



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jan 18, 2020 – 08:22 PM EST

PDB ID : 6KMX
EMDB ID: : EMD-0727
Title : Structure of PSI from *H. hongdechloris* grown under far-red light condition
Authors : Kato, K.; Nagao, R.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on : 2019-08-01
Resolution : 2.41 Å(reported)
Based on PDB ID : 1JB0

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

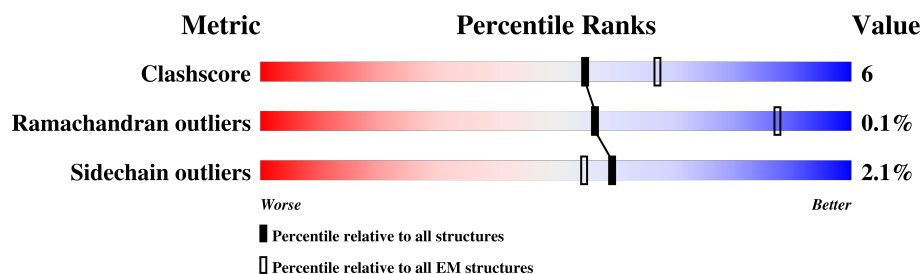
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.41 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.

















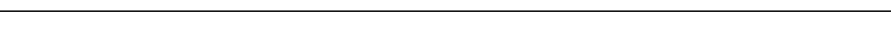
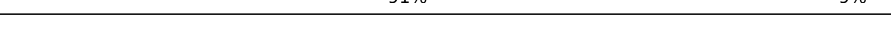
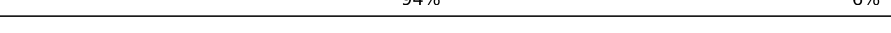
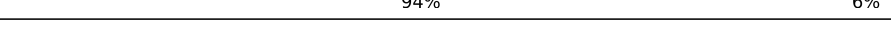
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	aA	784	
1	bA	784	
1	cA	784	
2	aB	743	
2	bB	743	
2	cB	743	
3	aC	81	
3	bC	81	
3	cC	81	

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Mol	Chain	Length	Quality of chain
4	aD	142	
4	bD	142	
4	cD	142	
5	aE	68	
5	bE	68	
5	cE	68	
6	aI	63	
6	bI	63	
6	cI	63	
7	aK	96	
7	bK	96	
7	cK	96	
8	aL	189	
8	bL	189	
8	cL	189	
9	aM	31	
9	bM	31	
9	cM	31	

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
10	CL0	aA	801	X	-	-	-
10	CL0	bA	801	X	-	-	-
10	CL0	cA	801	X	-	-	-
11	CLA	aA	802	X	-	-	-
11	CLA	aA	803	X	-	-	-
11	CLA	aA	804	X	-	-	-
11	CLA	aA	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	aA	806	X	-	-	-
11	CLA	aA	807	X	-	-	-
11	CLA	aA	808	X	-	-	-
11	CLA	aA	809	X	-	-	-
11	CLA	aA	810	X	-	-	-
11	CLA	aA	811	X	-	-	-
11	CLA	aA	812	X	-	-	-
11	CLA	aA	813	X	-	-	-
11	CLA	aA	814	X	-	-	-
11	CLA	aA	815	X	-	-	-
11	CLA	aA	816	X	-	-	-
11	CLA	aA	817	X	-	-	-
11	CLA	aA	818	X	-	-	-
11	CLA	aA	819	X	-	-	-
11	CLA	aA	820	X	-	-	-
11	CLA	aA	821	X	-	-	-
11	CLA	aA	822	X	-	-	-
11	CLA	aA	823	X	-	-	-
11	CLA	aA	824	X	-	-	-
11	CLA	aA	825	X	-	-	-
11	CLA	aA	828	X	-	-	-
11	CLA	aA	829	X	-	-	-
11	CLA	aA	831	X	-	-	-
11	CLA	aA	833	X	-	-	-
11	CLA	aA	834	X	-	-	-
11	CLA	aA	835	X	-	-	-
11	CLA	aA	836	X	-	-	-
11	CLA	aA	837	X	-	-	-
11	CLA	aA	838	X	-	-	-
11	CLA	aA	839	X	-	-	-
11	CLA	aA	840	X	-	-	-
11	CLA	aA	841	X	-	-	-
11	CLA	aA	842	X	-	-	-
11	CLA	aA	843	X	-	-	-
11	CLA	aB	801	X	-	-	-
11	CLA	aB	802	X	-	-	-
11	CLA	aB	803	X	-	-	-
11	CLA	aB	804	X	-	-	-
11	CLA	aB	805	X	-	-	-
11	CLA	aB	806	X	-	-	-
11	CLA	aB	807	X	-	-	-
11	CLA	aB	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	aB	809	X	-	-	-
11	CLA	aB	810	X	-	-	-
11	CLA	aB	811	X	-	-	-
11	CLA	aB	812	X	-	-	-
11	CLA	aB	813	X	-	-	-
11	CLA	aB	814	X	-	-	-
11	CLA	aB	815	X	-	-	-
11	CLA	aB	816	X	-	-	-
11	CLA	aB	817	X	-	-	-
11	CLA	aB	818	X	-	-	-
11	CLA	aB	819	X	-	-	-
11	CLA	aB	820	X	-	-	-
11	CLA	aB	821	X	-	-	-
11	CLA	aB	822	X	-	-	-
11	CLA	aB	823	X	-	-	-
11	CLA	aB	825	X	-	-	-
11	CLA	aB	826	X	-	-	-
11	CLA	aB	827	X	-	-	-
11	CLA	aB	828	X	-	-	-
11	CLA	aB	829	X	-	-	-
11	CLA	aB	830	X	-	-	-
11	CLA	aB	831	X	-	-	-
11	CLA	aB	832	X	-	-	-
11	CLA	aB	833	X	-	-	-
11	CLA	aB	834	X	-	-	-
11	CLA	aB	835	X	-	-	-
11	CLA	aB	836	X	-	-	-
11	CLA	aB	837	X	-	-	-
11	CLA	aB	838	X	-	-	-
11	CLA	aB	839	X	-	-	-
11	CLA	aB	840	X	-	-	-
11	CLA	aK	101	X	-	-	-
11	CLA	aK	103	X	-	-	-
11	CLA	aL	204	X	-	-	-
11	CLA	aL	205	X	-	-	-
11	CLA	aL	206	X	-	-	-
11	CLA	bA	802	X	-	-	-
11	CLA	bA	803	X	-	-	-
11	CLA	bA	804	X	-	-	-
11	CLA	bA	805	X	-	-	-
11	CLA	bA	806	X	-	-	-
11	CLA	bA	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	bA	808	X	-	-	-
11	CLA	bA	809	X	-	-	-
11	CLA	bA	810	X	-	-	-
11	CLA	bA	811	X	-	-	-
11	CLA	bA	812	X	-	-	-
11	CLA	bA	813	X	-	-	-
11	CLA	bA	814	X	-	-	-
11	CLA	bA	815	X	-	-	-
11	CLA	bA	816	X	-	-	-
11	CLA	bA	817	X	-	-	-
11	CLA	bA	818	X	-	-	-
11	CLA	bA	819	X	-	-	-
11	CLA	bA	820	X	-	-	-
11	CLA	bA	821	X	-	-	-
11	CLA	bA	822	X	-	-	-
11	CLA	bA	823	X	-	-	-
11	CLA	bA	824	X	-	-	-
11	CLA	bA	825	X	-	-	-
11	CLA	bA	828	X	-	-	-
11	CLA	bA	829	X	-	-	-
11	CLA	bA	831	X	-	-	-
11	CLA	bA	833	X	-	-	-
11	CLA	bA	834	X	-	-	-
11	CLA	bA	835	X	-	-	-
11	CLA	bA	836	X	-	-	-
11	CLA	bA	837	X	-	-	-
11	CLA	bA	838	X	-	-	-
11	CLA	bA	839	X	-	-	-
11	CLA	bA	840	X	-	-	-
11	CLA	bA	841	X	-	-	-
11	CLA	bA	842	X	-	-	-
11	CLA	bA	843	X	-	-	-
11	CLA	bB	801	X	-	-	-
11	CLA	bB	802	X	-	-	-
11	CLA	bB	803	X	-	-	-
11	CLA	bB	804	X	-	-	-
11	CLA	bB	805	X	-	-	-
11	CLA	bB	806	X	-	-	-
11	CLA	bB	807	X	-	-	-
11	CLA	bB	808	X	-	-	-
11	CLA	bB	809	X	-	-	-
11	CLA	bB	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	bB	811	X	-	-	-
11	CLA	bB	812	X	-	-	-
11	CLA	bB	813	X	-	-	-
11	CLA	bB	814	X	-	-	-
11	CLA	bB	815	X	-	-	-
11	CLA	bB	816	X	-	-	-
11	CLA	bB	817	X	-	-	-
11	CLA	bB	818	X	-	-	-
11	CLA	bB	819	X	-	-	-
11	CLA	bB	820	X	-	-	-
11	CLA	bB	821	X	-	-	-
11	CLA	bB	822	X	-	-	-
11	CLA	bB	823	X	-	-	-
11	CLA	bB	825	X	-	-	-
11	CLA	bB	826	X	-	-	-
11	CLA	bB	827	X	-	-	-
11	CLA	bB	828	X	-	-	-
11	CLA	bB	829	X	-	-	-
11	CLA	bB	830	X	-	-	-
11	CLA	bB	831	X	-	-	-
11	CLA	bB	832	X	-	-	-
11	CLA	bB	833	X	-	-	-
11	CLA	bB	834	X	-	-	-
11	CLA	bB	835	X	-	-	-
11	CLA	bB	836	X	-	-	-
11	CLA	bB	837	X	-	-	-
11	CLA	bB	838	X	-	-	-
11	CLA	bB	839	X	-	-	-
11	CLA	bB	840	X	-	-	-
11	CLA	bK	101	X	-	-	-
11	CLA	bK	103	X	-	-	-
11	CLA	bL	204	X	-	-	-
11	CLA	bL	205	X	-	-	-
11	CLA	bL	206	X	-	-	-
11	CLA	cA	802	X	-	-	-
11	CLA	cA	803	X	-	-	-
11	CLA	cA	804	X	-	-	-
11	CLA	cA	805	X	-	-	-
11	CLA	cA	806	X	-	-	-
11	CLA	cA	807	X	-	-	-
11	CLA	cA	808	X	-	-	-
11	CLA	cA	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	cA	810	X	-	-	-
11	CLA	cA	811	X	-	-	-
11	CLA	cA	812	X	-	-	-
11	CLA	cA	813	X	-	-	-
11	CLA	cA	814	X	-	-	-
11	CLA	cA	815	X	-	-	-
11	CLA	cA	816	X	-	-	-
11	CLA	cA	817	X	-	-	-
11	CLA	cA	818	X	-	-	-
11	CLA	cA	819	X	-	-	-
11	CLA	cA	820	X	-	-	-
11	CLA	cA	821	X	-	-	-
11	CLA	cA	822	X	-	-	-
11	CLA	cA	823	X	-	-	-
11	CLA	cA	824	X	-	-	-
11	CLA	cA	825	X	-	-	-
11	CLA	cA	828	X	-	-	-
11	CLA	cA	829	X	-	-	-
11	CLA	cA	831	X	-	-	-
11	CLA	cA	833	X	-	-	-
11	CLA	cA	834	X	-	-	-
11	CLA	cA	835	X	-	-	-
11	CLA	cA	836	X	-	-	-
11	CLA	cA	837	X	-	-	-
11	CLA	cA	838	X	-	-	-
11	CLA	cA	839	X	-	-	-
11	CLA	cA	840	X	-	-	-
11	CLA	cA	841	X	-	-	-
11	CLA	cA	842	X	-	-	-
11	CLA	cA	843	X	-	-	-
11	CLA	cB	801	X	-	-	-
11	CLA	cB	802	X	-	-	-
11	CLA	cB	803	X	-	-	-
11	CLA	cB	804	X	-	-	-
11	CLA	cB	805	X	-	-	-
11	CLA	cB	806	X	-	-	-
11	CLA	cB	807	X	-	-	-
11	CLA	cB	808	X	-	-	-
11	CLA	cB	809	X	-	-	-
11	CLA	cB	810	X	-	-	-
11	CLA	cB	811	X	-	-	-
11	CLA	cB	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	cB	813	X	-	-	-
11	CLA	cB	814	X	-	-	-
11	CLA	cB	815	X	-	-	-
11	CLA	cB	816	X	-	-	-
11	CLA	cB	817	X	-	-	-
11	CLA	cB	818	X	-	-	-
11	CLA	cB	819	X	-	-	-
11	CLA	cB	820	X	-	-	-
11	CLA	cB	821	X	-	-	-
11	CLA	cB	822	X	-	-	-
11	CLA	cB	823	X	-	-	-
11	CLA	cB	825	X	-	-	-
11	CLA	cB	826	X	-	-	-
11	CLA	cB	827	X	-	-	-
11	CLA	cB	828	X	-	-	-
11	CLA	cB	829	X	-	-	-
11	CLA	cB	830	X	-	-	-
11	CLA	cB	831	X	-	-	-
11	CLA	cB	832	X	-	-	-
11	CLA	cB	833	X	-	-	-
11	CLA	cB	834	X	-	-	-
11	CLA	cB	835	X	-	-	-
11	CLA	cB	836	X	-	-	-
11	CLA	cB	837	X	-	-	-
11	CLA	cB	838	X	-	-	-
11	CLA	cB	839	X	-	-	-
11	CLA	cB	840	X	-	-	-
11	CLA	cK	101	X	-	-	-
11	CLA	cK	103	X	-	-	-
11	CLA	cL	204	X	-	-	-
11	CLA	cL	205	X	-	-	-
11	CLA	cL	206	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 65112 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	717	Total	C	N	O	S	0	0
			5669	3724	966	950	29		
1	bA	717	Total	C	N	O	S	0	0
			5669	3724	966	950	29		
1	cA	717	Total	C	N	O	S	0	0
			5669	3724	966	950	29		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	727	Total	C	N	O	S	0	0
			5783	3786	976	996	25		
2	bB	727	Total	C	N	O	S	0	0
			5783	3786	976	996	25		
2	cB	727	Total	C	N	O	S	0	0
			5783	3786	976	996	25		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	aC	80	Total	C	N	O	S	0	0
			596	366	102	117	11		
3	bC	80	Total	C	N	O	S	0	0
			596	366	102	117	11		
3	cC	80	Total	C	N	O	S	0	0
			596	366	102	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	98	Total	C	N	O	S	0	0
			768	492	130	143	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	98	Total	C	N	O	S	0	0
			768	492	130	143	3		
4	cD	98	Total	C	N	O	S	0	0
			768	492	130	143	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	aE	61	Total	C	N	O		0	0
			499	317	87	95			
5	bE	61	Total	C	N	O		0	0
			499	317	87	95			
5	cE	61	Total	C	N	O		0	0
			499	317	87	95			

- Molecule 6 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aI	41	Total	C	N	O	S	0	0
			349	247	48	52	2		
6	bI	41	Total	C	N	O	S	0	0
			349	247	48	52	2		
6	cI	41	Total	C	N	O	S	0	0
			349	247	48	52	2		

- Molecule 7 is a protein called Photosystem I reaction center subunit Psak.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aK	46	Total	C	N	O	S	0	0
			317	206	55	54	2		
7	bK	46	Total	C	N	O	S	0	0
			317	206	55	54	2		
7	cK	46	Total	C	N	O	S	0	0
			317	206	55	54	2		

- Molecule 8 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	aL	172	Total	C	N	O	S	0	0
			1303	838	223	239	3		
8	bL	172	Total	C	N	O	S	0	0
			1303	838	223	239	3		

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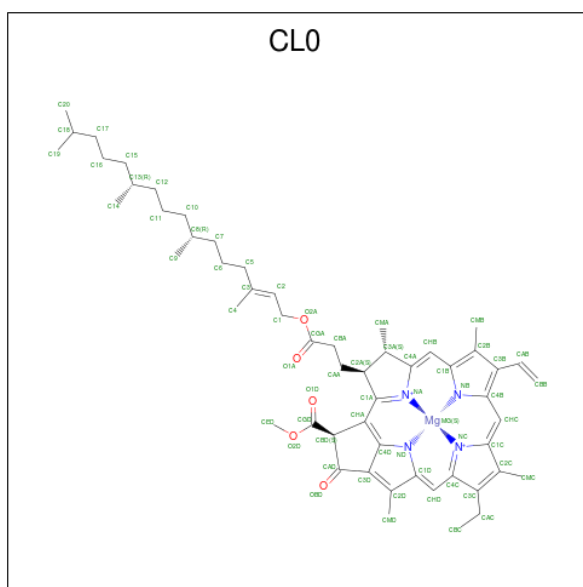
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Mol	Chain	Residues	Atoms					AltConf	Trace
8	cL	172	Total	C	N	O	S	0	0
			1303	838	223	239	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit XII.

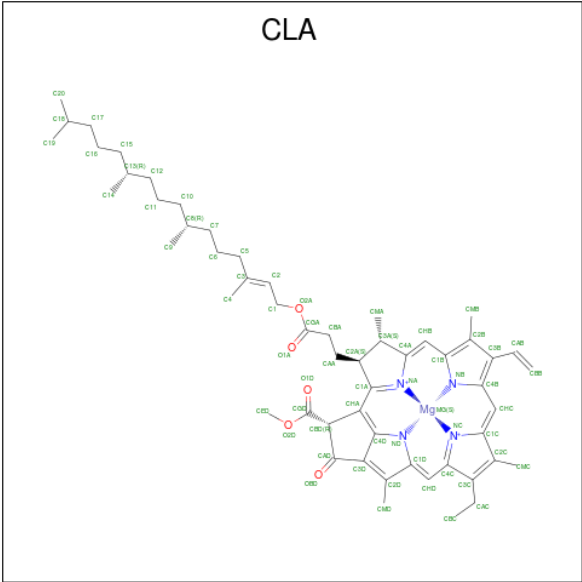
Mol	Chain	Residues	Atoms					AltConf	Trace
9	aM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		
9	bM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		
9	cM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		

- Molecule 10 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
10	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	bA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	cA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 11 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
11	aA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	aA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	aA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	aA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	aA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	aA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	aA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	aA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	aA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	aA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	aA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	aA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	

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Mol	Chain	Residues	Atoms					AltConf
11	aA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	aA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	aA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0
11	aB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0

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Mol	Chain	Residues	Atoms					AltConf
11	aK	1	Total	C	Mg	N	O	0
			89	73	2	8	6	
11	aK	1	Total	C	Mg	N	O	0
			89	73	2	8	6	
11	aL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
11	aL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
11	aL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	
11	bA	1	Total	C	Mg	N	O	0
			2112	1732	38	152	190	

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Mol	Chain	Residues	Atoms					AltConf
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	bK	1	Total	C	Mg	N	O	0
			89	73	2	8	6	
11	bK	1	Total	C	Mg	N	O	0
			89	73	2	8	6	

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Mol	Chain	Residues	Atoms					AltConf
11	bL	1	Total 195	C 165	Mg 3	N 12	O 15	0
11	bL	1	Total 195	C 165	Mg 3	N 12	O 15	0
11	bL	1	Total 195	C 165	Mg 3	N 12	O 15	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0

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Mol	Chain	Residues	Atoms					AltConf
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cA	1	Total 2112	C 1732	Mg 38	N 152	O 190	0
11	cB	1	Total 2116	C 1726	Mg 39	N 156	O 195	0

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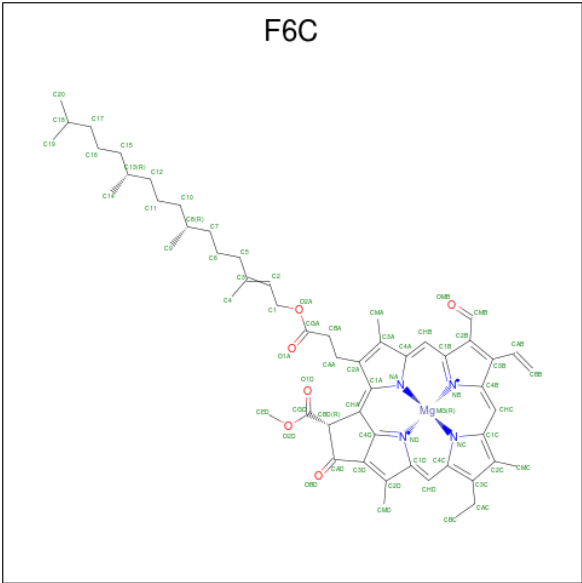
Mol	Chain	Residues	Atoms					AltConf
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cB	1	Total	C	Mg	N	O	0
			2116	1726	39	156	195	
11	cK	1	Total	C	Mg	N	O	0
			89	73	2	8	6	
11	cK	1	Total	C	Mg	N	O	0
			89	73	2	8	6	
11	cL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	
11	cL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	

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Mol	Chain	Residues	Atoms					AltConf
11	cL	1	Total	C	Mg	N	O	0
			195	165	3	12	15	

- Molecule 12 is Chlorophyll F (three-letter code: F6C) (formula: C₅₅H₆₈MgN₄O₆).



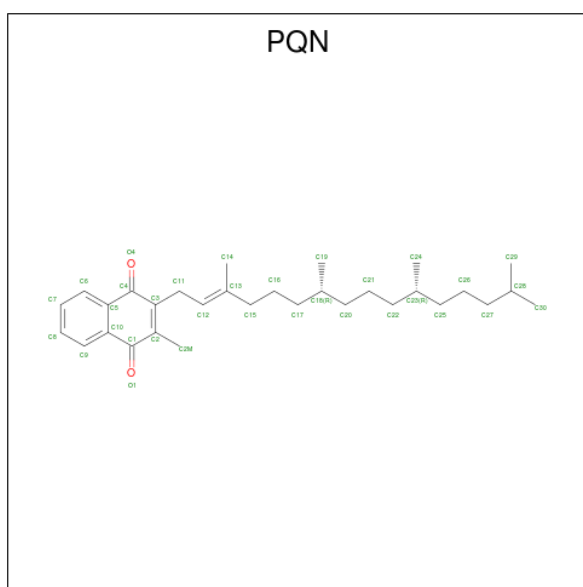
Mol	Chain	Residues	Atoms					AltConf
12	aA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	aA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	aA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	aA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	aA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	aB	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
12	aL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	bA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	bA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	bA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	

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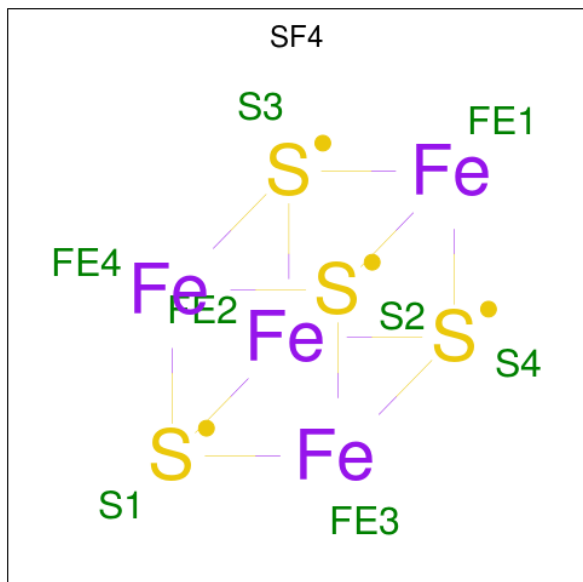
Mol	Chain	Residues	Atoms					AltConf
12	bA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	bA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	bB	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
12	bL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
12	cA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	cA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	cA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	cA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	cA	1	Total	C	Mg	N	O	0
			305	250	5	20	30	
12	cB	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
12	cL	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 13 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
13	aA	1	Total	C	O	0
			33	31	2	
13	aB	1	Total	C	O	0
			28	26	2	
13	bA	1	Total	C	O	0
			33	31	2	
13	bB	1	Total	C	O	0
			28	26	2	
13	cA	1	Total	C	O	0
			33	31	2	
13	cB	1	Total	C	O	0
			28	26	2	

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



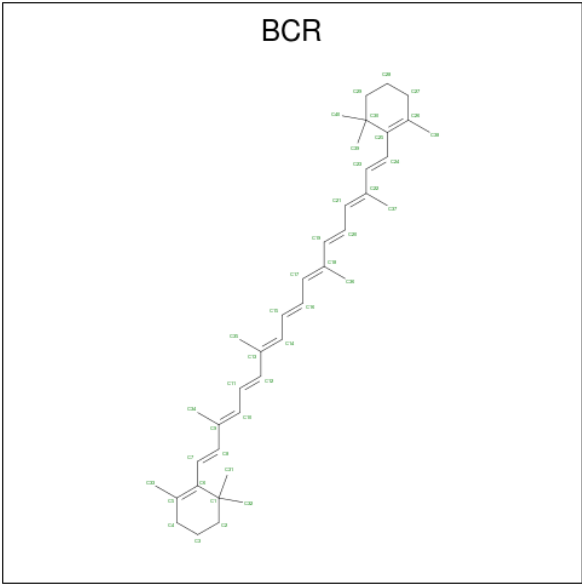
Mol	Chain	Residues	Atoms			AltConf
14	aA	1	Total	Fe	S	0
			8	4	4	
14	aC	1	Total	Fe	S	0
			16	8	8	
14	aC	1	Total	Fe	S	0
			16	8	8	
14	bA	1	Total	Fe	S	0
			8	4	4	
14	bC	1	Total	Fe	S	0
			16	8	8	
14	bC	1	Total	Fe	S	0
			16	8	8	

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Mol	Chain	Residues	Atoms			AltConf
14	cA	1	Total	Fe	S	0
			8	4	4	
14	cC	1	Total	Fe	S	0
			16	8	8	
14	cC	1	Total	Fe	S	0
			16	8	8	

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
15	aA	1	Total	C	0
			200	200	
15	aA	1	Total	C	0
			200	200	
15	aA	1	Total	C	0
			200	200	
15	aA	1	Total	C	0
			200	200	
15	aA	1	Total	C	0
			200	200	
15	aB	1	Total	C	0
			240	240	
15	aB	1	Total	C	0
			240	240	
15	aB	1	Total	C	0
			240	240	

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Mol	Chain	Residues	Atoms		AltConf
15	aB	1	Total 240	C 240	0
15	aB	1	Total 240	C 240	0
15	aB	1	Total 240	C 240	0
15	aI	1	Total 40	C 40	0
15	aK	1	Total 40	C 40	0
15	aL	1	Total 120	C 120	0
15	aL	1	Total 120	C 120	0
15	aL	1	Total 120	C 120	0
15	aM	1	Total 40	C 40	0
15	bA	1	Total 200	C 200	0
15	bA	1	Total 200	C 200	0
15	bA	1	Total 200	C 200	0
15	bA	1	Total 200	C 200	0
15	bA	1	Total 200	C 200	0
15	bB	1	Total 240	C 240	0
15	bB	1	Total 240	C 240	0
15	bB	1	Total 240	C 240	0
15	bB	1	Total 240	C 240	0
15	bB	1	Total 240	C 240	0
15	bB	1	Total 240	C 240	0
15	bI	1	Total 40	C 40	0

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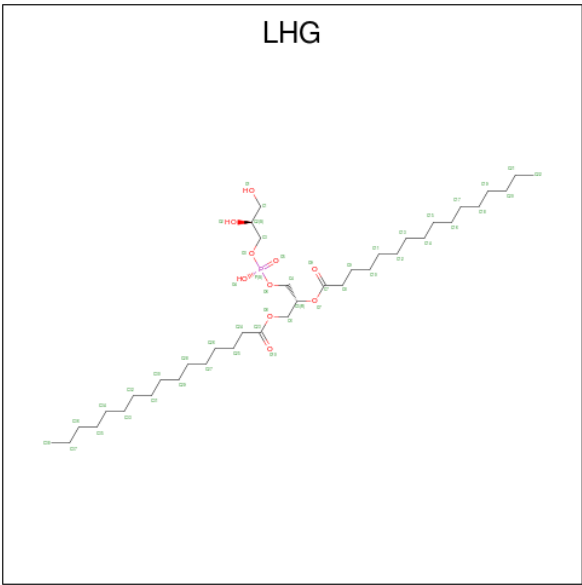
Mol	Chain	Residues	Atoms		AltConf
15	bK	1	Total 40	C 40	0
15	bL	1	Total 120	C 120	0
15	bL	1	Total 120	C 120	0
15	bL	1	Total 120	C 120	0
15	bM	1	Total 40	C 40	0
15	cA	1	Total 200	C 200	0
15	cA	1	Total 200	C 200	0
15	cA	1	Total 200	C 200	0
15	cA	1	Total 200	C 200	0
15	cA	1	Total 200	C 200	0
15	cA	1	Total 200	C 200	0
15	cB	1	Total 240	C 240	0
15	cB	1	Total 240	C 240	0
15	cB	1	Total 240	C 240	0
15	cB	1	Total 240	C 240	0
15	cB	1	Total 240	C 240	0
15	cB	1	Total 240	C 240	0
15	cI	1	Total 40	C 40	0
15	cK	1	Total 40	C 40	0
15	cL	1	Total 120	C 120	0
15	cL	1	Total 120	C 120	0
15	cL	1	Total 120	C 120	0

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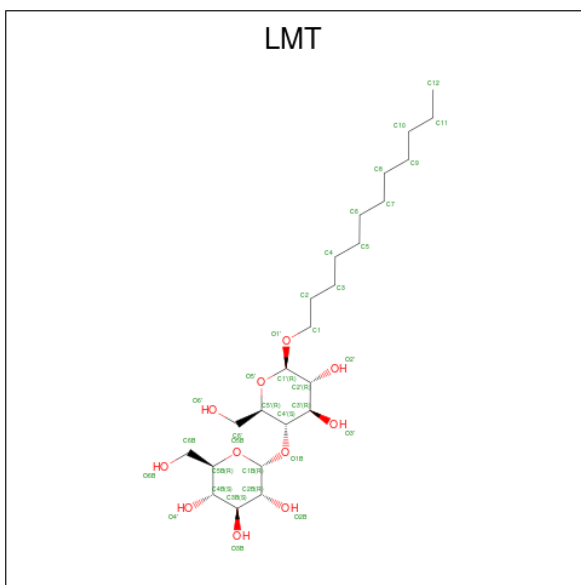
Mol	Chain	Residues	Atoms		AltConf
15	cM	1	Total	C	0
			40	40	

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



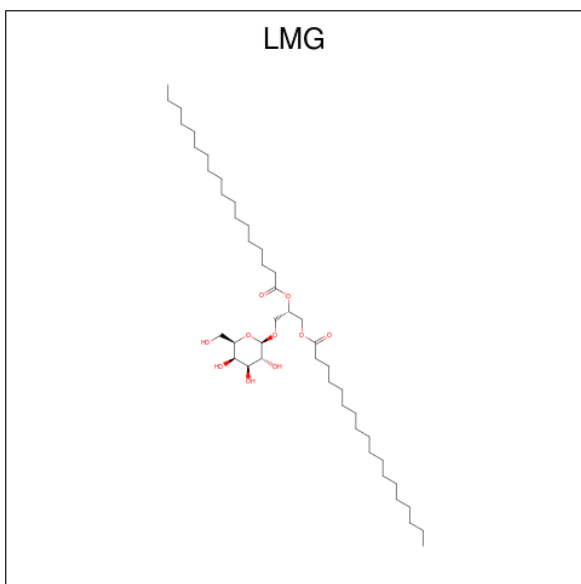
Mol	Chain	Residues	Atoms				AltConf
16	aA	1	Total	C	O	P	0
			49	38	10	1	
16	bA	1	Total	C	O	P	0
			49	38	10	1	
16	cA	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 17 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
17	aA	1	Total 35	C 24	O 11	0
17	bA	1	Total 35	C 24	O 11	0
17	cA	1	Total 35	C 24	O 11	0

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
18	aB	1	Total	C	O	0
			46	36	10	
18	bB	1	Total	C	O	0
			46	36	10	
18	cB	1	Total	C	O	0
			46	36	10	

- Molecule 19 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			AltConf
19	bL	4	Total	C	O	0
			56	52	4	
19	aL	4	Total	C	O	0
			56	52	4	
19	aI	1	Total	C		0
			9	9		
19	cI	2	Total	C	O	0
			25	23	2	
19	bI	1	Total	C		0
			9	9		
19	cL	3	Total	C	O	0
			40	38	2	

- Molecule 20 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
20	bL	1	Total	Ca	0
			1	1	
20	aL	1	Total	Ca	0
			1	1	
20	cL	1	Total	Ca	0
			1	1	

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	aA	72	Total	O	0
			72	72	
21	aB	72	Total	O	0
			72	72	
21	aC	21	Total	O	0
			21	21	

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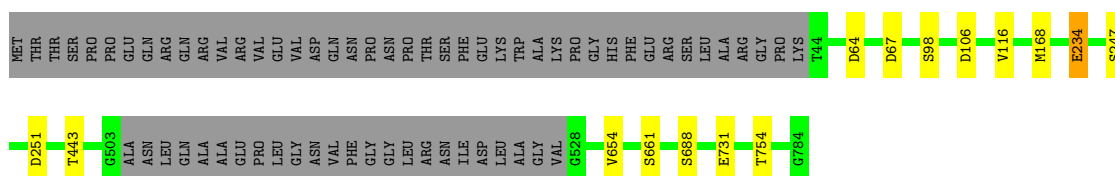
Mol	Chain	Residues	Atoms		AltConf
21	aD	15	Total 15	O 15	0
21	aI	5	Total 5	O 5	0
21	aK	1	Total 1	O 1	0
21	aL	25	Total 25	O 25	0
21	aM	1	Total 1	O 1	0
21	bA	72	Total 72	O 72	0
21	bB	72	Total 72	O 72	0
21	bC	20	Total 20	O 20	0
21	bD	16	Total 16	O 16	0
21	bI	6	Total 6	O 6	0
21	bK	1	Total 1	O 1	0
21	bL	24	Total 24	O 24	0
21	bM	1	Total 1	O 1	0
21	cA	72	Total 72	O 72	0
21	cB	72	Total 72	O 72	0
21	cC	21	Total 21	O 21	0
21	cD	15	Total 15	O 15	0
21	cI	6	Total 6	O 6	0
21	cK	1	Total 1	O 1	0
21	cL	24	Total 24	O 24	0
21	cM	1	Total 1	O 1	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

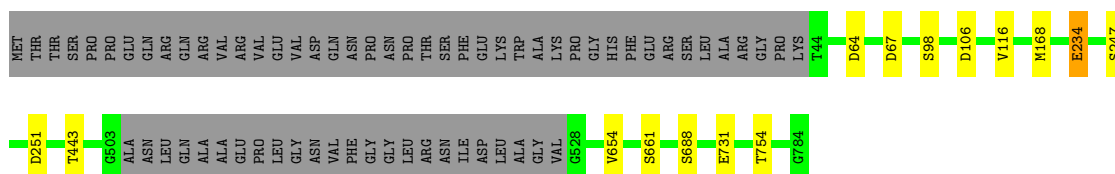
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain aA: 




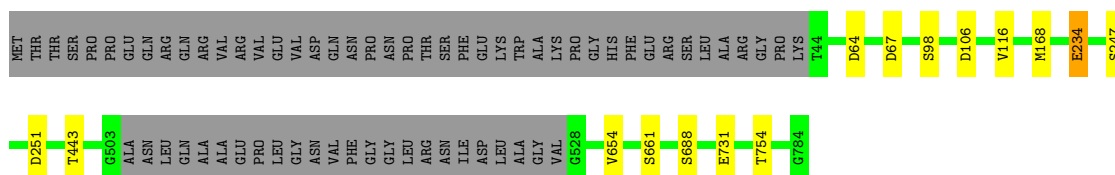
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain bA: 



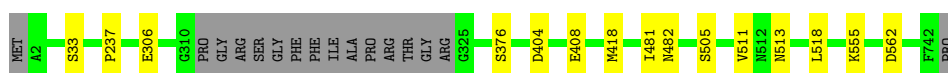
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain cA: 



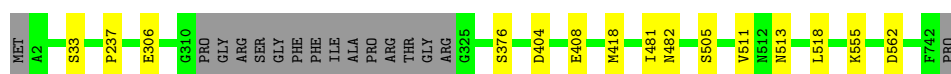
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain aB: 



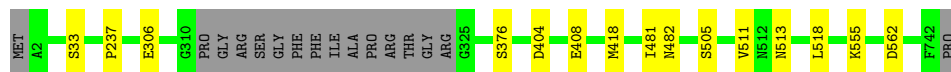
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB: 



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain cB: 96%



- Molecule 3: Photosystem I iron-sulfur center

Chain aC: 99%



- Molecule 3: Photosystem I iron-sulfur center

Chain bC: 99%



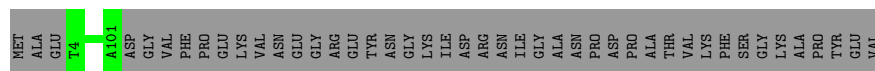
- Molecule 3: Photosystem I iron-sulfur center

Chain cC: 99%



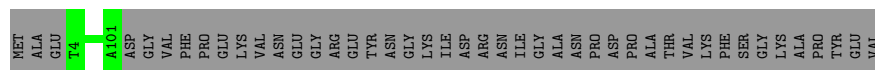
- Molecule 4: Photosystem I reaction center subunit II

Chain aD: 69% 31%



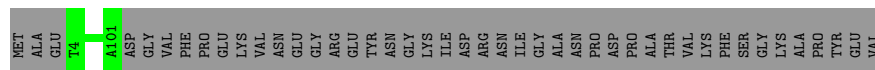
- Molecule 4: Photosystem I reaction center subunit II

Chain bD: 69% 31%




- Molecule 4: Photosystem I reaction center subunit II

Chain cD: 69% 31%




- Molecule 5: Photosystem I reaction center subunit IV

Chain aE:  82% 7% 10%




- Molecule 5: Photosystem I reaction center subunit IV

Chain bE:  82% 7% 10%



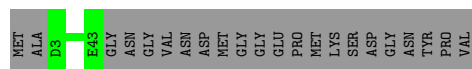
- Molecule 5: Photosystem I reaction center subunit IV

Chain cE:  82% 7% 10%



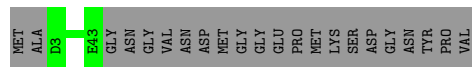
- Molecule 6: Photosystem I reaction center subunit VIII

Chain aI:  65% 35%



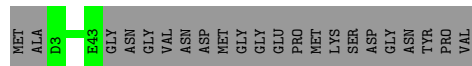
- Molecule 6: Photosystem I reaction center subunit VIII

Chain bI:  65% 35%



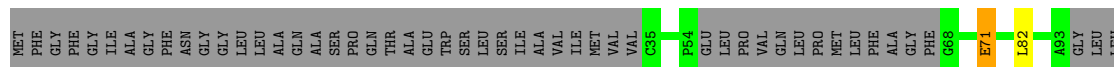
- Molecule 6: Photosystem I reaction center subunit VIII

Chain cI:  65% 35%



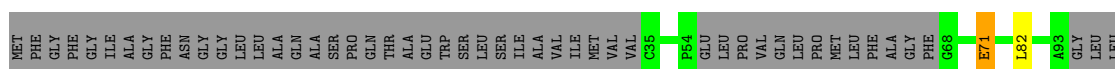
- Molecule 7: Photosystem I reaction center subunit PsaK

Chain aK:  46% .. 52%

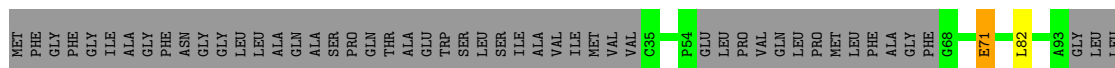


- Molecule 7: Photosystem I reaction center subunit PsaK

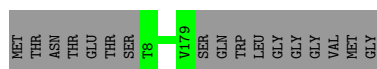
Chain bK:  46% .. 52%



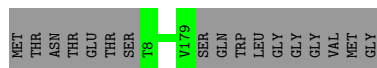
- Molecule 7: Photosystem I reaction center subunit Psak



- Molecule 8: Photosystem I reaction center subunit XI



- Molecule 8: Photosystem I reaction center subunit XI



- Molecule 8: Photosystem I reaction center subunit XI



- Molecule 9: Photosystem I reaction center subunit XII



- Molecule 9: Photosystem I reaction center subunit XII



- Molecule 9: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	311993	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 ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, CL0, LMT, SF4, F6C, CLA, PQN, UNL, CA, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	aA	0.29	0/5868	0.52	2/7993 (0.0%)
1	bA	0.29	0/5868	0.52	2/7993 (0.0%)
1	cA	0.29	0/5868	0.52	2/7993 (0.0%)
2	aB	0.30	0/5993	0.52	1/8185 (0.0%)
2	bB	0.30	0/5993	0.52	1/8185 (0.0%)
2	cB	0.30	0/5993	0.52	1/8185 (0.0%)
3	aC	0.26	0/606	0.55	0/820
3	bC	0.27	0/606	0.55	0/820
3	cC	0.27	0/606	0.55	0/820
4	aD	0.29	0/785	0.51	0/1061
4	bD	0.29	0/785	0.51	0/1061
4	cD	0.29	0/785	0.51	0/1061
5	aE	0.37	0/509	0.70	0/689
5	bE	0.37	0/509	0.70	0/689
5	cE	0.37	0/509	0.70	0/689
6	aI	0.33	0/365	0.63	0/503
6	bI	0.33	0/365	0.63	0/503
6	cI	0.33	0/365	0.63	0/503
7	aK	0.34	0/321	0.71	1/433 (0.2%)
7	bK	0.34	0/321	0.71	1/433 (0.2%)
7	cK	0.34	0/321	0.71	1/433 (0.2%)
8	aL	0.28	0/1334	0.50	0/1819
8	bL	0.28	0/1334	0.51	0/1819
8	cL	0.28	0/1334	0.50	0/1819
9	aM	0.27	0/244	0.60	0/332
9	bM	0.27	0/244	0.59	0/332
9	cM	0.27	0/244	0.60	0/332
All	All	0.30	0/48075	0.53	12/65505 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	aB	0	1
2	bB	0	1
2	cB	0	1
9	aM	0	1
9	bM	0	1
9	cM	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bA	64	ASP	CB-CG-OD2	7.17	124.75	118.30
1	cA	64	ASP	CB-CG-OD2	7.16	124.74	118.30
1	aA	64	ASP	CB-CG-OD2	7.13	124.72	118.30
1	cA	234	GLU	CA-CB-CG	7.04	128.89	113.40
1	bA	234	GLU	CA-CB-CG	7.02	128.84	113.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	aB	481	ILE	Peptide
9	aM	29	LEU	Peptide
2	bB	481	ILE	Peptide
9	bM	29	LEU	Peptide
2	cB	481	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5669	0	5487	0	0
1	bA	5669	0	5487	0	0
1	cA	5669	0	5487	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	aB	5783	0	5519	0	0
2	bB	5783	0	5519	0	0
2	cB	5783	0	5519	0	0
3	aC	596	0	576	0	0
3	bC	596	0	576	0	0
3	cC	596	0	576	0	0
4	aD	768	0	774	0	0
4	bD	768	0	774	0	0
4	cD	768	0	774	0	0
5	aE	499	0	488	0	0
5	bE	499	0	488	0	0
5	cE	499	0	488	0	0
6	aI	349	0	353	0	0
6	bI	349	0	353	0	0
6	cI	349	0	353	0	0
7	aK	317	0	336	0	0
7	bK	317	0	336	0	0
7	cK	317	0	336	0	0
8	aL	1303	0	1301	0	0
8	bL	1303	0	1301	0	0
8	cL	1303	0	1301	0	0
9	aM	241	0	266	0	0
9	bM	241	0	266	0	0
9	cM	241	0	266	0	0
10	aA	65	0	72	0	0
10	bA	65	0	72	0	0
10	cA	65	0	72	0	0
11	aA	2112	0	1999	0	0
11	aB	2116	0	1932	0	0
11	aK	89	0	68	0	0
11	aL	195	0	216	0	0
11	bA	2112	0	1999	0	0
11	bB	2116	0	1932	0	0
11	bK	89	0	68	0	0
11	bL	195	0	216	0	0
11	cA	2112	0	1999	0	0
11	cB	2116	0	1932	0	0
11	cK	89	0	68	0	0
11	cL	195	0	216	0	0
12	aA	305	0	0	0	0
12	aB	58	0	0	0	0
12	aL	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	bA	305	0	0	0	0
12	bB	58	0	0	0	0
12	bL	66	0	0	0	0
12	cA	305	0	0	0	0
12	cB	58	0	0	0	0
12	cL	66	0	0	0	0
13	aA	33	0	46	0	0
13	aB	28	0	33	0	0
13	bA	33	0	46	0	0
13	bB	28	0	33	0	0
13	cA	33	0	46	0	0
13	cB	28	0	33	0	0
14	aA	8	0	0	0	0
14	aC	16	0	0	0	0
14	bA	8	0	0	0	0
14	bC	16	0	0	0	0
14	cA	8	0	0	0	0
14	cC	16	0	0	0	0
15	aA	200	0	280	0	0
15	aB	240	0	336	0	0
15	aI	40	0	56	0	0
15	aK	40	0	56	0	0
15	aL	120	0	168	0	0
15	aM	40	0	56	0	0
15	bA	200	0	280	0	0
15	bB	240	0	336	0	0
15	bI	40	0	56	0	0
15	bK	40	0	56	0	0
15	bL	120	0	168	0	0
15	bM	40	0	56	0	0
15	cA	200	0	280	0	0
15	cB	240	0	336	0	0
15	cI	40	0	56	0	0
15	cK	40	0	56	0	0
15	cL	120	0	168	0	0
15	cM	40	0	56	0	0
16	aA	49	0	74	0	0
16	bA	49	0	74	0	0
16	cA	49	0	74	0	0
17	aA	35	0	46	0	0
17	bA	35	0	46	0	0
17	cA	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	aB	46	0	65	0	0
18	bB	46	0	65	0	0
18	cB	46	0	65	0	0
19	aI	9	0	0	0	0
19	aL	56	0	0	0	0
19	bI	9	0	0	0	0
19	bL	56	0	0	0	0
19	cI	25	0	0	0	0
19	cL	40	0	0	0	0
20	aL	1	0	0	0	0
20	bL	1	0	0	0	0
20	cL	1	0	0	0	0
21	aA	72	0	0	0	0
21	aB	72	0	0	0	0
21	aC	21	0	0	0	0
21	aD	15	0	0	0	0
21	aI	5	0	0	0	0
21	aK	1	0	0	0	0
21	aL	25	0	0	0	0
21	aM	1	0	0	0	0
21	bA	72	0	0	0	0
21	bB	72	0	0	0	0
21	bC	20	0	0	0	0
21	bD	16	0	0	0	0
21	bI	6	0	0	0	0
21	bK	1	0	0	0	0
21	bL	24	0	0	0	0
21	bM	1	0	0	0	0
21	cA	72	0	0	0	0
21	cB	72	0	0	0	0
21	cC	21	0	0	0	0
21	cD	15	0	0	0	0
21	cI	6	0	0	0	0
21	cK	1	0	0	0	0
21	cL	24	0	0	0	0
21	cM	1	0	0	0	0
All	All	65112	0	61809	0	0

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

There are no clashes within the asymmetric unit.

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	aA	713/784 (91%)	696 (98%)	17 (2%)	0	100	100
1	bA	713/784 (91%)	696 (98%)	17 (2%)	0	100	100
1	cA	713/784 (91%)	696 (98%)	17 (2%)	0	100	100
2	aB	723/743 (97%)	696 (96%)	26 (4%)	1 (0%)	53	69
2	bB	723/743 (97%)	696 (96%)	26 (4%)	1 (0%)	53	69
2	cB	723/743 (97%)	696 (96%)	26 (4%)	1 (0%)	53	69
3	aC	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	bC	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	cC	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
4	aD	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
4	bD	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
4	cD	96/142 (68%)	94 (98%)	2 (2%)	0	100	100
5	aE	59/68 (87%)	54 (92%)	5 (8%)	0	100	100
5	bE	59/68 (87%)	54 (92%)	5 (8%)	0	100	100
5	cE	59/68 (87%)	54 (92%)	5 (8%)	0	100	100
6	aI	39/63 (62%)	36 (92%)	3 (8%)	0	100	100
6	bI	39/63 (62%)	36 (92%)	3 (8%)	0	100	100
6	cI	39/63 (62%)	36 (92%)	3 (8%)	0	100	100
7	aK	42/96 (44%)	40 (95%)	2 (5%)	0	100	100
7	bK	42/96 (44%)	40 (95%)	2 (5%)	0	100	100
7	cK	42/96 (44%)	40 (95%)	2 (5%)	0	100	100
8	aL	170/189 (90%)	169 (99%)	1 (1%)	0	100	100
8	bL	170/189 (90%)	169 (99%)	1 (1%)	0	100	100
8	cL	170/189 (90%)	169 (99%)	1 (1%)	0	100	100
9	aM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	bM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
9	cM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
All	All	5847/6591 (89%)	5661 (97%)	183 (3%)	3 (0%)	56	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	aB	237	PRO
2	bB	237	PRO
2	cB	237	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	aA	578/633 (91%)	564 (98%)	14 (2%)	52	70
1	bA	578/633 (91%)	564 (98%)	14 (2%)	52	70
1	cA	578/633 (91%)	564 (98%)	14 (2%)	52	70
2	aB	586/598 (98%)	574 (98%)	12 (2%)	58	75
2	bB	586/598 (98%)	574 (98%)	12 (2%)	58	75
2	cB	586/598 (98%)	574 (98%)	12 (2%)	58	75
3	aC	68/69 (99%)	68 (100%)	0	100	100
3	bC	68/69 (99%)	68 (100%)	0	100	100
3	cC	68/69 (99%)	68 (100%)	0	100	100
4	aD	80/115 (70%)	80 (100%)	0	100	100
4	bD	80/115 (70%)	80 (100%)	0	100	100
4	cD	80/115 (70%)	80 (100%)	0	100	100
5	aE	54/61 (88%)	49 (91%)	5 (9%)	10	14
5	bE	54/61 (88%)	49 (91%)	5 (9%)	10	14
5	cE	54/61 (88%)	49 (91%)	5 (9%)	10	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	aI	36/52 (69%)	36 (100%)	0	100	100
6	bI	36/52 (69%)	36 (100%)	0	100	100
6	cI	36/52 (69%)	36 (100%)	0	100	100
7	aK	30/67 (45%)	28 (93%)	2 (7%)	18	27
7	bK	30/67 (45%)	28 (93%)	2 (7%)	18	27
7	cK	30/67 (45%)	28 (93%)	2 (7%)	18	27
8	aL	136/149 (91%)	136 (100%)	0	100	100
8	bL	136/149 (91%)	136 (100%)	0	100	100
8	cL	136/149 (91%)	136 (100%)	0	100	100
9	aM	27/27 (100%)	26 (96%)	1 (4%)	37	55
9	bM	27/27 (100%)	26 (96%)	1 (4%)	37	55
9	cM	27/27 (100%)	26 (96%)	1 (4%)	37	55
All	All	4785/5313 (90%)	4683 (98%)	102 (2%)	59	74

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	bA	731	GLU
2	bB	513	ASN
5	cE	9	ARG
1	bA	754	THR
2	bB	404	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	bA	755	GLN
2	bB	512	ASN
4	cD	56	ASN
2	bB	83	ASN
2	bB	262	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 363 ligands modelled in this entry, 15 are unknown and 3 are monoatomic - leaving 345 for Mogul analysis.

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
10	CL0	aA	801	1	57,73,73	1.98	13 (22%)	66,113,113	2.26	23 (34%)
11	CLA	aA	802	-	57,73,73	1.92	13 (22%)	66,113,113	2.42	29 (43%)
11	CLA	aA	803	-	48,64,73	2.17	11 (22%)	55,102,113	2.26	22 (40%)
11	CLA	aA	804	1	34,53,73	2.49	12 (35%)	37,89,113	2.51	17 (45%)
11	CLA	aA	805	1	34,53,73	2.50	13 (38%)	37,89,113	2.60	17 (45%)
11	CLA	aA	806	1	57,73,73	1.93	12 (21%)	66,113,113	2.06	22 (33%)
11	CLA	aA	807	1	57,73,73	1.94	13 (22%)	66,113,113	2.11	23 (34%)
11	CLA	aA	808	1	43,59,73	2.29	14 (32%)	49,96,113	2.34	19 (38%)
11	CLA	aA	809	1	34,53,73	2.45	13 (38%)	37,89,113	2.60	18 (48%)
11	CLA	aA	810	1	34,53,73	2.44	13 (38%)	37,89,113	2.58	19 (51%)
11	CLA	aA	811	1	34,53,73	2.47	12 (35%)	37,89,113	2.55	16 (43%)
11	CLA	aA	812	1	57,73,73	2.00	14 (24%)	66,113,113	1.99	19 (28%)
11	CLA	aA	813	1	46,62,73	2.21	13 (28%)	52,99,113	2.23	19 (36%)
11	CLA	aA	814	1	57,73,73	1.98	13 (22%)	66,113,113	2.12	21 (31%)
11	CLA	aA	815	1	34,53,73	2.45	12 (35%)	37,89,113	2.62	18 (48%)
11	CLA	aA	816	1	34,53,73	2.46	13 (38%)	37,89,113	2.51	16 (43%)
11	CLA	aA	817	-	41,57,73	2.35	14 (34%)	46,93,113	2.41	18 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	aA	818	1	46,62,73	2.20	13 (28%)	52,99,113	2.42	20 (38%)
11	CLA	aA	819	1	46,62,73	2.19	13 (28%)	52,99,113	2.31	20 (38%)
11	CLA	aA	820	1	57,73,73	1.93	13 (22%)	66,113,113	2.13	22 (33%)
11	CLA	aA	821	1	53,69,73	2.03	14 (26%)	61,108,113	2.14	20 (32%)
11	CLA	aA	822	-	57,73,73	1.96	13 (22%)	66,113,113	2.00	18 (27%)
11	CLA	aA	823	1	34,53,73	2.43	12 (35%)	37,89,113	2.67	16 (43%)
11	CLA	aA	824	-	43,59,73	2.23	12 (27%)	49,96,113	2.38	21 (42%)
11	CLA	aA	825	1	57,73,73	1.93	13 (22%)	66,113,113	2.07	23 (34%)
12	F6C	aA	826	-	54,74,74	2.28	14 (25%)	50,114,114	2.65	14 (28%)
12	F6C	aA	827	-	44,64,74	2.41	14 (31%)	38,102,114	4.41	12 (31%)
11	CLA	aA	828	1	52,68,73	2.03	12 (23%)	60,107,113	2.23	22 (36%)
11	CLA	aA	829	1	57,73,73	1.99	14 (24%)	66,113,113	4.55	24 (36%)
12	F6C	aA	830	1	54,74,74	2.18	14 (25%)	50,114,114	3.17	13 (26%)
11	CLA	aA	831	1	57,73,73	1.97	13 (22%)	66,113,113	2.21	22 (33%)
12	F6C	aA	832	1	39,59,74	2.53	14 (35%)	32,96,114	4.01	15 (46%)
11	CLA	aA	833	1	57,73,73	1.99	13 (22%)	66,113,113	2.06	21 (31%)
11	CLA	aA	834	1	57,73,73	1.93	13 (22%)	66,113,113	2.09	22 (33%)
11	CLA	aA	835	1	57,73,73	1.94	13 (22%)	66,113,113	2.06	19 (28%)
11	CLA	aA	836	1	34,53,73	2.35	12 (35%)	37,89,113	2.55	16 (43%)
11	CLA	aA	837	1	34,53,73	2.48	13 (38%)	37,89,113	2.58	17 (45%)
11	CLA	aA	838	1	43,59,73	2.27	13 (30%)	49,96,113	2.48	21 (42%)
11	CLA	aA	839	1	57,73,73	1.91	13 (22%)	66,113,113	2.09	20 (30%)
11	CLA	aA	840	1	57,73,73	1.95	13 (22%)	66,113,113	2.31	21 (31%)
11	CLA	aA	841	1	42,58,73	2.33	14 (33%)	48,95,113	2.33	21 (43%)
11	CLA	aA	842	-	34,53,73	2.47	13 (38%)	37,89,113	2.54	17 (45%)
11	CLA	aA	843	1	43,59,73	2.27	13 (30%)	49,96,113	2.39	20 (40%)
12	F6C	aA	844	-	54,74,74	2.20	14 (25%)	50,114,114	3.20	14 (28%)
13	PQN	aA	845	-	34,34,34	1.43	2 (5%)	42,45,45	1.06	4 (9%)
14	SF4	aA	846	1,2	0,12,12	0.00	-	-	-	-
15	BCR	aA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.34	7 (12%)
15	BCR	aA	848	-	41,41,41	1.07	2 (4%)	56,56,56	1.23	5 (8%)
15	BCR	aA	849	-	41,41,41	1.06	2 (4%)	56,56,56	1.29	5 (8%)
15	BCR	aA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	4 (7%)
15	BCR	aA	851	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	8 (14%)
16	LHG	aA	852	-	48,48,48	0.60	1 (2%)	51,54,54	1.23	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LMT	aA	853	-	36,36,36	0.40	0	47,47,47	1.36	5 (10%)
11	CLA	aB	801	2	57,73,73	1.89	13 (22%)	66,113,113	2.24	25 (37%)
11	CLA	aB	802	-	49,65,73	2.12	13 (26%)	56,103,113	2.47	22 (39%)
11	CLA	aB	803	-	53,69,73	2.02	14 (26%)	61,108,113	2.06	17 (27%)
11	CLA	aB	804	2	42,58,73	2.32	14 (33%)	48,95,113	2.45	23 (47%)
11	CLA	aB	805	2	57,73,73	1.95	13 (22%)	66,113,113	2.16	22 (33%)
11	CLA	aB	806	2	57,73,73	1.93	12 (21%)	66,113,113	2.02	20 (30%)
11	CLA	aB	807	2	53,69,73	2.00	13 (24%)	61,108,113	2.24	21 (34%)
11	CLA	aB	808	2	57,73,73	1.92	12 (21%)	66,113,113	2.23	21 (31%)
11	CLA	aB	809	2	39,55,73	2.30	13 (33%)	44,91,113	2.49	18 (40%)
11	CLA	aB	810	2	34,53,73	2.42	12 (35%)	37,89,113	2.66	19 (51%)
11	CLA	aB	811	2	34,53,73	2.48	13 (38%)	37,89,113	2.50	16 (43%)
11	CLA	aB	812	2	57,73,73	1.97	14 (24%)	66,113,113	2.12	23 (34%)
11	CLA	aB	813	2	48,64,73	2.14	14 (29%)	55,102,113	2.23	21 (38%)
11	CLA	aB	814	2	34,53,73	2.43	12 (35%)	37,89,113	2.62	18 (48%)
11	CLA	aB	815	2	47,63,73	2.17	14 (29%)	54,101,113	2.23	20 (37%)
11	CLA	aB	816	2	51,67,73	2.11	13 (25%)	58,105,113	2.12	21 (36%)
11	CLA	aB	817	2	52,68,73	2.05	12 (23%)	60,107,113	2.27	22 (36%)
11	CLA	aB	818	-	57,73,73	1.97	13 (22%)	66,113,113	1.99	17 (25%)
11	CLA	aB	819	2	39,55,73	2.39	14 (35%)	44,91,113	2.37	19 (43%)
11	CLA	aB	820	2	34,53,73	2.44	12 (35%)	37,89,113	2.48	16 (43%)
11	CLA	aB	821	-	47,63,73	2.22	14 (29%)	54,101,113	2.24	19 (35%)
11	CLA	aB	822	2	34,53,73	2.42	10 (29%)	37,89,113	2.62	16 (43%)
11	CLA	aB	823	2	46,62,73	2.18	14 (30%)	52,99,113	2.39	21 (40%)
12	F6C	aB	824	-	46,66,74	2.34	14 (30%)	40,104,114	4.16	14 (35%)
11	CLA	aB	825	2	57,73,73	1.99	13 (22%)	66,113,113	2.11	21 (31%)
11	CLA	aB	826	2	53,69,73	2.01	14 (26%)	61,108,113	2.24	23 (37%)
11	CLA	aB	827	2	57,73,73	1.95	12 (21%)	66,113,113	2.10	18 (27%)
11	CLA	aB	828	2	47,63,73	2.14	12 (25%)	54,101,113	2.36	22 (40%)
11	CLA	aB	829	2	34,53,73	2.35	12 (35%)	37,89,113	2.66	16 (43%)
11	CLA	aB	830	2	41,57,73	2.33	14 (34%)	46,93,113	2.33	18 (39%)
11	CLA	aB	831	2	48,64,73	2.15	13 (27%)	55,102,113	2.50	22 (40%)
11	CLA	aB	832	2	34,53,73	2.47	13 (38%)	37,89,113	2.45	16 (43%)
11	CLA	aB	833	2	34,53,73	2.48	12 (35%)	37,89,113	2.54	19 (51%)
11	CLA	aB	834	-	34,53,73	2.45	13 (38%)	37,89,113	2.52	17 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	aB	835	-	34,53,73	2.46	13 (38%)	37,89,113	2.58	17 (45%)
11	CLA	aB	836	2	43,59,73	2.23	13 (30%)	49,96,113	2.40	22 (44%)
11	CLA	aB	837	2	47,63,73	2.16	13 (27%)	54,101,113	2.21	20 (37%)
11	CLA	aB	838	2	39,55,73	2.36	13 (33%)	44,91,113	2.46	19 (43%)
11	CLA	aB	839	-	57,73,73	1.93	12 (21%)	66,113,113	2.05	20 (30%)
11	CLA	aB	840	2	34,53,73	2.39	11 (32%)	37,89,113	2.60	16 (43%)
13	PQN	aB	841	-	29,29,34	1.50	2 (6%)	36,39,45	1.13	2 (5%)
15	BCR	aB	842	-	41,41,41	1.03	2 (4%)	56,56,56	1.24	4 (7%)
15	BCR	aB	843	-	41,41,41	1.04	2 (4%)	56,56,56	1.14	3 (5%)
15	BCR	aB	844	-	41,41,41	1.02	2 (4%)	56,56,56	1.22	5 (8%)
15	BCR	aB	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	5 (8%)
15	BCR	aB	846	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	5 (8%)
18	LMG	aB	847	-	46,46,55	0.82	1 (2%)	54,54,63	1.35	8 (14%)
15	BCR	aB	848	-	41,41,41	0.99	2 (4%)	56,56,56	1.42	8 (14%)
14	SF4	aC	101	3	0,12,12	0.00	-	-		
14	SF4	aC	102	3	0,12,12	0.00	-	-		
15	BCR	aI	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.23	6 (10%)
11	CLA	aK	101	7	30,46,73	2.43	11 (36%)	32,79,113	2.56	16 (50%)
15	BCR	aK	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	8 (14%)
11	CLA	aK	103	-	43,59,73	2.26	14 (32%)	49,96,113	2.33	20 (40%)
12	F6C	aL	202	2	54,74,74	2.22	15 (27%)	50,114,114	2.28	13 (26%)
15	BCR	aL	203	-	41,41,41	1.11	3 (7%)	56,56,56	1.25	6 (10%)
11	CLA	aL	204	8	57,73,73	1.99	14 (24%)	66,113,113	2.12	18 (27%)
11	CLA	aL	205	8	57,73,73	1.96	14 (24%)	66,113,113	2.03	19 (28%)
11	CLA	aL	206	-	57,73,73	1.96	13 (22%)	66,113,113	2.10	20 (30%)
15	BCR	aL	207	-	41,41,41	1.04	2 (4%)	56,56,56	1.41	9 (16%)
15	BCR	aL	208	-	41,41,41	1.04	2 (4%)	56,56,56	1.26	7 (12%)
15	BCR	aM	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	7 (12%)
10	CL0	bA	801	1	57,73,73	1.97	13 (22%)	66,113,113	2.25	23 (34%)
11	CLA	bA	802	-	57,73,73	1.91	13 (22%)	66,113,113	2.42	29 (43%)
11	CLA	bA	803	-	48,64,73	2.18	11 (22%)	55,102,113	2.26	22 (40%)
11	CLA	bA	804	1	34,53,73	2.50	12 (35%)	37,89,113	2.51	17 (45%)
11	CLA	bA	805	1	34,53,73	2.51	13 (38%)	37,89,113	2.60	17 (45%)
11	CLA	bA	806	1	57,73,73	1.93	12 (21%)	66,113,113	2.06	21 (31%)
11	CLA	bA	807	1	57,73,73	1.94	13 (22%)	66,113,113	2.11	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	bA	808	1	43,59,73	2.29	14 (32%)	49,96,113	2.33	19 (38%)
11	CLA	bA	809	1	34,53,73	2.45	13 (38%)	37,89,113	2.60	18 (48%)
11	CLA	bA	810	1	34,53,73	2.44	13 (38%)	37,89,113	2.58	19 (51%)
11	CLA	bA	811	1	34,53,73	2.47	12 (35%)	37,89,113	2.55	16 (43%)
11	CLA	bA	812	1	57,73,73	2.00	13 (22%)	66,113,113	1.99	19 (28%)
11	CLA	bA	813	1	46,62,73	2.21	13 (28%)	52,99,113	2.22	19 (36%)
11	CLA	bA	814	1	57,73,73	1.98	14 (24%)	66,113,113	2.13	21 (31%)
11	CLA	bA	815	1	34,53,73	2.45	12 (35%)	37,89,113	2.62	18 (48%)
11	CLA	bA	816	1	34,53,73	2.46	12 (35%)	37,89,113	2.50	16 (43%)
11	CLA	bA	817	-	41,57,73	2.35	14 (34%)	46,93,113	2.41	18 (39%)
11	CLA	bA	818	1	46,62,73	2.20	13 (28%)	52,99,113	2.42	20 (38%)
11	CLA	bA	819	1	46,62,73	2.18	12 (26%)	52,99,113	2.31	19 (36%)
11	CLA	bA	820	1	57,73,73	1.93	13 (22%)	66,113,113	2.13	22 (33%)
11	CLA	bA	821	1	53,69,73	2.03	14 (26%)	61,108,113	2.14	20 (32%)
11	CLA	bA	822	-	57,73,73	1.96	13 (22%)	66,113,113	2.00	18 (27%)
11	CLA	bA	823	1	34,53,73	2.44	12 (35%)	37,89,113	2.67	16 (43%)
11	CLA	bA	824	-	43,59,73	2.23	12 (27%)	49,96,113	2.38	22 (44%)
11	CLA	bA	825	1	57,73,73	1.93	13 (22%)	66,113,113	2.07	23 (34%)
12	F6C	bA	826	-	54,74,74	2.28	14 (25%)	50,114,114	2.65	14 (28%)
12	F6C	bA	827	-	44,64,74	2.41	14 (31%)	38,102,114	4.41	12 (31%)
11	CLA	bA	828	1	52,68,73	2.02	12 (23%)	60,107,113	2.23	22 (36%)
11	CLA	bA	829	1	57,73,73	2.00	14 (24%)	66,113,113	4.55	24 (36%)
12	F6C	bA	830	1	54,74,74	2.19	14 (25%)	50,114,114	3.17	13 (26%)
11	CLA	bA	831	1	57,73,73	1.96	13 (22%)	66,113,113	2.21	22 (33%)
12	F6C	bA	832	1	39,59,74	2.54	14 (35%)	32,96,114	4.02	13 (40%)
11	CLA	bA	833	1	57,73,73	1.98	13 (22%)	66,113,113	2.06	21 (31%)
11	CLA	bA	834	1	57,73,73	1.93	13 (22%)	66,113,113	2.09	22 (33%)
11	CLA	bA	835	1	57,73,73	1.94	13 (22%)	66,113,113	2.07	19 (28%)
11	CLA	bA	836	1	34,53,73	2.35	12 (35%)	37,89,113	2.56	16 (43%)
11	CLA	bA	837	1	34,53,73	2.48	13 (38%)	37,89,113	2.59	17 (45%)
11	CLA	bA	838	1	43,59,73	2.26	13 (30%)	49,96,113	2.49	24 (48%)
11	CLA	bA	839	1	57,73,73	1.91	13 (22%)	66,113,113	2.10	20 (30%)
11	CLA	bA	840	1	57,73,73	1.95	13 (22%)	66,113,113	2.31	22 (33%)
11	CLA	bA	841	1	42,58,73	2.33	14 (33%)	48,95,113	2.34	21 (43%)
11	CLA	bA	842	-	34,53,73	2.46	13 (38%)	37,89,113	2.53	17 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	bA	843	1	43,59,73	2.27	13 (30%)	49,96,113	2.40	20 (40%)
12	F6C	bA	844	-	54,74,74	2.19	14 (25%)	50,114,114	3.20	14 (28%)
13	PQN	bA	845	-	34,34,34	1.42	2 (5%)	42,45,45	1.06	3 (7%)
14	SF4	bA	846	1,2	0,12,12	0.00	-	-		
15	BCR	bA	847	-	41,41,41	1.02	2 (4%)	56,56,56	1.35	7 (12%)
15	BCR	bA	848	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	5 (8%)
15	BCR	bA	849	-	41,41,41	1.06	2 (4%)	56,56,56	1.29	6 (10%)
15	BCR	bA	850	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	4 (7%)
15	BCR	bA	851	-	41,41,41	1.03	2 (4%)	56,56,56	1.23	8 (14%)
16	LHG	bA	852	-	48,48,48	0.60	1 (2%)	51,54,54	1.23	6 (11%)
17	LMT	bA	853	-	36,36,36	0.40	0	47,47,47	1.36	5 (10%)
11	CLA	bB	801	2	57,73,73	1.89	12 (21%)	66,113,113	2.24	25 (37%)
11	CLA	bB	802	-	49,65,73	2.12	13 (26%)	56,103,113	2.47	22 (39%)
11	CLA	bB	803	-	53,69,73	2.01	14 (26%)	61,108,113	2.06	17 (27%)
11	CLA	bB	804	2	42,58,73	2.33	14 (33%)	48,95,113	2.46	23 (47%)
11	CLA	bB	805	2	57,73,73	1.95	13 (22%)	66,113,113	2.15	22 (33%)
11	CLA	bB	806	2	57,73,73	1.92	12 (21%)	66,113,113	2.03	20 (30%)
11	CLA	bB	807	2	53,69,73	2.00	13 (24%)	61,108,113	2.23	21 (34%)
11	CLA	bB	808	2	57,73,73	1.92	12 (21%)	66,113,113	2.23	21 (31%)
11	CLA	bB	809	2	39,55,73	2.30	13 (33%)	44,91,113	2.50	18 (40%)
11	CLA	bB	810	2	34,53,73	2.41	12 (35%)	37,89,113	2.65	19 (51%)
11	CLA	bB	811	2	34,53,73	2.49	12 (35%)	37,89,113	2.49	16 (43%)
11	CLA	bB	812	2	57,73,73	1.97	13 (22%)	66,113,113	2.12	22 (33%)
11	CLA	bB	813	2	48,64,73	2.13	14 (29%)	55,102,113	2.22	21 (38%)
11	CLA	bB	814	2	34,53,73	2.43	13 (38%)	37,89,113	2.62	18 (48%)
11	CLA	bB	815	2	47,63,73	2.17	14 (29%)	54,101,113	2.23	20 (37%)
11	CLA	bB	816	2	51,67,73	2.10	13 (25%)	58,105,113	2.12	21 (36%)
11	CLA	bB	817	2	52,68,73	2.05	12 (23%)	60,107,113	2.27	22 (36%)
11	CLA	bB	818	-	57,73,73	1.97	13 (22%)	66,113,113	1.99	18 (27%)
11	CLA	bB	819	2	39,55,73	2.39	14 (35%)	44,91,113	2.39	19 (43%)
11	CLA	bB	820	2	34,53,73	2.44	12 (35%)	37,89,113	2.48	16 (43%)
11	CLA	bB	821	-	47,63,73	2.22	14 (29%)	54,101,113	2.25	19 (35%)
11	CLA	bB	822	2	34,53,73	2.42	10 (29%)	37,89,113	2.62	16 (43%)
11	CLA	bB	823	2	46,62,73	2.19	14 (30%)	52,99,113	2.40	21 (40%)
12	F6C	bB	824	-	46,66,74	2.34	14 (30%)	40,104,114	4.16	14 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	bB	825	2	57,73,73	1.99	13 (22%)	66,113,113	2.11	21 (31%)
11	CLA	bB	826	2	53,69,73	2.02	14 (26%)	61,108,113	2.25	23 (37%)
11	CLA	bB	827	2	57,73,73	1.95	12 (21%)	66,113,113	2.10	18 (27%)
11	CLA	bB	828	2	47,63,73	2.14	12 (25%)	54,101,113	2.37	19 (35%)
11	CLA	bB	829	2	34,53,73	2.35	12 (35%)	37,89,113	2.65	16 (43%)
11	CLA	bB	830	2	41,57,73	2.33	14 (34%)	46,93,113	2.35	18 (39%)
11	CLA	bB	831	2	48,64,73	2.14	13 (27%)	55,102,113	2.51	23 (41%)
11	CLA	bB	832	2	34,53,73	2.47	13 (38%)	37,89,113	2.45	16 (43%)
11	CLA	bB	833	2	34,53,73	2.48	12 (35%)	37,89,113	2.54	19 (51%)
11	CLA	bB	834	-	34,53,73	2.45	13 (38%)	37,89,113	2.52	17 (45%)
11	CLA	bB	835	-	34,53,73	2.46	13 (38%)	37,89,113	2.58	17 (45%)
11	CLA	bB	836	2	43,59,73	2.23	13 (30%)	49,96,113	2.41	22 (44%)
11	CLA	bB	837	2	47,63,73	2.16	13 (27%)	54,101,113	2.21	20 (37%)
11	CLA	bB	838	2	39,55,73	2.37	13 (33%)	44,91,113	2.46	19 (43%)
11	CLA	bB	839	-	57,73,73	1.94	12 (21%)	66,113,113	2.05	20 (30%)
11	CLA	bB	840	2	34,53,73	2.39	11 (32%)	37,89,113	2.60	16 (43%)
13	PQN	bB	841	-	29,29,34	1.51	2 (6%)	36,39,45	1.13	3 (8%)
15	BCR	bB	842	-	41,41,41	1.02	2 (4%)	56,56,56	1.24	4 (7%)
15	BCR	bB	843	-	41,41,41	1.03	2 (4%)	56,56,56	1.15	3 (5%)
15	BCR	bB	844	-	41,41,41	1.02	2 (4%)	56,56,56	1.22	5 (8%)
15	BCR	bB	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	5 (8%)
15	BCR	bB	846	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	5 (8%)
18	LMG	bB	847	-	46,46,55	0.82	1 (2%)	54,54,63	1.35	8 (14%)
15	BCR	bB	848	-	41,41,41	0.99	2 (4%)	56,56,56	1.42	8 (14%)
14	SF4	bC	101	3	0,12,12	0.00	-	-		
14	SF4	bC	102	3	0,12,12	0.00	-	-		
15	BCR	bI	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.23	6 (10%)
11	CLA	bK	101	7	30,46,73	2.43	11 (36%)	32,79,113	2.55	16 (50%)
15	BCR	bK	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.30	7 (12%)
11	CLA	bK	103	-	43,59,73	2.27	14 (32%)	49,96,113	2.33	20 (40%)
12	F6C	bL	202	2	54,74,74	2.23	15 (27%)	50,114,114	2.28	13 (26%)
15	BCR	bL	203	-	41,41,41	1.11	3 (7%)	56,56,56	1.23	6 (10%)
11	CLA	bL	204	8	57,73,73	1.99	14 (24%)	66,113,113	2.12	19 (28%)
11	CLA	bL	205	8	57,73,73	1.96	13 (22%)	66,113,113	2.04	18 (27%)
11	CLA	bL	206	-	57,73,73	1.96	13 (22%)	66,113,113	2.10	20 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	bL	207	-	41,41,41	1.05	2 (4%)	56,56,56	1.41	9 (16%)
15	BCR	bL	208	-	41,41,41	1.03	2 (4%)	56,56,56	1.26	7 (12%)
15	BCR	bM	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.28	8 (14%)
10	CL0	cA	801	1	57,73,73	1.98	13 (22%)	66,113,113	2.26	23 (34%)
11	CLA	cA	802	-	57,73,73	1.92	13 (22%)	66,113,113	2.43	29 (43%)
11	CLA	cA	803	-	48,64,73	2.18	12 (25%)	55,102,113	2.27	22 (40%)
11	CLA	cA	804	1	34,53,73	2.49	12 (35%)	37,89,113	2.51	17 (45%)
11	CLA	cA	805	1	34,53,73	2.50	13 (38%)	37,89,113	2.60	17 (45%)
11	CLA	cA	806	1	57,73,73	1.93	12 (21%)	66,113,113	2.06	22 (33%)
11	CLA	cA	807	1	57,73,73	1.94	13 (22%)	66,113,113	2.12	23 (34%)
11	CLA	cA	808	1	43,59,73	2.29	14 (32%)	49,96,113	2.34	19 (38%)
11	CLA	cA	809	1	34,53,73	2.45	13 (38%)	37,89,113	2.60	18 (48%)
11	CLA	cA	810	1	34,53,73	2.43	12 (35%)	37,89,113	2.58	19 (51%)
11	CLA	cA	811	1	34,53,73	2.47	12 (35%)	37,89,113	2.56	17 (45%)
11	CLA	cA	812	1	57,73,73	2.00	13 (22%)	66,113,113	1.99	19 (28%)
11	CLA	cA	813	1	46,62,73	2.21	13 (28%)	52,99,113	2.22	19 (36%)
11	CLA	cA	814	1	57,73,73	1.98	13 (22%)	66,113,113	2.12	21 (31%)
11	CLA	cA	815	1	34,53,73	2.45	12 (35%)	37,89,113	2.62	18 (48%)
11	CLA	cA	816	1	34,53,73	2.47	13 (38%)	37,89,113	2.51	16 (43%)
11	CLA	cA	817	-	41,57,73	2.35	14 (34%)	46,93,113	2.41	18 (39%)
11	CLA	cA	818	1	46,62,73	2.20	13 (28%)	52,99,113	2.42	20 (38%)
11	CLA	cA	819	1	46,62,73	2.19	13 (28%)	52,99,113	2.31	20 (38%)
11	CLA	cA	820	1	57,73,73	1.93	13 (22%)	66,113,113	2.12	22 (33%)
11	CLA	cA	821	1	53,69,73	2.03	14 (26%)	61,108,113	2.14	20 (32%)
11	CLA	cA	822	-	57,73,73	1.96	13 (22%)	66,113,113	1.99	18 (27%)
11	CLA	cA	823	1	34,53,73	2.43	12 (35%)	37,89,113	2.67	16 (43%)
11	CLA	cA	824	-	43,59,73	2.23	12 (27%)	49,96,113	2.38	22 (44%)
11	CLA	cA	825	1	57,73,73	1.92	13 (22%)	66,113,113	2.07	23 (34%)
12	F6C	cA	826	-	54,74,74	2.28	14 (25%)	50,114,114	2.65	14 (28%)
12	F6C	cA	827	-	44,64,74	2.42	14 (31%)	38,102,114	4.41	12 (31%)
11	CLA	cA	828	1	52,68,73	2.03	12 (23%)	60,107,113	2.24	22 (36%)
11	CLA	cA	829	1	57,73,73	2.00	14 (24%)	66,113,113	4.55	24 (36%)
12	F6C	cA	830	1	54,74,74	2.19	14 (25%)	50,114,114	3.17	13 (26%)
11	CLA	cA	831	1	57,73,73	1.97	13 (22%)	66,113,113	2.21	22 (33%)
12	F6C	cA	832	1	39,59,74	2.54	14 (35%)	32,96,114	4.02	14 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	cA	833	1	57,73,73	1.98	13 (22%)	66,113,113	2.06	21 (31%)
11	CLA	cA	834	1	57,73,73	1.93	13 (22%)	66,113,113	2.09	22 (33%)
11	CLA	cA	835	1	57,73,73	1.94	13 (22%)	66,113,113	2.07	19 (28%)
11	CLA	cA	836	1	34,53,73	2.34	12 (35%)	37,89,113	2.56	16 (43%)
11	CLA	cA	837	1	34,53,73	2.49	13 (38%)	37,89,113	2.58	17 (45%)
11	CLA	cA	838	1	43,59,73	2.27	13 (30%)	49,96,113	2.48	21 (42%)
11	CLA	cA	839	1	57,73,73	1.91	13 (22%)	66,113,113	2.09	20 (30%)
11	CLA	cA	840	1	57,73,73	1.95	13 (22%)	66,113,113	2.31	22 (33%)
11	CLA	cA	841	1	42,58,73	2.33	14 (33%)	48,95,113	2.33	21 (43%)
11	CLA	cA	842	-	34,53,73	2.47	13 (38%)	37,89,113	2.54	17 (45%)
11	CLA	cA	843	1	43,59,73	2.27	13 (30%)	49,96,113	2.40	20 (40%)
12	F6C	cA	844	-	54,74,74	2.20	14 (25%)	50,114,114	3.20	14 (28%)
13	PQN	cA	845	-	34,34,34	1.43	2 (5%)	42,45,45	1.07	3 (7%)
14	SF4	cA	846	1,2	0,12,12	0.00	-	-	-	-
15	BCR	cA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.34	7 (12%)
15	BCR	cA	848	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	5 (8%)
15	BCR	cA	849	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	5 (8%)
15	BCR	cA	850	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	3 (5%)
15	BCR	cA	851	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	8 (14%)
16	LHG	cA	852	-	48,48,48	0.60	1 (2%)	51,54,54	1.23	6 (11%)
17	LMT	cA	853	-	36,36,36	0.39	0	47,47,47	1.36	5 (10%)
11	CLA	cB	801	2	57,73,73	1.89	13 (22%)	66,113,113	2.24	25 (37%)
11	CLA	cB	802	-	49,65,73	2.12	13 (26%)	56,103,113	2.47	22 (39%)
11	CLA	cB	803	-	53,69,73	2.02	14 (26%)	61,108,113	2.06	17 (27%)
11	CLA	cB	804	2	42,58,73	2.32	14 (33%)	48,95,113	2.46	23 (47%)
11	CLA	cB	805	2	57,73,73	1.95	13 (22%)	66,113,113	2.16	22 (33%)
11	CLA	cB	806	2	57,73,73	1.93	12 (21%)	66,113,113	2.03	21 (31%)
11	CLA	cB	807	2	53,69,73	1.99	13 (24%)	61,108,113	2.23	21 (34%)
11	CLA	cB	808	2	57,73,73	1.91	12 (21%)	66,113,113	2.23	21 (31%)
11	CLA	cB	809	2	39,55,73	2.30	13 (33%)	44,91,113	2.50	18 (40%)
11	CLA	cB	810	2	34,53,73	2.41	12 (35%)	37,89,113	2.66	19 (51%)
11	CLA	cB	811	2	34,53,73	2.48	12 (35%)	37,89,113	2.48	16 (43%)
11	CLA	cB	812	2	57,73,73	1.97	14 (24%)	66,113,113	2.12	22 (33%)
11	CLA	cB	813	2	48,64,73	2.14	14 (29%)	55,102,113	2.23	21 (38%)
11	CLA	cB	814	2	34,53,73	2.43	12 (35%)	37,89,113	2.61	18 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	cB	815	2	47,63,73	2.17	14 (29%)	54,101,113	2.23	20 (37%)
11	CLA	cB	816	2	51,67,73	2.11	13 (25%)	58,105,113	2.12	21 (36%)
11	CLA	cB	817	2	52,68,73	2.05	12 (23%)	60,107,113	2.27	22 (36%)
11	CLA	cB	818	-	57,73,73	1.96	13 (22%)	66,113,113	1.99	17 (25%)
11	CLA	cB	819	2	39,55,73	2.39	14 (35%)	44,91,113	2.38	18 (40%)
11	CLA	cB	820	2	34,53,73	2.44	12 (35%)	37,89,113	2.49	16 (43%)
11	CLA	cB	821	-	47,63,73	2.22	14 (29%)	54,101,113	2.24	19 (35%)
11	CLA	cB	822	2	34,53,73	2.41	10 (29%)	37,89,113	2.61	16 (43%)
11	CLA	cB	823	2	46,62,73	2.18	14 (30%)	52,99,113	2.40	21 (40%)
12	F6C	cB	824	-	46,66,74	2.33	14 (30%)	40,104,114	4.16	14 (35%)
11	CLA	cB	825	2	57,73,73	1.99	13 (22%)	66,113,113	2.10	20 (30%)
11	CLA	cB	826	2	53,69,73	2.01	14 (26%)	61,108,113	2.24	23 (37%)
11	CLA	cB	827	2	57,73,73	1.96	12 (21%)	66,113,113	2.11	18 (27%)
11	CLA	cB	828	2	47,63,73	2.15	12 (25%)	54,101,113	2.36	21 (38%)
11	CLA	cB	829	2	34,53,73	2.35	12 (35%)	37,89,113	2.66	16 (43%)
11	CLA	cB	830	2	41,57,73	2.33	14 (34%)	46,93,113	2.34	19 (41%)
11	CLA	cB	831	2	48,64,73	2.15	13 (27%)	55,102,113	2.51	22 (40%)
11	CLA	cB	832	2	34,53,73	2.47	13 (38%)	37,89,113	2.45	16 (43%)
11	CLA	cB	833	2	34,53,73	2.49	12 (35%)	37,89,113	2.54	19 (51%)
11	CLA	cB	834	-	34,53,73	2.45	13 (38%)	37,89,113	2.52	17 (45%)
11	CLA	cB	835	-	34,53,73	2.46	13 (38%)	37,89,113	2.59	17 (45%)
11	CLA	cB	836	2	43,59,73	2.24	13 (30%)	49,96,113	2.40	22 (44%)
11	CLA	cB	837	2	47,63,73	2.17	13 (27%)	54,101,113	2.22	20 (37%)
11	CLA	cB	838	2	39,55,73	2.37	13 (33%)	44,91,113	2.46	19 (43%)
11	CLA	cB	839	-	57,73,73	1.94	12 (21%)	66,113,113	2.05	19 (28%)
11	CLA	cB	840	2	34,53,73	2.39	11 (32%)	37,89,113	2.60	16 (43%)
13	PQN	cB	841	-	29,29,34	1.52	2 (6%)	36,39,45	1.14	3 (8%)
15	BCR	cB	842	-	41,41,41	1.03	2 (4%)	56,56,56	1.24	4 (7%)
15	BCR	cB	843	-	41,41,41	1.04	2 (4%)	56,56,56	1.14	3 (5%)
15	BCR	cB	844	-	41,41,41	1.02	2 (4%)	56,56,56	1.22	5 (8%)
15	BCR	cB	845	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	5 (8%)
15	BCR	cB	846	-	41,41,41	1.04	2 (4%)	56,56,56	1.19	5 (8%)
18	LMG	cB	847	-	46,46,55	0.82	1 (2%)	54,54,63	1.36	8 (14%)
15	BCR	cB	848	-	41,41,41	0.99	2 (4%)	56,56,56	1.42	8 (14%)
14	SF4	cC	101	3	0,12,12	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	SF4	cC	102	3	0,12,12	0.00	-	-		
15	BCR	cI	103	-	41,41,41	1.01	2 (4%)	56,56,56	1.23	6 (10%)
11	CLA	cK	101	7	30,46,73	2.43	11 (36%)	32,79,113	2.55	16 (50%)
15	BCR	cK	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.30	8 (14%)
11	CLA	cK	103	-	43,59,73	2.27	14 (32%)	49,96,113	2.33	19 (38%)
12	F6C	cL	202	2	54,74,74	2.23	15 (27%)	50,114,114	2.28	13 (26%)
15	BCR	cL	203	-	41,41,41	1.10	3 (7%)	56,56,56	1.24	6 (10%)
11	CLA	cL	204	8	57,73,73	1.99	14 (24%)	66,113,113	2.12	19 (28%)
11	CLA	cL	205	8	57,73,73	1.96	13 (22%)	66,113,113	2.04	19 (28%)
11	CLA	cL	206	-	57,73,73	1.96	13 (22%)	66,113,113	2.10	20 (30%)
15	BCR	cL	207	-	41,41,41	1.05	2 (4%)	56,56,56	1.41	9 (16%)
15	BCR	cL	208	-	41,41,41	1.04	2 (4%)	56,56,56	1.26	7 (12%)
15	BCR	cM	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.29	7 (12%)

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
10	CL0	aA	801	1	3/3/20/25	5/37/135/135	-
11	CLA	aA	802	-	1/1/20/25	6/37/135/135	-
11	CLA	aA	803	-	3/3/18/25	7/27/125/135	-
11	CLA	aA	804	1	3/3/16/25	7/11/111/135	-
11	CLA	aA	805	1	3/3/16/25	4/11/111/135	-
11	CLA	aA	806	1	3/3/20/25	14/37/135/135	-
11	CLA	aA	807	1	3/3/20/25	15/37/135/135	-
11	CLA	aA	808	1	3/3/17/25	3/21/119/135	-
11	CLA	aA	809	1	3/3/16/25	7/11/111/135	-
11	CLA	aA	810	1	3/3/16/25	2/11/111/135	-
11	CLA	aA	811	1	3/3/16/25	3/11/111/135	-
11	CLA	aA	812	1	3/3/20/25	11/37/135/135	-
11	CLA	aA	813	1	3/3/17/25	8/24/122/135	-
11	CLA	aA	814	1	3/3/20/25	12/37/135/135	-
11	CLA	aA	815	1	3/3/16/25	5/11/111/135	-
11	CLA	aA	816	1	3/3/16/25	3/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	aA	817	-	3/3/16/25	6/18/116/135	-
11	CLA	aA	818	1	3/3/17/25	10/24/122/135	-
11	CLA	aA	819	1	3/3/17/25	10/24/122/135	-
11	CLA	aA	820	1	3/3/20/25	10/37/135/135	-
11	CLA	aA	821	1	3/3/19/25	14/33/131/135	-
11	CLA	aA	822	-	3/3/20/25	17/37/135/135	-
11	CLA	aA	823	1	3/3/16/25	5/11/111/135	-
11	CLA	aA	824	-	3/3/17/25	10/21/119/135	-
11	CLA	aA	825	1	3/3/20/25	12/37/135/135	-
12	F6C	aA	826	-	-	11/37/97/97	-
12	F6C	aA	827	-	-	8/25/85/97	-
11	CLA	aA	828	1	3/3/19/25	10/31/129/135	-
11	CLA	aA	829	1	2/2/20/25	12/37/135/135	-
12	F6C	aA	830	1	-	7/37/97/97	-
11	CLA	aA	831	1	3/3/20/25	12/37/135/135	-
12	F6C	aA	832	1	-	6/19/79/97	-
11	CLA	aA	833	1	3/3/20/25	14/37/135/135	-
11	CLA	aA	834	1	3/3/20/25	7/37/135/135	-
11	CLA	aA	835	1	3/3/20/25	11/37/135/135	-
11	CLA	aA	836	1	3/3/16/25	2/11/111/135	-
11	CLA	aA	837	1	3/3/16/25	4/11/111/135	-
11	CLA	aA	838	1	3/3/17/25	9/21/119/135	-
11	CLA	aA	839	1	3/3/20/25	5/37/135/135	-
11	CLA	aA	840	1	3/3/20/25	20/37/135/135	-
11	CLA	aA	841	1	3/3/17/25	4/19/117/135	-
11	CLA	aA	842	-	3/3/16/25	4/11/111/135	-
11	CLA	aA	843	1	3/3/17/25	7/21/119/135	-
12	F6C	aA	844	-	-	12/37/97/97	-
13	PQN	aA	845	-	-	3/23/43/43	0/2/2/2
14	SF4	aA	846	1,2	-	-	0/6/5/5
15	BCR	aA	847	-	-	9/29/63/63	0/2/2/2
15	BCR	aA	848	-	-	13/29/63/63	0/2/2/2
15	BCR	aA	849	-	-	12/29/63/63	0/2/2/2
15	BCR	aA	850	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	aA	851	-	-	19/29/63/63	0/2/2/2
16	LHG	aA	852	-	-	26/53/53/53	-
17	LMT	aA	853	-	-	11/21/61/61	0/2/2/2
11	CLA	aB	801	2	2/2/20/25	9/37/135/135	-
11	CLA	aB	802	-	1/1/18/25	10/28/126/135	-
11	CLA	aB	803	-	3/3/19/25	5/33/131/135	-
11	CLA	aB	804	2	3/3/17/25	7/19/117/135	-
11	CLA	aB	805	2	3/3/20/25	13/37/135/135	-
11	CLA	aB	806	2	3/3/20/25	18/37/135/135	-
11	CLA	aB	807	2	2/2/19/25	0/33/131/135	-
11	CLA	aB	808	2	2/2/20/25	10/37/135/135	-
11	CLA	aB	809	2	3/3/16/25	9/16/114/135	-
11	CLA	aB	810	2	3/3/16/25	3/11/111/135	-
11	CLA	aB	811	2	3/3/16/25	1/11/111/135	-
11	CLA	aB	812	2	3/3/20/25	16/37/135/135	-
11	CLA	aB	813	2	3/3/18/25	10/27/125/135	-
11	CLA	aB	814	2	3/3/16/25	4/11/111/135	-
11	CLA	aB	815	2	3/3/18/25	11/25/123/135	-
11	CLA	aB	816	2	3/3/18/25	10/30/128/135	-
11	CLA	aB	817	2	3/3/19/25	12/31/129/135	-
11	CLA	aB	818	-	3/3/20/25	5/37/135/135	-
11	CLA	aB	819	2	3/3/16/25	7/16/114/135	-
11	CLA	aB	820	2	3/3/16/25	4/11/111/135	-
11	CLA	aB	821	-	3/3/18/25	8/25/123/135	-
11	CLA	aB	822	2	1/1/16/25	4/11/111/135	-
11	CLA	aB	823	2	3/3/17/25	7/24/122/135	-
12	F6C	aB	824	-	-	7/28/88/97	-
11	CLA	aB	825	2	3/3/20/25	10/37/135/135	-
11	CLA	aB	826	2	2/2/19/25	10/33/131/135	-
11	CLA	aB	827	2	3/3/20/25	8/37/135/135	-
11	CLA	aB	828	2	3/3/18/25	7/25/123/135	-
11	CLA	aB	829	2	3/3/16/25	4/11/111/135	-
11	CLA	aB	830	2	3/3/16/25	7/18/116/135	-
11	CLA	aB	831	2	3/3/18/25	5/27/125/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	aB	832	2	3/3/16/25	5/11/111/135	-
11	CLA	aB	833	2	3/3/16/25	3/11/111/135	-
11	CLA	aB	834	-	3/3/16/25	3/11/111/135	-
11	CLA	aB	835	-	3/3/16/25	0/11/111/135	-
11	CLA	aB	836	2	3/3/17/25	8/21/119/135	-
11	CLA	aB	837	2	3/3/18/25	6/25/123/135	-
11	CLA	aB	838	2	3/3/16/25	4/16/114/135	-
11	CLA	aB	839	-	3/3/20/25	8/37/135/135	-
11	CLA	aB	840	2	3/3/16/25	3/11/111/135	-
13	PQN	aB	841	-	-	2/17/37/43	0/2/2/2
15	BCR	aB	842	-	-	14/29/63/63	0/2/2/2
15	BCR	aB	843	-	-	9/29/63/63	0/2/2/2
15	BCR	aB	844	-	-	12/29/63/63	0/2/2/2
15	BCR	aB	845	-	-	9/29/63/63	0/2/2/2
15	BCR	aB	846	-	-	13/29/63/63	0/2/2/2
18	LMG	aB	847	-	-	17/41/61/70	0/1/1/1
15	BCR	aB	848	-	-	18/29/63/63	0/2/2/2
14	SF4	aC	101	3	-	-	0/6/5/5
14	SF4	aC	102	3	-	-	0/6/5/5
15	BCR	aI	101	-	-	11/29/63/63	0/2/2/2
11	CLA	aK	101	7	3/3/13/25	0/4/98/135	-
15	BCR	aK	102	-	-	8/29/63/63	0/2/2/2
11	CLA	aK	103	-	2/2/17/25	4/21/119/135	-
12	F6C	aL	202	2	-	14/37/97/97	-
15	BCR	aL	203	-	-	8/29/63/63	0/2/2/2
11	CLA	aL	204	8	3/3/20/25	5/37/135/135	-
11	CLA	aL	205	8	3/3/20/25	13/37/135/135	-
11	CLA	aL	206	-	3/3/20/25	13/37/135/135	-
15	BCR	aL	207	-	-	9/29/63/63	0/2/2/2
15	BCR	aL	208	-	-	7/29/63/63	0/2/2/2
15	BCR	aM	101	-	-	7/29/63/63	0/2/2/2
10	CL0	bA	801	1	3/3/20/25	5/37/135/135	-
11	CLA	bA	802	-	1/1/20/25	6/37/135/135	-
11	CLA	bA	803	-	3/3/18/25	7/27/125/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	bA	804	1	3/3/16/25	7/11/111/135	-
11	CLA	bA	805	1	3/3/16/25	4/11/111/135	-
11	CLA	bA	806	1	3/3/20/25	14/37/135/135	-
11	CLA	bA	807	1	3/3/20/25	15/37/135/135	-
11	CLA	bA	808	1	3/3/17/25	3/21/119/135	-
11	CLA	bA	809	1	3/3/16/25	7/11/111/135	-
11	CLA	bA	810	1	3/3/16/25	2/11/111/135	-
11	CLA	bA	811	1	3/3/16/25	3/11/111/135	-
11	CLA	bA	812	1	3/3/20/25	11/37/135/135	-
11	CLA	bA	813	1	3/3/17/25	8/24/122/135	-
11	CLA	bA	814	1	3/3/20/25	12/37/135/135	-
11	CLA	bA	815	1	3/3/16/25	5/11/111/135	-
11	CLA	bA	816	1	3/3/16/25	3/11/111/135	-
11	CLA	bA	817	-	3/3/16/25	6/18/116/135	-
11	CLA	bA	818	1	3/3/17/25	10/24/122/135	-
11	CLA	bA	819	1	3/3/17/25	10/24/122/135	-
11	CLA	bA	820	1	3/3/20/25	10/37/135/135	-
11	CLA	bA	821	1	3/3/19/25	14/33/131/135	-
11	CLA	bA	822	-	3/3/20/25	17/37/135/135	-
11	CLA	bA	823	1	3/3/16/25	5/11/111/135	-
11	CLA	bA	824	-	3/3/17/25	10/21/119/135	-
11	CLA	bA	825	1	3/3/20/25	12/37/135/135	-
12	F6C	bA	826	-	-	11/37/97/97	-
12	F6C	bA	827	-	-	8/25/85/97	-
11	CLA	bA	828	1	3/3/19/25	10/31/129/135	-
11	CLA	bA	829	1	2/2/20/25	12/37/135/135	-
12	F6C	bA	830	1	-	7/37/97/97	-
11	CLA	bA	831	1	3/3/20/25	12/37/135/135	-
12	F6C	bA	832	1	-	7/19/79/97	-
11	CLA	bA	833	1	3/3/20/25	14/37/135/135	-
11	CLA	bA	834	1	3/3/20/25	7/37/135/135	-
11	CLA	bA	835	1	3/3/20/25	11/37/135/135	-
11	CLA	bA	836	1	3/3/16/25	2/11/111/135	-
11	CLA	bA	837	1	3/3/16/25	4/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	bA	838	1	3/3/17/25	9/21/119/135	-
11	CLA	bA	839	1	3/3/20/25	5/37/135/135	-
11	CLA	bA	840	1	3/3/20/25	20/37/135/135	-
11	CLA	bA	841	1	3/3/17/25	4/19/117/135	-
11	CLA	bA	842	-	3/3/16/25	4/11/111/135	-
11	CLA	bA	843	1	3/3/17/25	7/21/119/135	-
12	F6C	bA	844	-	-	12/37/97/97	-
13	PQN	bA	845	-	-	3/23/43/43	0/2/2/2
14	SF4	bA	846	1,2	-	-	0/6/5/5
15	BCR	bA	847	-	-	9/29/63/63	0/2/2/2
15	BCR	bA	848	-	-	13/29/63/63	0/2/2/2
15	BCR	bA	849	-	-	12/29/63/63	0/2/2/2
15	BCR	bA	850	-	-	6/29/63/63	0/2/2/2
15	BCR	bA	851	-	-	19/29/63/63	0/2/2/2
16	LHG	bA	852	-	-	26/53/53/53	-
17	LMT	bA	853	-	-	11/21/61/61	0/2/2/2
11	CLA	bB	801	2	2/2/20/25	9/37/135/135	-
11	CLA	bB	802	-	1/1/18/25	10/28/126/135	-
11	CLA	bB	803	-	3/3/19/25	5/33/131/135	-
11	CLA	bB	804	2	3/3/17/25	7/19/117/135	-
11	CLA	bB	805	2	3/3/20/25	13/37/135/135	-
11	CLA	bB	806	2	3/3/20/25	18/37/135/135	-
11	CLA	bB	807	2	2/2/19/25	0/33/131/135	-
11	CLA	bB	808	2	2/2/20/25	10/37/135/135	-
11	CLA	bB	809	2	3/3/16/25	9/16/114/135	-
11	CLA	bB	810	2	3/3/16/25	3/11/111/135	-
11	CLA	bB	811	2	3/3/16/25	1/11/111/135	-
11	CLA	bB	812	2	3/3/20/25	16/37/135/135	-
11	CLA	bB	813	2	3/3/18/25	10/27/125/135	-
11	CLA	bB	814	2	3/3/16/25	4/11/111/135	-
11	CLA	bB	815	2	3/3/18/25	11/25/123/135	-
11	CLA	bB	816	2	3/3/18/25	10/30/128/135	-
11	CLA	bB	817	2	3/3/19/25	12/31/129/135	-
11	CLA	bB	818	-	3/3/20/25	5/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	bB	819	2	3/3/16/25	7/16/114/135	-
11	CLA	bB	820	2	3/3/16/25	4/11/111/135	-
11	CLA	bB	821	-	3/3/18/25	7/25/123/135	-
11	CLA	bB	822	2	1/1/16/25	4/11/111/135	-
11	CLA	bB	823	2	3/3/17/25	7/24/122/135	-
12	F6C	bB	824	-	-	7/28/88/97	-
11	CLA	bB	825	2	3/3/20/25	10/37/135/135	-
11	CLA	bB	826	2	2/2/19/25	10/33/131/135	-
11	CLA	bB	827	2	3/3/20/25	8/37/135/135	-
11	CLA	bB	828	2	3/3/18/25	7/25/123/135	-
11	CLA	bB	829	2	3/3/16/25	4/11/111/135	-
11	CLA	bB	830	2	3/3/16/25	7/18/116/135	-
11	CLA	bB	831	2	3/3/18/25	5/27/125/135	-
11	CLA	bB	832	2	3/3/16/25	5/11/111/135	-
11	CLA	bB	833	2	3/3/16/25	3/11/111/135	-
11	CLA	bB	834	-	3/3/16/25	3/11/111/135	-
11	CLA	bB	835	-	3/3/16/25	0/11/111/135	-
11	CLA	bB	836	2	3/3/17/25	8/21/119/135	-
11	CLA	bB	837	2	3/3/18/25	6/25/123/135	-
11	CLA	bB	838	2	3/3/16/25	4/16/114/135	-
11	CLA	bB	839	-	3/3/20/25	8/37/135/135	-
11	CLA	bB	840	2	3/3/16/25	3/11/111/135	-
13	PQN	bB	841	-	-	2/17/37/43	0/2/2/2
15	BCR	bB	842	-	-	14/29/63/63	0/2/2/2
15	BCR	bB	843	-	-	9/29/63/63	0/2/2/2
15	BCR	bB	844	-	-	12/29/63/63	0/2/2/2
15	BCR	bB	845	-	-	9/29/63/63	0/2/2/2
15	BCR	bB	846	-	-	13/29/63/63	0/2/2/2
18	LMG	bB	847	-	-	17/41/61/70	0/1/1/1
15	BCR	bB	848	-	-	18/29/63/63	0/2/2/2
14	SF4	bC	101	3	-	-	0/6/5/5
14	SF4	bC	102	3	-	-	0/6/5/5
15	BCR	bI	101	-	-	11/29/63/63	0/2/2/2
11	CLA	bK	101	7	3/3/13/25	0/4/98/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	bK	102	-	-	8/29/63/63	0/2/2/2
11	CLA	bK	103	-	2/2/17/25	4/21/119/135	-
12	F6C	bL	202	2	-	14/37/97/97	-
15	BCR	bL	203	-	-	8/29/63/63	0/2/2/2
11	CLA	bL	204	8	3/3/20/25	5/37/135/135	-
11	CLA	bL	205	8	3/3/20/25	13/37/135/135	-
11	CLA	bL	206	-	3/3/20/25	13/37/135/135	-
15	BCR	bL	207	-	-	9/29/63/63	0/2/2/2
15	BCR	bL	208	-	-	7/29/63/63	0/2/2/2
15	BCR	bM	101	-	-	7/29/63/63	0/2/2/2
10	CL0	cA	801	1	3/3/20/25	5/37/135/135	-
11	CLA	cA	802	-	1/1/20/25	6/37/135/135	-
11	CLA	cA	803	-	3/3/18/25	7/27/125/135	-
11	CLA	cA	804	1	3/3/16/25	7/11/111/135	-
11	CLA	cA	805	1	3/3/16/25	4/11/111/135	-
11	CLA	cA	806	1	3/3/20/25	14/37/135/135	-
11	CLA	cA	807	1	3/3/20/25	15/37/135/135	-
11	CLA	cA	808	1	3/3/17/25	3/21/119/135	-
11	CLA	cA	809	1	3/3/16/25	7/11/111/135	-
11	CLA	cA	810	1	3/3/16/25	2/11/111/135	-
11	CLA	cA	811	1	3/3/16/25	3/11/111/135	-
11	CLA	cA	812	1	3/3/20/25	11/37/135/135	-
11	CLA	cA	813	1	3/3/17/25	8/24/122/135	-
11	CLA	cA	814	1	3/3/20/25	12/37/135/135	-
11	CLA	cA	815	1	3/3/16/25	5/11/111/135	-
11	CLA	cA	816	1	3/3/16/25	3/11/111/135	-
11	CLA	cA	817	-	3/3/16/25	6/18/116/135	-
11	CLA	cA	818	1	3/3/17/25	10/24/122/135	-
11	CLA	cA	819	1	3/3/17/25	10/24/122/135	-
11	CLA	cA	820	1	3/3/20/25	10/37/135/135	-
11	CLA	cA	821	1	3/3/19/25	14/33/131/135	-
11	CLA	cA	822	-	3/3/20/25	17/37/135/135	-
11	CLA	cA	823	1	3/3/16/25	5/11/111/135	-
11	CLA	cA	824	-	3/3/17/25	10/21/119/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	cA	825	1	3/3/20/25	12/37/135/135	-
12	F6C	cA	826	-	-	11/37/97/97	-
12	F6C	cA	827	-	-	8/25/85/97	-
11	CLA	cA	828	1	3/3/19/25	10/31/129/135	-
11	CLA	cA	829	1	2/2/20/25	12/37/135/135	-
12	F6C	cA	830	1	-	7/37/97/97	-
11	CLA	cA	831	1	3/3/20/25	12/37/135/135	-
12	F6C	cA	832	1	-	6/19/79/97	-
11	CLA	cA	833	1	3/3/20/25	14/37/135/135	-
11	CLA	cA	834	1	3/3/20/25	7/37/135/135	-
11	CLA	cA	835	1	3/3/20/25	11/37/135/135	-
11	CLA	cA	836	1	3/3/16/25	2/11/111/135	-
11	CLA	cA	837	1	3/3/16/25	4/11/111/135	-
11	CLA	cA	838	1	3/3/17/25	9/21/119/135	-
11	CLA	cA	839	1	3/3/20/25	5/37/135/135	-
11	CLA	cA	840	1	3/3/20/25	20/37/135/135	-
11	CLA	cA	841	1	3/3/17/25	4/19/117/135	-
11	CLA	cA	842	-	3/3/16/25	4/11/111/135	-
11	CLA	cA	843	1	3/3/17/25	7/21/119/135	-
12	F6C	cA	844	-	-	12/37/97/97	-
13	PQN	cA	845	-	-	3/23/43/43	0/2/2/2
14	SF4	cA	846	1,2	-	-	0/6/5/5
15	BCR	cA	847	-	-	9/29/63/63	0/2/2/2
15	BCR	cA	848	-	-	13/29/63/63	0/2/2/2
15	BCR	cA	849	-	-	12/29/63/63	0/2/2/2
15	BCR	cA	850	-	-	6/29/63/63	0/2/2/2
15	BCR	cA	851	-	-	19/29/63/63	0/2/2/2
16	LHG	cA	852	-	-	26/53/53/53	-
17	LMT	cA	853	-	-	11/21/61/61	0/2/2/2
11	CLA	cB	801	2	2/2/20/25	9/37/135/135	-
11	CLA	cB	802	-	1/1/18/25	10/28/126/135	-
11	CLA	cB	803	-	3/3/19/25	5/33/131/135	-
11	CLA	cB	804	2	3/3/17/25	7/19/117/135	-
11	CLA	cB	805	2	3/3/20/25	13/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	cB	806	2	3/3/20/25	18/37/135/135	-
11	CLA	cB	807	2	2/2/19/25	0/33/131/135	-
11	CLA	cB	808	2	2/2/20/25	9/37/135/135	-
11	CLA	cB	809	2	3/3/16/25	9/16/114/135	-
11	CLA	cB	810	2	3/3/16/25	3/11/111/135	-
11	CLA	cB	811	2	3/3/16/25	1/11/111/135	-
11	CLA	cB	812	2	3/3/20/25	16/37/135/135	-
11	CLA	cB	813	2	3/3/18/25	10/27/125/135	-
11	CLA	cB	814	2	3/3/16/25	4/11/111/135	-
11	CLA	cB	815	2	3/3/18/25	11/25/123/135	-
11	CLA	cB	816	2	3/3/18/25	10/30/128/135	-
11	CLA	cB	817	2	3/3/19/25	12/31/129/135	-
11	CLA	cB	818	-	3/3/20/25	5/37/135/135	-
11	CLA	cB	819	2	3/3/16/25	7/16/114/135	-
11	CLA	cB	820	2	3/3/16/25	4/11/111/135	-
11	CLA	cB	821	-	3/3/18/25	7/25/123/135	-
11	CLA	cB	822	2	1/1/16/25	4/11/111/135	-
11	CLA	cB	823	2	3/3/17/25	7/24/122/135	-
12	F6C	cB	824	-	-	7/28/88/97	-
11	CLA	cB	825	2	3/3/20/25	10/37/135/135	-
11	CLA	cB	826	2	2/2/19/25	10/33/131/135	-
11	CLA	cB	827	2	3/3/20/25	8/37/135/135	-
11	CLA	cB	828	2	3/3/18/25	7/25/123/135	-
11	CLA	cB	829	2	3/3/16/25	4/11/111/135	-
11	CLA	cB	830	2	3/3/16/25	7/18/116/135	-
11	CLA	cB	831	2	3/3/18/25	5/27/125/135	-
11	CLA	cB	832	2	3/3/16/25	5/11/111/135	-
11	CLA	cB	833	2	3/3/16/25	3/11/111/135	-
11	CLA	cB	834	-	3/3/16/25	2/11/111/135	-
11	CLA	cB	835	-	3/3/16/25	0/11/111/135	-
11	CLA	cB	836	2	3/3/17/25	8/21/119/135	-
11	CLA	cB	837	2	3/3/18/25	6/25/123/135	-
11	CLA	cB	838	2	3/3/16/25	4/16/114/135	-
11	CLA	cB	839	-	3/3/20/25	8/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	cB	840	2	3/3/16/25	3/11/111/135	-
13	PQN	cB	841	-	-	2/17/37/43	0/2/2/2
15	BCR	cB	842	-	-	14/29/63/63	0/2/2/2
15	BCR	cB	843	-	-	9/29/63/63	0/2/2/2
15	BCR	cB	844	-	-	12/29/63/63	0/2/2/2
15	BCR	cB	845	-	-	9/29/63/63	0/2/2/2
15	BCR	cB	846	-	-	13/29/63/63	0/2/2/2
18	LMG	cB	847	-	-	17/41/61/70	0/1/1/1
15	BCR	cB	848	-	-	18/29/63/63	0/2/2/2
14	SF4	cC	101	3	-	-	0/6/5/5
14	SF4	cC	102	3	-	-	0/6/5/5
15	BCR	cI	103	-	-	11/29/63/63	0/2/2/2
11	CLA	cK	101	7	3/3/13/25	0/4/98/135	-
15	BCR	cK	102	-	-	8/29/63/63	0/2/2/2
11	CLA	cK	103	-	2/2/17/25	4/21/119/135	-
12	F6C	cL	202	2	-	14/37/97/97	-
15	BCR	cL	203	-	-	8/29/63/63	0/2/2/2
11	CLA	cL	204	8	3/3/20/25	5/37/135/135	-
11	CLA	cL	205	8	3/3/20/25	13/37/135/135	-
11	CLA	cL	206	-	3/3/20/25	13/37/135/135	-
15	BCR	cL	207	-	-	9/29/63/63	0/2/2/2
15	BCR	cL	208	-	-	7/29/63/63	0/2/2/2
15	BCR	cM	101	-	-	7/29/63/63	0/2/2/2

The worst 5 of 3620 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	838	CLA	C3B-C2B	6.57	1.49	1.40
11	aA	838	CLA	C3B-C2B	6.55	1.49	1.40
11	bA	838	CLA	C3B-C2B	6.54	1.49	1.40
11	cA	818	CLA	C3B-C2B	6.50	1.49	1.40
11	aA	818	CLA	C3B-C2B	6.49	1.49	1.40

The worst 5 of 5569 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	cA	827	F6C	CAA-C2A-C1A	-21.51	104.11	127.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	bA	827	F6C	CAA-C2A-C1A	-21.48	104.14	127.48
12	aA	827	F6C	CAA-C2A-C1A	-21.47	104.14	127.48
11	aA	829	CLA	C4-C3-C5	-21.43	78.37	115.29
11	cA	829	CLA	C4-C3-C5	-21.42	78.38	115.29

5 of 711 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	cB	813	CLA	NC
11	cB	813	CLA	ND
11	cB	813	CLA	NA
11	cB	819	CLA	NC
11	cB	819	CLA	ND

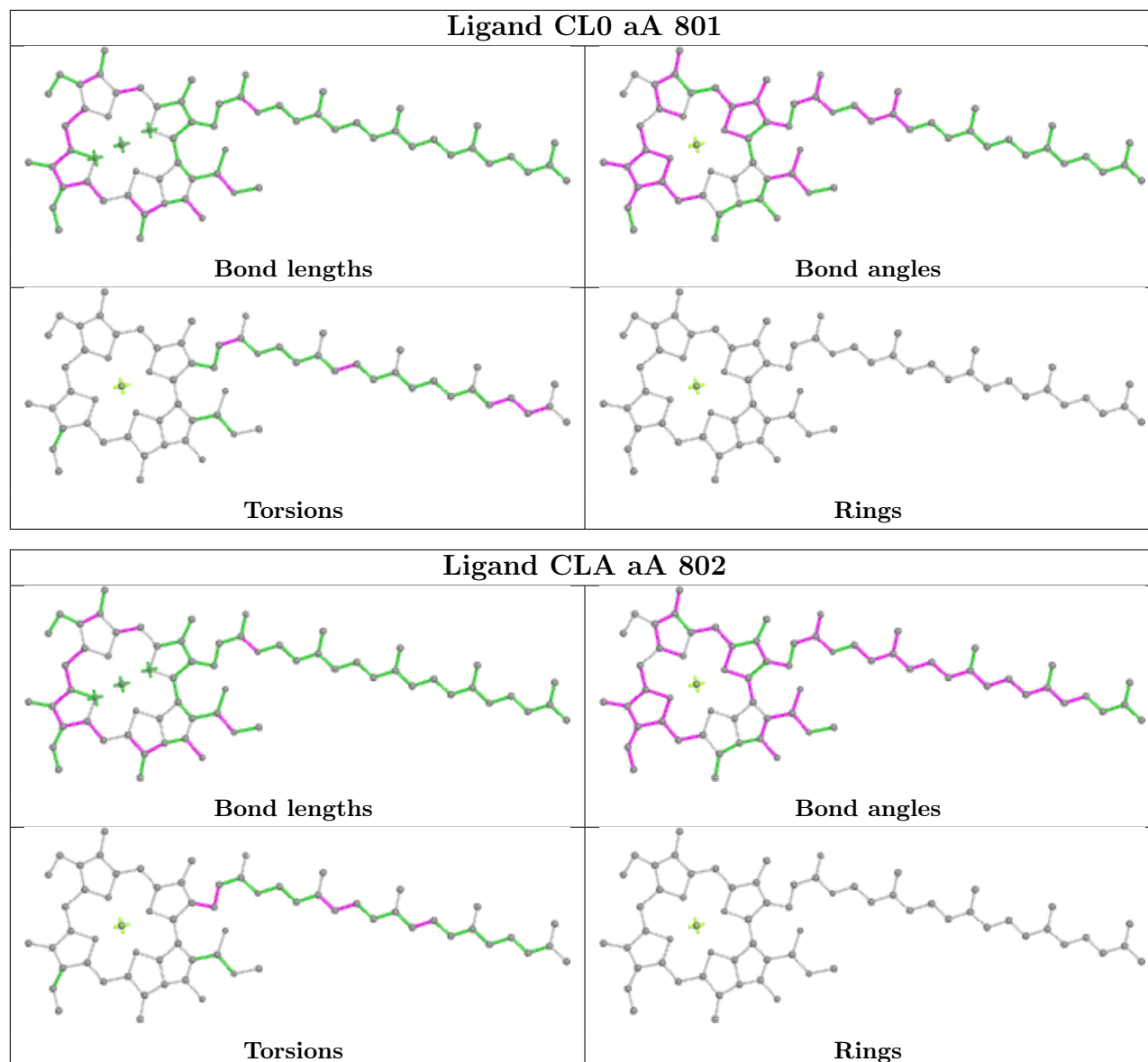
5 of 2829 torsion outliers are listed below:

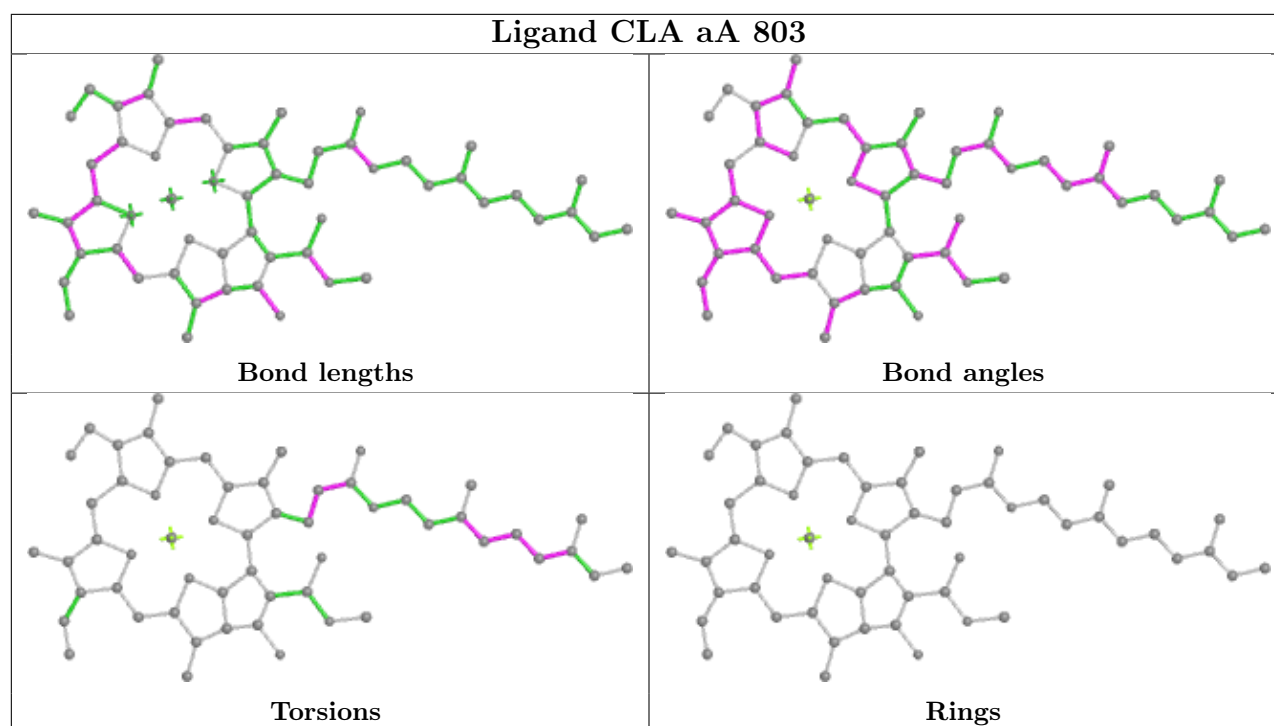
Mol	Chain	Res	Type	Atoms
11	cB	819	CLA	C3A-C2A-CAA-CBA
11	bB	811	CLA	C2A-CAA-CBA-CGA
11	bL	205	CLA	C1A-C2A-CAA-CBA
11	bL	205	CLA	C3A-C2A-CAA-CBA
11	bL	205	CLA	C6-C7-C8-C9

There are no ring outliers.

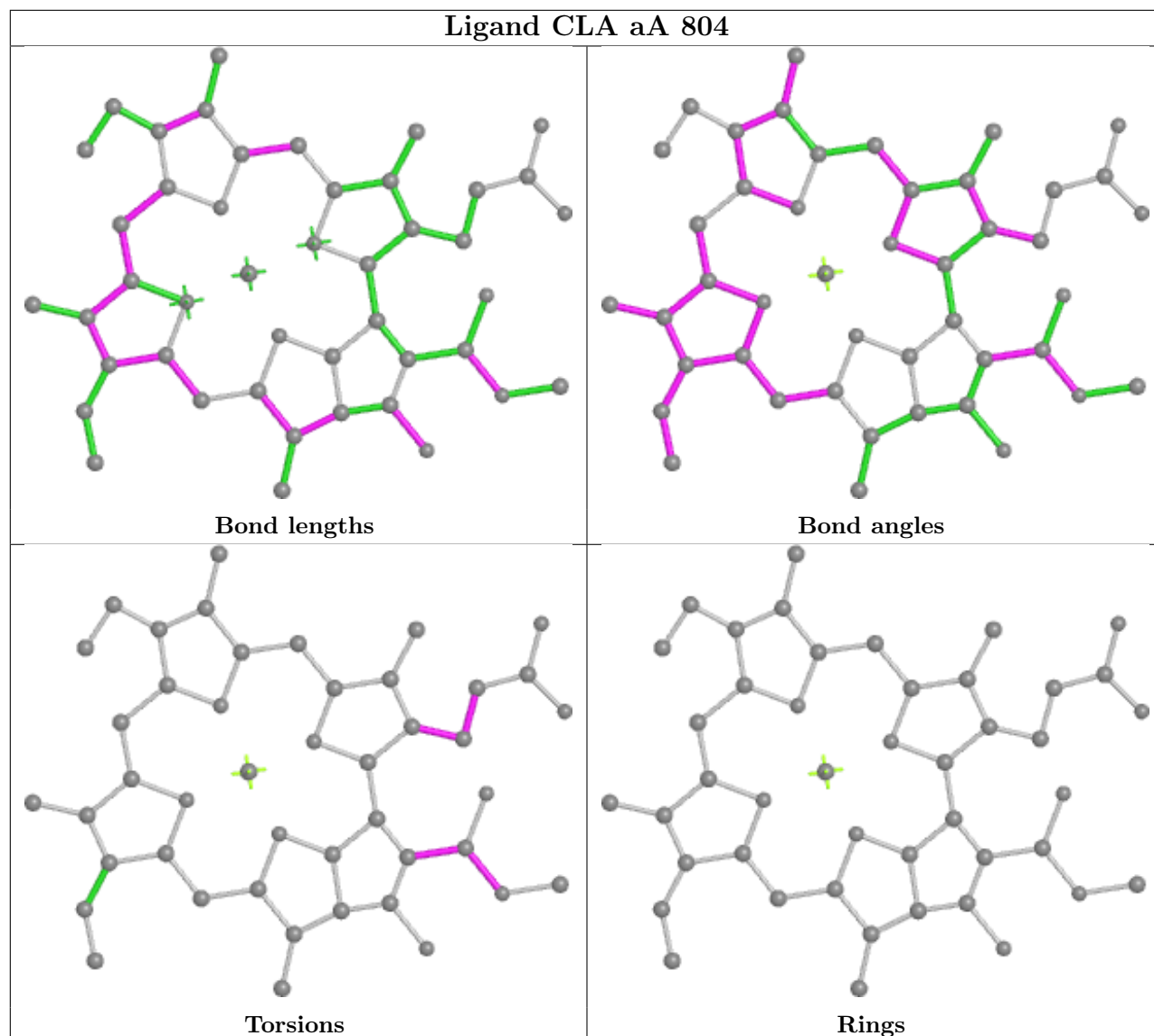
No monomer is involved in short contacts.

