



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jan 6, 2020 – 01:45 PM EST

PDB ID : 6KMW
EMDB ID: : EMD-0726
Title : Structure of PSI from *H. hongdechloris* grown under white light condition
Authors : Kato, K.; Nagao, R.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on : 2019-08-01
Resolution : 2.35 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

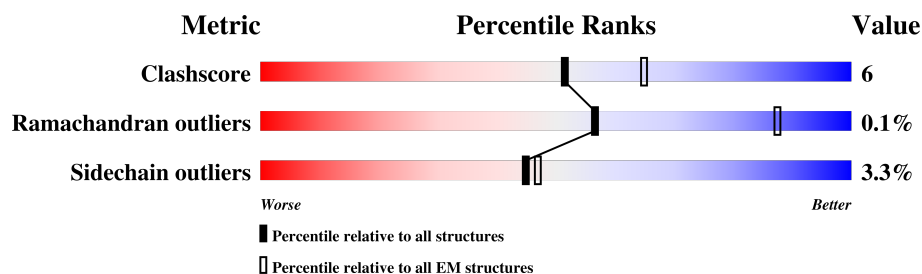
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.35 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	764	91% 6%
1	bA	764	91% 6%
1	cA	764	91% 6%
2	aB	742	97% .
2	bB	742	97% .
2	cB	742	97% .
3	aC	81	98% ..
3	bC	81	98% ..
3	cC	81	98% ..

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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	38	
6	bI	38	
6	cI	38	
7	aL	159	
7	bL	159	
7	cL	159	
8	aM	31	
8	bM	31	
8	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	CLA	aA	802	X	-	-	-
10	CLA	aA	803	X	-	-	-
10	CLA	aA	804	X	-	-	-
10	CLA	aA	805	X	-	-	-
10	CLA	aA	806	X	-	-	-
10	CLA	aA	807	X	-	-	-
10	CLA	aA	808	X	-	-	-
10	CLA	aA	809	X	-	-	-
10	CLA	aA	810	X	-	-	-
10	CLA	aA	811	X	-	-	-
10	CLA	aA	812	X	-	-	-
10	CLA	aA	813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	aA	814	X	-	-	-
10	CLA	aA	815	X	-	-	-
10	CLA	aA	816	X	-	-	-
10	CLA	aA	817	X	-	-	-
10	CLA	aA	818	X	-	-	-
10	CLA	aA	819	X	-	-	-
10	CLA	aA	820	X	-	-	-
10	CLA	aA	821	X	-	-	-
10	CLA	aA	822	X	-	-	-
10	CLA	aA	823	X	-	-	-
10	CLA	aA	824	X	-	-	-
10	CLA	aA	825	X	-	-	-
10	CLA	aA	826	X	-	-	-
10	CLA	aA	827	X	-	-	-
10	CLA	aA	828	X	-	-	-
10	CLA	aA	829	X	-	-	-
10	CLA	aA	830	X	-	-	-
10	CLA	aA	831	X	-	-	-
10	CLA	aA	832	X	-	-	-
10	CLA	aA	833	X	-	-	-
10	CLA	aA	834	X	-	-	-
10	CLA	aA	835	X	-	-	-
10	CLA	aA	836	X	-	-	-
10	CLA	aA	837	X	-	-	-
10	CLA	aA	838	X	-	-	-
10	CLA	aA	839	X	-	-	-
10	CLA	aA	840	X	-	-	-
10	CLA	aA	841	X	-	-	-
10	CLA	aA	842	X	-	-	-
10	CLA	aA	843	X	-	-	-
10	CLA	aA	854	X	-	-	-
10	CLA	aA	856	X	-	-	-
10	CLA	aB	801	X	-	-	-
10	CLA	aB	802	X	-	-	-
10	CLA	aB	803	X	-	-	-
10	CLA	aB	804	X	-	-	-
10	CLA	aB	805	X	-	-	-
10	CLA	aB	806	X	-	-	-
10	CLA	aB	807	X	-	-	-
10	CLA	aB	808	X	-	-	-
10	CLA	aB	809	X	-	-	-
10	CLA	aB	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	aB	811	X	-	-	-
10	CLA	aB	812	X	-	-	-
10	CLA	aB	813	X	-	-	-
10	CLA	aB	814	X	-	-	-
10	CLA	aB	815	X	-	-	-
10	CLA	aB	816	X	-	-	-
10	CLA	aB	817	X	-	-	-
10	CLA	aB	818	X	-	-	-
10	CLA	aB	819	X	-	-	-
10	CLA	aB	820	X	-	-	-
10	CLA	aB	821	X	-	-	-
10	CLA	aB	822	X	-	-	-
10	CLA	aB	823	X	-	-	-
10	CLA	aB	824	X	-	-	-
10	CLA	aB	825	X	-	-	-
10	CLA	aB	826	X	-	-	-
10	CLA	aB	827	X	-	-	-
10	CLA	aB	828	X	-	-	-
10	CLA	aB	829	X	-	-	-
10	CLA	aB	830	X	-	-	-
10	CLA	aB	831	X	-	-	-
10	CLA	aB	832	X	-	-	-
10	CLA	aB	833	X	-	-	-
10	CLA	aB	834	X	-	-	-
10	CLA	aB	835	X	-	-	-
10	CLA	aB	836	X	-	-	-
10	CLA	aB	837	X	-	-	-
10	CLA	aB	838	X	-	-	-
10	CLA	aB	839	X	-	-	-
10	CLA	aB	840	X	-	-	-
10	CLA	aB	841	X	-	-	-
10	CLA	aL	202	X	-	-	-
10	CLA	aL	203	X	-	-	-
10	CLA	aL	204	X	-	-	-
10	CLA	aL	205	X	-	-	-
10	CLA	bA	802	X	-	-	-
10	CLA	bA	803	X	-	-	-
10	CLA	bA	804	X	-	-	-
10	CLA	bA	805	X	-	-	-
10	CLA	bA	806	X	-	-	-
10	CLA	bA	807	X	-	-	-
10	CLA	bA	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	bA	809	X	-	-	-
10	CLA	bA	810	X	-	-	-
10	CLA	bA	811	X	-	-	-
10	CLA	bA	812	X	-	-	-
10	CLA	bA	813	X	-	-	-
10	CLA	bA	814	X	-	-	-
10	CLA	bA	815	X	-	-	-
10	CLA	bA	816	X	-	-	-
10	CLA	bA	817	X	-	-	-
10	CLA	bA	818	X	-	-	-
10	CLA	bA	819	X	-	-	-
10	CLA	bA	820	X	-	-	-
10	CLA	bA	821	X	-	-	-
10	CLA	bA	822	X	-	-	-
10	CLA	bA	823	X	-	-	-
10	CLA	bA	824	X	-	-	-
10	CLA	bA	825	X	-	-	-
10	CLA	bA	826	X	-	-	-
10	CLA	bA	827	X	-	-	-
10	CLA	bA	828	X	-	-	-
10	CLA	bA	829	X	-	-	-
10	CLA	bA	830	X	-	-	-
10	CLA	bA	831	X	-	-	-
10	CLA	bA	832	X	-	-	-
10	CLA	bA	833	X	-	-	-
10	CLA	bA	834	X	-	-	-
10	CLA	bA	835	X	-	-	-
10	CLA	bA	836	X	-	-	-
10	CLA	bA	837	X	-	-	-
10	CLA	bA	838	X	-	-	-
10	CLA	bA	839	X	-	-	-
10	CLA	bA	840	X	-	-	-
10	CLA	bA	841	X	-	-	-
10	CLA	bA	842	X	-	-	-
10	CLA	bA	843	X	-	-	-
10	CLA	bA	854	X	-	-	-
10	CLA	bA	856	X	-	-	-
10	CLA	bB	801	X	-	-	-
10	CLA	bB	802	X	-	-	-
10	CLA	bB	803	X	-	-	-
10	CLA	bB	804	X	-	-	-
10	CLA	bB	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	bB	806	X	-	-	-
10	CLA	bB	807	X	-	-	-
10	CLA	bB	808	X	-	-	-
10	CLA	bB	809	X	-	-	-
10	CLA	bB	810	X	-	-	-
10	CLA	bB	811	X	-	-	-
10	CLA	bB	812	X	-	-	-
10	CLA	bB	813	X	-	-	-
10	CLA	bB	814	X	-	-	-
10	CLA	bB	815	X	-	-	-
10	CLA	bB	816	X	-	-	-
10	CLA	bB	817	X	-	-	-
10	CLA	bB	818	X	-	-	-
10	CLA	bB	819	X	-	-	-
10	CLA	bB	820	X	-	-	-
10	CLA	bB	821	X	-	-	-
10	CLA	bB	822	X	-	-	-
10	CLA	bB	823	X	-	-	-
10	CLA	bB	824	X	-	-	-
10	CLA	bB	825	X	-	-	-
10	CLA	bB	826	X	-	-	-
10	CLA	bB	827	X	-	-	-
10	CLA	bB	828	X	-	-	-
10	CLA	bB	829	X	-	-	-
10	CLA	bB	830	X	-	-	-
10	CLA	bB	831	X	-	-	-
10	CLA	bB	832	X	-	-	-
10	CLA	bB	833	X	-	-	-
10	CLA	bB	834	X	-	-	-
10	CLA	bB	835	X	-	-	-
10	CLA	bB	836	X	-	-	-
10	CLA	bB	837	X	-	-	-
10	CLA	bB	838	X	-	-	-
10	CLA	bB	839	X	-	-	-
10	CLA	bB	840	X	-	-	-
10	CLA	bB	841	X	-	-	-
10	CLA	bL	202	X	-	-	-
10	CLA	bL	203	X	-	-	-
10	CLA	bL	204	X	-	-	-
10	CLA	bL	205	X	-	-	-
10	CLA	cA	802	X	-	-	-
10	CLA	cA	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	cA	804	X	-	-	-
10	CLA	cA	805	X	-	-	-
10	CLA	cA	806	X	-	-	-
10	CLA	cA	807	X	-	-	-
10	CLA	cA	808	X	-	-	-
10	CLA	cA	809	X	-	-	-
10	CLA	cA	810	X	-	-	-
10	CLA	cA	811	X	-	-	-
10	CLA	cA	812	X	-	-	-
10	CLA	cA	813	X	-	-	-
10	CLA	cA	814	X	-	-	-
10	CLA	cA	815	X	-	-	-
10	CLA	cA	816	X	-	-	-
10	CLA	cA	817	X	-	-	-
10	CLA	cA	818	X	-	-	-
10	CLA	cA	819	X	-	-	-
10	CLA	cA	820	X	-	-	-
10	CLA	cA	821	X	-	-	-
10	CLA	cA	822	X	-	-	-
10	CLA	cA	823	X	-	-	-
10	CLA	cA	824	X	-	-	-
10	CLA	cA	825	X	-	-	-
10	CLA	cA	826	X	-	-	-
10	CLA	cA	827	X	-	-	-
10	CLA	cA	828	X	-	-	-
10	CLA	cA	829	X	-	-	-
10	CLA	cA	830	X	-	-	-
10	CLA	cA	831	X	-	-	-
10	CLA	cA	832	X	-	-	-
10	CLA	cA	833	X	-	-	-
10	CLA	cA	834	X	-	-	-
10	CLA	cA	835	X	-	-	-
10	CLA	cA	836	X	-	-	-
10	CLA	cA	837	X	-	-	-
10	CLA	cA	838	X	-	-	-
10	CLA	cA	839	X	-	-	-
10	CLA	cA	840	X	-	-	-
10	CLA	cA	841	X	-	-	-
10	CLA	cA	842	X	-	-	-
10	CLA	cA	843	X	-	-	-
10	CLA	cA	854	X	-	-	-
10	CLA	cA	856	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	cB	801	X	-	-	-
10	CLA	cB	802	X	-	-	-
10	CLA	cB	803	X	-	-	-
10	CLA	cB	804	X	-	-	-
10	CLA	cB	805	X	-	-	-
10	CLA	cB	806	X	-	-	-
10	CLA	cB	807	X	-	-	-
10	CLA	cB	808	X	-	-	-
10	CLA	cB	809	X	-	-	-
10	CLA	cB	810	X	-	-	-
10	CLA	cB	811	X	-	-	-
10	CLA	cB	812	X	-	-	-
10	CLA	cB	813	X	-	-	-
10	CLA	cB	814	X	-	-	-
10	CLA	cB	815	X	-	-	-
10	CLA	cB	816	X	-	-	-
10	CLA	cB	817	X	-	-	-
10	CLA	cB	818	X	-	-	-
10	CLA	cB	819	X	-	-	-
10	CLA	cB	820	X	-	-	-
10	CLA	cB	821	X	-	-	-
10	CLA	cB	822	X	-	-	-
10	CLA	cB	823	X	-	-	-
10	CLA	cB	824	X	-	-	-
10	CLA	cB	825	X	-	-	-
10	CLA	cB	826	X	-	-	-
10	CLA	cB	827	X	-	-	-
10	CLA	cB	828	X	-	-	-
10	CLA	cB	829	X	-	-	-
10	CLA	cB	830	X	-	-	-
10	CLA	cB	831	X	-	-	-
10	CLA	cB	832	X	-	-	-
10	CLA	cB	833	X	-	-	-
10	CLA	cB	834	X	-	-	-
10	CLA	cB	835	X	-	-	-
10	CLA	cB	836	X	-	-	-
10	CLA	cB	837	X	-	-	-
10	CLA	cB	838	X	-	-	-
10	CLA	cB	839	X	-	-	-
10	CLA	cB	840	X	-	-	-
10	CLA	cB	841	X	-	-	-
10	CLA	cL	202	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	cL	203	X	-	-	-
10	CLA	cL	204	X	-	-	-
10	CLA	cL	205	X	-	-	-
9	CL0	aA	801	X	-	-	-
9	CL0	bA	801	X	-	-	-
9	CL0	cA	801	X	-	-	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 64083 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	721	Total	C	N	O	S	0	0
			5629	3692	953	958	26		
1	bA	721	Total	C	N	O	S	0	0
			5629	3692	953	958	26		
1	cA	721	Total	C	N	O	S	0	0
			5629	3692	953	958	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	740	Total	C	N	O	S	0	0
			5884	3866	990	1005	23		
2	bB	740	Total	C	N	O	S	0	0
			5884	3866	990	1005	23		
2	cB	740	Total	C	N	O	S	0	0
			5884	3866	990	1005	23		

- 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	38	Total	C	N	O	S	0	0
			305	210	41	51	3		
6	bI	38	Total	C	N	O	S	0	0
			305	210	41	51	3		
6	cI	38	Total	C	N	O	S	0	0
			305	210	41	51	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aL	144	Total	C	N	O	S	0	0
			1065	694	173	192	6		
7	bL	144	Total	C	N	O	S	0	0
			1065	694	173	192	6		
7	cL	144	Total	C	N	O	S	0	0
			1065	694	173	192	6		

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

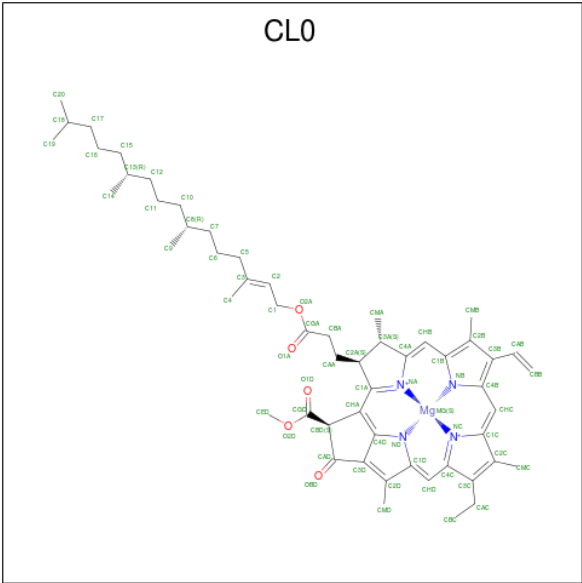
Mol	Chain	Residues	Atoms					AltConf	Trace
8	aM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		
8	bM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		

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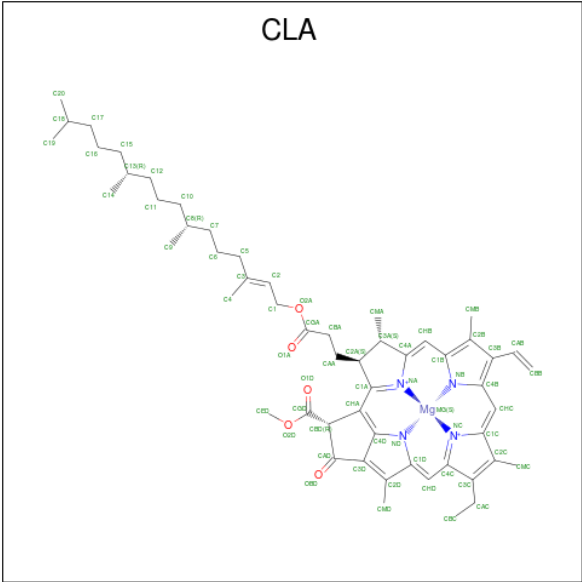
Mol	Chain	Residues	Atoms					AltConf	Trace
8	cM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		

- Molecule 9 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 10 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	

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Mol	Chain	Residues	Atoms					AltConf
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	

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Mol	Chain	Residues	Atoms					AltConf
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	aL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	aL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	aL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	aL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	

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Mol	Chain	Residues	Atoms					AltConf
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	

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Mol	Chain	Residues	Atoms					AltConf
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	bL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	bL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	bL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	bL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	

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Mol	Chain	Residues	Atoms					AltConf
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cA	1	Total	C	Mg	N	O	0
			2491	2053	44	176	218	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	

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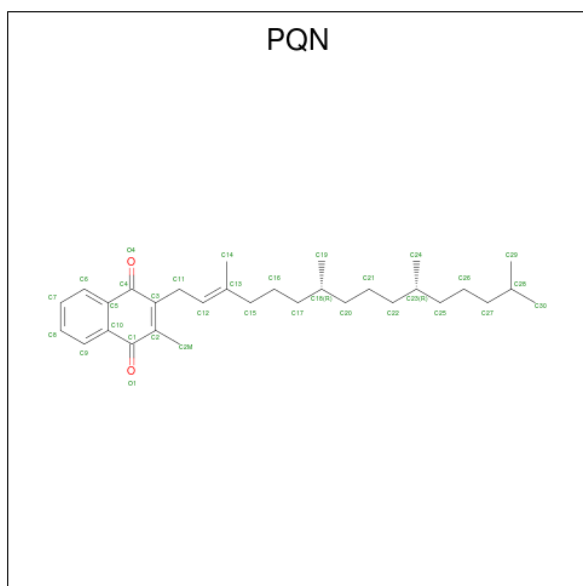
Mol	Chain	Residues	Atoms					AltConf
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cB	1	Total	C	Mg	N	O	0
			2357	1947	41	164	205	
10	cL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	cL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	
10	cL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	

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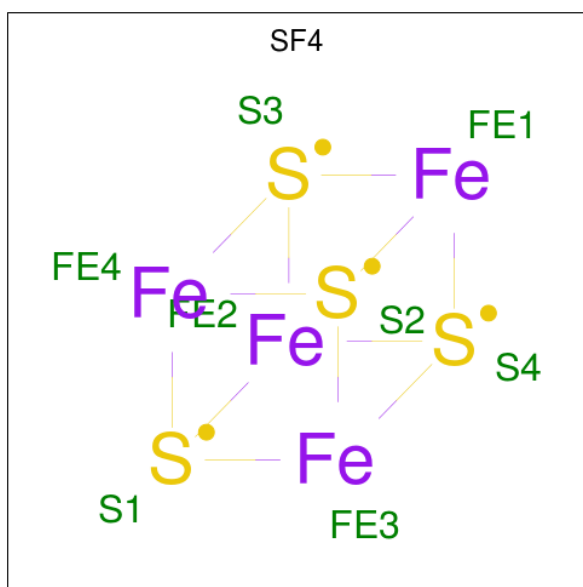
Mol	Chain	Residues	Atoms					AltConf
10	cL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	

- Molecule 11 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



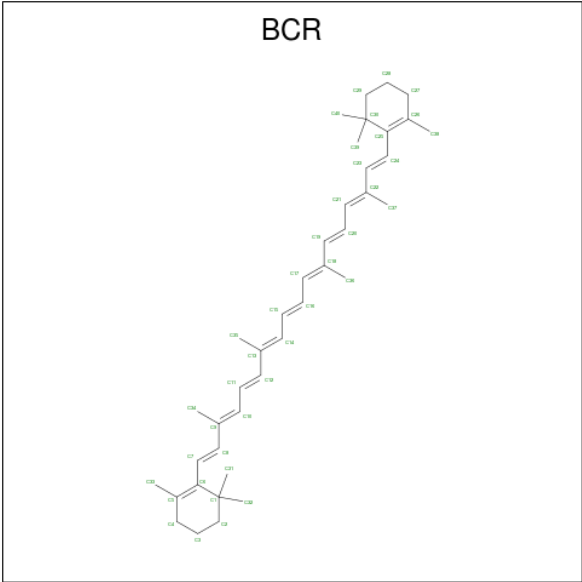
Mol	Chain	Residues	Atoms			AltConf
11	aA	1	Total	C	O	0
			33	31	2	
11	aB	1	Total	C	O	0
			33	31	2	
11	bA	1	Total	C	O	0
			33	31	2	
11	bB	1	Total	C	O	0
			33	31	2	
11	cA	1	Total	C	O	0
			33	31	2	
11	cB	1	Total	C	O	0
			33	31	2	

- Molecule 12 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 13 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
13	aA	1	Total	C	0
			240	240	
13	aA	1	Total	C	0
			240	240	
13	aA	1	Total	C	0
			240	240	
13	aA	1	Total	C	0
			240	240	
13	aA	1	Total	C	0
			240	240	
13	aA	1	Total	C	0
			240	240	
13	aB	1	Total	C	0
			240	240	
13	aB	1	Total	C	0
			240	240	
13	aB	1	Total	C	0
			240	240	
13	aB	1	Total	C	0
			240	240	
13	aB	1	Total	C	0
			240	240	
13	aB	1	Total	C	0
			240	240	
13	aI	1	Total	C	0
			80	80	
13	aI	1	Total	C	0
			80	80	

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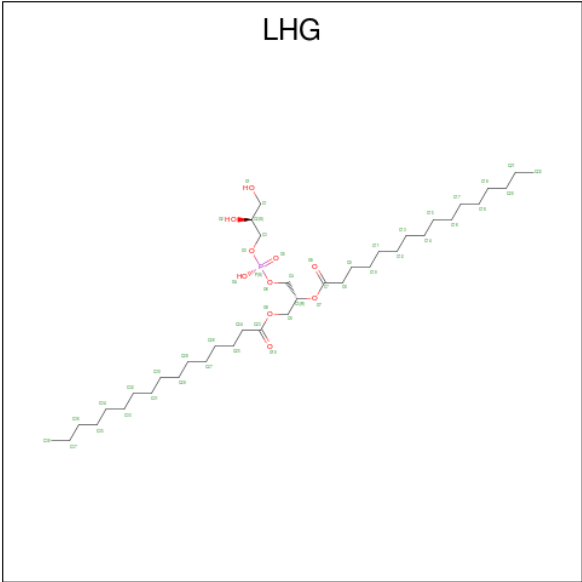
Mol	Chain	Residues	Atoms		AltConf
13	aL	1	Total 80	C 80	0
13	aL	1	Total 80	C 80	0
13	aM	1	Total 40	C 40	0
13	bA	1	Total 240	C 240	0
13	bA	1	Total 240	C 240	0
13	bA	1	Total 240	C 240	0
13	bA	1	Total 240	C 240	0
13	bA	1	Total 240	C 240	0
13	bA	1	Total 240	C 240	0
13	bB	1	Total 240	C 240	0
13	bB	1	Total 240	C 240	0
13	bB	1	Total 240	C 240	0
13	bB	1	Total 240	C 240	0
13	bB	1	Total 240	C 240	0
13	bB	1	Total 240	C 240	0
13	bB	1	Total 240	C 240	0
13	bI	1	Total 80	C 80	0
13	bI	1	Total 80	C 80	0
13	bL	1	Total 80	C 80	0
13	bL	1	Total 80	C 80	0
13	bM	1	Total 40	C 40	0
13	cA	1	Total 240	C 240	0

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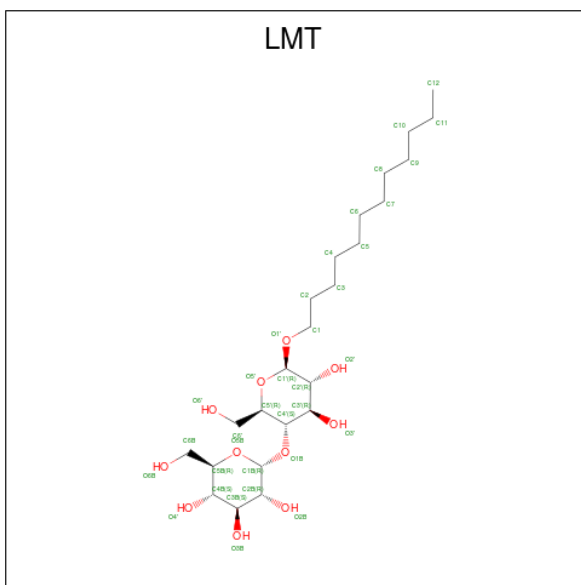
Mol	Chain	Residues	Atoms		AltConf
13	cA	1	Total	C	0
			240	240	
13	cA	1	Total	C	0
			240	240	
13	cA	1	Total	C	0
			240	240	
13	cA	1	Total	C	0
			240	240	
13	cA	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cI	1	Total	C	0
			80	80	
13	cI	1	Total	C	0
			80	80	
13	cL	1	Total	C	0
			80	80	
13	cL	1	Total	C	0
			80	80	
13	cM	1	Total	C	0
			40	40	

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



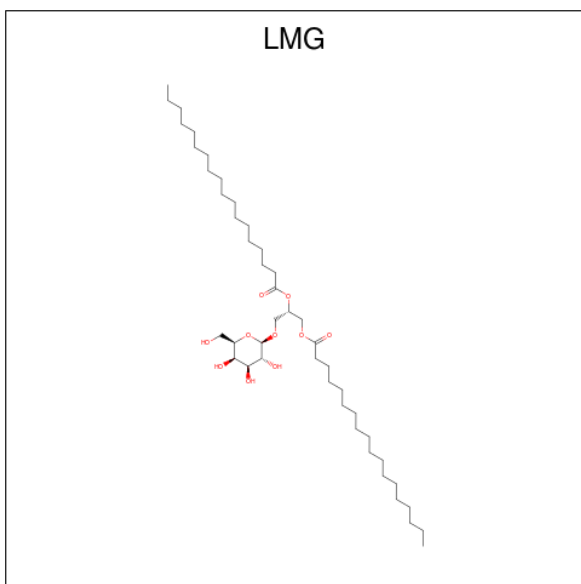
Mol	Chain	Residues	Atoms				AltConf
14	aA	1	Total	C	O	P	0
			76	54	20	2	
14	aA	1	Total	C	O	P	0
			76	54	20	2	
14	bA	1	Total	C	O	P	0
			76	54	20	2	
14	bA	1	Total	C	O	P	0
			76	54	20	2	
14	cA	1	Total	C	O	P	0
			76	54	20	2	
14	cA	1	Total	C	O	P	0
			76	54	20	2	

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
16	aB	1	Total	C	O	0
			55	45	10	
16	bB	1	Total	C	O	0
			55	45	10	
16	cB	1	Total	C	O	0
			55	45	10	

- Molecule 17 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			AltConf
17	bL	4	Total	C	O	0
			56	52	4	
17	aL	4	Total	C	O	0
			56	52	4	
17	aI	1	Total	C		0
			9	9		
17	cI	1	Total	C		0
			9	9		
17	bI	1	Total	C		0
			9	9		
17	cL	4	Total	C	O	0
			56	52	4	

- Molecule 18 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 19 is water.

Mol	Chain	Residues	Atoms		AltConf
19	aA	64	Total	O	0
			64	64	
19	aB	85	Total	O	0
			85	85	
19	aC	16	Total	O	0
			16	16	

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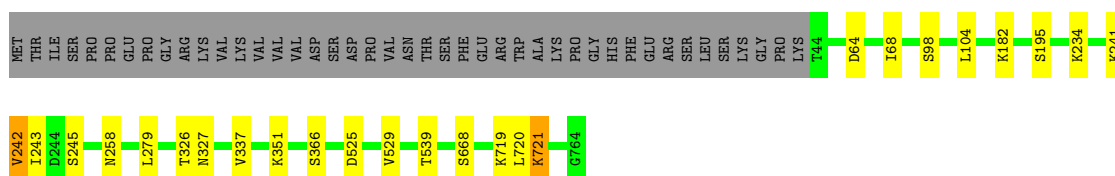
Mol	Chain	Residues	Atoms		AltConf
19	aD	12	Total 12	O 12	0
19	aI	1	Total 1	O 1	0
19	aL	30	Total 30	O 30	0
19	aM	1	Total 1	O 1	0
19	bA	63	Total 63	O 63	0
19	bB	85	Total 85	O 85	0
19	bC	17	Total 17	O 17	0
19	bD	12	Total 12	O 12	0
19	bI	1	Total 1	O 1	0
19	bL	30	Total 30	O 30	0
19	bM	1	Total 1	O 1	0
19	cA	63	Total 63	O 63	0
19	cB	86	Total 86	O 86	0
19	cC	15	Total 15	O 15	0
19	cD	13	Total 13	O 13	0
19	cI	1	Total 1	O 1	0
19	cL	30	Total 30	O 30	0
19	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.

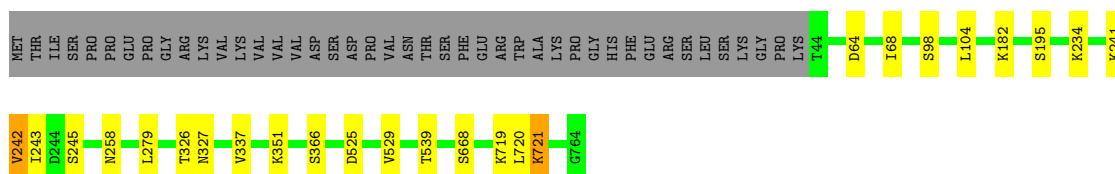
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain aA: 



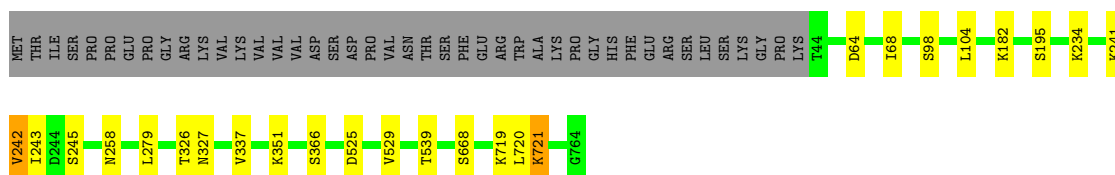
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

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 5: Photosystem I reaction center subunit IV

Chain aE:  84% 6% 10%




- Molecule 5: Photosystem I reaction center subunit IV

Chain bE:  84% 6% 10%



- Molecule 5: Photosystem I reaction center subunit IV

Chain cE:  84% 6% 10%



- Molecule 6: Photosystem I reaction center subunit VIII

Chain aI:  97% .



- Molecule 6: Photosystem I reaction center subunit VIII

Chain bI:  97% .




- Molecule 6: Photosystem I reaction center subunit VIII

Chain cI:  97% .



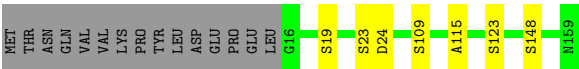
- Molecule 7: Photosystem I reaction center subunit XI

Chain aL:  86% . 9%

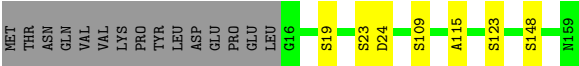
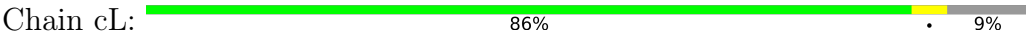


- Molecule 7: Photosystem I reaction center subunit XI

Chain bL:  86% . 9%



• Molecule 7: Photosystem I reaction center subunit XI



• Molecule 8: Photosystem I reaction center subunit XII



• Molecule 8: Photosystem I reaction center subunit XII



• Molecule 8: 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	546366	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, UNL, SF4, LMT, CLA, PQN, CL0, 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	0.34	0/5825	0.52	1/7944 (0.0%)
1	bA	0.34	0/5825	0.52	1/7944 (0.0%)
1	cA	0.34	0/5825	0.52	1/7944 (0.0%)
2	aB	0.35	0/6105	0.53	2/8343 (0.0%)
2	bB	0.35	0/6105	0.53	2/8343 (0.0%)
2	cB	0.35	0/6105	0.53	2/8343 (0.0%)
3	aC	0.32	0/606	0.59	1/820 (0.1%)
3	bC	0.33	0/606	0.59	1/820 (0.1%)
3	cC	0.33	0/606	0.59	1/820 (0.1%)
4	aD	0.31	0/785	0.52	0/1061
4	bD	0.31	0/785	0.51	0/1061
4	cD	0.31	0/785	0.51	0/1061
5	aE	0.31	0/509	0.59	1/689 (0.1%)
5	bE	0.31	0/509	0.59	1/689 (0.1%)
5	cE	0.31	0/509	0.59	1/689 (0.1%)
6	aI	0.36	0/317	0.60	0/436
6	bI	0.36	0/317	0.60	0/436
6	cI	0.36	0/317	0.60	0/436
7	aL	0.34	0/1093	0.52	0/1481
7	bL	0.34	0/1093	0.52	0/1481
7	cL	0.34	0/1093	0.52	0/1481
8	aM	0.30	0/244	0.56	0/332
8	bM	0.30	0/244	0.56	0/332
8	cM	0.30	0/244	0.56	0/332
All	All	0.34	0/46452	0.53	15/63318 (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
1	aA	0	4
1	bA	0	4
1	cA	0	4
2	aB	0	3
2	bB	0	3
2	cB	0	3
All	All	0	21

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	cC	32	ASP	CB-CG-OD1	7.78	125.30	118.30
3	aC	32	ASP	CB-CG-OD1	7.78	125.30	118.30
3	bC	32	ASP	CB-CG-OD1	7.75	125.27	118.30
2	bB	310	PRO	C-N-CD	-6.41	106.49	120.60
2	aB	310	PRO	C-N-CD	-6.41	106.51	120.60

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	aA	242	VAL	Peptide
1	aA	529	VAL	Peptide
1	aA	720	LEU	Peptide
1	aA	721	LYS	Peptide
2	aB	314	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5629	0	5454	0	0
1	bA	5629	0	5454	0	0
1	cA	5629	0	5454	0	0
2	aB	5884	0	5623	0	0
2	bB	5884	0	5623	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	cB	5884	0	5623	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	305	0	304	0	0
6	bI	305	0	304	0	0
6	cI	305	0	304	0	0
7	aL	1065	0	1064	0	0
7	bL	1065	0	1064	0	0
7	cL	1065	0	1064	0	0
8	aM	241	0	266	0	0
8	bM	241	0	266	0	0
8	cM	241	0	266	0	0
9	aA	65	0	72	0	0
9	bA	65	0	72	0	0
9	cA	65	0	72	0	0
10	aA	2491	0	2400	0	0
10	aB	2357	0	2305	0	0
10	aL	250	0	265	0	0
10	bA	2491	0	2400	0	0
10	bB	2357	0	2305	0	0
10	bL	250	0	265	0	0
10	cA	2491	0	2400	0	0
10	cB	2357	0	2305	0	0
10	cL	250	0	265	0	0
11	aA	33	0	46	0	0
11	aB	33	0	46	0	0
11	bA	33	0	46	0	0
11	bB	33	0	46	0	0
11	cA	33	0	46	0	0
11	cB	33	0	46	0	0
12	aA	8	0	0	0	0
12	aC	16	0	0	0	0
12	bA	8	0	0	0	0
12	bC	16	0	0	0	0
12	cA	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	cC	16	0	0	0	0
13	aA	240	0	336	0	0
13	aB	240	0	333	0	0
13	aI	80	0	112	0	0
13	aL	80	0	112	0	0
13	aM	40	0	56	0	0
13	bA	240	0	336	0	0
13	bB	240	0	333	0	0
13	bI	80	0	112	0	0
13	bL	80	0	112	0	0
13	bM	40	0	56	0	0
13	cA	240	0	336	0	0
13	cB	240	0	333	0	0
13	cI	80	0	112	0	0
13	cL	80	0	112	0	0
13	cM	40	0	56	0	0
14	aA	76	0	98	0	0
14	bA	76	0	98	0	0
14	cA	76	0	98	0	0
15	aA	35	0	46	0	0
15	bA	35	0	46	0	0
15	cA	35	0	46	0	0
16	aB	55	0	84	0	0
16	bB	55	0	84	0	0
16	cB	55	0	84	0	0
17	aI	9	0	0	0	0
17	aL	56	0	0	0	0
17	bI	9	0	0	0	0
17	bL	56	0	0	0	0
17	cI	9	0	0	0	0
17	cL	56	0	0	0	0
18	aL	1	0	0	0	0
18	bL	1	0	0	0	0
18	cL	1	0	0	0	0
19	aA	64	0	0	0	0
19	aB	85	0	0	0	0
19	aC	16	0	0	0	0
19	aD	12	0	0	0	0
19	aI	1	0	0	0	0
19	aL	30	0	0	0	0
19	aM	1	0	0	0	0
19	bA	63	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	bB	85	0	0	0	0
19	bC	17	0	0	0	0
19	bD	12	0	0	0	0
19	bI	1	0	0	0	0
19	bL	30	0	0	0	0
19	bM	1	0	0	0	0
19	cA	63	0	0	0	0
19	cB	86	0	0	0	0
19	cC	15	0	0	0	0
19	cD	13	0	0	0	0
19	cI	1	0	0	0	0
19	cL	30	0	0	0	0
19	cM	1	0	0	0	0
All	All	64083	0	62580	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	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	53	65
1	bA	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	53	65
1	cA	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	53	65
2	aB	738/742 (100%)	705 (96%)	33 (4%)	0	100	100
2	bB	738/742 (100%)	705 (96%)	33 (4%)	0	100	100
2	cB	738/742 (100%)	705 (96%)	33 (4%)	0	100	100
3	aC	78/81 (96%)	73 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	bC	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
3	cC	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	aD	96/142 (68%)	93 (97%)	3 (3%)	0	100	100
4	bD	96/142 (68%)	93 (97%)	3 (3%)	0	100	100
4	cD	96/142 (68%)	93 (97%)	3 (3%)	0	100	100
5	aE	59/68 (87%)	51 (86%)	8 (14%)	0	100	100
5	bE	59/68 (87%)	51 (86%)	8 (14%)	0	100	100
5	cE	59/68 (87%)	51 (86%)	8 (14%)	0	100	100
6	aI	36/38 (95%)	36 (100%)	0	0	100	100
6	bI	36/38 (95%)	36 (100%)	0	0	100	100
6	cI	36/38 (95%)	36 (100%)	0	0	100	100
7	aL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	24	25
7	bL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	24	25
7	cL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	24	25
8	aM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
8	bM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
8	cM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
All	All	5691/6075 (94%)	5442 (96%)	243 (4%)	6 (0%)	56	65

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	aL	115	ALA
7	bL	115	ALA
7	cL	115	ALA
1	aA	242	VAL
1	bA	242	VAL

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	574/614 (94%)	553 (96%)	21 (4%)	37	45
1	bA	574/614 (94%)	553 (96%)	21 (4%)	37	45
1	cA	574/614 (94%)	553 (96%)	21 (4%)	37	45
2	aB	597/598 (100%)	581 (97%)	16 (3%)	48	58
2	bB	597/598 (100%)	581 (97%)	16 (3%)	48	58
2	cB	597/598 (100%)	581 (97%)	16 (3%)	48	58
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%)	77 (96%)	3 (4%)	36	44
4	bD	80/115 (70%)	77 (96%)	3 (4%)	36	44
4	cD	80/115 (70%)	77 (96%)	3 (4%)	36	44
5	aE	54/61 (88%)	51 (94%)	3 (6%)	23	25
5	bE	54/61 (88%)	51 (94%)	3 (6%)	23	25
5	cE	54/61 (88%)	51 (94%)	3 (6%)	23	25
6	aI	32/32 (100%)	31 (97%)	1 (3%)	43	52
6	bI	32/32 (100%)	31 (97%)	1 (3%)	43	52
6	cI	32/32 (100%)	31 (97%)	1 (3%)	43	52
7	aL	108/123 (88%)	102 (94%)	6 (6%)	23	25
7	bL	108/123 (88%)	102 (94%)	6 (6%)	23	25
7	cL	108/123 (88%)	102 (94%)	6 (6%)	23	25
8	aM	27/27 (100%)	26 (96%)	1 (4%)	37	45
8	bM	27/27 (100%)	26 (96%)	1 (4%)	37	45
8	cM	27/27 (100%)	26 (96%)	1 (4%)	37	45
All	All	4620/4917 (94%)	4467 (97%)	153 (3%)	45	50

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	bA	539	THR
2	bB	425	SER
4	cD	37	LYS
1	bA	719	LYS
2	bB	160	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	bA	571	ASN
2	bB	496	ASN
2	cB	641	ASN
1	bA	727	GLN
2	bB	332	ASN

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 366 ligands modelled in this entry, 15 are unknown and 3 are monoatomic - leaving 348 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	$\# Z > 2$
9	CL0	aA	801	1	57,73,73	1.86	12 (21%)	66,113,113	2.29	25 (37%)
10	CLA	aA	802	1	34,53,73	2.45	12 (35%)	37,89,113	2.63	18 (48%)
10	CLA	aA	803	1	34,53,73	2.48	13 (38%)	37,89,113	2.68	19 (51%)
10	CLA	aA	804	1	57,73,73	1.89	13 (22%)	66,113,113	2.16	20 (30%)
10	CLA	aA	805	1	57,73,73	1.94	13 (22%)	66,113,113	2.26	24 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	aA	806	1	43,59,73	2.24	13 (30%)	49,96,113	2.38	22 (44%)
10	CLA	aA	807	1	34,53,73	2.39	13 (38%)	37,89,113	2.64	19 (51%)
10	CLA	aA	808	1	34,53,73	2.38	12 (35%)	37,89,113	2.56	15 (40%)
10	CLA	aA	809	1	34,53,73	2.41	11 (32%)	37,89,113	2.62	17 (45%)
10	CLA	aA	810	1	57,73,73	1.98	13 (22%)	66,113,113	2.13	21 (31%)
10	CLA	aA	811	1	46,62,73	2.17	13 (28%)	52,99,113	2.28	21 (40%)
10	CLA	aA	812	1	57,73,73	1.96	13 (22%)	66,113,113	2.14	22 (33%)
10	CLA	aA	813	1	34,53,73	2.46	12 (35%)	37,89,113	2.58	17 (45%)
10	CLA	aA	814	1	34,53,73	2.42	12 (35%)	37,89,113	2.58	17 (45%)
10	CLA	aA	815	-	41,57,73	2.32	13 (31%)	46,93,113	2.36	18 (39%)
10	CLA	aA	816	1	46,62,73	2.15	13 (28%)	52,99,113	2.38	22 (42%)
10	CLA	aA	817	1	46,62,73	2.16	12 (26%)	52,99,113	2.28	22 (42%)
10	CLA	aA	818	1	57,73,73	1.98	11 (19%)	66,113,113	2.37	22 (33%)
10	CLA	aA	819	1	53,69,73	2.06	13 (24%)	61,108,113	2.15	20 (32%)
10	CLA	aA	820	-	57,73,73	1.96	12 (21%)	66,113,113	2.00	21 (31%)
10	CLA	aA	821	1	41,57,73	2.33	12 (29%)	46,93,113	2.53	20 (43%)
10	CLA	aA	822	1	43,59,73	2.27	12 (27%)	49,96,113	2.50	21 (42%)
10	CLA	aA	823	1	57,73,73	1.92	14 (24%)	66,113,113	2.05	19 (28%)
10	CLA	aA	824	-	57,73,73	1.90	13 (22%)	66,113,113	2.15	18 (27%)
10	CLA	aA	825	-	47,63,73	2.08	12 (25%)	54,101,113	2.35	21 (38%)
10	CLA	aA	826	1	57,73,73	1.90	12 (21%)	66,113,113	2.08	21 (31%)
10	CLA	aA	827	1	57,73,73	1.96	14 (24%)	66,113,113	2.19	22 (33%)
10	CLA	aA	828	1	57,73,73	1.93	12 (21%)	66,113,113	2.17	22 (33%)
10	CLA	aA	829	1	57,73,73	1.94	13 (22%)	66,113,113	2.26	21 (31%)
10	CLA	aA	830	1	42,58,73	2.21	13 (30%)	48,95,113	2.40	21 (43%)
10	CLA	aA	831	1	57,73,73	1.93	12 (21%)	66,113,113	2.09	19 (28%)
10	CLA	aA	832	1	57,73,73	1.88	13 (22%)	66,113,113	2.11	23 (34%)
10	CLA	aA	833	1	57,73,73	1.88	12 (21%)	66,113,113	2.20	21 (31%)
10	CLA	aA	834	1	46,62,73	2.13	12 (26%)	52,99,113	2.34	23 (44%)
10	CLA	aA	835	1	57,73,73	1.94	13 (22%)	66,113,113	2.10	22 (33%)
10	CLA	aA	836	1	43,59,73	2.16	13 (30%)	49,96,113	6.08	25 (51%)
10	CLA	aA	837	1	57,73,73	1.85	13 (22%)	66,113,113	2.12	21 (31%)
10	CLA	aA	838	1	42,58,73	2.18	14 (33%)	48,95,113	2.79	24 (50%)
10	CLA	aA	839	1	57,73,73	1.96	13 (22%)	66,113,113	2.06	20 (30%)
10	CLA	aA	840	-	43,59,73	2.32	13 (30%)	49,96,113	2.48	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	aA	841	-	57,73,73	1.95	13 (22%)	66,113,113	2.11	20 (30%)
10	CLA	aA	842	-	57,73,73	1.86	13 (22%)	66,113,113	2.11	23 (34%)
10	CLA	aA	843	-	30,49,73	2.45	11 (36%)	31,83,113	2.58	15 (48%)
11	PQN	aA	844	-	34,34,34	1.36	2 (5%)	42,45,45	1.17	4 (9%)
12	SF4	aA	845	1,2	0,12,12	0.00	-	-		
13	BCR	aA	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.23	5 (8%)
13	BCR	aA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.28	5 (8%)
13	BCR	aA	848	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	7 (12%)
13	BCR	aA	849	-	41,41,41	1.10	3 (7%)	56,56,56	1.26	7 (12%)
13	BCR	aA	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.18	5 (8%)
13	BCR	aA	851	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	3 (5%)
14	LHG	aA	852	-	48,48,48	0.66	1 (2%)	51,54,54	1.22	7 (13%)
15	LMT	aA	853	-	36,36,36	0.45	0	47,47,47	0.90	3 (6%)
10	CLA	aA	854	-	44,60,73	2.22	13 (29%)	50,97,113	2.41	20 (40%)
14	LHG	aA	855	-	26,26,48	0.82	0	29,32,54	1.32	3 (10%)
10	CLA	aA	856	2	41,57,73	2.34	13 (31%)	46,93,113	2.31	18 (39%)
10	CLA	aB	801	-	57,73,73	1.87	13 (22%)	66,113,113	2.37	23 (34%)
10	CLA	aB	802	-	57,73,73	1.93	12 (21%)	66,113,113	2.08	20 (30%)
10	CLA	aB	803	2	57,73,73	1.87	13 (22%)	66,113,113	2.20	23 (34%)
10	CLA	aB	804	-	49,65,73	2.07	12 (24%)	56,103,113	2.57	23 (41%)
10	CLA	aB	805	-	57,73,73	1.89	14 (24%)	66,113,113	1.89	16 (24%)
10	CLA	aB	806	2	46,62,73	2.16	13 (28%)	52,99,113	2.42	25 (48%)
10	CLA	aB	807	2	57,73,73	1.89	14 (24%)	66,113,113	2.22	24 (36%)
10	CLA	aB	808	2	57,73,73	1.88	13 (22%)	66,113,113	2.10	21 (31%)
10	CLA	aB	809	2	57,73,73	1.90	14 (24%)	66,113,113	2.15	20 (30%)
10	CLA	aB	810	2	47,63,73	2.02	12 (25%)	54,101,113	2.47	23 (42%)
10	CLA	aB	811	2	57,73,73	1.84	13 (22%)	66,113,113	2.22	19 (28%)
10	CLA	aB	812	2	34,53,73	2.35	11 (32%)	37,89,113	2.63	16 (43%)
10	CLA	aB	813	2	34,53,73	2.46	12 (35%)	37,89,113	2.55	16 (43%)
10	CLA	aB	814	2	57,73,73	1.94	14 (24%)	66,113,113	2.20	21 (31%)
10	CLA	aB	815	2	48,64,73	2.12	13 (27%)	55,102,113	2.27	21 (38%)
10	CLA	aB	816	2	34,53,73	2.38	12 (35%)	37,89,113	2.69	19 (51%)
10	CLA	aB	817	2	47,63,73	2.13	14 (29%)	54,101,113	2.24	21 (38%)
10	CLA	aB	818	2	51,67,73	2.09	14 (27%)	58,105,113	2.24	21 (36%)
10	CLA	aB	819	2	52,68,73	1.98	12 (23%)	60,107,113	2.41	24 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	aB	820	-	57,73,73	1.97	13 (22%)	66,113,113	2.04	22 (33%)
10	CLA	aB	821	2	39,55,73	2.38	13 (33%)	44,91,113	2.44	20 (45%)
10	CLA	aB	822	2	34,53,73	2.47	12 (35%)	37,89,113	2.66	16 (43%)
10	CLA	aB	823	2	47,63,73	2.20	13 (27%)	54,101,113	2.26	21 (38%)
10	CLA	aB	824	2	34,53,73	2.46	12 (35%)	37,89,113	2.59	18 (48%)
10	CLA	aB	825	2	46,62,73	2.17	13 (28%)	52,99,113	2.49	22 (42%)
10	CLA	aB	826	-	57,73,73	1.98	13 (22%)	66,113,113	2.27	24 (36%)
10	CLA	aB	827	2	57,73,73	1.92	13 (22%)	66,113,113	2.21	21 (31%)
10	CLA	aB	828	2	57,73,73	1.89	12 (21%)	66,113,113	2.20	21 (31%)
10	CLA	aB	829	2	57,73,73	1.93	12 (21%)	66,113,113	2.08	19 (28%)
10	CLA	aB	830	2	57,73,73	1.92	13 (22%)	66,113,113	2.20	22 (33%)
10	CLA	aB	831	2	34,53,73	2.41	12 (35%)	37,89,113	2.59	19 (51%)
10	CLA	aB	832	2	57,73,73	1.95	14 (24%)	66,113,113	2.11	22 (33%)
10	CLA	aB	833	2	50,66,73	2.10	13 (26%)	57,104,113	2.25	22 (38%)
10	CLA	aB	834	2	34,53,73	2.41	12 (35%)	37,89,113	2.59	20 (54%)
10	CLA	aB	835	-	34,53,73	2.42	12 (35%)	37,89,113	2.50	18 (48%)
10	CLA	aB	836	-	34,53,73	2.46	12 (35%)	37,89,113	2.61	18 (48%)
10	CLA	aB	837	2	52,68,73	2.00	14 (26%)	60,107,113	2.31	21 (35%)
10	CLA	aB	838	2	57,73,73	1.93	12 (21%)	66,113,113	2.12	22 (33%)
10	CLA	aB	839	2	39,55,73	2.30	13 (33%)	44,91,113	2.50	19 (43%)
10	CLA	aB	840	-	57,73,73	1.87	13 (22%)	66,113,113	2.06	20 (30%)
10	CLA	aB	841	2	57,73,73	1.87	13 (22%)	66,113,113	2.09	20 (30%)
11	PQN	aB	842	-	34,34,34	1.34	2 (5%)	42,45,45	1.02	2 (4%)
13	BCR	aB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)
13	BCR	aB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.32	5 (8%)
13	BCR	aB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
13	BCR	aB	846	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	3 (5%)
13	BCR	aB	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	6 (10%)
16	LMG	aB	848	-	55,55,55	0.76	1 (1%)	63,63,63	1.35	9 (14%)
13	BCR	aB	849	-	41,41,41	1.01	2 (4%)	56,56,56	1.16	4 (7%)
12	SF4	aC	101	3	0,12,12	0.00	-	-	-	-
12	SF4	aC	102	3	0,12,12	0.00	-	-	-	-
13	BCR	aI	101	-	41,41,41	1.06	3 (7%)	56,56,56	1.27	6 (10%)
13	BCR	aI	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	5 (8%)
10	CLA	aL	202	2	47,63,73	2.05	14 (29%)	54,101,113	2.35	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	aL	203	7	57,73,73	1.92	13 (22%)	66,113,113	2.03	21 (31%)
10	CLA	aL	204	7	57,73,73	1.89	11 (19%)	66,113,113	2.05	20 (30%)
10	CLA	aL	205	-	57,73,73	1.91	14 (24%)	66,113,113	2.08	19 (28%)
13	BCR	aL	206	-	41,41,41	1.01	2 (4%)	56,56,56	1.29	6 (10%)
13	BCR	aL	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	3 (5%)
13	BCR	aM	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	11 (19%)
9	CL0	bA	801	1	57,73,73	1.87	11 (19%)	66,113,113	2.29	24 (36%)
10	CLA	bA	802	1	34,53,73	2.44	12 (35%)	37,89,113	2.63	18 (48%)
10	CLA	bA	803	1	34,53,73	2.48	13 (38%)	37,89,113	2.69	19 (51%)
10	CLA	bA	804	1	57,73,73	1.89	13 (22%)	66,113,113	2.17	20 (30%)
10	CLA	bA	805	1	57,73,73	1.95	13 (22%)	66,113,113	2.26	24 (36%)
10	CLA	bA	806	1	43,59,73	2.25	13 (30%)	49,96,113	2.39	22 (44%)
10	CLA	bA	807	1	34,53,73	2.40	13 (38%)	37,89,113	2.65	19 (51%)
10	CLA	bA	808	1	34,53,73	2.37	12 (35%)	37,89,113	2.55	15 (40%)
10	CLA	bA	809	1	34,53,73	2.41	12 (35%)	37,89,113	2.61	17 (45%)
10	CLA	bA	810	1	57,73,73	1.99	13 (22%)	66,113,113	2.14	21 (31%)
10	CLA	bA	811	1	46,62,73	2.17	13 (28%)	52,99,113	2.28	21 (40%)
10	CLA	bA	812	1	57,73,73	1.96	13 (22%)	66,113,113	2.15	22 (33%)
10	CLA	bA	813	1	34,53,73	2.46	12 (35%)	37,89,113	2.57	17 (45%)
10	CLA	bA	814	1	34,53,73	2.42	12 (35%)	37,89,113	2.58	17 (45%)
10	CLA	bA	815	-	41,57,73	2.32	13 (31%)	46,93,113	2.36	18 (39%)
10	CLA	bA	816	1	46,62,73	2.15	13 (28%)	52,99,113	2.37	22 (42%)
10	CLA	bA	817	1	46,62,73	2.16	12 (26%)	52,99,113	2.27	22 (42%)
10	CLA	bA	818	1	57,73,73	1.97	11 (19%)	66,113,113	2.37	22 (33%)
10	CLA	bA	819	1	53,69,73	2.06	13 (24%)	61,108,113	2.15	20 (32%)
10	CLA	bA	820	-	57,73,73	1.96	13 (22%)	66,113,113	2.00	21 (31%)
10	CLA	bA	821	1	41,57,73	2.33	12 (29%)	46,93,113	2.54	20 (43%)
10	CLA	bA	822	1	43,59,73	2.27	12 (27%)	49,96,113	2.50	22 (44%)
10	CLA	bA	823	1	57,73,73	1.92	13 (22%)	66,113,113	2.05	19 (28%)
10	CLA	bA	824	-	57,73,73	1.90	13 (22%)	66,113,113	2.16	18 (27%)
10	CLA	bA	825	-	47,63,73	2.09	13 (27%)	54,101,113	2.35	21 (38%)
10	CLA	bA	826	1	57,73,73	1.90	12 (21%)	66,113,113	2.07	21 (31%)
10	CLA	bA	827	1	57,73,73	1.96	14 (24%)	66,113,113	2.19	22 (33%)
10	CLA	bA	828	1	57,73,73	1.94	12 (21%)	66,113,113	2.18	22 (33%)
10	CLA	bA	829	1	57,73,73	1.94	13 (22%)	66,113,113	2.26	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	bA	830	1	42,58,73	2.21	13 (30%)	48,95,113	2.40	21 (43%)
10	CLA	bA	831	1	57,73,73	1.93	12 (21%)	66,113,113	2.09	19 (28%)
10	CLA	bA	832	1	57,73,73	1.89	13 (22%)	66,113,113	2.12	23 (34%)
10	CLA	bA	833	1	57,73,73	1.89	12 (21%)	66,113,113	2.20	21 (31%)
10	CLA	bA	834	1	46,62,73	2.14	12 (26%)	52,99,113	2.34	23 (44%)
10	CLA	bA	835	1	57,73,73	1.94	13 (22%)	66,113,113	2.10	22 (33%)
10	CLA	bA	836	1	43,59,73	2.16	13 (30%)	49,96,113	6.08	25 (51%)
10	CLA	bA	837	1	57,73,73	1.85	12 (21%)	66,113,113	2.11	21 (31%)
10	CLA	bA	838	1	42,58,73	2.17	12 (28%)	48,95,113	2.79	24 (50%)
10	CLA	bA	839	1	57,73,73	1.96	13 (22%)	66,113,113	2.06	20 (30%)
10	CLA	bA	840	-	43,59,73	2.32	13 (30%)	49,96,113	2.48	20 (40%)
10	CLA	bA	841	1	57,73,73	1.95	13 (22%)	66,113,113	2.11	20 (30%)
10	CLA	bA	842	-	57,73,73	1.86	13 (22%)	66,113,113	2.11	23 (34%)
10	CLA	bA	843	-	30,49,73	2.44	11 (36%)	31,83,113	2.58	15 (48%)
11	PQN	bA	844	-	34,34,34	1.37	2 (5%)	42,45,45	1.17	4 (9%)
12	SF4	bA	845	1,2	0,12,12	0.00	-	-		
13	BCR	bA	846	-	41,41,41	1.09	3 (7%)	56,56,56	1.23	6 (10%)
13	BCR	bA	847	-	41,41,41	1.02	2 (4%)	56,56,56	1.30	5 (8%)
13	BCR	bA	848	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	8 (14%)
13	BCR	bA	849	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	7 (12%)
13	BCR	bA	850	-	41,41,41	1.11	2 (4%)	56,56,56	1.18	5 (8%)
13	BCR	bA	851	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	3 (5%)
14	LHG	bA	852	-	48,48,48	0.66	1 (2%)	51,54,54	1.22	7 (13%)
15	LMT	bA	853	-	36,36,36	0.45	0	47,47,47	0.90	3 (6%)
10	CLA	bA	854	-	44,60,73	2.22	12 (27%)	50,97,113	2.40	20 (40%)
14	LHG	bA	855	-	26,26,48	0.82	0	29,32,54	1.32	3 (10%)
10	CLA	bA	856	2	41,57,73	2.35	13 (31%)	46,93,113	2.32	18 (39%)
10	CLA	bB	801	-	57,73,73	1.86	13 (22%)	66,113,113	2.36	24 (36%)
10	CLA	bB	802	-	57,73,73	1.93	12 (21%)	66,113,113	2.08	20 (30%)
10	CLA	bB	803	2	57,73,73	1.88	13 (22%)	66,113,113	2.21	23 (34%)
10	CLA	bB	804	-	49,65,73	2.07	12 (24%)	56,103,113	2.57	23 (41%)
10	CLA	bB	805	-	57,73,73	1.88	14 (24%)	66,113,113	1.88	16 (24%)
10	CLA	bB	806	2	46,62,73	2.16	13 (28%)	52,99,113	2.41	25 (48%)
10	CLA	bB	807	2	57,73,73	1.89	14 (24%)	66,113,113	2.21	24 (36%)
10	CLA	bB	808	2	57,73,73	1.88	13 (22%)	66,113,113	2.10	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	bB	809	2	57,73,73	1.90	14 (24%)	66,113,113	2.15	20 (30%)
10	CLA	bB	810	2	47,63,73	2.02	12 (25%)	54,101,113	2.48	23 (42%)
10	CLA	bB	811	2	57,73,73	1.85	13 (22%)	66,113,113	2.22	19 (28%)
10	CLA	bB	812	2	34,53,73	2.36	11 (32%)	37,89,113	2.64	16 (43%)
10	CLA	bB	813	2	34,53,73	2.45	12 (35%)	37,89,113	2.55	16 (43%)
10	CLA	bB	814	2	57,73,73	1.94	13 (22%)	66,113,113	2.19	21 (31%)
10	CLA	bB	815	2	48,64,73	2.12	13 (27%)	55,102,113	2.27	21 (38%)
10	CLA	bB	816	2	34,53,73	2.38	12 (35%)	37,89,113	2.69	19 (51%)
10	CLA	bB	817	2	47,63,73	2.13	14 (29%)	54,101,113	2.24	21 (38%)
10	CLA	bB	818	2	51,67,73	2.09	13 (25%)	58,105,113	2.23	21 (36%)
10	CLA	bB	819	2	52,68,73	1.98	12 (23%)	60,107,113	2.41	24 (40%)
10	CLA	bB	820	-	57,73,73	1.97	13 (22%)	66,113,113	2.05	21 (31%)
10	CLA	bB	821	2	39,55,73	2.39	13 (33%)	44,91,113	2.45	20 (45%)
10	CLA	bB	822	2	34,53,73	2.46	12 (35%)	37,89,113	2.66	16 (43%)
10	CLA	bB	823	2	47,63,73	2.20	13 (27%)	54,101,113	2.26	21 (38%)
10	CLA	bB	824	2	34,53,73	2.45	12 (35%)	37,89,113	2.59	18 (48%)
10	CLA	bB	825	2	46,62,73	2.17	12 (26%)	52,99,113	2.49	22 (42%)
10	CLA	bB	826	-	57,73,73	1.99	13 (22%)	66,113,113	2.27	24 (36%)
10	CLA	bB	827	2	57,73,73	1.92	13 (22%)	66,113,113	2.20	22 (33%)
10	CLA	bB	828	2	57,73,73	1.89	12 (21%)	66,113,113	2.20	21 (31%)
10	CLA	bB	829	2	57,73,73	1.93	12 (21%)	66,113,113	2.08	19 (28%)
10	CLA	bB	830	2	57,73,73	1.92	13 (22%)	66,113,113	2.20	22 (33%)
10	CLA	bB	831	2	34,53,73	2.42	12 (35%)	37,89,113	2.59	19 (51%)
10	CLA	bB	832	2	57,73,73	1.95	14 (24%)	66,113,113	2.10	22 (33%)
10	CLA	bB	833	2	50,66,73	2.09	13 (26%)	57,104,113	2.25	22 (38%)
10	CLA	bB	834	2	34,53,73	2.42	12 (35%)	37,89,113	2.60	20 (54%)
10	CLA	bB	835	-	34,53,73	2.41	13 (38%)	37,89,113	2.49	18 (48%)
10	CLA	bB	836	-	34,53,73	2.47	12 (35%)	37,89,113	2.61	18 (48%)
10	CLA	bB	837	2	52,68,73	2.00	14 (26%)	60,107,113	2.31	21 (35%)
10	CLA	bB	838	2	57,73,73	1.93	12 (21%)	66,113,113	2.12	22 (33%)
10	CLA	bB	839	2	39,55,73	2.30	13 (33%)	44,91,113	2.50	19 (43%)
10	CLA	bB	840	-	57,73,73	1.87	13 (22%)	66,113,113	2.07	20 (30%)
10	CLA	bB	841	2	57,73,73	1.87	13 (22%)	66,113,113	2.09	20 (30%)
11	PQN	bB	842	-	34,34,34	1.34	2 (5%)	42,45,45	1.01	2 (4%)
13	BCR	bB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCR	bB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.32	5 (8%)
13	BCR	bB	845	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	7 (12%)
13	BCR	bB	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	3 (5%)
13	BCR	bB	847	-	41,41,41	1.07	3 (7%)	56,56,56	1.30	6 (10%)
16	LMG	bB	848	-	55,55,55	0.77	1 (1%)	63,63,63	1.34	9 (14%)
13	BCR	bB	849	-	41,41,41	1.01	2 (4%)	56,56,56	1.15	4 (7%)
12	SF4	bC	101	3	0,12,12	0.00	-	-		
12	SF4	bC	102	3	0,12,12	0.00	-	-		
13	BCR	bI	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	6 (10%)
13	BCR	bI	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	6 (10%)
10	CLA	bL	202	2	47,63,73	2.04	14 (29%)	54,101,113	2.35	20 (37%)
10	CLA	bL	203	7	57,73,73	1.91	13 (22%)	66,113,113	2.03	21 (31%)
10	CLA	bL	204	7	57,73,73	1.89	11 (19%)	66,113,113	2.05	20 (30%)
10	CLA	bL	205	-	57,73,73	1.91	14 (24%)	66,113,113	2.08	19 (28%)
13	BCR	bL	206	-	41,41,41	1.01	2 (4%)	56,56,56	1.29	7 (12%)
13	BCR	bL	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.17	3 (5%)
13	BCR	bM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	11 (19%)
9	CL0	cA	801	1	57,73,73	1.87	12 (21%)	66,113,113	2.29	24 (36%)
10	CLA	cA	802	1	34,53,73	2.45	12 (35%)	37,89,113	2.63	18 (48%)
10	CLA	cA	803	1	34,53,73	2.49	13 (38%)	37,89,113	2.68	19 (51%)
10	CLA	cA	804	1	57,73,73	1.89	14 (24%)	66,113,113	2.16	20 (30%)
10	CLA	cA	805	1	57,73,73	1.95	13 (22%)	66,113,113	2.25	24 (36%)
10	CLA	cA	806	1	43,59,73	2.25	13 (30%)	49,96,113	2.39	22 (44%)
10	CLA	cA	807	1	34,53,73	2.39	13 (38%)	37,89,113	2.64	19 (51%)
10	CLA	cA	808	1	34,53,73	2.38	12 (35%)	37,89,113	2.55	15 (40%)
10	CLA	cA	809	1	34,53,73	2.42	12 (35%)	37,89,113	2.62	17 (45%)
10	CLA	cA	810	1	57,73,73	1.98	13 (22%)	66,113,113	2.14	21 (31%)
10	CLA	cA	811	1	46,62,73	2.17	13 (28%)	52,99,113	2.28	21 (40%)
10	CLA	cA	812	1	57,73,73	1.97	13 (22%)	66,113,113	2.15	22 (33%)
10	CLA	cA	813	1	34,53,73	2.46	12 (35%)	37,89,113	2.58	18 (48%)
10	CLA	cA	814	1	34,53,73	2.42	12 (35%)	37,89,113	2.58	17 (45%)
10	CLA	cA	815	-	41,57,73	2.32	12 (29%)	46,93,113	2.36	18 (39%)
10	CLA	cA	816	1	46,62,73	2.16	12 (26%)	52,99,113	2.38	22 (42%)
10	CLA	cA	817	1	46,62,73	2.16	13 (28%)	52,99,113	2.27	22 (42%)
10	CLA	cA	818	1	57,73,73	1.98	12 (21%)	66,113,113	2.37	22 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	cA	819	1	53,69,73	2.05	13 (24%)	61,108,113	2.15	20 (32%)
10	CLA	cA	820	-	57,73,73	1.96	12 (21%)	66,113,113	2.00	21 (31%)
10	CLA	cA	821	1	41,57,73	2.33	12 (29%)	46,93,113	2.53	20 (43%)
10	CLA	cA	822	1	43,59,73	2.26	12 (27%)	49,96,113	2.50	22 (44%)
10	CLA	cA	823	1	57,73,73	1.92	13 (22%)	66,113,113	2.05	19 (28%)
10	CLA	cA	824	-	57,73,73	1.91	13 (22%)	66,113,113	2.15	18 (27%)
10	CLA	cA	825	-	47,63,73	2.09	14 (29%)	54,101,113	2.35	21 (38%)
10	CLA	cA	826	1	57,73,73	1.90	12 (21%)	66,113,113	2.08	21 (31%)
10	CLA	cA	827	1	57,73,73	1.96	14 (24%)	66,113,113	2.18	22 (33%)
10	CLA	cA	828	1	57,73,73	1.93	12 (21%)	66,113,113	2.17	22 (33%)
10	CLA	cA	829	1	57,73,73	1.94	13 (22%)	66,113,113	2.25	21 (31%)
10	CLA	cA	830	1	42,58,73	2.22	12 (28%)	48,95,113	2.41	21 (43%)
10	CLA	cA	831	1	57,73,73	1.93	12 (21%)	66,113,113	2.09	19 (28%)
10	CLA	cA	832	1	57,73,73	1.89	13 (22%)	66,113,113	2.11	23 (34%)
10	CLA	cA	833	1	57,73,73	1.88	12 (21%)	66,113,113	2.19	21 (31%)
10	CLA	cA	834	1	46,62,73	2.14	12 (26%)	52,99,113	2.34	23 (44%)
10	CLA	cA	835	1	57,73,73	1.94	13 (22%)	66,113,113	2.10	22 (33%)
10	CLA	cA	836	1	43,59,73	2.17	13 (30%)	49,96,113	6.09	25 (51%)
10	CLA	cA	837	1	57,73,73	1.85	13 (22%)	66,113,113	2.11	21 (31%)
10	CLA	cA	838	1	42,58,73	2.18	14 (33%)	48,95,113	2.79	24 (50%)
10	CLA	cA	839	1	57,73,73	1.96	13 (22%)	66,113,113	2.06	20 (30%)
10	CLA	cA	840	-	43,59,73	2.32	13 (30%)	49,96,113	2.48	20 (40%)
10	CLA	cA	841	1	57,73,73	1.96	14 (24%)	66,113,113	2.11	20 (30%)
10	CLA	cA	842	-	57,73,73	1.86	13 (22%)	66,113,113	2.11	23 (34%)
10	CLA	cA	843	-	30,49,73	2.44	11 (36%)	31,83,113	2.58	15 (48%)
11	PQN	cA	844	-	34,34,34	1.37	2 (5%)	42,45,45	1.17	4 (9%)
12	SF4	cA	845	1,2	0,12,12	0.00	-	-	-	-
13	BCR	cA	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.23	6 (10%)
13	BCR	cA	847	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	5 (8%)
13	BCR	cA	848	-	41,41,41	1.01	2 (4%)	56,56,56	1.29	8 (14%)
13	BCR	cA	849	-	41,41,41	1.10	3 (7%)	56,56,56	1.27	7 (12%)
13	BCR	cA	850	-	41,41,41	1.11	2 (4%)	56,56,56	1.18	5 (8%)
13	BCR	cA	851	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	3 (5%)
14	LHG	cA	852	-	48,48,48	0.66	1 (2%)	51,54,54	1.21	7 (13%)
15	LMT	cA	853	-	36,36,36	0.45	0	47,47,47	0.90	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	cA	854	14	44,60,73	2.22	13 (29%)	50,97,113	2.40	20 (40%)
14	LHG	cA	855	10	26,26,48	0.82	0	29,32,54	1.32	3 (10%)
10	CLA	cA	856	2	41,57,73	2.35	13 (31%)	46,93,113	2.32	18 (39%)
10	CLA	cB	801	-	57,73,73	1.86	13 (22%)	66,113,113	2.36	23 (34%)
10	CLA	cB	802	-	57,73,73	1.94	12 (21%)	66,113,113	2.08	20 (30%)
10	CLA	cB	803	2	57,73,73	1.88	13 (22%)	66,113,113	2.20	23 (34%)
10	CLA	cB	804	-	49,65,73	2.07	12 (24%)	56,103,113	2.57	23 (41%)
10	CLA	cB	805	-	57,73,73	1.88	14 (24%)	66,113,113	1.88	16 (24%)
10	CLA	cB	806	2	46,62,73	2.16	13 (28%)	52,99,113	2.41	25 (48%)
10	CLA	cB	807	2	57,73,73	1.89	14 (24%)	66,113,113	2.21	24 (36%)
10	CLA	cB	808	2	57,73,73	1.88	13 (22%)	66,113,113	2.10	22 (33%)
10	CLA	cB	809	2	57,73,73	1.90	14 (24%)	66,113,113	2.15	20 (30%)
10	CLA	cB	810	2	47,63,73	2.02	12 (25%)	54,101,113	2.48	24 (44%)
10	CLA	cB	811	2	57,73,73	1.85	13 (22%)	66,113,113	2.23	19 (28%)
10	CLA	cB	812	2	34,53,73	2.35	11 (32%)	37,89,113	2.64	16 (43%)
10	CLA	cB	813	2	34,53,73	2.46	13 (38%)	37,89,113	2.55	16 (43%)
10	CLA	cB	814	2	57,73,73	1.94	14 (24%)	66,113,113	2.20	21 (31%)
10	CLA	cB	815	2	48,64,73	2.12	13 (27%)	55,102,113	2.27	21 (38%)
10	CLA	cB	816	2	34,53,73	2.38	12 (35%)	37,89,113	2.69	19 (51%)
10	CLA	cB	817	2	47,63,73	2.13	14 (29%)	54,101,113	2.24	21 (38%)
10	CLA	cB	818	2	51,67,73	2.09	14 (27%)	58,105,113	2.23	21 (36%)
10	CLA	cB	819	2	52,68,73	1.98	12 (23%)	60,107,113	2.41	24 (40%)
10	CLA	cB	820	-	57,73,73	1.97	13 (22%)	66,113,113	2.04	21 (31%)
10	CLA	cB	821	2	39,55,73	2.38	13 (33%)	44,91,113	2.44	20 (45%)
10	CLA	cB	822	2	34,53,73	2.47	12 (35%)	37,89,113	2.66	16 (43%)
10	CLA	cB	823	2	47,63,73	2.20	13 (27%)	54,101,113	2.26	21 (38%)
10	CLA	cB	824	2	34,53,73	2.44	12 (35%)	37,89,113	2.59	18 (48%)
10	CLA	cB	825	2	46,62,73	2.18	13 (28%)	52,99,113	2.49	22 (42%)
10	CLA	cB	826	-	57,73,73	1.99	13 (22%)	66,113,113	2.28	24 (36%)
10	CLA	cB	827	2	57,73,73	1.92	13 (22%)	66,113,113	2.21	22 (33%)
10	CLA	cB	828	2	57,73,73	1.89	12 (21%)	66,113,113	2.19	21 (31%)
10	CLA	cB	829	2	57,73,73	1.93	13 (22%)	66,113,113	2.08	19 (28%)
10	CLA	cB	830	2	57,73,73	1.92	12 (21%)	66,113,113	2.20	22 (33%)
10	CLA	cB	831	2	34,53,73	2.42	12 (35%)	37,89,113	2.60	20 (54%)
10	CLA	cB	832	2	57,73,73	1.95	14 (24%)	66,113,113	2.10	22 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	cB	833	2	50,66,73	2.09	13 (26%)	57,104,113	2.25	22 (38%)
10	CLA	cB	834	2	34,53,73	2.42	12 (35%)	37,89,113	2.58	20 (54%)
10	CLA	cB	835	-	34,53,73	2.41	12 (35%)	37,89,113	2.49	18 (48%)
10	CLA	cB	836	-	34,53,73	2.47	12 (35%)	37,89,113	2.60	18 (48%)
10	CLA	cB	837	2	52,68,73	2.00	14 (26%)	60,107,113	2.32	21 (35%)
10	CLA	cB	838	2	57,73,73	1.93	12 (21%)	66,113,113	2.11	22 (33%)
10	CLA	cB	839	2	39,55,73	2.30	14 (35%)	44,91,113	2.50	19 (43%)
10	CLA	cB	840	-	57,73,73	1.87	13 (22%)	66,113,113	2.07	20 (30%)
10	CLA	cB	841	2	57,73,73	1.87	13 (22%)	66,113,113	2.09	20 (30%)
11	PQN	cB	842	-	34,34,34	1.34	2 (5%)	42,45,45	1.01	2 (4%)
13	BCR	cB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.13	4 (7%)
13	BCR	cB	844	-	41,41,41	1.03	2 (4%)	56,56,56	1.32	5 (8%)
13	BCR	cB	845	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	7 (12%)
13	BCR	cB	846	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	3 (5%)
13	BCR	cB	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	6 (10%)
16	LMG	cB	848	-	55,55,55	0.76	1 (1%)	63,63,63	1.35	9 (14%)
13	BCR	cB	849	-	41,41,41	1.01	2 (4%)	56,56,56	1.16	4 (7%)
12	SF4	cC	101	3	0,12,12	0.00	-	-		
12	SF4	cC	102	3	0,12,12	0.00	-	-		
13	BCR	cI	102	-	41,41,41	1.07	3 (7%)	56,56,56	1.27	6 (10%)
13	BCR	cI	103	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	5 (8%)
10	CLA	cL	202	2	47,63,73	2.05	14 (29%)	54,101,113	2.35	20 (37%)
10	CLA	cL	203	7	57,73,73	1.91	13 (22%)	66,113,113	2.02	21 (31%)
10	CLA	cL	204	7	57,73,73	1.89	11 (19%)	66,113,113	2.05	20 (30%)
10	CLA	cL	205	-	57,73,73	1.91	14 (24%)	66,113,113	2.08	19 (28%)
13	BCR	cL	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	6 (10%)
13	BCR	cL	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	3 (5%)
13	BCR	cM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	11 (19%)

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
9	CL0	aA	801	1	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	aA	802	1	2/2/16/25	5/11/111/135	-
10	CLA	aA	803	1	3/3/16/25	3/11/111/135	-
10	CLA	aA	804	1	3/3/20/25	10/37/135/135	-
10	CLA	aA	805	1	3/3/20/25	9/37/135/135	-
10	CLA	aA	806	1	3/3/17/25	3/21/119/135	-
10	CLA	aA	807	1	3/3/16/25	7/11/111/135	-
10	CLA	aA	808	1	3/3/16/25	2/11/111/135	-
10	CLA	aA	809	1	3/3/16/25	2/11/111/135	-
10	CLA	aA	810	1	3/3/20/25	10/37/135/135	-
10	CLA	aA	811	1	3/3/17/25	8/24/122/135	-
10	CLA	aA	812	1	3/3/20/25	15/37/135/135	-
10	CLA	aA	813	1	3/3/16/25	1/11/111/135	-
10	CLA	aA	814	1	3/3/16/25	2/11/111/135	-
10	CLA	aA	815	-	3/3/16/25	3/18/116/135	-
10	CLA	aA	816	1	2/2/17/25	10/24/122/135	-
10	CLA	aA	817	1	2/2/17/25	10/24/122/135	-
10	CLA	aA	818	1	2/2/20/25	13/37/135/135	-
10	CLA	aA	819	1	3/3/19/25	11/33/131/135	-
10	CLA	aA	820	-	3/3/20/25	13/37/135/135	-
10	CLA	aA	821	1	3/3/16/25	4/18/116/135	-
10	CLA	aA	822	1	2/2/17/25	10/21/119/135	-
10	CLA	aA	823	1	3/3/20/25	12/37/135/135	-
10	CLA	aA	824	-	3/3/20/25	11/37/135/135	-
10	CLA	aA	825	-	3/3/18/25	9/25/123/135	-
10	CLA	aA	826	1	3/3/20/25	8/37/135/135	-
10	CLA	aA	827	1	2/2/20/25	17/37/135/135	-
10	CLA	aA	828	1	3/3/20/25	6/37/135/135	-
10	CLA	aA	829	1	3/3/20/25	12/37/135/135	-
10	CLA	aA	830	1	3/3/17/25	5/19/117/135	-
10	CLA	aA	831	1	3/3/20/25	13/37/135/135	-
10	CLA	aA	832	1	3/3/20/25	6/37/135/135	-
10	CLA	aA	833	1	3/3/20/25	10/37/135/135	-
10	CLA	aA	834	1	3/3/17/25	8/24/122/135	-
10	CLA	aA	835	1	3/3/20/25	11/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	aA	836	1	3/3/17/25	7/21/119/135	-
10	CLA	aA	837	1	3/3/20/25	7/37/135/135	-
10	CLA	aA	838	1	3/3/17/25	9/19/117/135	-
10	CLA	aA	839	1	2/2/20/25	6/37/135/135	-
10	CLA	aA	840	-	3/3/17/25	6/21/119/135	-
10	CLA	aA	841	-	3/3/20/25	11/37/135/135	-
10	CLA	aA	842	-	3/3/20/25	14/37/135/135	-
10	CLA	aA	843	-	3/3/14/25	0/5/101/135	-
11	PQN	aA	844	-	-	8/23/43/43	0/2/2/2
12	SF4	aA	845	1,2	-	-	0/6/5/5
13	BCR	aA	846	-	-	14/29/63/63	0/2/2/2
13	BCR	aA	847	-	-	9/29/63/63	0/2/2/2
13	BCR	aA	848	-	-	16/29/63/63	0/2/2/2
13	BCR	aA	849	-	-	13/29/63/63	0/2/2/2
13	BCR	aA	850	-	-	9/29/63/63	0/2/2/2
13	BCR	aA	851	-	-	13/29/63/63	0/2/2/2
14	LHG	aA	852	-	-	31/53/53/53	-
15	LMT	aA	853	-	-	9/21/61/61	0/2/2/2
10	CLA	aA	854	-	2/2/17/25	8/22/120/135	-
14	LHG	aA	855	-	-	15/31/31/53	-
10	CLA	aA	856	2	3/3/16/25	7/18/116/135	-
10	CLA	aB	801	-	1/1/20/25	7/37/135/135	-
10	CLA	aB	802	-	3/3/20/25	12/37/135/135	-
10	CLA	aB	803	2	2/2/20/25	5/37/135/135	-
10	CLA	aB	804	-	1/1/18/25	14/28/126/135	-
10	CLA	aB	805	-	2/2/20/25	10/37/135/135	-
10	CLA	aB	806	2	3/3/17/25	11/24/122/135	-
10	CLA	aB	807	2	3/3/20/25	12/37/135/135	-
10	CLA	aB	808	2	3/3/20/25	12/37/135/135	-
10	CLA	aB	809	2	2/2/20/25	6/37/135/135	-
10	CLA	aB	810	2	2/2/18/25	8/25/123/135	-
10	CLA	aB	811	2	2/2/20/25	17/37/135/135	-
10	CLA	aB	812	2	3/3/16/25	1/11/111/135	-
10	CLA	aB	813	2	2/2/16/25	2/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	aB	814	2	3/3/20/25	14/37/135/135	-
10	CLA	aB	815	2	3/3/18/25	7/27/125/135	-
10	CLA	aB	816	2	3/3/16/25	2/11/111/135	-
10	CLA	aB	817	2	3/3/18/25	10/25/123/135	-
10	CLA	aB	818	2	3/3/18/25	11/30/128/135	-
10	CLA	aB	819	2	3/3/19/25	10/31/129/135	-
10	CLA	aB	820	-	3/3/20/25	11/37/135/135	-
10	CLA	aB	821	2	3/3/16/25	5/16/114/135	-
10	CLA	aB	822	2	2/2/16/25	7/11/111/135	-
10	CLA	aB	823	2	3/3/18/25	13/25/123/135	-
10	CLA	aB	824	2	3/3/16/25	3/11/111/135	-
10	CLA	aB	825	2	3/3/17/25	7/24/122/135	-
10	CLA	aB	826	-	3/3/20/25	11/37/135/135	-
10	CLA	aB	827	2	3/3/20/25	9/37/135/135	-
10	CLA	aB	828	2	1/1/20/25	11/37/135/135	-
10	CLA	aB	829	2	3/3/20/25	12/37/135/135	-
10	CLA	aB	830	2	3/3/20/25	9/37/135/135	-
10	CLA	aB	831	2	3/3/16/25	4/11/111/135	-
10	CLA	aB	832	2	3/3/20/25	14/37/135/135	-
10	CLA	aB	833	2	3/3/18/25	14/29/127/135	-
10	CLA	aB	834	2	3/3/16/25	0/11/111/135	-
10	CLA	aB	835	-	3/3/16/25	3/11/111/135	-
10	CLA	aB	836	-	2/2/16/25	1/11/111/135	-
10	CLA	aB	837	2	3/3/19/25	10/31/129/135	-
10	CLA	aB	838	2	3/3/20/25	9/37/135/135	-
10	CLA	aB	839	2	3/3/16/25	5/16/114/135	-
10	CLA	aB	840	-	3/3/20/25	2/37/135/135	-
10	CLA	aB	841	2	3/3/20/25	10/37/135/135	-
11	PQN	aB	842	-	-	2/23/43/43	0/2/2/2
13	BCR	aB	843	-	-	11/29/63/63	0/2/2/2
13	BCR	aB	844	-	-	10/29/63/63	0/2/2/2
13	BCR	aB	845	-	-	12/29/63/63	0/2/2/2
13	BCR	aB	846	-	-	8/29/63/63	0/2/2/2
13	BCR	aB	847	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LMG	aB	848	-	-	19/50/70/70	0/1/1/1
13	BCR	aB	849	-	-	18/29/63/63	0/2/2/2
12	SF4	aC	101	3	-	-	0/6/5/5
12	SF4	aC	102	3	-	-	0/6/5/5
13	BCR	aI	101	-	-	8/29/63/63	0/2/2/2
13	BCR	aI	102	-	-	8/29/63/63	0/2/2/2
10	CLA	aL	202	2	3/3/18/25	7/25/123/135	-
10	CLA	aL	203	7	2/2/20/25	11/37/135/135	-
10	CLA	aL	204	7	3/3/20/25	8/37/135/135	-
10	CLA	aL	205	-	2/2/20/25	10/37/135/135	-
13	BCR	aL	206	-	-	8/29/63/63	0/2/2/2
13	BCR	aL	207	-	-	7/29/63/63	0/2/2/2
13	BCR	aM	101	-	-	13/29/63/63	0/2/2/2
9	CL0	bA	801	1	3/3/20/25	6/37/135/135	-
10	CLA	bA	802	1	2/2/16/25	5/11/111/135	-
10	CLA	bA	803	1	3/3/16/25	3/11/111/135	-
10	CLA	bA	804	1	3/3/20/25	10/37/135/135	-
10	CLA	bA	805	1	3/3/20/25	9/37/135/135	-
10	CLA	bA	806	1	3/3/17/25	3/21/119/135	-
10	CLA	bA	807	1	3/3/16/25	7/11/111/135	-
10	CLA	bA	808	1	3/3/16/25	2/11/111/135	-
10	CLA	bA	809	1	3/3/16/25	2/11/111/135	-
10	CLA	bA	810	1	3/3/20/25	10/37/135/135	-
10	CLA	bA	811	1	3/3/17/25	8/24/122/135	-
10	CLA	bA	812	1	3/3/20/25	15/37/135/135	-
10	CLA	bA	813	1	3/3/16/25	1/11/111/135	-
10	CLA	bA	814	1	3/3/16/25	2/11/111/135	-
10	CLA	bA	815	-	3/3/16/25	3/18/116/135	-
10	CLA	bA	816	1	2/2/17/25	10/24/122/135	-
10	CLA	bA	817	1	2/2/17/25	10/24/122/135	-
10	CLA	bA	818	1	2/2/20/25	13/37/135/135	-
10	CLA	bA	819	1	3/3/19/25	11/33/131/135	-
10	CLA	bA	820	-	3/3/20/25	13/37/135/135	-
10	CLA	bA	821	1	3/3/16/25	4/18/116/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bA	822	1	2/2/17/25	10/21/119/135	-
10	CLA	bA	823	1	3/3/20/25	12/37/135/135	-
10	CLA	bA	824	-	3/3/20/25	11/37/135/135	-
10	CLA	bA	825	-	3/3/18/25	9/25/123/135	-
10	CLA	bA	826	1	3/3/20/25	8/37/135/135	-
10	CLA	bA	827	1	2/2/20/25	17/37/135/135	-
10	CLA	bA	828	1	3/3/20/25	6/37/135/135	-
10	CLA	bA	829	1	3/3/20/25	12/37/135/135	-
10	CLA	bA	830	1	3/3/17/25	5/19/117/135	-
10	CLA	bA	831	1	3/3/20/25	13/37/135/135	-
10	CLA	bA	832	1	3/3/20/25	6/37/135/135	-
10	CLA	bA	833	1	3/3/20/25	10/37/135/135	-
10	CLA	bA	834	1	3/3/17/25	8/24/122/135	-
10	CLA	bA	835	1	3/3/20/25	11/37/135/135	-
10	CLA	bA	836	1	3/3/17/25	7/21/119/135	-
10	CLA	bA	837	1	3/3/20/25	7/37/135/135	-
10	CLA	bA	838	1	3/3/17/25	9/19/117/135	-
10	CLA	bA	839	1	2/2/20/25	6/37/135/135	-
10	CLA	bA	840	-	3/3/17/25	6/21/119/135	-
10	CLA	bA	841	1	3/3/20/25	11/37/135/135	-
10	CLA	bA	842	-	3/3/20/25	14/37/135/135	-
10	CLA	bA	843	-	3/3/14/25	0/5/101/135	-
11	PQN	bA	844	-	-	8/23/43/43	0/2/2/2
12	SF4	bA	845	1,2	-	-	0/6/5/5
13	BCR	bA	846	-	-	14/29/63/63	0/2/2/2
13	BCR	bA	847	-	-	9/29/63/63	0/2/2/2
13	BCR	bA	848	-	-	16/29/63/63	0/2/2/2
13	BCR	bA	849	-	-	13/29/63/63	0/2/2/2
13	BCR	bA	850	-	-	9/29/63/63	0/2/2/2
13	BCR	bA	851	-	-	13/29/63/63	0/2/2/2
14	LHG	bA	852	-	-	31/53/53/53	-
15	LMT	bA	853	-	-	9/21/61/61	0/2/2/2
10	CLA	bA	854	-	2/2/17/25	8/22/120/135	-
14	LHG	bA	855	-	-	15/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bA	856	2	3/3/16/25	7/18/116/135	-
10	CLA	bB	801	-	1/1/20/25	7/37/135/135	-
10	CLA	bB	802	-	3/3/20/25	12/37/135/135	-
10	CLA	bB	803	2	2/2/20/25	5/37/135/135	-
10	CLA	bB	804	-	1/1/18/25	14/28/126/135	-
10	CLA	bB	805	-	2/2/20/25	10/37/135/135	-
10	CLA	bB	806	2	3/3/17/25	12/24/122/135	-
10	CLA	bB	807	2	3/3/20/25	12/37/135/135	-
10	CLA	bB	808	2	3/3/20/25	12/37/135/135	-
10	CLA	bB	809	2	2/2/20/25	6/37/135/135	-
10	CLA	bB	810	2	2/2/18/25	8/25/123/135	-
10	CLA	bB	811	2	2/2/20/25	17/37/135/135	-
10	CLA	bB	812	2	3/3/16/25	1/11/111/135	-
10	CLA	bB	813	2	2/2/16/25	2/11/111/135	-
10	CLA	bB	814	2	3/3/20/25	14/37/135/135	-
10	CLA	bB	815	2	3/3/18/25	7/27/125/135	-
10	CLA	bB	816	2	3/3/16/25	2/11/111/135	-
10	CLA	bB	817	2	3/3/18/25	10/25/123/135	-
10	CLA	bB	818	2	3/3/18/25	11/30/128/135	-
10	CLA	bB	819	2	3/3/19/25	10/31/129/135	-
10	CLA	bB	820	-	3/3/20/25	11/37/135/135	-
10	CLA	bB	821	2	3/3/16/25	4/16/114/135	-
10	CLA	bB	822	2	2/2/16/25	7/11/111/135	-
10	CLA	bB	823	2	3/3/18/25	13/25/123/135	-
10	CLA	bB	824	2	3/3/16/25	3/11/111/135	-
10	CLA	bB	825	2	3/3/17/25	7/24/122/135	-
10	CLA	bB	826	-	3/3/20/25	11/37/135/135	-
10	CLA	bB	827	2	3/3/20/25	9/37/135/135	-
10	CLA	bB	828	2	1/1/20/25	11/37/135/135	-
10	CLA	bB	829	2	3/3/20/25	12/37/135/135	-
10	CLA	bB	830	2	3/3/20/25	9/37/135/135	-
10	CLA	bB	831	2	3/3/16/25	4/11/111/135	-
10	CLA	bB	832	2	3/3/20/25	14/37/135/135	-
10	CLA	bB	833	2	3/3/18/25	14/29/127/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bB	834	2	3/3/16/25	0/11/111/135	-
10	CLA	bB	835	-	3/3/16/25	3/11/111/135	-
10	CLA	bB	836	-	2/2/16/25	1/11/111/135	-
10	CLA	bB	837	2	3/3/19/25	10/31/129/135	-
10	CLA	bB	838	2	3/3/20/25	9/37/135/135	-
10	CLA	bB	839	2	3/3/16/25	5/16/114/135	-
10	CLA	bB	840	-	3/3/20/25	2/37/135/135	-
10	CLA	bB	841	2	3/3/20/25	10/37/135/135	-
11	PQN	bB	842	-	-	2/23/43/43	0/2/2/2
13	BCR	bB	843	-	-	11/29/63/63	0/2/2/2
13	BCR	bB	844	-	-	10/29/63/63	0/2/2/2
13	BCR	bB	845	-	-	12/29/63/63	0/2/2/2
13	BCR	bB	846	-	-	8/29/63/63	0/2/2/2
13	BCR	bB	847	-	-	10/29/63/63	0/2/2/2
16	LMG	bB	848	-	-	19/50/70/70	0/1/1/1
13	BCR	bB	849	-	-	18/29/63/63	0/2/2/2
12	SF4	bC	101	3	-	-	0/6/5/5
12	SF4	bC	102	3	-	-	0/6/5/5
13	BCR	bI	101	-	-	8/29/63/63	0/2/2/2
13	BCR	bI	102	-	-	8/29/63/63	0/2/2/2
10	CLA	bL	202	2	3/3/18/25	7/25/123/135	-
10	CLA	bL	203	7	2/2/20/25	11/37/135/135	-
10	CLA	bL	204	7	3/3/20/25	8/37/135/135	-
10	CLA	bL	205	-	2/2/20/25	10/37/135/135	-
13	BCR	bL	206	-	-	8/29/63/63	0/2/2/2
13	BCR	bL	207	-	-	7/29/63/63	0/2/2/2
13	BCR	bM	101	-	-	13/29/63/63	0/2/2/2
9	CL0	cA	801	1	3/3/20/25	6/37/135/135	-
10	CLA	cA	802	1	2/2/16/25	5/11/111/135	-
10	CLA	cA	803	1	3/3/16/25	3/11/111/135	-
10	CLA	cA	804	1	3/3/20/25	10/37/135/135	-
10	CLA	cA	805	1	3/3/20/25	9/37/135/135	-
10	CLA	cA	806	1	3/3/17/25	3/21/119/135	-
10	CLA	cA	807	1	3/3/16/25	7/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cA	808	1	3/3/16/25	2/11/111/135	-
10	CLA	cA	809	1	3/3/16/25	2/11/111/135	-
10	CLA	cA	810	1	3/3/20/25	10/37/135/135	-
10	CLA	cA	811	1	3/3/17/25	8/24/122/135	-
10	CLA	cA	812	1	3/3/20/25	15/37/135/135	-
10	CLA	cA	813	1	3/3/16/25	1/11/111/135	-
10	CLA	cA	814	1	3/3/16/25	2/11/111/135	-
10	CLA	cA	815	-	3/3/16/25	3/18/116/135	-
10	CLA	cA	816	1	2/2/17/25	10/24/122/135	-
10	CLA	cA	817	1	2/2/17/25	10/24/122/135	-
10	CLA	cA	818	1	2/2/20/25	13/37/135/135	-
10	CLA	cA	819	1	3/3/19/25	11/33/131/135	-
10	CLA	cA	820	-	3/3/20/25	13/37/135/135	-
10	CLA	cA	821	1	3/3/16/25	4/18/116/135	-
10	CLA	cA	822	1	2/2/17/25	10/21/119/135	-
10	CLA	cA	823	1	3/3/20/25	12/37/135/135	-
10	CLA	cA	824	-	3/3/20/25	11/37/135/135	-
10	CLA	cA	825	-	3/3/18/25	9/25/123/135	-
10	CLA	cA	826	1	3/3/20/25	8/37/135/135	-
10	CLA	cA	827	1	2/2/20/25	17/37/135/135	-
10	CLA	cA	828	1	3/3/20/25	6/37/135/135	-
10	CLA	cA	829	1	3/3/20/25	12/37/135/135	-
10	CLA	cA	830	1	3/3/17/25	5/19/117/135	-
10	CLA	cA	831	1	3/3/20/25	13/37/135/135	-
10	CLA	cA	832	1	3/3/20/25	6/37/135/135	-
10	CLA	cA	833	1	3/3/20/25	10/37/135/135	-
10	CLA	cA	834	1	3/3/17/25	8/24/122/135	-
10	CLA	cA	835	1	3/3/20/25	11/37/135/135	-
10	CLA	cA	836	1	3/3/17/25	7/21/119/135	-
10	CLA	cA	837	1	3/3/20/25	7/37/135/135	-
10	CLA	cA	838	1	3/3/17/25	9/19/117/135	-
10	CLA	cA	839	1	2/2/20/25	6/37/135/135	-
10	CLA	cA	840	-	3/3/17/25	6/21/119/135	-
10	CLA	cA	841	1	3/3/20/25	11/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cA	842	-	3/3/20/25	14/37/135/135	-
10	CLA	cA	843	-	3/3/14/25	0/5/101/135	-
11	PQN	cA	844	-	-	8/23/43/43	0/2/2/2
12	SF4	cA	845	1,2	-	-	0/6/5/5
13	BCR	cA	846	-	-	14/29/63/63	0/2/2/2
13	BCR	cA	847	-	-	9/29/63/63	0/2/2/2
13	BCR	cA	848	-	-	16/29/63/63	0/2/2/2
13	BCR	cA	849	-	-	13/29/63/63	0/2/2/2
13	BCR	cA	850	-	-	9/29/63/63	0/2/2/2
13	BCR	cA	851	-	-	13/29/63/63	0/2/2/2
14	LHG	cA	852	-	-	31/53/53/53	-
15	LMT	cA	853	-	-	9/21/61/61	0/2/2/2
10	CLA	cA	854	14	2/2/17/25	8/22/120/135	-
14	LHG	cA	855	10	-	15/31/31/53	-
10	CLA	cA	856	2	3/3/16/25	7/18/116/135	-
10	CLA	cB	801	-	1/1/20/25	7/37/135/135	-
10	CLA	cB	802	-	3/3/20/25	12/37/135/135	-
10	CLA	cB	803	2	2/2/20/25	5/37/135/135	-
10	CLA	cB	804	-	1/1/18/25	14/28/126/135	-
10	CLA	cB	805	-	2/2/20/25	10/37/135/135	-
10	CLA	cB	806	2	3/3/17/25	11/24/122/135	-
10	CLA	cB	807	2	3/3/20/25	12/37/135/135	-
10	CLA	cB	808	2	3/3/20/25	12/37/135/135	-
10	CLA	cB	809	2	2/2/20/25	6/37/135/135	-
10	CLA	cB	810	2	2/2/18/25	8/25/123/135	-
10	CLA	cB	811	2	2/2/20/25	17/37/135/135	-
10	CLA	cB	812	2	3/3/16/25	1/11/111/135	-
10	CLA	cB	813	2	2/2/16/25	2/11/111/135	-
10	CLA	cB	814	2	3/3/20/25	14/37/135/135	-
10	CLA	cB	815	2	3/3/18/25	7/27/125/135	-
10	CLA	cB	816	2	3/3/16/25	2/11/111/135	-
10	CLA	cB	817	2	3/3/18/25	10/25/123/135	-
10	CLA	cB	818	2	3/3/18/25	11/30/128/135	-
10	CLA	cB	819	2	3/3/19/25	10/31/129/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cB	820	-	3/3/20/25	11/37/135/135	-
10	CLA	cB	821	2	3/3/16/25	5/16/114/135	-
10	CLA	cB	822	2	2/2/16/25	7/11/111/135	-
10	CLA	cB	823	2	3/3/18/25	13/25/123/135	-
10	CLA	cB	824	2	3/3/16/25	3/11/111/135	-
10	CLA	cB	825	2	3/3/17/25	7/24/122/135	-
10	CLA	cB	826	-	3/3/20/25	11/37/135/135	-
10	CLA	cB	827	2	3/3/20/25	9/37/135/135	-
10	CLA	cB	828	2	1/1/20/25	11/37/135/135	-
10	CLA	cB	829	2	3/3/20/25	12/37/135/135	-
10	CLA	cB	830	2	3/3/20/25	9/37/135/135	-
10	CLA	cB	831	2	3/3/16/25	4/11/111/135	-
10	CLA	cB	832	2	3/3/20/25	14/37/135/135	-
10	CLA	cB	833	2	3/3/18/25	14/29/127/135	-
10	CLA	cB	834	2	3/3/16/25	0/11/111/135	-
10	CLA	cB	835	-	3/3/16/25	3/11/111/135	-
10	CLA	cB	836	-	2/2/16/25	1/11/111/135	-
10	CLA	cB	837	2	3/3/19/25	10/31/129/135	-
10	CLA	cB	838	2	3/3/20/25	9/37/135/135	-
10	CLA	cB	839	2	3/3/16/25	5/16/114/135	-
10	CLA	cB	840	-	3/3/20/25	2/37/135/135	-
10	CLA	cB	841	2	3/3/20/25	10/37/135/135	-
11	PQN	cB	842	-	-	2/23/43/43	0/2/2/2
13	BCR	cB	843	-	-	11/29/63/63	0/2/2/2
13	BCR	cB	844	-	-	10/29/63/63	0/2/2/2
13	BCR	cB	845	-	-	12/29/63/63	0/2/2/2
13	BCR	cB	846	-	-	8/29/63/63	0/2/2/2
13	BCR	cB	847	-	-	10/29/63/63	0/2/2/2
16	LMG	cB	848	-	-	19/50/70/70	0/1/1/1
13	BCR	cB	849	-	-	18/29/63/63	0/2/2/2
12	SF4	cC	101	3	-	-	0/6/5/5
12	SF4	cC	102	3	-	-	0/6/5/5
13	BCR	cI	102	-	-	8/29/63/63	0/2/2/2
13	BCR	cI	103	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cL	202	2	3/3/18/25	7/25/123/135	-
10	CLA	cL	203	7	2/2/20/25	11/37/135/135	-
10	CLA	cL	204	7	3/3/20/25	8/37/135/135	-
10	CLA	cL	205	-	2/2/20/25	10/37/135/135	-
13	BCR	cL	206	-	-	8/29/63/63	0/2/2/2
13	BCR	cL	207	-	-	7/29/63/63	0/2/2/2
13	BCR	cM	101	-	-	13/29/63/63	0/2/2/2

The worst 5 of 3560 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	aA	828	CLA	C3B-C2B	6.54	1.49	1.40
10	bA	828	CLA	C3B-C2B	6.52	1.49	1.40
10	cA	828	CLA	C3B-C2B	6.52	1.49	1.40
10	cA	836	CLA	C3B-C2B	6.39	1.49	1.40
10	bA	836	CLA	C3B-C2B	6.32	1.49	1.40

The worst 5 of 5907 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	836	CLA	C4-C3-C5	-31.28	79.75	115.99
10	bA	836	CLA	C4-C3-C5	-31.26	79.77	115.99
10	aA	836	CLA	C4-C3-C5	-31.22	79.81	115.99
10	cA	836	CLA	C4-C3-C2	-16.94	79.65	123.68
10	aA	836	CLA	C4-C3-C2	-16.93	79.68	123.68

5 of 738 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	cA	818	CLA	NC
10	cA	818	CLA	ND
10	bB	822	CLA	NC
10	bB	822	CLA	NA
10	bB	806	CLA	NC

5 of 3024 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	cA	818	CLA	C1A-C2A-CAA-CBA
10	cA	818	CLA	CHA-CBD-CGD-O1D

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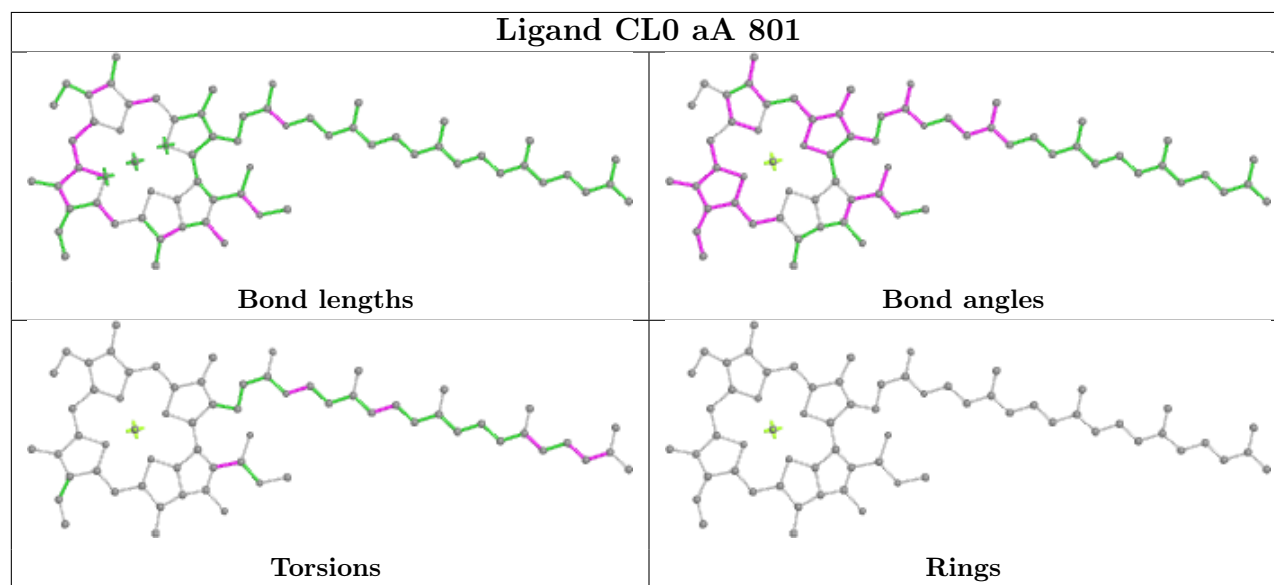
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Mol	Chain	Res	Type	Atoms
10	cA	818	CLA	CHA-CBD-CGD-O2D
15	cA	853	LMT	C2'-C1'-O1'-C1
15	cA	853	LMT	O5'-C1'-O1'-C1

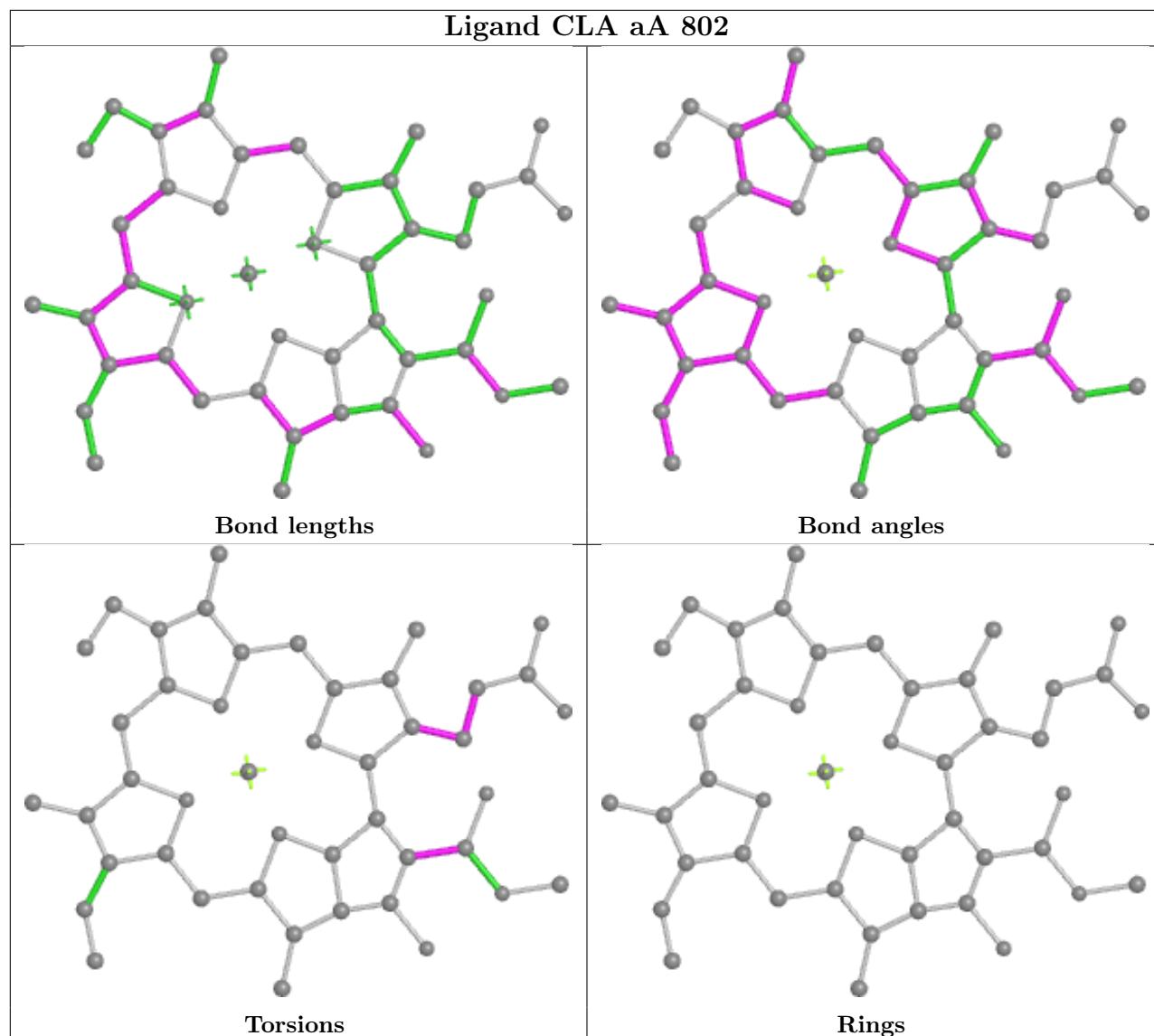
There are no ring outliers.

No monomer is involved in short contacts.

