



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 06:17 PM JST

PDB ID : 6JEO / pdb_00006jeo
EMDB ID : EMD-9807
Title : Structure of PSI tetramer from Anabaena
Authors : Kato, K.; Nagao, R.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on : 2019-02-06
Resolution : 3.30 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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

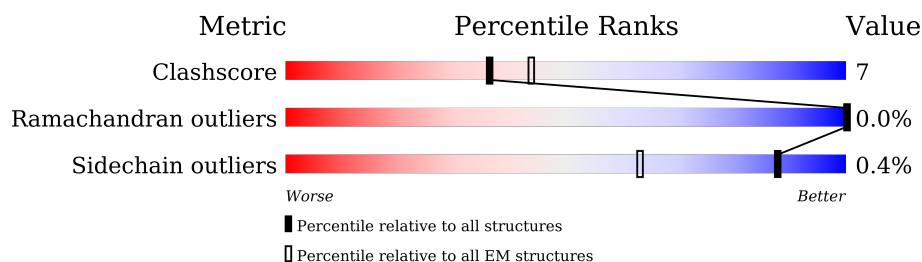
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



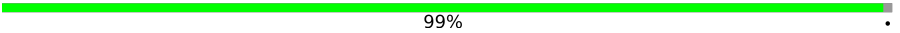
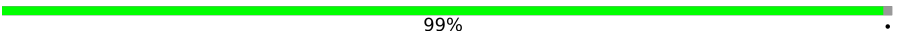
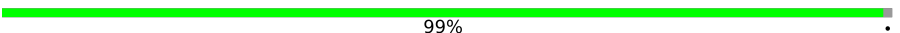






















Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	aA	752	
1	bA	752	
1	cA	752	
1	dA	752	
2	aB	741	
2	bB	741	
2	cB	741	
2	dB	741	
3	aC	81	

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Mol	Chain	Length	Quality of chain
3	bC	81	 99% .
3	cC	81	 99% .
3	dC	81	 99% .
4	aD	139	 53% 47%
4	bD	139	 69% 31%
4	cD	139	 53% 47%
4	dD	139	 69% 31%
5	aE	70	 87% 13%
5	bE	70	 87% 13%
5	cE	70	 87% 13%
5	dE	70	 87% 13%
6	aF	164	 85% . 15%
6	bF	164	 86% 14%
6	cF	164	 85% . 15%
6	dF	164	 86% 14%
7	aI	46	 67% 33%
7	bI	46	 67% 33%
7	cI	46	 67% 33%
7	dI	46	 67% 33%
8	aJ	49	 88% 12%
8	bJ	49	 88% 12%
8	cJ	49	 88% 12%
8	dJ	49	 88% 12%
9	aK	86	 76% . 23%
9	bK	86	 76% . 23%

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Mol	Chain	Length	Quality of chain
9	cK	86	
9	dK	86	
10	aL	172	
10	bL	172	
10	cL	172	
10	dL	172	
11	aM	40	
11	bM	40	
11	cM	40	
11	dM	40	
12	aX	44	
12	bX	44	
12	cX	44	
12	dX	44	

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
13	CL0	aA	801	X	-	-	-
13	CL0	bA	801	X	-	-	-
13	CL0	cA	801	X	-	-	-
13	CL0	dA	801	X	-	-	-
14	CLA	aA	802	X	-	-	-
14	CLA	aA	803	X	-	-	-
14	CLA	aA	804	X	-	-	-
14	CLA	aA	805	X	-	-	-
14	CLA	aA	806	X	-	-	-
14	CLA	aA	807	X	-	-	-
14	CLA	aA	808	X	-	-	-
14	CLA	aA	809	X	-	-	-
14	CLA	aA	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	aA	811	X	-	-	-
14	CLA	aA	812	X	-	-	-
14	CLA	aA	814	X	-	-	-
14	CLA	aA	815	X	-	-	-
14	CLA	aA	817	X	-	-	-
14	CLA	aA	818	X	-	-	-
14	CLA	aA	819	X	-	-	-
14	CLA	aA	820	X	-	-	-
14	CLA	aA	821	X	-	-	-
14	CLA	aA	822	X	-	-	-
14	CLA	aA	823	X	-	-	-
14	CLA	aA	824	X	-	-	-
14	CLA	aA	825	X	-	-	-
14	CLA	aA	826	X	-	-	-
14	CLA	aA	827	X	-	-	-
14	CLA	aA	828	X	-	-	-
14	CLA	aA	829	X	-	-	-
14	CLA	aA	830	X	-	-	-
14	CLA	aA	831	X	-	-	-
14	CLA	aA	832	X	-	-	-
14	CLA	aA	833	X	-	-	-
14	CLA	aA	834	X	-	-	-
14	CLA	aA	835	X	-	-	-
14	CLA	aA	836	X	-	-	-
14	CLA	aA	837	X	-	-	-
14	CLA	aA	838	X	-	-	-
14	CLA	aA	839	X	-	-	-
14	CLA	aA	840	X	-	-	-
14	CLA	aA	841	X	-	-	-
14	CLA	aA	842	X	-	-	-
14	CLA	aA	843	X	-	-	-
14	CLA	aB	801	X	-	-	-
14	CLA	aB	802	X	-	-	-
14	CLA	aB	803	X	-	-	-
14	CLA	aB	804	X	-	-	-
14	CLA	aB	805	X	-	-	-
14	CLA	aB	806	X	-	-	-
14	CLA	aB	807	X	-	-	-
14	CLA	aB	808	X	-	-	-
14	CLA	aB	809	X	-	-	-
14	CLA	aB	810	X	-	-	-
14	CLA	aB	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	aB	812	X	-	-	-
14	CLA	aB	813	X	-	-	-
14	CLA	aB	814	X	-	-	-
14	CLA	aB	815	X	-	-	-
14	CLA	aB	816	X	-	-	-
14	CLA	aB	817	X	-	-	-
14	CLA	aB	818	X	-	-	-
14	CLA	aB	819	X	-	-	-
14	CLA	aB	820	X	-	-	-
14	CLA	aB	821	X	-	-	-
14	CLA	aB	822	X	-	-	-
14	CLA	aB	823	X	-	-	-
14	CLA	aB	825	X	-	-	-
14	CLA	aB	826	X	-	-	-
14	CLA	aB	827	X	-	-	-
14	CLA	aB	828	X	-	-	-
14	CLA	aB	829	X	-	-	-
14	CLA	aB	830	X	-	-	-
14	CLA	aB	831	X	-	-	-
14	CLA	aB	832	X	-	-	-
14	CLA	aB	833	X	-	-	-
14	CLA	aB	834	X	-	-	-
14	CLA	aB	835	X	-	-	-
14	CLA	aB	837	X	-	-	-
14	CLA	aB	838	X	-	-	-
14	CLA	aB	840	X	-	-	-
14	CLA	aB	841	X	-	-	-
14	CLA	aF	201	X	-	-	-
14	CLA	aF	203	X	-	-	-
14	CLA	aJ	101	X	-	-	-
14	CLA	aJ	102	X	-	-	-
14	CLA	aK	101	X	-	-	-
14	CLA	aK	102	X	-	-	-
14	CLA	aL	202	X	-	-	-
14	CLA	aL	203	X	-	-	-
14	CLA	aL	204	X	-	-	-
14	CLA	aX	101	X	-	-	-
14	CLA	bA	802	X	-	-	-
14	CLA	bA	803	X	-	-	-
14	CLA	bA	804	X	-	-	-
14	CLA	bA	805	X	-	-	-
14	CLA	bA	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	bA	807	X	-	-	-
14	CLA	bA	808	X	-	-	-
14	CLA	bA	809	X	-	-	-
14	CLA	bA	810	X	-	-	-
14	CLA	bA	811	X	-	-	-
14	CLA	bA	812	X	-	-	-
14	CLA	bA	814	X	-	-	-
14	CLA	bA	815	X	-	-	-
14	CLA	bA	817	X	-	-	-
14	CLA	bA	818	X	-	-	-
14	CLA	bA	819	X	-	-	-
14	CLA	bA	820	X	-	-	-
14	CLA	bA	821	X	-	-	-
14	CLA	bA	822	X	-	-	-
14	CLA	bA	823	X	-	-	-
14	CLA	bA	824	X	-	-	-
14	CLA	bA	825	X	-	-	-
14	CLA	bA	826	X	-	-	-
14	CLA	bA	827	X	-	-	-
14	CLA	bA	828	X	-	-	-
14	CLA	bA	829	X	-	-	-
14	CLA	bA	830	X	-	-	-
14	CLA	bA	831	X	-	-	-
14	CLA	bA	832	X	-	-	-
14	CLA	bA	833	X	-	-	-
14	CLA	bA	834	X	-	-	-
14	CLA	bA	835	X	-	-	-
14	CLA	bA	836	X	-	-	-
14	CLA	bA	837	X	-	-	-
14	CLA	bA	838	X	-	-	-
14	CLA	bA	839	X	-	-	-
14	CLA	bA	840	X	-	-	-
14	CLA	bA	841	X	-	-	-
14	CLA	bA	842	X	-	-	-
14	CLA	bB	801	X	-	-	-
14	CLA	bB	802	X	-	-	-
14	CLA	bB	803	X	-	-	-
14	CLA	bB	804	X	-	-	-
14	CLA	bB	805	X	-	-	-
14	CLA	bB	806	X	-	-	-
14	CLA	bB	807	X	-	-	-
14	CLA	bB	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	bB	809	X	-	-	-
14	CLA	bB	810	X	-	-	-
14	CLA	bB	811	X	-	-	-
14	CLA	bB	812	X	-	-	-
14	CLA	bB	813	X	-	-	-
14	CLA	bB	814	X	-	-	-
14	CLA	bB	815	X	-	-	-
14	CLA	bB	816	X	-	-	-
14	CLA	bB	817	X	-	-	-
14	CLA	bB	818	X	-	-	-
14	CLA	bB	819	X	-	-	-
14	CLA	bB	820	X	-	-	-
14	CLA	bB	821	X	-	-	-
14	CLA	bB	822	X	-	-	-
14	CLA	bB	823	X	-	-	-
14	CLA	bB	824	X	-	-	-
14	CLA	bB	826	X	-	-	-
14	CLA	bB	827	X	-	-	-
14	CLA	bB	828	X	-	-	-
14	CLA	bB	829	X	-	-	-
14	CLA	bB	830	X	-	-	-
14	CLA	bB	831	X	-	-	-
14	CLA	bB	832	X	-	-	-
14	CLA	bB	833	X	-	-	-
14	CLA	bB	834	X	-	-	-
14	CLA	bB	835	X	-	-	-
14	CLA	bB	836	X	-	-	-
14	CLA	bB	838	X	-	-	-
14	CLA	bB	839	X	-	-	-
14	CLA	bB	841	X	-	-	-
14	CLA	bB	842	X	-	-	-
14	CLA	bF	201	X	-	-	-
14	CLA	bF	203	X	-	-	-
14	CLA	bJ	101	X	-	-	-
14	CLA	bJ	102	X	-	-	-
14	CLA	bK	101	X	-	-	-
14	CLA	bK	103	X	-	-	-
14	CLA	bL	201	X	-	-	-
14	CLA	bL	202	X	-	-	-
14	CLA	bL	204	X	-	-	-
14	CLA	bL	205	X	-	-	-
14	CLA	bL	206	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	bX	101	X	-	-	-
14	CLA	cA	802	X	-	-	-
14	CLA	cA	803	X	-	-	-
14	CLA	cA	804	X	-	-	-
14	CLA	cA	805	X	-	-	-
14	CLA	cA	806	X	-	-	-
14	CLA	cA	807	X	-	-	-
14	CLA	cA	808	X	-	-	-
14	CLA	cA	809	X	-	-	-
14	CLA	cA	810	X	-	-	-
14	CLA	cA	811	X	-	-	-
14	CLA	cA	812	X	-	-	-
14	CLA	cA	814	X	-	-	-
14	CLA	cA	815	X	-	-	-
14	CLA	cA	817	X	-	-	-
14	CLA	cA	818	X	-	-	-
14	CLA	cA	819	X	-	-	-
14	CLA	cA	820	X	-	-	-
14	CLA	cA	821	X	-	-	-
14	CLA	cA	822	X	-	-	-
14	CLA	cA	823	X	-	-	-
14	CLA	cA	824	X	-	-	-
14	CLA	cA	825	X	-	-	-
14	CLA	cA	826	X	-	-	-
14	CLA	cA	827	X	-	-	-
14	CLA	cA	828	X	-	-	-
14	CLA	cA	829	X	-	-	-
14	CLA	cA	830	X	-	-	-
14	CLA	cA	831	X	-	-	-
14	CLA	cA	832	X	-	-	-
14	CLA	cA	833	X	-	-	-
14	CLA	cA	834	X	-	-	-
14	CLA	cA	835	X	-	-	-
14	CLA	cA	836	X	-	-	-
14	CLA	cA	837	X	-	-	-
14	CLA	cA	838	X	-	-	-
14	CLA	cA	839	X	-	-	-
14	CLA	cA	840	X	-	-	-
14	CLA	cA	841	X	-	-	-
14	CLA	cA	842	X	-	-	-
14	CLA	cA	843	X	-	-	-
14	CLA	cB	801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	cB	802	X	-	-	-
14	CLA	cB	803	X	-	-	-
14	CLA	cB	804	X	-	-	-
14	CLA	cB	805	X	-	-	-
14	CLA	cB	806	X	-	-	-
14	CLA	cB	807	X	-	-	-
14	CLA	cB	808	X	-	-	-
14	CLA	cB	809	X	-	-	-
14	CLA	cB	810	X	-	-	-
14	CLA	cB	811	X	-	-	-
14	CLA	cB	812	X	-	-	-
14	CLA	cB	813	X	-	-	-
14	CLA	cB	814	X	-	-	-
14	CLA	cB	815	X	-	-	-
14	CLA	cB	816	X	-	-	-
14	CLA	cB	817	X	-	-	-
14	CLA	cB	818	X	-	-	-
14	CLA	cB	819	X	-	-	-
14	CLA	cB	820	X	-	-	-
14	CLA	cB	821	X	-	-	-
14	CLA	cB	822	X	-	-	-
14	CLA	cB	823	X	-	-	-
14	CLA	cB	825	X	-	-	-
14	CLA	cB	826	X	-	-	-
14	CLA	cB	827	X	-	-	-
14	CLA	cB	828	X	-	-	-
14	CLA	cB	829	X	-	-	-
14	CLA	cB	830	X	-	-	-
14	CLA	cB	831	X	-	-	-
14	CLA	cB	832	X	-	-	-
14	CLA	cB	833	X	-	-	-
14	CLA	cB	834	X	-	-	-
14	CLA	cB	835	X	-	-	-
14	CLA	cB	837	X	-	-	-
14	CLA	cB	838	X	-	-	-
14	CLA	cB	840	X	-	-	-
14	CLA	cB	841	X	-	-	-
14	CLA	cF	201	X	-	-	-
14	CLA	cF	203	X	-	-	-
14	CLA	cJ	101	X	-	-	-
14	CLA	cJ	102	X	-	-	-
14	CLA	cK	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	cK	102	X	-	-	-
14	CLA	cL	202	X	-	-	-
14	CLA	cL	203	X	-	-	-
14	CLA	cL	204	X	-	-	-
14	CLA	cX	101	X	-	-	-
14	CLA	dA	802	X	-	-	-
14	CLA	dA	803	X	-	-	-
14	CLA	dA	804	X	-	-	-
14	CLA	dA	805	X	-	-	-
14	CLA	dA	806	X	-	-	-
14	CLA	dA	807	X	-	-	-
14	CLA	dA	808	X	-	-	-
14	CLA	dA	809	X	-	-	-
14	CLA	dA	810	X	-	-	-
14	CLA	dA	811	X	-	-	-
14	CLA	dA	812	X	-	-	-
14	CLA	dA	814	X	-	-	-
14	CLA	dA	815	X	-	-	-
14	CLA	dA	817	X	-	-	-
14	CLA	dA	818	X	-	-	-
14	CLA	dA	819	X	-	-	-
14	CLA	dA	820	X	-	-	-
14	CLA	dA	821	X	-	-	-
14	CLA	dA	822	X	-	-	-
14	CLA	dA	823	X	-	-	-
14	CLA	dA	824	X	-	-	-
14	CLA	dA	825	X	-	-	-
14	CLA	dA	826	X	-	-	-
14	CLA	dA	827	X	-	-	-
14	CLA	dA	828	X	-	-	-
14	CLA	dA	829	X	-	-	-
14	CLA	dA	830	X	-	-	-
14	CLA	dA	831	X	-	-	-
14	CLA	dA	832	X	-	-	-
14	CLA	dA	833	X	-	-	-
14	CLA	dA	834	X	-	-	-
14	CLA	dA	835	X	-	-	-
14	CLA	dA	836	X	-	-	-
14	CLA	dA	837	X	-	-	-
14	CLA	dA	838	X	-	-	-
14	CLA	dA	839	X	-	-	-
14	CLA	dA	840	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	dA	841	X	-	-	-
14	CLA	dA	842	X	-	-	-
14	CLA	dB	801	X	-	-	-
14	CLA	dB	802	X	-	-	-
14	CLA	dB	803	X	-	-	-
14	CLA	dB	804	X	-	-	-
14	CLA	dB	805	X	-	-	-
14	CLA	dB	806	X	-	-	-
14	CLA	dB	807	X	-	-	-
14	CLA	dB	808	X	-	-	-
14	CLA	dB	809	X	-	-	-
14	CLA	dB	810	X	-	-	-
14	CLA	dB	811	X	-	-	-
14	CLA	dB	812	X	-	-	-
14	CLA	dB	813	X	-	-	-
14	CLA	dB	814	X	-	-	-
14	CLA	dB	815	X	-	-	-
14	CLA	dB	816	X	-	-	-
14	CLA	dB	817	X	-	-	-
14	CLA	dB	818	X	-	-	-
14	CLA	dB	819	X	-	-	-
14	CLA	dB	820	X	-	-	-
14	CLA	dB	821	X	-	-	-
14	CLA	dB	822	X	-	-	-
14	CLA	dB	823	X	-	-	-
14	CLA	dB	824	X	-	-	-
14	CLA	dB	826	X	-	-	-
14	CLA	dB	827	X	-	-	-
14	CLA	dB	828	X	-	-	-
14	CLA	dB	829	X	-	-	-
14	CLA	dB	830	X	-	-	-
14	CLA	dB	831	X	-	-	-
14	CLA	dB	832	X	-	-	-
14	CLA	dB	833	X	-	-	-
14	CLA	dB	834	X	-	-	-
14	CLA	dB	835	X	-	-	-
14	CLA	dB	836	X	-	-	-
14	CLA	dB	838	X	-	-	-
14	CLA	dB	839	X	-	-	-
14	CLA	dB	841	X	-	-	-
14	CLA	dB	842	X	-	-	-
14	CLA	dF	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	dF	203	X	-	-	-
14	CLA	dJ	101	X	-	-	-
14	CLA	dJ	102	X	-	-	-
14	CLA	dK	101	X	-	-	-
14	CLA	dK	103	X	-	-	-
14	CLA	dL	201	X	-	-	-
14	CLA	dL	202	X	-	-	-
14	CLA	dL	204	X	-	-	-
14	CLA	dL	205	X	-	-	-
14	CLA	dL	206	X	-	-	-
14	CLA	dX	101	X	-	-	-