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

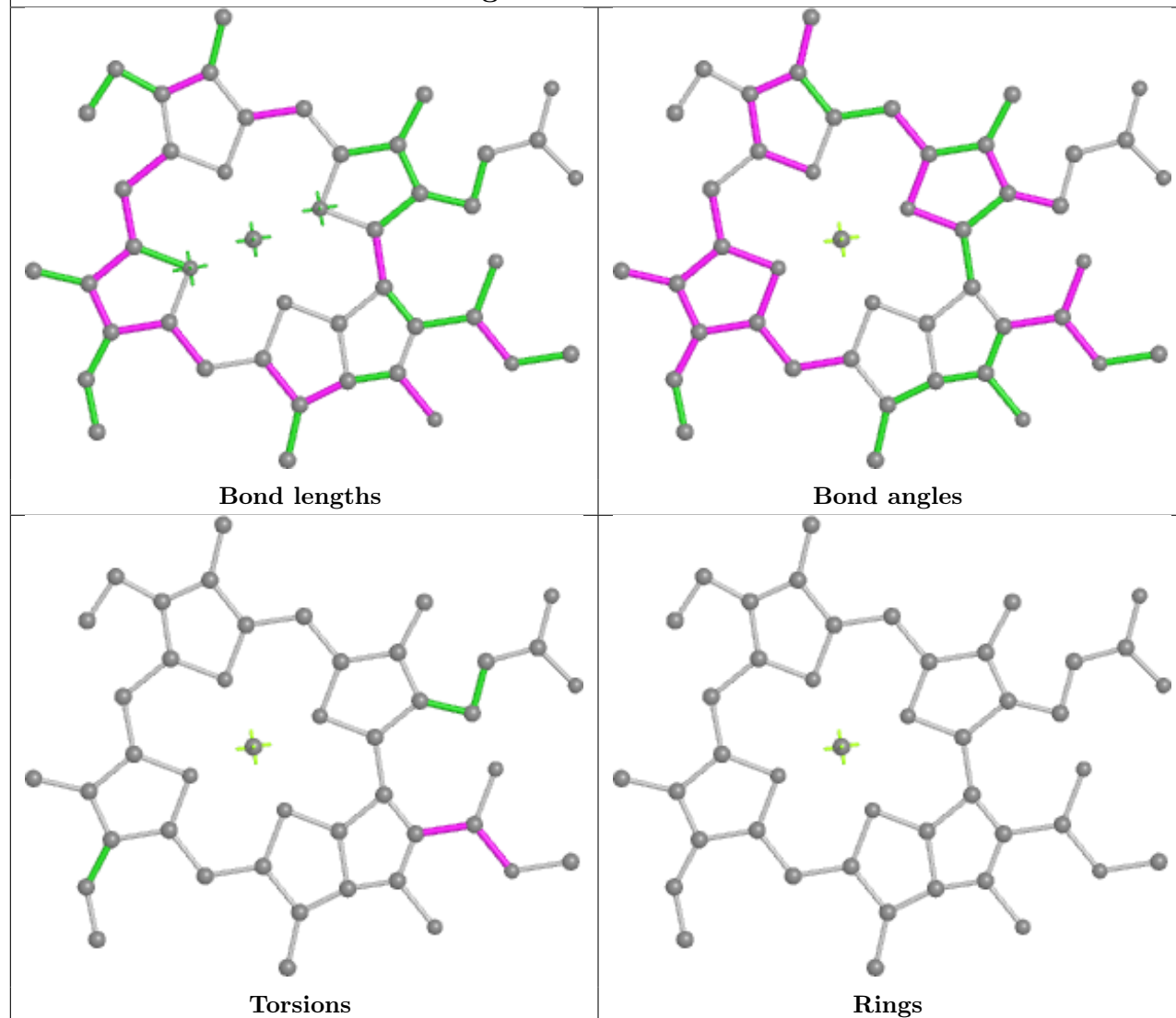




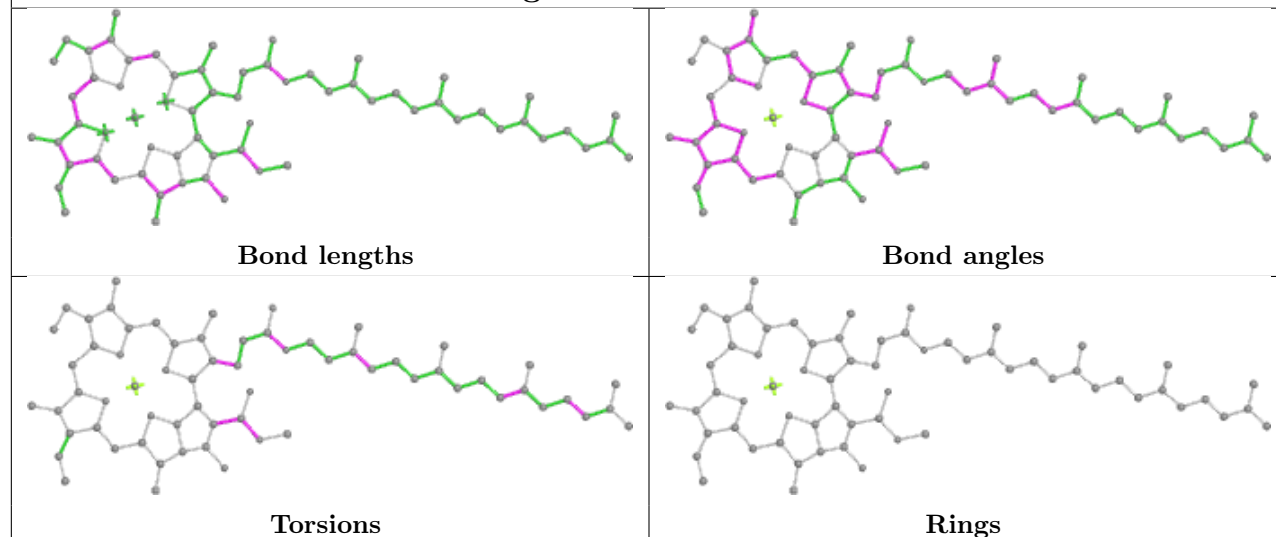
Ligand CLA aA 804



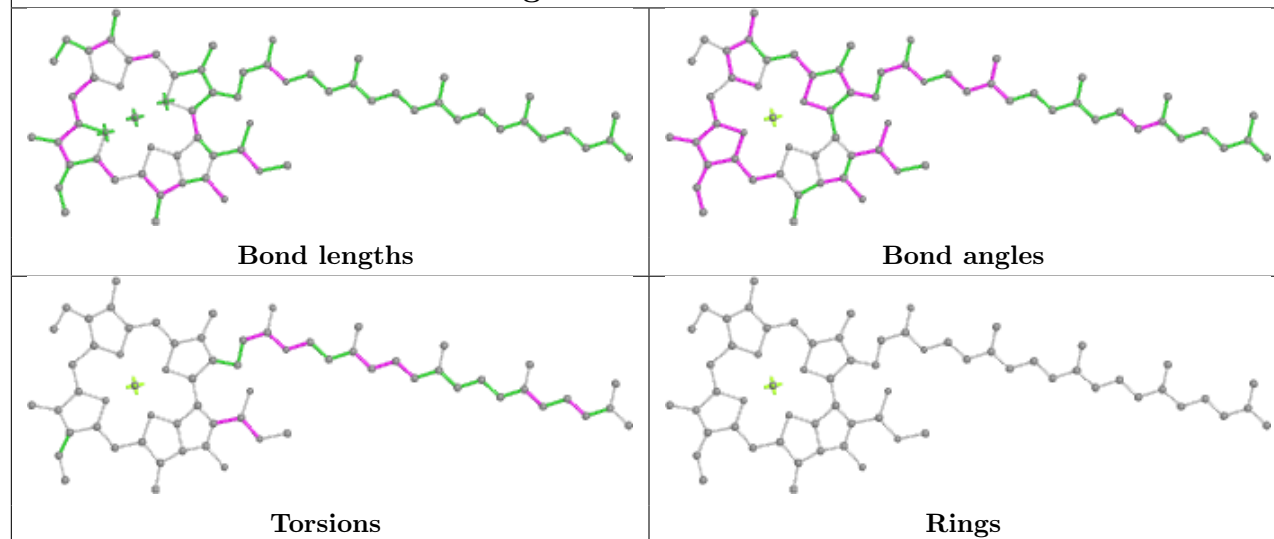
Ligand CLA aA 805



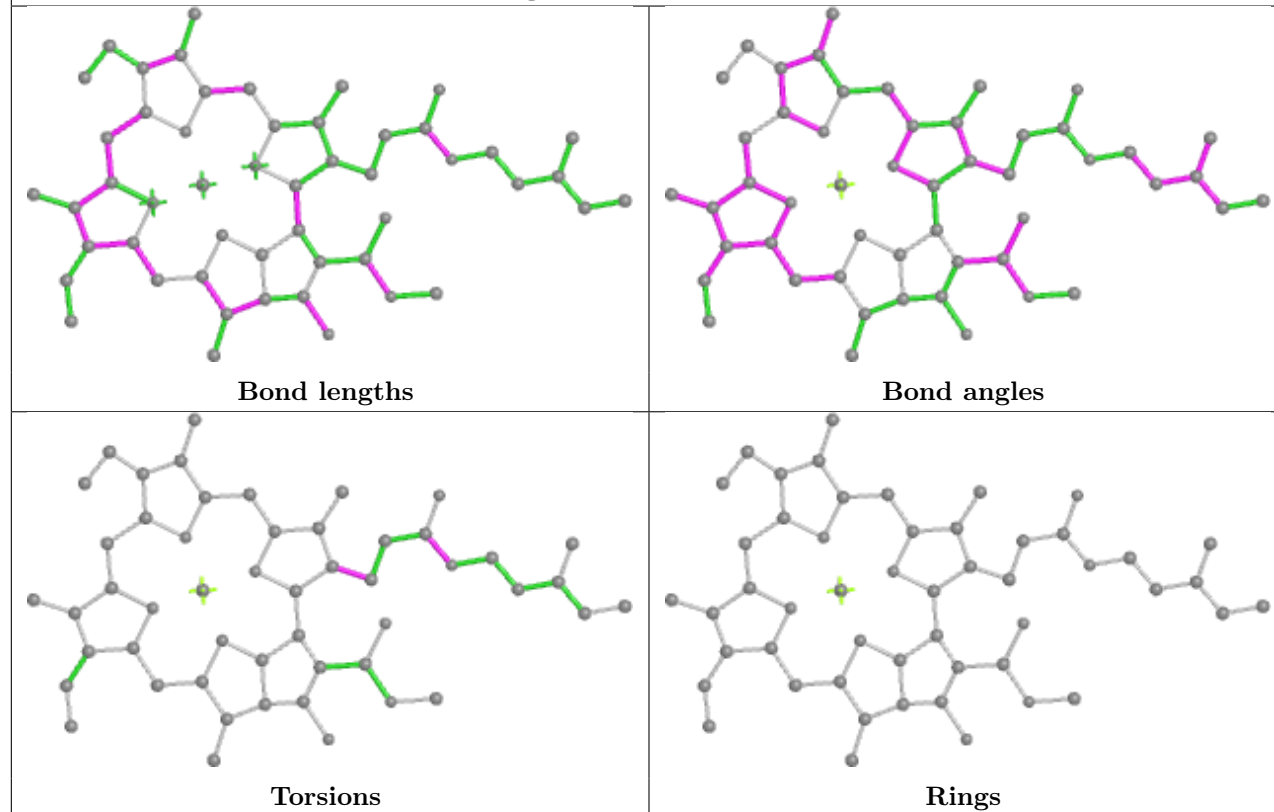
Ligand CLA aA 806



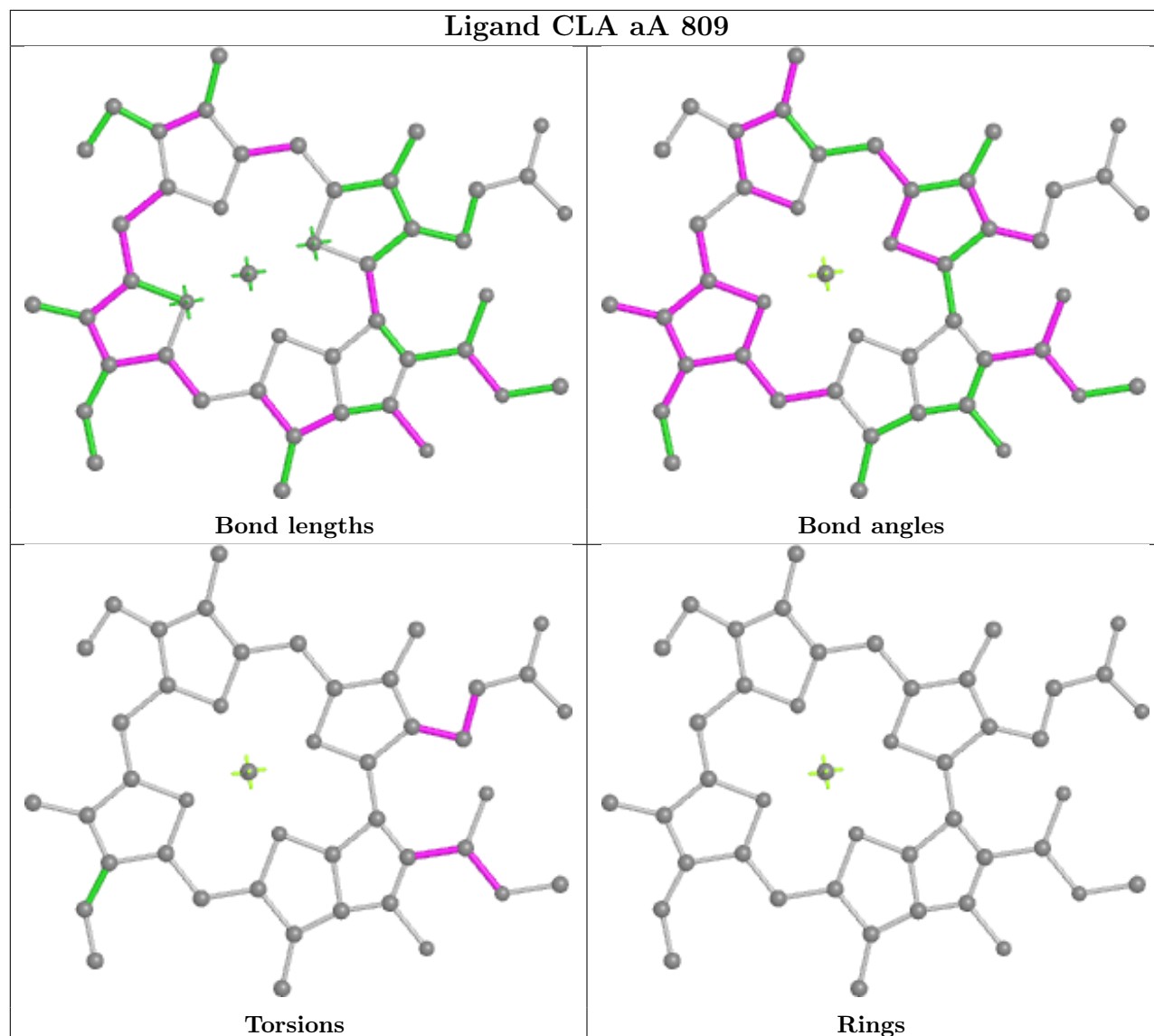
Ligand CLA aA 807



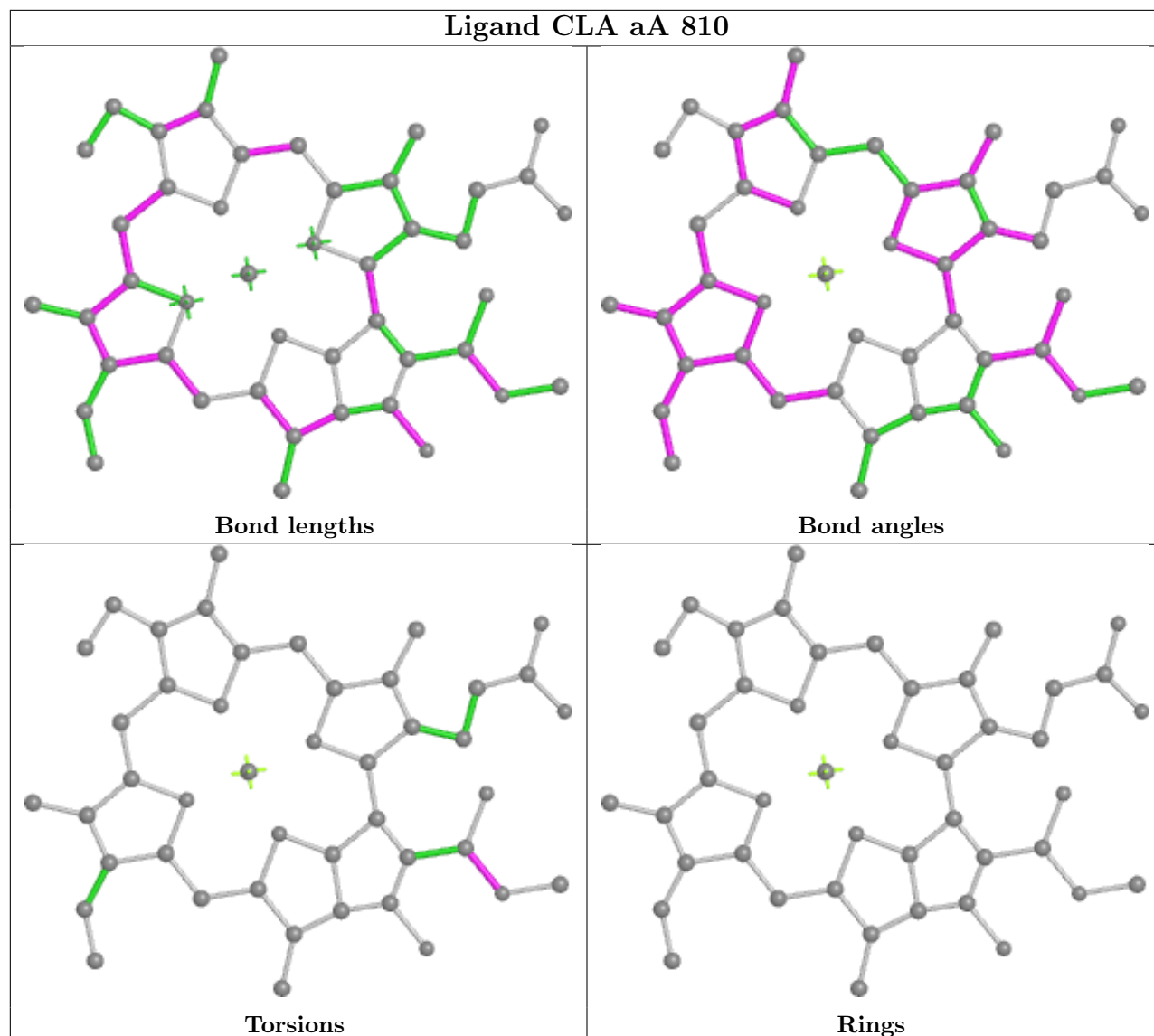
Ligand CLA aA 808



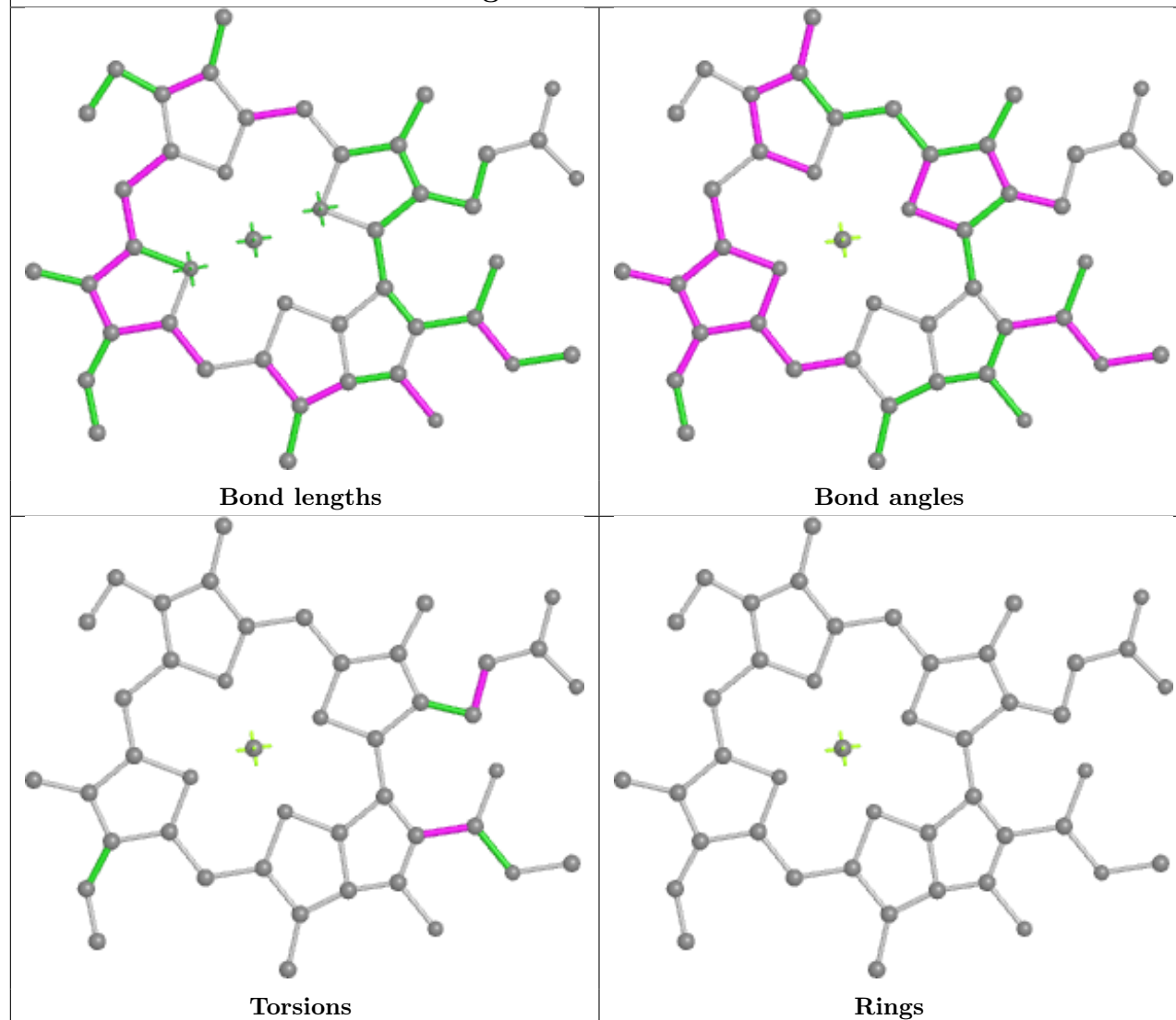
Ligand CLA aA 809



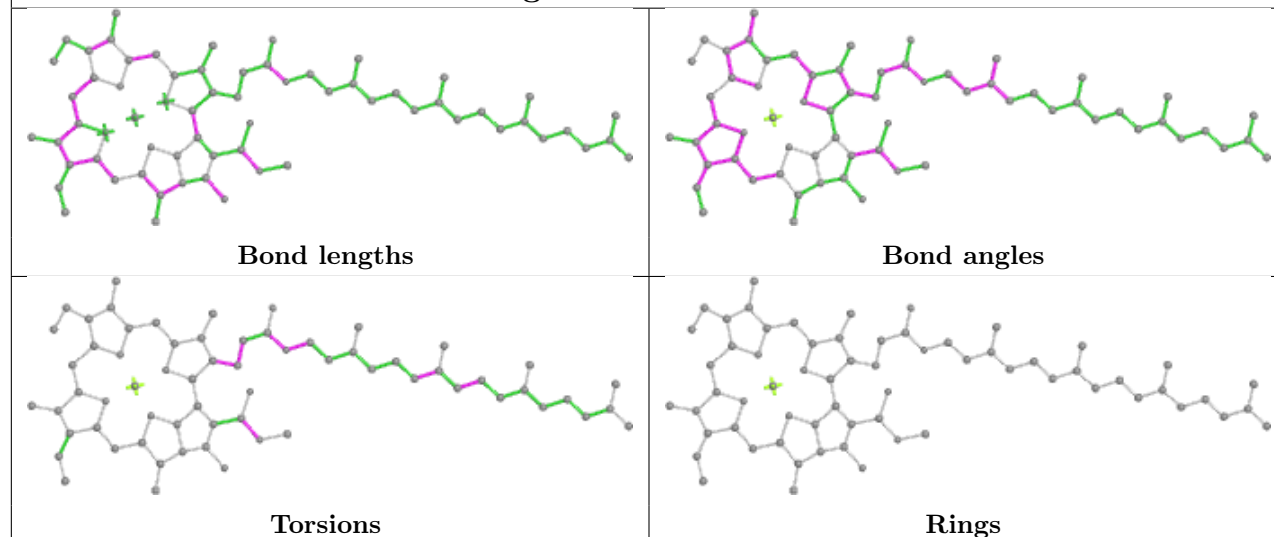
Ligand CLA aA 810

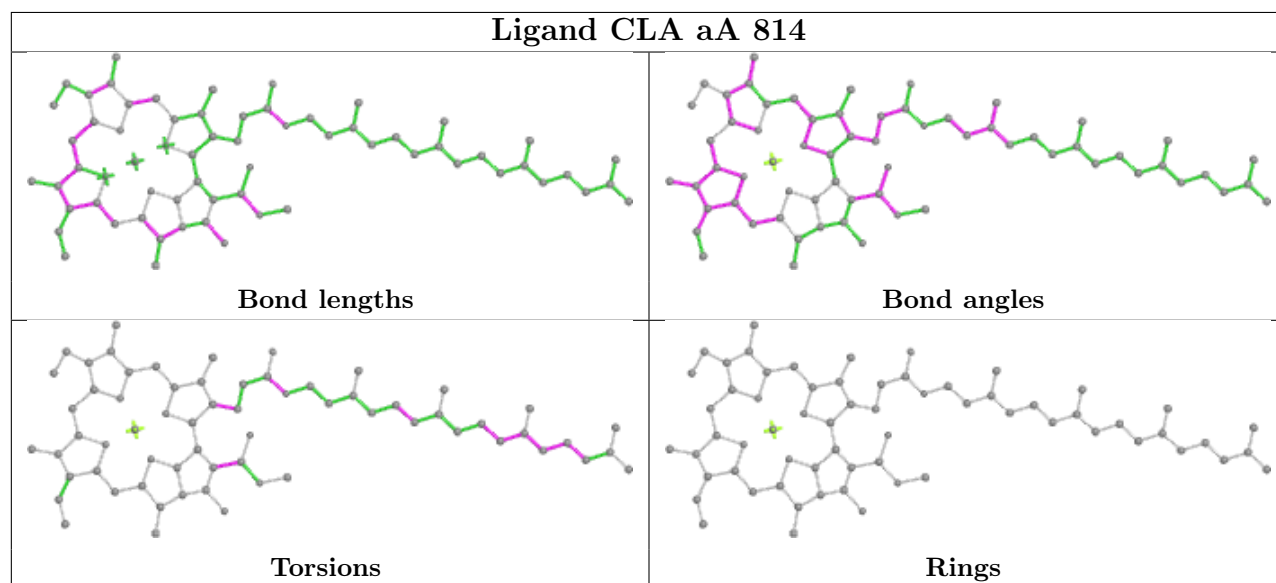
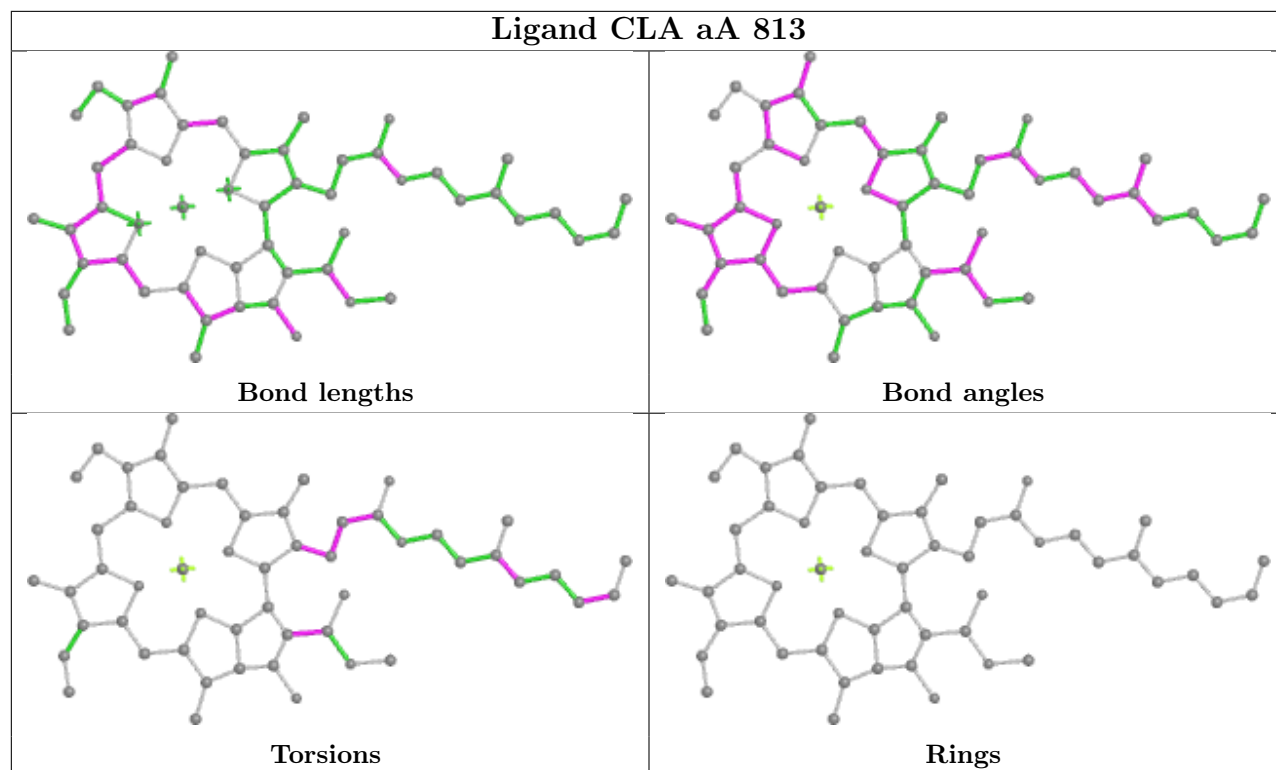


Ligand CLA aA 811

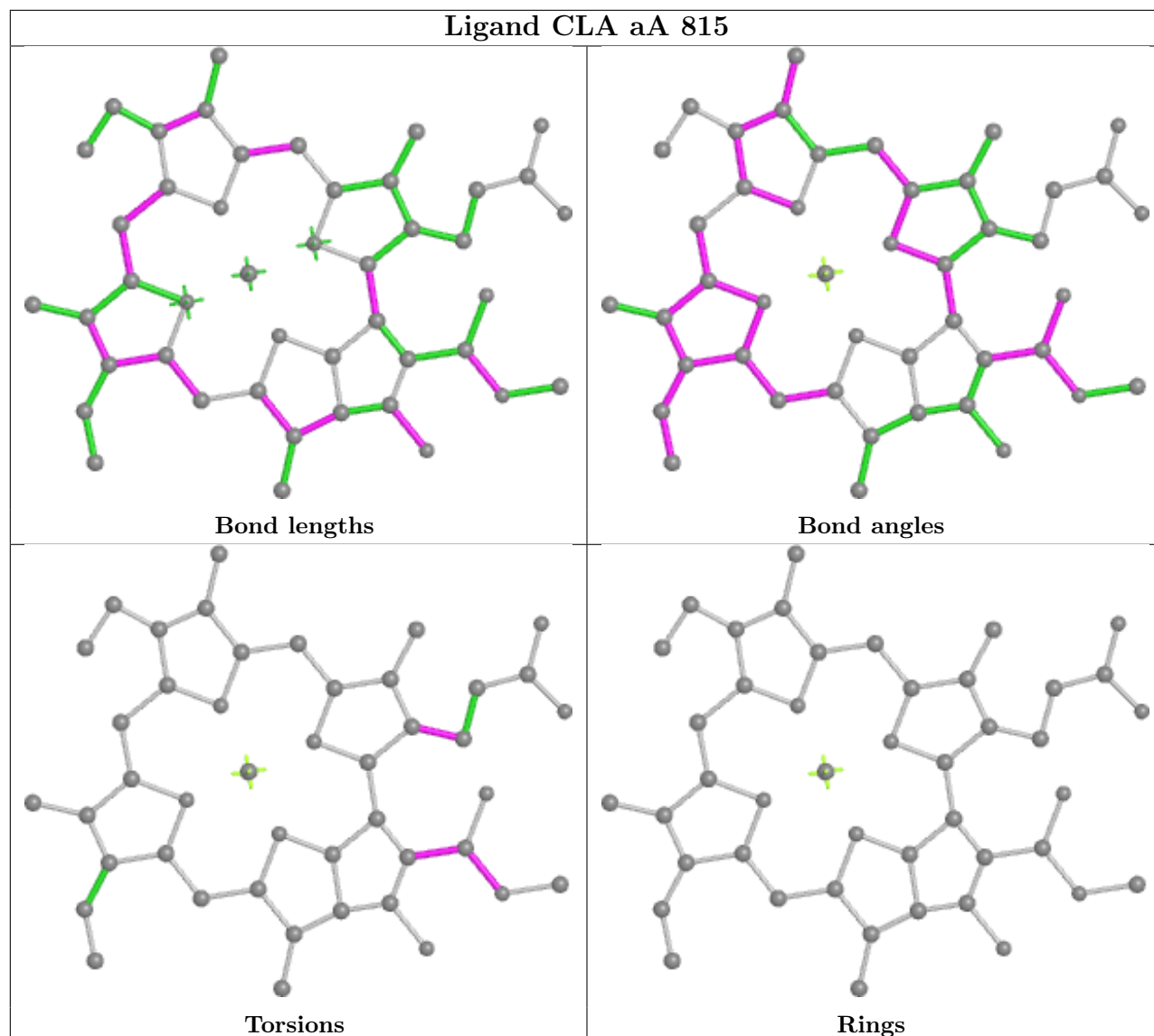


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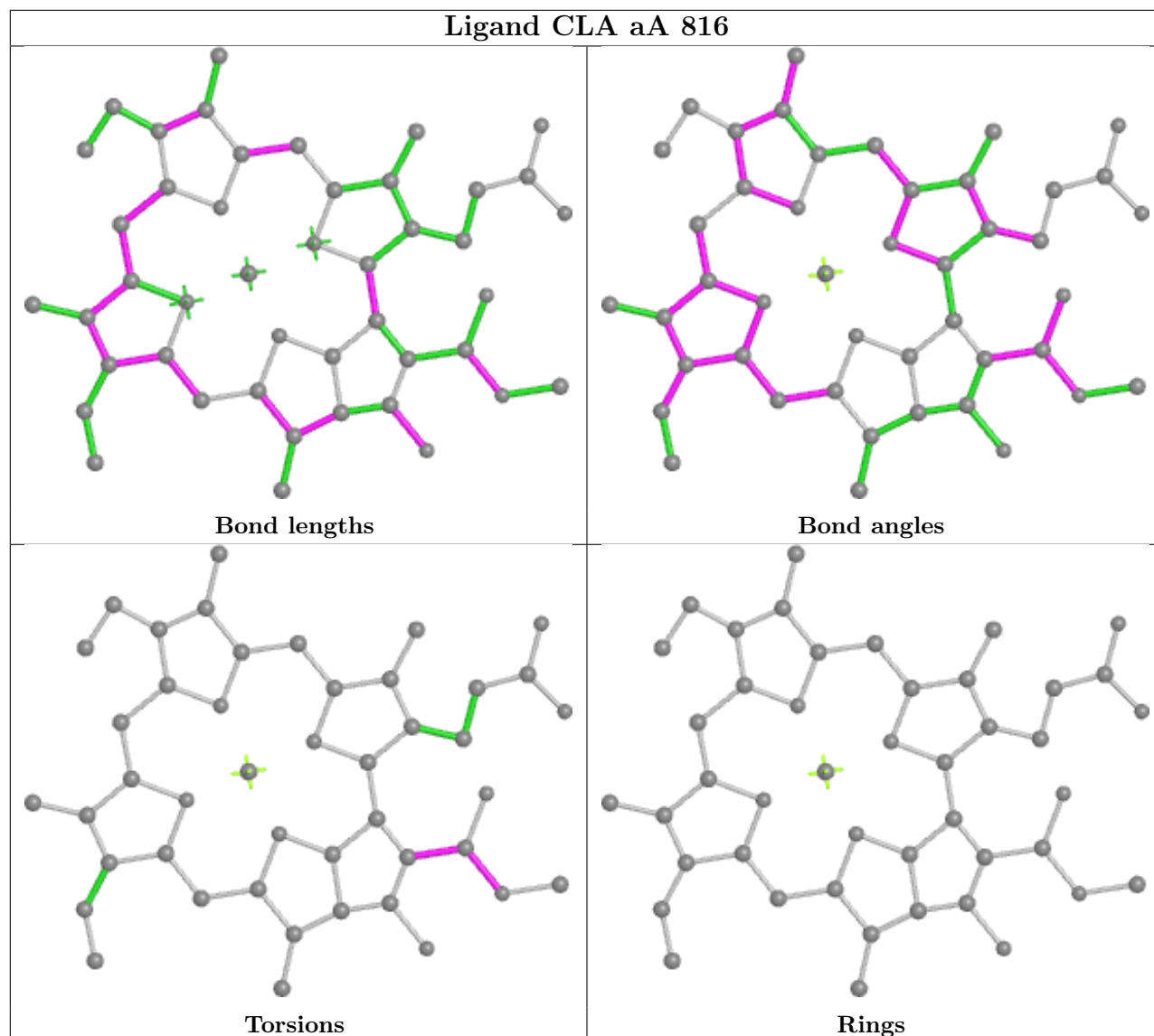




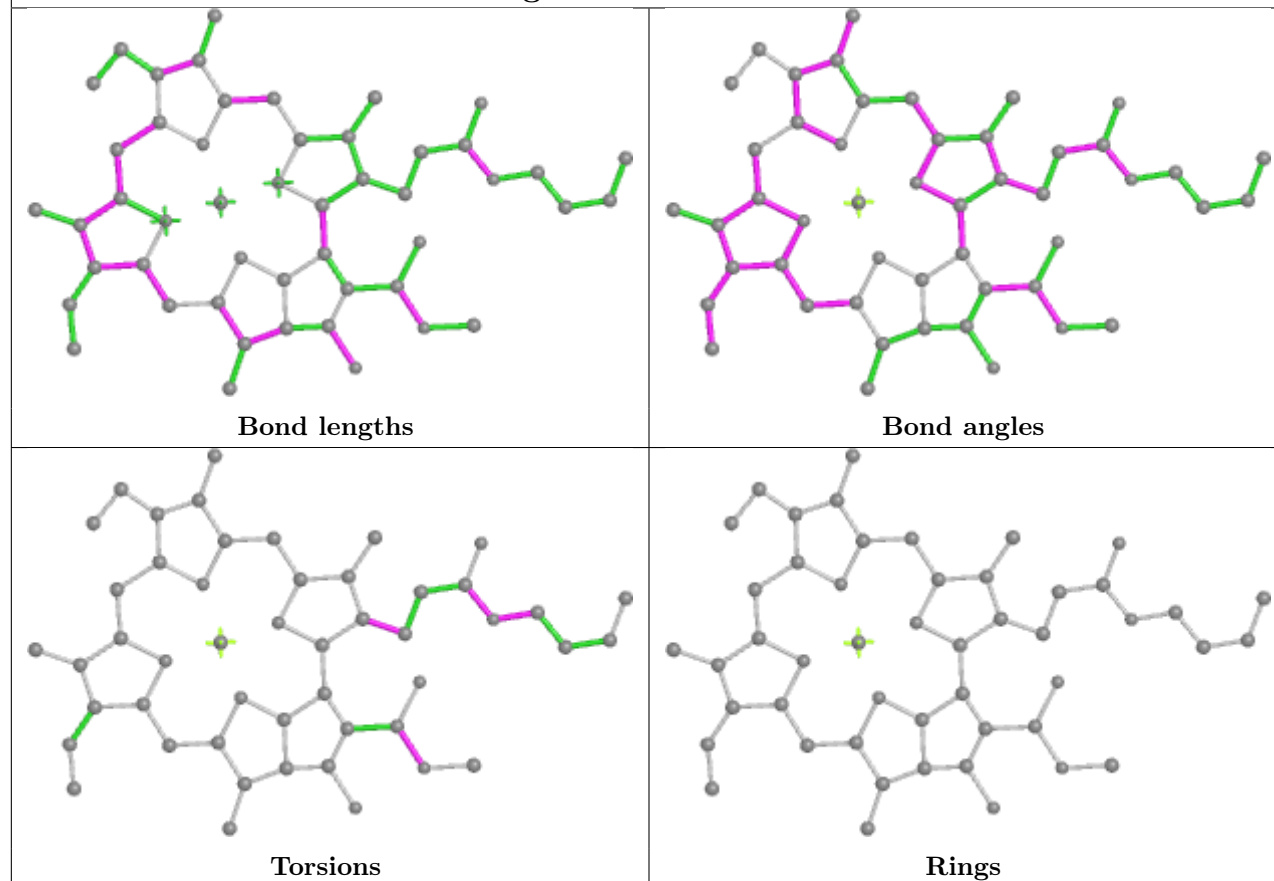
Ligand CLA aA 815



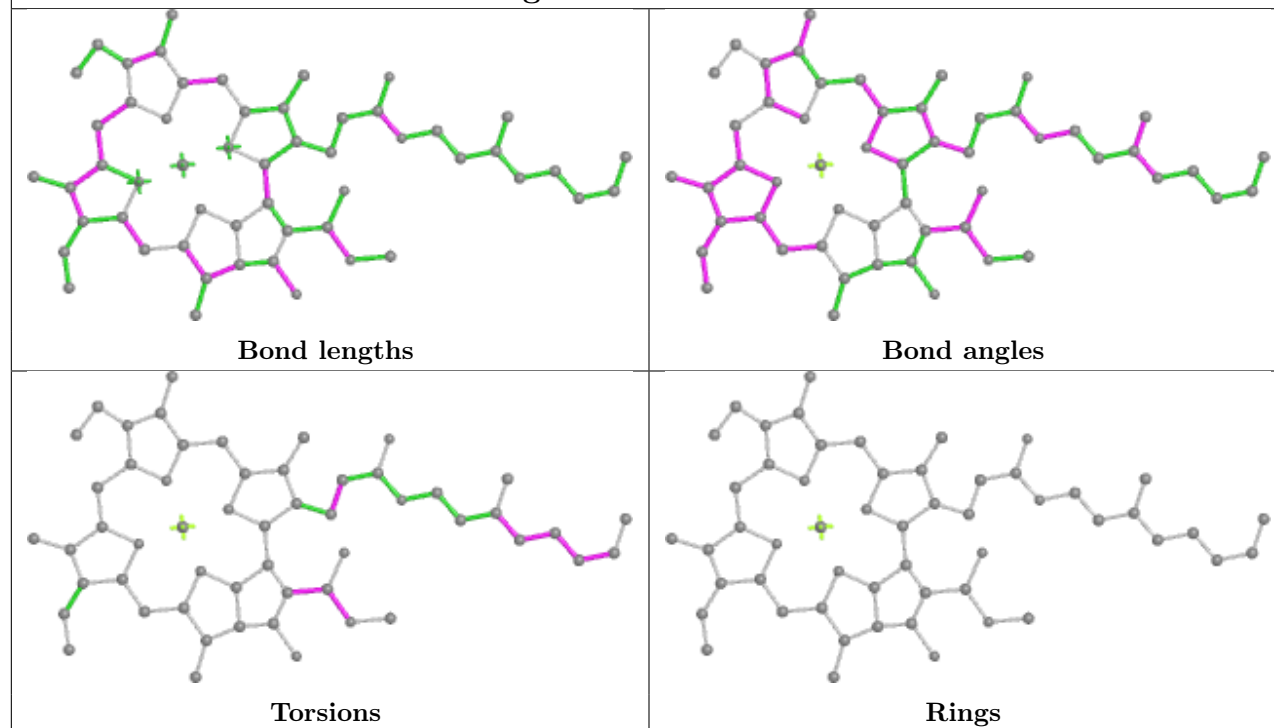
Ligand CLA aA 816

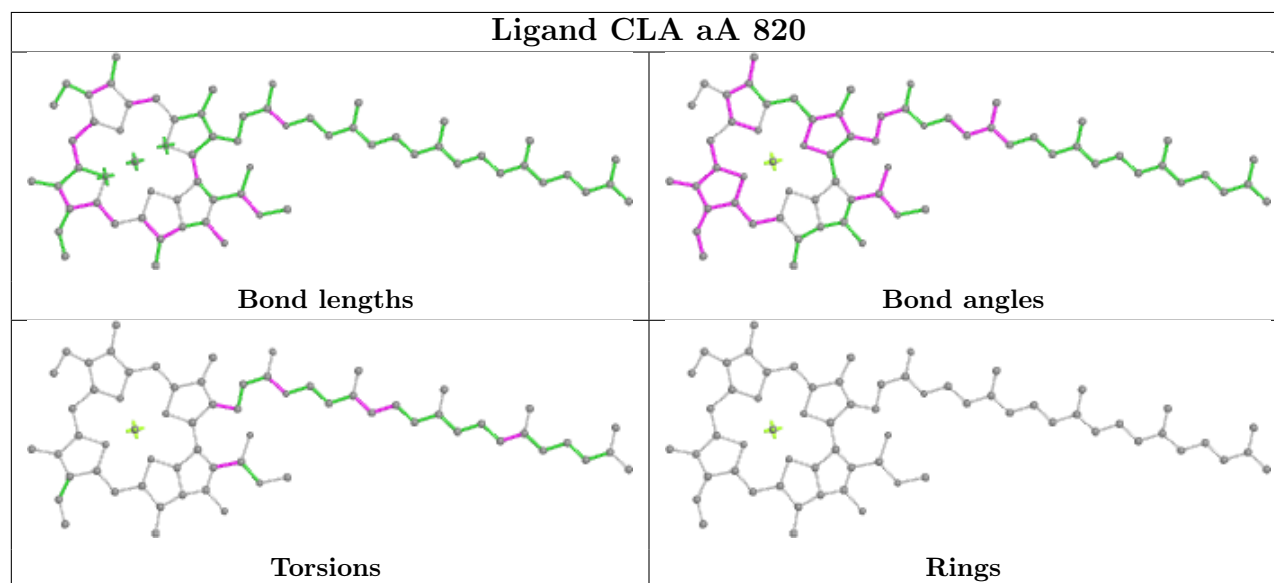
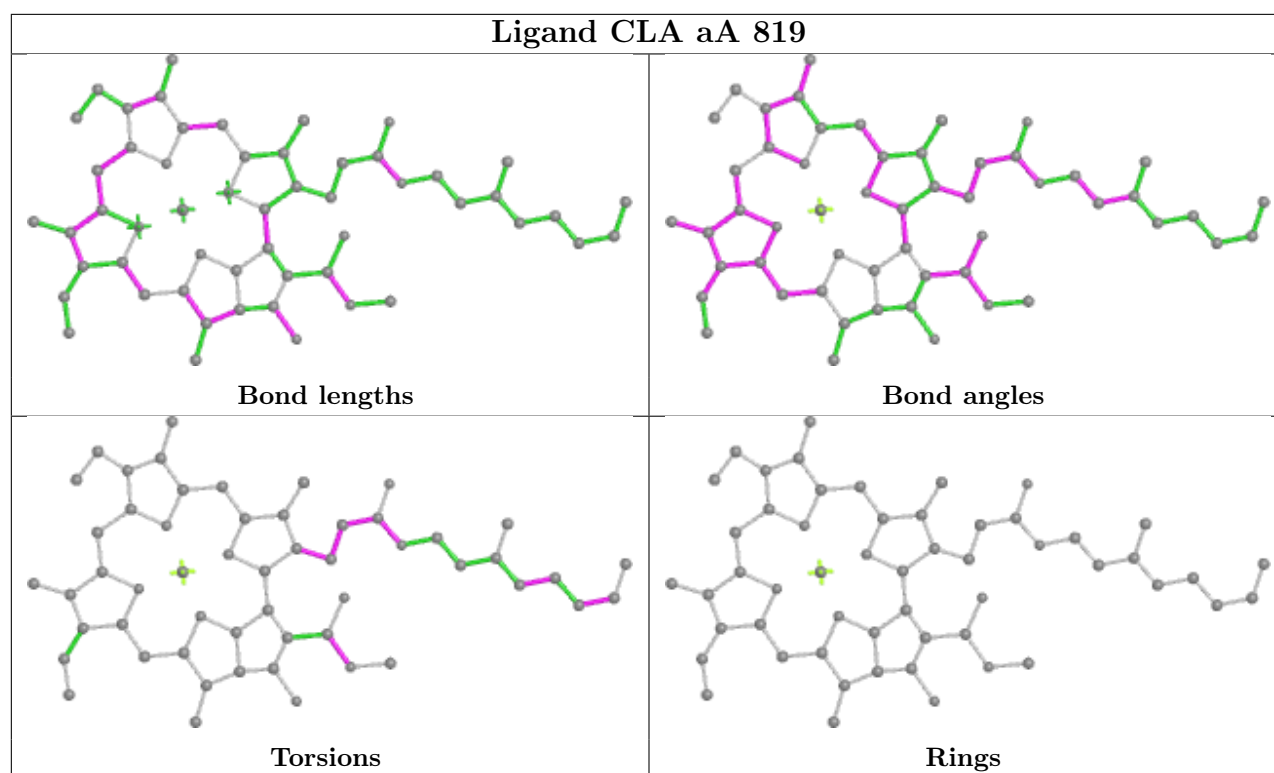


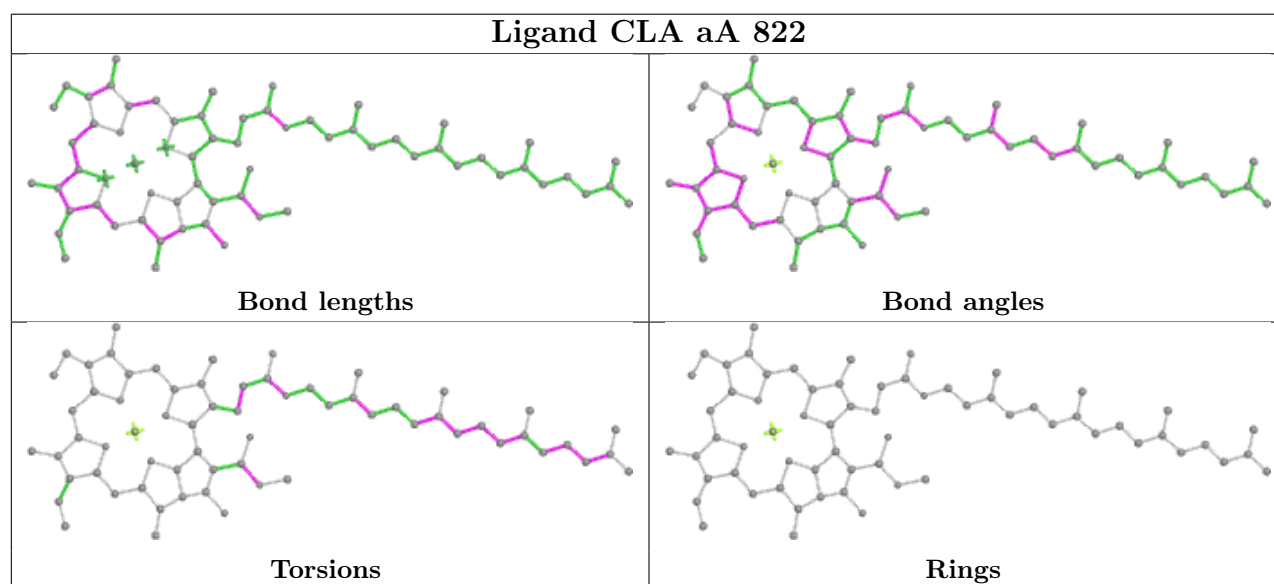
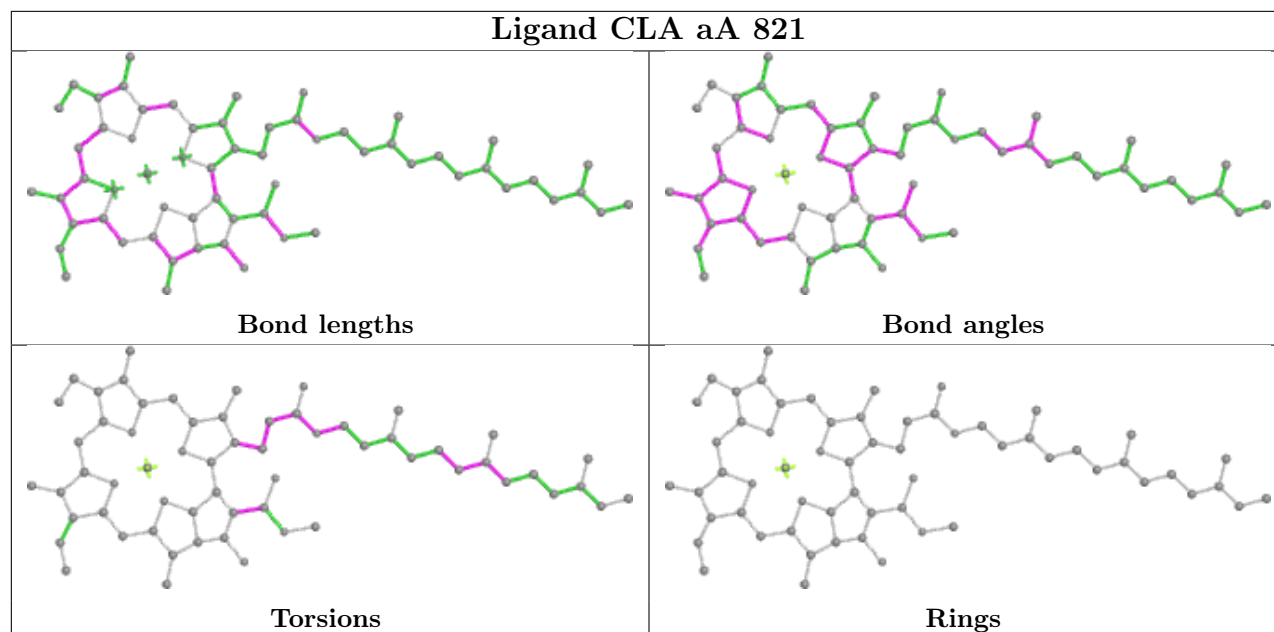
Ligand CLA aA 817



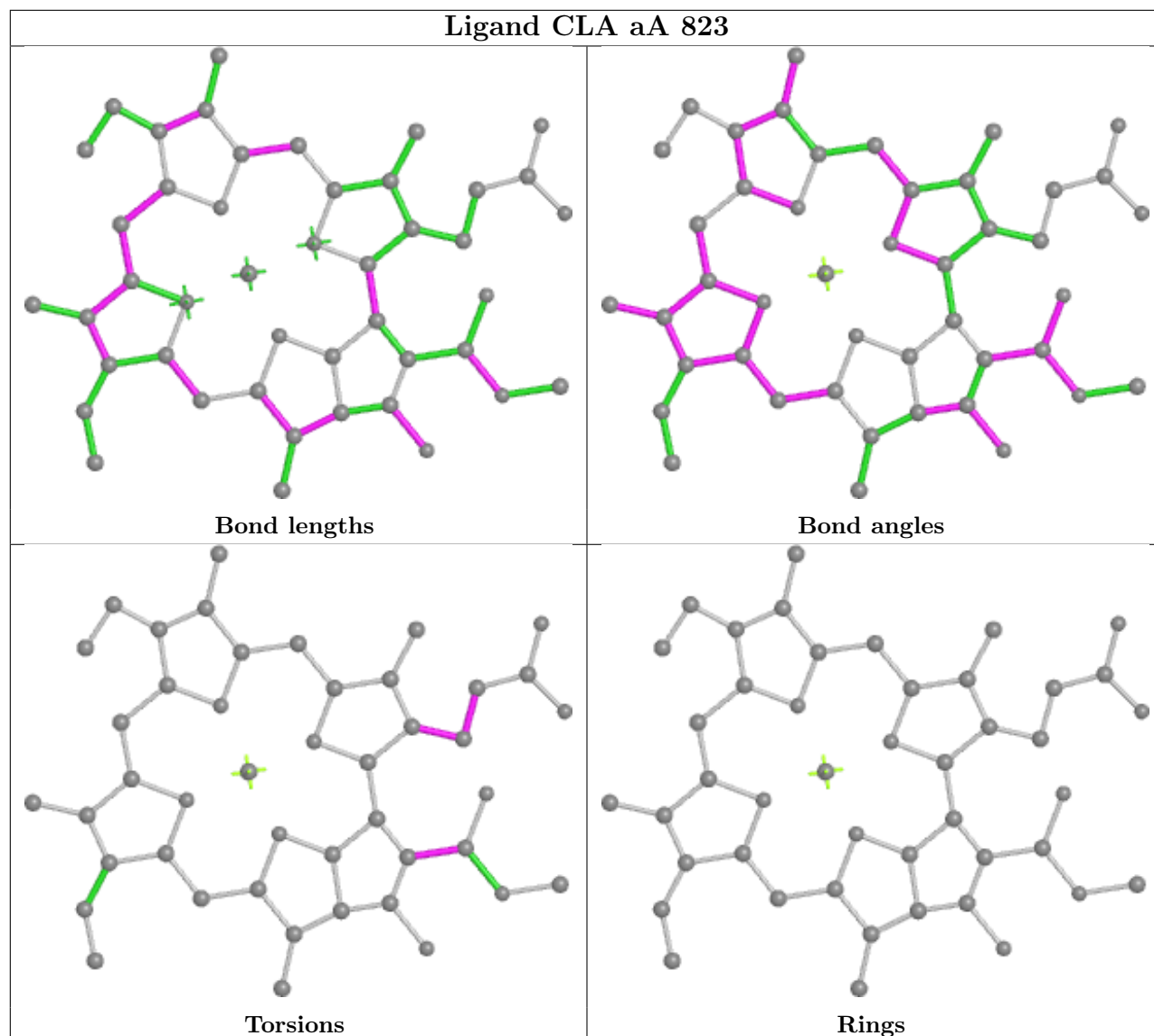
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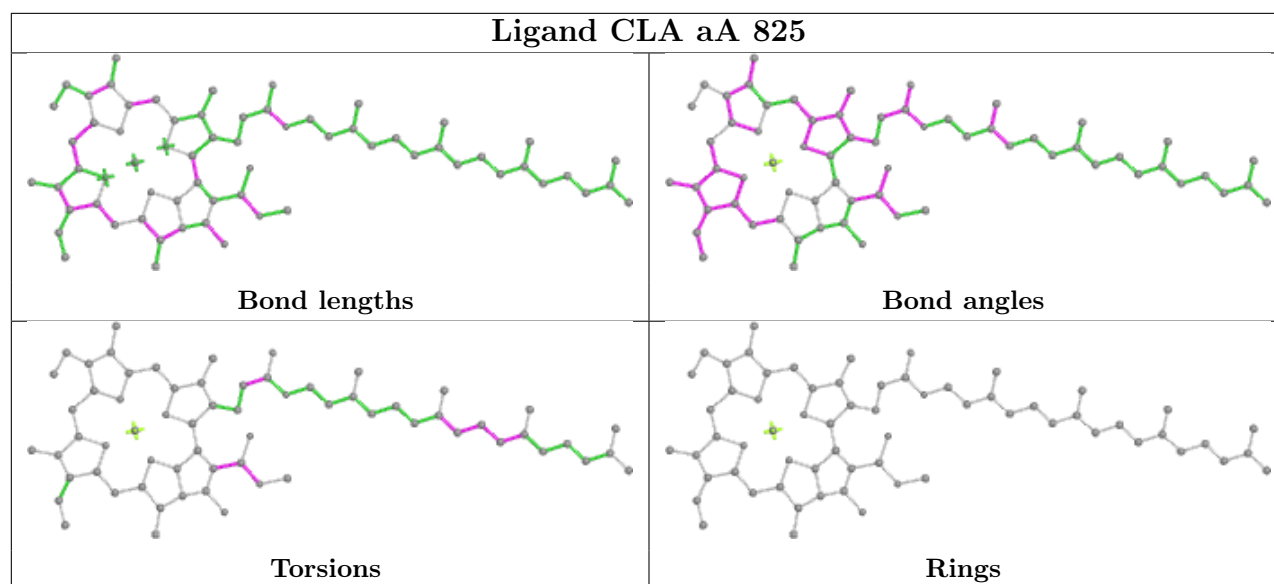
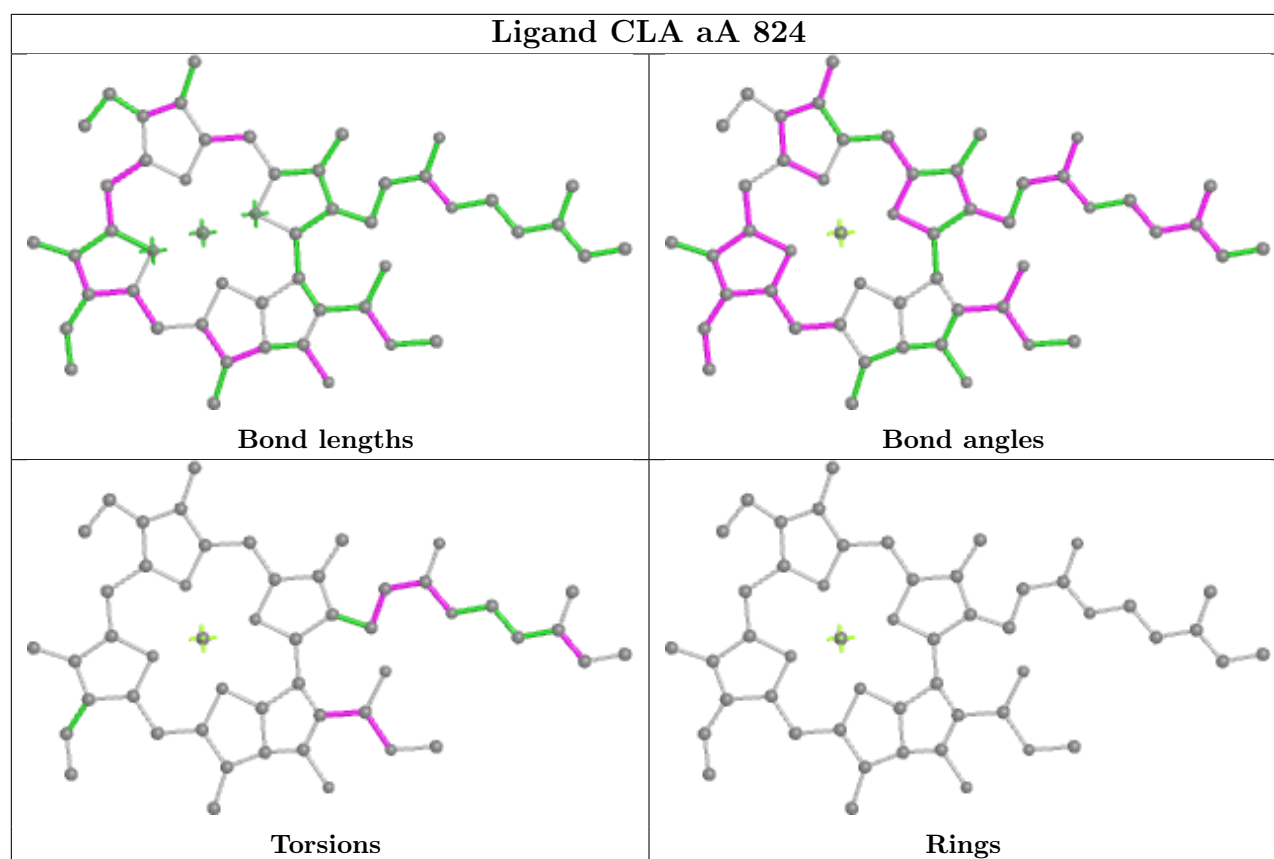


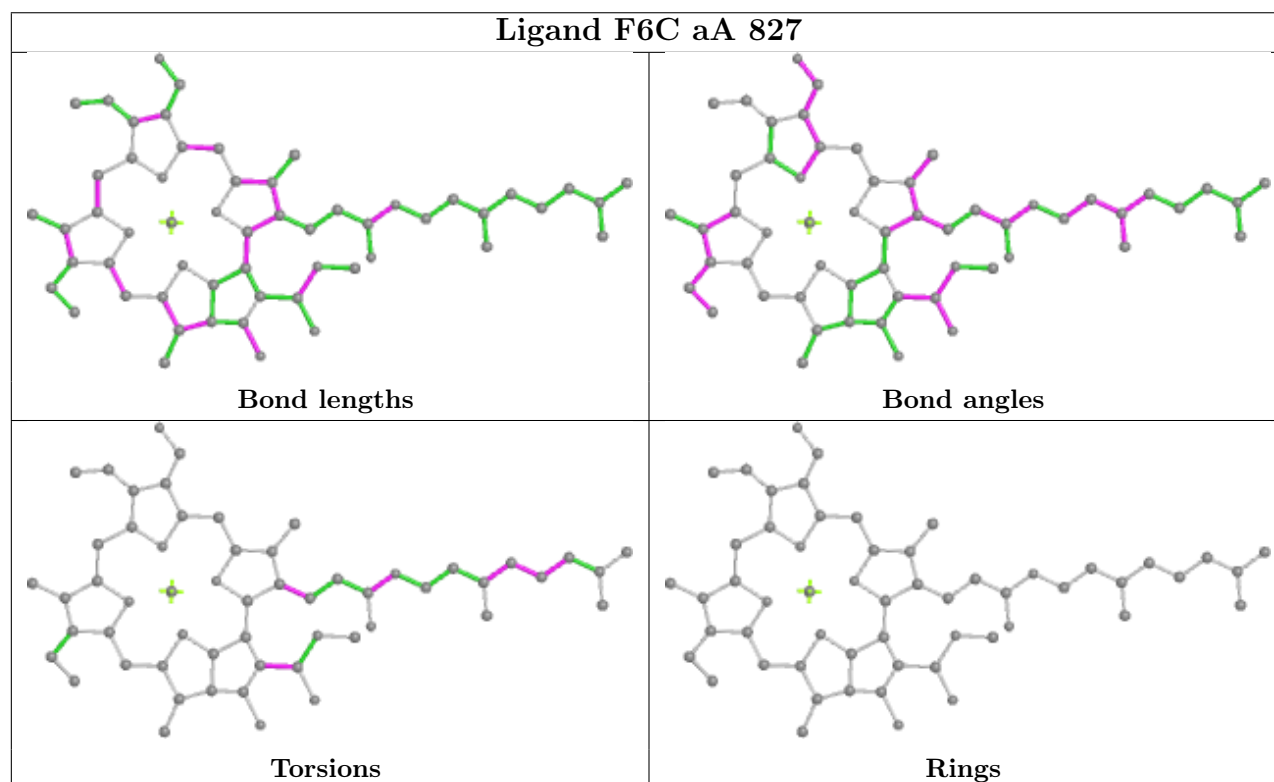
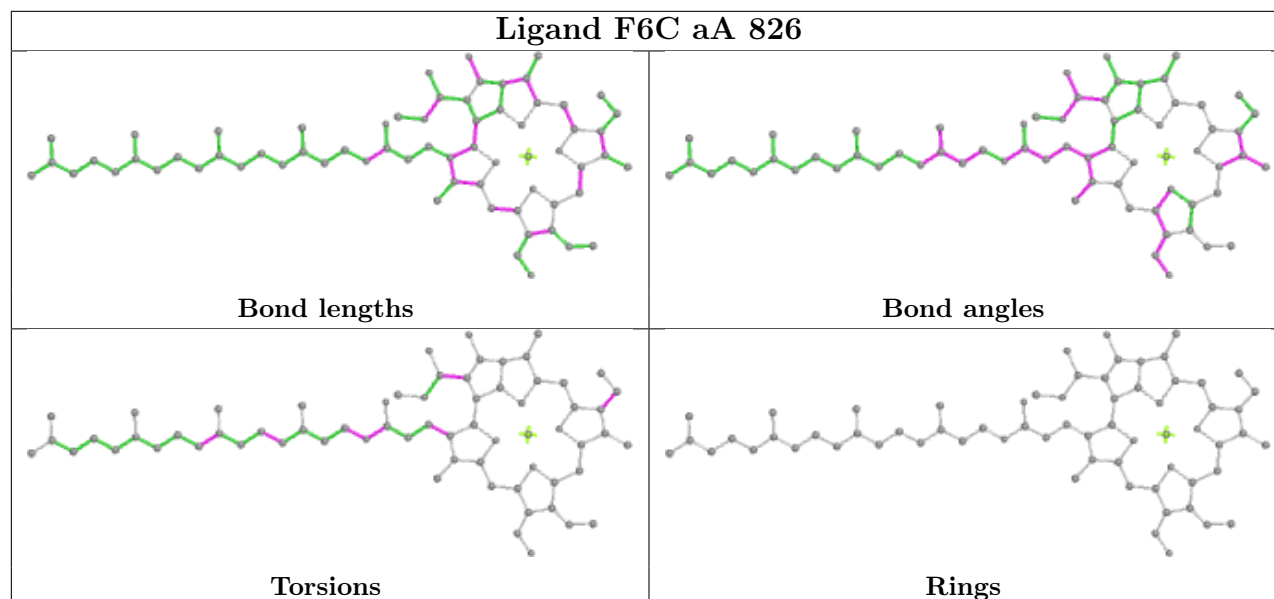




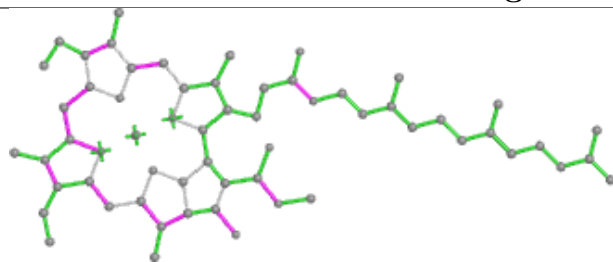
Ligand CLA aA 823



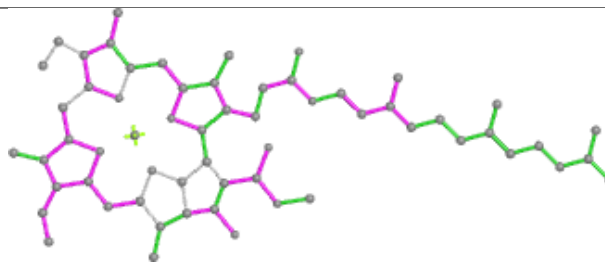




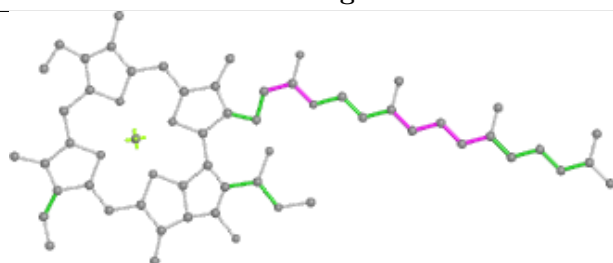
Ligand CLA aA 828



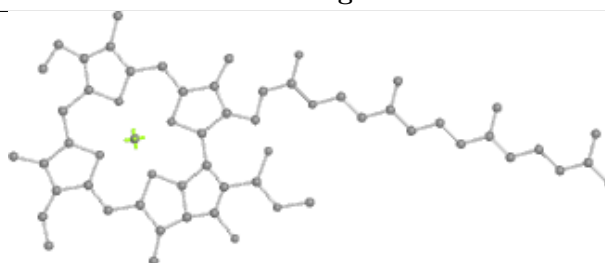
Bond lengths



Bond angles

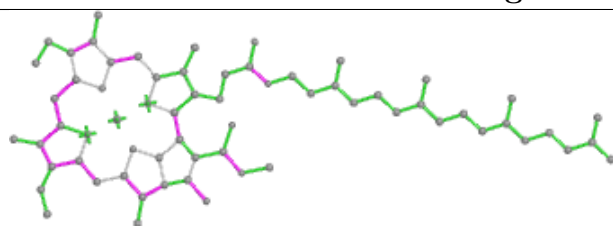


Torsions

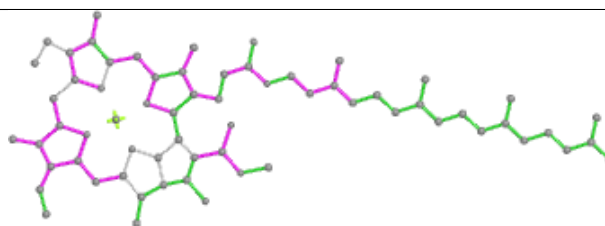


Rings

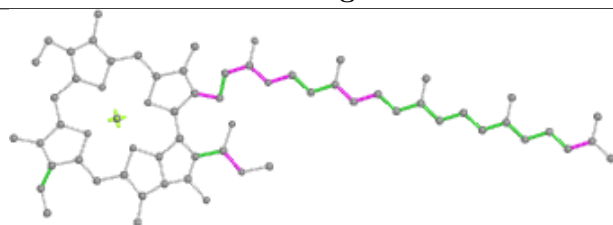
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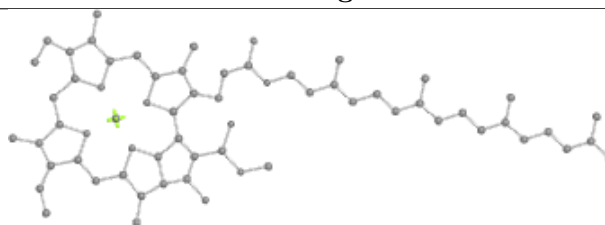
Bond lengths



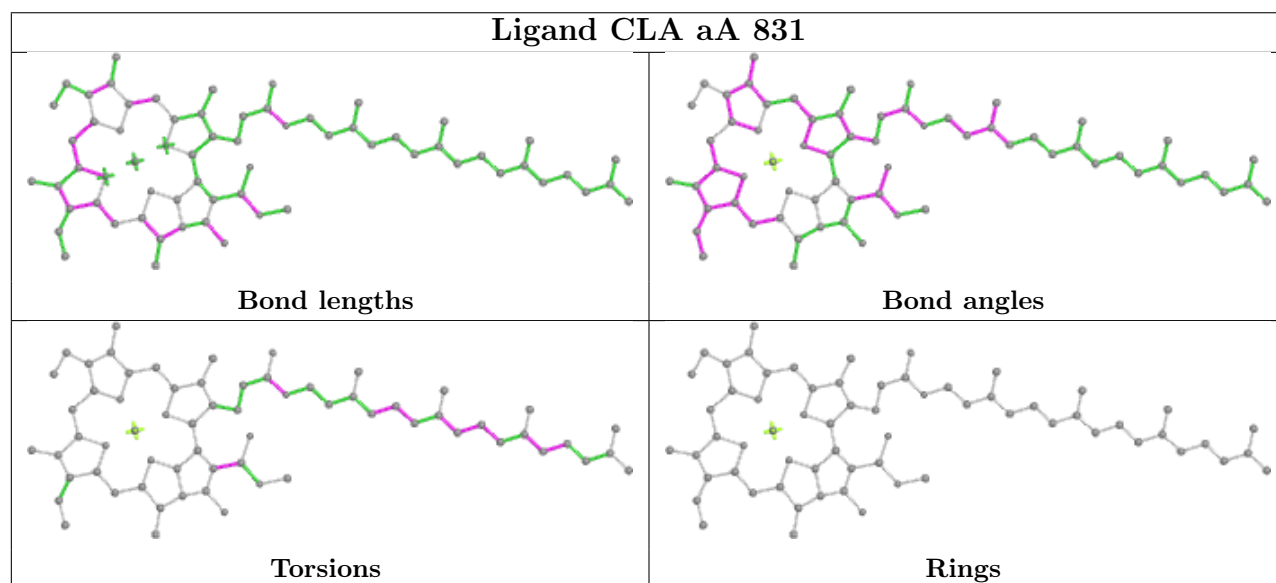
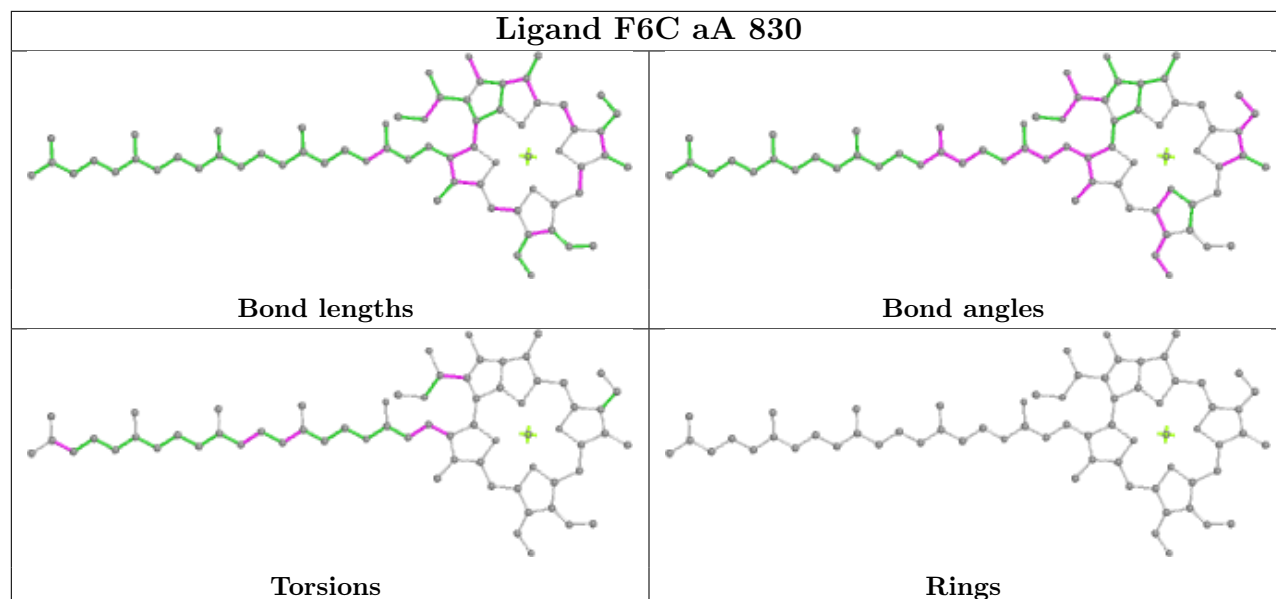
Bond angles

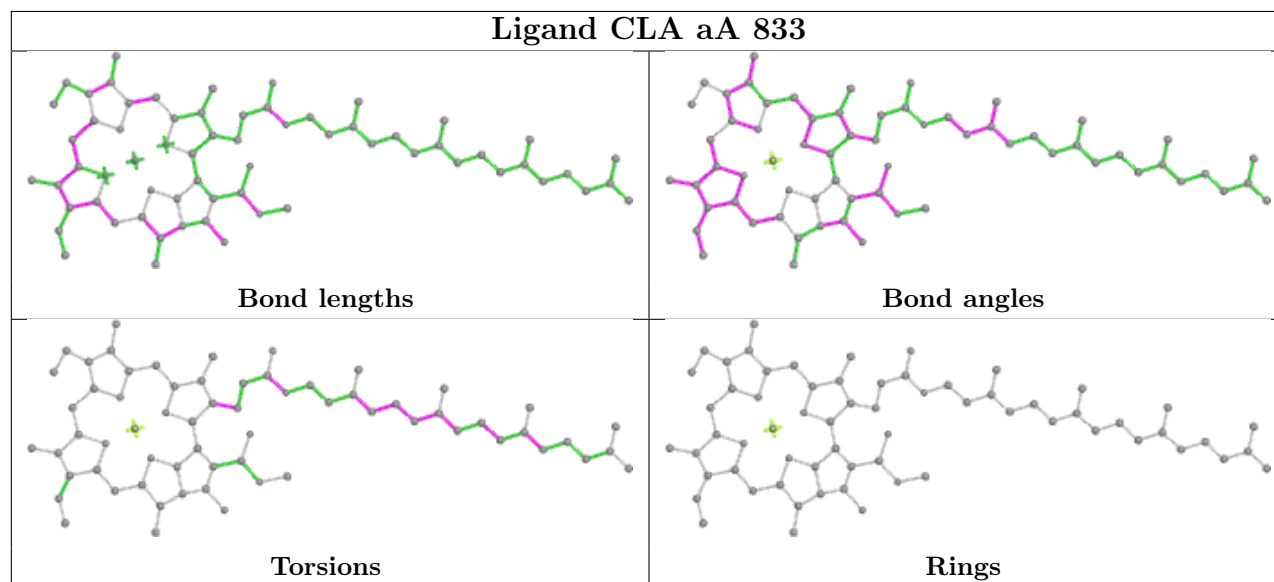
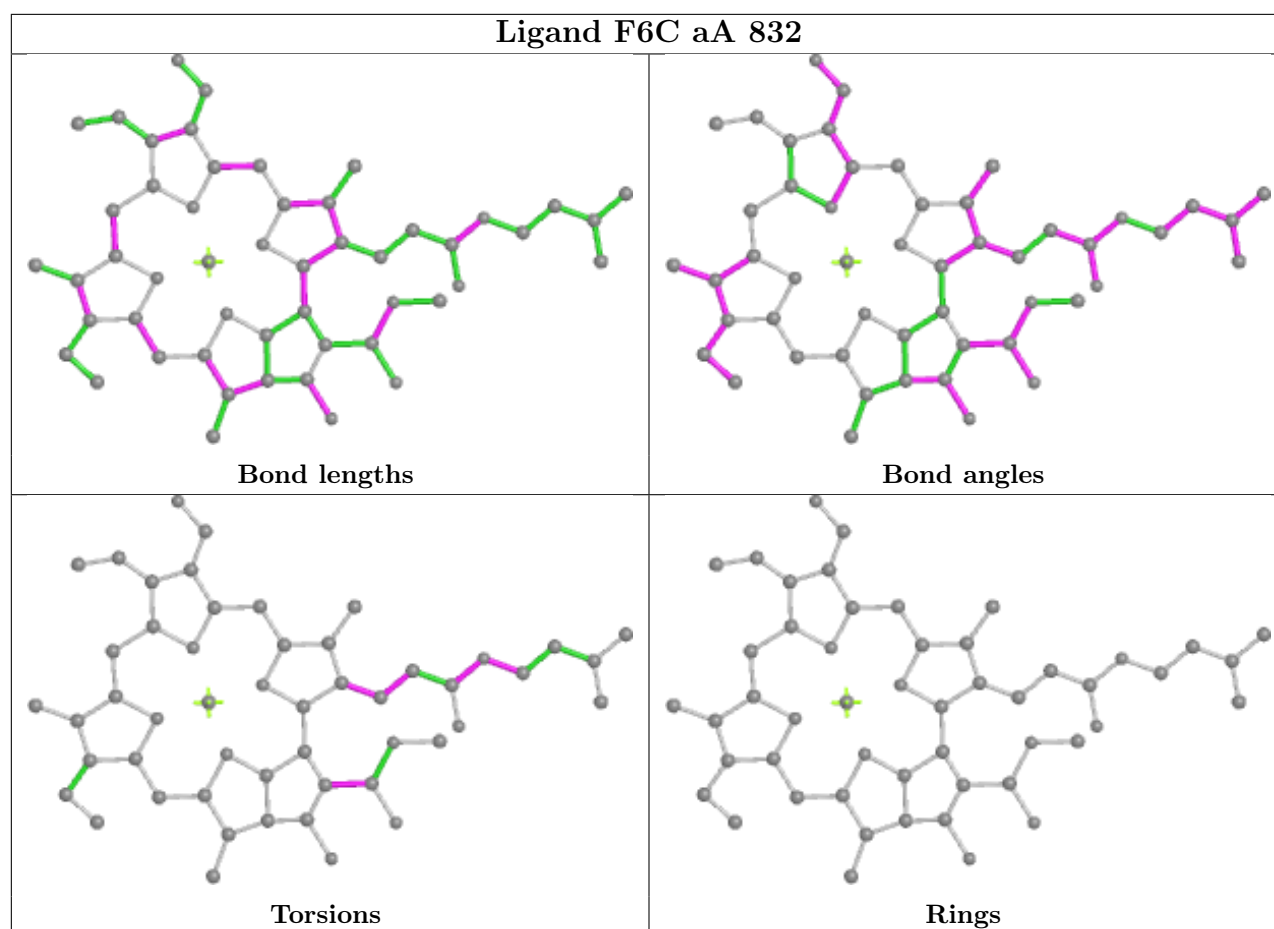


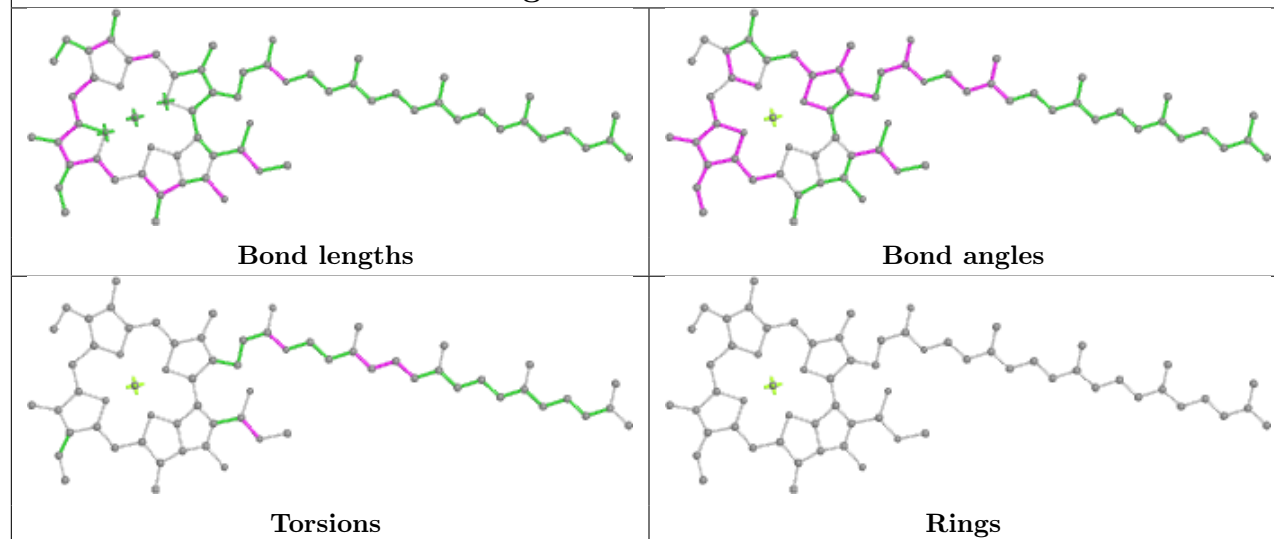
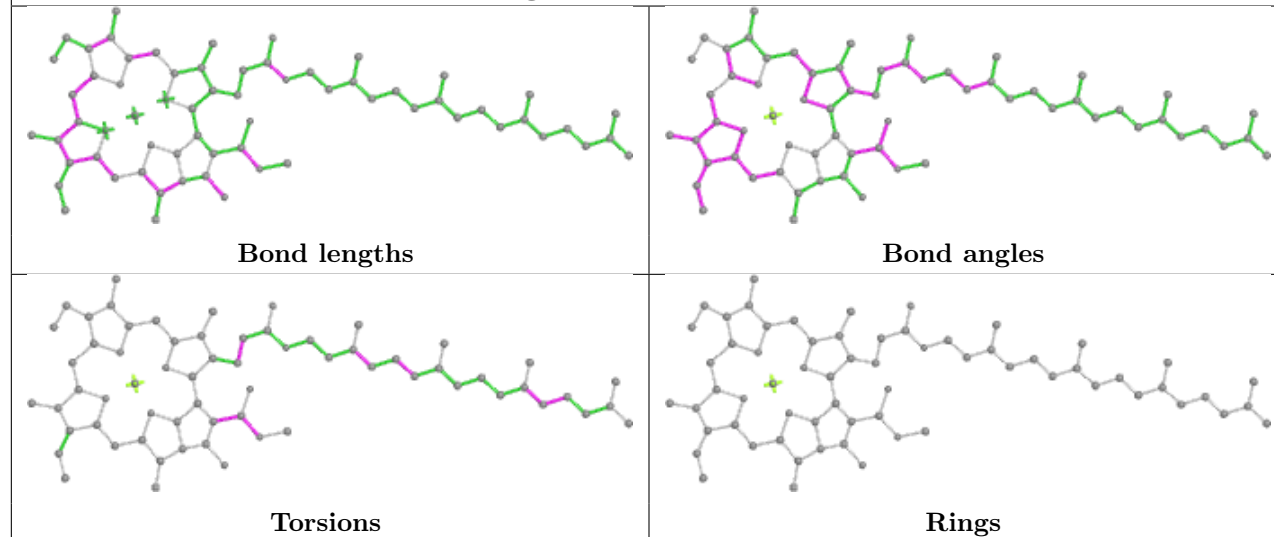
Torsions



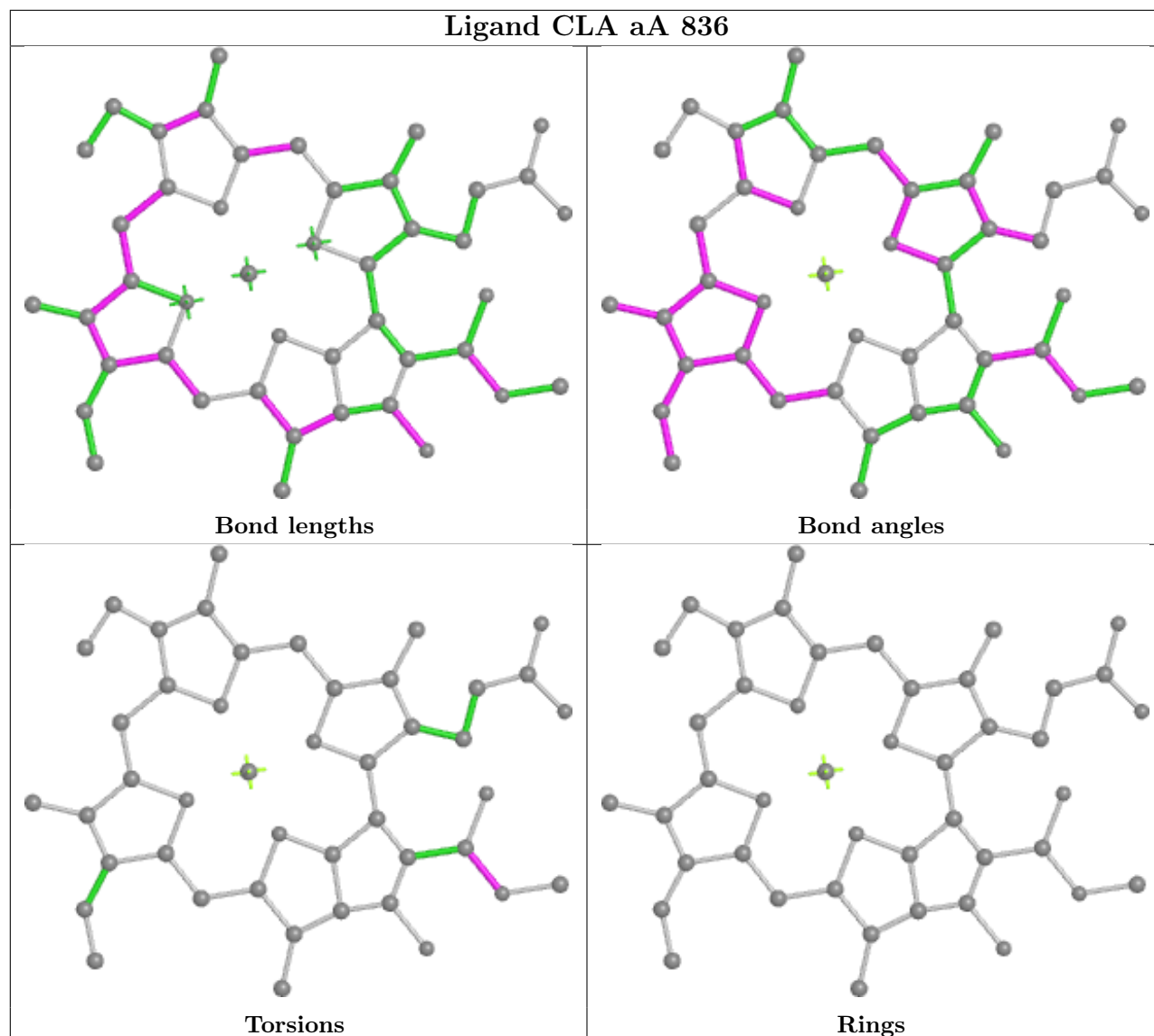
Rings



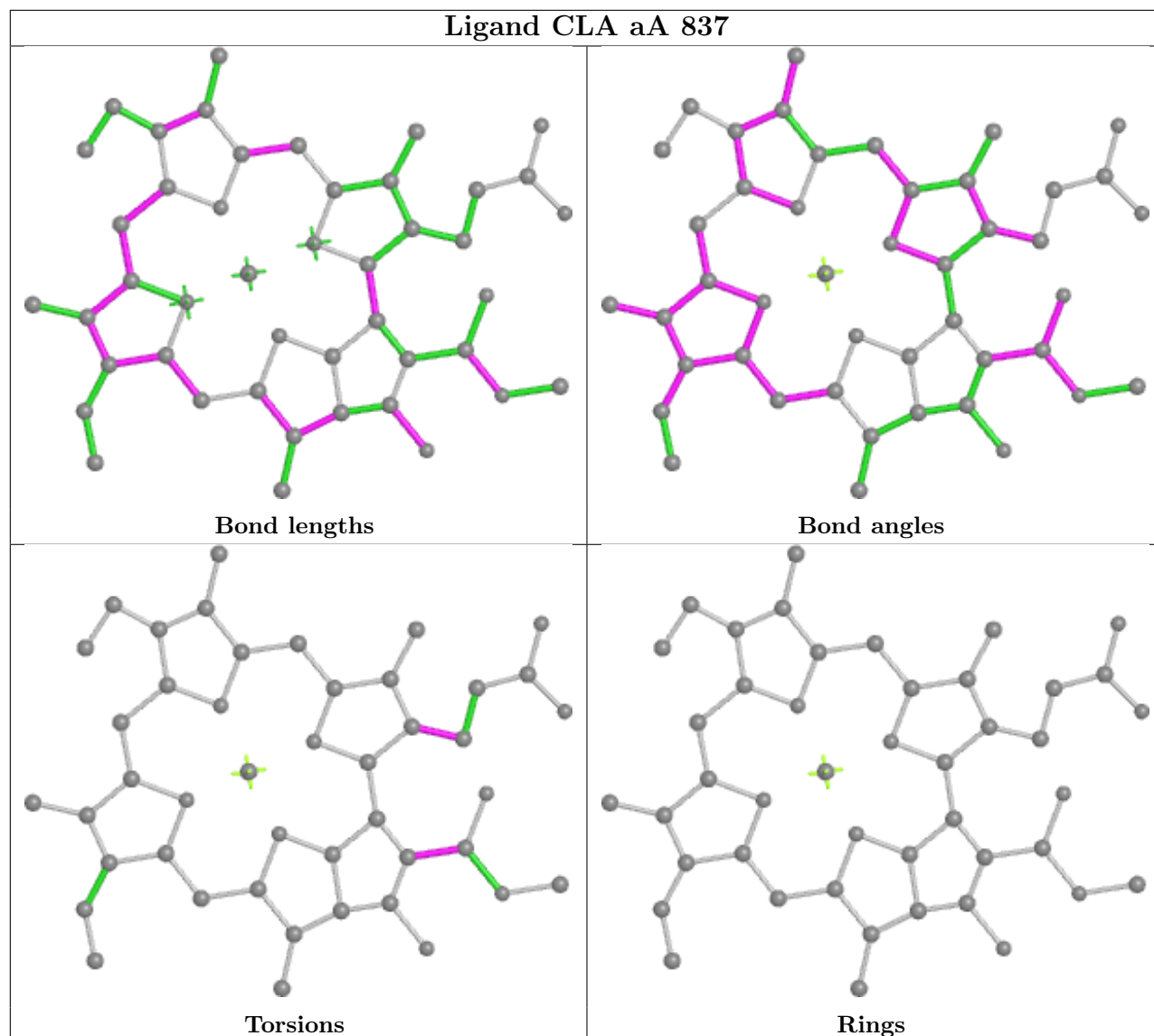


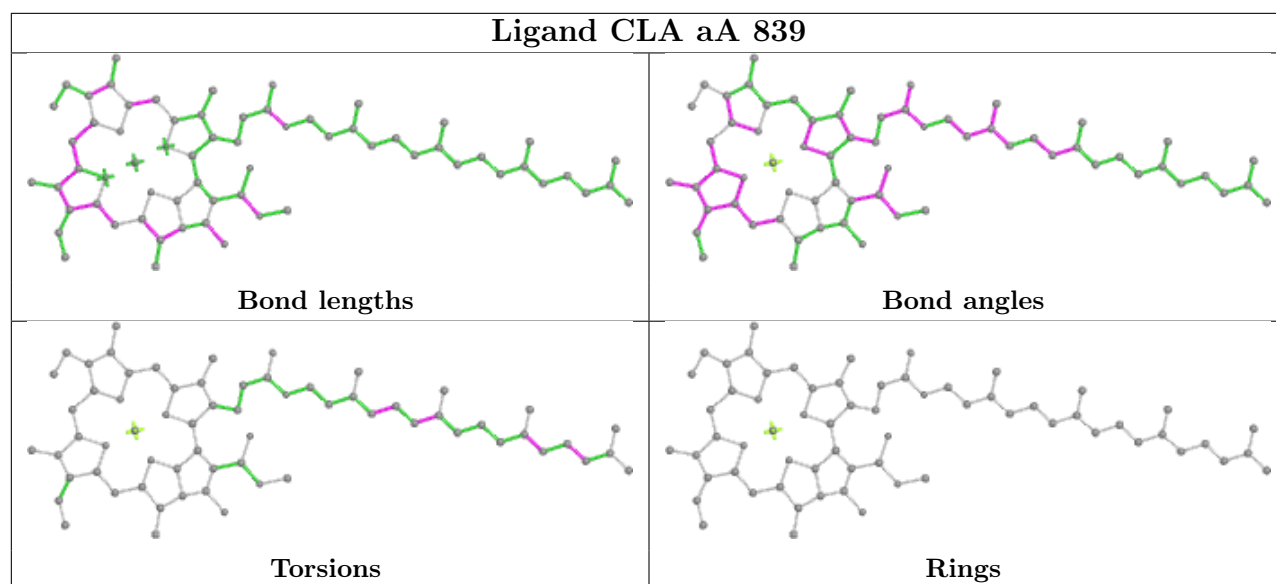
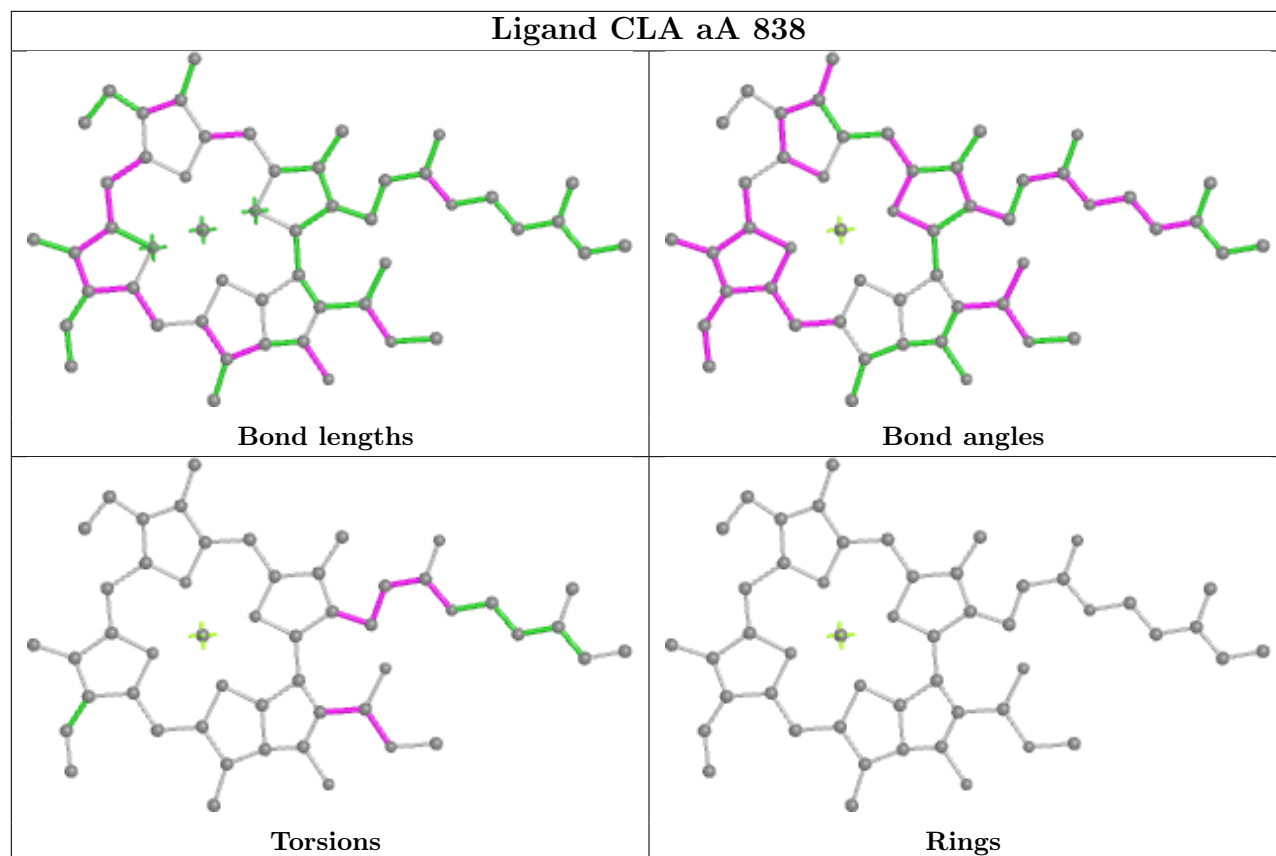
Ligand CLA aA 834**Ligand CLA aA 835**

Ligand CLA aA 836

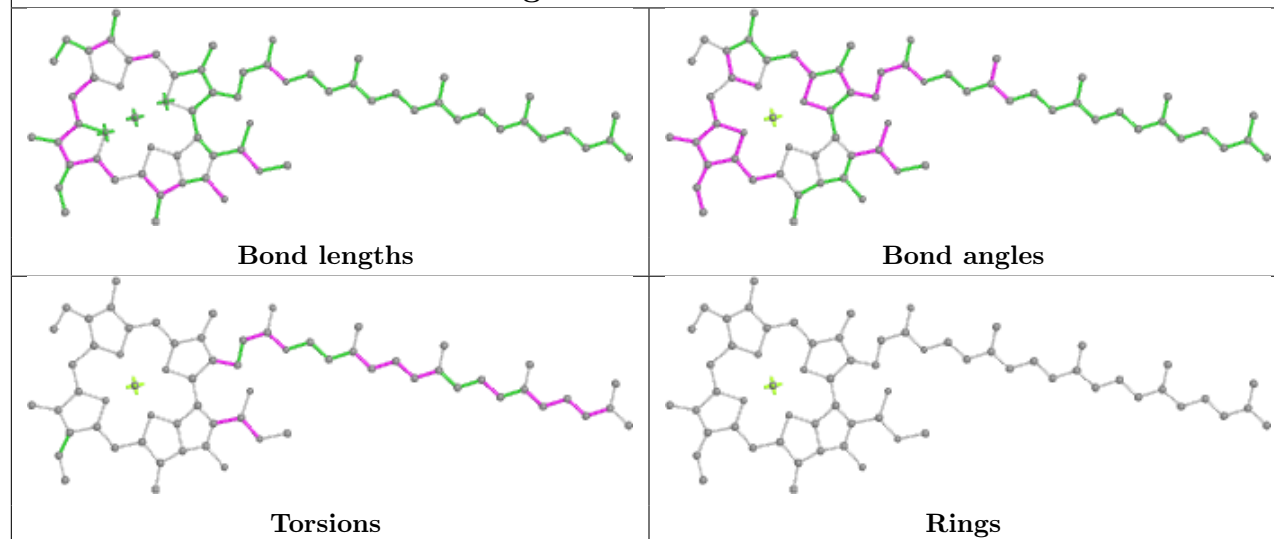


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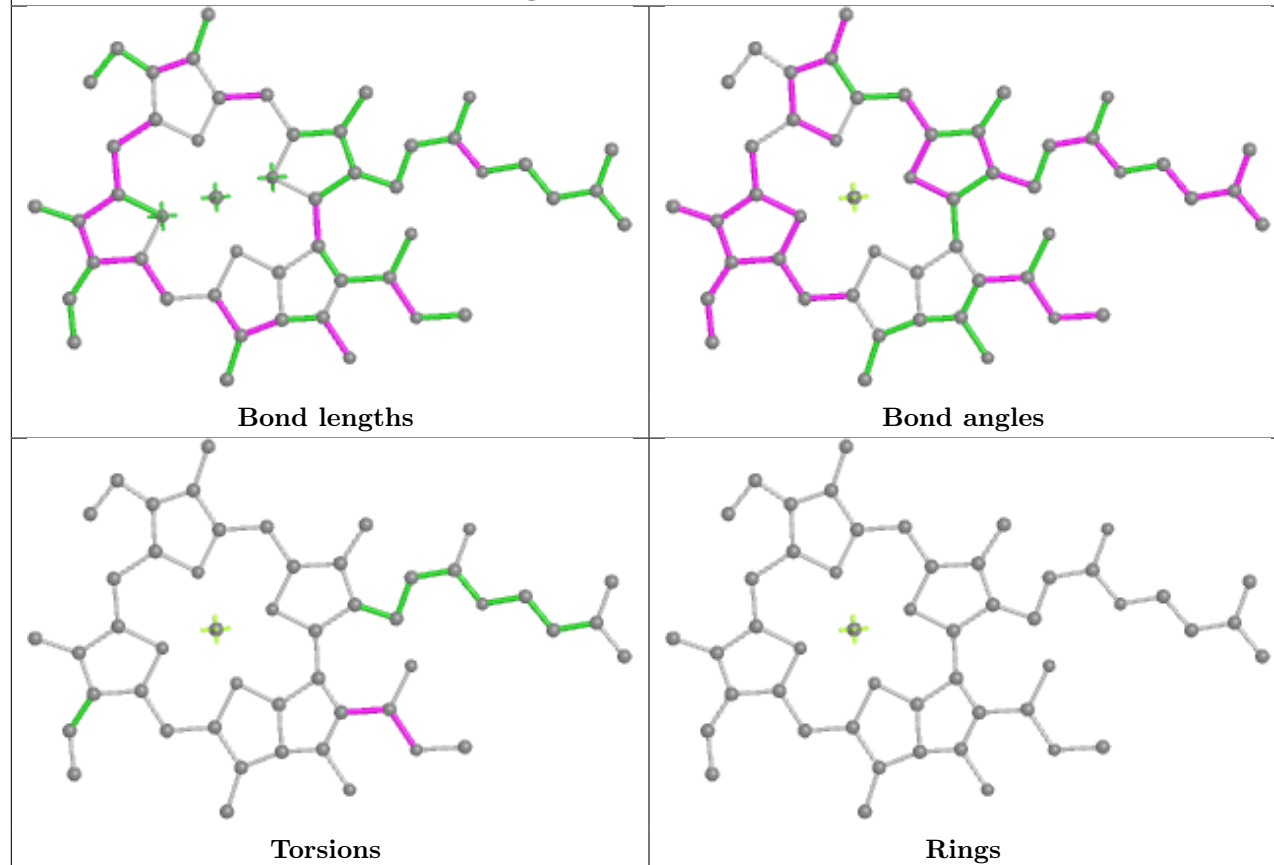




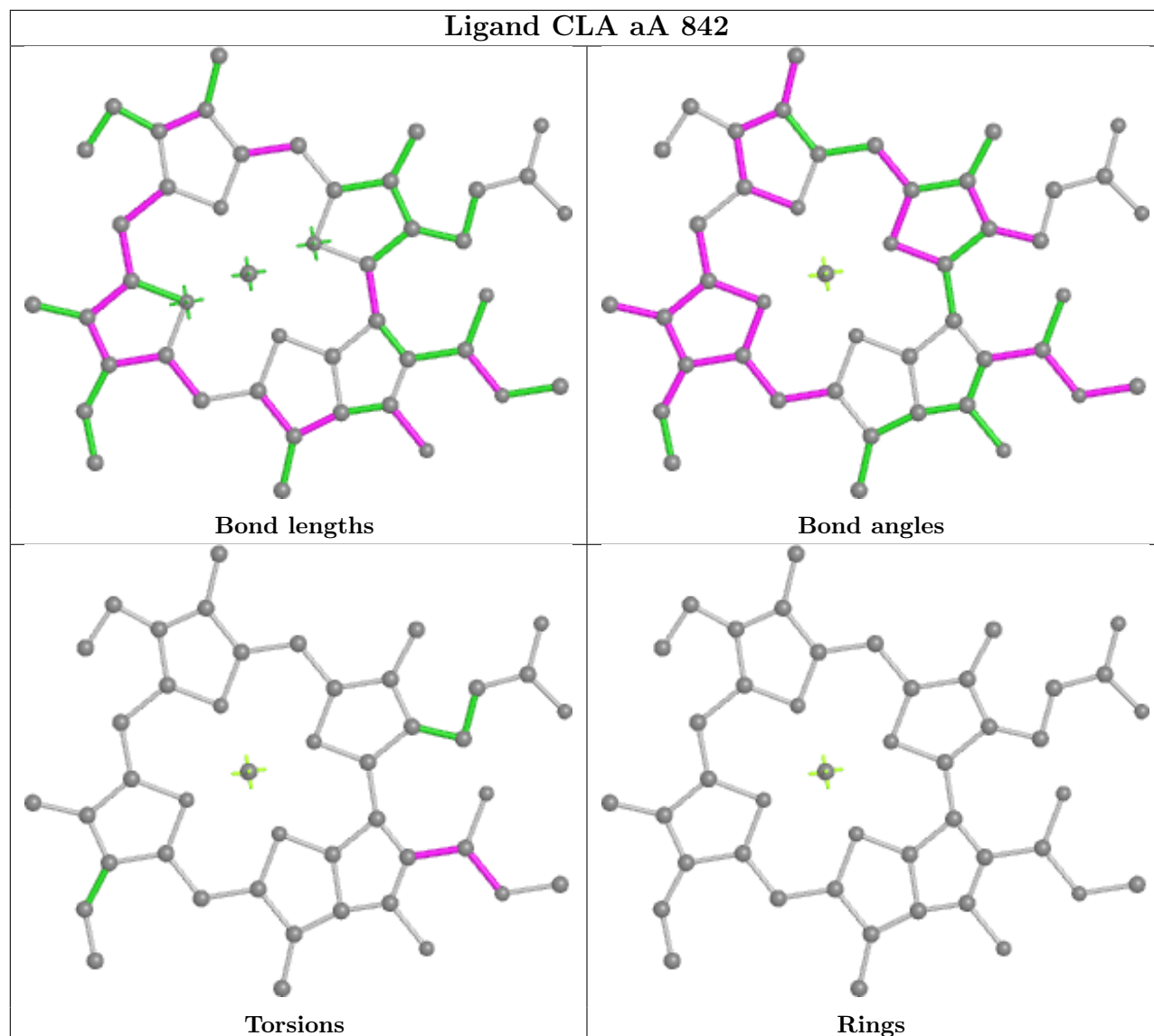
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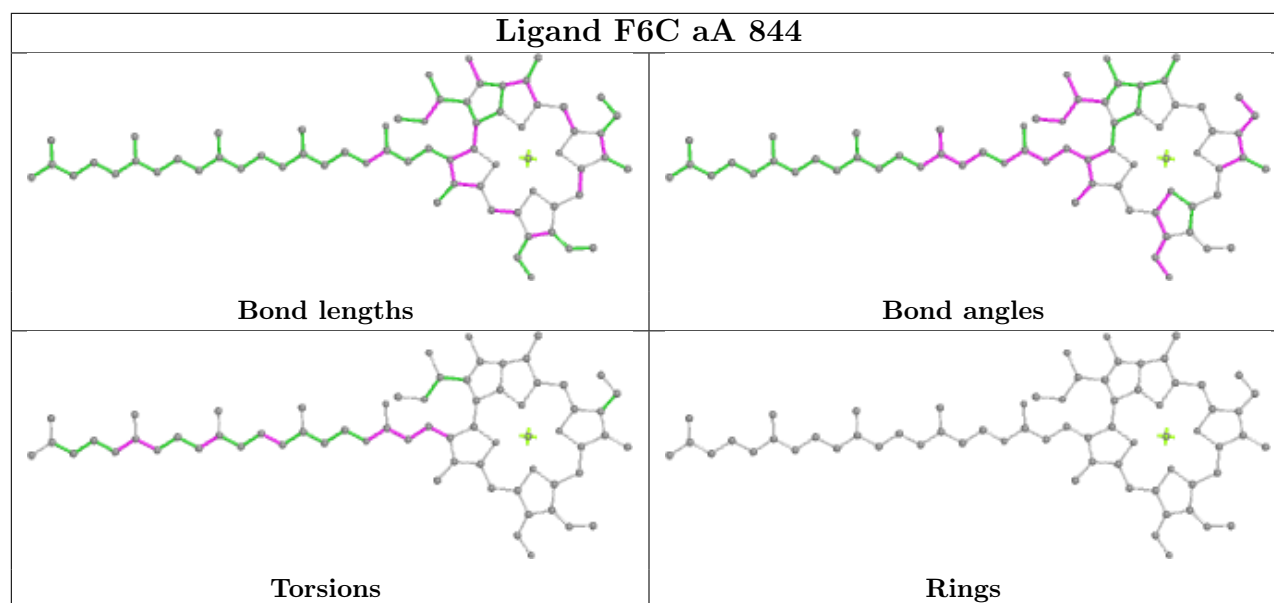
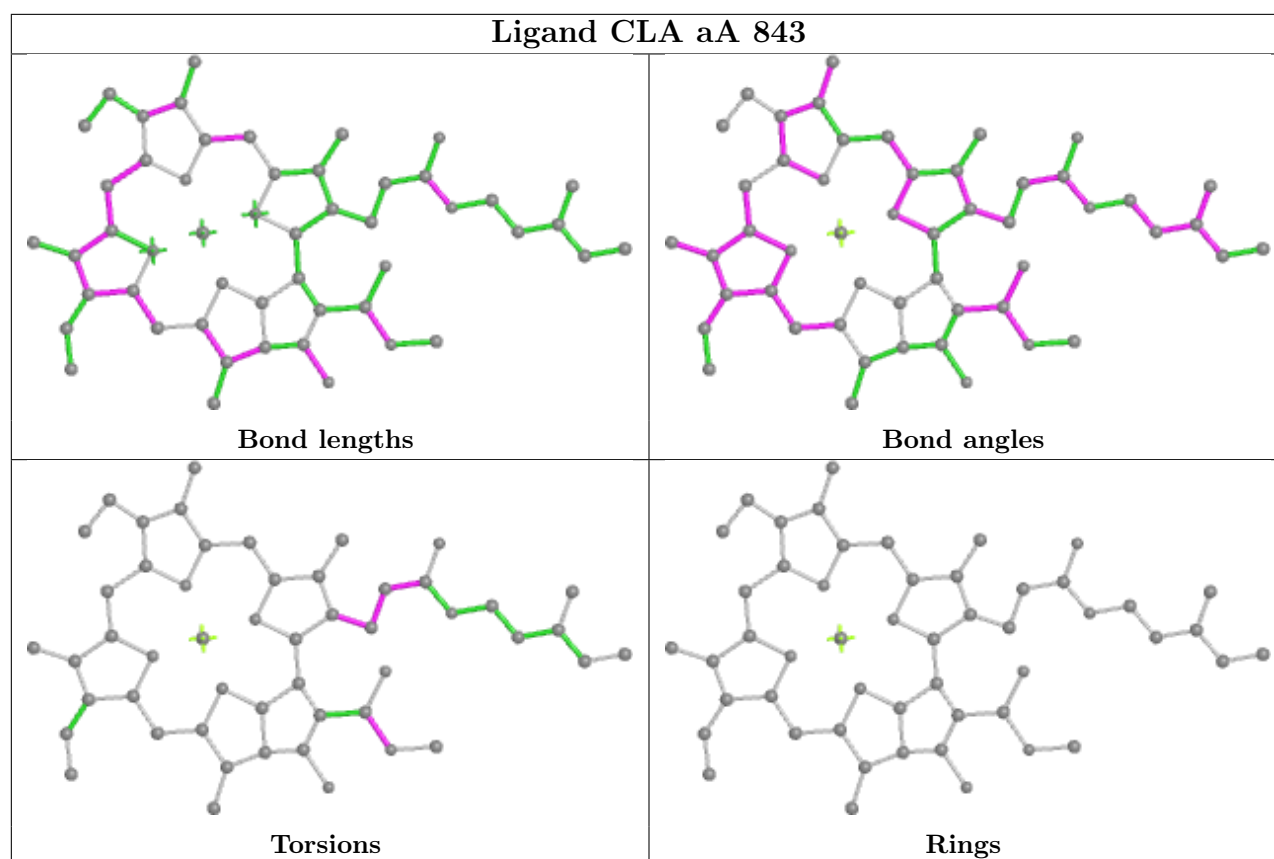


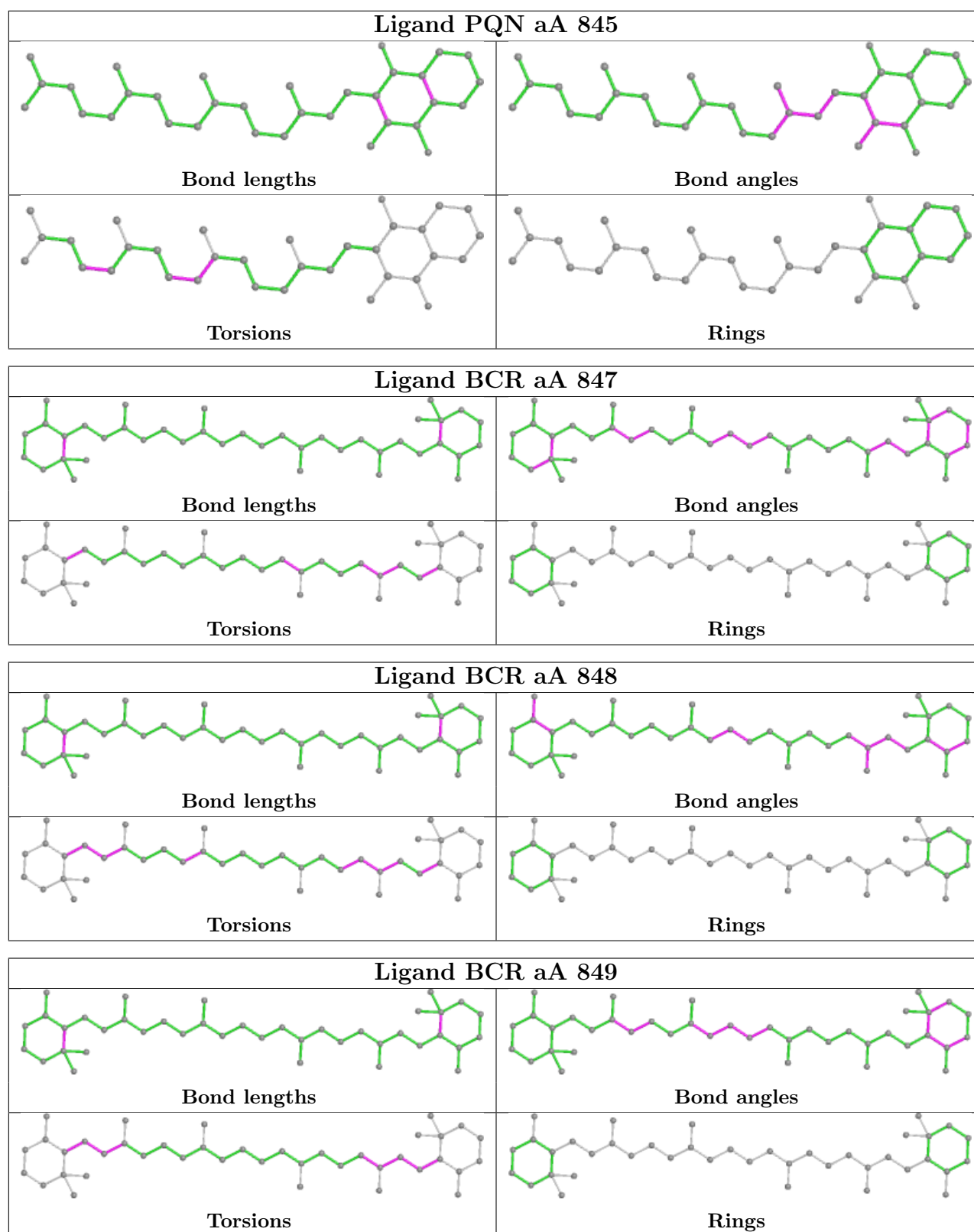
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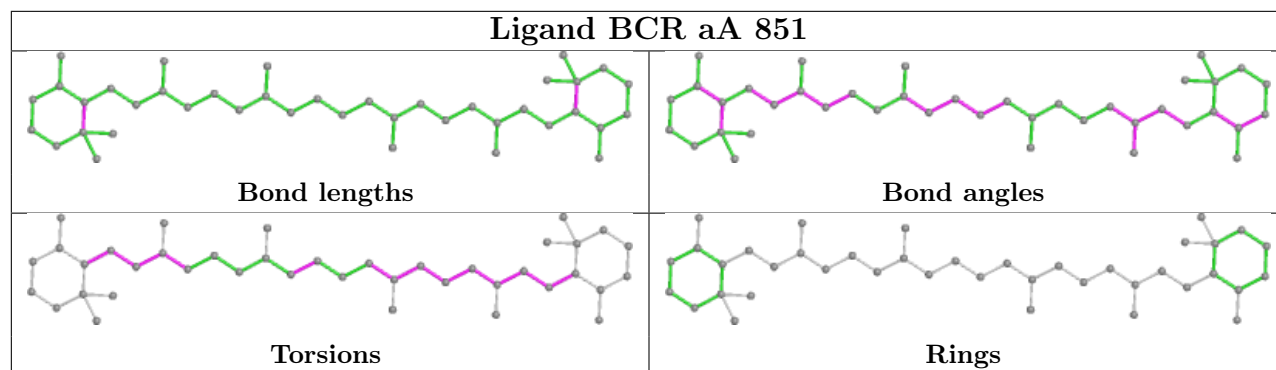
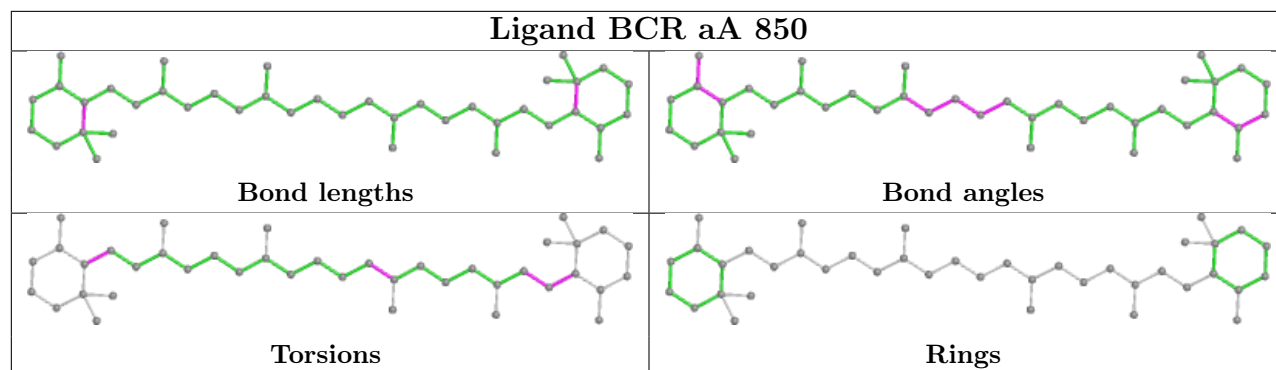


