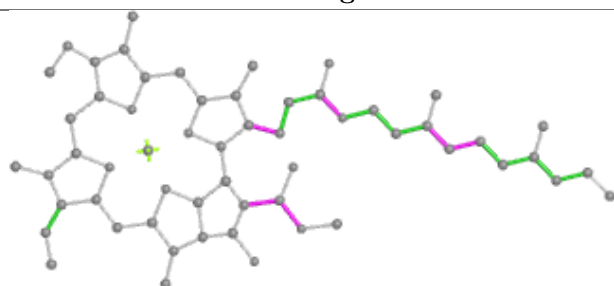
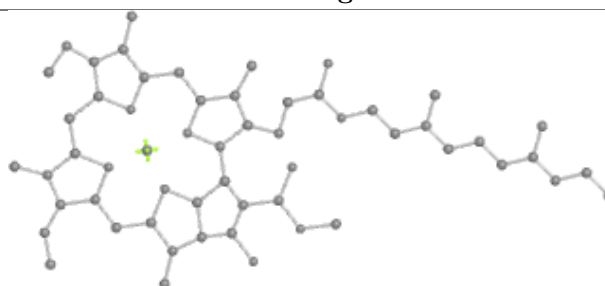


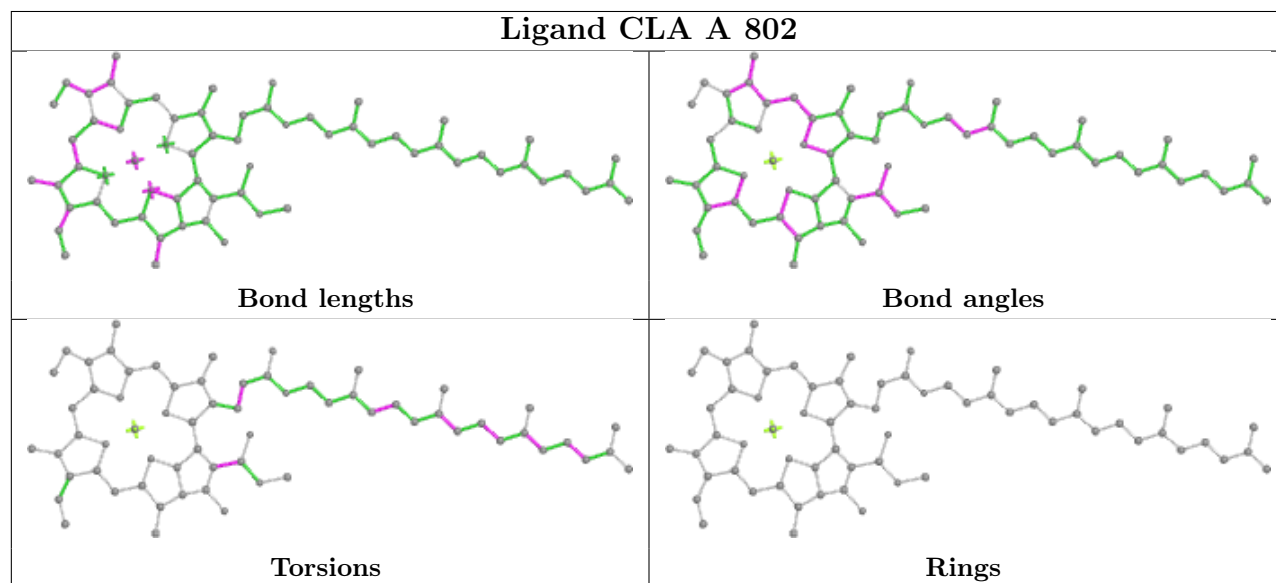
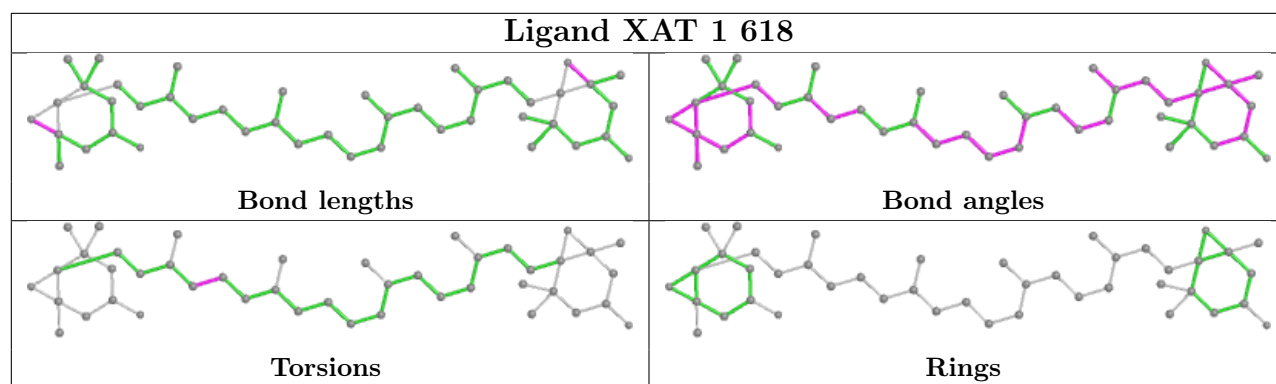
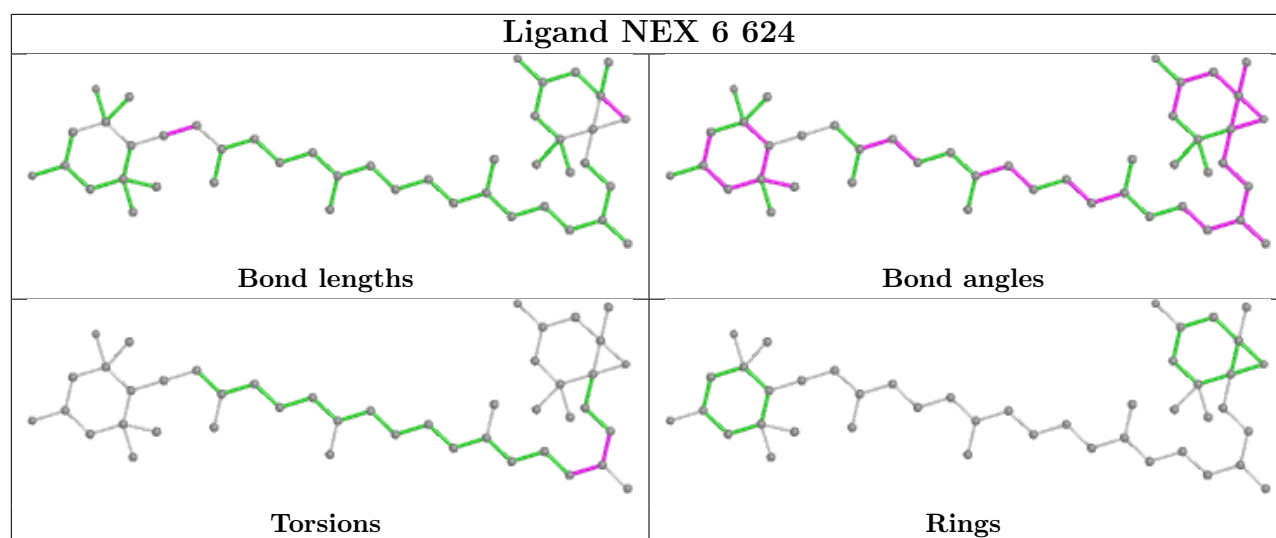
Ligand XAT 7 620

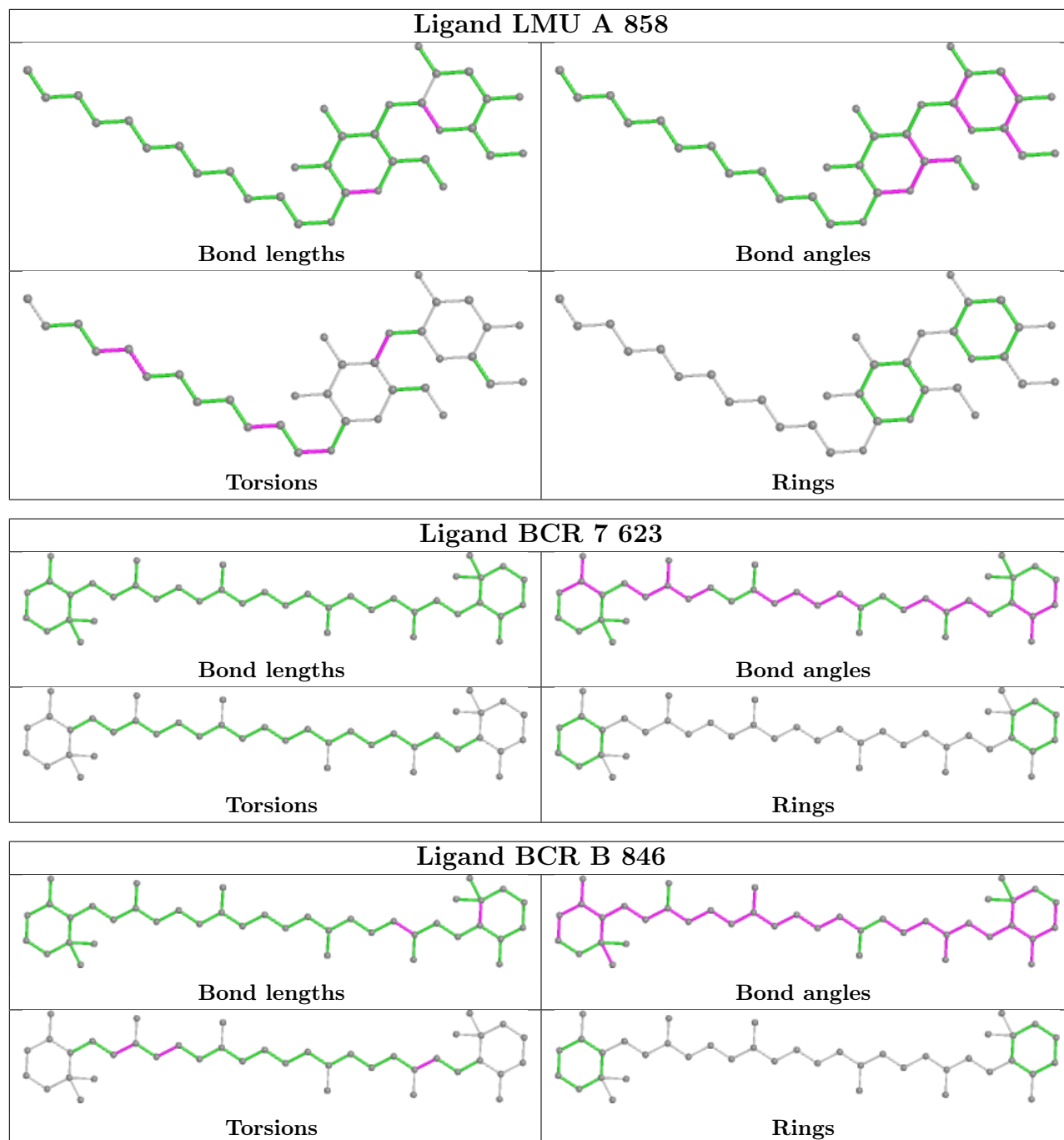


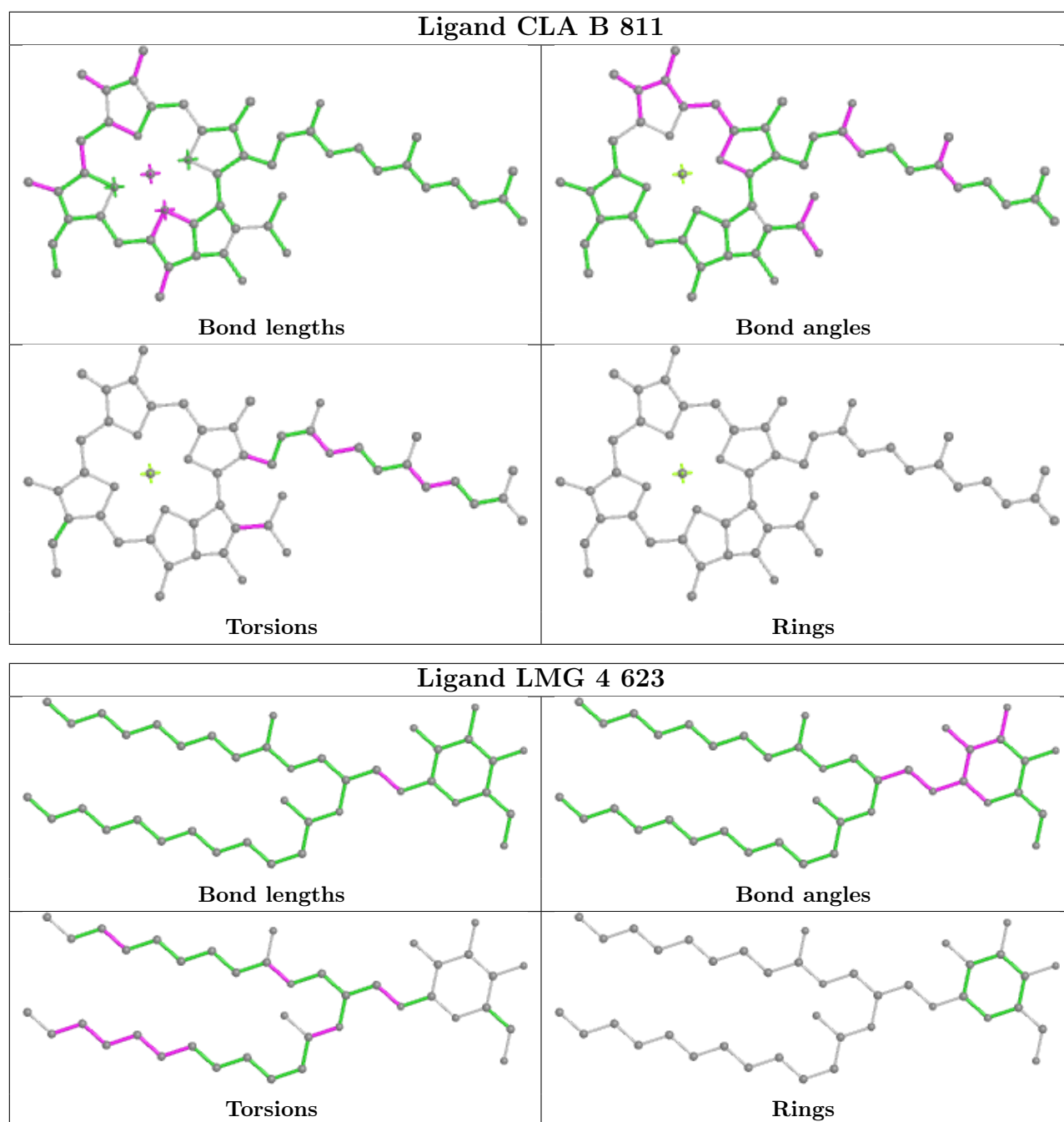
Ligand CLA a 606

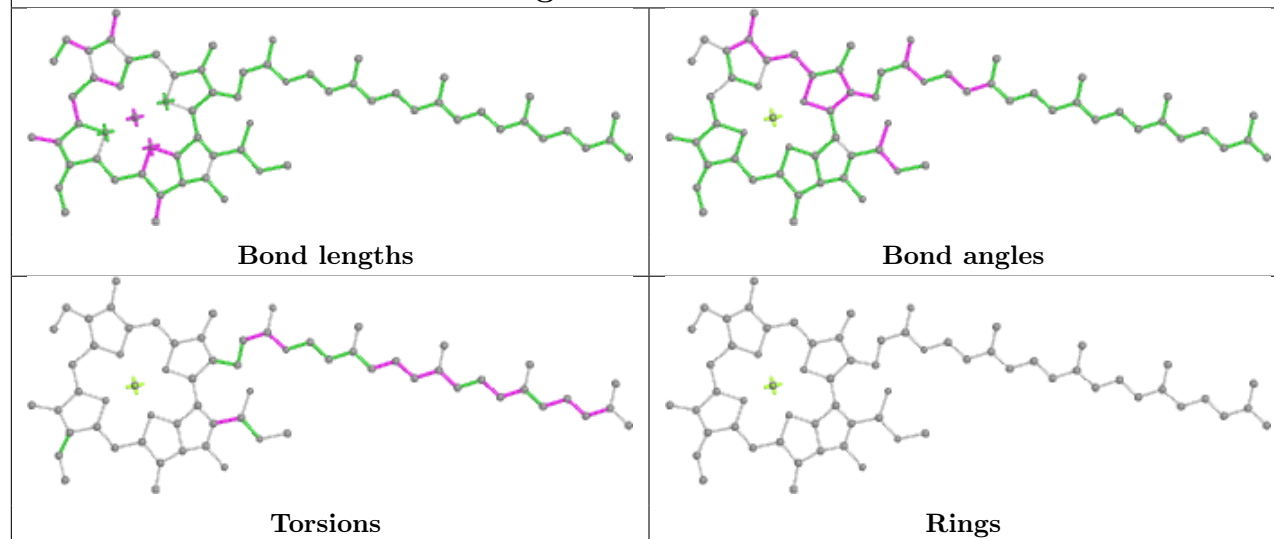
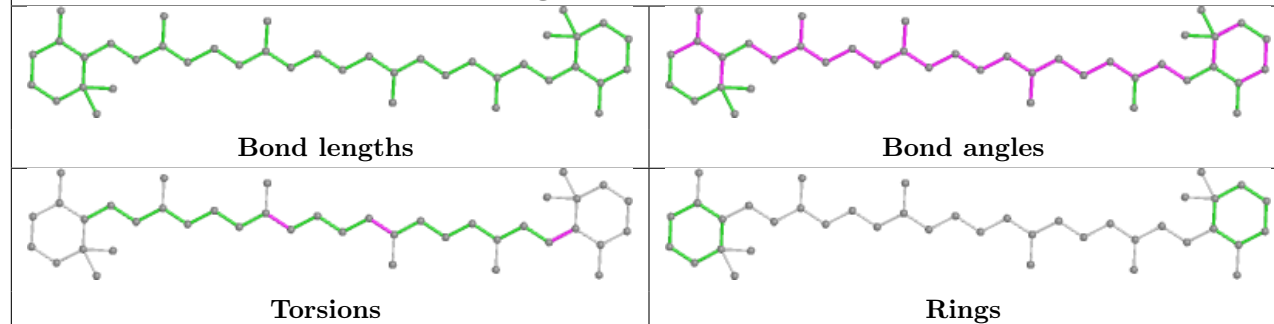
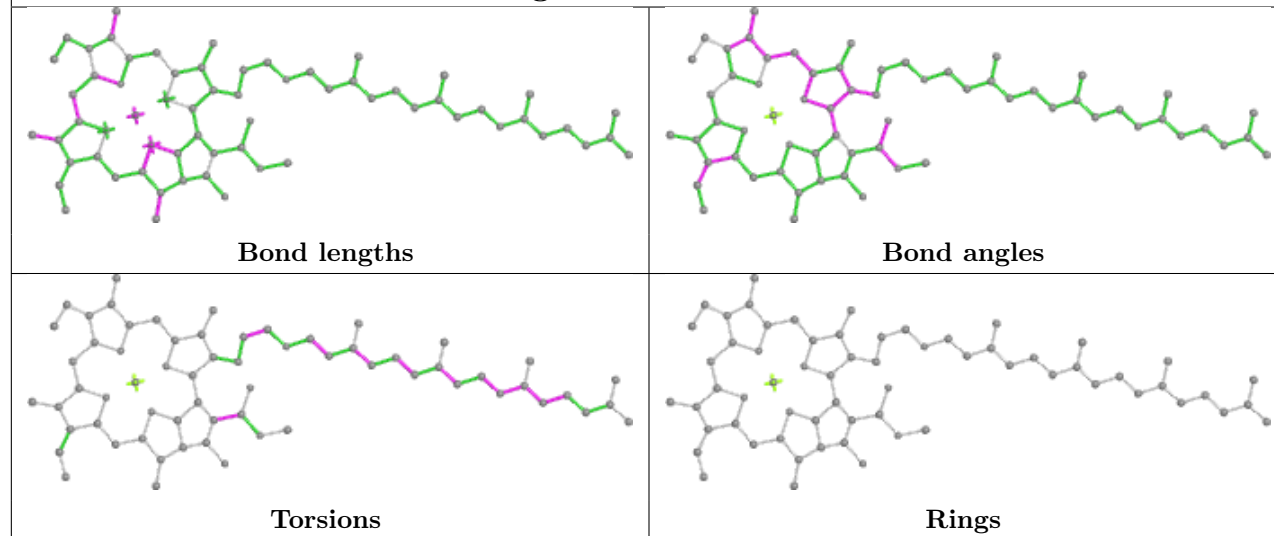


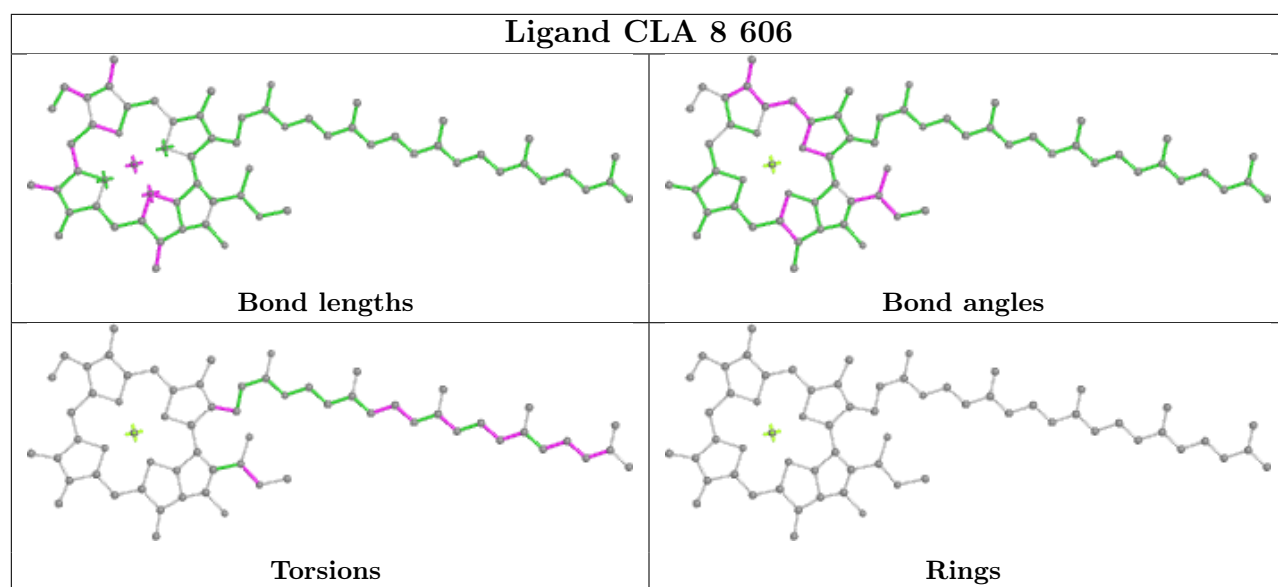
Ligand CLA 6 616**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA F 301****Bond lengths****Bond angles****Torsions****Rings**



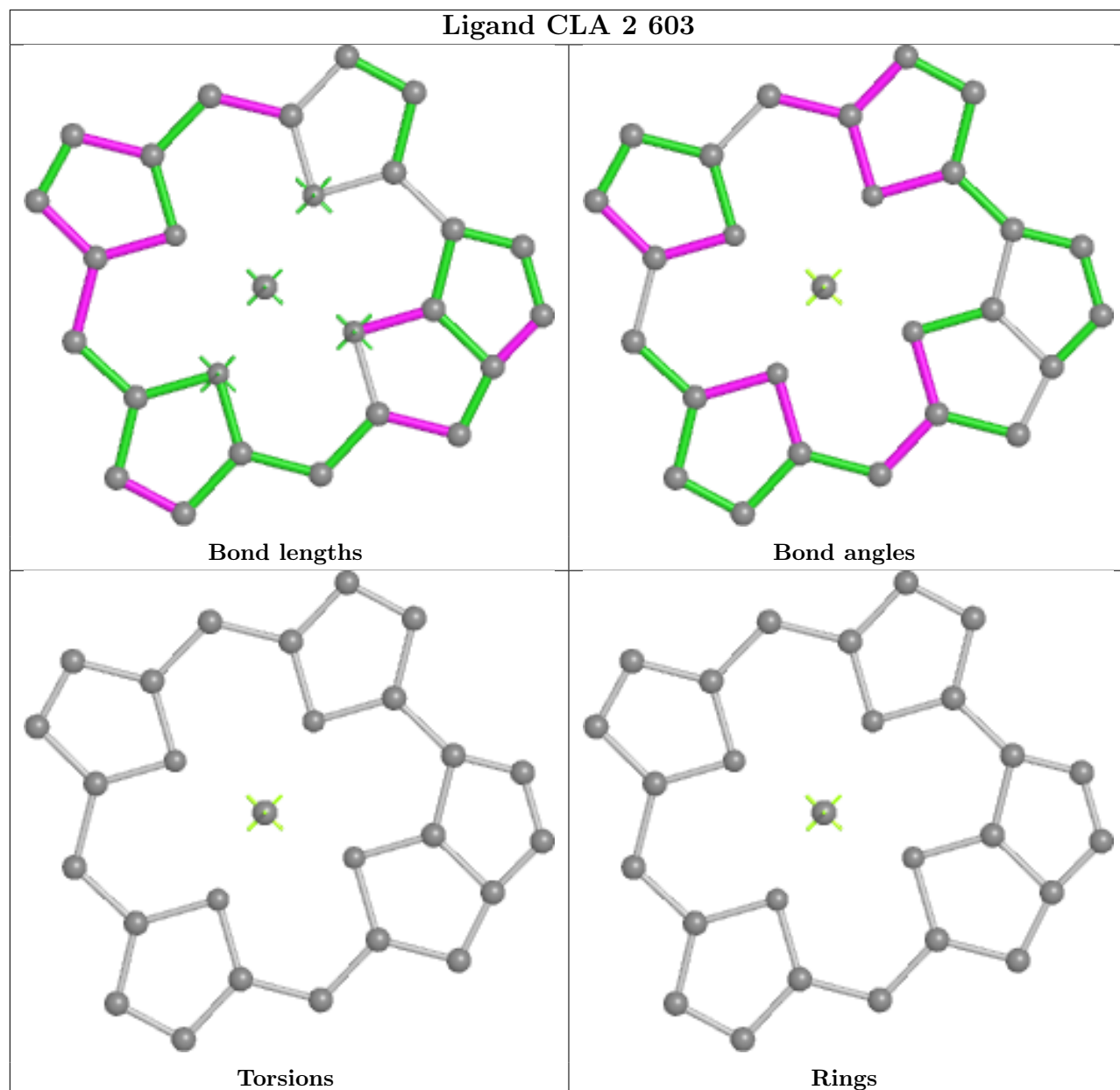




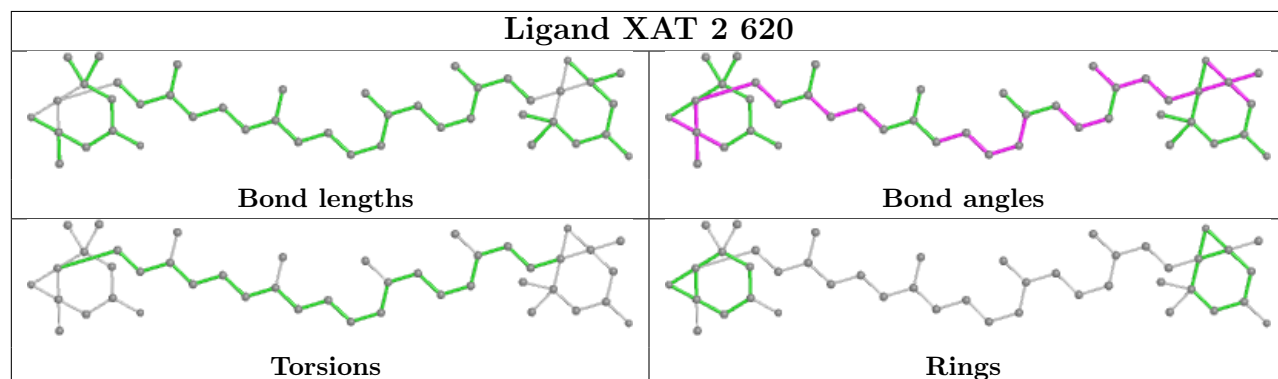
Ligand CLA 8 601**Ligand BCR 3 621****Ligand CLA A 826**