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 94576 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	739	Total	C	N	O	S	0	0
			5801	3806	998	976	21		
1	bA	739	Total	C	N	O	S	0	0
			5801	3806	998	976	21		
1	cA	739	Total	C	N	O	S	0	0
			5801	3806	998	976	21		
1	dA	739	Total	C	N	O	S	0	0
			5801	3806	998	976	21		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		
2	bB	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		
2	cB	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		
2	dB	739	Total	C	N	O	S	0	0
			5919	3906	990	1005	18		

- 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
			599	367	103	118	11		
3	bC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		
3	cC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		
3	dC	80	Total	C	N	O	S	0	0
			599	367	103	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	73	Total	C	N	O	S	0	0
			581	378	97	105	1		
4	bD	96	Total	C	N	O	S	0	0
			740	479	122	138	1		
4	cD	73	Total	C	N	O	S	0	0
			581	378	97	105	1		
4	dD	96	Total	C	N	O	S	0	0
			740	479	122	138	1		

- 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
			490	313	84	93		
5	bE	61	Total	C	N	O	0	0
			490	313	84	93		
5	cE	61	Total	C	N	O	0	0
			490	313	84	93		
5	dE	61	Total	C	N	O	0	0
			490	313	84	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	140	Total	C	N	O	S	0	0
			1072	684	183	203	2		
6	bF	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		
6	cF	140	Total	C	N	O	S	0	0
			1072	684	183	203	2		
6	dF	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	aI	31	Total	C	N	O	0	0
			253	177	35	41		
7	bI	31	Total	C	N	O	0	0
			253	177	35	41		
7	cI	31	Total	C	N	O	0	0
			253	177	35	41		

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Mol	Chain	Residues	Atoms				AltConf	Trace
7	dI	31	Total	C	N	O	0	0
			253	177	35	41		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	aJ	43	Total	C	N	O	0	0
			347	236	52	59		
8	bJ	43	Total	C	N	O	0	0
			347	236	52	59		
8	cJ	43	Total	C	N	O	0	0
			347	236	52	59		
8	dJ	43	Total	C	N	O	0	0
			347	236	52	59		

- Molecule 9 is a protein called Photosystem I reaction center subunit Psak 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	aK	66	Total	C	N	O	S	0	0
			480	322	78	79	1		
9	bK	66	Total	C	N	O	S	0	0
			480	322	78	79	1		
9	cK	66	Total	C	N	O	S	0	0
			480	322	78	79	1		
9	dK	66	Total	C	N	O	S	0	0
			480	322	78	79	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aL	140	Total	C	N	O	S	0	0
			1037	684	172	180	1		
10	bL	161	Total	C	N	O	S	0	0
			1210	792	206	211	1		
10	cL	140	Total	C	N	O	S	0	0
			1037	684	172	180	1		
10	dL	161	Total	C	N	O	S	0	0
			1210	792	206	211	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	aM	30	Total 235	C 157	N 36	O 42	0	0
11	bM	30	Total 235	C 157	N 36	O 42	0	0
11	cM	30	Total 235	C 157	N 36	O 42	0	0
11	dM	30	Total 235	C 157	N 36	O 42	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
aM	1	MET	-	see sequence details	UNP Q8YNB0
aM	2	PRO	-	see sequence details	UNP Q8YNB0
aM	3	THR	-	see sequence details	UNP Q8YNB0
aM	4	LEU	-	see sequence details	UNP Q8YNB0
aM	5	TYR	-	see sequence details	UNP Q8YNB0
aM	6	LEU	-	see sequence details	UNP Q8YNB0
aM	7	ALA	-	see sequence details	UNP Q8YNB0
aM	8	GLN	-	see sequence details	UNP Q8YNB0
aM	9	VAL	-	see sequence details	UNP Q8YNB0
bM	1	MET	-	see sequence details	UNP Q8YNB0
bM	2	PRO	-	see sequence details	UNP Q8YNB0
bM	3	THR	-	see sequence details	UNP Q8YNB0
bM	4	LEU	-	see sequence details	UNP Q8YNB0
bM	5	TYR	-	see sequence details	UNP Q8YNB0
bM	6	LEU	-	see sequence details	UNP Q8YNB0
bM	7	ALA	-	see sequence details	UNP Q8YNB0
bM	8	GLN	-	see sequence details	UNP Q8YNB0
bM	9	VAL	-	see sequence details	UNP Q8YNB0
cM	1	MET	-	see sequence details	UNP Q8YNB0
cM	2	PRO	-	see sequence details	UNP Q8YNB0
cM	3	THR	-	see sequence details	UNP Q8YNB0
cM	4	LEU	-	see sequence details	UNP Q8YNB0
cM	5	TYR	-	see sequence details	UNP Q8YNB0
cM	6	LEU	-	see sequence details	UNP Q8YNB0
cM	7	ALA	-	see sequence details	UNP Q8YNB0
cM	8	GLN	-	see sequence details	UNP Q8YNB0
cM	9	VAL	-	see sequence details	UNP Q8YNB0
dM	1	MET	-	see sequence details	UNP Q8YNB0
dM	2	PRO	-	see sequence details	UNP Q8YNB0
dM	3	THR	-	see sequence details	UNP Q8YNB0
dM	4	LEU	-	see sequence details	UNP Q8YNB0

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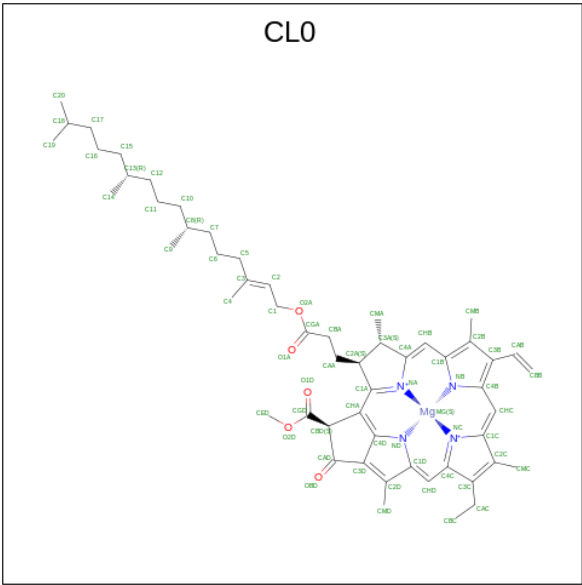
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Chain	Residue	Modelled	Actual	Comment	Reference
dM	5	TYR	-	see sequence details	UNP Q8YNB0
dM	6	LEU	-	see sequence details	UNP Q8YNB0
dM	7	ALA	-	see sequence details	UNP Q8YNB0
dM	8	GLN	-	see sequence details	UNP Q8YNB0
dM	9	VAL	-	see sequence details	UNP Q8YNB0

- Molecule 12 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	aX	29	Total	C	N	O	0	0
			243	170	37	36		
12	bX	29	Total	C	N	O	0	0
			243	170	37	36		
12	cX	29	Total	C	N	O	0	0
			243	170	37	36		
12	dX	29	Total	C	N	O	0	0
			243	170	37	36		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



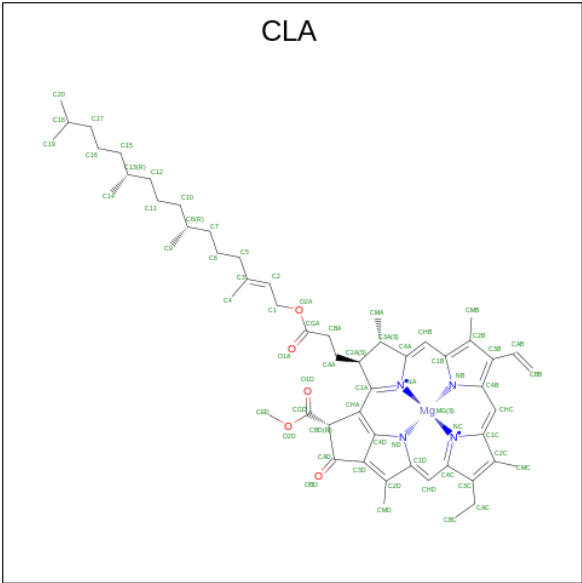
Mol	Chain	Residues	Atoms					AltConf
13	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	aA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aA	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	aB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aF	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	aF	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aJ	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	aK	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	aK	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	aL	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	aX	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bA	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	bF	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	bF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	bJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bJ	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	bK	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	bK	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bL	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	bL	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	bX	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 61	C 51	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	cA	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cA	1	Total 52	C 42	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 56	C 46	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cB	1	Total 59	C 49	Mg 1	N 4	O 5	0
14	cB	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	cB	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	cB	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	cB	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cF	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	cF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cJ	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	cK	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
14	cK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	cL	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	cX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	dA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	dA	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dB	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	dB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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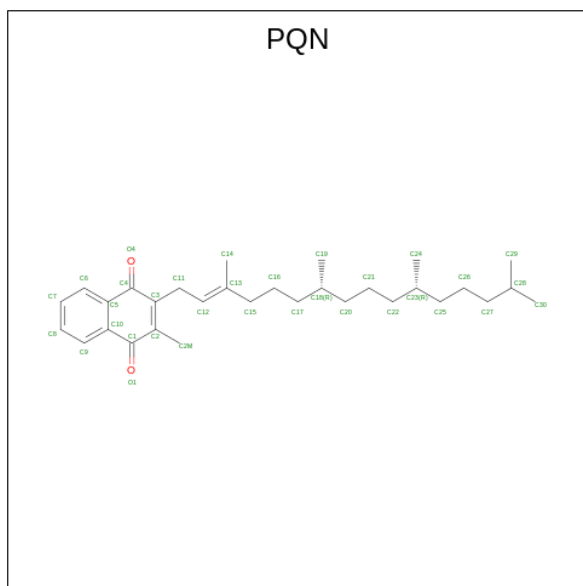
Mol	Chain	Residues	Atoms					AltConf
14	dB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dF	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	dF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	dJ	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	dK	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
14	dK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dL	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	dL	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
14	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	dX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



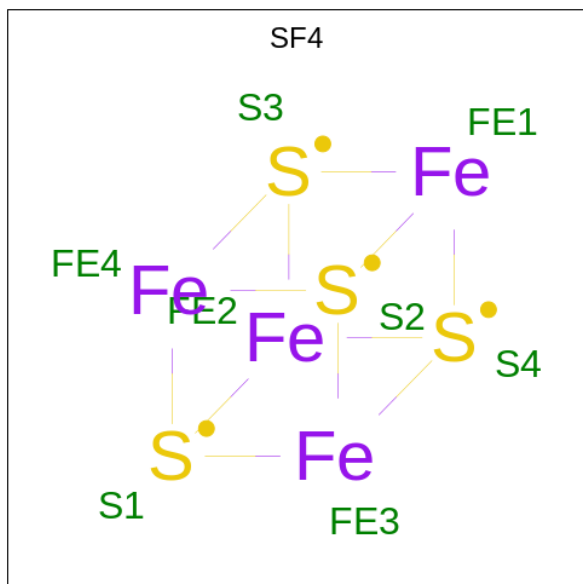
Mol	Chain	Residues	Atoms			AltConf
15	aA	1	Total	C	O	0
			33	31	2	
15	aB	1	Total	C	O	0
			33	31	2	

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Mol	Chain	Residues	Atoms			AltConf
15	bA	1	Total	C	O	0
			33	31	2	
15	bB	1	Total	C	O	0
			33	31	2	
15	cA	1	Total	C	O	0
			33	31	2	
15	cB	1	Total	C	O	0
			33	31	2	
15	dA	1	Total	C	O	0
			33	31	2	
15	dB	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



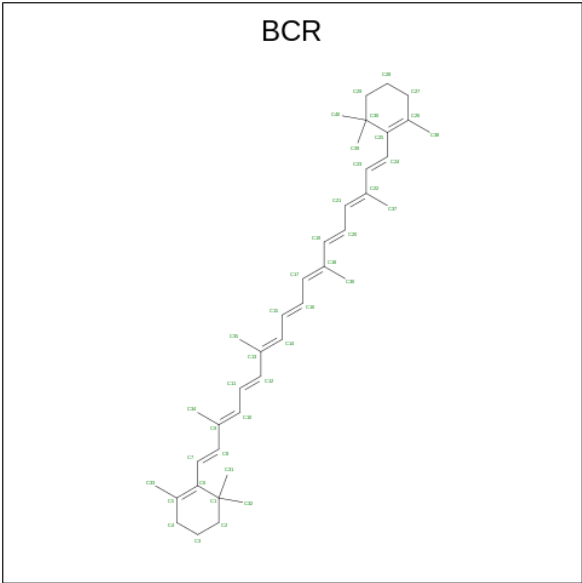
Mol	Chain	Residues	Atoms			AltConf
16	aA	1	Total	Fe	S	0
			8	4	4	
16	aC	1	Total	Fe	S	0
			8	4	4	
16	aC	1	Total	Fe	S	0
			8	4	4	
16	bA	1	Total	Fe	S	0
			8	4	4	
16	bC	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
16	bC	1	Total	Fe	S	0
			8	4	4	
16	cA	1	Total	Fe	S	0
			8	4	4	
16	cC	1	Total	Fe	S	0
			8	4	4	
16	cC	1	Total	Fe	S	0
			8	4	4	
16	dA	1	Total	Fe	S	0
			8	4	4	
16	dC	1	Total	Fe	S	0
			8	4	4	
16	dC	1	Total	Fe	S	0
			8	4	4	

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	
17	aA	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
17	aA	1	Total C 40 40	0
17	aA	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aB	1	Total C 40 40	0
17	aF	1	Total C 40 40	0
17	aF	1	Total C 40 40	0
17	aI	1	Total C 40 40	0
17	aJ	1	Total C 40 40	0
17	aJ	1	Total C 40 40	0
17	aL	1	Total C 40 40	0
17	aL	1	Total C 40 40	0
17	aL	1	Total C 40 40	0
17	aM	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	bA	1	Total C 40 40	0
17	bA	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bB	1	Total C 40 40	0
17	bF	1	Total C 40 40	0
17	bF	1	Total C 40 40	0
17	bI	1	Total C 40 40	0
17	bJ	1	Total C 40 40	0
17	bJ	1	Total C 40 40	0
17	bK	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bL	1	Total C 40 40	0
17	bM	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0

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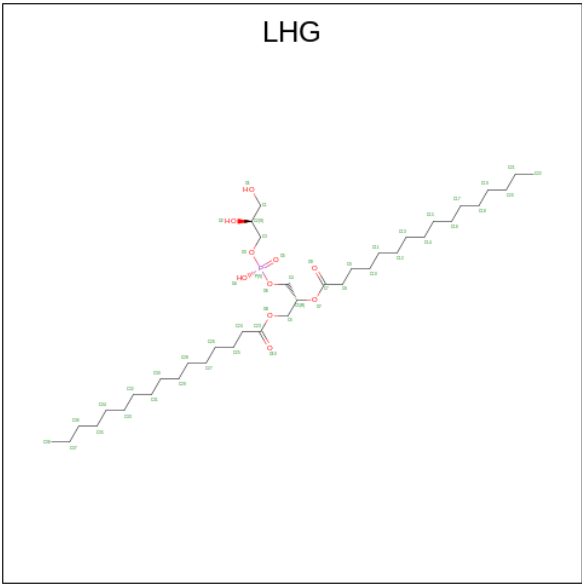
Mol	Chain	Residues	Atoms	AltConf
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cA	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cB	1	Total C 40 40	0
17	cF	1	Total C 40 40	0
17	cF	1	Total C 40 40	0
17	cI	1	Total C 40 40	0
17	cJ	1	Total C 40 40	0
17	cJ	1	Total C 40 40	0
17	cL	1	Total C 40 40	0
17	cL	1	Total C 40 40	0
17	cL	1	Total C 40 40	0
17	cM	1	Total C 40 40	0
17	dA	1	Total C 40 40	0

