



## wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 07:09 AM JST

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 initial model : 1JB0

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

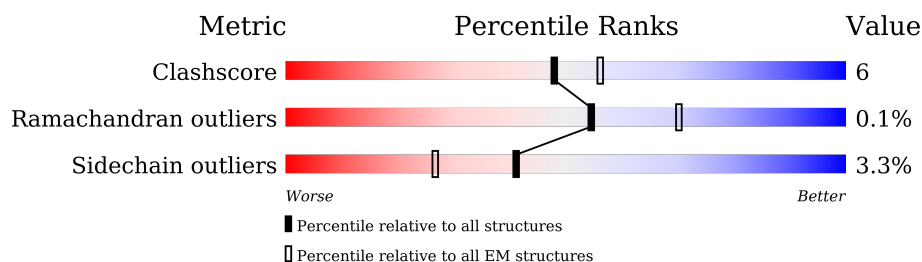
# 1 Overall quality at a glance

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	aA	764	
1	bA	764	
1	cA	764	
2	aB	742	
2	bB	742	
2	cB	742	
3	aC	81	
3	bC	81	

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Mol	Chain	Length	Quality of chain
3	cC	81	
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	aA	812	X	-	-	-
10	CLA	aA	813	X	-	-	-
10	CLA	aA	814	X	-	-	-
10	CLA	aA	815	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	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	-	-	-
10	CLA	aB	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	aB	812	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	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	204	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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	bA	814	X	-	-	-
10	CLA	bA	815	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	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	-	-	-
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	814	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	204	X	-	-	-
10	CLA	cA	802	X	-	-	-
10	CLA	cA	803	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	856	X	-	-	-
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	814	X	-	-	-
10	CLA	cB	815	X	-	-	-
10	CLA	cB	816	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	-	-	-
10	CLA	cL	204	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.

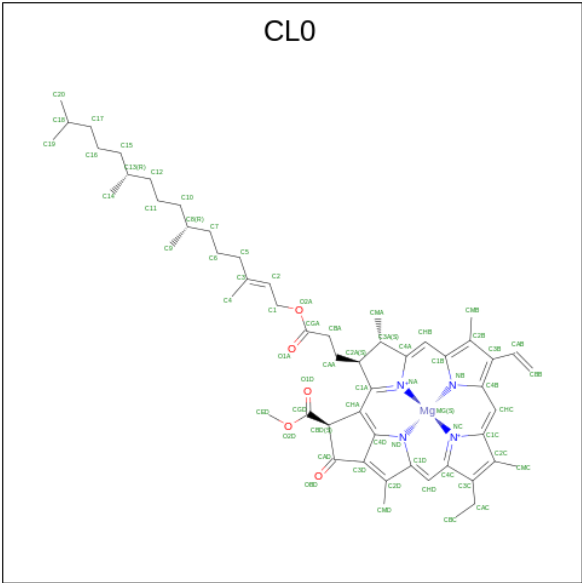
Mol	Chain	Residues	Atoms					AltConf	Trace
8	aM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		
8	bM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		

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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		

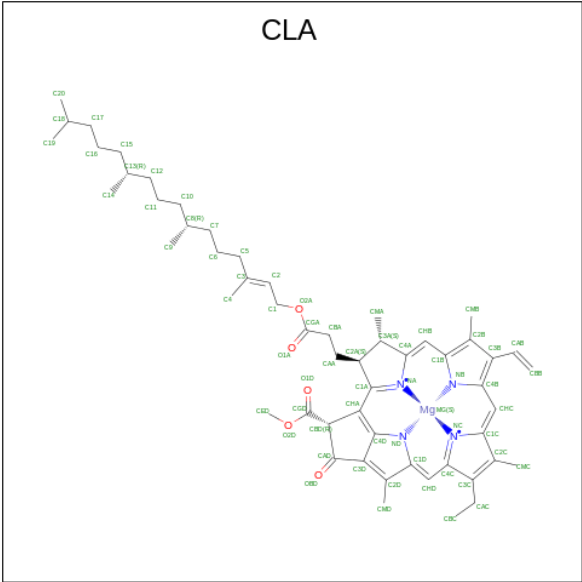
- Molecule 9 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).





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	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 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	aB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0

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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 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	bB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0

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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	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 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0

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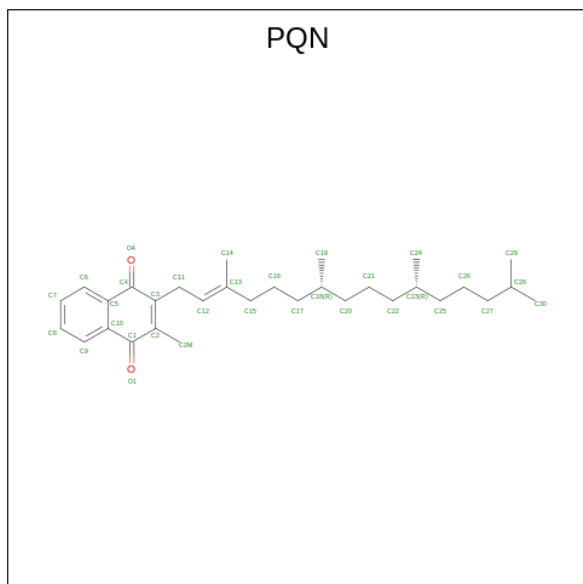
Mol	Chain	Residues	Atoms					AltConf
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N 164	O 205	0
10	cB	1	Total 2357	C 1947	Mg 41	N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

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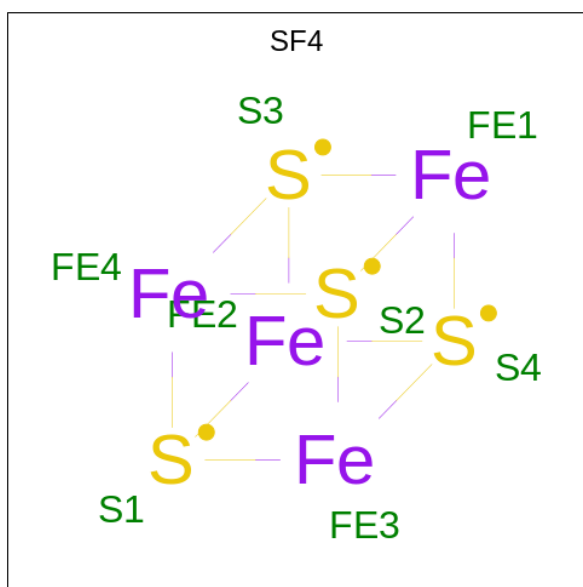
Mol	Chain	Residues	Atoms					AltConf
10	cL	1	Total	C	Mg	N	O	0
			250	210	4	16	20	

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



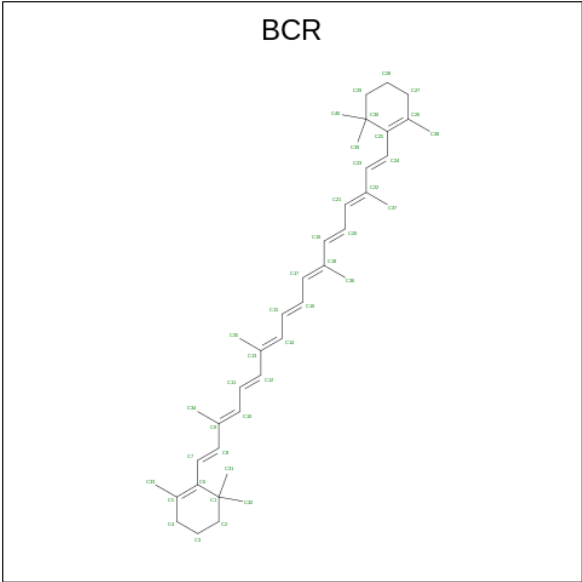
Mol	Chain	Residues	Atoms			AltConf
11	aA	1	Total	C	O	0
			33	31	2	
11	aB	1	Total	C	O	0
			33	31	2	
11	bA	1	Total	C	O	0
			33	31	2	
11	bB	1	Total	C	O	0
			33	31	2	
11	cA	1	Total	C	O	0
			33	31	2	
11	cB	1	Total	C	O	0
			33	31	2	

- 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: C<sub>40</sub>H<sub>56</sub>).



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	aI	1	Total	C	0
			80	80	
13	aI	1	Total	C	0
			80	80	

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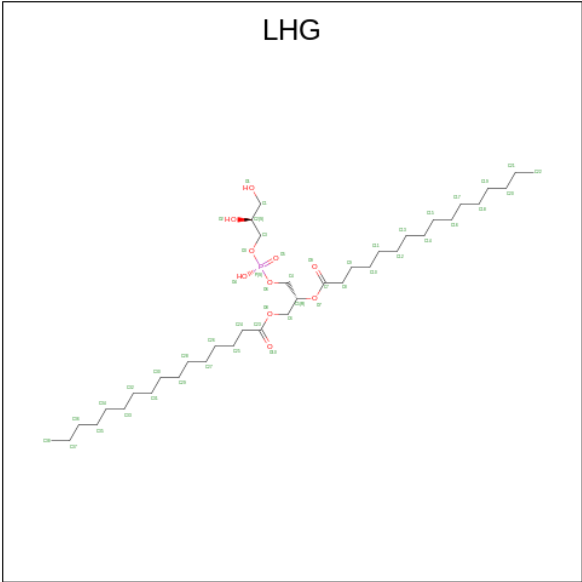
Mol	Chain	Residues	Atoms	AltConf
13	aL	1	Total C 80 80	0
13	aL	1	Total C 80 80	0
13	aM	1	Total C 40 40	0
13	bA	1	Total C 240 240	0
13	bA	1	Total C 240 240	0
13	bA	1	Total C 240 240	0
13	bA	1	Total C 240 240	0
13	bA	1	Total C 240 240	0
13	bA	1	Total C 240 240	0
13	bB	1	Total C 240 240	0
13	bB	1	Total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

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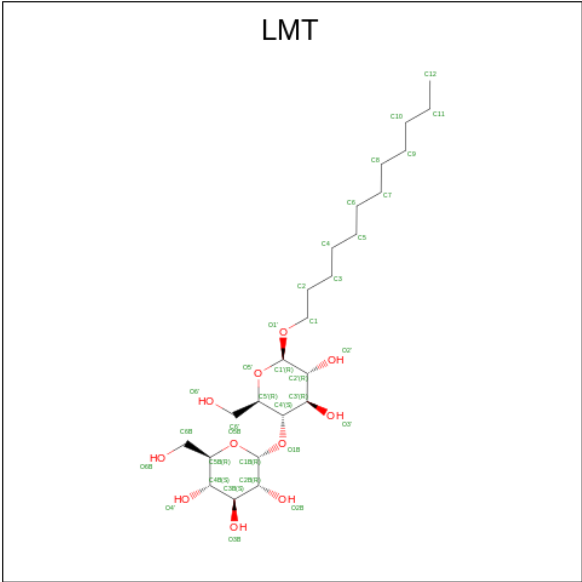
Mol	Chain	Residues	Atoms		AltConf
13	cA	1	Total	C	0
			240	240	
13	cA	1	Total	C	0
			240	240	
13	cA	1	Total	C	0
			240	240	
13	cA	1	Total	C	0
			240	240	
13	cA	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
13	cB	1	Total	C	0
			240	240	
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: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



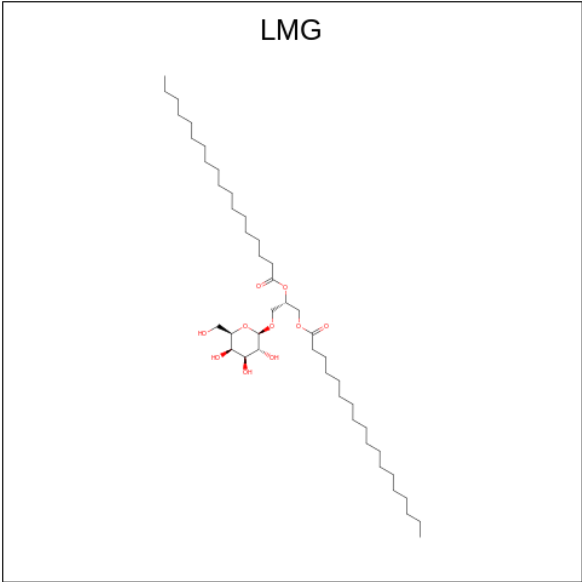
Mol	Chain	Residues	Atoms				AltConf
14	aA	1	Total	C	O	P	0
			76	54	20	2	
14	aA	1	Total	C	O	P	0
			76	54	20	2	
14	bA	1	Total	C	O	P	0
			76	54	20	2	
14	bA	1	Total	C	O	P	0
			76	54	20	2	
14	cA	1	Total	C	O	P	0
			76	54	20	2	
14	cA	1	Total	C	O	P	0
			76	54	20	2	

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



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

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



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	aI	1	Total	C		0
			9	9		
17	aL	4	Total	C	O	0
			56	52	4	
17	bI	1	Total	C		0
			9	9		
17	bL	4	Total	C	O	0
			56	52	4	
17	cI	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	aL	1	Total	Ca	0
			1	1	
18	bL	1	Total	Ca	0
			1	1	
18	cL	1	Total	Ca	0
			1	1	

- Molecule 19 is water.

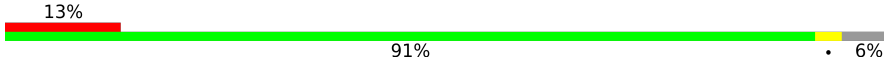
Mol	Chain	Residues	Atoms		AltConf
19	aA	64	Total	O	0
			64	64	
19	aB	85	Total	O	0
			85	85	
19	aC	16	Total	O	0
			16	16	

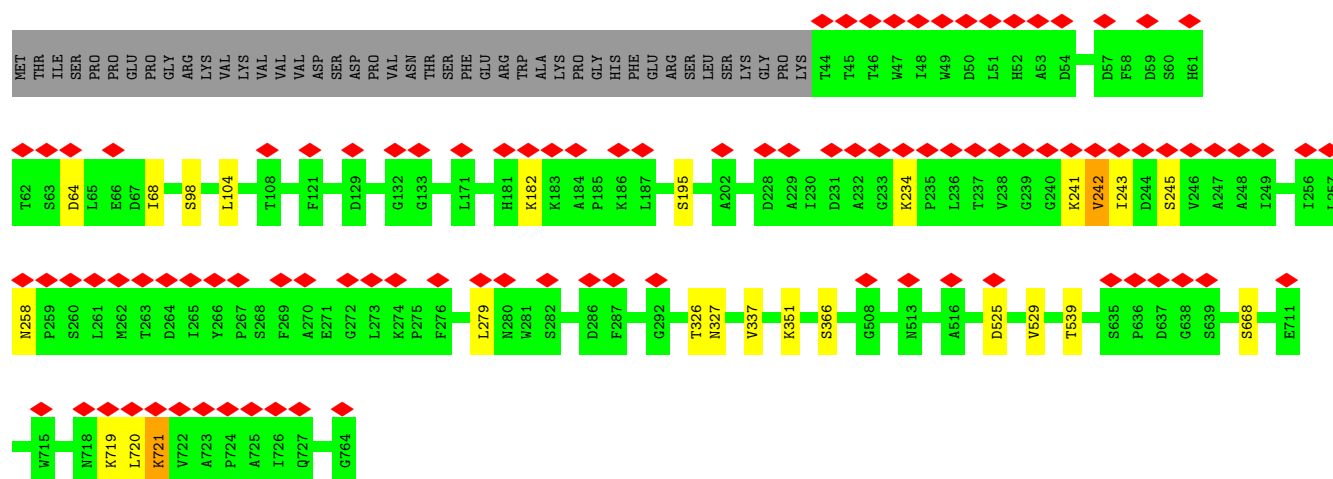
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Mol	Chain	Residues	Atoms		AltConf
19	aD	12	Total 12	O 12	0
19	aI	1	Total 1	O 1	0
19	aL	30	Total 30	O 30	0
19	aM	1	Total 1	O 1	0
19	bA	63	Total 63	O 63	0
19	bB	85	Total 85	O 85	0
19	bC	17	Total 17	O 17	0
19	bD	12	Total 12	O 12	0
19	bI	1	Total 1	O 1	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

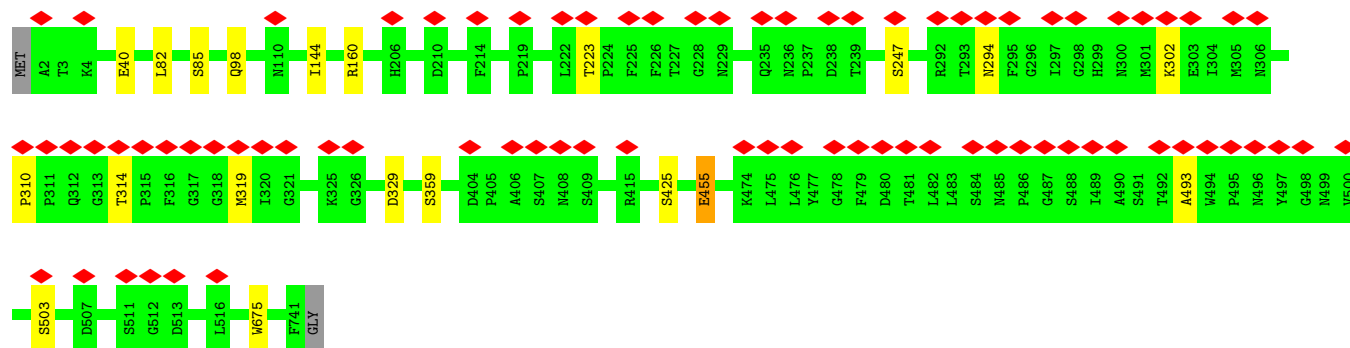


Chain cA: 



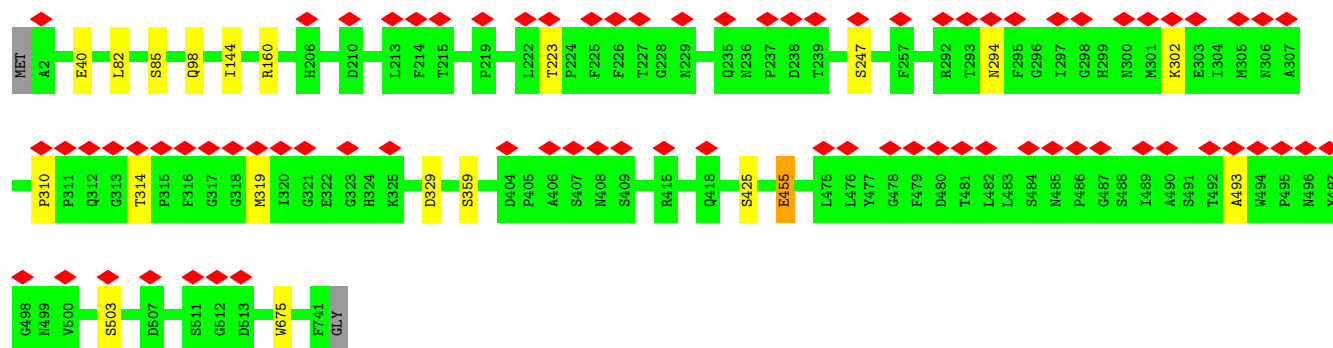
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain aB: 



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

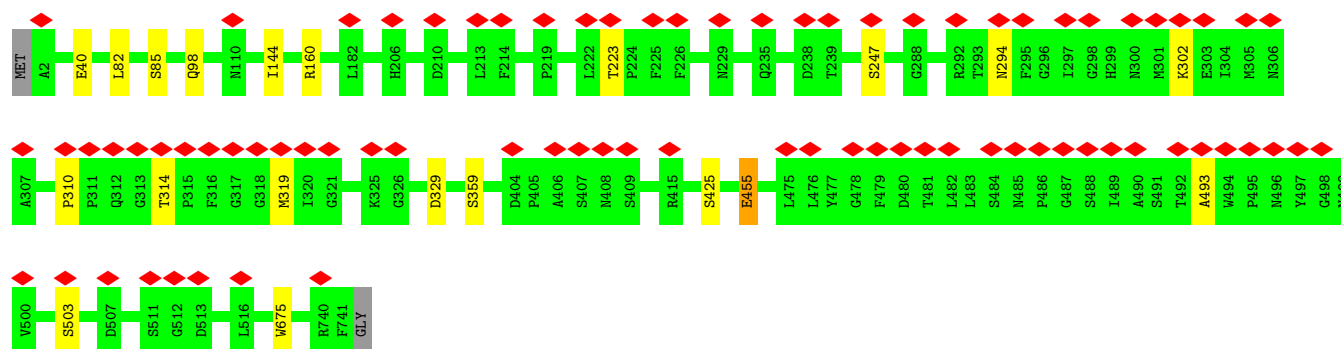
Chain bB: 



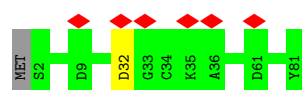
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain cB: 

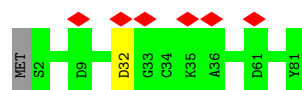




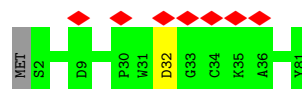
- Molecule 3: Photosystem I iron-sulfur center



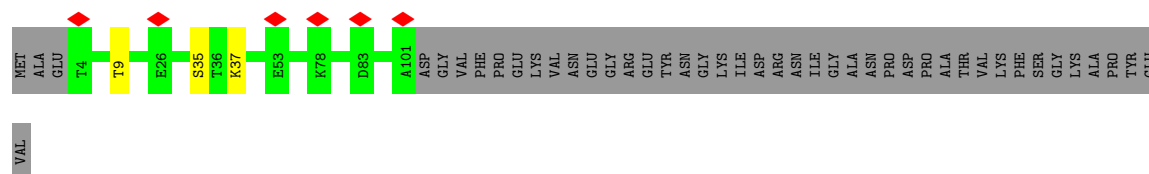
- Molecule 3: Photosystem I iron-sulfur center



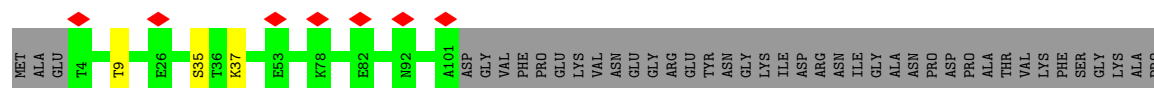
- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II

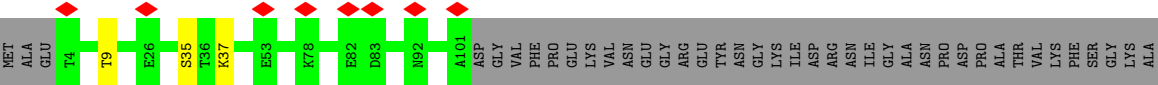


- Molecule 4: Photosystem I reaction center subunit II



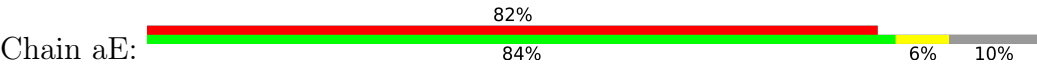
TYR  
GLU  
VAL

• Molecule 4: Photosystem I reaction center subunit II



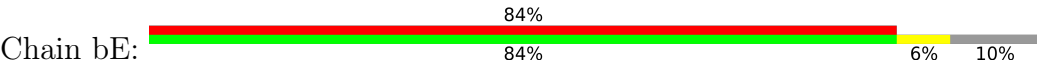
PRO  
TYR  
GLU  
VAL

• Molecule 5: Photosystem I reaction center subunit IV



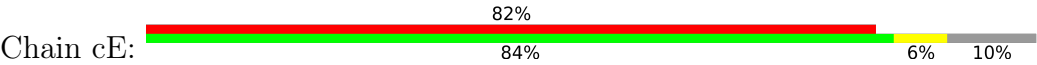
PRO  
PRO  
LYS  
LYS  
LYS

• Molecule 5: Photosystem I reaction center subunit IV



E62  
PRO  
PRO  
LYS  
LYS  
LYS

• Molecule 5: Photosystem I reaction center subunit IV



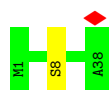
PRO  
PRO  
LYS  
LYS  
LYS

• Molecule 6: Photosystem I reaction center subunit VIII



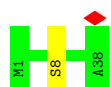
- Molecule 6: Photosystem I reaction center subunit VIII

Chain bI:  97%




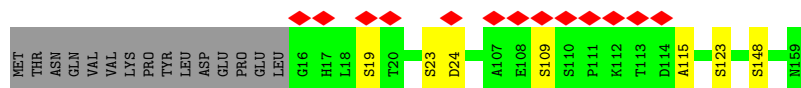
- Molecule 6: Photosystem I reaction center subunit VIII

Chain cI:  97%




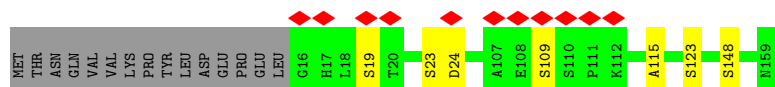
- Molecule 7: Photosystem I reaction center subunit XI

Chain aL:  8% 86% 9%




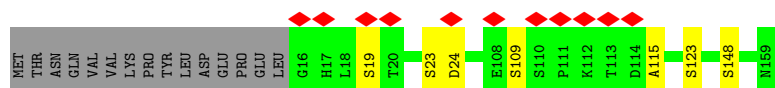
- Molecule 7: Photosystem I reaction center subunit XI

Chain bL:  7% 86% 9%



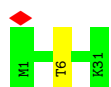
- Molecule 7: Photosystem I reaction center subunit XI

Chain cL:  7% 86% 9%



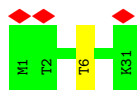
- Molecule 8: Photosystem I reaction center subunit XII

Chain aM:  97%



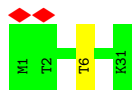
- Molecule 8: Photosystem I reaction center subunit XII

Chain bM:  10% 97%



- Molecule 8: Photosystem I reaction center subunit XII

Chain cM: 6% 97% .



## 4 Experimental information

Property	Value	Source
EM 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	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.453	Depositor
Minimum map value	-0.267	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	313.2, 313.2, 313.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	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%)	51	63
1	bA	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	51	63
1	cA	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	51	63
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%)	22	23
7	bL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	22	23
7	cL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	22	23
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%)	54	63

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%)	34	42
1	bA	574/614 (94%)	553 (96%)	21 (4%)	34	42
1	cA	574/614 (94%)	553 (96%)	21 (4%)	34	42
2	aB	597/598 (100%)	581 (97%)	16 (3%)	44	55
2	bB	597/598 (100%)	581 (97%)	16 (3%)	44	55
2	cB	597/598 (100%)	581 (97%)	16 (3%)	44	55
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%)	33	41
4	bD	80/115 (70%)	77 (96%)	3 (4%)	33	41
4	cD	80/115 (70%)	77 (96%)	3 (4%)	33	41
5	aE	54/61 (88%)	51 (94%)	3 (6%)	21	23
5	bE	54/61 (88%)	51 (94%)	3 (6%)	21	23
5	cE	54/61 (88%)	51 (94%)	3 (6%)	21	23
6	aI	32/32 (100%)	31 (97%)	1 (3%)	40	48
6	bI	32/32 (100%)	31 (97%)	1 (3%)	40	48
6	cI	32/32 (100%)	31 (97%)	1 (3%)	40	48
7	aL	108/123 (88%)	102 (94%)	6 (6%)	21	23
7	bL	108/123 (88%)	102 (94%)	6 (6%)	21	23
7	cL	108/123 (88%)	102 (94%)	6 (6%)	21	23
8	aM	27/27 (100%)	26 (96%)	1 (4%)	34	42
8	bM	27/27 (100%)	26 (96%)	1 (4%)	34	42
8	cM	27/27 (100%)	26 (96%)	1 (4%)	34	42
All	All	4620/4917 (94%)	4467 (97%)	153 (3%)	41	46

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

Mol	Chain	Res	Type
1	cA	327	ASN
5	cE	29	GLN
1	cA	525	ASP
2	cB	247	SER
7	cL	123	SER

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

Mol	Chain	Res	Type
2	cB	333	ASN
2	cB	373	GLN
4	cD	99	HIS
1	bA	150	ASN
1	bA	135	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
10	CLA	cB	819	2	60,68,73	2.08	15 (25%)	70,107,113	2.89	30 (42%)
10	CLA	bA	816	1	54,62,73	2.20	16 (29%)	62,99,113	3.05	28 (45%)
9	CL0	aA	801	1	65,73,73	1.93	17 (26%)	76,113,113	2.69	31 (40%)
10	CLA	cA	837	1	65,73,73	1.94	18 (27%)	76,113,113	2.72	27 (35%)
10	CLA	cA	811	1	54,62,73	2.22	17 (31%)	62,99,113	2.90	27 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	bA	808	1	45,53,73	2.38	17 (37%)	52,89,113	3.14	23 (44%)
10	CLA	aA	838	1	50,58,73	2.24	17 (34%)	58,95,113	3.35	30 (51%)
10	CLA	aB	831	2	45,53,73	2.46	16 (35%)	52,89,113	3.12	25 (48%)
13	BCR	bA	848	-	41,41,41	1.03	2 (4%)	56,56,56	1.29	8 (14%)
10	CLA	bA	835	1	65,73,73	2.02	17 (26%)	76,113,113	2.64	28 (36%)
13	BCR	bL	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	3 (5%)
10	CLA	bB	805	-	65,73,73	1.94	18 (27%)	76,113,113	2.59	23 (30%)
10	CLA	cB	808	2	65,73,73	1.98	18 (27%)	76,113,113	2.68	27 (35%)
10	CLA	cB	829	2	65,73,73	2.01	19 (29%)	76,113,113	2.51	26 (34%)
10	CLA	aB	836	-	45,53,73	2.49	17 (37%)	52,89,113	3.12	25 (48%)
13	BCR	cA	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.18	5 (8%)
10	CLA	aA	827	1	65,73,73	2.04	19 (29%)	76,113,113	2.78	28 (36%)
13	BCR	cA	849	-	41,41,41	1.11	3 (7%)	56,56,56	1.27	7 (12%)
10	CLA	bB	841	2	65,73,73	1.95	16 (24%)	76,113,113	2.70	27 (35%)
10	CLA	aA	821	1	49,57,73	2.34	16 (32%)	55,93,113	3.17	26 (47%)
10	CLA	aB	805	-	65,73,73	1.94	18 (27%)	76,113,113	2.59	23 (30%)
10	CLA	cB	830	2	65,73,73	2.04	16 (24%)	76,113,113	2.67	29 (38%)
10	CLA	aA	814	1	45,53,73	2.45	17 (37%)	52,89,113	3.12	24 (46%)
10	CLA	bA	856	2	49,57,73	2.38	17 (34%)	55,93,113	3.00	24 (43%)
10	CLA	aA	843	-	42,49,73	2.42	14 (33%)	48,83,113	3.19	21 (43%)
10	CLA	cB	802	-	65,73,73	1.99	17 (26%)	76,113,113	2.64	27 (35%)
10	CLA	cA	843	-	42,49,73	2.42	14 (33%)	48,83,113	3.18	21 (43%)
10	CLA	bA	807	1	45,53,73	2.42	19 (42%)	52,89,113	3.25	26 (50%)
13	BCR	bA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.30	5 (8%)
10	CLA	cA	821	1	49,57,73	2.34	16 (32%)	55,93,113	3.18	26 (47%)
10	CLA	cA	804	1	65,73,73	1.97	17 (26%)	76,113,113	2.74	26 (34%)
10	CLA	aA	839	1	65,73,73	2.04	16 (24%)	76,113,113	2.66	26 (34%)
9	CL0	bA	801	1	65,73,73	1.93	17 (26%)	76,113,113	2.69	30 (39%)
10	CLA	aB	824	2	45,53,73	2.48	16 (35%)	52,89,113	3.14	24 (46%)
13	BCR	aB	849	-	41,41,41	1.02	2 (4%)	56,56,56	1.16	4 (7%)
10	CLA	bB	822	2	45,53,73	2.45	17 (37%)	52,89,113	3.31	22 (42%)
10	CLA	cA	813	1	45,53,73	2.50	18 (40%)	52,89,113	3.11	25 (48%)
10	CLA	aB	840	-	65,73,73	1.97	17 (26%)	76,113,113	2.65	28 (36%)
13	BCR	bB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.32	5 (8%)
10	CLA	bB	816	2	45,53,73	2.41	16 (35%)	52,89,113	3.15	25 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	cL	205	-	65,73,73	1.99	19 (29%)	76,113,113	2.72	26 (34%)
10	CLA	aA	802	1	45,53,73	2.48	16 (35%)	52,89,113	3.21	24 (46%)
13	BCR	aA	846	-	41,41,41	1.11	3 (7%)	56,56,56	1.23	6 (10%)
13	BCR	cI	102	-	41,41,41	1.08	3 (7%)	56,56,56	1.27	6 (10%)
10	CLA	aA	806	1	51,59,73	2.29	16 (31%)	59,96,113	3.05	28 (47%)
10	CLA	aA	833	1	65,73,73	1.97	16 (24%)	76,113,113	2.77	27 (35%)
10	CLA	cB	838	2	65,73,73	2.01	15 (23%)	76,113,113	2.73	28 (36%)
10	CLA	cA	823	1	65,73,73	2.02	16 (24%)	76,113,113	2.62	25 (32%)
10	CLA	aB	830	2	65,73,73	2.04	17 (26%)	76,113,113	2.67	29 (38%)
10	CLA	bL	205	-	65,73,73	1.99	19 (29%)	76,113,113	2.73	26 (34%)
10	CLA	bB	835	-	45,53,73	2.46	18 (40%)	52,89,113	3.10	24 (46%)
10	CLA	cA	854	14	52,60,73	2.26	17 (32%)	60,97,113	3.11	26 (43%)
10	CLA	bB	814	2	65,73,73	2.03	18 (27%)	76,113,113	2.67	28 (36%)
10	CLA	cB	837	2	60,68,73	2.05	18 (30%)	70,107,113	2.84	27 (38%)
10	CLA	aB	839	2	47,55,73	2.33	17 (36%)	54,91,113	3.17	25 (46%)
13	BCR	bB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)
10	CLA	bA	809	1	45,53,73	2.43	16 (35%)	52,89,113	3.20	23 (44%)
10	CLA	cB	836	-	45,53,73	2.49	17 (37%)	52,89,113	3.11	24 (46%)
10	CLA	aA	840	-	51,59,73	2.34	17 (33%)	59,96,113	3.05	27 (45%)
10	CLA	bB	837	2	60,68,73	2.05	18 (30%)	70,107,113	2.84	27 (38%)
15	LMT	bA	853	-	36,36,36	0.45	0	47,47,47	0.91	3 (6%)
10	CLA	aB	814	2	65,73,73	2.04	19 (29%)	76,113,113	2.68	28 (36%)
14	LHG	aA	852	-	48,48,48	0.67	2 (4%)	51,54,54	1.23	7 (13%)
10	CLA	aA	837	1	65,73,73	1.94	18 (27%)	76,113,113	2.72	27 (35%)
10	CLA	bA	830	1	50,58,73	2.26	17 (34%)	58,95,113	3.00	27 (46%)
10	CLA	bA	817	1	54,62,73	2.22	16 (29%)	62,99,113	2.94	28 (45%)
10	CLA	aA	826	1	65,73,73	1.99	16 (24%)	76,113,113	2.70	27 (35%)
10	CLA	aB	811	2	65,73,73	1.94	17 (26%)	76,113,113	2.65	25 (32%)
10	CLA	cA	827	1	65,73,73	2.04	19 (29%)	76,113,113	2.77	28 (36%)
10	CLA	cB	831	2	45,53,73	2.45	15 (33%)	52,89,113	3.11	26 (50%)
16	LMG	bB	848	-	55,55,55	0.77	1 (1%)	63,63,63	1.36	9 (14%)
10	CLA	cB	827	2	65,73,73	2.01	17 (26%)	76,113,113	2.79	28 (36%)
10	CLA	cB	823	2	55,63,73	2.27	17 (30%)	64,101,113	2.86	27 (42%)
10	CLA	cA	807	1	45,53,73	2.42	18 (40%)	52,89,113	3.24	26 (50%)
13	BCR	cL	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	3 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	cB	821	2	47,55,73	2.39	16 (34%)	54,91,113	3.00	26 (48%)
10	CLA	cB	812	2	45,53,73	2.41	16 (35%)	52,89,113	3.19	23 (44%)
10	CLA	bA	829	1	65,73,73	2.01	17 (26%)	76,113,113	2.77	27 (35%)
10	CLA	aA	841	-	65,73,73	2.02	17 (26%)	76,113,113	2.69	27 (35%)
10	CLA	bB	806	2	54,62,73	2.20	17 (31%)	62,99,113	3.06	31 (50%)
12	SF4	bA	845	2,1	0,12,12	-	-	-	-	-
10	CLA	bB	813	2	45,53,73	2.46	17 (37%)	52,89,113	3.09	22 (42%)
10	CLA	bB	809	2	65,73,73	1.97	19 (29%)	76,113,113	2.75	26 (34%)
10	CLA	aB	804	-	57,65,73	2.10	15 (26%)	66,103,113	3.08	29 (43%)
10	CLA	aA	832	1	65,73,73	1.96	16 (24%)	76,113,113	2.73	29 (38%)
13	BCR	aB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)
10	CLA	bB	810	2	55,63,73	2.11	14 (25%)	64,101,113	2.90	30 (46%)
13	BCR	cB	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	6 (10%)
10	CLA	bA	802	1	45,53,73	2.47	16 (35%)	52,89,113	3.20	24 (46%)
10	CLA	cL	202	2	55,63,73	2.13	18 (32%)	64,101,113	2.94	27 (42%)
10	CLA	bA	826	1	65,73,73	1.99	16 (24%)	76,113,113	2.69	27 (35%)
10	CLA	bA	843	-	42,49,73	2.42	14 (33%)	48,83,113	3.19	21 (43%)
12	SF4	aC	101	3	0,12,12	-	-	-	-	-
10	CLA	cA	830	1	50,58,73	2.26	16 (32%)	58,95,113	3.00	27 (46%)
10	CLA	cA	825	-	55,63,73	2.16	18 (32%)	64,101,113	2.98	26 (40%)
10	CLA	cA	815	-	49,57,73	2.35	16 (32%)	55,93,113	3.11	24 (43%)
10	CLA	cB	809	2	65,73,73	1.96	19 (29%)	76,113,113	2.74	26 (34%)
10	CLA	cB	826	-	65,73,73	2.08	16 (24%)	76,113,113	2.79	30 (39%)
10	CLA	bA	813	1	45,53,73	2.49	18 (40%)	52,89,113	3.12	24 (46%)
10	CLA	cB	811	2	65,73,73	1.94	17 (26%)	76,113,113	2.66	25 (32%)
10	CLA	bA	810	1	65,73,73	2.07	15 (23%)	76,113,113	2.73	27 (35%)
10	CLA	aA	824	-	65,73,73	1.96	17 (26%)	76,113,113	2.77	24 (31%)
10	CLA	bA	838	1	50,58,73	2.23	15 (30%)	58,95,113	3.35	30 (51%)
10	CLA	bA	834	1	54,62,73	2.17	16 (29%)	62,99,113	2.88	29 (46%)
10	CLA	cA	856	2	49,57,73	2.38	16 (32%)	55,93,113	2.99	24 (43%)
10	CLA	aB	826	-	65,73,73	2.08	16 (24%)	76,113,113	2.79	30 (39%)
10	CLA	cB	824	2	45,53,73	2.48	16 (35%)	52,89,113	3.14	24 (46%)
10	CLA	bA	823	1	65,73,73	2.02	16 (24%)	76,113,113	2.62	25 (32%)
13	BCR	cA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.29	5 (8%)
10	CLA	aA	825	-	55,63,73	2.15	16 (29%)	64,101,113	2.98	26 (40%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	aA	817	1	54,62,73	2.22	16 (29%)	62,99,113	2.94	29 (46%)
10	CLA	aB	835	-	45,53,73	2.46	17 (37%)	52,89,113	3.10	24 (46%)
10	CLA	aL	202	2	55,63,73	2.13	19 (34%)	64,101,113	2.94	26 (40%)
10	CLA	aB	813	2	45,53,73	2.46	17 (37%)	52,89,113	3.10	22 (42%)
10	CLA	bA	854	-	52,60,73	2.27	16 (30%)	60,97,113	3.10	26 (43%)
10	CLA	bA	812	1	65,73,73	2.04	16 (24%)	76,113,113	2.75	28 (36%)
10	CLA	aA	811	1	54,62,73	2.22	17 (31%)	62,99,113	2.91	27 (43%)
10	CLA	cB	814	2	65,73,73	2.03	19 (29%)	76,113,113	2.68	27 (35%)
10	CLA	bA	836	1	51,59,73	2.26	17 (33%)	59,96,113	5.96	30 (50%)
13	BCR	cB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)
10	CLA	bA	820	-	65,73,73	2.03	16 (24%)	76,113,113	2.62	27 (35%)
10	CLA	aB	822	2	45,53,73	2.46	17 (37%)	52,89,113	3.32	22 (42%)
13	BCR	cA	848	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	8 (14%)
10	CLA	aA	822	1	51,59,73	2.31	16 (31%)	59,96,113	3.05	27 (45%)
10	CLA	aB	816	2	45,53,73	2.41	16 (35%)	52,89,113	3.16	25 (48%)
12	SF4	cC	102	3	0,12,12	-	-	-	-	-
10	CLA	bB	807	2	65,73,73	1.99	19 (29%)	76,113,113	2.78	29 (38%)
10	CLA	aA	819	1	61,69,73	2.12	17 (27%)	71,108,113	2.71	26 (36%)
13	BCR	bA	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.18	5 (8%)
10	CLA	aB	807	2	65,73,73	1.99	19 (29%)	76,113,113	2.78	30 (39%)
14	LHG	bA	855	-	26,26,48	0.83	0	29,32,54	1.33	3 (10%)
10	CLA	aB	818	2	59,67,73	2.16	17 (28%)	68,105,113	2.84	27 (39%)
10	CLA	cB	806	2	54,62,73	2.19	17 (31%)	62,99,113	3.06	31 (50%)
10	CLA	bA	827	1	65,73,73	2.04	19 (29%)	76,113,113	2.77	28 (36%)
10	CLA	cA	842	-	65,73,73	1.93	17 (26%)	76,113,113	2.64	29 (38%)
10	CLA	cA	809	1	45,53,73	2.44	17 (37%)	52,89,113	3.21	23 (44%)
13	BCR	aA	849	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	7 (12%)
10	CLA	bL	203	7	65,73,73	2.00	18 (27%)	76,113,113	2.69	27 (35%)
10	CLA	cB	828	2	65,73,73	1.94	19 (29%)	76,113,113	2.76	27 (35%)
10	CLA	bA	818	1	65,73,73	2.07	16 (24%)	76,113,113	2.91	29 (38%)
10	CLA	bA	821	1	49,57,73	2.34	16 (32%)	55,93,113	3.18	26 (47%)
10	CLA	aA	805	1	65,73,73	2.03	18 (27%)	76,113,113	2.81	30 (39%)
10	CLA	cB	804	-	57,65,73	2.09	15 (26%)	66,103,113	3.08	29 (43%)
13	BCR	cA	851	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	3 (5%)
10	CLA	bB	823	2	55,63,73	2.27	17 (30%)	64,101,113	2.86	27 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	PQN	cA	844	-	34,34,34	1.53	2 (5%)	42,45,45	1.21	4 (9%)
12	SF4	cA	845	2,1	0,12,12	-	-	-		
13	BCR	bB	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	3 (5%)
10	CLA	bA	839	1	65,73,73	2.04	16 (24%)	76,113,113	2.66	26 (34%)
10	CLA	aB	815	2	56,64,73	2.18	16 (28%)	65,102,113	2.80	27 (41%)
10	CLA	cA	834	1	54,62,73	2.17	16 (29%)	62,99,113	2.90	29 (46%)
10	CLA	aA	830	1	50,58,73	2.26	17 (34%)	58,95,113	2.99	27 (46%)
10	CLA	bB	808	2	65,73,73	1.98	18 (27%)	76,113,113	2.69	27 (35%)
10	CLA	cB	816	2	45,53,73	2.41	16 (35%)	52,89,113	3.15	25 (48%)
10	CLA	aA	815	-	49,57,73	2.35	17 (34%)	55,93,113	3.11	24 (43%)
10	CLA	cA	802	1	45,53,73	2.47	16 (35%)	52,89,113	3.20	24 (46%)
10	CLA	bA	824	-	65,73,73	1.96	17 (26%)	76,113,113	2.77	24 (31%)
13	BCR	aB	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	3 (5%)
14	LHG	cA	855	10	26,26,48	0.83	0	29,32,54	1.33	3 (10%)
16	LMG	aB	848	-	55,55,55	0.76	1 (1%)	63,63,63	1.36	9 (14%)
11	PQN	bB	842	-	34,34,34	1.51	2 (5%)	42,45,45	1.05	3 (7%)
10	CLA	bL	202	2	55,63,73	2.12	19 (34%)	64,101,113	2.94	26 (40%)
10	CLA	cB	841	2	65,73,73	1.95	16 (24%)	76,113,113	2.70	27 (35%)
10	CLA	cA	810	1	65,73,73	2.06	15 (23%)	76,113,113	2.73	27 (35%)
10	CLA	cB	822	2	45,53,73	2.46	17 (37%)	52,89,113	3.32	22 (42%)
10	CLA	cA	820	-	65,73,73	2.03	15 (23%)	76,113,113	2.62	27 (35%)
13	BCR	cB	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	3 (5%)
13	BCR	aB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	5 (8%)
14	LHG	bA	852	-	48,48,48	0.66	2 (4%)	51,54,54	1.23	7 (13%)
13	BCR	bL	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	7 (12%)
13	BCR	aA	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.18	5 (8%)
10	CLA	cA	831	1	65,73,73	2.01	17 (26%)	76,113,113	2.68	25 (32%)
10	CLA	cB	801	-	65,73,73	1.98	16 (24%)	76,113,113	2.78	28 (36%)
13	BCR	bB	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	6 (10%)
10	CLA	bA	825	-	55,63,73	2.15	17 (30%)	64,101,113	2.99	26 (40%)
13	BCR	bM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	10 (17%)
10	CLA	bA	815	-	49,57,73	2.35	17 (34%)	55,93,113	3.11	24 (43%)
10	CLA	aB	828	2	65,73,73	1.95	19 (29%)	76,113,113	2.76	27 (35%)
10	CLA	bB	821	2	47,55,73	2.39	16 (34%)	54,91,113	2.99	26 (48%)
10	CLA	aA	808	1	45,53,73	2.38	17 (37%)	52,89,113	3.14	23 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	cA	808	1	45,53,73	2.39	17 (37%)	52,89,113	3.13	23 (44%)
10	CLA	bA	822	1	51,59,73	2.31	16 (31%)	59,96,113	3.05	28 (47%)
10	CLA	cB	805	-	65,73,73	1.94	18 (27%)	76,113,113	2.59	23 (30%)
10	CLA	bA	814	1	45,53,73	2.45	17 (37%)	52,89,113	3.12	24 (46%)
10	CLA	bA	833	1	65,73,73	1.98	16 (24%)	76,113,113	2.78	28 (36%)
10	CLA	bB	803	2	65,73,73	1.94	17 (26%)	76,113,113	2.78	29 (38%)
13	BCR	bB	849	-	41,41,41	1.02	2 (4%)	56,56,56	1.15	4 (7%)
10	CLA	bB	839	2	47,55,73	2.33	17 (36%)	54,91,113	3.16	25 (46%)
10	CLA	aA	818	1	65,73,73	2.08	16 (24%)	76,113,113	2.91	29 (38%)
12	SF4	bC	102	3	0,12,12	-	-	-	-	-
16	LMG	cB	848	-	55,55,55	0.76	1 (1%)	63,63,63	1.36	9 (14%)
10	CLA	bA	804	1	65,73,73	1.97	16 (24%)	76,113,113	2.74	26 (34%)
10	CLA	aB	817	2	55,63,73	2.19	17 (30%)	64,101,113	2.89	27 (42%)
10	CLA	bA	842	-	65,73,73	1.94	16 (24%)	76,113,113	2.64	29 (38%)
10	CLA	cA	840	-	51,59,73	2.34	17 (33%)	59,96,113	3.06	27 (45%)
10	CLA	aA	842	-	65,73,73	1.93	17 (26%)	76,113,113	2.64	29 (38%)
13	BCR	bI	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	6 (10%)
10	CLA	cL	204	7	65,73,73	1.93	16 (24%)	76,113,113	2.80	26 (34%)
10	CLA	bB	829	2	65,73,73	2.01	18 (27%)	76,113,113	2.51	26 (34%)
13	BCR	cB	849	-	41,41,41	1.02	2 (4%)	56,56,56	1.15	4 (7%)
10	CLA	bB	820	-	65,73,73	2.05	16 (24%)	76,113,113	2.65	27 (35%)
10	CLA	bB	815	2	56,64,73	2.17	16 (28%)	65,102,113	2.80	27 (41%)
10	CLA	aB	809	2	65,73,73	1.96	19 (29%)	76,113,113	2.74	26 (34%)
10	CLA	bA	819	1	61,69,73	2.11	17 (27%)	71,108,113	2.70	26 (36%)
10	CLA	bA	806	1	51,59,73	2.30	16 (31%)	59,96,113	3.07	29 (49%)
10	CLA	cB	834	2	45,53,73	2.45	17 (37%)	52,89,113	3.22	27 (51%)
10	CLA	aA	813	1	45,53,73	2.49	17 (37%)	52,89,113	3.11	24 (46%)
10	CLA	bA	841	1	65,73,73	2.03	17 (26%)	76,113,113	2.69	27 (35%)
11	PQN	bA	844	-	34,34,34	1.53	2 (5%)	42,45,45	1.22	4 (9%)
13	BCR	cA	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.23	7 (12%)
10	CLA	bB	830	2	65,73,73	2.04	17 (26%)	76,113,113	2.67	29 (38%)
12	SF4	aC	102	3	0,12,12	-	-	-	-	-
10	CLA	bB	834	2	45,53,73	2.45	17 (37%)	52,89,113	3.23	27 (51%)
10	CLA	cL	203	7	65,73,73	2.00	18 (27%)	76,113,113	2.69	27 (35%)
10	CLA	cB	820	-	65,73,73	2.05	16 (24%)	76,113,113	2.65	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	cB	815	2	56,64,73	2.18	16 (28%)	65,102,113	2.80	27 (41%)
10	CLA	aB	834	2	45,53,73	2.44	17 (37%)	52,89,113	3.23	27 (51%)
13	BCR	bB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
10	CLA	cA	838	1	50,58,73	2.23	17 (34%)	58,95,113	3.35	30 (51%)
13	BCR	cI	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	5 (8%)
10	CLA	aA	834	1	54,62,73	2.17	16 (29%)	62,99,113	2.89	29 (46%)
10	CLA	bB	812	2	45,53,73	2.41	16 (35%)	52,89,113	3.20	23 (44%)
10	CLA	aB	808	2	65,73,73	1.98	18 (27%)	76,113,113	2.68	28 (36%)
14	LHG	cA	852	-	48,48,48	0.67	1 (2%)	51,54,54	1.23	7 (13%)
14	LHG	aA	855	-	26,26,48	0.83	0	29,32,54	1.33	3 (10%)
10	CLA	aB	810	2	55,63,73	2.11	15 (27%)	64,101,113	2.90	30 (46%)
10	CLA	bL	204	7	65,73,73	1.93	16 (24%)	76,113,113	2.79	26 (34%)
10	CLA	aB	820	-	65,73,73	2.05	16 (24%)	76,113,113	2.65	28 (36%)
10	CLA	cA	817	1	54,62,73	2.23	17 (31%)	62,99,113	2.95	29 (46%)
10	CLA	aA	828	1	65,73,73	2.02	17 (26%)	76,113,113	2.64	28 (36%)
13	BCR	bI	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
10	CLA	bA	837	1	65,73,73	1.94	16 (24%)	76,113,113	2.72	27 (35%)
13	BCR	cL	206	-	41,41,41	1.03	2 (4%)	56,56,56	1.29	6 (10%)
13	BCR	cB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
10	CLA	bB	818	2	59,67,73	2.16	16 (27%)	68,105,113	2.83	27 (39%)
13	BCR	cM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	10 (17%)
10	CLA	cA	818	1	65,73,73	2.08	17 (26%)	76,113,113	2.91	29 (38%)
10	CLA	aB	838	2	65,73,73	2.01	15 (23%)	76,113,113	2.74	28 (36%)
10	CLA	aA	816	1	54,62,73	2.20	16 (29%)	62,99,113	3.06	28 (45%)
10	CLA	aL	203	7	65,73,73	2.01	18 (27%)	76,113,113	2.69	27 (35%)
10	CLA	cB	803	2	65,73,73	1.93	17 (26%)	76,113,113	2.77	29 (38%)
10	CLA	cA	803	1	45,53,73	2.50	17 (37%)	52,89,113	3.21	25 (48%)
10	CLA	bA	831	1	65,73,73	2.01	17 (26%)	76,113,113	2.67	25 (32%)
13	BCR	aB	847	-	41,41,41	1.09	3 (7%)	56,56,56	1.30	6 (10%)
10	CLA	aB	837	2	60,68,73	2.05	18 (30%)	70,107,113	2.84	27 (38%)
15	LMT	aA	853	-	36,36,36	0.45	0	47,47,47	0.91	3 (6%)
10	CLA	cB	817	2	55,63,73	2.18	17 (30%)	64,101,113	2.88	27 (42%)
10	CLA	aB	827	2	65,73,73	2.01	17 (26%)	76,113,113	2.79	27 (35%)
10	CLA	aA	807	1	45,53,73	2.42	19 (42%)	52,89,113	3.24	26 (50%)
13	BCR	aA	847	-	41,41,41	1.04	2 (4%)	56,56,56	1.29	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	BCR	aA	848	-	41,41,41	1.03	2 (4%)	56,56,56	1.29	8 (14%)
10	CLA	aA	835	1	65,73,73	2.02	17 (26%)	76,113,113	2.64	28 (36%)
10	CLA	aA	854	-	52,60,73	2.27	17 (32%)	60,97,113	3.11	26 (43%)
10	CLA	aB	823	2	55,63,73	2.27	17 (30%)	64,101,113	2.86	27 (42%)
10	CLA	aB	801	-	65,73,73	1.98	16 (24%)	76,113,113	2.77	28 (36%)
13	BCR	aM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	10 (17%)
10	CLA	aB	821	2	47,55,73	2.39	16 (34%)	54,91,113	3.00	26 (48%)
10	CLA	cA	814	1	45,53,73	2.46	17 (37%)	52,89,113	3.12	24 (46%)
13	BCR	aL	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	6 (10%)
10	CLA	bA	805	1	65,73,73	2.03	18 (27%)	76,113,113	2.81	30 (39%)
10	CLA	cA	829	1	65,73,73	2.01	17 (26%)	76,113,113	2.76	27 (35%)
10	CLA	cA	833	1	65,73,73	1.98	16 (24%)	76,113,113	2.77	27 (35%)
10	CLA	bB	838	2	65,73,73	2.01	15 (23%)	76,113,113	2.73	28 (36%)
10	CLA	bA	828	1	65,73,73	2.02	17 (26%)	76,113,113	2.64	28 (36%)
12	SF4	bC	101	3	0,12,12	-	-	-	-	-
11	PQN	aA	844	-	34,34,34	1.53	2 (5%)	42,45,45	1.22	4 (9%)
12	SF4	aA	845	2,1	0,12,12	-	-	-	-	-
10	CLA	cA	832	1	65,73,73	1.96	16 (24%)	76,113,113	2.73	29 (38%)
10	CLA	cB	810	2	55,63,73	2.11	14 (25%)	64,101,113	2.90	30 (46%)
10	CLA	cA	839	1	65,73,73	2.04	16 (24%)	76,113,113	2.67	26 (34%)
10	CLA	cB	813	2	45,53,73	2.46	18 (40%)	52,89,113	3.08	22 (42%)
13	BCR	bA	849	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	7 (12%)
10	CLA	bA	832	1	65,73,73	1.96	16 (24%)	76,113,113	2.74	29 (38%)
10	CLA	cA	806	1	51,59,73	2.29	16 (31%)	59,96,113	3.07	28 (47%)
10	CLA	cA	841	1	65,73,73	2.03	18 (27%)	76,113,113	2.68	27 (35%)
10	CLA	aB	833	2	58,66,73	2.16	17 (29%)	67,104,113	2.85	29 (43%)
10	CLA	cA	812	1	65,73,73	2.04	16 (24%)	76,113,113	2.75	28 (36%)
10	CLA	bA	840	-	51,59,73	2.34	17 (33%)	59,96,113	3.06	27 (45%)
10	CLA	aA	810	1	65,73,73	2.06	15 (23%)	76,113,113	2.73	27 (35%)
10	CLA	bB	831	2	45,53,73	2.45	15 (33%)	52,89,113	3.11	25 (48%)
10	CLA	cA	826	1	65,73,73	1.99	16 (24%)	76,113,113	2.69	27 (35%)
10	CLA	aB	825	2	54,62,73	2.22	17 (31%)	62,99,113	2.93	28 (45%)
10	CLA	aA	809	1	45,53,73	2.43	16 (35%)	52,89,113	3.21	23 (44%)
10	CLA	cA	835	1	65,73,73	2.03	17 (26%)	76,113,113	2.64	28 (36%)
10	CLA	bB	825	2	54,62,73	2.22	15 (27%)	62,99,113	2.94	28 (45%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	CLA	bB	817	2	55,63,73	2.18	17 (30%)	64,101,113	2.88	27 (42%)
10	CLA	bB	827	2	65,73,73	2.02	18 (27%)	76,113,113	2.79	28 (36%)
10	CLA	bA	803	1	45,53,73	2.50	18 (40%)	52,89,113	3.21	25 (48%)
10	CLA	bA	811	1	54,62,73	2.22	17 (31%)	62,99,113	2.90	27 (43%)
11	PQN	cB	842	-	34,34,34	1.50	2 (5%)	42,45,45	1.05	3 (7%)
10	CLA	cB	835	-	45,53,73	2.46	17 (37%)	52,89,113	3.10	24 (46%)
10	CLA	bB	819	2	60,68,73	2.08	15 (25%)	70,107,113	2.88	30 (42%)
10	CLA	cA	816	1	54,62,73	2.20	15 (27%)	62,99,113	3.06	28 (45%)
10	CLA	cA	819	1	61,69,73	2.11	17 (27%)	71,108,113	2.70	26 (36%)
10	CLA	bB	811	2	65,73,73	1.94	17 (26%)	76,113,113	2.66	25 (32%)
10	CLA	aA	836	1	51,59,73	2.26	17 (33%)	59,96,113	5.96	30 (50%)
10	CLA	cB	825	2	54,62,73	2.22	16 (29%)	62,99,113	2.93	28 (45%)
10	CLA	aA	820	-	65,73,73	2.03	15 (23%)	76,113,113	2.62	27 (35%)
10	CLA	cA	836	1	51,59,73	2.27	17 (33%)	59,96,113	5.96	30 (50%)
10	CLA	bB	802	-	65,73,73	1.99	17 (26%)	76,113,113	2.63	27 (35%)
13	BCR	cB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.32	5 (8%)
10	CLA	aB	803	2	65,73,73	1.93	17 (26%)	76,113,113	2.77	29 (38%)
10	CLA	bB	824	2	45,53,73	2.47	16 (35%)	52,89,113	3.13	24 (46%)
10	CLA	cB	833	2	58,66,73	2.16	17 (29%)	67,104,113	2.85	28 (41%)
10	CLA	cB	818	2	59,67,73	2.16	17 (28%)	68,105,113	2.83	27 (39%)
10	CLA	aA	803	1	45,53,73	2.50	18 (40%)	52,89,113	3.21	25 (48%)
10	CLA	bB	840	-	65,73,73	1.97	17 (26%)	76,113,113	2.66	28 (36%)
10	CLA	aA	831	1	65,73,73	2.01	17 (26%)	76,113,113	2.68	25 (32%)
10	CLA	aB	802	-	65,73,73	1.98	17 (26%)	76,113,113	2.64	27 (35%)
13	BCR	aB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
10	CLA	bB	833	2	58,66,73	2.16	17 (29%)	67,104,113	2.84	28 (41%)
10	CLA	cB	839	2	47,55,73	2.33	18 (38%)	54,91,113	3.17	25 (46%)
10	CLA	cB	832	2	65,73,73	2.03	18 (27%)	76,113,113	2.72	28 (36%)
10	CLA	aB	819	2	60,68,73	2.09	15 (25%)	70,107,113	2.89	30 (42%)
10	CLA	aB	841	2	65,73,73	1.95	16 (24%)	76,113,113	2.70	27 (35%)
10	CLA	cA	828	1	65,73,73	2.02	17 (26%)	76,113,113	2.64	28 (36%)
10	CLA	aA	804	1	65,73,73	1.97	16 (24%)	76,113,113	2.75	26 (34%)
10	CLA	cA	824	-	65,73,73	1.96	17 (26%)	76,113,113	2.77	24 (31%)
10	CLA	aB	829	2	65,73,73	2.01	18 (27%)	76,113,113	2.51	26 (34%)
10	CLA	bB	826	-	65,73,73	2.08	16 (24%)	76,113,113	2.79	30 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	BCR	bA	851	-	41,41,41	1.06	2 (4%)	56,56,56	1.20	3 (5%)
10	CLA	bB	836	-	45,53,73	2.49	17 (37%)	52,89,113	3.11	25 (48%)
10	CLA	bB	832	2	65,73,73	2.03	17 (26%)	76,113,113	2.72	28 (36%)
10	CLA	aL	205	-	65,73,73	1.99	19 (29%)	76,113,113	2.73	26 (34%)
10	CLA	aA	829	1	65,73,73	2.01	17 (26%)	76,113,113	2.77	27 (35%)
10	CLA	cB	840	-	65,73,73	1.97	17 (26%)	76,113,113	2.66	28 (36%)
10	CLA	cA	805	1	65,73,73	2.03	18 (27%)	76,113,113	2.80	30 (39%)
10	CLA	aL	204	7	65,73,73	1.93	16 (24%)	76,113,113	2.80	26 (34%)
10	CLA	aA	856	2	49,57,73	2.38	17 (34%)	55,93,113	3.00	24 (43%)
9	CL0	cA	801	1	65,73,73	1.93	17 (26%)	76,113,113	2.69	30 (39%)
10	CLA	aB	832	2	65,73,73	2.03	17 (26%)	76,113,113	2.72	28 (36%)
13	BCR	aA	851	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	3 (5%)
10	CLA	cB	807	2	65,73,73	1.99	19 (29%)	76,113,113	2.77	30 (39%)
13	BCR	bA	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.23	7 (12%)
15	LMT	cA	853	-	36,36,36	0.45	0	47,47,47	0.91	3 (6%)
13	BCR	aI	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.27	6 (10%)
13	BCR	aL	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	3 (5%)
10	CLA	aB	806	2	54,62,73	2.20	17 (31%)	62,99,113	3.06	31 (50%)
10	CLA	cA	822	1	51,59,73	2.31	16 (31%)	59,96,113	3.05	28 (47%)
10	CLA	bB	828	2	65,73,73	1.95	19 (29%)	76,113,113	2.76	27 (35%)
10	CLA	aB	812	2	45,53,73	2.40	16 (35%)	52,89,113	3.19	23 (44%)
10	CLA	aA	823	1	65,73,73	2.02	17 (26%)	76,113,113	2.62	25 (32%)
10	CLA	bB	804	-	57,65,73	2.10	15 (26%)	66,103,113	3.08	29 (43%)
13	BCR	aI	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	5 (8%)
11	PQN	aB	842	-	34,34,34	1.51	2 (5%)	42,45,45	1.05	3 (7%)
10	CLA	aA	812	1	65,73,73	2.04	17 (26%)	76,113,113	2.75	28 (36%)
12	SF4	cC	101	3	0,12,12	-	-	-	-	-
10	CLA	bB	801	-	65,73,73	1.97	16 (24%)	76,113,113	2.77	29 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cB	819	2	1/1/14/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bA	816	1	-	10/24/102/115	-
9	CL0	aA	801	1	3/3/20/25	6/37/135/135	-
10	CLA	cA	837	1	1/1/15/20	7/37/115/115	-
10	CLA	cA	811	1	1/1/12/20	8/24/102/115	-
10	CLA	bA	808	1	1/1/11/20	4/13/91/115	-
10	CLA	aA	838	1	1/1/12/20	9/19/97/115	-
10	CLA	aB	831	2	1/1/11/20	6/13/91/115	-
13	BCR	bA	848	-	-	16/29/63/63	0/2/2/2
10	CLA	bA	835	1	1/1/15/20	12/37/115/115	-
13	BCR	bL	207	-	-	7/29/63/63	0/2/2/2
10	CLA	bB	805	-	1/1/15/20	10/37/115/115	-
10	CLA	cB	808	2	1/1/15/20	12/37/115/115	-
10	CLA	cB	829	2	1/1/15/20	12/37/115/115	-
10	CLA	aB	836	-	1/1/11/20	2/13/91/115	-
13	BCR	cA	850	-	-	9/29/63/63	0/2/2/2
10	CLA	aA	827	1	1/1/15/20	17/37/115/115	-
13	BCR	cA	849	-	-	13/29/63/63	0/2/2/2
10	CLA	bB	841	2	1/1/15/20	10/37/115/115	-
10	CLA	aA	821	1	1/1/11/20	4/18/96/115	-
10	CLA	aB	805	-	1/1/15/20	10/37/115/115	-
10	CLA	cB	830	2	1/1/15/20	9/37/115/115	-
10	CLA	aA	814	1	1/1/11/20	2/13/91/115	-
10	CLA	bA	856	2	1/1/11/20	7/18/96/115	-
10	CLA	aA	843	-	1/1/9/20	2/7/81/115	-
10	CLA	cB	802	-	1/1/15/20	13/37/115/115	-
10	CLA	cA	843	-	1/1/9/20	2/7/81/115	-
10	CLA	bA	807	1	1/1/11/20	7/13/91/115	-
13	BCR	bA	847	-	-	9/29/63/63	0/2/2/2
10	CLA	cA	821	1	1/1/11/20	4/18/96/115	-
10	CLA	cA	804	1	1/1/15/20	10/37/115/115	-
10	CLA	aA	839	1	1/1/15/20	6/37/115/115	-
9	CL0	bA	801	1	3/3/20/25	6/37/135/135	-
10	CLA	aB	824	2	1/1/11/20	5/13/91/115	-
13	BCR	aB	849	-	-	18/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bB	822	2	-	7/13/91/115	-
10	CLA	cA	813	1	1/1/11/20	1/13/91/115	-
10	CLA	aB	840	-	1/1/15/20	2/37/115/115	-
13	BCR	bB	844	-	-	10/29/63/63	0/2/2/2
10	CLA	bB	816	2	1/1/11/20	2/13/91/115	-
10	CLA	cL	205	-	-	11/37/115/115	-
10	CLA	aA	802	1	1/1/11/20	7/13/91/115	-
13	BCR	aA	846	-	-	14/29/63/63	0/2/2/2
13	BCR	cI	102	-	-	8/29/63/63	0/2/2/2
10	CLA	aA	806	1	1/1/12/20	3/21/99/115	-
10	CLA	aA	833	1	1/1/15/20	10/37/115/115	-
10	CLA	cB	838	2	1/1/15/20	9/37/115/115	-
10	CLA	cA	823	1	1/1/15/20	12/37/115/115	-
10	CLA	aB	830	2	1/1/15/20	9/37/115/115	-
10	CLA	bL	205	-	-	11/37/115/115	-
10	CLA	bB	835	-	1/1/11/20	5/13/91/115	-
10	CLA	cA	854	14	-	8/22/100/115	-
10	CLA	bB	814	2	1/1/15/20	14/37/115/115	-
10	CLA	cB	837	2	1/1/14/20	10/31/109/115	-
10	CLA	aB	839	2	1/1/11/20	5/16/94/115	-
13	BCR	bB	843	-	-	11/29/63/63	0/2/2/2
10	CLA	bA	809	1	1/1/11/20	2/13/91/115	-
10	CLA	cB	836	-	1/1/11/20	2/13/91/115	-
10	CLA	aA	840	-	1/1/12/20	6/21/99/115	-
10	CLA	bB	837	2	1/1/14/20	10/31/109/115	-
15	LMT	bA	853	-	-	9/21/61/61	0/2/2/2
10	CLA	aB	814	2	1/1/15/20	14/37/115/115	-
14	LHG	aA	852	-	-	31/53/53/53	-
10	CLA	aA	837	1	1/1/15/20	7/37/115/115	-
10	CLA	bA	830	1	1/1/12/20	5/19/97/115	-
10	CLA	bA	817	1	-	10/24/102/115	-
10	CLA	aA	826	1	1/1/15/20	8/37/115/115	-
10	CLA	aB	811	2	1/1/15/20	17/37/115/115	-
10	CLA	cA	827	1	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cB	831	2	1/1/11/20	6/13/91/115	-
16	LMG	bB	848	-	-	19/50/70/70	0/1/1/1
10	CLA	cB	827	2	1/1/15/20	9/37/115/115	-
10	CLA	cB	823	2	1/1/13/20	13/25/103/115	-
10	CLA	cA	807	1	1/1/11/20	7/13/91/115	-
13	BCR	cL	207	-	-	7/29/63/63	0/2/2/2
10	CLA	cB	821	2	1/1/11/20	4/16/94/115	-
10	CLA	cB	812	2	1/1/11/20	1/13/91/115	-
10	CLA	bA	829	1	1/1/15/20	12/37/115/115	-
10	CLA	aA	841	-	1/1/15/20	11/37/115/115	-
10	CLA	bB	806	2	1/1/12/20	12/24/102/115	-
12	SF4	bA	845	2,1	-	-	0/6/5/5
10	CLA	bB	813	2	-	4/13/91/115	-
10	CLA	bB	809	2	1/1/15/20	6/37/115/115	-
10	CLA	aB	804	-	1/1/13/20	14/28/106/115	-
10	CLA	aA	832	1	1/1/15/20	6/37/115/115	-
13	BCR	aB	843	-	-	11/29/63/63	0/2/2/2
10	CLA	bB	810	2	1/1/13/20	9/25/103/115	-
13	BCR	cB	847	-	-	10/29/63/63	0/2/2/2
10	CLA	bA	802	1	1/1/11/20	7/13/91/115	-
10	CLA	cL	202	2	1/1/13/20	7/25/103/115	-
10	CLA	bA	826	1	1/1/15/20	8/37/115/115	-
10	CLA	bA	843	-	1/1/9/20	2/7/81/115	-
12	SF4	aC	101	3	-	-	0/6/5/5
10	CLA	cA	830	1	1/1/12/20	5/19/97/115	-
10	CLA	cA	825	-	1/1/13/20	9/25/103/115	-
10	CLA	cA	815	-	1/1/11/20	3/18/96/115	-
10	CLA	cB	809	2	1/1/15/20	6/37/115/115	-
10	CLA	cB	826	-	1/1/15/20	12/37/115/115	-
10	CLA	bA	813	1	1/1/11/20	1/13/91/115	-
10	CLA	cB	811	2	1/1/15/20	17/37/115/115	-
10	CLA	bA	810	1	1/1/15/20	10/37/115/115	-
10	CLA	aA	824	-	1/1/15/20	11/37/115/115	-
10	CLA	bA	838	1	1/1/12/20	9/19/97/115	-
10	CLA	bA	834	1	1/1/12/20	8/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cA	856	2	1/1/11/20	7/18/96/115	-
10	CLA	aB	826	-	1/1/15/20	12/37/115/115	-
10	CLA	cB	824	2	1/1/11/20	5/13/91/115	-
10	CLA	bA	823	1	1/1/15/20	12/37/115/115	-
13	BCR	cA	847	-	-	9/29/63/63	0/2/2/2
10	CLA	aA	825	-	1/1/13/20	9/25/103/115	-
10	CLA	aB	835	-	1/1/11/20	5/13/91/115	-
10	CLA	aL	202	2	1/1/13/20	7/25/103/115	-
10	CLA	aA	817	1	-	10/24/102/115	-
10	CLA	aB	813	2	-	4/13/91/115	-
10	CLA	bA	854	-	-	8/22/100/115	-
10	CLA	bA	812	1	1/1/15/20	15/37/115/115	-
10	CLA	aA	811	1	1/1/12/20	8/24/102/115	-
10	CLA	cB	814	2	1/1/15/20	14/37/115/115	-
10	CLA	bA	836	1	1/1/12/20	7/21/99/115	-
13	BCR	cB	843	-	-	11/29/63/63	0/2/2/2
10	CLA	bA	820	-	1/1/15/20	13/37/115/115	-
10	CLA	aB	822	2	-	7/13/91/115	-
13	BCR	cA	848	-	-	16/29/63/63	0/2/2/2
10	CLA	aA	822	1	1/1/12/20	10/21/99/115	-
10	CLA	aB	816	2	1/1/11/20	2/13/91/115	-
12	SF4	cC	102	3	-	-	0/6/5/5
10	CLA	bB	807	2	1/1/15/20	12/37/115/115	-
10	CLA	aA	819	1	1/1/14/20	11/33/111/115	-
13	BCR	bA	850	-	-	9/29/63/63	0/2/2/2
10	CLA	aB	807	2	1/1/15/20	12/37/115/115	-
14	LHG	bA	855	-	-	15/31/31/53	-
10	CLA	aB	818	2	1/1/13/20	11/30/108/115	-
10	CLA	cB	806	2	1/1/12/20	11/24/102/115	-
10	CLA	bA	827	1	1/1/15/20	17/37/115/115	-
10	CLA	cA	842	-	1/1/15/20	13/37/115/115	-
10	CLA	cA	809	1	1/1/11/20	2/13/91/115	-
13	BCR	aA	849	-	-	13/29/63/63	0/2/2/2
10	CLA	bL	203	7	-	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cB	828	2	1/1/15/20	11/37/115/115	-
10	CLA	bA	818	1	1/1/15/20	13/37/115/115	-
10	CLA	bA	821	1	1/1/11/20	4/18/96/115	-
10	CLA	aA	805	1	1/1/15/20	10/37/115/115	-
10	CLA	cB	804	-	1/1/13/20	14/28/106/115	-
13	BCR	cA	851	-	-	13/29/63/63	0/2/2/2
10	CLA	bB	823	2	1/1/13/20	13/25/103/115	-
11	PQN	cA	844	-	-	8/23/43/43	0/2/2/2
12	SF4	cA	845	2,1	-	-	0/6/5/5
13	BCR	bB	846	-	-	8/29/63/63	0/2/2/2
10	CLA	bA	839	1	1/1/15/20	6/37/115/115	-
10	CLA	aB	815	2	1/1/13/20	7/27/105/115	-
10	CLA	cA	834	1	1/1/12/20	8/24/102/115	-
10	CLA	aA	830	1	1/1/12/20	5/19/97/115	-
10	CLA	bB	808	2	1/1/15/20	12/37/115/115	-
10	CLA	cB	816	2	1/1/11/20	2/13/91/115	-
10	CLA	aA	815	-	1/1/11/20	3/18/96/115	-
10	CLA	cA	802	1	1/1/11/20	7/13/91/115	-
10	CLA	bA	824	-	1/1/15/20	11/37/115/115	-
13	BCR	aB	846	-	-	8/29/63/63	0/2/2/2
14	LHG	cA	855	10	-	15/31/31/53	-
16	LMG	aB	848	-	-	19/50/70/70	0/1/1/1
11	PQN	bB	842	-	-	2/23/43/43	0/2/2/2
10	CLA	bL	202	2	1/1/13/20	7/25/103/115	-
10	CLA	cB	841	2	1/1/15/20	10/37/115/115	-
10	CLA	cA	810	1	1/1/15/20	10/37/115/115	-
10	CLA	cB	822	2	-	7/13/91/115	-
10	CLA	cA	820	-	1/1/15/20	13/37/115/115	-
13	BCR	cB	846	-	-	8/29/63/63	0/2/2/2
13	BCR	aB	844	-	-	10/29/63/63	0/2/2/2
14	LHG	bA	852	-	-	31/53/53/53	-
13	BCR	bL	206	-	-	8/29/63/63	0/2/2/2
13	BCR	aA	850	-	-	9/29/63/63	0/2/2/2
10	CLA	cA	831	1	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cB	801	-	1/1/15/20	7/37/115/115	-
13	BCR	bB	847	-	-	10/29/63/63	0/2/2/2
10	CLA	bA	825	-	1/1/13/20	9/25/103/115	-
13	BCR	bM	101	-	-	13/29/63/63	0/2/2/2
10	CLA	bA	815	-	1/1/11/20	3/18/96/115	-
10	CLA	aB	828	2	1/1/15/20	11/37/115/115	-
10	CLA	bB	821	2	1/1/11/20	4/16/94/115	-
10	CLA	aA	808	1	1/1/11/20	4/13/91/115	-
10	CLA	cA	808	1	1/1/11/20	4/13/91/115	-
10	CLA	bA	822	1	1/1/12/20	10/21/99/115	-
10	CLA	cB	805	-	1/1/15/20	10/37/115/115	-
10	CLA	bA	814	1	1/1/11/20	2/13/91/115	-
10	CLA	bA	833	1	1/1/15/20	10/37/115/115	-
10	CLA	bB	803	2	1/1/15/20	4/37/115/115	-
13	BCR	bB	849	-	-	18/29/63/63	0/2/2/2
10	CLA	bB	839	2	1/1/11/20	5/16/94/115	-
10	CLA	aA	818	1	1/1/15/20	13/37/115/115	-
12	SF4	bC	102	3	-	-	0/6/5/5
16	LMG	cB	848	-	-	19/50/70/70	0/1/1/1
10	CLA	bA	804	1	1/1/15/20	10/37/115/115	-
10	CLA	aB	817	2	1/1/13/20	10/25/103/115	-
10	CLA	bA	842	-	1/1/15/20	13/37/115/115	-
10	CLA	cA	840	-	1/1/12/20	6/21/99/115	-
10	CLA	aA	842	-	1/1/15/20	13/37/115/115	-
13	BCR	bI	102	-	-	8/29/63/63	0/2/2/2
10	CLA	cL	204	7	1/1/15/20	8/37/115/115	-
10	CLA	bB	829	2	1/1/15/20	12/37/115/115	-
13	BCR	cB	849	-	-	18/29/63/63	0/2/2/2
10	CLA	bB	820	-	1/1/15/20	11/37/115/115	-
10	CLA	bB	815	2	1/1/13/20	7/27/105/115	-
10	CLA	aB	809	2	1/1/15/20	6/37/115/115	-
10	CLA	bA	819	1	1/1/14/20	11/33/111/115	-
10	CLA	bA	806	1	1/1/12/20	3/21/99/115	-
10	CLA	cB	834	2	1/1/11/20	0/13/91/115	-
10	CLA	aA	813	1	1/1/11/20	1/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bA	841	1	1/1/15/20	11/37/115/115	-
11	PQN	bA	844	-	-	8/23/43/43	0/2/2/2
13	BCR	cA	846	-	-	14/29/63/63	0/2/2/2
10	CLA	bB	830	2	1/1/15/20	9/37/115/115	-
12	SF4	aC	102	3	-	-	0/6/5/5
10	CLA	bB	834	2	1/1/11/20	0/13/91/115	-
10	CLA	cL	203	7	-	11/37/115/115	-
10	CLA	cB	820	-	1/1/15/20	11/37/115/115	-
10	CLA	cB	815	2	1/1/13/20	7/27/105/115	-
10	CLA	aB	834	2	1/1/11/20	0/13/91/115	-
13	BCR	bB	845	-	-	12/29/63/63	0/2/2/2
10	CLA	cA	838	1	1/1/12/20	9/19/97/115	-
13	BCR	cI	103	-	-	8/29/63/63	0/2/2/2
10	CLA	aA	834	1	1/1/12/20	8/24/102/115	-
10	CLA	bB	812	2	1/1/11/20	1/13/91/115	-
10	CLA	aB	808	2	1/1/15/20	12/37/115/115	-
14	LHG	cA	852	-	-	31/53/53/53	-
14	LHG	aA	855	-	-	15/31/31/53	-
10	CLA	aB	810	2	1/1/13/20	9/25/103/115	-
10	CLA	bL	204	7	1/1/15/20	8/37/115/115	-
10	CLA	aB	820	-	1/1/15/20	11/37/115/115	-
10	CLA	cA	817	1	-	10/24/102/115	-
10	CLA	aA	828	1	1/1/15/20	6/37/115/115	-
13	BCR	bI	101	-	-	8/29/63/63	0/2/2/2
10	CLA	bA	837	1	1/1/15/20	7/37/115/115	-
13	BCR	cL	206	-	-	8/29/63/63	0/2/2/2
13	BCR	cB	845	-	-	12/29/63/63	0/2/2/2
10	CLA	bB	818	2	1/1/13/20	11/30/108/115	-
13	BCR	cM	101	-	-	13/29/63/63	0/2/2/2
10	CLA	cA	818	1	1/1/15/20	13/37/115/115	-
10	CLA	aB	838	2	1/1/15/20	9/37/115/115	-
10	CLA	aA	816	1	-	10/24/102/115	-
10	CLA	aL	203	7	-	11/37/115/115	-
10	CLA	cB	803	2	1/1/15/20	4/37/115/115	-
10	CLA	cA	803	1	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bA	831	1	1/1/15/20	13/37/115/115	-
13	BCR	aB	847	-	-	10/29/63/63	0/2/2/2
10	CLA	aB	837	2	1/1/14/20	10/31/109/115	-
15	LMT	aA	853	-	-	9/21/61/61	0/2/2/2
10	CLA	cB	817	2	1/1/13/20	10/25/103/115	-
10	CLA	aB	827	2	1/1/15/20	9/37/115/115	-
10	CLA	aA	807	1	1/1/11/20	7/13/91/115	-
13	BCR	aA	847	-	-	9/29/63/63	0/2/2/2
13	BCR	aA	848	-	-	16/29/63/63	0/2/2/2
10	CLA	aA	835	1	1/1/15/20	12/37/115/115	-
10	CLA	aA	854	-	-	8/22/100/115	-
10	CLA	aB	823	2	1/1/13/20	13/25/103/115	-
10	CLA	aB	801	-	1/1/15/20	7/37/115/115	-
13	BCR	aM	101	-	-	13/29/63/63	0/2/2/2
10	CLA	aB	821	2	1/1/11/20	4/16/94/115	-
10	CLA	cA	814	1	1/1/11/20	2/13/91/115	-
13	BCR	aL	206	-	-	8/29/63/63	0/2/2/2
10	CLA	bA	805	1	1/1/15/20	10/37/115/115	-
10	CLA	cA	829	1	1/1/15/20	12/37/115/115	-
10	CLA	cA	833	1	1/1/15/20	10/37/115/115	-
10	CLA	bB	838	2	1/1/15/20	9/37/115/115	-
10	CLA	bA	828	1	1/1/15/20	6/37/115/115	-
12	SF4	bC	101	3	-	-	0/6/5/5
11	PQN	aA	844	-	-	8/23/43/43	0/2/2/2
12	SF4	aA	845	2,1	-	-	0/6/5/5
10	CLA	cA	832	1	1/1/15/20	6/37/115/115	-
10	CLA	cB	810	2	1/1/13/20	9/25/103/115	-
10	CLA	cA	839	1	1/1/15/20	6/37/115/115	-
10	CLA	cB	813	2	-	4/13/91/115	-
13	BCR	bA	849	-	-	13/29/63/63	0/2/2/2
10	CLA	bA	832	1	1/1/15/20	6/37/115/115	-
10	CLA	cA	806	1	1/1/12/20	3/21/99/115	-
10	CLA	cA	841	1	1/1/15/20	11/37/115/115	-
10	CLA	aB	833	2	1/1/13/20	14/29/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cA	812	1	1/1/15/20	15/37/115/115	-
10	CLA	bA	840	-	1/1/12/20	6/21/99/115	-
10	CLA	aA	810	1	1/1/15/20	10/37/115/115	-
10	CLA	bB	831	2	1/1/11/20	6/13/91/115	-
10	CLA	cA	826	1	1/1/15/20	8/37/115/115	-
10	CLA	aB	825	2	1/1/12/20	7/24/102/115	-
10	CLA	aA	809	1	1/1/11/20	2/13/91/115	-
10	CLA	cA	835	1	1/1/15/20	12/37/115/115	-
10	CLA	bB	825	2	1/1/12/20	7/24/102/115	-
10	CLA	bB	817	2	1/1/13/20	10/25/103/115	-
10	CLA	bB	827	2	1/1/15/20	9/37/115/115	-
10	CLA	bA	803	1	1/1/11/20	3/13/91/115	-
10	CLA	bA	811	1	1/1/12/20	8/24/102/115	-
11	PQN	cB	842	-	-	2/23/43/43	0/2/2/2
10	CLA	cB	835	-	1/1/11/20	5/13/91/115	-
10	CLA	bB	819	2	1/1/14/20	10/31/109/115	-
10	CLA	cA	816	1	-	10/24/102/115	-
10	CLA	cA	819	1	1/1/14/20	11/33/111/115	-
10	CLA	bB	811	2	1/1/15/20	17/37/115/115	-
10	CLA	aA	836	1	1/1/12/20	7/21/99/115	-
10	CLA	cB	825	2	1/1/12/20	7/24/102/115	-
10	CLA	aA	820	-	1/1/15/20	13/37/115/115	-
10	CLA	cA	836	1	1/1/12/20	7/21/99/115	-
10	CLA	bB	802	-	1/1/15/20	13/37/115/115	-
13	BCR	cB	844	-	-	10/29/63/63	0/2/2/2
10	CLA	aB	803	2	1/1/15/20	4/37/115/115	-
10	CLA	bB	824	2	1/1/11/20	5/13/91/115	-
10	CLA	cB	833	2	1/1/13/20	14/29/107/115	-
10	CLA	cB	818	2	1/1/13/20	11/30/108/115	-
10	CLA	aA	803	1	1/1/11/20	3/13/91/115	-
10	CLA	bB	840	-	1/1/15/20	2/37/115/115	-
10	CLA	aA	831	1	1/1/15/20	13/37/115/115	-
10	CLA	aB	802	-	1/1/15/20	13/37/115/115	-
13	BCR	aB	845	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bB	833	2	1/1/13/20	14/29/107/115	-
10	CLA	cB	839	2	1/1/11/20	5/16/94/115	-
10	CLA	cB	832	2	1/1/15/20	14/37/115/115	-
10	CLA	aB	819	2	1/1/14/20	10/31/109/115	-
10	CLA	aB	841	2	1/1/15/20	10/37/115/115	-
10	CLA	cA	828	1	1/1/15/20	6/37/115/115	-
10	CLA	aA	804	1	1/1/15/20	10/37/115/115	-
10	CLA	cA	824	-	1/1/15/20	11/37/115/115	-
10	CLA	aB	829	2	1/1/15/20	12/37/115/115	-
10	CLA	bB	826	-	1/1/15/20	12/37/115/115	-
13	BCR	bA	851	-	-	13/29/63/63	0/2/2/2
10	CLA	bB	836	-	1/1/11/20	2/13/91/115	-
10	CLA	bB	832	2	1/1/15/20	14/37/115/115	-
10	CLA	aL	205	-	-	11/37/115/115	-
10	CLA	aA	829	1	1/1/15/20	12/37/115/115	-
10	CLA	cB	840	-	1/1/15/20	2/37/115/115	-
10	CLA	cA	805	1	1/1/15/20	10/37/115/115	-
10	CLA	aL	204	7	1/1/15/20	8/37/115/115	-
10	CLA	aA	856	2	1/1/11/20	7/18/96/115	-
9	CL0	cA	801	1	3/3/20/25	6/37/135/135	-
10	CLA	aB	832	2	1/1/15/20	14/37/115/115	-
13	BCR	aA	851	-	-	13/29/63/63	0/2/2/2
10	CLA	cB	807	2	1/1/15/20	12/37/115/115	-
13	BCR	bA	846	-	-	14/29/63/63	0/2/2/2
15	LMT	cA	853	-	-	9/21/61/61	0/2/2/2
13	BCR	aI	101	-	-	8/29/63/63	0/2/2/2
13	BCR	aL	207	-	-	7/29/63/63	0/2/2/2
10	CLA	aB	806	2	1/1/12/20	11/24/102/115	-
10	CLA	cA	822	1	1/1/12/20	10/21/99/115	-
10	CLA	bB	828	2	1/1/15/20	11/37/115/115	-
10	CLA	aB	812	2	1/1/11/20	1/13/91/115	-
10	CLA	aA	823	1	1/1/15/20	12/37/115/115	-
10	CLA	bB	804	-	1/1/13/20	14/28/106/115	-
13	BCR	aI	102	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PQN	aB	842	-	-	2/23/43/43	0/2/2/2
10	CLA	aA	812	1	1/1/15/20	15/37/115/115	-
12	SF4	cC	101	3	-	-	0/6/5/5
10	CLA	bB	801	-	1/1/15/20	7/37/115/115	-

The worst 5 of 4662 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	cA	844	PQN	C3-C2	7.31	1.48	1.35
11	bA	844	PQN	C3-C2	7.31	1.48	1.35
11	aA	844	PQN	C3-C2	7.31	1.48	1.35
11	aB	842	PQN	C3-C2	7.23	1.48	1.35
11	cB	842	PQN	C3-C2	7.22	1.48	1.35

The worst 5 of 7586 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	cA	836	CLA	C4-C3-C5	-31.70	79.75	115.98
10	bA	836	CLA	C4-C3-C5	-31.68	79.77	115.98
10	aA	836	CLA	C4-C3-C5	-31.64	79.81	115.98
10	cA	836	CLA	C4-C3-C2	-17.16	79.65	123.68
10	aA	836	CLA	C4-C3-C2	-17.15	79.68	123.68

5 of 255 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	aA	801	CL0	ND
9	aA	801	CL0	NC
9	aA	801	CL0	NA
9	bA	801	CL0	ND
9	bA	801	CL0	NC

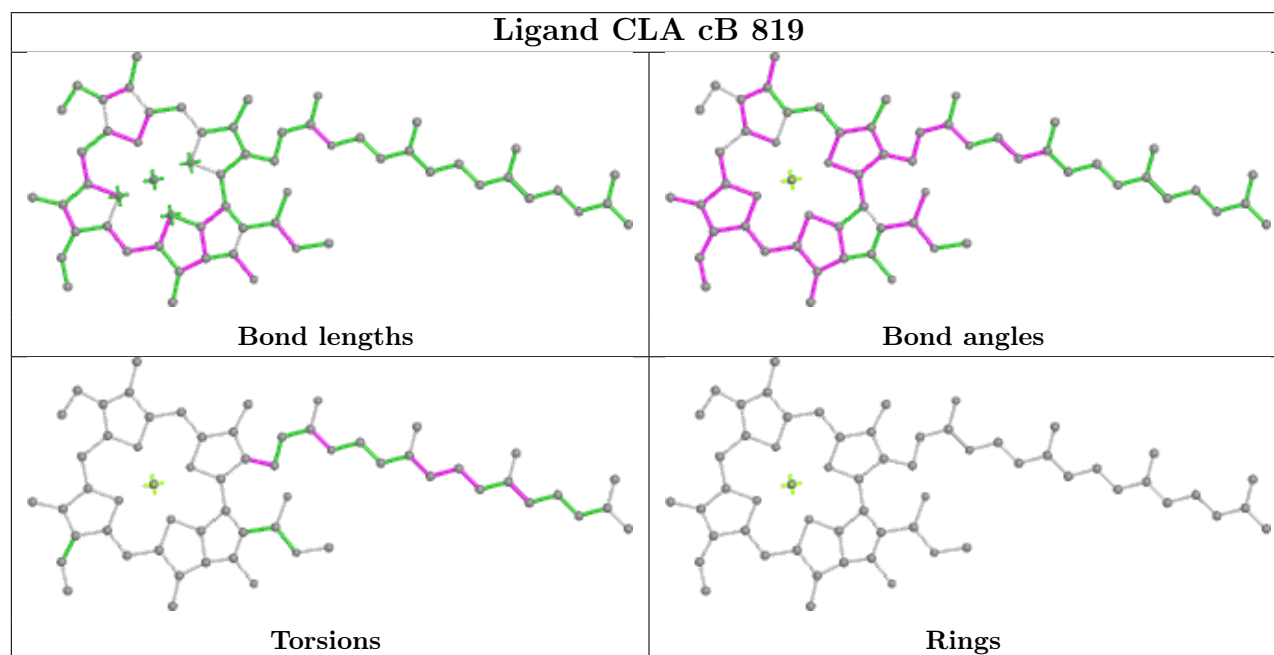
5 of 3079 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	aA	805	CLA	C1A-C2A-CAA-CBA
10	aA	806	CLA	C2-C3-C5-C6
10	aA	806	CLA	C4-C3-C5-C6
10	aA	807	CLA	C3A-C2A-CAA-CBA
10	aA	807	CLA	CHA-CBD-CGD-O2D

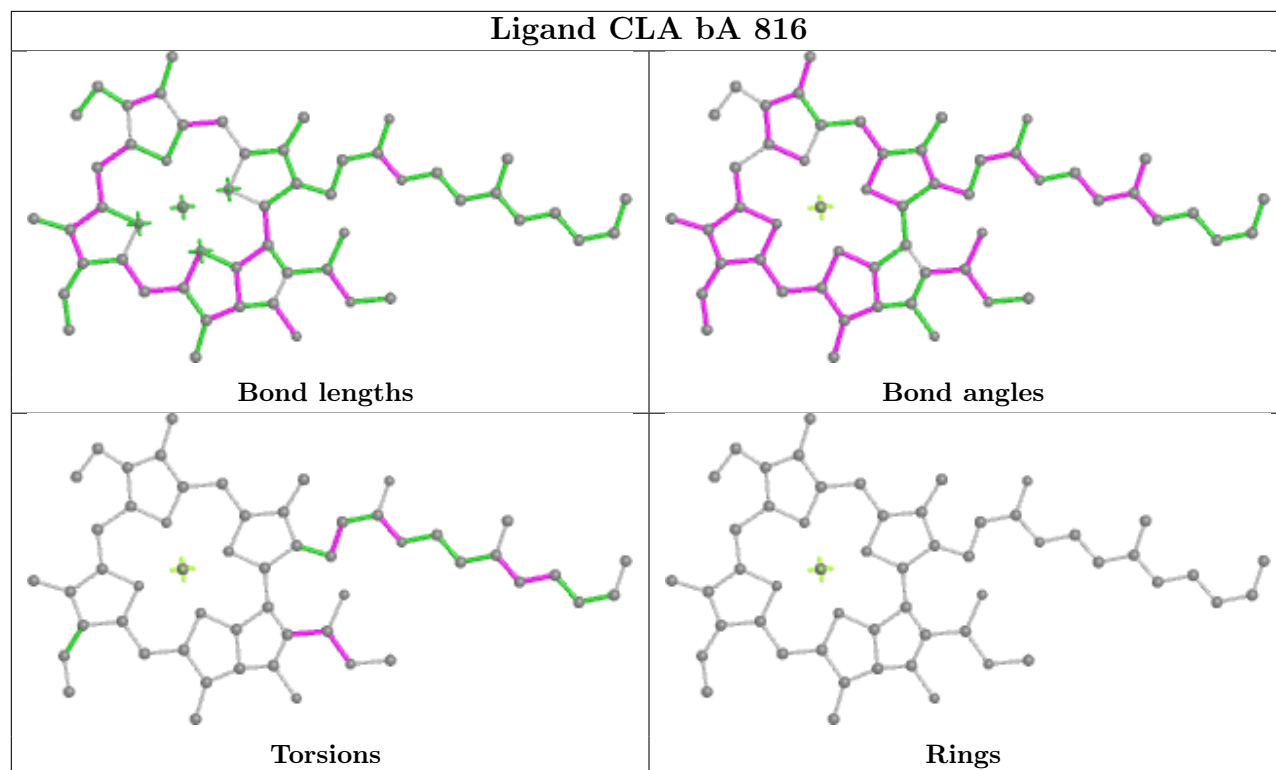
There are no ring outliers.

No monomer is involved in short contacts.

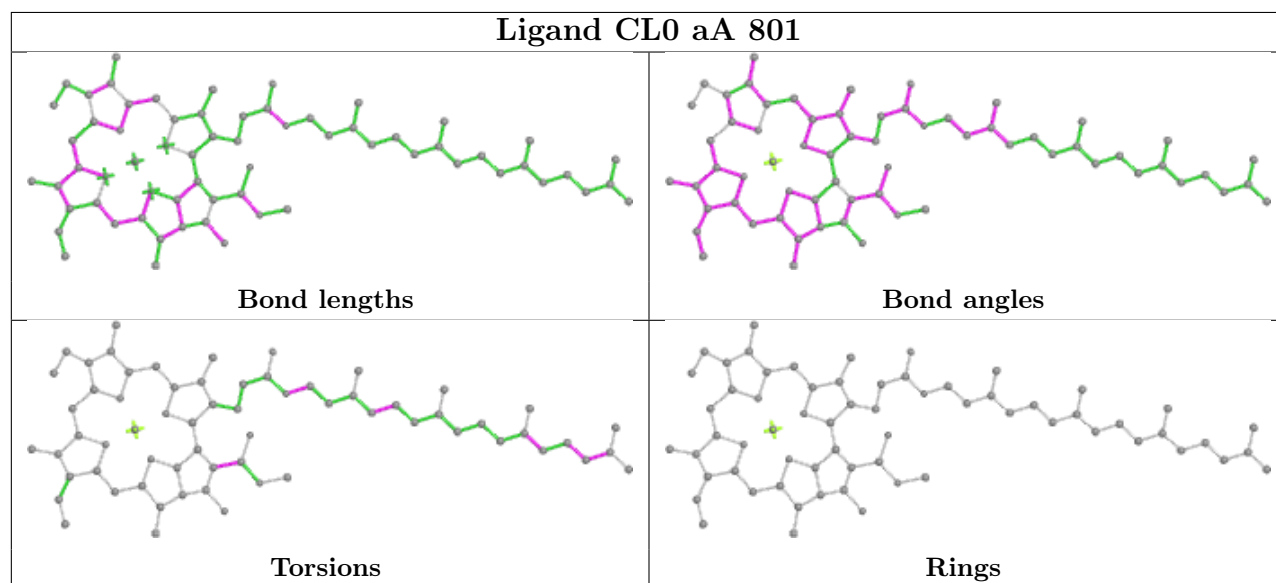
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



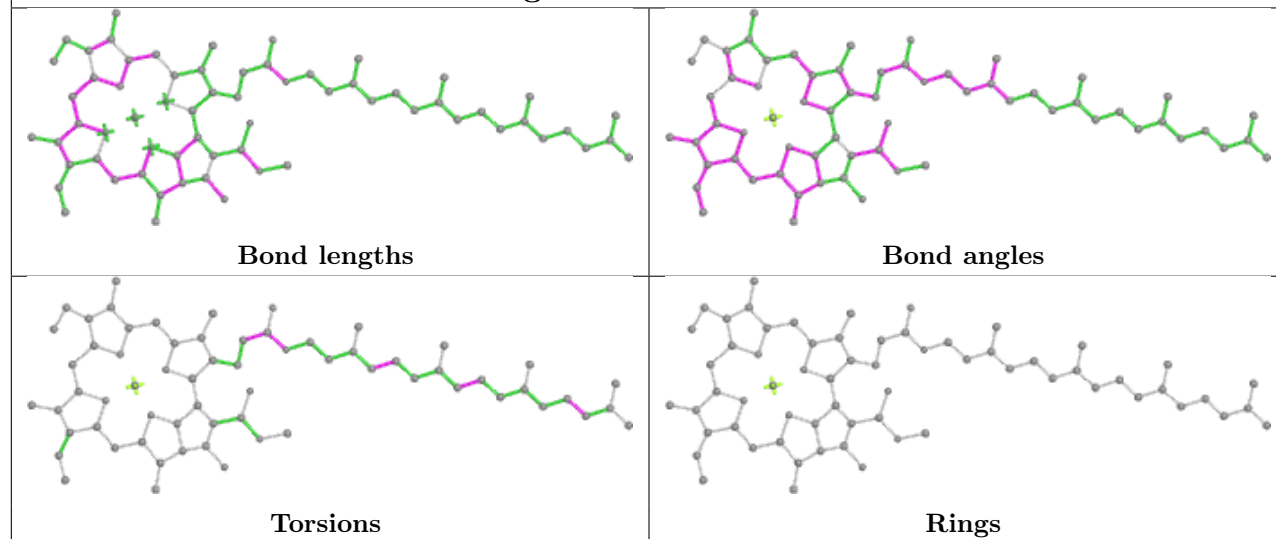
## Ligand CLA bA 816



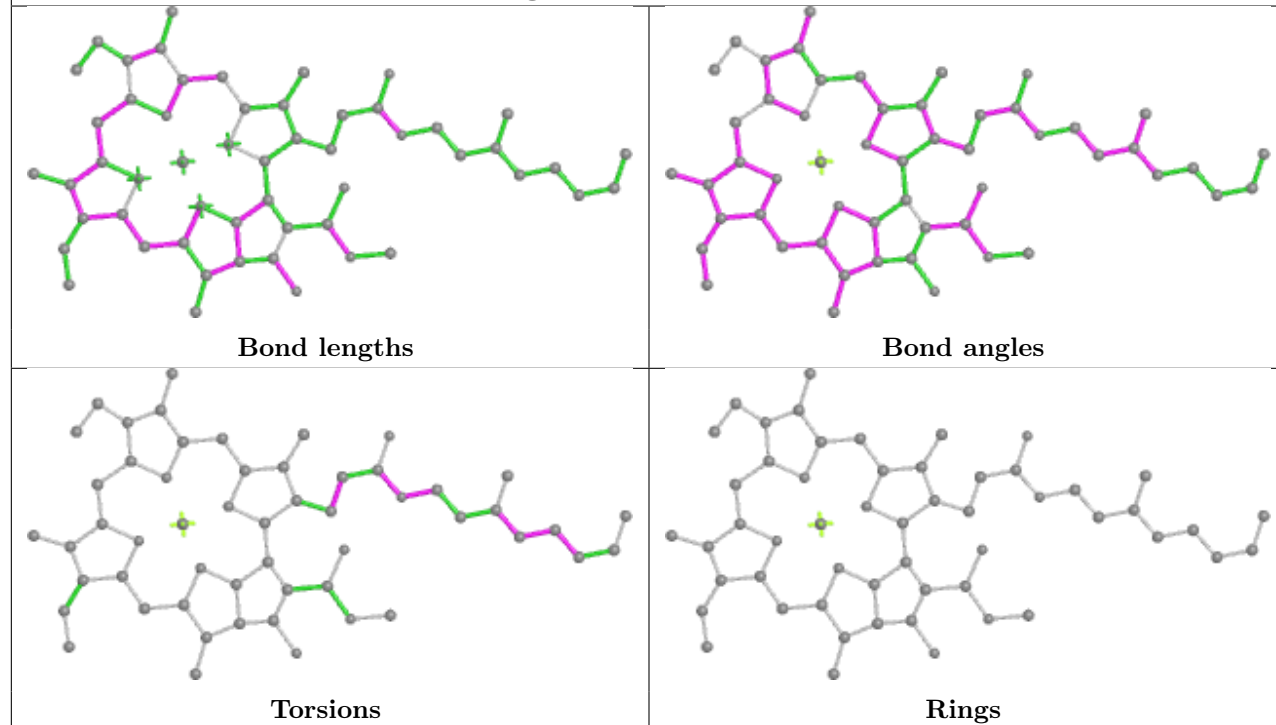
## Ligand CL0 aA 801

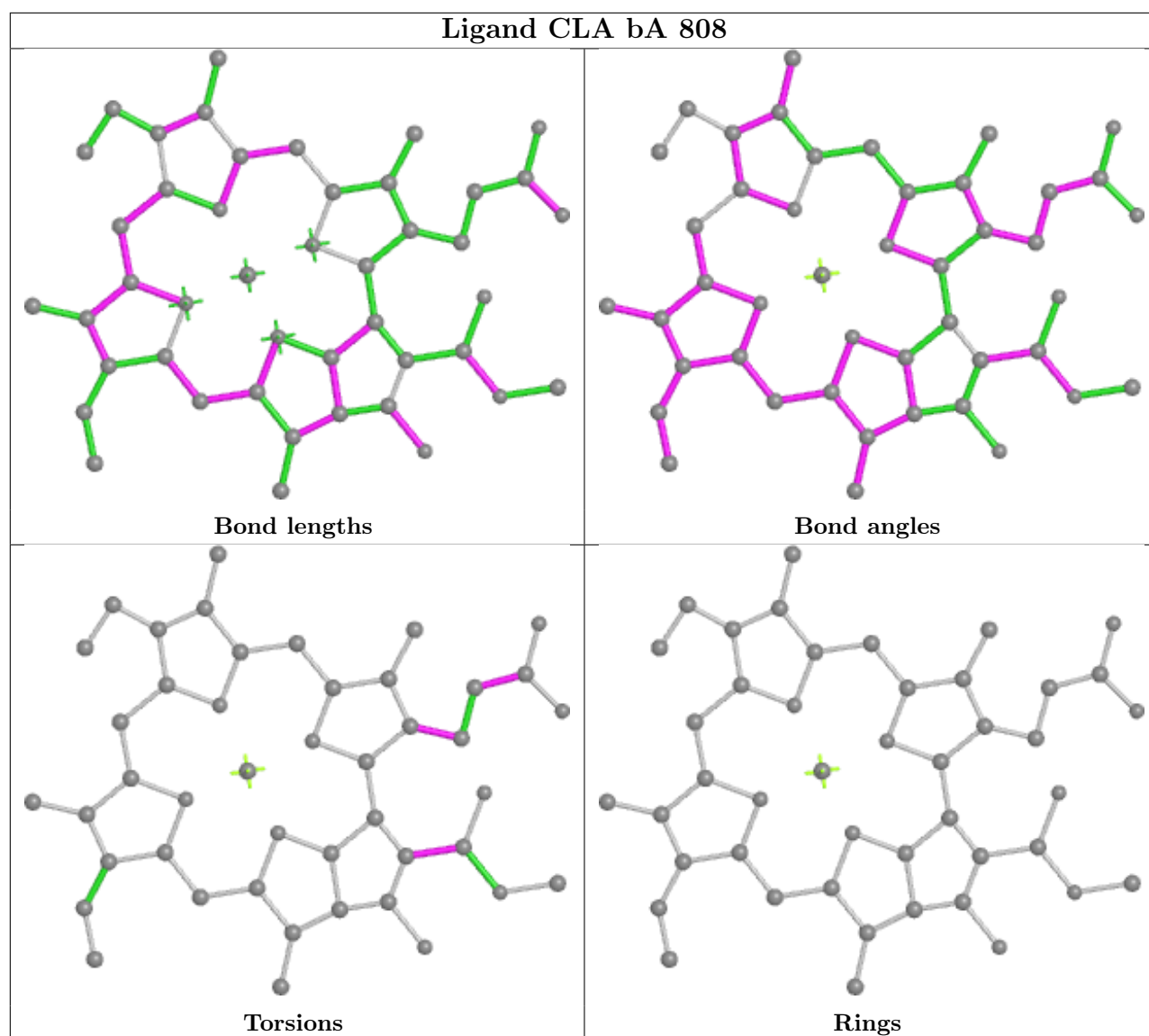


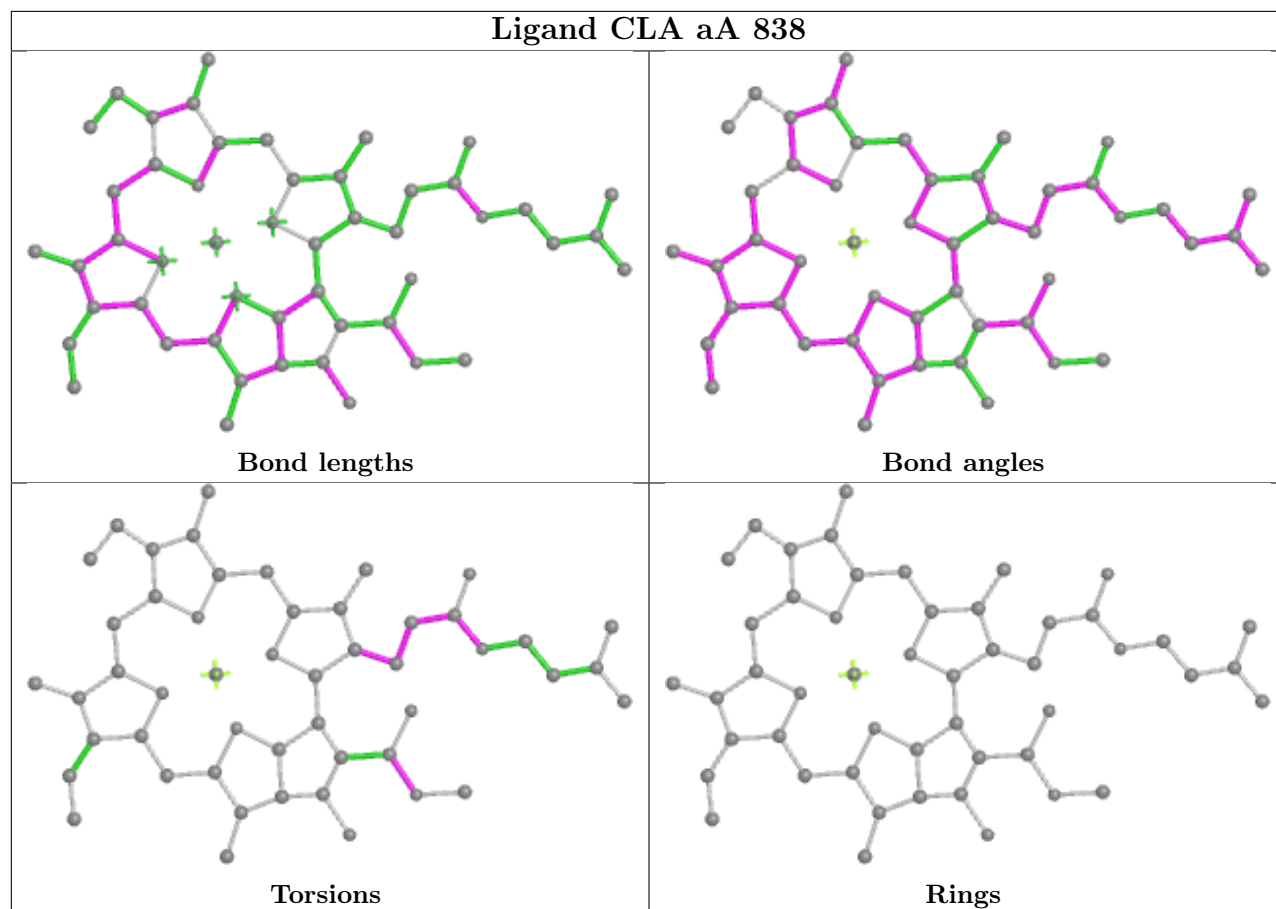
## Ligand CLA cA 837

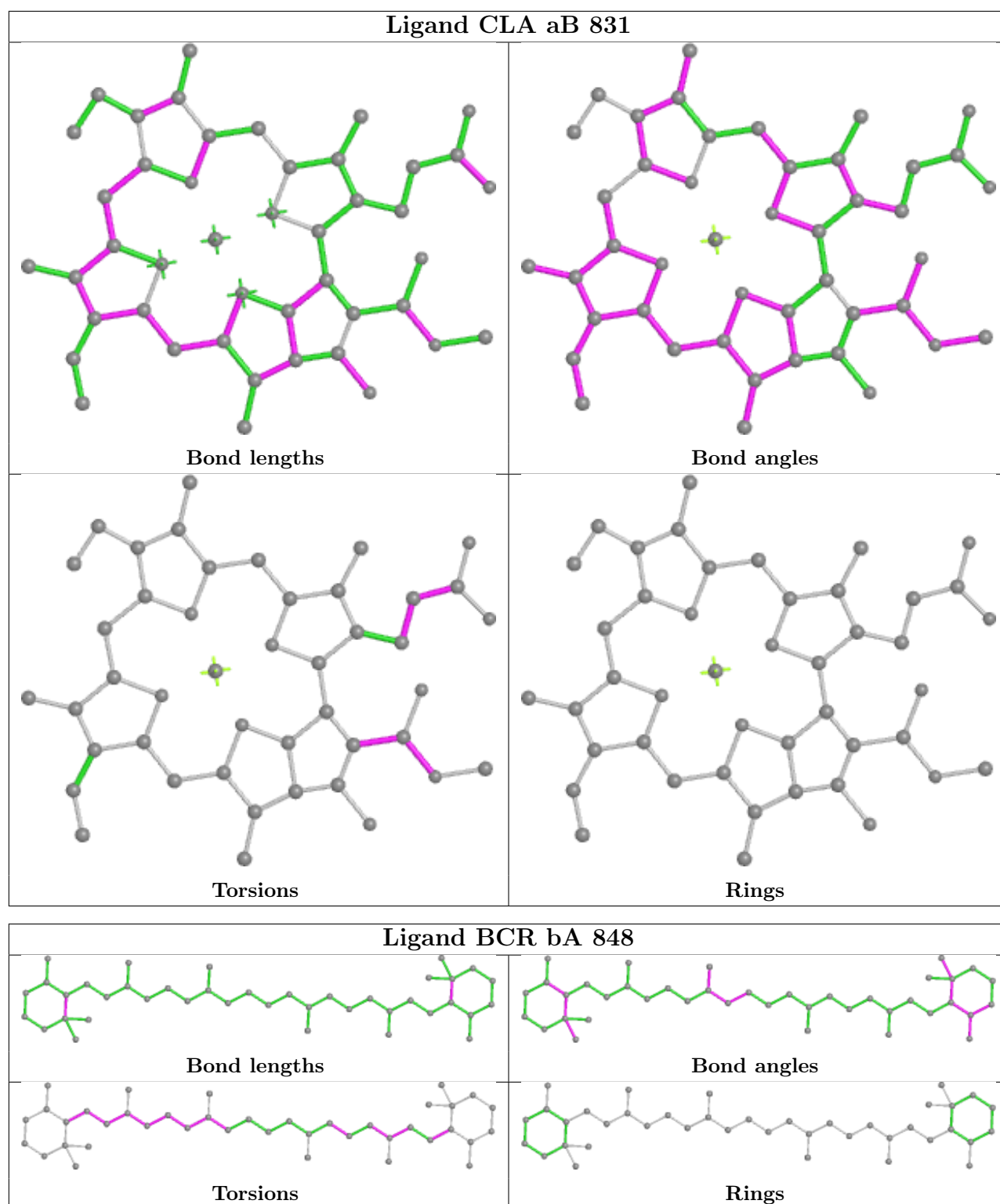


## Ligand CLA cA 811

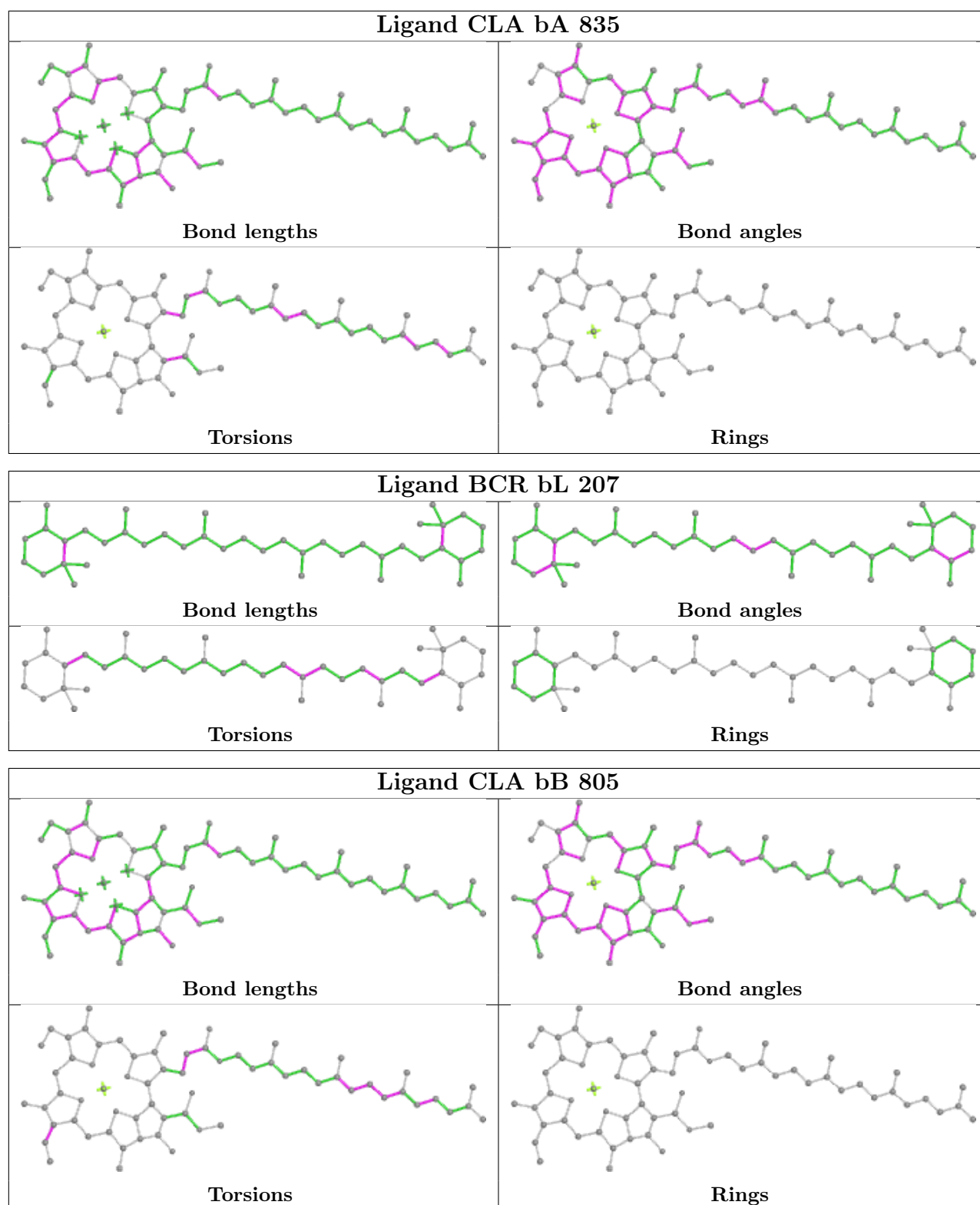


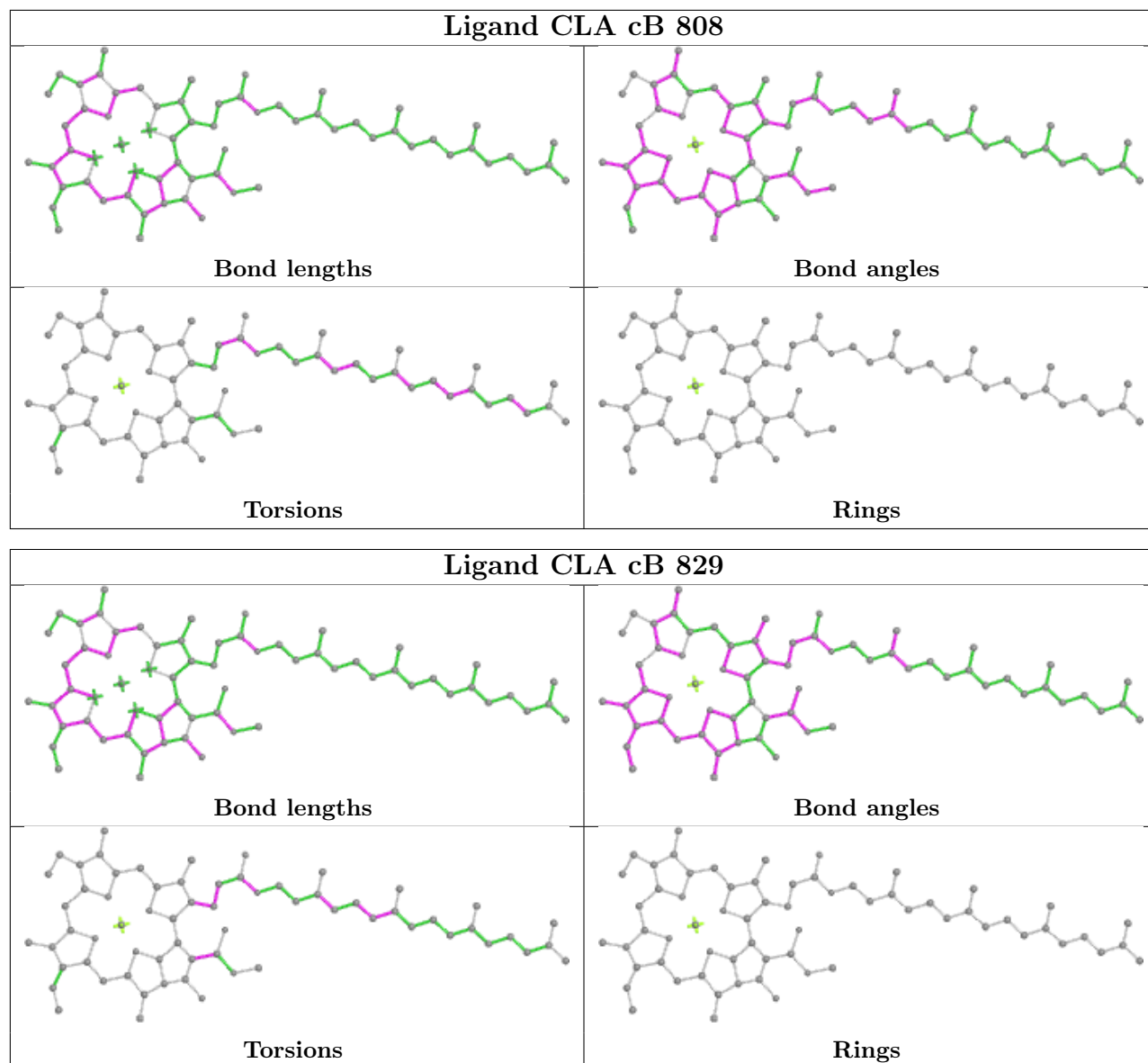


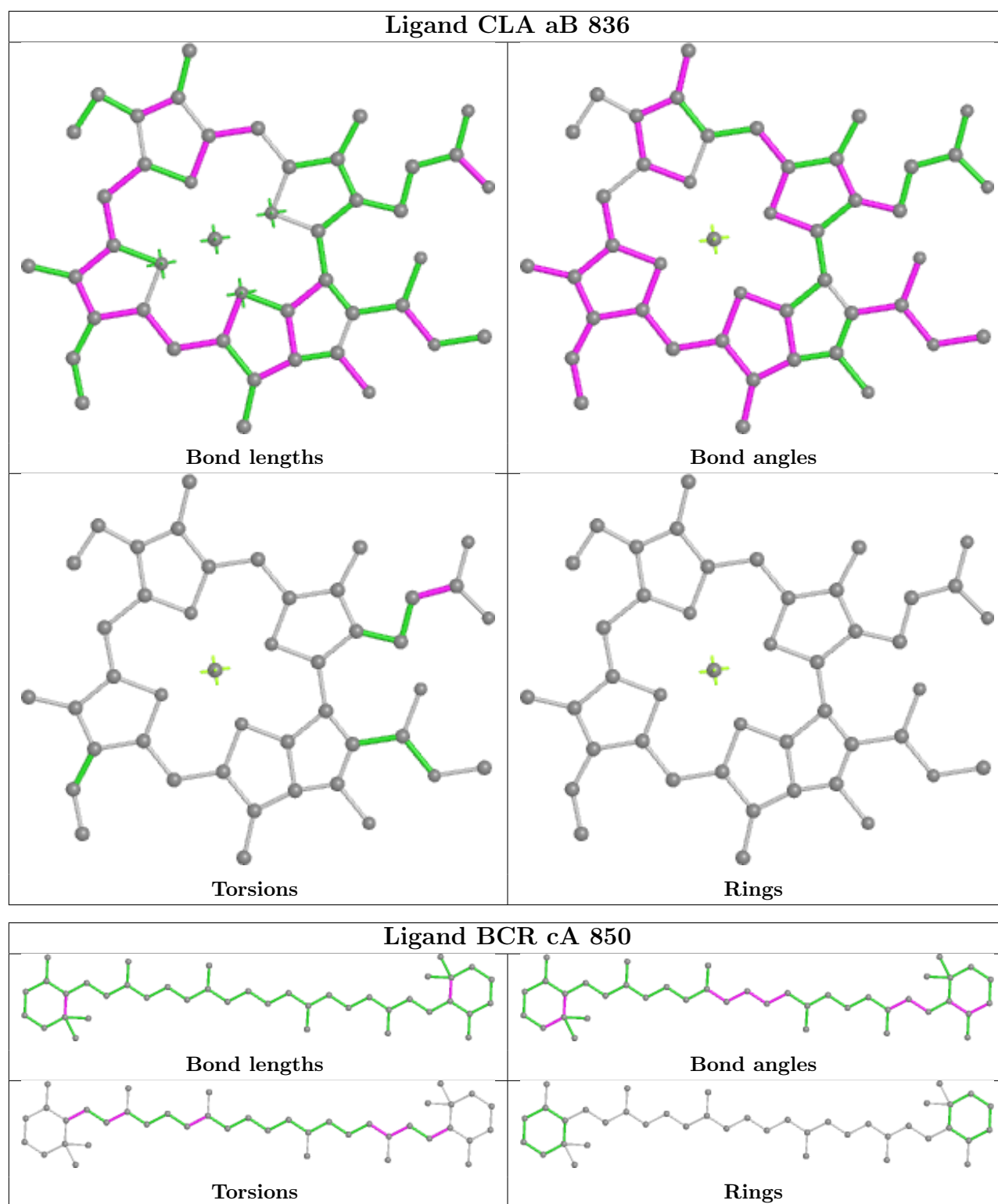


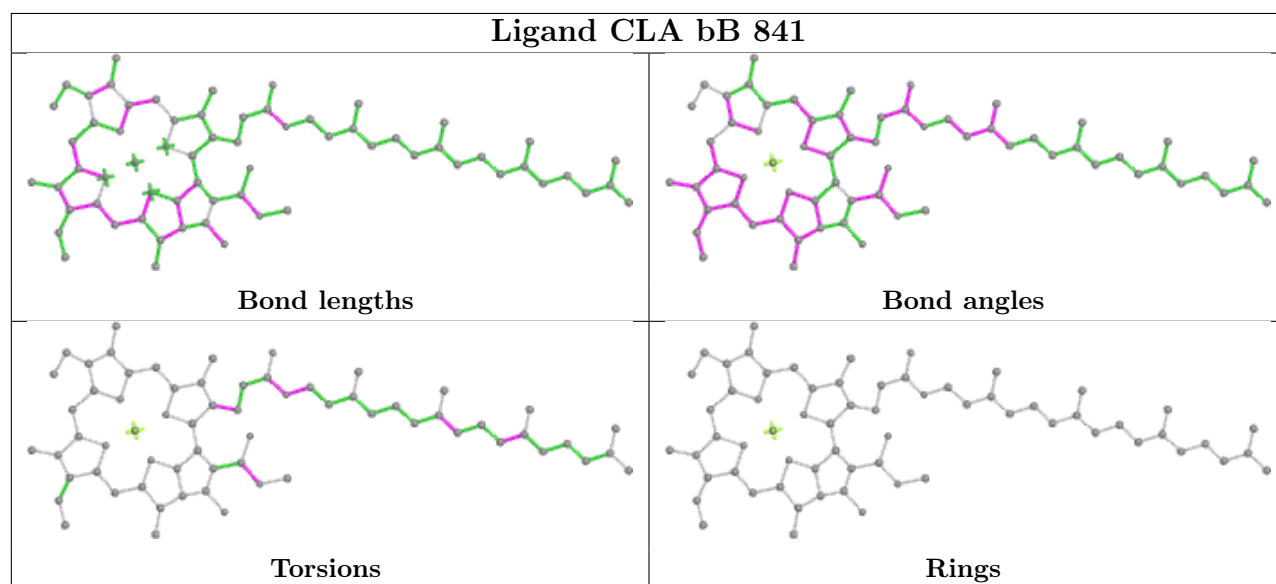
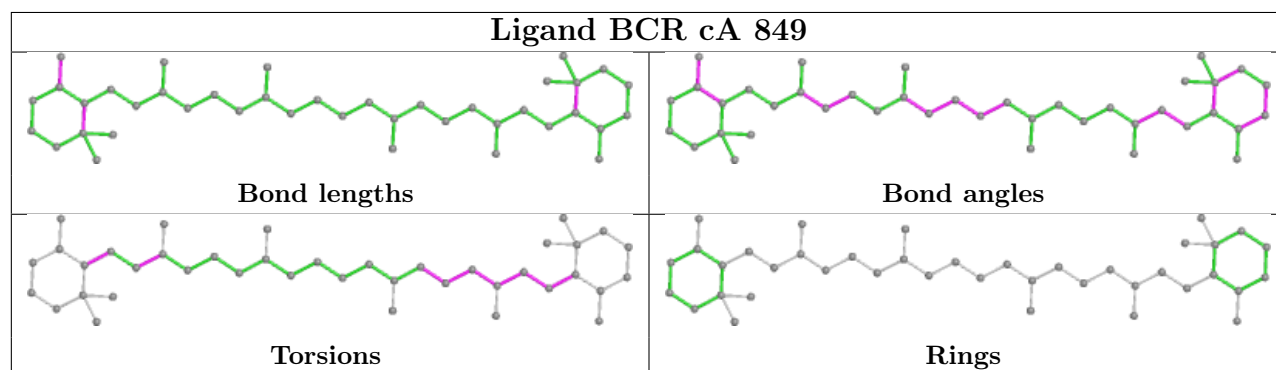
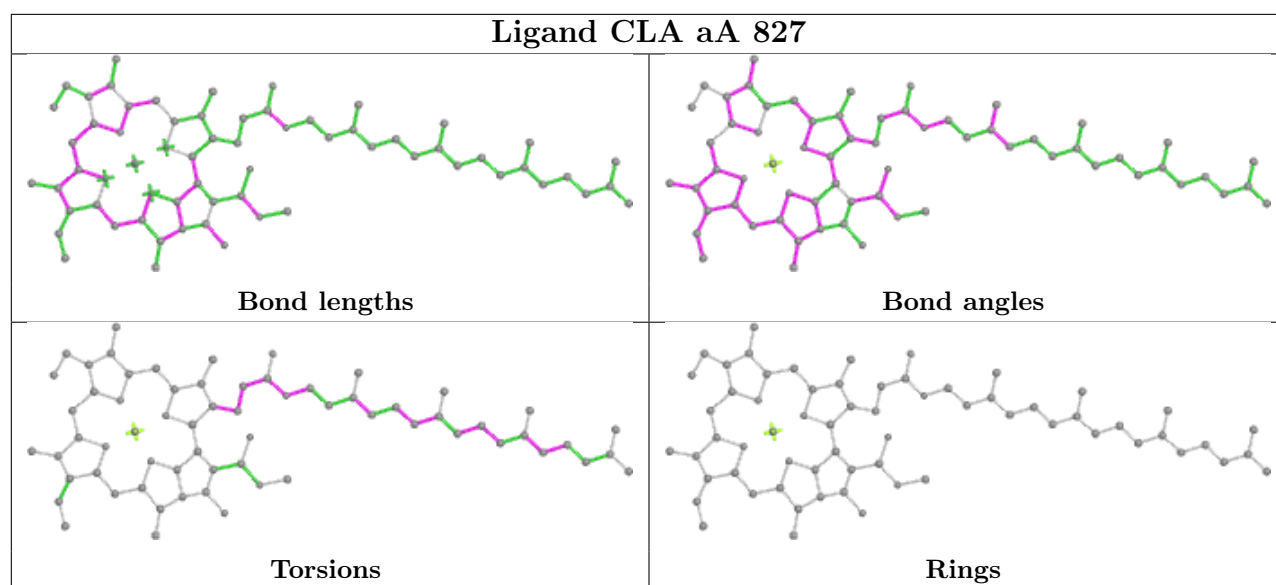