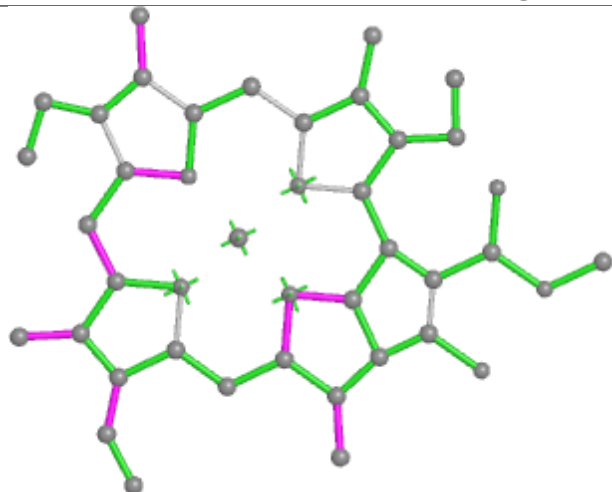
Ligand CLA 2 603



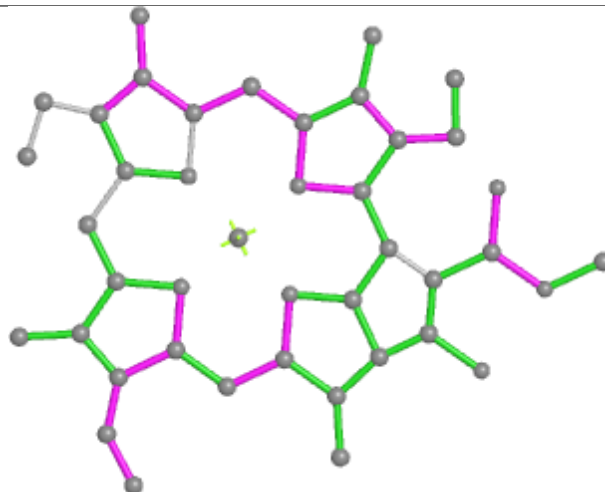
Ligand XAT 2 620



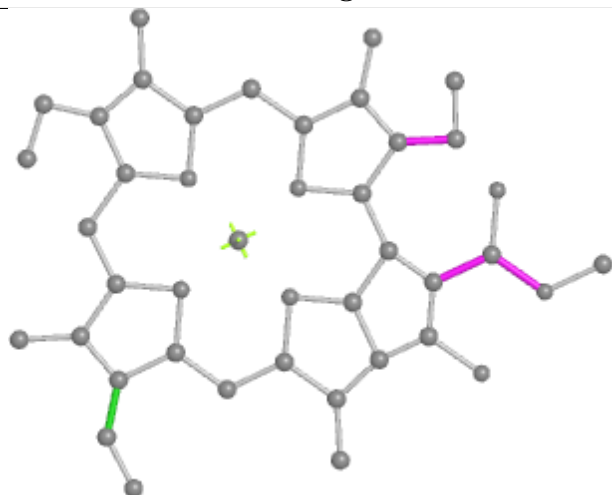
Ligand CLA F 303



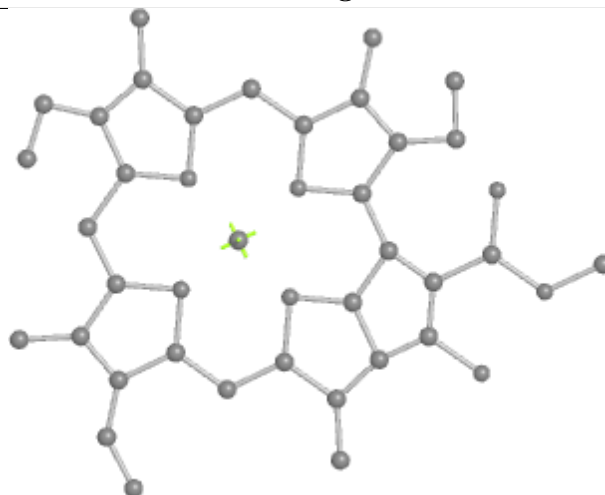
Bond lengths



Bond angles

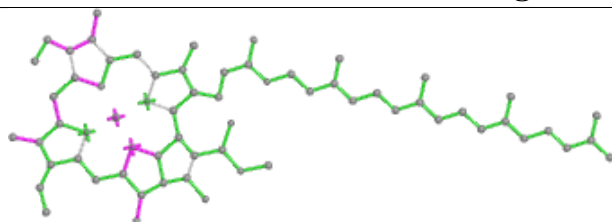


Torsions

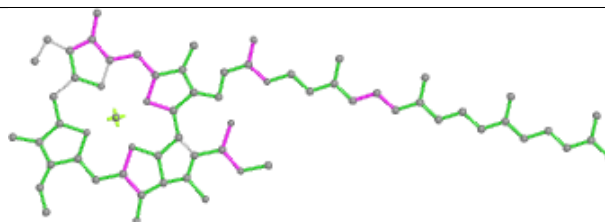


Rings

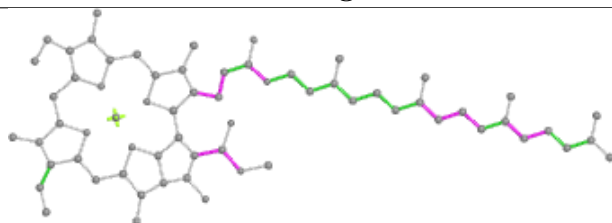
Ligand CLA B 828



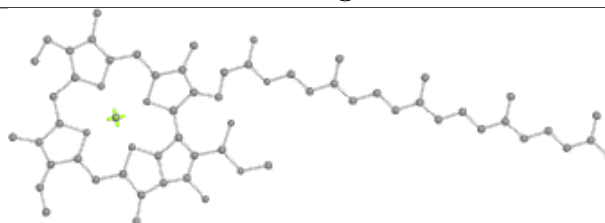
Bond lengths



Bond angles

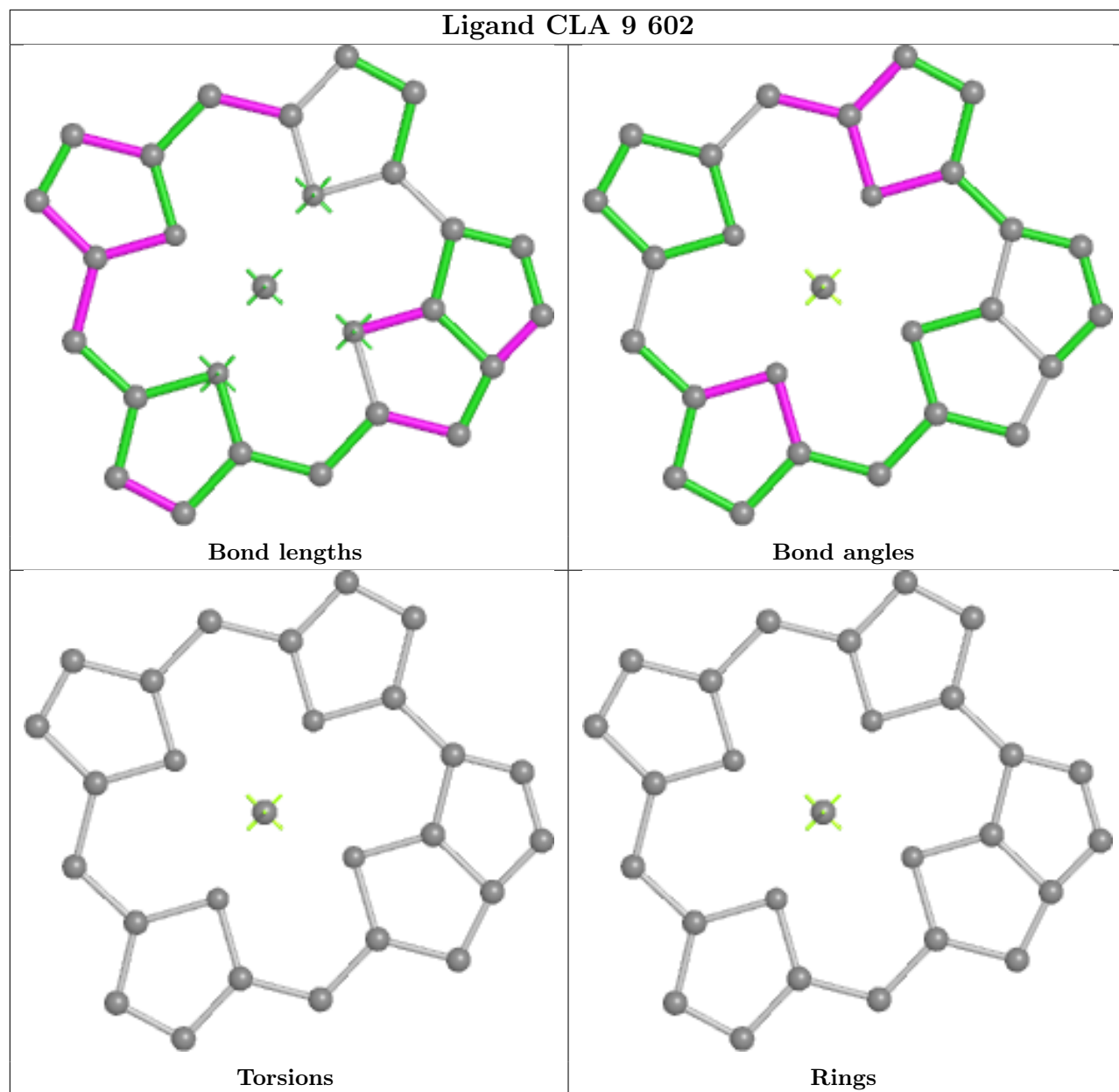


Torsions

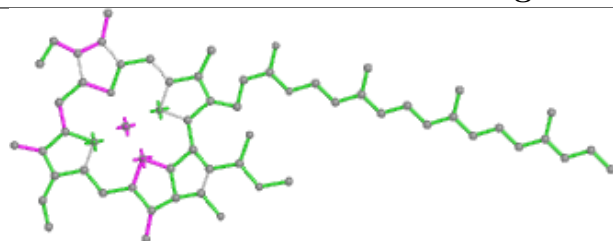


Rings

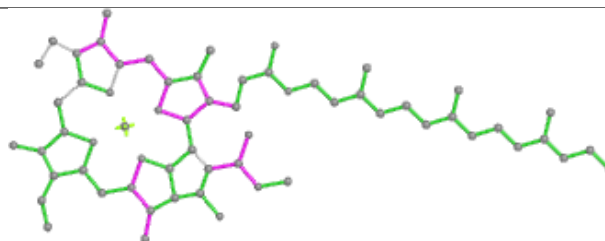
Ligand CLA 9 602



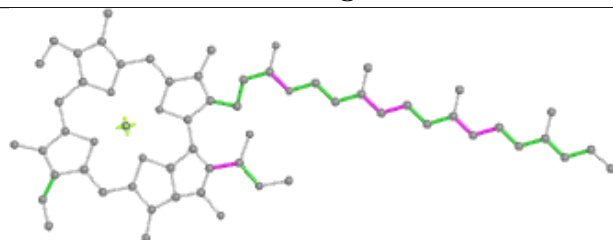
Ligand CLA B 825



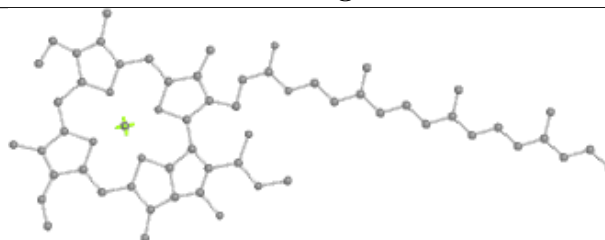
Bond lengths



Bond angles

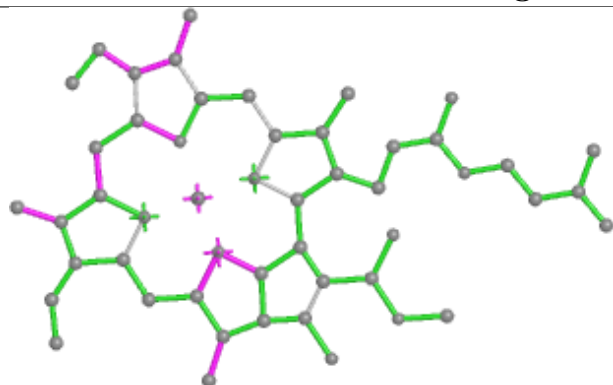


Torsions

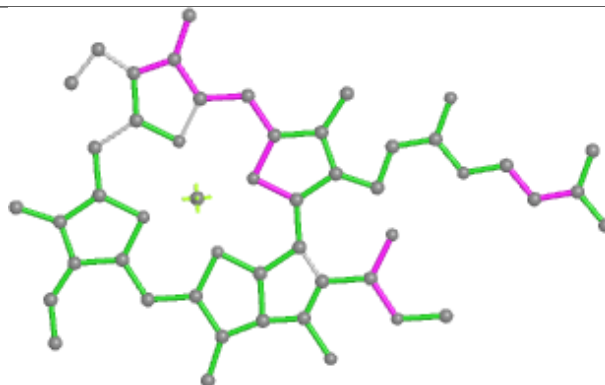


Rings

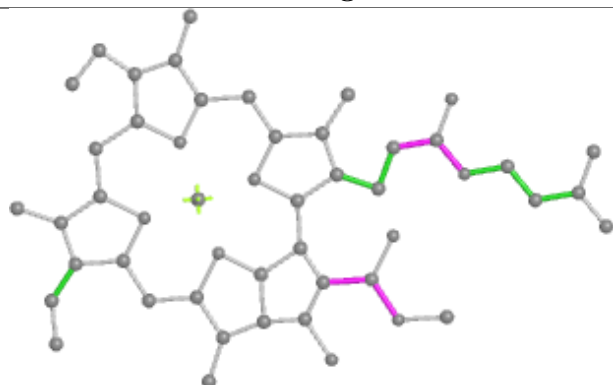
Ligand CLA A 845



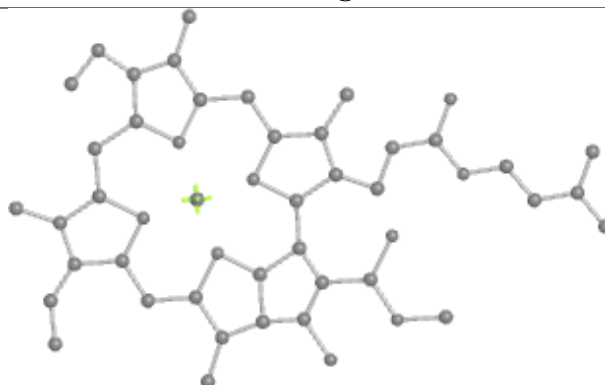
Bond lengths



Bond angles

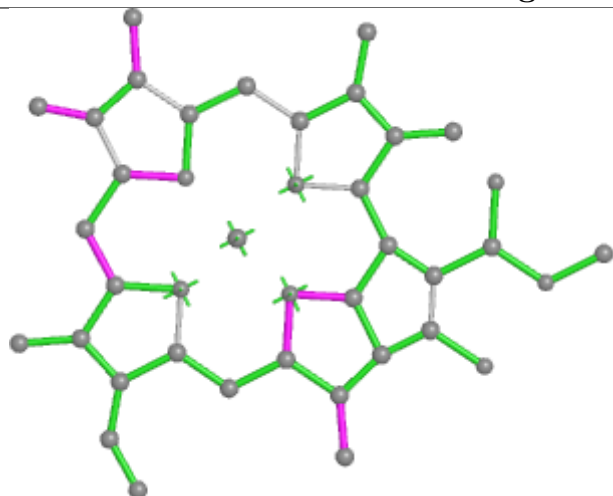


Torsions

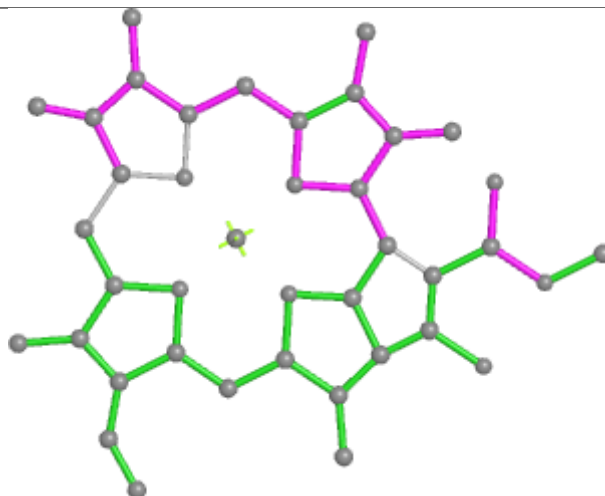


Rings

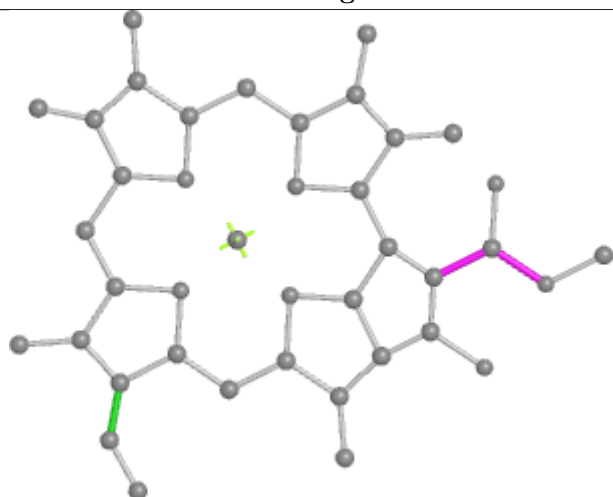
Ligand CLA 1 609



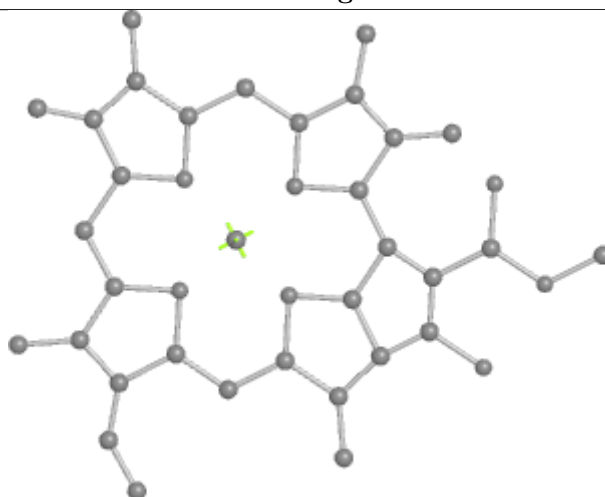
Bond lengths



Bond angles

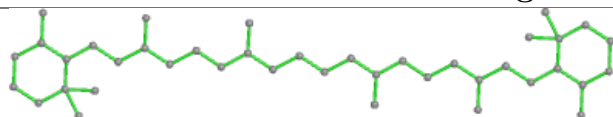


Torsions

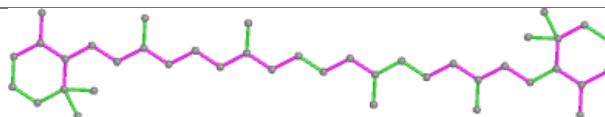


Rings

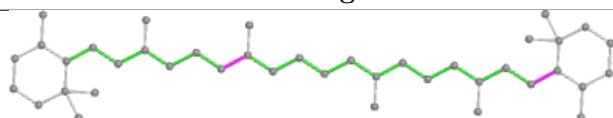
Ligand BCR 1 619



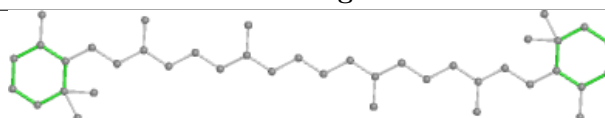
Bond lengths



Bond angles

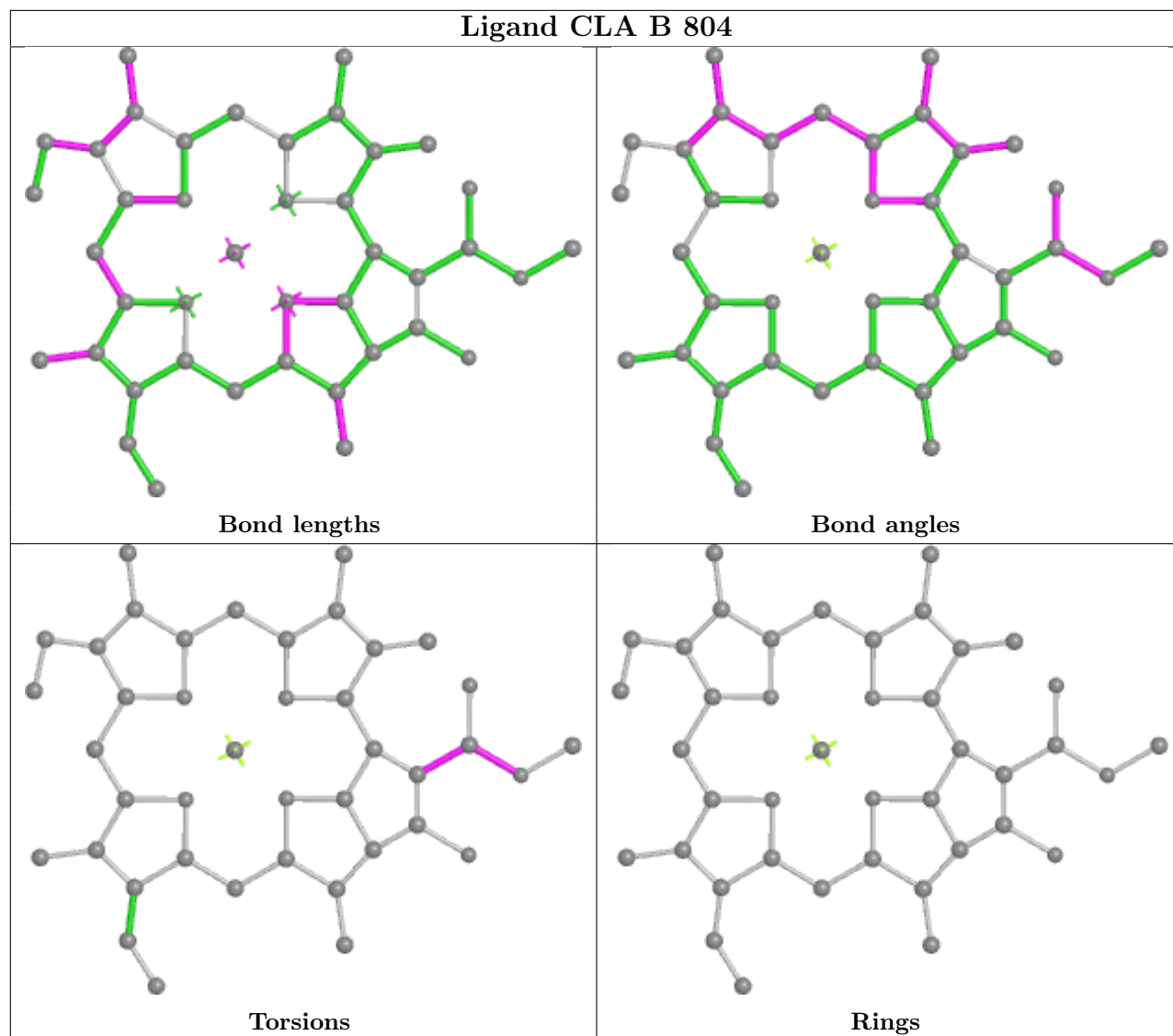


Torsions

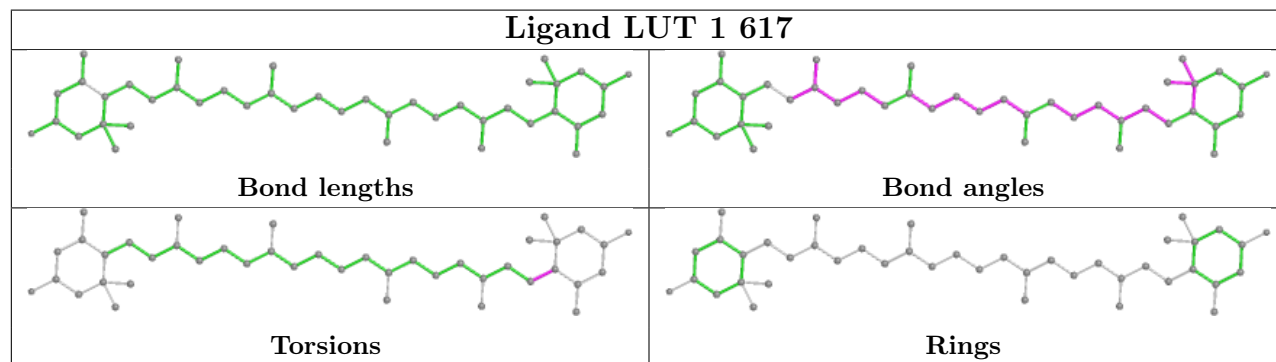


Rings

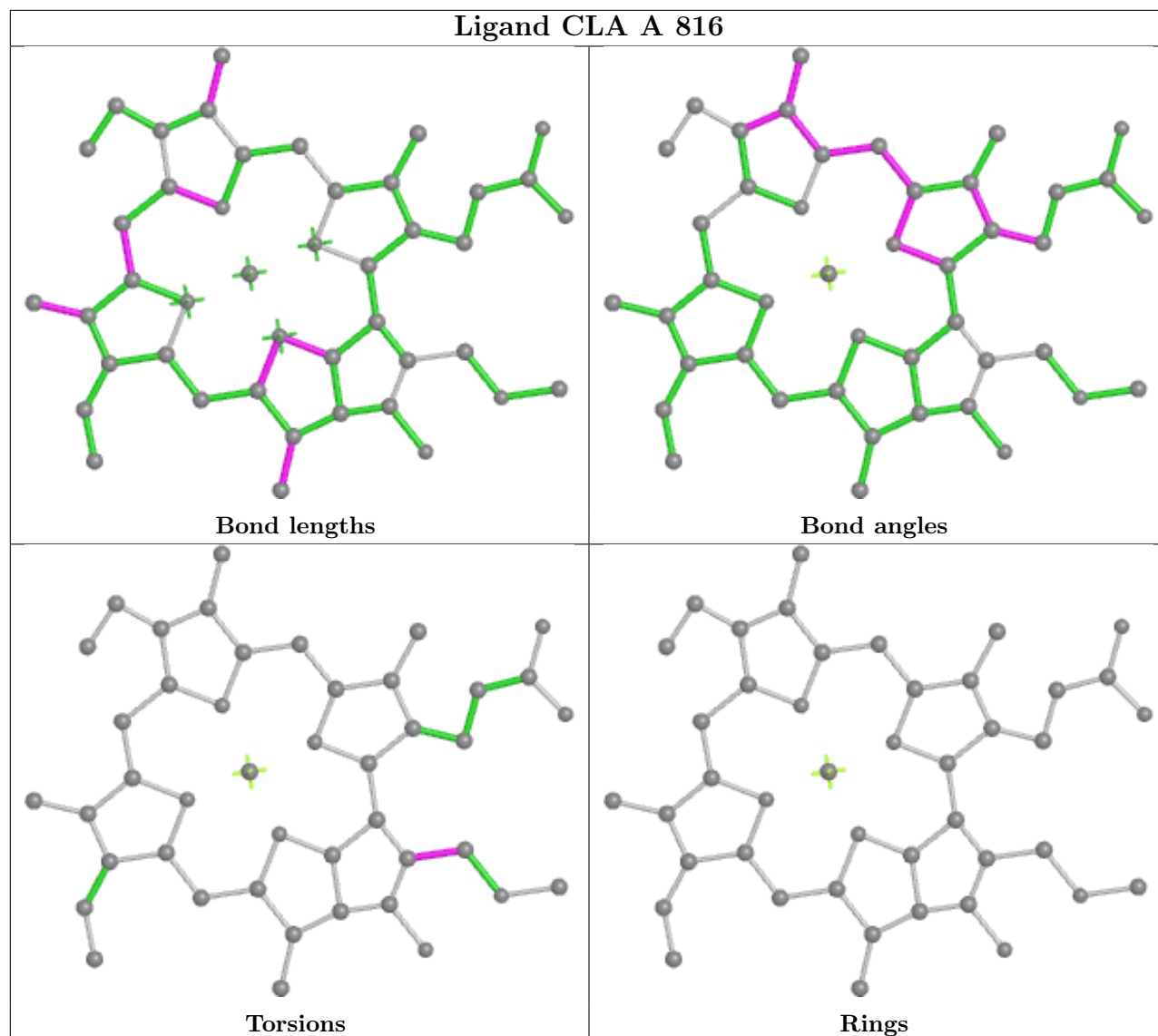
Ligand CLA B 804



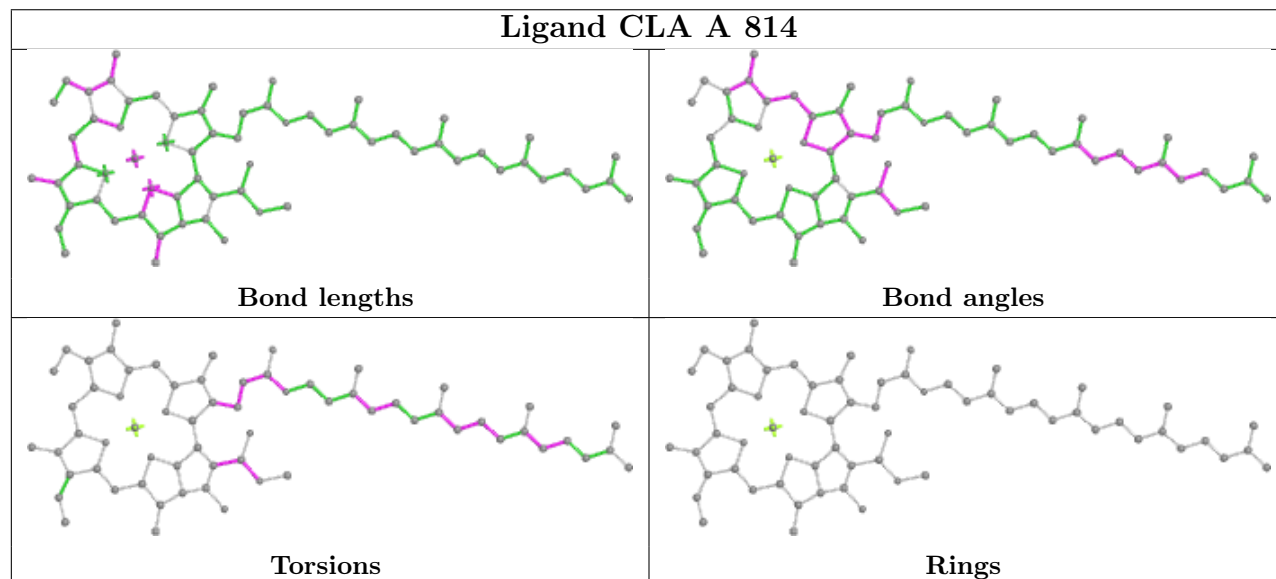
Ligand LUT 1 617



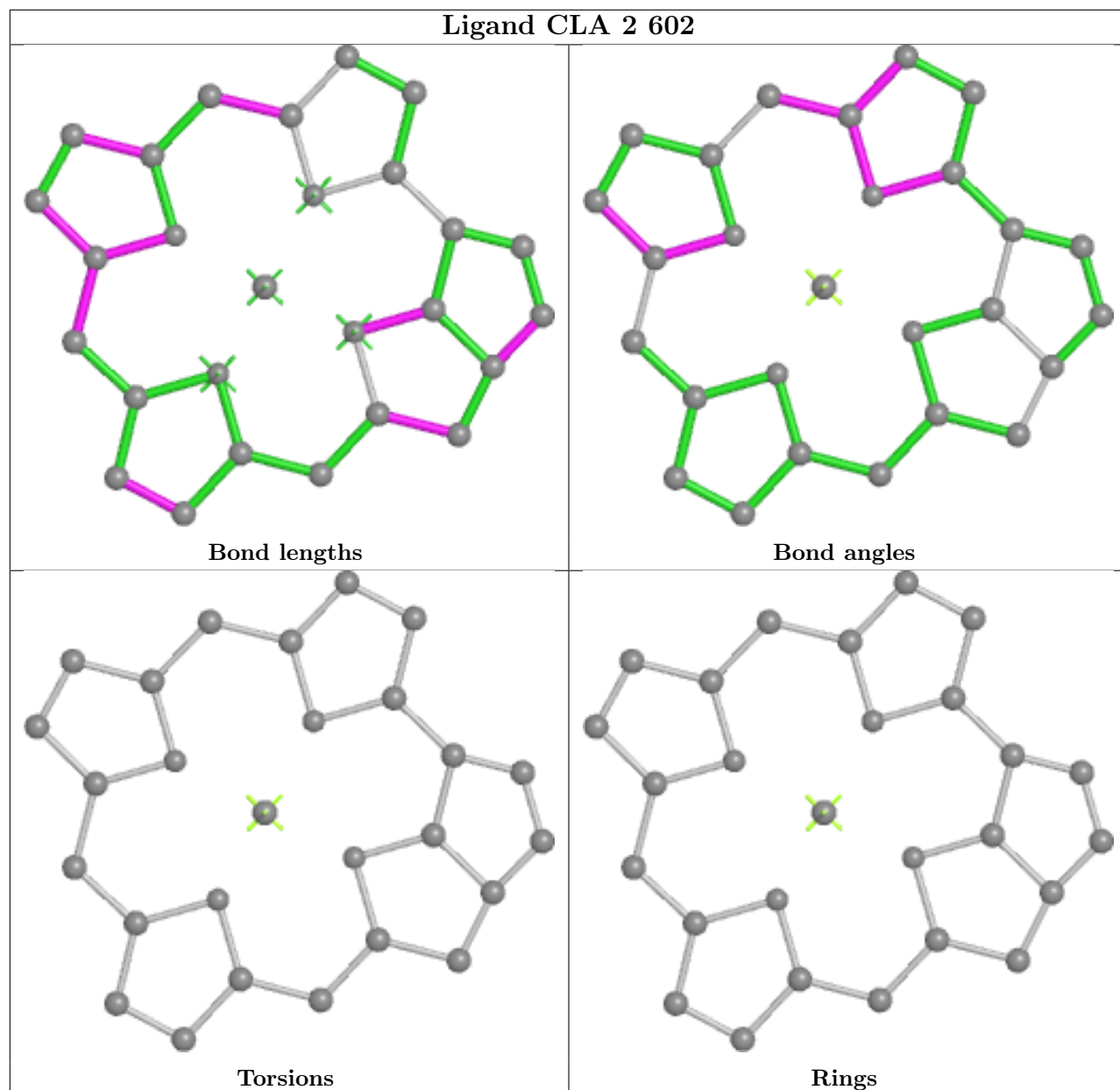
Ligand CLA A 816



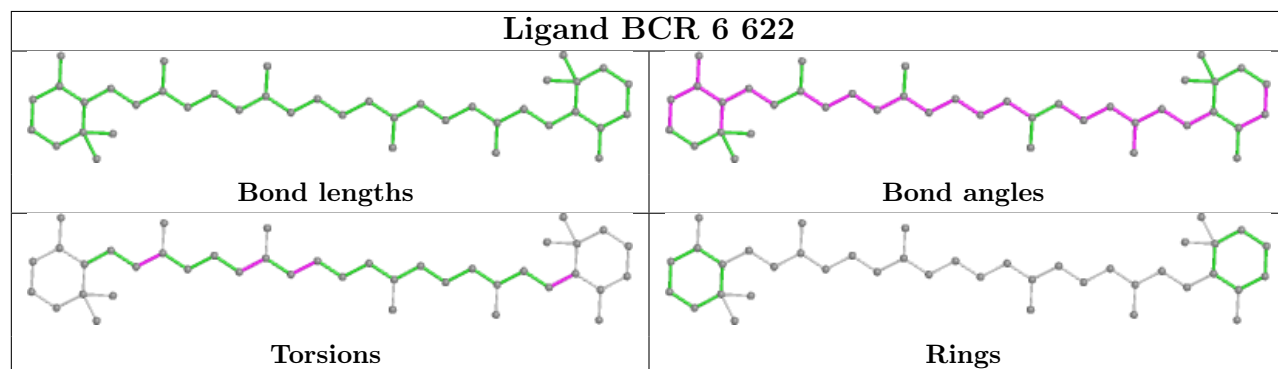
Ligand CLA A 814



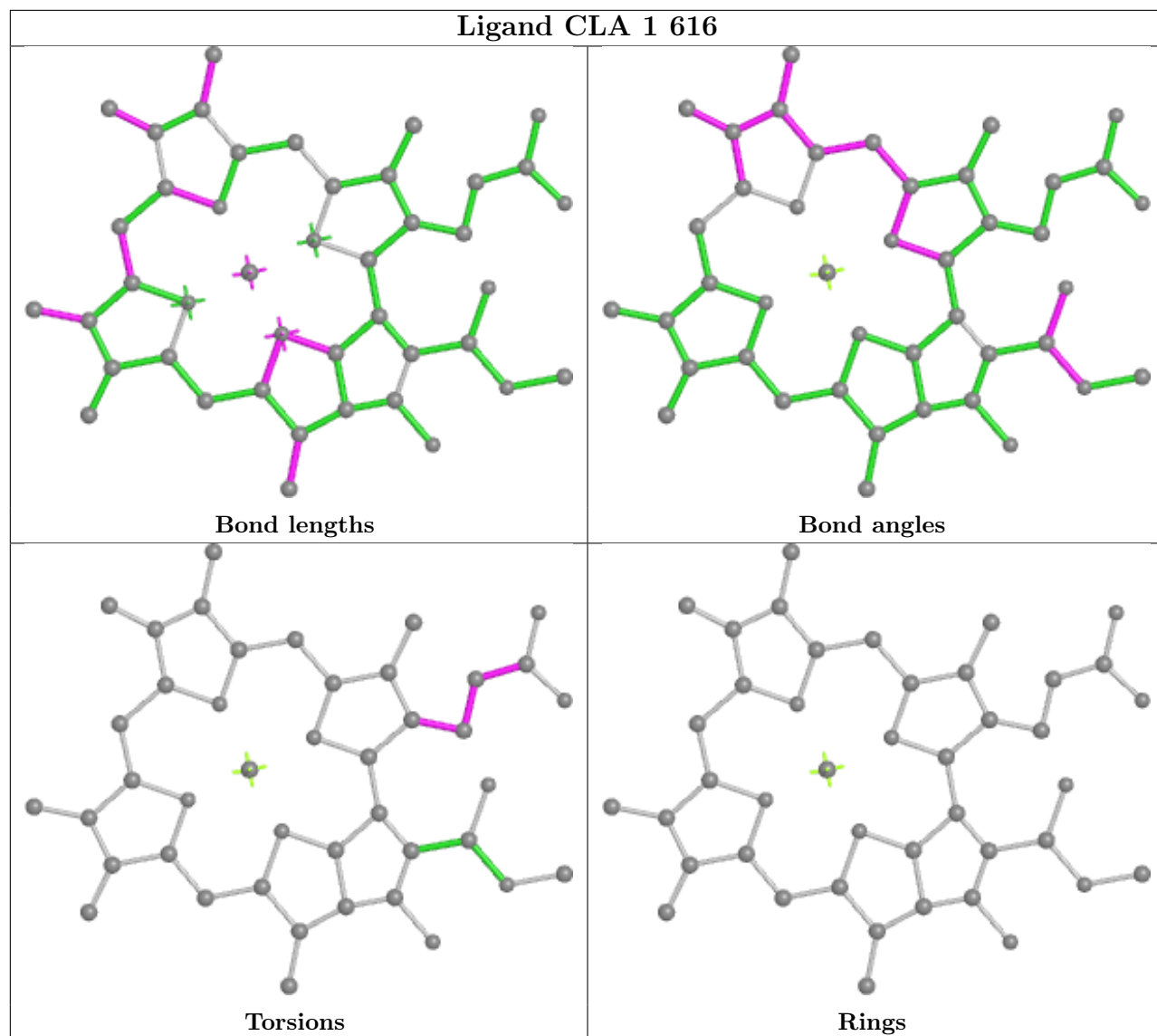
Ligand CLA 2 602

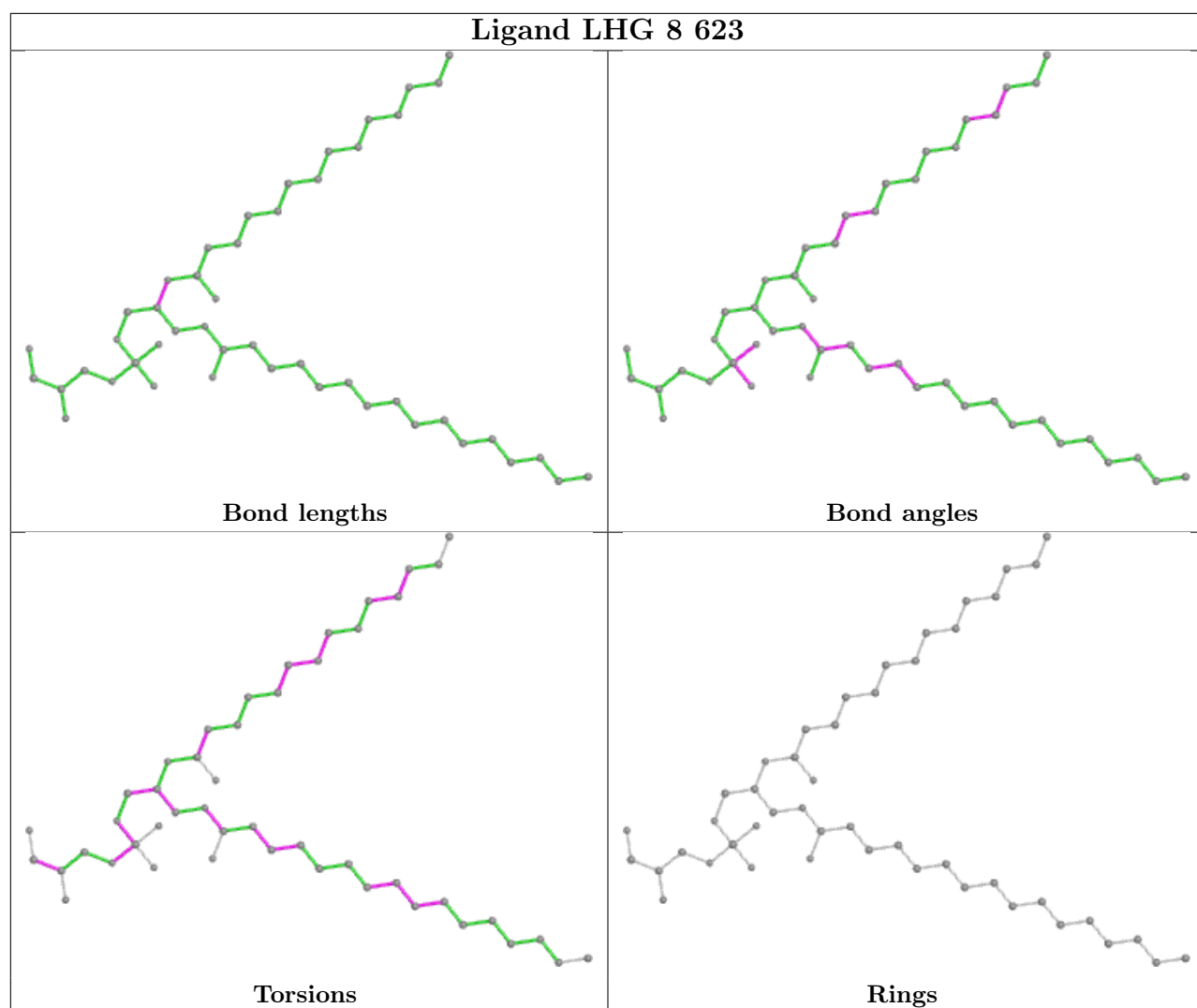


Ligand BCR 6 622

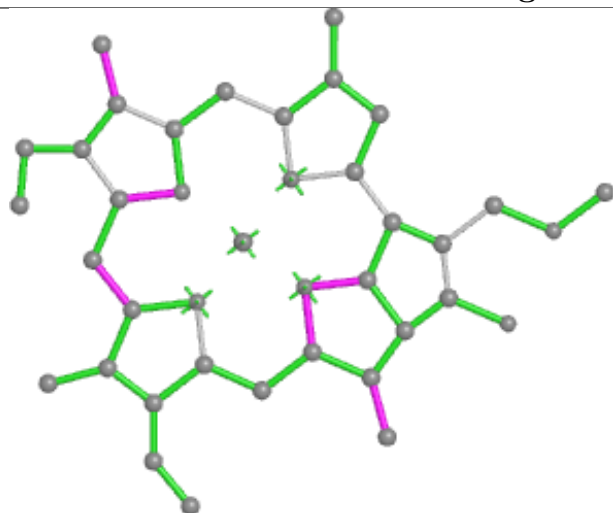


Ligand CLA 1 616

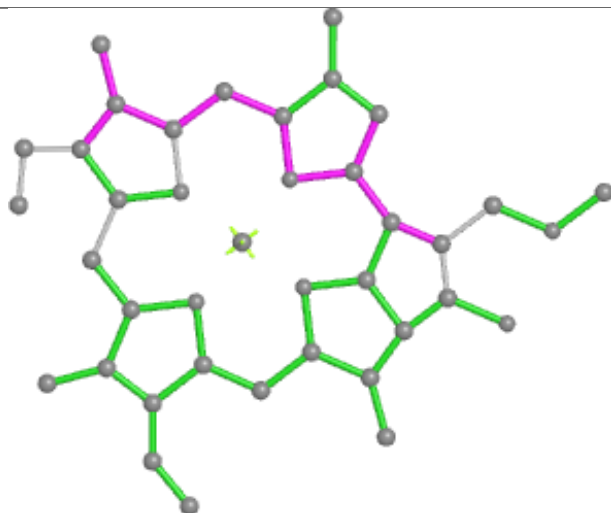




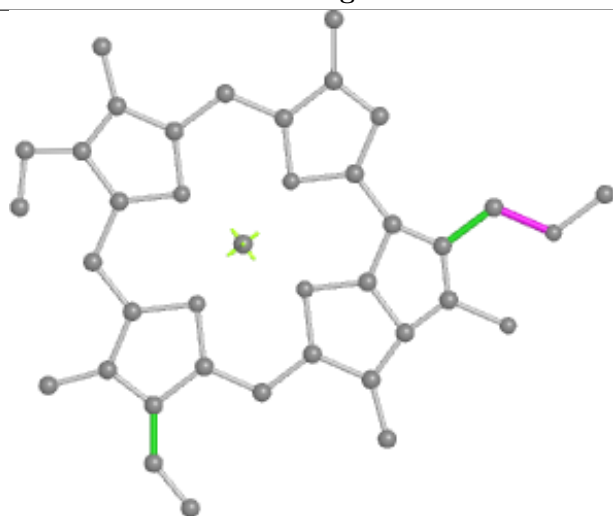
Ligand CLA 1 606



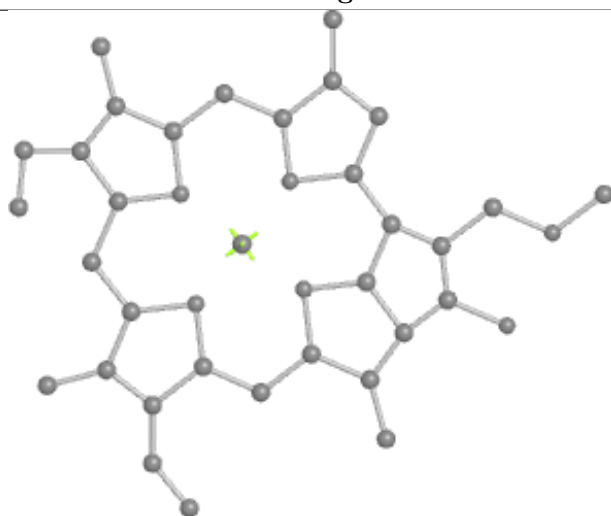
Bond lengths



Bond angles

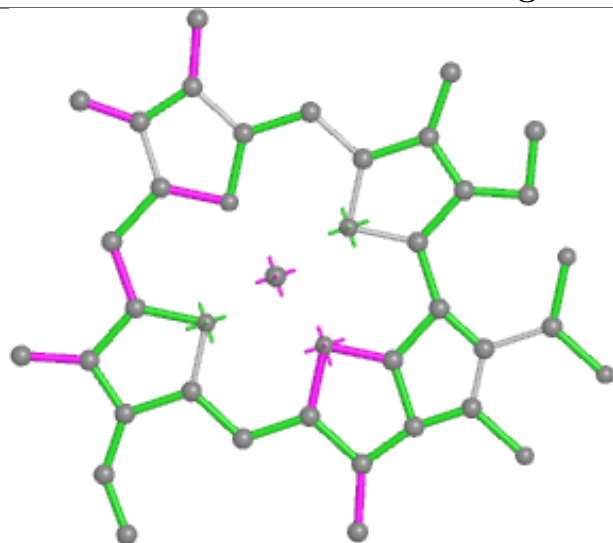


Torsions

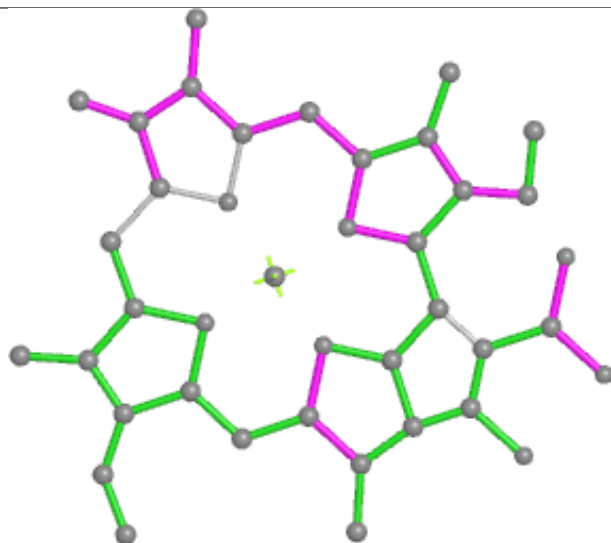


Rings

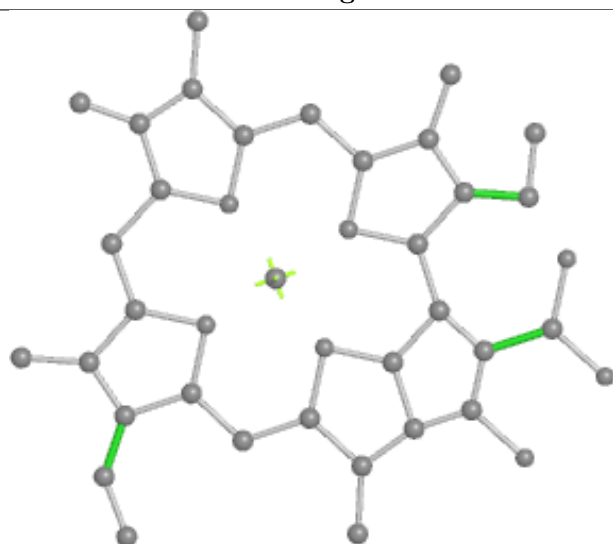
Ligand CLA 4 618



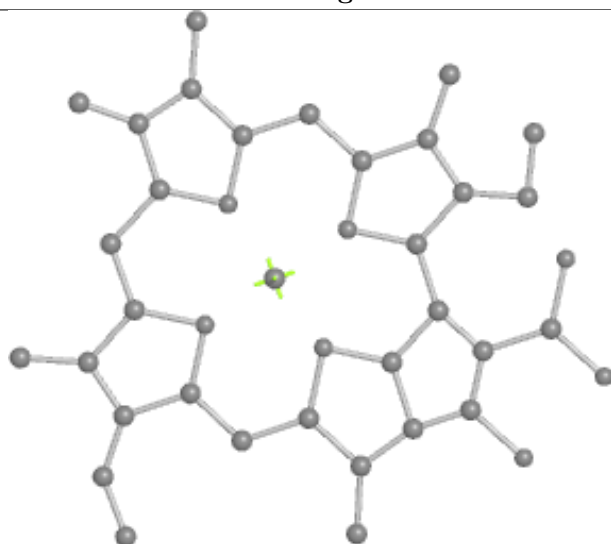
Bond lengths



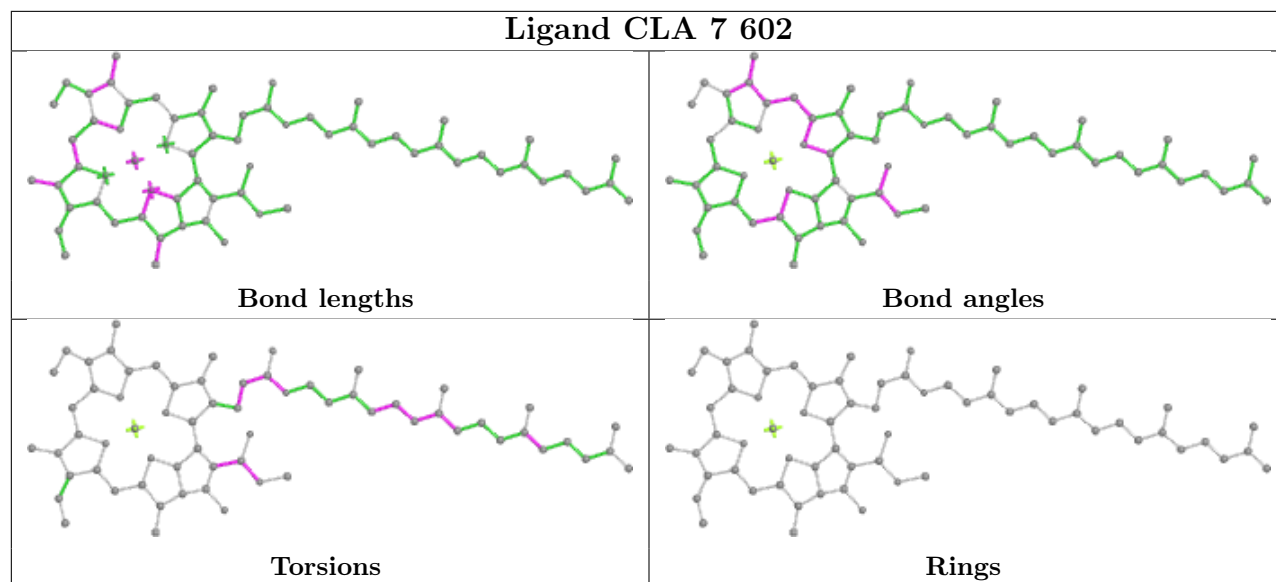
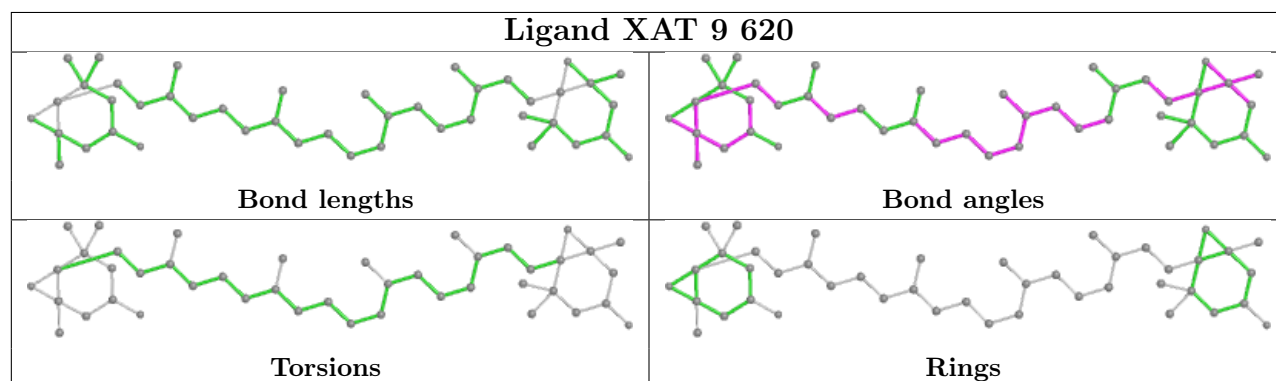
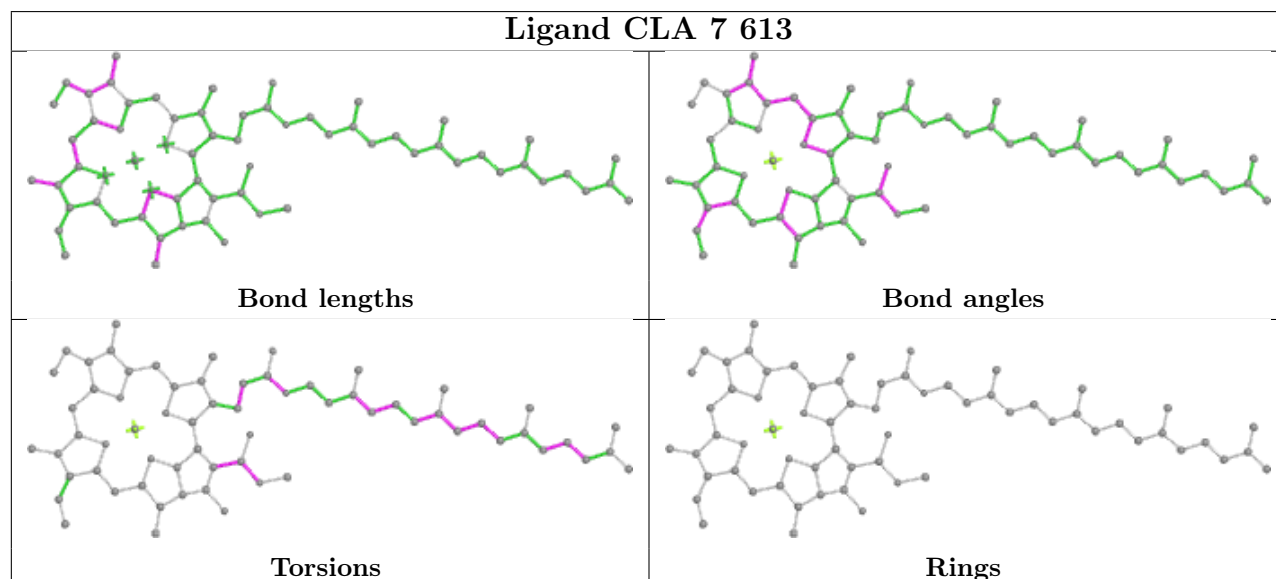
Bond angles



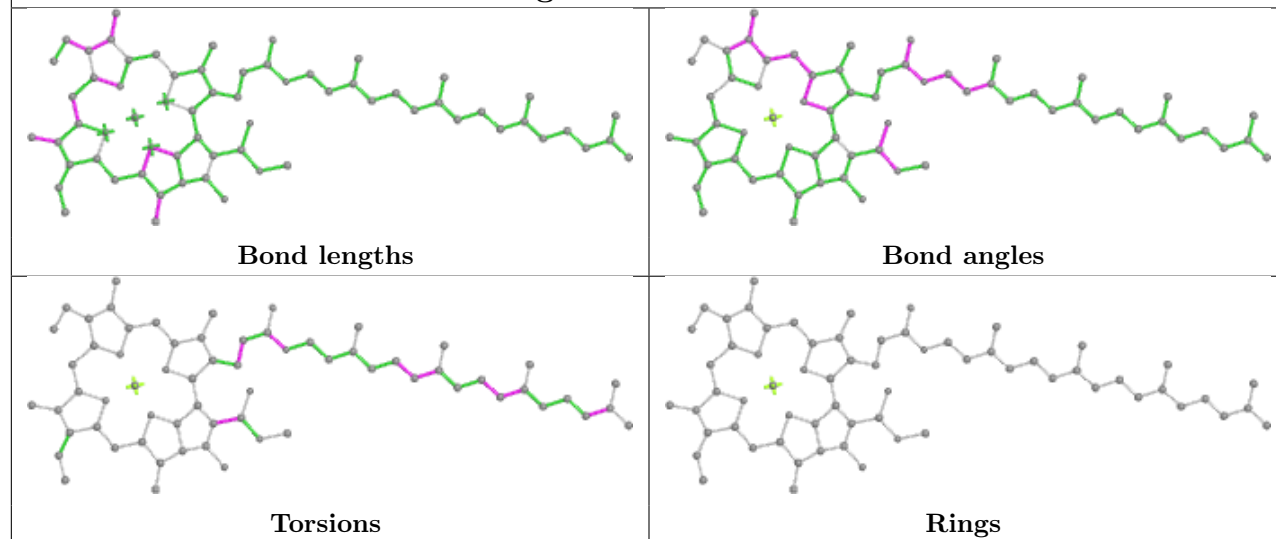
Torsions



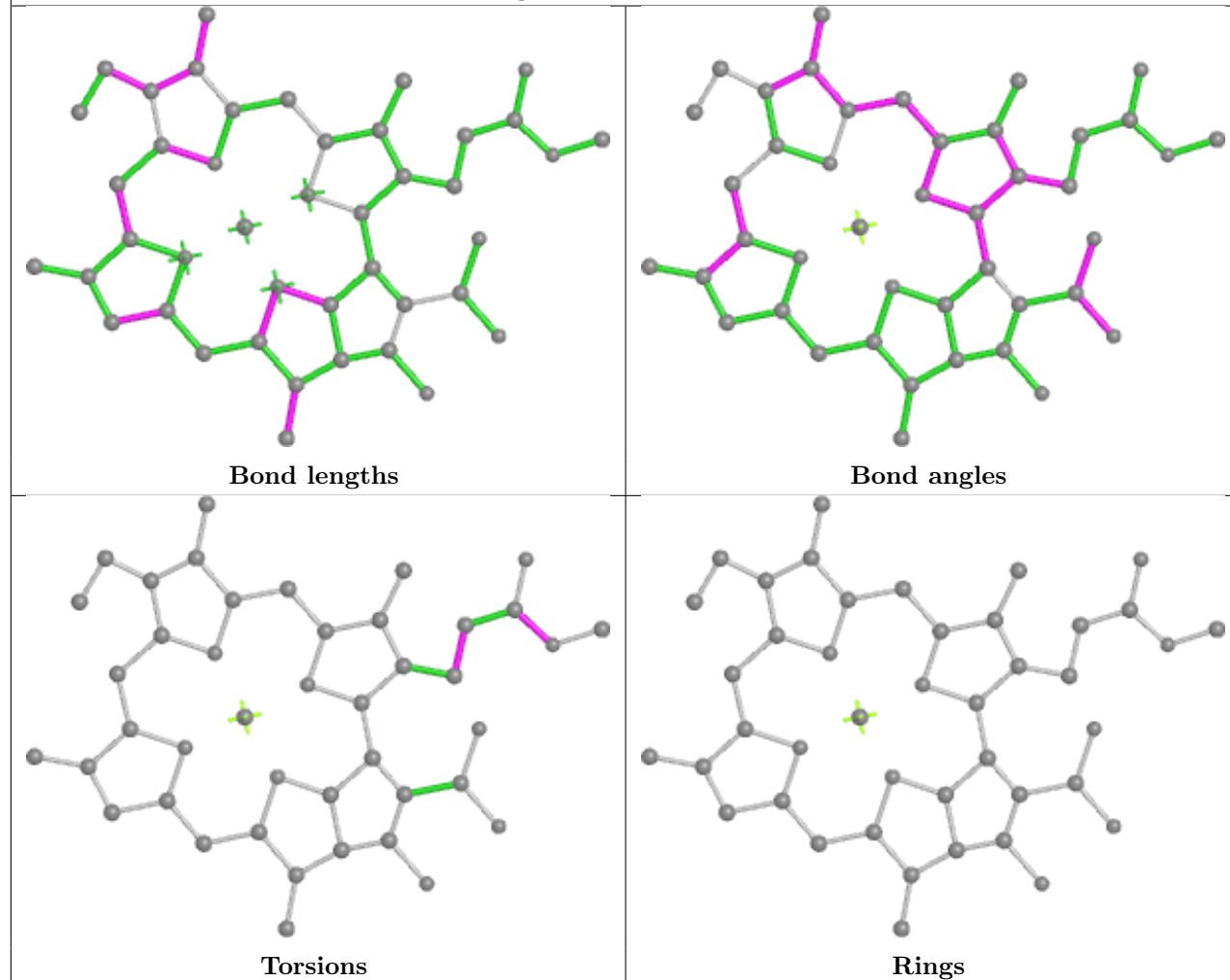
Rings

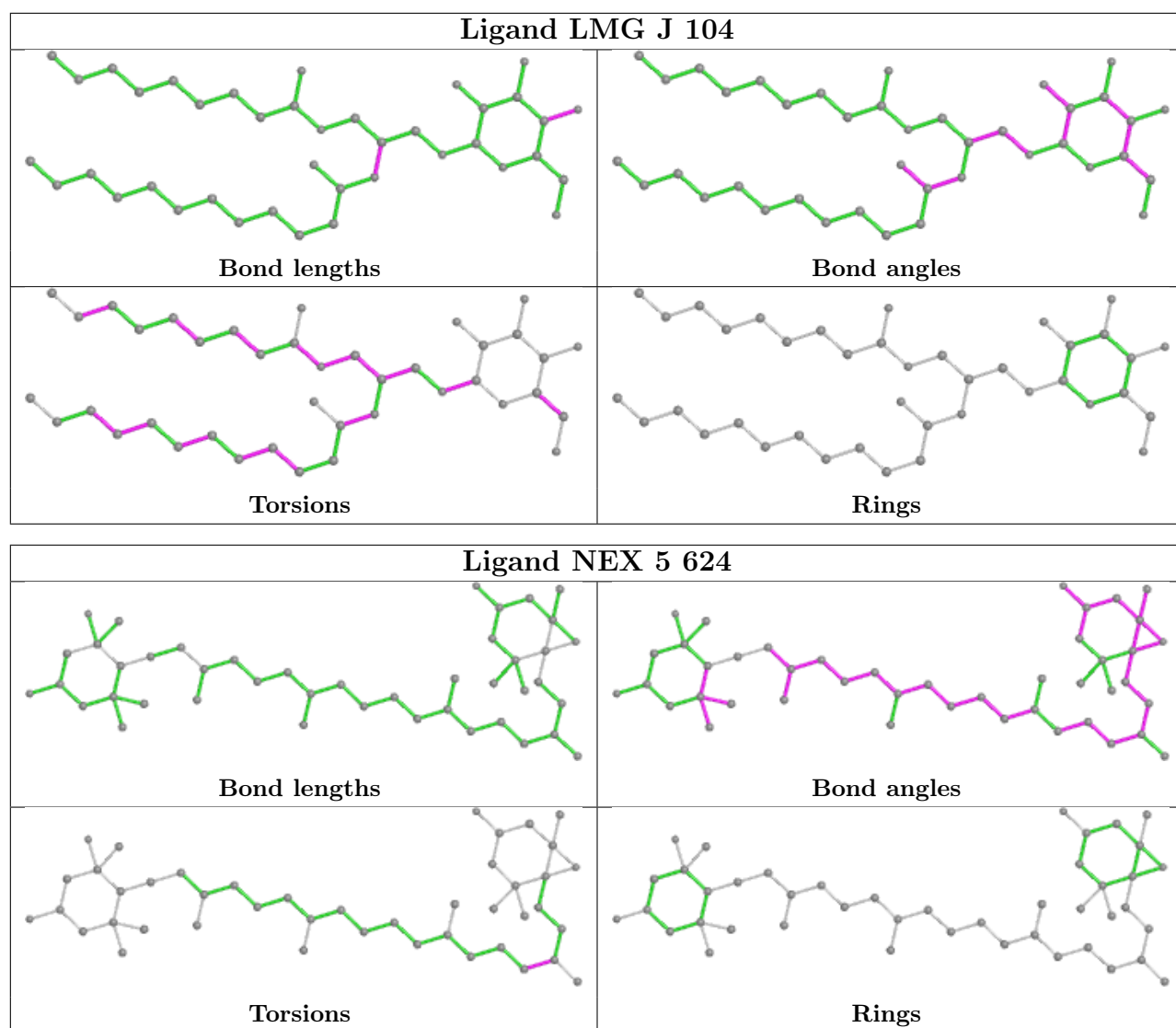
Ligand CLA 7 602**Ligand XAT 9 620****Ligand CLA 7 613**