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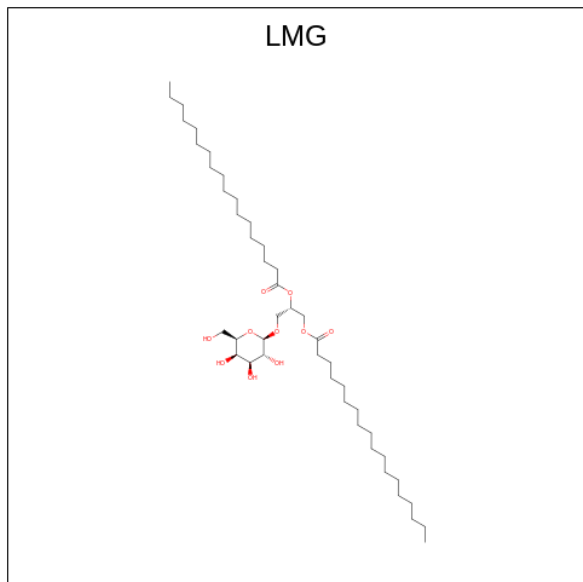
Mol	Chain	Residues	Atoms	AltConf
17	dA	1	Total C 40 40	0
17	dA	1	Total C 40 40	0
17	dA	1	Total C 40 40	0
17	dA	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dB	1	Total C 40 40	0
17	dF	1	Total C 40 40	0
17	dF	1	Total C 40 40	0
17	dI	1	Total C 40 40	0
17	dJ	1	Total C 40 40	0
17	dJ	1	Total C 40 40	0
17	dK	1	Total C 40 40	0
17	dL	1	Total C 40 40	0
17	dL	1	Total C 40 40	0
17	dL	1	Total C 40 40	0
17	dM	1	Total C 40 40	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
18	aA	1	Total	C	O	P	0
			49	38	10	1	
18	aA	1	Total	C	O	P	0
			27	16	10	1	
18	aB	1	Total	C	O	P	0
			23	12	10	1	
18	bA	1	Total	C	O	P	0
			49	38	10	1	
18	bA	1	Total	C	O	P	0
			27	16	10	1	
18	bB	1	Total	C	O	P	0
			23	12	10	1	
18	cA	1	Total	C	O	P	0
			49	38	10	1	
18	cA	1	Total	C	O	P	0
			27	16	10	1	
18	cB	1	Total	C	O	P	0
			23	12	10	1	
18	dA	1	Total	C	O	P	0
			49	38	10	1	
18	dA	1	Total	C	O	P	0
			27	16	10	1	
18	dB	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



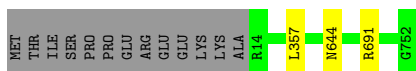
Mol	Chain	Residues	Atoms			AltConf
19	aB	1	Total	C	O	0
			55	45	10	
19	bB	1	Total	C	O	0
			55	45	10	
19	cB	1	Total	C	O	0
			55	45	10	
19	dB	1	Total	C	O	0
			55	45	10	

3 Residue-property plots

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

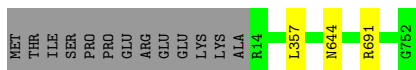
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain aA:  98%



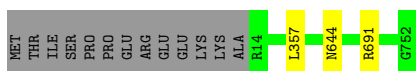
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain bA:  98%



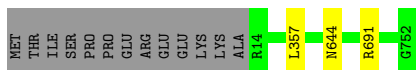
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain cA:  98%



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain dA:  98%



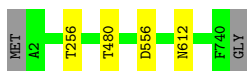
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain aB:  99%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain bB:  99%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain cB: 99%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain dB: 99%



- Molecule 3: Photosystem I iron-sulfur center

Chain aC: 99%



- Molecule 3: Photosystem I iron-sulfur center

Chain bC: 99%



- Molecule 3: Photosystem I iron-sulfur center

Chain cC: 99%



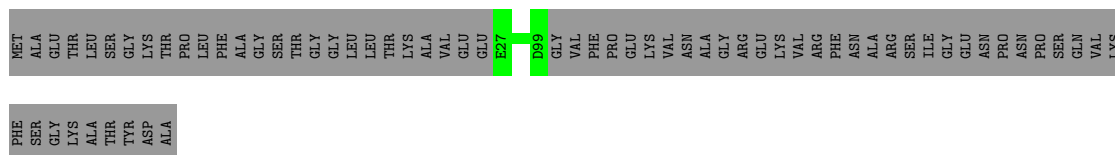
- Molecule 3: Photosystem I iron-sulfur center

Chain dC: 99%



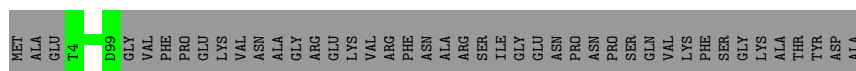
- Molecule 4: Photosystem I reaction center subunit II

Chain aD: 53%



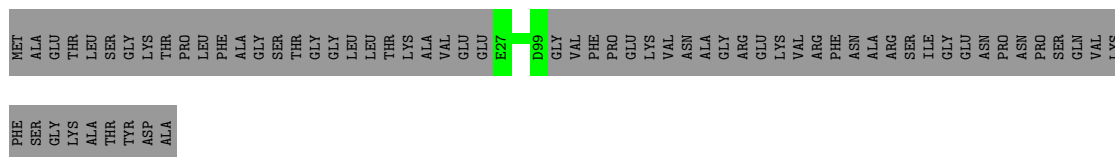
- Molecule 4: Photosystem I reaction center subunit II

Chain bD: 69% 31%



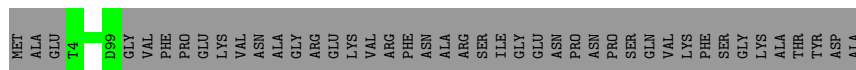
- Molecule 4: Photosystem I reaction center subunit II

Chain cD: 53% 47%



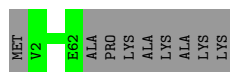
- Molecule 4: Photosystem I reaction center subunit II

Chain dD: 69% 31%



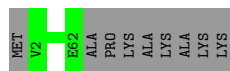
- Molecule 5: Photosystem I reaction center subunit IV

Chain aE: 87% 13%



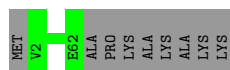
- Molecule 5: Photosystem I reaction center subunit IV

Chain bE: 87% 13%



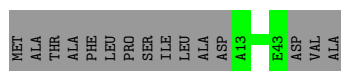
- Molecule 5: Photosystem I reaction center subunit IV

Chain cE: 87% 13%



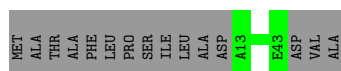
- Molecule 7: Photosystem I reaction center subunit VIII

Chain cI:  67% 33%




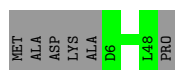
- Molecule 7: Photosystem I reaction center subunit VIII

Chain dI:  67% 33%



- Molecule 8: Photosystem I reaction center subunit IX

Chain aJ:  88% 12%



- Molecule 8: Photosystem I reaction center subunit IX

Chain bJ:  88% 12%




- Molecule 8: Photosystem I reaction center subunit IX

Chain cJ:  88% 12%




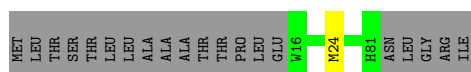
- Molecule 8: Photosystem I reaction center subunit IX

Chain dJ:  88% 12%




- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain aK:  76% 23%




- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain bK:  76% 23%


MET LEU THR SER THR LEU ALA ALA THR PRO LEU W16 M24 H81 ASN LEU GLY ARG ILE

- Molecule 9: Photosystem I reaction center subunit Psak 1

Chain cK:  76% 23%


MET LEU THR SER THR LEU ALA ALA THR PRO LEU W16 M24 H81 ASN LEU GLY ARG ILE

- Molecule 9: Photosystem I reaction center subunit Psak 1

Chain dK:  76% 23%

MET LEU THR SER THR LEU ALA ALA THR PRO LEU W16 M24 H81 ASN LEU GLY ARG ILE

- Molecule 10: Photosystem I reaction center subunit XI

Chain aL:  81% 19%


MET ALA GLN VAL ASP ALA SER LYS ASN LEU PRO SER ASP PRO ARG ASN ARG VAL VAL PHE PRO ALA GLY ARG ASP PRO GLN TRP GLY ASN L33 G172

- Molecule 10: Photosystem I reaction center subunit XI

Chain bL:  91% 6%

MET ALA GLN VAL ASP ALA SER LYS ASN LEU PRO SER ASP PRO ARG ASN ARG VAL VAL PHE PRO ALA GLY ARG ASP PRO GLN TRP GLY ASN L33 G172

- Molecule 10: Photosystem I reaction center subunit XI

Chain cL:  81% 19%


MET ALA GLN VAL ASP ALA SER LYS ASN LEU PRO SER ASP PRO ARG ASN ARG VAL VAL PHE PRO ALA GLY ARG ASP PRO GLN TRP GLY ASN L33 G172

- Molecule 10: Photosystem I reaction center subunit XI

Chain dL:  91% 6%


MET ALA GLN VAL ASP ALA SER LYS ASN LEU PRO SER ASP PRO ARG ASN ARG VAL VAL PHE PRO ALA GLY ARG ASP PRO GLN TRP GLY ASN L33 G172

- Molecule 11: Photosystem I reaction center subunit XII

Chain aM:  75% 25%


MET PRO THR LEU TYR LEU ALA GLN VAL SER S11 K40

- Molecule 11: Photosystem I reaction center subunit XII

Chain bM:  75% 25%


MET PRO THR LEU TYR LEU ALA GLN VAL SER S11 K40

- Molecule 11: Photosystem I reaction center subunit XII

Chain cM:  75% 25%

MET PRO THR LEU TYR LEU ALA GLN VAL SER S11 K40

- Molecule 11: Photosystem I reaction center subunit XII

Chain dM:  75% 25%

MET PRO THR LEU TYR LEU ALA GLN VAL SER S11 K40

- Molecule 12: Photosystem I 4.8 kDa protein

Chain aX:  64% 34%

MET ALA LYS LYS ILE SER PRO VAL ALA ALA ASN THR GLY ALA LYS P16 N32 Q44

- Molecule 12: Photosystem I 4.8 kDa protein

Chain bX:  64% 34%

MET ALA LYS LYS ILE SER PRO VAL ALA ALA ASN THR GLY ALA LYS P16 N32 Q44

- Molecule 12: Photosystem I 4.8 kDa protein

Chain cX:  64% 34%

MET ALA LYS LYS ILE SER PRO VAL ALA ALA ASN THR GLY ALA LYS P16 N32 Q44

- Molecule 12: Photosystem I 4.8 kDa protein



MET	ALA	LYS	ALA	LYS	ILE	SER	PRO	VAL	ALA	ASN	THR	GLY	ALA	LYS	P16	N32	Q44
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	111400	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	aA	0.40	0/6000	0.52	1/8187 (0.0%)
1	bA	0.40	0/6000	0.52	1/8187 (0.0%)
1	cA	0.40	0/6000	0.52	1/8187 (0.0%)
1	dA	0.40	0/6000	0.52	1/8187 (0.0%)
2	aB	0.44	0/6143	0.55	1/8398 (0.0%)
2	bB	0.44	0/6143	0.55	1/8398 (0.0%)
2	cB	0.44	0/6143	0.55	1/8398 (0.0%)
2	dB	0.44	0/6143	0.55	1/8398 (0.0%)
3	aC	0.37	0/609	0.54	0/826
3	bC	0.37	0/609	0.54	0/826
3	cC	0.37	0/609	0.54	0/826
3	dC	0.37	0/609	0.54	0/826
4	aD	0.33	0/596	0.53	0/806
4	bD	0.36	0/757	0.58	0/1024
4	cD	0.33	0/596	0.53	0/806
4	dD	0.36	0/757	0.58	0/1024
5	aE	0.41	0/499	0.50	0/677
5	bE	0.41	0/499	0.50	0/677
5	cE	0.41	0/499	0.50	0/677
5	dE	0.41	0/499	0.50	0/677
6	aF	0.33	0/1096	0.55	0/1489
6	bF	0.37	0/1104	0.61	0/1500
6	cF	0.33	0/1096	0.55	0/1489
6	dF	0.37	0/1104	0.61	0/1500
7	aI	0.40	0/262	0.59	0/358
7	bI	0.40	0/262	0.59	0/358
7	cI	0.40	0/262	0.59	0/358
7	dI	0.39	0/262	0.59	0/358
8	aJ	0.33	0/358	0.51	0/490
8	bJ	0.34	0/358	0.51	0/490
8	cJ	0.34	0/358	0.51	0/490
8	dJ	0.33	0/358	0.51	0/490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	aK	0.34	0/494	0.70	0/675
9	bK	0.34	0/494	0.70	0/675
9	cK	0.34	0/494	0.70	0/675
9	dK	0.34	0/494	0.70	0/675
10	aL	0.38	0/1067	0.58	0/1462
10	bL	0.41	0/1247	0.67	1/1710 (0.1%)
10	cL	0.38	0/1067	0.58	0/1462
10	dL	0.41	0/1247	0.68	1/1710 (0.1%)
11	aM	0.32	0/239	0.50	0/326
11	bM	0.32	0/239	0.50	0/326
11	cM	0.32	0/239	0.50	0/326
11	dM	0.32	0/239	0.50	0/326
12	aX	0.37	0/253	0.44	0/347
12	bX	0.37	0/253	0.44	0/347
12	cX	0.37	0/253	0.44	0/347
12	dX	0.37	0/253	0.45	0/347
All	All	0.41	0/71162	0.55	10/97118 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	aB	0	1
2	bB	0	1
2	cB	0	1
2	dB	0	1
6	aF	0	1
6	cF	0	1
10	bL	0	3
10	dL	0	3
All	All	0	12

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	dL	21	VAL	CG1-CB-CG2	-9.94	95.00	110.90
10	bL	21	VAL	CG1-CB-CG2	-9.93	95.01	110.90
2	bB	556	ASP	CB-CG-OD1	5.99	123.69	118.30
2	cB	556	ASP	CB-CG-OD1	5.92	123.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	aB	556	ASP	CB-CG-OD1	5.92	123.63	118.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	aB	480	THR	Peptide
6	aF	135	THR	Peptide
2	bB	480	THR	Peptide
10	bL	14	ASP	Peptide
10	bL	19	GLU	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	5801	0	5667	0	0
1	bA	5801	0	5667	0	0
1	cA	5801	0	5667	0	0
1	dA	5801	0	5667	0	0
2	aB	5919	0	5675	0	0
2	bB	5919	0	5675	0	0
2	cB	5919	0	5675	0	0
2	dB	5919	0	5675	0	0
3	aC	599	0	577	0	0
3	bC	599	0	577	0	0
3	cC	599	0	577	0	0
3	dC	599	0	577	0	0
4	aD	581	0	584	0	0
4	bD	740	0	751	0	0
4	cD	581	0	584	0	0
4	dD	740	0	751	0	0
5	aE	490	0	484	0	0
5	bE	490	0	484	0	0
5	cE	490	0	484	0	0
5	dE	490	0	484	0	0
6	aF	1072	0	1065	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	bF	1080	0	1076	0	0
6	cF	1072	0	1065	0	0
6	dF	1080	0	1076	0	0
7	aI	253	0	255	0	0
7	bI	253	0	255	0	0
7	cI	253	0	255	0	0
7	dI	253	0	255	0	0
8	aJ	347	0	352	0	0
8	bJ	347	0	352	0	0
8	cJ	347	0	352	0	0
8	dJ	347	0	352	0	0
9	aK	480	0	501	0	0
9	bK	480	0	501	0	0
9	cK	480	0	501	0	0
9	dK	480	0	501	0	0
10	aL	1037	0	1051	0	0
10	bL	1210	0	1213	0	0
10	cL	1037	0	1051	0	0
10	dL	1210	0	1213	0	0
11	aM	235	0	251	0	0
11	bM	235	0	251	0	0
11	cM	235	0	251	0	0
11	dM	235	0	251	0	0
12	aX	243	0	244	0	0
12	bX	243	0	244	0	0
12	cX	243	0	244	0	0
12	dX	243	0	244	0	0
13	aA	65	0	72	0	0
13	bA	65	0	72	0	0
13	cA	65	0	72	0	0
13	dA	65	0	72	0	0
14	aA	2332	0	2197	0	0
14	aB	2340	0	2282	0	0
14	aF	96	0	74	0	0
14	aJ	82	0	58	0	0
14	aK	86	0	62	0	0
14	aL	182	0	187	0	0
14	aX	45	0	33	0	0
14	bA	2280	0	2154	0	0
14	bB	2405	0	2354	0	0
14	bF	96	0	74	0	0
14	bJ	82	0	58	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	bK	86	0	62	0	0
14	bL	299	0	301	0	0
14	bX	45	0	33	0	0
14	cA	2332	0	2197	0	0
14	cB	2340	0	2282	0	0
14	cF	96	0	74	0	0
14	cJ	82	0	58	0	0
14	cK	86	0	62	0	0
14	cL	182	0	187	0	0
14	cX	45	0	33	0	0
14	dA	2280	0	2154	0	0
14	dB	2405	0	2354	0	0
14	dF	96	0	74	0	0
14	dJ	82	0	58	0	0
14	dK	86	0	62	0	0
14	dL	299	0	301	0	0
14	dX	45	0	33	0	0
15	aA	33	0	46	0	0
15	aB	33	0	46	0	0
15	bA	33	0	46	0	0
15	bB	33	0	46	0	0
15	cA	33	0	46	0	0
15	cB	33	0	46	0	0
15	dA	33	0	46	0	0
15	dB	33	0	46	0	0
16	aA	8	0	0	0	0
16	aC	16	0	0	0	0
16	bA	8	0	0	0	0
16	bC	16	0	0	0	0
16	cA	8	0	0	0	0
16	cC	16	0	0	0	0
16	dA	8	0	0	0	0
16	dC	16	0	0	0	0
17	aA	240	0	336	0	0
17	aB	280	0	392	0	0
17	aF	80	0	112	0	0
17	aI	40	0	56	0	0
17	aJ	80	0	112	0	0
17	aL	120	0	168	0	0
17	aM	40	0	56	0	0
17	bA	200	0	280	0	0
17	bB	280	0	392	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	bF	80	0	112	0	0
17	bI	40	0	56	0	0
17	bJ	80	0	112	0	0
17	bK	40	0	56	0	0
17	bL	120	0	168	0	0
17	bM	40	0	56	0	0
17	cA	240	0	336	0	0
17	cB	280	0	392	0	0
17	cF	80	0	112	0	0
17	cI	40	0	56	0	0
17	cJ	80	0	112	0	0
17	cL	120	0	168	0	0
17	cM	40	0	56	0	0
17	dA	200	0	280	0	0
17	dB	280	0	392	0	0
17	dF	80	0	112	0	0
17	dI	40	0	56	0	0
17	dJ	80	0	112	0	0
17	dK	40	0	56	0	0
17	dL	120	0	168	0	0
17	dM	40	0	56	0	0
18	aA	76	0	98	0	0
18	aB	23	0	16	0	0
18	bA	76	0	98	0	0
18	bB	23	0	16	0	0
18	cA	76	0	98	0	0
18	cB	23	0	16	0	0
18	dA	76	0	98	0	0
18	dB	23	0	16	0	0
19	aB	55	0	86	0	0
19	bB	55	0	86	0	0
19	cB	55	0	86	0	0
19	dB	55	0	86	0	0
All	All	94576	0	93746	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 7.