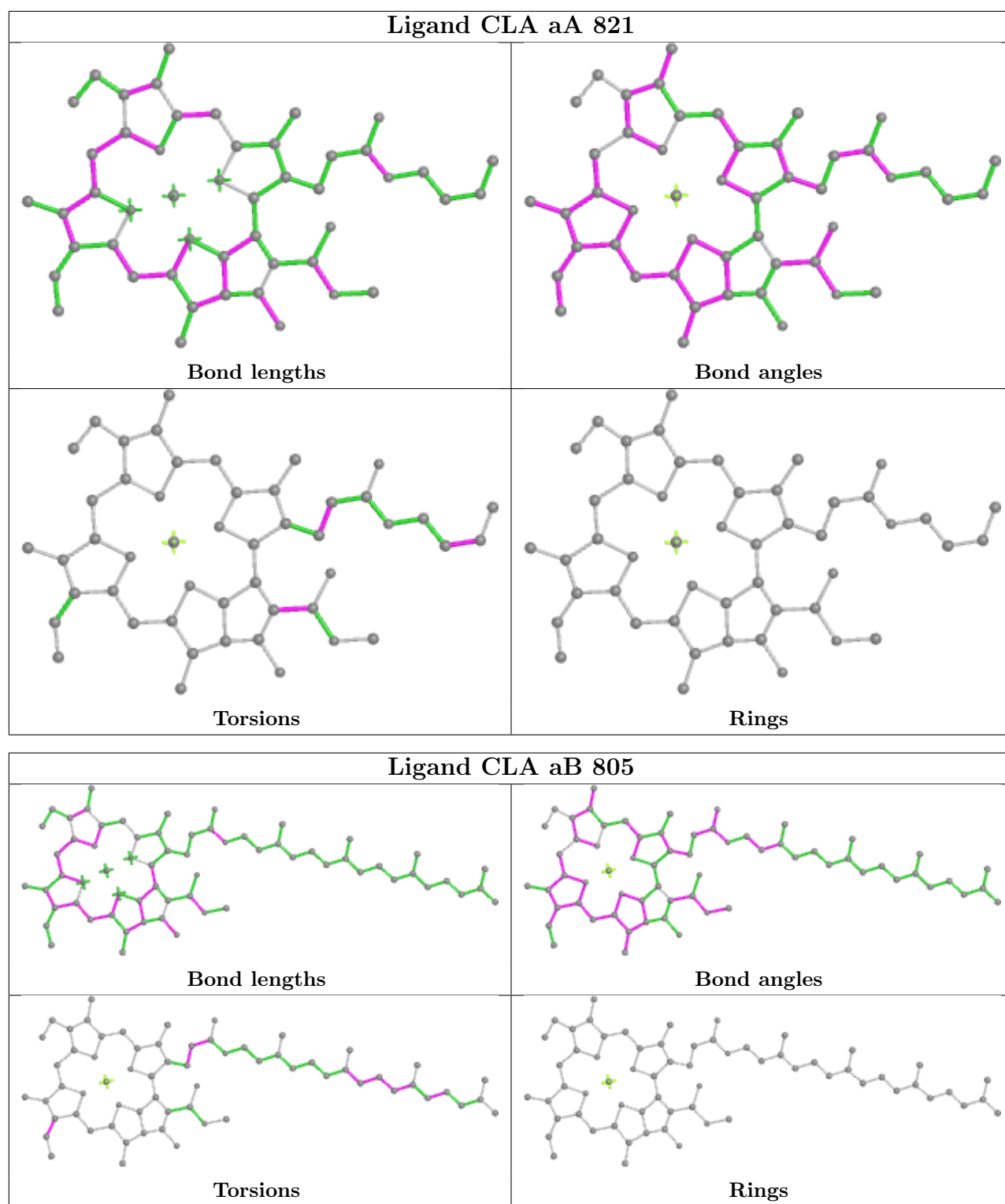


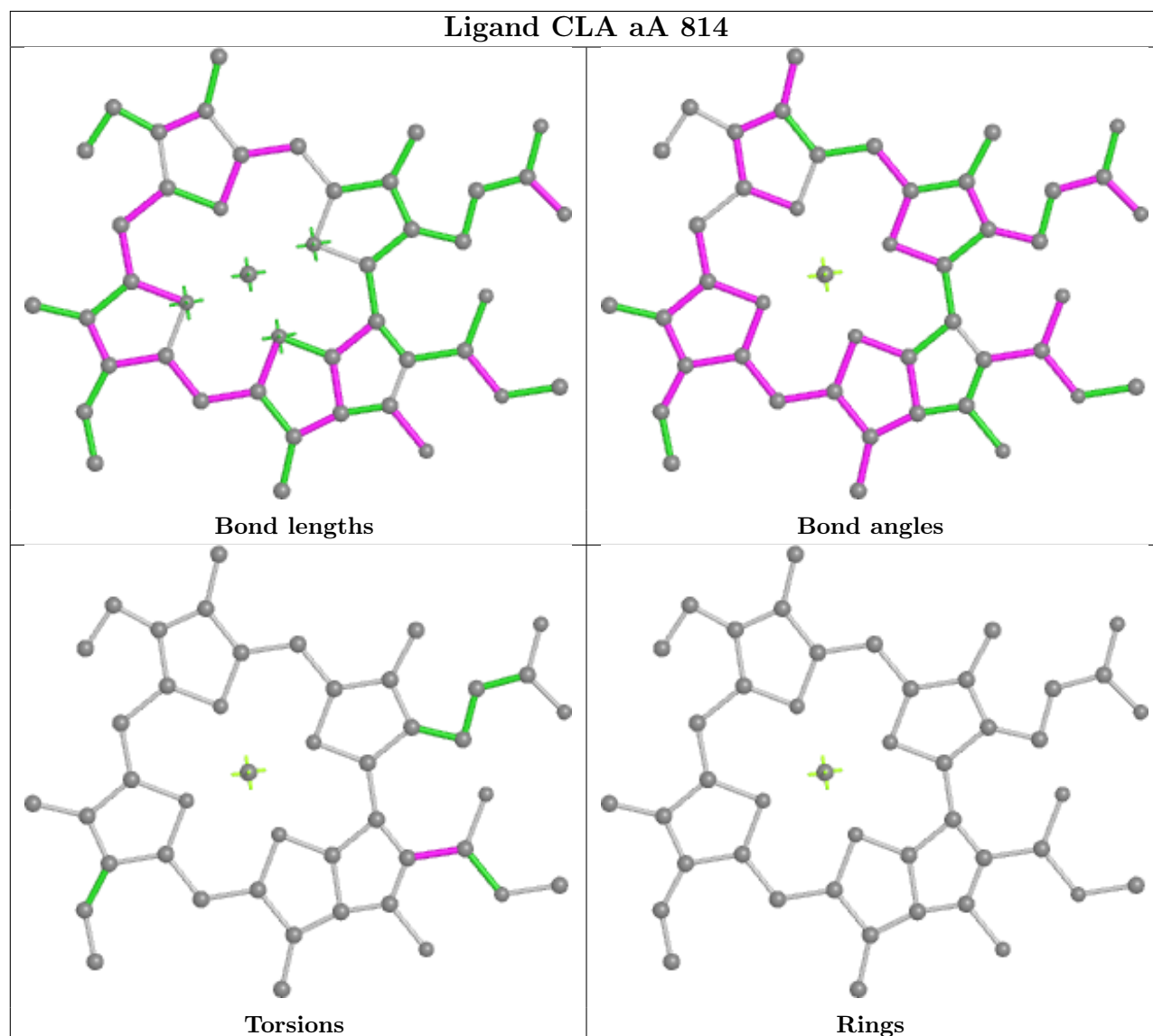
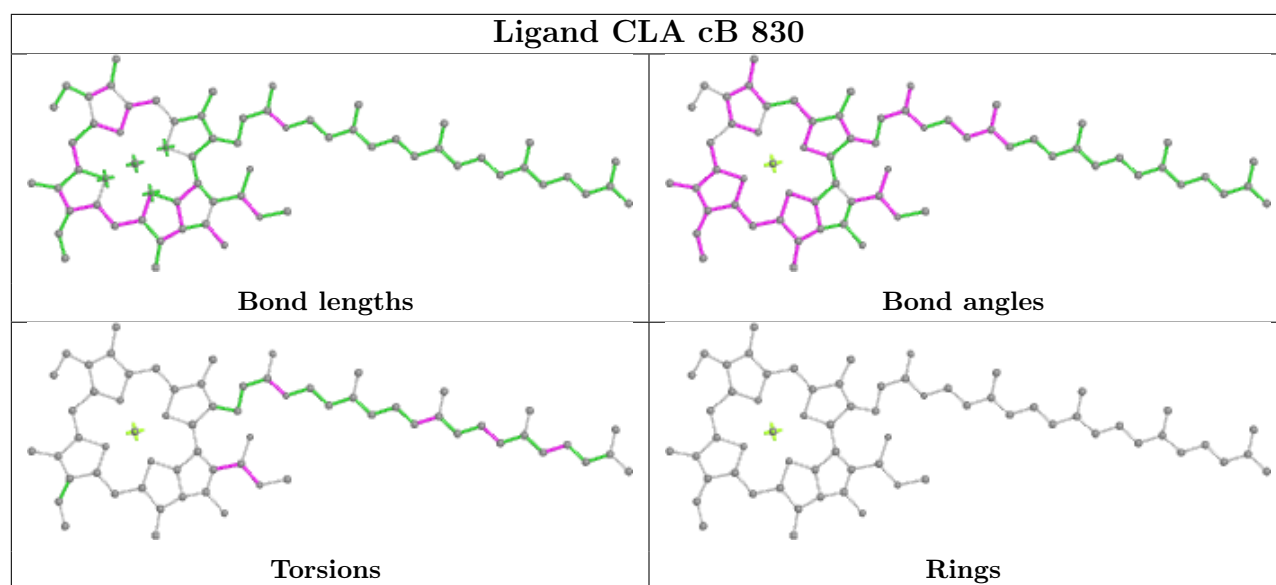


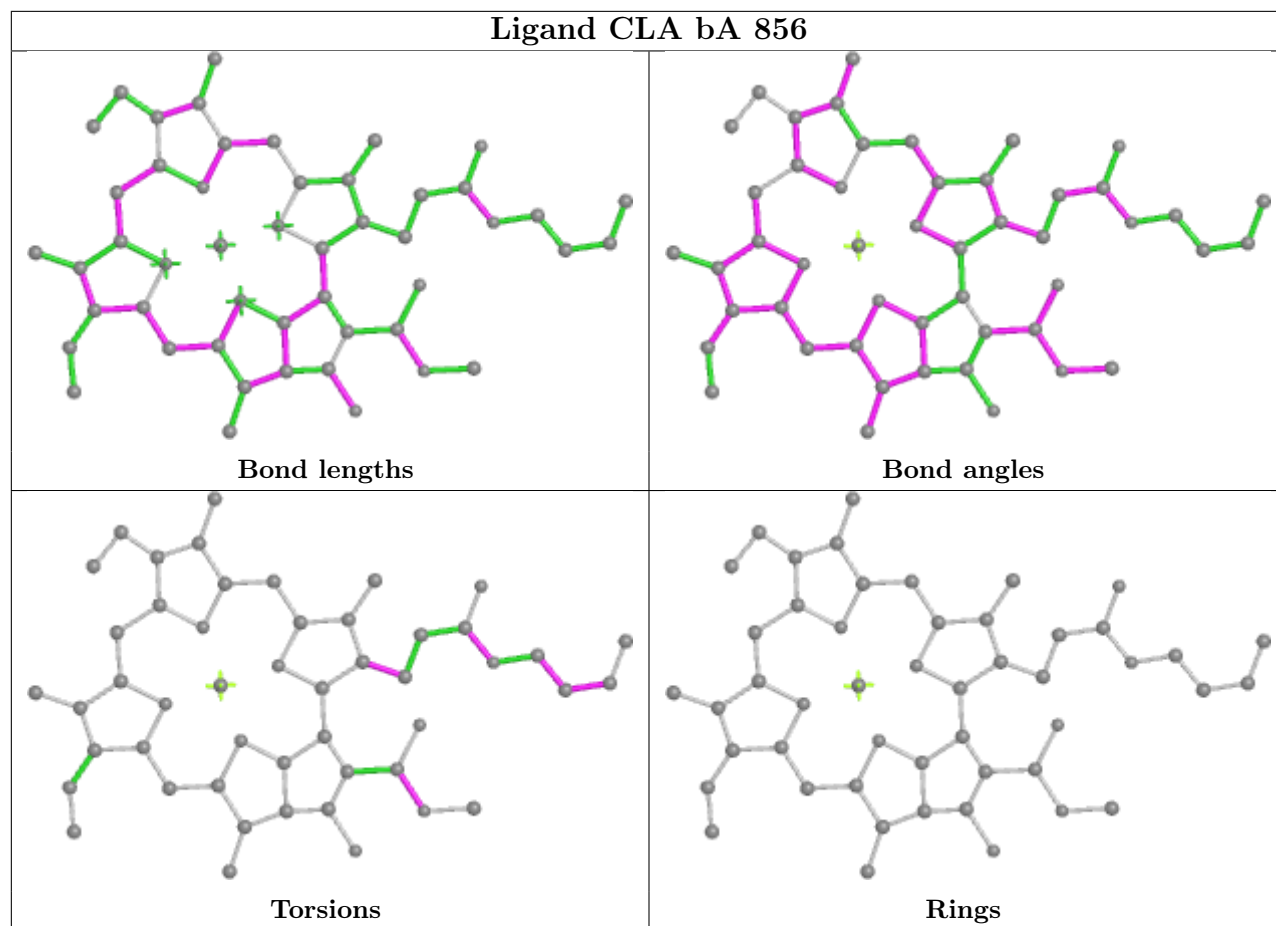




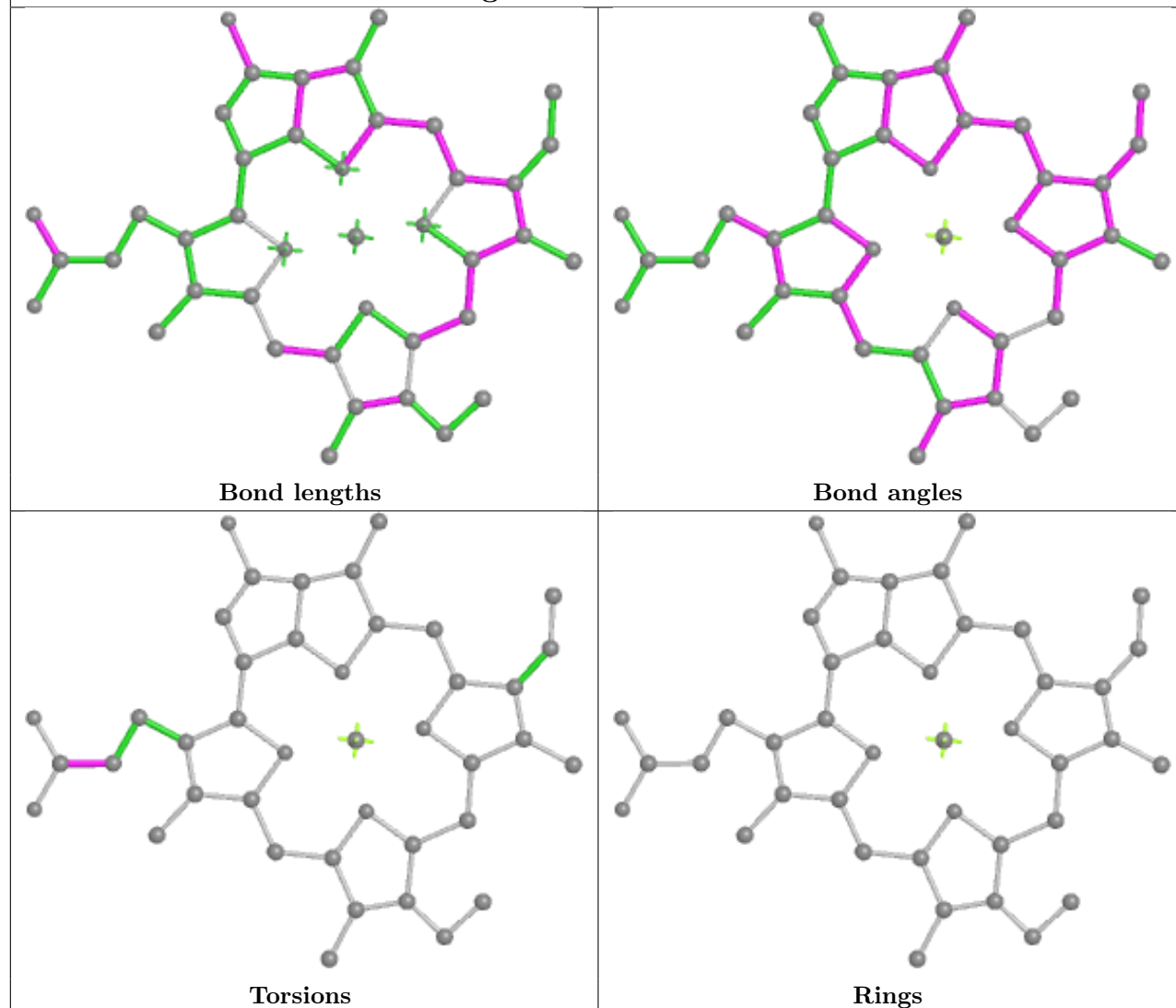




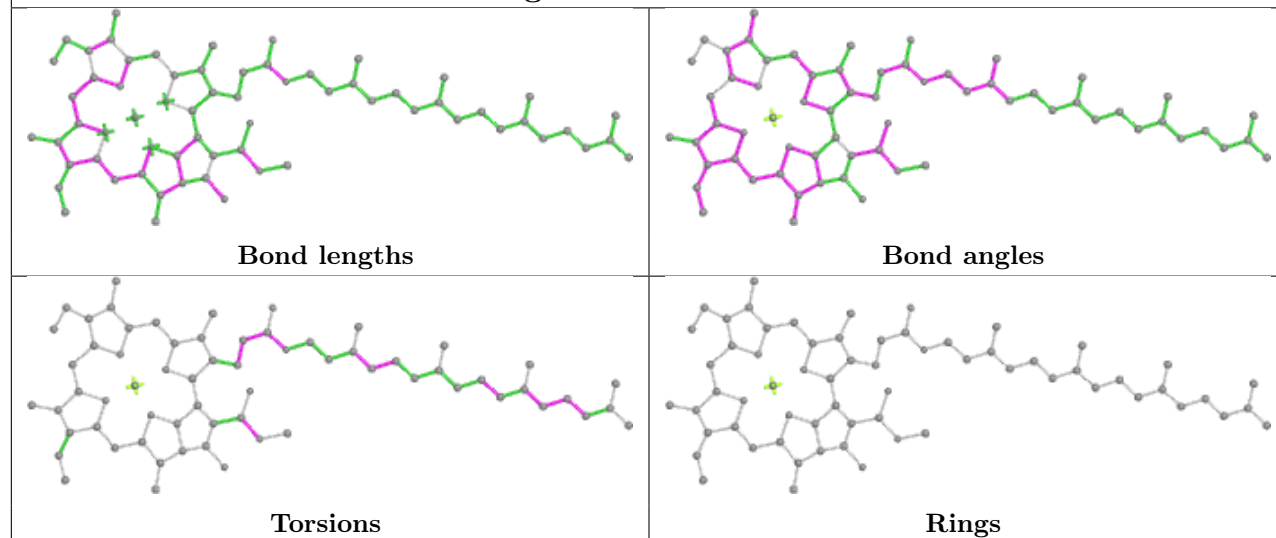




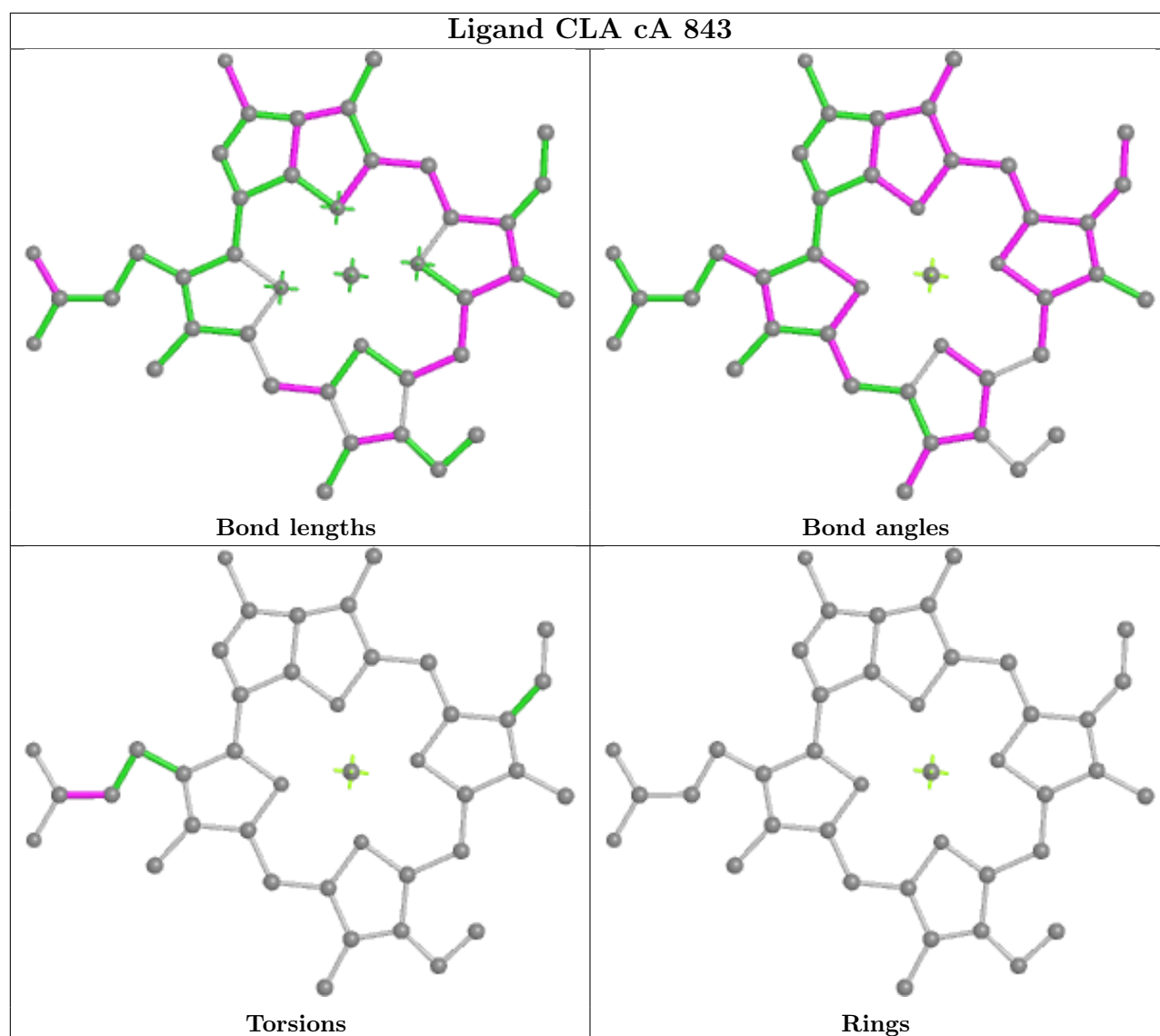
## Ligand CLA aA 843



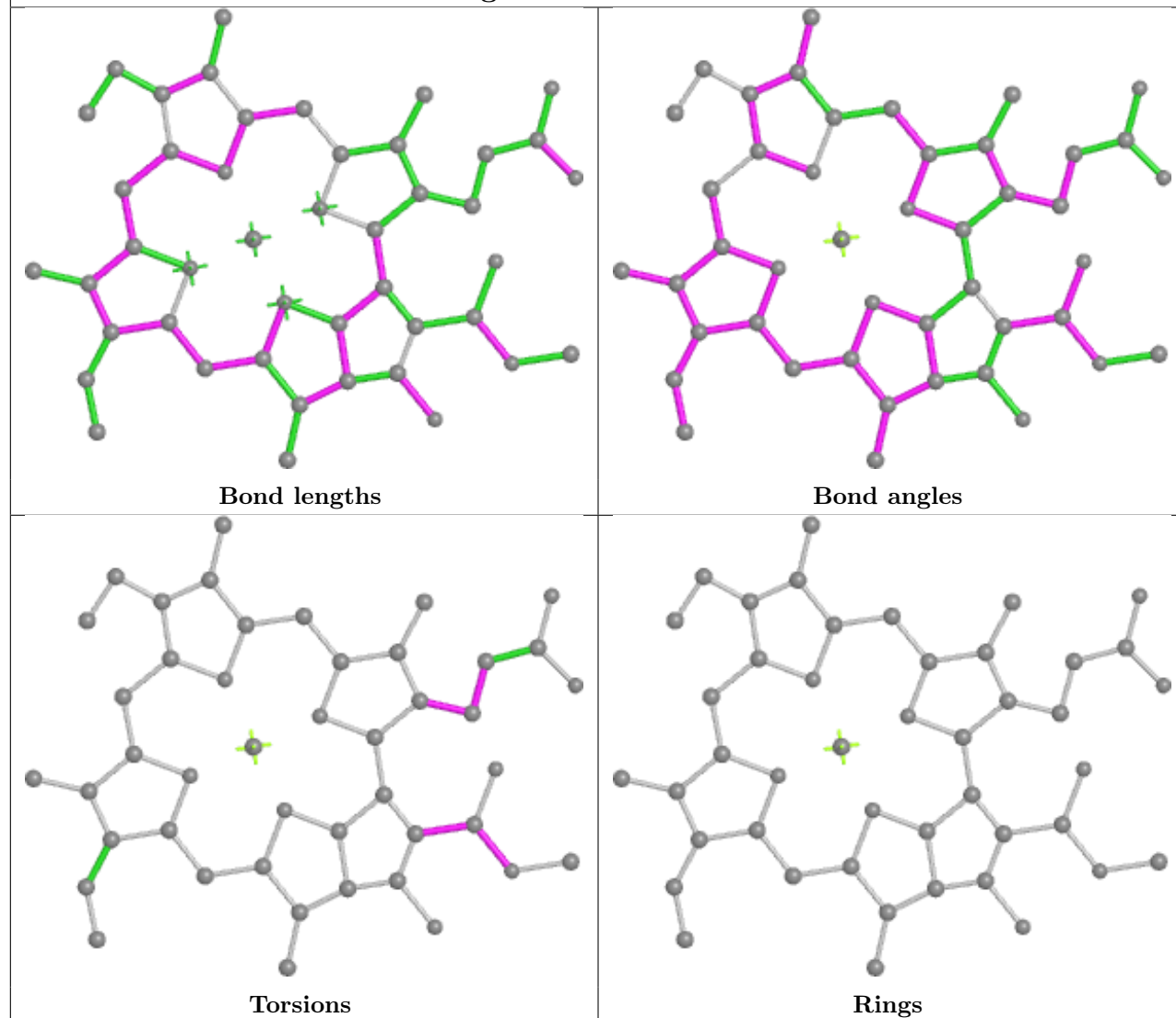
## Ligand CLA cB 802



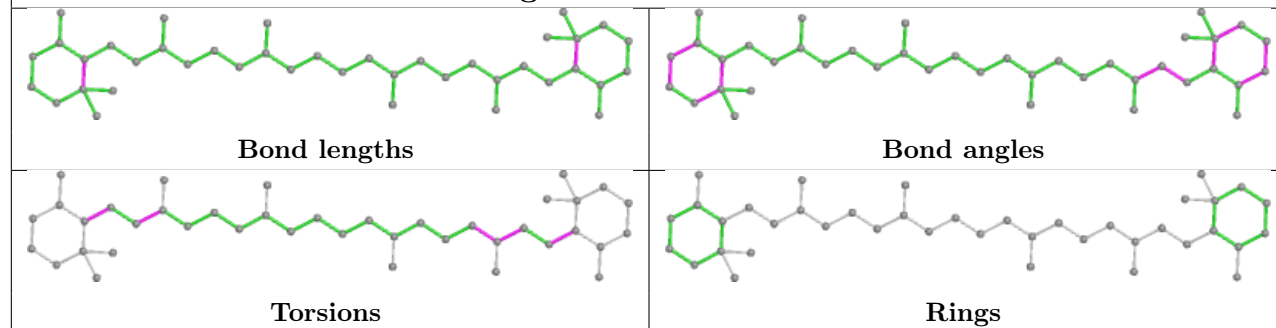


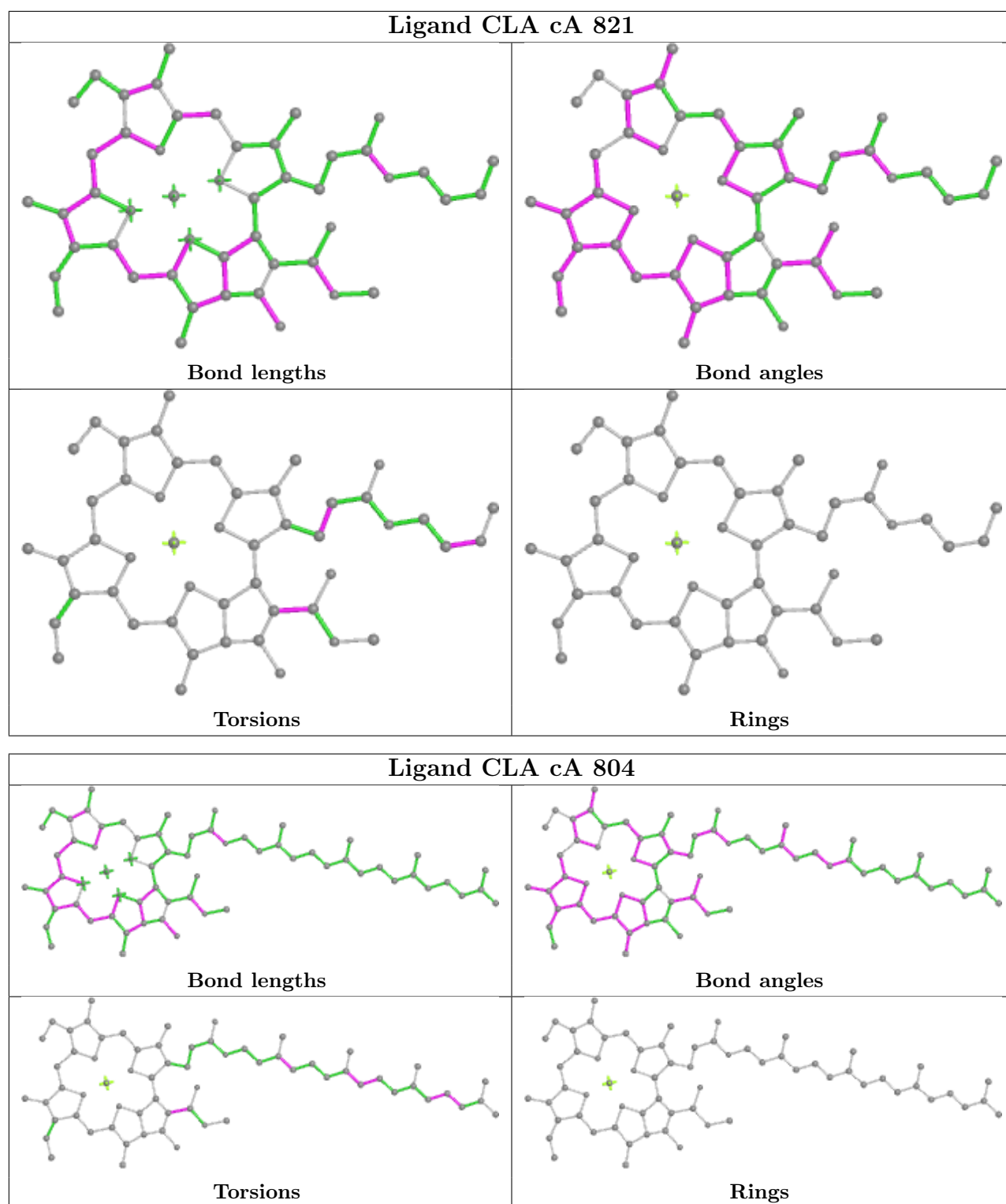


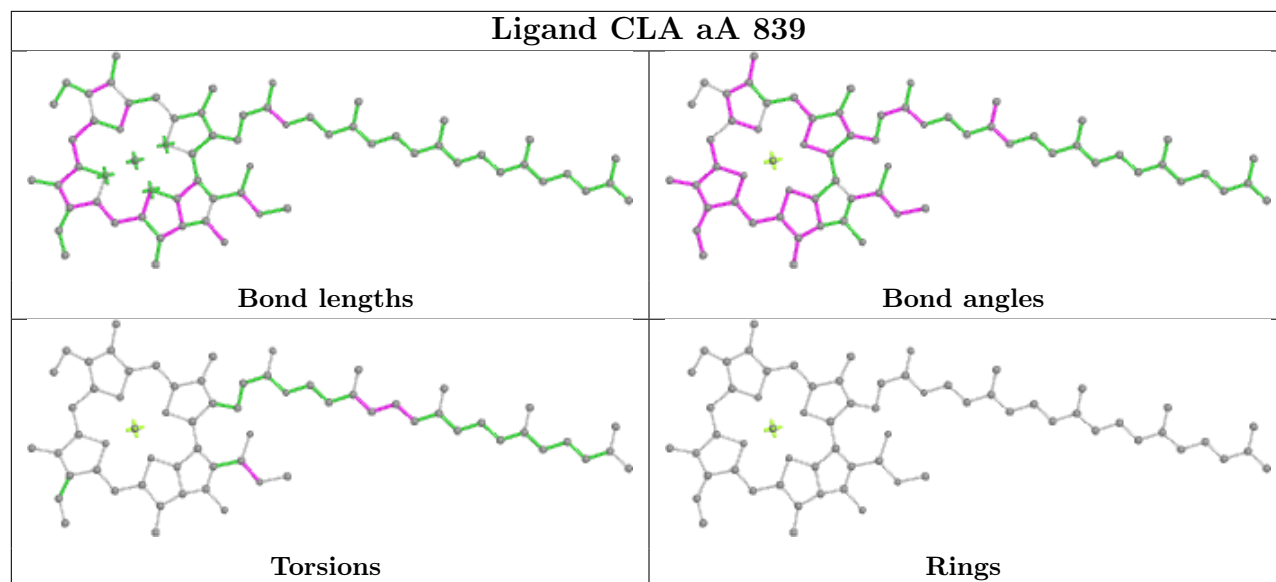
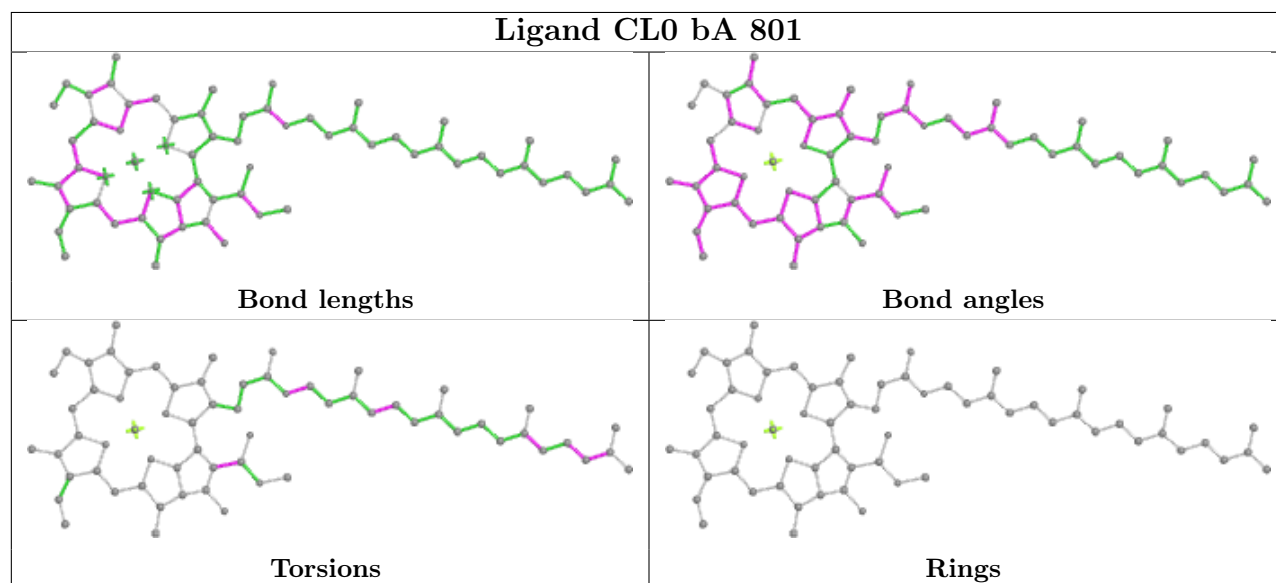
## Ligand CLA bA 807

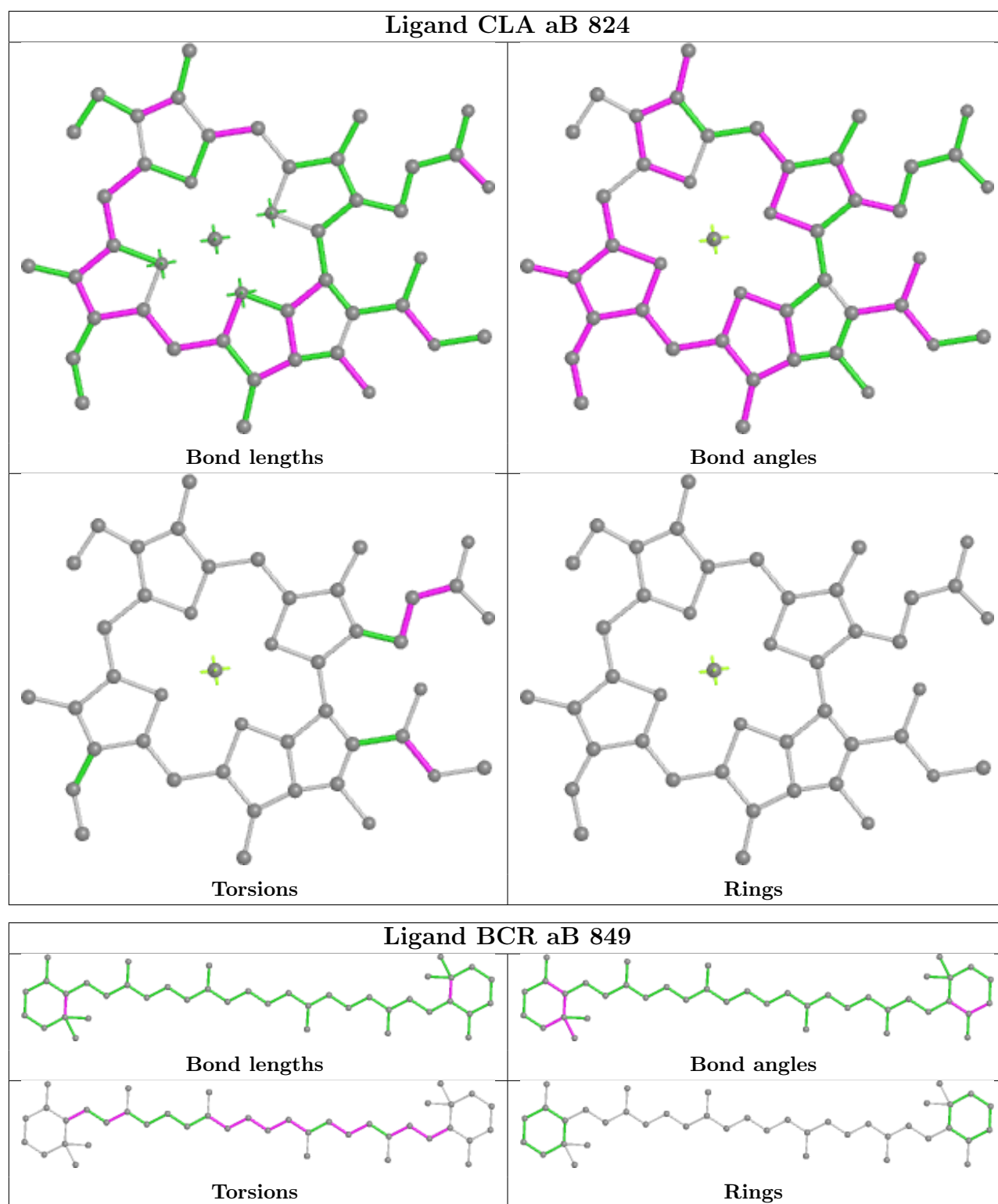


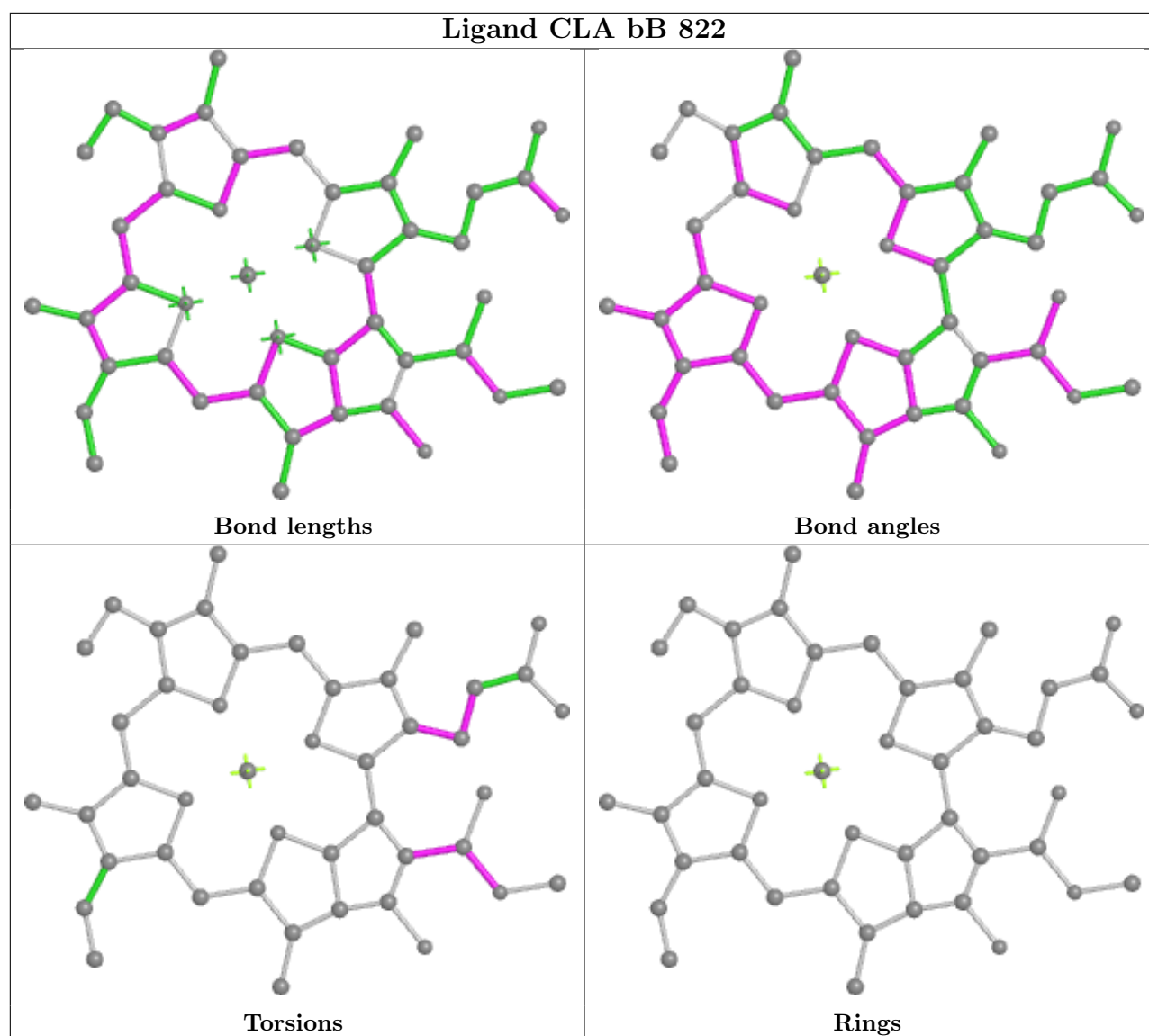
## Ligand BCR bA 847

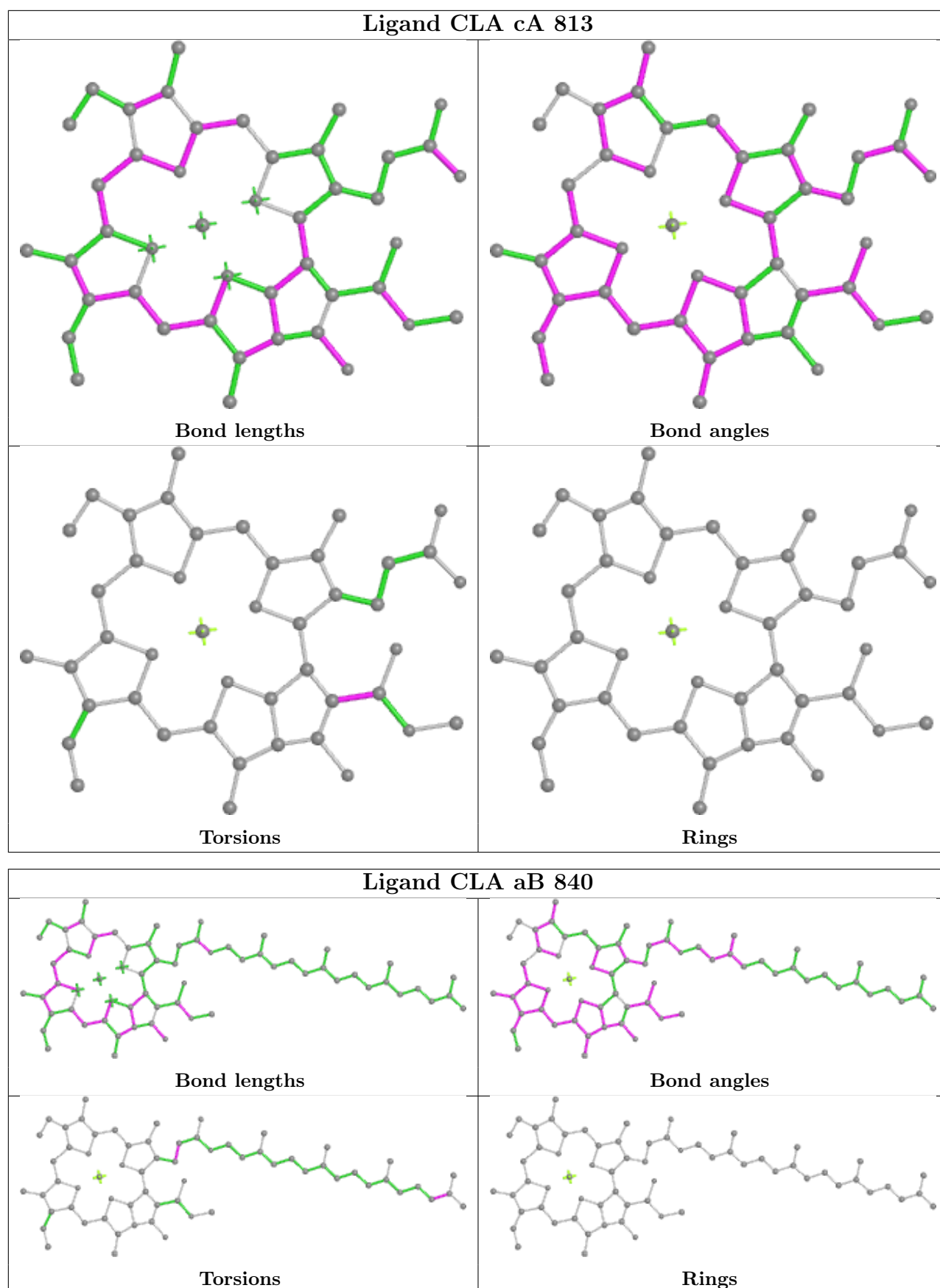


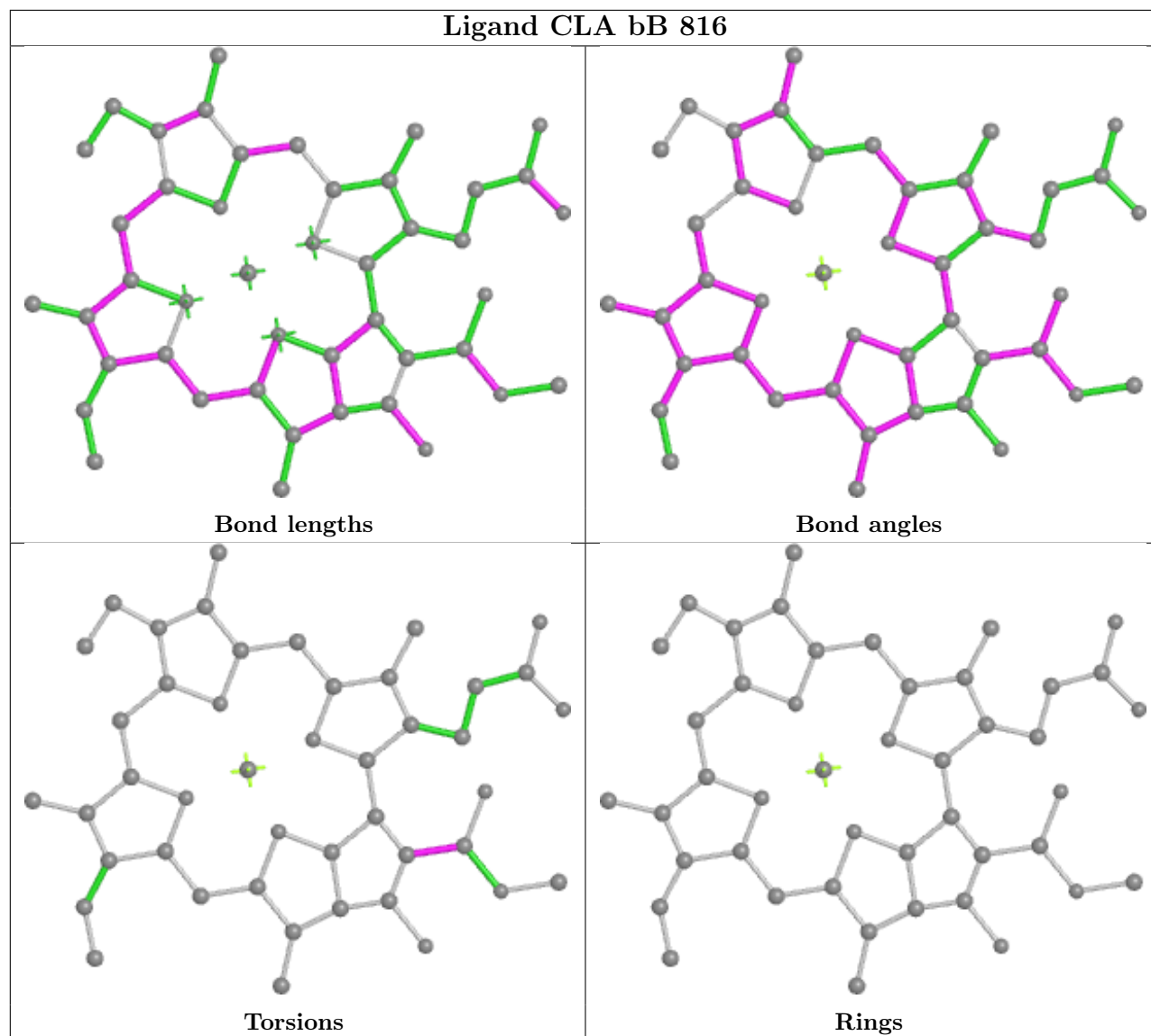
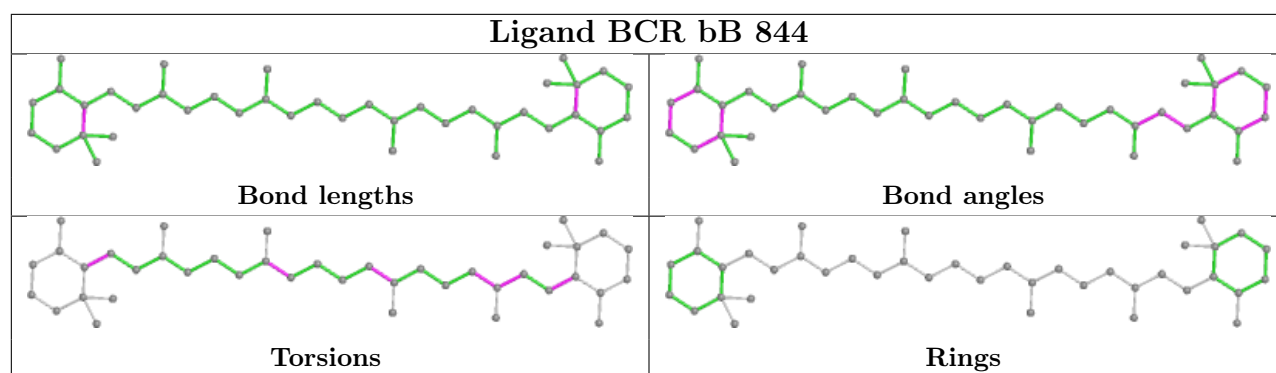


**Ligand CLA aA 839****Ligand CL0 bA 801**

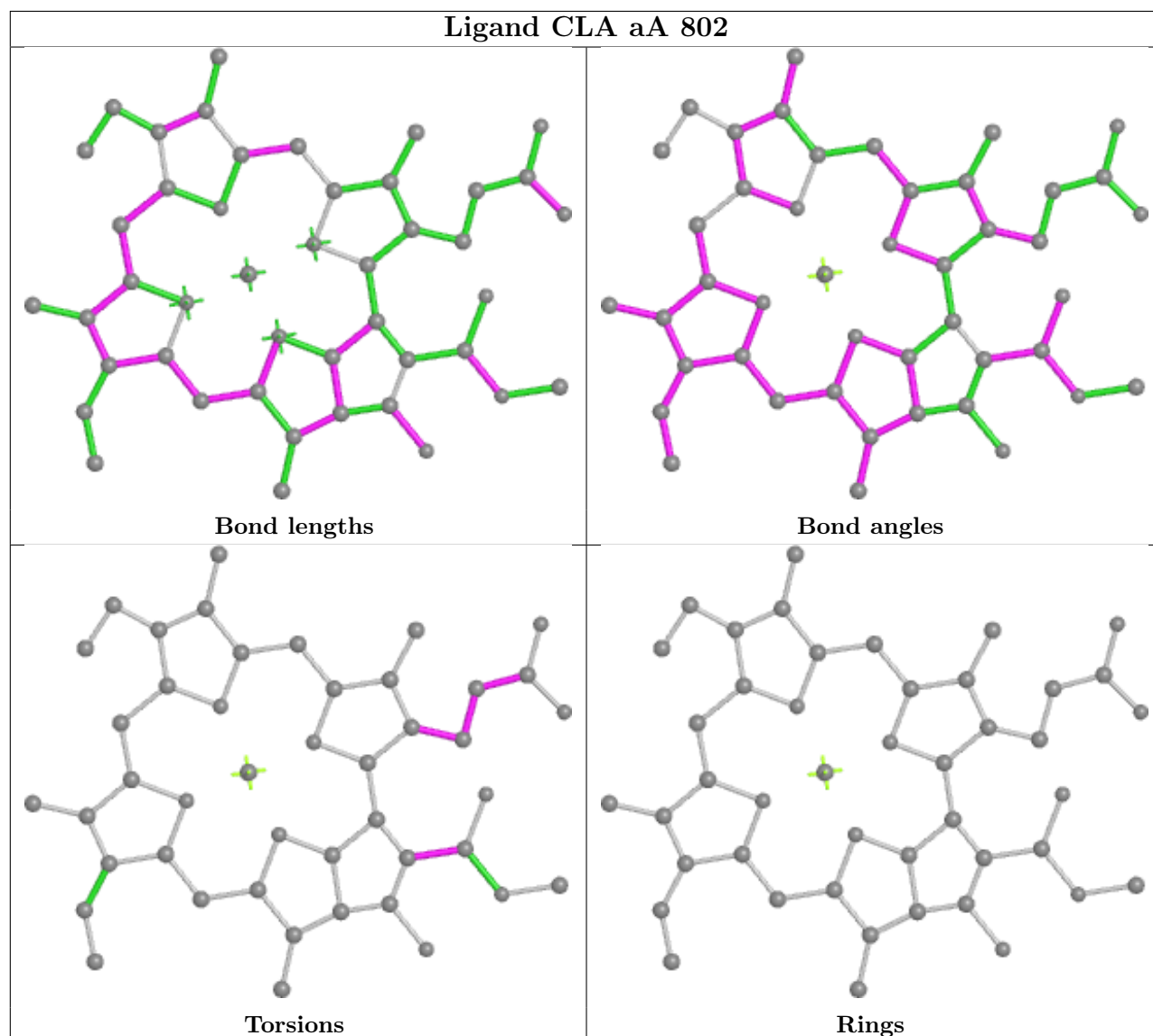
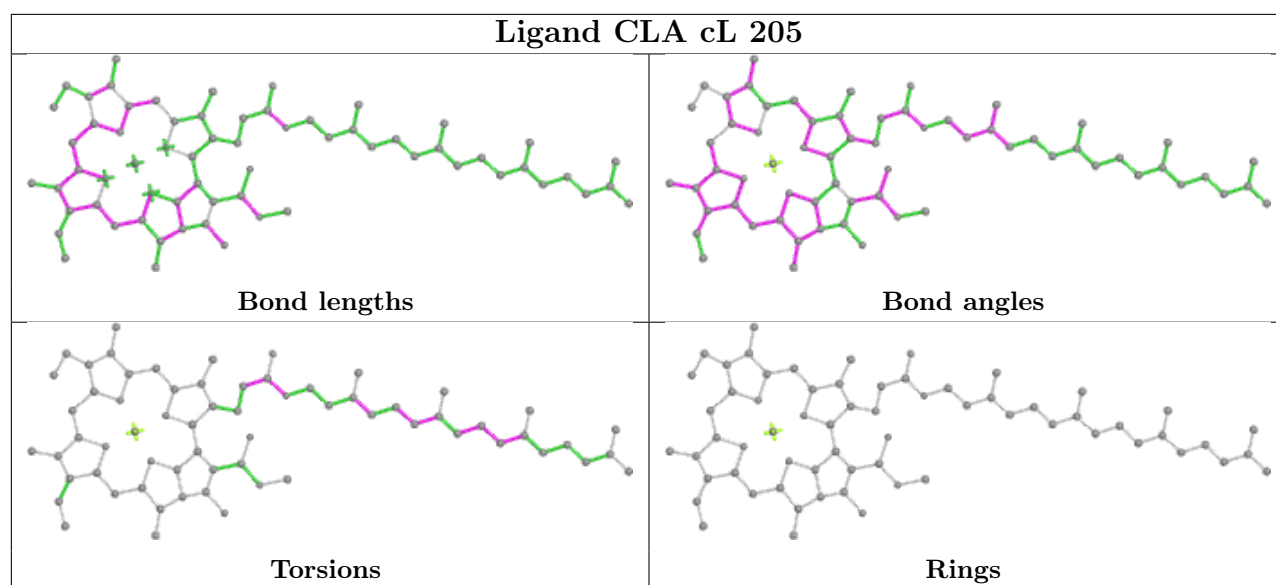


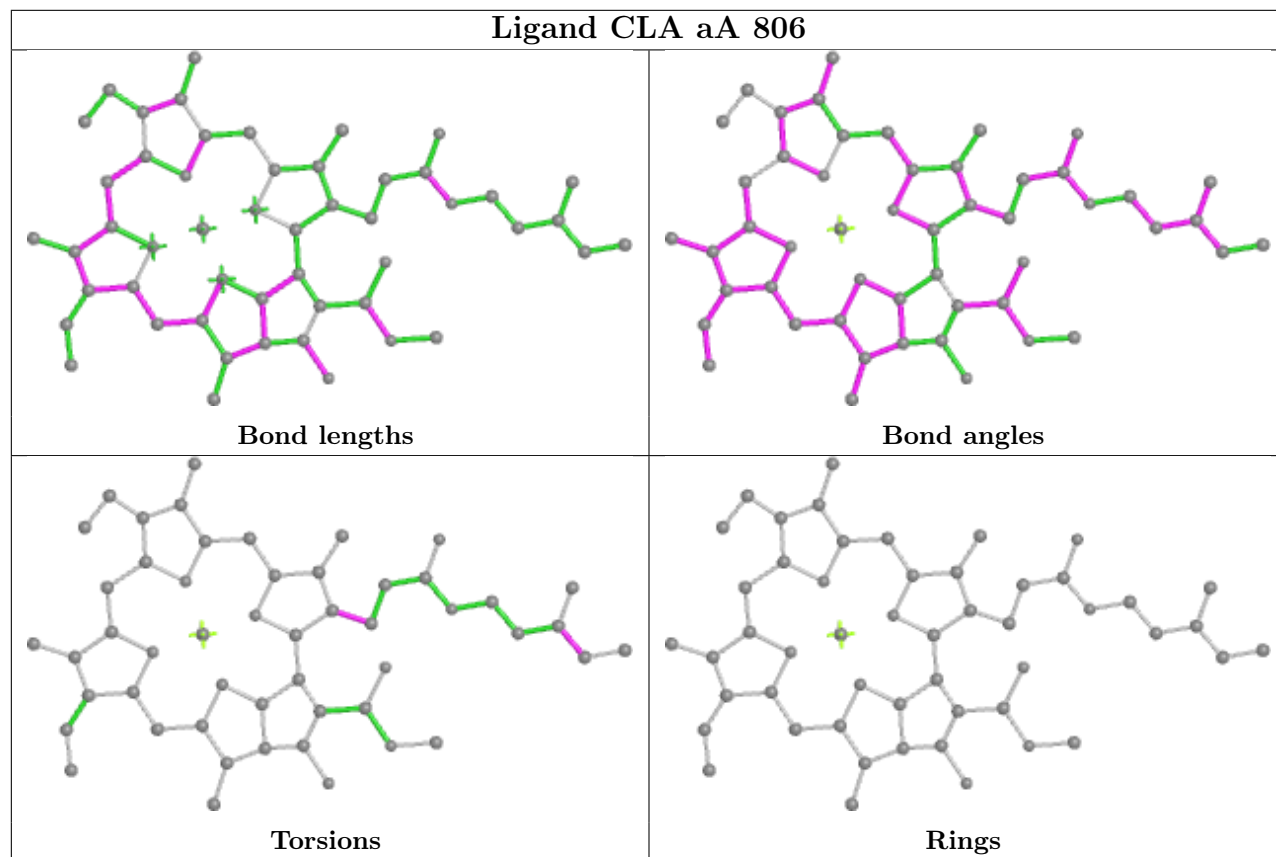
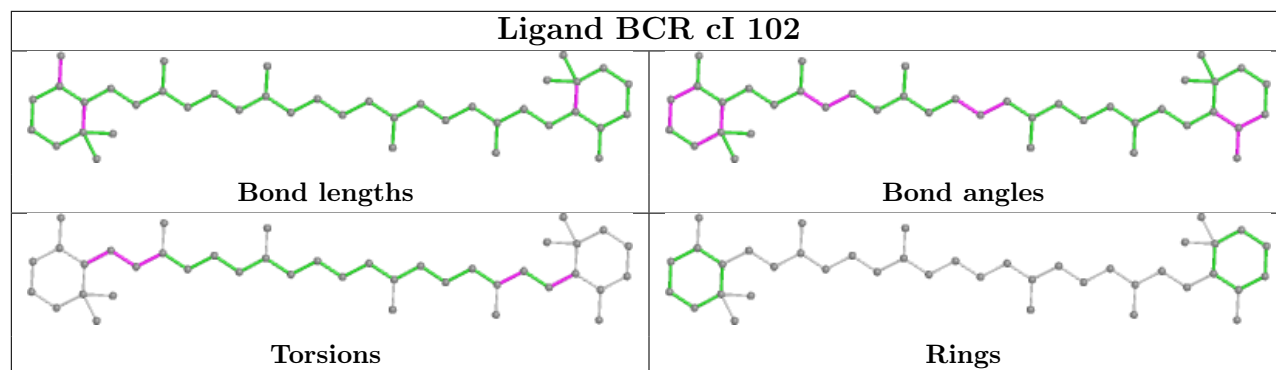
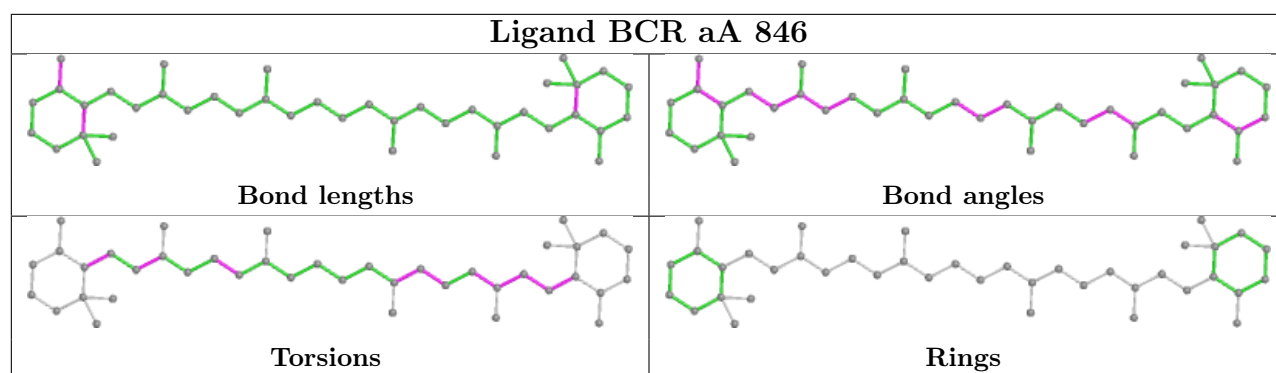




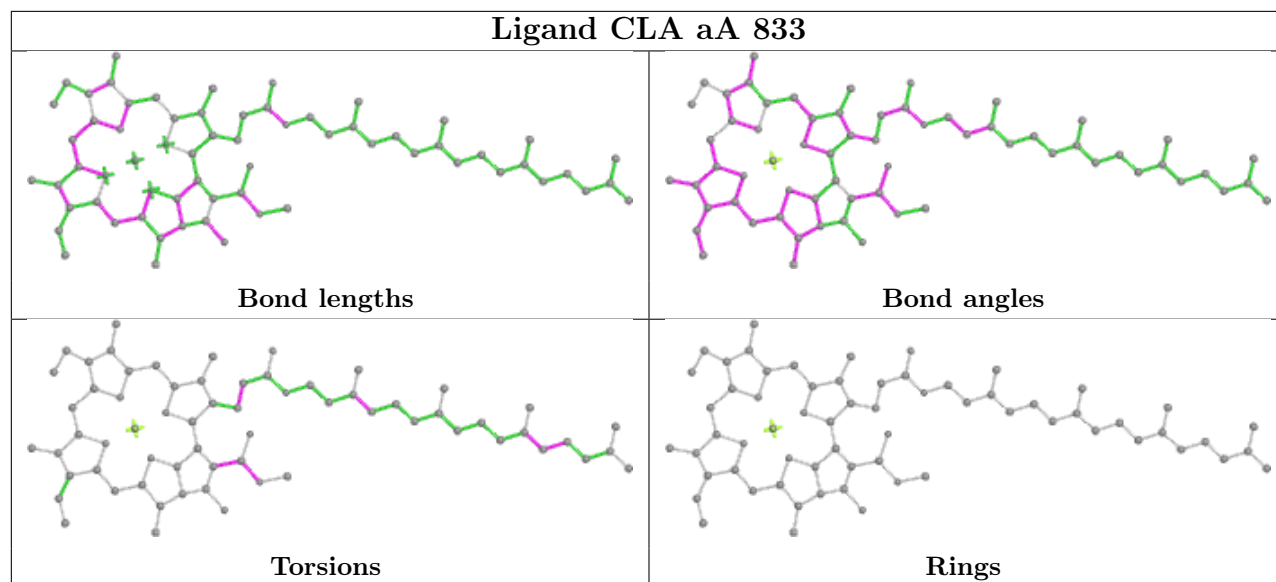




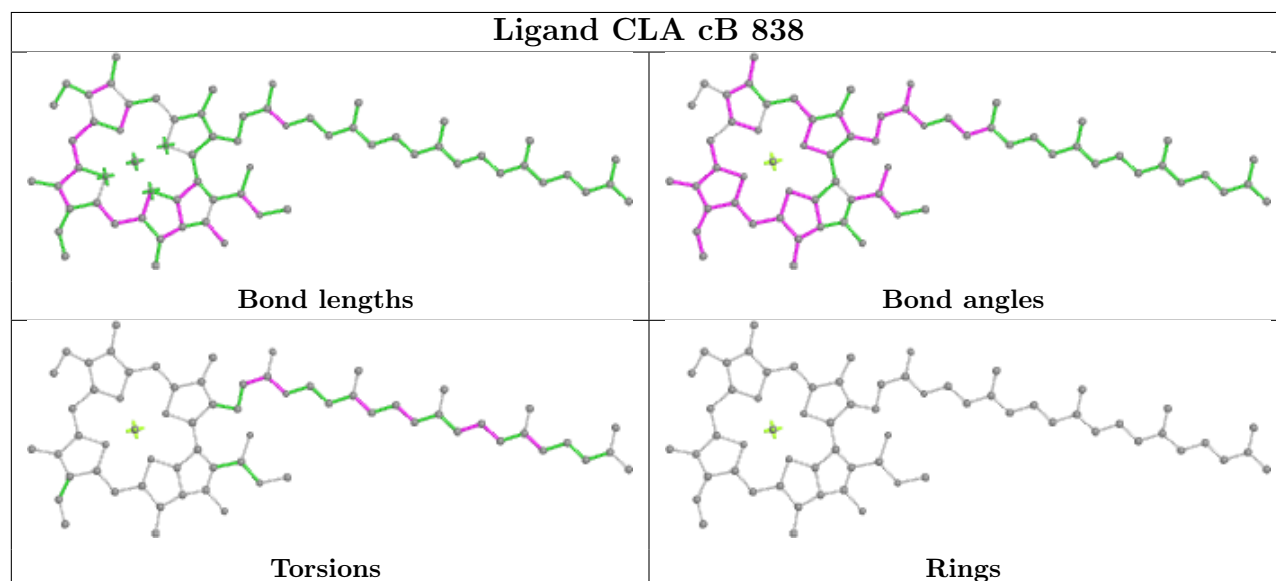




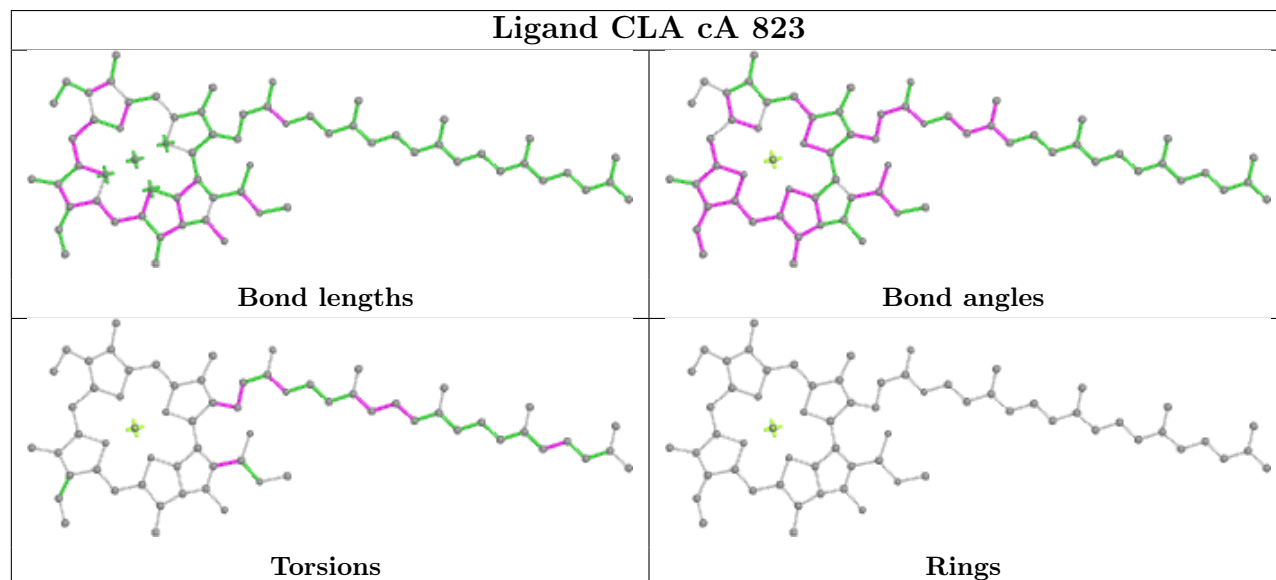
## Ligand CLA aA 833

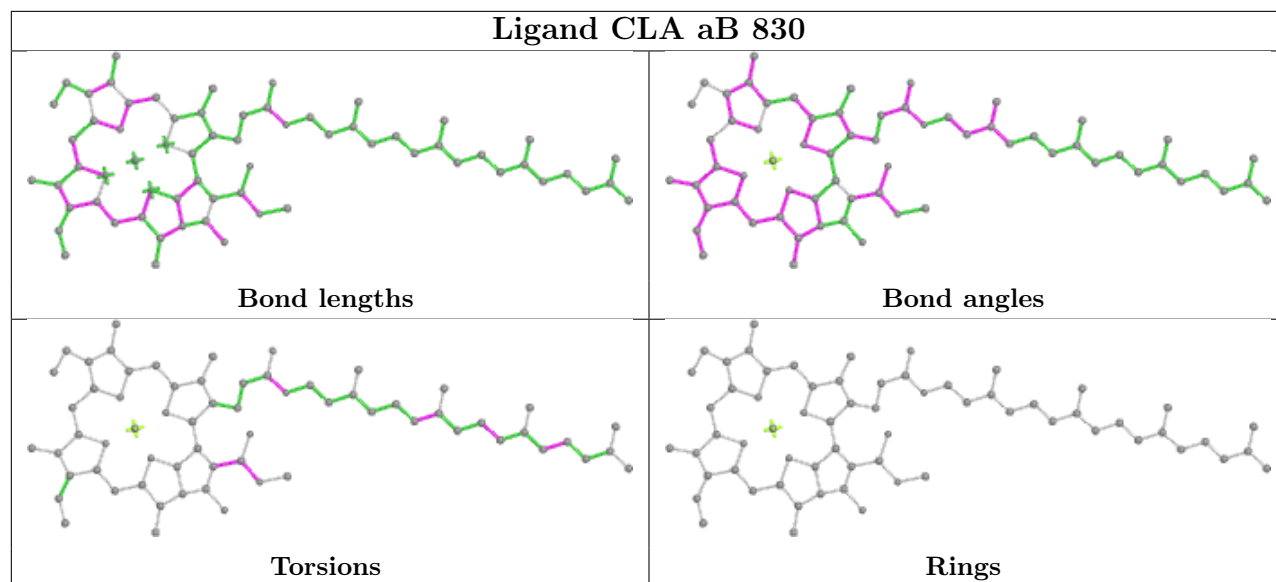
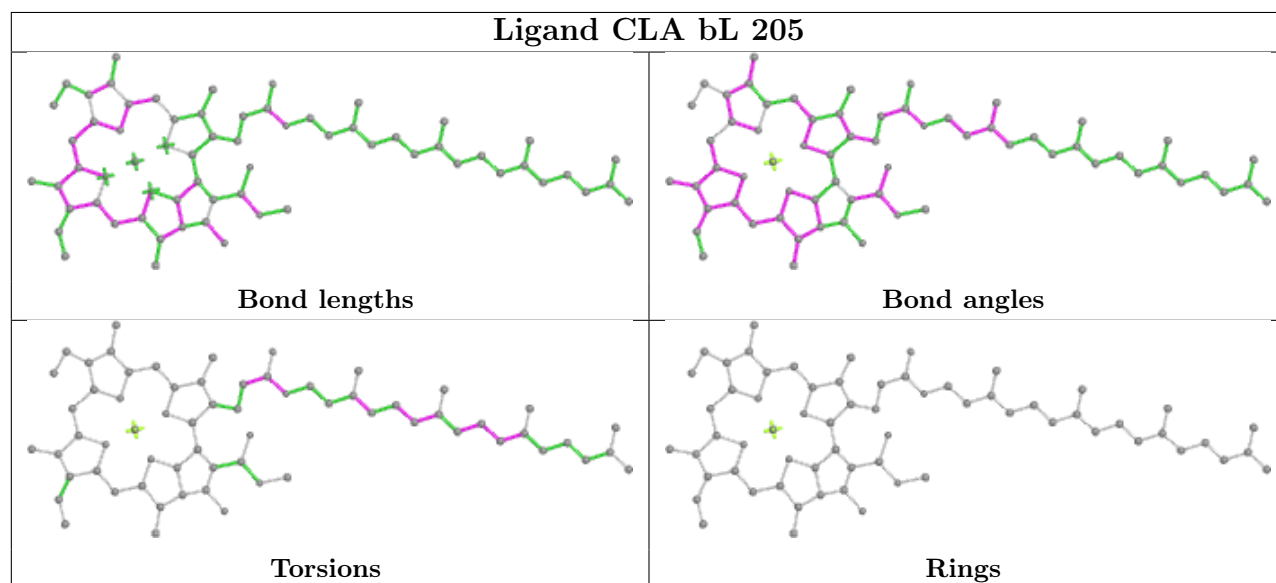


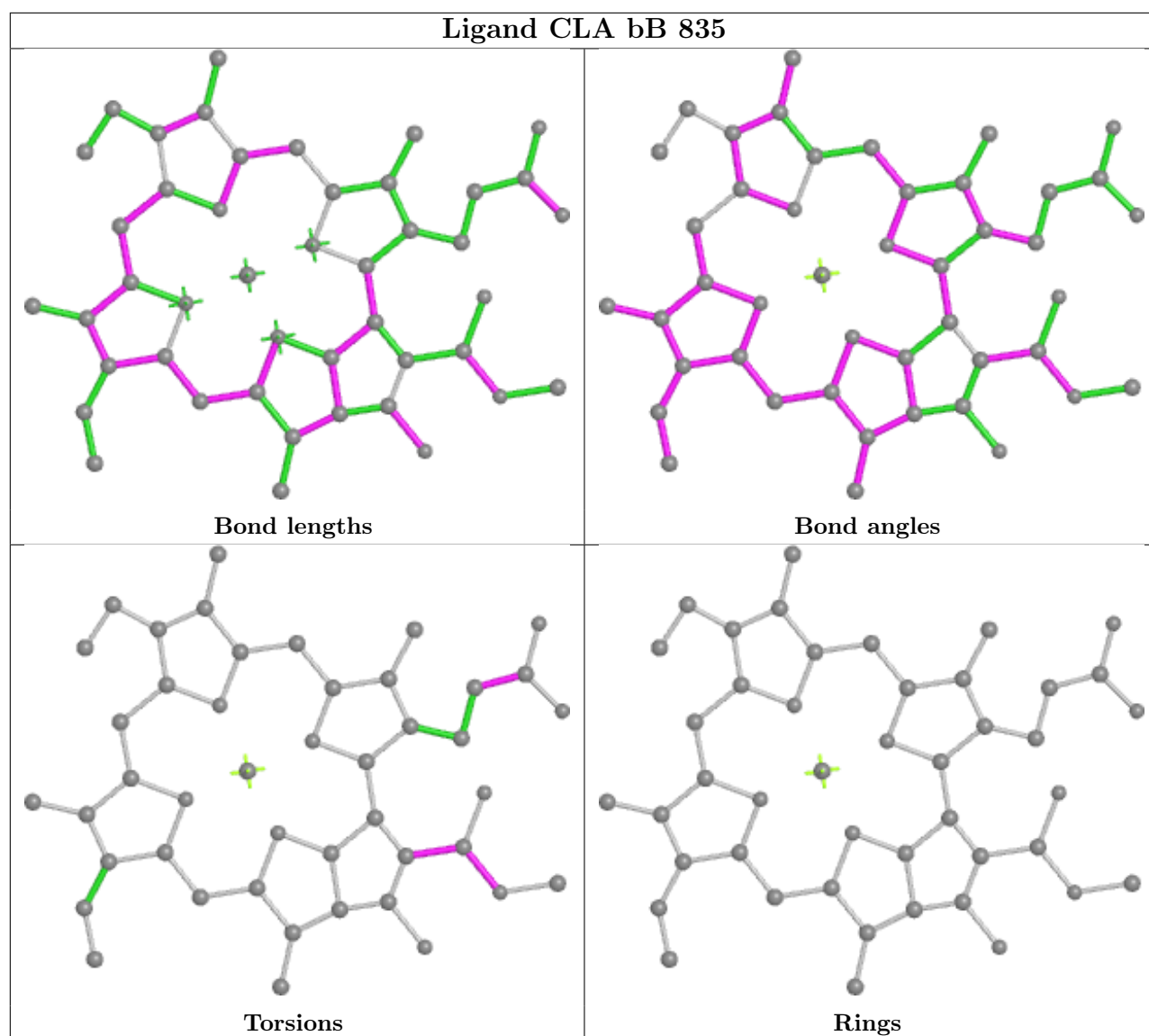
## Ligand CLA cB 838

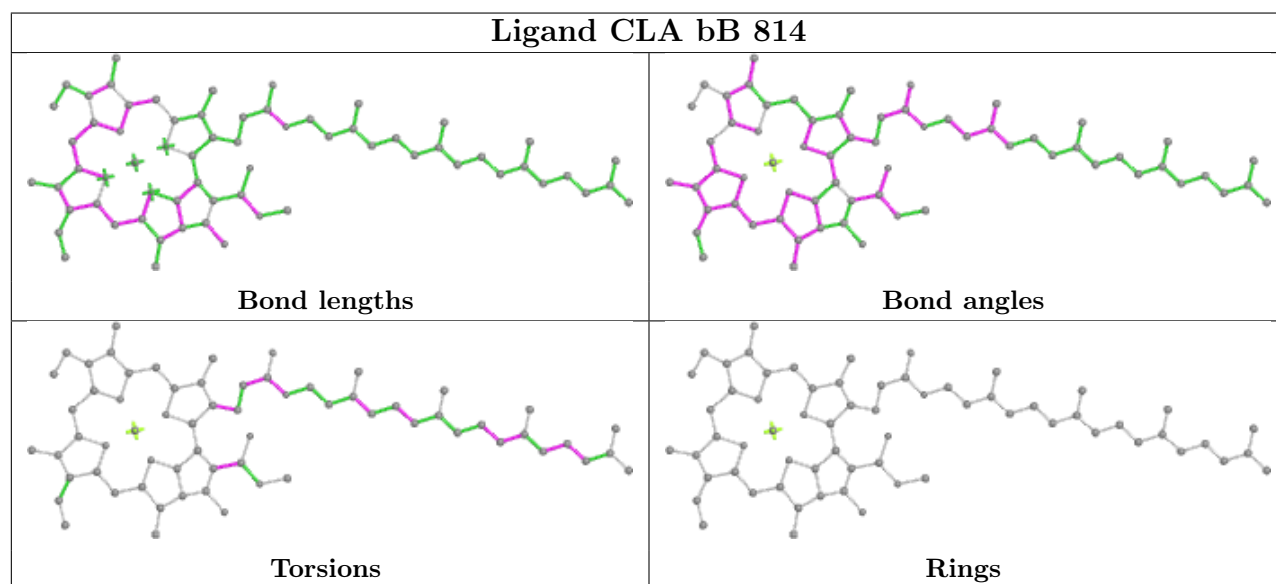
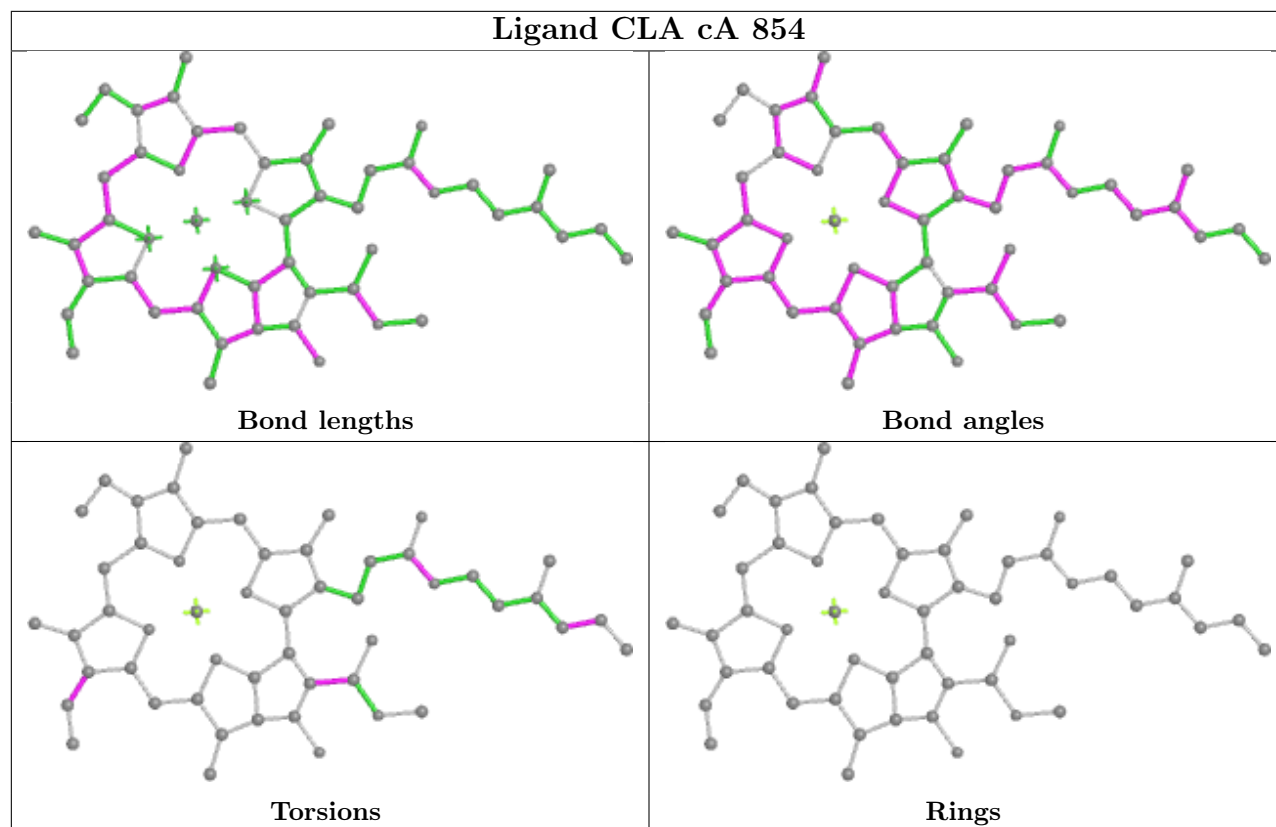


## Ligand CLA cA 823

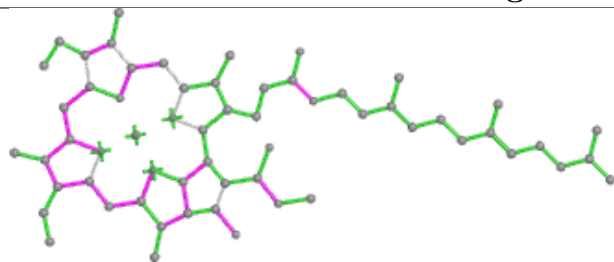


**Ligand CLA aB 830****Ligand CLA bL 205**

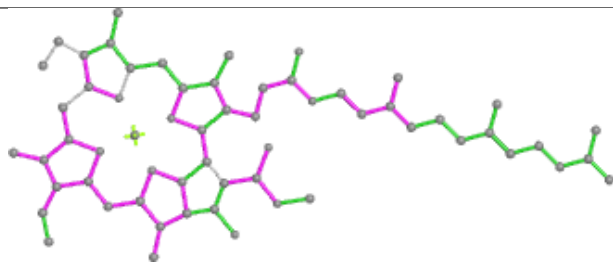




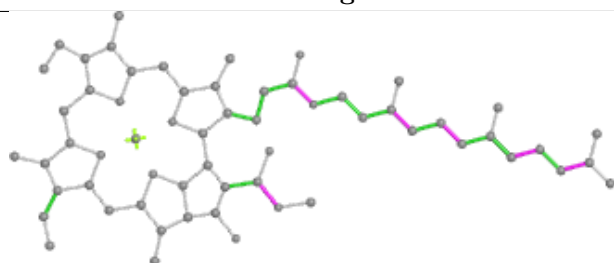
## Ligand CLA cB 837



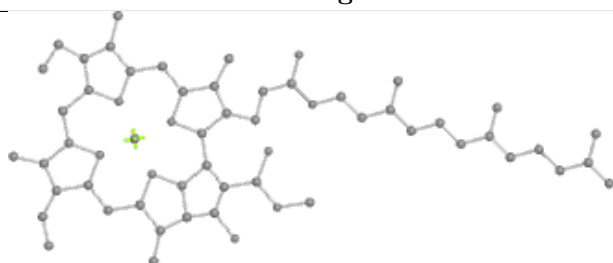
Bond lengths



Bond angles

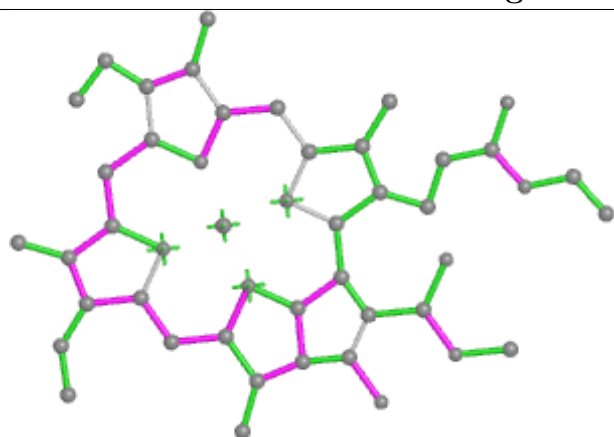


Torsions

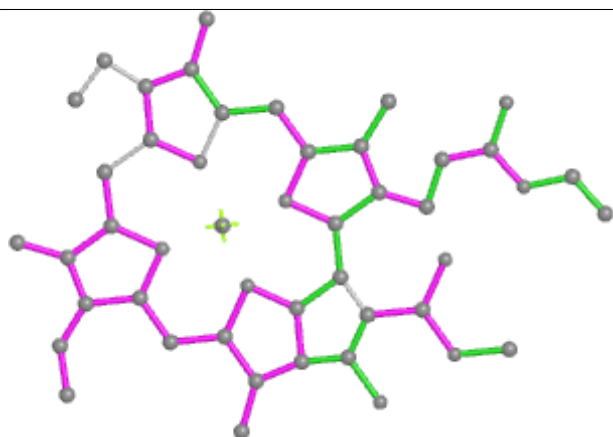


Rings

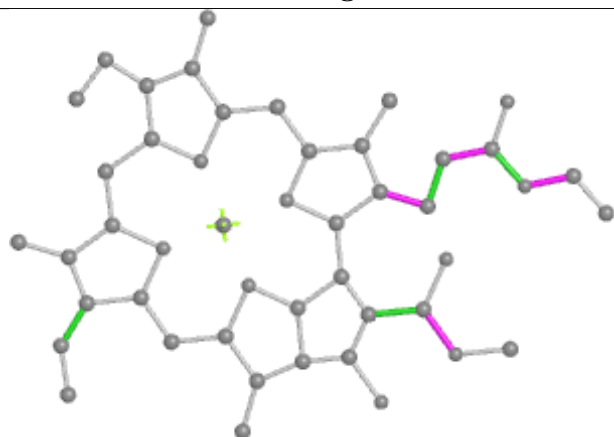
## Ligand CLA aB 839



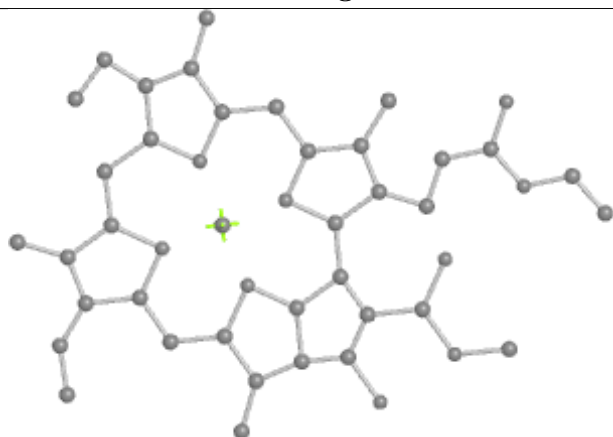
Bond lengths



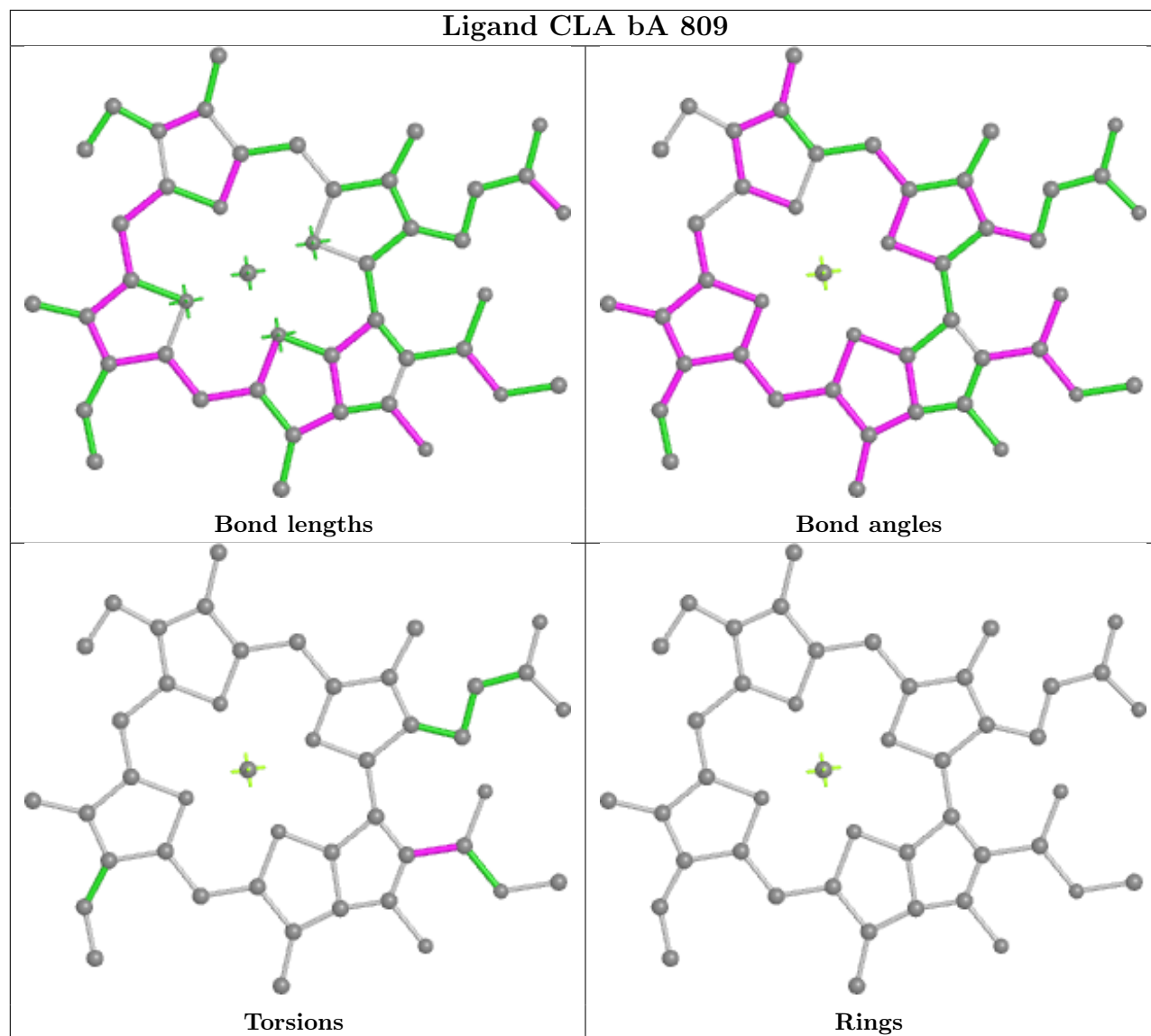
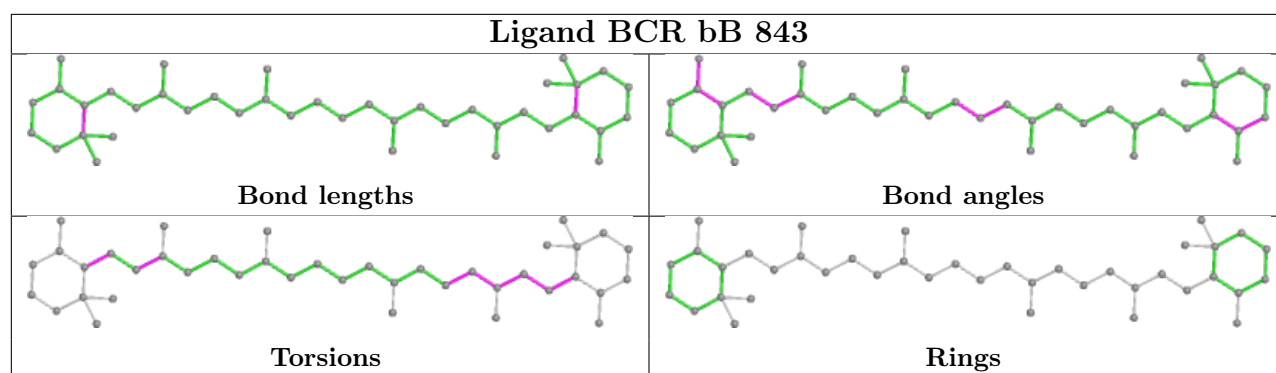
Bond angles



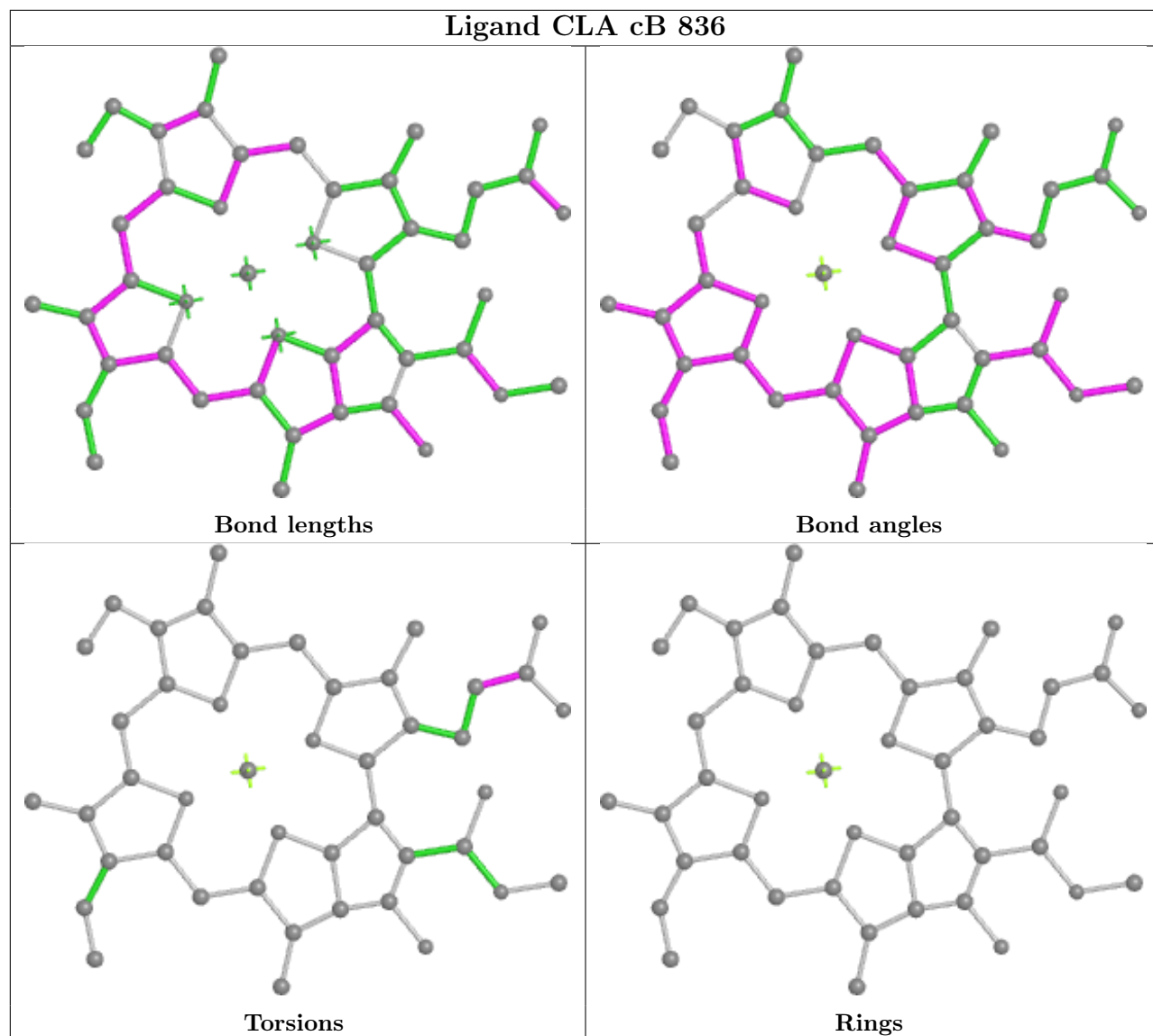
Torsions

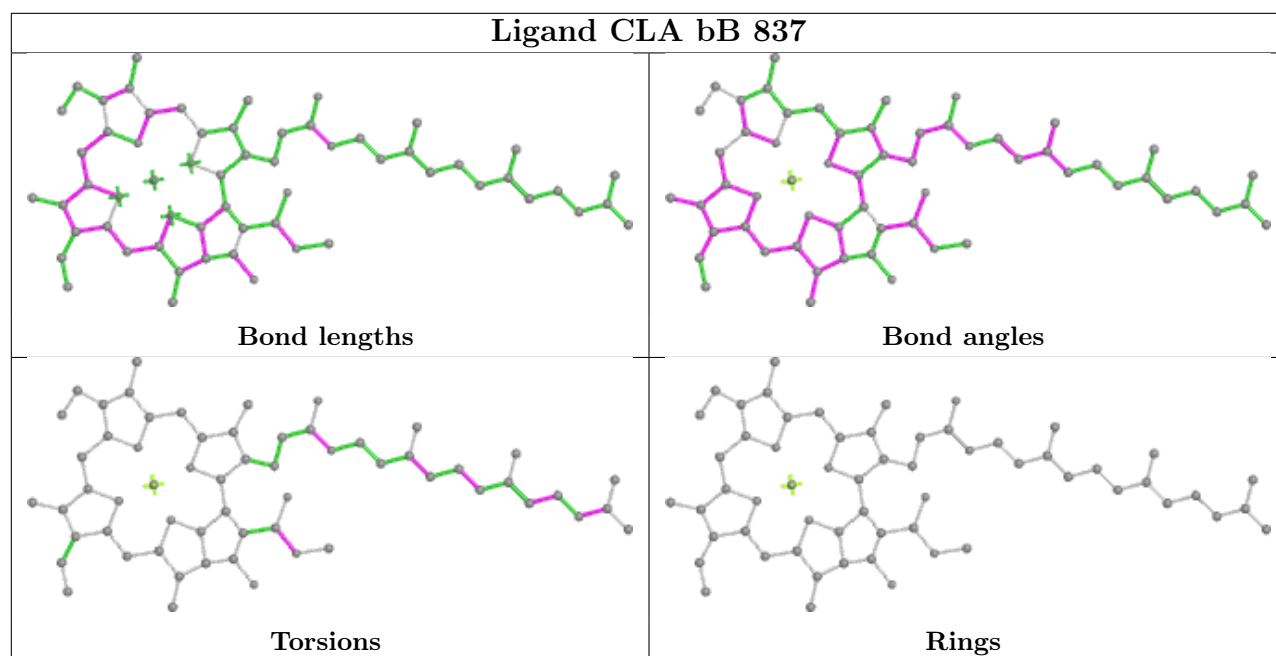
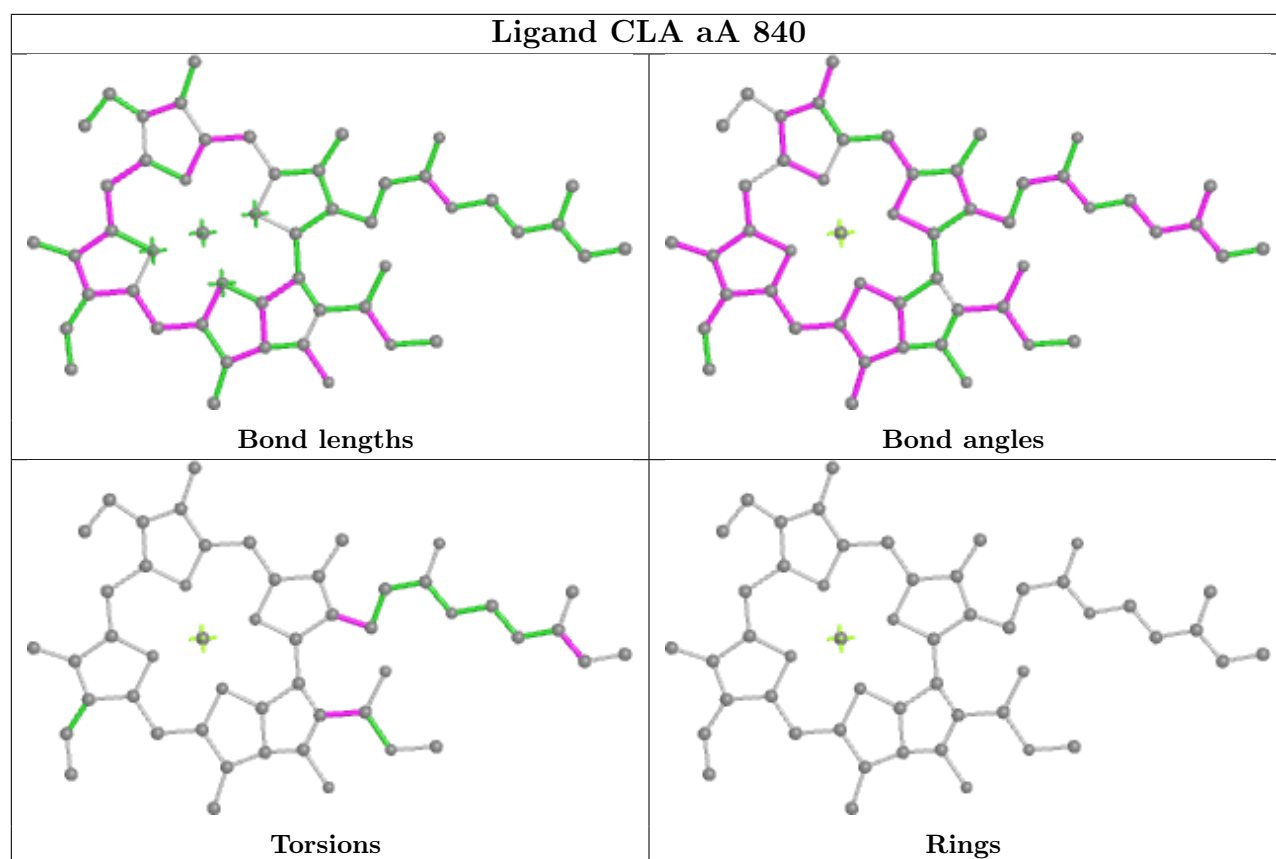