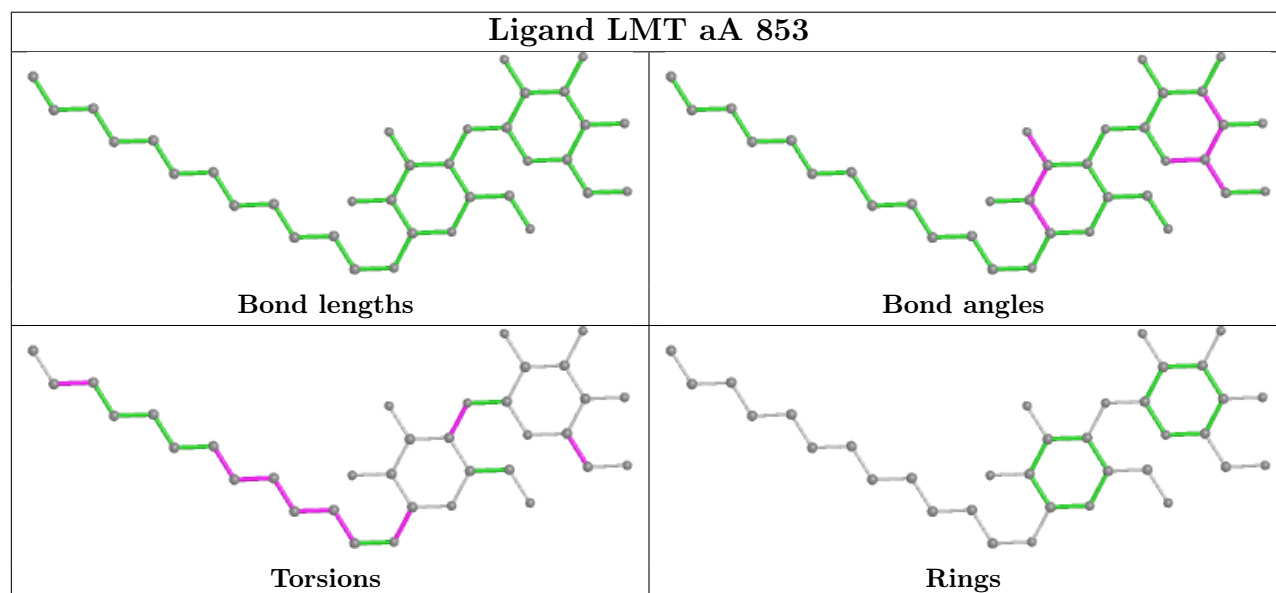
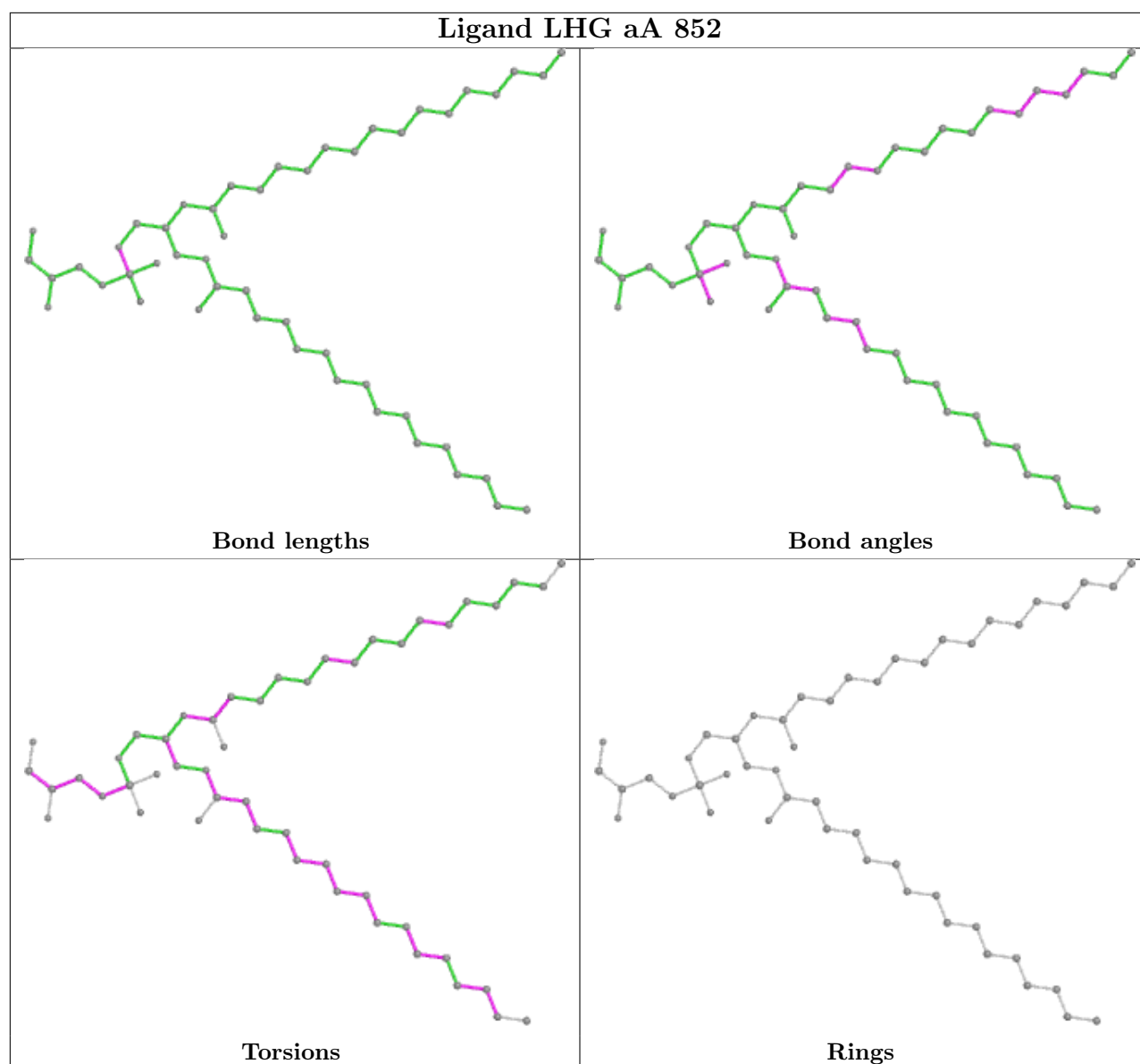
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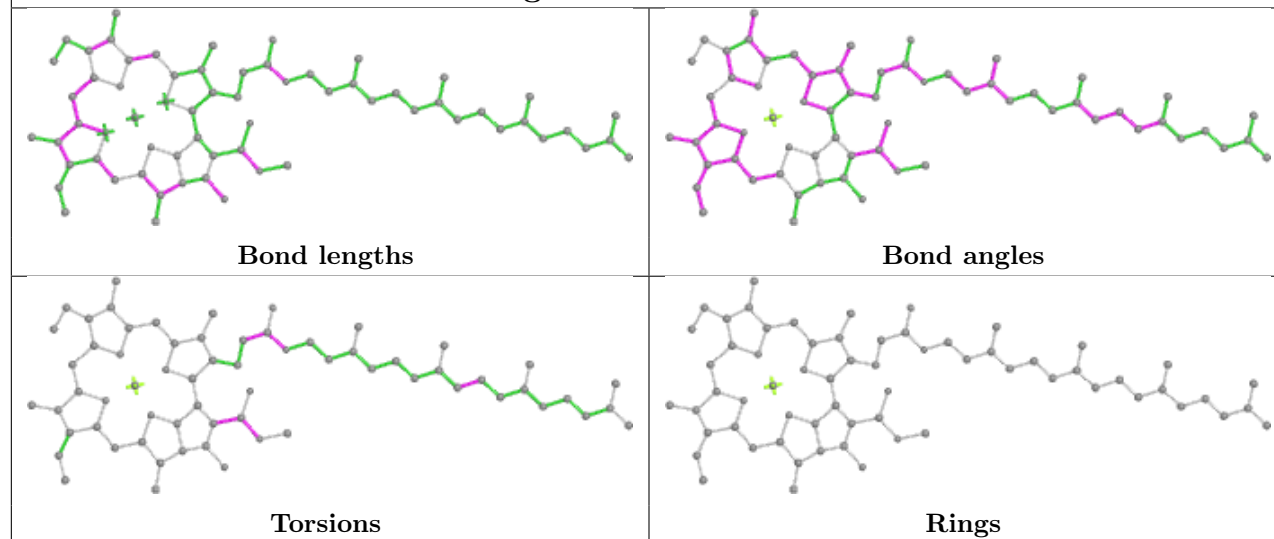




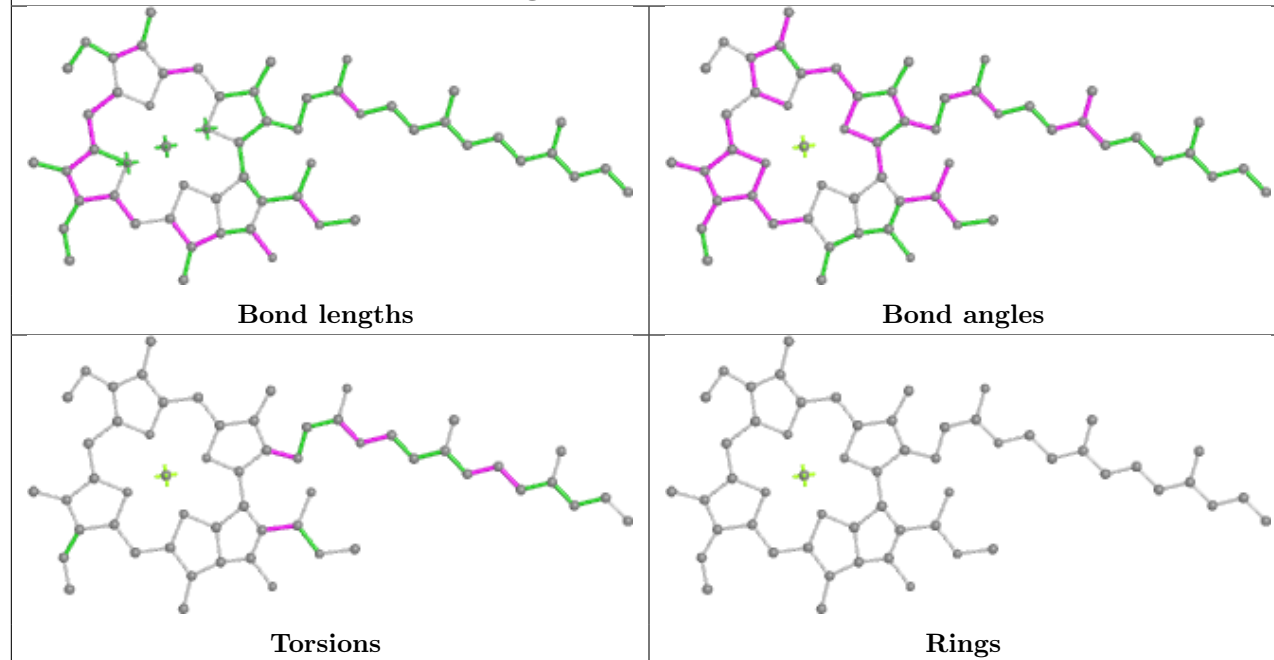


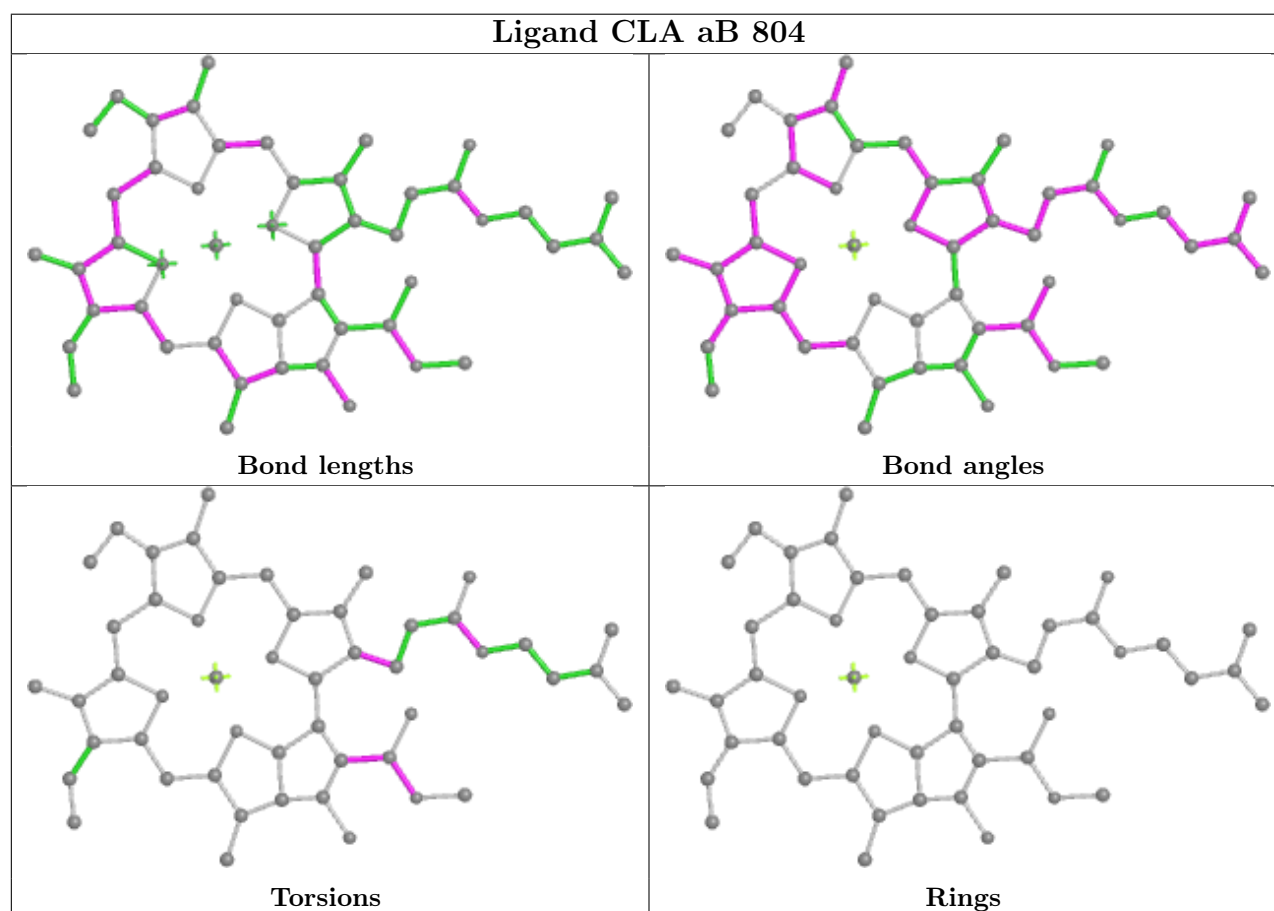
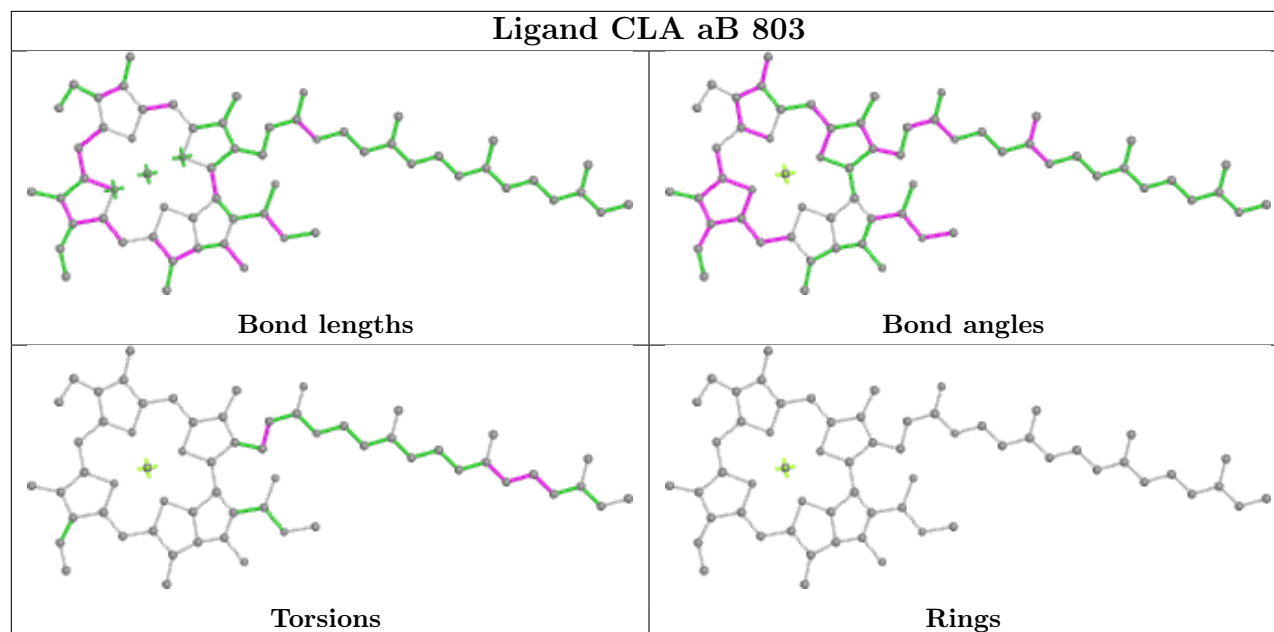


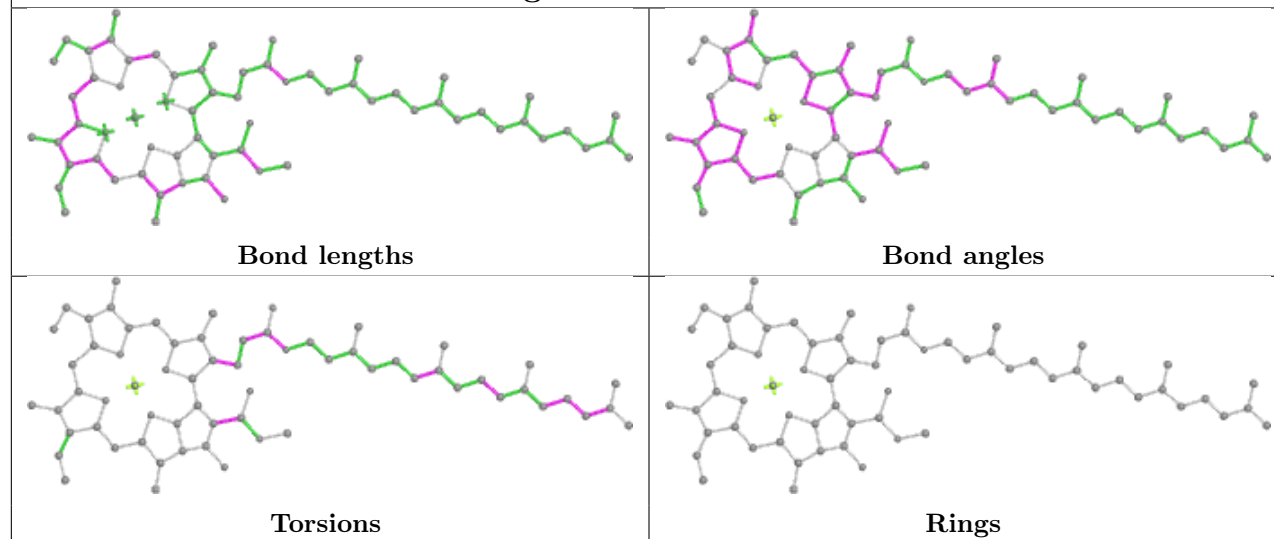
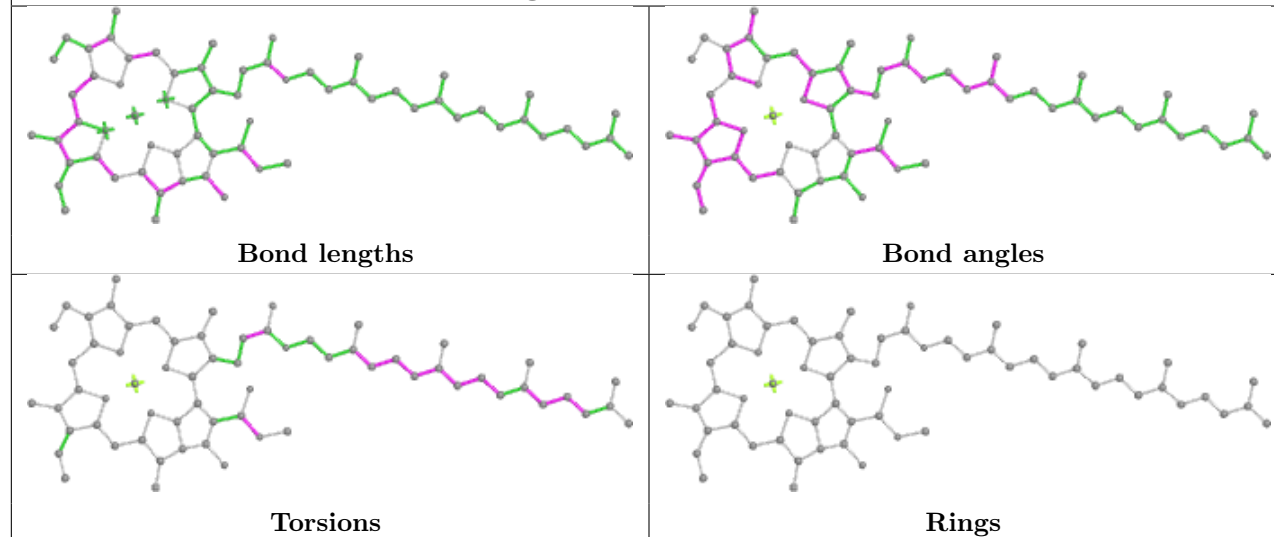
Ligand CLA aB 801

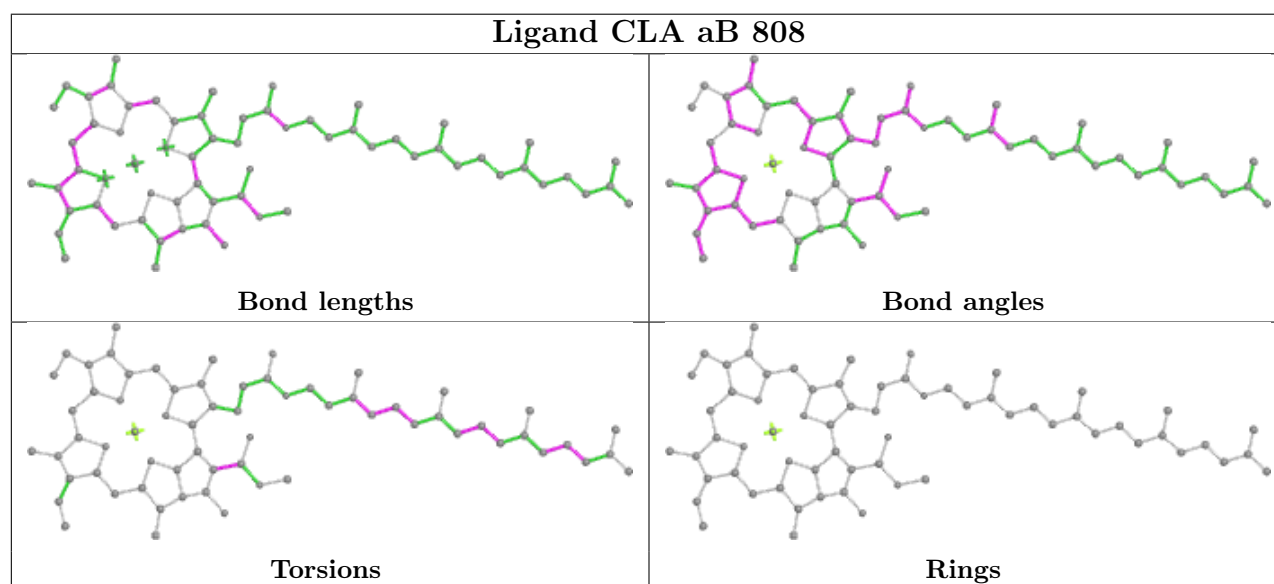
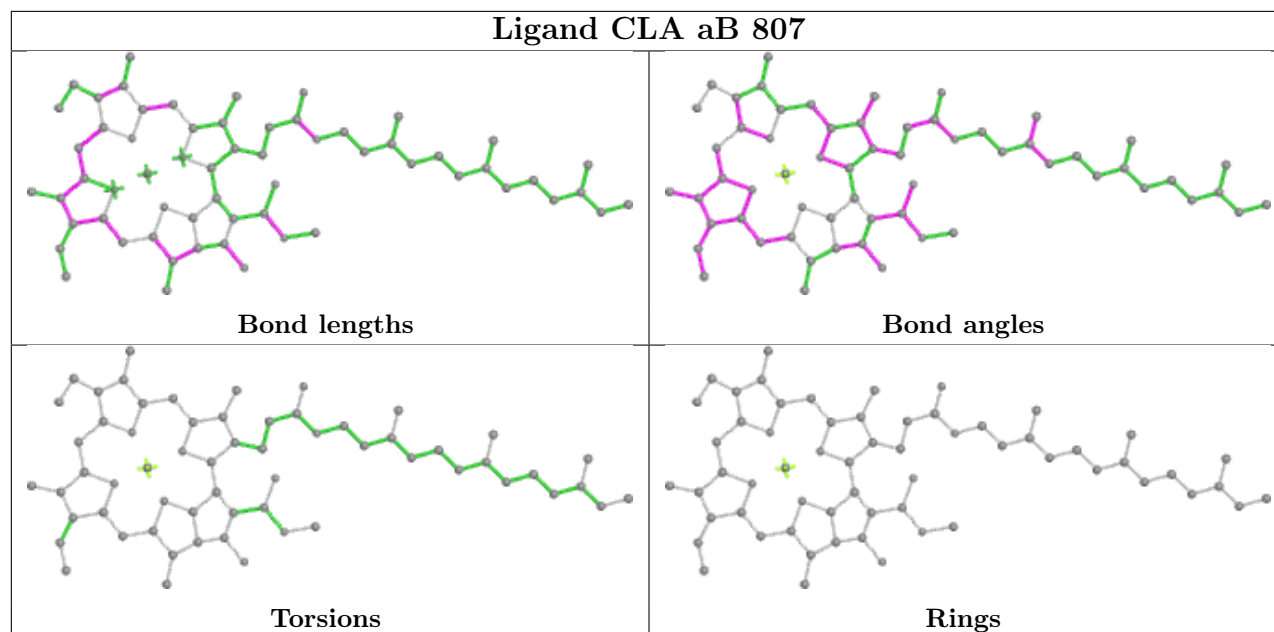


Ligand CLA aB 802

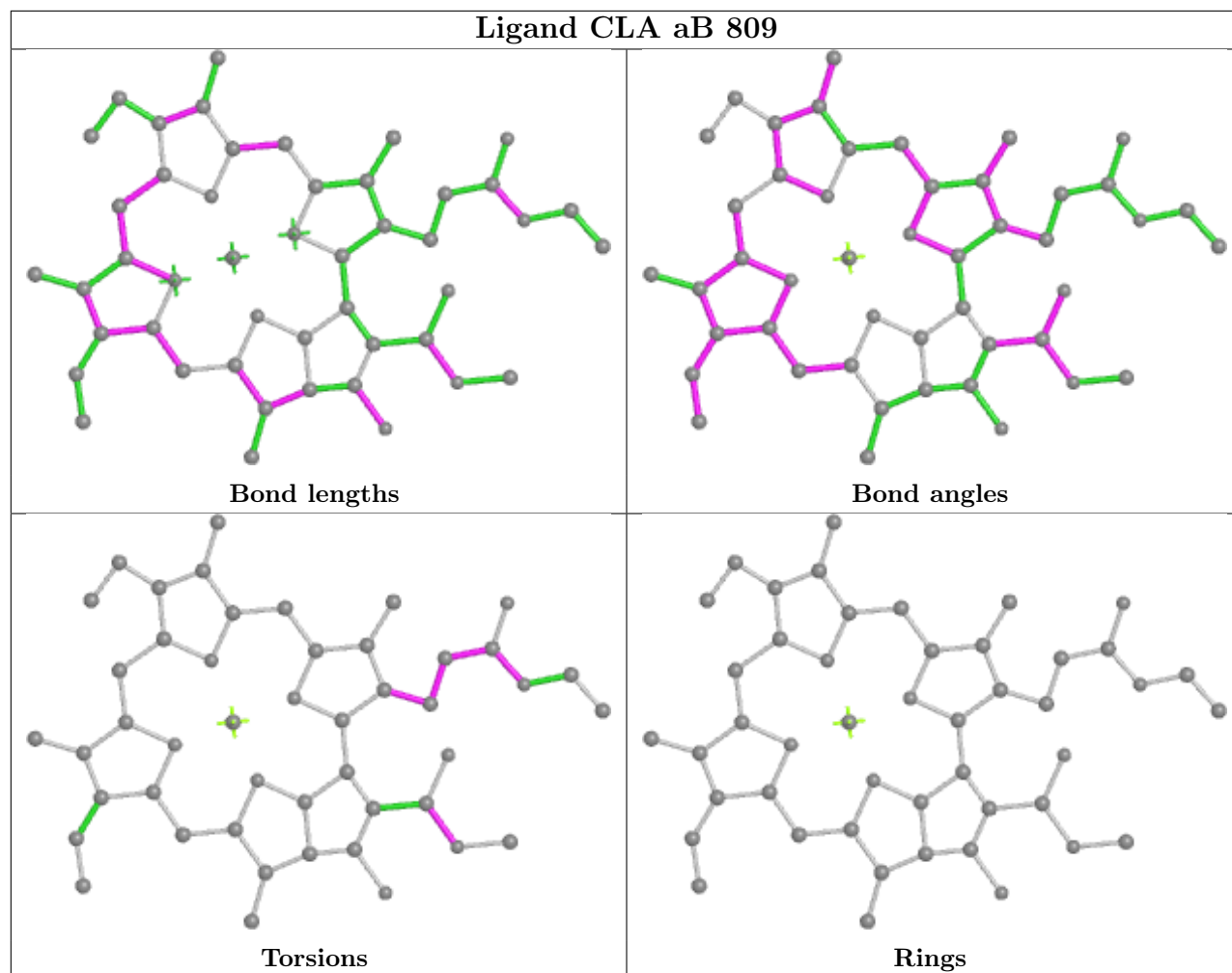




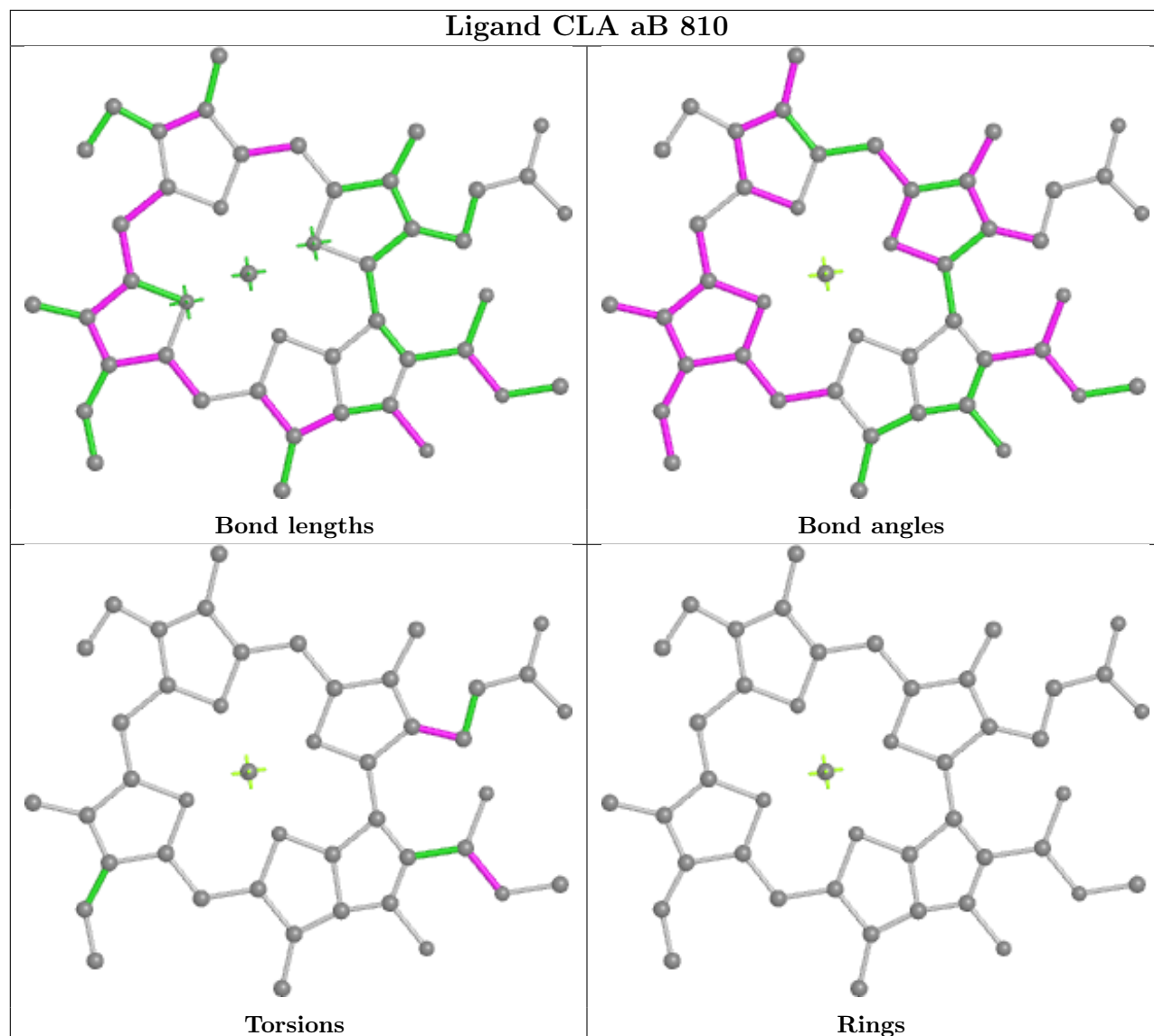
Ligand CLA aB 805**Ligand CLA aB 806**



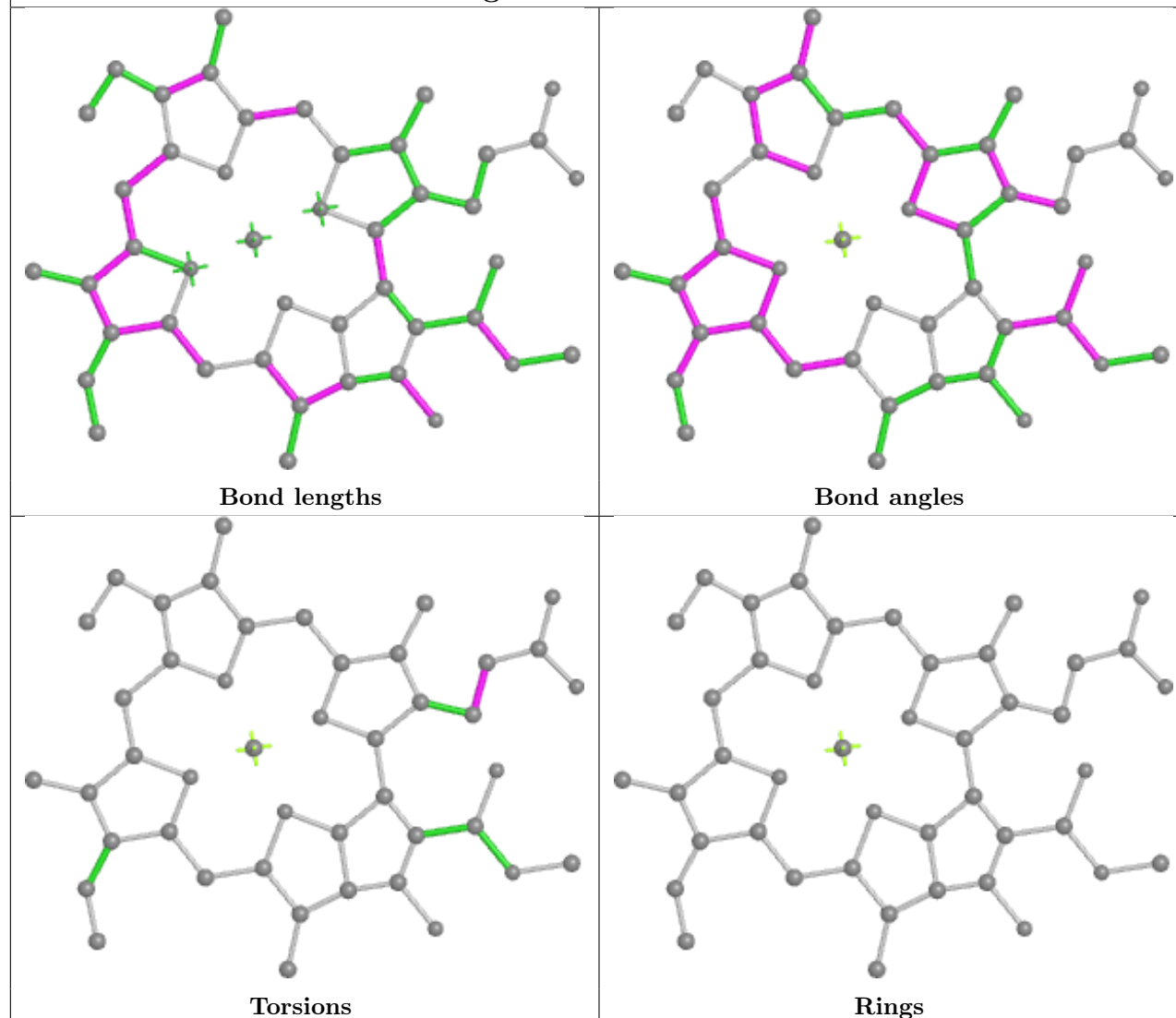
Ligand CLA aB 809



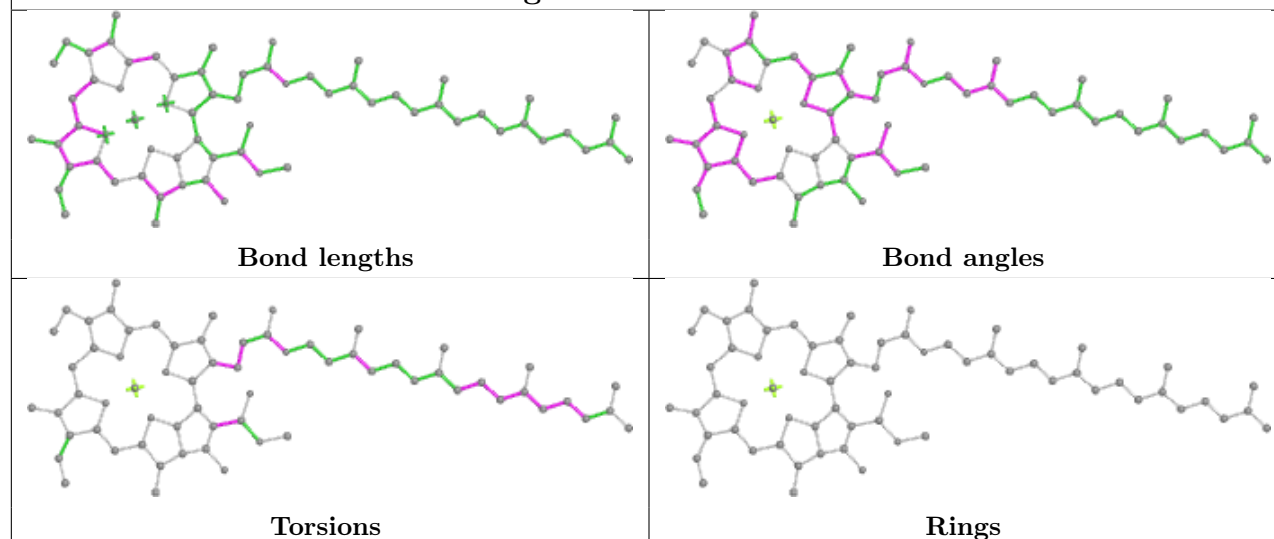
Ligand CLA aB 810

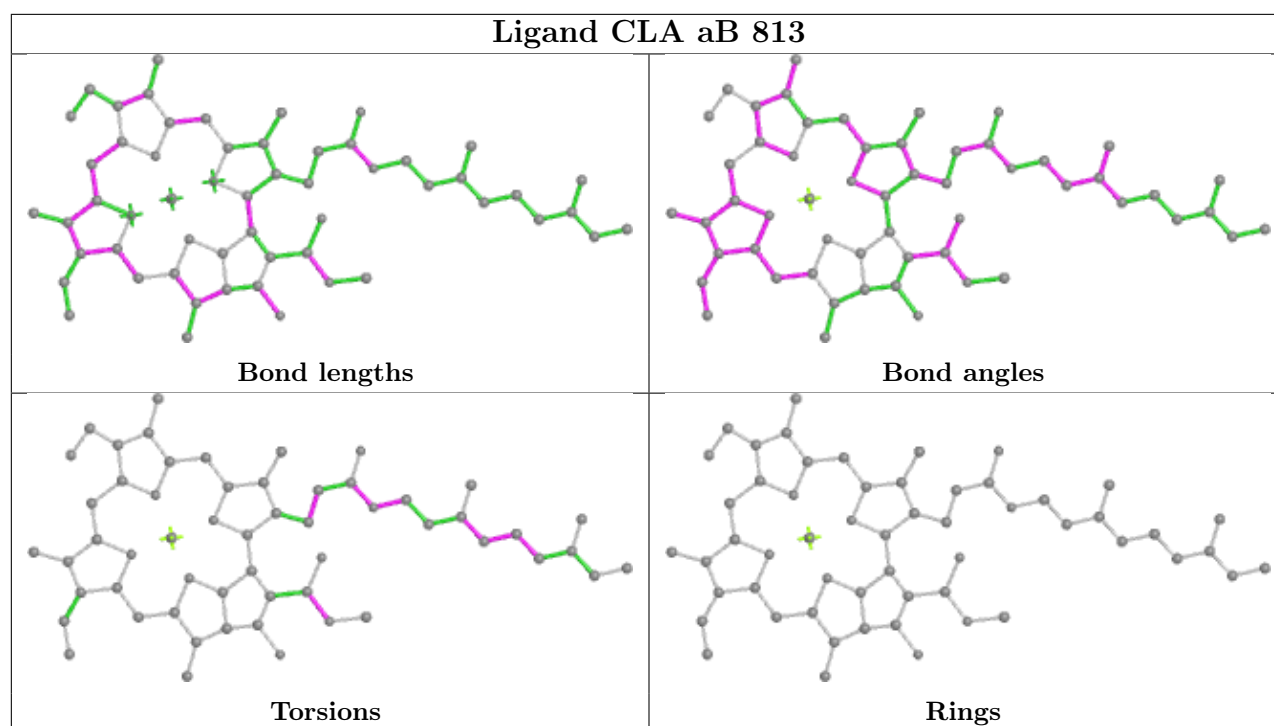


Ligand CLA aB 811

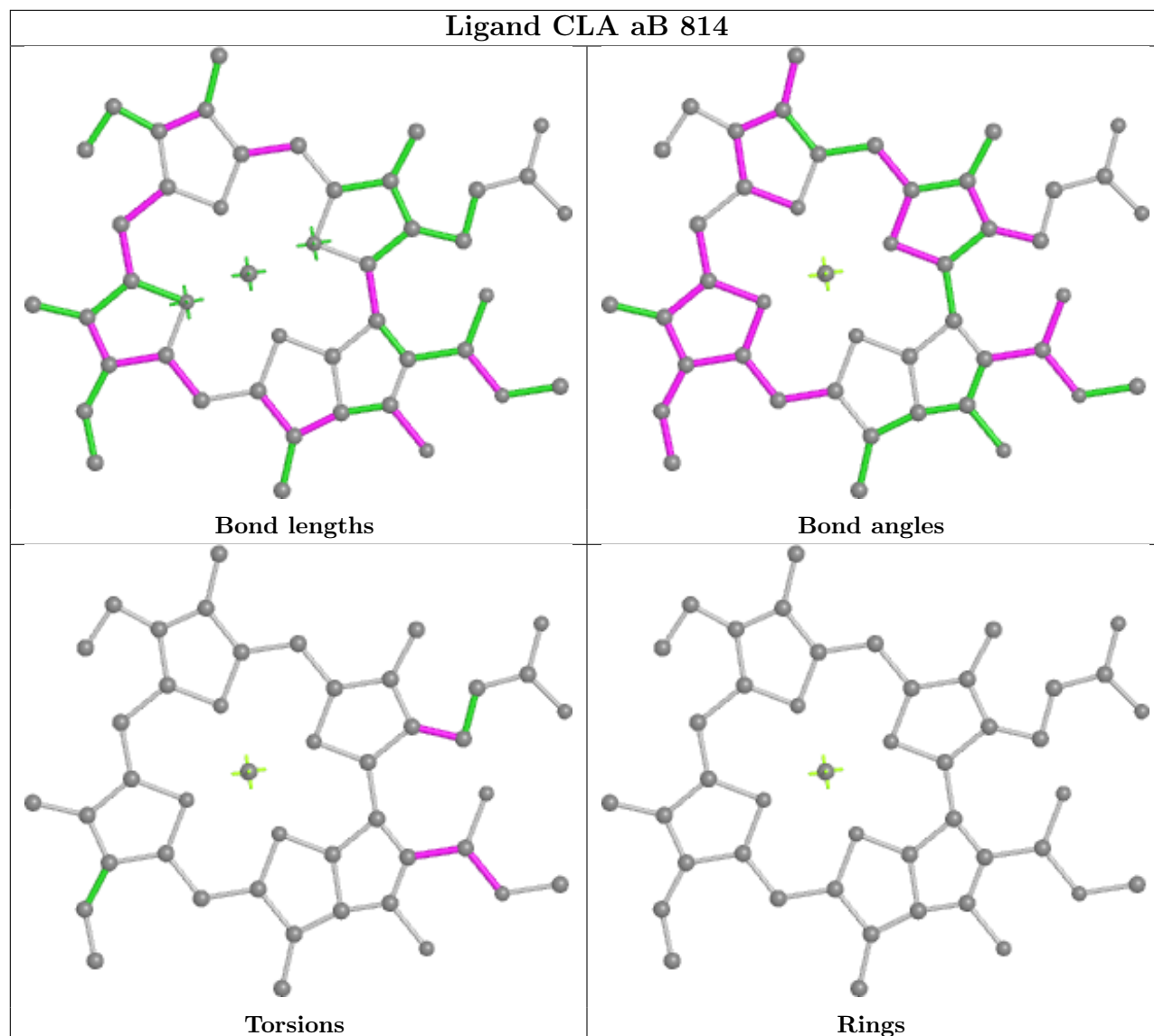


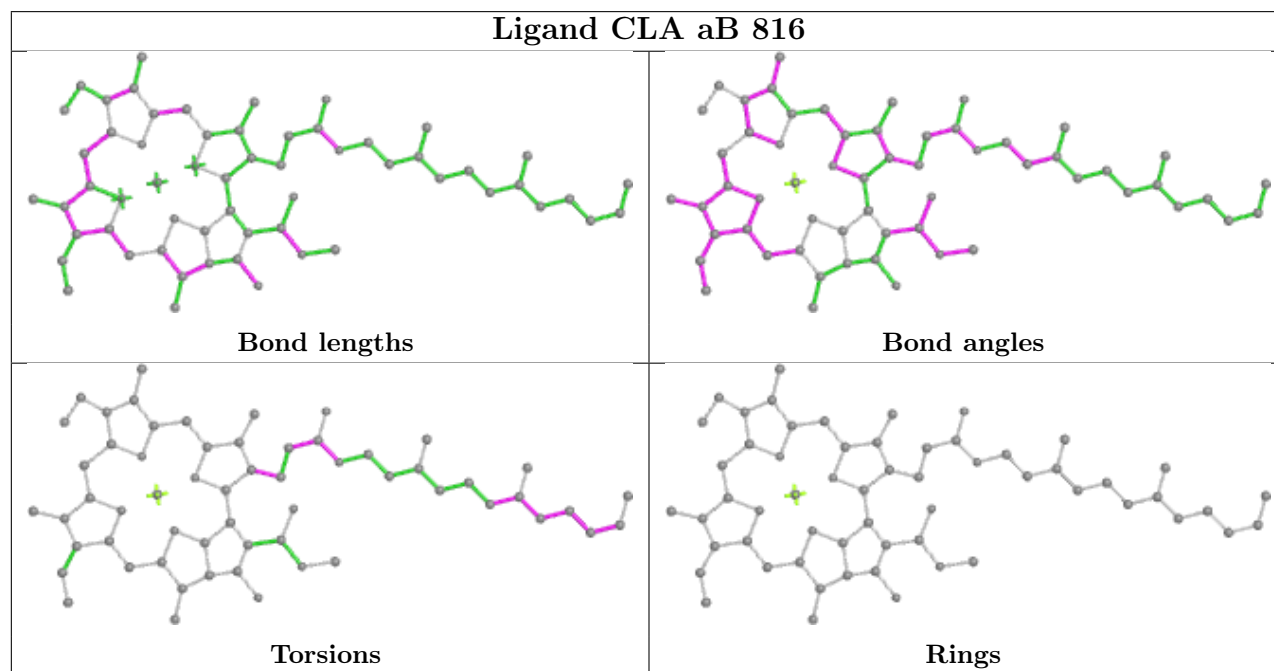
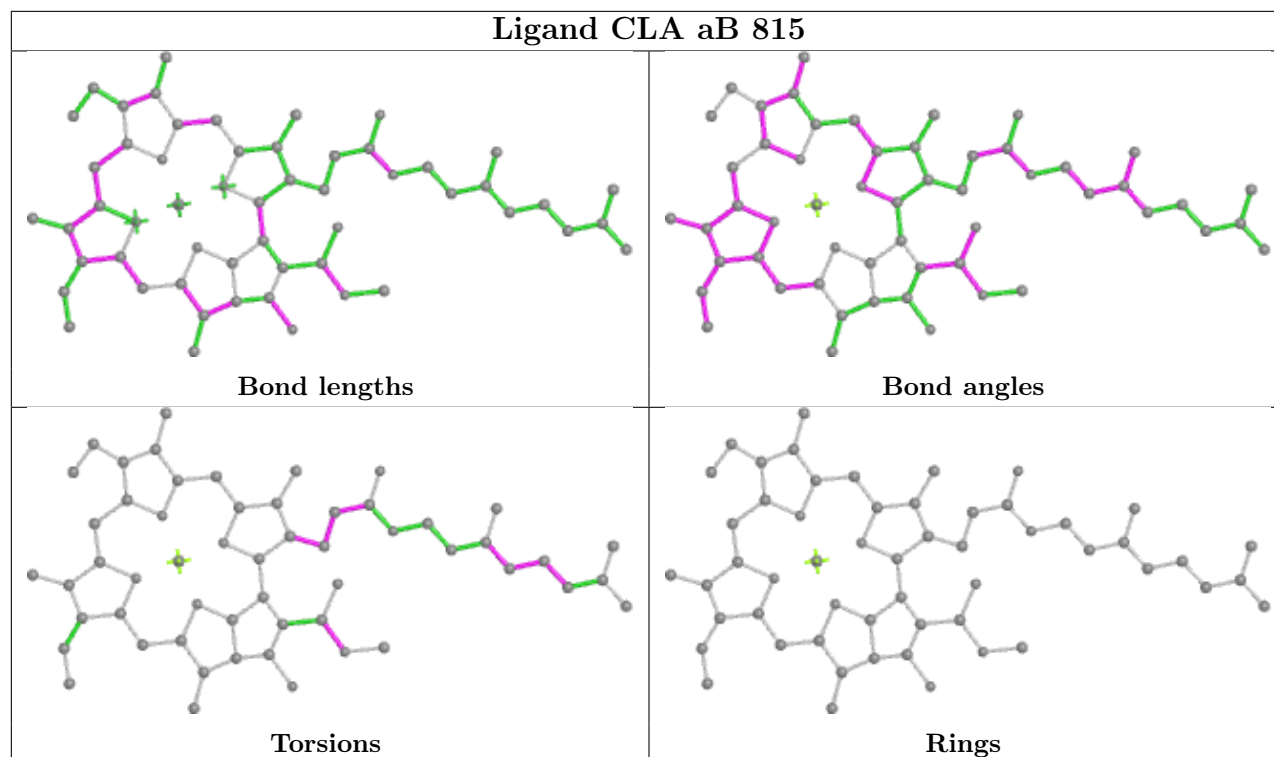
Ligand CLA aB 812

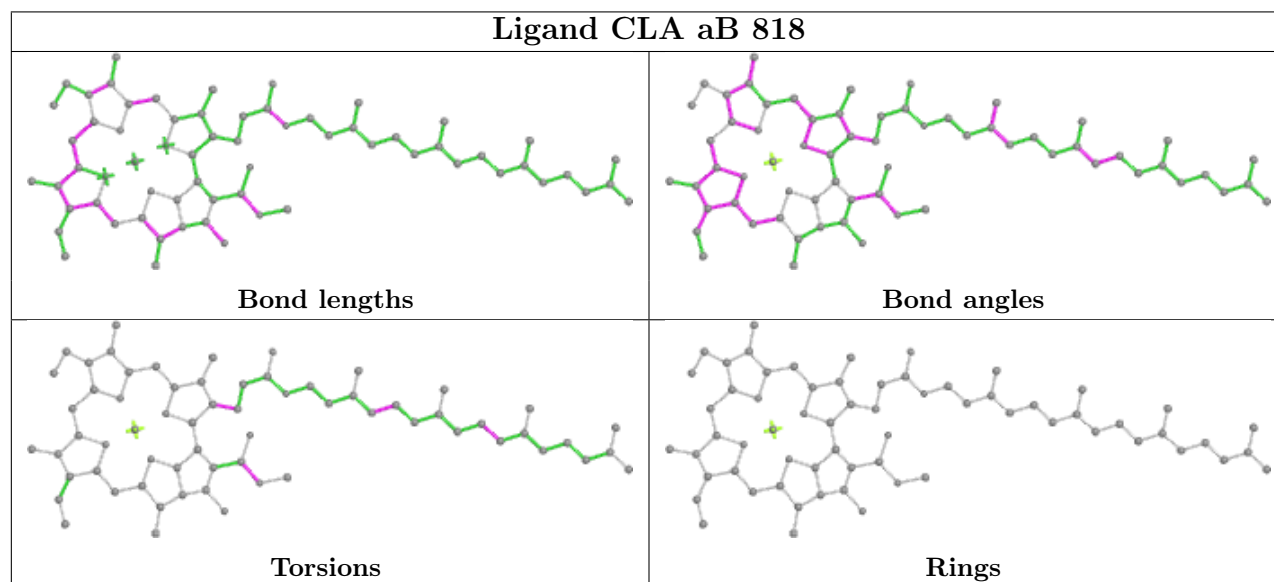
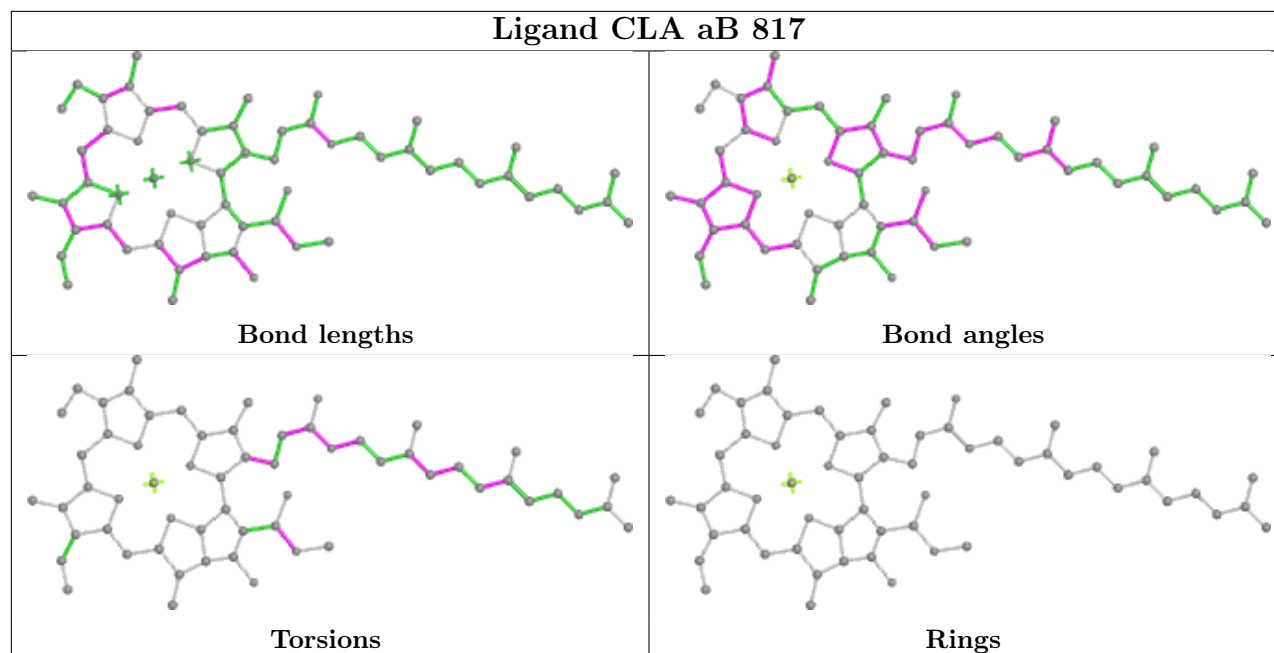




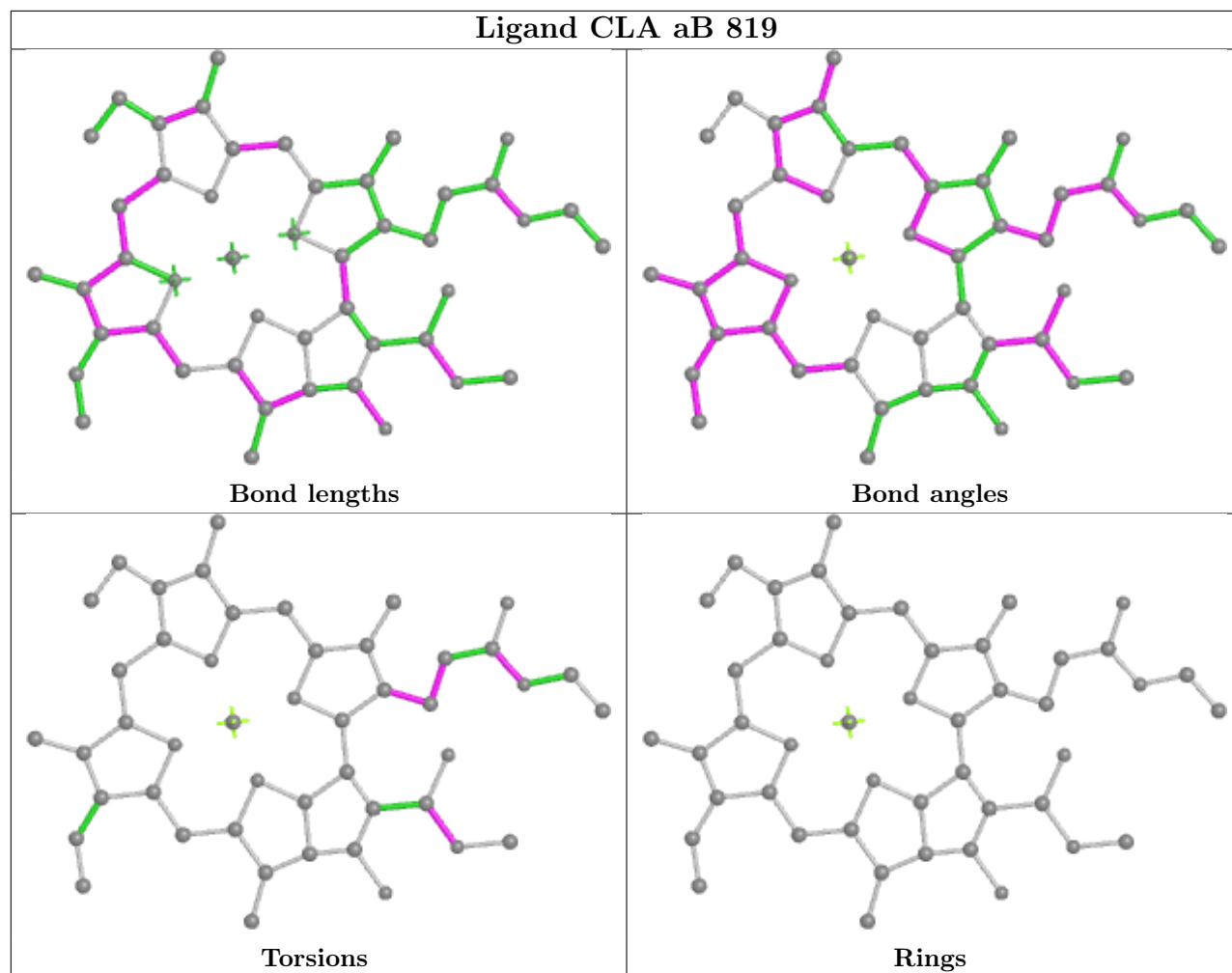
Ligand CLA aB 814



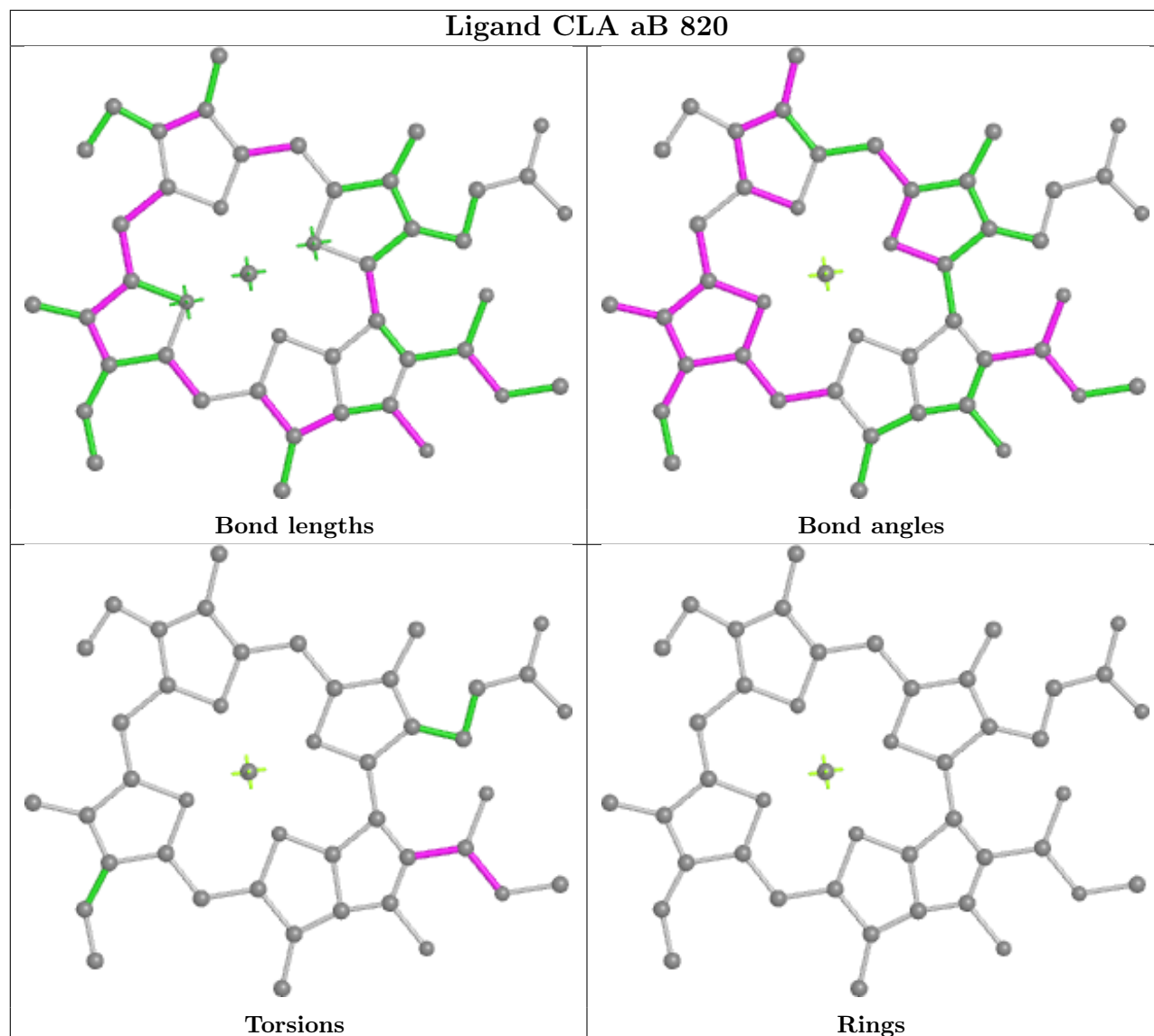


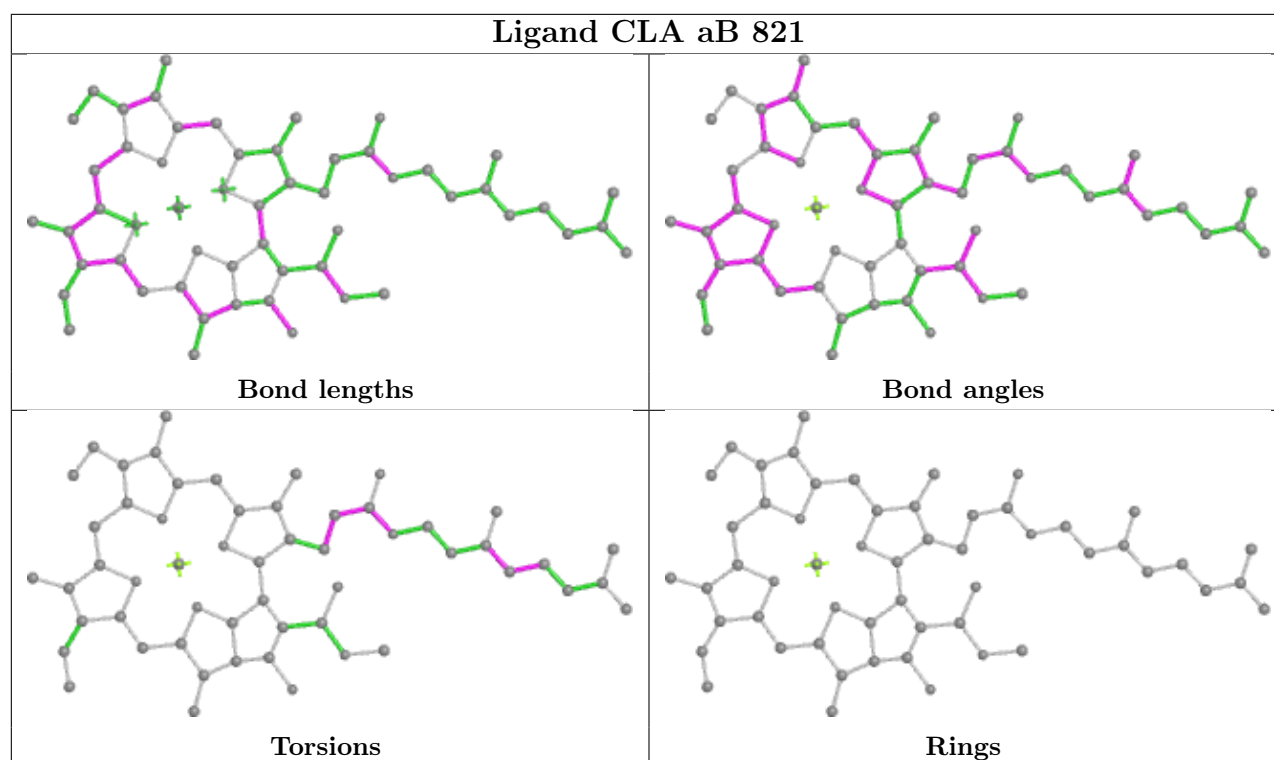


Ligand CLA aB 819

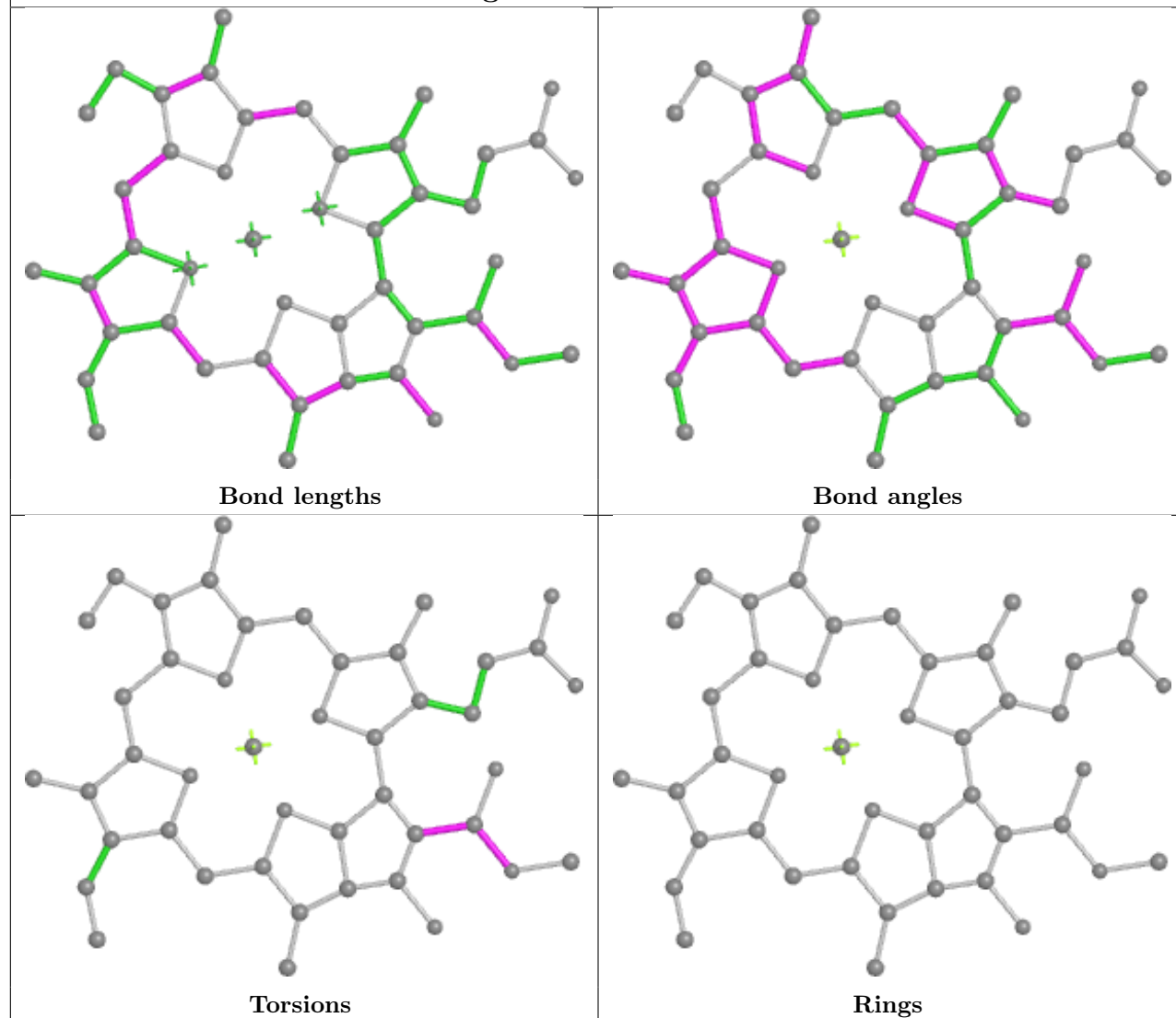


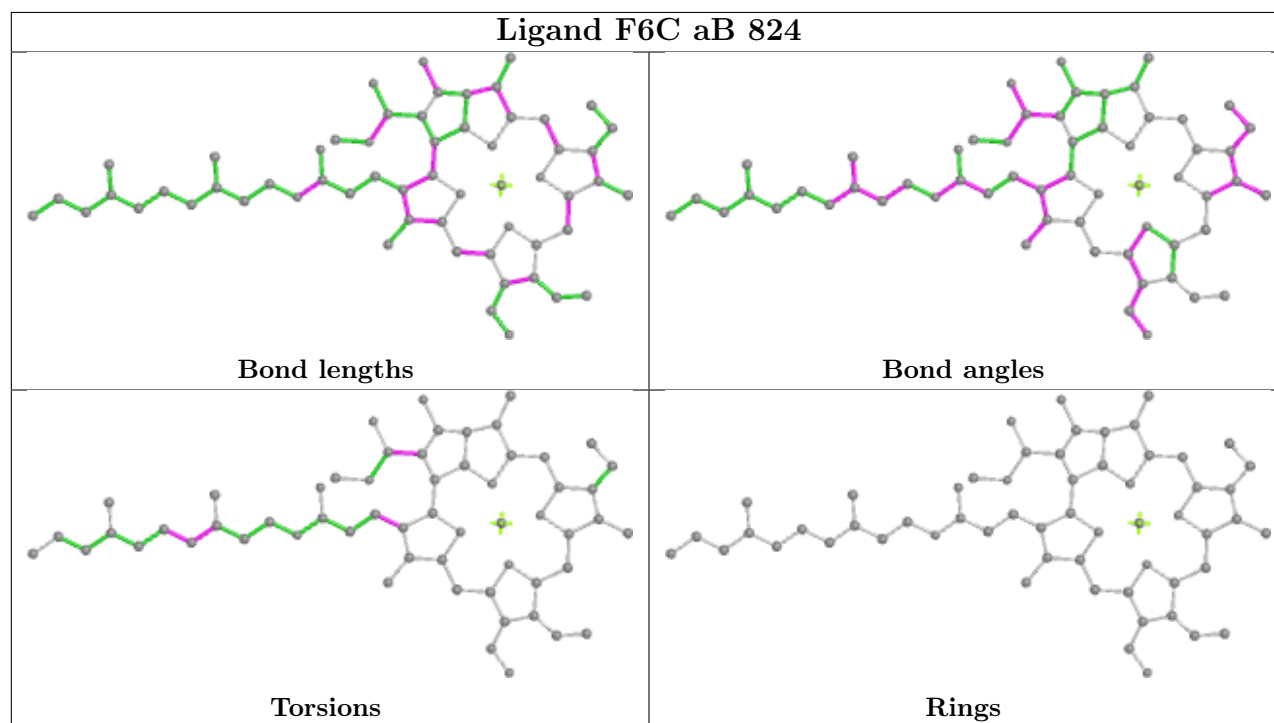
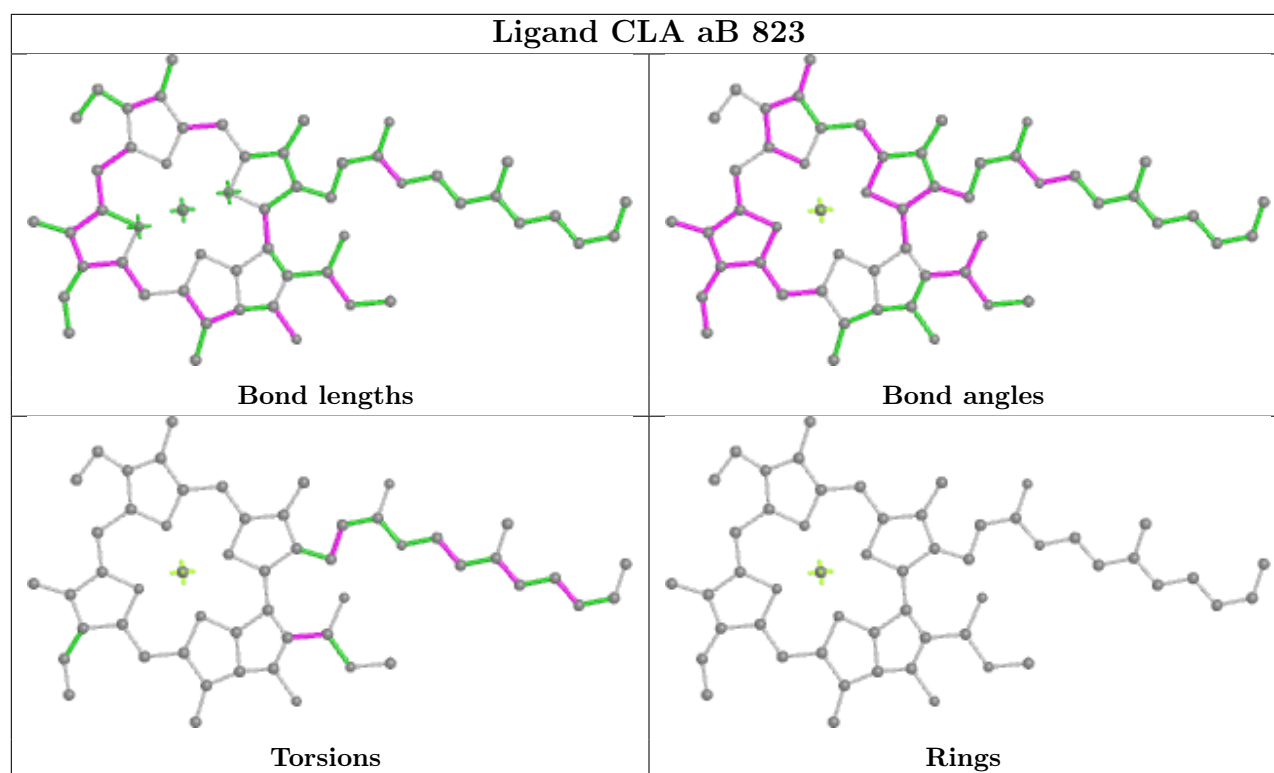
Ligand CLA aB 820



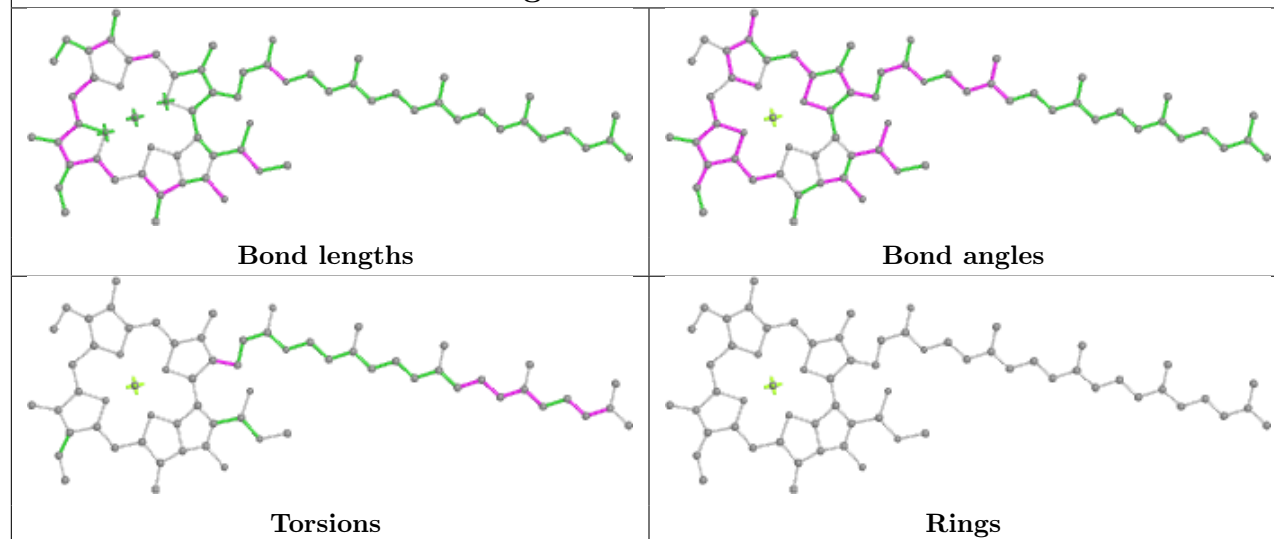


Ligand CLA aB 822

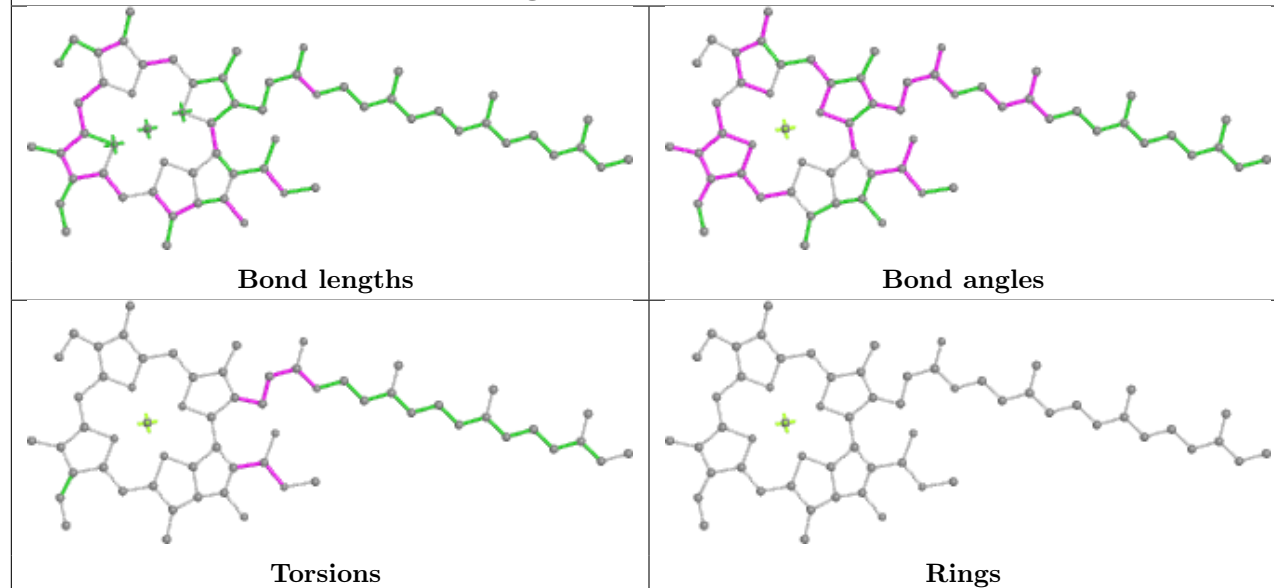




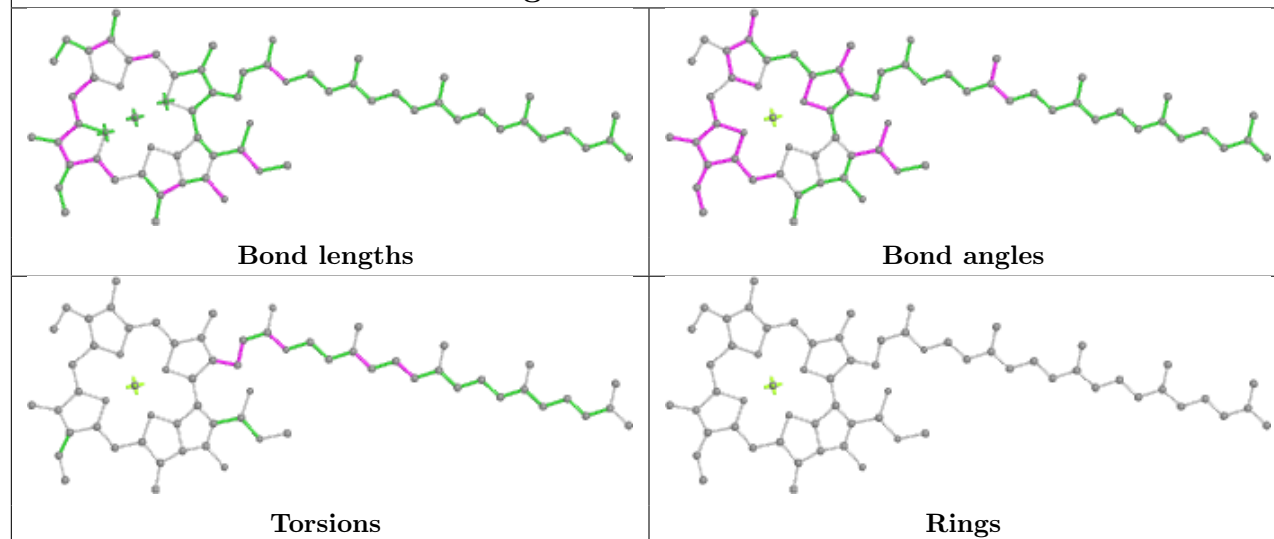
Ligand CLA aB 825



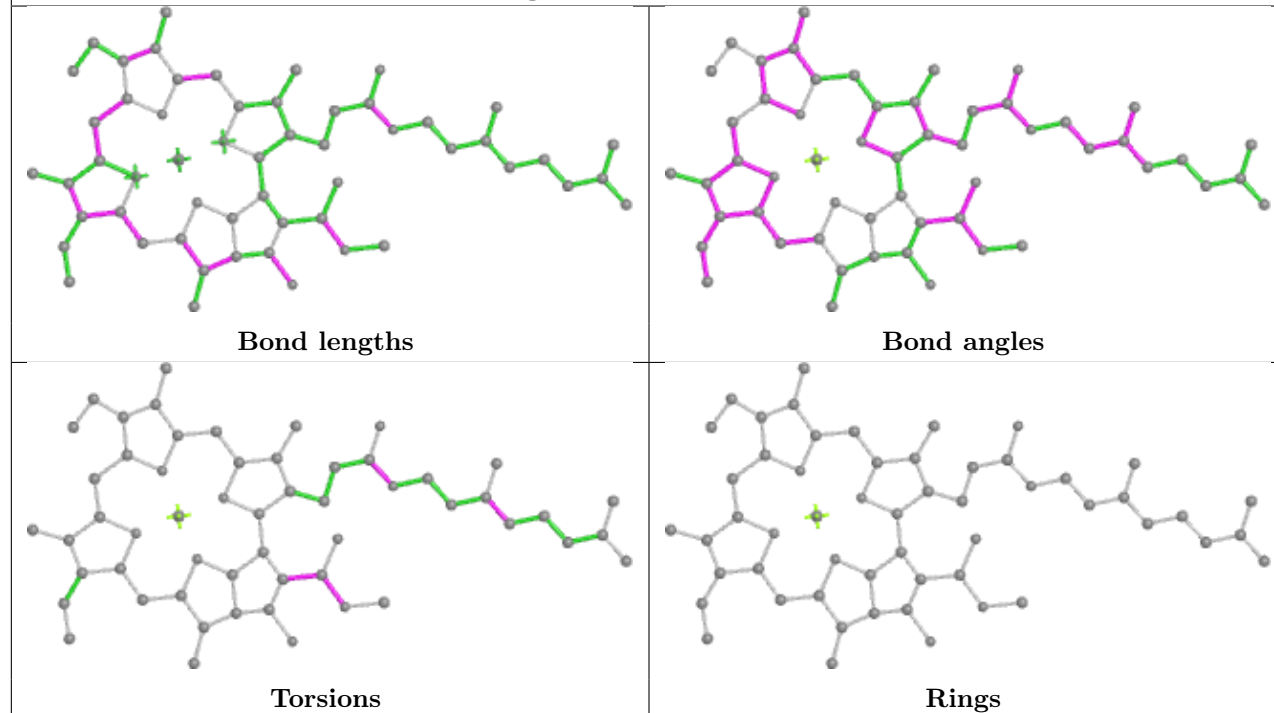
Ligand CLA aB 826



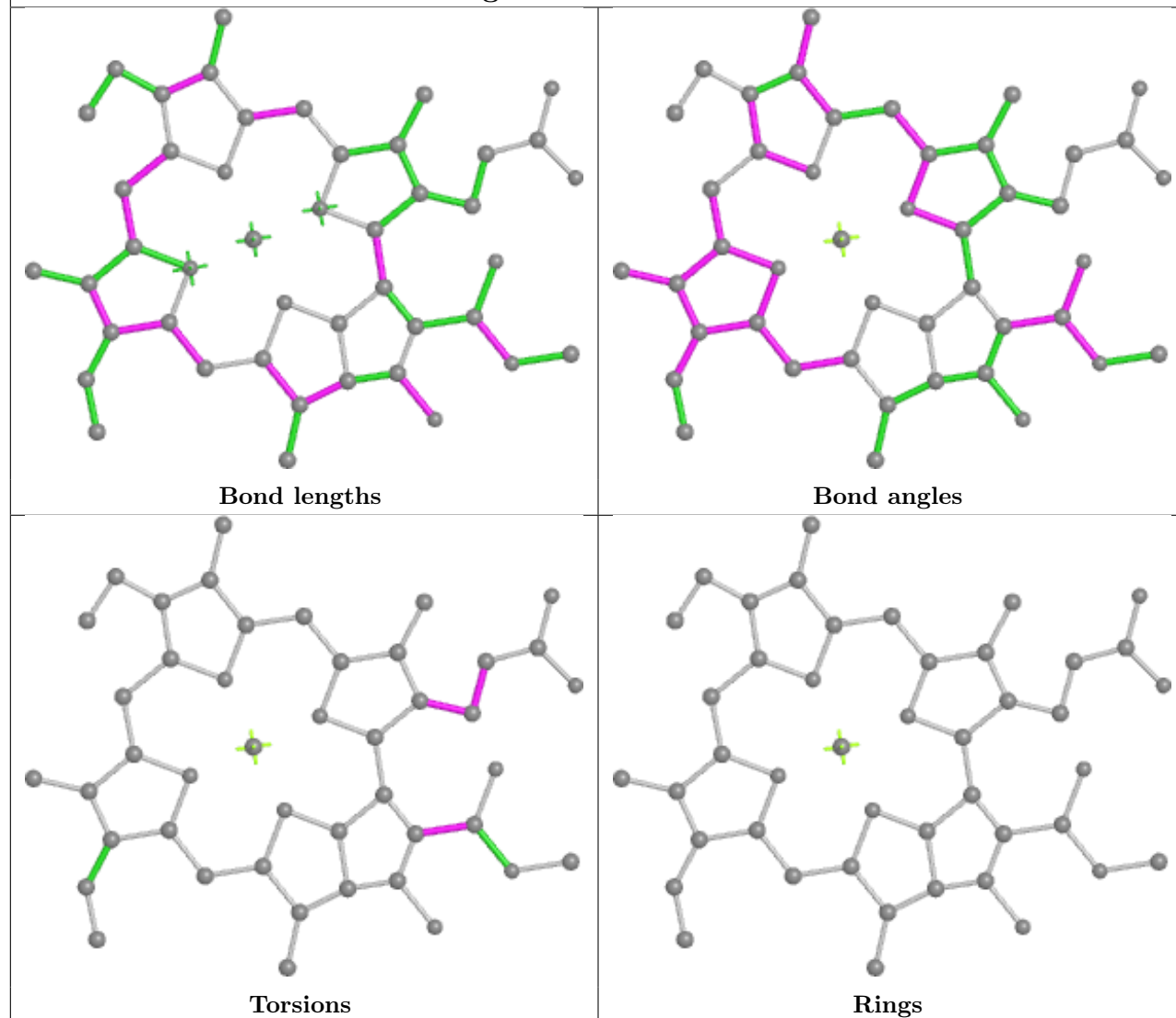
Ligand CLA aB 827



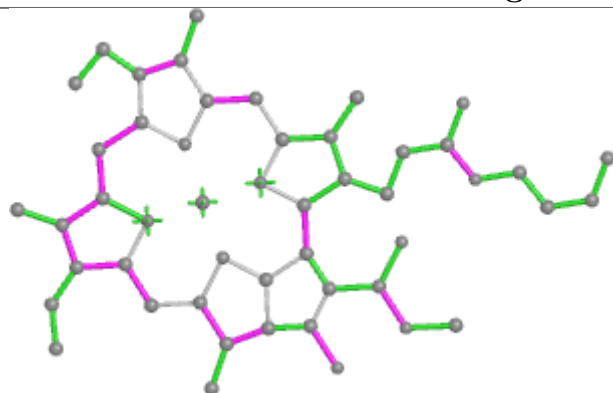
Ligand CLA aB 828



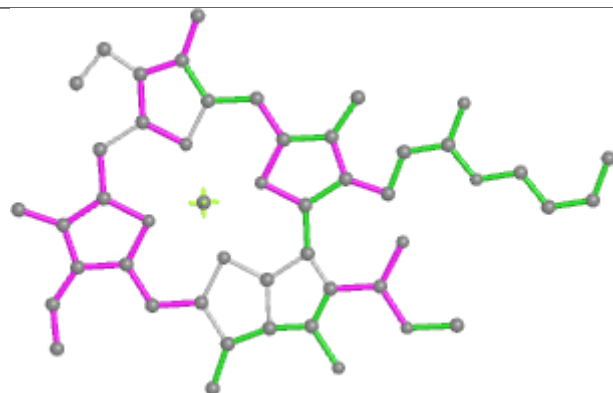
Ligand CLA aB 829



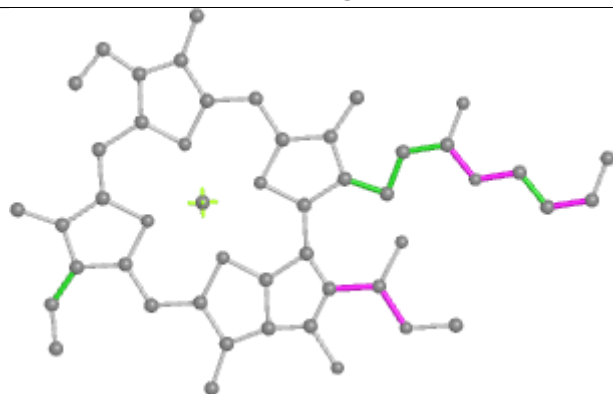
Ligand CLA aB 830



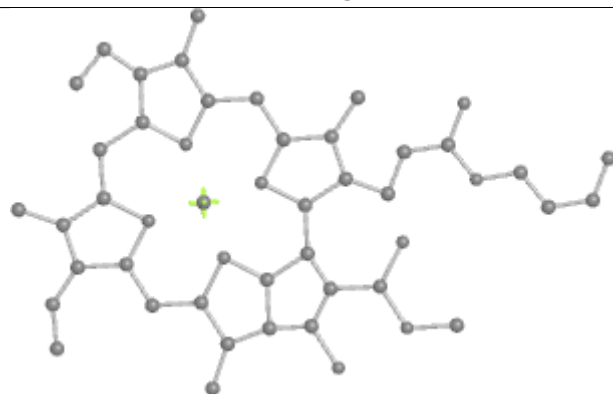
Bond lengths



Bond angles

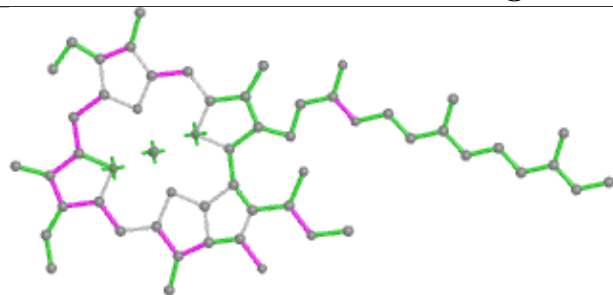


Torsions

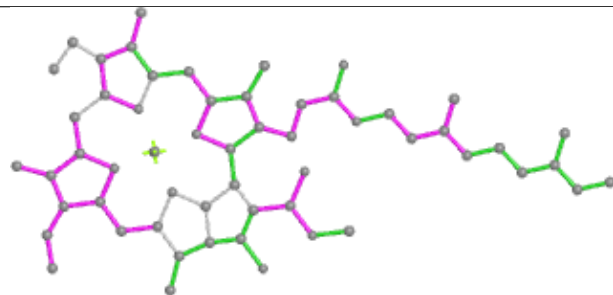


Rings

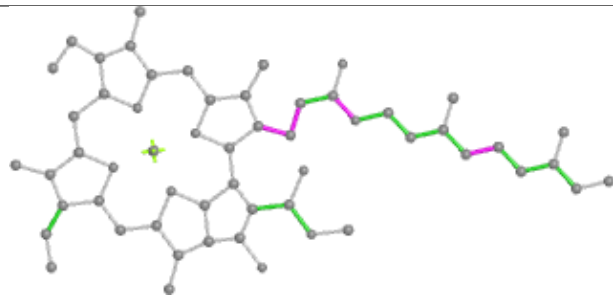
Ligand CLA aB 831



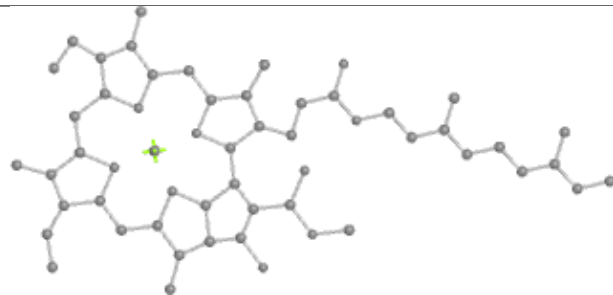
Bond lengths



Bond angles

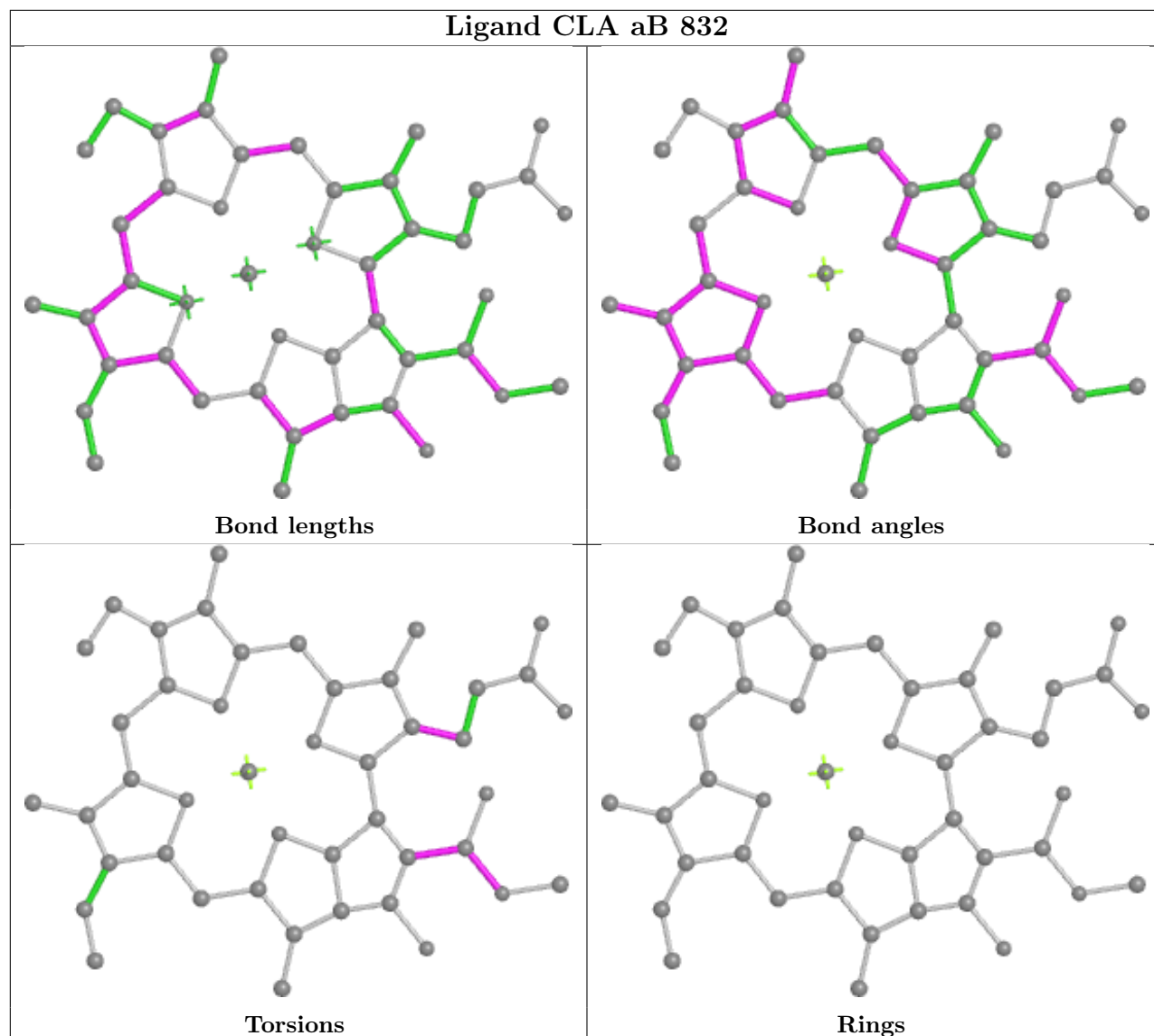


Torsions

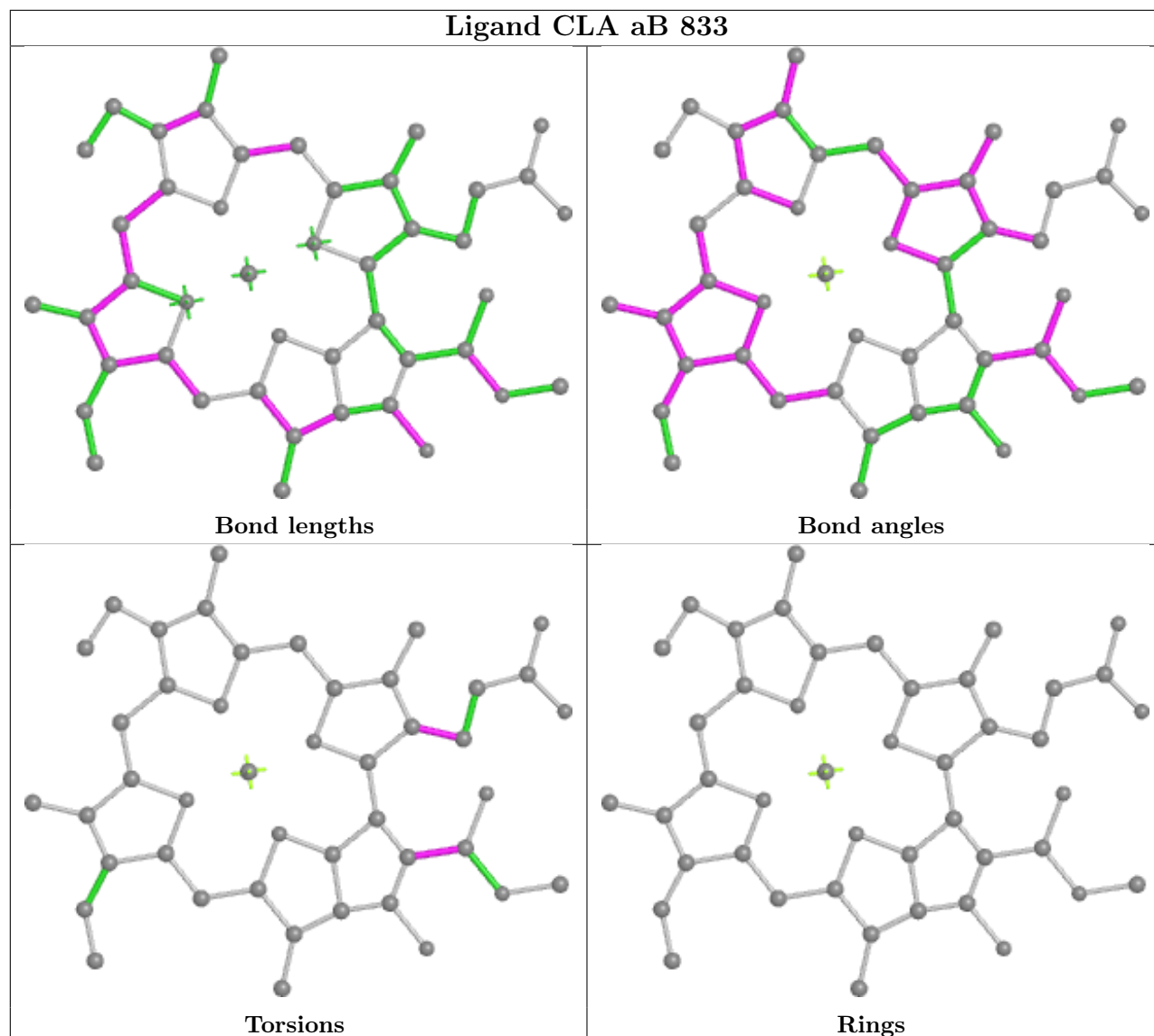


Rings

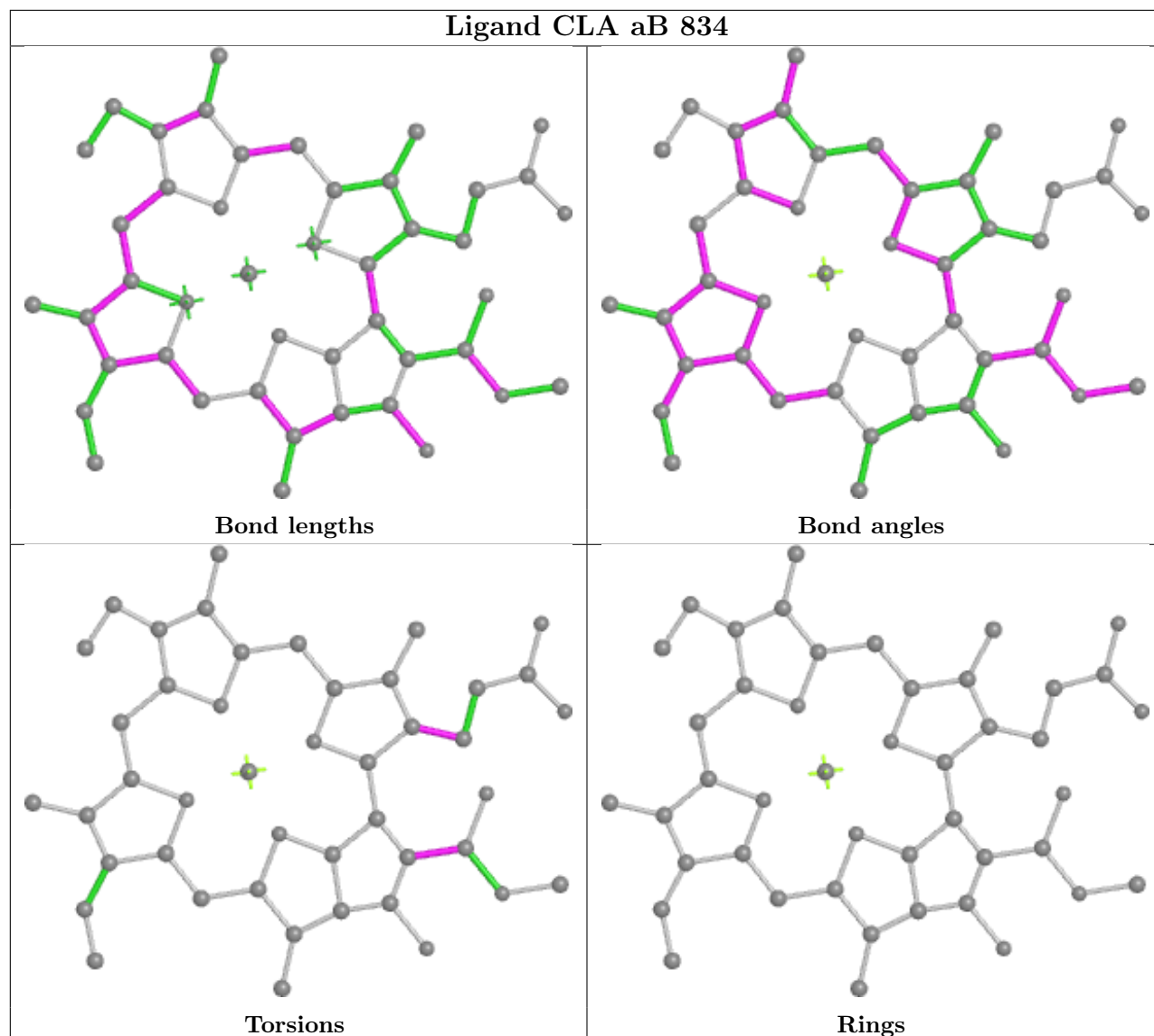
Ligand CLA aB 832



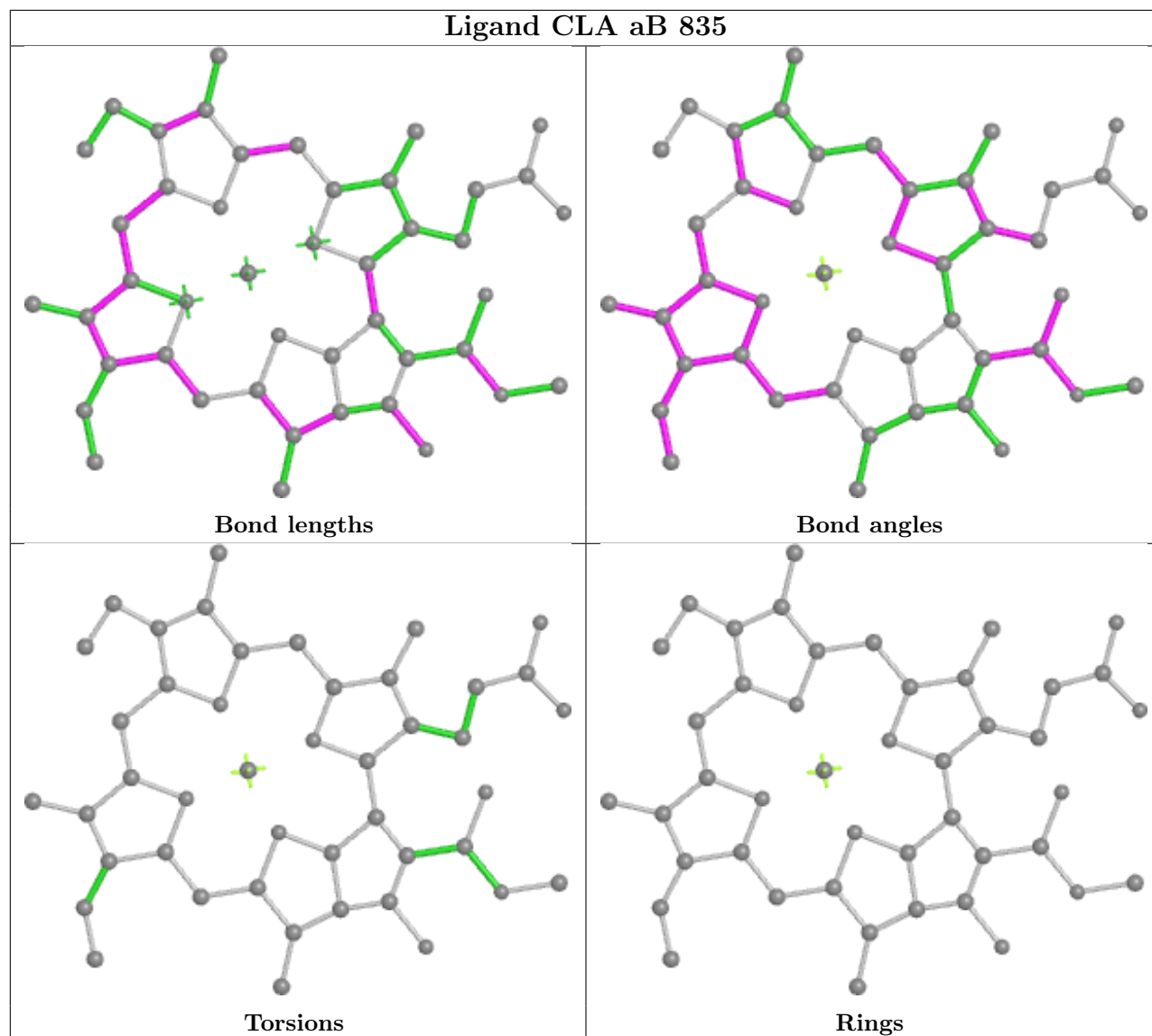
Ligand CLA aB 833

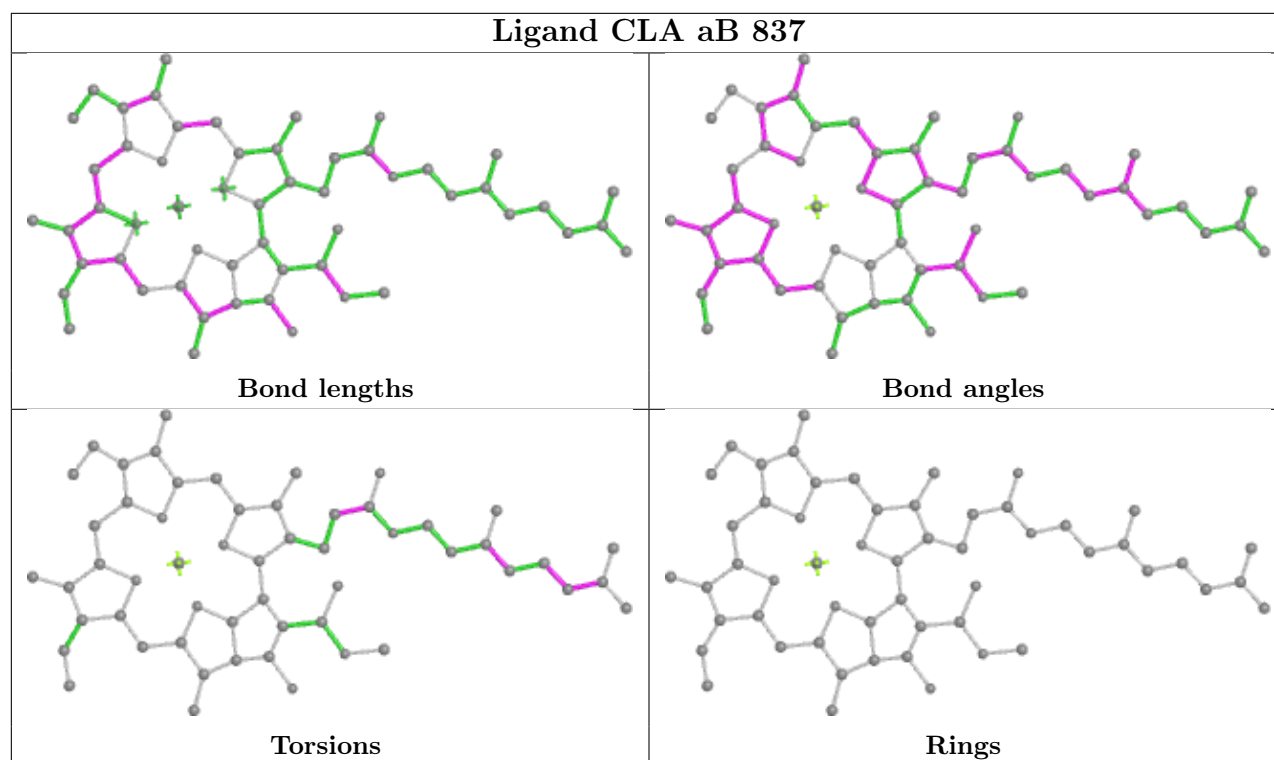
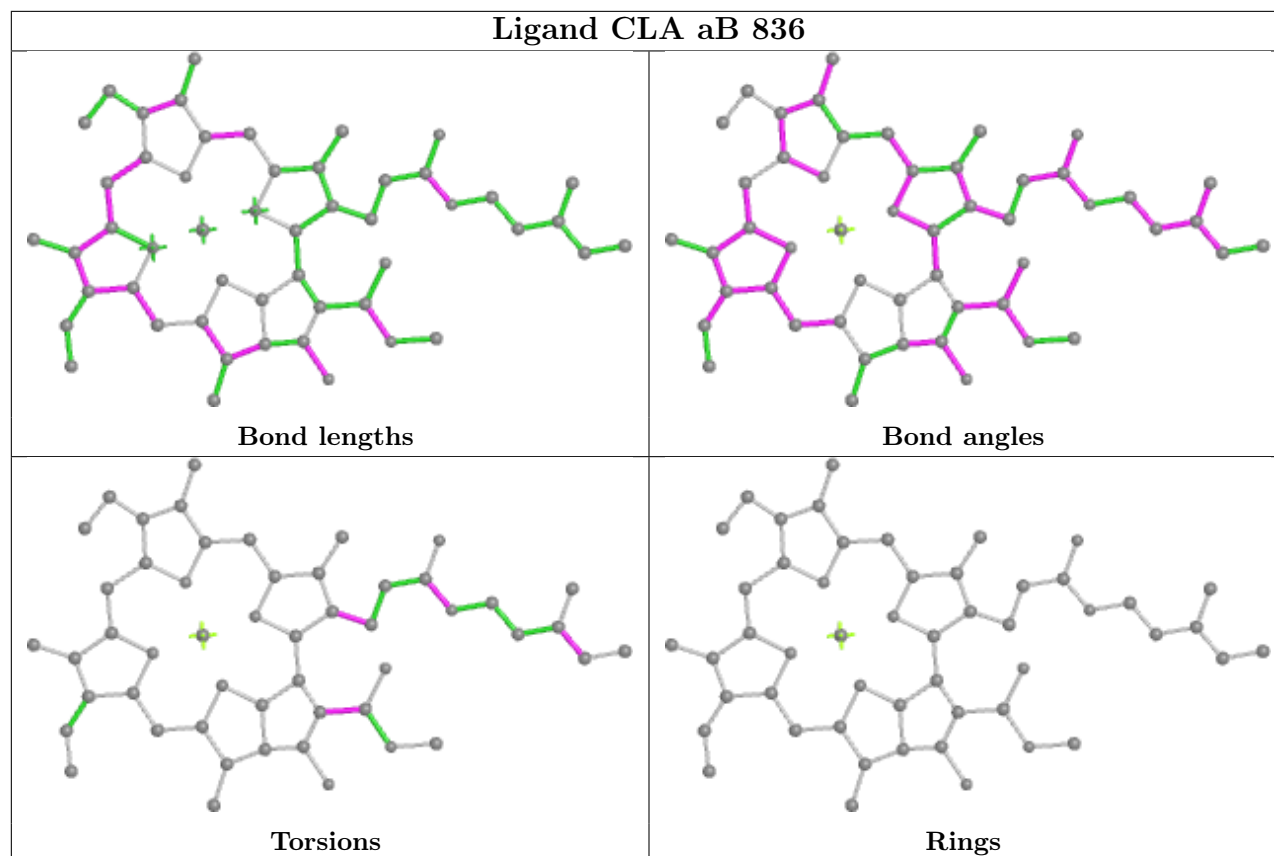


Ligand CLA aB 834

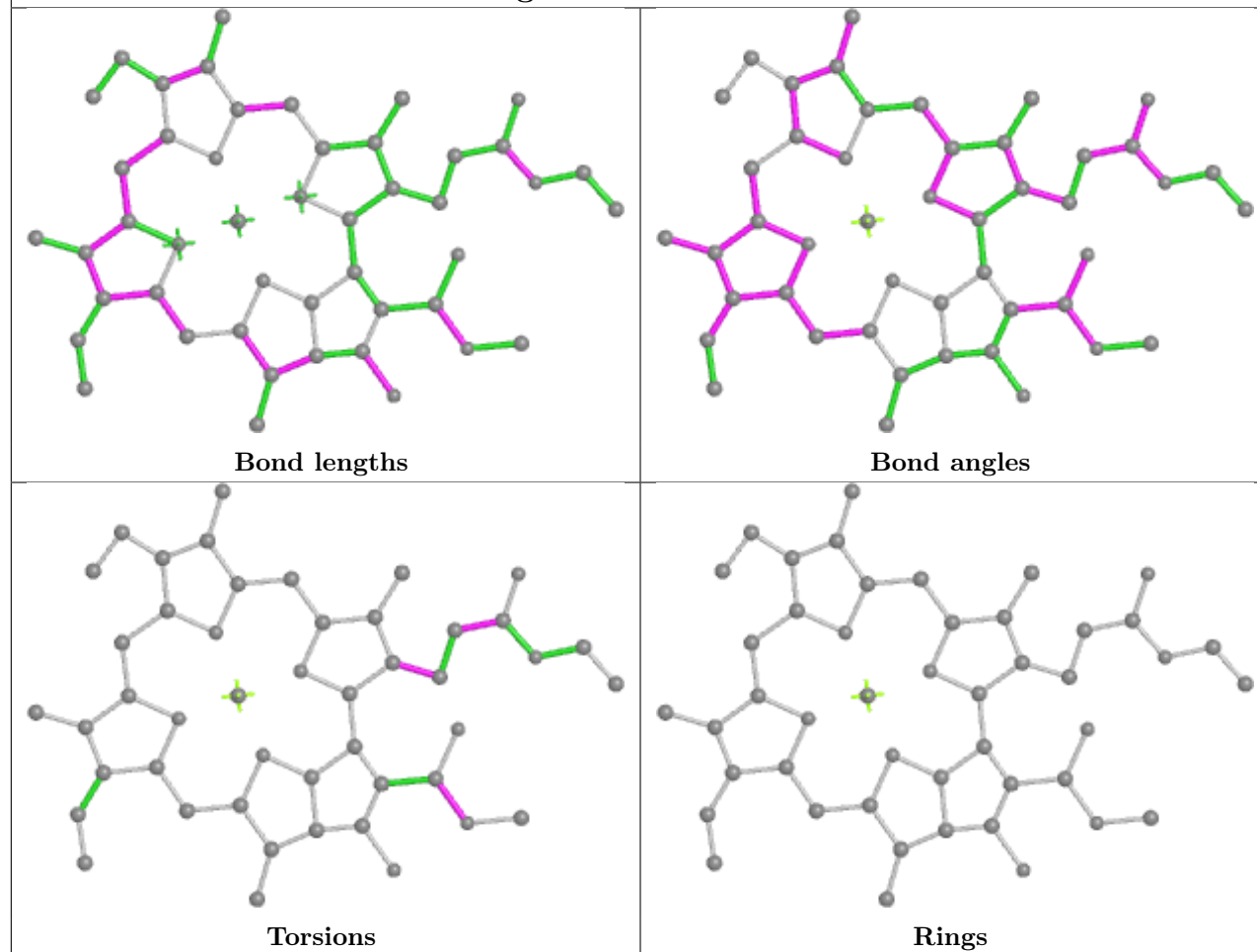


Ligand CLA aB 835

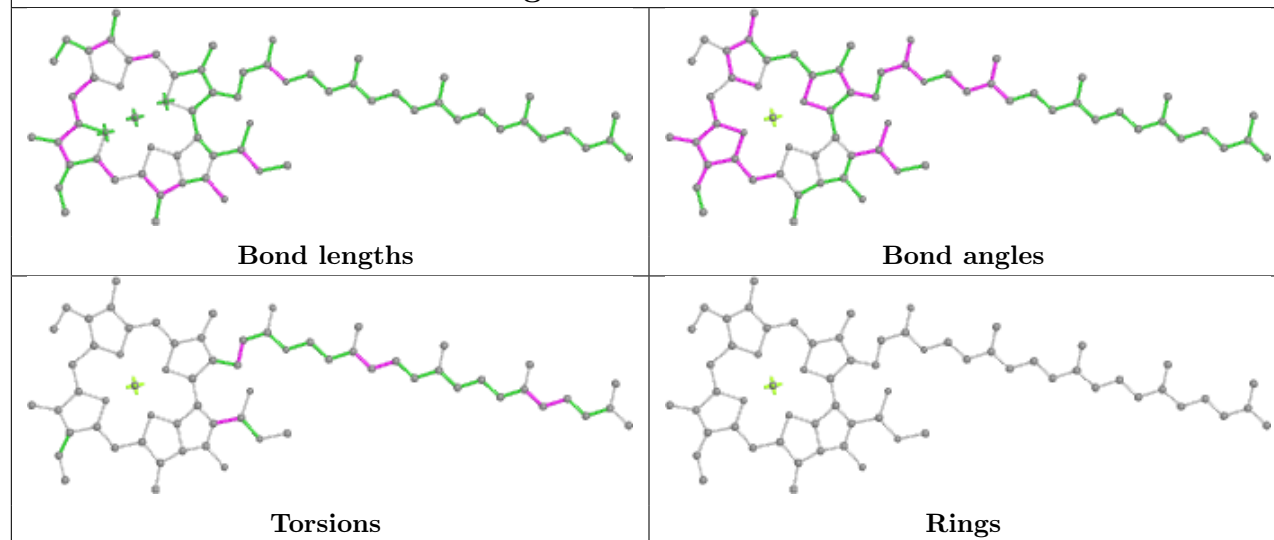




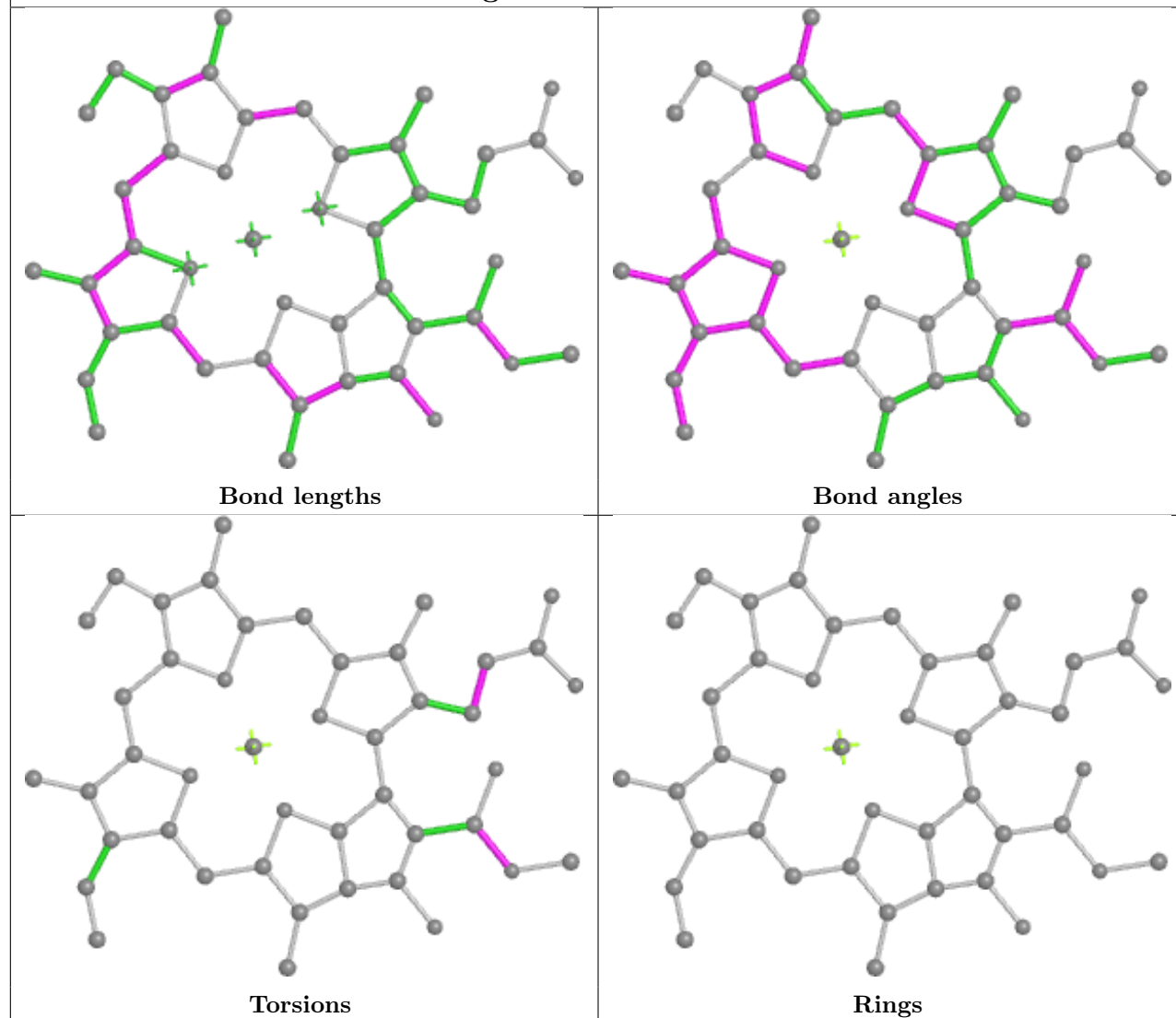
Ligand CLA aB 838



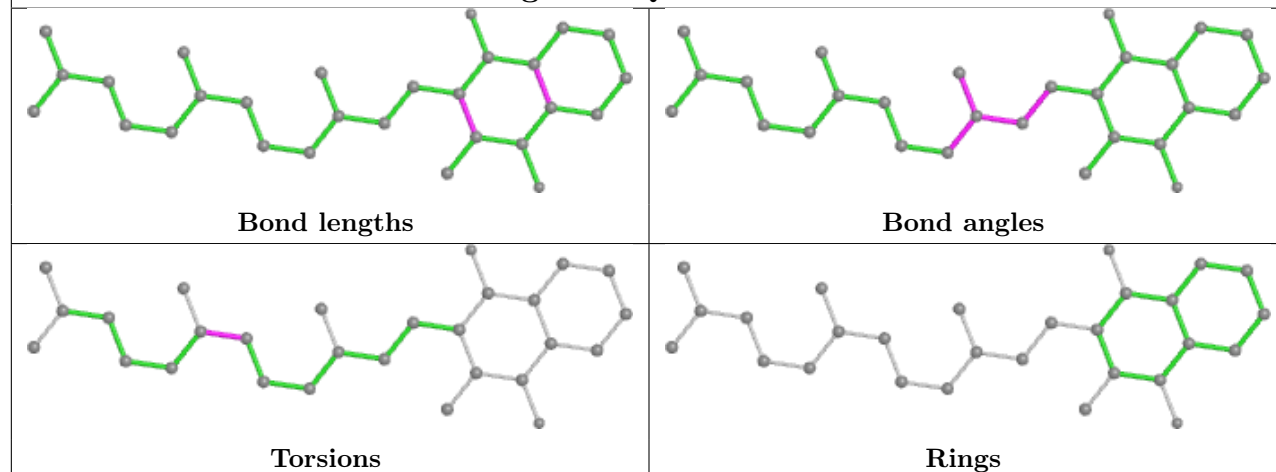
Ligand CLA aB 839

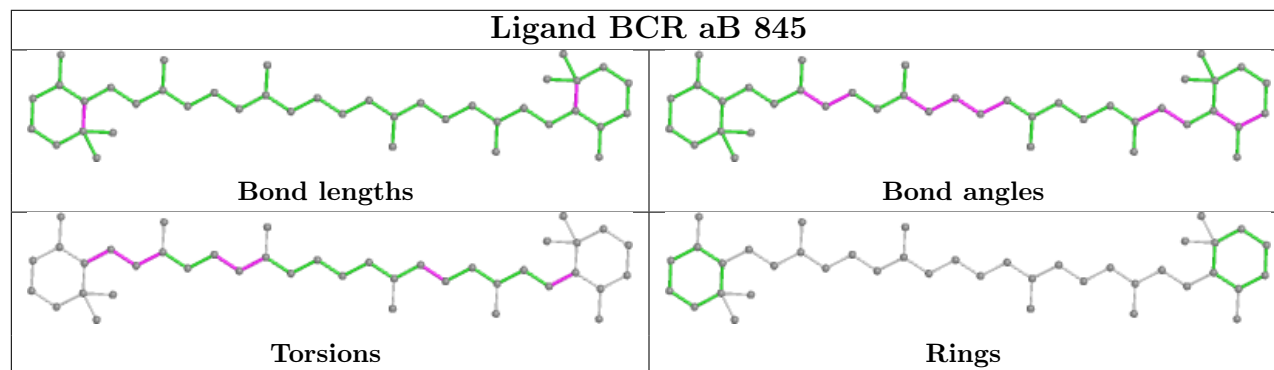
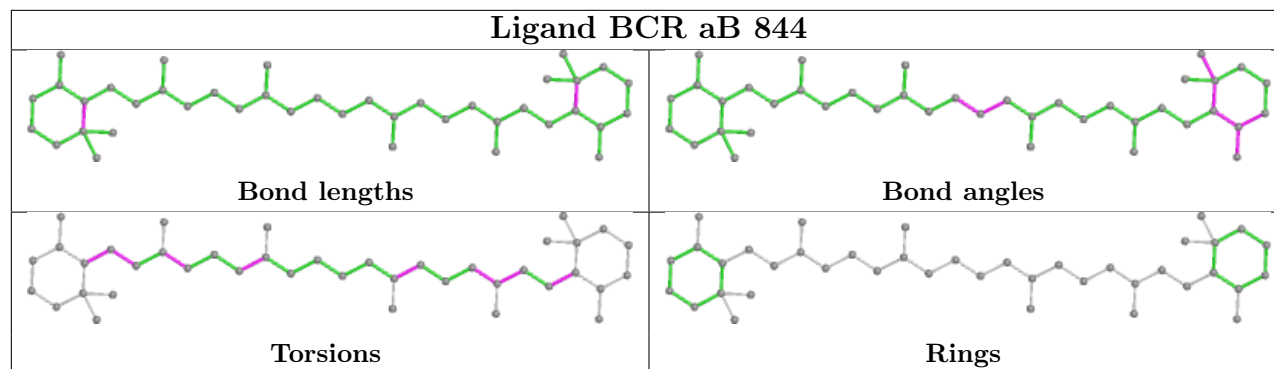
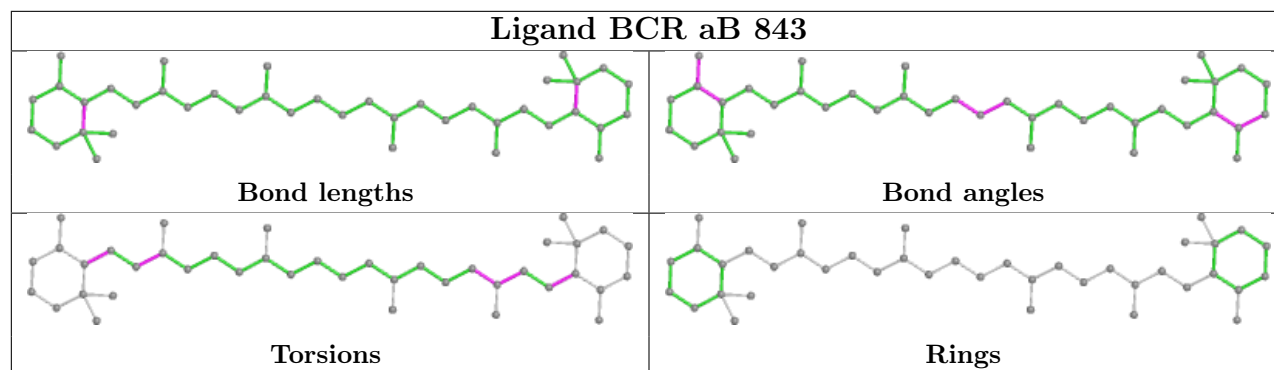
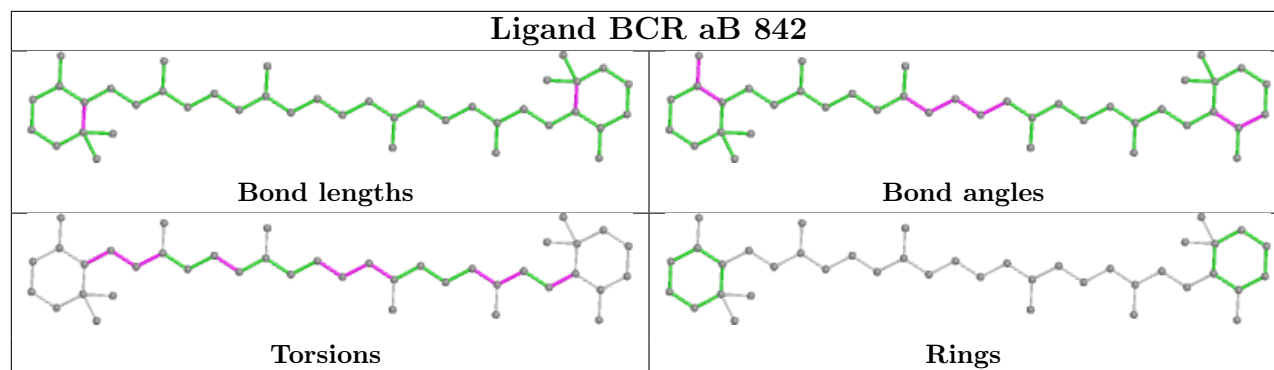