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	737/752 (98%)	704 (96%)	33 (4%)	0	100	100
1	bA	737/752 (98%)	703 (95%)	34 (5%)	0	100	100
1	cA	737/752 (98%)	704 (96%)	33 (4%)	0	100	100
1	dA	737/752 (98%)	703 (95%)	34 (5%)	0	100	100
2	aB	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	bB	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	cB	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
2	dB	737/741 (100%)	707 (96%)	30 (4%)	0	100	100
3	aC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	bC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	cC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	dC	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	aD	71/139 (51%)	69 (97%)	2 (3%)	0	100	100
4	bD	94/139 (68%)	89 (95%)	5 (5%)	0	100	100
4	cD	71/139 (51%)	69 (97%)	2 (3%)	0	100	100
4	dD	94/139 (68%)	89 (95%)	5 (5%)	0	100	100
5	aE	59/70 (84%)	53 (90%)	6 (10%)	0	100	100
5	bE	59/70 (84%)	53 (90%)	6 (10%)	0	100	100
5	cE	59/70 (84%)	53 (90%)	6 (10%)	0	100	100
5	dE	59/70 (84%)	53 (90%)	6 (10%)	0	100	100
6	aF	138/164 (84%)	129 (94%)	9 (6%)	0	100	100
6	bF	139/164 (85%)	131 (94%)	8 (6%)	0	100	100
6	cF	138/164 (84%)	130 (94%)	8 (6%)	0	100	100
6	dF	139/164 (85%)	131 (94%)	8 (6%)	0	100	100
7	aI	29/46 (63%)	28 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	bI	29/46 (63%)	28 (97%)	1 (3%)	0	100	100
7	cI	29/46 (63%)	28 (97%)	1 (3%)	0	100	100
7	dI	29/46 (63%)	28 (97%)	1 (3%)	0	100	100
8	aJ	41/49 (84%)	41 (100%)	0	0	100	100
8	bJ	41/49 (84%)	41 (100%)	0	0	100	100
8	cJ	41/49 (84%)	41 (100%)	0	0	100	100
8	dJ	41/49 (84%)	41 (100%)	0	0	100	100
9	aK	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
9	bK	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
9	cK	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
9	dK	64/86 (74%)	55 (86%)	9 (14%)	0	100	100
10	aL	138/172 (80%)	134 (97%)	4 (3%)	0	100	100
10	bL	159/172 (92%)	145 (91%)	12 (8%)	2 (1%)	10	36
10	cL	138/172 (80%)	134 (97%)	4 (3%)	0	100	100
10	dL	159/172 (92%)	144 (91%)	13 (8%)	2 (1%)	10	36
11	aM	28/40 (70%)	28 (100%)	0	0	100	100
11	bM	28/40 (70%)	28 (100%)	0	0	100	100
11	cM	28/40 (70%)	28 (100%)	0	0	100	100
11	dM	28/40 (70%)	28 (100%)	0	0	100	100
12	aX	27/44 (61%)	27 (100%)	0	0	100	100
12	bX	27/44 (61%)	27 (100%)	0	0	100	100
12	cX	27/44 (61%)	27 (100%)	0	0	100	100
12	dX	27/44 (61%)	27 (100%)	0	0	100	100
All	All	8678/9536 (91%)	8260 (95%)	414 (5%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	bL	15	PRO
10	dL	15	PRO
10	dL	21	VAL
10	bL	21	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	593/605 (98%)	591 (100%)	2 (0%)	91	94
1	bA	593/605 (98%)	591 (100%)	2 (0%)	91	94
1	cA	593/605 (98%)	591 (100%)	2 (0%)	91	94
1	dA	593/605 (98%)	591 (100%)	2 (0%)	91	94
2	aB	601/602 (100%)	599 (100%)	2 (0%)	91	94
2	bB	601/602 (100%)	599 (100%)	2 (0%)	91	94
2	cB	601/602 (100%)	599 (100%)	2 (0%)	91	94
2	dB	601/602 (100%)	599 (100%)	2 (0%)	91	94
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
3	dC	68/69 (99%)	68 (100%)	0	100	100
4	aD	59/110 (54%)	59 (100%)	0	100	100
4	bD	76/110 (69%)	76 (100%)	0	100	100
4	cD	59/110 (54%)	59 (100%)	0	100	100
4	dD	76/110 (69%)	76 (100%)	0	100	100
5	aE	54/60 (90%)	54 (100%)	0	100	100
5	bE	54/60 (90%)	54 (100%)	0	100	100
5	cE	54/60 (90%)	54 (100%)	0	100	100
5	dE	54/60 (90%)	54 (100%)	0	100	100
6	aF	109/129 (84%)	109 (100%)	0	100	100
6	bF	110/129 (85%)	110 (100%)	0	100	100
6	cF	109/129 (84%)	109 (100%)	0	100	100
6	dF	110/129 (85%)	110 (100%)	0	100	100
7	aI	28/39 (72%)	28 (100%)	0	100	100
7	bI	28/39 (72%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	cI	28/39 (72%)	28 (100%)	0	100	100
7	dI	28/39 (72%)	28 (100%)	0	100	100
8	aJ	38/42 (90%)	38 (100%)	0	100	100
8	bJ	38/42 (90%)	38 (100%)	0	100	100
8	cJ	38/42 (90%)	38 (100%)	0	100	100
8	dJ	38/42 (90%)	38 (100%)	0	100	100
9	aK	48/64 (75%)	47 (98%)	1 (2%)	48	70
9	bK	48/64 (75%)	47 (98%)	1 (2%)	48	70
9	cK	48/64 (75%)	47 (98%)	1 (2%)	48	70
9	dK	48/64 (75%)	47 (98%)	1 (2%)	48	70
10	aL	105/131 (80%)	105 (100%)	0	100	100
10	bL	124/131 (95%)	123 (99%)	1 (1%)	79	87
10	cL	105/131 (80%)	105 (100%)	0	100	100
10	dL	124/131 (95%)	123 (99%)	1 (1%)	79	87
11	aM	25/34 (74%)	25 (100%)	0	100	100
11	bM	25/34 (74%)	25 (100%)	0	100	100
11	cM	25/34 (74%)	25 (100%)	0	100	100
11	dM	25/34 (74%)	25 (100%)	0	100	100
12	aX	24/34 (71%)	23 (96%)	1 (4%)	25	53
12	bX	24/34 (71%)	23 (96%)	1 (4%)	25	53
12	cX	24/34 (71%)	23 (96%)	1 (4%)	25	53
12	dX	24/34 (71%)	23 (96%)	1 (4%)	25	53
All	All	7082/7676 (92%)	7056 (100%)	26 (0%)	88	93

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	cA	691	ARG
9	cK	24	MET
10	dL	20	VAL
2	cB	612	ASN
12	cX	32	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
2	dB	114	ASN
2	dB	354	GLN
2	dB	640	ASN
2	bB	407	ASN
2	bB	262	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