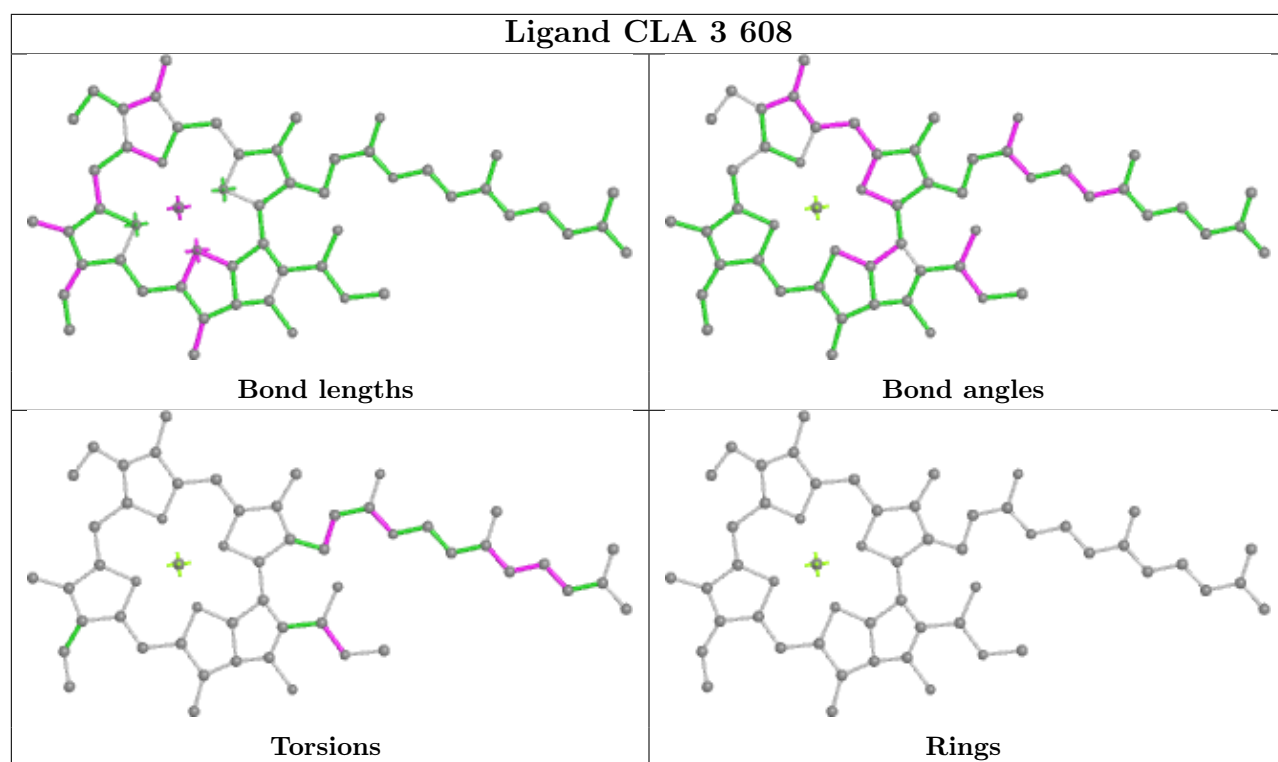
Ligand CLA 1 613



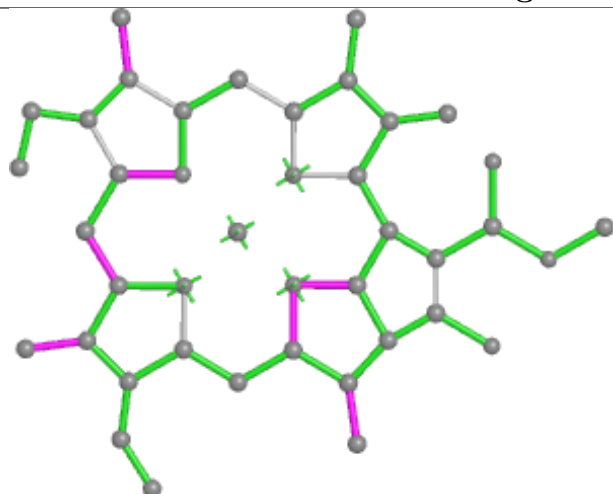
Ligand CLA B 821



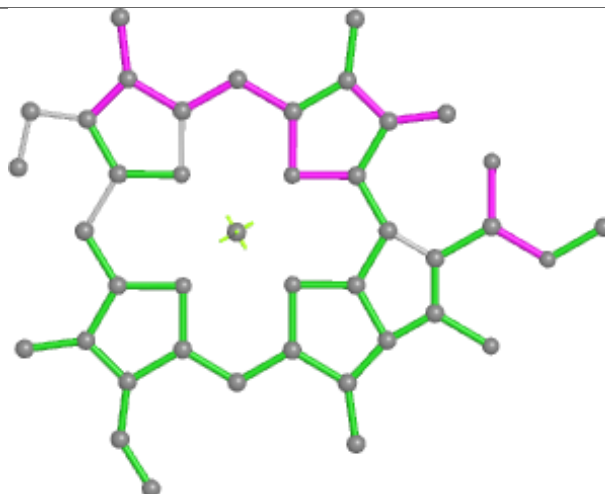




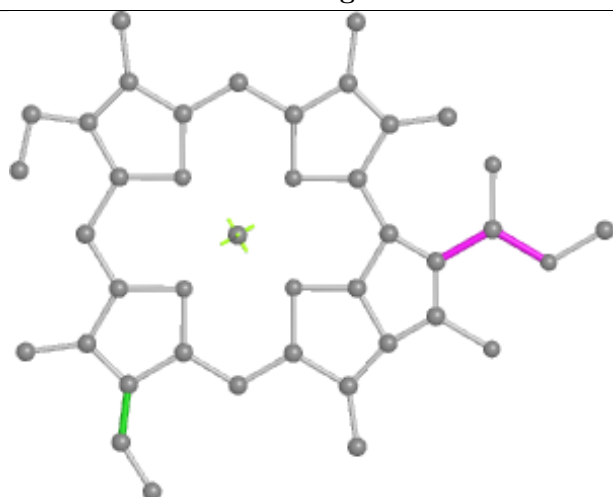
Ligand CLA F 304



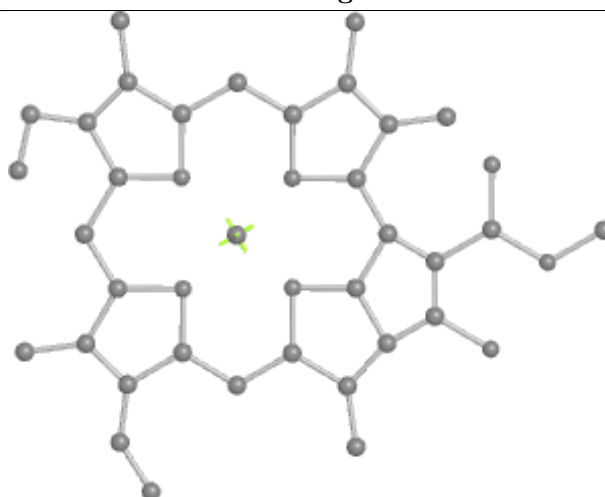
Bond lengths



Bond angles

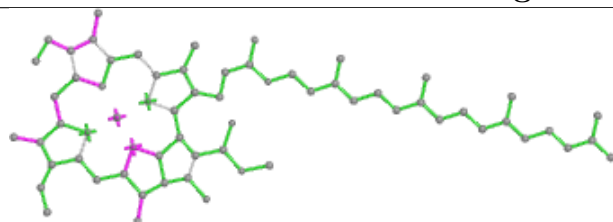


Torsions

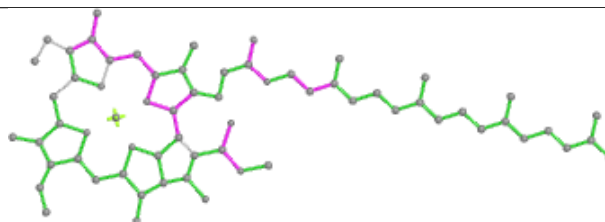


Rings

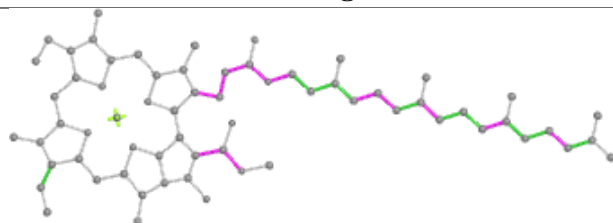
Ligand CLA A 841



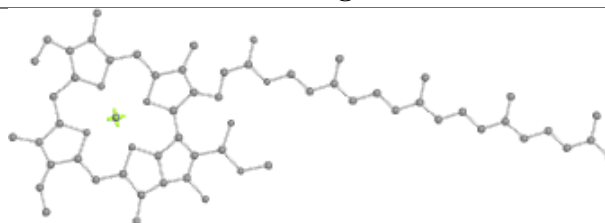
Bond lengths



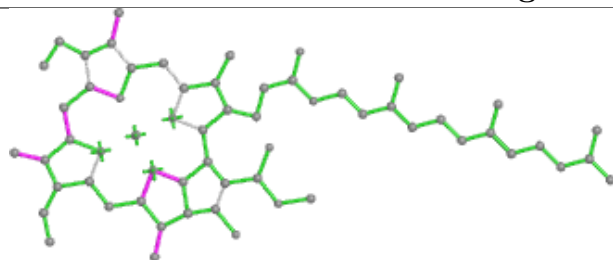
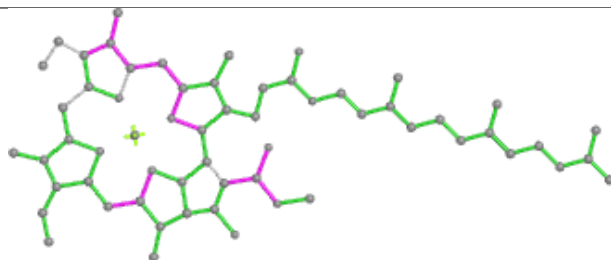
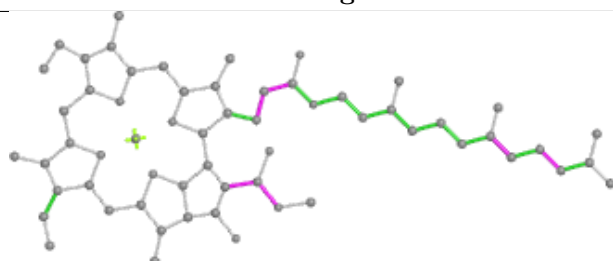
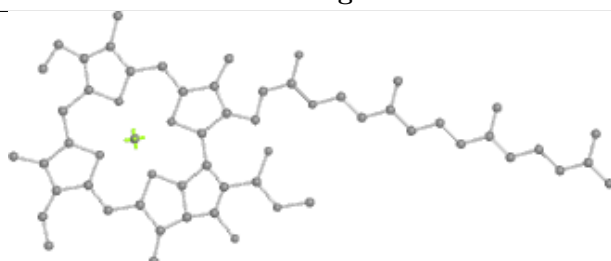
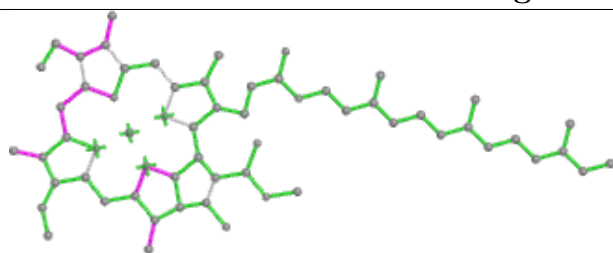
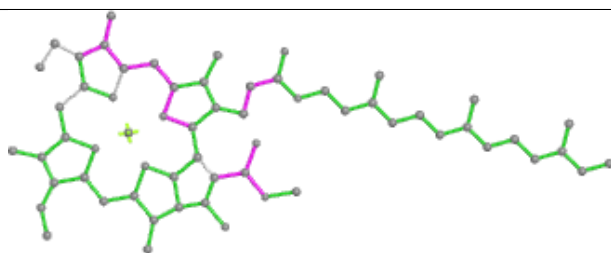
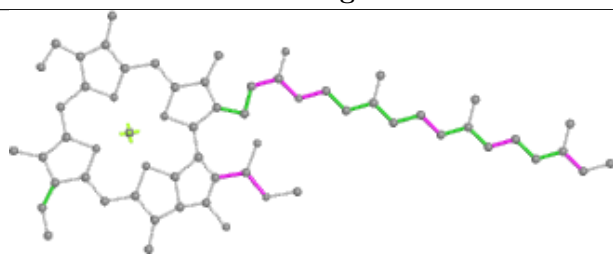
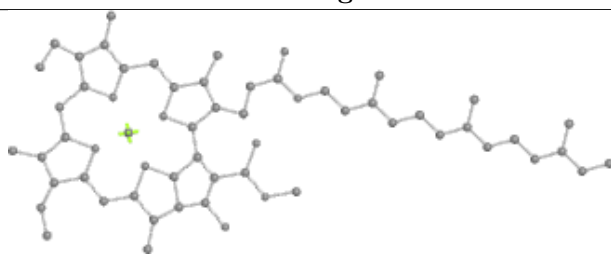
Bond angles

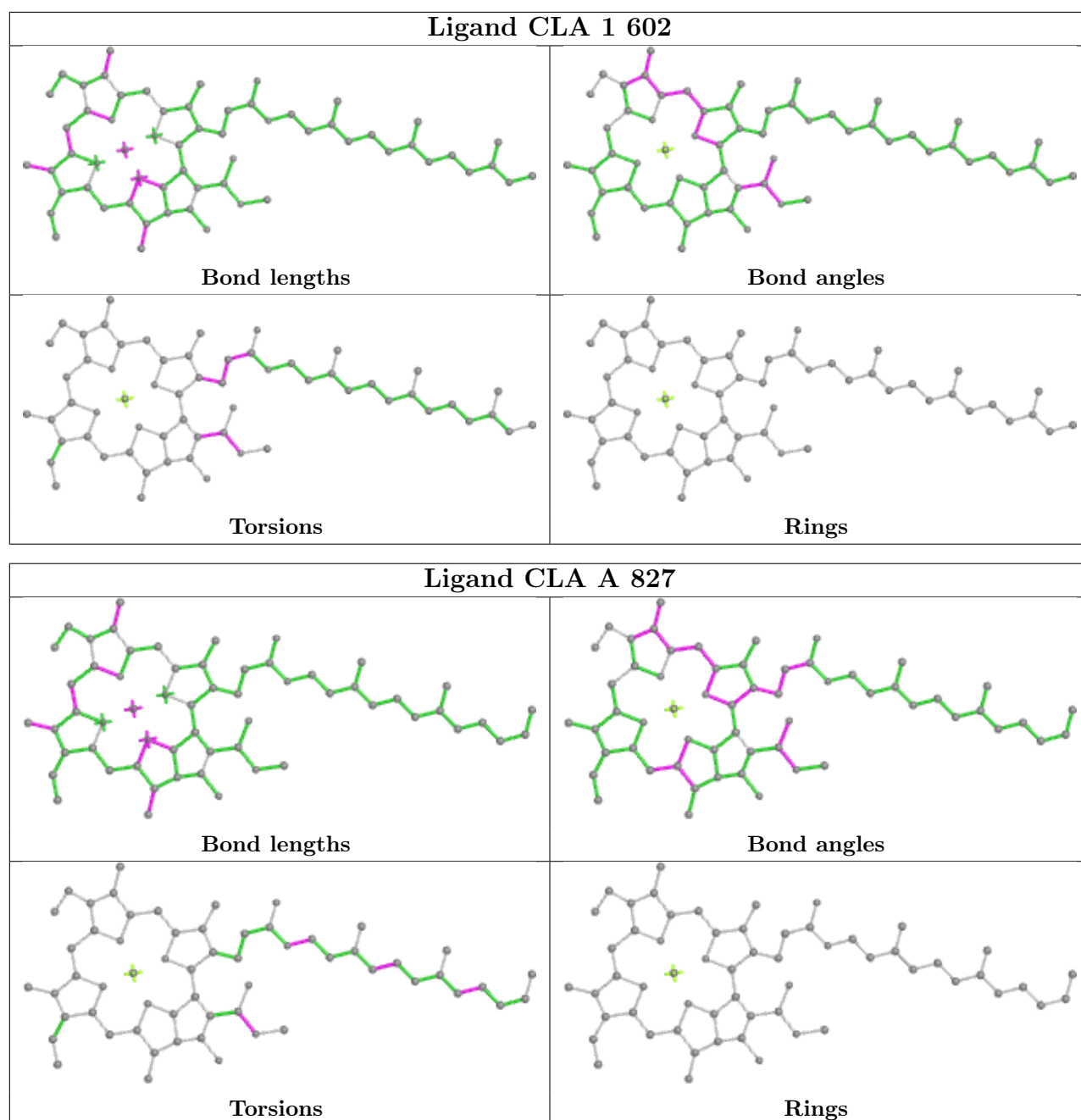


Torsions

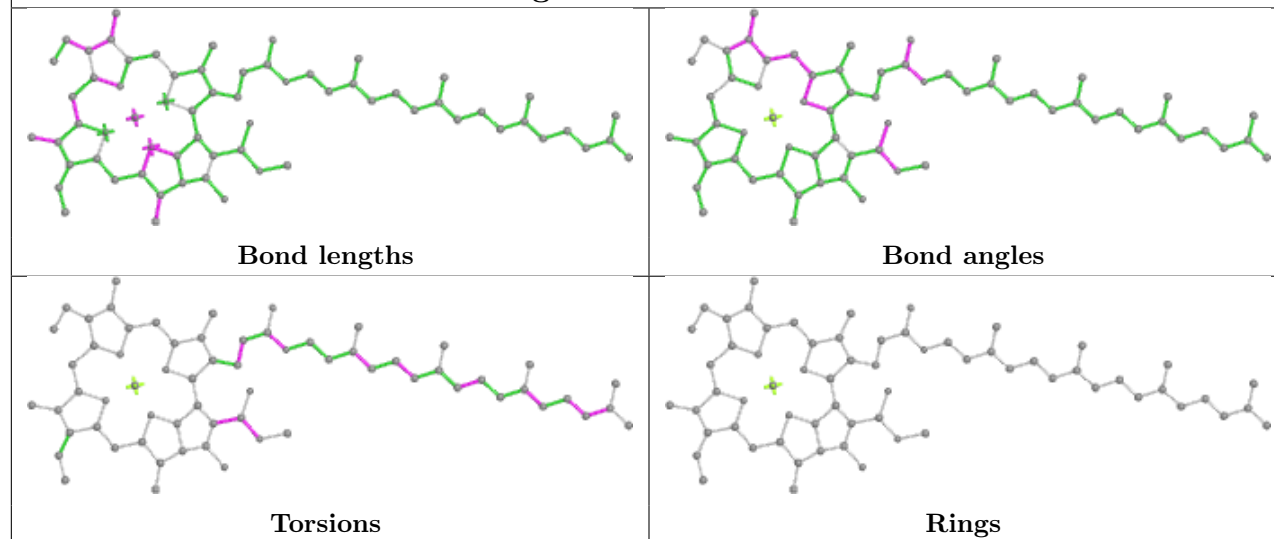


Rings

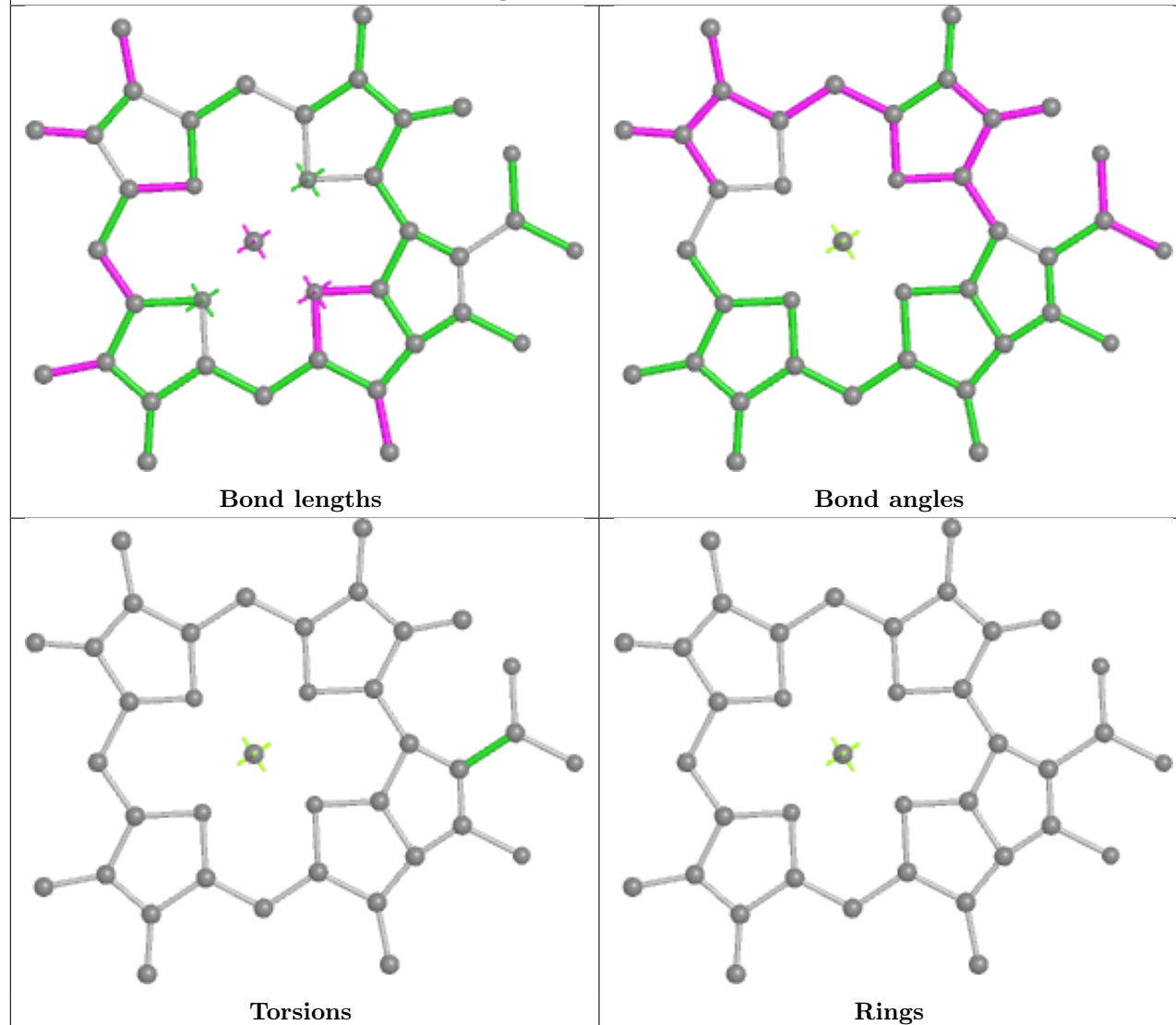
Ligand CLA 4 602**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 835****Bond lengths****Bond angles****Torsions****Rings**

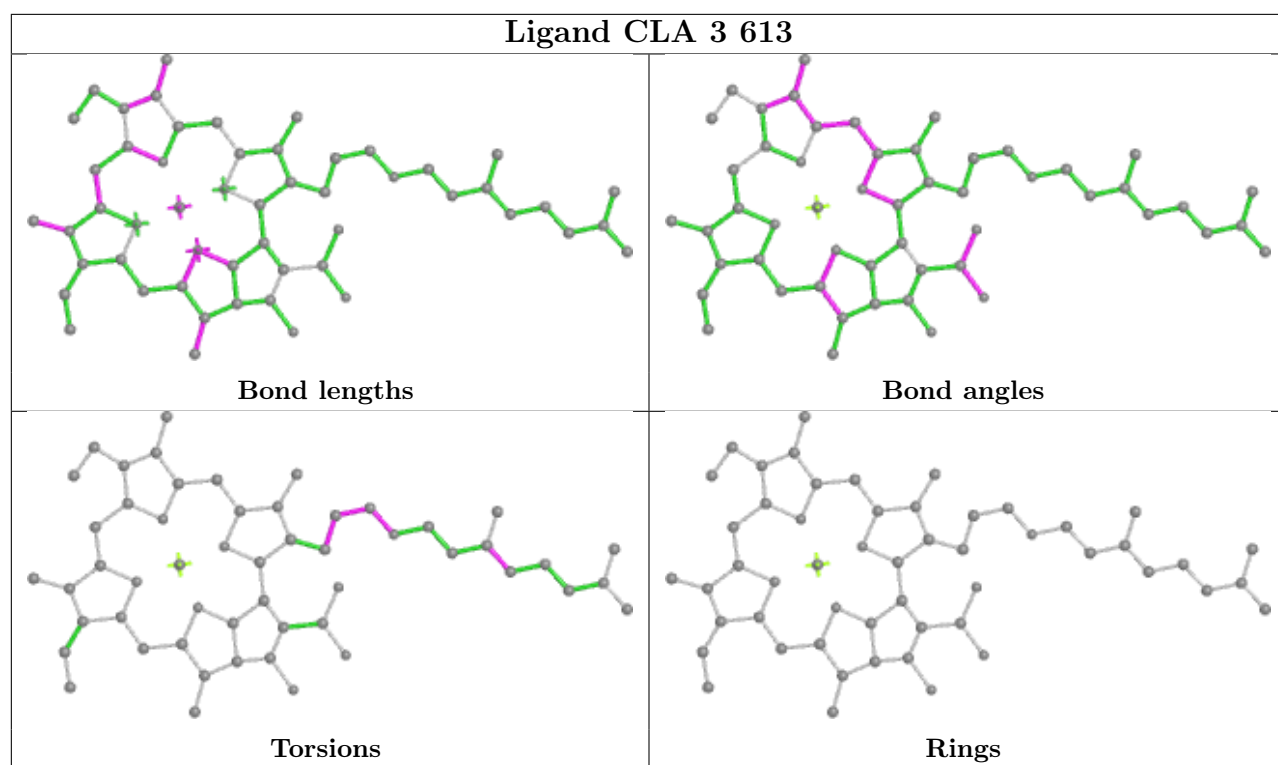


Ligand CLA B 837

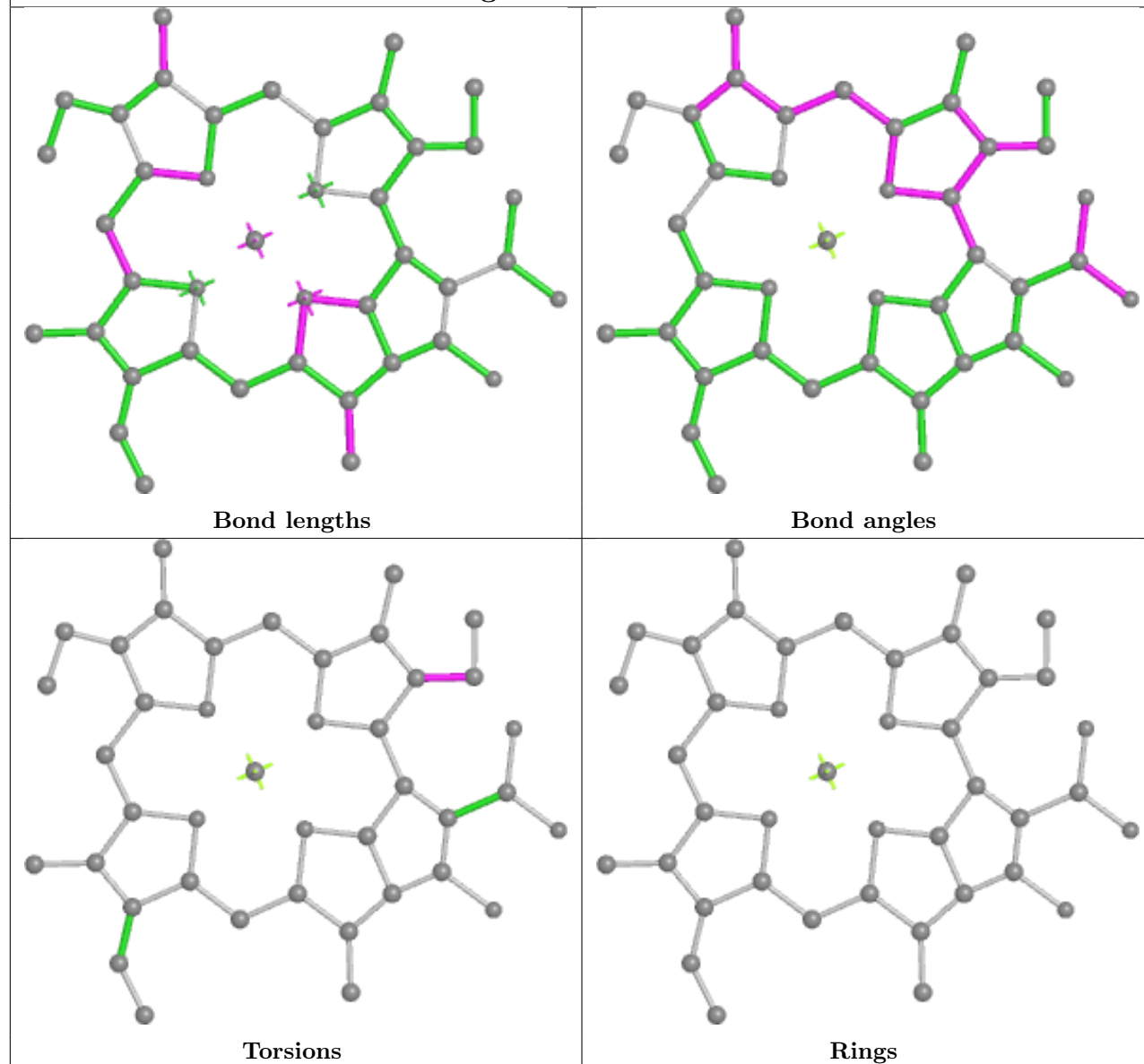


Ligand CLA a 611

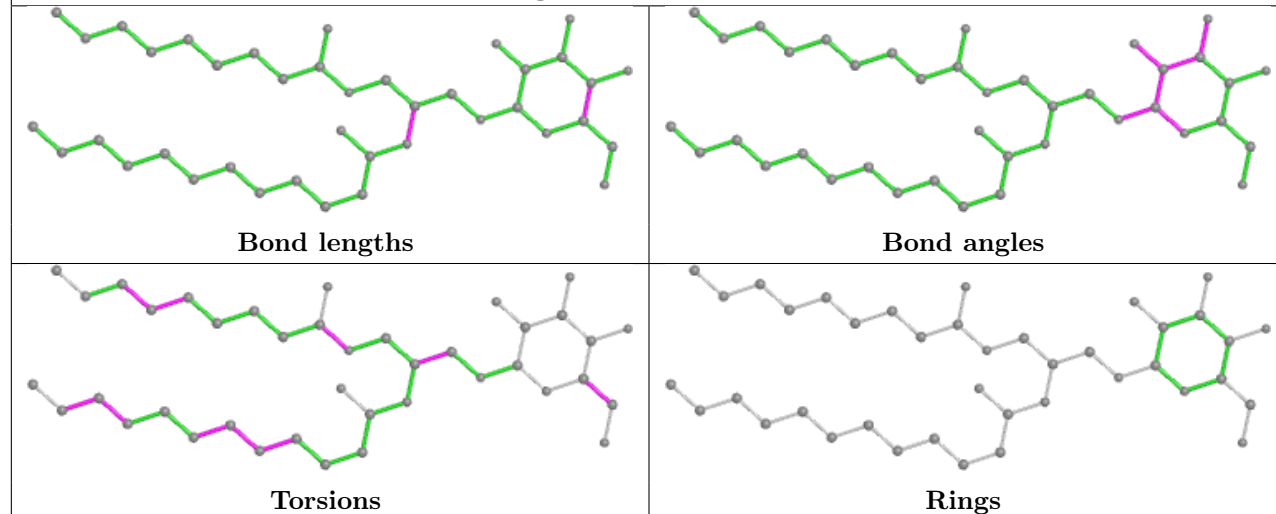


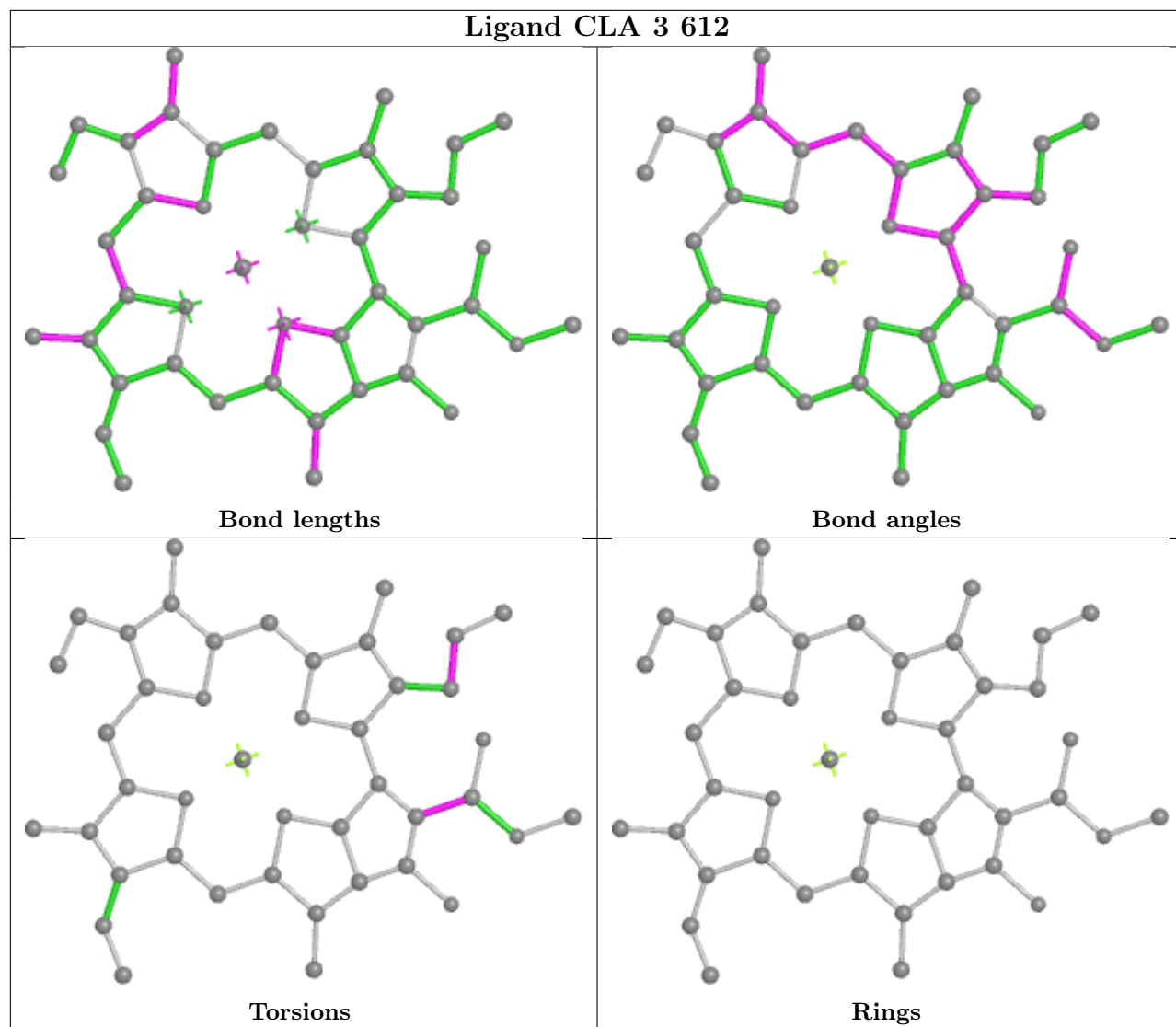
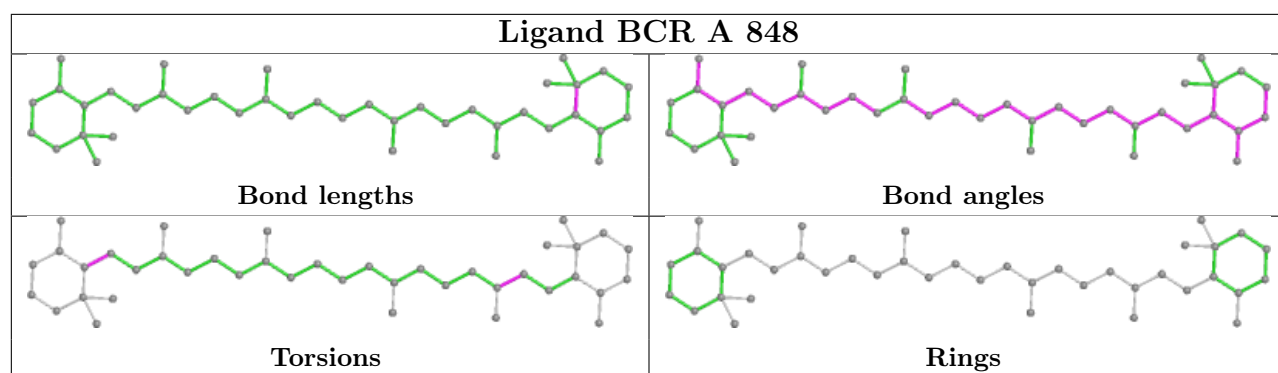


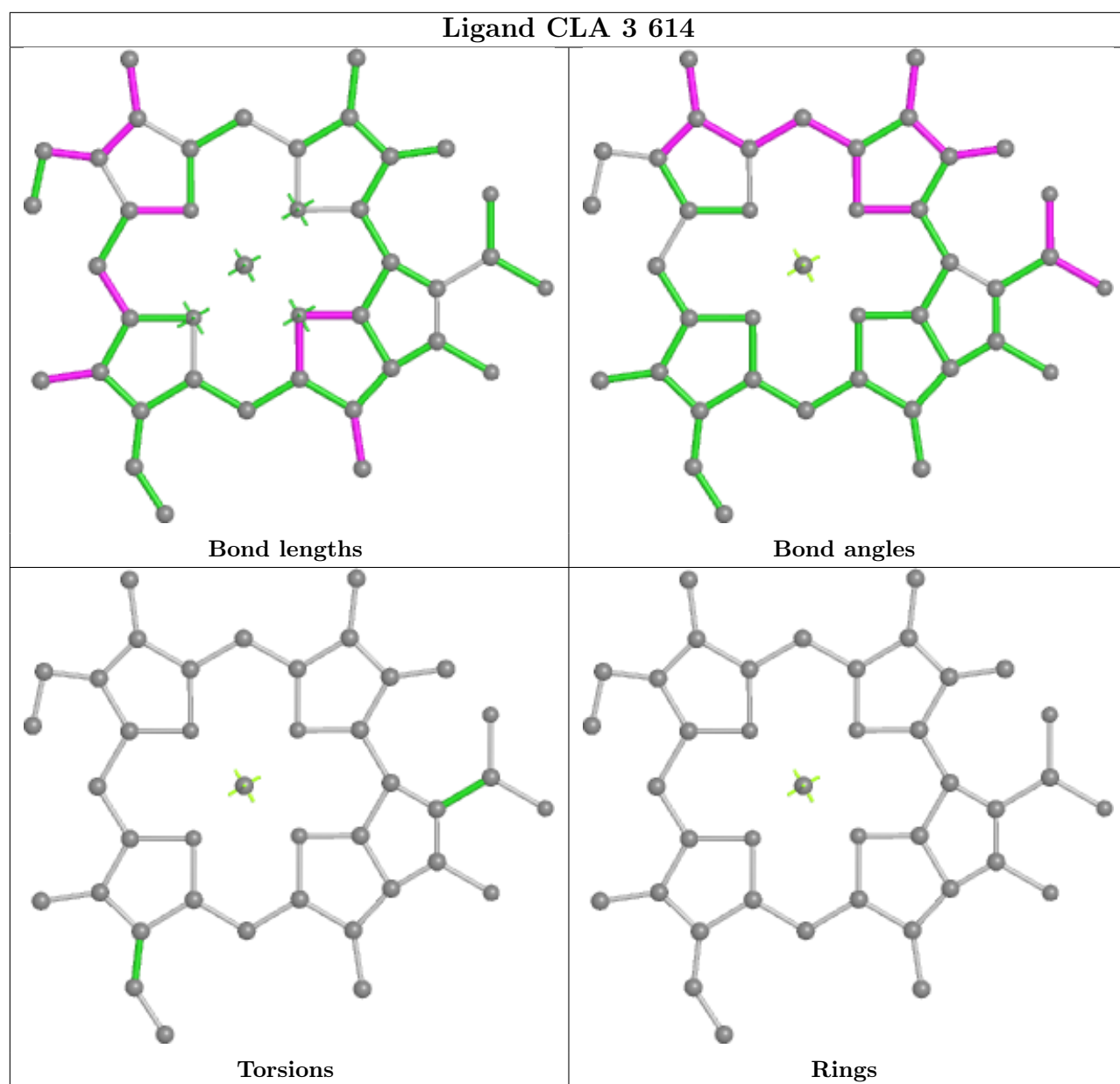
Ligand CLA 6 612

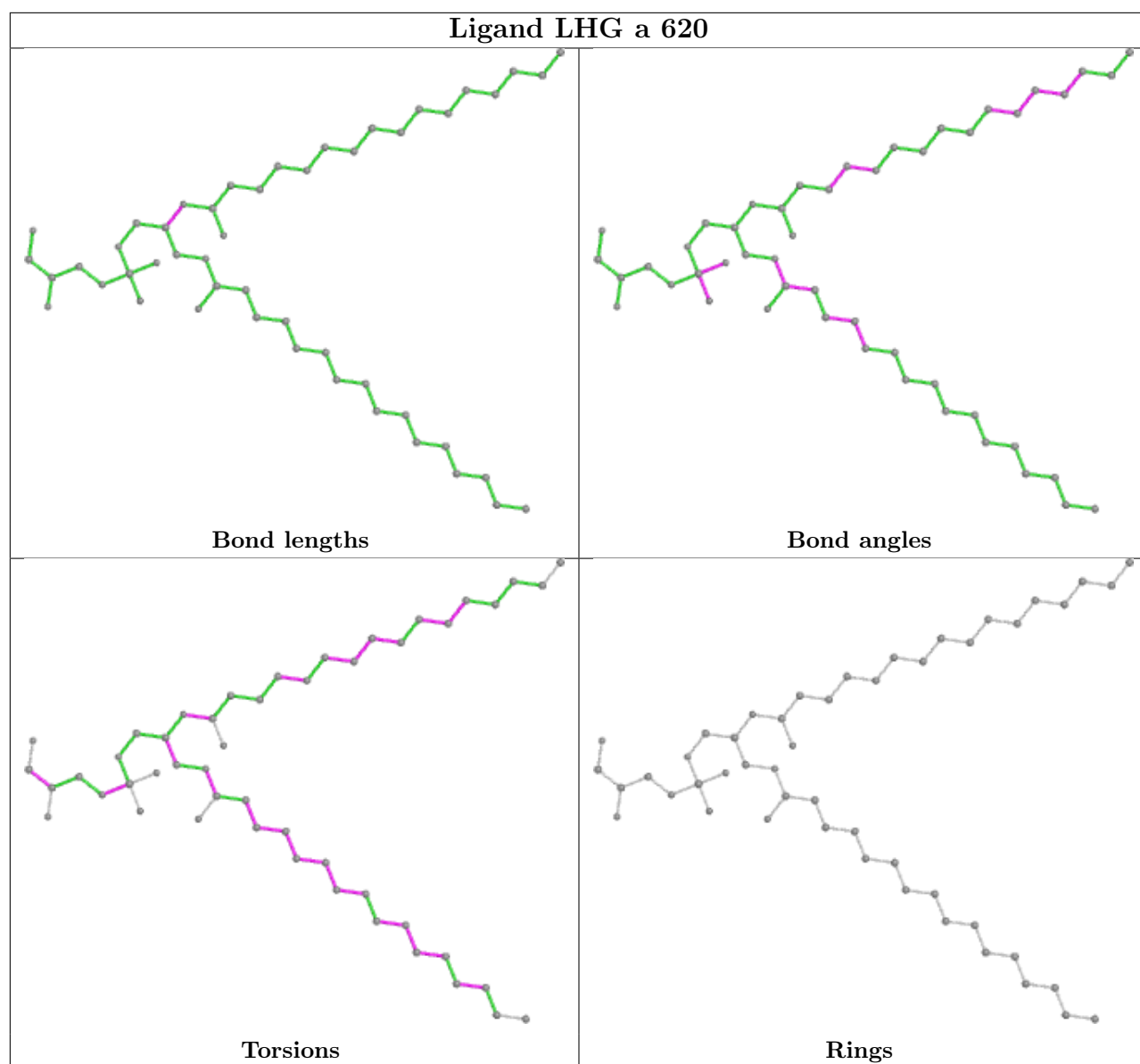


Ligand LMG 5 627

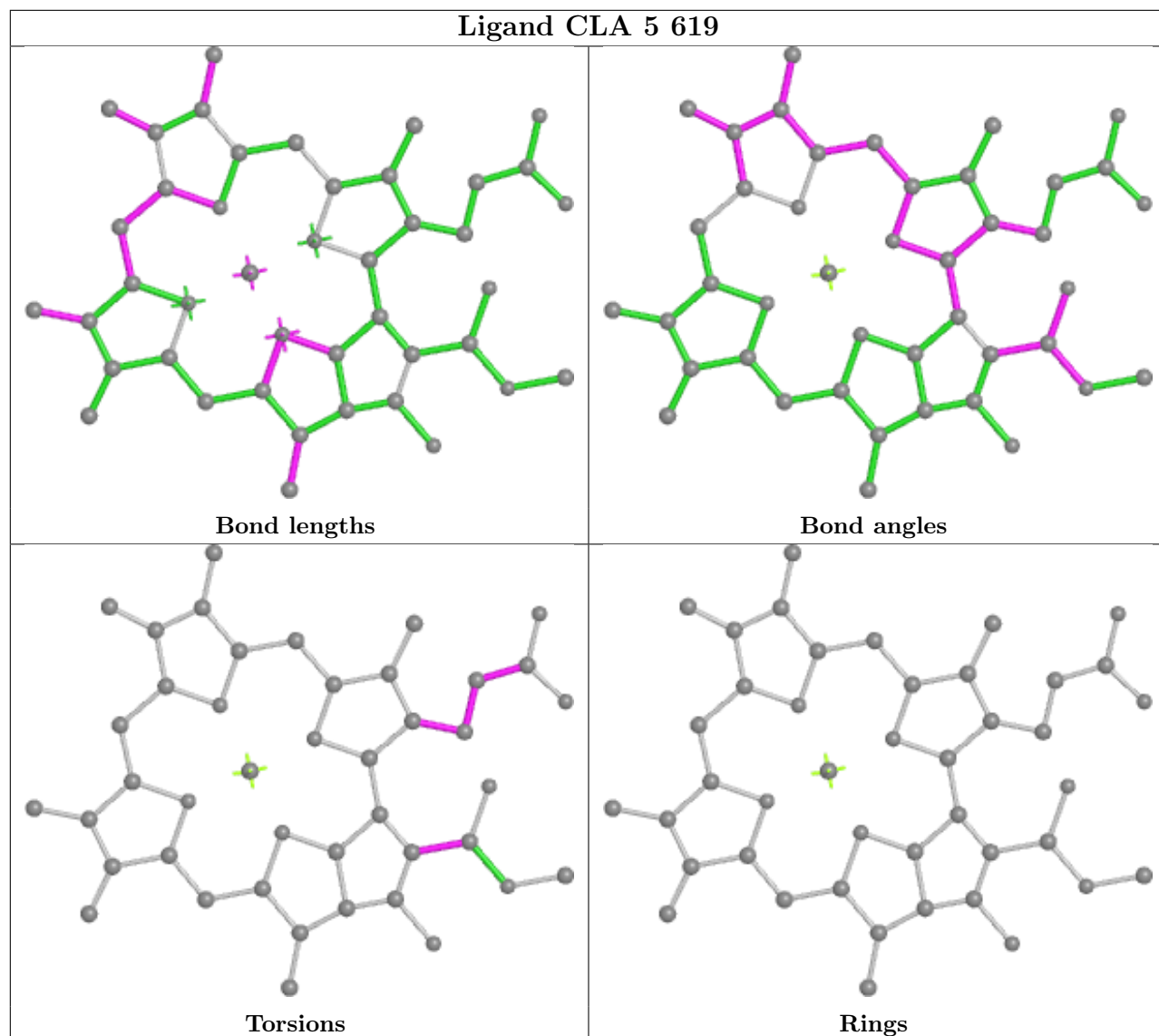




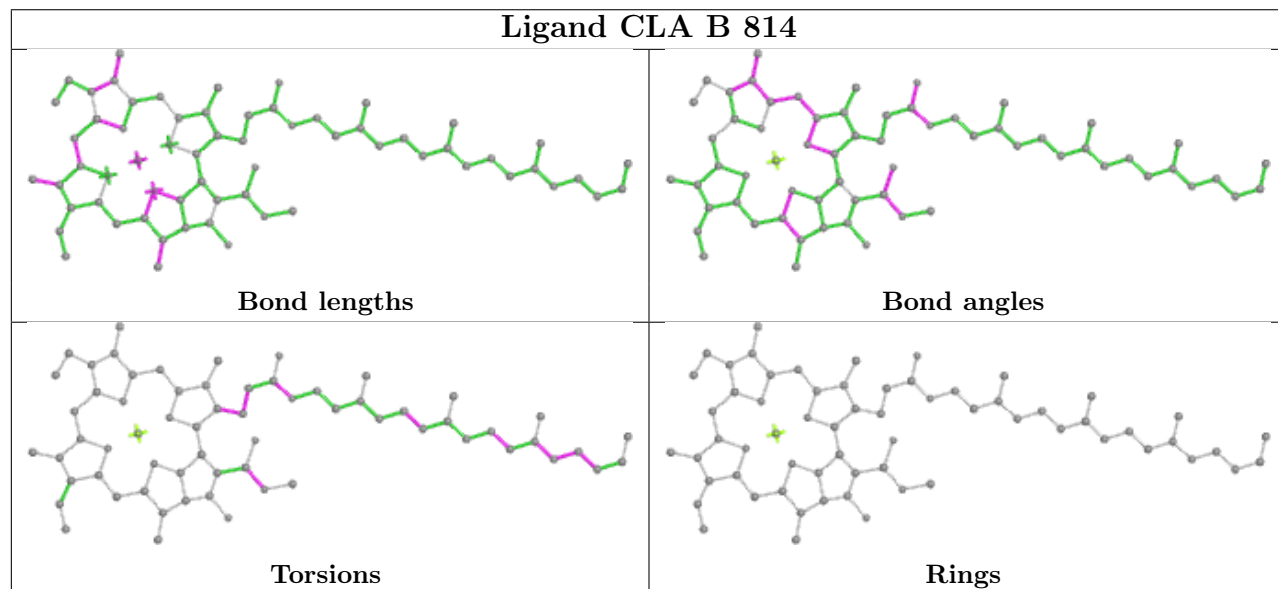


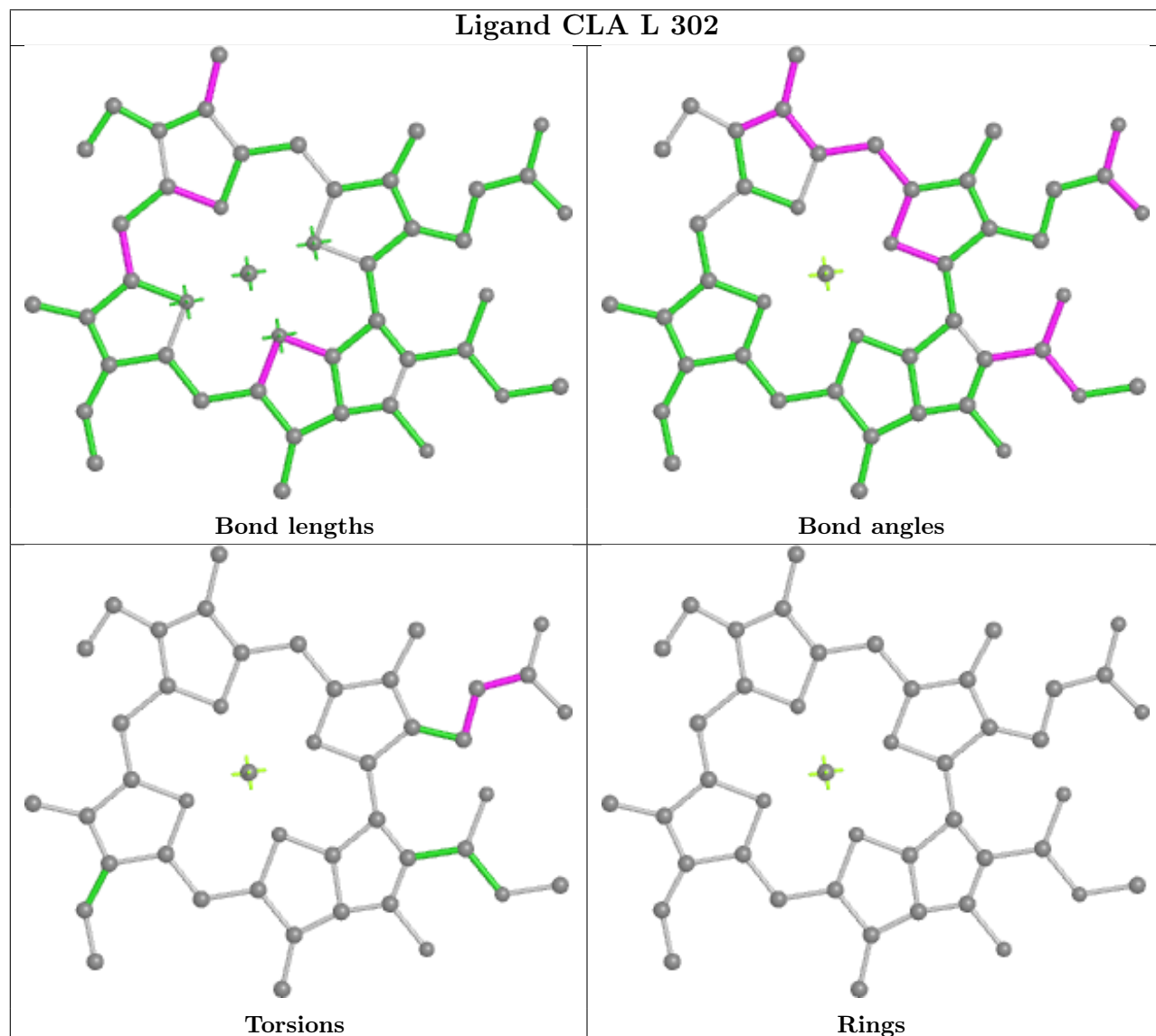
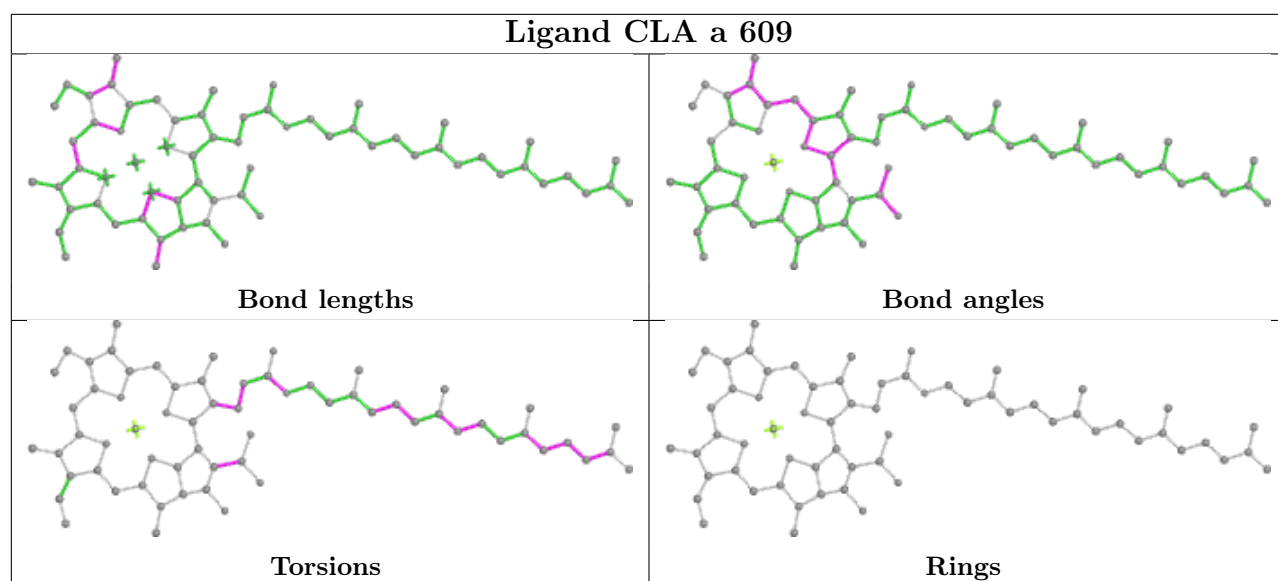