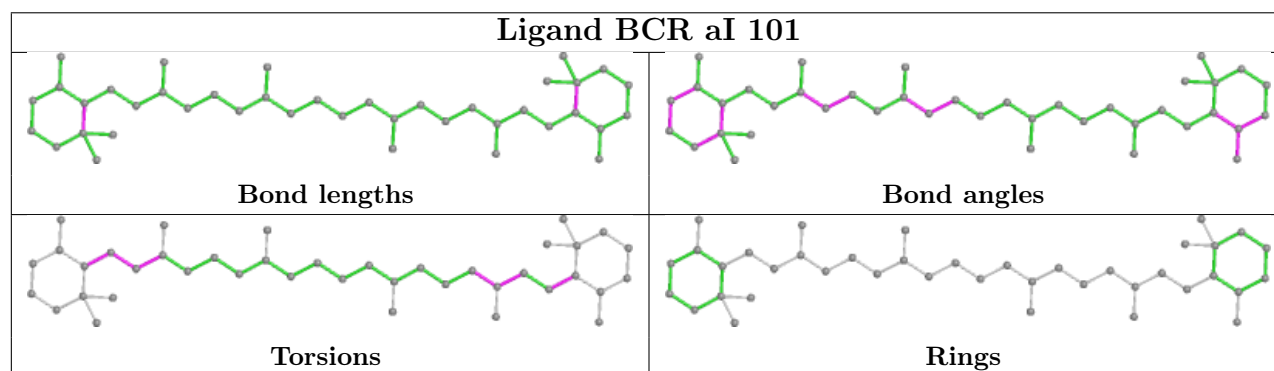
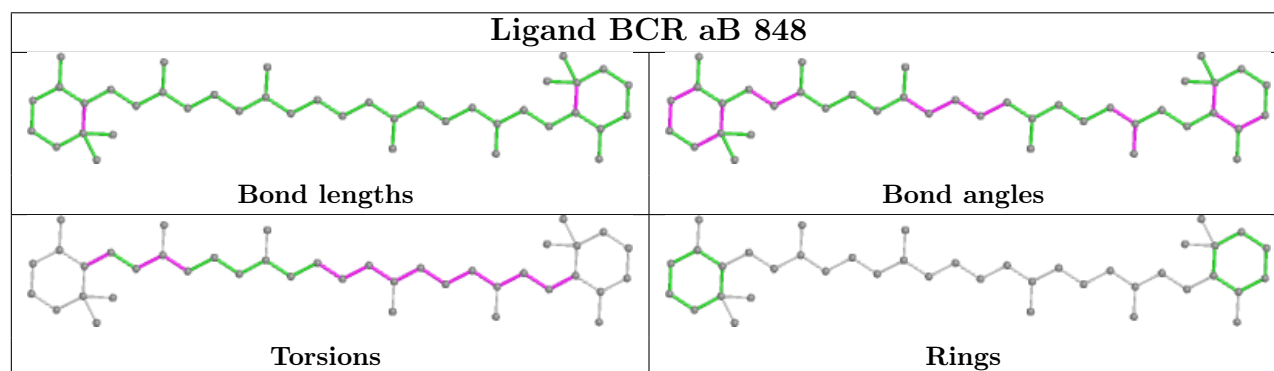
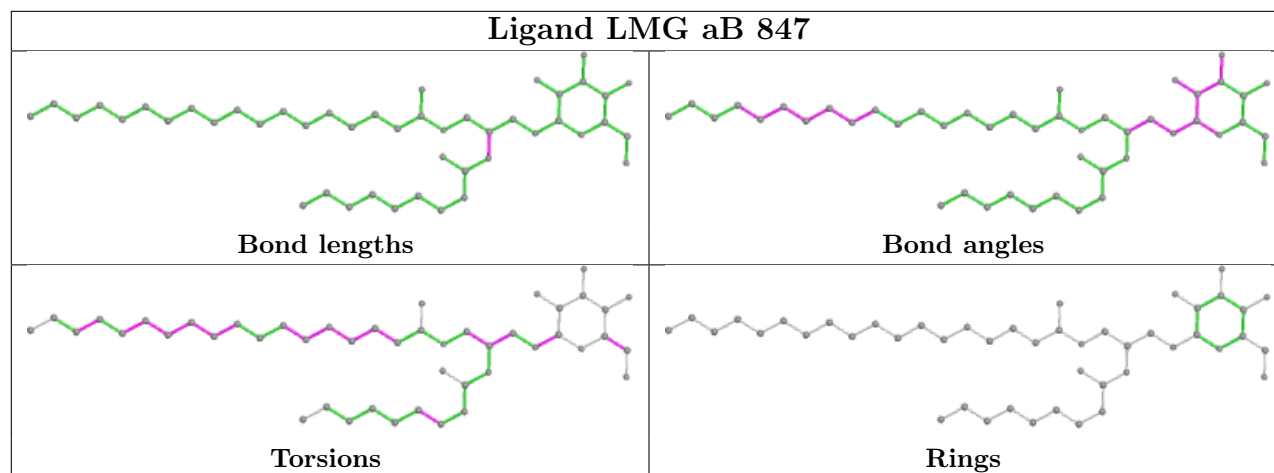
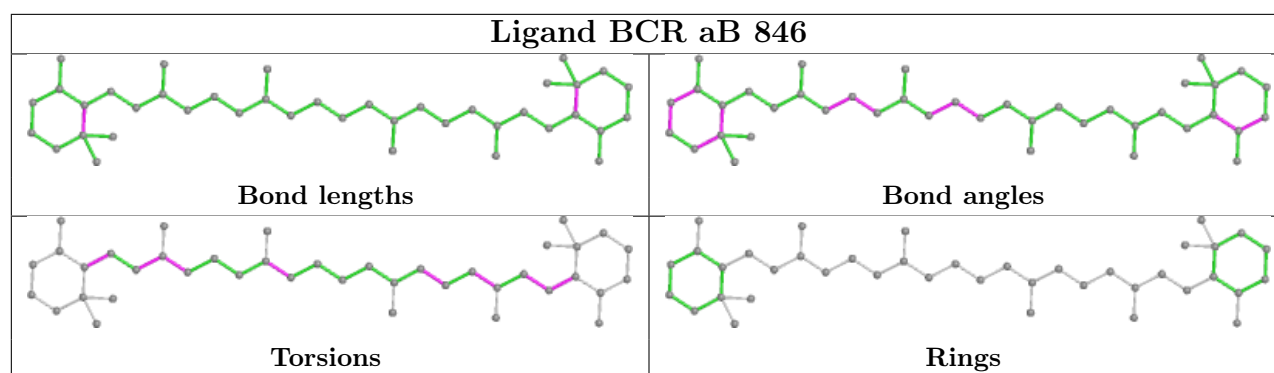
Ligand CLA aB 840



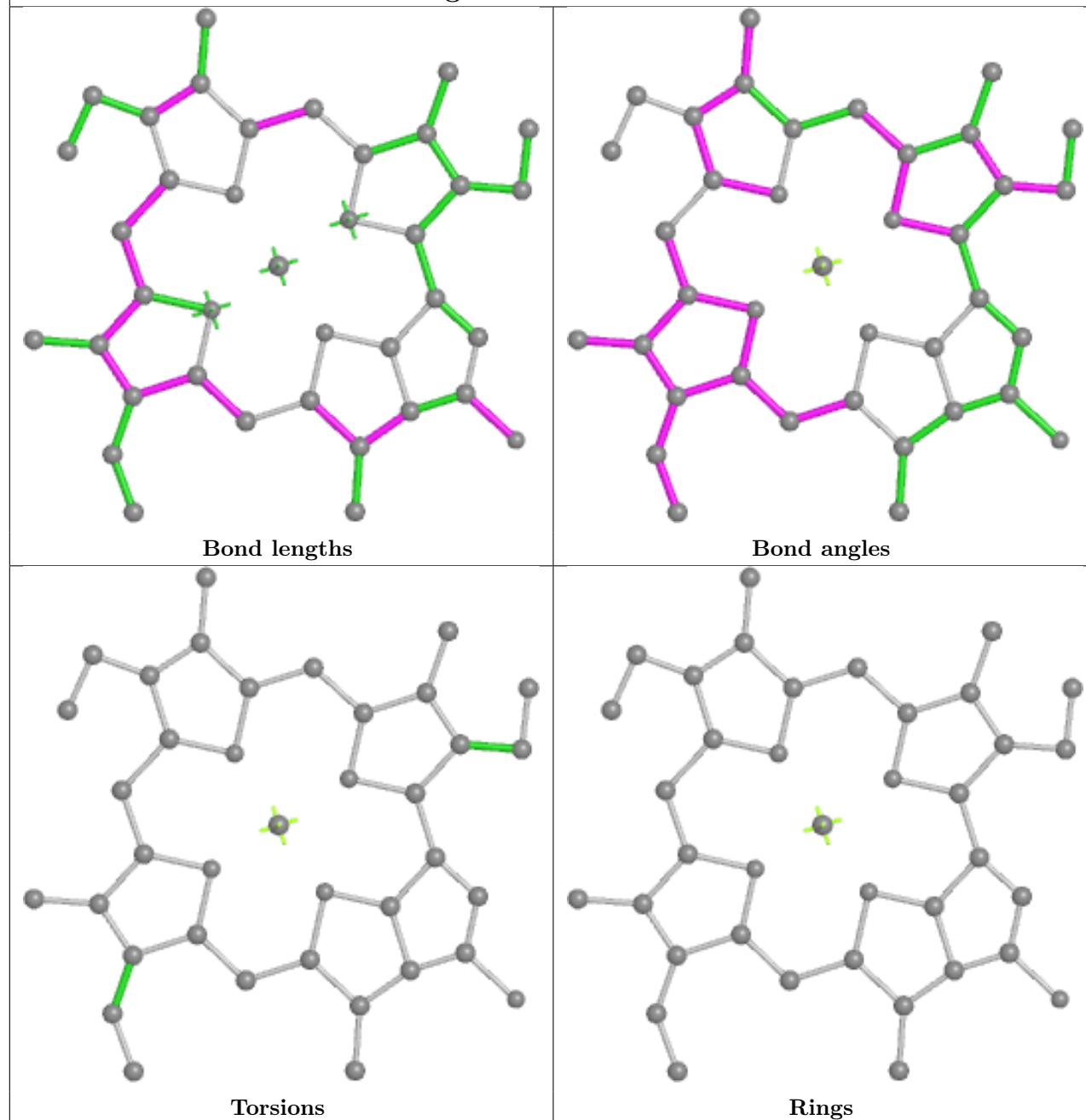
Ligand PQN aB 841



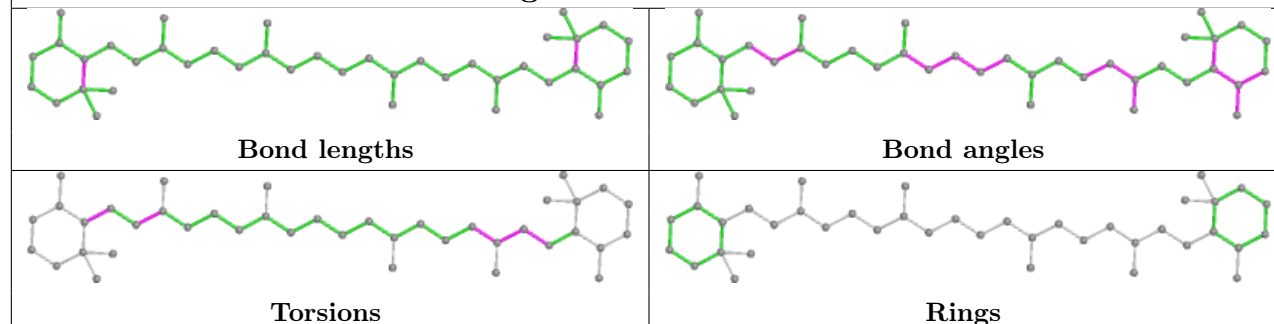




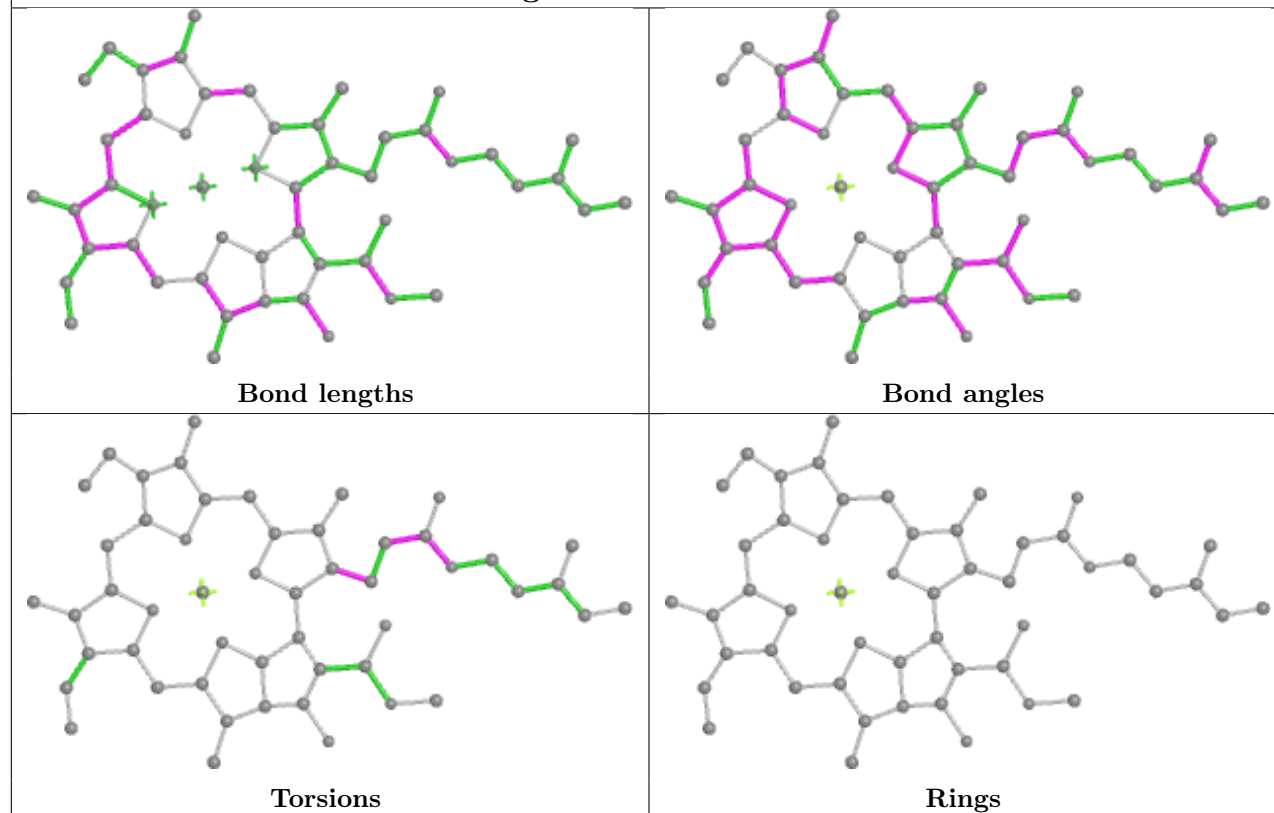
Ligand CLA aK 101



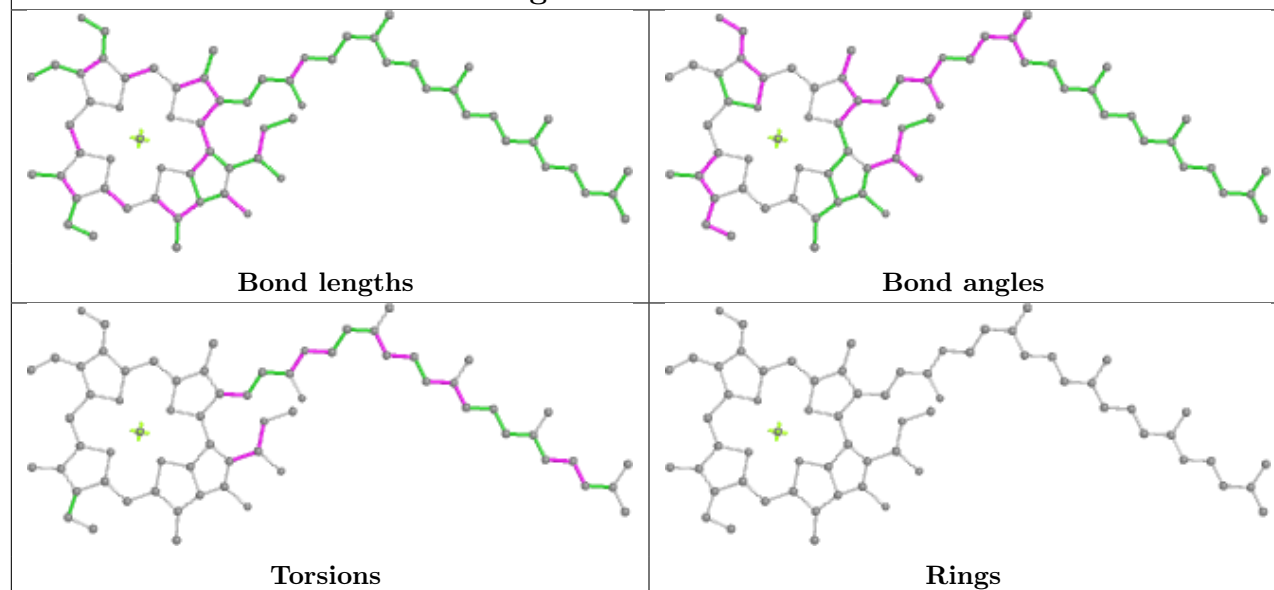
Ligand BCR aK 102

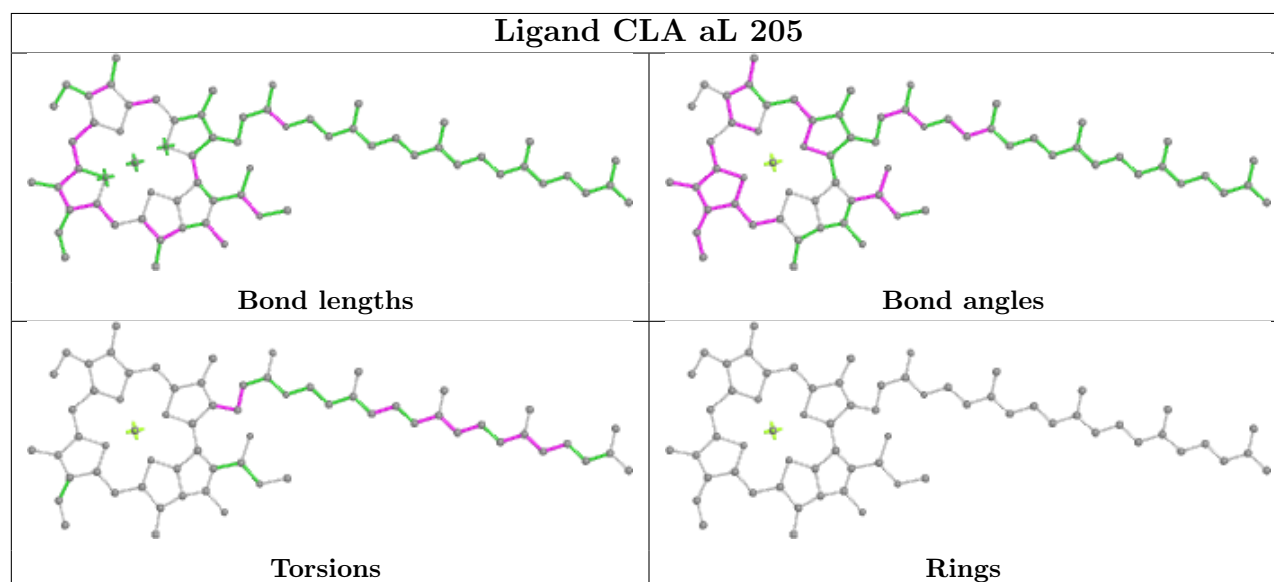
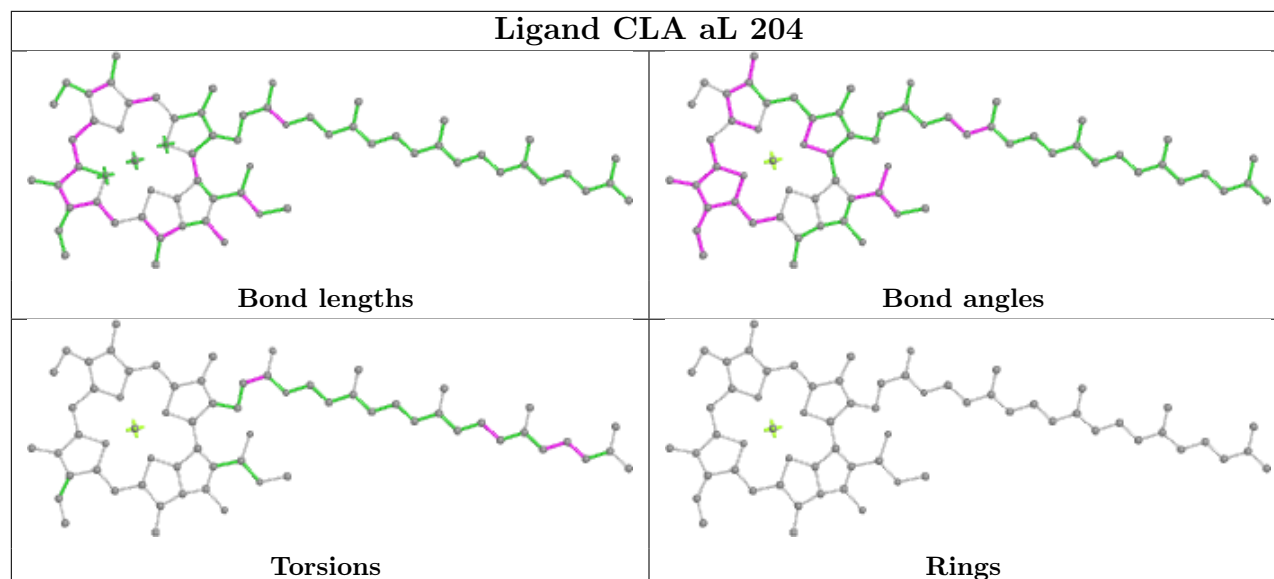
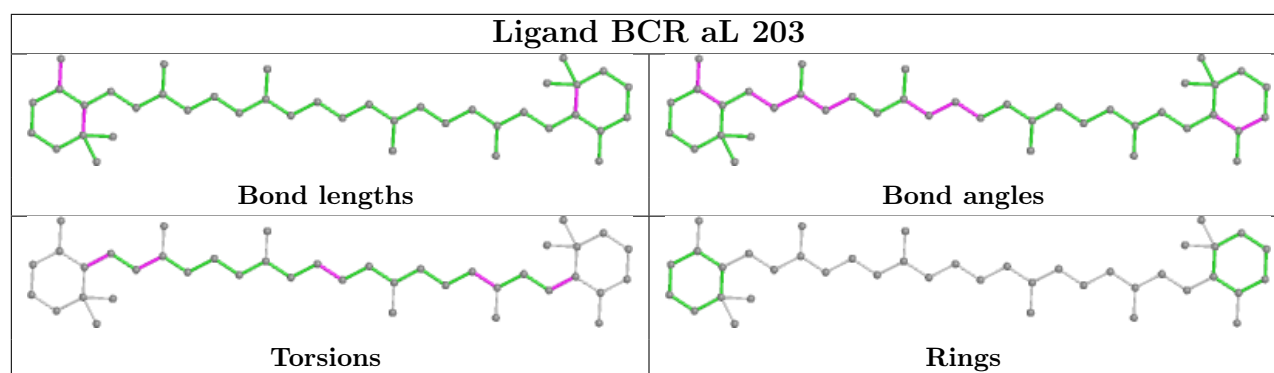


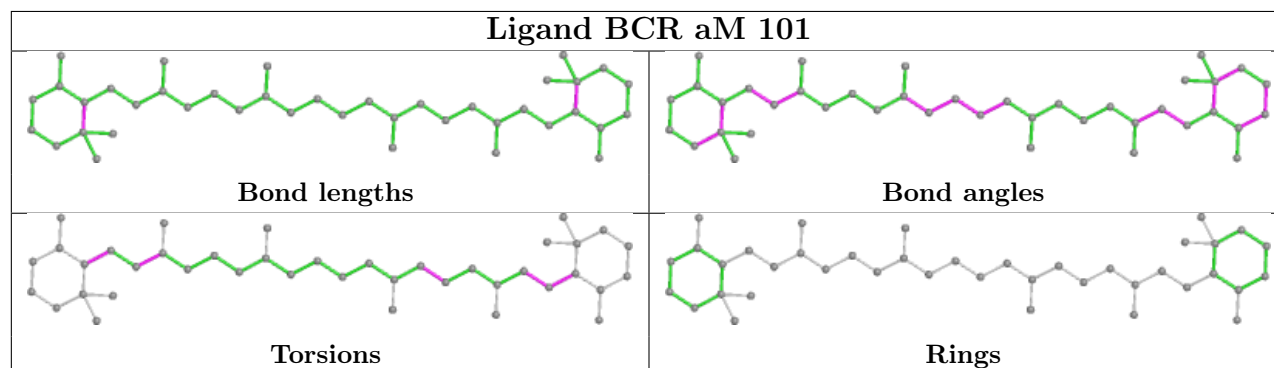
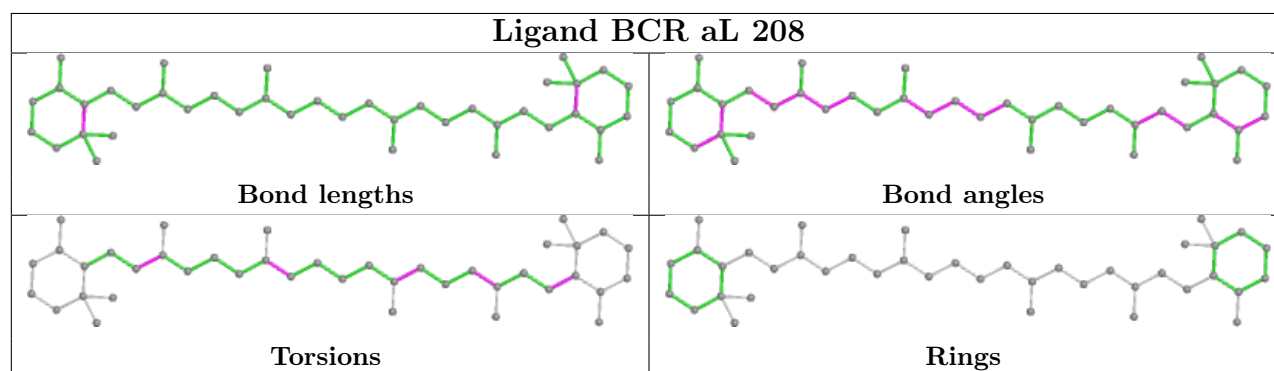
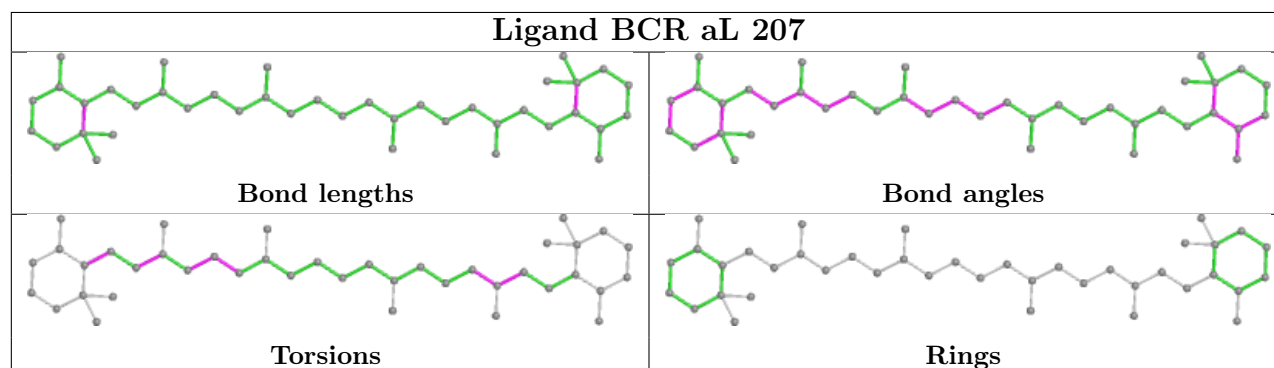
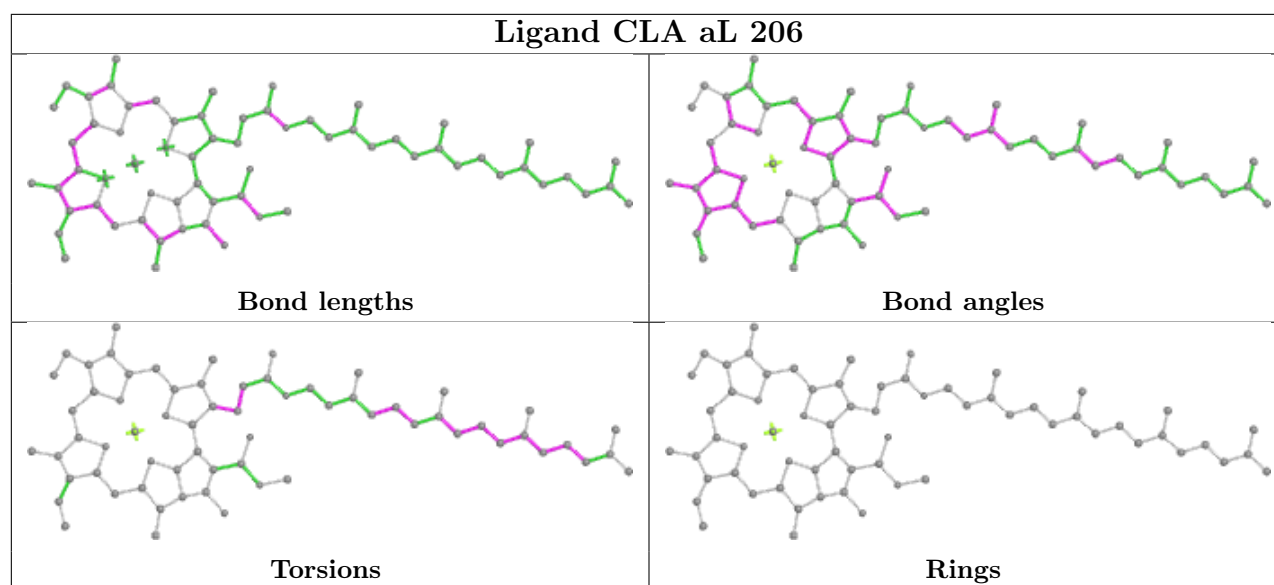
Ligand CLA aK 103

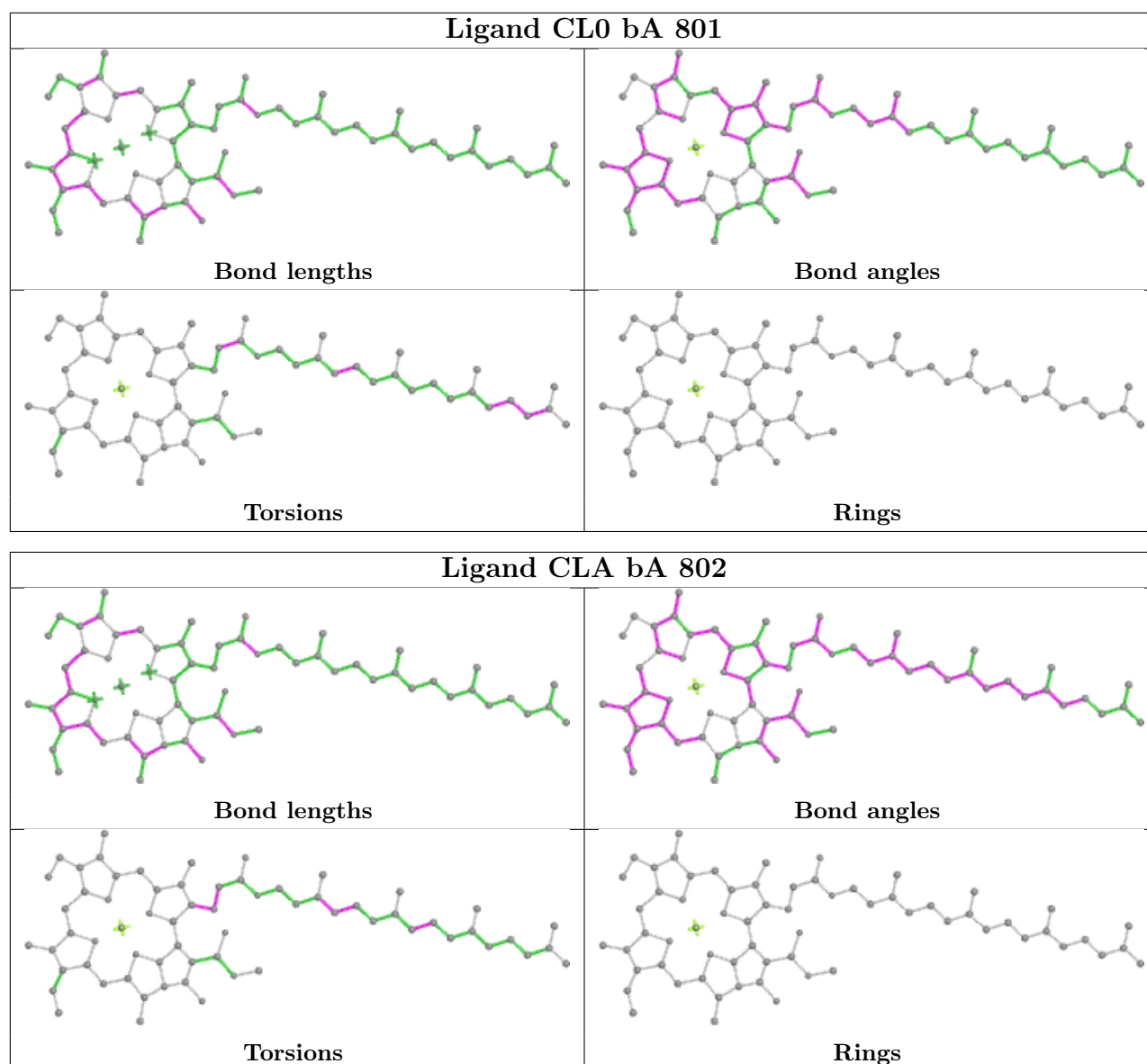


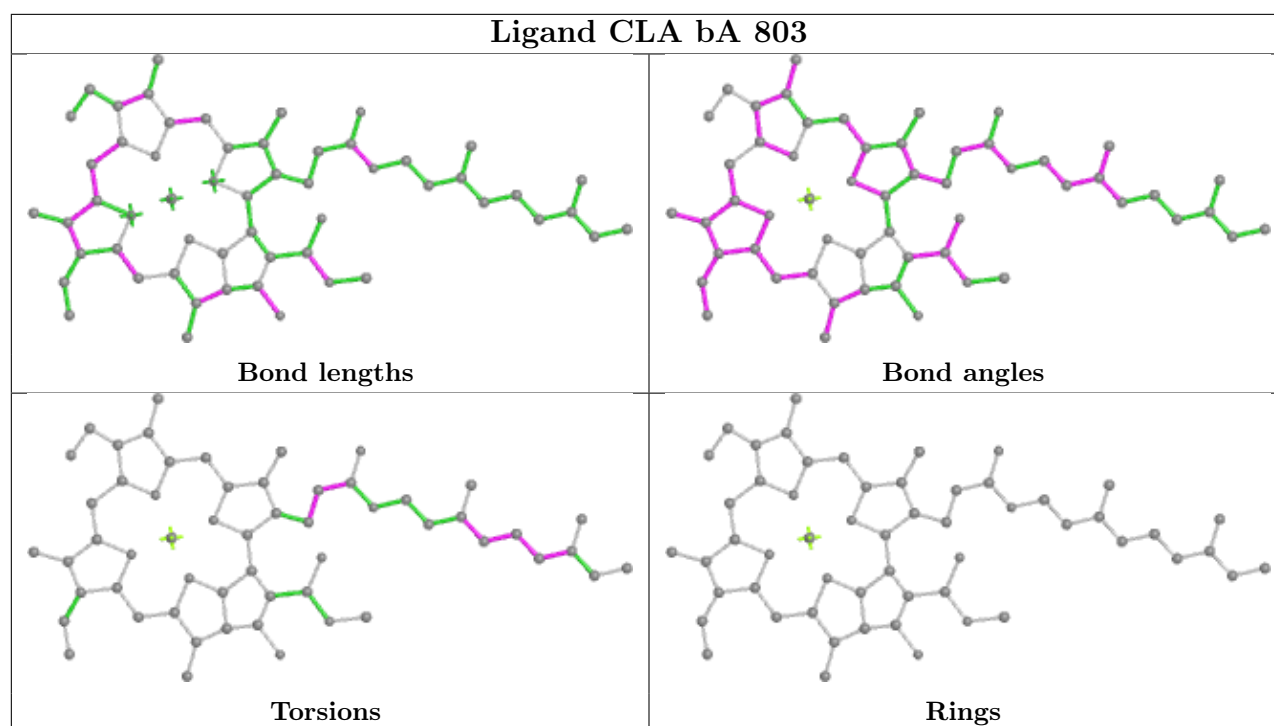
Ligand F6C aL 202



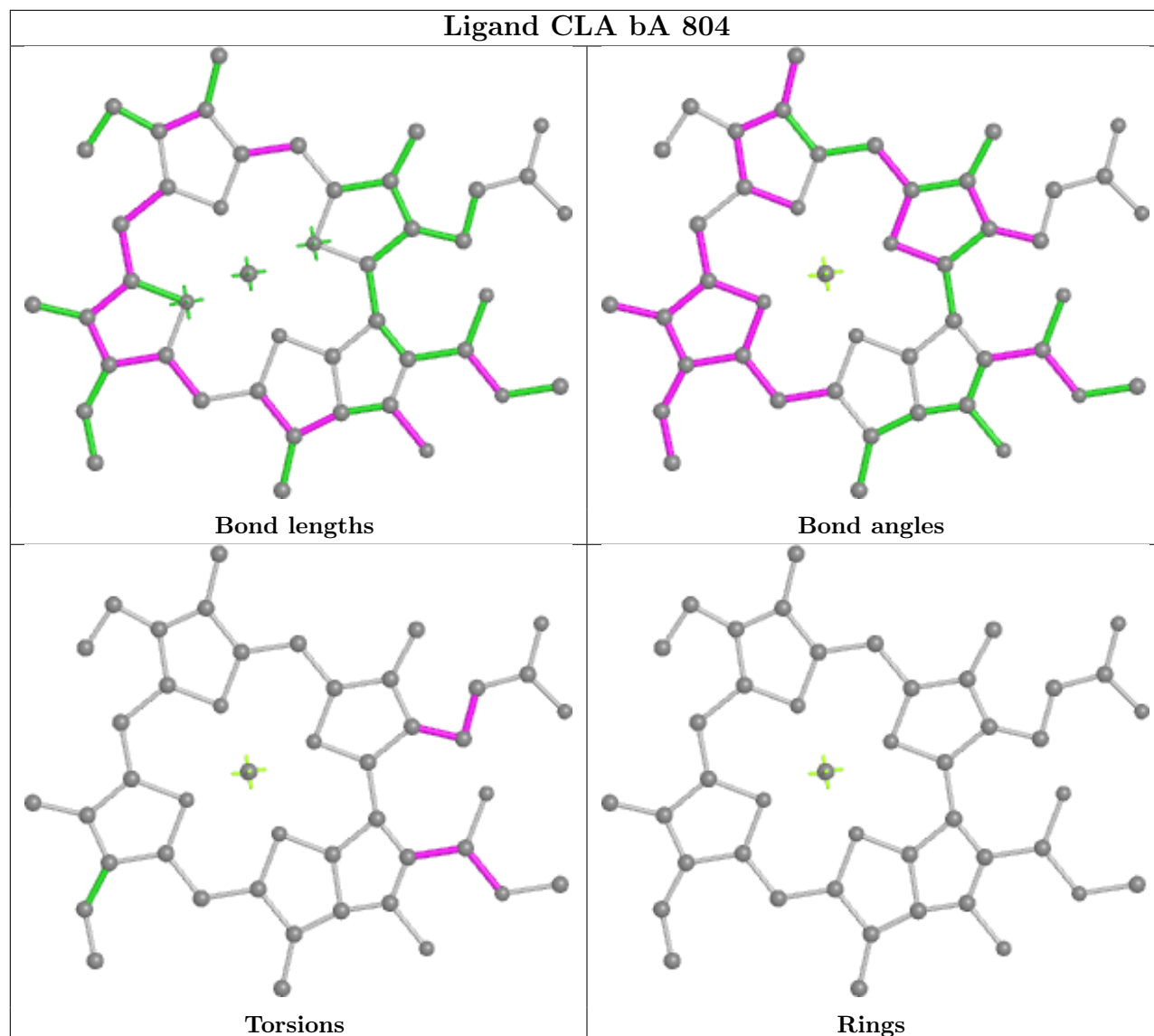




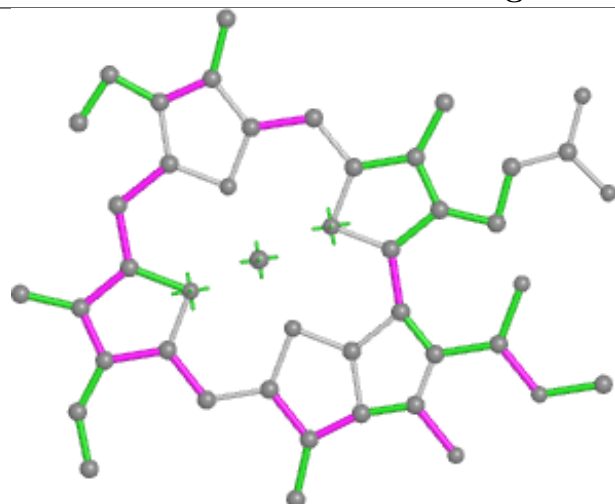




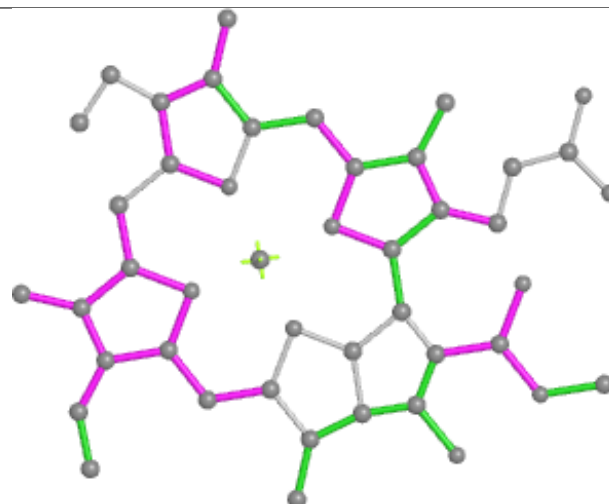
Ligand CLA bA 804



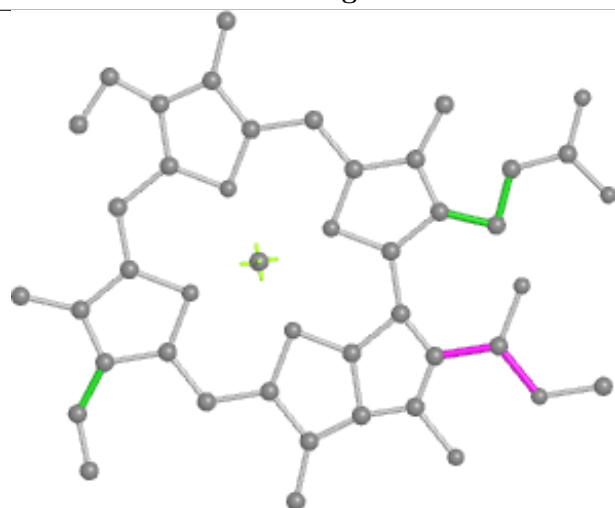
Ligand CLA bA 805



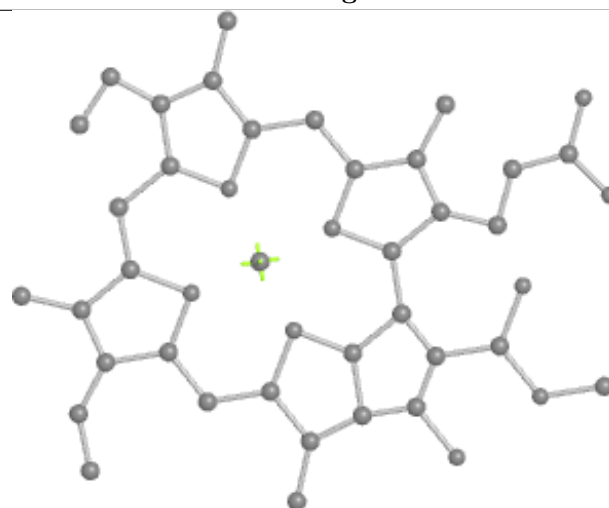
Bond lengths



Bond angles

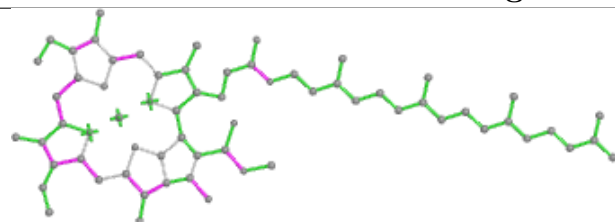


Torsions

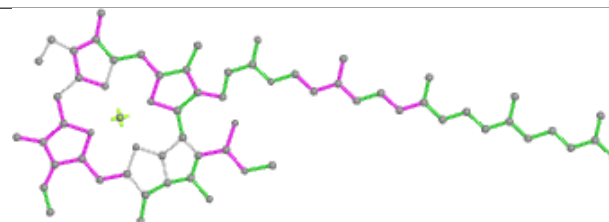


Rings

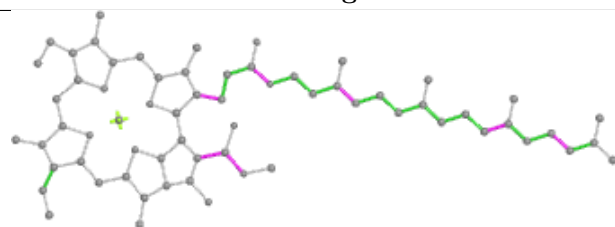
Ligand CLA bA 806



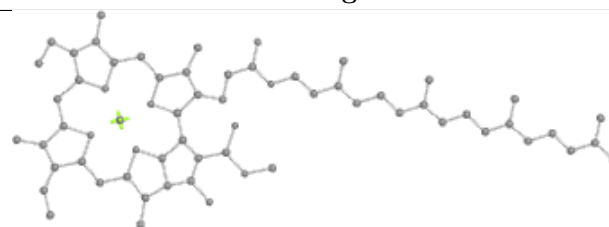
Bond lengths



Bond angles

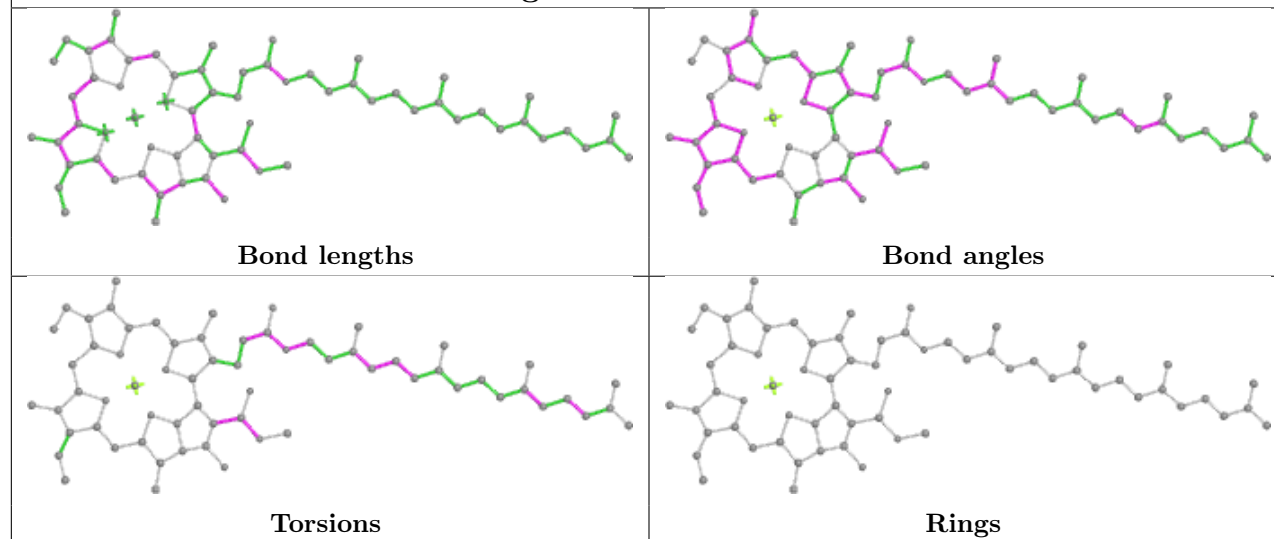


Torsions

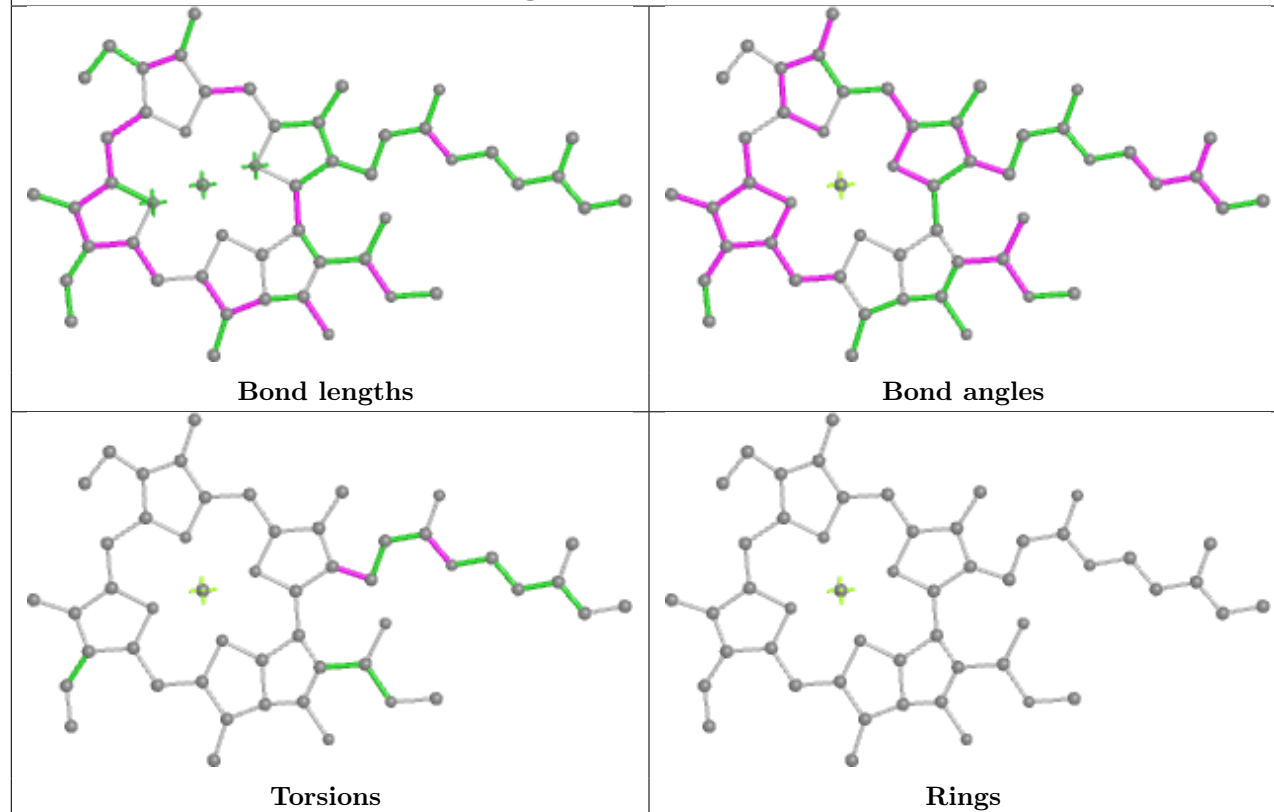


Rings

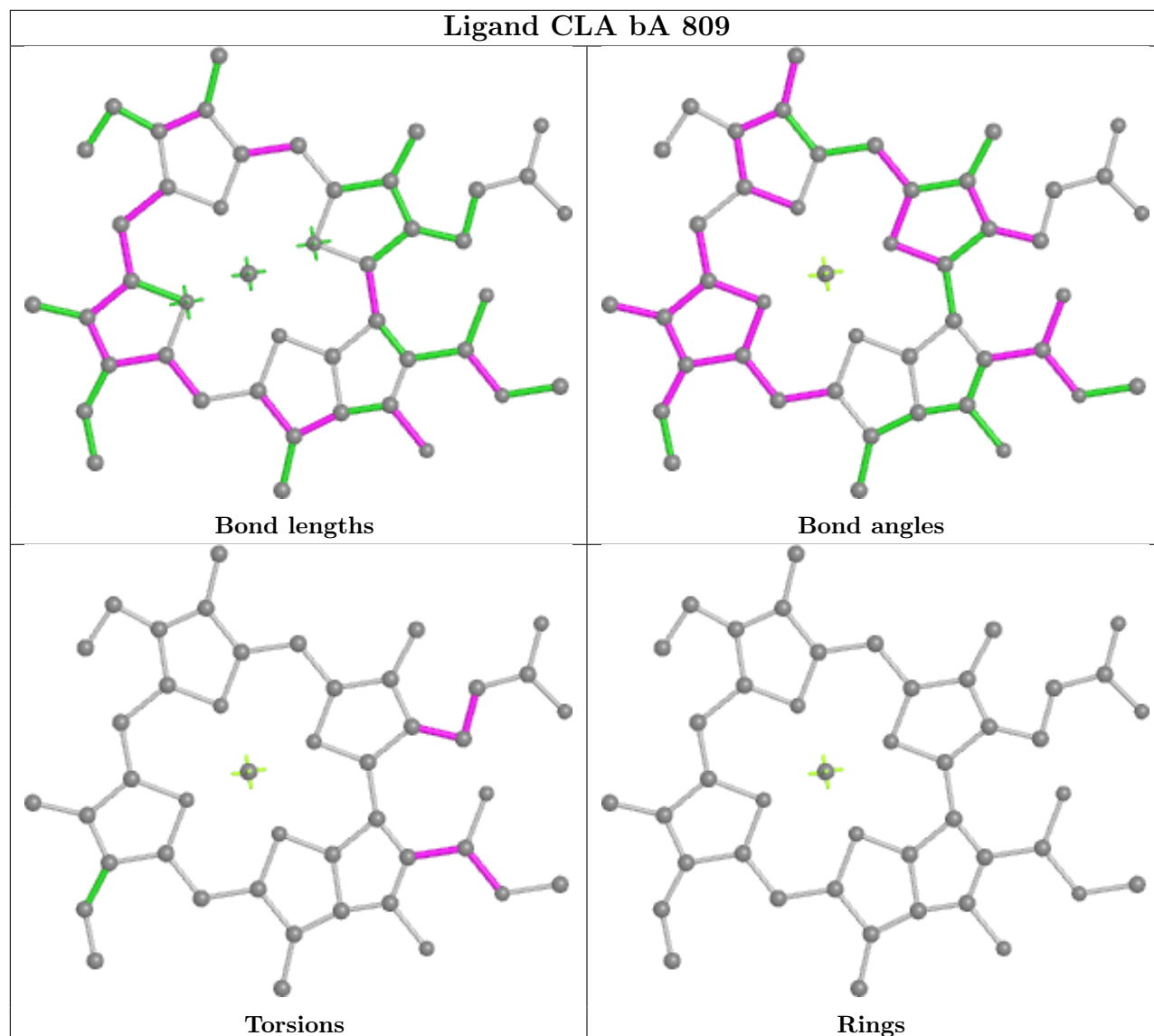
Ligand CLA bA 807



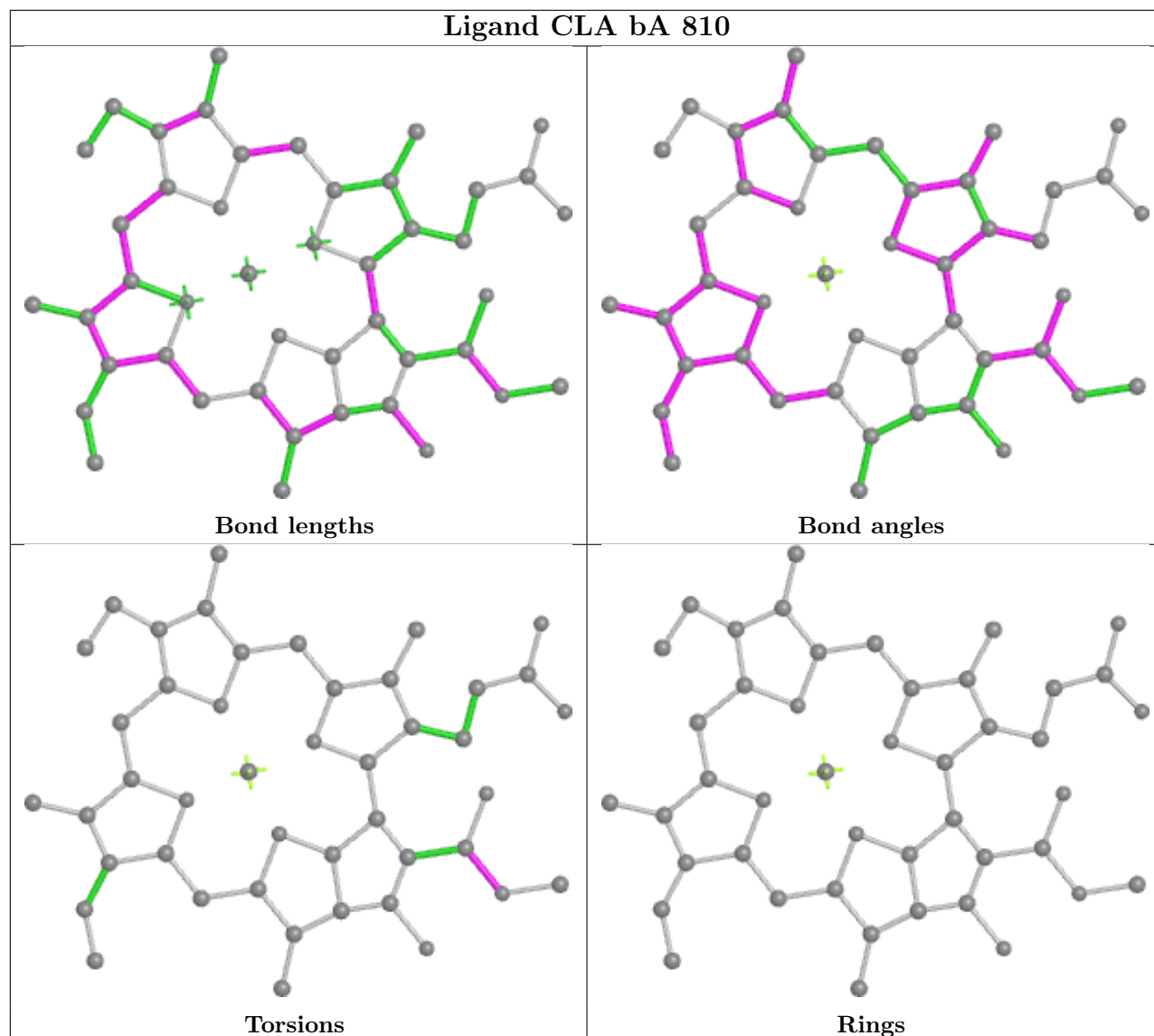
Ligand CLA bA 808



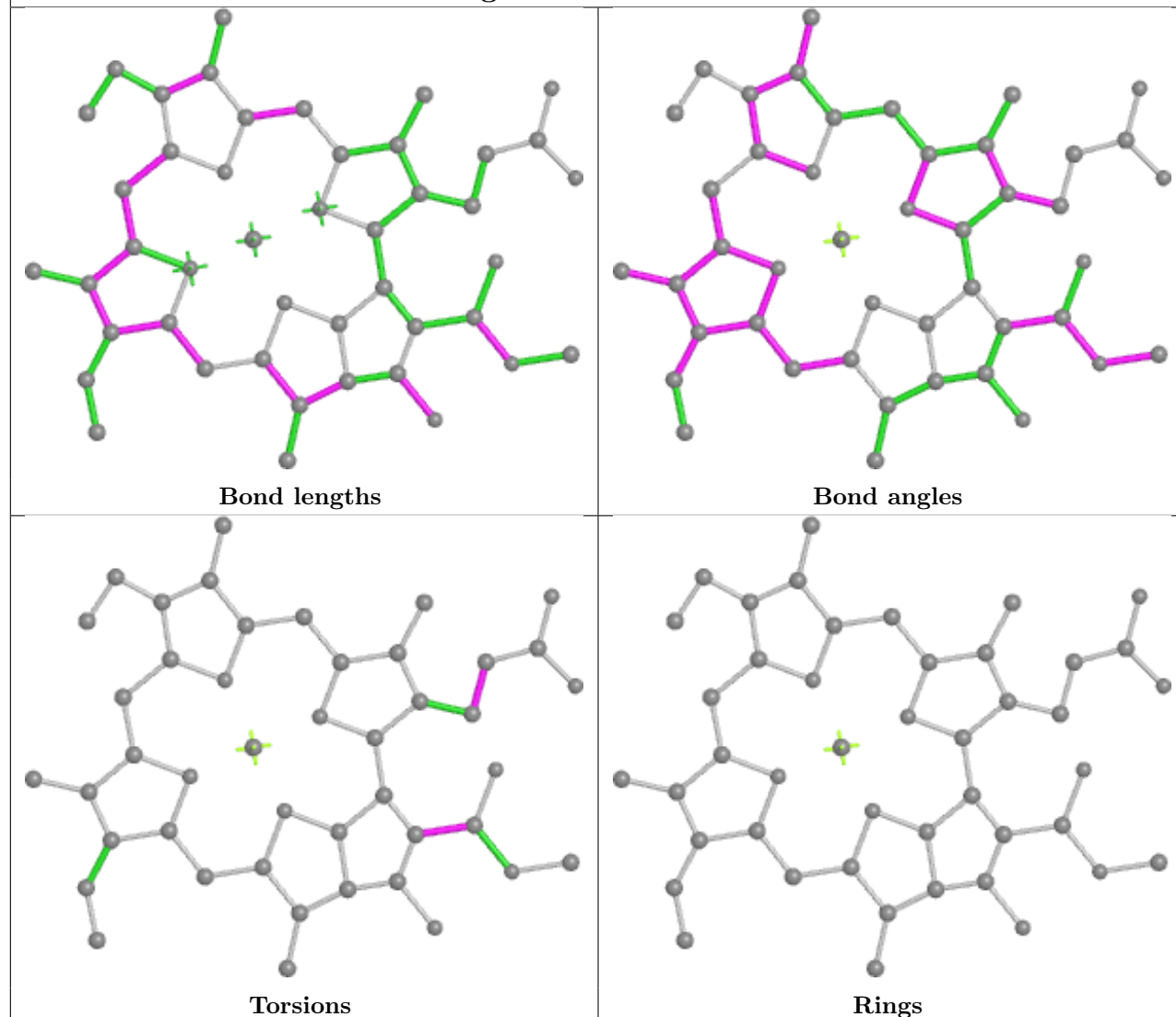
Ligand CLA bA 809



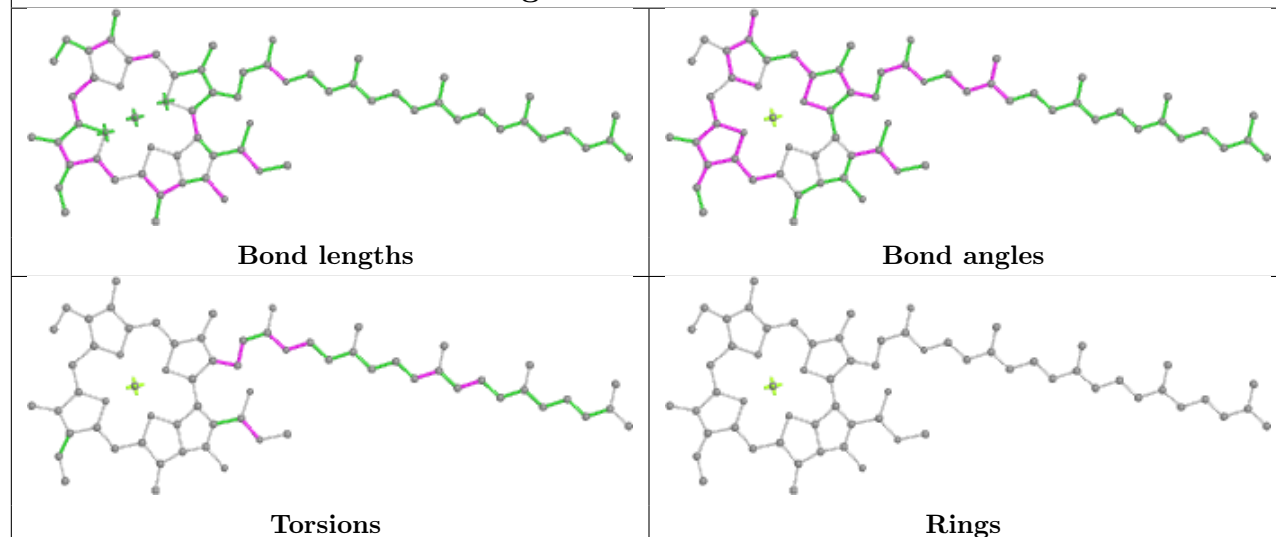
Ligand CLA bA 810

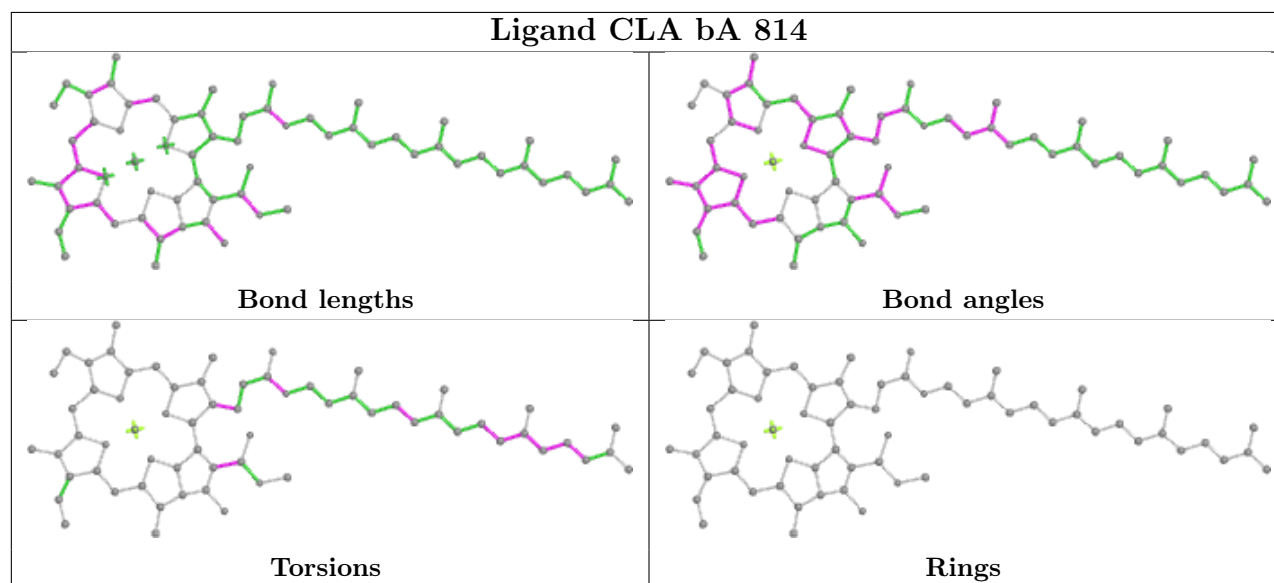
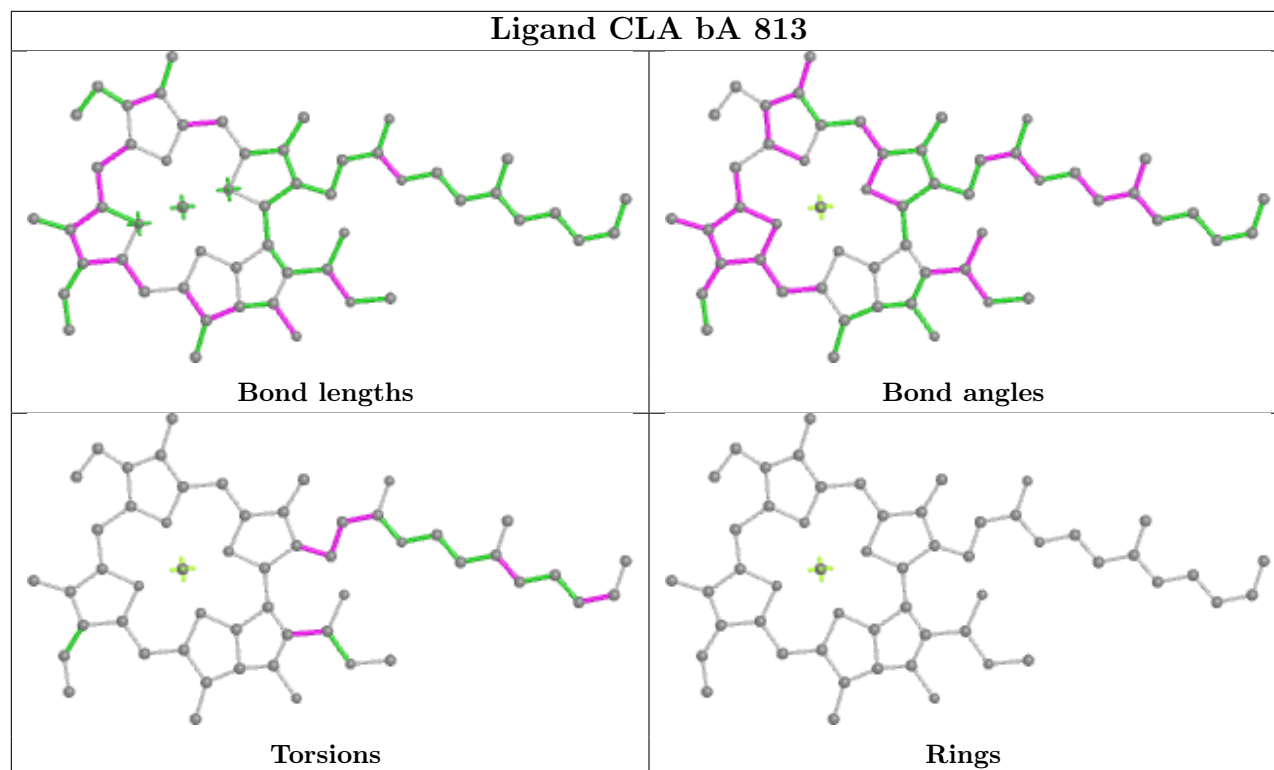


Ligand CLA bA 811

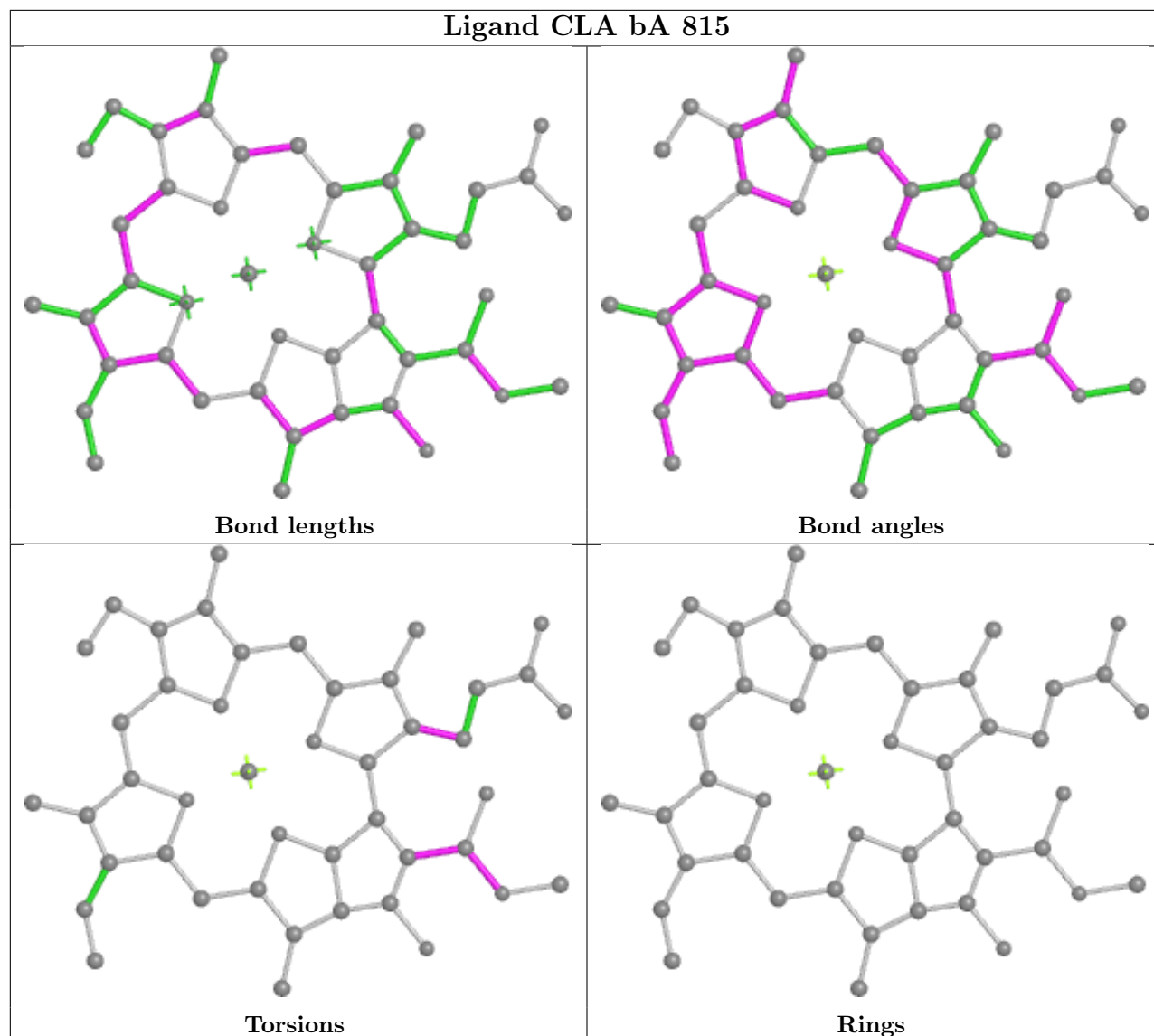


Ligand CLA bA 812

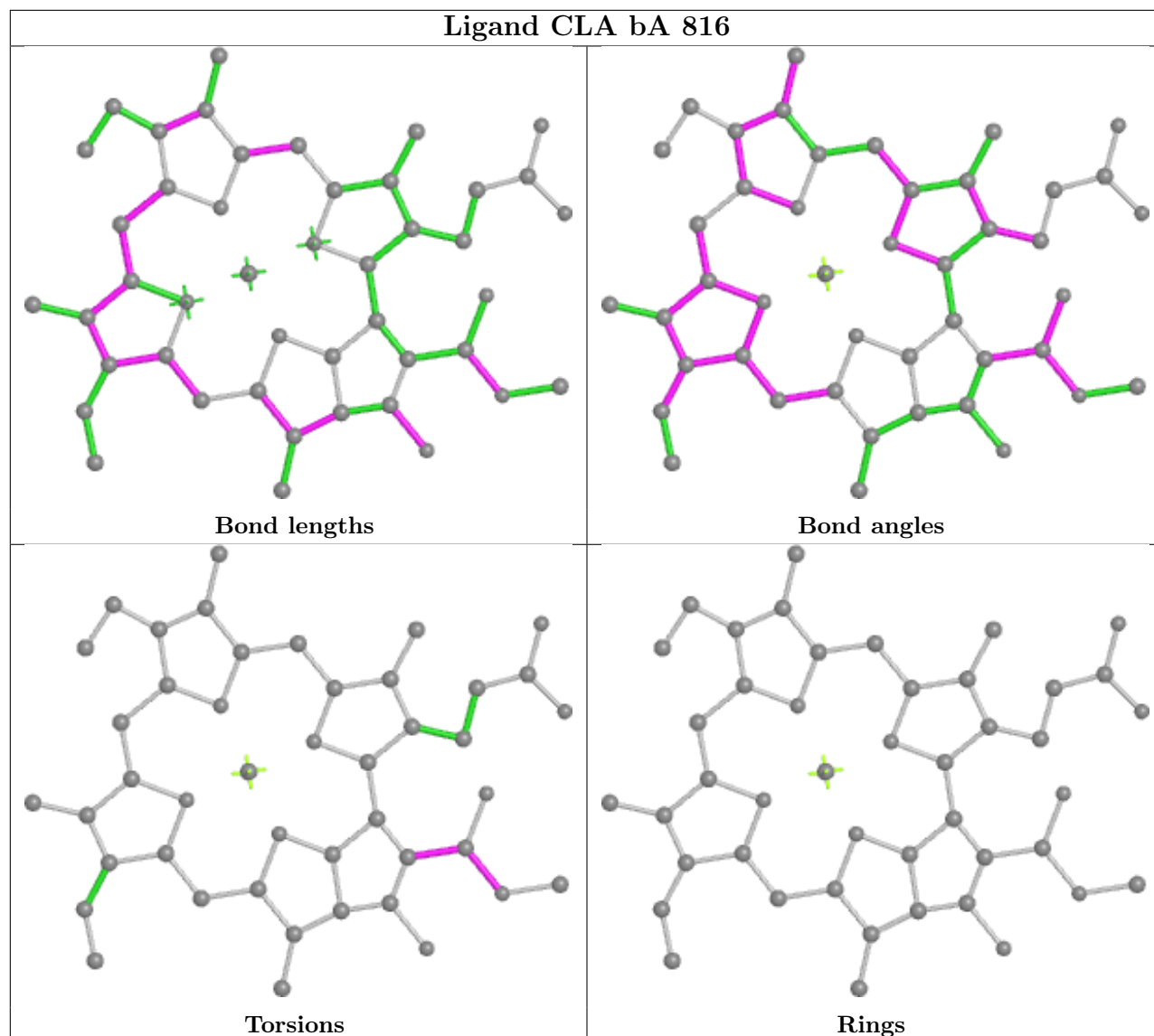




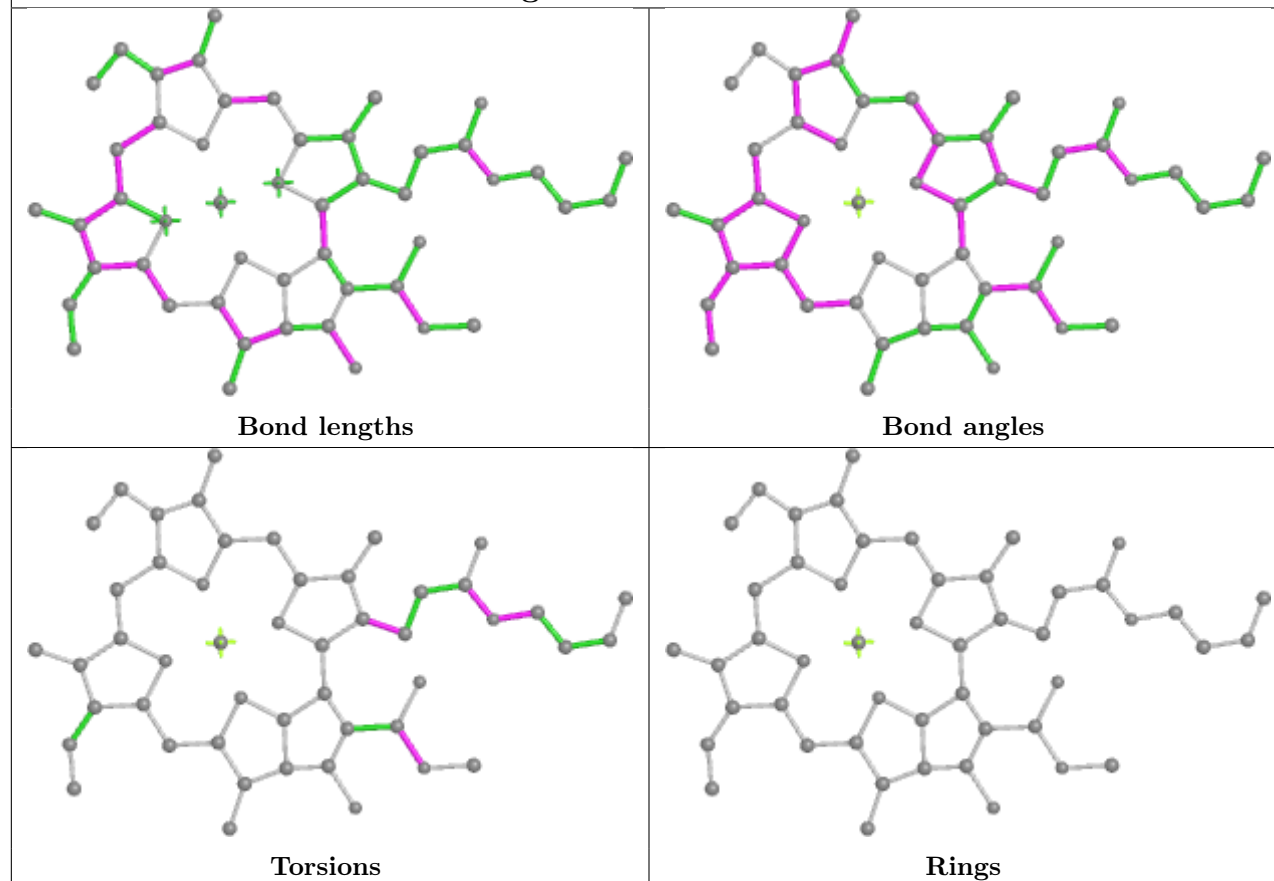
Ligand CLA bA 815



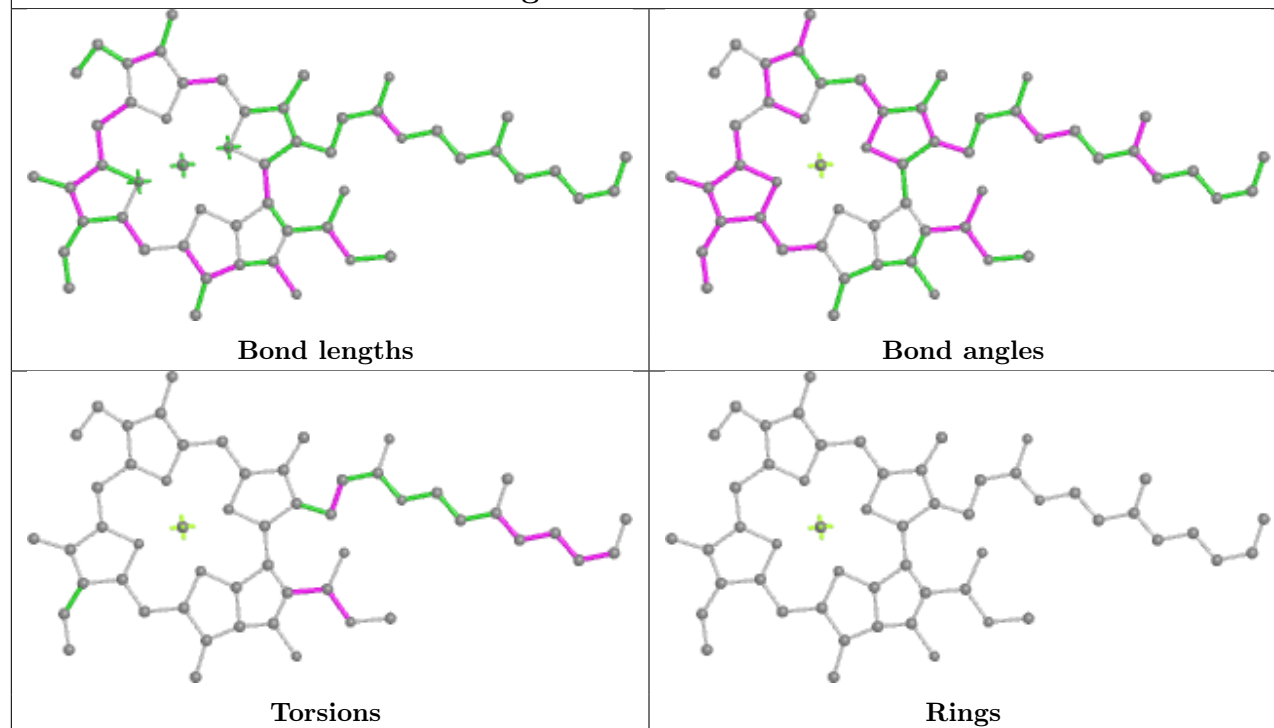
Ligand CLA bA 816



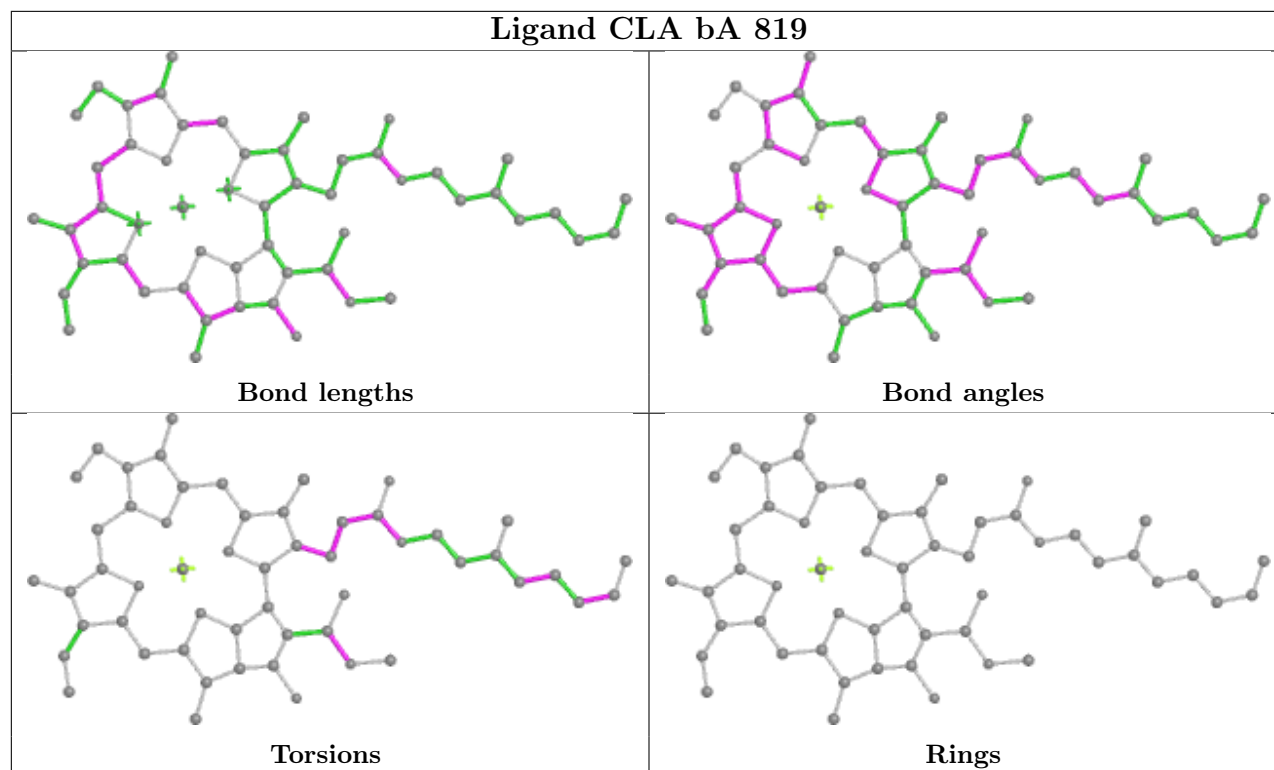
Ligand CLA bA 817



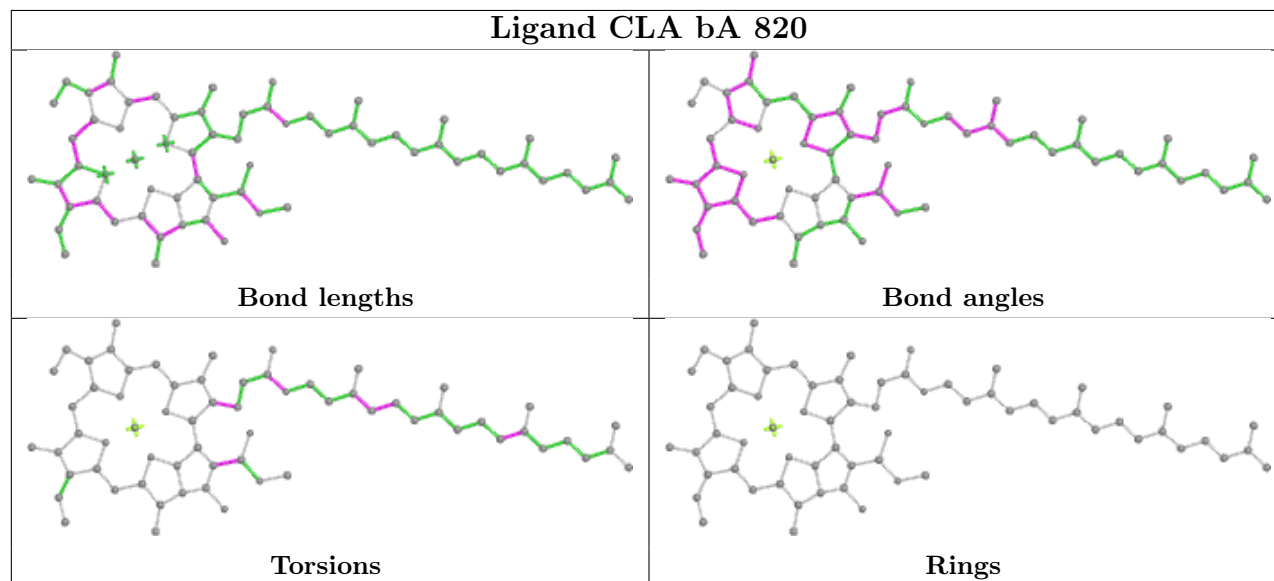
Ligand CLA bA 818

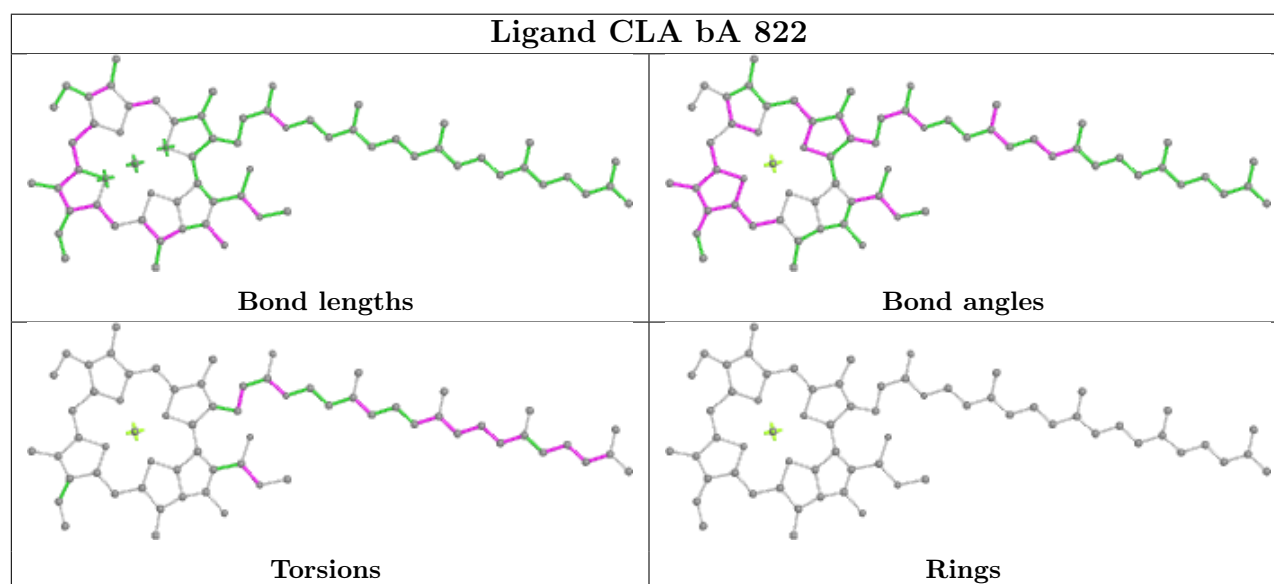
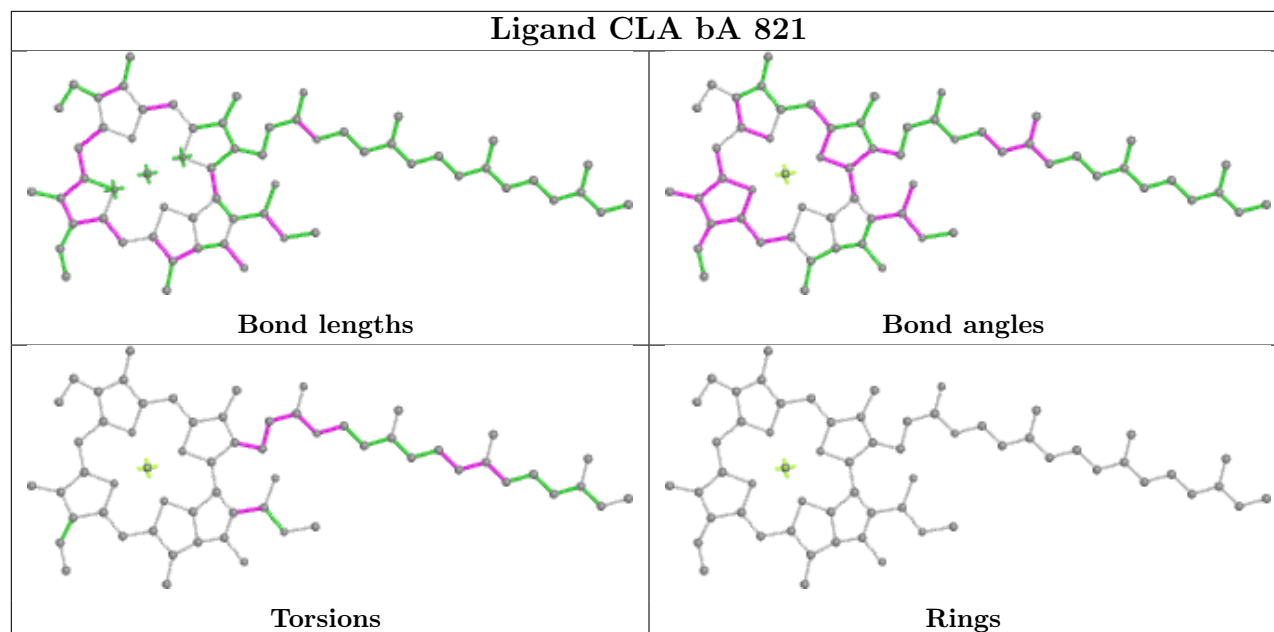


Ligand CLA bA 819

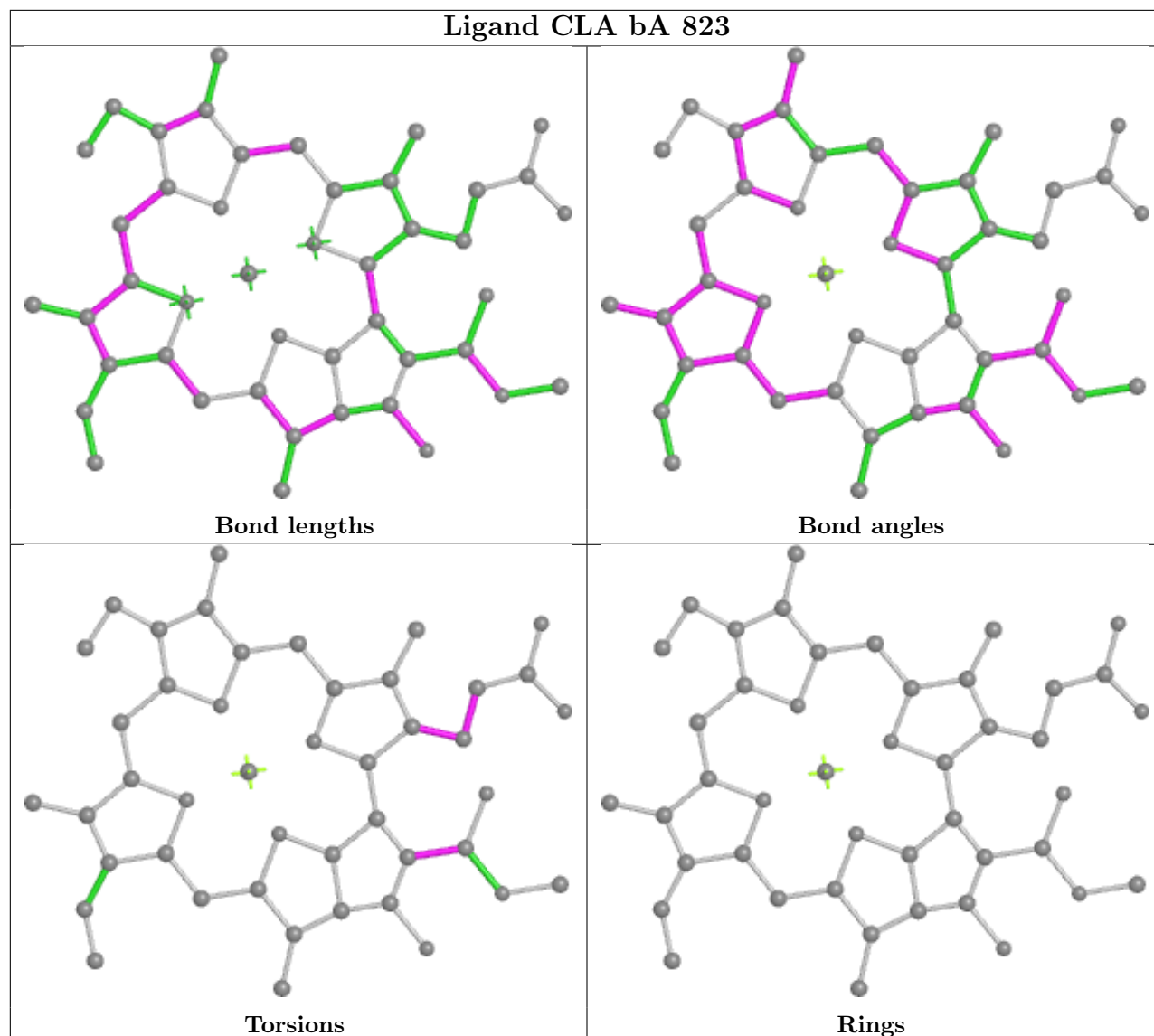


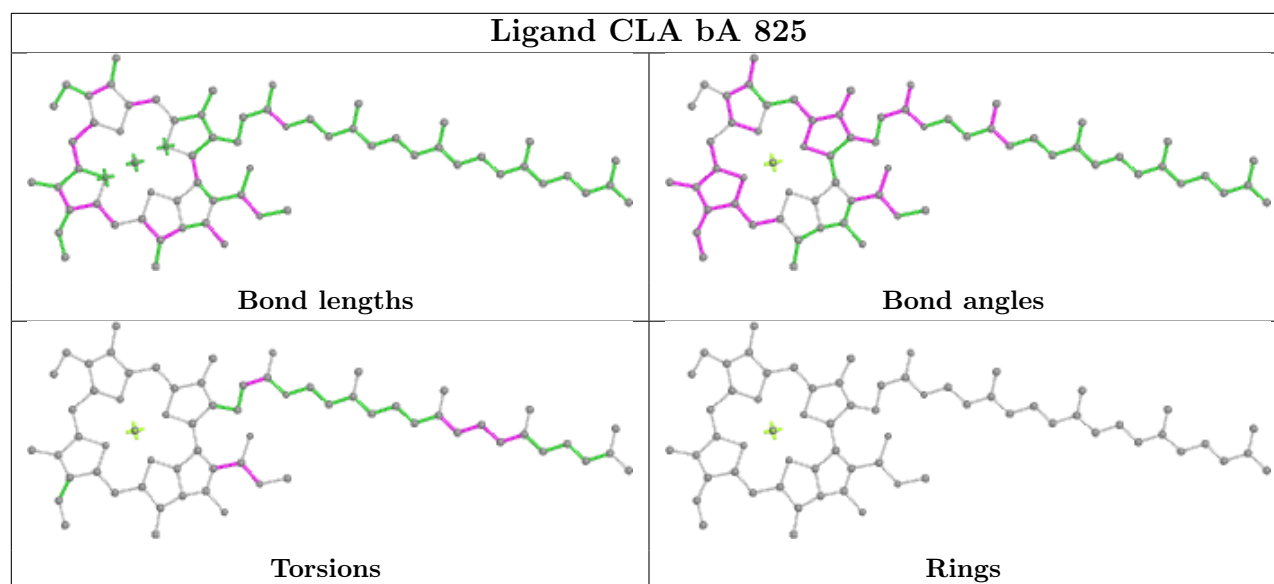
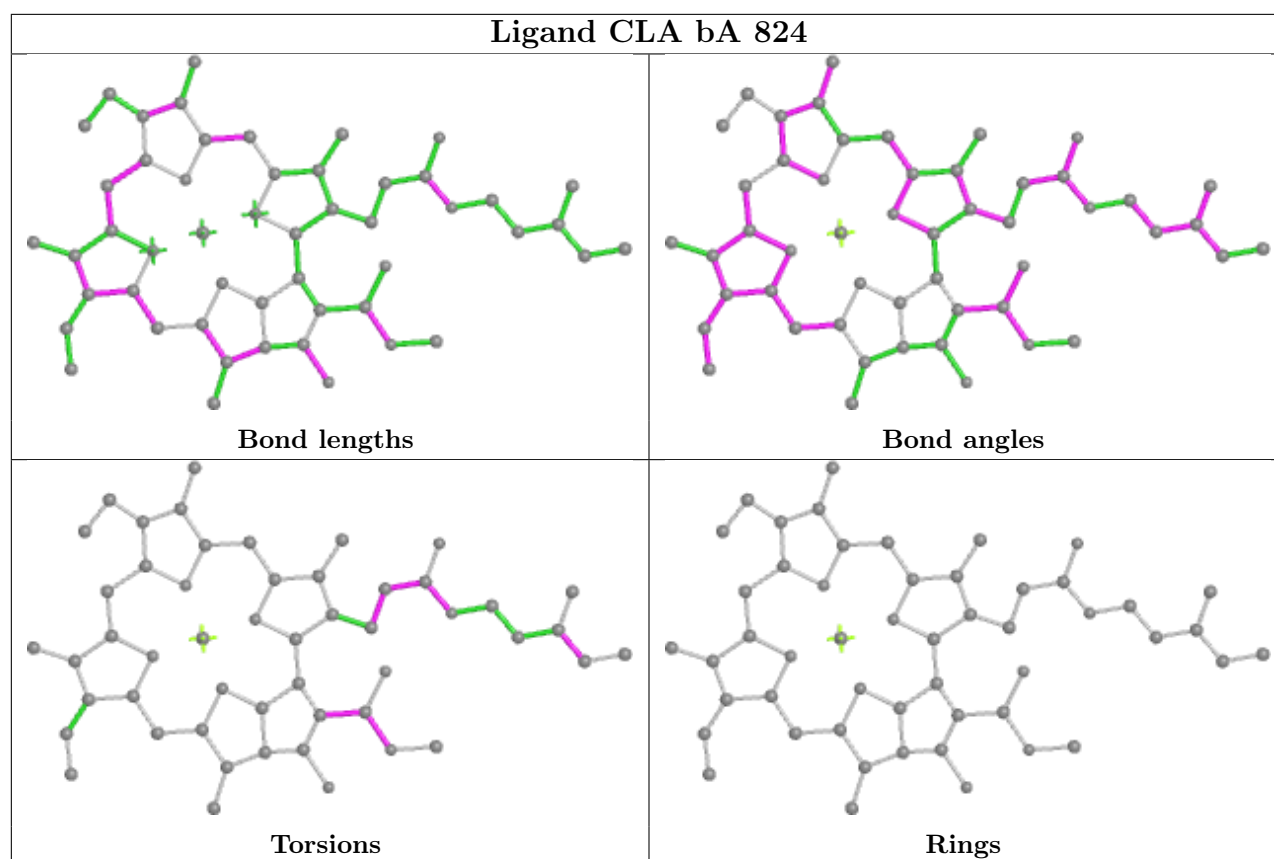
Ligand CLA bA 820

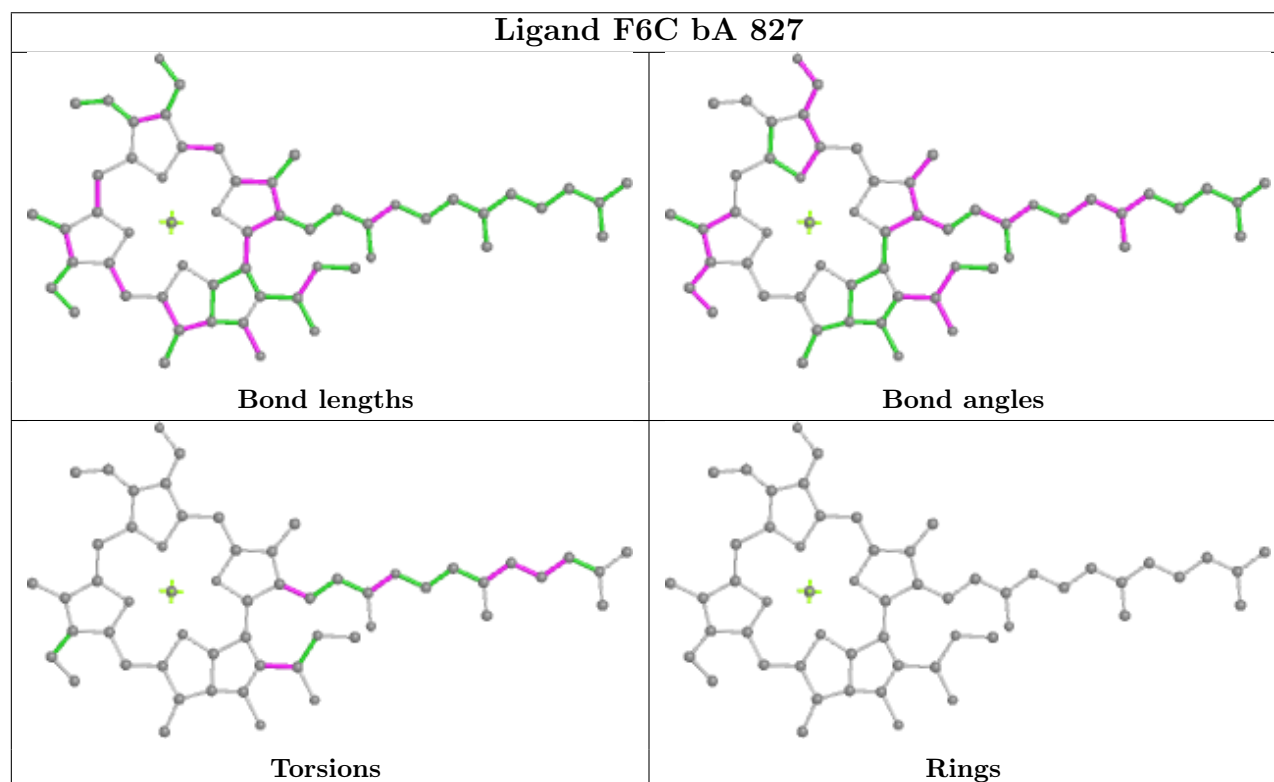
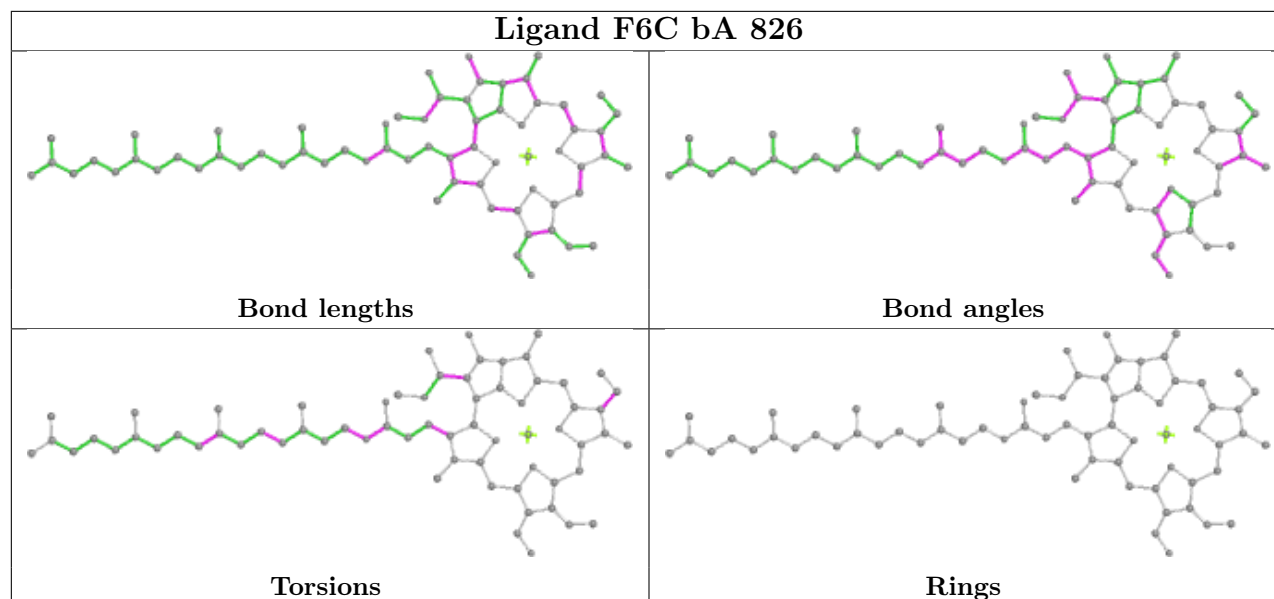


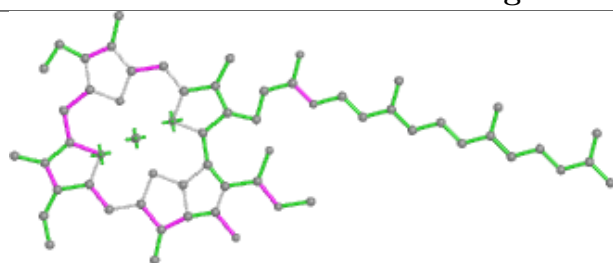


Ligand CLA bA 823

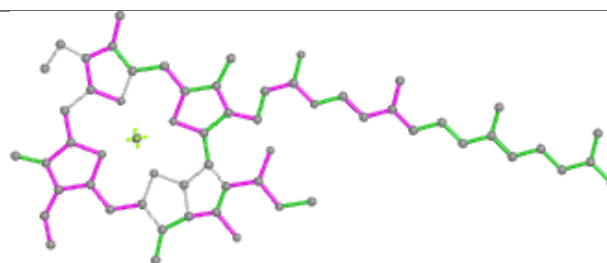




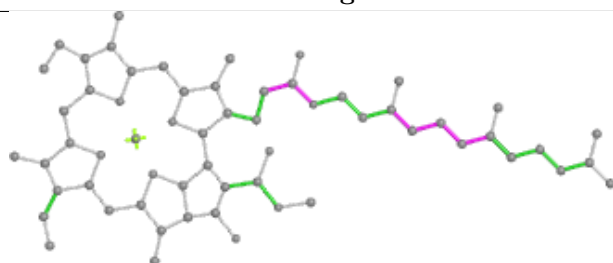


Ligand CLA bA 828

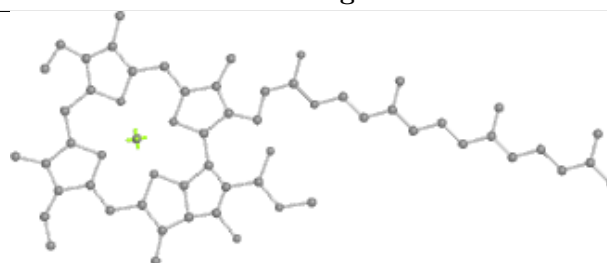
Bond lengths



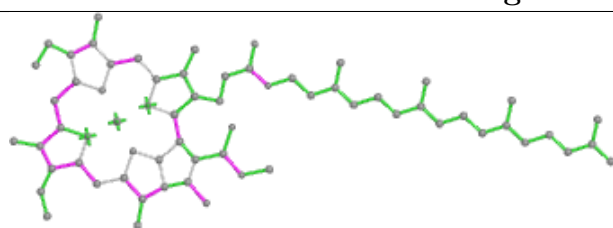
Bond angles



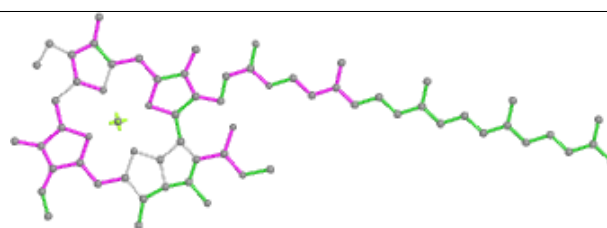
Torsions



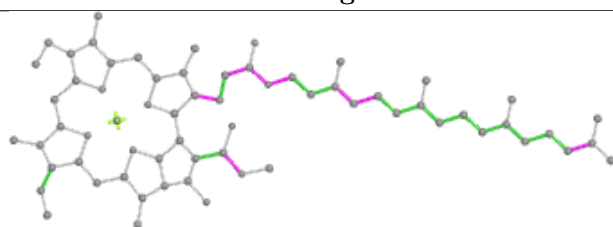
Rings

Ligand CLA bA 829

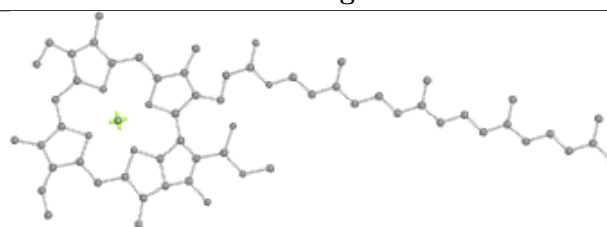
Bond lengths



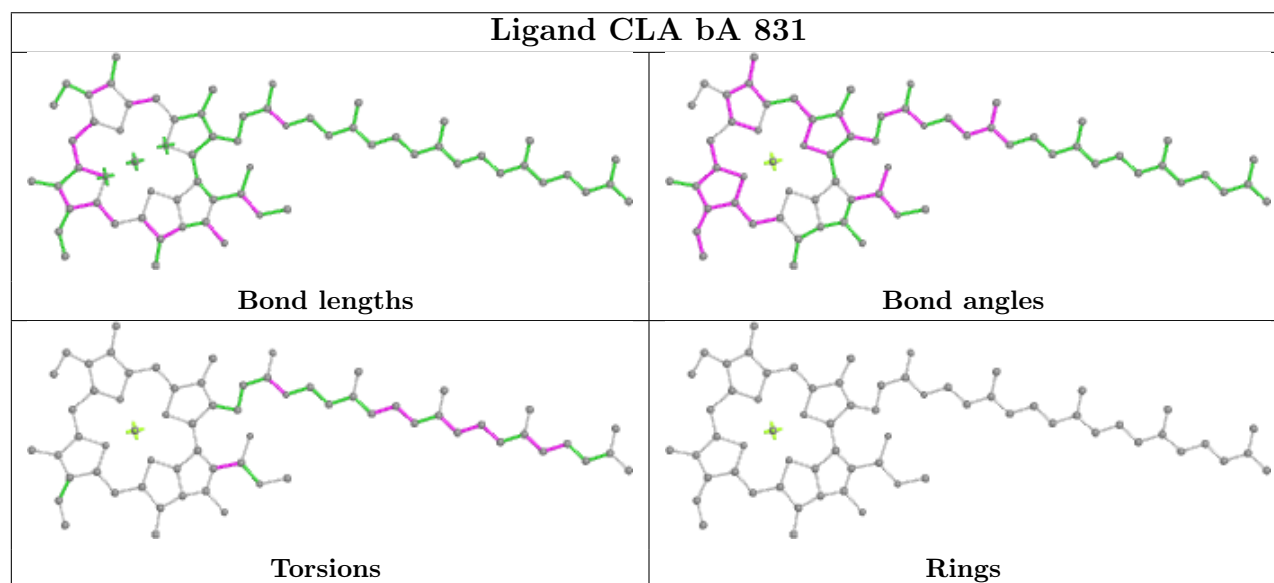
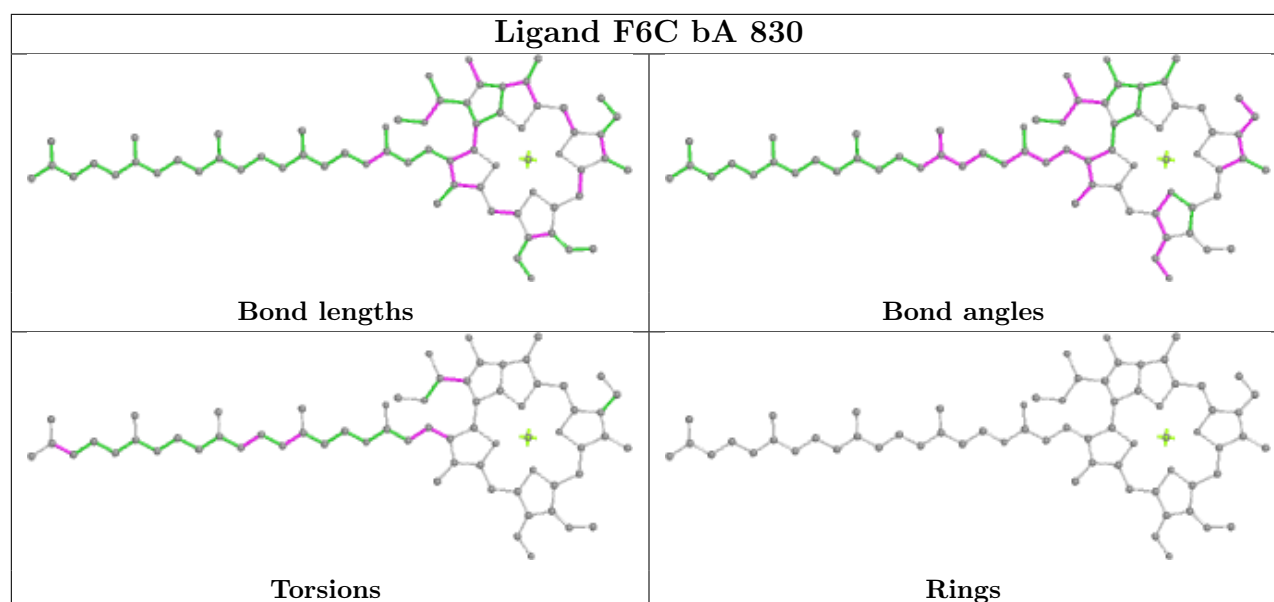
Bond angles