504 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	CLA	aB	815	2	45,53,73	1.74	7 (15%)	52,89,113	1.74	7 (13%)
17	BCR	cF	204	-	41,41,41	1.10	2 (4%)	56,56,56	1.29	8 (14%)
17	BCR	bB	852	-	41,41,41	1.19	2 (4%)	56,56,56	1.37	8 (14%)
14	CLA	aB	813	2	65,73,73	1.43	10 (15%)	76,113,113	1.52	9 (11%)
17	BCR	dA	846	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	8 (14%)
14	CLA	dB	842	2	65,73,73	1.47	9 (13%)	76,113,113	1.51	7 (9%)
14	CLA	aB	811	2	45,53,73	1.72	8 (17%)	52,89,113	1.68	7 (13%)
14	CLA	dA	827	14,1	65,73,73	1.42	8 (12%)	76,113,113	1.53	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	aA	812	1	54,62,73	1.61	8 (14%)	62,99,113	1.55	6 (9%)
14	CLA	aA	809	1	45,53,73	1.71	8 (17%)	52,89,113	1.73	8 (15%)
14	CLA	bA	818	1	54,62,73	1.57	9 (16%)	62,99,113	1.63	7 (11%)
14	CLA	cJ	102	-	38,45,73	1.86	8 (21%)	43,78,113	1.70	7 (16%)
14	CLA	aB	818	2	60,68,73	1.54	10 (16%)	70,107,113	1.47	7 (10%)
14	CLA	aA	805	1	45,53,73	1.82	10 (22%)	52,89,113	1.72	9 (17%)
14	CLA	aB	834	2	45,53,73	1.71	7 (15%)	52,89,113	1.88	7 (13%)
14	CLA	aA	803	1	45,53,73	1.76	8 (17%)	52,89,113	1.70	9 (17%)
14	CLA	bA	834	1	65,73,73	1.46	8 (12%)	76,113,113	1.43	7 (9%)
14	CLA	aA	841	1	65,73,73	1.46	9 (13%)	76,113,113	1.43	7 (9%)
14	CLA	dB	829	2	65,73,73	1.43	10 (15%)	76,113,113	1.45	8 (10%)
14	CLA	aJ	101	-	45,53,73	1.75	7 (15%)	52,89,113	1.64	6 (11%)
17	BCR	aF	202	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	5 (8%)
17	BCR	cJ	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	6 (10%)
17	BCR	bB	844	-	41,41,41	1.14	2 (4%)	56,56,56	1.31	6 (10%)
14	CLA	bB	836	-	45,53,73	1.79	8 (17%)	52,89,113	1.71	9 (17%)
17	BCR	dL	203	-	41,41,41	1.24	3 (7%)	56,56,56	1.25	5 (8%)
14	CLA	cA	840	1	65,73,73	1.46	10 (15%)	76,113,113	1.49	7 (9%)
14	CLA	bB	832	2	49,57,73	1.69	7 (14%)	55,93,113	1.71	9 (16%)
14	CLA	dB	802	2	65,73,73	1.46	9 (13%)	76,113,113	1.35	6 (7%)
14	CLA	bA	836	1	45,53,73	1.72	7 (15%)	52,89,113	1.81	8 (15%)
14	CLA	bB	809	2	65,73,73	1.46	12 (18%)	76,113,113	1.61	9 (11%)
14	CLA	aB	838	2	65,73,73	1.43	7 (10%)	76,113,113	1.61	9 (11%)
14	CLA	dB	835	2	45,53,73	1.71	7 (15%)	52,89,113	1.88	7 (13%)
17	BCR	cB	846	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	4 (7%)
14	CLA	aB	804	-	65,73,73	1.39	9 (13%)	76,113,113	1.80	12 (15%)
14	CLA	aB	809	2	65,73,73	1.45	11 (16%)	76,113,113	1.61	9 (11%)
14	CLA	bA	809	1	45,53,73	1.71	8 (17%)	52,89,113	1.72	8 (15%)
14	CLA	bB	841	-	65,73,73	1.47	10 (15%)	76,113,113	1.33	7 (9%)
14	CLA	bL	202	18,10	52,60,73	1.62	8 (15%)	60,97,113	2.13	12 (20%)
14	CLA	dB	840	2	47,55,73	1.66	7 (14%)	54,91,113	1.74	8 (14%)
17	BCR	dB	848	-	41,41,41	1.17	2 (4%)	56,56,56	1.32	5 (8%)
17	BCR	dA	849	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	6 (10%)
16	SF4	aC	101	3	0,12,12	-	-	-	-	-
14	CLA	cB	807	2	65,73,73	1.45	8 (12%)	76,113,113	1.47	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	dB	832	2	49,57,73	1.69	7 (14%)	55,93,113	1.71	9 (16%)
14	CLA	cB	815	2	45,53,73	1.73	7 (15%)	52,89,113	1.73	7 (13%)
14	CLA	cA	808	1	45,53,73	1.73	9 (20%)	52,89,113	1.68	8 (15%)
14	CLA	aB	820	2	47,55,73	1.67	8 (17%)	54,91,113	1.58	6 (11%)
14	CLA	aA	815	1	45,53,73	1.77	8 (17%)	52,89,113	1.70	6 (11%)
14	CLA	bF	201	-	51,59,73	1.64	7 (13%)	59,96,113	1.61	7 (11%)
14	CLA	bA	805	1	45,53,73	1.82	10 (22%)	52,89,113	1.72	9 (17%)
14	CLA	cA	815	1	45,53,73	1.78	8 (17%)	52,89,113	1.72	6 (11%)
14	CLA	dX	101	12	45,53,73	1.75	9 (20%)	52,89,113	1.64	6 (11%)
18	LHG	bA	851	14	26,26,48	0.87	1 (3%)	29,32,54	1.31	3 (10%)
14	CLA	dA	835	1	54,62,73	1.64	9 (16%)	62,99,113	1.56	8 (12%)
14	CLA	bK	101	9	42,49,73	1.73	7 (16%)	48,83,113	1.67	6 (12%)
14	CLA	cA	839	1	65,73,73	1.48	8 (12%)	76,113,113	1.49	8 (10%)
14	CLA	aA	833	1	65,73,73	1.45	9 (13%)	76,113,113	1.53	10 (13%)
17	BCR	bF	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
14	CLA	aA	814	1	45,53,73	1.73	7 (15%)	52,89,113	1.67	8 (15%)
17	BCR	aB	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.38	8 (14%)
14	CLA	aA	818	1	54,62,73	1.56	9 (16%)	62,99,113	1.61	7 (11%)
14	CLA	cB	820	2	47,55,73	1.67	8 (17%)	54,91,113	1.58	6 (11%)
17	BCR	dK	102	-	41,41,41	1.19	3 (7%)	56,56,56	1.42	10 (17%)
14	CLA	cA	813	1	45,53,73	1.73	9 (20%)	52,89,113	1.69	12 (23%)
17	BCR	aA	848	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	8 (14%)
17	BCR	cL	201	-	41,41,41	1.24	3 (7%)	56,56,56	1.25	5 (8%)
19	LMG	bB	850	-	55,55,55	0.79	2 (3%)	63,63,63	1.46	9 (14%)
18	LHG	aA	853	14	26,26,48	0.86	1 (3%)	29,32,54	1.31	3 (10%)
14	CLA	cA	829	1	65,73,73	1.48	10 (15%)	76,113,113	1.39	8 (10%)
14	CLA	dK	101	9	42,49,73	1.74	7 (16%)	48,83,113	1.67	6 (12%)
14	CLA	bB	804	-	65,73,73	1.40	9 (13%)	76,113,113	1.79	12 (15%)
14	CLA	bB	815	2	56,64,73	1.54	7 (12%)	65,102,113	1.53	6 (9%)
17	BCR	cA	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	8 (14%)
14	CLA	cL	202	10	65,73,73	1.47	7 (10%)	76,113,113	1.39	9 (11%)
14	CLA	cB	823	2	45,53,73	1.76	8 (17%)	52,89,113	1.57	8 (15%)
14	CLA	dB	810	2	65,73,73	1.48	10 (15%)	76,113,113	1.47	6 (7%)
14	CLA	dB	830	2	65,73,73	1.46	10 (15%)	76,113,113	1.70	9 (11%)
14	CLA	dJ	101	-	45,53,73	1.76	7 (15%)	52,89,113	1.64	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	bM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	6 (10%)
17	BCR	bJ	103	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	7 (12%)
14	CLA	bA	829	1	65,73,73	1.47	10 (15%)	76,113,113	1.38	7 (9%)
17	BCR	dJ	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	7 (12%)
16	SF4	bC	101	3	0,12,12	-	-	-	-	-
17	BCR	aL	205	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	7 (12%)
14	CLA	aA	838	1	65,73,73	1.46	9 (13%)	76,113,113	1.51	9 (11%)
17	BCR	bL	208	-	41,41,41	1.12	2 (4%)	56,56,56	1.38	10 (17%)
14	CLA	bA	816	-	49,57,73	1.69	6 (12%)	55,93,113	1.65	7 (12%)
14	CLA	cA	838	1	65,73,73	1.46	9 (13%)	76,113,113	1.51	9 (11%)
14	CLA	dB	837	-	45,53,73	1.81	8 (17%)	52,89,113	1.57	7 (13%)
17	BCR	bB	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.32	5 (8%)
14	CLA	aB	816	2	55,63,73	1.64	9 (16%)	64,101,113	1.47	9 (14%)
16	SF4	dA	844	2,1	0,12,12	-	-	-	-	-
14	CLA	bA	840	1	65,73,73	1.46	10 (15%)	76,113,113	1.50	7 (9%)
14	CLA	dA	811	14,1	65,73,73	1.48	9 (13%)	76,113,113	1.41	8 (10%)
17	BCR	bA	848	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	6 (10%)
14	CLA	cB	810	2	65,73,73	1.48	10 (15%)	76,113,113	1.48	6 (7%)
15	PQN	cB	842	-	34,34,34	1.52	2 (5%)	42,45,45	1.23	5 (11%)
17	BCR	dB	852	-	41,41,41	1.18	2 (4%)	56,56,56	1.38	8 (14%)
14	CLA	dA	810	1	45,53,73	1.71	6 (13%)	52,89,113	1.65	6 (11%)
15	PQN	aB	842	-	34,34,34	1.52	2 (5%)	42,45,45	1.23	5 (11%)
14	CLA	aX	101	12	45,53,73	1.75	8 (17%)	52,89,113	1.65	6 (11%)
17	BCR	aB	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.31	5 (8%)
14	CLA	cA	826	-	55,63,73	1.56	8 (14%)	64,101,113	1.55	8 (12%)
17	BCR	cA	846	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	11 (19%)
14	CLA	aA	824	1	47,55,73	1.71	8 (17%)	54,91,113	1.65	8 (14%)
14	CLA	cB	816	2	55,63,73	1.64	9 (16%)	64,101,113	1.47	9 (14%)
17	BCR	aB	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	6 (10%)
17	BCR	aM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	6 (10%)
14	CLA	bB	808	2	65,73,73	1.50	7 (10%)	76,113,113	1.49	9 (11%)
14	CLA	aK	102	-	45,53,73	1.72	8 (17%)	52,89,113	1.66	6 (11%)
14	CLA	aA	806	1	65,73,73	1.47	10 (15%)	76,113,113	1.46	9 (11%)
14	CLA	bB	816	2	45,53,73	1.73	7 (15%)	52,89,113	1.73	7 (13%)
14	CLA	dA	842	-	65,73,73	1.49	10 (15%)	76,113,113	1.45	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	cA	843	18	52,60,73	1.62	8 (15%)	60,97,113	2.12	11 (18%)
14	CLA	dB	826	-	46,54,73	1.66	10 (21%)	53,90,113	1.70	8 (15%)
19	LMG	aB	849	-	55,55,55	0.79	2 (3%)	63,63,63	1.46	9 (14%)
17	BCR	dB	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	6 (10%)
14	CLA	aA	836	1	45,53,73	1.72	7 (15%)	52,89,113	1.81	8 (15%)
14	CLA	bB	833	2	65,73,73	1.53	8 (12%)	76,113,113	1.41	8 (10%)
17	BCR	cB	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.38	8 (14%)
14	CLA	cA	836	1	45,53,73	1.72	7 (15%)	52,89,113	1.82	8 (15%)
13	CL0	cA	801	1	65,73,73	2.03	18 (27%)	76,113,113	2.76	26 (34%)
14	CLA	dA	807	1	51,59,73	1.65	8 (15%)	59,96,113	1.61	6 (10%)
17	BCR	cA	851	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	6 (10%)
14	CLA	dB	828	2	65,73,73	1.40	7 (10%)	76,113,113	1.55	9 (11%)
14	CLA	bB	824	2	45,53,73	1.77	8 (17%)	52,89,113	1.57	8 (15%)
14	CLA	cL	203	10	65,73,73	1.45	10 (15%)	76,113,113	1.55	9 (11%)
14	CLA	cA	827	14,1	65,73,73	1.42	7 (10%)	76,113,113	1.53	8 (10%)
14	CLA	cA	830	1	65,73,73	1.49	10 (15%)	76,113,113	1.53	7 (9%)
14	CLA	aA	813	1	45,53,73	1.73	9 (20%)	52,89,113	1.69	11 (21%)
14	CLA	aB	824	2	54,62,73	1.65	10 (18%)	62,99,113	1.45	8 (12%)
14	CLA	bB	806	2	65,73,73	1.38	8 (12%)	76,113,113	1.57	8 (10%)
17	BCR	aF	204	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	9 (16%)
14	CLA	dB	811	2	65,73,73	1.45	10 (15%)	76,113,113	1.37	8 (10%)
17	BCR	dJ	104	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	cA	842	-	65,73,73	1.49	10 (15%)	76,113,113	1.45	7 (9%)
18	LHG	dA	850	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	5 (9%)
14	CLA	dA	808	1	45,53,73	1.74	9 (20%)	52,89,113	1.67	8 (15%)
14	CLA	dA	802	-	45,53,73	1.69	8 (17%)	52,89,113	1.83	6 (11%)
14	CLA	bA	802	-	45,53,73	1.68	8 (17%)	52,89,113	1.83	6 (11%)
14	CLA	aA	825	-	65,73,73	1.40	8 (12%)	76,113,113	1.55	9 (11%)
17	BCR	aJ	103	-	41,41,41	1.16	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	bB	838	2	60,68,73	1.52	8 (13%)	70,107,113	1.49	9 (12%)
14	CLA	aB	808	2	65,73,73	1.49	8 (12%)	76,113,113	1.49	9 (11%)
14	CLA	bL	204	10	52,60,73	1.65	9 (17%)	60,97,113	1.63	9 (15%)
14	CLA	bA	806	1	65,73,73	1.46	10 (15%)	76,113,113	1.47	9 (11%)
14	CLA	aB	828	2	65,73,73	1.44	10 (15%)	76,113,113	1.46	8 (10%)
14	CLA	cB	821	2	45,53,73	1.72	9 (20%)	52,89,113	1.67	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	dB	841	-	65,73,73	1.47	10 (15%)	76,113,113	1.33	7 (9%)
14	CLA	dA	834	1	65,73,73	1.46	8 (12%)	76,113,113	1.44	7 (9%)
14	CLA	cB	818	2	60,68,73	1.54	10 (16%)	70,107,113	1.47	7 (10%)
14	CLA	dA	832	1	65,73,73	1.46	10 (15%)	76,113,113	1.49	10 (13%)
14	CLA	bB	813	2	45,53,73	1.76	9 (20%)	52,89,113	1.64	7 (13%)
14	CLA	cB	841	2	65,73,73	1.46	9 (13%)	76,113,113	1.52	7 (9%)
14	CLA	cB	814	2	56,64,73	1.54	8 (14%)	65,102,113	1.54	6 (9%)
14	CLA	cB	813	2	65,73,73	1.44	10 (15%)	76,113,113	1.52	9 (11%)
14	CLA	dB	819	2	60,68,73	1.53	10 (16%)	70,107,113	1.47	7 (10%)
18	LHG	cA	852	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	5 (9%)
14	CLA	aB	836	-	45,53,73	1.82	9 (20%)	52,89,113	1.56	7 (13%)
17	BCR	bB	846	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	3 (5%)
14	CLA	aA	829	1	65,73,73	1.47	10 (15%)	76,113,113	1.38	7 (9%)
14	CLA	dA	837	1	51,59,73	1.57	8 (15%)	59,96,113	1.70	8 (13%)
14	CLA	dB	838	2	60,68,73	1.52	9 (15%)	70,107,113	1.49	9 (12%)
14	CLA	bB	802	2	65,73,73	1.46	9 (13%)	76,113,113	1.35	6 (7%)
14	CLA	aA	804	14,1	45,53,73	1.81	9 (20%)	52,89,113	1.78	8 (15%)