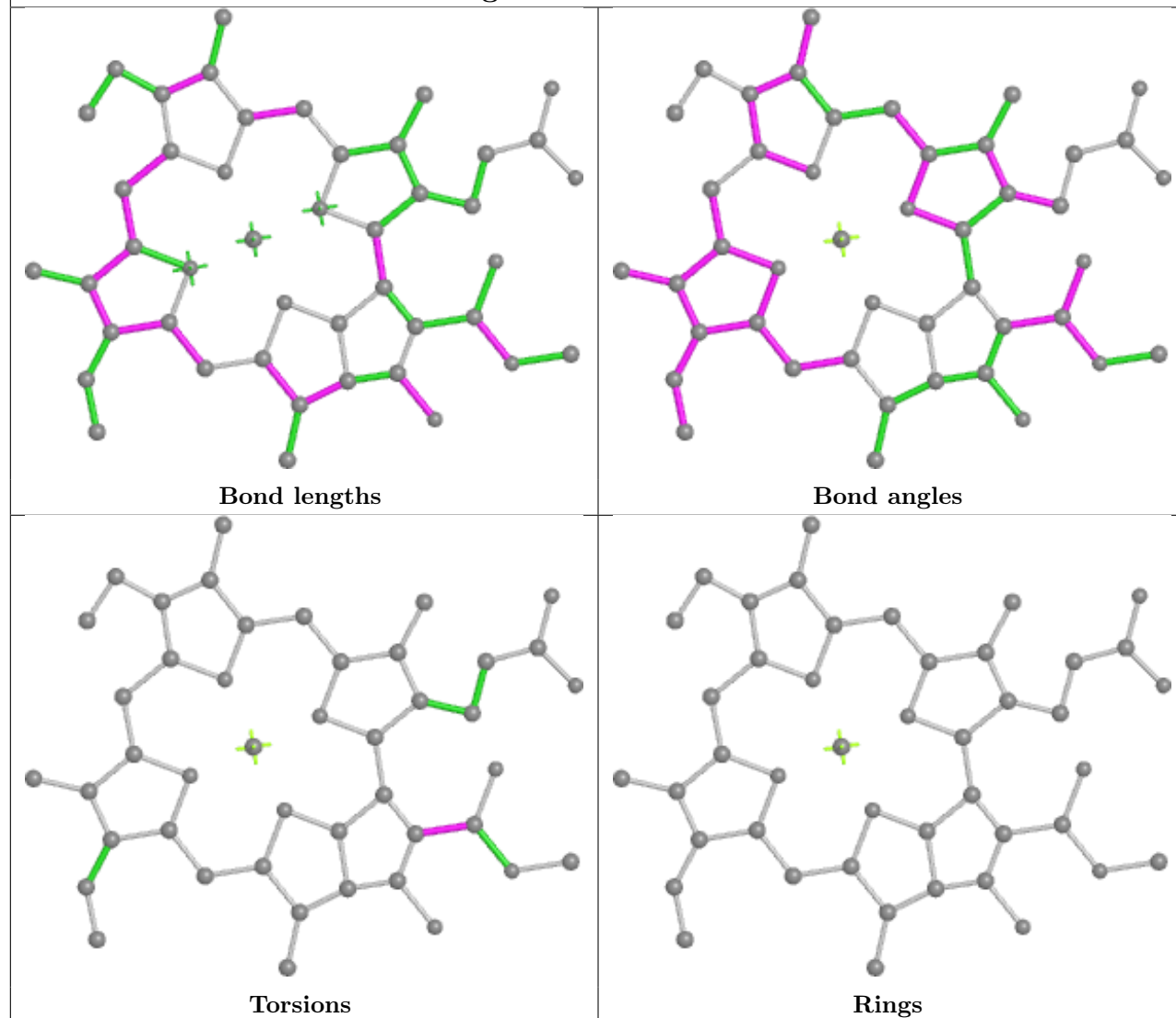
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



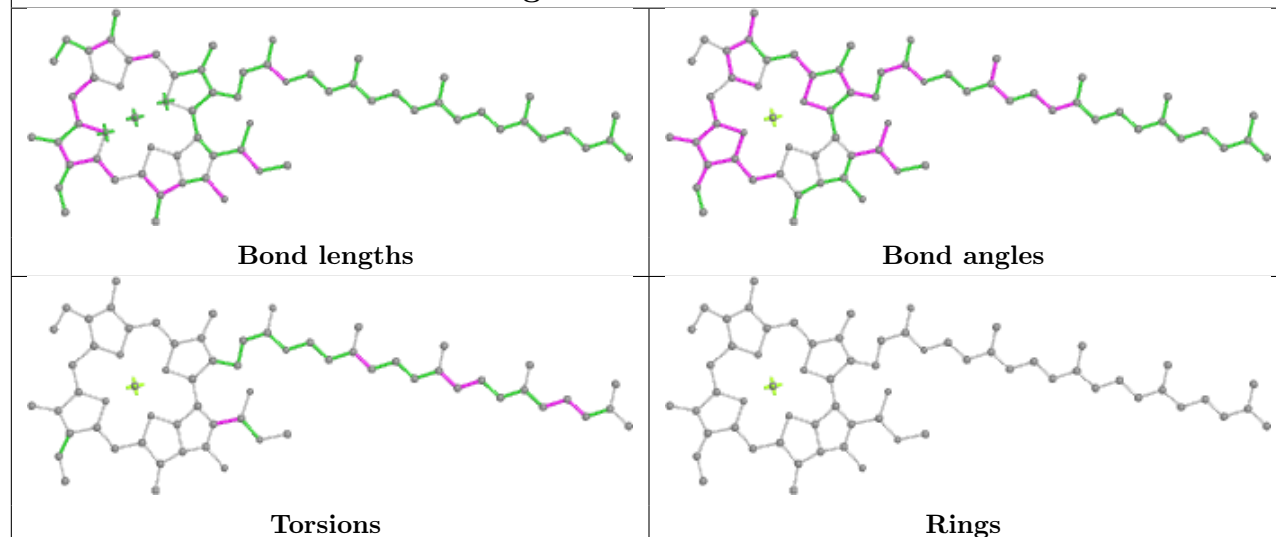
Ligand CLA aA 802



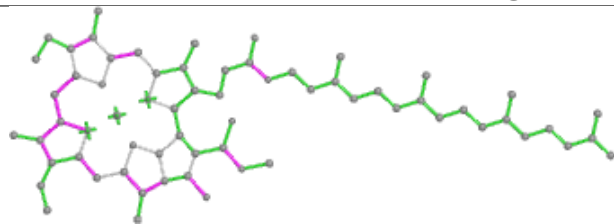
Ligand CLA aA 803



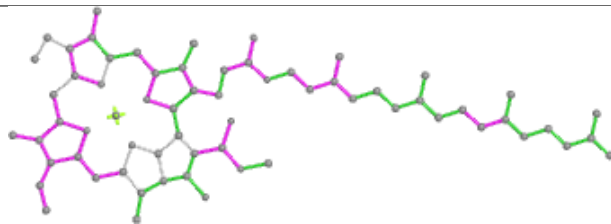
Ligand CLA aA 804



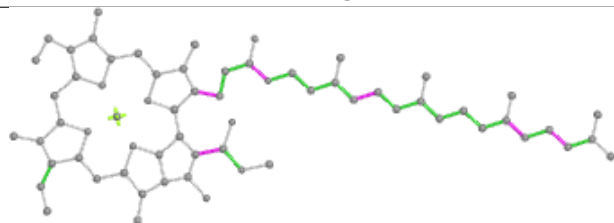
Ligand CLA aA 805



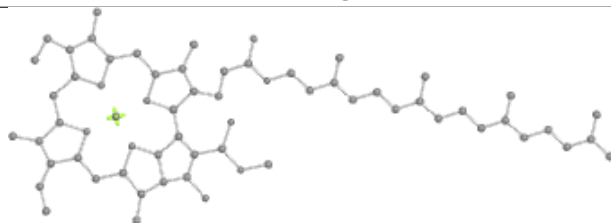
Bond lengths



Bond angles

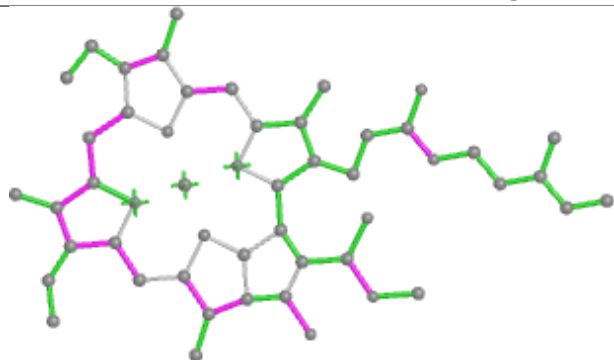


Torsions

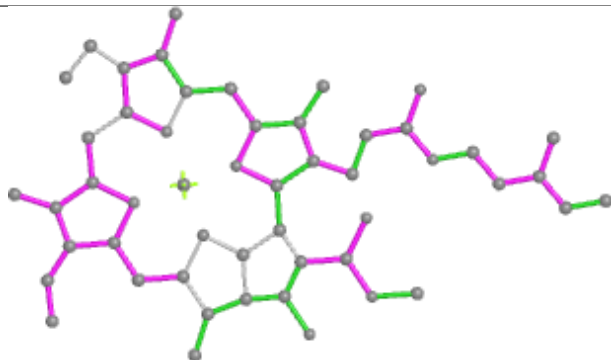


Rings

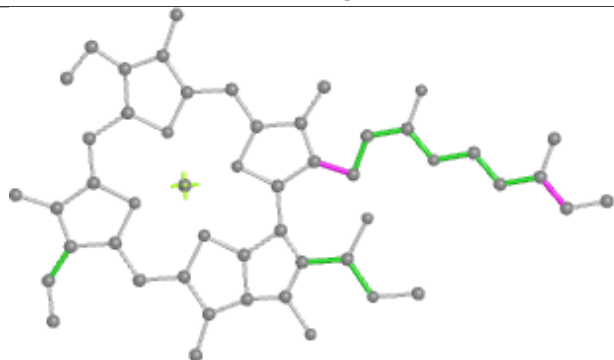
Ligand CLA aA 806



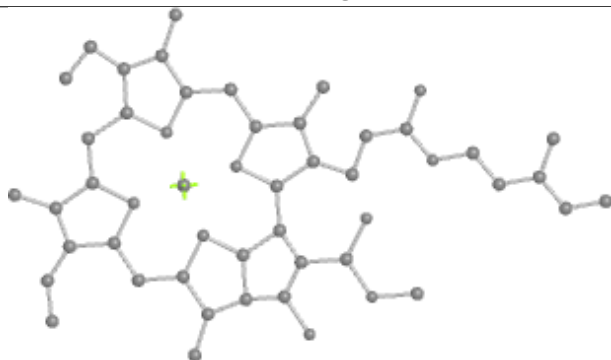
Bond lengths



Bond angles

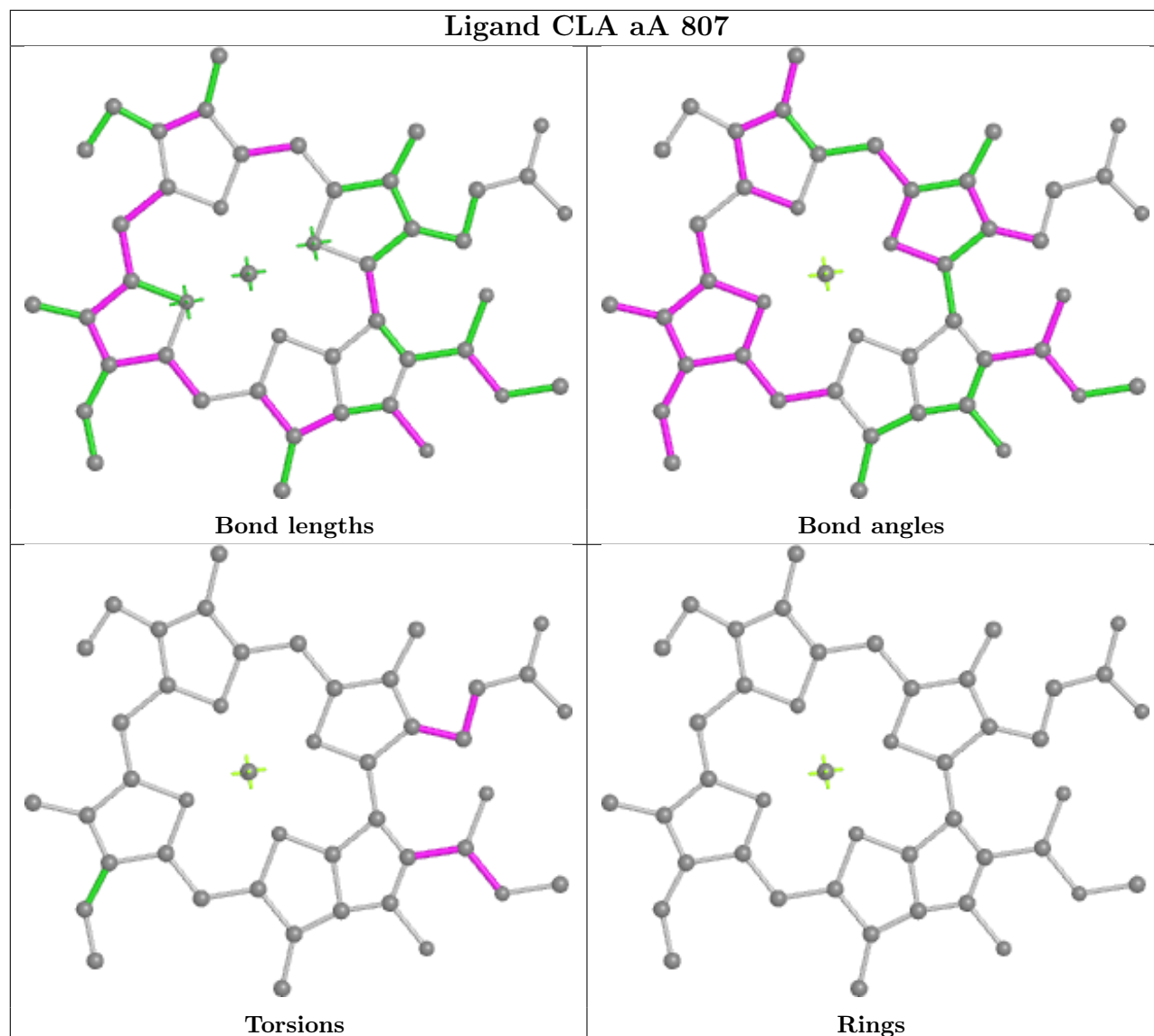


Torsions

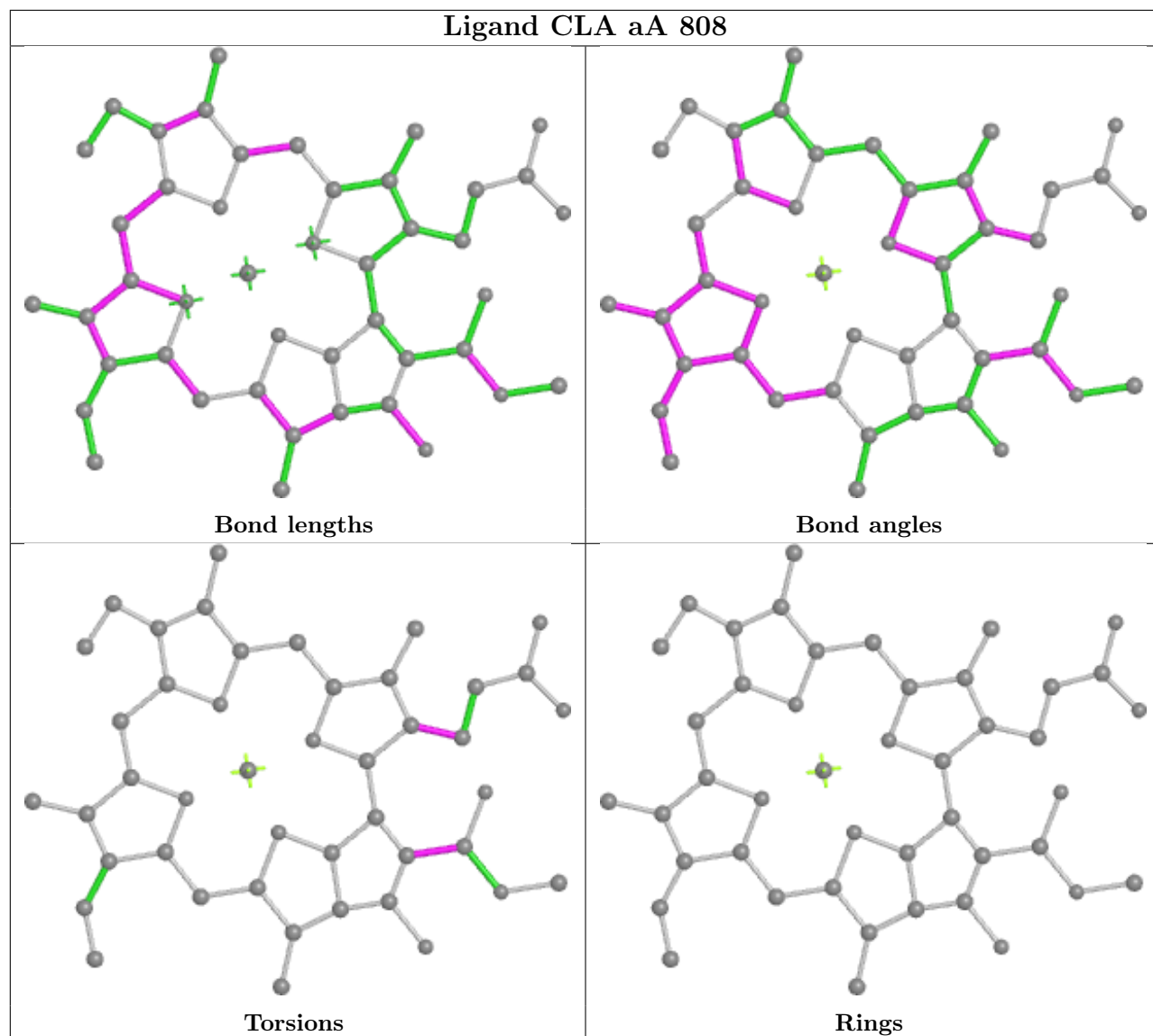


Rings

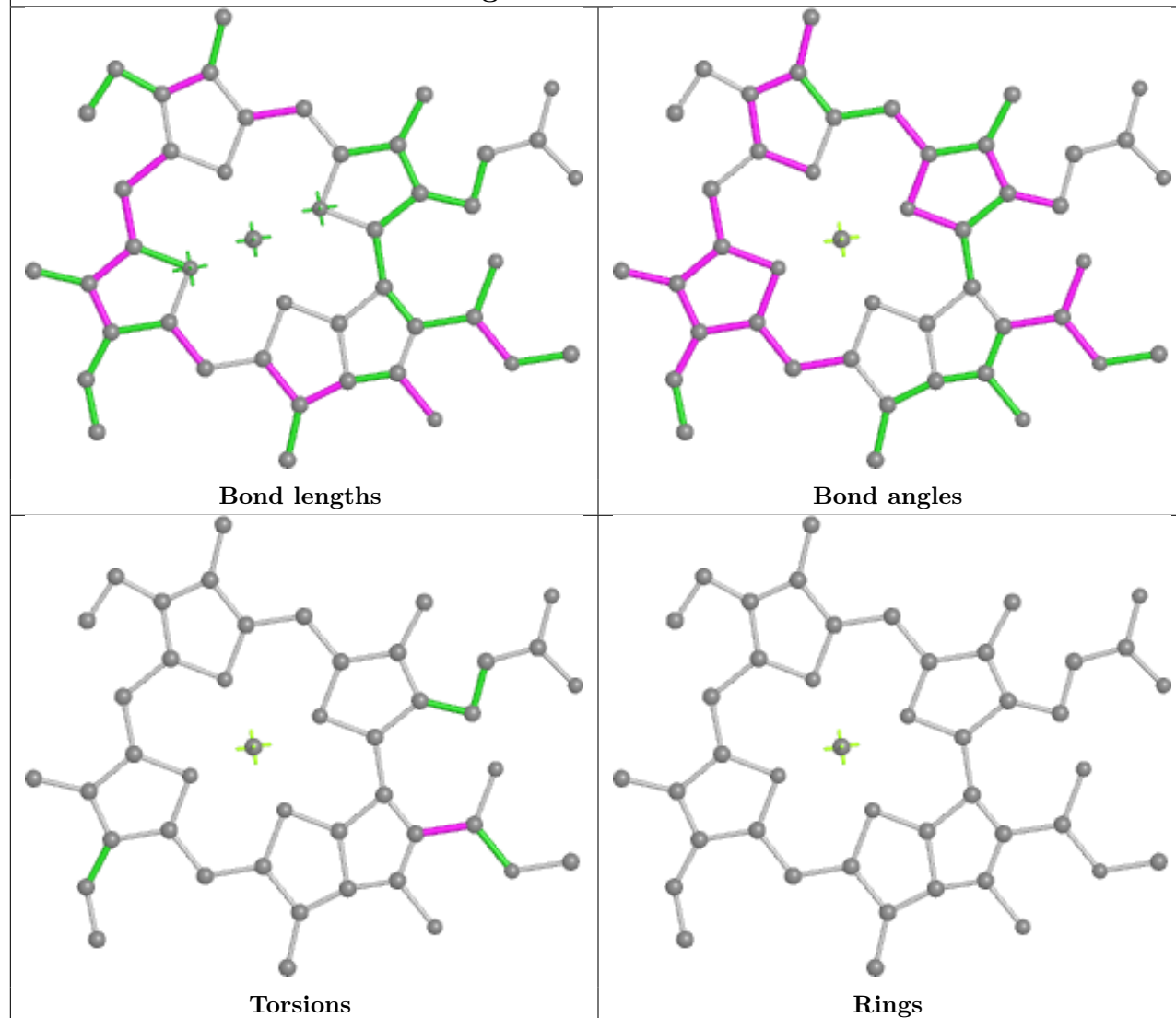
Ligand CLA aA 807



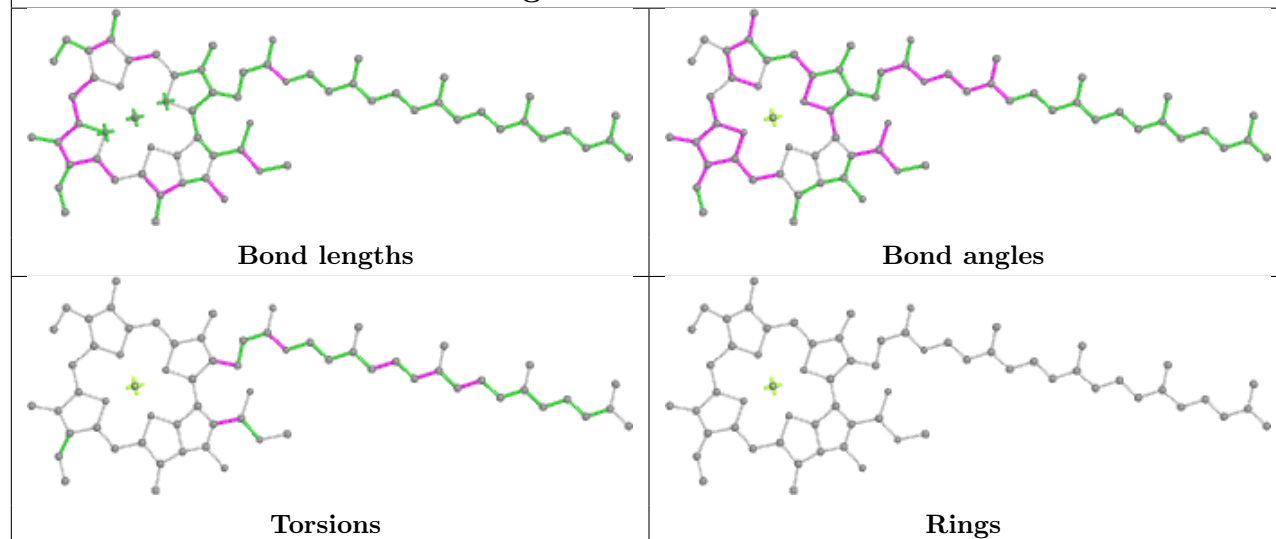
Ligand CLA aA 808

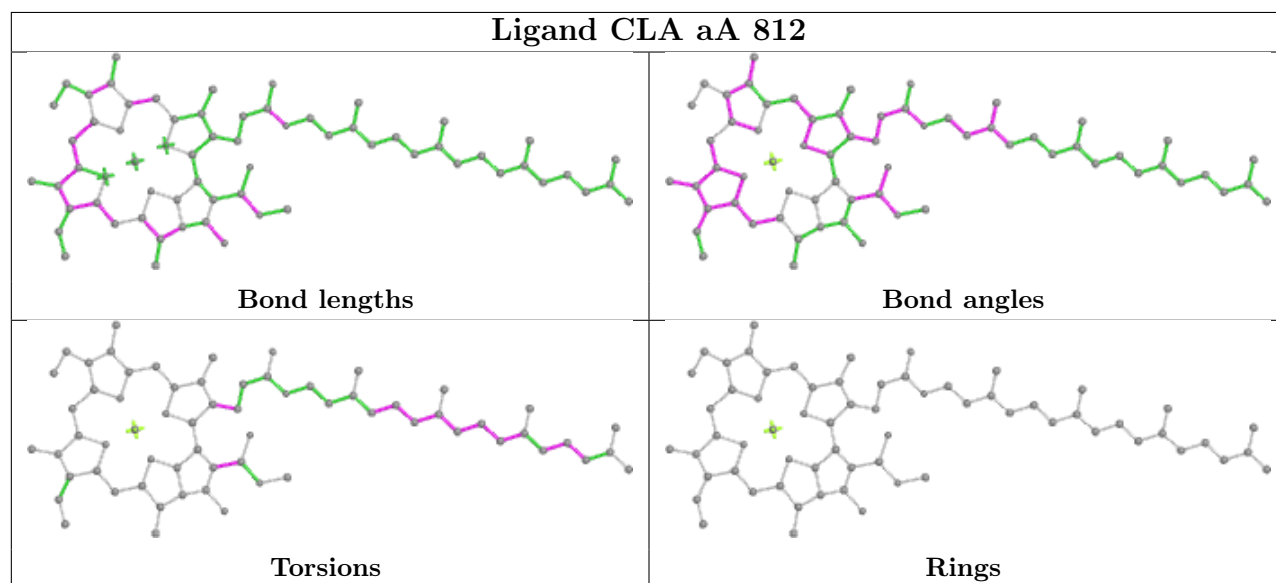
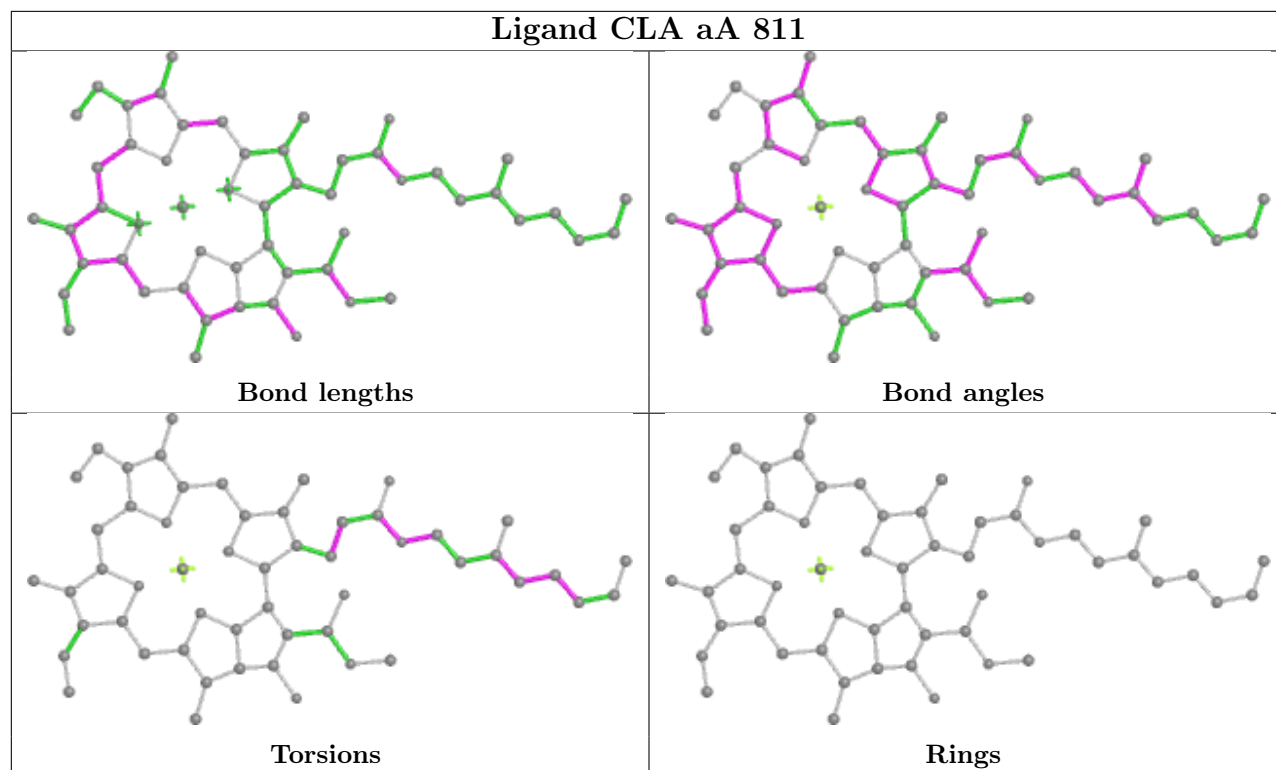


Ligand CLA aA 809

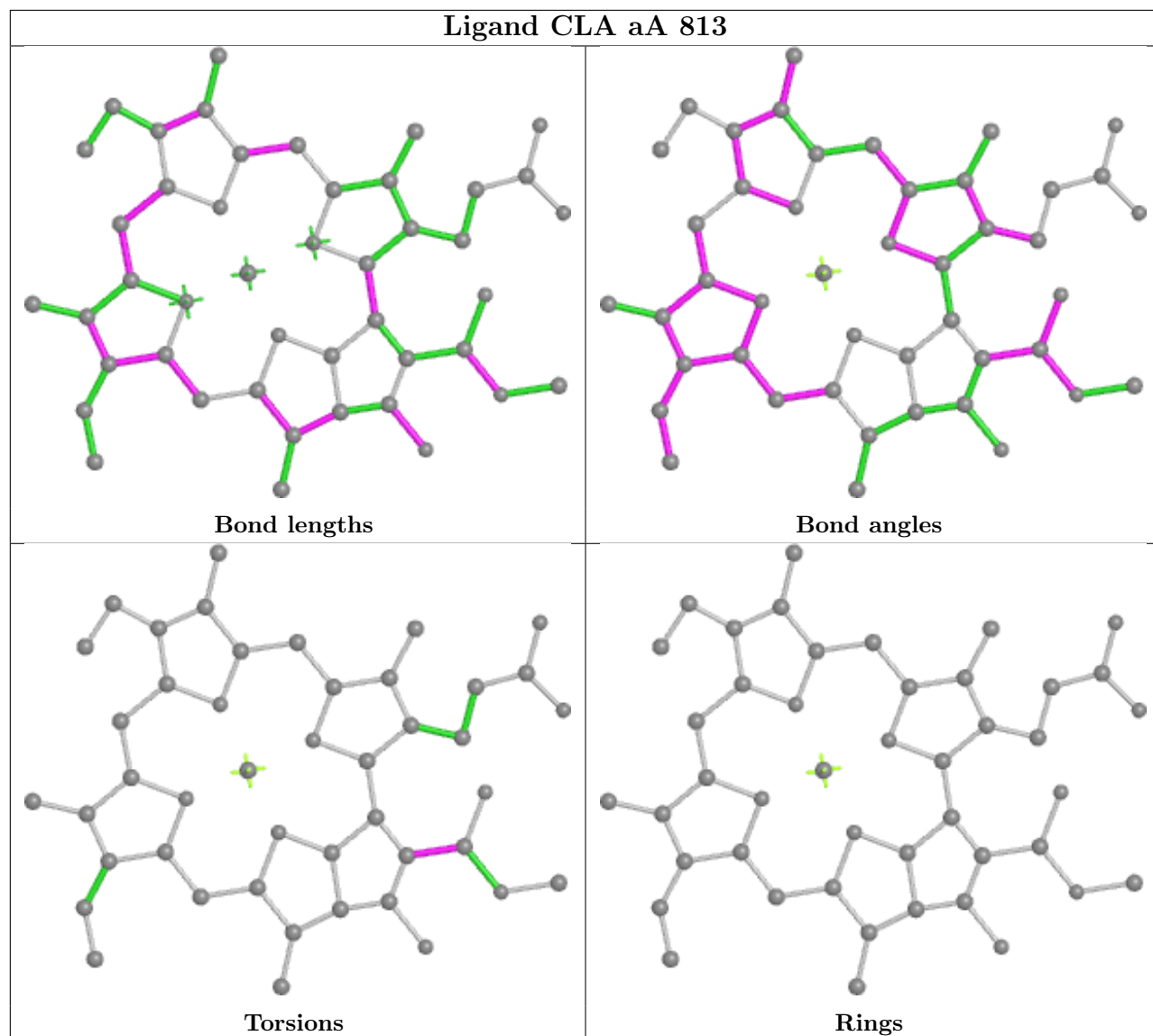


Ligand CLA aA 810

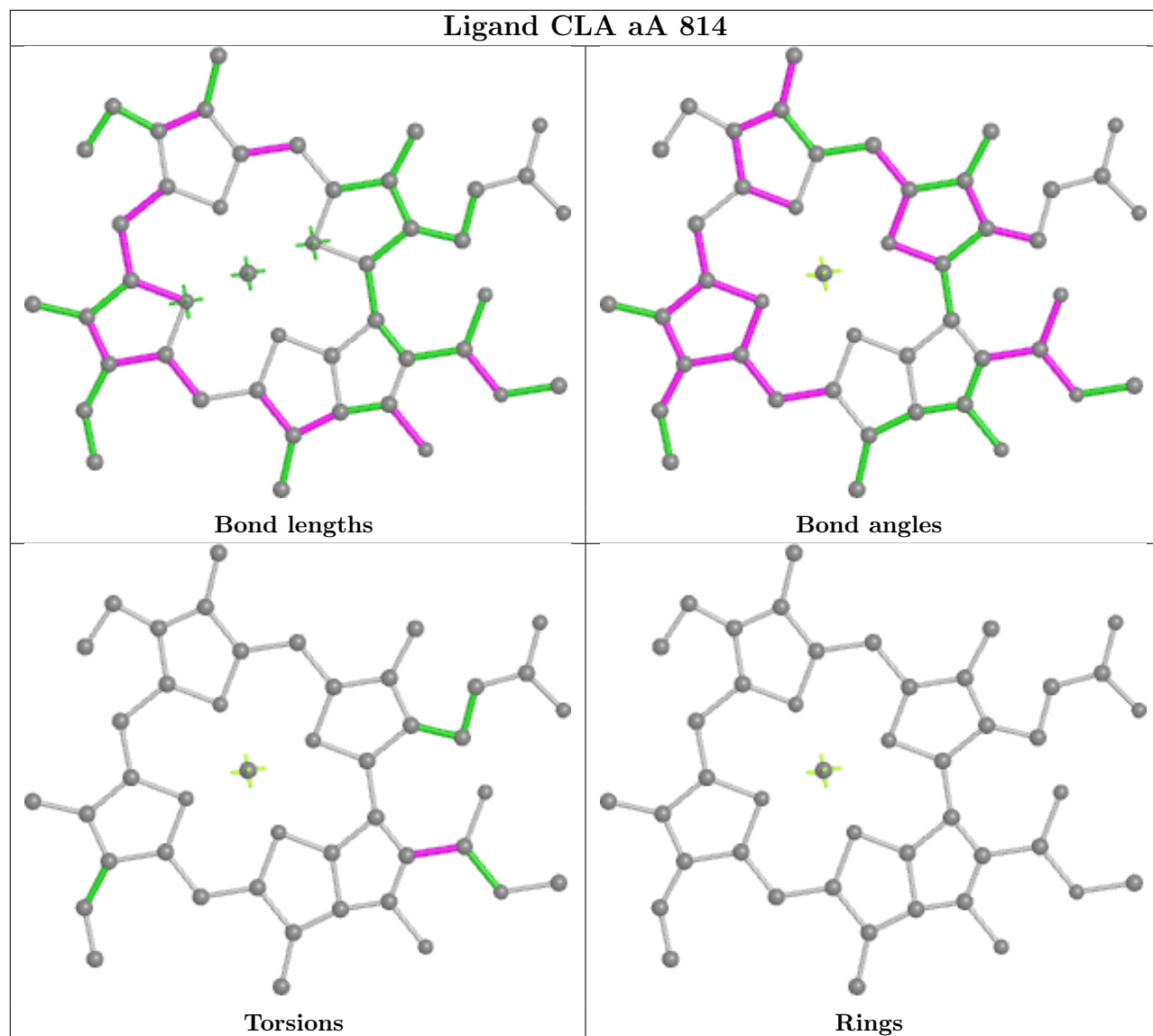




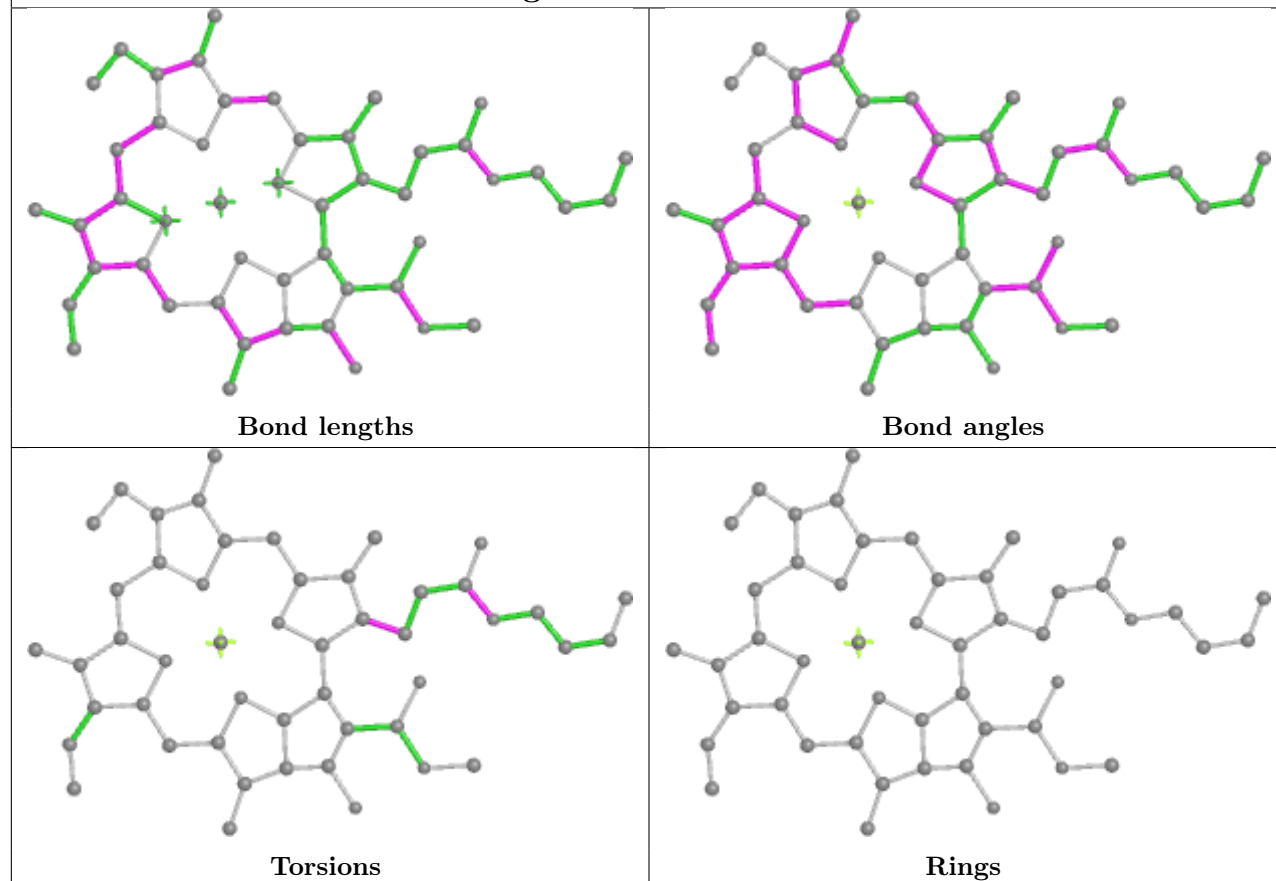
Ligand CLA aA 813



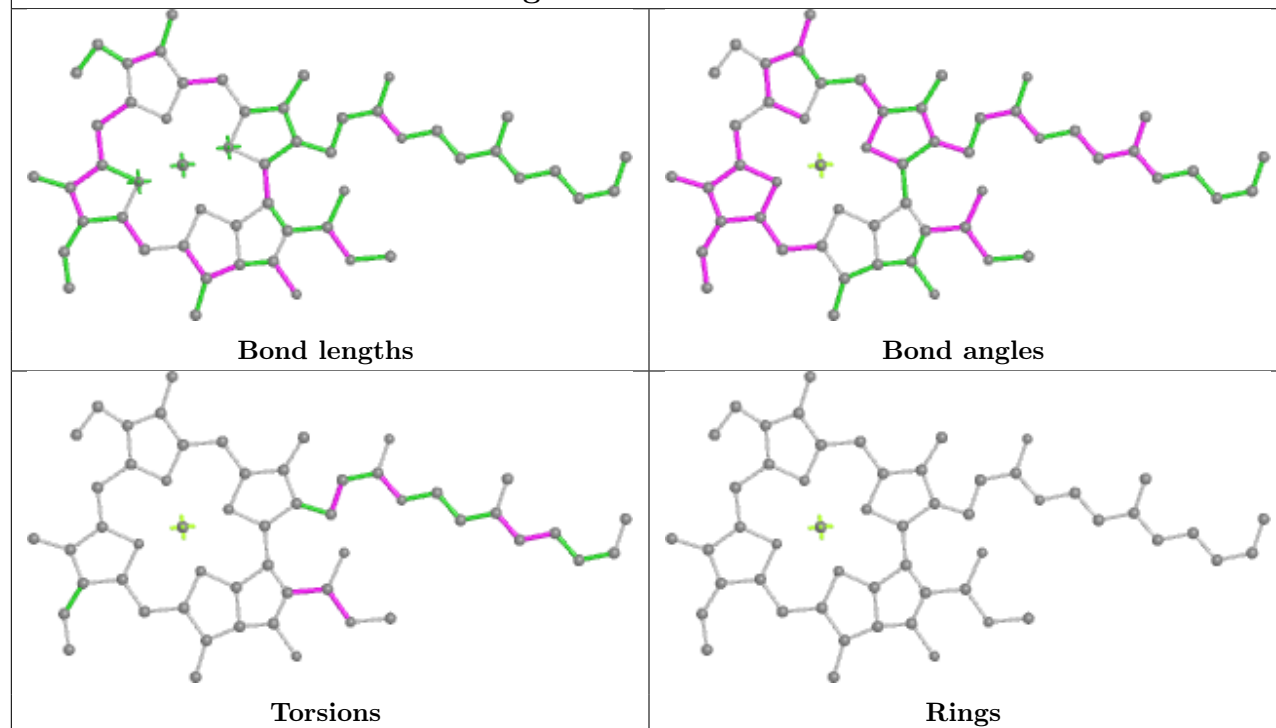
Ligand CLA aA 814

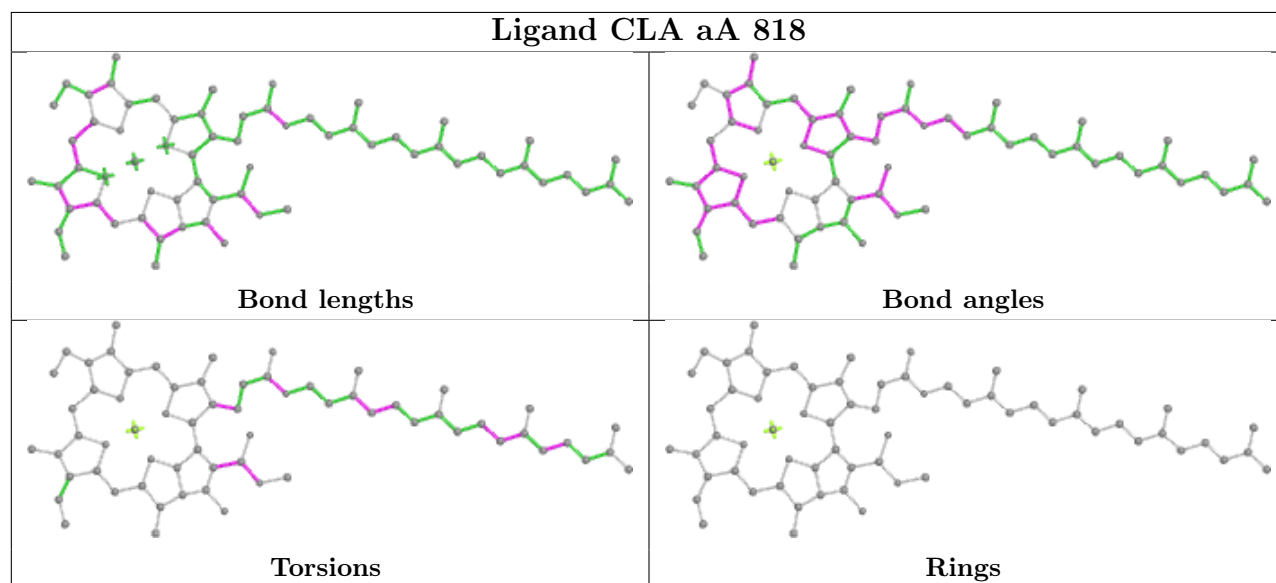
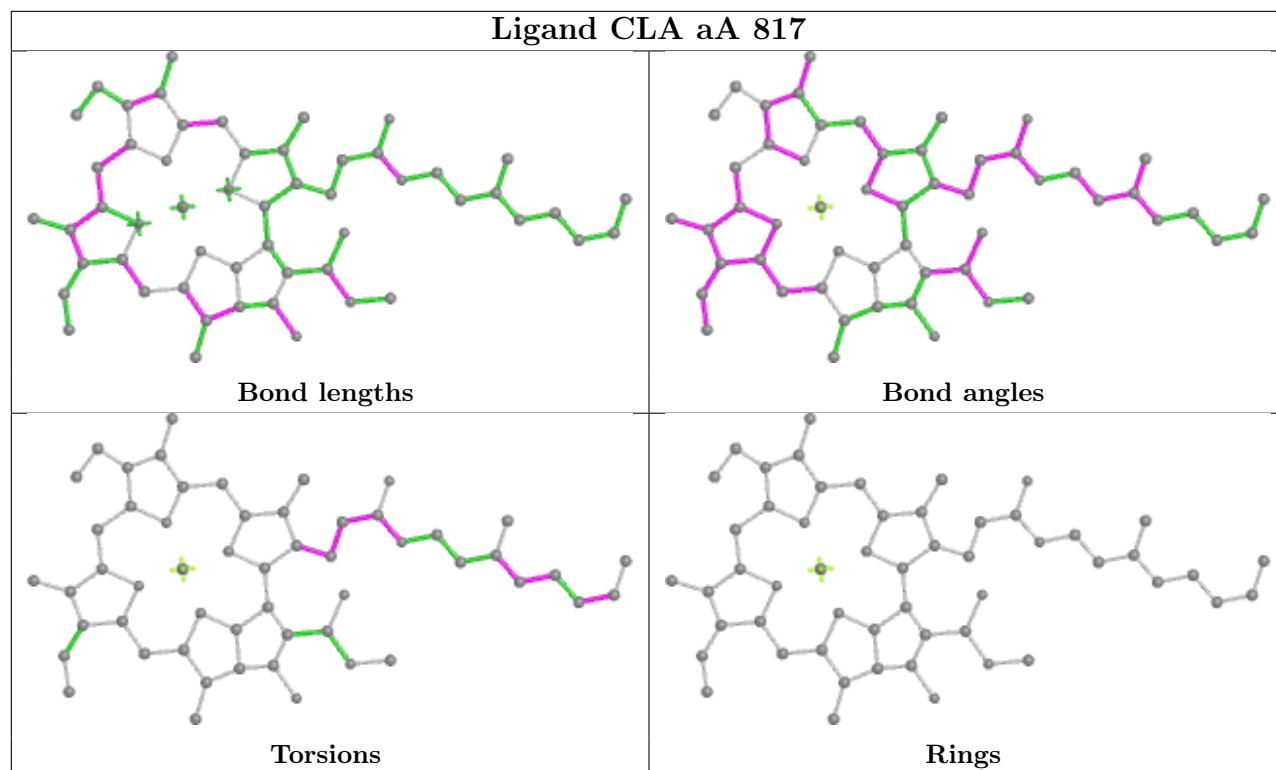


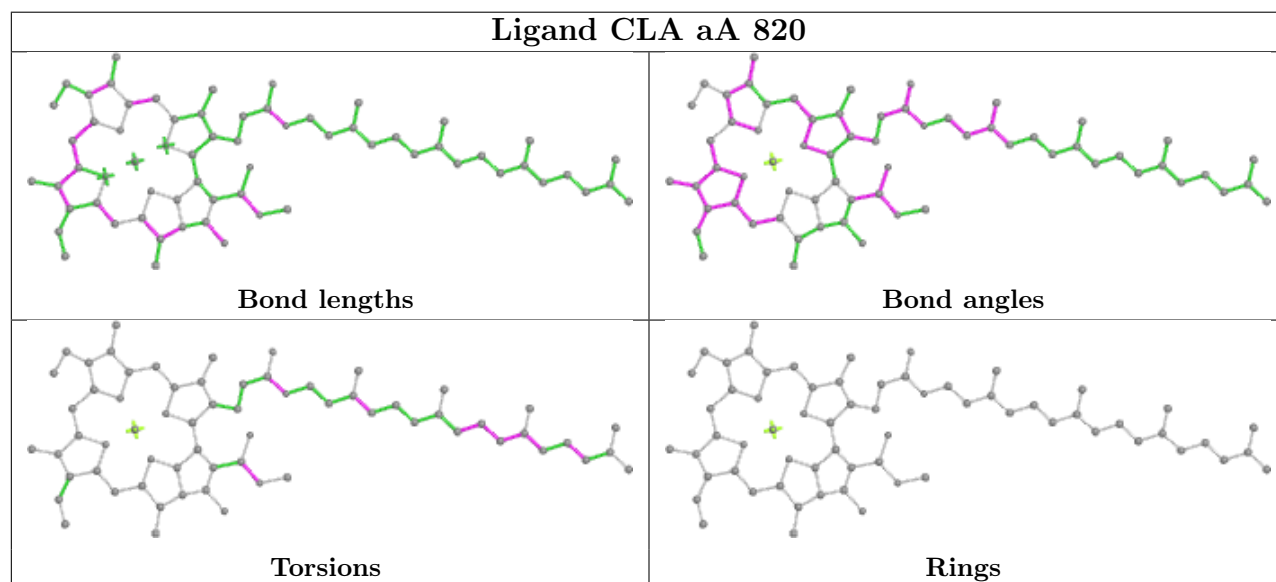
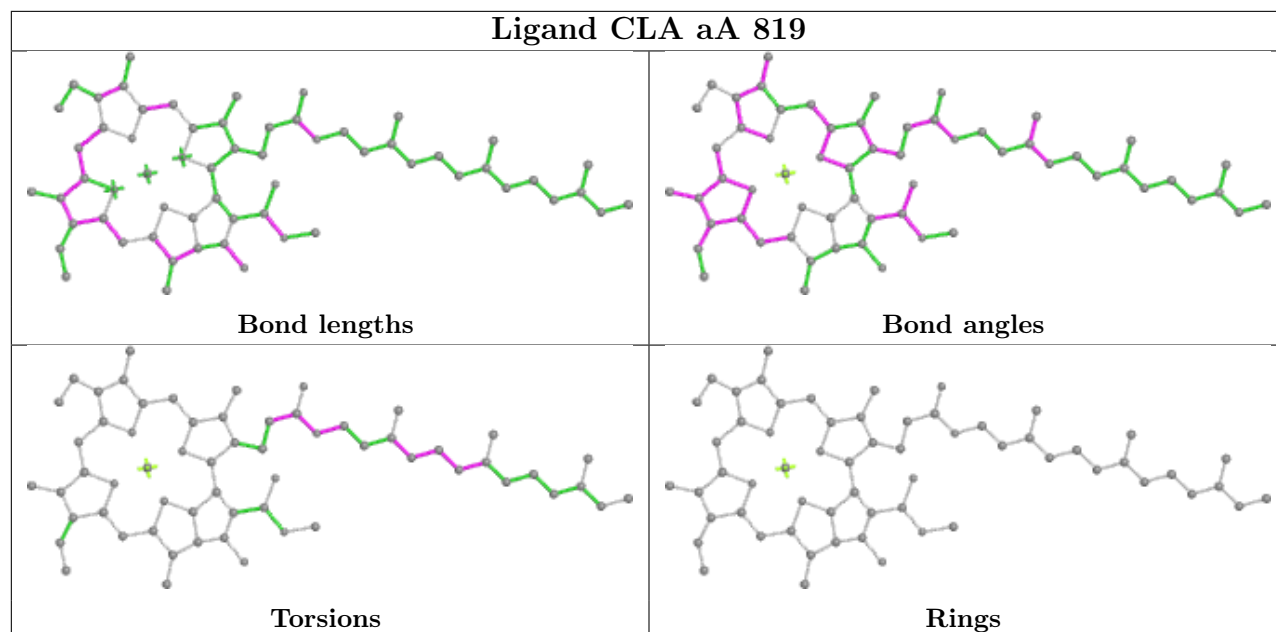
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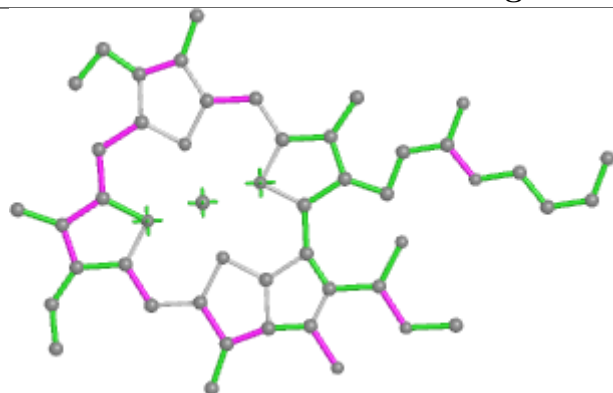
Ligand CLA aA 816



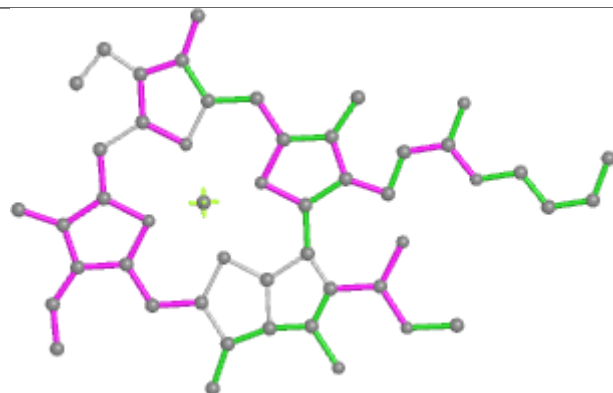




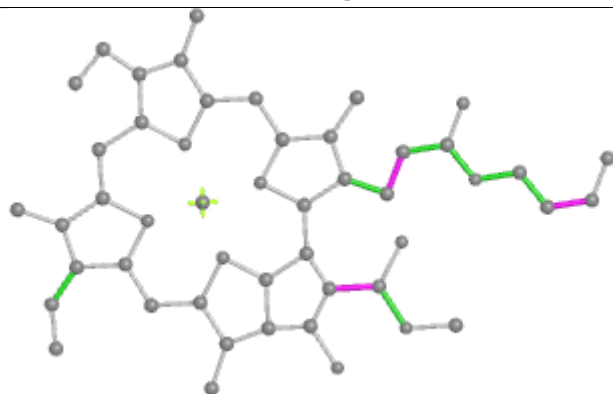
Ligand CLA aA 821



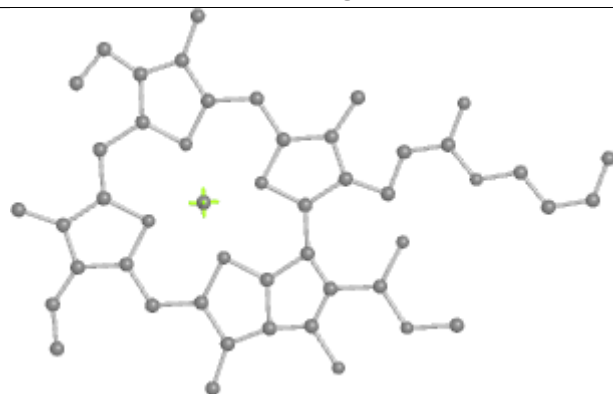
Bond lengths



Bond angles

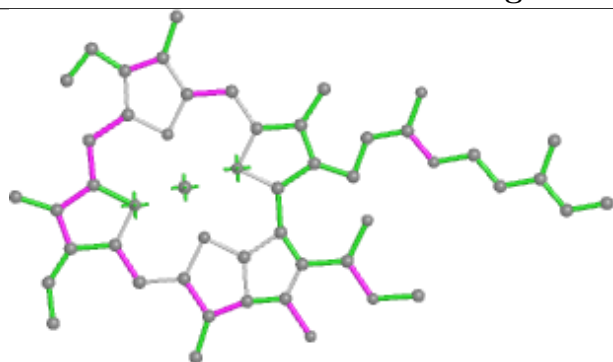


Torsions

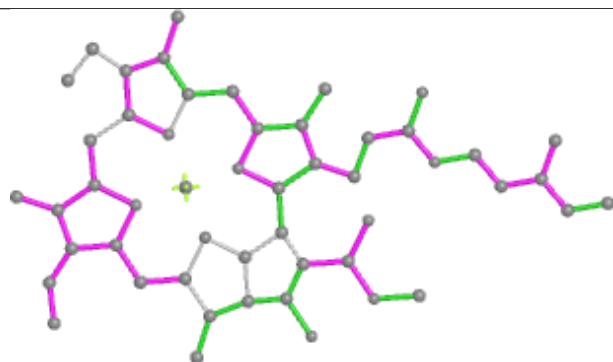


Rings

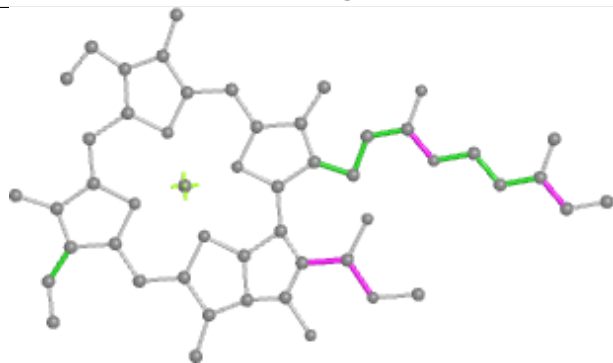
Ligand CLA aA 822



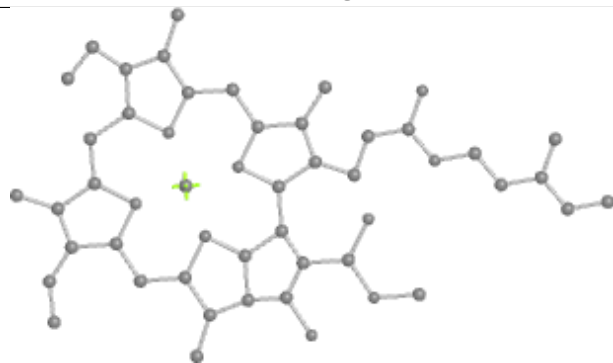
Bond lengths



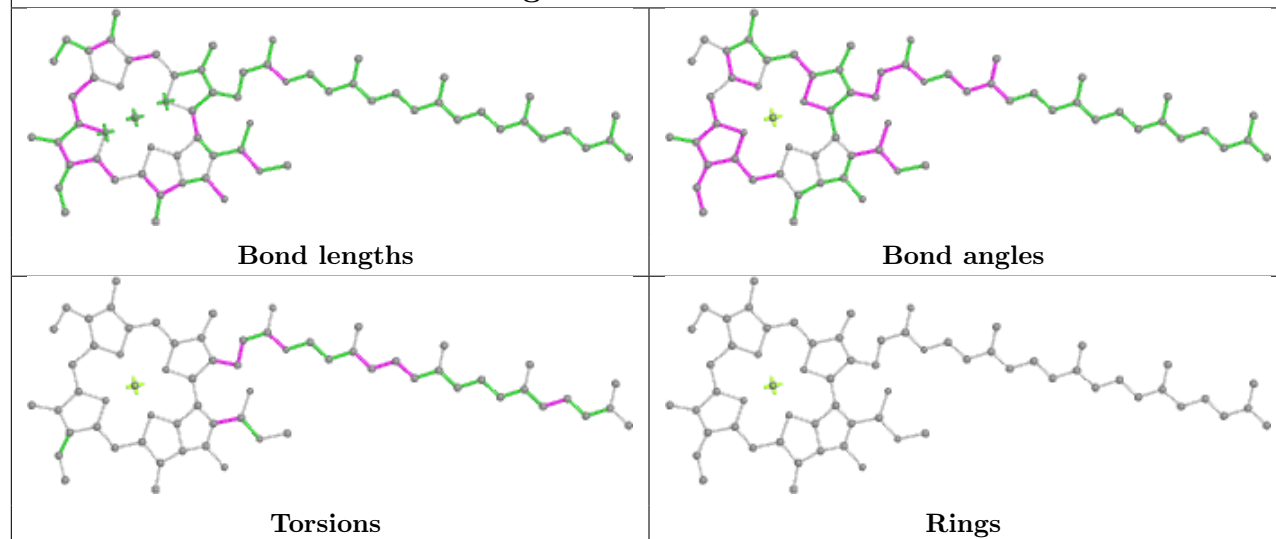
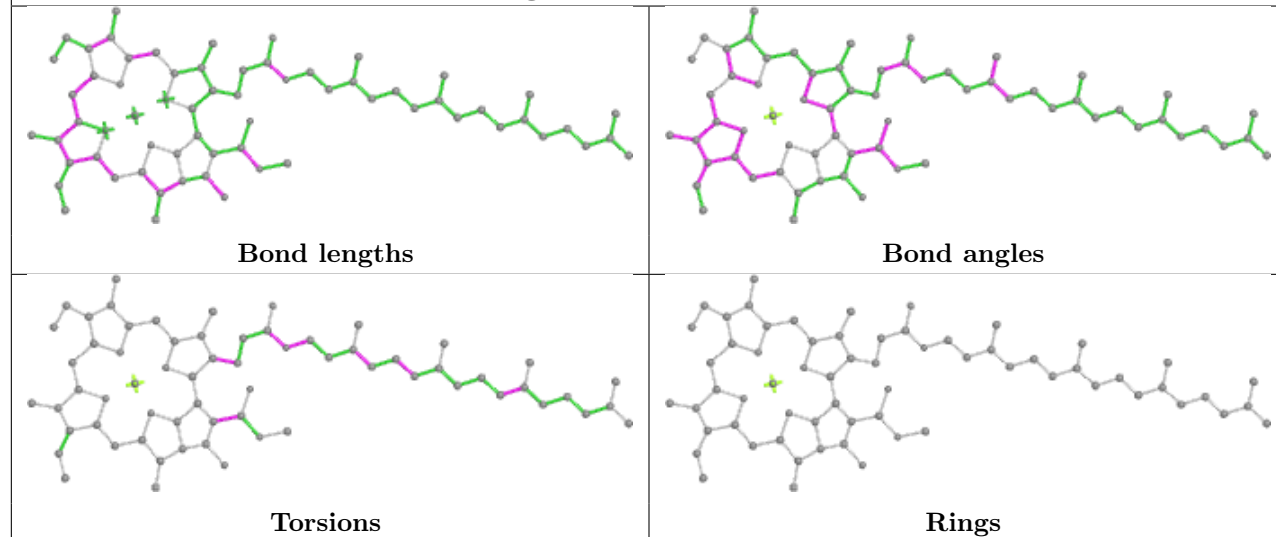
Bond angles

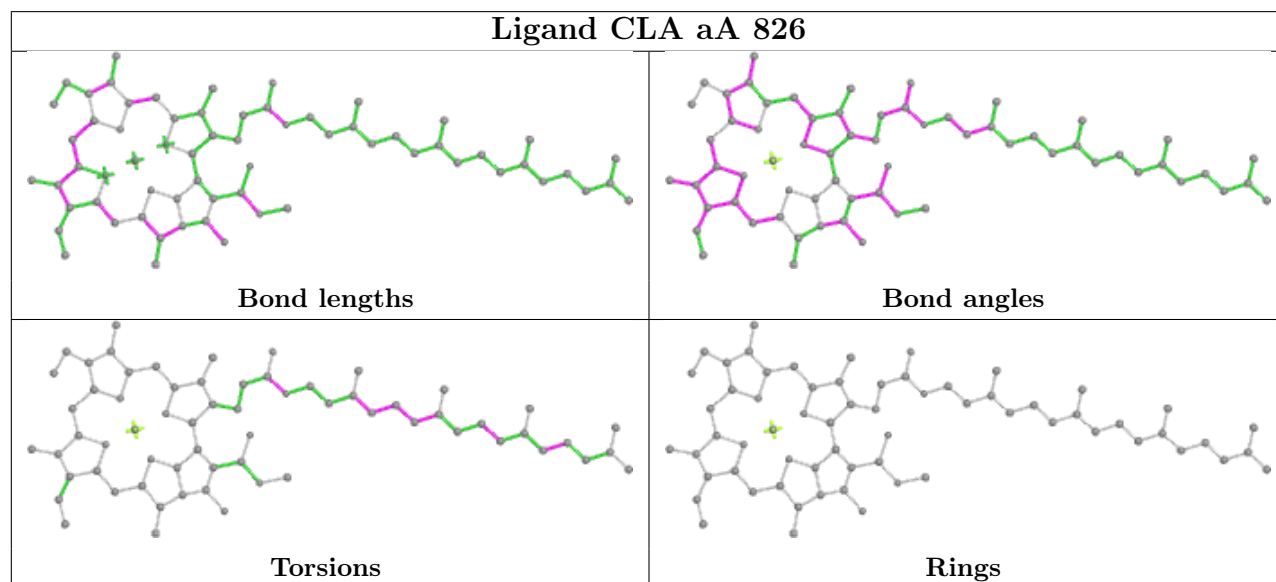
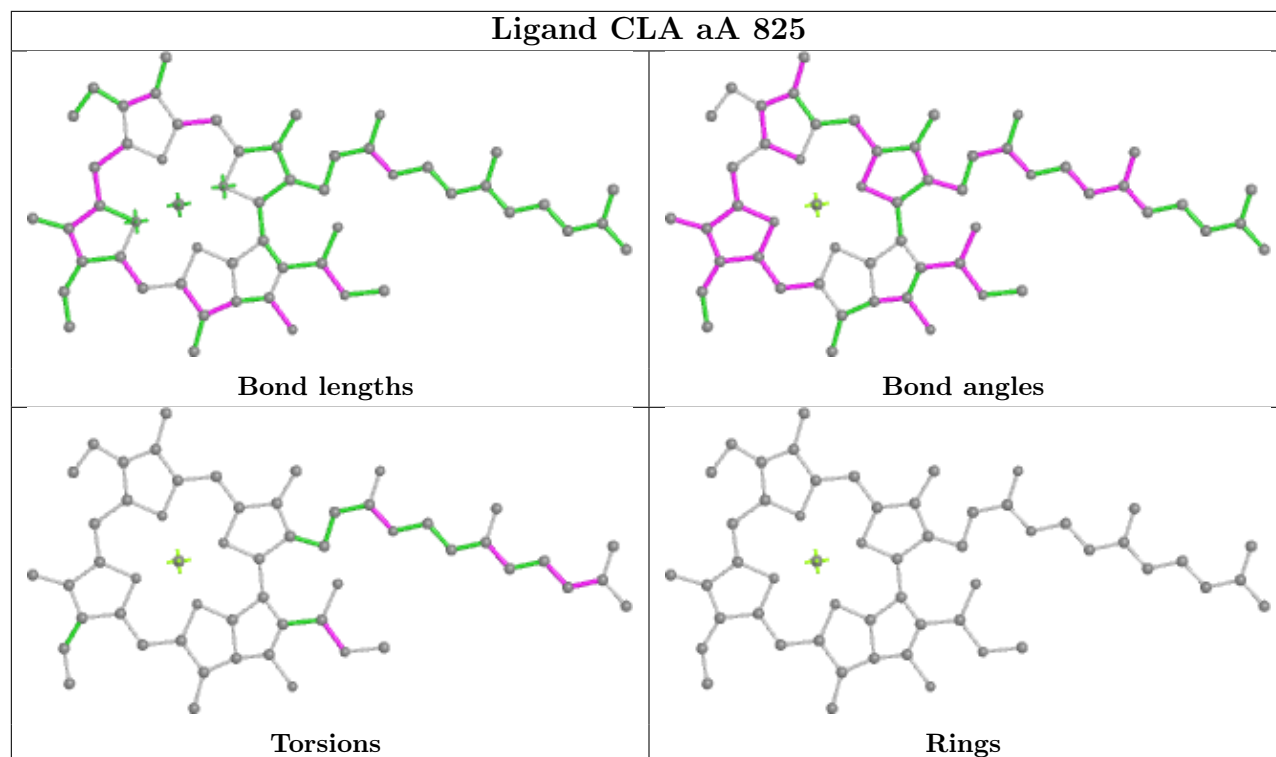


Torsions

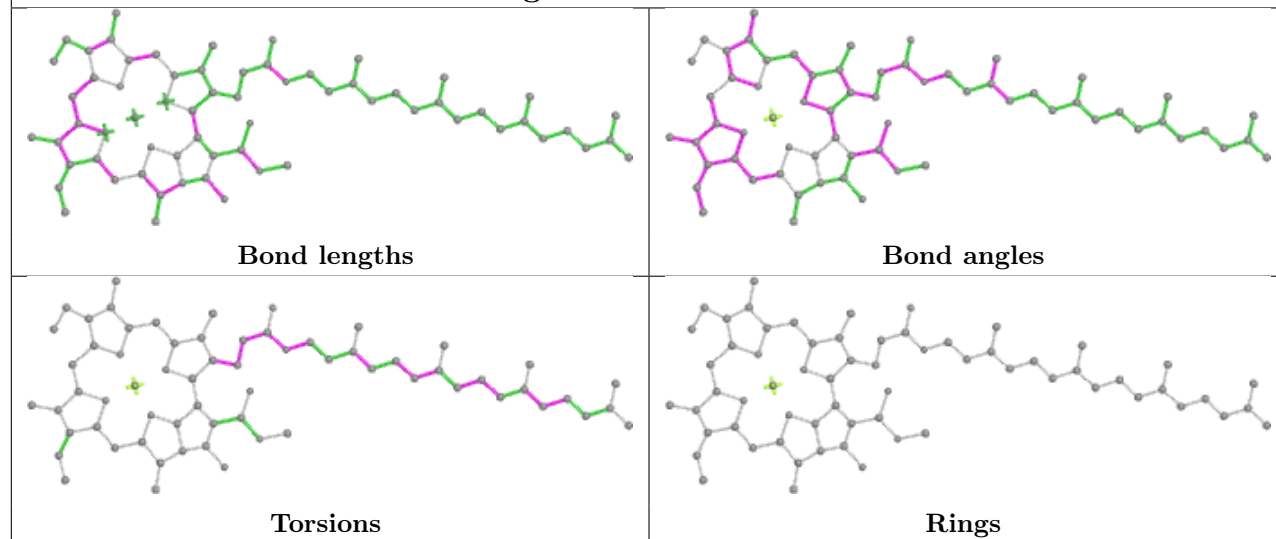


Rings

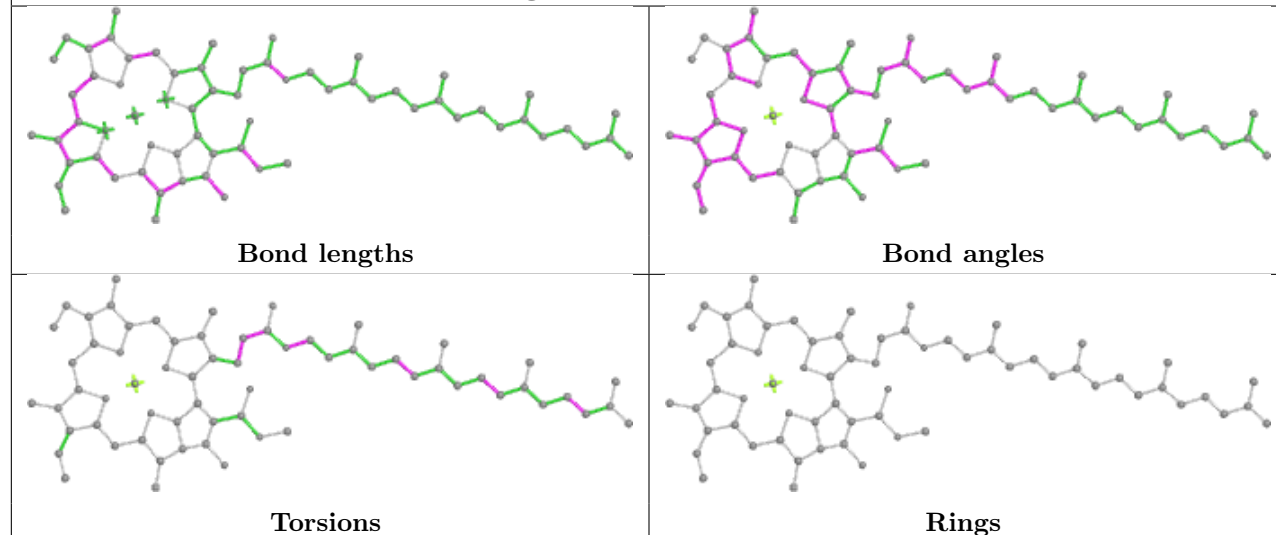
Ligand CLA aA 823**Ligand CLA aA 824**



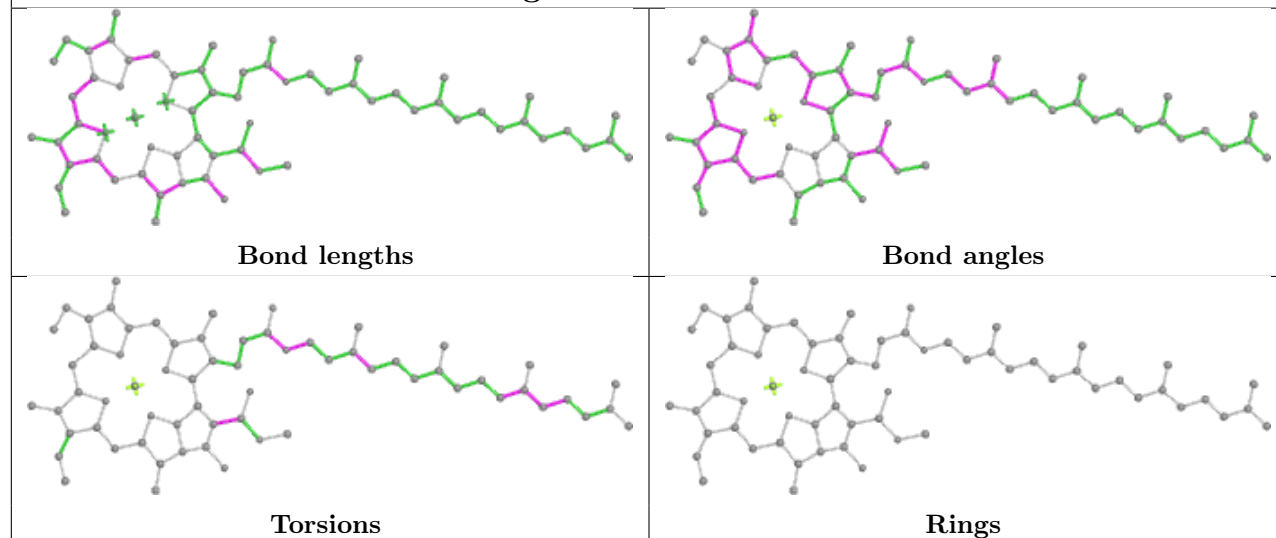
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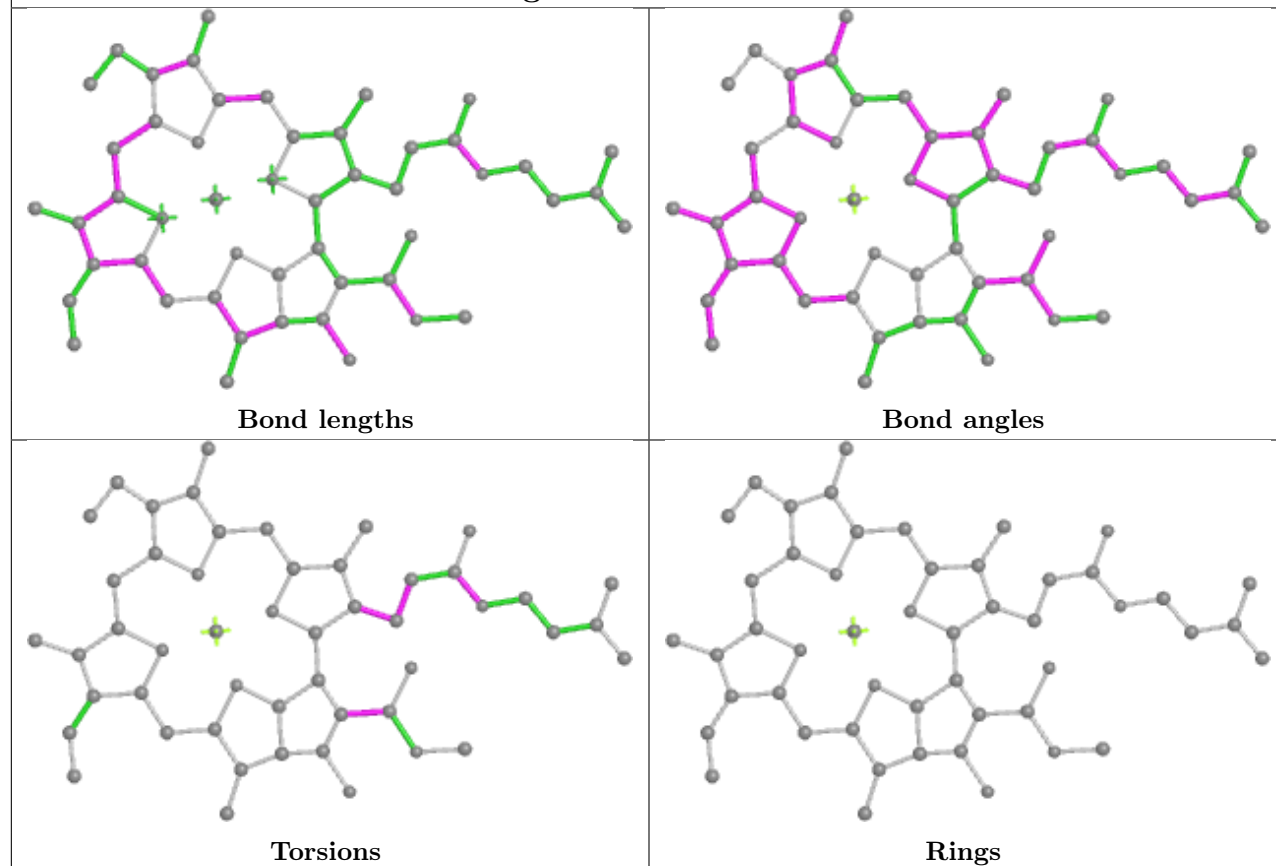
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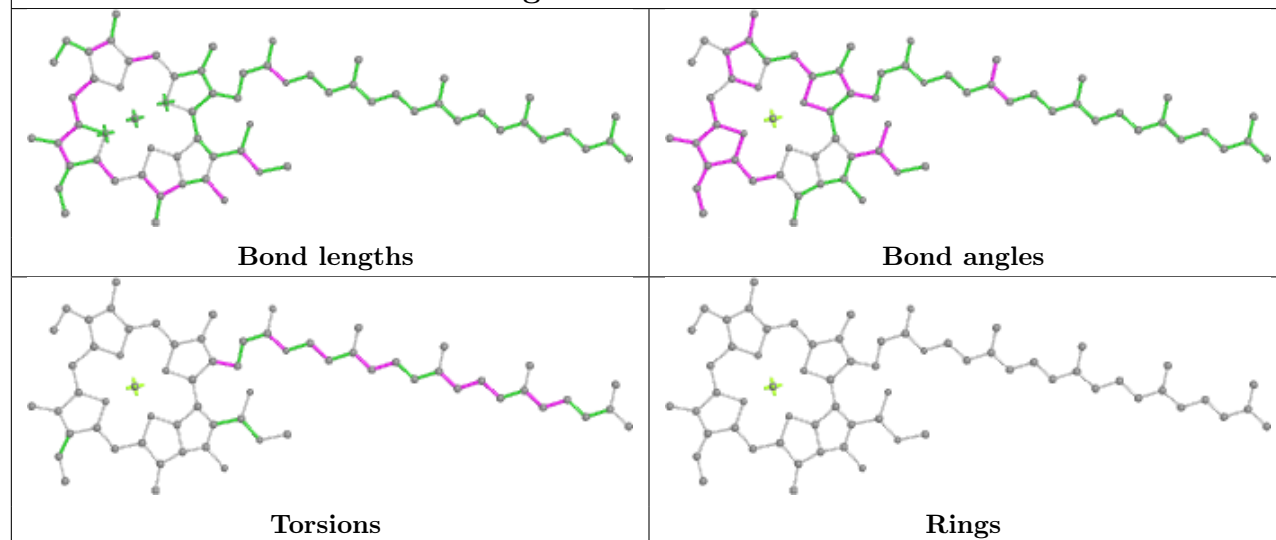
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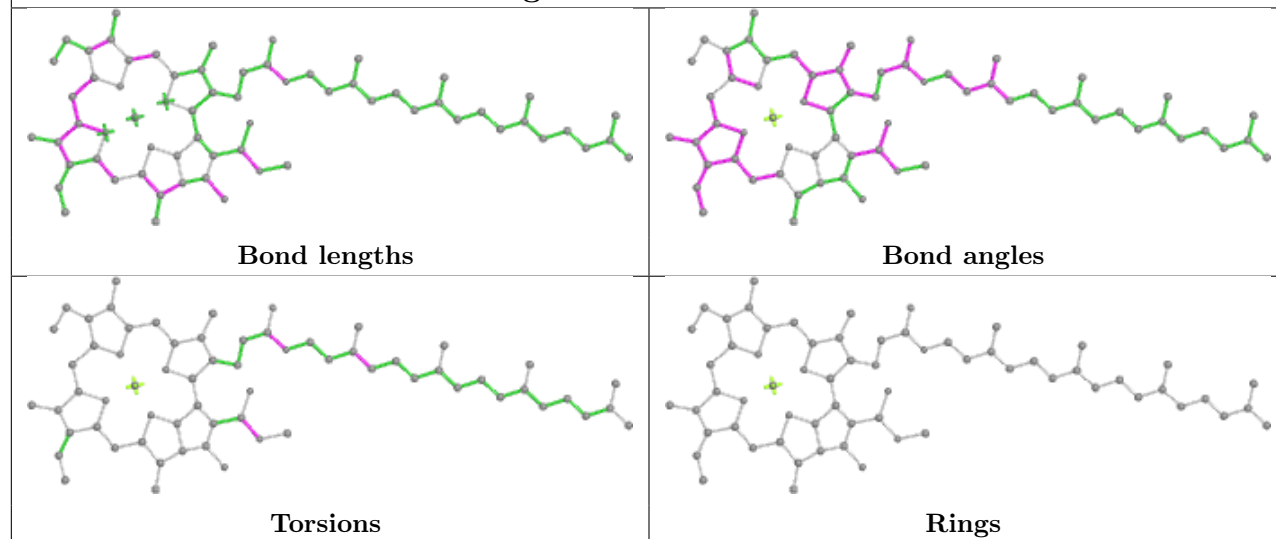
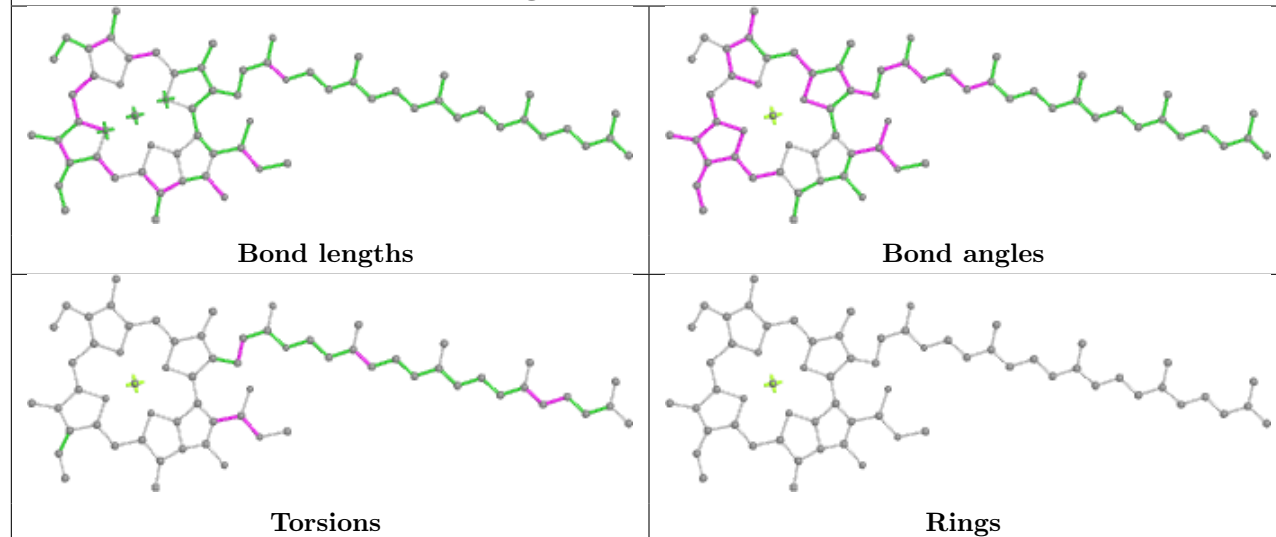


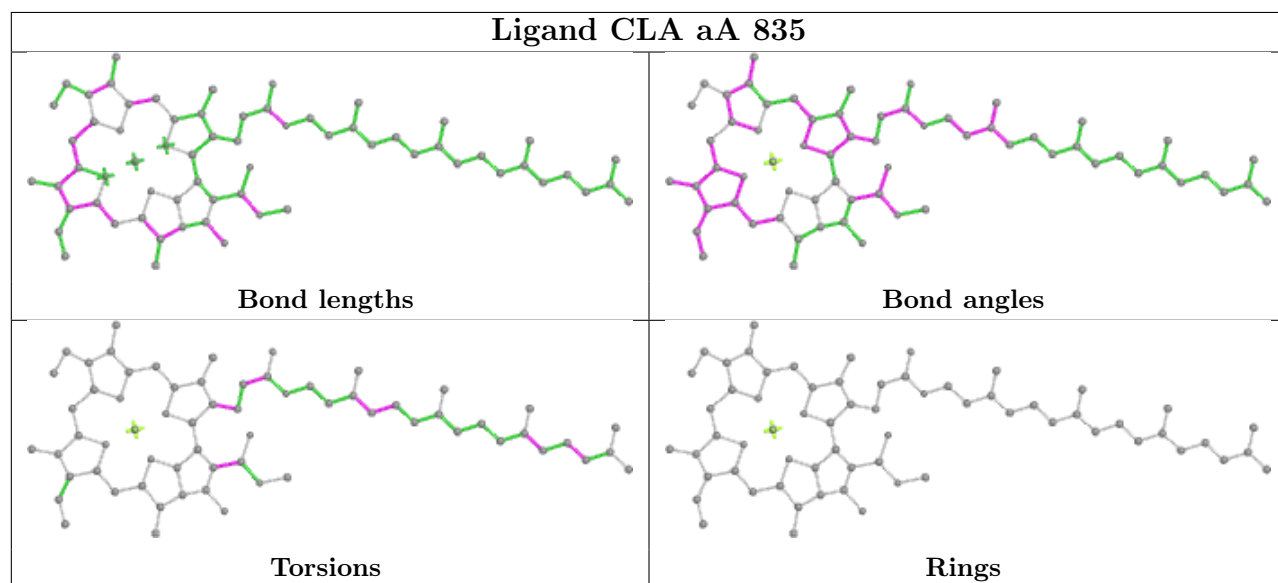
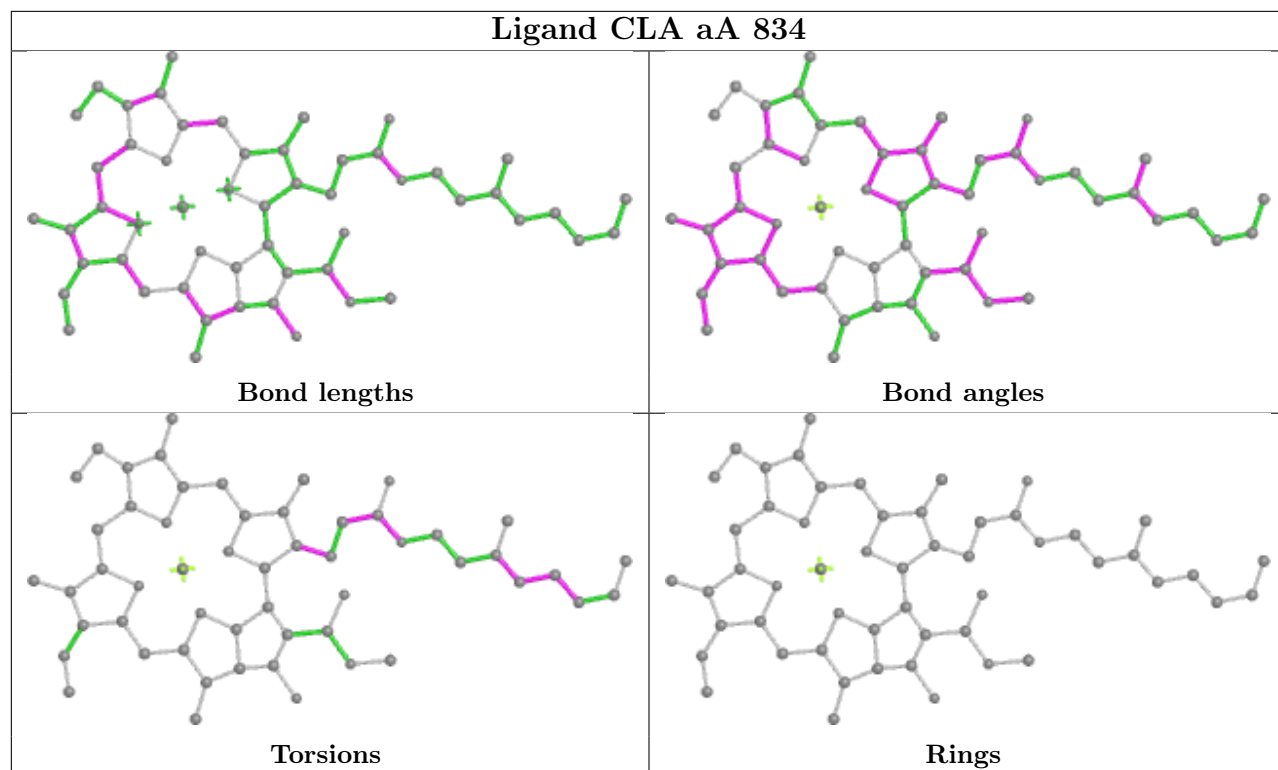
Ligand CLA aA 830

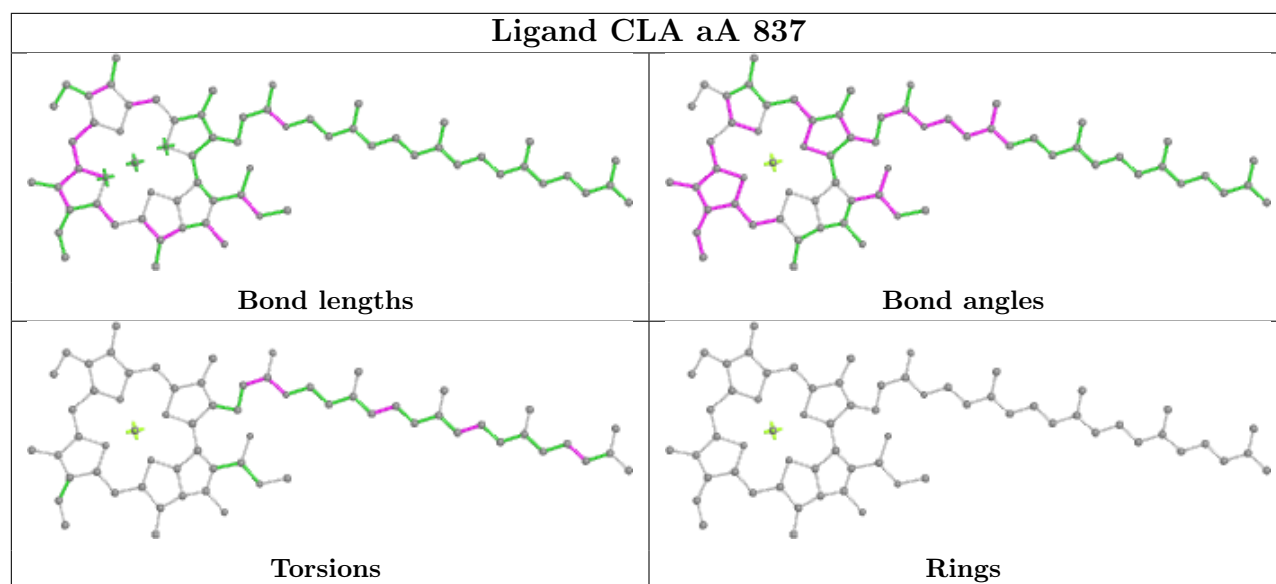
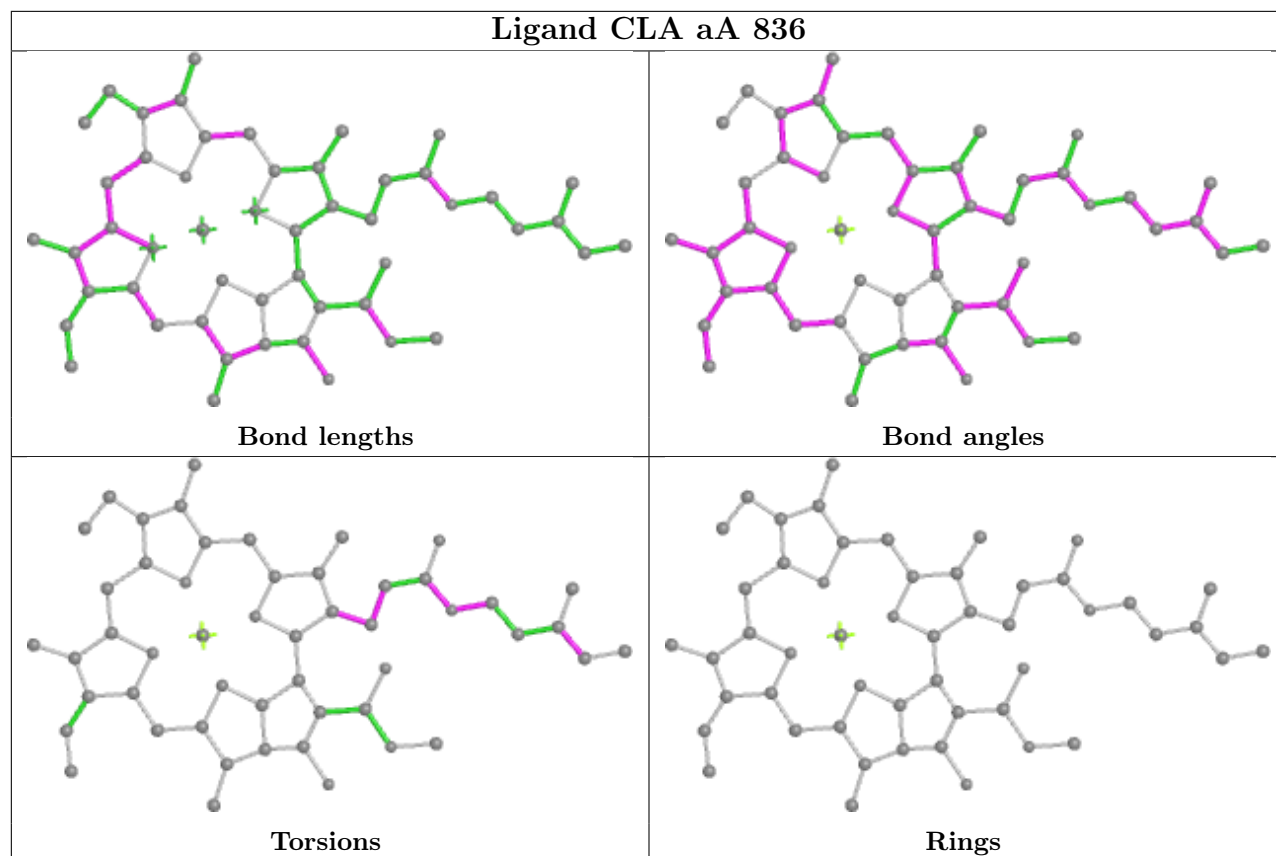


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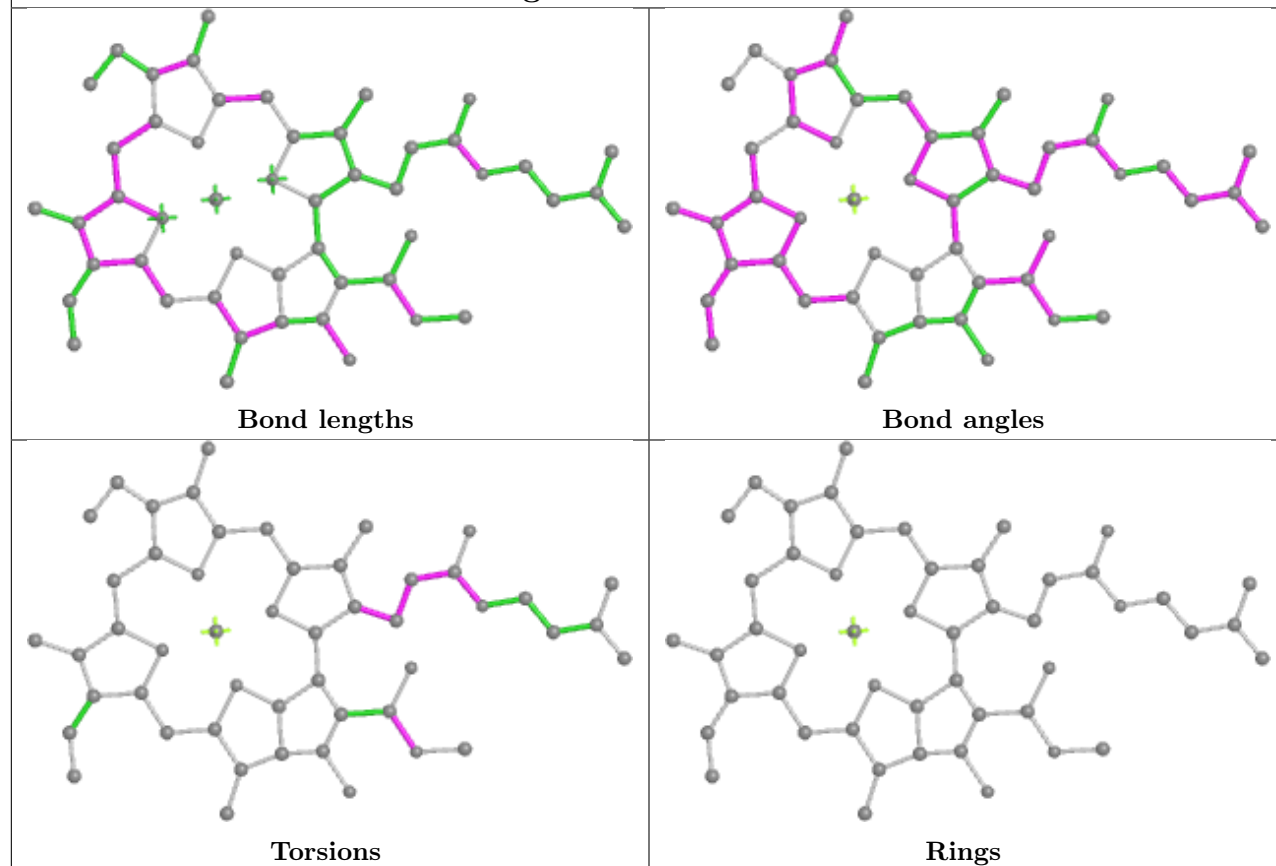


Ligand CLA aA 832**Ligand CLA aA 833**

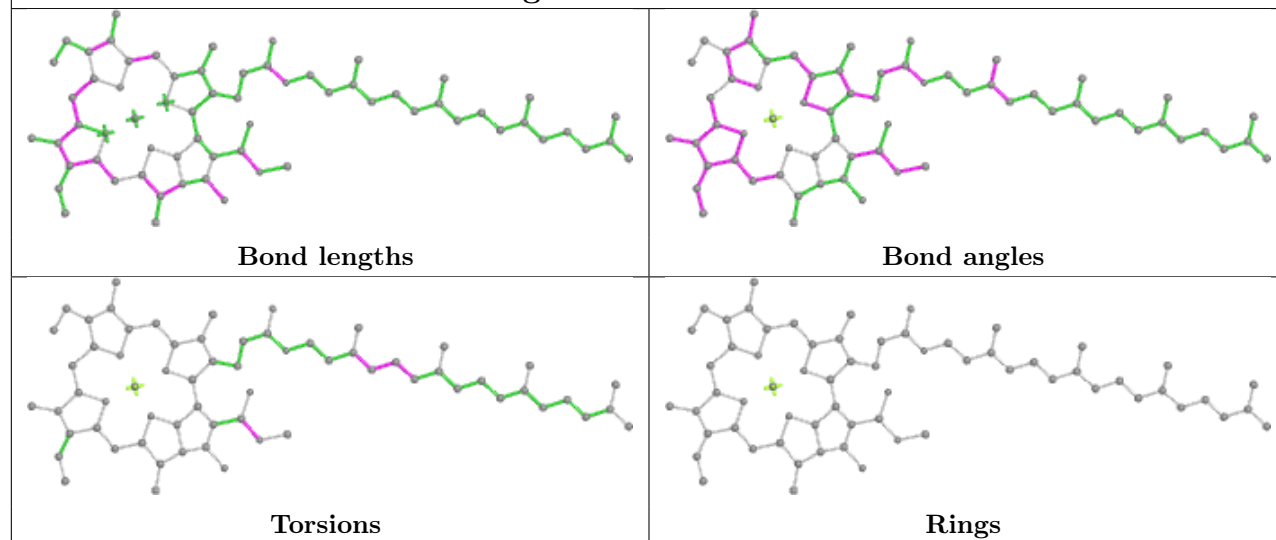


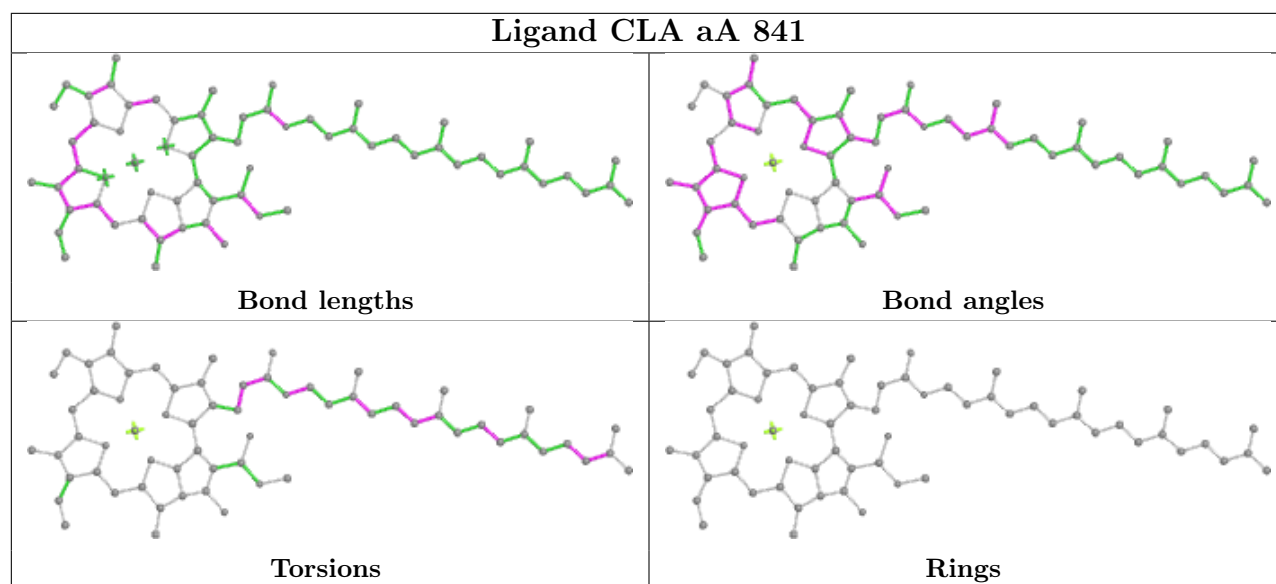
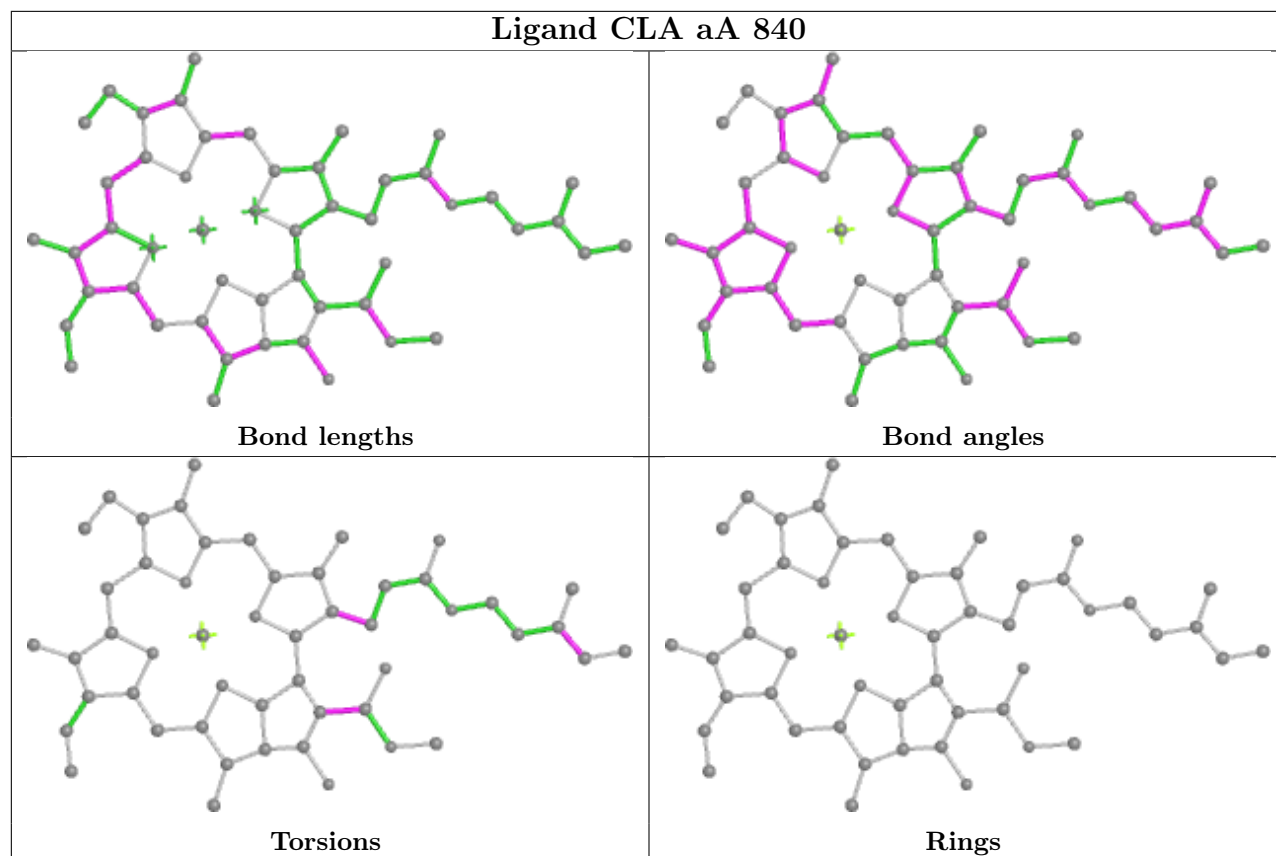


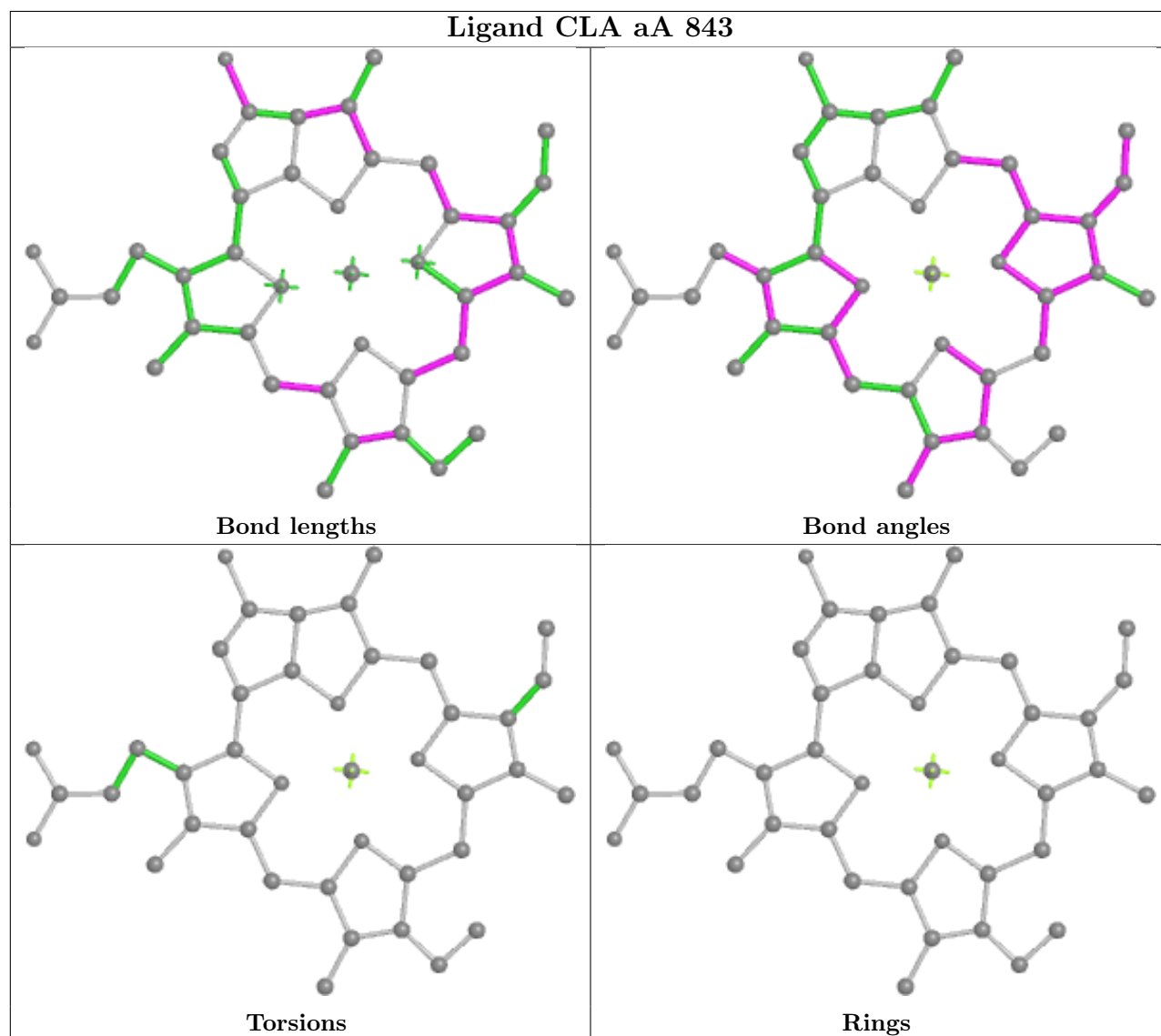
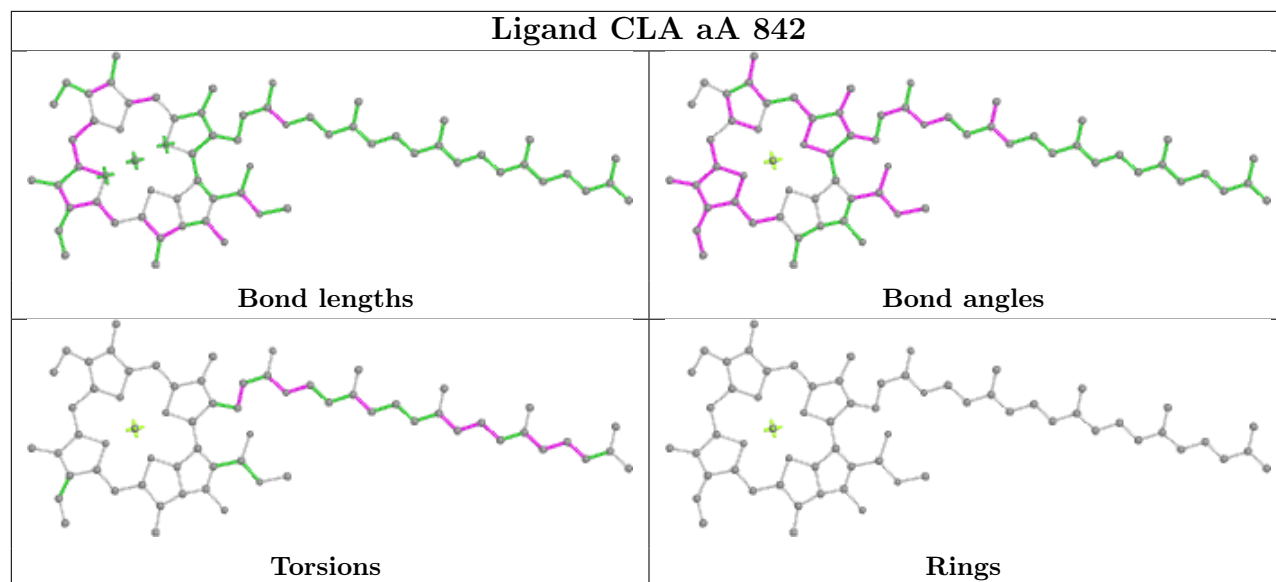
Ligand CLA aA 838

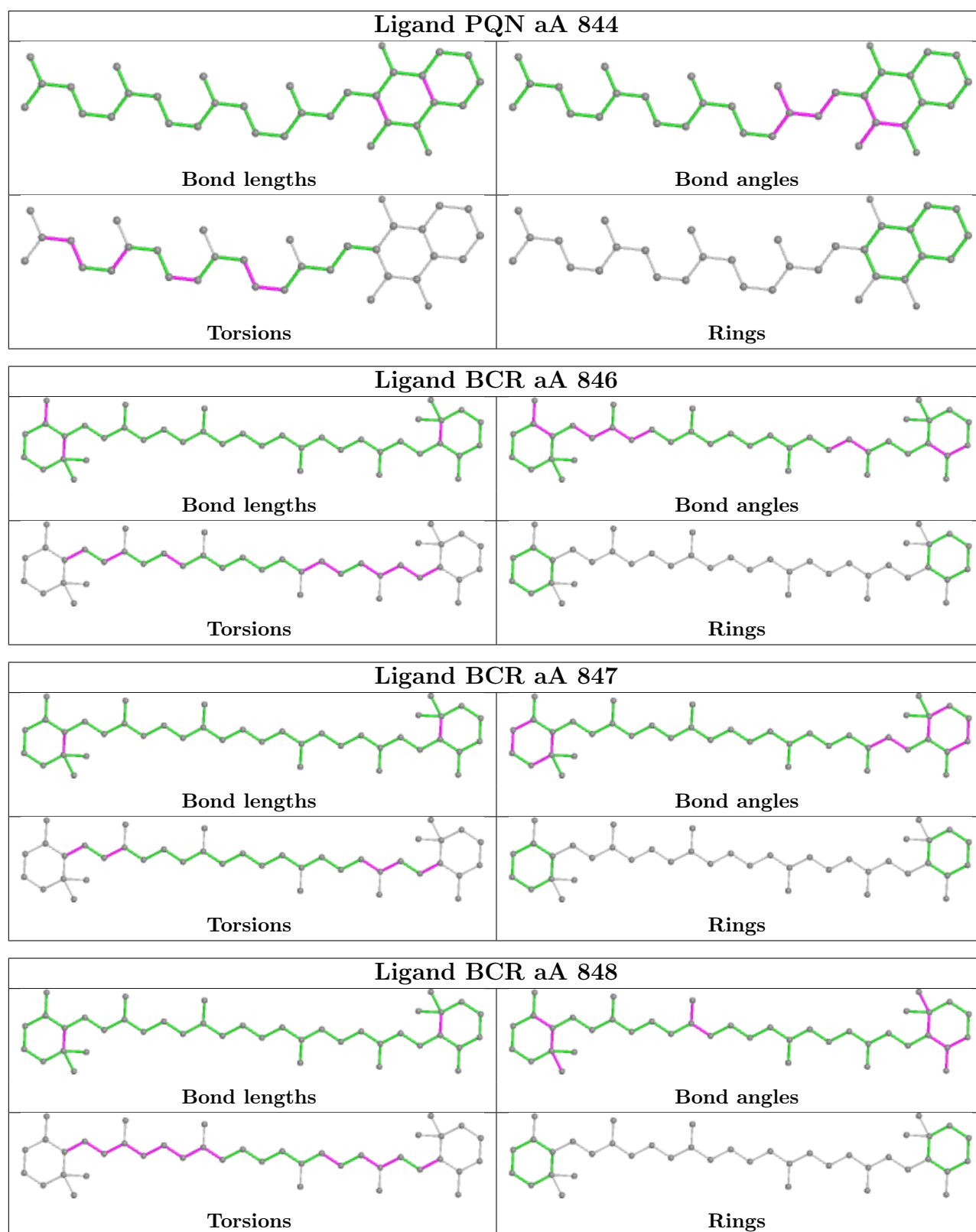


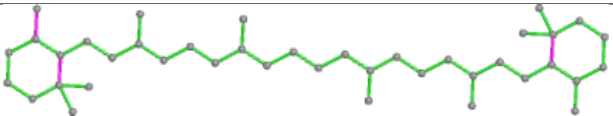
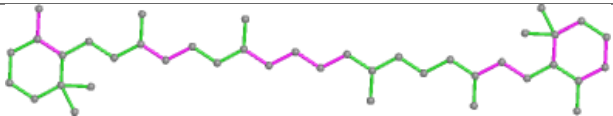
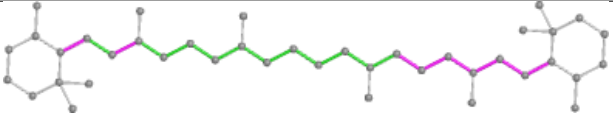
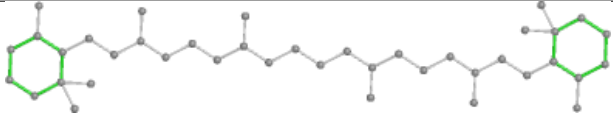
Ligand CLA aA 839

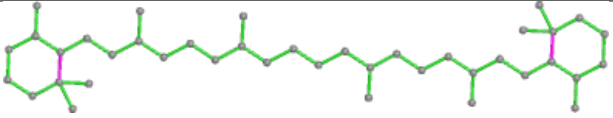
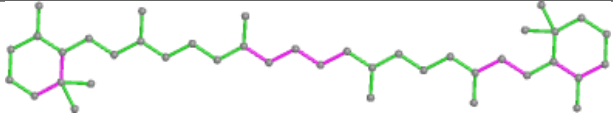
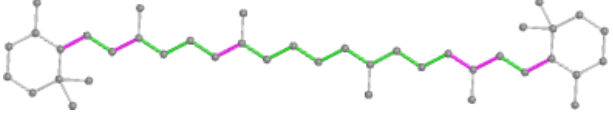
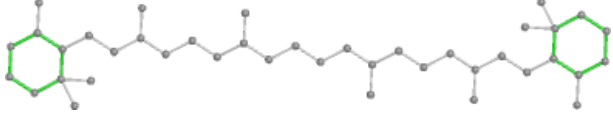


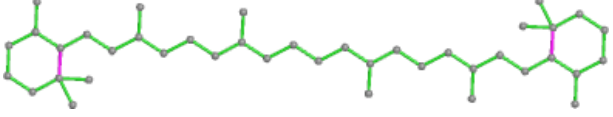
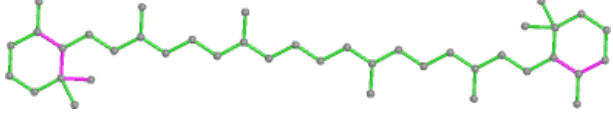
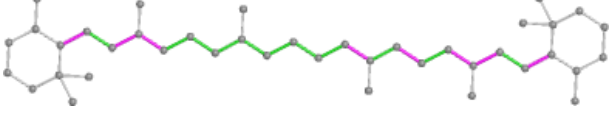
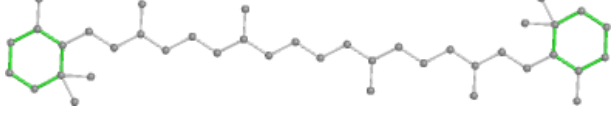


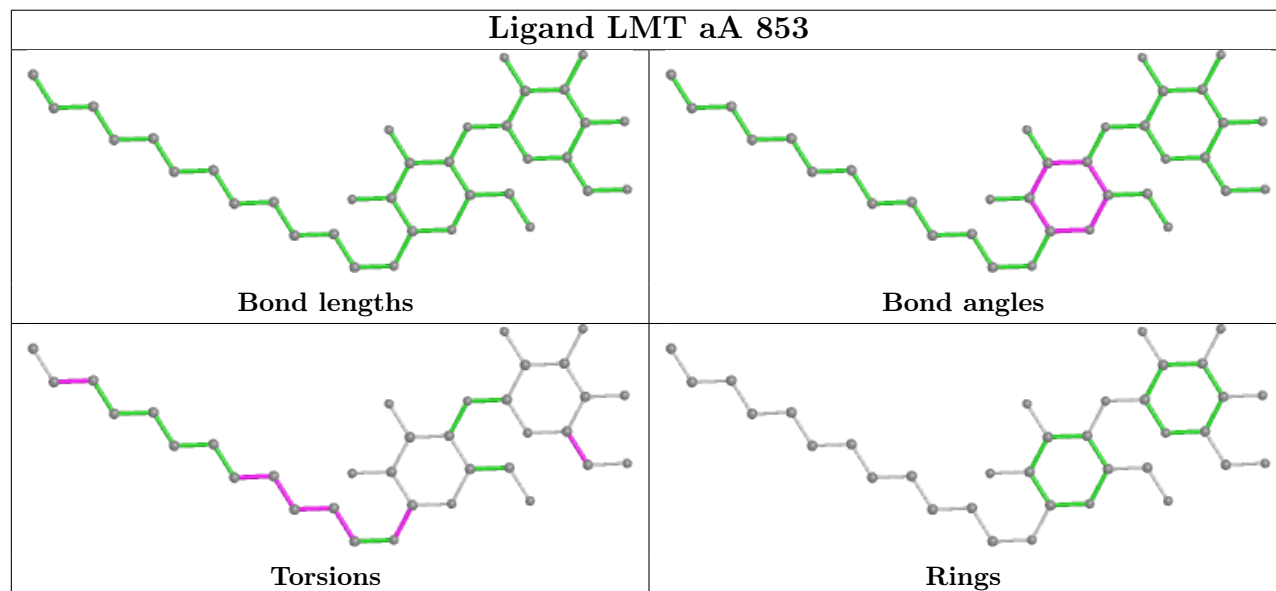
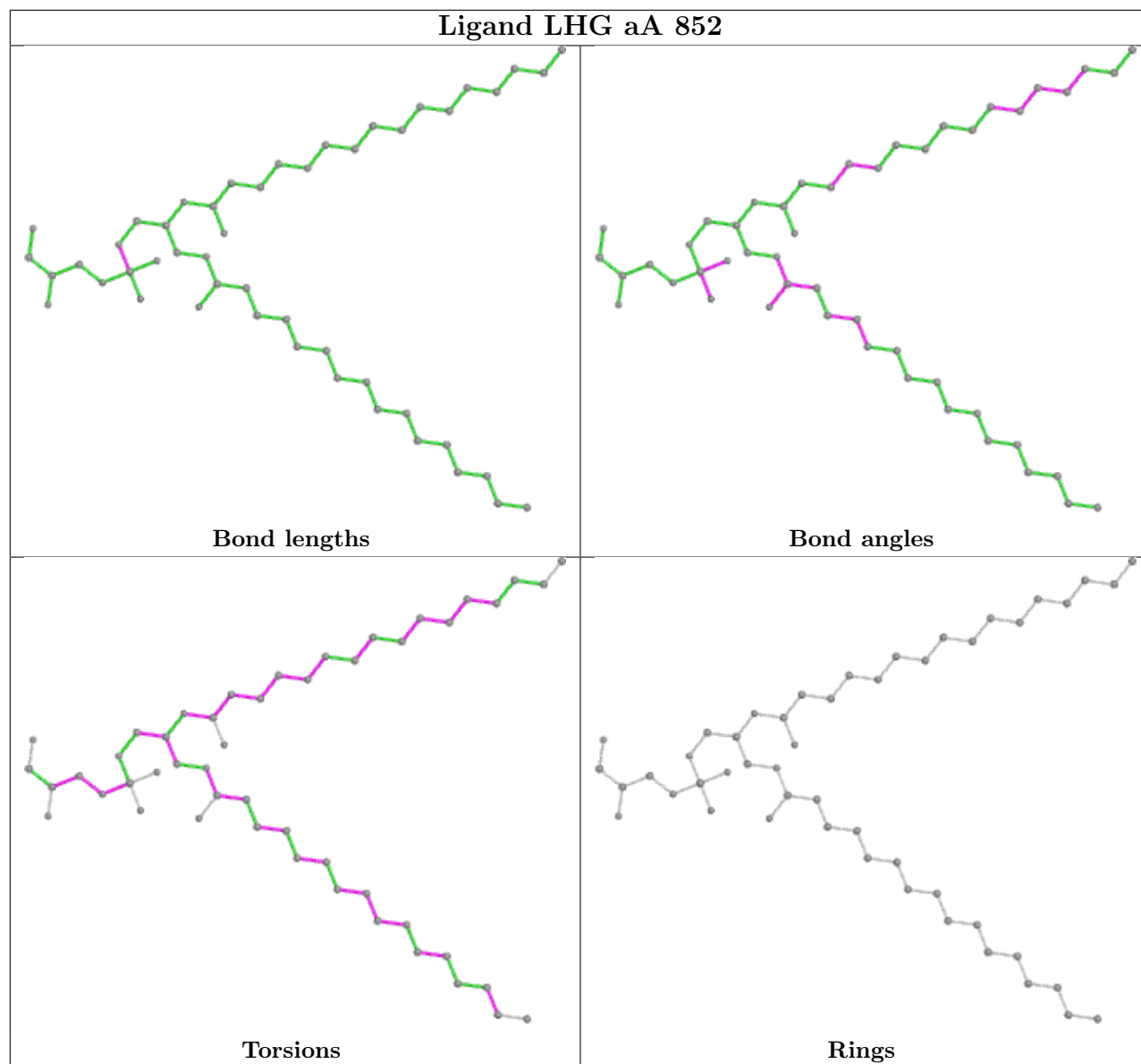