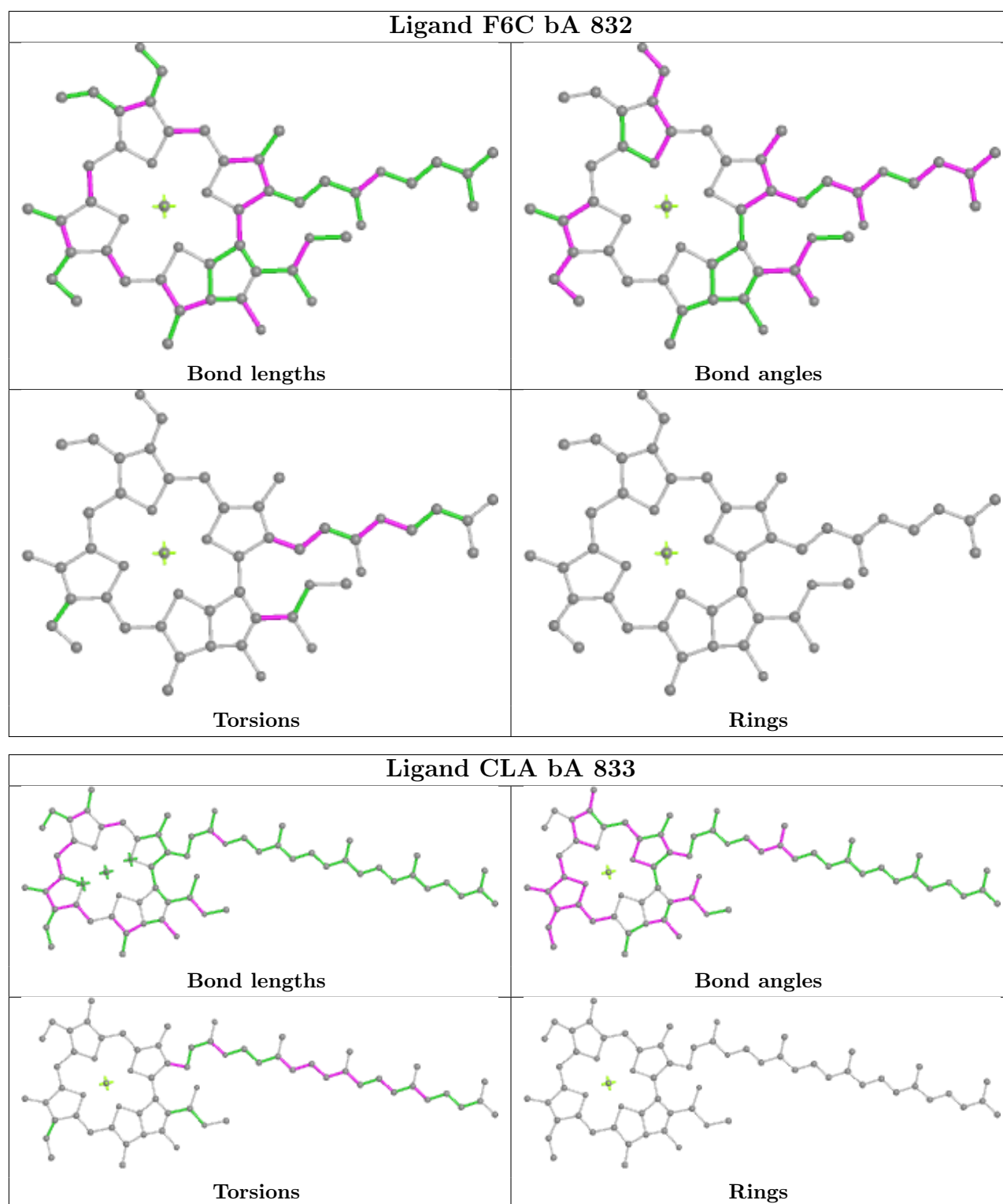


Torsions

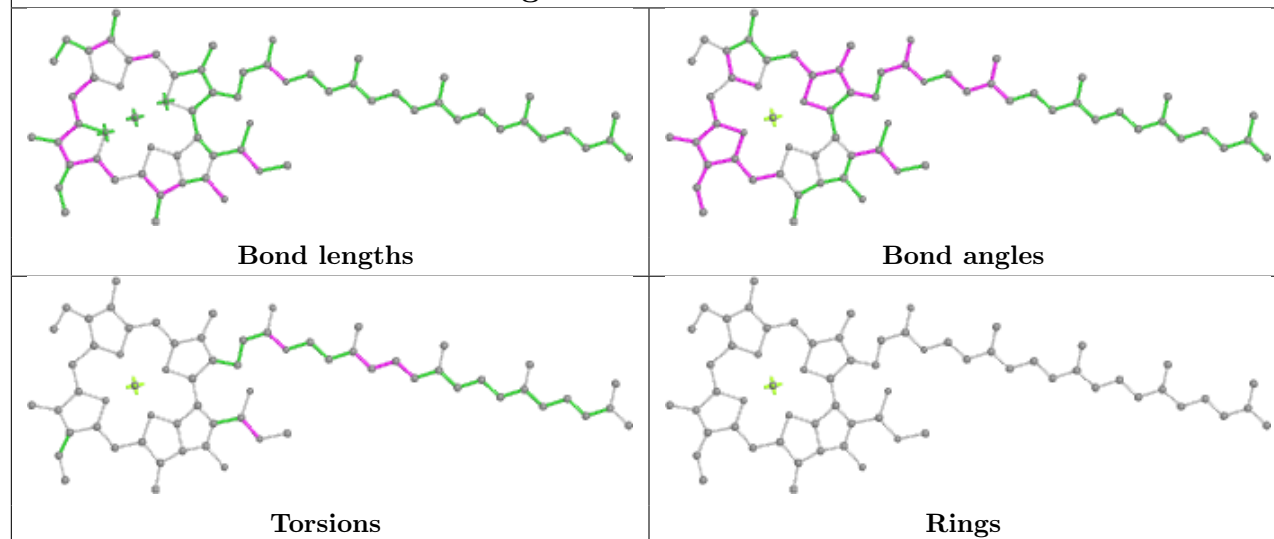


Rings

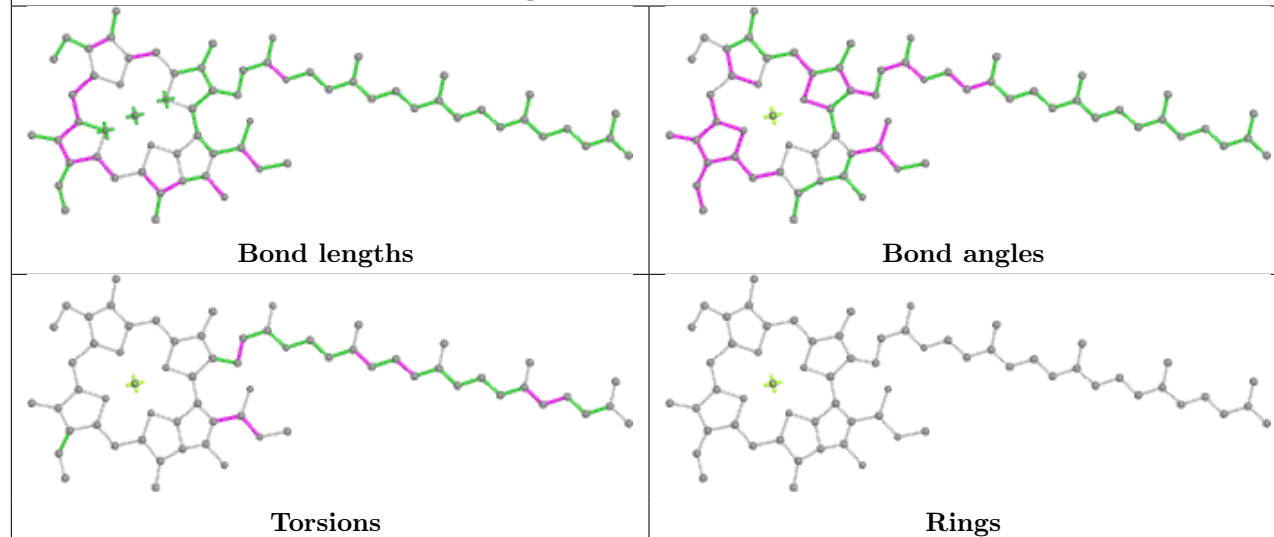




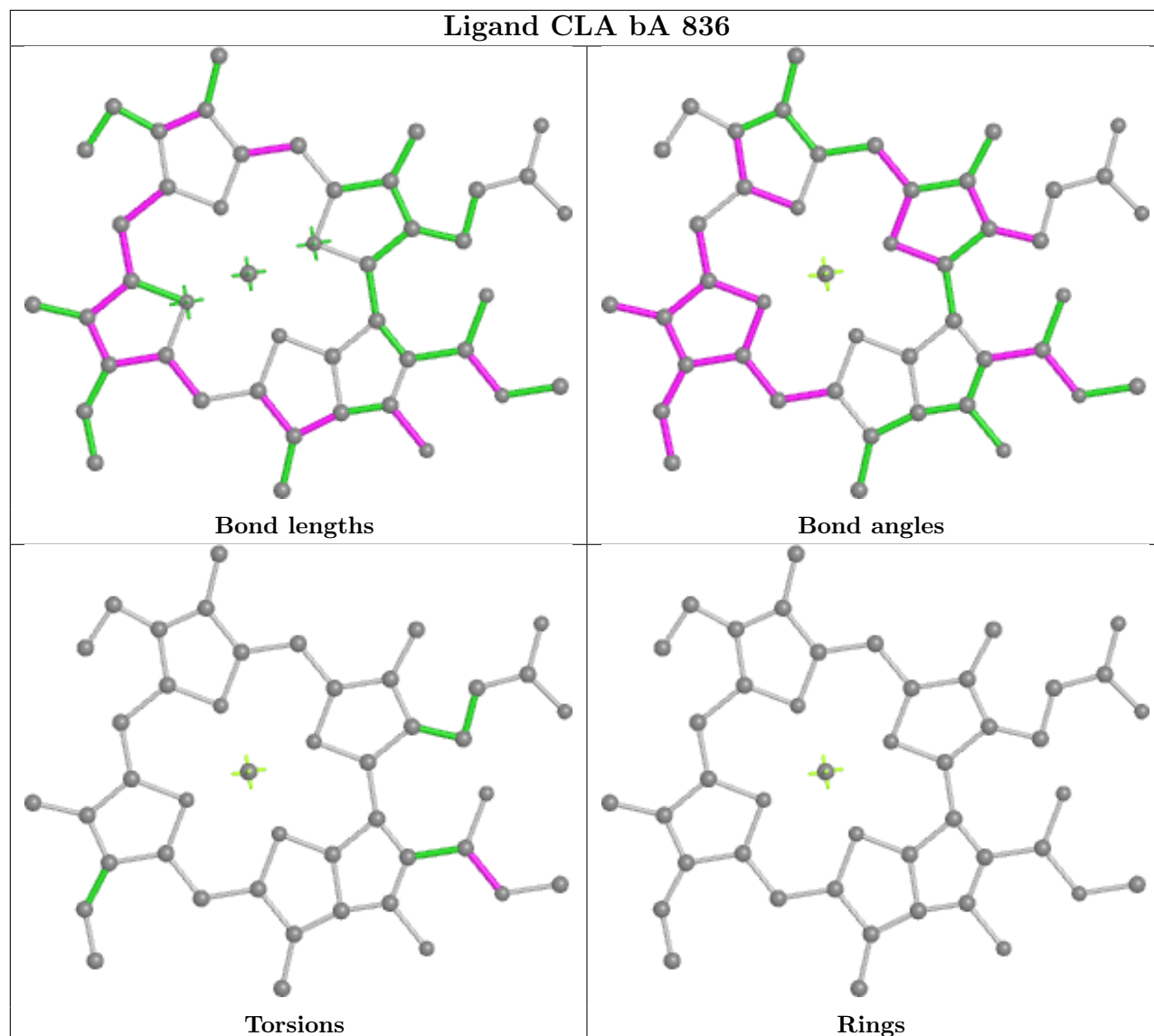
Ligand CLA bA 834



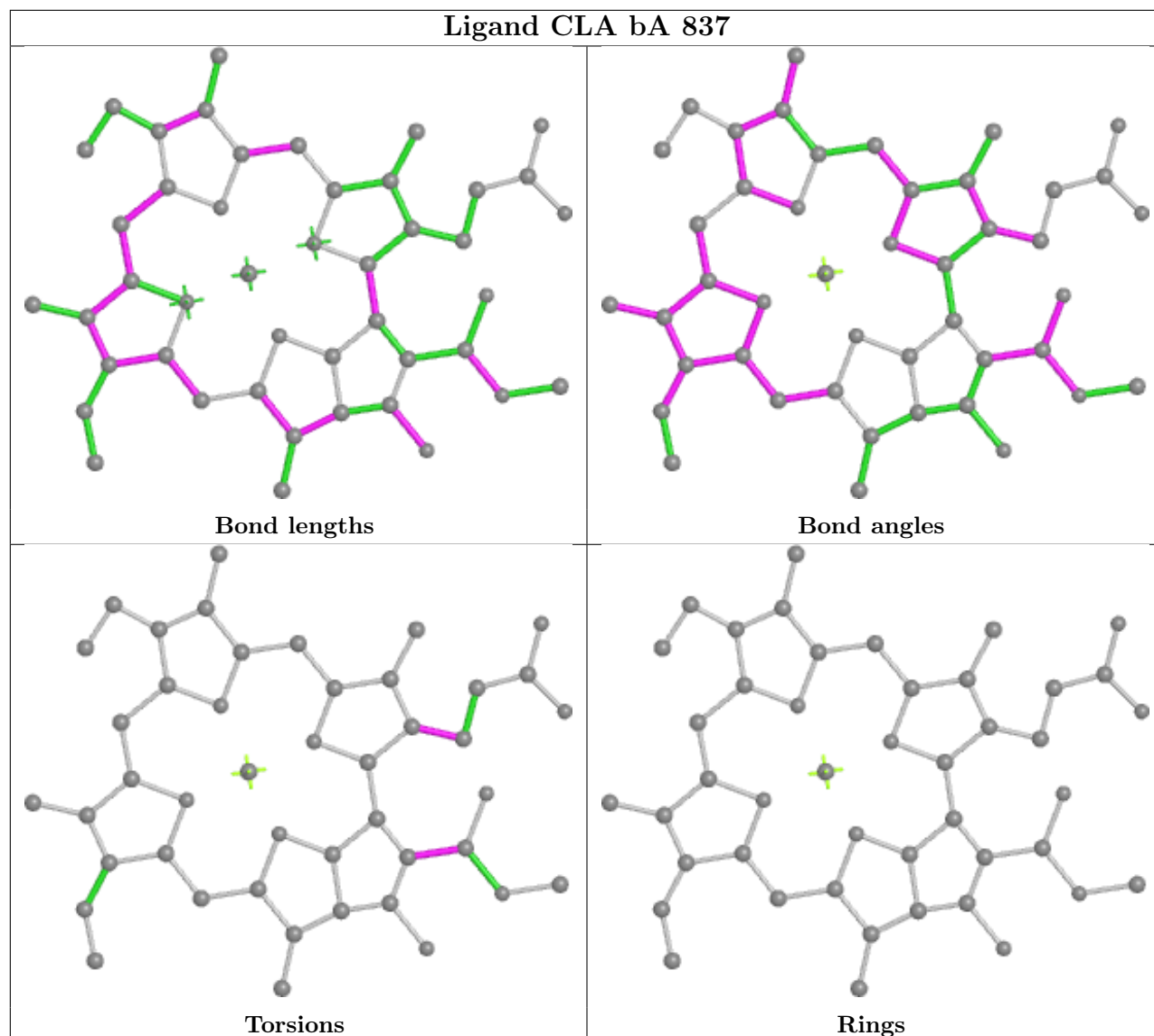
Ligand CLA bA 835

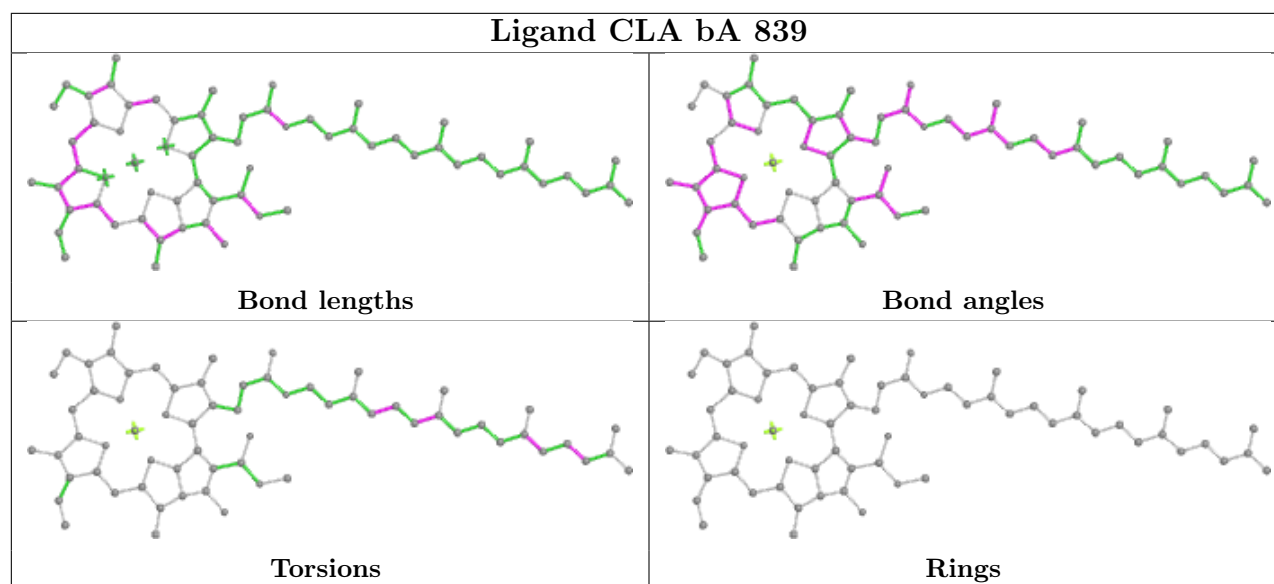
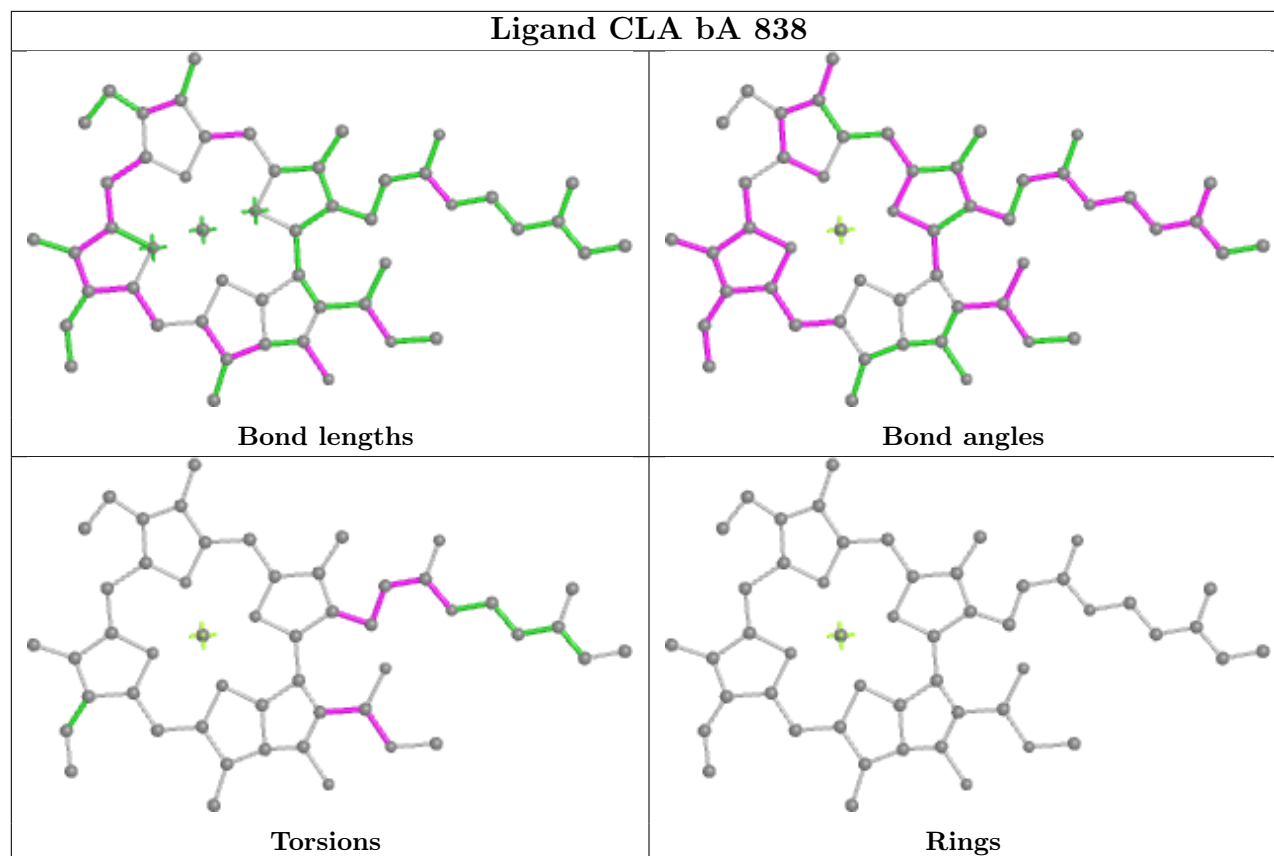


Ligand CLA bA 836

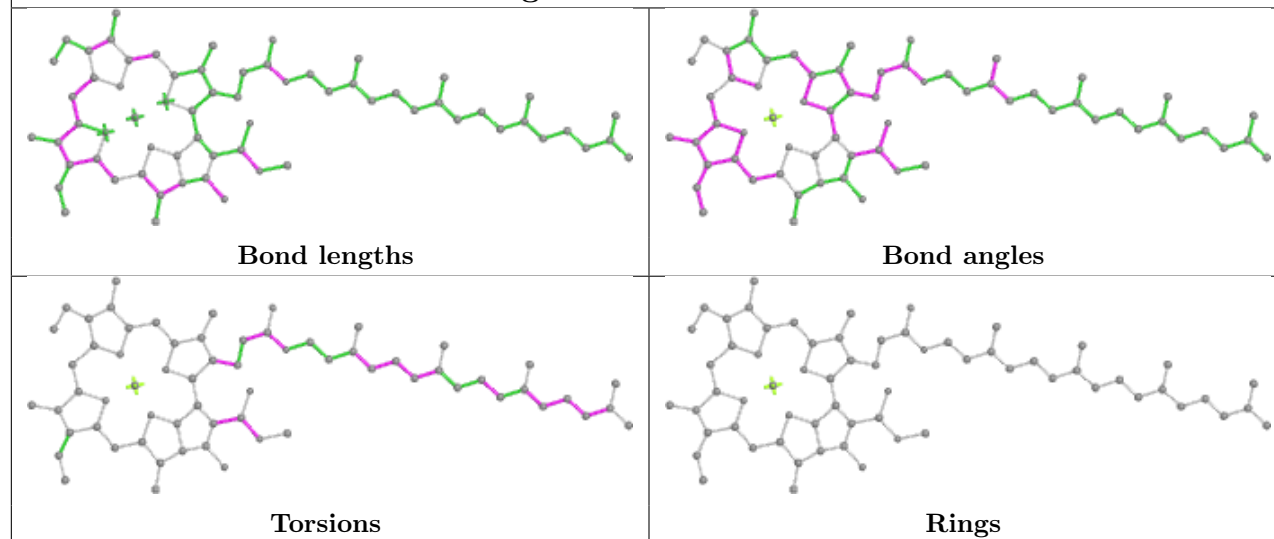


Ligand CLA bA 837

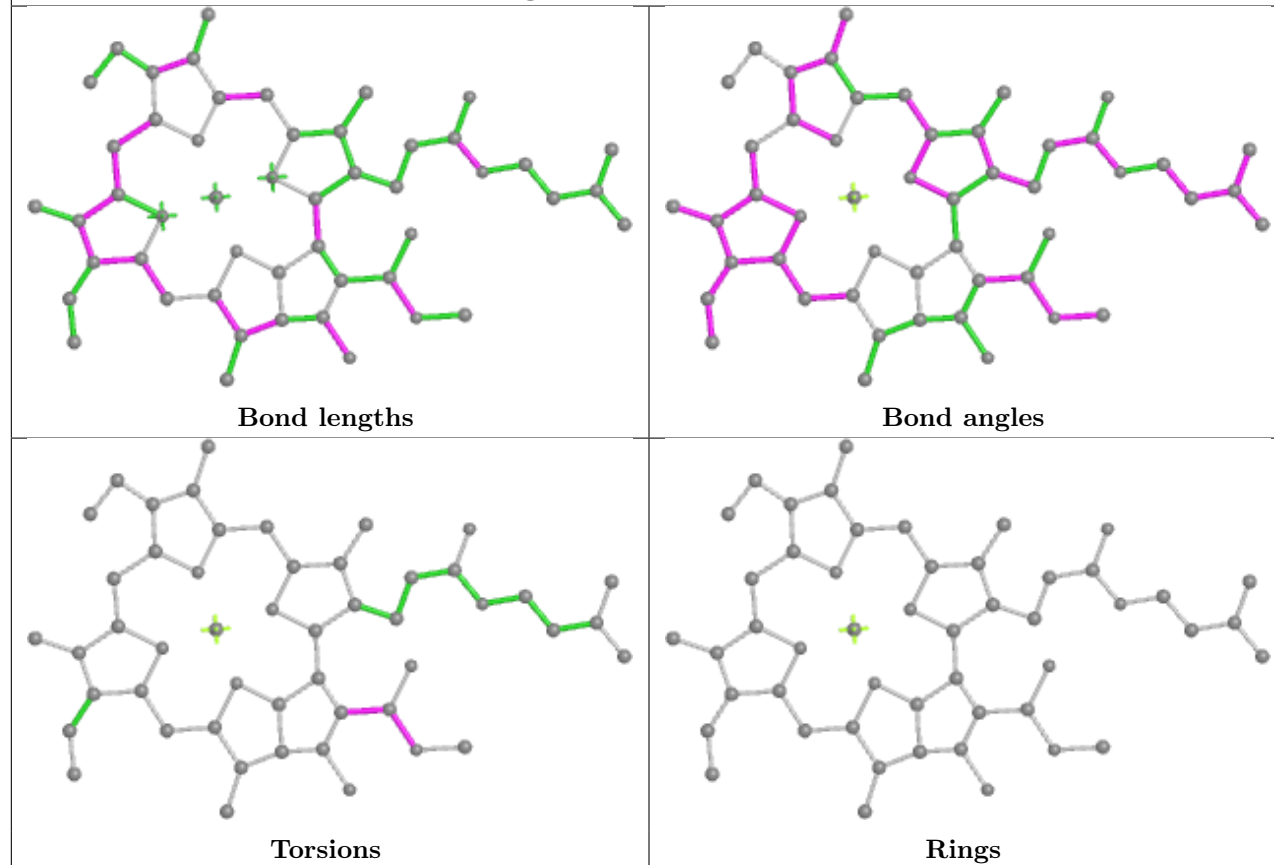




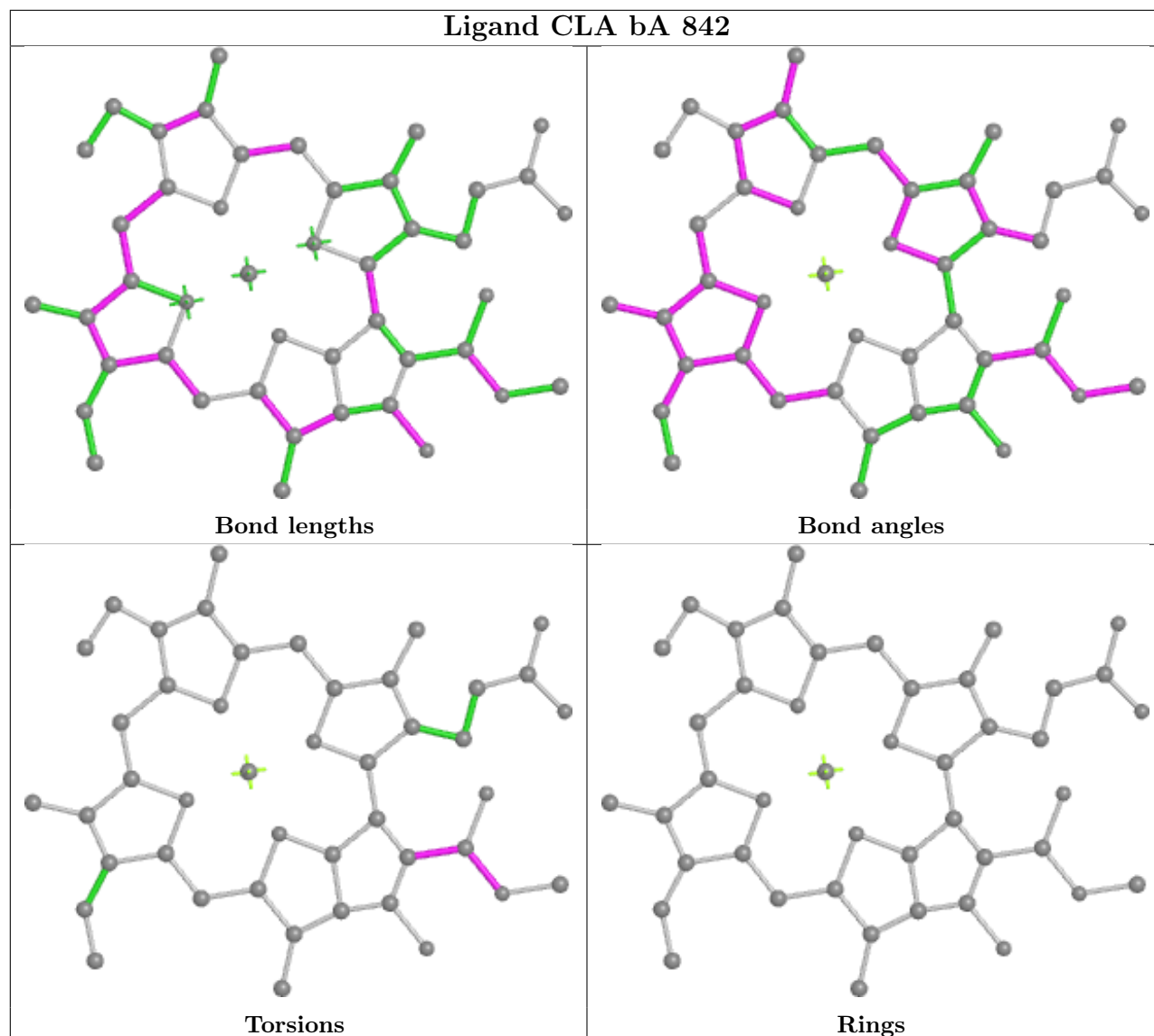
Ligand CLA bA 840



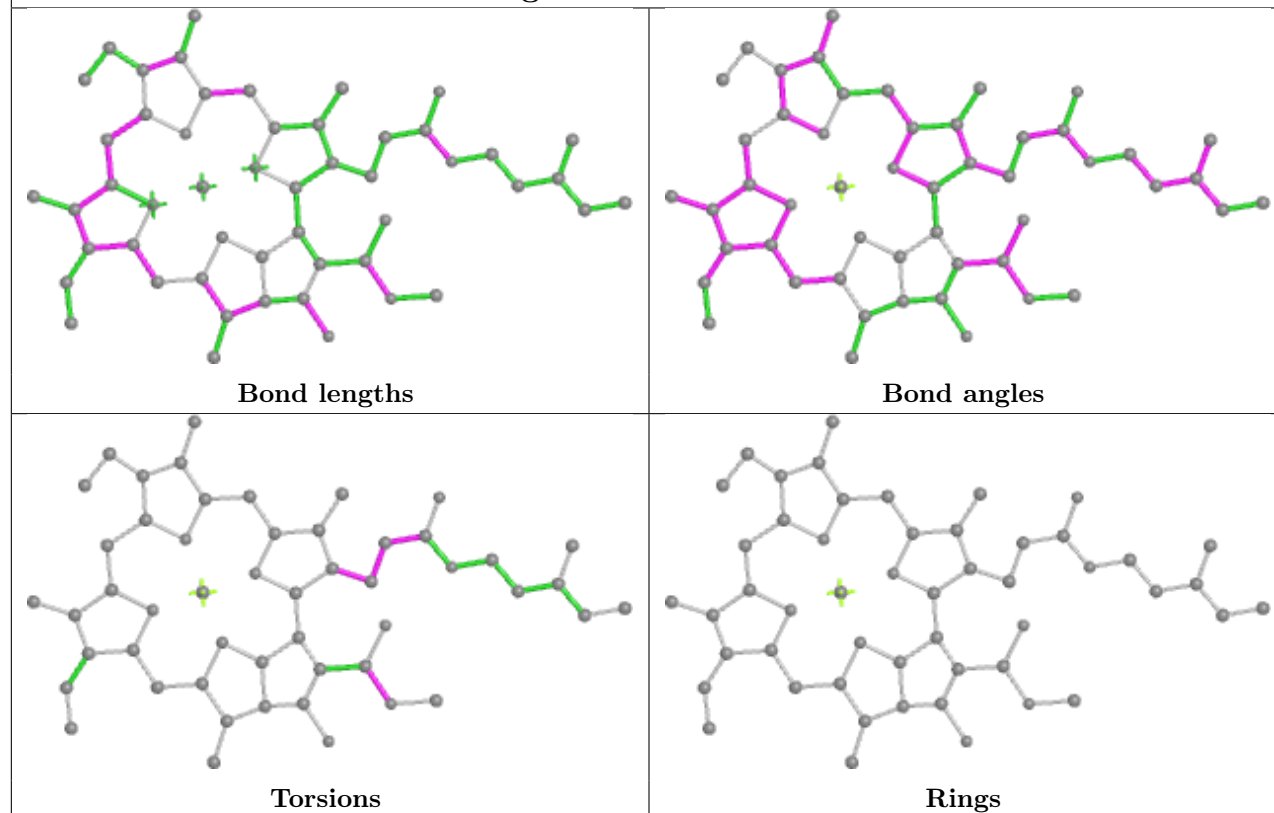
Ligand CLA bA 841



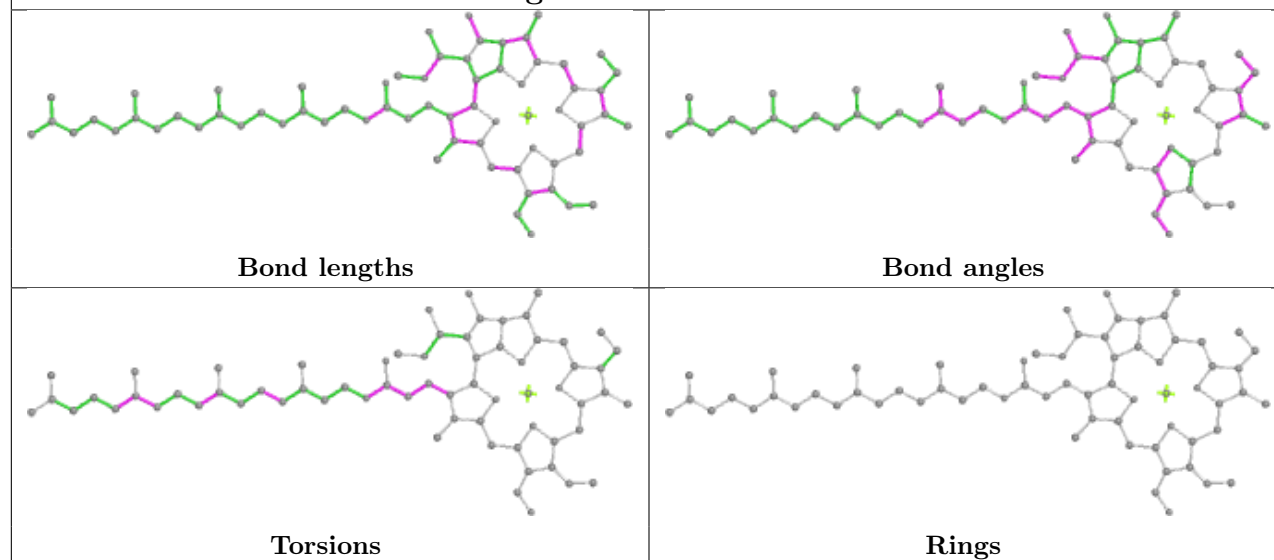
Ligand CLA bA 842

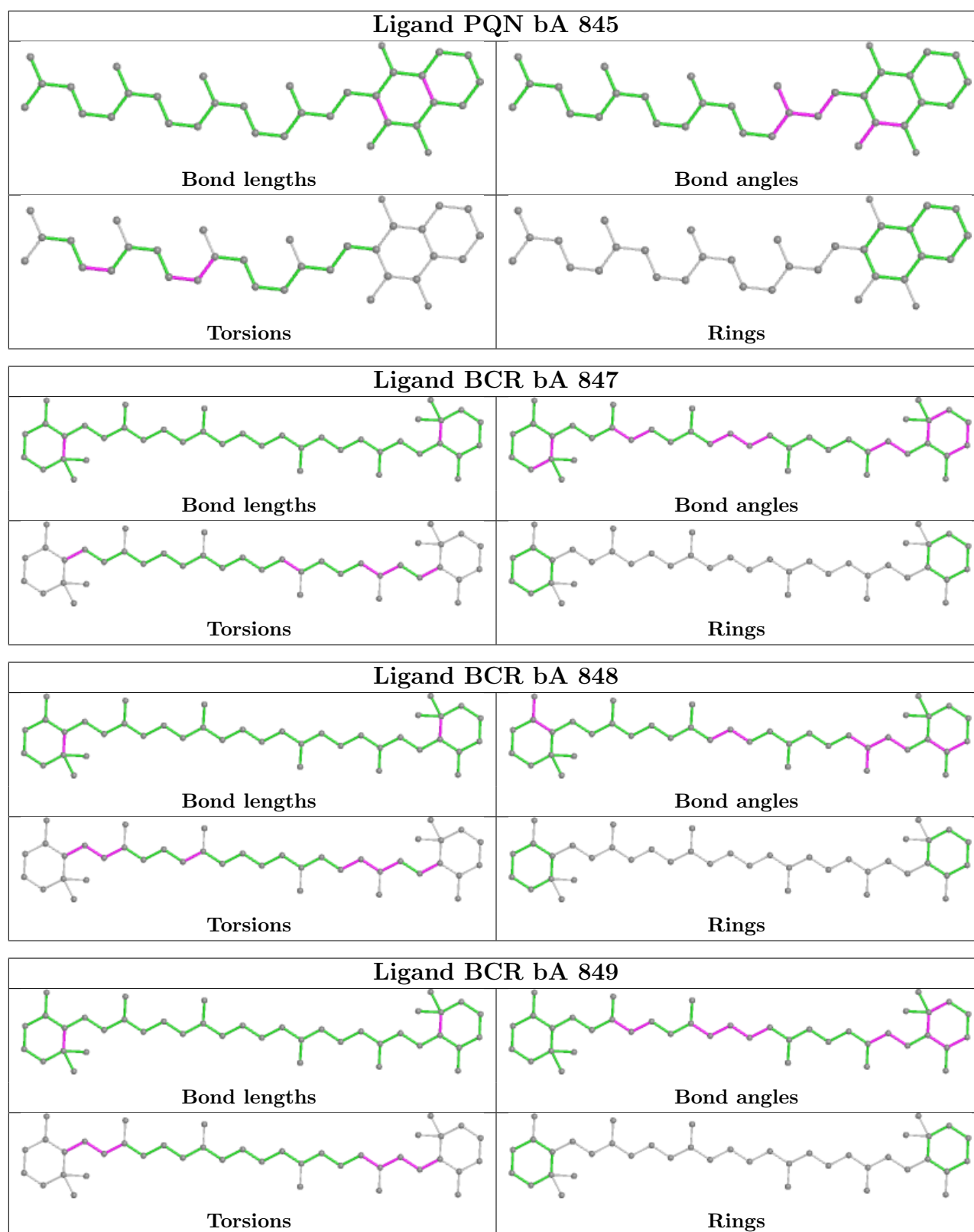


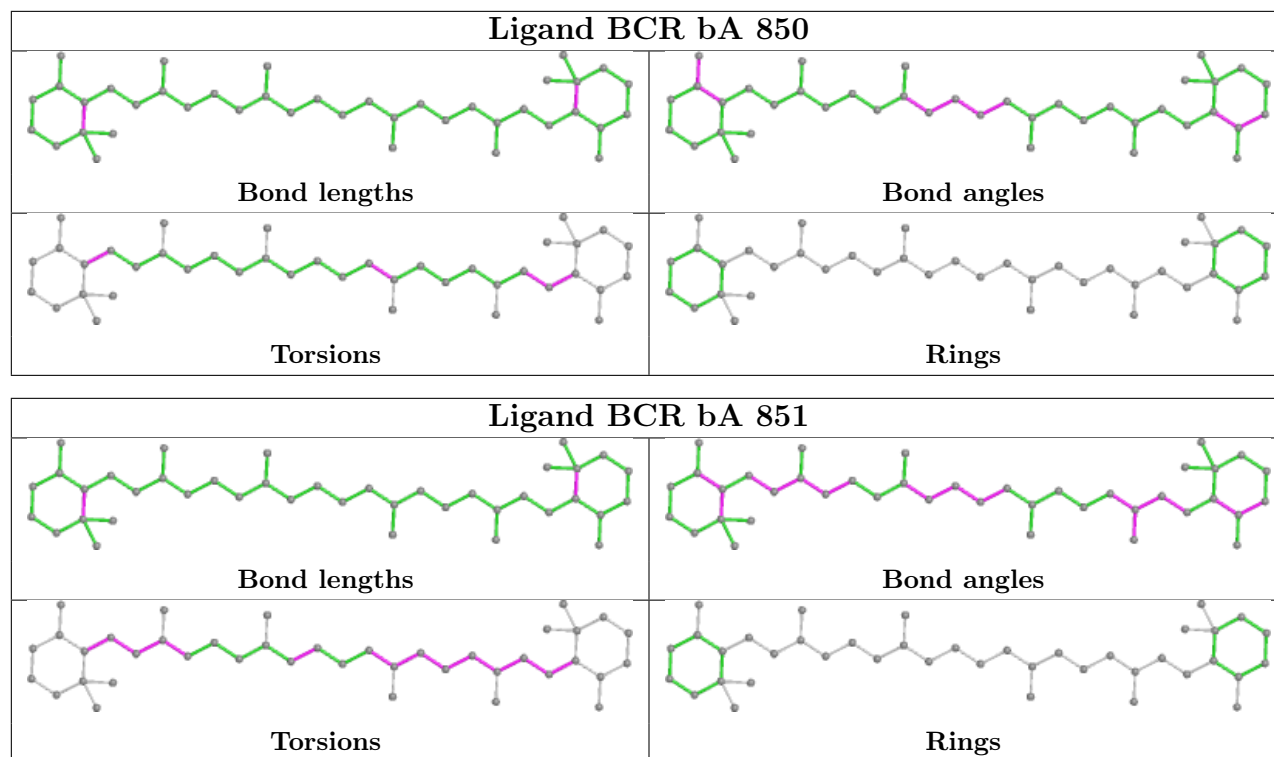
Ligand CLA bA 843

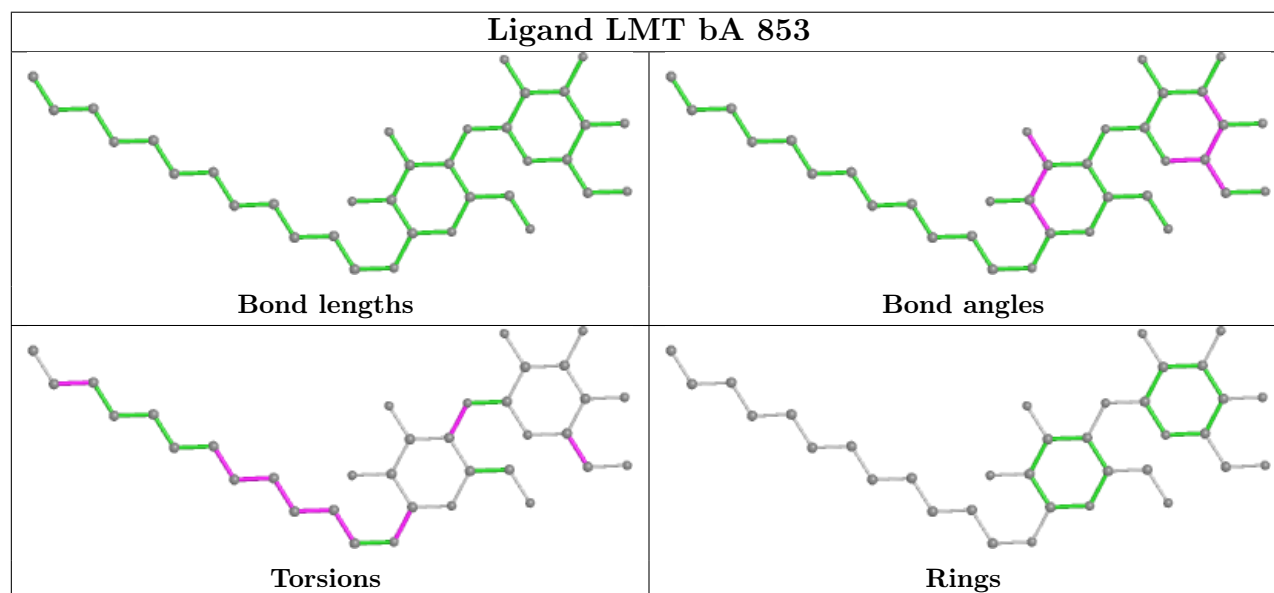
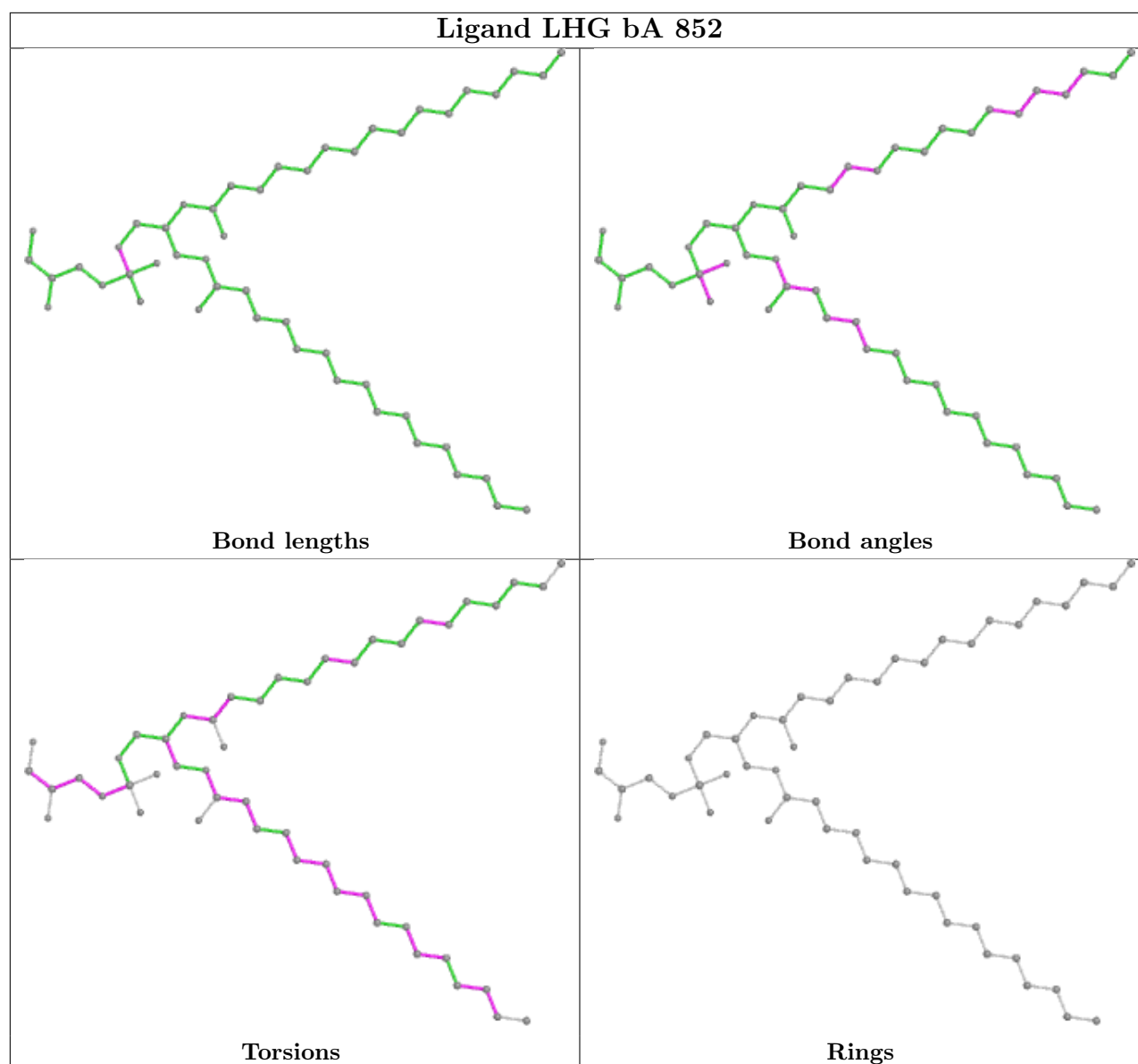


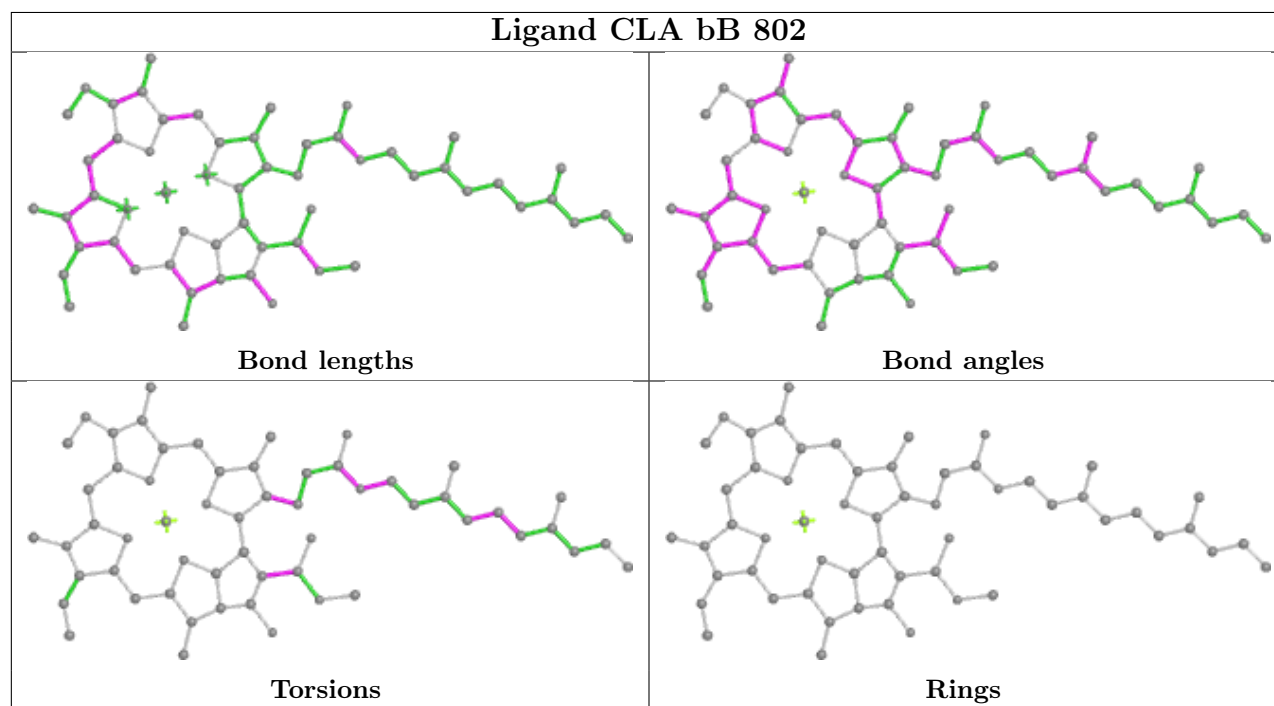
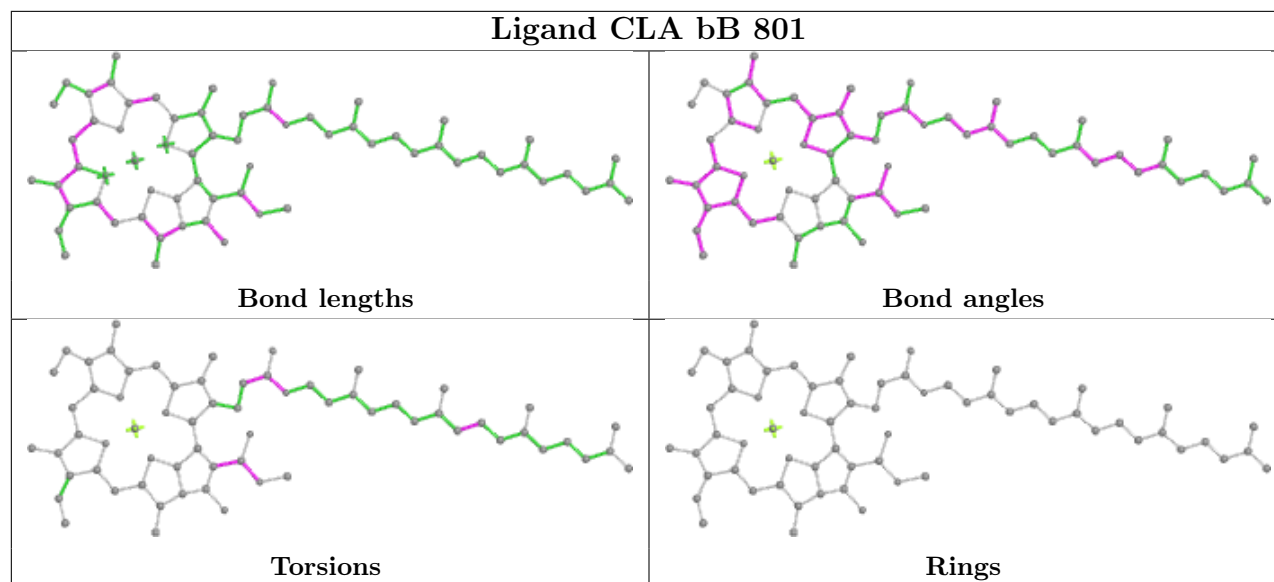
Ligand F6C bA 844



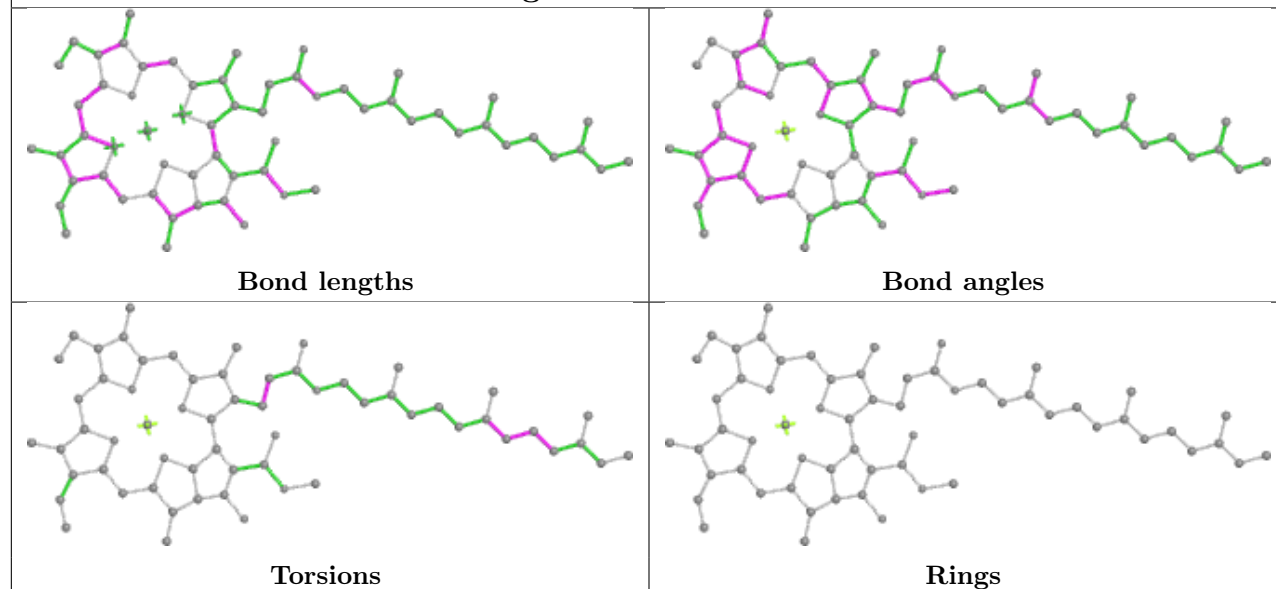




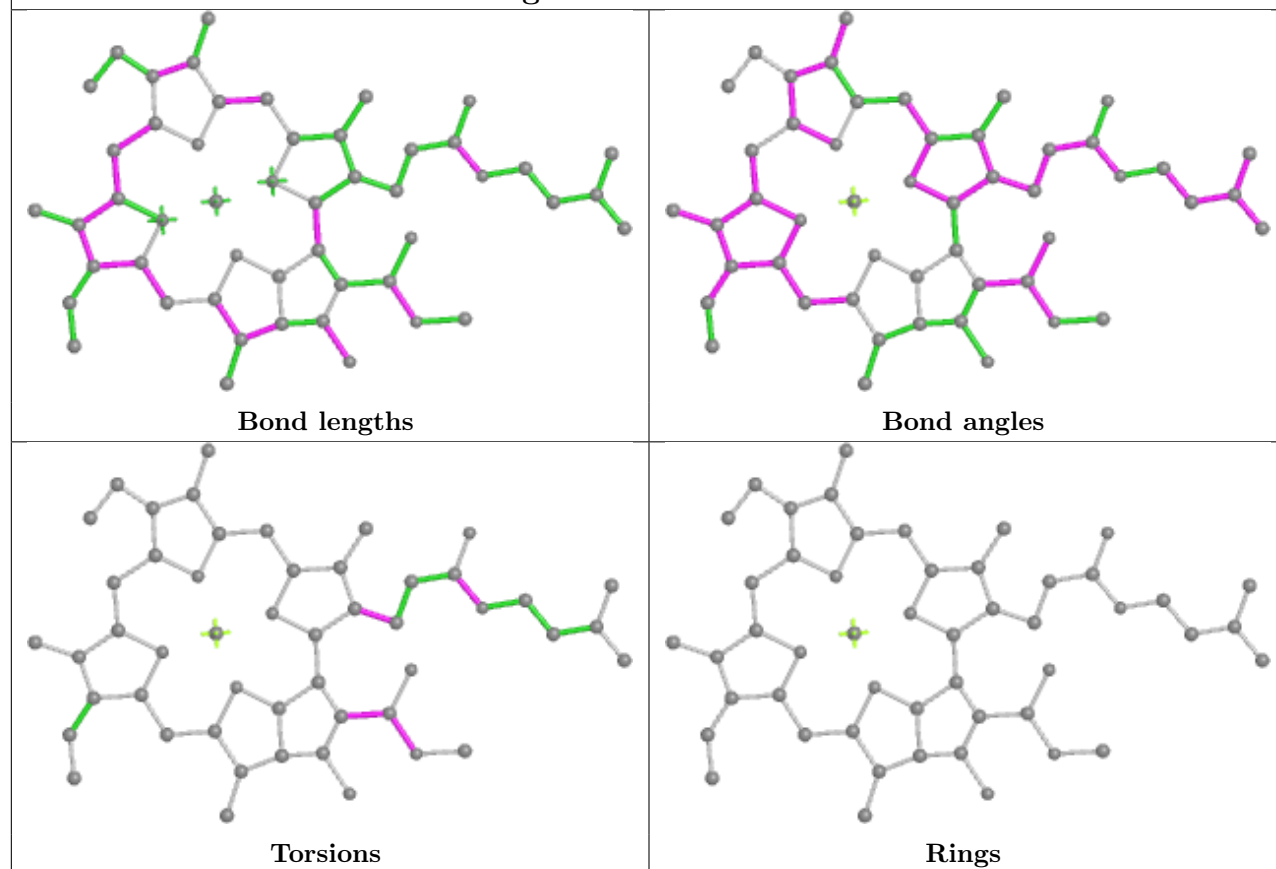


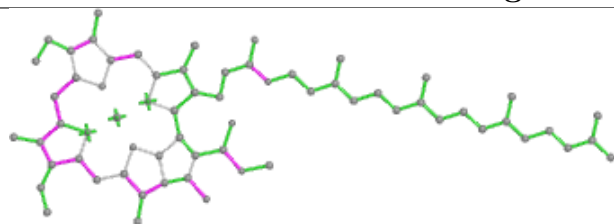
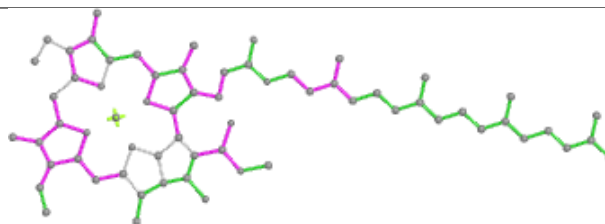
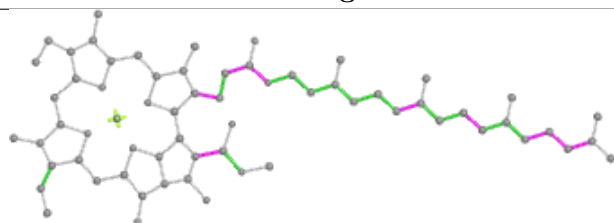
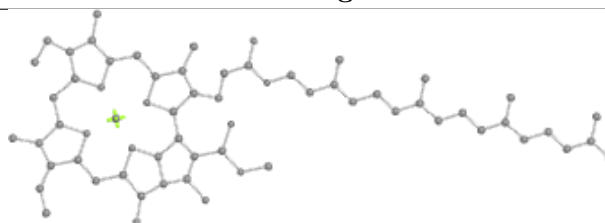
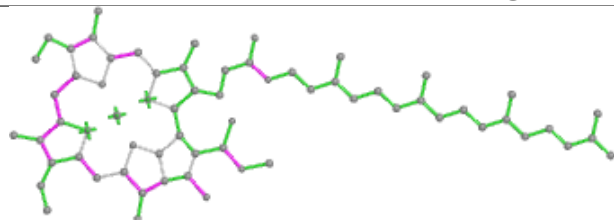
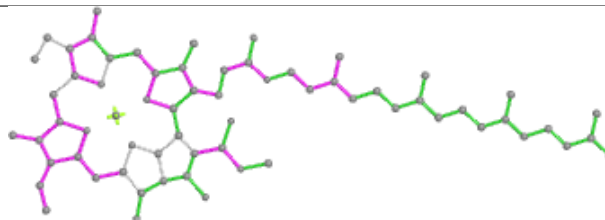
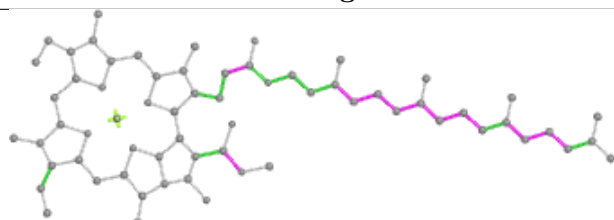
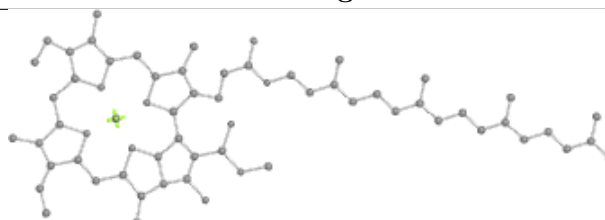


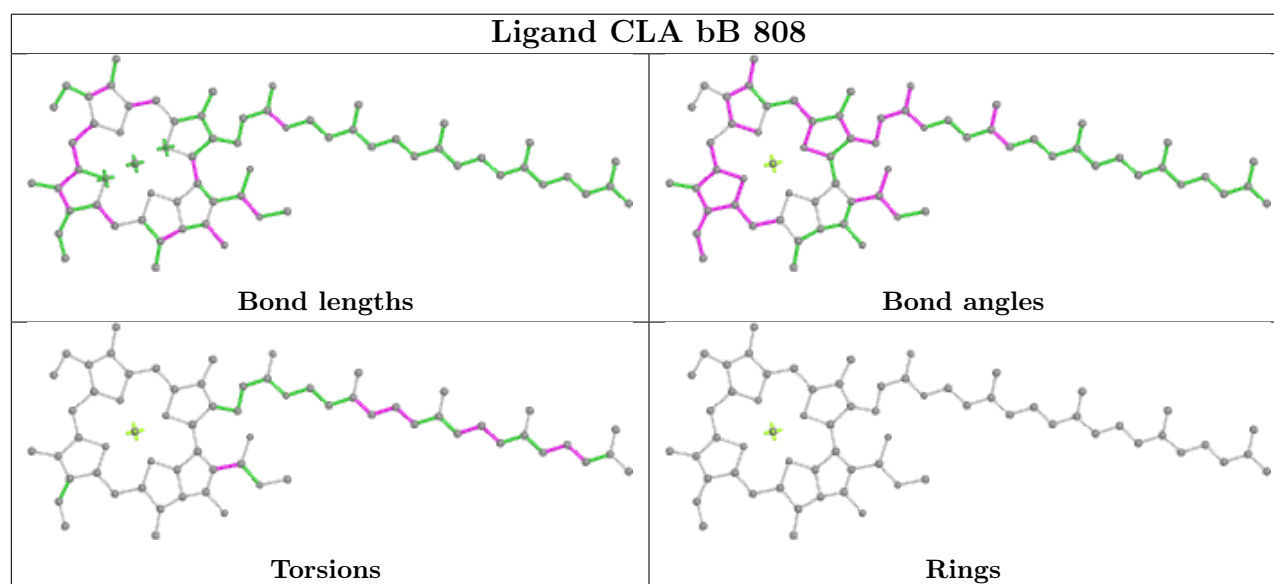
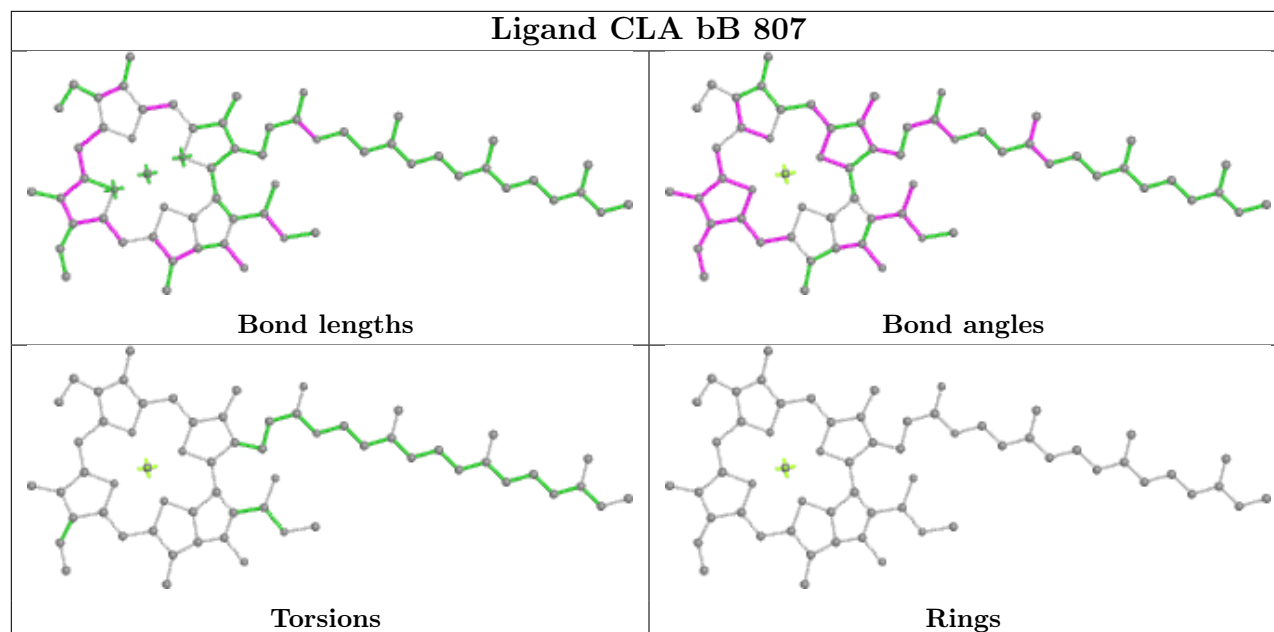
Ligand CLA bB 803



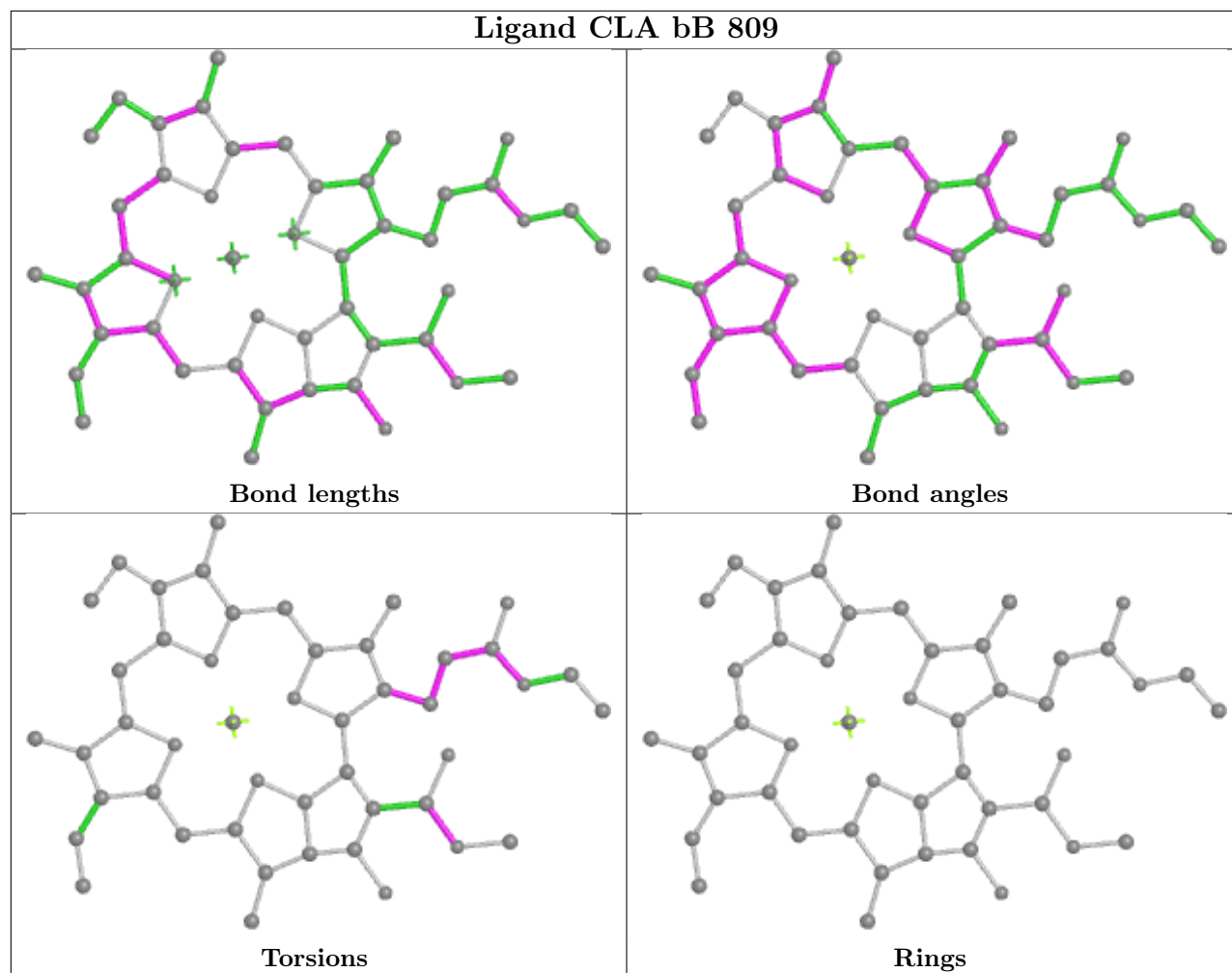
Ligand CLA bB 804



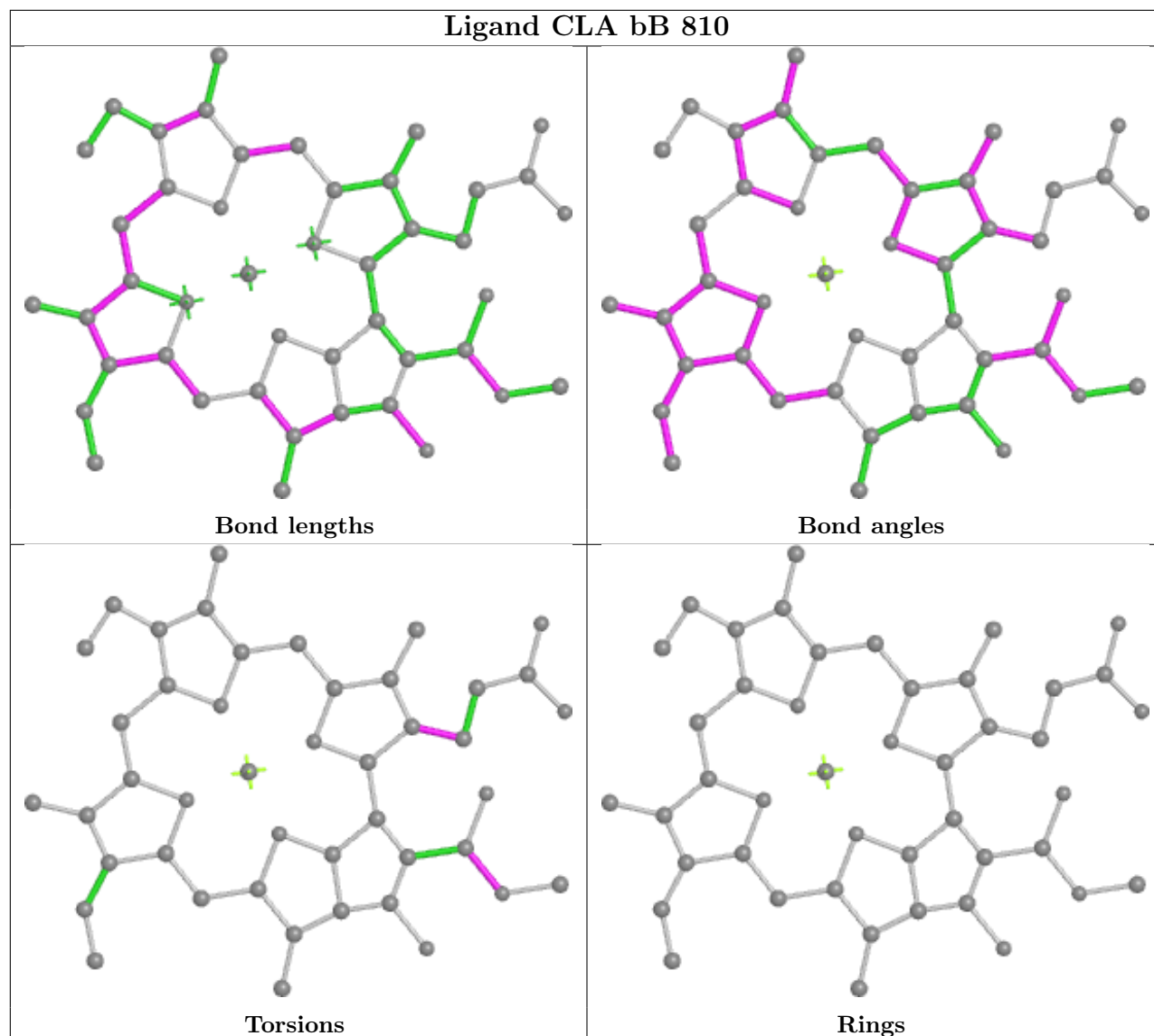
Ligand CLA bB 805**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA bB 806****Bond lengths****Bond angles****Torsions****Rings**



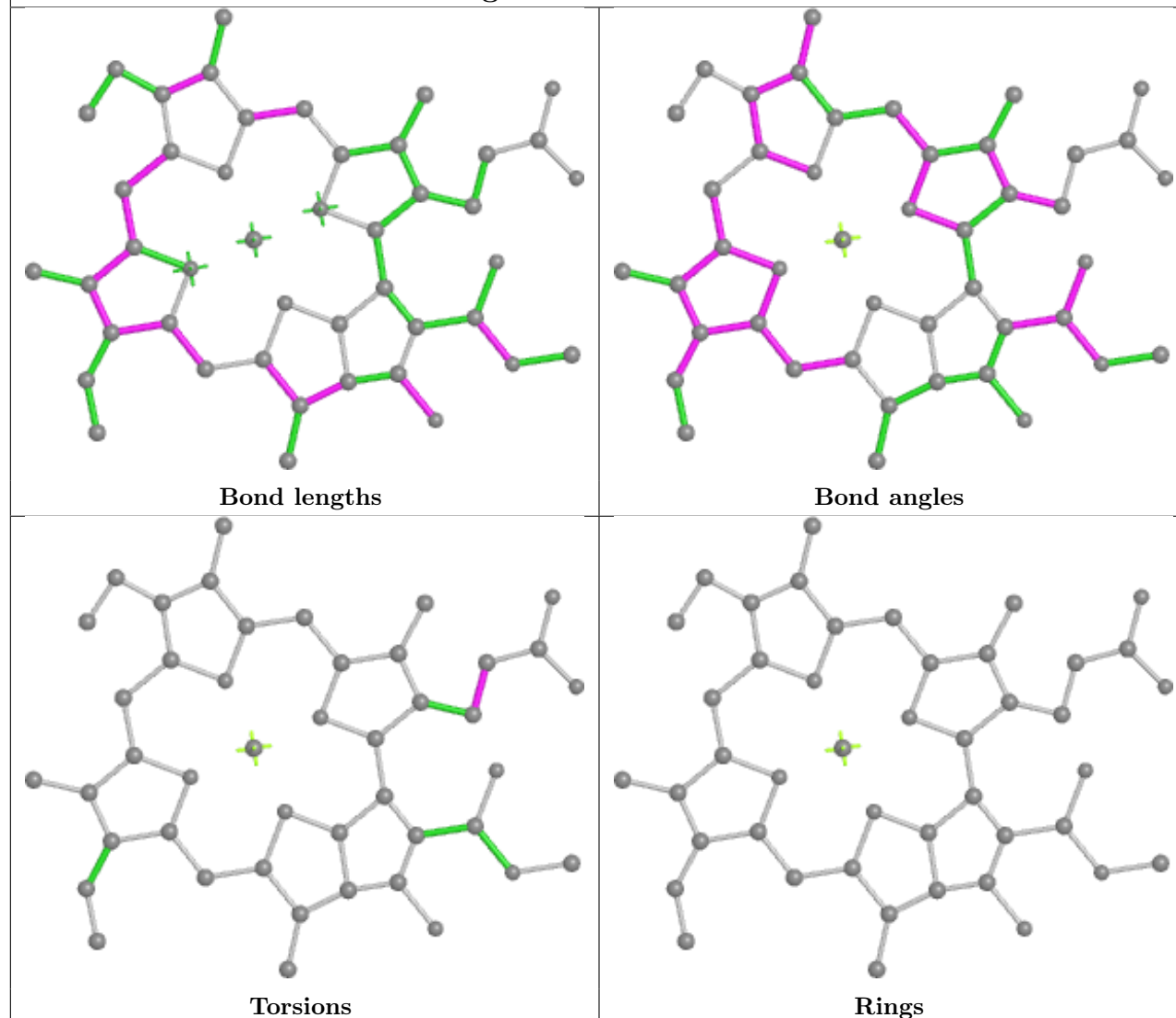
Ligand CLA bB 809



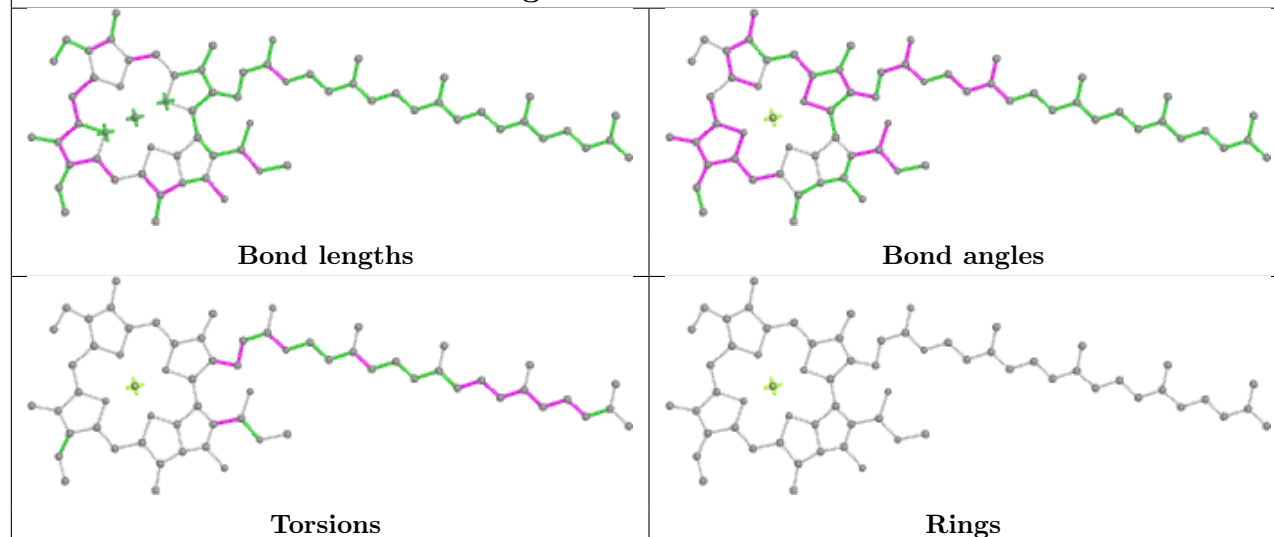
Ligand CLA bB 810

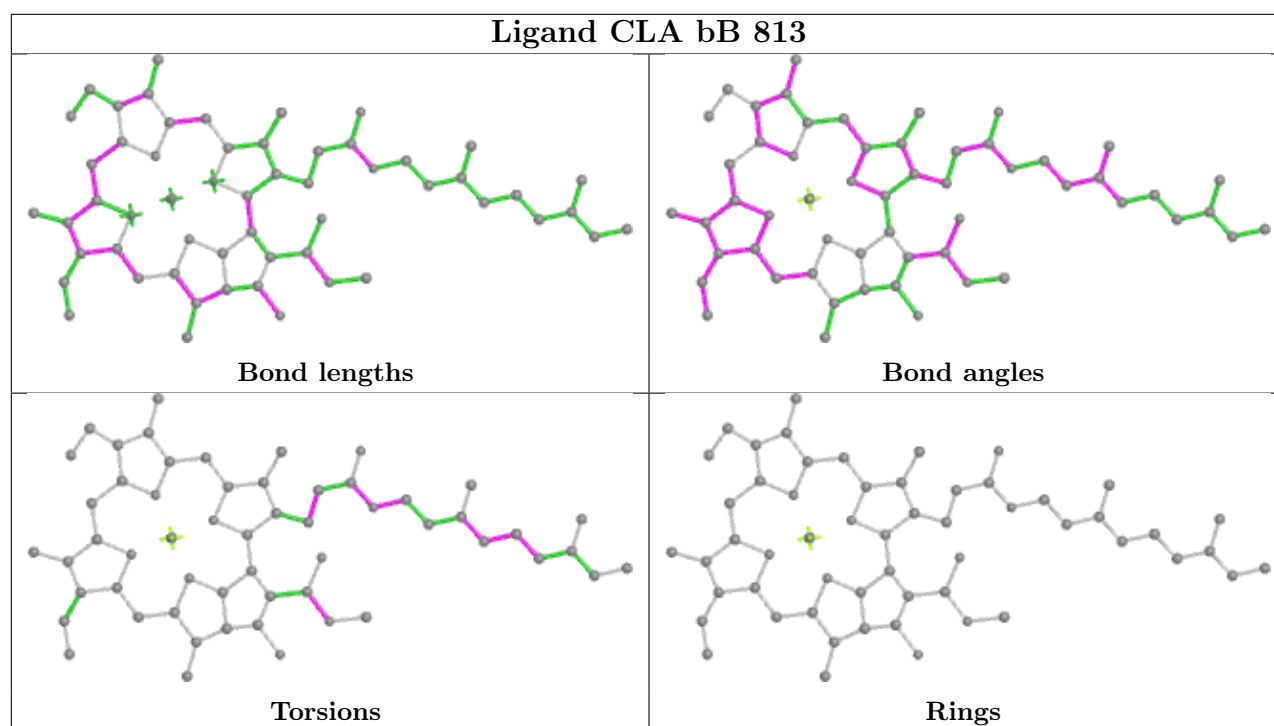


Ligand CLA bB 811

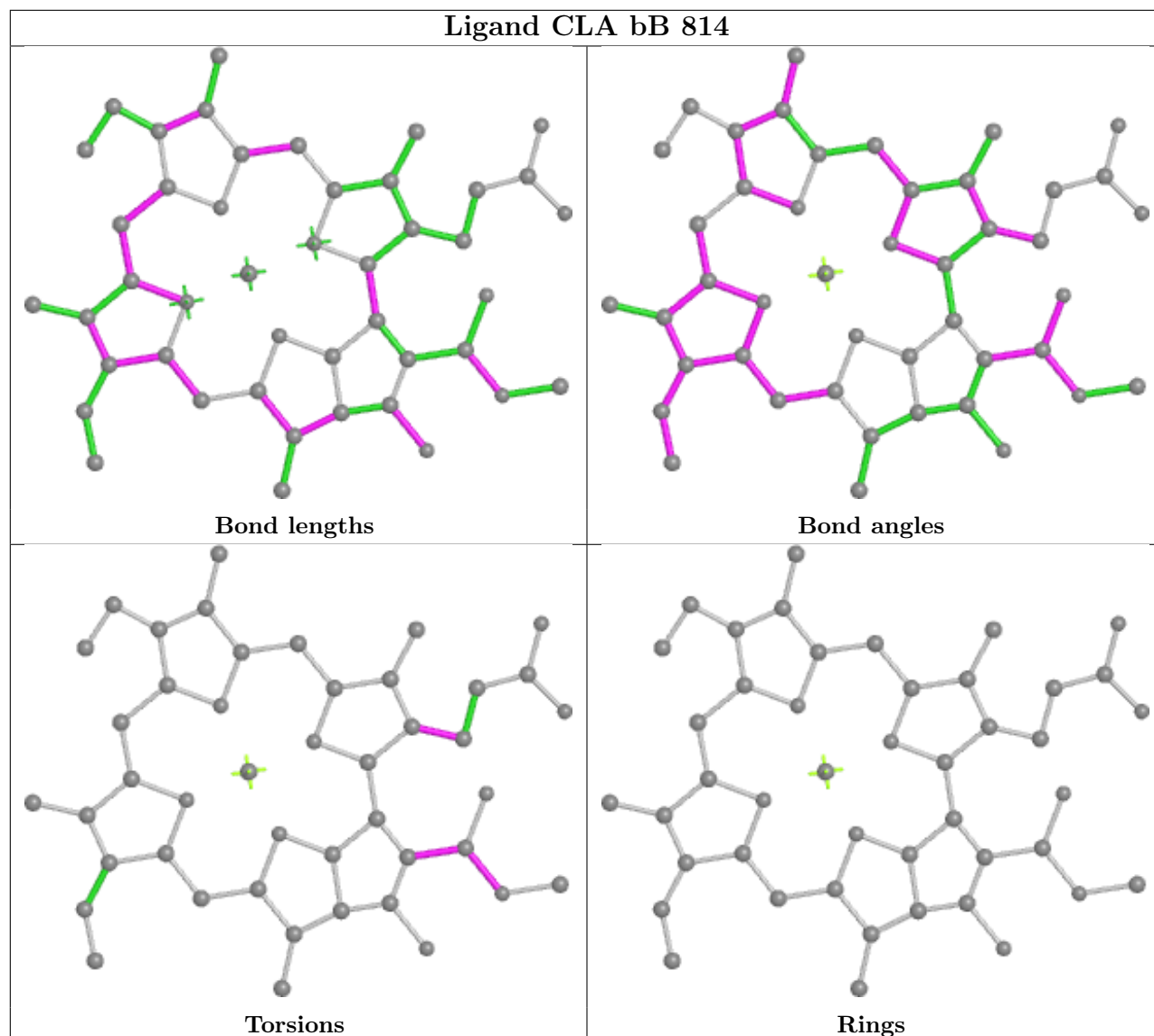


Ligand CLA bB 812

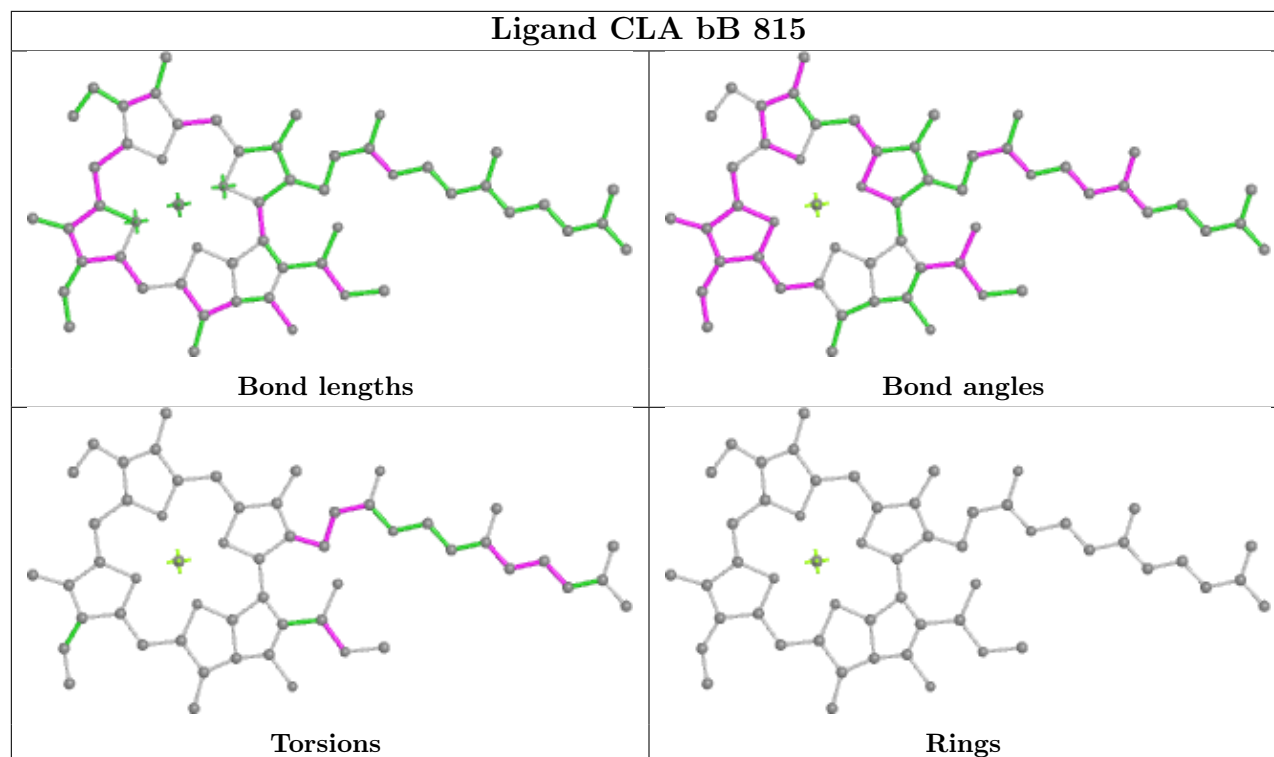




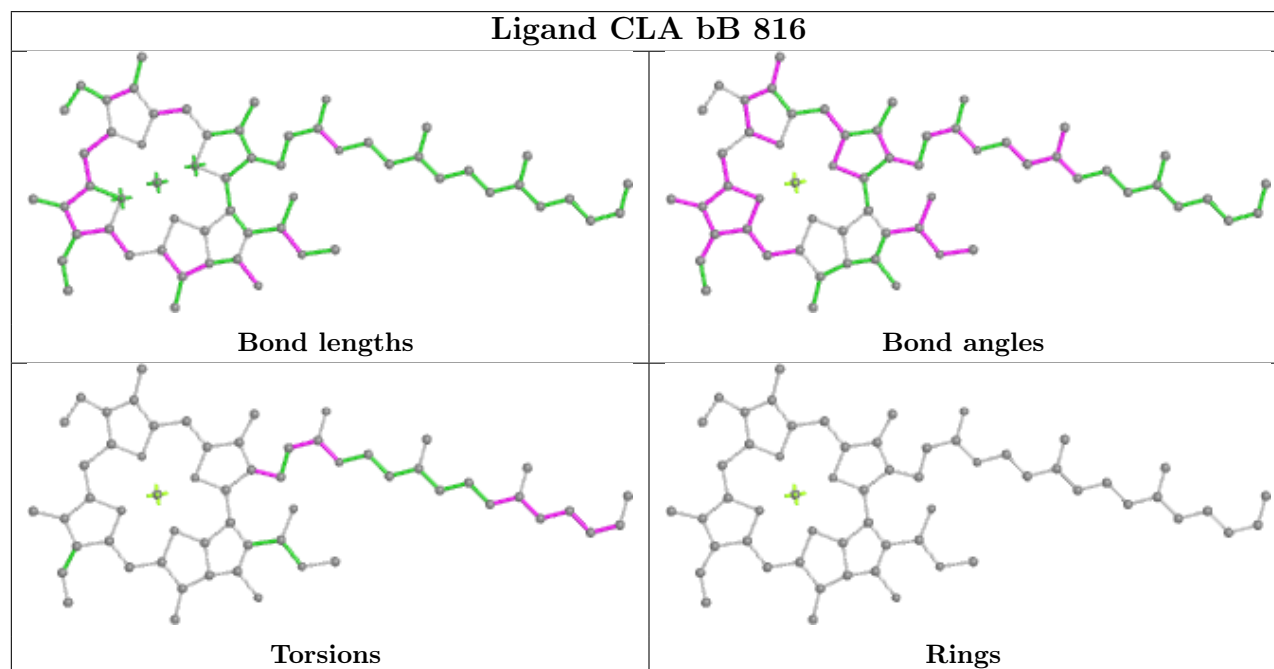
Ligand CLA bB 814

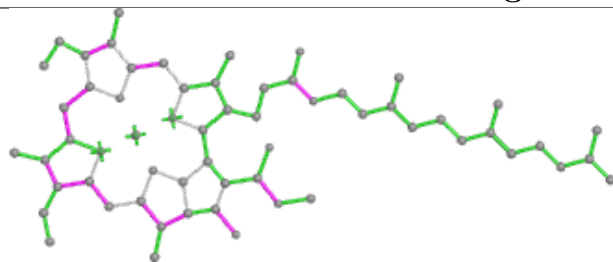
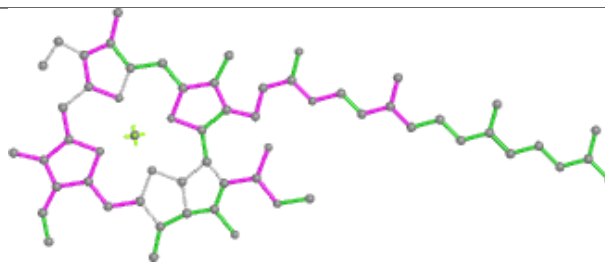
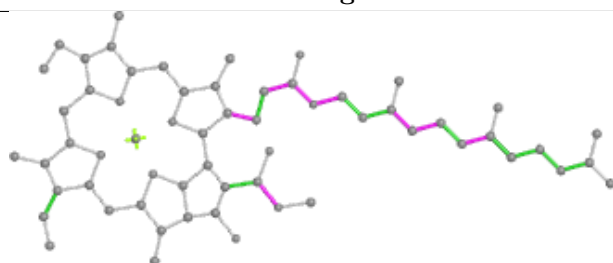
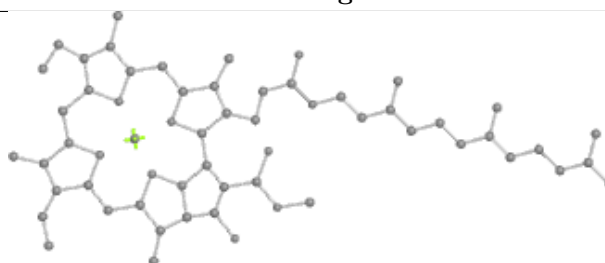
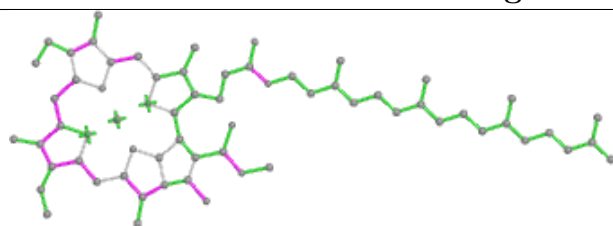
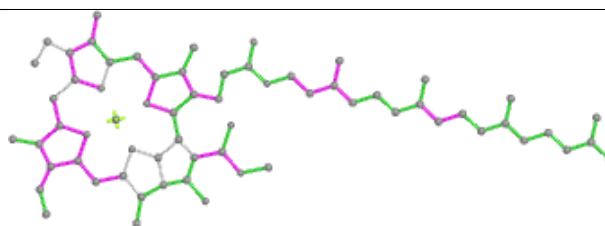
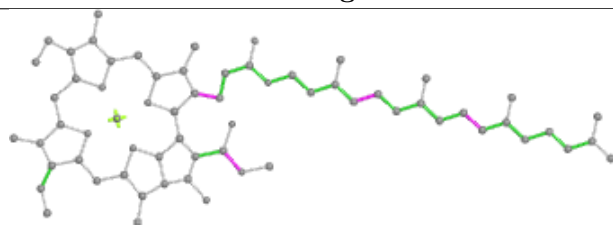
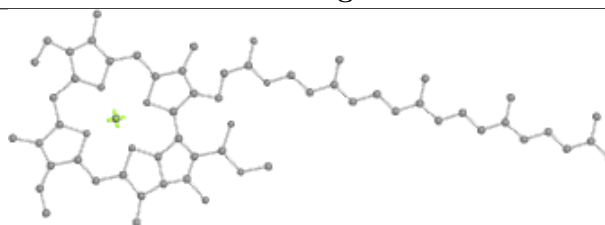


Ligand CLA bB 815

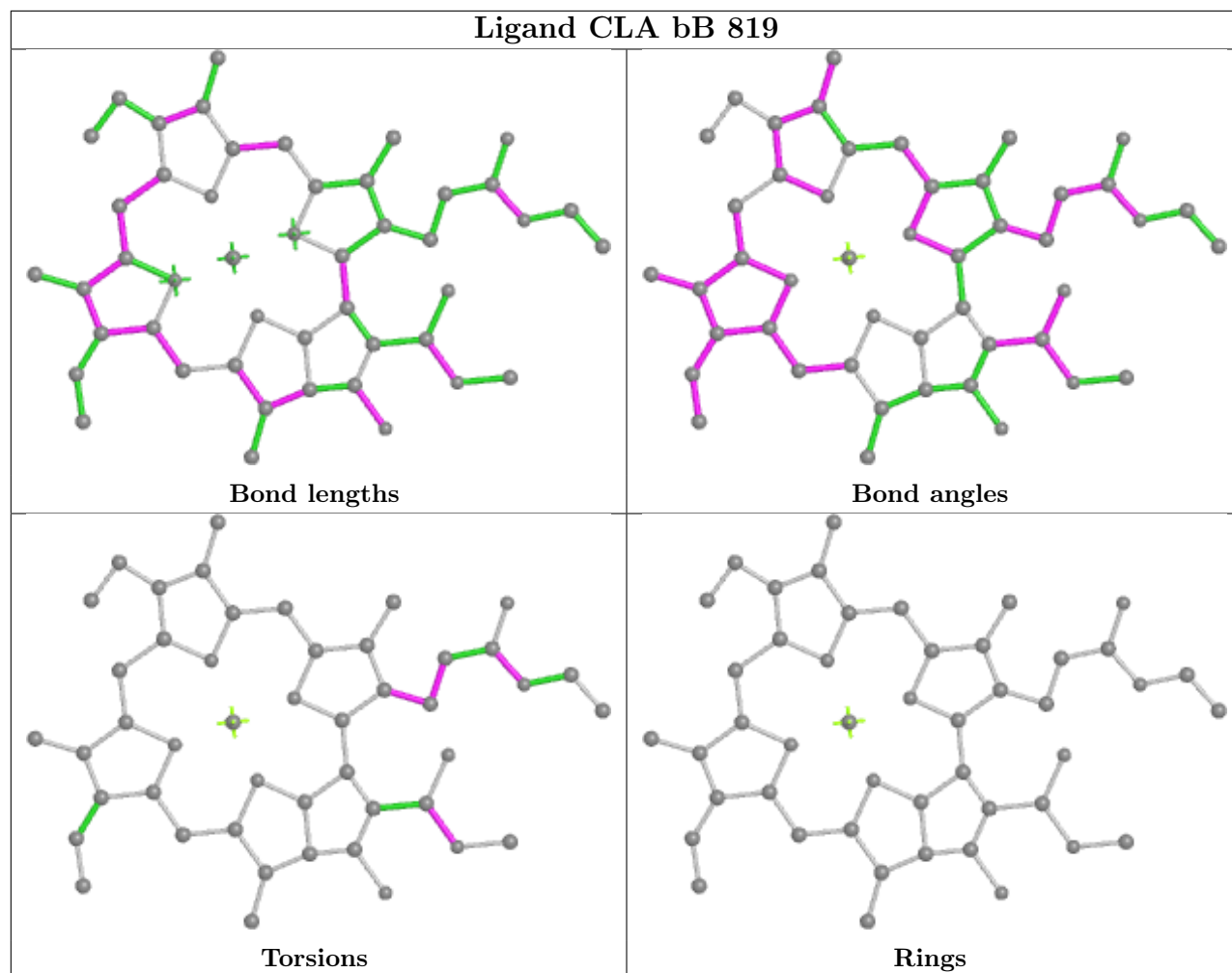


Ligand CLA bB 816

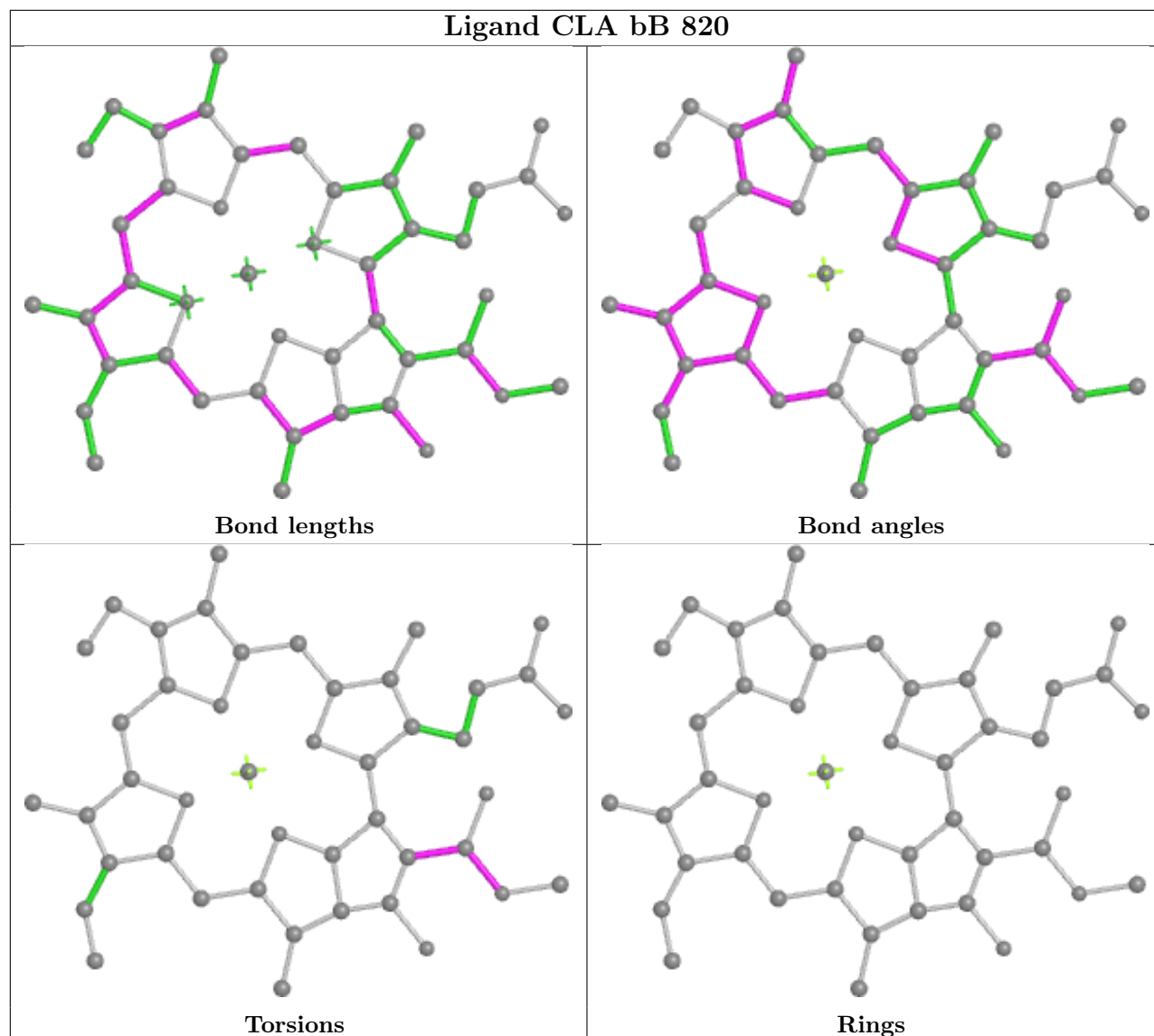


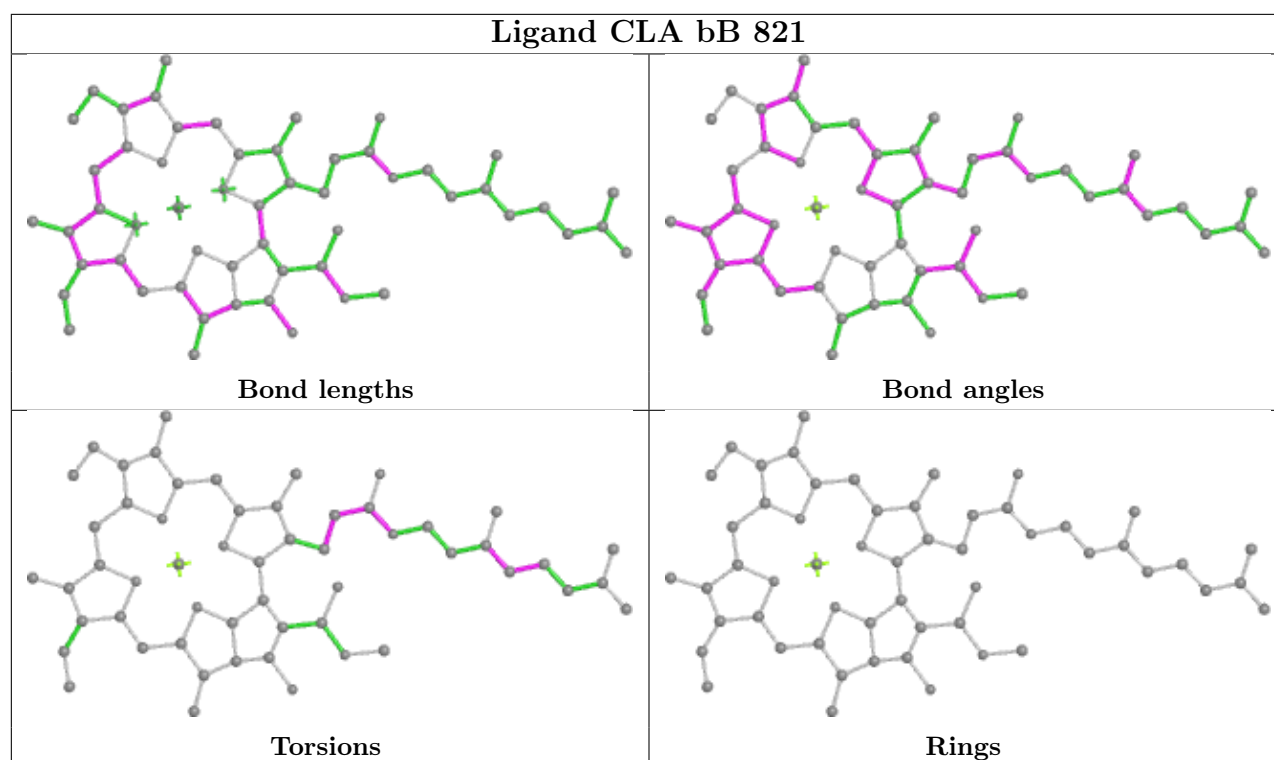
Ligand CLA bB 817**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA bB 818****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA bB 819

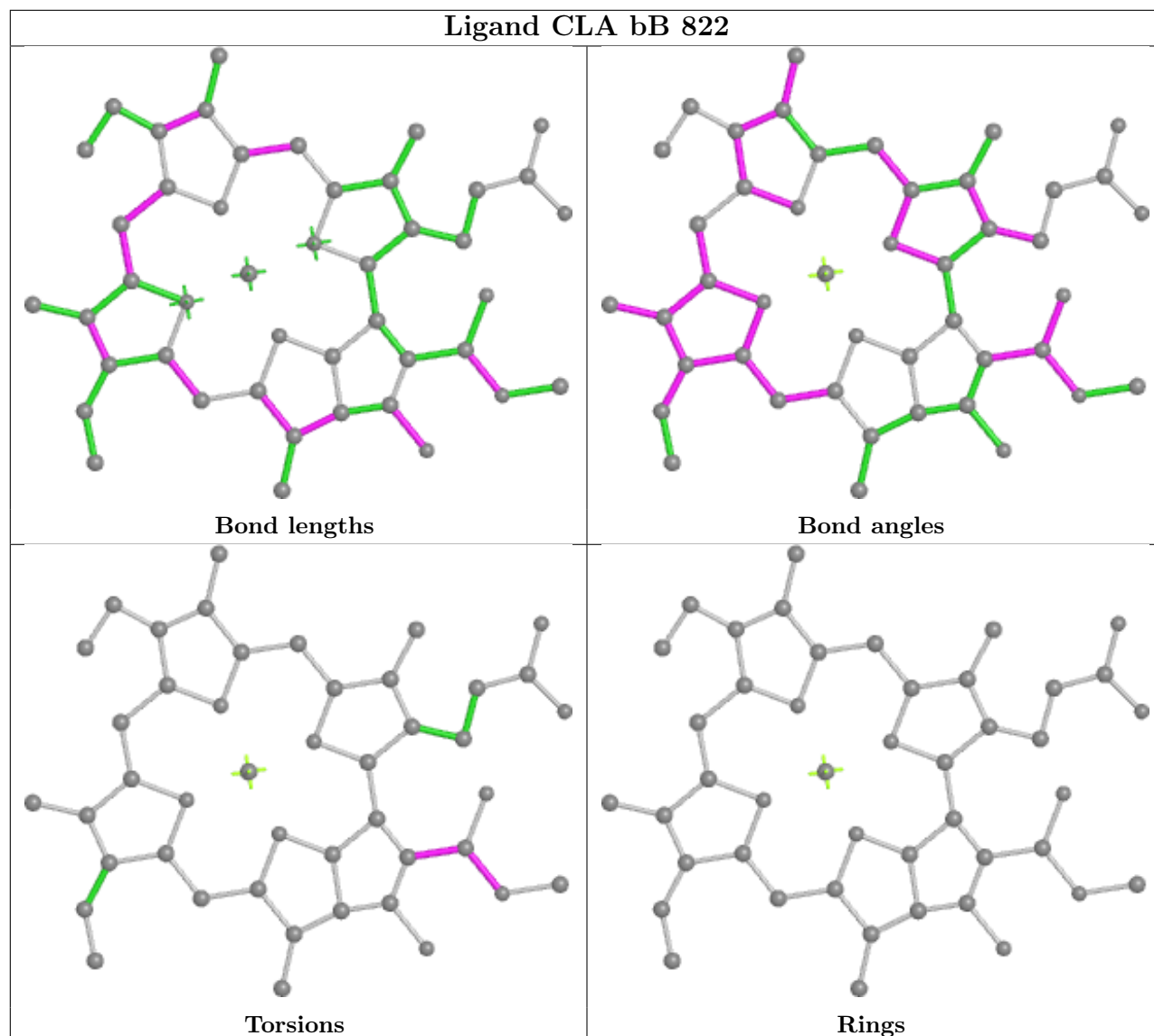


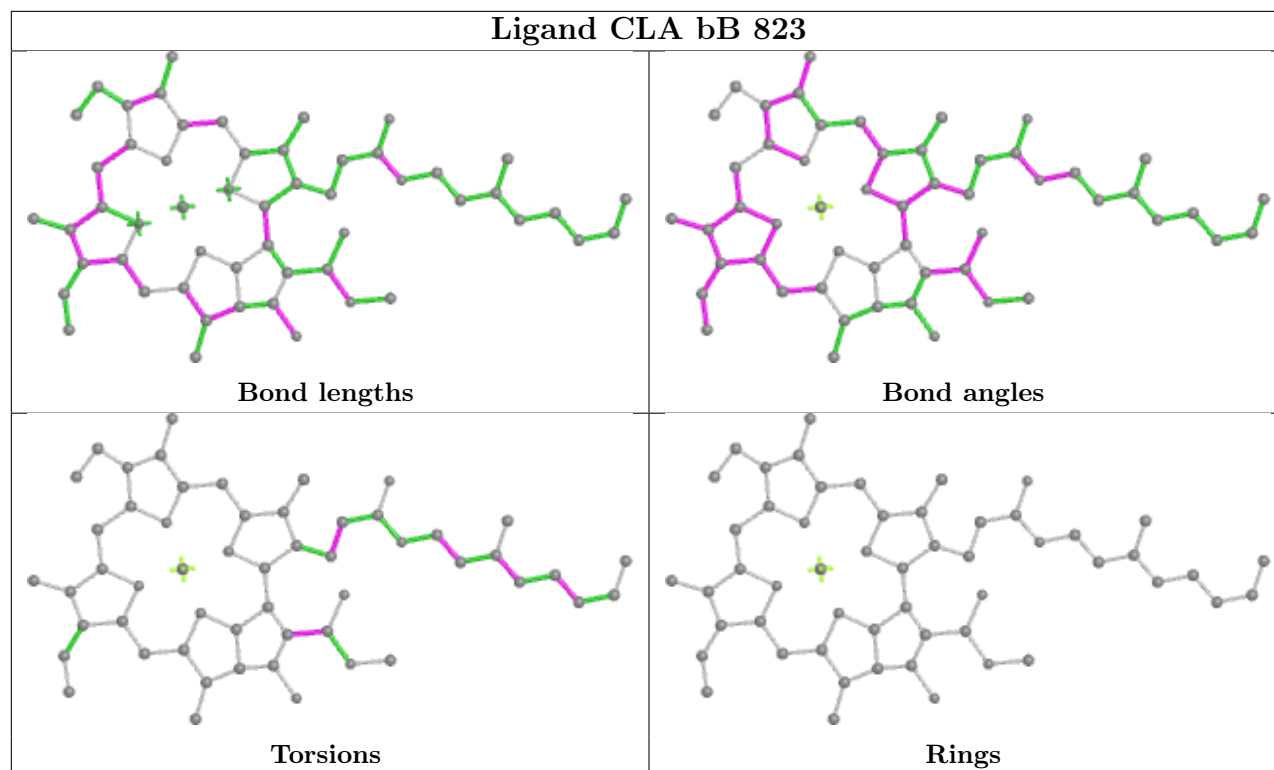
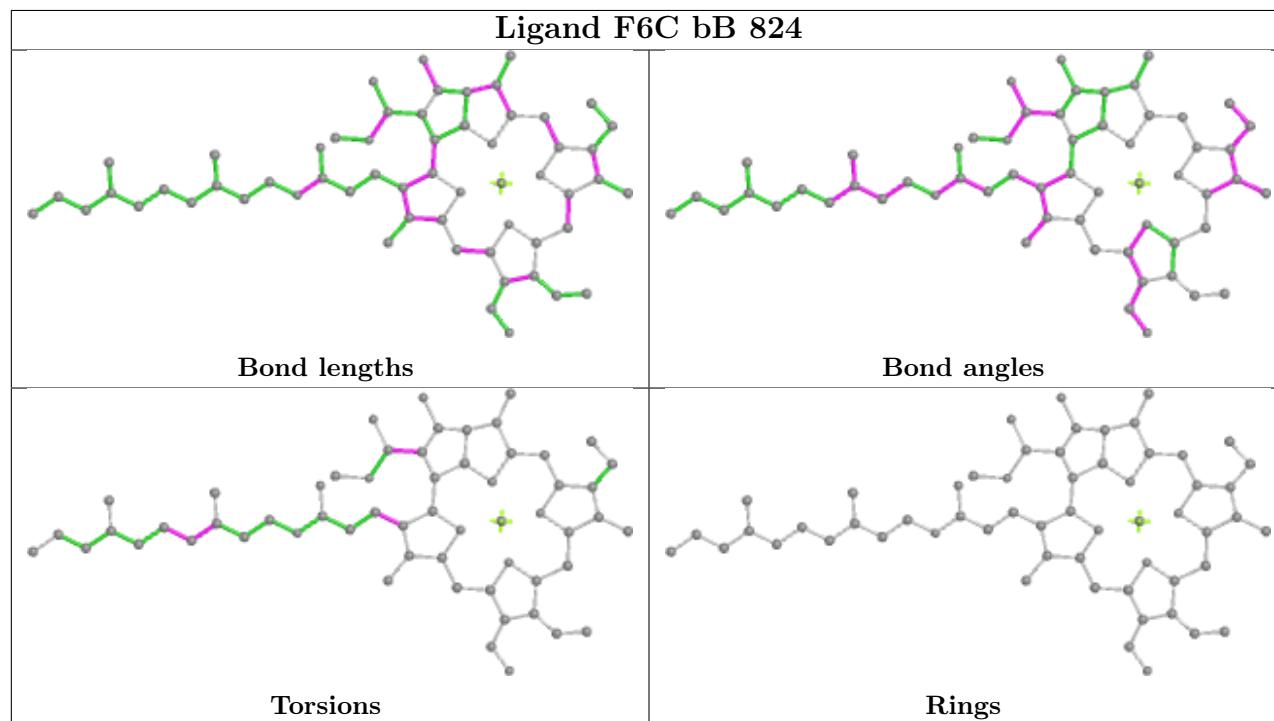
Ligand CLA bB 820

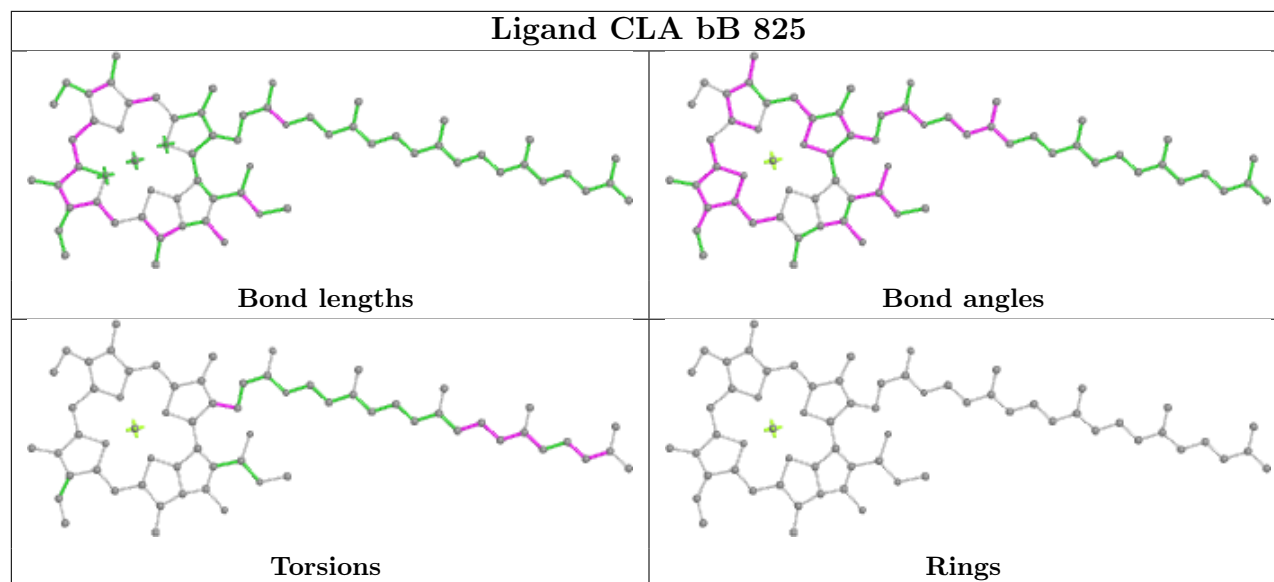
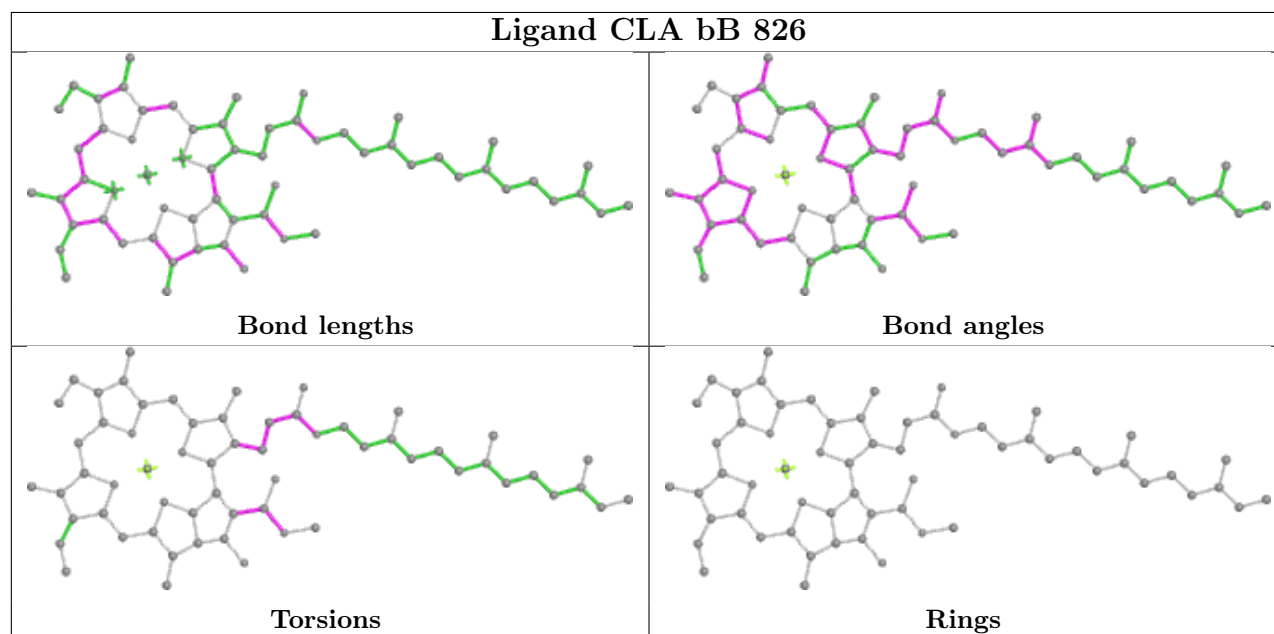