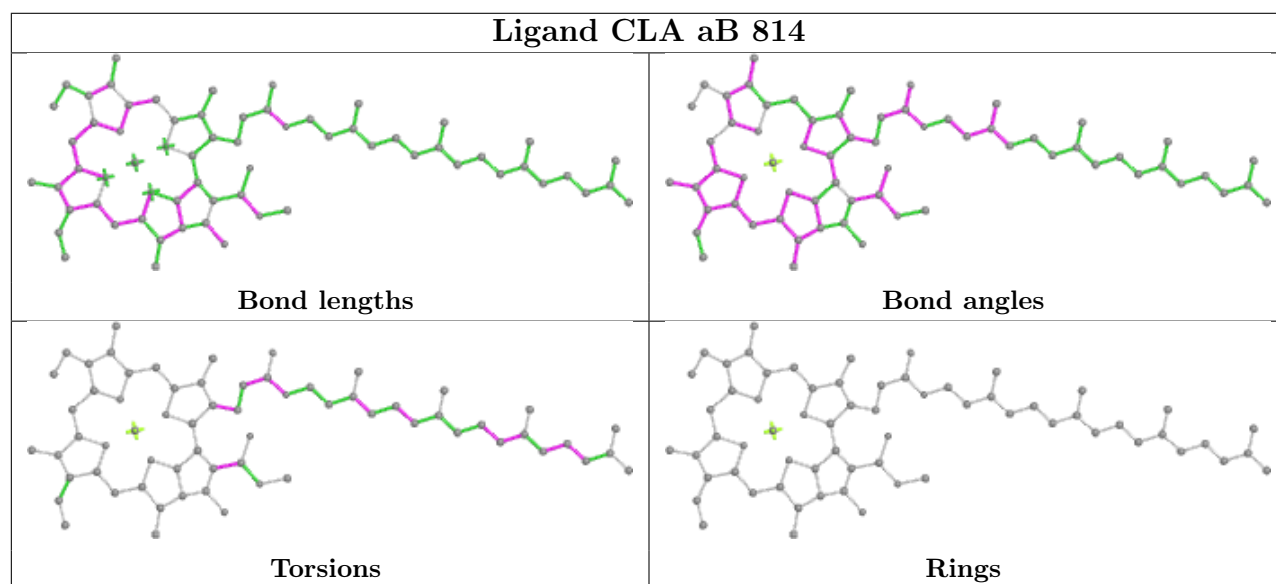
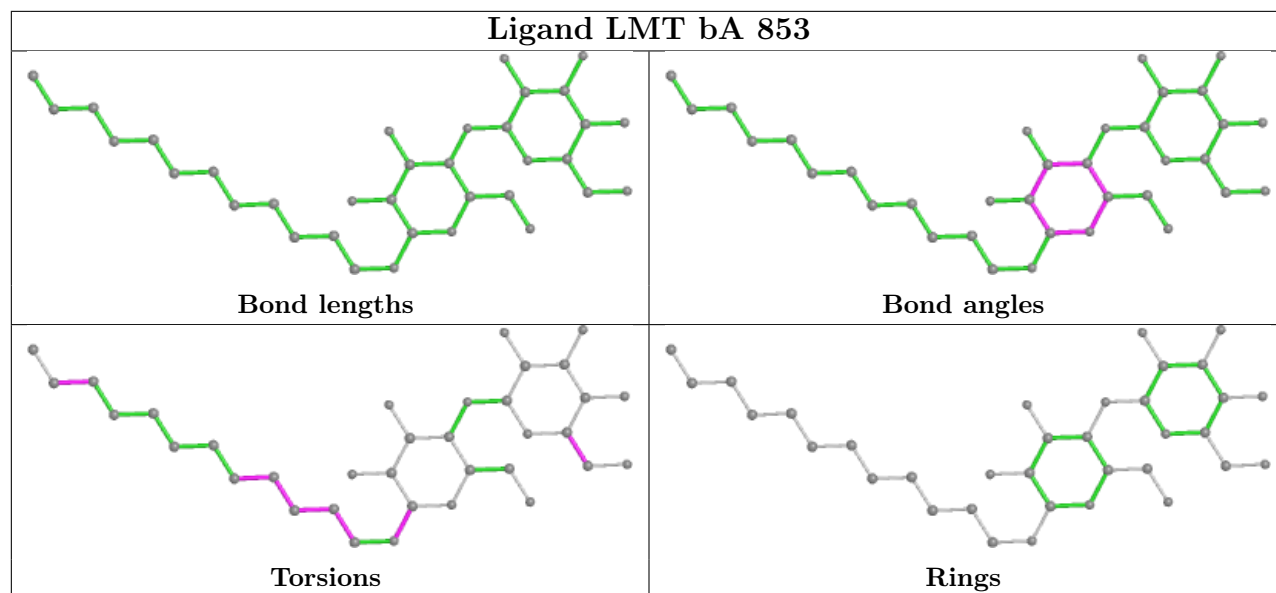
Rings

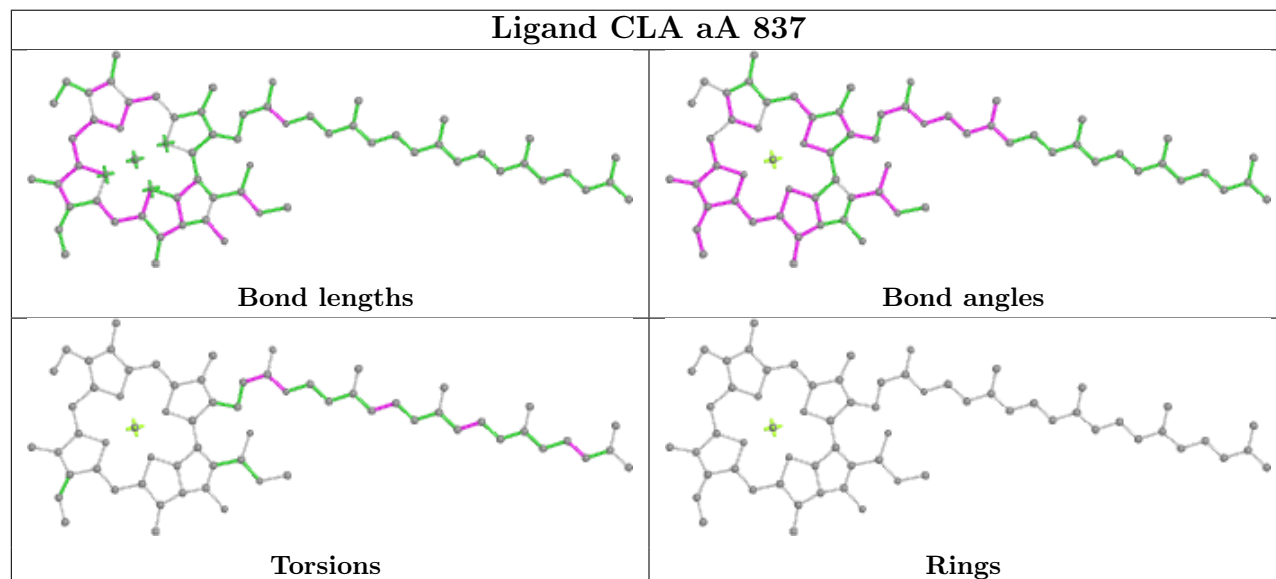
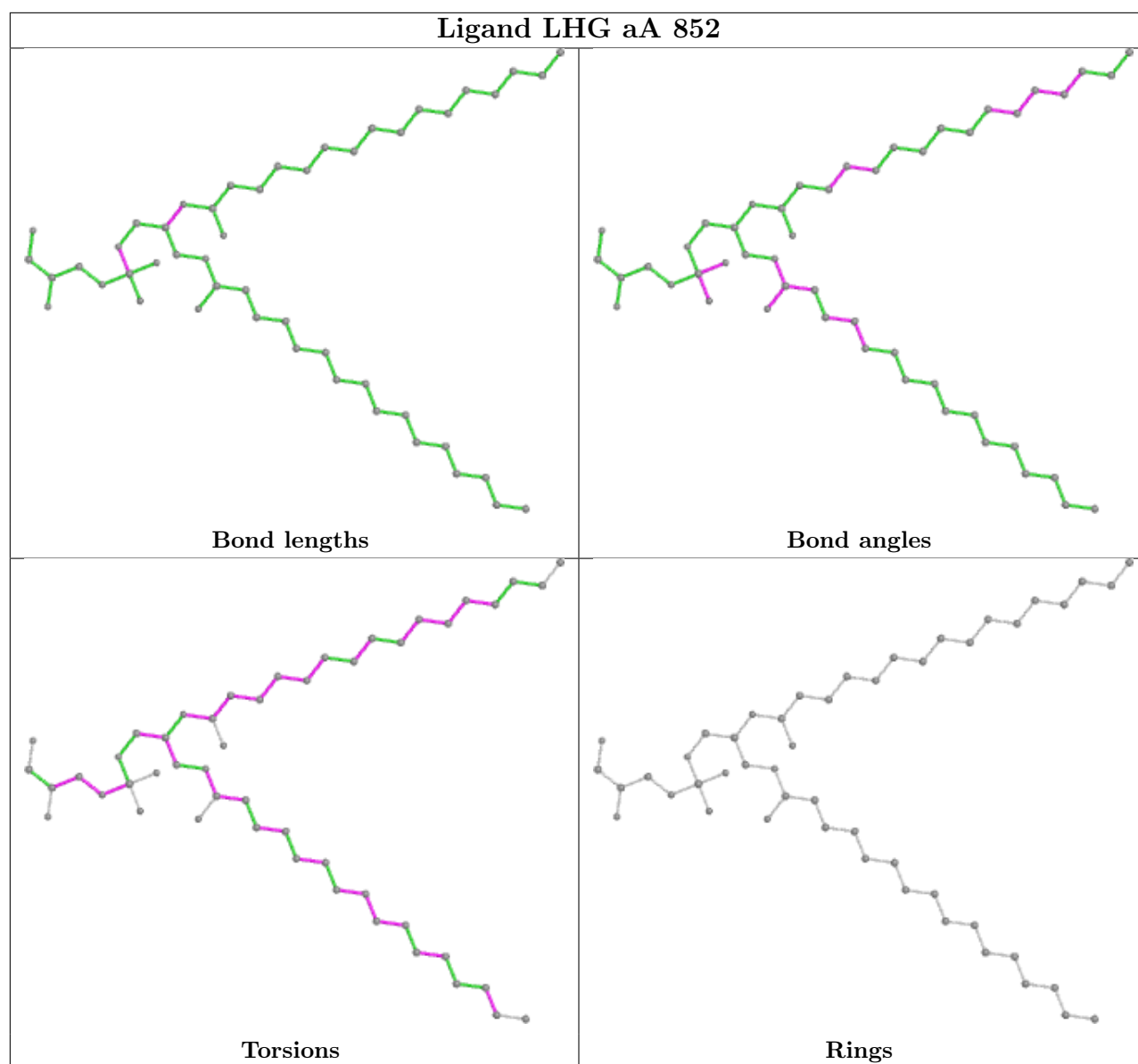




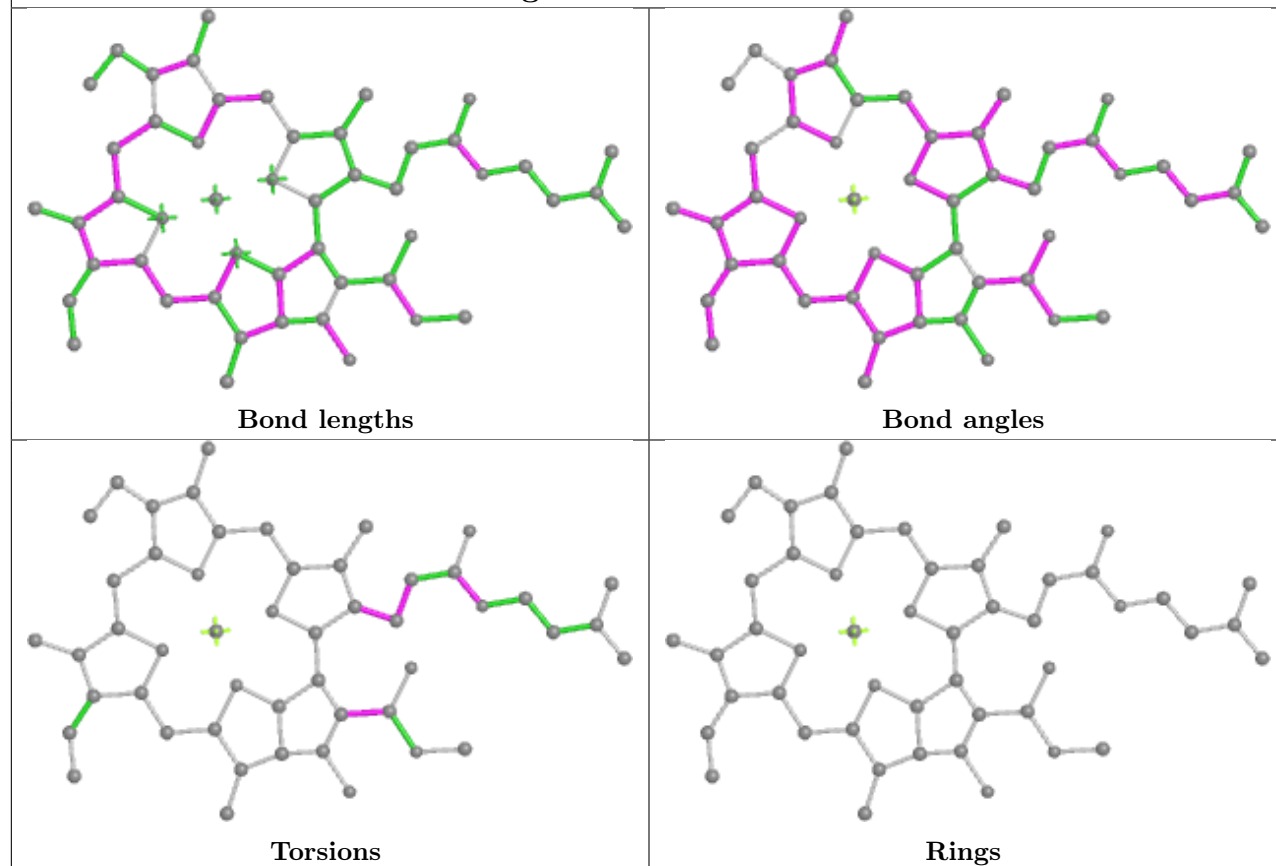




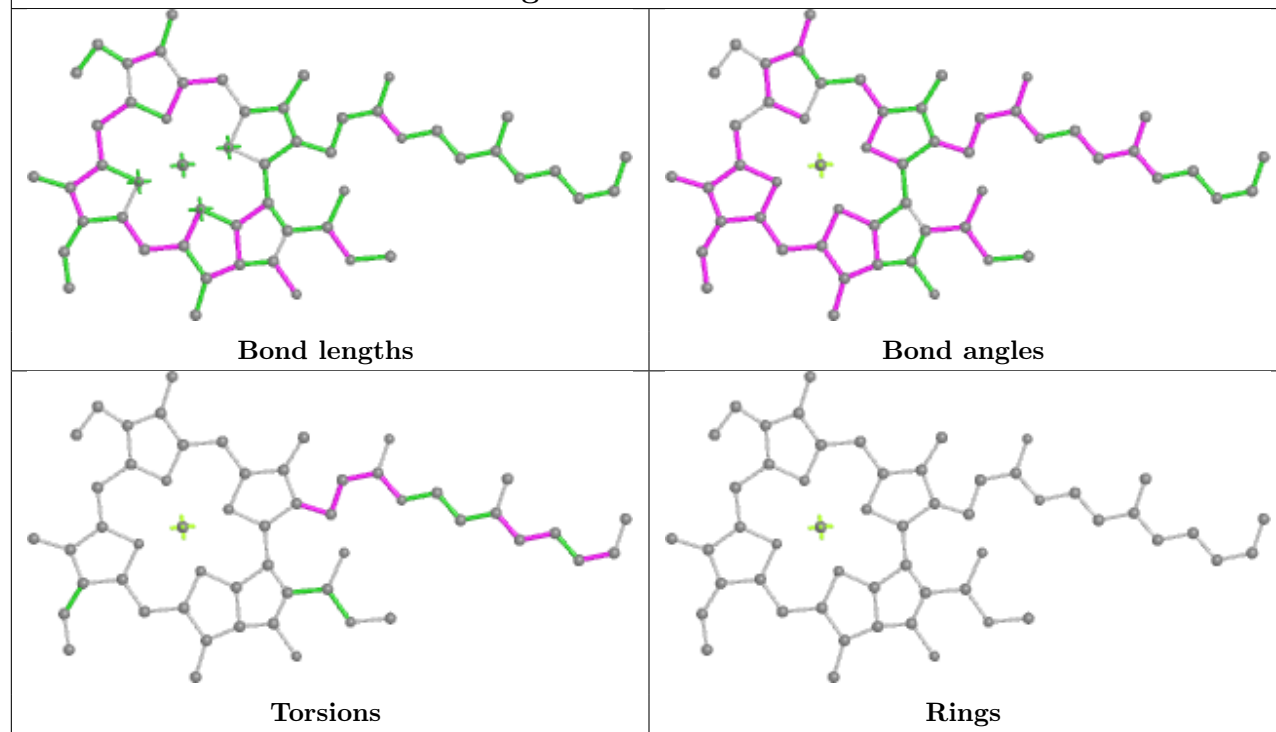




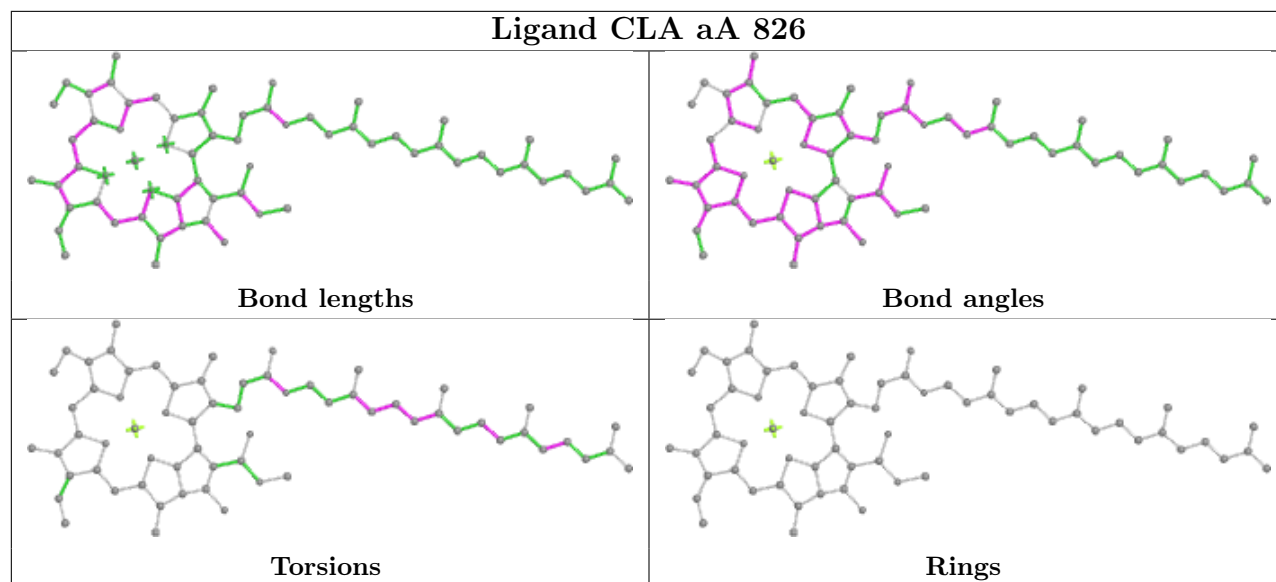
## Ligand CLA bA 830



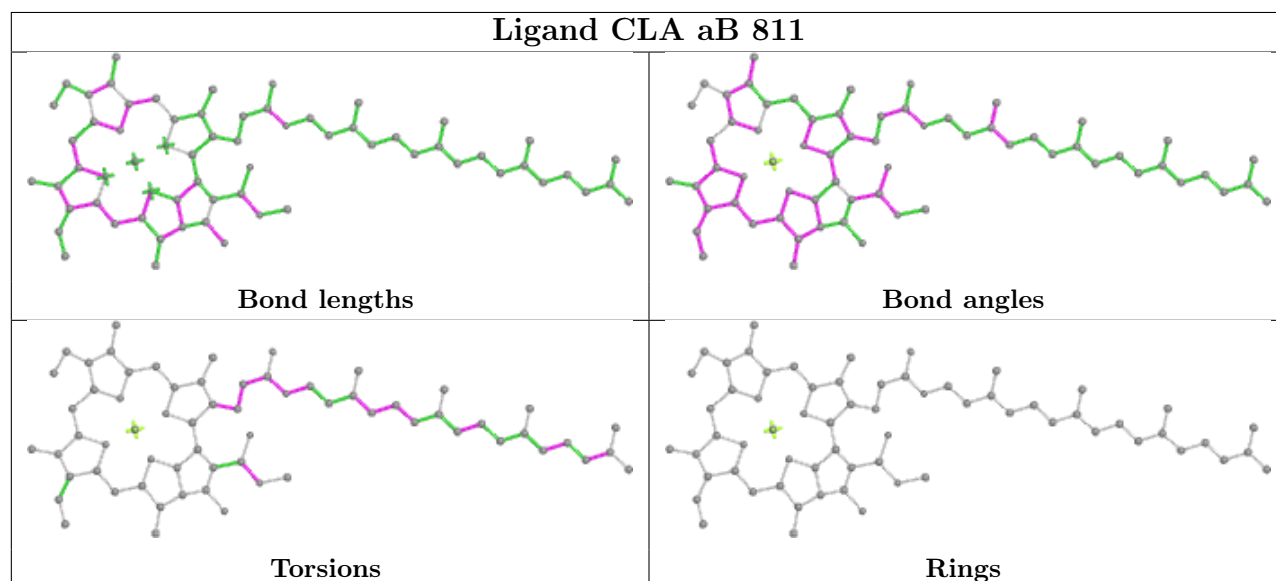
## Ligand CLA bA 817



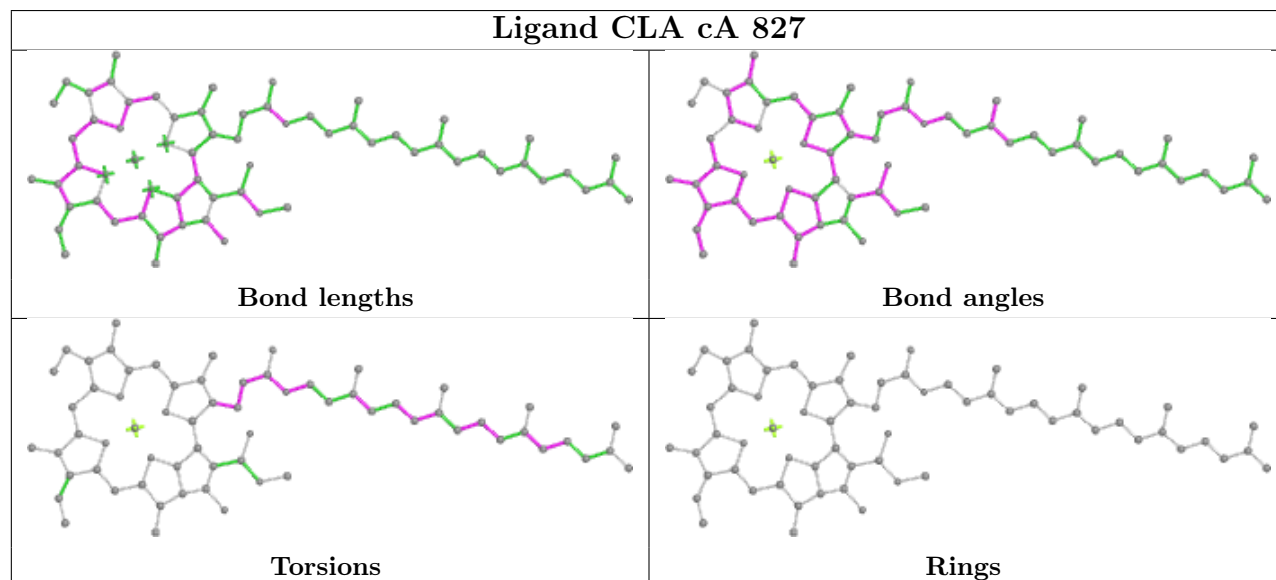
## Ligand CLA aA 826

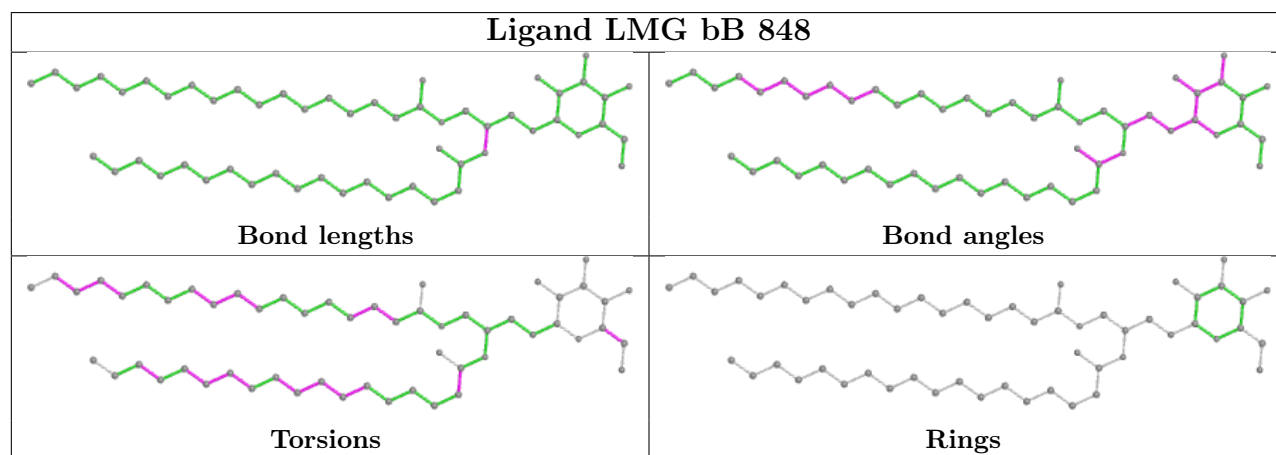
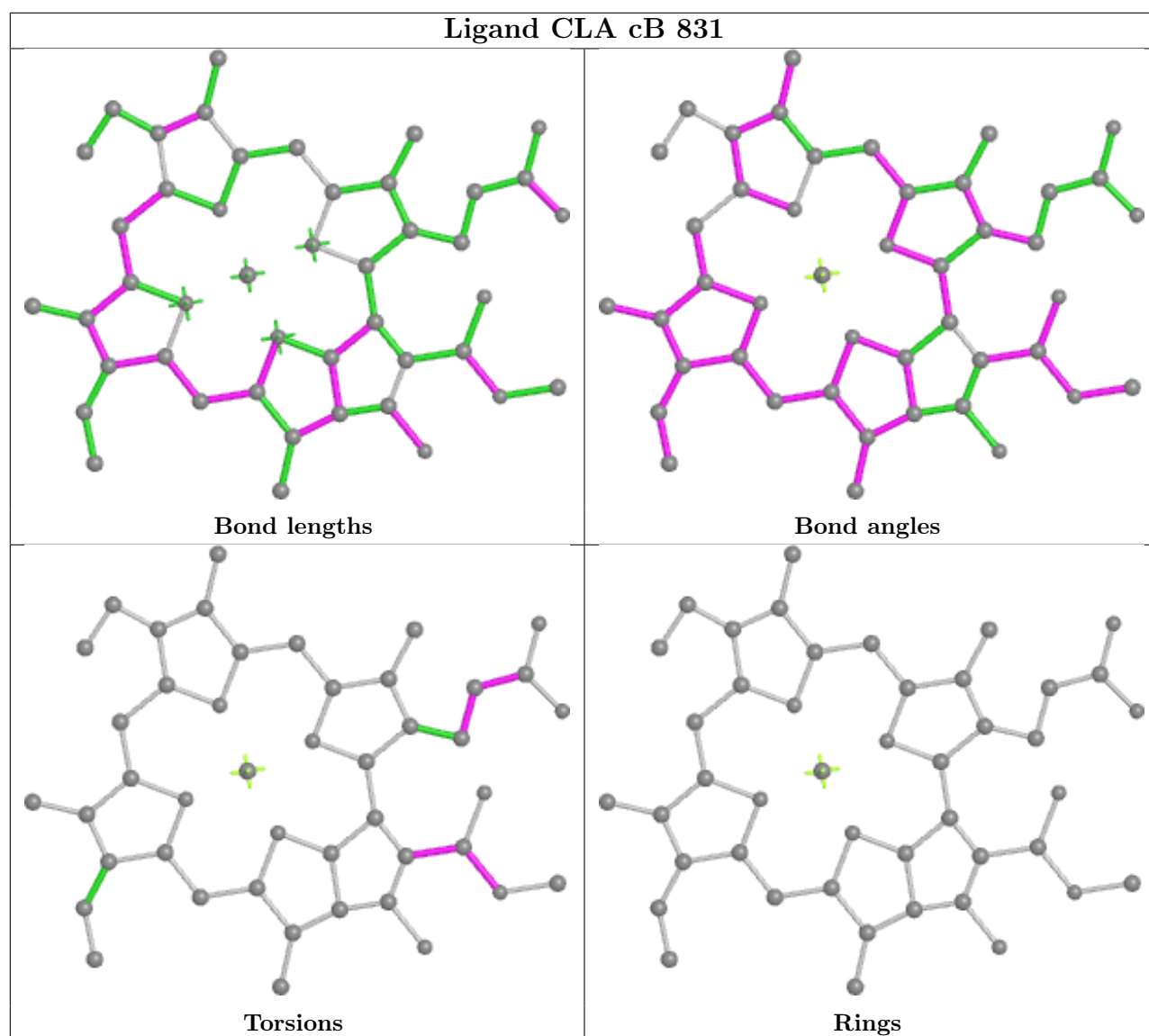


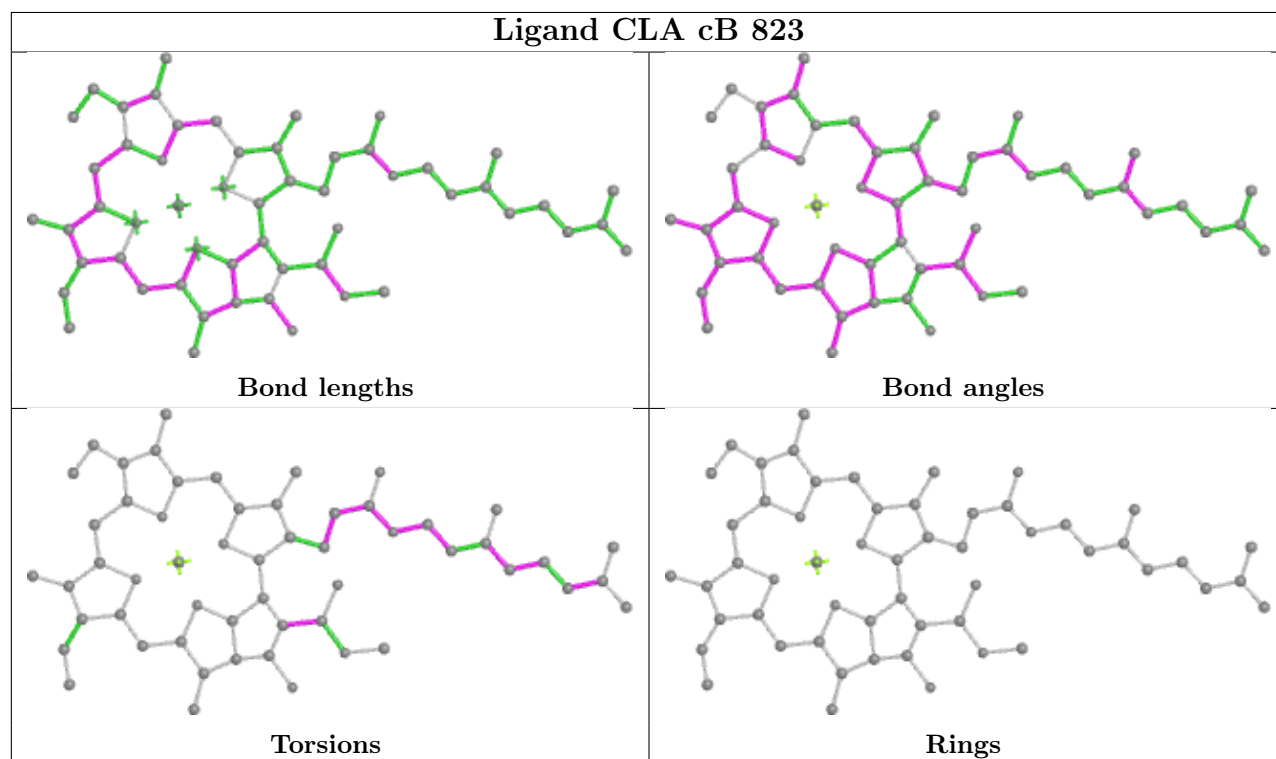
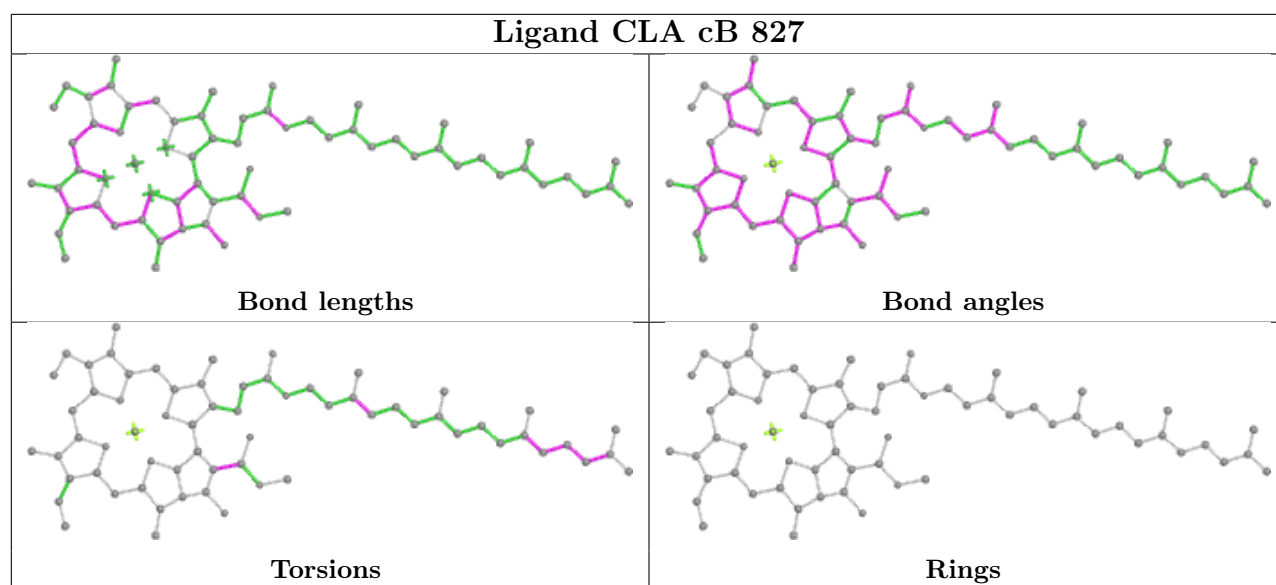
## Ligand CLA aB 811



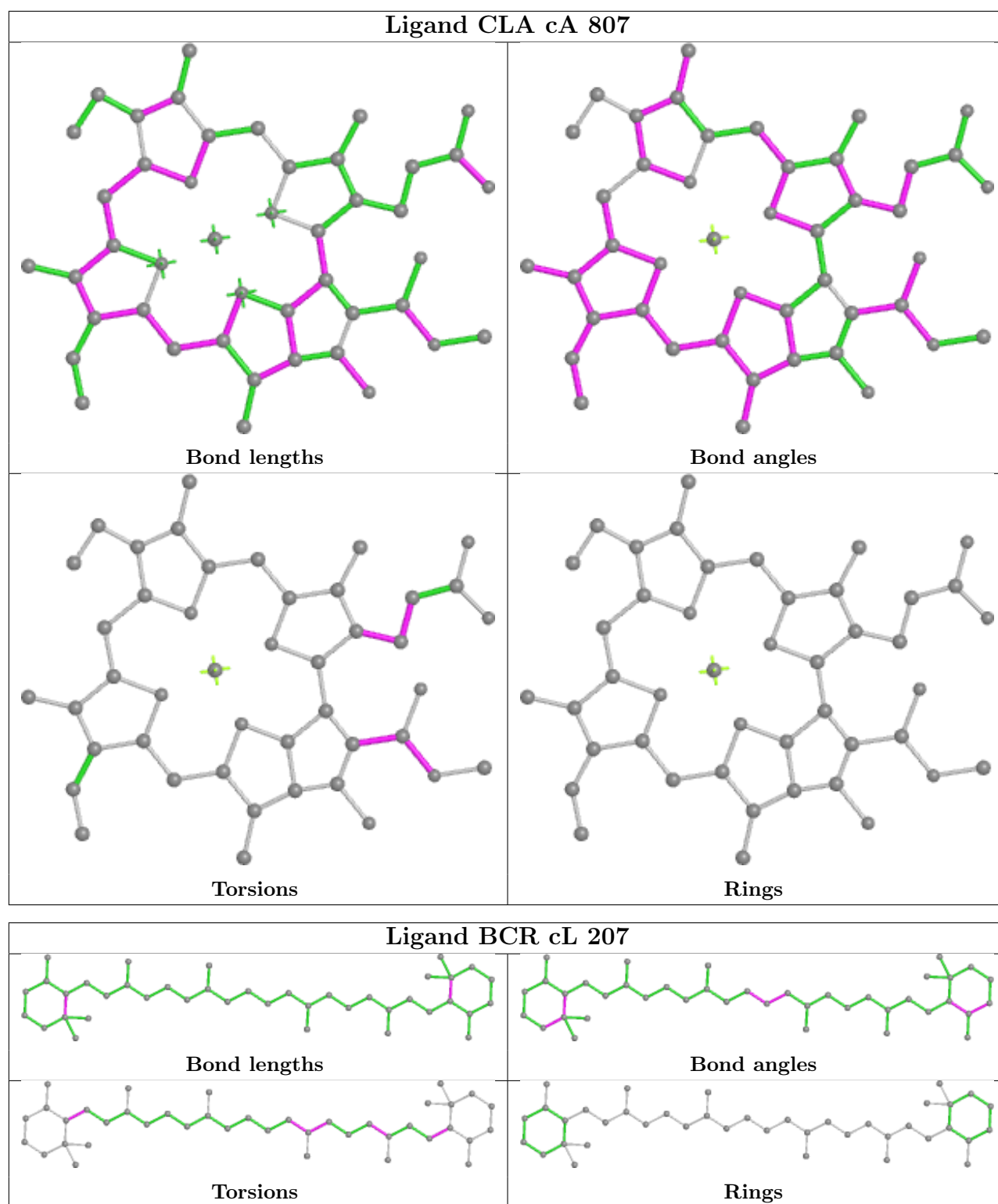
## Ligand CLA cA 827

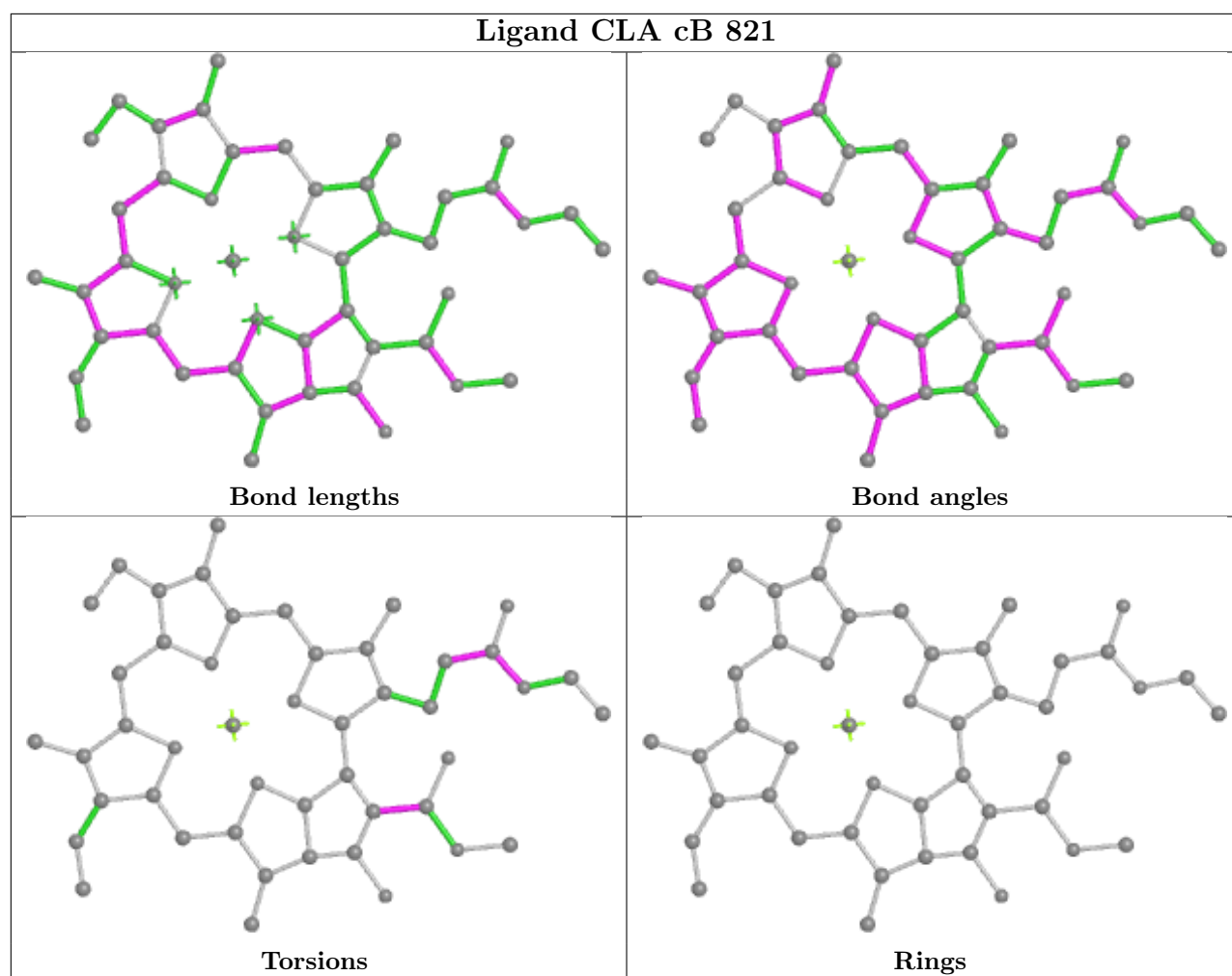


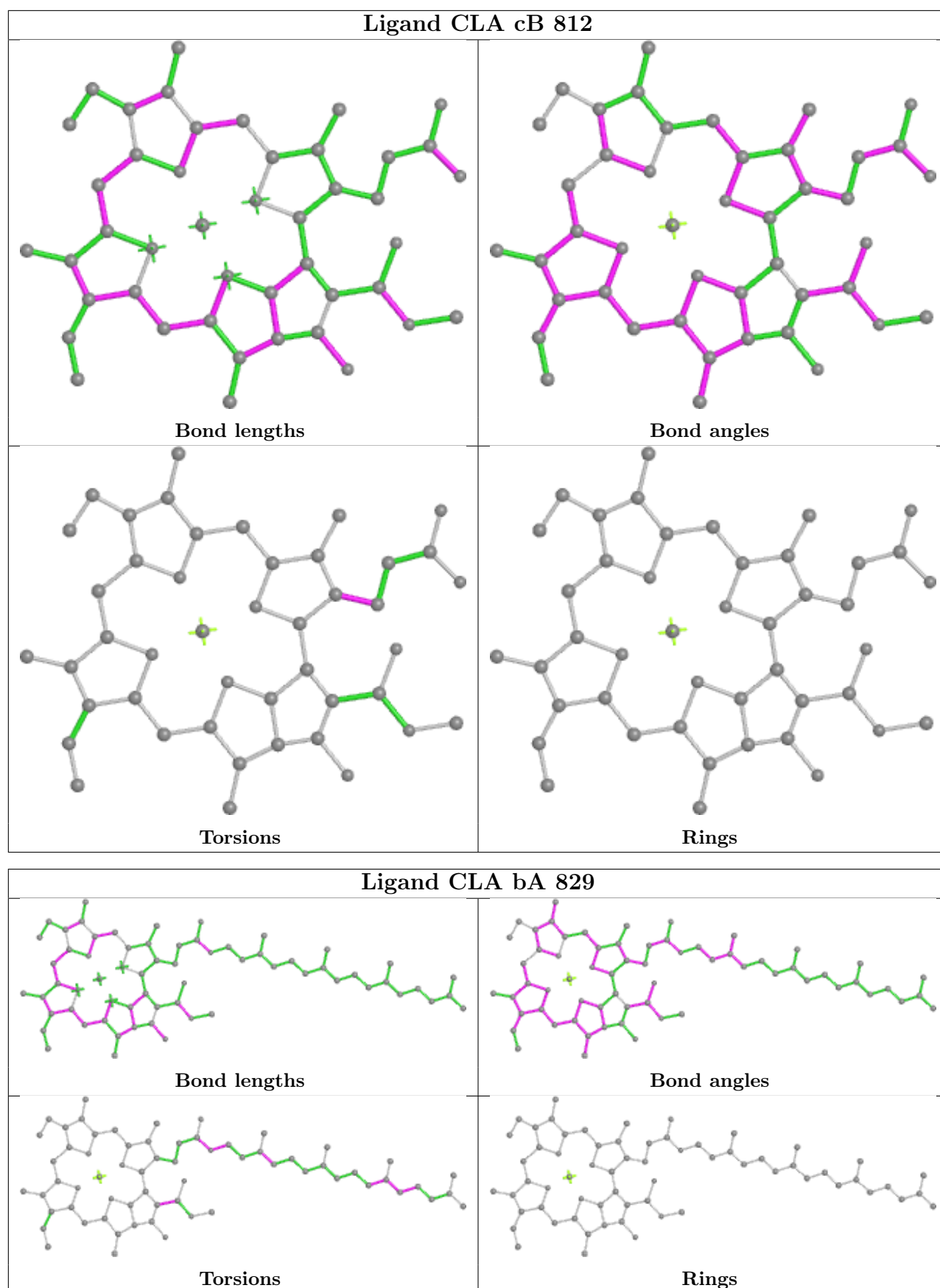




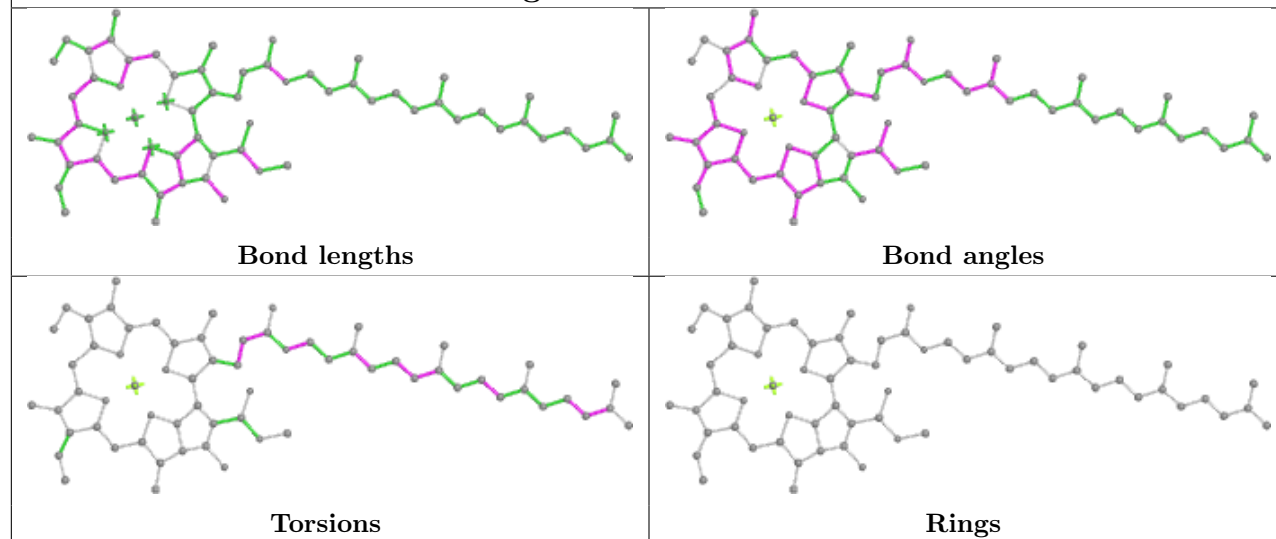




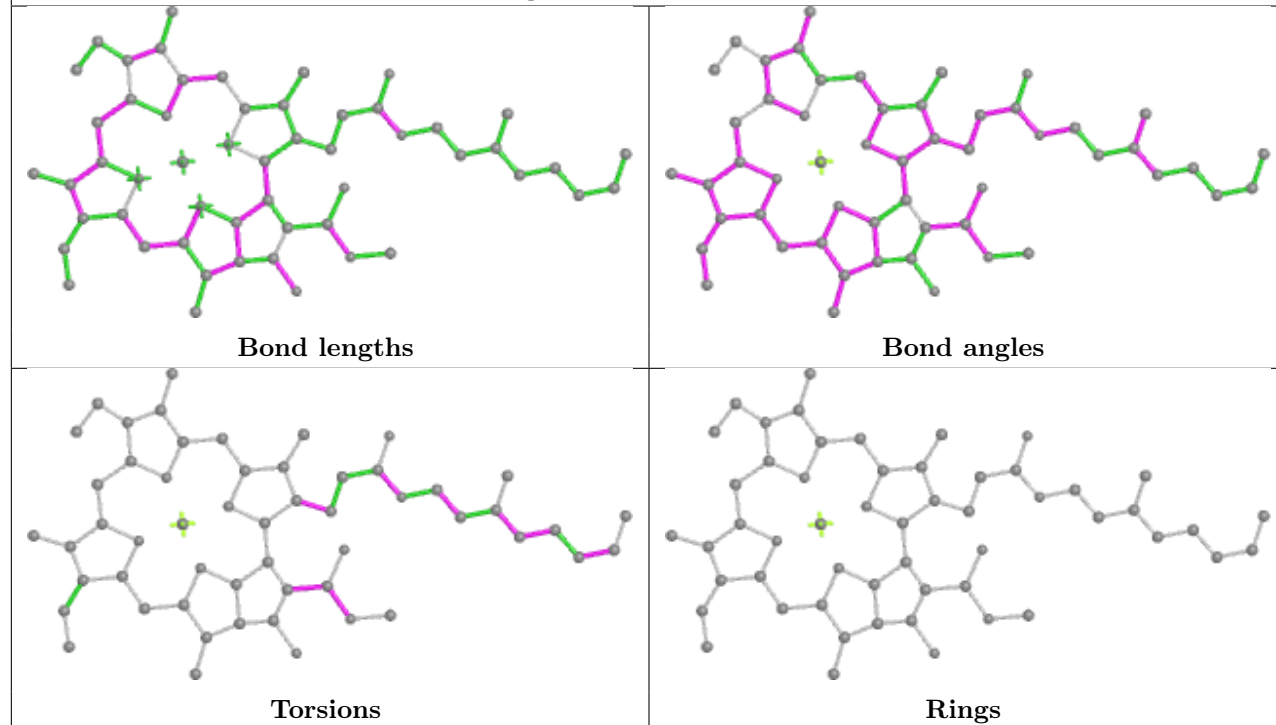




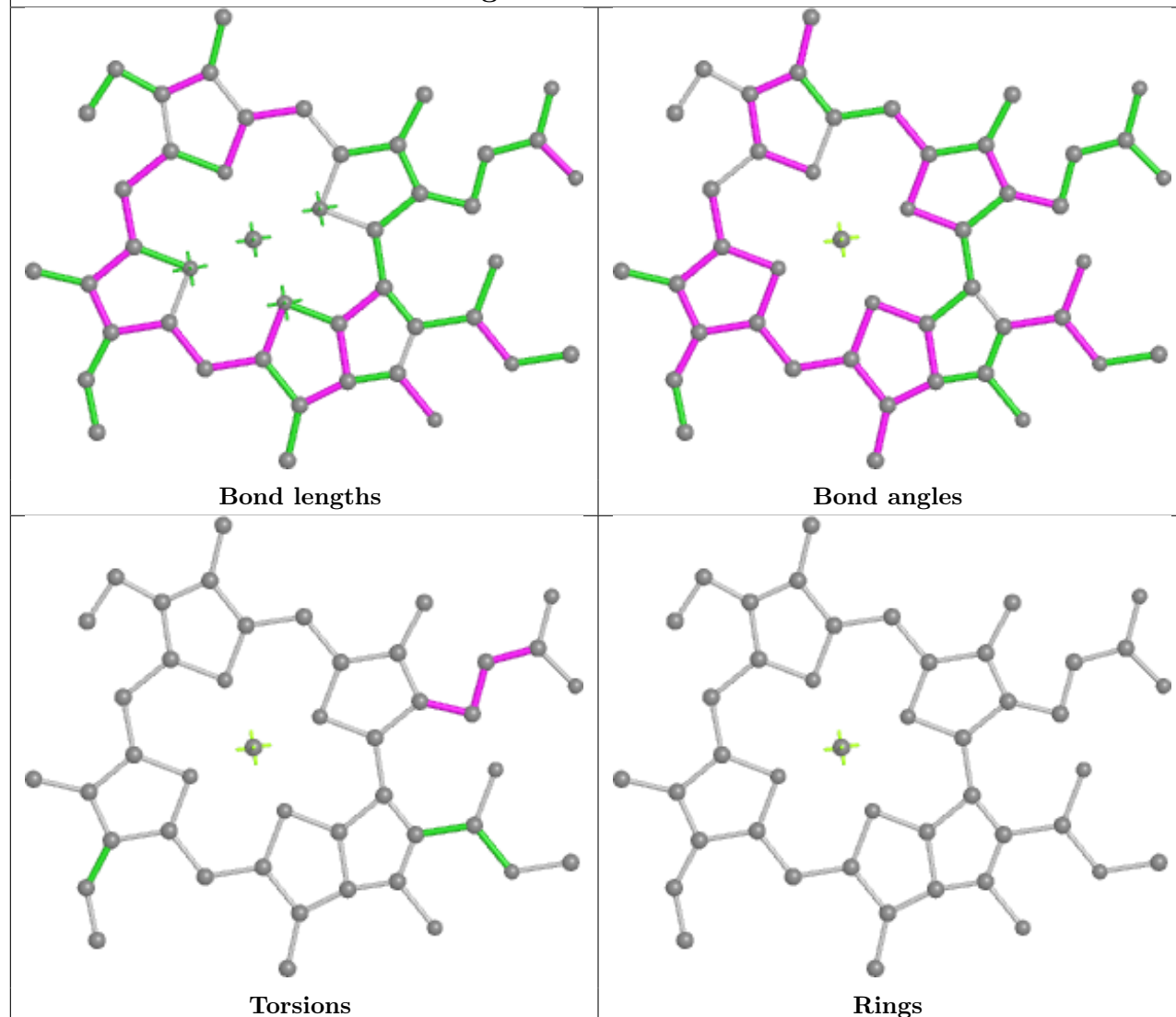
## Ligand CLA aA 841



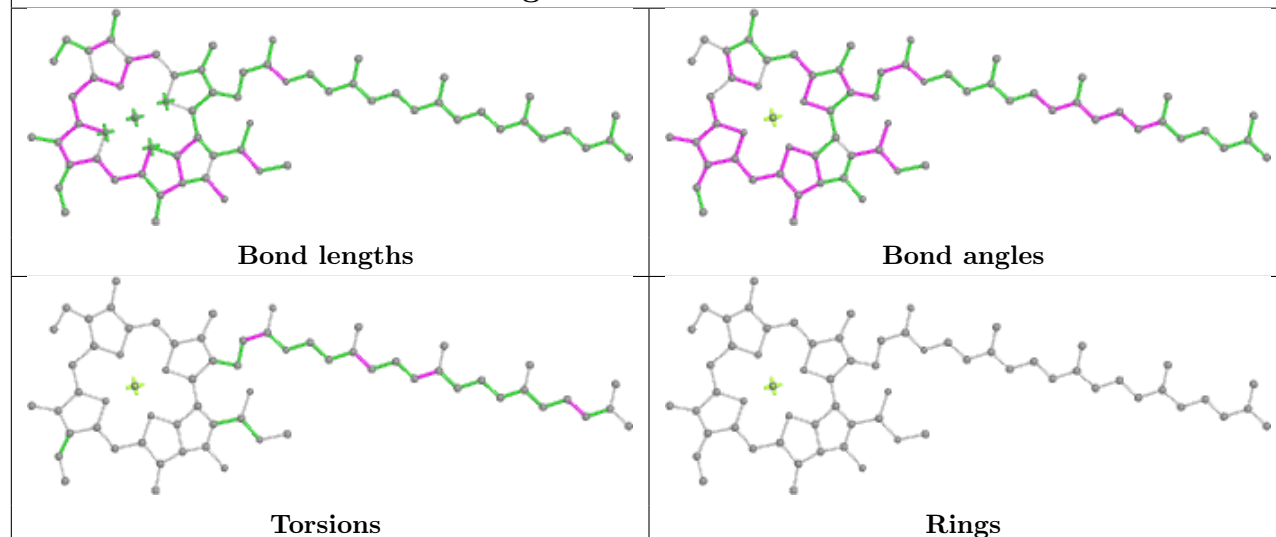
## Ligand CLA bB 806

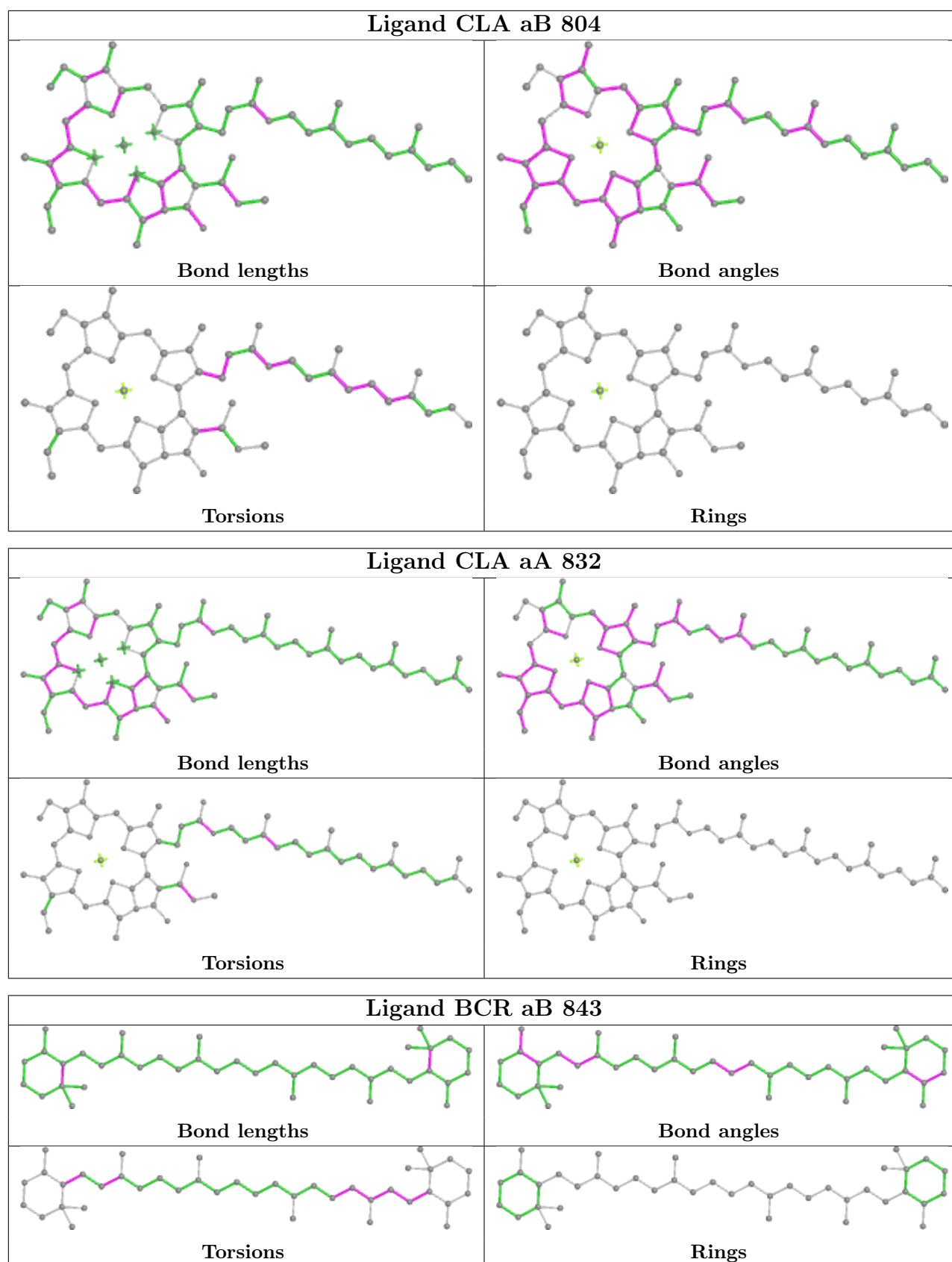


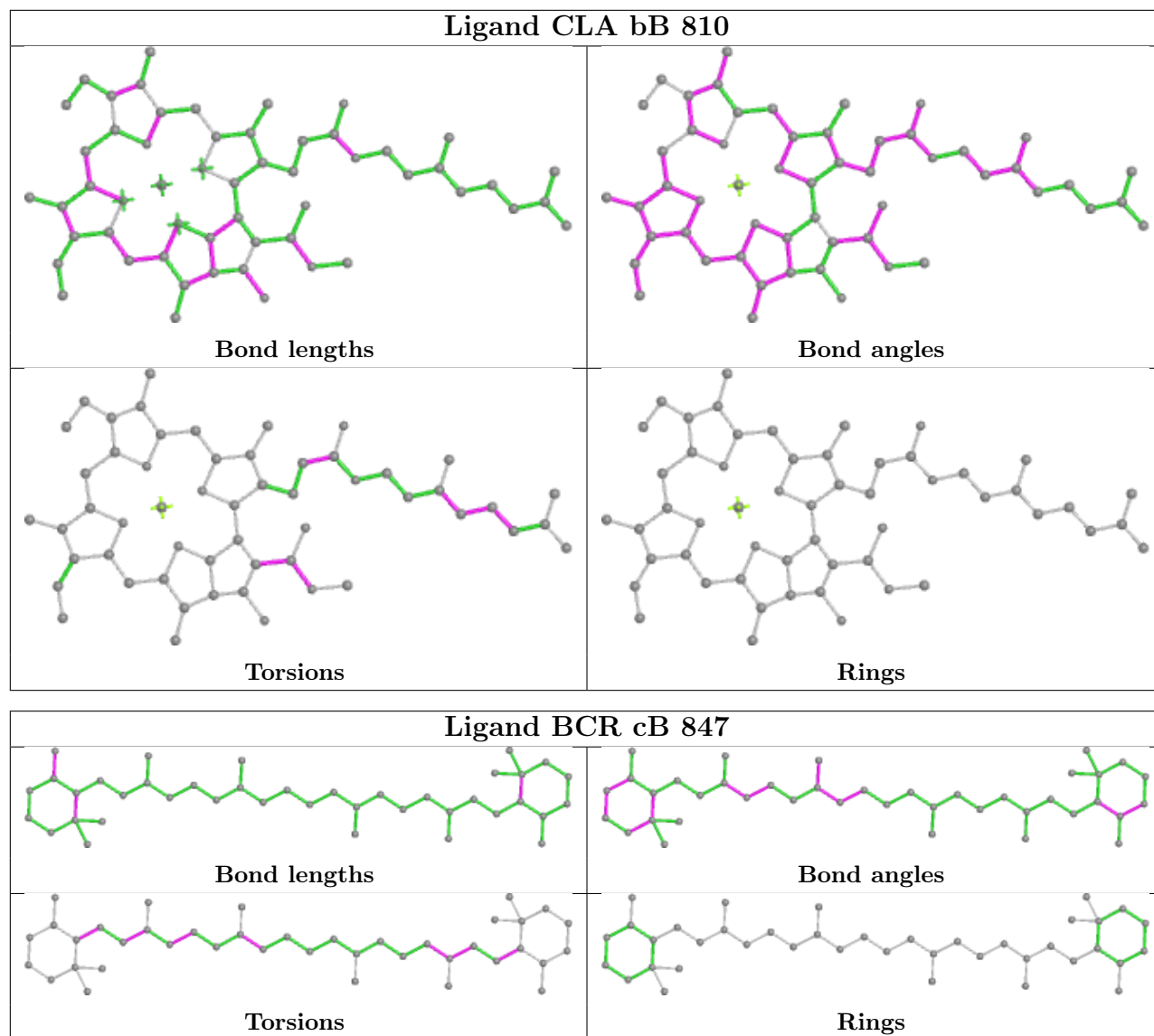
## Ligand CLA bB 813

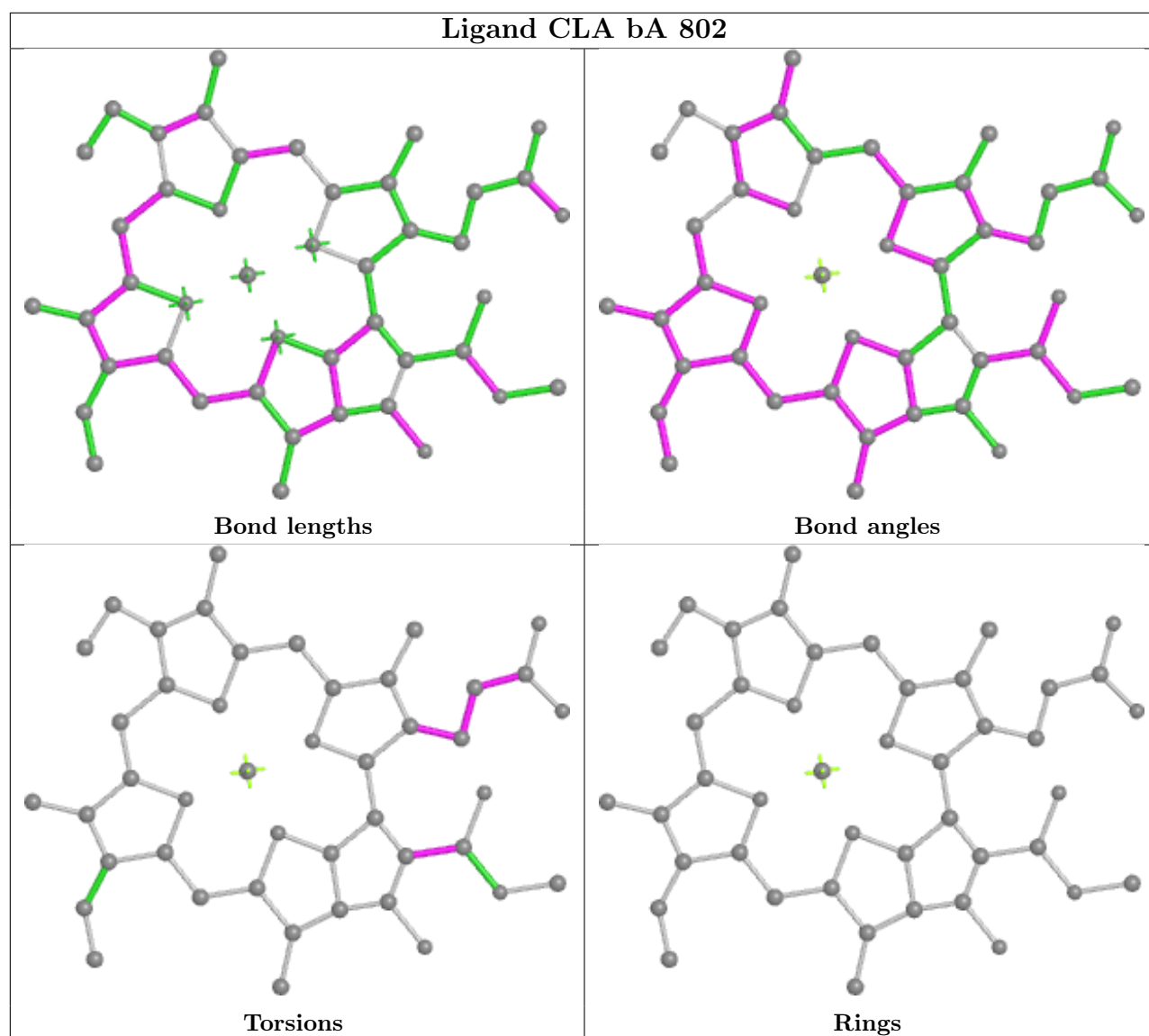


## Ligand CLA bB 809

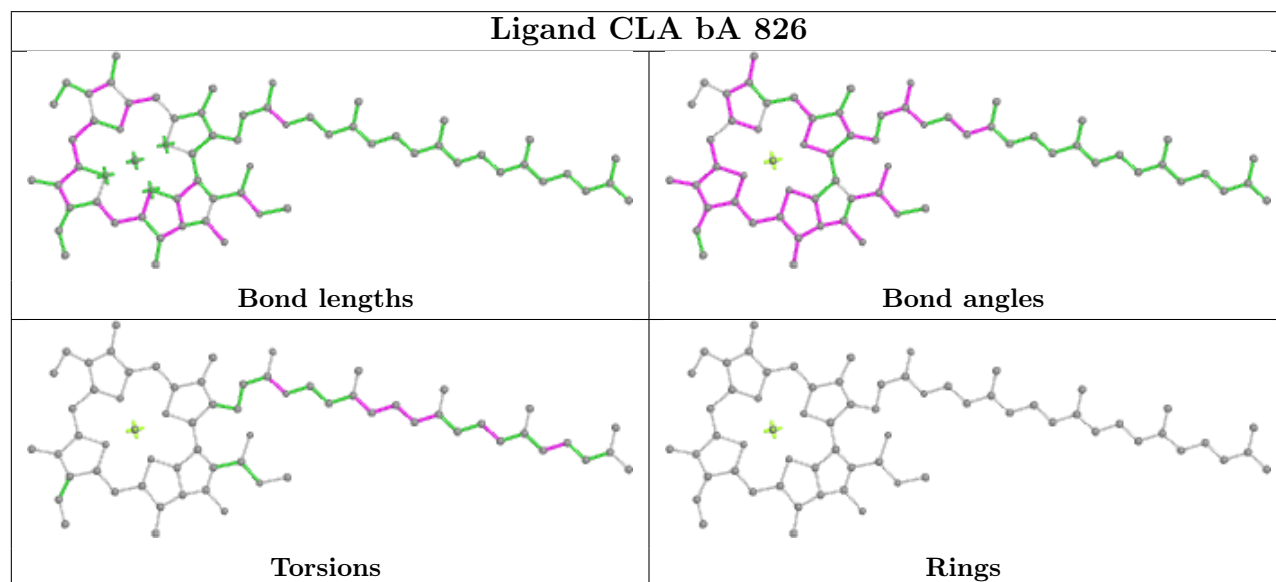
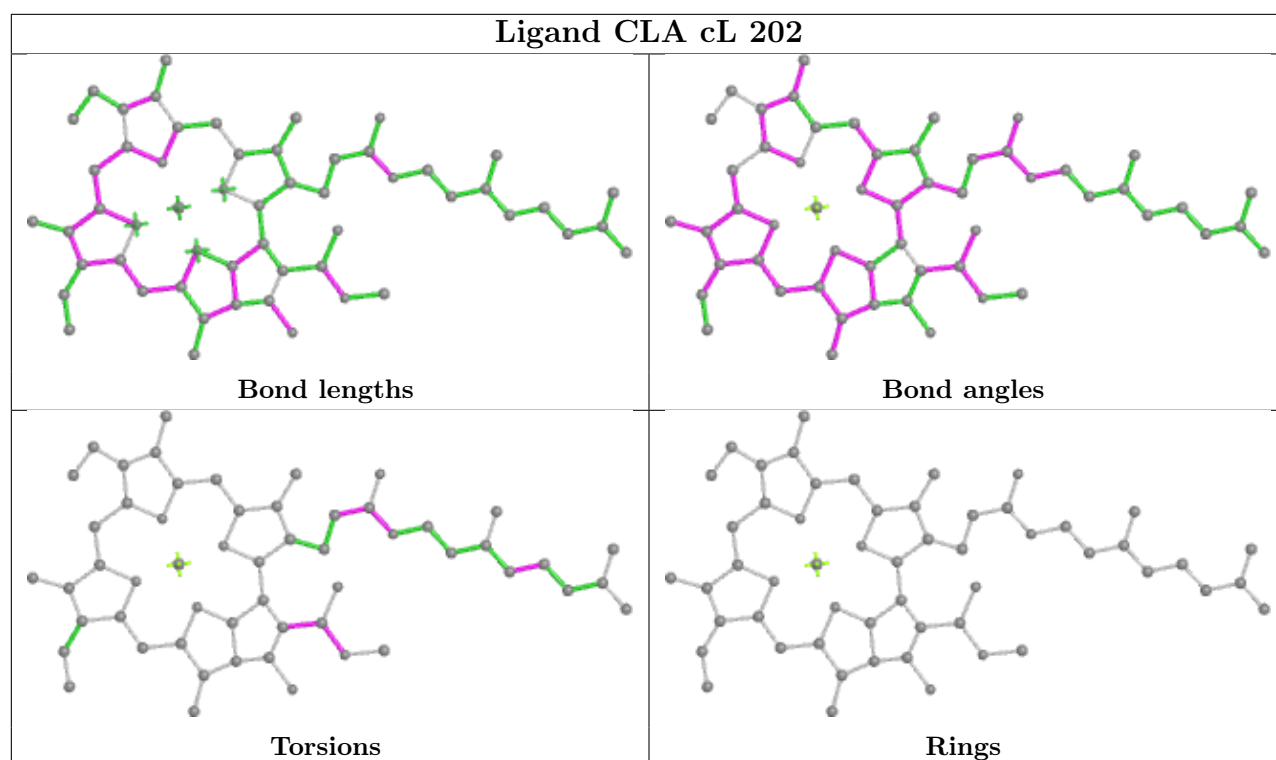


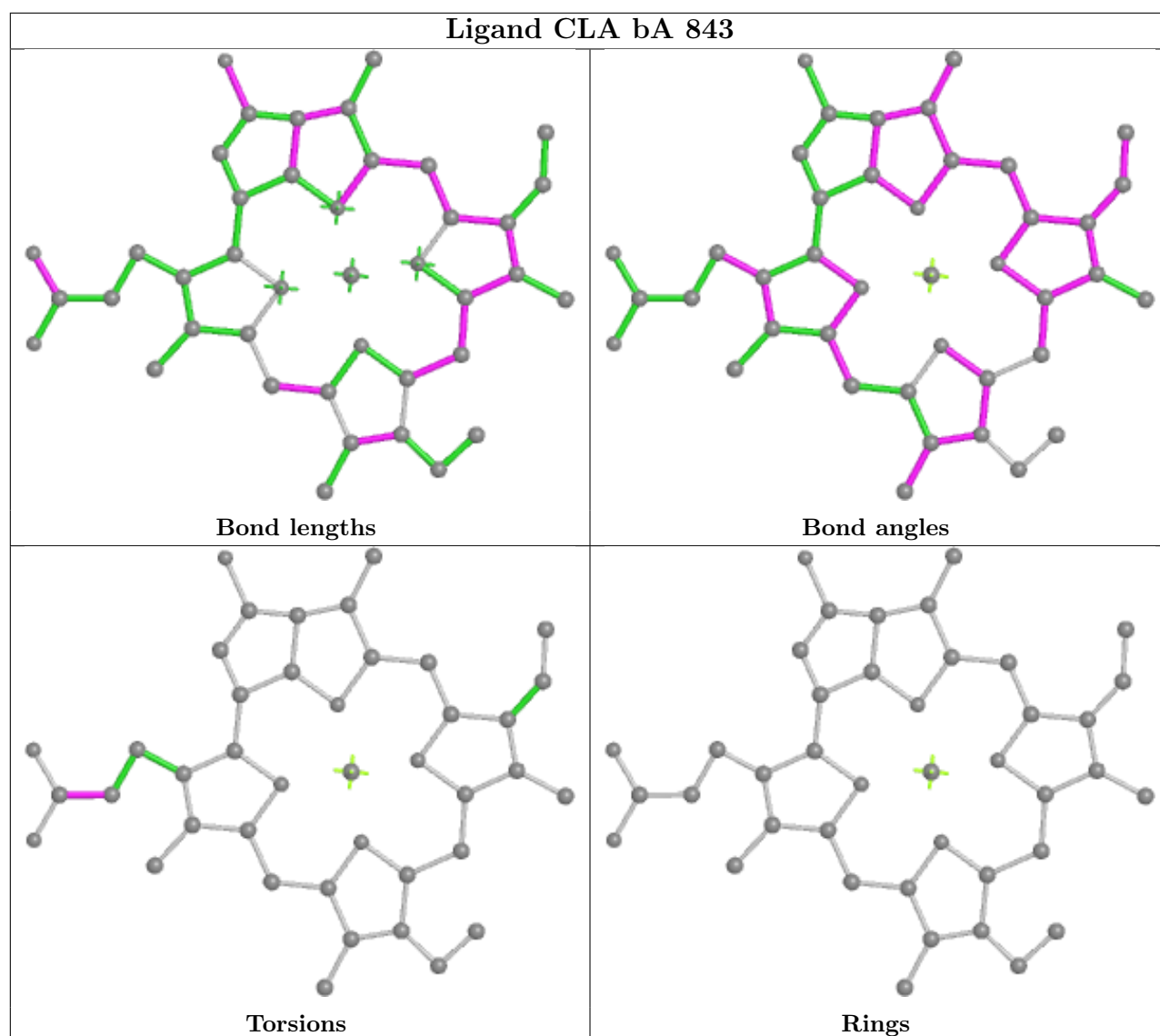




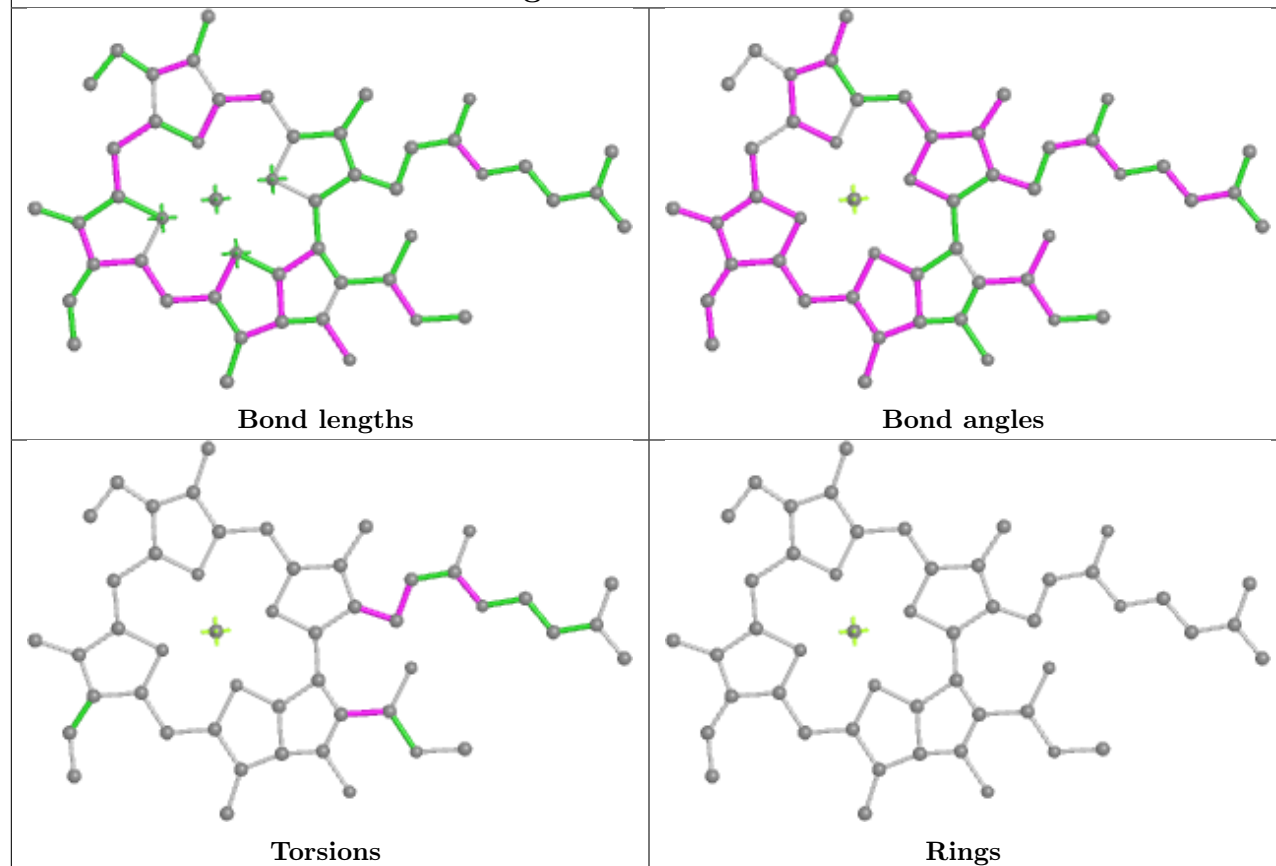




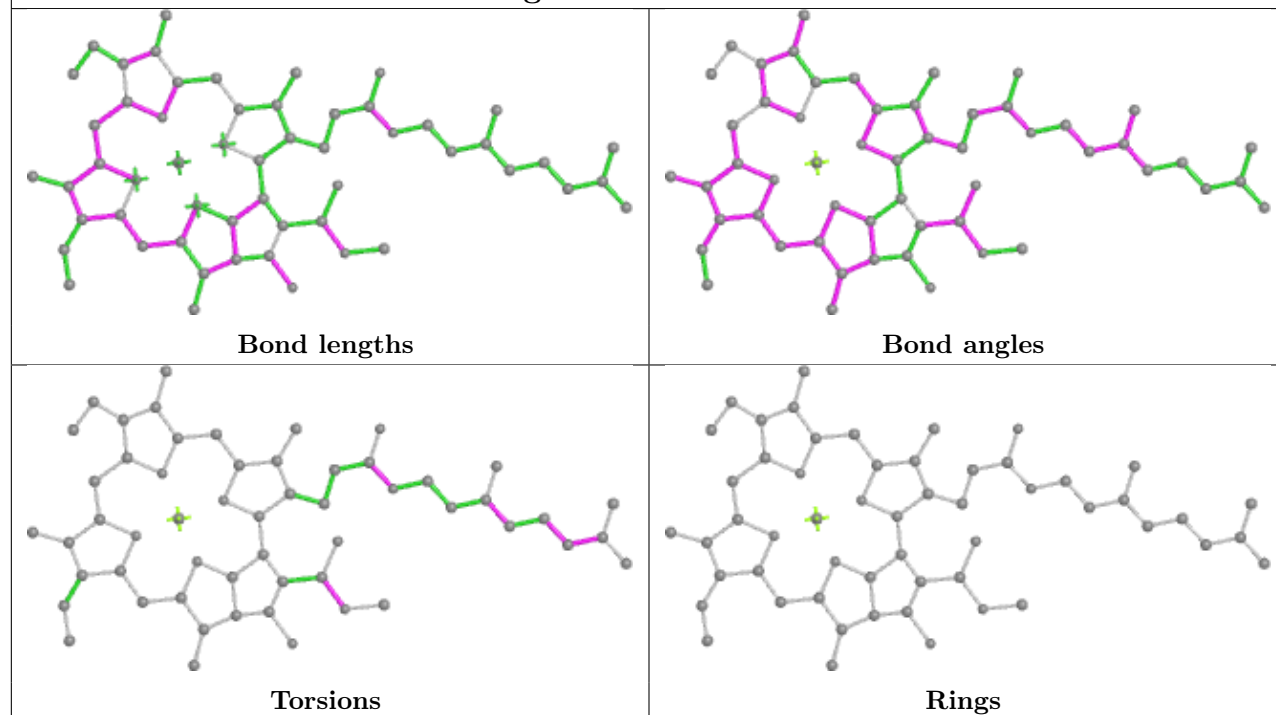


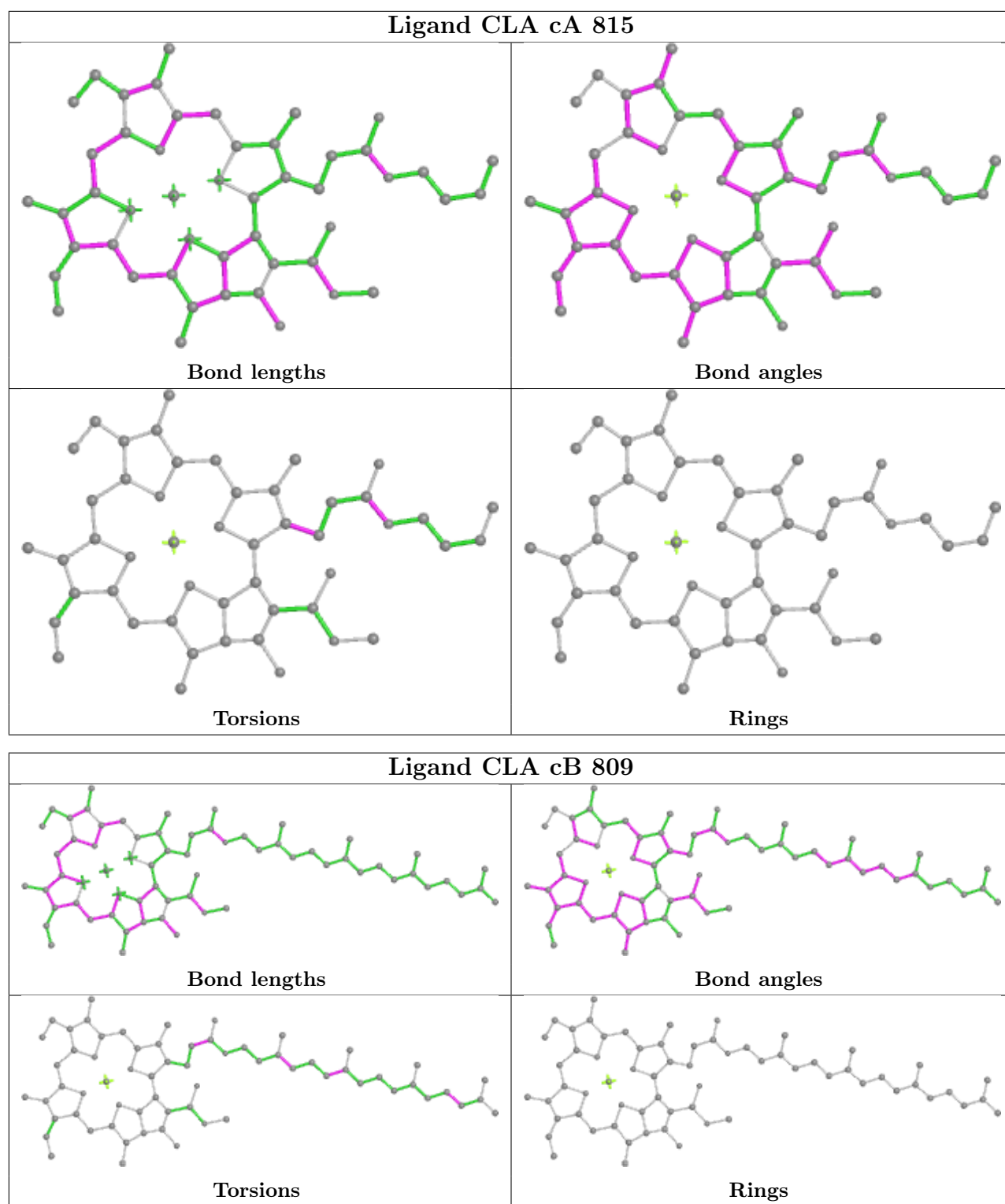


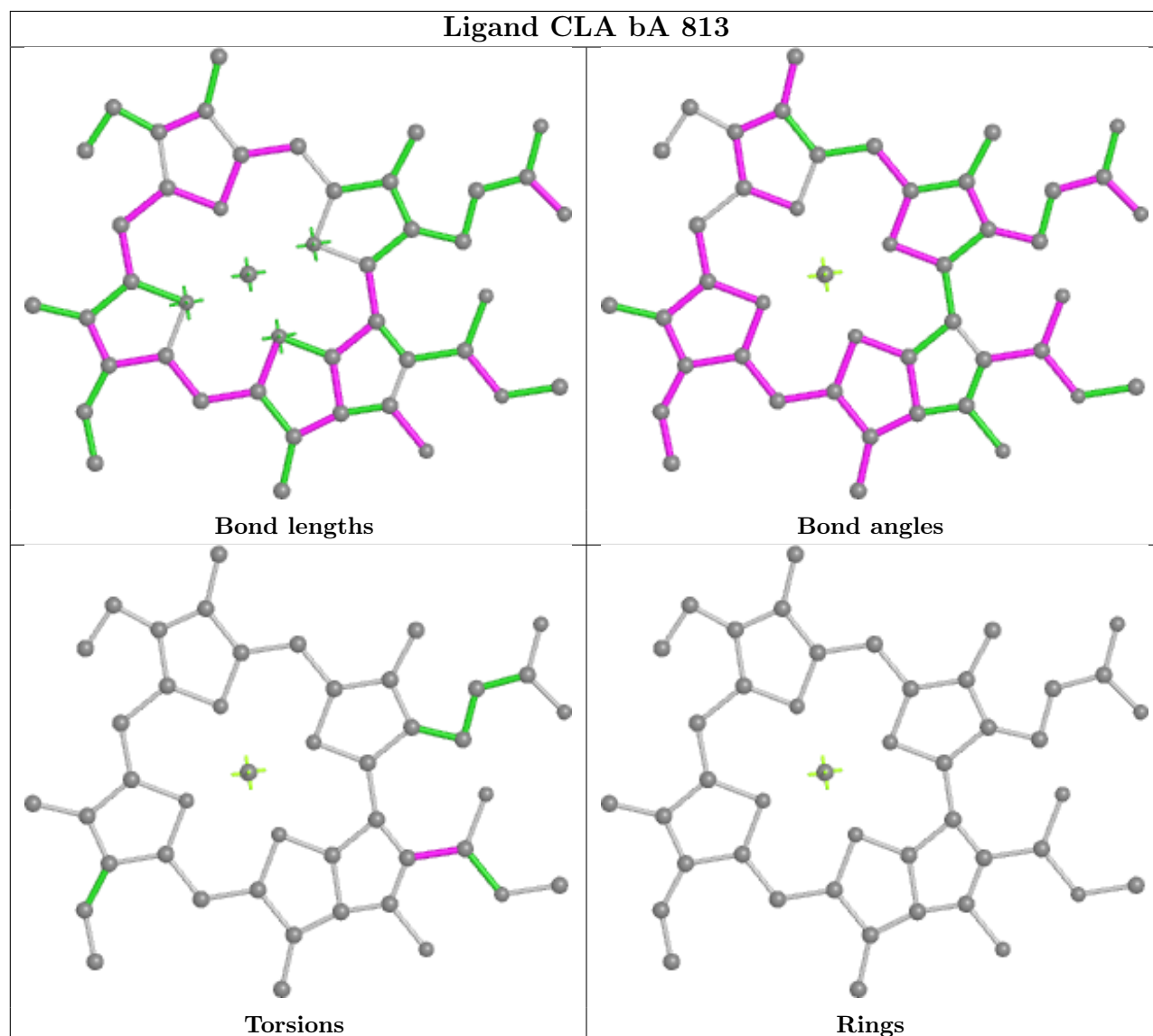
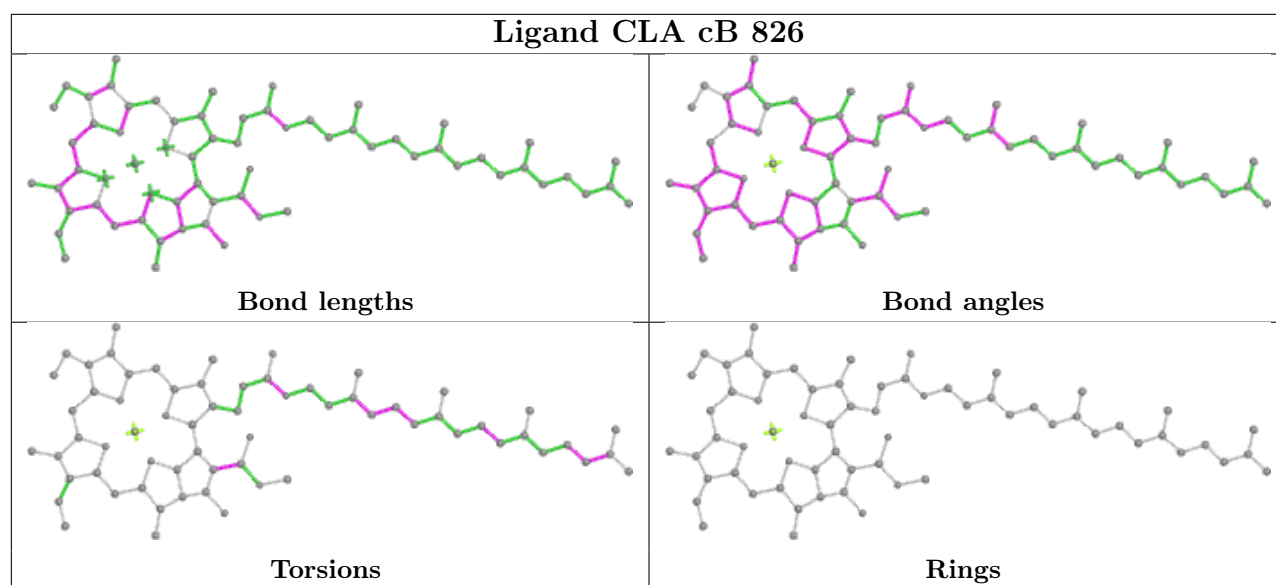
## Ligand CLA cA 830

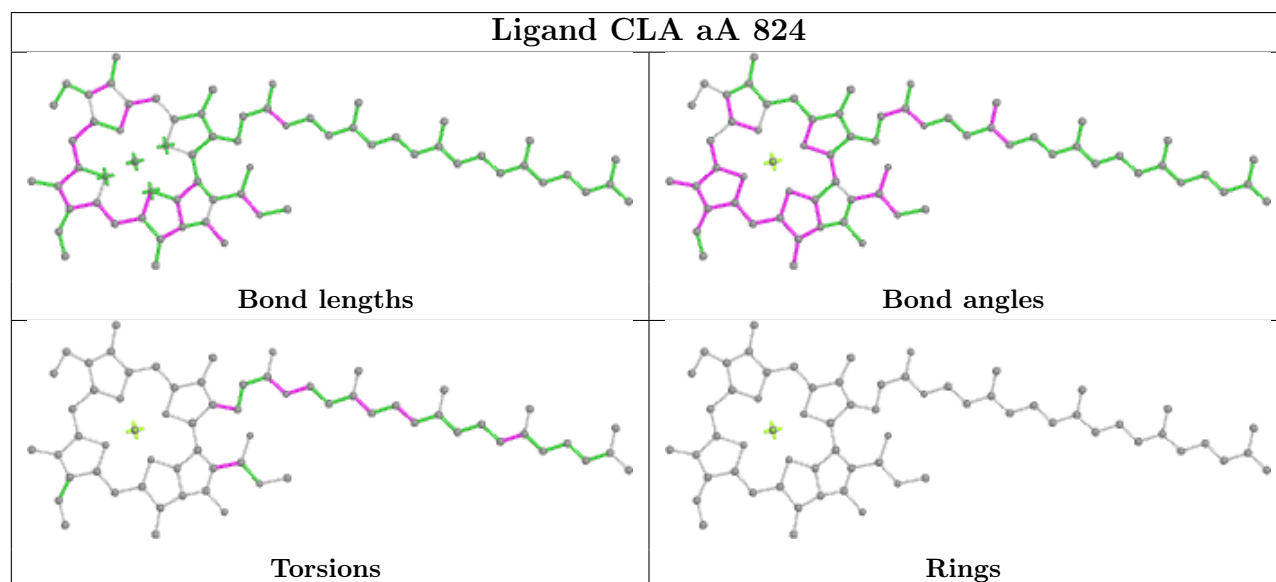
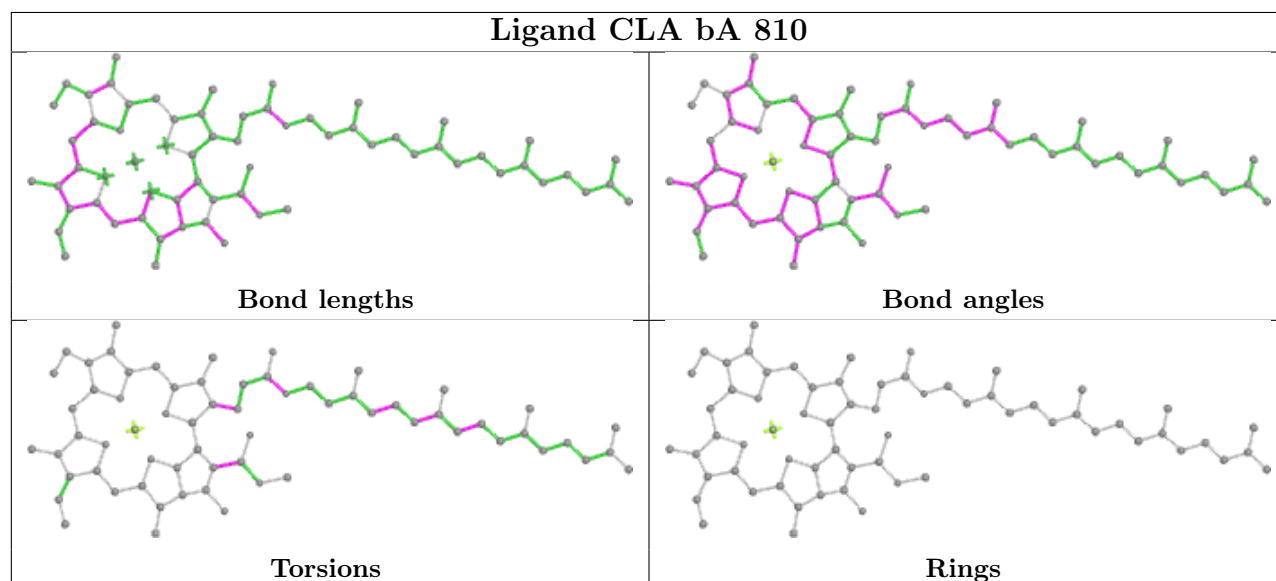
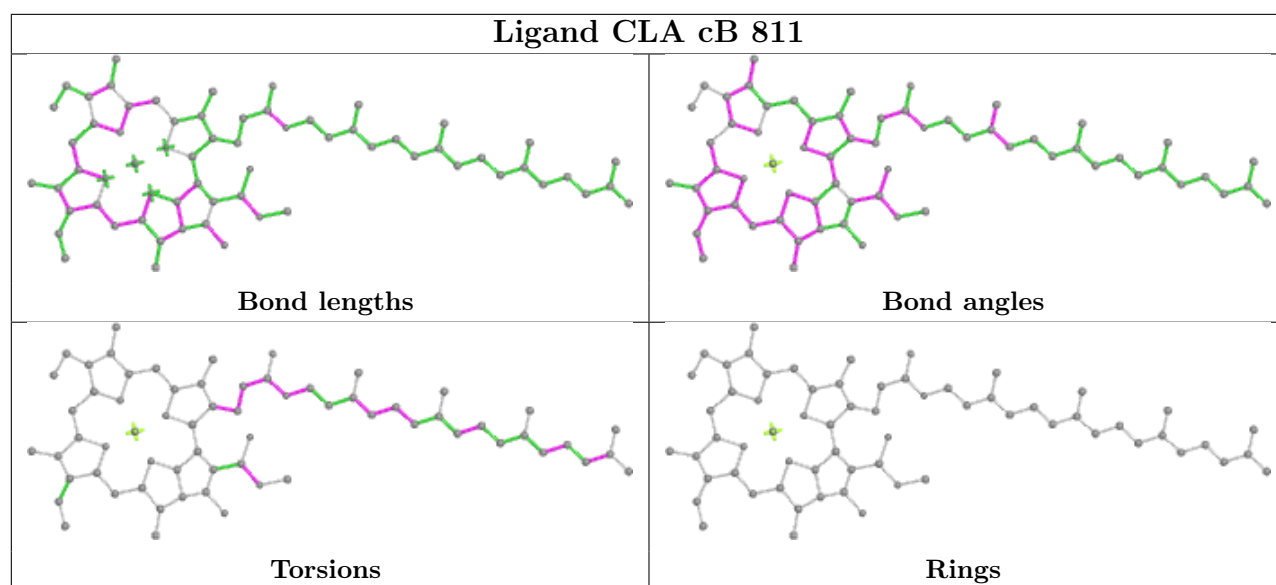


## Ligand CLA cA 825

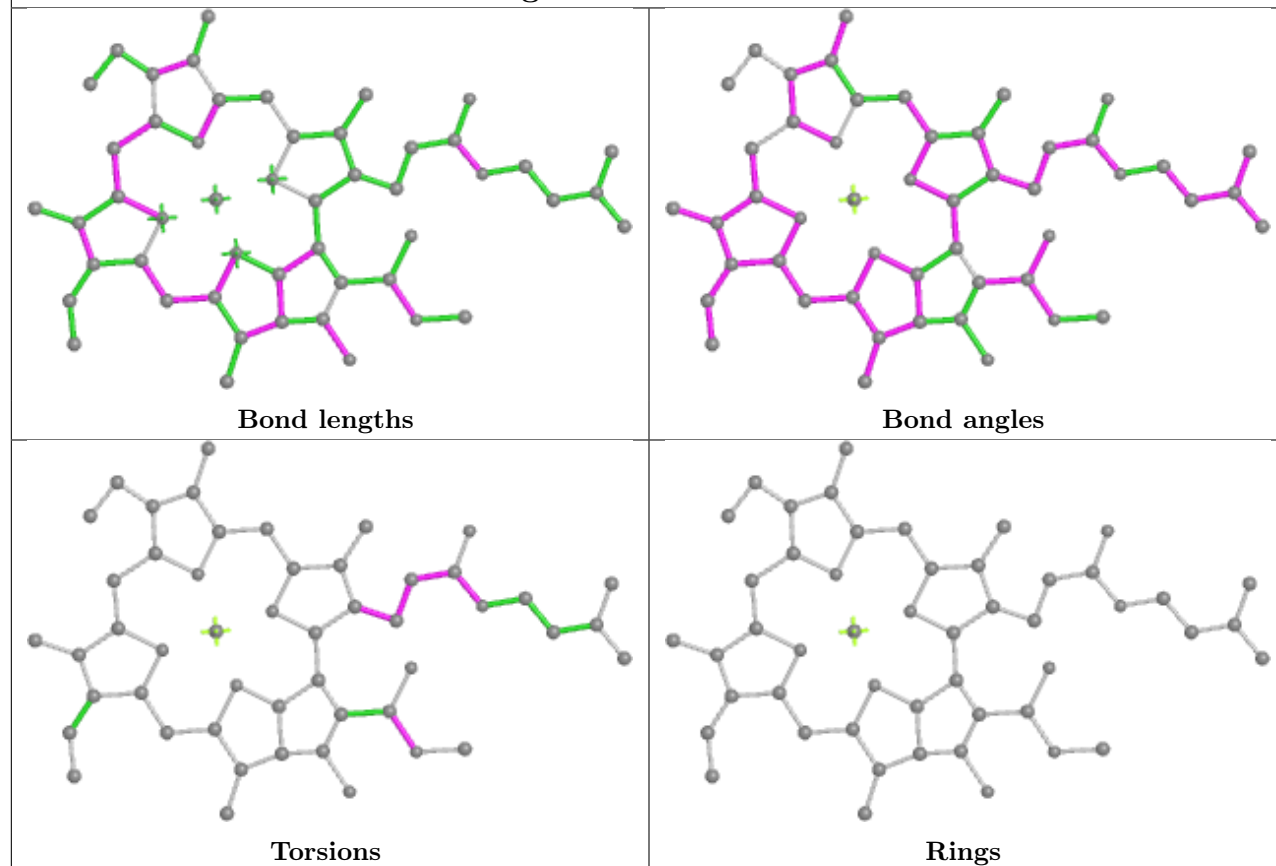




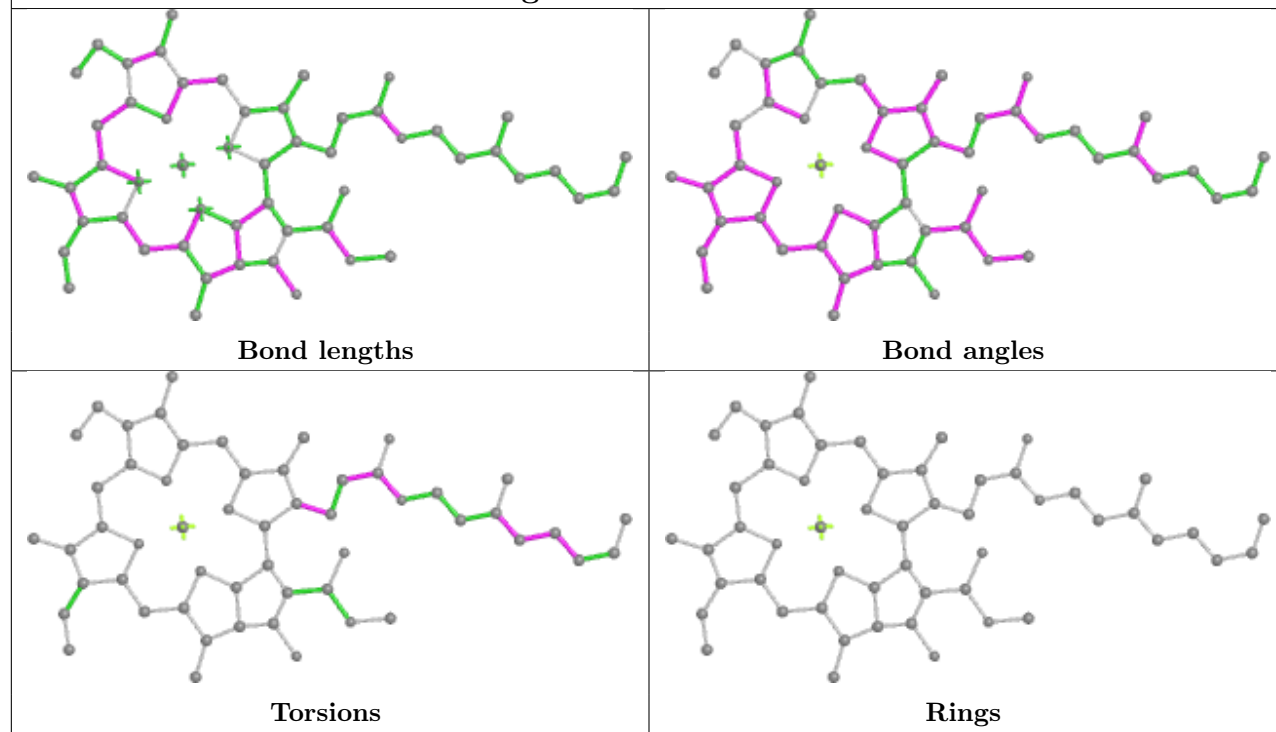


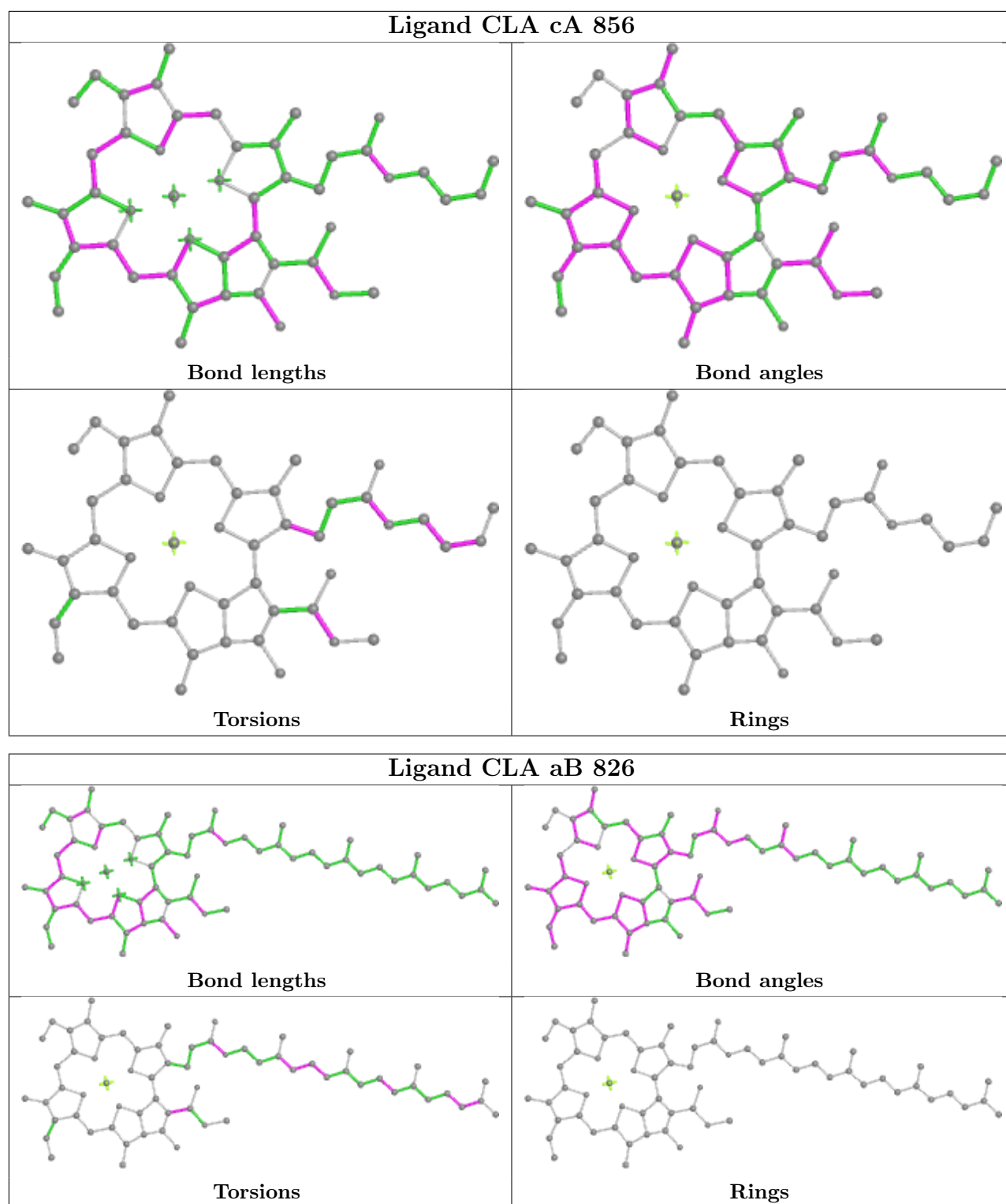


## Ligand CLA bA 838

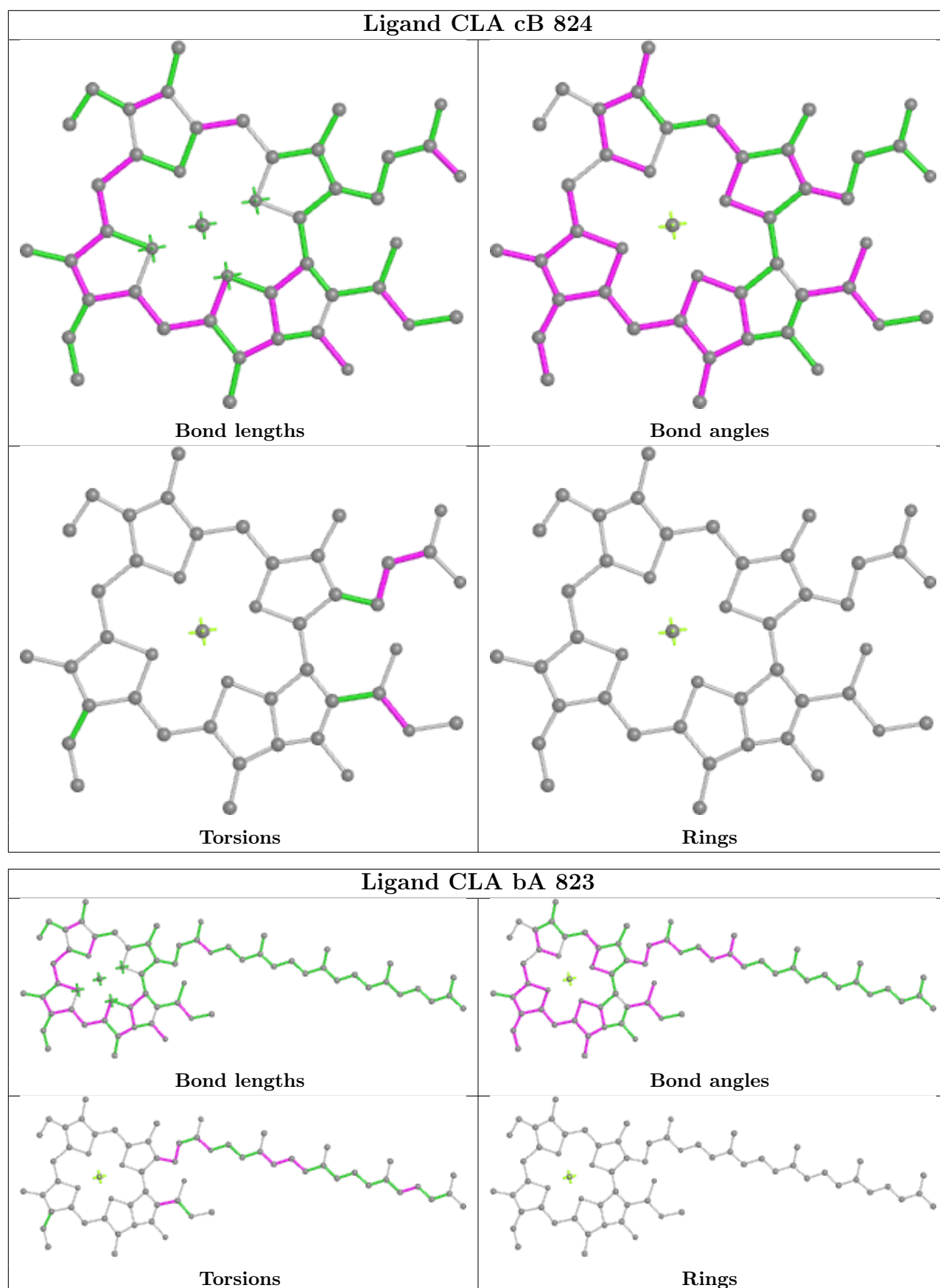


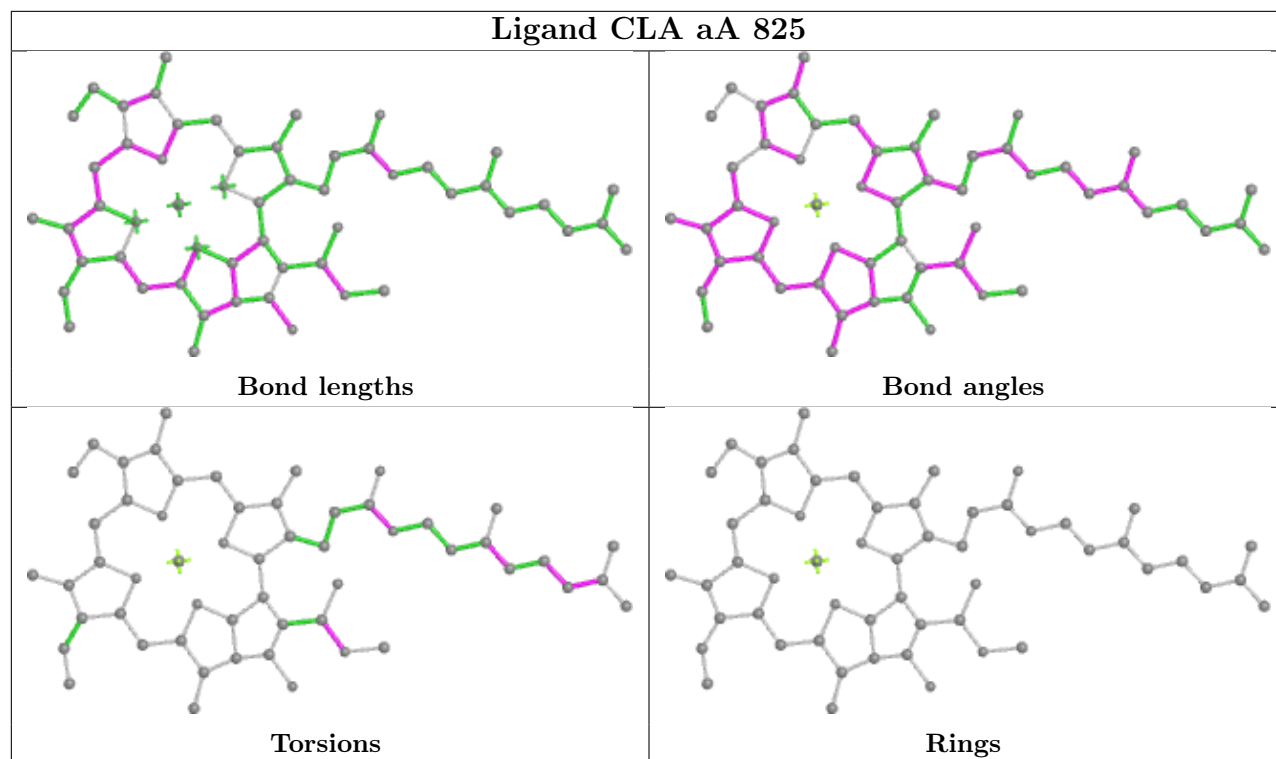
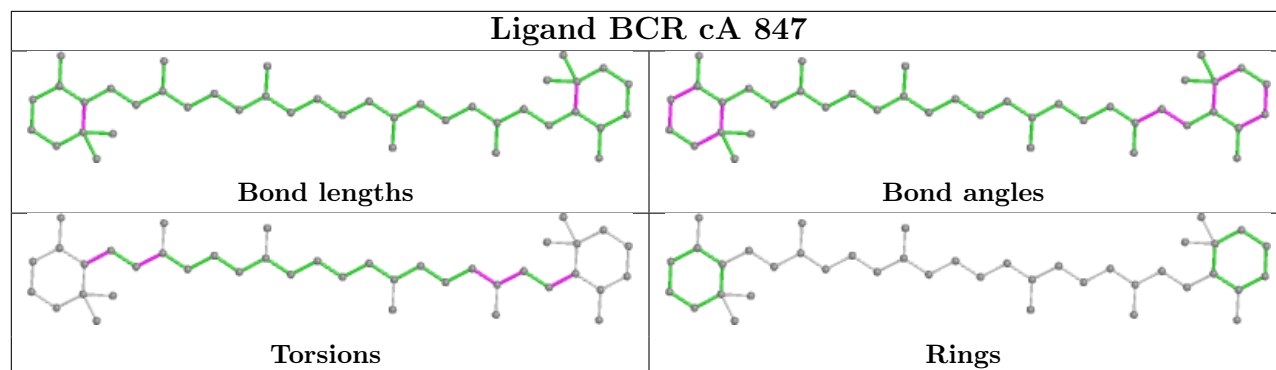
## Ligand CLA bA 834