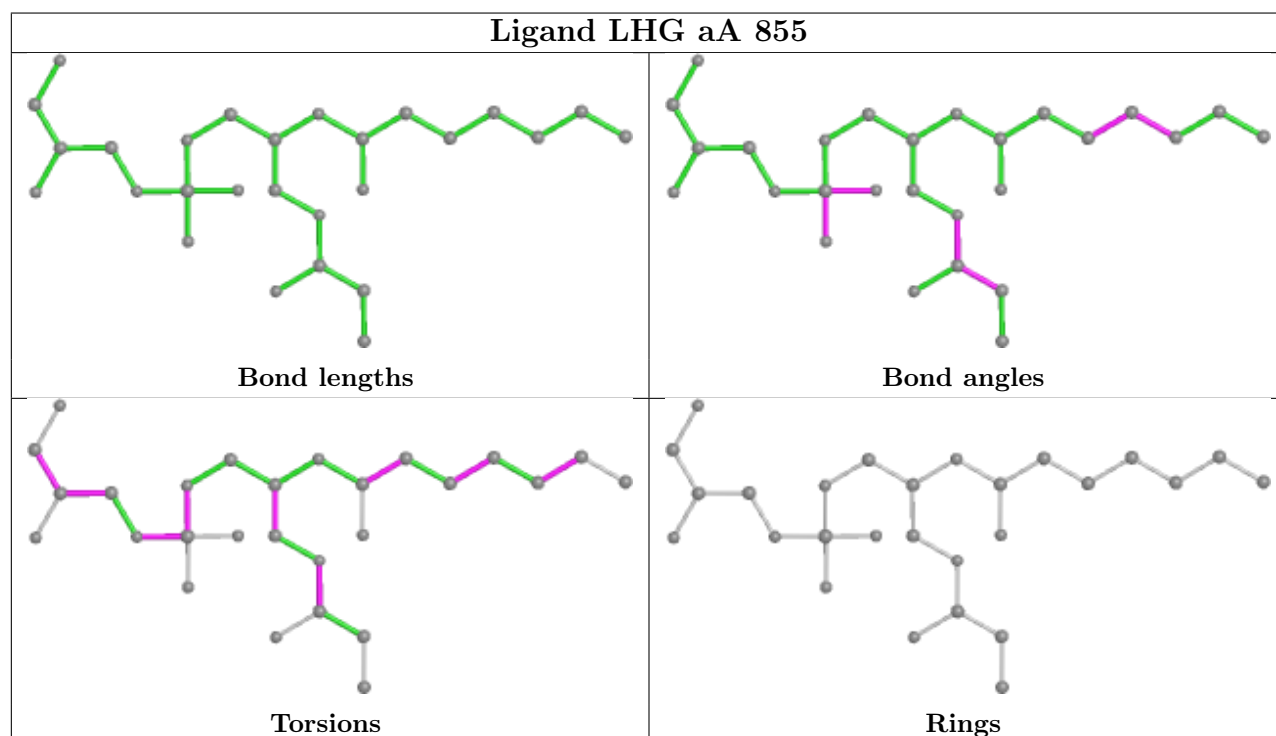
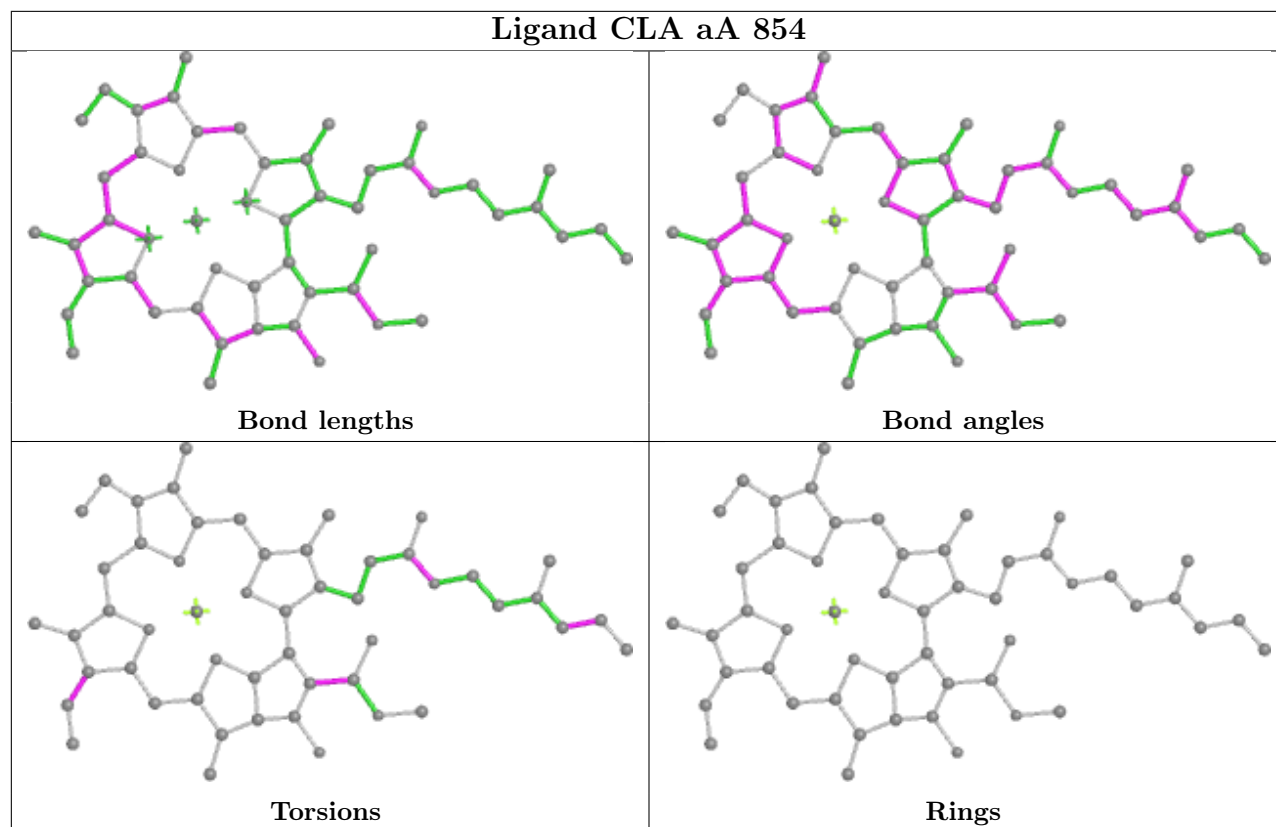


Ligand BCR aA 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

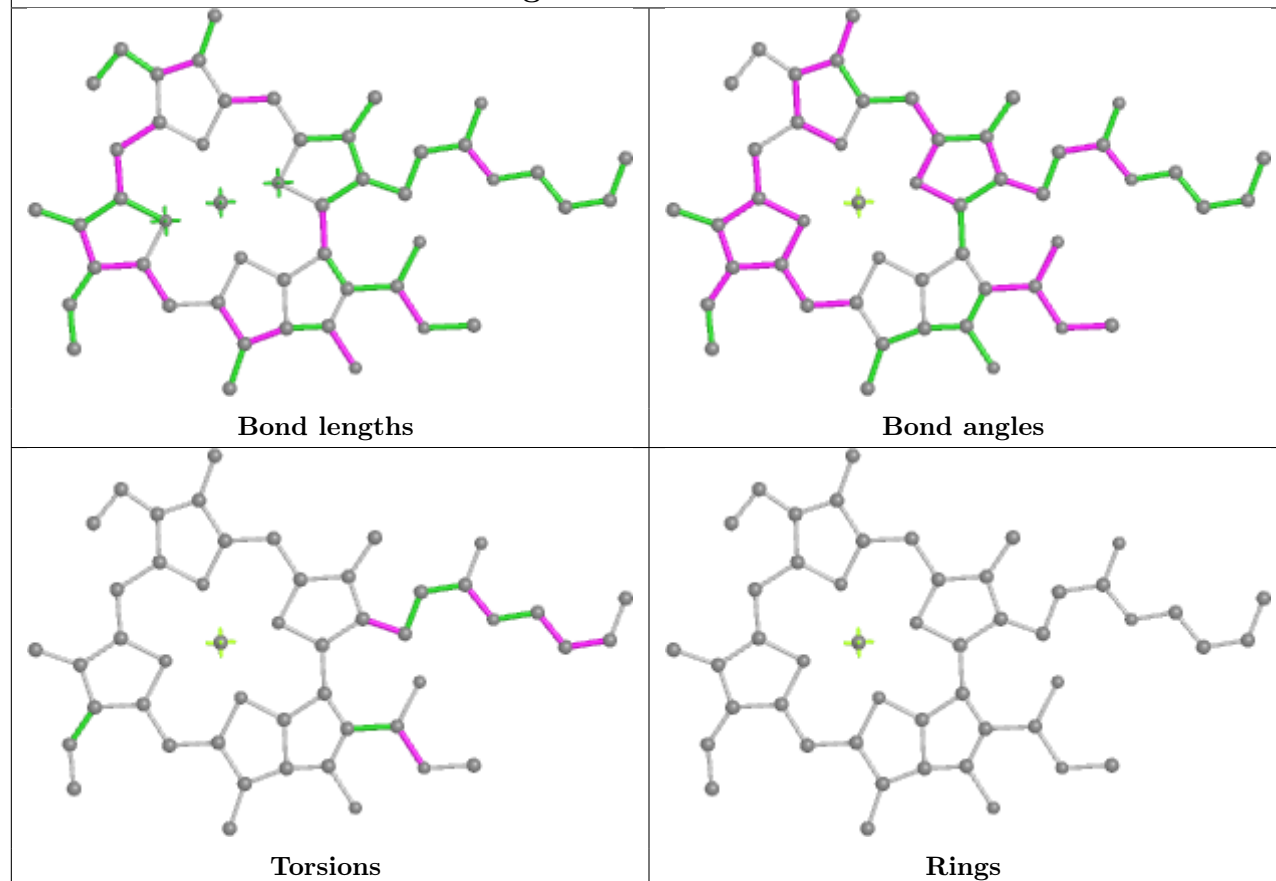
Ligand BCR aA 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR aA 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

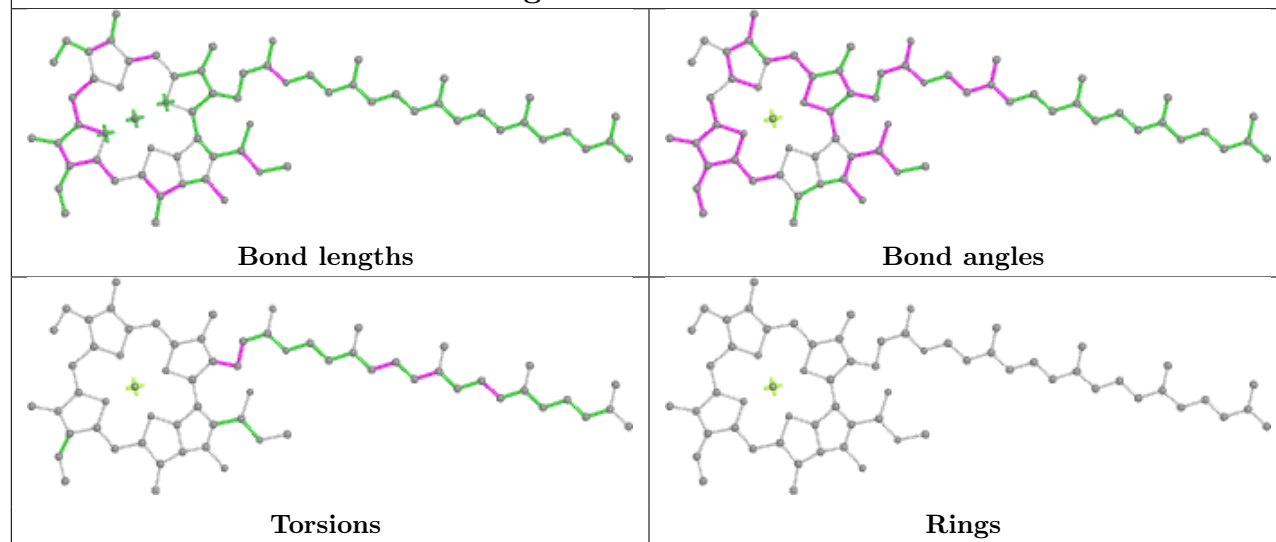


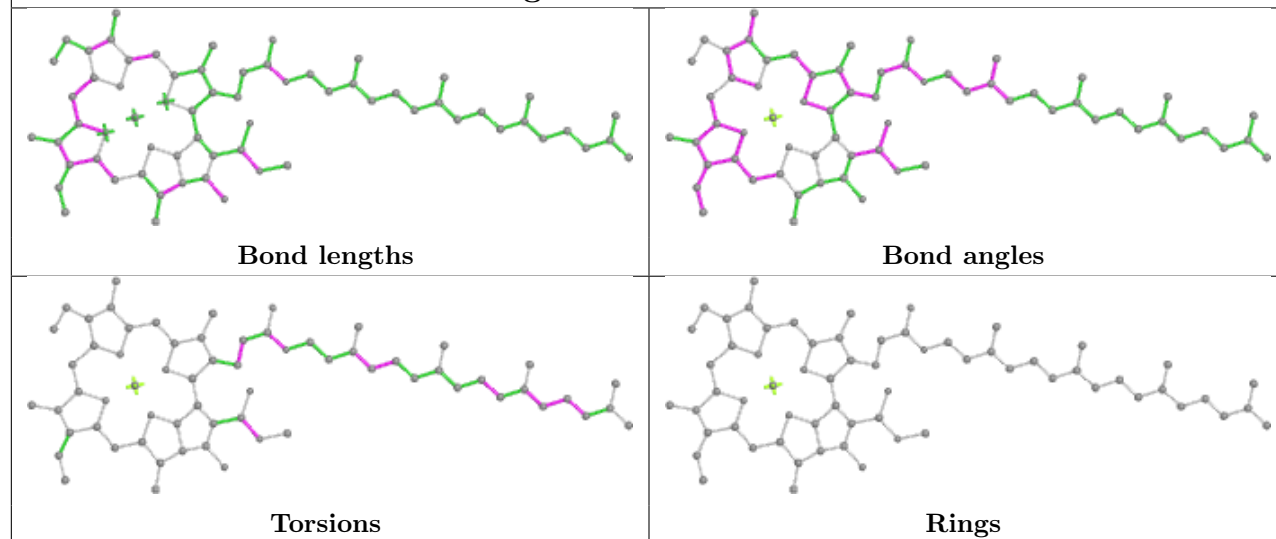
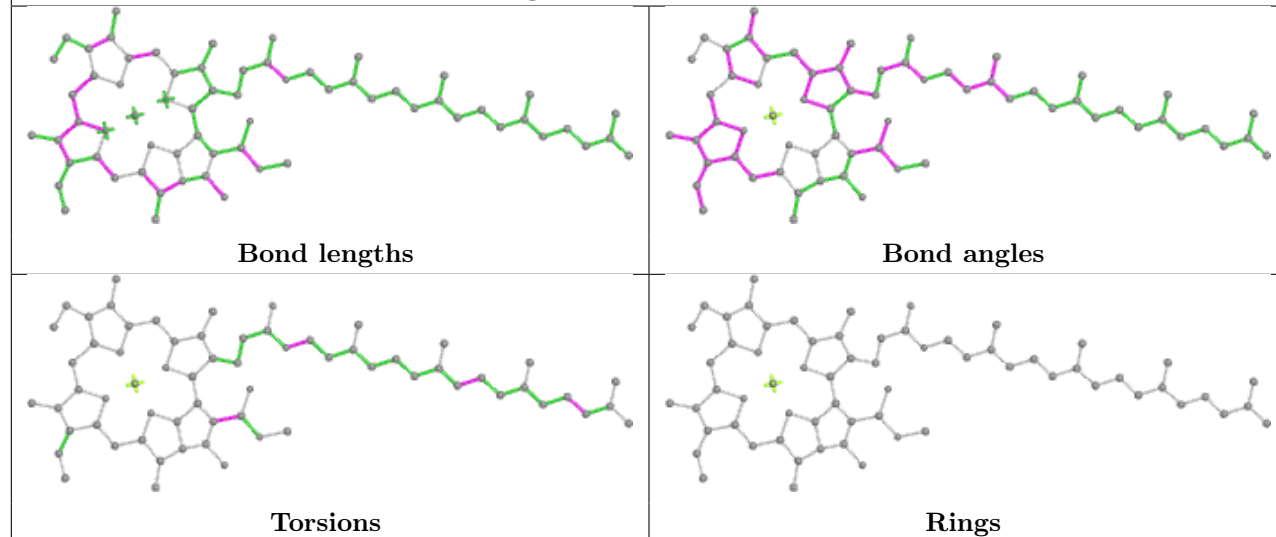


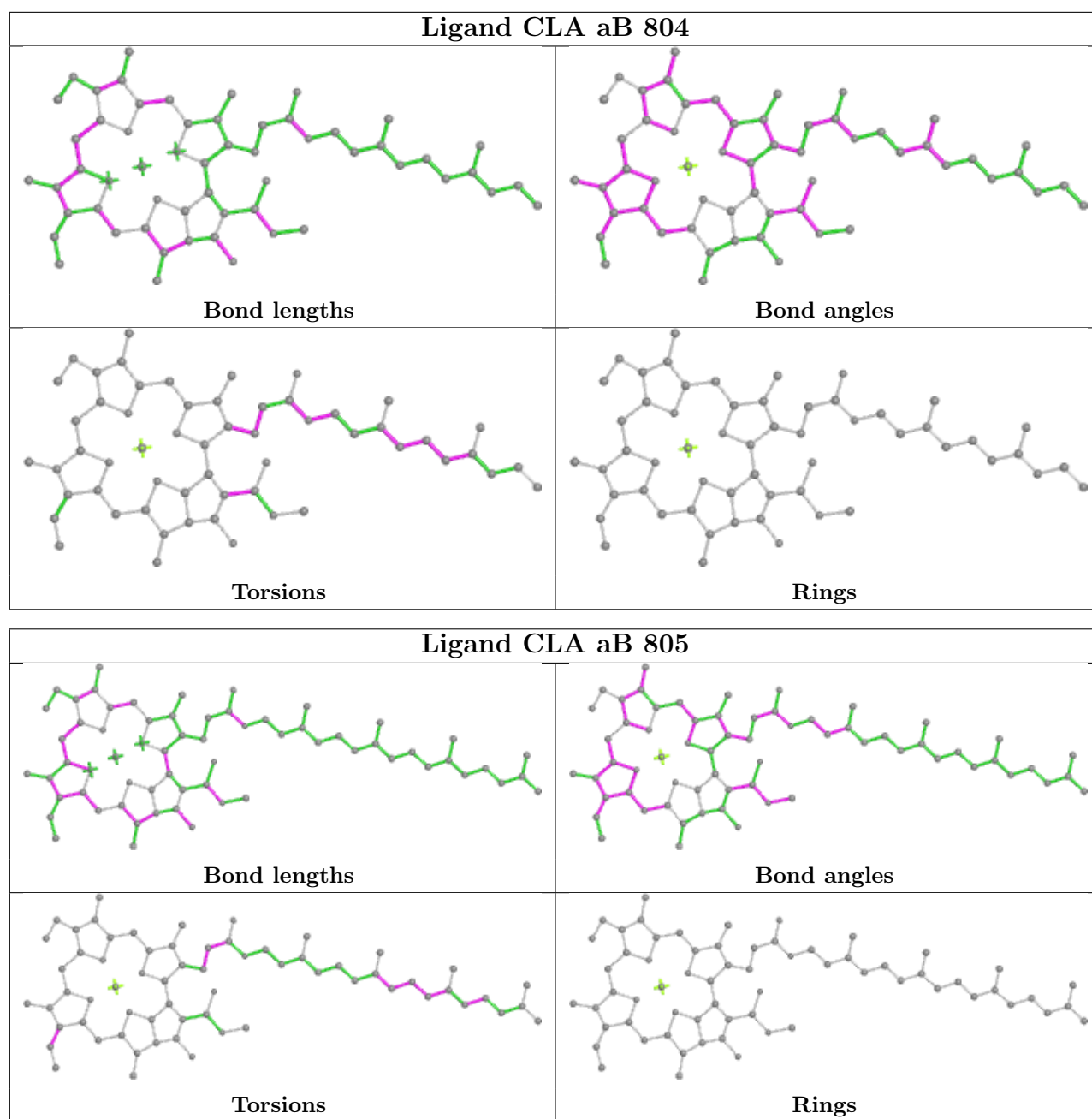
Ligand CLA aA 856

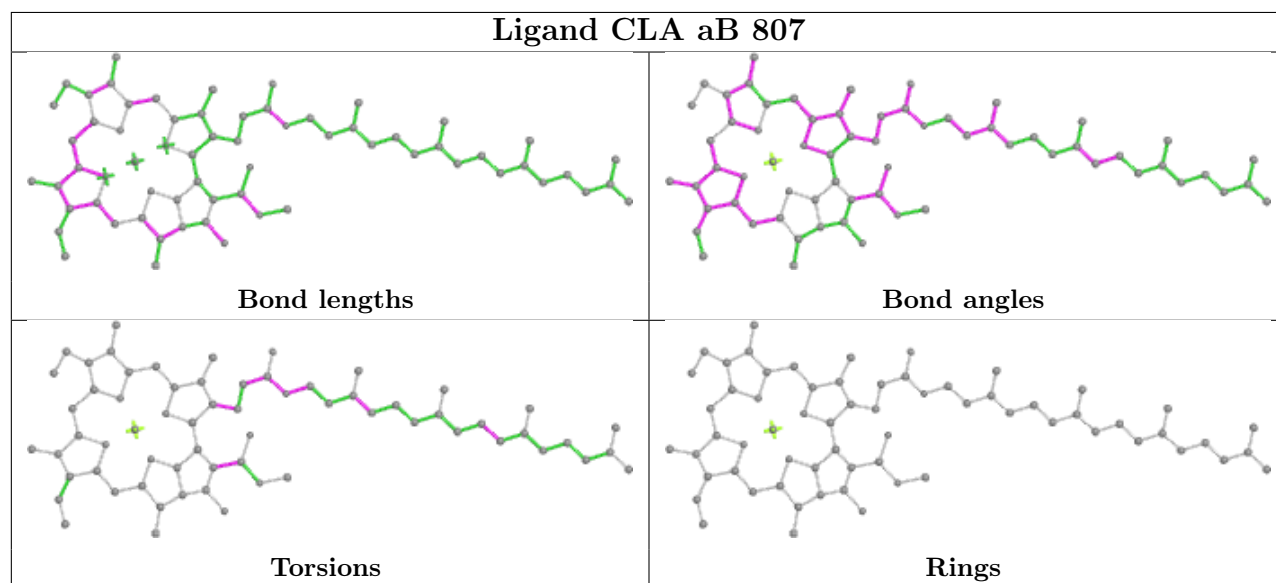
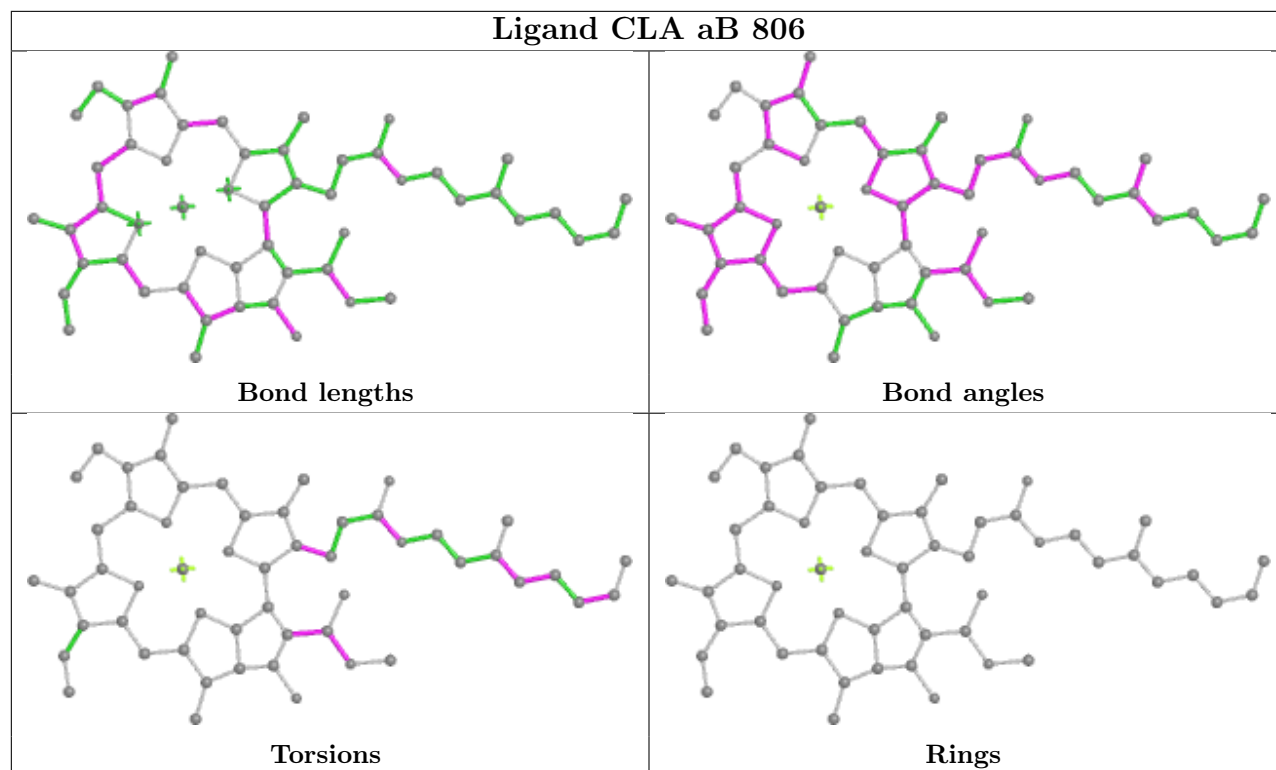


Ligand CLA aB 801

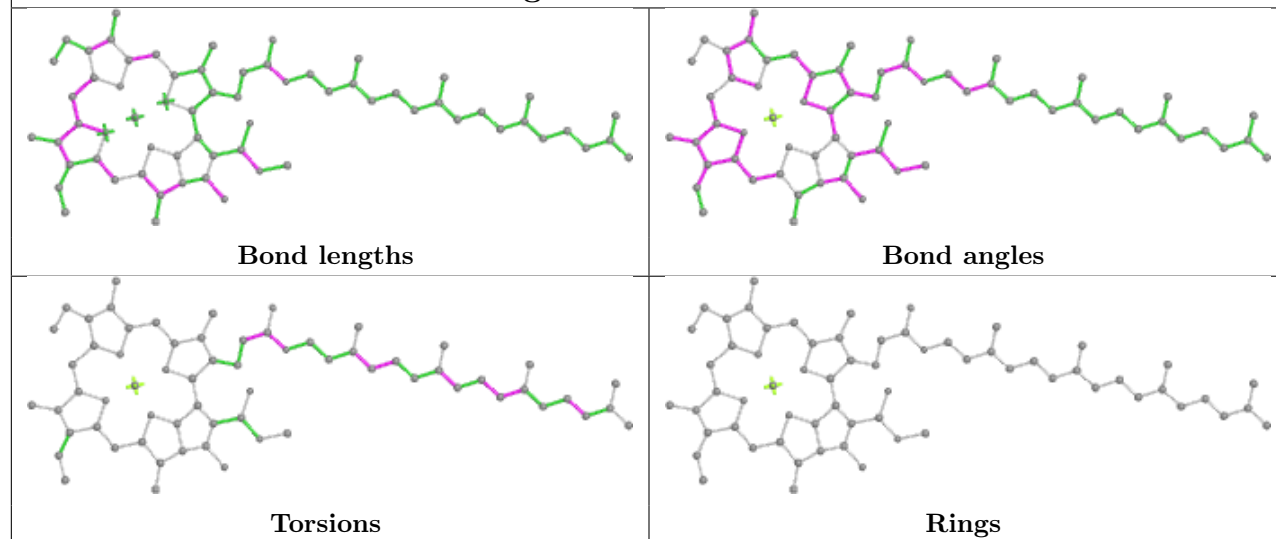


Ligand CLA aB 802**Ligand CLA aB 803**

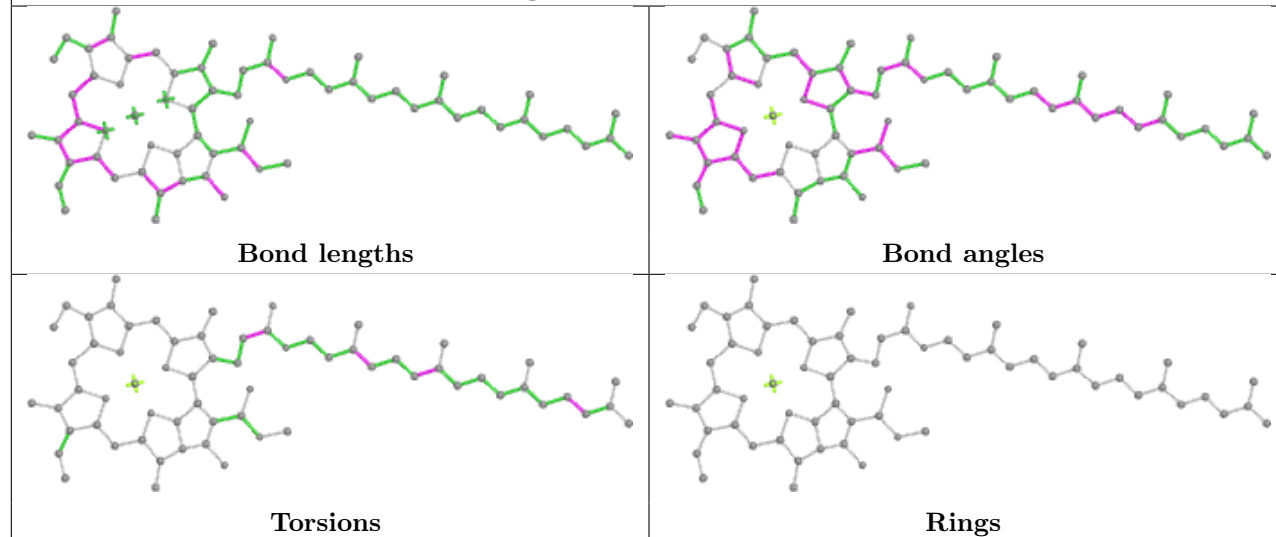


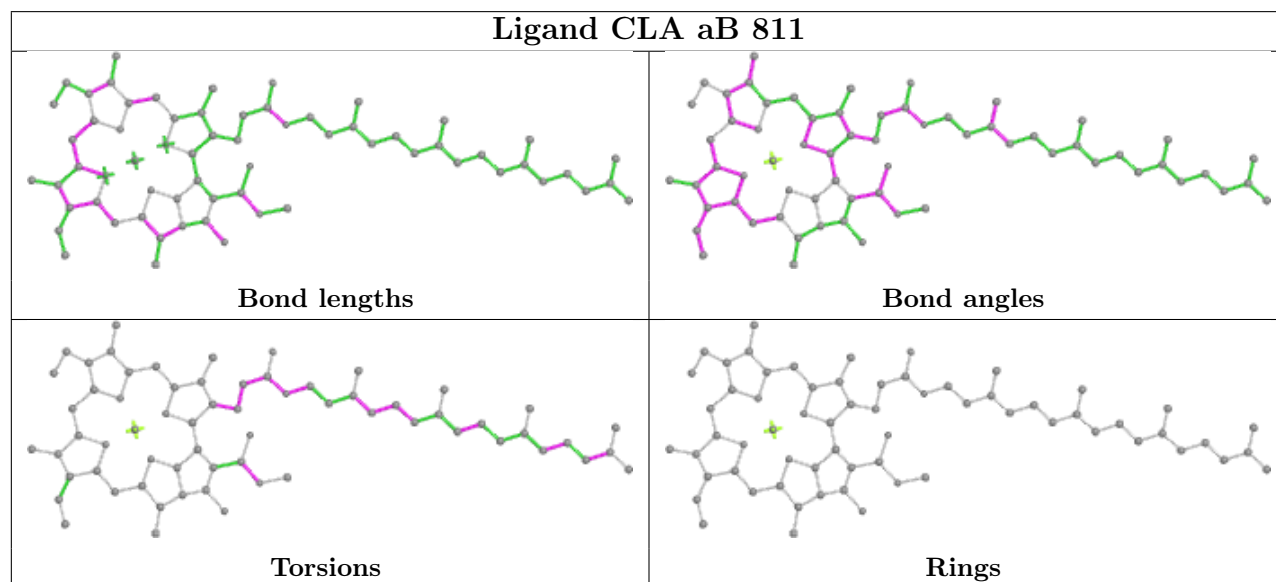
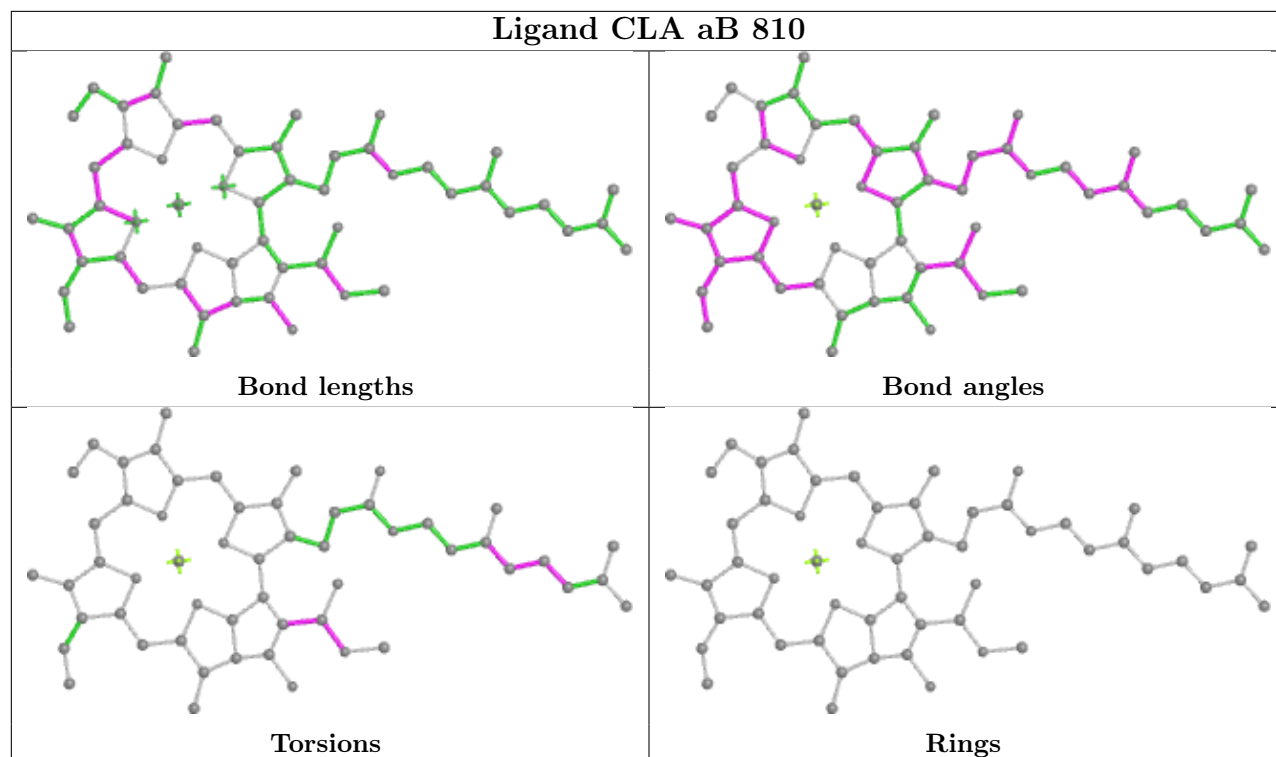


Ligand CLA aB 808

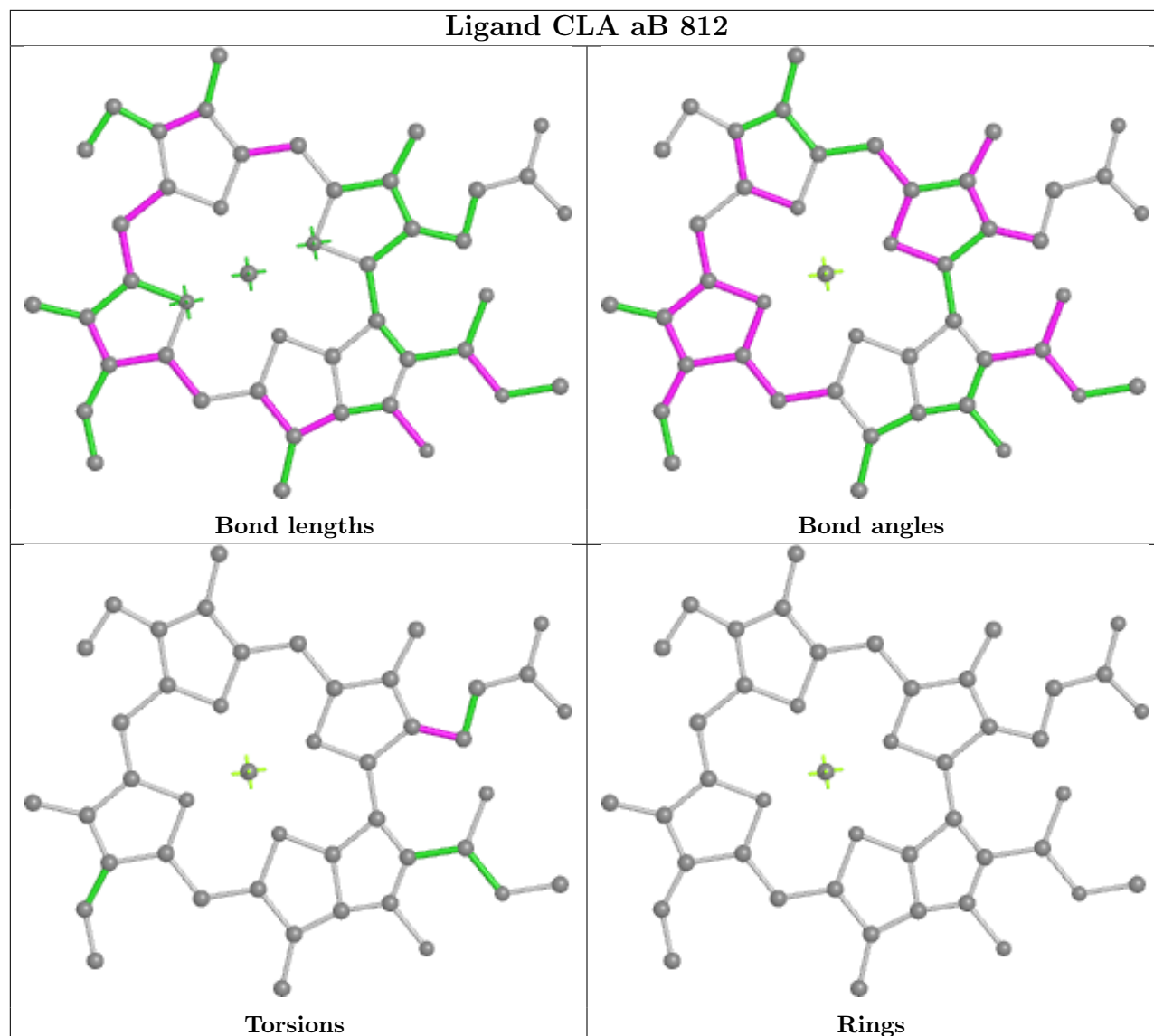


Ligand CLA aB 809

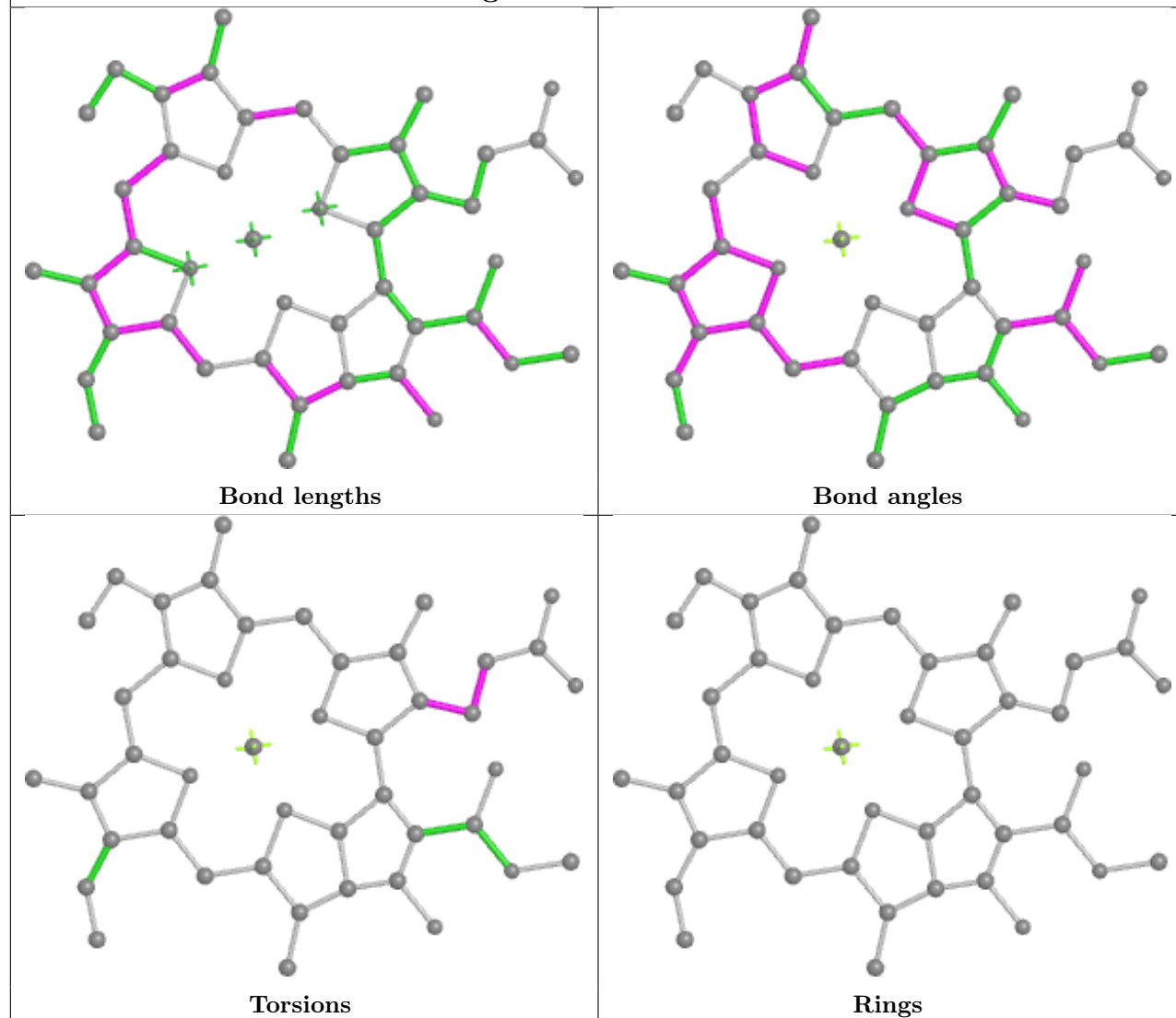




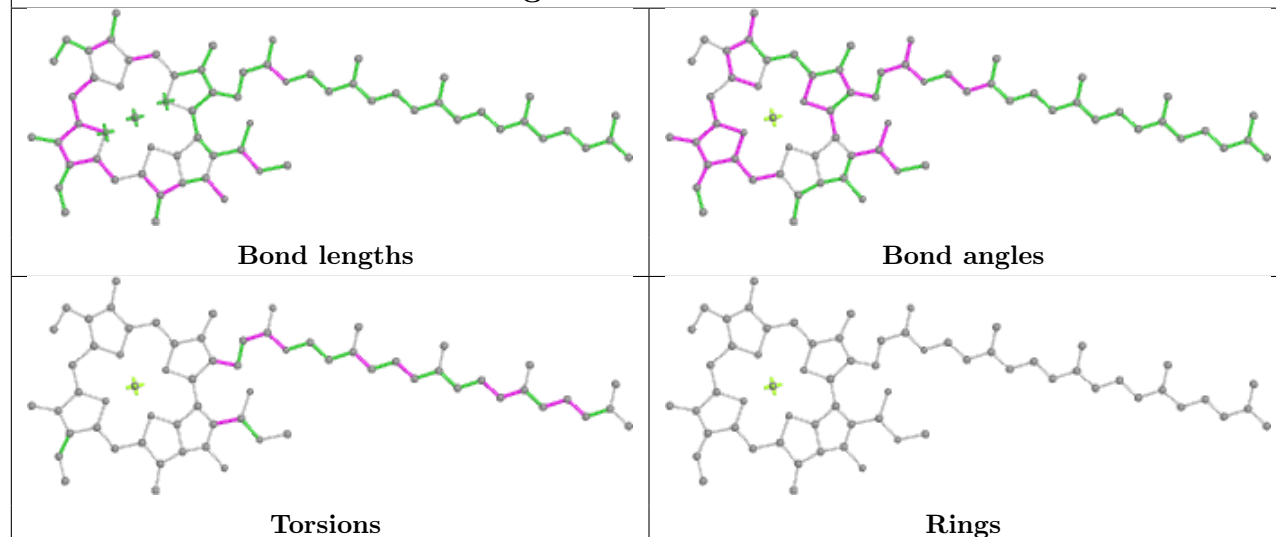
Ligand CLA aB 812

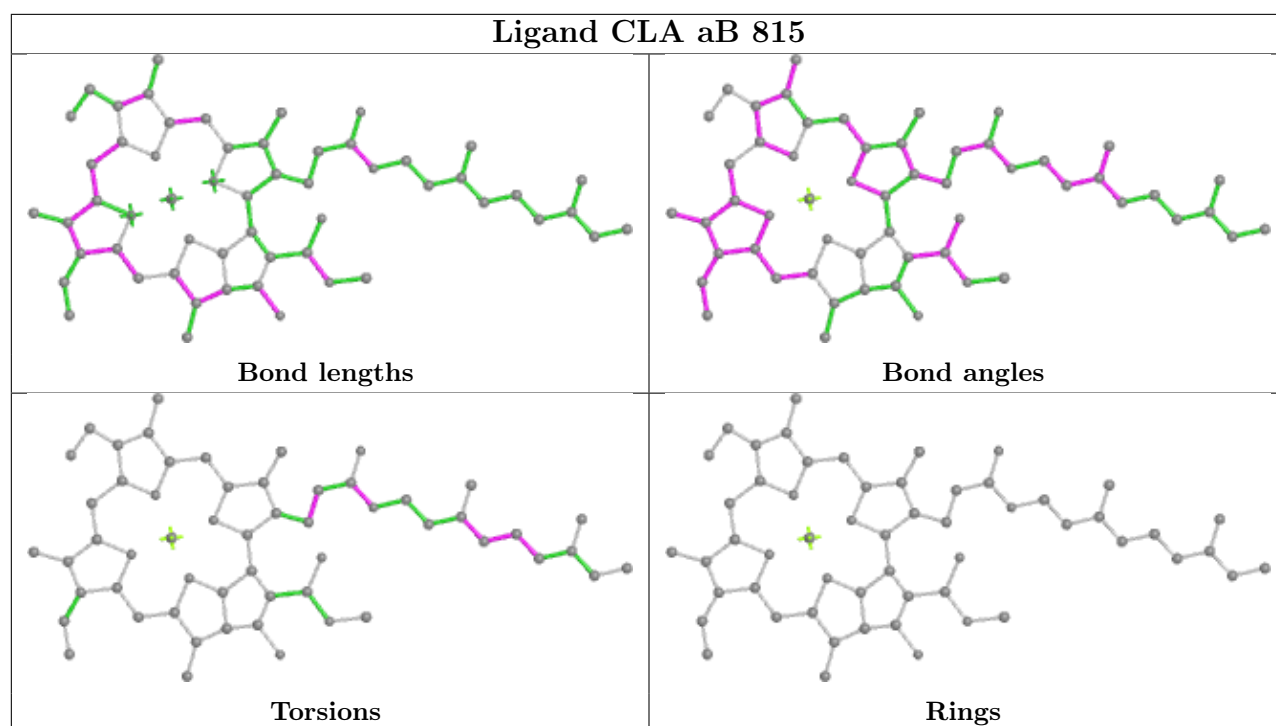


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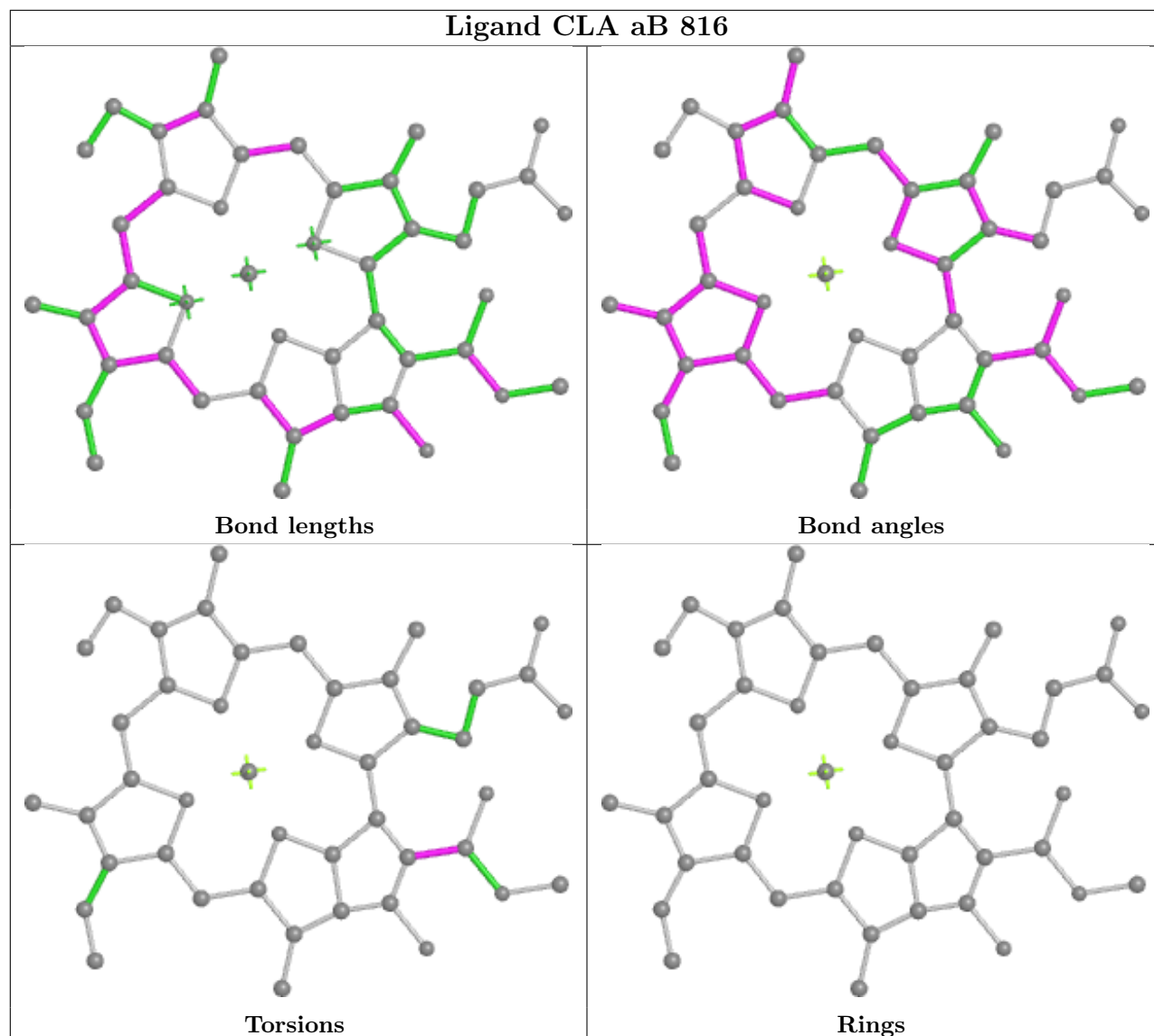


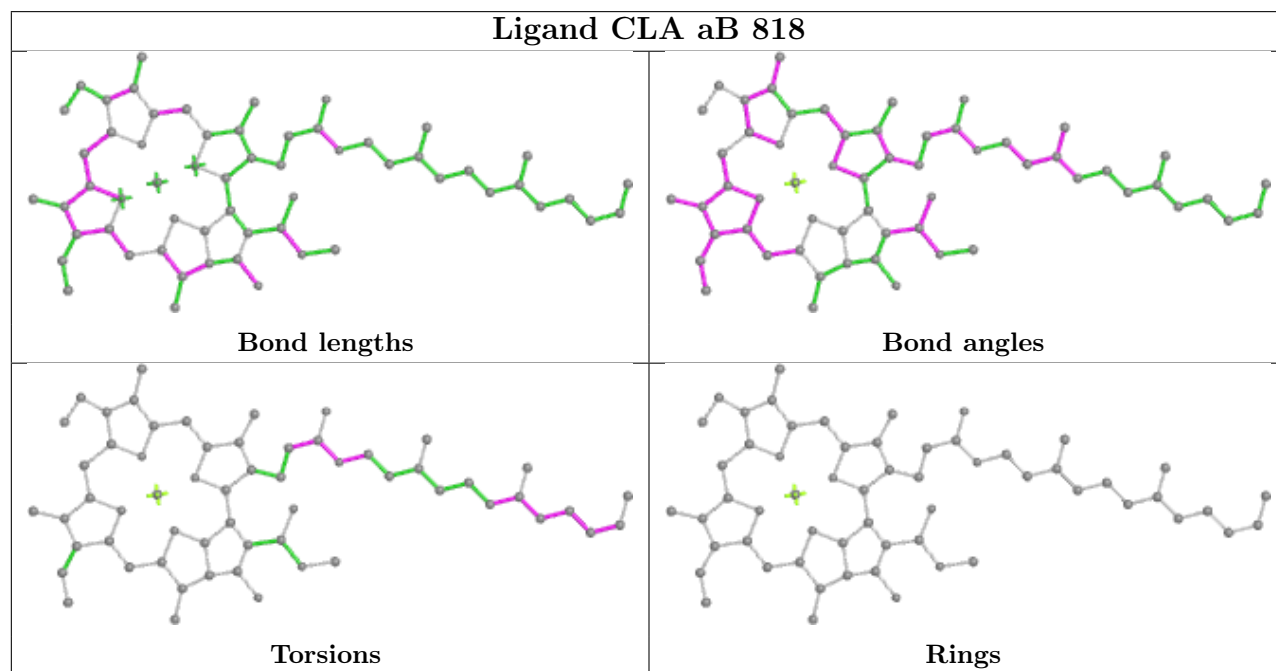
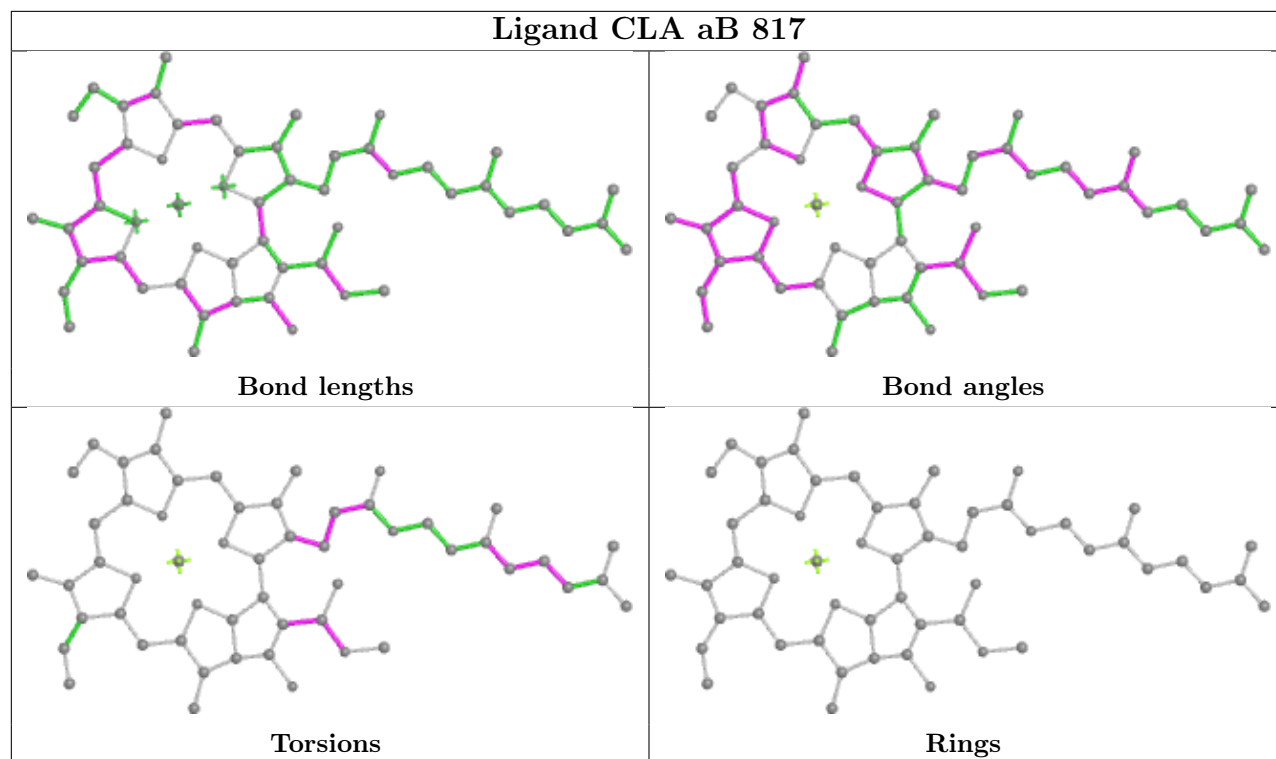
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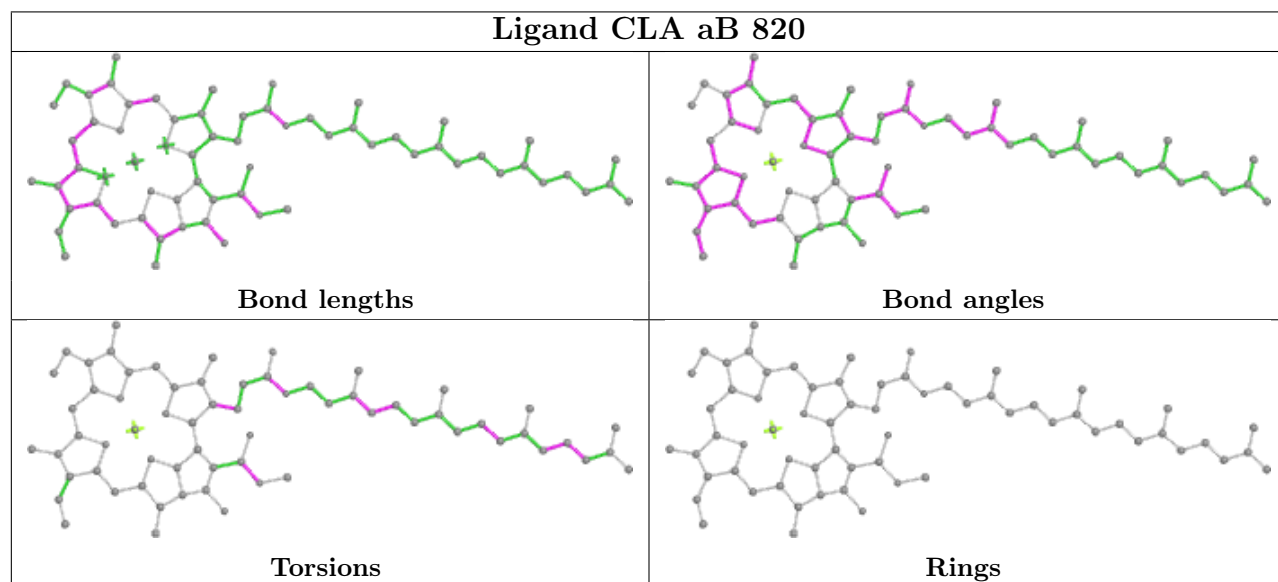
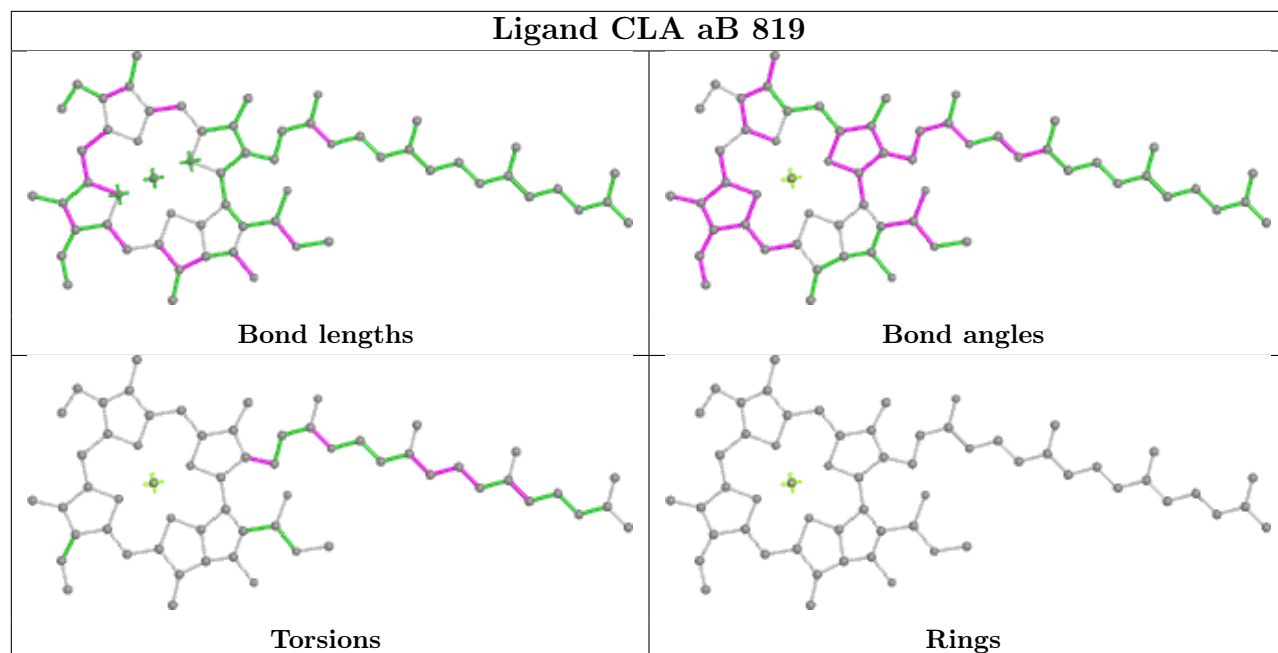




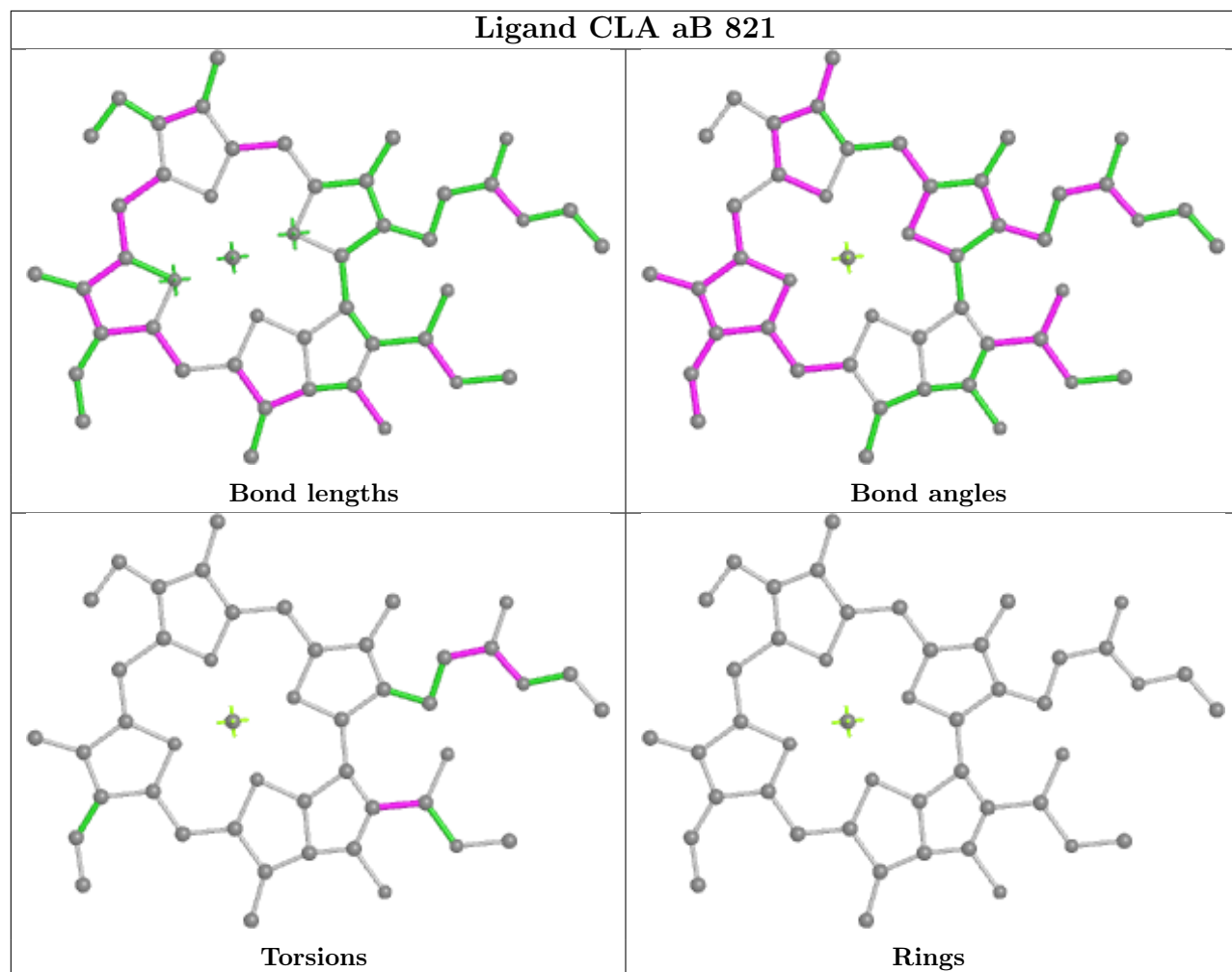
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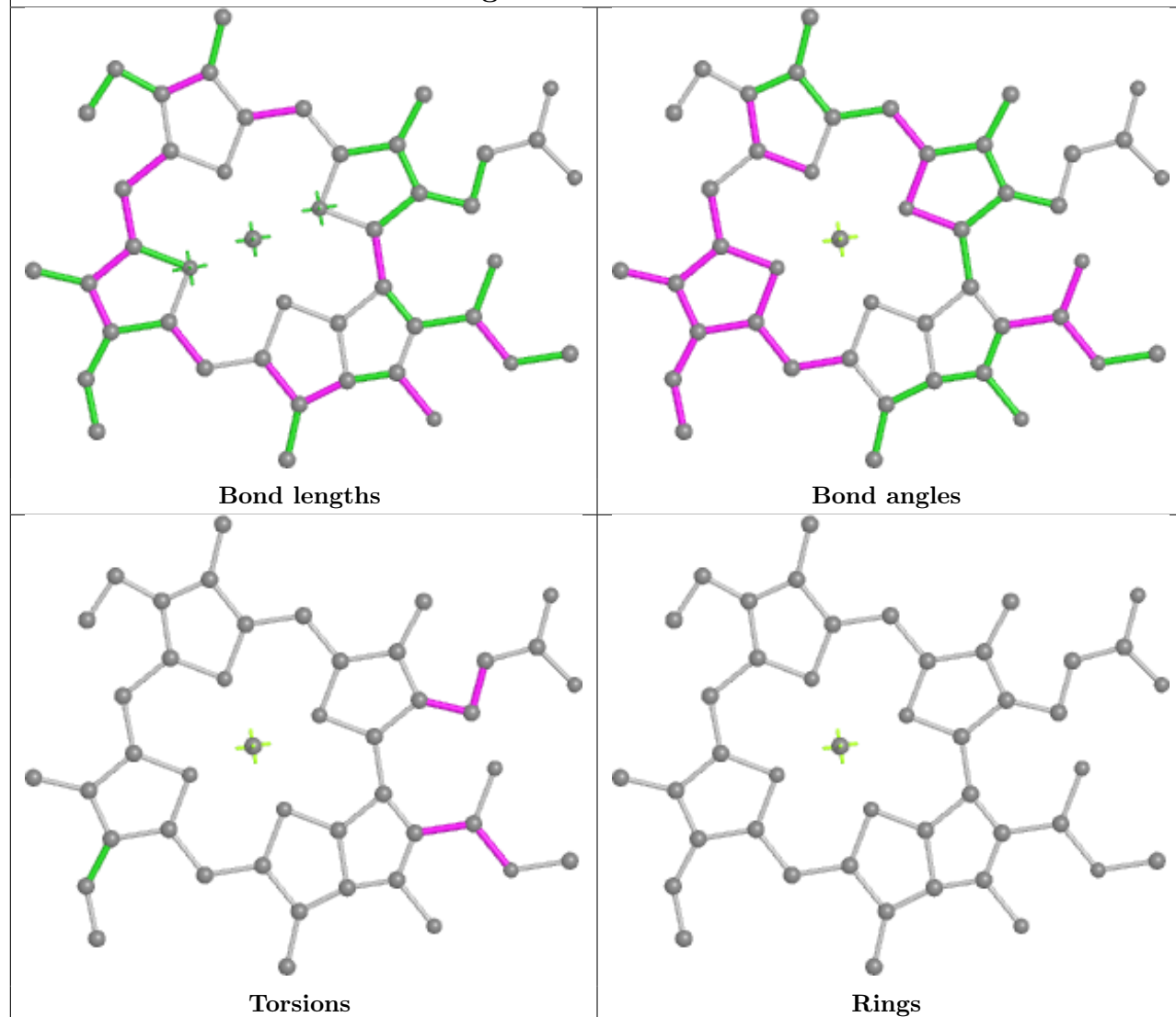


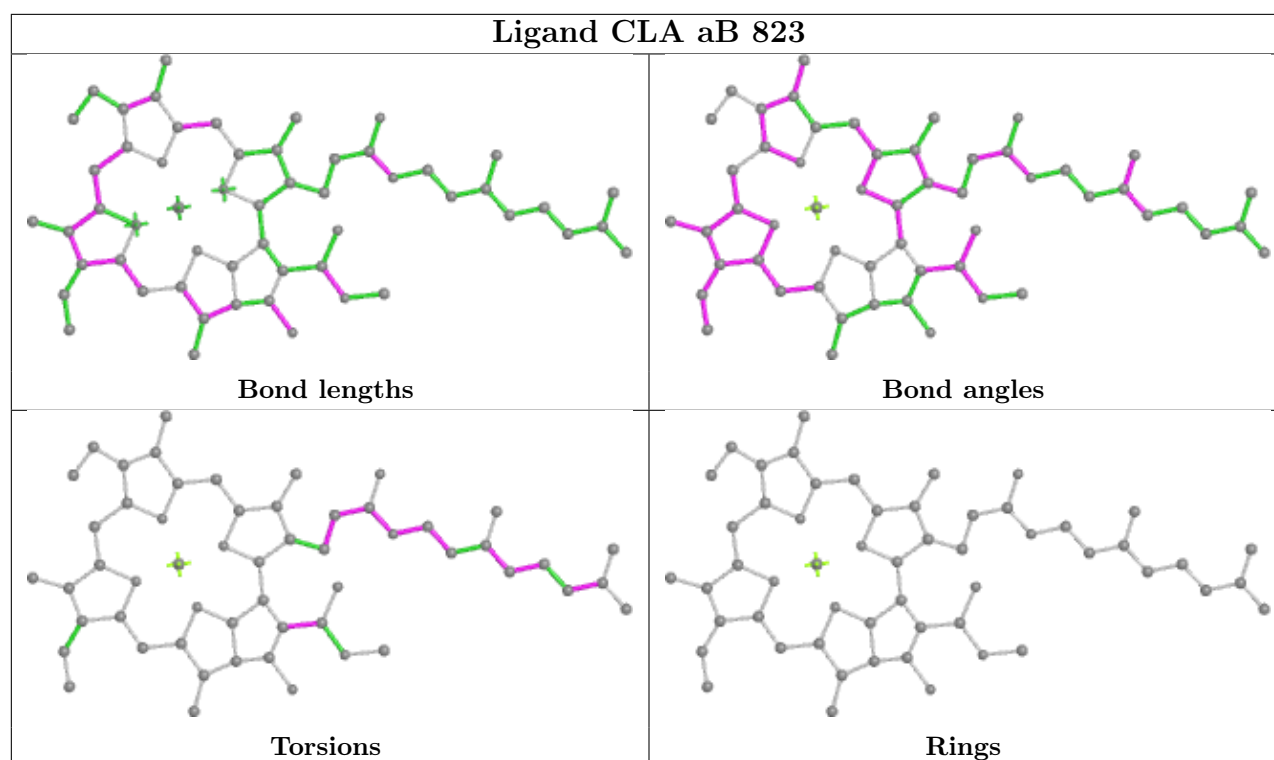


Ligand CLA aB 821

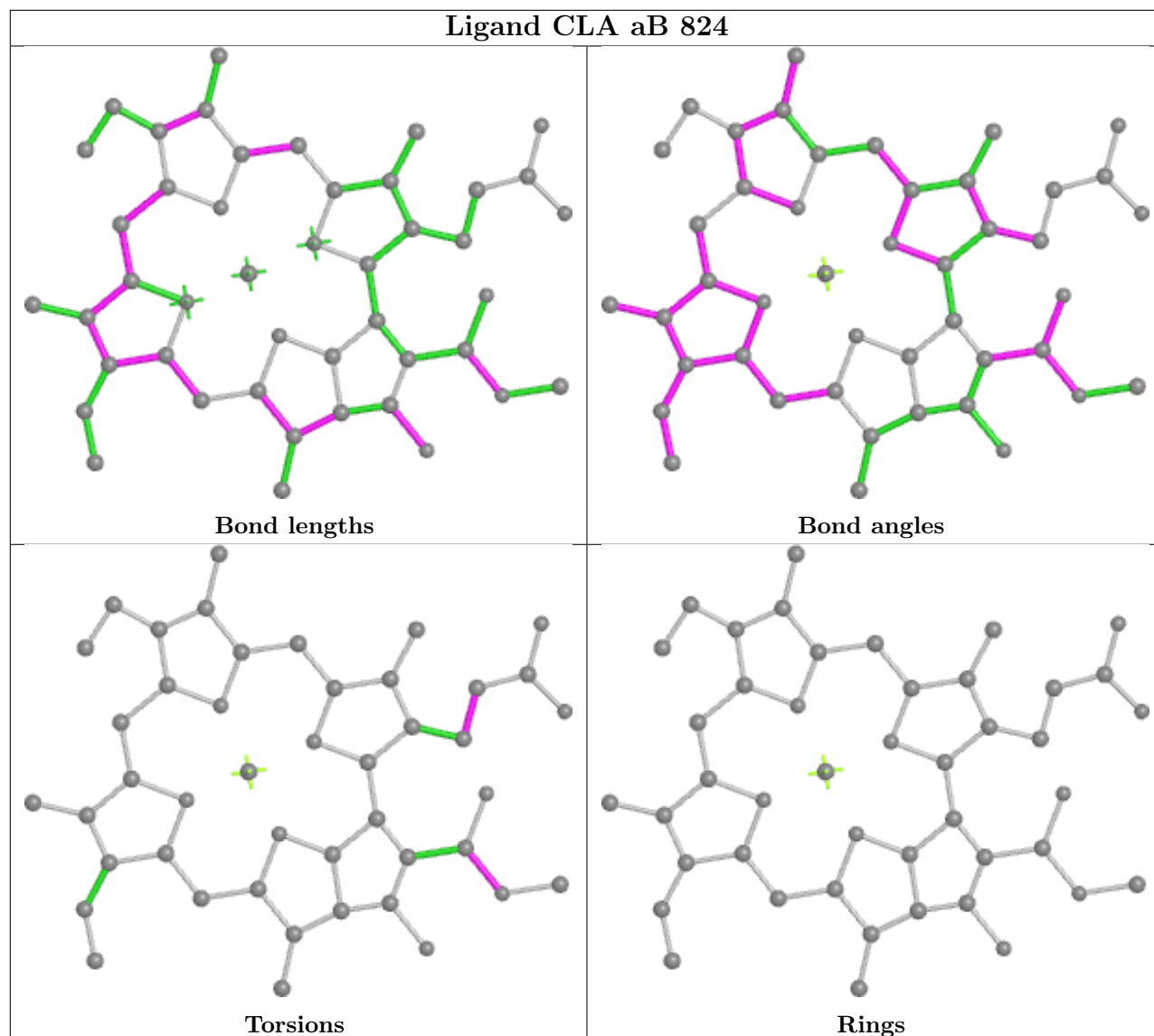


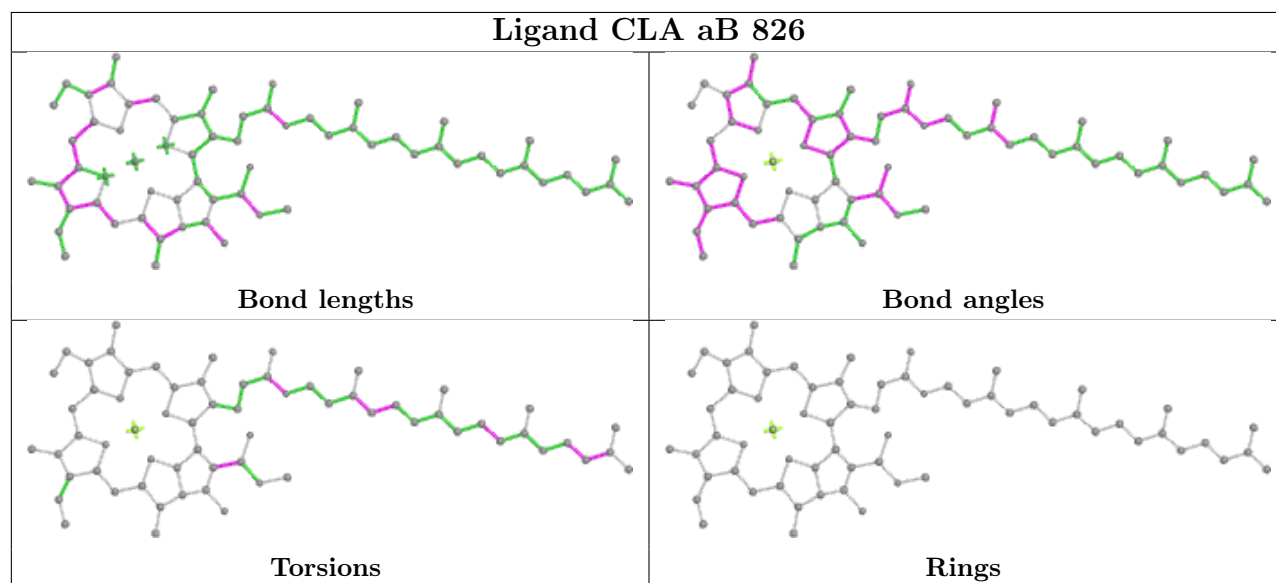
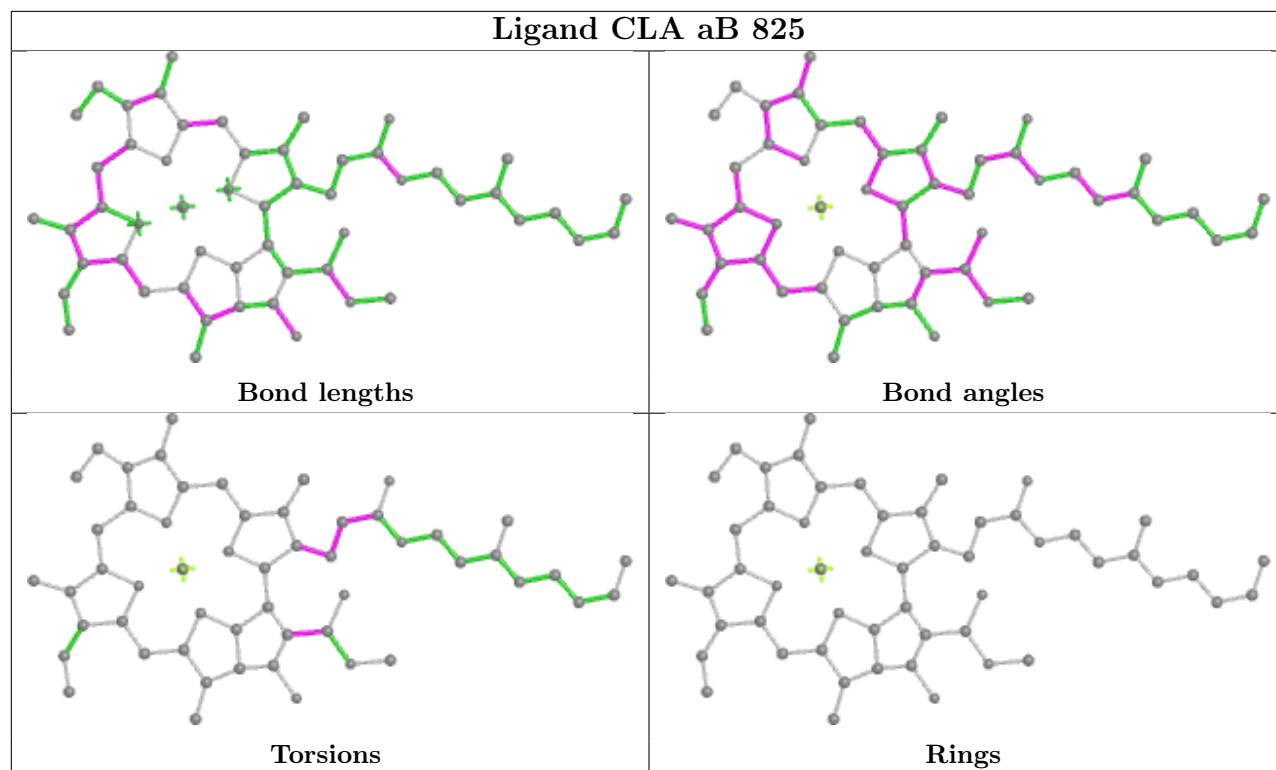
Ligand CLA aB 822



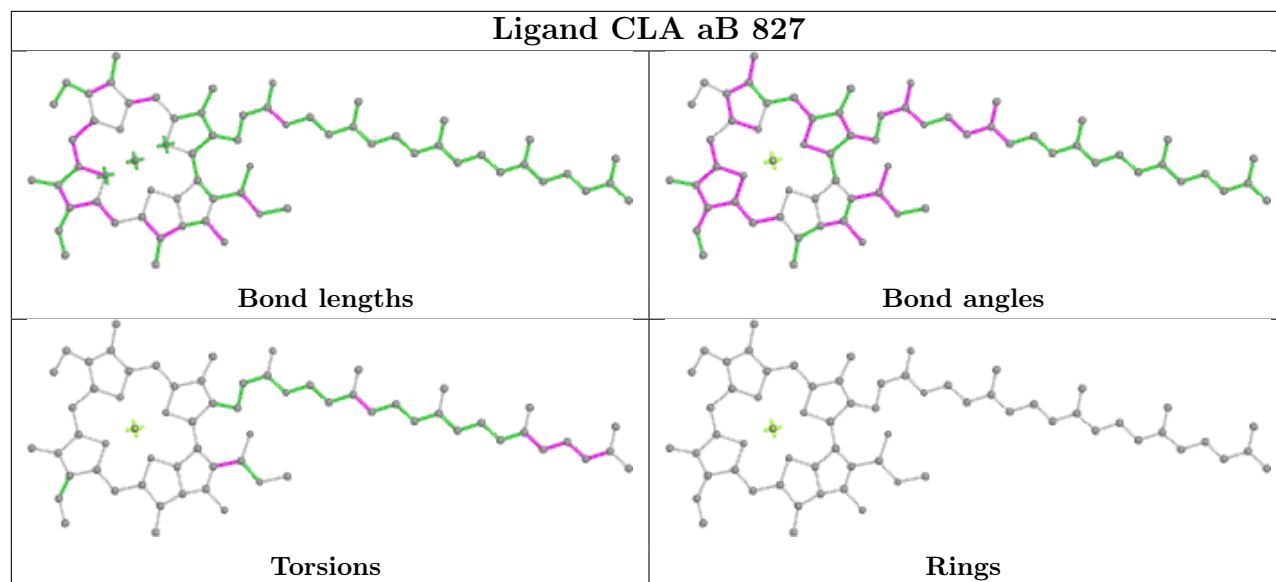


Ligand CLA aB 824

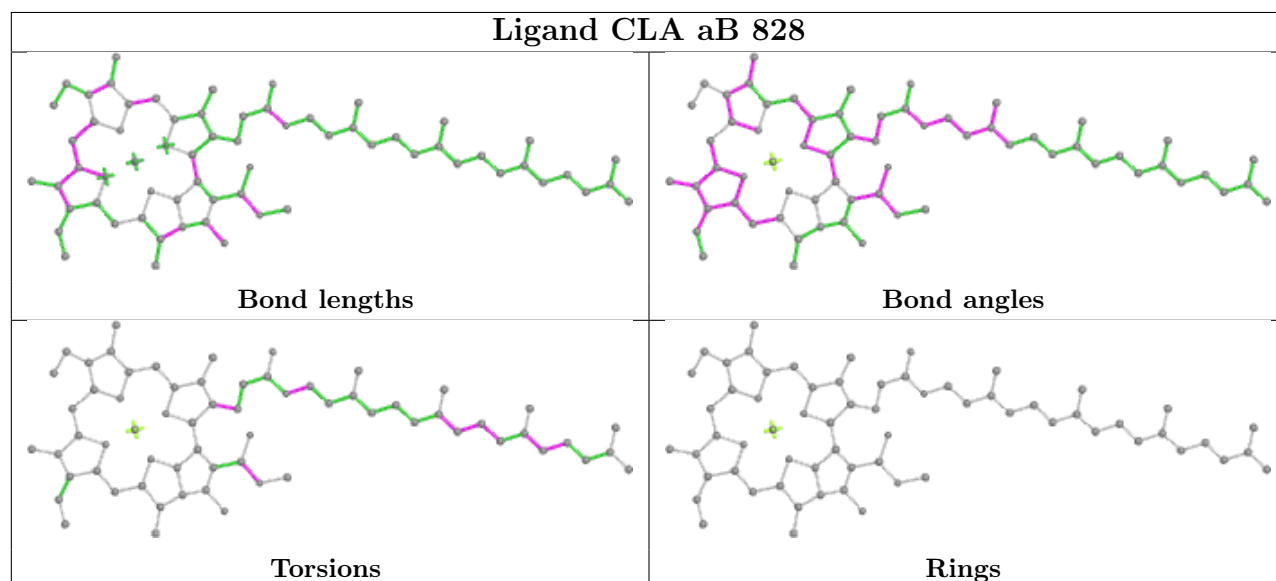




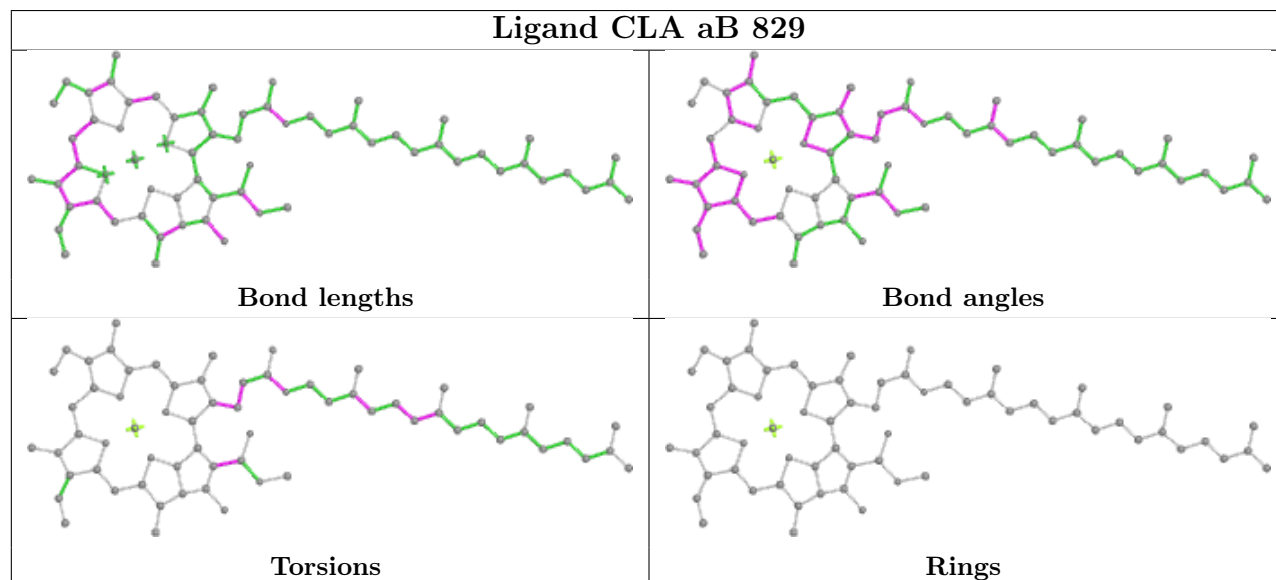
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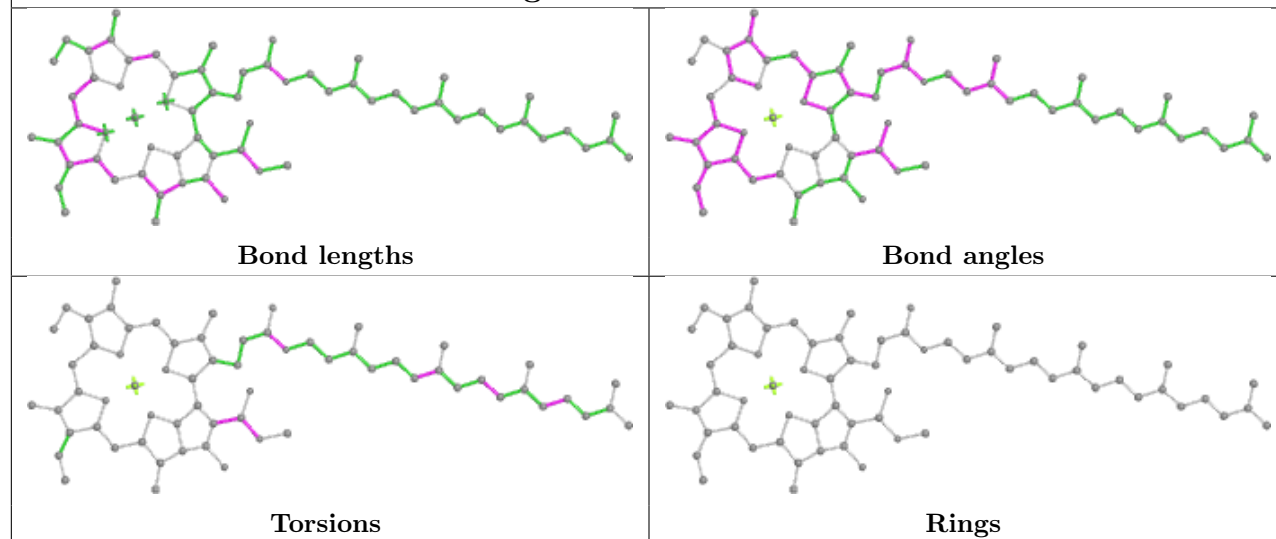
Ligand CLA aB 828



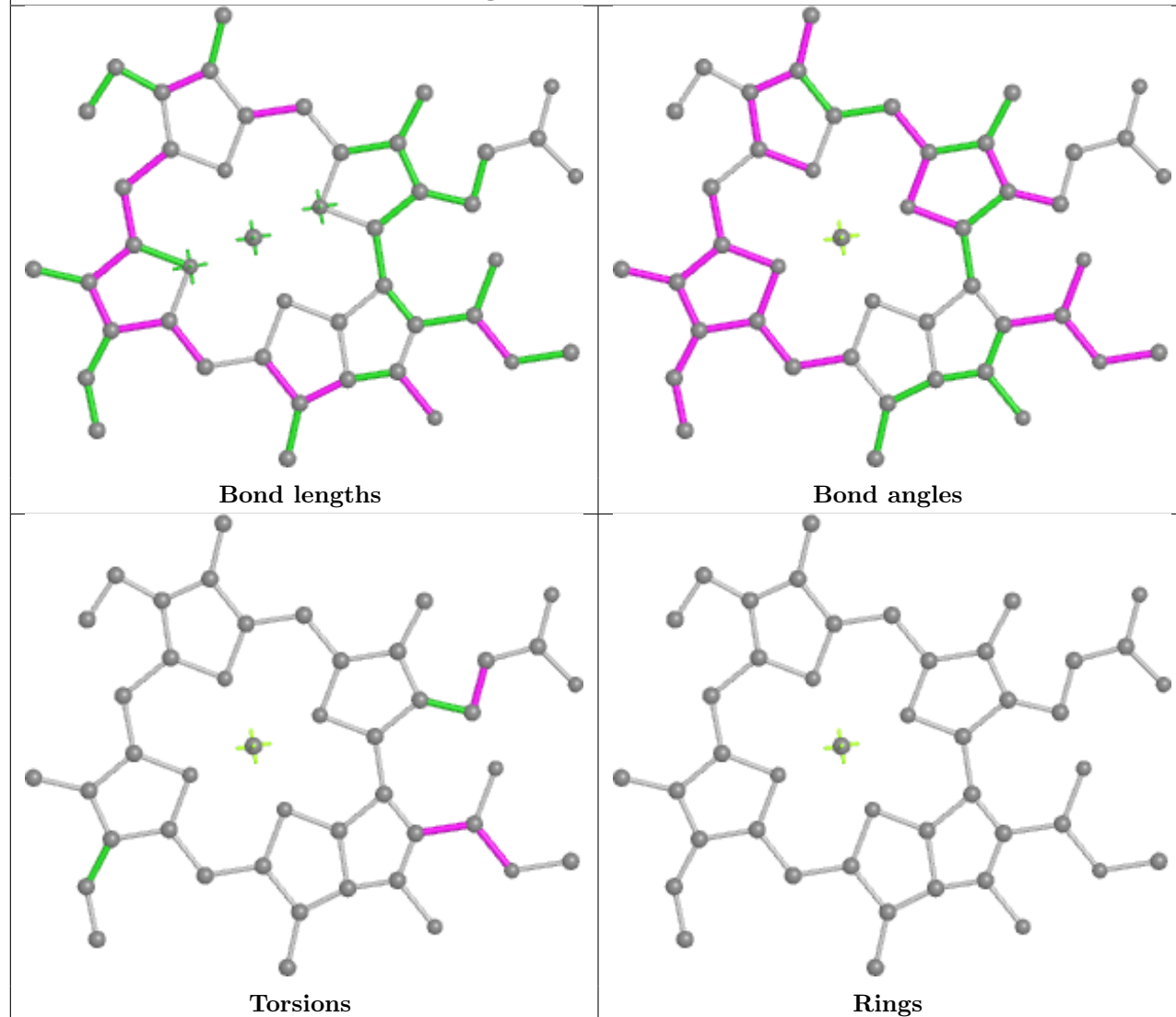
Ligand CLA aB 829

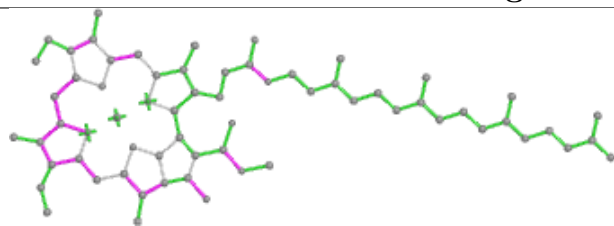
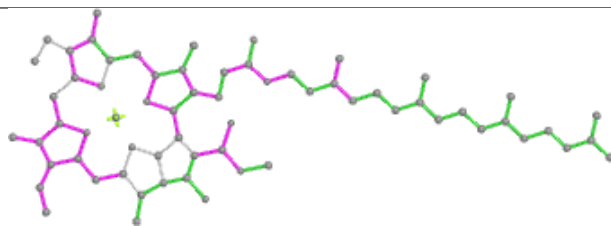
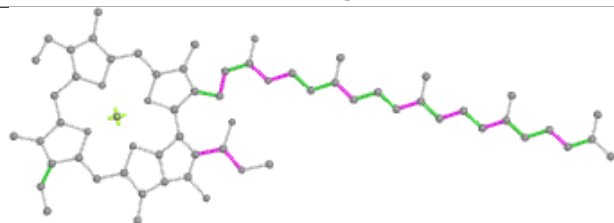
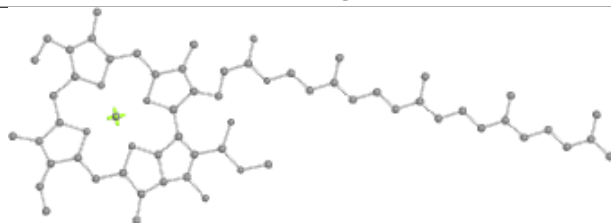
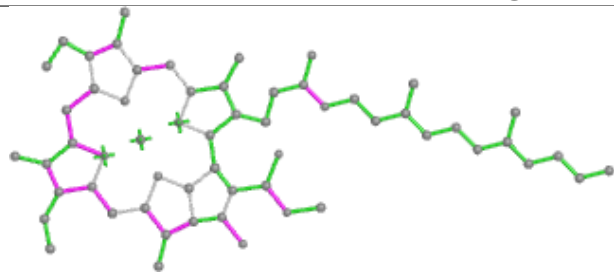
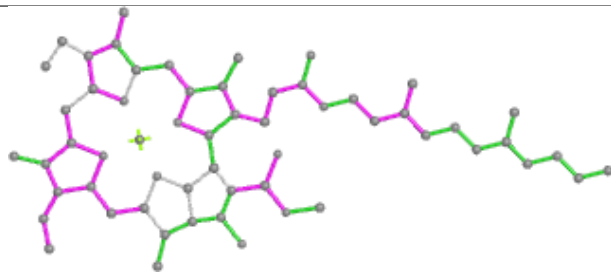
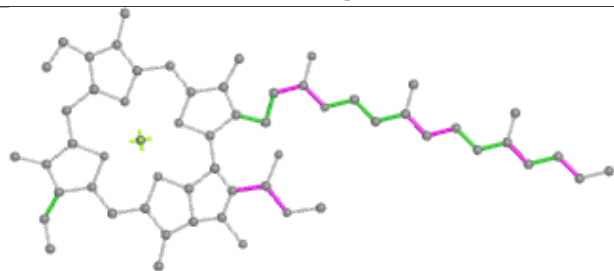
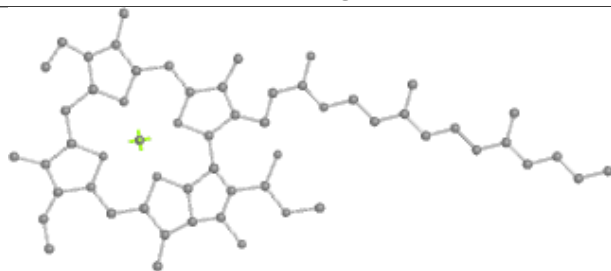


Ligand CLA aB 830

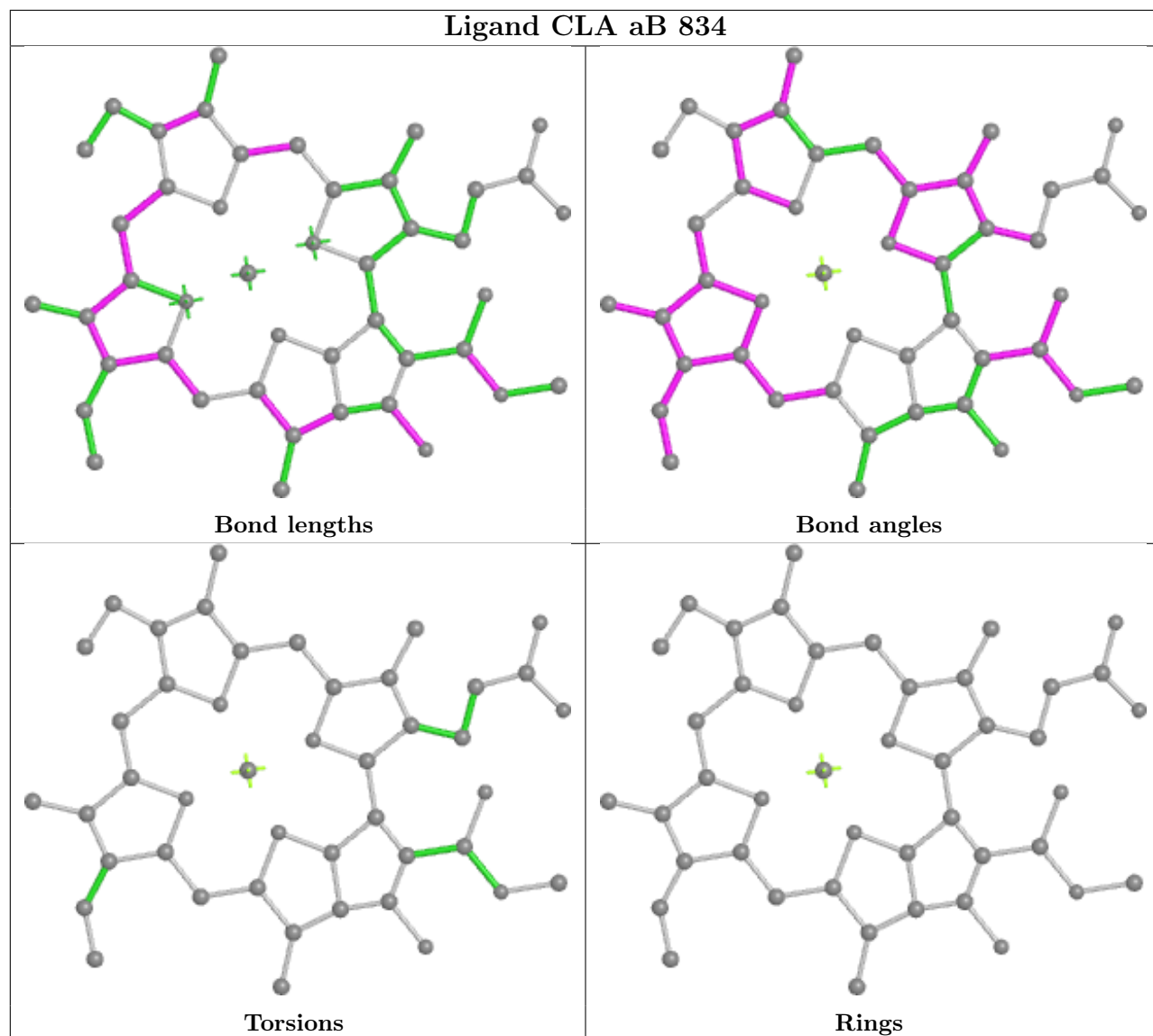


Ligand CLA aB 831

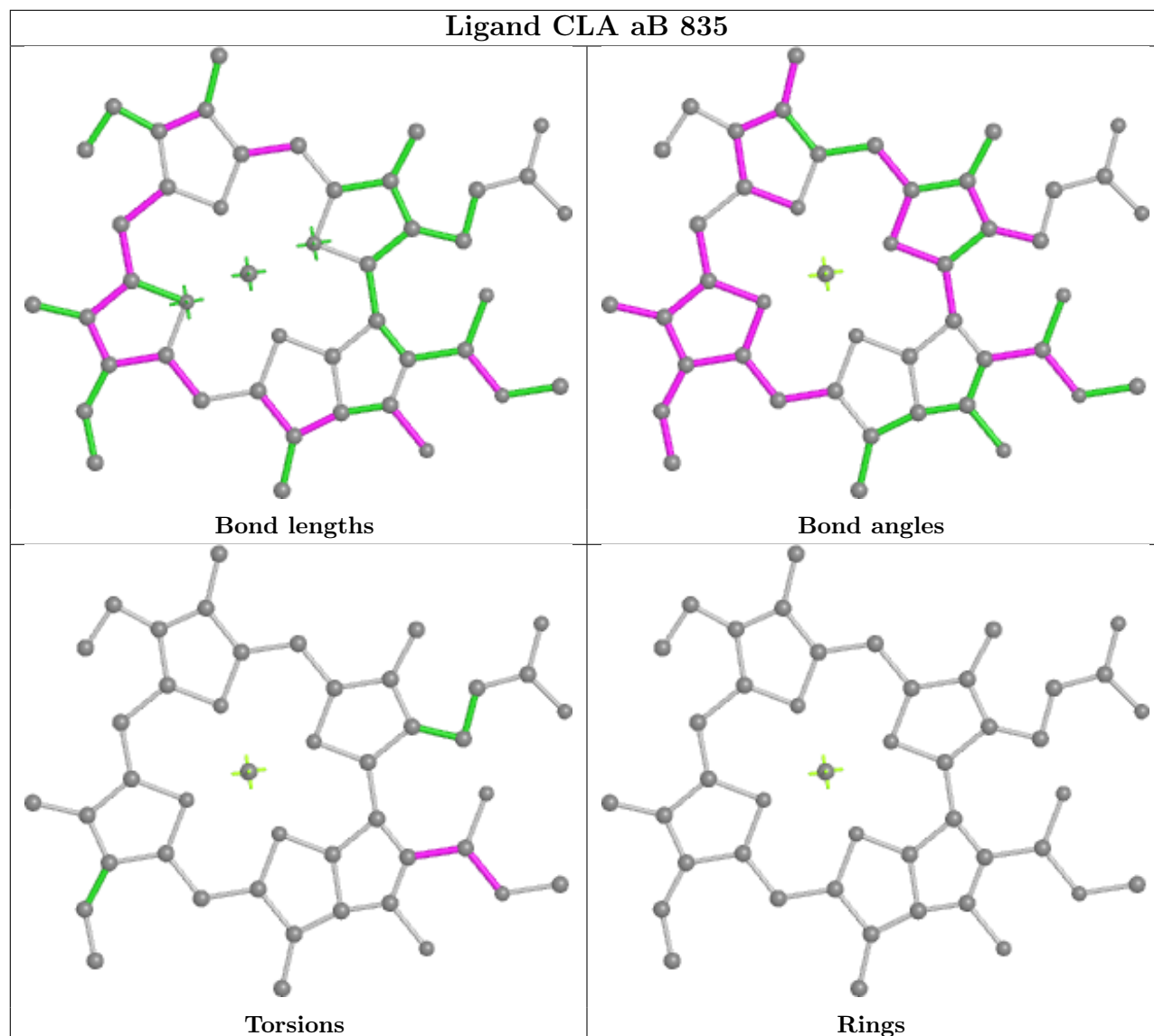


Ligand CLA aB 832**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA aB 833****Bond lengths****Bond angles****Torsions****Rings**

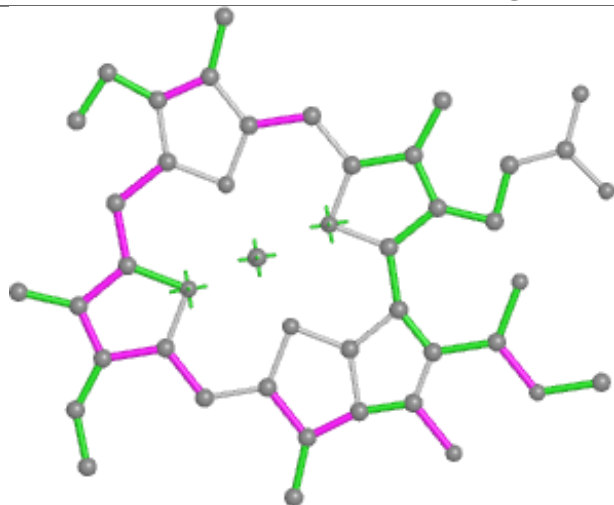
Ligand CLA aB 834



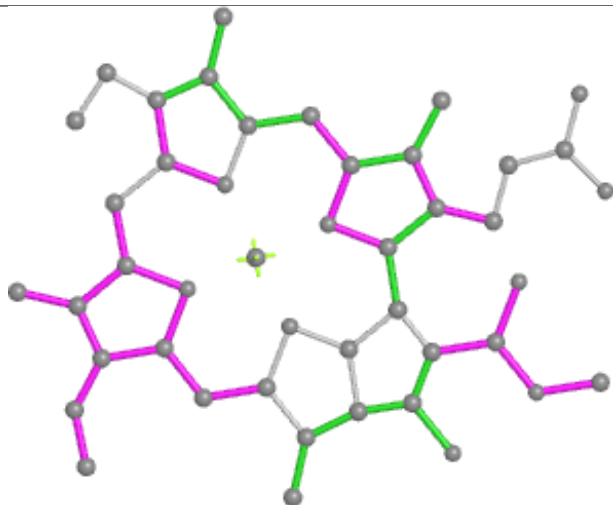
Ligand CLA aB 835



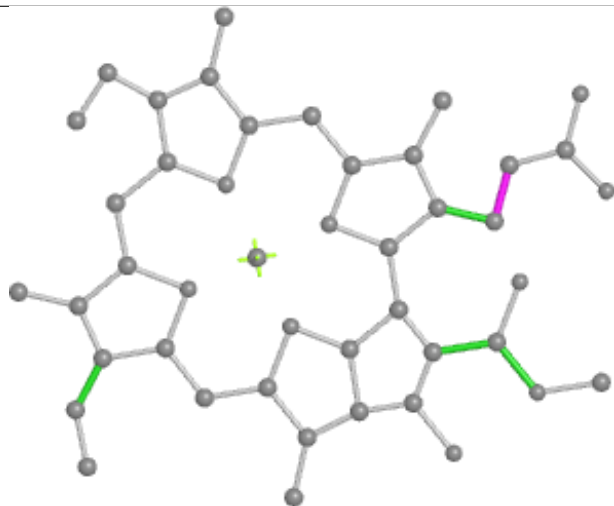
Ligand CLA aB 836



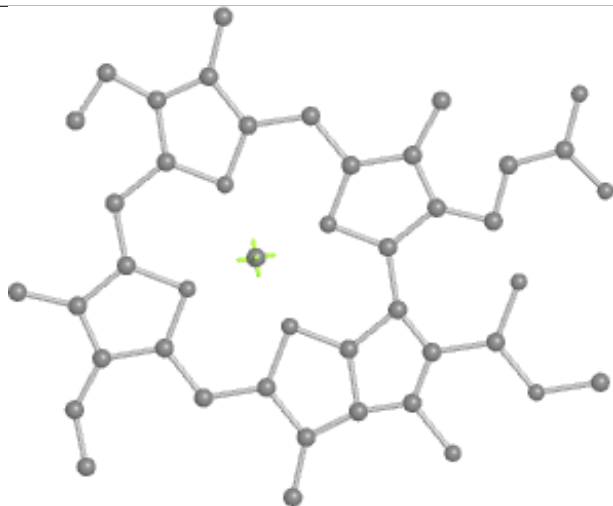
Bond lengths



Bond angles

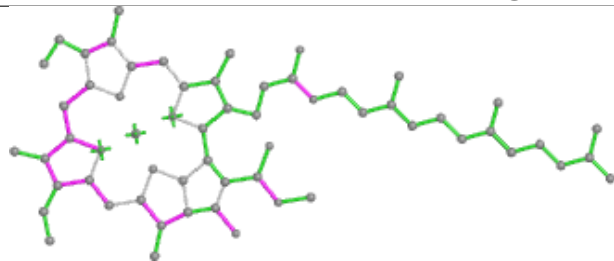


Torsions

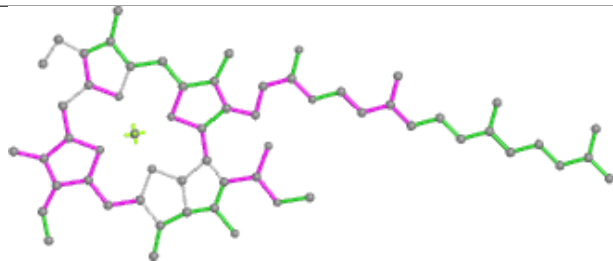


Rings

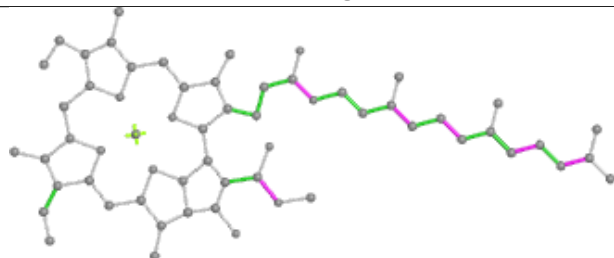
Ligand CLA aB 837



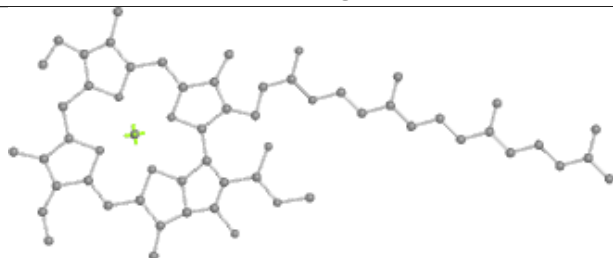
Bond lengths



Bond angles

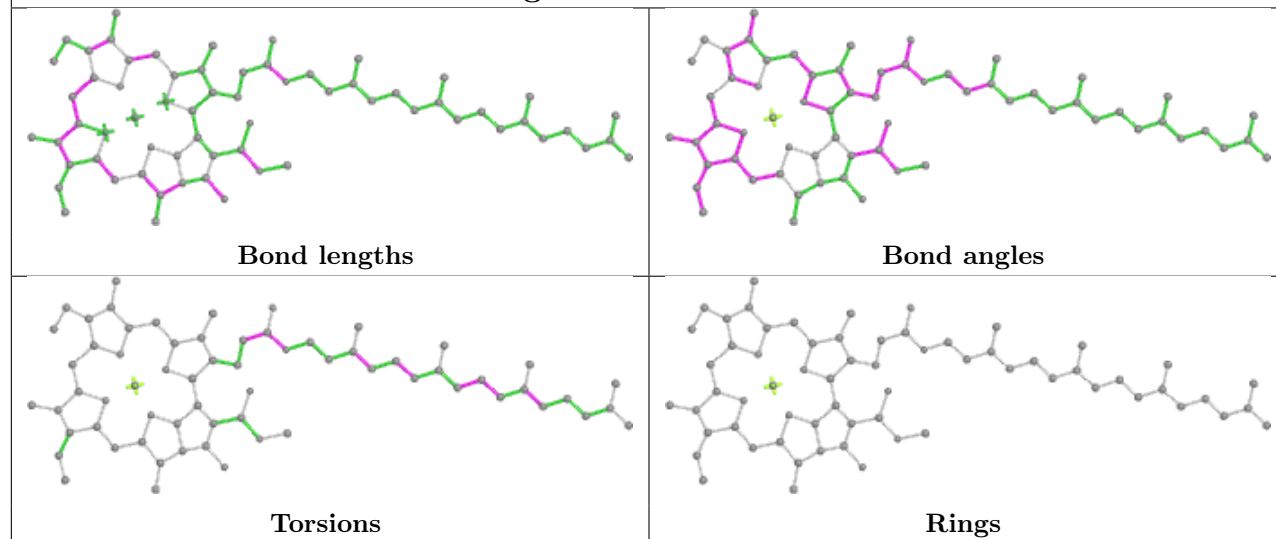


Torsions

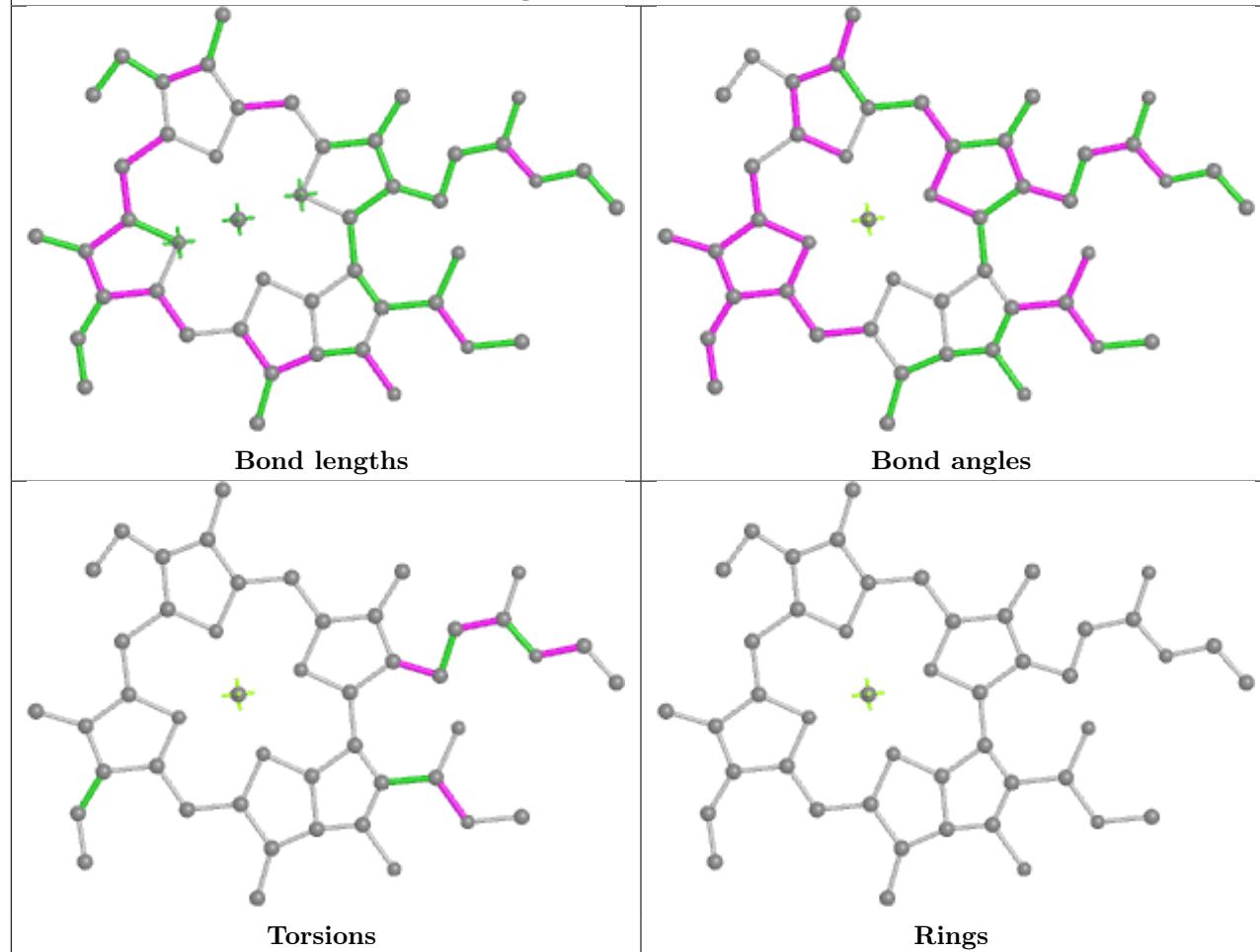


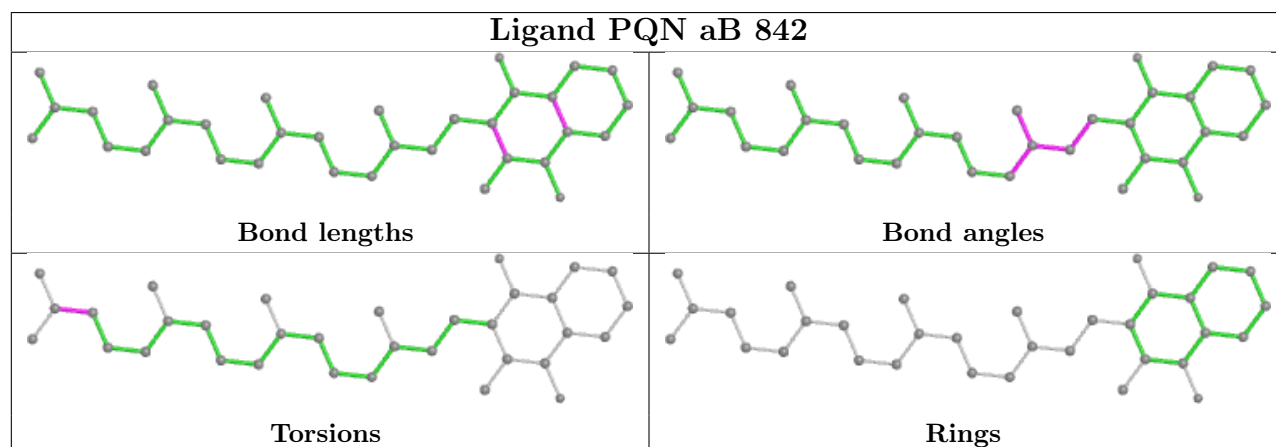
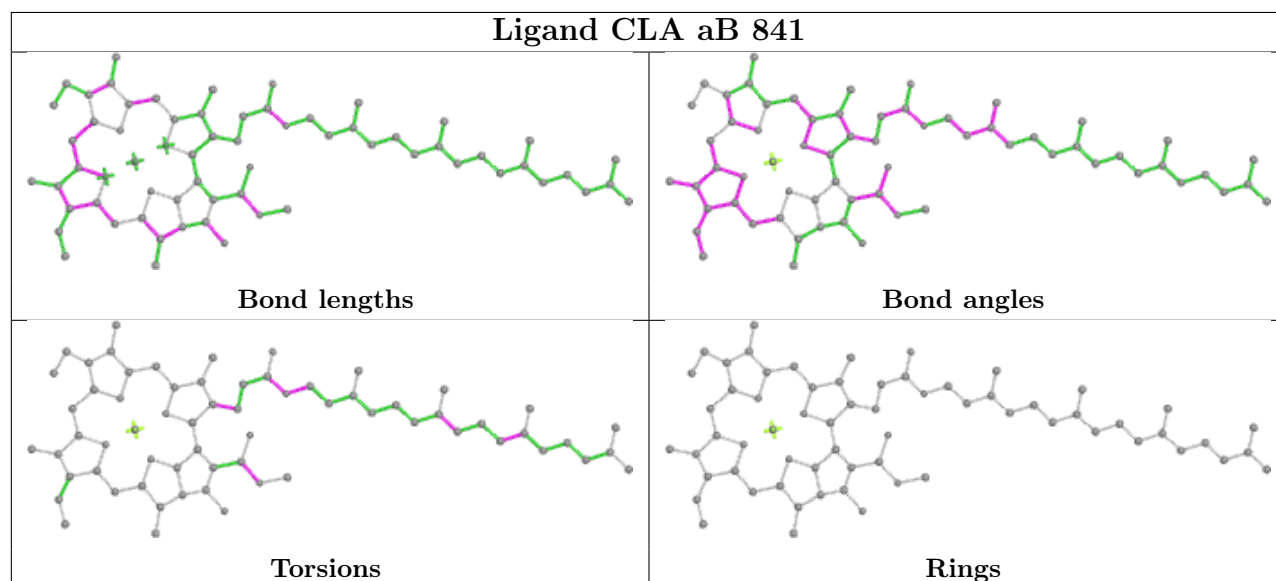
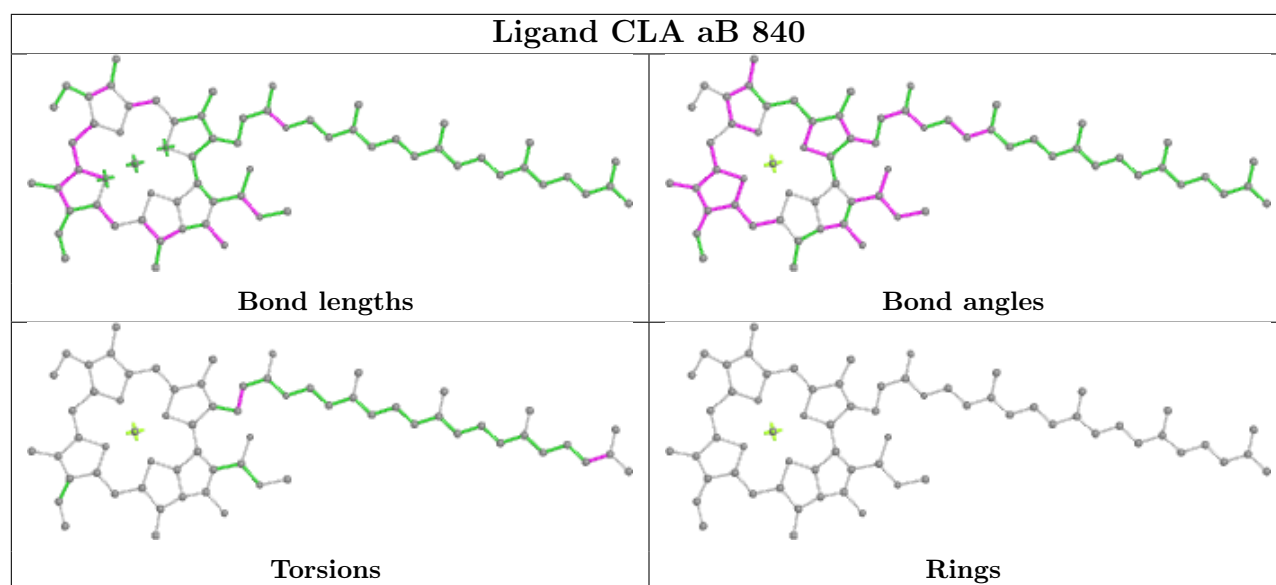
Rings