14	CLA	bA	814	1	45,53,73	1.74	7 (15%)	52,89,113	1.66	8 (15%)
14	CLA	dA	841	1	65,73,73	1.47	9 (13%)	76,113,113	1.42	6 (7%)
15	PQN	dA	843	-	34,34,34	1.50	2 (5%)	42,45,45	1.27	6 (14%)
14	CLA	cA	804	14,1	45,53,73	1.80	9 (20%)	52,89,113	1.79	8 (15%)
17	BCR	bA	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.22	3 (5%)
14	CLA	dB	817	2	55,63,73	1.63	9 (16%)	64,101,113	1.47	9 (14%)
14	CLA	bA	813	1	45,53,73	1.73	9 (20%)	52,89,113	1.69	11 (21%)
14	CLA	cB	834	2	45,53,73	1.72	7 (15%)	52,89,113	1.87	7 (13%)
14	CLA	dB	823	-	55,63,73	1.56	9 (16%)	64,101,113	1.60	6 (9%)
14	CLA	bB	821	2	47,55,73	1.67	8 (17%)	54,91,113	1.59	6 (11%)
14	CLA	bB	818	2	59,67,73	1.54	9 (15%)	68,105,113	1.53	9 (13%)
14	CLA	bA	825	-	65,73,73	1.40	8 (12%)	76,113,113	1.56	10 (13%)
14	CLA	cL	204	-	52,60,73	1.60	8 (15%)	60,97,113	1.56	8 (13%)
14	CLA	dA	812	1	54,62,73	1.61	9 (16%)	62,99,113	1.56	6 (9%)
17	BCR	aB	845	-	41,41,41	1.17	3 (7%)	56,56,56	1.17	3 (5%)
14	CLA	dB	806	2	65,73,73	1.37	8 (12%)	76,113,113	1.58	8 (10%)
14	CLA	bB	814	2	65,73,73	1.43	10 (15%)	76,113,113	1.52	9 (11%)
17	BCR	dB	849	-	41,41,41	1.21	2 (4%)	56,56,56	1.16	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	dA	805	1	45,53,73	1.84	10 (22%)	52,89,113	1.72	9 (17%)
14	CLA	bB	827	2	65,73,73	1.45	10 (15%)	76,113,113	1.45	8 (10%)
14	CLA	bJ	102	-	38,45,73	1.85	7 (18%)	43,78,113	1.70	7 (16%)
14	CLA	dB	839	2	65,73,73	1.43	7 (10%)	76,113,113	1.62	9 (11%)
17	BCR	dB	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.15	5 (8%)
17	BCR	aA	851	-	41,41,41	1.15	2 (4%)	56,56,56	1.24	6 (10%)
14	CLA	dA	829	1	65,73,73	1.48	10 (15%)	76,113,113	1.38	7 (9%)
14	CLA	cA	802	-	45,53,73	1.68	8 (17%)	52,89,113	1.83	6 (11%)
17	BCR	cB	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.32	5 (8%)
17	BCR	cB	845	-	41,41,41	1.17	2 (4%)	56,56,56	1.16	3 (5%)
14	CLA	bA	827	14,1	65,73,73	1.42	7 (10%)	76,113,113	1.52	8 (10%)
14	CLA	aB	826	2	65,73,73	1.45	10 (15%)	76,113,113	1.45	8 (10%)
14	CLA	bB	834	2	58,66,73	1.56	8 (13%)	67,104,113	1.48	10 (14%)
14	CLA	aB	829	2	65,73,73	1.47	10 (15%)	76,113,113	1.69	9 (11%)
14	CLA	bA	826	-	55,63,73	1.57	8 (14%)	64,101,113	1.56	8 (12%)
14	CLA	dA	815	1	45,53,73	1.76	7 (15%)	52,89,113	1.72	6 (11%)
17	BCR	bJ	104	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	5 (8%)
14	CLA	aB	825	-	46,54,73	1.67	10 (21%)	53,90,113	1.69	8 (15%)
14	CLA	bB	805	2	54,62,73	1.57	7 (12%)	62,99,113	1.61	7 (11%)
14	CLA	dL	202	18,10	52,60,73	1.62	8 (15%)	60,97,113	2.12	11 (18%)
16	SF4	bC	102	3	0,12,12	-	-	-	-	-
14	CLA	aA	843	18	52,60,73	1.62	8 (15%)	60,97,113	2.13	11 (18%)
14	CLA	aA	822	1	49,57,73	1.65	9 (18%)	55,93,113	1.64	6 (10%)
14	CLA	aB	835	-	45,53,73	1.80	8 (17%)	52,89,113	1.71	9 (17%)
14	CLA	bA	804	14,1	45,53,73	1.81	9 (20%)	52,89,113	1.77	8 (15%)
14	CLA	aA	816	-	49,57,73	1.69	6 (12%)	55,93,113	1.65	7 (12%)
17	BCR	cL	206	-	41,41,41	1.07	1 (2%)	56,56,56	1.33	7 (12%)
13	CL0	aA	801	1	65,73,73	2.04	18 (27%)	76,113,113	2.77	25 (32%)
17	BCR	dI	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	7 (12%)
16	SF4	cC	101	3	0,12,12	-	-	-	-	-
14	CLA	dA	814	1	45,53,73	1.74	7 (15%)	52,89,113	1.67	8 (15%)
16	SF4	cA	845	2,1	0,12,12	-	-	-	-	-
14	CLA	dA	818	1	54,62,73	1.56	9 (16%)	62,99,113	1.62	7 (11%)
14	CLA	aB	821	2	45,53,73	1.71	8 (17%)	52,89,113	1.67	7 (13%)
14	CLA	bB	810	2	65,73,73	1.48	10 (15%)	76,113,113	1.47	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	aA	839	1	65,73,73	1.48	9 (13%)	76,113,113	1.49	8 (10%)
17	BCR	dA	848	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	6 (10%)
14	CLA	dL	206	-	65,73,73	1.45	10 (15%)	76,113,113	1.38	7 (9%)
14	CLA	dB	833	2	65,73,73	1.53	8 (12%)	76,113,113	1.41	8 (10%)
17	BCR	bB	849	-	41,41,41	1.21	2 (4%)	56,56,56	1.17	4 (7%)
14	CLA	dB	825	2	54,62,73	1.65	10 (18%)	62,99,113	1.44	8 (12%)
14	CLA	cA	837	1	51,59,73	1.56	8 (15%)	59,96,113	1.69	8 (13%)
14	CLA	dL	201	2,10	65,73,73	1.45	10 (15%)	76,113,113	1.36	8 (10%)
14	CLA	bA	822	1	49,57,73	1.65	9 (18%)	55,93,113	1.64	7 (12%)
14	CLA	cK	101	9	42,49,73	1.74	7 (16%)	48,83,113	1.68	6 (12%)
17	BCR	bB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	5 (8%)
14	CLA	dA	826	-	55,63,73	1.57	8 (14%)	64,101,113	1.56	8 (12%)
18	LHG	bB	851	-	22,22,48	0.89	1 (4%)	25,28,54	1.20	1 (4%)
14	CLA	aA	830	1	65,73,73	1.50	10 (15%)	76,113,113	1.53	7 (9%)
14	CLA	bA	817	1	54,62,73	1.61	8 (14%)	62,99,113	1.54	8 (12%)
14	CLA	cA	814	1	45,53,73	1.73	8 (17%)	52,89,113	1.66	9 (17%)
14	CLA	cA	818	1	54,62,73	1.56	9 (16%)	62,99,113	1.63	7 (11%)
17	BCR	aB	846	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	4 (7%)
14	CLA	bB	825	2	54,62,73	1.65	10 (18%)	62,99,113	1.43	8 (12%)
14	CLA	bL	205	10	65,73,73	1.44	9 (13%)	76,113,113	1.55	9 (11%)
14	CLA	aB	827	2	65,73,73	1.40	7 (10%)	76,113,113	1.55	9 (11%)
14	CLA	aA	842	-	65,73,73	1.49	10 (15%)	76,113,113	1.46	7 (9%)
14	CLA	dB	814	2	65,73,73	1.43	10 (15%)	76,113,113	1.52	9 (11%)
14	CLA	dA	823	1	51,59,73	1.66	9 (17%)	59,96,113	1.55	8 (13%)
14	CLA	bB	822	2	45,53,73	1.72	8 (17%)	52,89,113	1.67	7 (13%)
17	BCR	dL	208	-	41,41,41	1.12	2 (4%)	56,56,56	1.38	10 (17%)
17	BCR	dB	847	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	4 (7%)
14	CLA	cB	805	2	54,62,73	1.57	7 (12%)	62,99,113	1.61	7 (11%)
14	CLA	aB	817	2	59,67,73	1.53	9 (15%)	68,105,113	1.54	9 (13%)
14	CLA	cB	839	2	47,55,73	1.66	7 (14%)	54,91,113	1.74	8 (14%)
17	BCR	cB	848	-	41,41,41	1.22	2 (4%)	56,56,56	1.16	4 (7%)
14	CLA	bA	808	1	45,53,73	1.73	9 (20%)	52,89,113	1.67	8 (15%)
14	CLA	bB	839	2	65,73,73	1.43	7 (10%)	76,113,113	1.61	9 (11%)
14	CLA	dA	816	-	49,57,73	1.69	6 (12%)	55,93,113	1.65	7 (12%)
14	CLA	aA	840	1	65,73,73	1.46	10 (15%)	76,113,113	1.50	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	bB	835	2	45,53,73	1.71	7 (15%)	52,89,113	1.88	7 (13%)
14	CLA	bA	811	14,1	65,73,73	1.47	9 (13%)	76,113,113	1.40	8 (10%)
14	CLA	cB	827	2	65,73,73	1.40	7 (10%)	76,113,113	1.55	9 (11%)
14	CLA	cB	830	2	45,53,73	1.77	10 (22%)	52,89,113	1.60	6 (11%)
17	BCR	cB	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	6 (10%)
17	BCR	dM	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.28	6 (10%)
14	CLA	dB	801	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	7 (9%)
14	CLA	bA	839	1	65,73,73	1.48	9 (13%)	76,113,113	1.49	8 (10%)
19	LMG	dB	850	-	55,55,55	0.79	2 (3%)	63,63,63	1.46	9 (14%)
18	LHG	aA	852	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	5 (9%)
14	CLA	cB	838	2	65,73,73	1.43	7 (10%)	76,113,113	1.61	9 (11%)
13	CL0	bA	801	1	65,73,73	2.03	17 (26%)	76,113,113	2.79	28 (36%)
14	CLA	cB	817	2	59,67,73	1.54	9 (15%)	68,105,113	1.52	9 (13%)
17	BCR	dA	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	3 (5%)
14	CLA	cB	801	-	65,73,73	1.45	10 (15%)	76,113,113	1.42	7 (9%)
14	CLA	cF	201	-	51,59,73	1.65	7 (13%)	59,96,113	1.61	7 (11%)
14	CLA	dA	833	1	65,73,73	1.44	9 (13%)	76,113,113	1.53	10 (13%)
14	CLA	bB	817	2	55,63,73	1.63	9 (16%)	64,101,113	1.47	9 (14%)
17	BCR	aJ	104	-	41,41,41	1.13	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	aB	801	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	7 (9%)
14	CLA	cA	824	1	47,55,73	1.71	8 (17%)	54,91,113	1.64	8 (14%)
14	CLA	aB	810	2	65,73,73	1.48	10 (15%)	76,113,113	1.47	6 (7%)
14	CLA	cA	823	1	51,59,73	1.66	8 (15%)	59,96,113	1.54	8 (13%)
14	CLA	dA	830	1	65,73,73	1.50	9 (13%)	76,113,113	1.52	7 (9%)
14	CLA	bA	830	1	65,73,73	1.49	9 (13%)	76,113,113	1.52	7 (9%)
14	CLA	aB	839	2	47,55,73	1.66	7 (14%)	54,91,113	1.74	8 (14%)
14	CLA	dA	824	1	47,55,73	1.70	8 (17%)	54,91,113	1.65	8 (14%)
14	CLA	aA	820	1	61,69,73	1.52	8 (13%)	71,108,113	1.50	7 (9%)
14	CLA	cB	840	-	65,73,73	1.47	10 (15%)	76,113,113	1.34	7 (9%)
14	CLA	cA	803	1	45,53,73	1.75	8 (17%)	52,89,113	1.70	9 (17%)
14	CLA	cF	203	-	45,53,73	1.74	8 (17%)	52,89,113	1.65	6 (11%)
14	CLA	dA	806	1	65,73,73	1.47	10 (15%)	76,113,113	1.46	9 (11%)
17	BCR	bF	202	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
17	BCR	bL	203	-	41,41,41	1.23	3 (7%)	56,56,56	1.25	5 (8%)
17	BCR	dB	846	-	41,41,41	1.16	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
17	BCR	cI	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	7 (12%)
14	CLA	dB	812	2	45,53,73	1.71	8 (17%)	52,89,113	1.68	7 (13%)
14	CLA	bJ	101	-	45,53,73	1.76	7 (15%)	52,89,113	1.63	6 (11%)
14	CLA	dB	831	2	45,53,73	1.76	9 (20%)	52,89,113	1.59	6 (11%)
14	CLA	cA	828	1	65,73,73	1.42	7 (10%)	76,113,113	1.59	9 (11%)
14	CLA	cA	835	1	54,62,73	1.65	9 (16%)	62,99,113	1.54	8 (12%)
14	CLA	dB	805	2	54,62,73	1.56	7 (12%)	62,99,113	1.61	8 (12%)
14	CLA	cB	831	2	49,57,73	1.69	7 (14%)	55,93,113	1.70	9 (16%)
14	CLA	dA	840	1	65,73,73	1.46	10 (15%)	76,113,113	1.50	7 (9%)
14	CLA	dA	838	1	65,73,73	1.47	9 (13%)	76,113,113	1.52	9 (11%)
14	CLA	dB	803	-	65,73,73	1.44	9 (13%)	76,113,113	1.40	6 (7%)
14	CLA	aA	831	1	50,58,73	1.62	10 (20%)	58,95,113	1.66	8 (13%)
15	PQN	dB	843	-	34,34,34	1.52	2 (5%)	42,45,45	1.27	4 (9%)
14	CLA	bB	801	-	65,73,73	1.45	10 (15%)	76,113,113	1.42	7 (9%)
14	CLA	cA	821	14	65,73,73	1.44	10 (15%)	76,113,113	1.52	7 (9%)
14	CLA	dB	808	2	65,73,73	1.48	8 (12%)	76,113,113	1.50	9 (11%)
14	CLA	dB	807	2	65,73,73	1.44	8 (12%)	76,113,113	1.46	6 (7%)
17	BCR	bA	845	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	8 (14%)
17	BCR	dF	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	8 (14%)
14	CLA	bA	838	1	65,73,73	1.47	9 (13%)	76,113,113	1.51	9 (11%)
14	CLA	bB	820	-	65,73,73	1.42	8 (12%)	76,113,113	1.53	6 (7%)
16	SF4	aA	845	2,1	0,12,12	-	-	-	-	-
14	CLA	dL	204	10	52,60,73	1.66	9 (17%)	60,97,113	1.63	9 (15%)
14	CLA	dA	813	1	45,53,73	1.73	8 (17%)	52,89,113	1.68	11 (21%)
14	CLA	bB	842	2	65,73,73	1.47	10 (15%)	76,113,113	1.51	7 (9%)
17	BCR	aL	201	-	41,41,41	1.23	3 (7%)	56,56,56	1.26	5 (8%)
17	BCR	aA	846	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	11 (19%)
14	CLA	cJ	101	-	45,53,73	1.75	7 (15%)	52,89,113	1.64	6 (11%)
14	CLA	aA	802	-	45,53,73	1.68	8 (17%)	52,89,113	1.84	6 (11%)
14	CLA	dB	827	2	65,73,73	1.46	9 (13%)	76,113,113	1.44	8 (10%)
14	CLA	dB	821	2	47,55,73	1.67	8 (17%)	54,91,113	1.58	6 (11%)
14	CLA	aB	802	2	65,73,73	1.47	9 (13%)	76,113,113	1.35	5 (6%)
14	CLA	cA	819	1	65,73,73	1.44	9 (13%)	76,113,113	1.56	9 (11%)
14	CLA	dA	825	-	65,73,73	1.40	8 (12%)	76,113,113	1.56	10 (13%)
14	CLA	cB	802	2	65,73,73	1.46	9 (13%)	76,113,113	1.36	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	dA	836	1	45,53,73	1.72	7 (15%)	52,89,113	1.82	8 (15%)
14	CLA	bB	831	2	45,53,73	1.77	9 (20%)	52,89,113	1.60	6 (11%)
14	CLA	dB	820	-	65,73,73	1.43	8 (12%)	76,113,113	1.53	6 (7%)
14	CLA	cB	828	2	65,73,73	1.43	10 (15%)	76,113,113	1.46	8 (10%)
14	CLA	cX	101	12	45,53,73	1.76	8 (17%)	52,89,113	1.65	6 (11%)
17	BCR	aB	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	5 (8%)
14	CLA	bA	828	1	65,73,73	1.42	8 (12%)	76,113,113	1.59	10 (13%)
14	CLA	cA	833	1	65,73,73	1.44	8 (12%)	76,113,113	1.53	10 (13%)
14	CLA	aA	828	1	65,73,73	1.42	7 (10%)	76,113,113	1.59	9 (11%)
14	CLA	bA	831	1	50,58,73	1.63	10 (20%)	58,95,113	1.66	8 (13%)