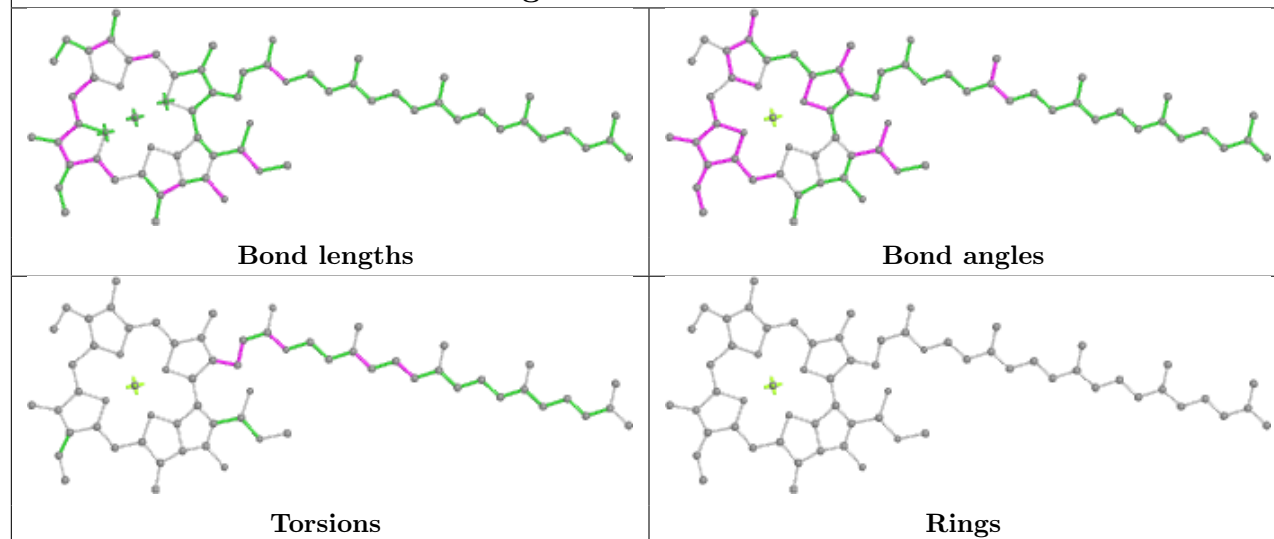
Ligand CLA bB 822



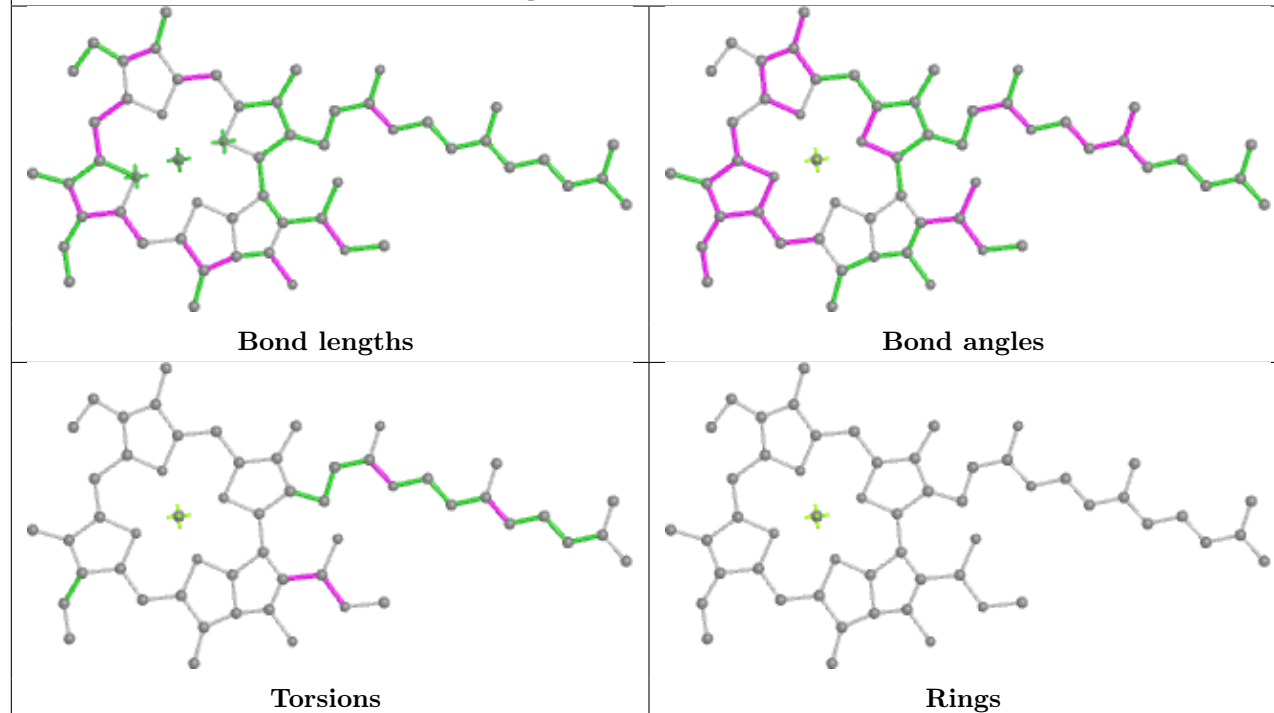
Ligand CLA bB 823**Ligand F6C bB 824**

Ligand CLA bB 825**Ligand CLA bB 826**

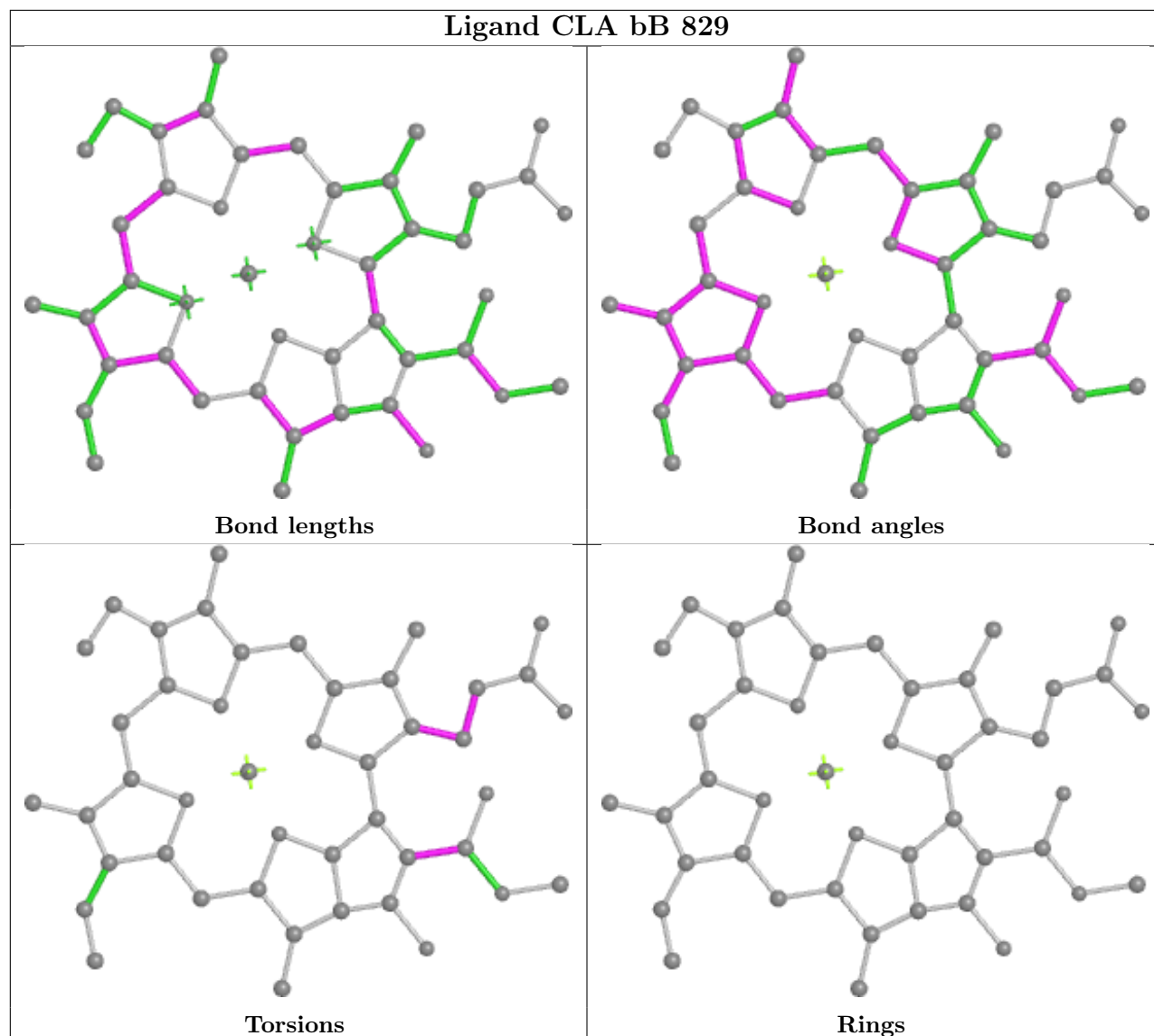
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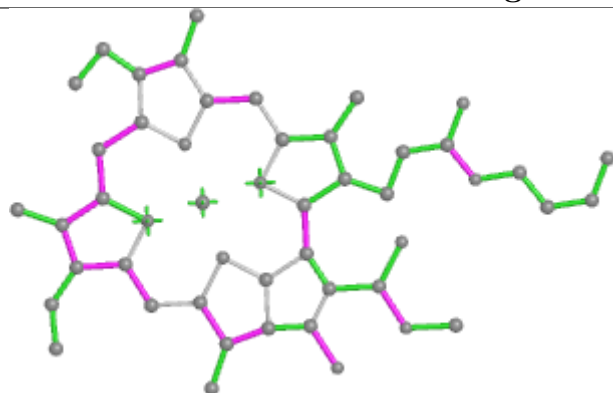
Ligand CLA bB 828



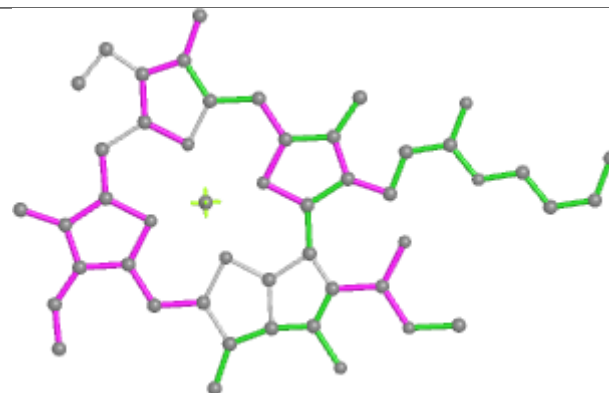
Ligand CLA bB 829



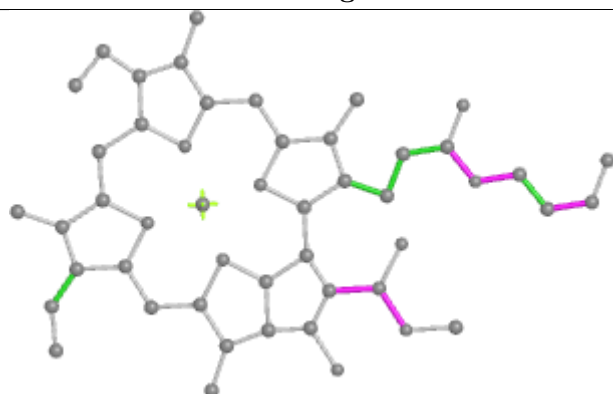
Ligand CLA bB 830



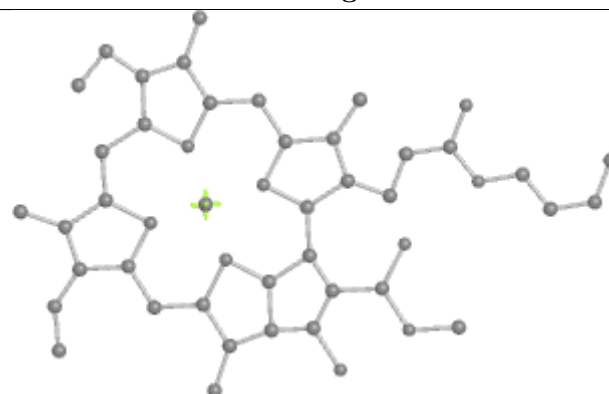
Bond lengths



Bond angles

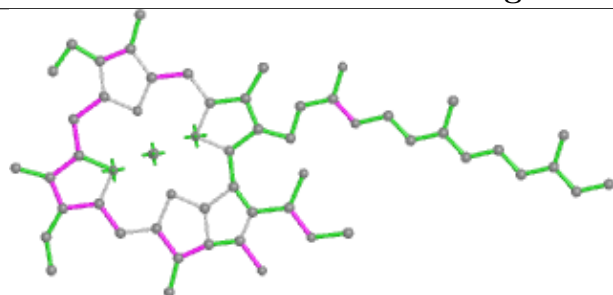


Torsions

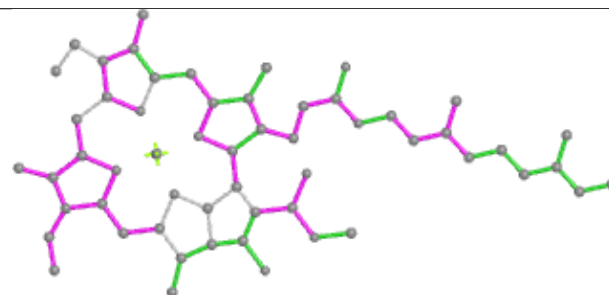


Rings

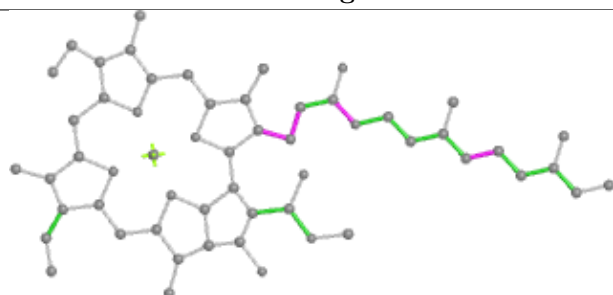
Ligand CLA bB 831



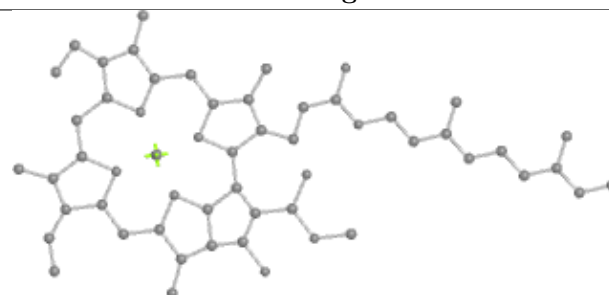
Bond lengths



Bond angles

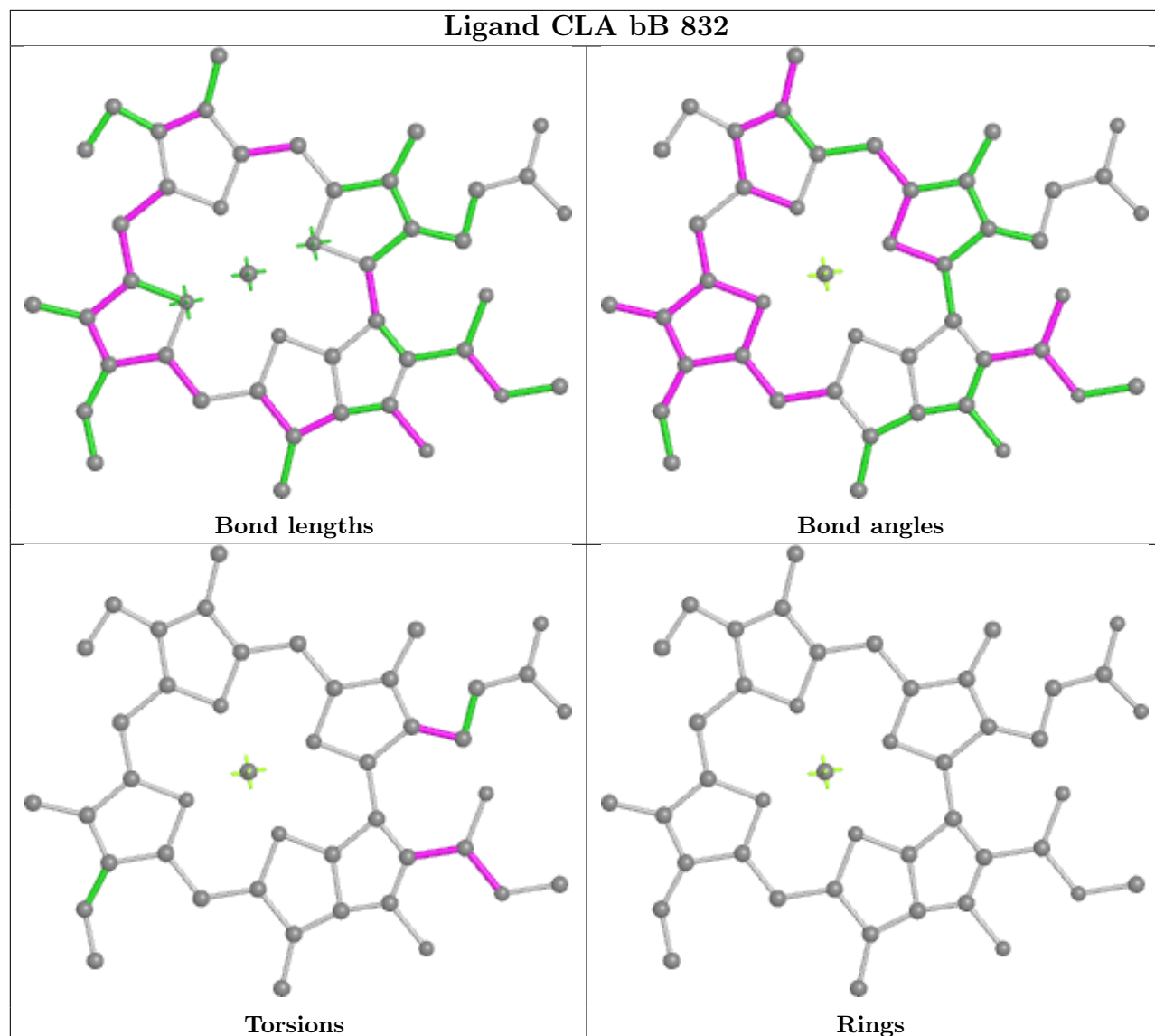


Torsions

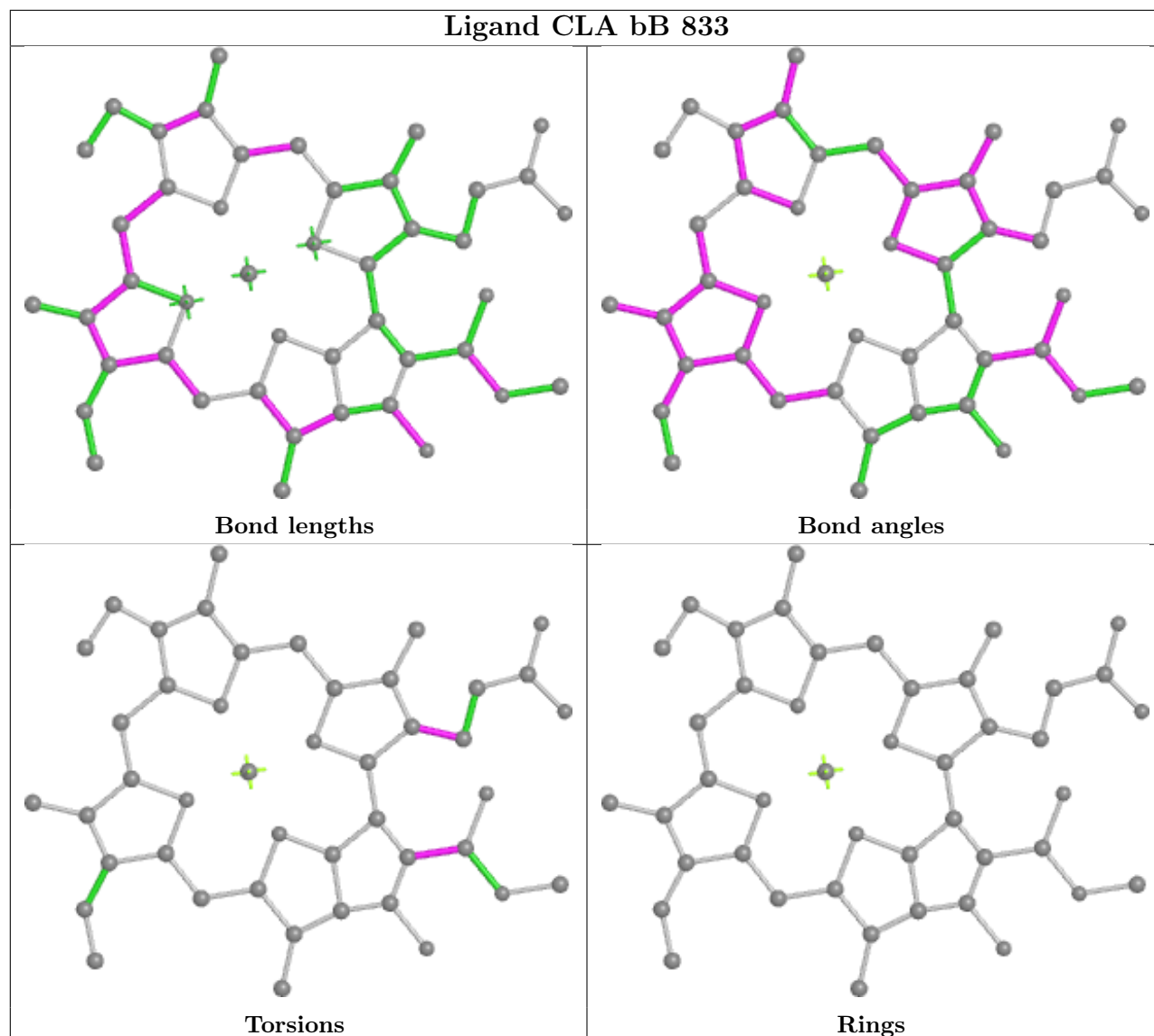


Rings

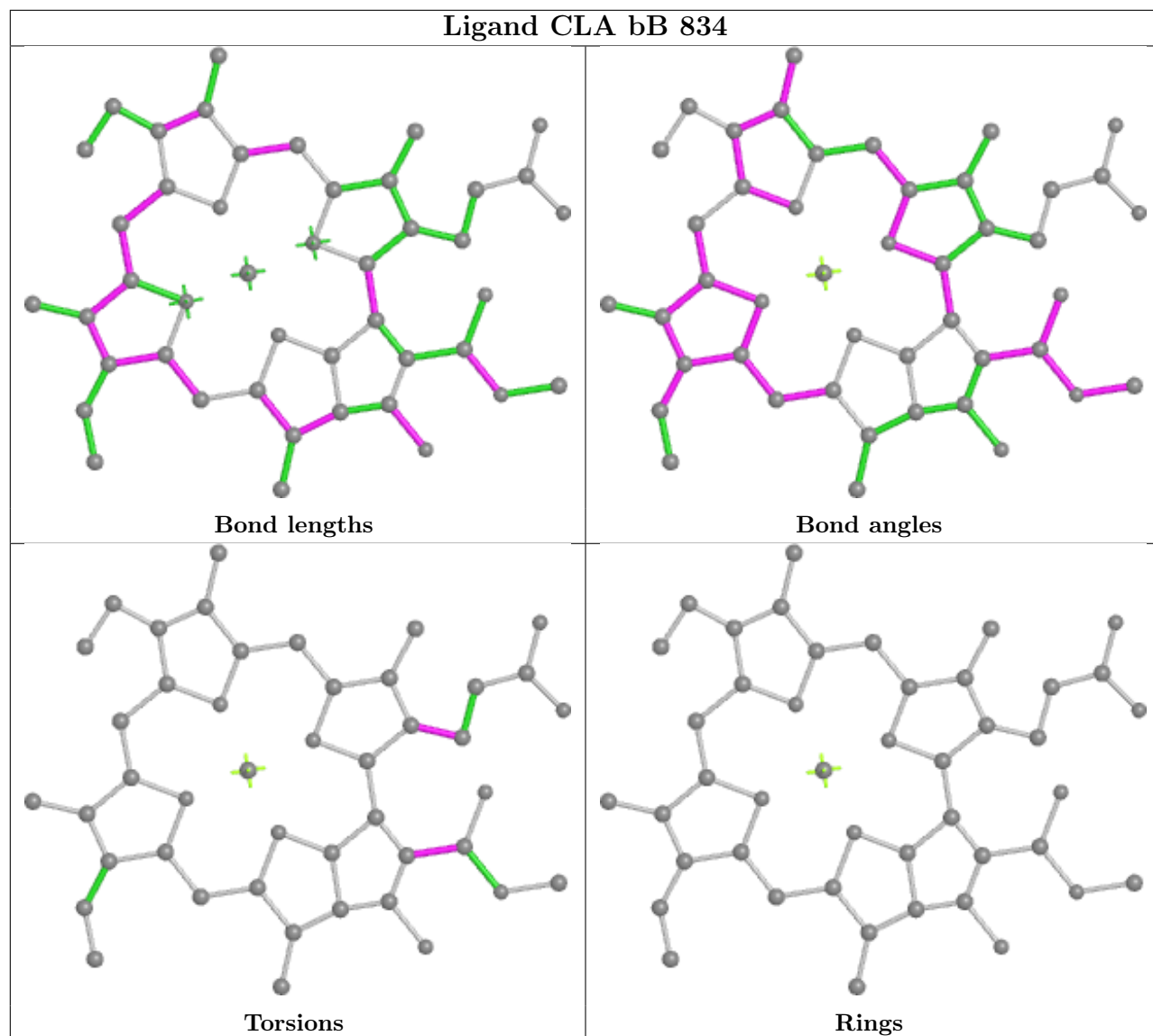
Ligand CLA bB 832



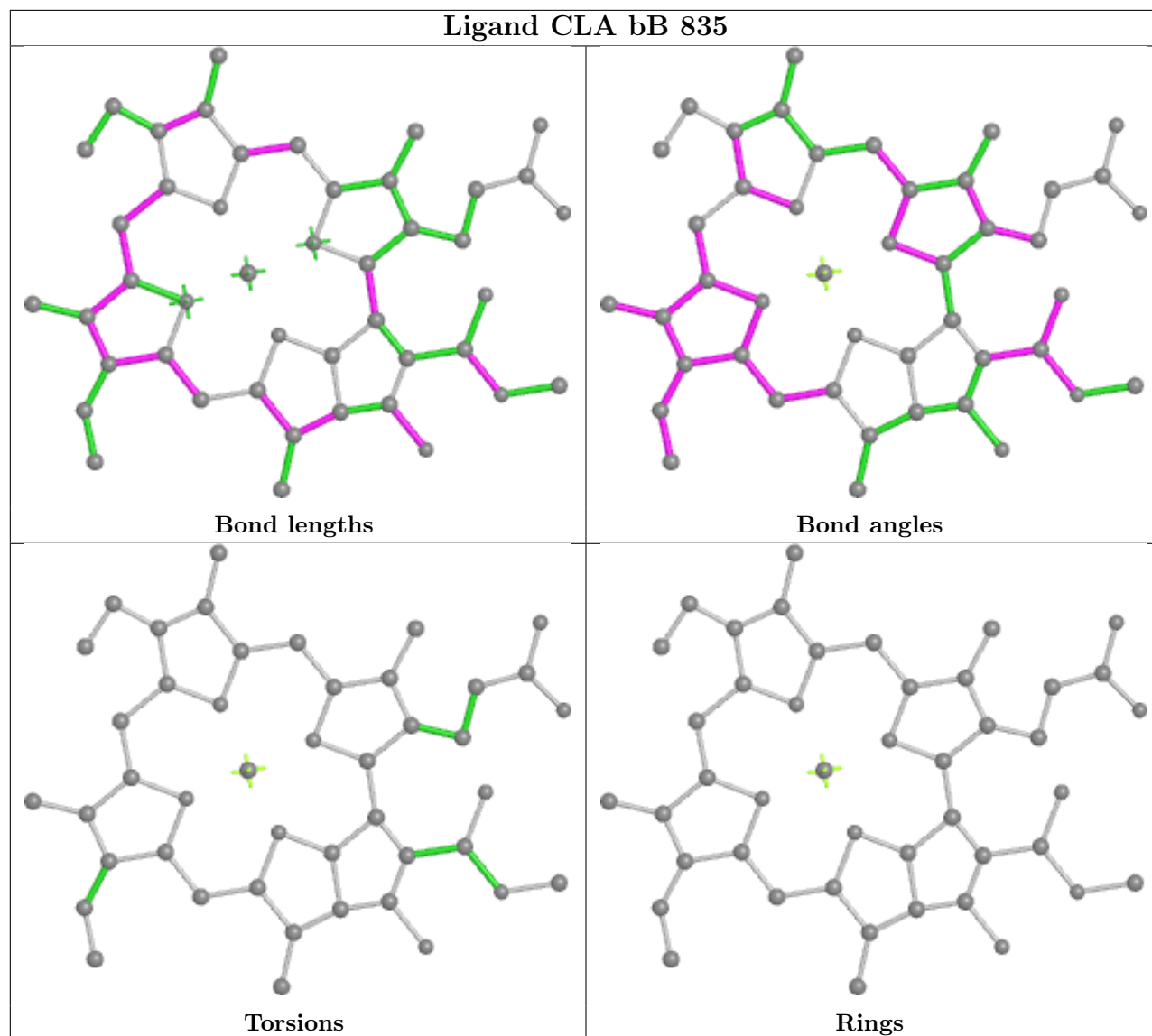
Ligand CLA bB 833



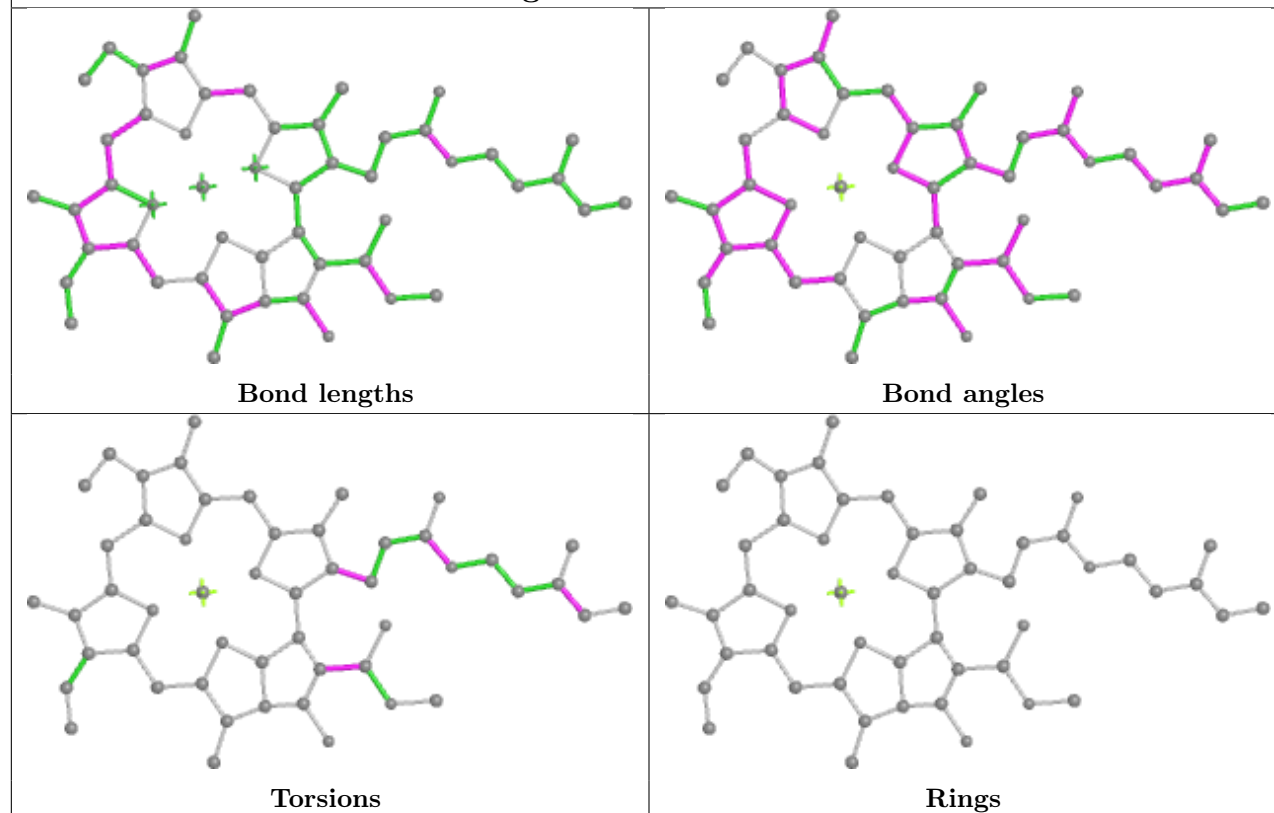
Ligand CLA bB 834



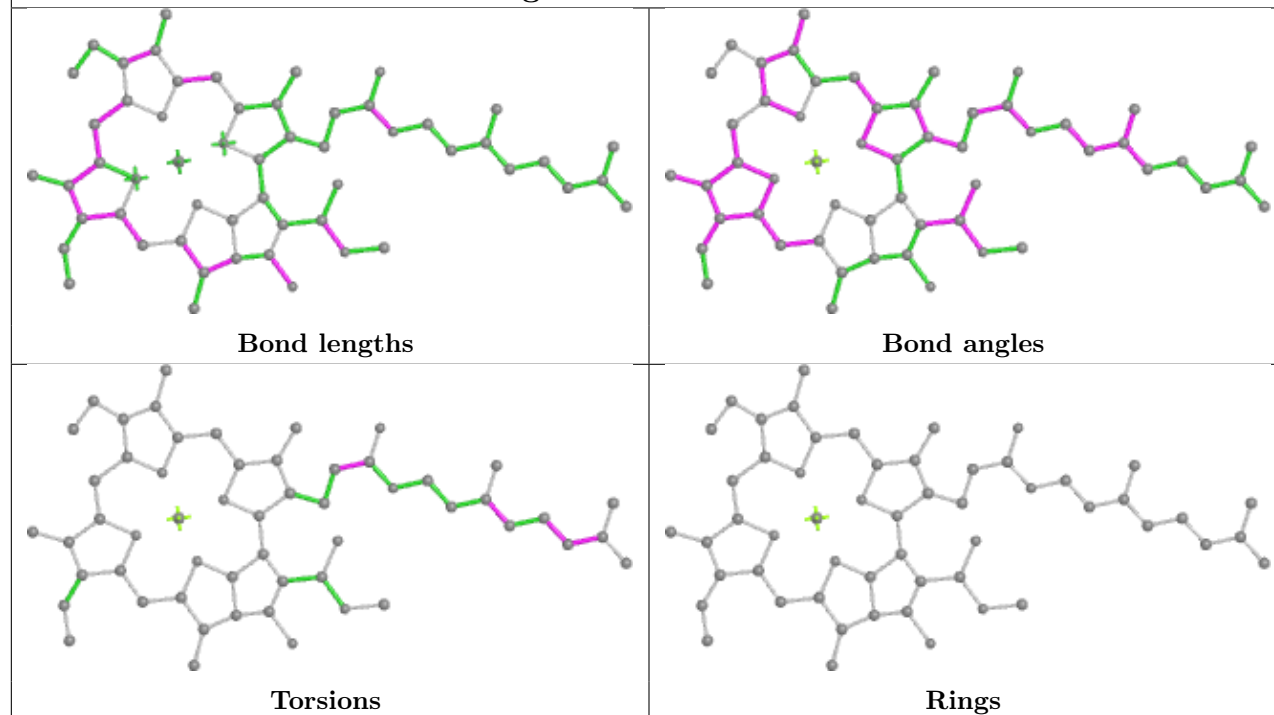
Ligand CLA bB 835



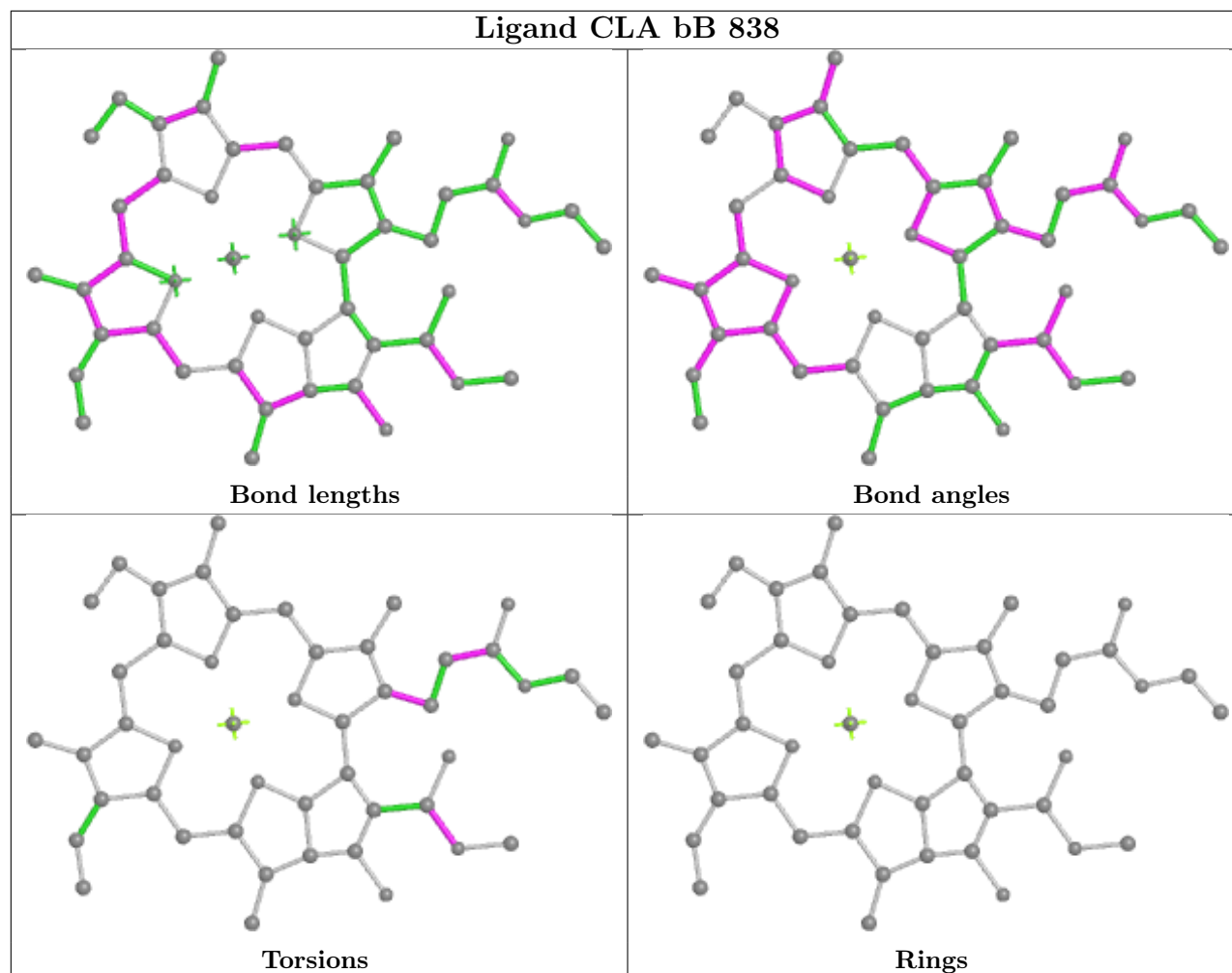
Ligand CLA bB 836



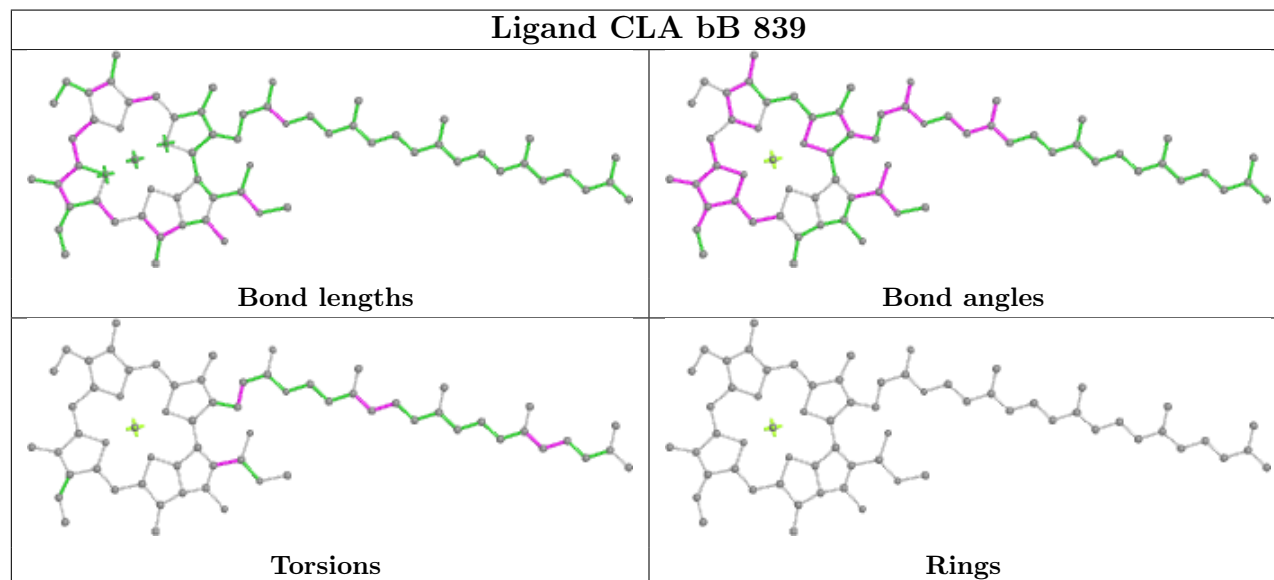
Ligand CLA bB 837



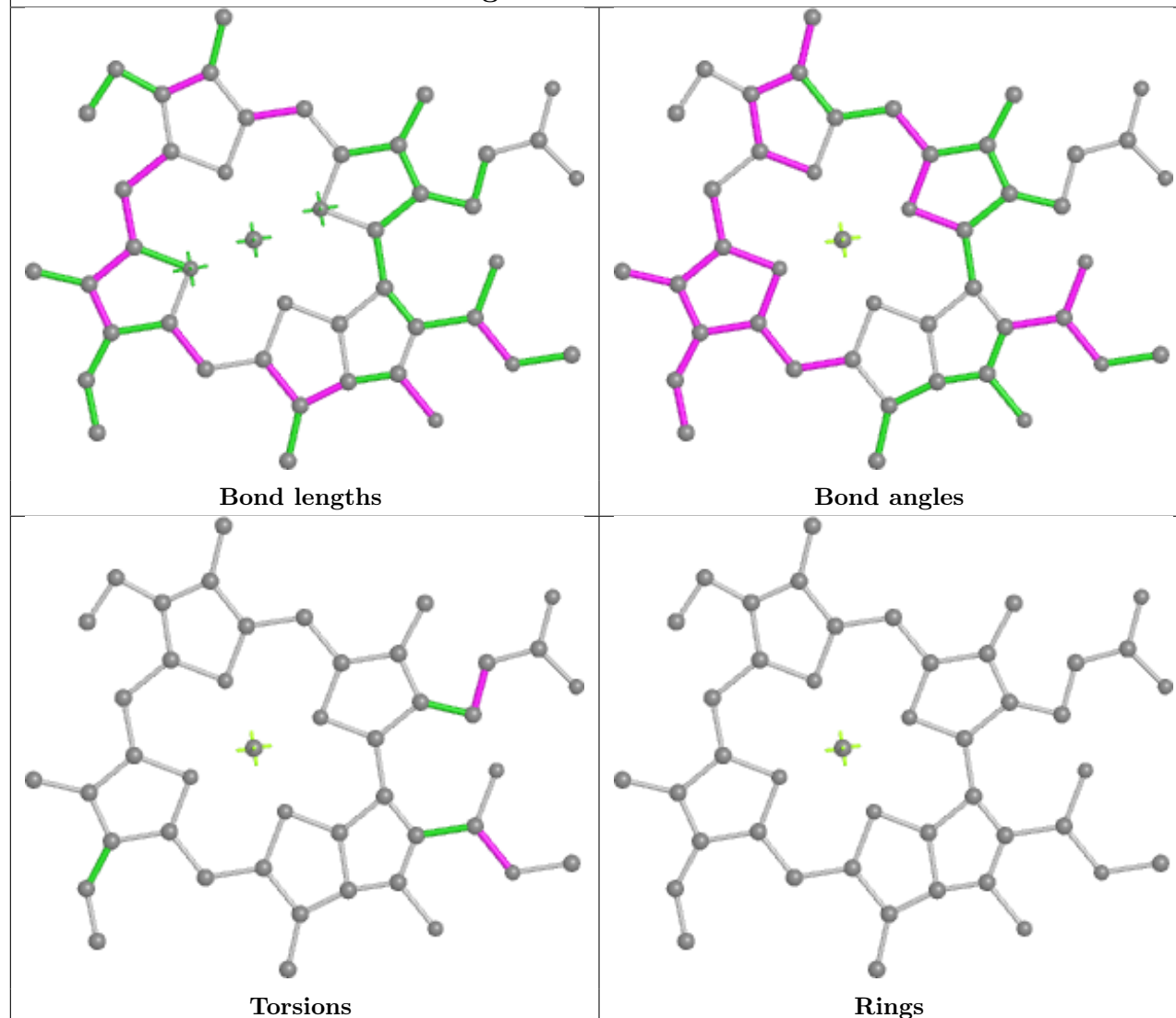
Ligand CLA bB 838



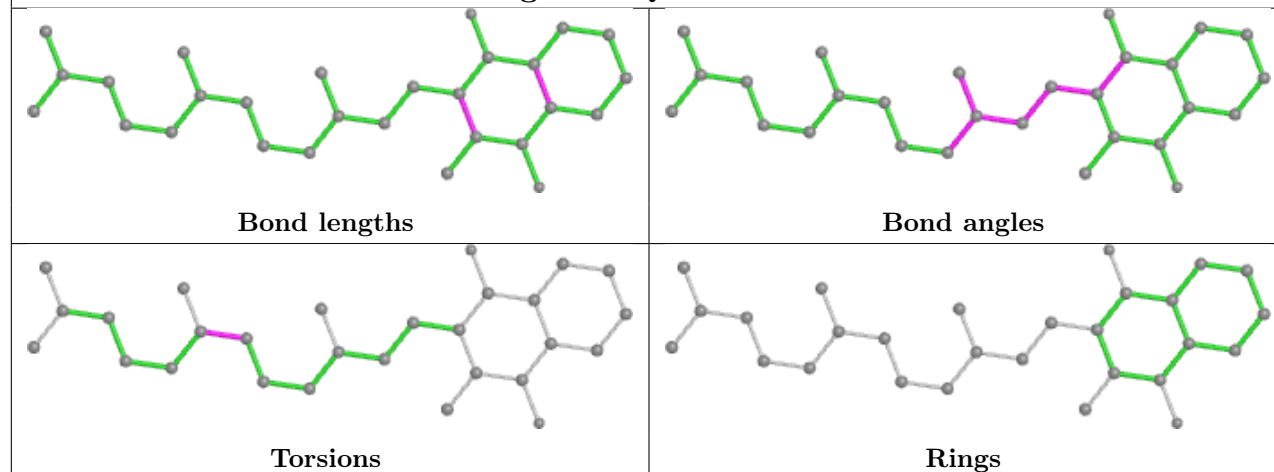
Ligand CLA bB 839

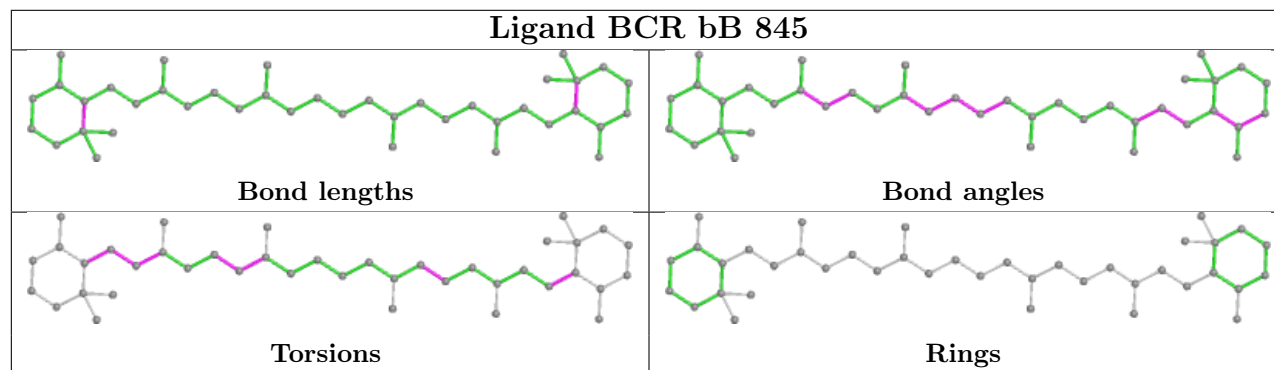
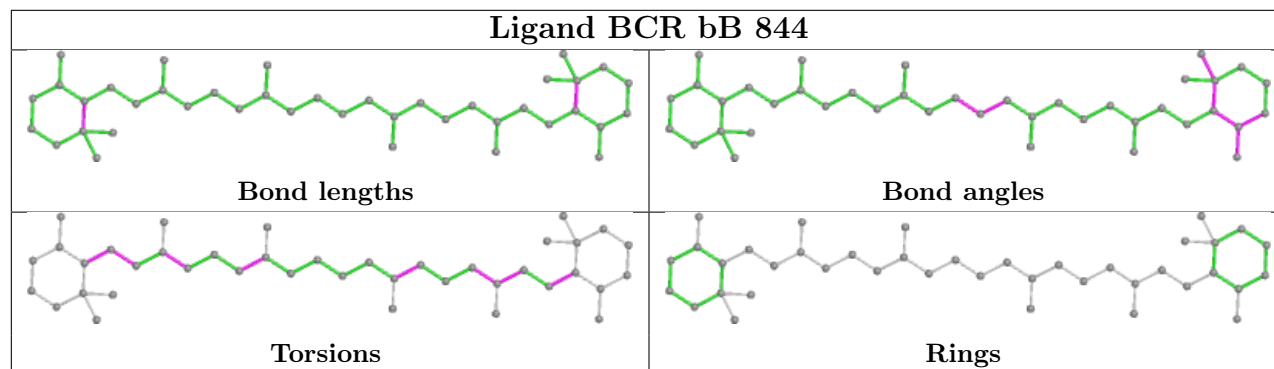
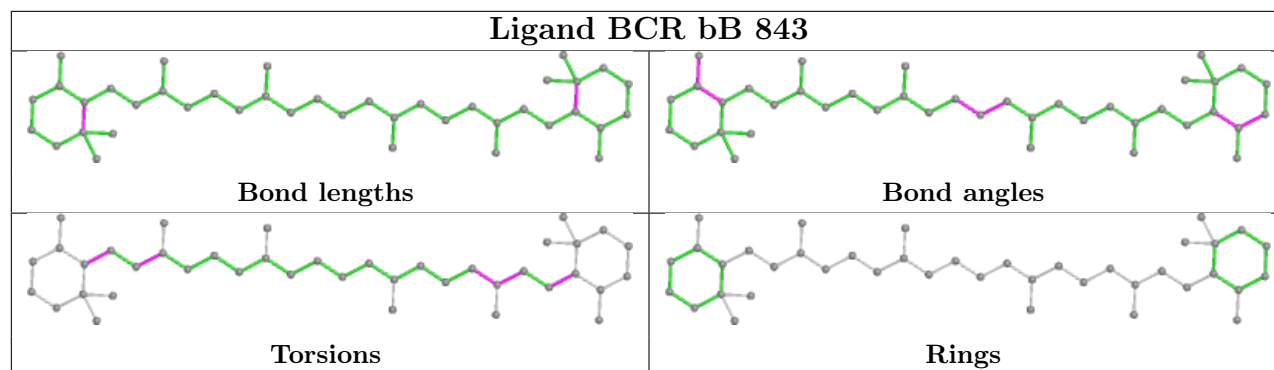
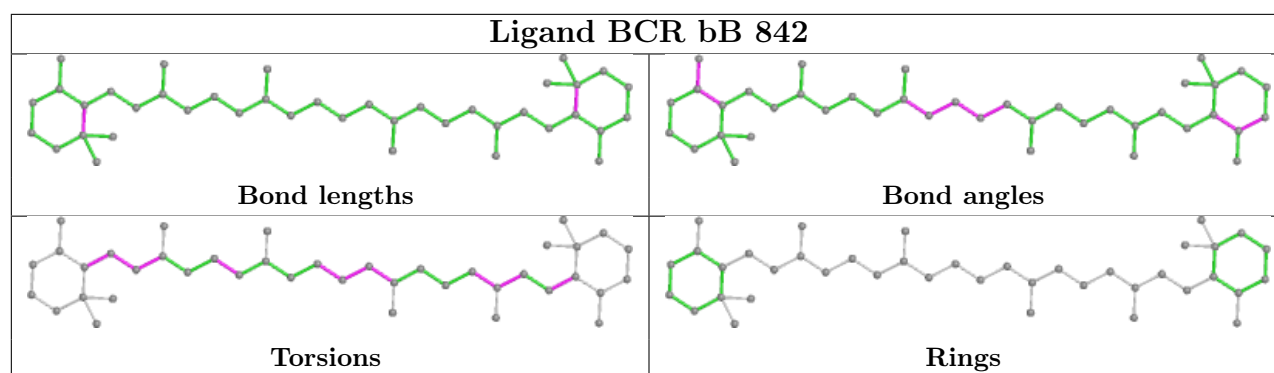


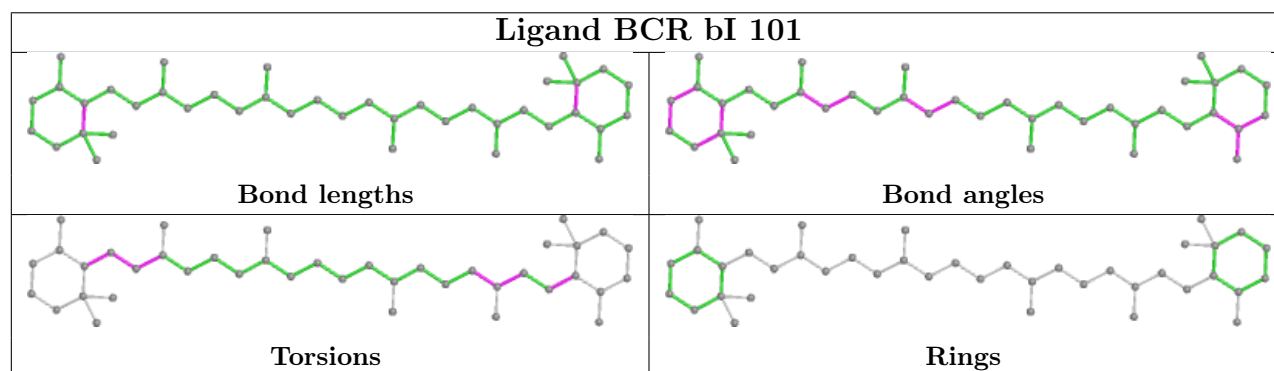
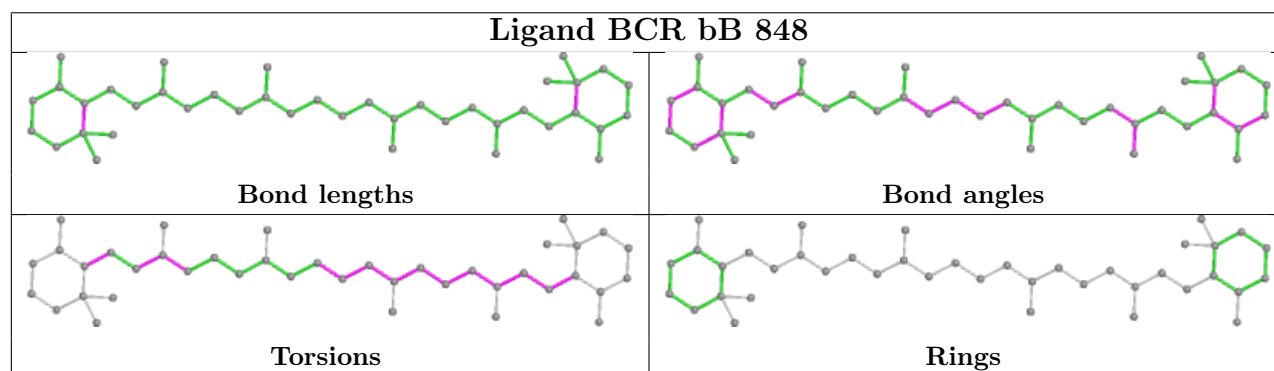
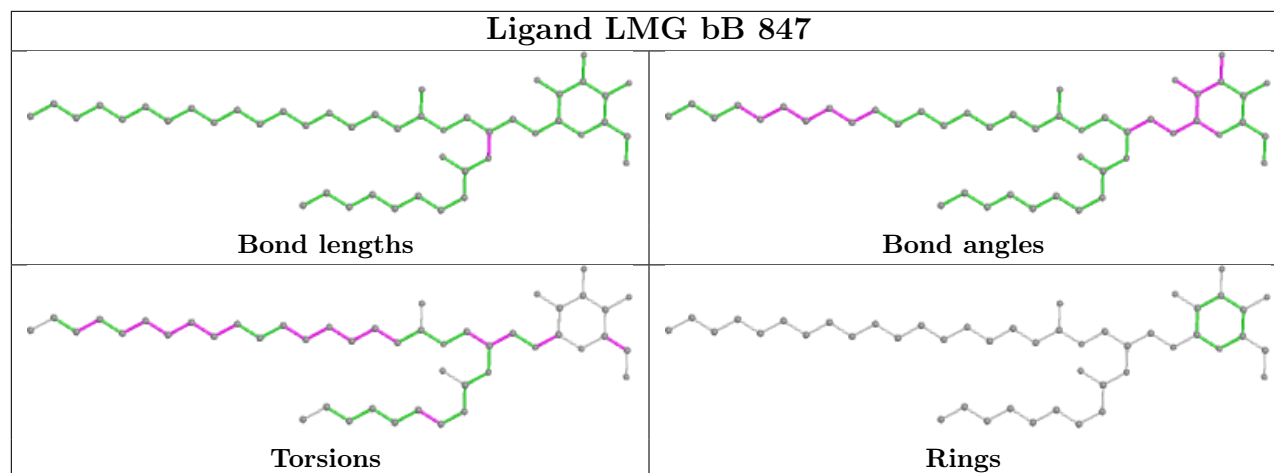
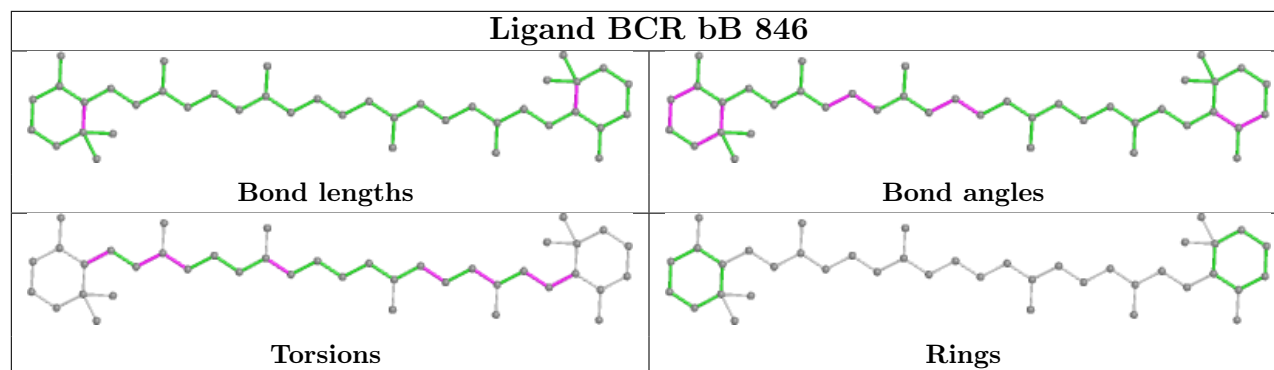
Ligand CLA bB 840



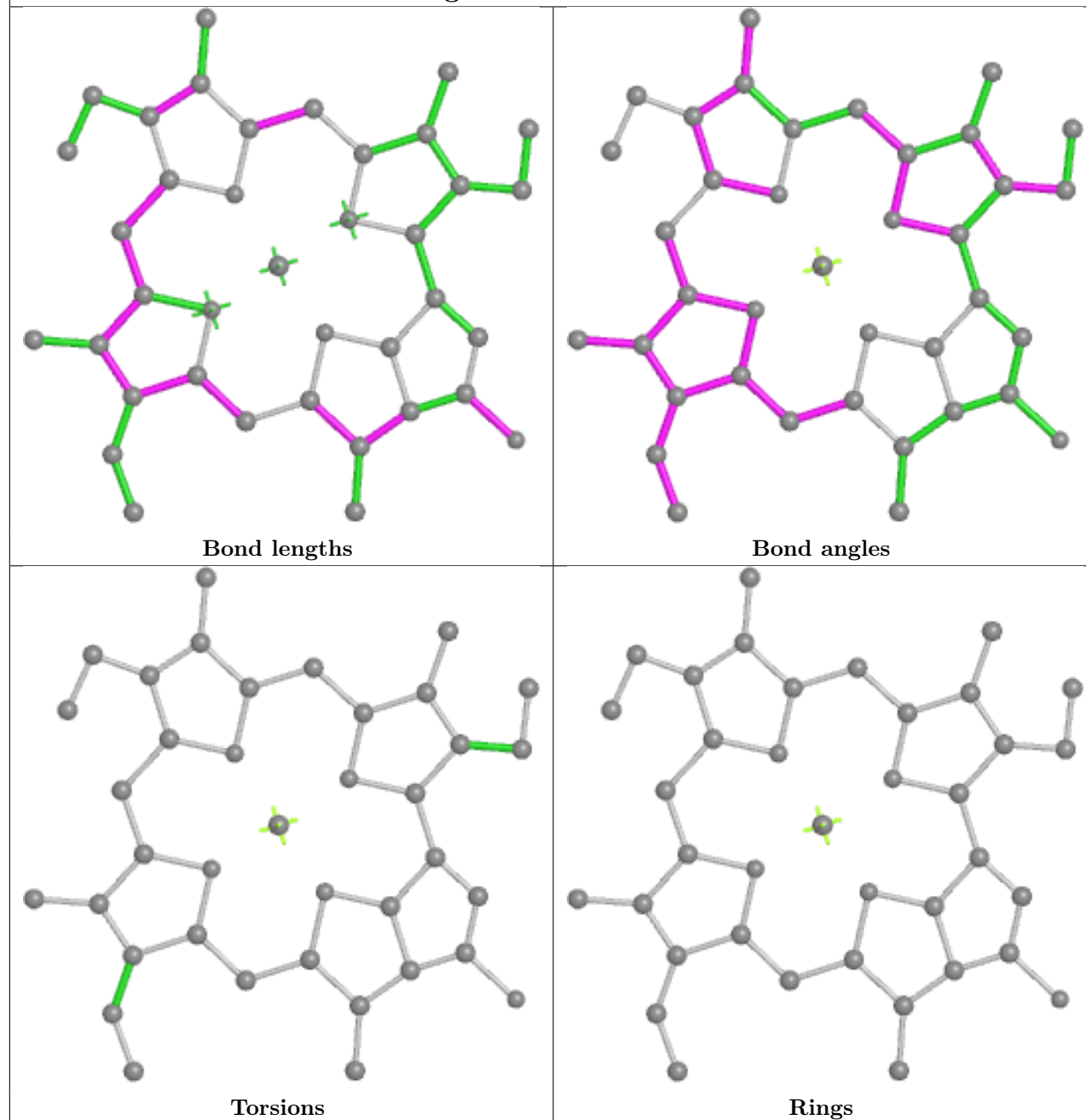
Ligand PQN bB 841



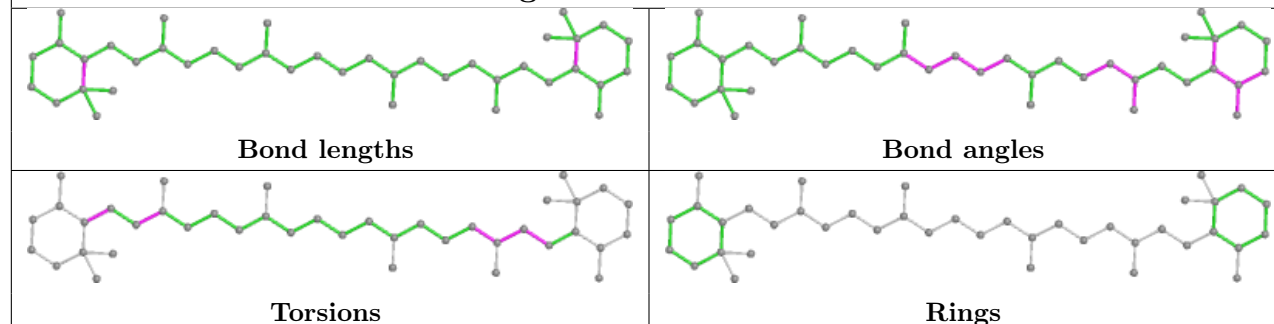




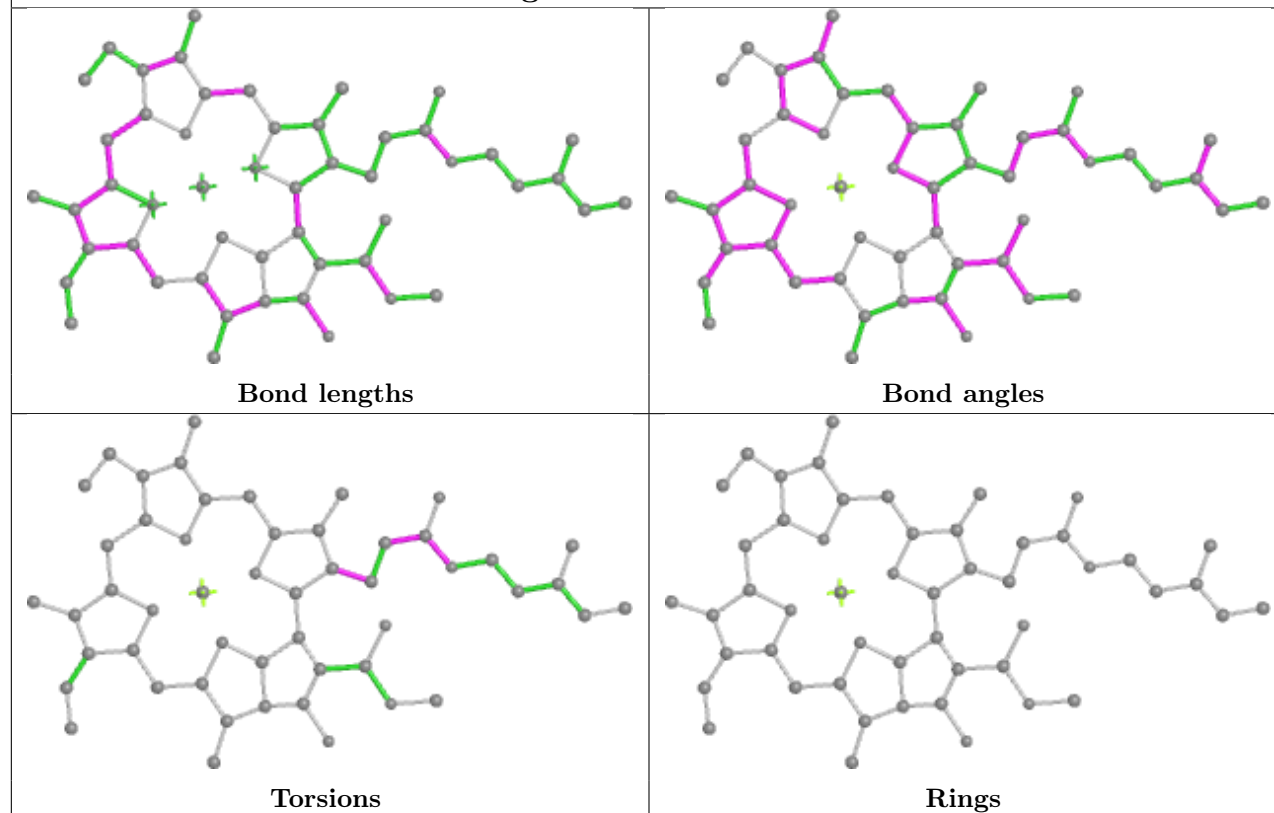
Ligand CLA bK 101



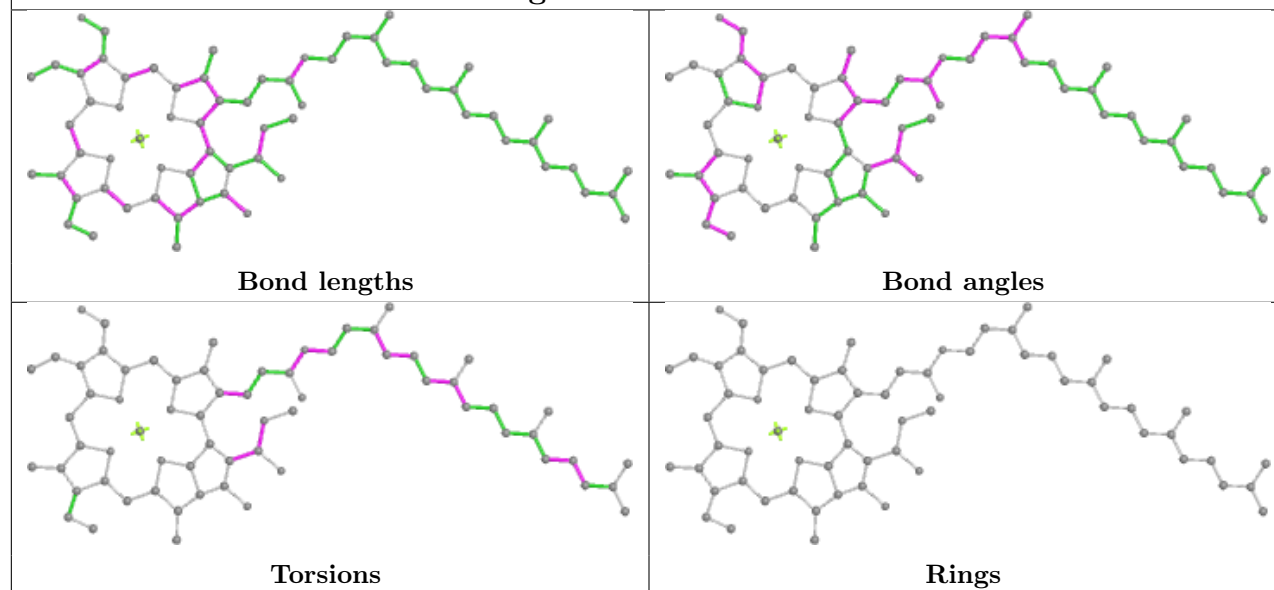
Ligand BCR bK 102

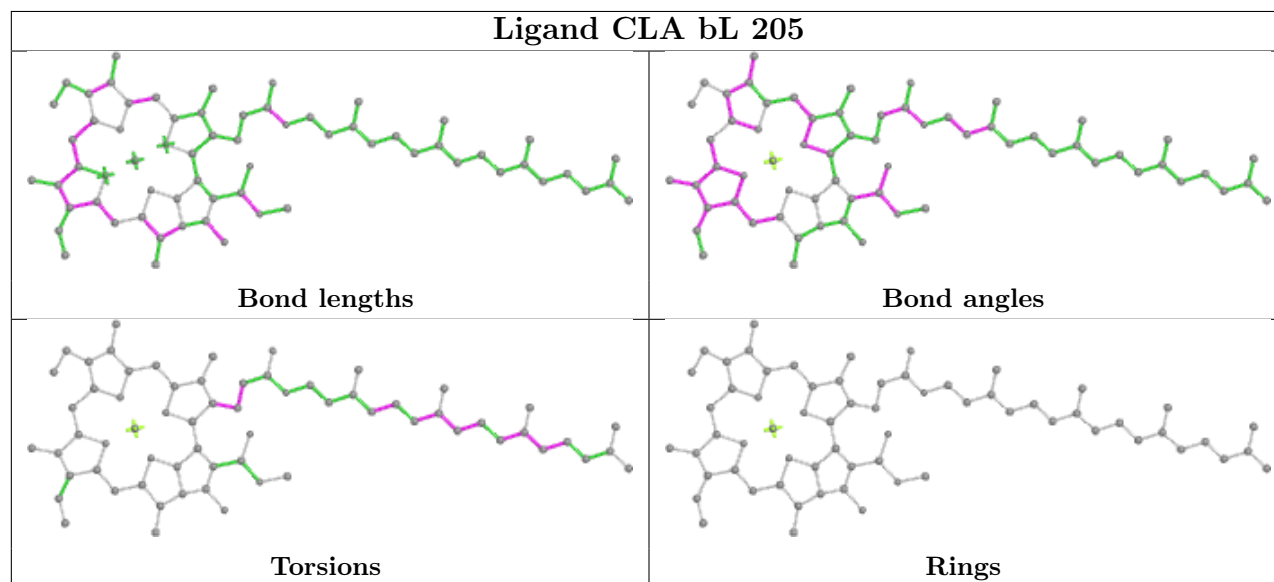
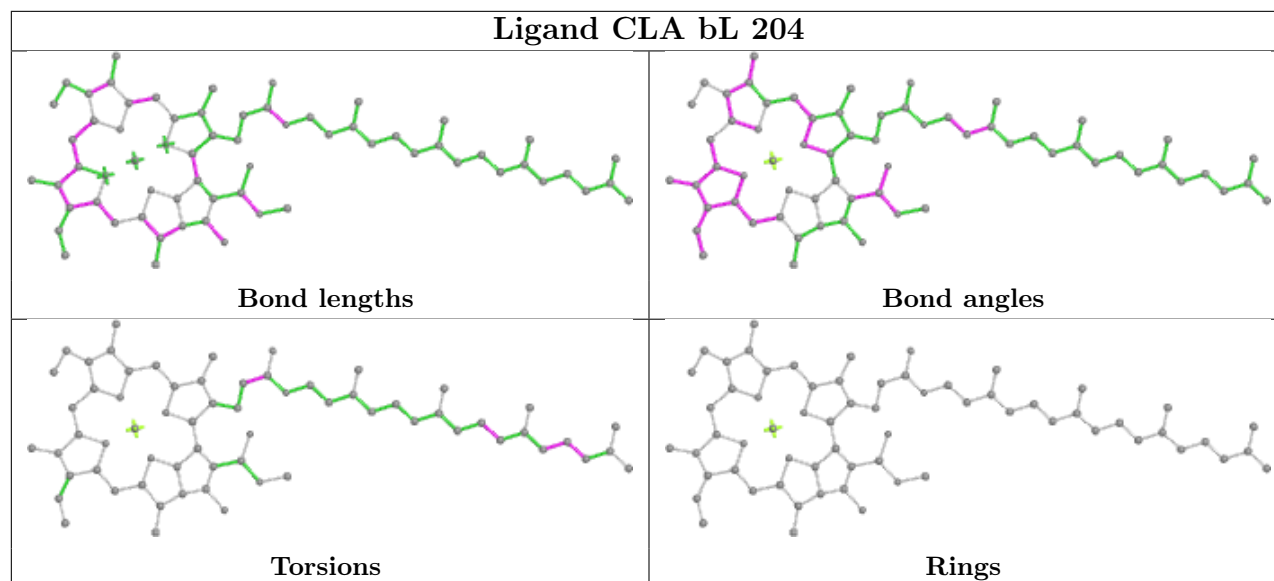
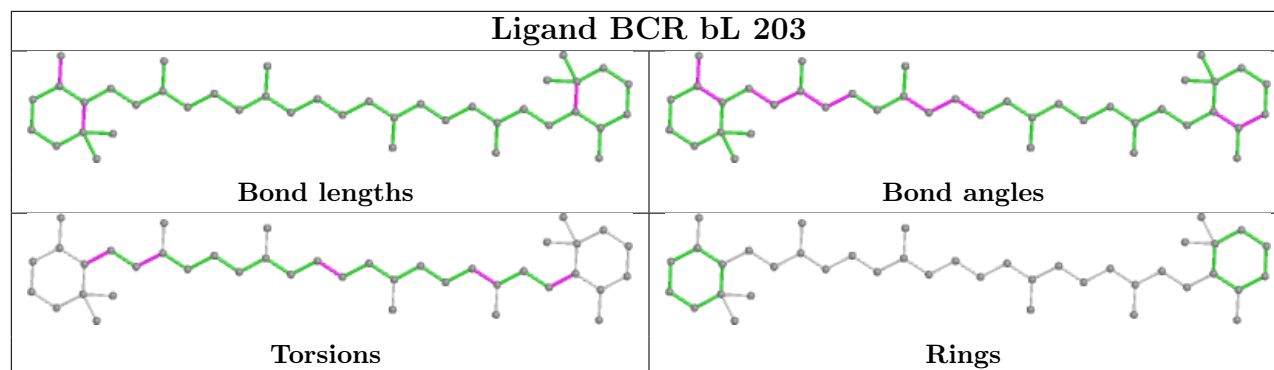


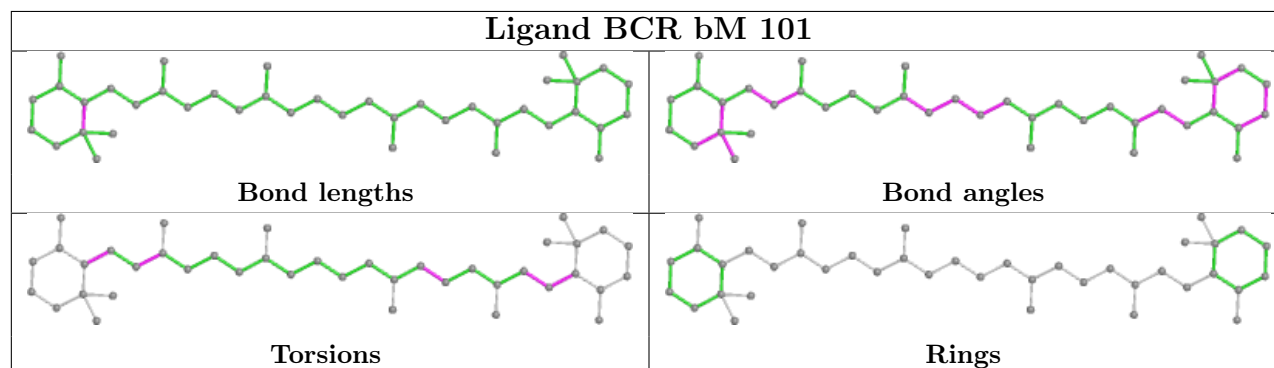
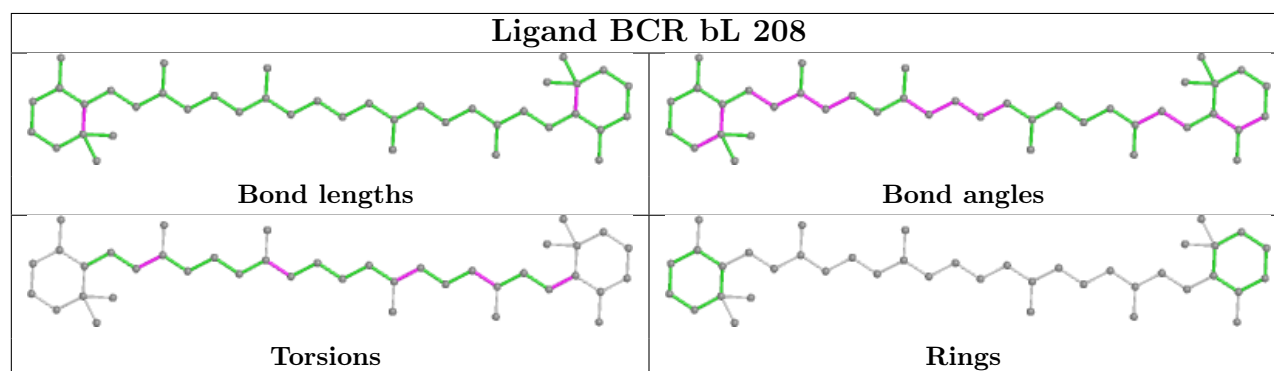
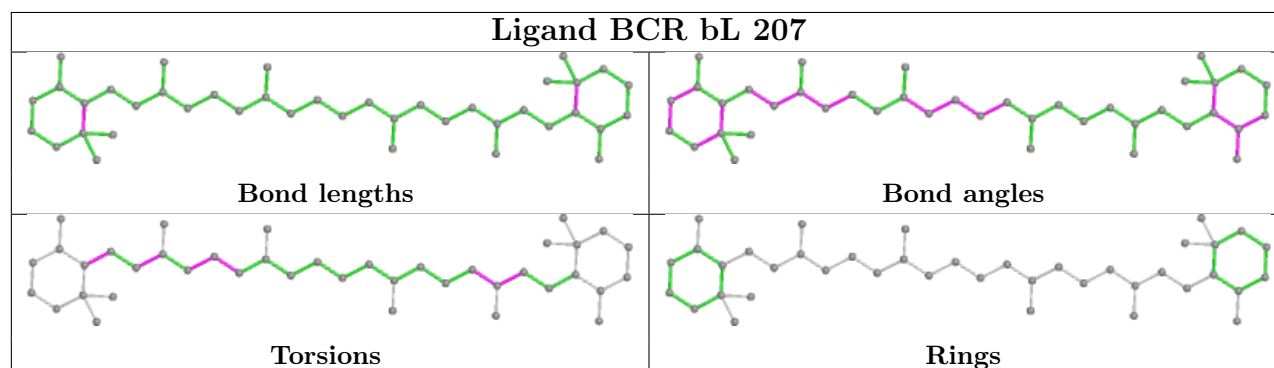
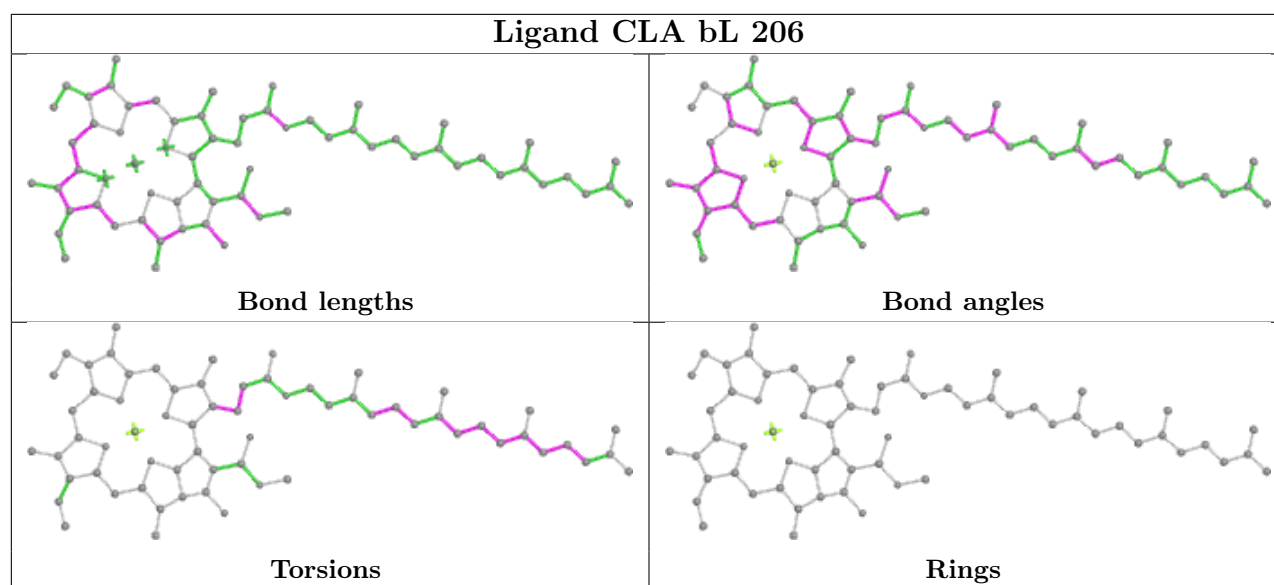
Ligand CLA bK 103

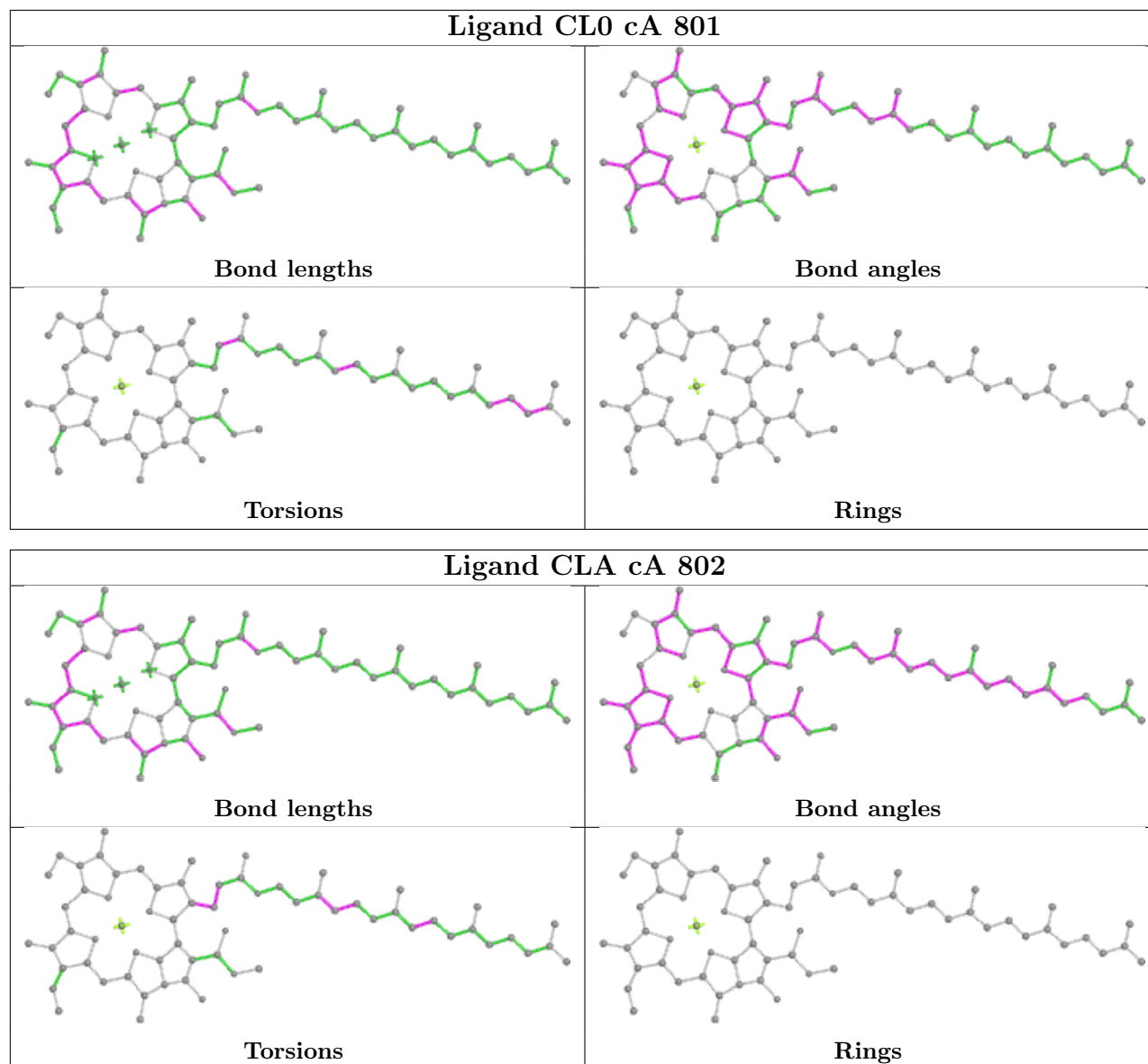


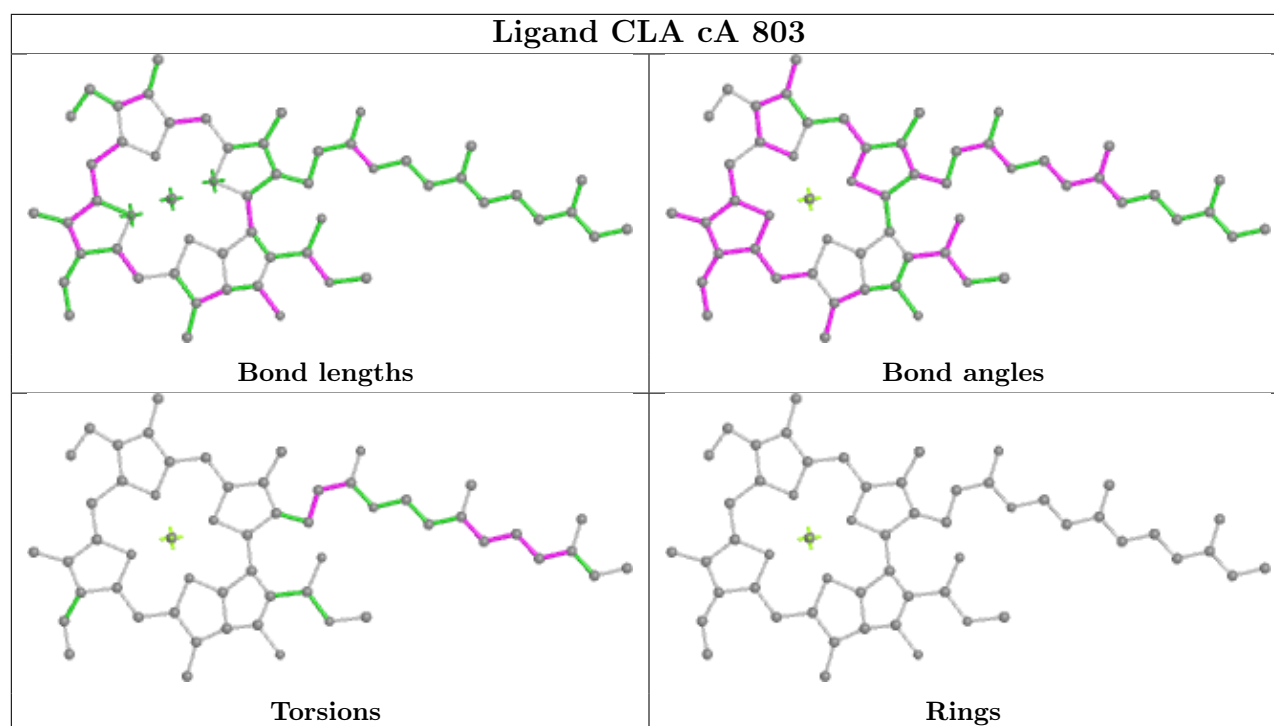
Ligand F6C bL 202



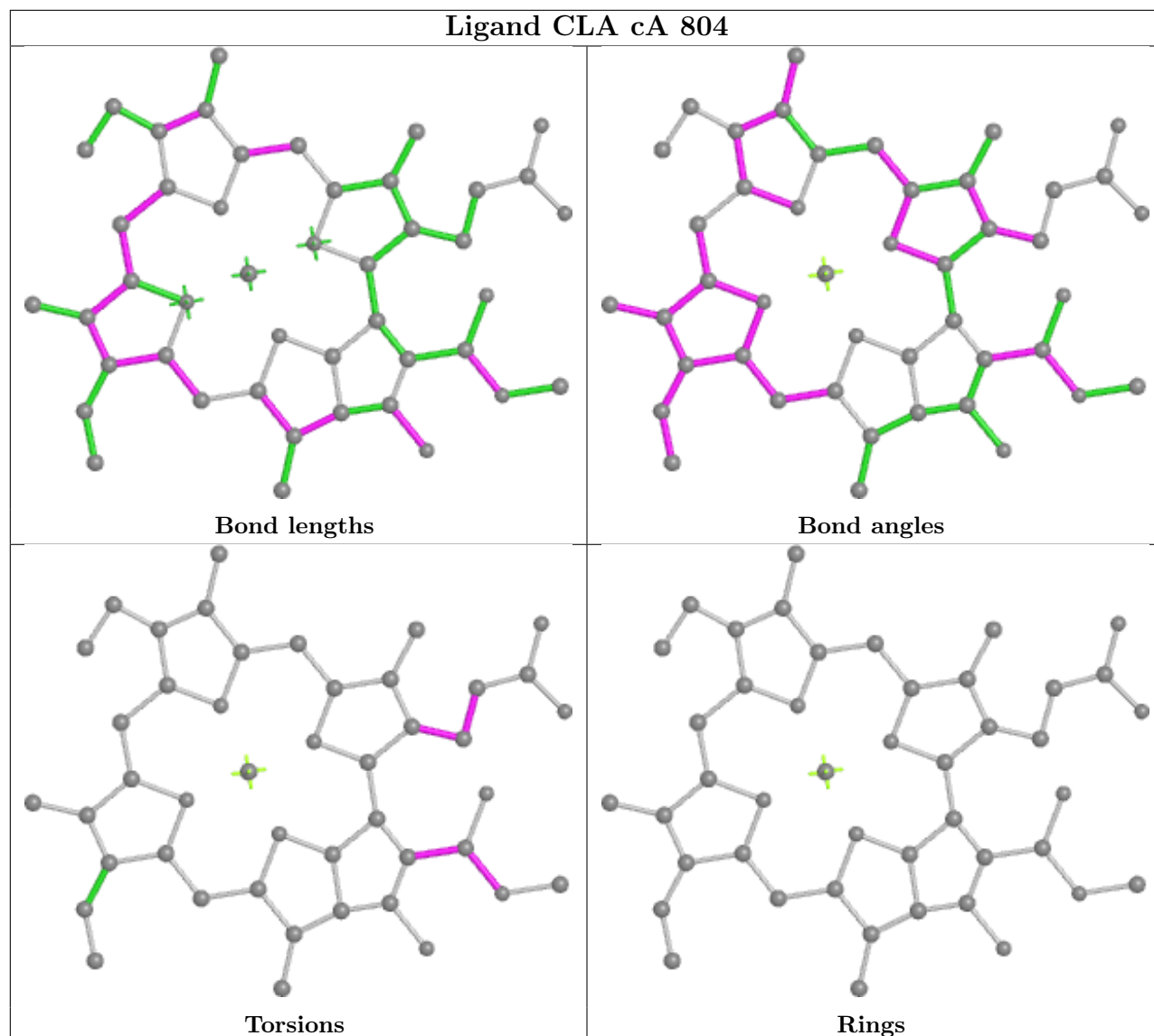




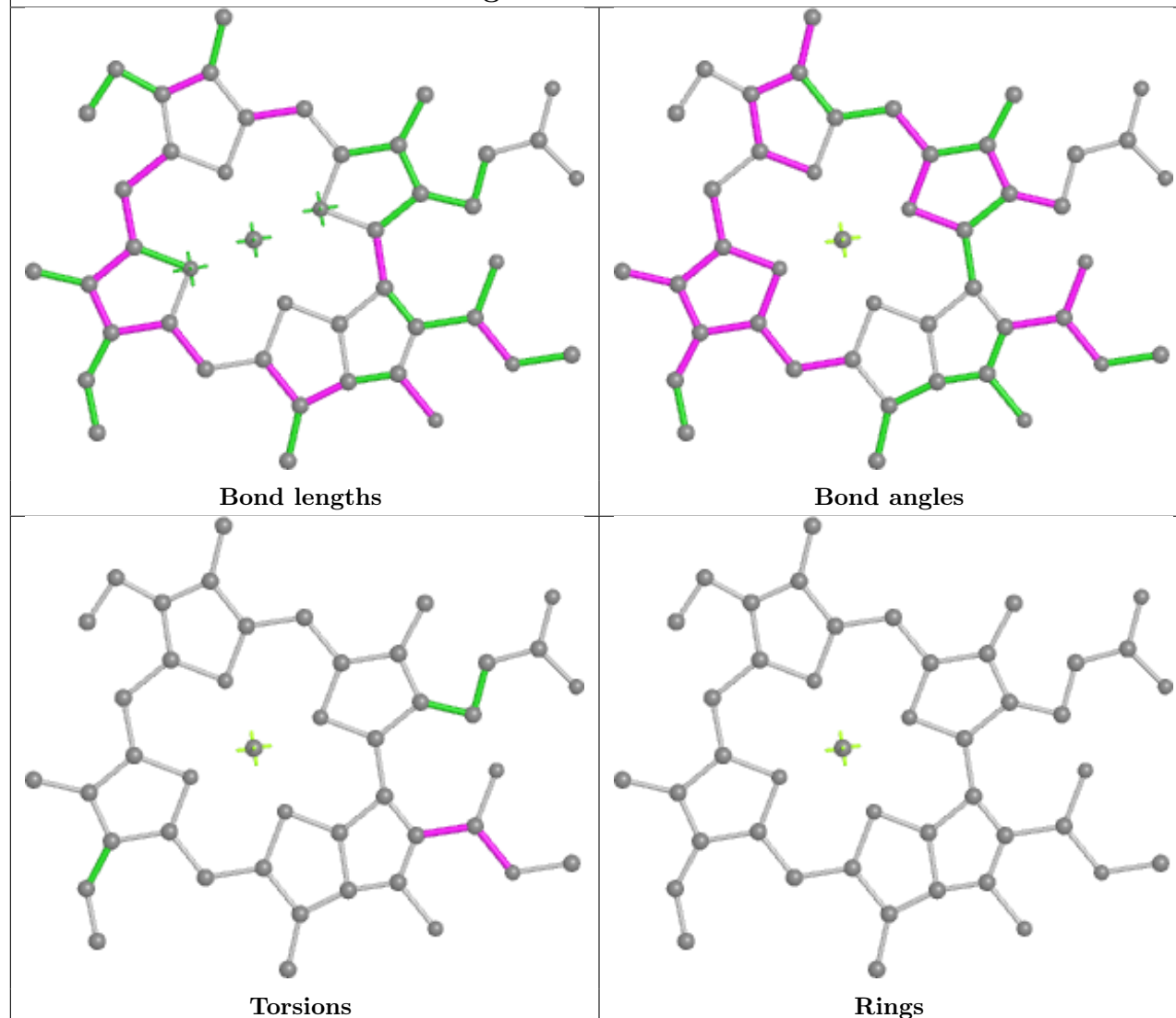




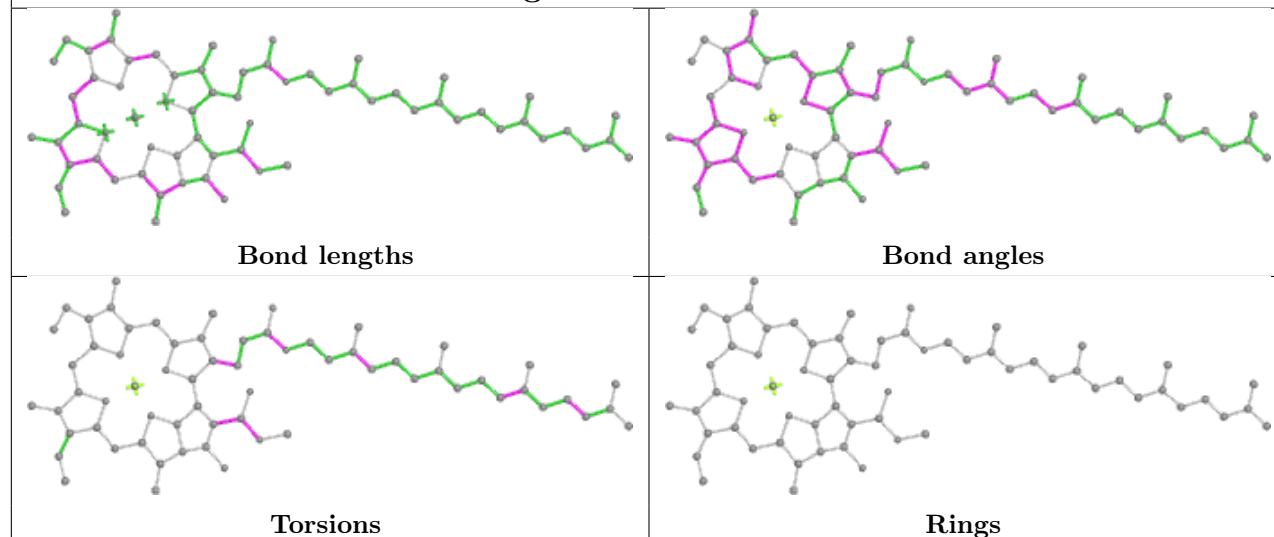
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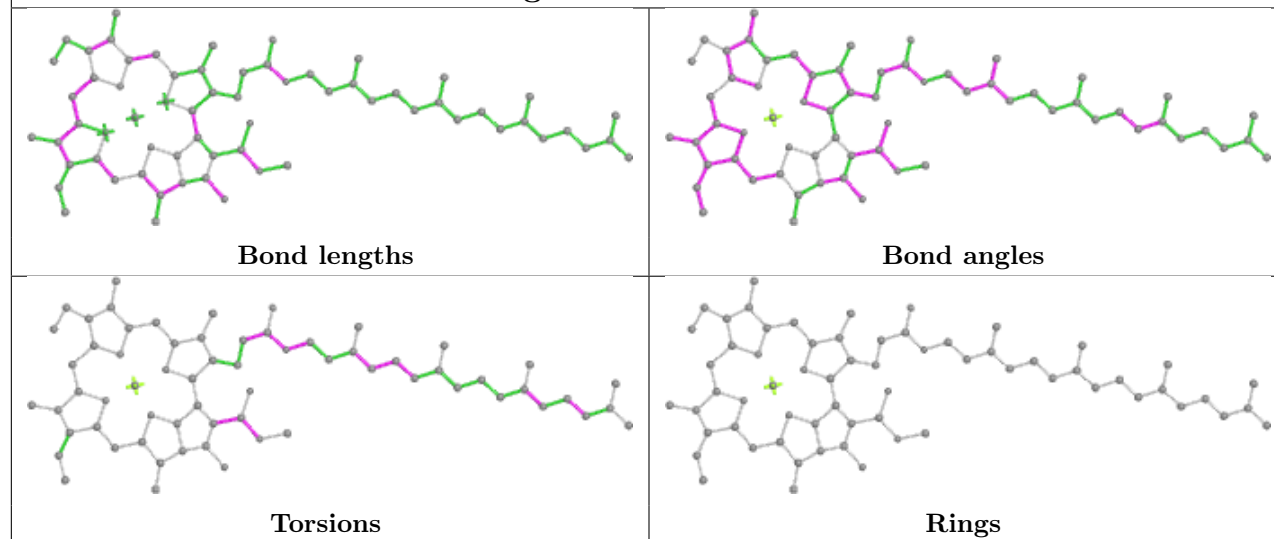
Ligand CLA cA 805



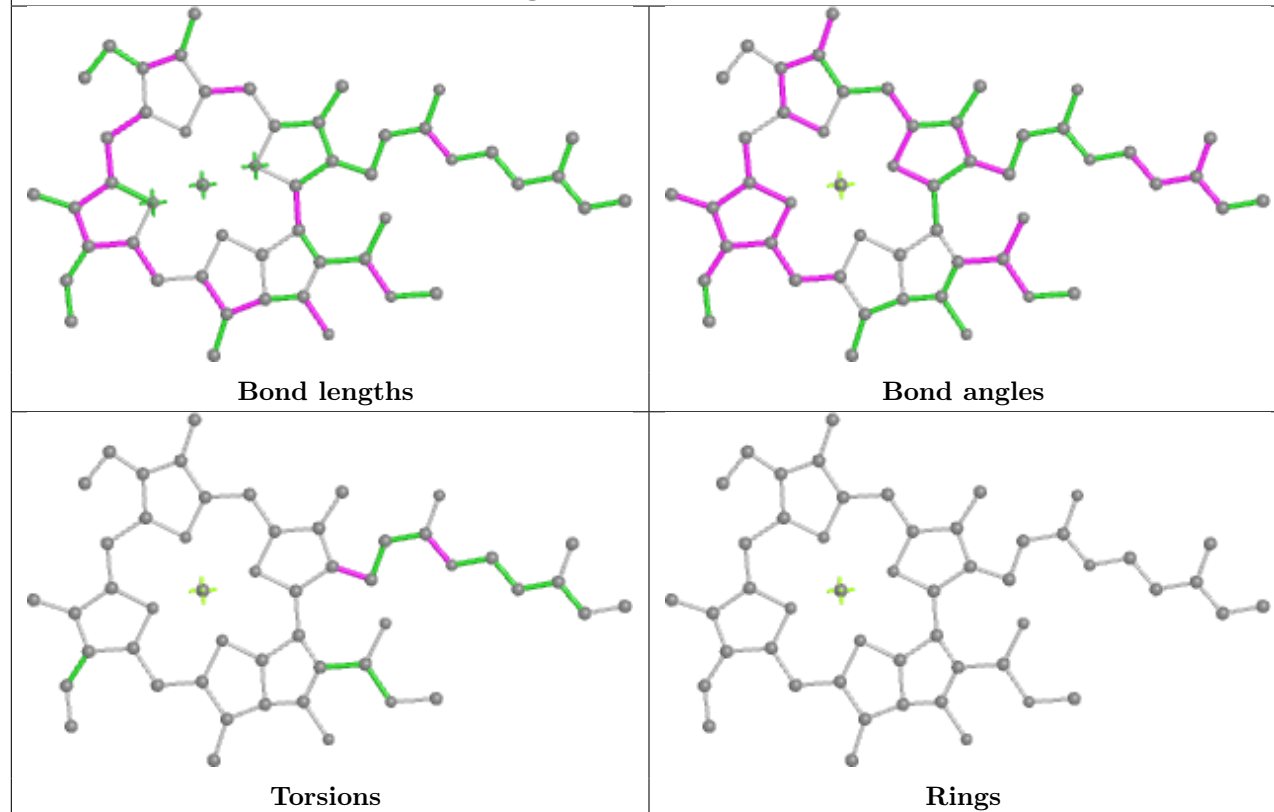
Ligand CLA cA 806



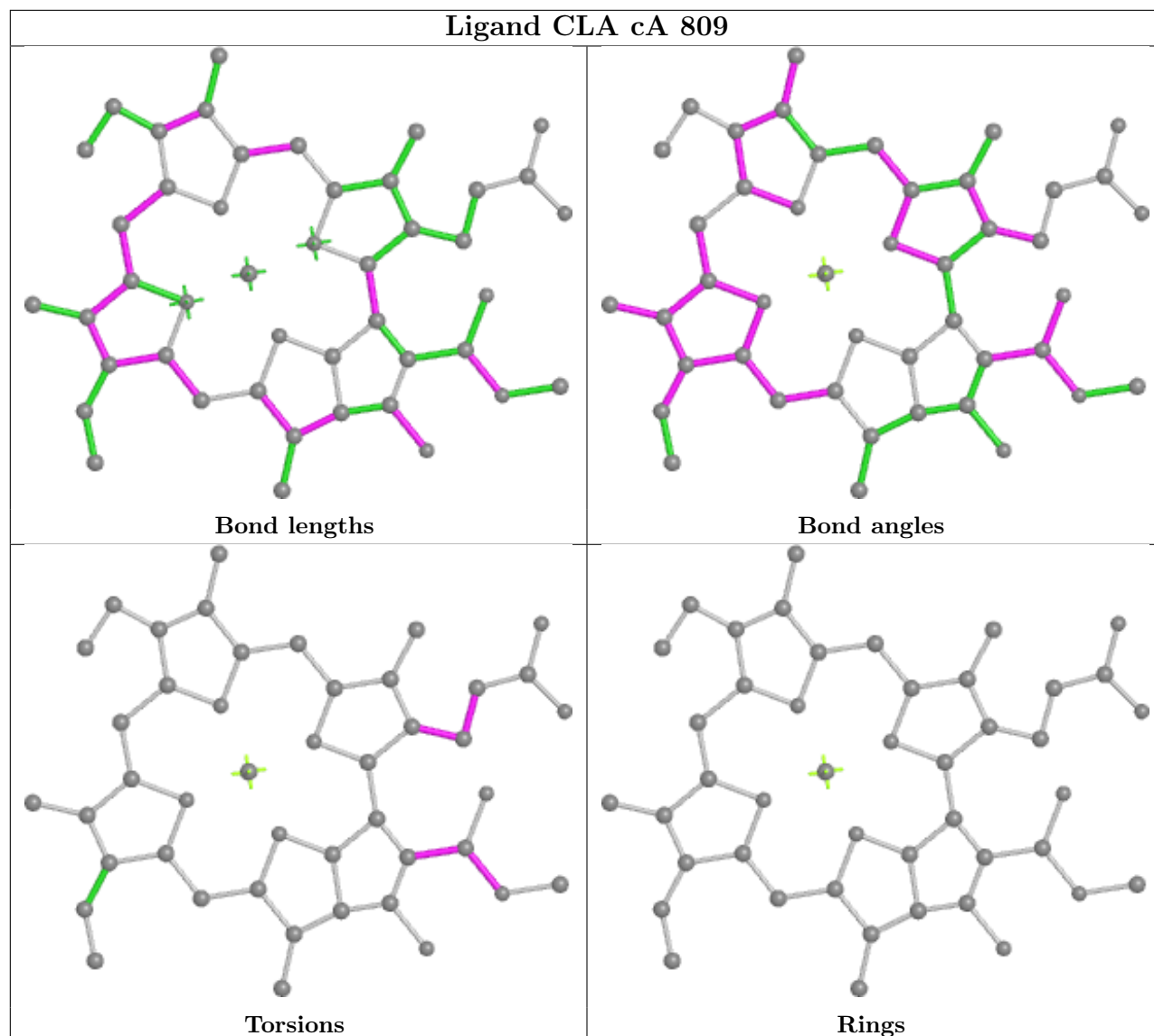
Ligand CLA cA 807



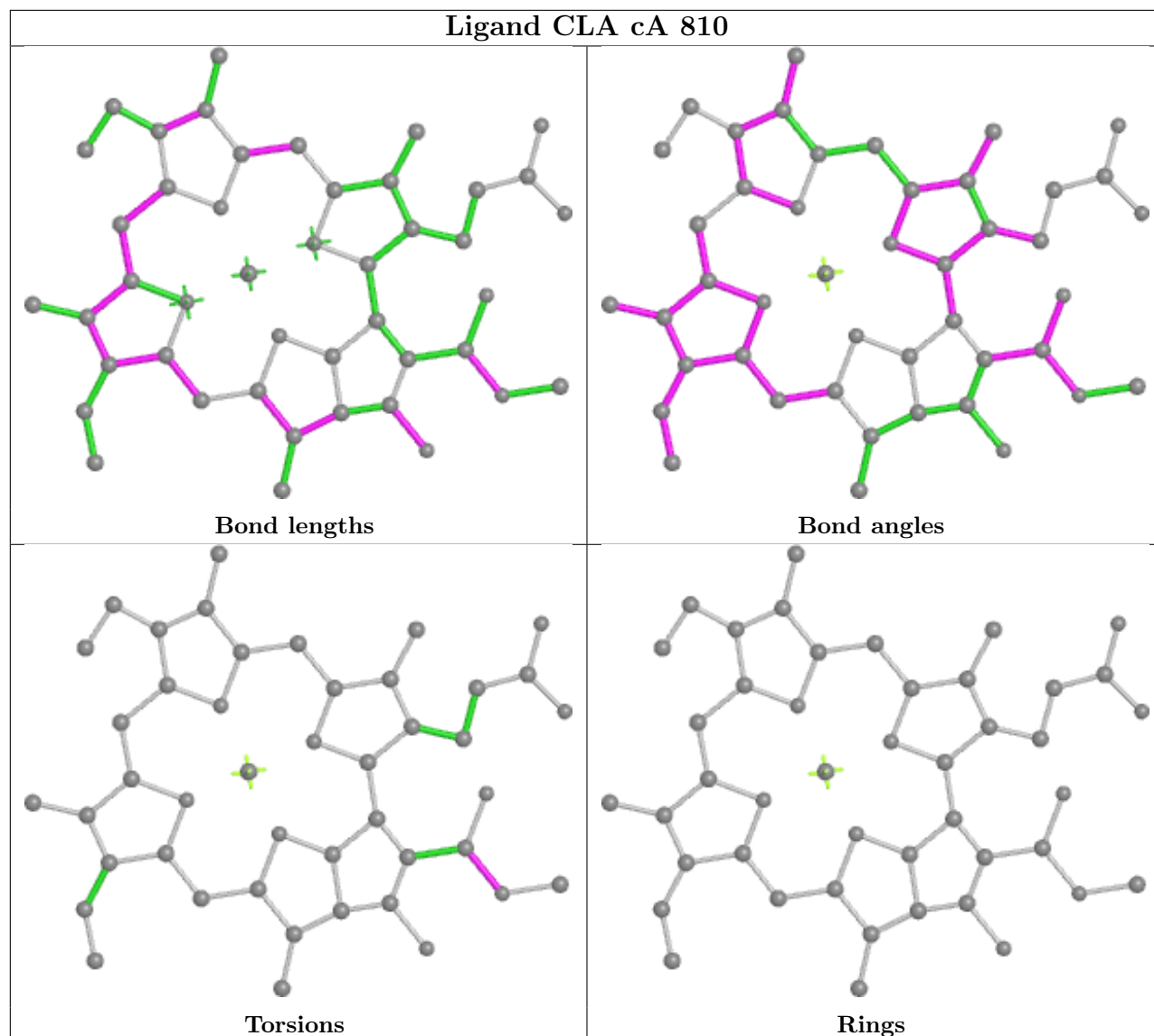
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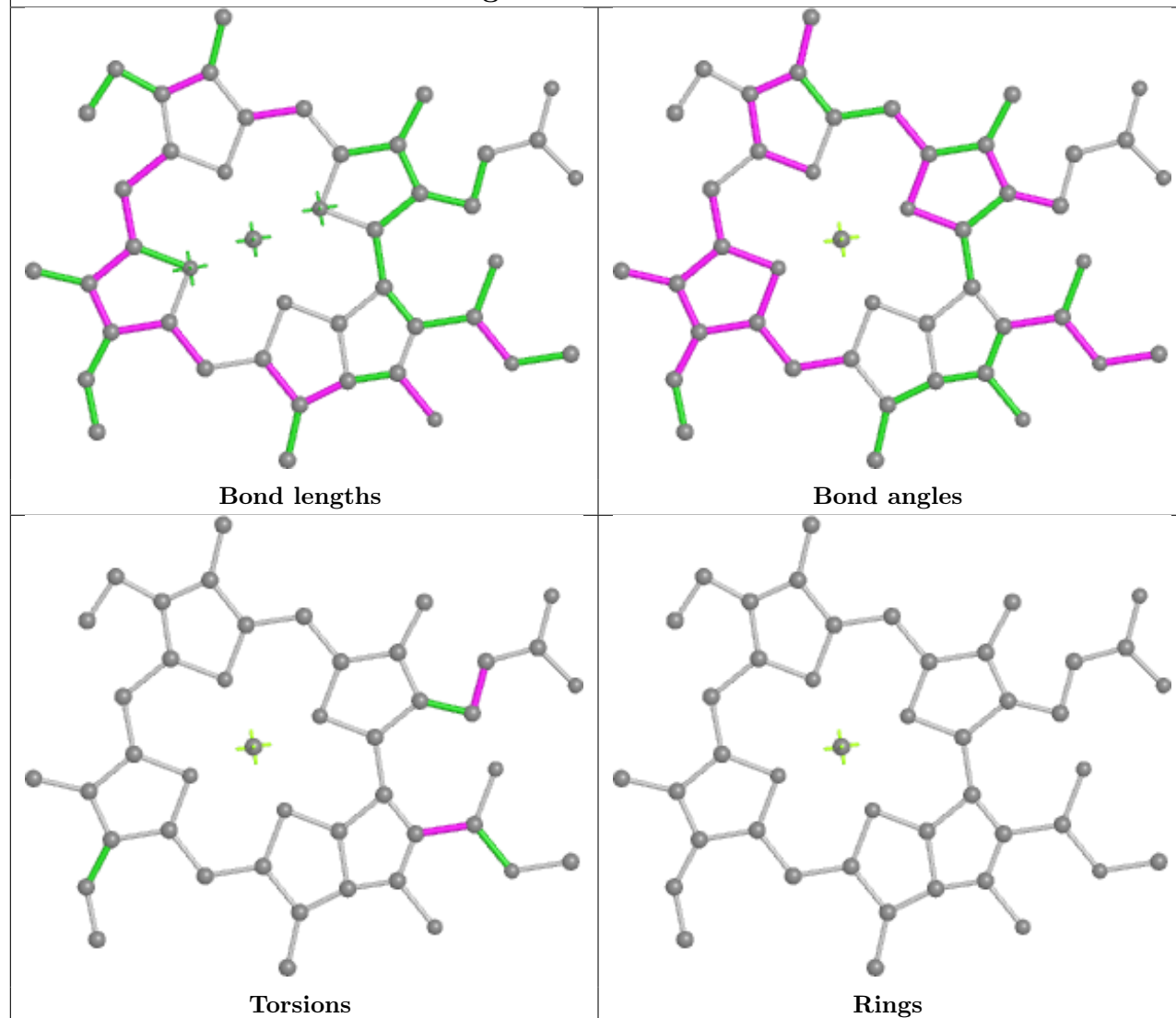
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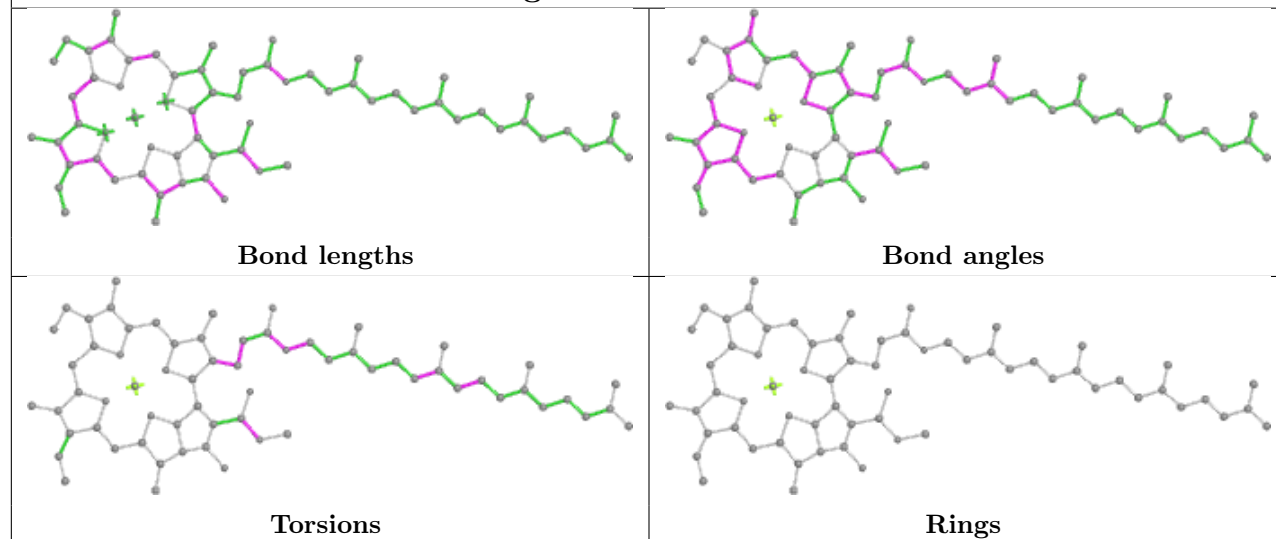
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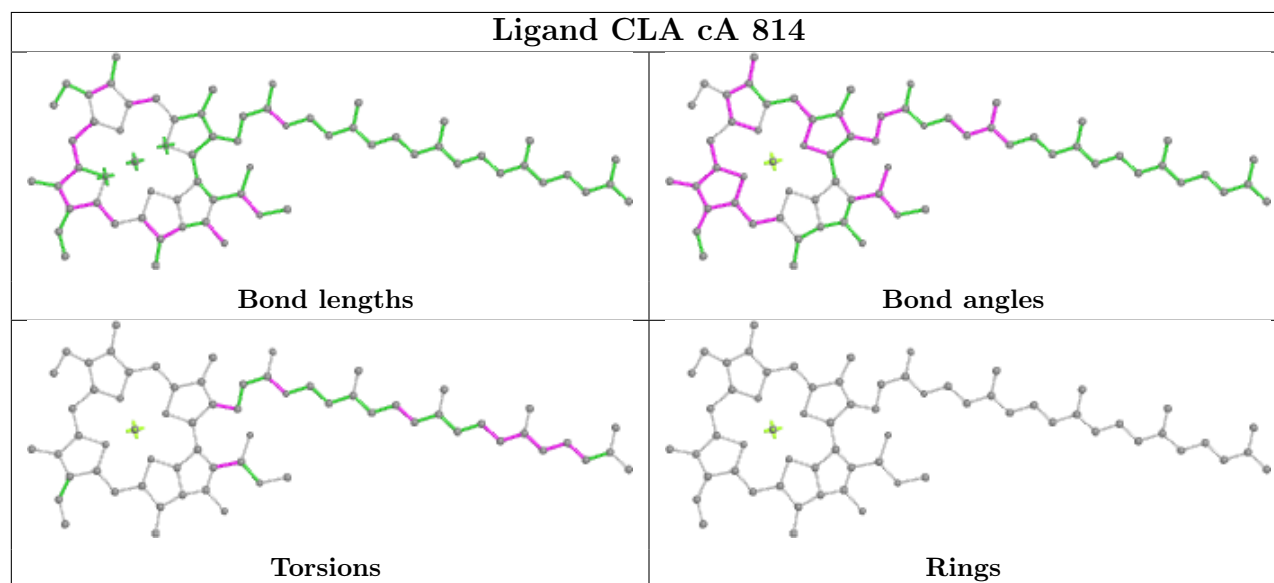
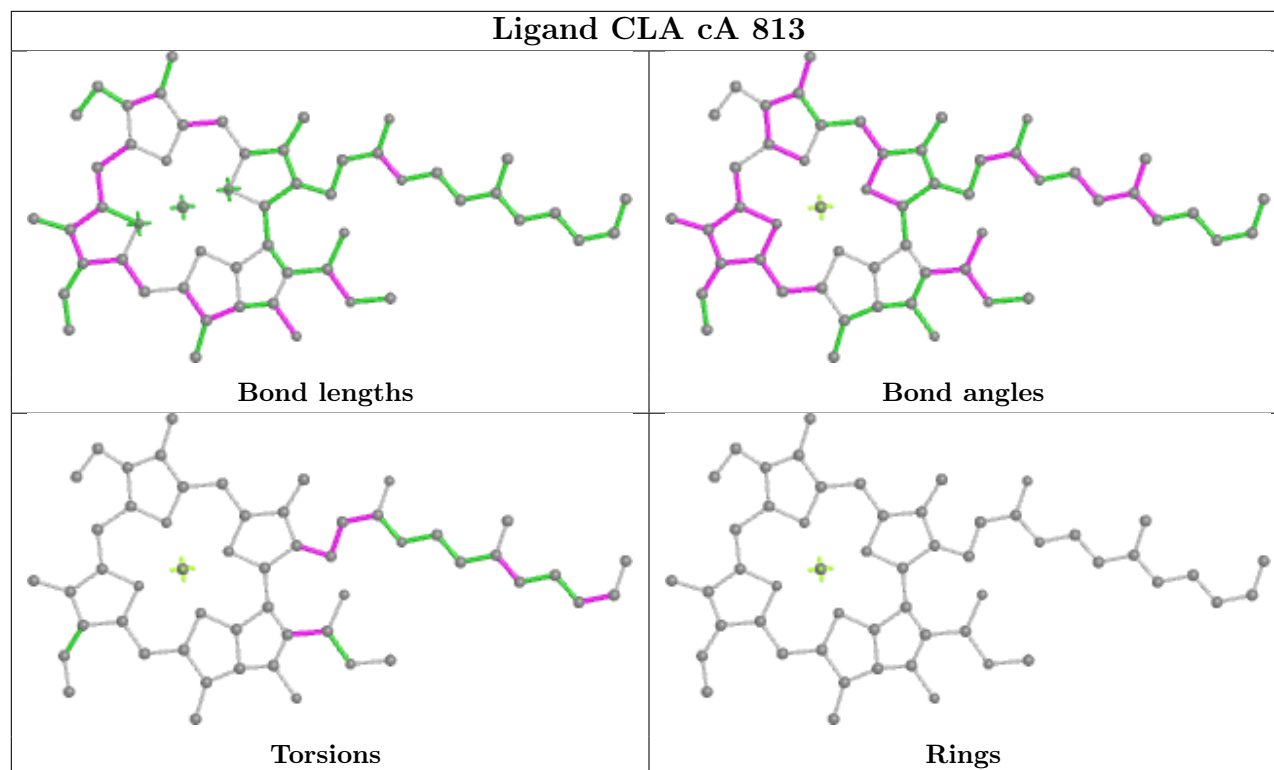