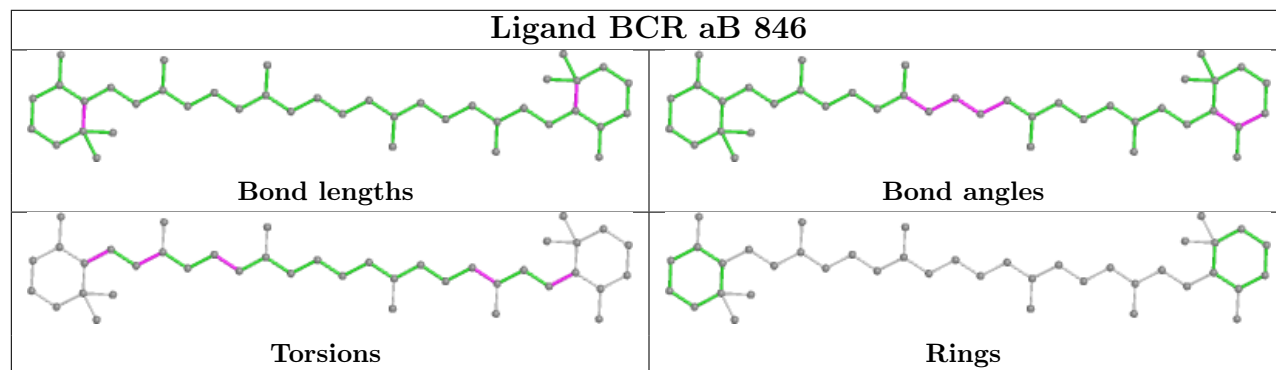
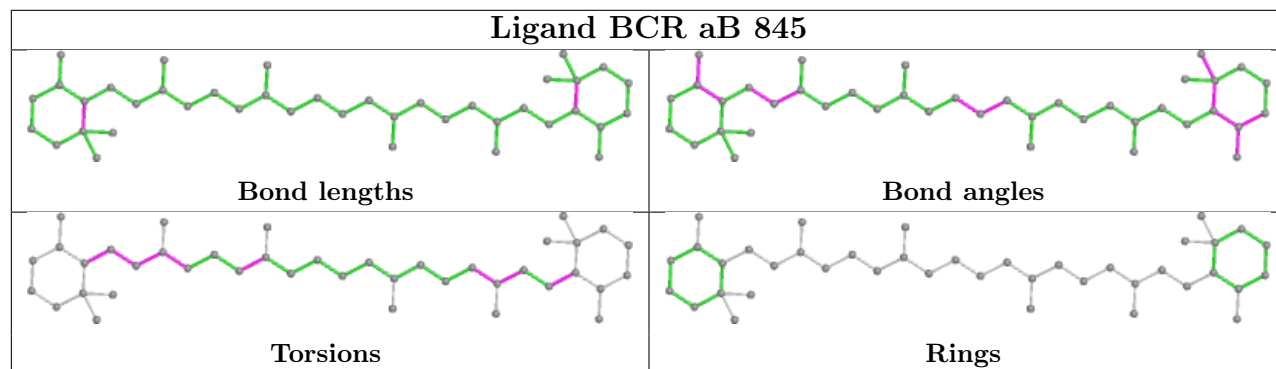
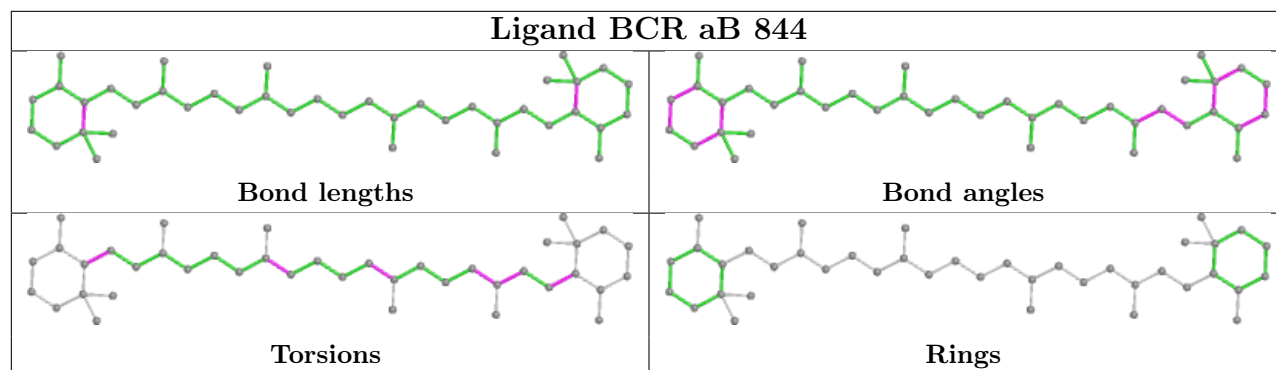
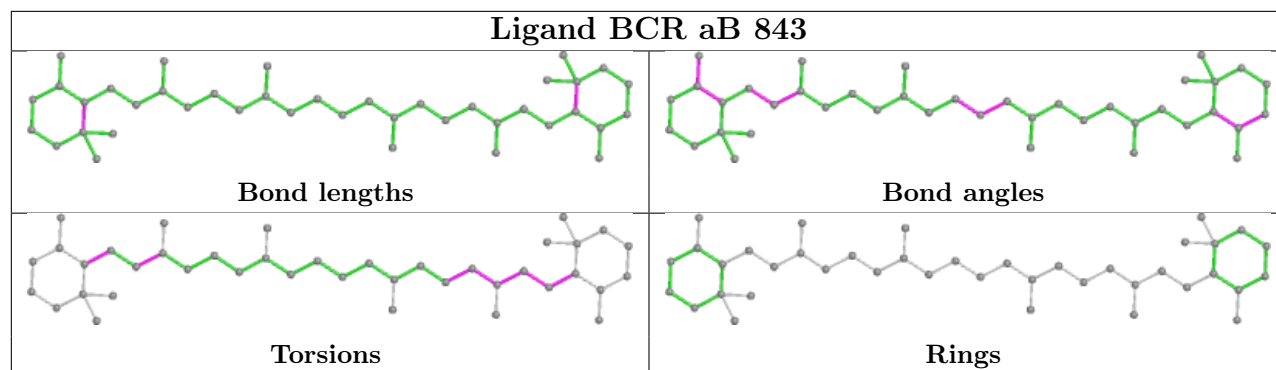
Ligand CLA aB 838

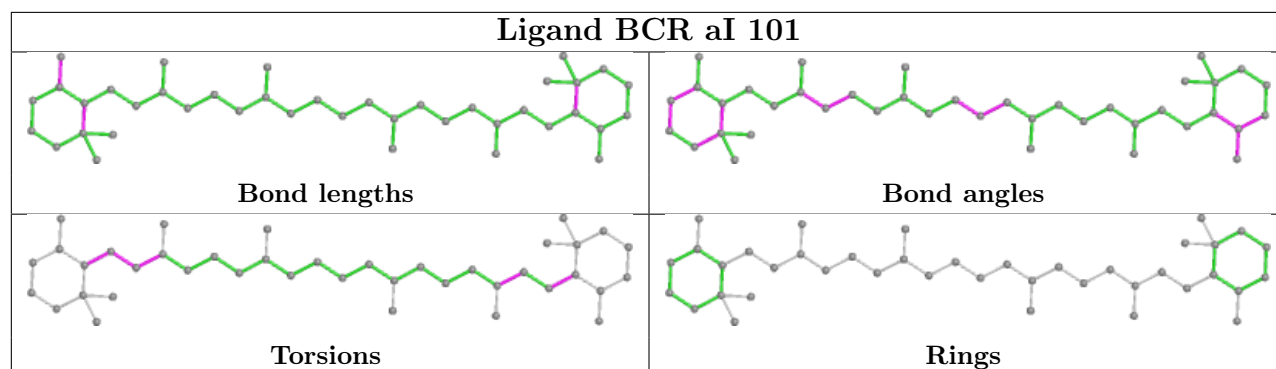
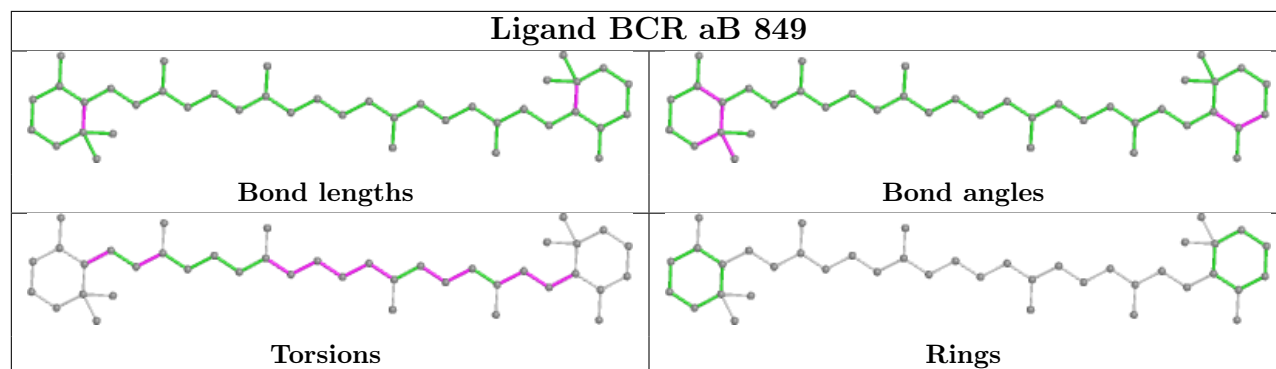
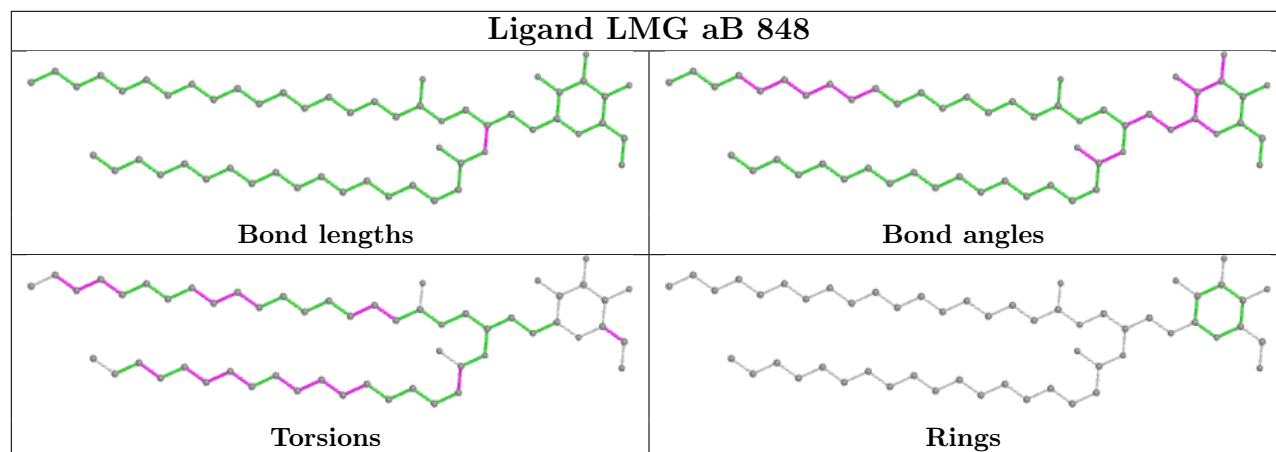
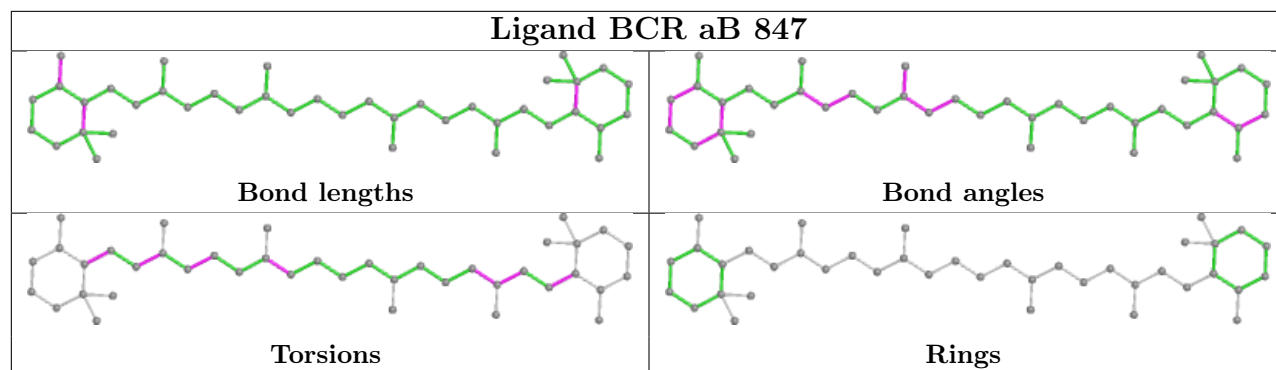


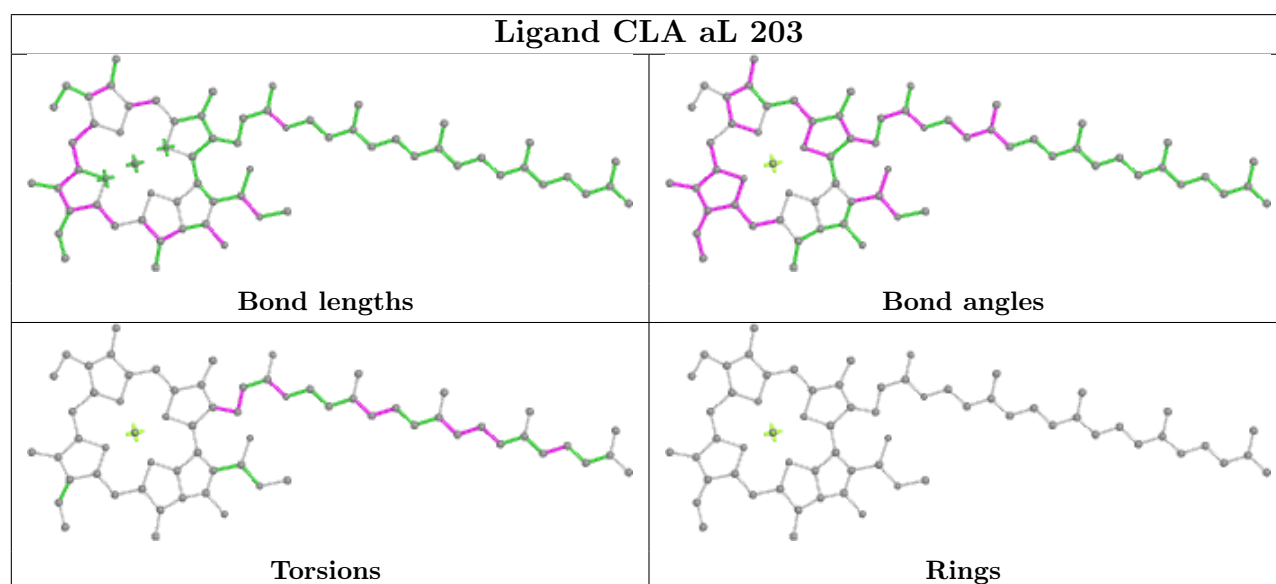
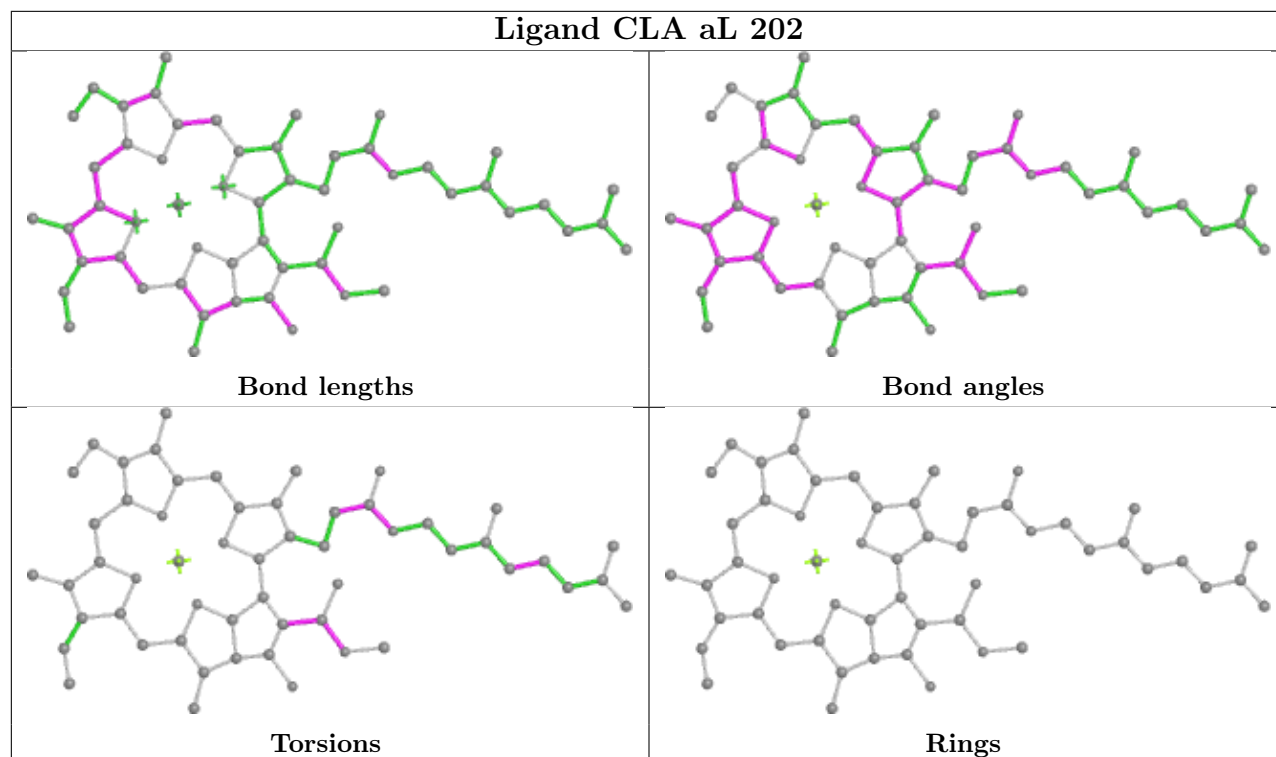
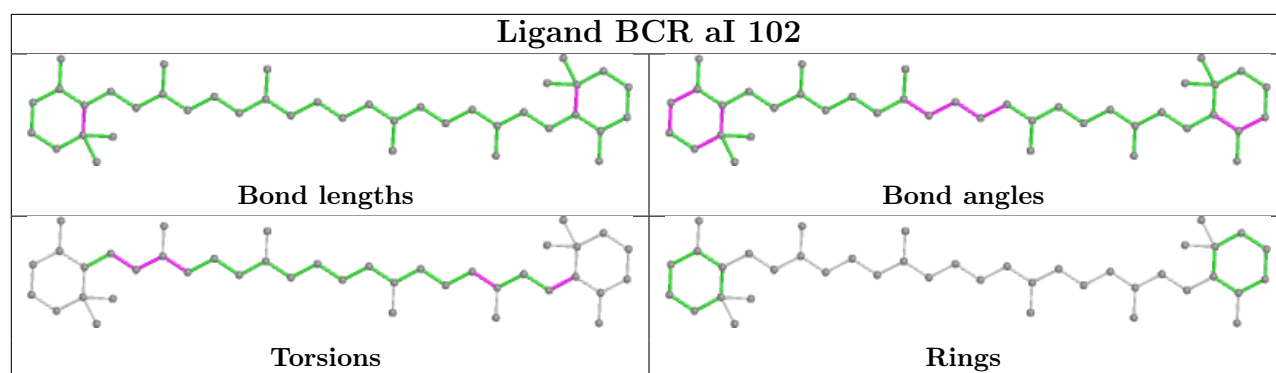
Ligand CLA aB 839

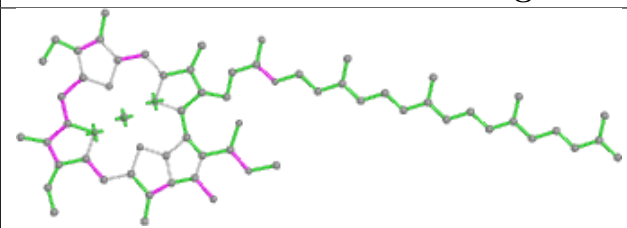
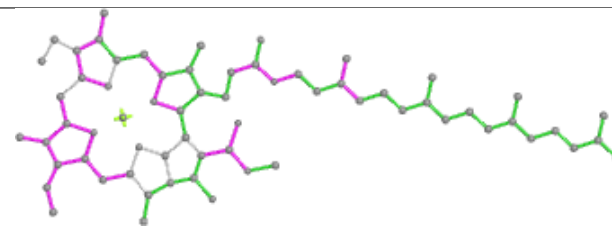
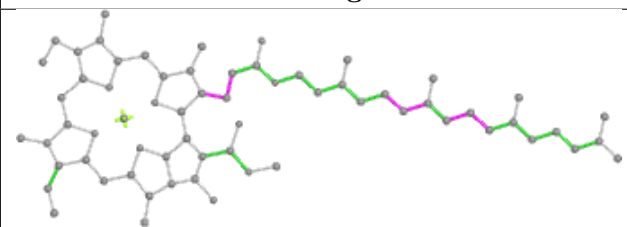
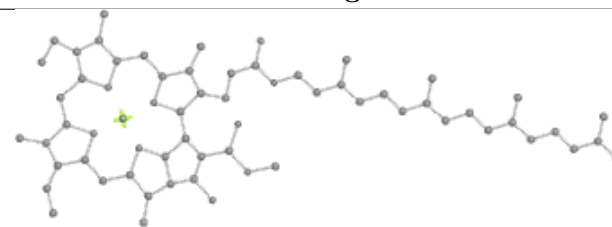
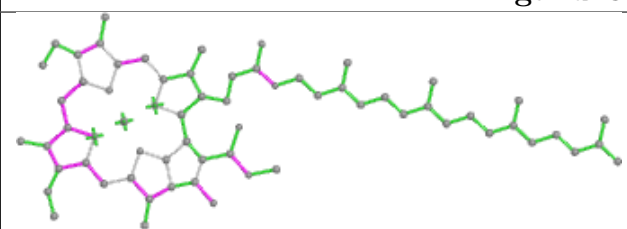
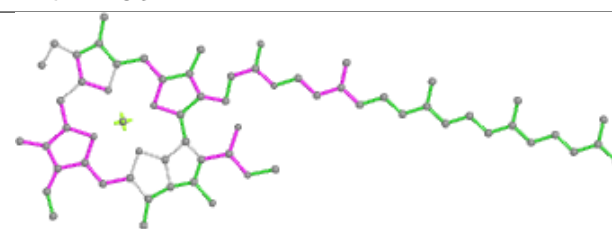
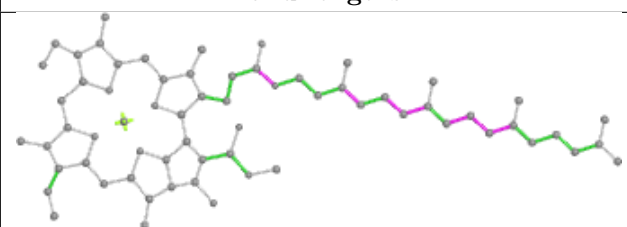
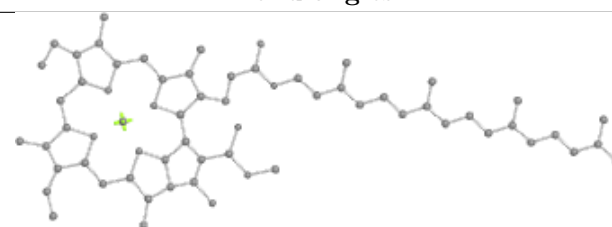
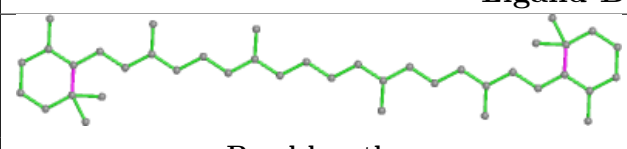
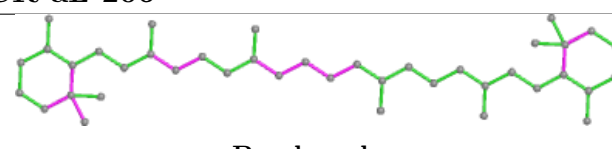
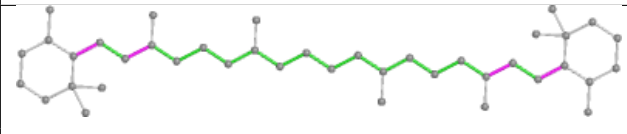
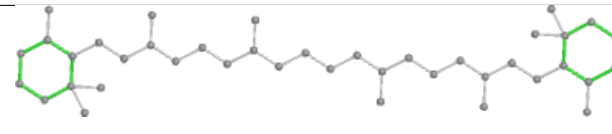


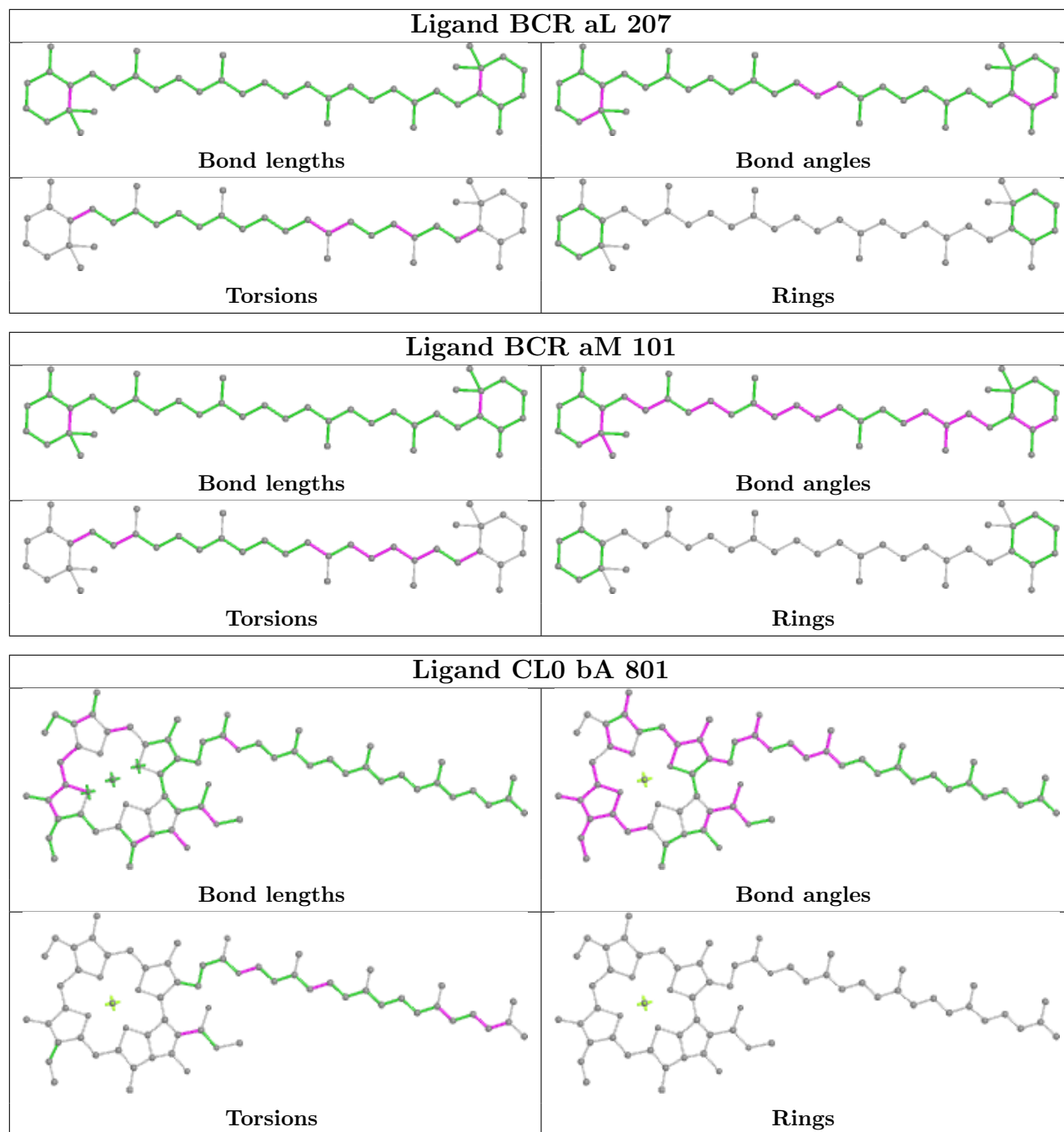




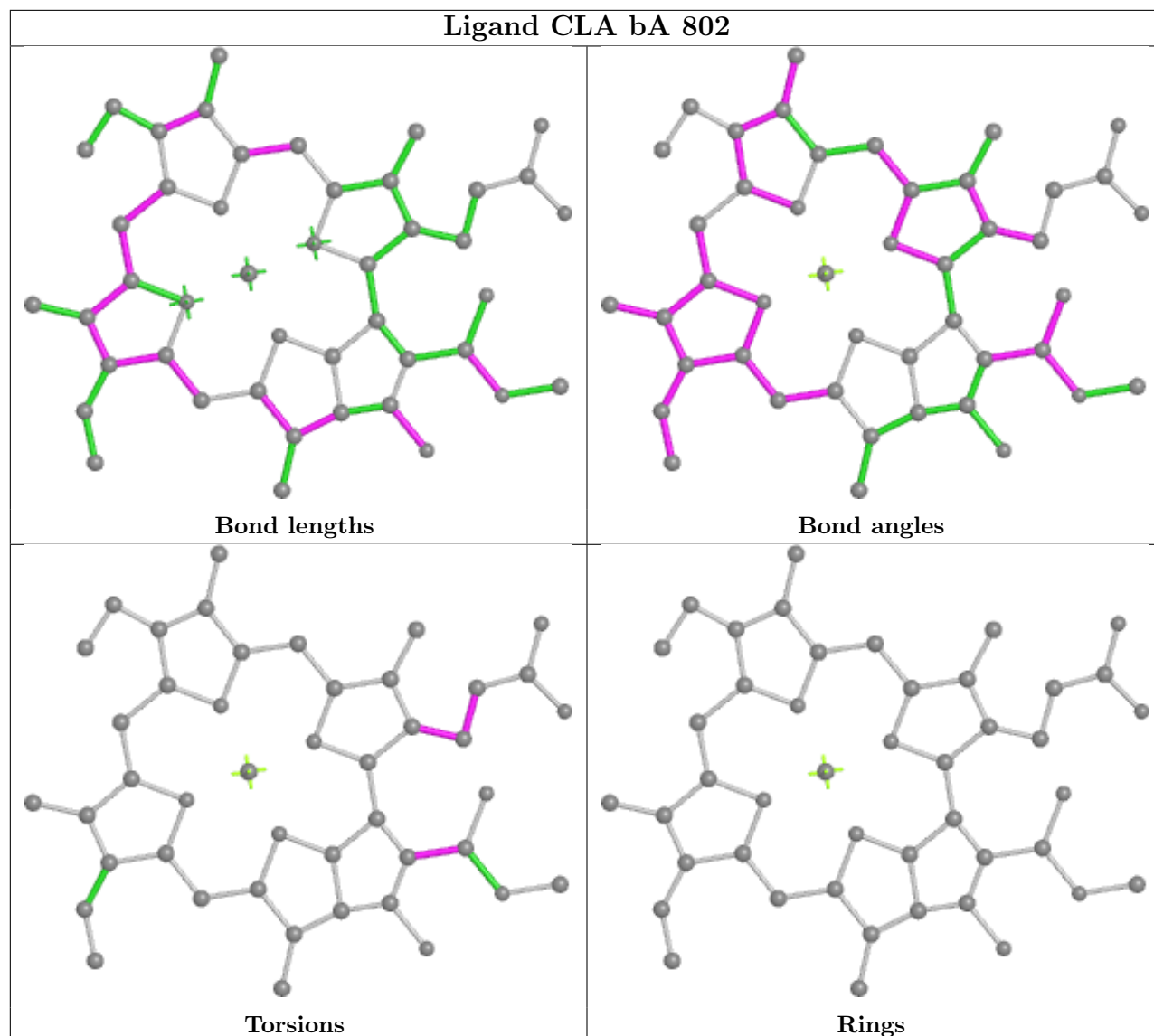




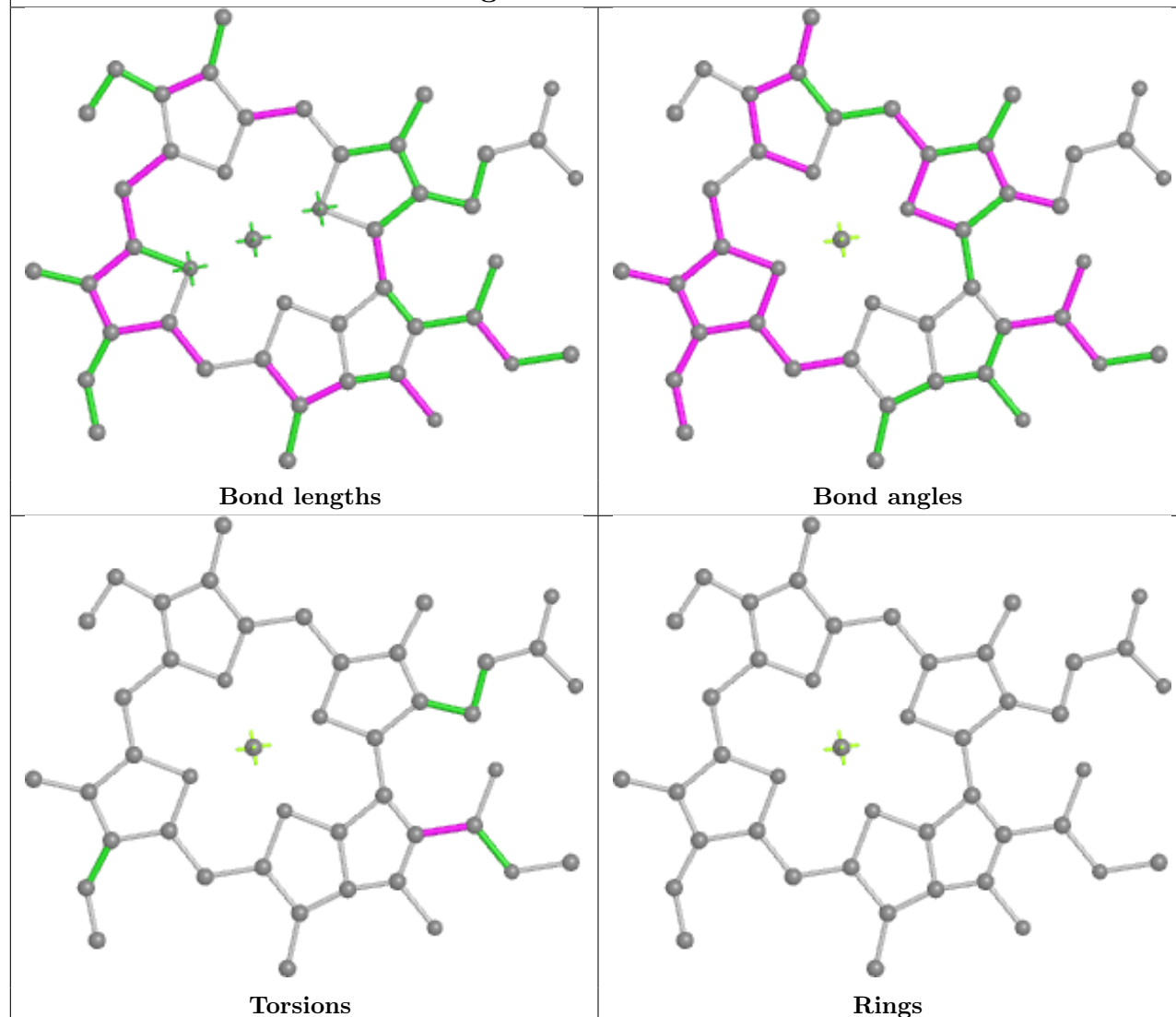
Ligand CLA aL 204	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA aL 205	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR aL 206	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



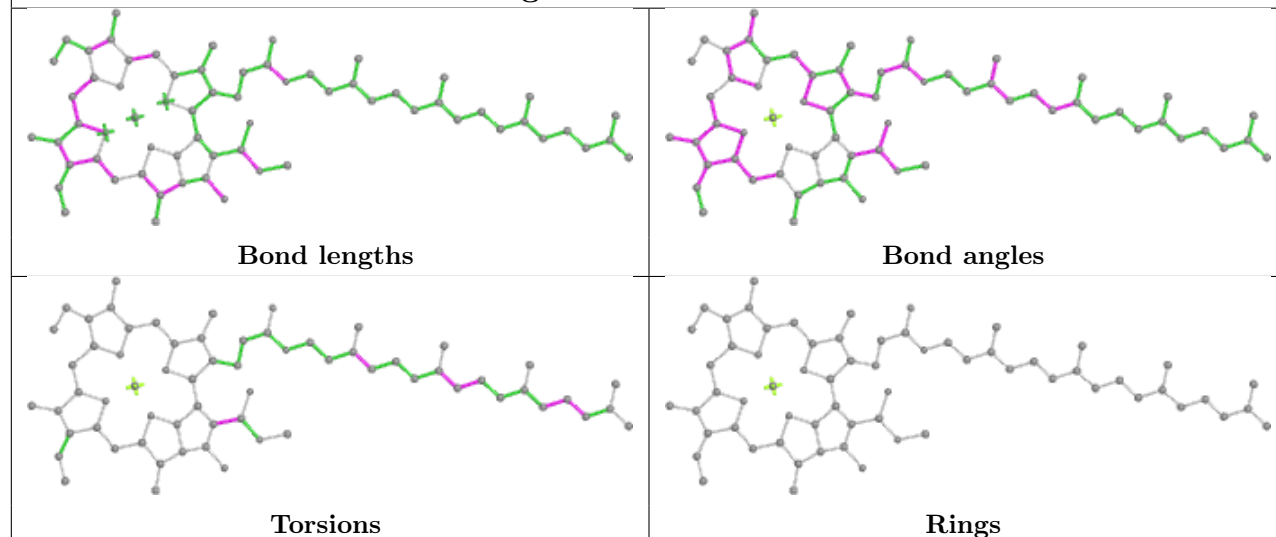
Ligand CLA bA 802



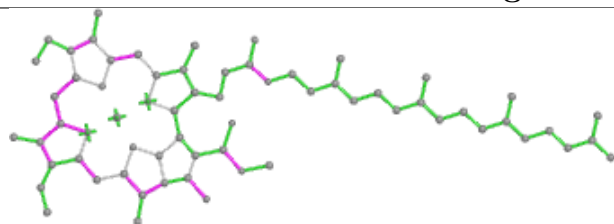
Ligand CLA bA 803



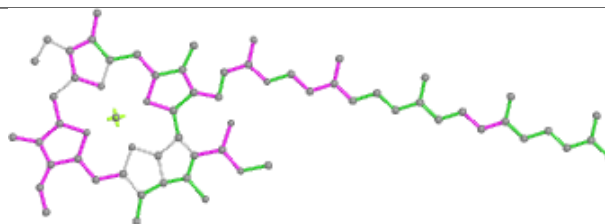
Ligand CLA bA 804



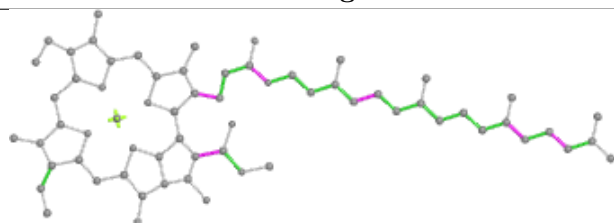
Ligand CLA bA 805



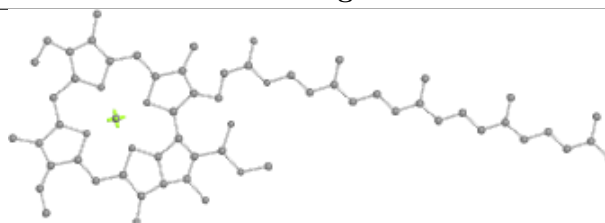
Bond lengths



Bond angles

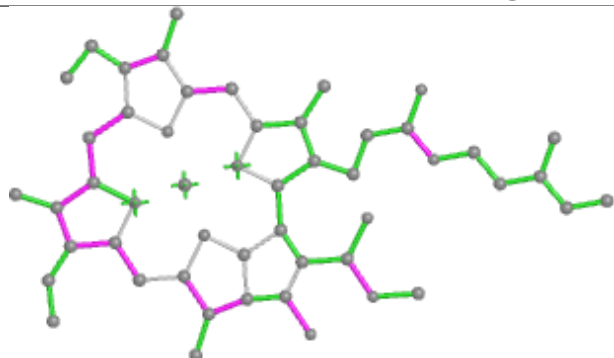


Torsions

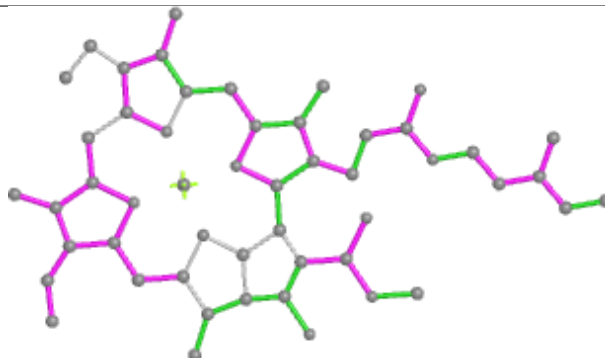


Rings

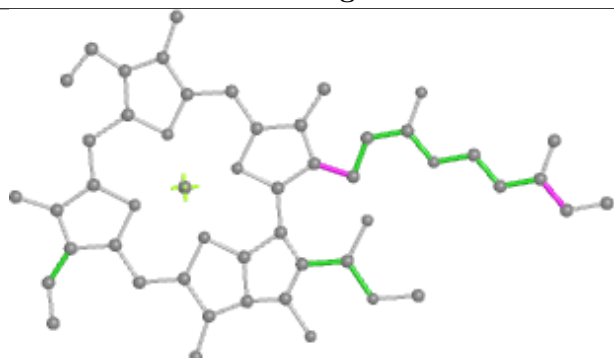
Ligand CLA bA 806



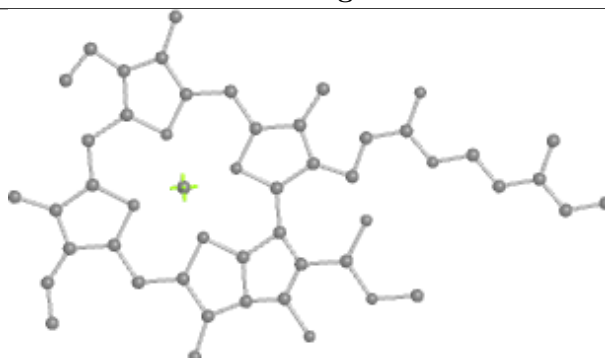
Bond lengths



Bond angles

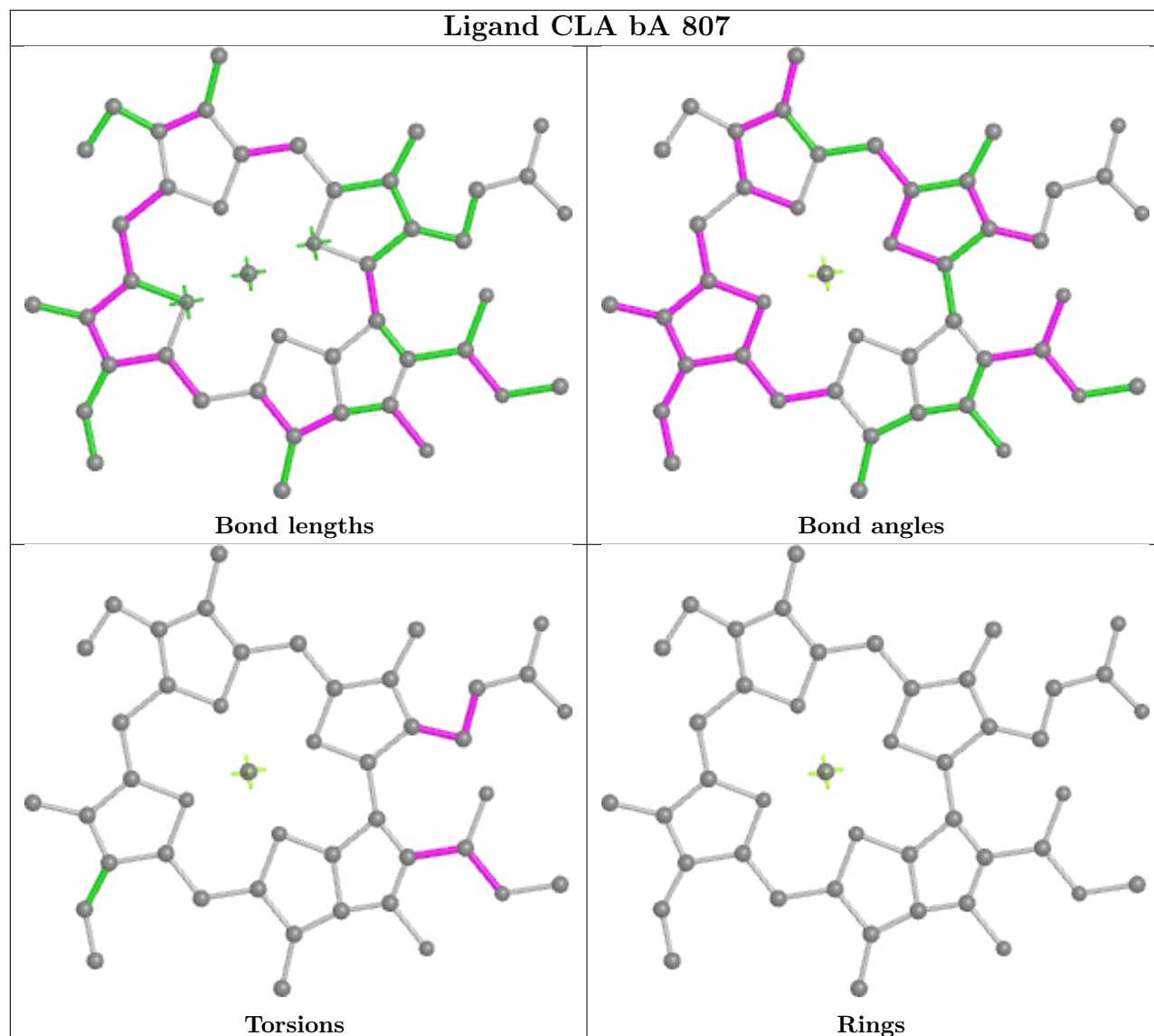


Torsions

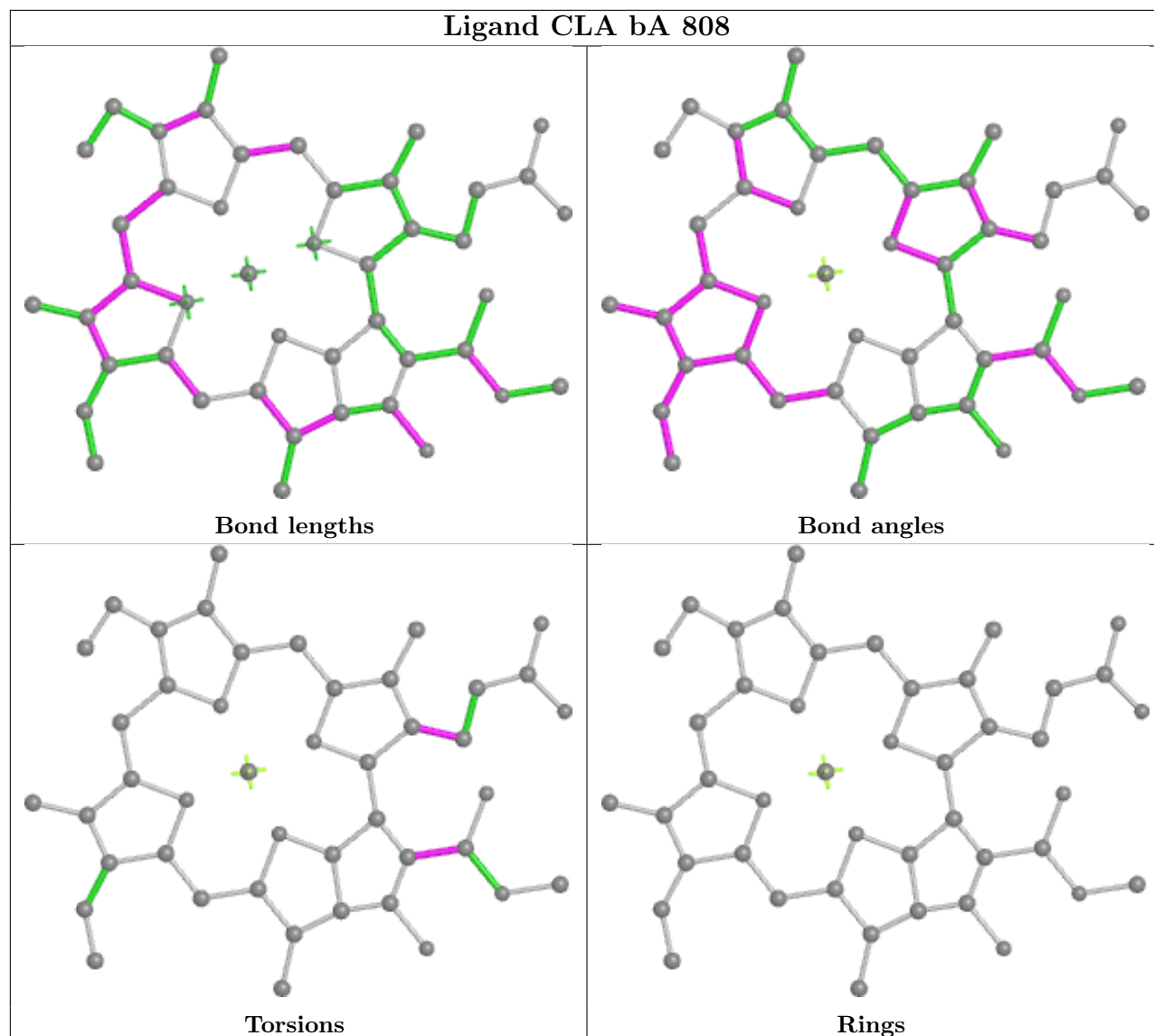


Rings

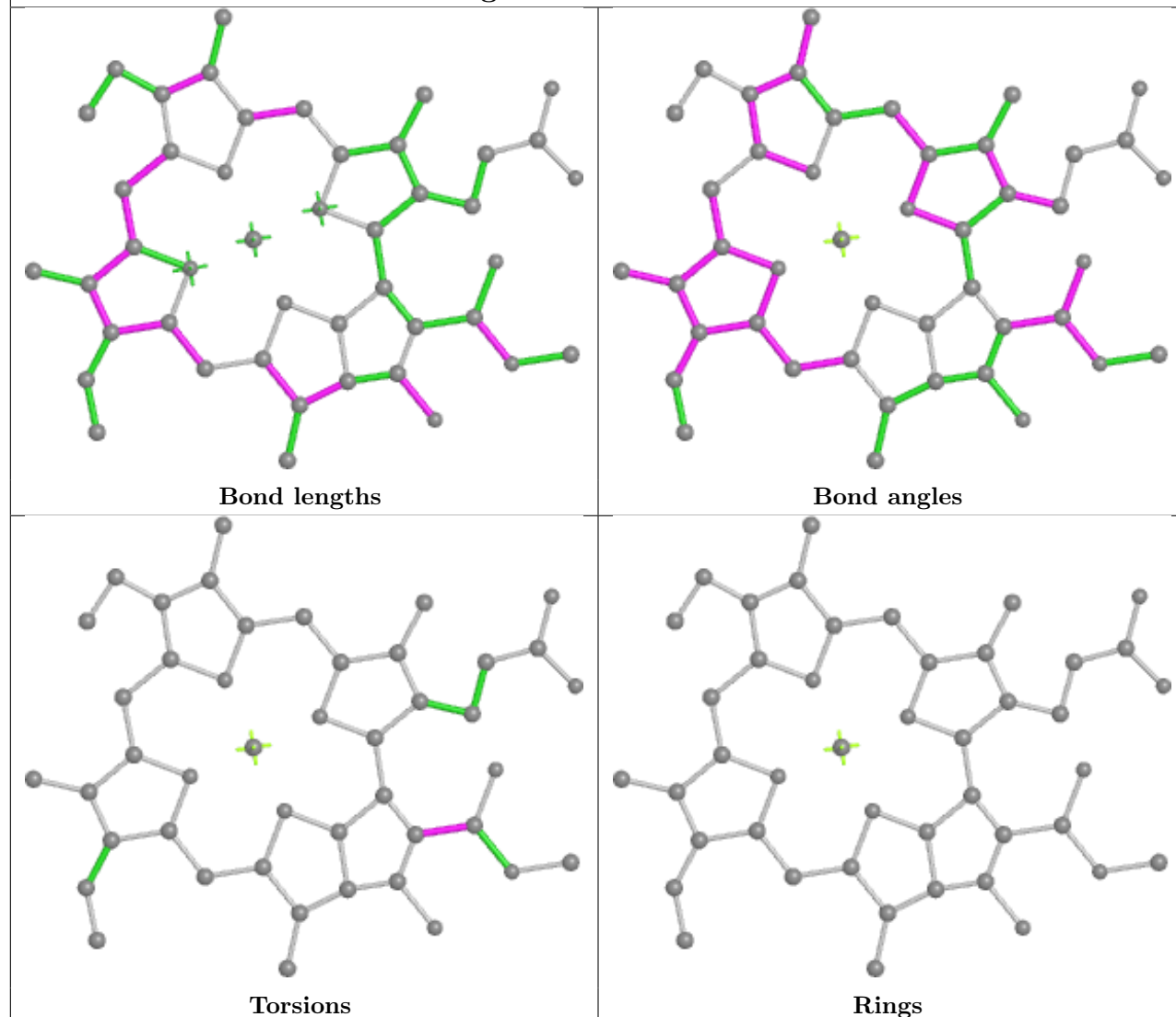
Ligand CLA bA 807



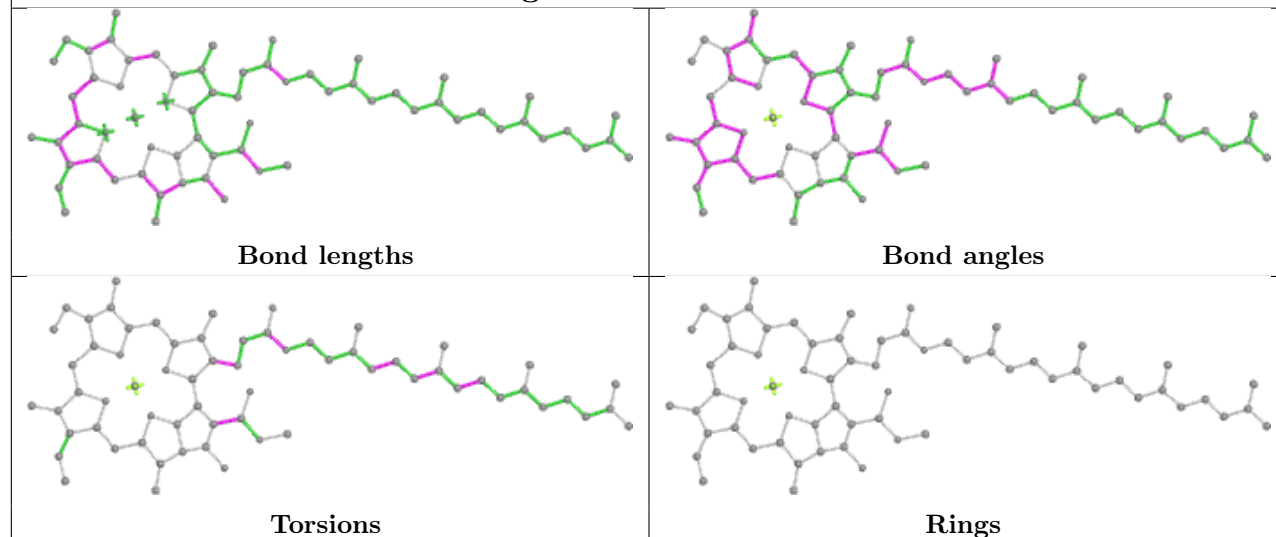
Ligand CLA bA 808



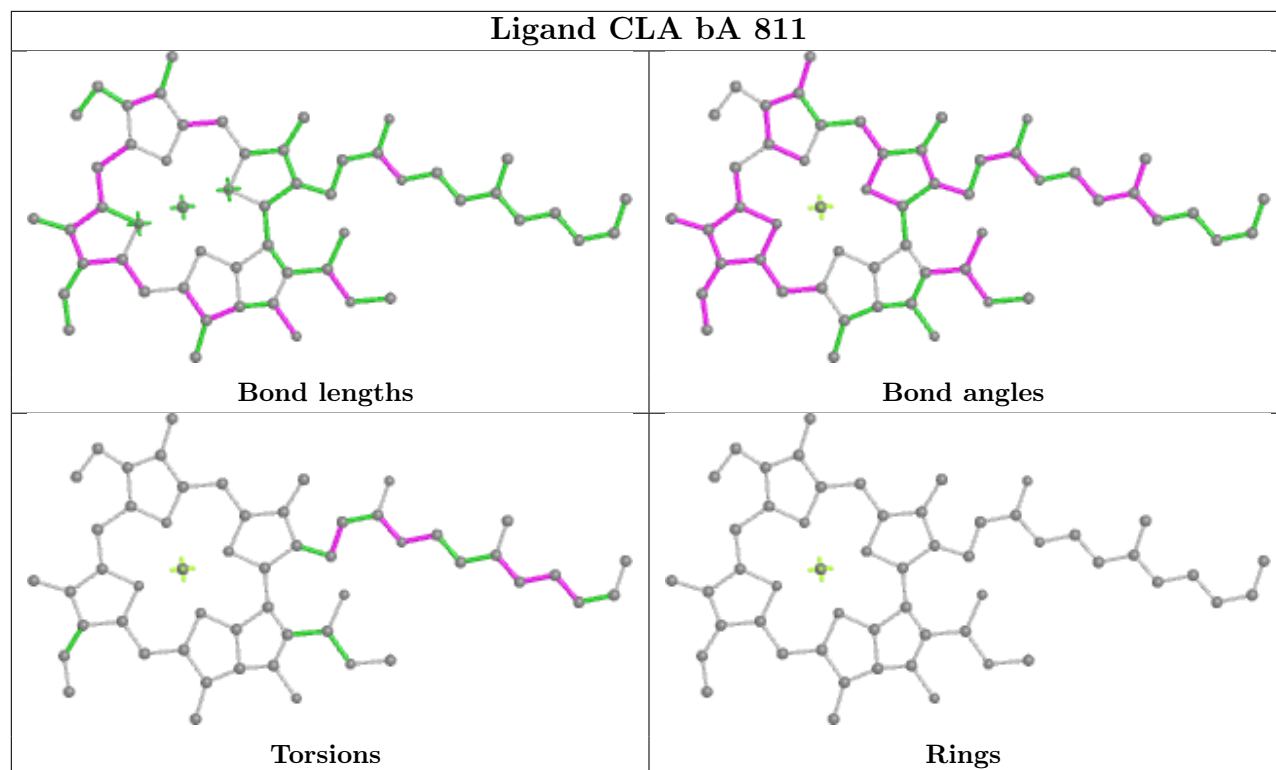
Ligand CLA bA 809



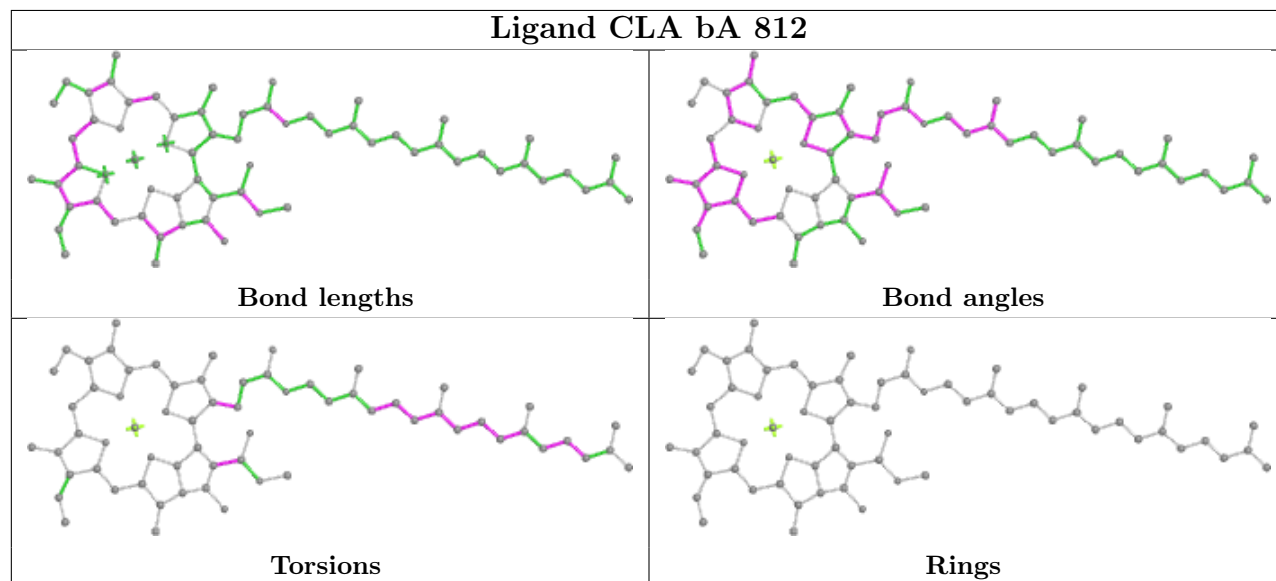
Ligand CLA bA 810



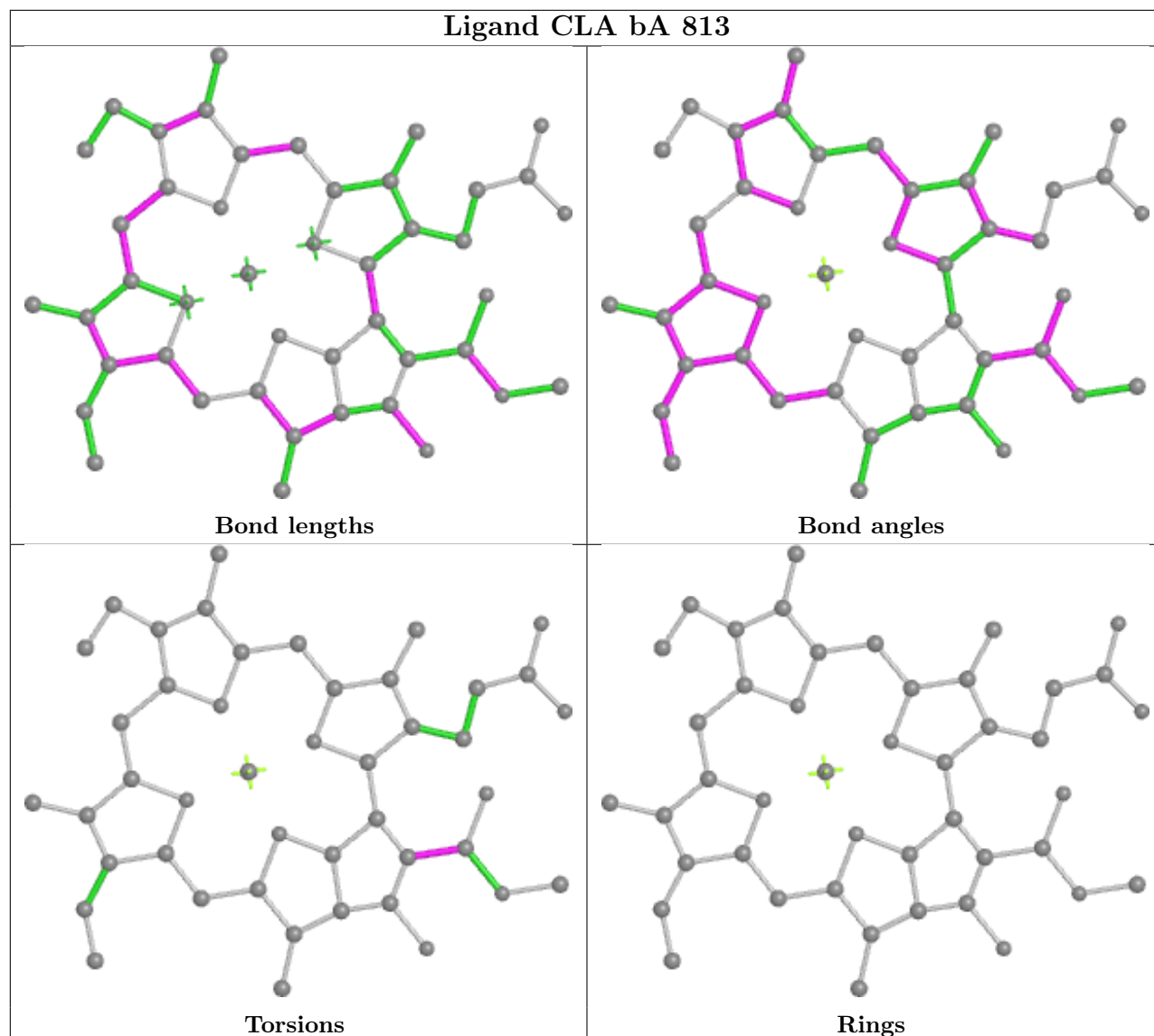
Ligand CLA ba 811



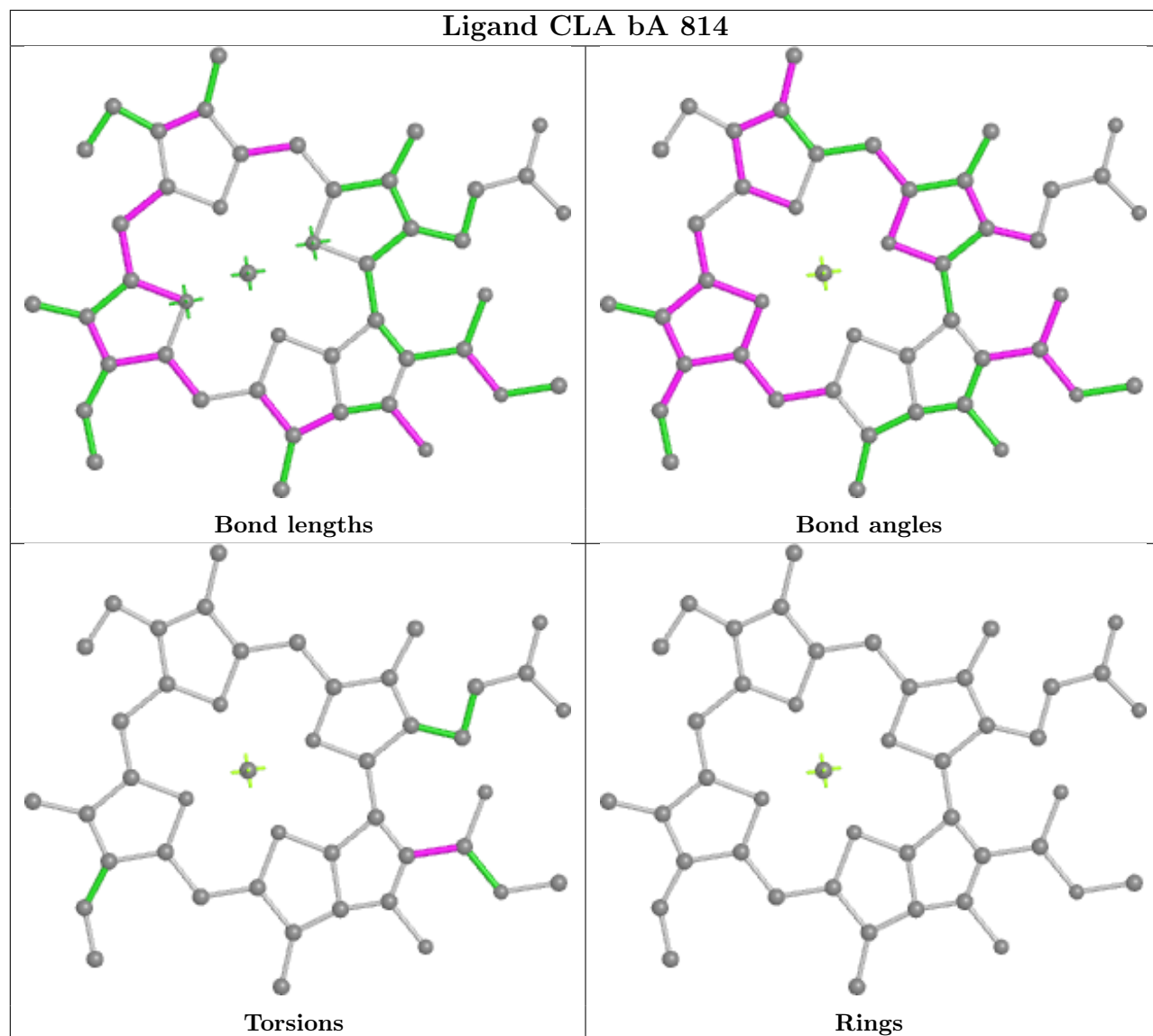
Ligand CLA ba 812



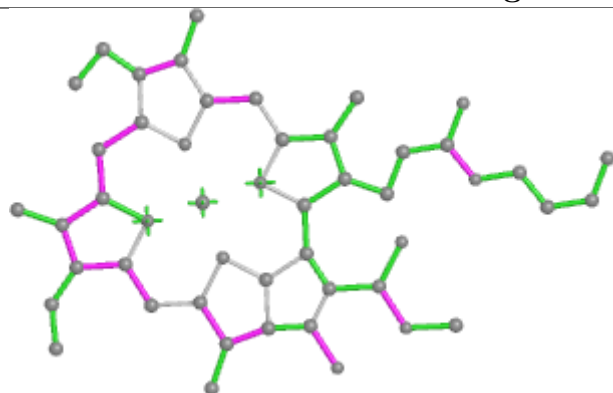
Ligand CLA bA 813



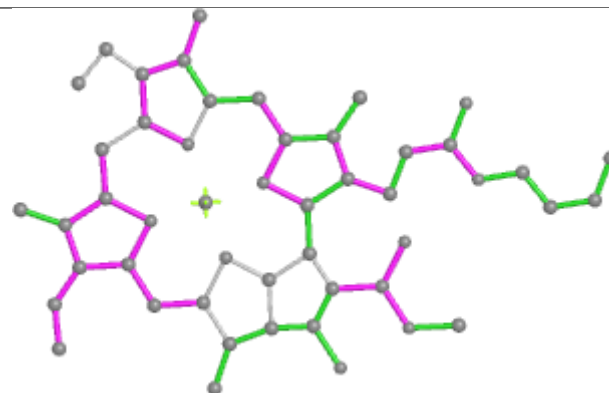
Ligand CLA bA 814



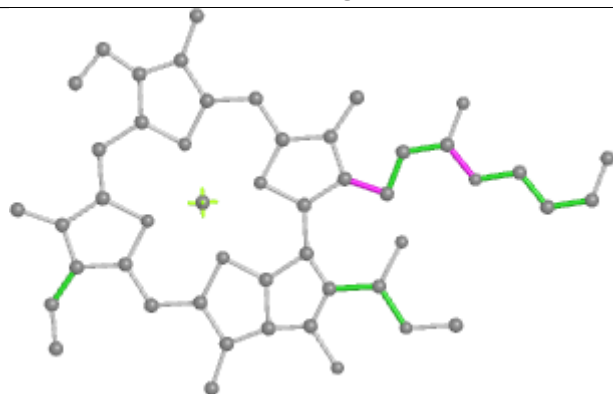
Ligand CLA bA 815



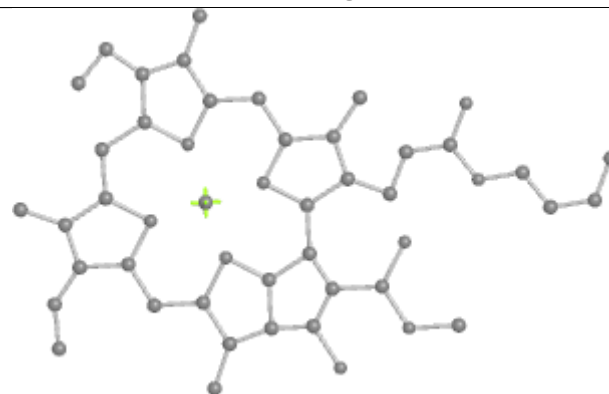
Bond lengths



Bond angles

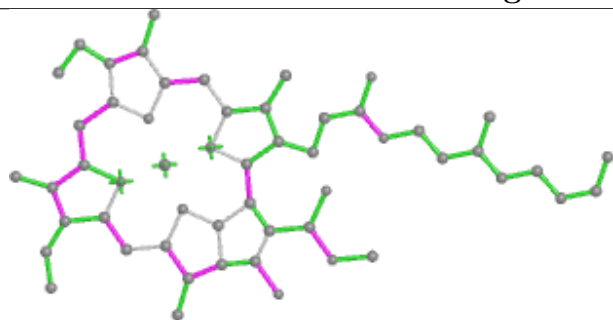


Torsions

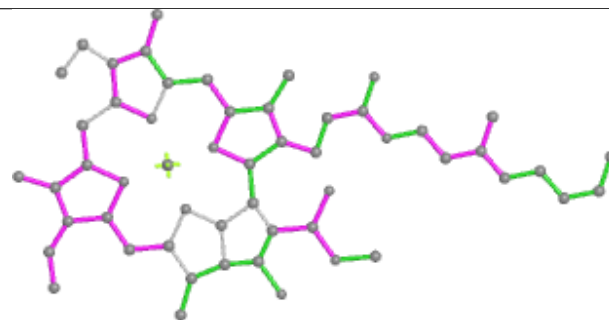


Rings

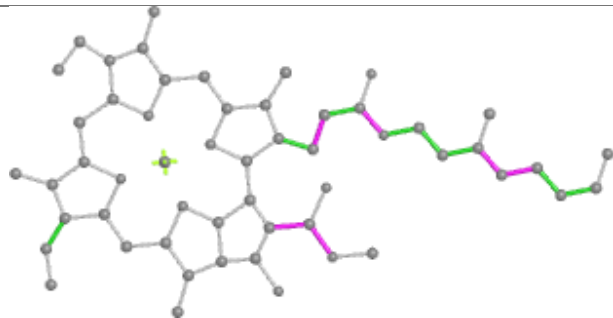
Ligand CLA bA 816



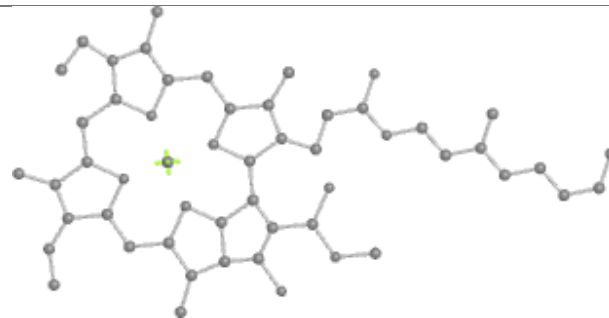
Bond lengths



Bond angles

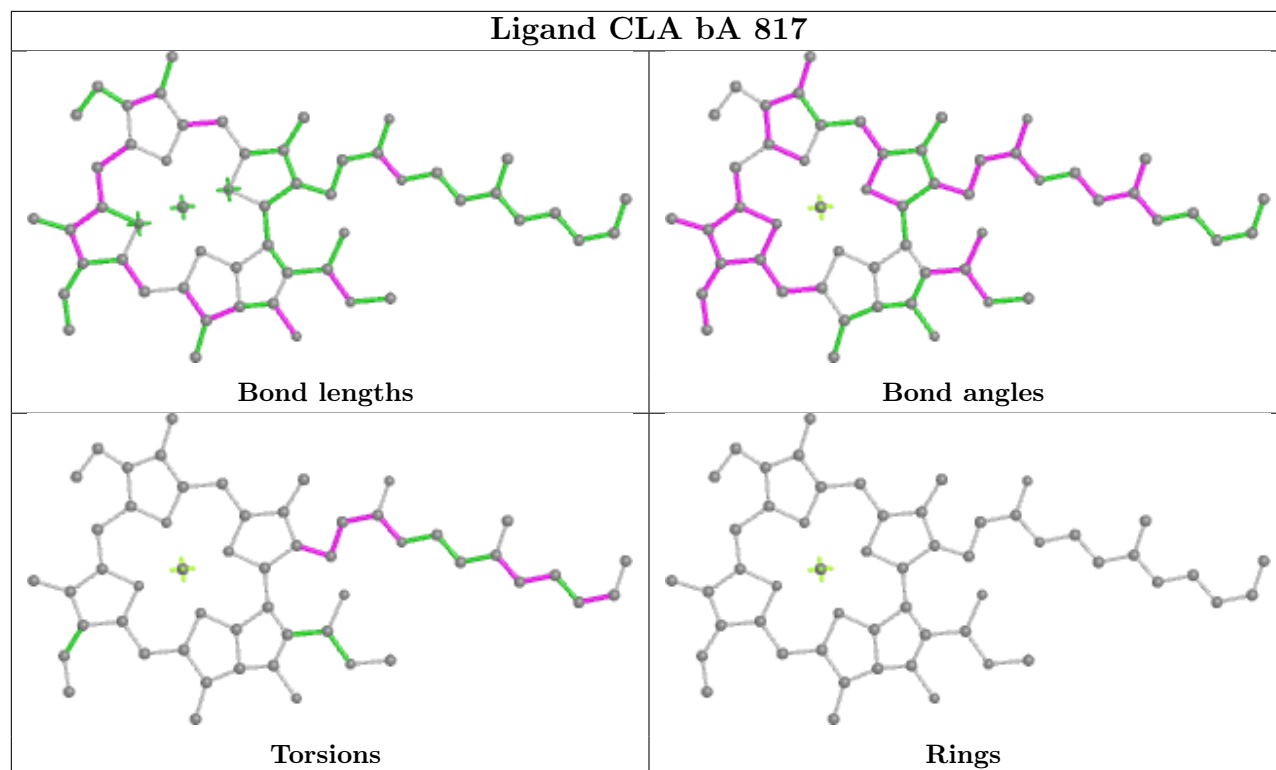


Torsions

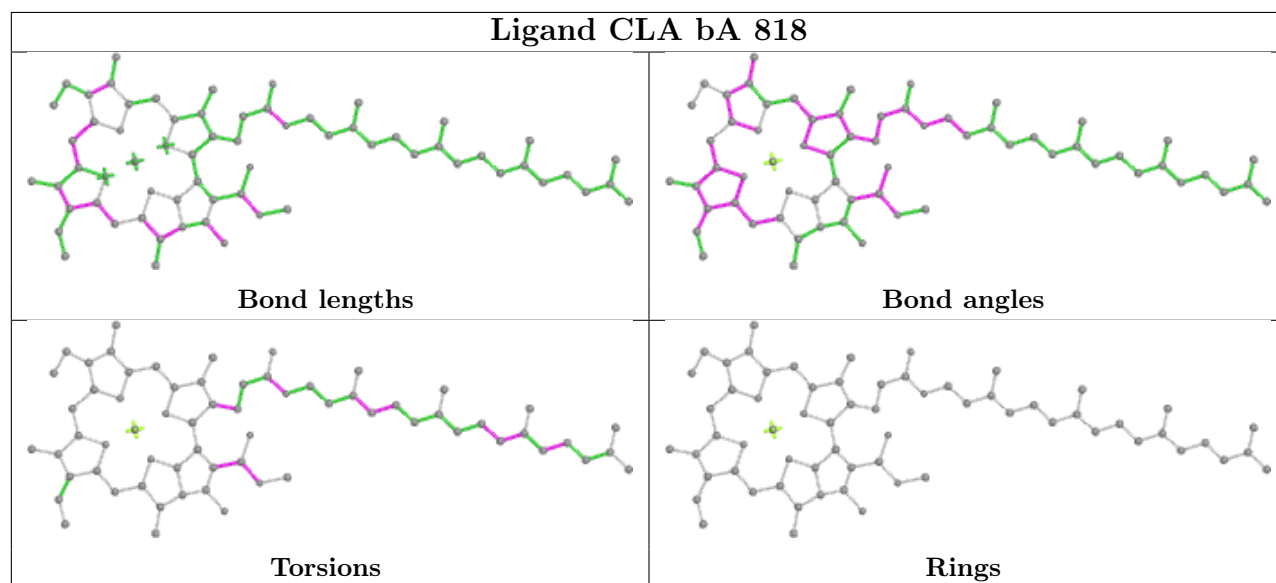


Rings

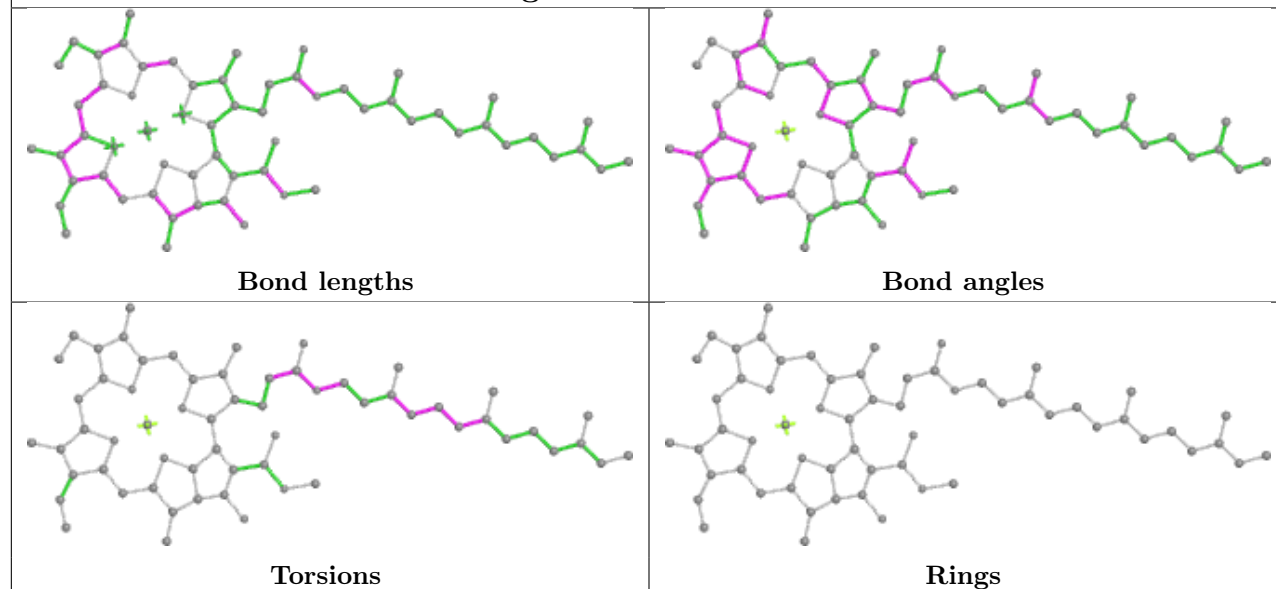
Ligand CLA bA 817



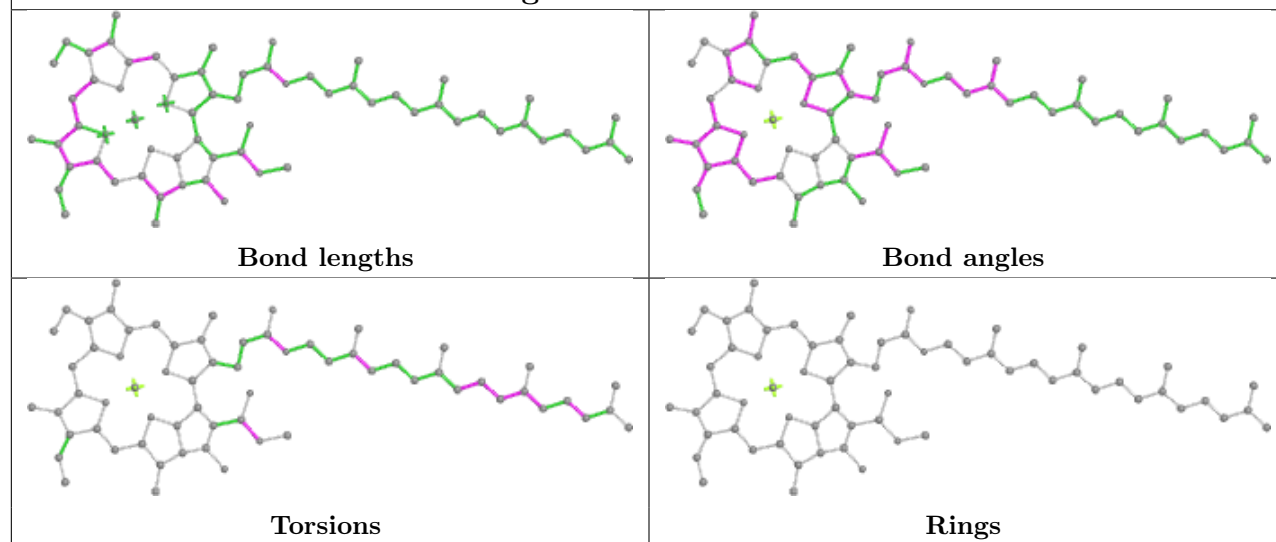
Ligand CLA bA 818



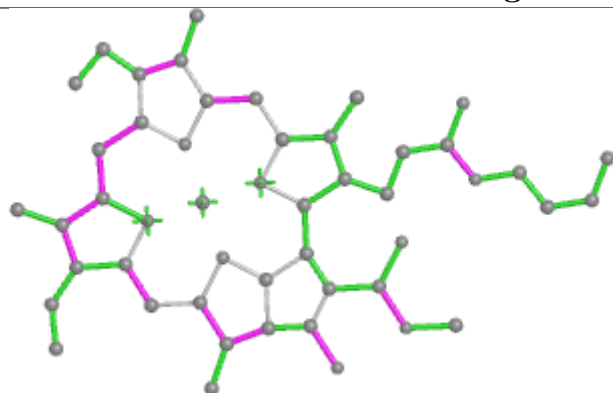
Ligand CLA bA 819



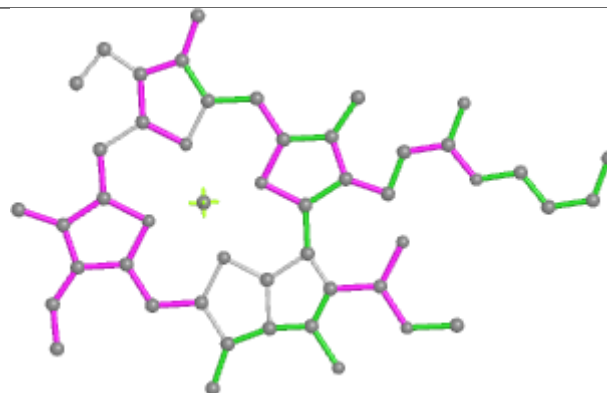
Ligand CLA bA 820



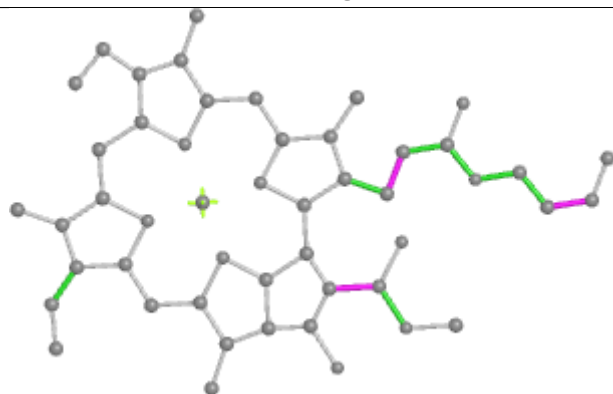
Ligand CLA bA 821



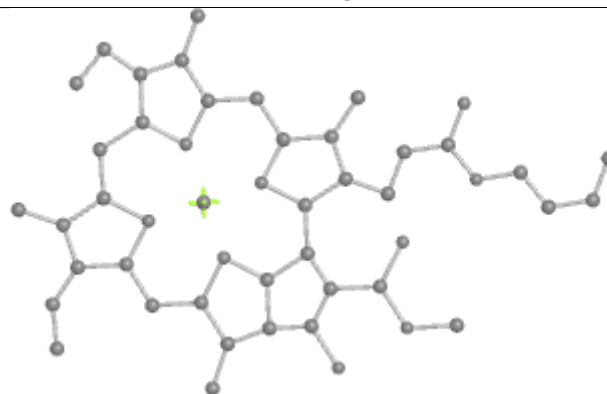
Bond lengths



Bond angles

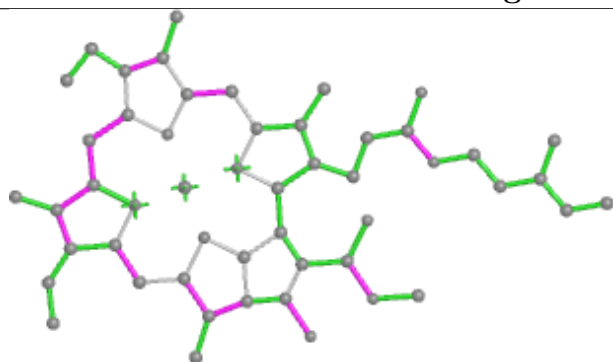


Torsions

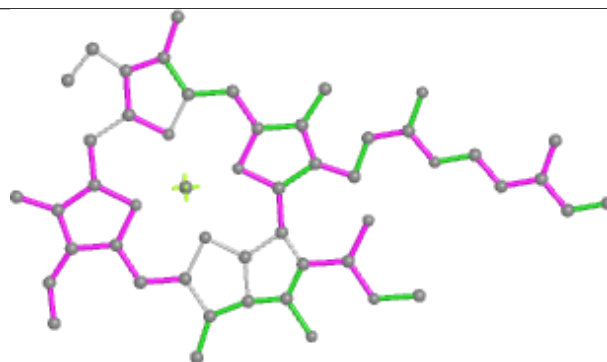


Rings

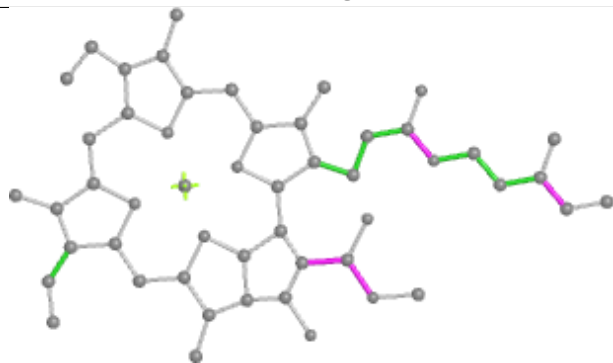
Ligand CLA bA 822



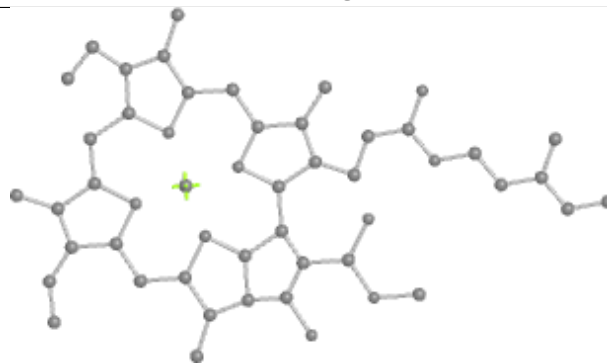
Bond lengths



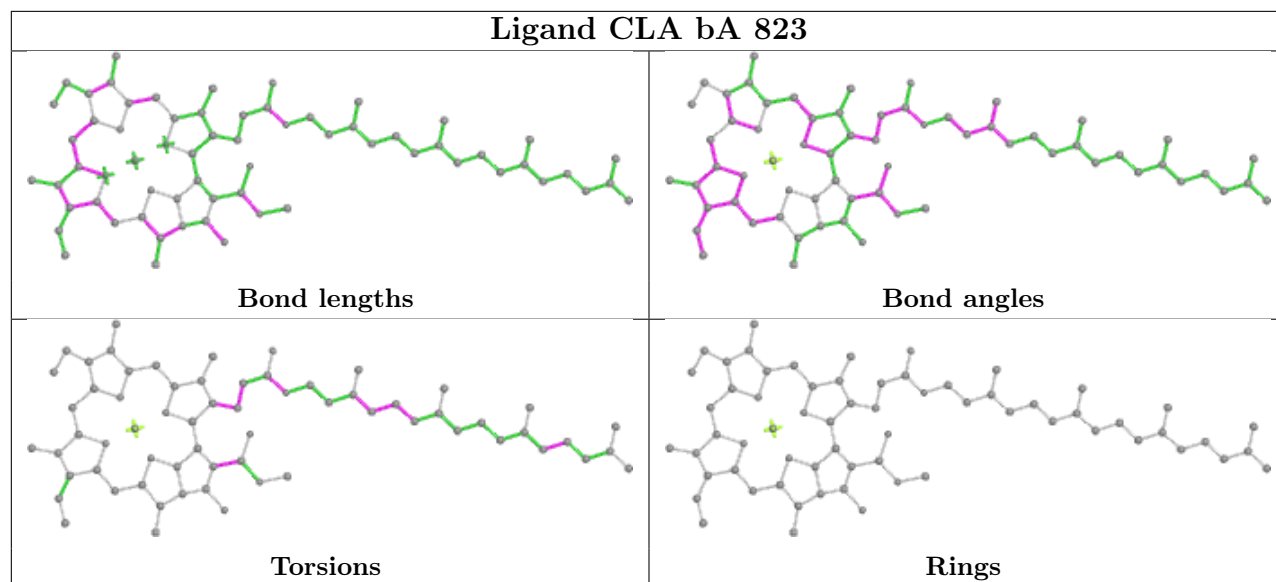
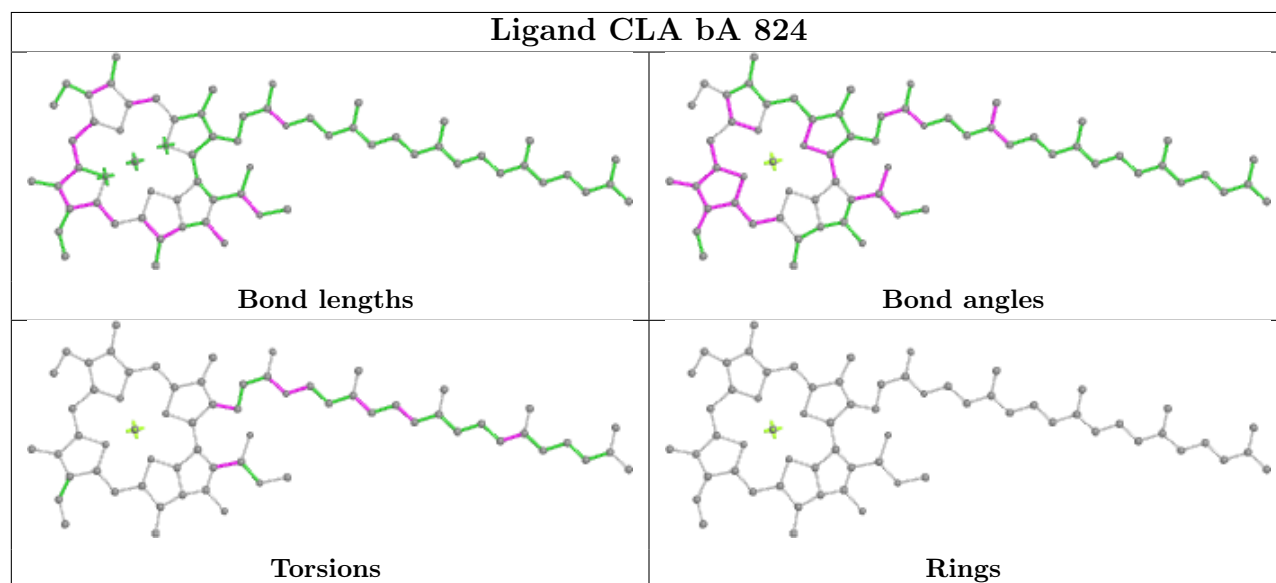
Bond angles



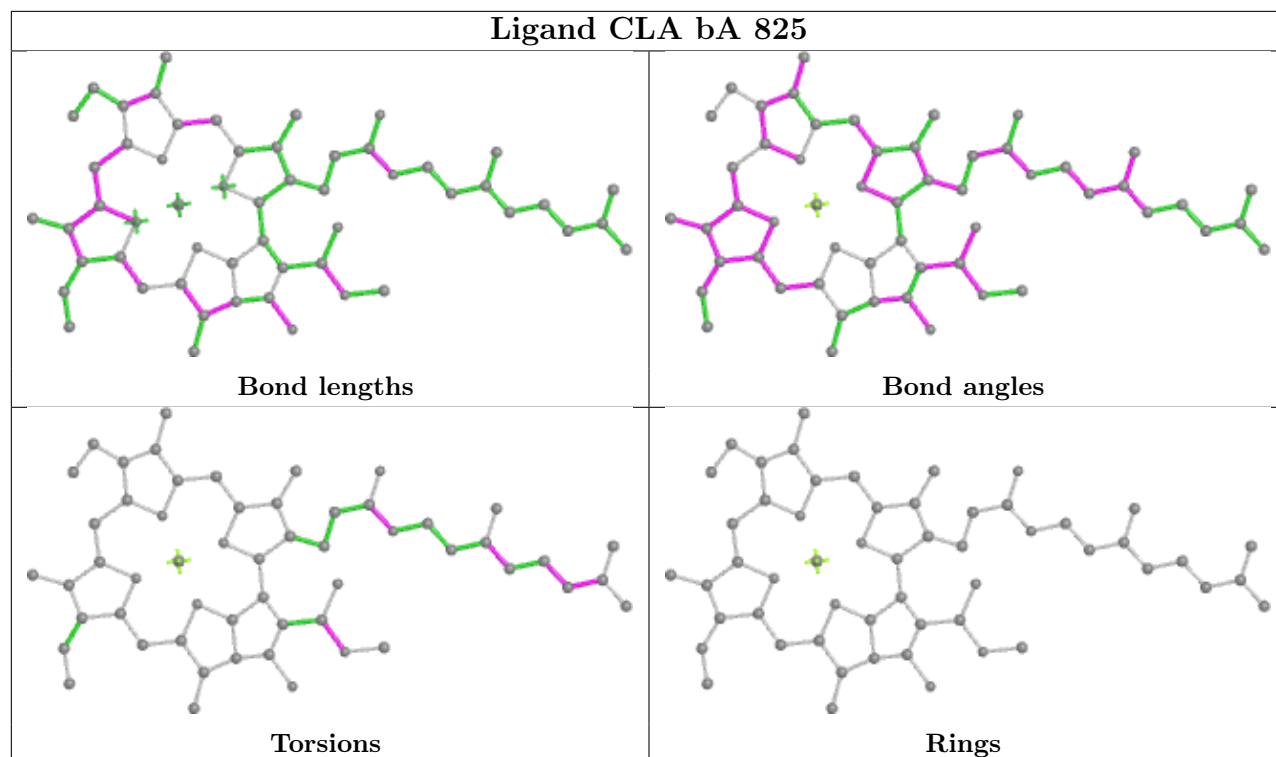
Torsions



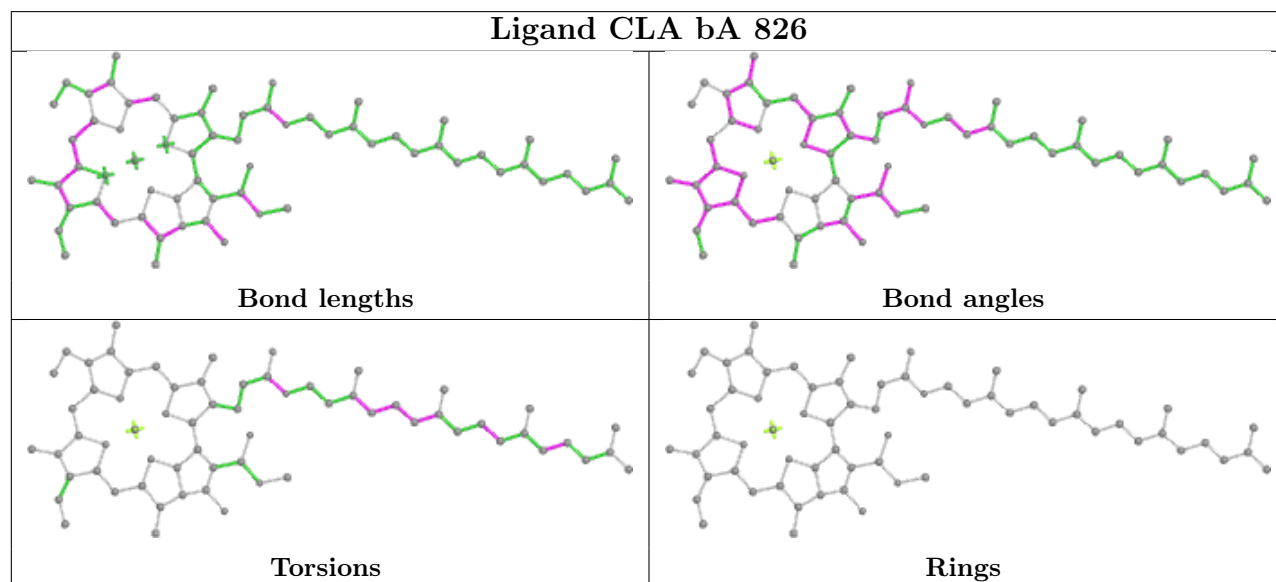
Rings

Ligand CLA bA 823**Ligand CLA bA 824**

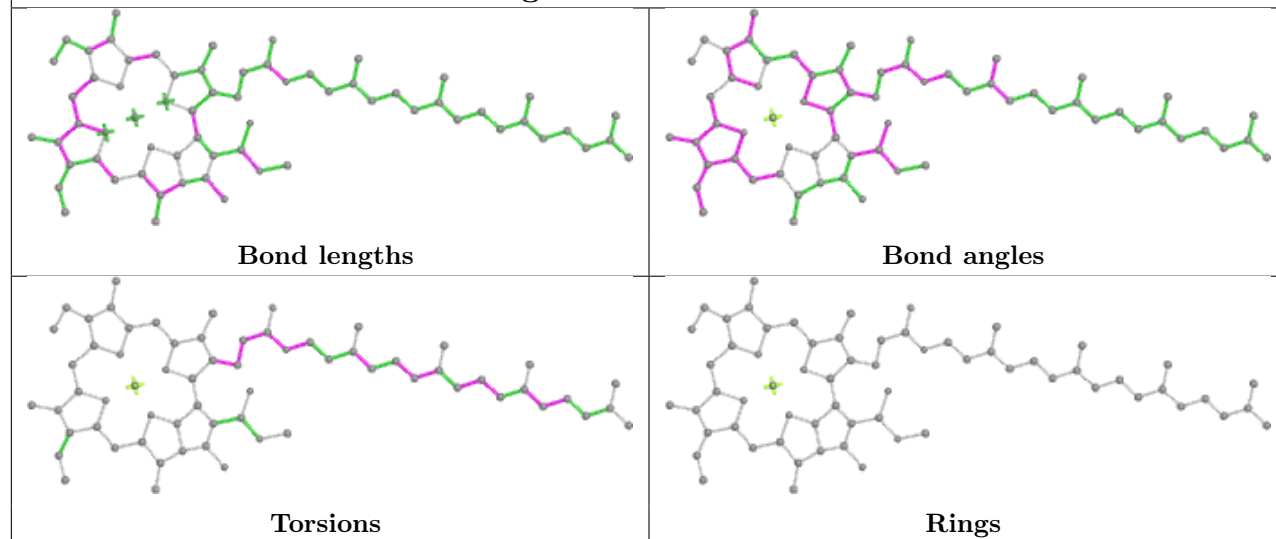
Ligand CLA bA 825



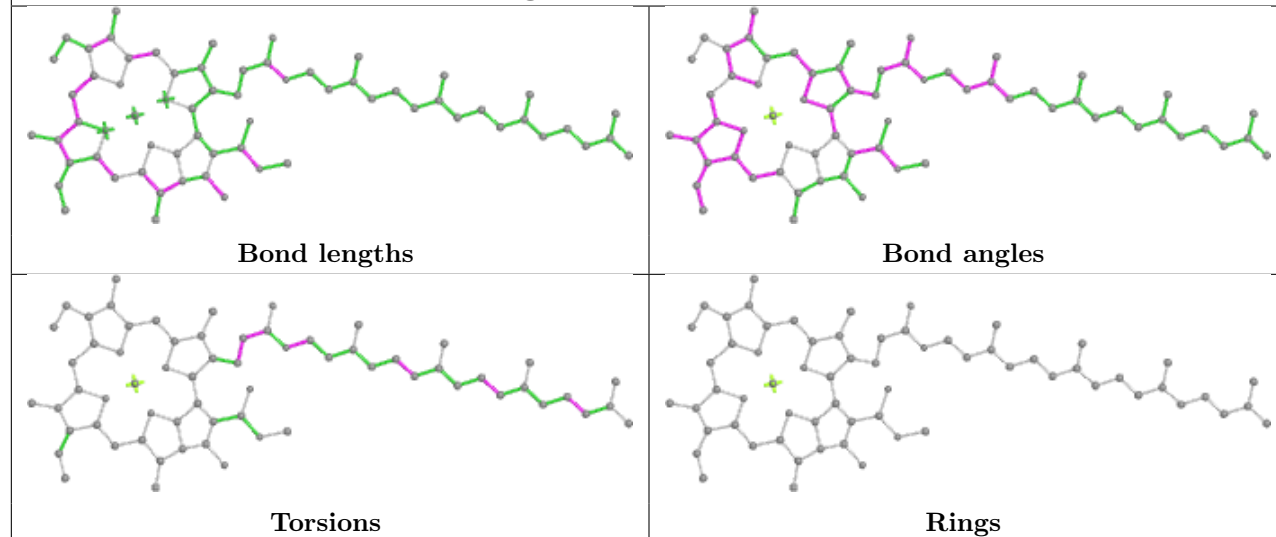
Ligand CLA bA 826



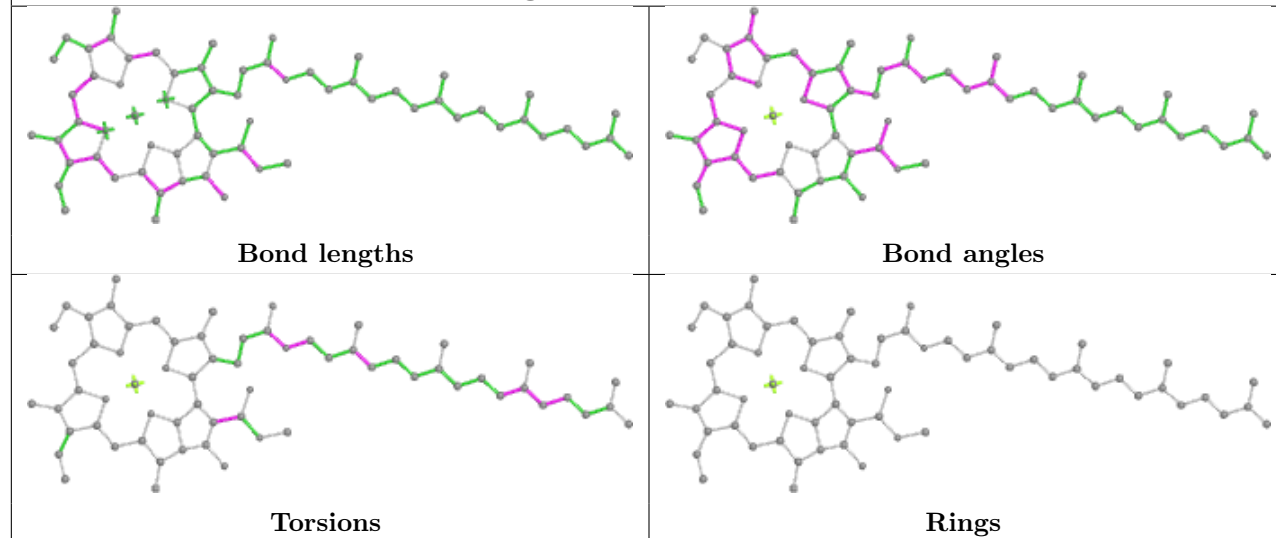
Ligand CLA ba 827



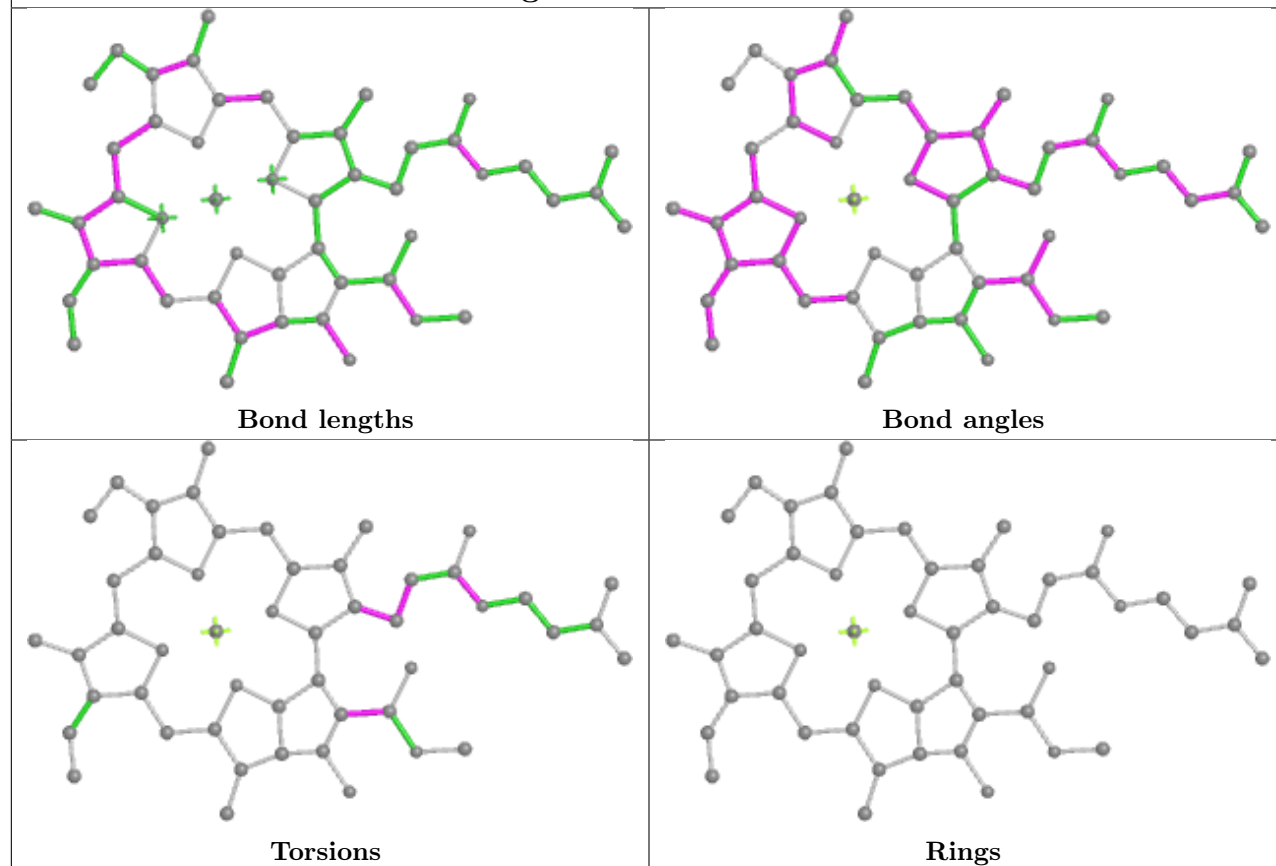
Ligand CLA ba 828



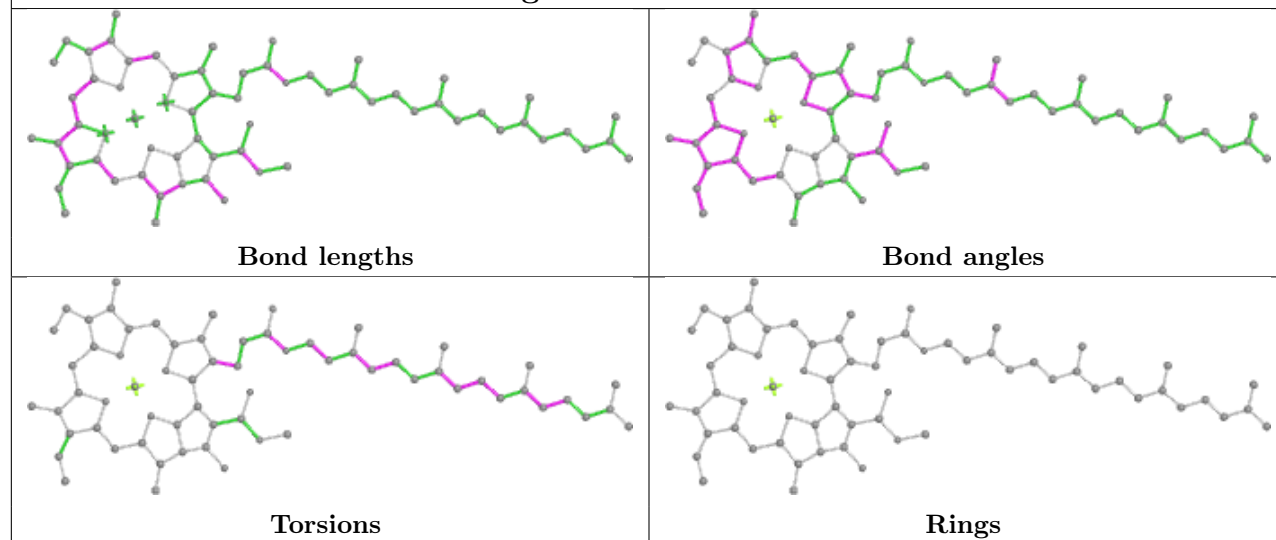
Ligand CLA ba 829

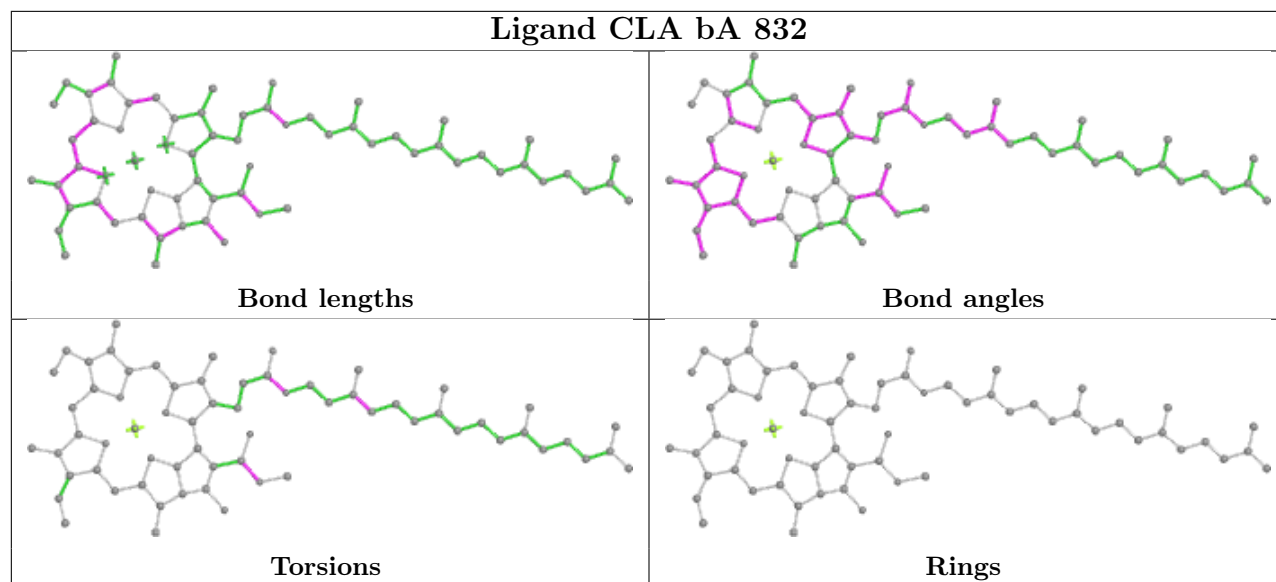
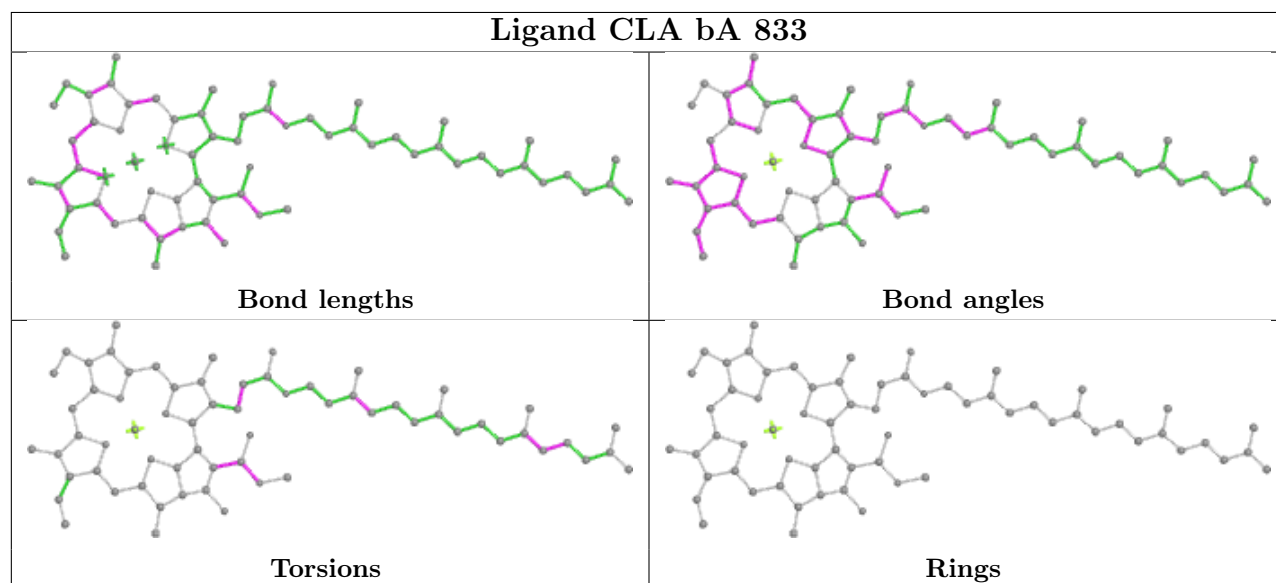