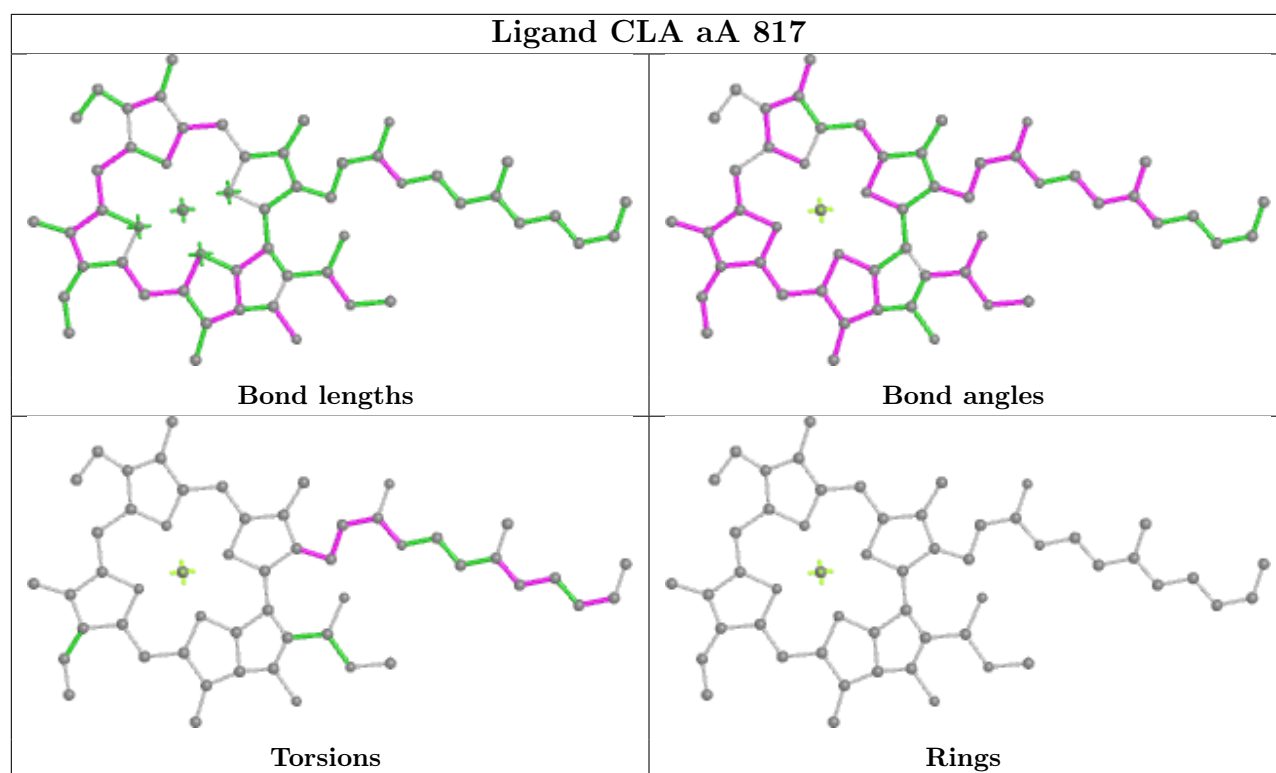


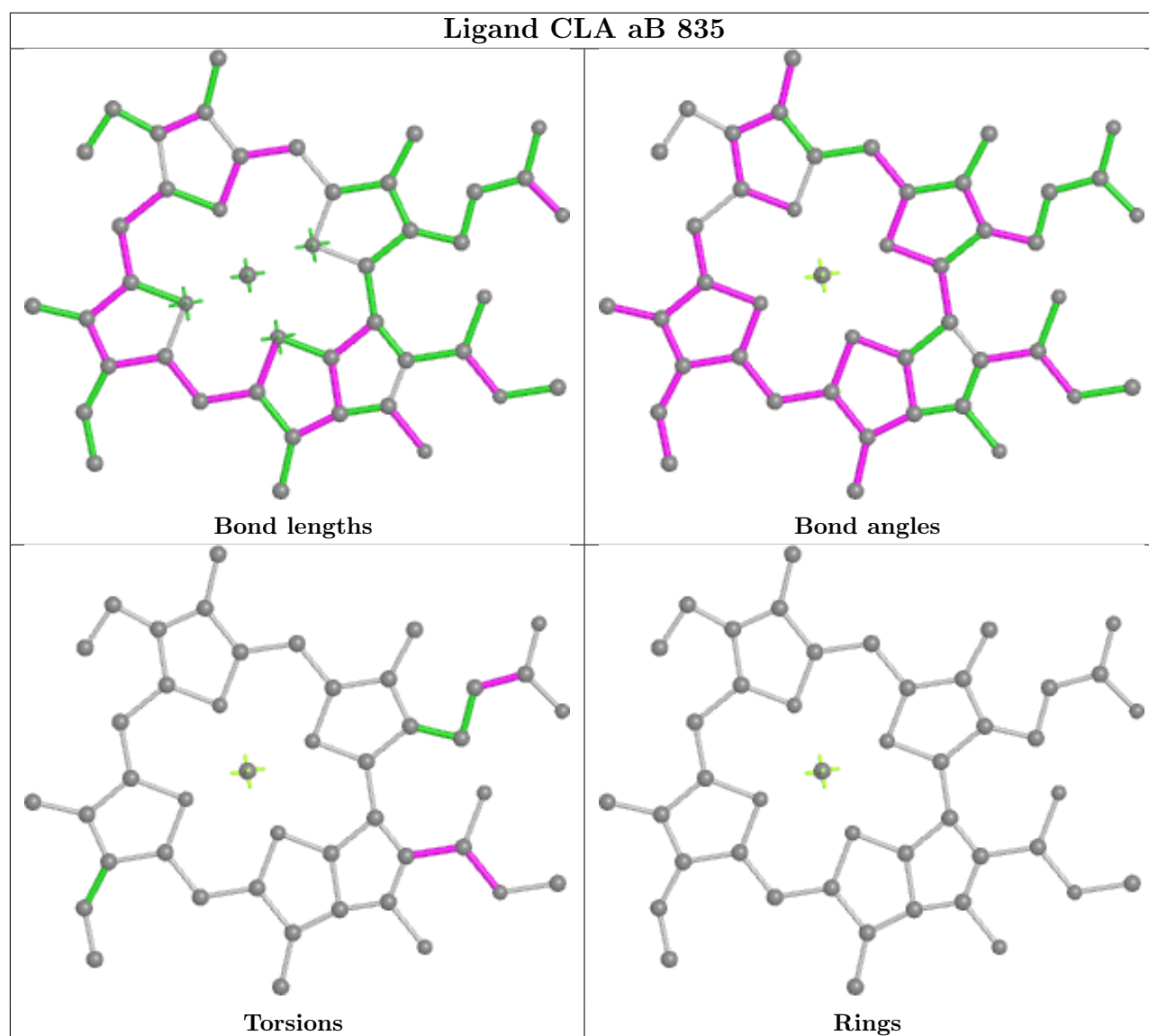


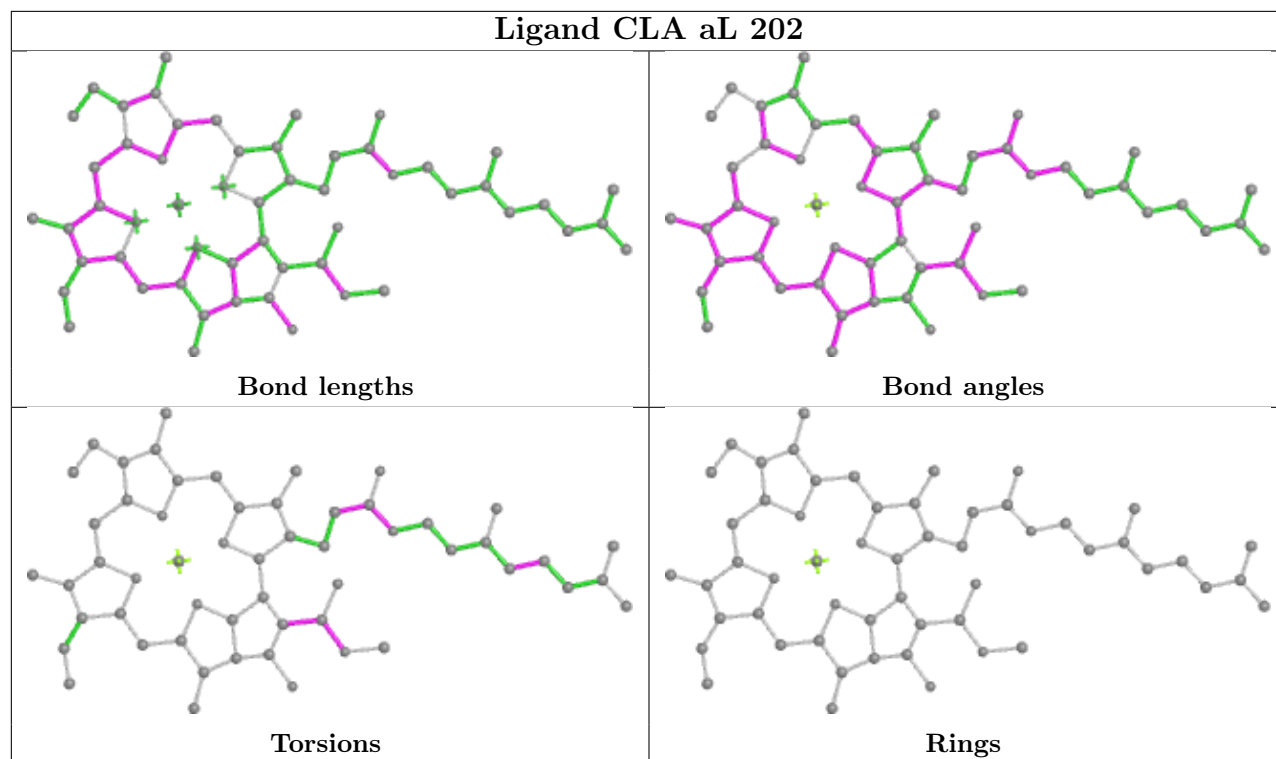


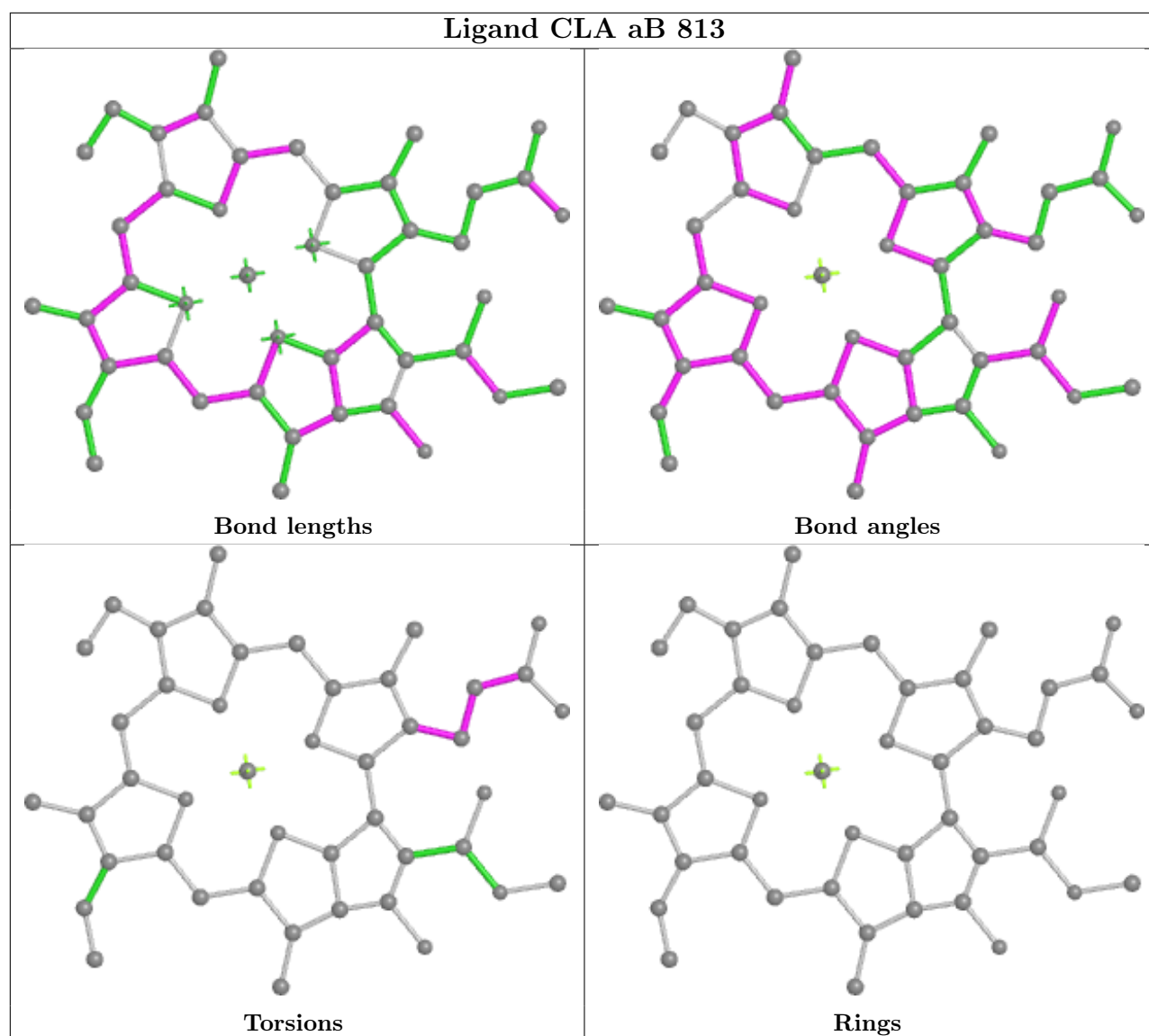


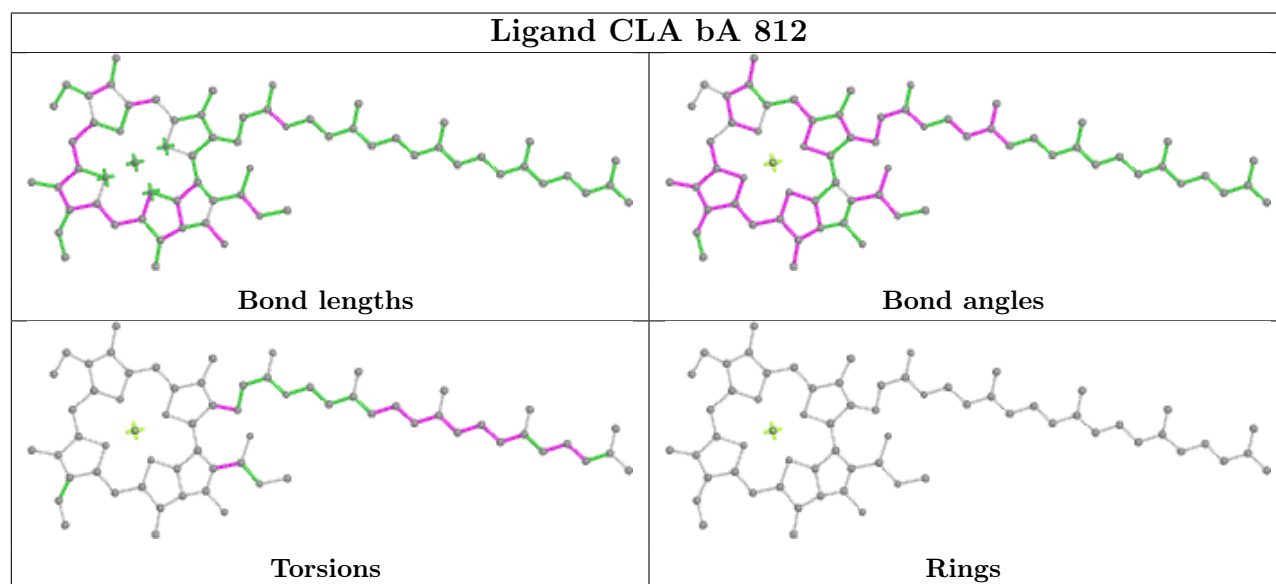
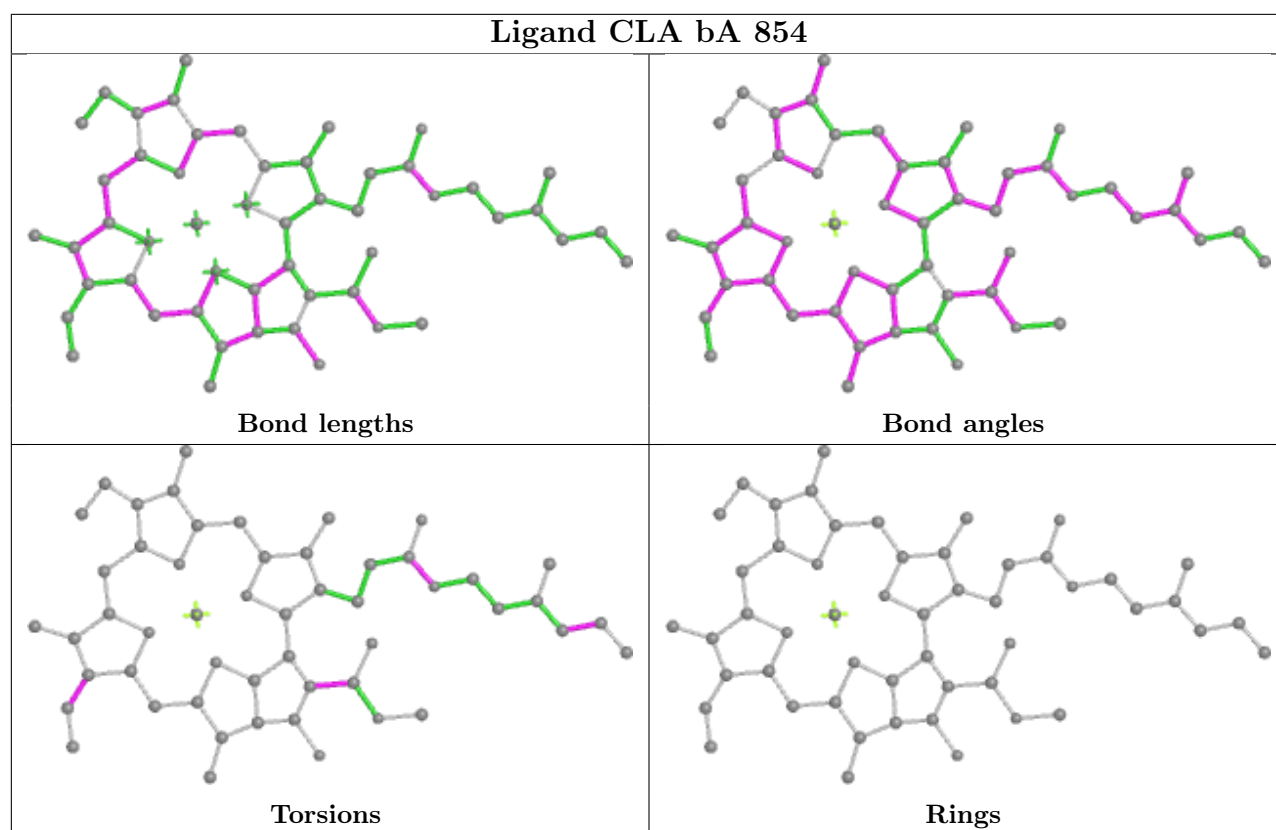




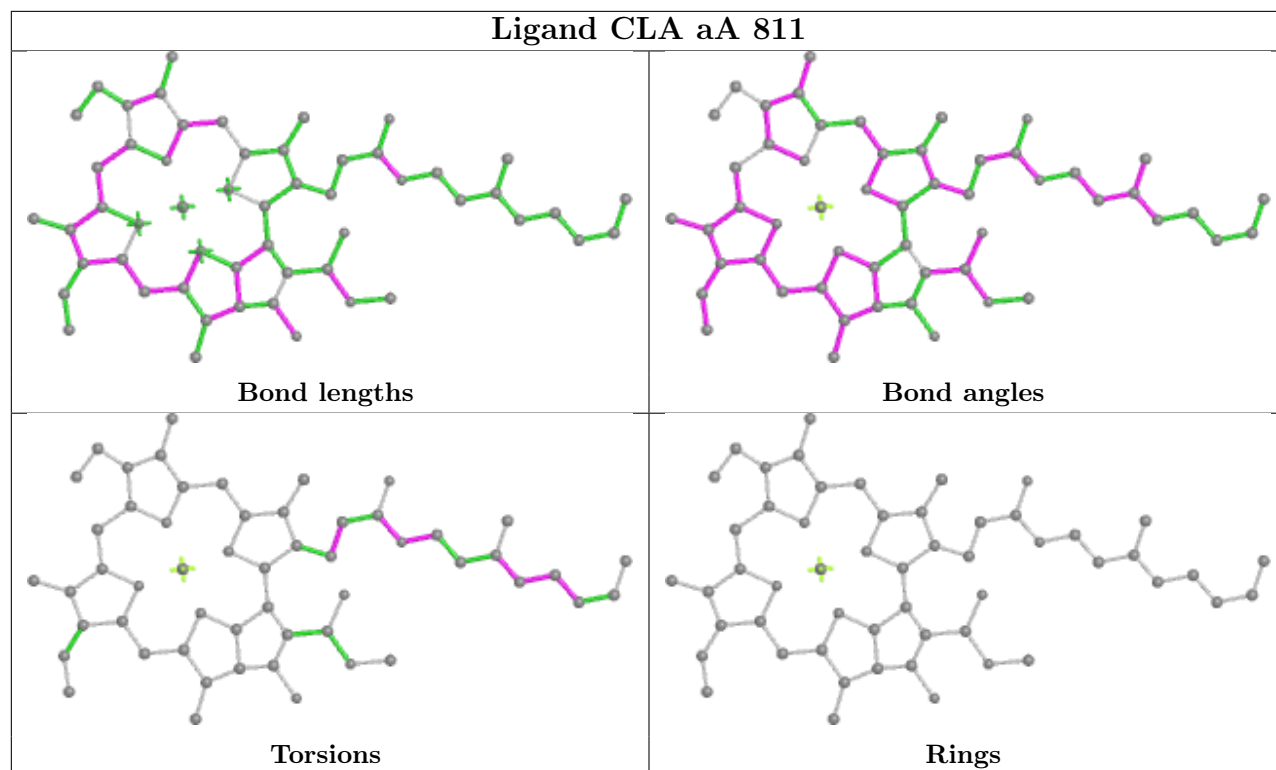




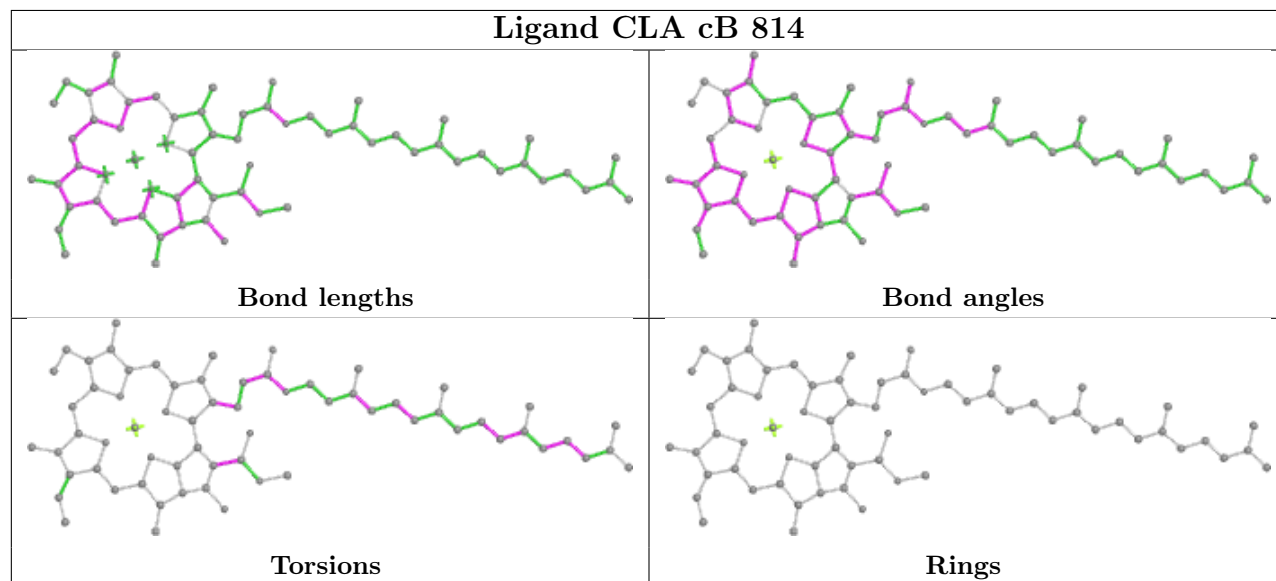




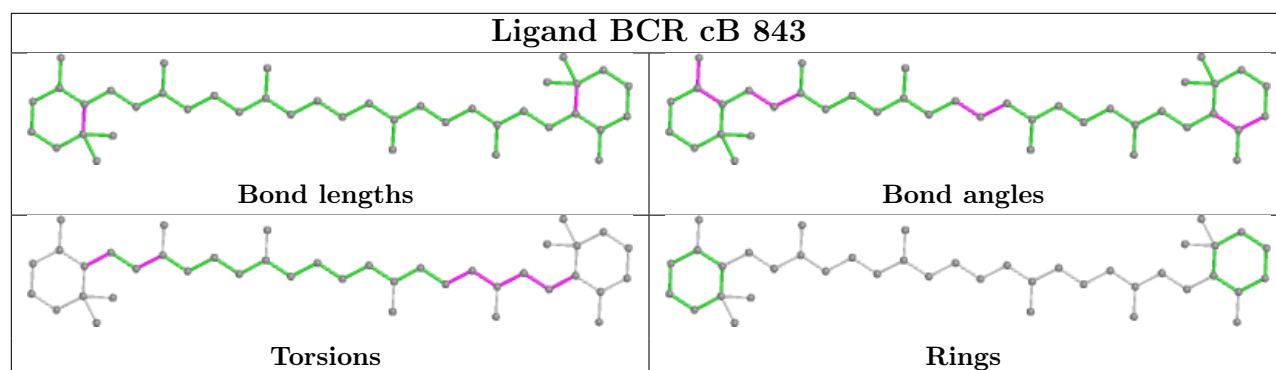
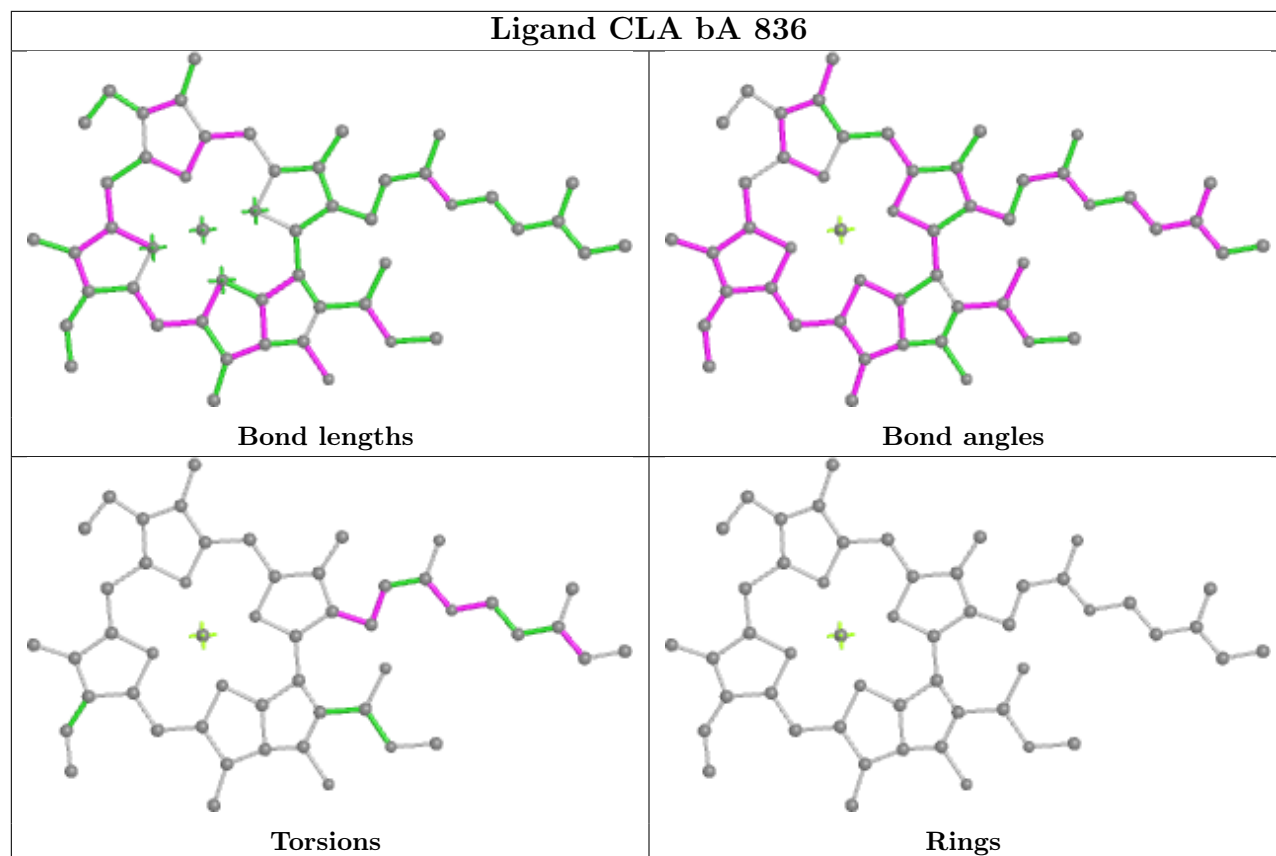
## Ligand CLA aA 811



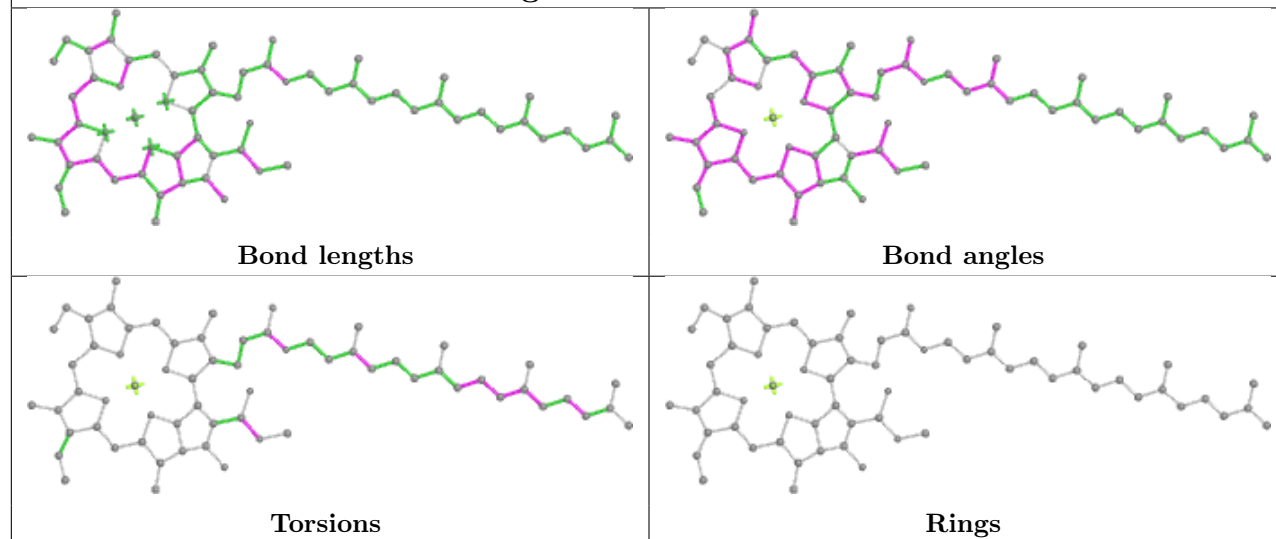
## Ligand CLA cB 814



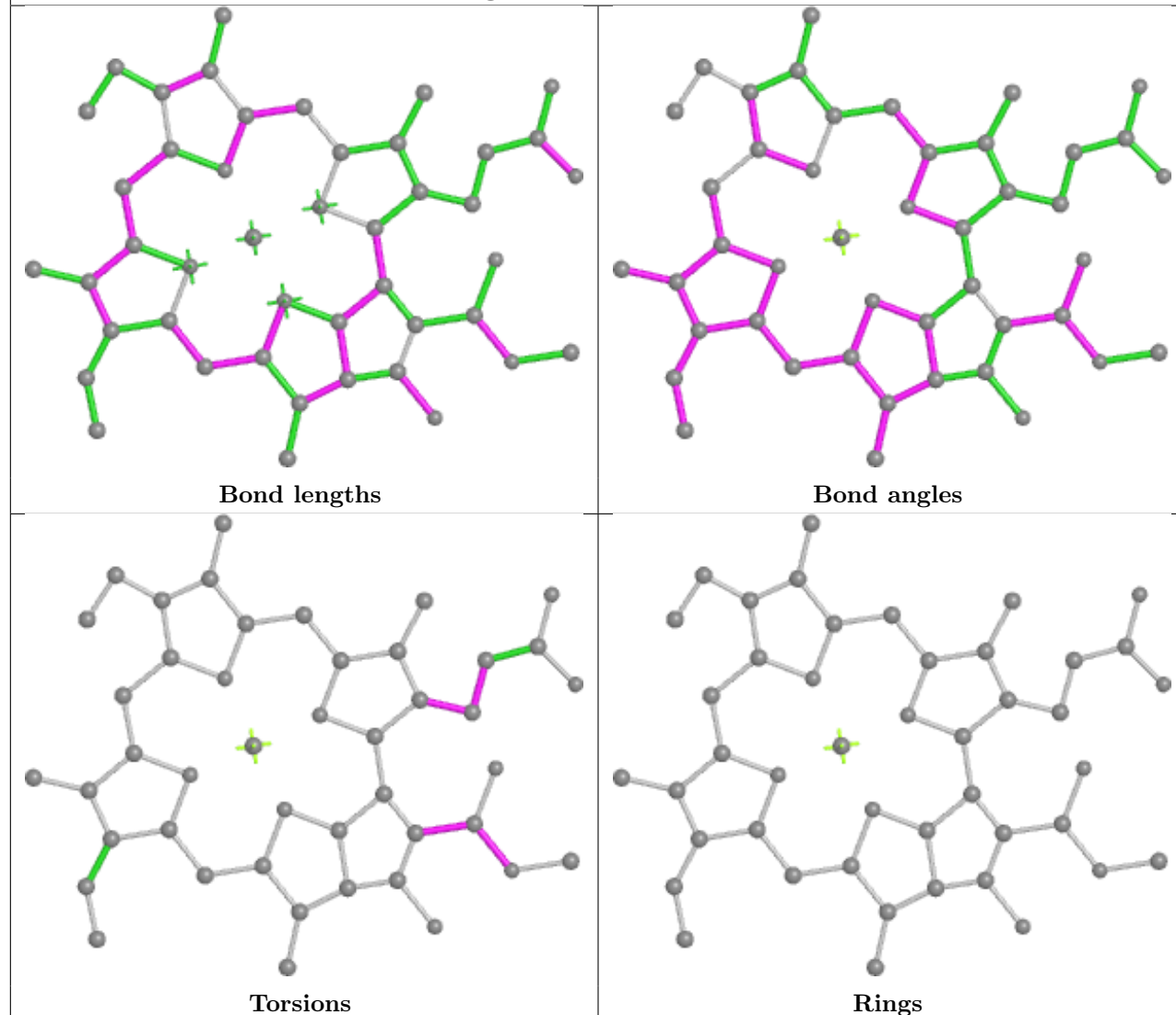


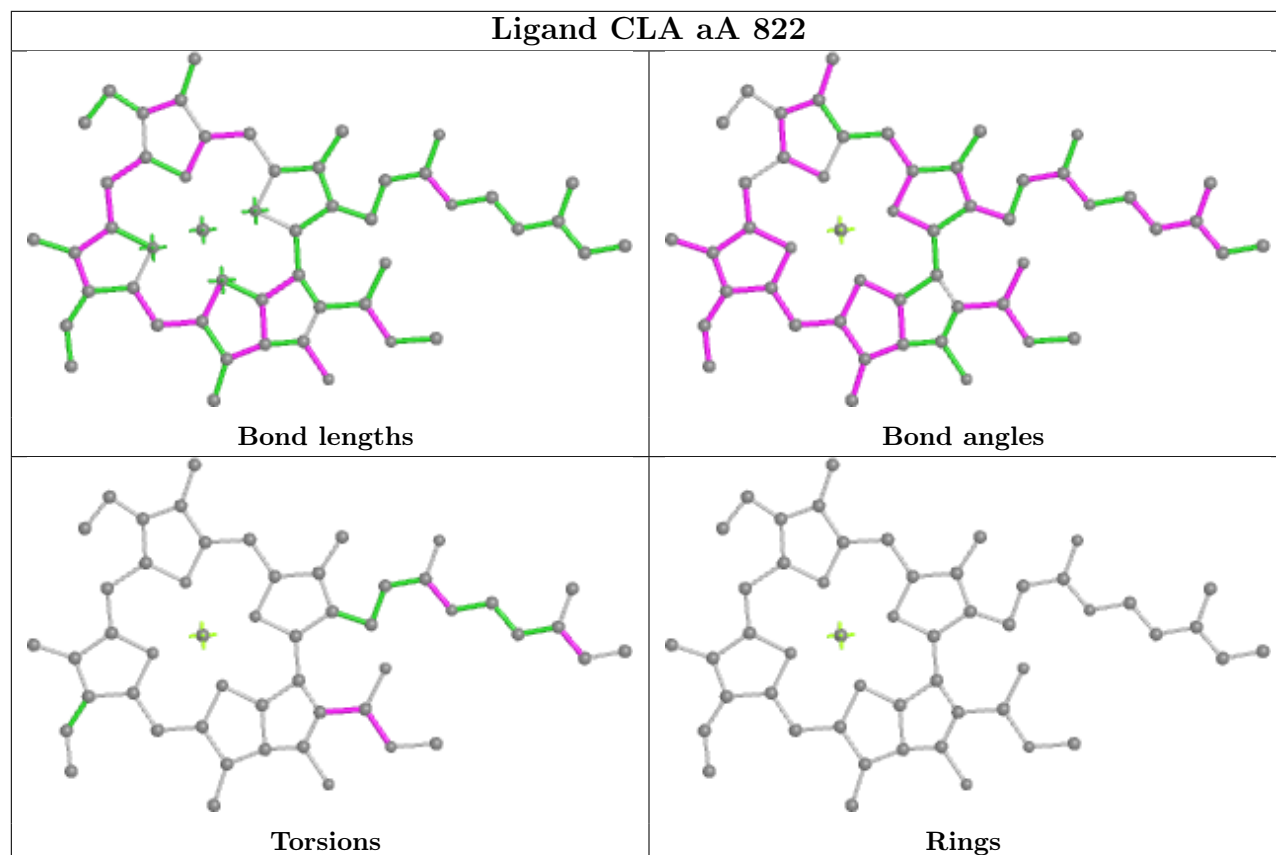
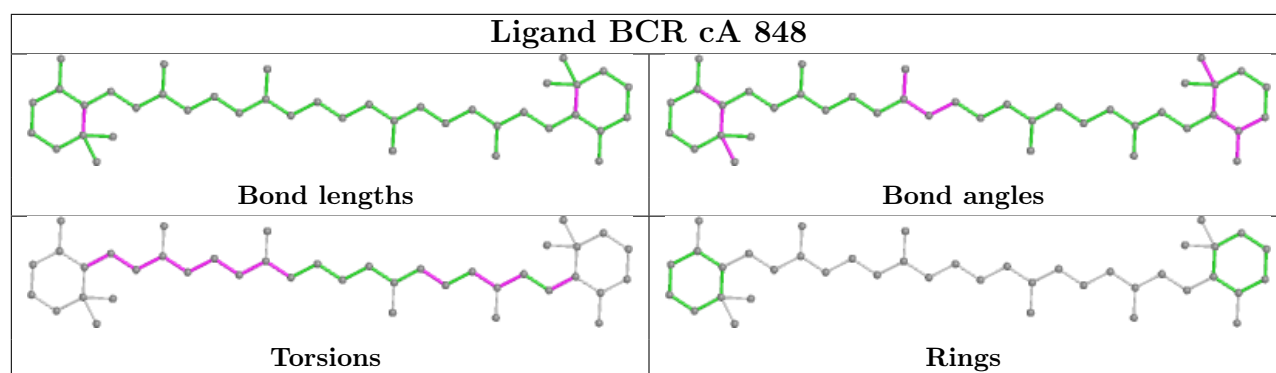


## Ligand CLA bA 820

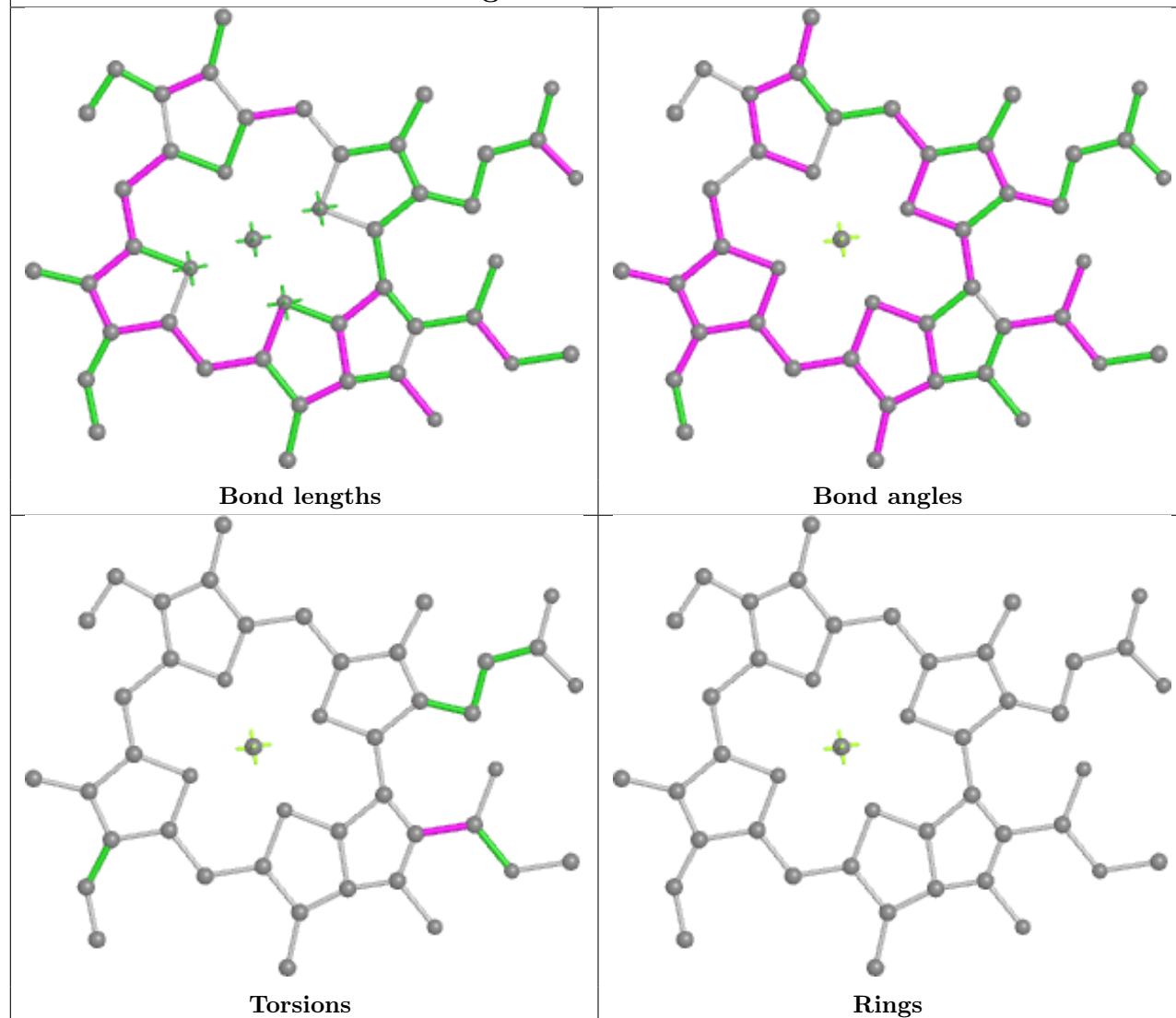


## Ligand CLA aB 822

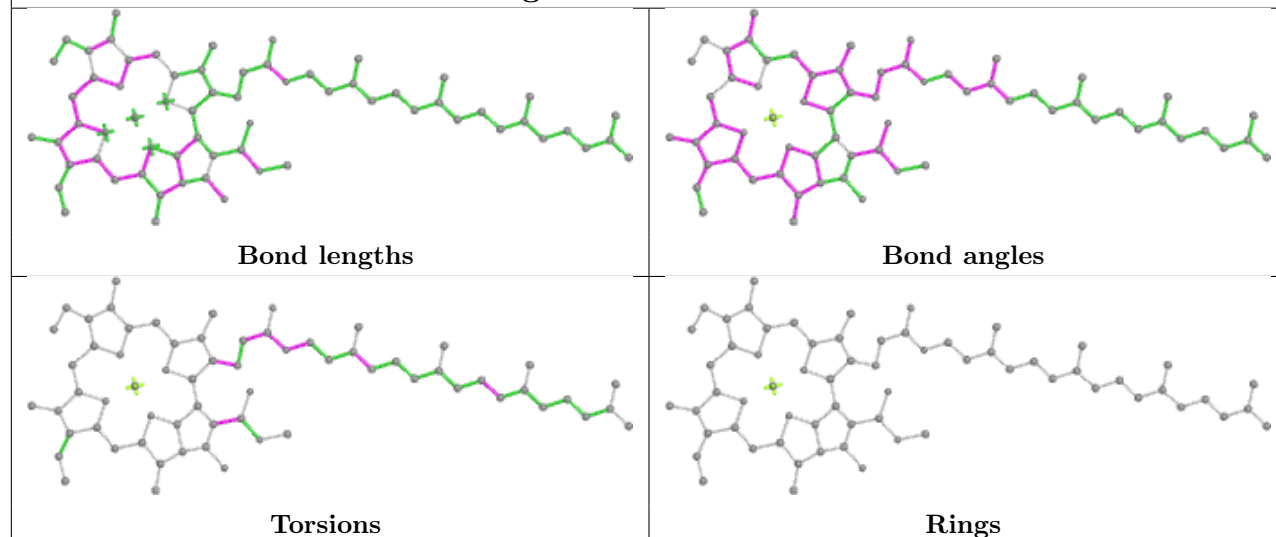


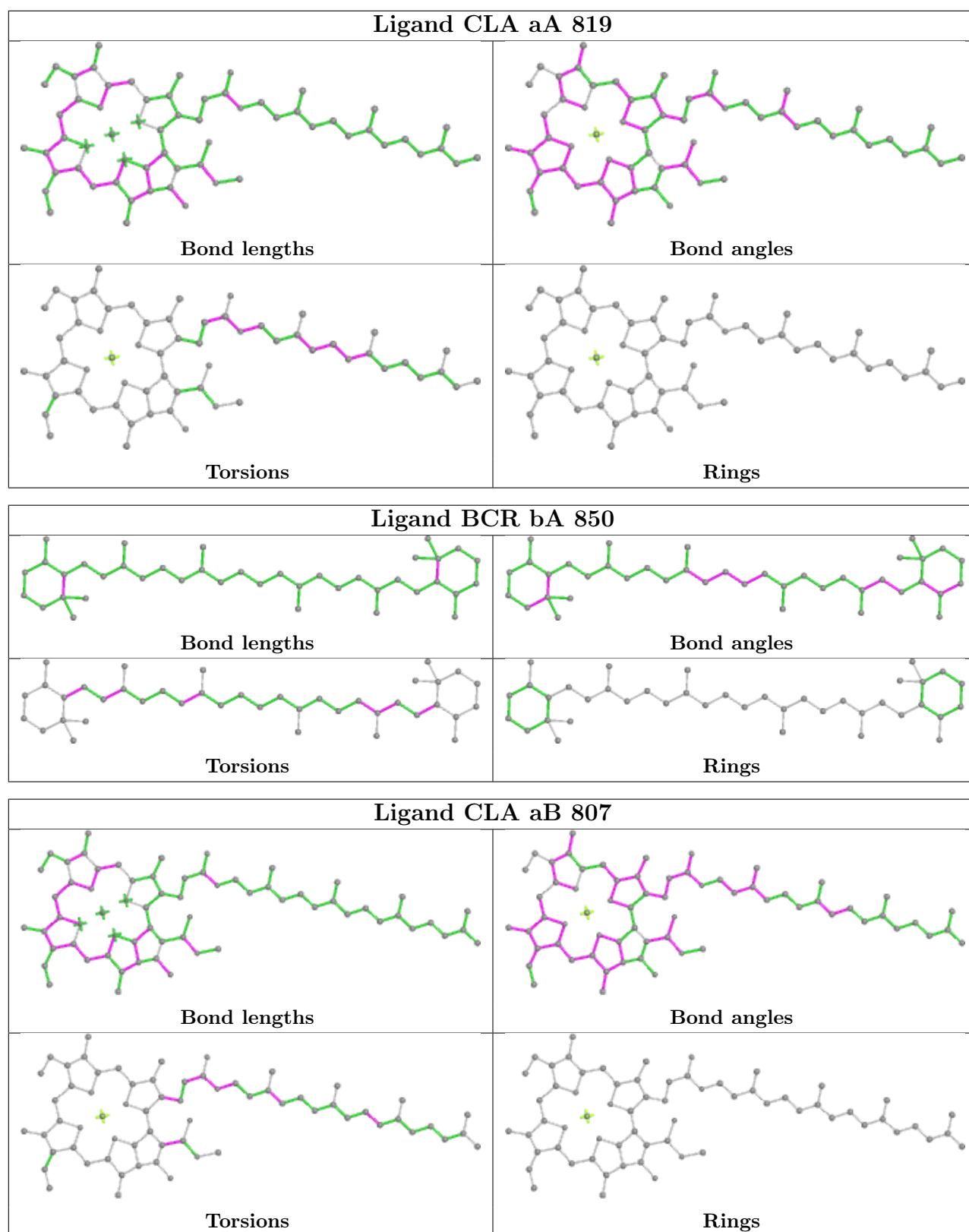


## Ligand CLA aB 816

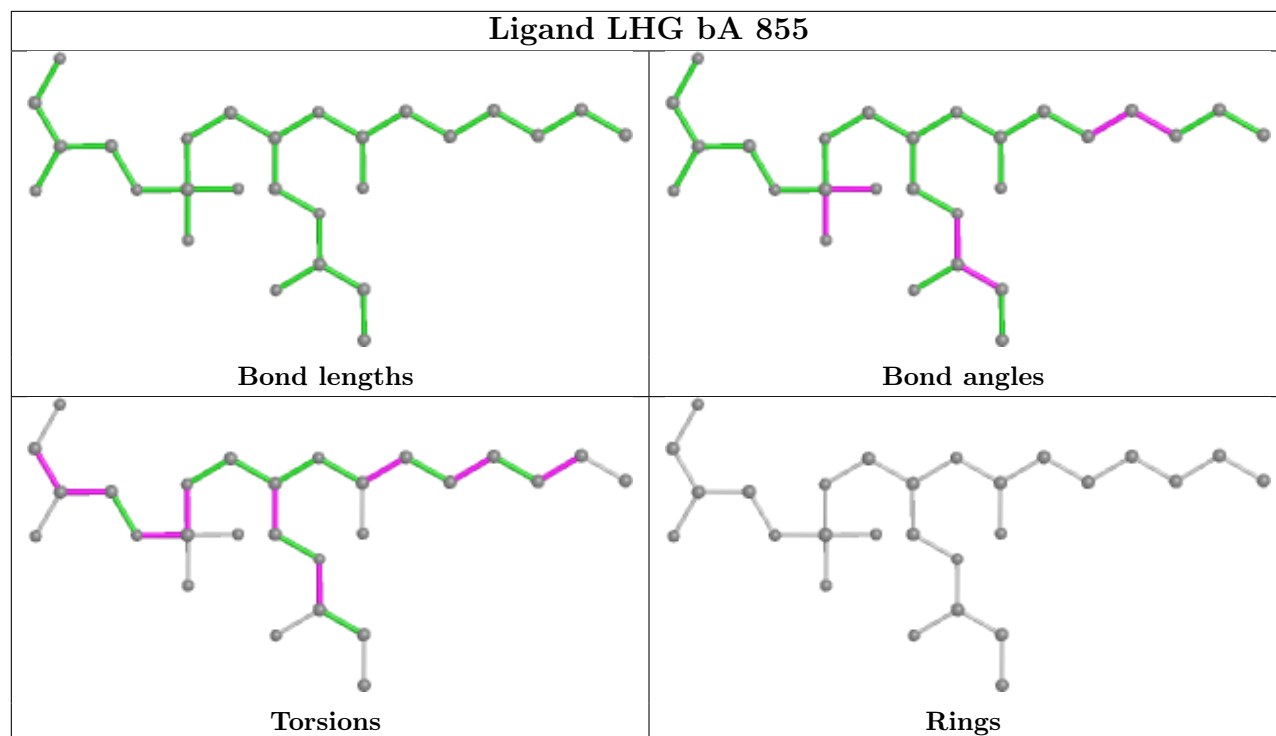


## Ligand CLA bB 807

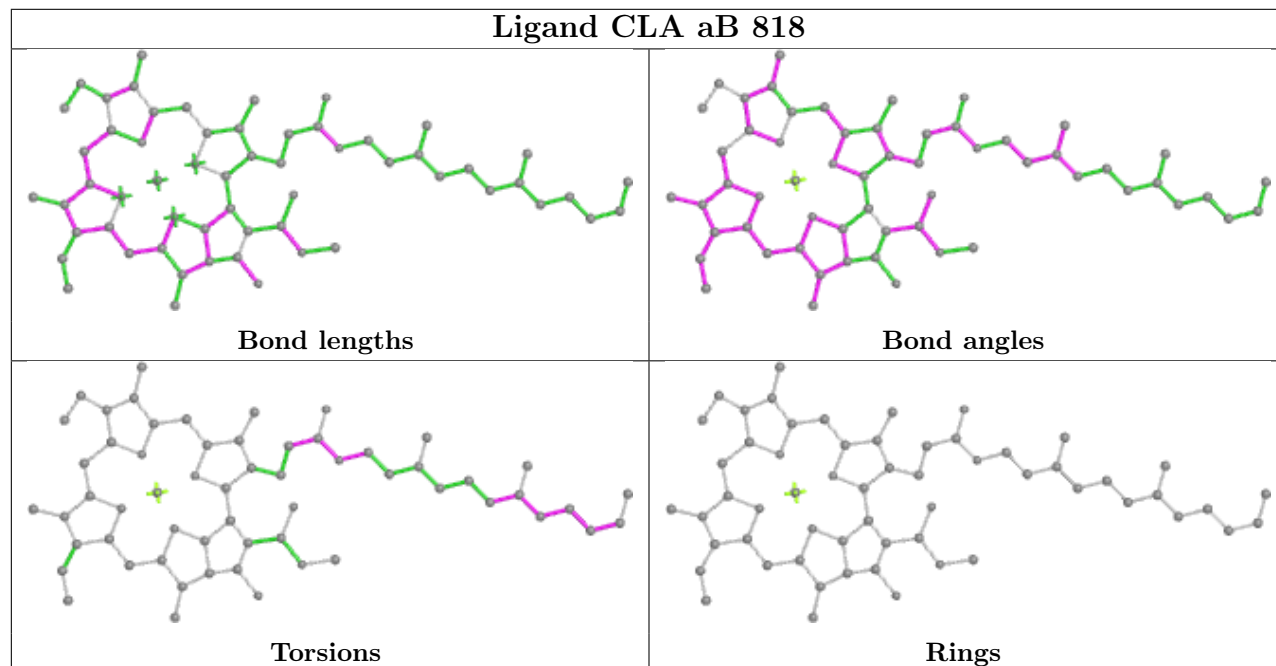


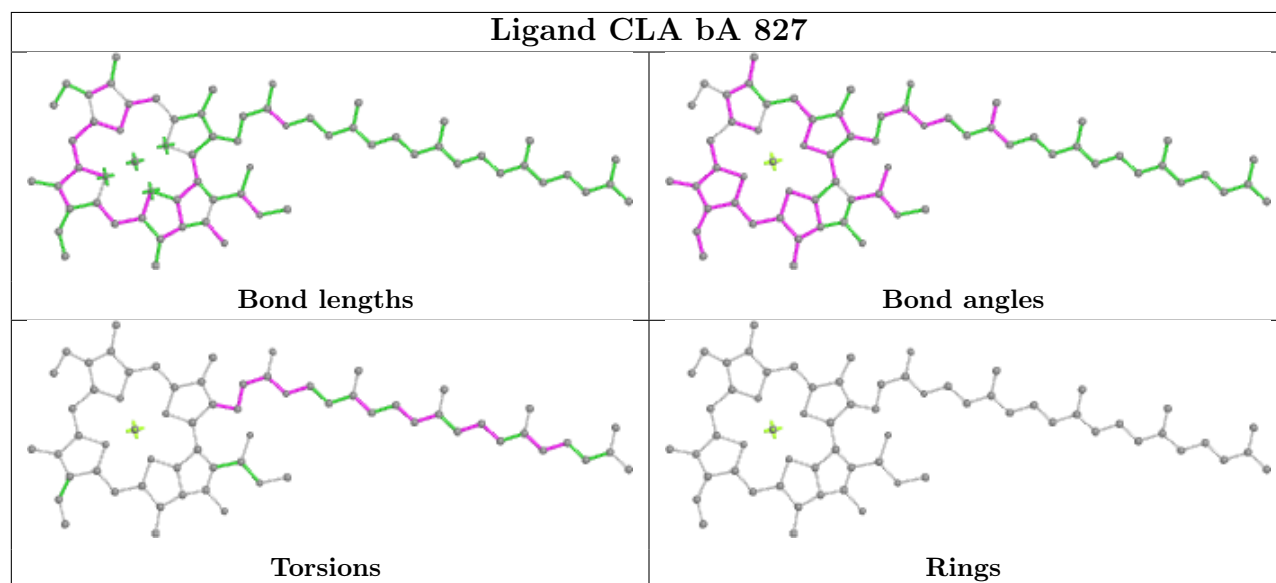
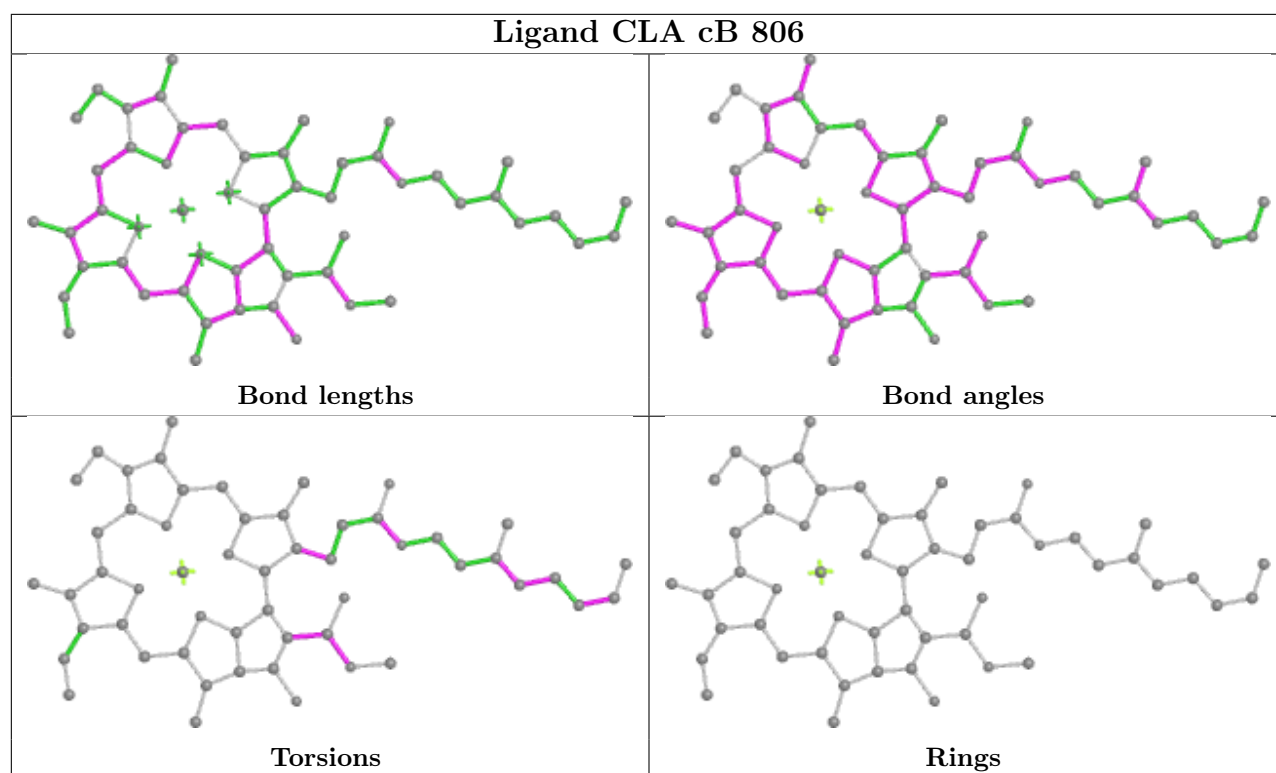


## Ligand LHG bA 855

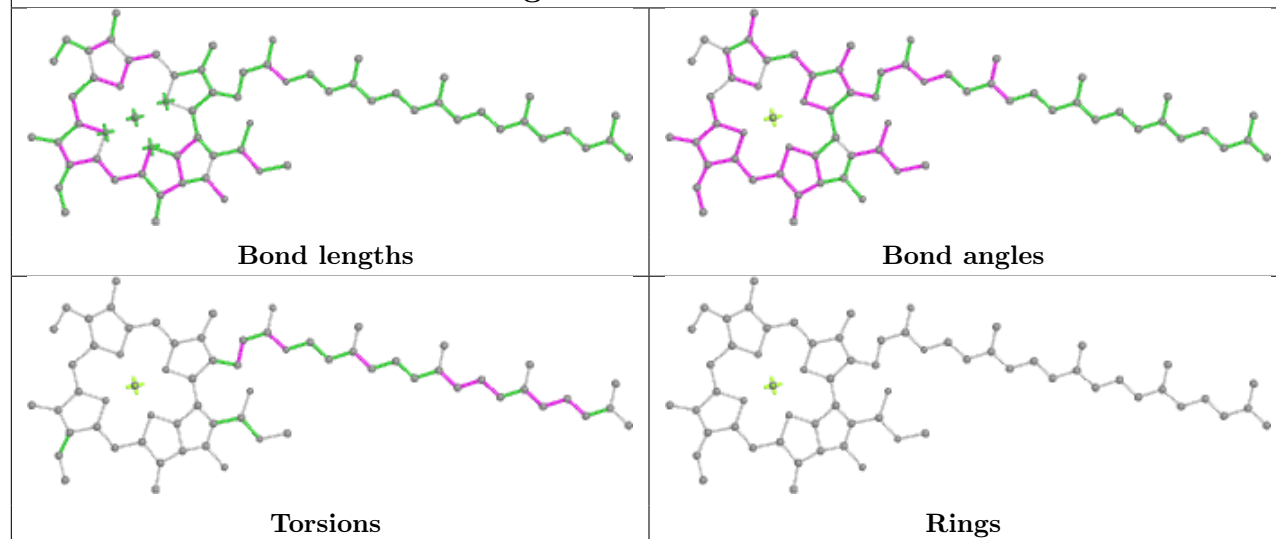


## Ligand CLA aB 818

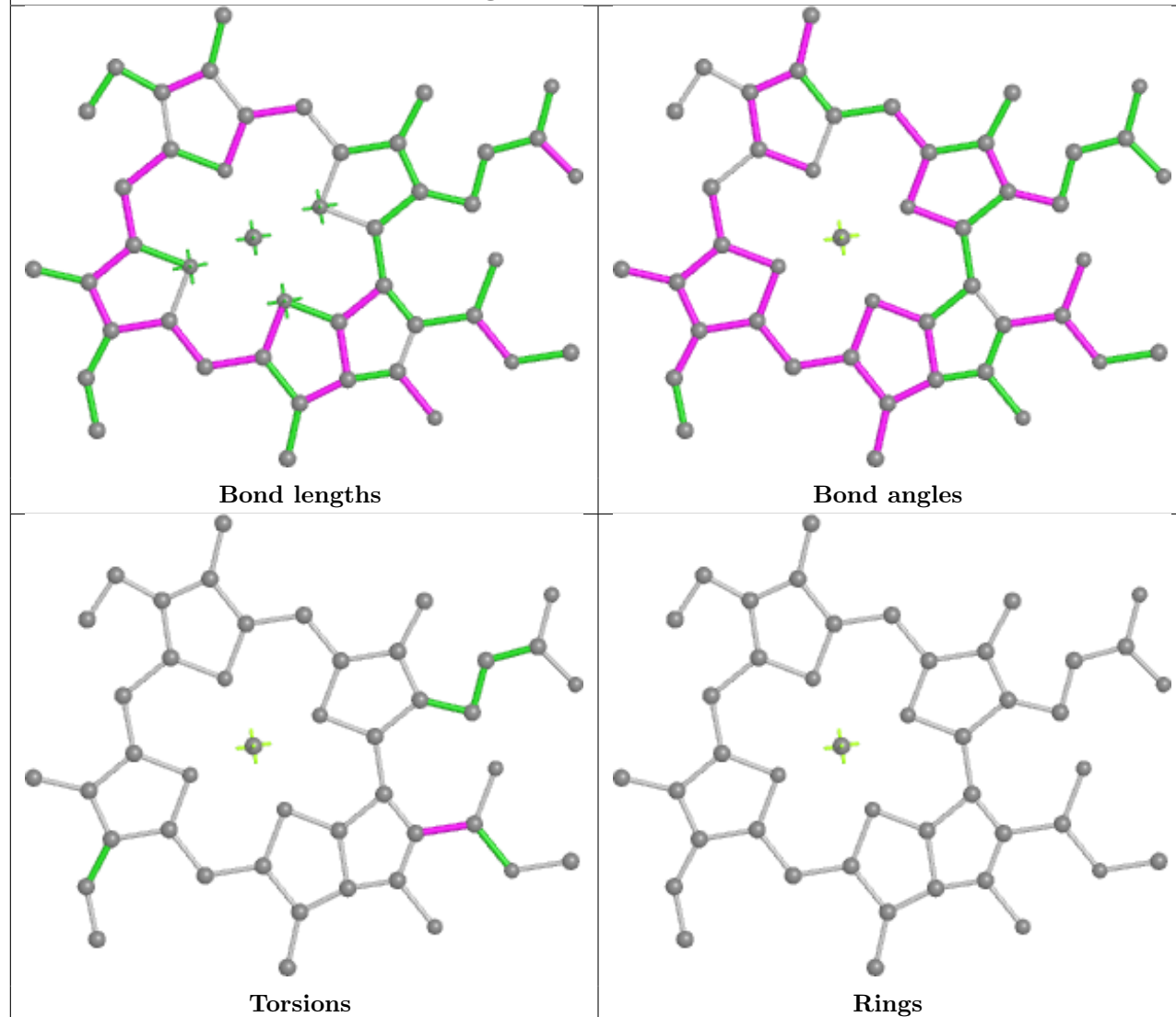




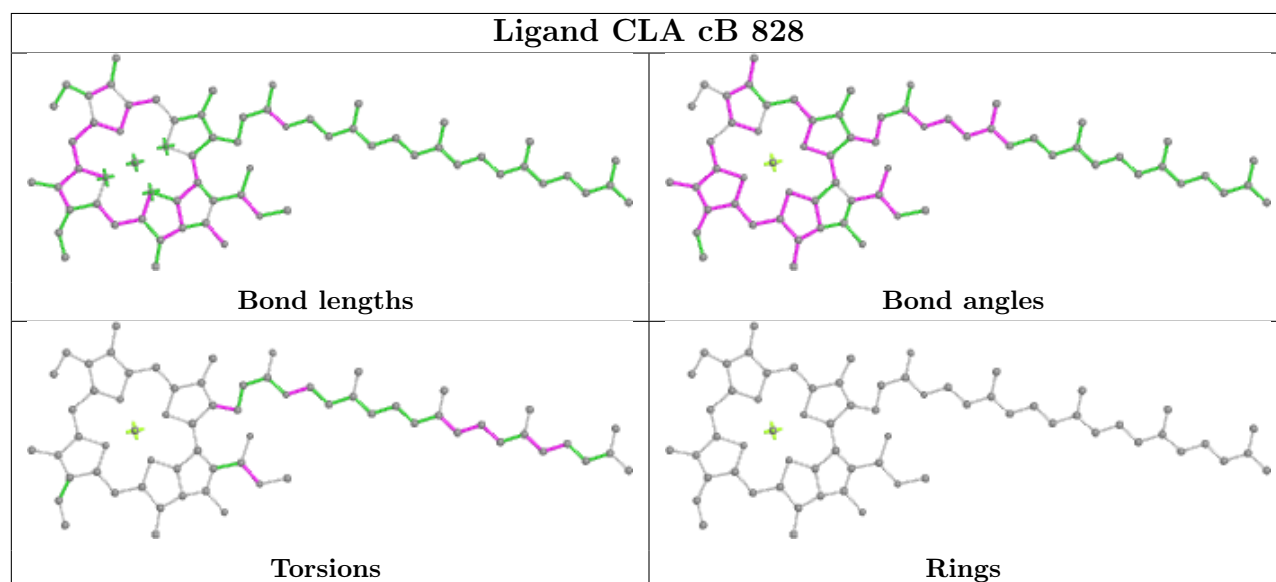
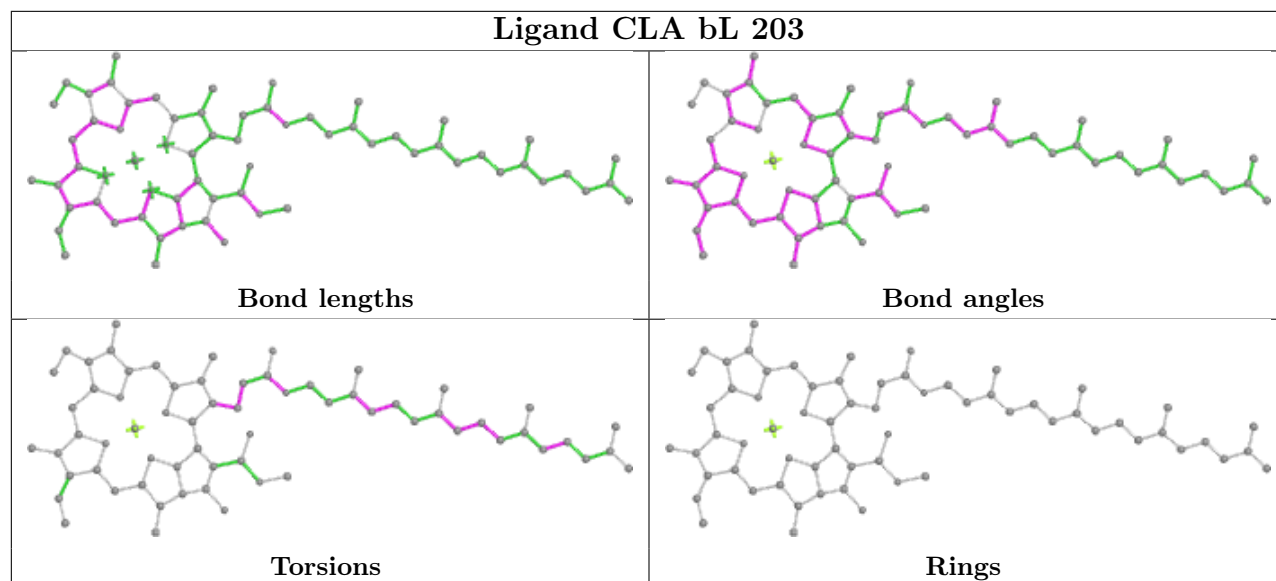
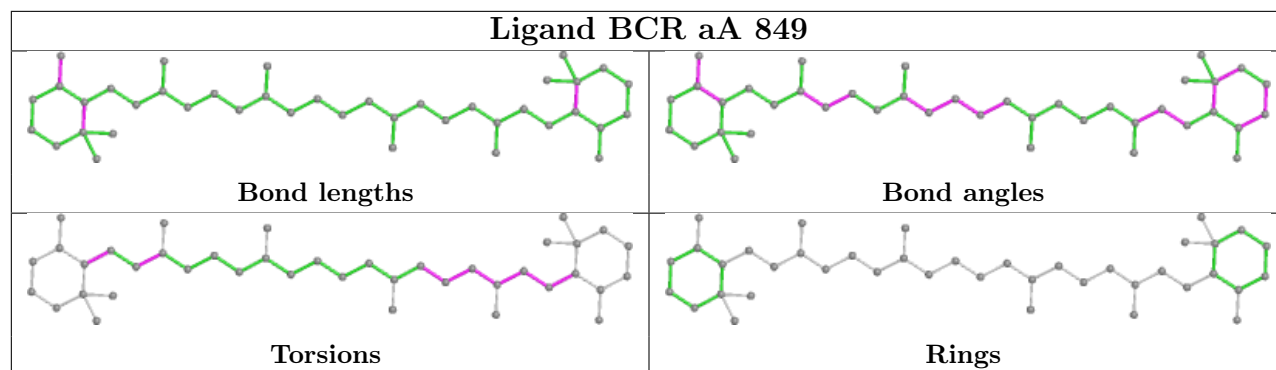
## Ligand CLA cA 842



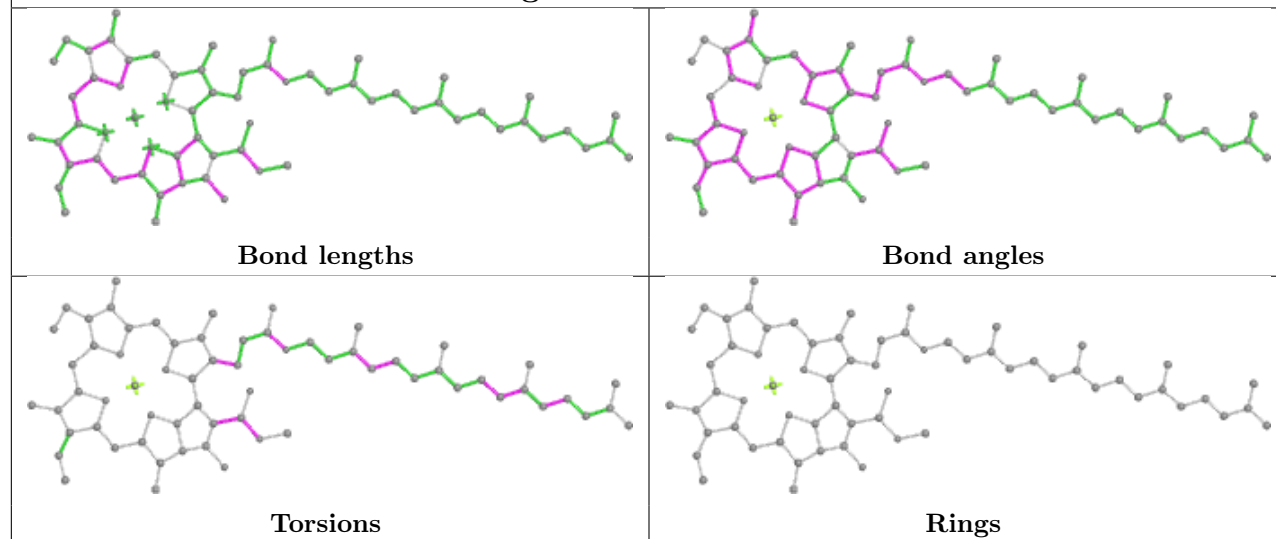
## Ligand CLA cA 809



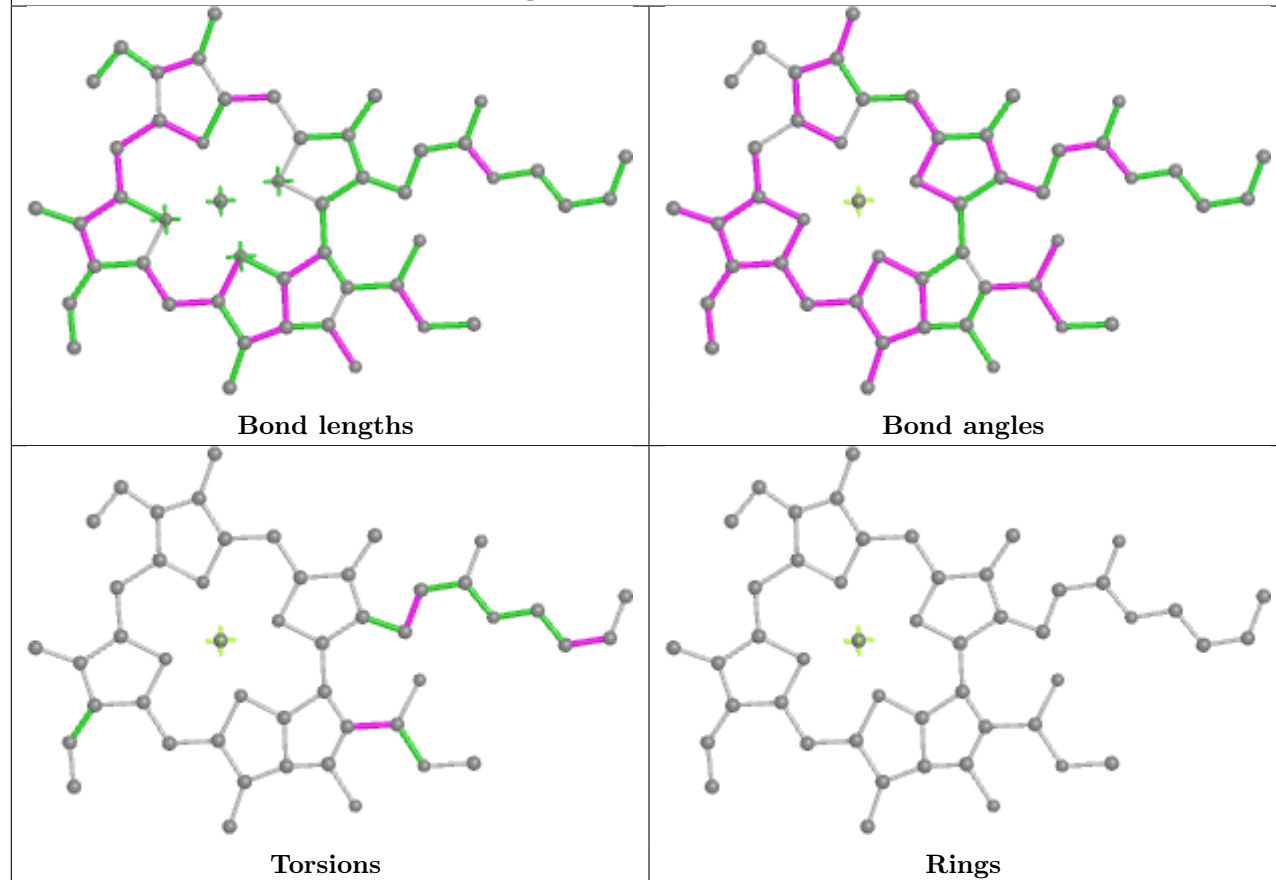


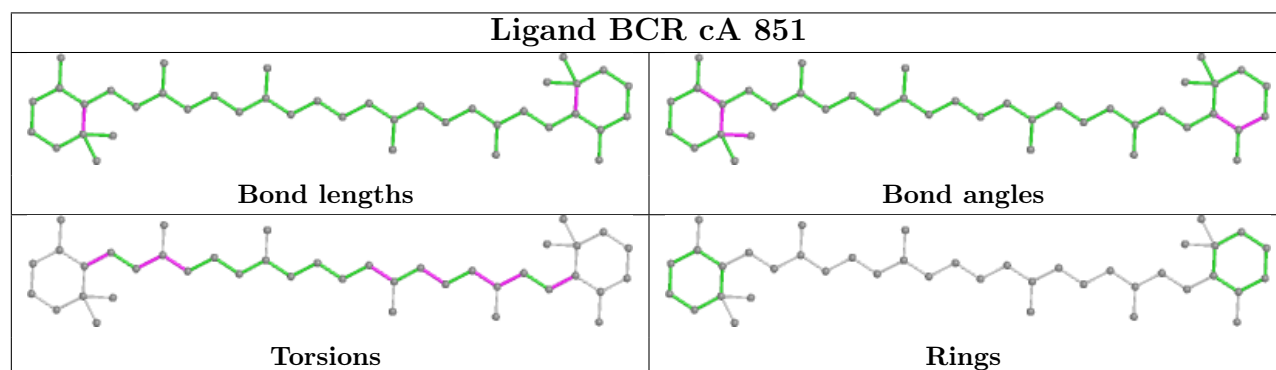
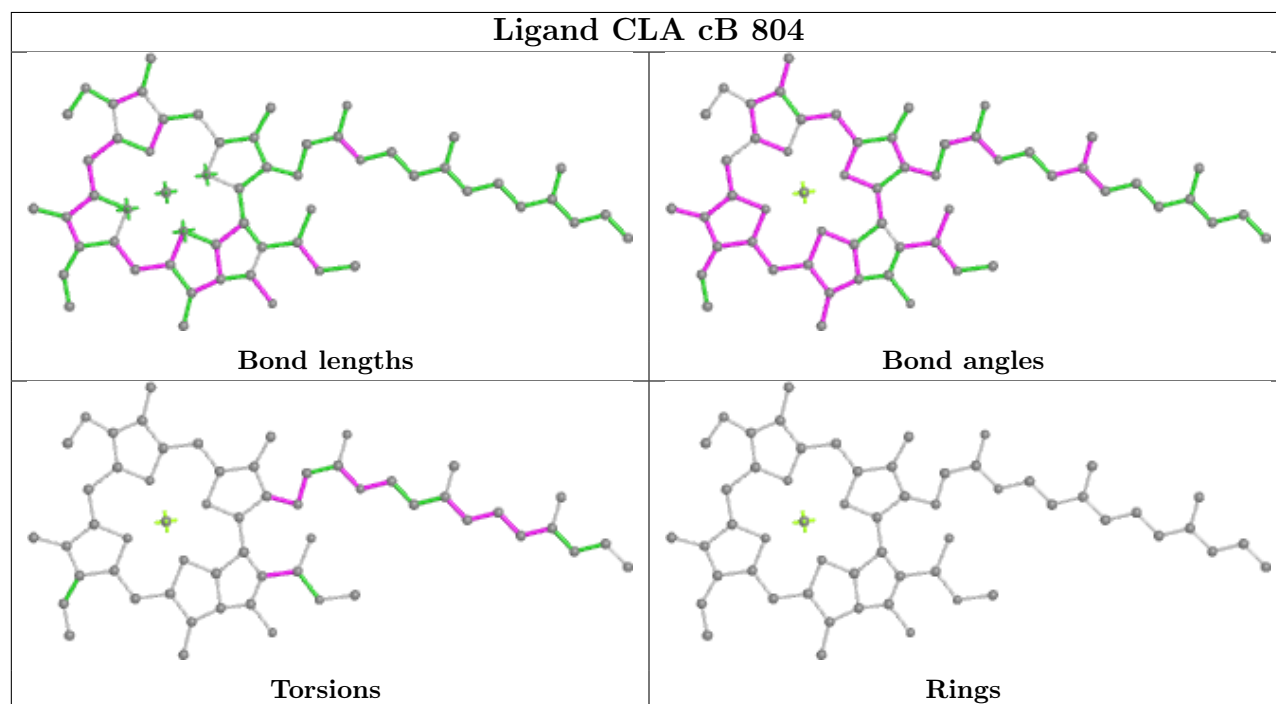
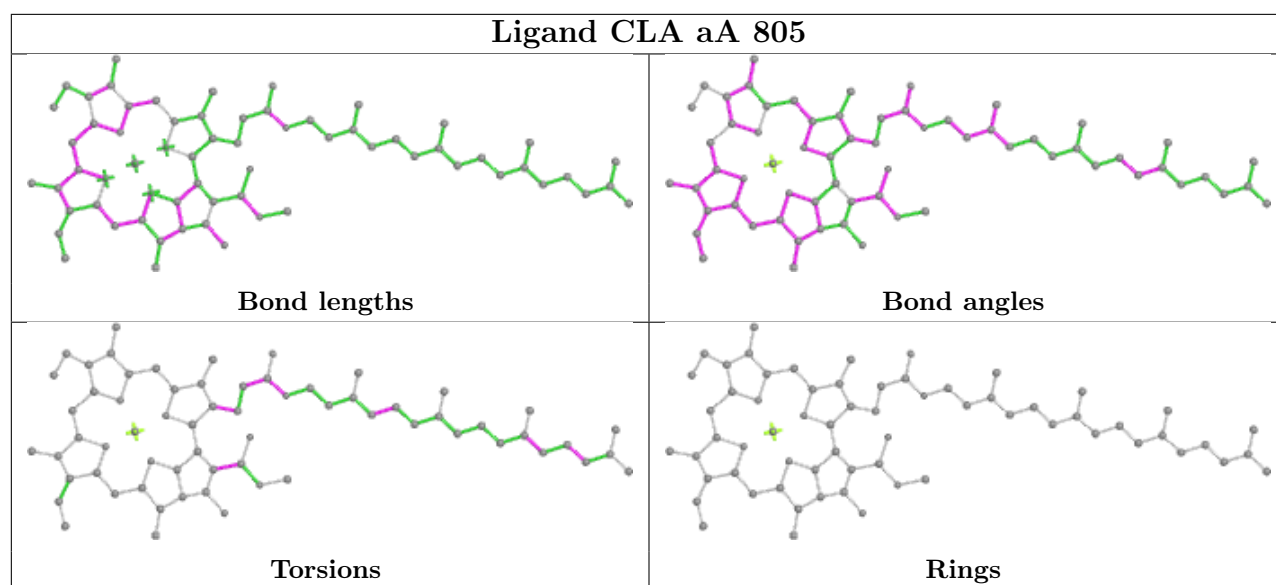


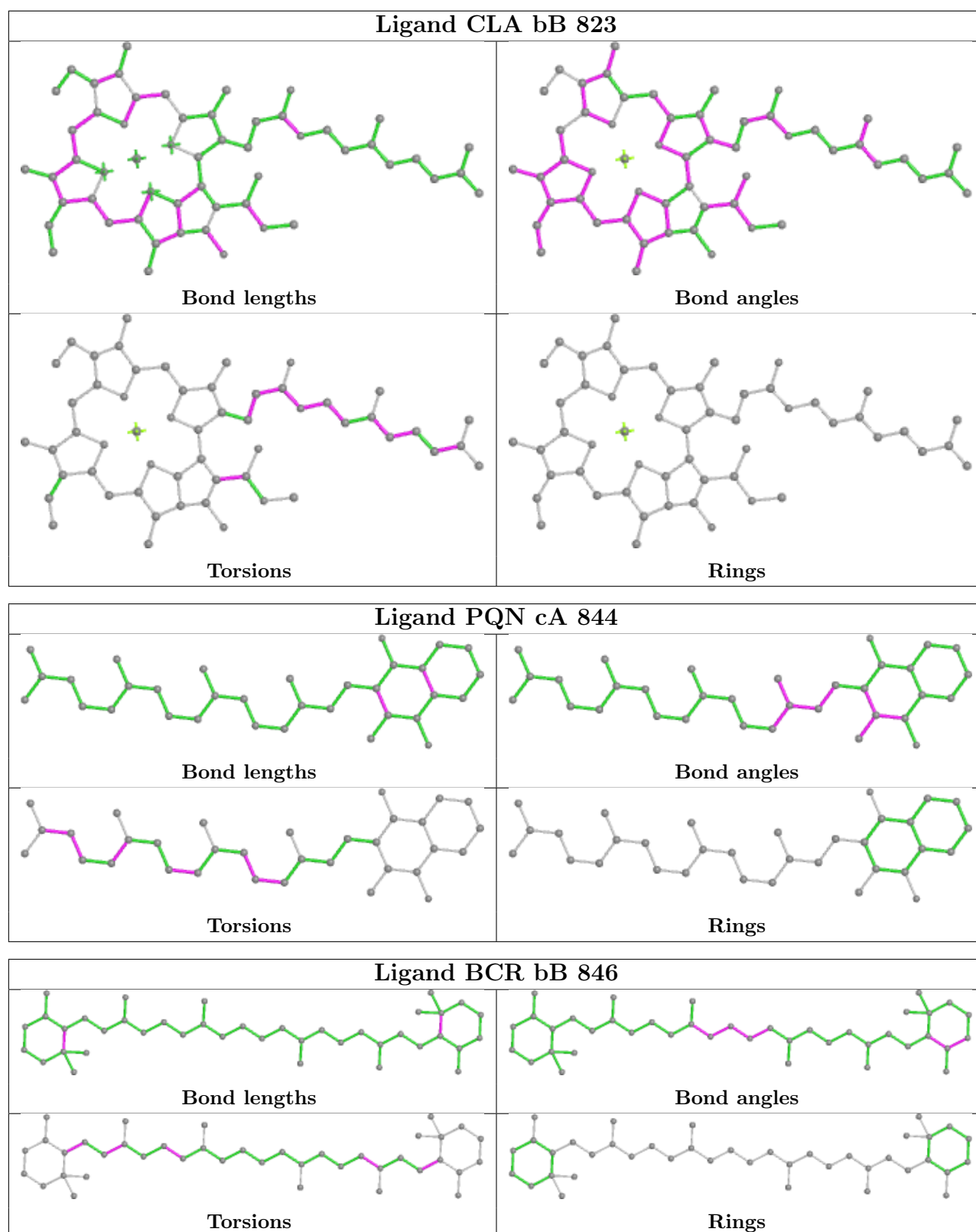
## Ligand CLA bA 818



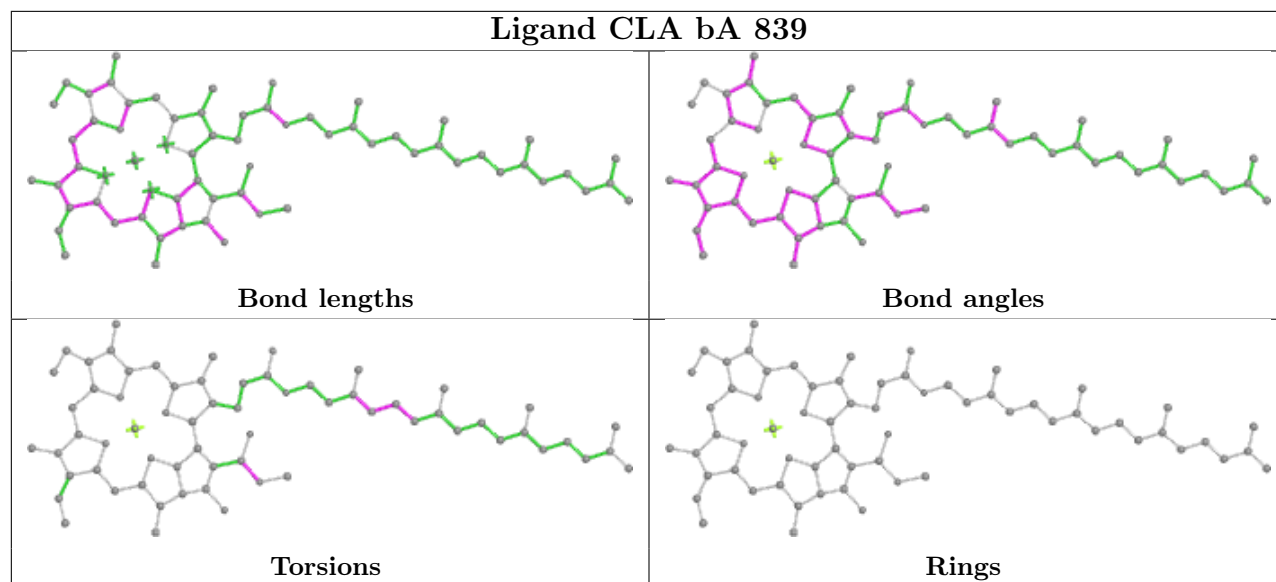
## Ligand CLA bA 821



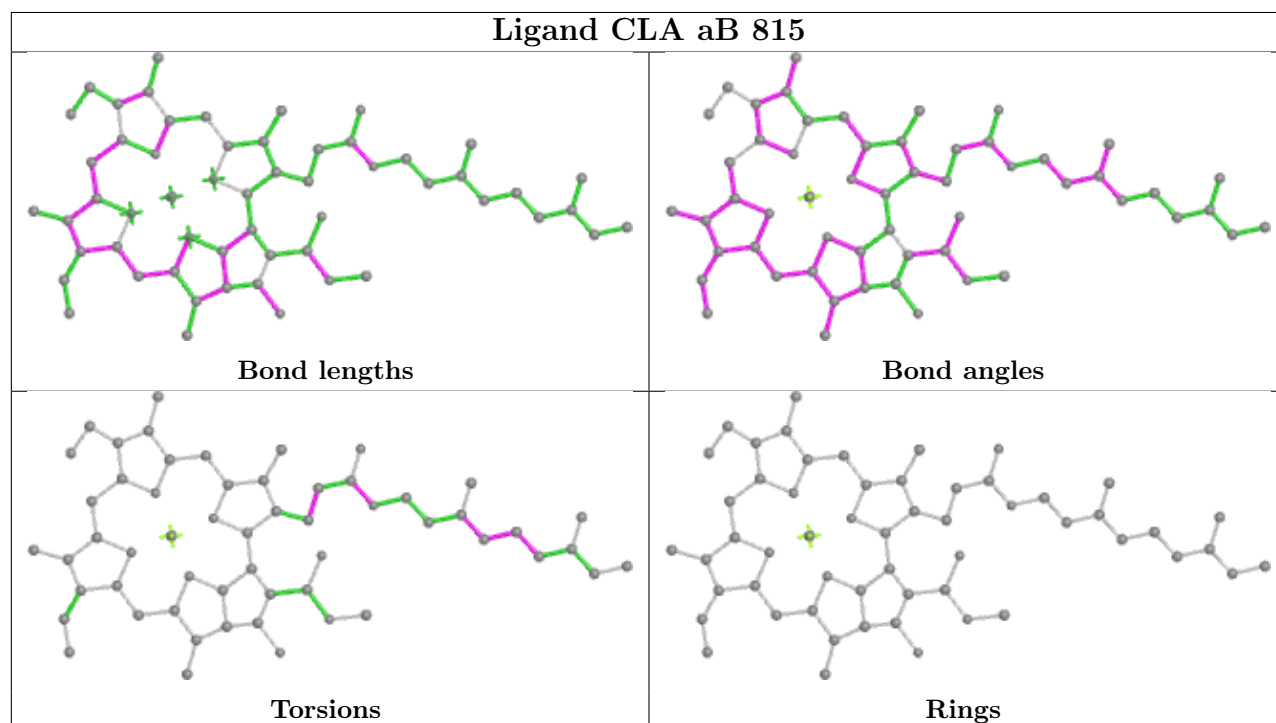




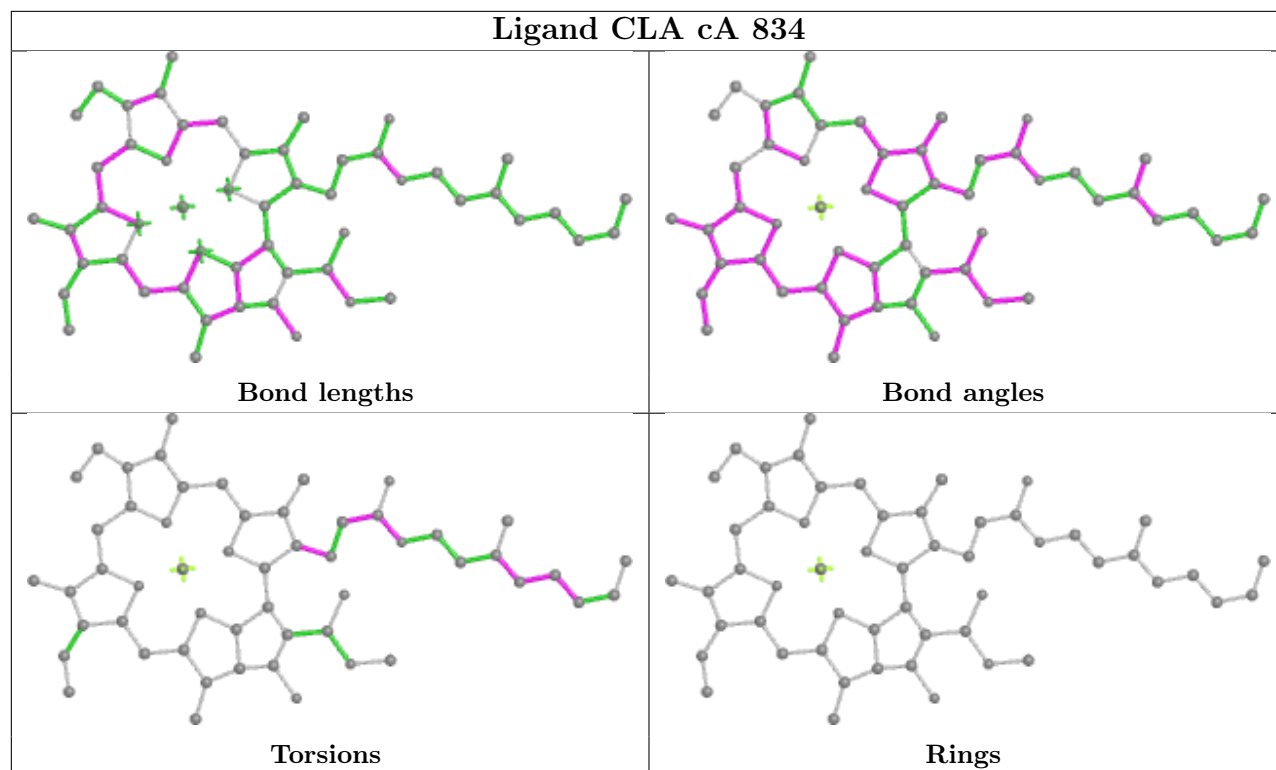
## Ligand CLA bA 839



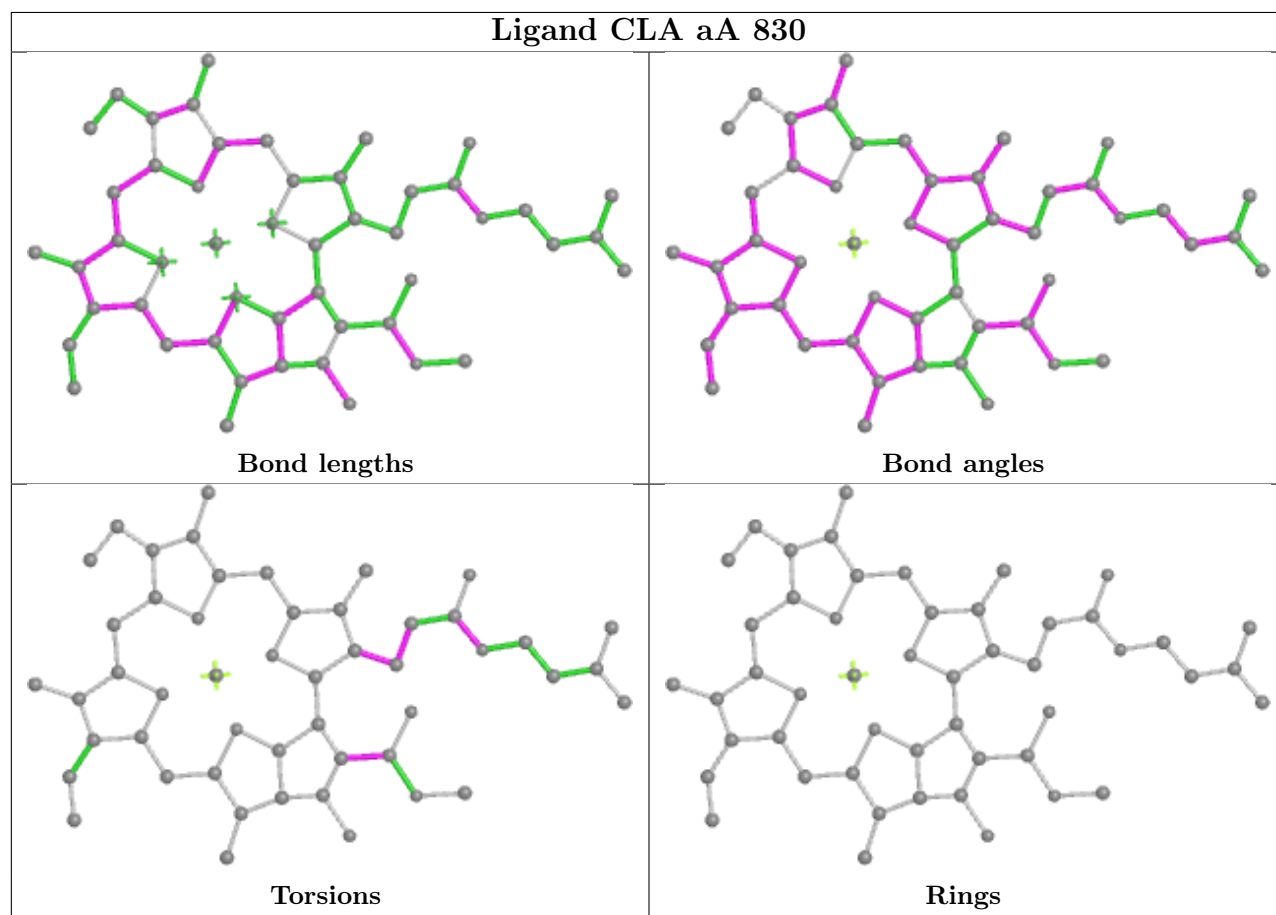
## Ligand CLA aB 815



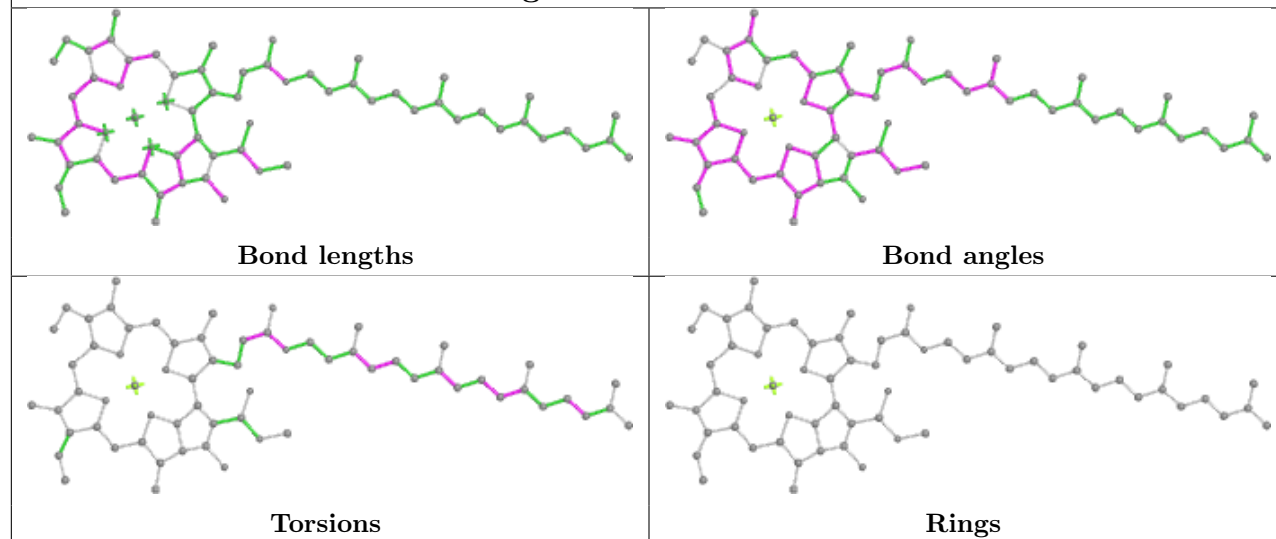
## Ligand CLA cA 834



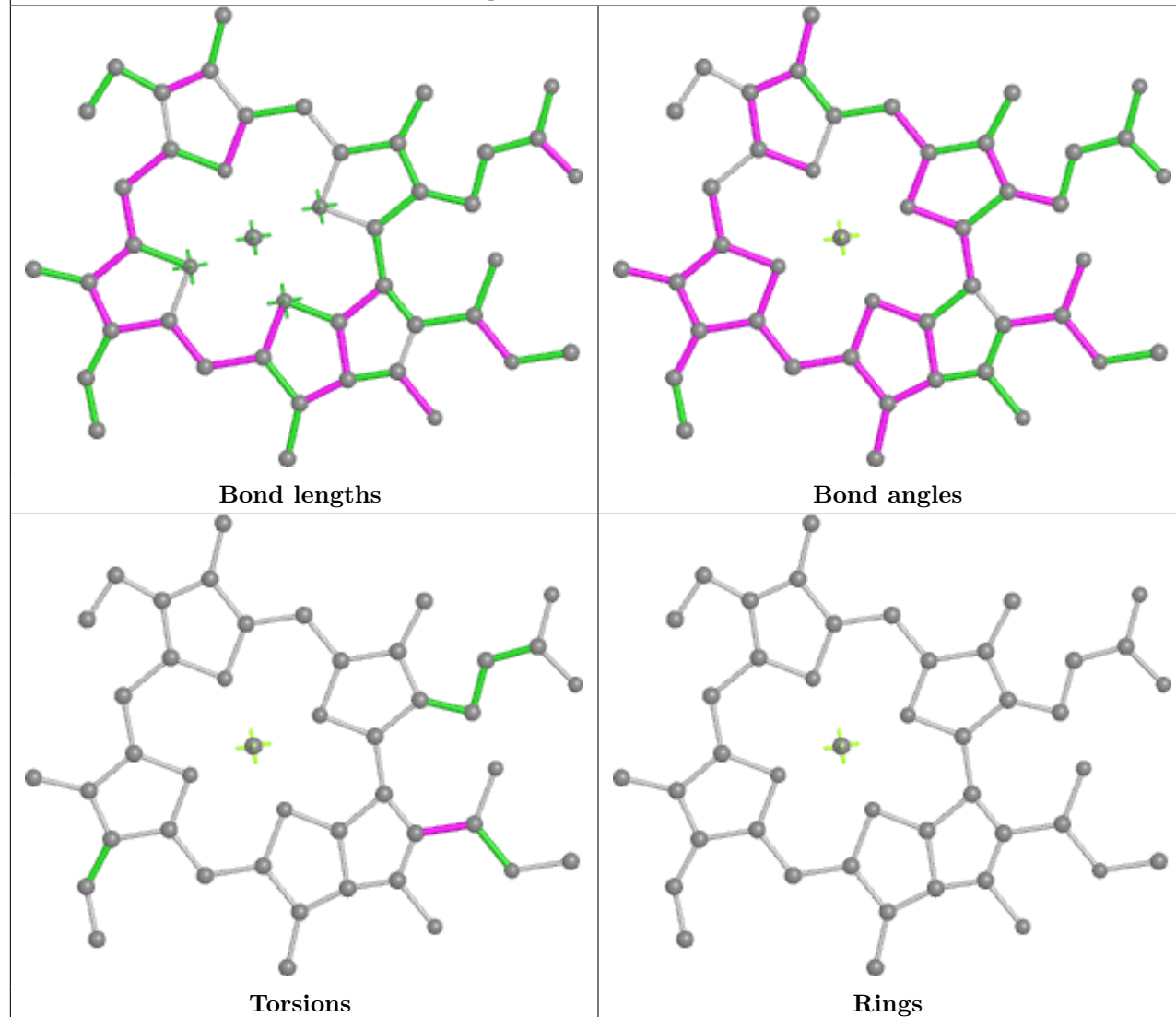
## Ligand CLA aA 830

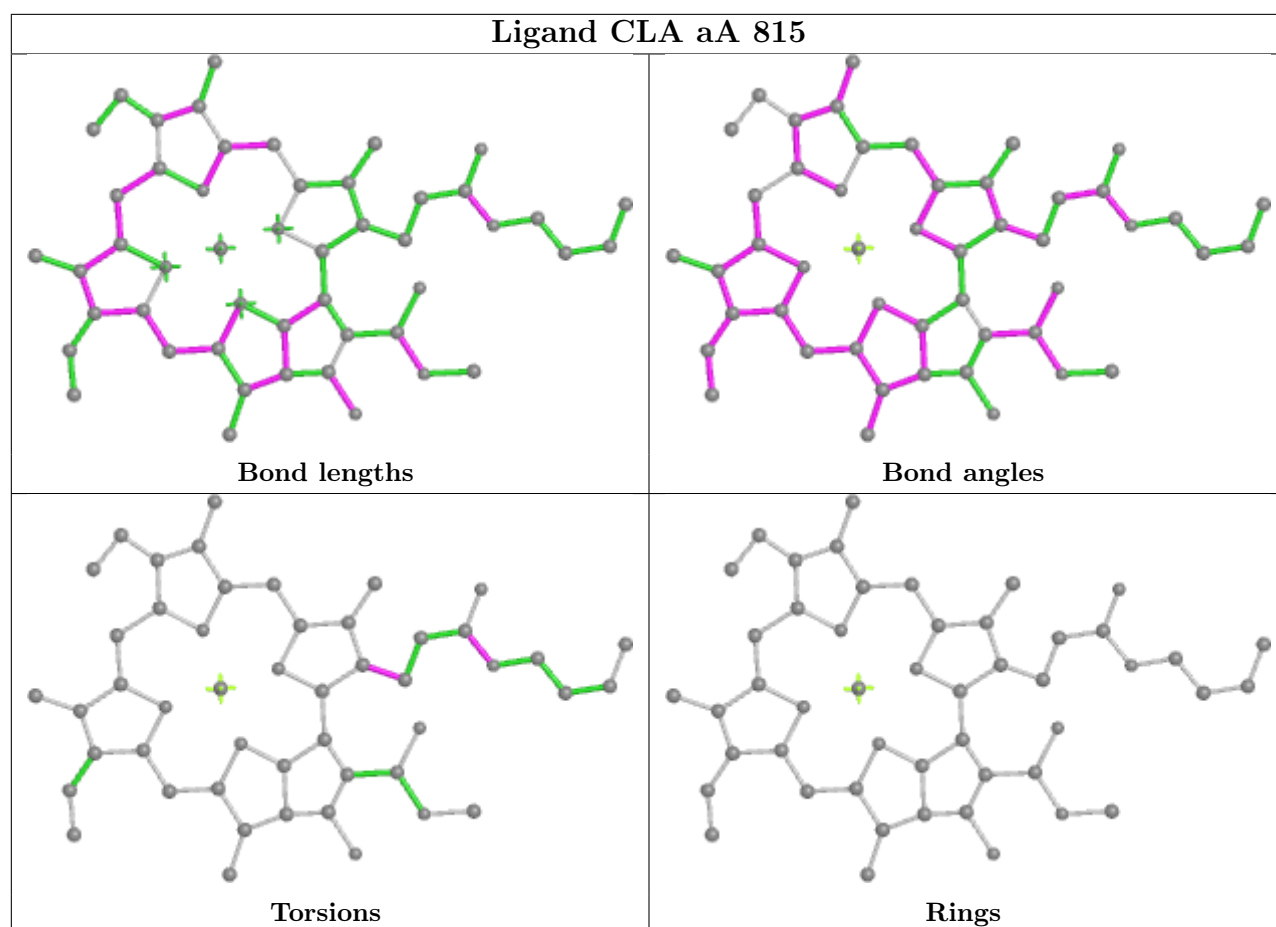


## Ligand CLA bB 808



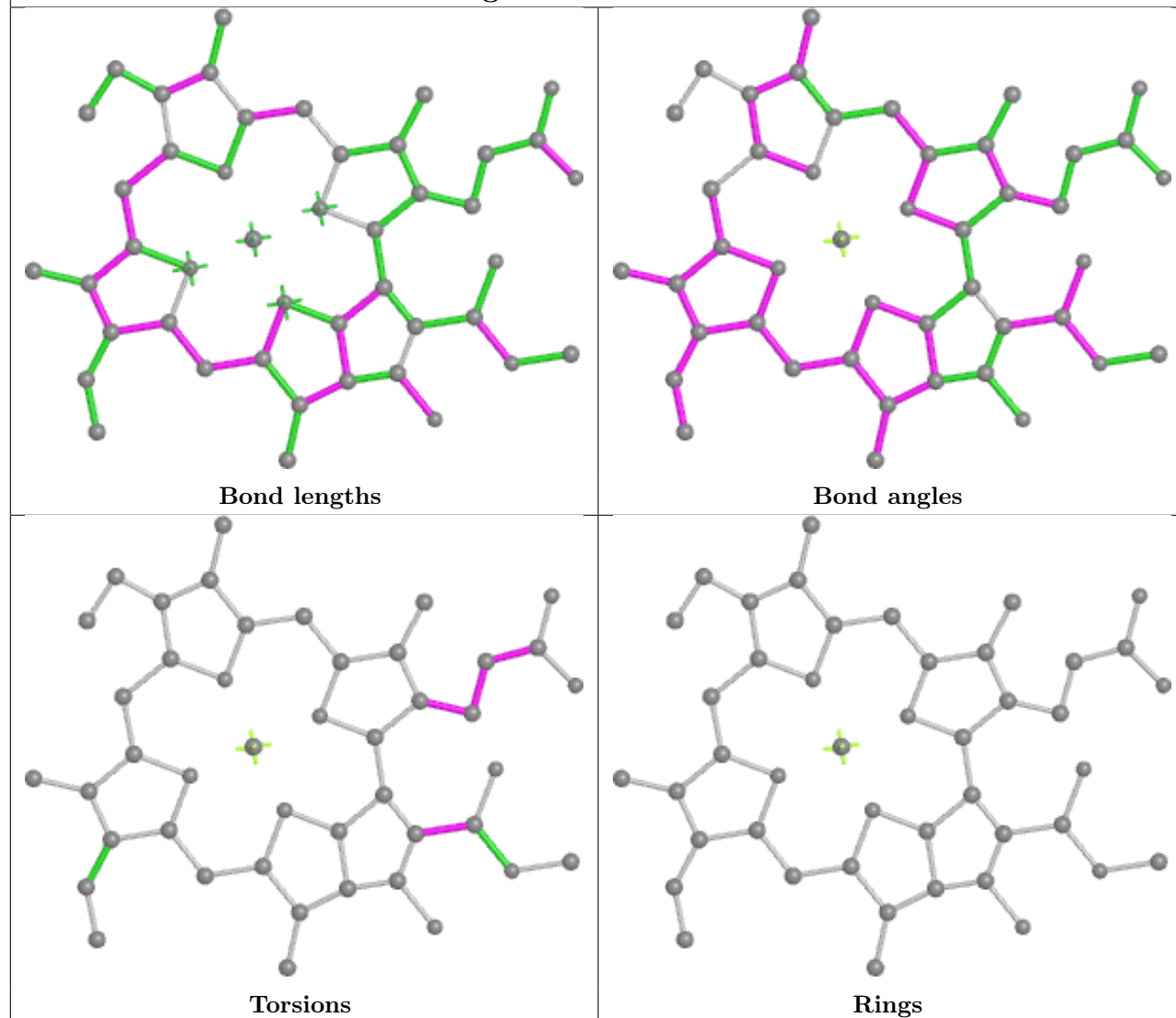
## Ligand CLA cB 816



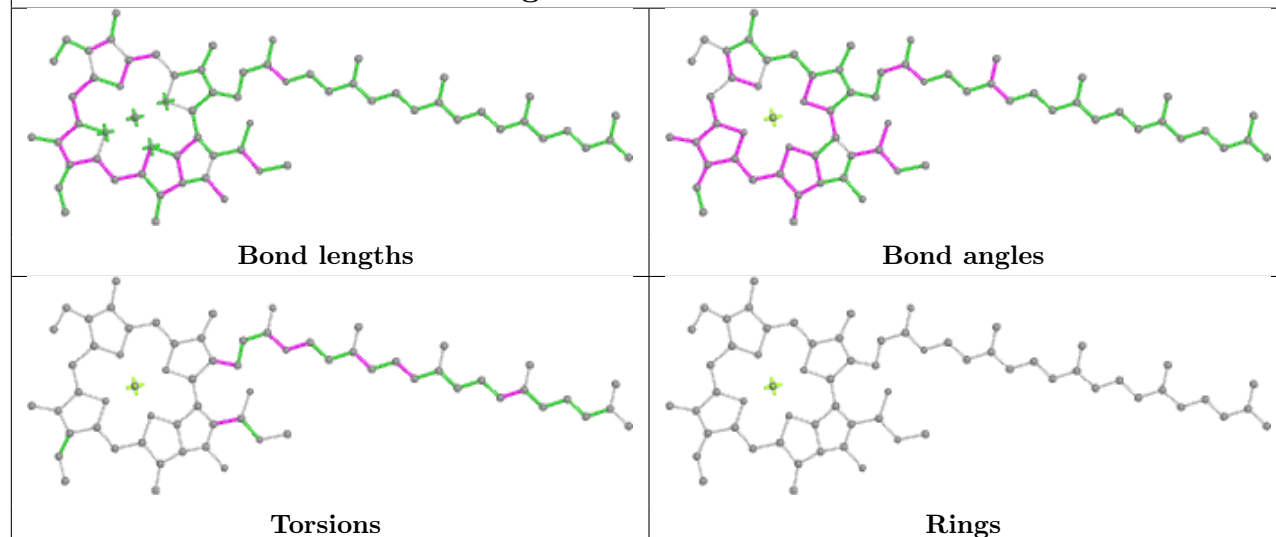


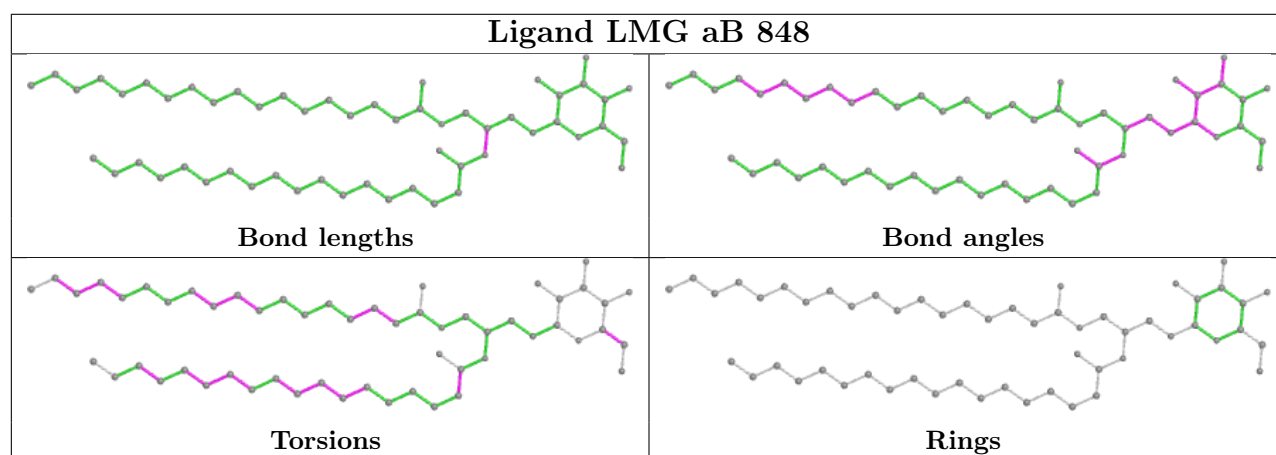
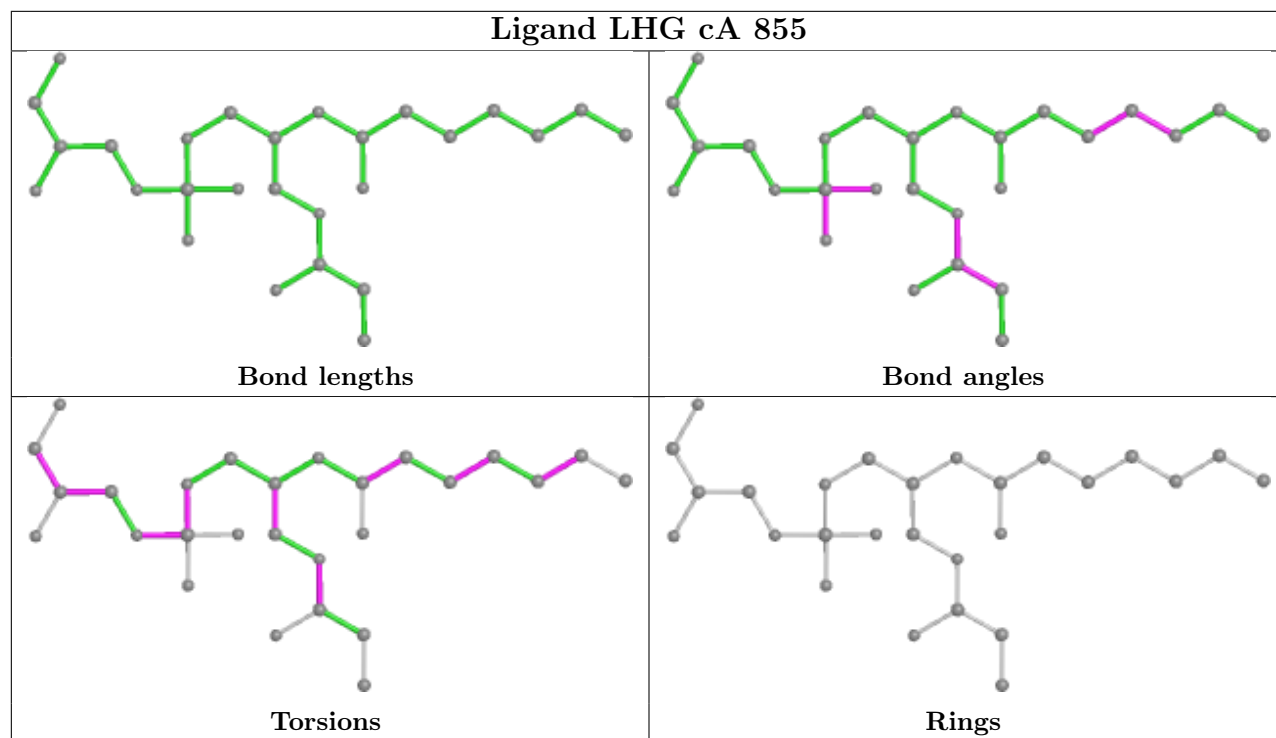
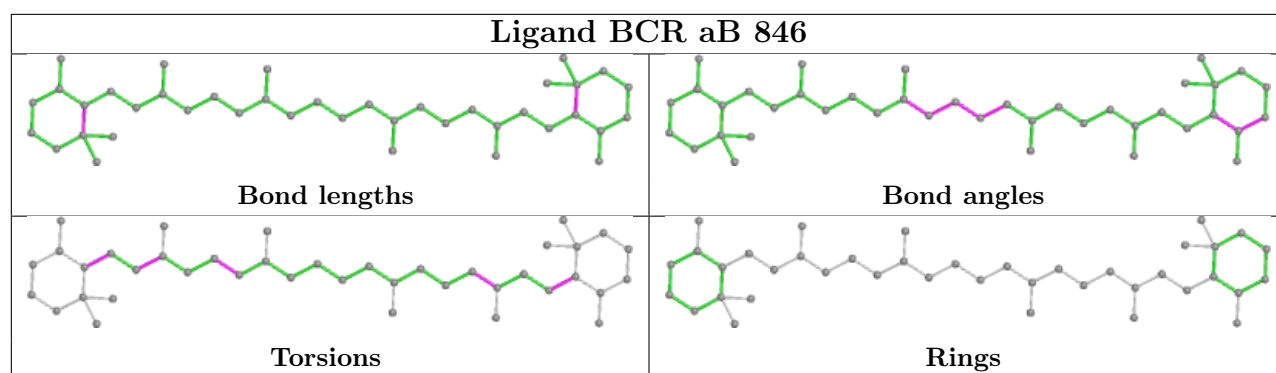