14	CLA	cA	812	1	54,62,73	1.61	9 (16%)	62,99,113	1.56	6 (9%)
14	CLA	cA	822	1	49,57,73	1.65	9 (18%)	55,93,113	1.64	7 (12%)
14	CLA	dB	815	2	56,64,73	1.53	7 (12%)	65,102,113	1.54	6 (9%)
14	CLA	bB	807	2	65,73,73	1.44	8 (12%)	76,113,113	1.46	6 (7%)
14	CLA	bX	101	12	45,53,73	1.75	8 (17%)	52,89,113	1.64	6 (11%)
14	CLA	bL	201	2,10	65,73,73	1.45	10 (15%)	76,113,113	1.36	7 (9%)
17	BCR	cJ	104	-	41,41,41	1.14	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	aA	827	14,1	65,73,73	1.42	8 (12%)	76,113,113	1.53	8 (10%)
14	CLA	cA	820	1	61,69,73	1.51	8 (13%)	71,108,113	1.50	7 (9%)
14	CLA	cA	810	1	45,53,73	1.72	6 (13%)	52,89,113	1.66	6 (11%)
15	PQN	cA	844	-	34,34,34	1.52	2 (5%)	42,45,45	1.27	5 (11%)
18	LHG	cA	853	14	26,26,48	0.87	1 (3%)	29,32,54	1.31	3 (10%)
14	CLA	aA	826	-	55,63,73	1.57	8 (14%)	64,101,113	1.56	8 (12%)
14	CLA	bA	832	1	65,73,73	1.45	10 (15%)	76,113,113	1.49	10 (13%)
14	CLA	cA	806	1	65,73,73	1.46	10 (15%)	76,113,113	1.46	9 (11%)
17	BCR	bK	102	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	10 (17%)
14	CLA	aB	837	2	60,68,73	1.51	8 (13%)	70,107,113	1.48	9 (12%)
17	BCR	cA	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	3 (5%)
14	CLA	aB	841	2	65,73,73	1.46	10 (15%)	76,113,113	1.51	7 (9%)
14	CLA	dB	809	2	65,73,73	1.45	12 (18%)	76,113,113	1.60	9 (11%)
14	CLA	aA	823	1	51,59,73	1.65	8 (15%)	59,96,113	1.55	8 (13%)
14	CLA	cB	837	2	60,68,73	1.51	9 (15%)	70,107,113	1.48	9 (12%)
14	CLA	bB	828	2	65,73,73	1.41	7 (10%)	76,113,113	1.55	9 (11%)
14	CLA	bA	841	1	65,73,73	1.46	9 (13%)	76,113,113	1.44	7 (9%)
18	LHG	bA	850	-	48,48,48	0.65	1 (2%)	51,54,54	1.29	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	aB	819	-	65,73,73	1.42	8 (12%)	76,113,113	1.54	6 (7%)
14	CLA	cB	811	2	45,53,73	1.72	8 (17%)	52,89,113	1.67	7 (13%)
14	CLA	aK	101	9	42,49,73	1.74	6 (14%)	48,83,113	1.68	6 (12%)
17	BCR	bL	207	-	41,41,41	1.18	3 (7%)	56,56,56	1.42	7 (12%)
17	BCR	bI	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	7 (12%)
14	CLA	aB	812	2	45,53,73	1.76	9 (20%)	52,89,113	1.63	7 (13%)
17	BCR	cM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	6 (10%)
14	CLA	aB	822	-	55,63,73	1.57	8 (14%)	64,101,113	1.61	6 (9%)
14	CLA	cB	812	2	45,53,73	1.76	9 (20%)	52,89,113	1.64	7 (13%)
14	CLA	bB	812	2	45,53,73	1.71	8 (17%)	52,89,113	1.68	7 (13%)
14	CLA	dA	804	14,1	45,53,73	1.80	8 (17%)	52,89,113	1.78	8 (15%)
14	CLA	dA	809	1	45,53,73	1.73	8 (17%)	52,89,113	1.73	8 (15%)
14	CLA	bB	823	-	55,63,73	1.56	9 (16%)	64,101,113	1.60	6 (9%)
14	CLA	cB	803	-	65,73,73	1.44	8 (12%)	76,113,113	1.41	6 (7%)
14	CLA	cB	824	2	54,62,73	1.65	10 (18%)	62,99,113	1.45	8 (12%)
14	CLA	aL	203	10	65,73,73	1.45	10 (15%)	76,113,113	1.54	9 (11%)
14	CLA	bA	812	1	54,62,73	1.61	8 (14%)	62,99,113	1.56	6 (9%)
14	CLA	bB	837	-	45,53,73	1.81	8 (17%)	52,89,113	1.57	7 (13%)
14	CLA	cA	834	1	65,73,73	1.45	9 (13%)	76,113,113	1.44	7 (9%)
17	BCR	dA	845	-	41,41,41	1.14	3 (7%)	56,56,56	1.29	8 (14%)
14	CLA	bA	823	1	51,59,73	1.66	8 (15%)	59,96,113	1.54	8 (13%)
14	CLA	bB	803	-	65,73,73	1.43	9 (13%)	76,113,113	1.41	6 (7%)
16	SF4	bA	844	2,1	0,12,12	-	-	-	-	-
17	BCR	cF	202	-	41,41,41	1.16	2 (4%)	56,56,56	1.30	5 (8%)
15	PQN	bB	843	-	34,34,34	1.53	2 (5%)	42,45,45	1.20	4 (9%)
17	BCR	cL	205	-	41,41,41	1.18	2 (4%)	56,56,56	1.37	9 (16%)
14	CLA	cB	819	-	65,73,73	1.42	8 (12%)	76,113,113	1.53	6 (7%)
14	CLA	bA	837	1	51,59,73	1.57	8 (15%)	59,96,113	1.70	8 (13%)
14	CLA	dA	822	1	49,57,73	1.65	9 (18%)	55,93,113	1.63	7 (12%)
14	CLA	dB	804	-	65,73,73	1.39	9 (13%)	76,113,113	1.80	12 (15%)
14	CLA	bA	803	1	45,53,73	1.75	8 (17%)	52,89,113	1.70	9 (17%)
13	CL0	dA	801	1	65,73,73	2.03	17 (26%)	76,113,113	2.79	28 (36%)
14	CLA	aA	819	1	65,73,73	1.44	9 (13%)	76,113,113	1.55	9 (11%)
18	LHG	dB	851	-	22,22,48	0.90	1 (4%)	25,28,54	1.20	1 (4%)
14	CLA	dA	817	1	54,62,73	1.60	8 (14%)	62,99,113	1.54	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PQN	bA	843	-	34,34,34	1.51	2 (5%)	42,45,45	1.27	6 (14%)
14	CLA	aA	835	1	54,62,73	1.66	9 (16%)	62,99,113	1.55	8 (12%)
14	CLA	bA	815	1	45,53,73	1.77	8 (17%)	52,89,113	1.71	6 (11%)
14	CLA	dB	834	2	58,66,73	1.55	8 (13%)	67,104,113	1.48	9 (13%)
16	SF4	dC	102	3	0,12,12	-	-	-	-	-
14	CLA	dL	205	10	65,73,73	1.43	9 (13%)	76,113,113	1.55	9 (11%)
14	CLA	cB	809	2	65,73,73	1.46	12 (18%)	76,113,113	1.60	9 (11%)
14	CLA	cA	811	14,1	65,73,73	1.47	9 (13%)	76,113,113	1.41	8 (10%)
17	BCR	cA	850	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	5 (8%)
14	CLA	dB	816	2	45,53,73	1.73	7 (15%)	52,89,113	1.74	7 (13%)
17	BCR	aB	848	-	41,41,41	1.22	2 (4%)	56,56,56	1.16	4 (7%)
14	CLA	cA	832	1	65,73,73	1.45	10 (15%)	76,113,113	1.48	10 (13%)
14	CLA	aA	821	14	65,73,73	1.44	10 (15%)	76,113,113	1.52	7 (9%)
14	CLA	bA	833	1	65,73,73	1.44	9 (13%)	76,113,113	1.53	10 (13%)
14	CLA	aA	817	1	54,62,73	1.60	8 (14%)	62,99,113	1.54	8 (12%)
14	CLA	cA	817	1	54,62,73	1.61	8 (14%)	62,99,113	1.54	8 (12%)
14	CLA	bF	203	-	45,53,73	1.72	8 (17%)	52,89,113	1.68	7 (13%)
14	CLA	aB	832	2	65,73,73	1.53	8 (12%)	76,113,113	1.41	8 (10%)
14	CLA	dK	103	-	45,53,73	1.73	8 (17%)	52,89,113	1.66	6 (11%)
18	LHG	dA	851	14	26,26,48	0.87	1 (3%)	29,32,54	1.31	3 (10%)
17	BCR	aA	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	8 (14%)
14	CLA	bB	829	2	65,73,73	1.43	10 (15%)	76,113,113	1.46	8 (10%)
14	CLA	dB	836	-	45,53,73	1.81	8 (17%)	52,89,113	1.72	9 (17%)
14	CLA	bA	824	1	47,55,73	1.70	7 (14%)	54,91,113	1.65	8 (14%)
16	SF4	cC	102	3	0,12,12	-	-	-	-	-
14	CLA	cA	841	1	65,73,73	1.47	9 (13%)	76,113,113	1.44	7 (9%)
14	CLA	aA	810	1	45,53,73	1.70	6 (13%)	52,89,113	1.65	6 (11%)
14	CLA	aB	823	2	45,53,73	1.77	8 (17%)	52,89,113	1.57	8 (15%)
14	CLA	cB	826	2	65,73,73	1.46	9 (13%)	76,113,113	1.44	8 (10%)
14	CLA	dA	803	1	45,53,73	1.75	8 (17%)	52,89,113	1.69	9 (17%)
14	CLA	bB	819	2	60,68,73	1.53	10 (16%)	70,107,113	1.48	7 (10%)
14	CLA	dB	818	2	59,67,73	1.54	9 (15%)	68,105,113	1.54	9 (13%)
14	CLA	dB	824	2	45,53,73	1.77	8 (17%)	52,89,113	1.58	8 (15%)
14	CLA	bL	206	-	65,73,73	1.46	10 (15%)	76,113,113	1.37	7 (9%)
17	BCR	cB	844	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	bB	840	2	47,55,73	1.65	7 (14%)	54,91,113	1.74	8 (14%)
14	CLA	bK	103	-	45,53,73	1.72	8 (17%)	52,89,113	1.66	6 (11%)
19	LMG	cB	849	-	55,55,55	0.79	2 (3%)	63,63,63	1.46	9 (14%)
14	CLA	cB	835	-	45,53,73	1.79	8 (17%)	52,89,113	1.71	8 (15%)
14	CLA	aB	803	-	65,73,73	1.43	8 (12%)	76,113,113	1.40	6 (7%)
14	CLA	bA	819	1	65,73,73	1.44	9 (13%)	76,113,113	1.55	9 (11%)
14	CLA	dA	839	1	65,73,73	1.48	8 (12%)	76,113,113	1.49	8 (10%)
14	CLA	cA	831	1	50,58,73	1.63	10 (20%)	58,95,113	1.66	8 (13%)
14	CLA	cA	809	1	45,53,73	1.71	8 (17%)	52,89,113	1.72	8 (15%)
14	CLA	aL	204	-	52,60,73	1.61	8 (15%)	60,97,113	1.56	9 (15%)
14	CLA	bA	821	14	65,73,73	1.44	10 (15%)	76,113,113	1.52	7 (9%)
14	CLA	aA	811	14,1	65,73,73	1.48	9 (13%)	76,113,113	1.41	8 (10%)
14	CLA	aB	833	2	58,66,73	1.56	8 (13%)	67,104,113	1.49	10 (14%)
17	BCR	dL	207	-	41,41,41	1.17	3 (7%)	56,56,56	1.43	7 (12%)
16	SF4	aC	102	3	0,12,12	-	-	-	-	-
14	CLA	cB	822	-	55,63,73	1.55	8 (14%)	64,101,113	1.60	6 (9%)
15	PQN	aA	844	-	34,34,34	1.52	2 (5%)	42,45,45	1.26	5 (11%)
14	CLA	aA	808	1	45,53,73	1.73	9 (20%)	52,89,113	1.66	8 (15%)
14	CLA	aB	830	2	45,53,73	1.77	9 (20%)	52,89,113	1.59	6 (11%)
17	BCR	dF	202	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	5 (8%)
18	LHG	cB	850	-	22,22,48	0.89	1 (4%)	25,28,54	1.20	1 (4%)
14	CLA	cA	807	1	51,59,73	1.64	7 (13%)	59,96,113	1.62	6 (10%)
14	CLA	bB	826	-	46,54,73	1.66	9 (19%)	53,90,113	1.70	8 (15%)
14	CLA	aF	201	-	51,59,73	1.64	7 (13%)	59,96,113	1.61	7 (11%)
14	CLA	cA	805	1	45,53,73	1.83	10 (22%)	52,89,113	1.72	9 (17%)
17	BCR	aA	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	3 (5%)
14	CLA	bA	820	1	61,69,73	1.52	9 (14%)	71,108,113	1.50	8 (11%)
14	CLA	bA	810	1	45,53,73	1.71	6 (13%)	52,89,113	1.66	6 (11%)
14	CLA	aB	806	2	65,73,73	1.39	8 (12%)	76,113,113	1.57	8 (10%)
14	CLA	cB	829	2	65,73,73	1.46	10 (15%)	76,113,113	1.69	9 (11%)
14	CLA	aB	807	2	65,73,73	1.45	8 (12%)	76,113,113	1.47	6 (7%)
14	CLA	cB	833	2	58,66,73	1.54	8 (13%)	67,104,113	1.48	10 (14%)
14	CLA	cB	825	-	46,54,73	1.66	10 (21%)	53,90,113	1.69	8 (15%)
17	BCR	aI	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	7 (12%)
14	CLA	aB	805	2	54,62,73	1.57	7 (12%)	62,99,113	1.61	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	dF	201	-	51,59,73	1.65	7 (13%)	59,96,113	1.62	8 (13%)
14	CLA	aB	840	-	65,73,73	1.47	10 (15%)	76,113,113	1.33	7 (9%)
14	CLA	bB	811	2	65,73,73	1.46	10 (15%)	76,113,113	1.37	7 (9%)
18	LHG	aB	850	-	22,22,48	0.89	1 (4%)	25,28,54	1.20	1 (4%)
14	CLA	dA	831	1	50,58,73	1.62	10 (20%)	58,95,113	1.66	8 (13%)
17	BCR	aL	206	-	41,41,41	1.08	1 (2%)	56,56,56	1.32	7 (12%)
17	BCR	cA	848	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	8 (14%)
14	CLA	aA	807	1	51,59,73	1.65	8 (15%)	59,96,113	1.61	6 (10%)
17	BCR	aA	850	-	41,41,41	1.20	2 (4%)	56,56,56	1.21	5 (8%)
14	CLA	dA	820	1	61,69,73	1.52	9 (14%)	71,108,113	1.49	7 (9%)
17	BCR	bB	847	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	4 (7%)
14	CLA	aJ	102	-	38,45,73	1.85	7 (18%)	43,78,113	1.70	7 (16%)
14	CLA	aB	831	2	49,57,73	1.69	7 (14%)	55,93,113	1.70	9 (16%)
14	CLA	cB	806	2	65,73,73	1.38	8 (12%)	76,113,113	1.58	8 (10%)
14	CLA	aB	814	2	56,64,73	1.54	7 (12%)	65,102,113	1.53	6 (9%)
14	CLA	dJ	102	-	38,45,73	1.85	8 (21%)	43,78,113	1.70	7 (16%)
14	CLA	aA	832	1	65,73,73	1.44	10 (15%)	76,113,113	1.49	10 (13%)
17	BCR	bA	846	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	8 (14%)
14	CLA	aL	202	10	65,73,73	1.47	7 (10%)	76,113,113	1.38	9 (11%)
14	CLA	bB	830	2	65,73,73	1.47	10 (15%)	76,113,113	1.69	9 (11%)
16	SF4	dC	101	3	0,12,12	-	-	-	-	-
14	CLA	cB	808	2	65,73,73	1.48	7 (10%)	76,113,113	1.49	9 (11%)
14	CLA	dB	822	2	45,53,73	1.72	9 (20%)	52,89,113	1.67	7 (13%)
17	BCR	bA	849	-	41,41,41	1.16	2 (4%)	56,56,56	1.24	6 (10%)
14	CLA	cB	804	-	65,73,73	1.39	9 (13%)	76,113,113	1.80	12 (15%)
14	CLA	aA	834	1	65,73,73	1.46	8 (12%)	76,113,113	1.43	7 (9%)
14	CLA	dB	813	2	45,53,73	1.76	9 (20%)	52,89,113	1.63	7 (13%)
14	CLA	bA	807	1	51,59,73	1.63	7 (13%)	59,96,113	1.61	6 (10%)
14	CLA	aF	203	-	45,53,73	1.72	8 (17%)	52,89,113	1.65	6 (11%)
14	CLA	aA	837	1	51,59,73	1.57	8 (15%)	59,96,113	1.70	8 (13%)
14	CLA	dA	819	1	65,73,73	1.44	9 (13%)	76,113,113	1.56	9 (11%)
14	CLA	cA	825	-	65,73,73	1.39	8 (12%)	76,113,113	1.55	10 (13%)
14	CLA	dA	821	14	65,73,73	1.44	10 (15%)	76,113,113	1.52	7 (9%)
14	CLA	cK	102	-	45,53,73	1.73	7 (15%)	52,89,113	1.66	6 (11%)
14	CLA	cA	816	-	49,57,73	1.69	6 (12%)	55,93,113	1.65	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	bA	835	1	54,62,73	1.65	10 (18%)	62,99,113	1.54	8 (12%)
14	CLA	dA	828	1	65,73,73	1.42	8 (12%)	76,113,113	1.60	10 (13%)
14	CLA	cB	836	-	45,53,73	1.82	9 (20%)	52,89,113	1.57	7 (13%)
14	CLA	bA	842	-	65,73,73	1.49	10 (15%)	76,113,113	1.46	7 (9%)
14	CLA	dF	203	-	45,53,73	1.71	8 (17%)	52,89,113	1.68	7 (13%)
14	CLA	cB	832	2	65,73,73	1.53	8 (12%)	76,113,113	1.42	8 (10%)