Ligand CLA bA 830

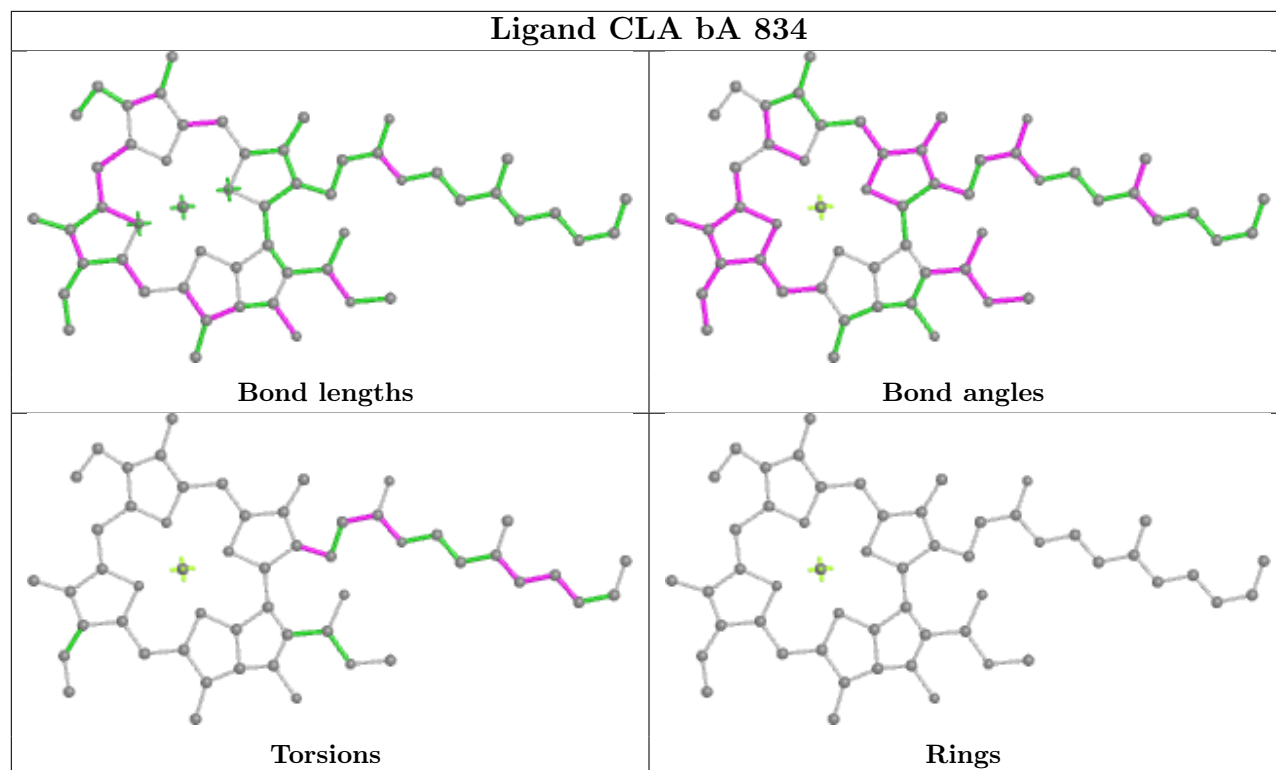


Ligand CLA bA 831

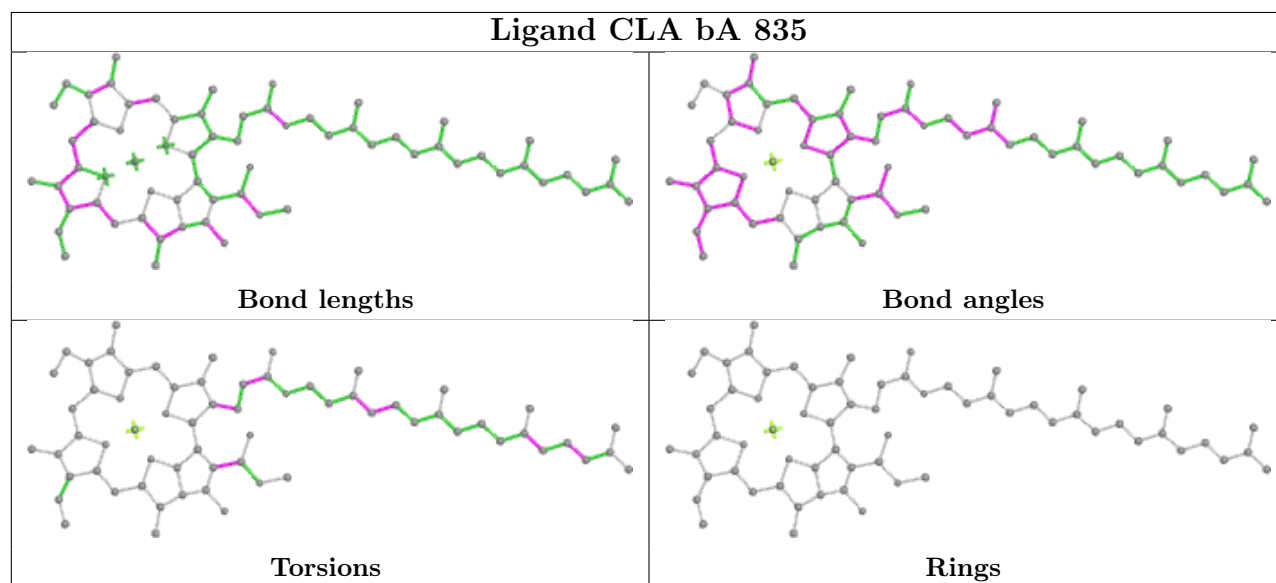


Ligand CLA bA 832**Ligand CLA bA 833**

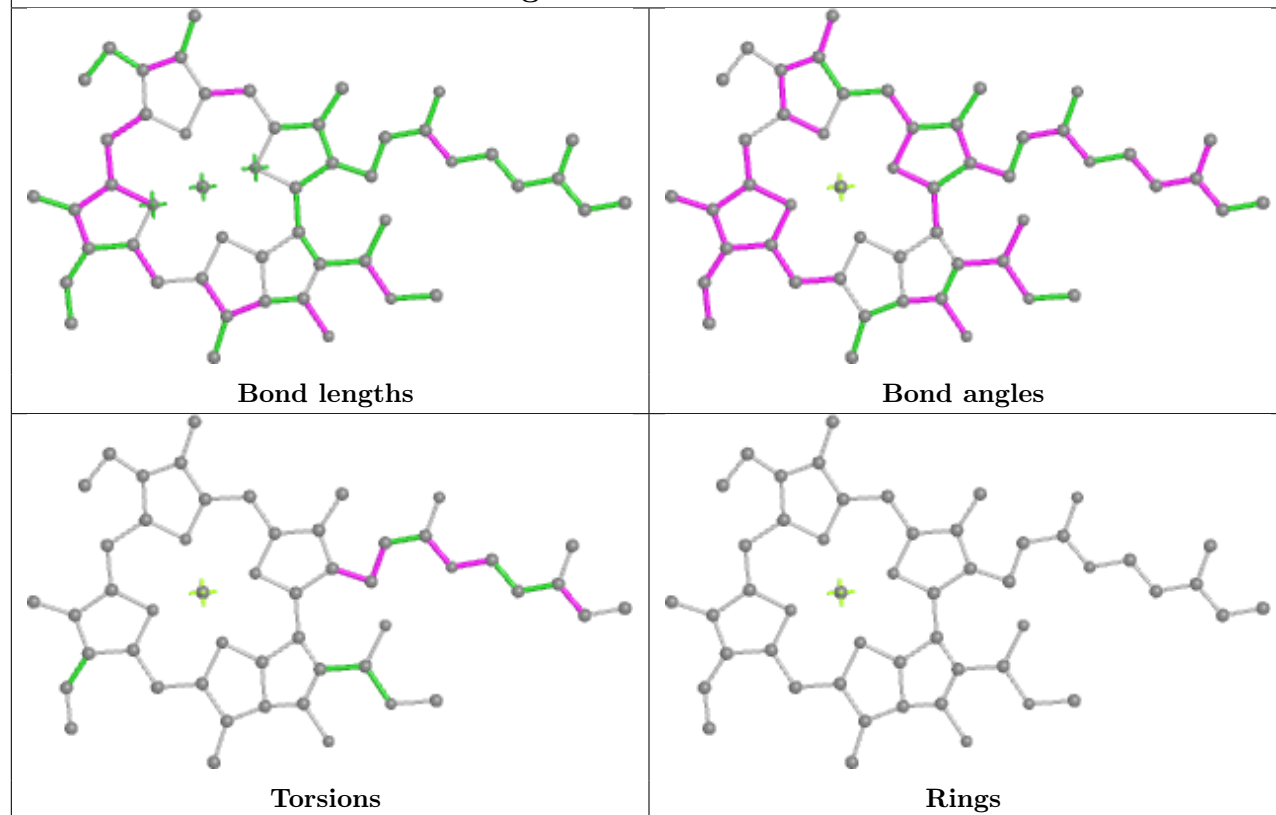
Ligand CLA bA 834



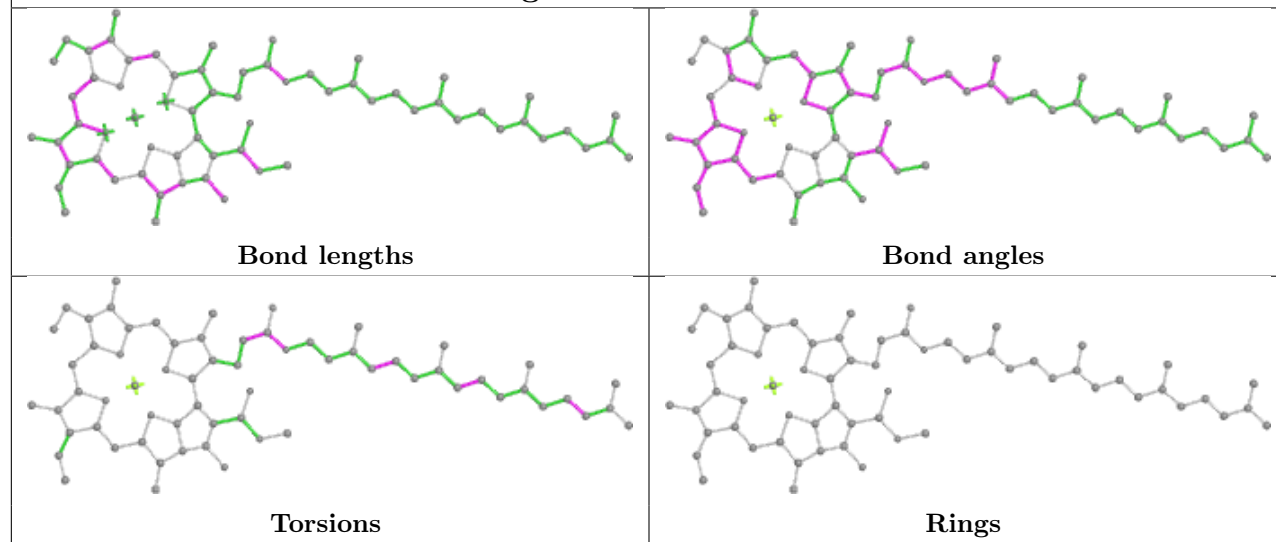
Ligand CLA bA 835



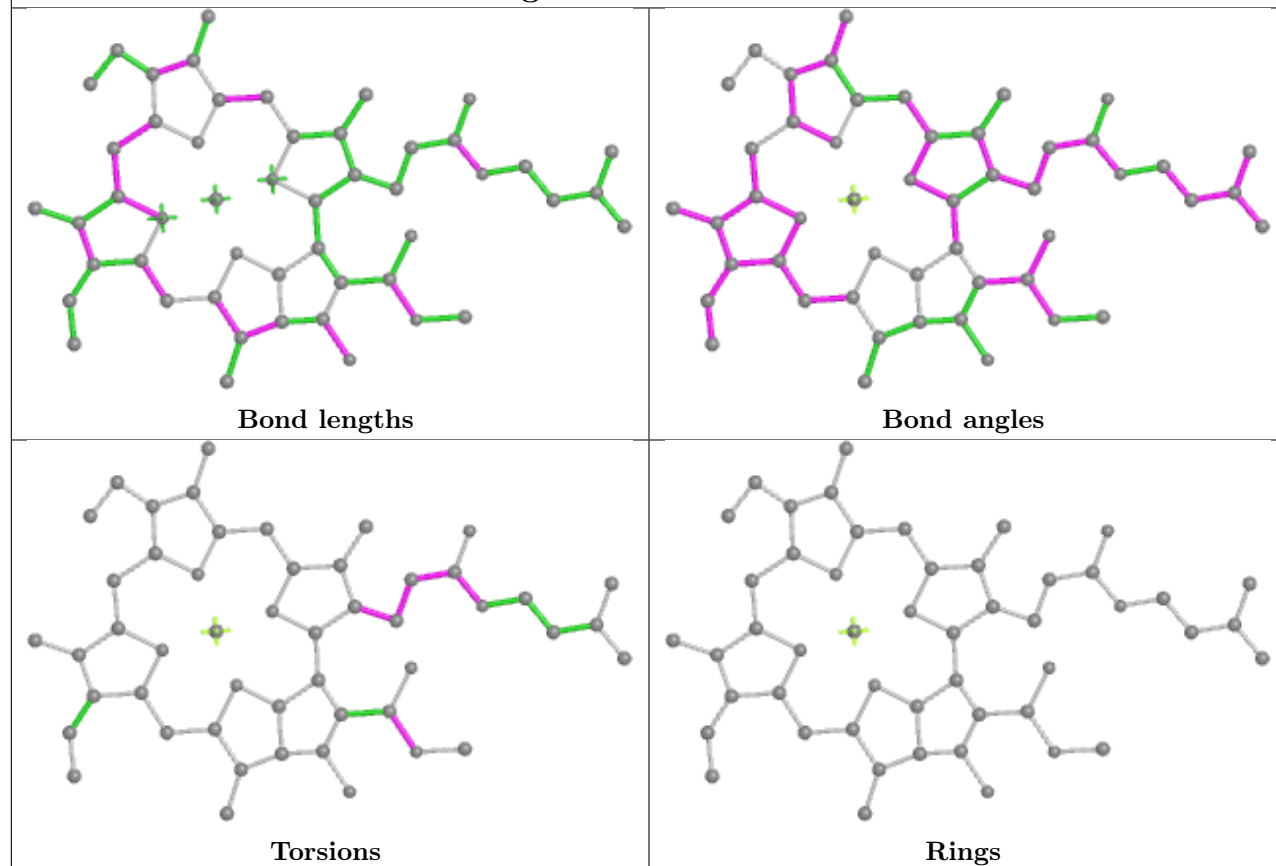
Ligand CLA bA 836



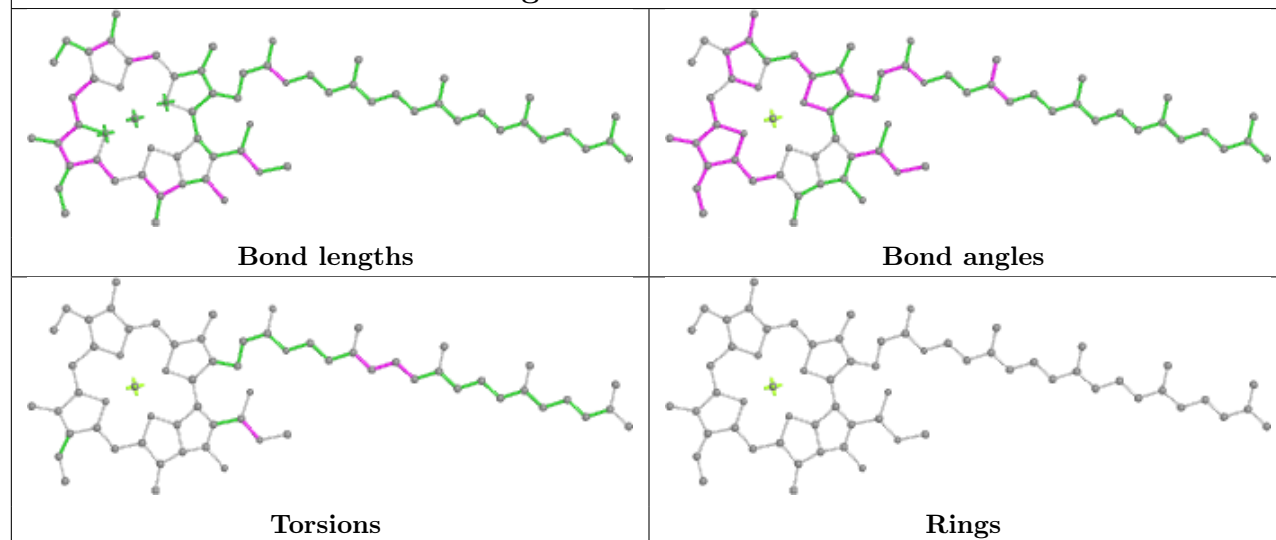
Ligand CLA bA 837

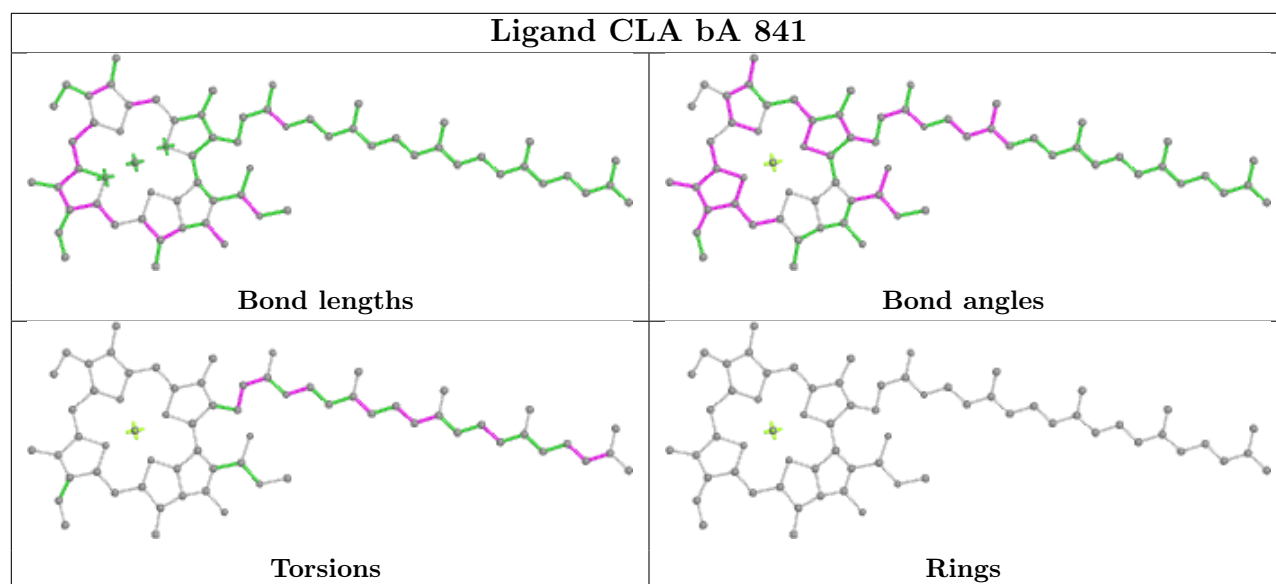
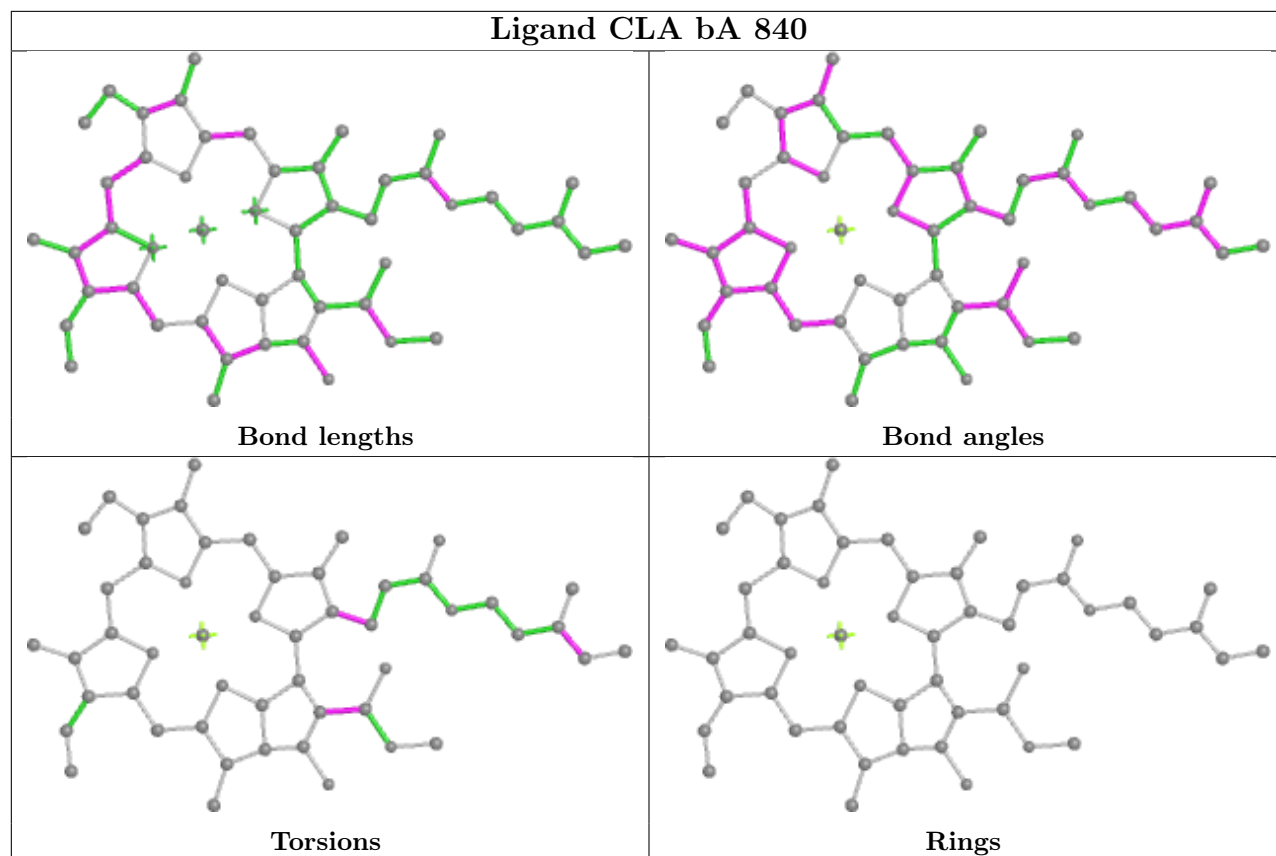


Ligand CLA bA 838

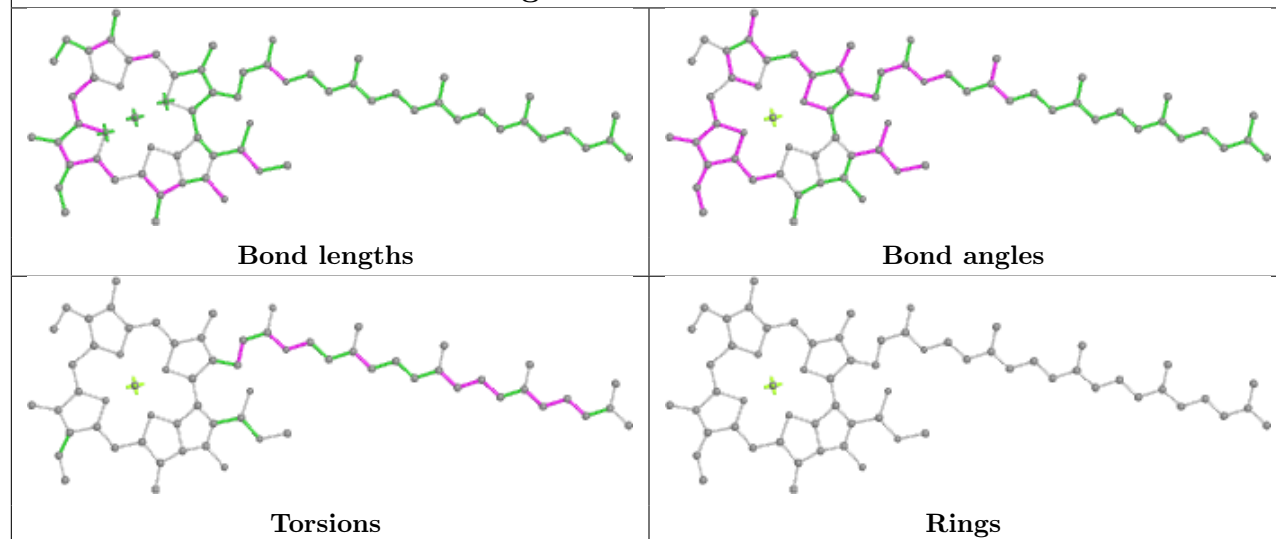


Ligand CLA bA 839

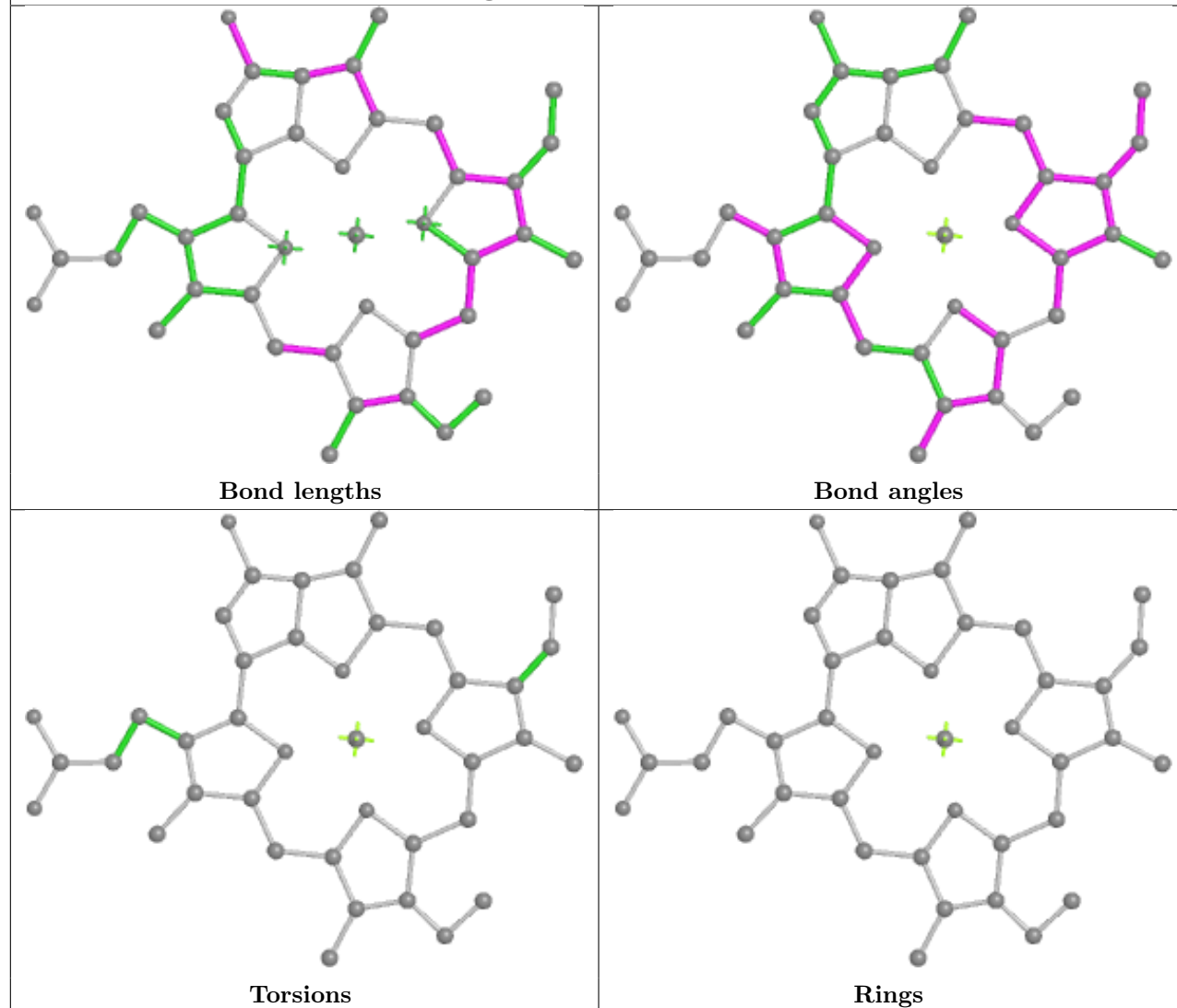


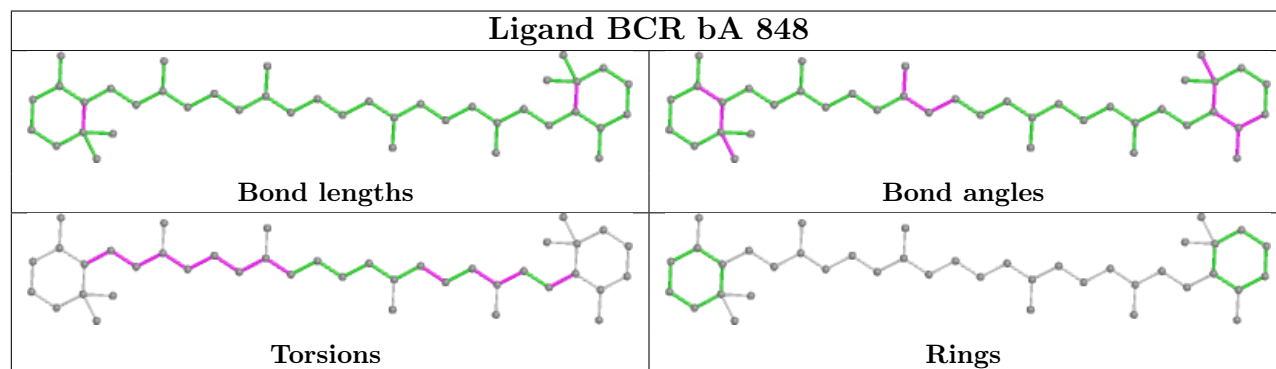
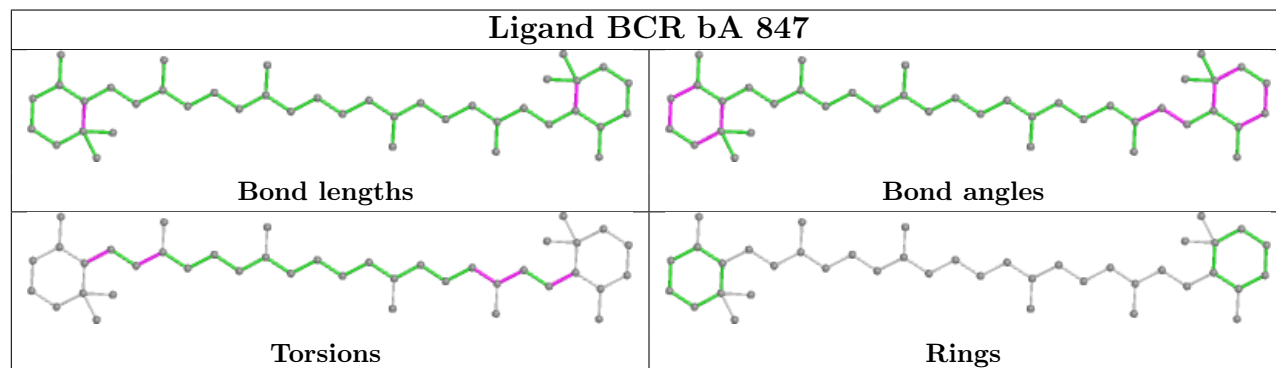
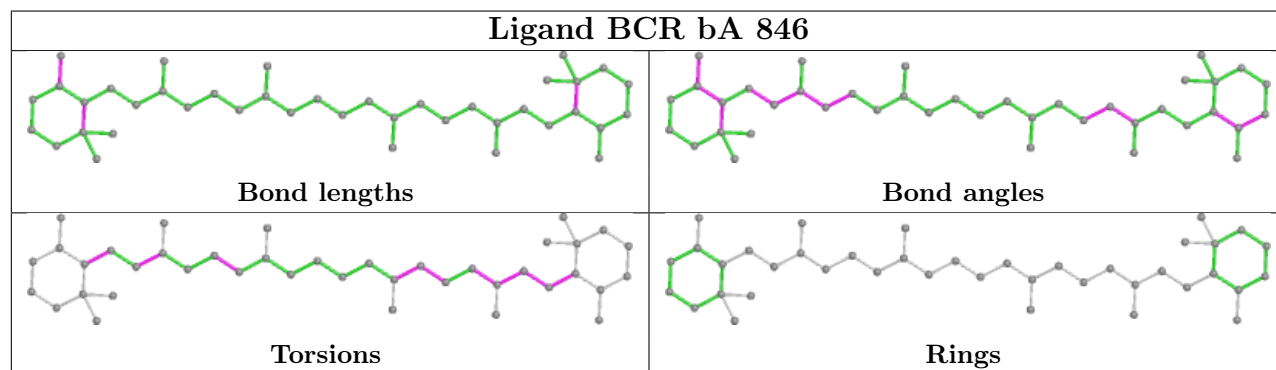
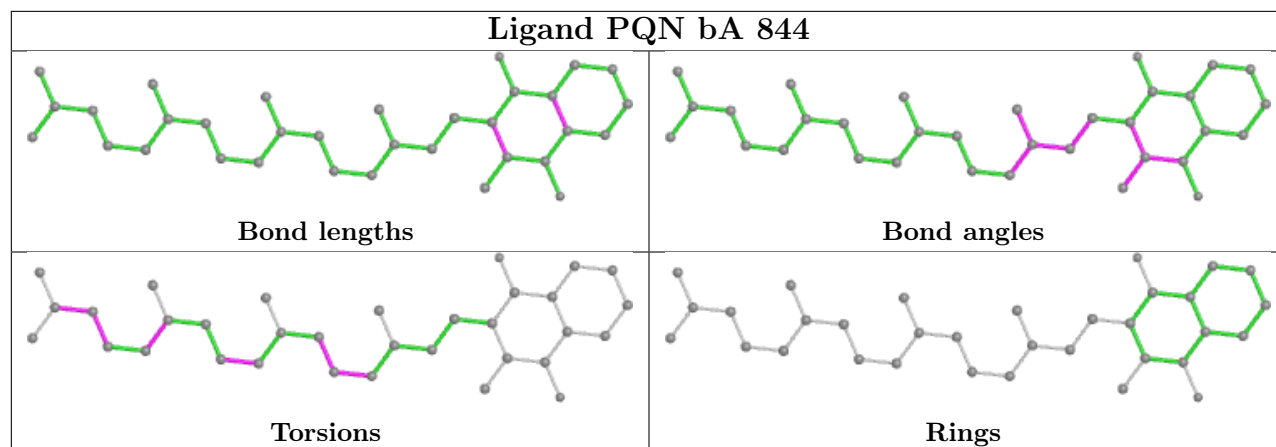


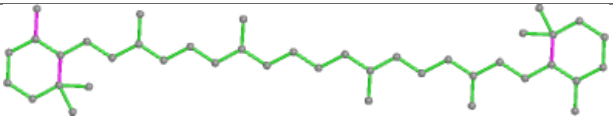
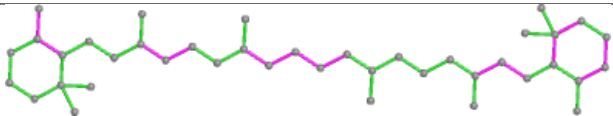
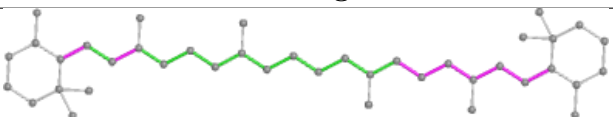
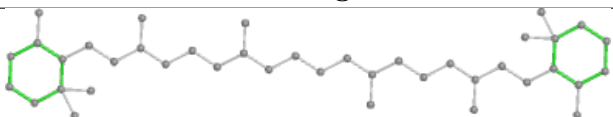
Ligand CLA bA 842

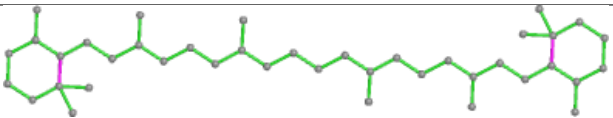
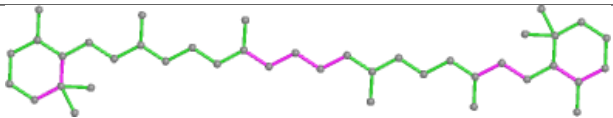
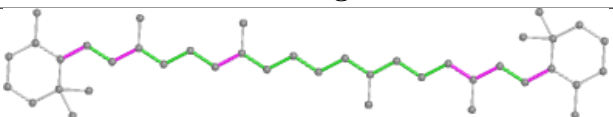
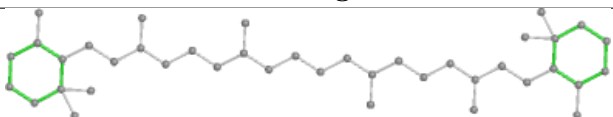


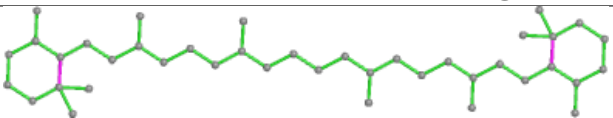
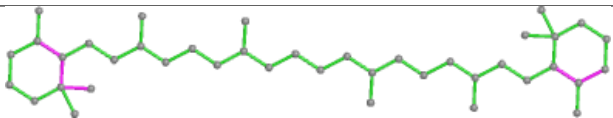
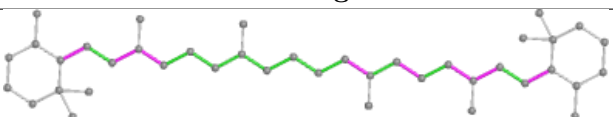
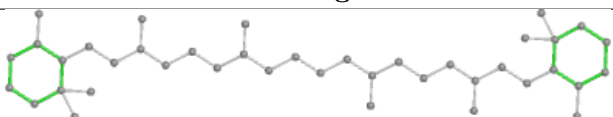
Ligand CLA bA 843

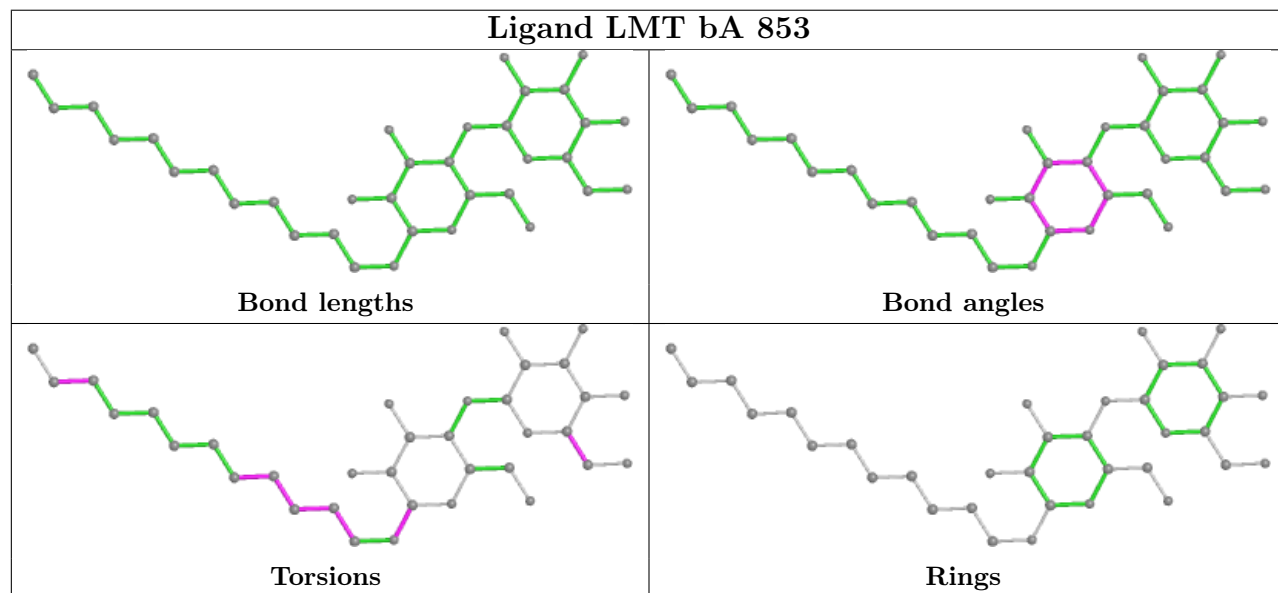
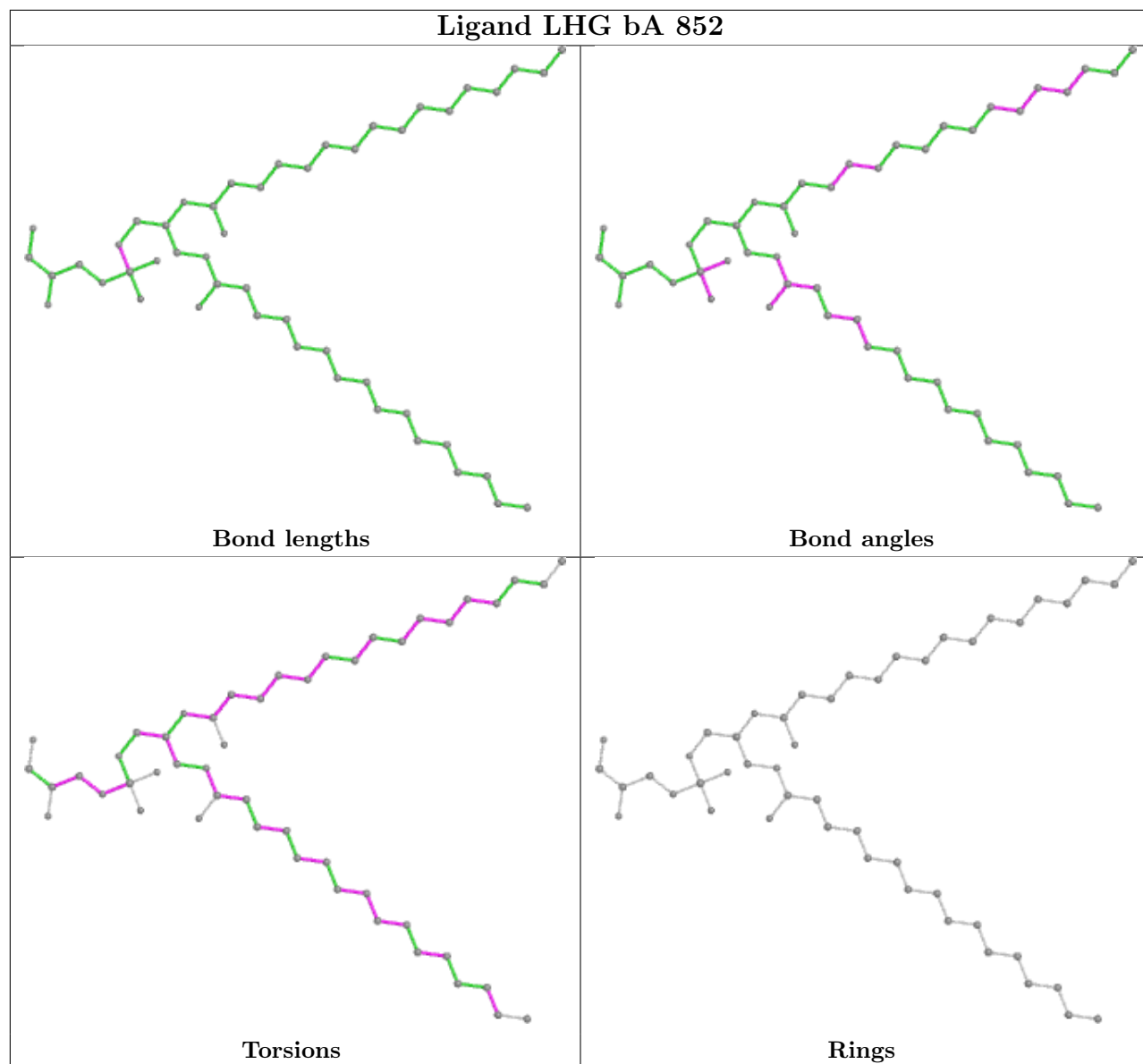


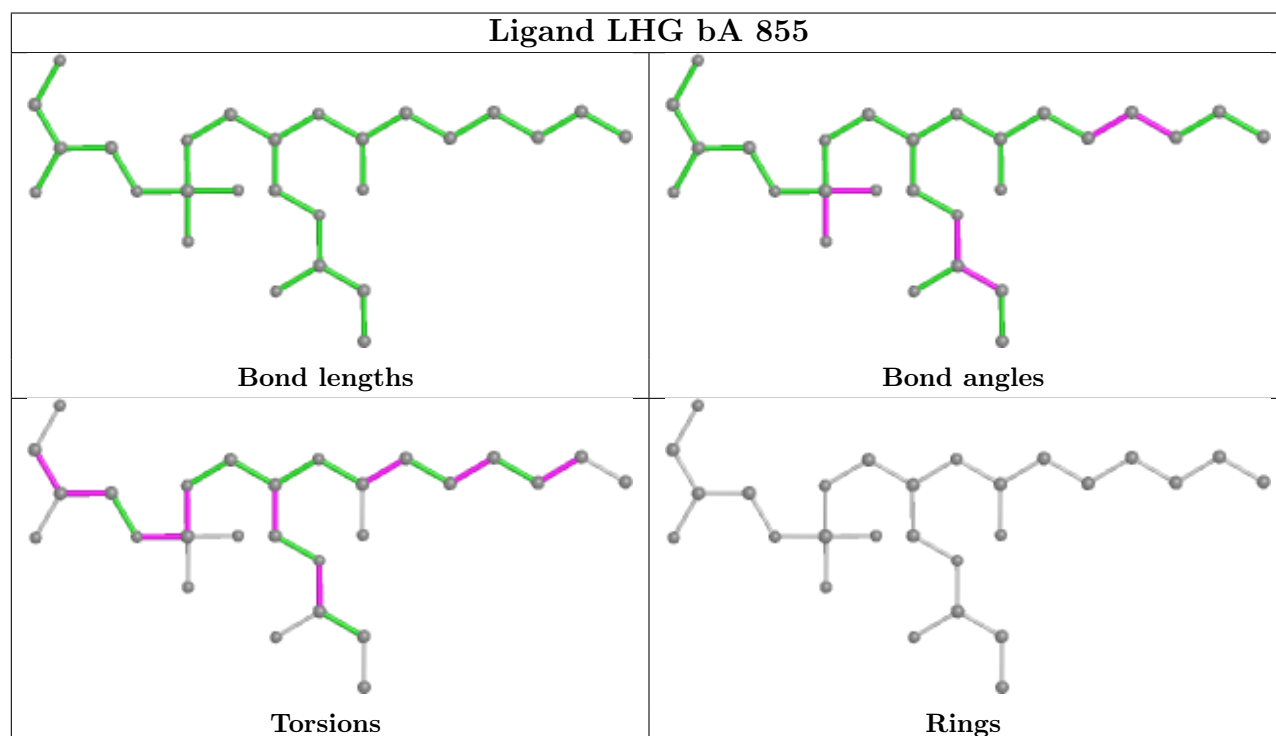
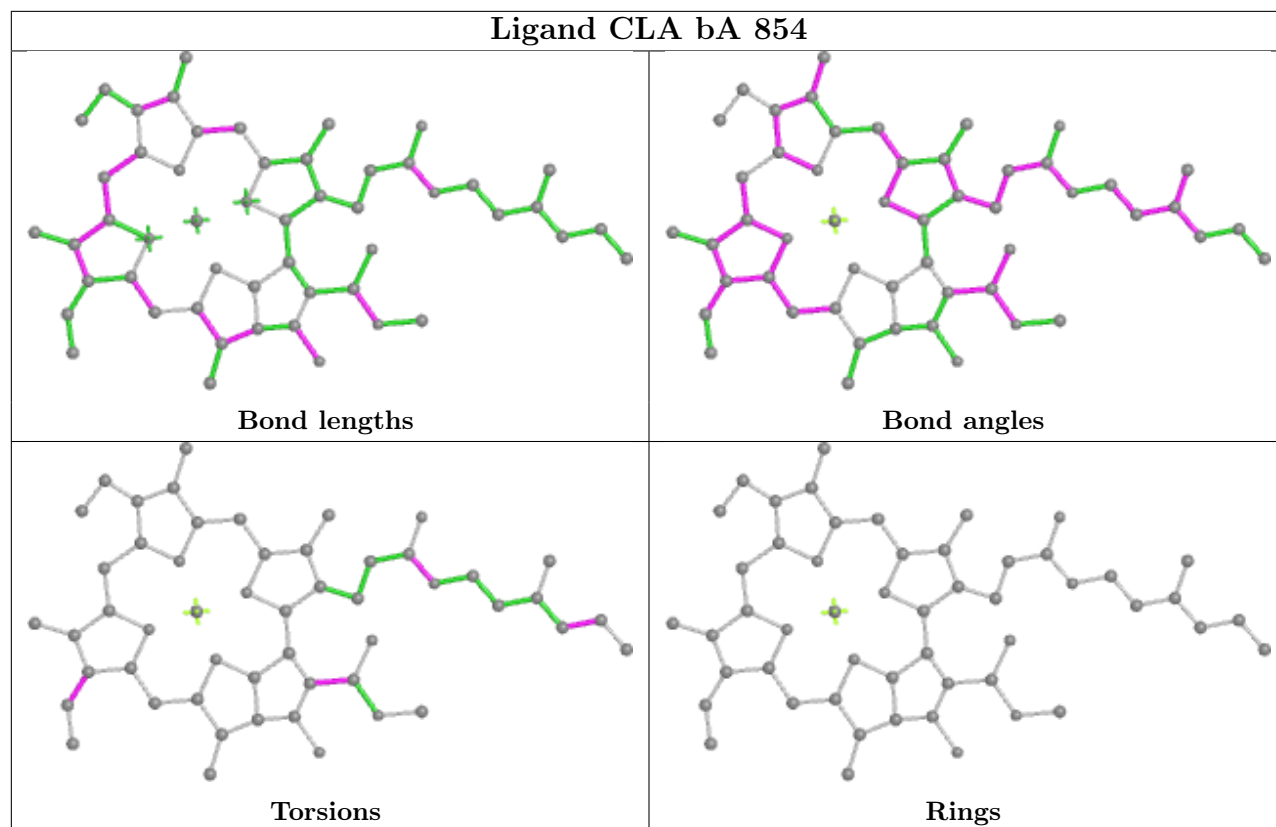


Ligand BCR bA 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

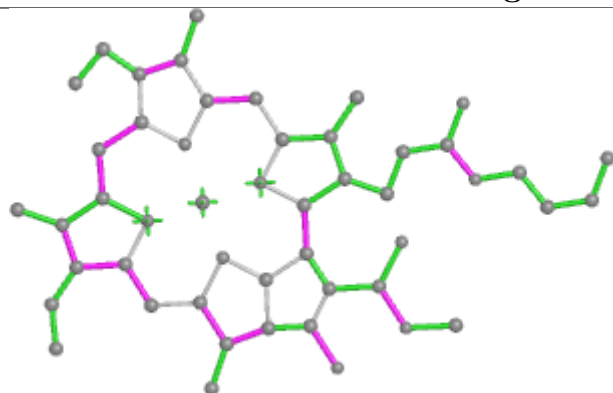
Ligand BCR bA 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR bA 851	
 Bond lengths	 Bond angles
 Torsions	 Rings

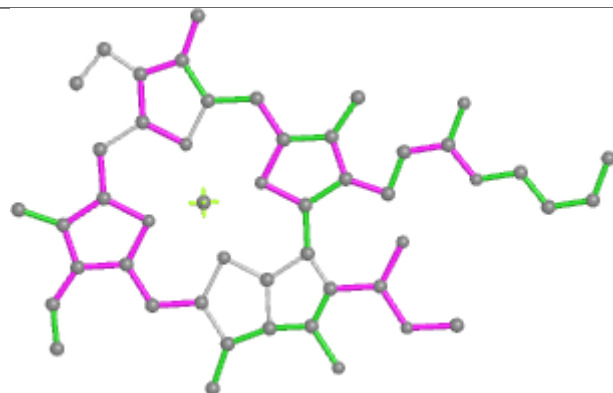




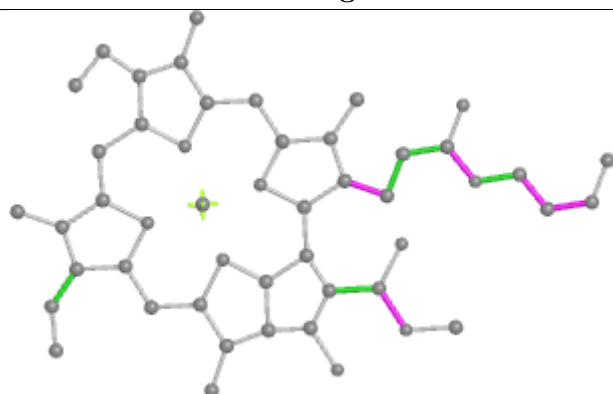
Ligand CLA bA 856



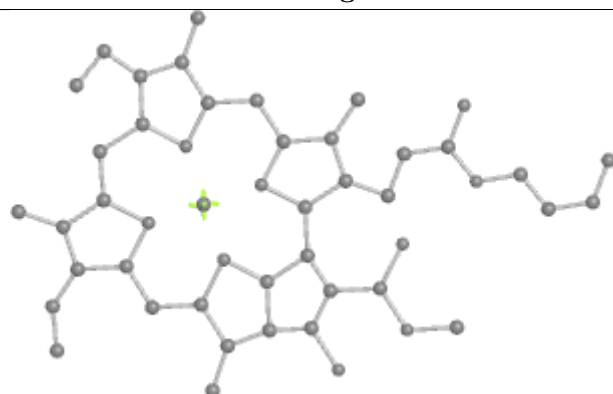
Bond lengths



Bond angles

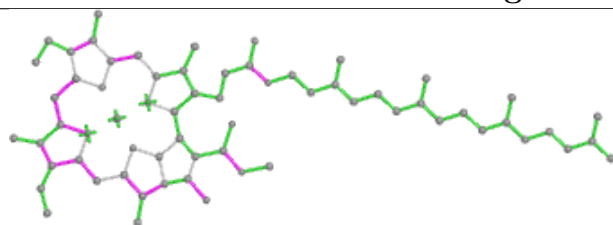


Torsions

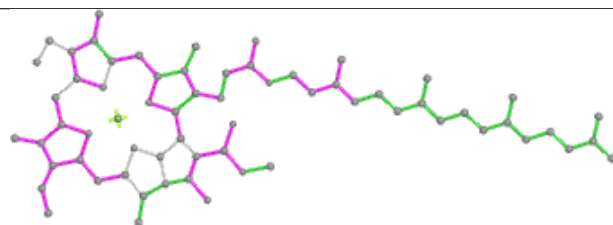


Rings

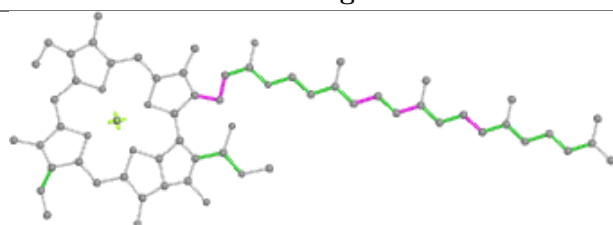
Ligand CLA bB 801



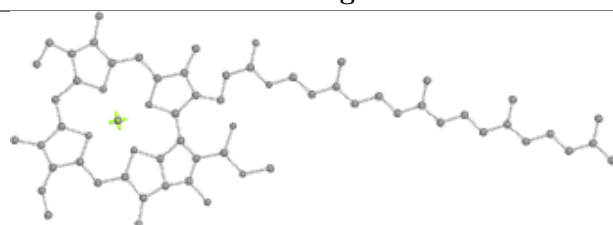
Bond lengths



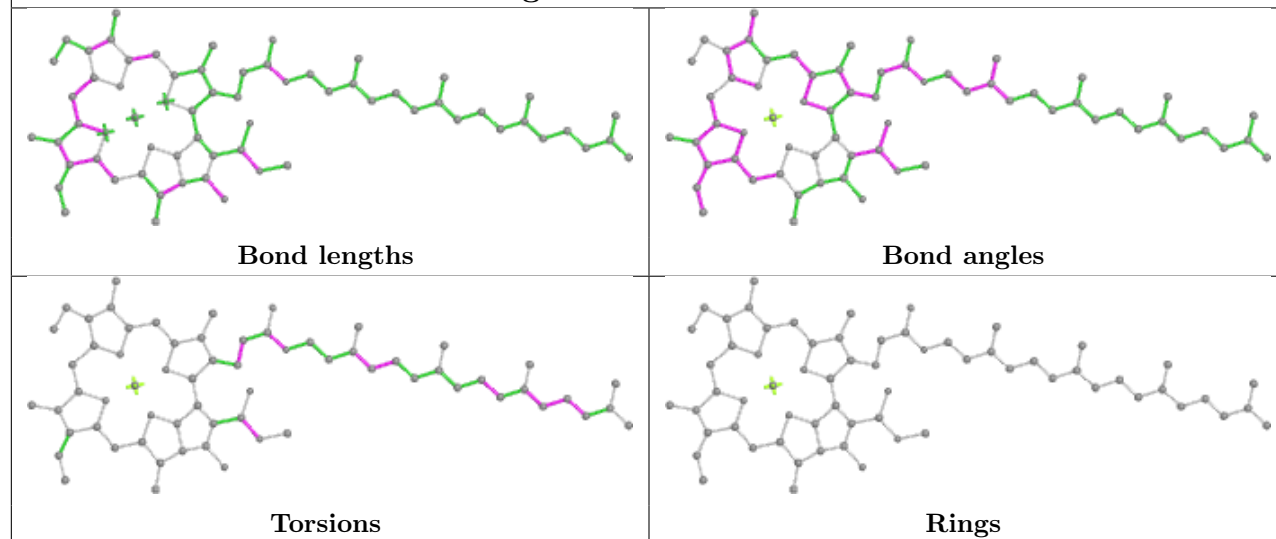
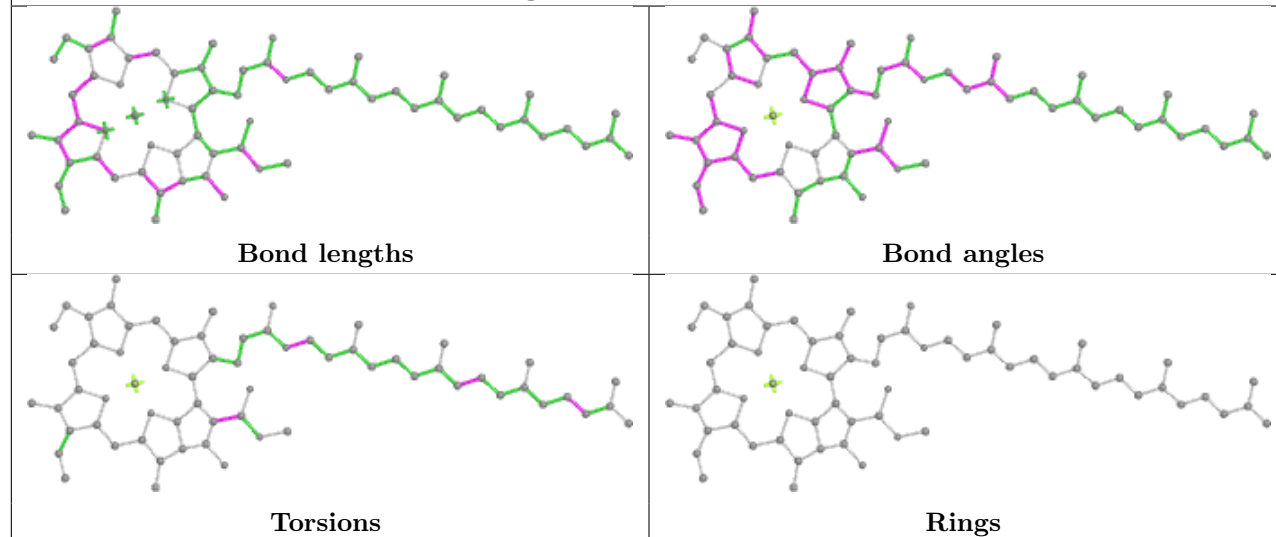
Bond angles



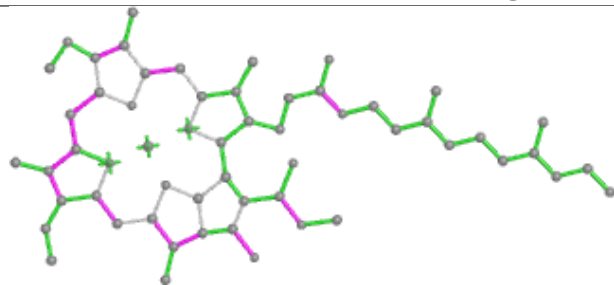
Torsions



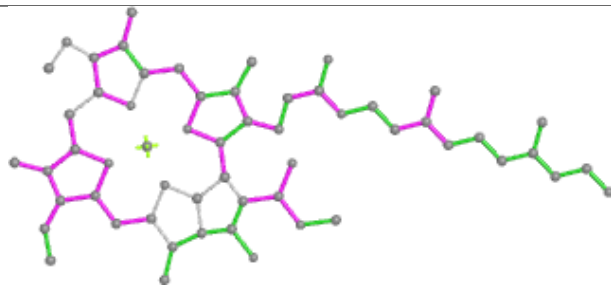
Rings

Ligand CLA bB 802**Ligand CLA bB 803**

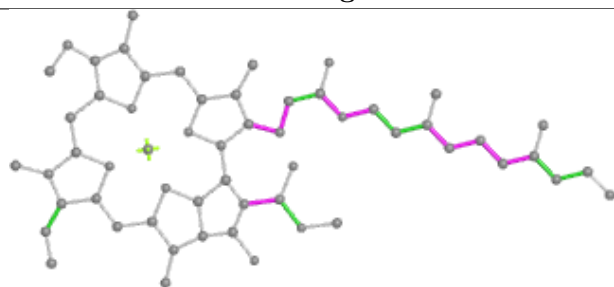
Ligand CLA bB 804



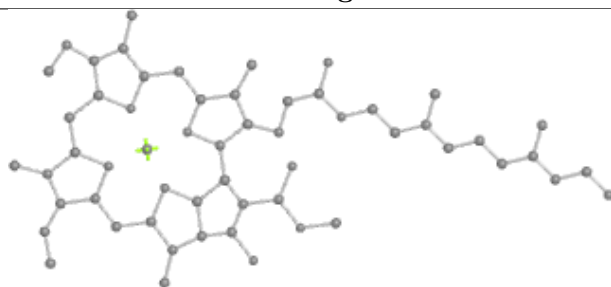
Bond lengths



Bond angles

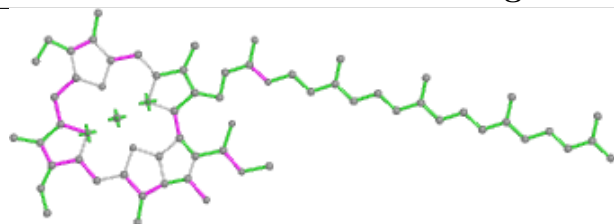


Torsions

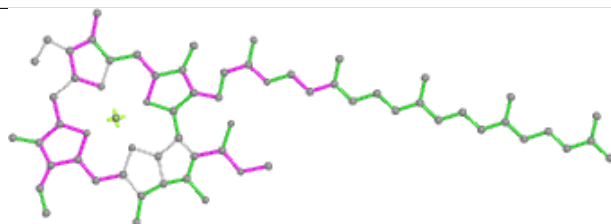


Rings

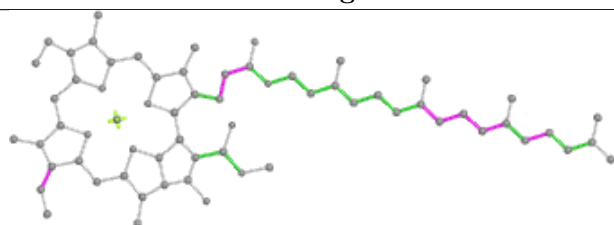
Ligand CLA bB 805



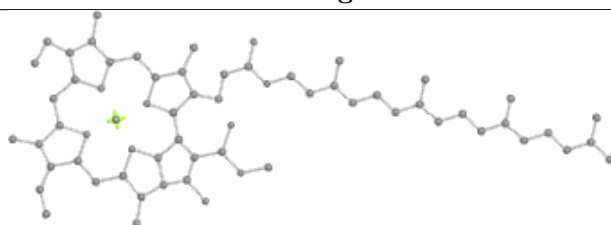
Bond lengths



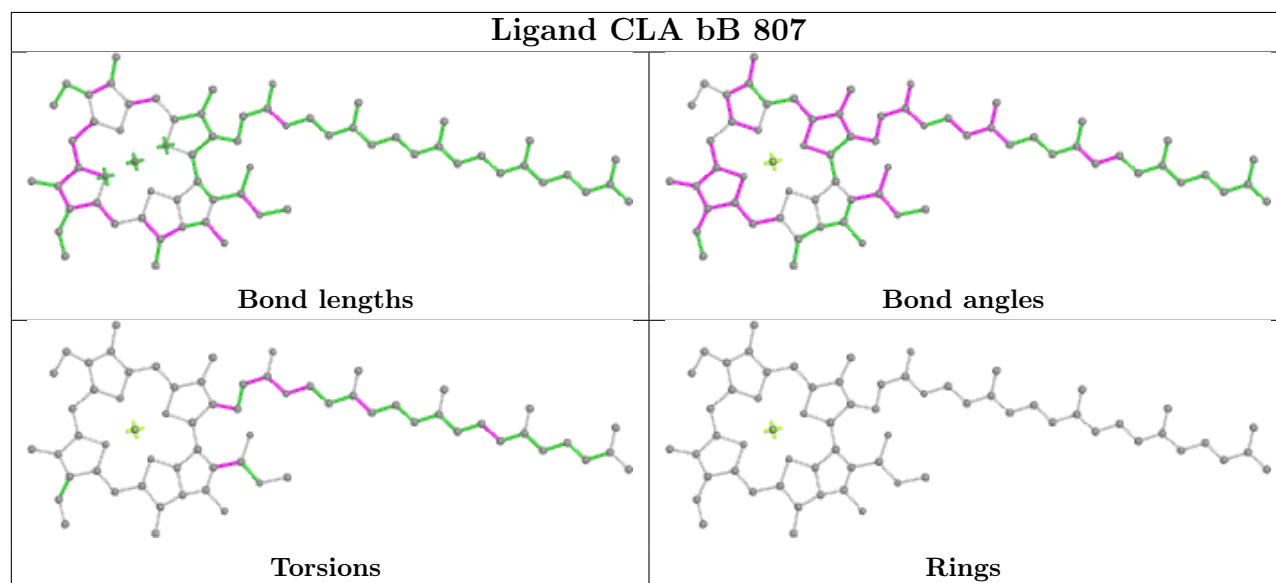
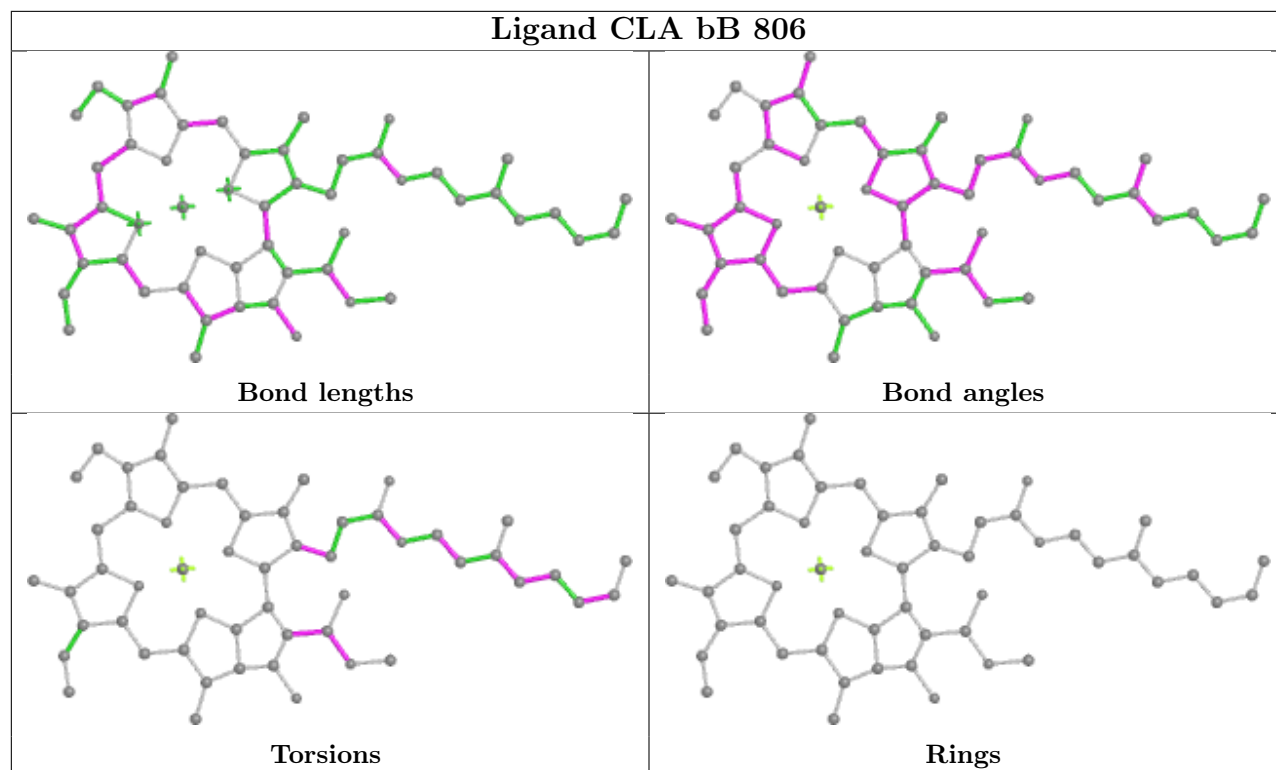
Bond angles

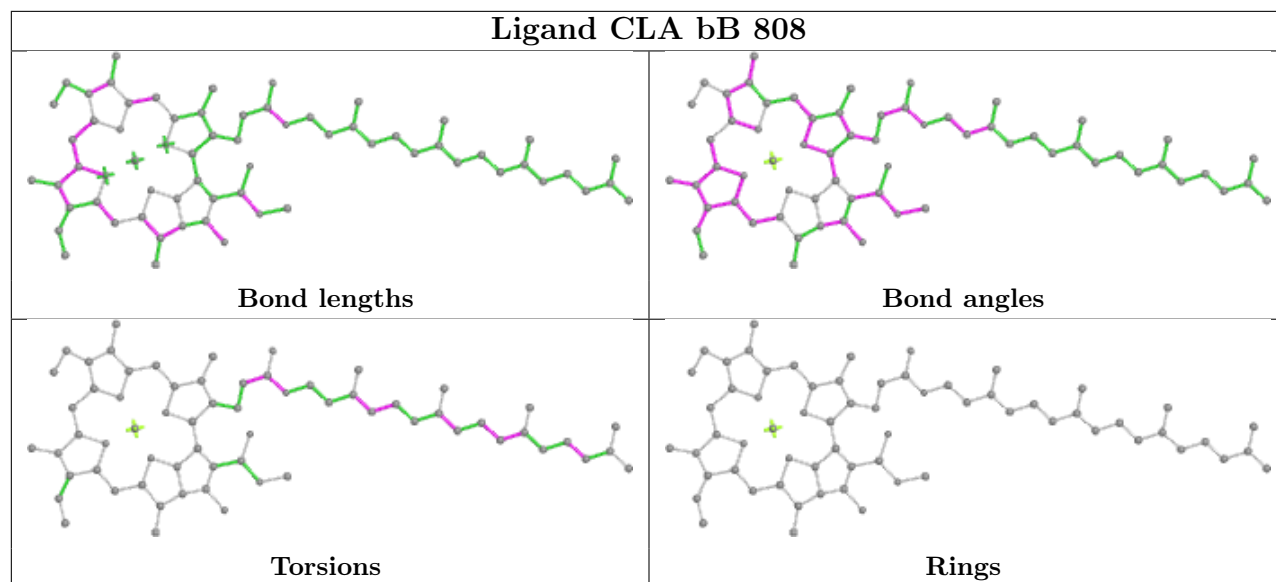
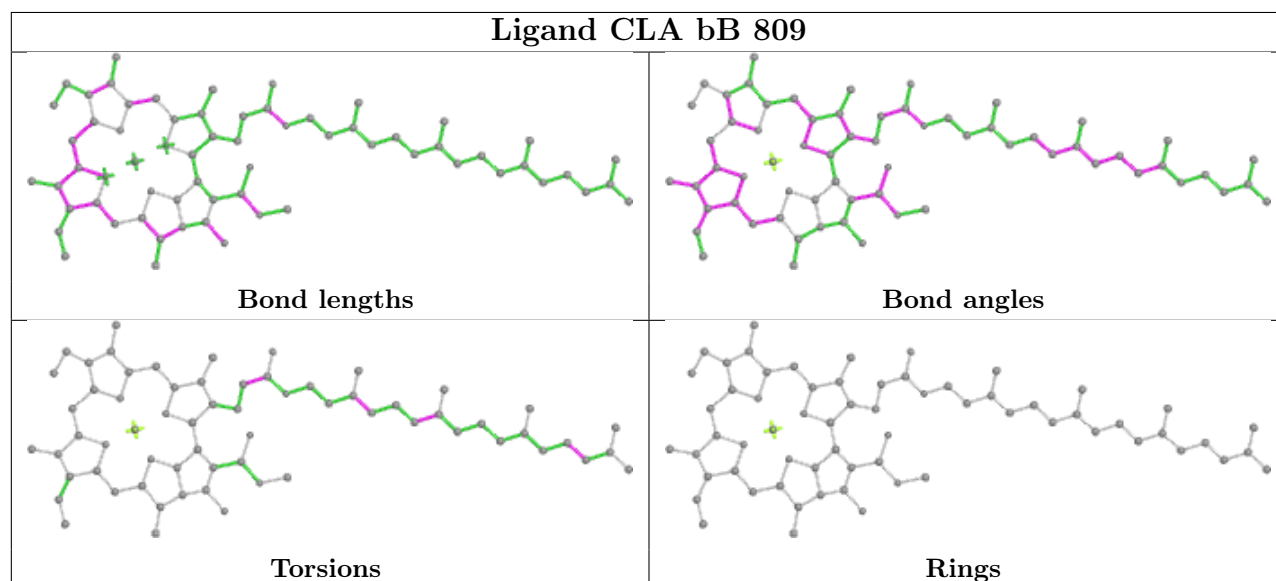


Torsions

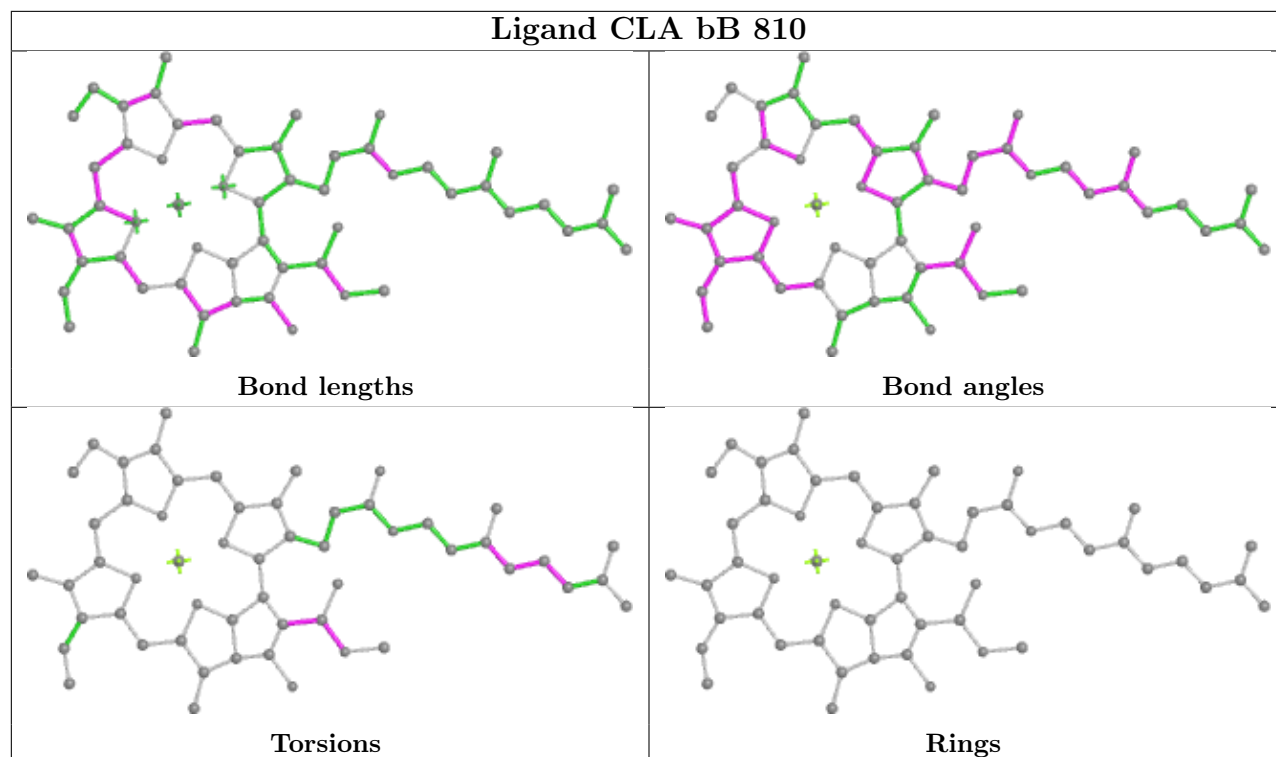


Rings

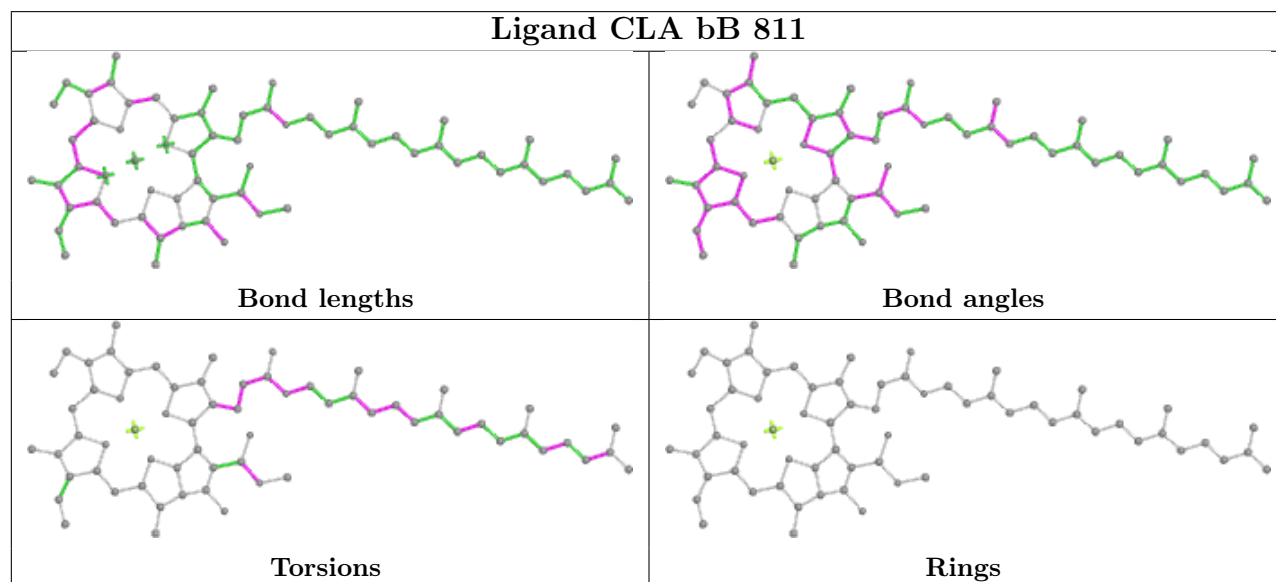


Ligand CLA bB 808**Ligand CLA bB 809**

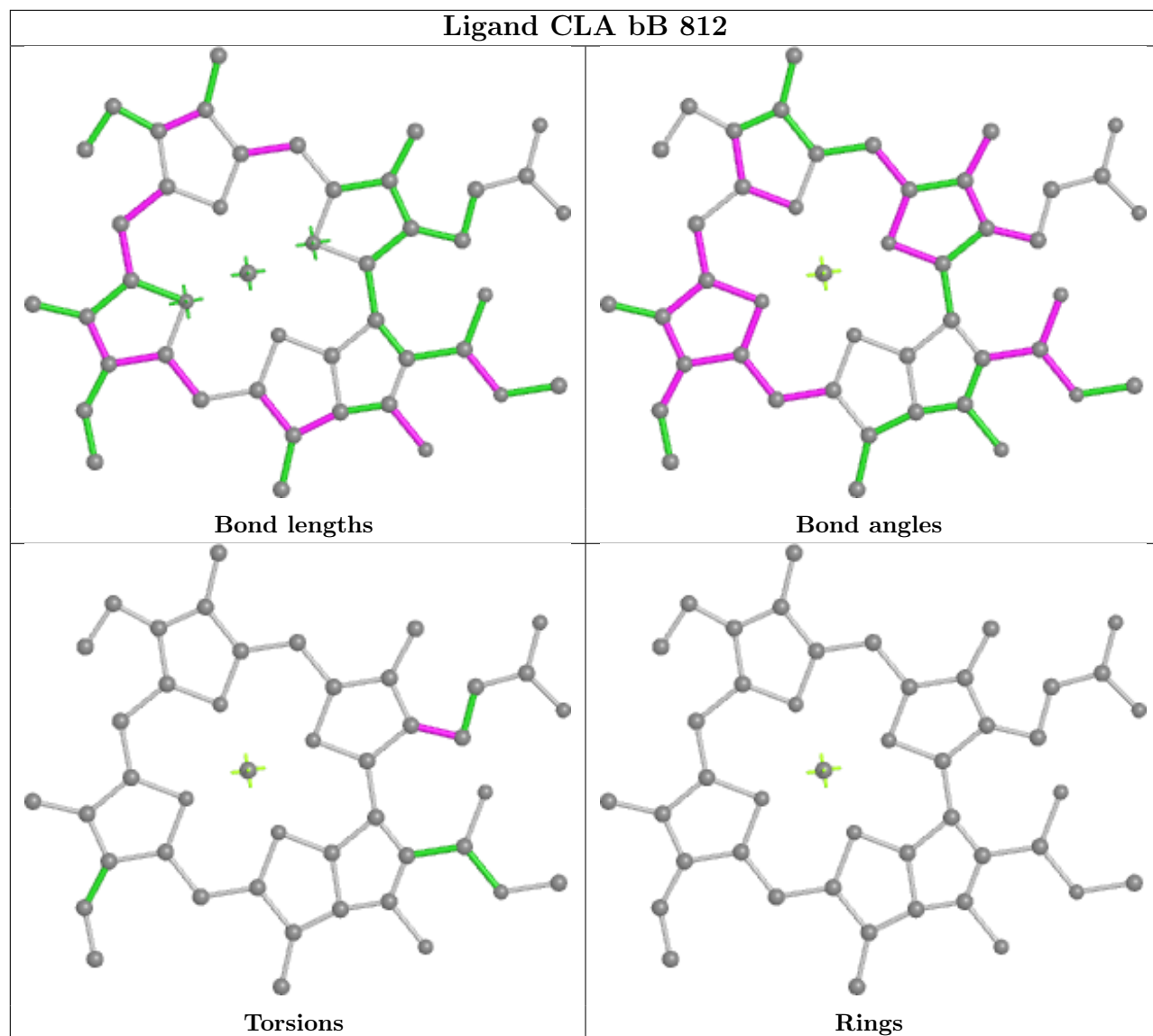
Ligand CLA bB 810



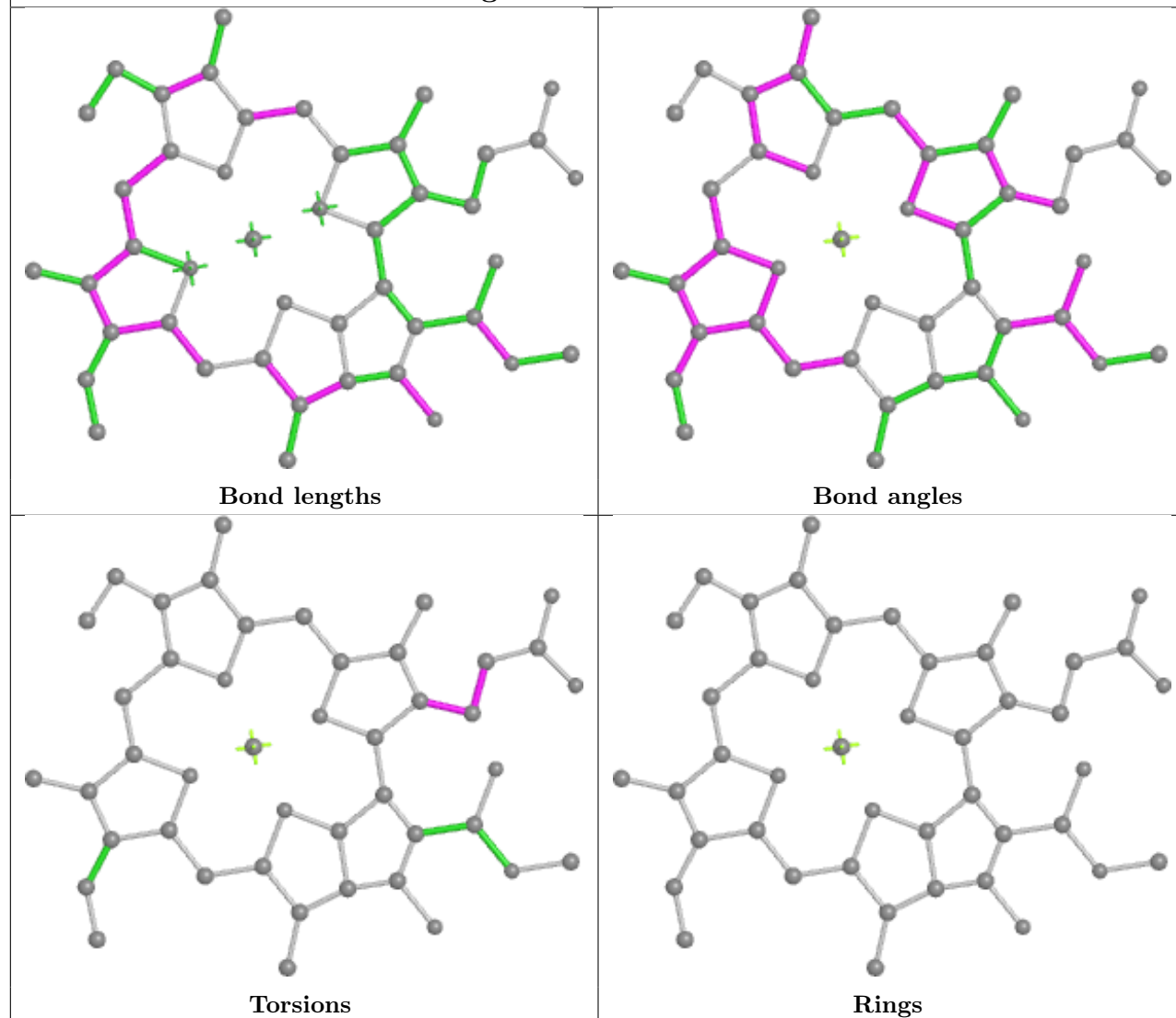
Ligand CLA bB 811



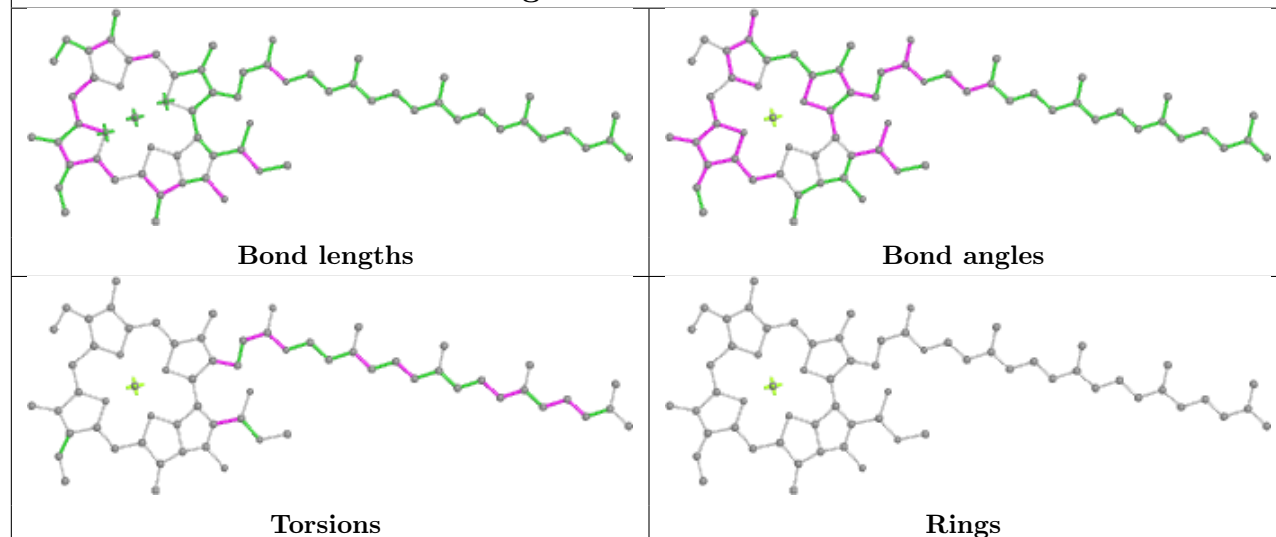
Ligand CLA bB 812

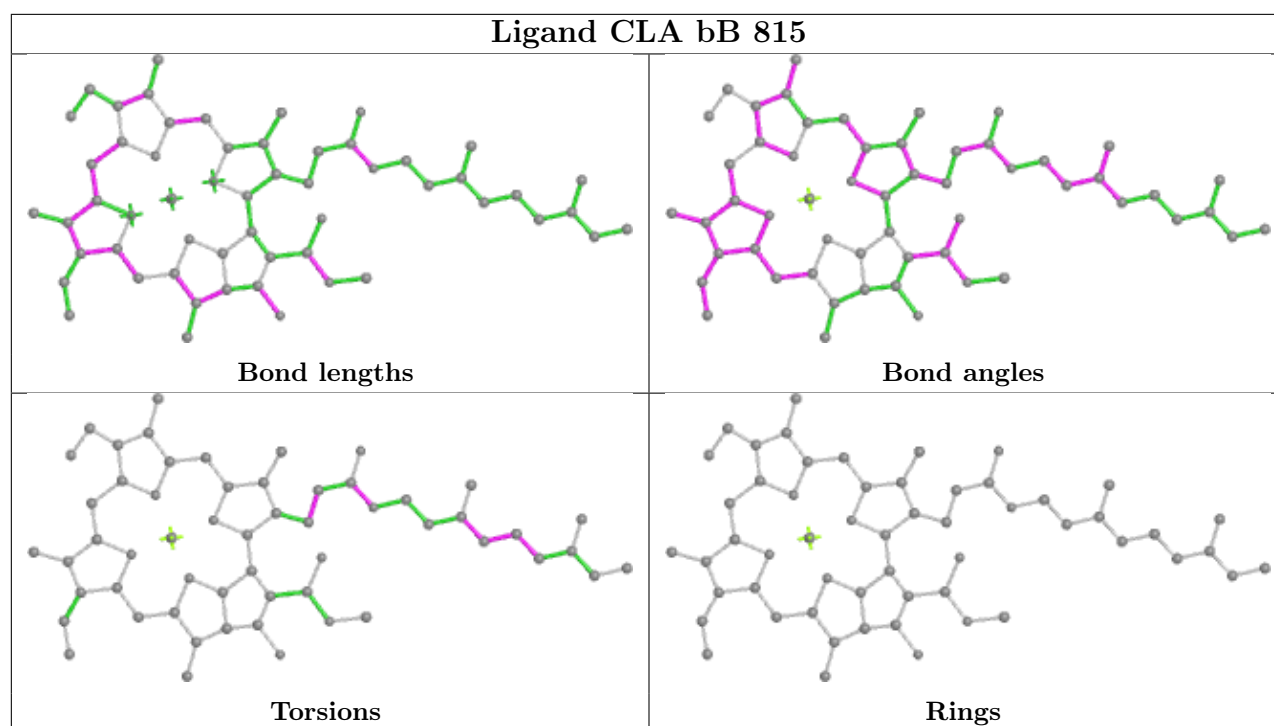


Ligand CLA bB 813

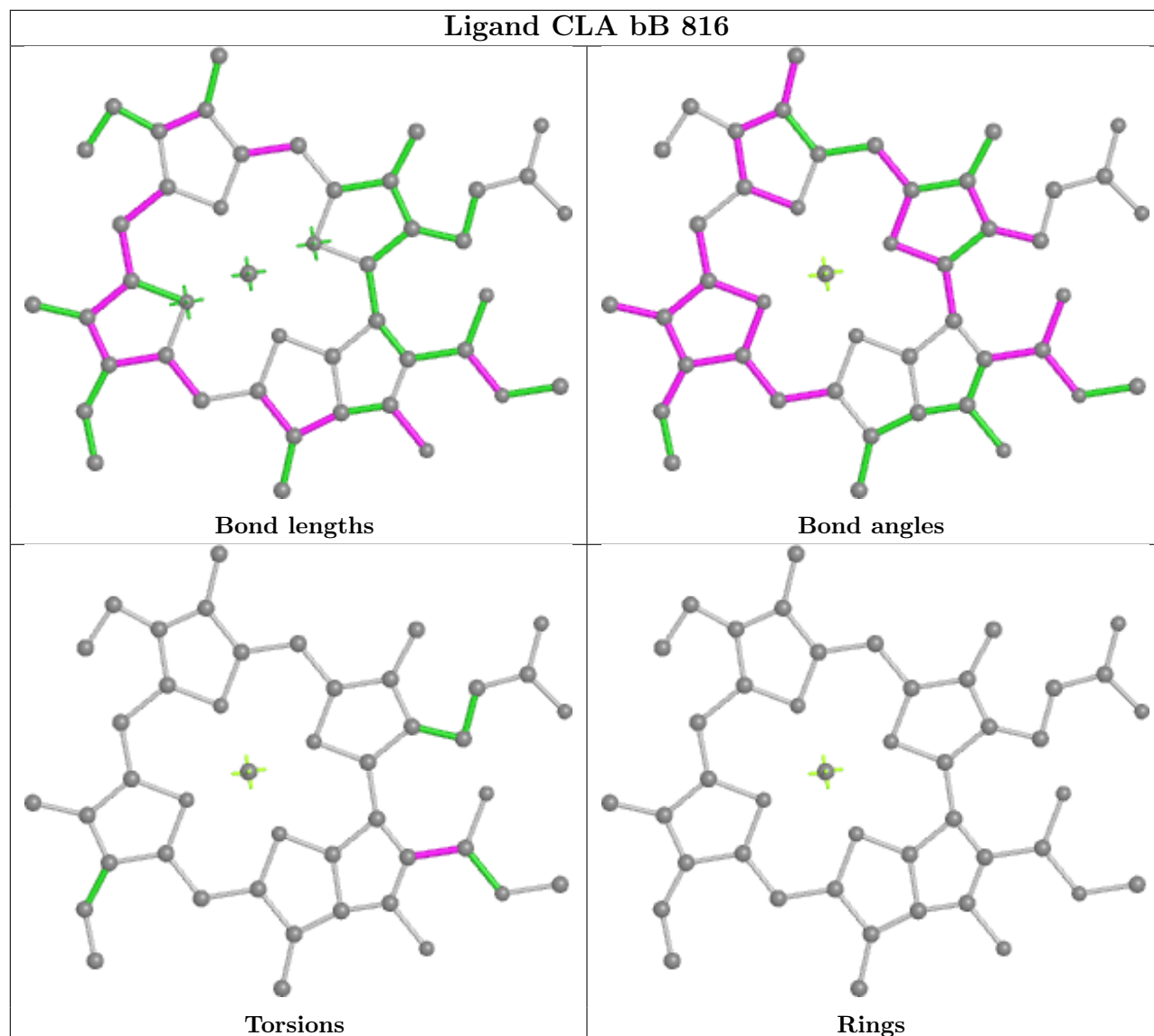


Ligand CLA bB 814

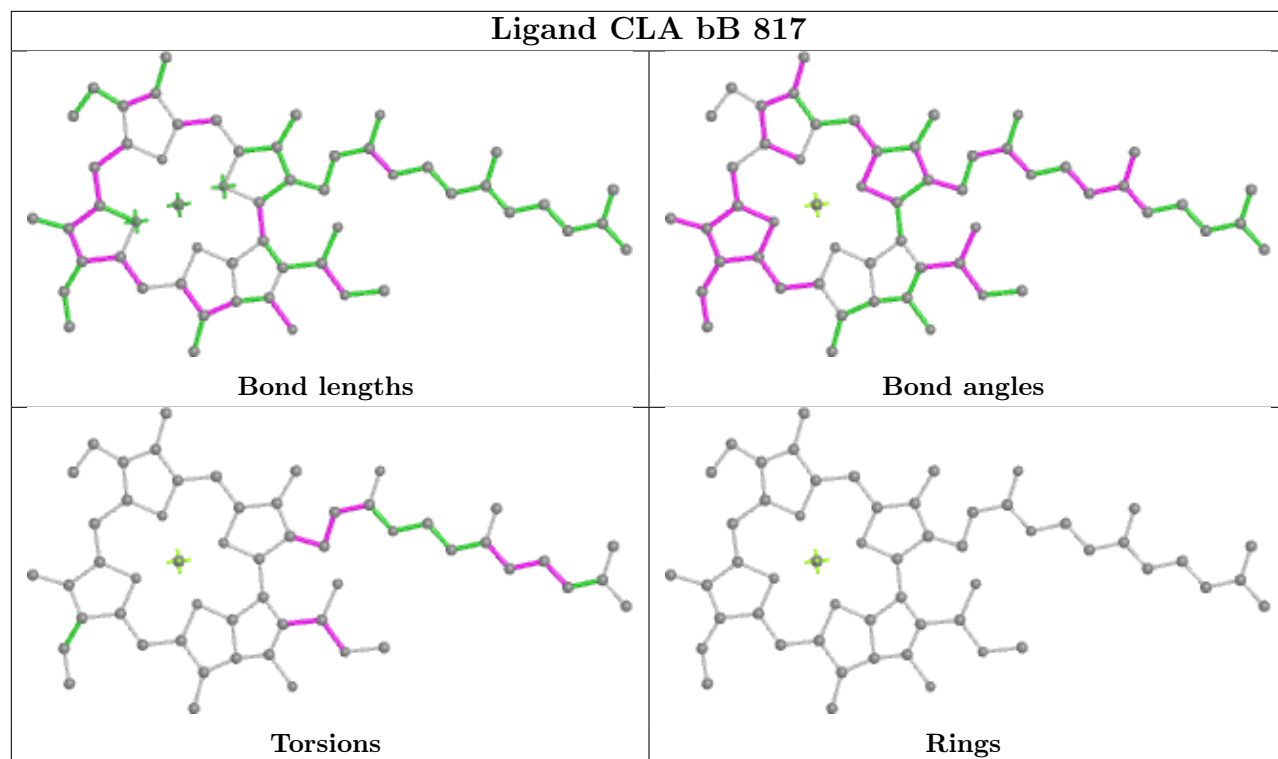




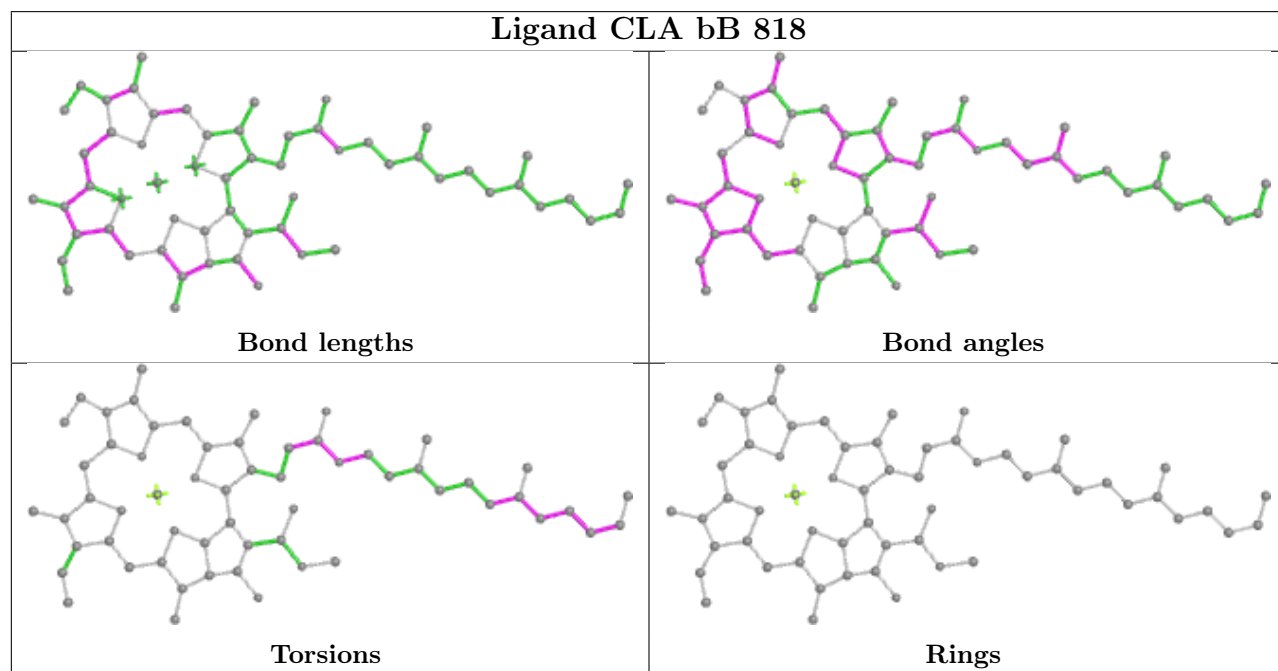
Ligand CLA bB 816

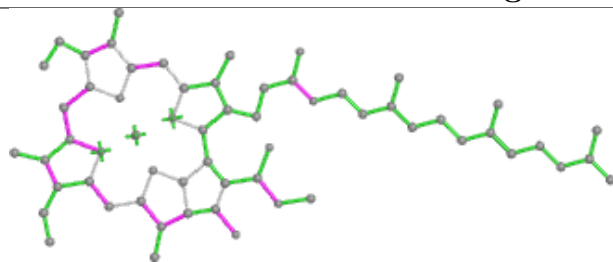
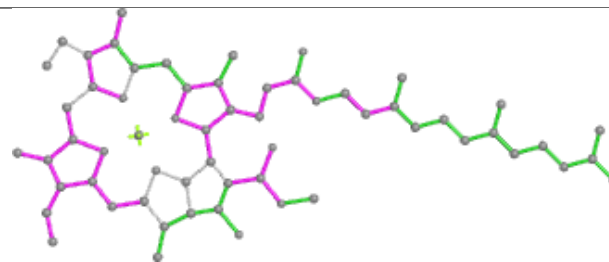
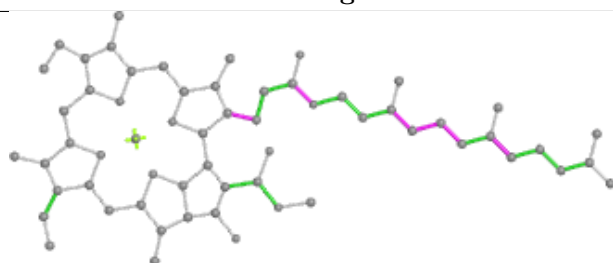
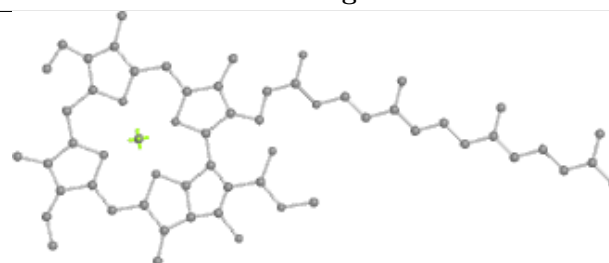
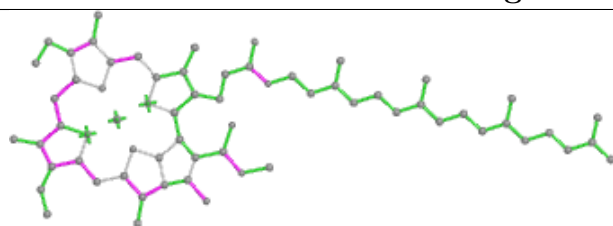
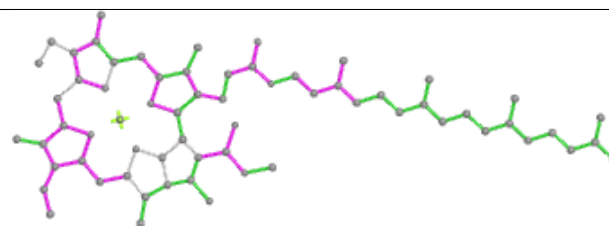
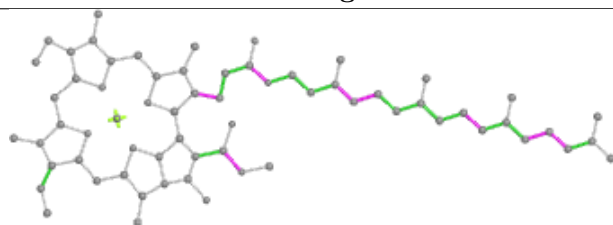
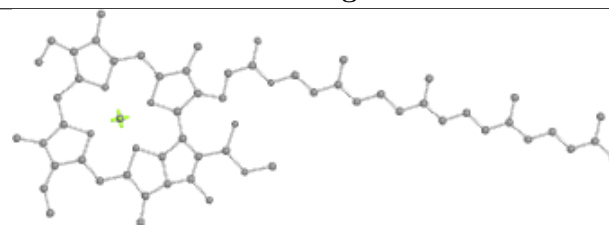


Ligand CLA bB 817

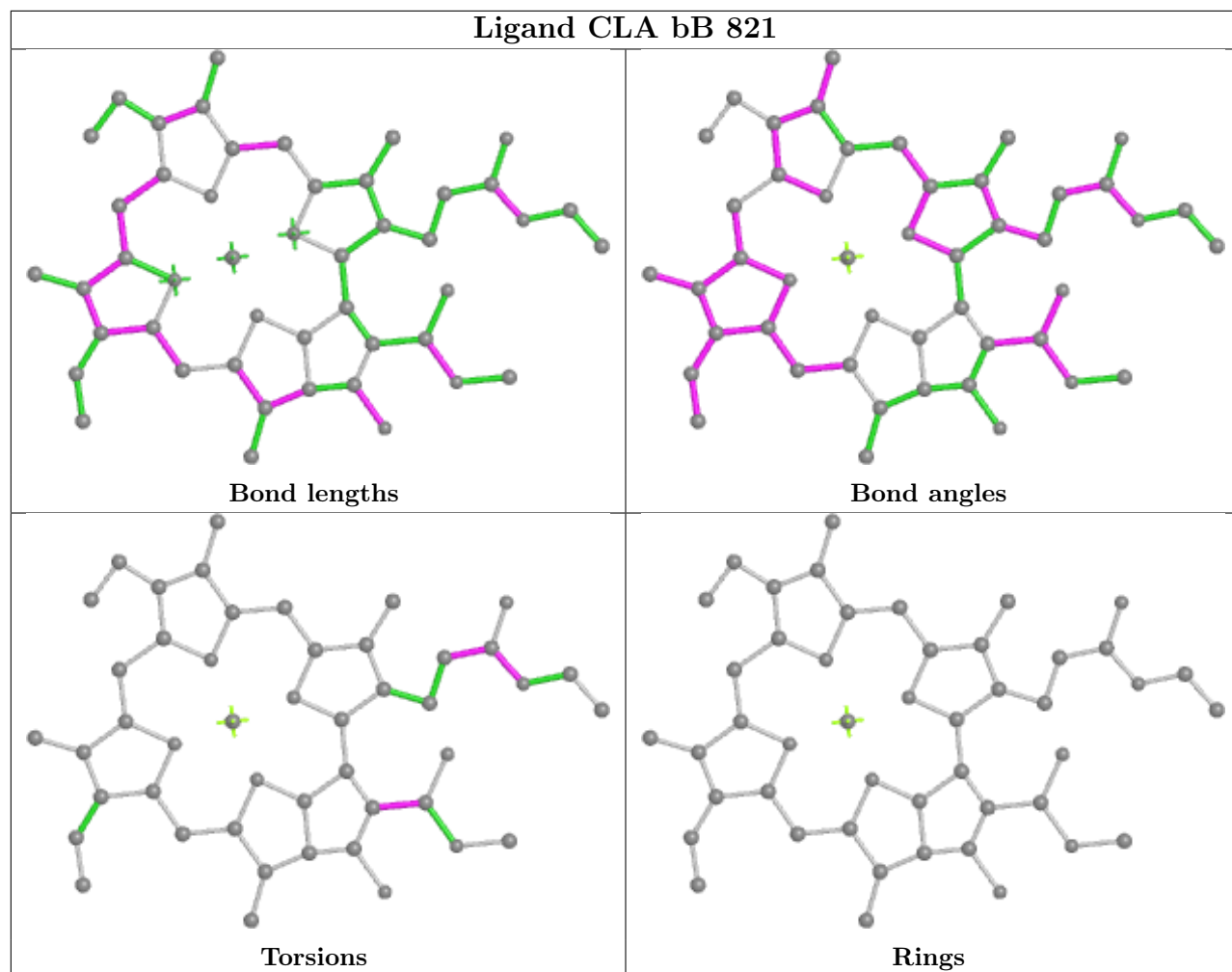


Ligand CLA bB 818

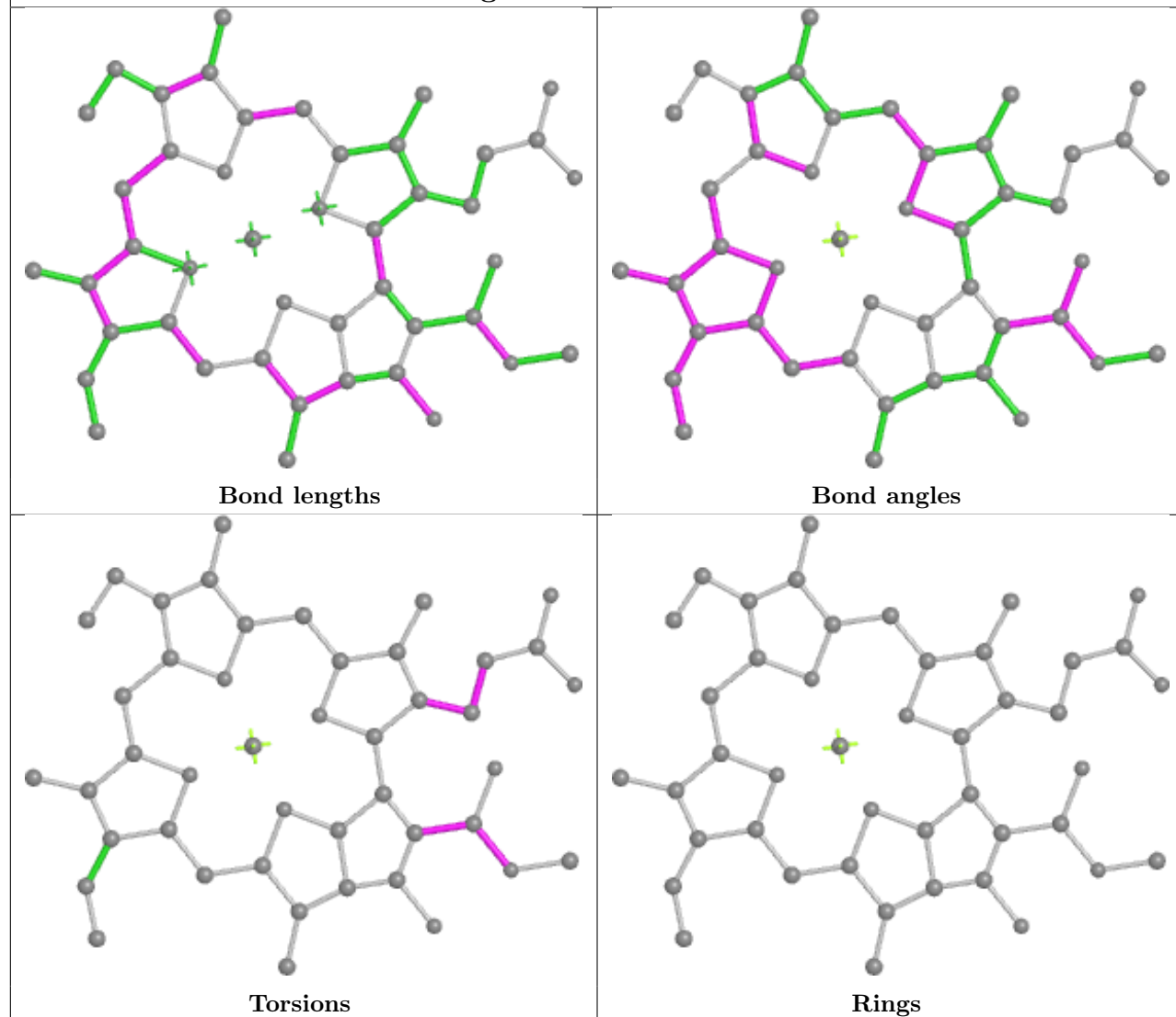


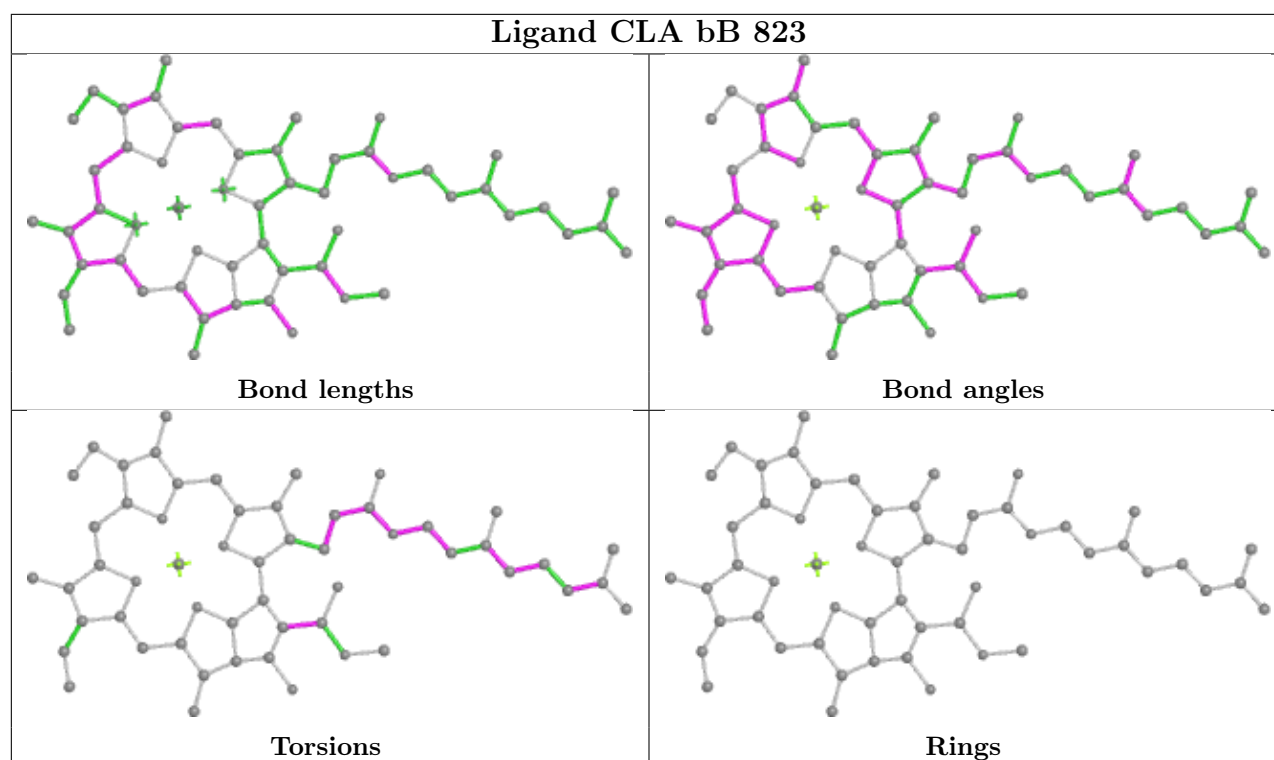
Ligand CLA bB 819**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA bB 820****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA bB 821