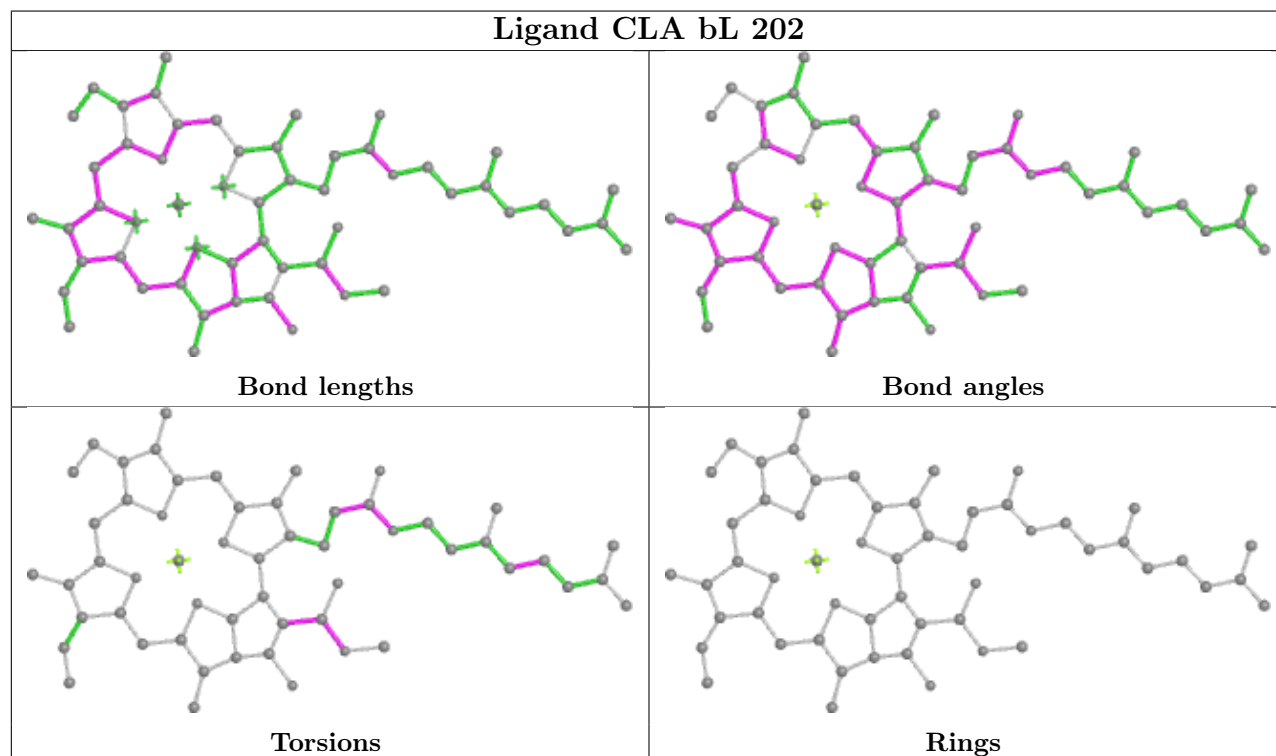
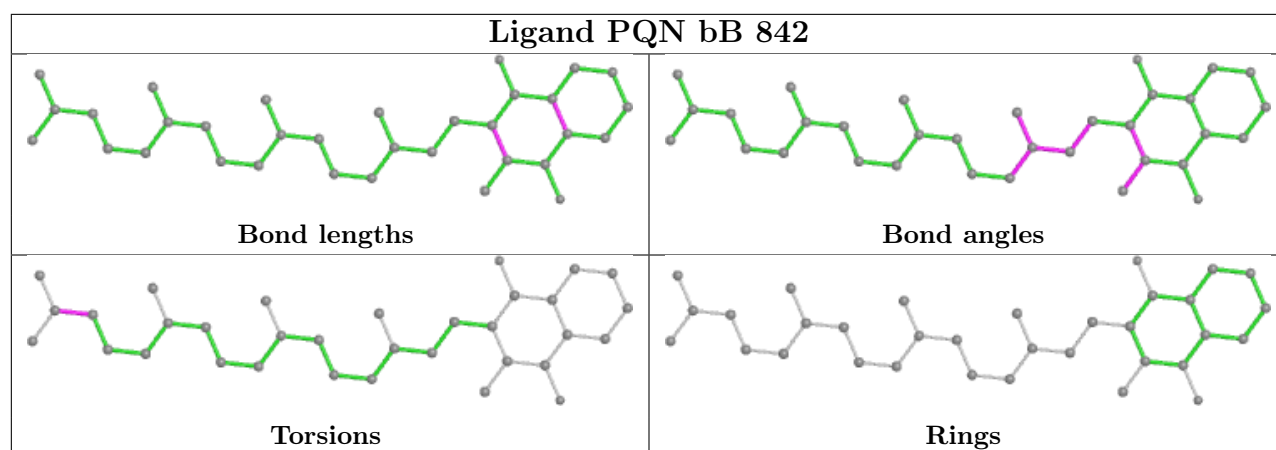
## Ligand CLA cA 802

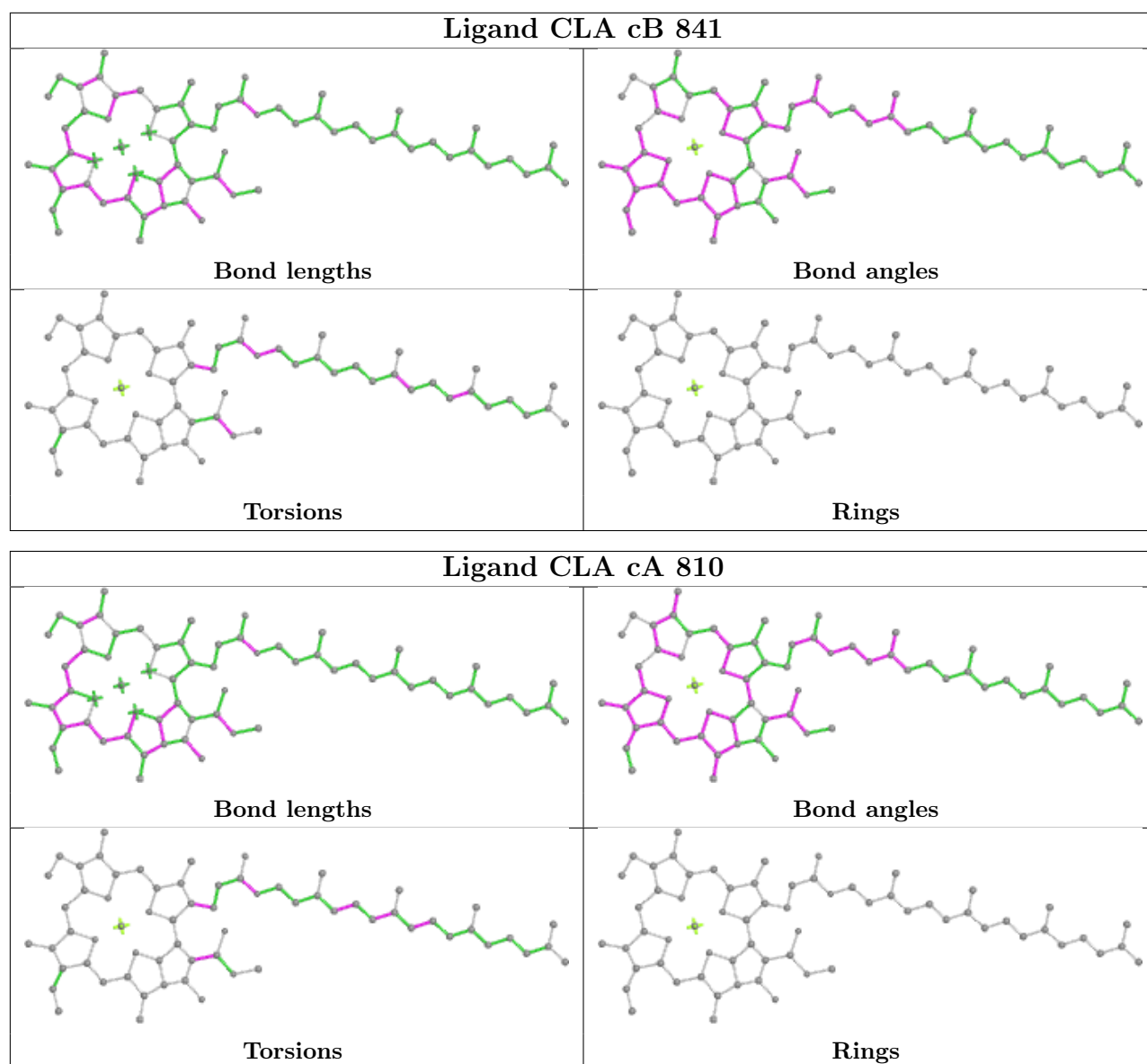


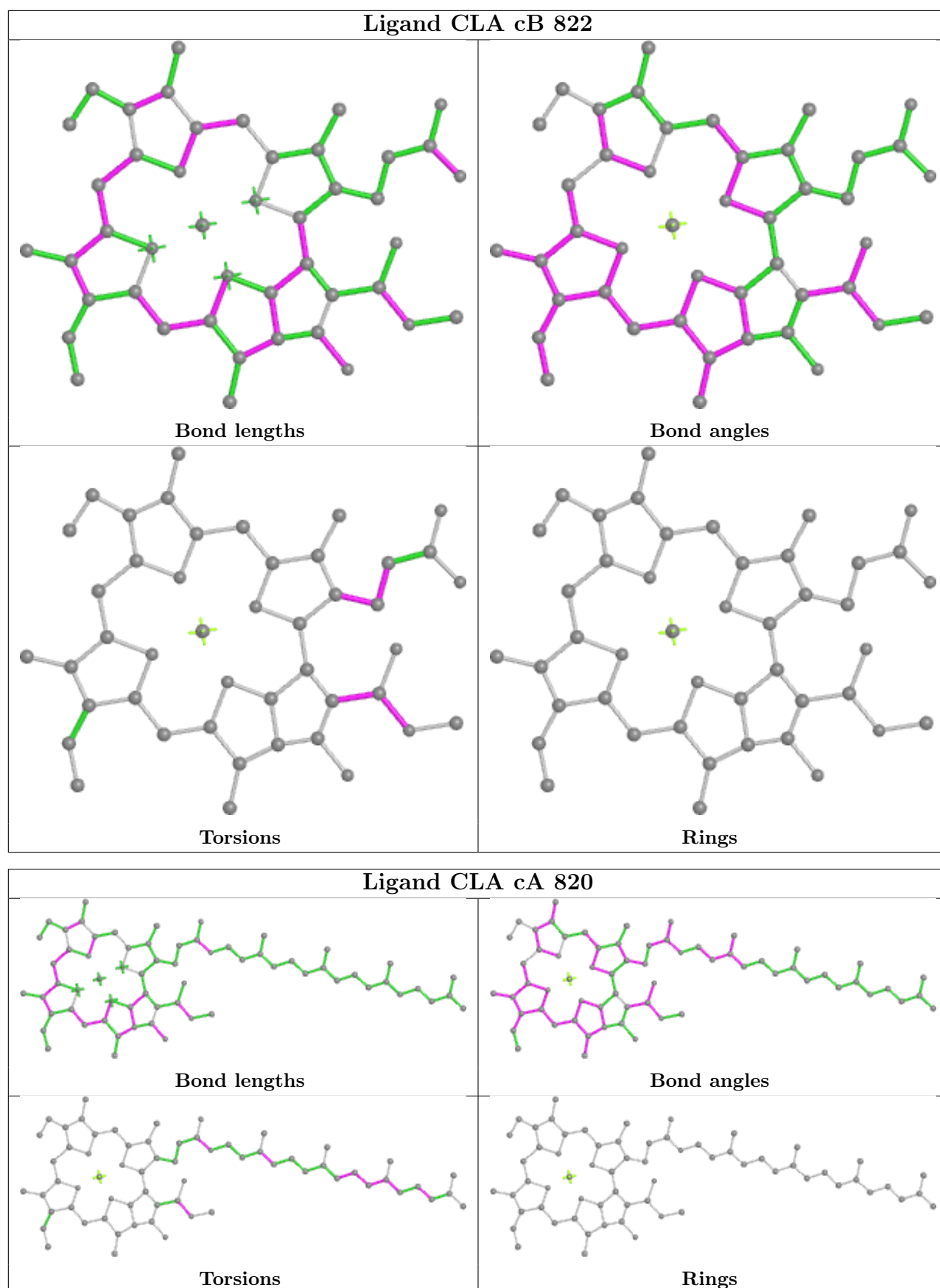
## Ligand CLA bA 824

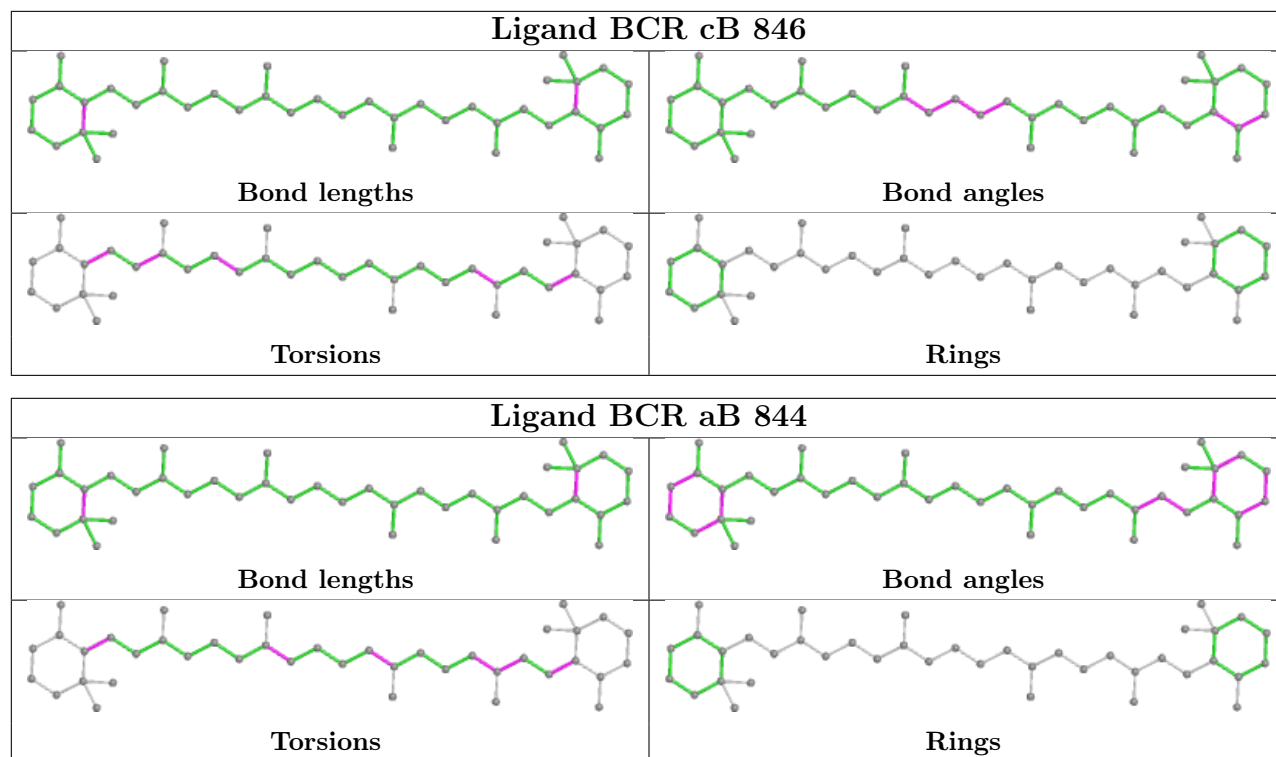




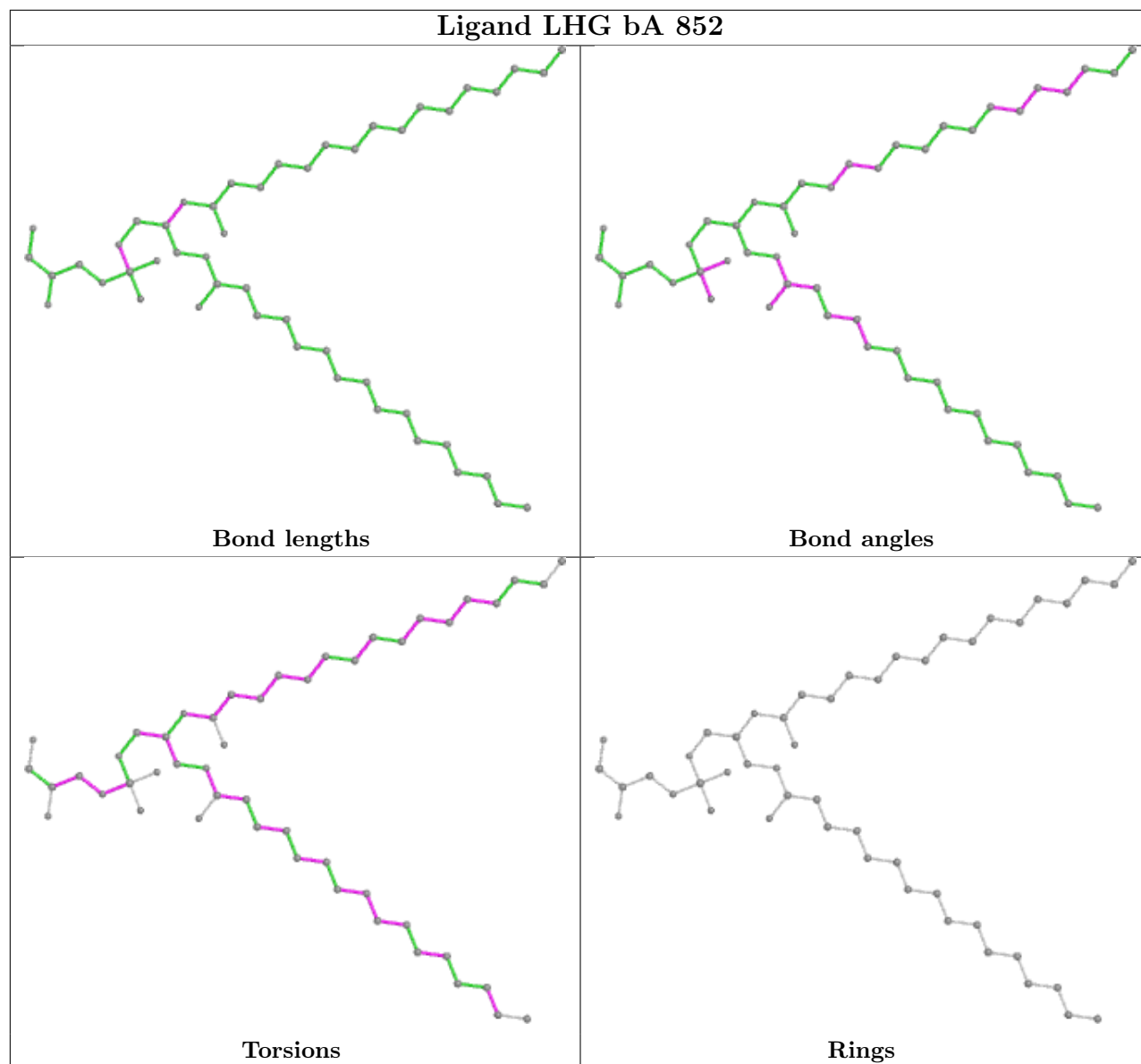




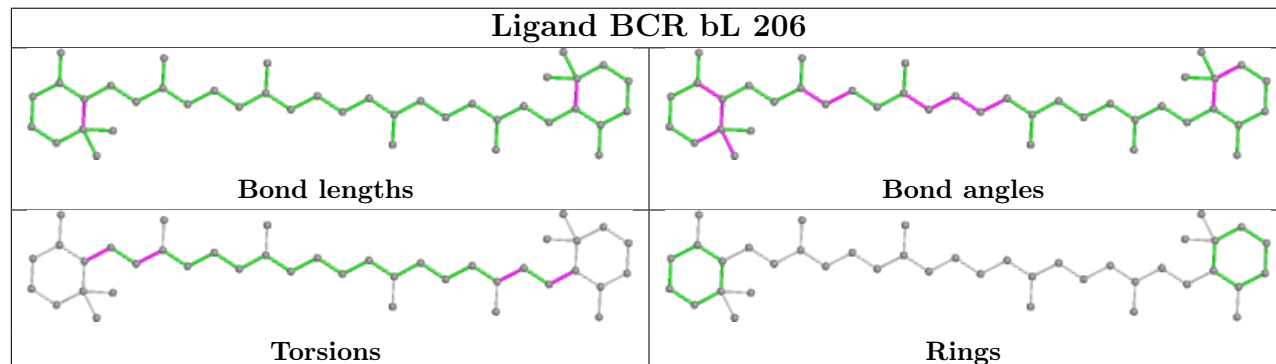


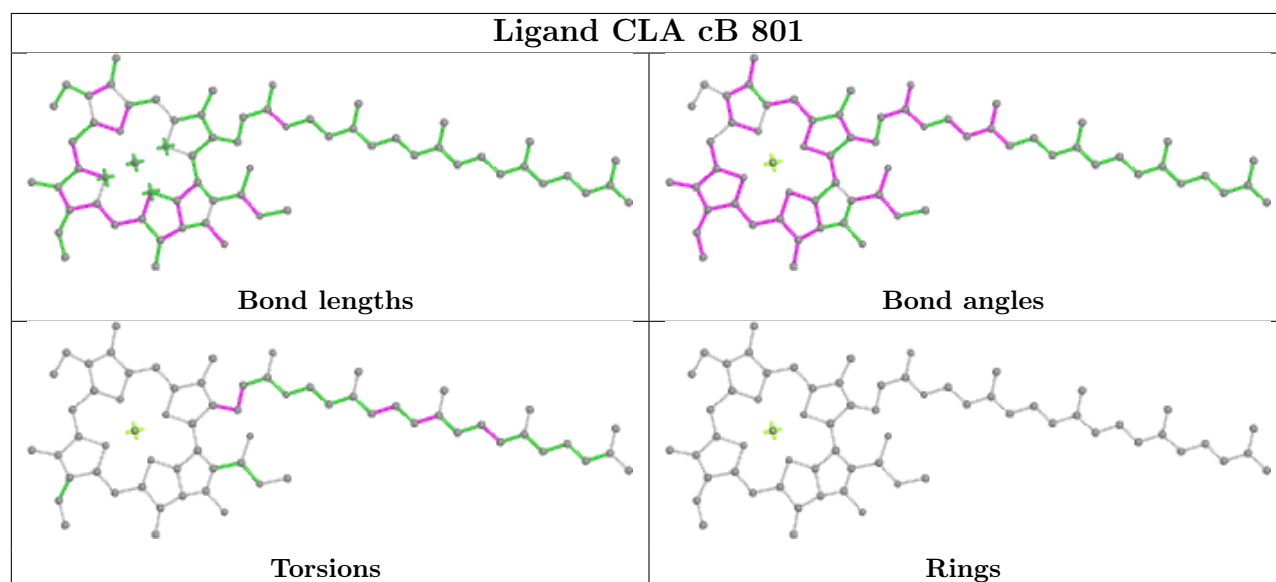
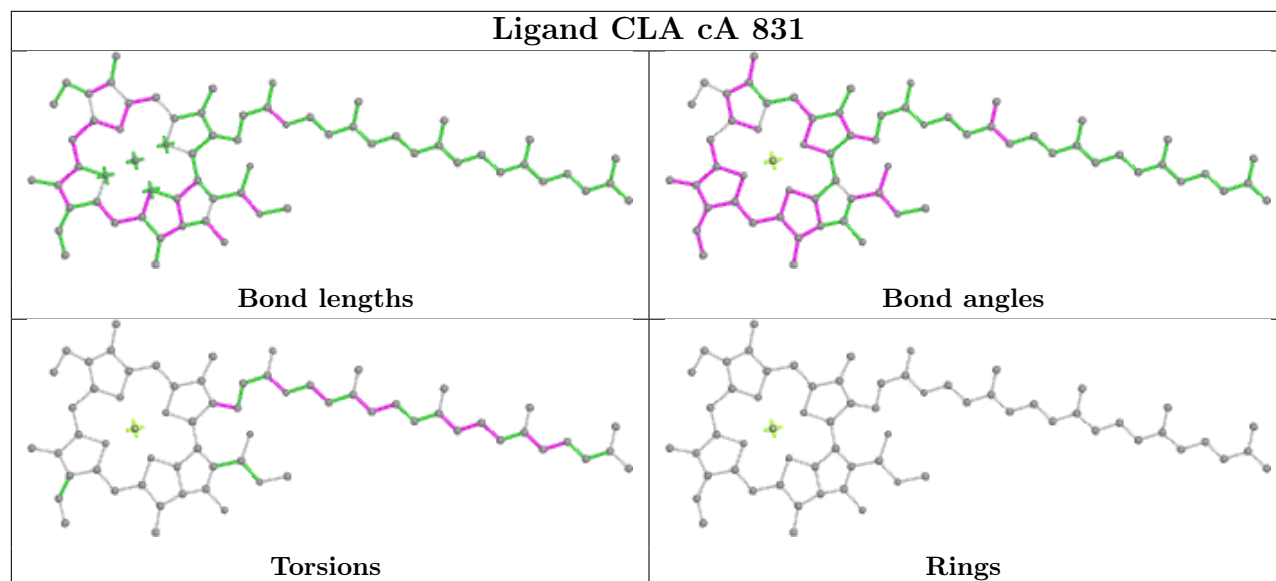
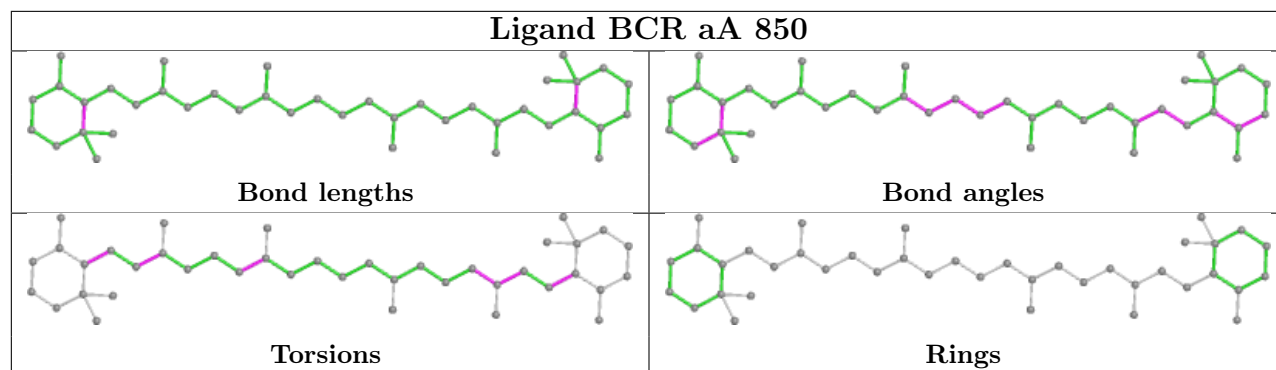


## Ligand LHG bA 852

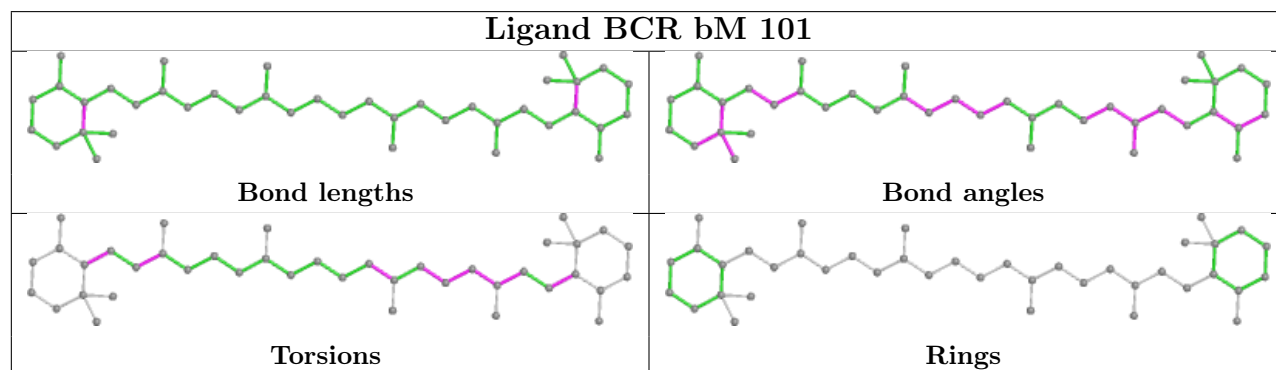
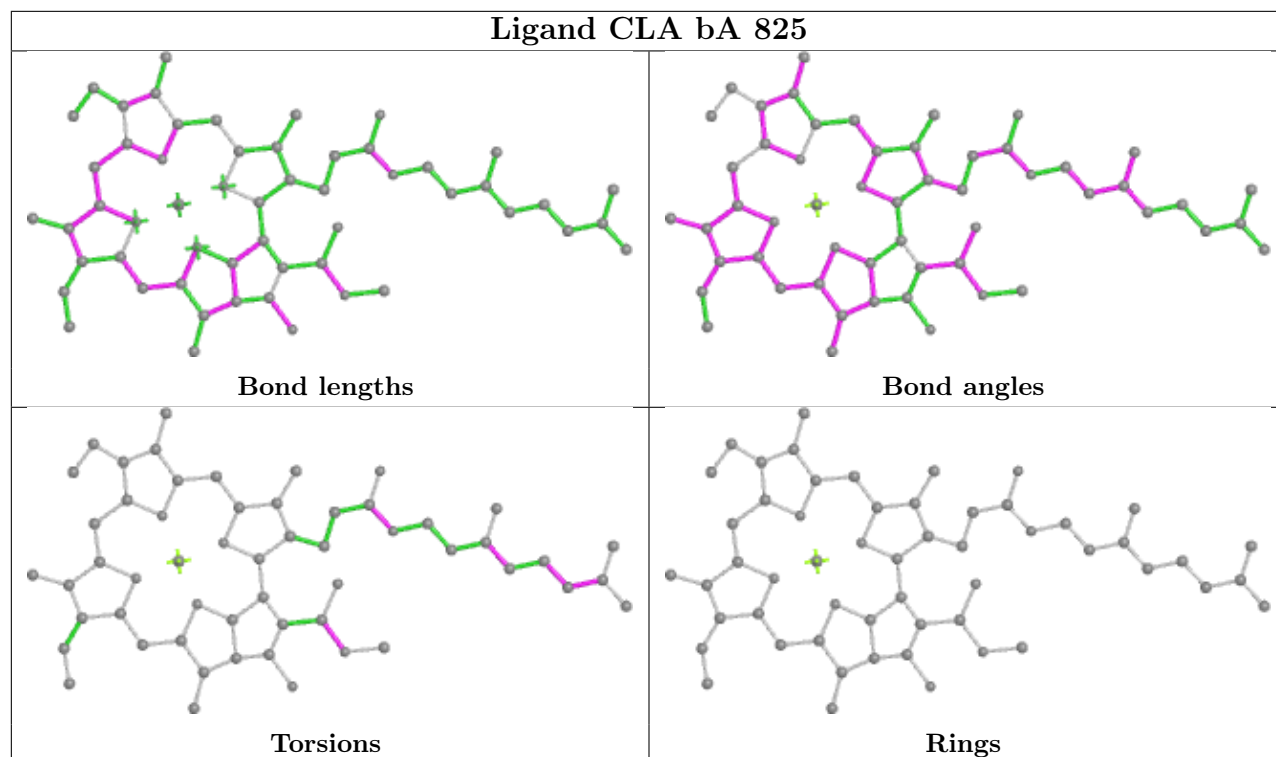
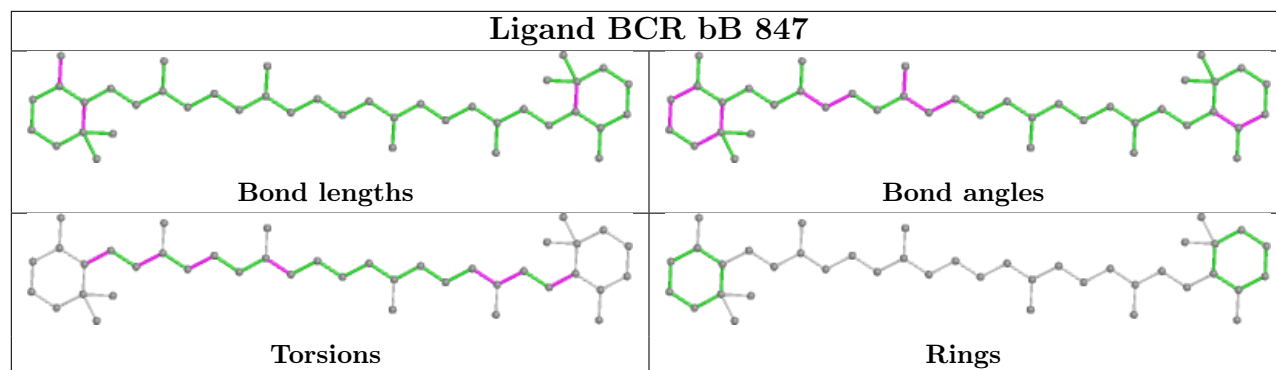


## Ligand BCR bL 206

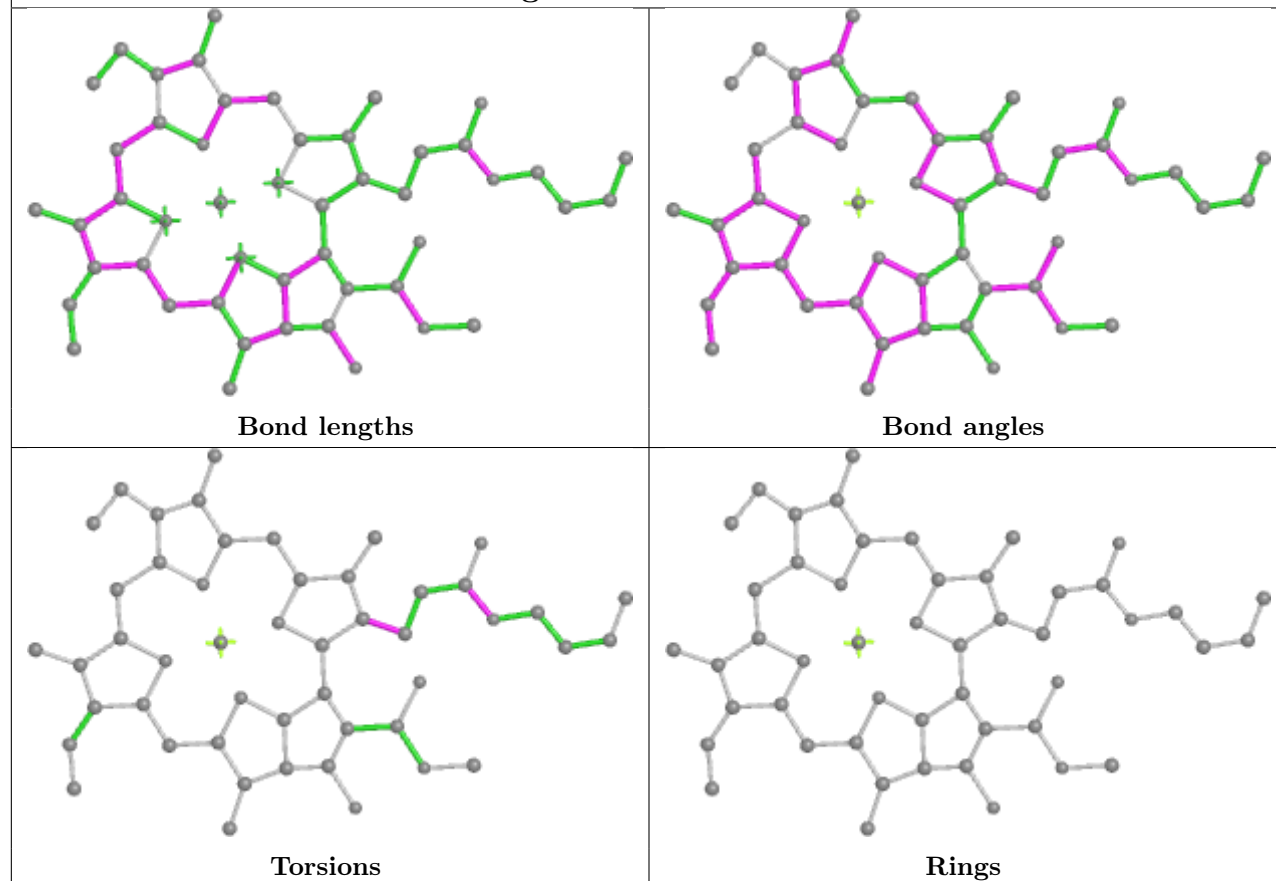




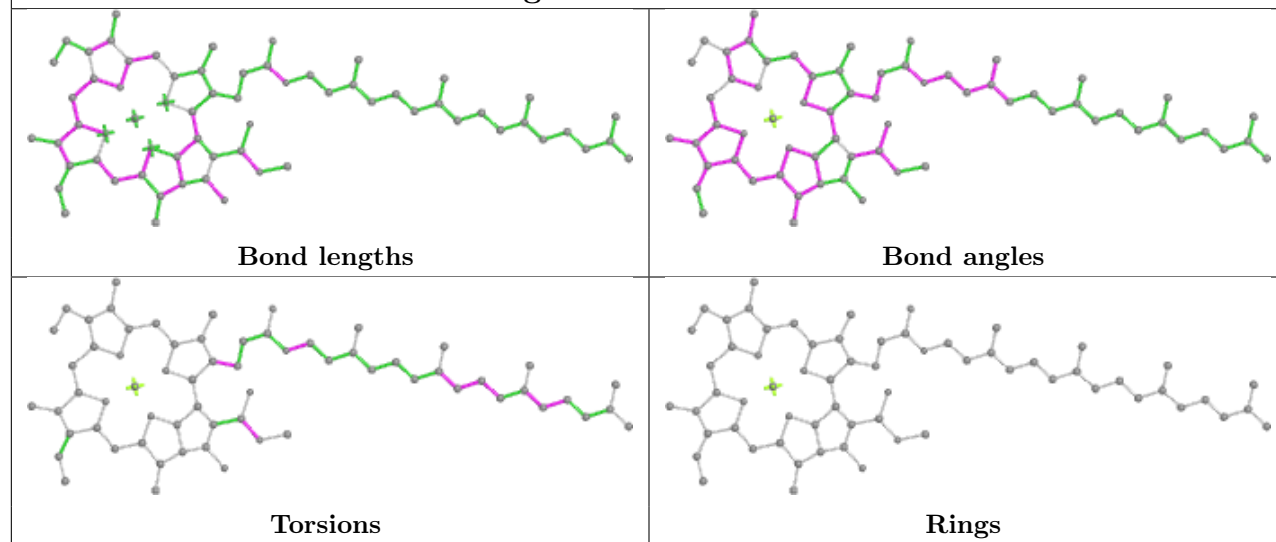




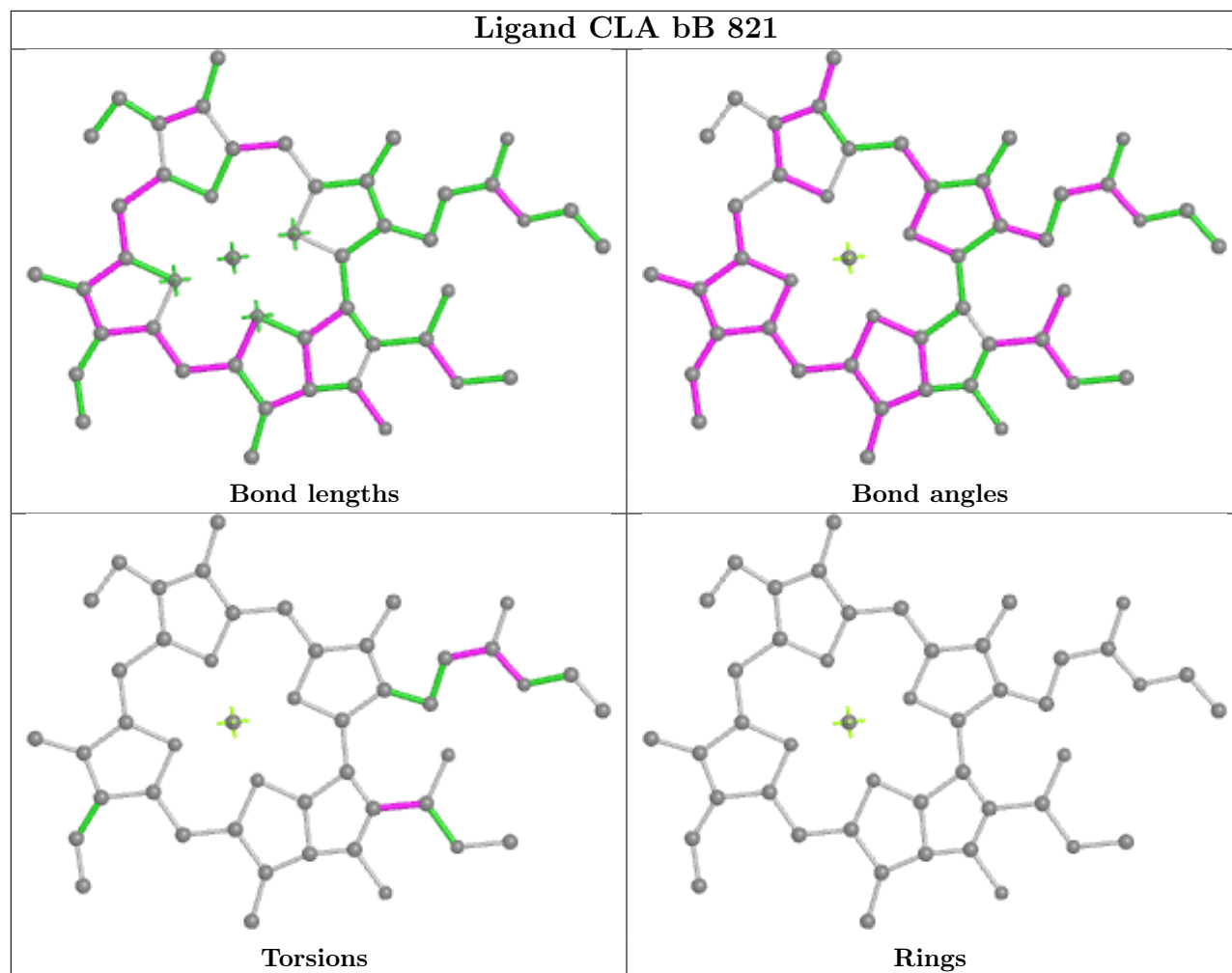
## Ligand CLA bA 815

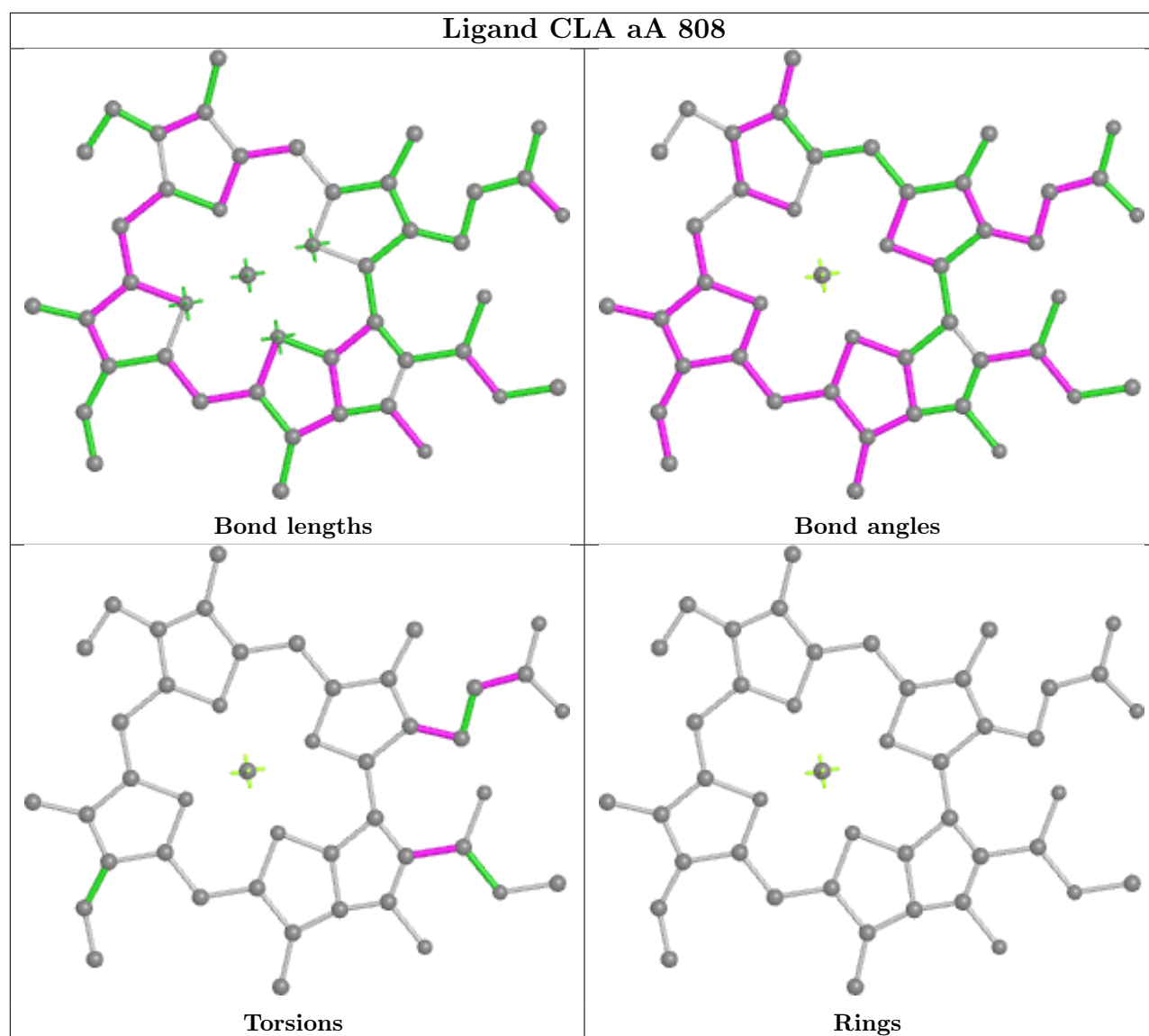


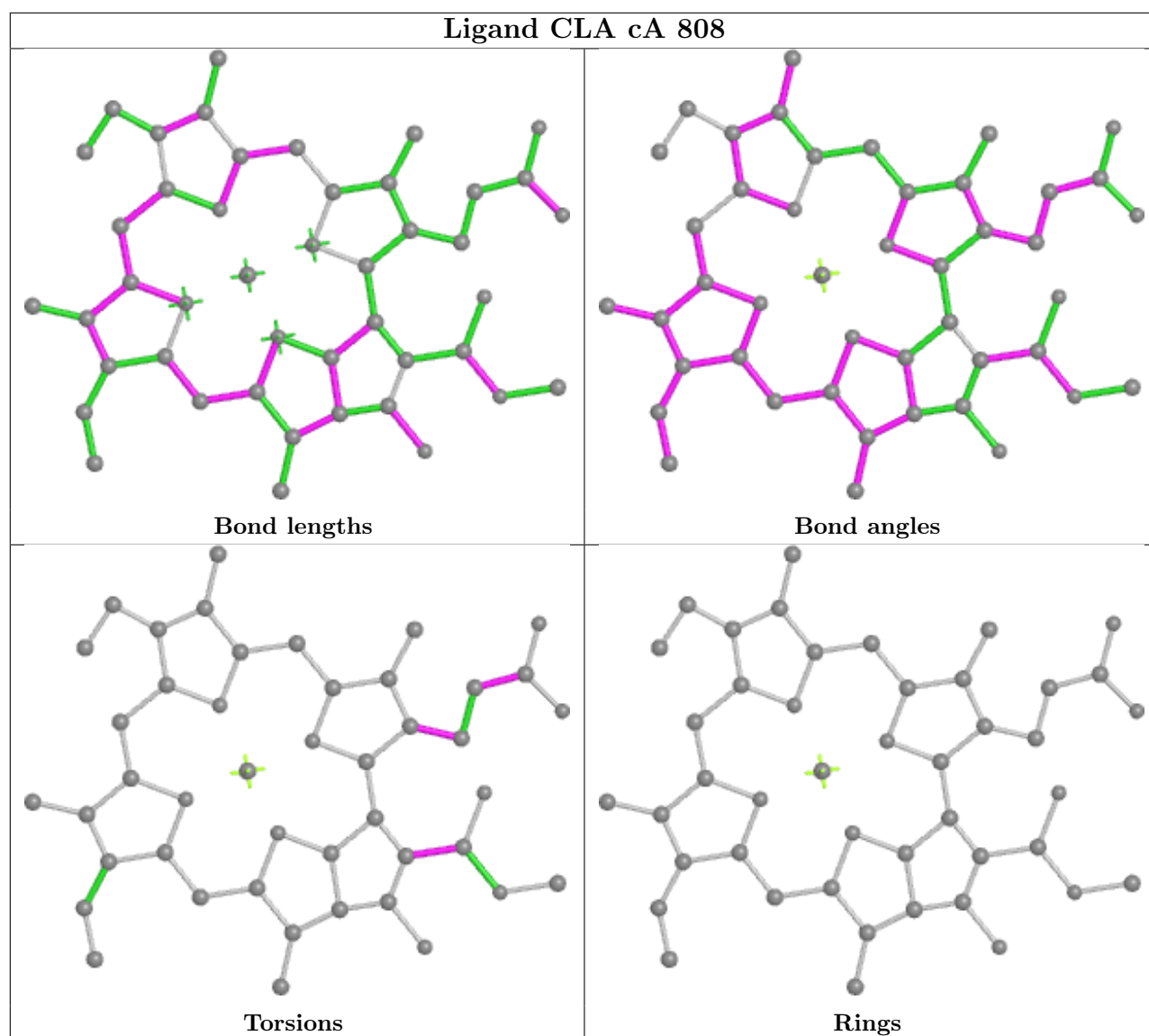
## Ligand CLA aB 828

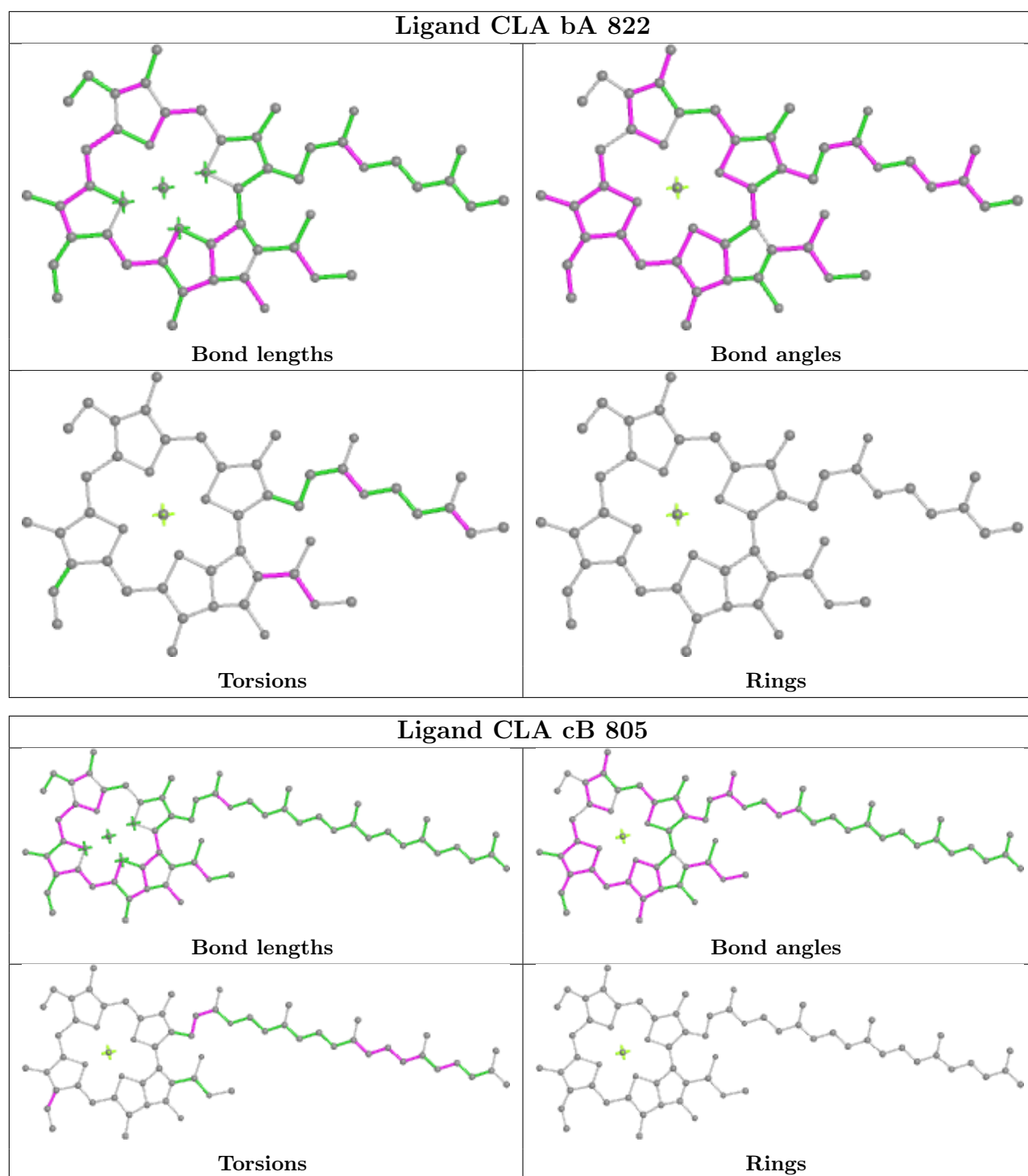


## Ligand CLA bB 821

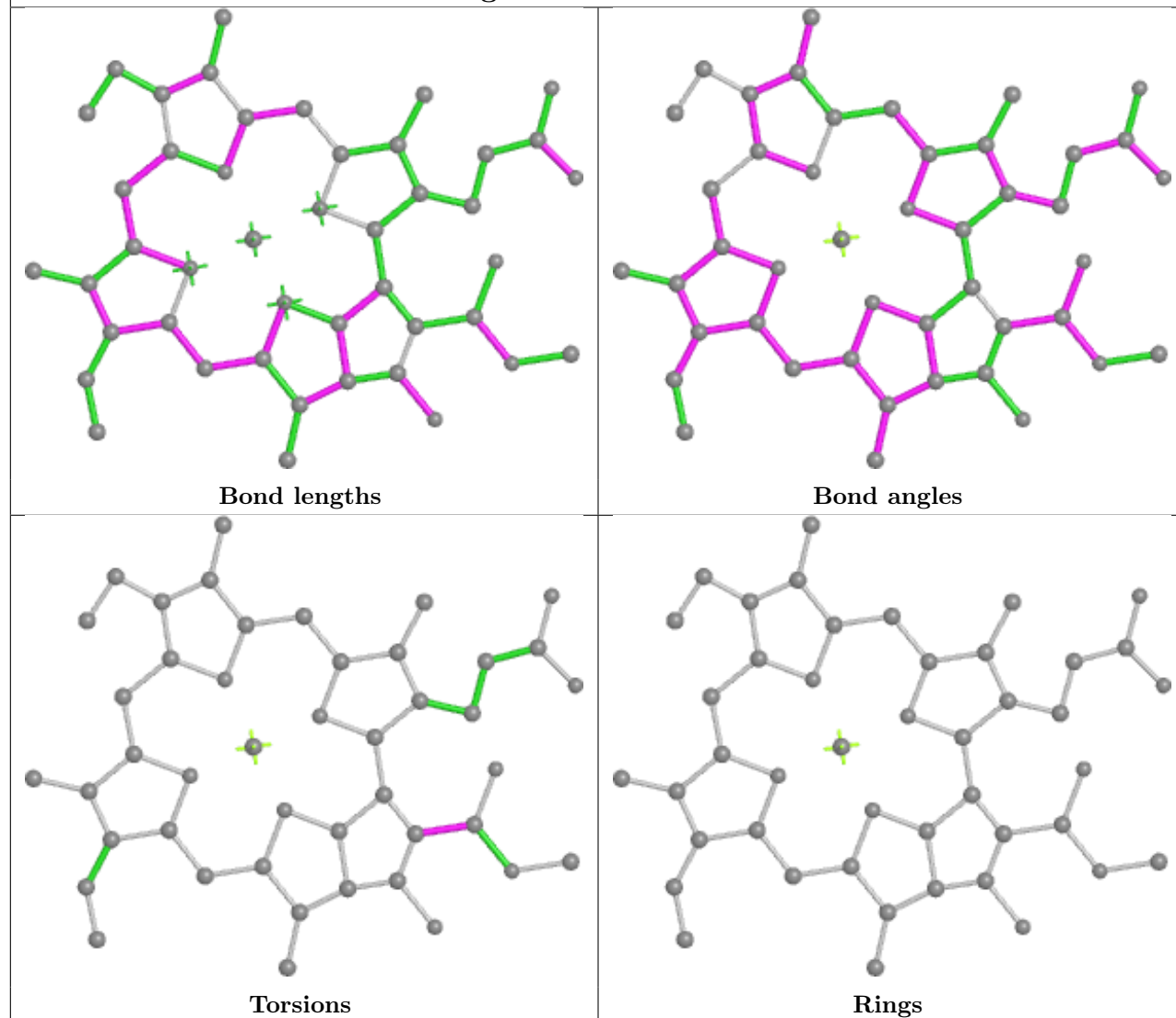




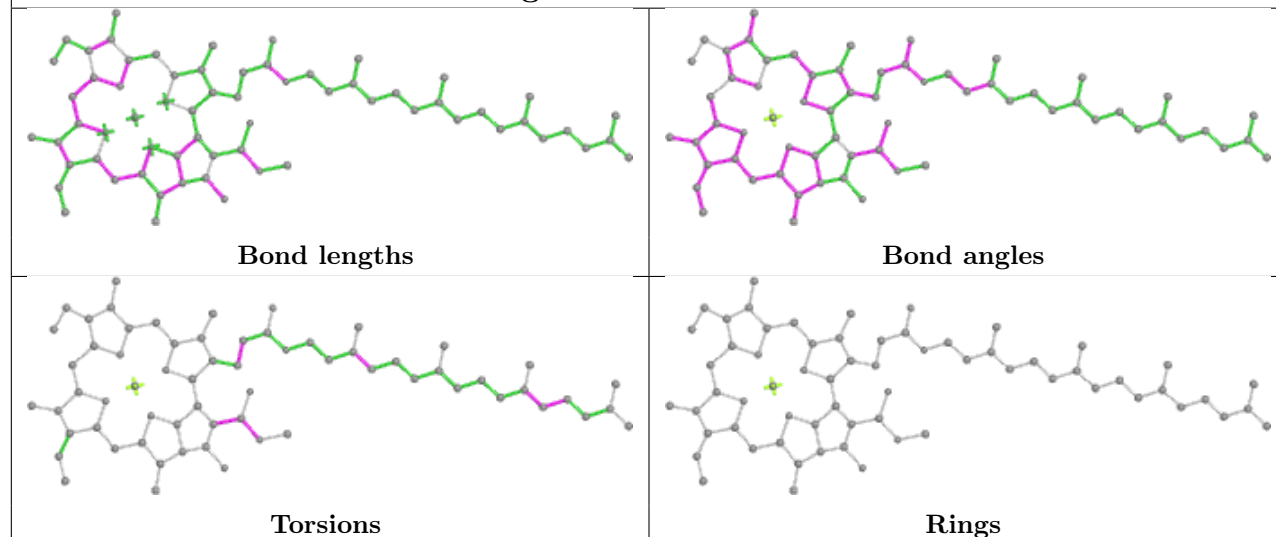


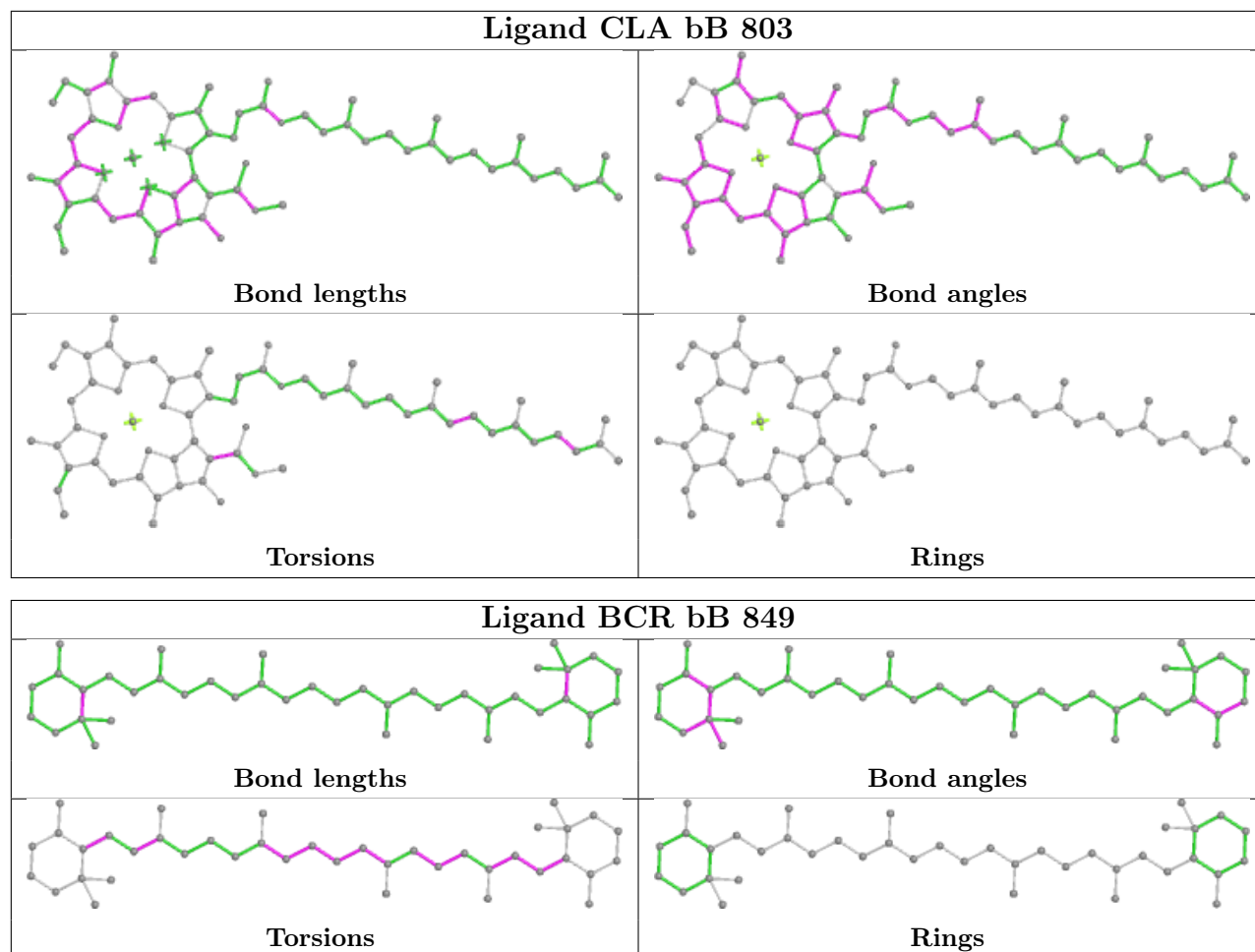


## Ligand CLA ba 814



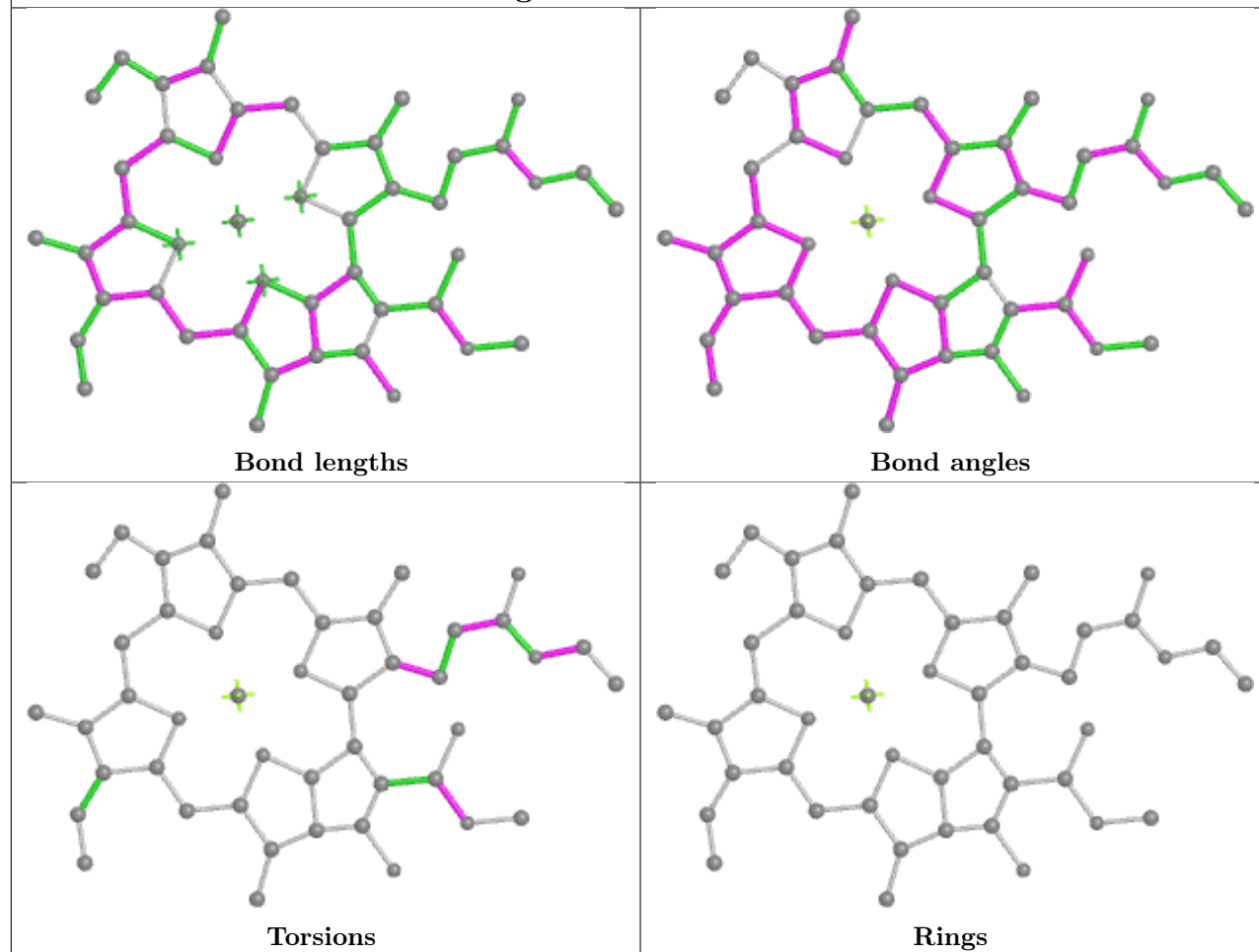
## Ligand CLA ba 833



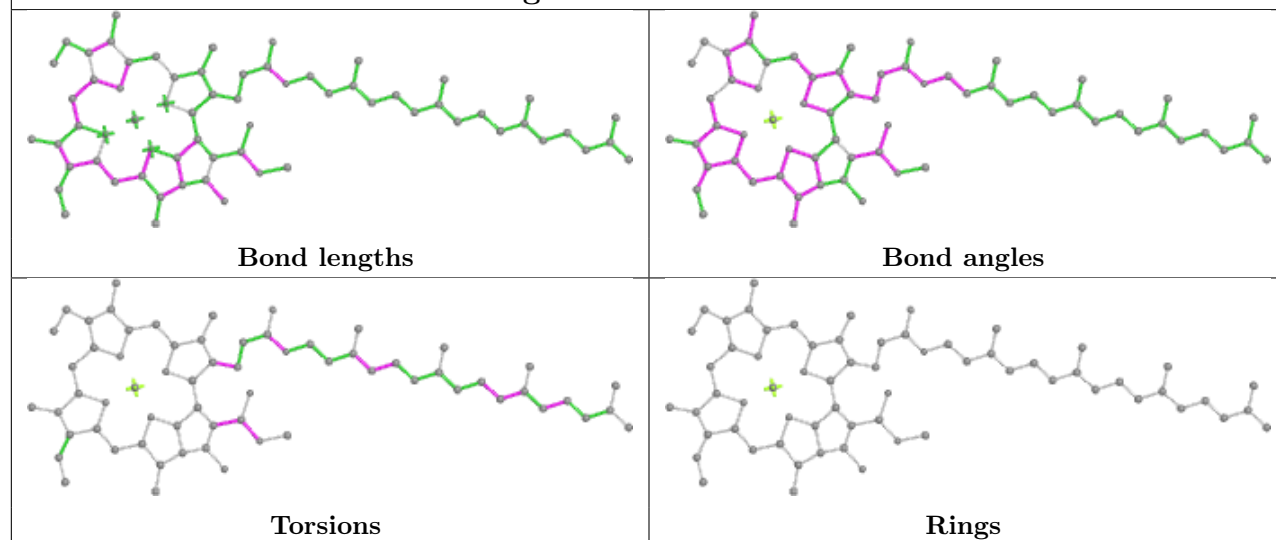


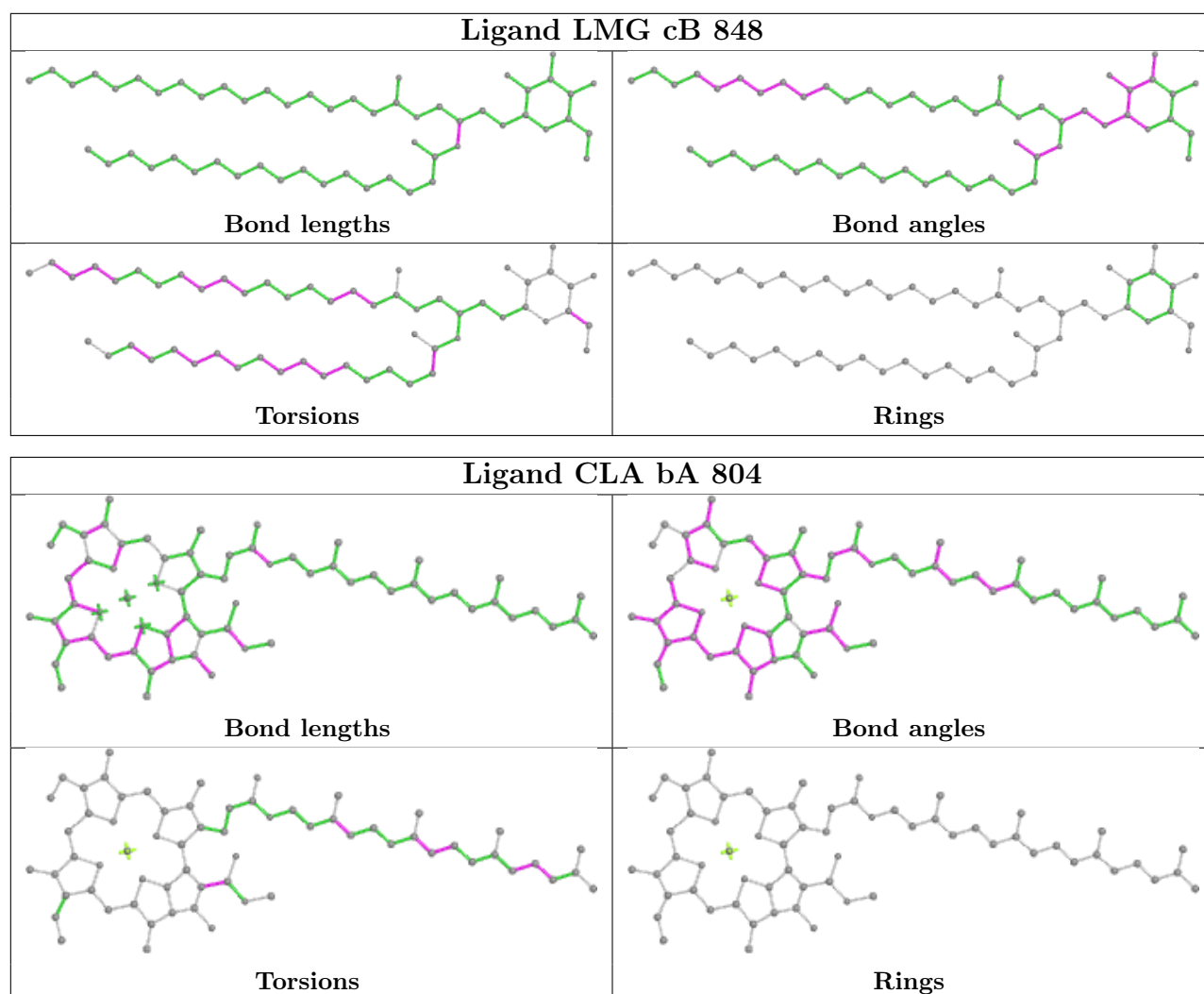


## Ligand CLA bB 839

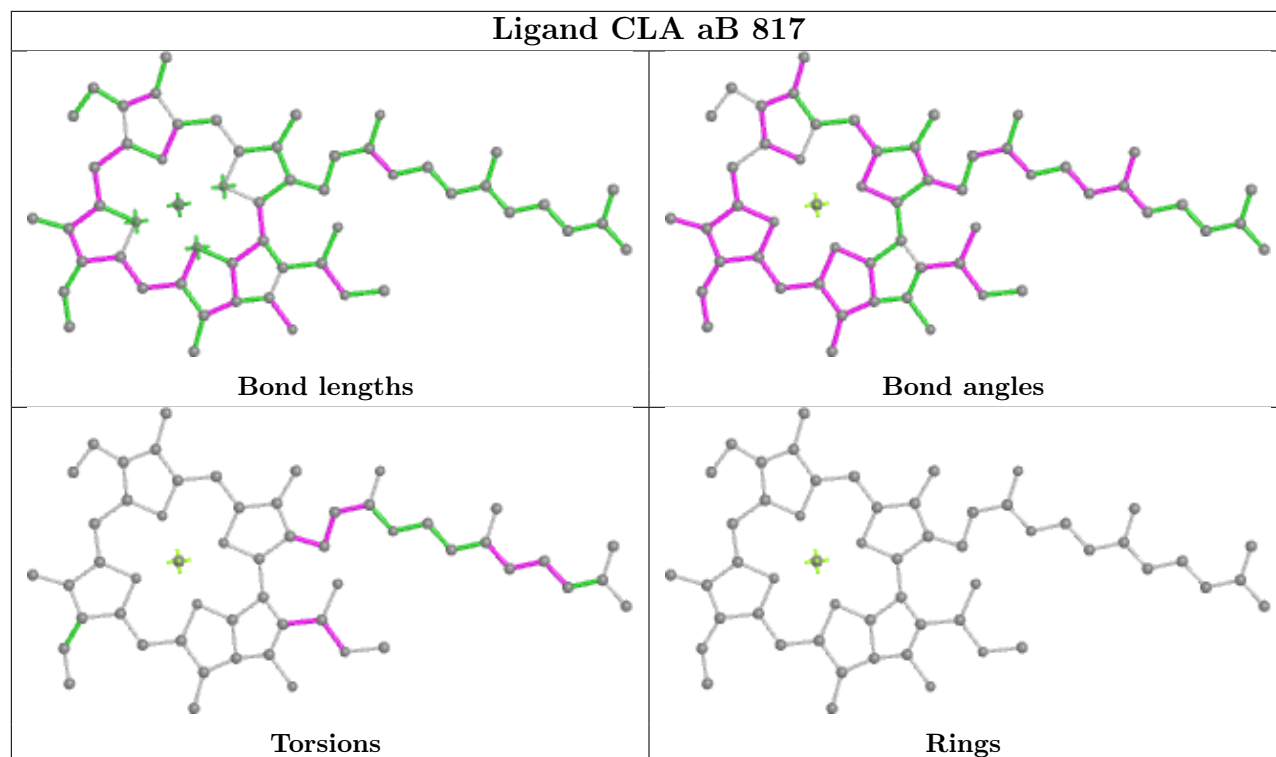


## Ligand CLA aA 818

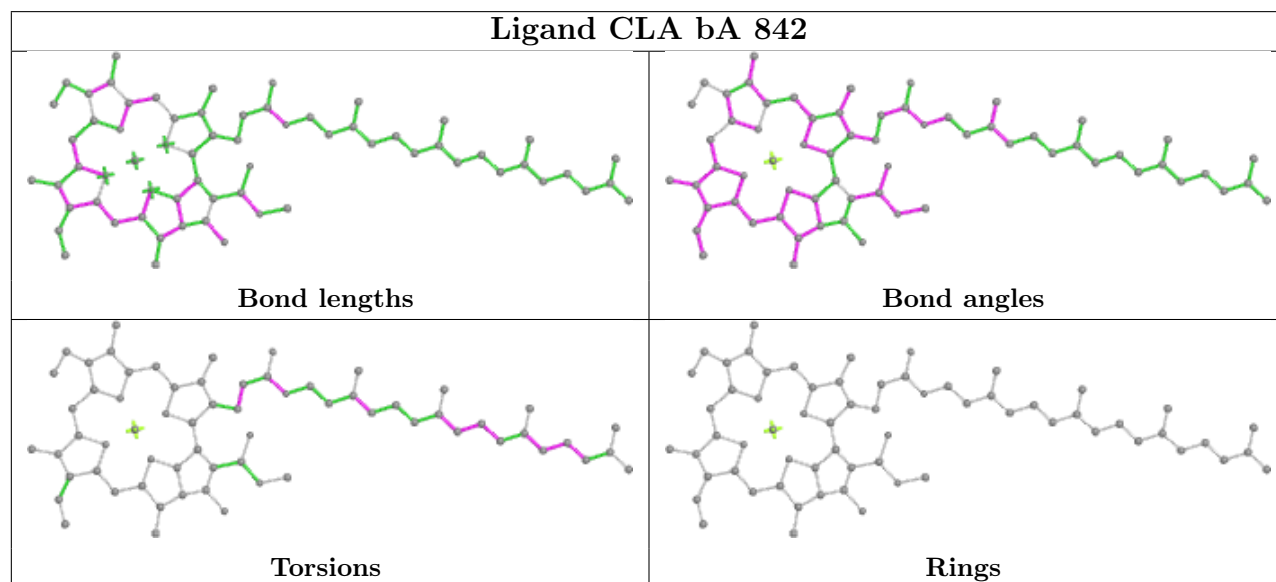


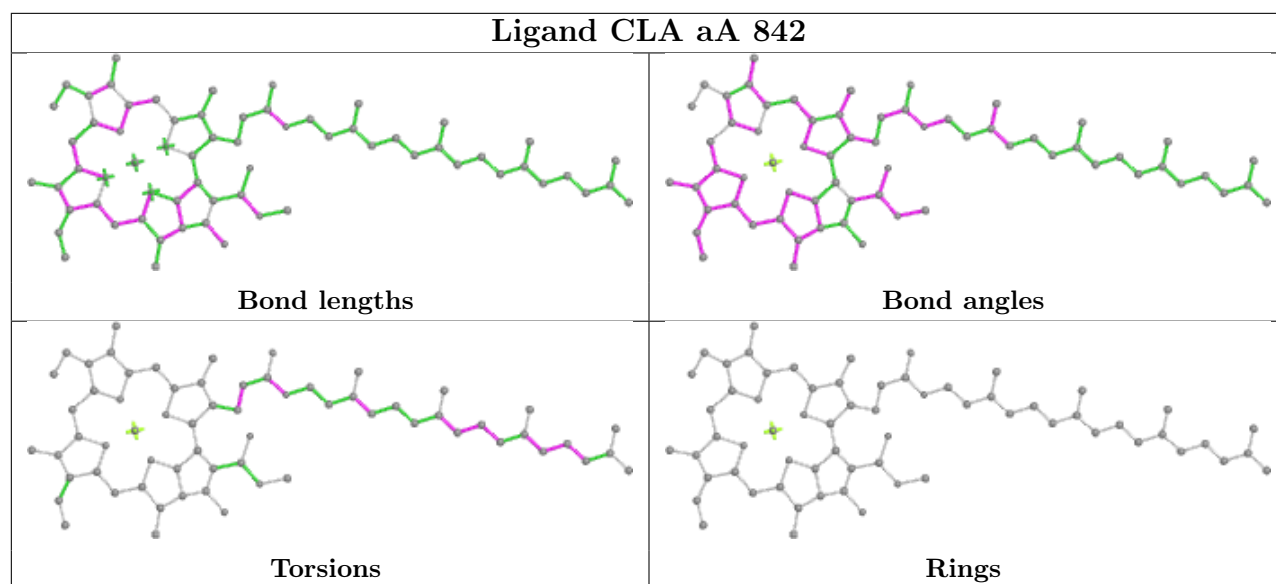
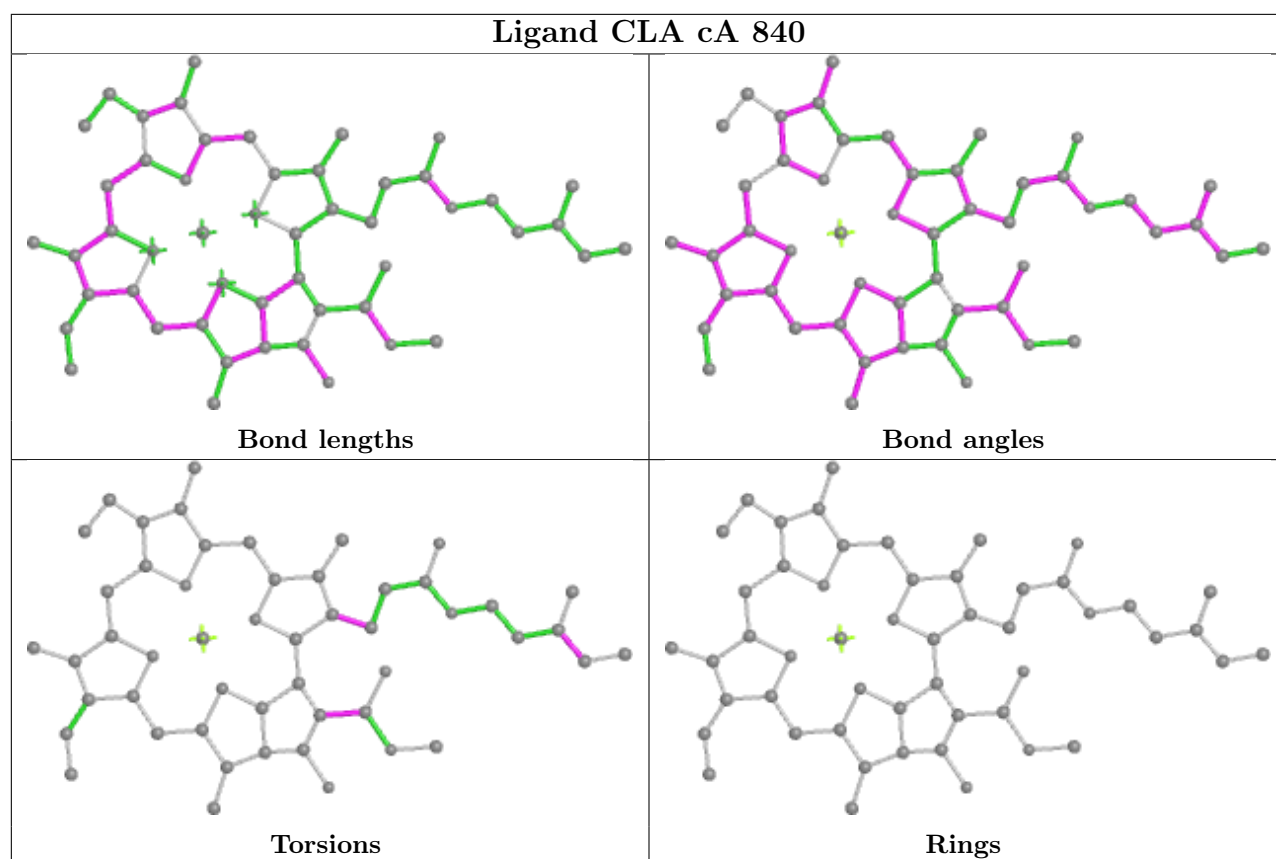


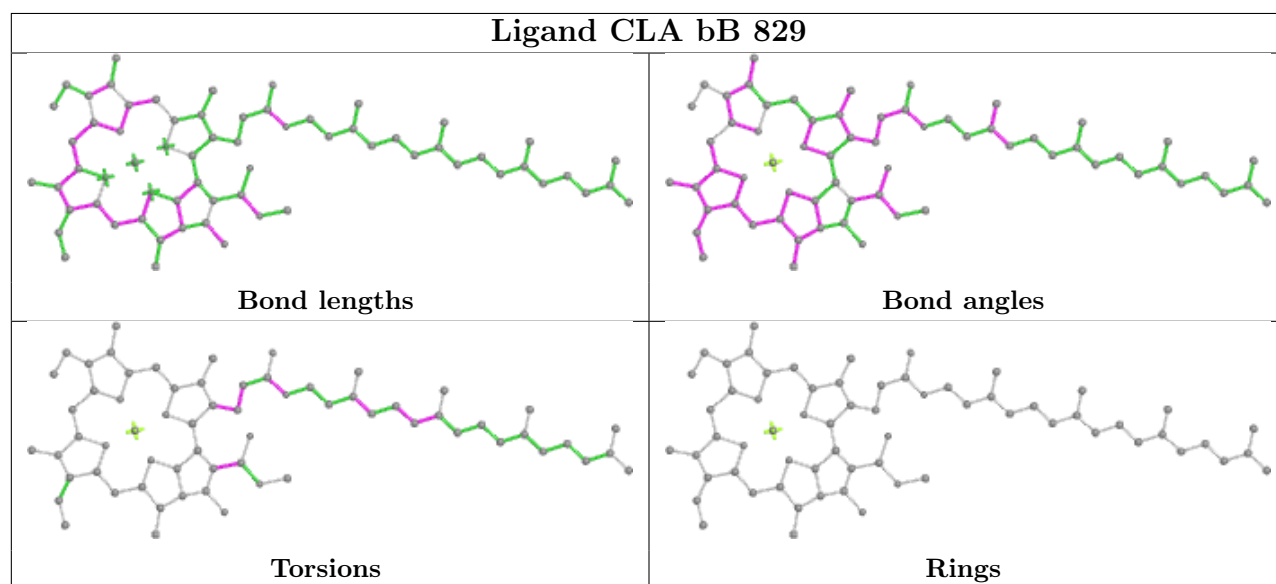
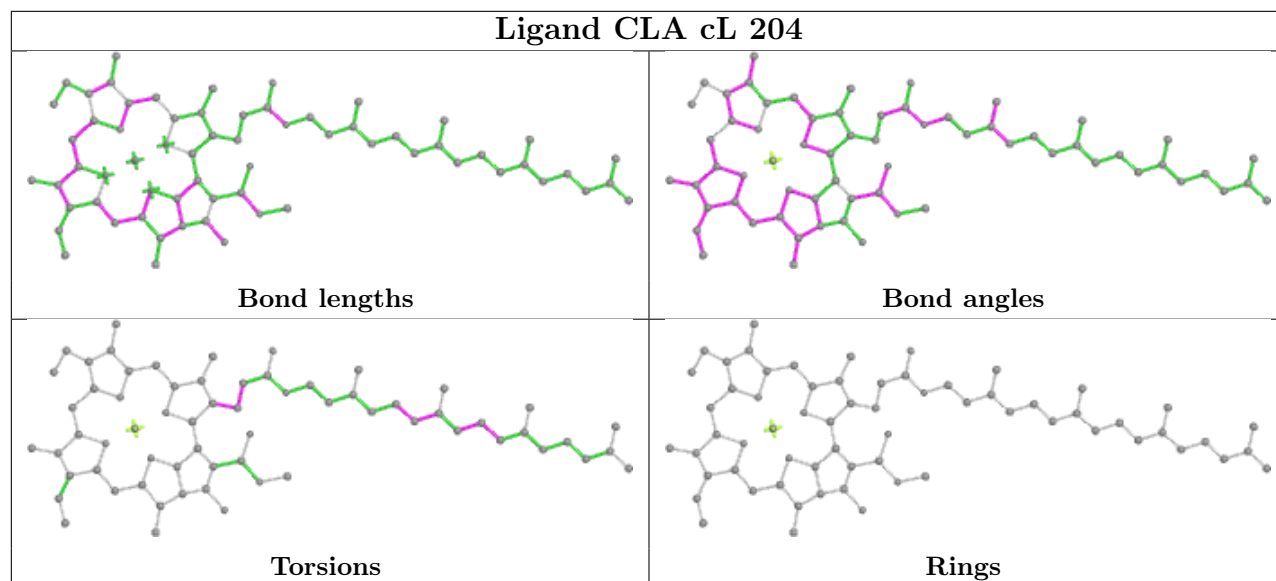
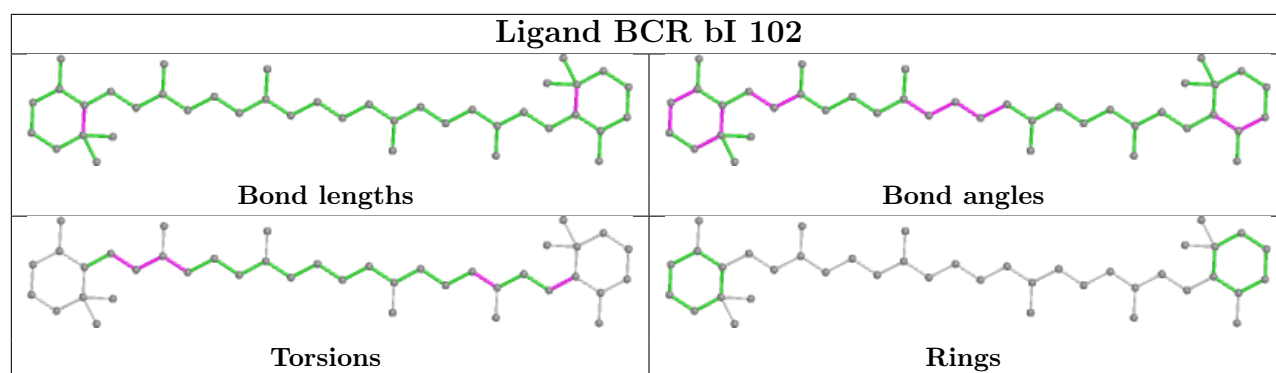
## Ligand CLA aB 817

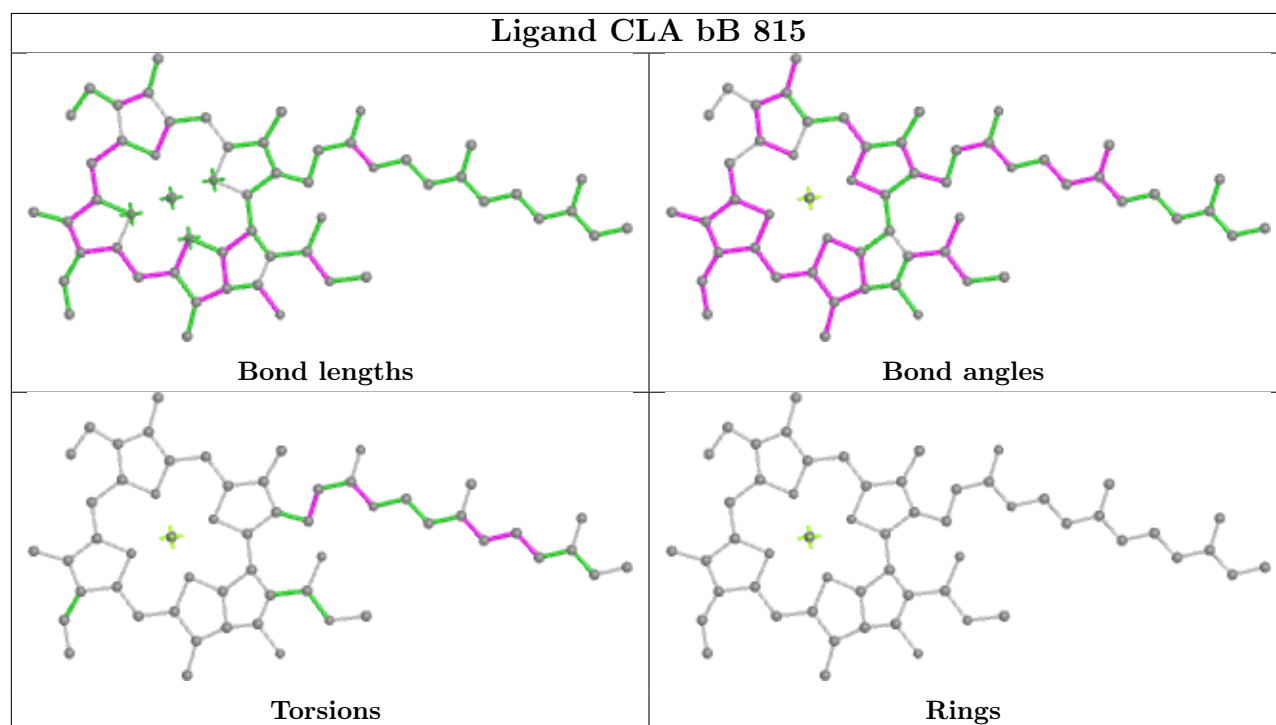
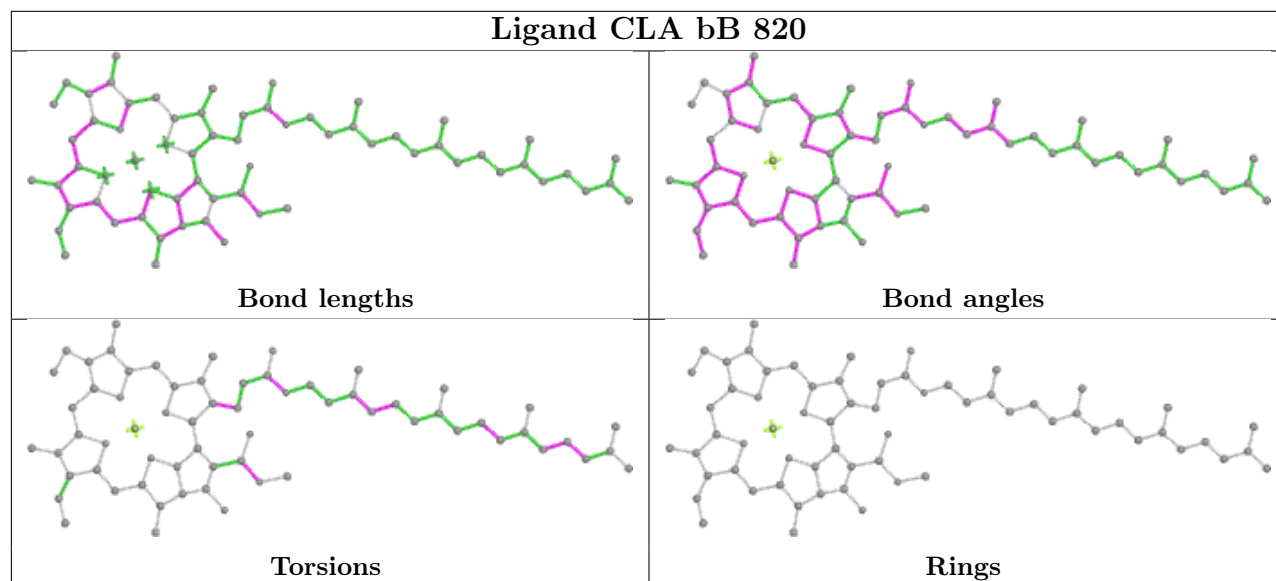
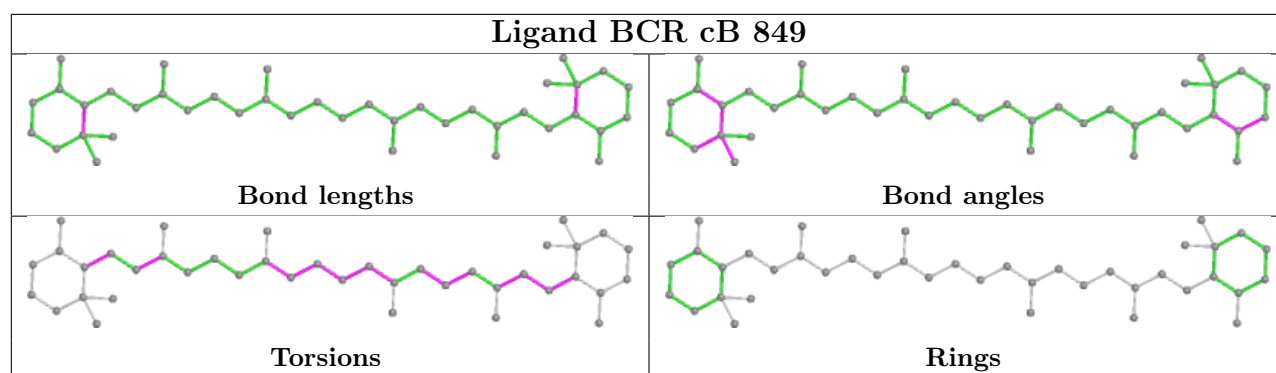


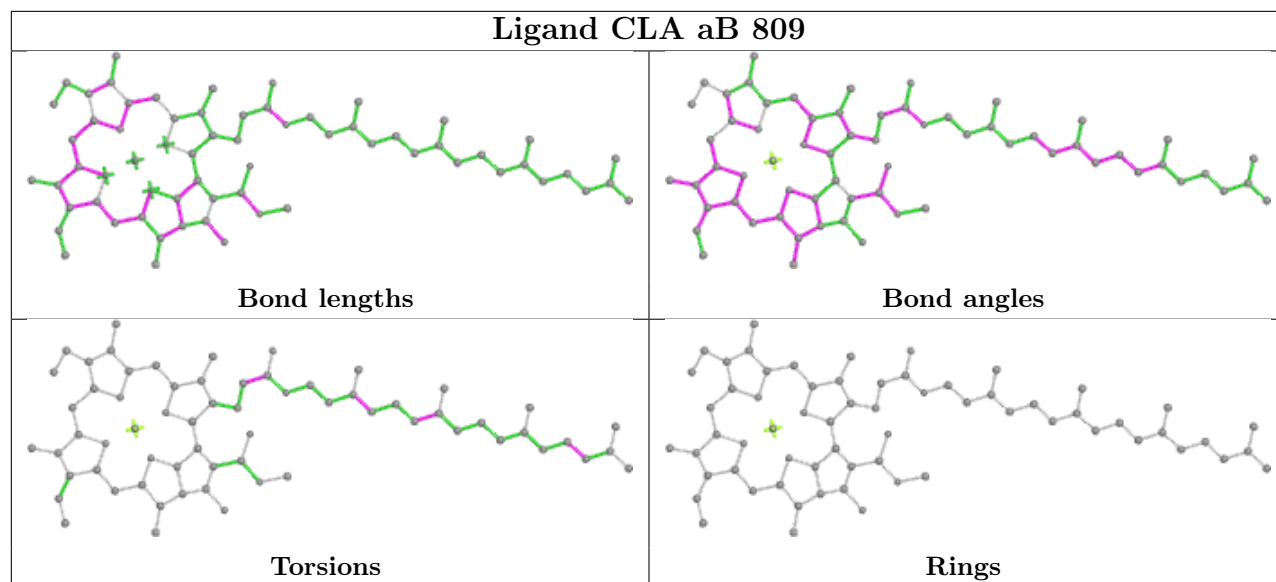
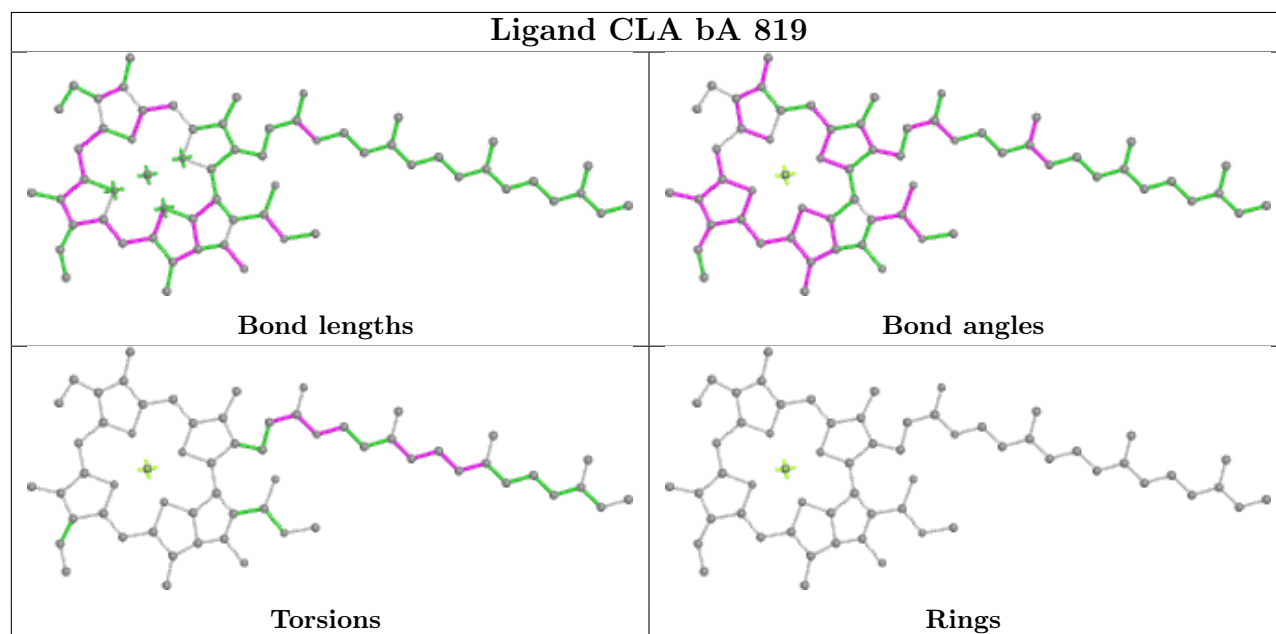
## Ligand CLA bA 842

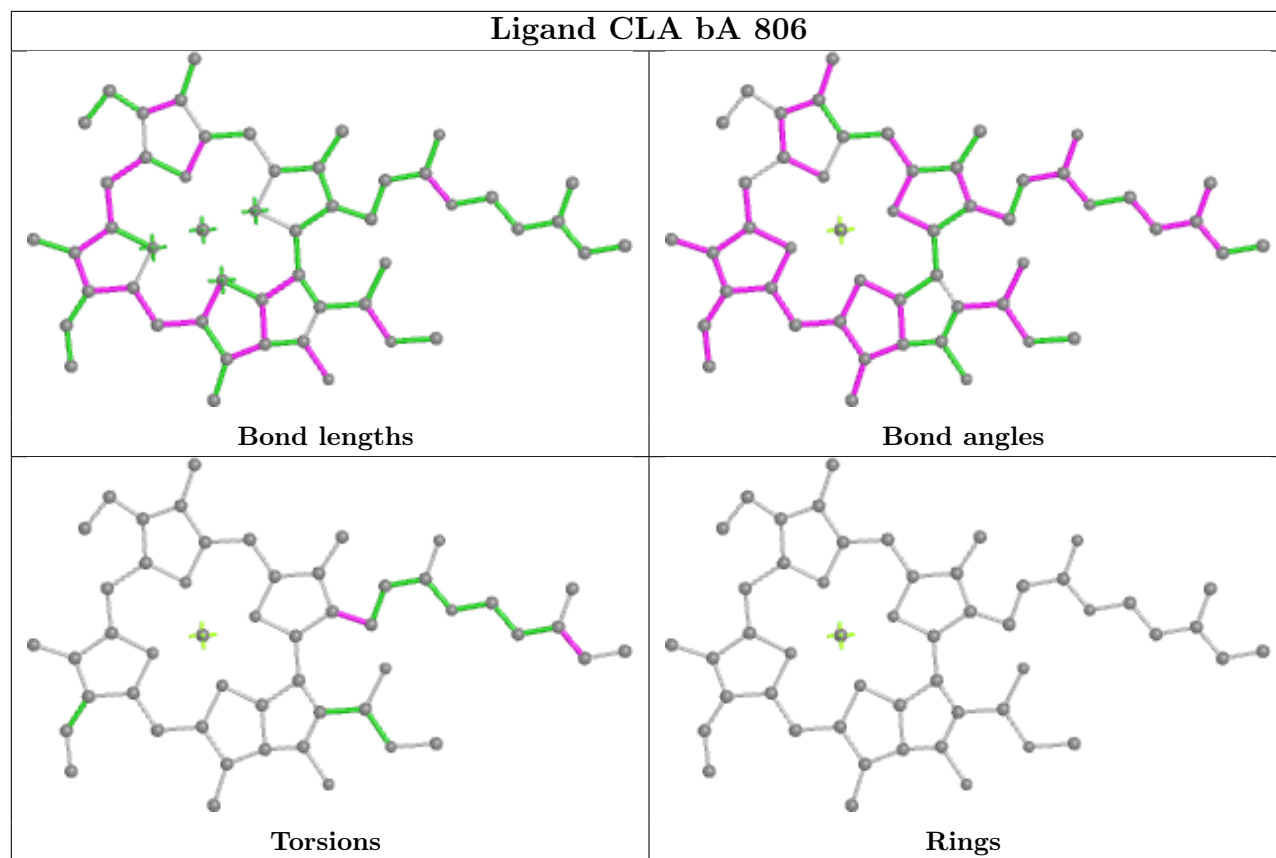




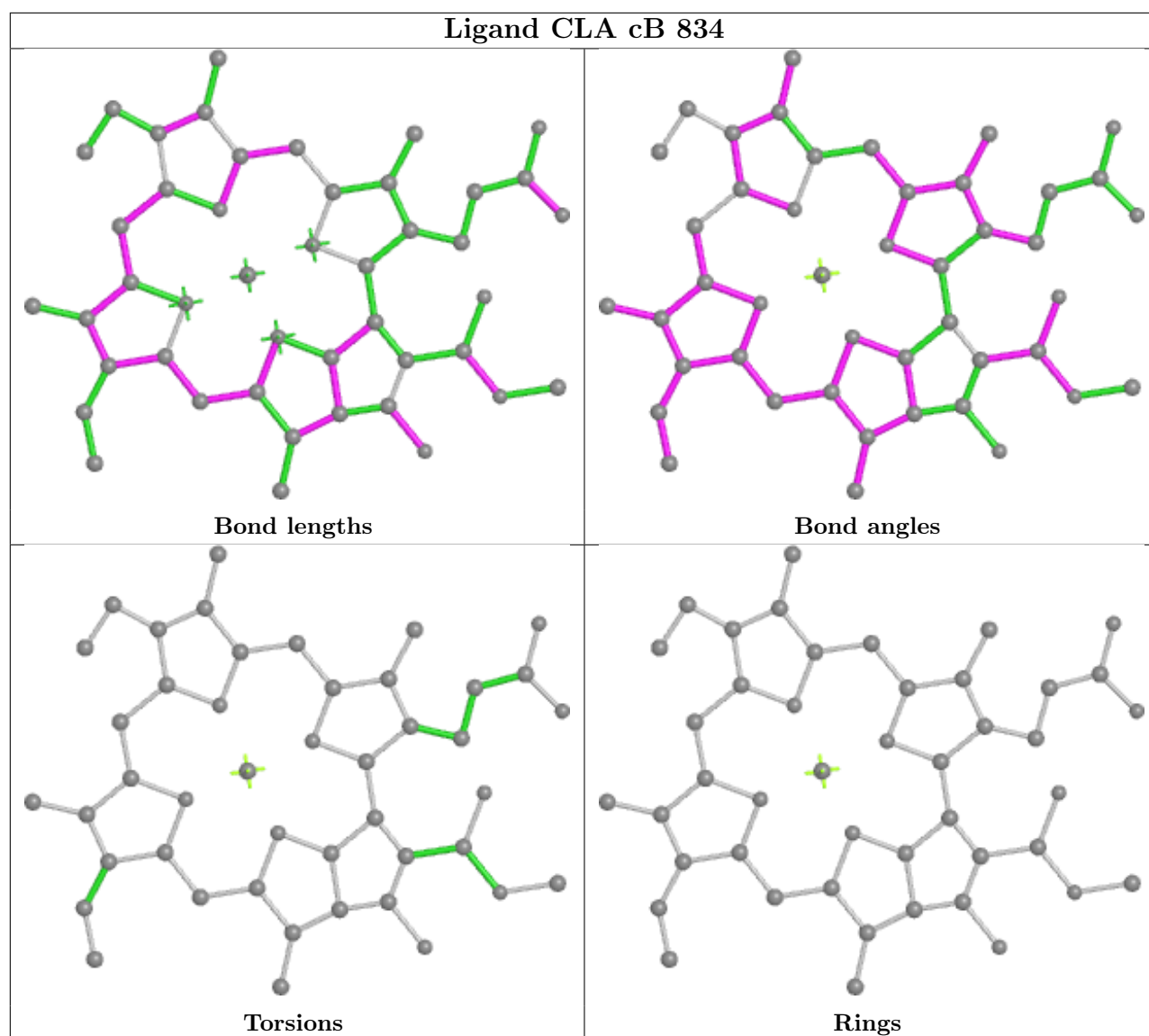




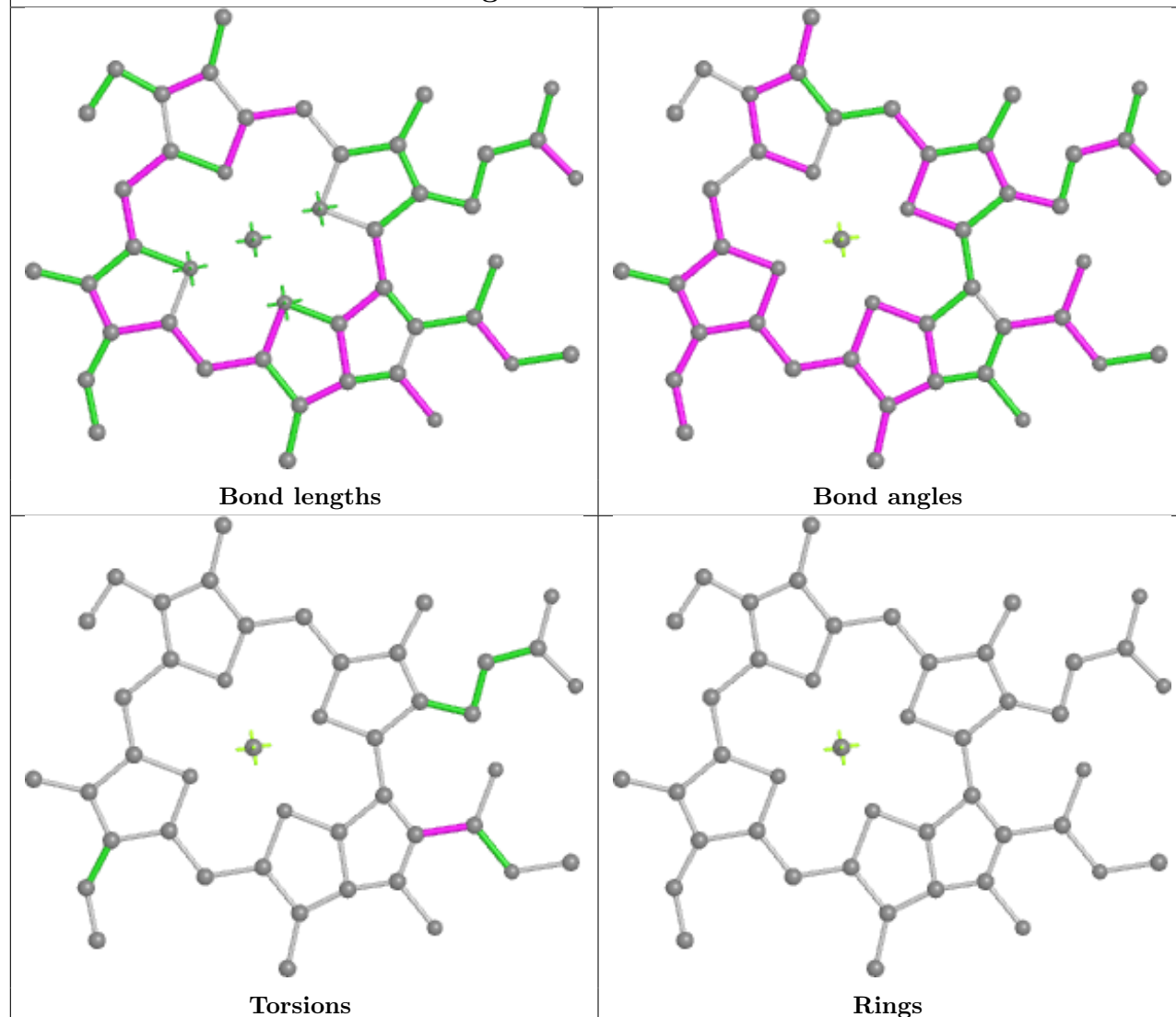
**Ligand CLA aB 809****Ligand CLA bA 819**