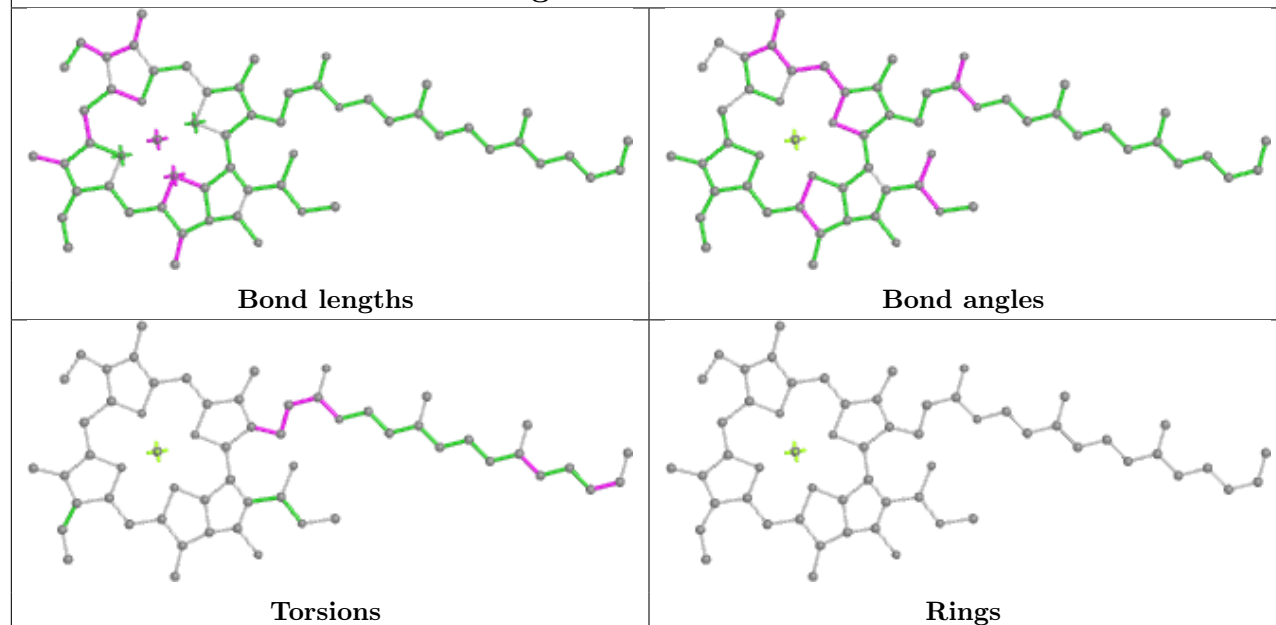
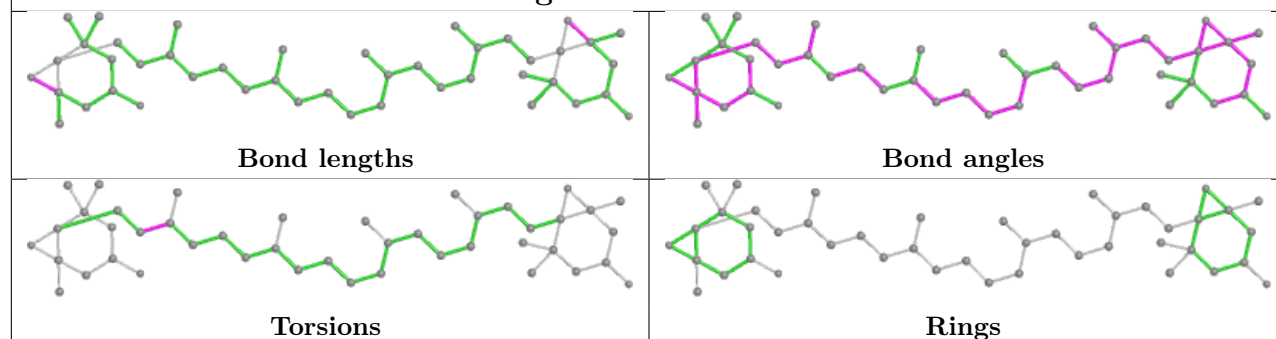
Ligand CLA 5 619



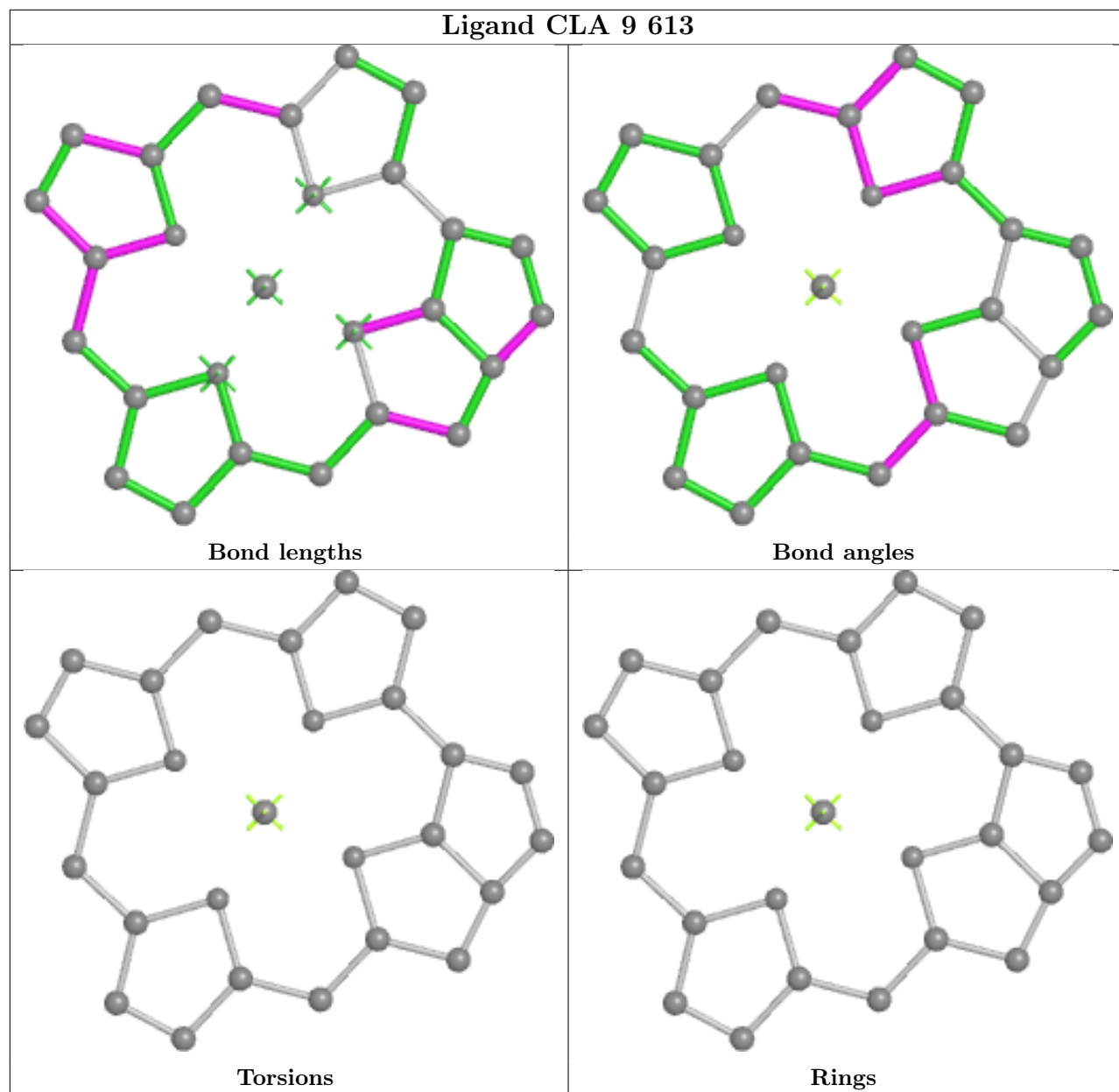
Ligand CLA B 814



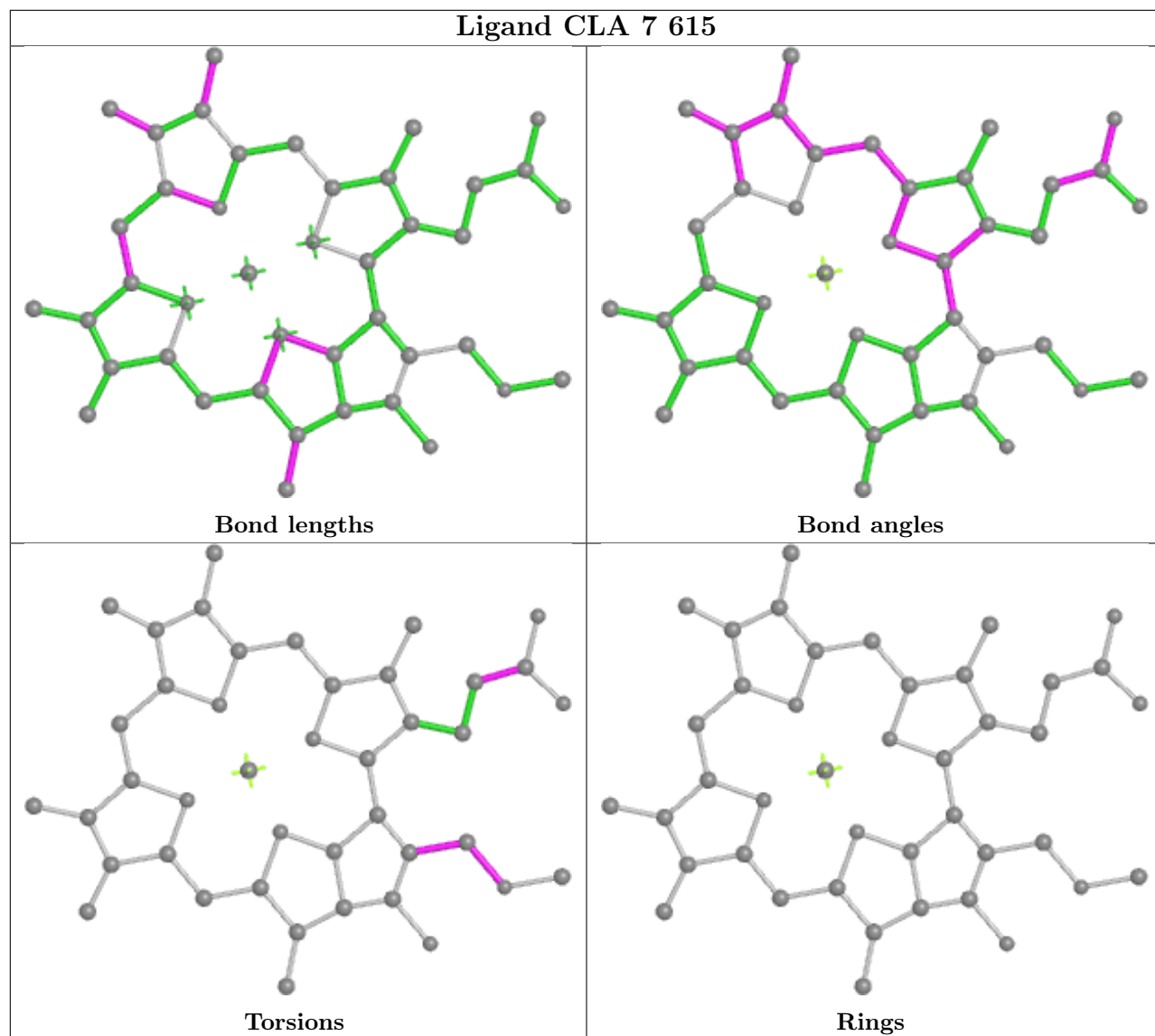


Ligand CLA A 819**Ligand XAT 8 620**

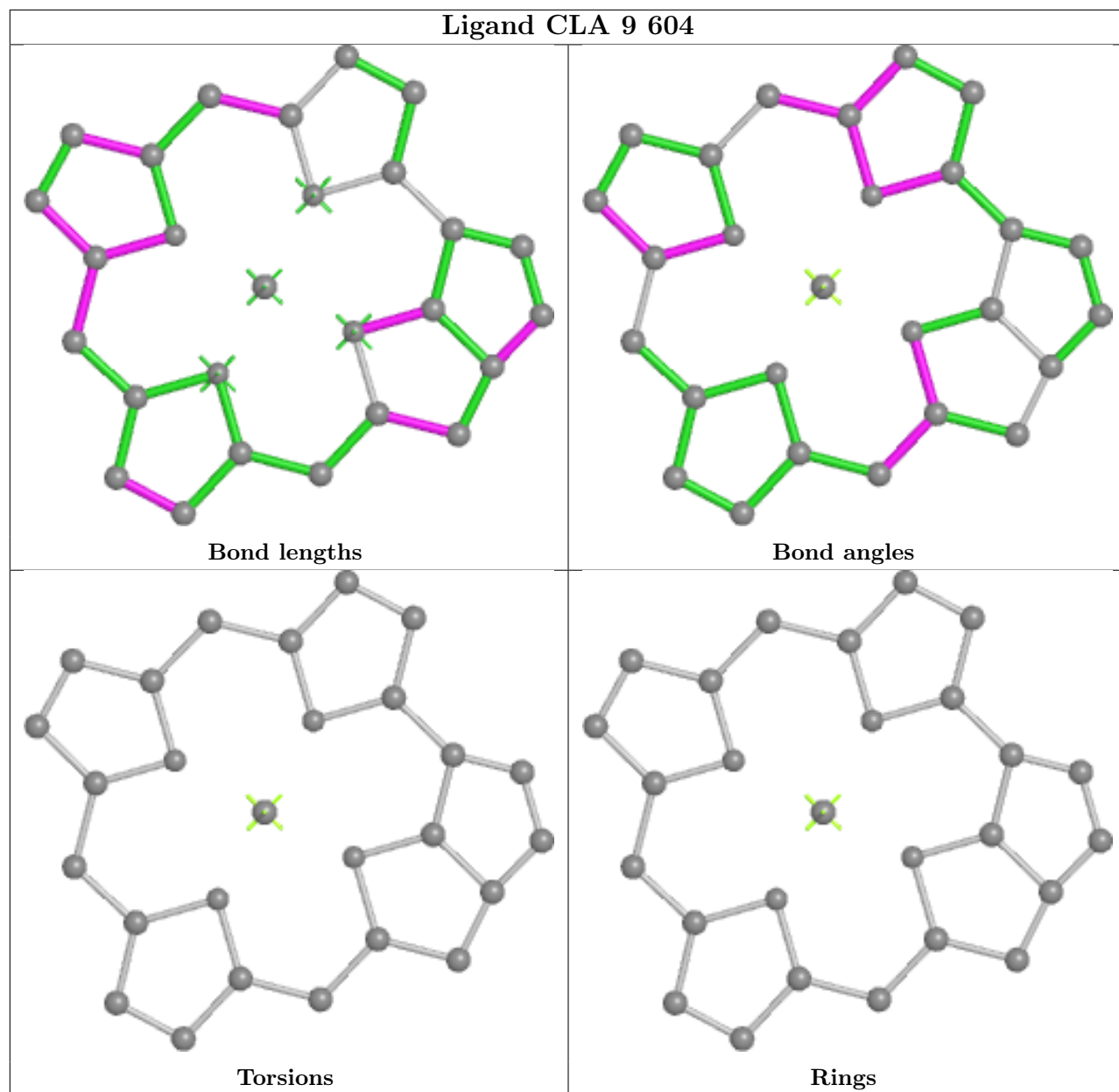
Ligand CLA 9 613

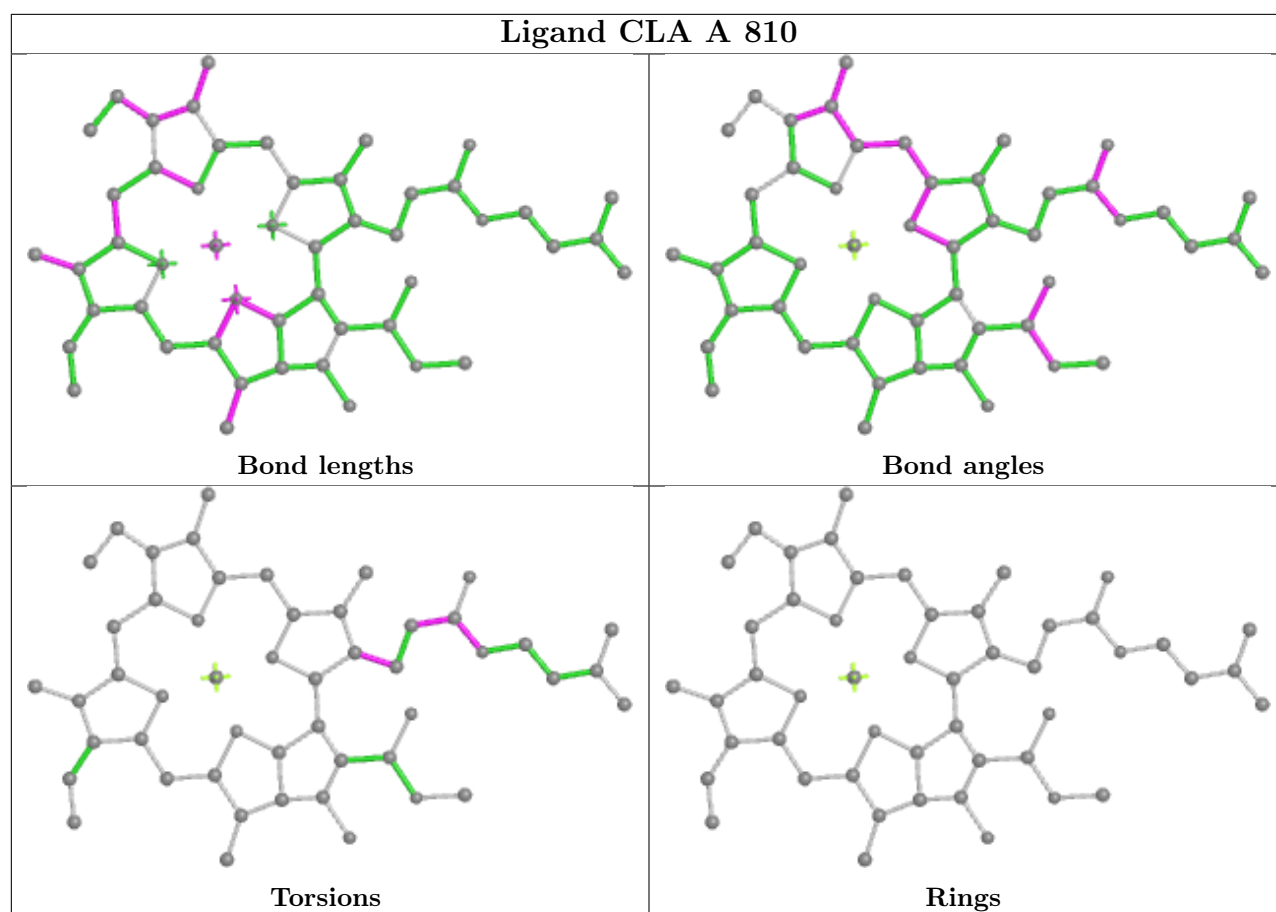


Ligand CLA 7 615

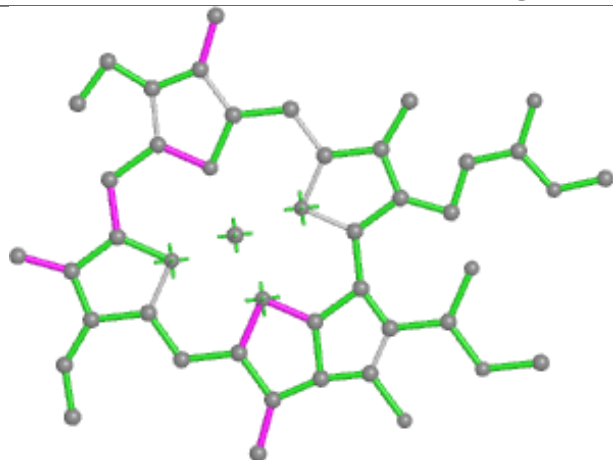


Ligand CLA 9 604

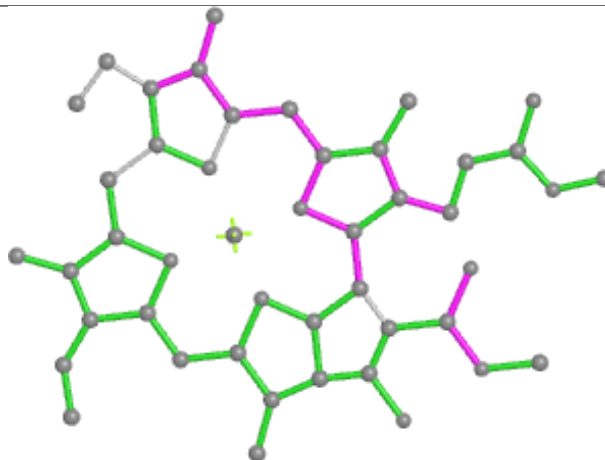




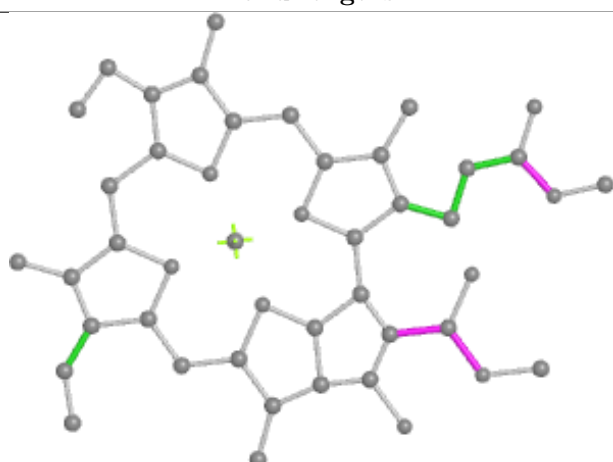
Ligand CLA K 204



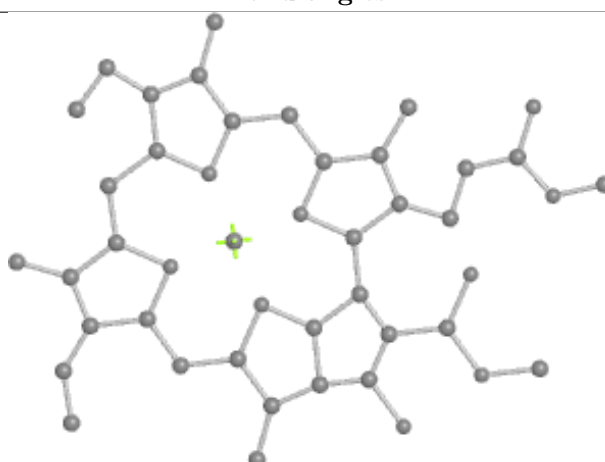
Bond lengths



Bond angles

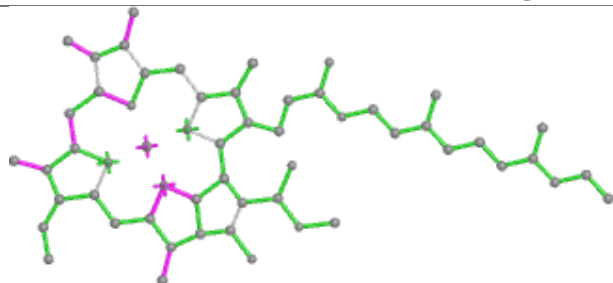


Torsions

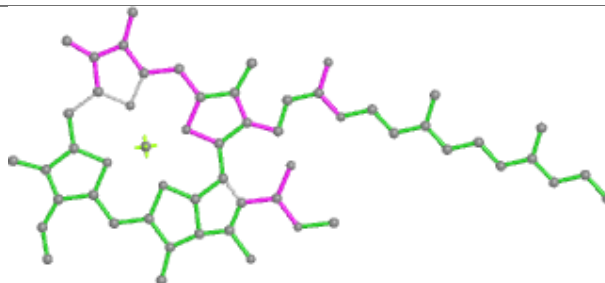


Rings

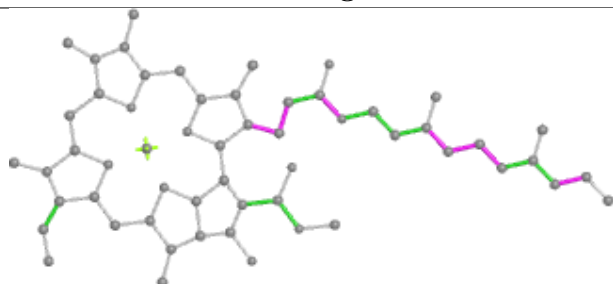
Ligand CLA 3 607



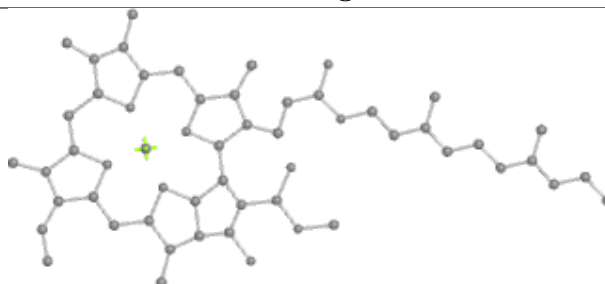
Bond lengths



Bond angles

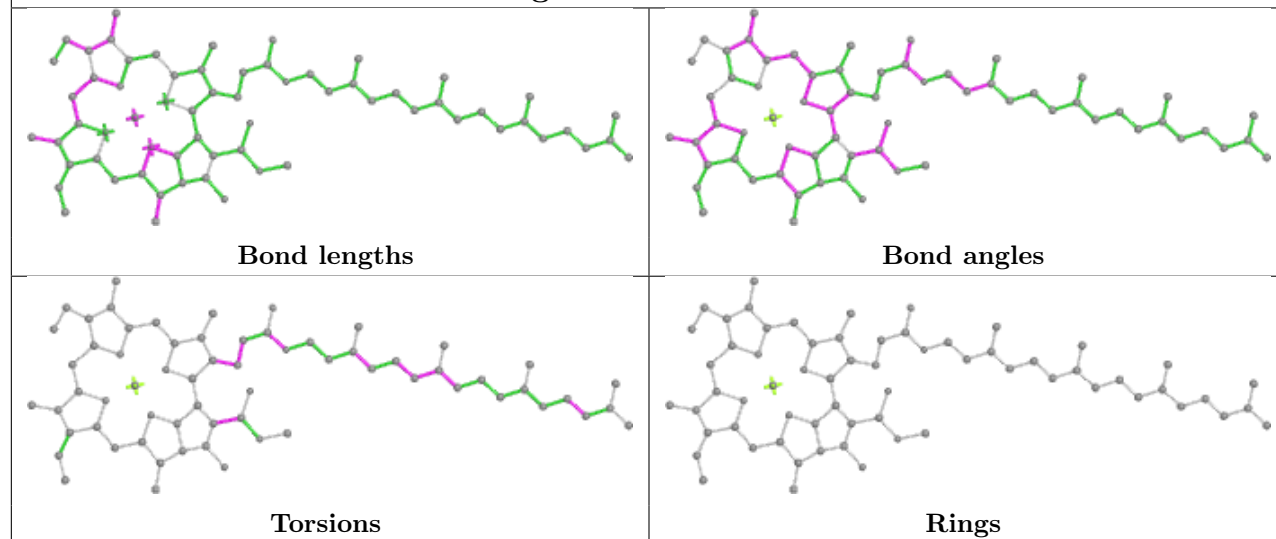


Torsions

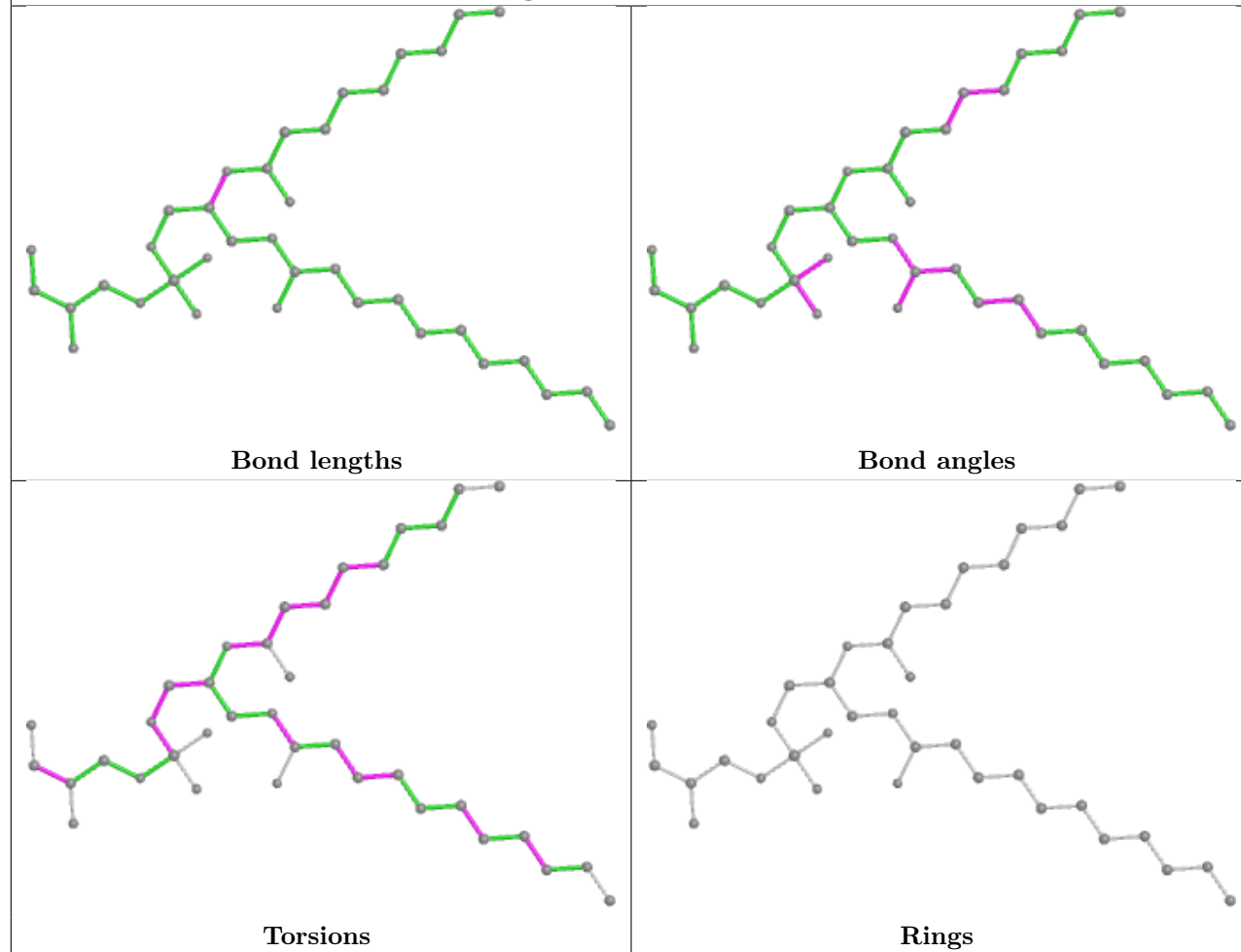


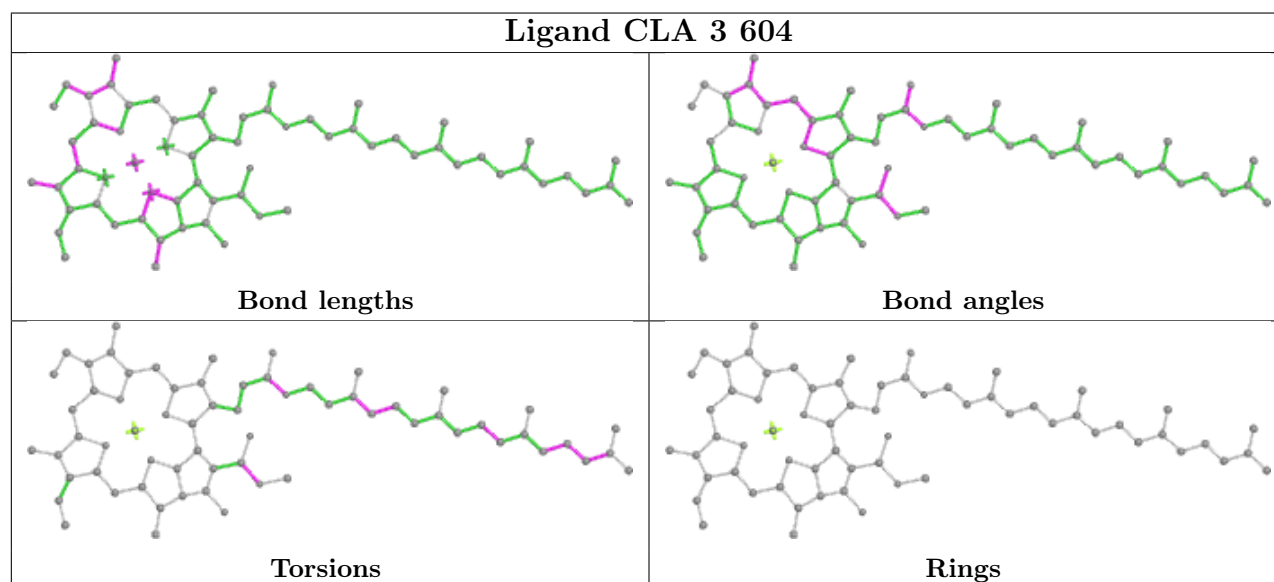
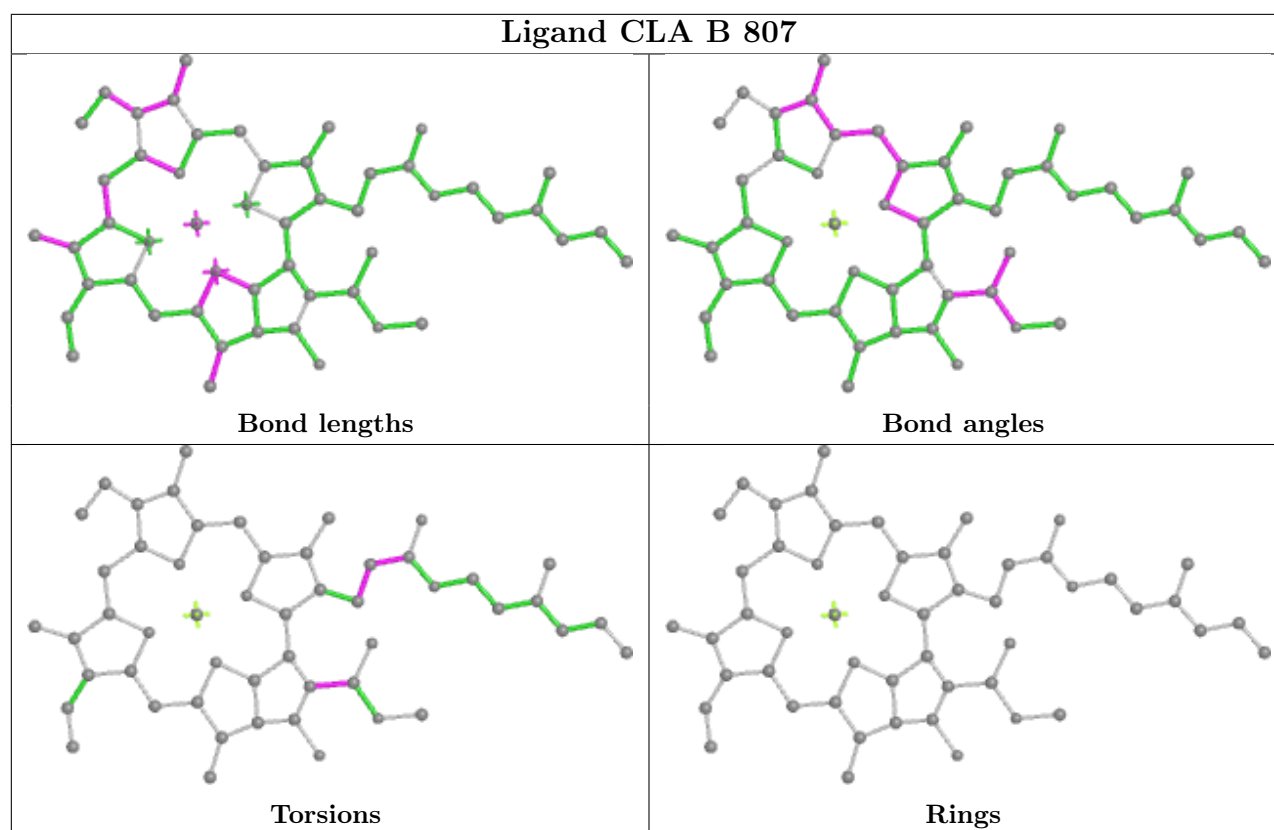
Rings