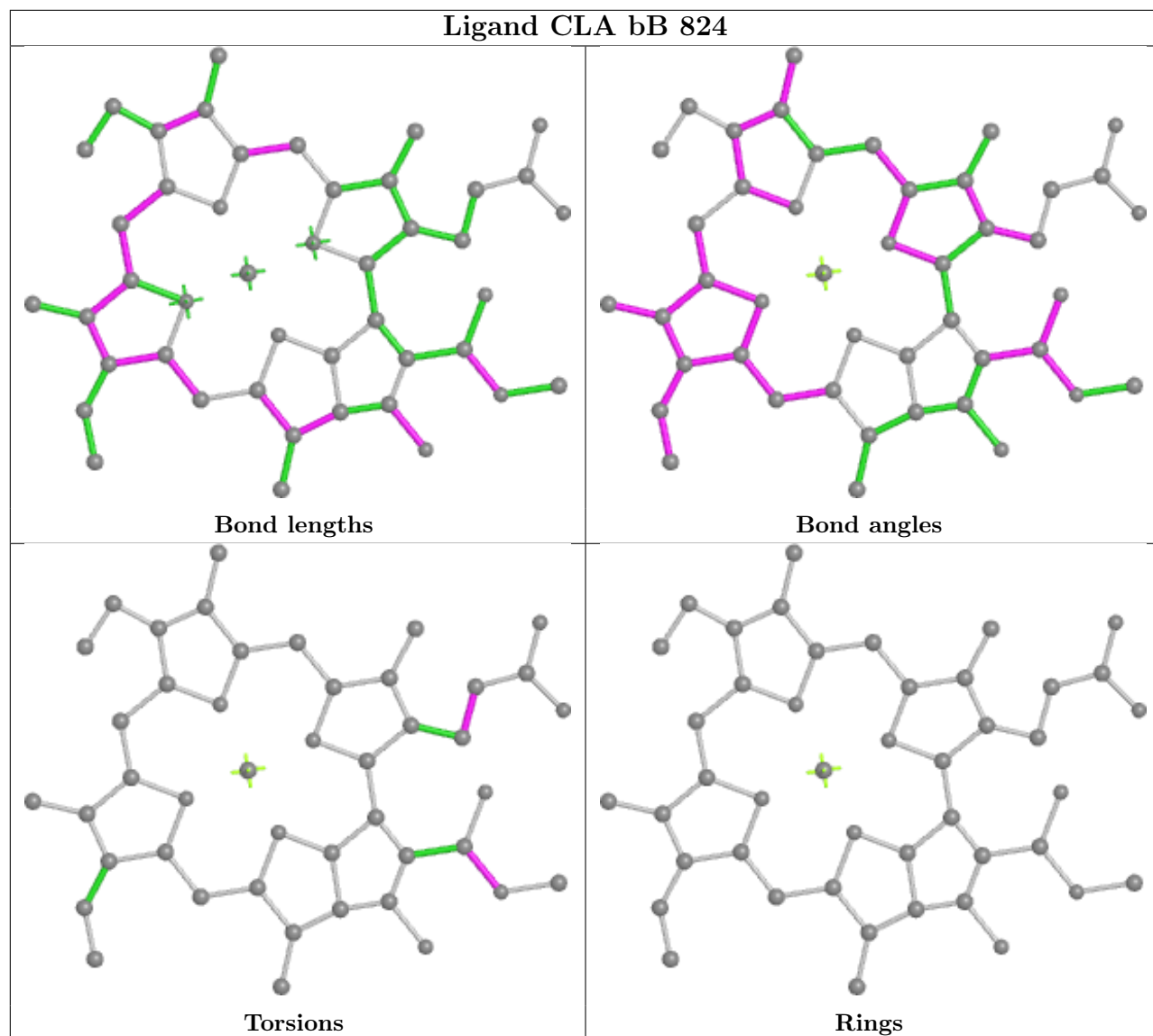


Ligand CLA bB 822

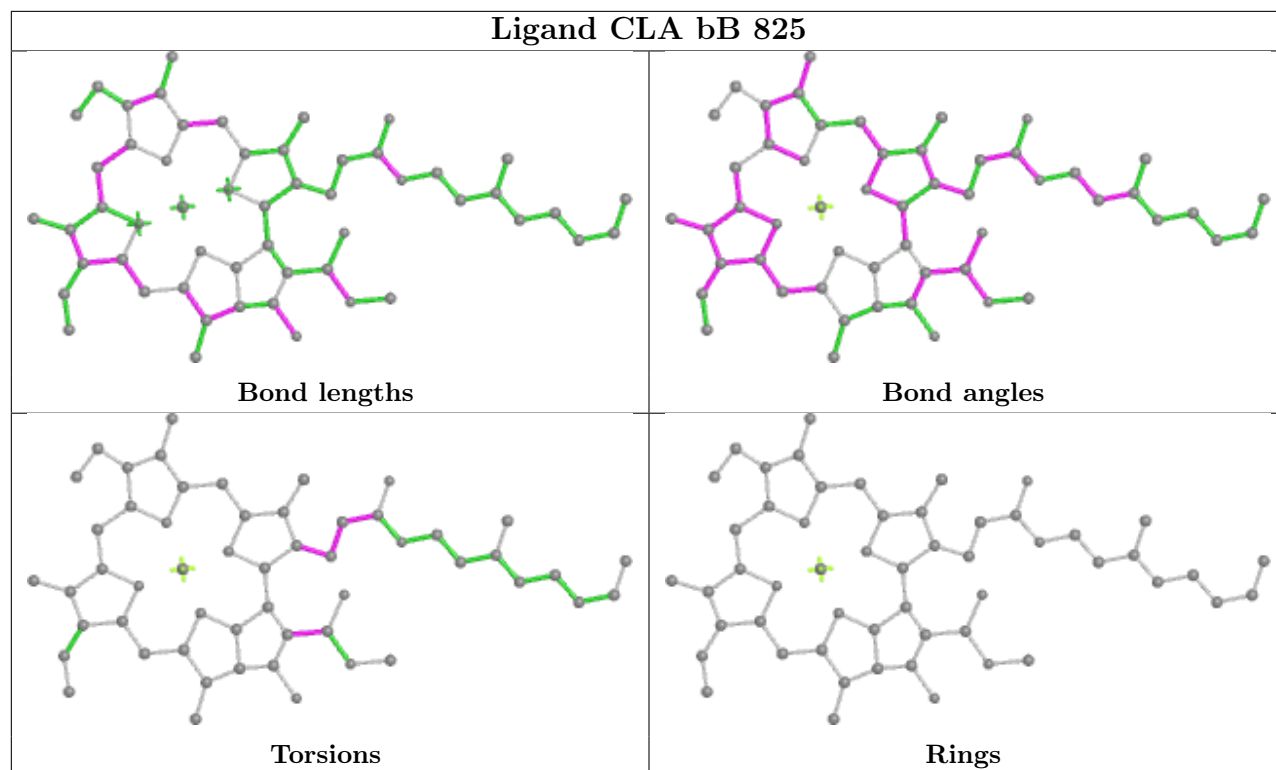




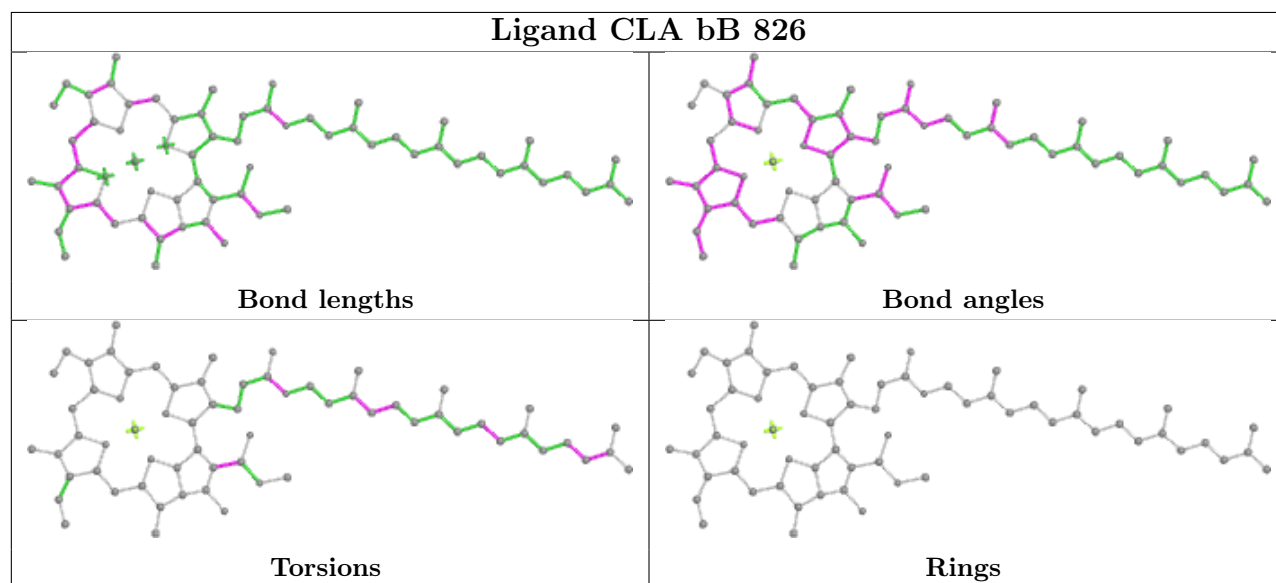
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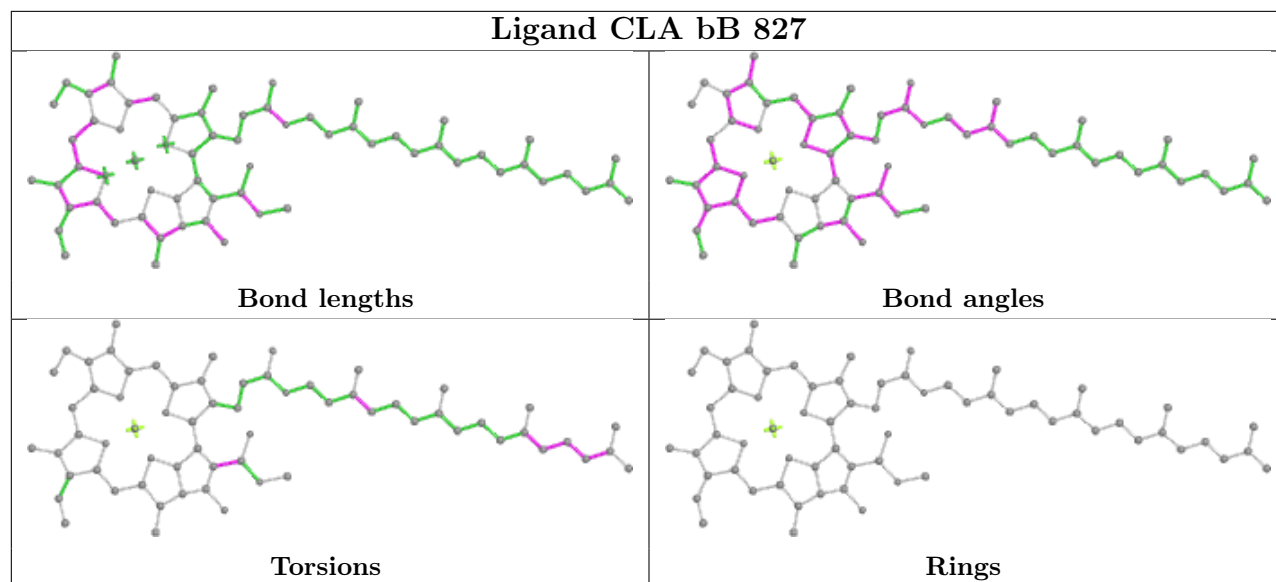
Ligand CLA bB 825



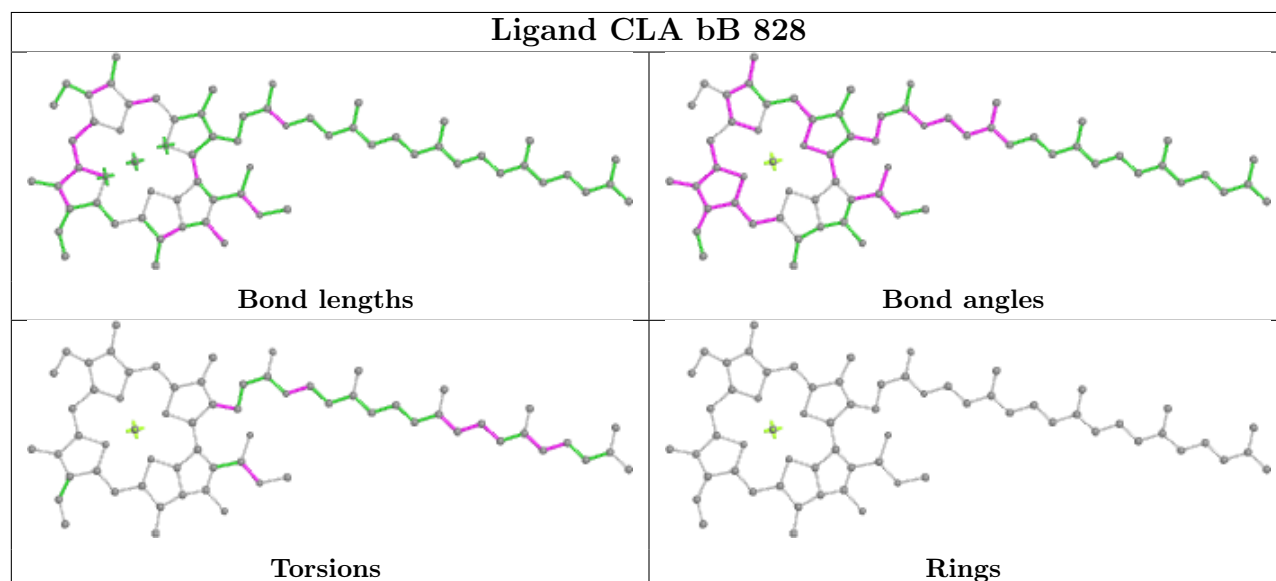
Ligand CLA bB 826



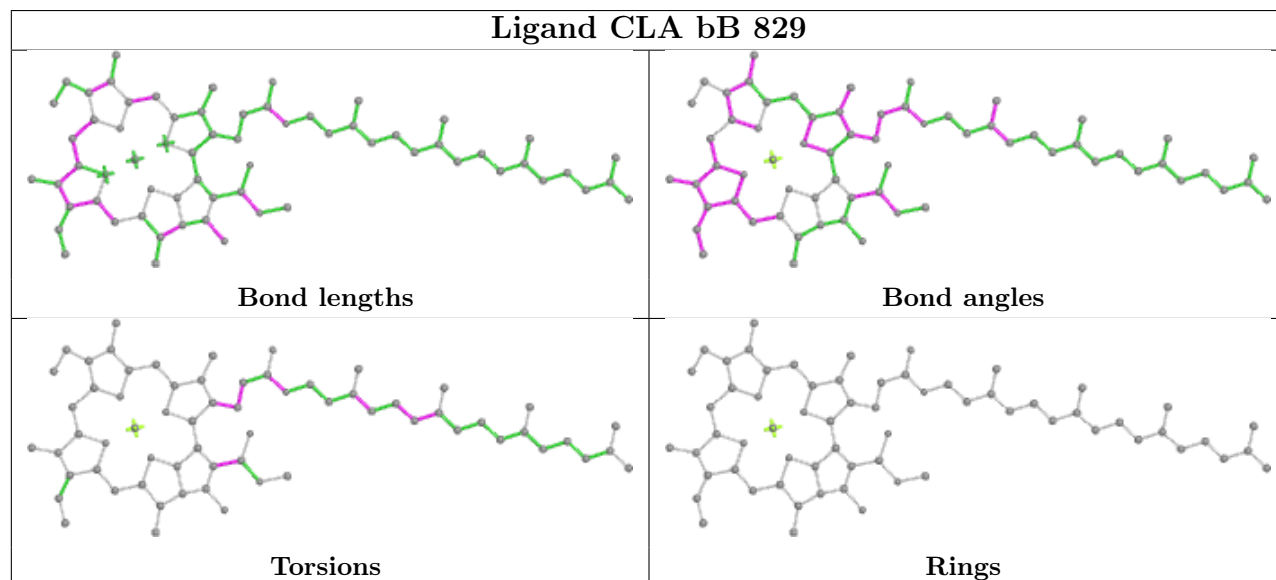
Ligand CLA bB 827



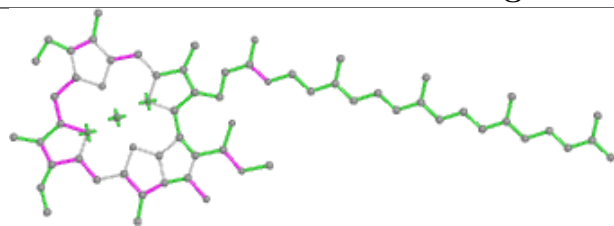
Ligand CLA bB 828



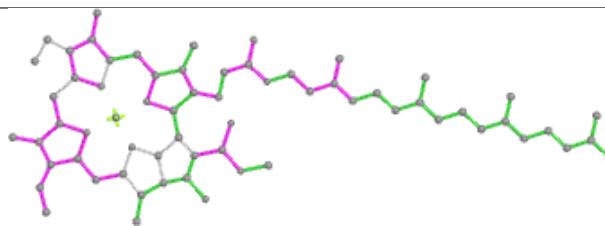
Ligand CLA bB 829



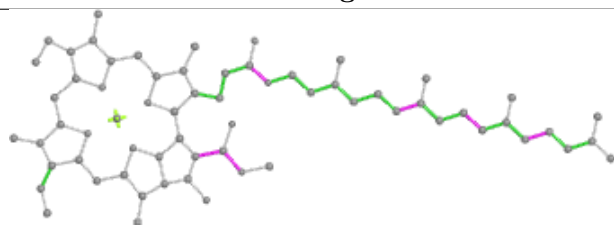
Ligand CLA bB 830



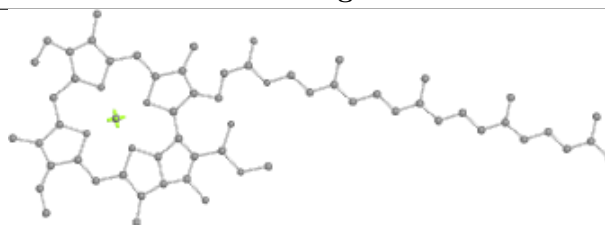
Bond lengths



Bond angles

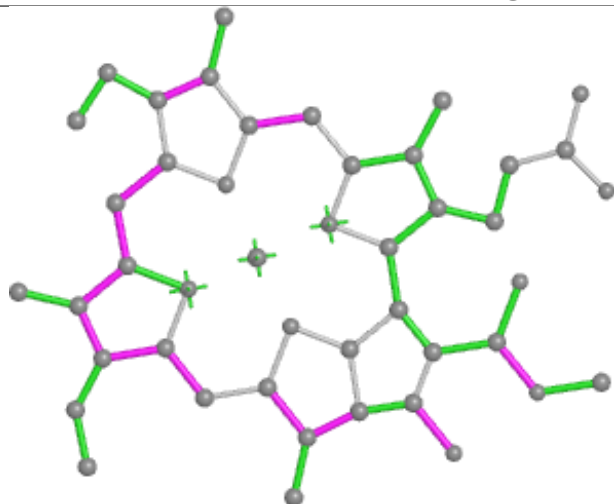


Torsions

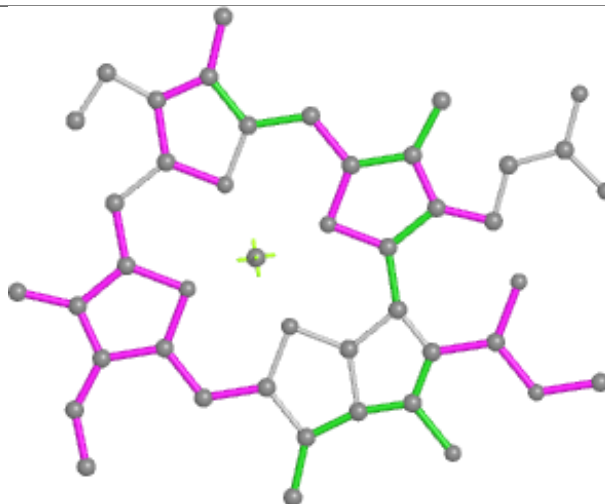


Rings

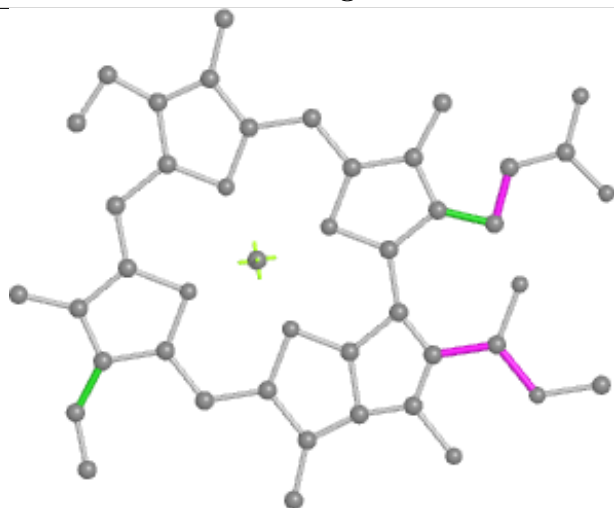
Ligand CLA bB 831



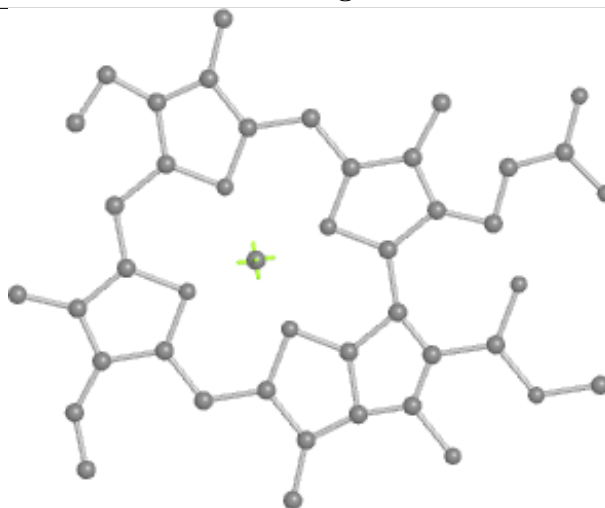
Bond lengths



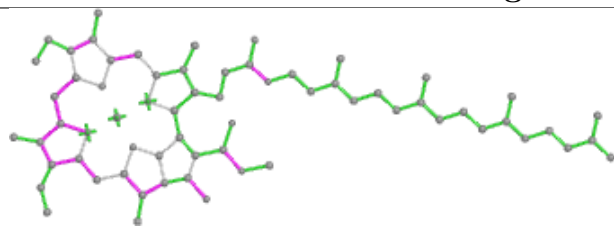
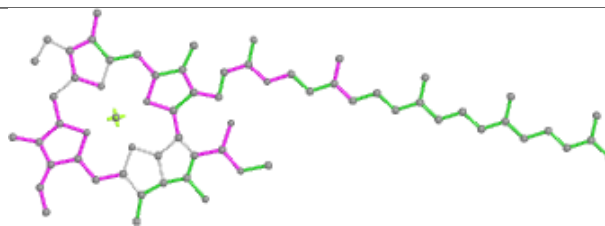
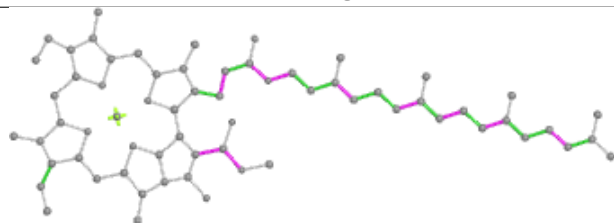
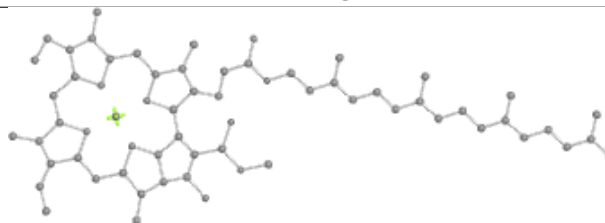
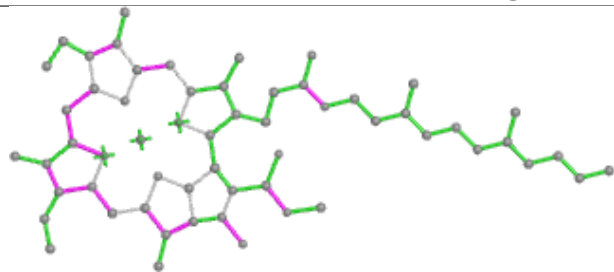
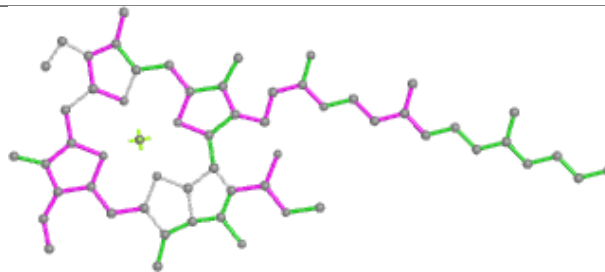
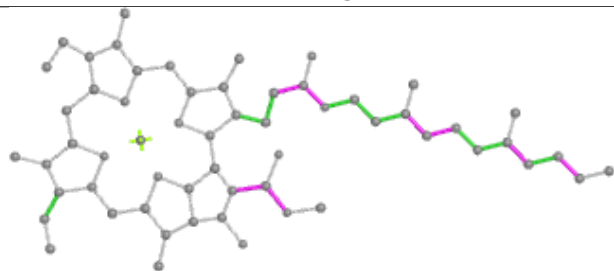
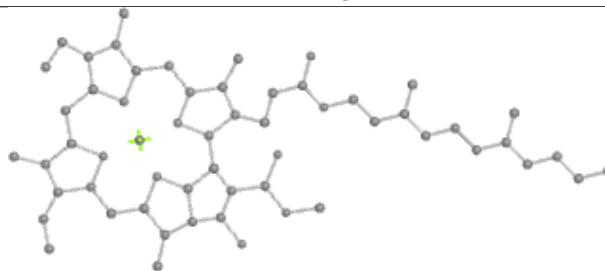
Bond angles



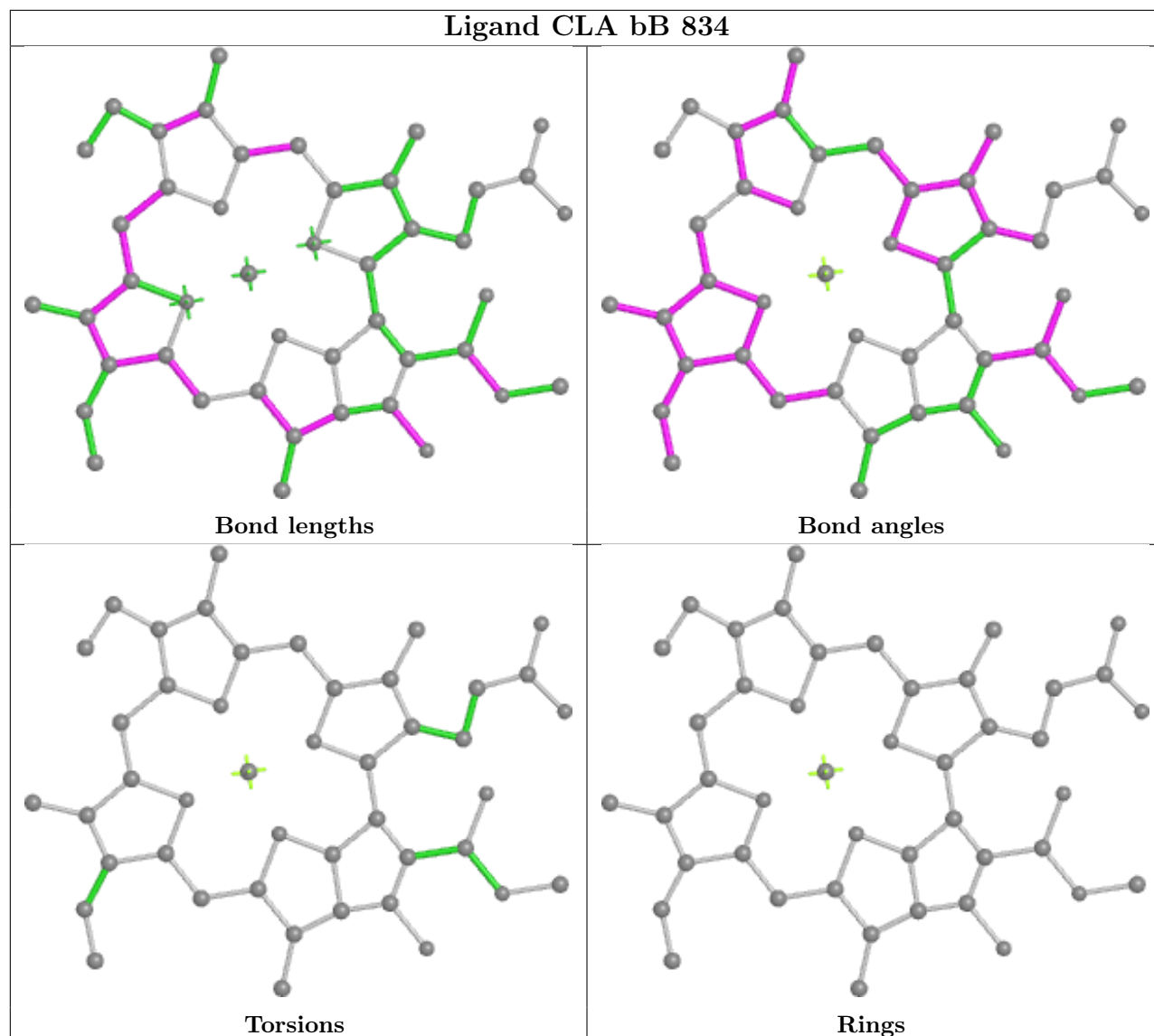
Torsions



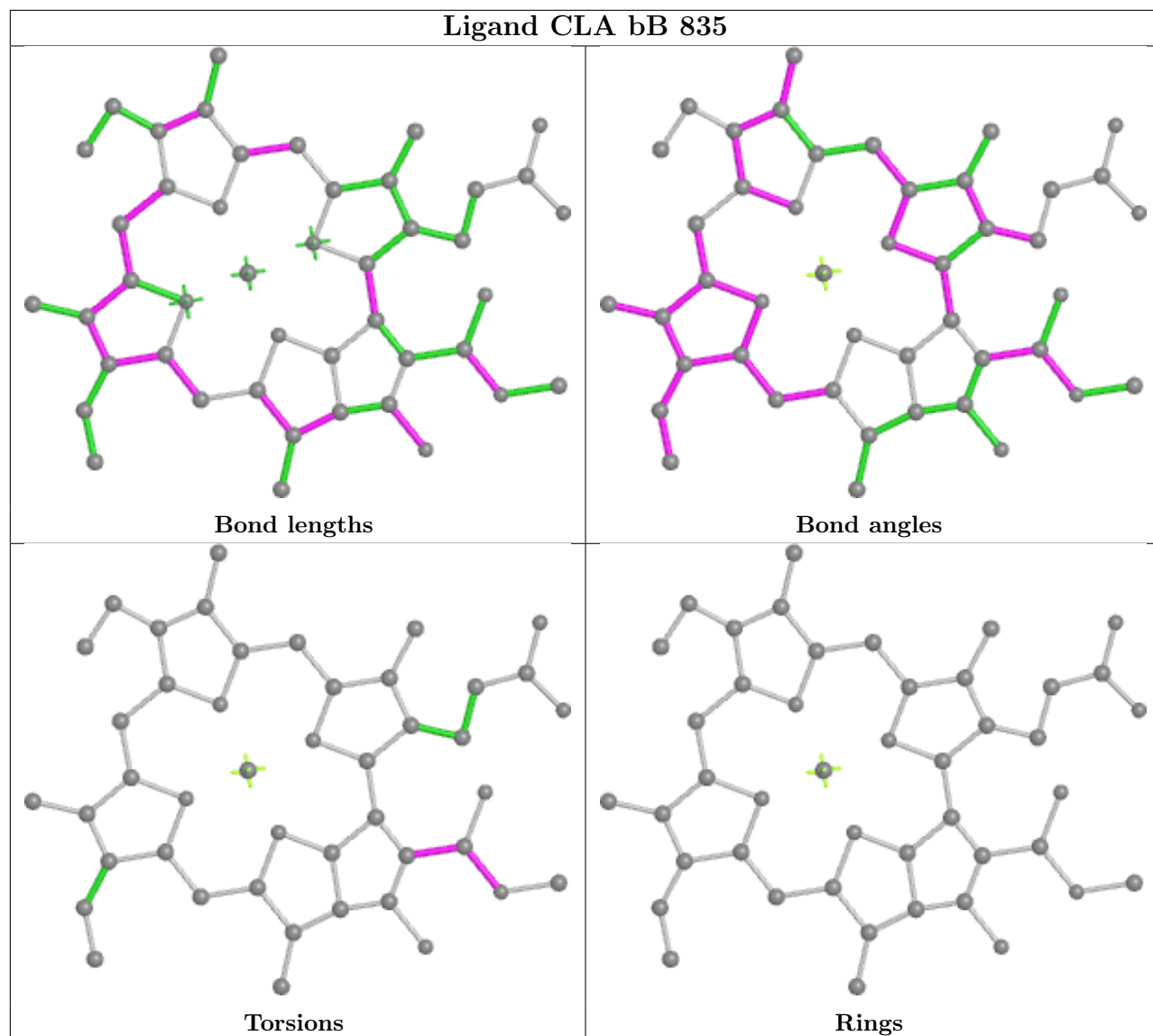
Rings

Ligand CLA bB 832**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA bB 833****Bond lengths****Bond angles****Torsions****Rings**

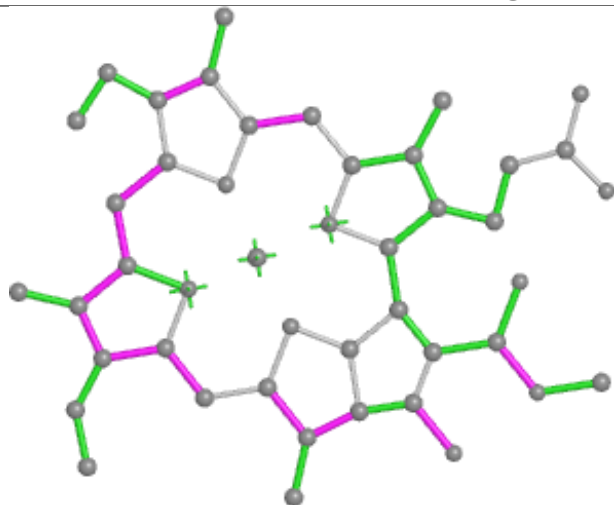
Ligand CLA bB 834



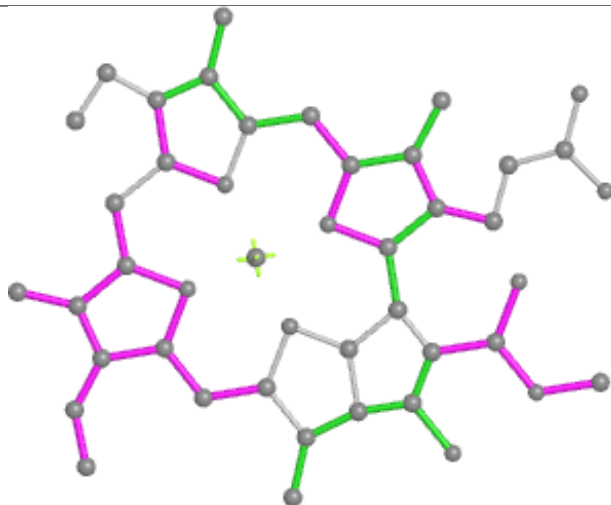
Ligand CLA bB 835



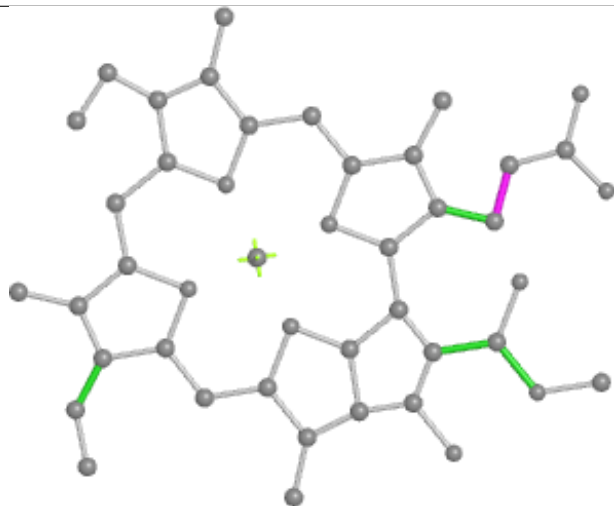
Ligand CLA bB 836



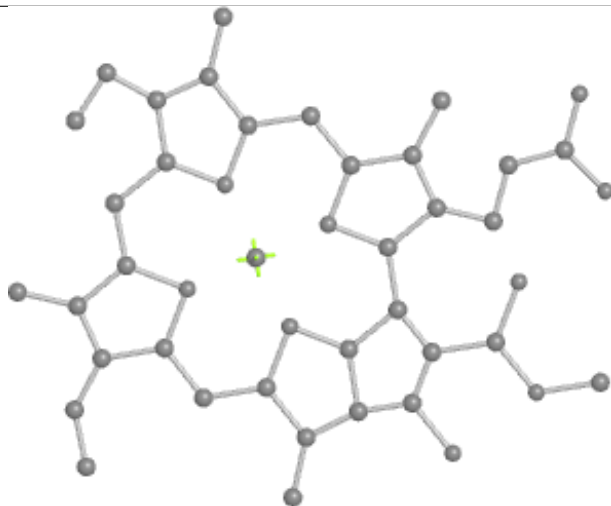
Bond lengths



Bond angles

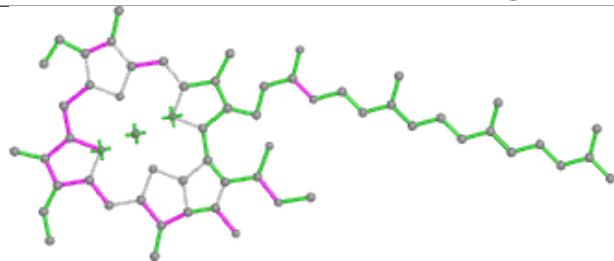


Torsions

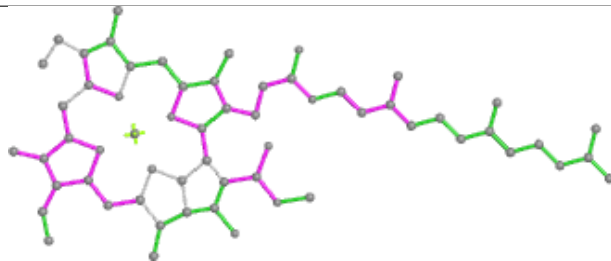


Rings

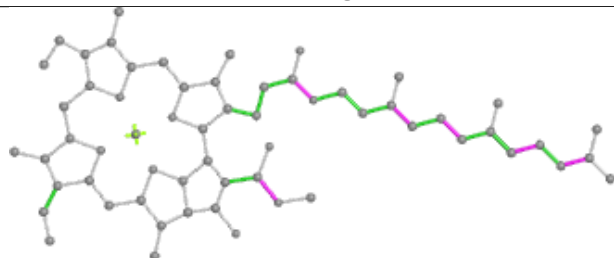
Ligand CLA bB 837



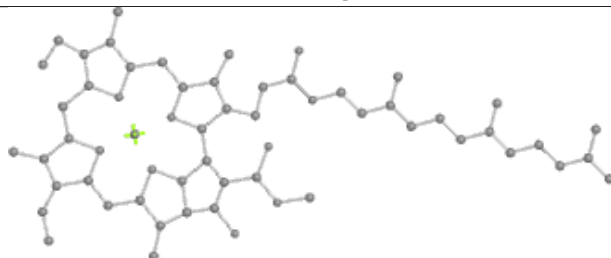
Bond lengths



Bond angles

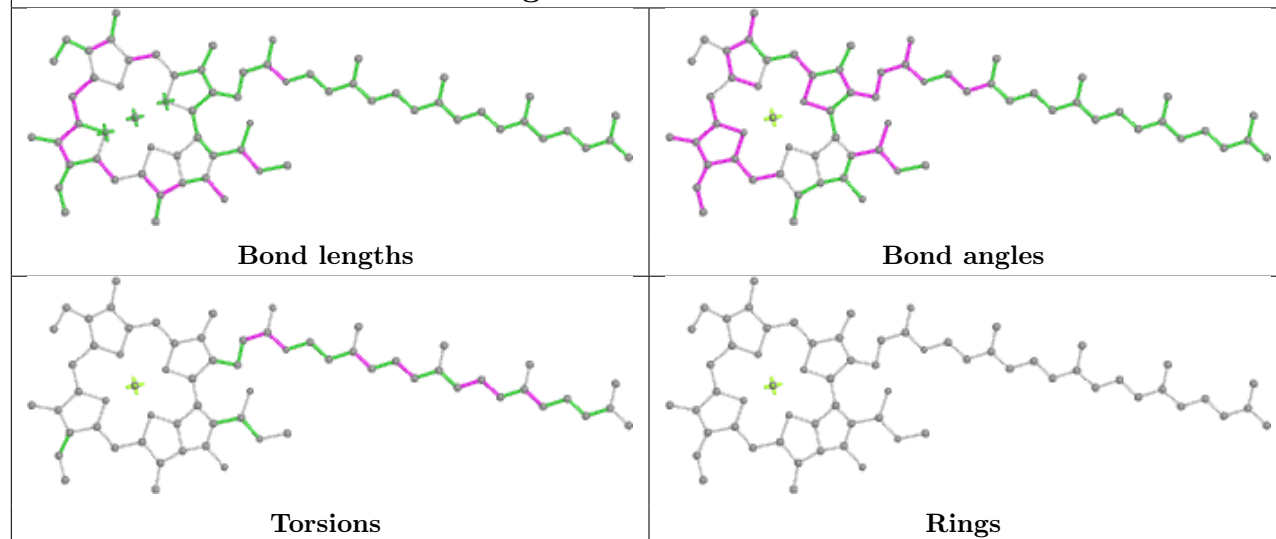


Torsions

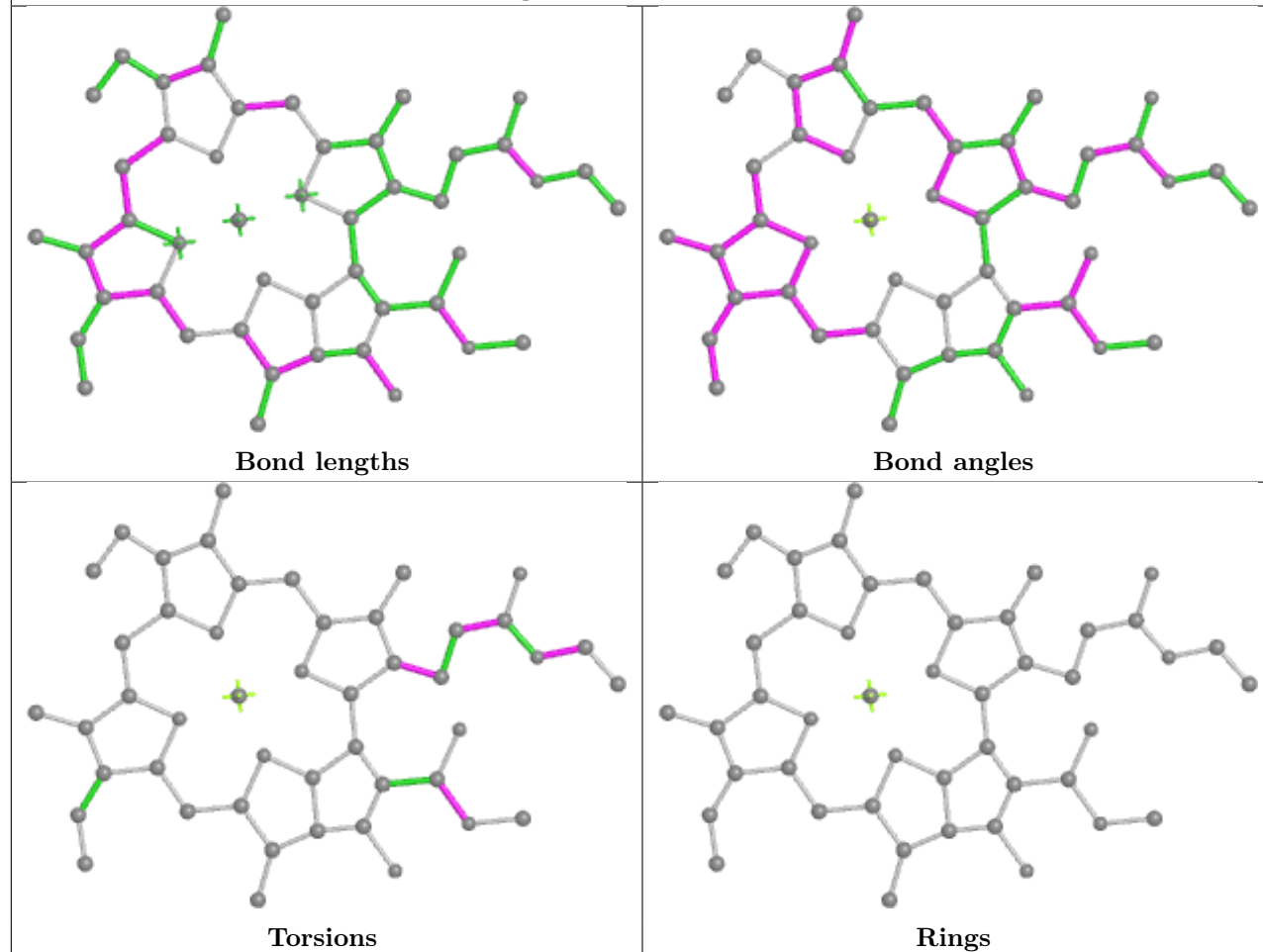


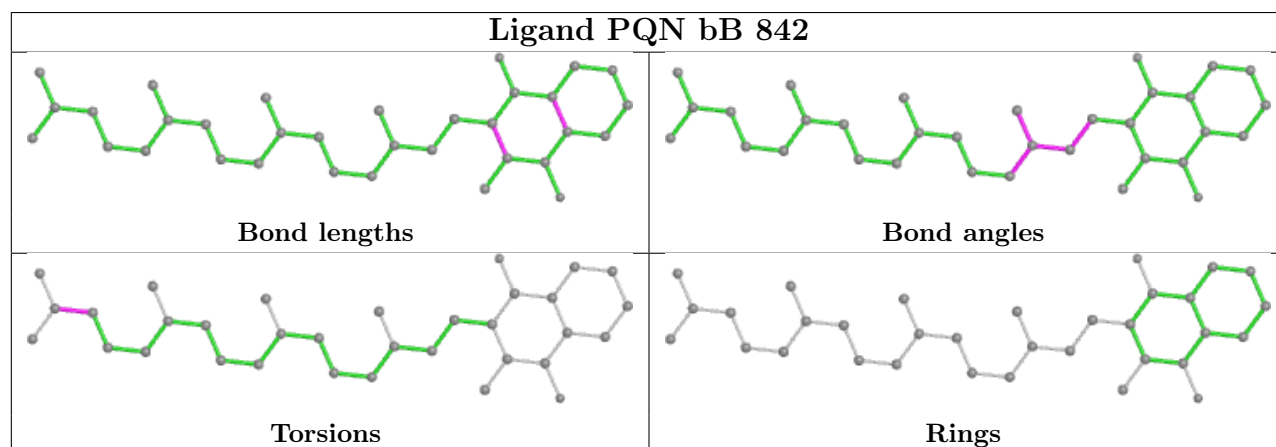
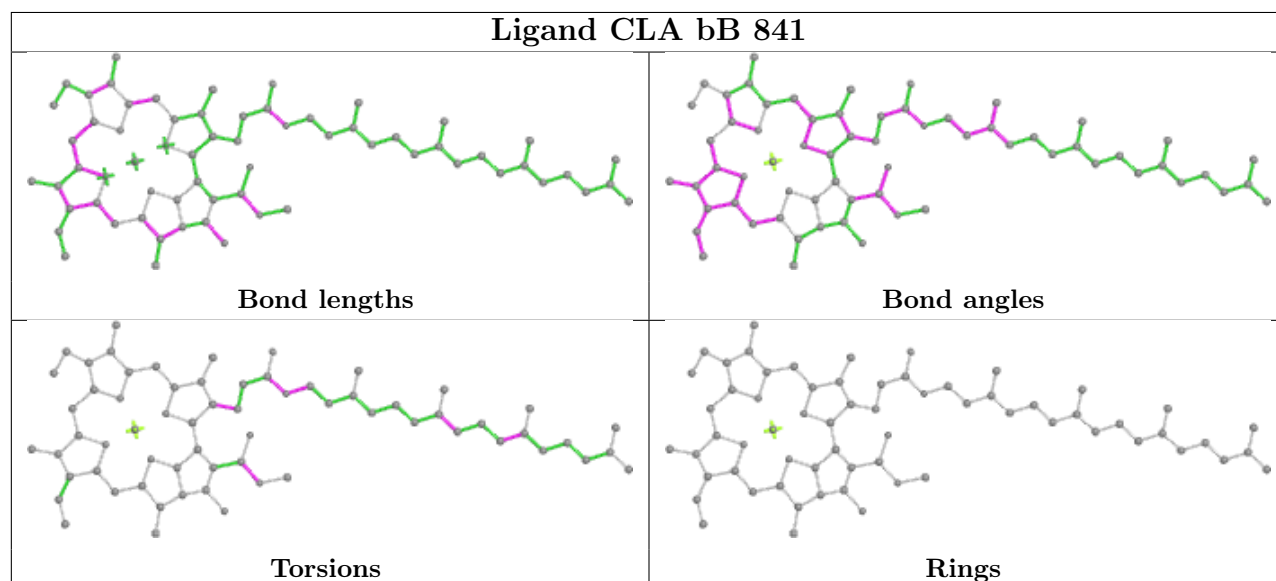
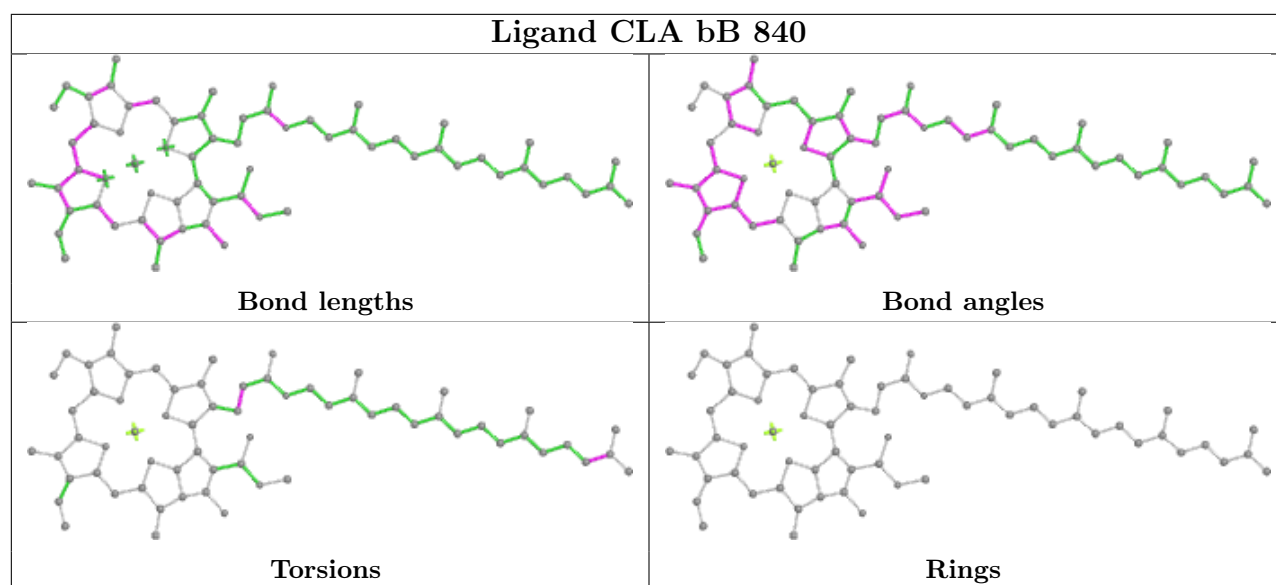
Rings

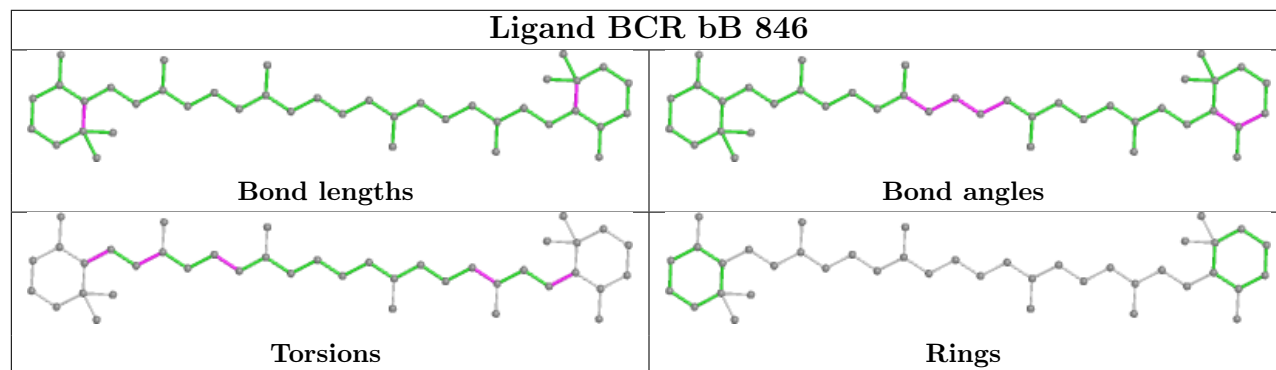
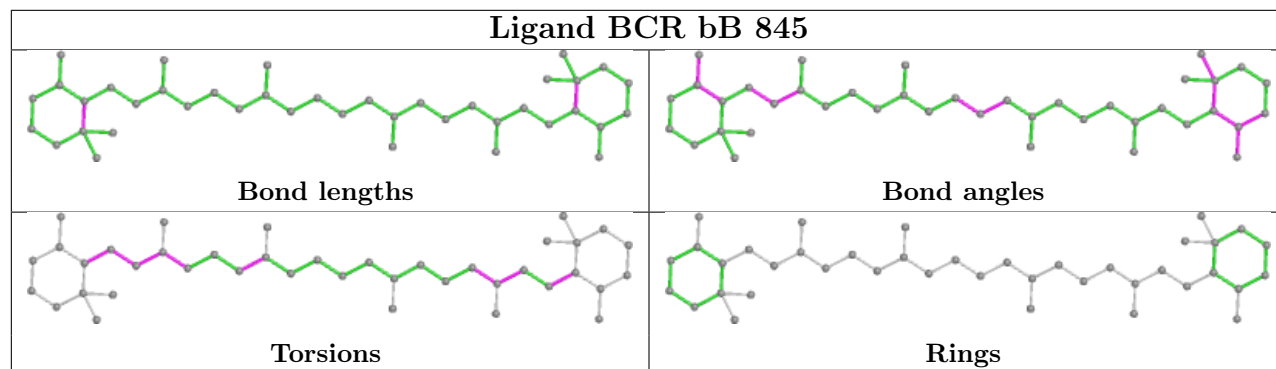
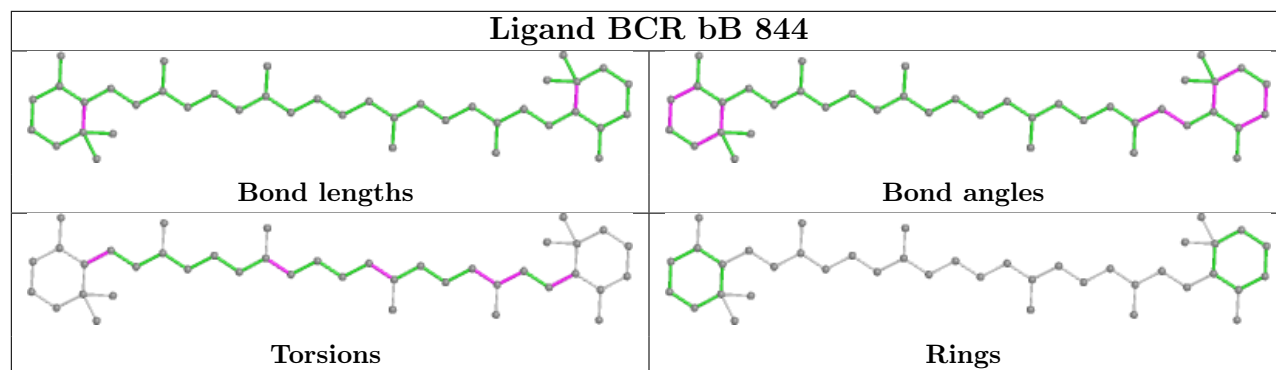
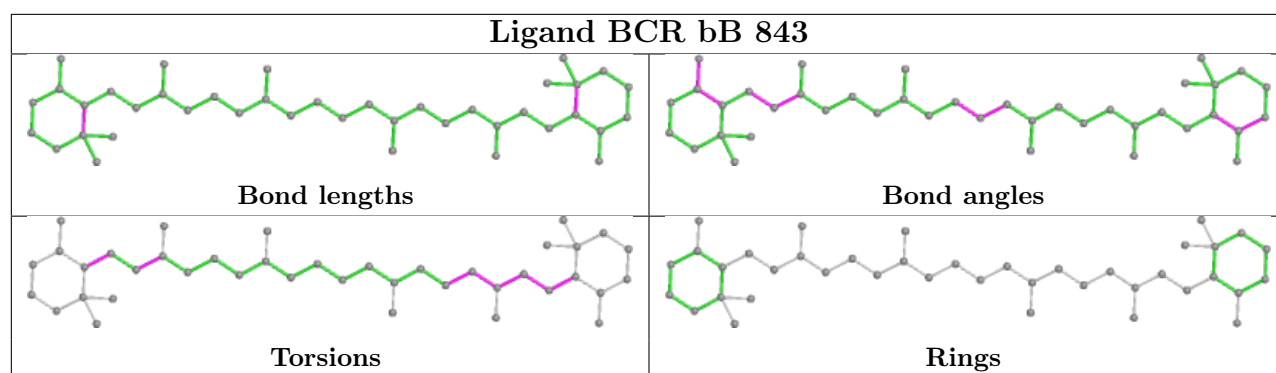
Ligand CLA bB 838

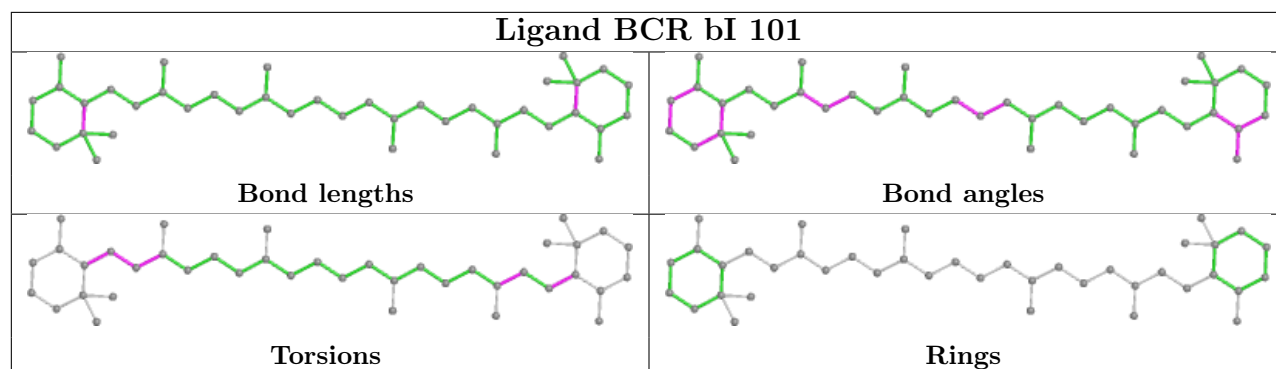
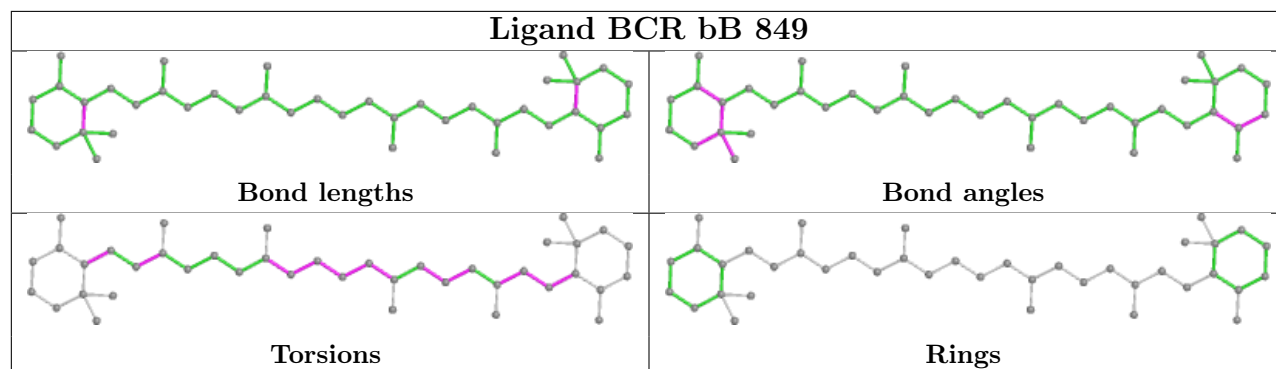
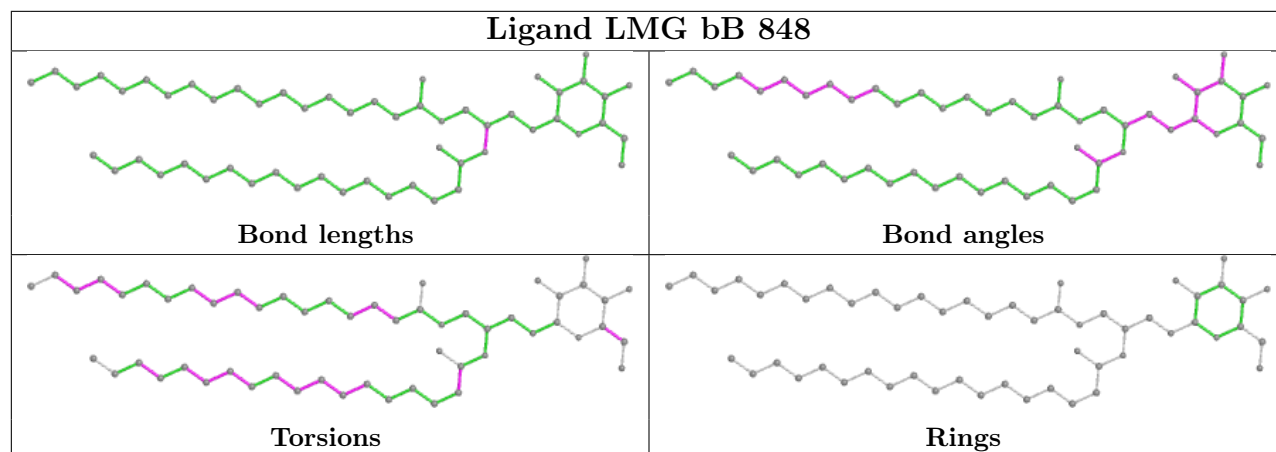
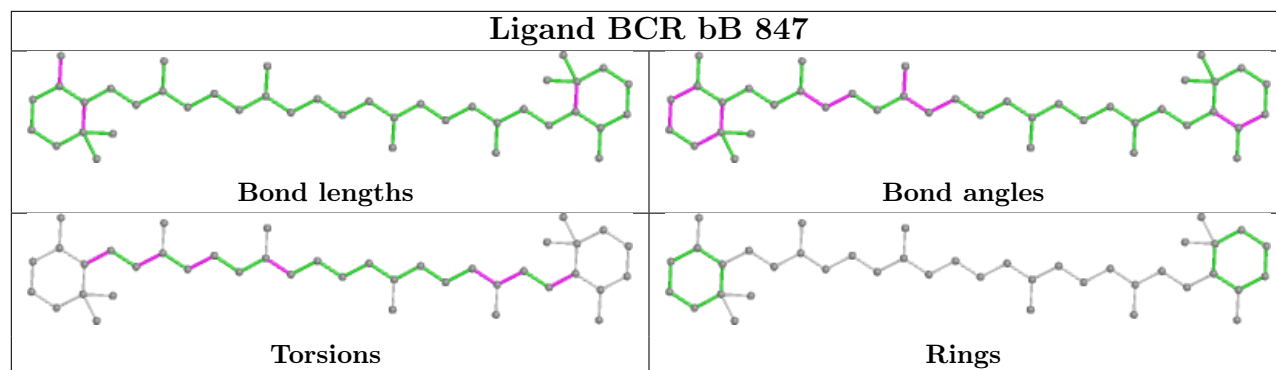


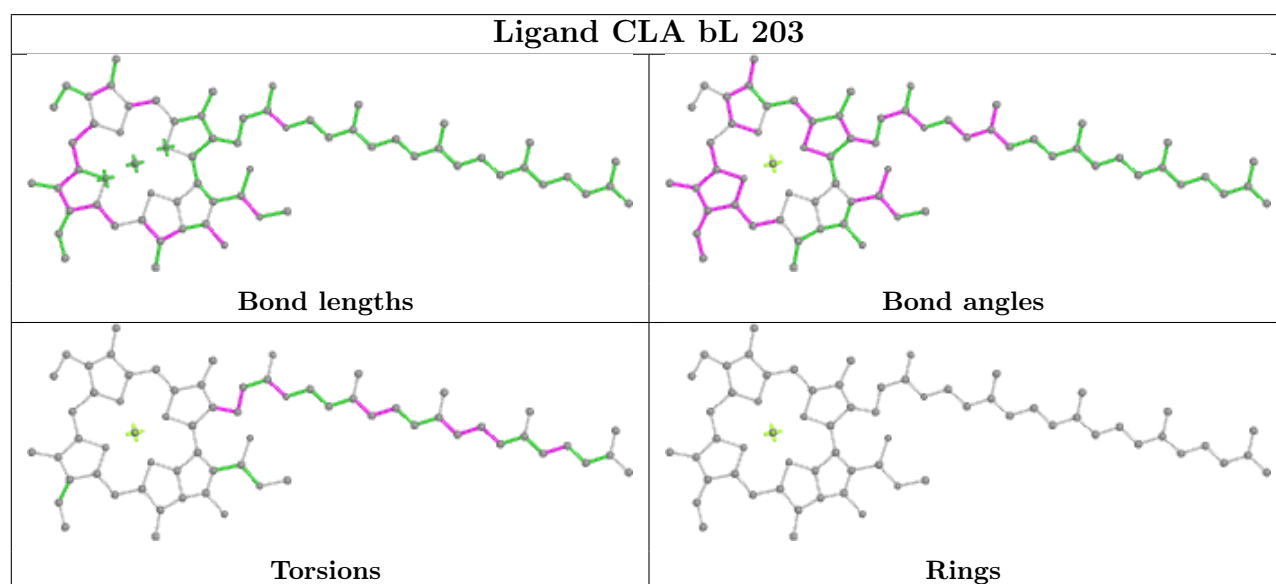
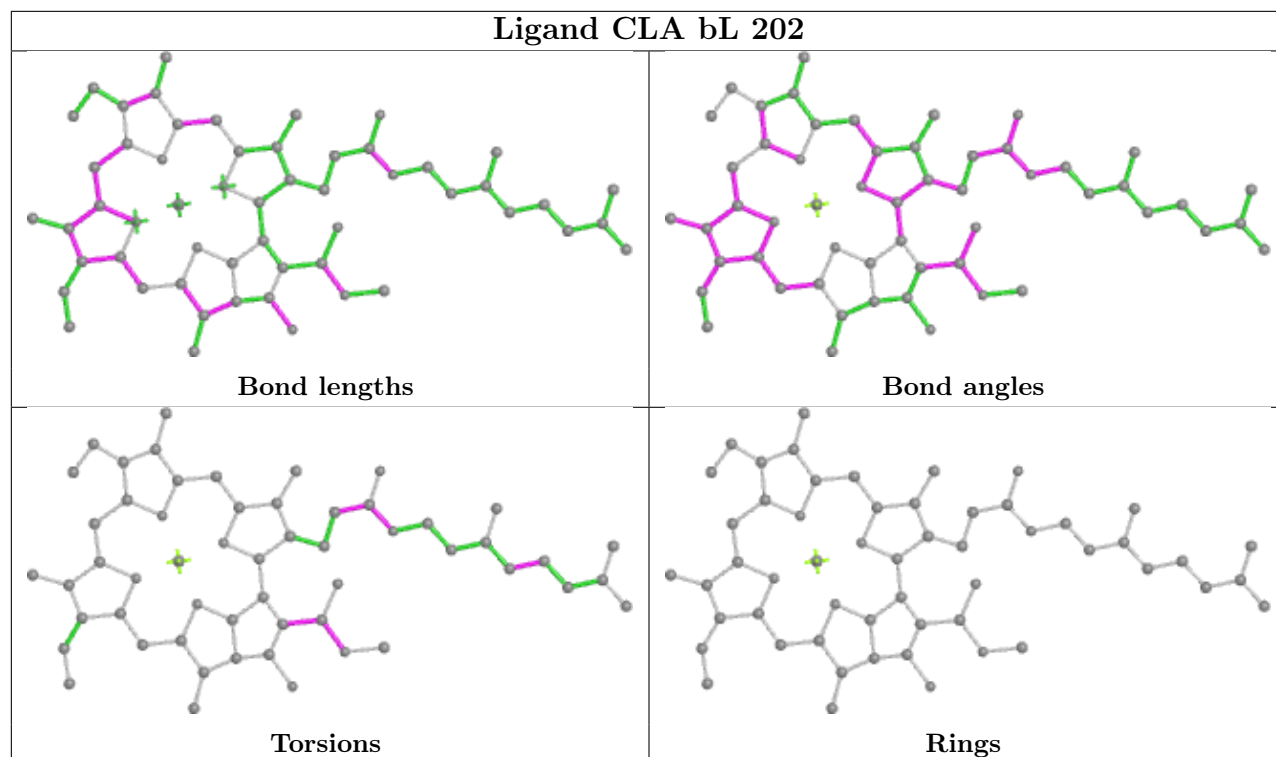
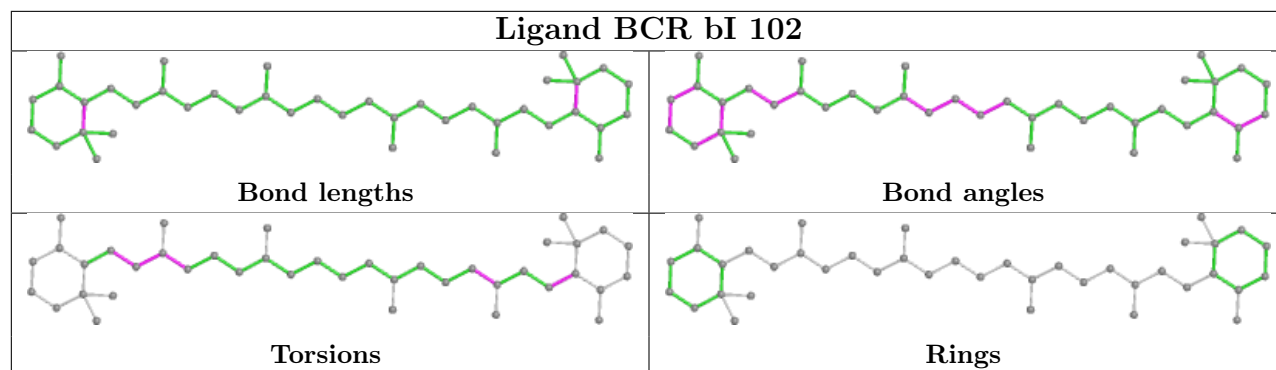
Ligand CLA bB 839

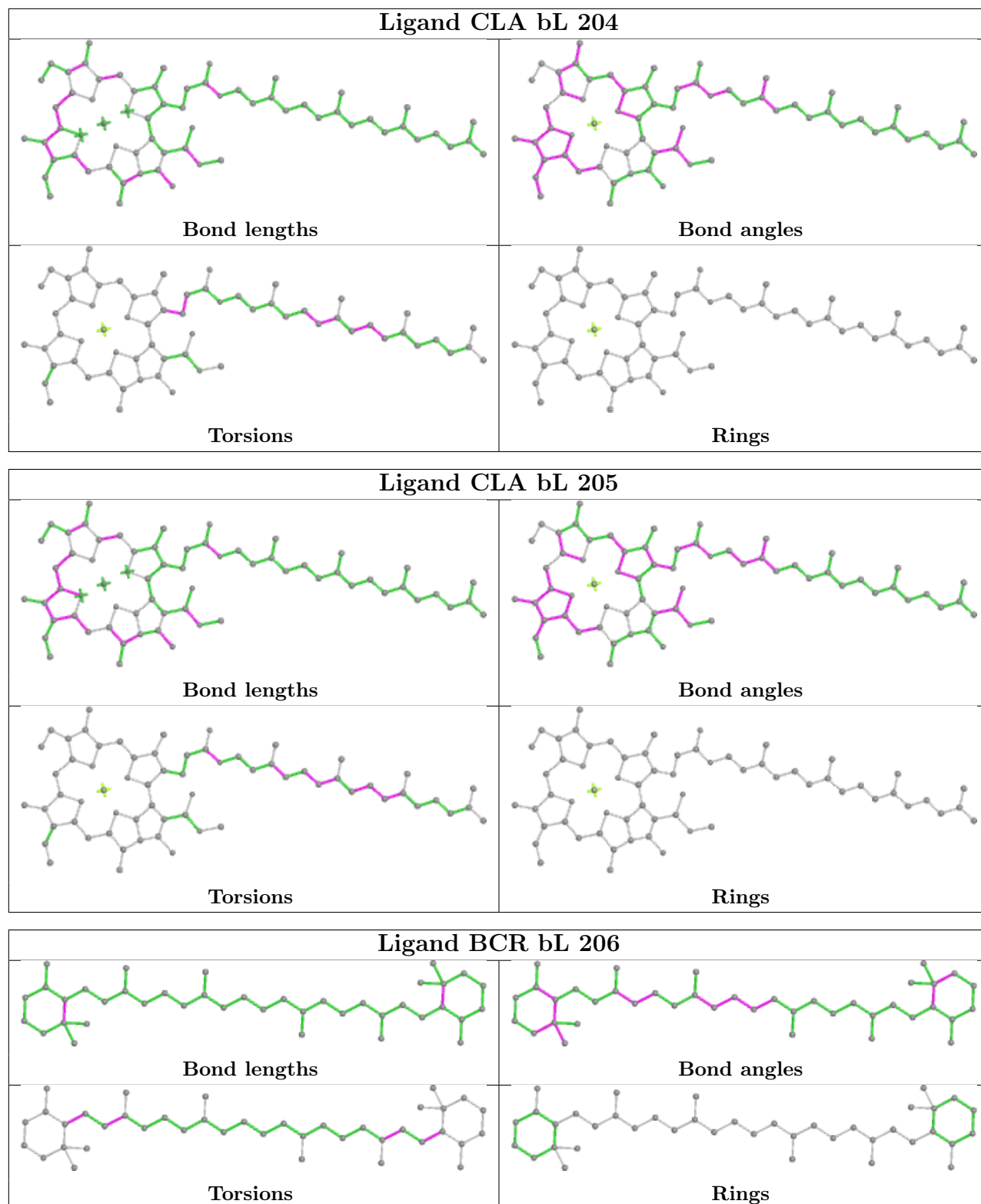


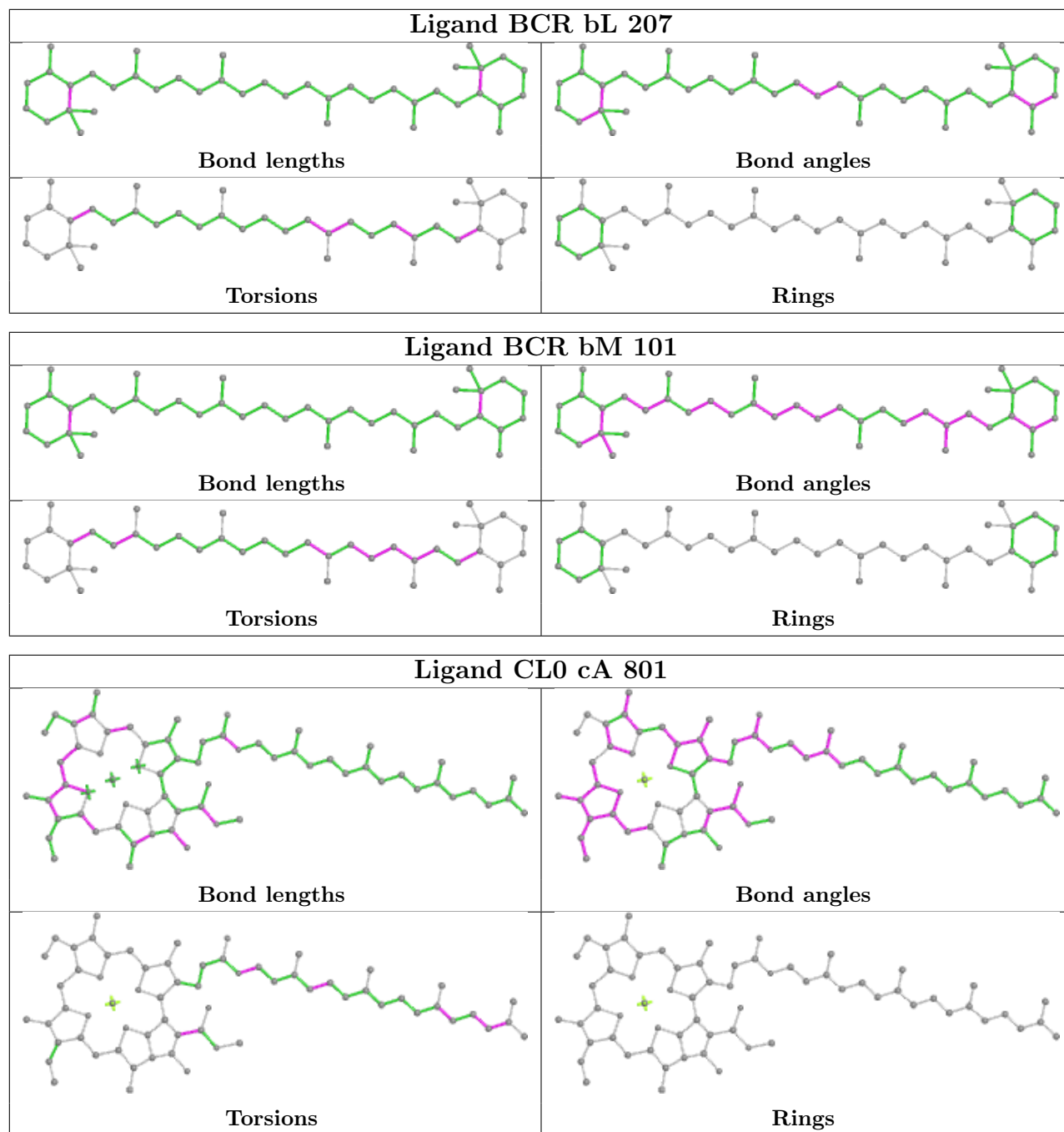




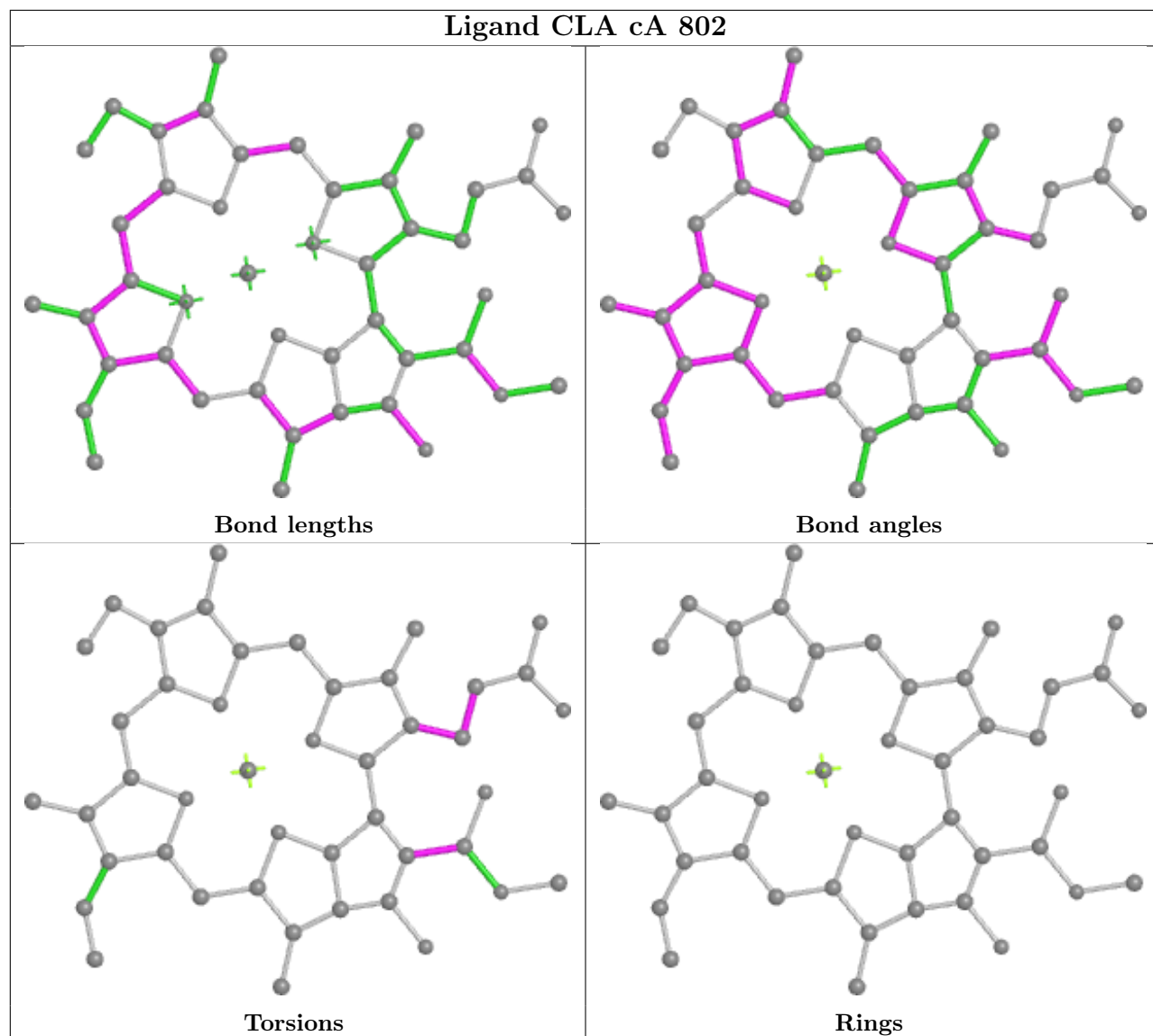




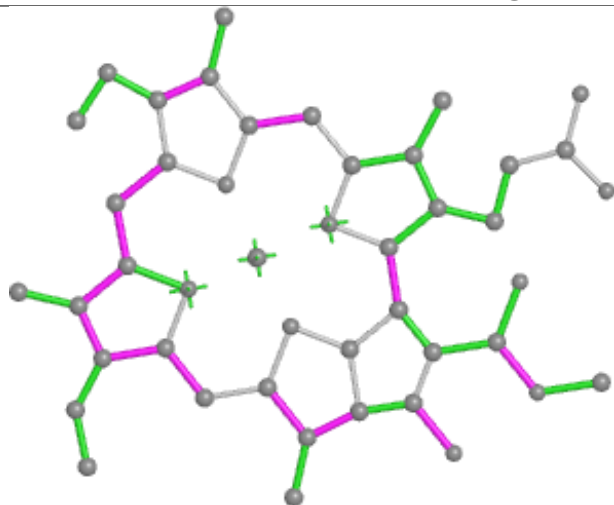




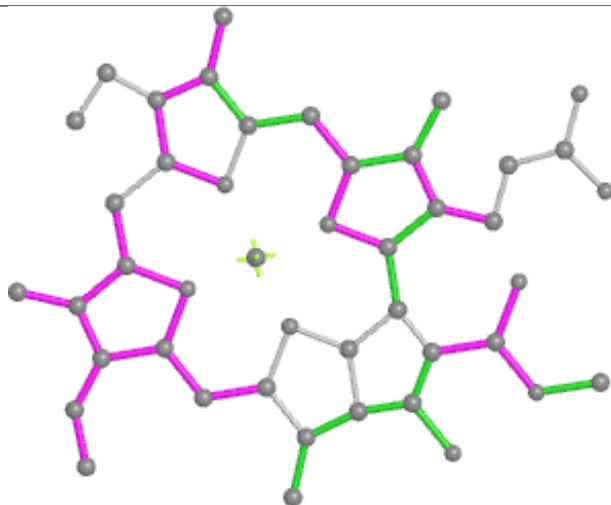
Ligand CLA cA 802



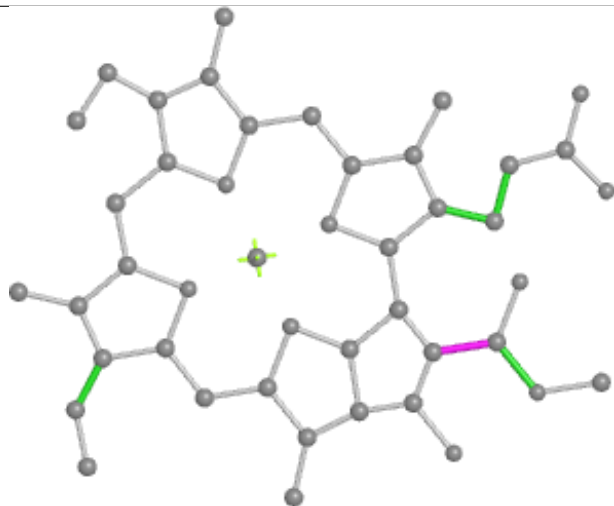
Ligand CLA cA 803



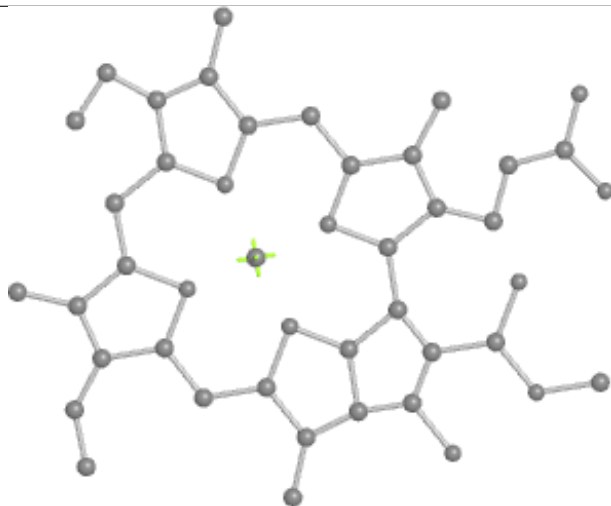
Bond lengths



Bond angles

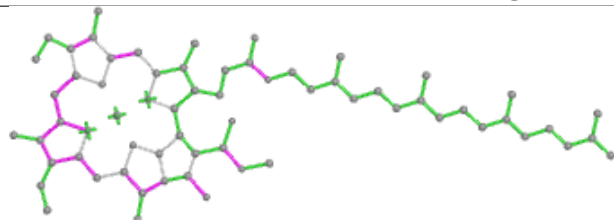


Torsions

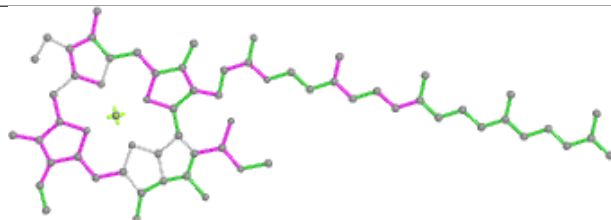


Rings

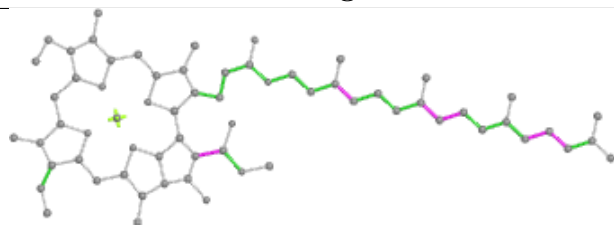
Ligand CLA cA 804



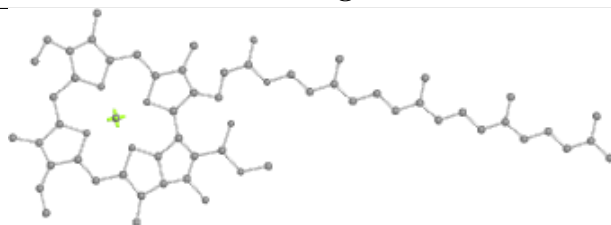
Bond lengths



Bond angles

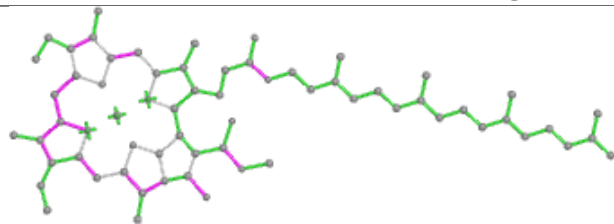


Torsions

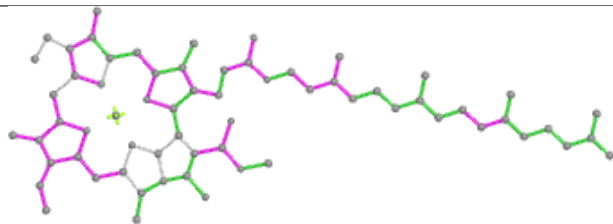


Rings

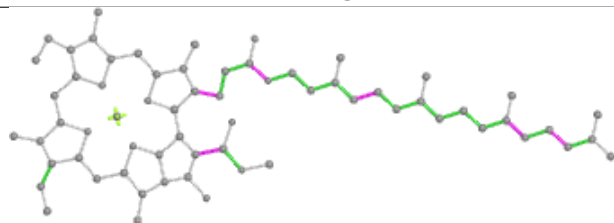
Ligand CLA cA 805



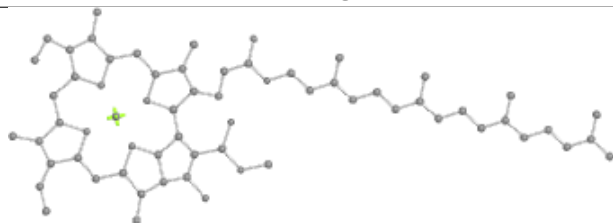
Bond lengths



Bond angles

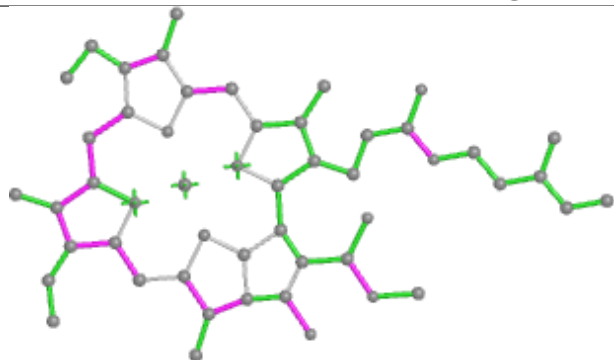


Torsions

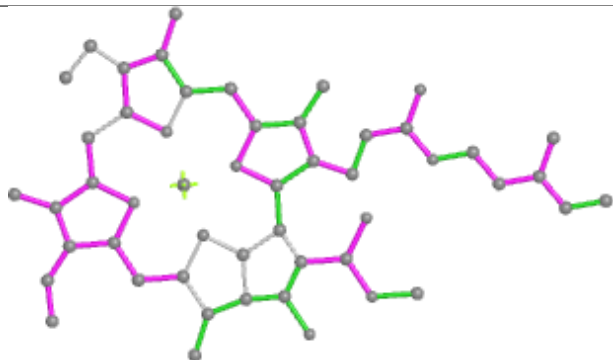


Rings

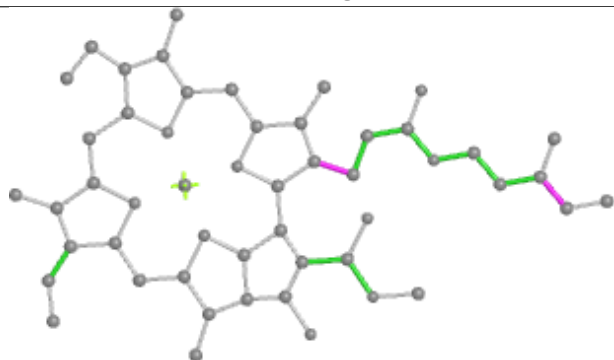
Ligand CLA cA 806



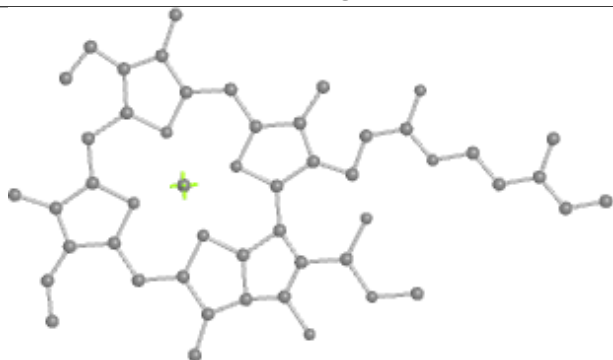
Bond lengths



Bond angles

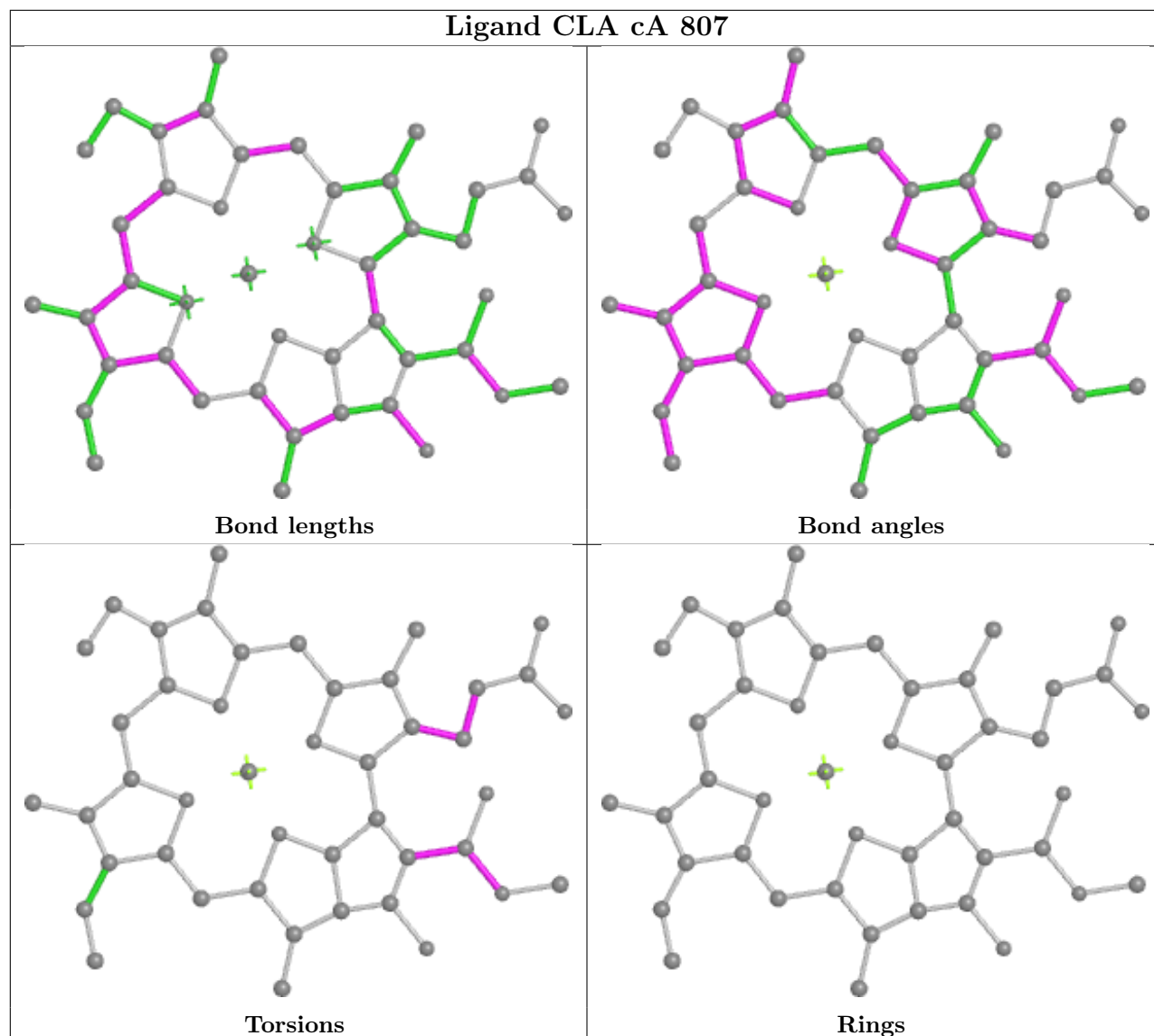


Torsions

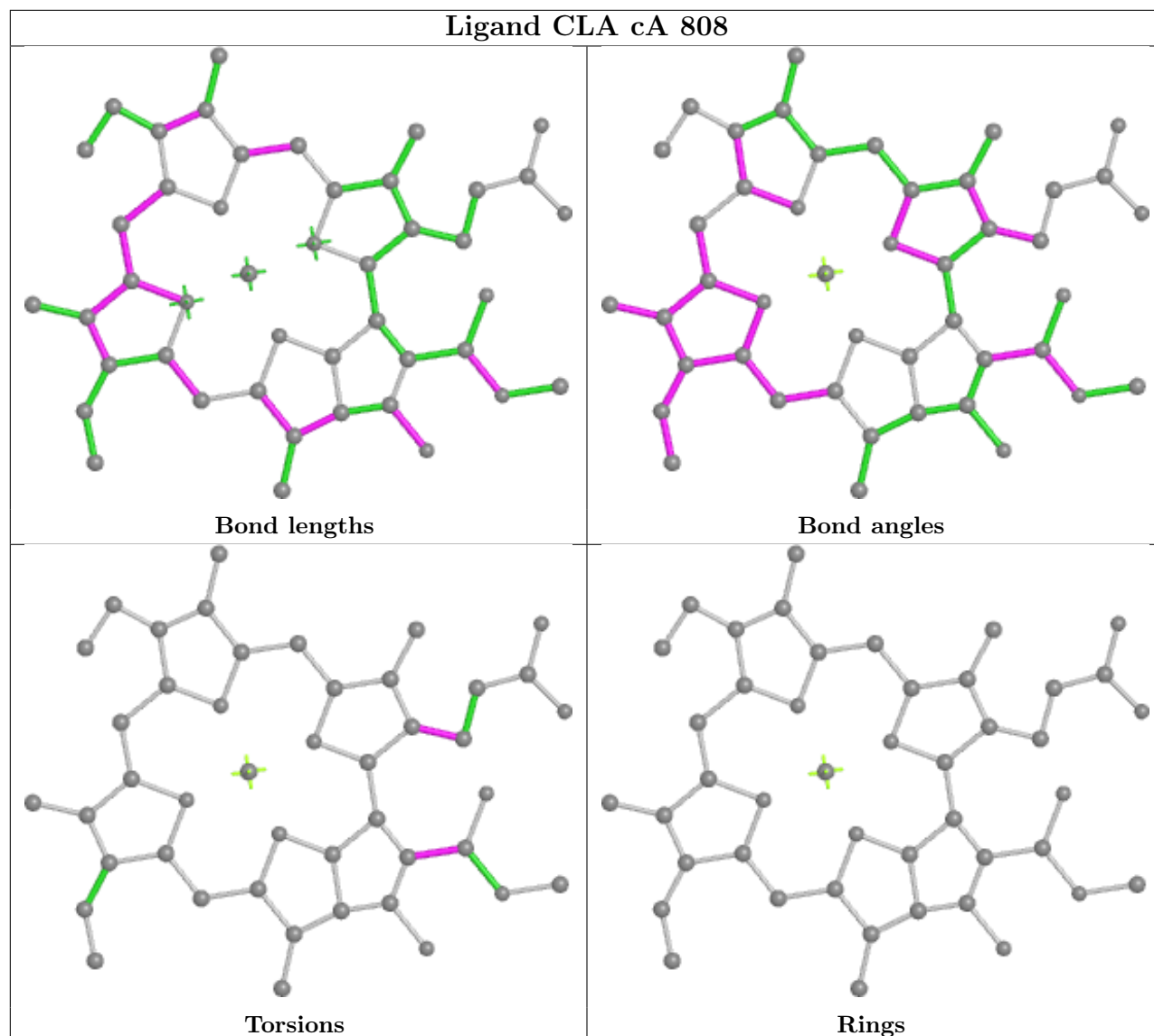


Rings

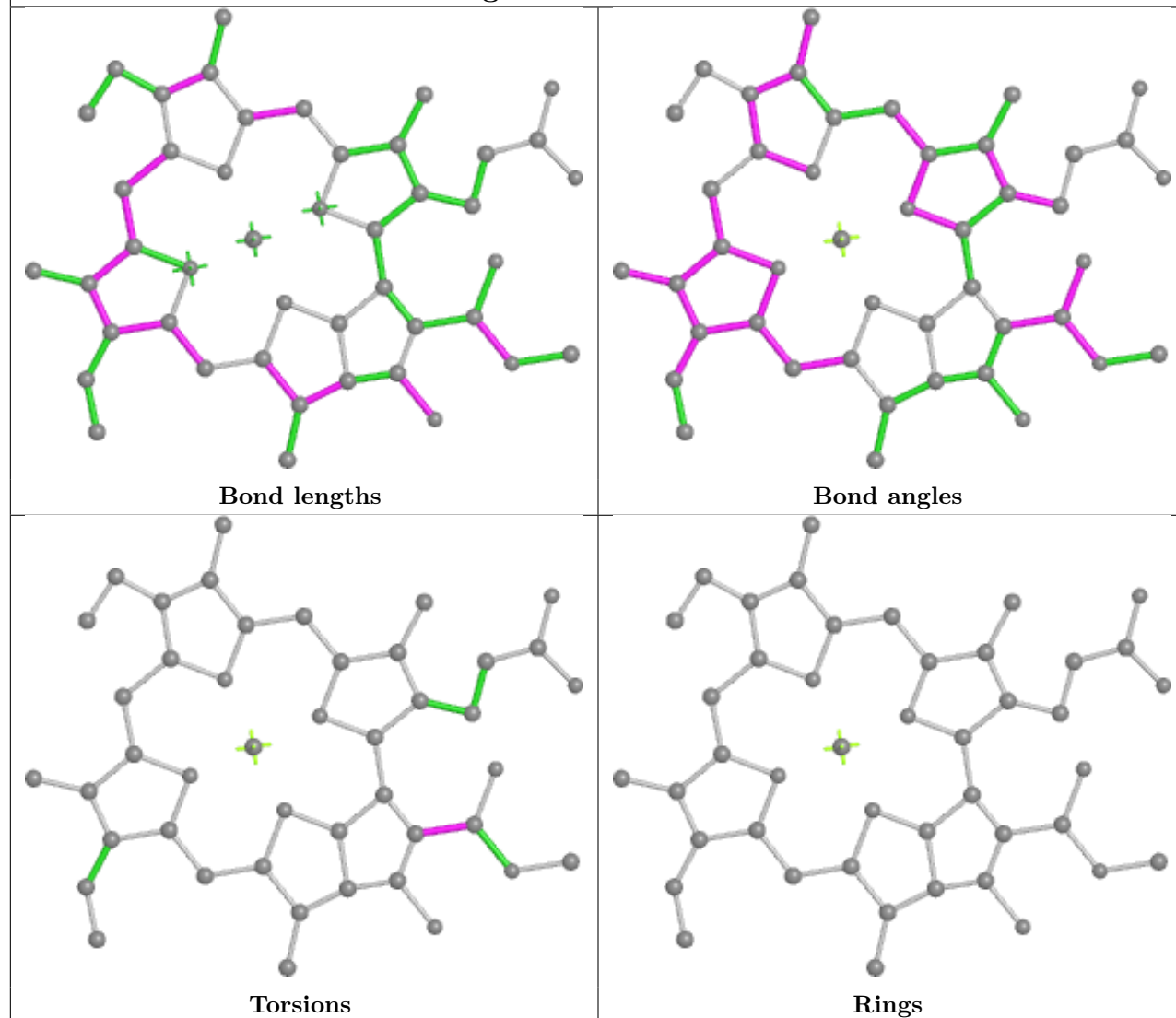
Ligand CLA cA 807



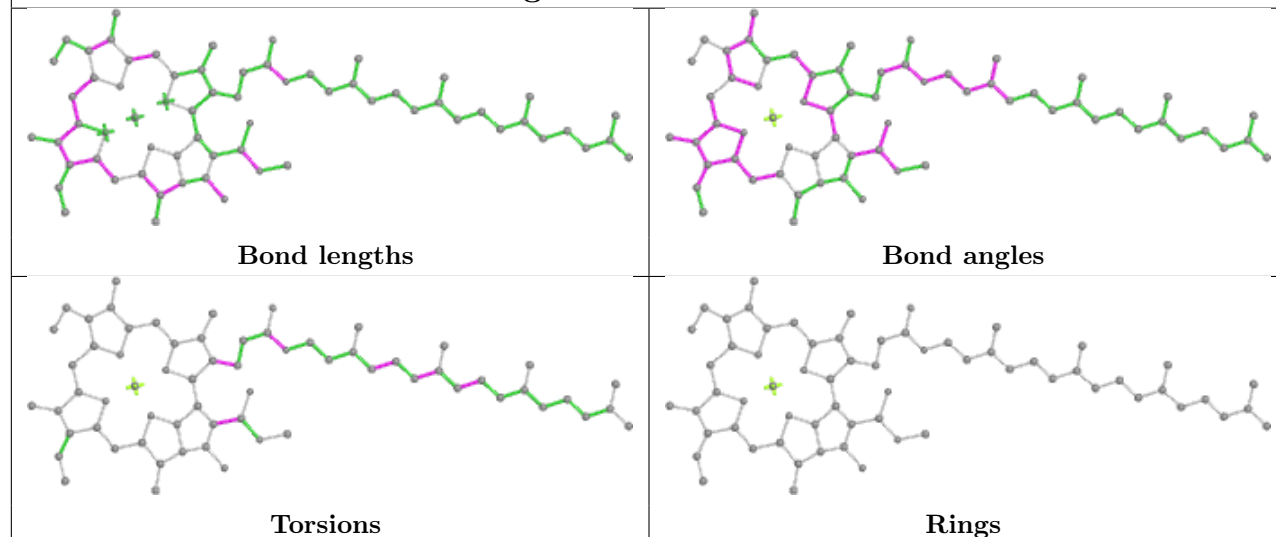
Ligand CLA cA 808

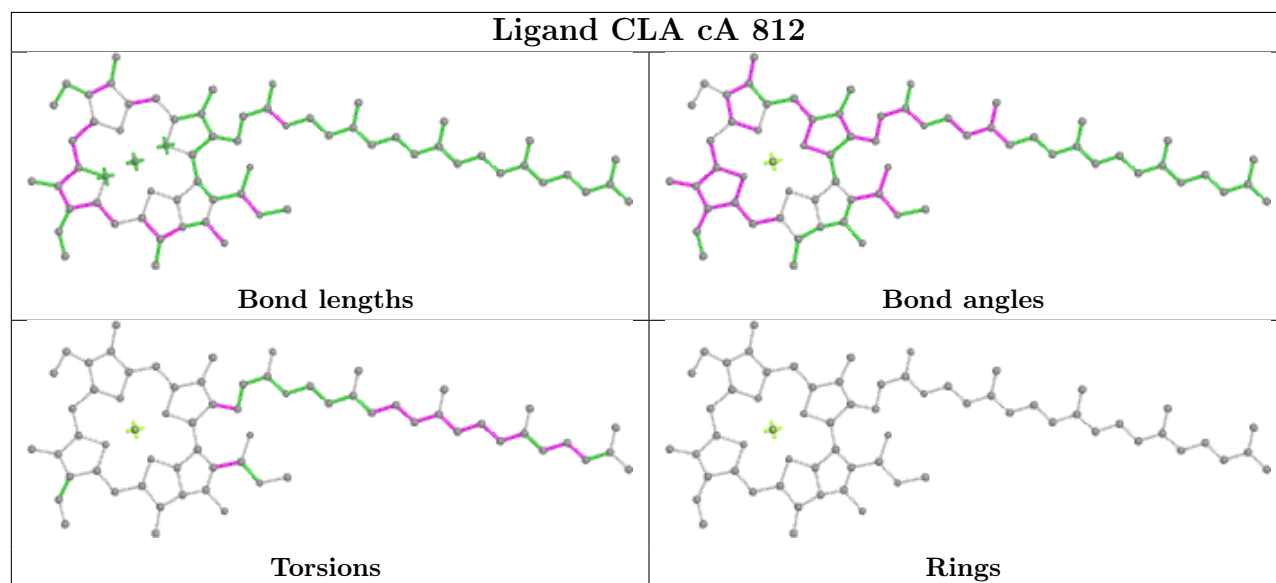
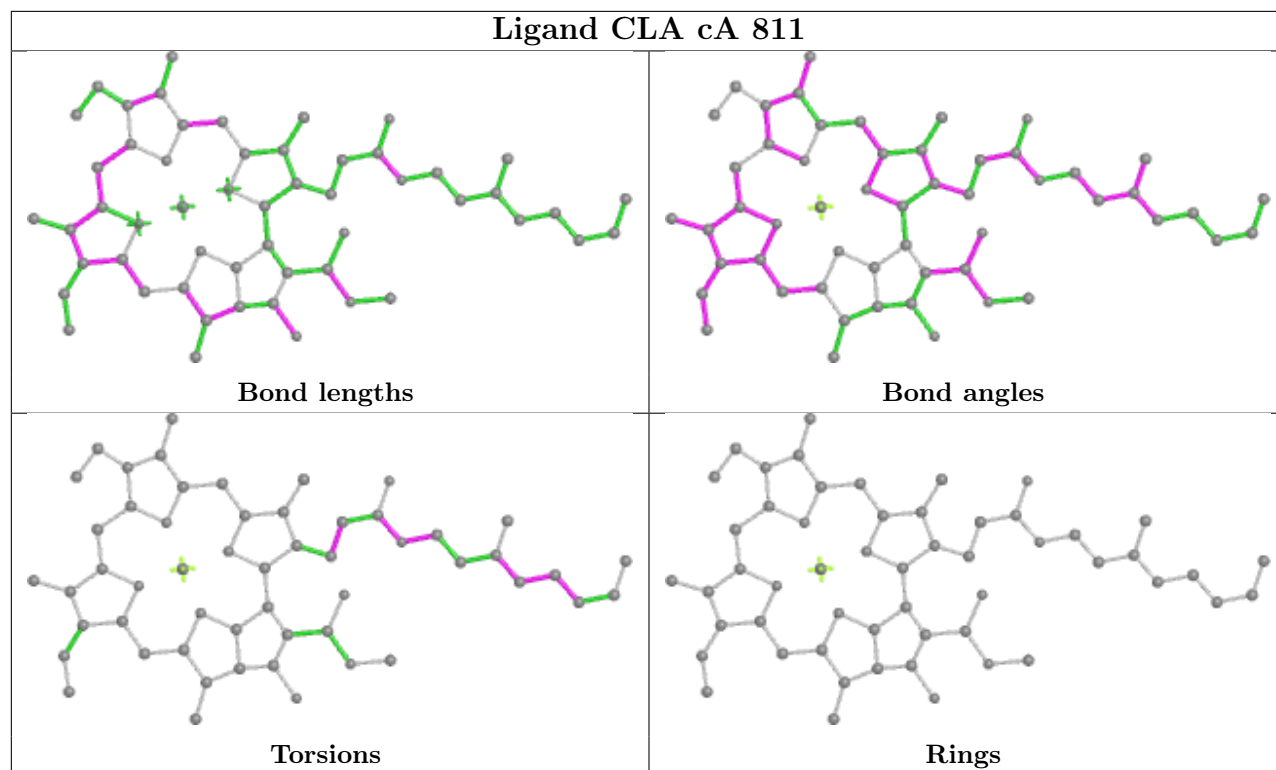