Ligand CLA cA 811

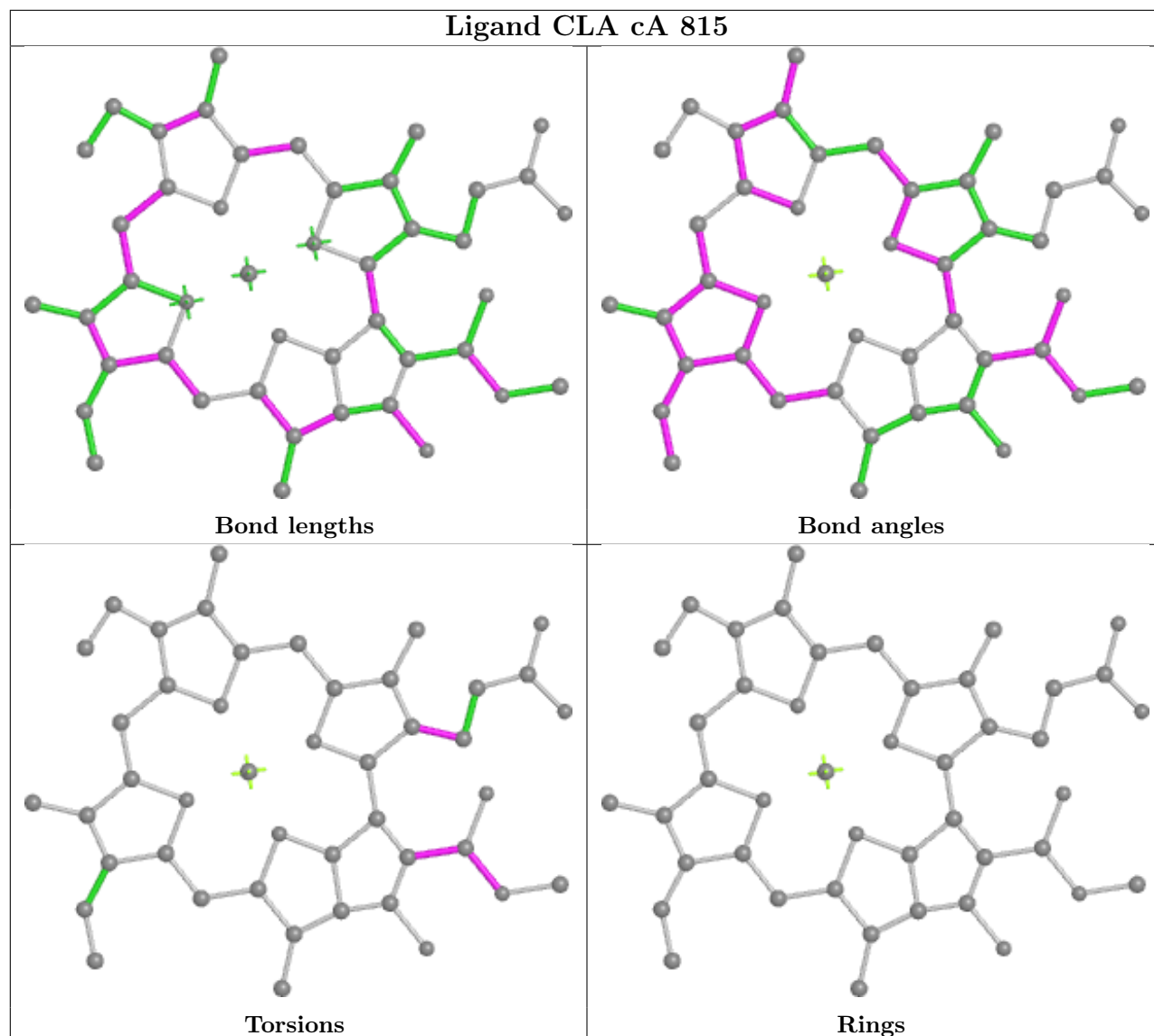


Ligand CLA cA 812

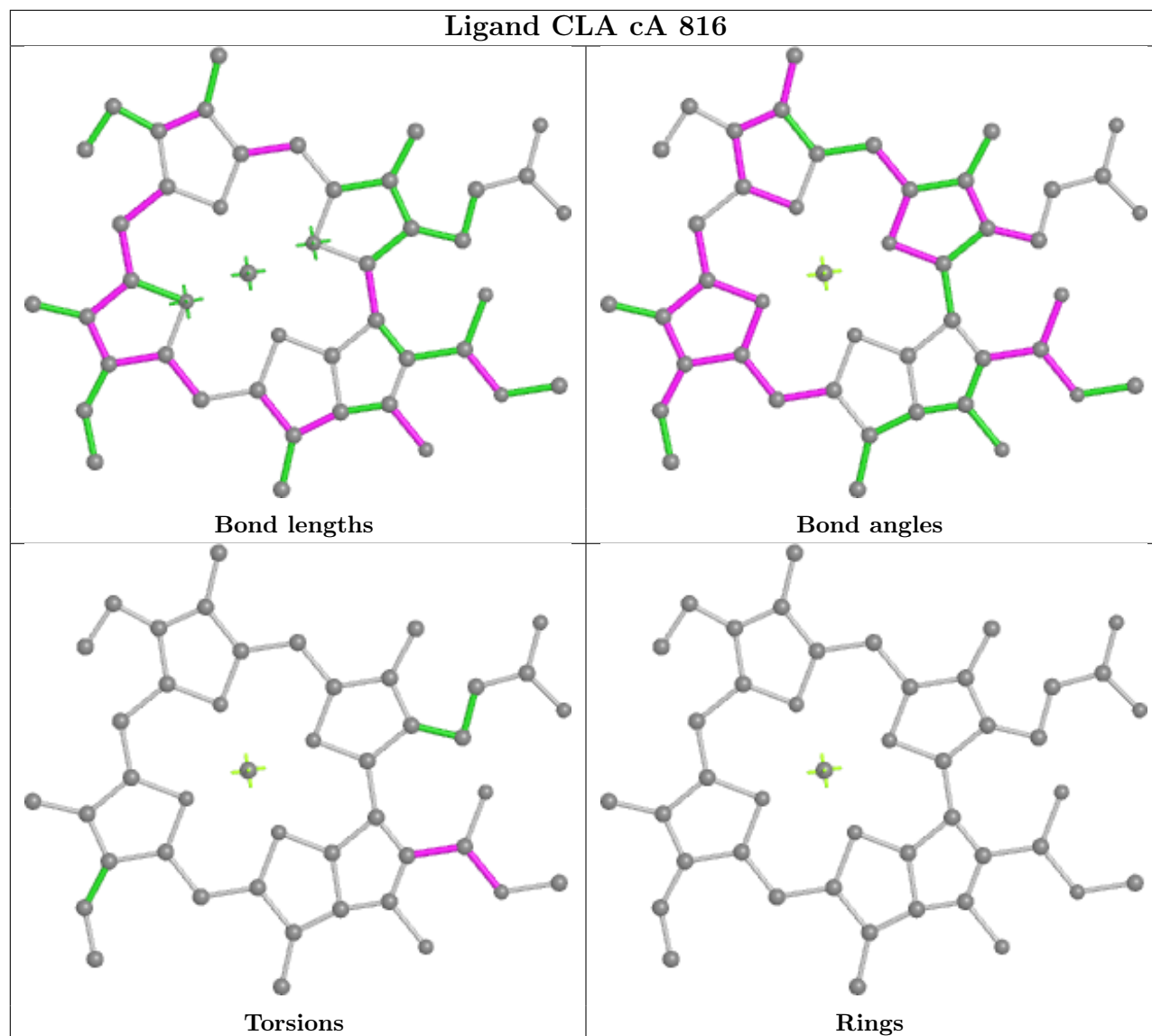




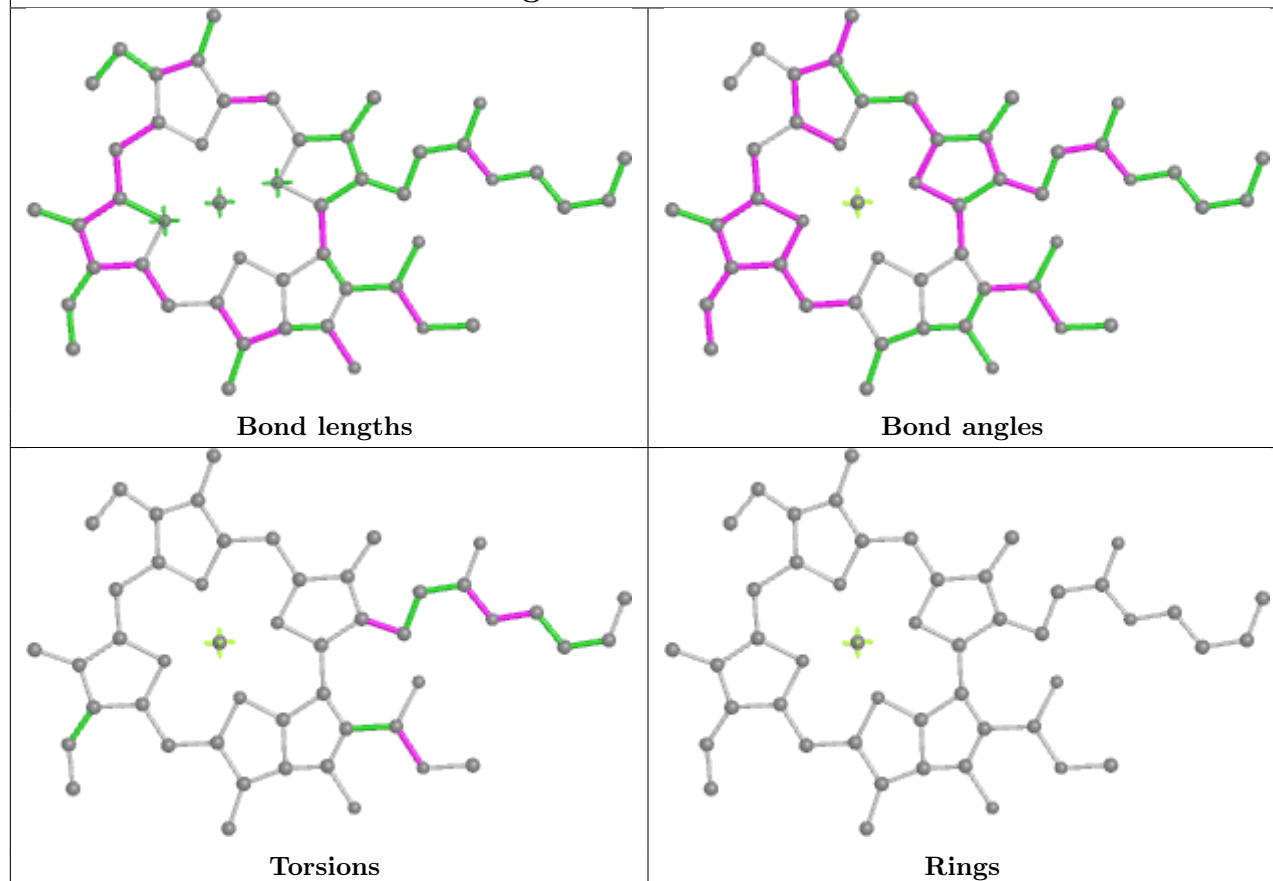
Ligand CLA cA 815



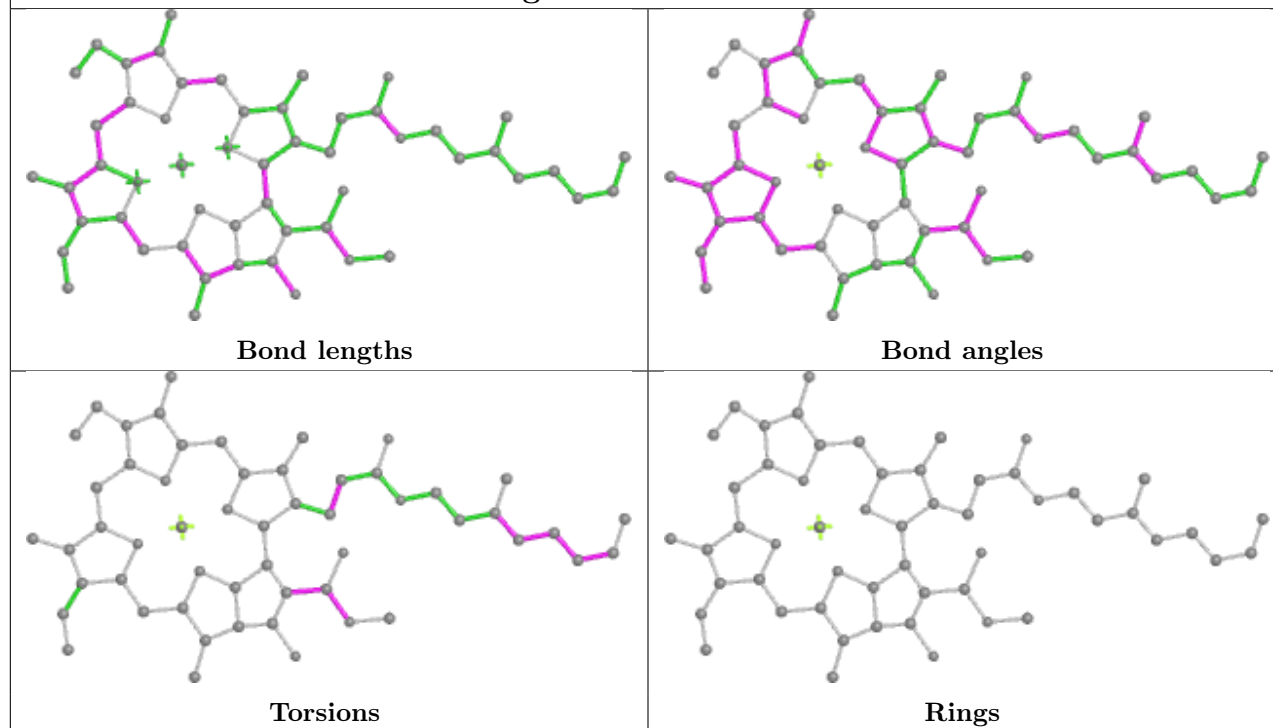
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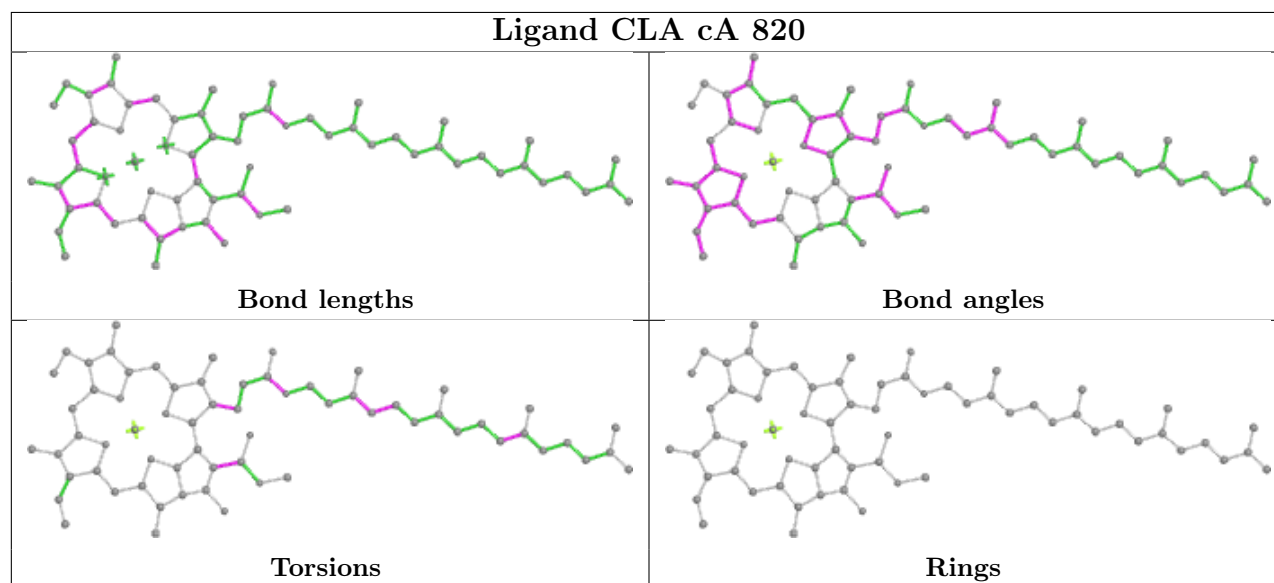
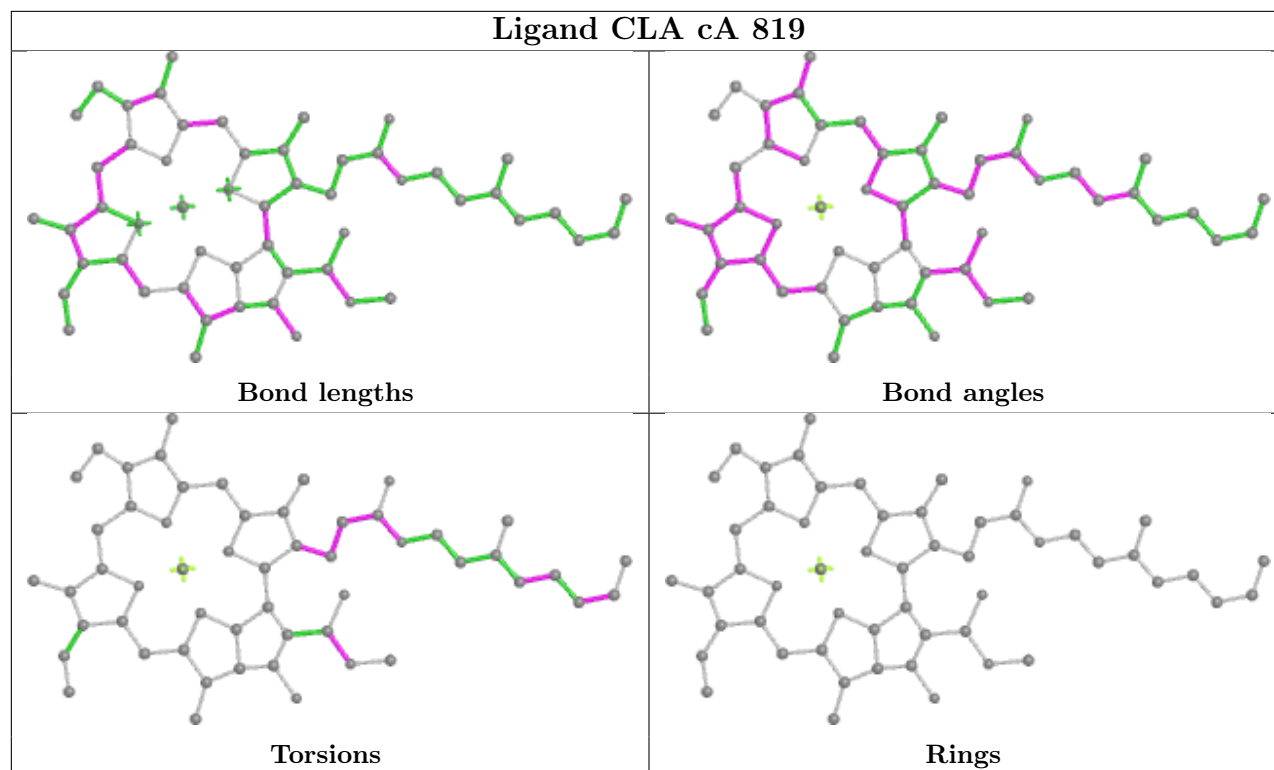


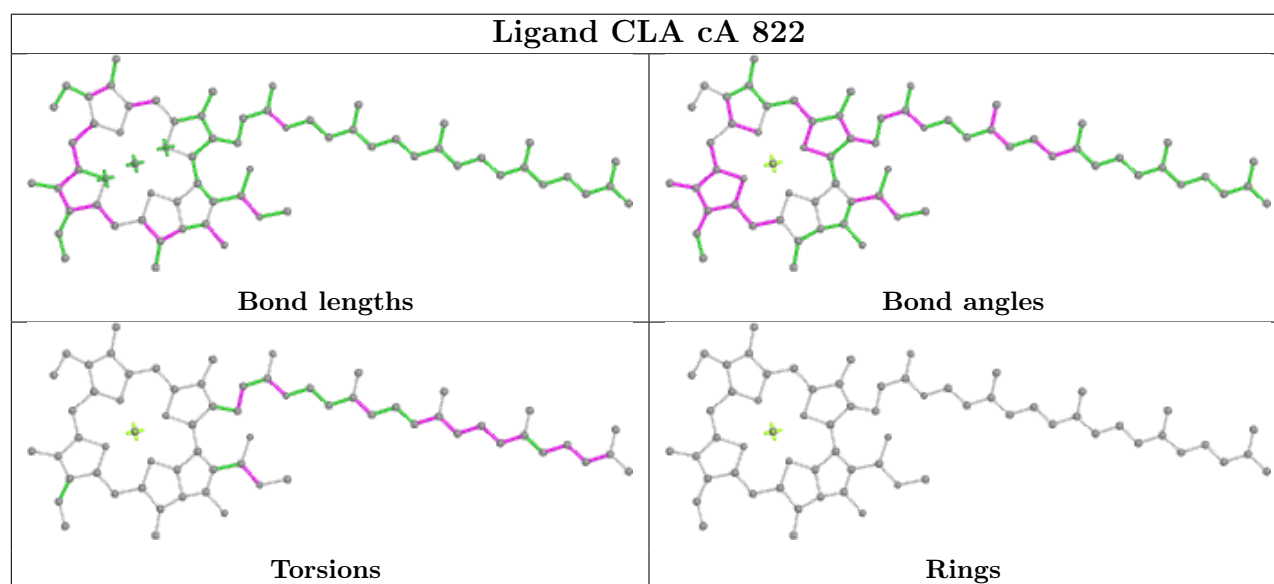
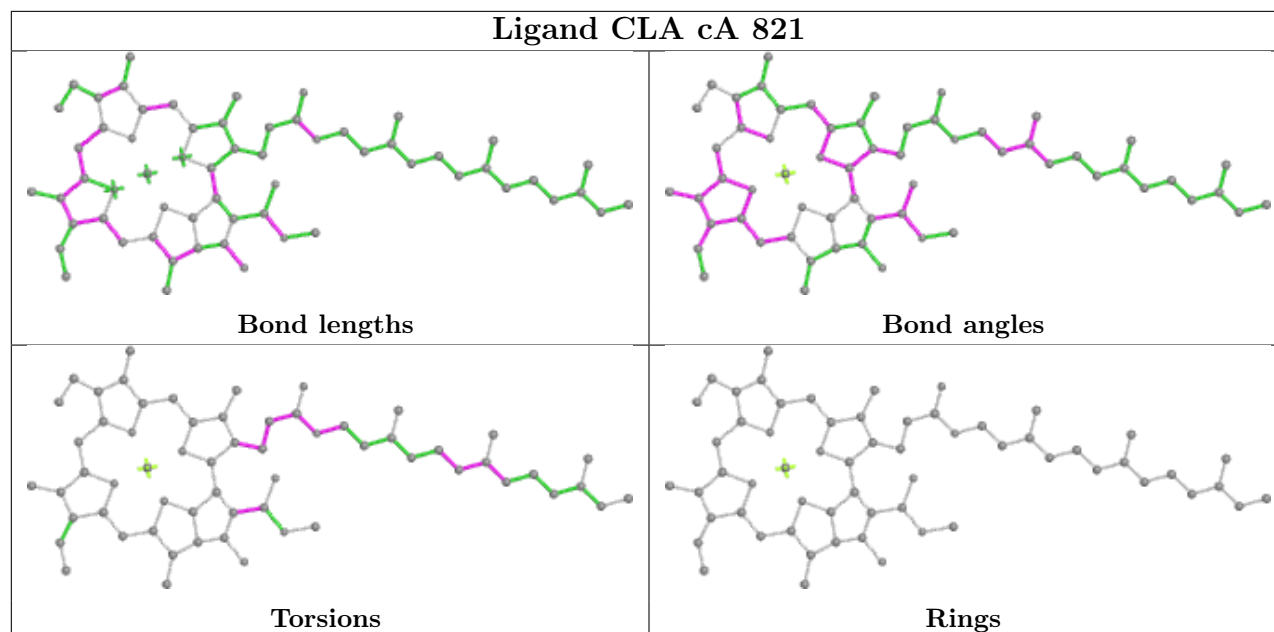
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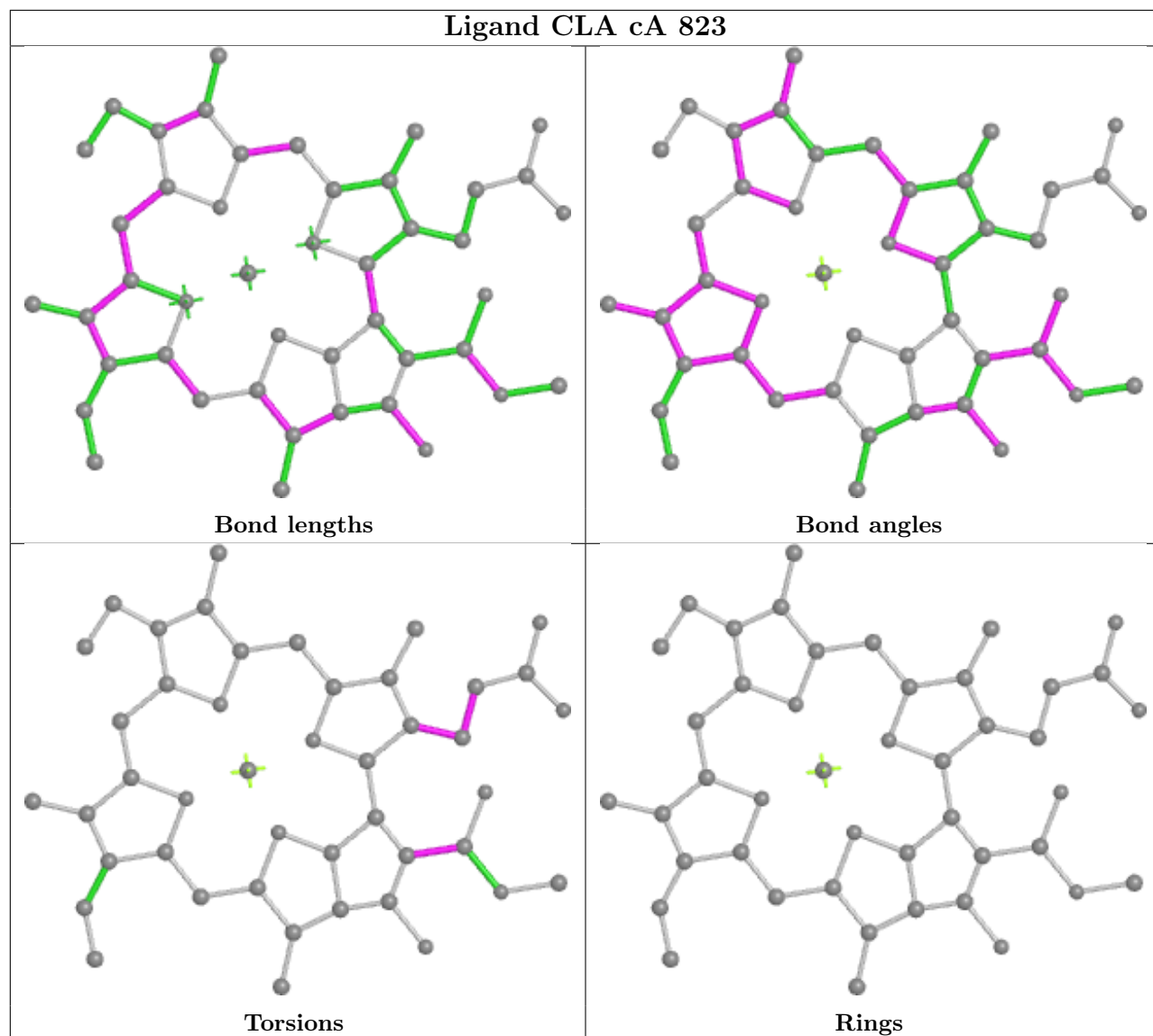
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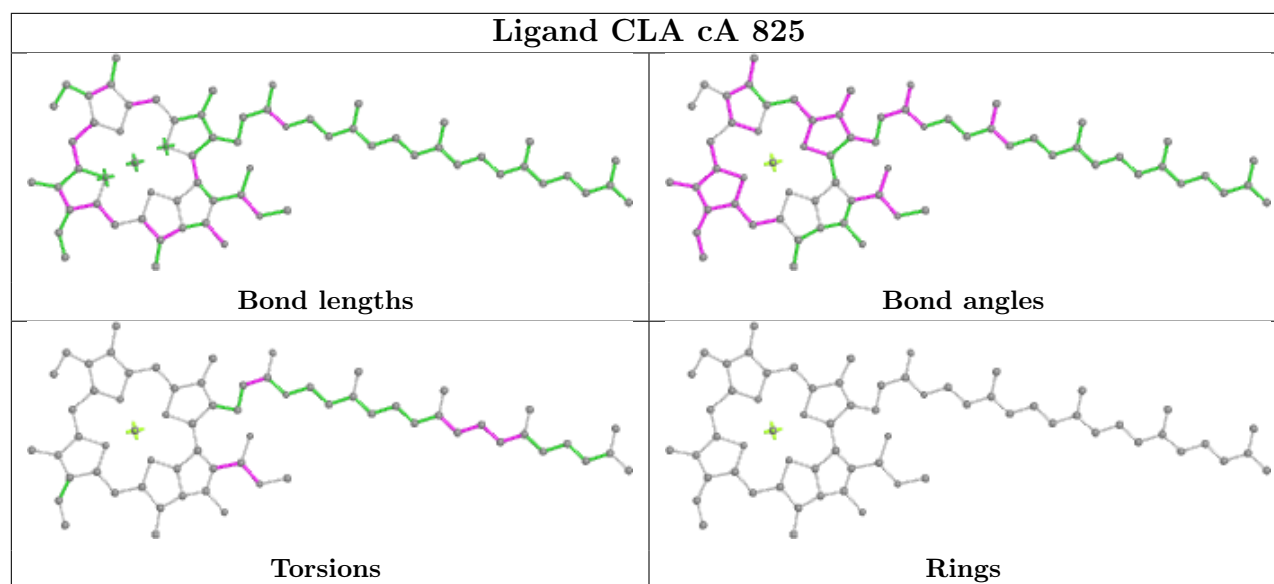
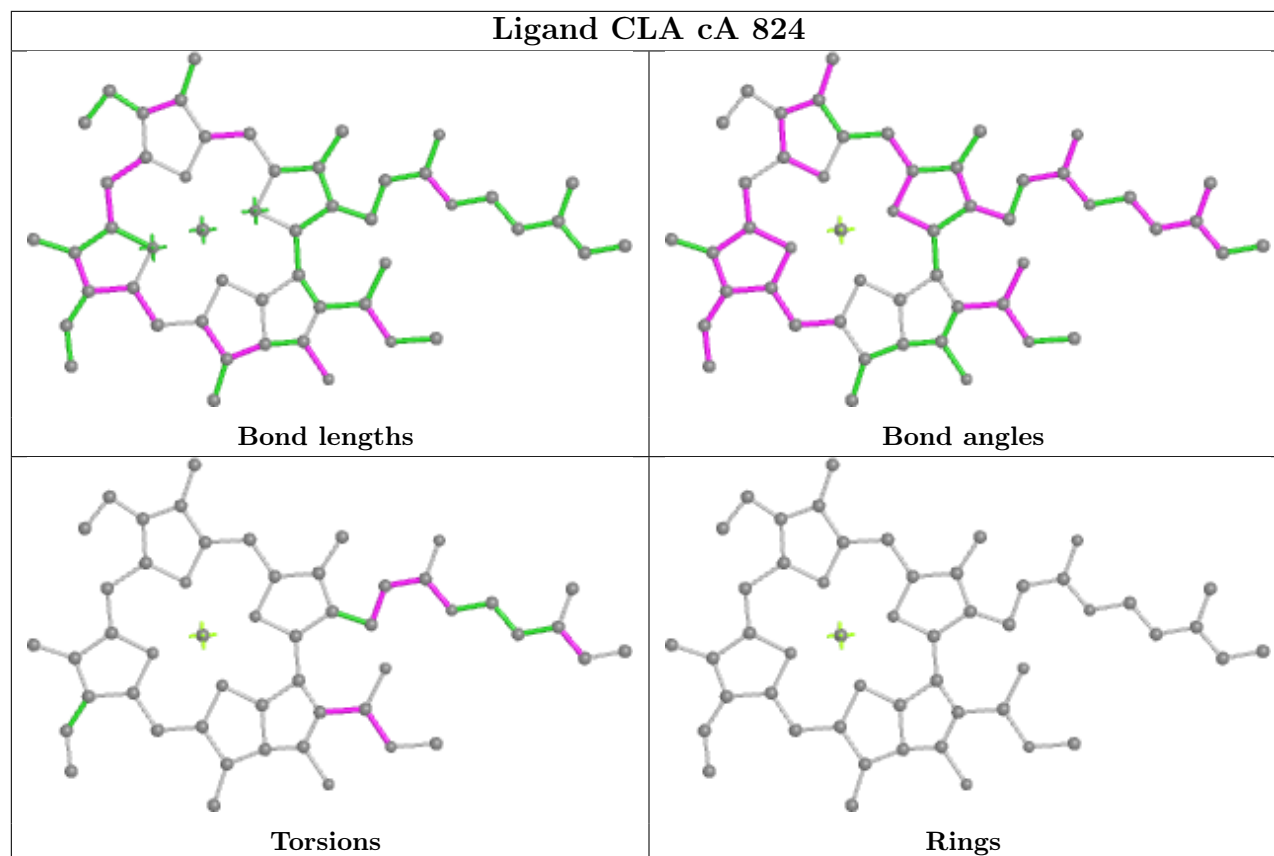


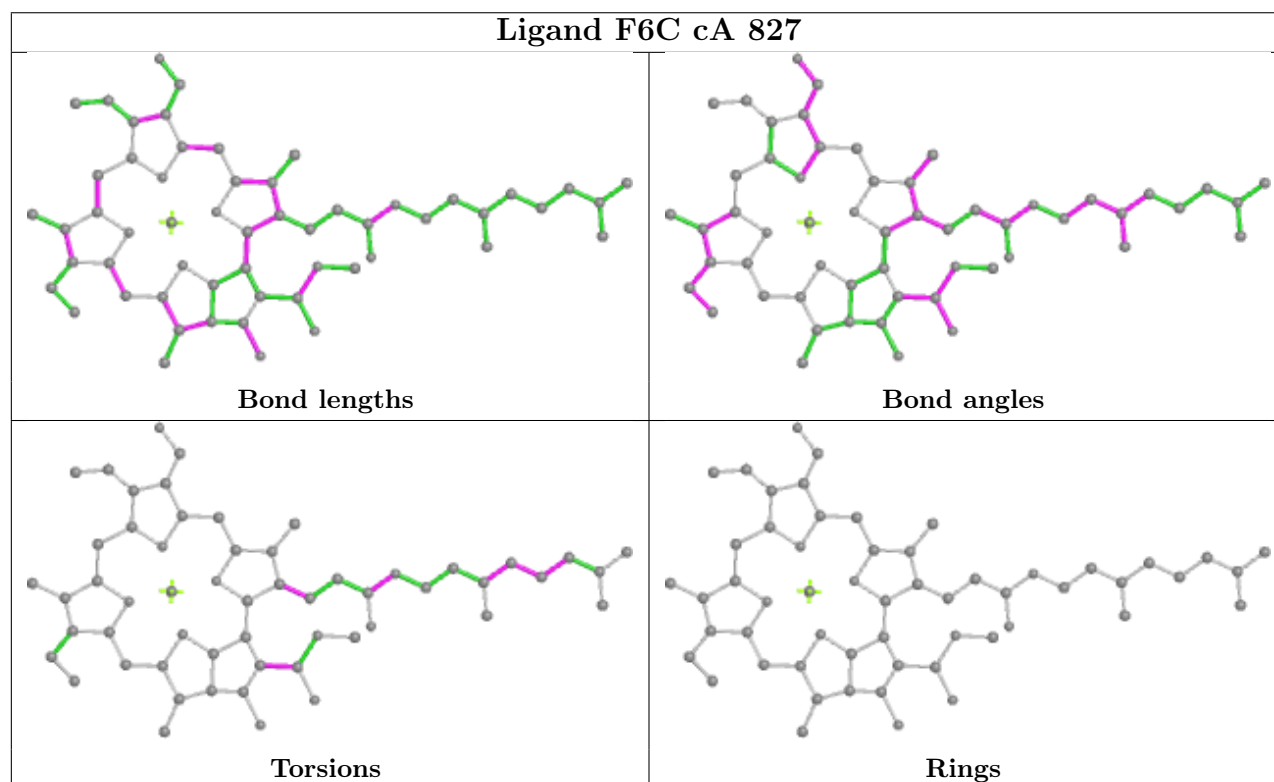
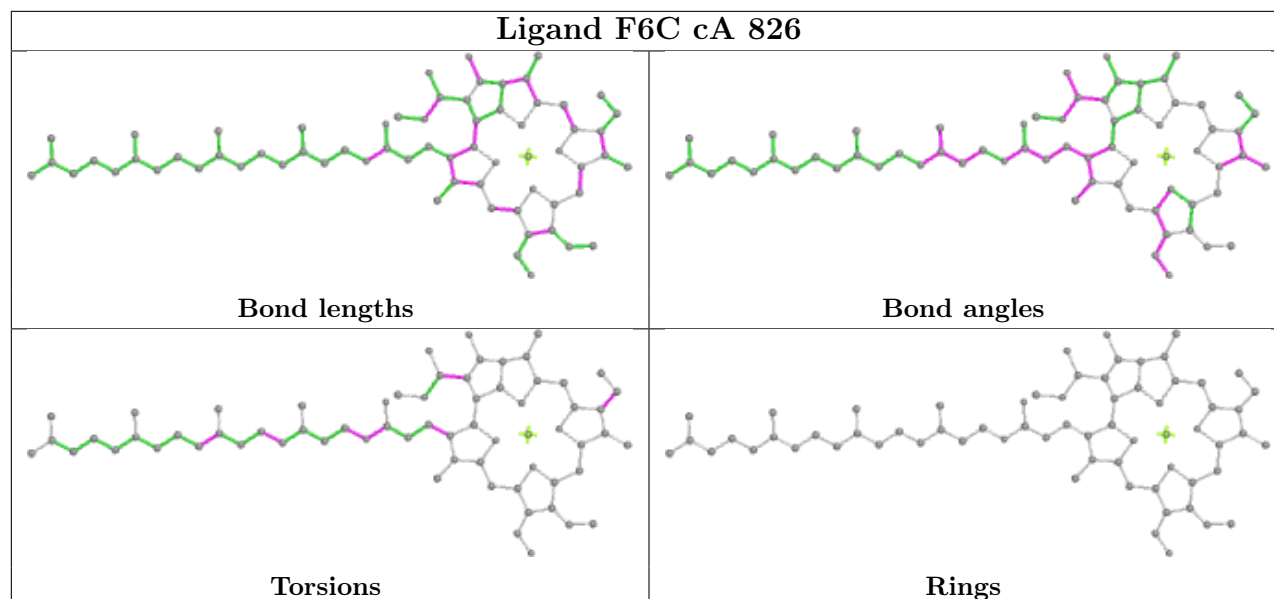


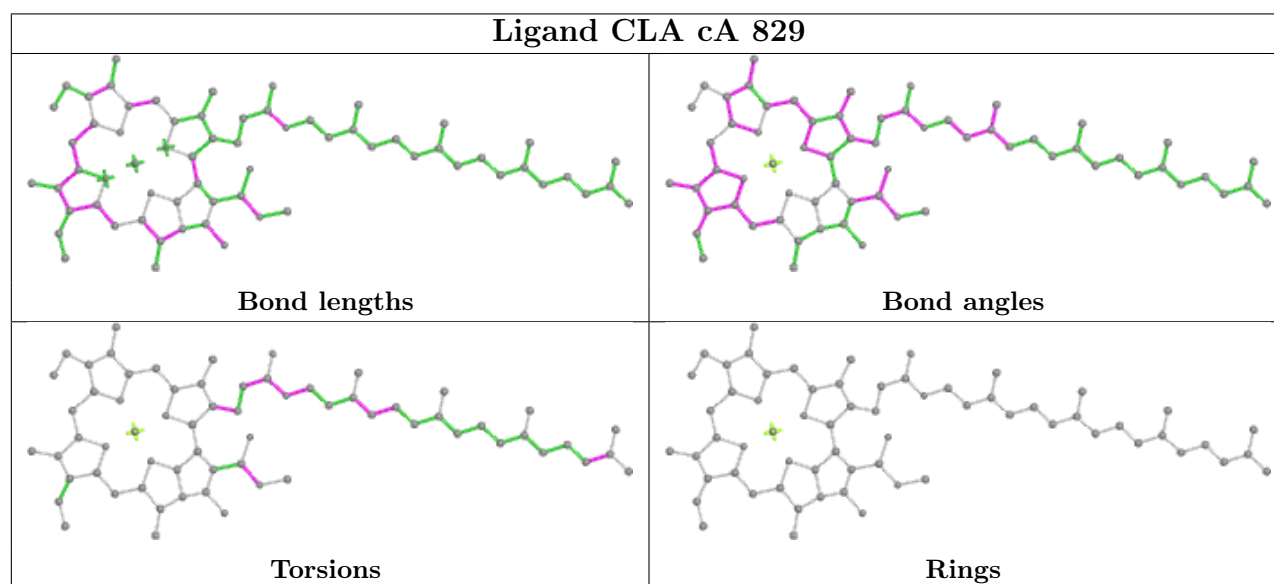
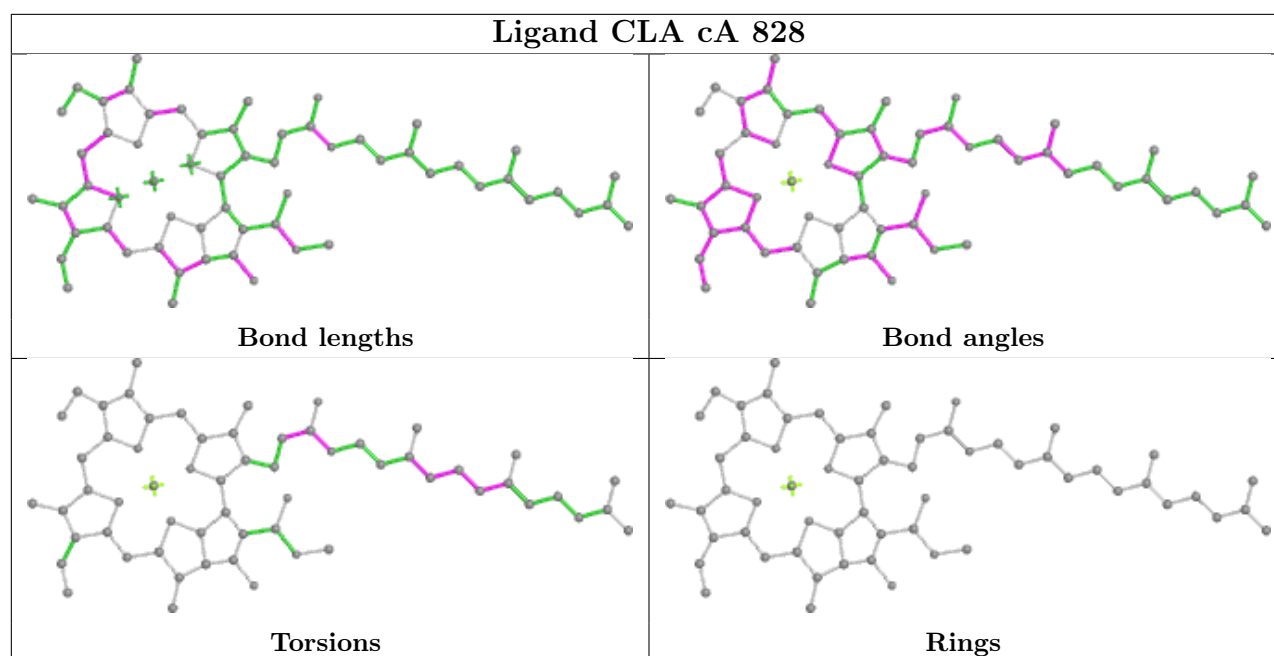


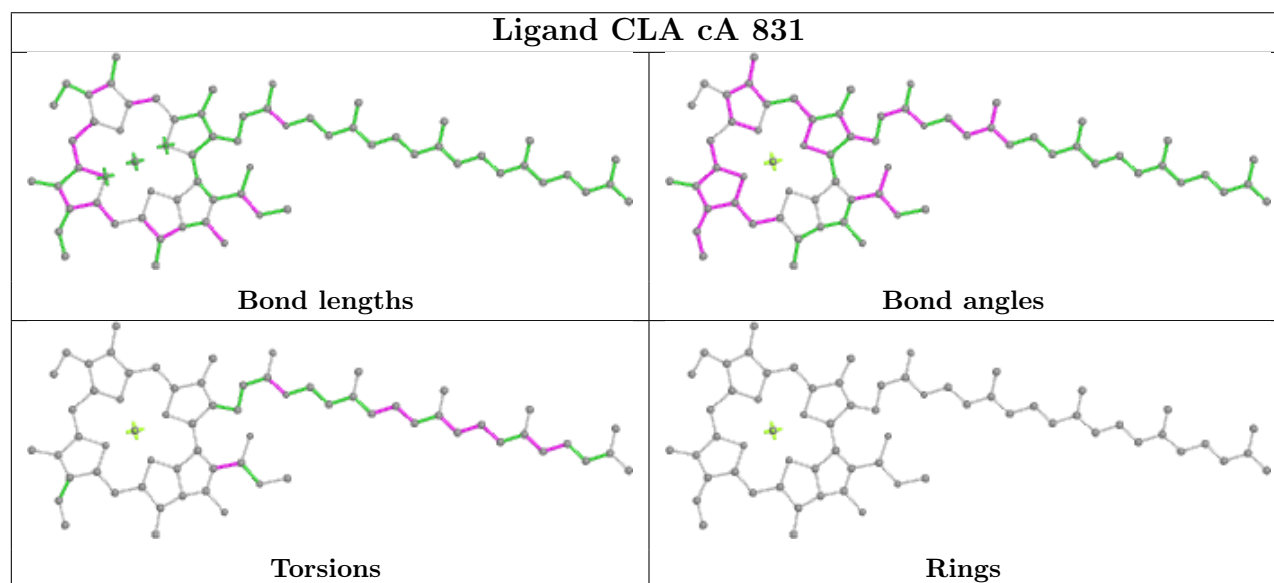
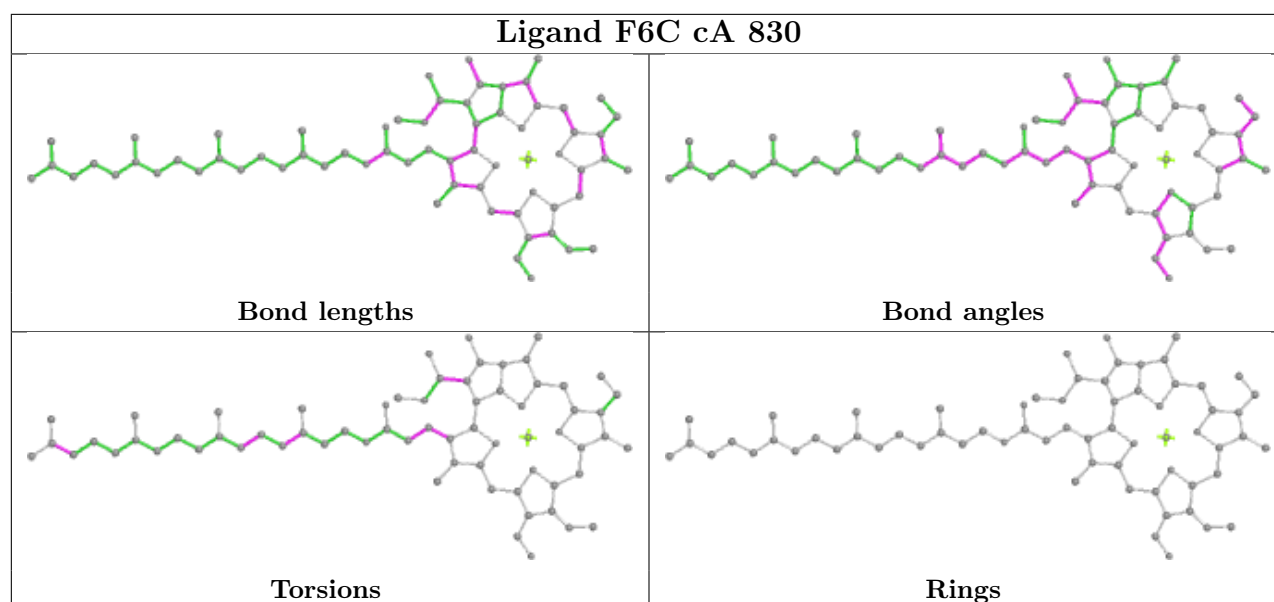
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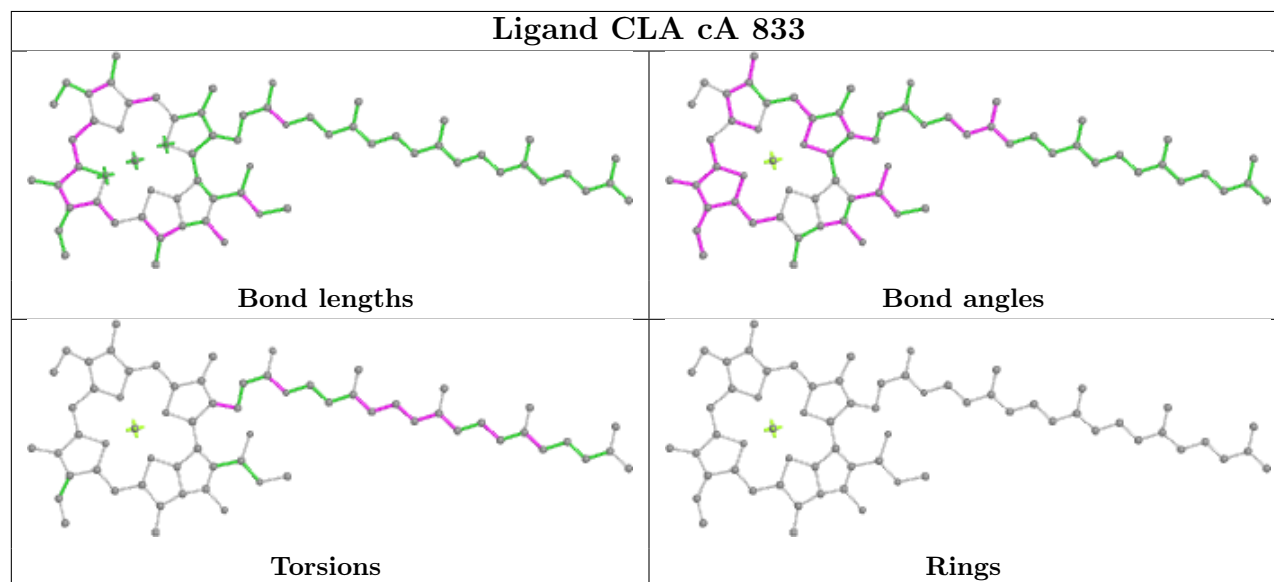
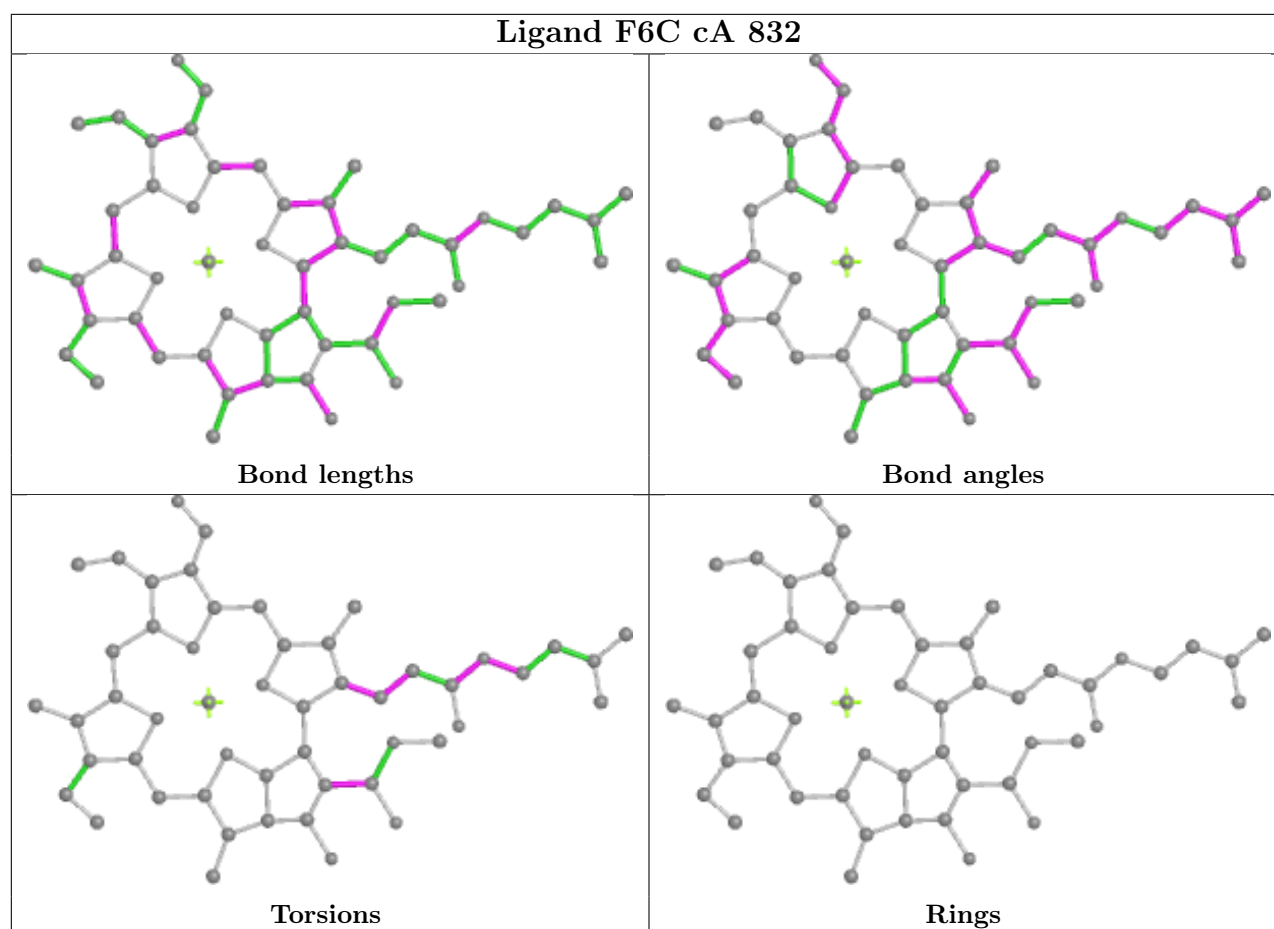


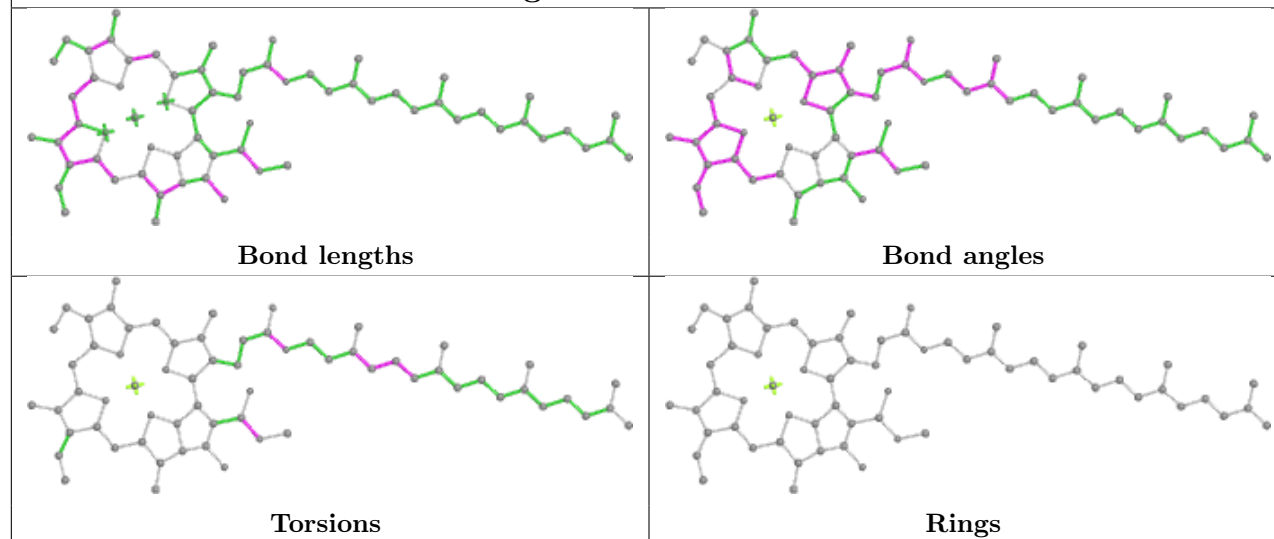
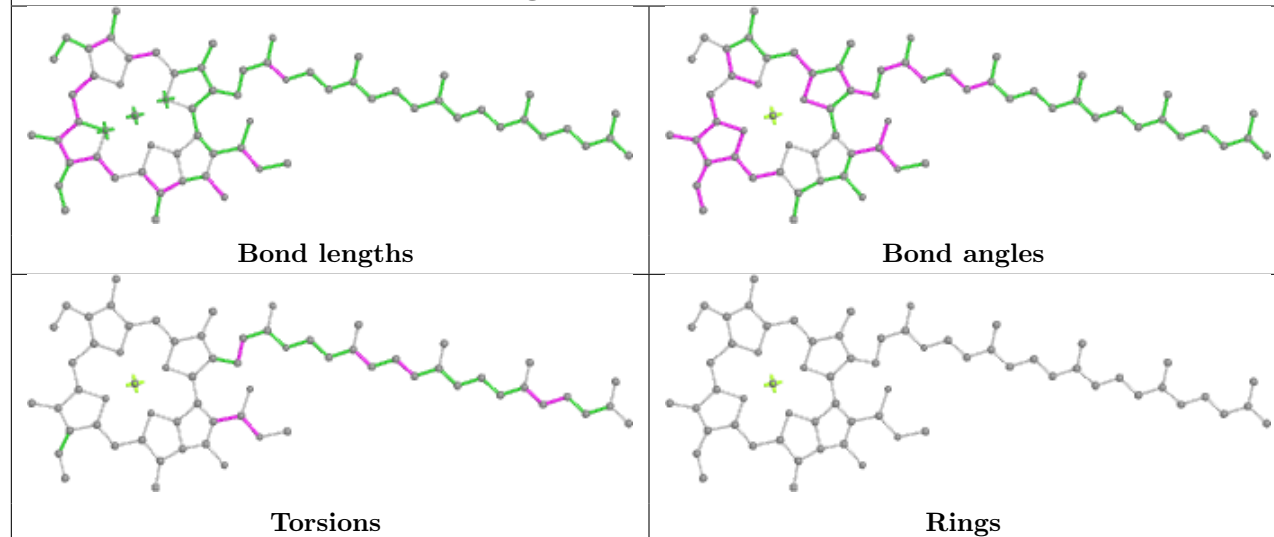




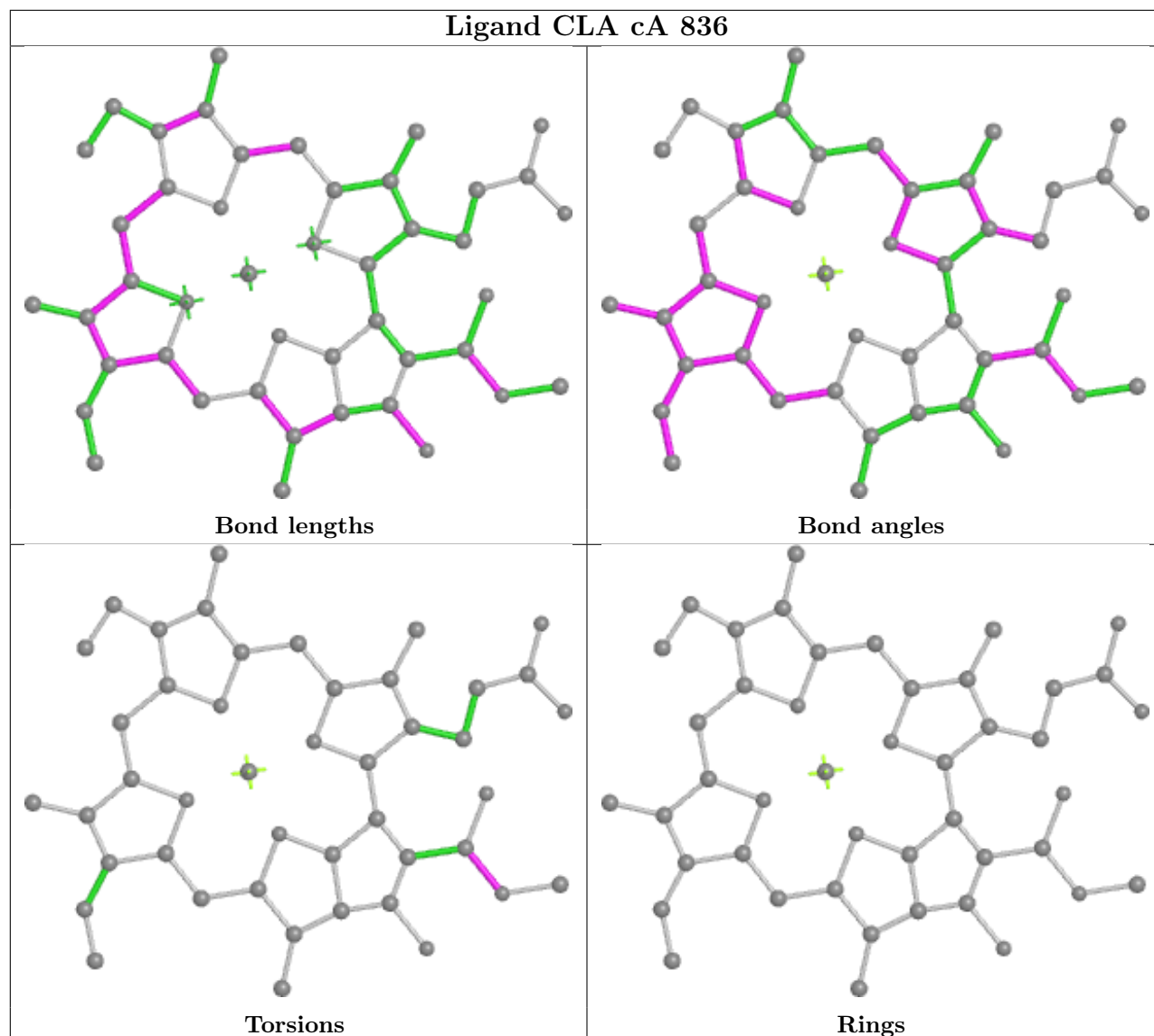




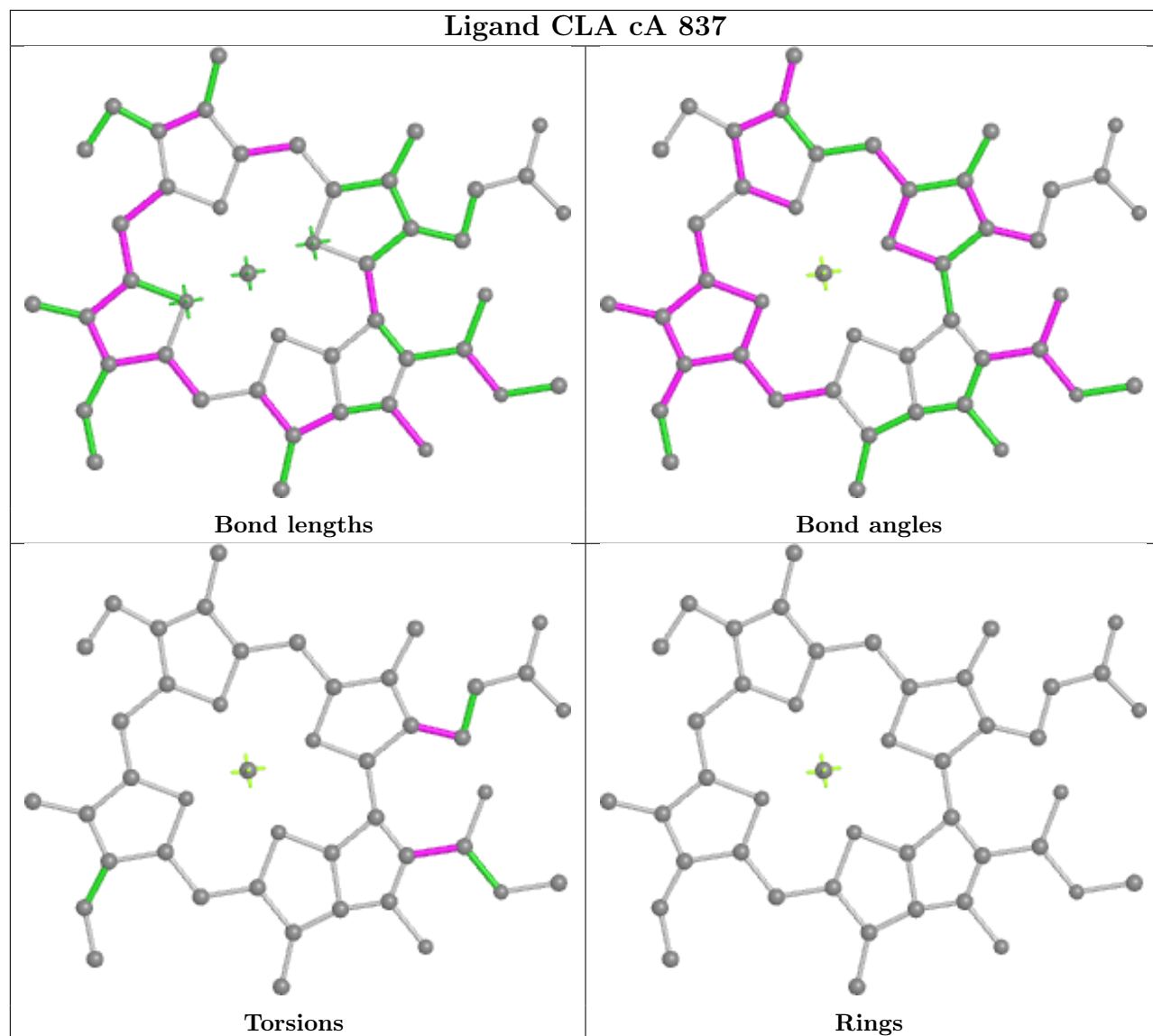


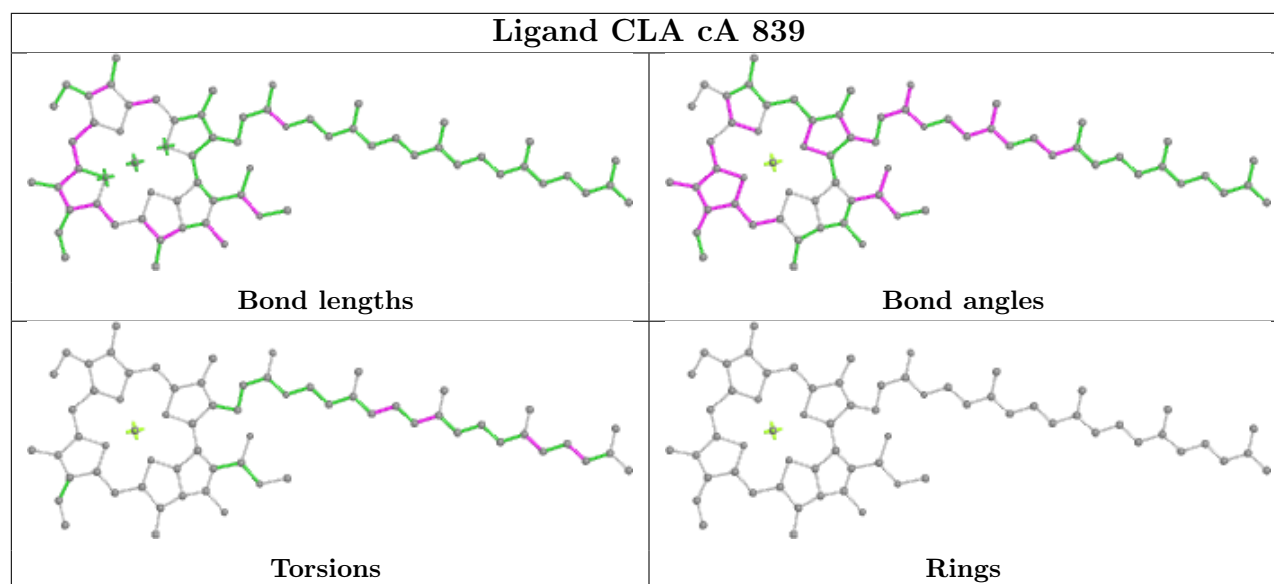
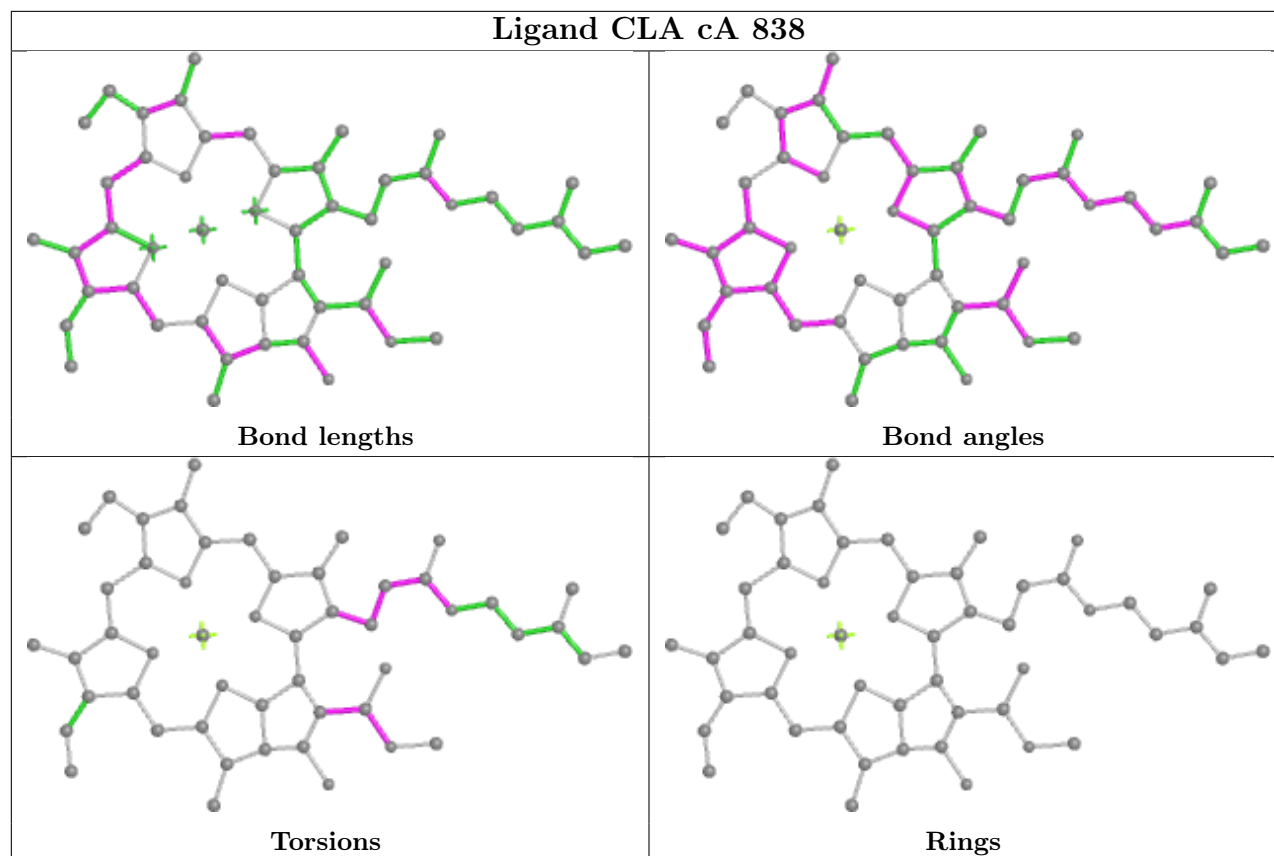
Ligand CLA cA 834**Ligand CLA cA 835**

Ligand CLA cA 836

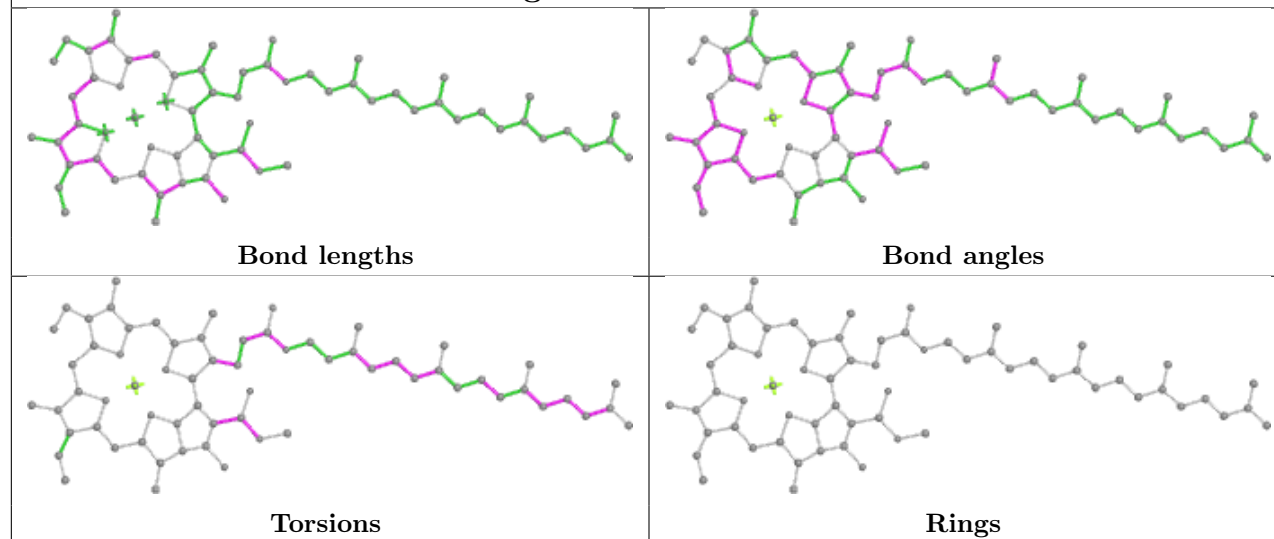


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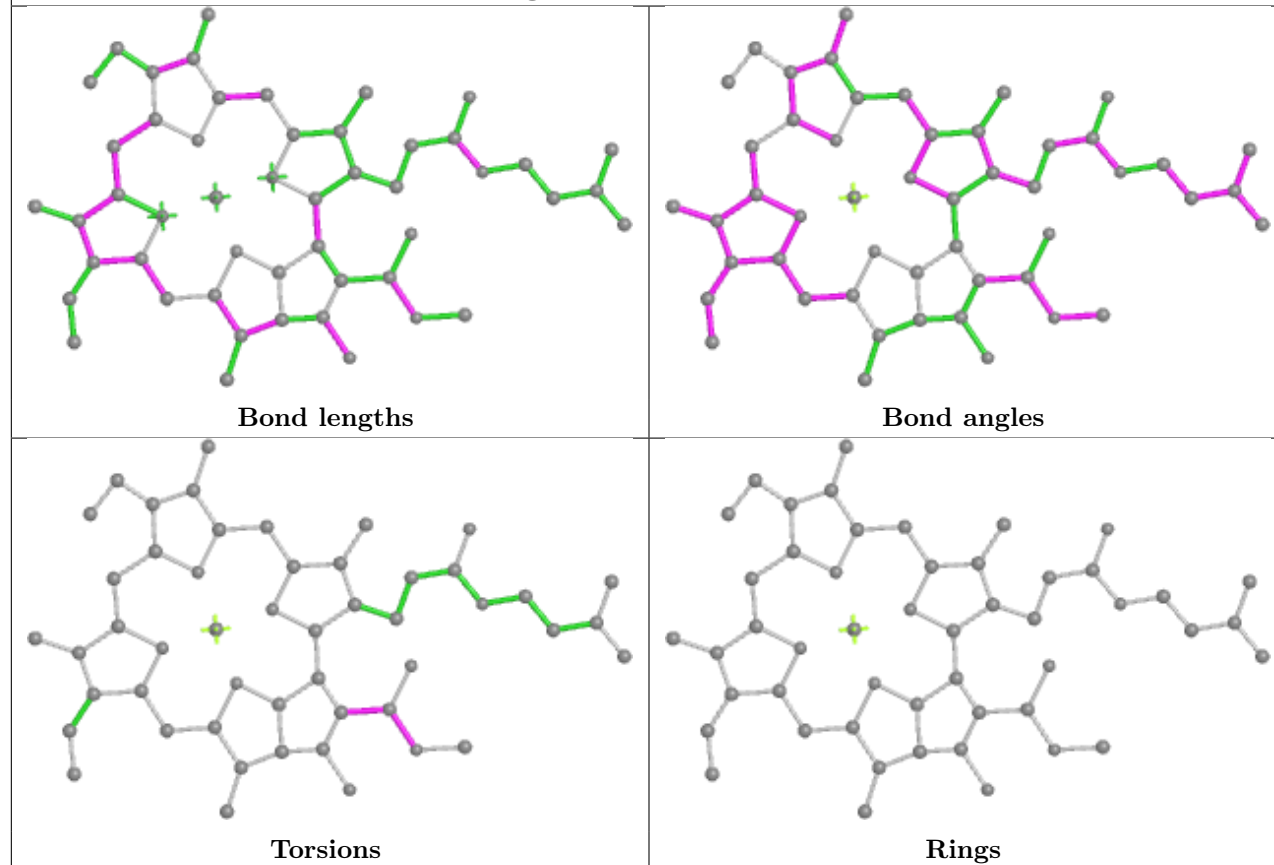




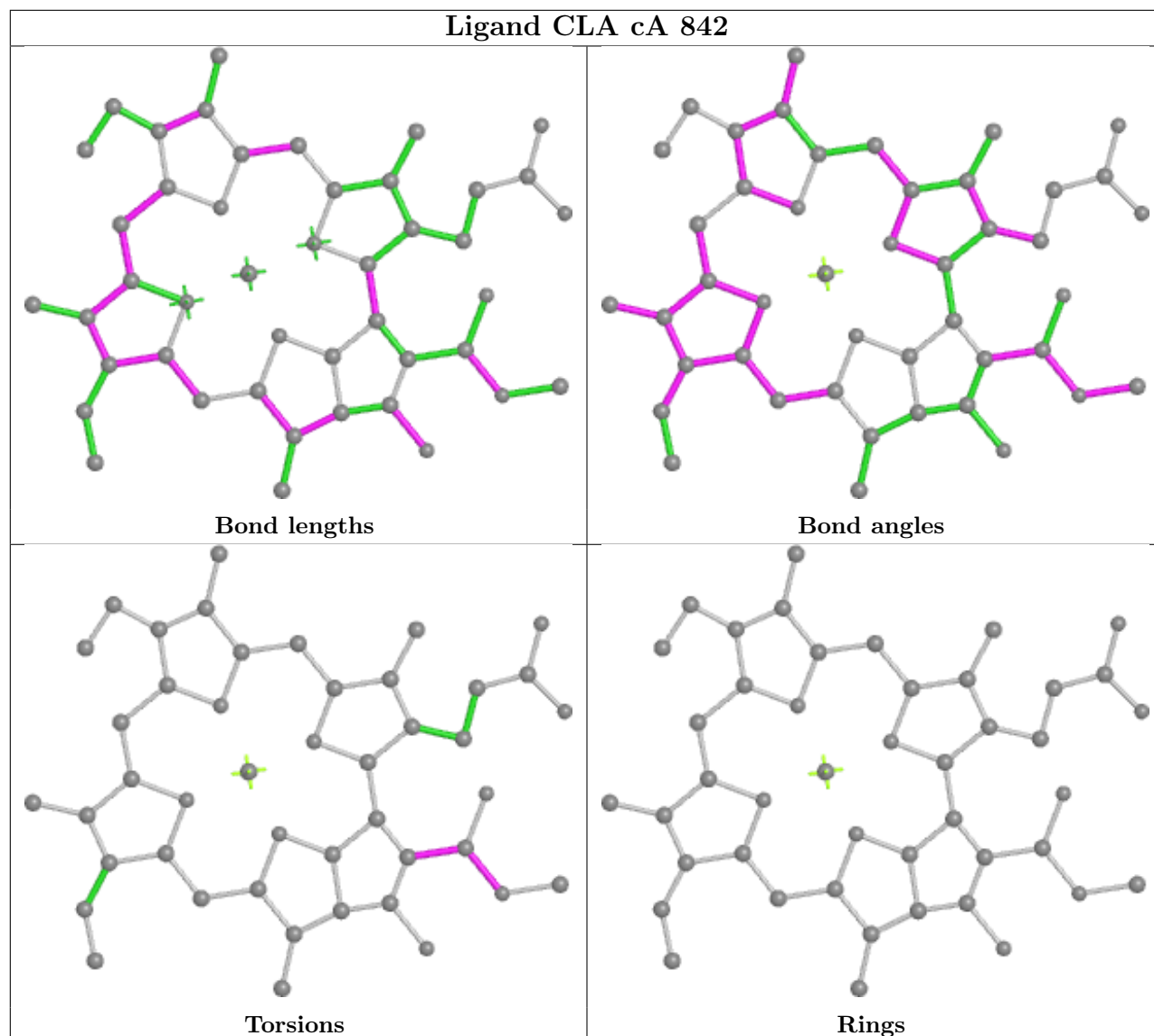
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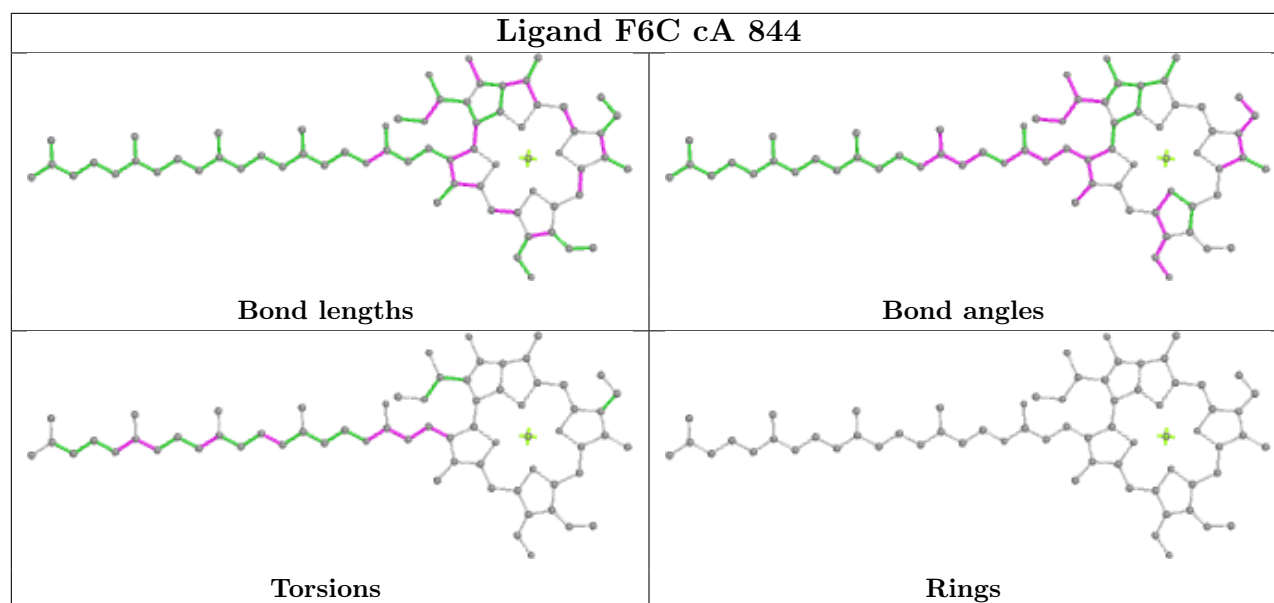
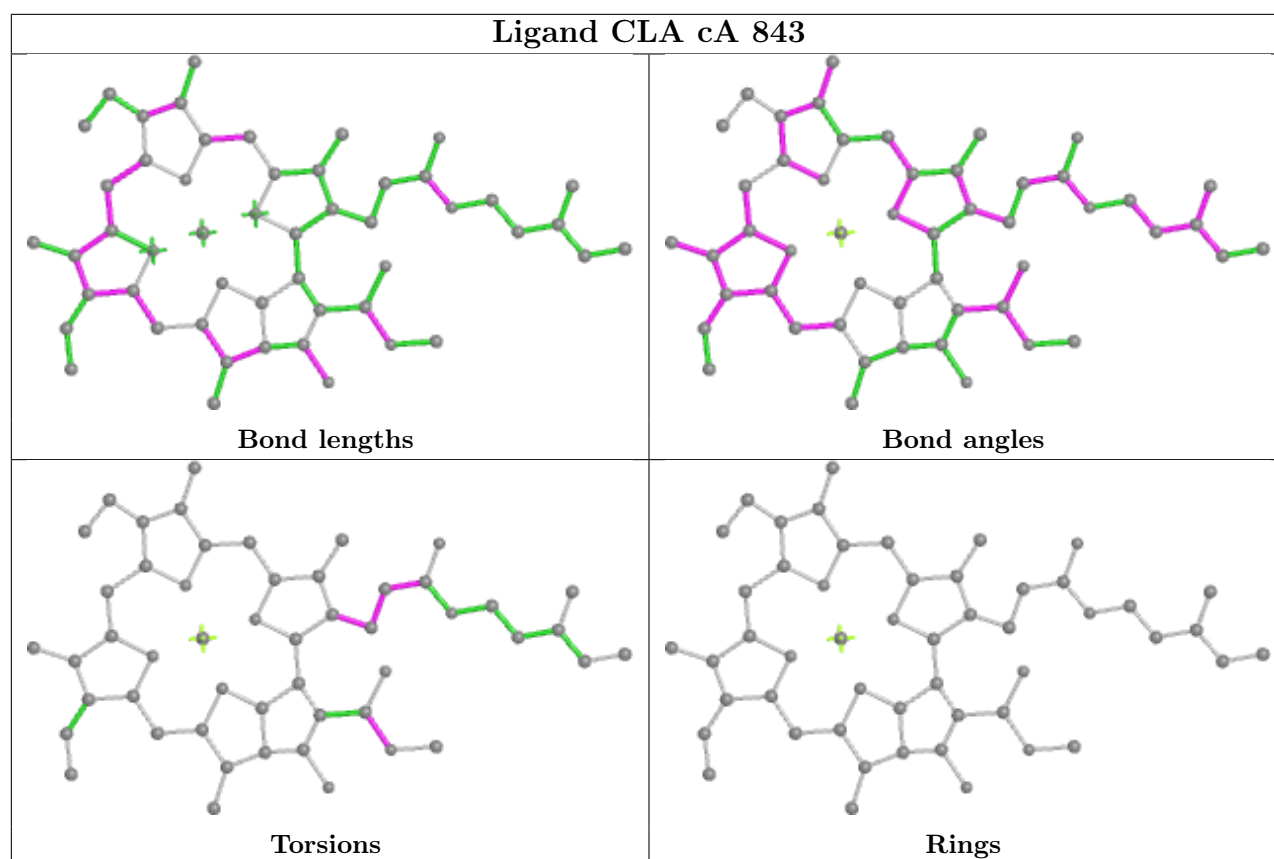


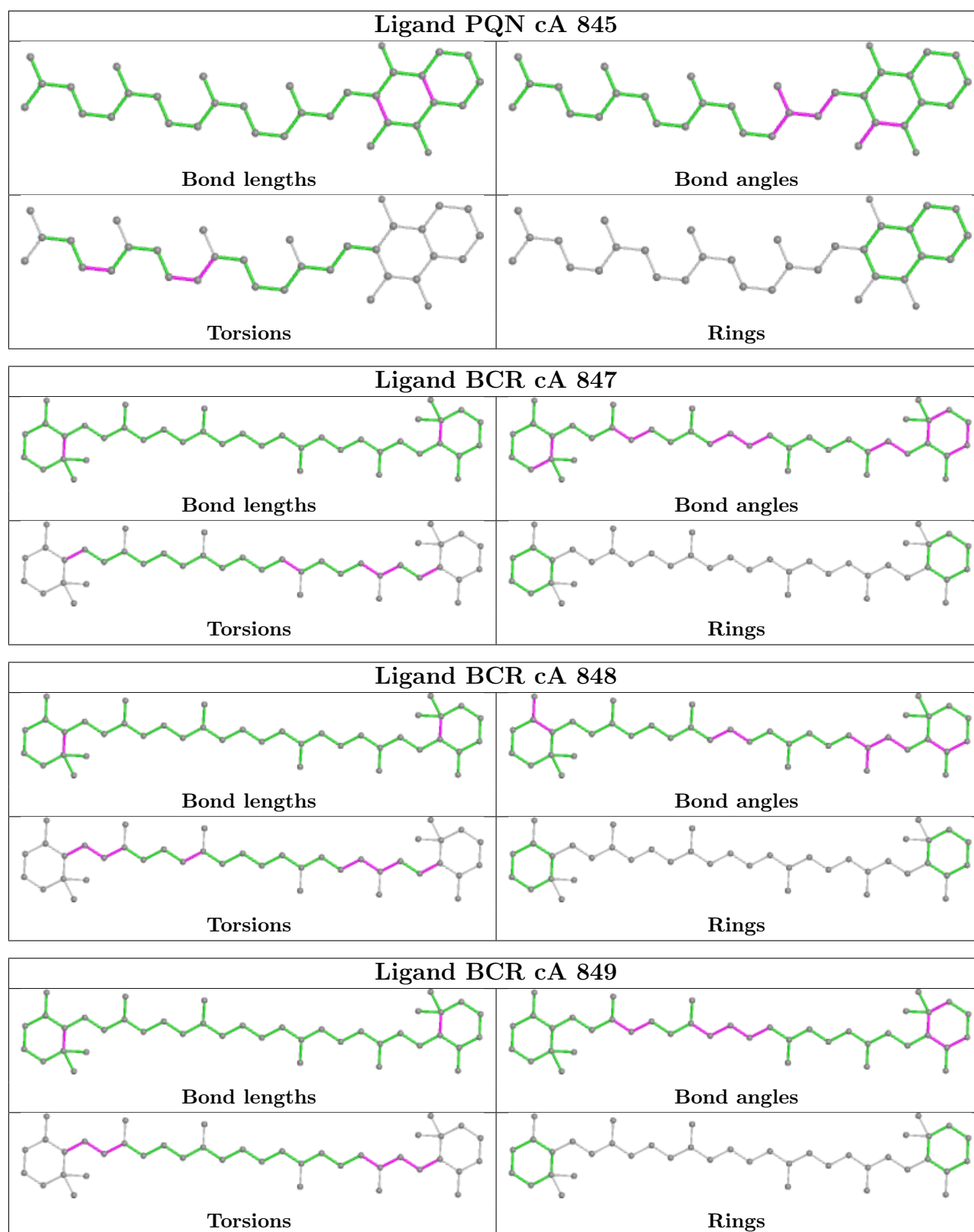
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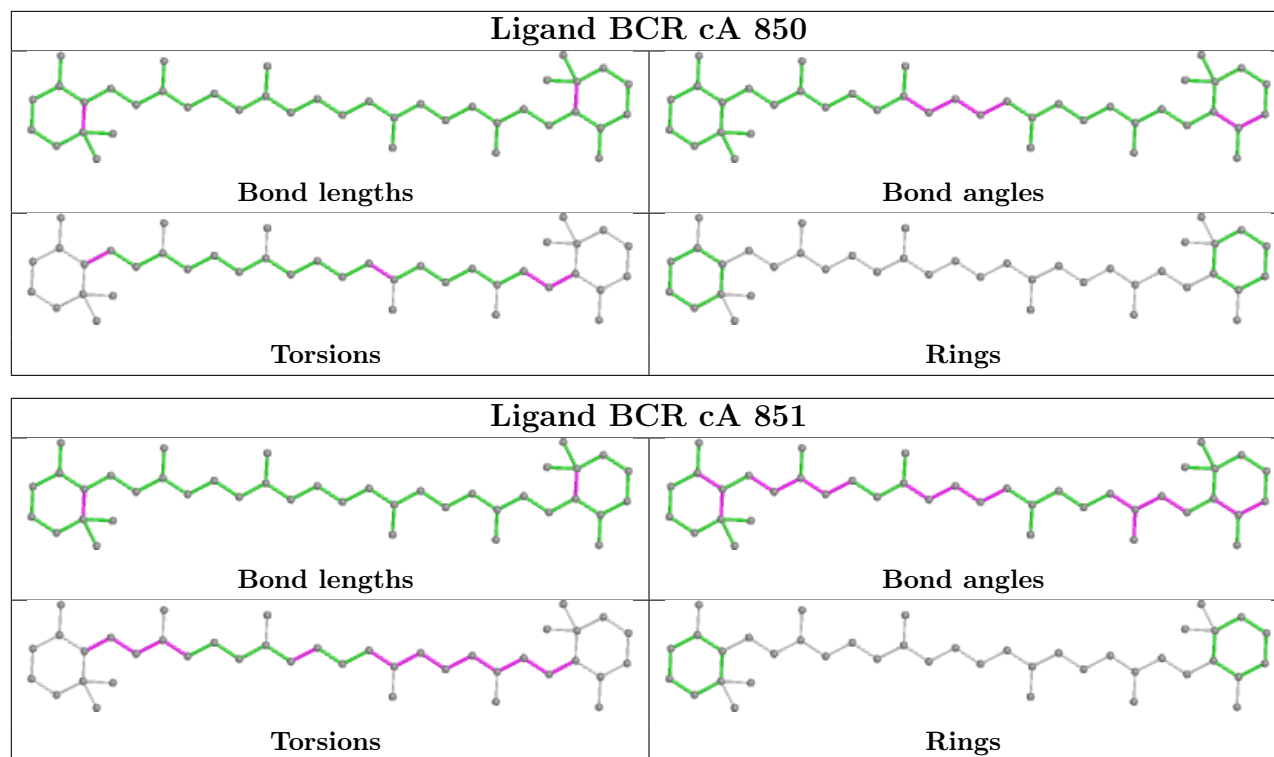


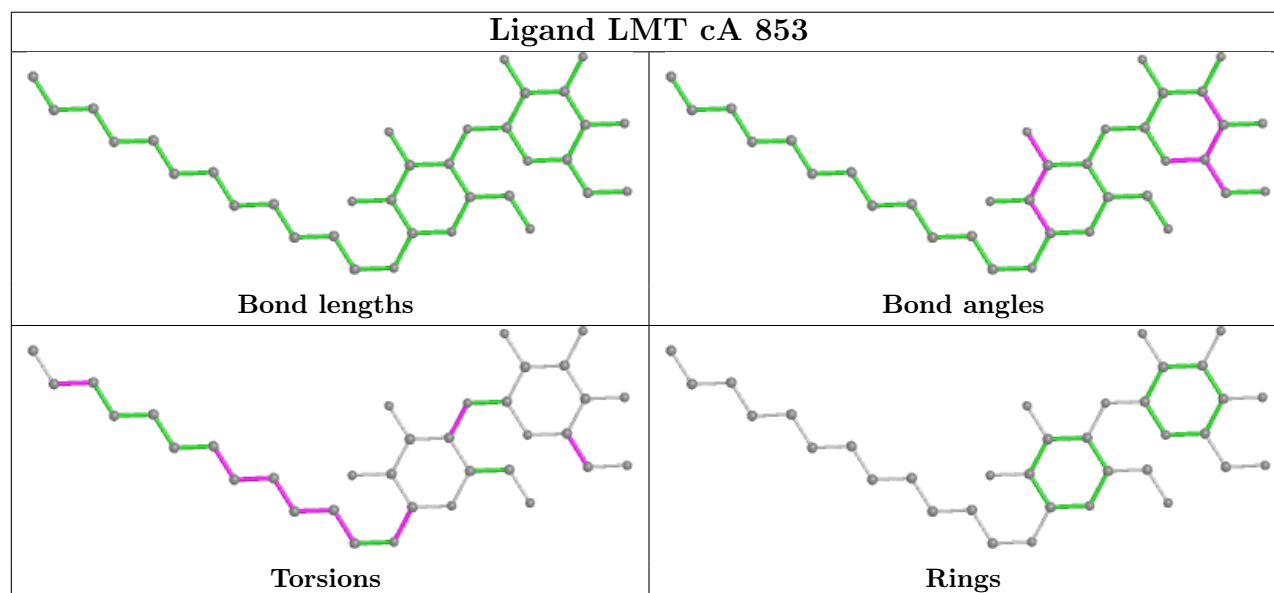
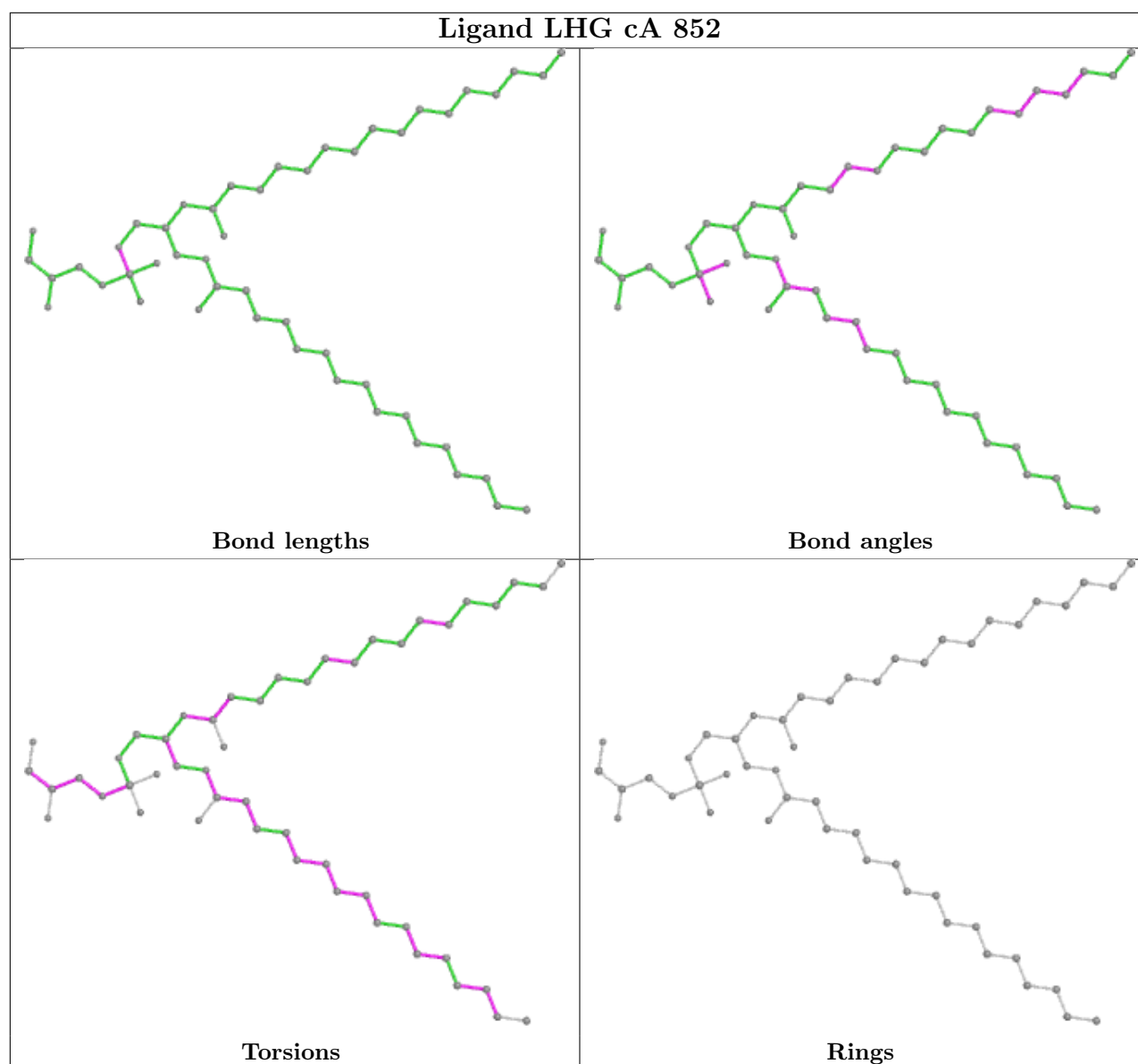
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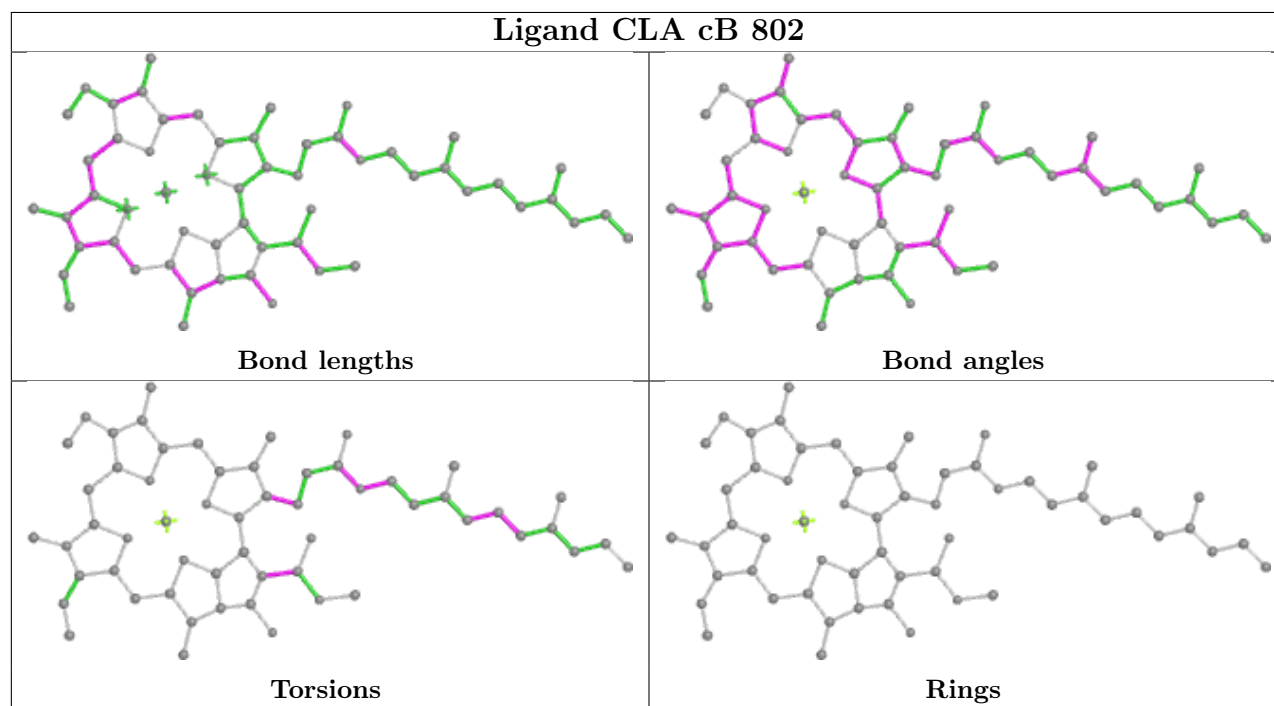
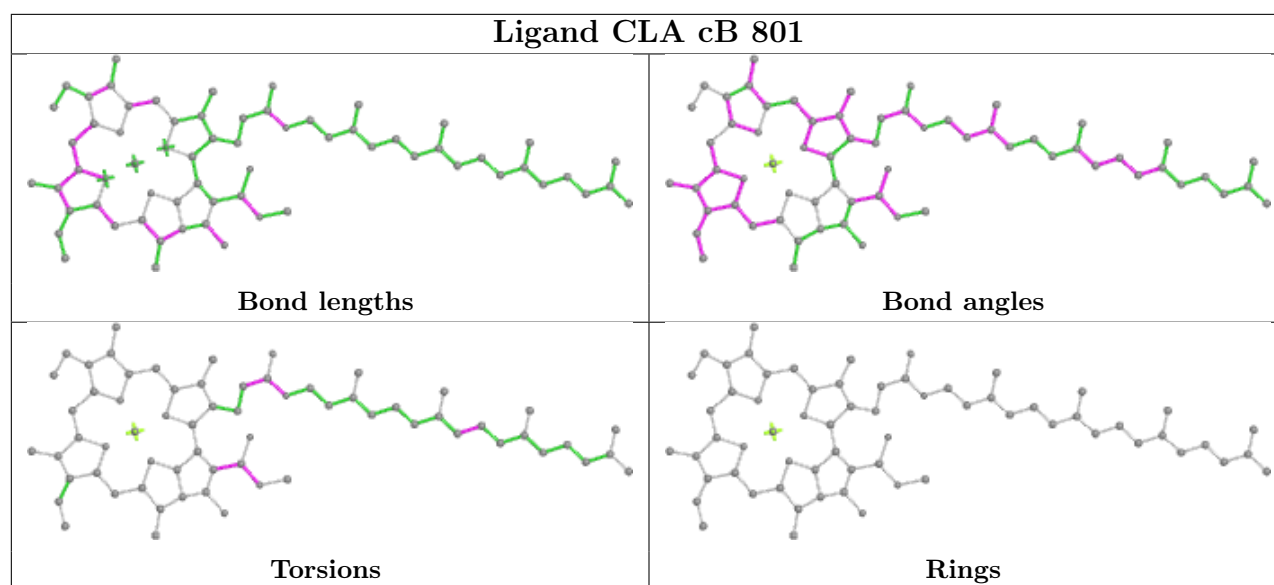


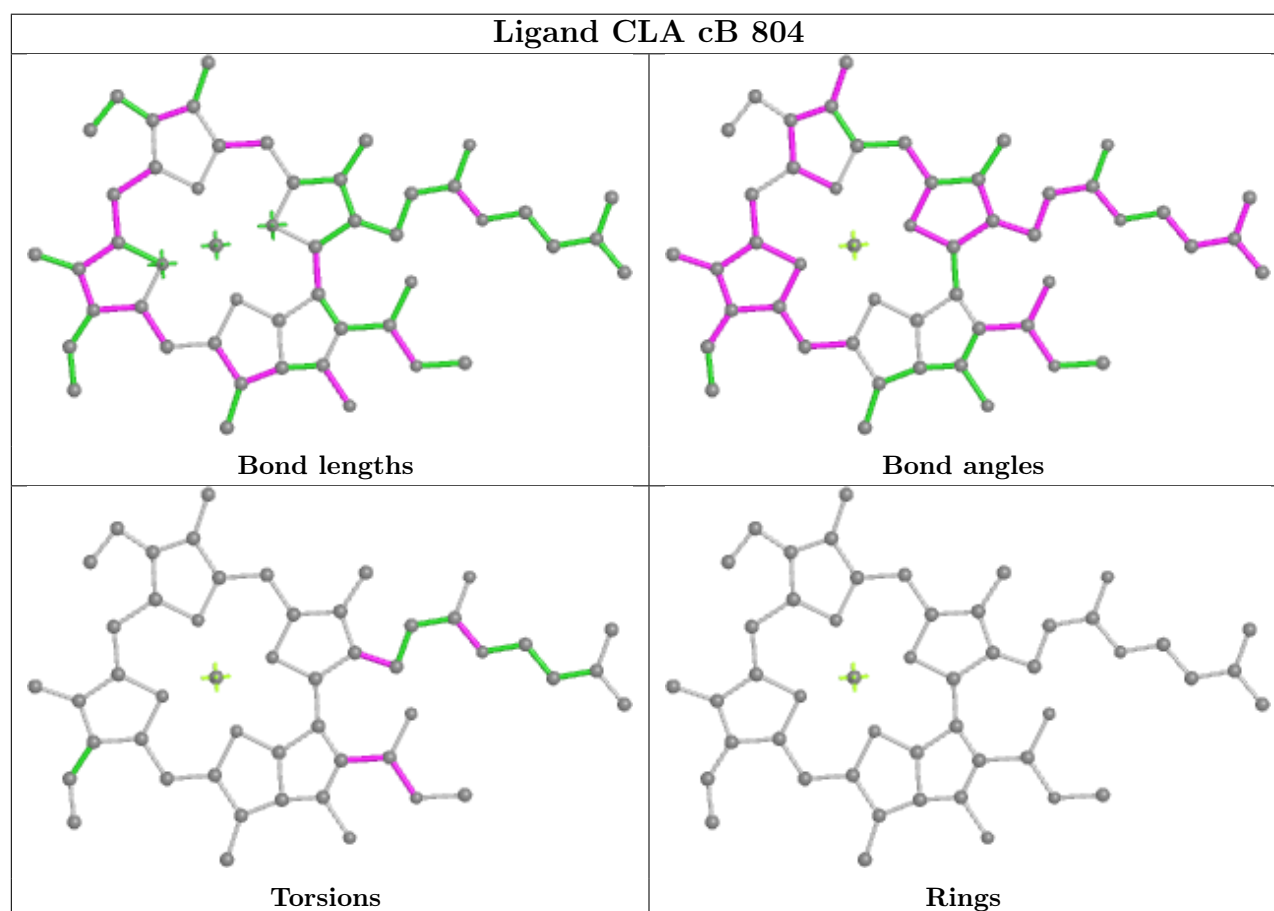
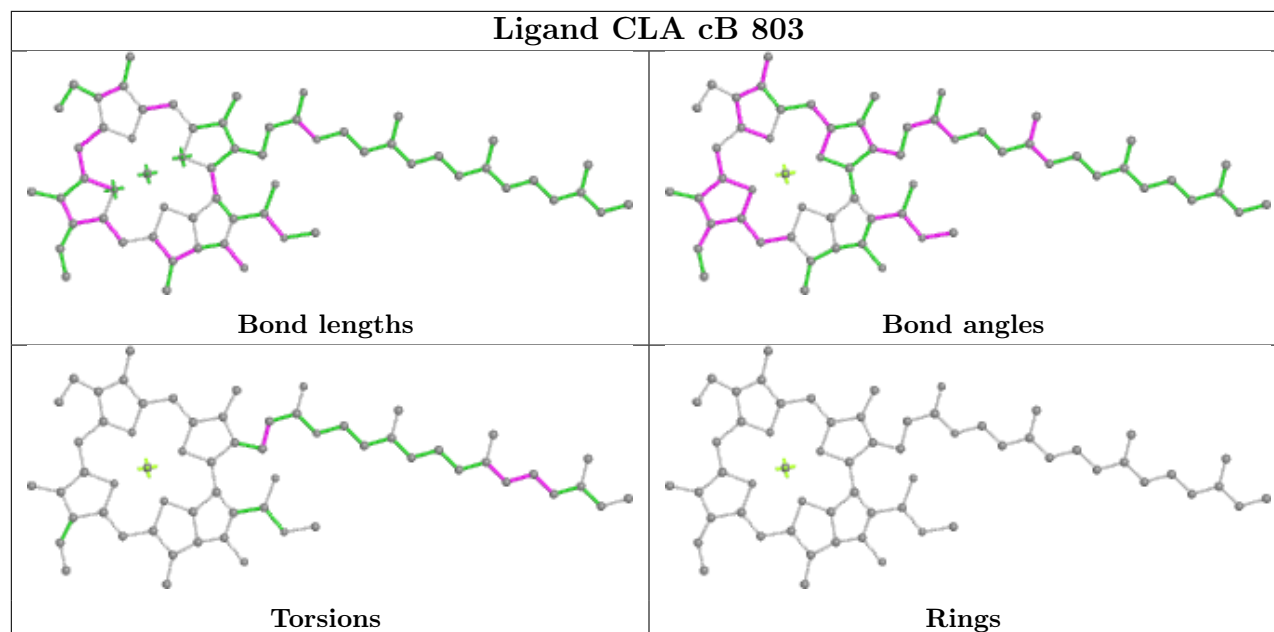


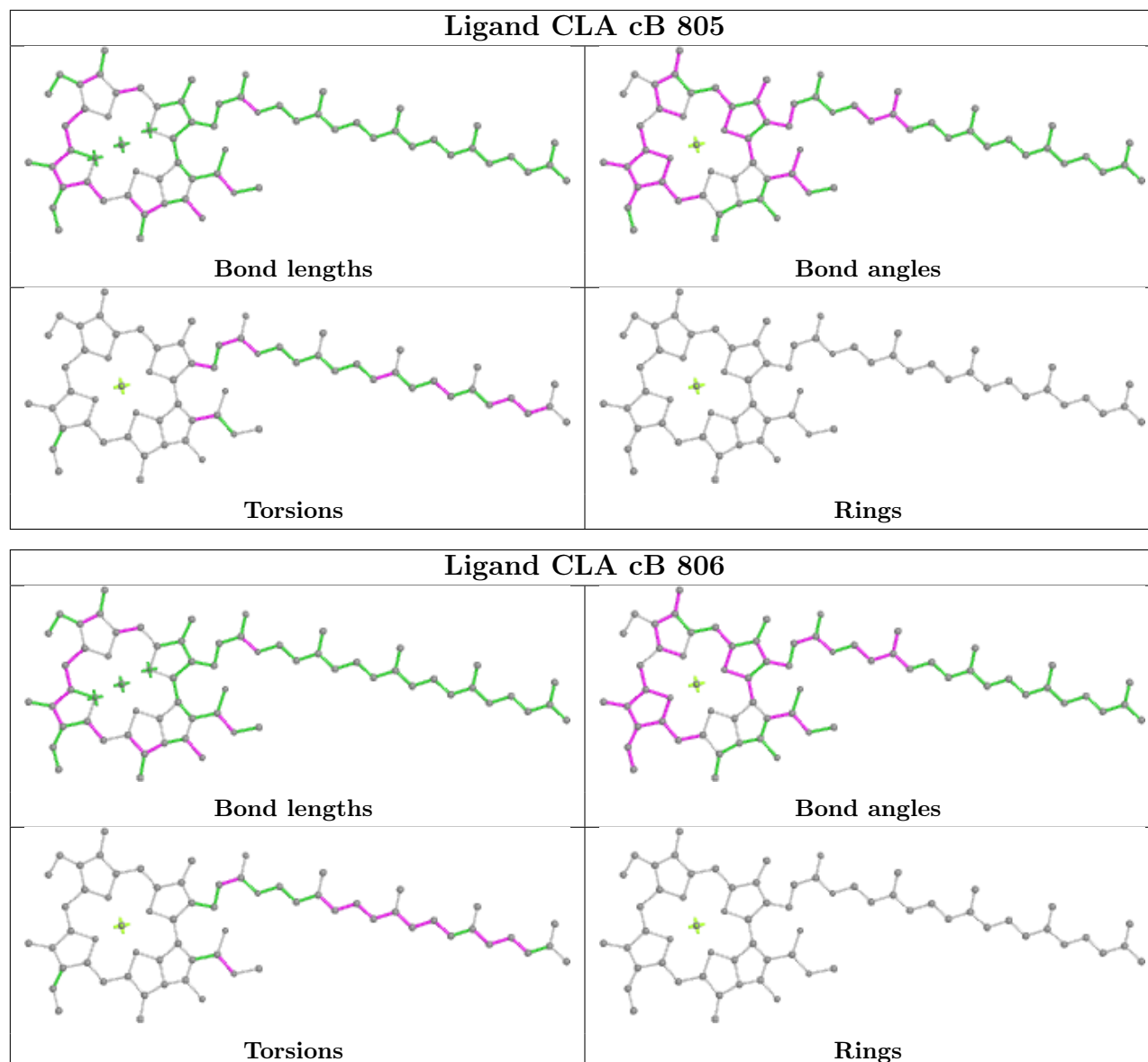


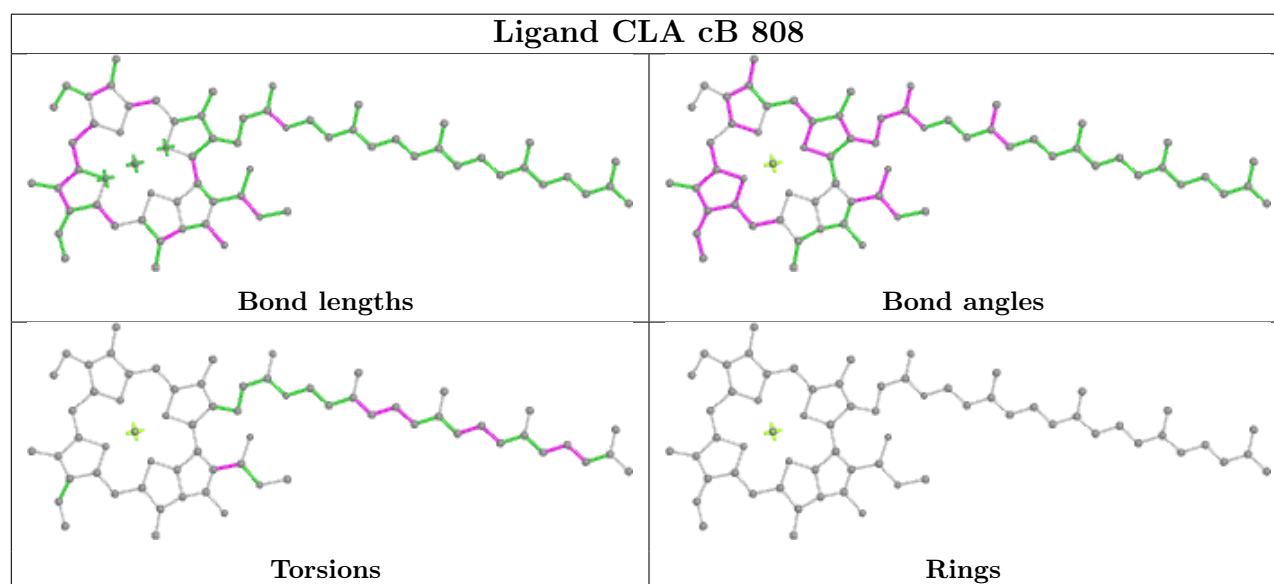
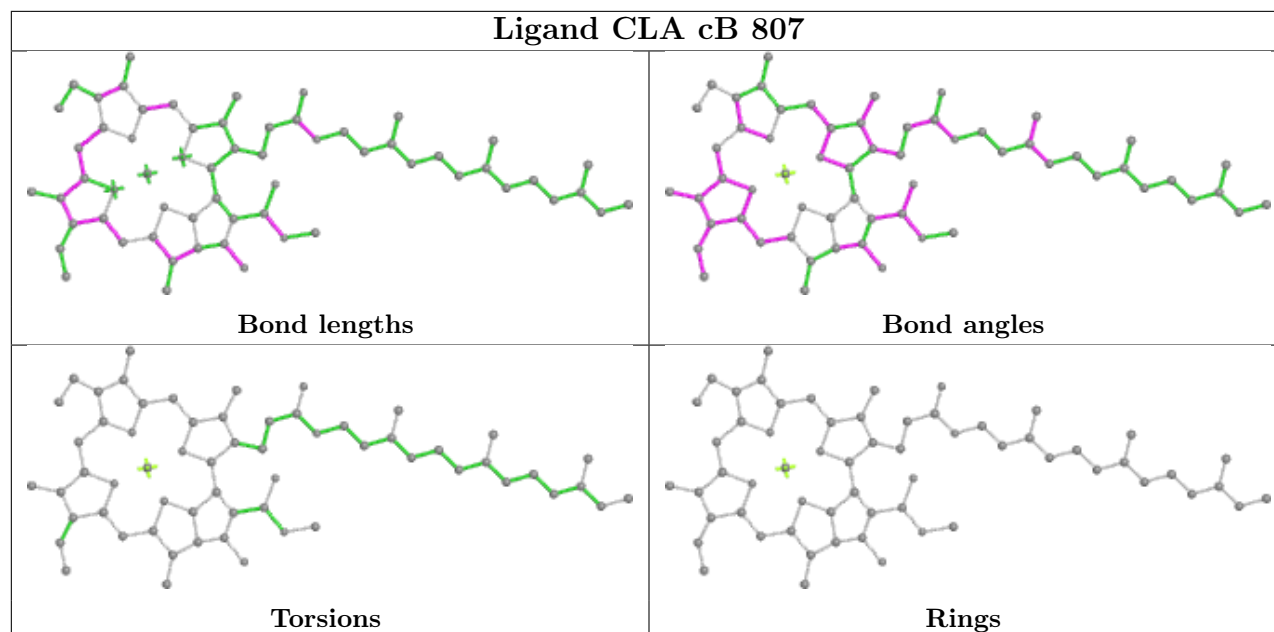




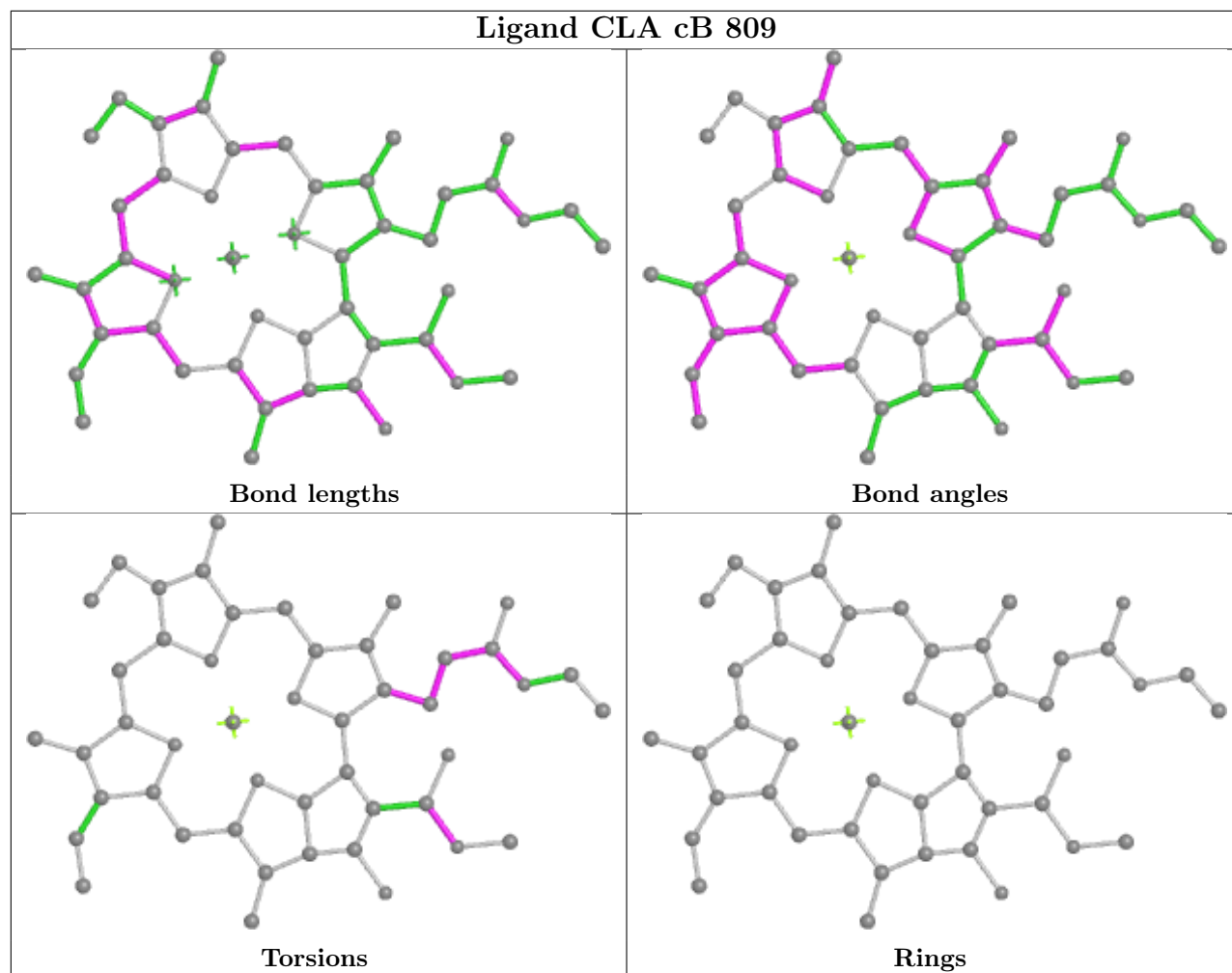




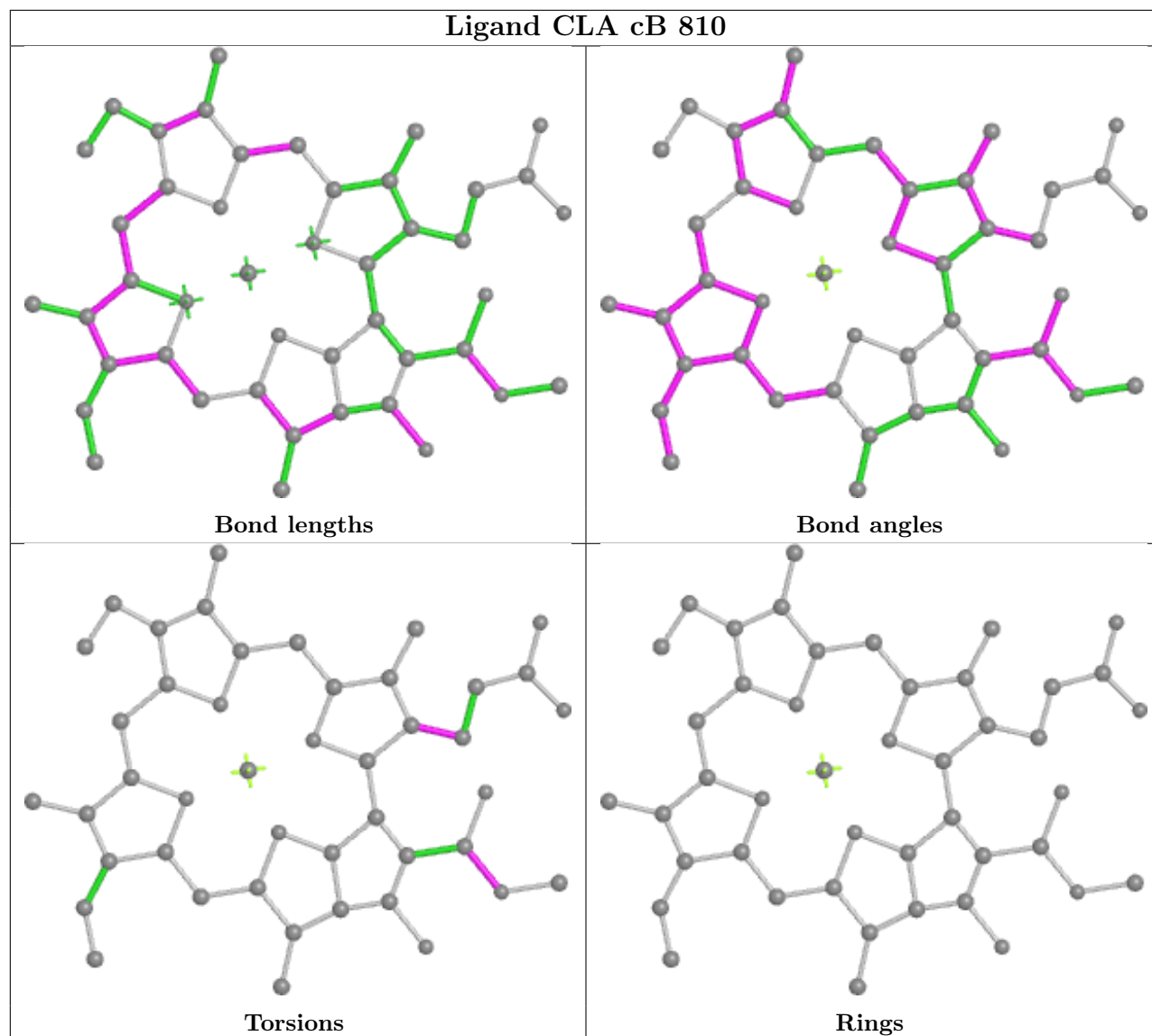




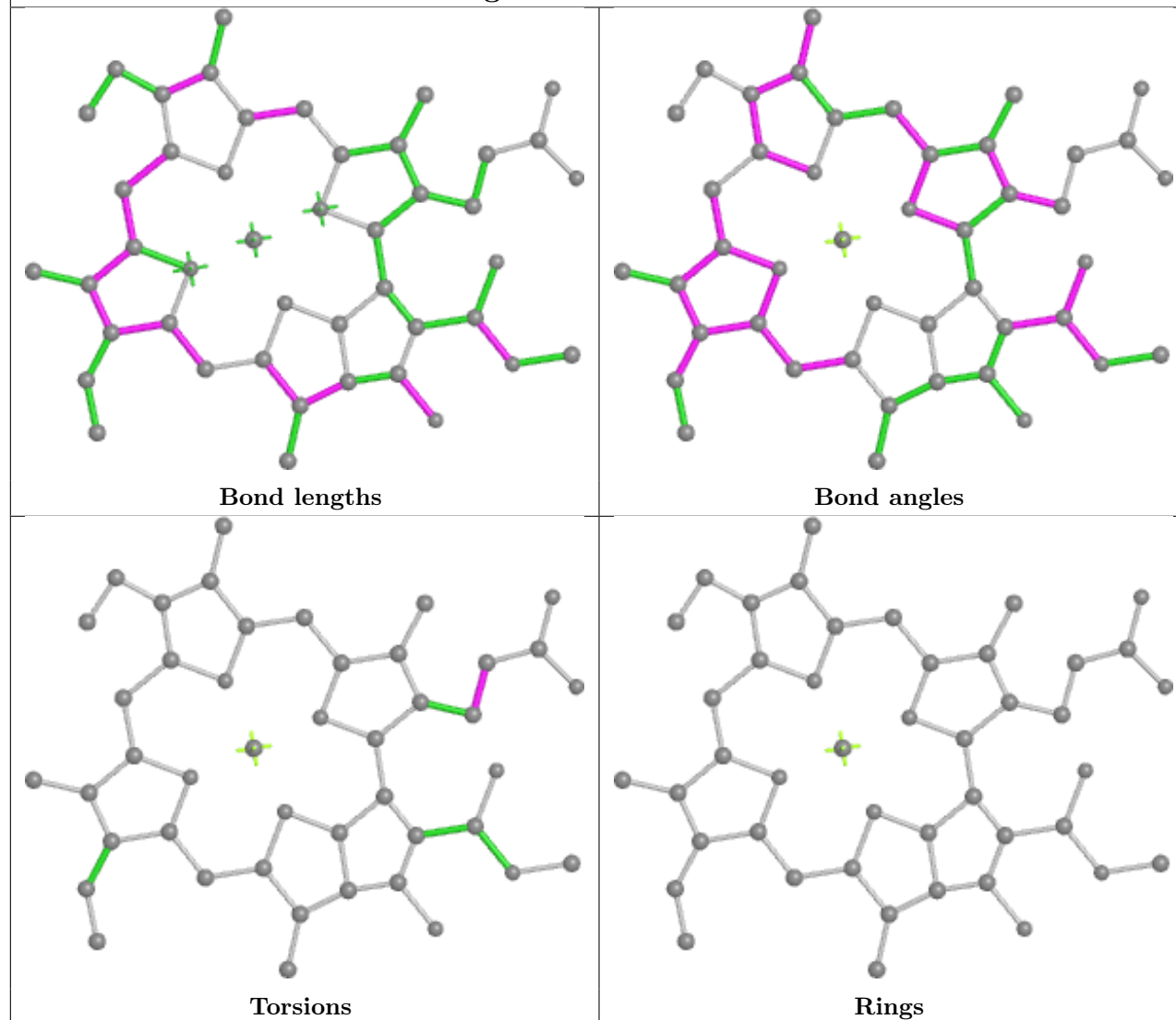
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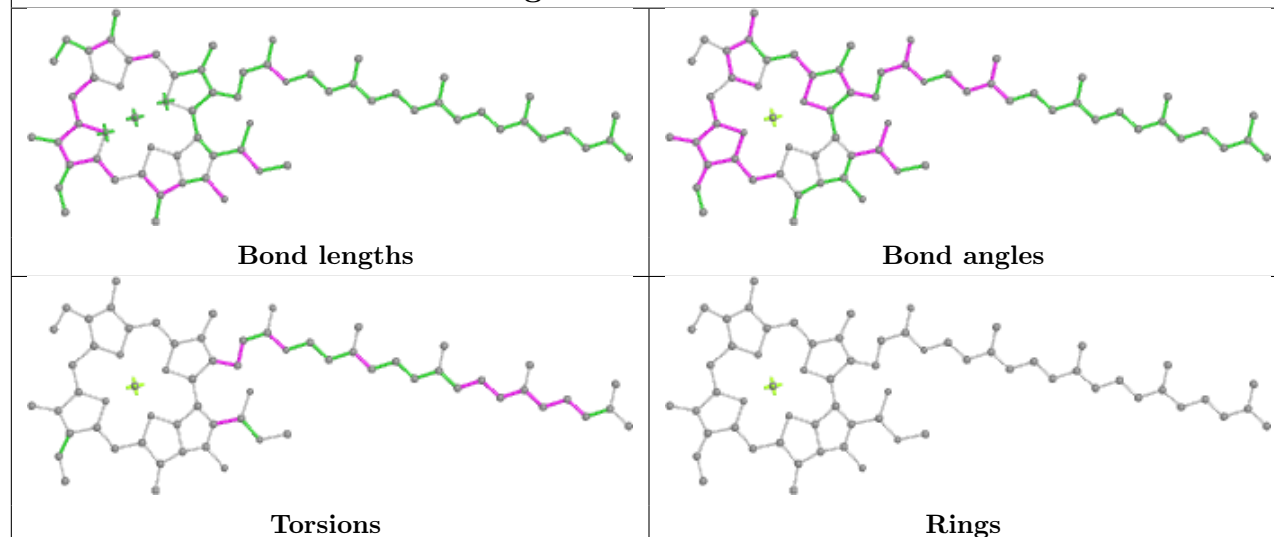
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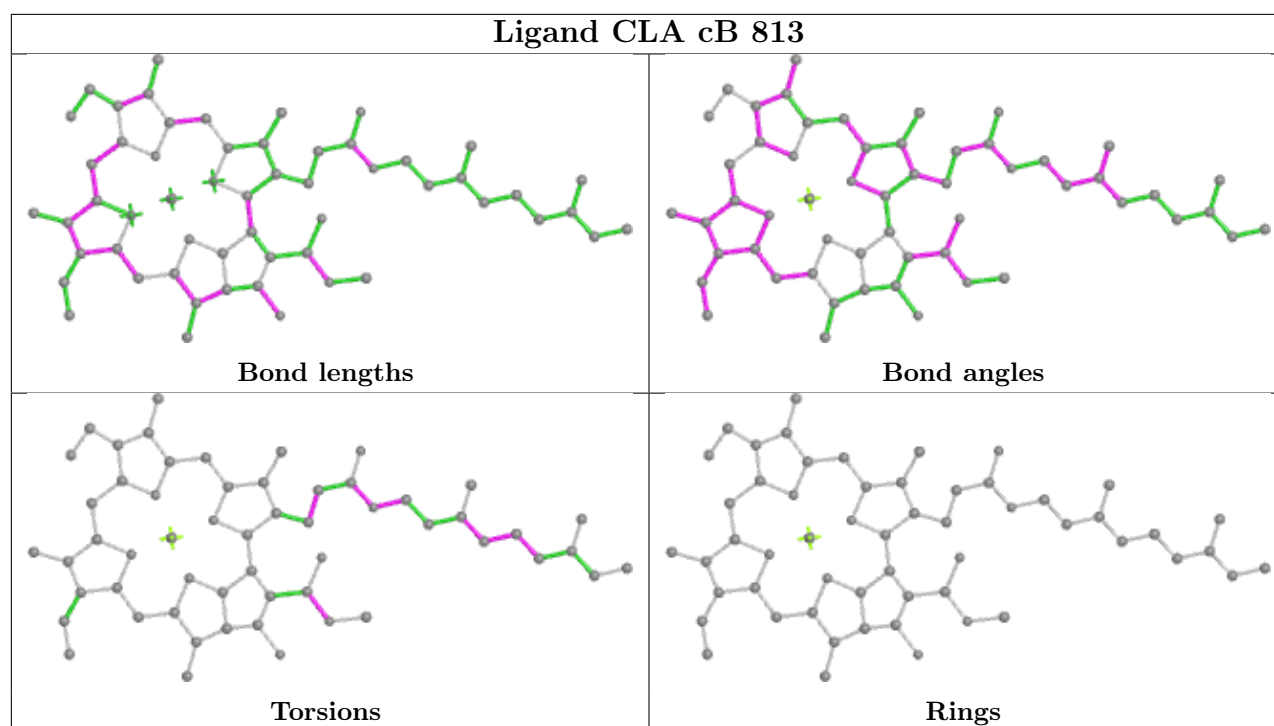