Ligand CLA A 820

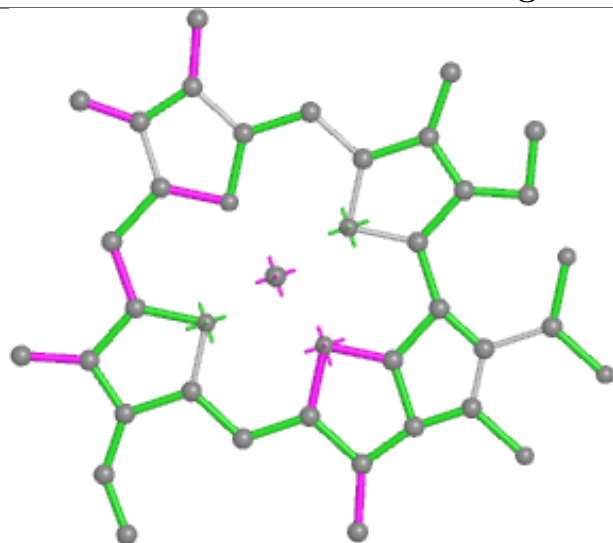


Ligand LHG 2 622

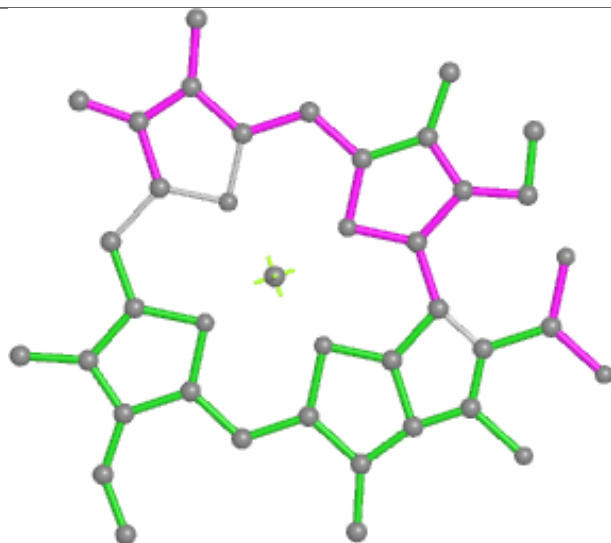




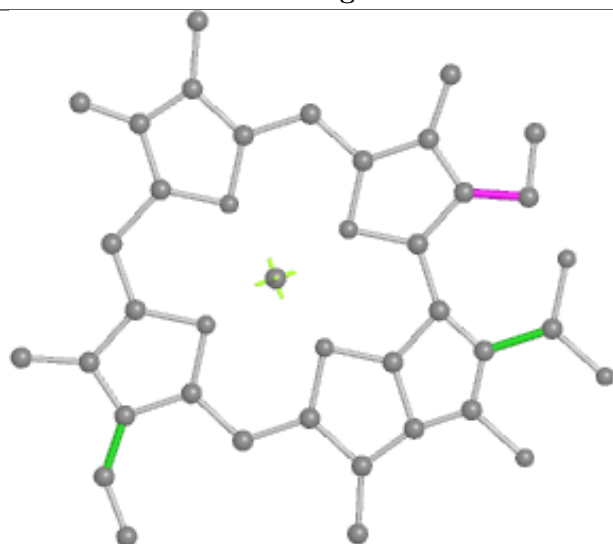
Ligand CLA 6 618



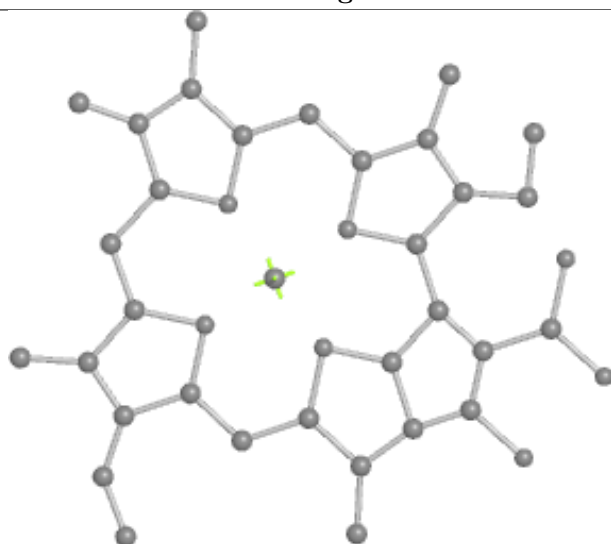
Bond lengths



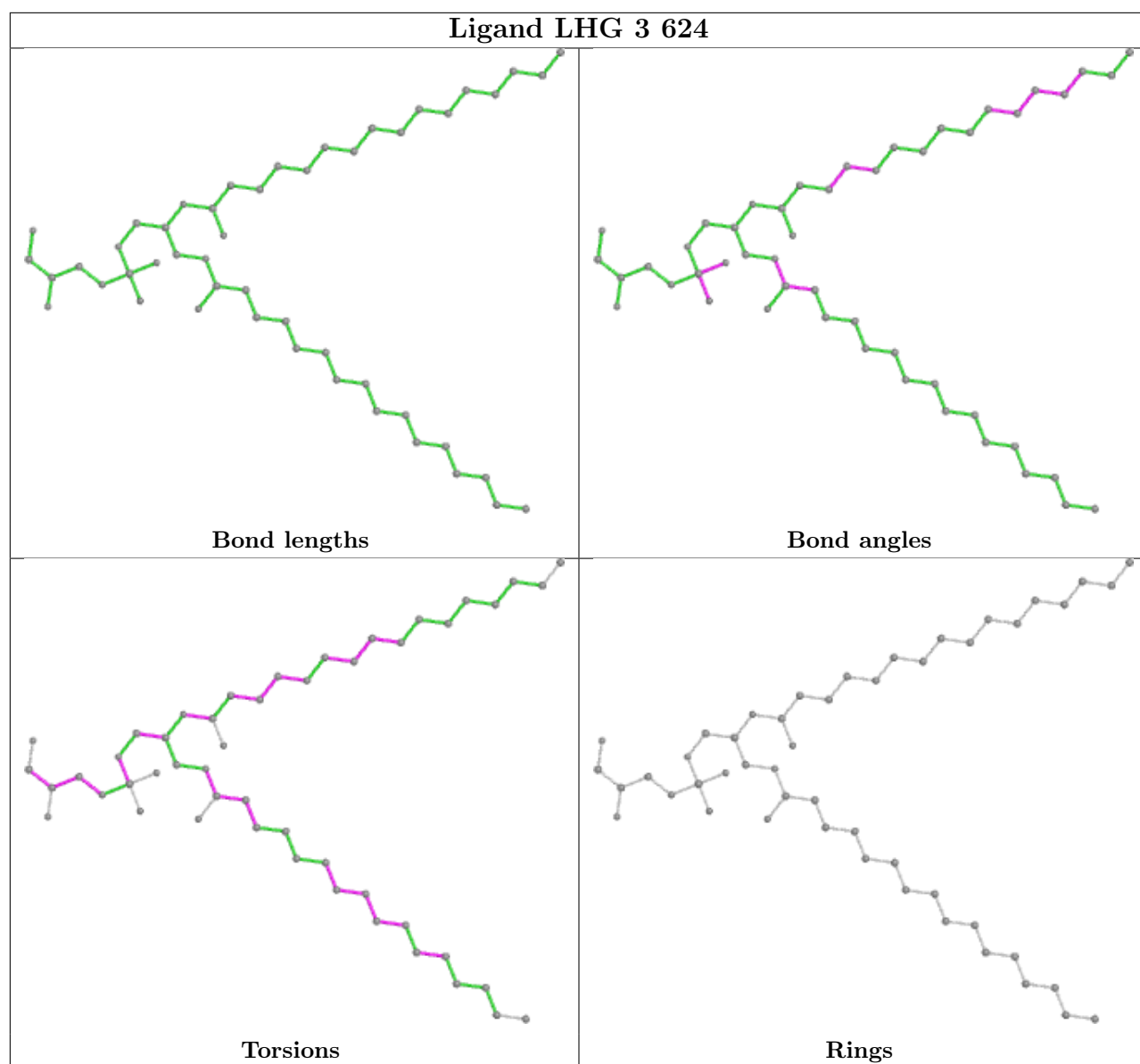
Bond angles



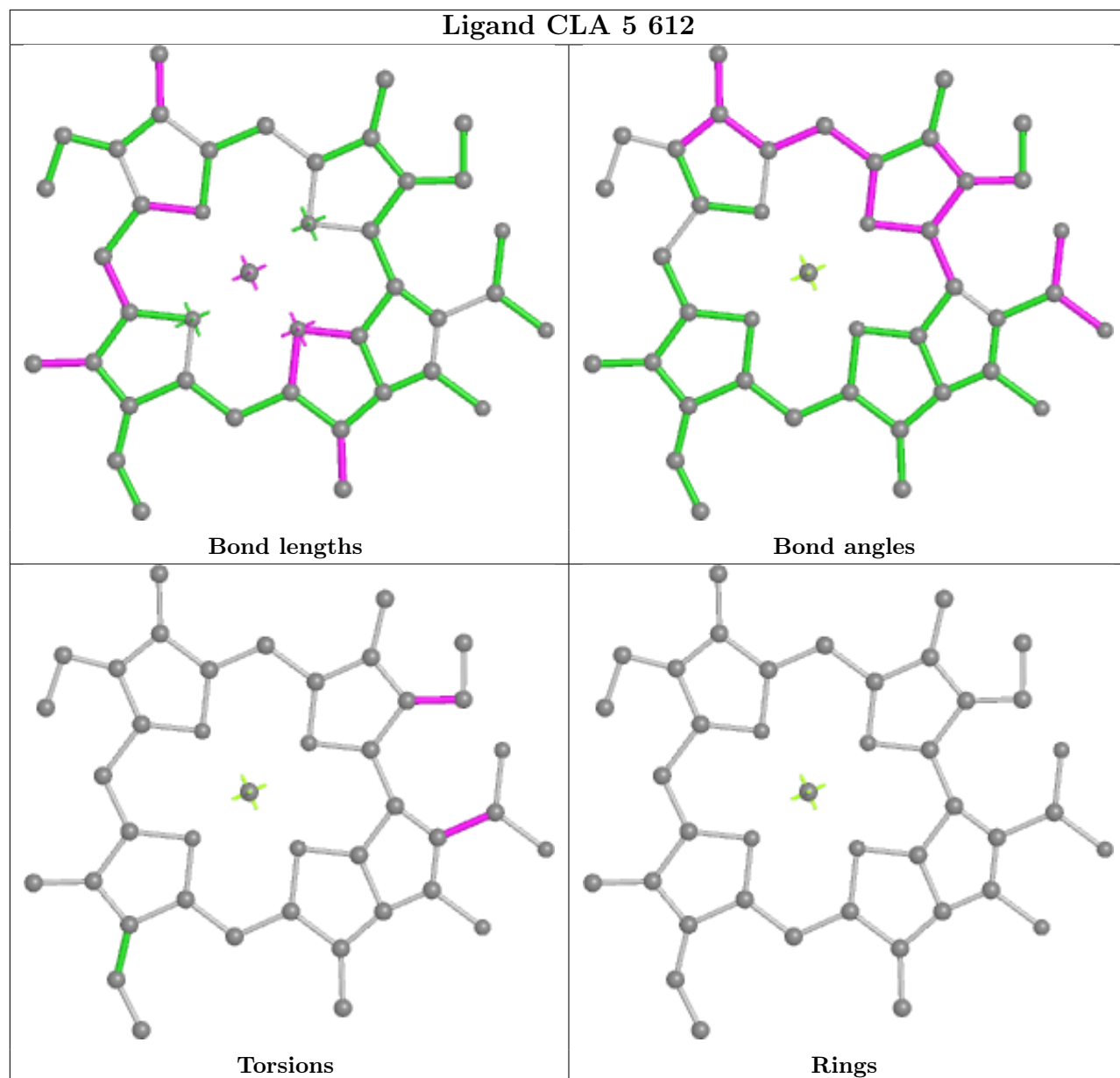
Torsions



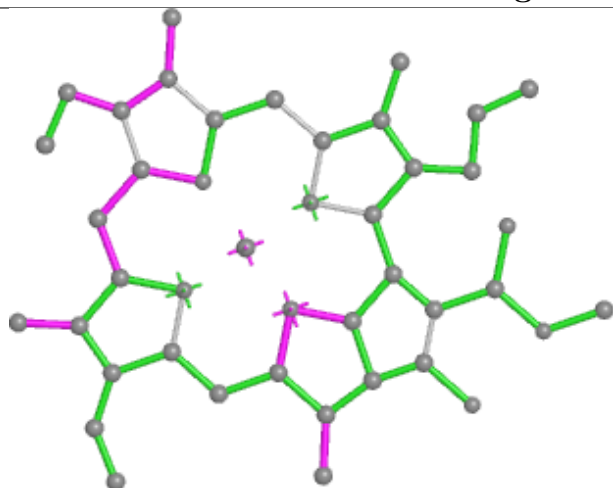
Rings



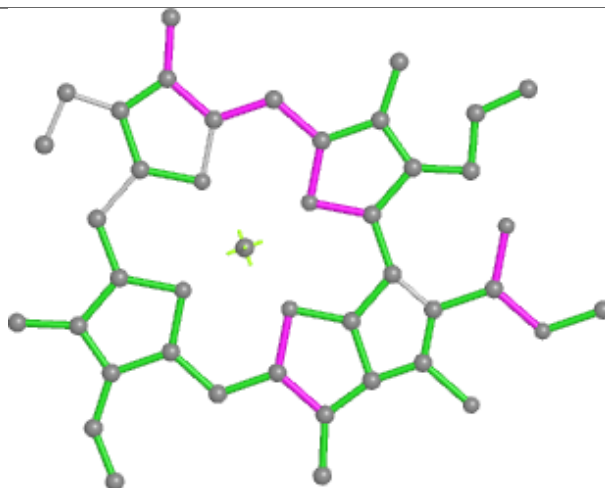
Ligand CLA 5 612



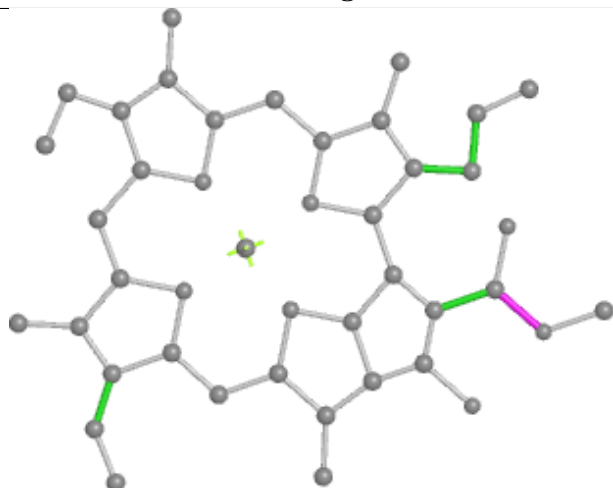
Ligand CLA B 830



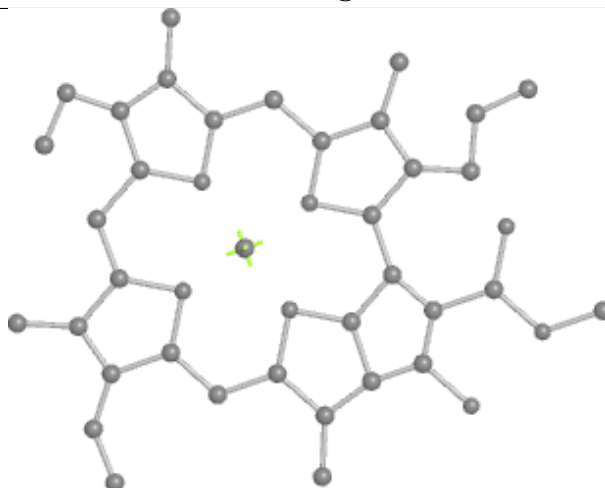
Bond lengths



Bond angles

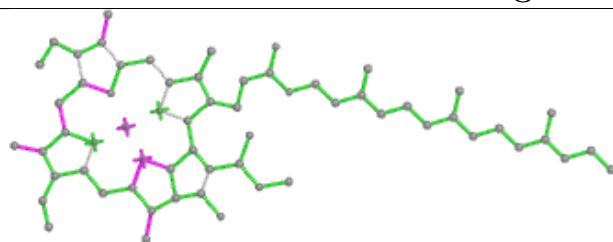


Torsions

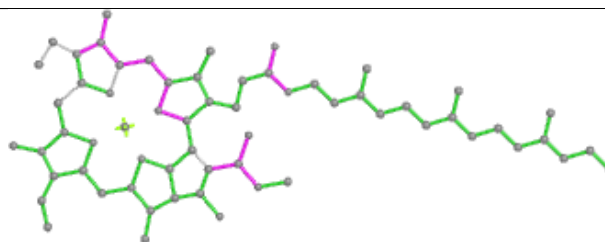


Rings

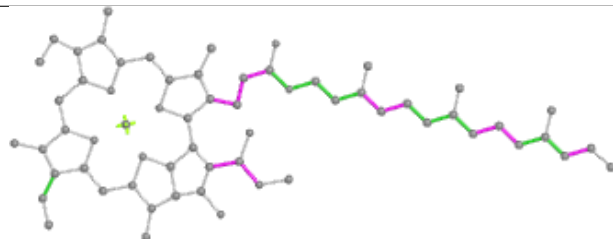
Ligand CLA B 827



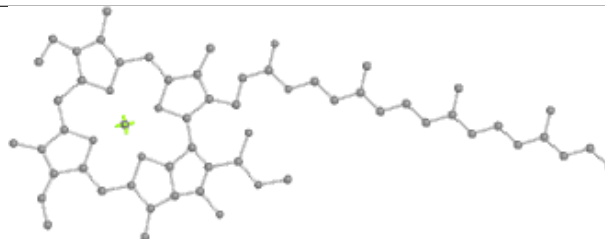
Bond lengths



Bond angles

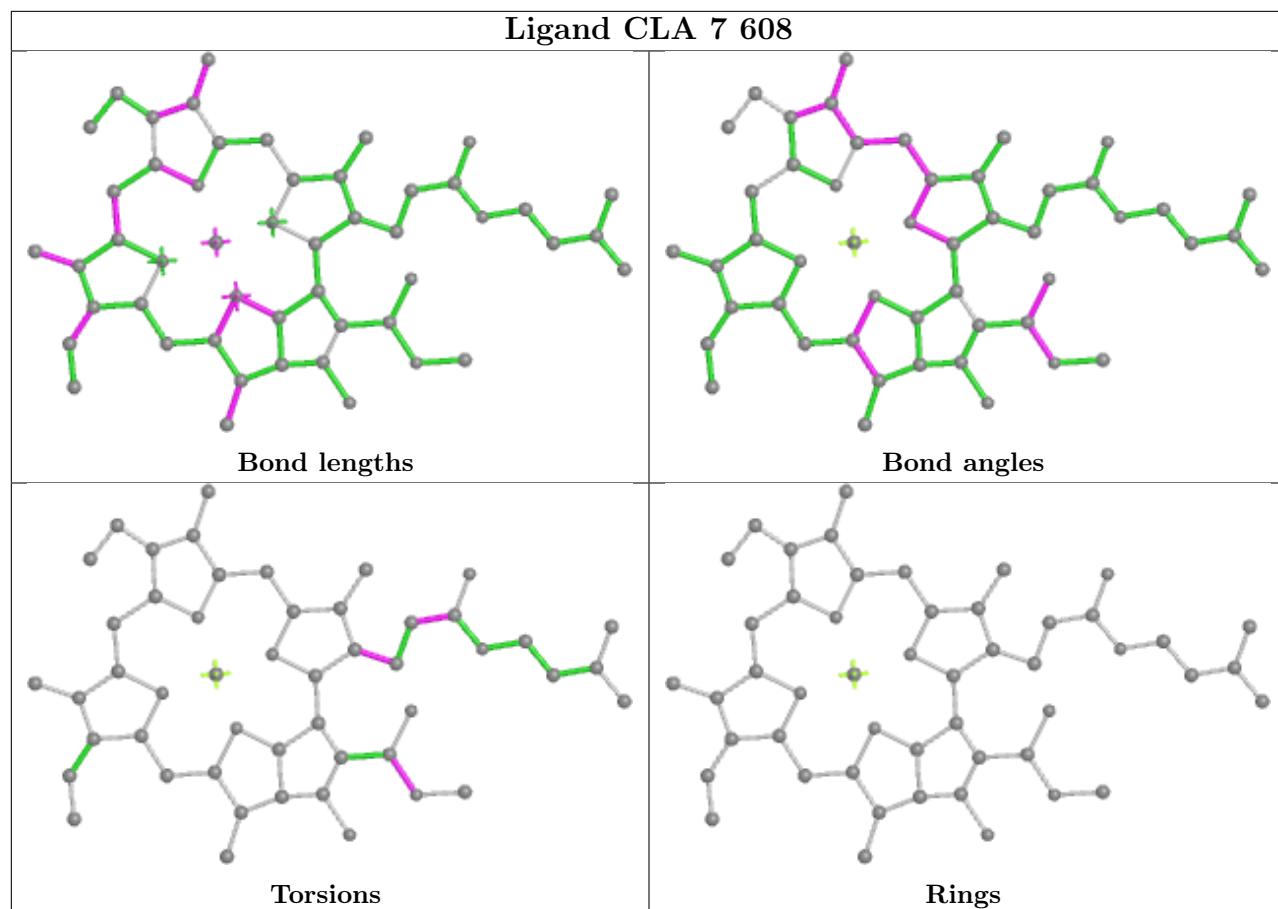


Torsions

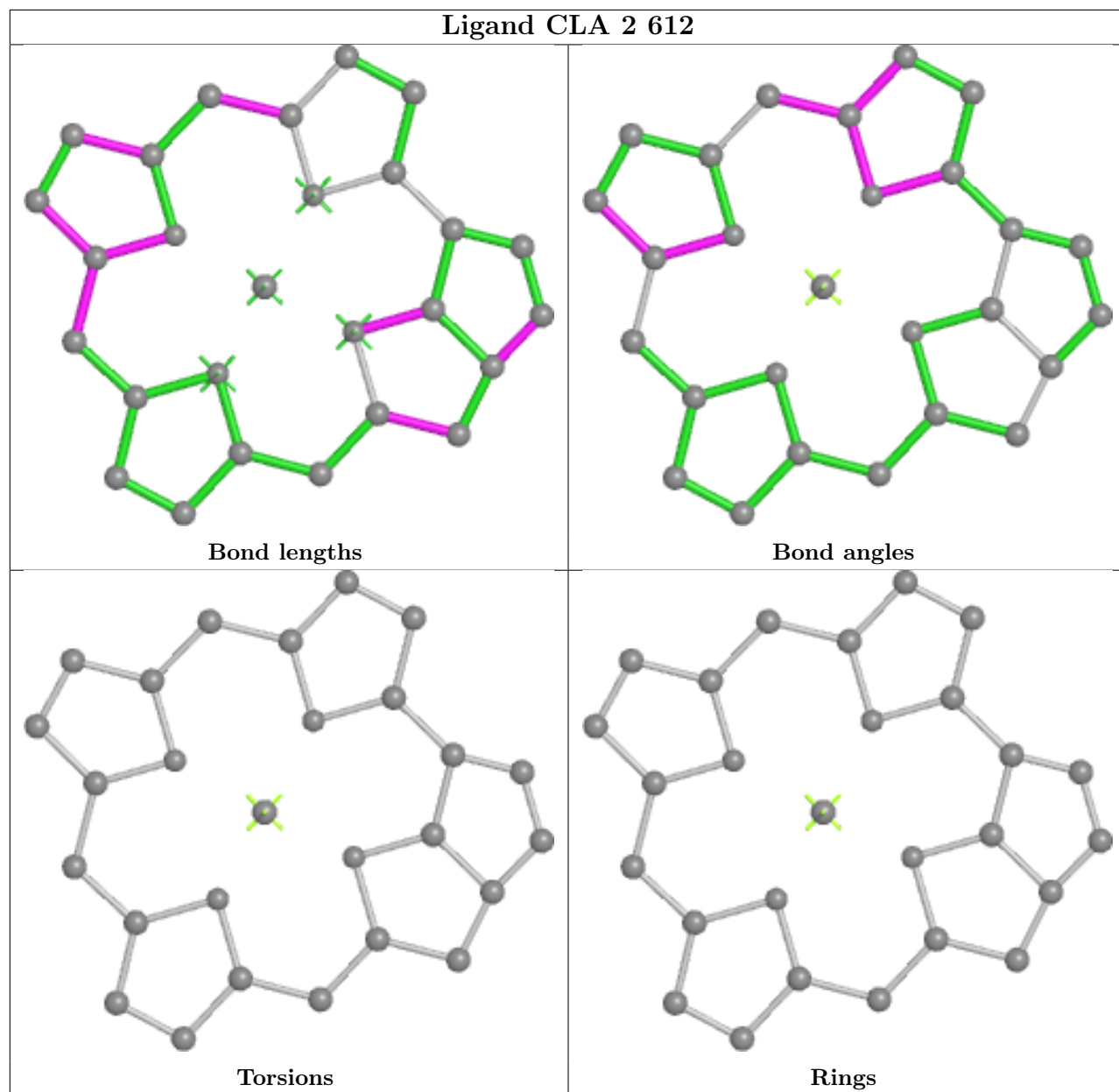


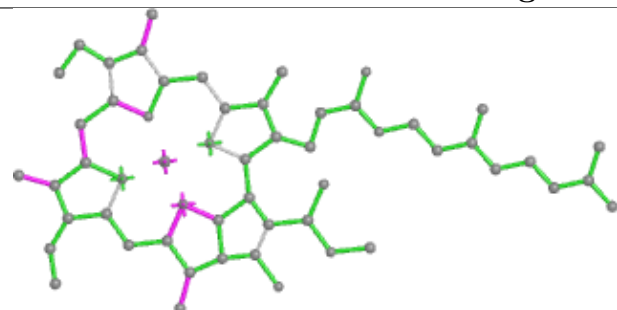
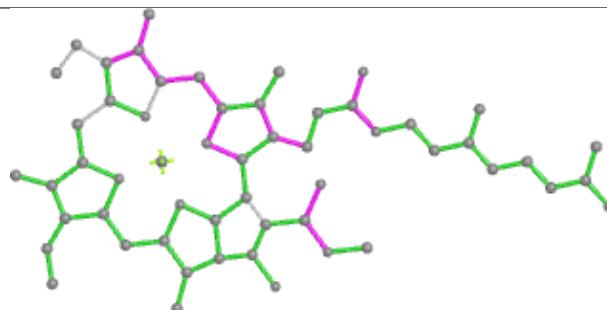
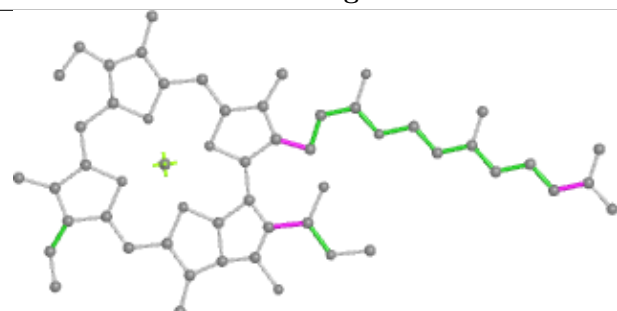
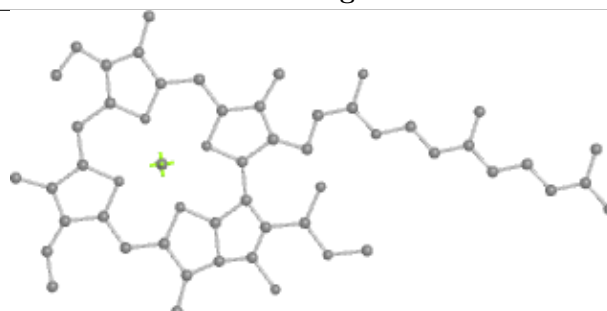
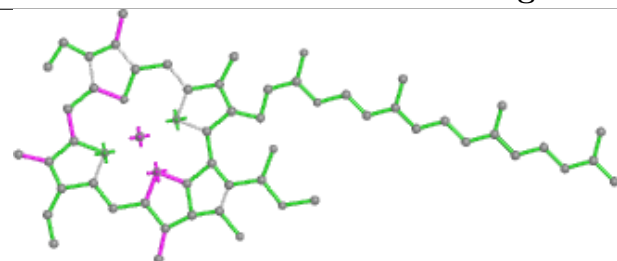
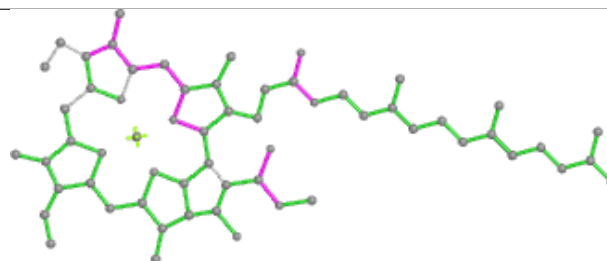
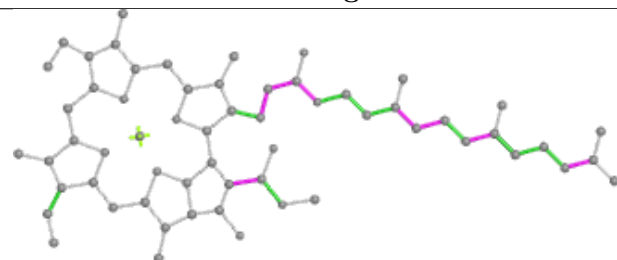
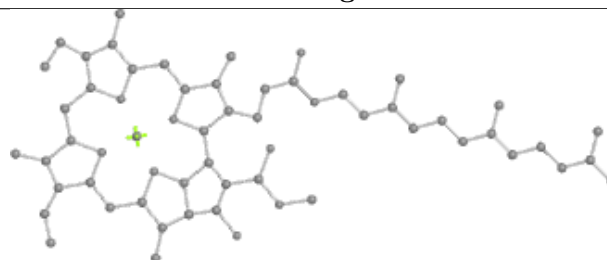
Rings

Ligand CLA 7 608

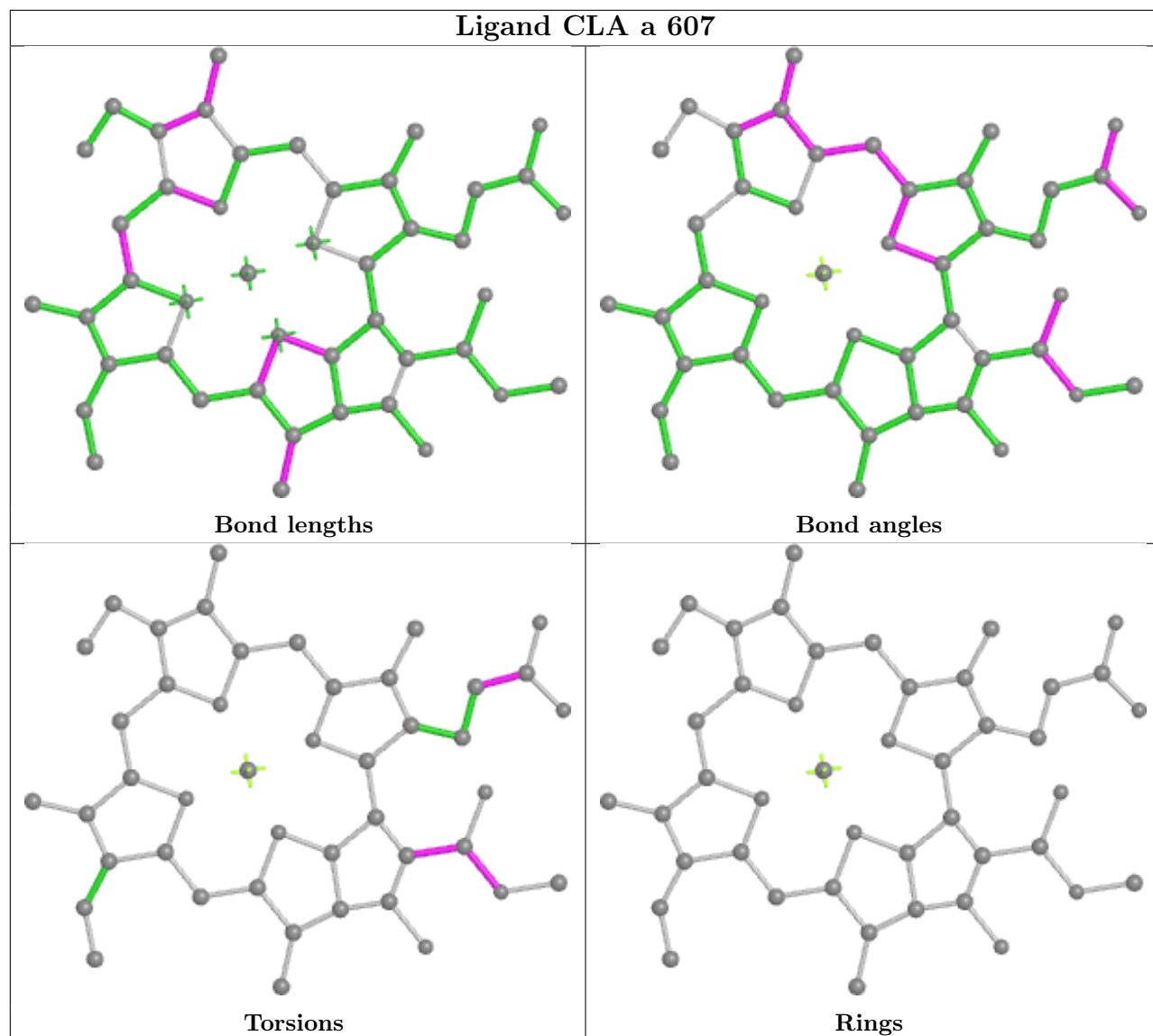


Ligand CLA 2 612

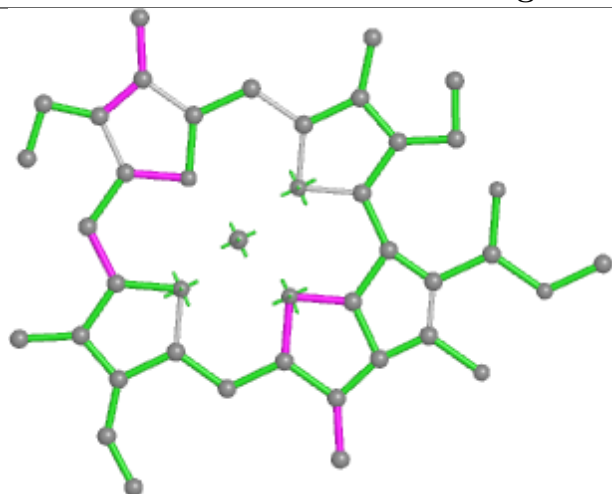


Ligand CLA B 826**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 818****Bond lengths****Bond angles****Torsions****Rings**

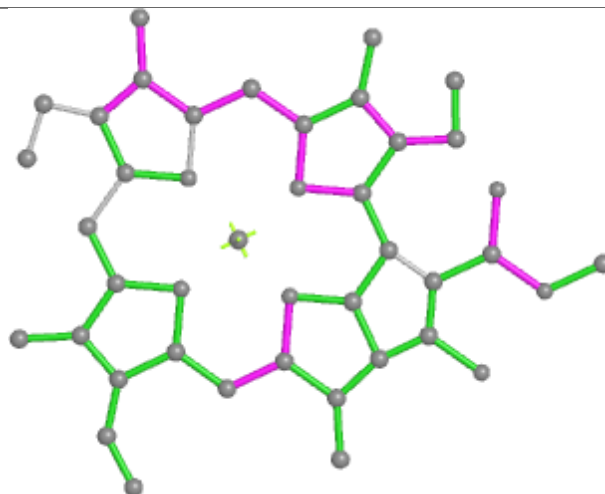
Ligand CLA a 607



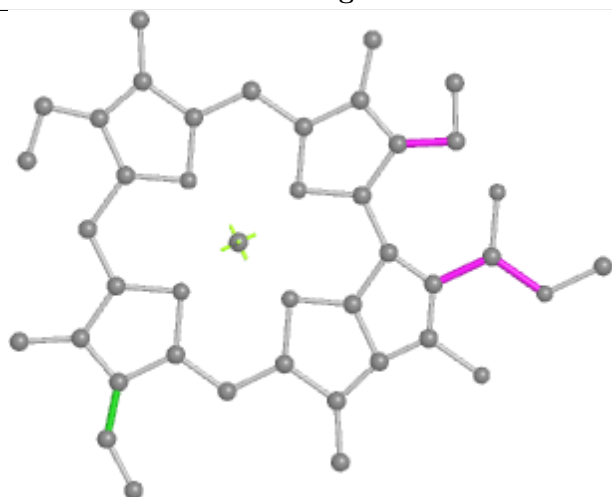
Ligand CLA J 101



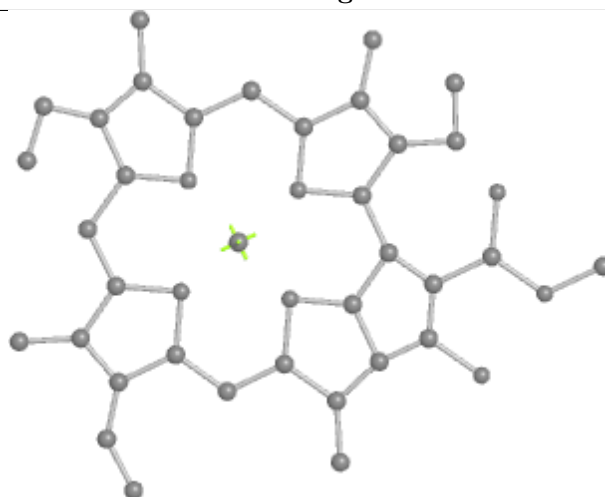
Bond lengths



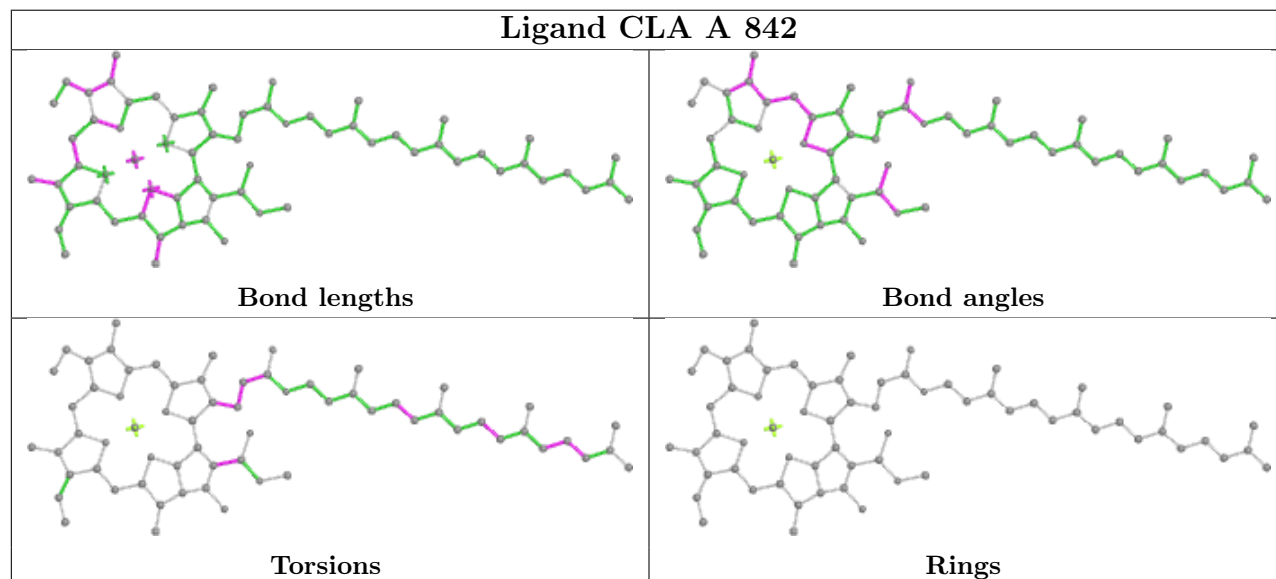
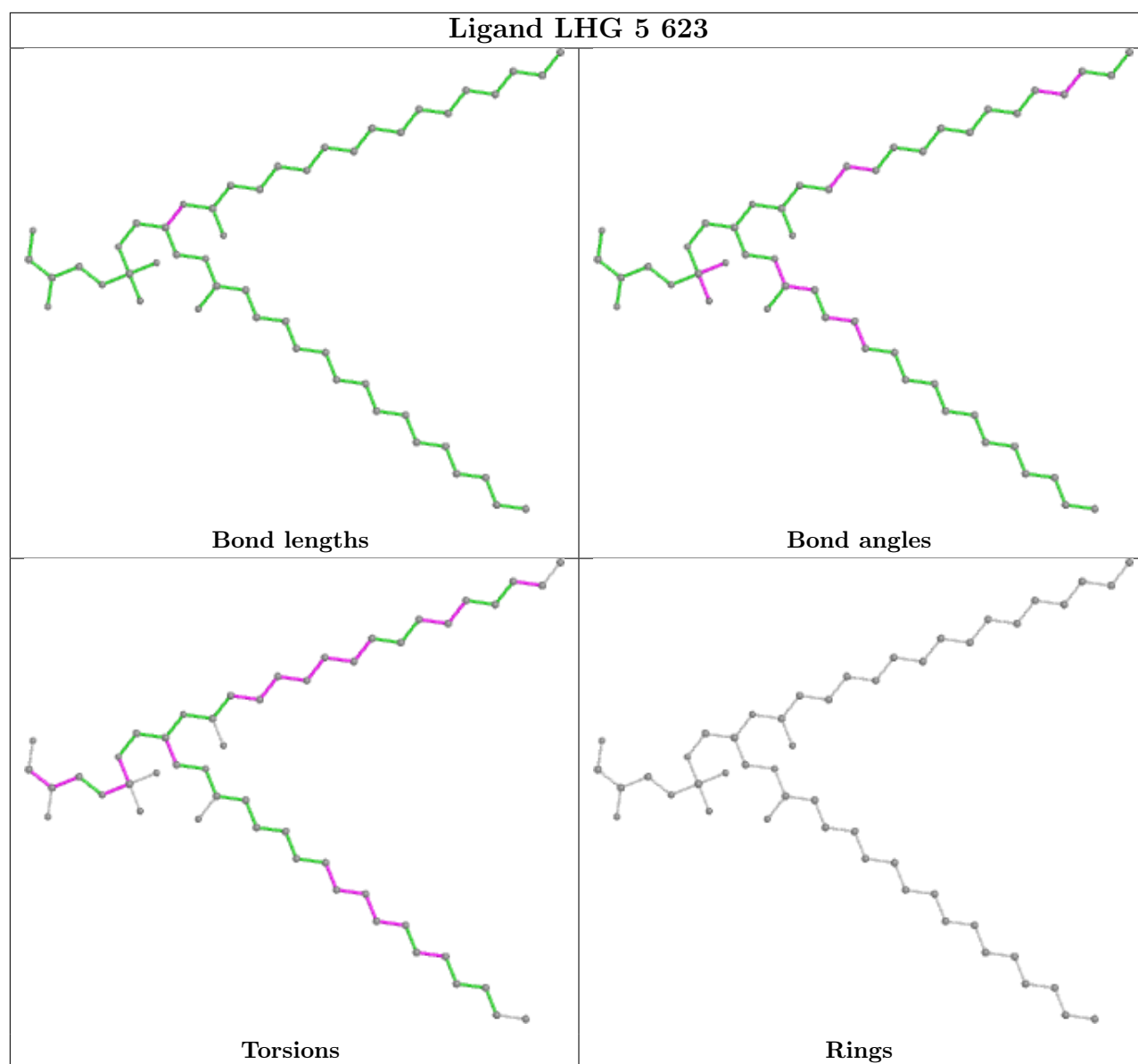
Bond angles