Ligand CLA cA 809

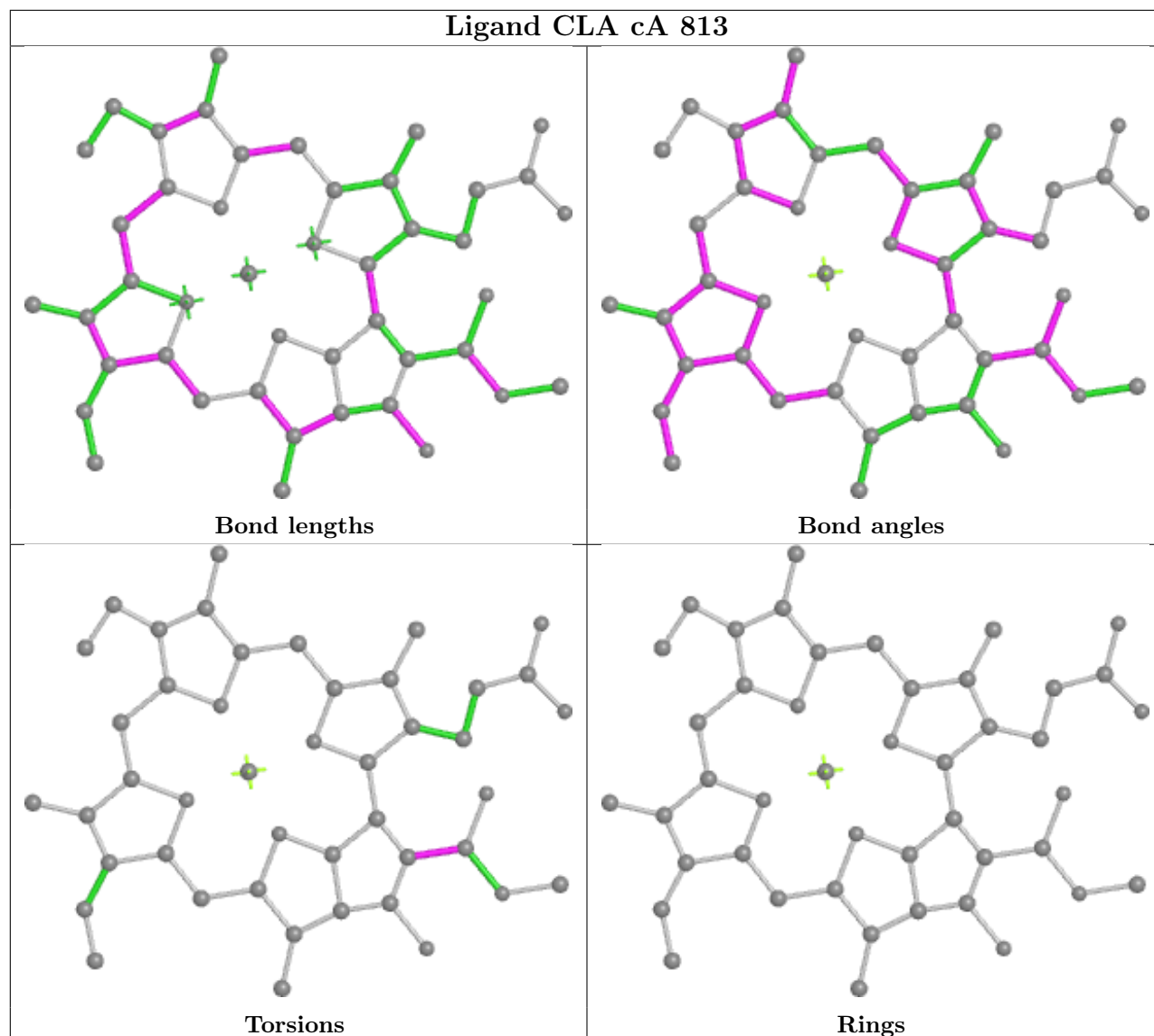


Ligand CLA cA 810

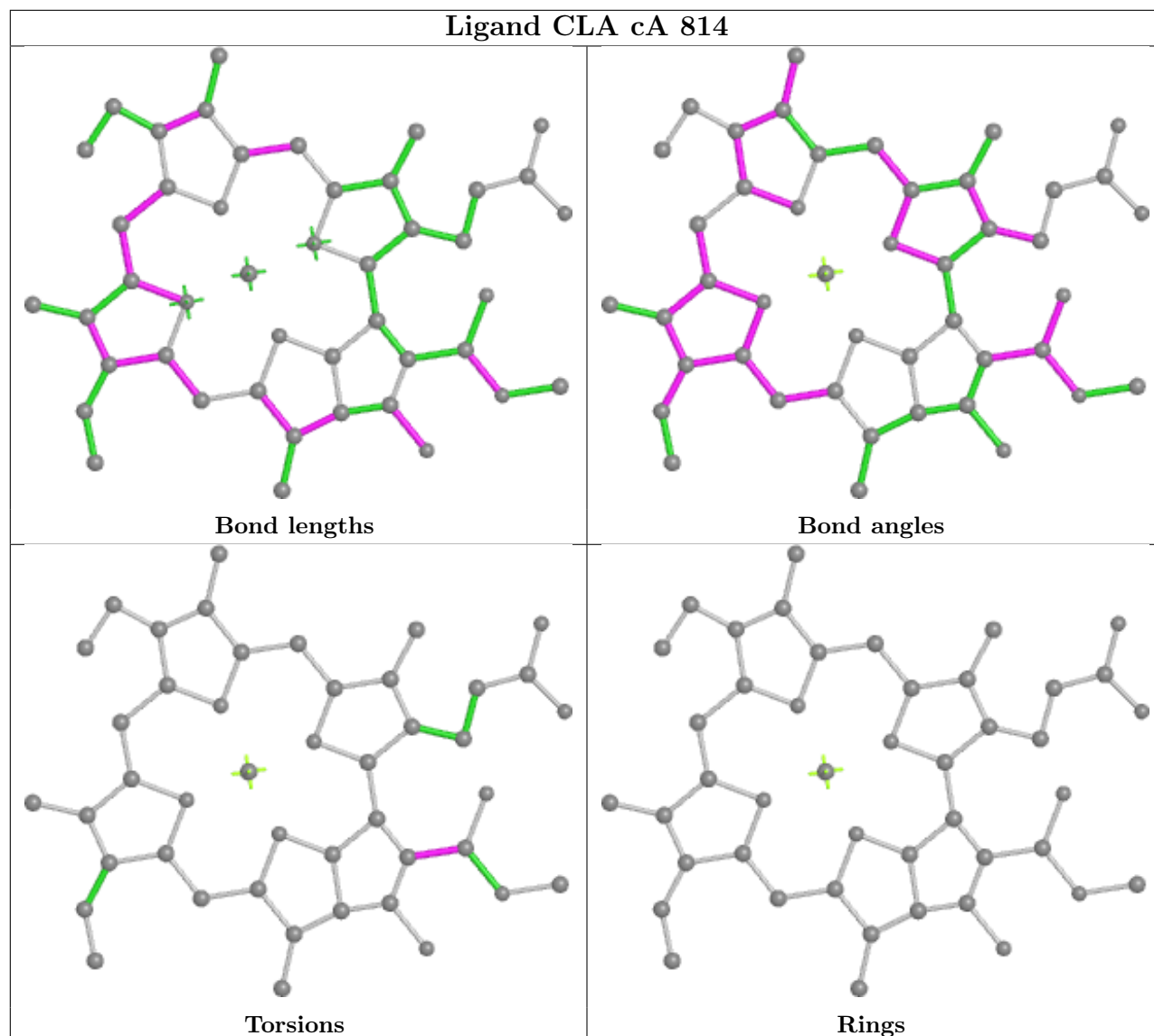


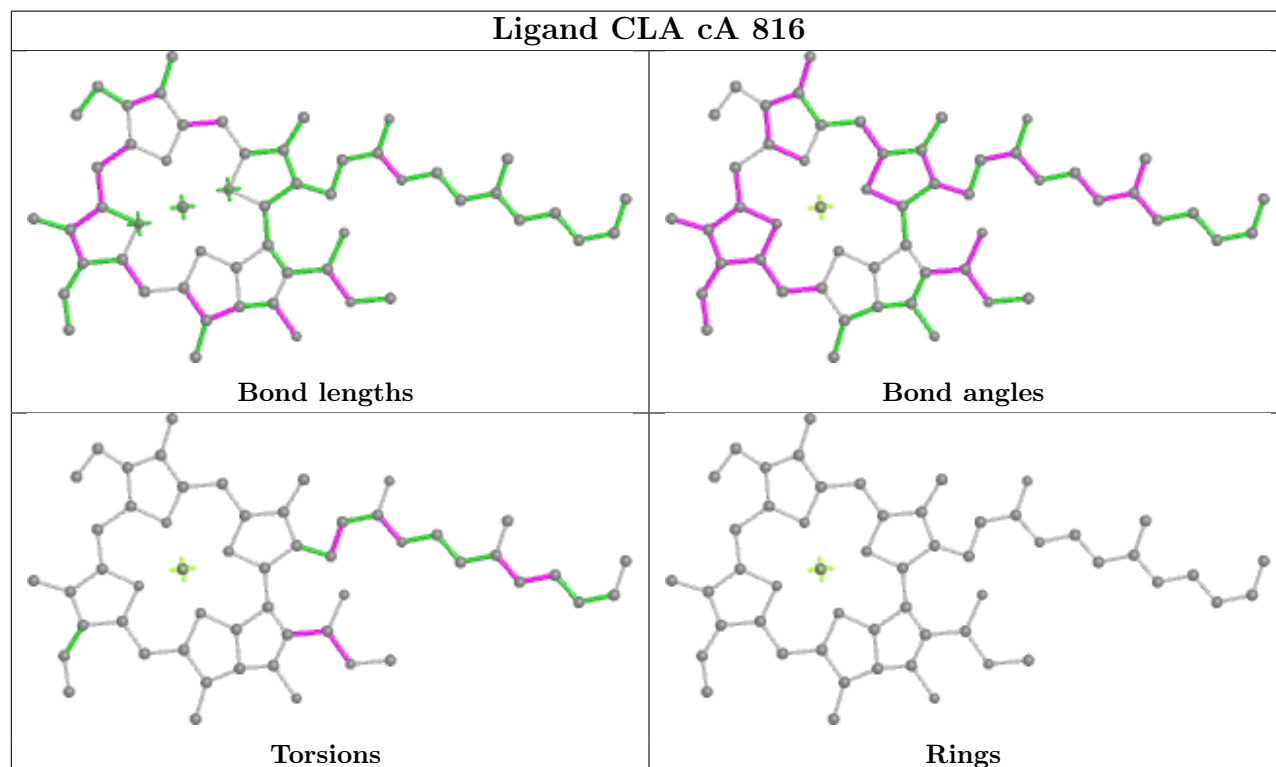
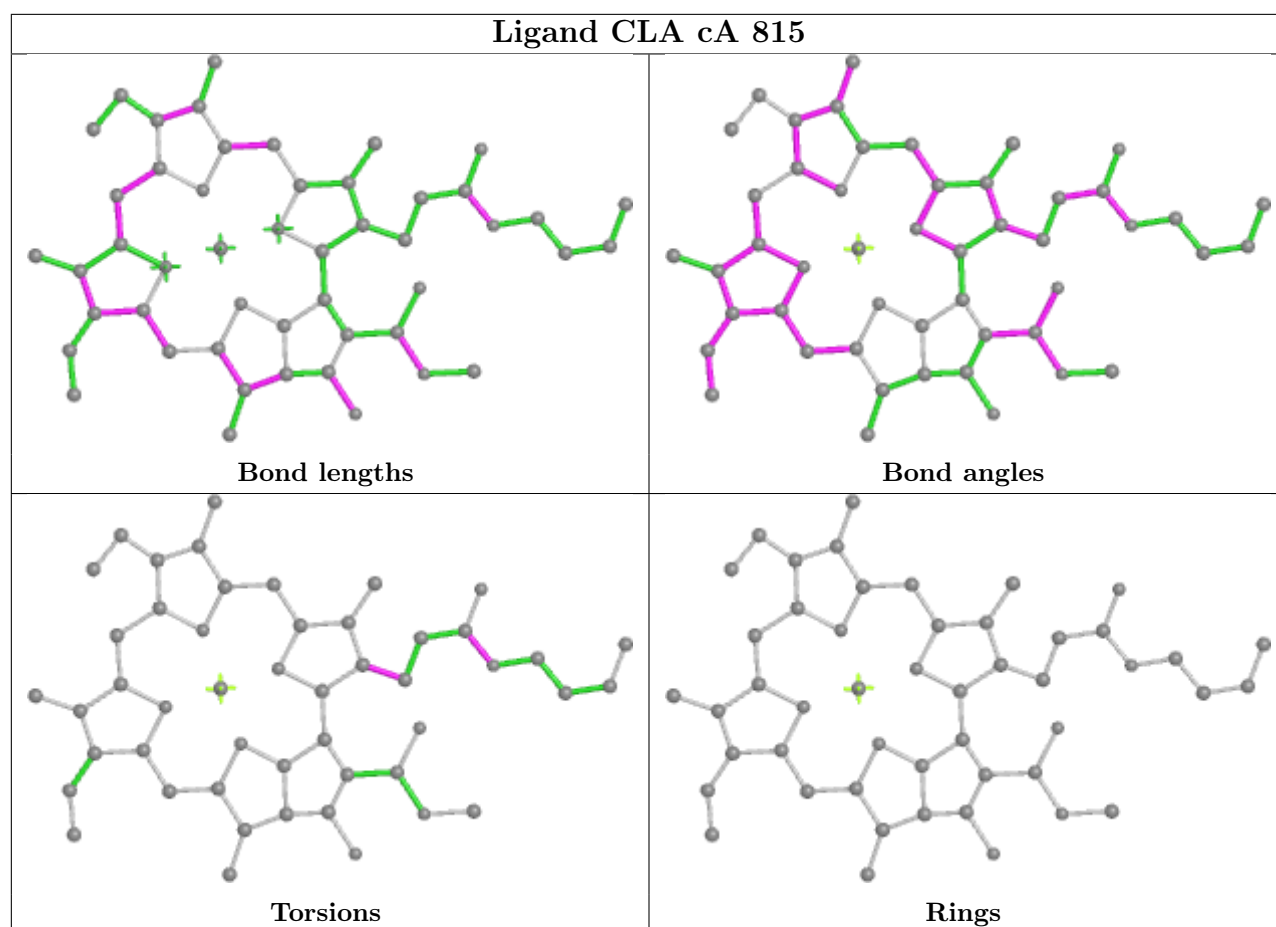


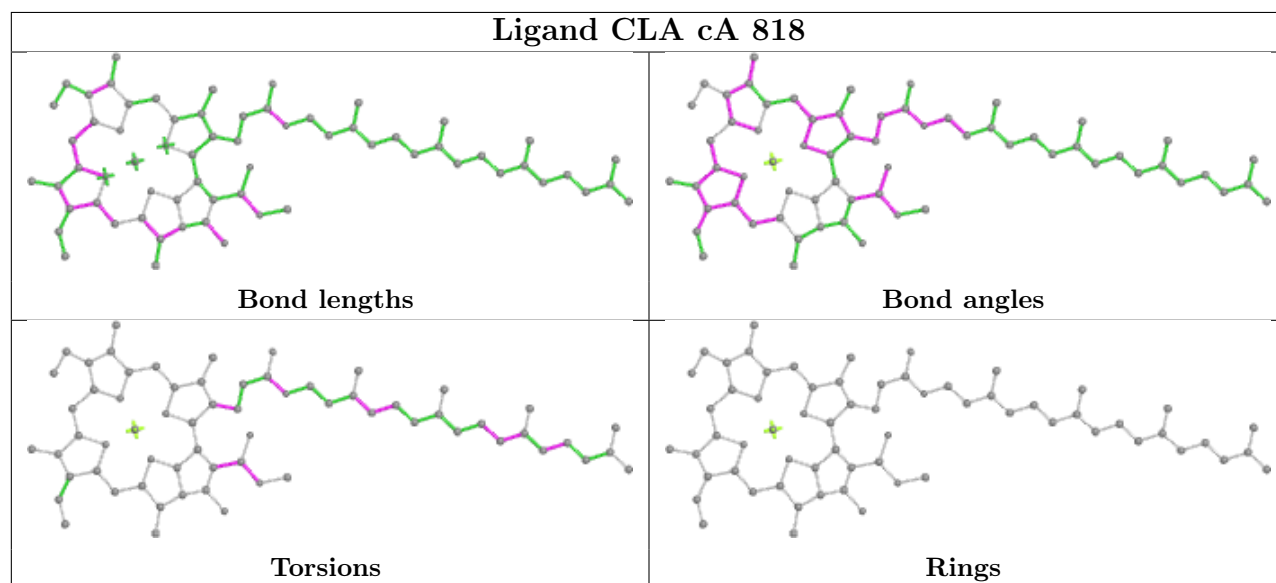
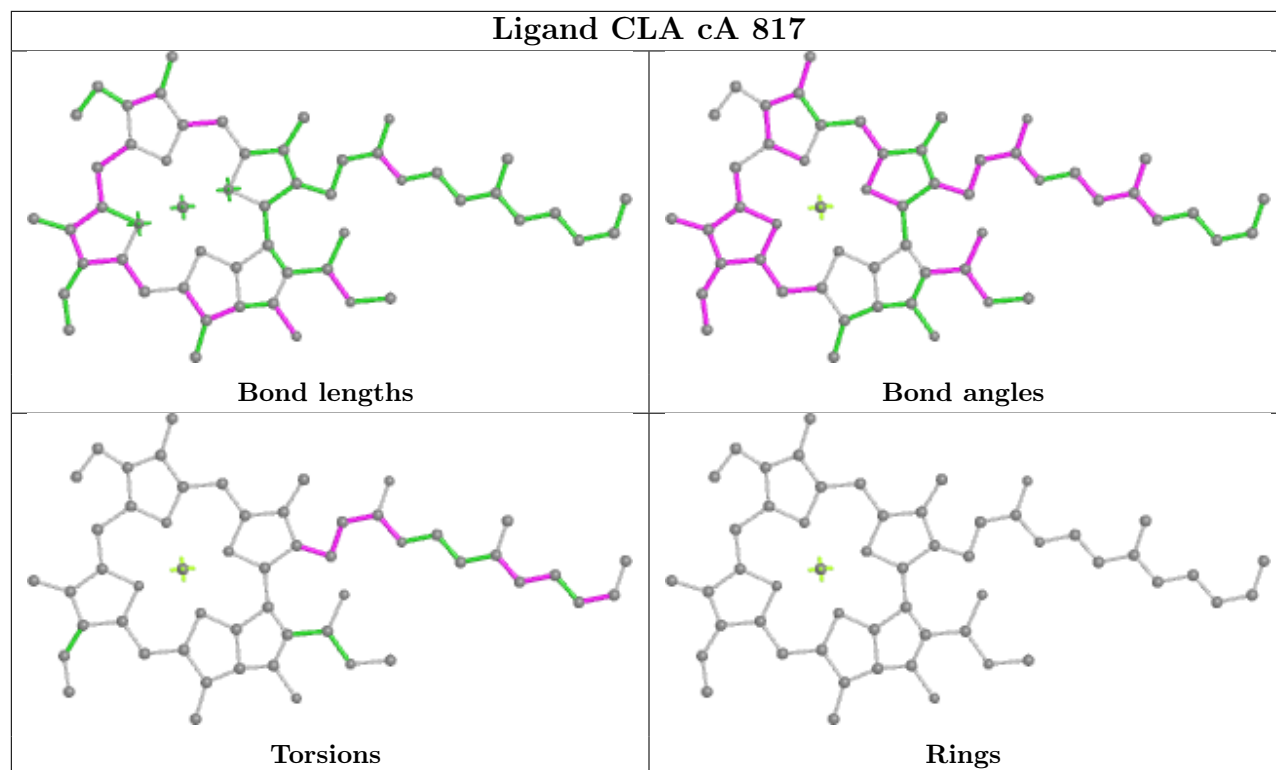
Ligand CLA cA 813

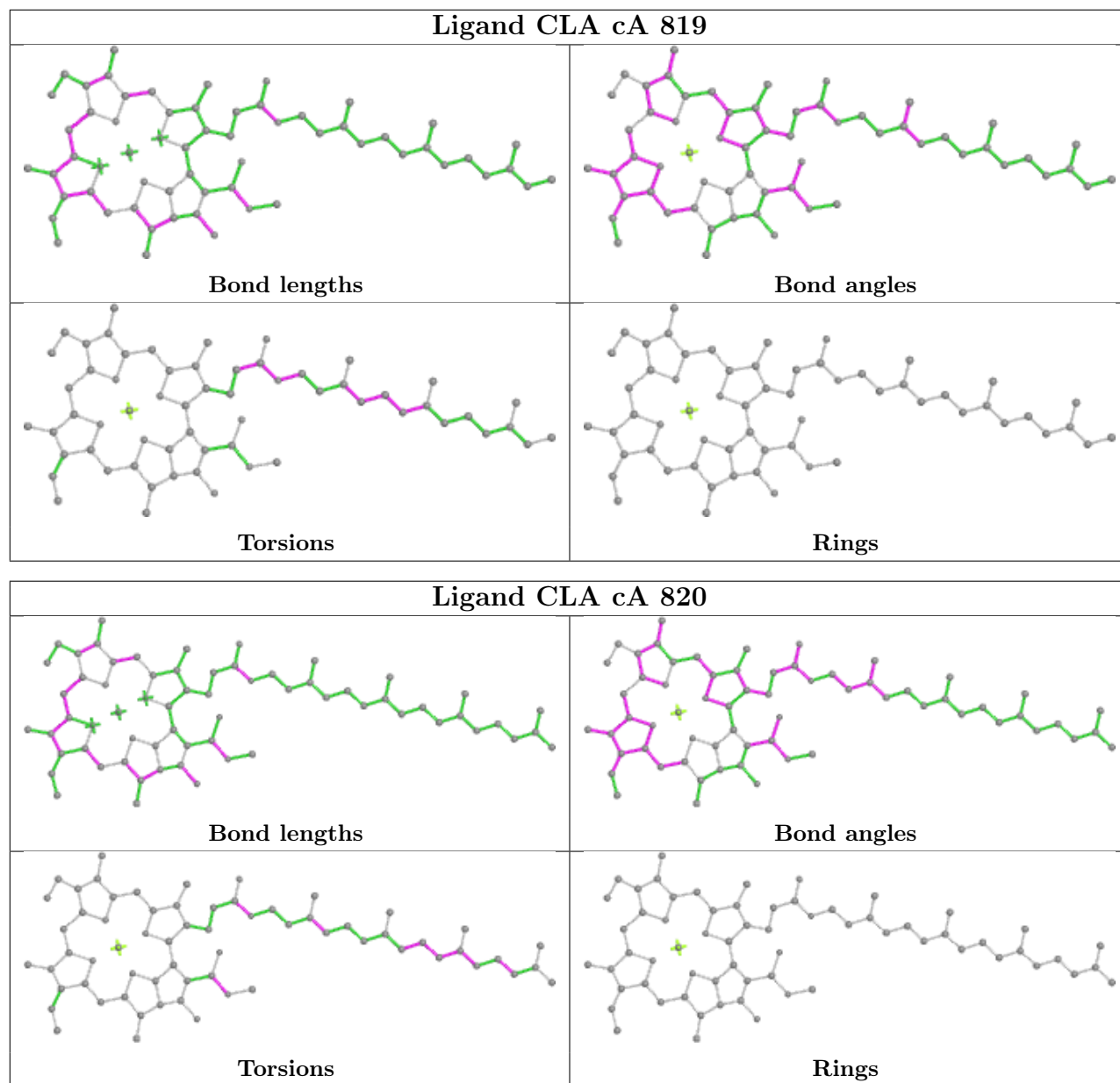


Ligand CLA cA 814

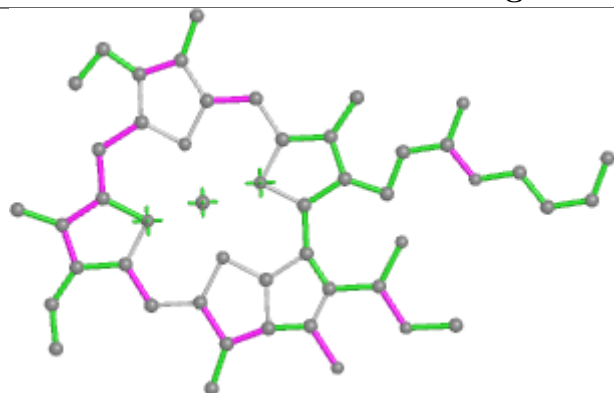




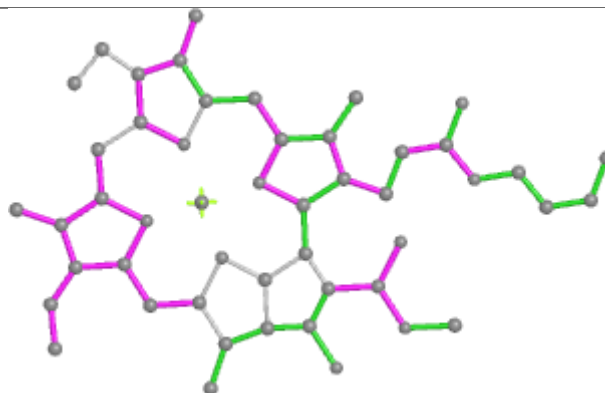




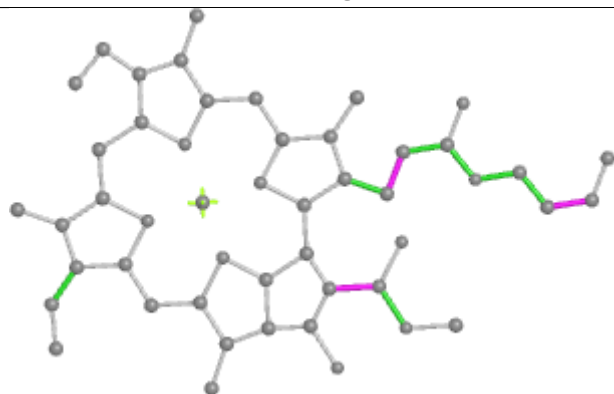
Ligand CLA cA 821



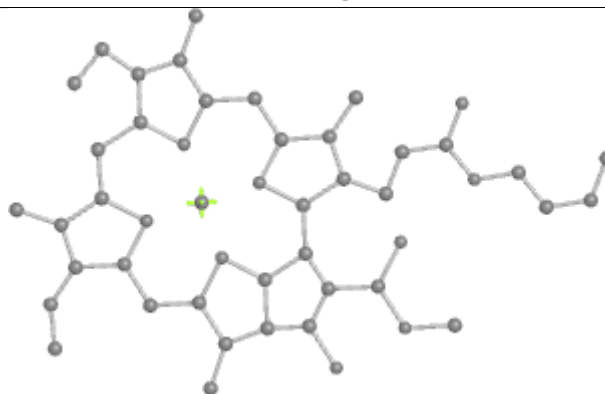
Bond lengths



Bond angles

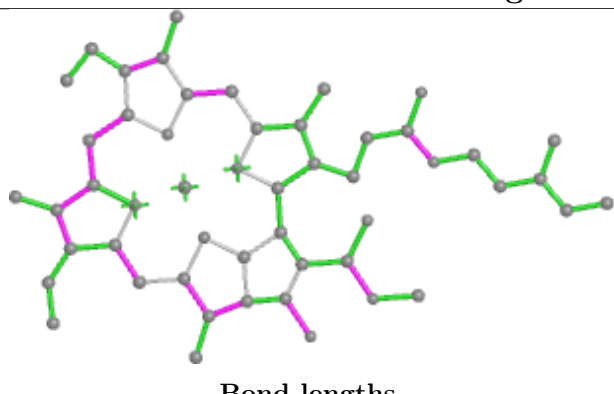


Torsions

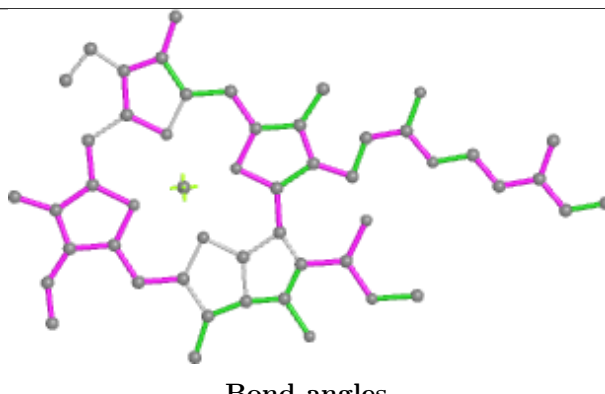


Rings

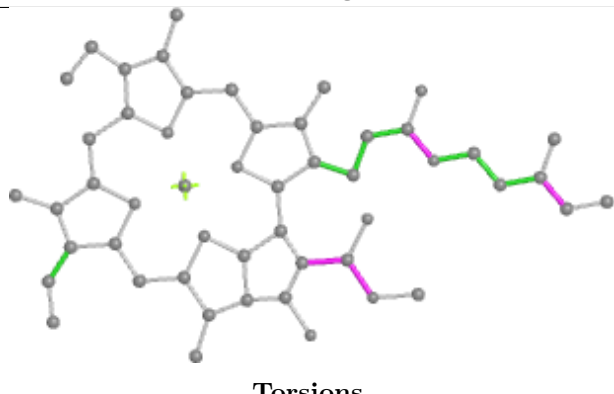
Ligand CLA cA 822



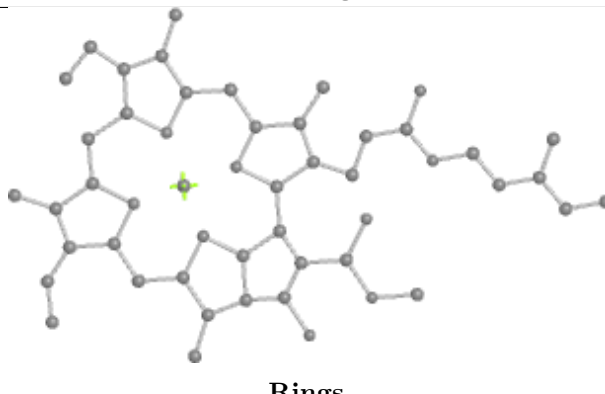
Bond lengths



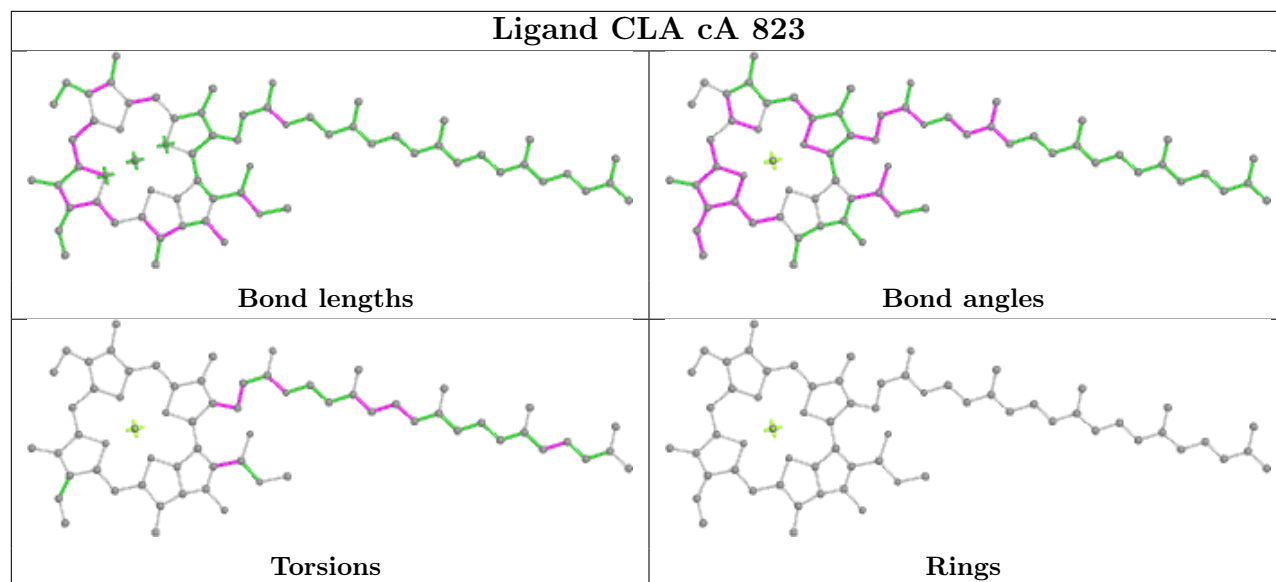
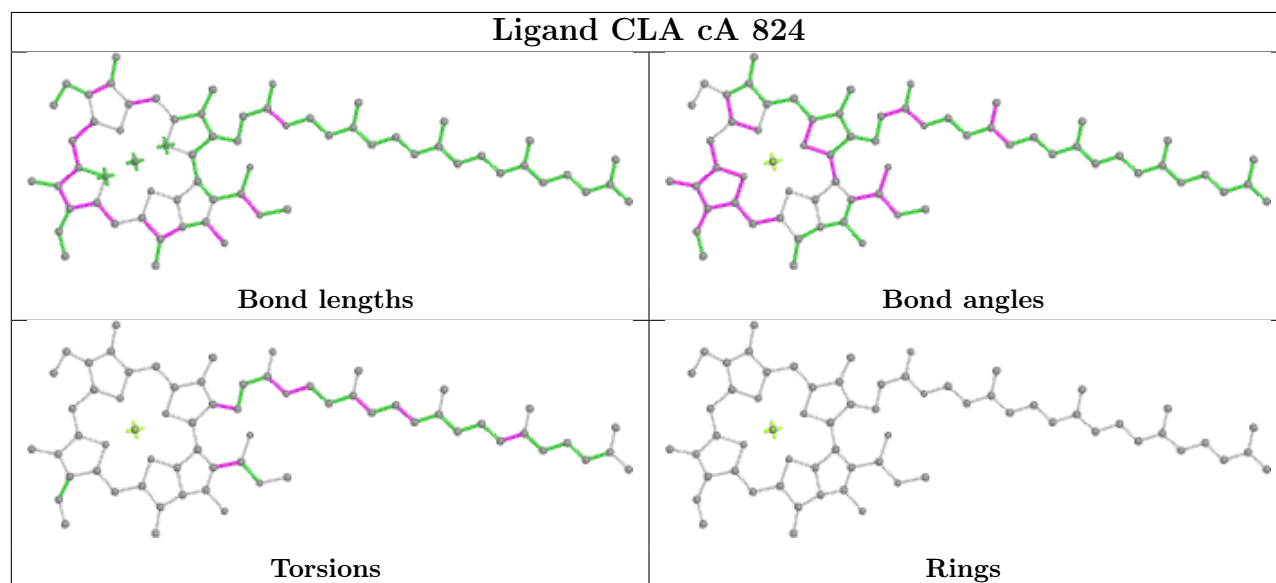
Bond angles



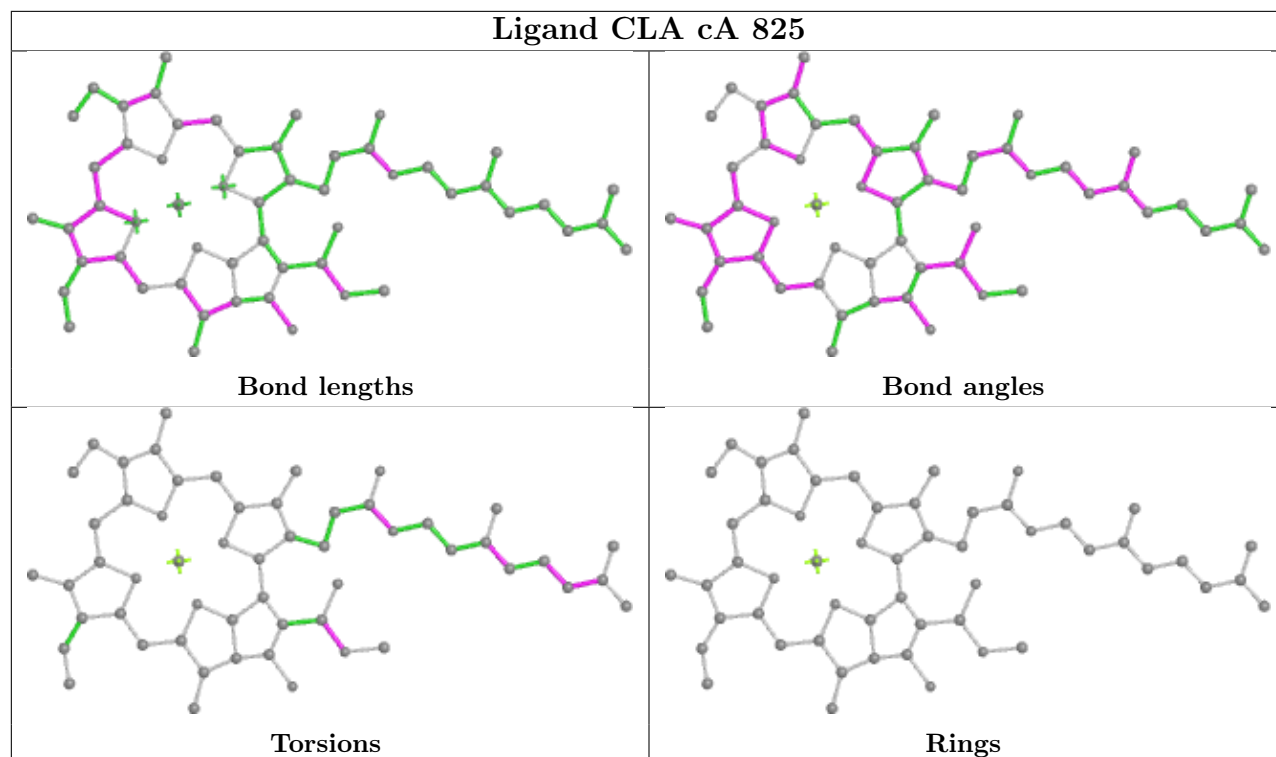
Torsions



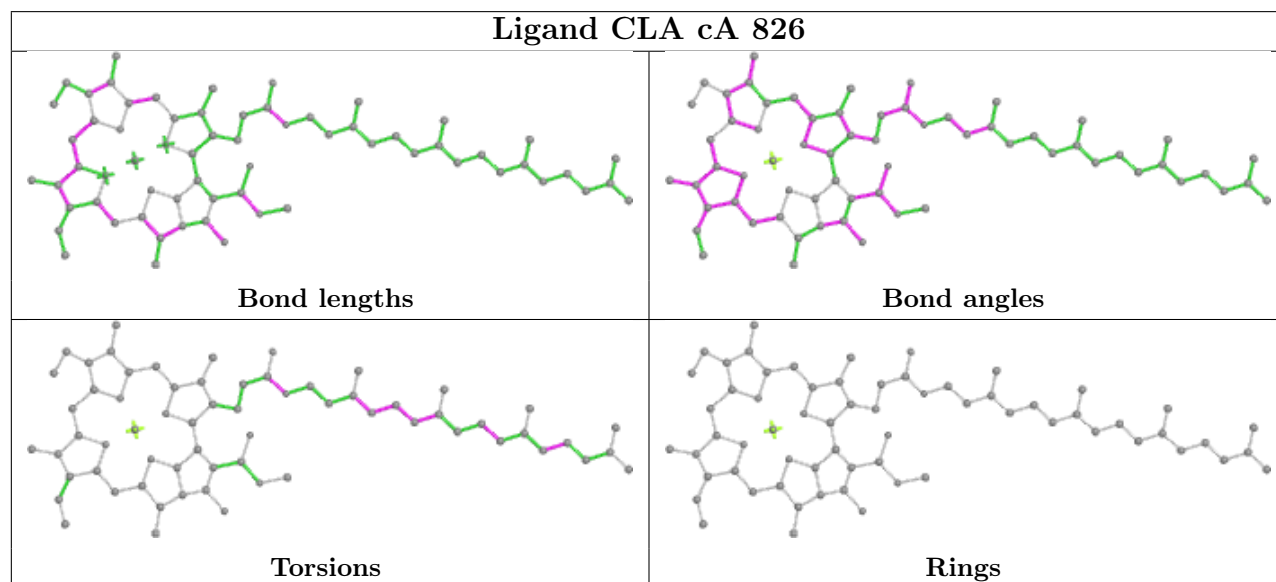
Rings

Ligand CLA cA 823**Ligand CLA cA 824**

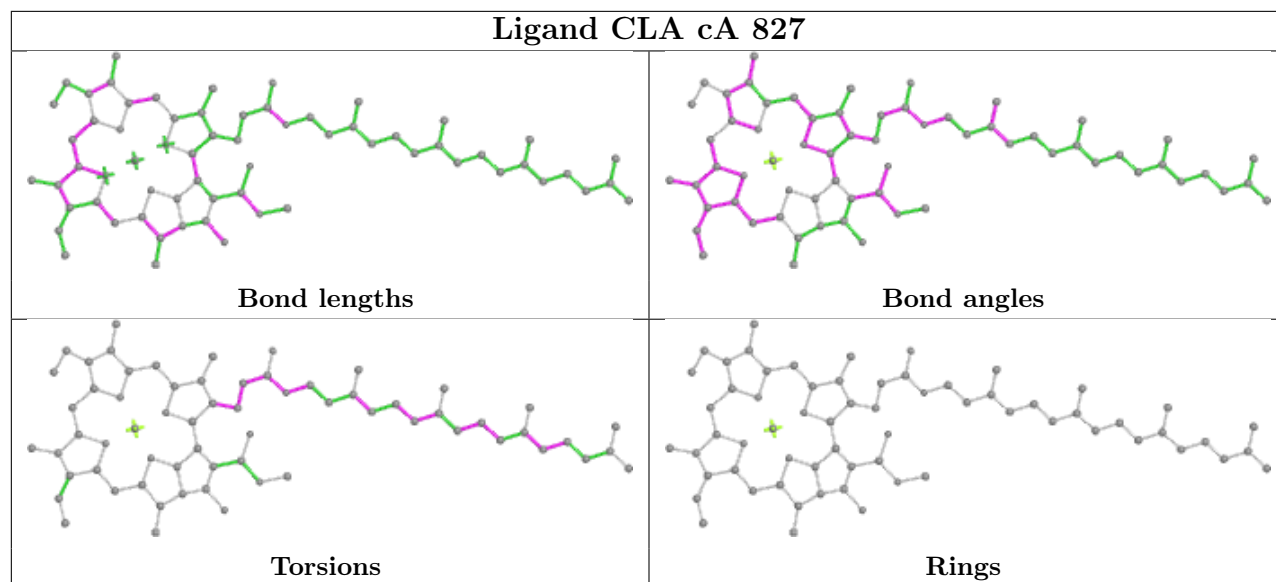
Ligand CLA cA 825



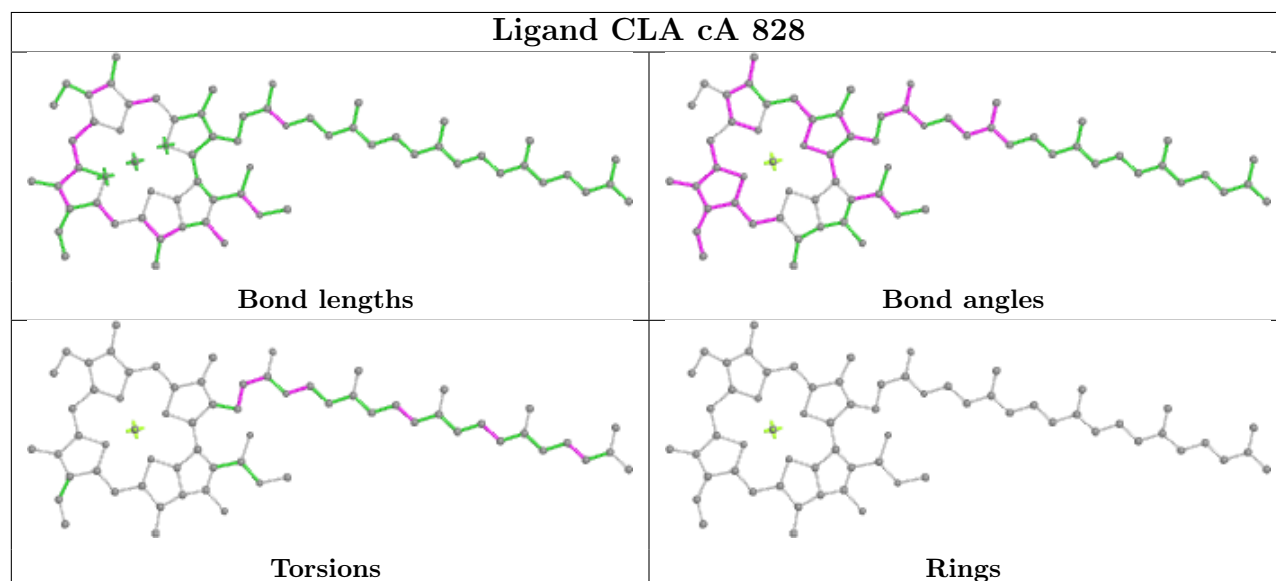
Ligand CLA cA 826



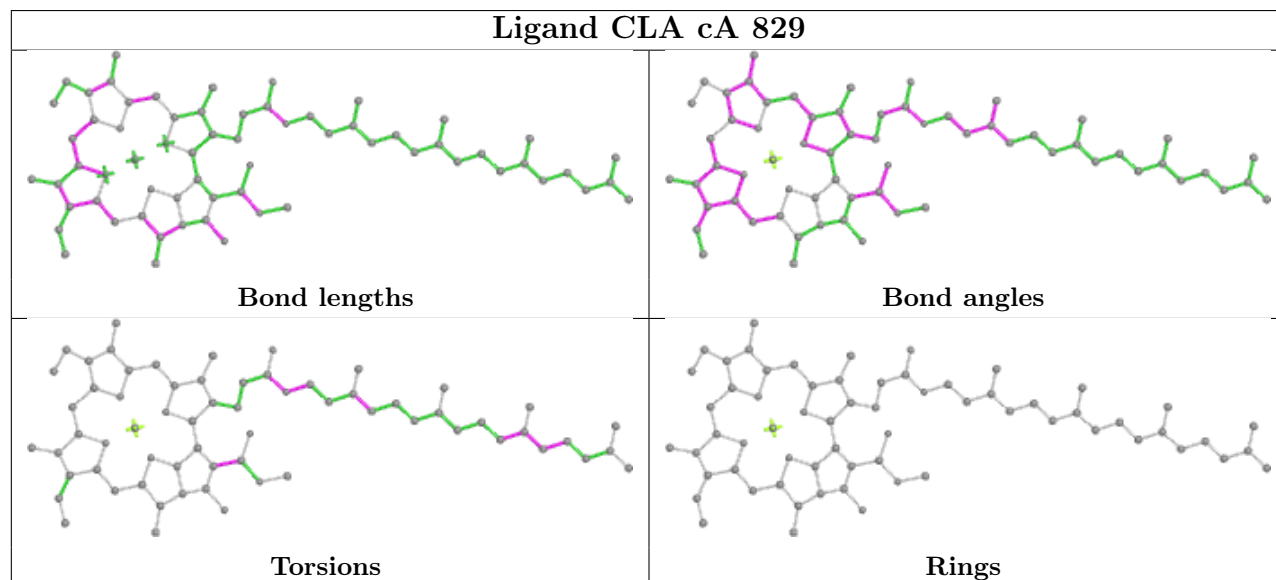
Ligand CLA cA 827

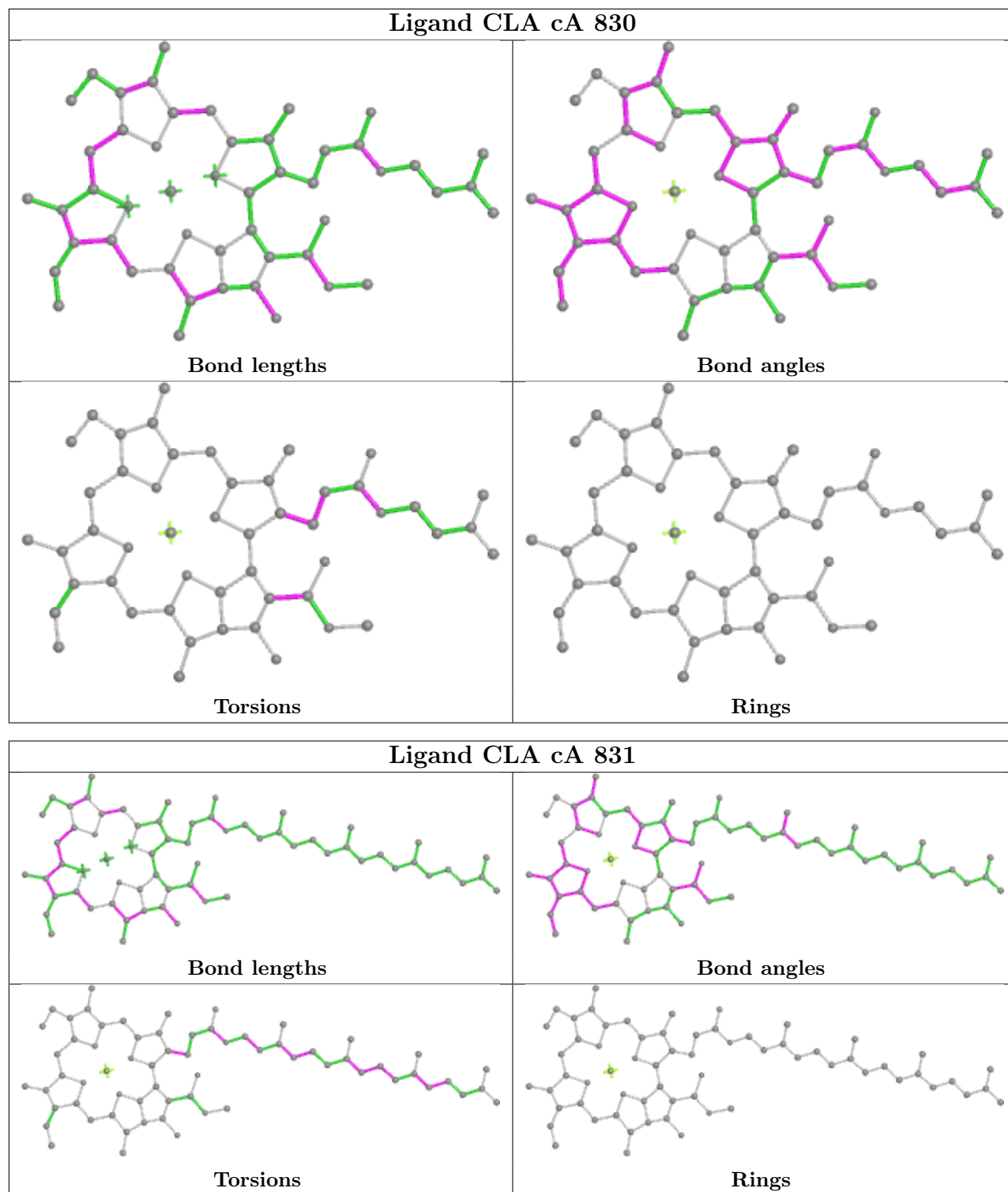


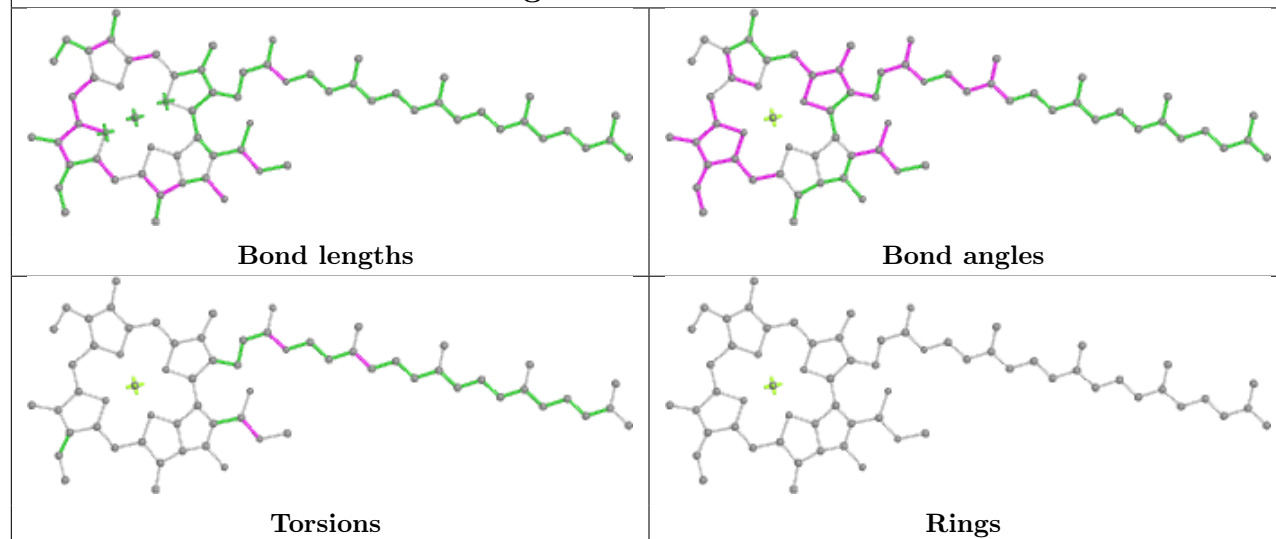
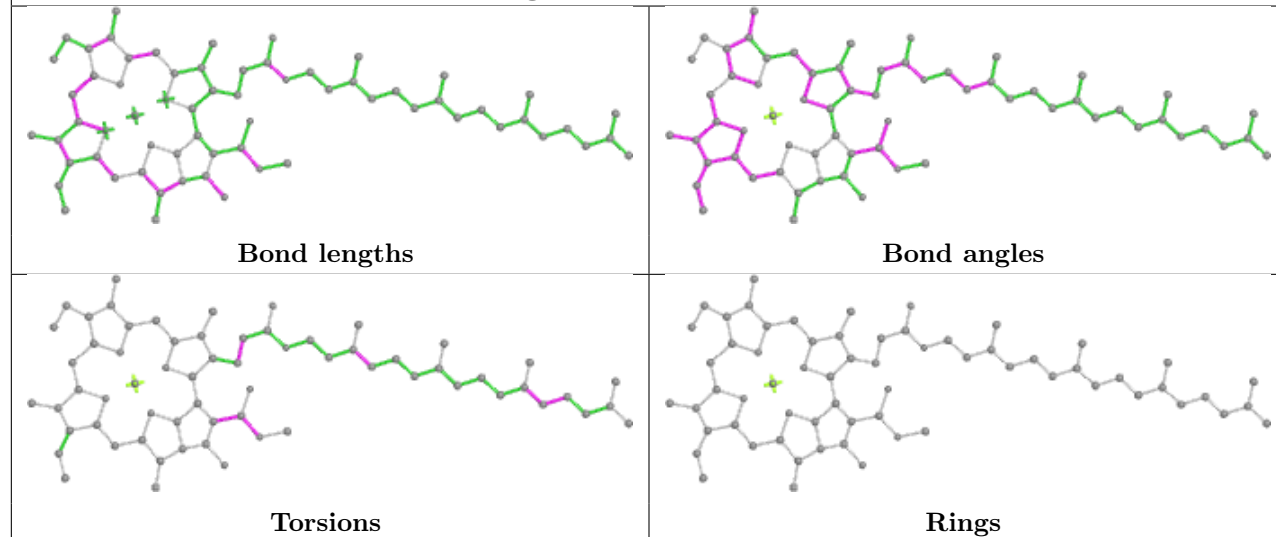
Ligand CLA cA 828

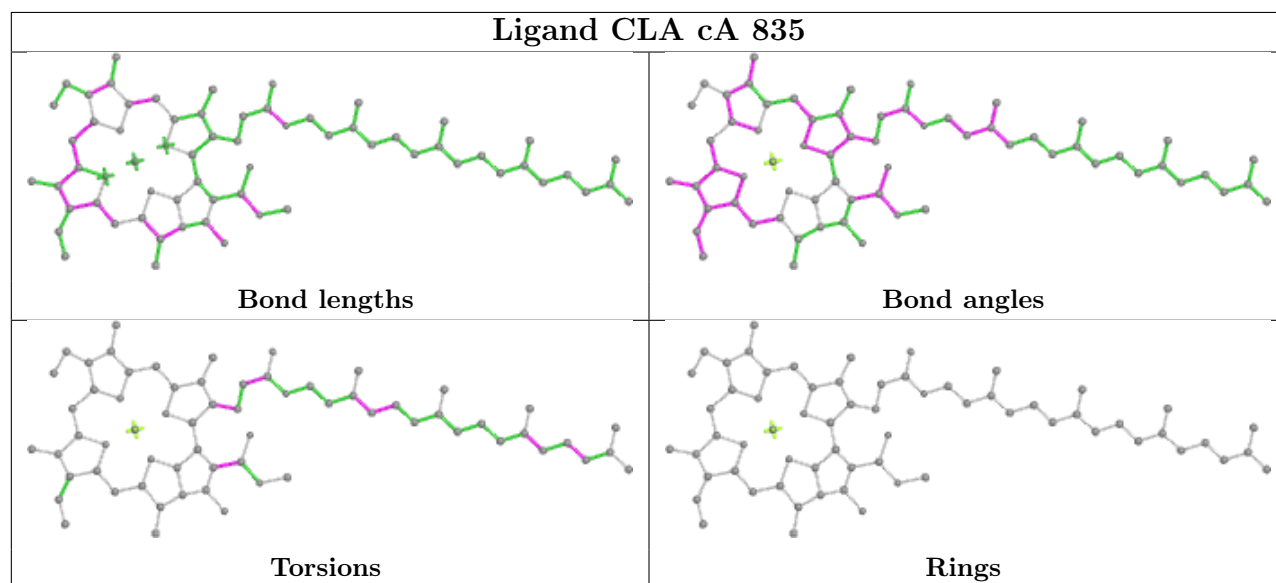
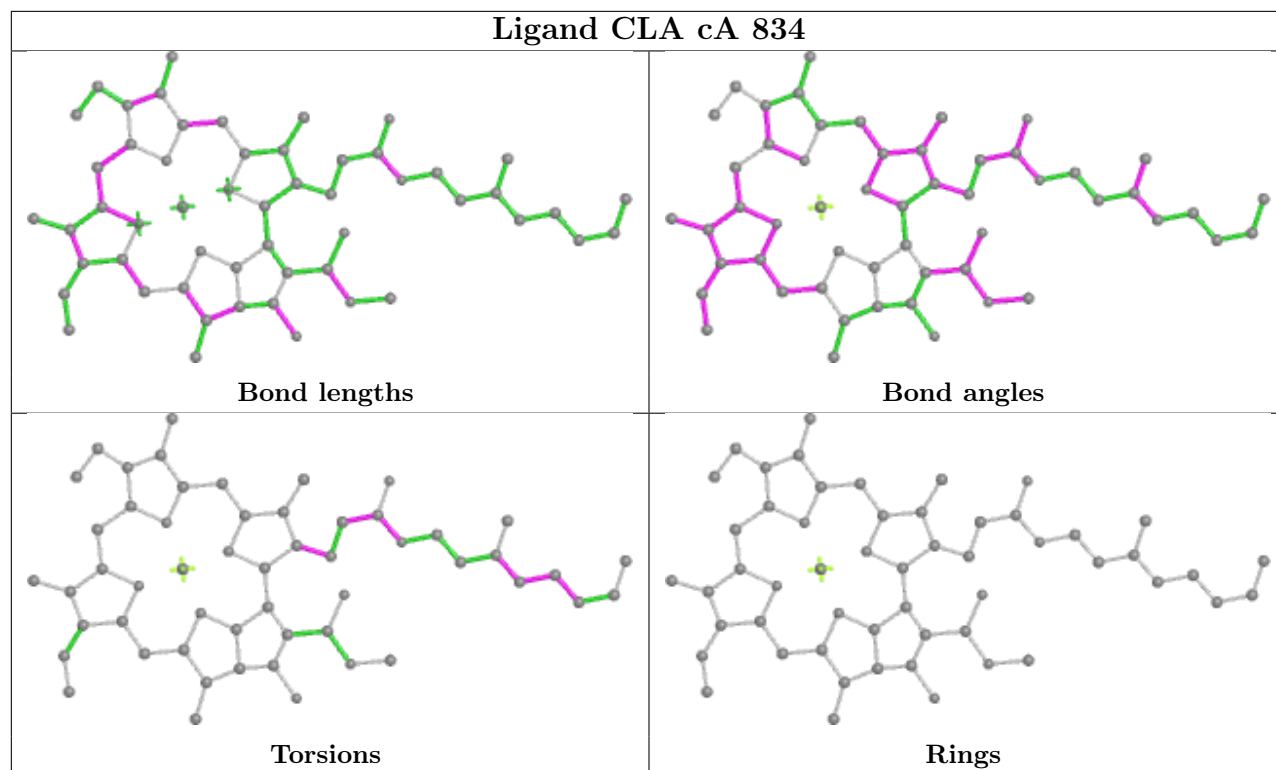


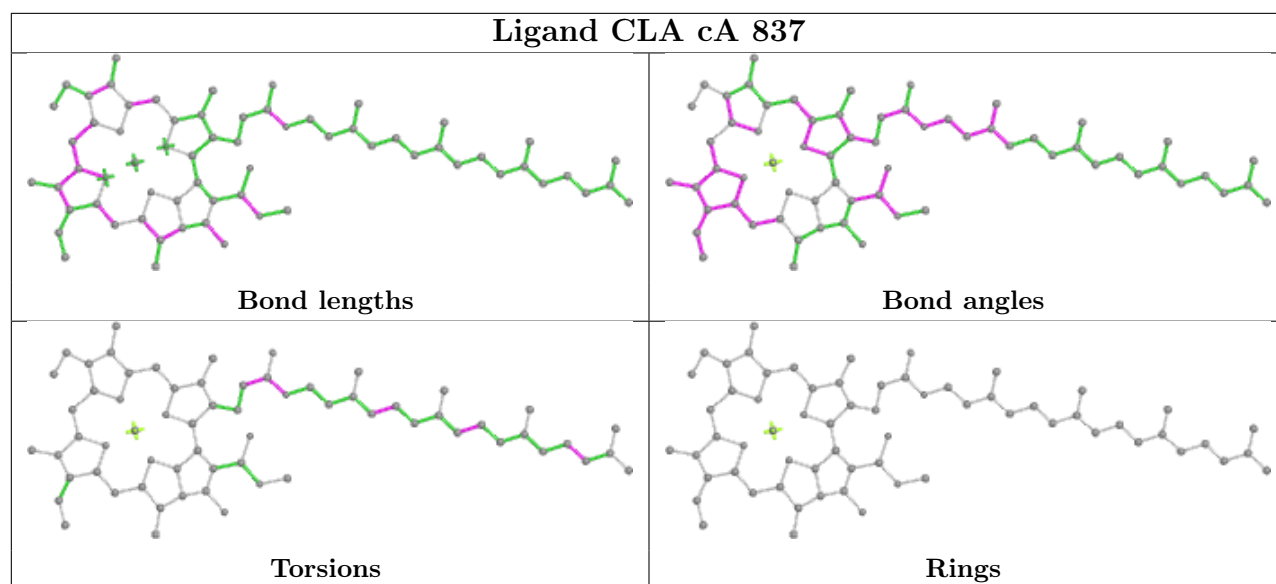
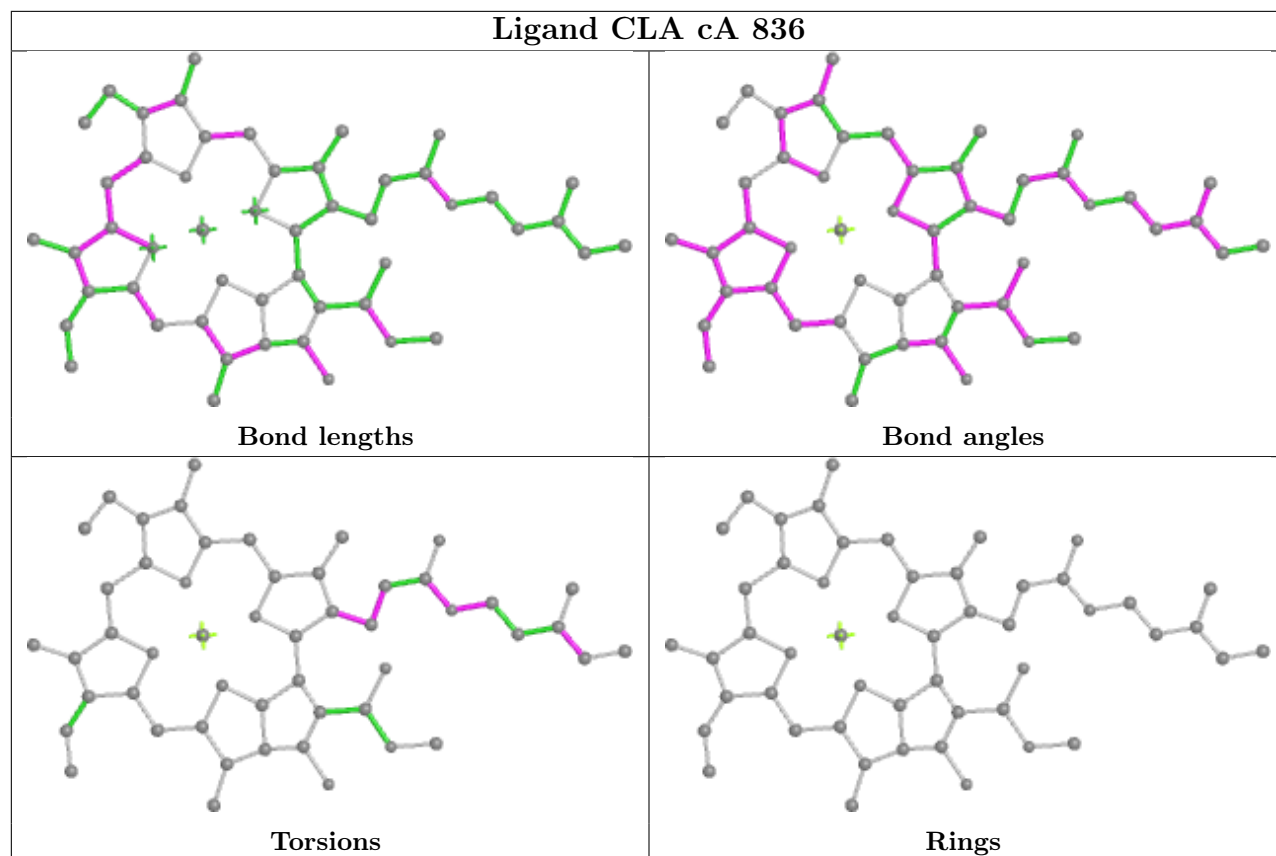
Ligand CLA cA 829

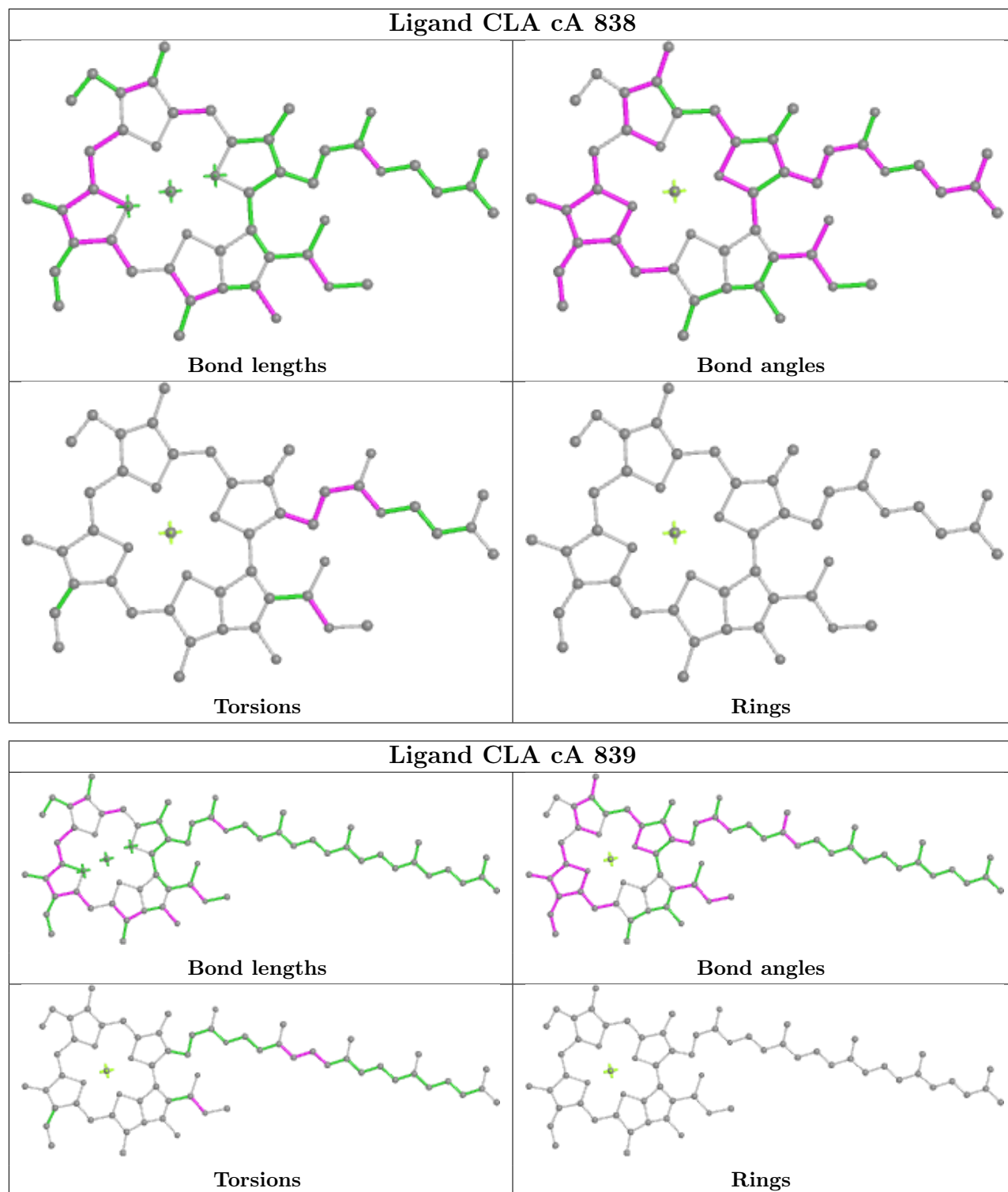


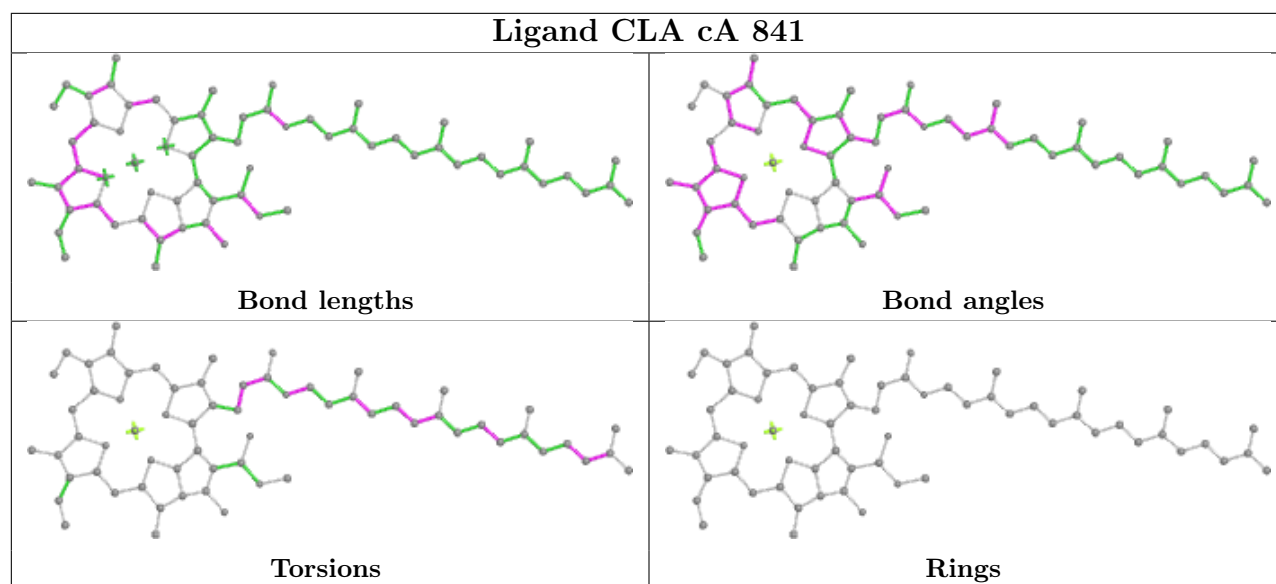
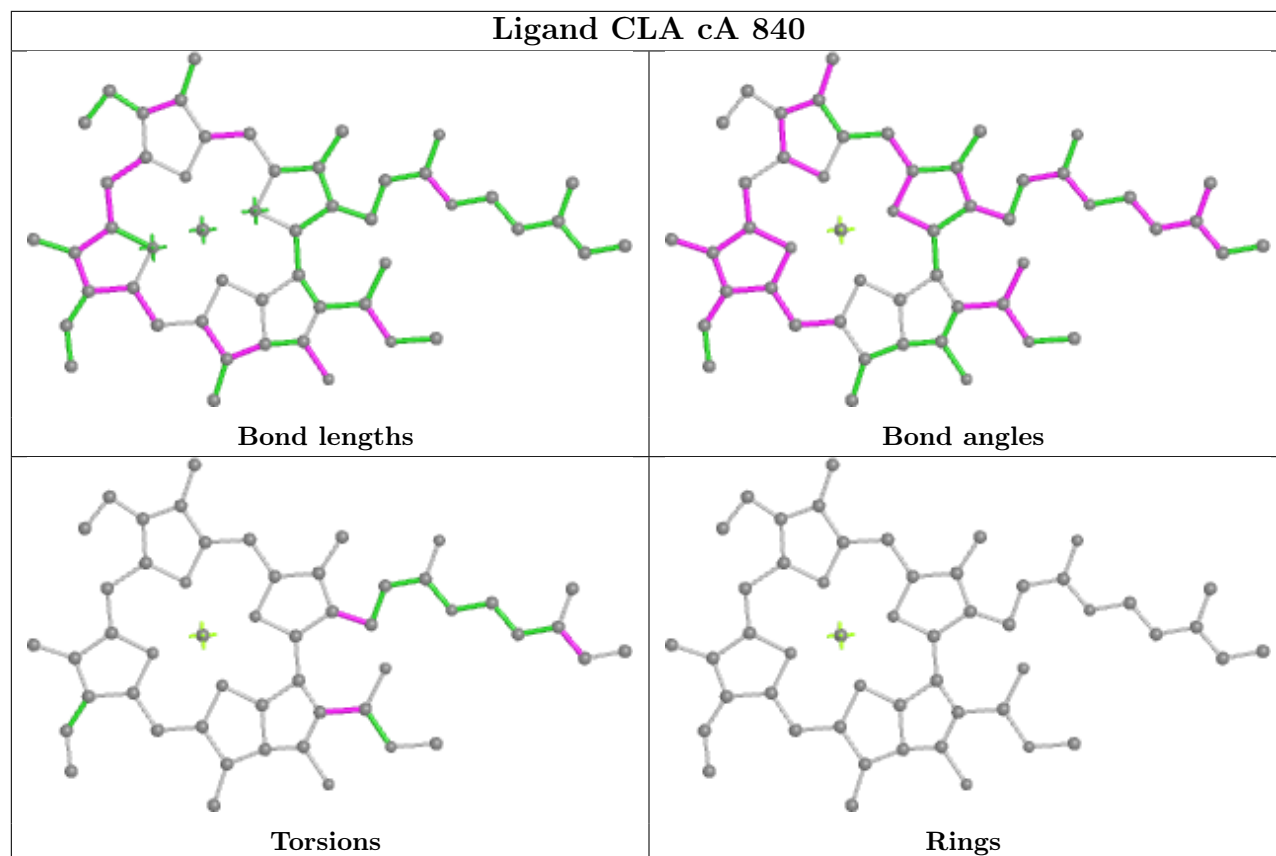


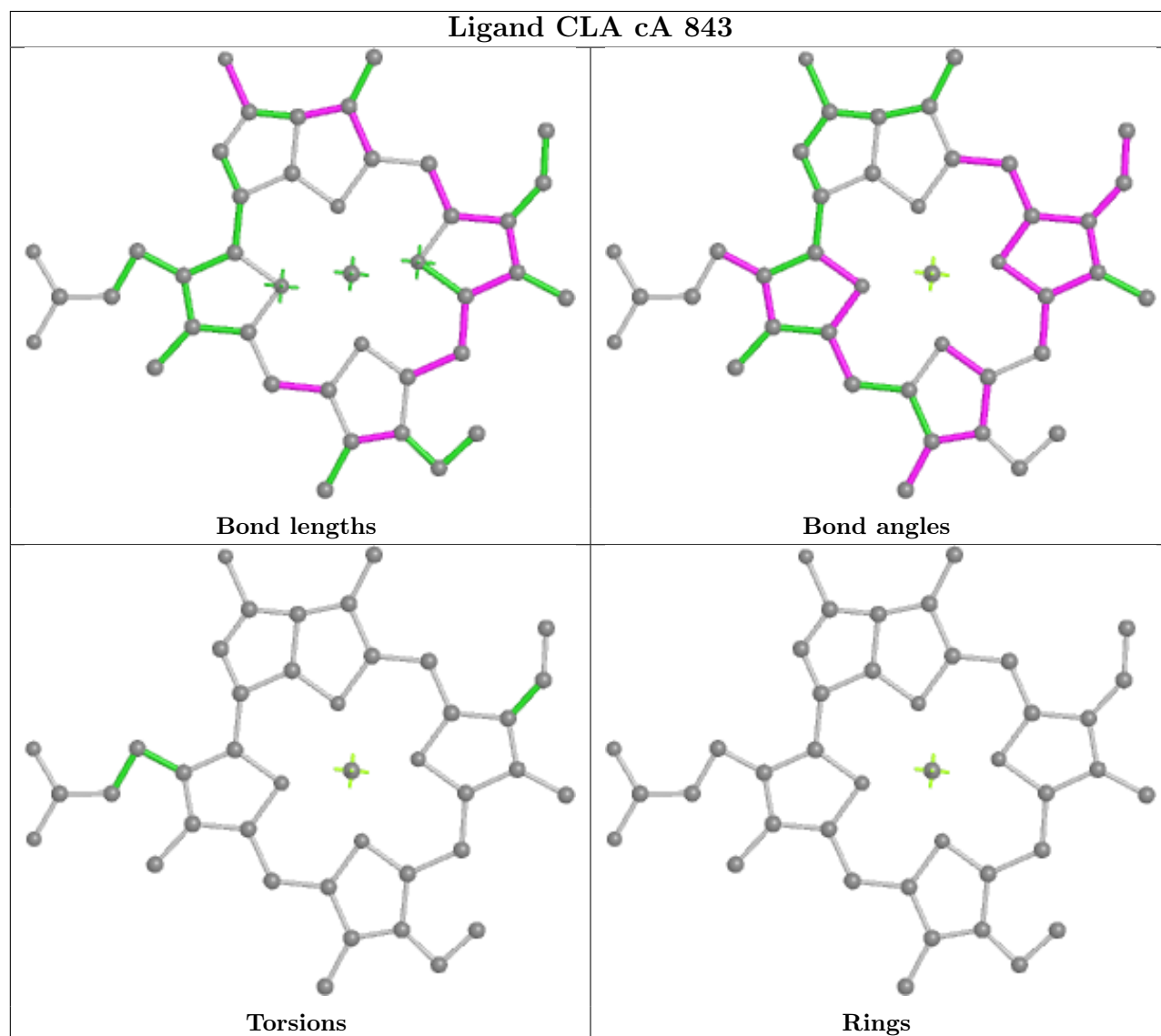
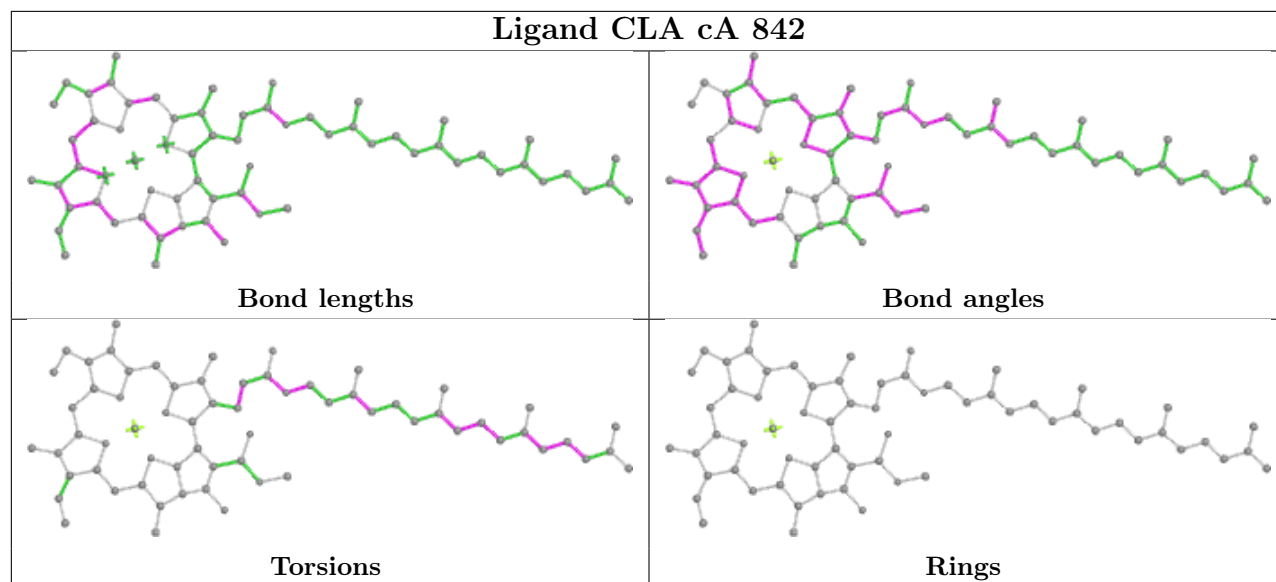
Ligand CLA cA 832**Ligand CLA cA 833**

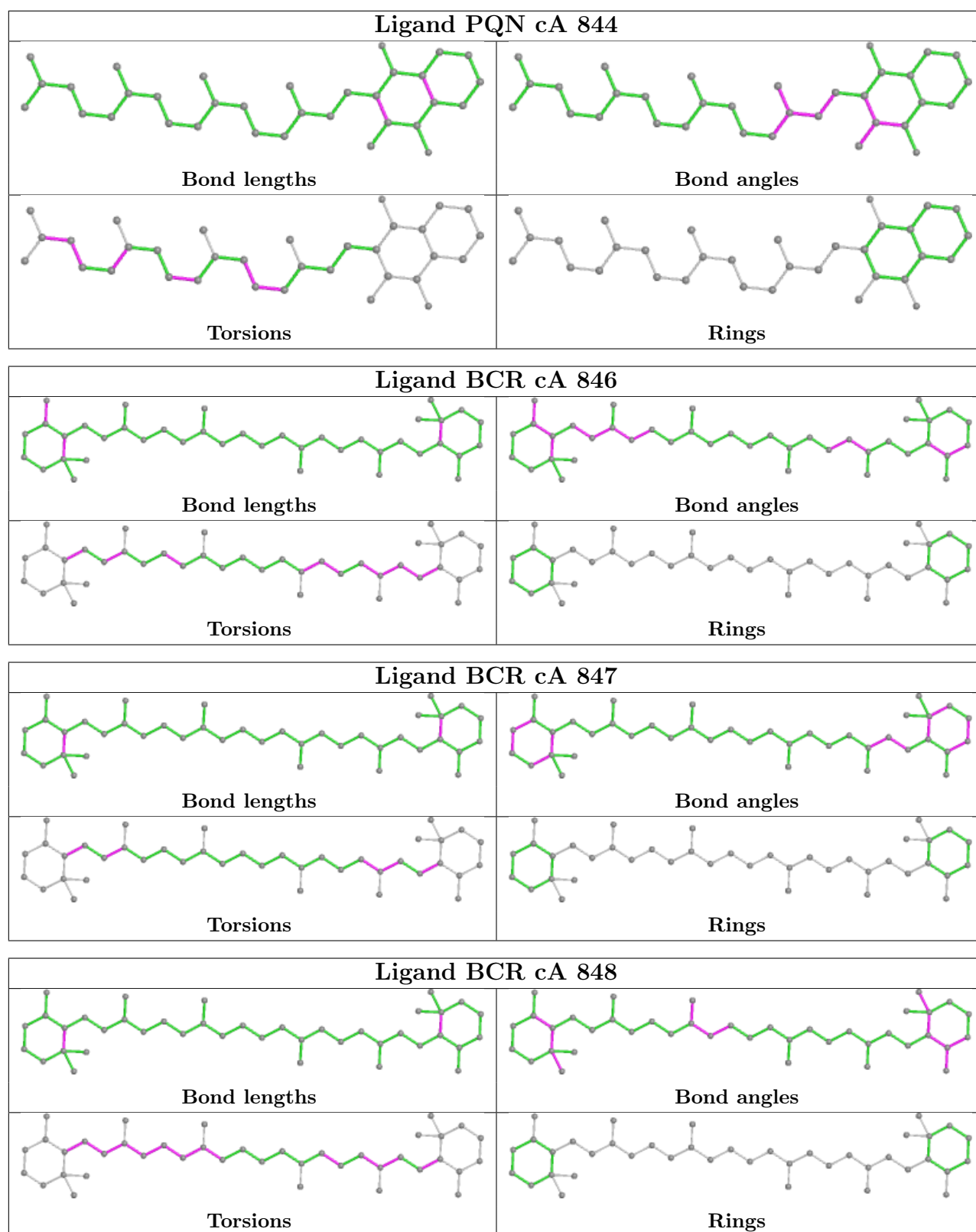


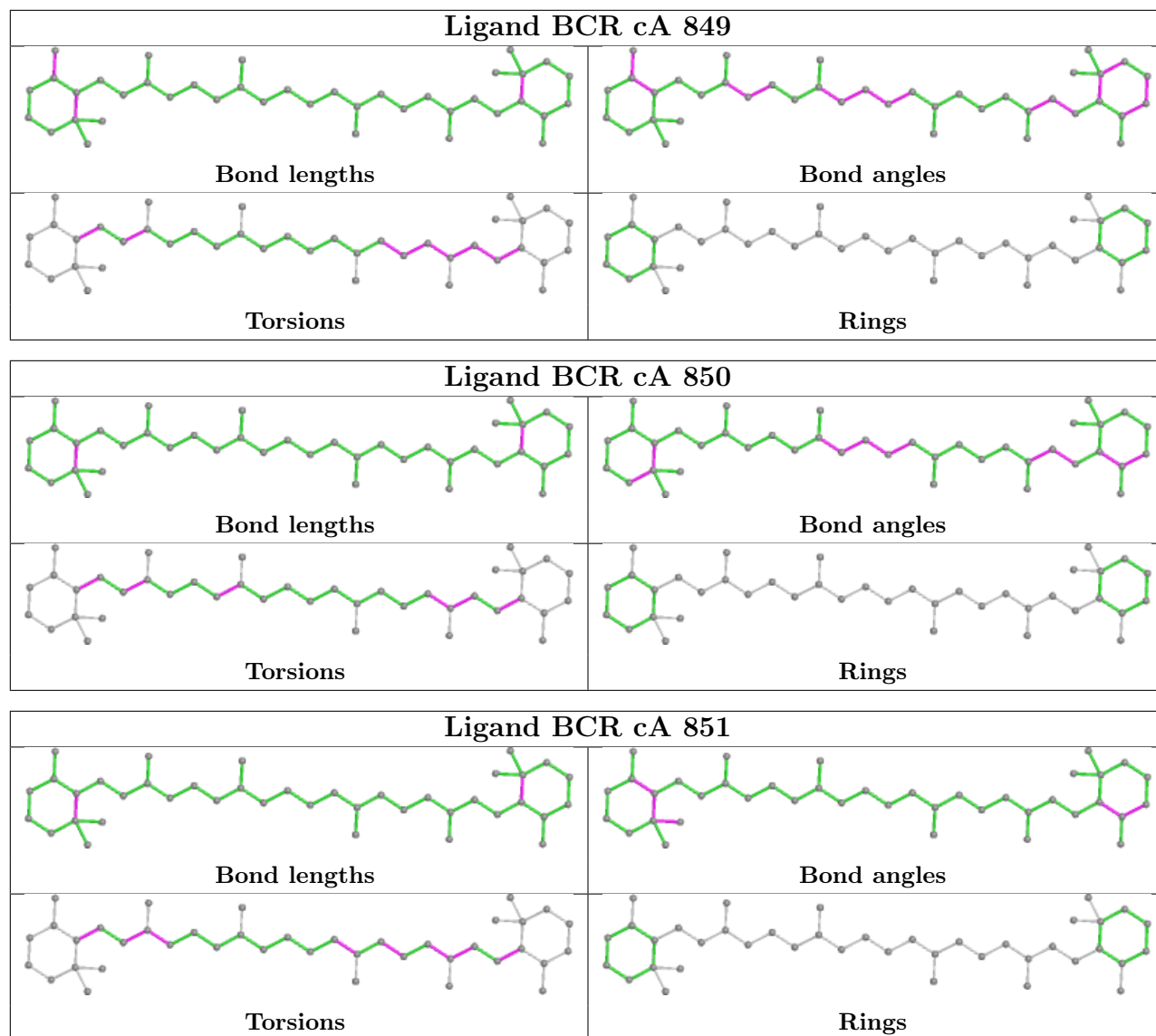


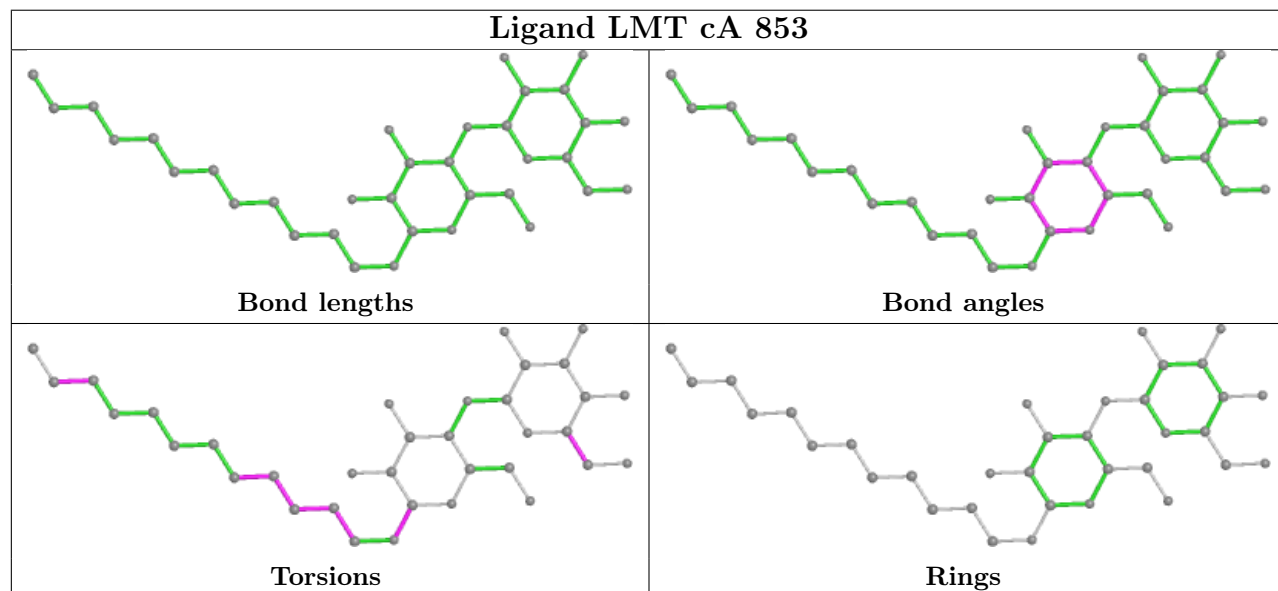
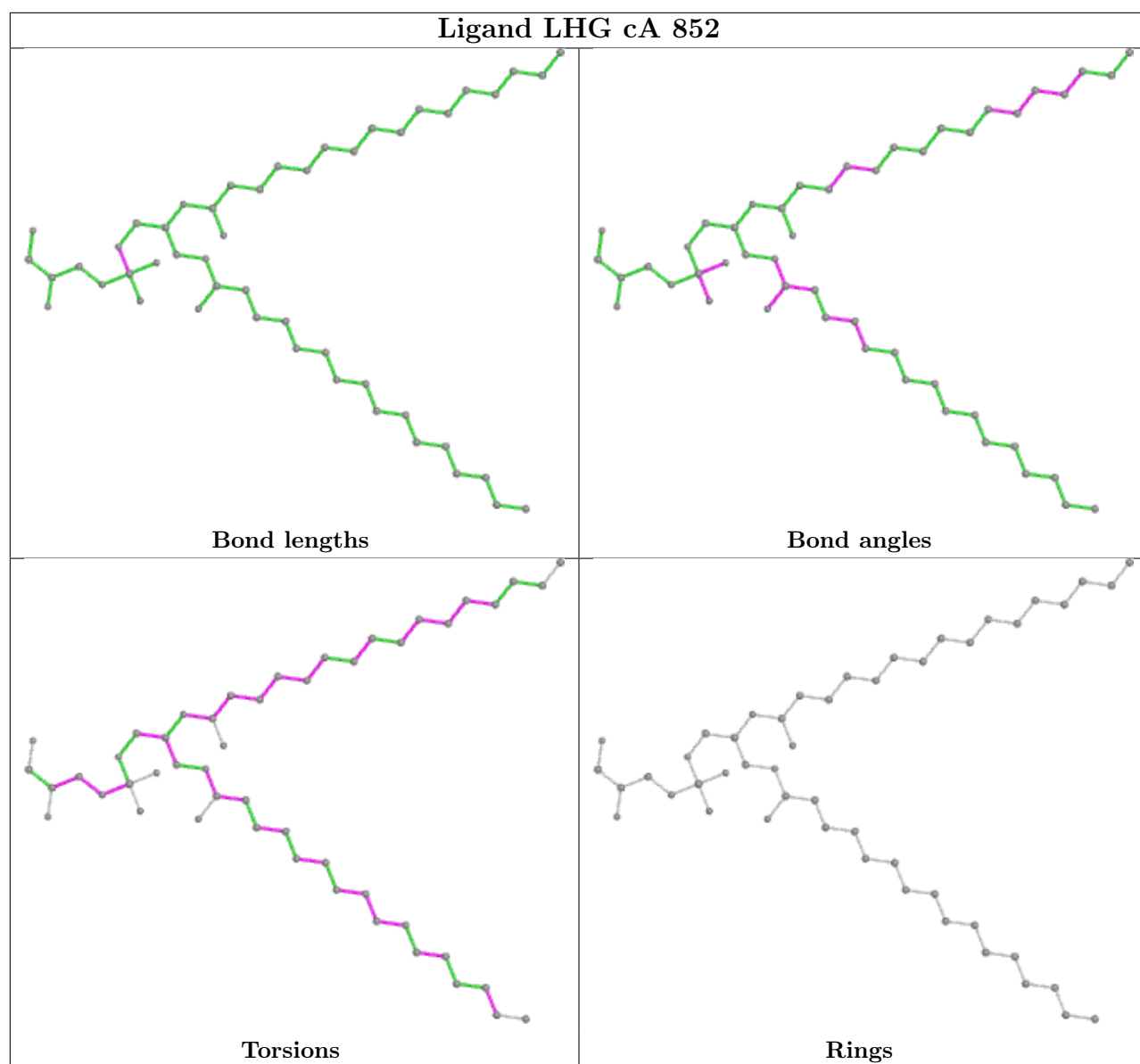


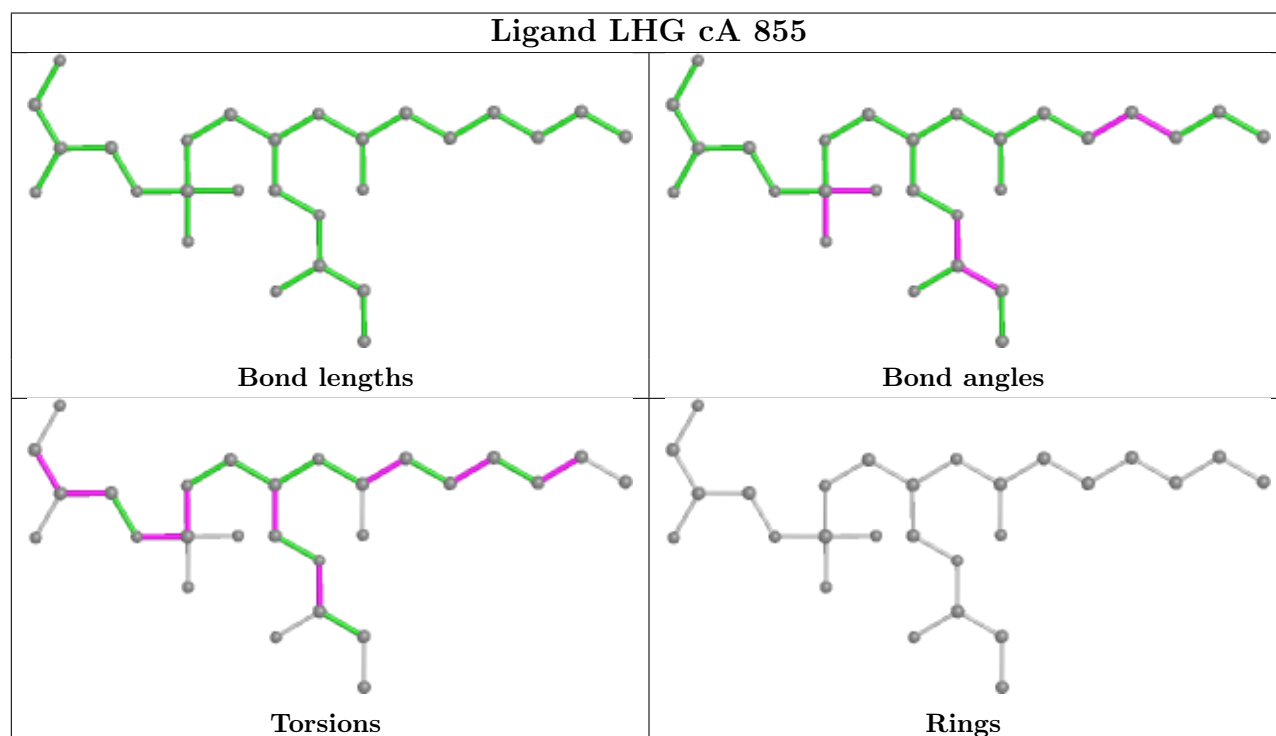
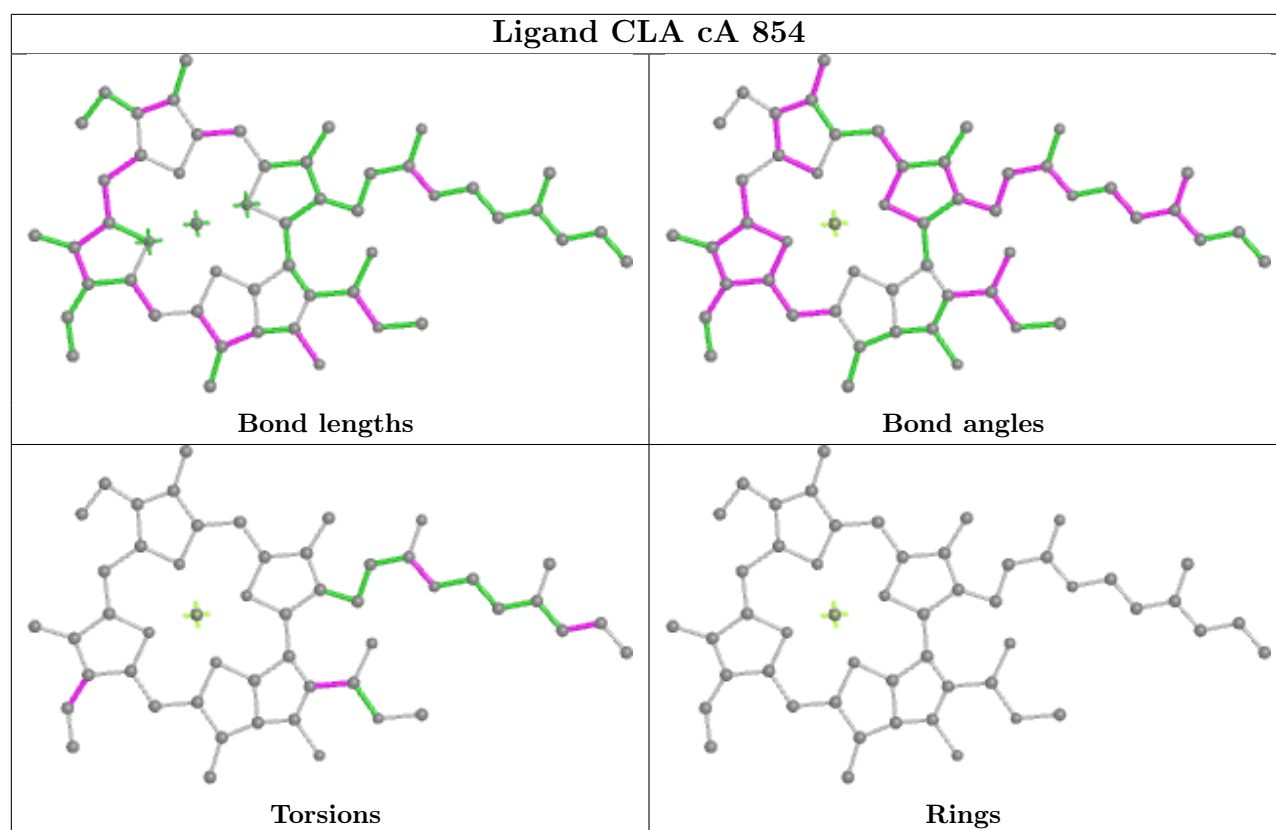


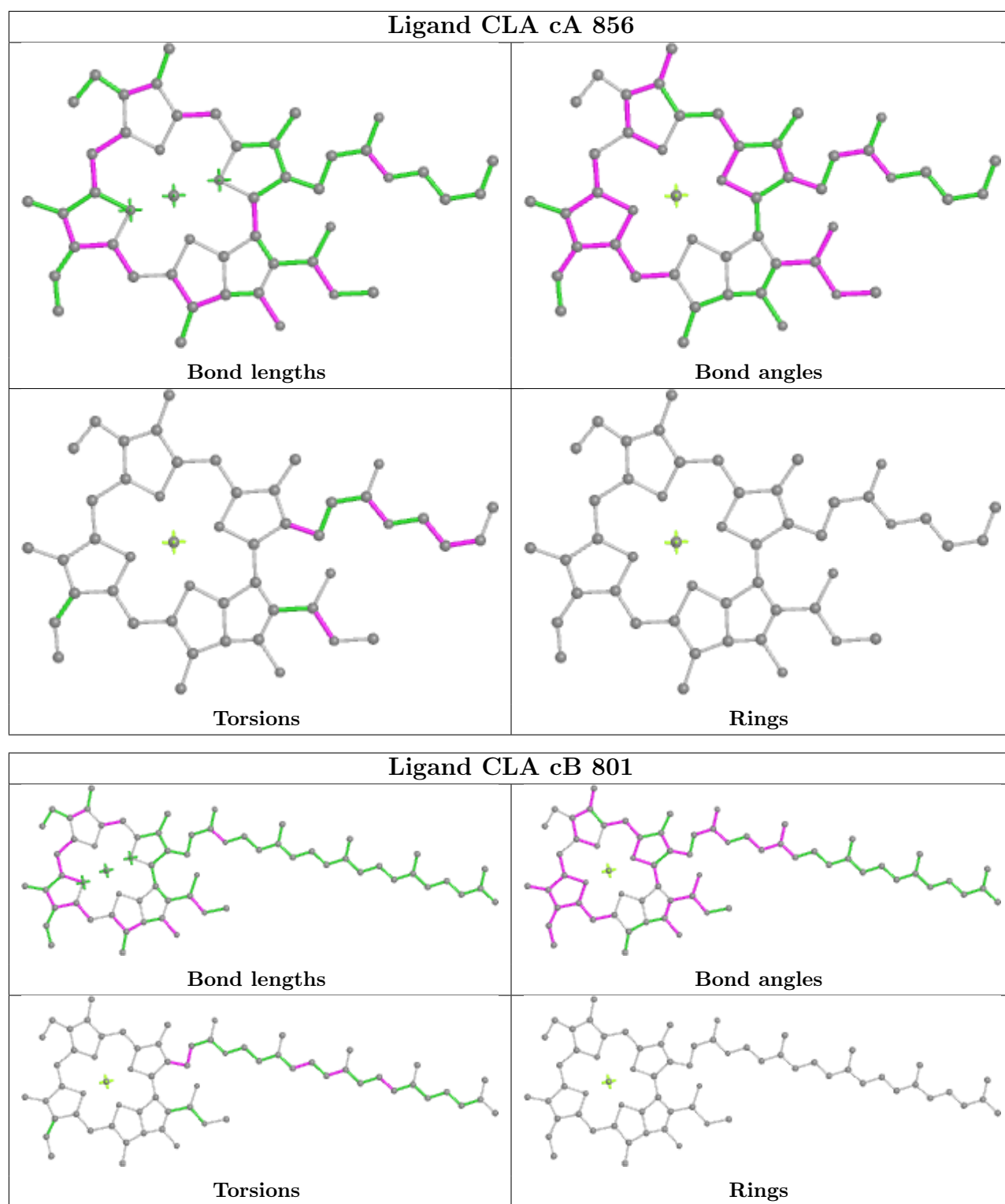


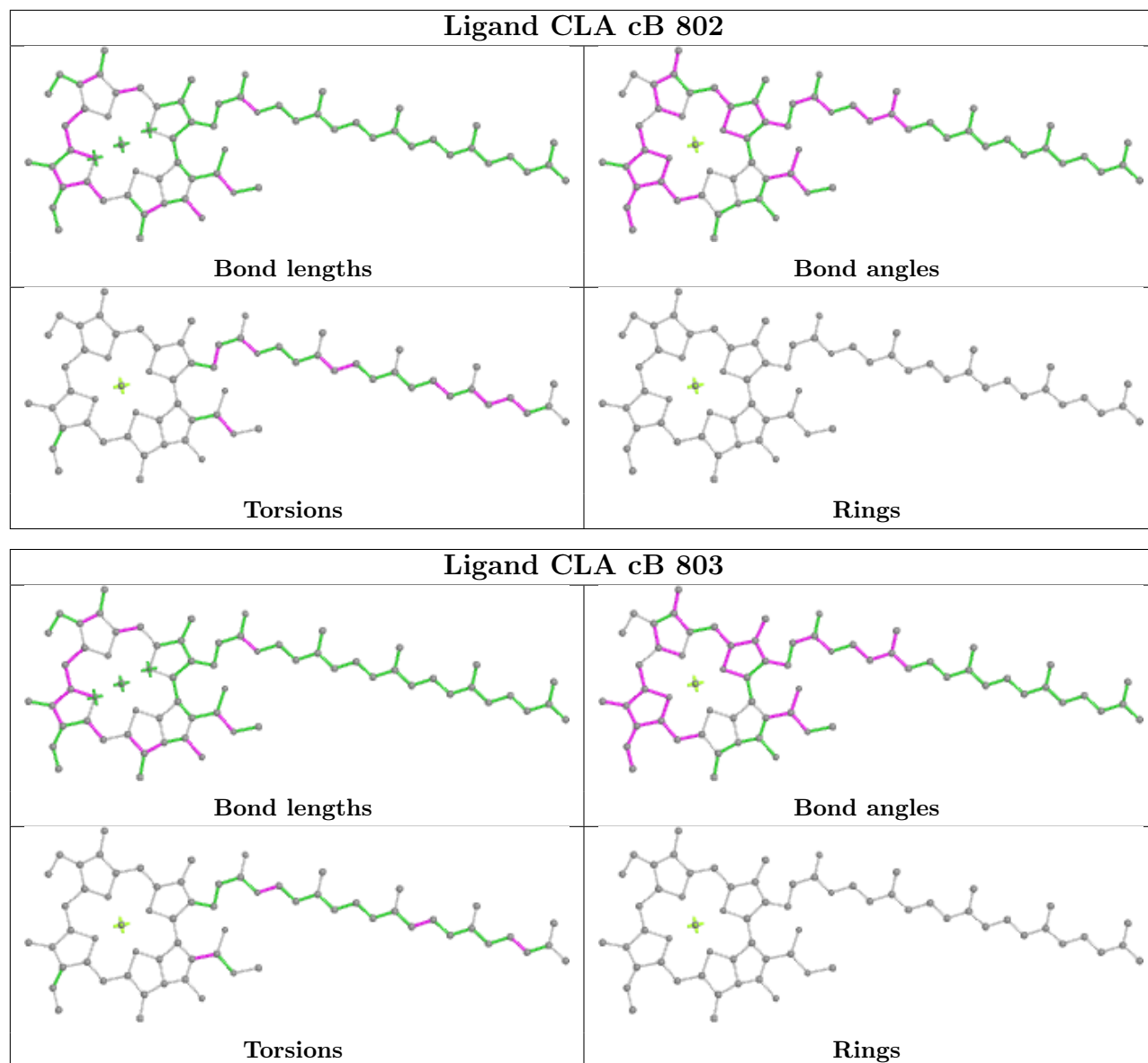


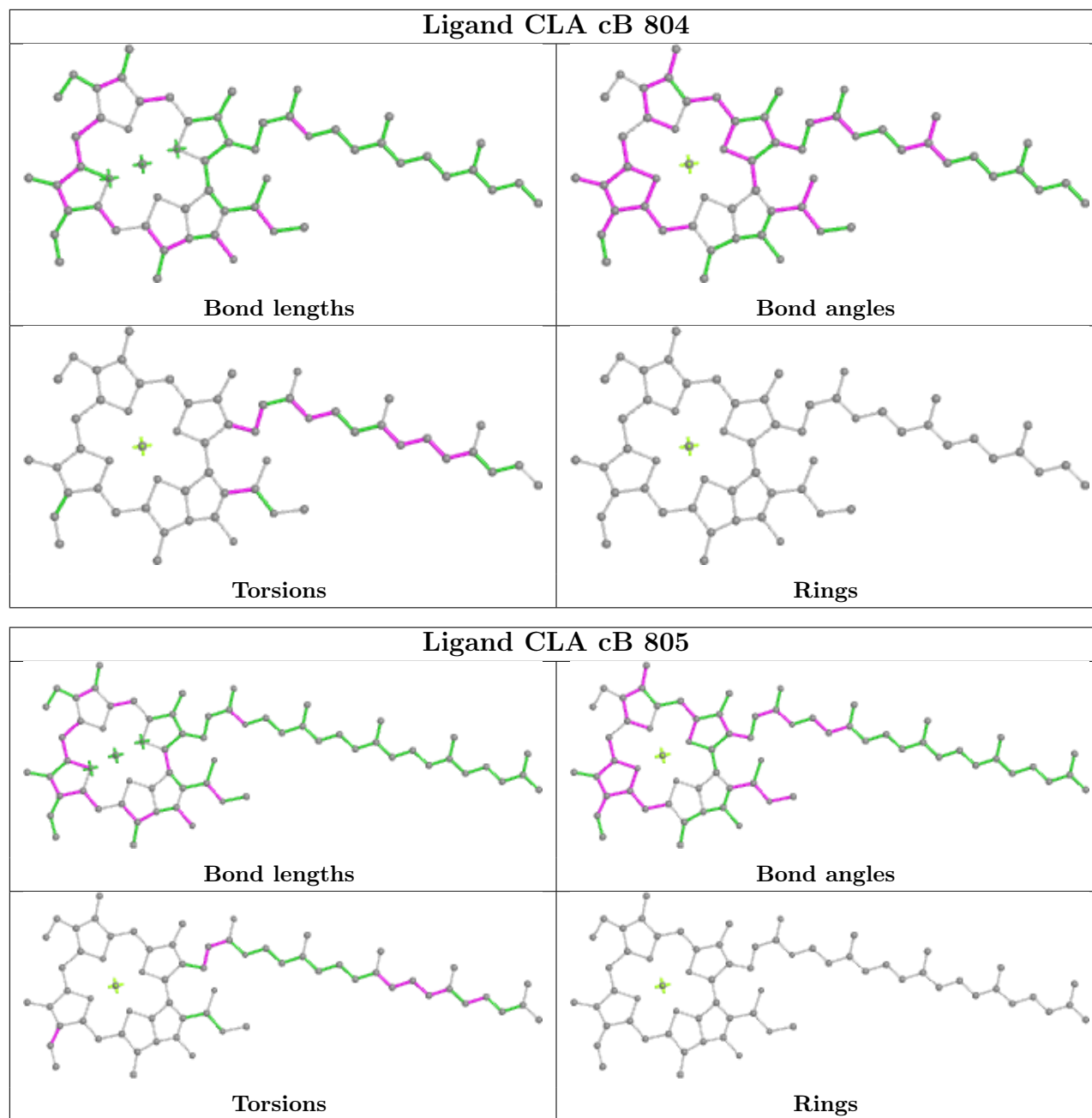


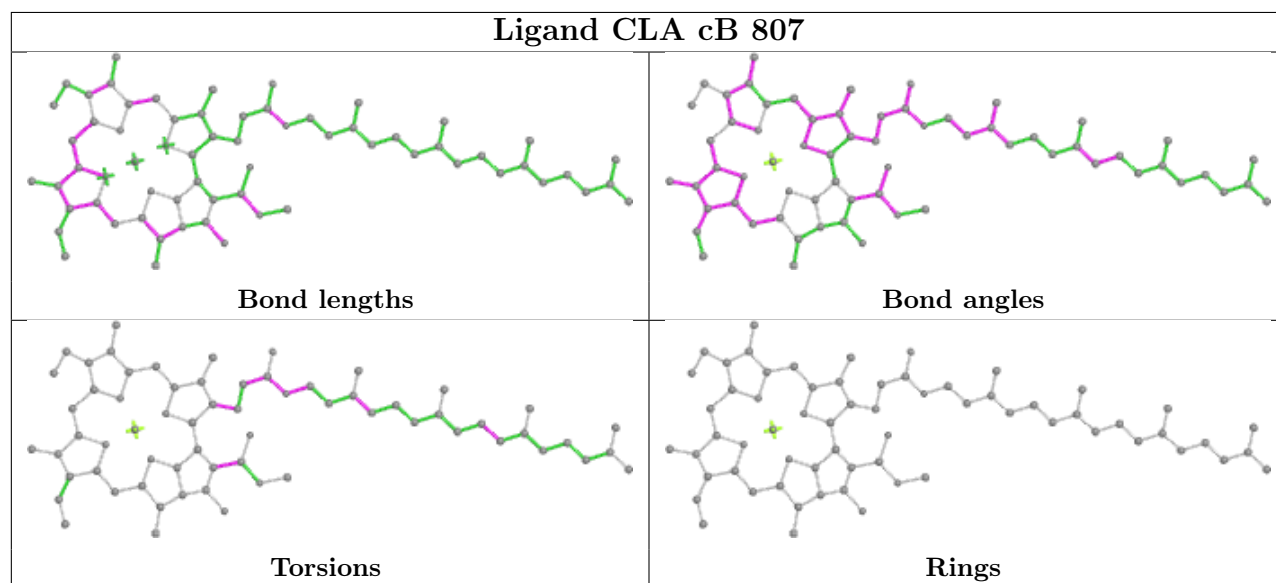
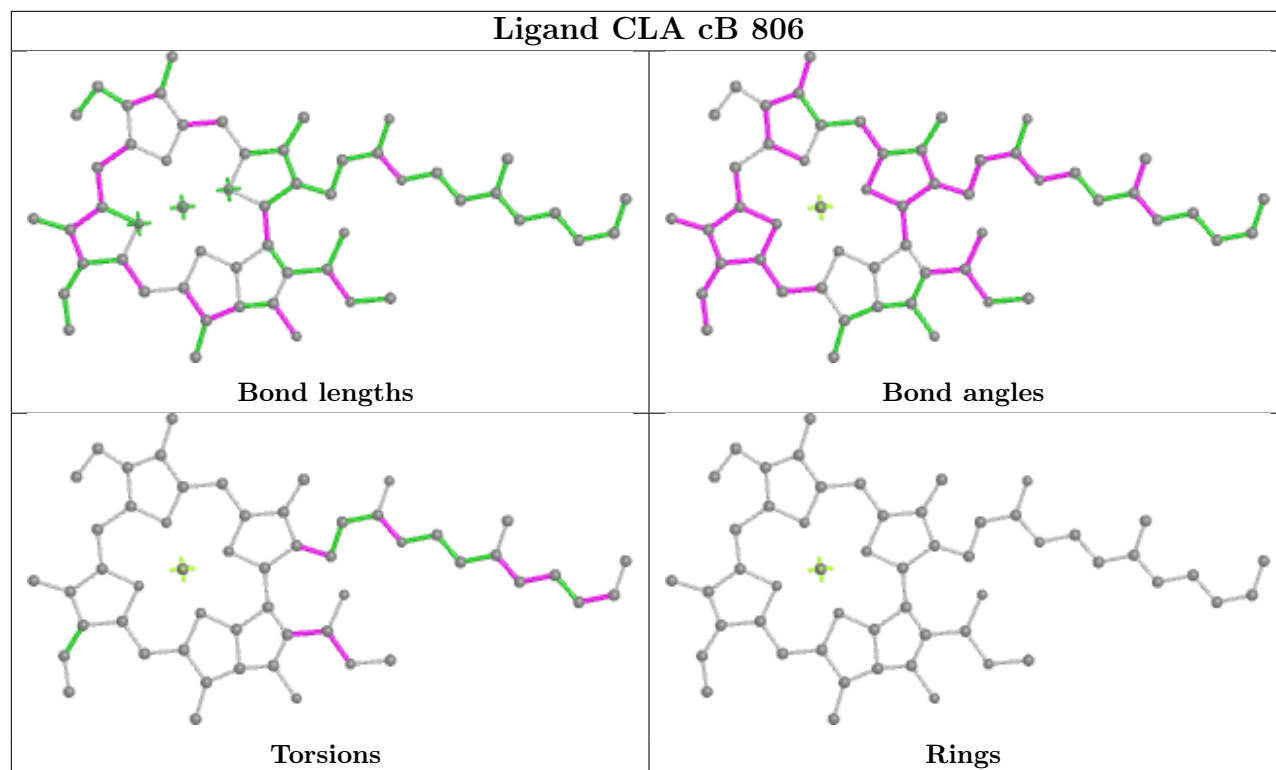


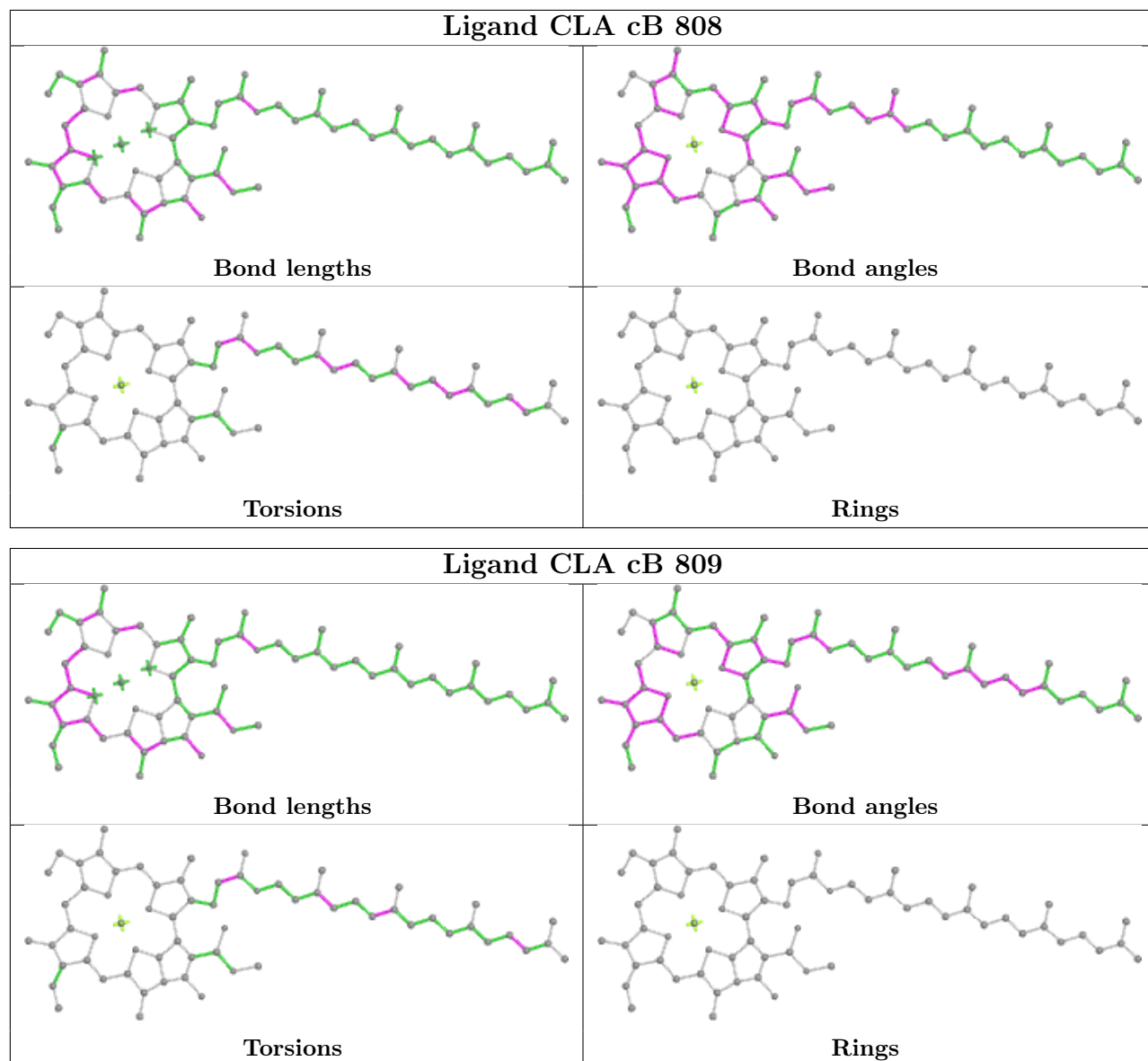


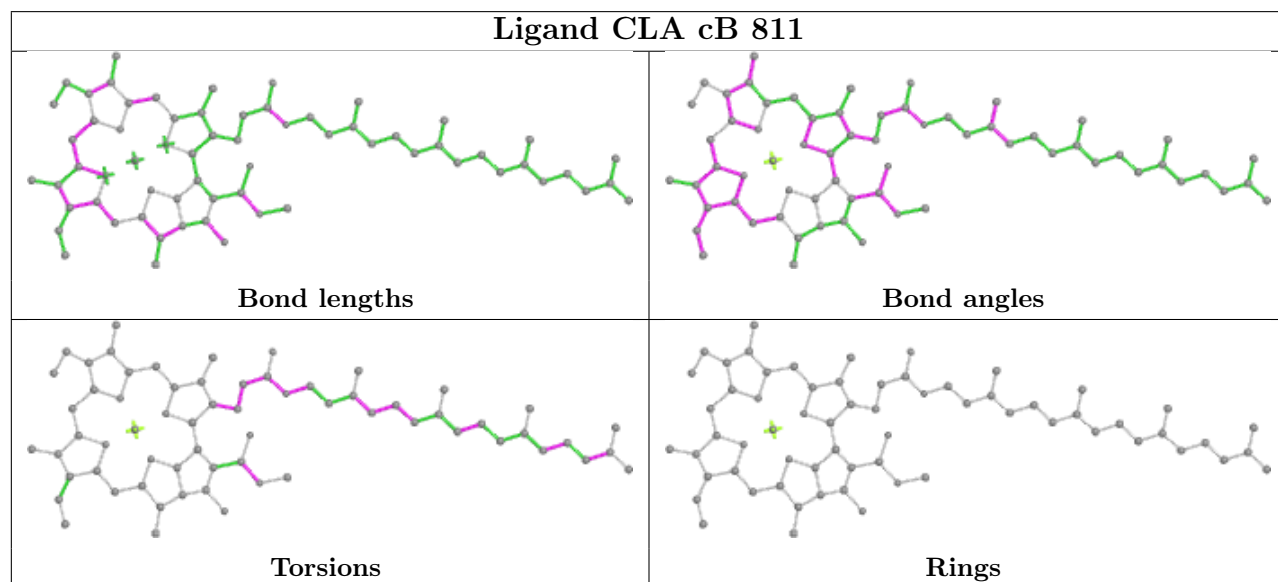
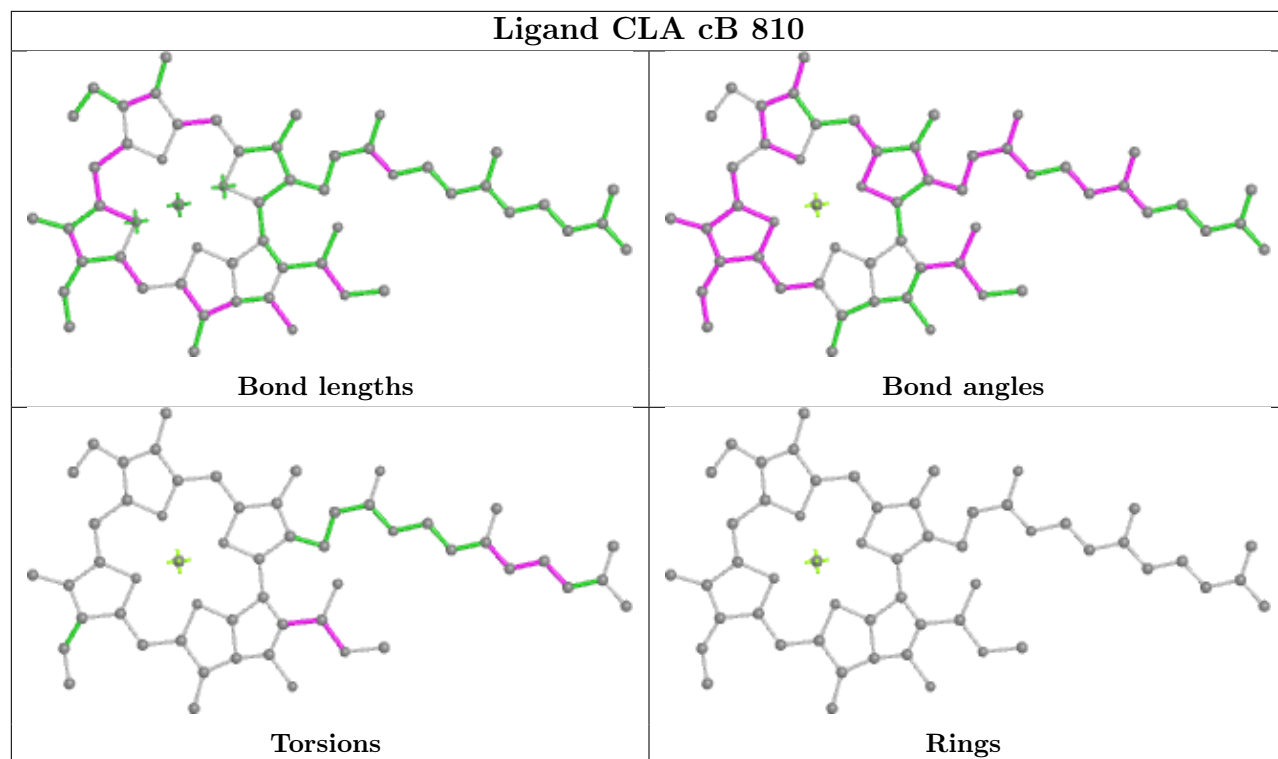