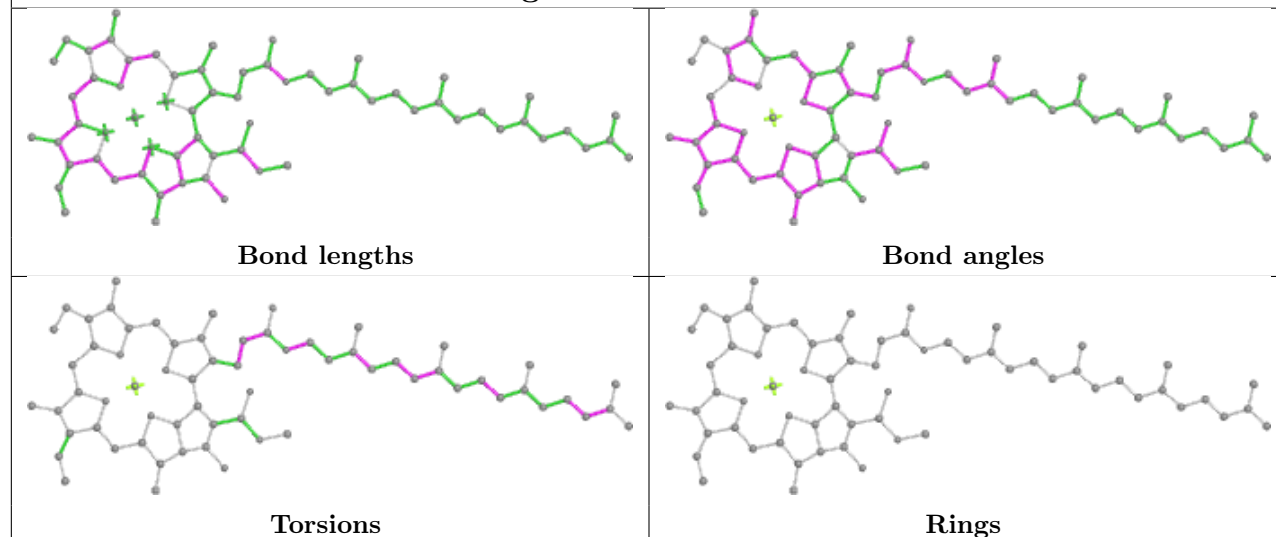


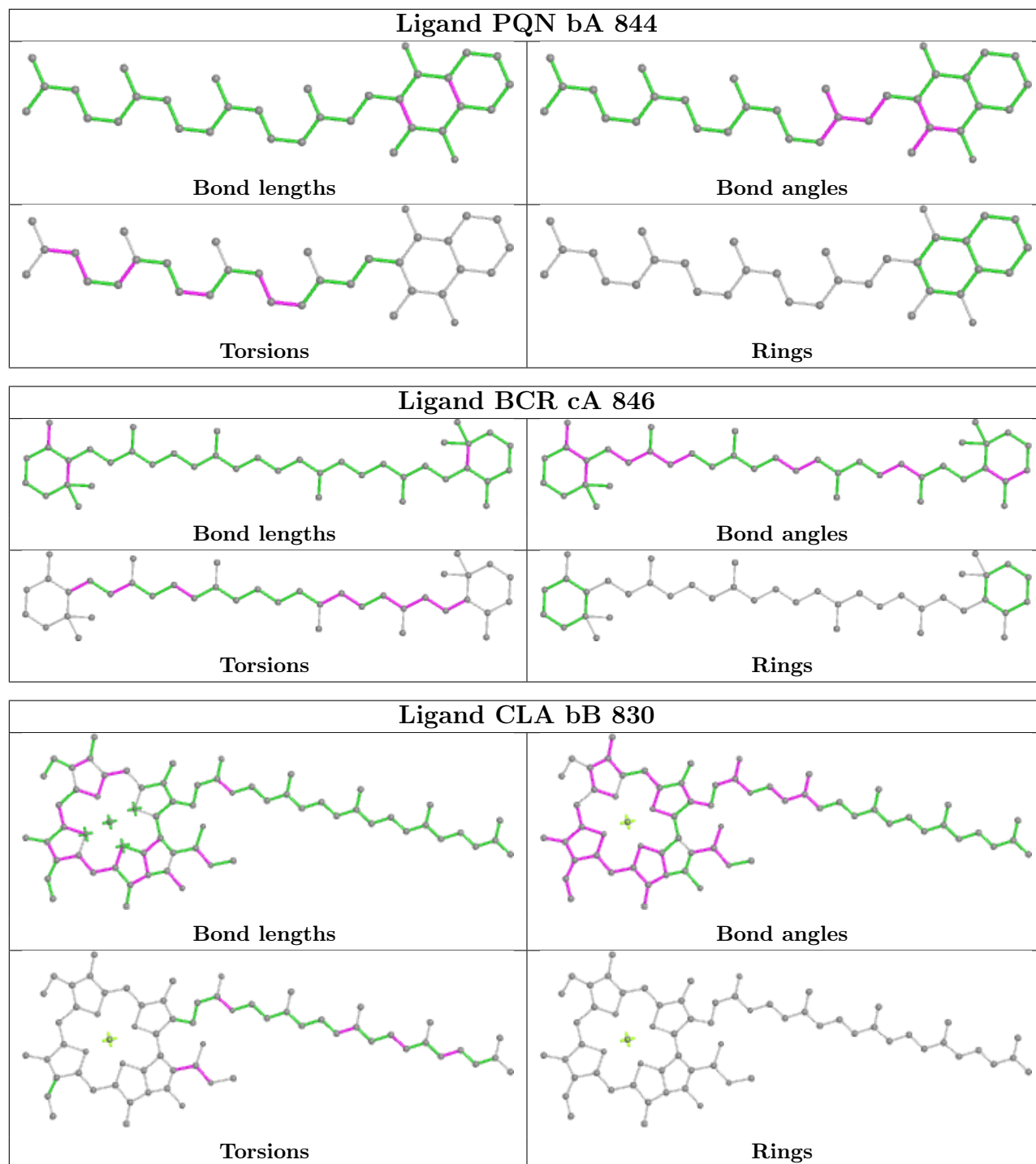


## Ligand CLA aA 813

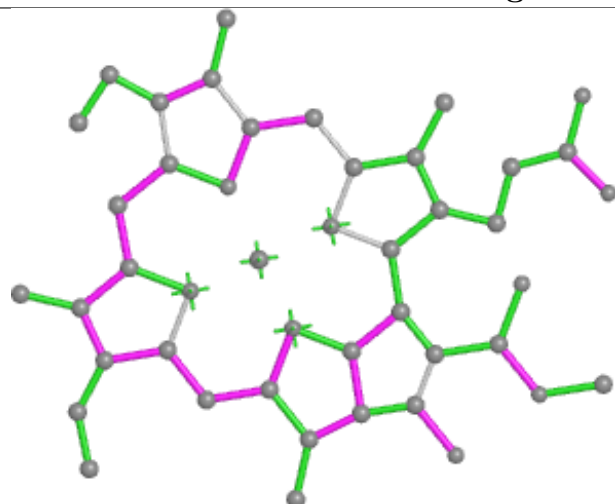


## Ligand CLA bA 841

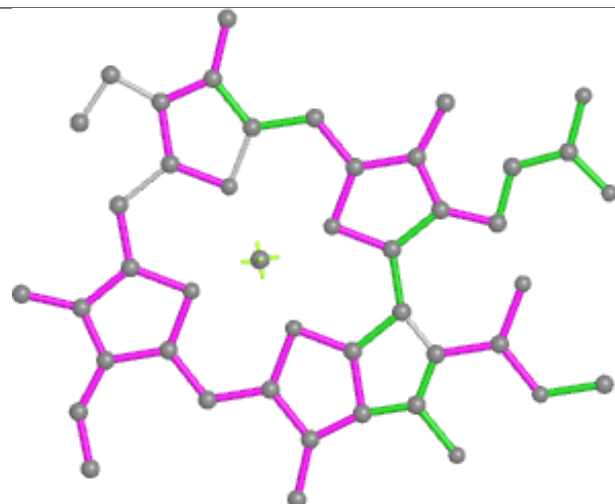




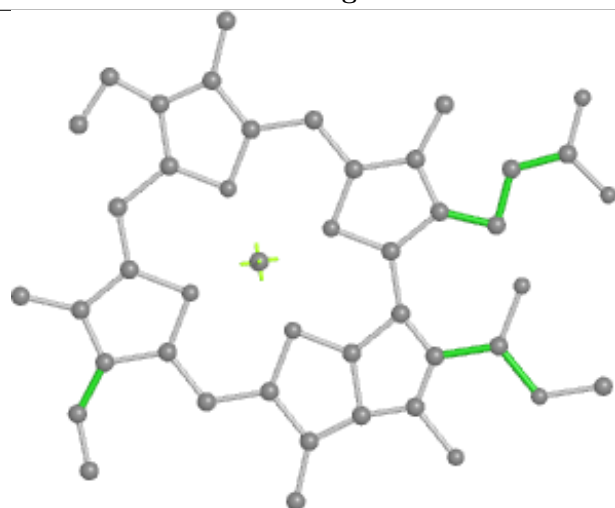
## Ligand CLA bB 834



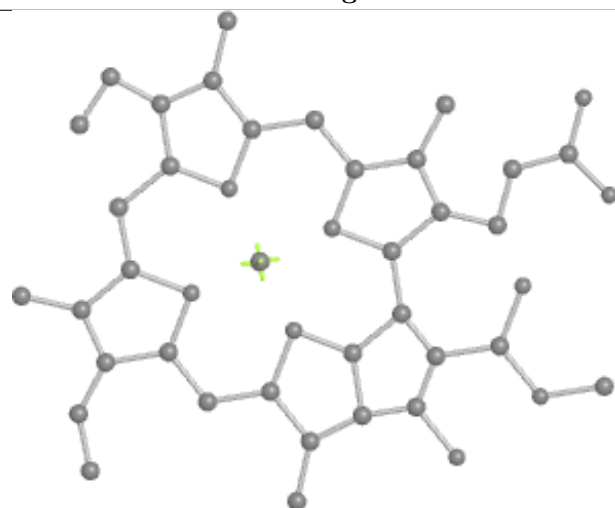
Bond lengths



Bond angles

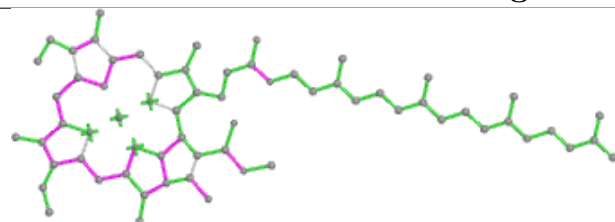


Torsions

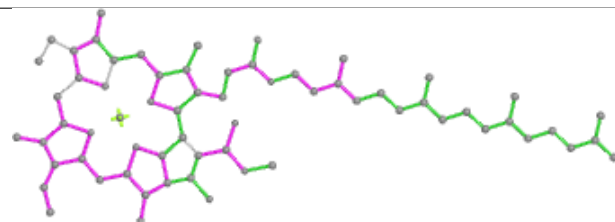


Rings

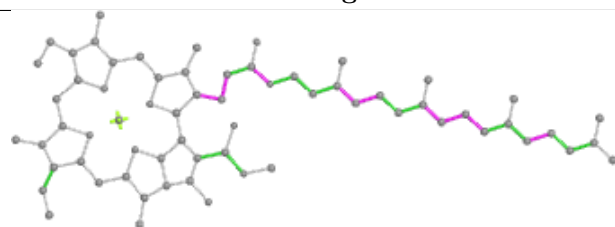
## Ligand CLA cL 203



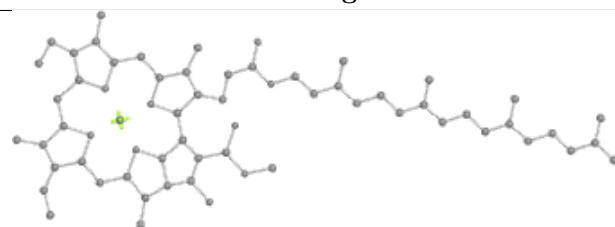
Bond lengths



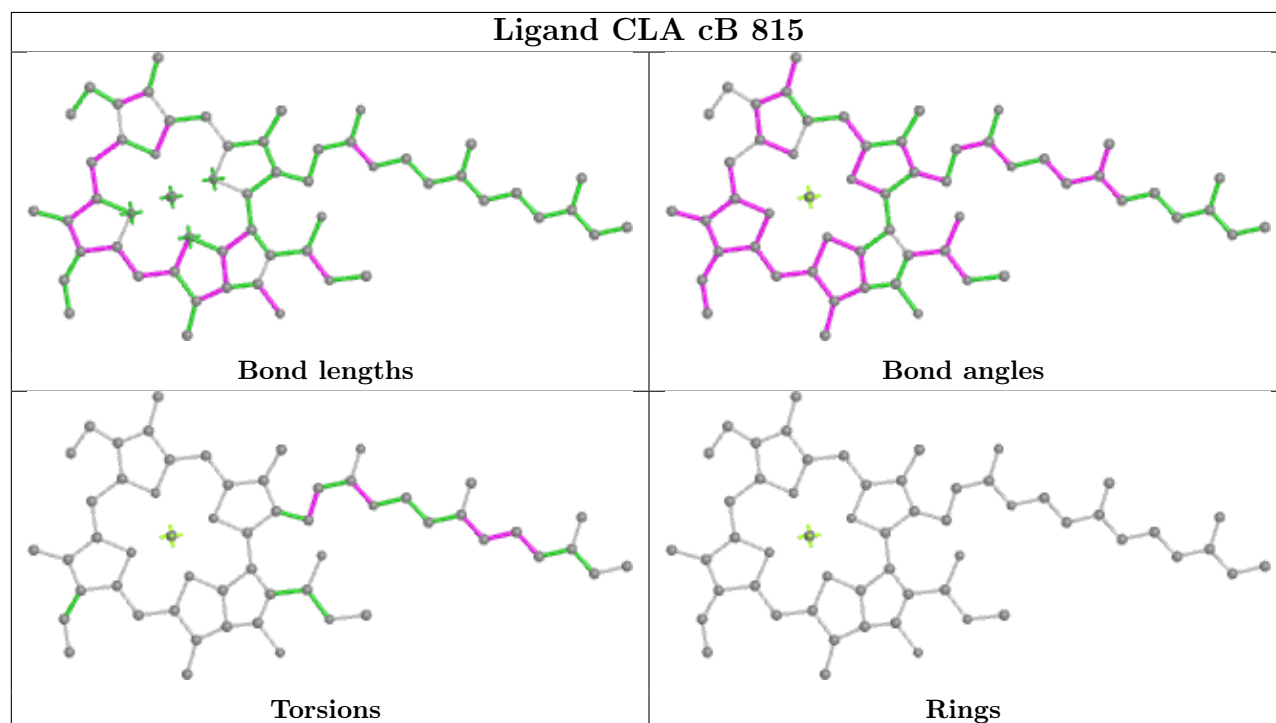
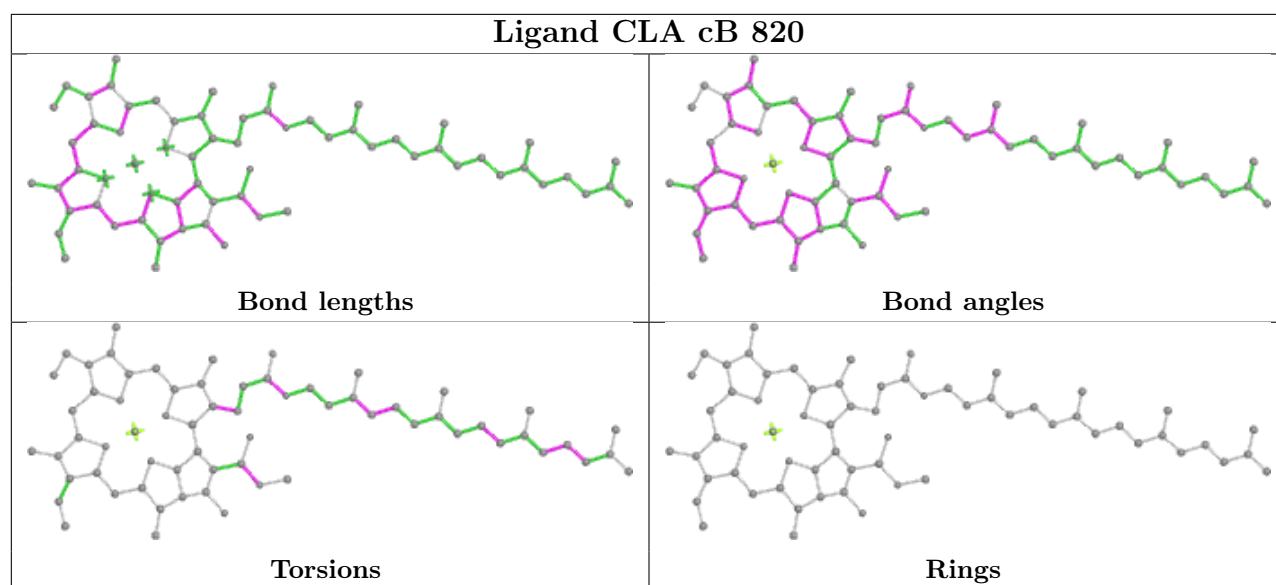
Bond angles

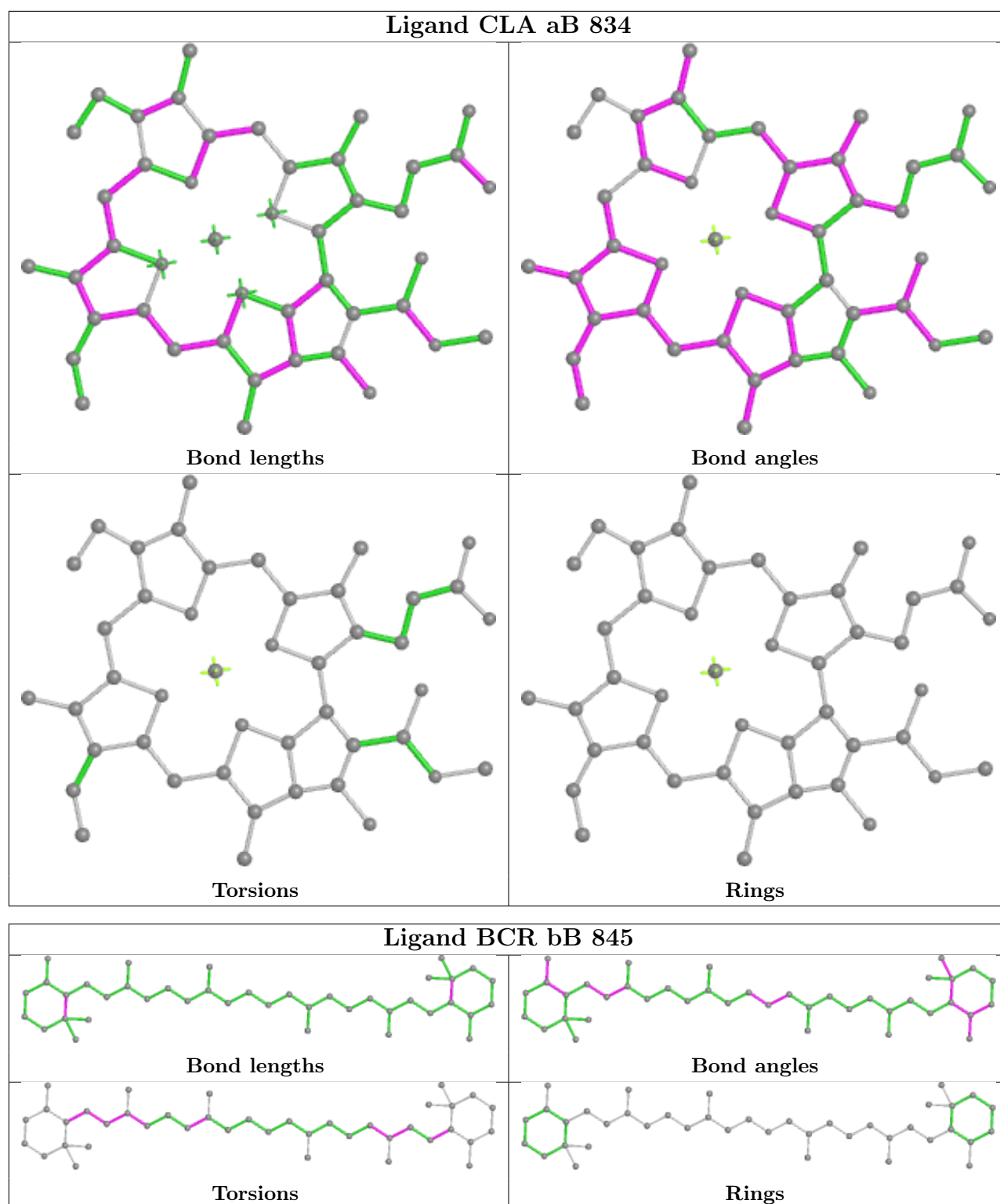


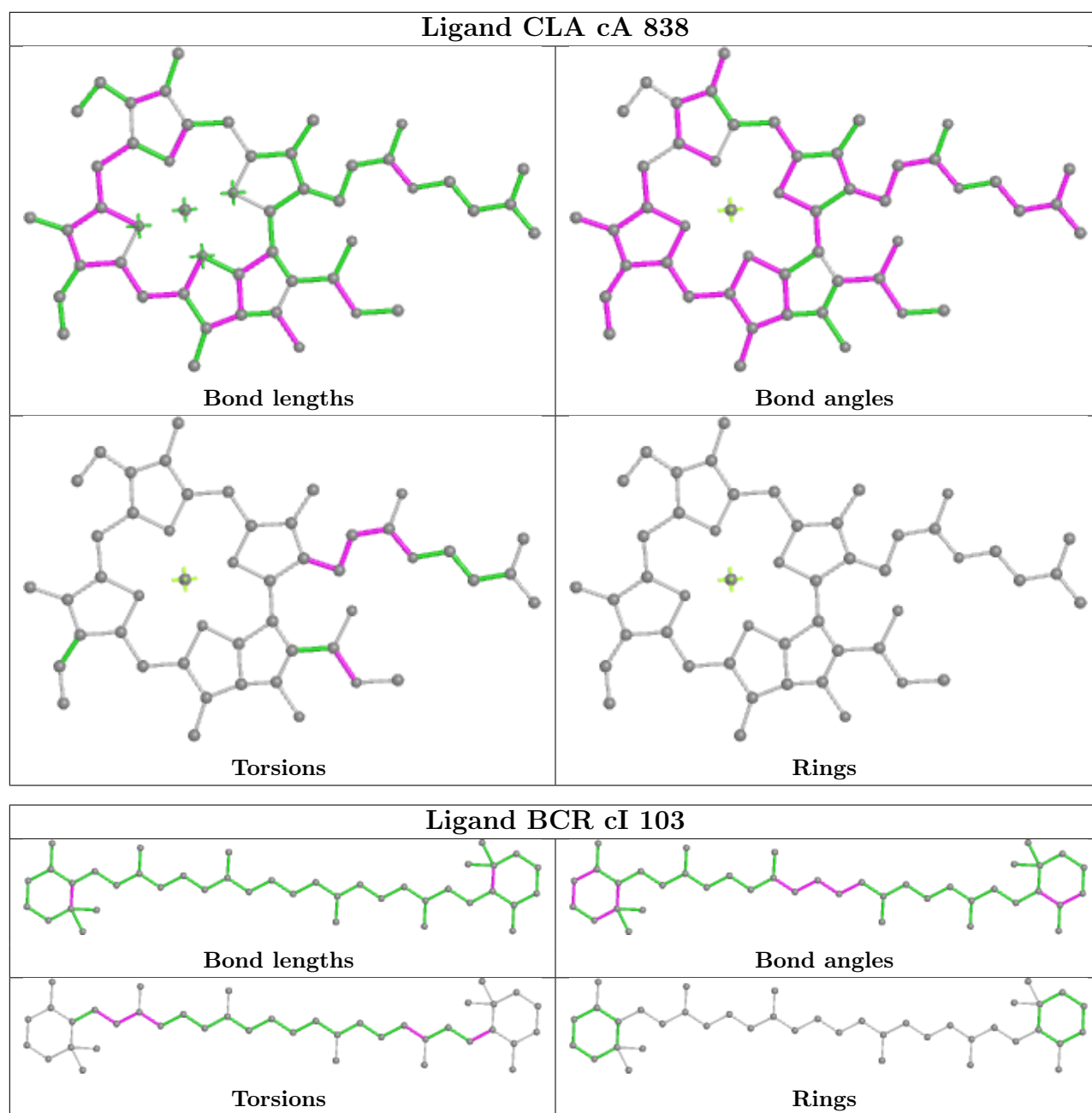
Torsions

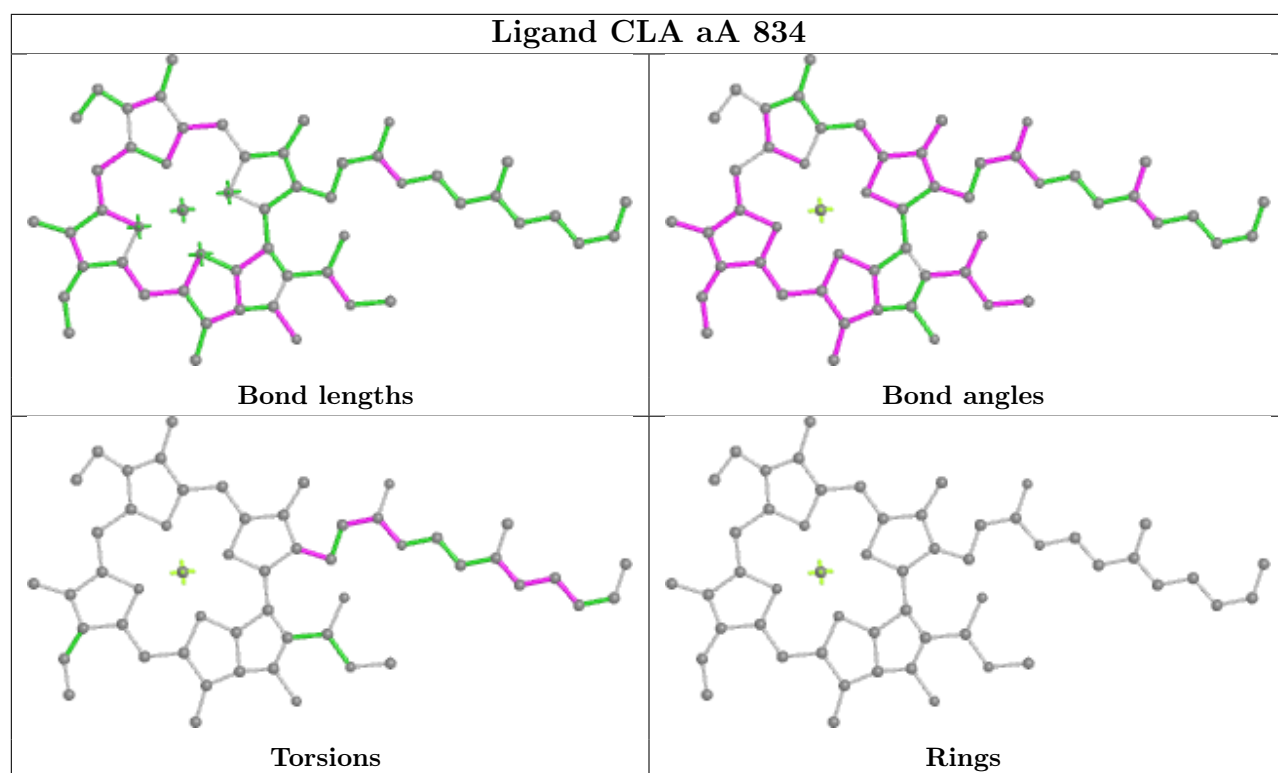


Rings



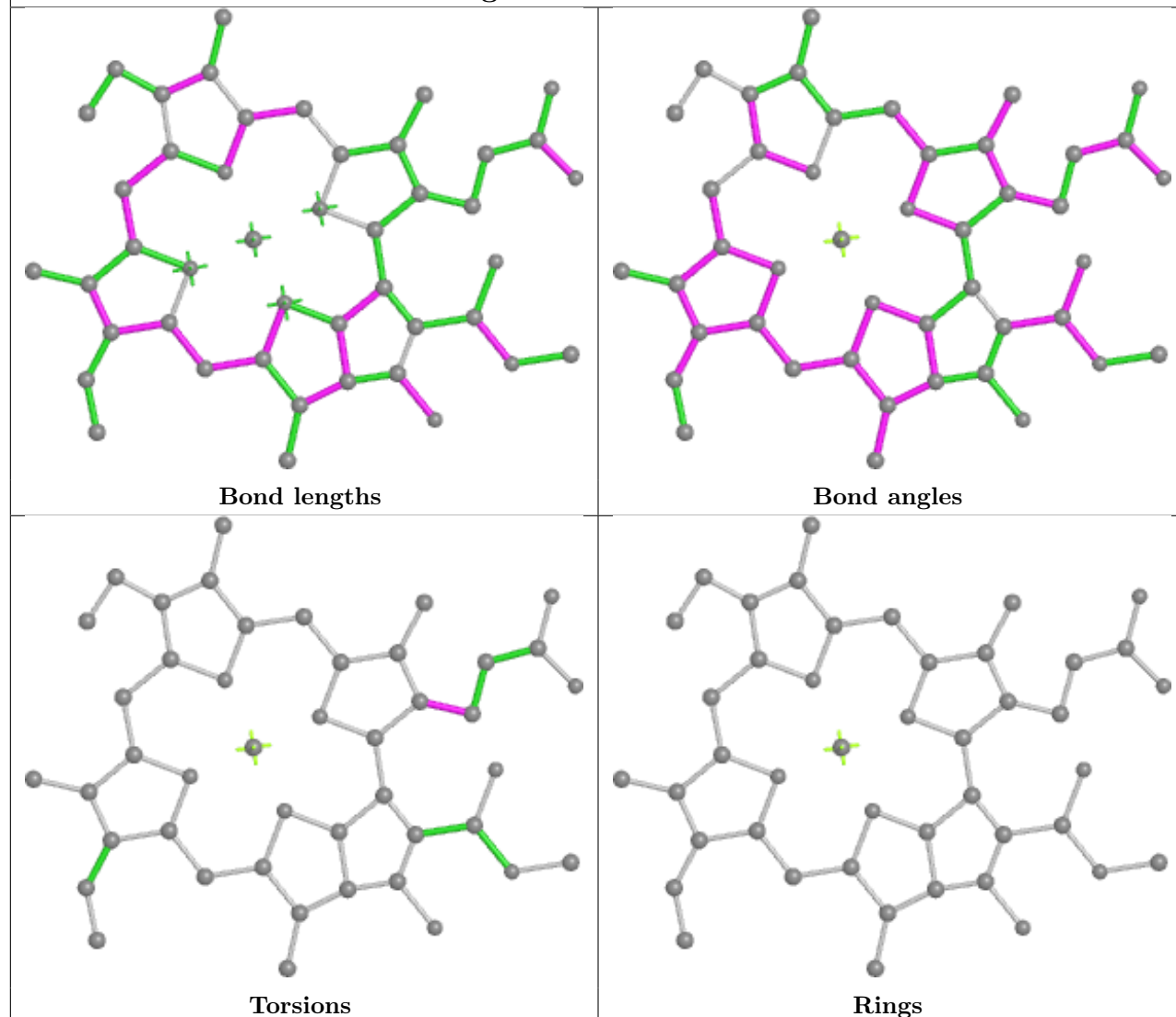




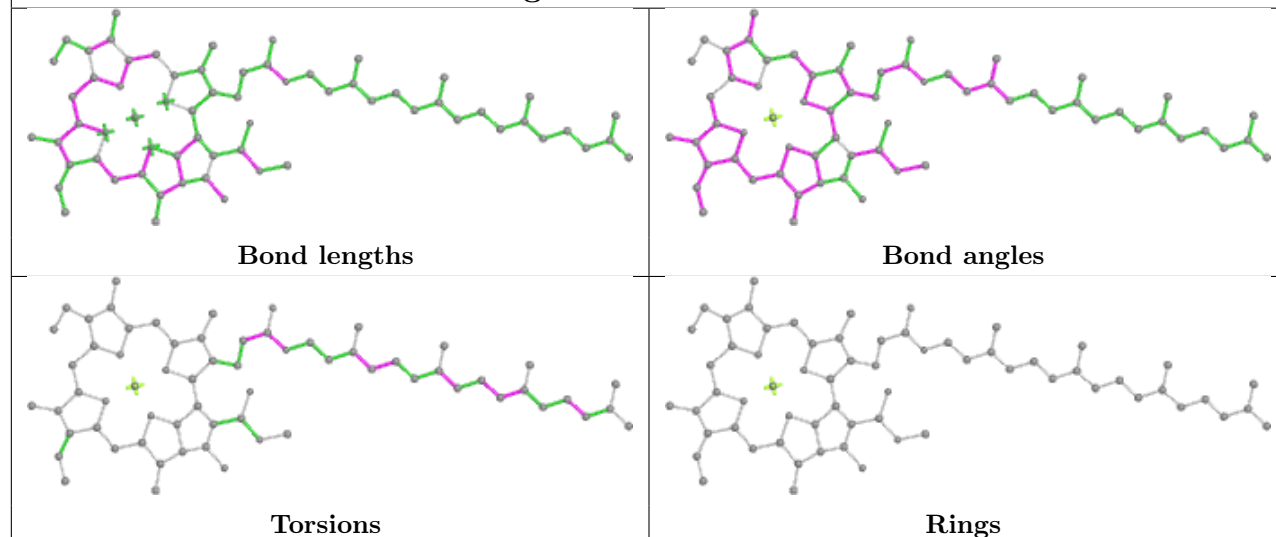


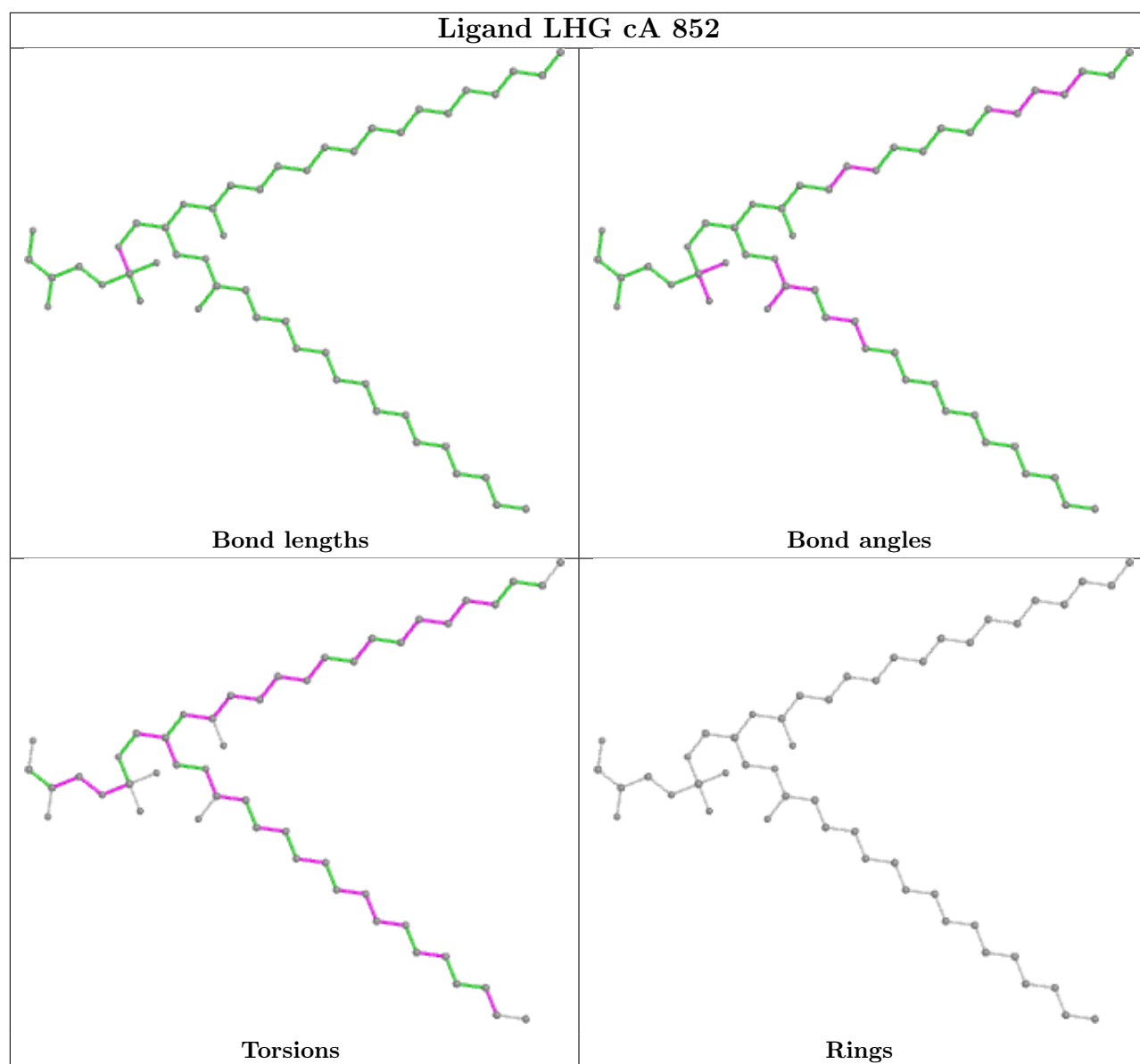


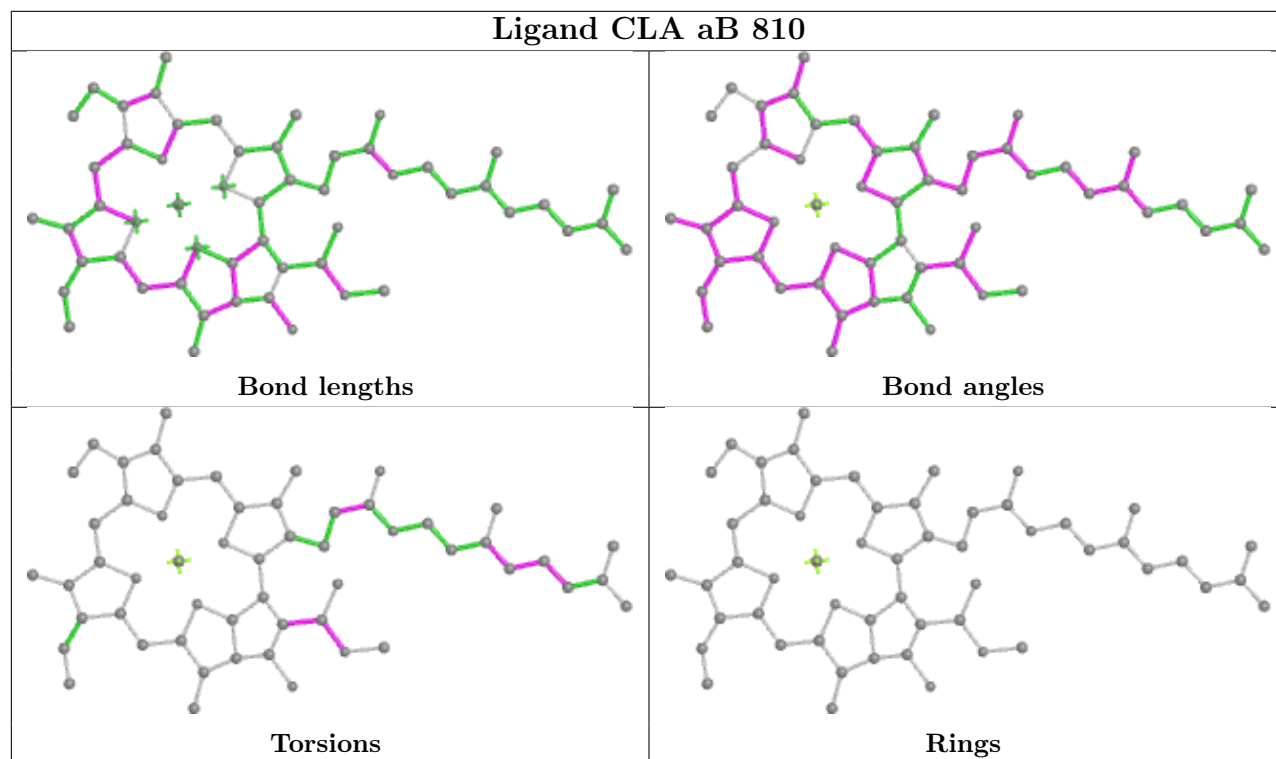
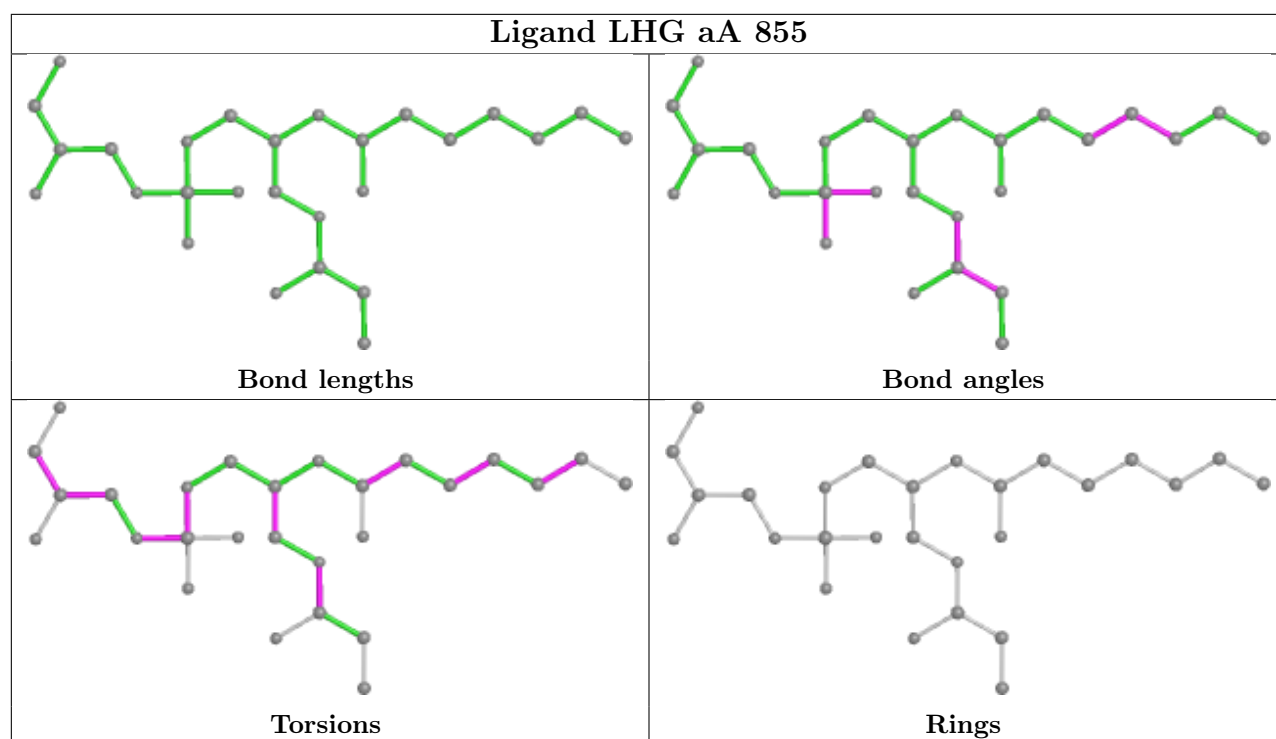
## Ligand CLA bB 812



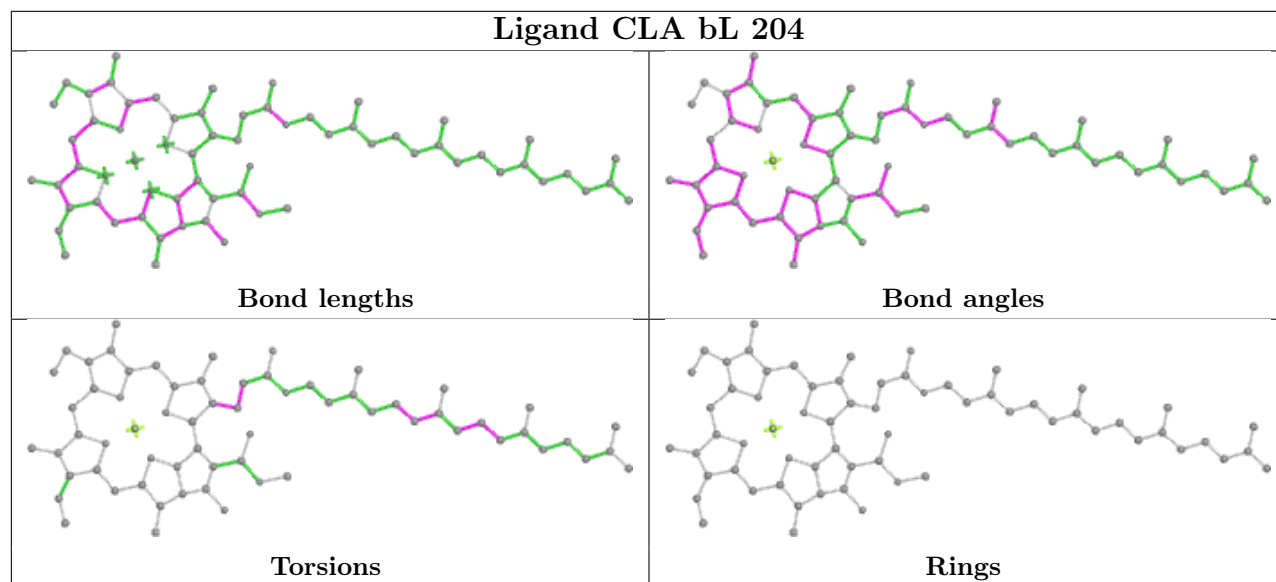
## Ligand CLA aB 808



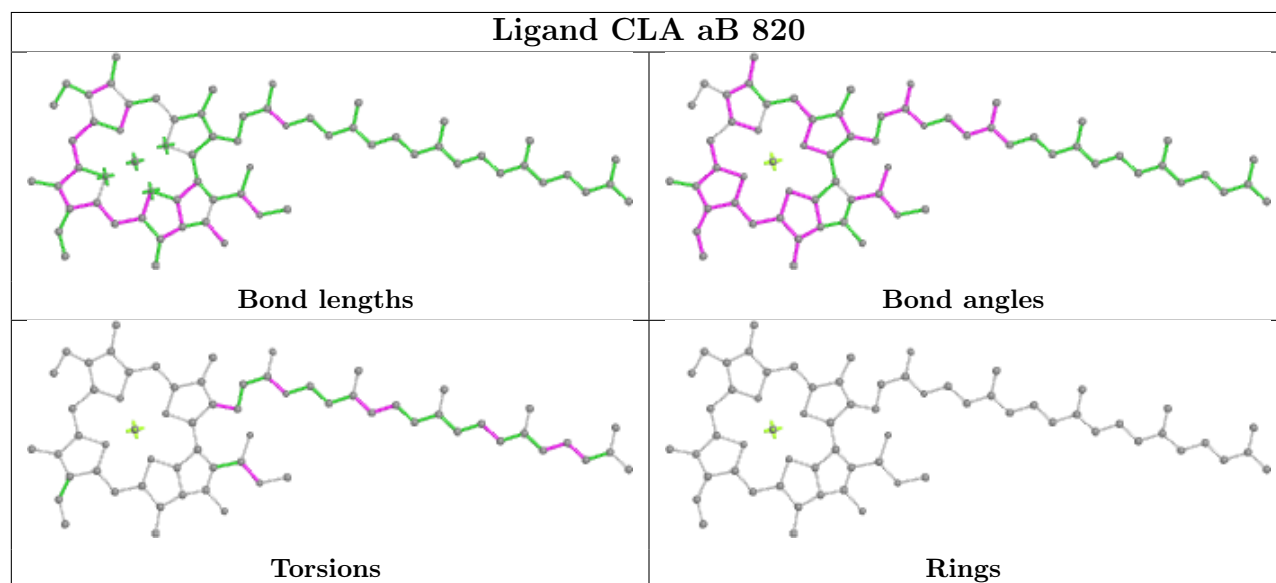


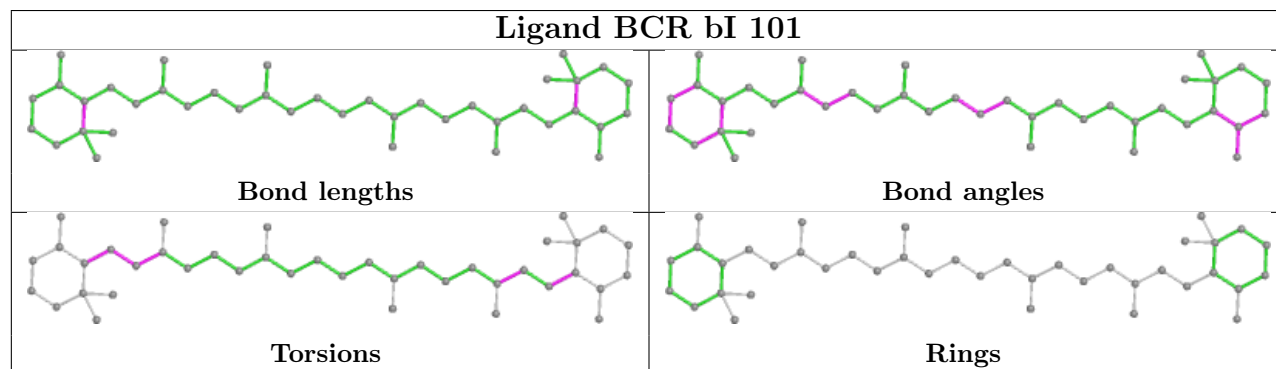
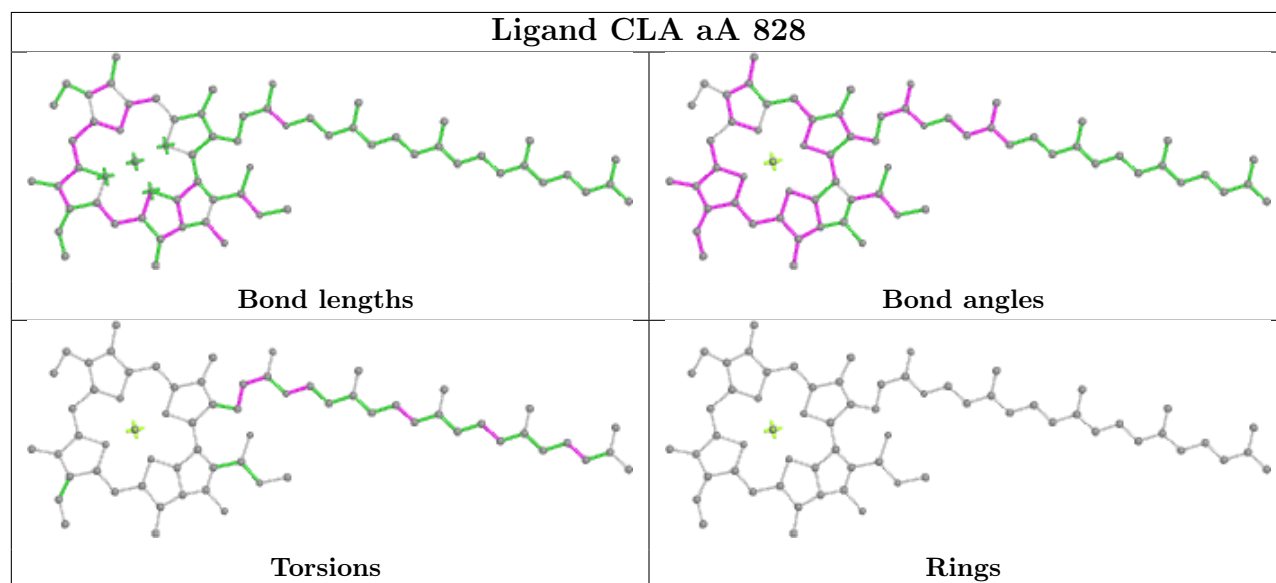
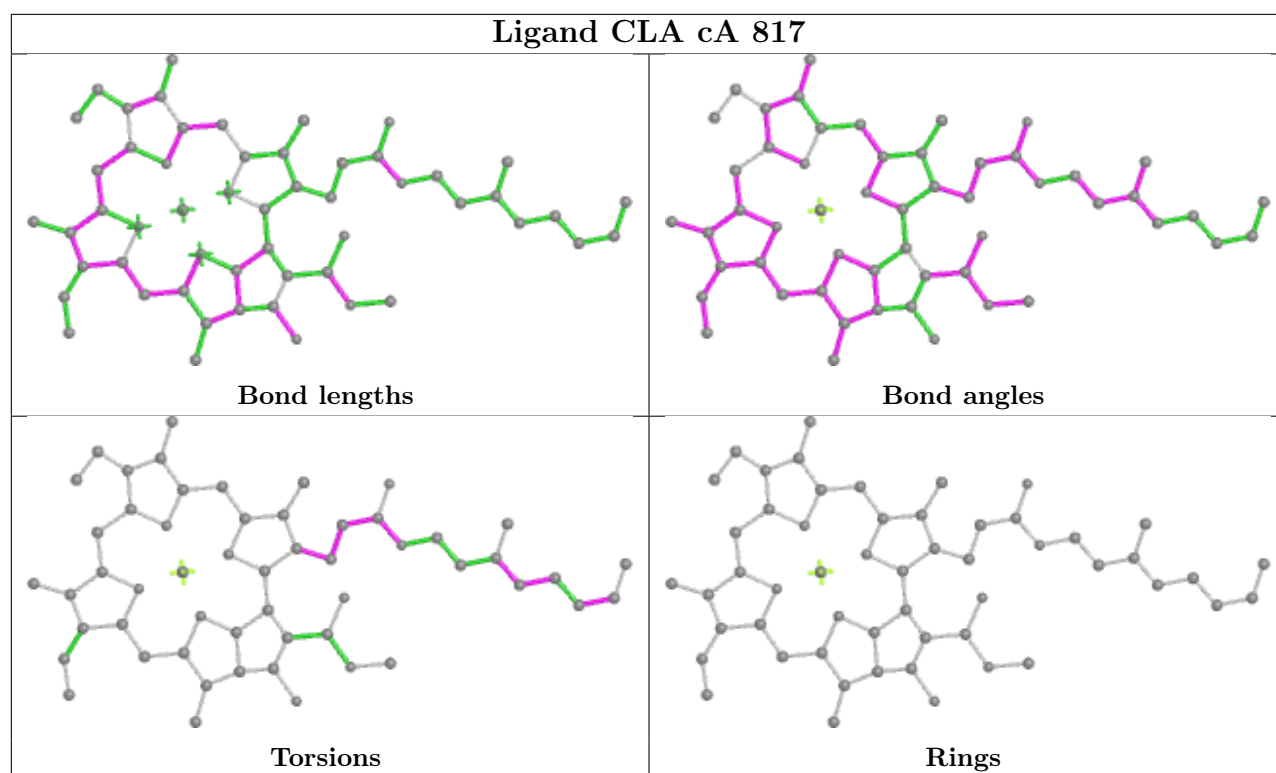


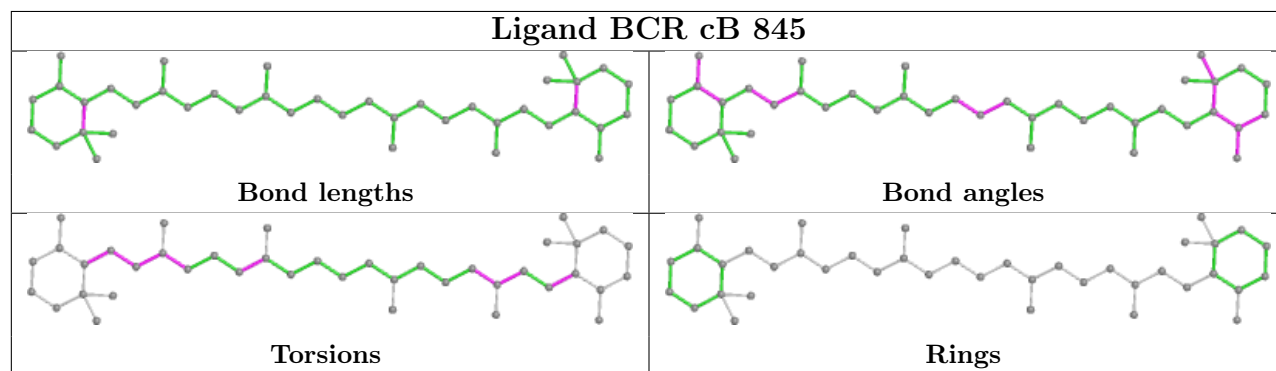
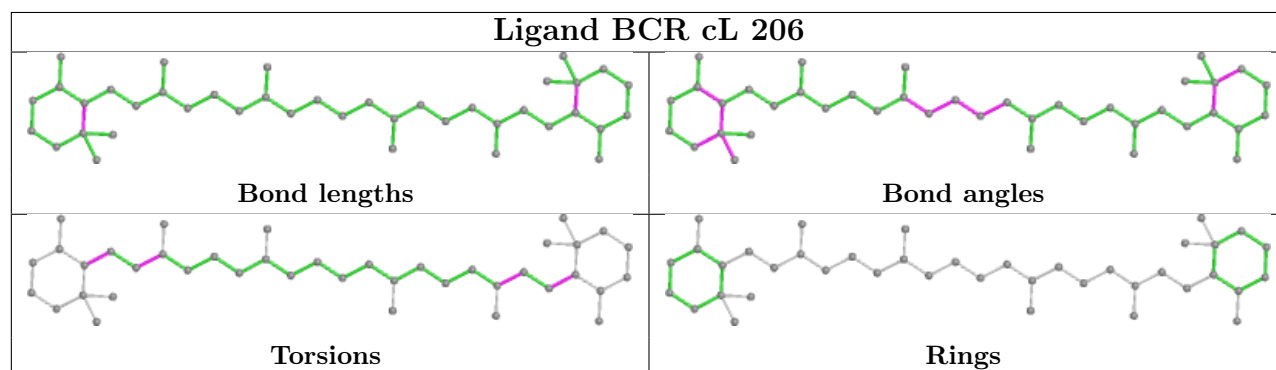
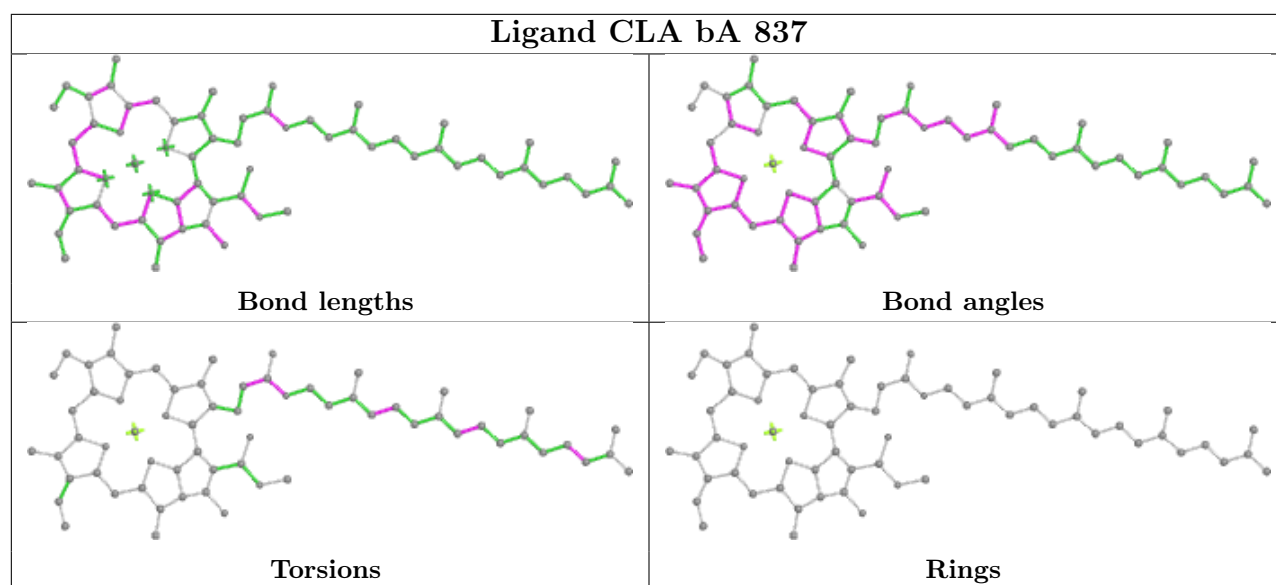
## Ligand CLA bL 204

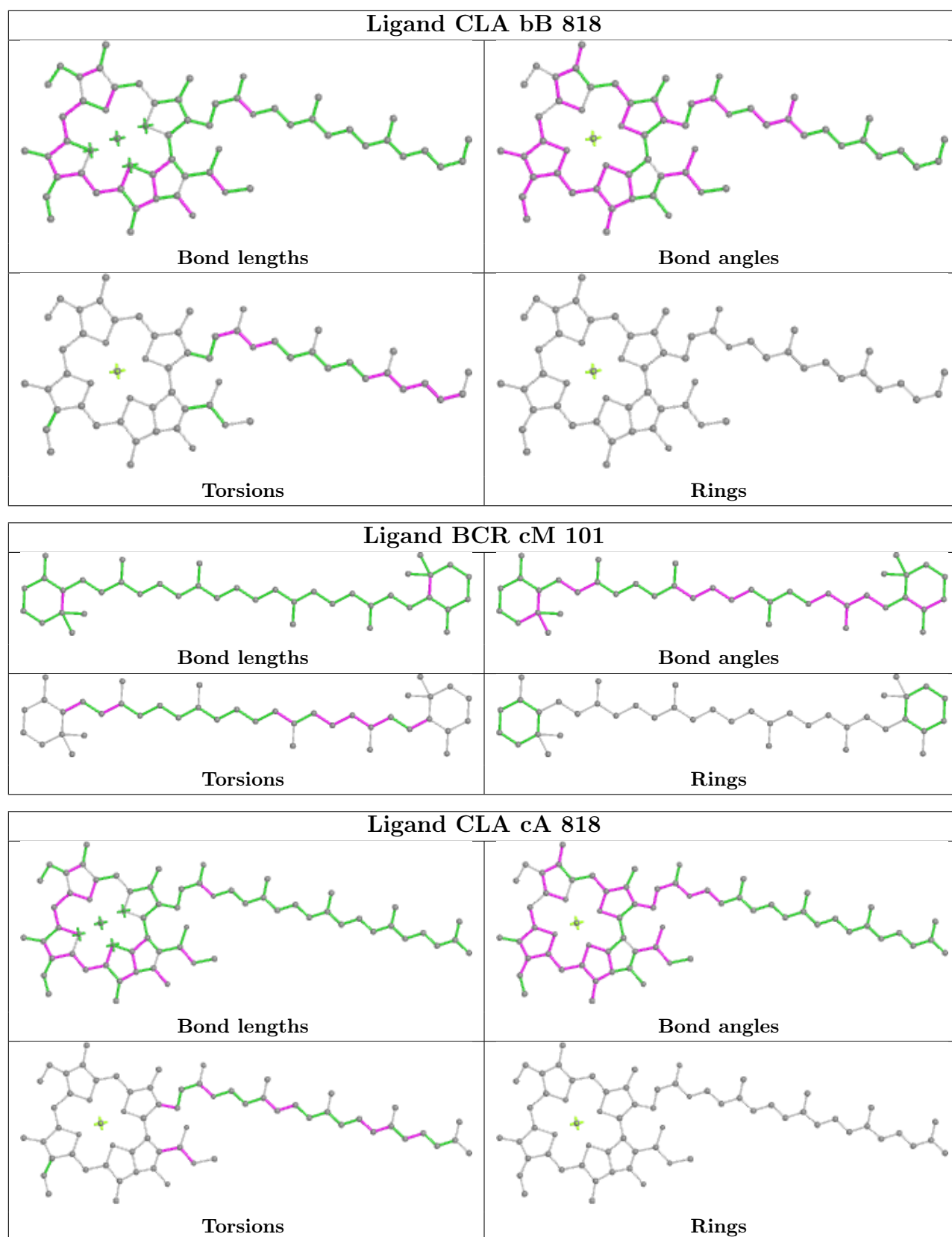


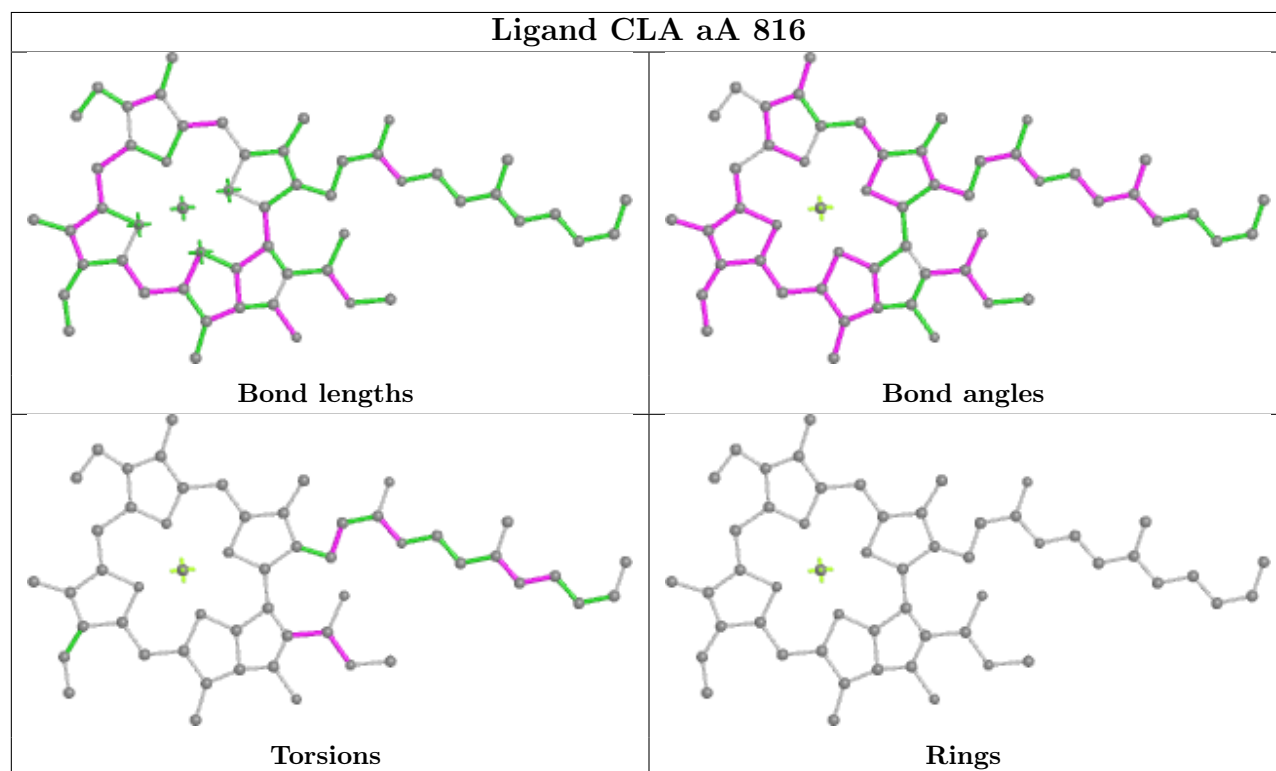
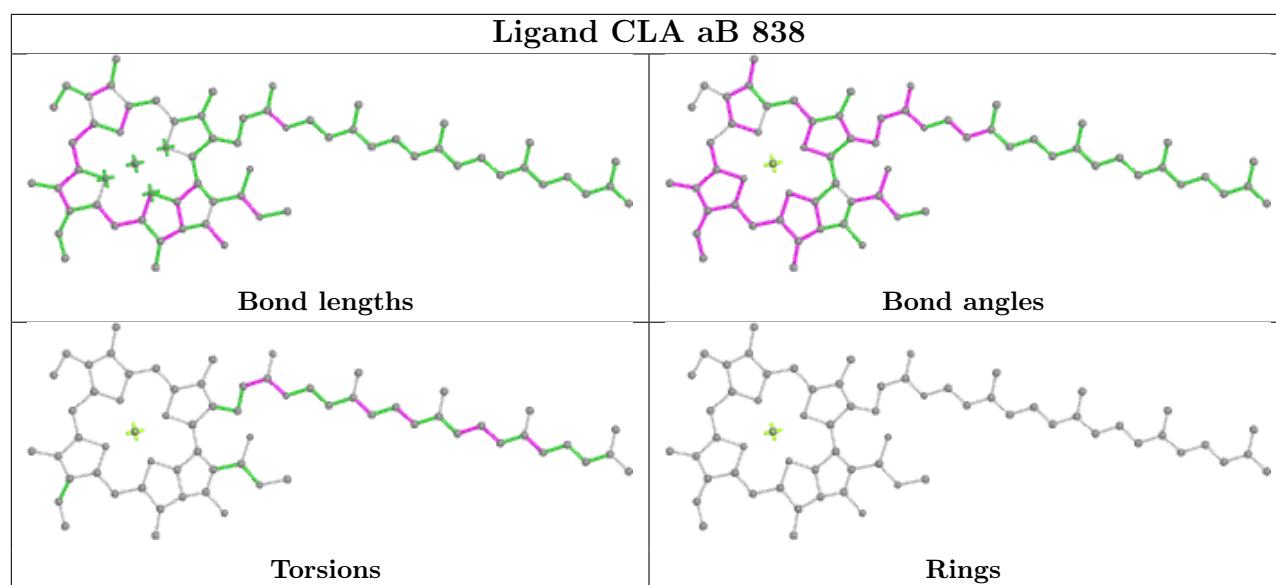
## Ligand CLA aB 820



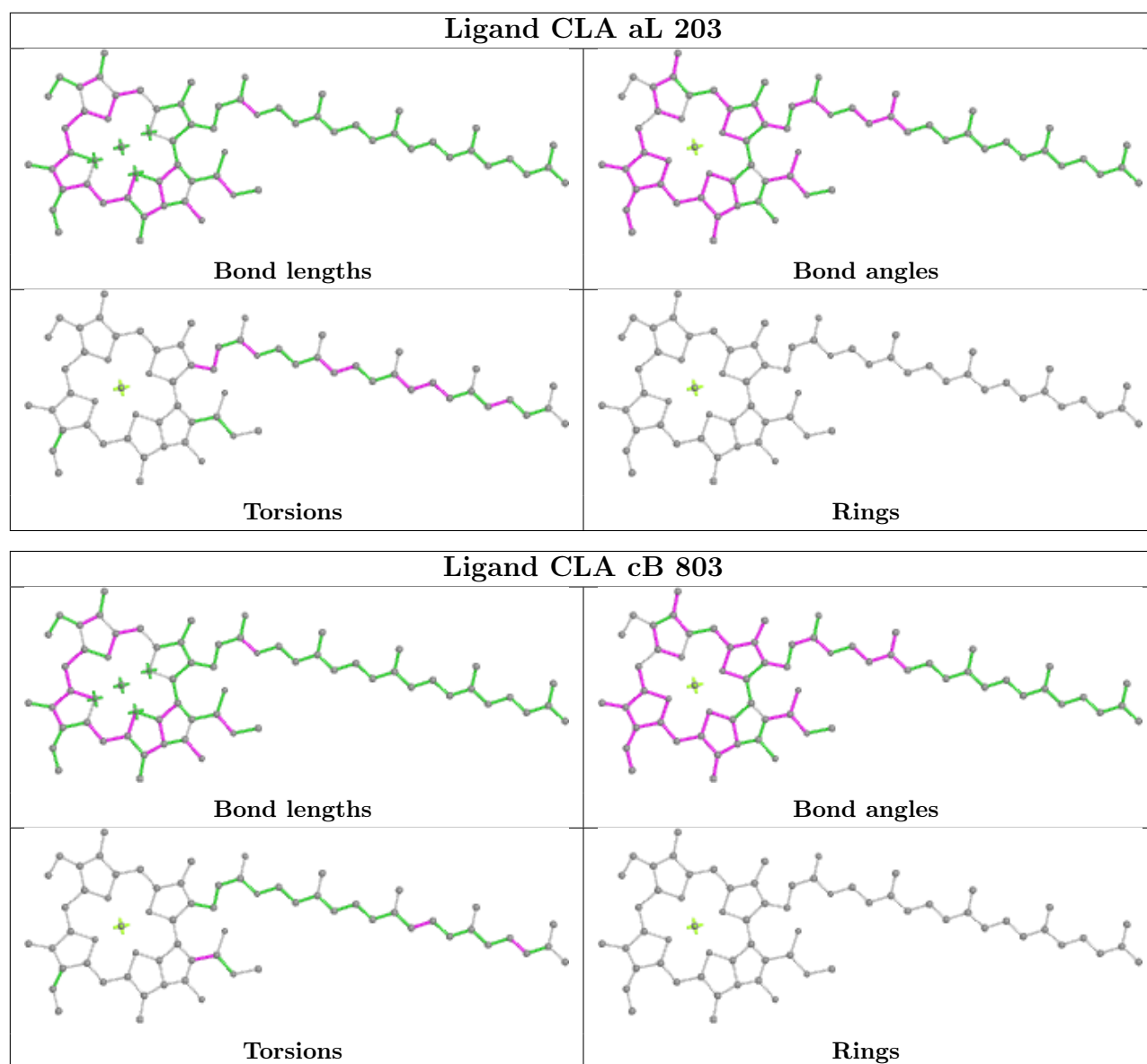


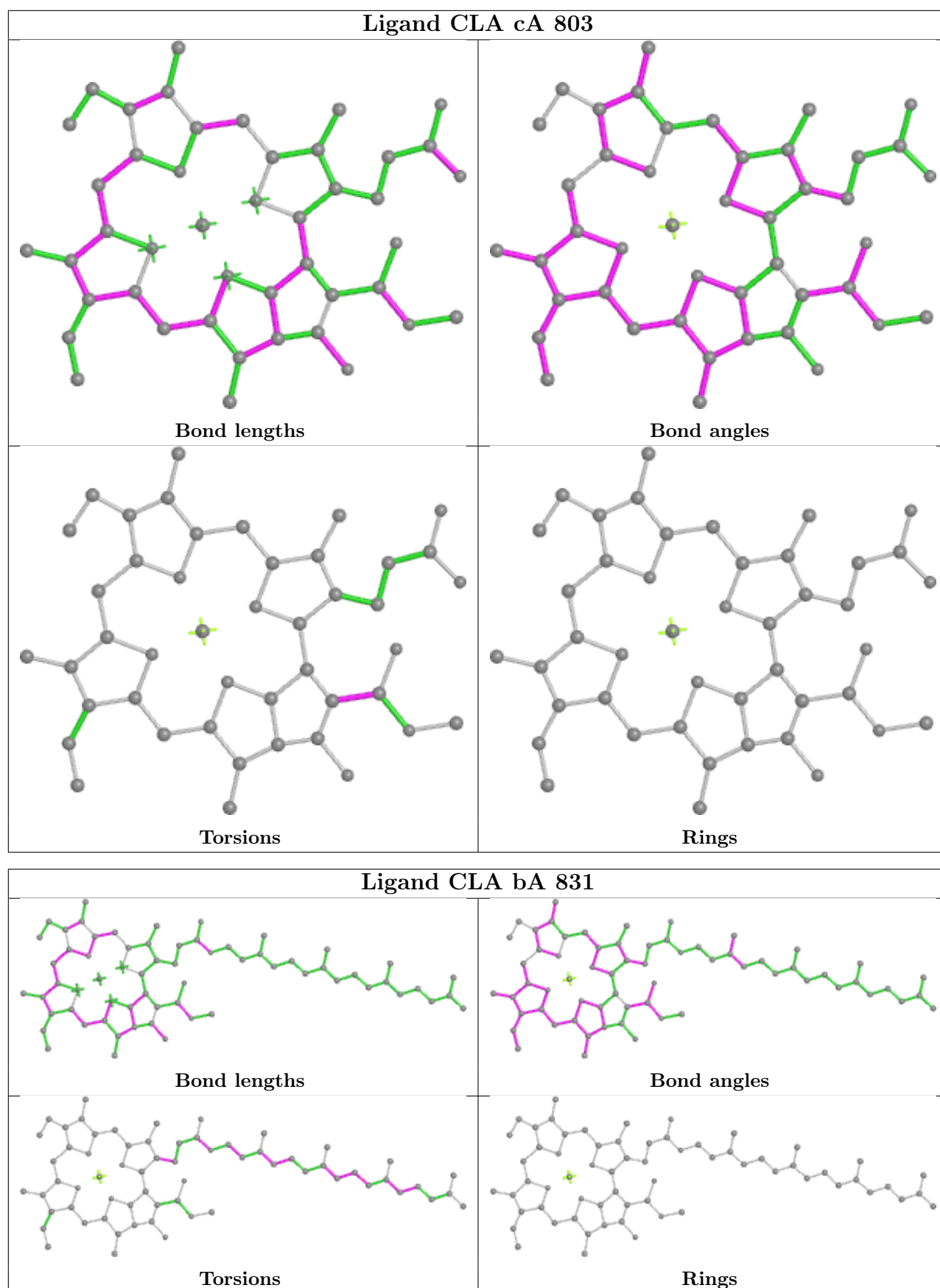


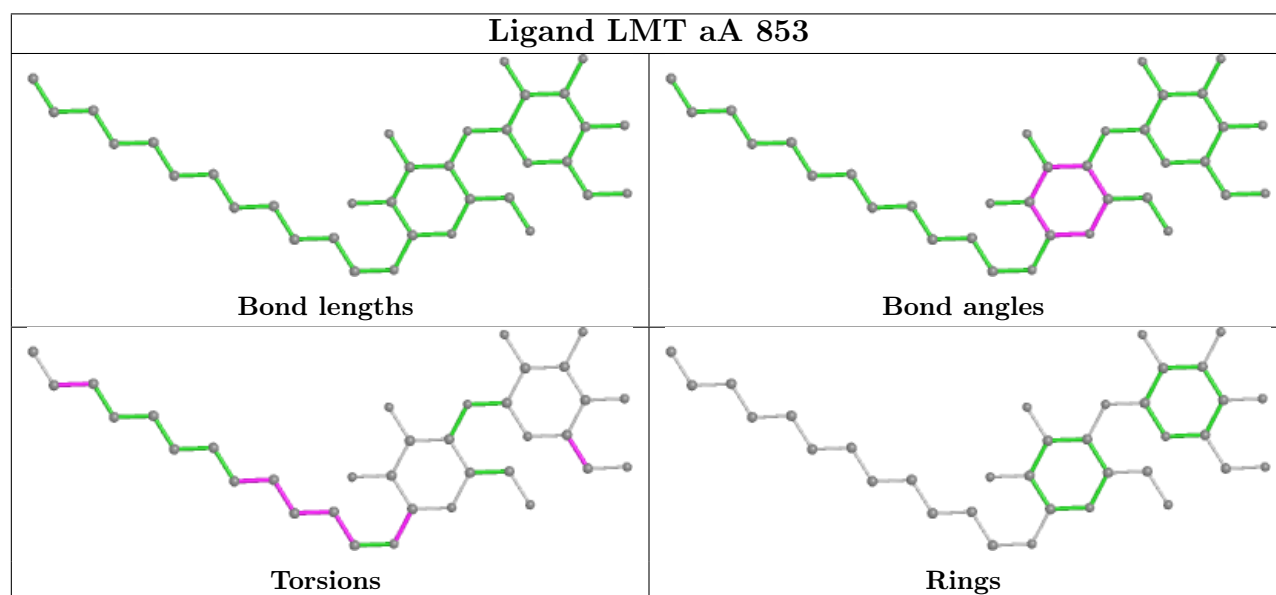
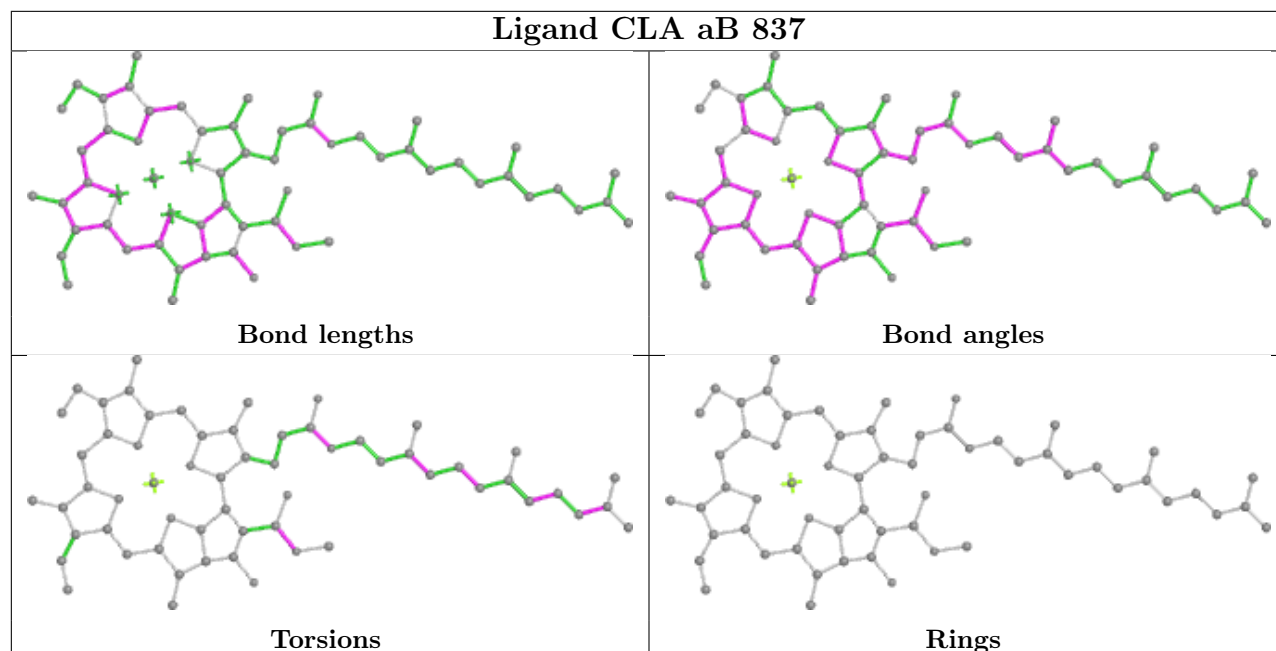
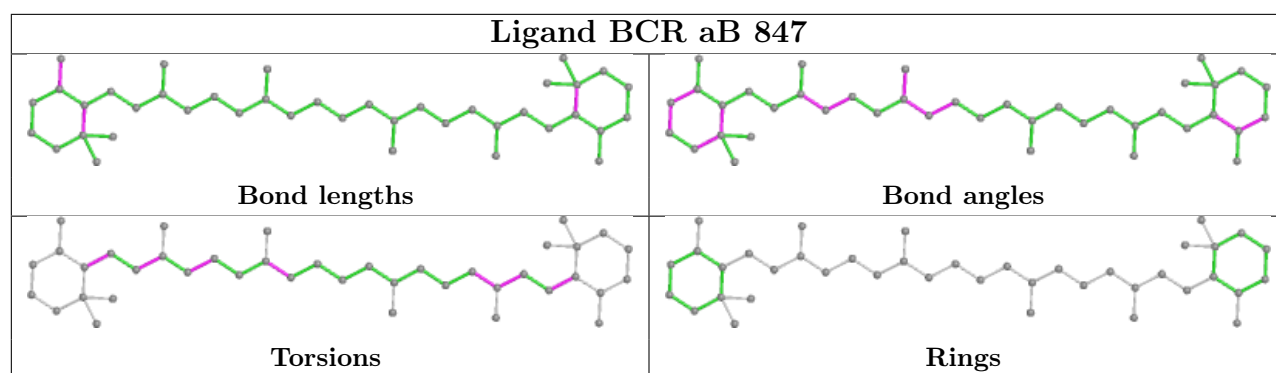


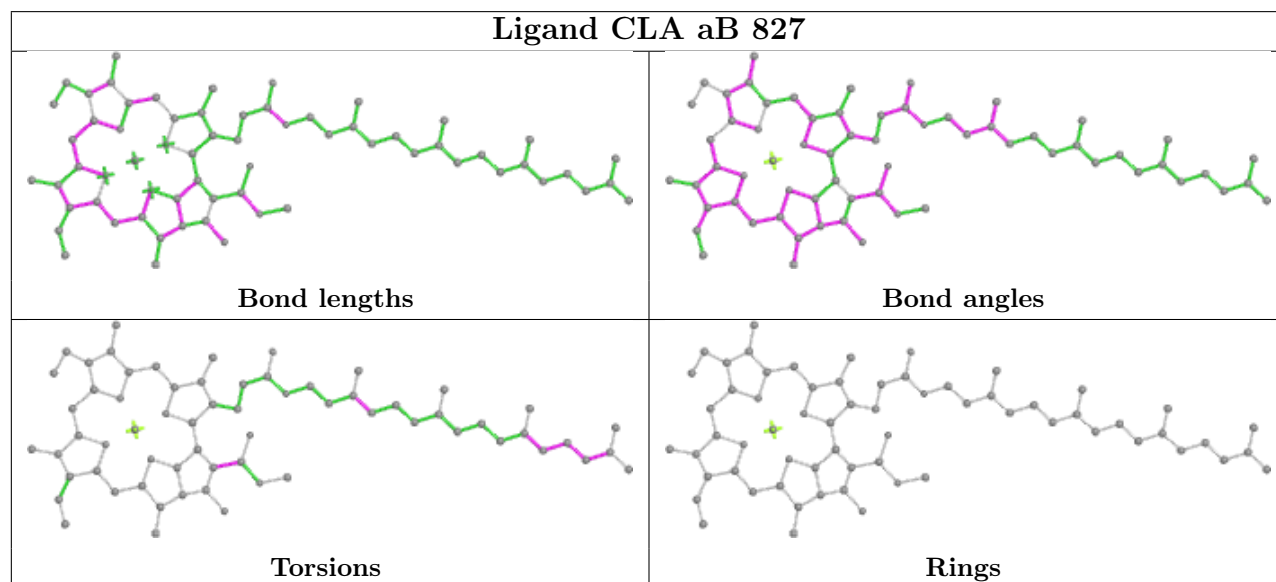
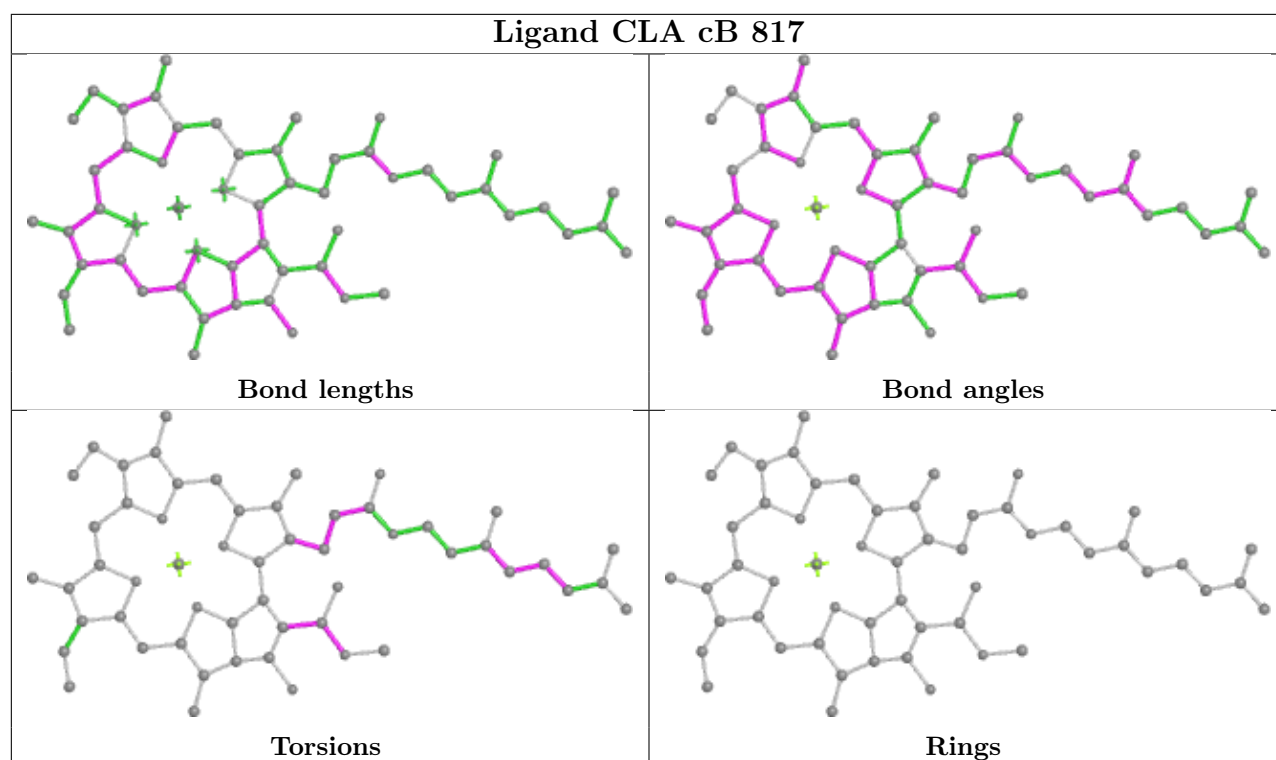




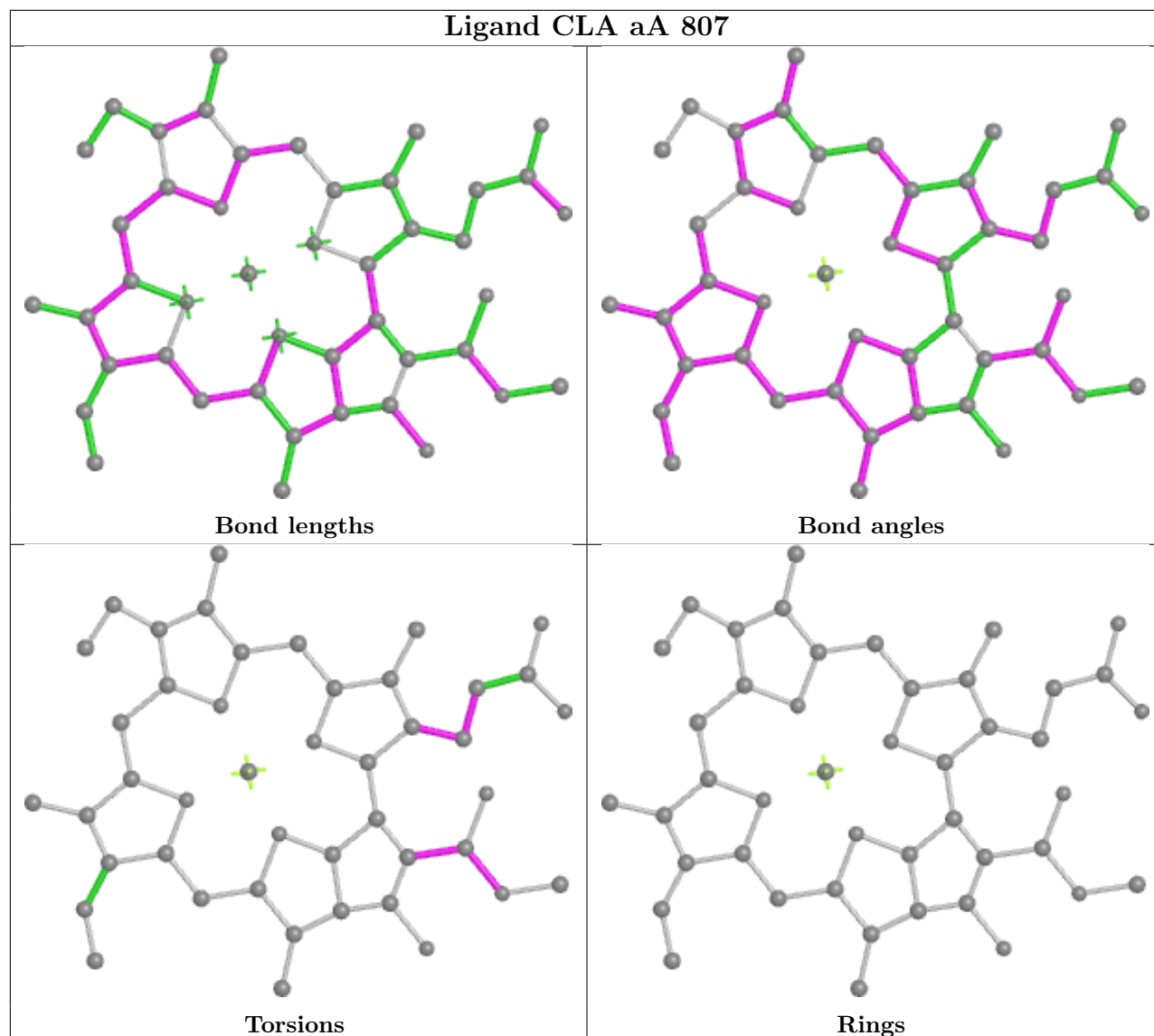




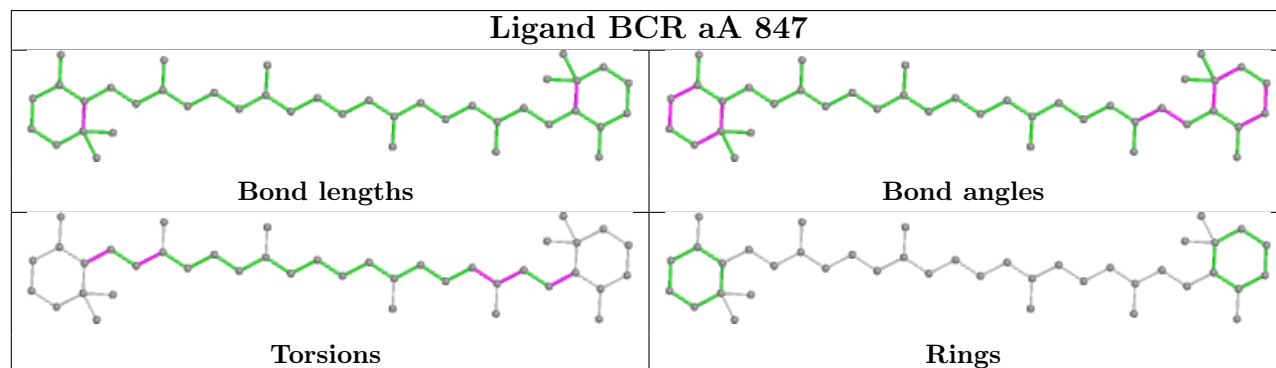


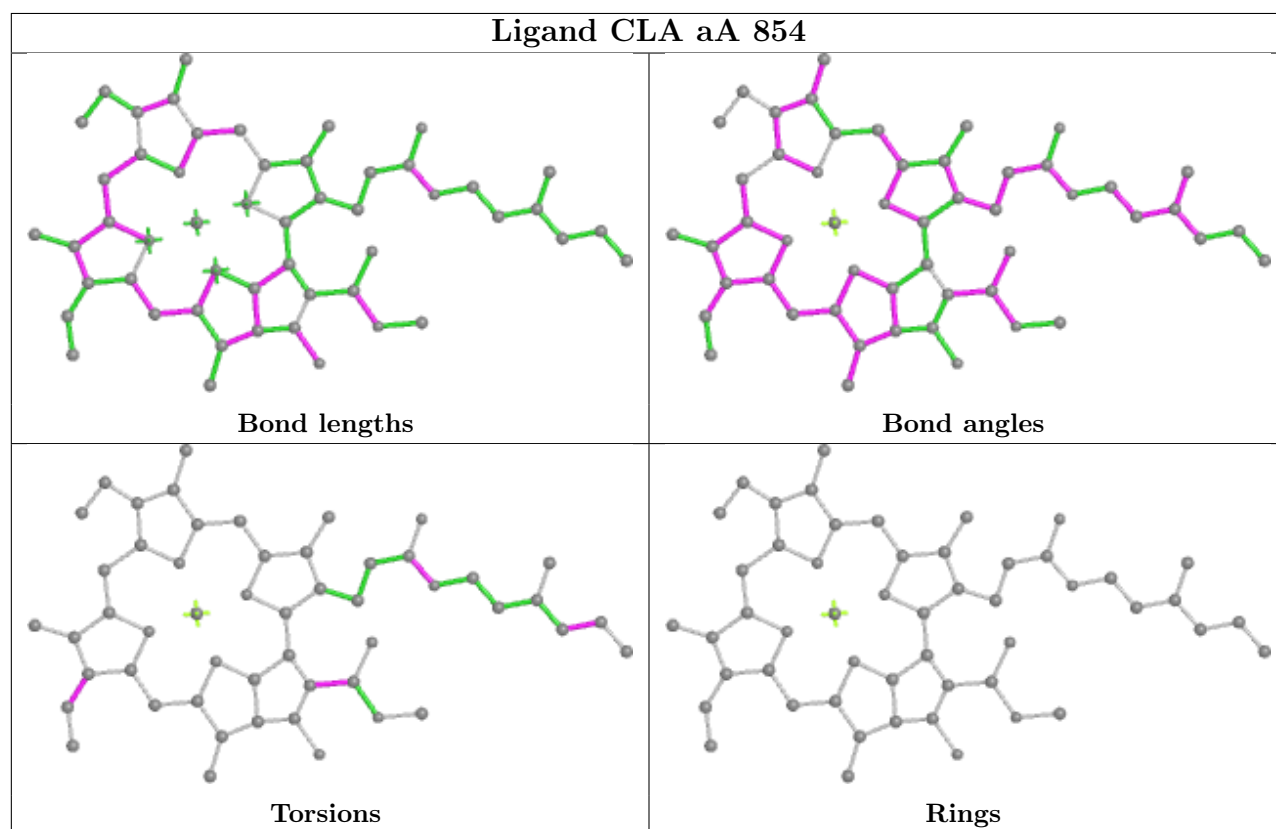
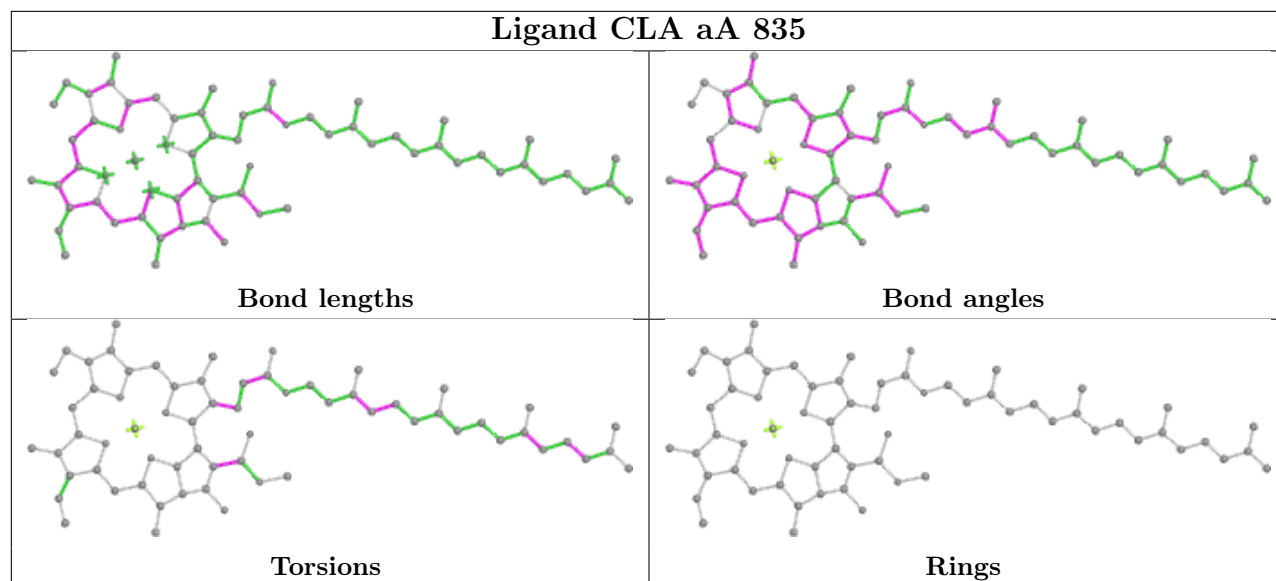
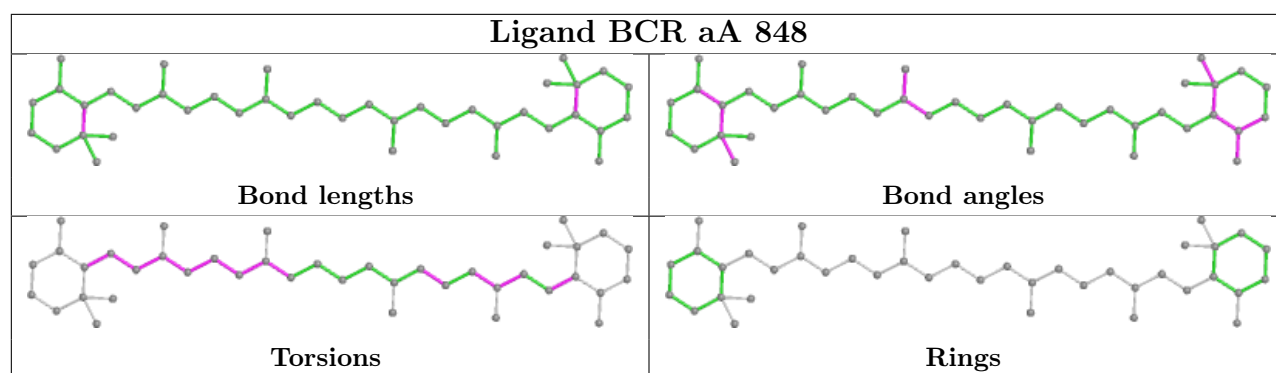


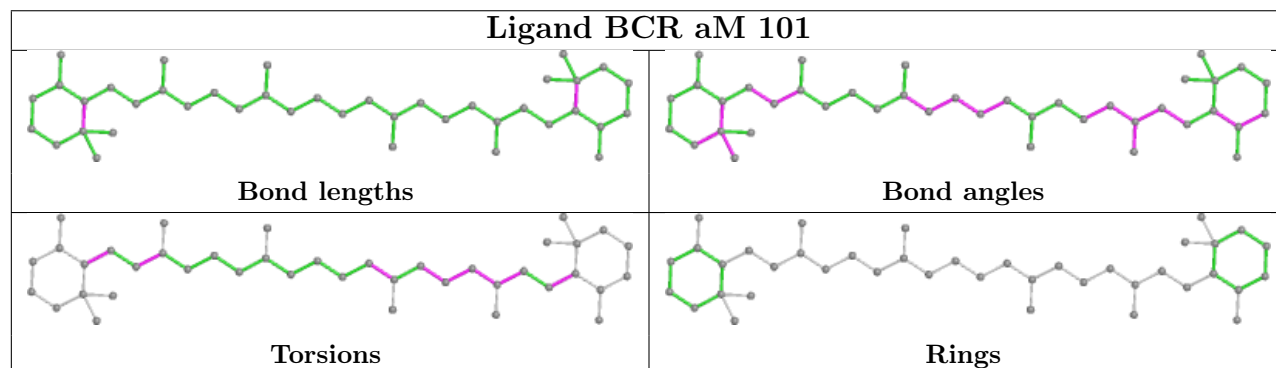
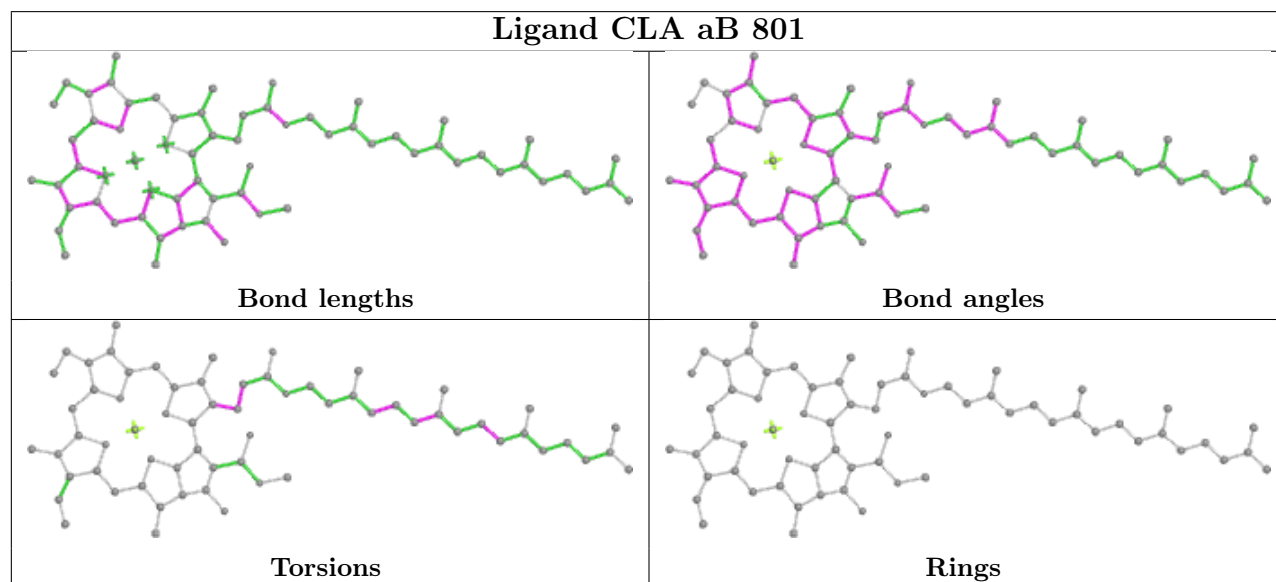
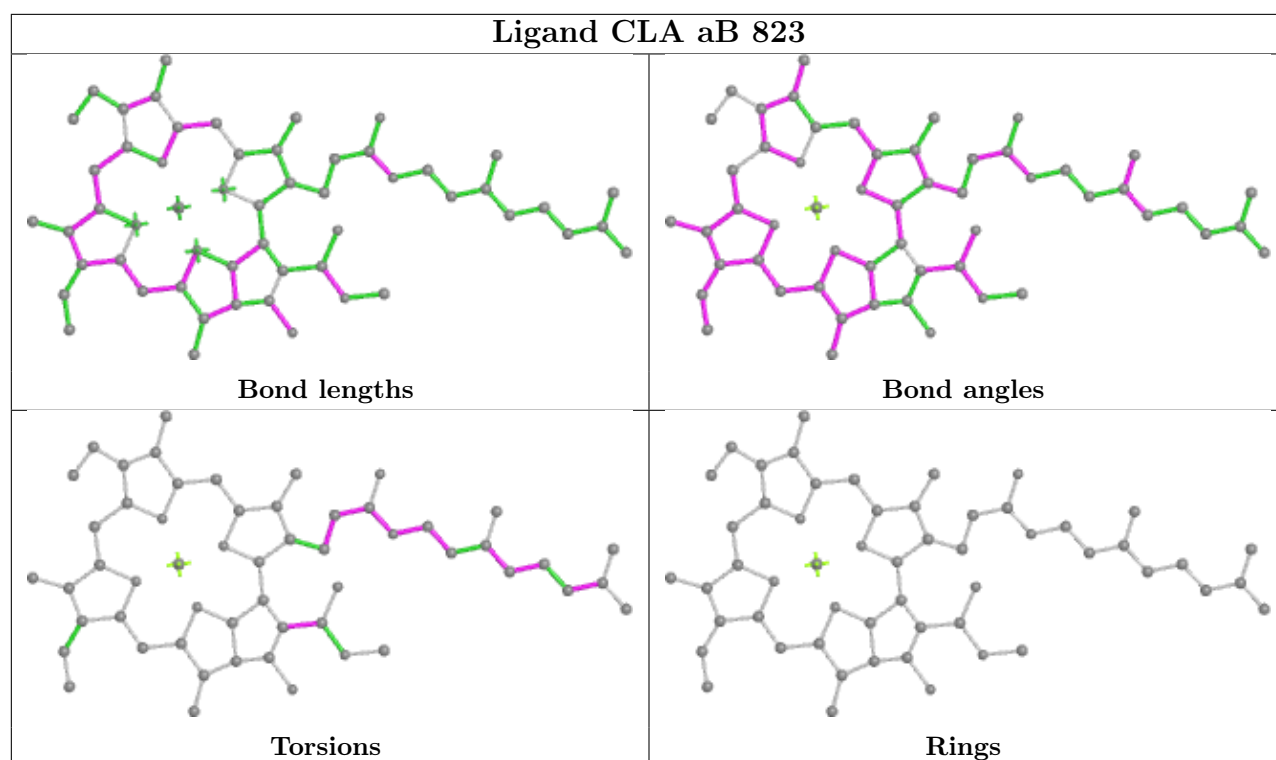
## Ligand CLA aA 807