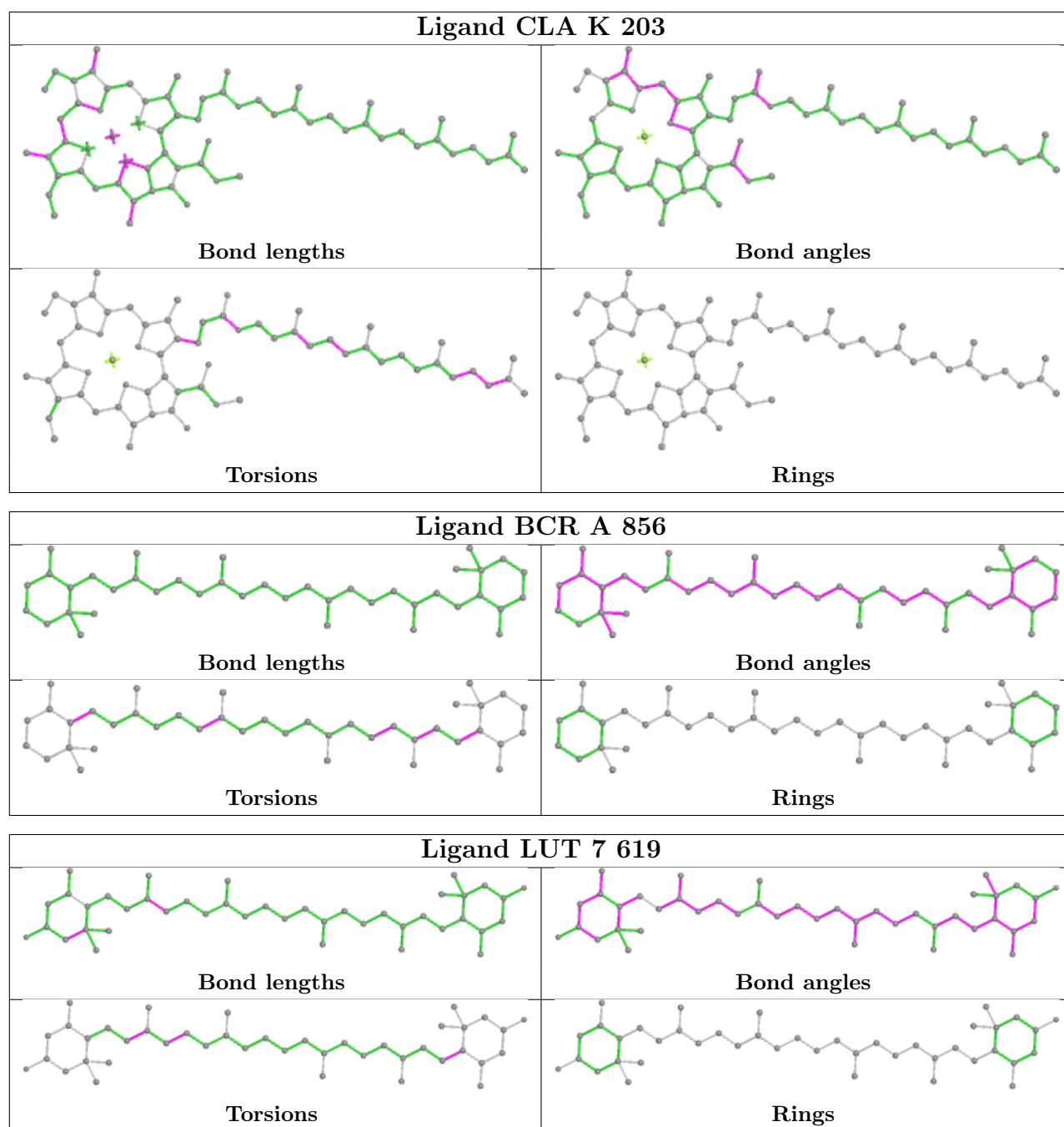


Torsions

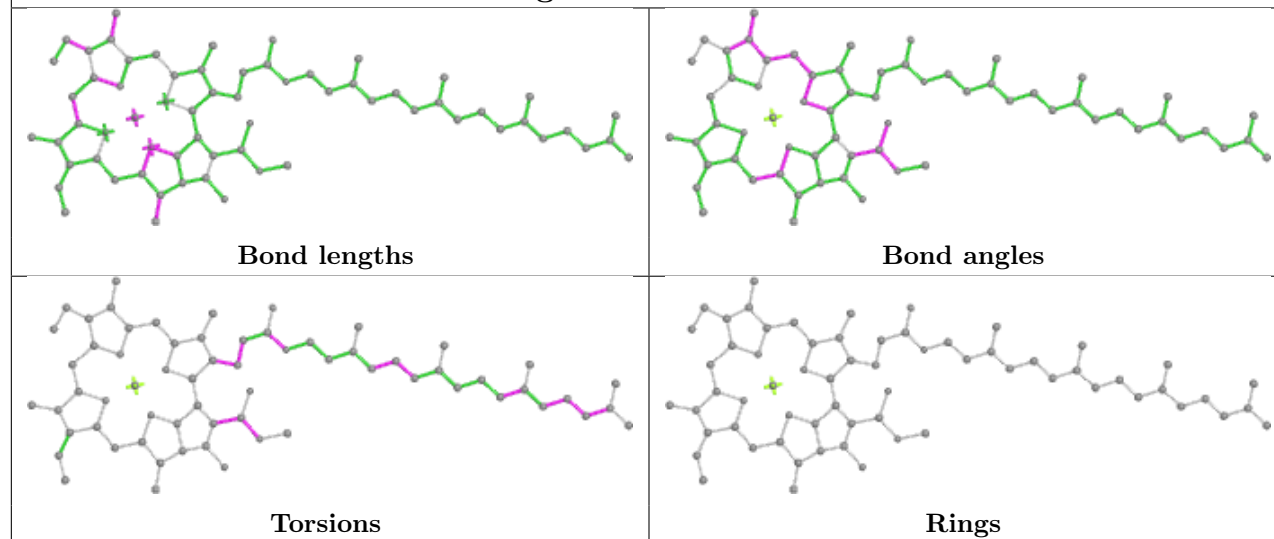


Rings

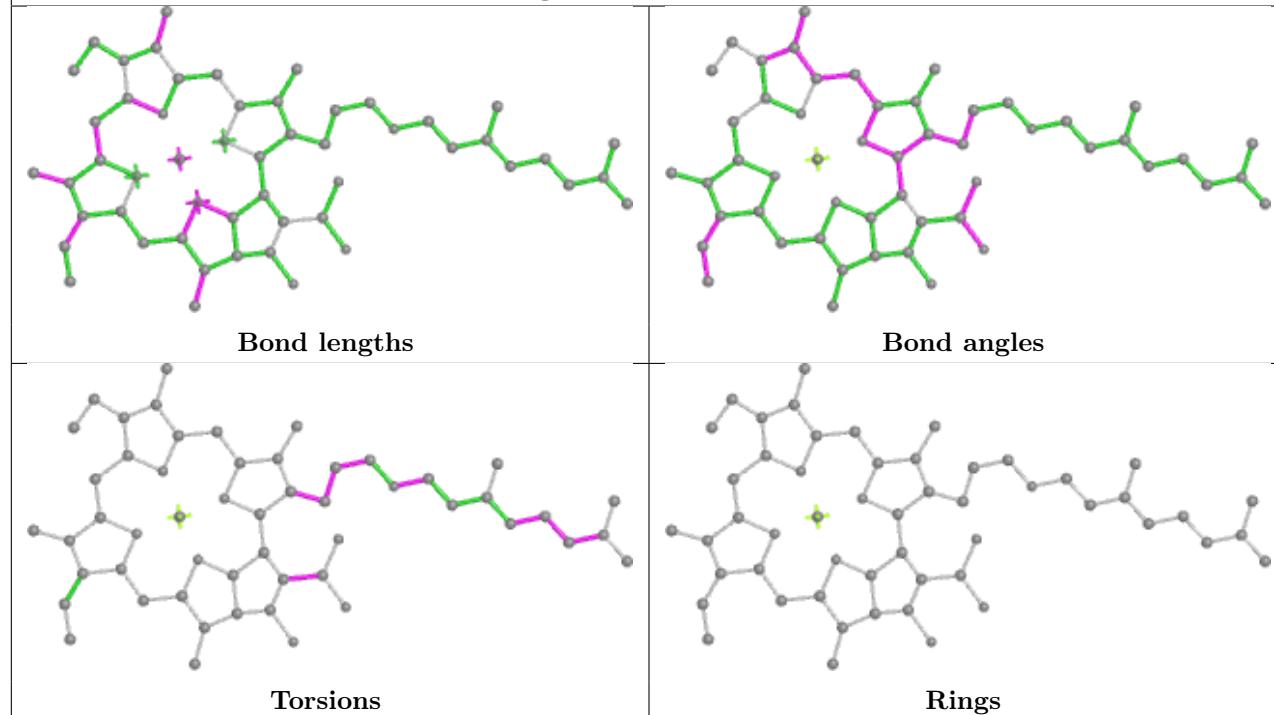




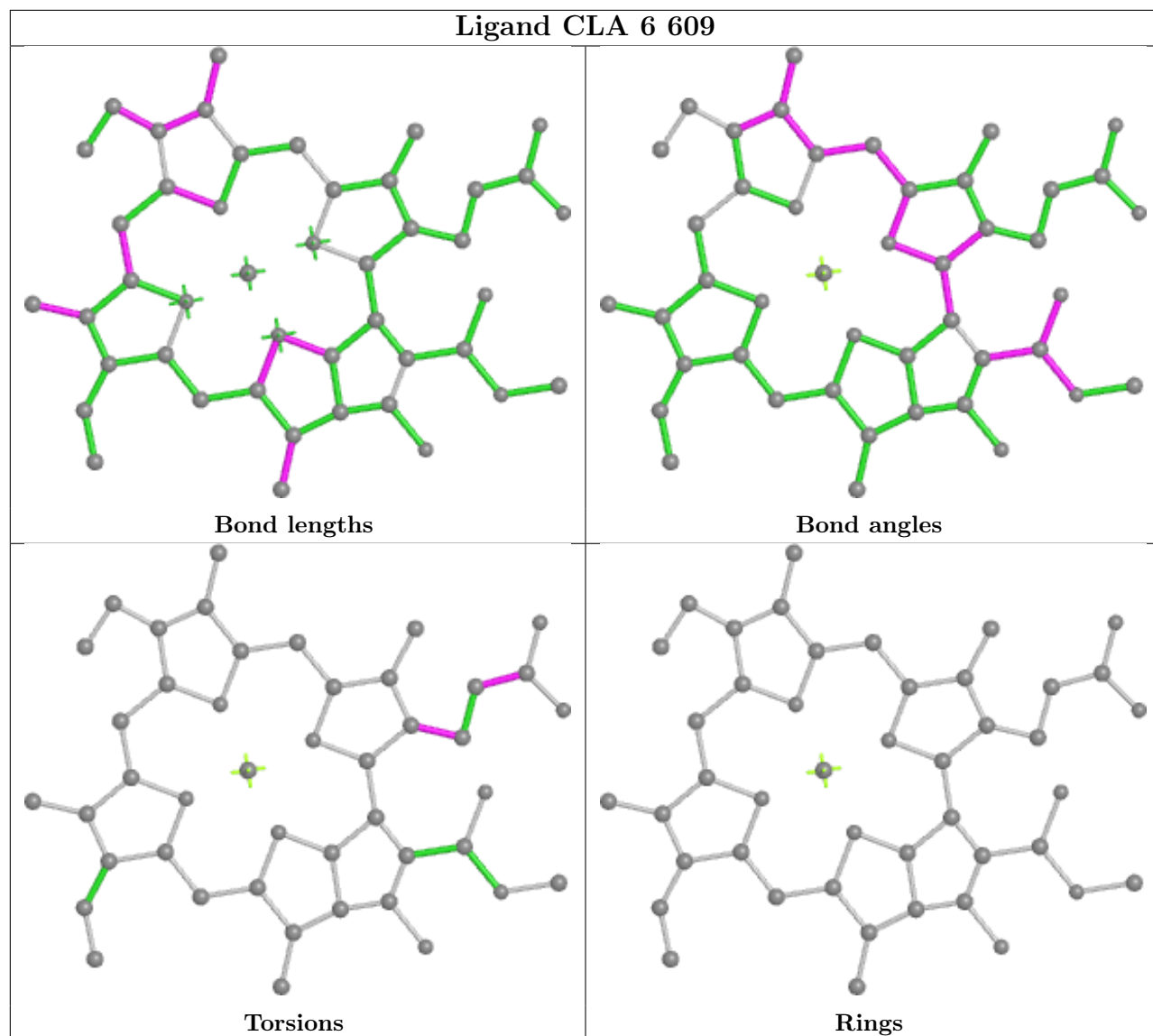
Ligand CLA 4 601



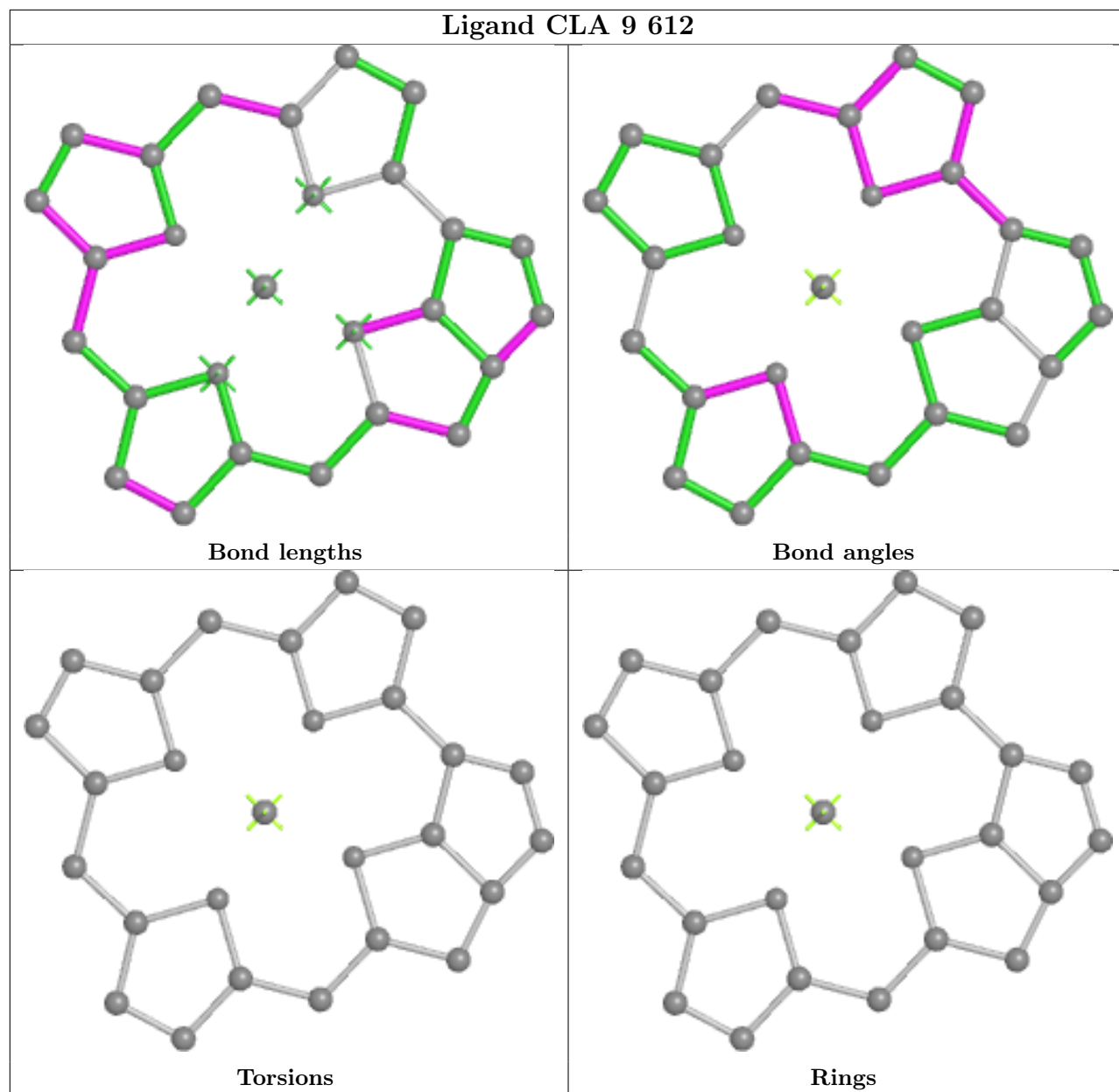
Ligand CLA 1 603



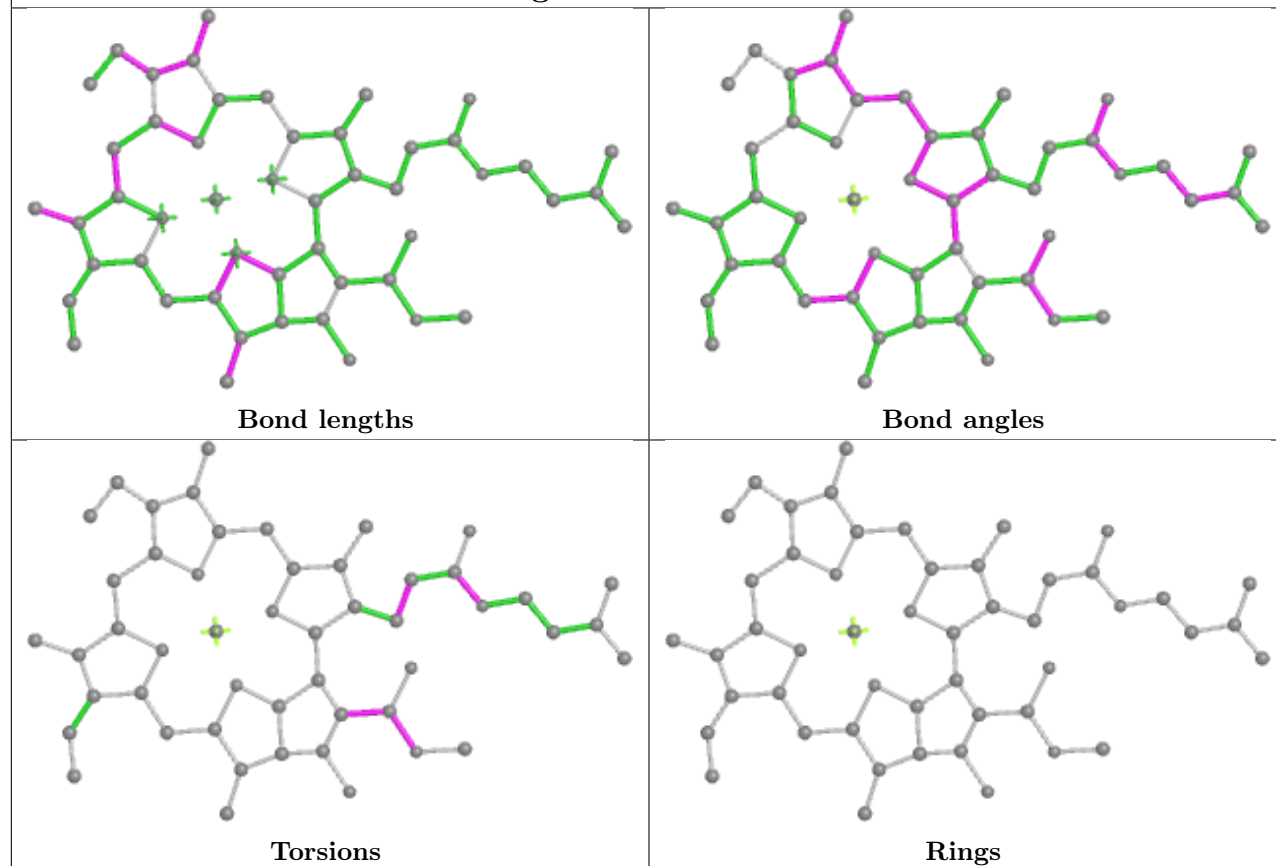
Ligand CLA 6 609



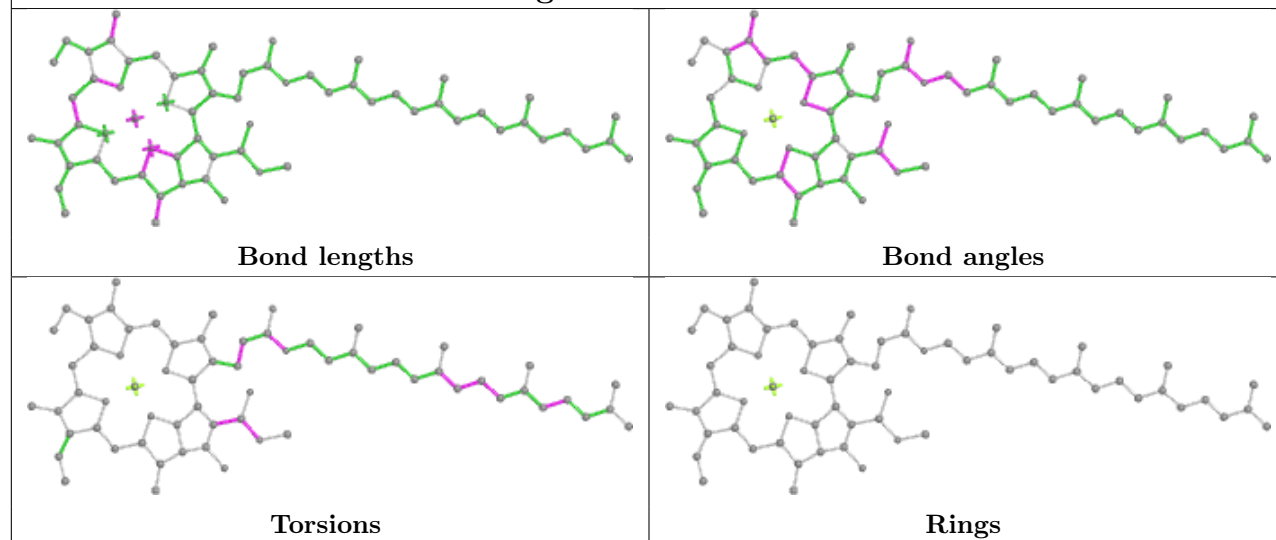
Ligand CLA 9 612



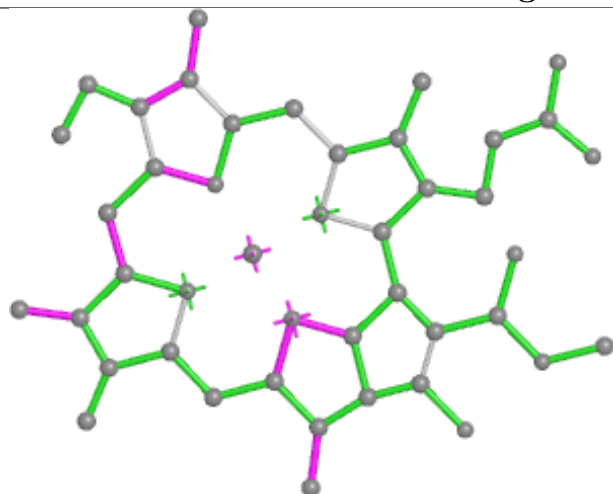
Ligand CLA A 815



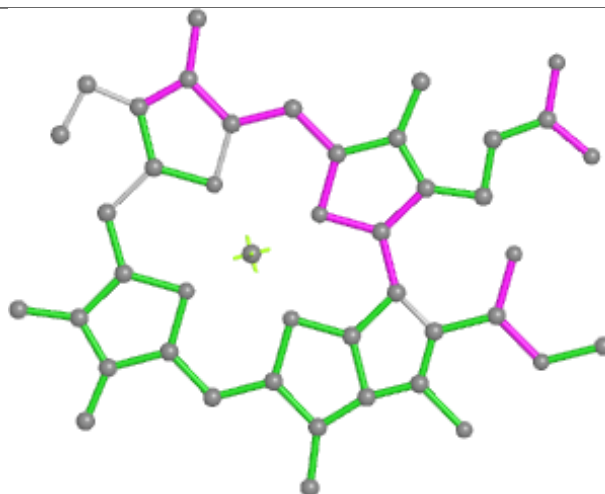
Ligand CLA 5 602



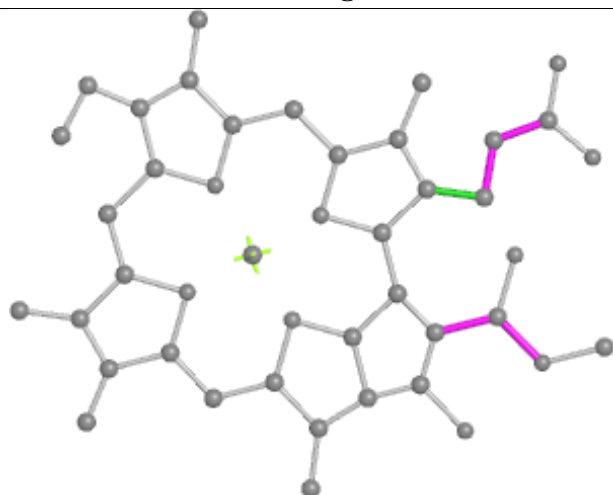
Ligand CLA 7 612



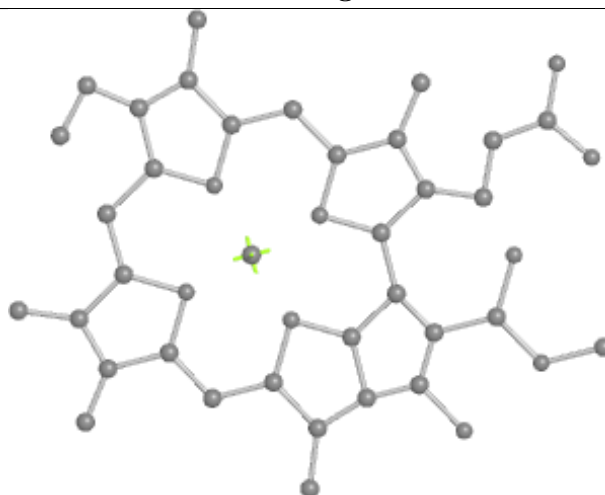
Bond lengths



Bond angles

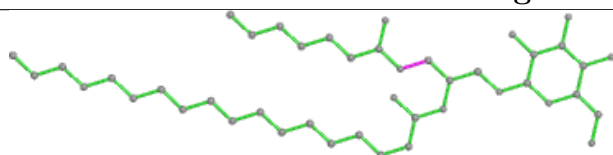


Torsions

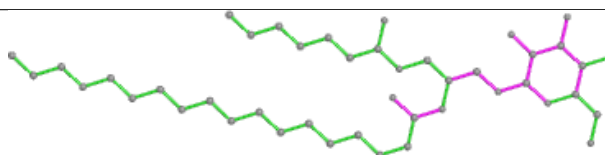


Rings

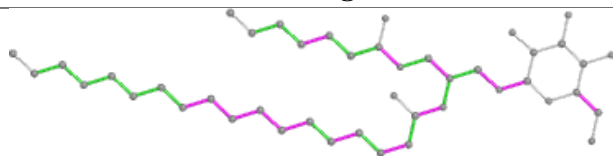
Ligand LMG 7 624



Bond lengths



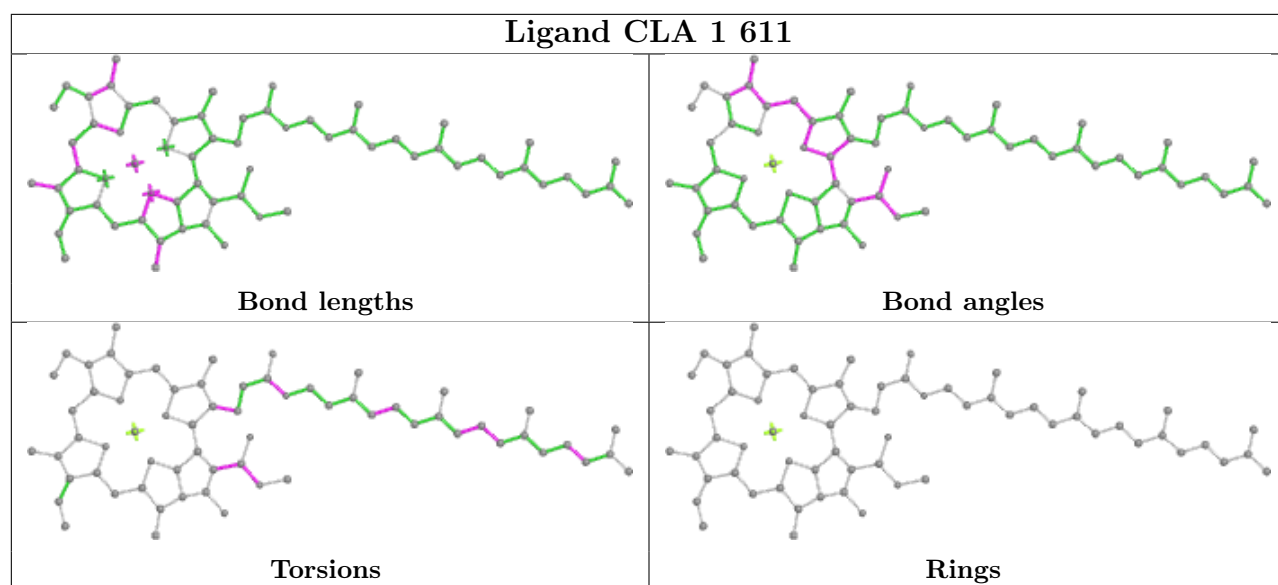
Bond angles



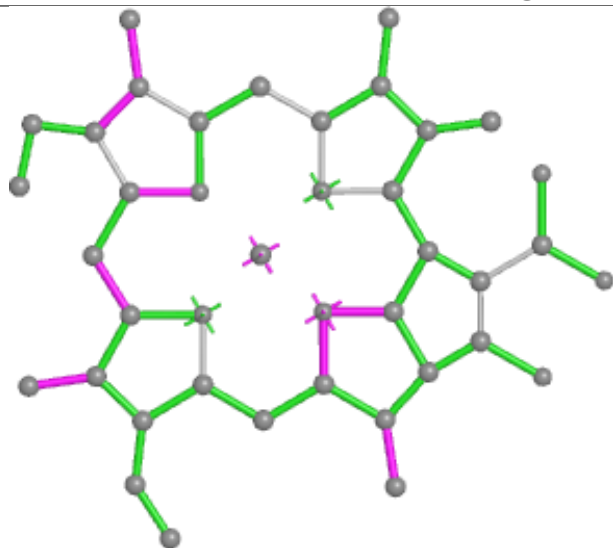
Torsions



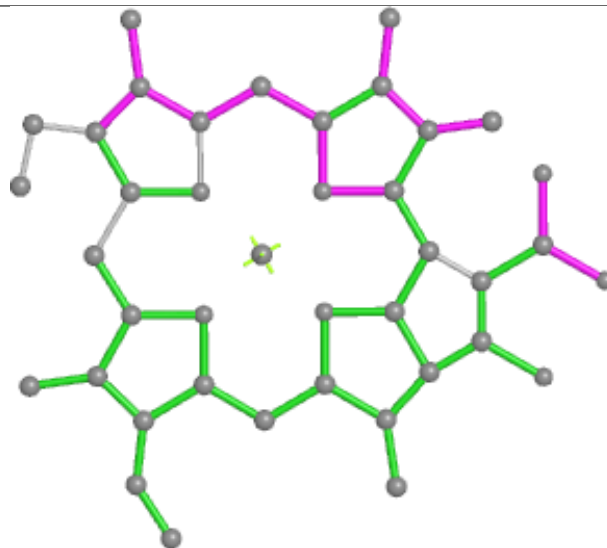
Rings



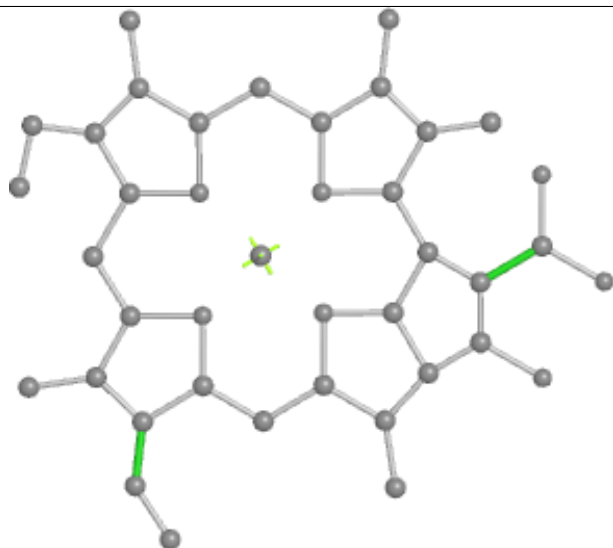
Ligand CLA 3 617



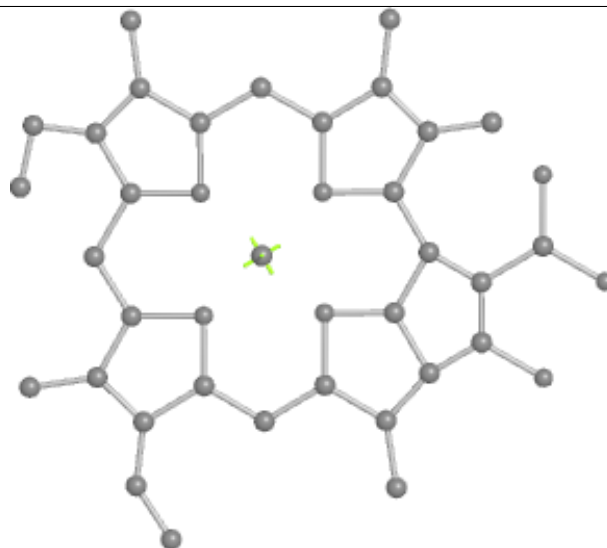
Bond lengths



Bond angles

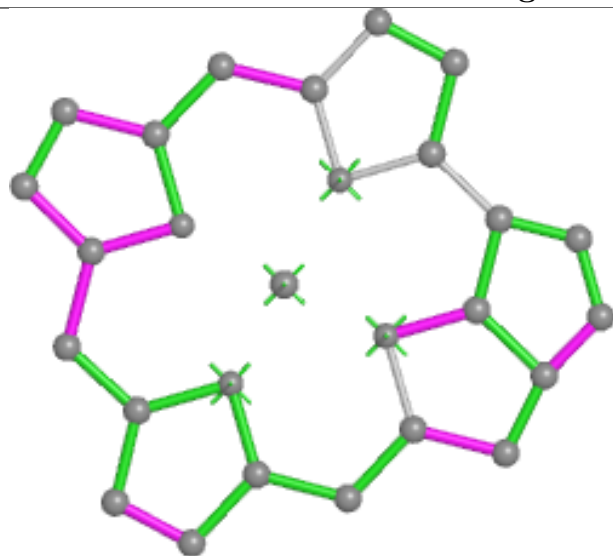


Torsions

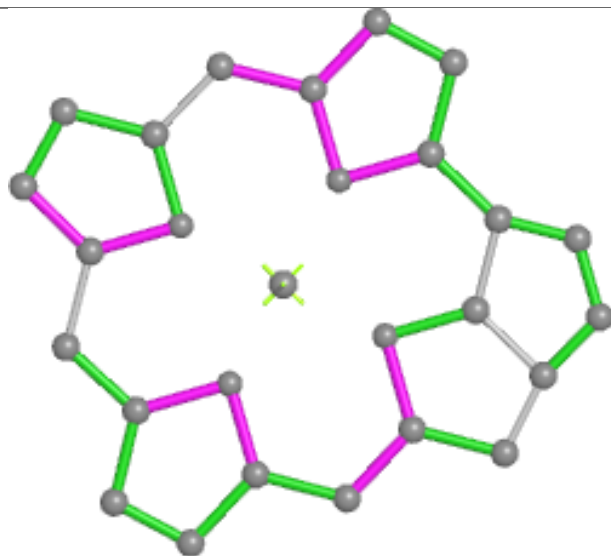


Rings

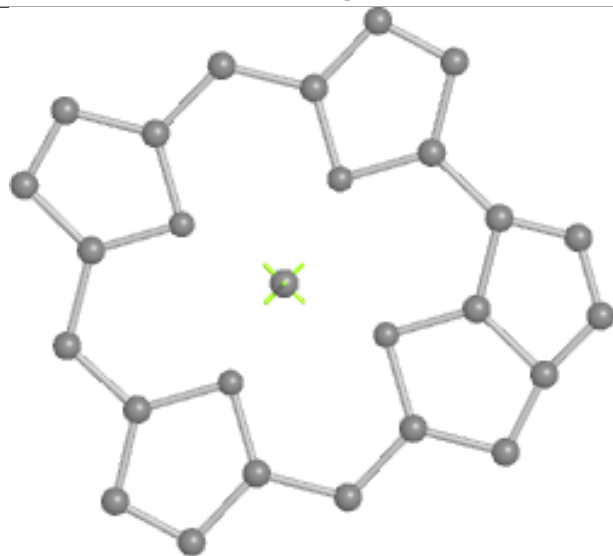
Ligand CLA 9 607



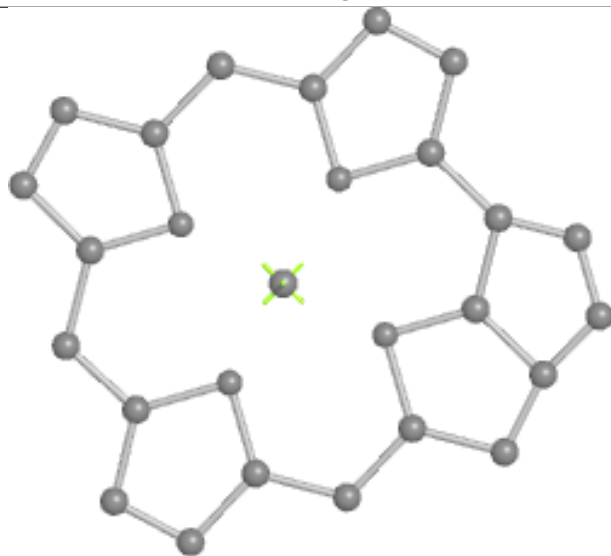
Bond lengths



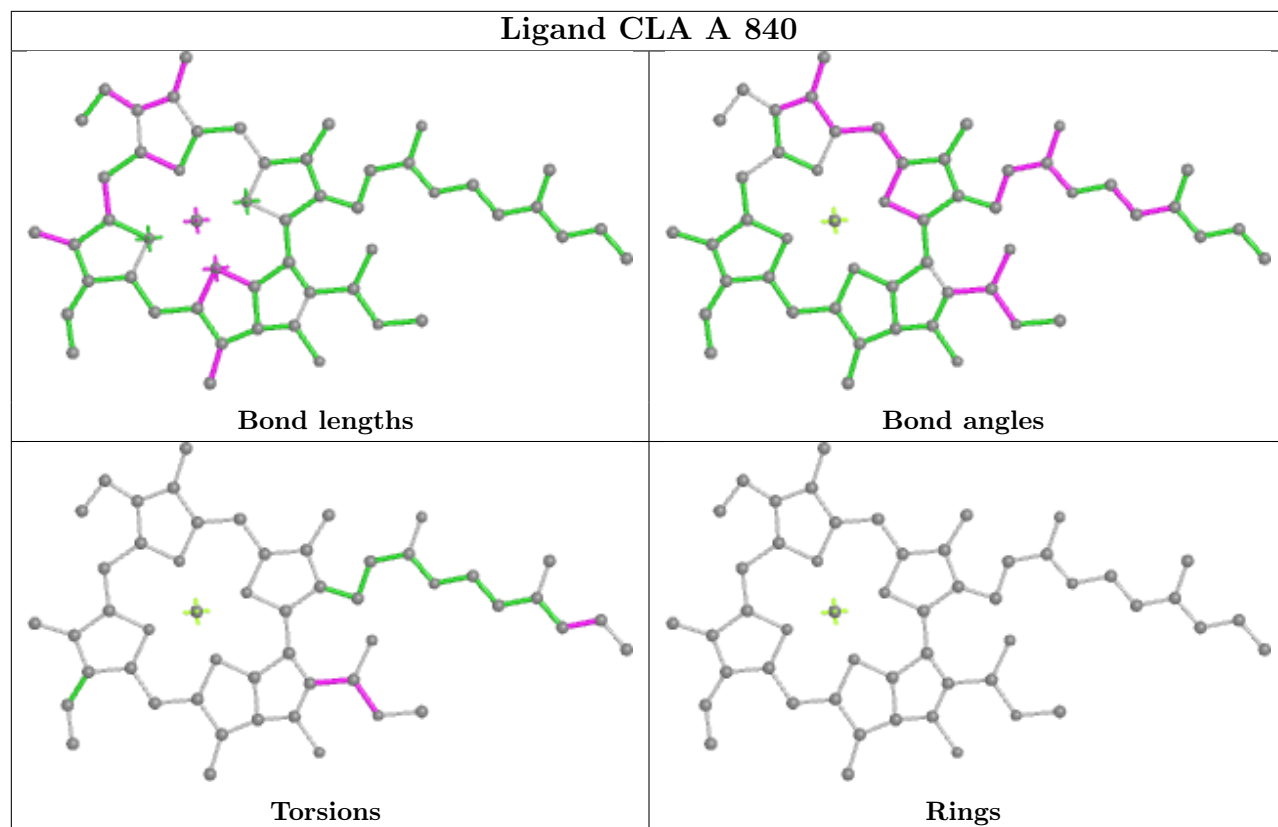
Bond angles



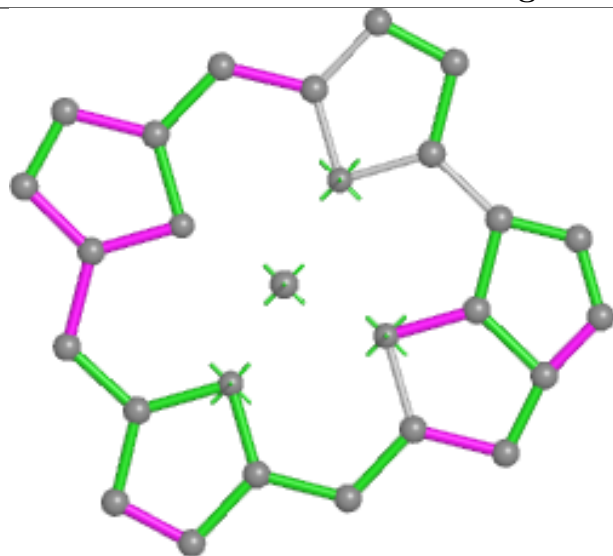
Torsions



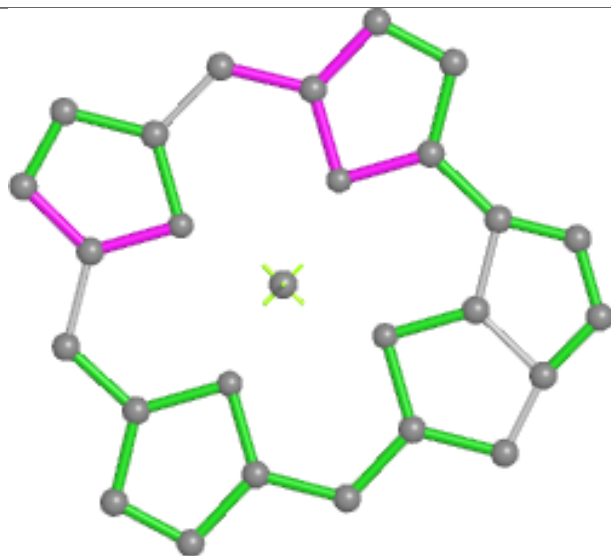
Rings



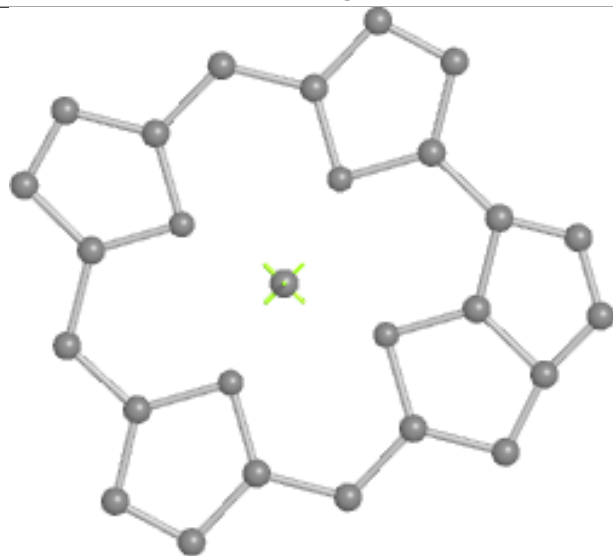
Ligand CLA 9 603



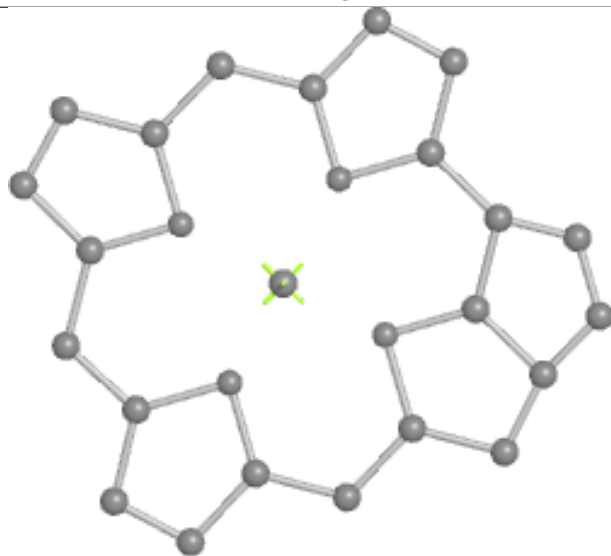
Bond lengths



Bond angles

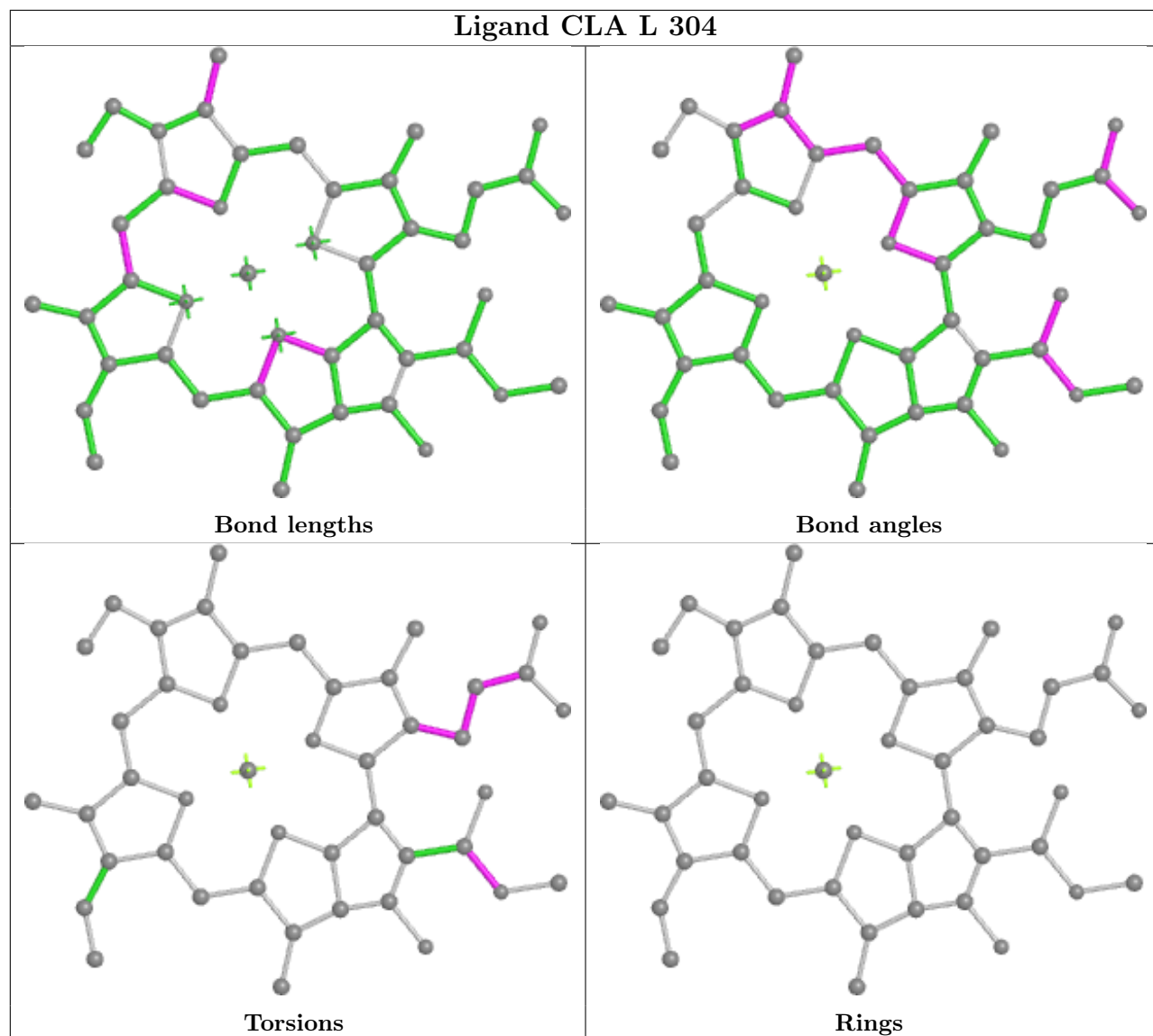


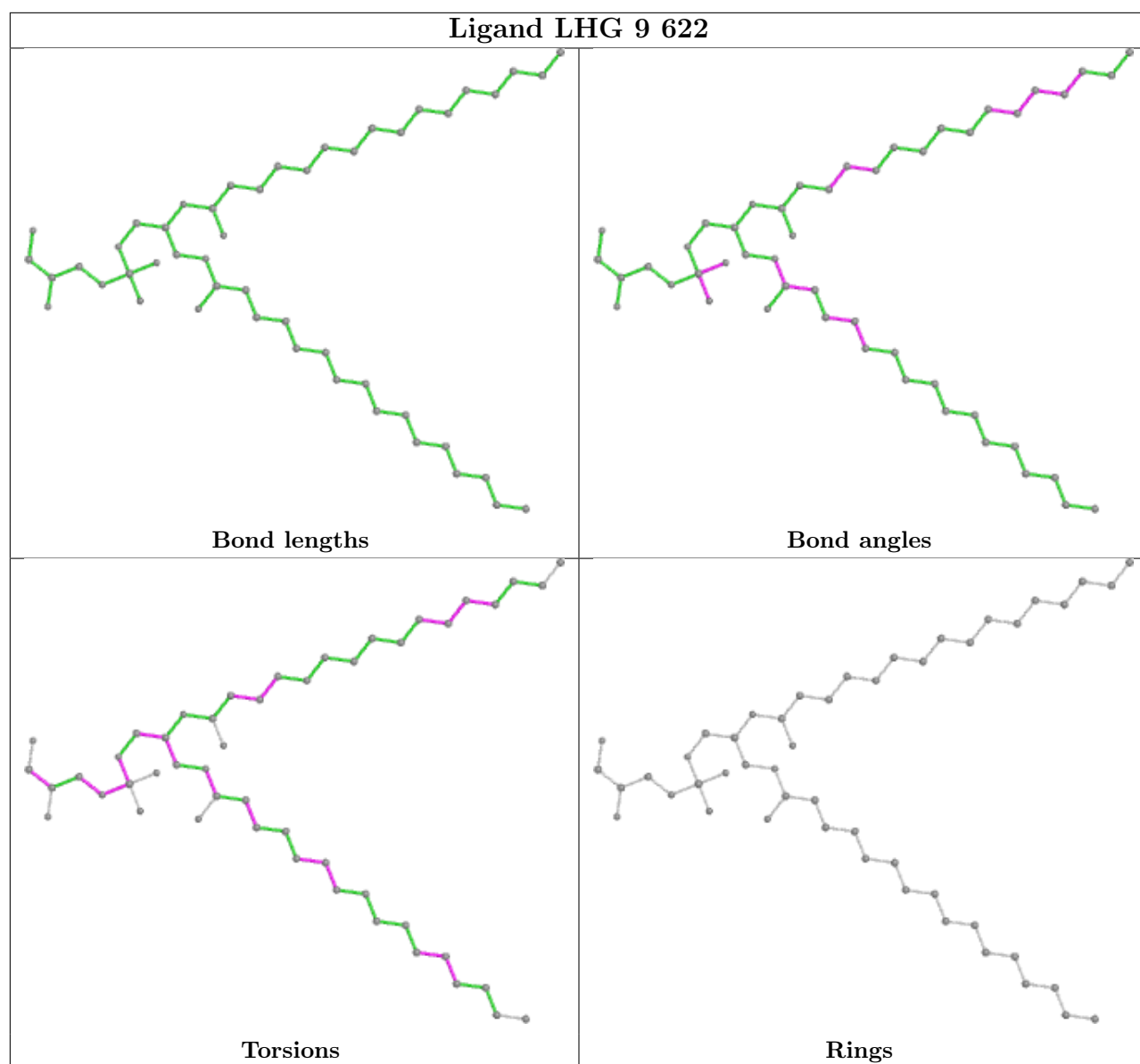
Torsions



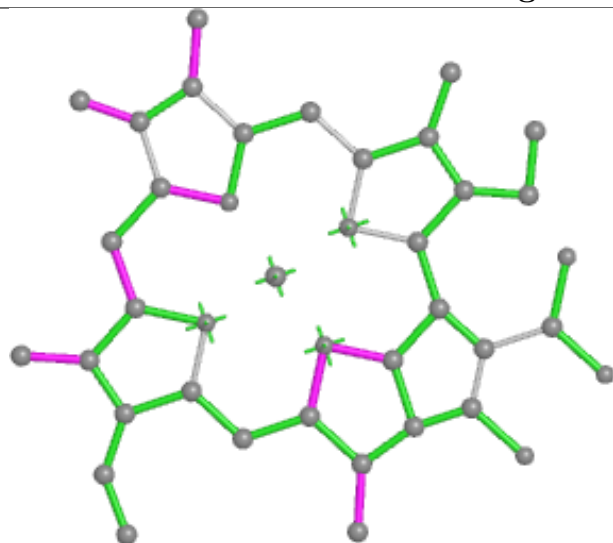
Rings

Ligand CLA L 304

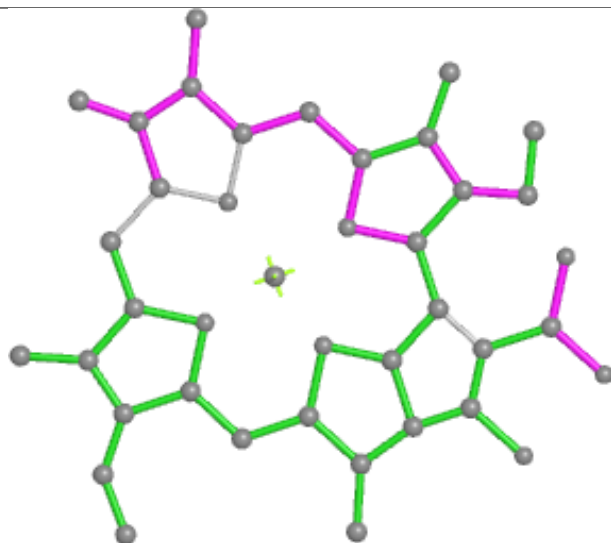




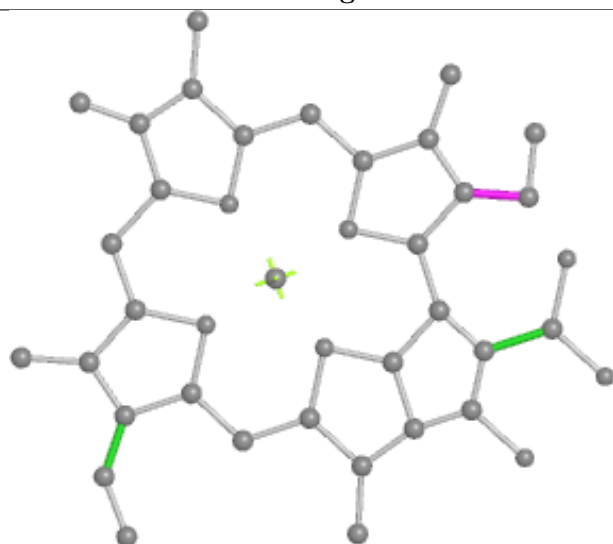
Ligand CLA 5 618



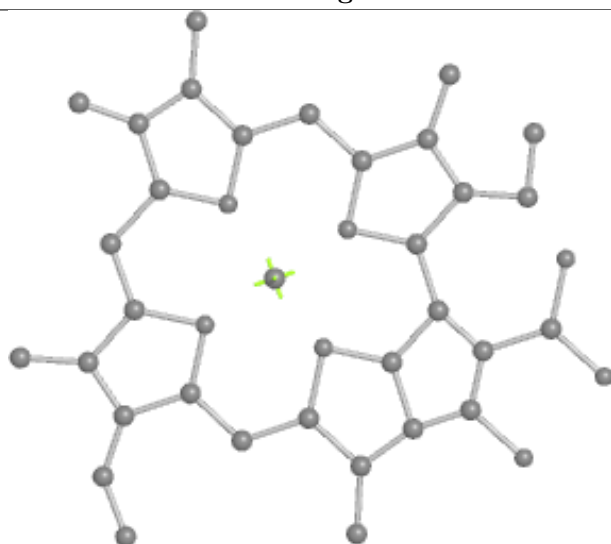
Bond lengths



Bond angles

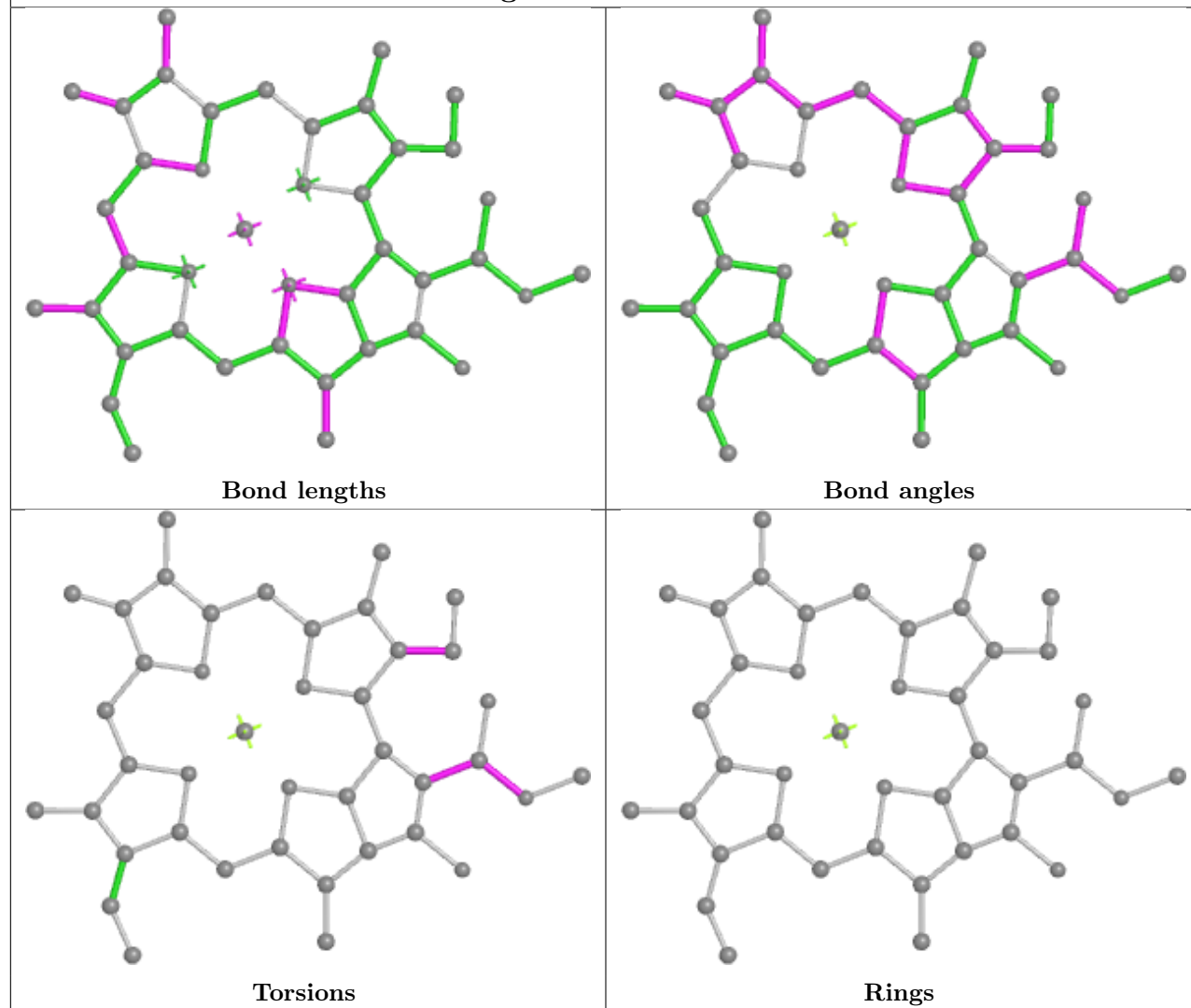


Torsions

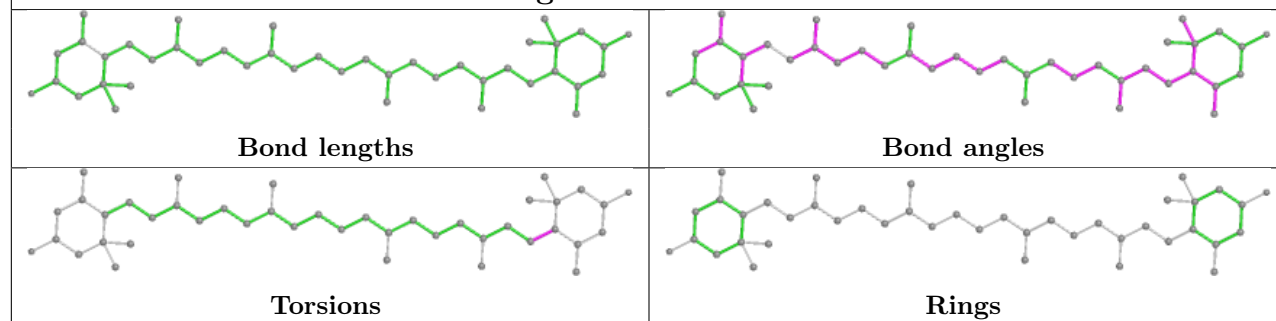


Rings

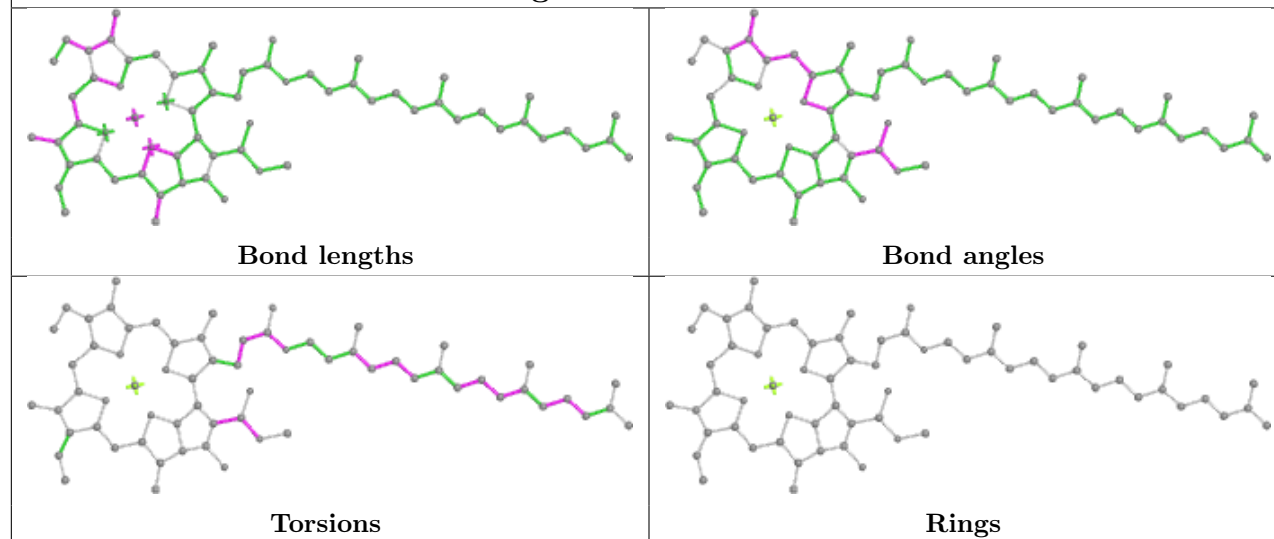
Ligand CLA 6 607



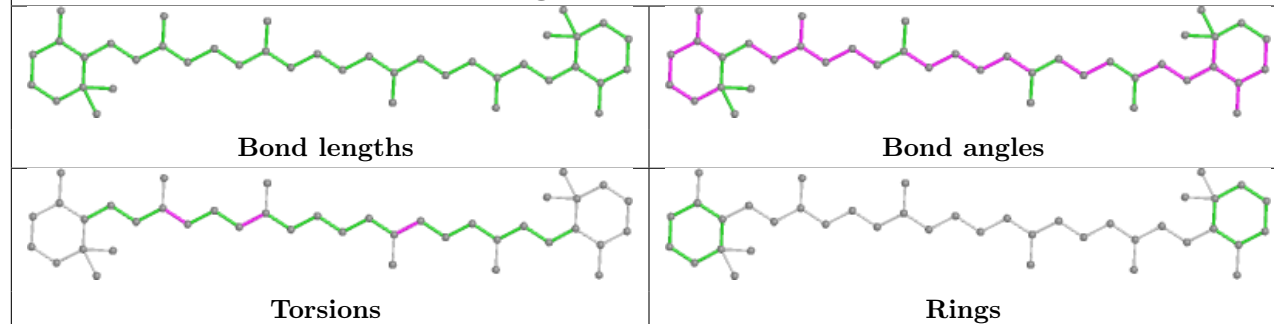