Ligand CLA cB 811

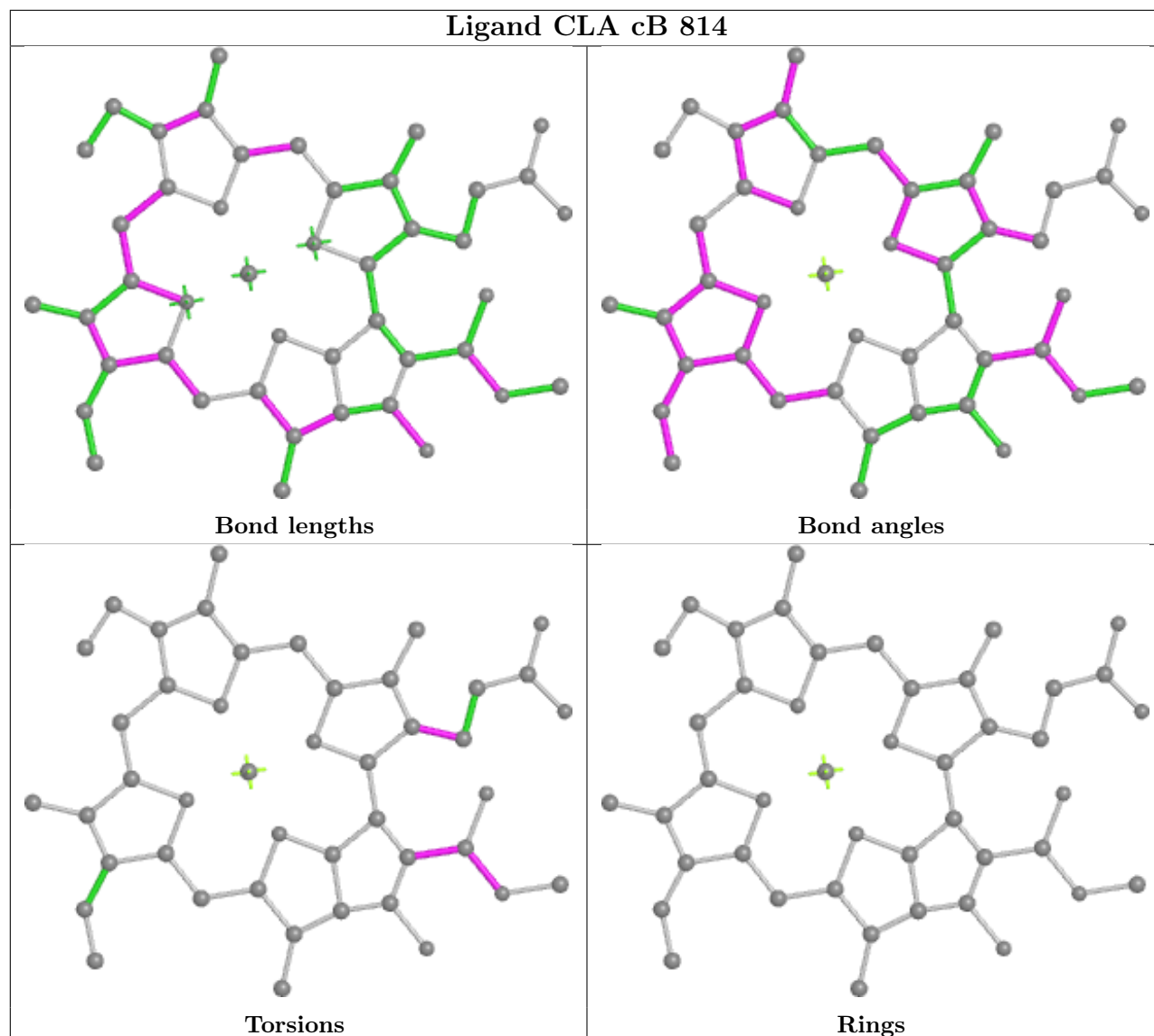


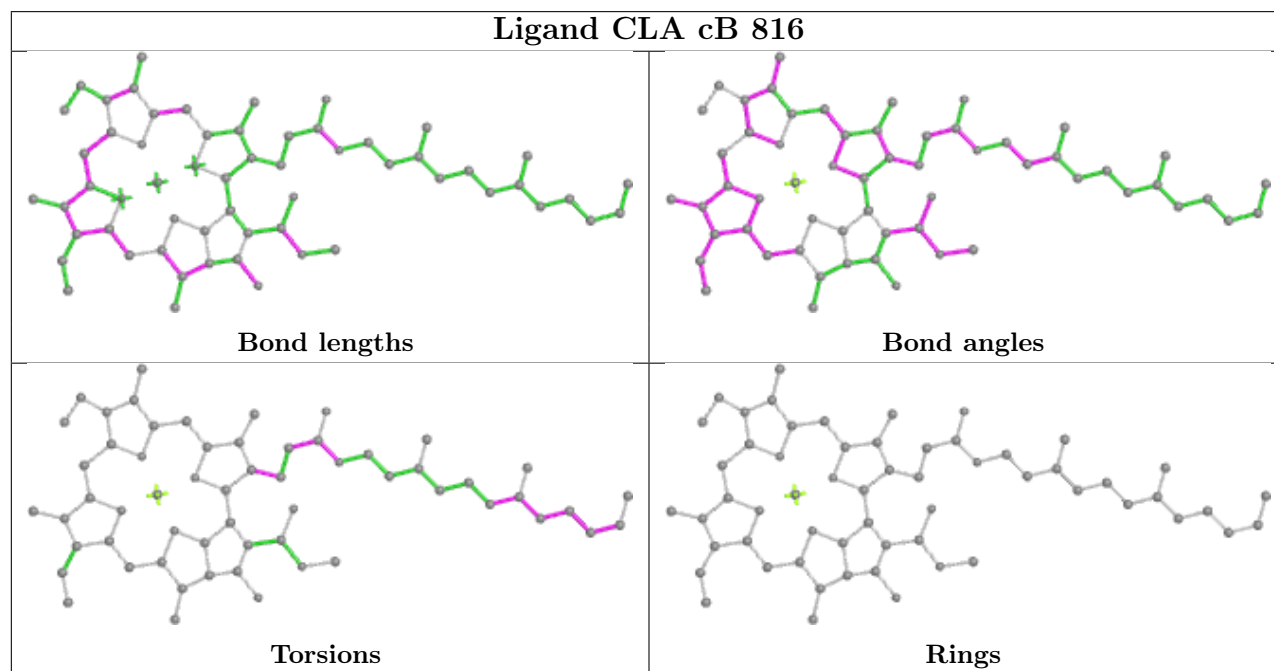
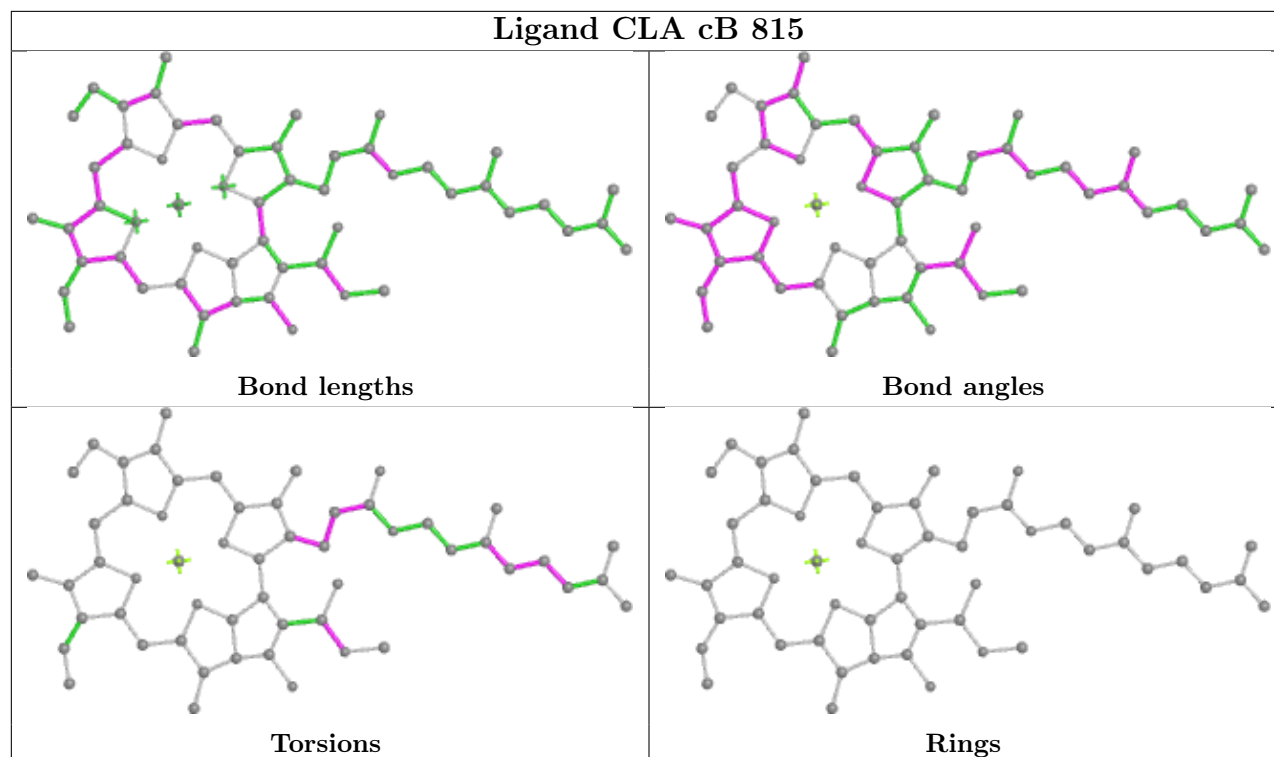
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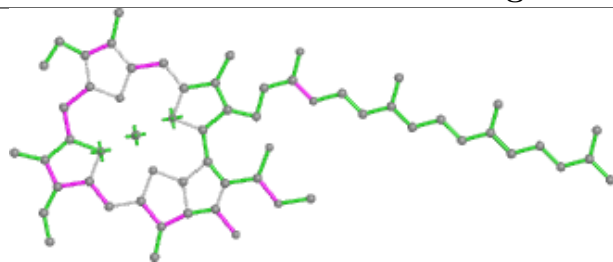




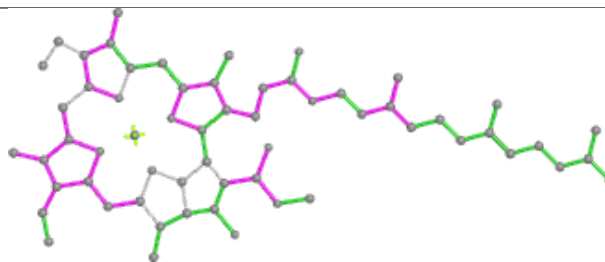
Ligand CLA cB 814



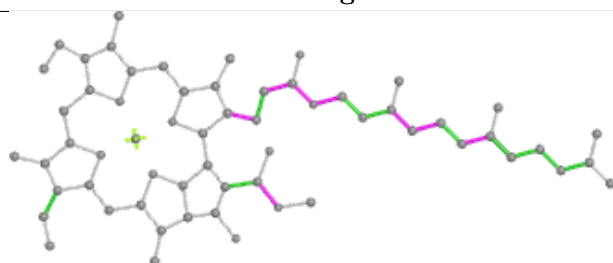


Ligand CLA cB 817

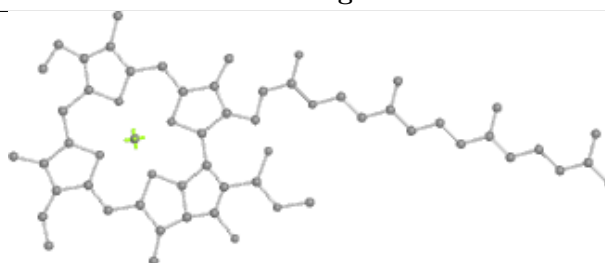
Bond lengths



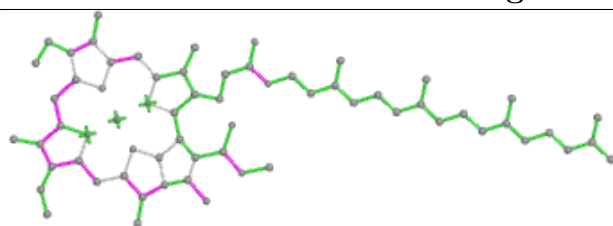
Bond angles



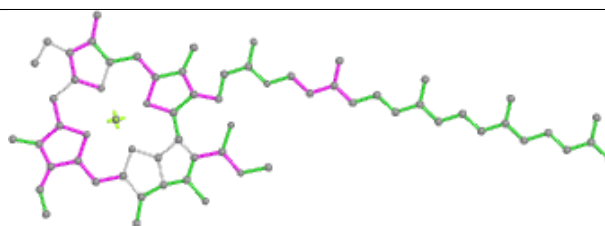
Torsions



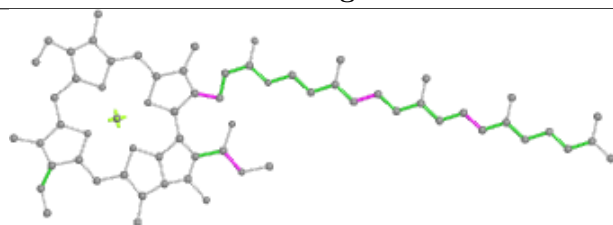
Rings

Ligand CLA cB 818

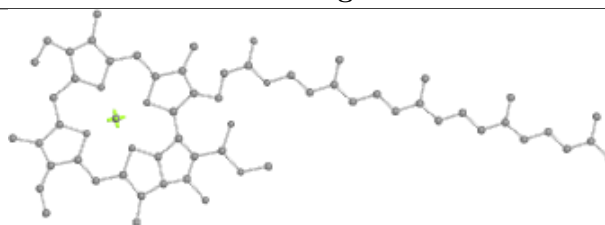
Bond lengths



Bond angles

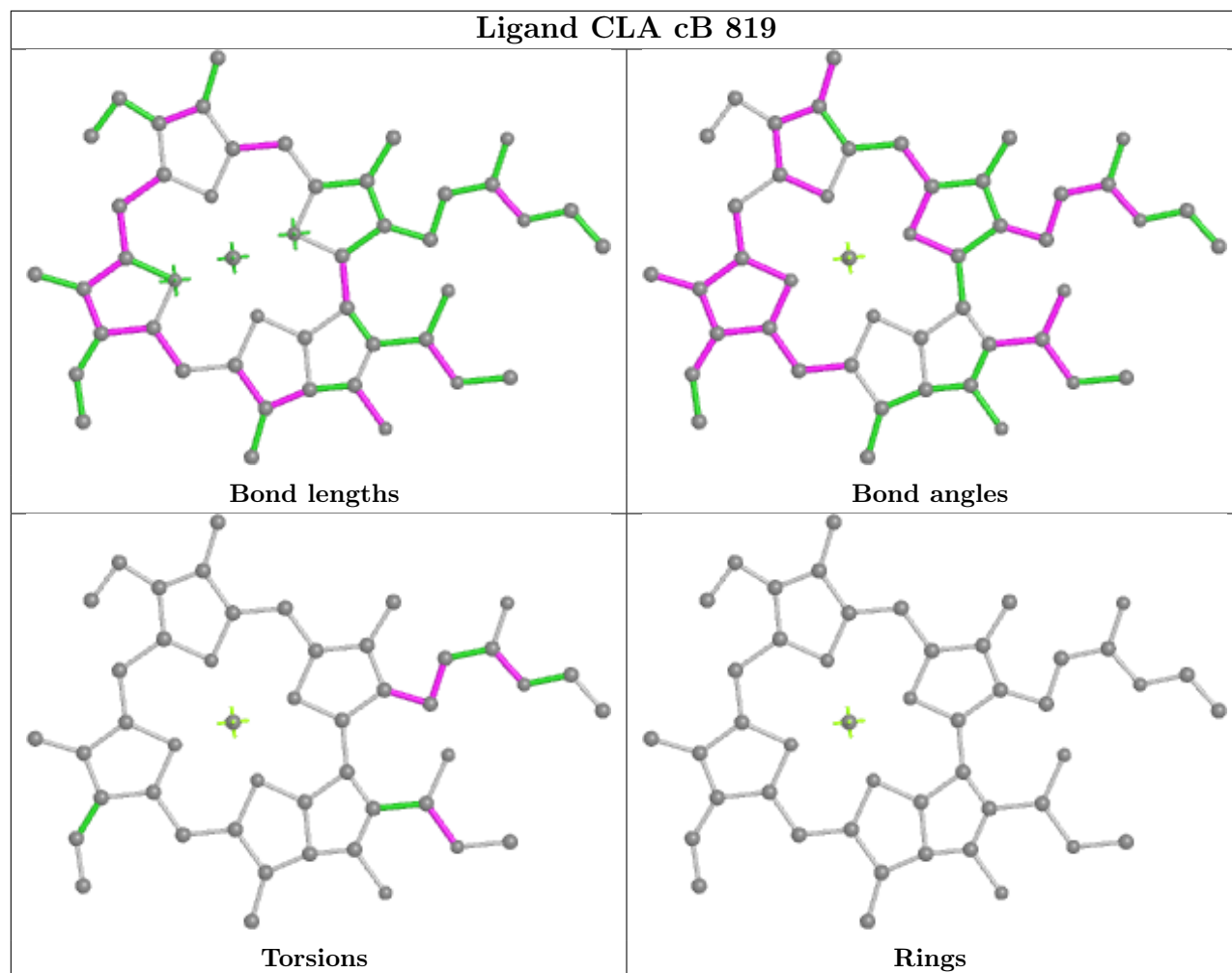


Torsions

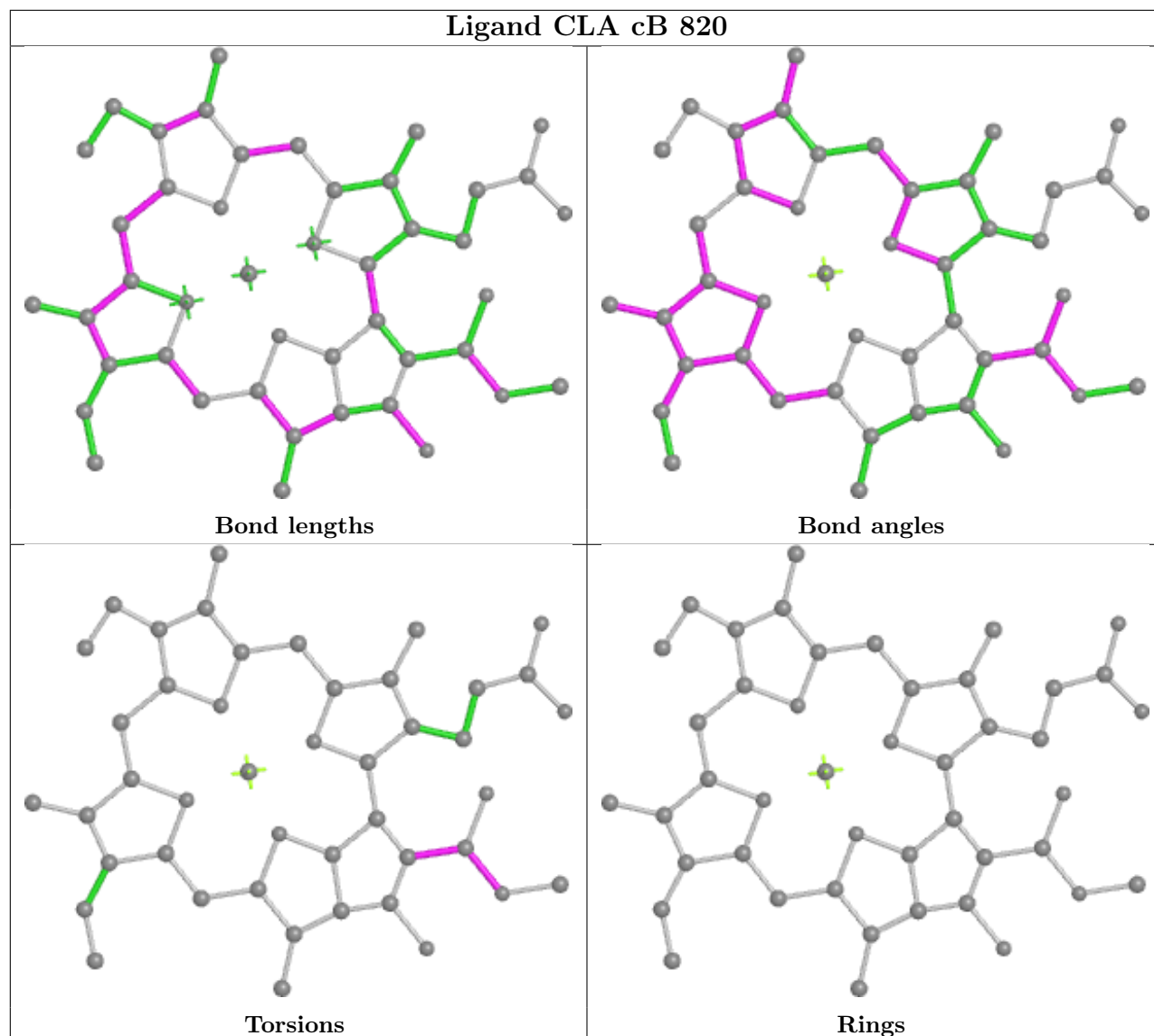


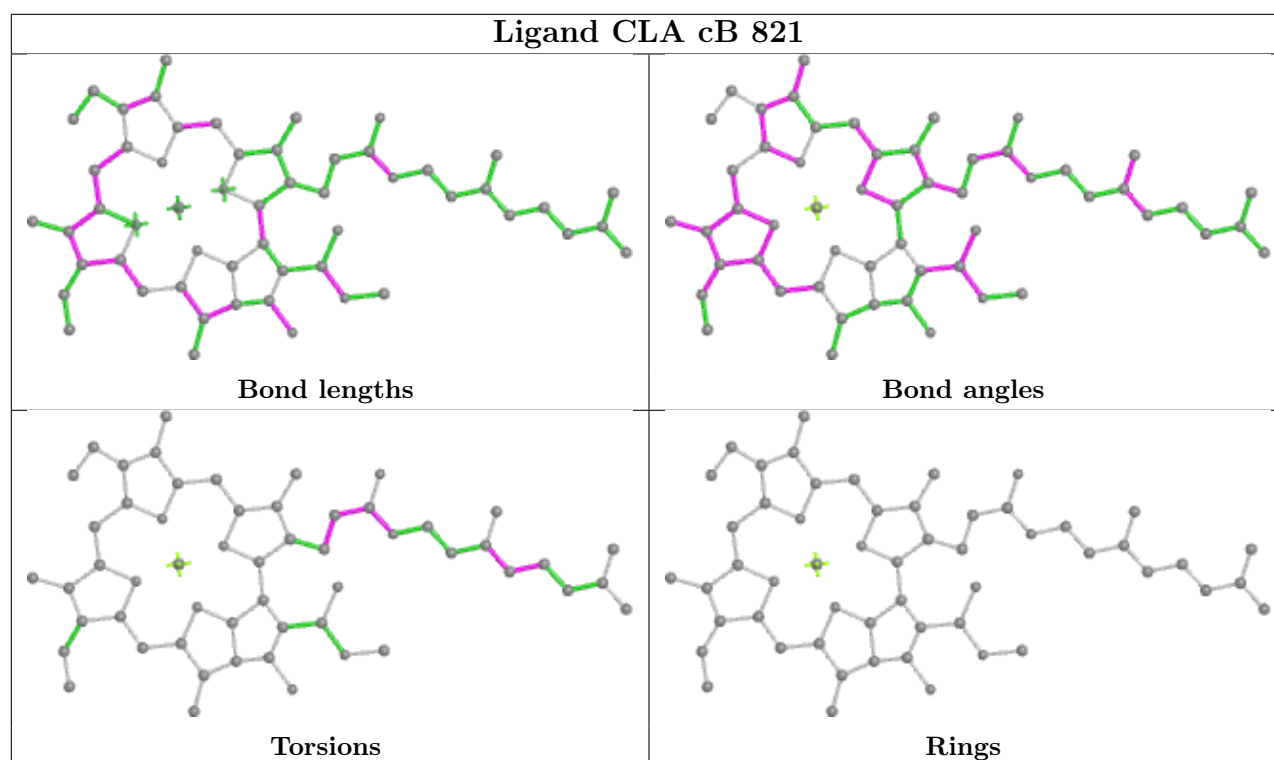
Rings

Ligand CLA cB 819

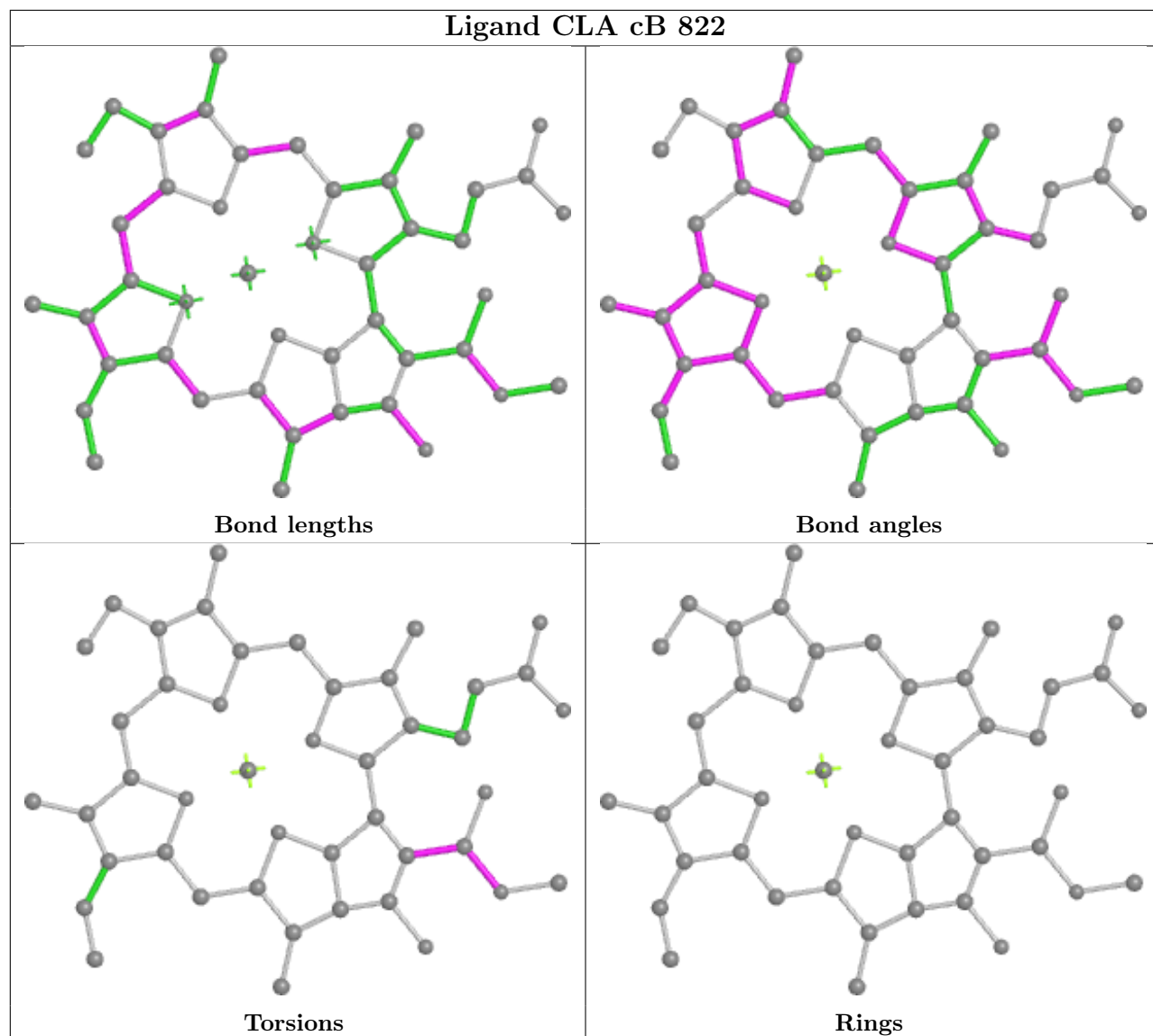


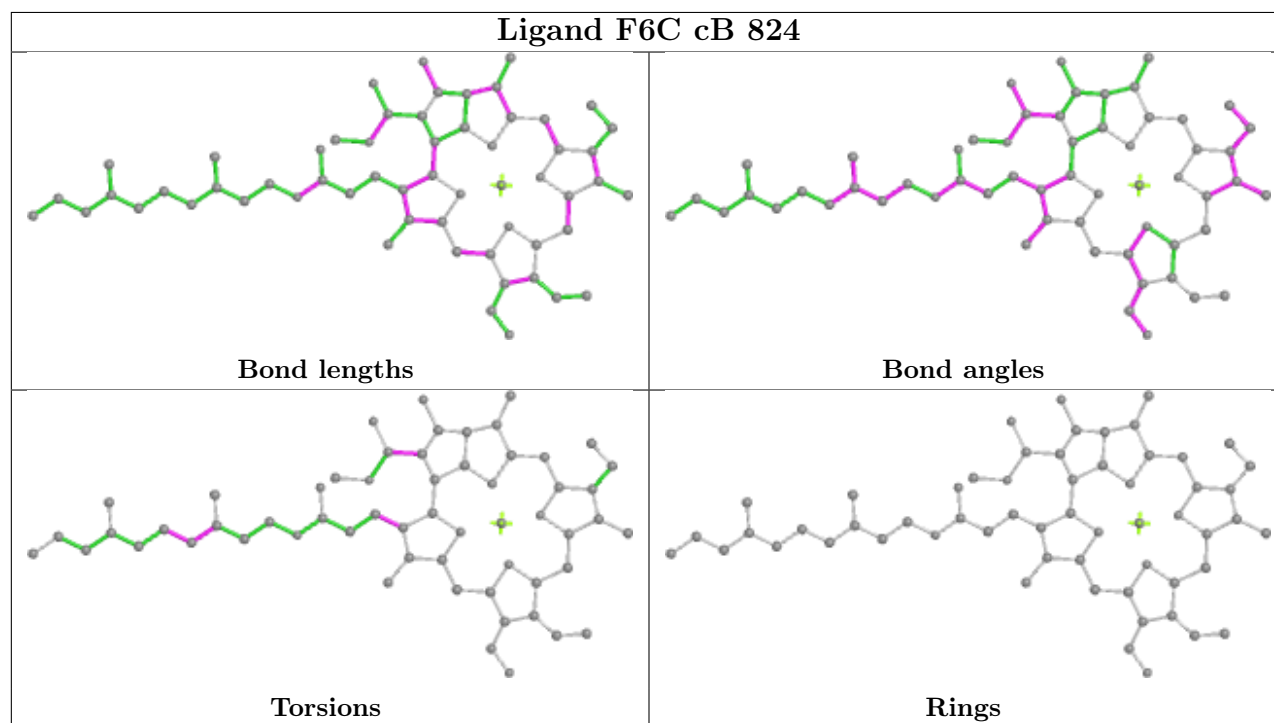
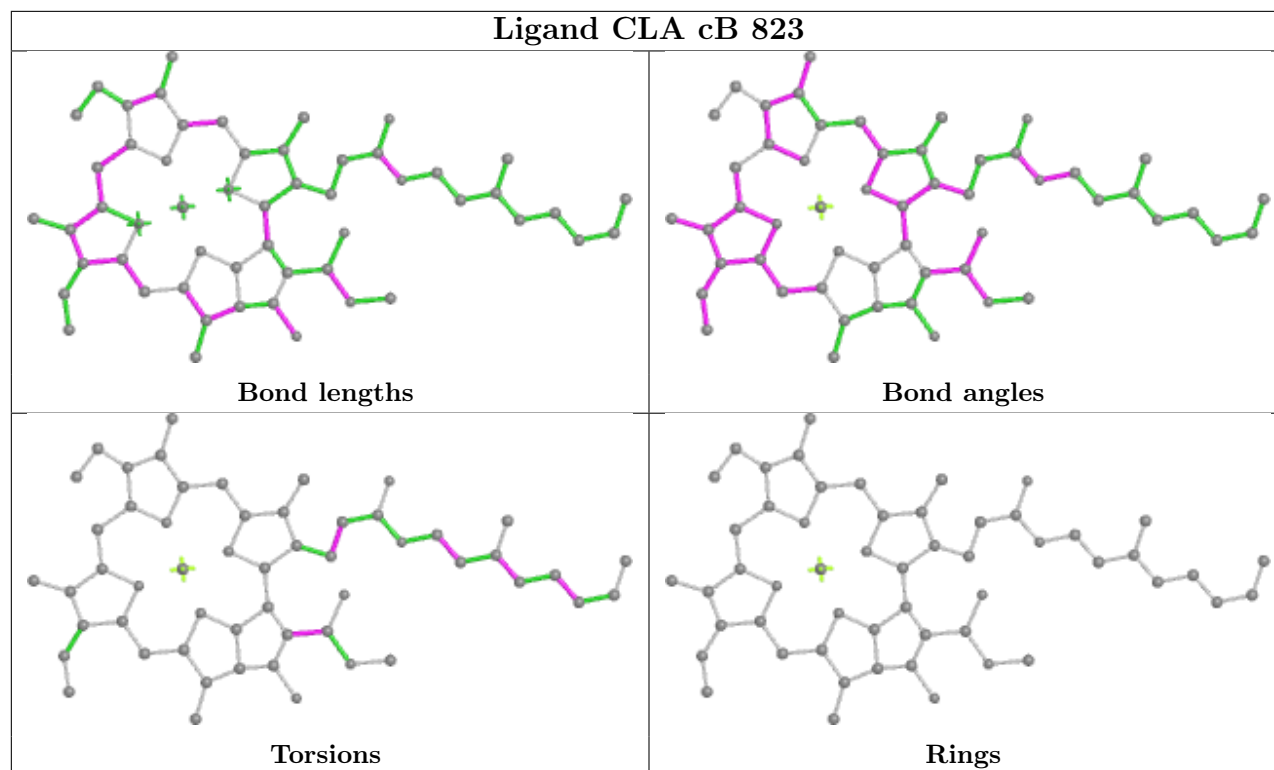
Ligand CLA cB 820

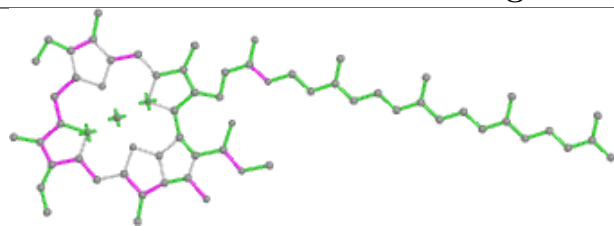
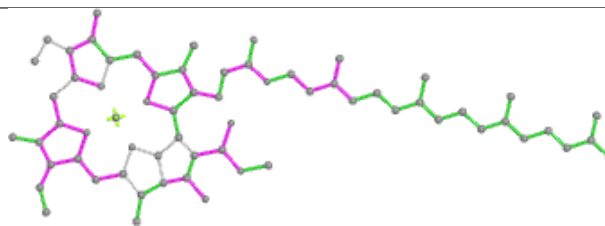
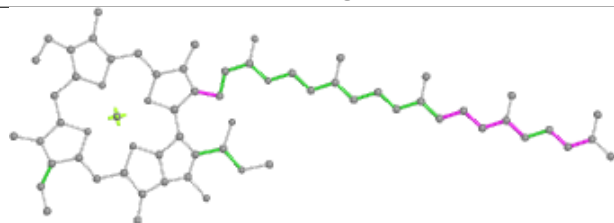
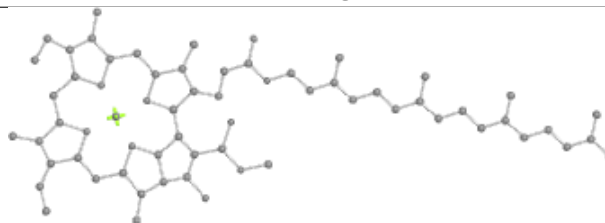
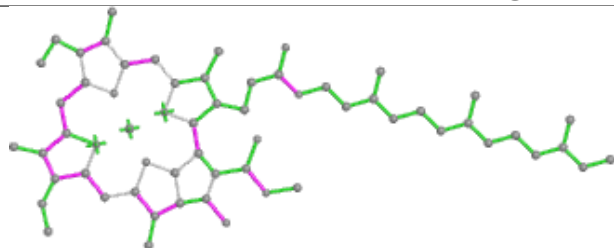
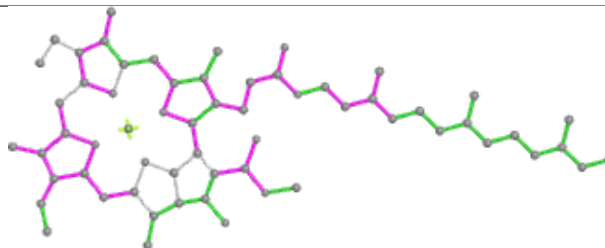
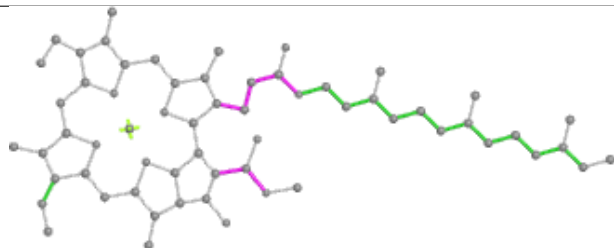
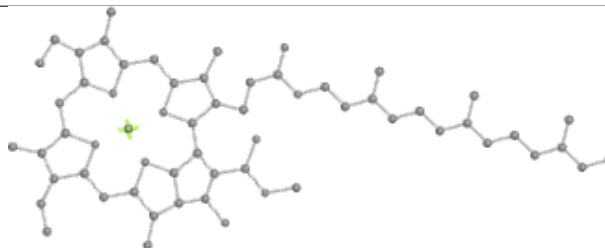


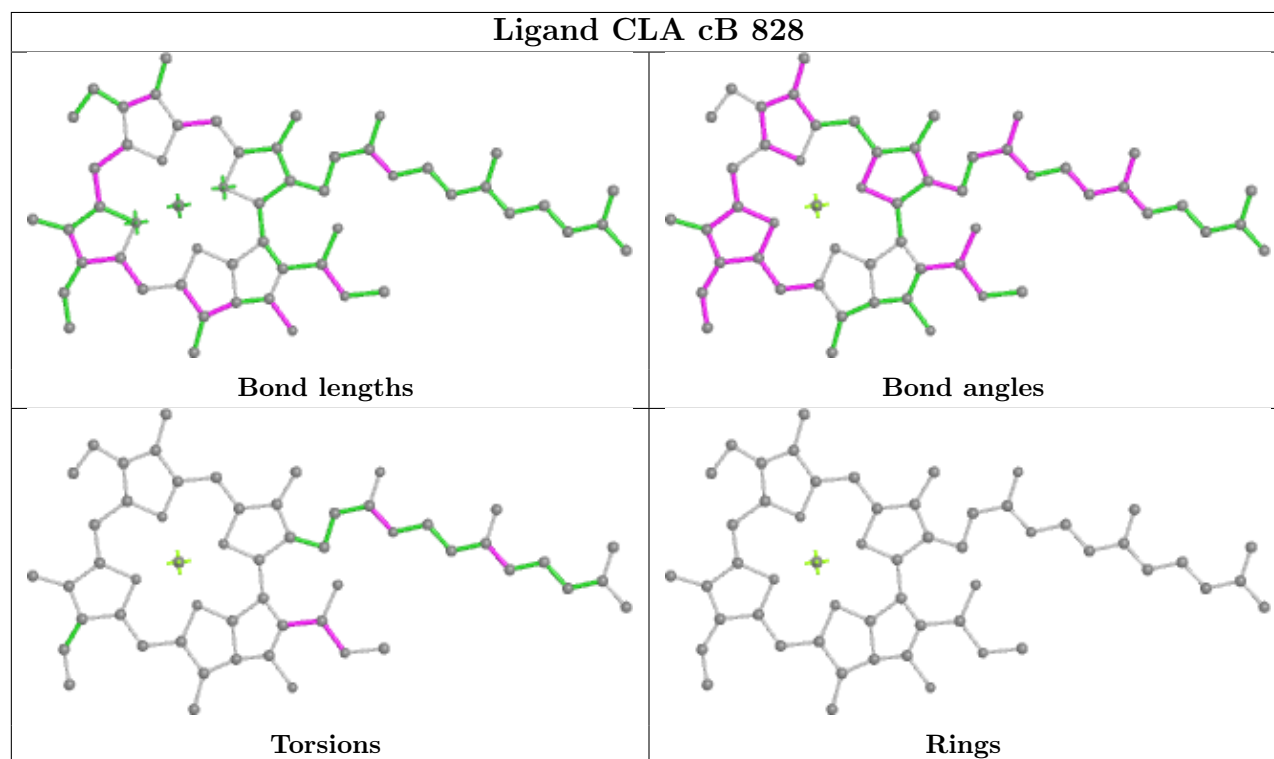
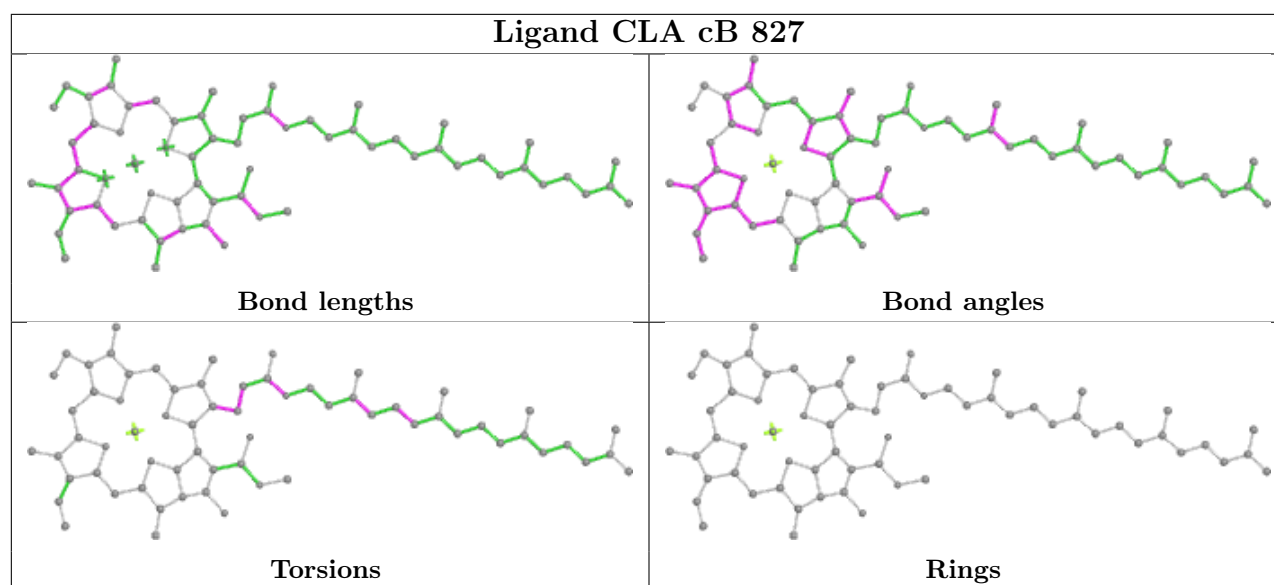


Ligand CLA cB 822

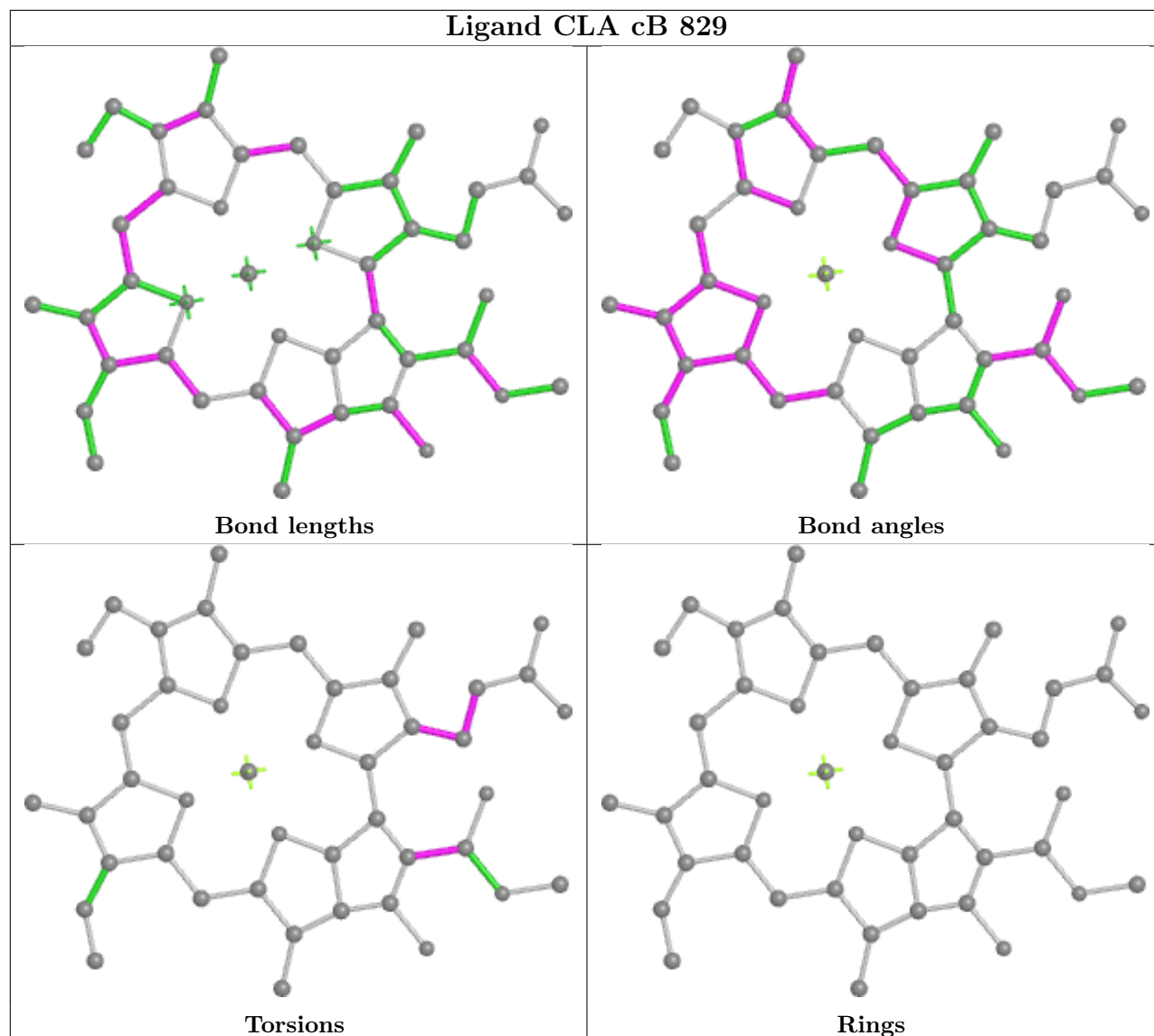




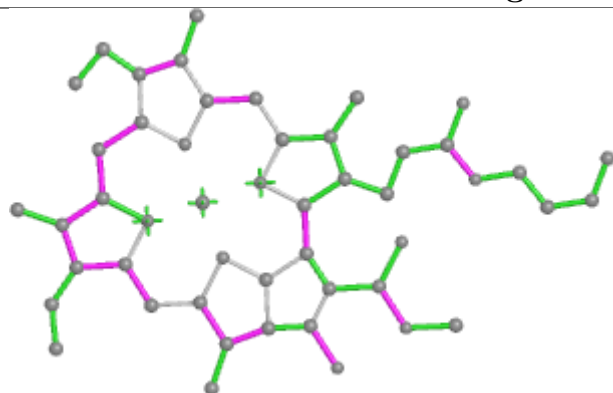
Ligand CLA cB 825**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA cB 826****Bond lengths****Bond angles****Torsions****Rings**



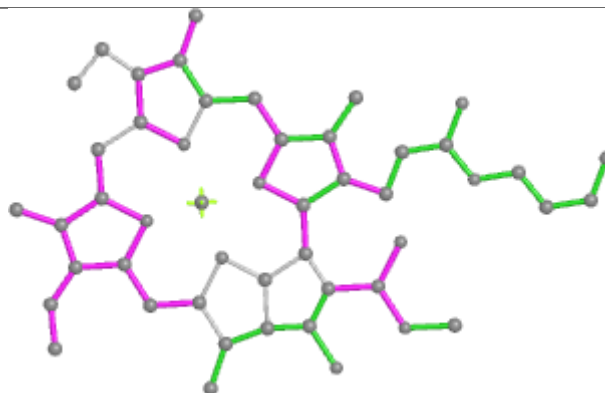
Ligand CLA cB 829



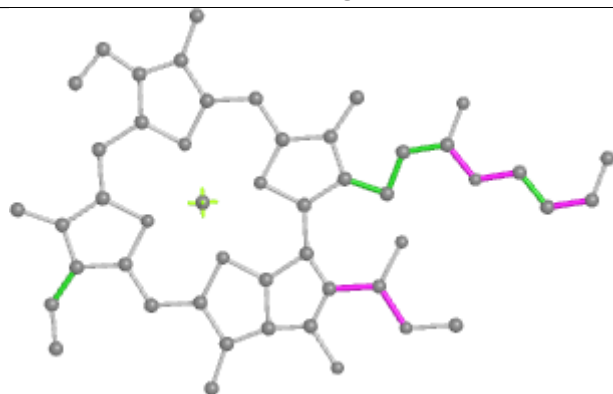
Ligand CLA cB 830



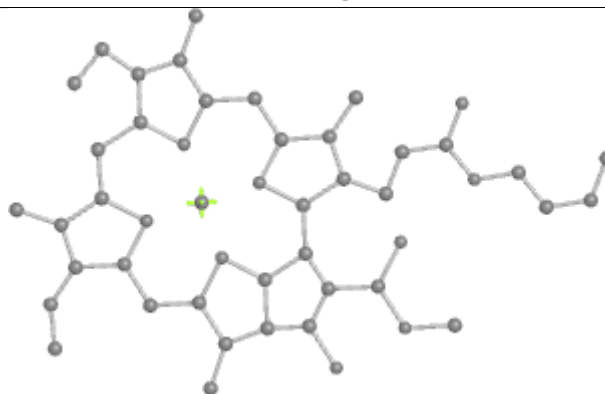
Bond lengths



Bond angles

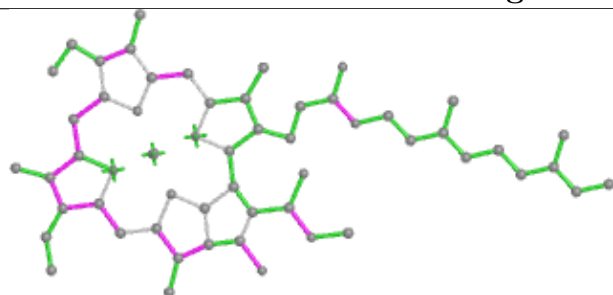


Torsions

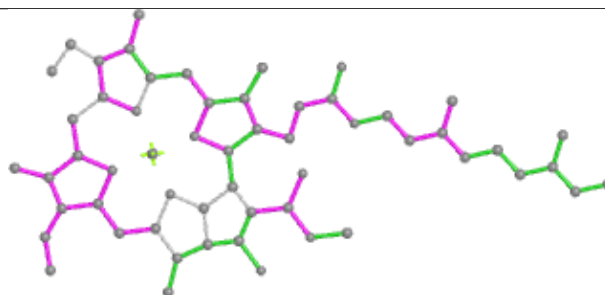


Rings

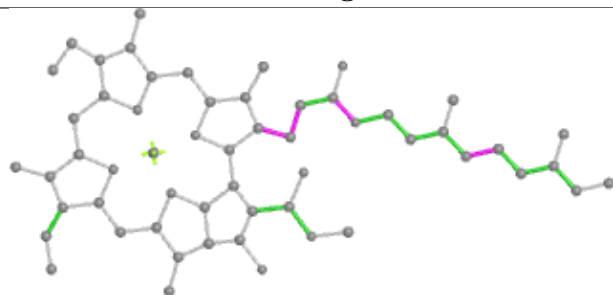
Ligand CLA cB 831



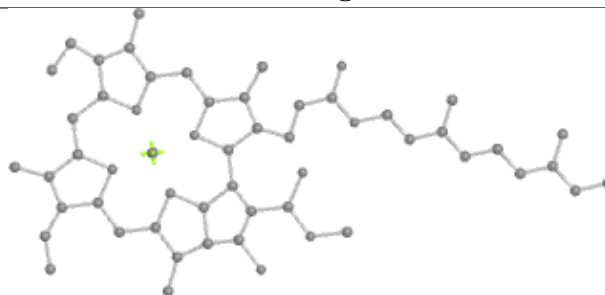
Bond lengths



Bond angles

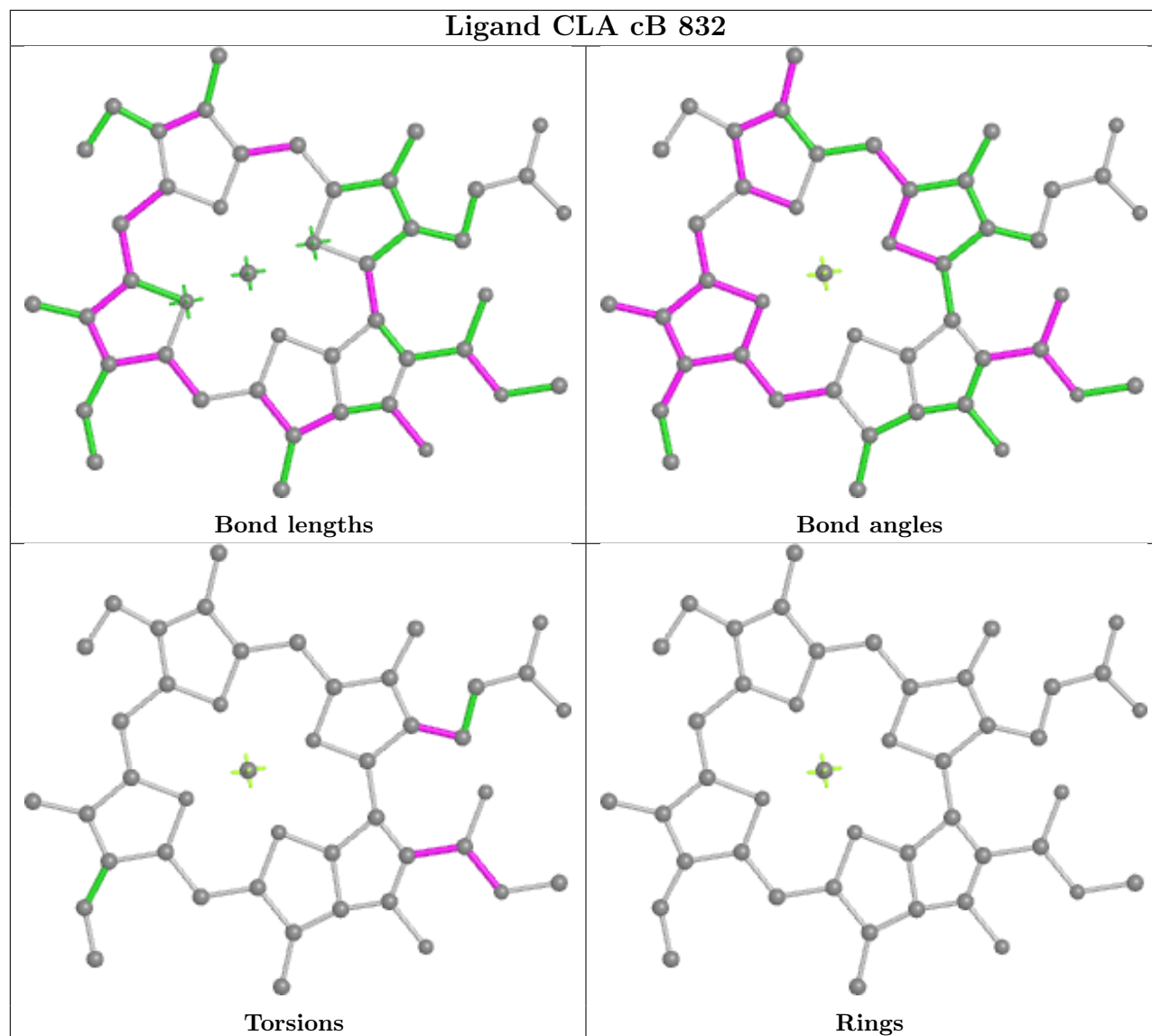


Torsions

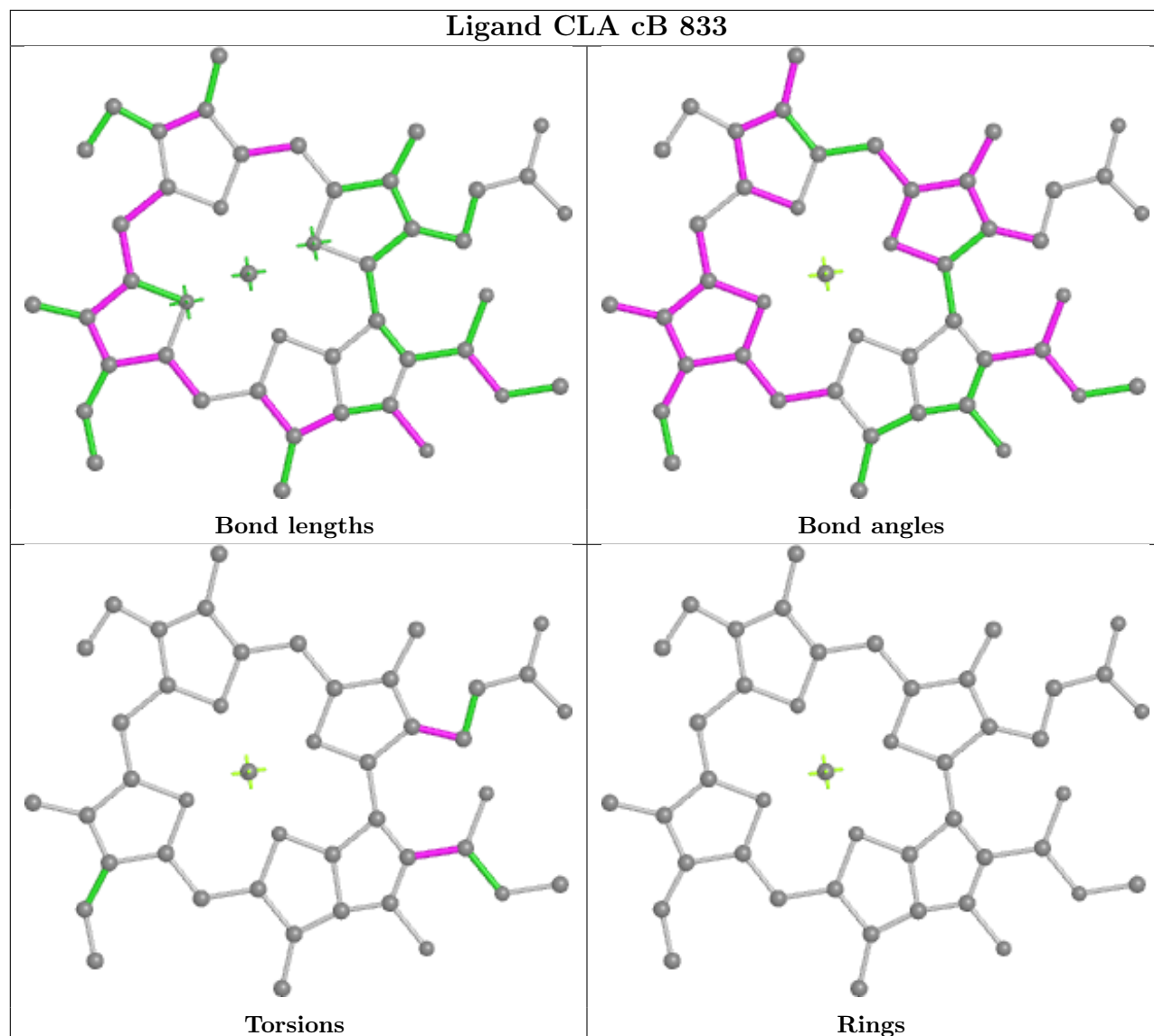


Rings

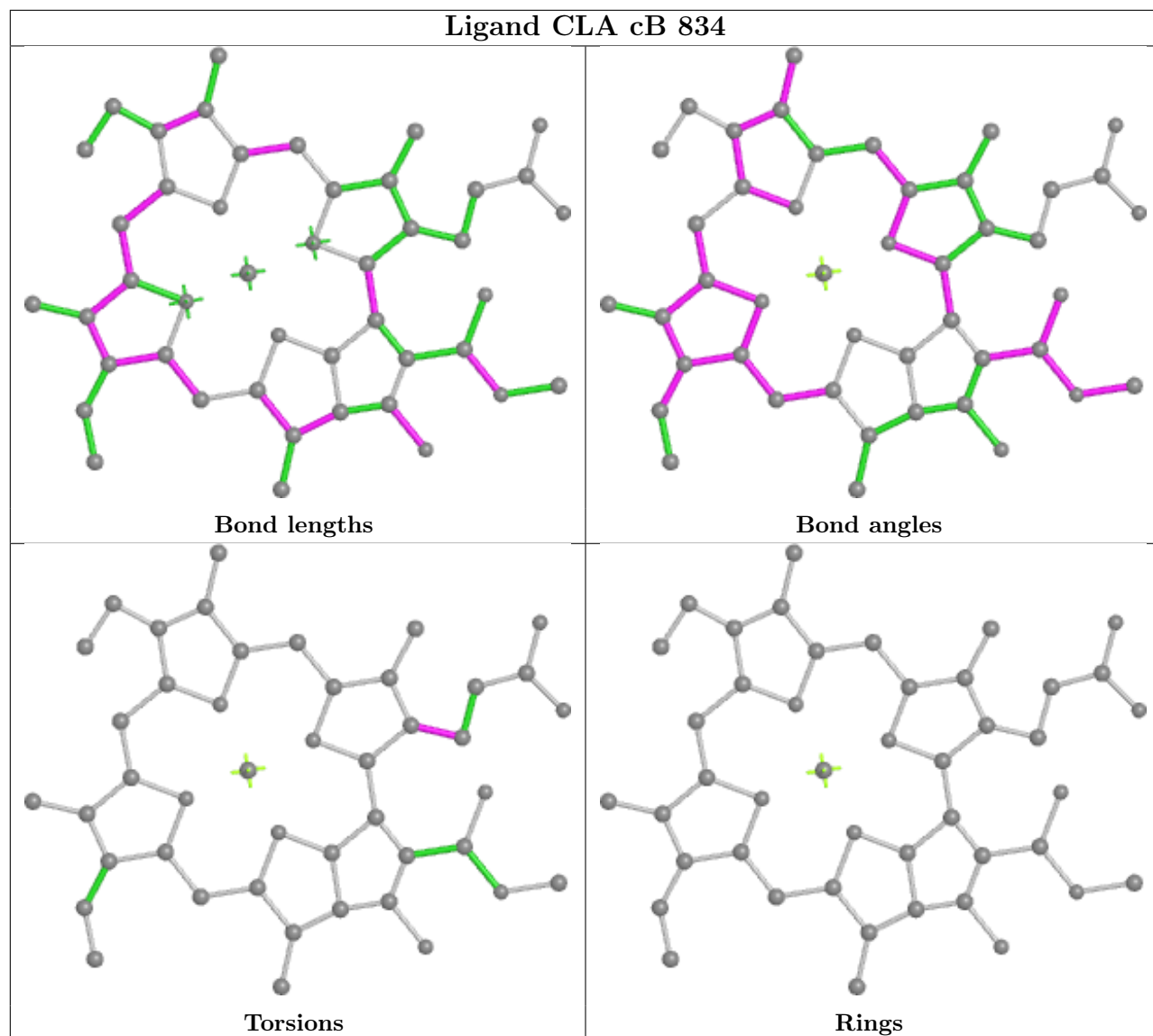
Ligand CLA cB 832



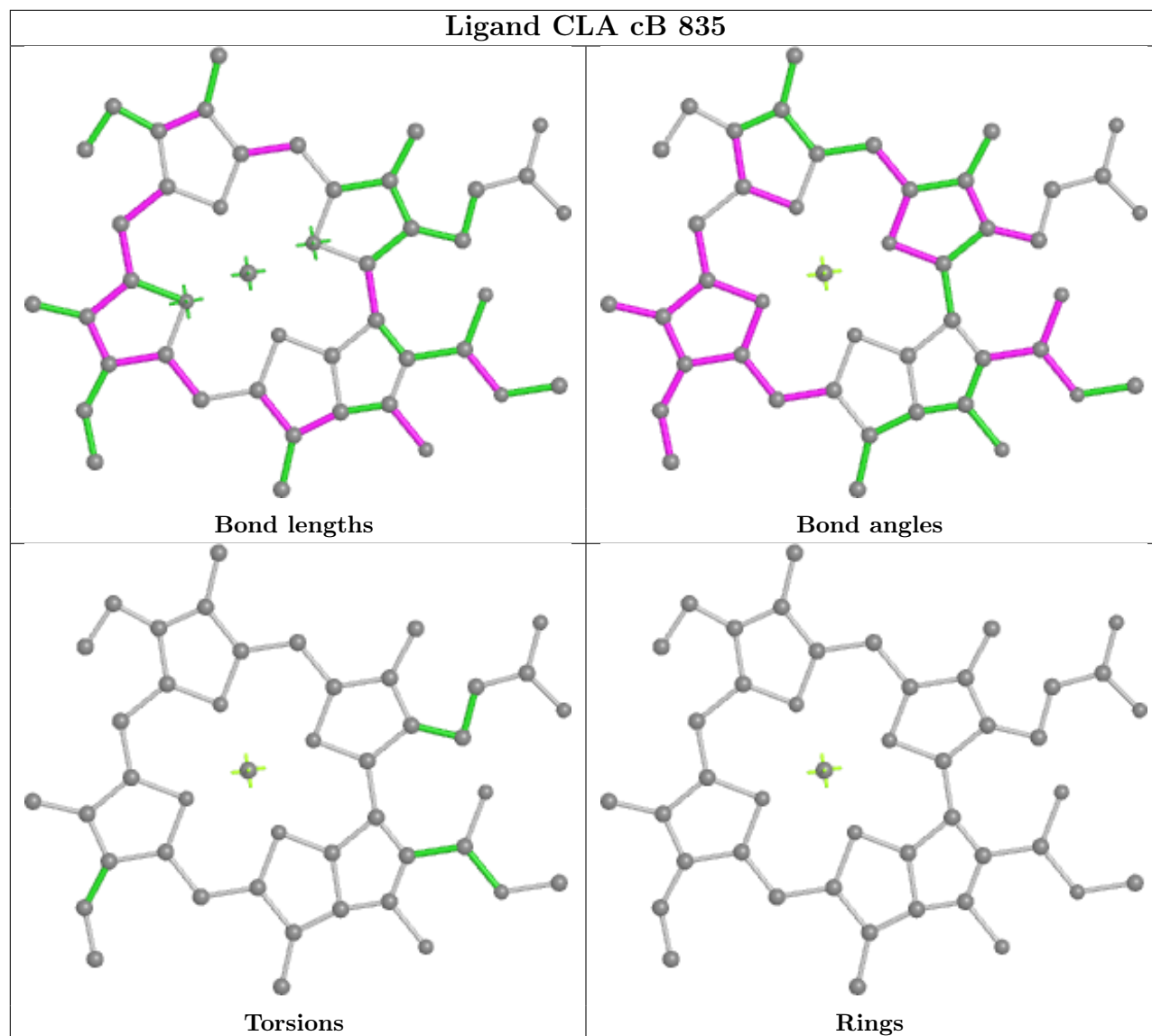
Ligand CLA cB 833

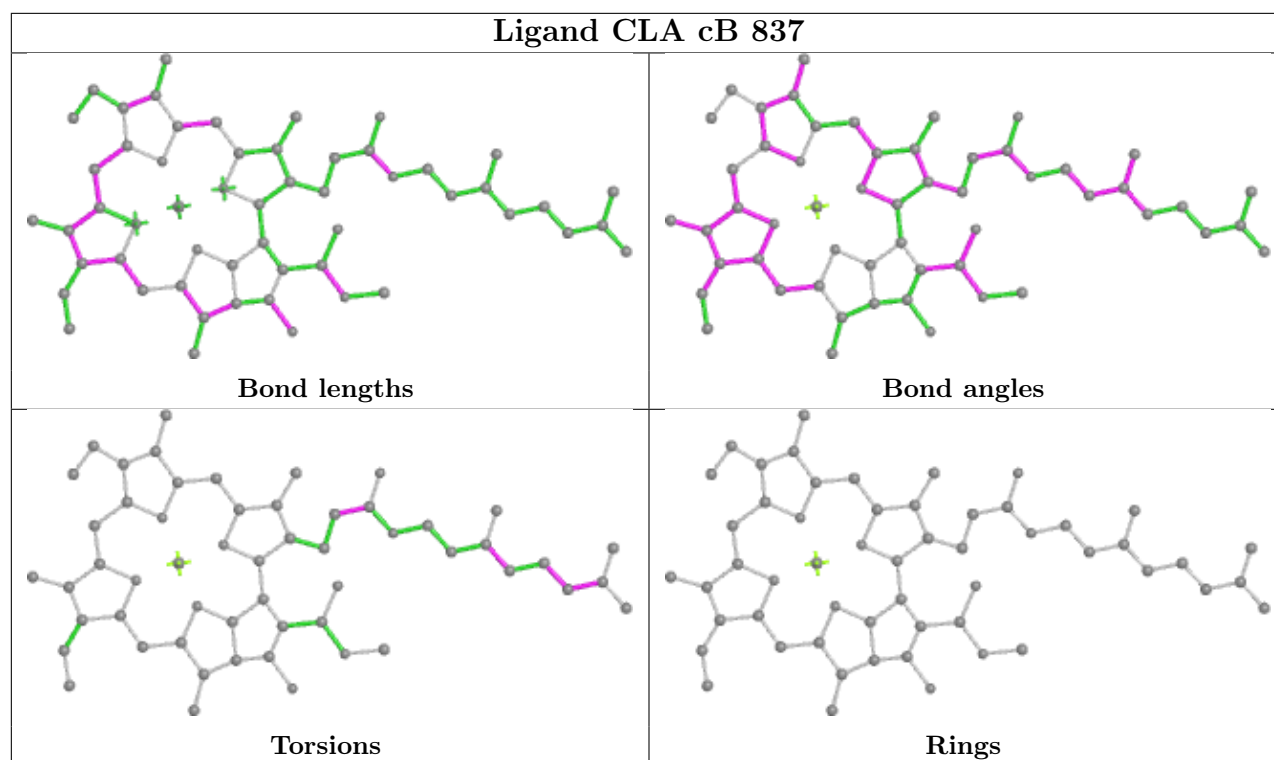
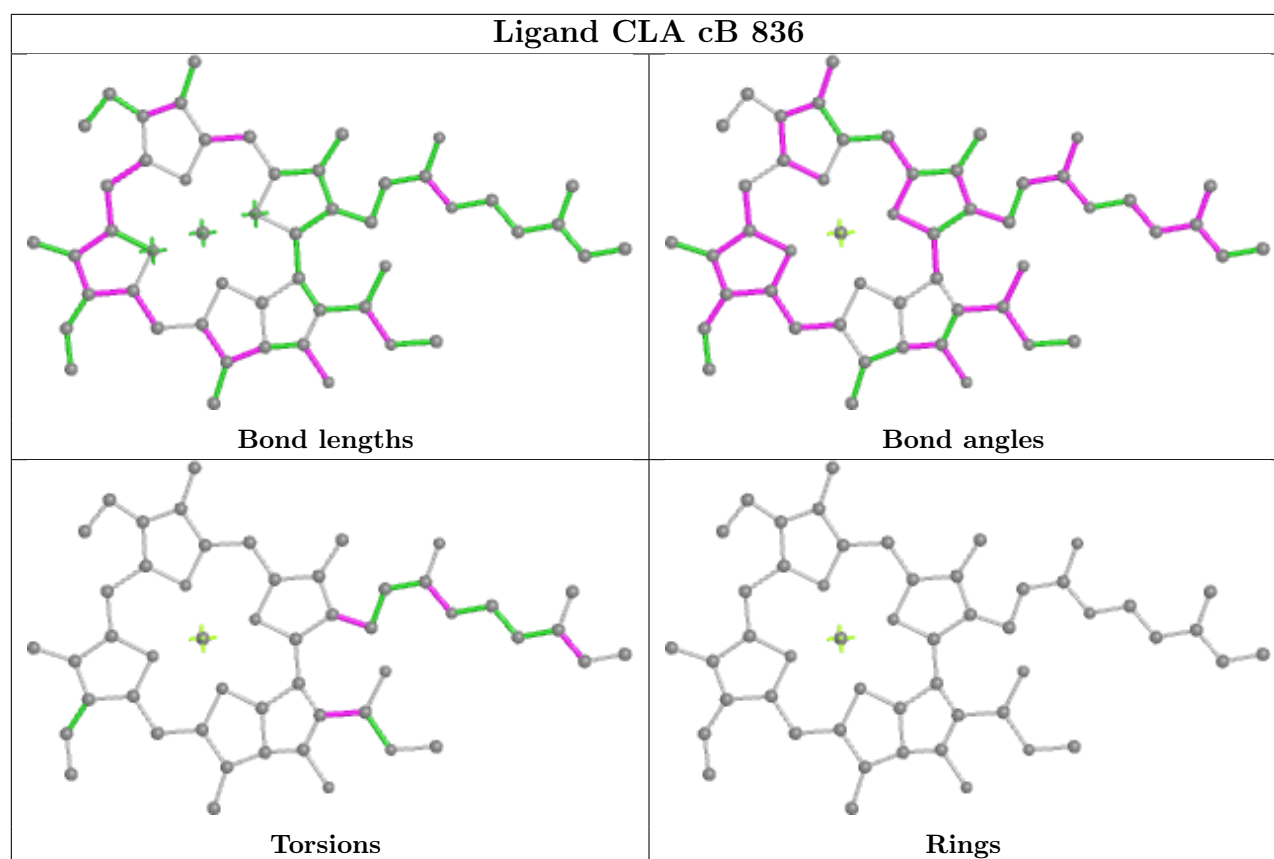


Ligand CLA cB 834

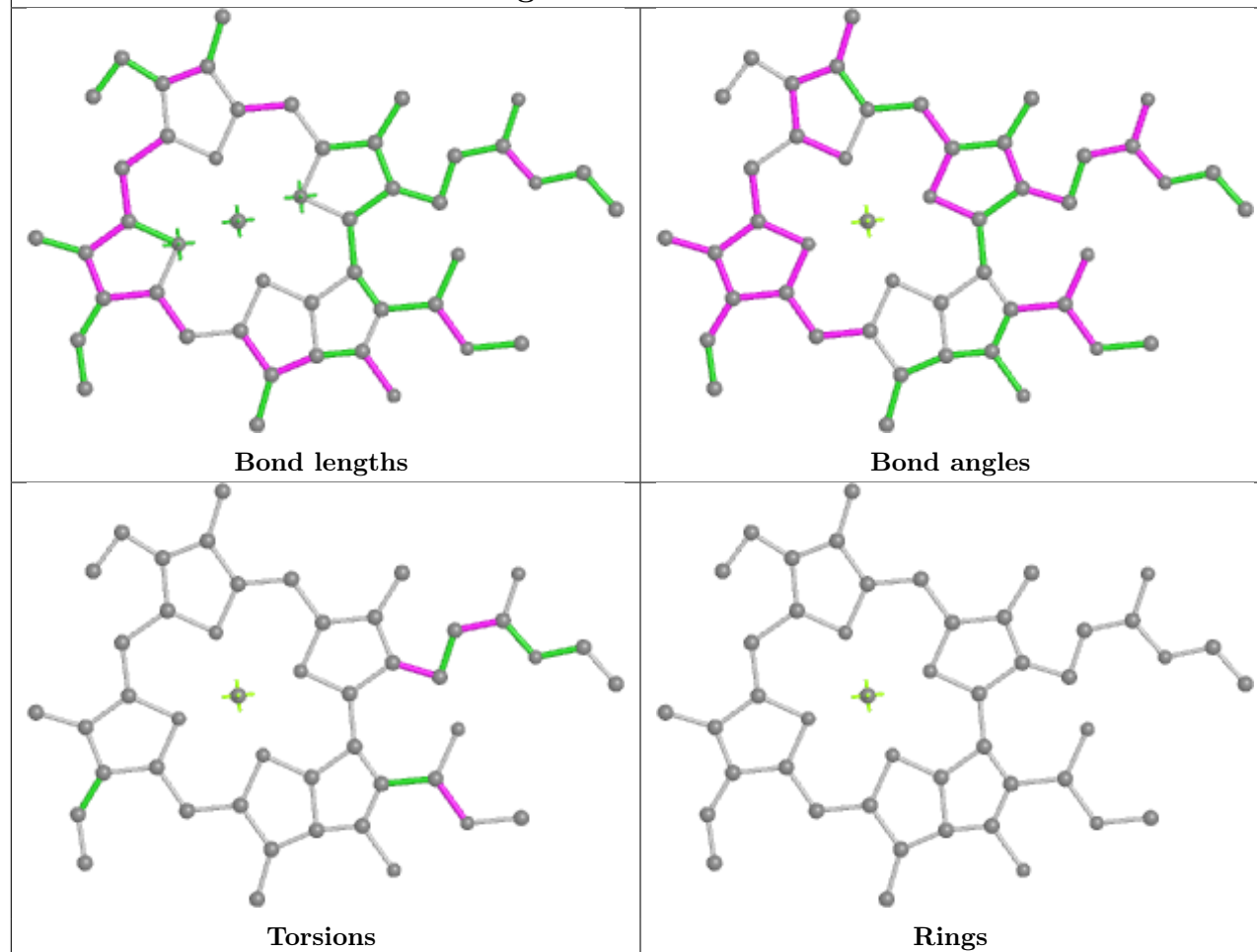


Ligand CLA cB 835

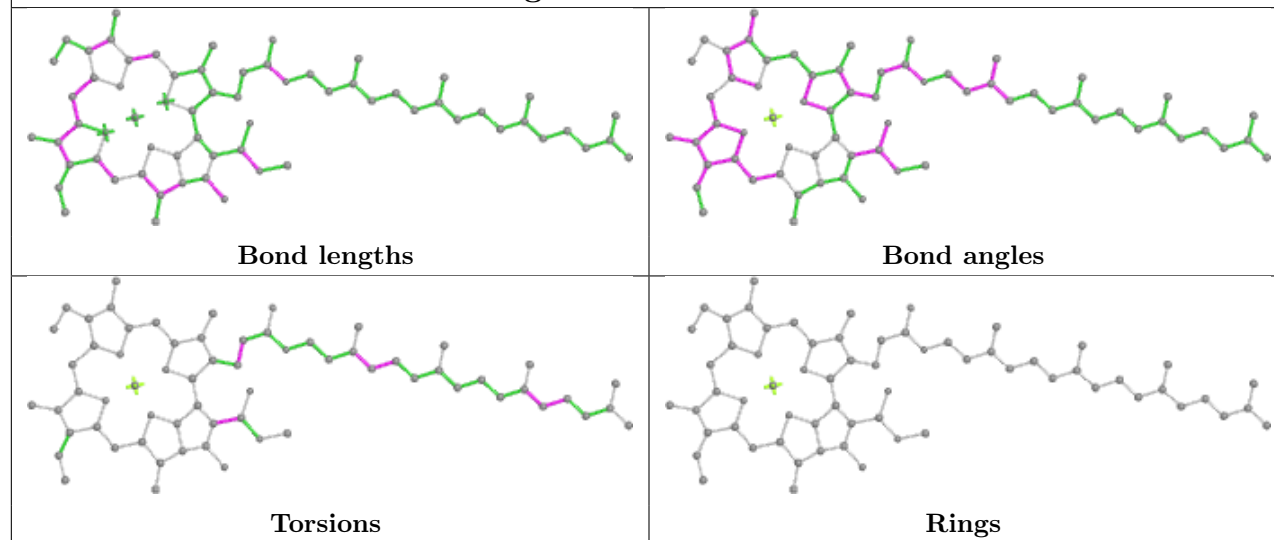


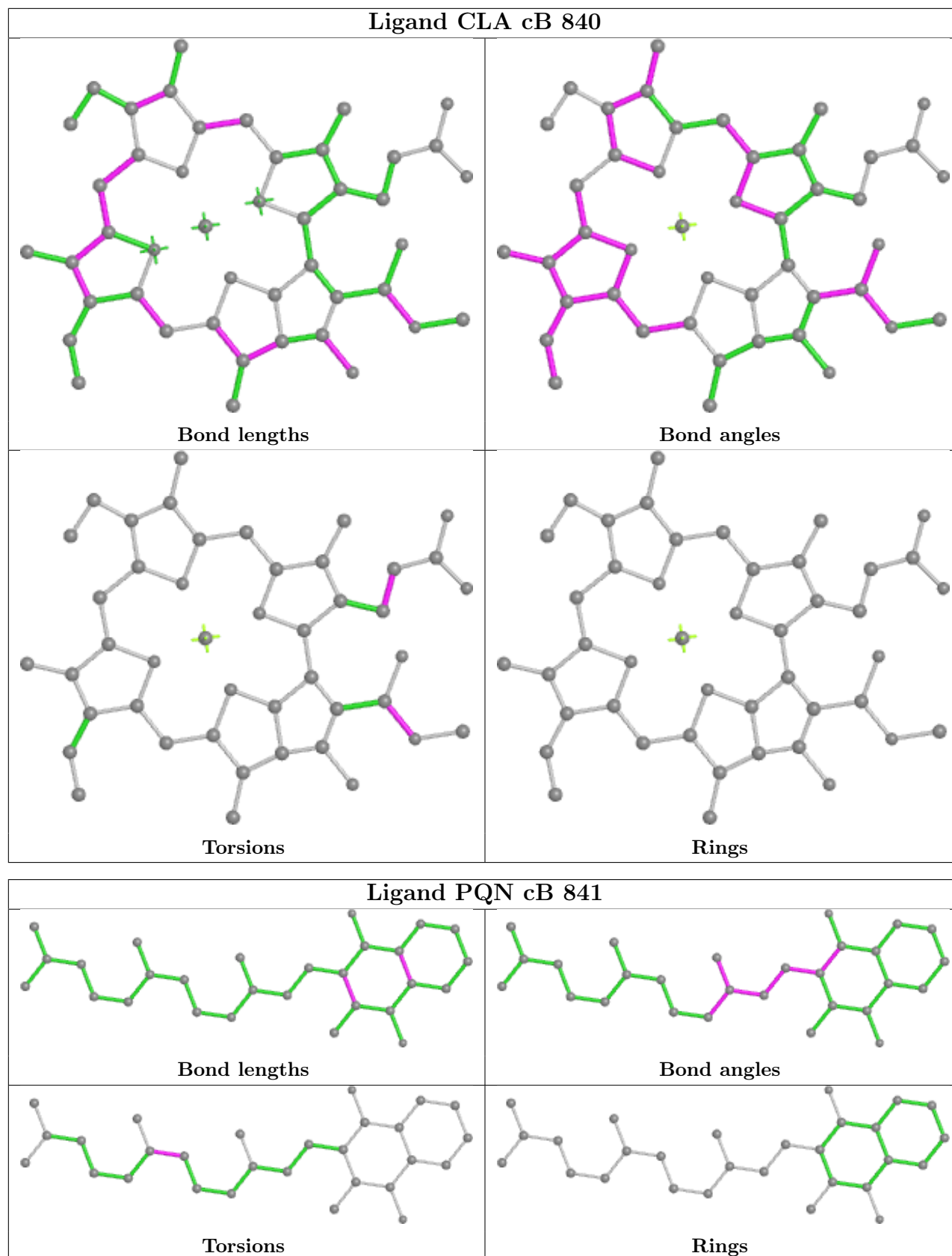


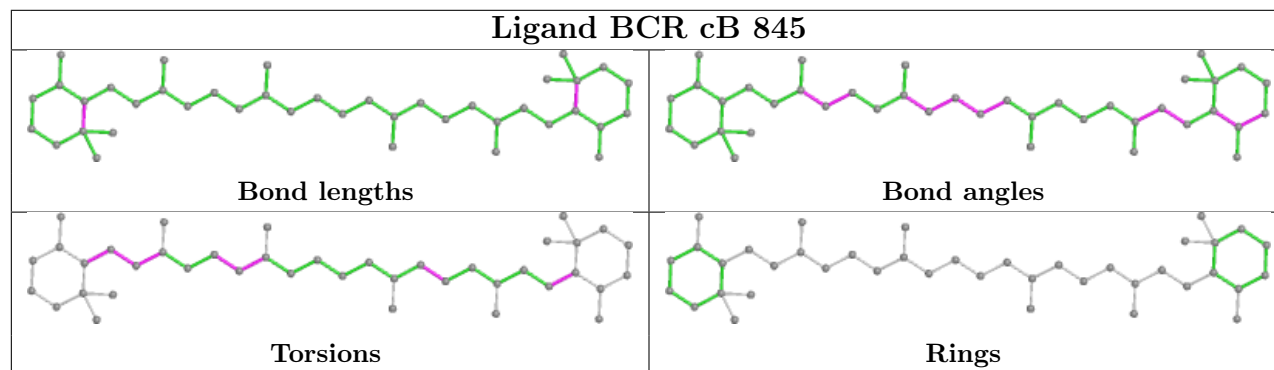
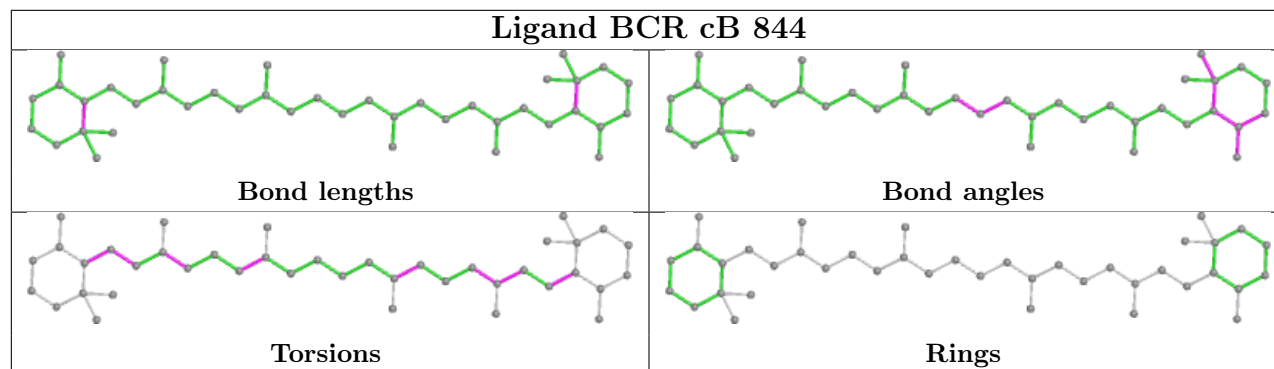
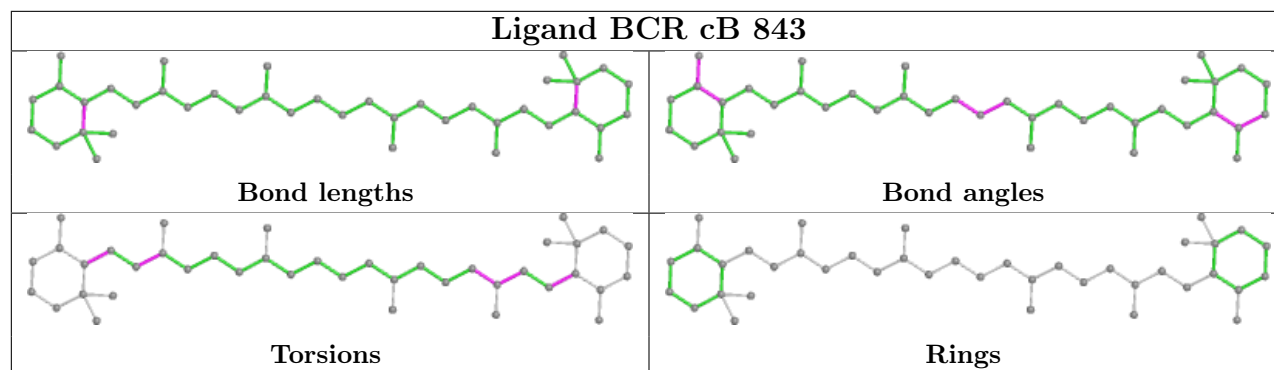
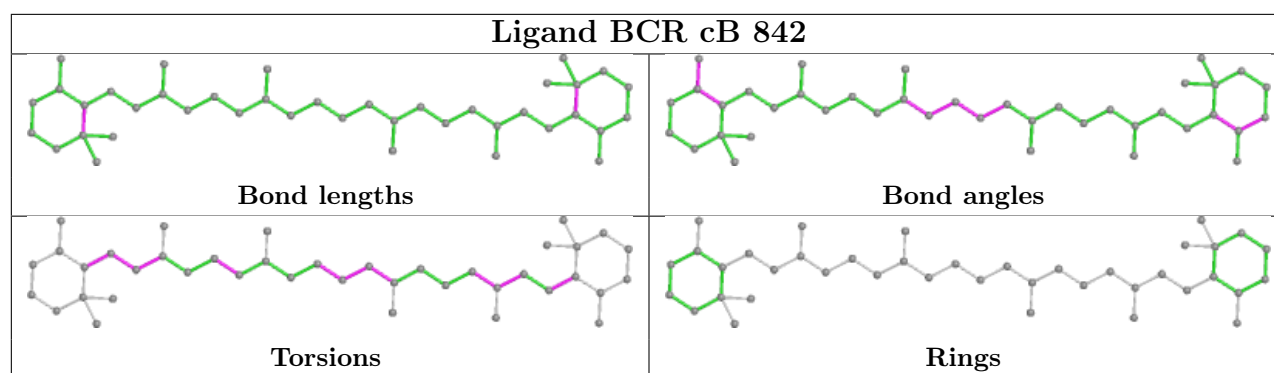
Ligand CLA cB 838

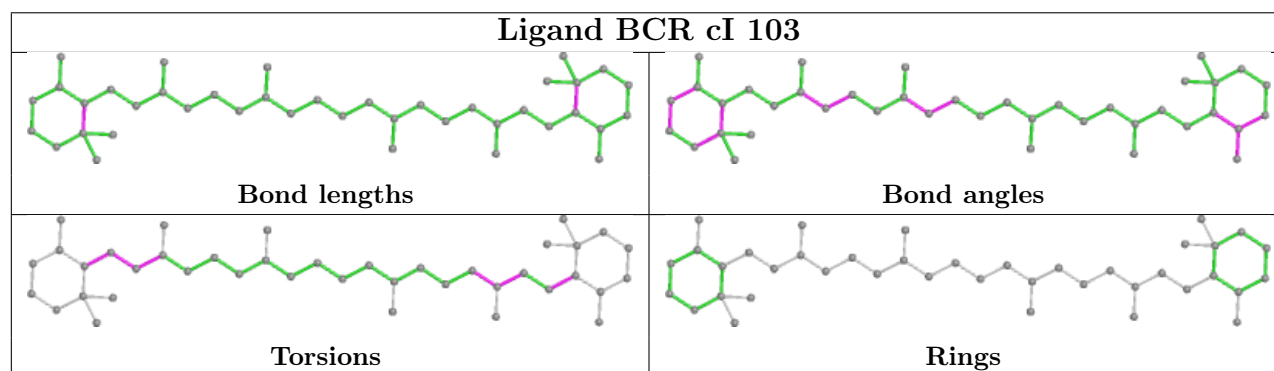
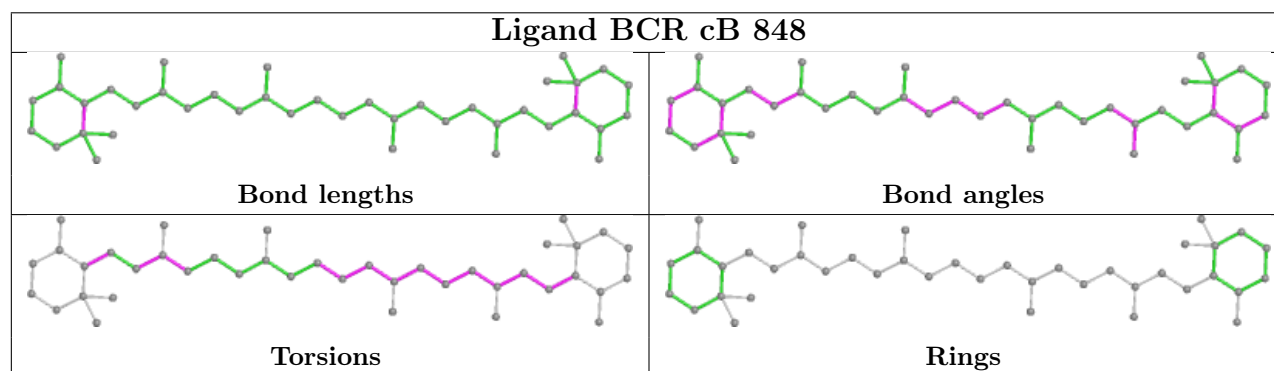
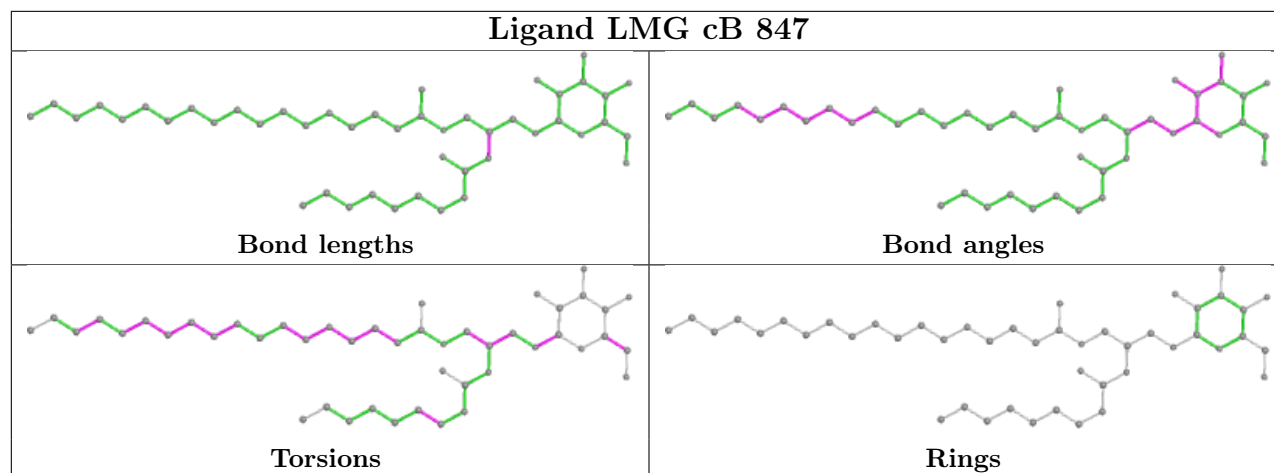
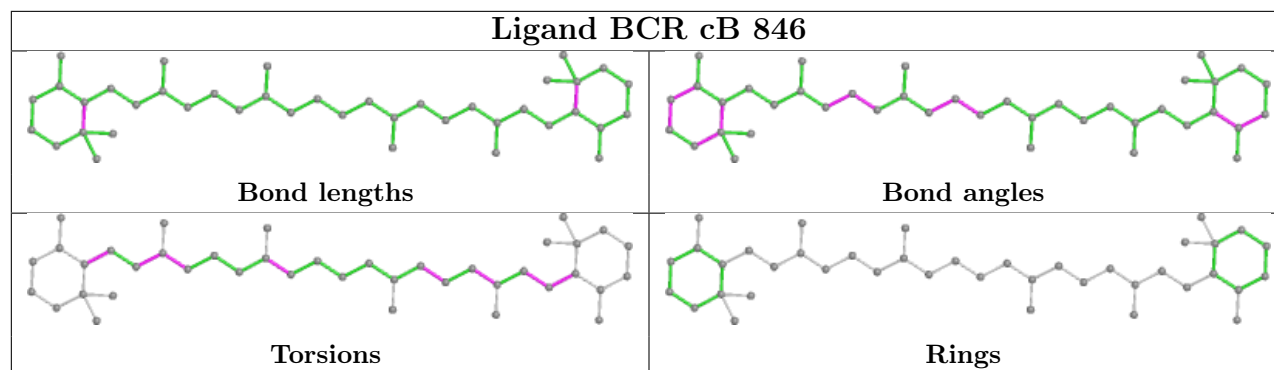


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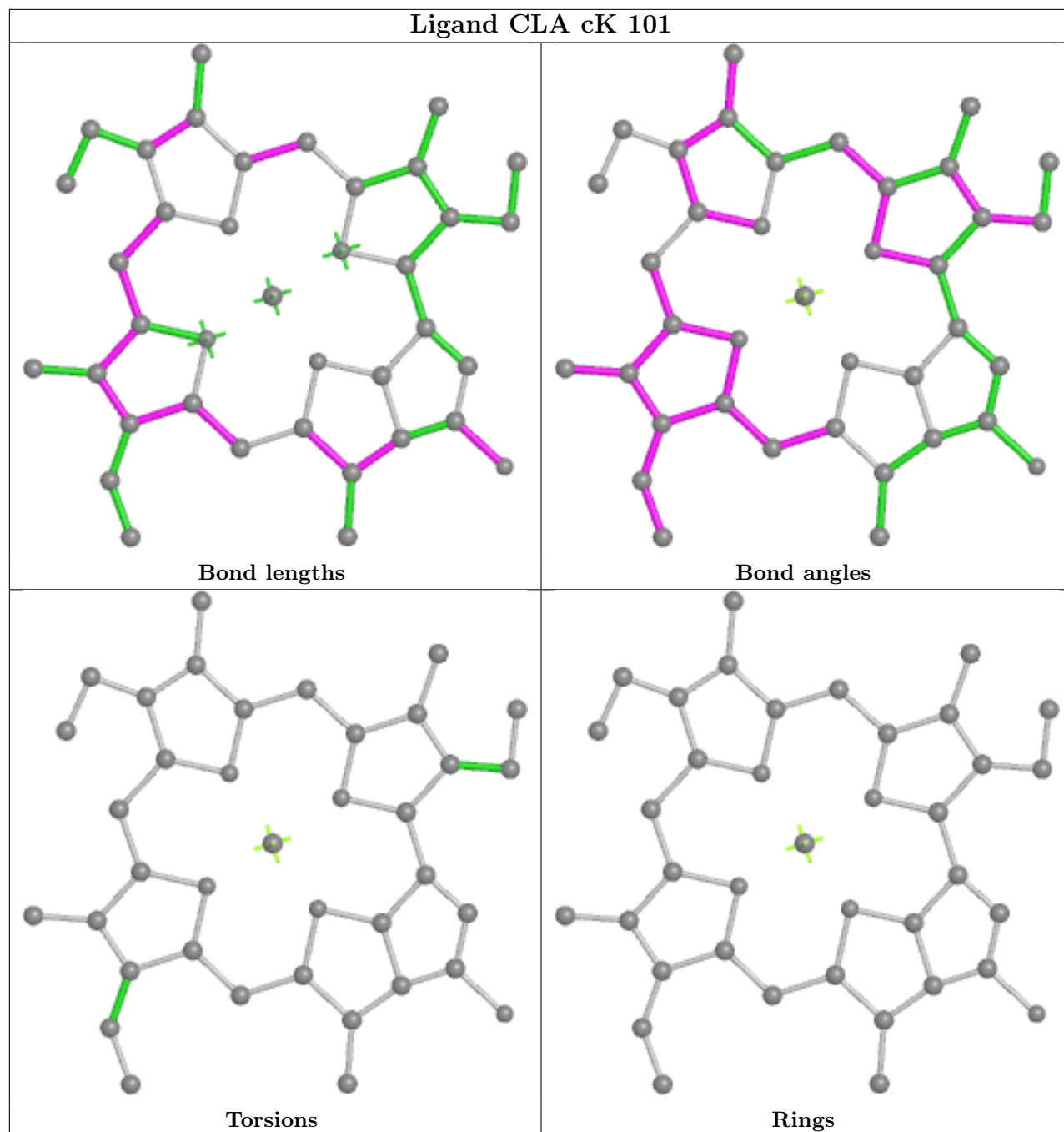




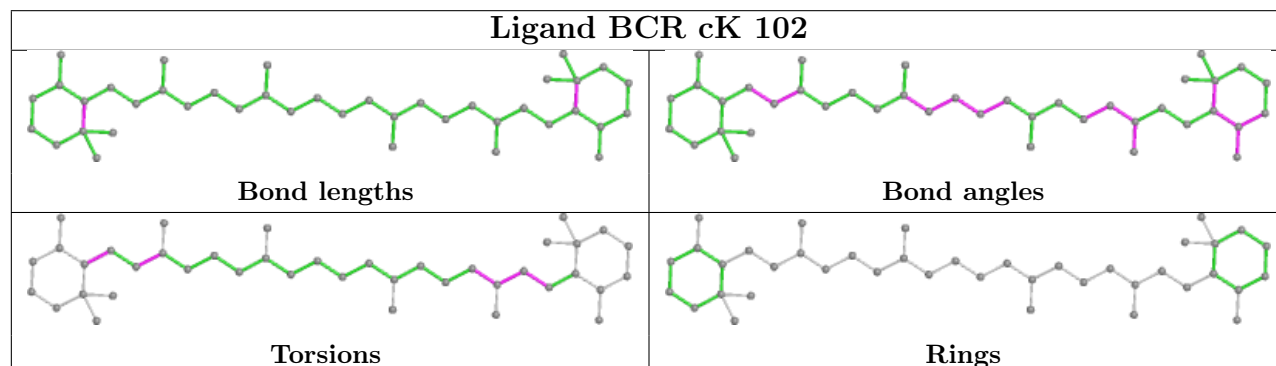


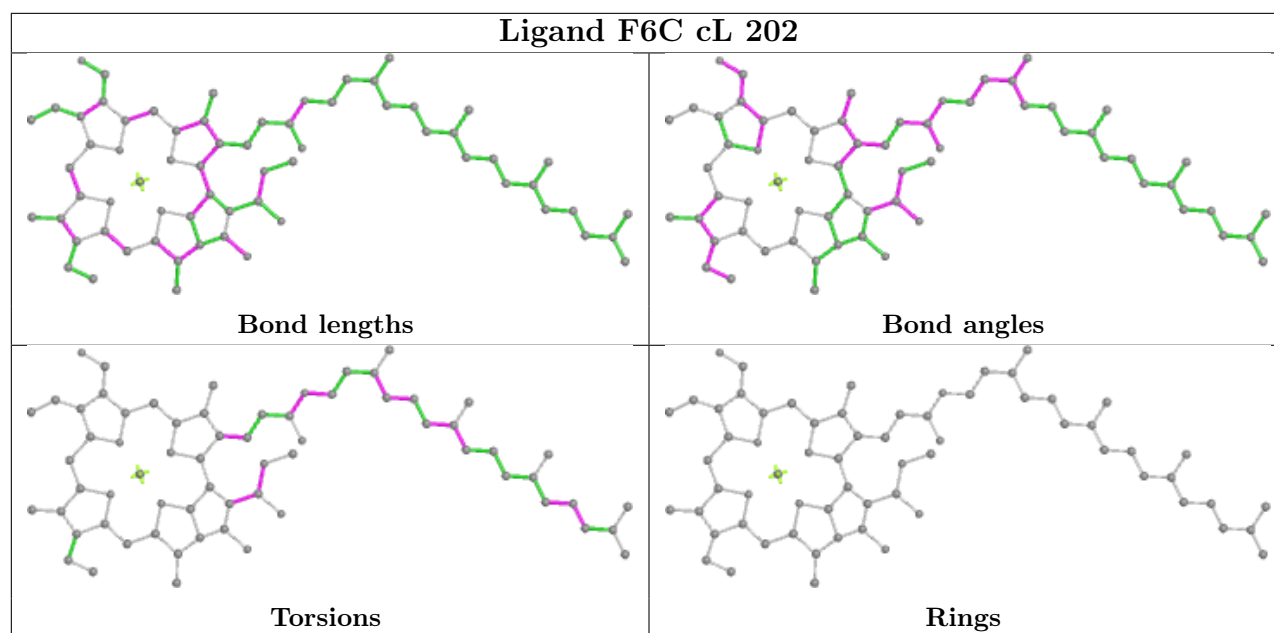
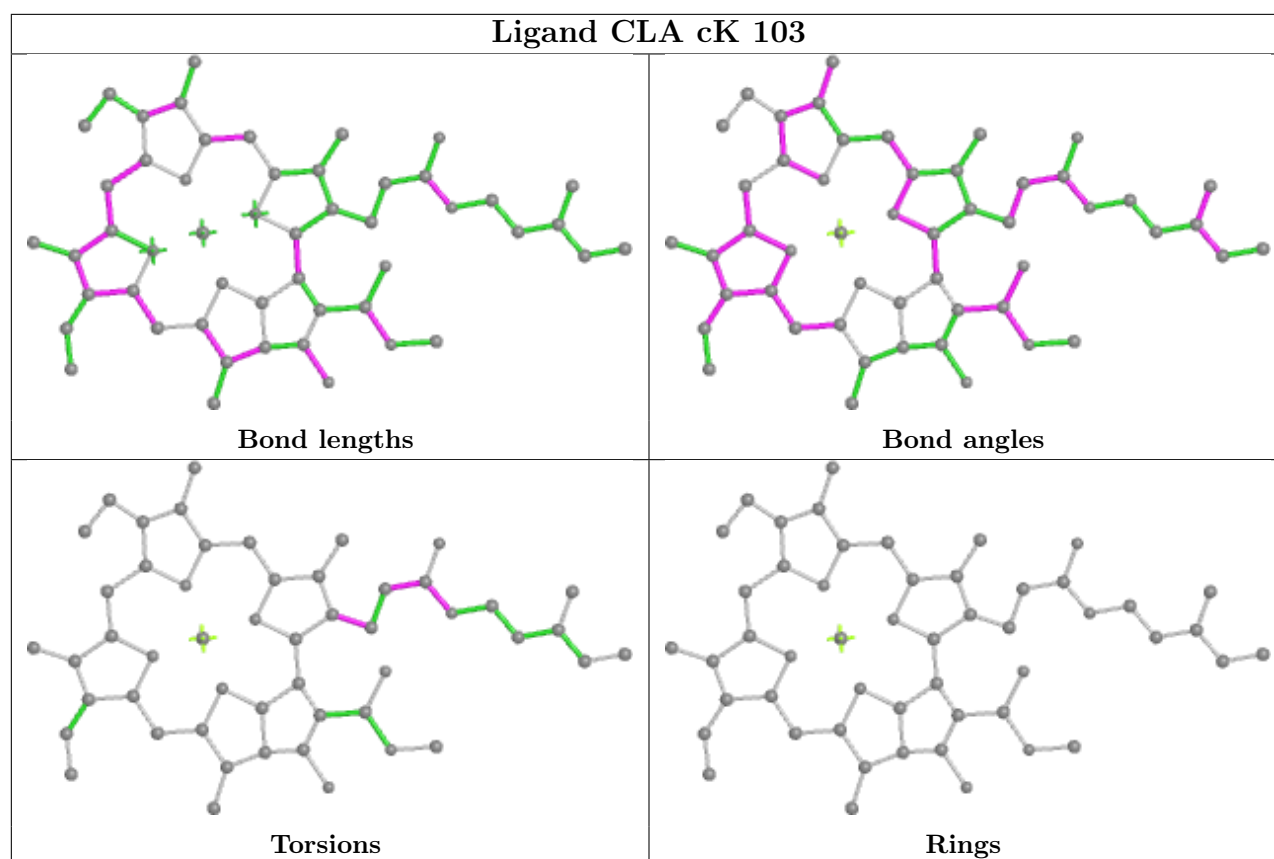


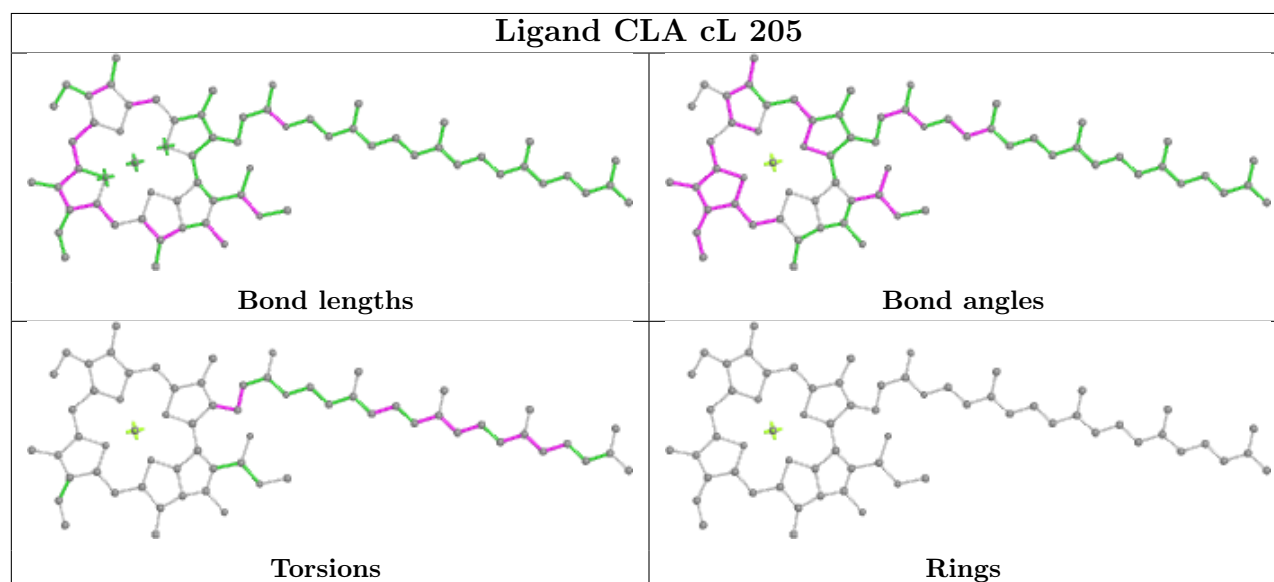
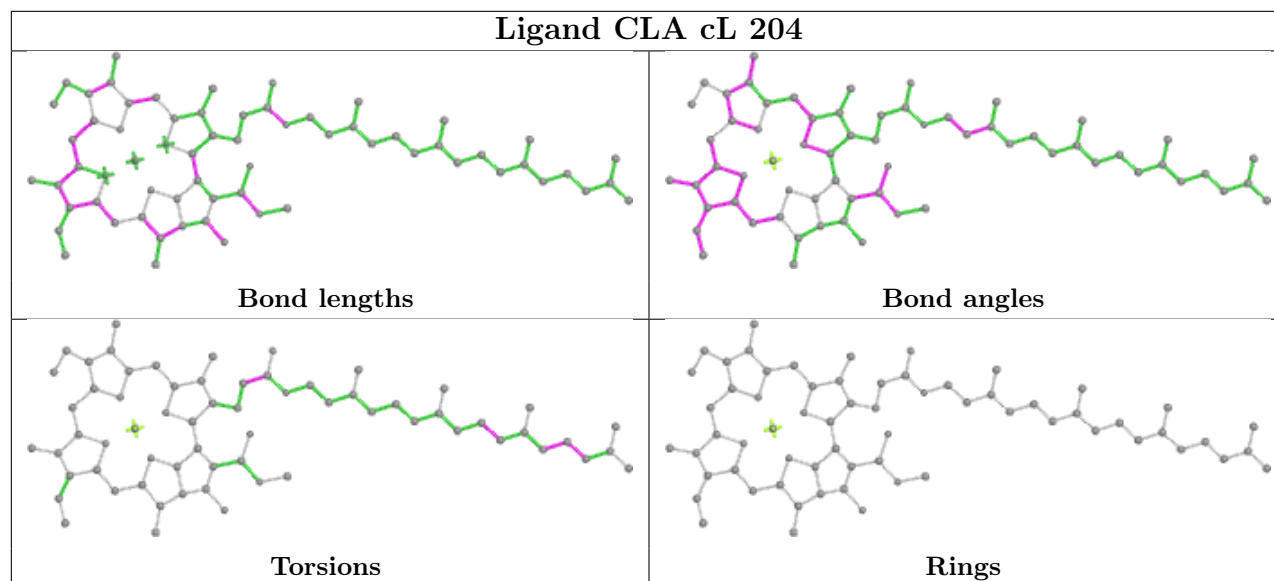
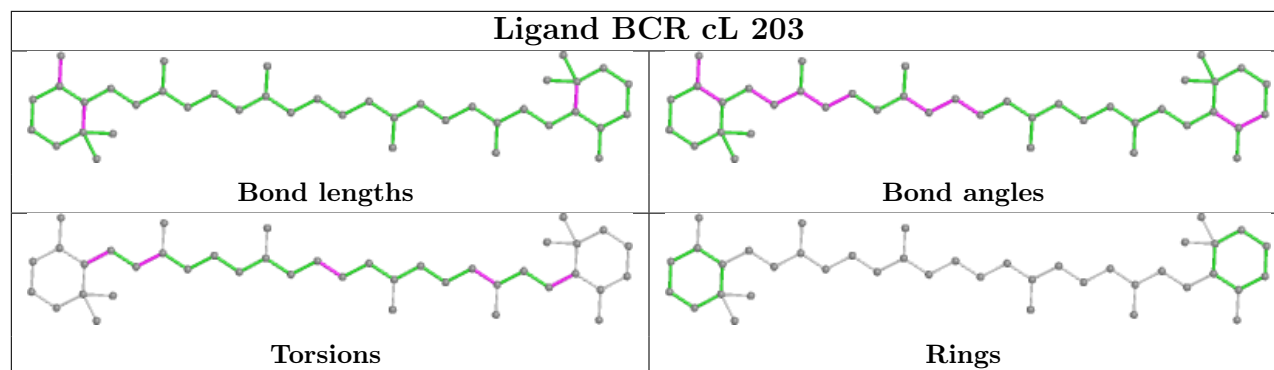
Ligand CLA cK 101

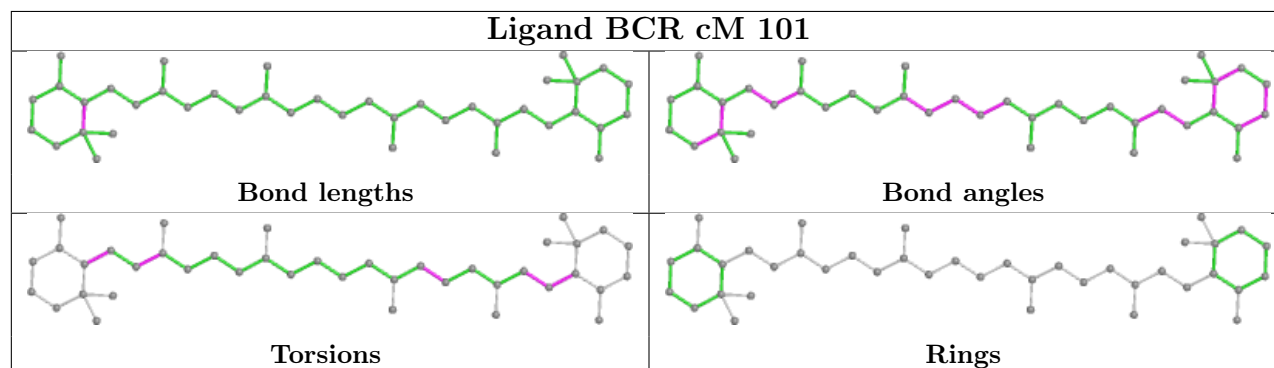
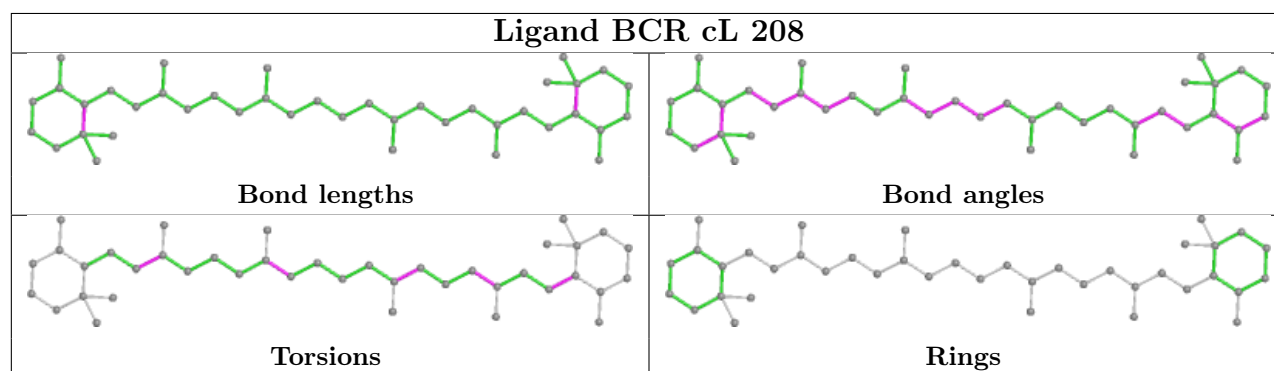
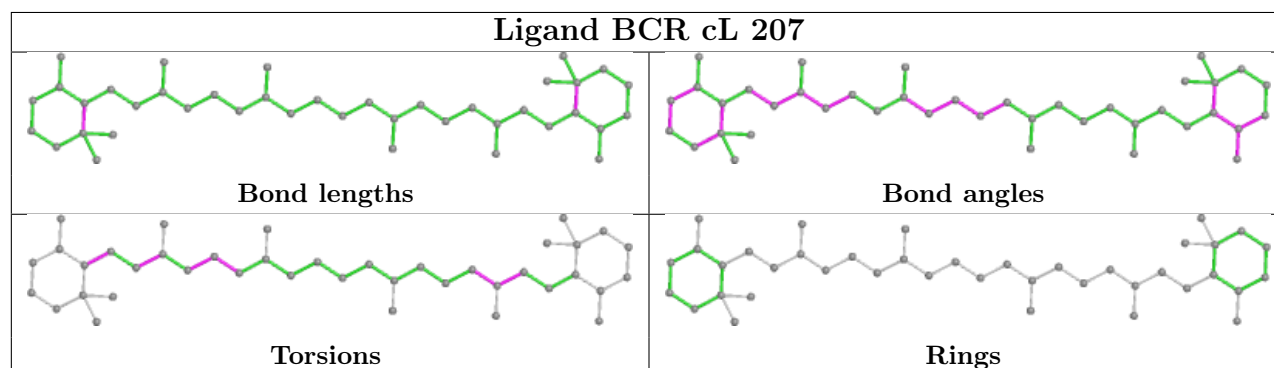
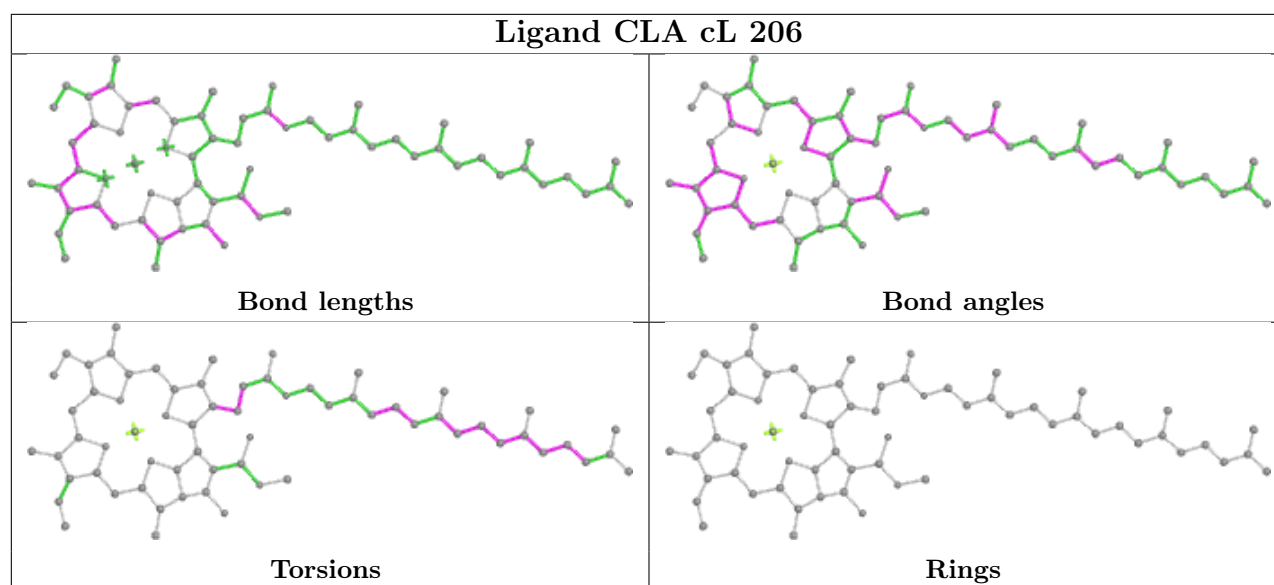


Ligand BCR cK 102









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.