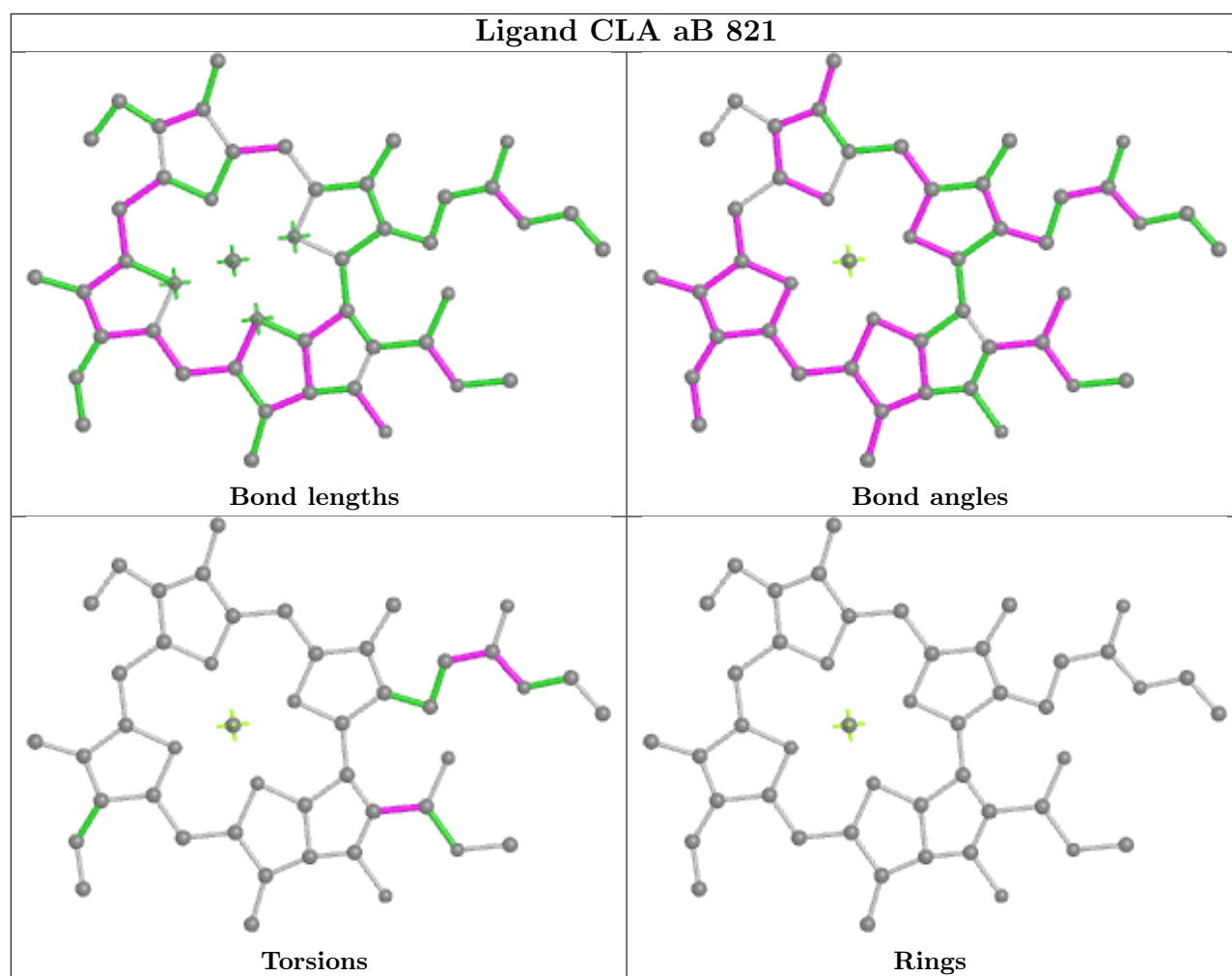


## Ligand BCR aA 847

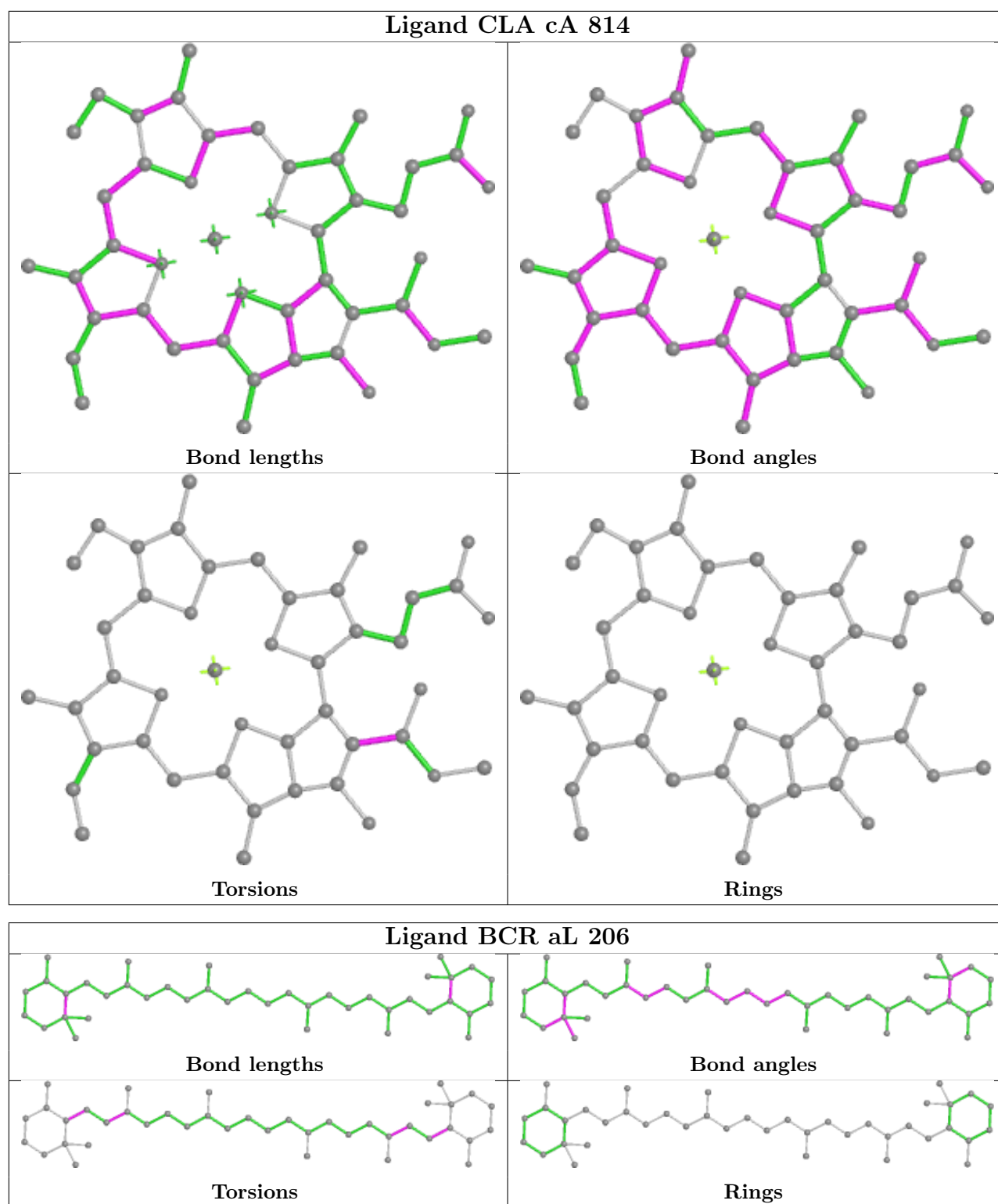




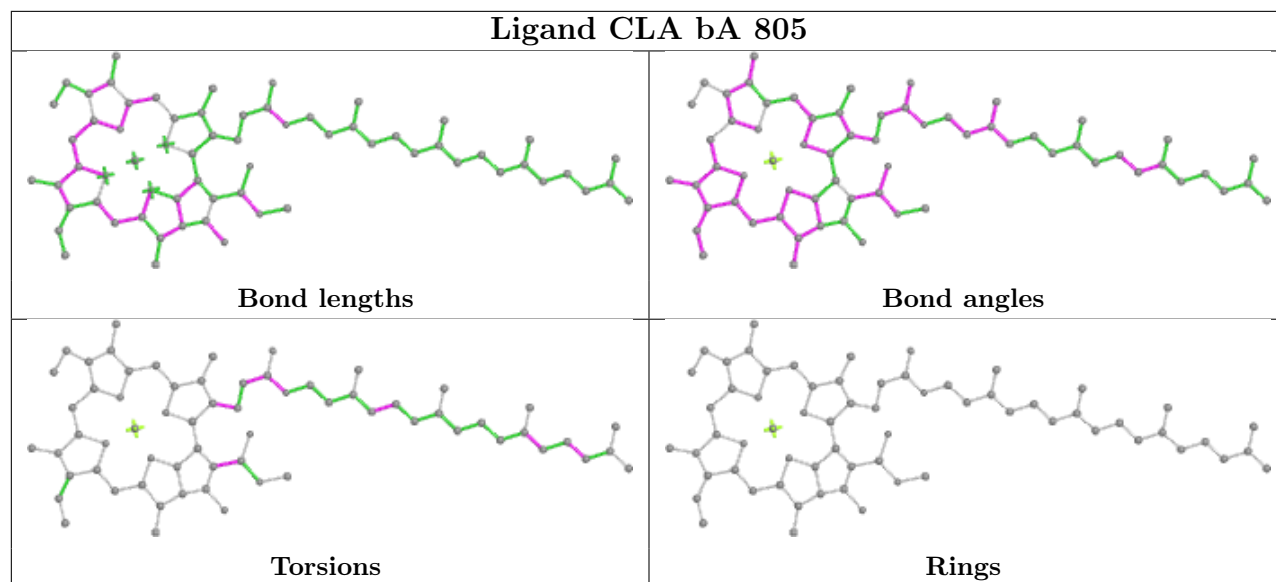




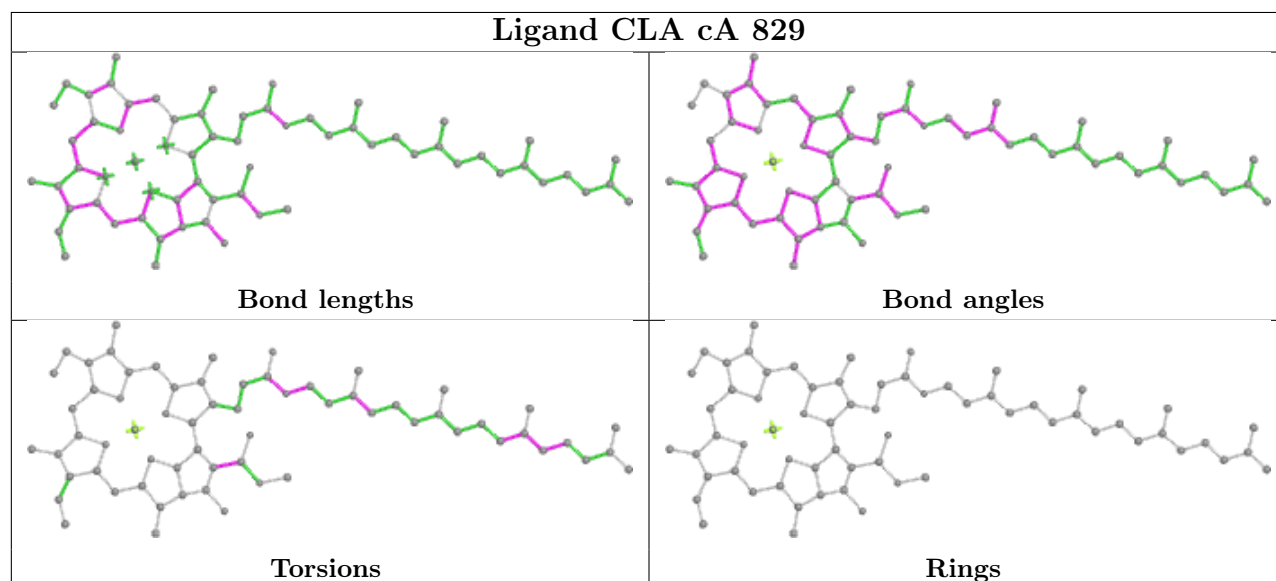




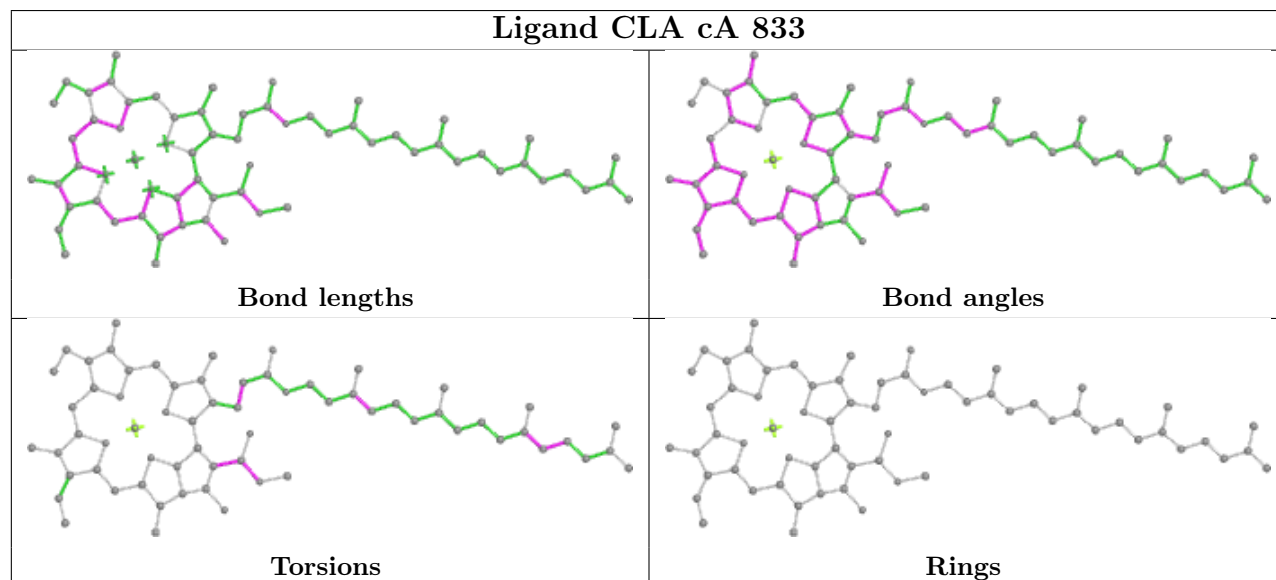
## Ligand CLA bA 805

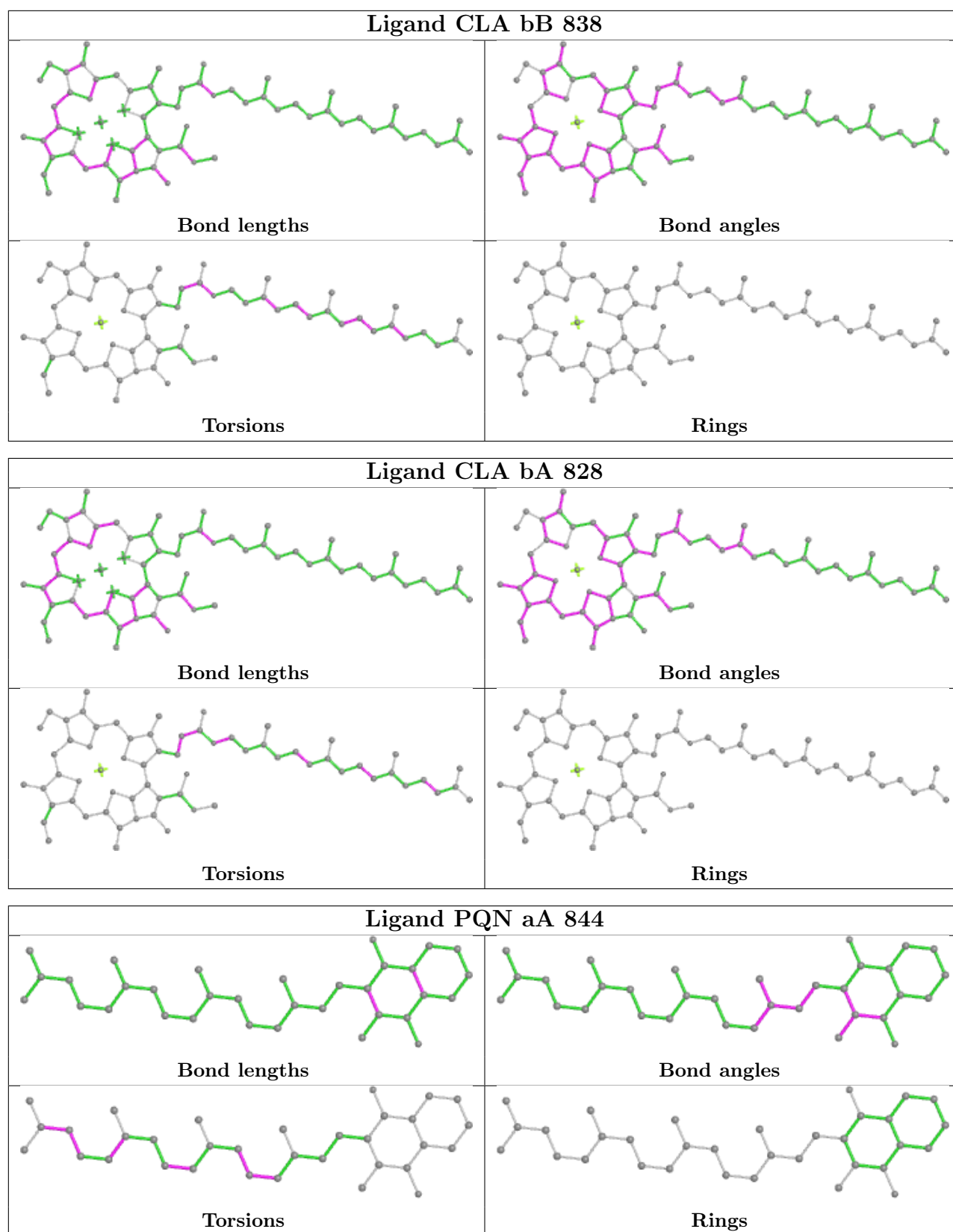


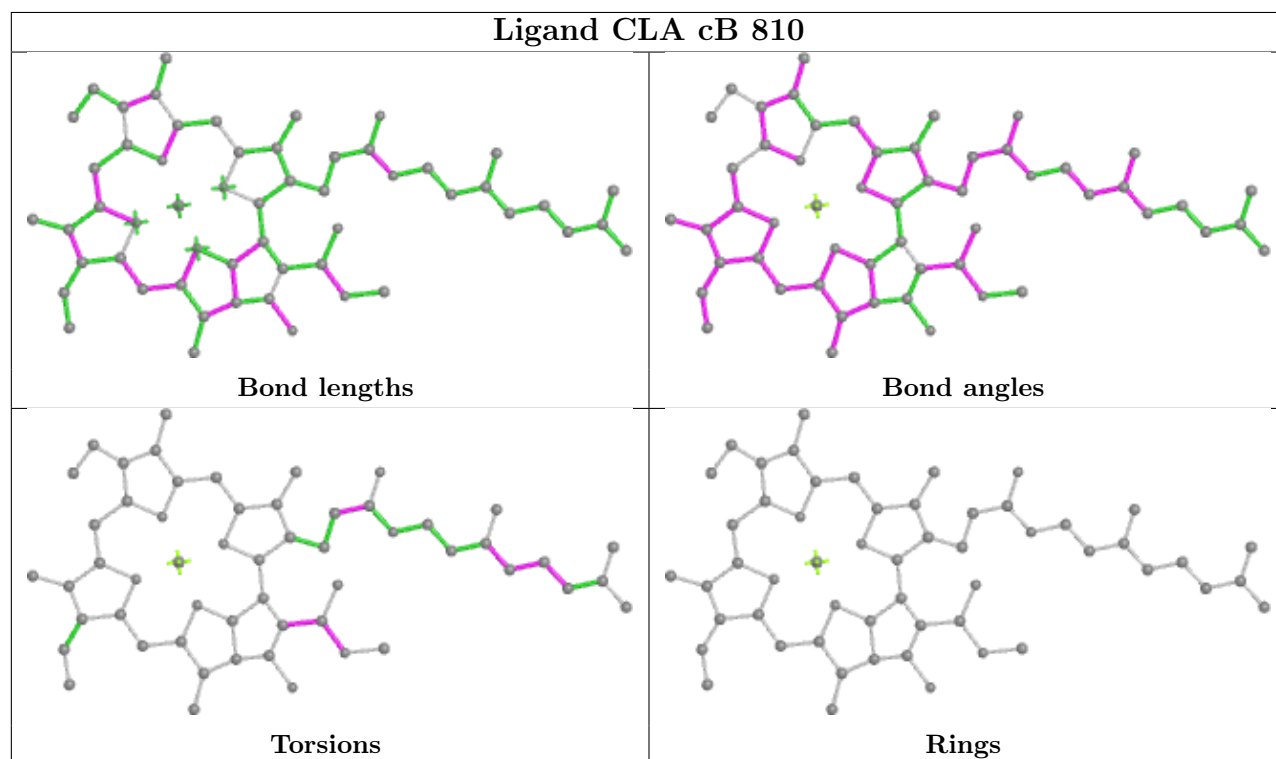
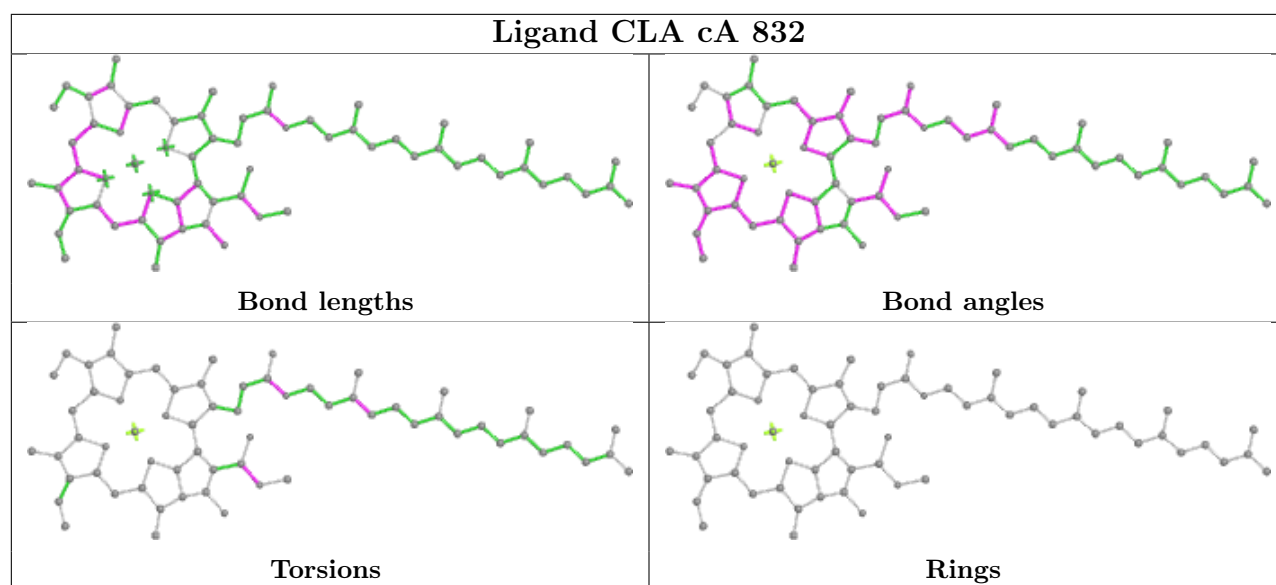
## Ligand CLA cA 829



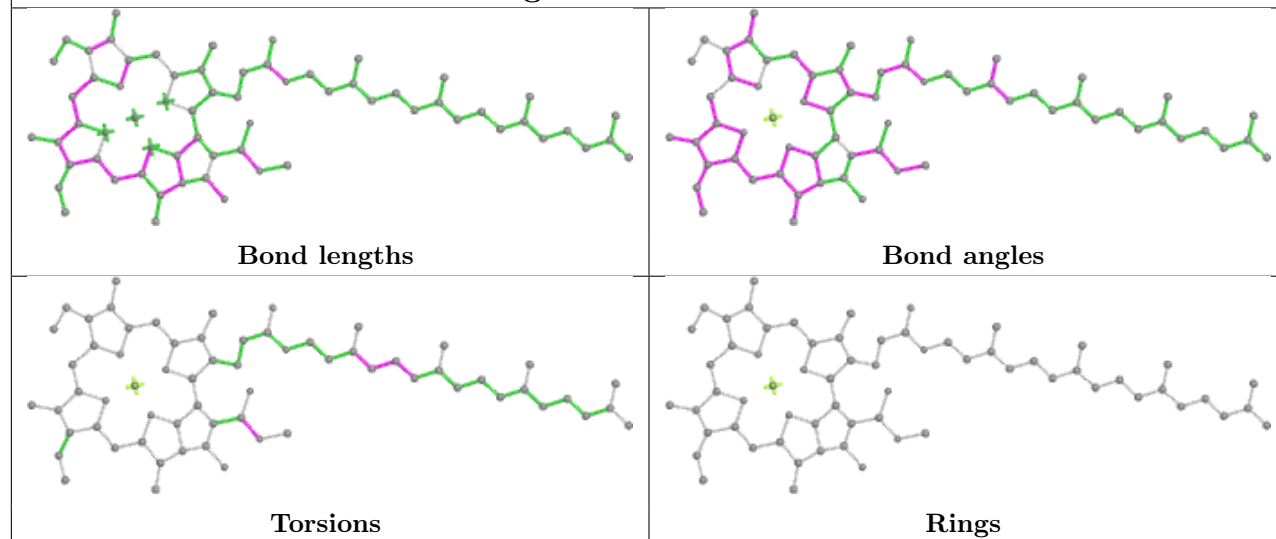
## Ligand CLA cA 833



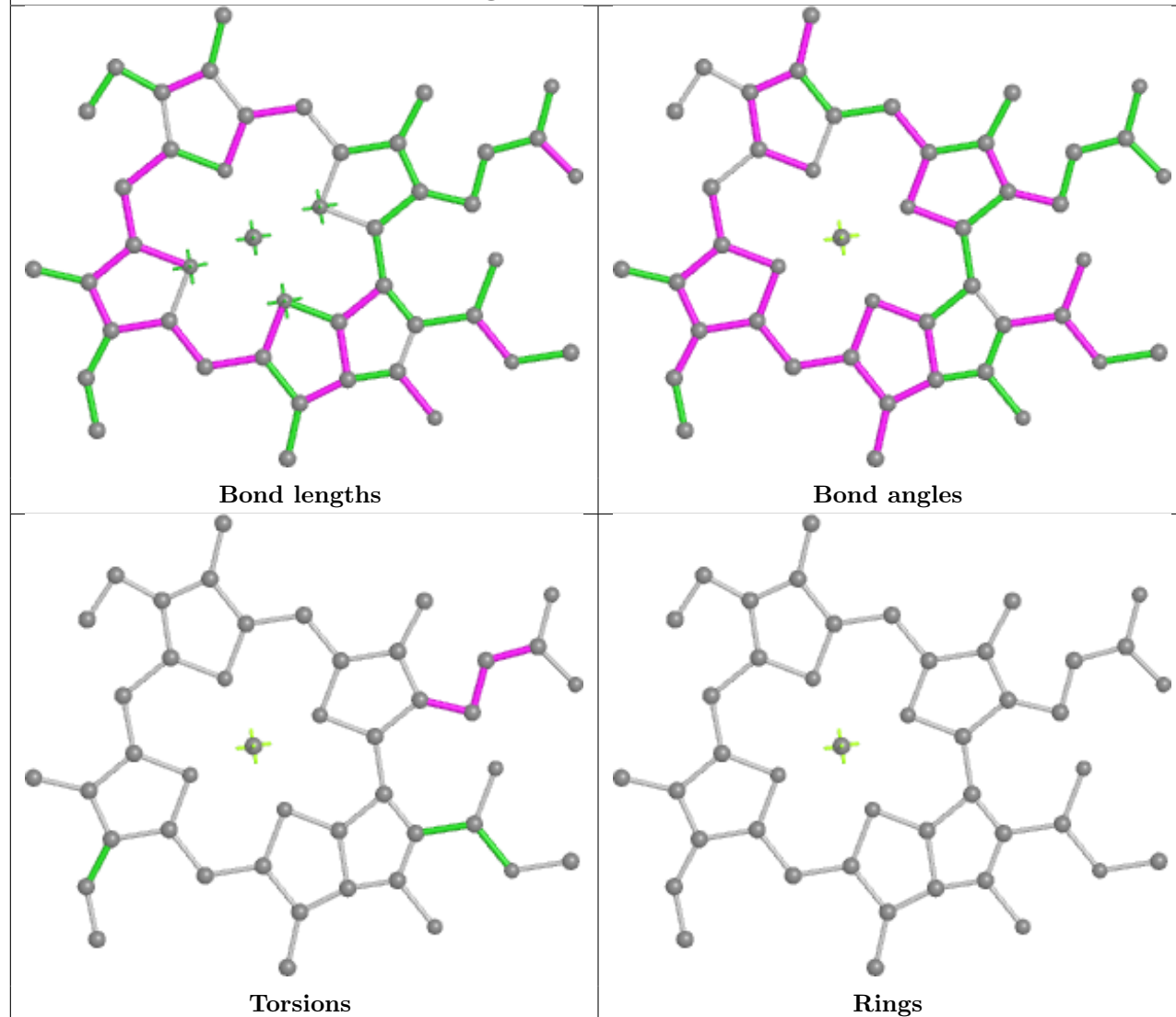


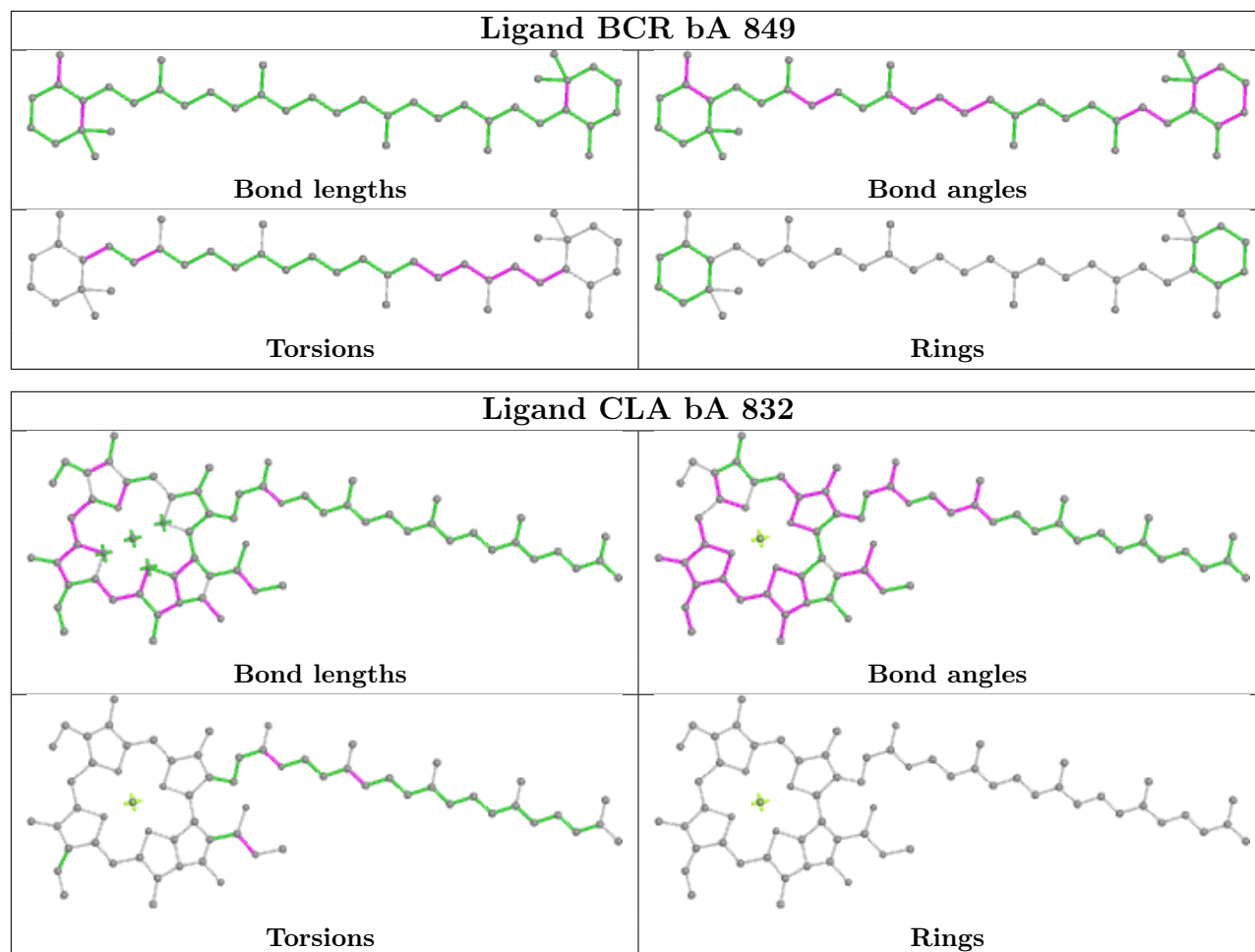


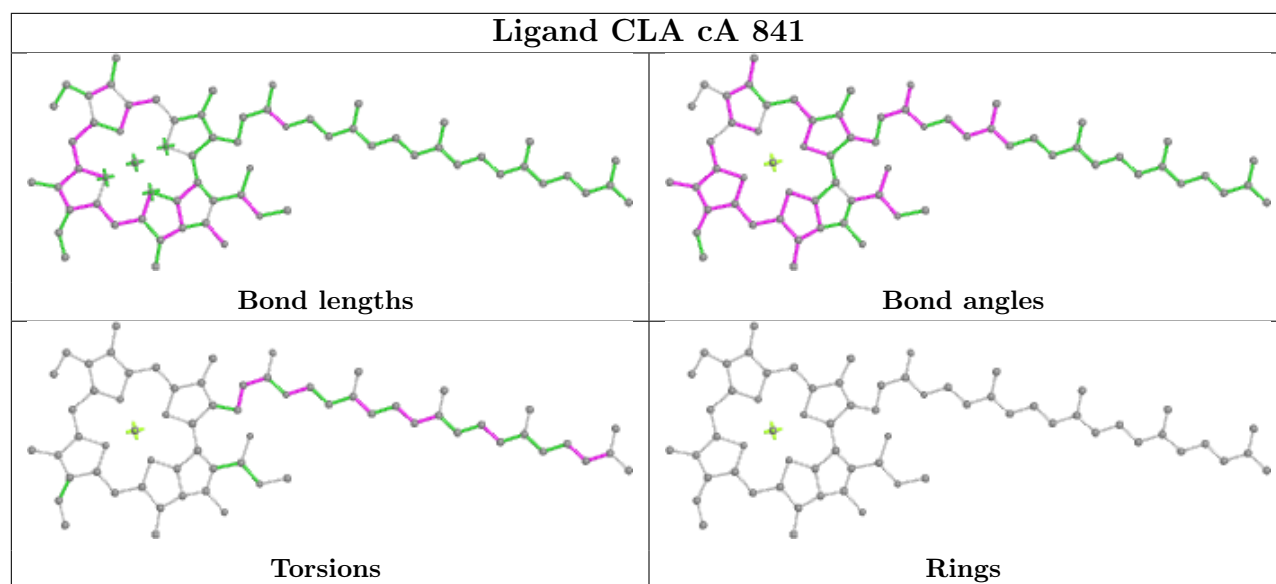
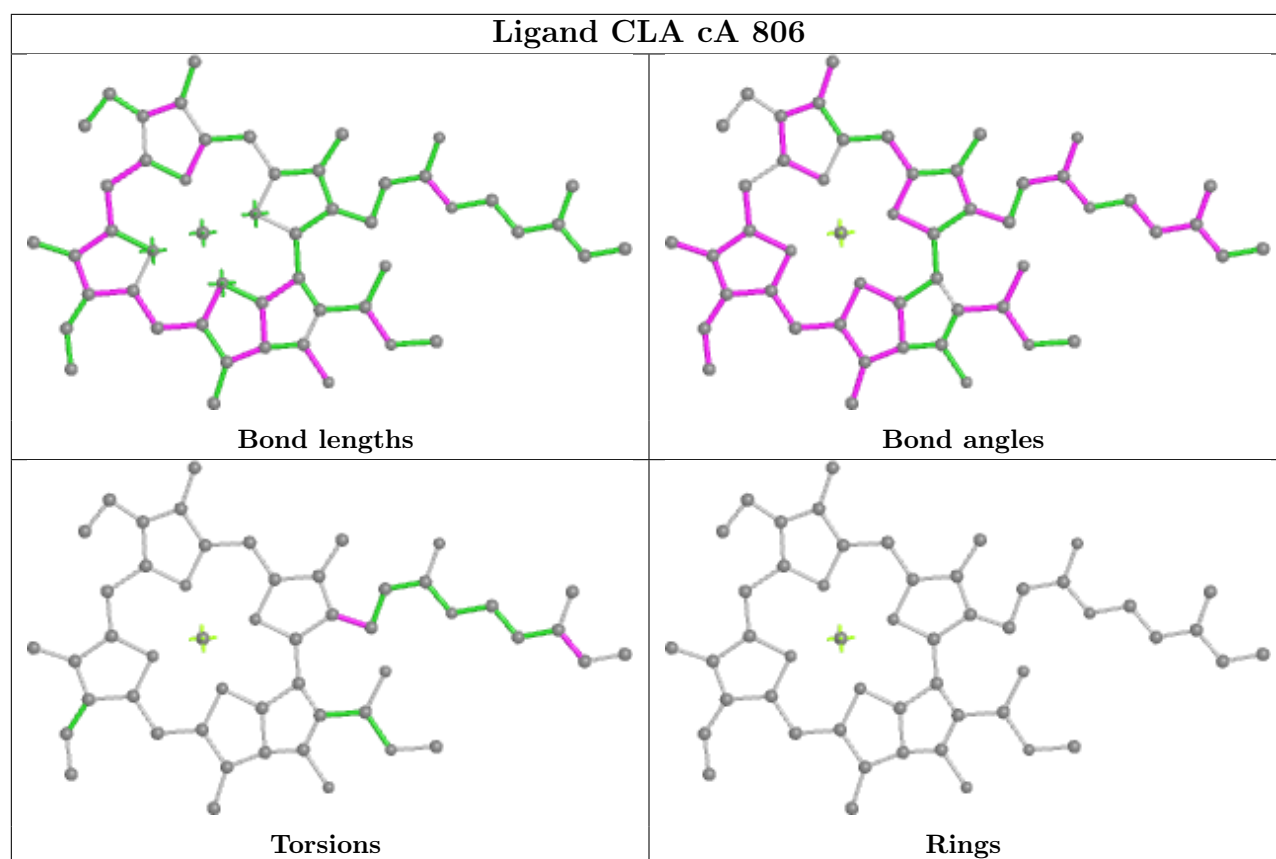
## Ligand CLA cA 839

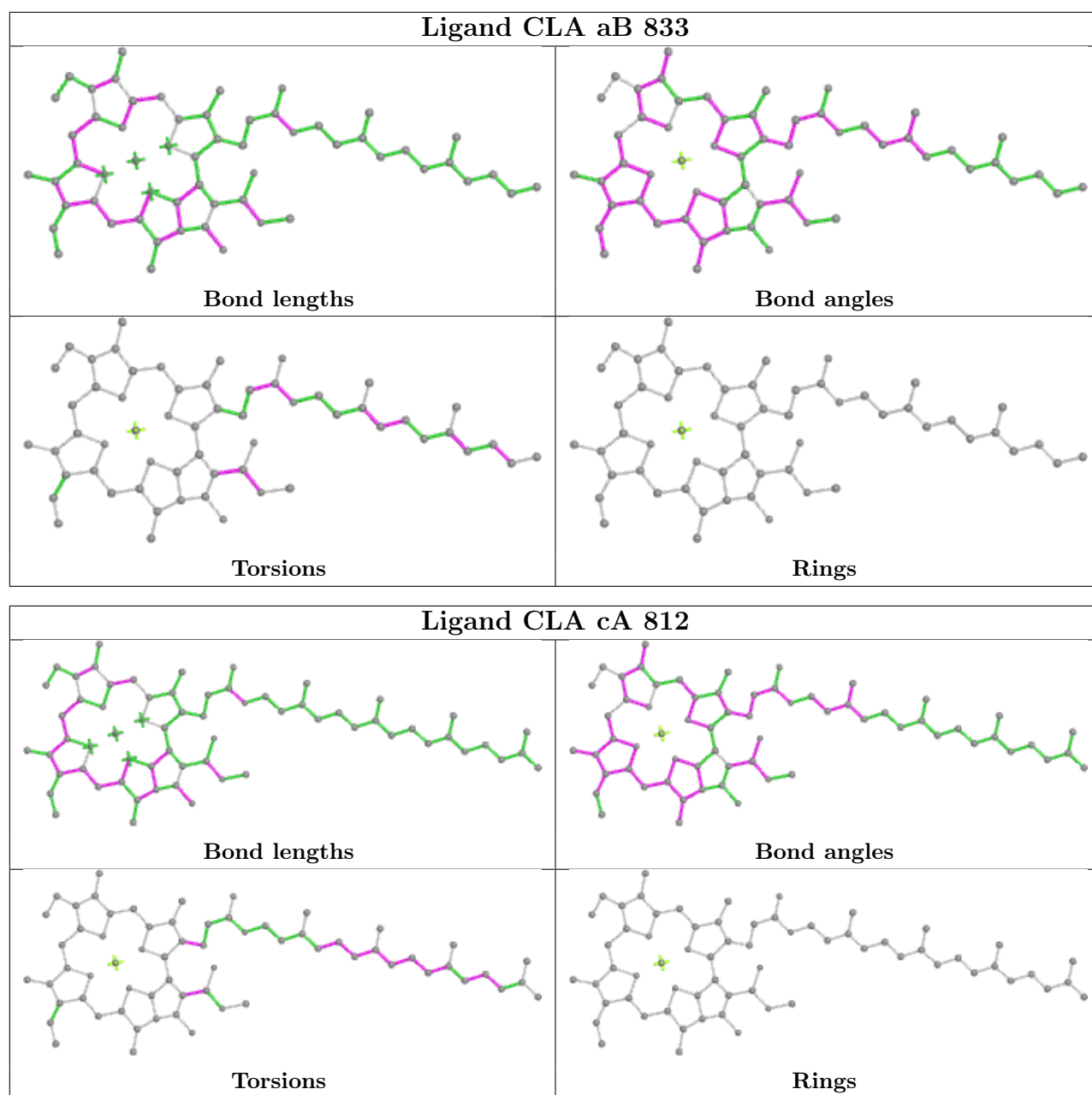


## Ligand CLA cB 813



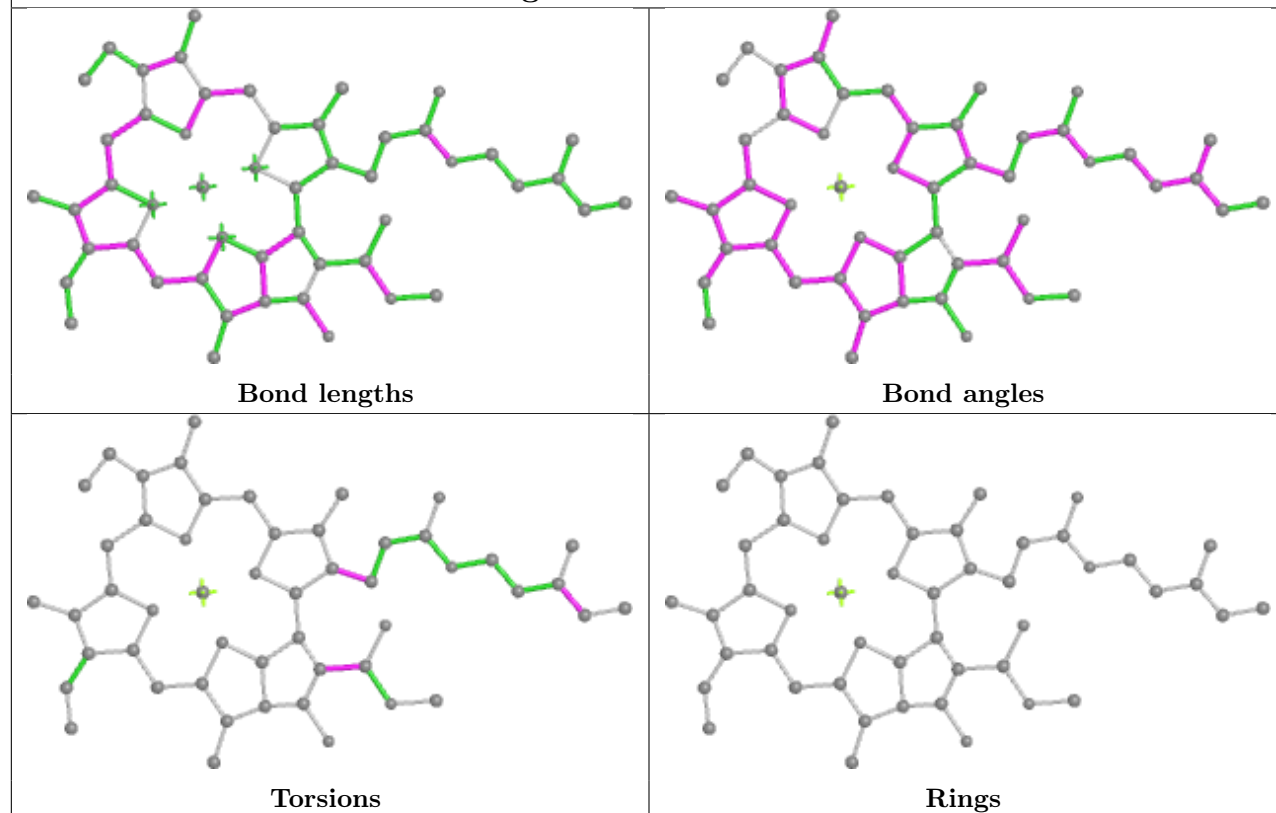




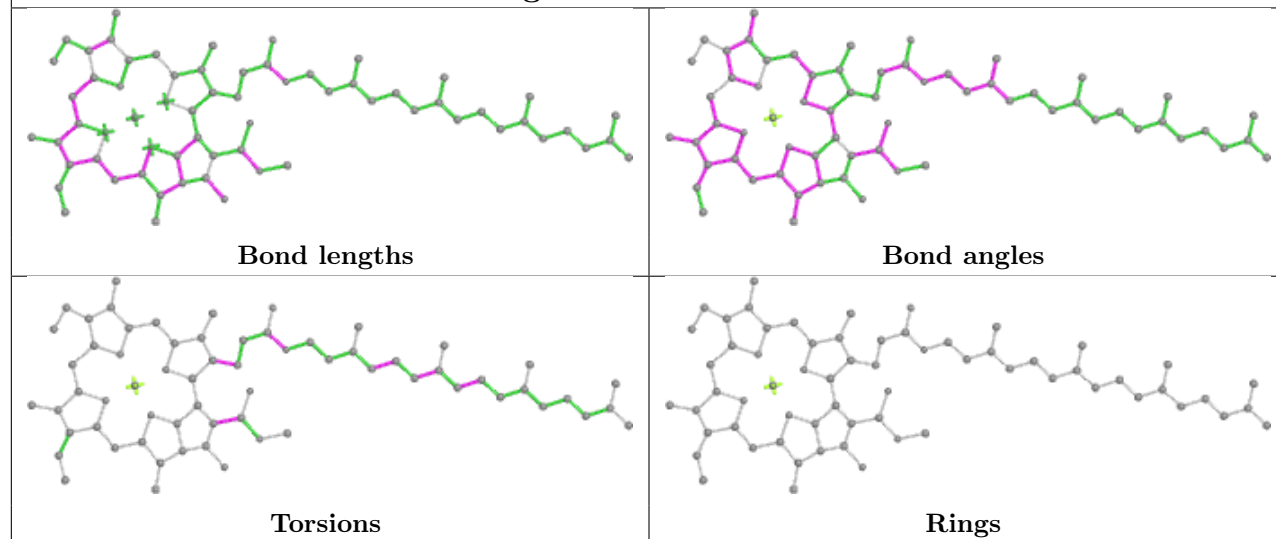




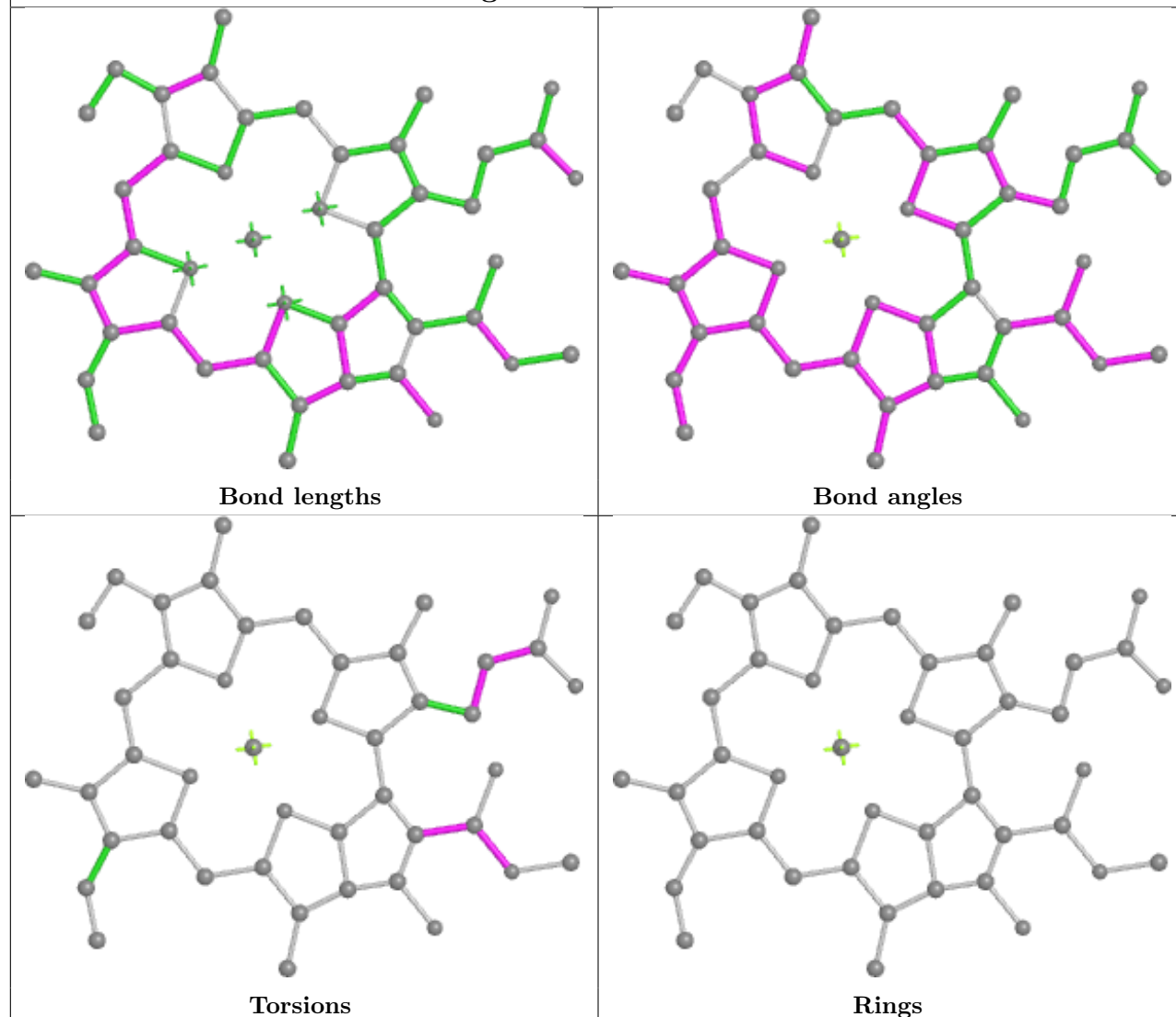
## Ligand CLA bA 840



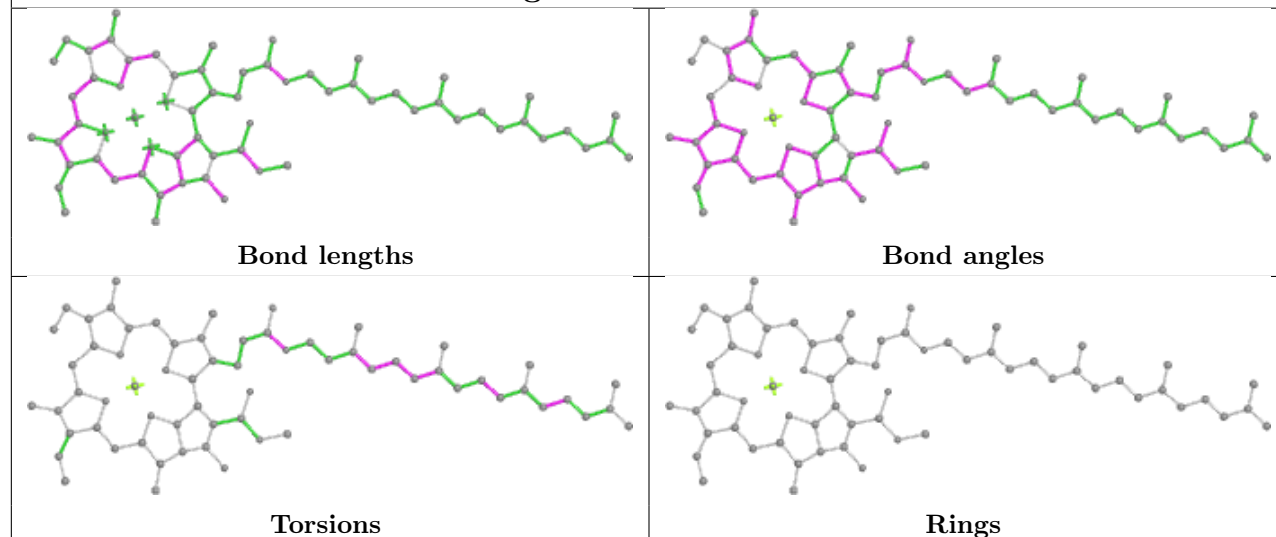
## Ligand CLA aA 810

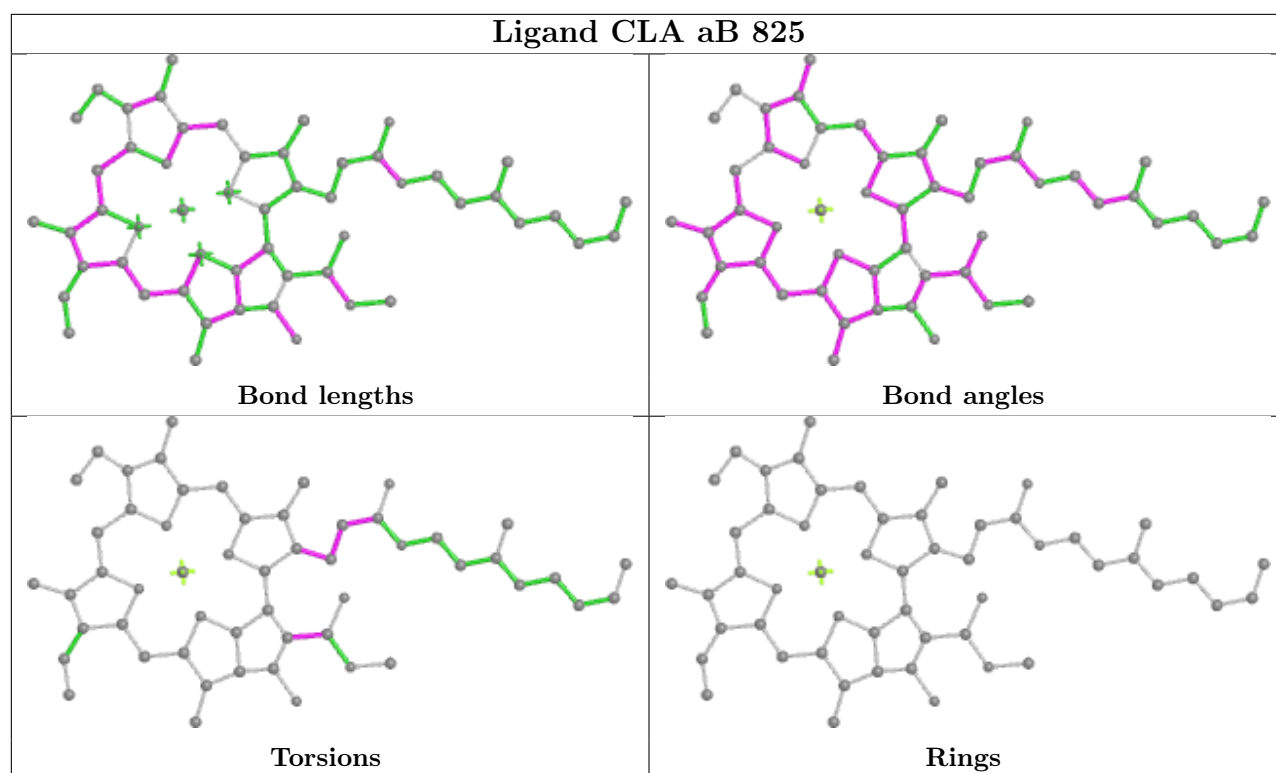


## Ligand CLA bB 831

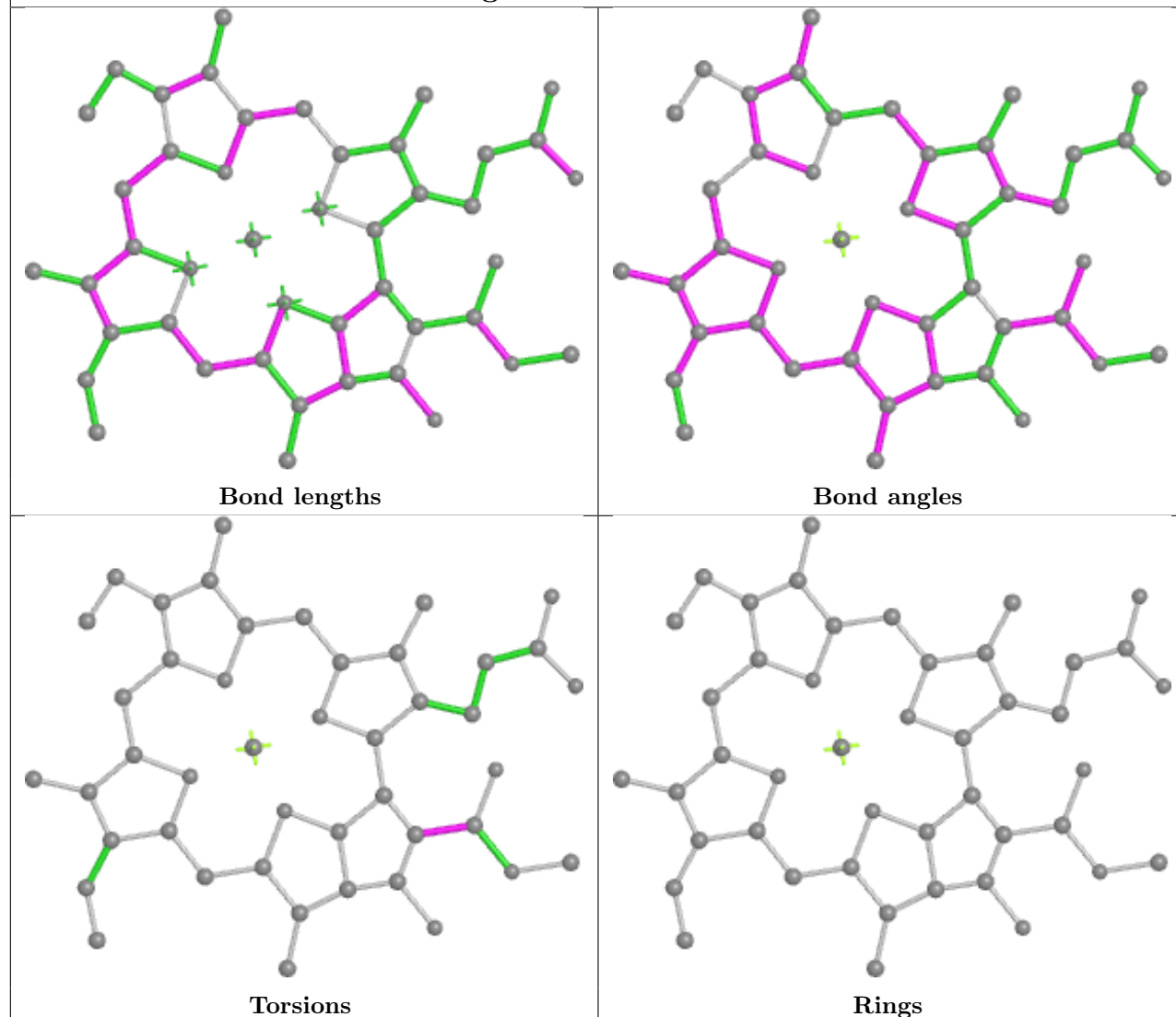


## Ligand CLA cA 826

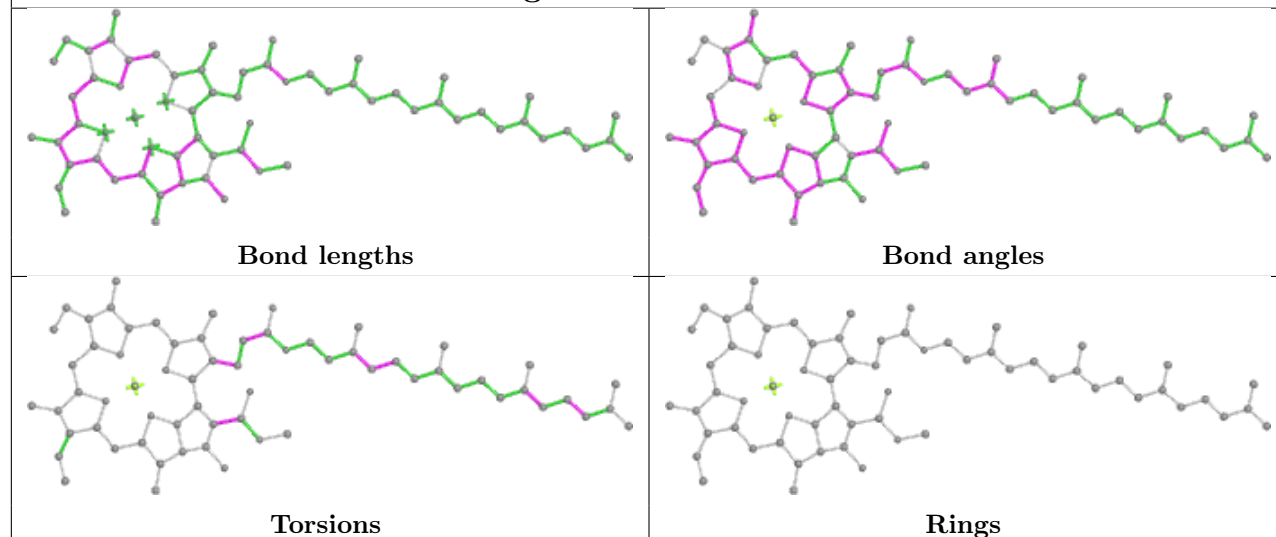




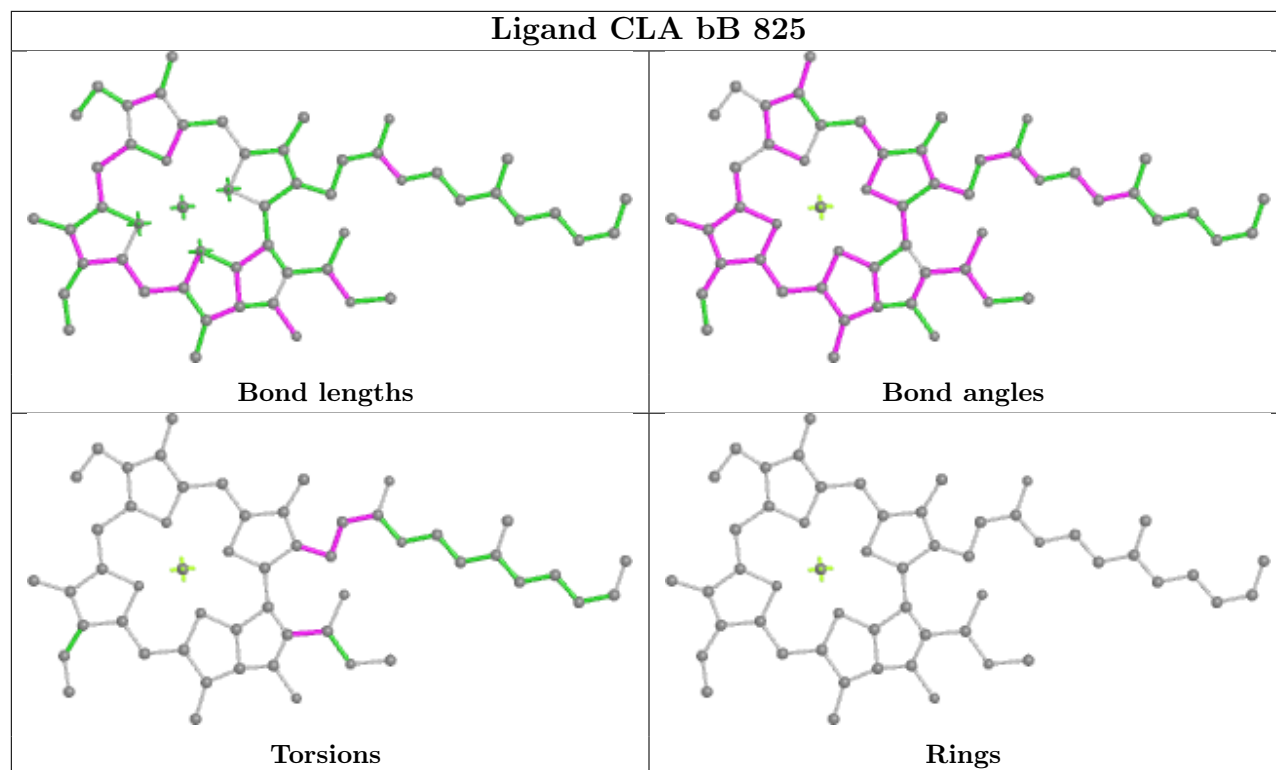
## Ligand CLA aA 809



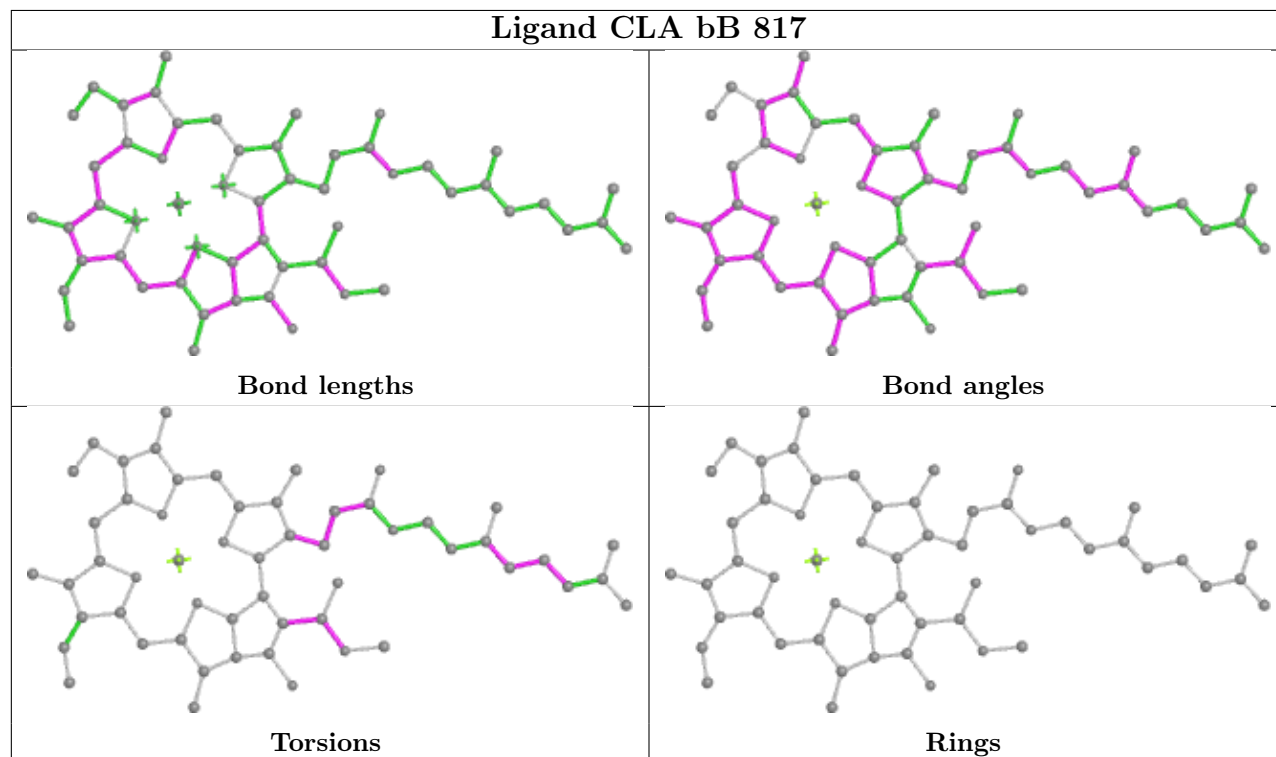
## Ligand CLA cA 835



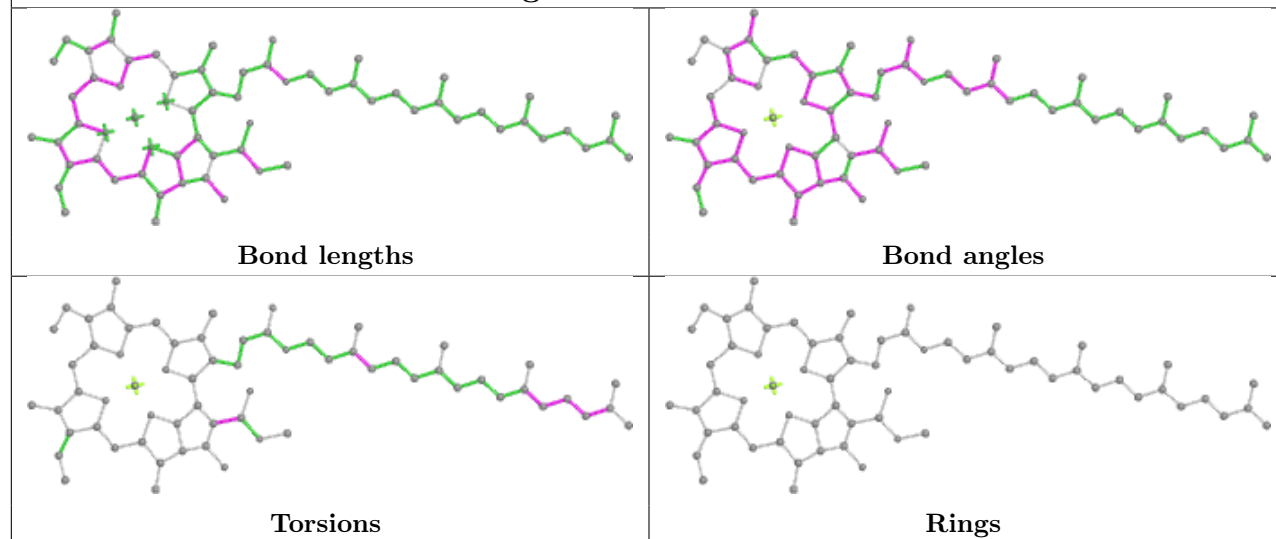
## Ligand CLA bB 825



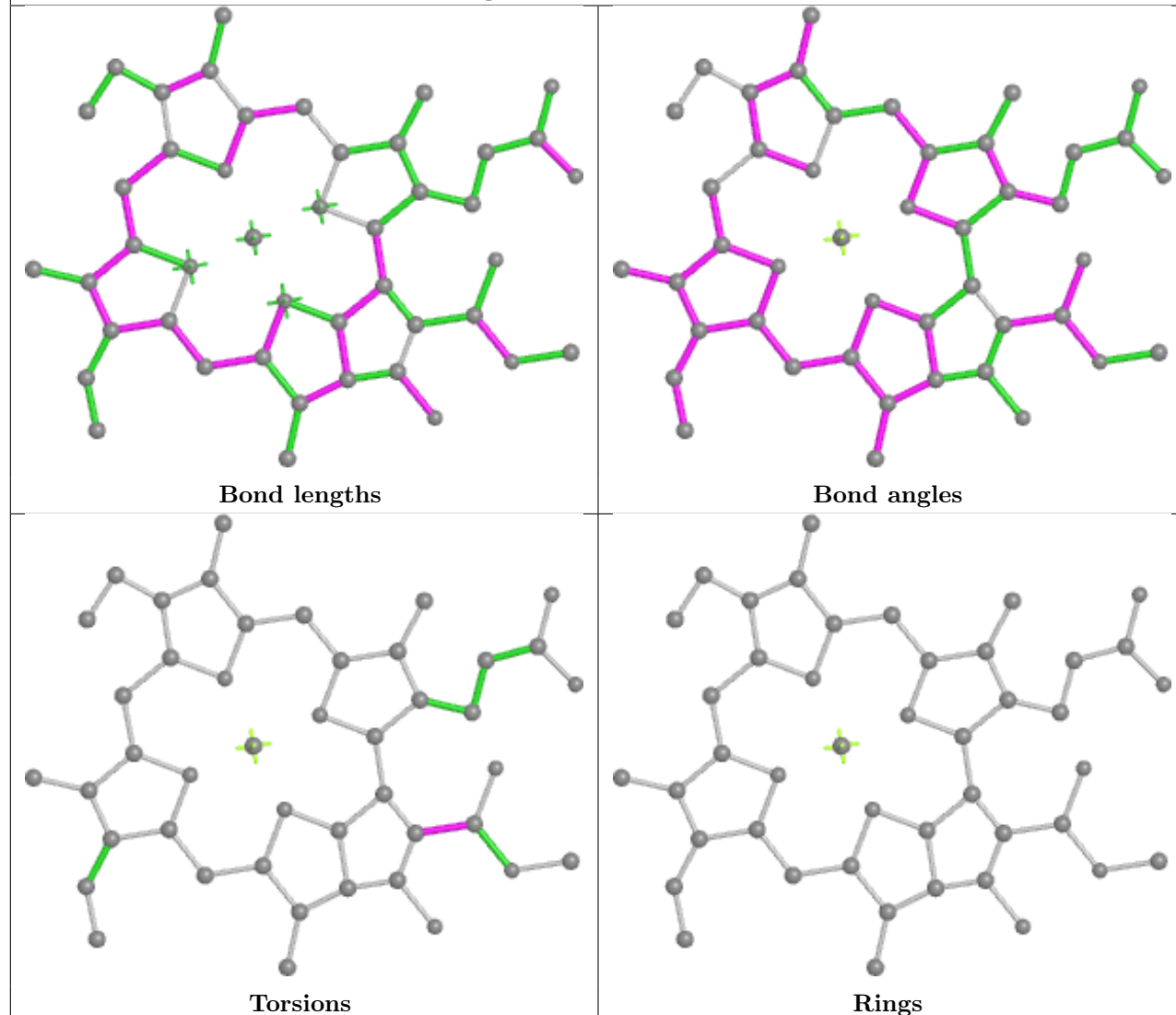
## Ligand CLA bB 817

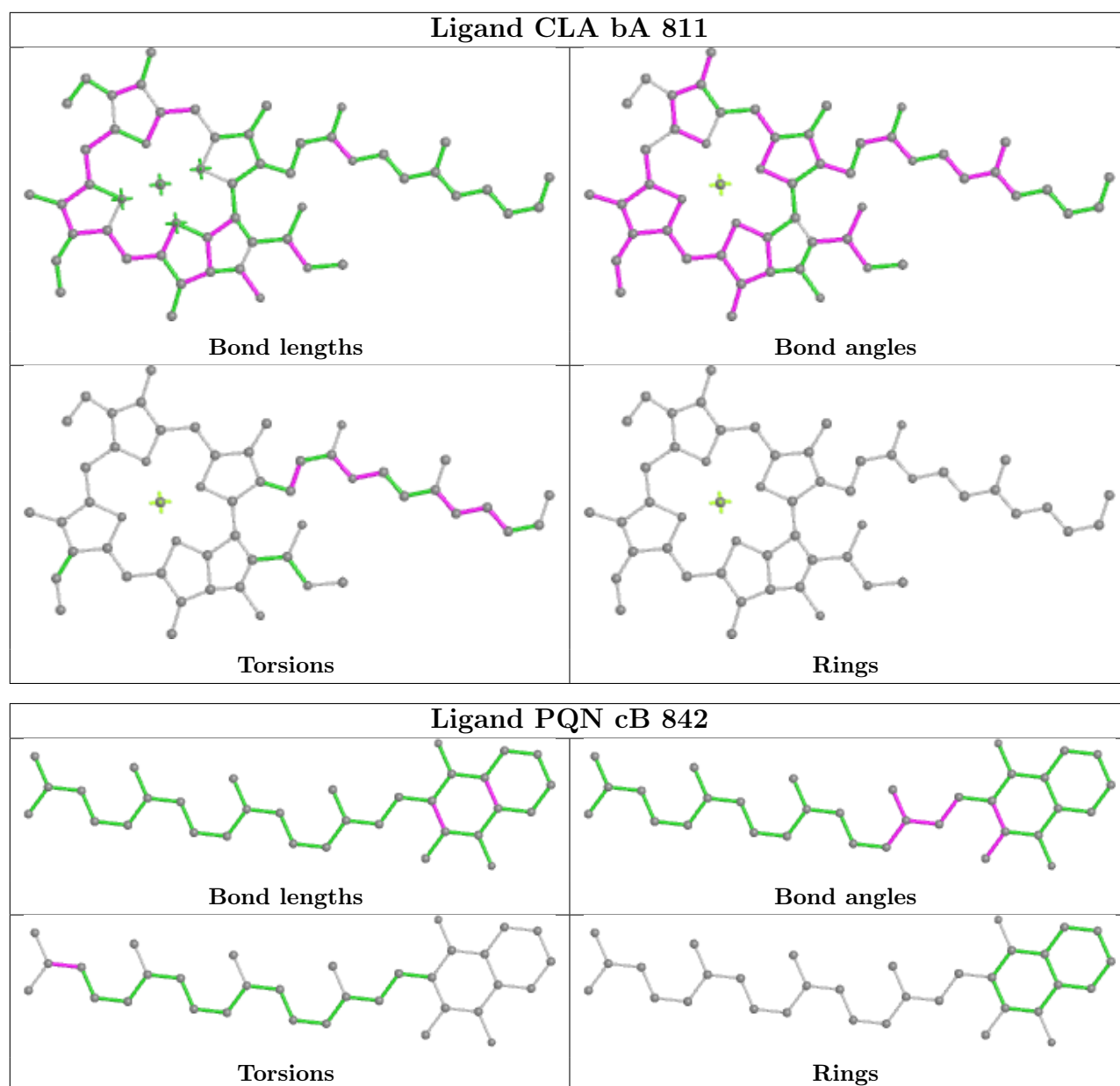


## Ligand CLA bB 827

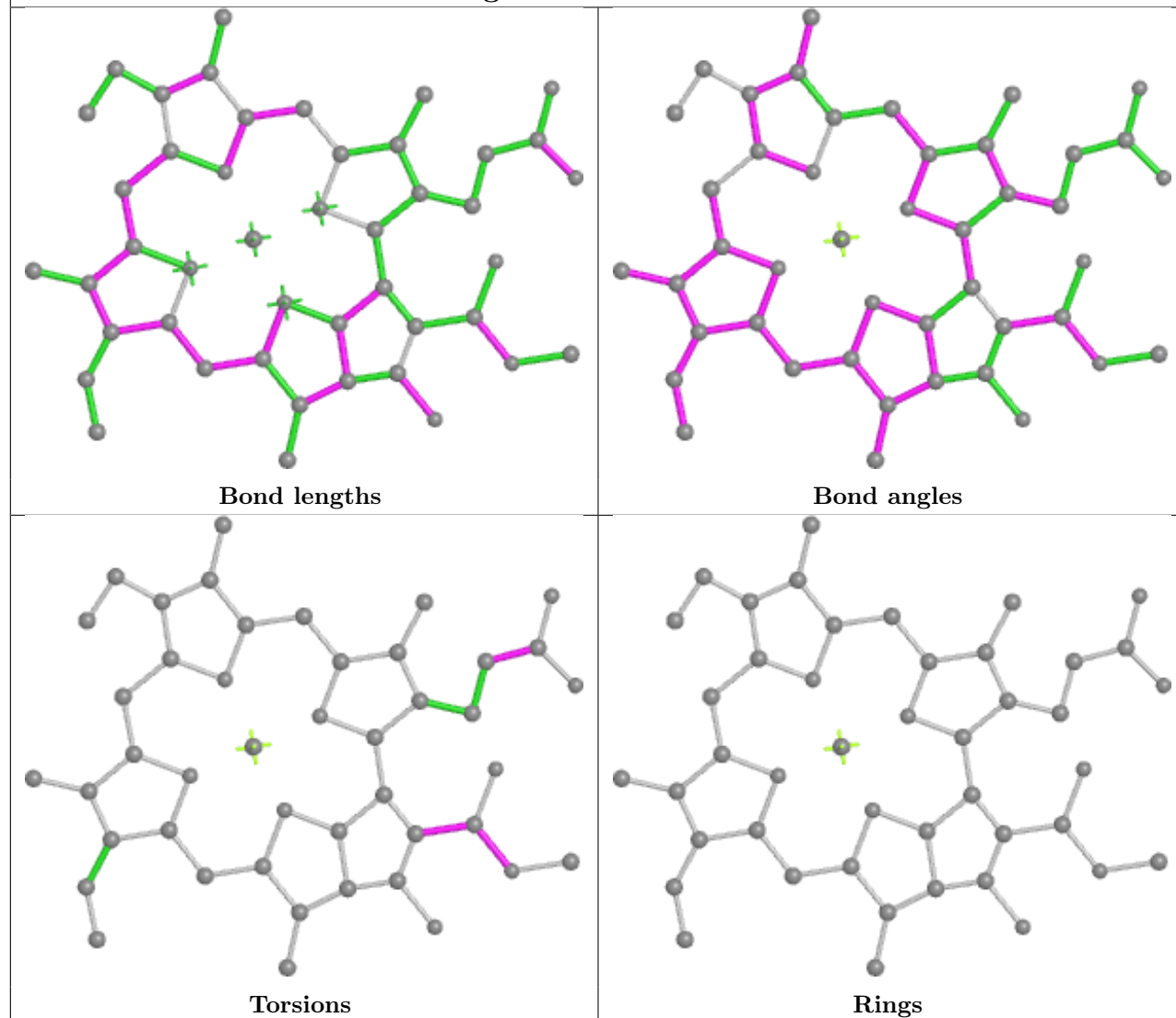


## Ligand CLA bA 803

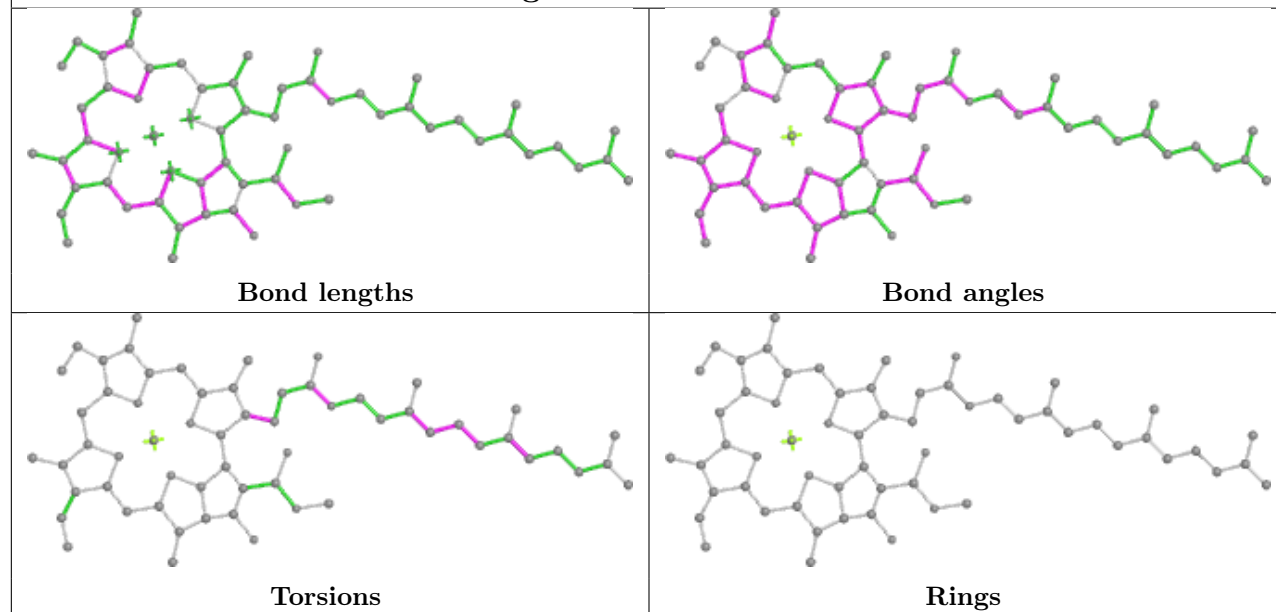




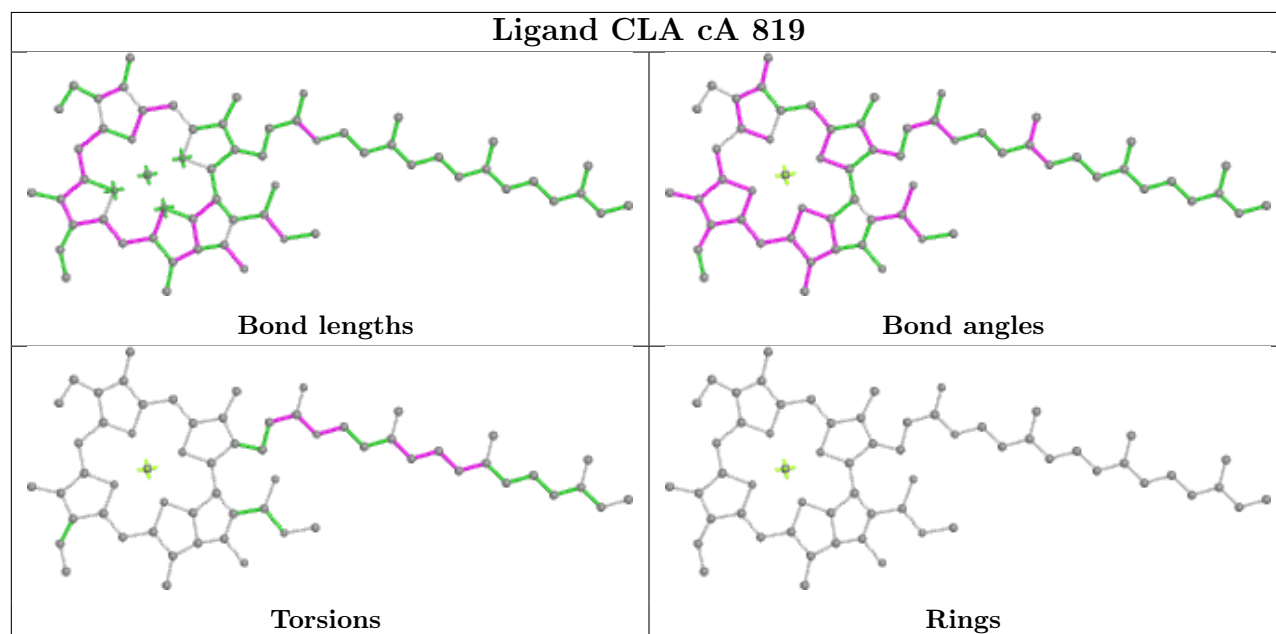
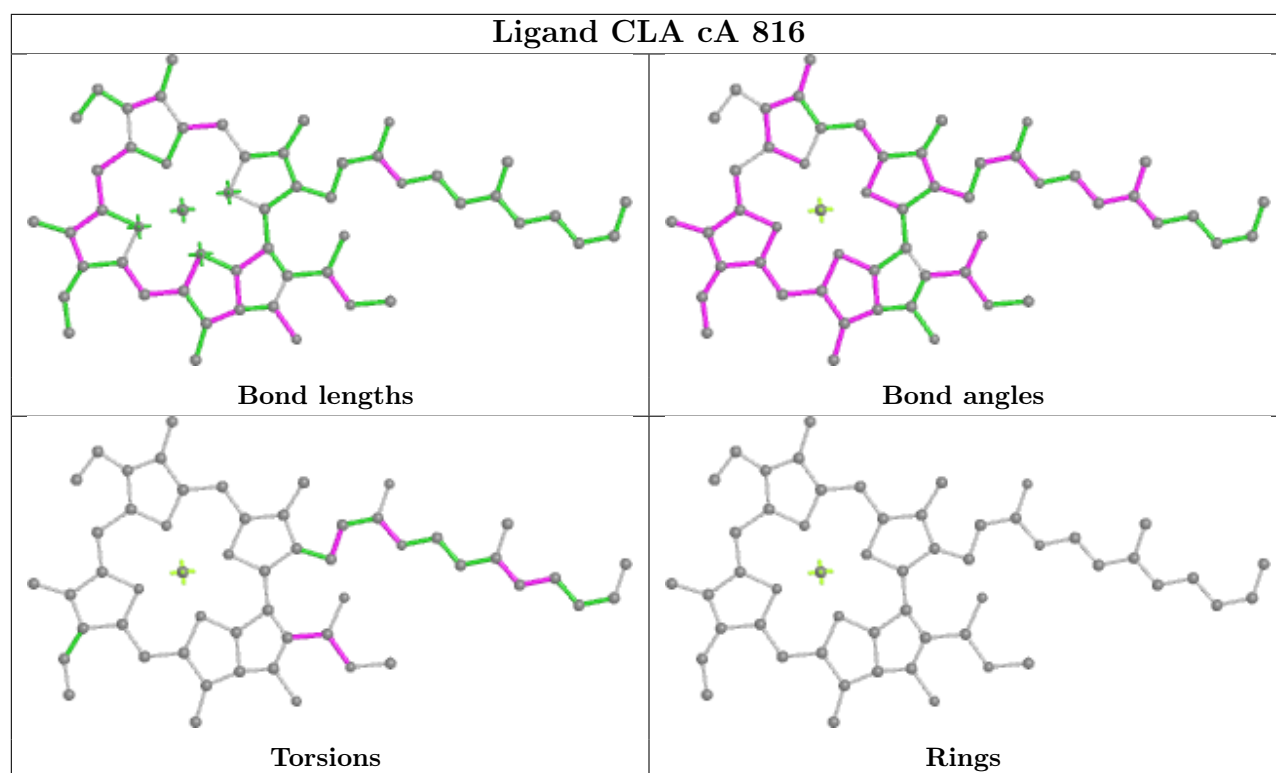
## Ligand CLA cB 835



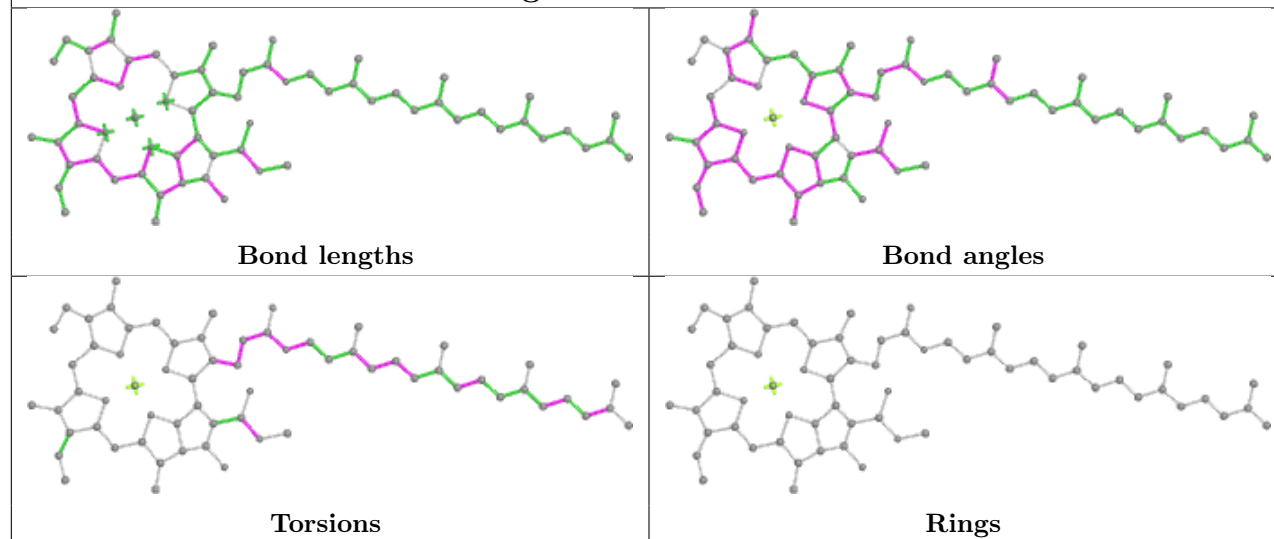
## Ligand CLA bB 819



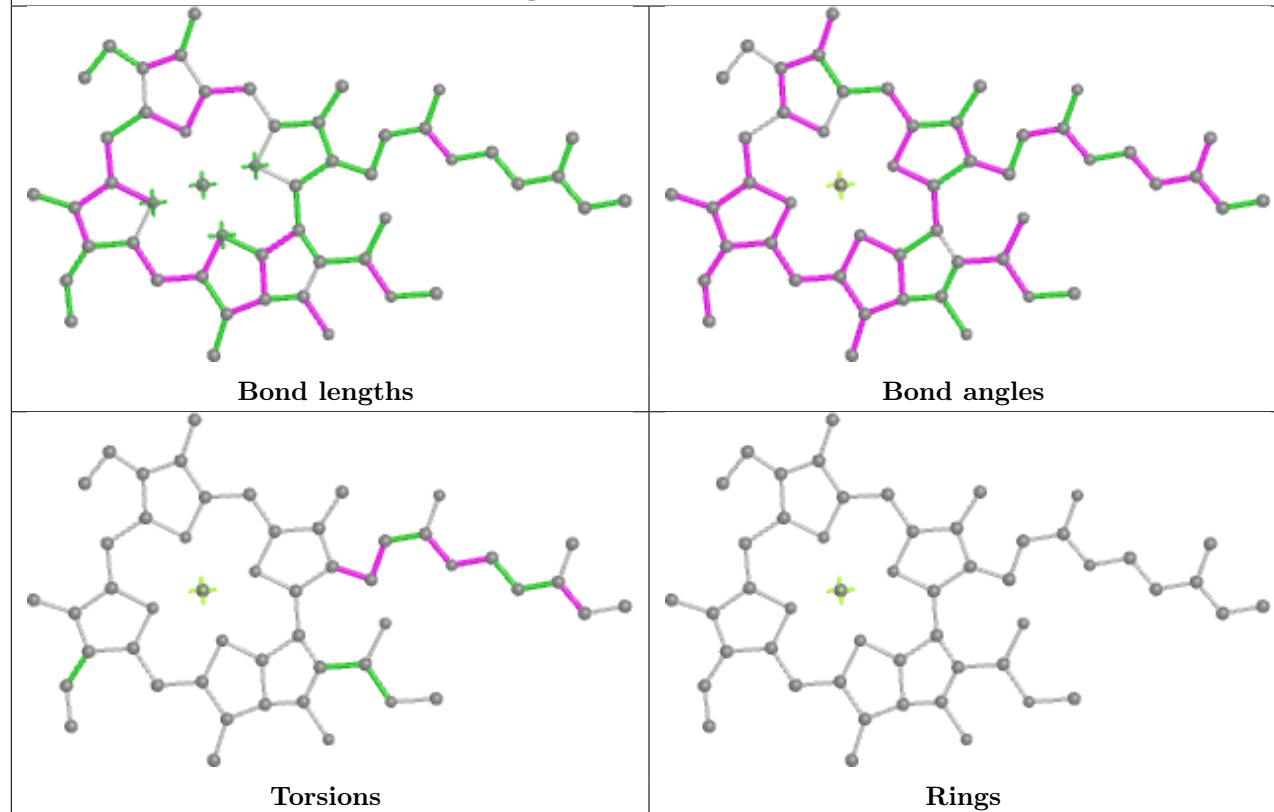


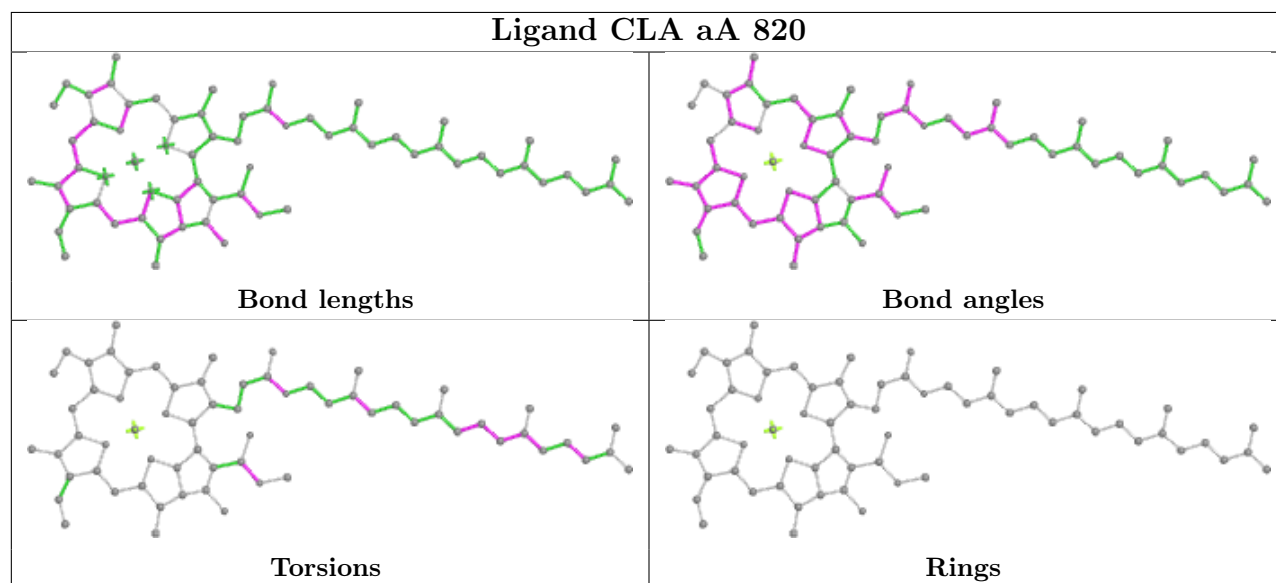
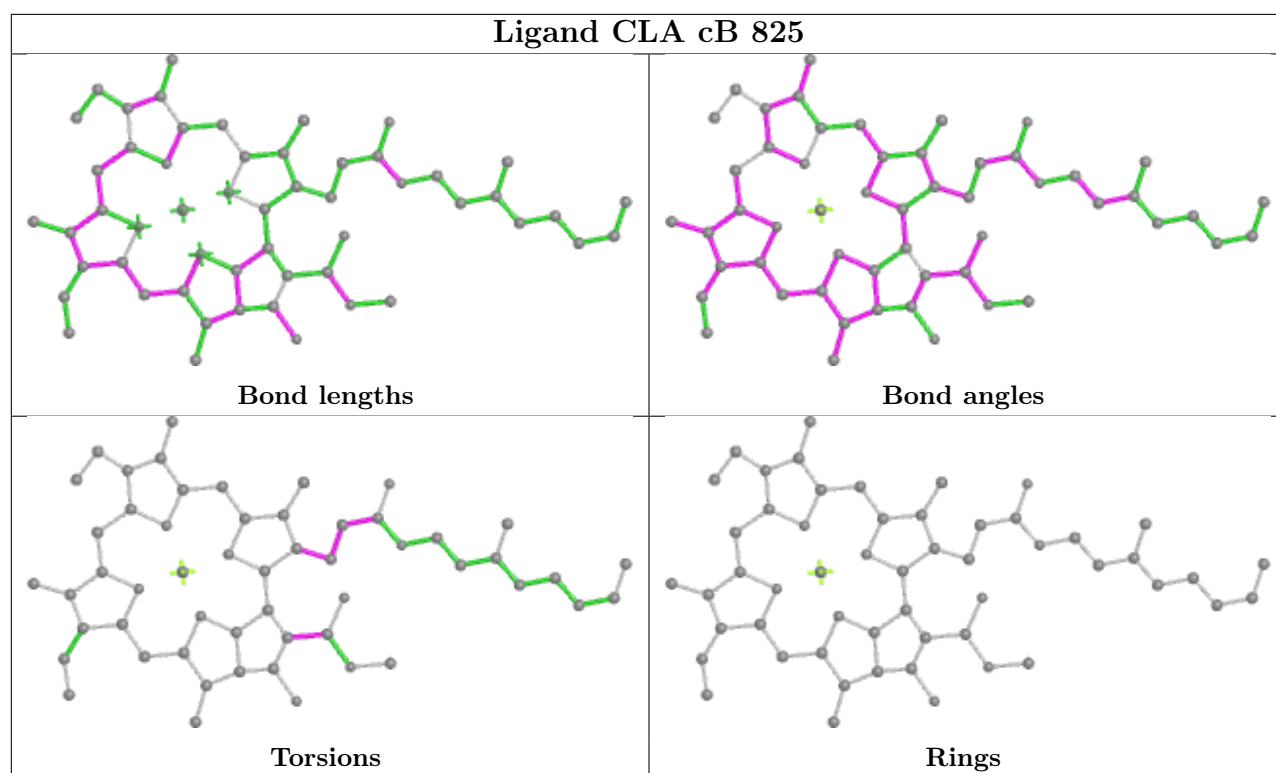


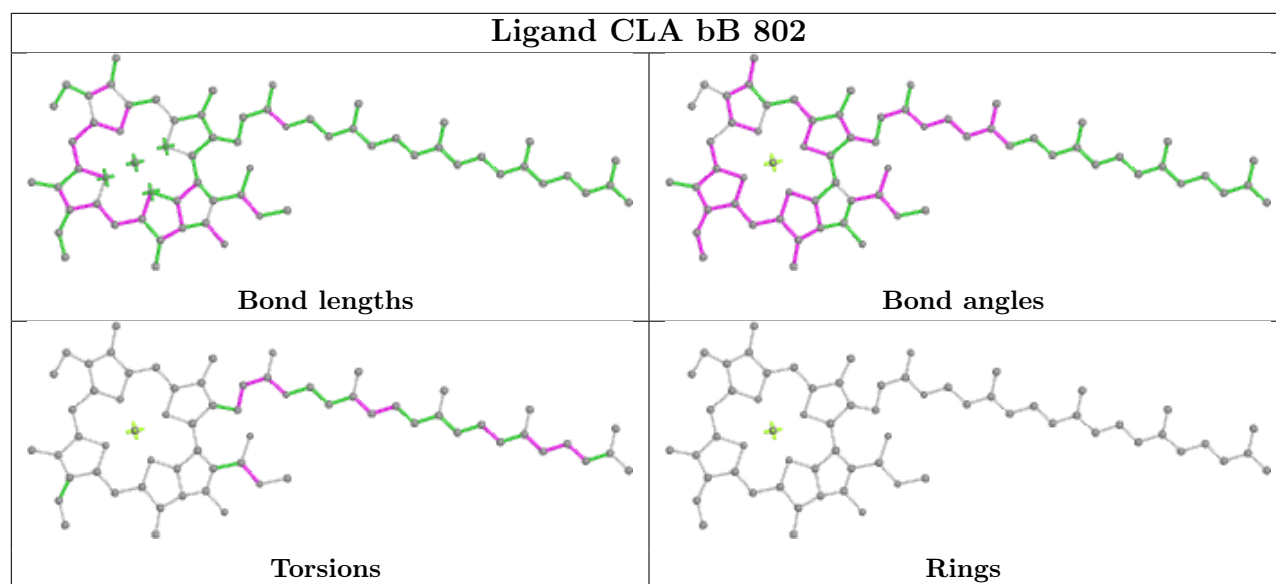
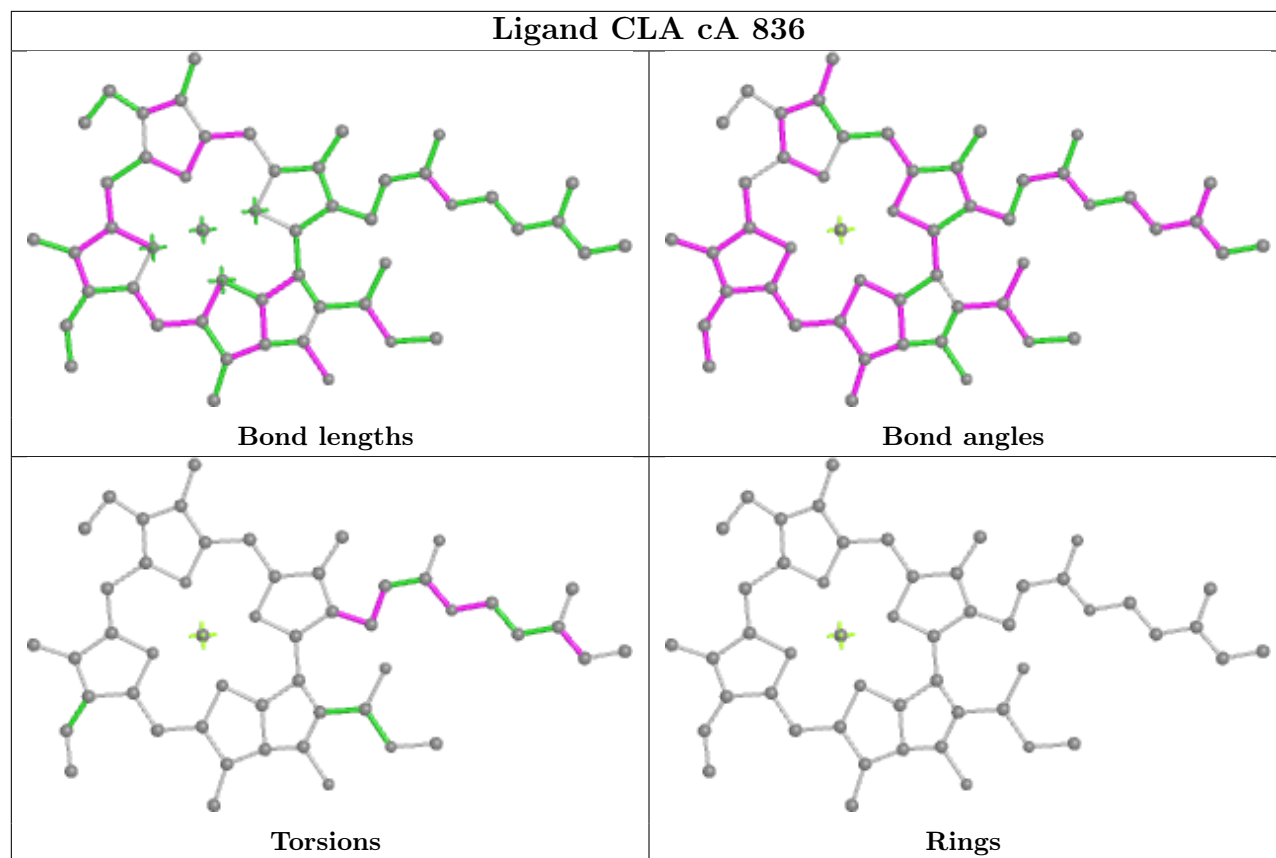
## Ligand CLA bB 811