Ligand LUT 5 620



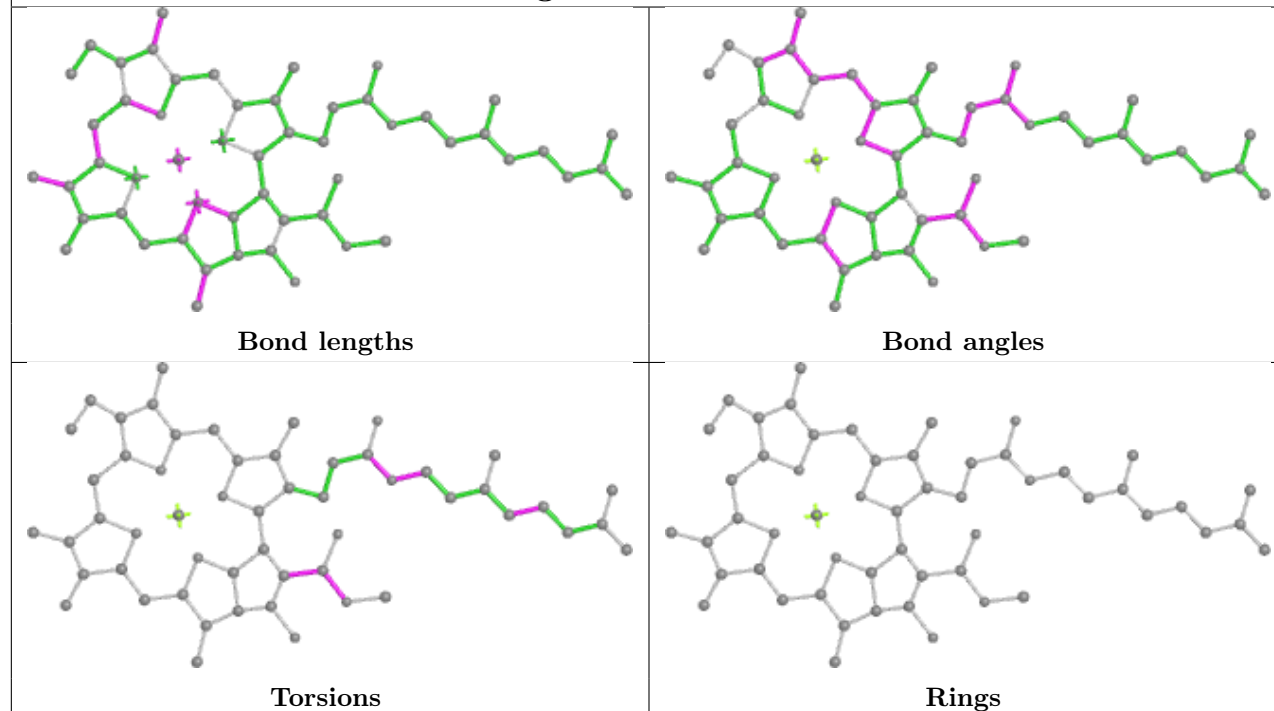
Ligand CLA A 834

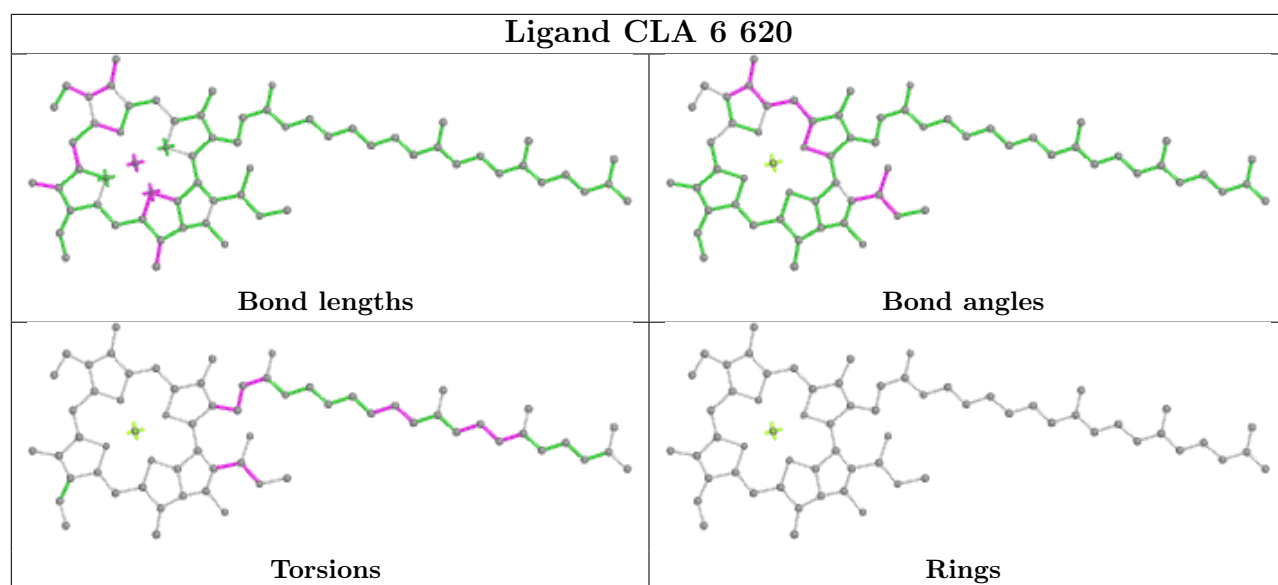


Ligand BCR L 301

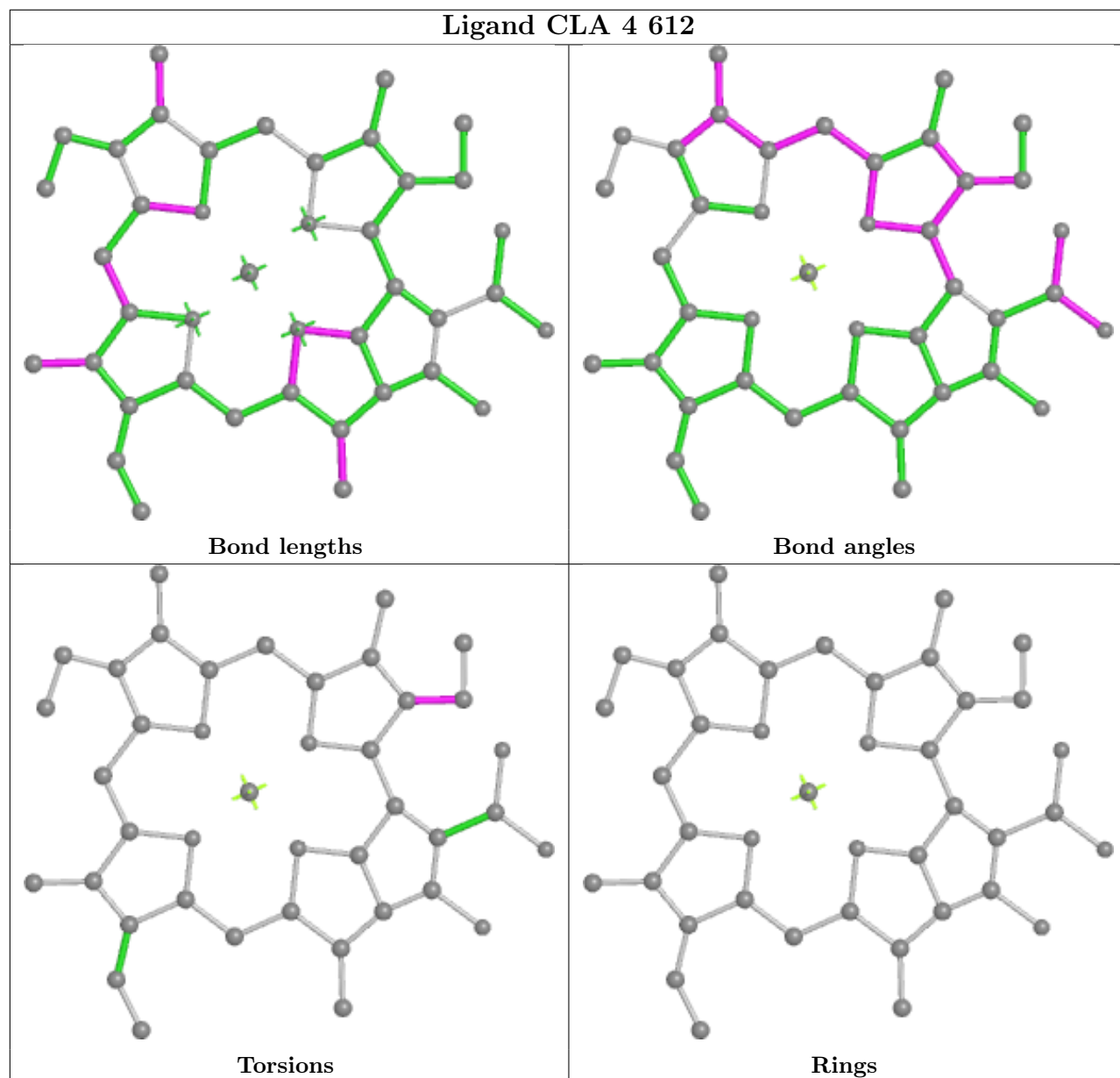


Ligand CLA 7 604

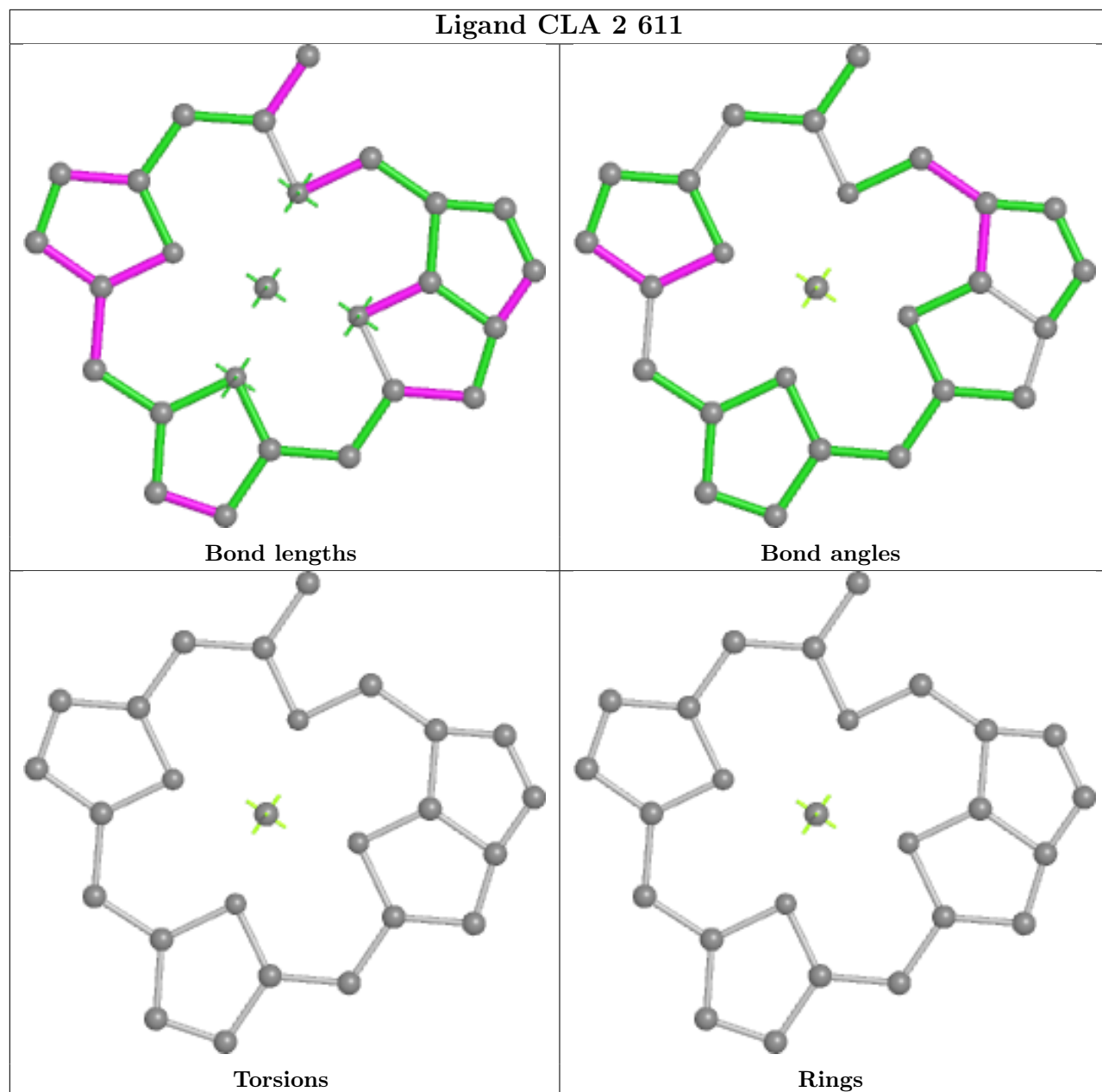


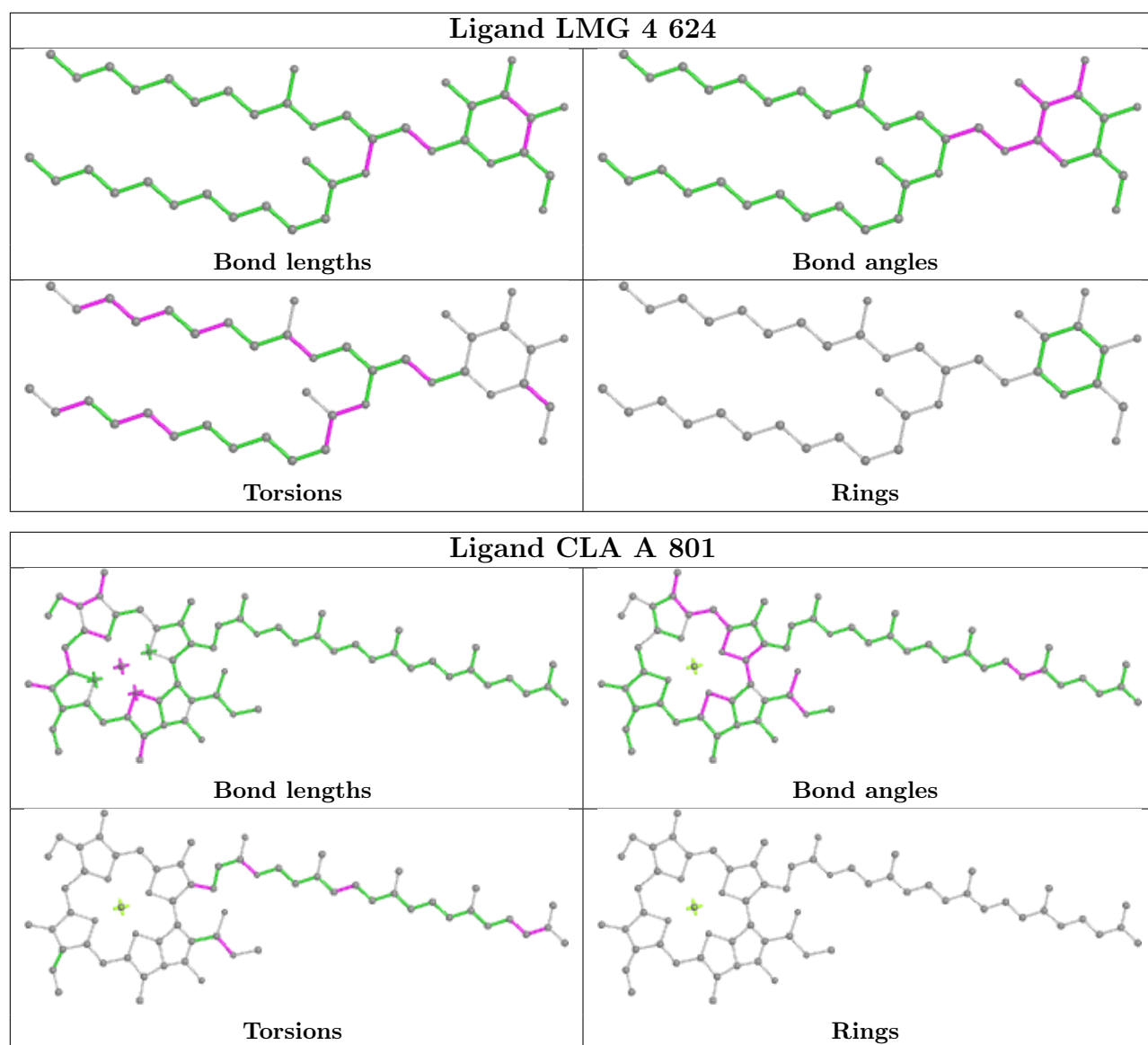


Ligand CLA 4 612

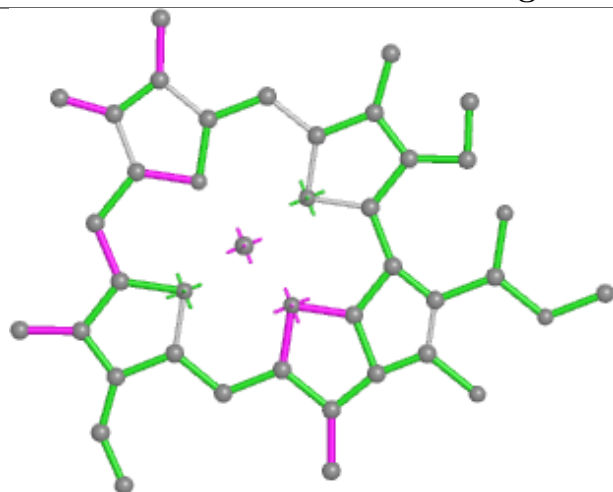


Ligand CLA 2 611

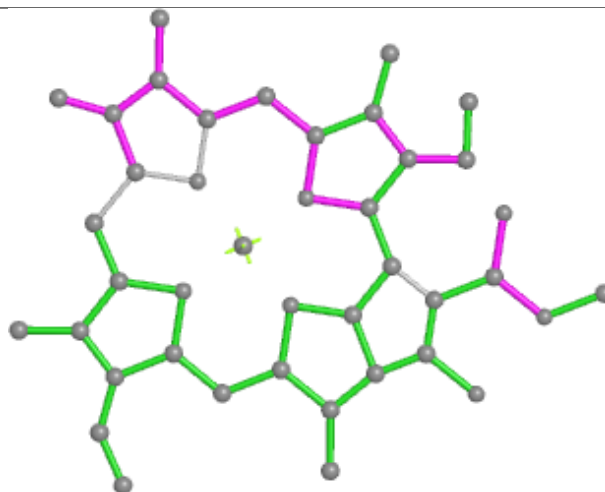




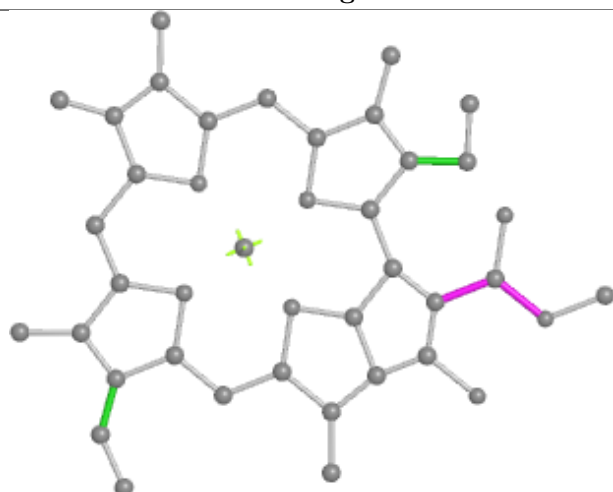
Ligand CLA 8 607



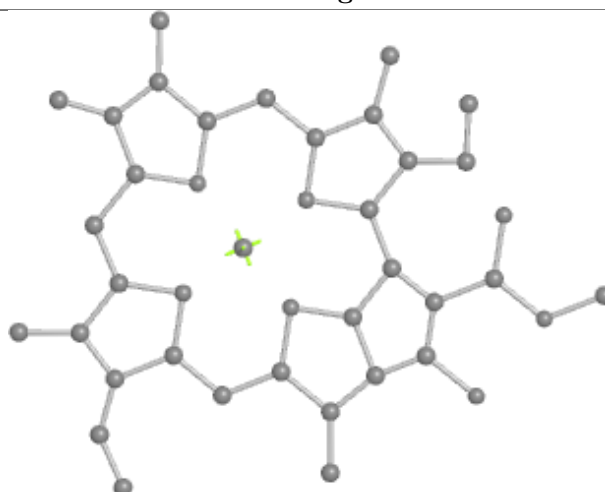
Bond lengths



Bond angles

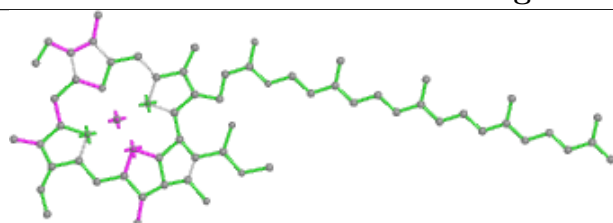


Torsions

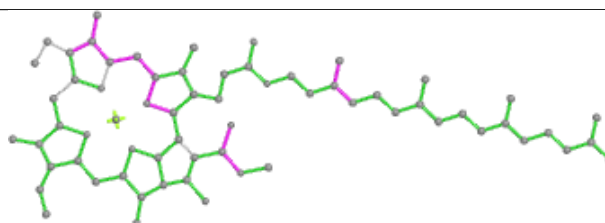


Rings

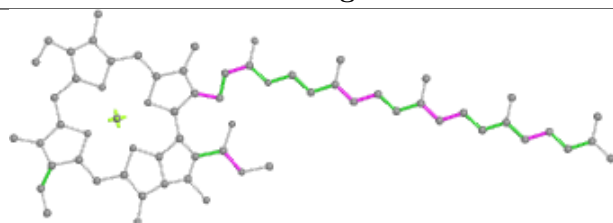
Ligand CLA A 836



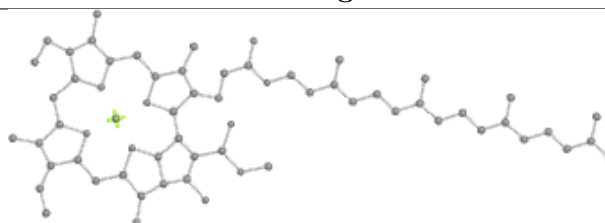
Bond lengths



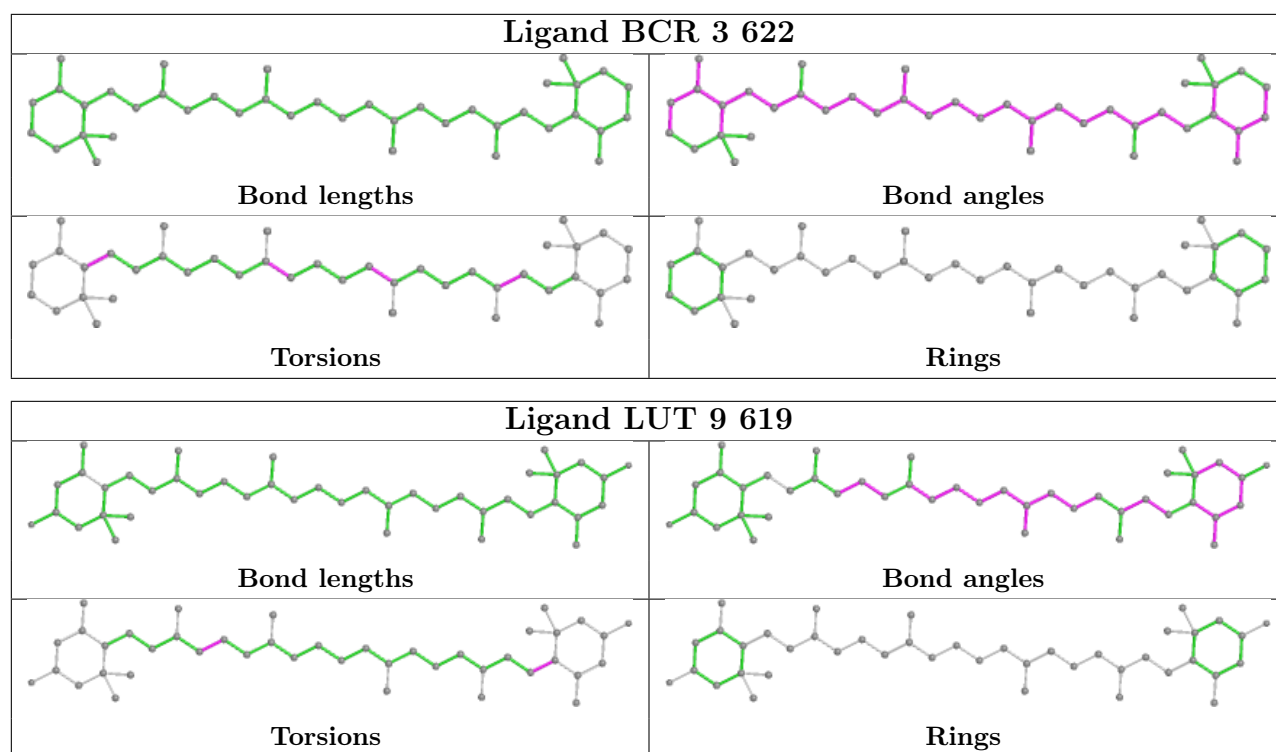
Bond angles



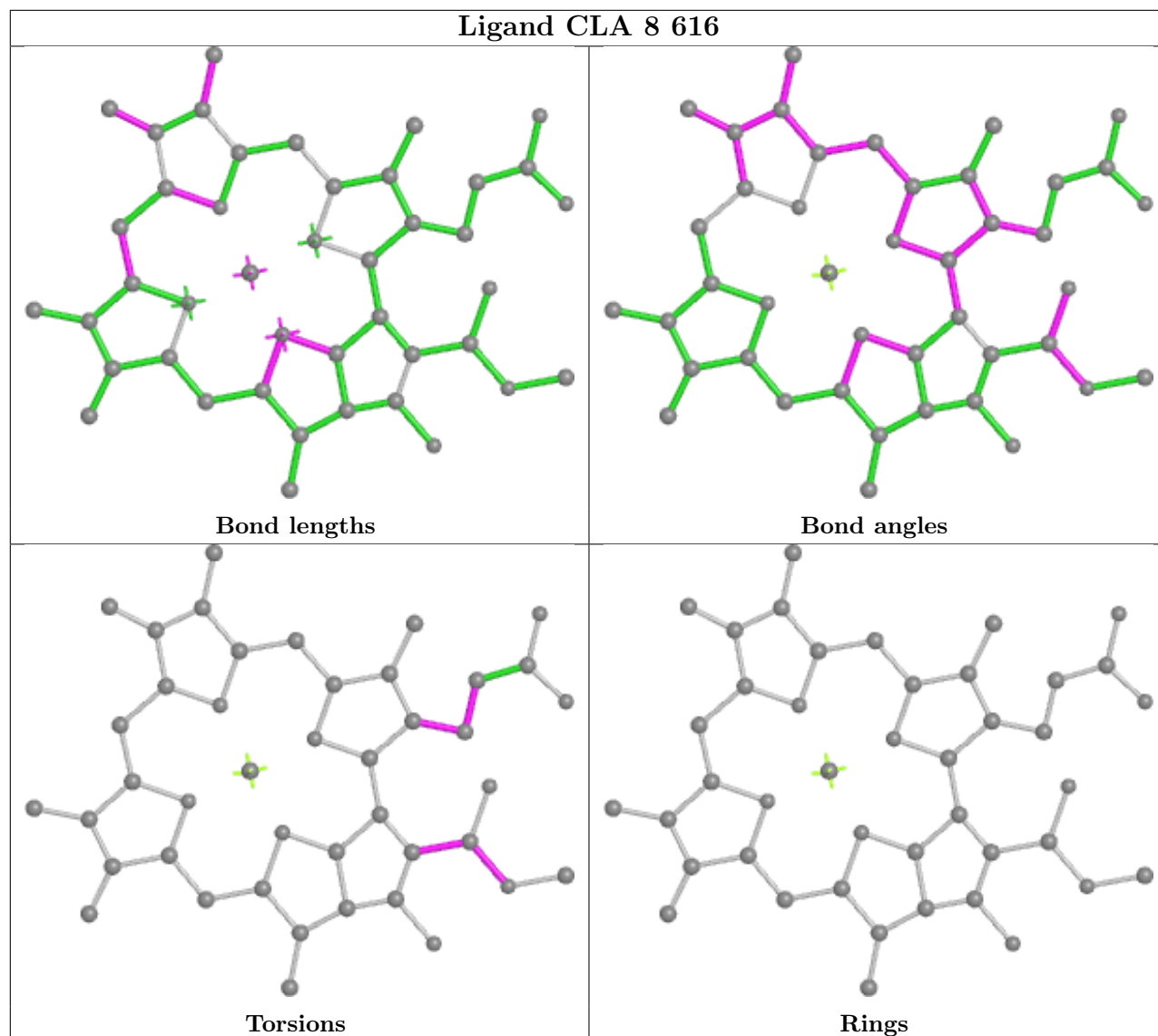
Torsions



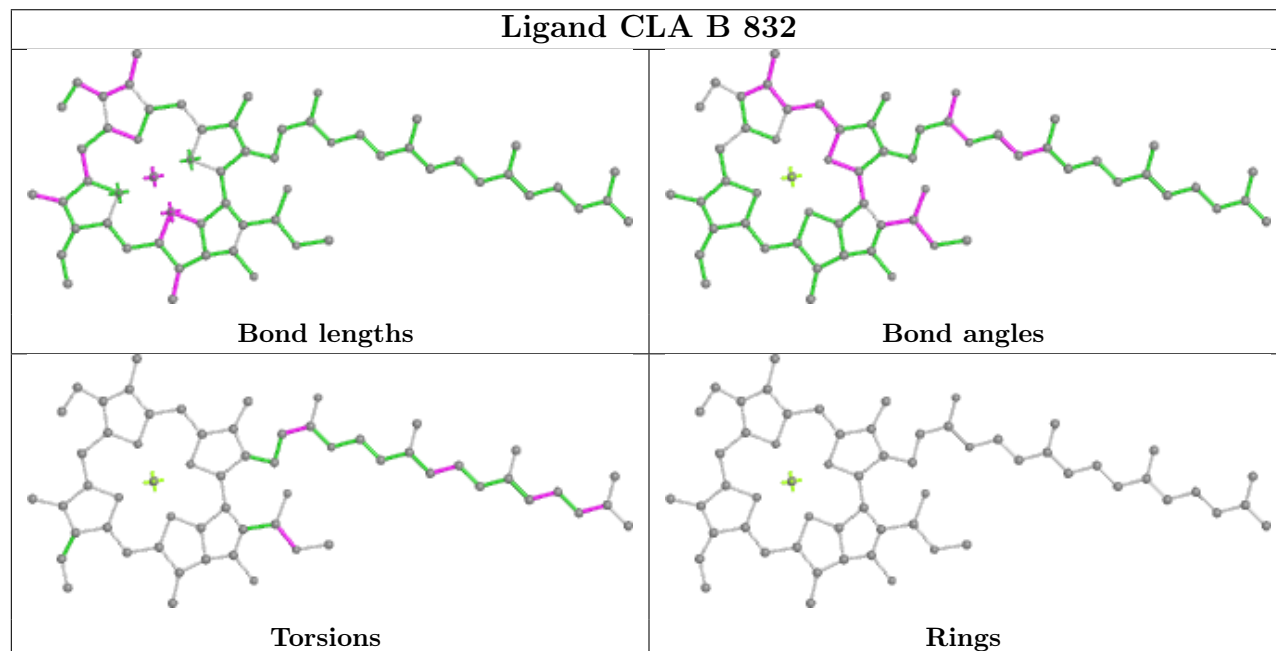
Rings



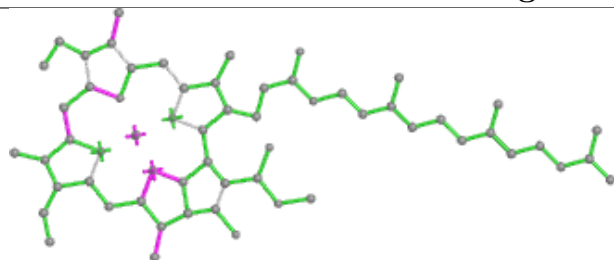
Ligand CLA 8 616



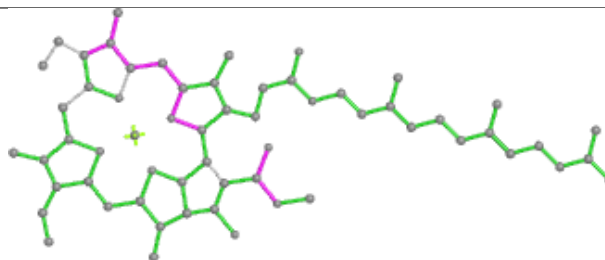
Ligand CLA B 832



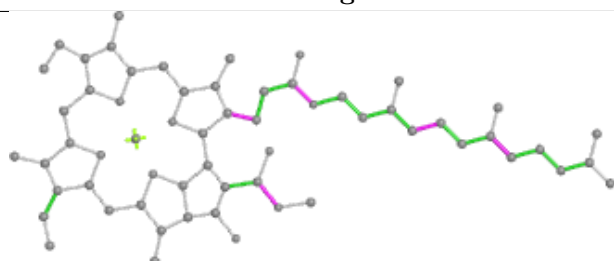
Ligand CLA 6 614



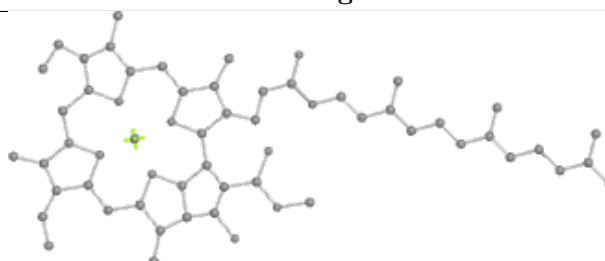
Bond lengths



Bond angles

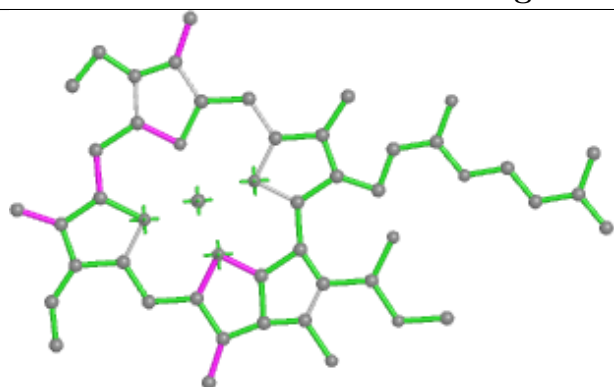


Torsions

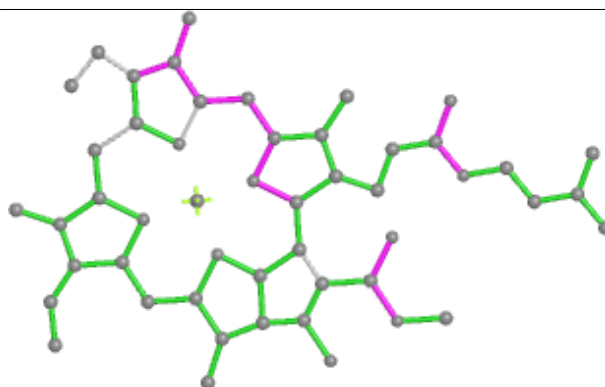


Rings

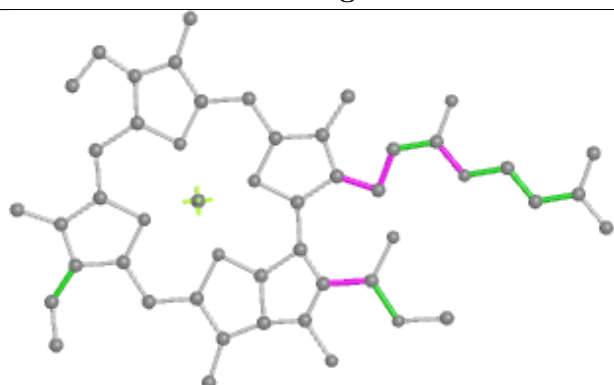
Ligand CLA B 820



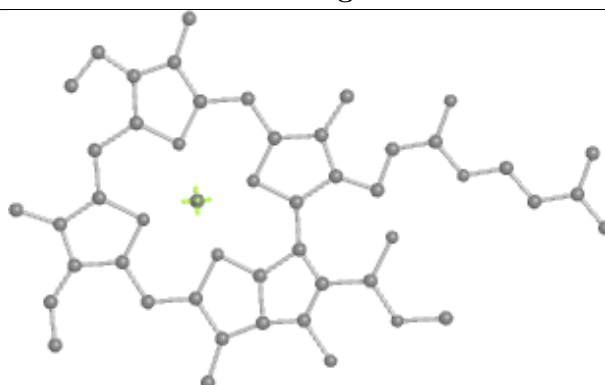
Bond lengths



Bond angles

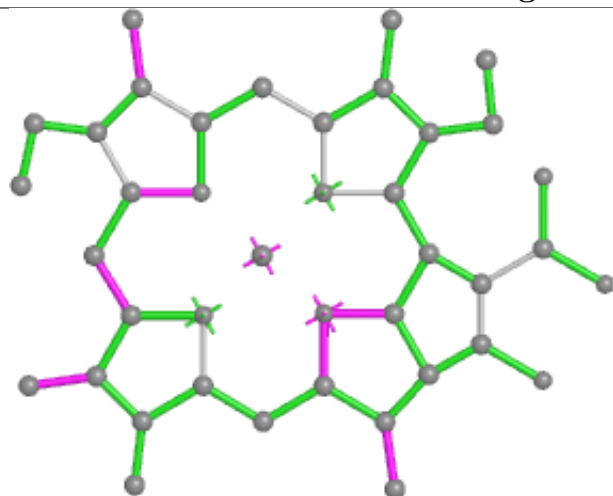


Torsions

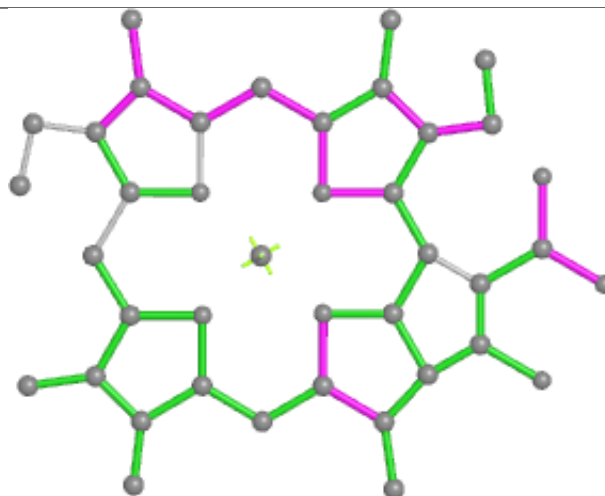


Rings

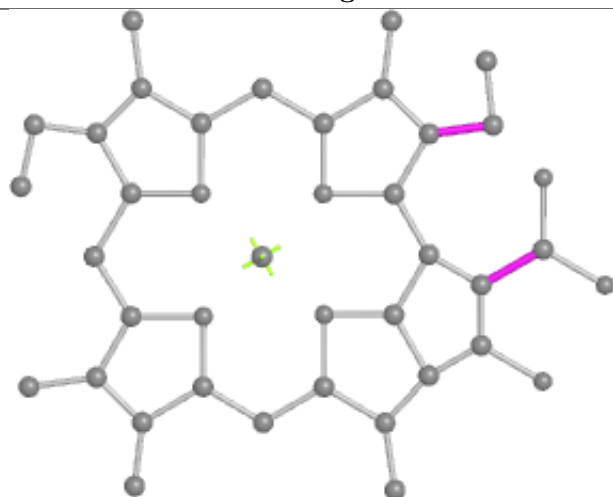
Ligand CLA 4 606



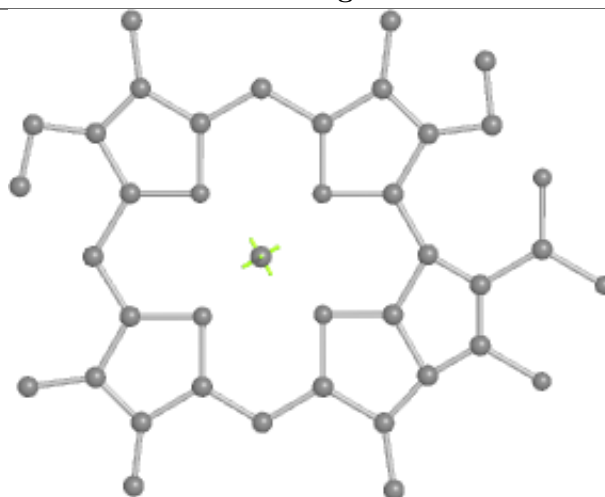
Bond lengths



Bond angles

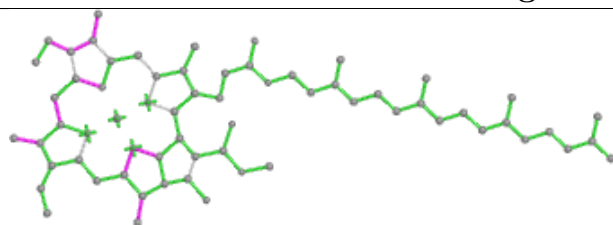


Torsions

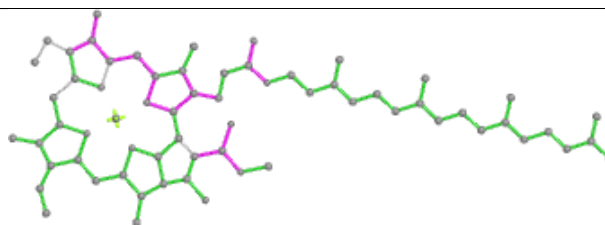


Rings

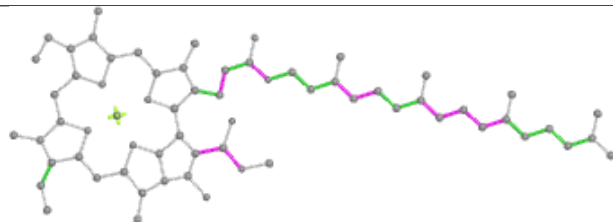
Ligand CLA 8 613



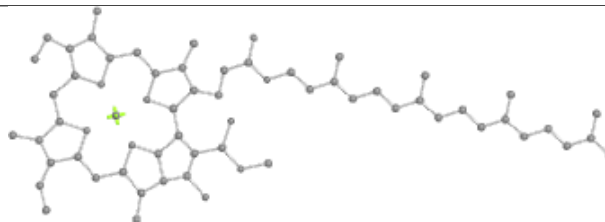
Bond lengths



Bond angles

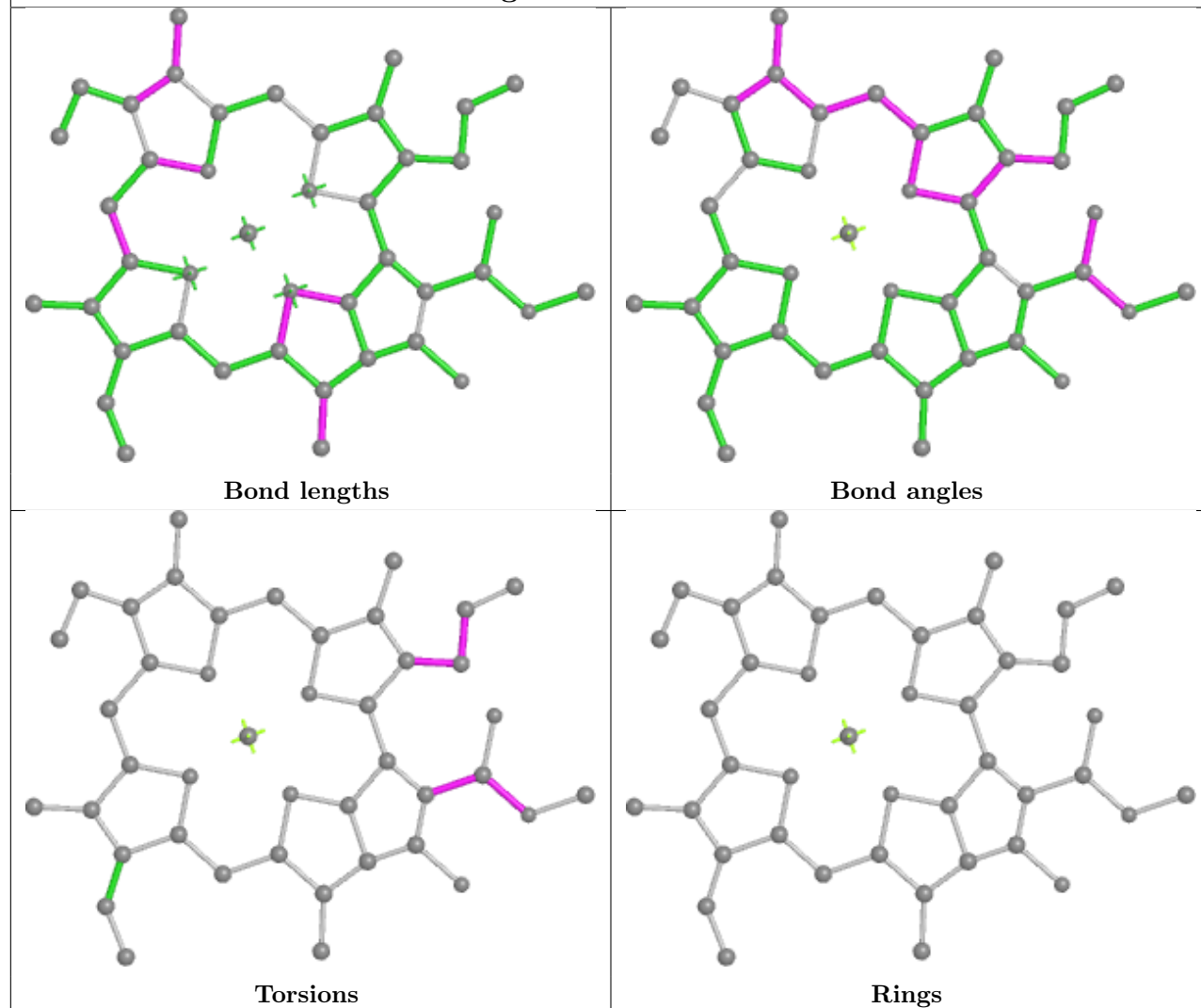


Torsions

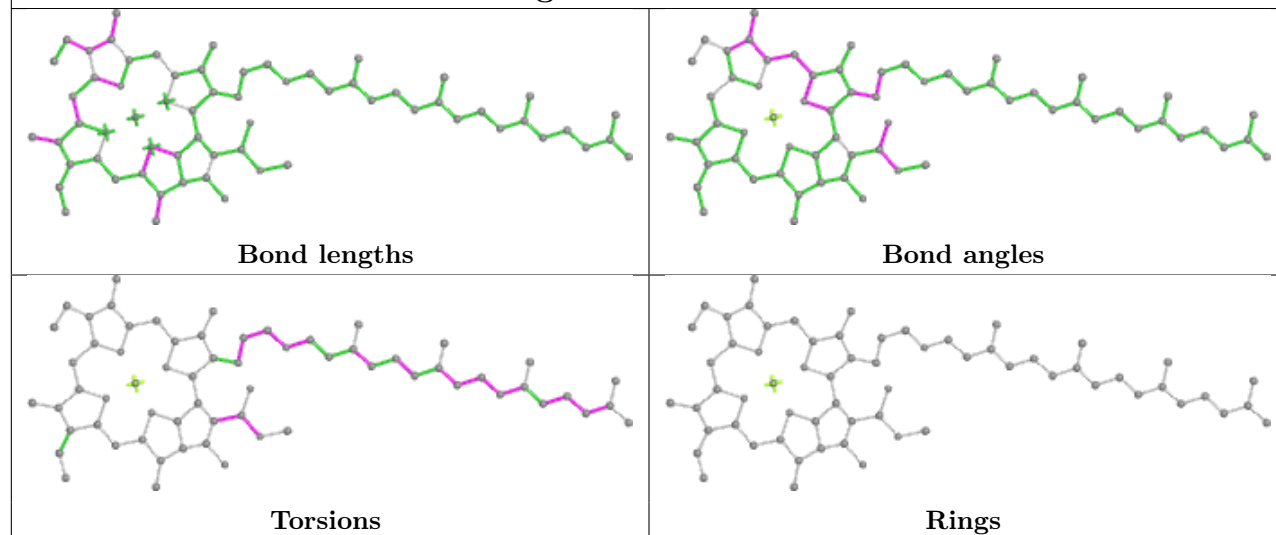


Rings

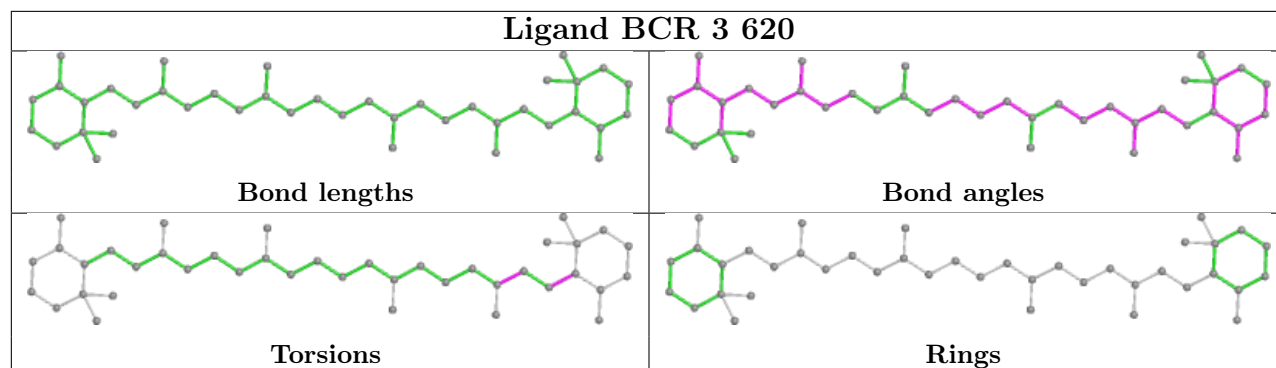
Ligand CLA B 812



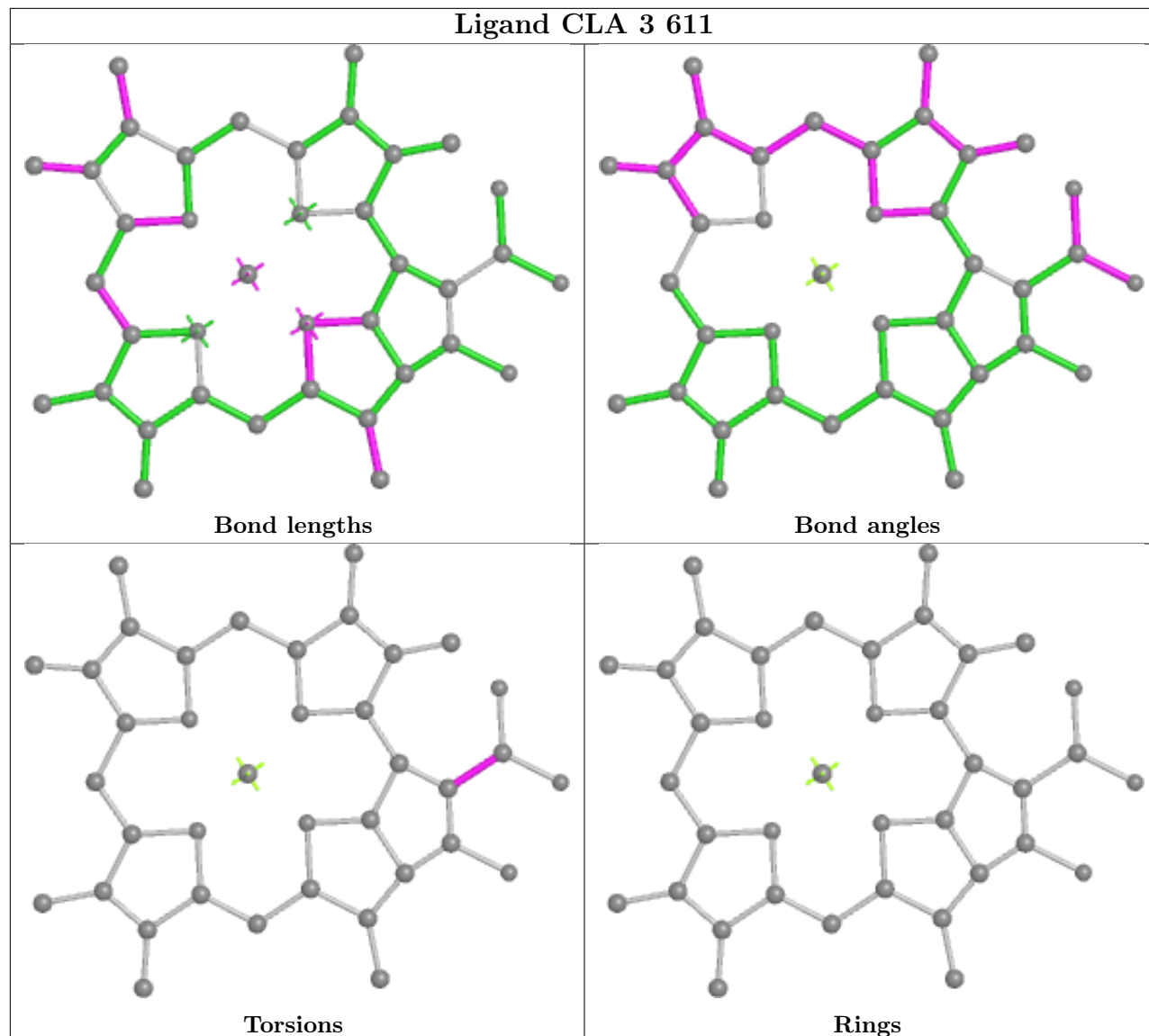
Ligand CLA 5 613

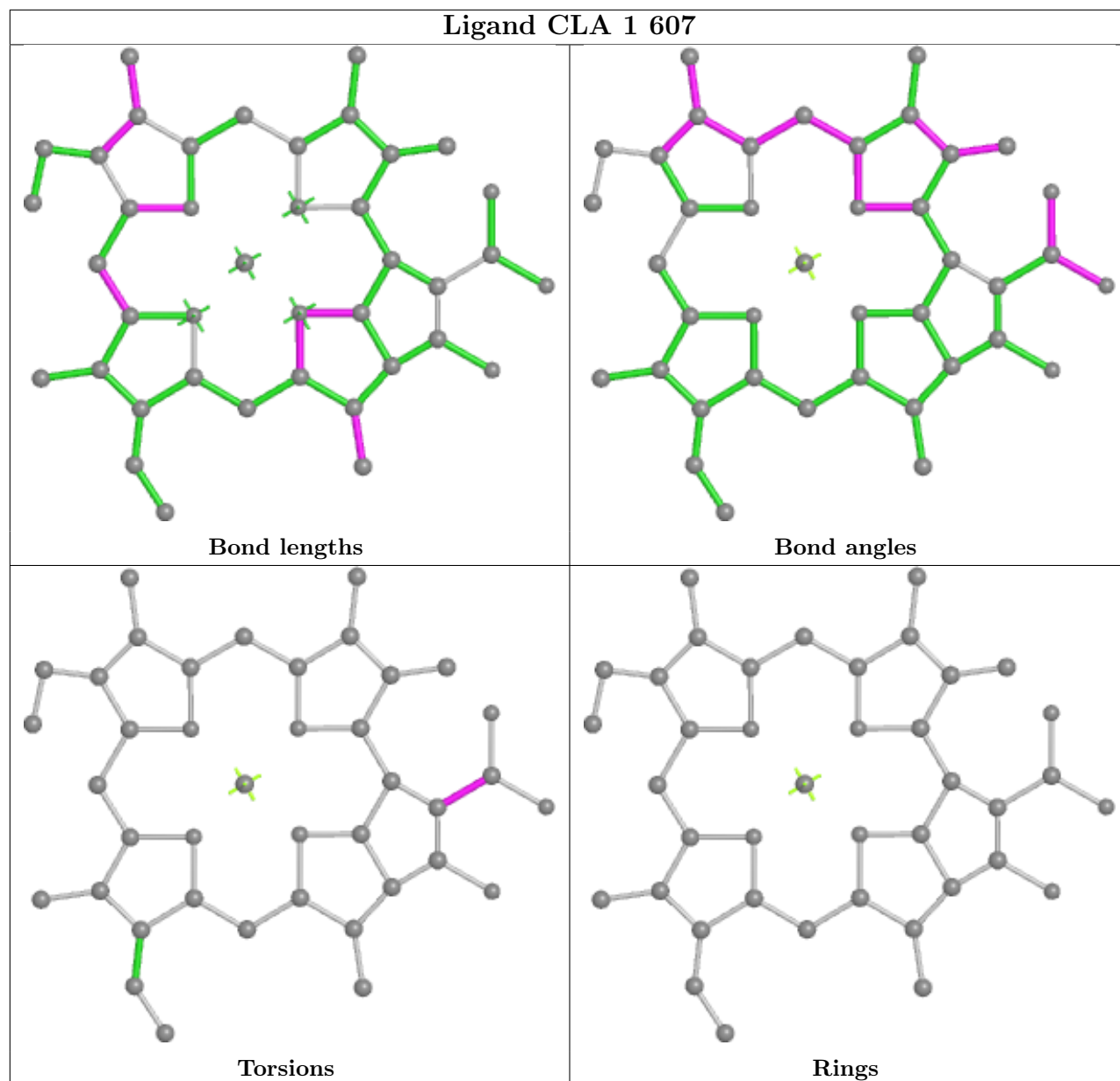
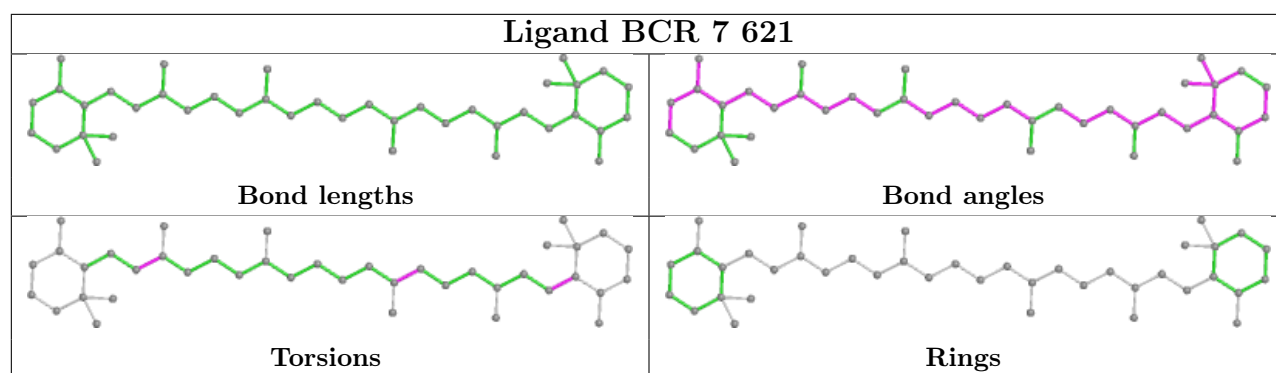