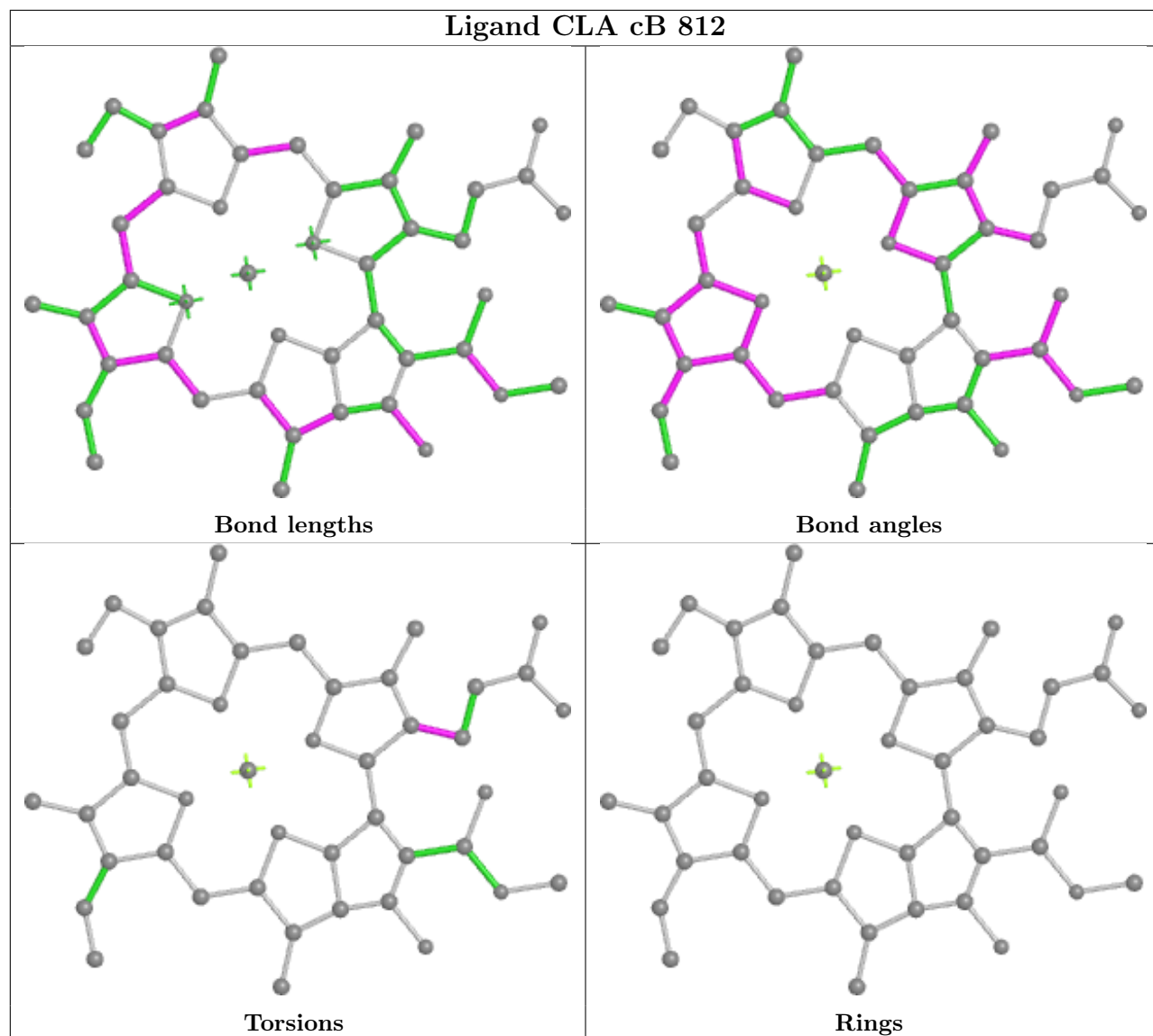




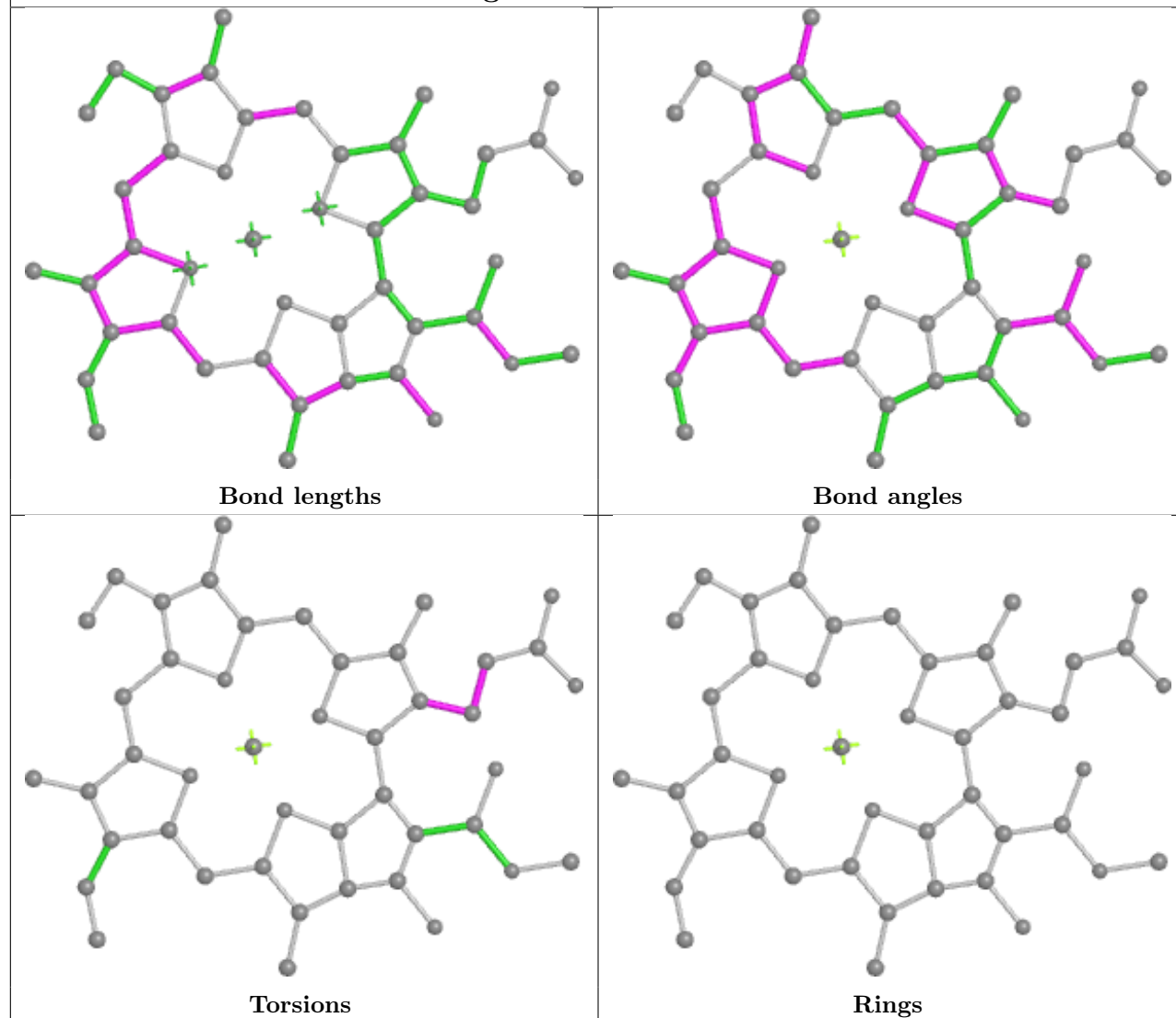




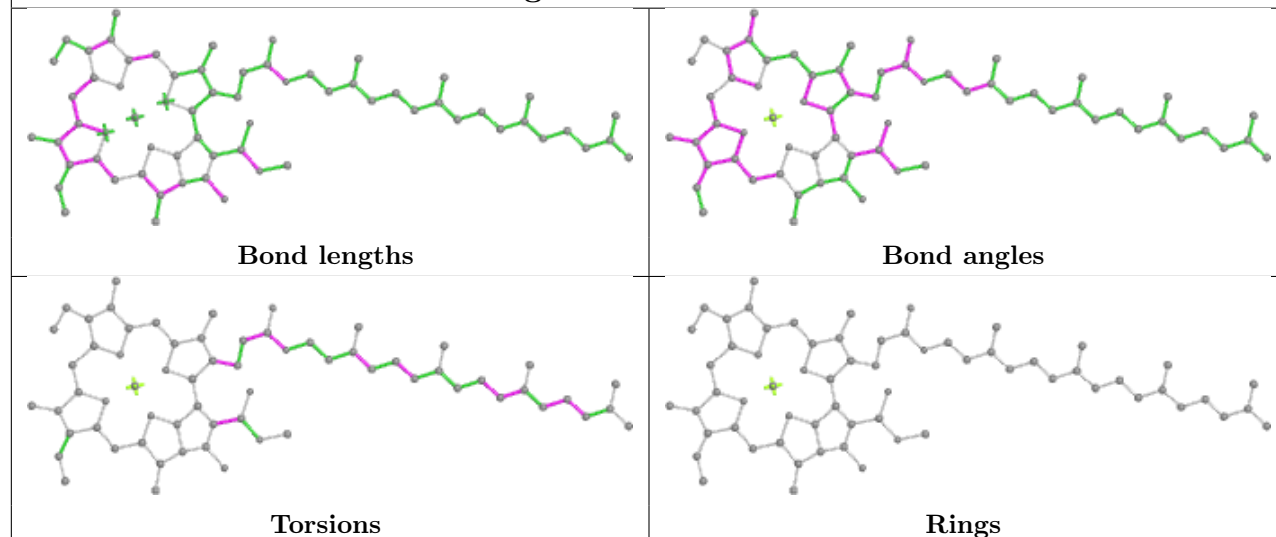
Ligand CLA cB 812

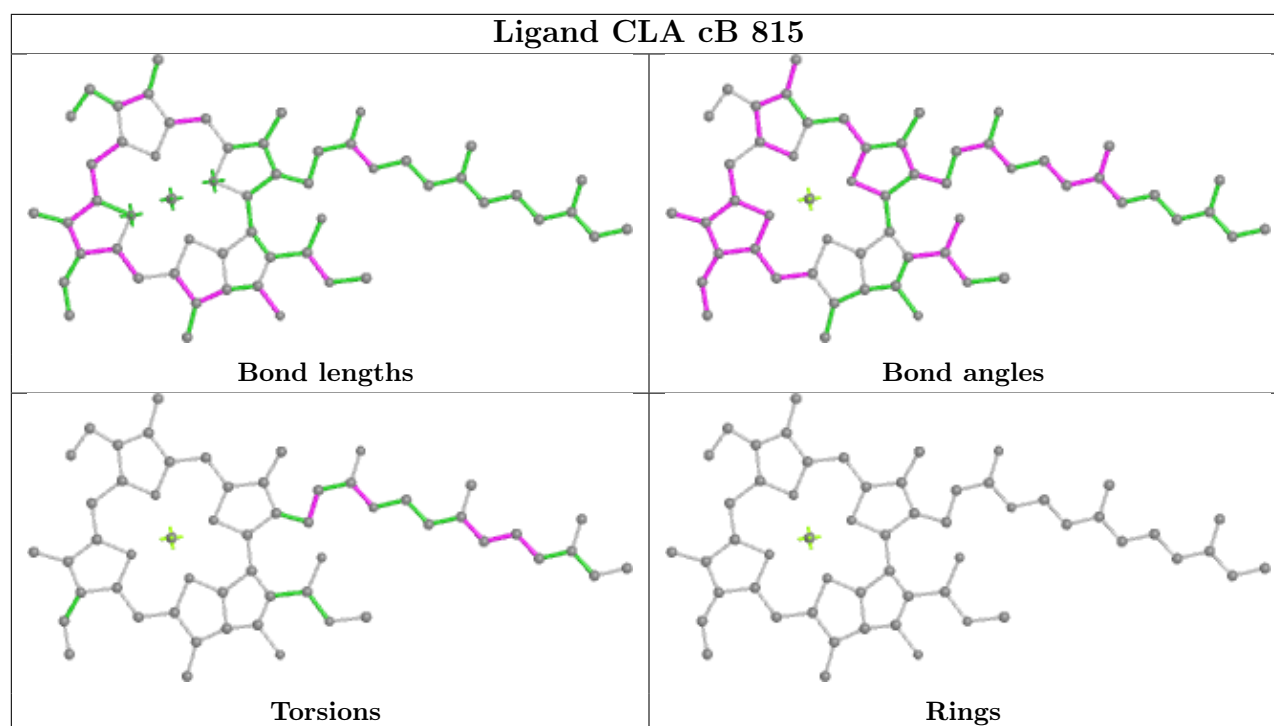


Ligand CLA cB 813

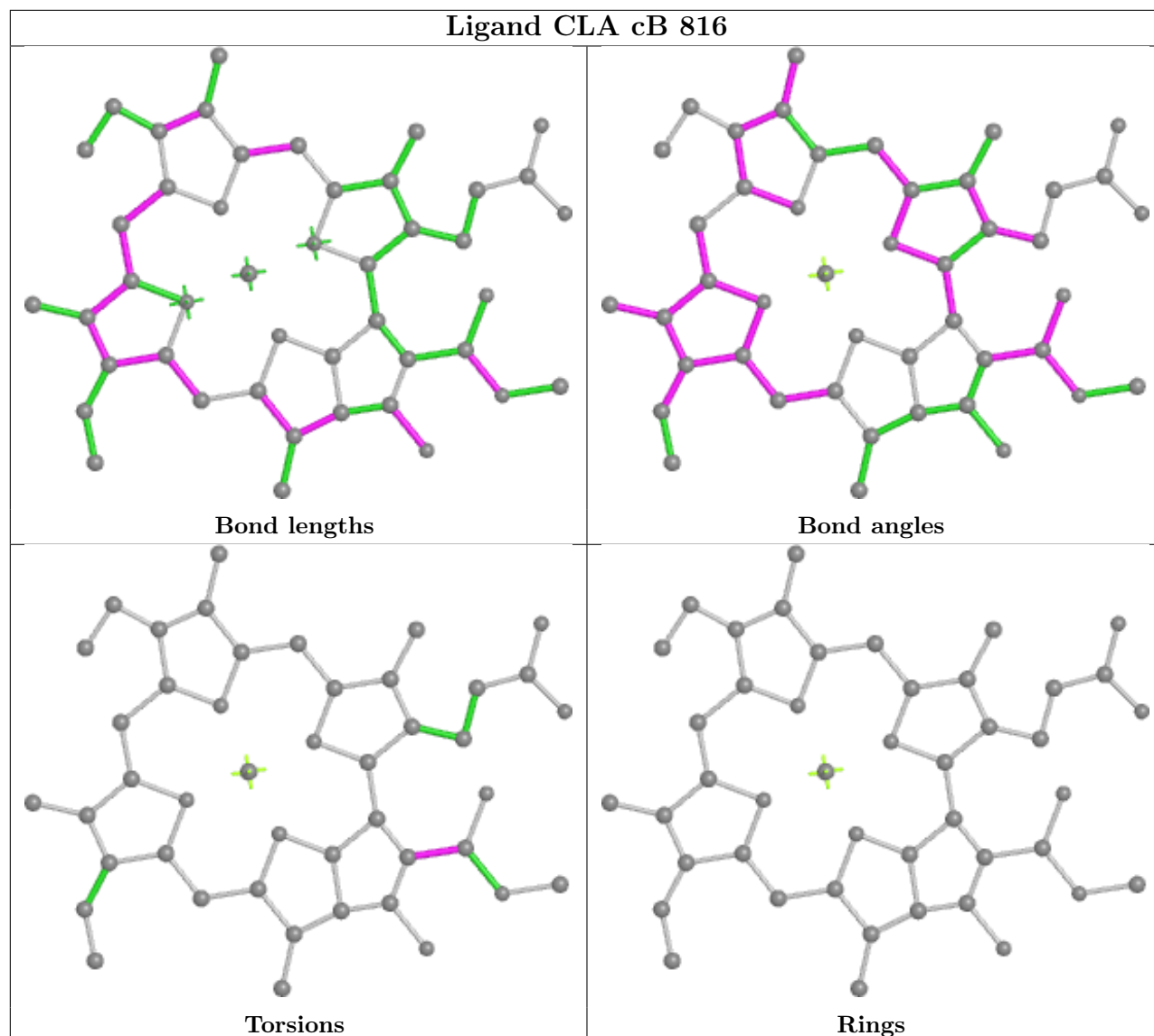


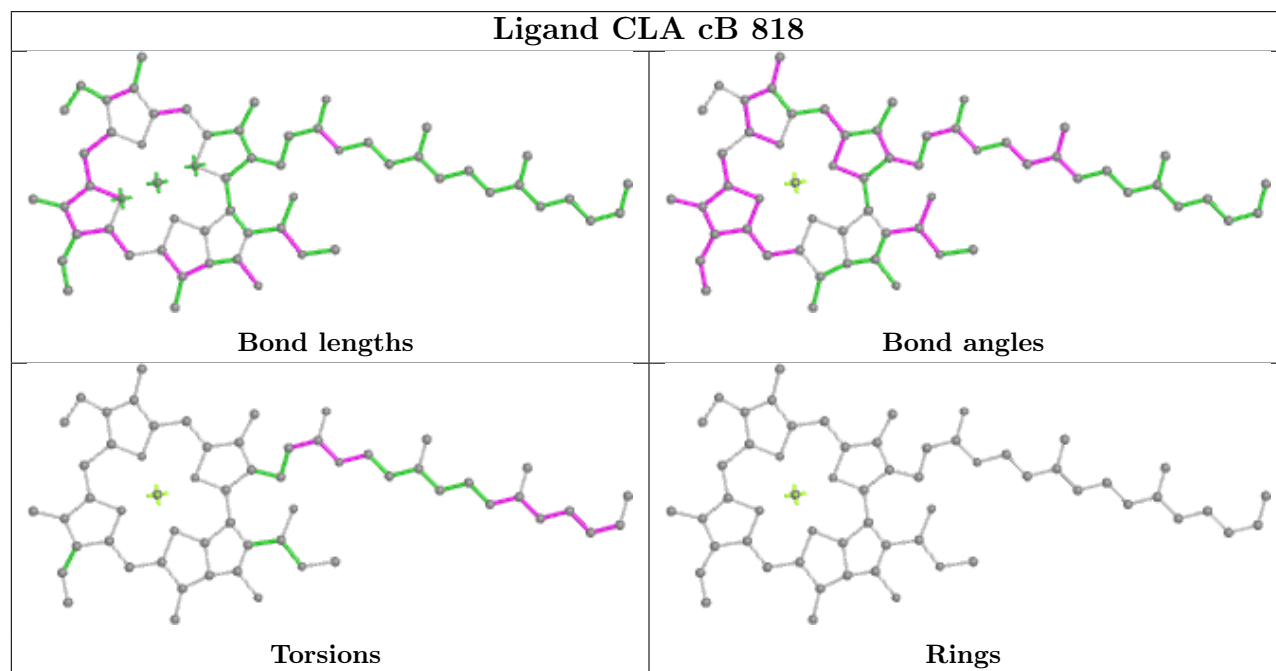
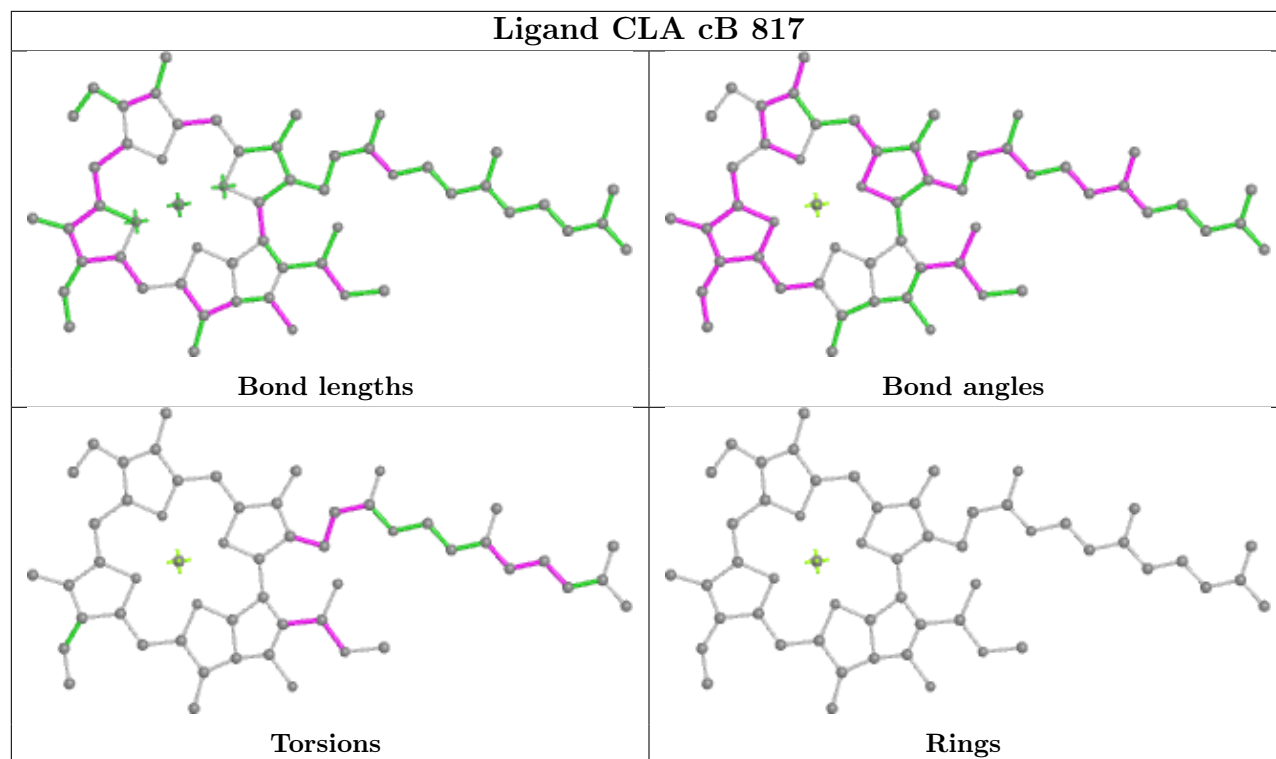
Ligand CLA cB 814

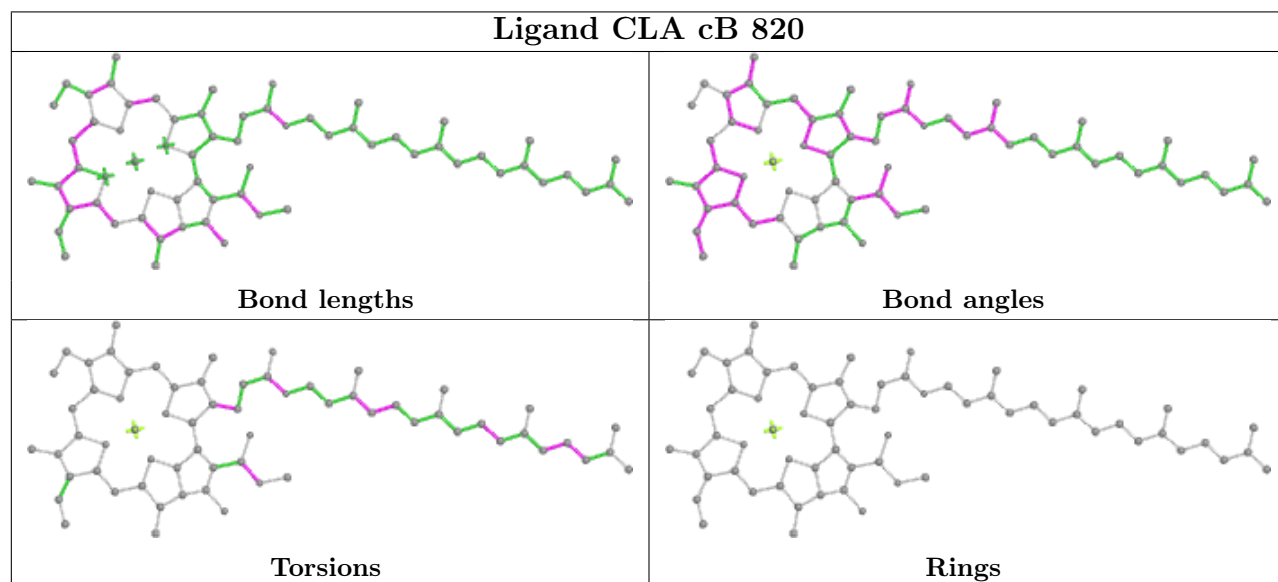
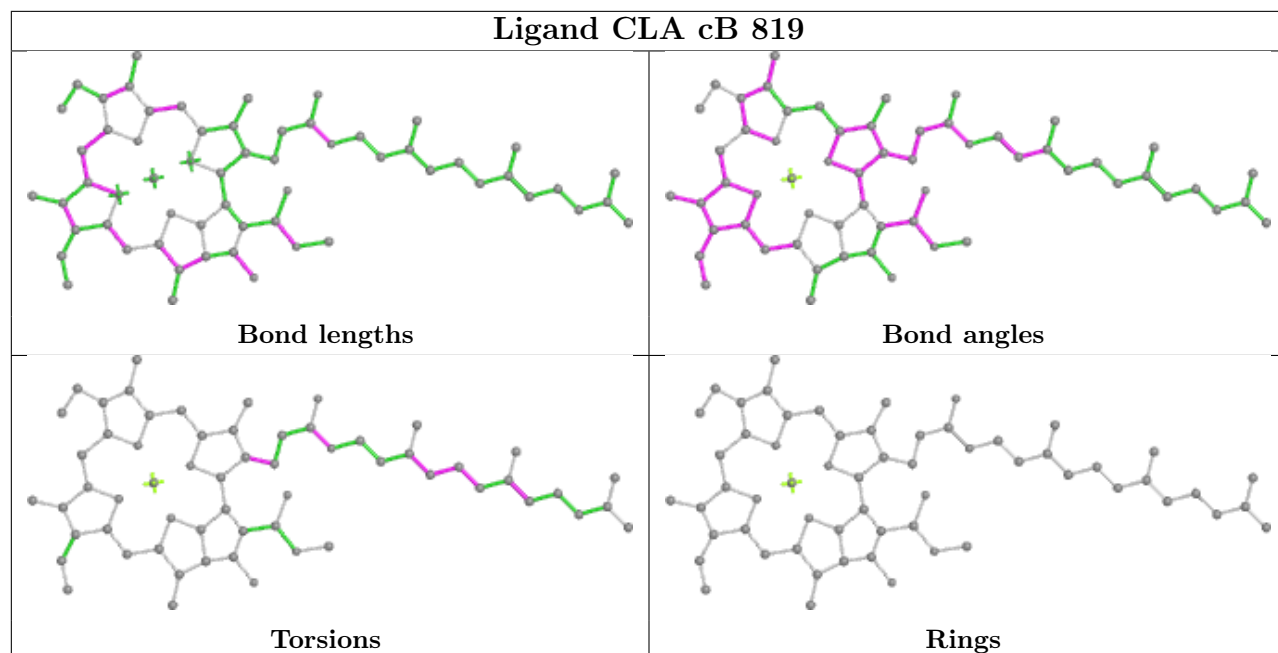


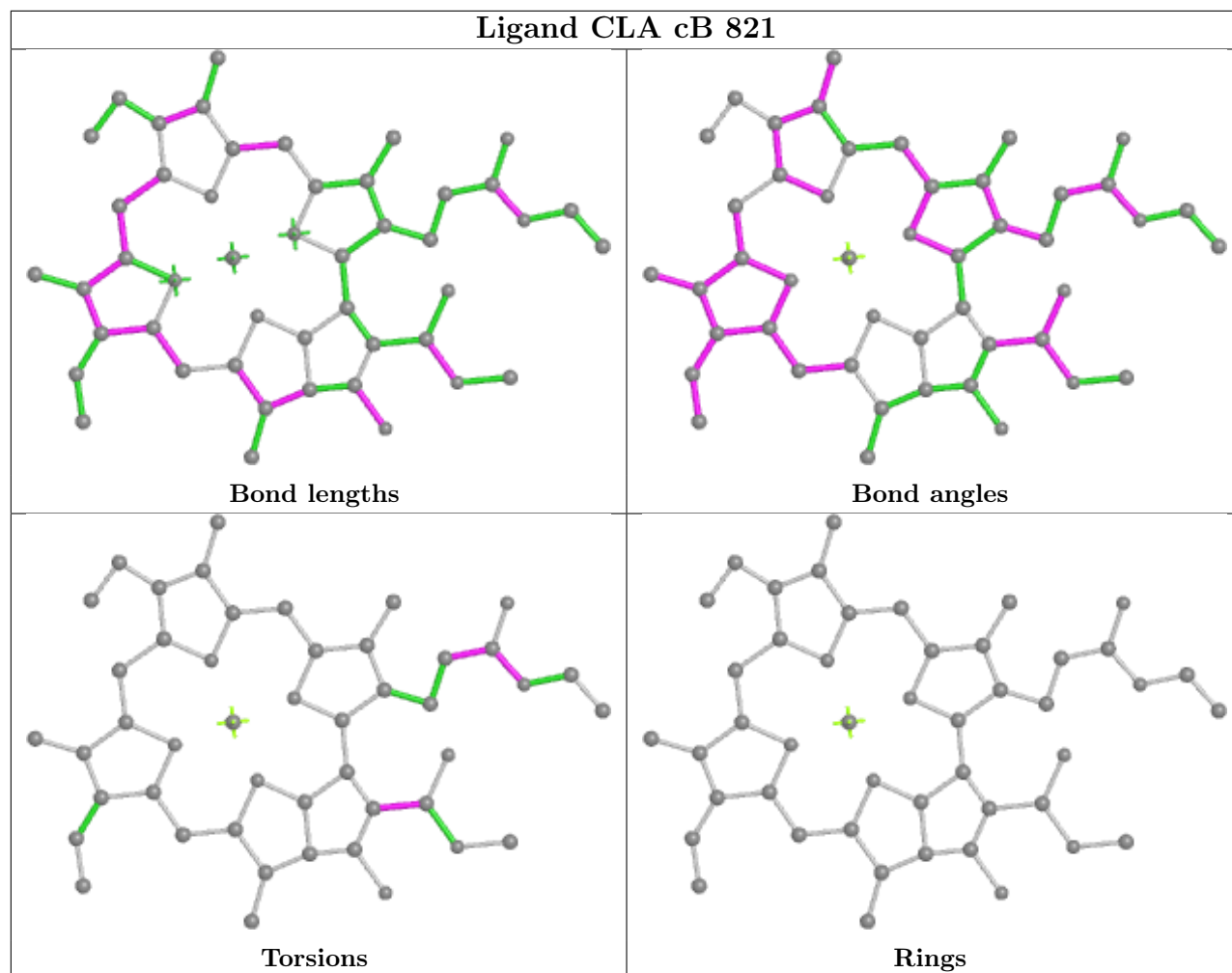


Ligand CLA cB 816

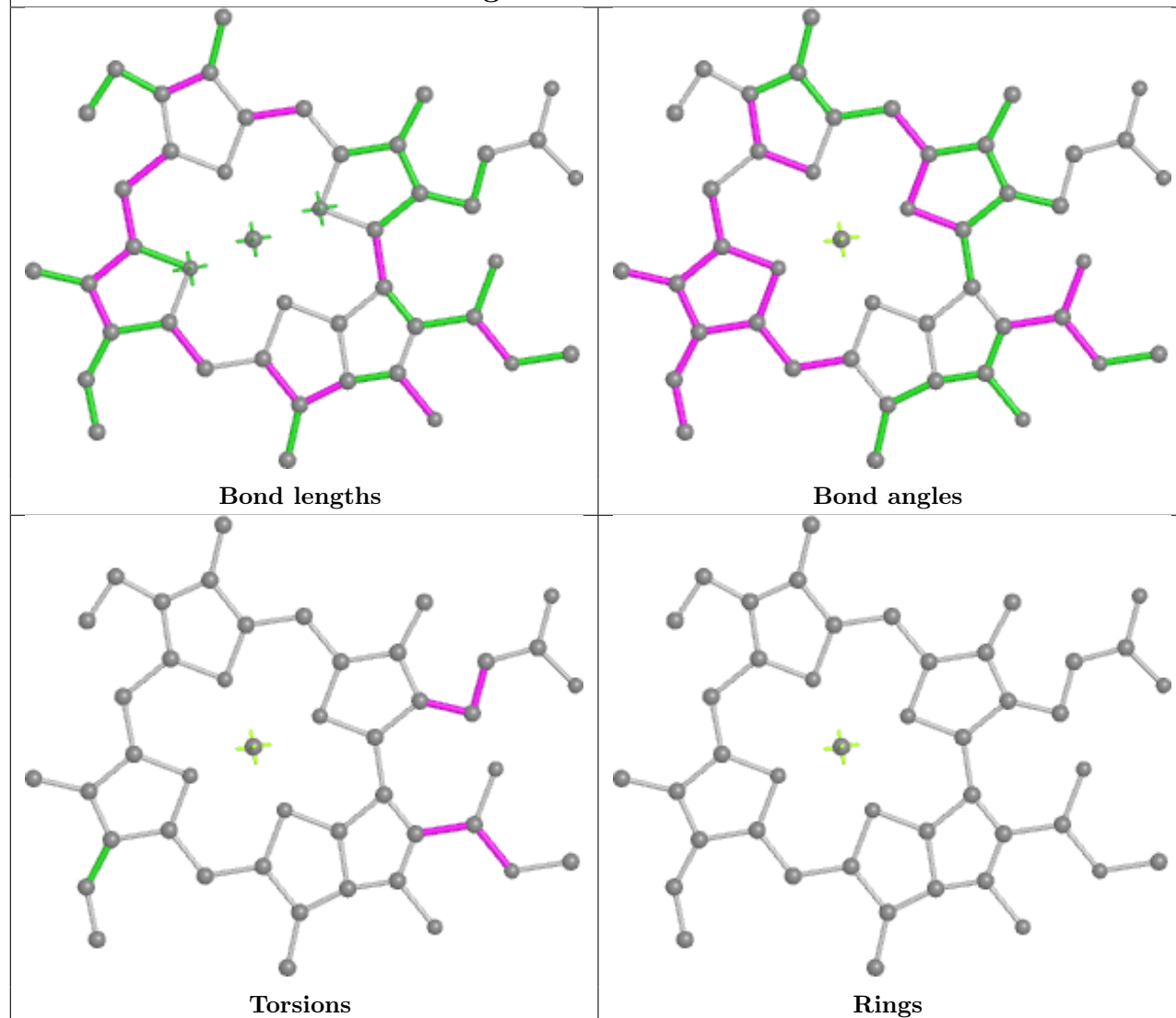


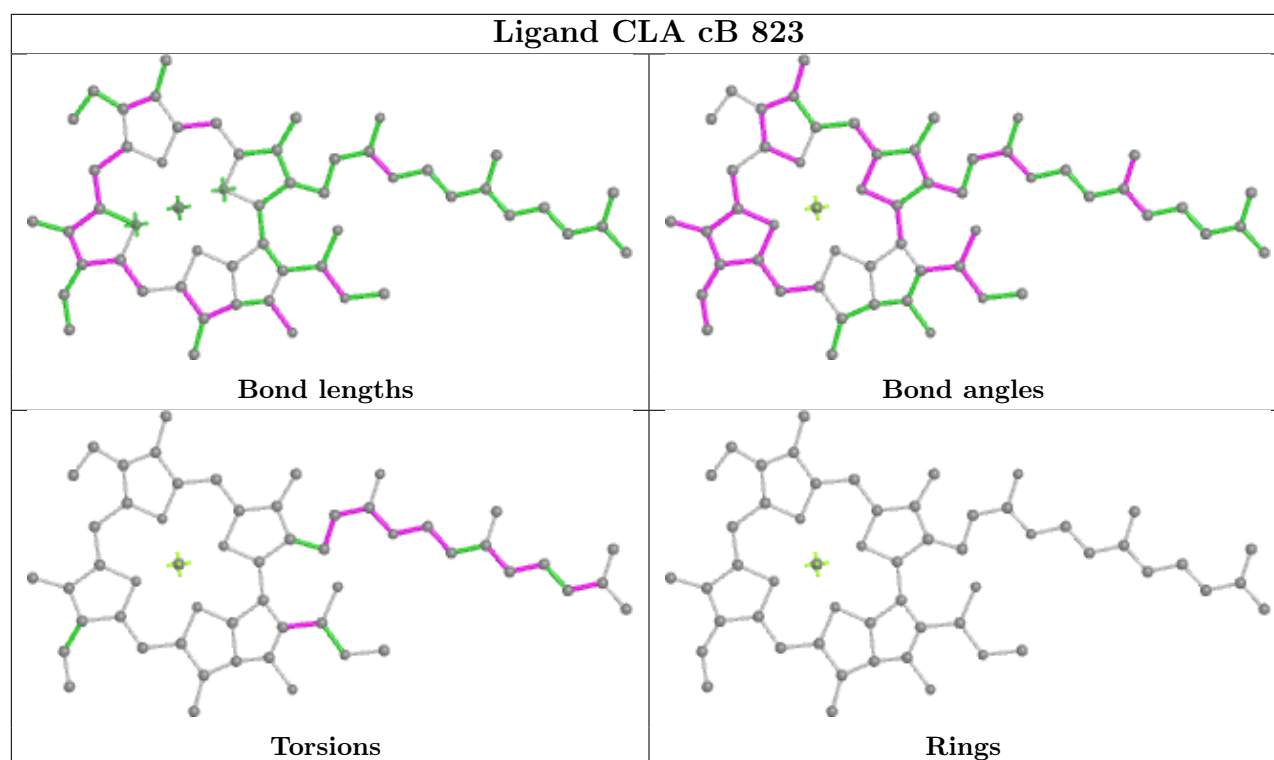




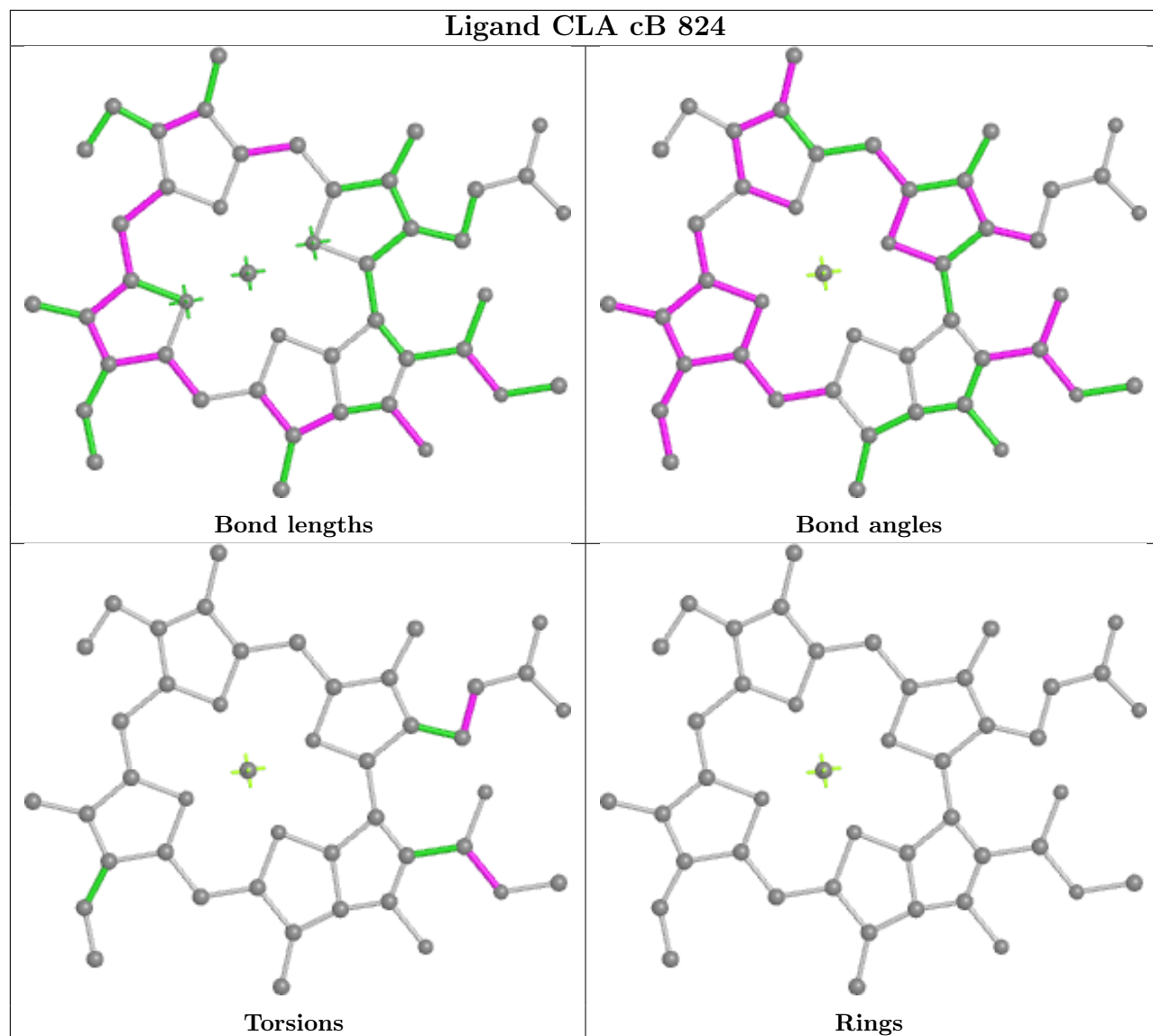


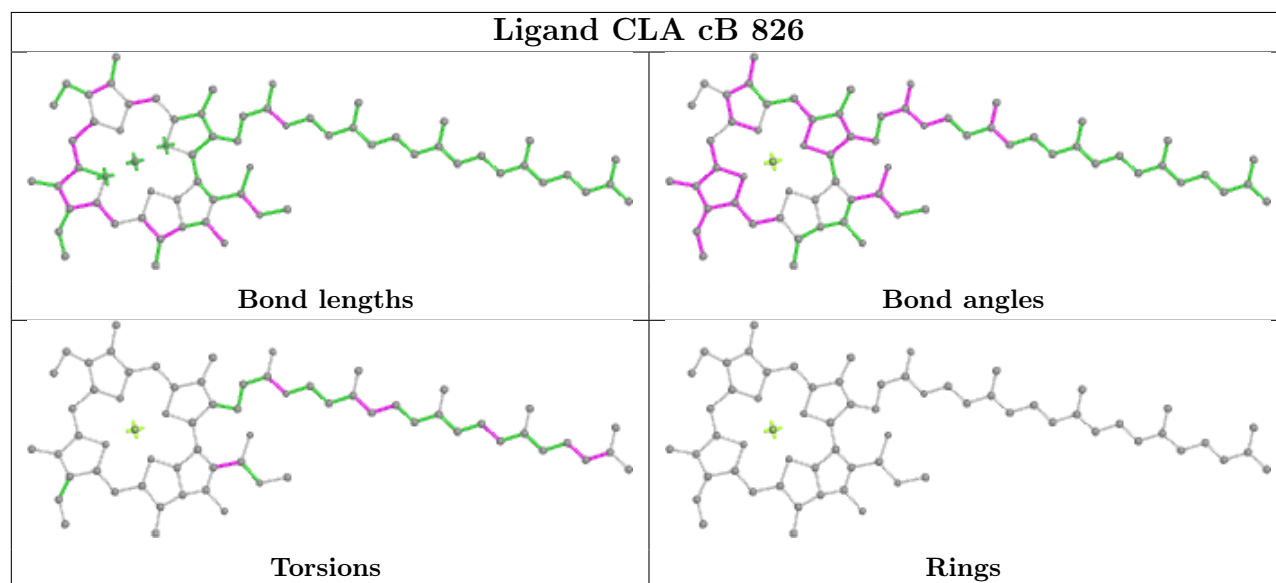
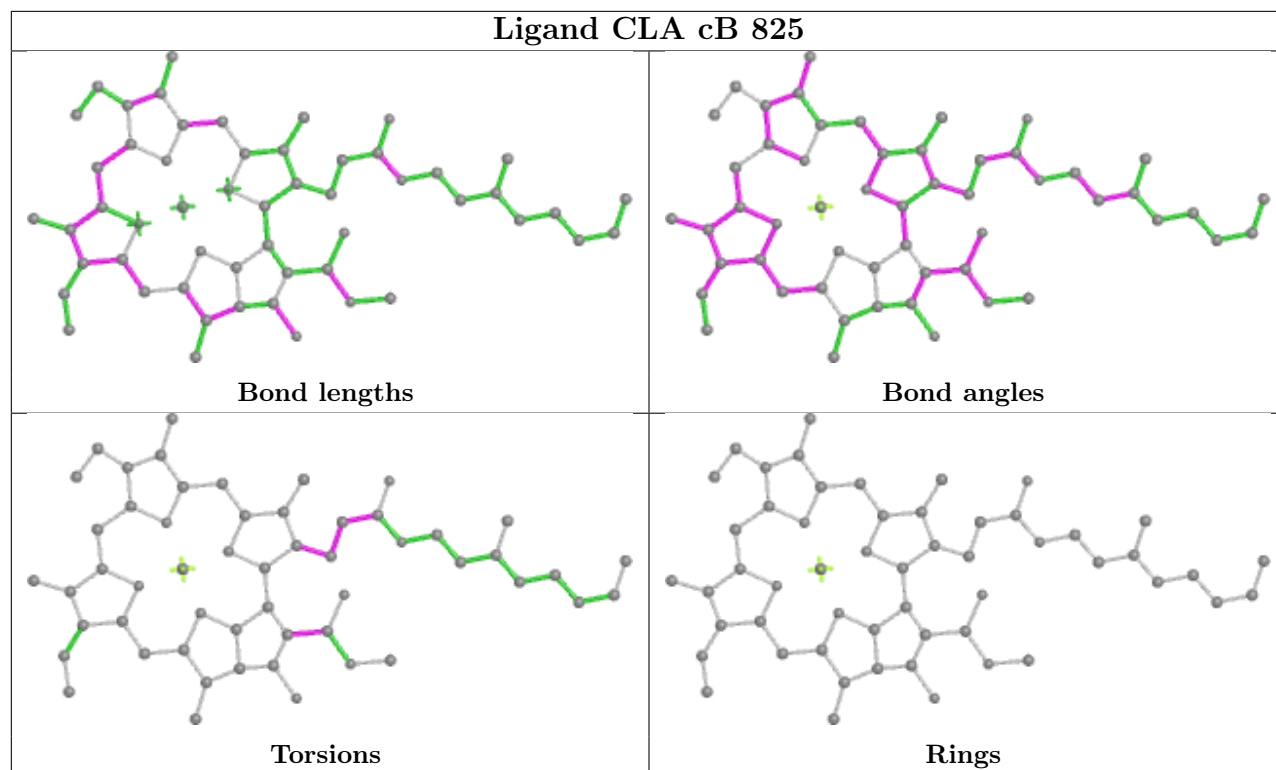
Ligand CLA cB 822

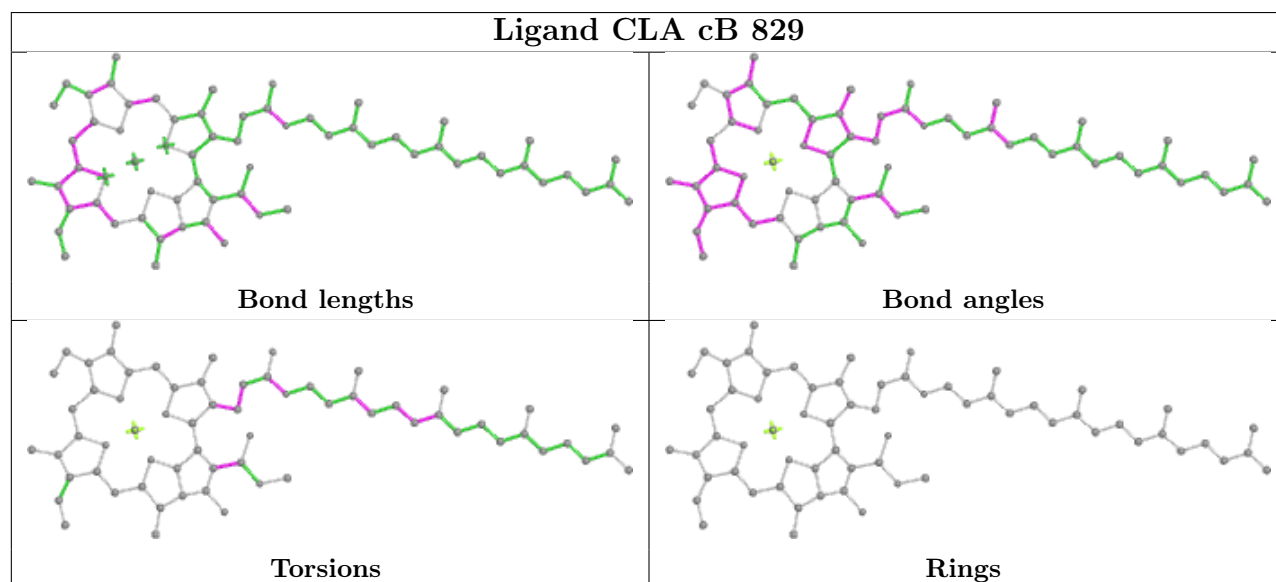
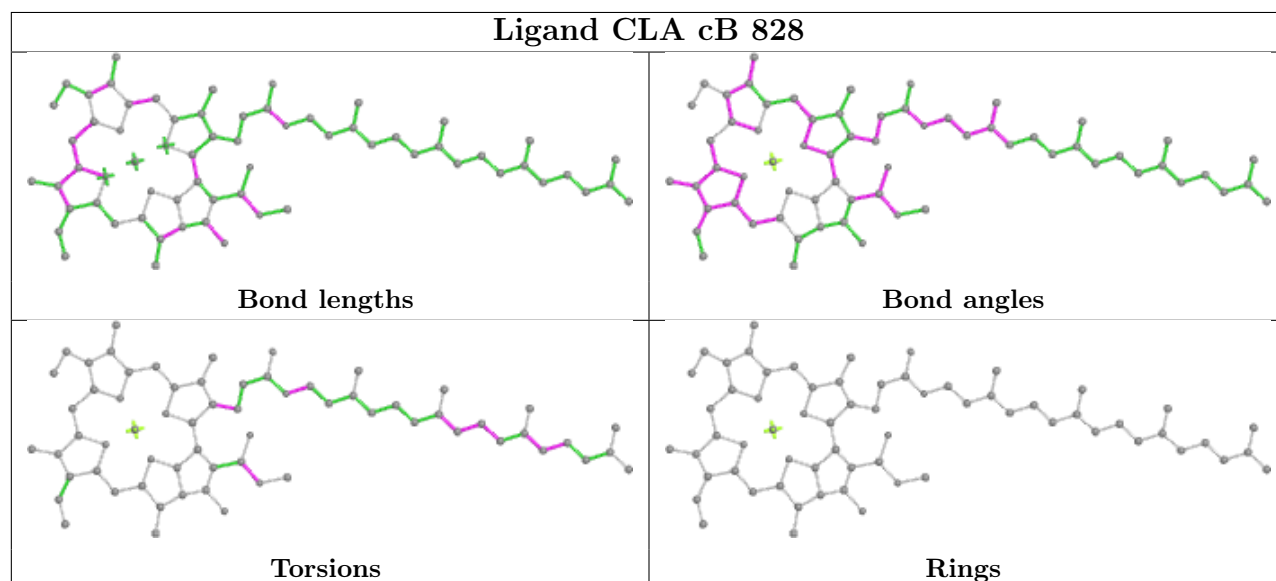
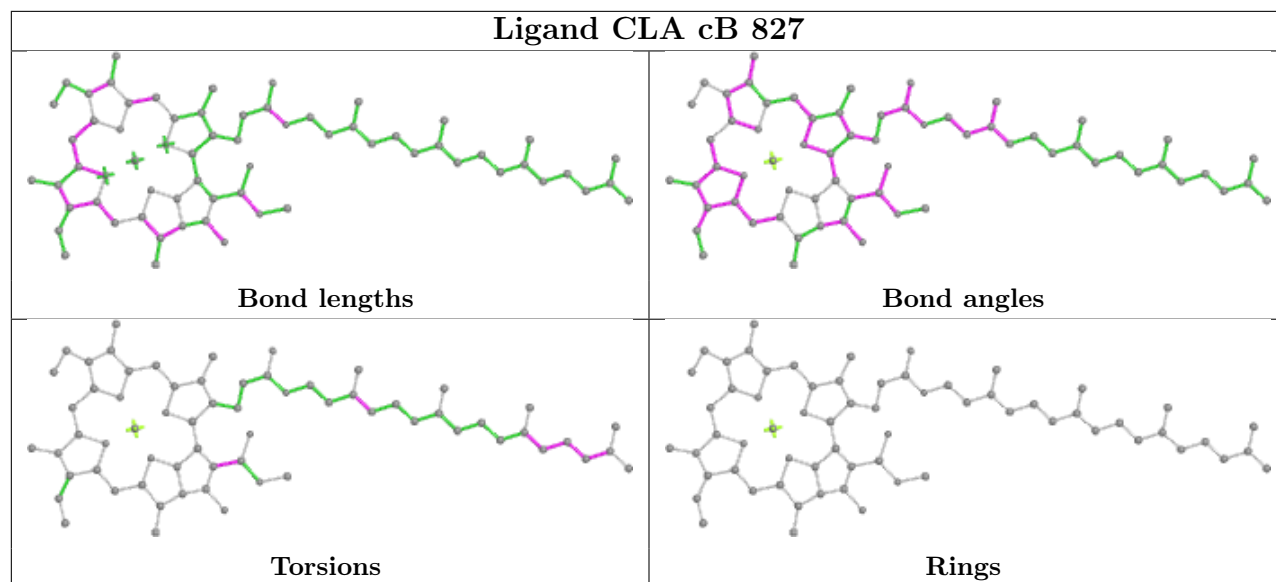


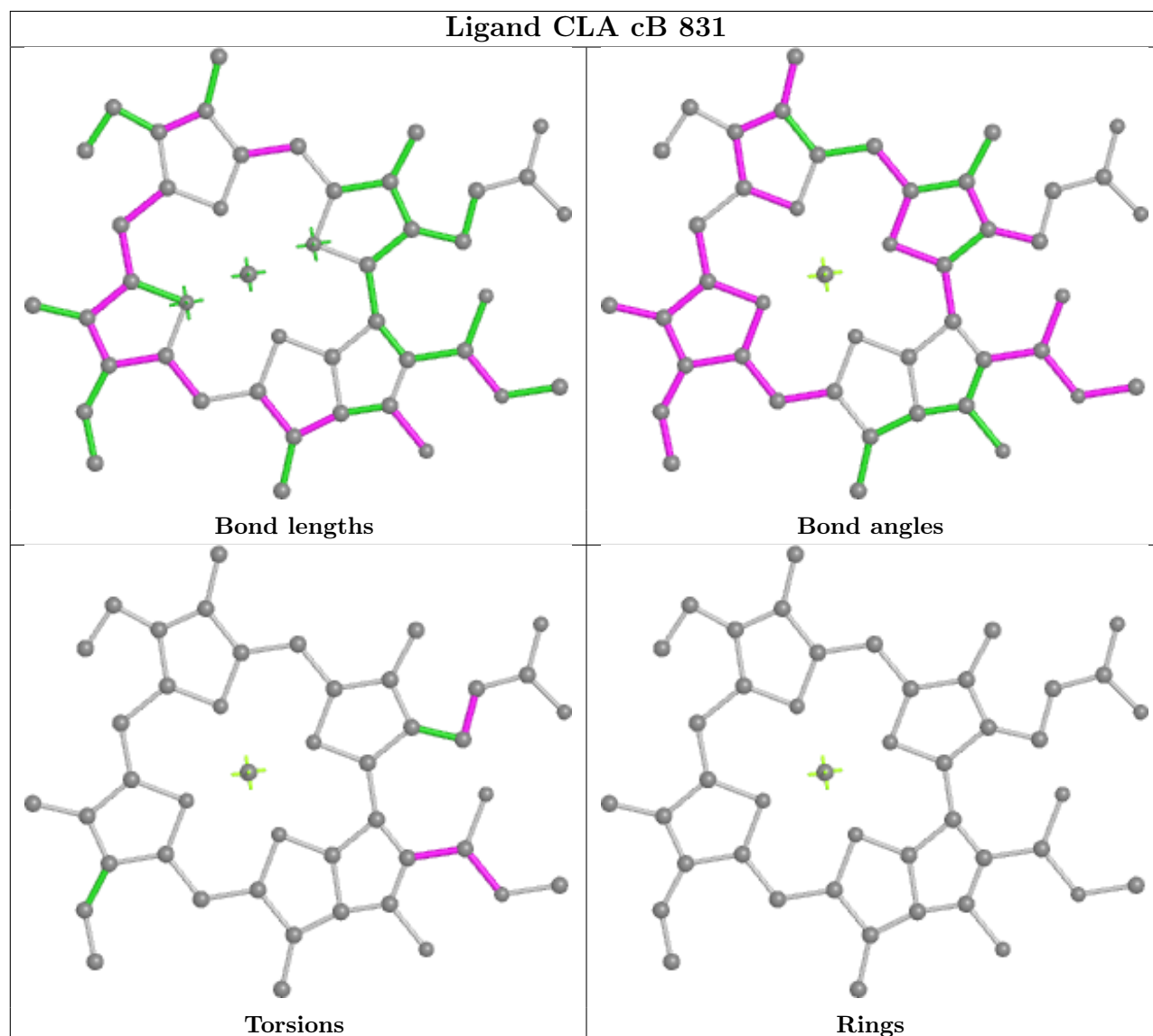
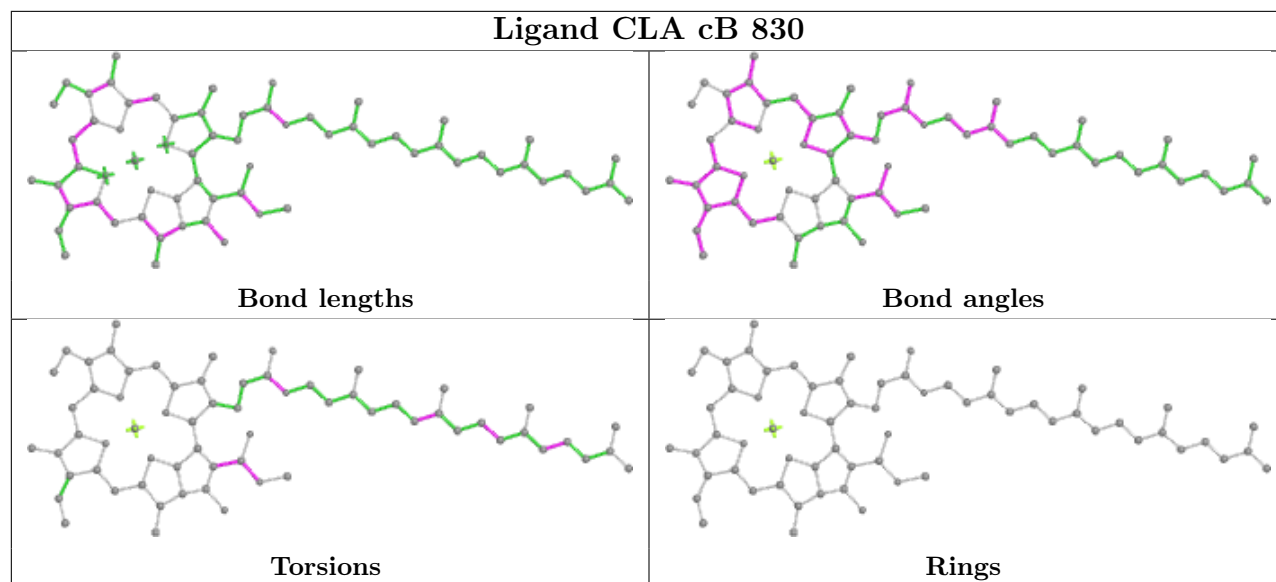


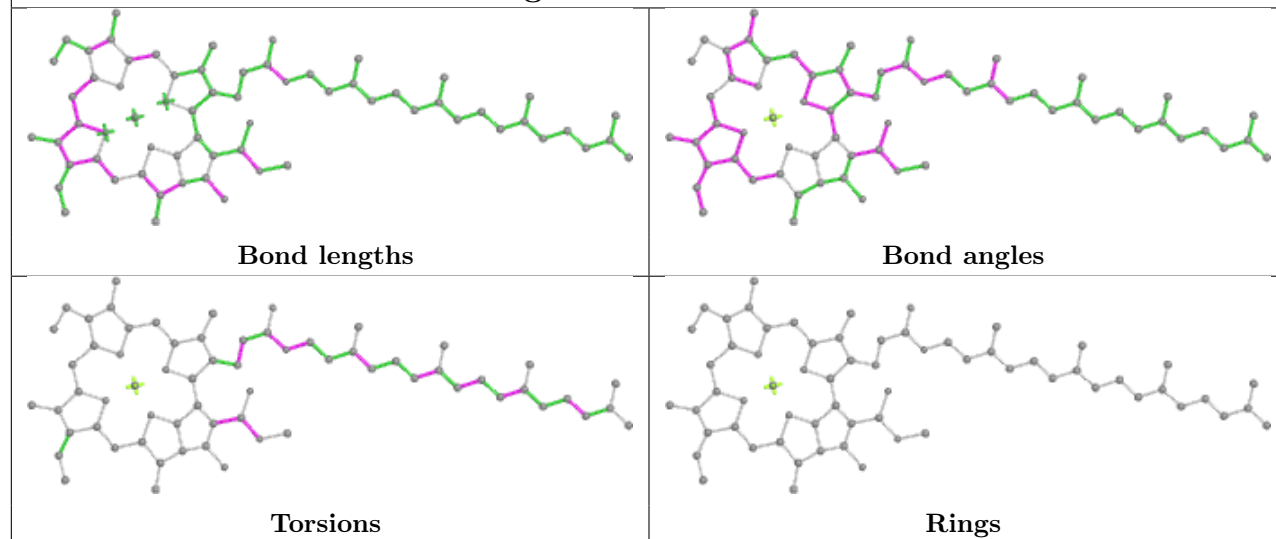
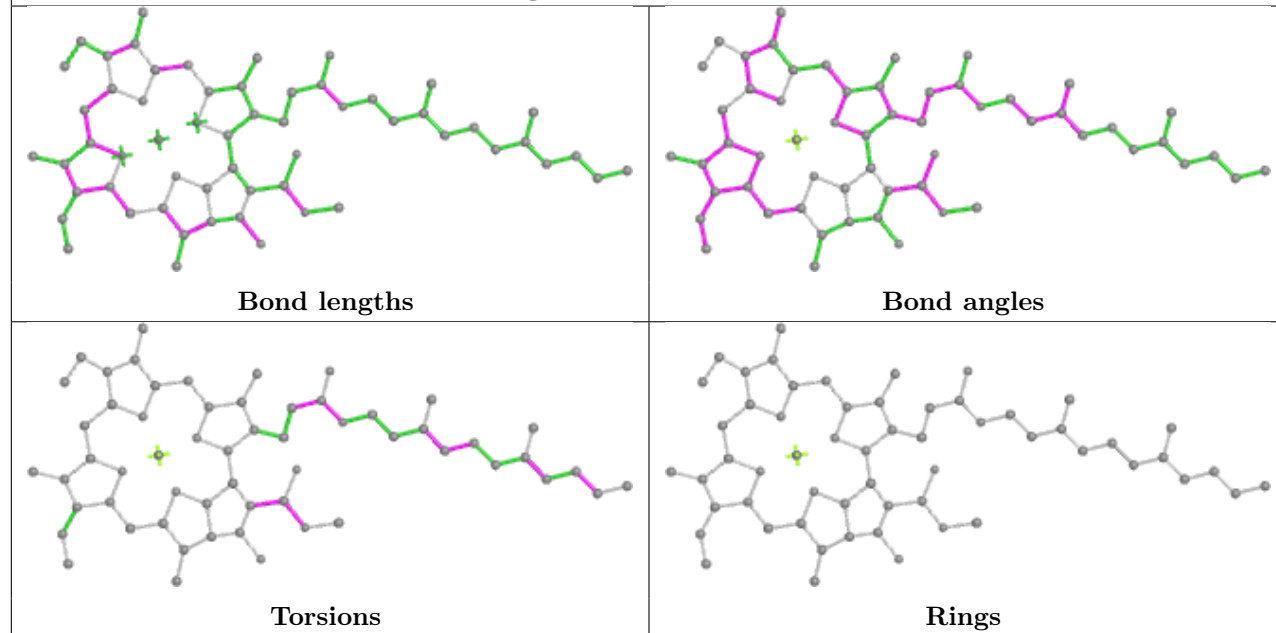
Ligand CLA cB 824



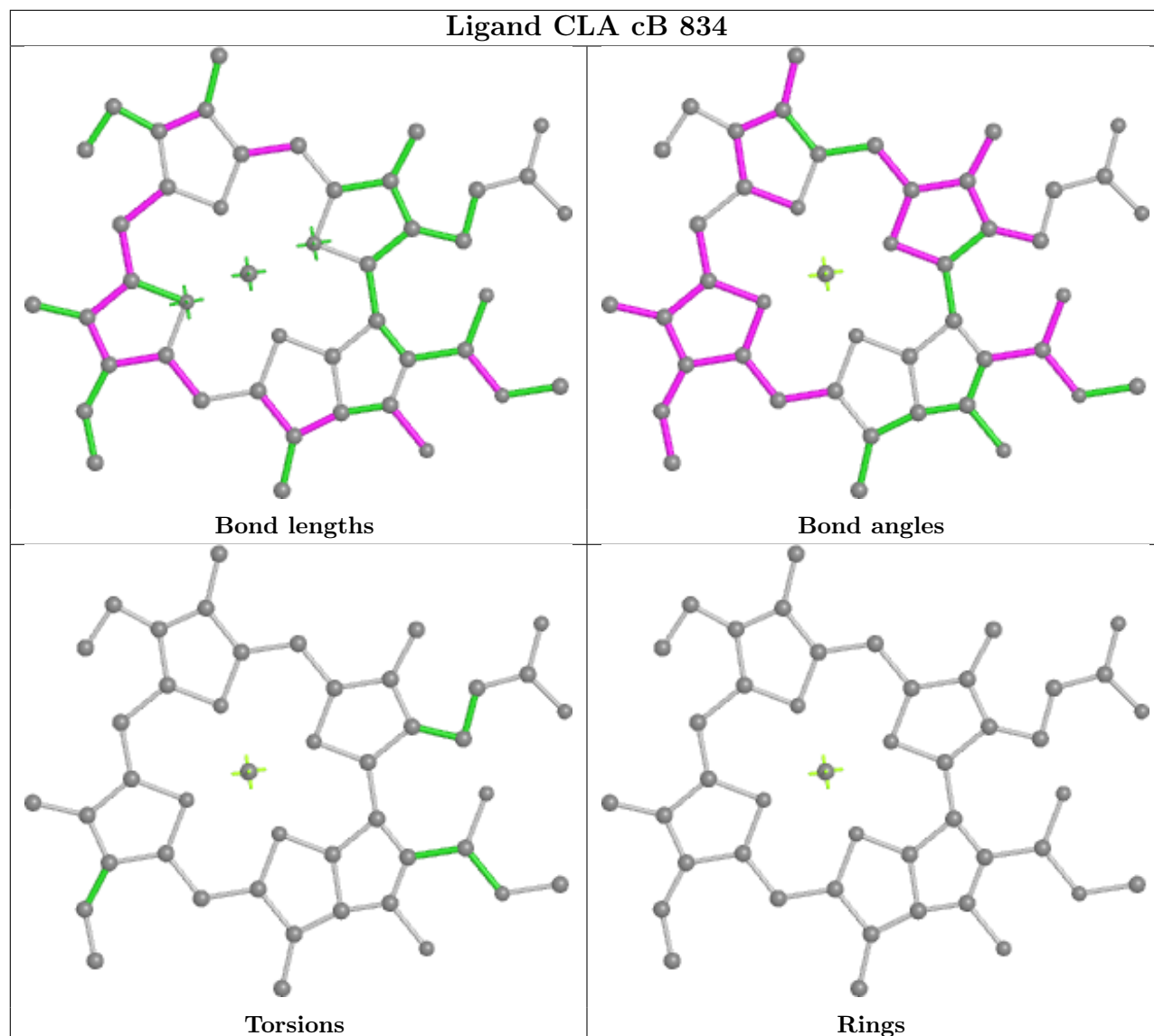




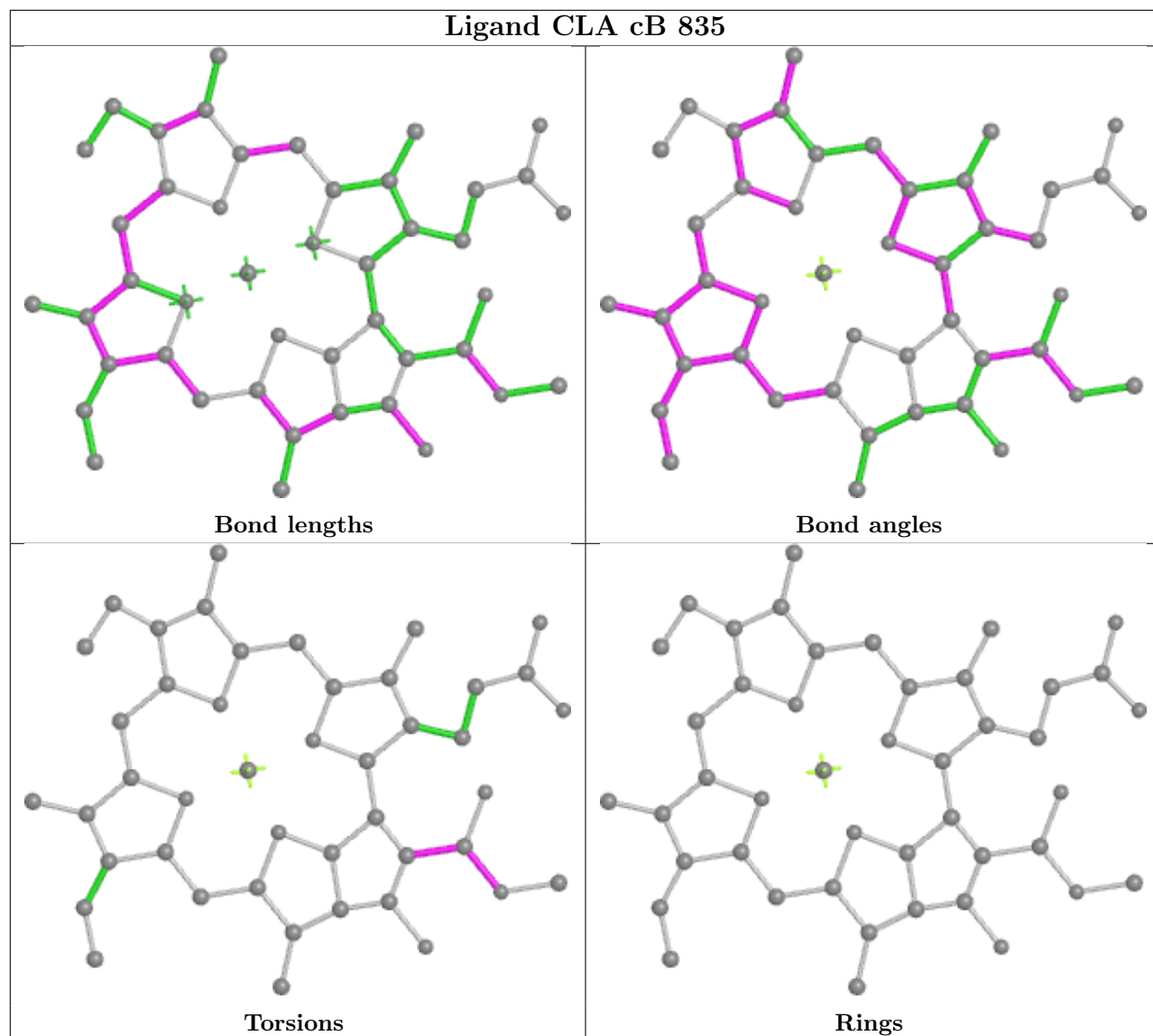


Ligand CLA cB 832**Ligand CLA cB 833**

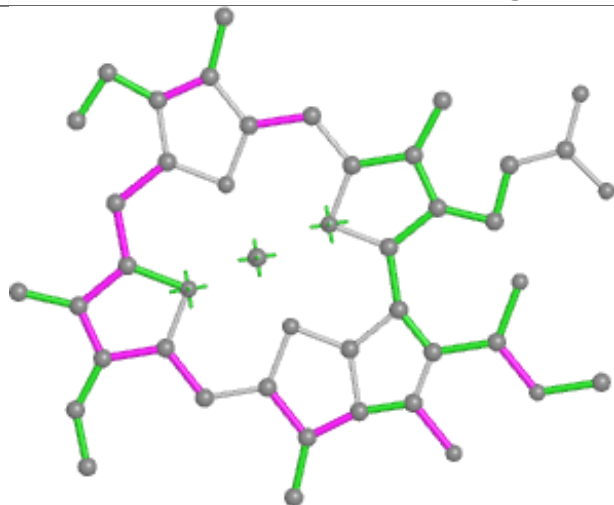
Ligand CLA cB 834



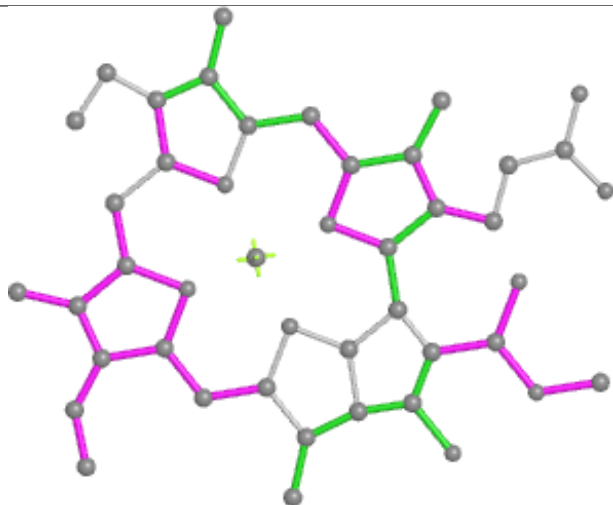
Ligand CLA cB 835



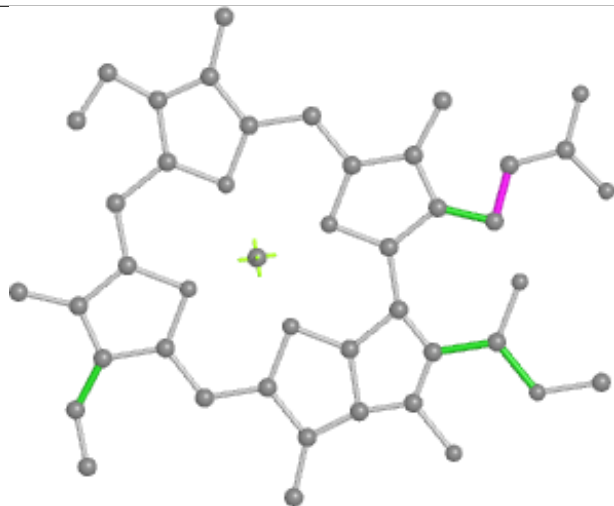
Ligand CLA cB 836



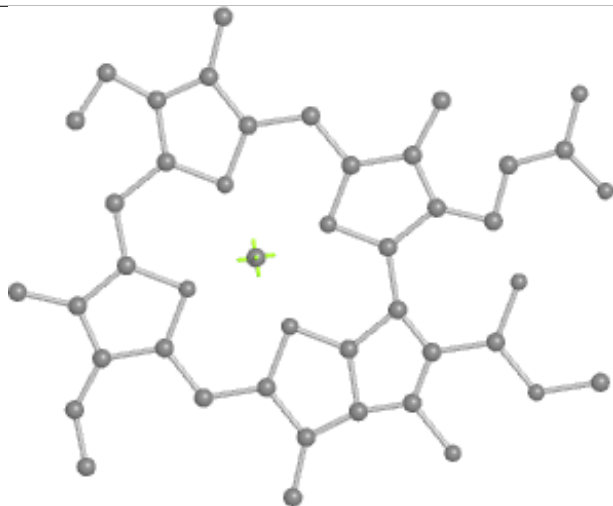
Bond lengths



Bond angles

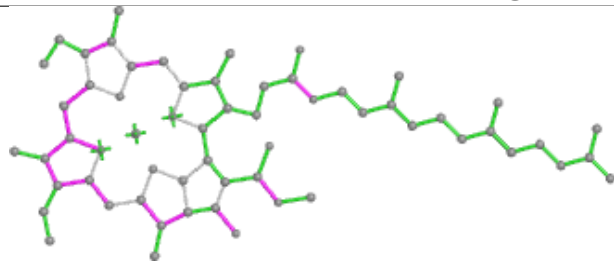


Torsions

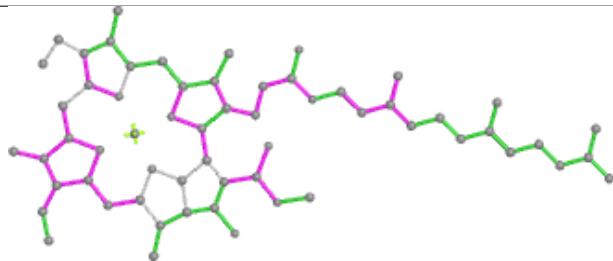


Rings

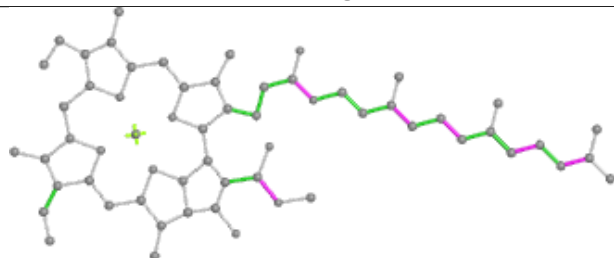
Ligand CLA cB 837



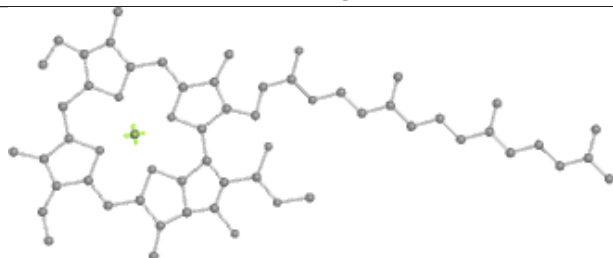
Bond lengths



Bond angles

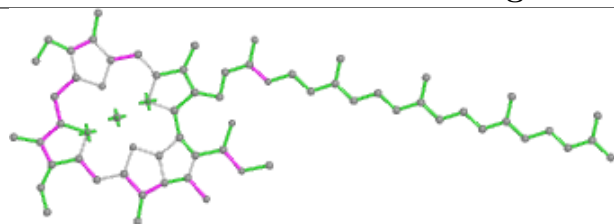


Torsions

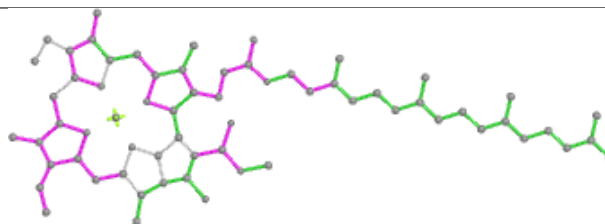


Rings

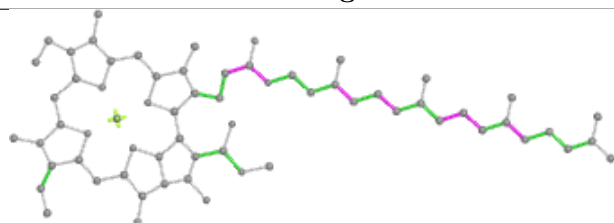
Ligand CLA cB 838



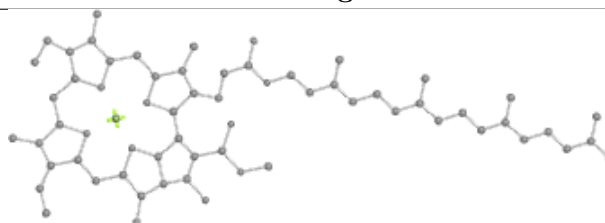
Bond lengths



Bond angles

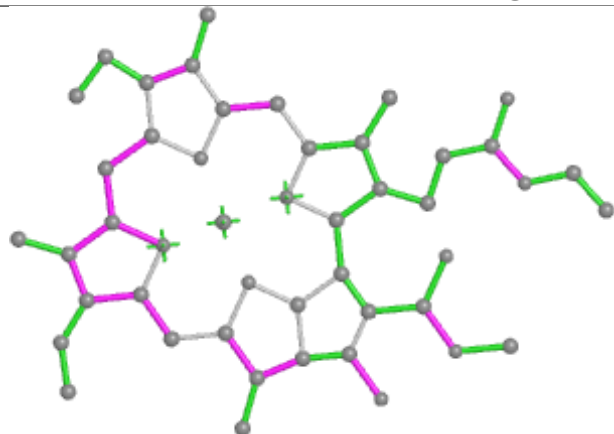


Torsions

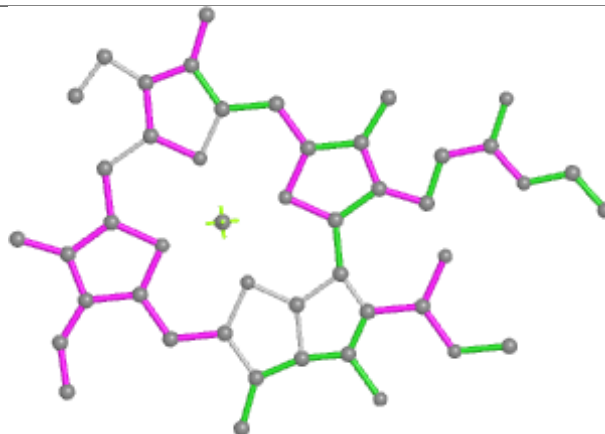


Rings

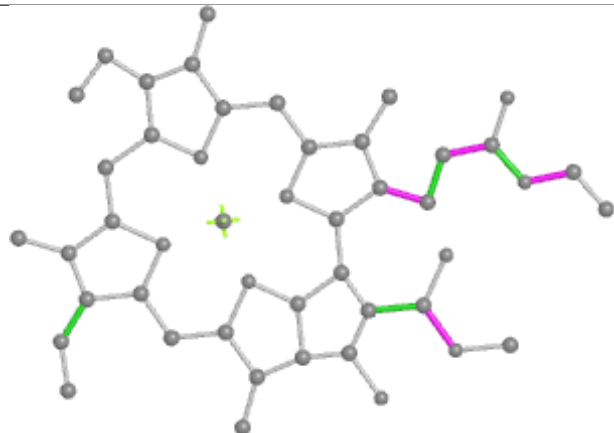
Ligand CLA cB 839



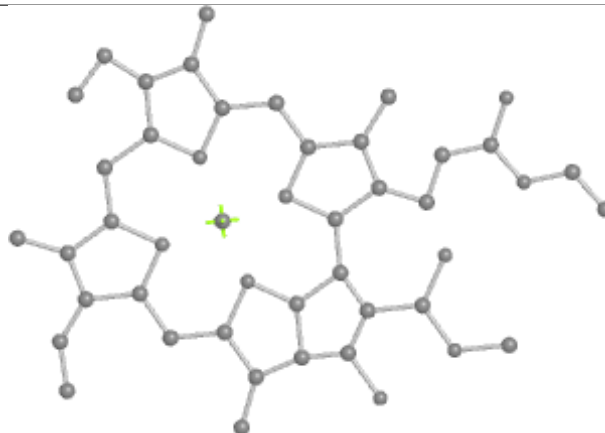
Bond lengths



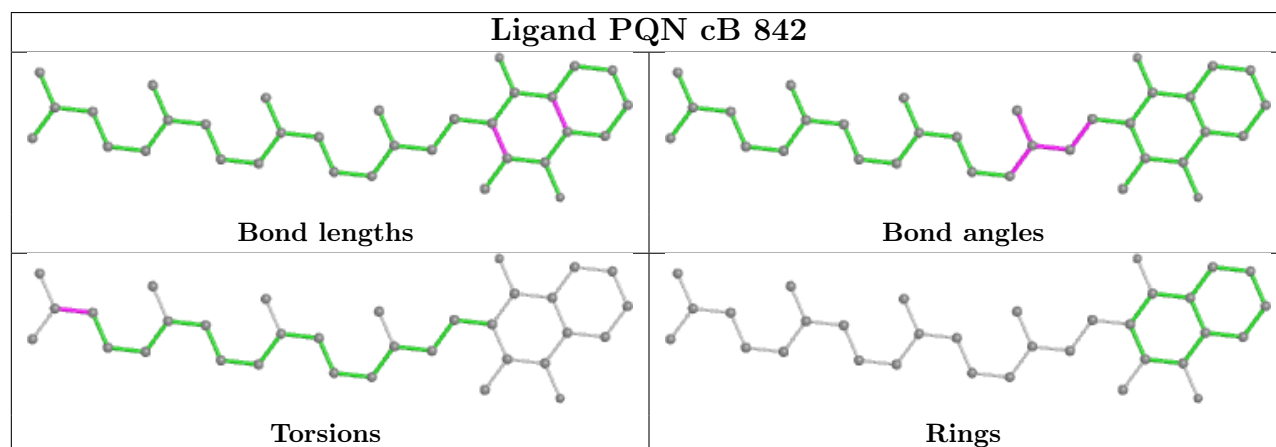
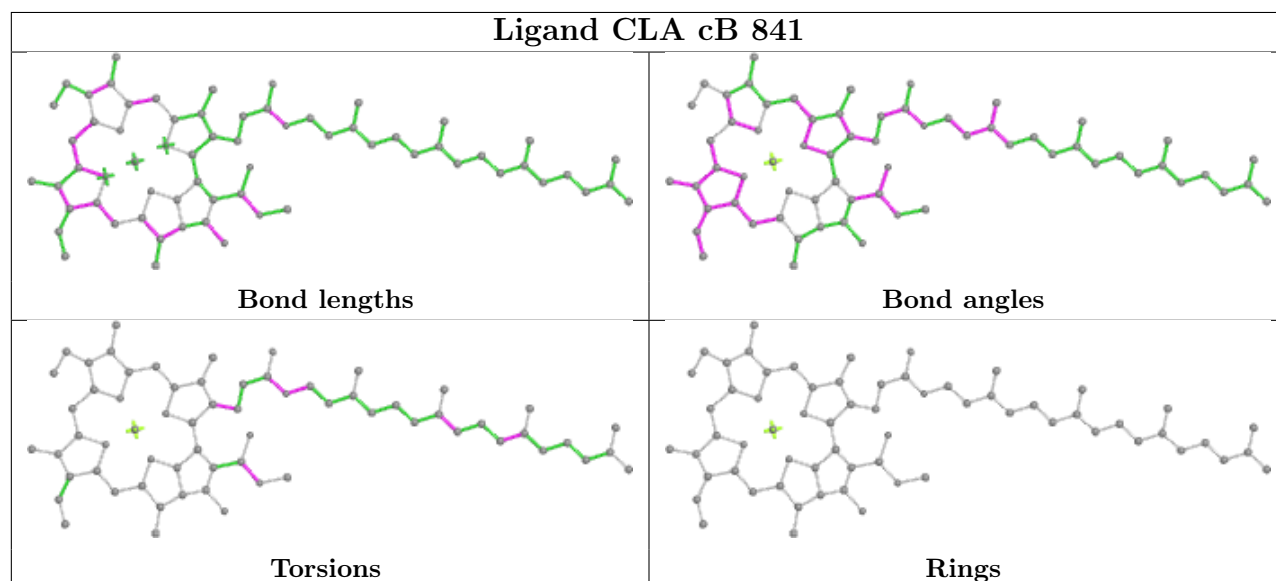
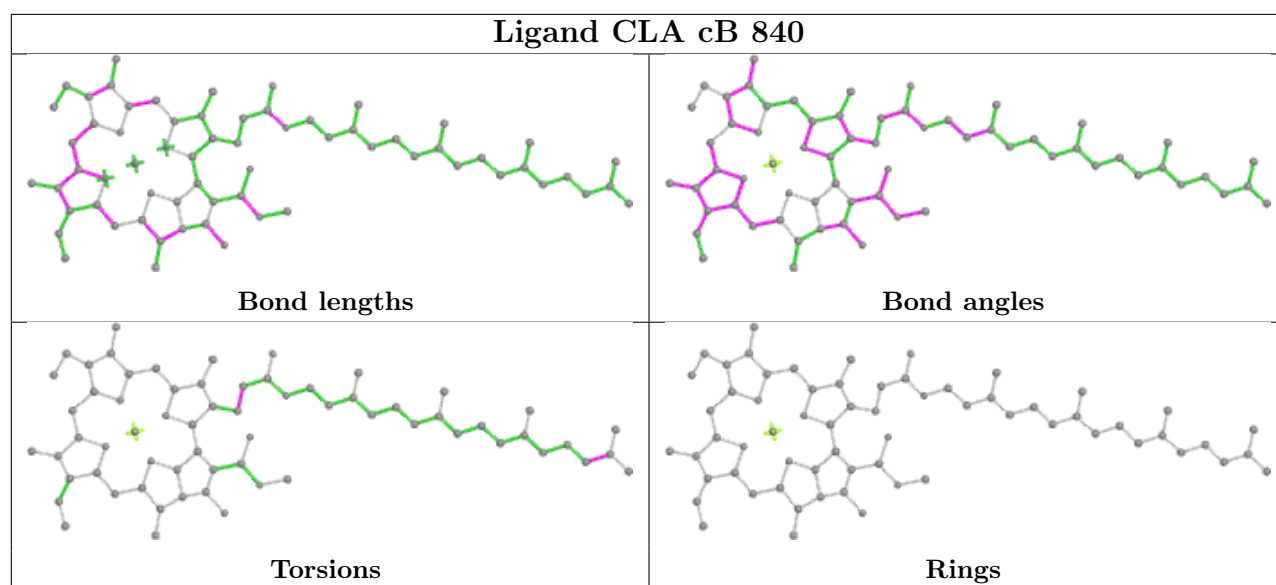
Bond angles

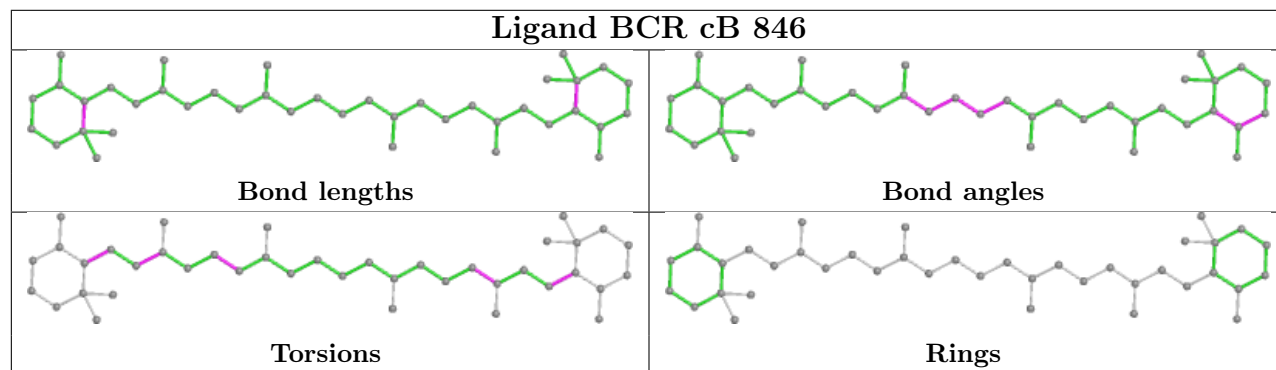
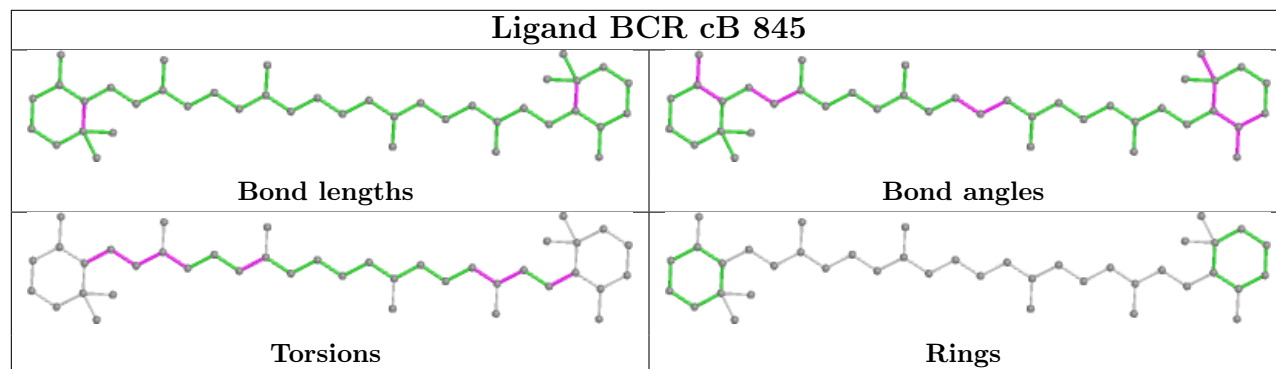
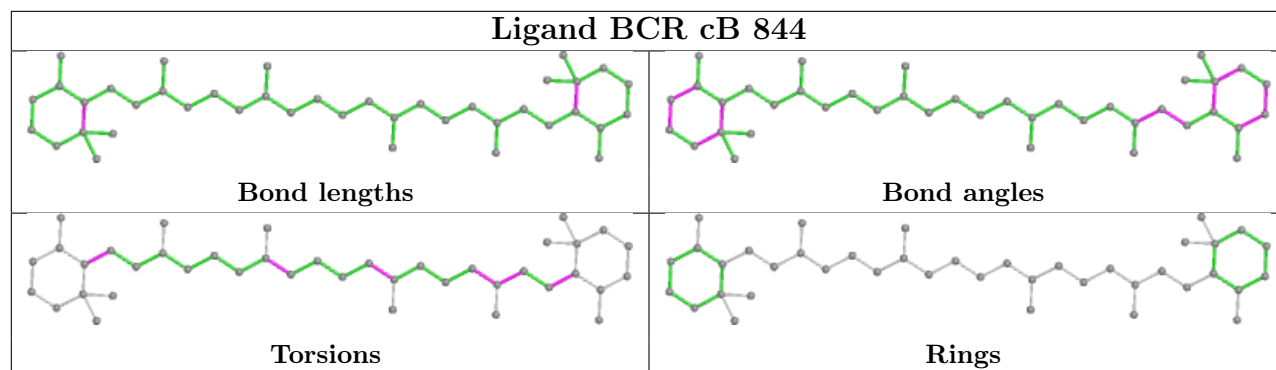
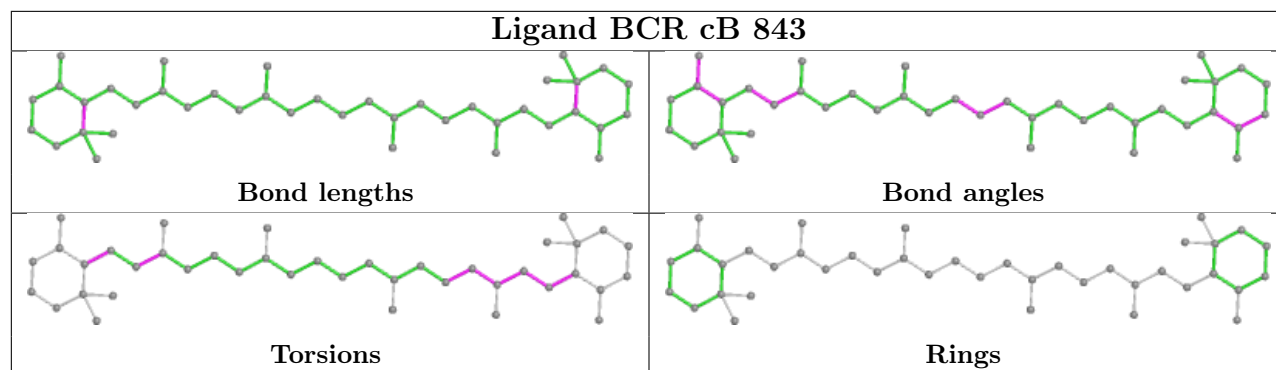


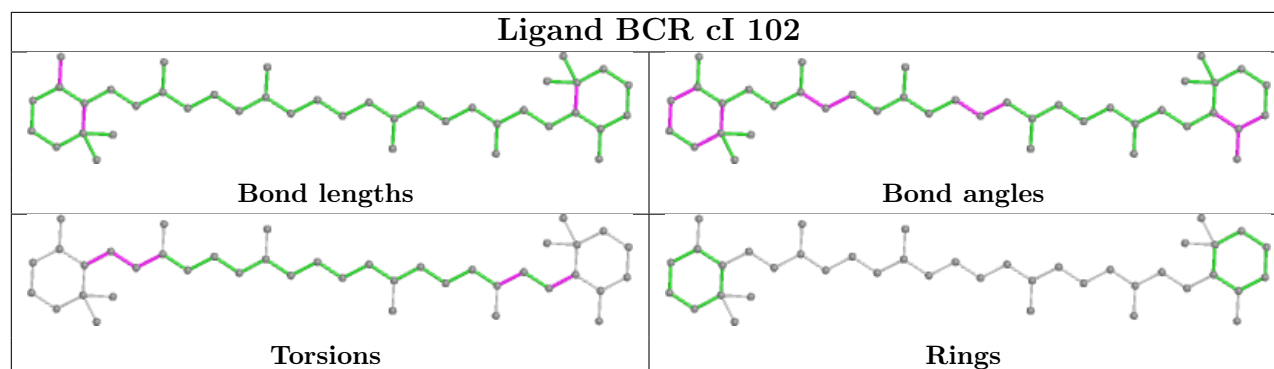
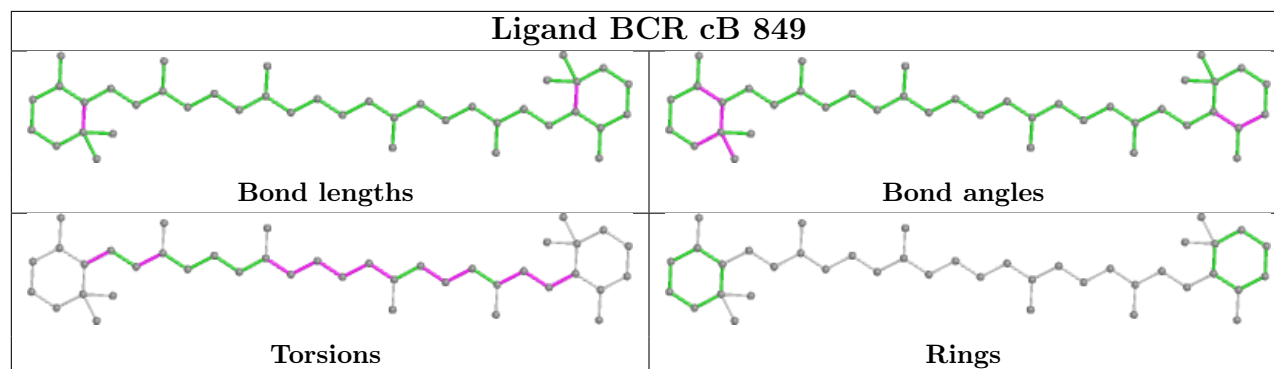
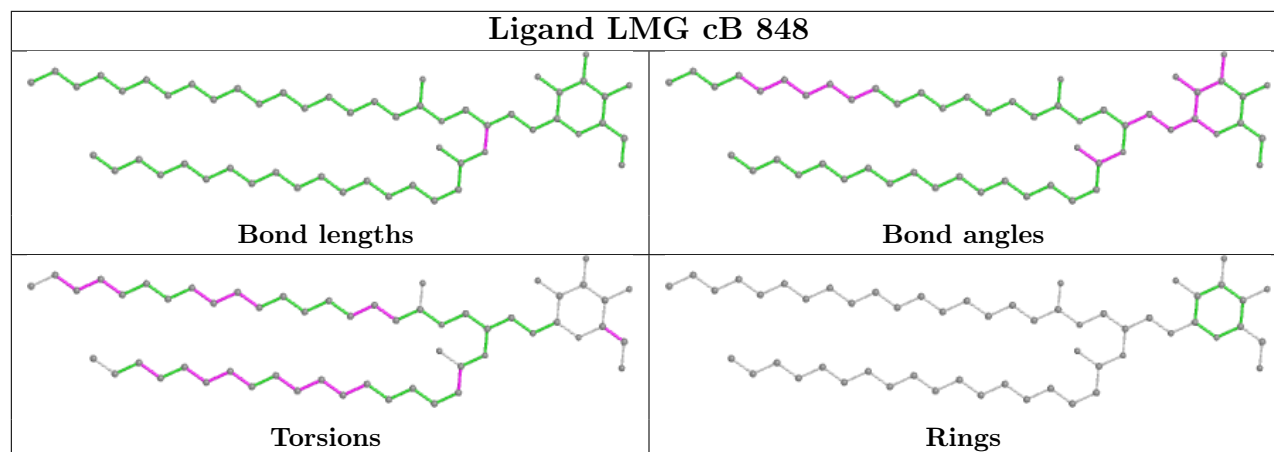
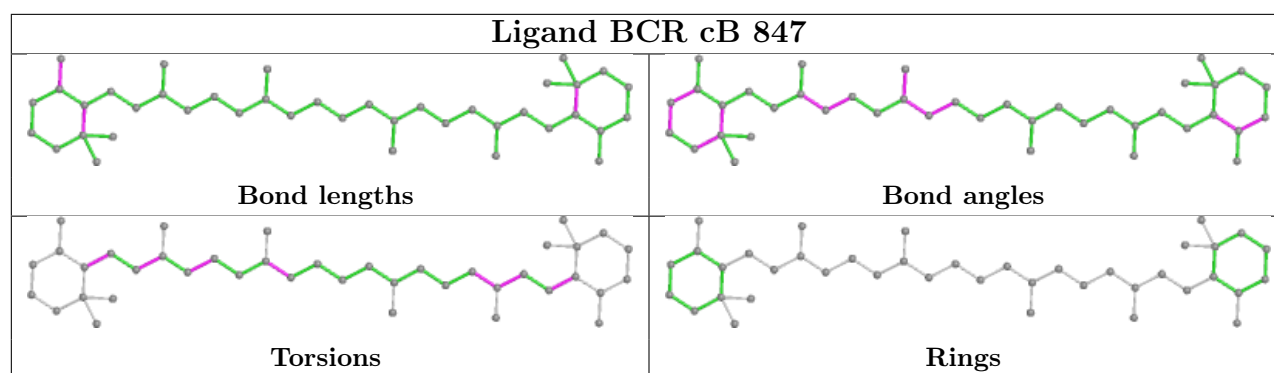
Torsions

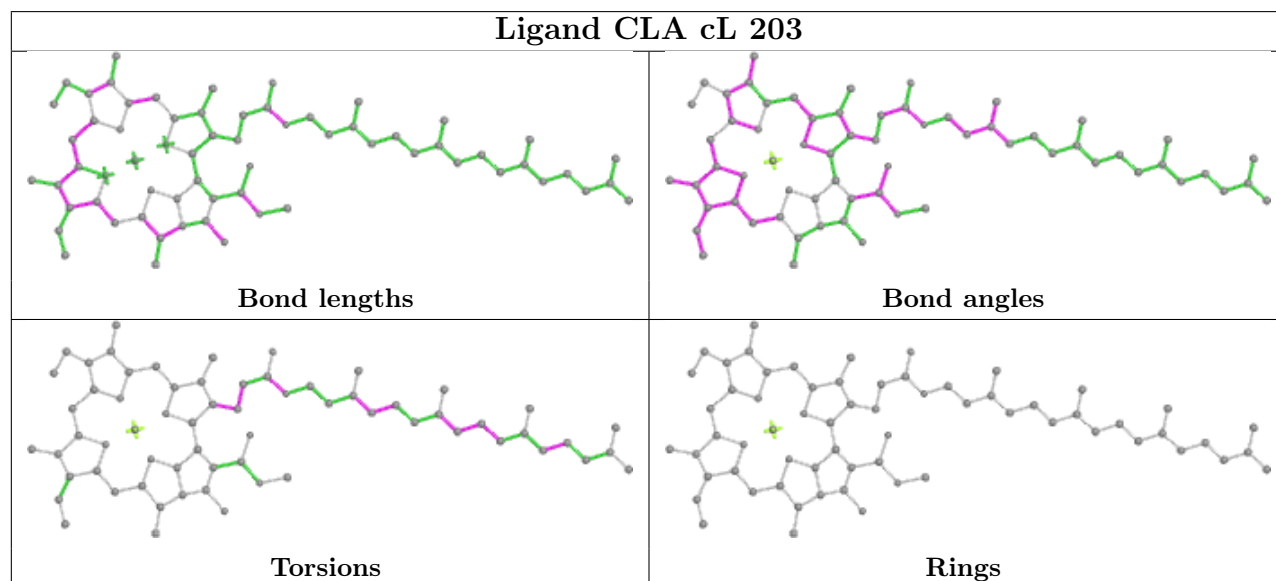
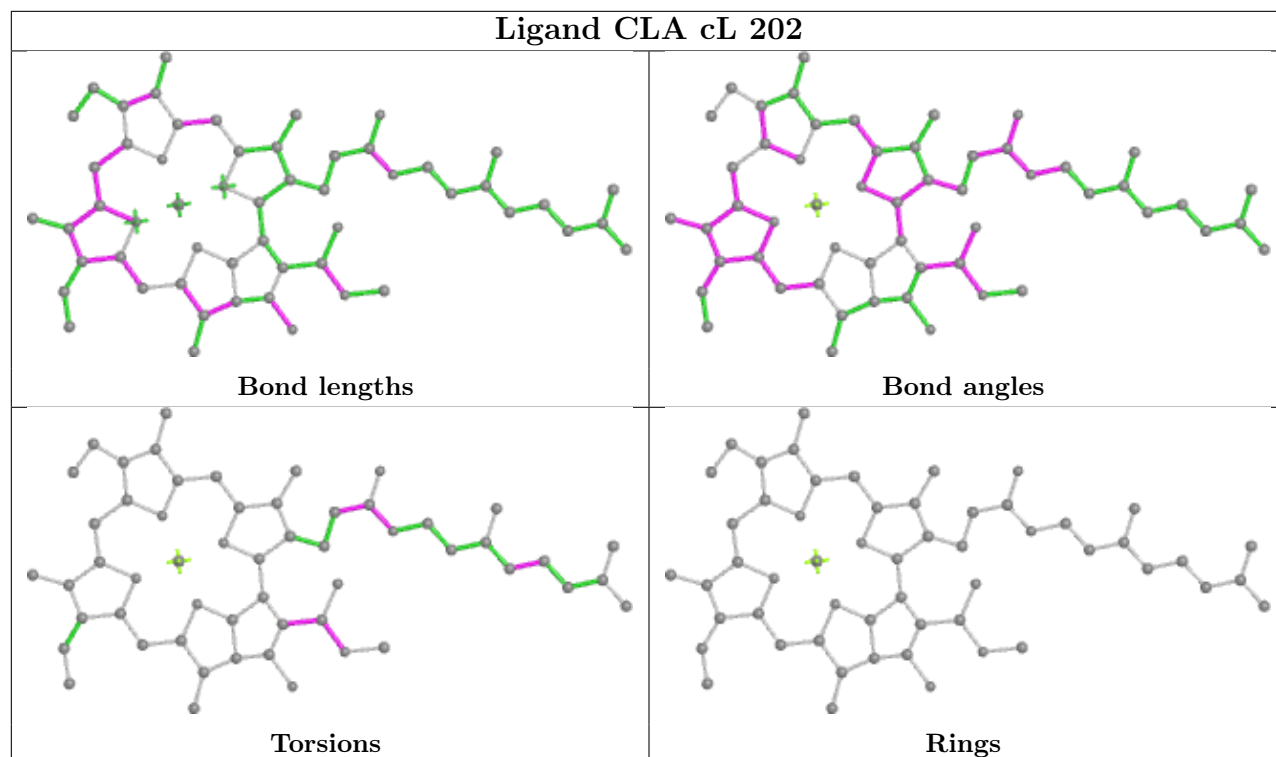
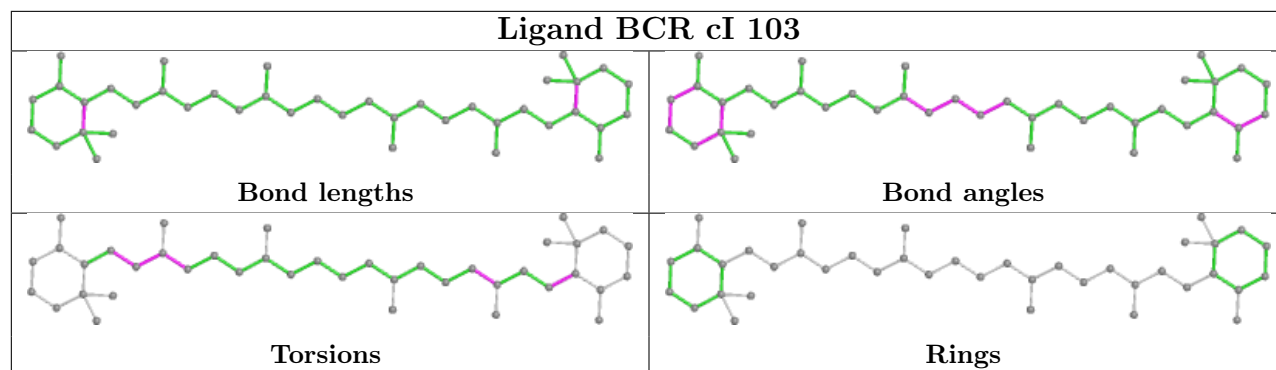


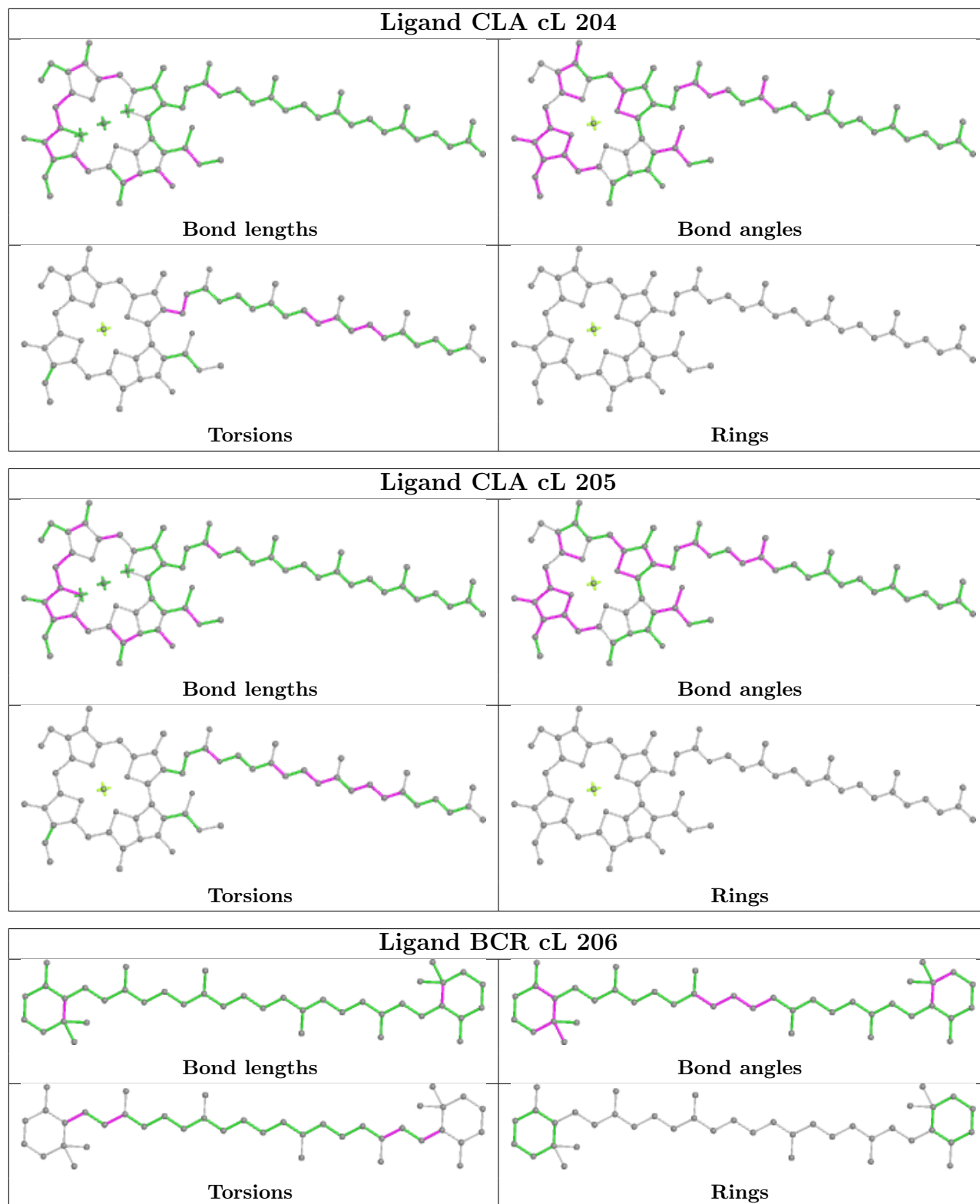
Rings

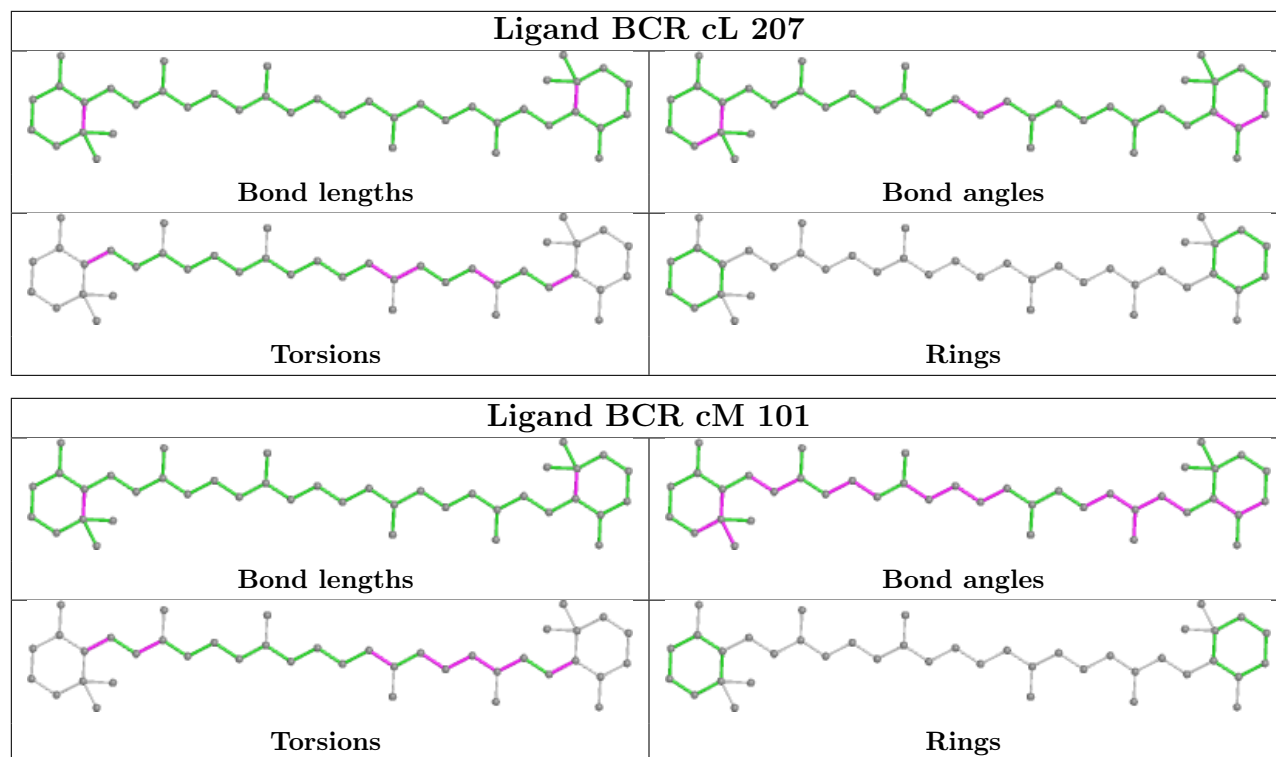












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.