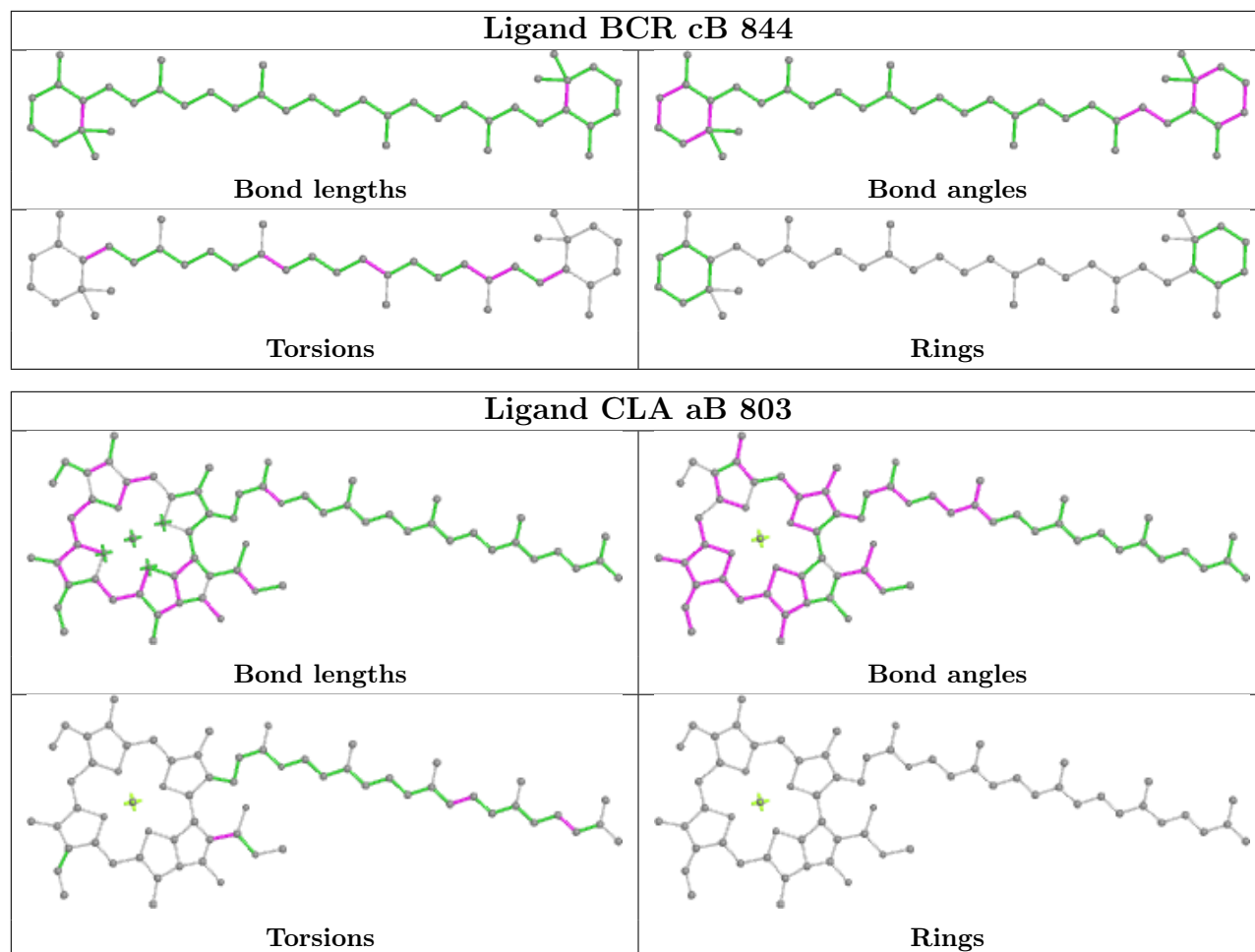


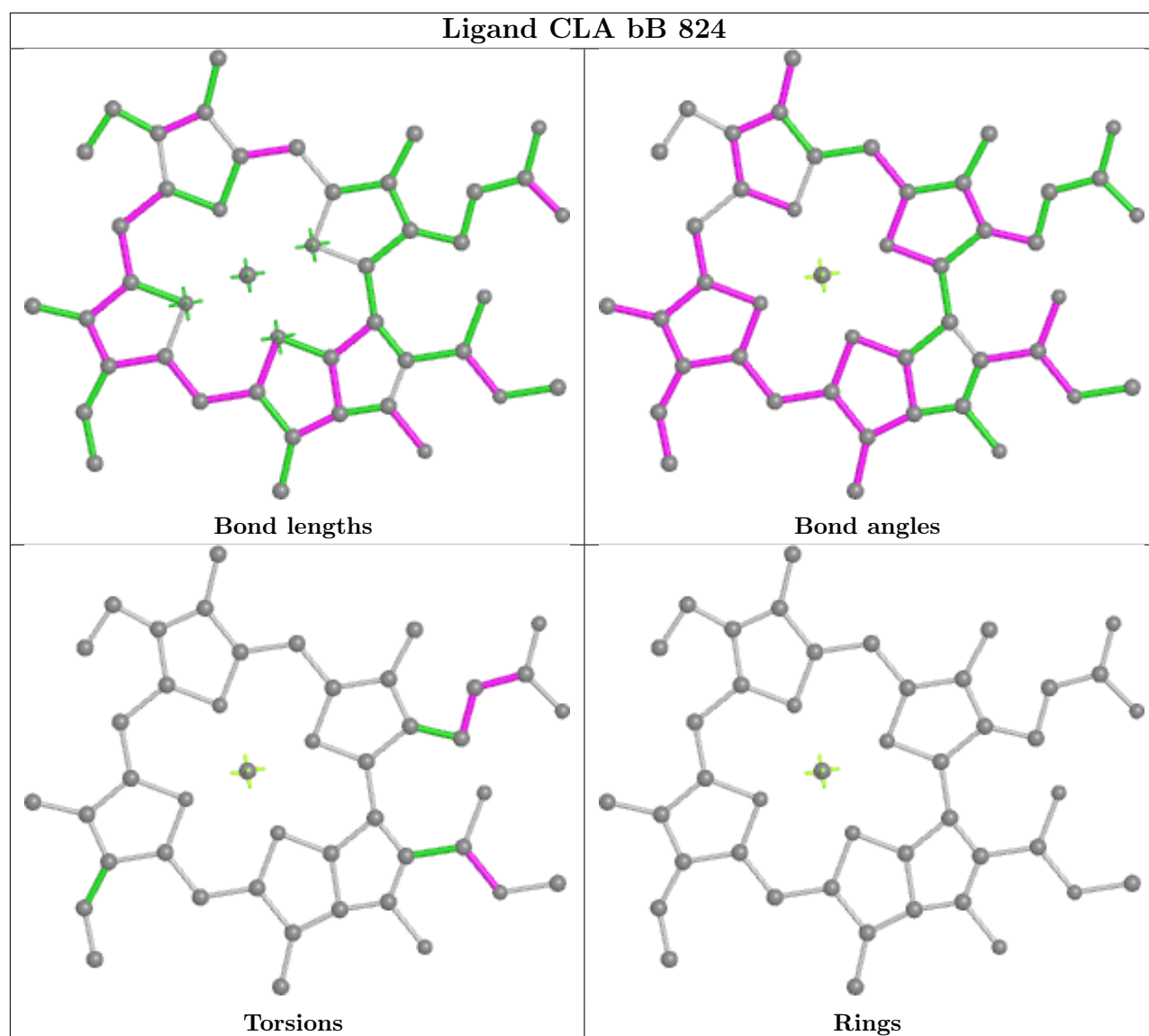
## Ligand CLA aA 836

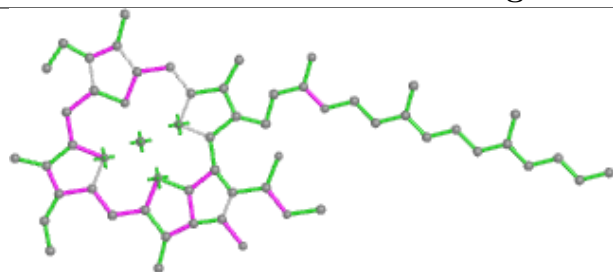




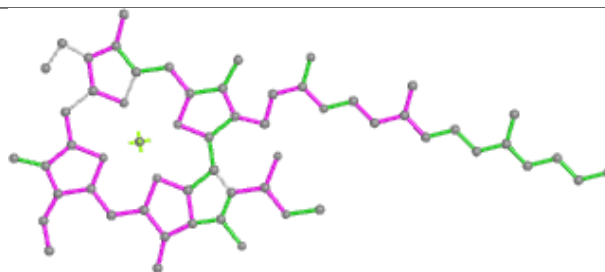




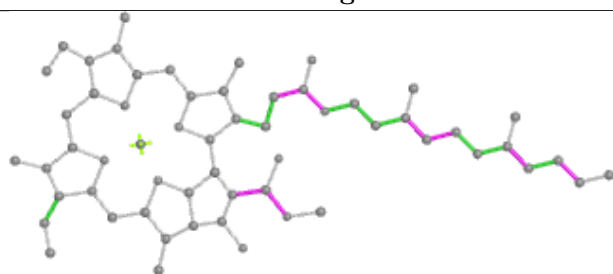


**Ligand CLA cB 833**

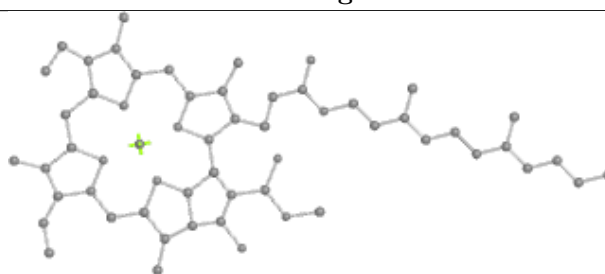
Bond lengths



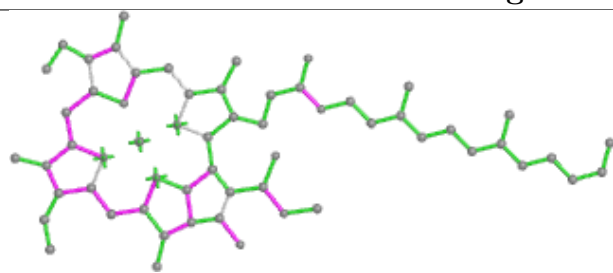
Bond angles



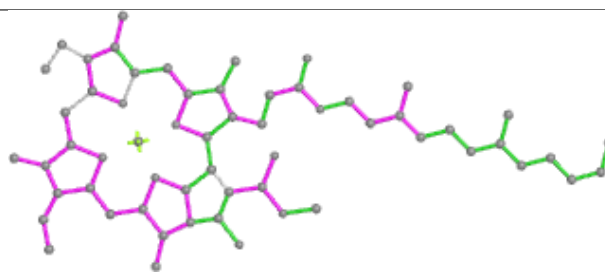
Torsions



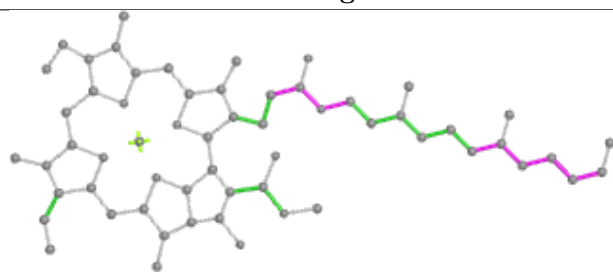
Rings

**Ligand CLA cB 818**

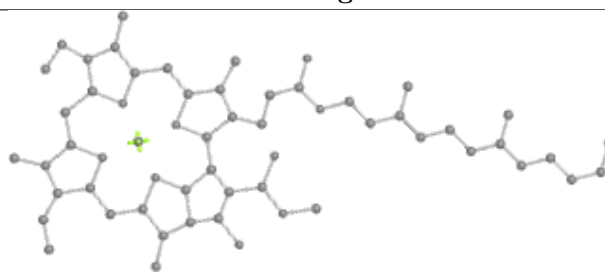
Bond lengths



Bond angles

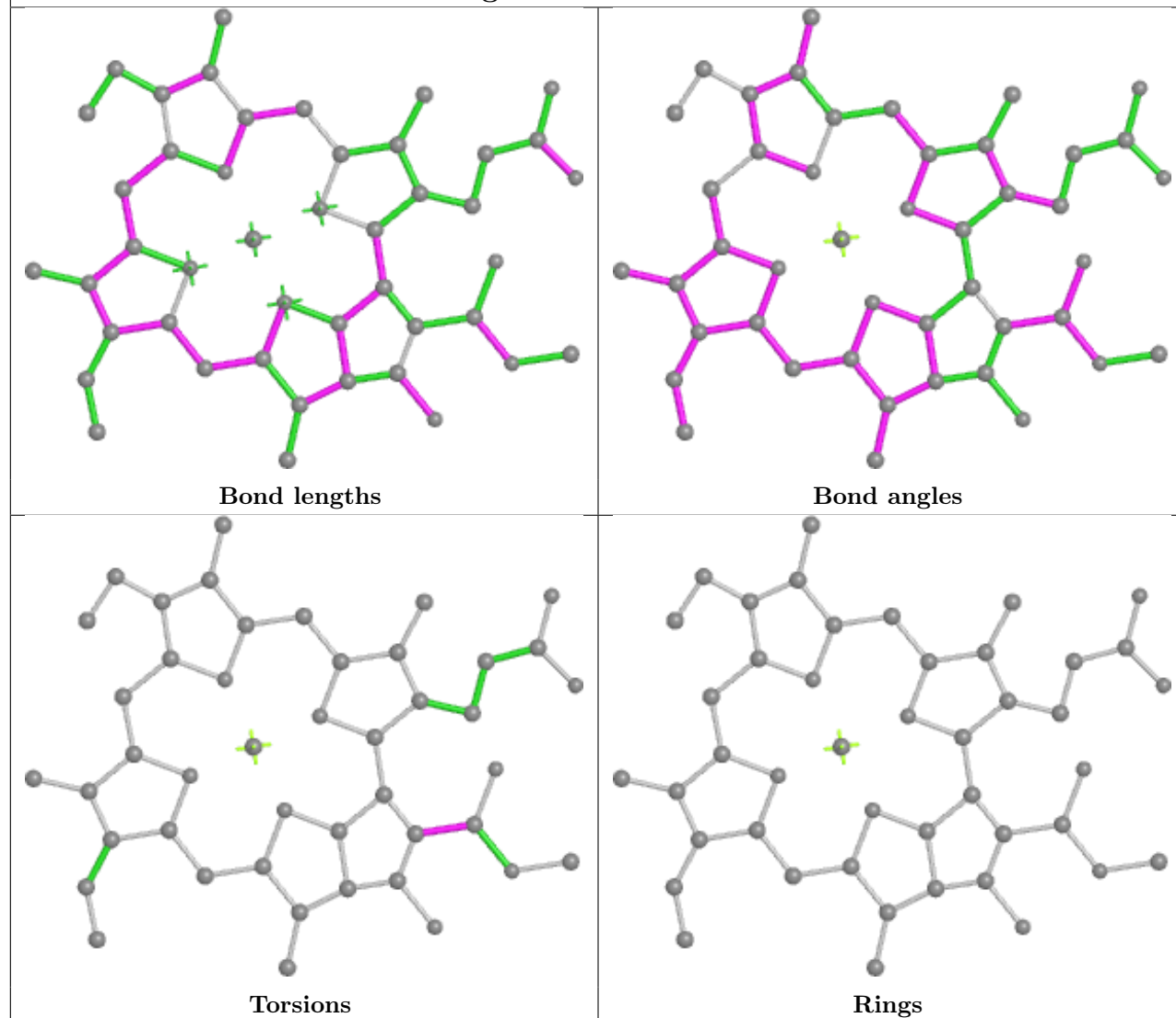


Torsions

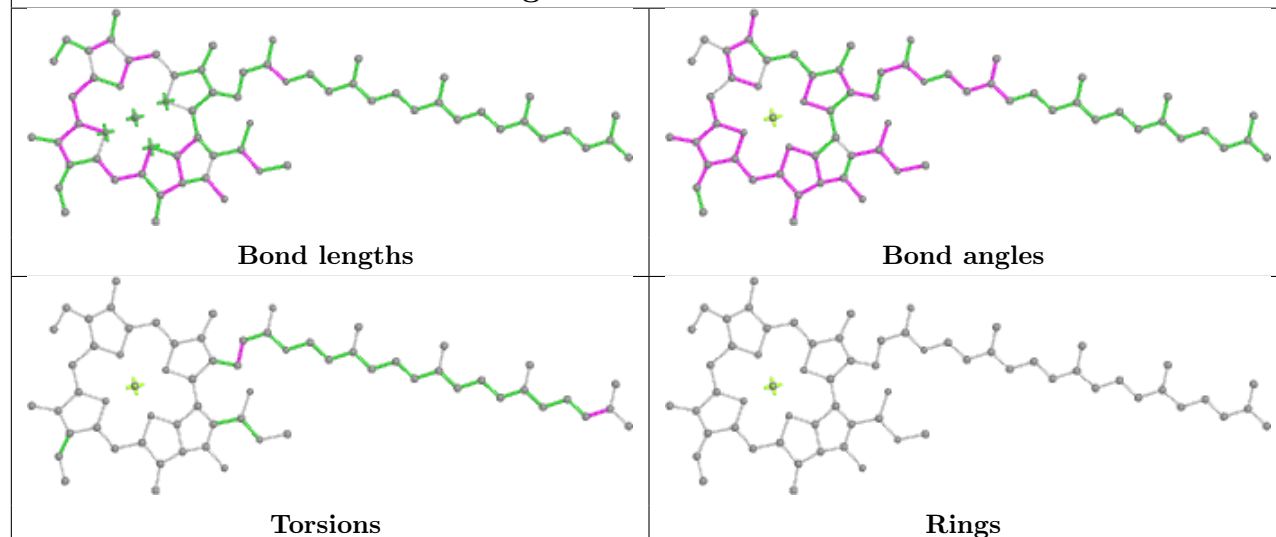


Rings

## Ligand CLA aA 803

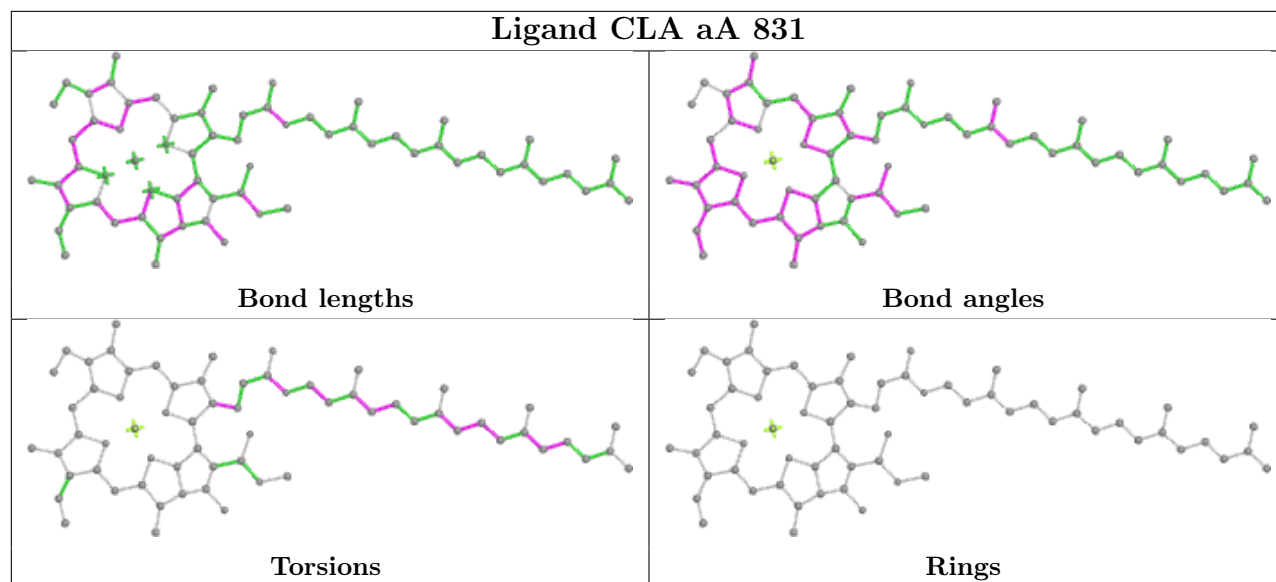


## Ligand CLA bB 840

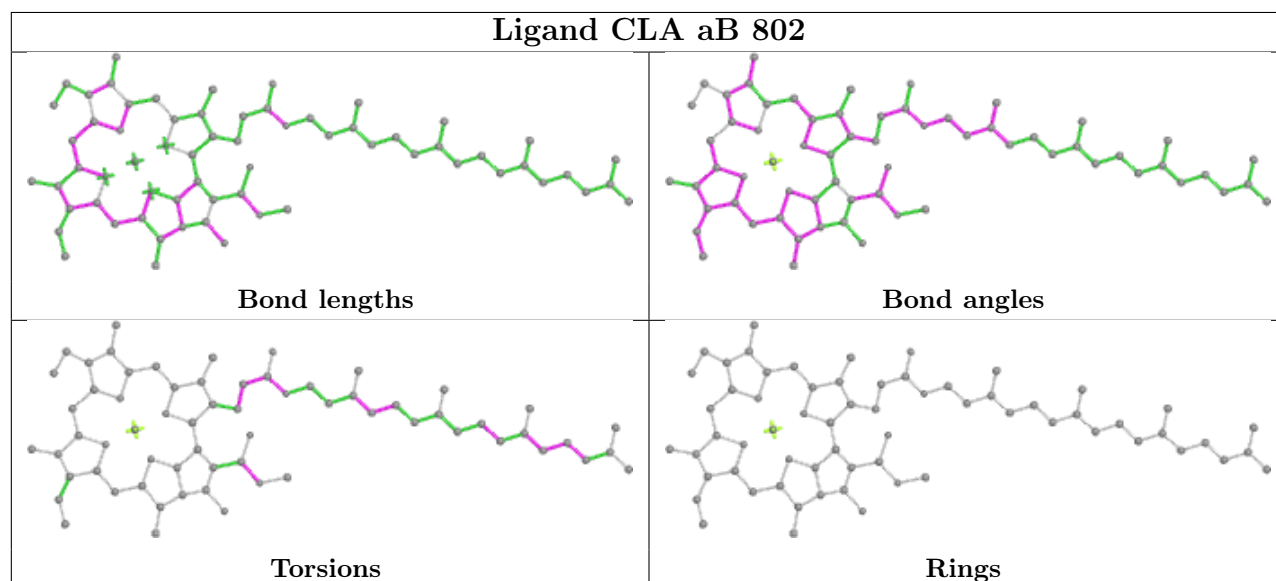




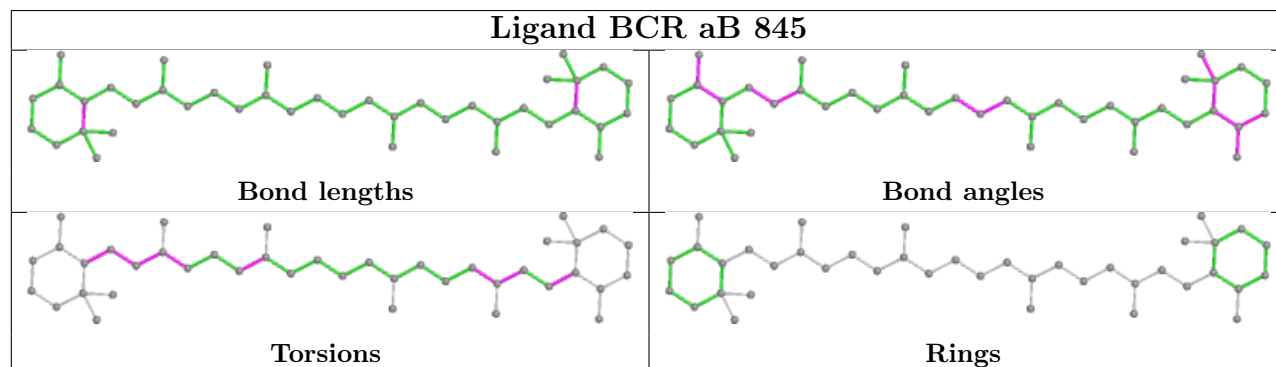
## Ligand CLA aA 831



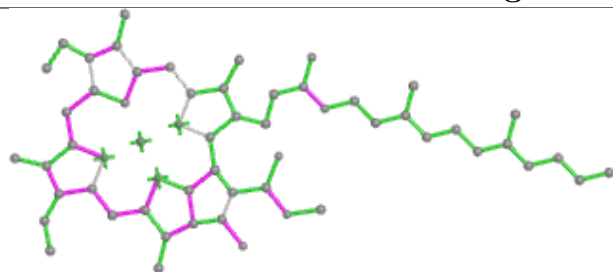
## Ligand CLA aB 802



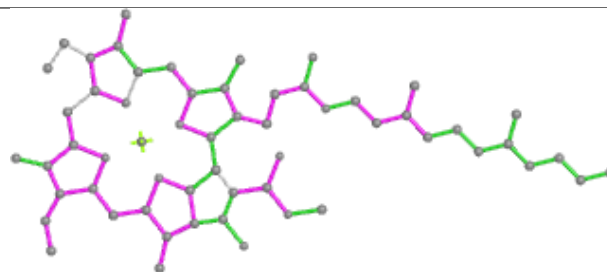
## Ligand BCR aB 845



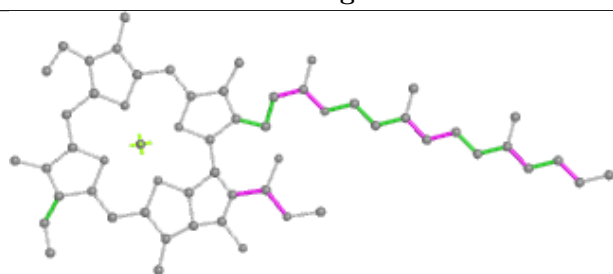
## Ligand CLA bB 833



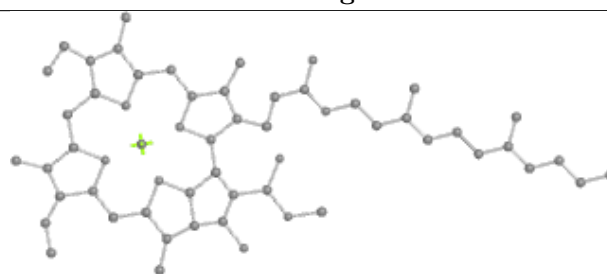
Bond lengths



Bond angles

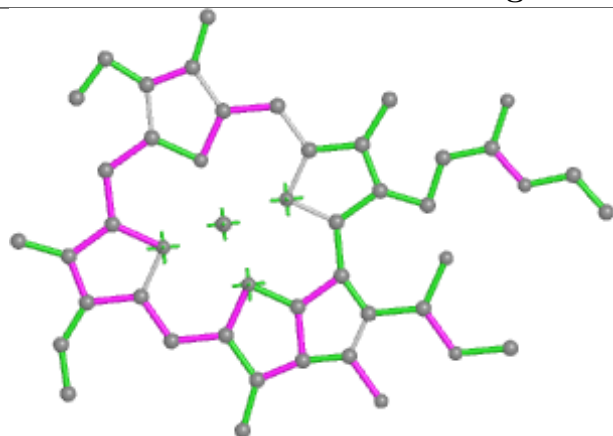


Torsions

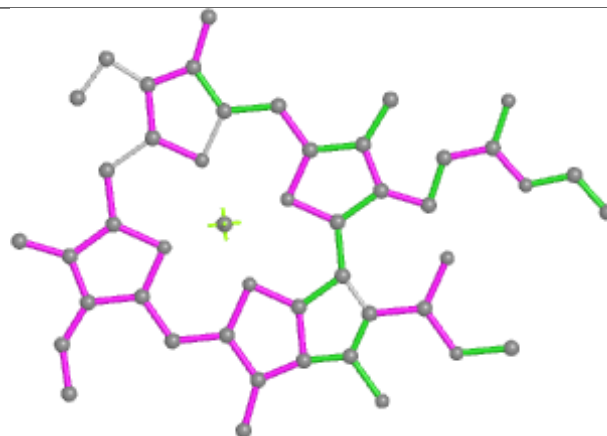


Rings

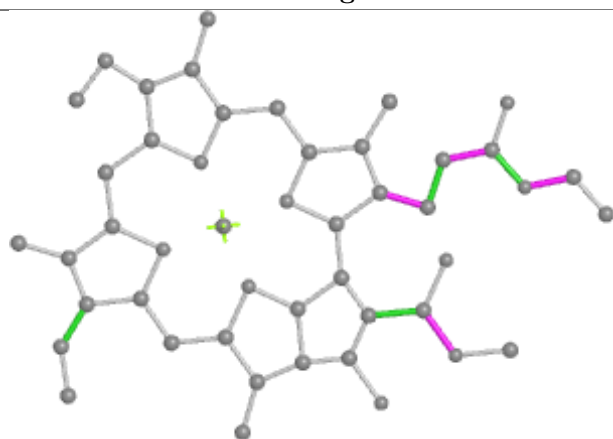
## Ligand CLA cB 839



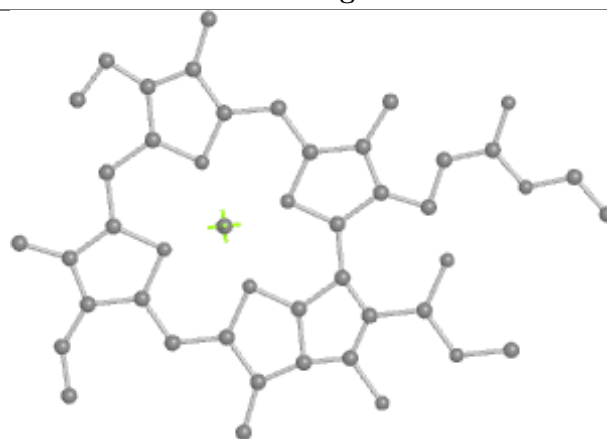
Bond lengths



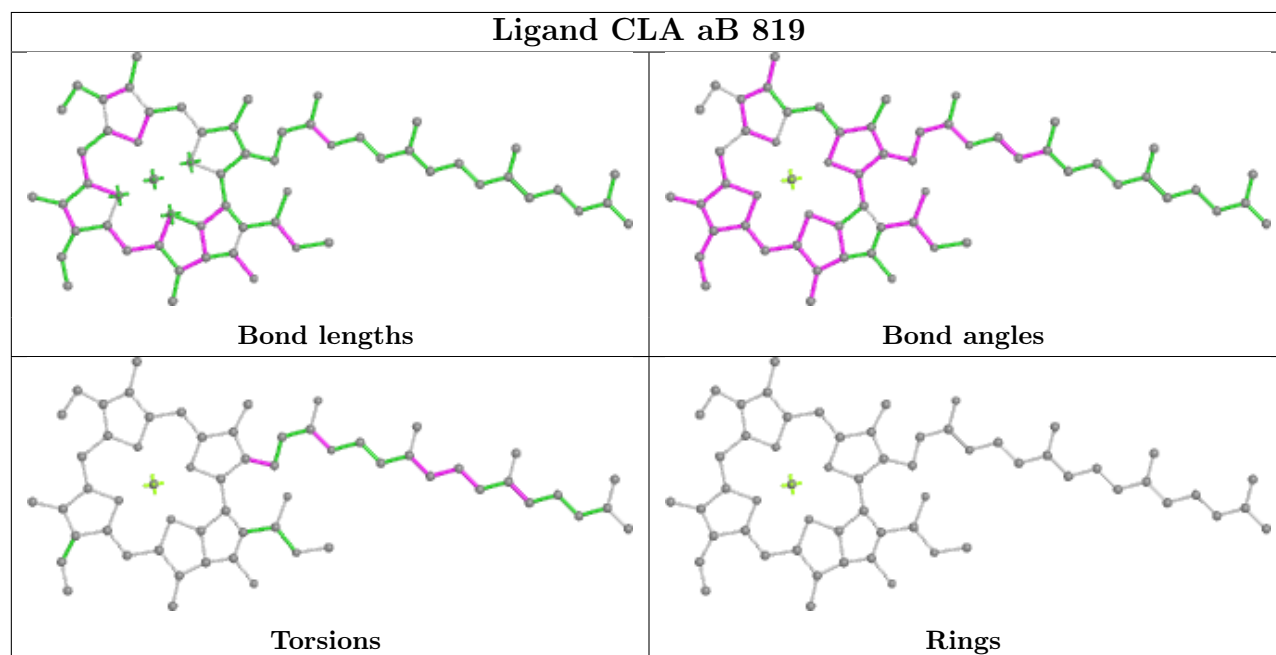
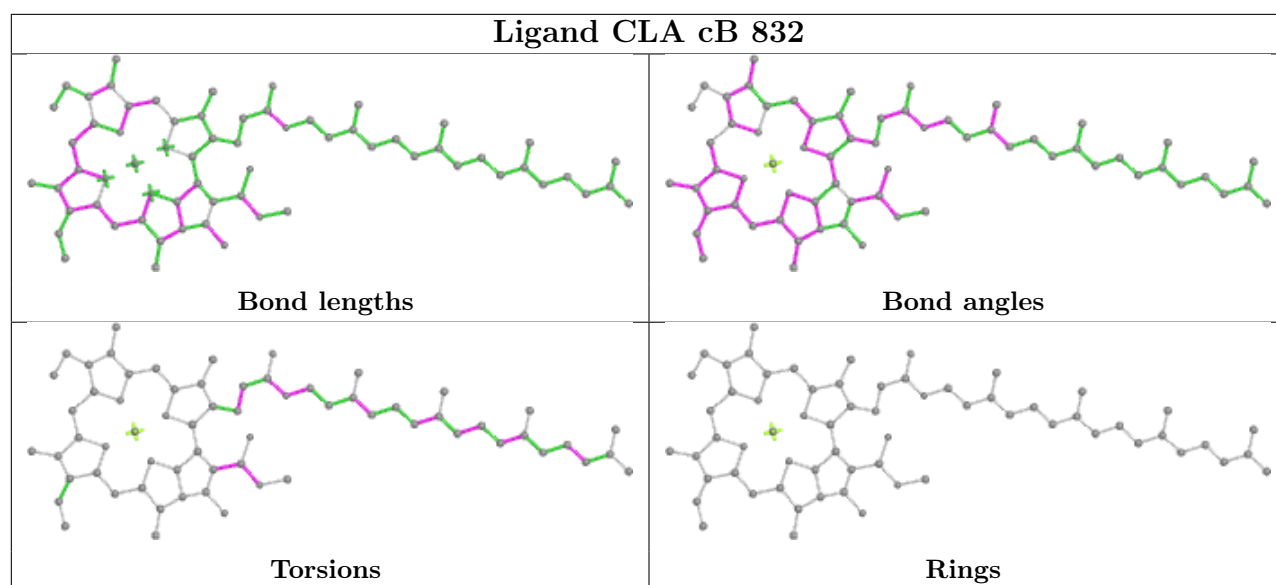
Bond angles

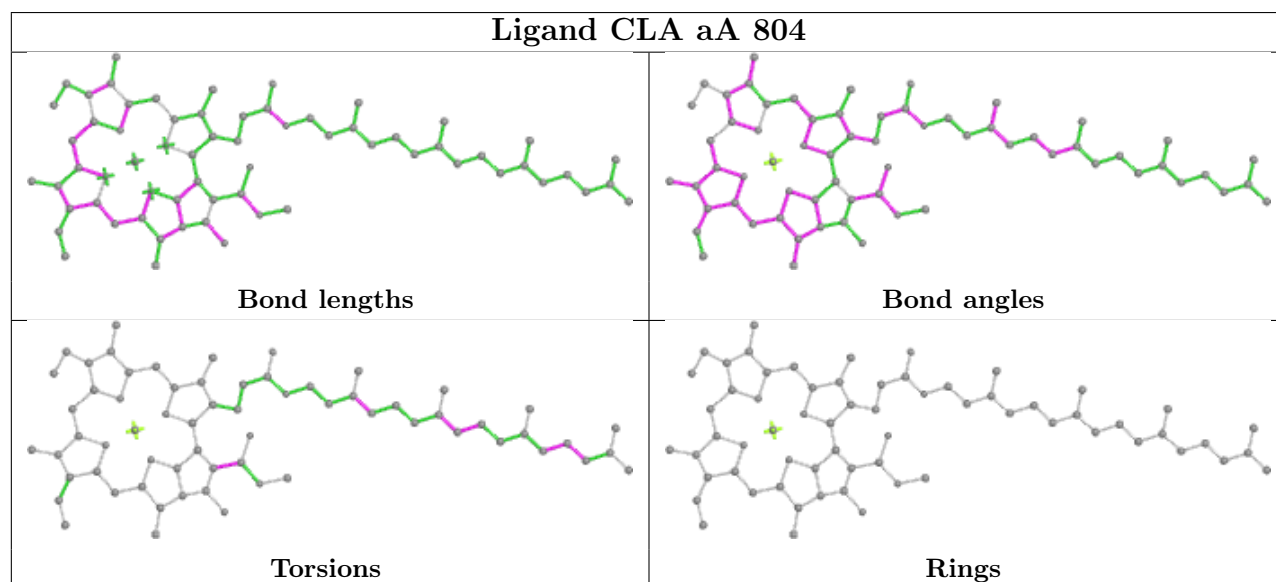
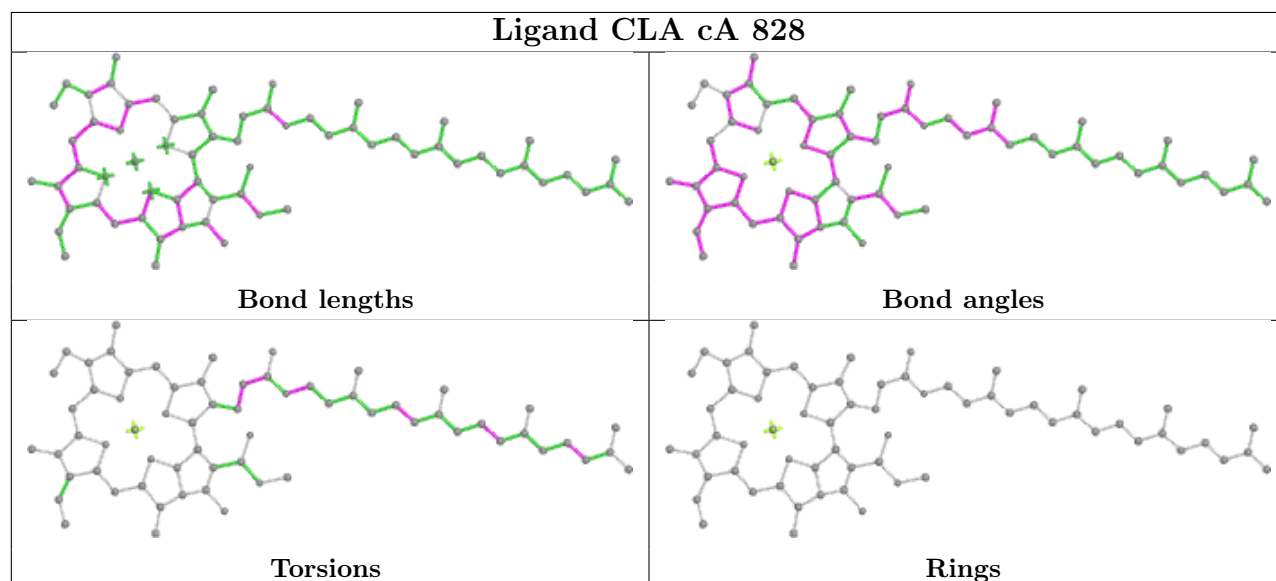
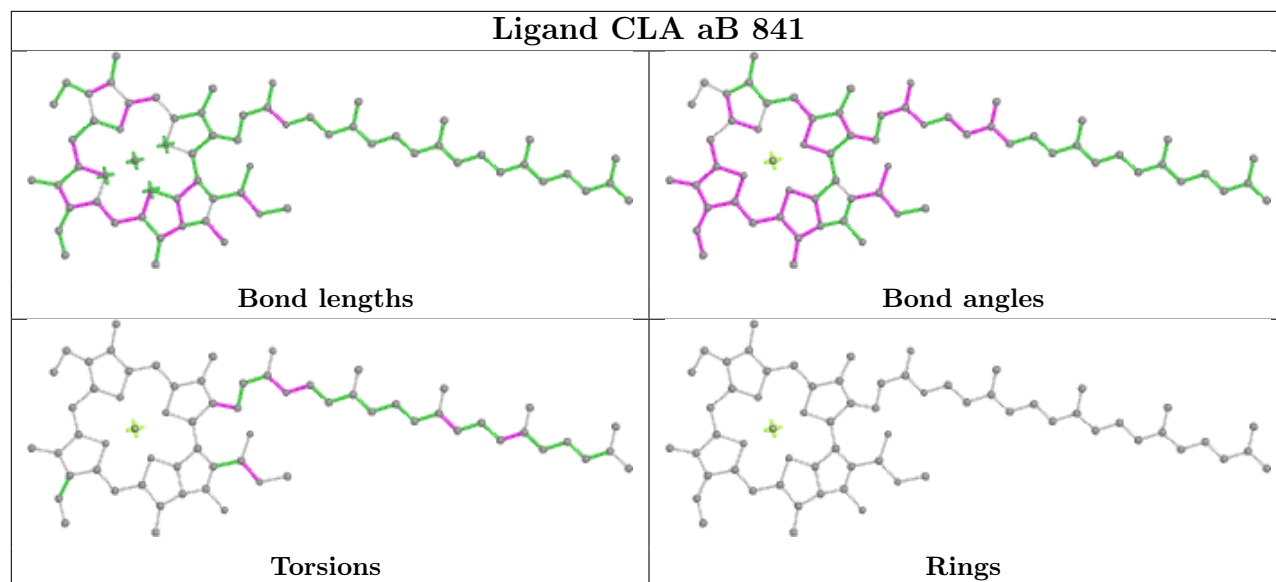


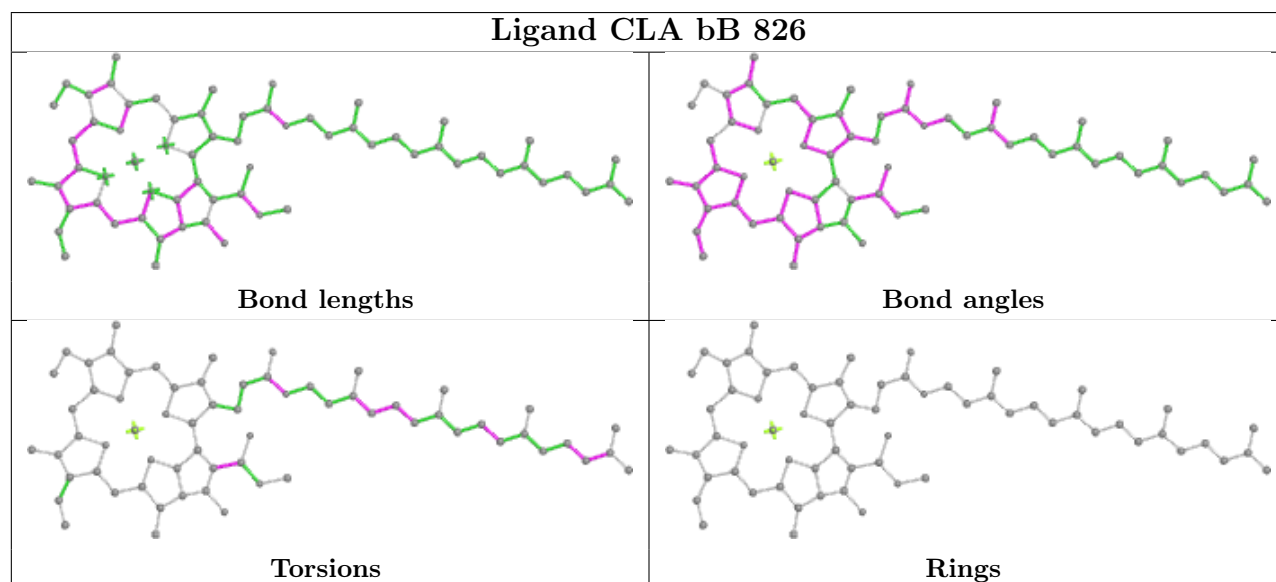
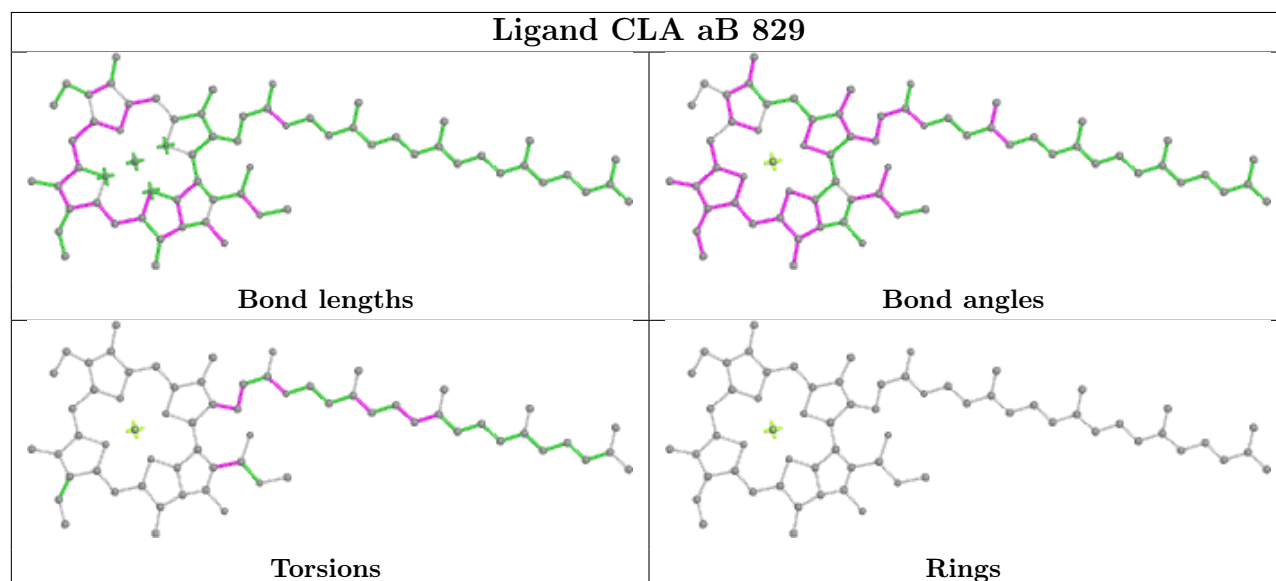
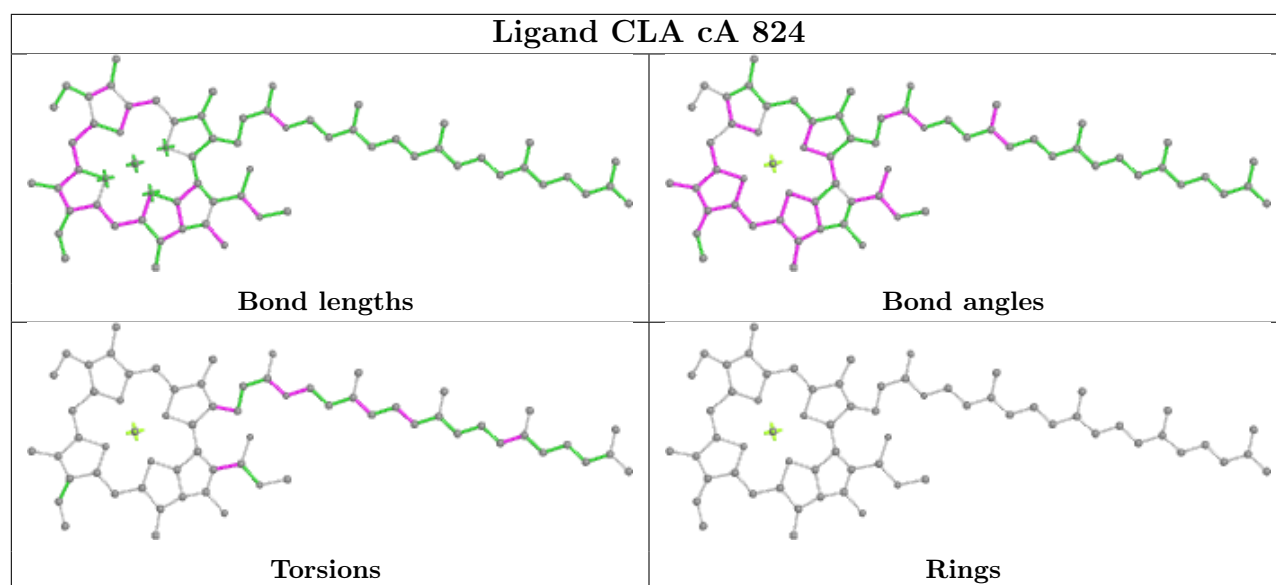
Torsions



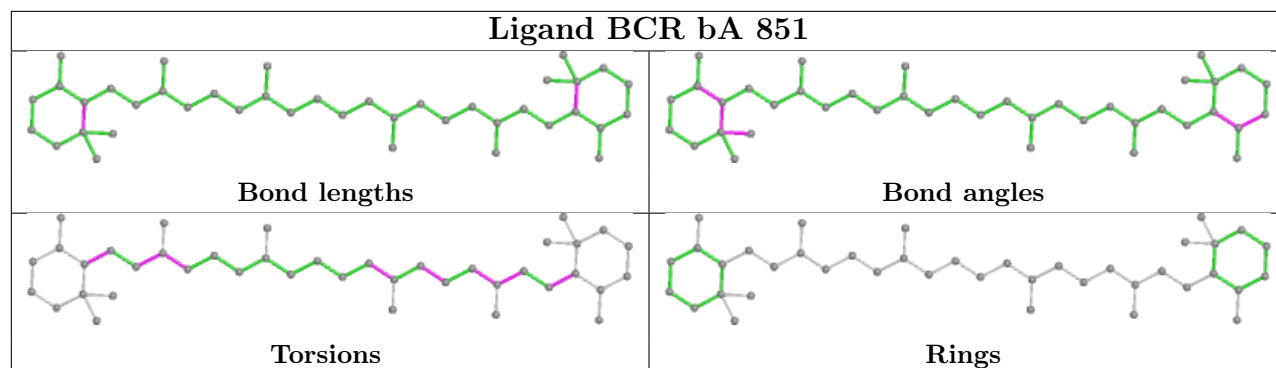
Rings



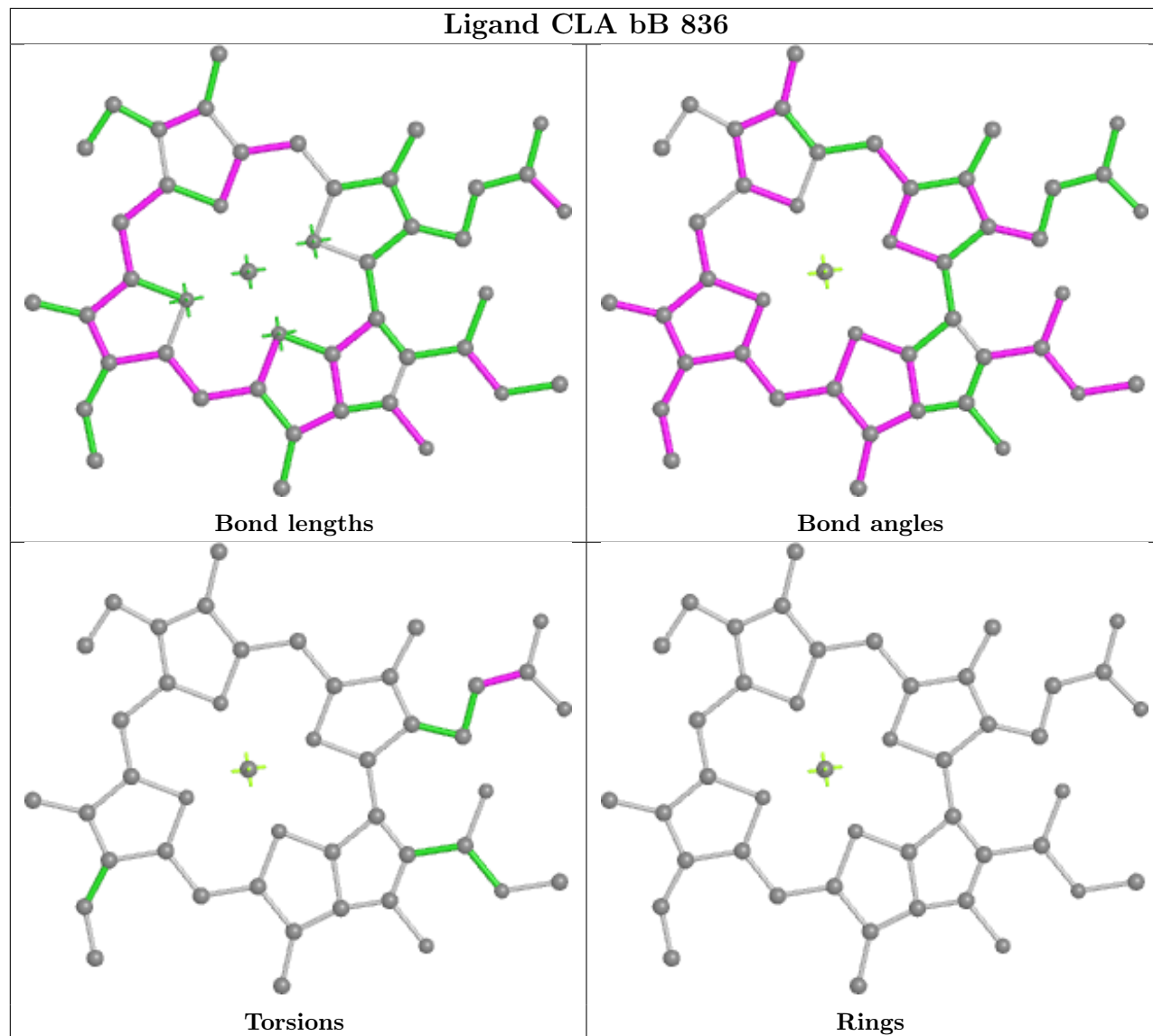




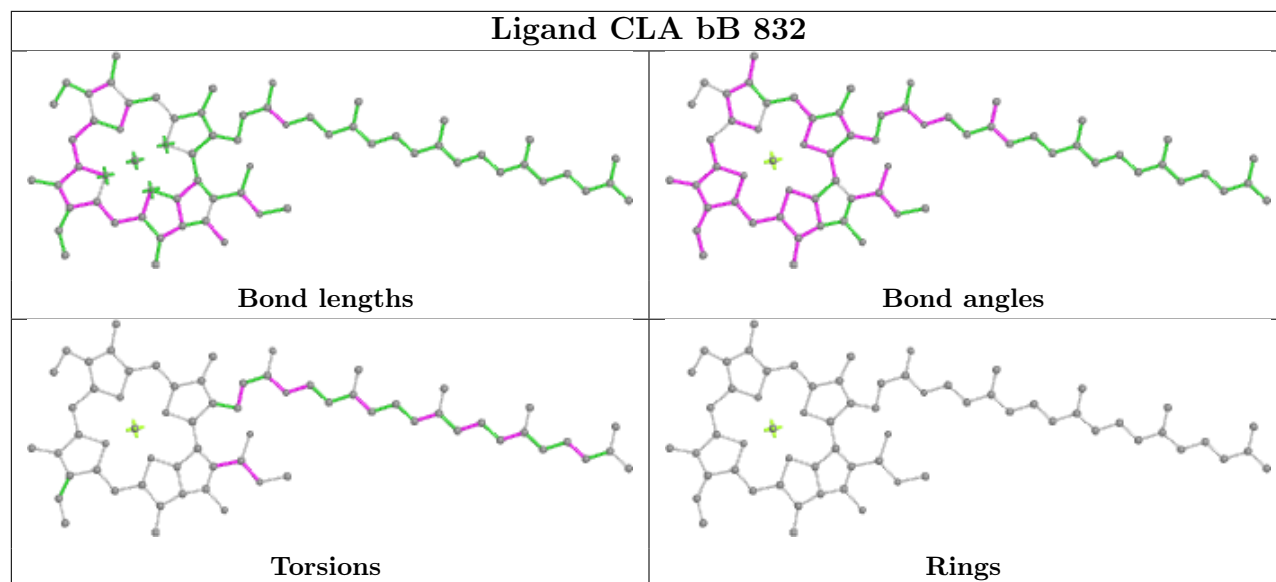
## Ligand BCR bA 851



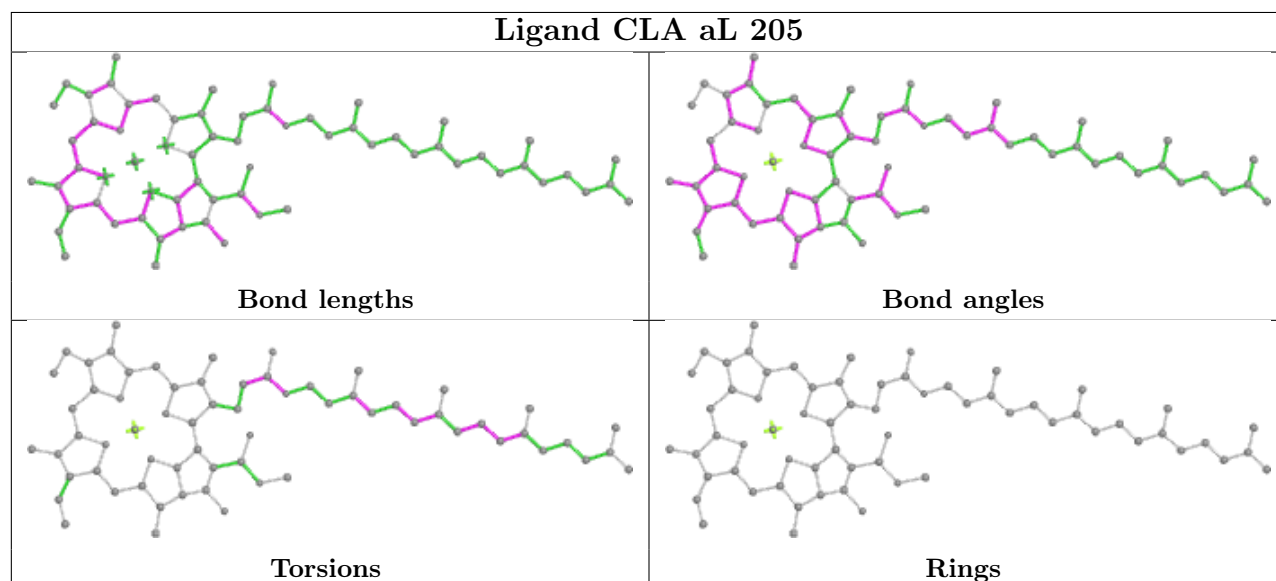
## Ligand CLA bB 836



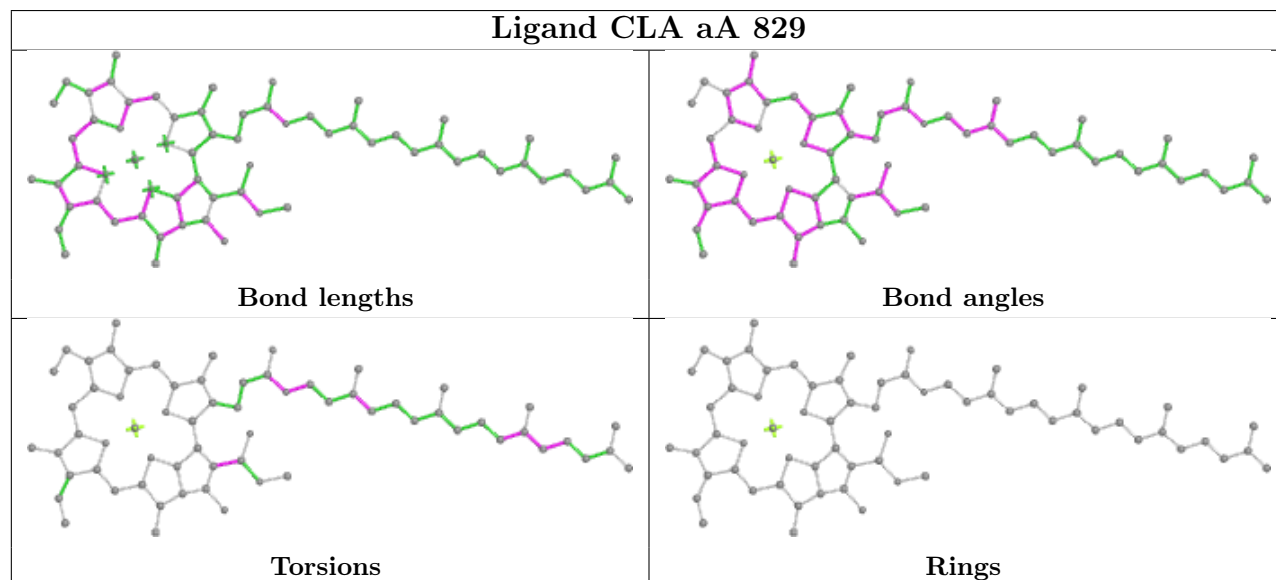
## Ligand CLA bB 832

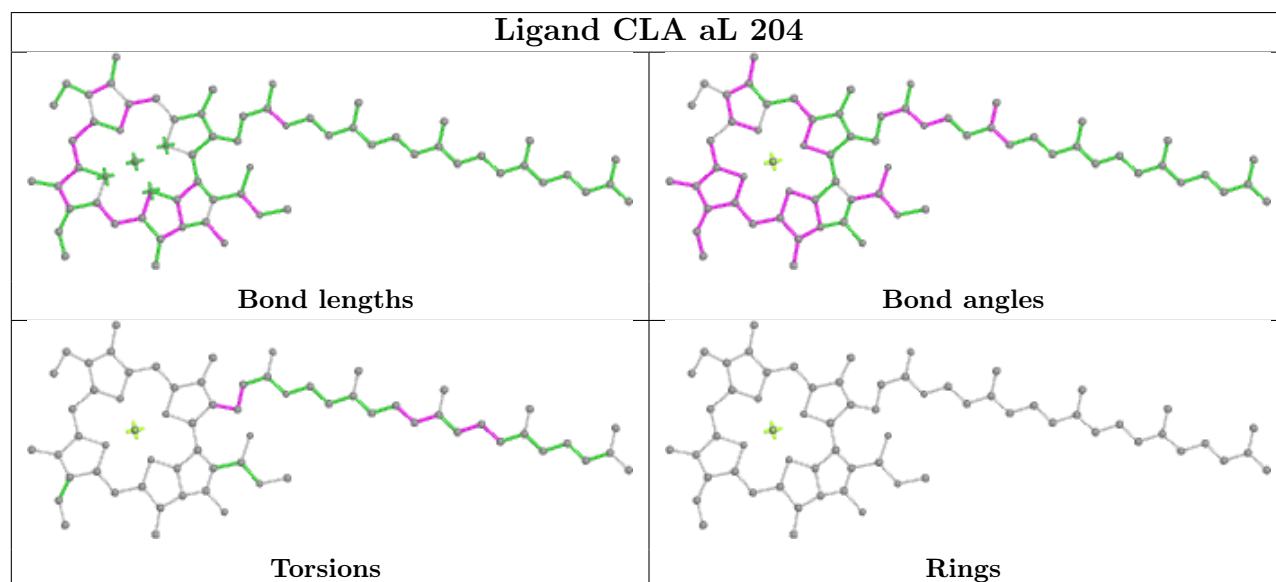
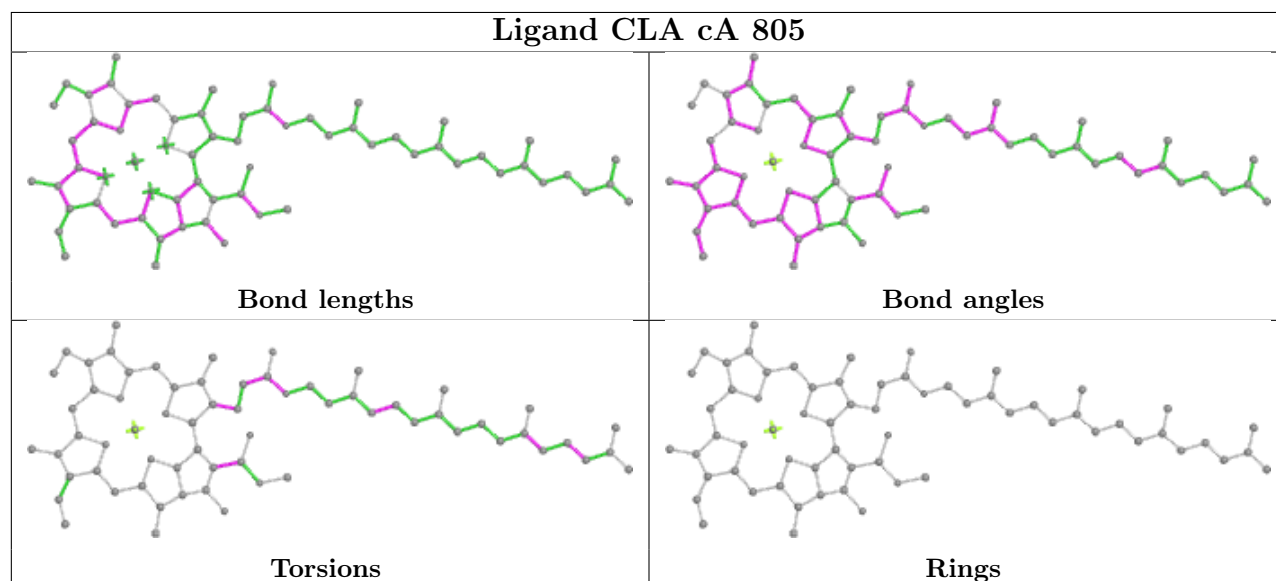
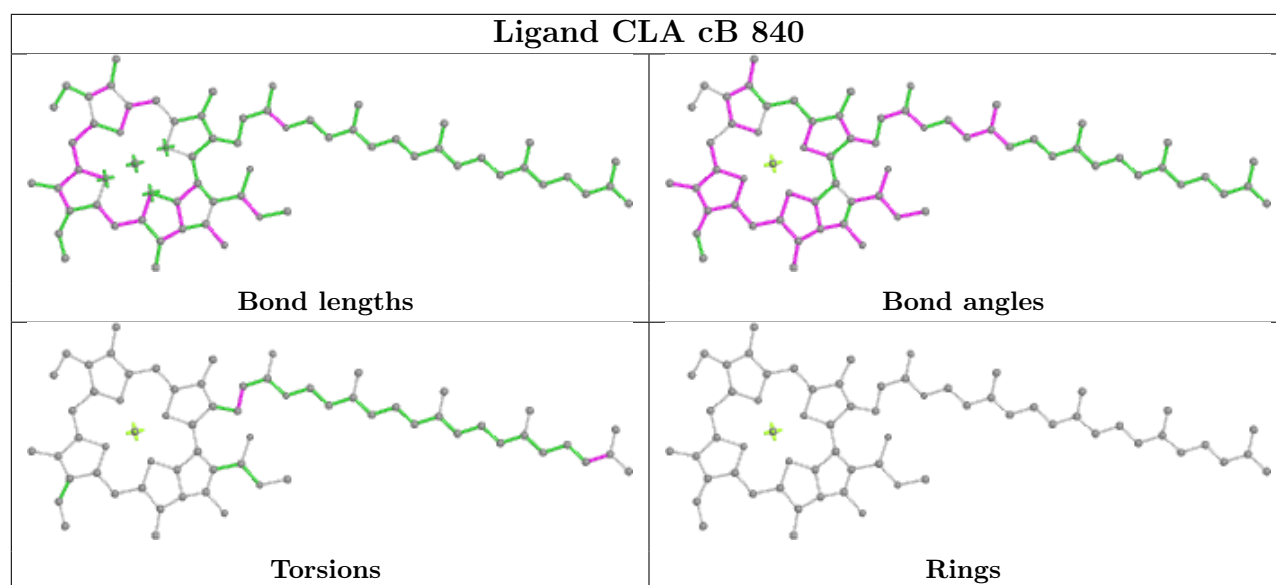


## Ligand CLA aL 205

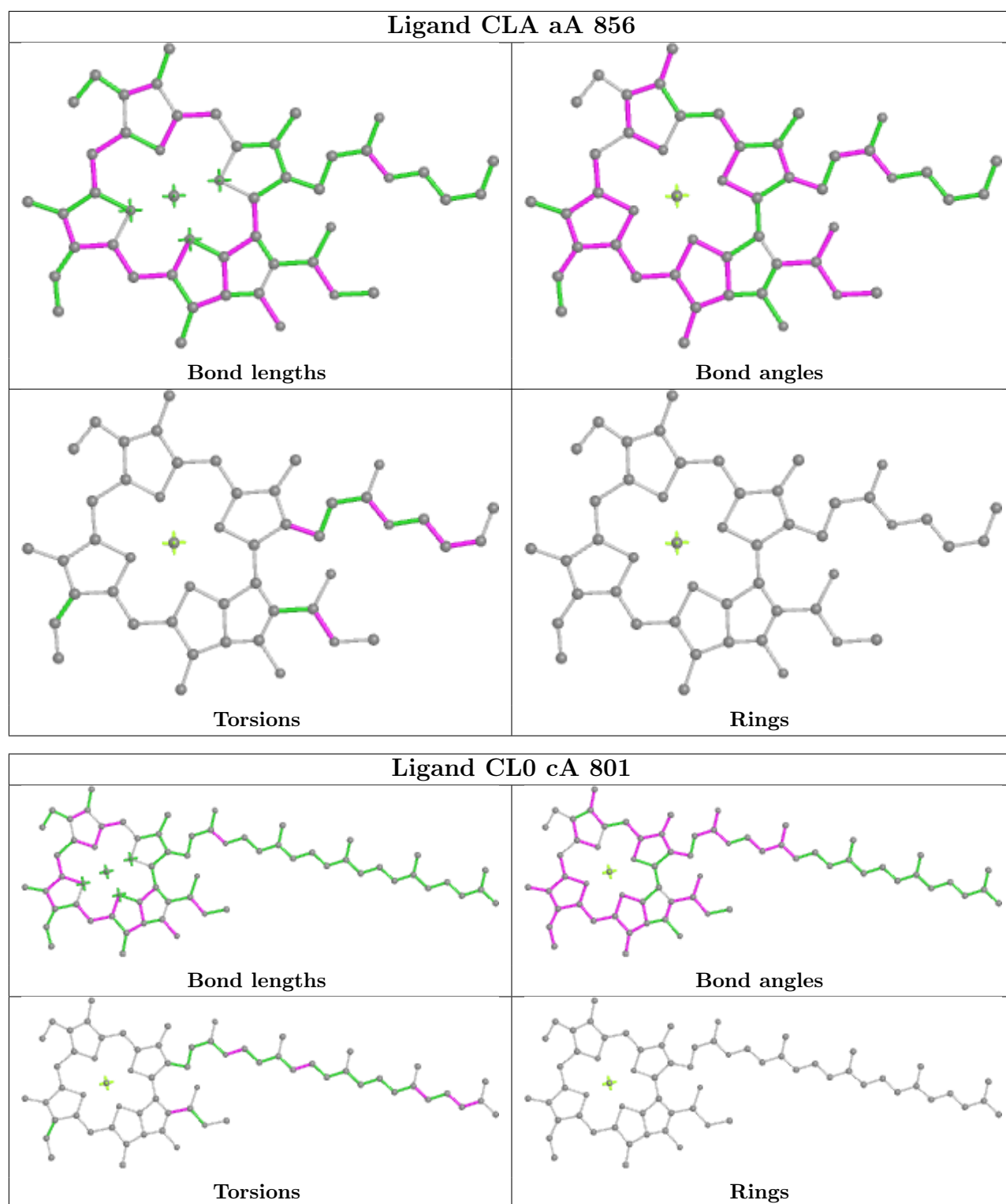


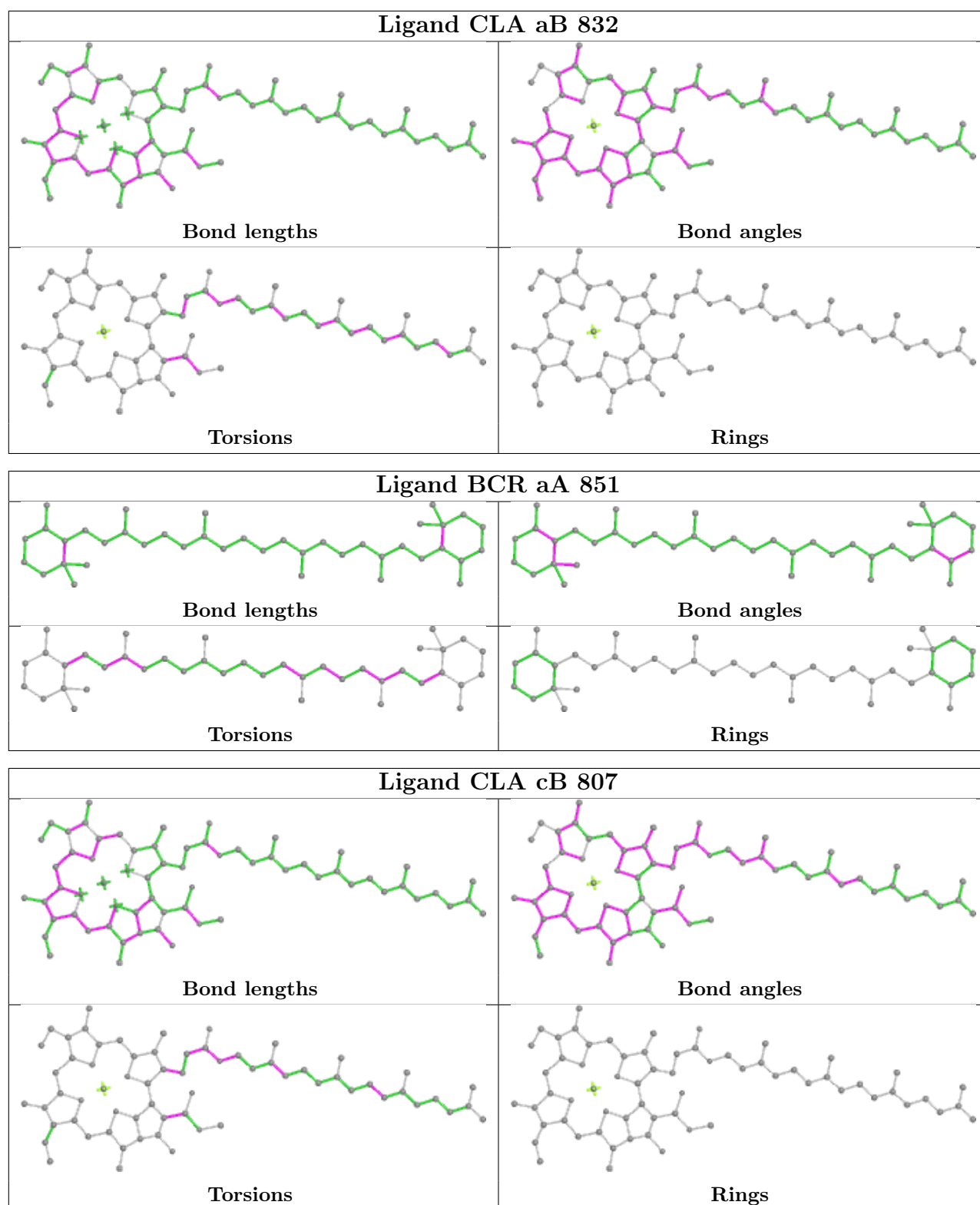
## Ligand CLA aA 829

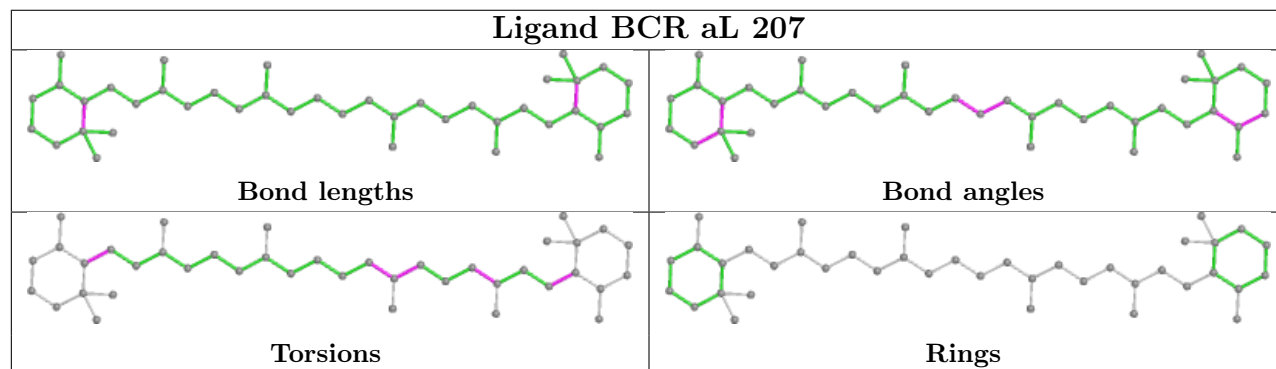
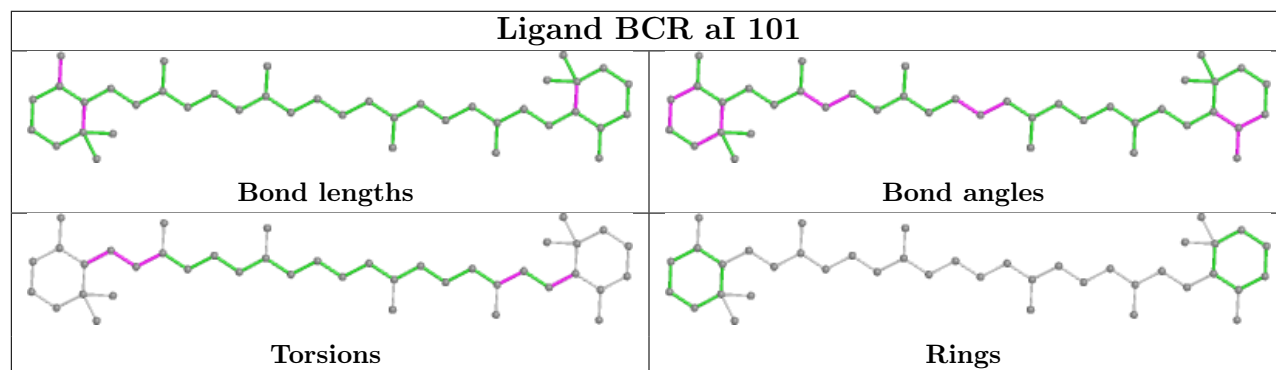
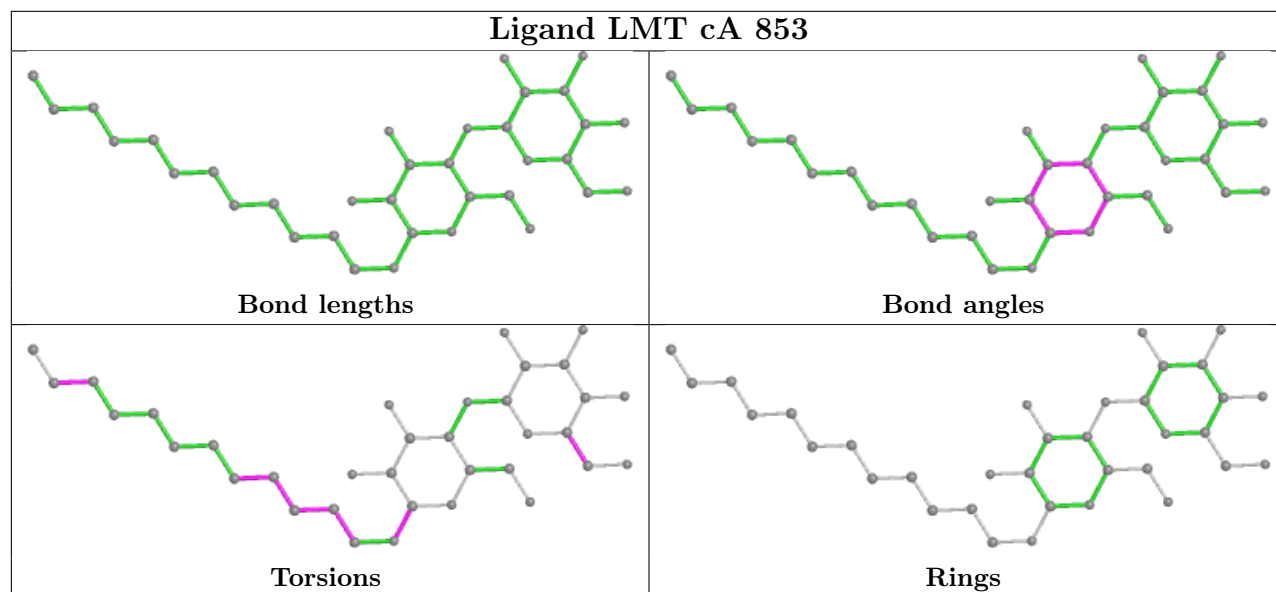
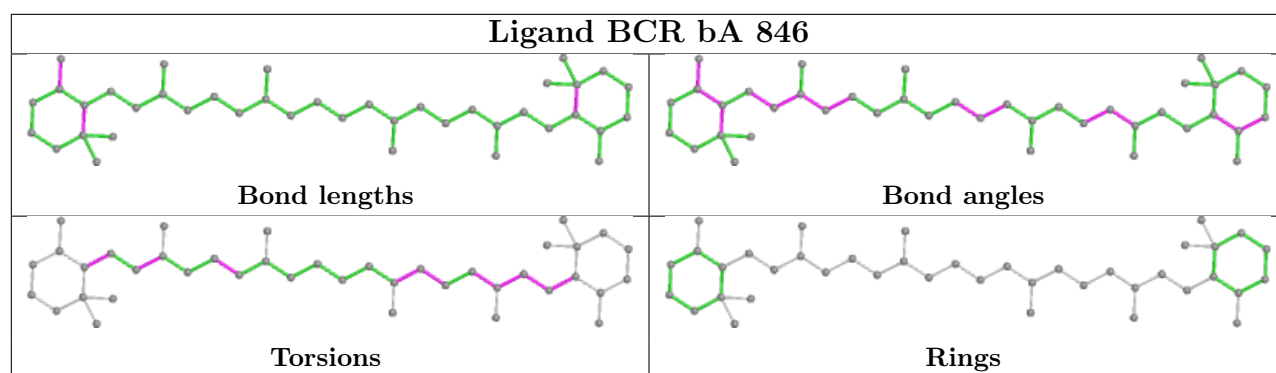




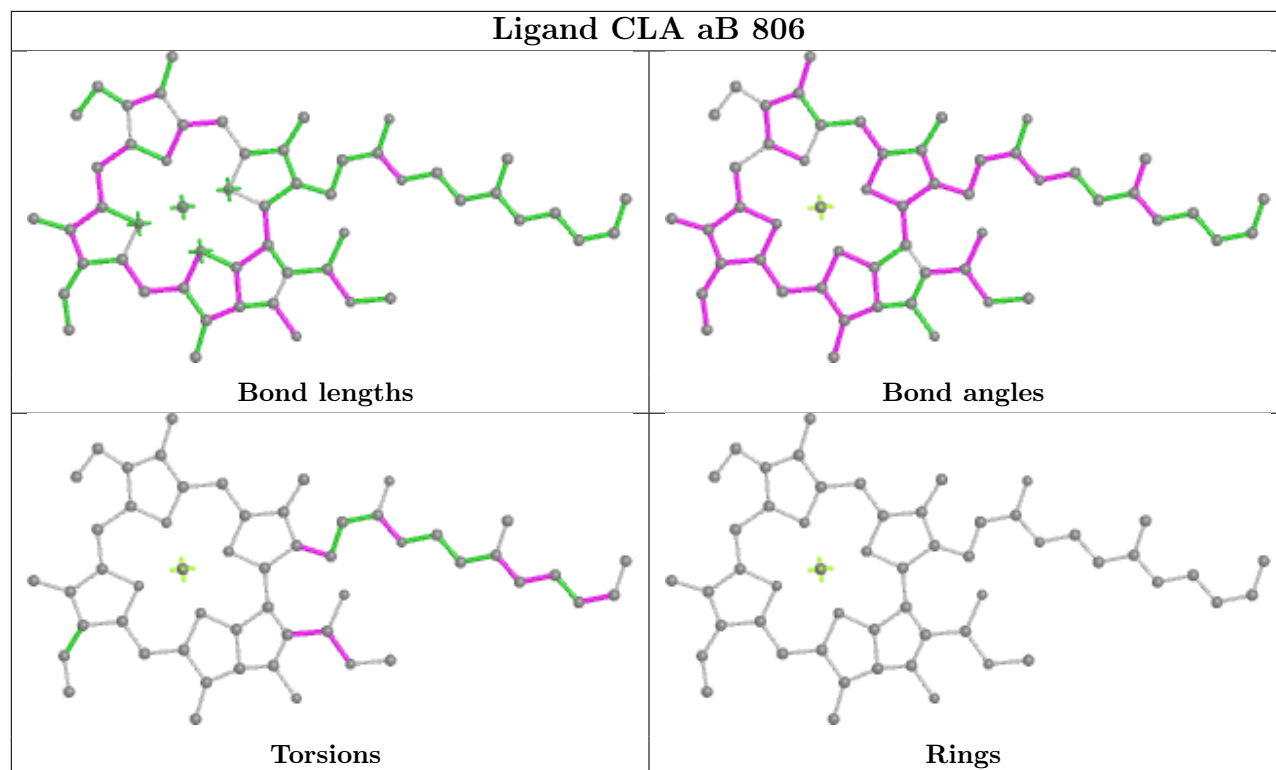




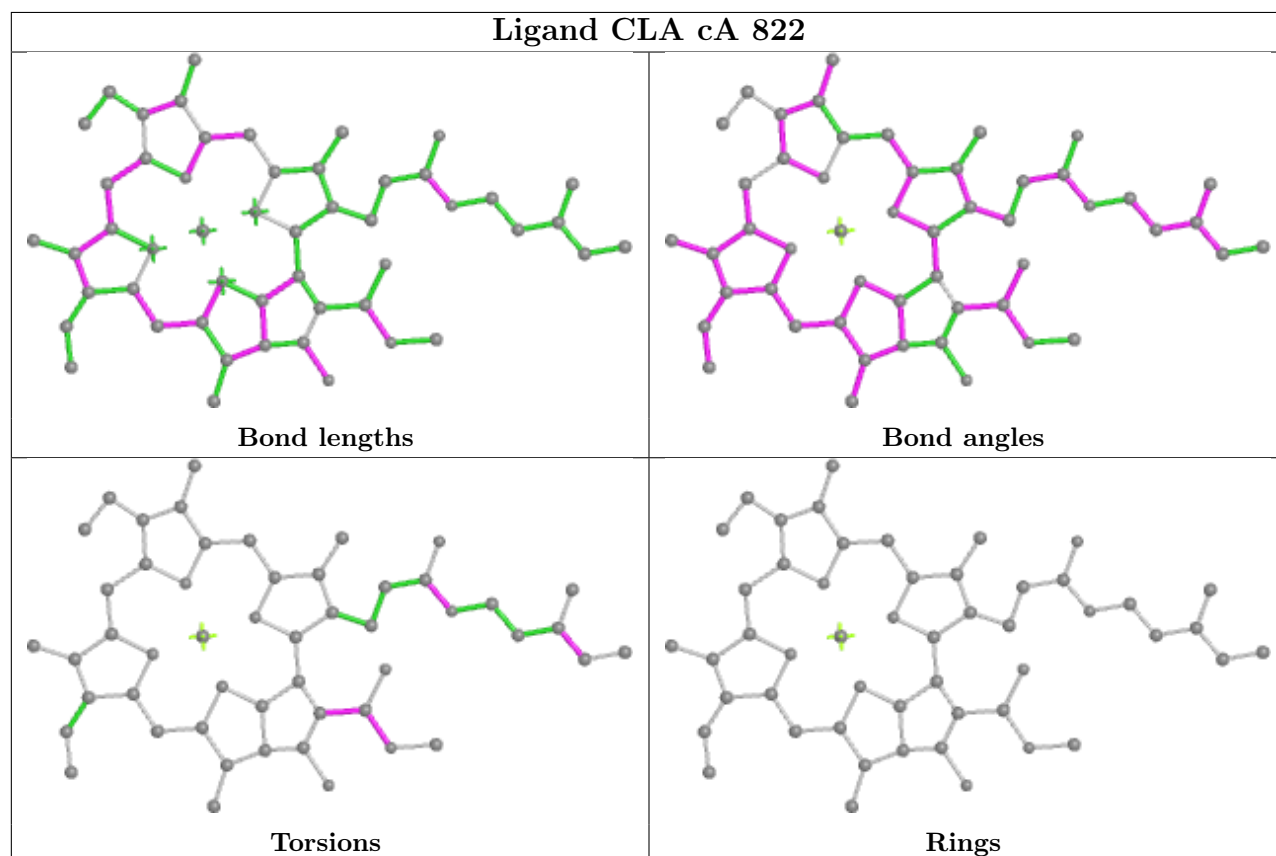




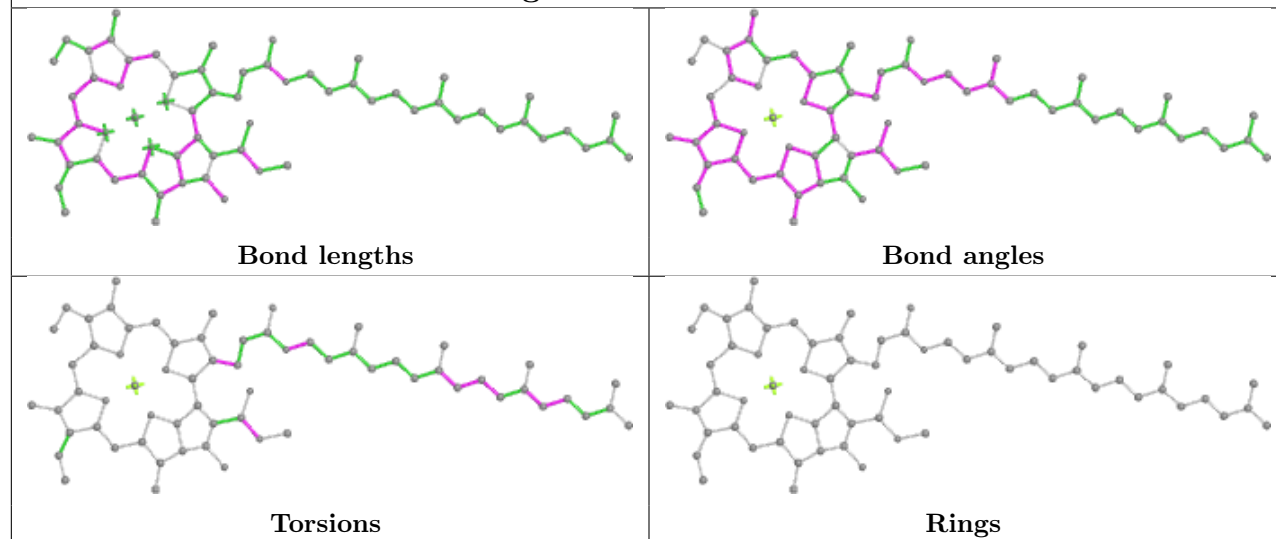
## Ligand CLA aB 806



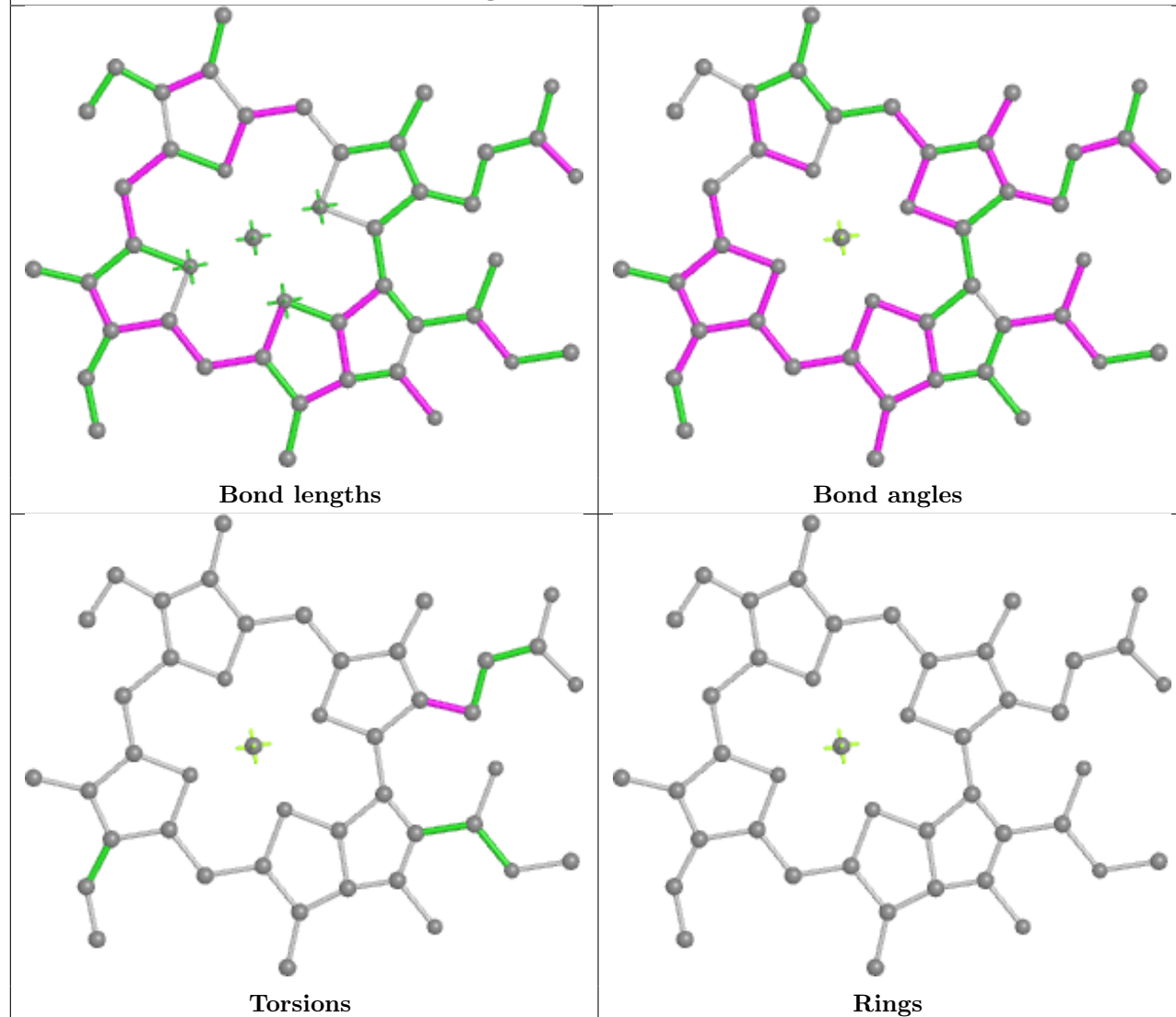
## Ligand CLA cA 822

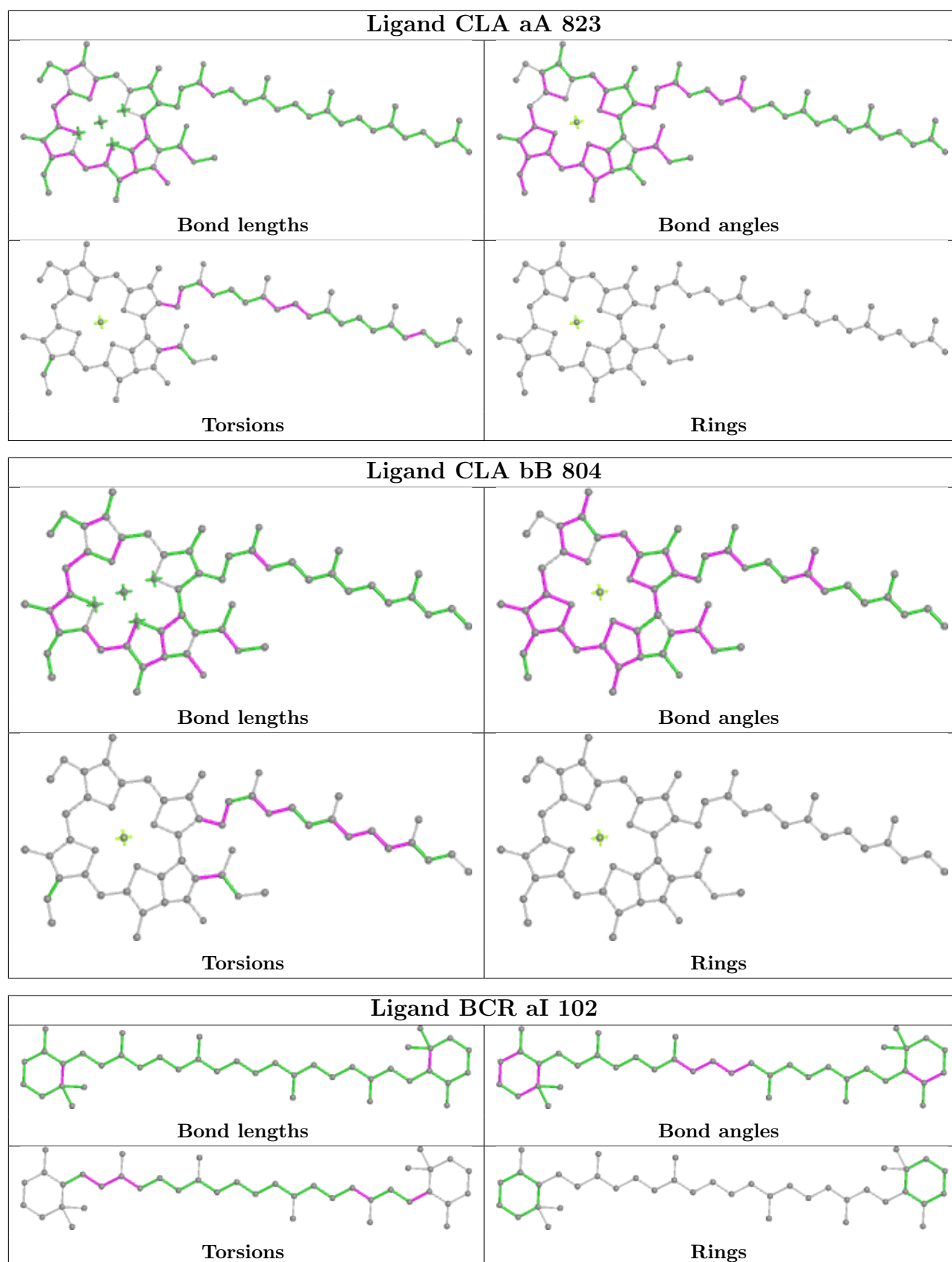


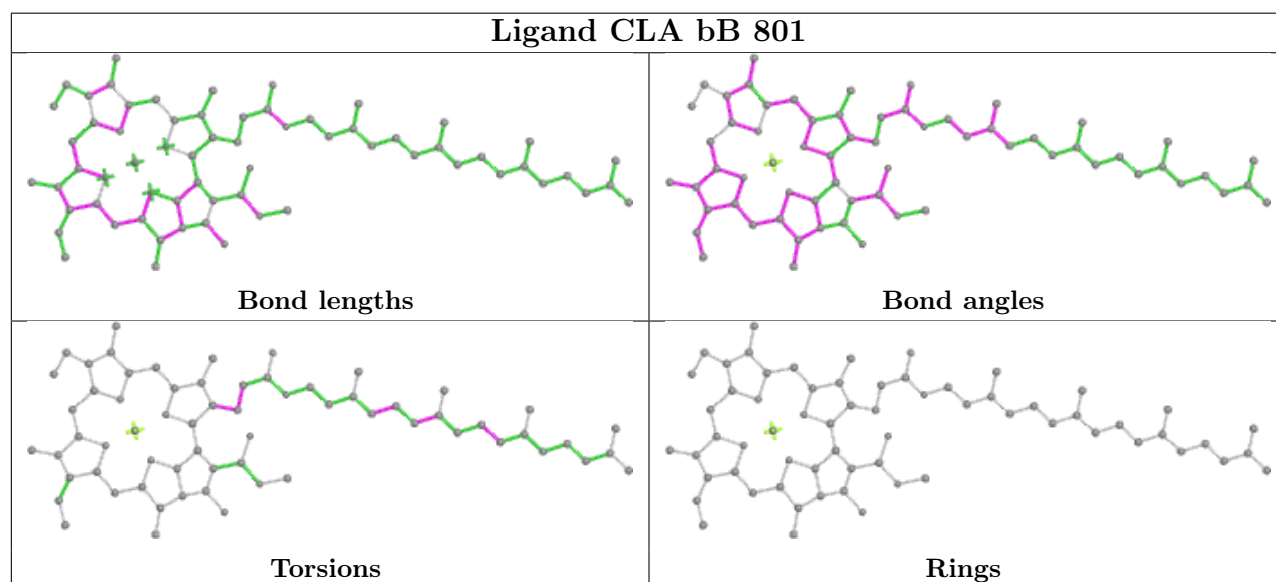
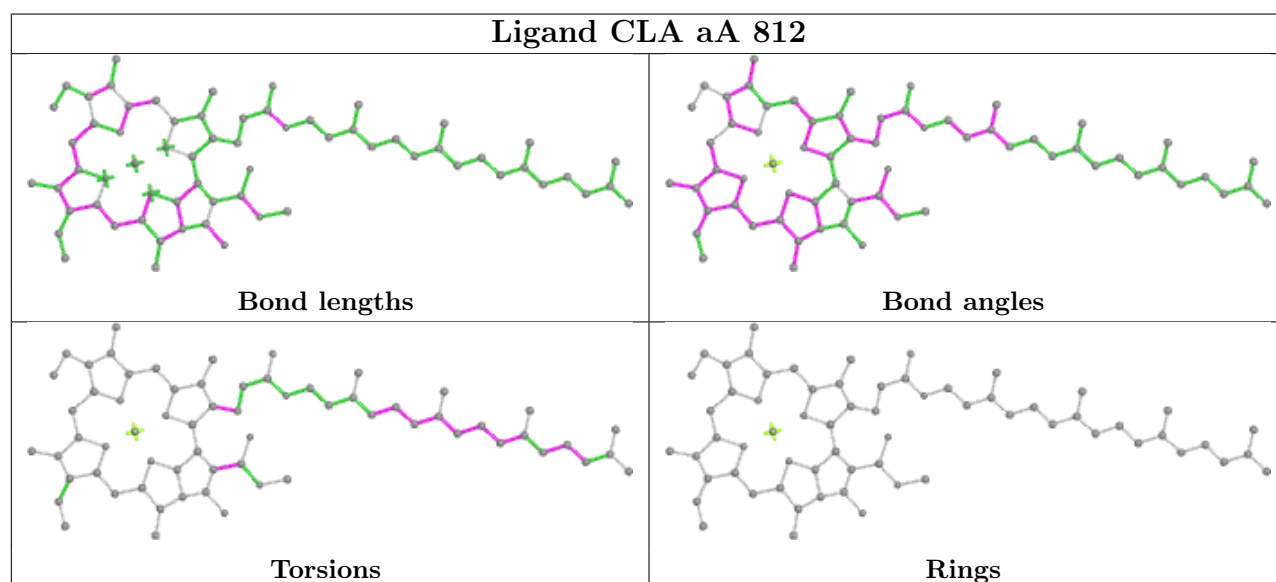
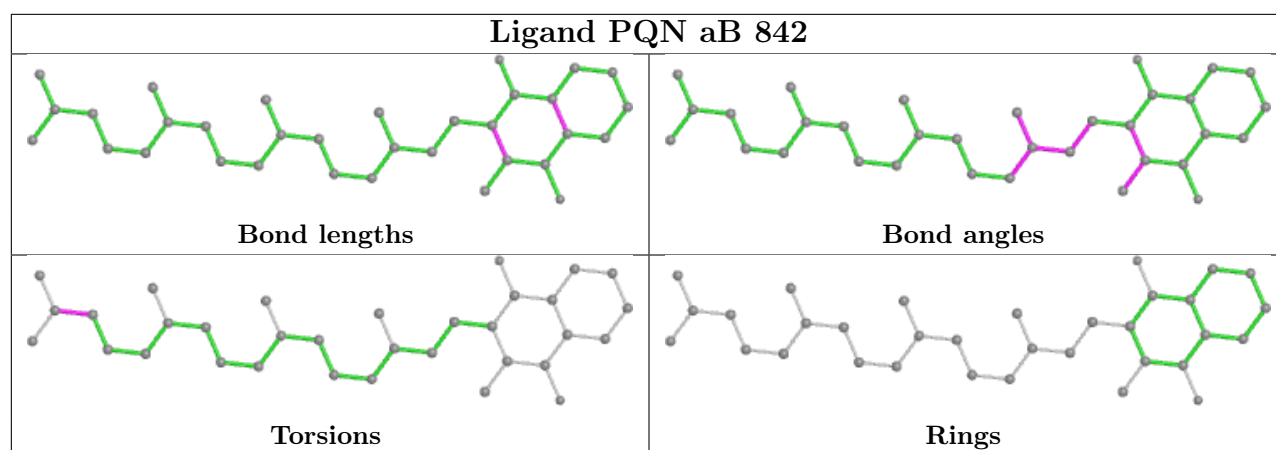
## Ligand CLA bB 828



## Ligand CLA aB 812







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



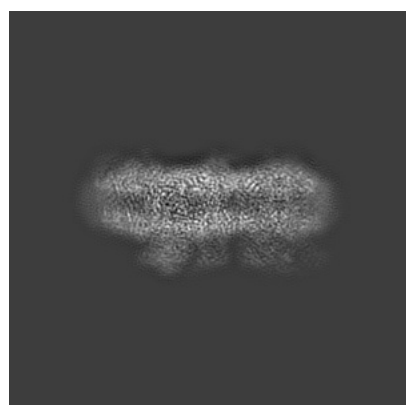
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0726. These allow visual inspection of the internal detail of the map and identification of artifacts.

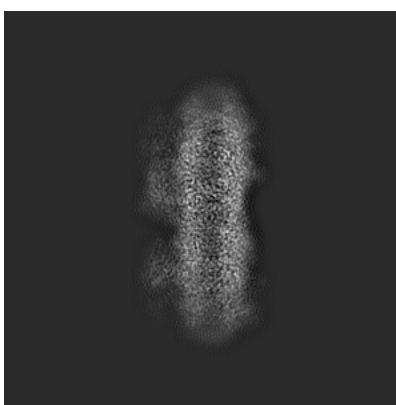
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

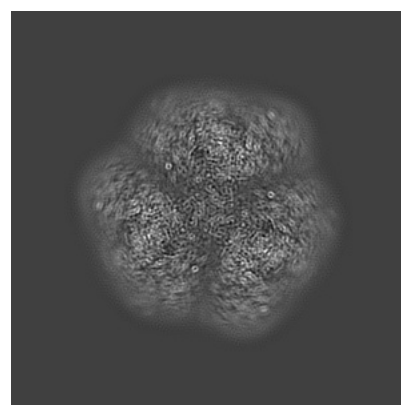
#### 6.1.1 Primary map



X



Y

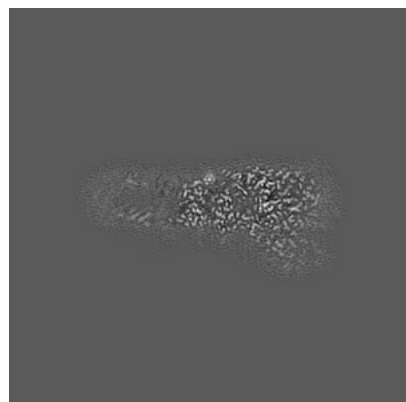


Z

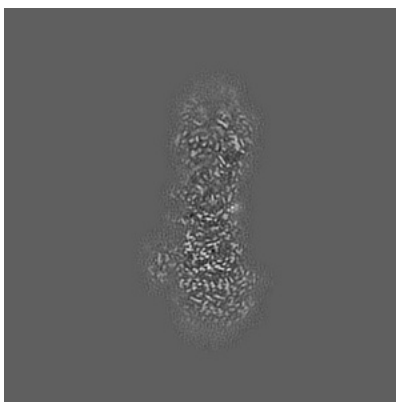
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

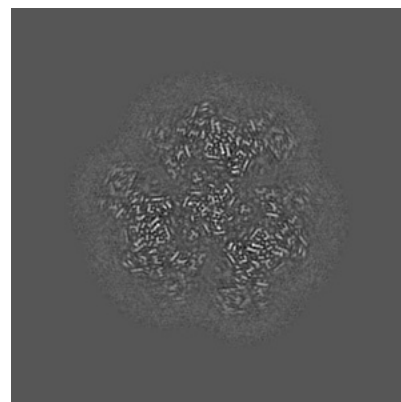
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

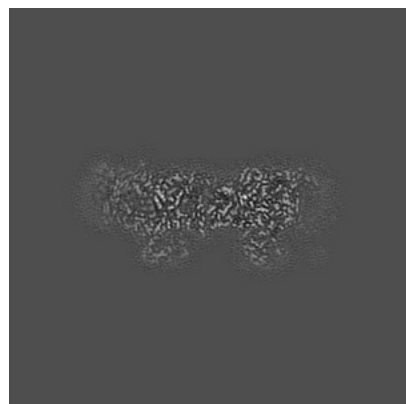


Z Index: 180

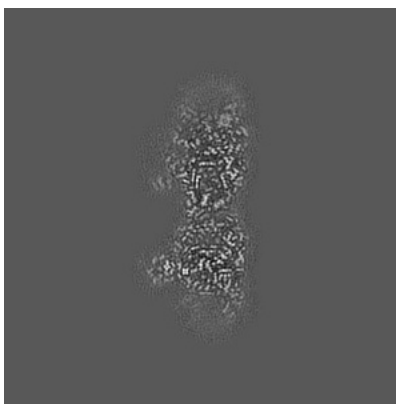
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

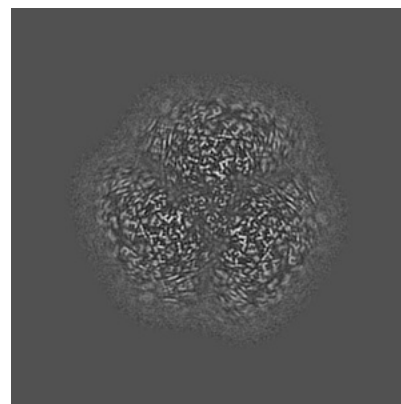
### 6.3.1 Primary map



X Index: 197



Y Index: 157

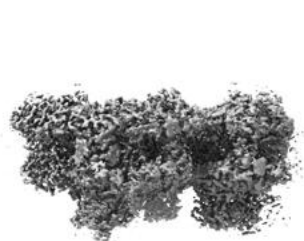


Z Index: 199

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

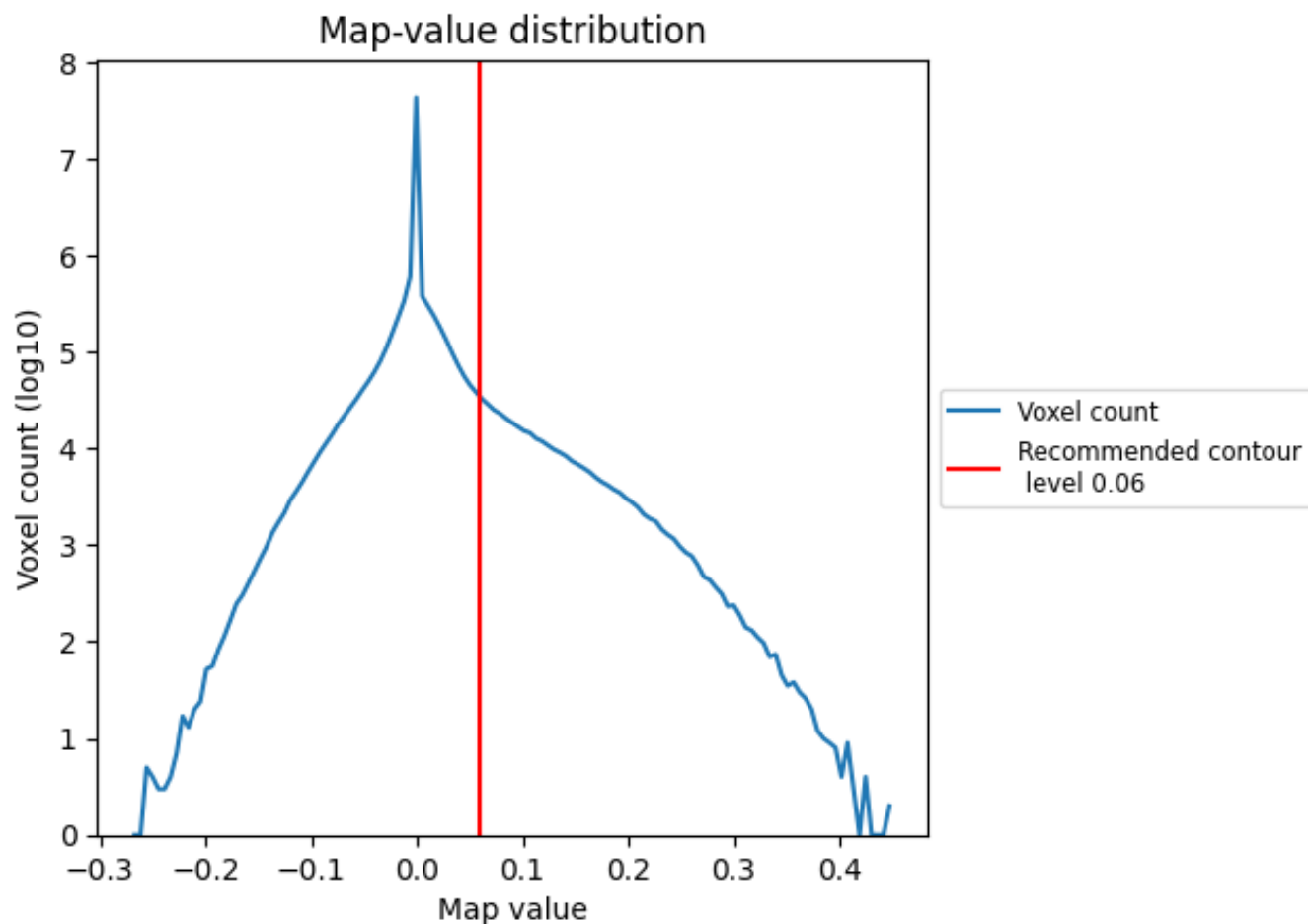
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

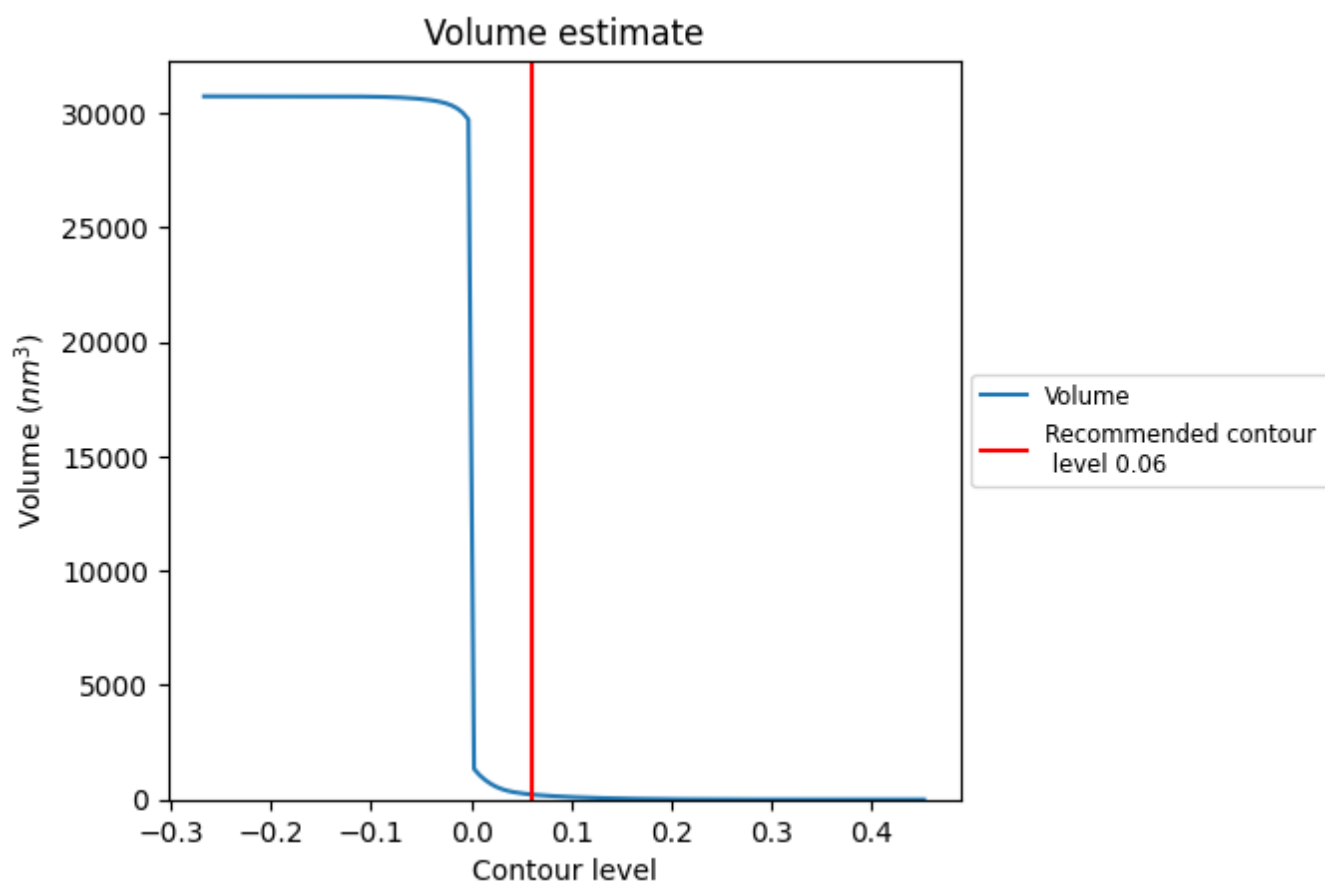
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

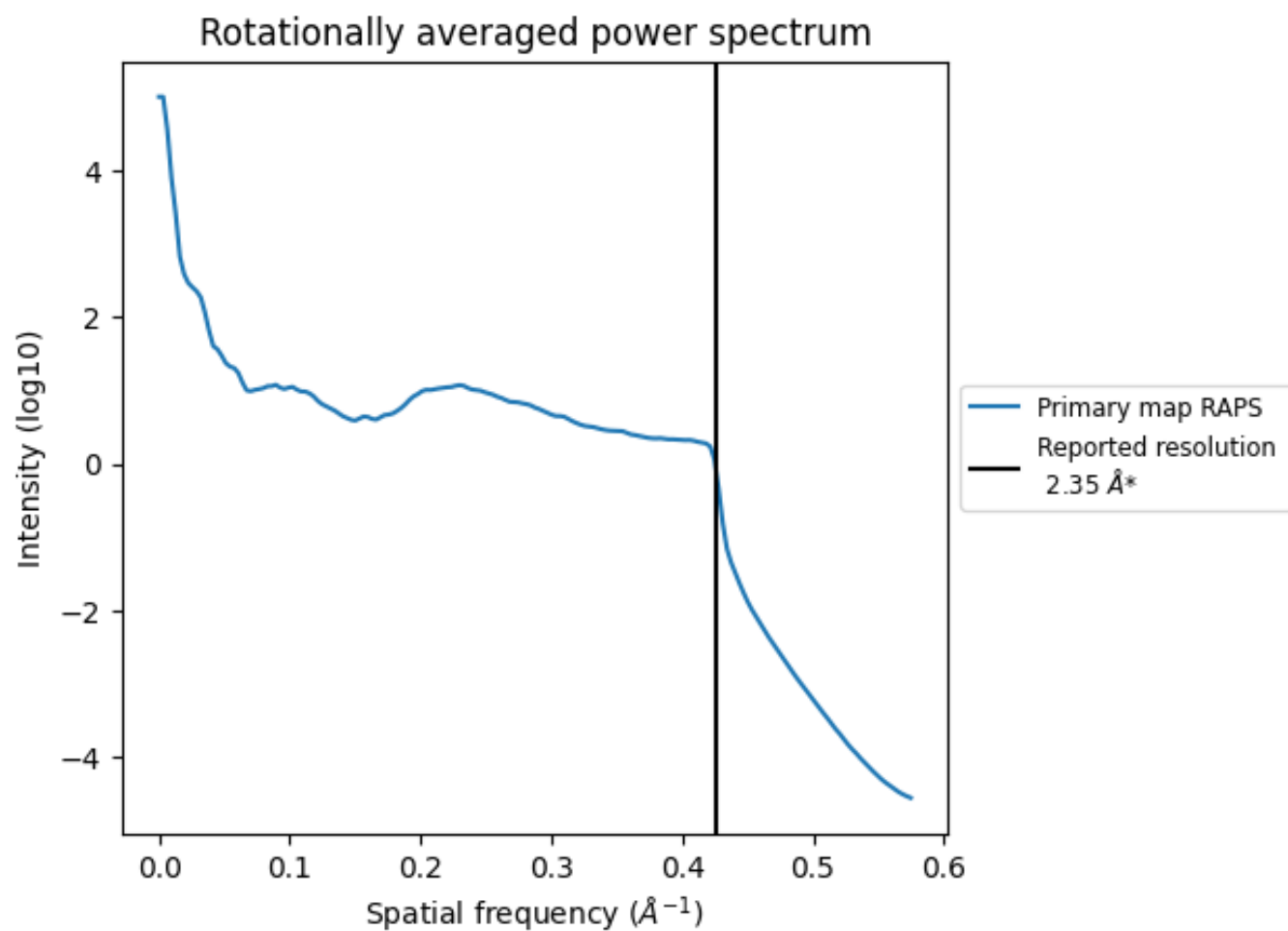
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 224 nm<sup>3</sup>; this corresponds to an approximate mass of 202 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

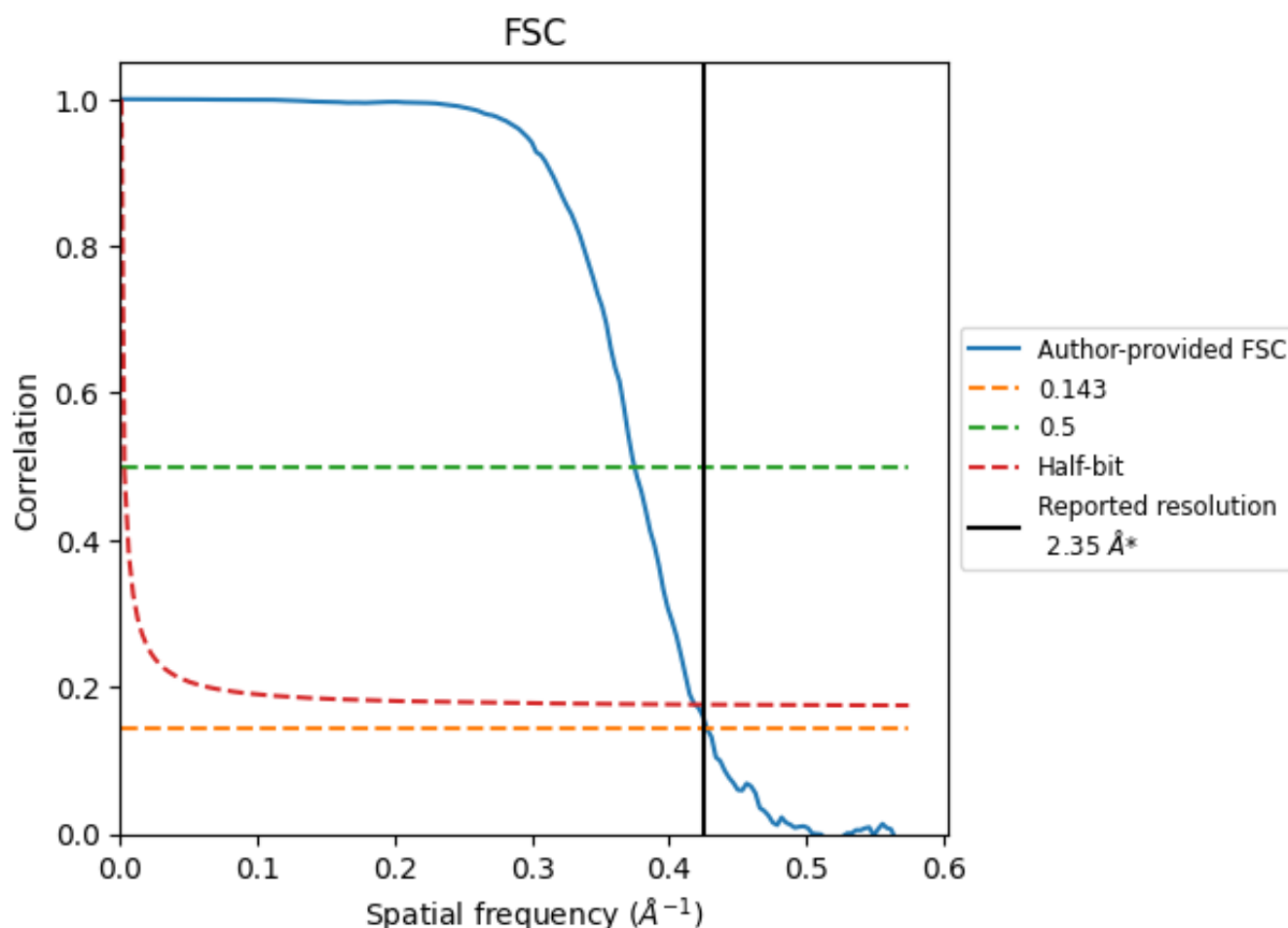


\*Reported resolution corresponds to spatial frequency of 0.426 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.426 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.34	2.67	2.39
Unmasked-calculated*	-	-	-

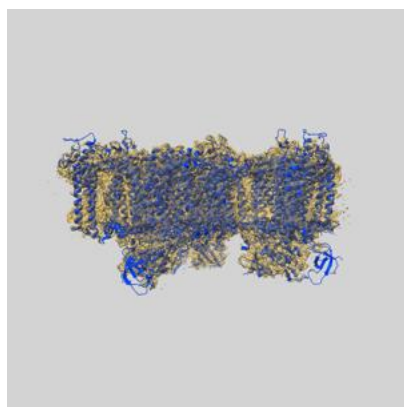
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



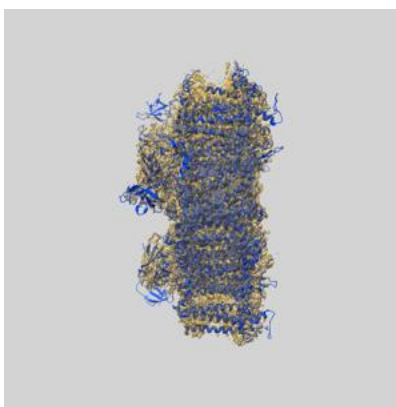
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0726 and PDB model 6KMW. Per-residue inclusion information can be found in section [3](#) on page [35](#).

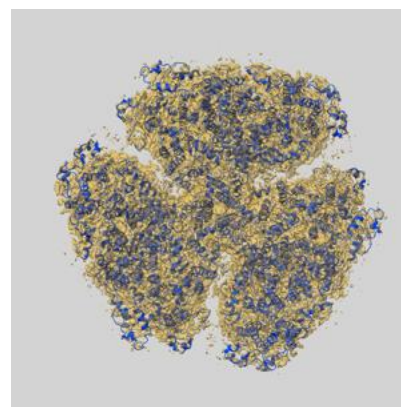
### 9.1 Map-model overlay [i](#)



X



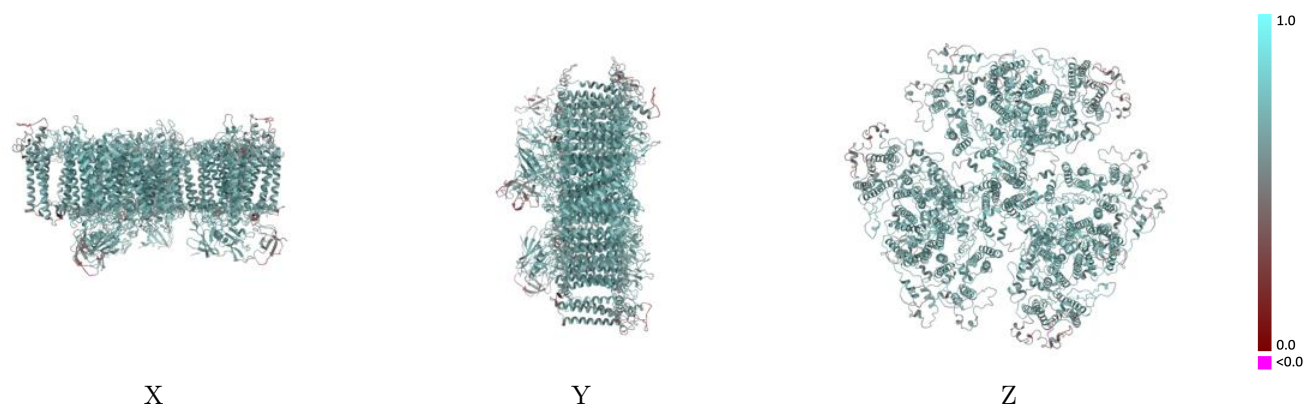
Y



Z

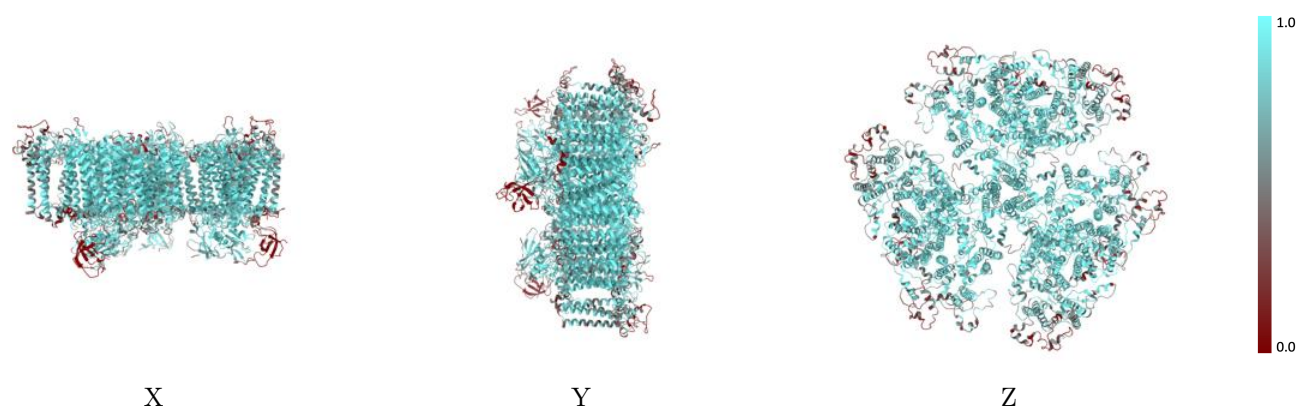
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



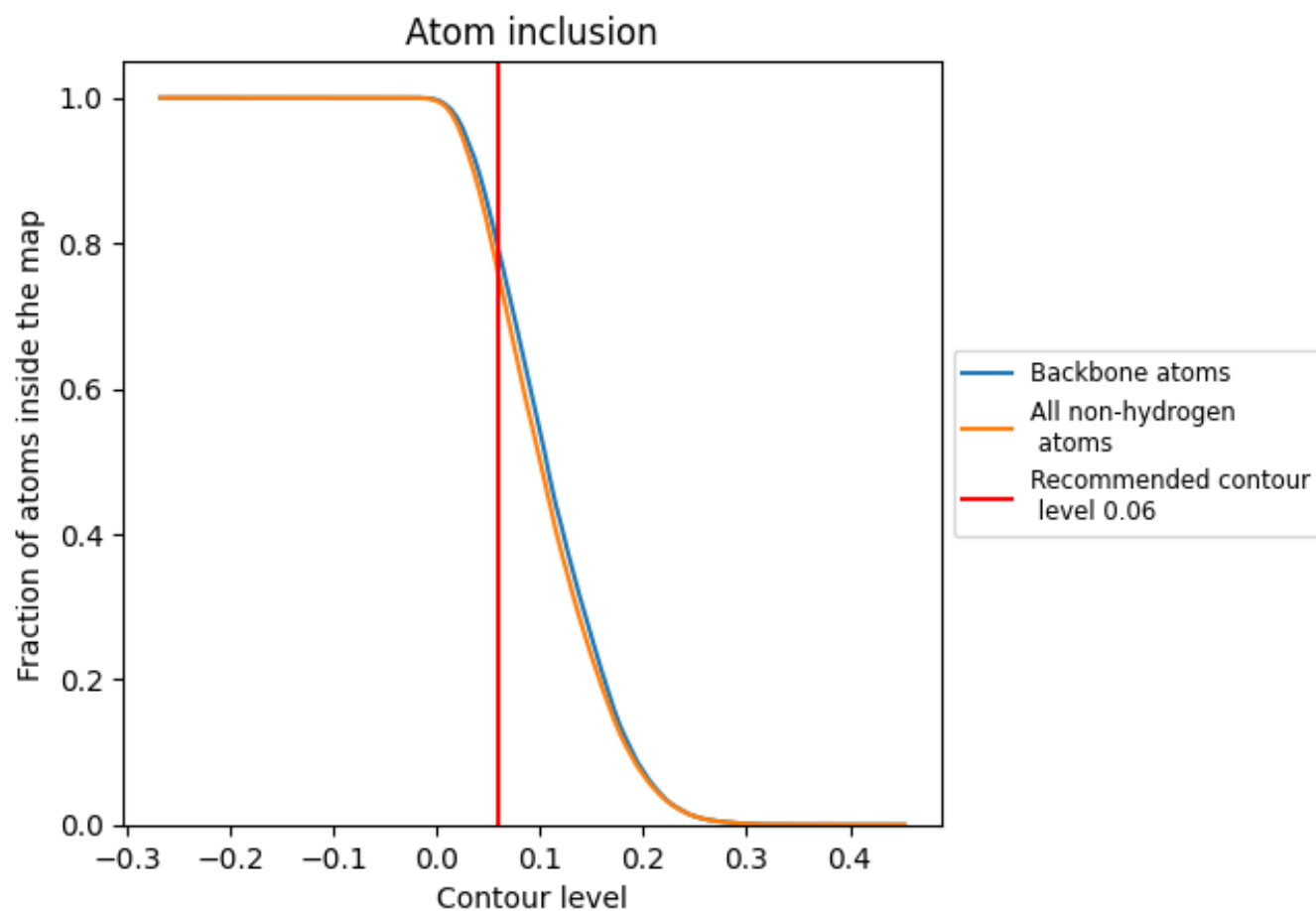
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7579	 0.6450
aA	 0.7318	 0.6360
aB	 0.7854	 0.6540
aC	 0.8211	 0.6660
aD	 0.7862	 0.6530
aE	 0.0998	 0.4610
aI	 0.9152	 0.7050
aL	 0.8676	 0.6930
aM	 0.8022	 0.6590
bA	 0.7317	 0.6370
bB	 0.7851	 0.6520
bC	 0.8261	 0.6650
bD	 0.7822	 0.6530
bE	 0.1164	 0.4620
bI	 0.9229	 0.7070
bL	 0.8655	 0.6920
bM	 0.7986	 0.6590
cA	 0.7301	 0.6350
cB	 0.7837	 0.6520
cC	 0.8294	 0.6620
cD	 0.7782	 0.6510
cE	 0.1081	 0.4530
cI	 0.9229	 0.7060
cL	 0.8676	 0.6920
cM	 0.8129	 0.6580