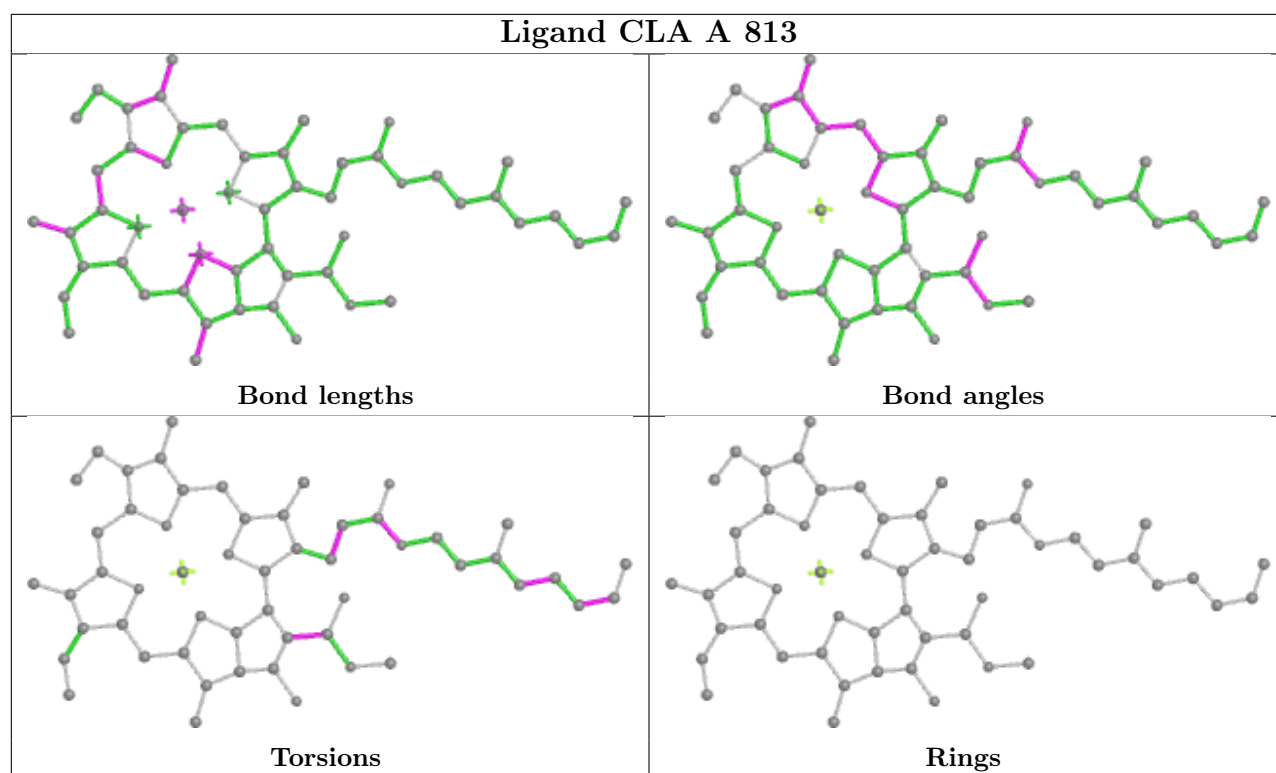
Ligand BCR 3 620



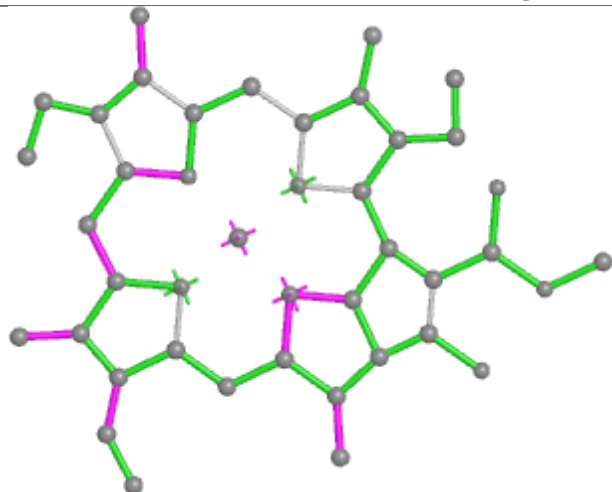
Ligand CLA 3 611



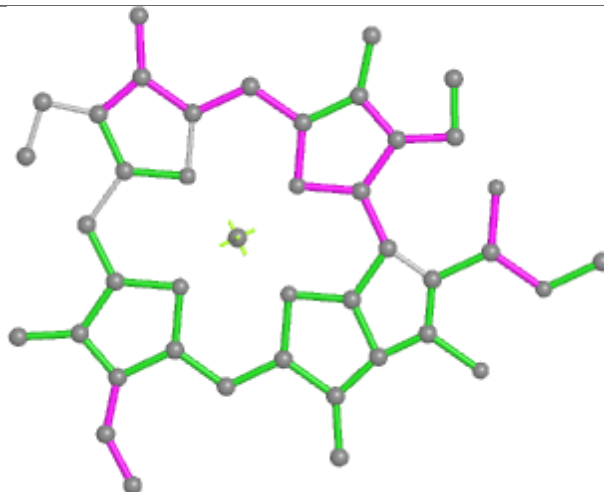




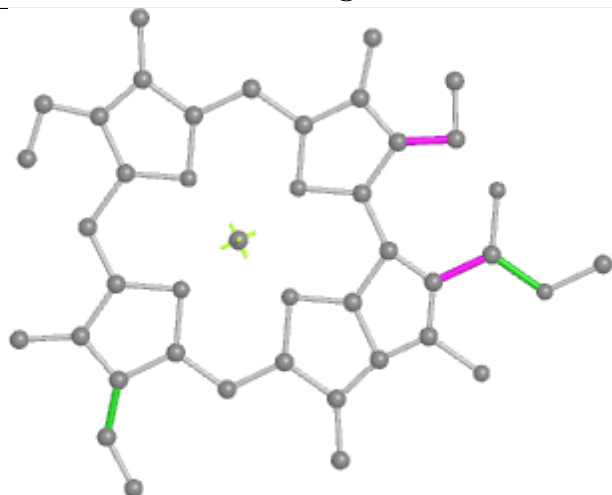
Ligand CLA a 603



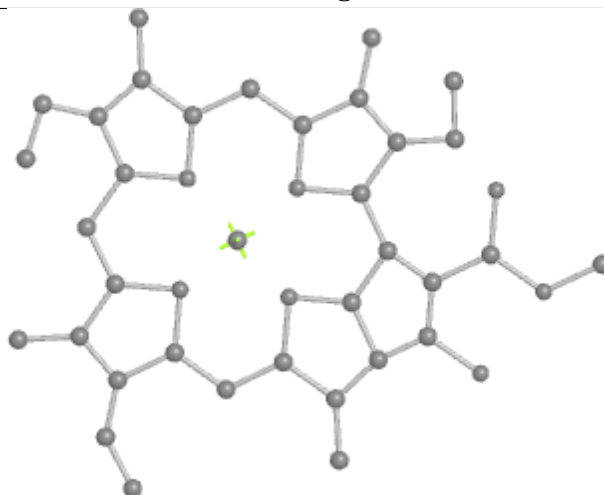
Bond lengths



Bond angles

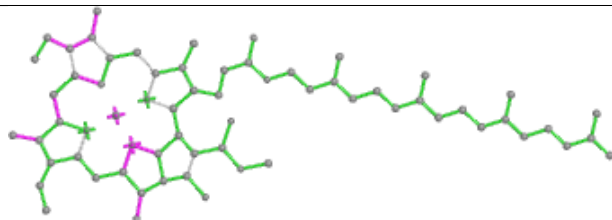


Torsions

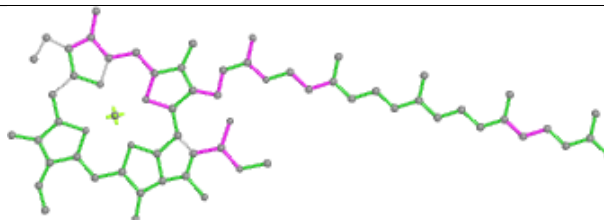


Rings

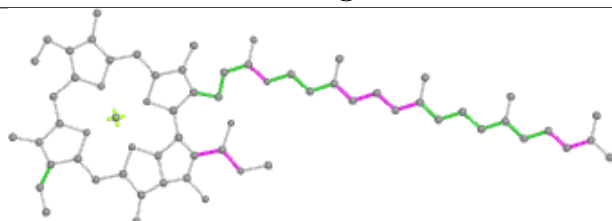
Ligand CLA B 808



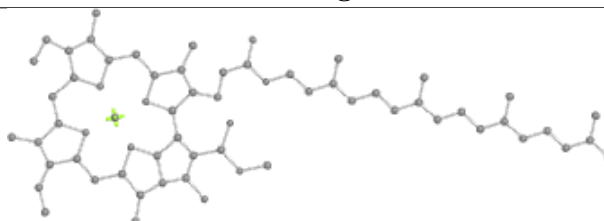
Bond lengths



Bond angles

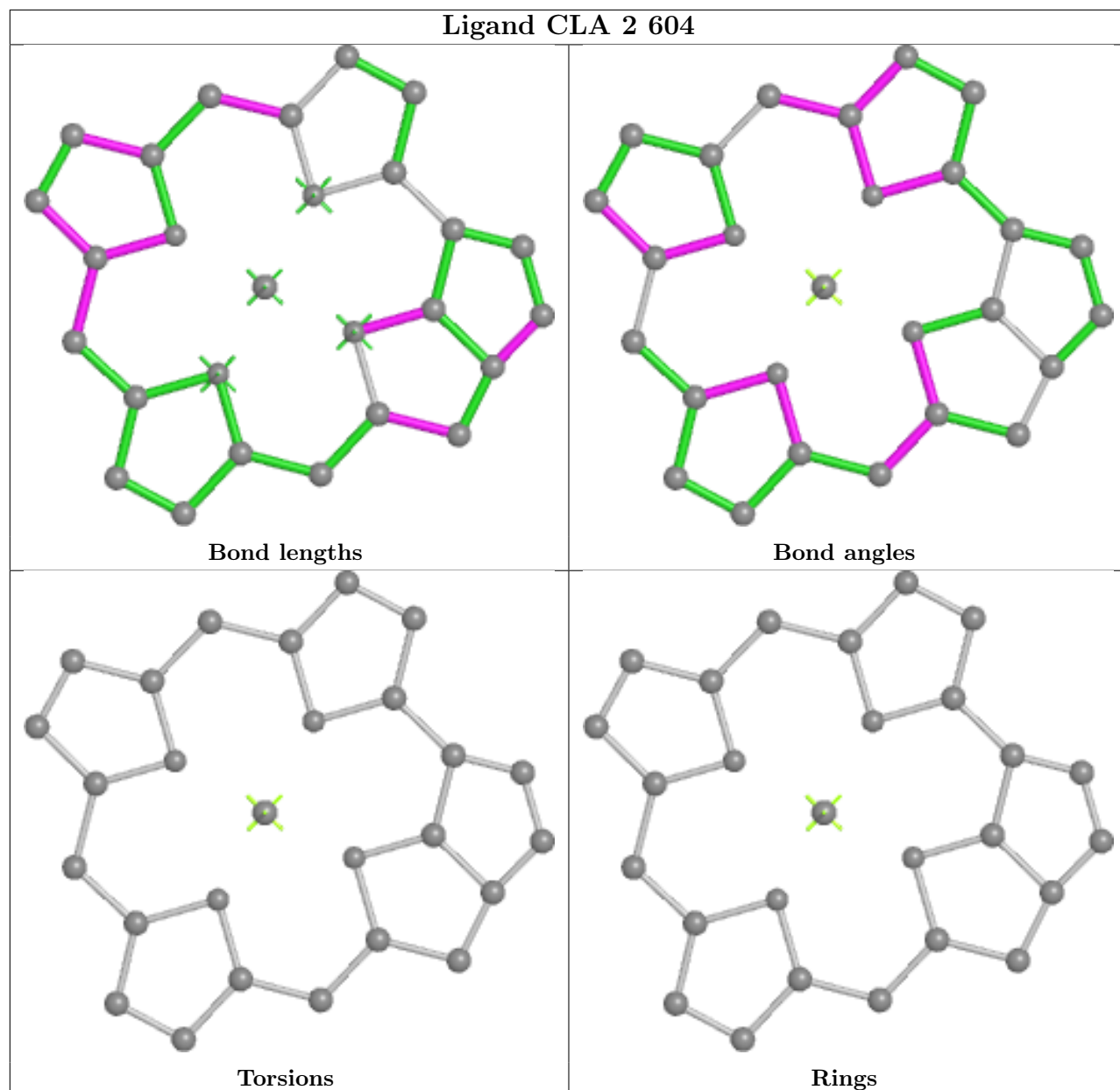


Torsions

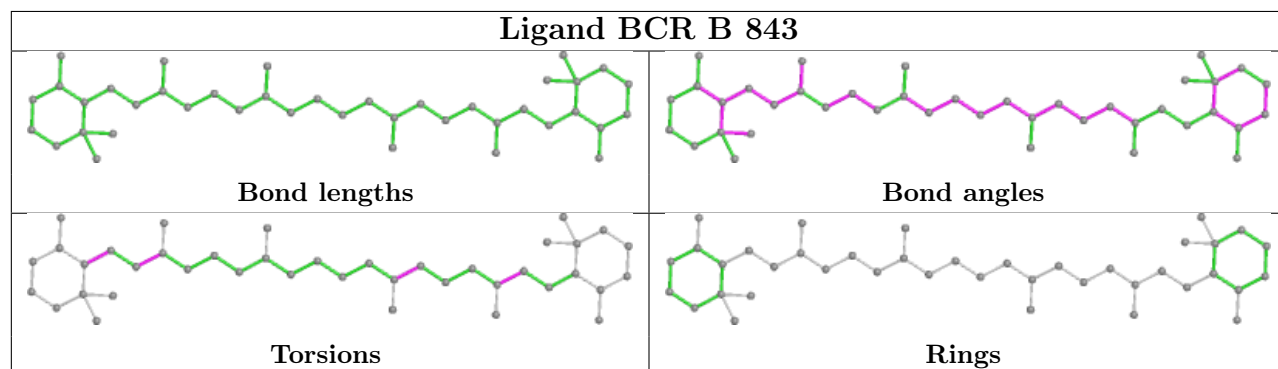


Rings

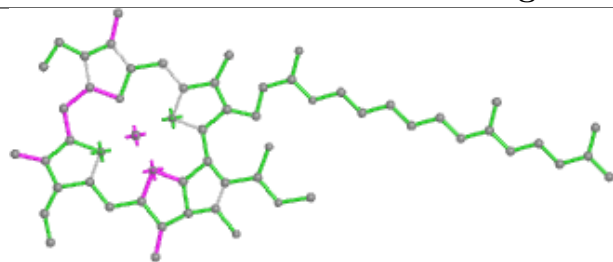
Ligand CLA 2 604



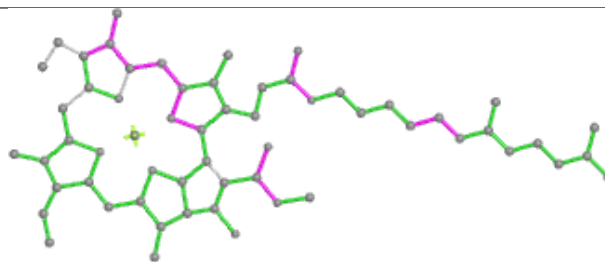
Ligand BCR B 843



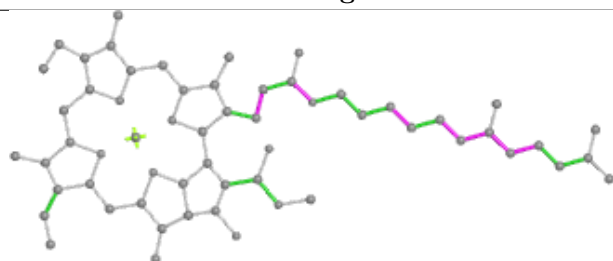
Ligand CLA 7 611



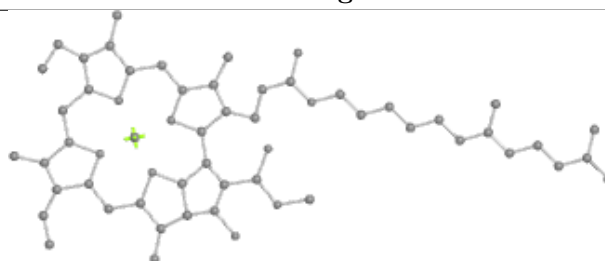
Bond lengths



Bond angles

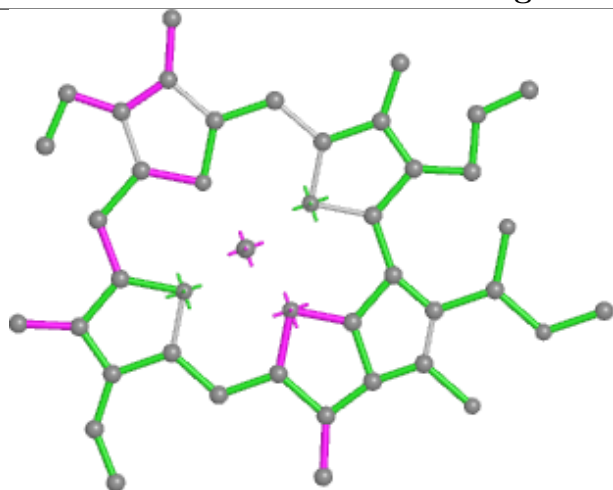


Torsions

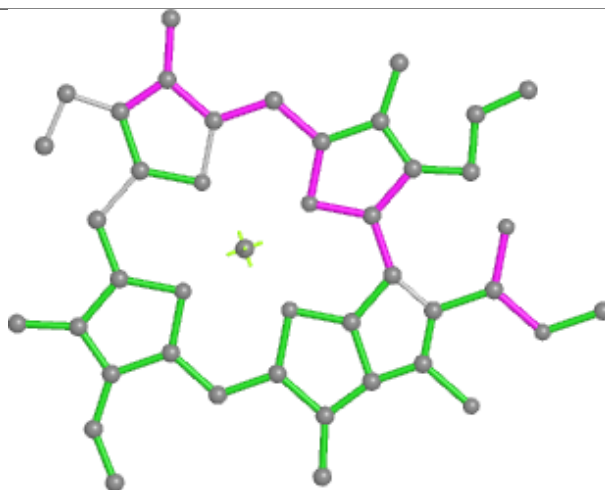


Rings

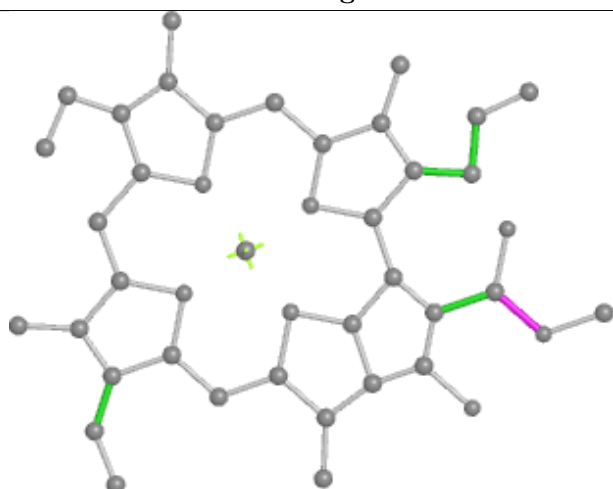
Ligand CLA B 815



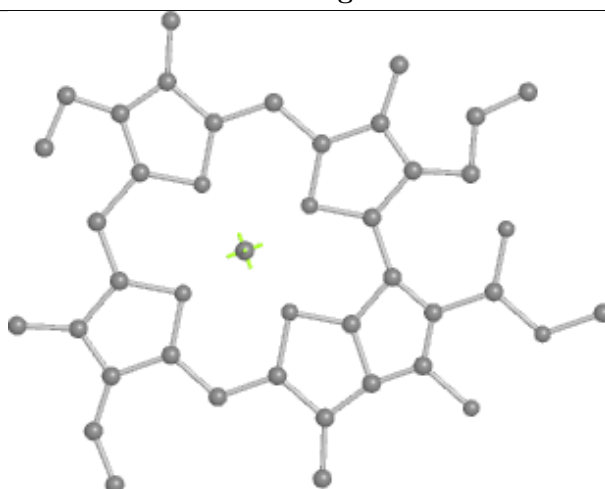
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

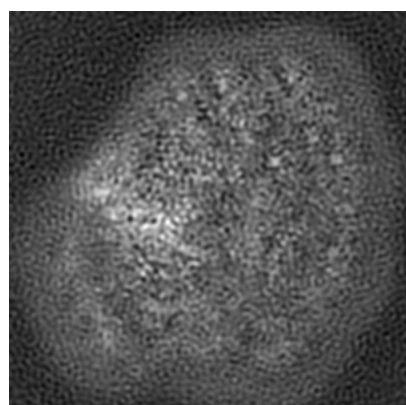
6 Map visualisation [i](#)

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

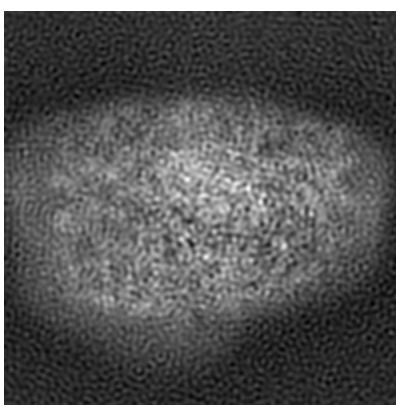
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

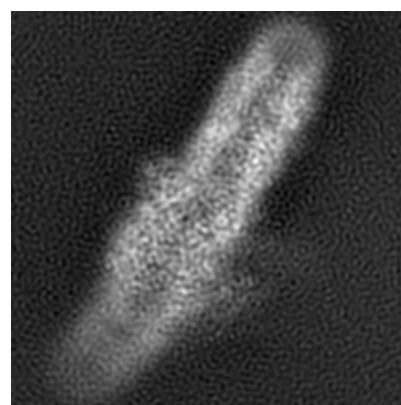
6.1.1 Primary map



X



Y

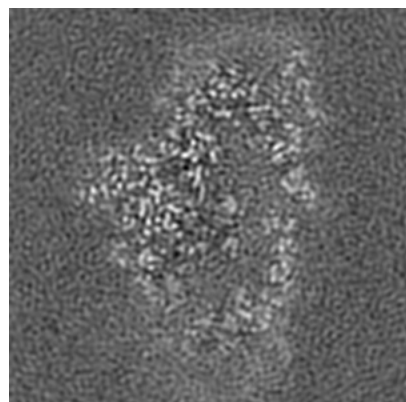


Z

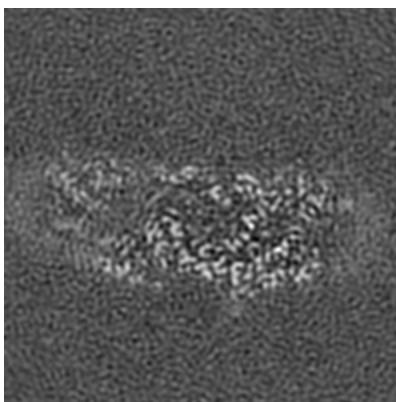
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

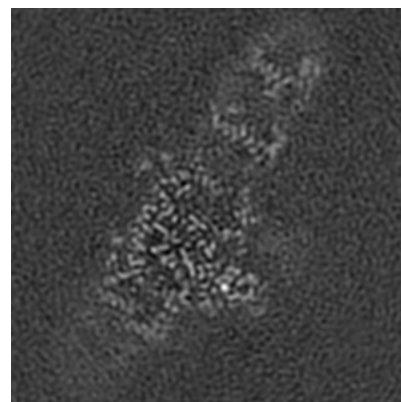
6.2.1 Primary map



X Index: 100



Y Index: 100

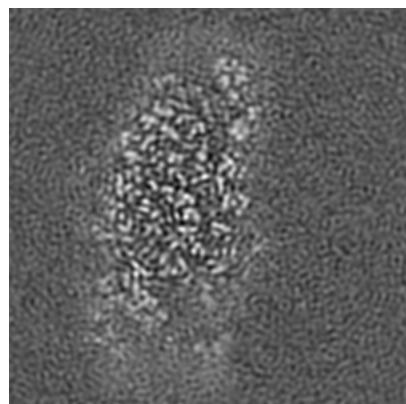


Z Index: 100

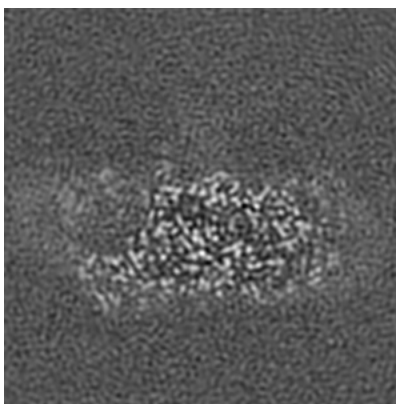
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

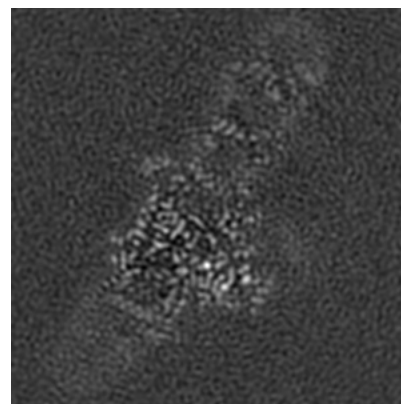
6.3.1 Primary map



X Index: 84



Y Index: 88

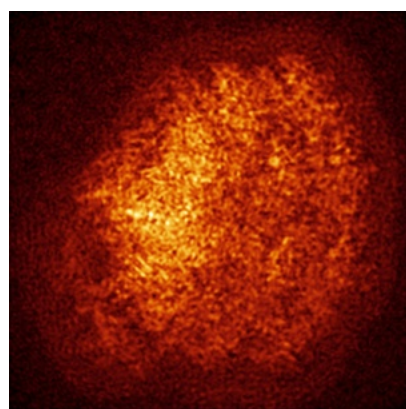


Z Index: 98

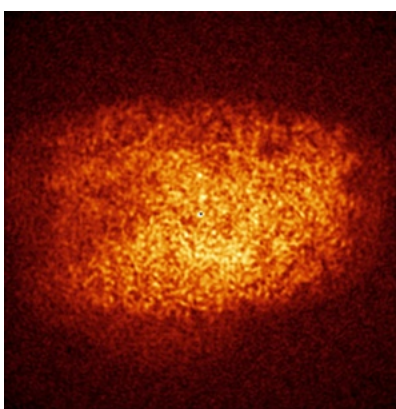
The images above show the largest variance slices of the map in three orthogonal directions.

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

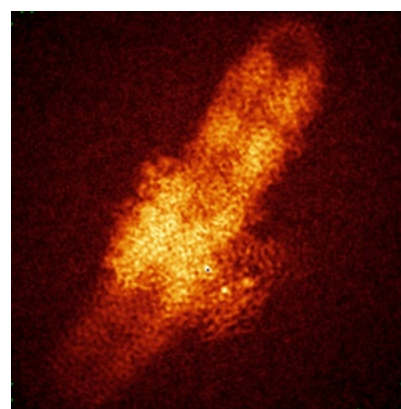
6.4.1 Primary map



X



Y

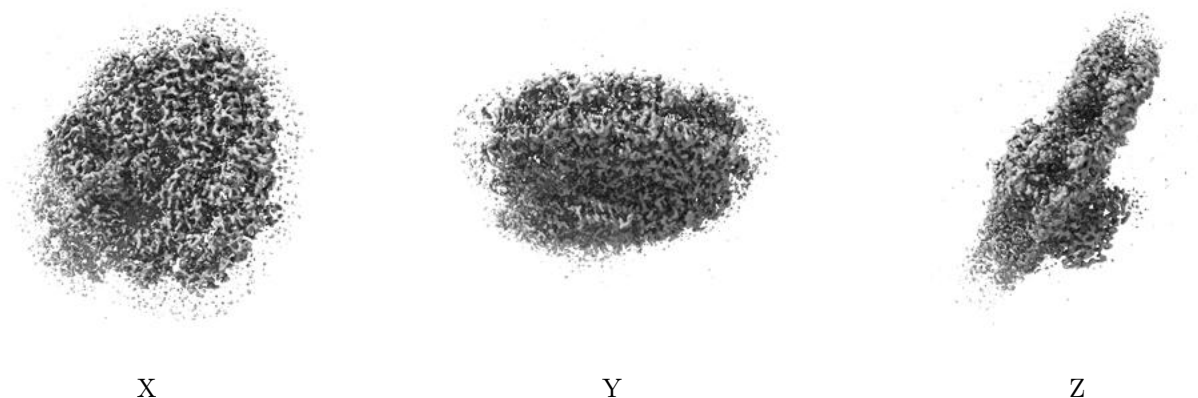


Z

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.

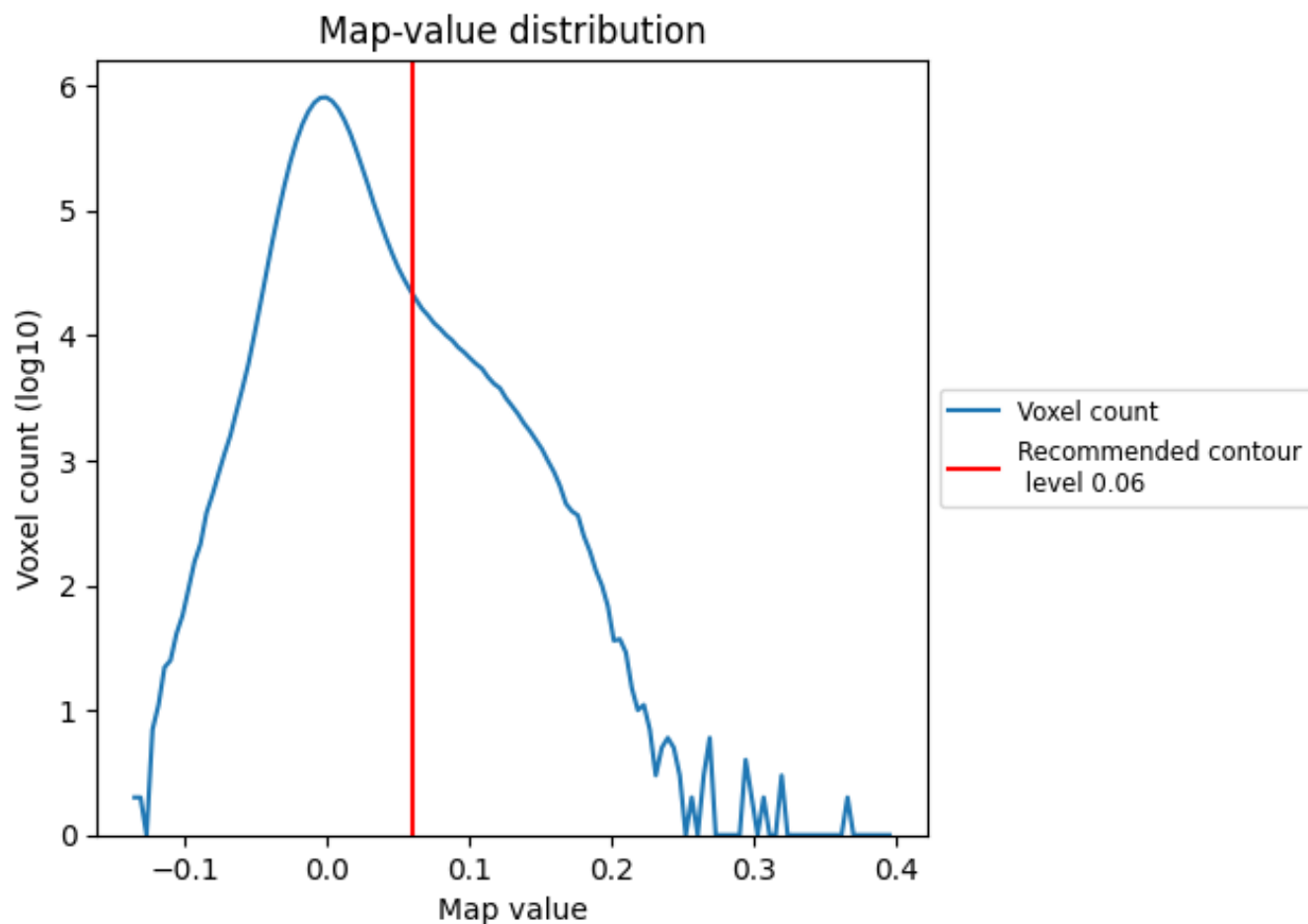
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

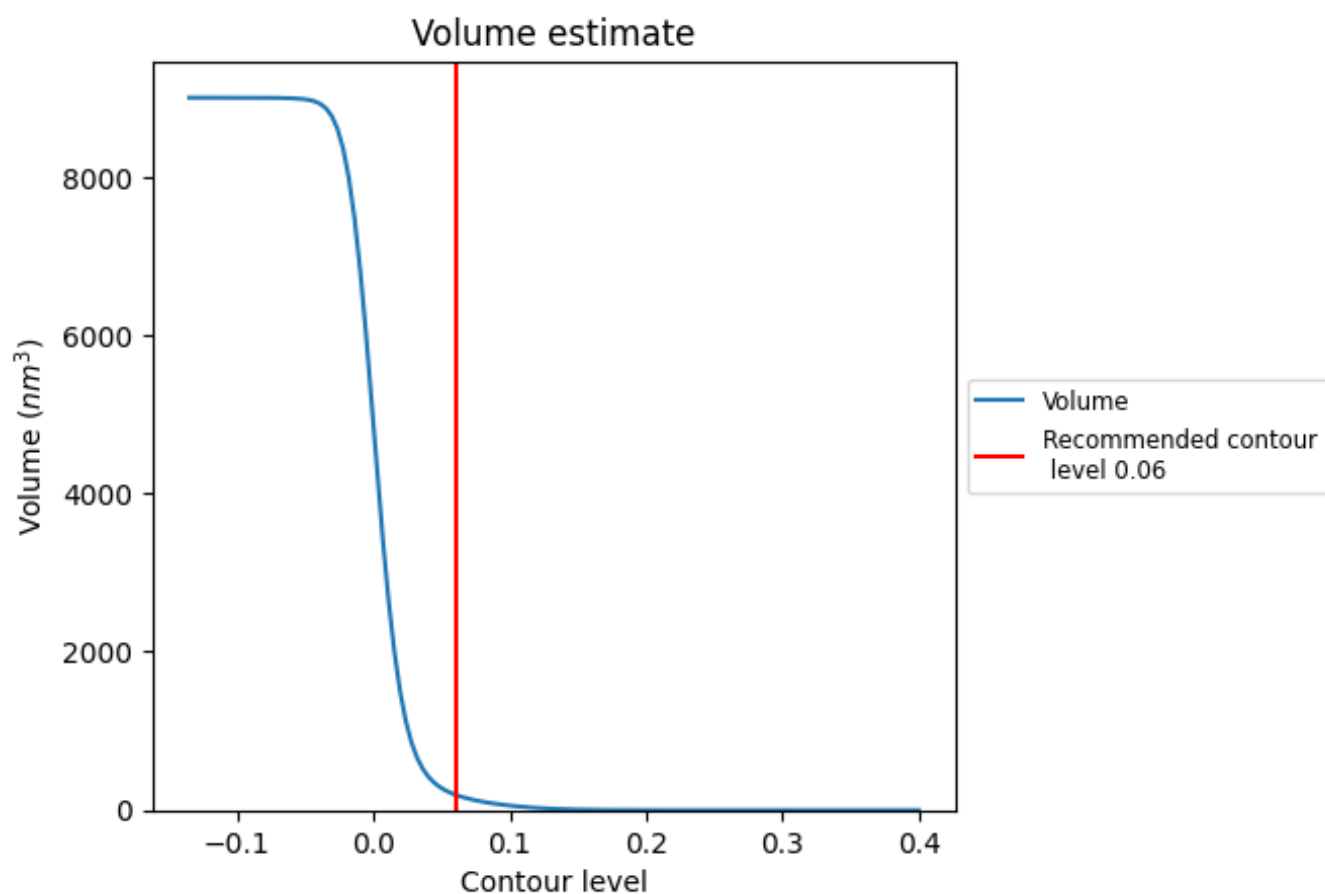
This section contains the results of statistical analysis of the map.

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.

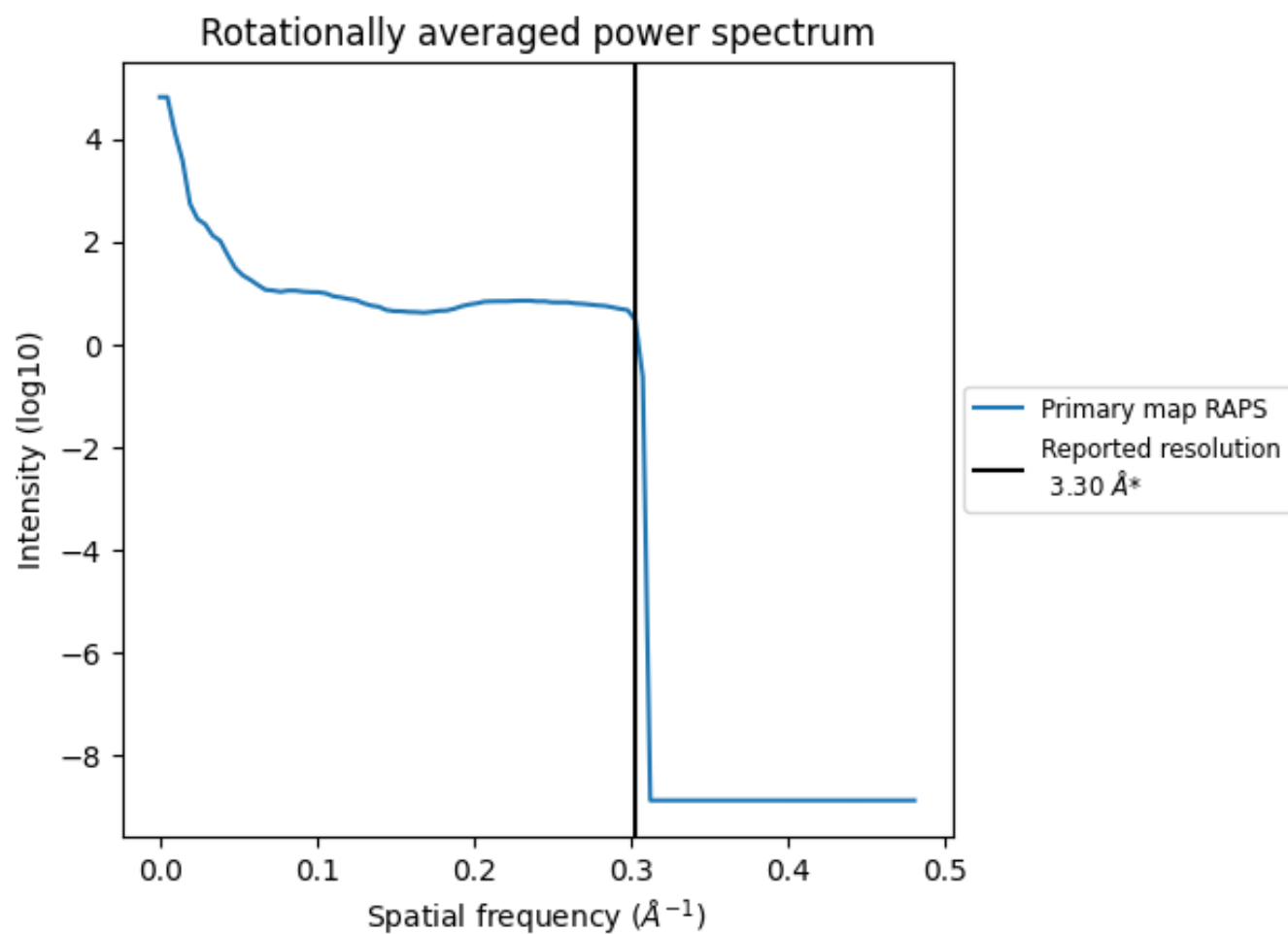
7.2 Volume estimate [i](#)



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

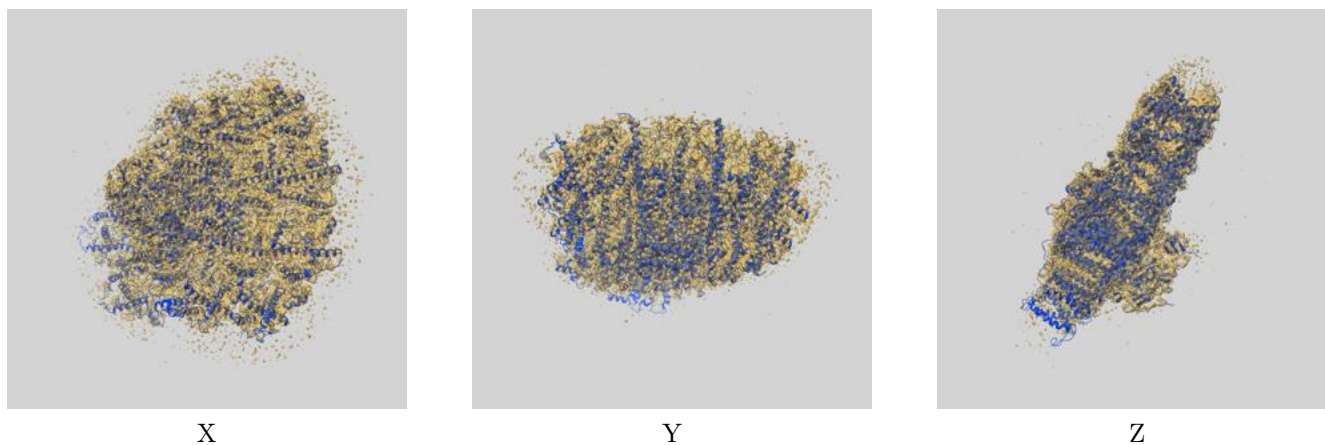
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

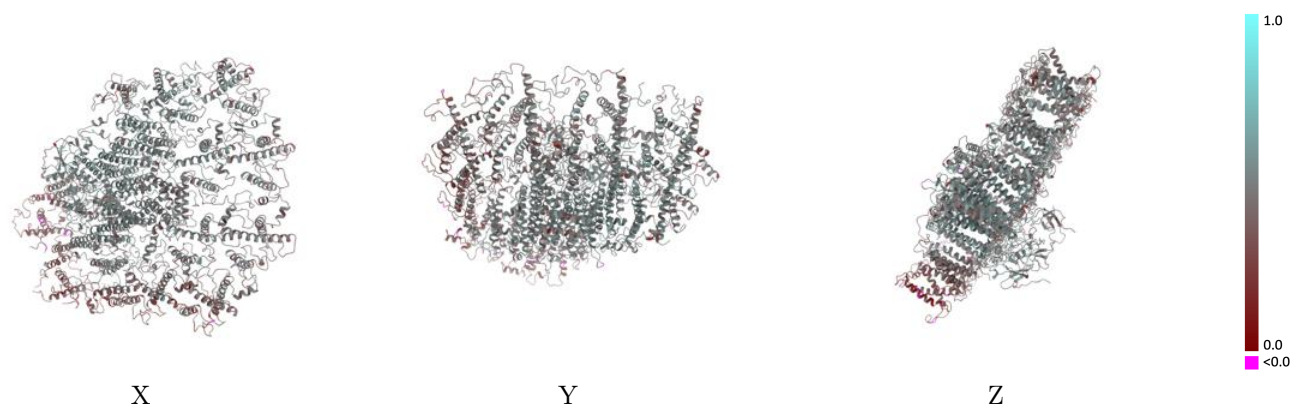
This section contains information regarding the fit between EMDB map EMD-9680 and PDB model 6IJO. Per-residue inclusion information can be found in section 3 on page 35.

9.1 Map-model overlay [i](#)



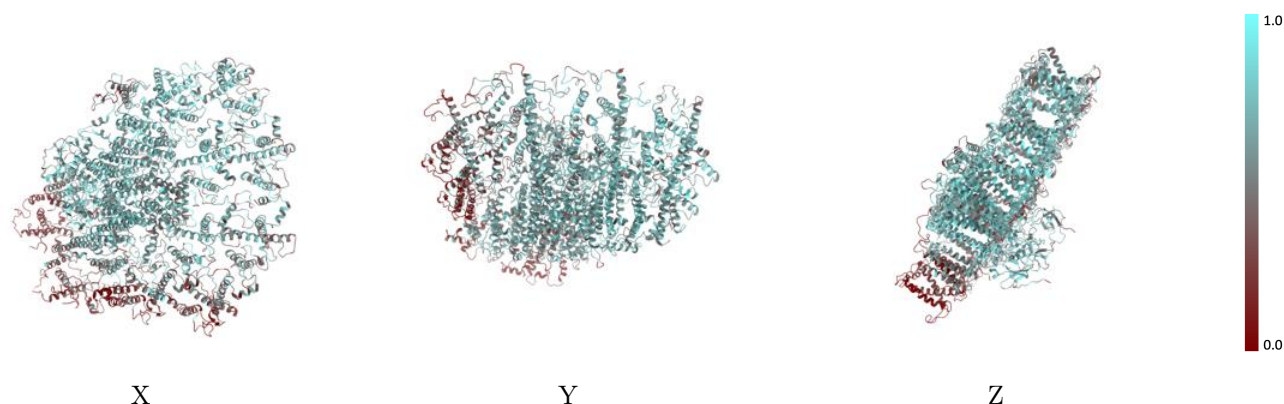
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



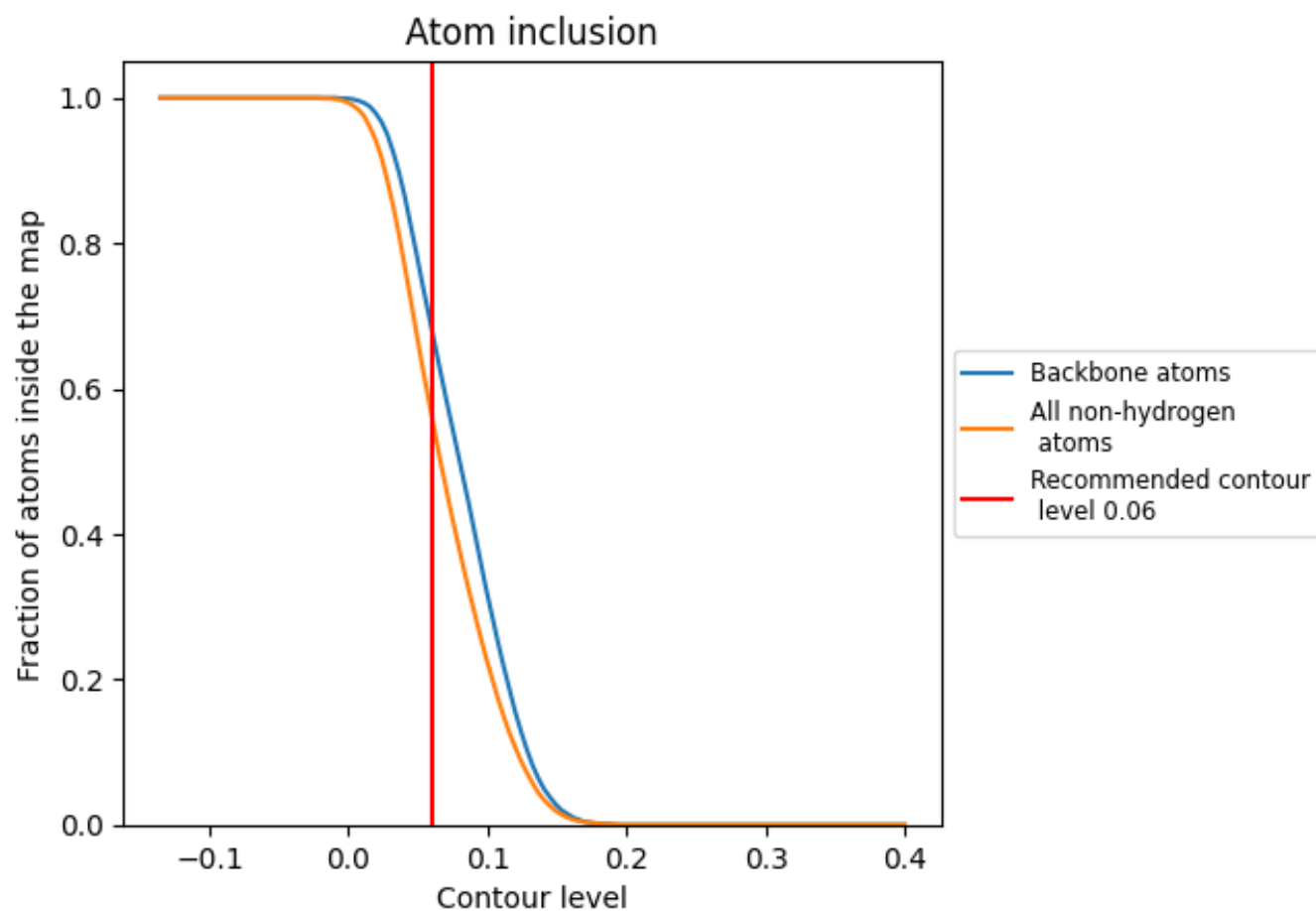
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

















































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