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
14	CLA	aB	815	2	1/1/11/20	5/13/91/115	-
17	BCR	cF	204	-	-	14/29/63/63	0/2/2/2
17	BCR	bB	852	-	-	8/29/63/63	0/2/2/2
14	CLA	aB	813	2	1/1/15/20	13/37/115/115	-
17	BCR	dA	846	-	-	8/29/63/63	0/2/2/2
14	CLA	dB	842	2	1/1/15/20	20/37/115/115	-
14	CLA	aB	811	2	1/1/11/20	4/13/91/115	-
14	CLA	dA	827	14,1	1/1/15/20	12/37/115/115	-
14	CLA	aA	812	1	1/1/12/20	11/24/102/115	-
14	CLA	aA	809	1	1/1/11/20	5/13/91/115	-
14	CLA	bA	818	1	1/1/12/20	7/24/102/115	-
14	CLA	cJ	102	-	1/1/8/20	0/2/76/115	-
14	CLA	aB	818	2	1/1/14/20	8/31/109/115	-
14	CLA	aA	805	1	1/1/11/20	5/13/91/115	-
14	CLA	aB	834	2	1/1/11/20	4/13/91/115	-
14	CLA	aA	803	1	1/1/11/20	6/13/91/115	-
14	CLA	bA	834	1	1/1/15/20	9/37/115/115	-
14	CLA	aA	841	1	1/1/15/20	12/37/115/115	-
14	CLA	dB	829	2	1/1/15/20	9/37/115/115	-
14	CLA	aJ	101	-	1/1/11/20	10/13/91/115	-
17	BCR	aF	202	-	-	11/29/63/63	0/2/2/2
17	BCR	cJ	103	-	-	15/29/63/63	0/2/2/2
17	BCR	bB	844	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bB	836	-	1/1/11/20	2/13/91/115	-
17	BCR	dL	203	-	-	13/29/63/63	0/2/2/2
14	CLA	cA	840	1	1/1/15/20	12/37/115/115	-
14	CLA	bB	832	2	1/1/11/20	11/18/96/115	-
14	CLA	dB	802	2	1/1/15/20	12/37/115/115	-
14	CLA	bA	836	1	1/1/11/20	7/13/91/115	-
14	CLA	bB	809	2	1/1/15/20	9/37/115/115	-
14	CLA	aB	838	2	1/1/15/20	8/37/115/115	-
14	CLA	dB	835	2	1/1/11/20	4/13/91/115	-
17	BCR	cB	846	-	-	17/29/63/63	0/2/2/2
14	CLA	aB	804	-	1/1/15/20	13/37/115/115	-
14	CLA	aB	809	2	1/1/15/20	9/37/115/115	-
14	CLA	bA	809	1	1/1/11/20	5/13/91/115	-
14	CLA	bB	841	-	1/1/15/20	3/37/115/115	-
14	CLA	bL	202	18,10	1/1/12/20	13/22/100/115	-
14	CLA	dB	840	2	-	1/16/94/115	-
17	BCR	dB	848	-	-	10/29/63/63	0/2/2/2
17	BCR	dA	849	-	-	20/29/63/63	0/2/2/2
16	SF4	aC	101	3	-	-	0/6/5/5
14	CLA	cB	807	2	1/1/15/20	20/37/115/115	-
14	CLA	dB	832	2	1/1/11/20	11/18/96/115	-
14	CLA	cB	815	2	1/1/11/20	5/13/91/115	-
14	CLA	cA	808	1	1/1/11/20	4/13/91/115	-
14	CLA	aB	820	2	1/1/11/20	8/16/94/115	-
14	CLA	aA	815	1	1/1/11/20	4/13/91/115	-
14	CLA	bF	201	-	1/1/12/20	5/21/99/115	-
14	CLA	bA	805	1	1/1/11/20	5/13/91/115	-
14	CLA	cA	815	1	1/1/11/20	4/13/91/115	-
14	CLA	dX	101	12	1/1/11/20	7/13/91/115	-
18	LHG	bA	851	14	-	10/31/31/53	-
14	CLA	dA	835	1	1/1/12/20	5/24/102/115	-
14	CLA	bK	101	9	1/1/9/20	3/7/81/115	-
14	CLA	cA	839	1	1/1/15/20	10/37/115/115	-
14	CLA	aA	833	1	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	bF	204	-	-	13/29/63/63	0/2/2/2
14	CLA	aA	814	1	1/1/11/20	5/13/91/115	-
17	BCR	aB	851	-	-	8/29/63/63	0/2/2/2
14	CLA	aA	818	1	1/1/12/20	7/24/102/115	-
14	CLA	cB	820	2	1/1/11/20	8/16/94/115	-
17	BCR	dK	102	-	-	6/29/63/63	0/2/2/2
14	CLA	cA	813	1	-	6/13/91/115	-
17	BCR	aA	848	-	-	8/29/63/63	0/2/2/2
17	BCR	cL	201	-	-	13/29/63/63	0/2/2/2
19	LMG	bB	850	-	-	23/50/70/70	0/1/1/1
18	LHG	aA	853	14	-	10/31/31/53	-
14	CLA	cA	829	1	1/1/15/20	14/37/115/115	-
14	CLA	dK	101	9	1/1/9/20	3/7/81/115	-
14	CLA	bB	804	-	1/1/15/20	13/37/115/115	-
14	CLA	bB	815	2	1/1/13/20	2/27/105/115	-
17	BCR	cA	847	-	-	7/29/63/63	0/2/2/2
14	CLA	cL	202	10	1/1/15/20	10/37/115/115	-
14	CLA	cB	823	2	1/1/11/20	6/13/91/115	-
14	CLA	dB	810	2	1/1/15/20	9/37/115/115	-
14	CLA	dB	830	2	1/1/15/20	13/37/115/115	-
14	CLA	dJ	101	-	1/1/11/20	10/13/91/115	-
17	BCR	bM	101	-	-	9/29/63/63	0/2/2/2
17	BCR	bJ	103	-	-	15/29/63/63	0/2/2/2
14	CLA	bA	829	1	1/1/15/20	14/37/115/115	-
17	BCR	dJ	103	-	-	15/29/63/63	0/2/2/2
16	SF4	bC	101	3	-	-	0/6/5/5
17	BCR	aL	205	-	-	9/29/63/63	0/2/2/2
14	CLA	aA	838	1	1/1/15/20	14/37/115/115	-
17	BCR	bL	208	-	-	15/29/63/63	0/2/2/2
14	CLA	cA	838	1	1/1/15/20	14/37/115/115	-
14	CLA	bA	816	-	-	8/18/96/115	-
14	CLA	dB	837	-	-	6/13/91/115	-
17	BCR	bB	848	-	-	10/29/63/63	0/2/2/2
14	CLA	aB	816	2	1/1/13/20	8/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SF4	dA	844	2,1	-	-	0/6/5/5
14	CLA	bA	840	1	1/1/15/20	12/37/115/115	-
14	CLA	dA	811	14,1	1/1/15/20	11/37/115/115	-
17	BCR	bA	848	-	-	9/29/63/63	0/2/2/2
14	CLA	cB	810	2	1/1/15/20	9/37/115/115	-
15	PQN	cB	842	-	-	9/23/43/43	0/2/2/2
17	BCR	dB	852	-	-	8/29/63/63	0/2/2/2
14	CLA	dA	810	1	1/1/11/20	5/13/91/115	-
15	PQN	aB	842	-	-	9/23/43/43	0/2/2/2
14	CLA	aX	101	12	1/1/11/20	7/13/91/115	-
17	BCR	aB	847	-	-	9/29/63/63	0/2/2/2
14	CLA	cA	826	-	1/1/13/20	5/25/103/115	-
17	BCR	cA	846	-	-	6/29/63/63	0/2/2/2
14	CLA	aA	824	1	1/1/11/20	5/16/94/115	-
14	CLA	cB	816	2	1/1/13/20	8/25/103/115	-
17	BCR	aB	843	-	-	10/29/63/63	0/2/2/2
17	BCR	aM	101	-	-	9/29/63/63	0/2/2/2
14	CLA	bB	808	2	1/1/15/20	8/37/115/115	-
14	CLA	aK	102	-	1/1/11/20	3/13/91/115	-
14	CLA	aA	806	1	1/1/15/20	10/37/115/115	-
14	CLA	bB	816	2	1/1/11/20	5/13/91/115	-
14	CLA	dA	842	-	1/1/15/20	12/37/115/115	-
14	CLA	cA	843	18	1/1/12/20	13/22/100/115	-
14	CLA	dB	826	-	1/1/11/20	6/15/93/115	-
19	LMG	aB	849	-	-	23/50/70/70	0/1/1/1
17	BCR	dB	844	-	-	10/29/63/63	0/2/2/2
14	CLA	aA	836	1	1/1/11/20	7/13/91/115	-
14	CLA	bB	833	2	1/1/15/20	15/37/115/115	-
17	BCR	cB	851	-	-	8/29/63/63	0/2/2/2
14	CLA	cA	836	1	1/1/11/20	7/13/91/115	-
13	CL0	cA	801	1	3/3/20/25	20/37/135/135	-
14	CLA	dA	807	1	1/1/12/20	2/21/99/115	-
17	BCR	cA	851	-	-	20/29/63/63	0/2/2/2
14	CLA	dB	828	2	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bB	824	2	1/1/11/20	6/13/91/115	-
14	CLA	cL	203	10	1/1/15/20	12/37/115/115	-
14	CLA	cA	827	14,1	1/1/15/20	12/37/115/115	-
14	CLA	cA	830	1	1/1/15/20	12/37/115/115	-
14	CLA	bB	806	2	1/1/15/20	15/37/115/115	-
14	CLA	aA	813	1	-	6/13/91/115	-
14	CLA	aB	824	2	-	6/24/102/115	-
17	BCR	aF	204	-	-	14/29/63/63	0/2/2/2
14	CLA	dB	811	2	1/1/15/20	6/37/115/115	-
17	BCR	dJ	104	-	-	9/29/63/63	0/2/2/2
14	CLA	cA	842	-	1/1/15/20	12/37/115/115	-
18	LHG	dA	850	-	-	18/53/53/53	-
14	CLA	dA	808	1	1/1/11/20	4/13/91/115	-
14	CLA	dA	802	-	1/1/11/20	3/13/91/115	-
14	CLA	bA	802	-	1/1/11/20	3/13/91/115	-
14	CLA	aA	825	-	1/1/15/20	13/37/115/115	-
17	BCR	aJ	103	-	-	15/29/63/63	0/2/2/2
14	CLA	bB	838	2	1/1/14/20	8/31/109/115	-
14	CLA	aB	808	2	1/1/15/20	8/37/115/115	-
14	CLA	bL	204	10	1/1/12/20	8/22/100/115	-
14	CLA	bA	806	1	1/1/15/20	10/37/115/115	-
14	CLA	aB	828	2	1/1/15/20	9/37/115/115	-
14	CLA	cB	821	2	1/1/11/20	5/13/91/115	-
14	CLA	dB	841	-	1/1/15/20	2/37/115/115	-
14	CLA	dA	834	1	1/1/15/20	9/37/115/115	-
14	CLA	cB	818	2	1/1/14/20	8/31/109/115	-
14	CLA	dA	832	1	1/1/15/20	11/37/115/115	-
14	CLA	bB	813	2	1/1/11/20	6/13/91/115	-
14	CLA	cB	841	2	1/1/15/20	20/37/115/115	-
14	CLA	cB	814	2	1/1/13/20	2/27/105/115	-
14	CLA	cB	813	2	1/1/15/20	13/37/115/115	-
14	CLA	dB	819	2	1/1/14/20	8/31/109/115	-
18	LHG	cA	852	-	-	18/53/53/53	-
14	CLA	aB	836	-	-	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	bB	846	-	-	12/29/63/63	0/2/2/2
14	CLA	aA	829	1	1/1/15/20	14/37/115/115	-
14	CLA	dA	837	1	1/1/12/20	7/21/99/115	-
14	CLA	dB	838	2	1/1/14/20	8/31/109/115	-
14	CLA	bB	802	2	1/1/15/20	12/37/115/115	-
14	CLA	aA	804	14,1	1/1/11/20	4/13/91/115	-
14	CLA	bA	814	1	1/1/11/20	5/13/91/115	-
14	CLA	dA	841	1	1/1/15/20	12/37/115/115	-
15	PQN	dA	843	-	-	5/23/43/43	0/2/2/2
14	CLA	cA	804	14,1	1/1/11/20	4/13/91/115	-
17	BCR	bA	847	-	-	18/29/63/63	0/2/2/2
14	CLA	dB	817	2	1/1/13/20	8/25/103/115	-
14	CLA	bA	813	1	-	6/13/91/115	-
14	CLA	cB	834	2	1/1/11/20	4/13/91/115	-
14	CLA	dB	823	-	1/1/13/20	12/25/103/115	-
14	CLA	bB	821	2	1/1/11/20	8/16/94/115	-
14	CLA	bB	818	2	1/1/13/20	9/30/108/115	-
14	CLA	bA	825	-	1/1/15/20	13/37/115/115	-
14	CLA	cL	204	-	1/1/12/20	7/22/100/115	-
14	CLA	dA	812	1	1/1/12/20	11/24/102/115	-
17	BCR	aB	845	-	-	12/29/63/63	0/2/2/2
14	CLA	dB	806	2	1/1/15/20	15/37/115/115	-
14	CLA	bB	814	2	1/1/15/20	13/37/115/115	-
17	BCR	dB	849	-	-	7/29/63/63	0/2/2/2
14	CLA	dA	805	1	1/1/11/20	5/13/91/115	-
14	CLA	bB	827	2	1/1/15/20	20/37/115/115	-
14	CLA	bJ	102	-	1/1/8/20	0/2/76/115	-
14	CLA	dB	839	2	1/1/15/20	8/37/115/115	-
17	BCR	dB	845	-	-	9/29/63/63	0/2/2/2
17	BCR	aA	851	-	-	20/29/63/63	0/2/2/2
14	CLA	dA	829	1	1/1/15/20	14/37/115/115	-
14	CLA	cA	802	-	1/1/11/20	3/13/91/115	-
17	BCR	cB	847	-	-	9/29/63/63	0/2/2/2
17	BCR	cB	845	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bA	827	14,1	1/1/15/20	12/37/115/115	-
14	CLA	aB	826	2	1/1/15/20	20/37/115/115	-
14	CLA	bB	834	2	1/1/13/20	11/29/107/115	-
14	CLA	aB	829	2	1/1/15/20	13/37/115/115	-
14	CLA	bA	826	-	1/1/13/20	5/25/103/115	-
14	CLA	dA	815	1	1/1/11/20	4/13/91/115	-
17	BCR	bJ	104	-	-	9/29/63/63	0/2/2/2
14	CLA	aB	825	-	1/1/11/20	6/15/93/115	-
14	CLA	bB	805	2	1/1/12/20	7/24/102/115	-
14	CLA	dL	202	18,10	1/1/12/20	13/22/100/115	-
16	SF4	bC	102	3	-	-	0/6/5/5
14	CLA	aA	843	18	1/1/12/20	13/22/100/115	-
14	CLA	aA	822	1	1/1/11/20	11/18/96/115	-
14	CLA	aB	835	-	1/1/11/20	2/13/91/115	-
14	CLA	bA	804	14,1	1/1/11/20	4/13/91/115	-
14	CLA	aA	816	-	-	8/18/96/115	-
17	BCR	cL	206	-	-	11/29/63/63	0/2/2/2
13	CL0	aA	801	1	3/3/20/25	17/37/135/135	-
17	BCR	dI	101	-	-	14/29/63/63	0/2/2/2
16	SF4	cC	101	3	-	-	0/6/5/5
14	CLA	dA	814	1	1/1/11/20	5/13/91/115	-
16	SF4	cA	845	2,1	-	-	0/6/5/5
14	CLA	dA	818	1	1/1/12/20	7/24/102/115	-
14	CLA	aB	821	2	1/1/11/20	5/13/91/115	-
14	CLA	bB	810	2	1/1/15/20	9/37/115/115	-
14	CLA	aA	839	1	1/1/15/20	10/37/115/115	-
17	BCR	dA	848	-	-	9/29/63/63	0/2/2/2
14	CLA	dL	206	-	1/1/15/20	20/37/115/115	-
14	CLA	dB	833	2	1/1/15/20	15/37/115/115	-
17	BCR	bB	849	-	-	7/29/63/63	0/2/2/2
14	CLA	dB	825	2	-	6/24/102/115	-
14	CLA	cA	837	1	1/1/12/20	7/21/99/115	-
14	CLA	dL	201	2,10	1/1/15/20	6/37/115/115	-
14	CLA	bA	822	1	1/1/11/20	11/18/96/115	-
14	CLA	cK	101	9	1/1/9/20	3/7/81/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	bB	845	-	-	9/29/63/63	0/2/2/2
14	CLA	dA	826	-	1/1/13/20	5/25/103/115	-
18	LHG	bB	851	-	-	11/26/26/53	-
14	CLA	aA	830	1	1/1/15/20	12/37/115/115	-
14	CLA	bA	817	1	1/1/12/20	9/24/102/115	-
14	CLA	cA	814	1	1/1/11/20	5/13/91/115	-
14	CLA	cA	818	1	1/1/12/20	7/24/102/115	-
17	BCR	aB	846	-	-	17/29/63/63	0/2/2/2
14	CLA	bB	825	2	-	6/24/102/115	-
14	CLA	bL	205	10	1/1/15/20	10/37/115/115	-
14	CLA	aB	827	2	1/1/15/20	13/37/115/115	-
14	CLA	aA	842	-	1/1/15/20	12/37/115/115	-
14	CLA	dB	814	2	1/1/15/20	13/37/115/115	-
14	CLA	dA	823	1	1/1/12/20	12/21/99/115	-
14	CLA	bB	822	2	1/1/11/20	5/13/91/115	-
17	BCR	dL	208	-	-	15/29/63/63	0/2/2/2
17	BCR	dB	847	-	-	17/29/63/63	0/2/2/2
14	CLA	cB	805	2	1/1/12/20	7/24/102/115	-
14	CLA	aB	817	2	1/1/13/20	9/30/108/115	-
14	CLA	cB	839	2	-	1/16/94/115	-
17	BCR	cB	848	-	-	7/29/63/63	0/2/2/2
14	CLA	bA	808	1	1/1/11/20	4/13/91/115	-
14	CLA	bB	839	2	1/1/15/20	8/37/115/115	-
14	CLA	dA	816	-	-	8/18/96/115	-
14	CLA	aA	840	1	1/1/15/20	12/37/115/115	-
14	CLA	bB	835	2	1/1/11/20	4/13/91/115	-
14	CLA	bA	811	14,1	1/1/15/20	11/37/115/115	-
14	CLA	cB	827	2	1/1/15/20	13/37/115/115	-
14	CLA	cB	830	2	1/1/11/20	6/13/91/115	-
17	BCR	cB	843	-	-	10/29/63/63	0/2/2/2
17	BCR	dM	101	-	-	9/29/63/63	0/2/2/2
14	CLA	dB	801	-	1/1/15/20	14/37/115/115	-
14	CLA	bA	839	1	1/1/15/20	10/37/115/115	-
19	LMG	dB	850	-	-	23/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	aA	852	-	-	18/53/53/53	-
14	CLA	cB	838	2	1/1/15/20	8/37/115/115	-
13	CL0	bA	801	1	2/2/20/25	12/37/135/135	-
14	CLA	cB	817	2	1/1/13/20	9/30/108/115	-
17	BCR	dA	847	-	-	18/29/63/63	0/2/2/2
14	CLA	cB	801	-	1/1/15/20	14/37/115/115	-
14	CLA	cF	201	-	1/1/12/20	5/21/99/115	-
14	CLA	dA	833	1	1/1/15/20	9/37/115/115	-
14	CLA	bB	817	2	1/1/13/20	8/25/103/115	-
17	BCR	aJ	104	-	-	9/29/63/63	0/2/2/2
14	CLA	aB	801	-	1/1/15/20	14/37/115/115	-
14	CLA	cA	824	1	1/1/11/20	5/16/94/115	-
14	CLA	aB	810	2	1/1/15/20	9/37/115/115	-
14	CLA	cA	823	1	1/1/12/20	12/21/99/115	-
14	CLA	dA	830	1	1/1/15/20	12/37/115/115	-
14	CLA	bA	830	1	1/1/15/20	12/37/115/115	-
14	CLA	aB	839	2	-	1/16/94/115	-
14	CLA	dA	824	1	1/1/11/20	5/16/94/115	-
14	CLA	aA	820	1	1/1/14/20	11/33/111/115	-
14	CLA	cB	840	-	1/1/15/20	3/37/115/115	-
14	CLA	cA	803	1	1/1/11/20	6/13/91/115	-
14	CLA	cF	203	-	1/1/11/20	4/13/91/115	-
14	CLA	dA	806	1	1/1/15/20	10/37/115/115	-
17	BCR	bF	202	-	-	11/29/63/63	0/2/2/2
17	BCR	bL	203	-	-	13/29/63/63	0/2/2/2
17	BCR	dB	846	-	-	12/29/63/63	0/2/2/2
17	BCR	cI	101	-	-	14/29/63/63	0/2/2/2
14	CLA	dB	812	2	1/1/11/20	4/13/91/115	-
14	CLA	bJ	101	-	1/1/11/20	10/13/91/115	-
14	CLA	dB	831	2	1/1/11/20	6/13/91/115	-
14	CLA	cA	828	1	1/1/15/20	6/37/115/115	-
14	CLA	cA	835	1	1/1/12/20	5/24/102/115	-
14	CLA	dB	805	2	1/1/12/20	7/24/102/115	-
14	CLA	cB	831	2	1/1/11/20	11/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	dA	840	1	1/1/15/20	12/37/115/115	-
14	CLA	dA	838	1	1/1/15/20	14/37/115/115	-
14	CLA	dB	803	-	1/1/15/20	18/37/115/115	-
14	CLA	aA	831	1	1/1/12/20	2/19/97/115	-
15	PQN	dB	843	-	-	5/23/43/43	0/2/2/2
14	CLA	bB	801	-	1/1/15/20	14/37/115/115	-
14	CLA	cA	821	14	1/1/15/20	14/37/115/115	-
14	CLA	dB	808	2	1/1/15/20	8/37/115/115	-
14	CLA	dB	807	2	1/1/15/20	20/37/115/115	-
17	BCR	bA	845	-	-	7/29/63/63	0/2/2/2
17	BCR	dF	204	-	-	13/29/63/63	0/2/2/2
14	CLA	bA	838	1	1/1/15/20	14/37/115/115	-
14	CLA	bB	820	-	1/1/15/20	9/37/115/115	-
16	SF4	aA	845	2,1	-	-	0/6/5/5
14	CLA	dL	204	10	1/1/12/20	8/22/100/115	-
14	CLA	dA	813	1	-	6/13/91/115	-
14	CLA	bB	842	2	1/1/15/20	20/37/115/115	-
17	BCR	aL	201	-	-	13/29/63/63	0/2/2/2
17	BCR	aA	846	-	-	6/29/63/63	0/2/2/2
14	CLA	cJ	101	-	1/1/11/20	10/13/91/115	-
14	CLA	aA	802	-	1/1/11/20	3/13/91/115	-
14	CLA	dB	827	2	1/1/15/20	20/37/115/115	-
14	CLA	dB	821	2	1/1/11/20	8/16/94/115	-
14	CLA	aB	802	2	1/1/15/20	12/37/115/115	-
14	CLA	cA	819	1	1/1/15/20	19/37/115/115	-
14	CLA	dA	825	-	1/1/15/20	13/37/115/115	-
14	CLA	cB	802	2	1/1/15/20	13/37/115/115	-
14	CLA	dA	836	1	1/1/11/20	7/13/91/115	-
14	CLA	bB	831	2	1/1/11/20	6/13/91/115	-
14	CLA	dB	820	-	1/1/15/20	9/37/115/115	-
14	CLA	cB	828	2	1/1/15/20	9/37/115/115	-
14	CLA	cX	101	12	1/1/11/20	7/13/91/115	-
17	BCR	aB	844	-	-	9/29/63/63	0/2/2/2
14	CLA	bA	828	1	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	cA	833	1	1/1/15/20	9/37/115/115	-
14	CLA	aA	828	1	1/1/15/20	6/37/115/115	-
14	CLA	bA	831	1	1/1/12/20	2/19/97/115	-
14	CLA	cA	812	1	1/1/12/20	11/24/102/115	-
14	CLA	cA	822	1	1/1/11/20	11/18/96/115	-
14	CLA	dB	815	2	1/1/13/20	2/27/105/115	-
14	CLA	bB	807	2	1/1/15/20	20/37/115/115	-
14	CLA	bX	101	12	1/1/11/20	7/13/91/115	-
14	CLA	bL	201	2,10	1/1/15/20	6/37/115/115	-
17	BCR	cJ	104	-	-	9/29/63/63	0/2/2/2
14	CLA	aA	827	14,1	1/1/15/20	12/37/115/115	-
14	CLA	cA	820	1	1/1/14/20	11/33/111/115	-
14	CLA	cA	810	1	1/1/11/20	5/13/91/115	-
15	PQN	cA	844	-	-	8/23/43/43	0/2/2/2
18	LHG	cA	853	14	-	10/31/31/53	-
14	CLA	aA	826	-	1/1/13/20	5/25/103/115	-
14	CLA	bA	832	1	1/1/15/20	11/37/115/115	-
14	CLA	cA	806	1	1/1/15/20	10/37/115/115	-
17	BCR	bK	102	-	-	6/29/63/63	0/2/2/2
14	CLA	aB	837	2	1/1/14/20	8/31/109/115	-
17	BCR	cA	849	-	-	18/29/63/63	0/2/2/2
14	CLA	aB	841	2	1/1/15/20	20/37/115/115	-
14	CLA	dB	809	2	1/1/15/20	9/37/115/115	-
14	CLA	aA	823	1	1/1/12/20	12/21/99/115	-
14	CLA	cB	837	2	1/1/14/20	8/31/109/115	-
14	CLA	bB	828	2	1/1/15/20	13/37/115/115	-
14	CLA	bA	841	1	1/1/15/20	12/37/115/115	-
18	LHG	bA	850	-	-	18/53/53/53	-
14	CLA	aB	819	-	1/1/15/20	9/37/115/115	-
14	CLA	cB	811	2	1/1/11/20	4/13/91/115	-
14	CLA	aK	101	9	1/1/9/20	3/7/81/115	-
17	BCR	bL	207	-	-	9/29/63/63	0/2/2/2
17	BCR	bI	101	-	-	14/29/63/63	0/2/2/2
14	CLA	aB	812	2	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	cM	101	-	-	9/29/63/63	0/2/2/2
14	CLA	aB	822	-	1/1/13/20	13/25/103/115	-
14	CLA	cB	812	2	1/1/11/20	6/13/91/115	-
14	CLA	bB	812	2	1/1/11/20	4/13/91/115	-
14	CLA	dA	804	14,1	1/1/11/20	4/13/91/115	-
14	CLA	dA	809	1	1/1/11/20	5/13/91/115	-
14	CLA	bB	823	-	1/1/13/20	13/25/103/115	-
14	CLA	cB	803	-	1/1/15/20	18/37/115/115	-
14	CLA	cB	824	2	-	6/24/102/115	-
14	CLA	aL	203	10	1/1/15/20	12/37/115/115	-
14	CLA	bA	812	1	1/1/12/20	11/24/102/115	-
14	CLA	cA	834	1	1/1/15/20	9/37/115/115	-
14	CLA	bB	837	-	-	6/13/91/115	-
17	BCR	dA	845	-	-	7/29/63/63	0/2/2/2
14	CLA	bA	823	1	1/1/12/20	12/21/99/115	-
14	CLA	bB	803	-	1/1/15/20	18/37/115/115	-
16	SF4	bA	844	2,1	-	-	0/6/5/5
17	BCR	cF	202	-	-	11/29/63/63	0/2/2/2
15	PQN	bB	843	-	-	7/23/43/43	0/2/2/2
17	BCR	cL	205	-	-	9/29/63/63	0/2/2/2
14	CLA	cB	819	-	1/1/15/20	9/37/115/115	-
14	CLA	bA	837	1	1/1/12/20	7/21/99/115	-
14	CLA	dA	822	1	1/1/11/20	11/18/96/115	-
14	CLA	dB	804	-	1/1/15/20	13/37/115/115	-
14	CLA	bA	803	1	1/1/11/20	6/13/91/115	-
13	CL0	dA	801	1	2/2/20/25	11/37/135/135	-
14	CLA	aA	819	1	1/1/15/20	19/37/115/115	-
18	LHG	dB	851	-	-	11/26/26/53	-
14	CLA	dA	817	1	1/1/12/20	9/24/102/115	-
15	PQN	bA	843	-	-	5/23/43/43	0/2/2/2
14	CLA	aA	835	1	1/1/12/20	5/24/102/115	-
14	CLA	bA	815	1	1/1/11/20	4/13/91/115	-
14	CLA	dB	834	2	1/1/13/20	11/29/107/115	-
16	SF4	dC	102	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	dL	205	10	1/1/15/20	10/37/115/115	-
14	CLA	cB	809	2	1/1/15/20	9/37/115/115	-
14	CLA	cA	811	14,1	1/1/15/20	11/37/115/115	-
17	BCR	cA	850	-	-	9/29/63/63	0/2/2/2
14	CLA	dB	816	2	1/1/11/20	5/13/91/115	-
17	BCR	aB	848	-	-	7/29/63/63	0/2/2/2
14	CLA	cA	832	1	1/1/15/20	12/37/115/115	-
14	CLA	aA	821	14	1/1/15/20	14/37/115/115	-
14	CLA	bA	833	1	1/1/15/20	9/37/115/115	-
14	CLA	aA	817	1	1/1/12/20	9/24/102/115	-
14	CLA	cA	817	1	1/1/12/20	9/24/102/115	-
14	CLA	bF	203	-	1/1/11/20	3/13/91/115	-
14	CLA	aB	832	2	1/1/15/20	15/37/115/115	-
14	CLA	dK	103	-	1/1/11/20	3/13/91/115	-
18	LHG	dA	851	14	-	10/31/31/53	-
17	BCR	aA	847	-	-	7/29/63/63	0/2/2/2
14	CLA	bB	829	2	1/1/15/20	9/37/115/115	-
14	CLA	dB	836	-	1/1/11/20	2/13/91/115	-
14	CLA	bA	824	1	1/1/11/20	5/16/94/115	-
16	SF4	cC	102	3	-	-	0/6/5/5
14	CLA	cA	841	1	1/1/15/20	12/37/115/115	-
14	CLA	aA	810	1	1/1/11/20	5/13/91/115	-
14	CLA	aB	823	2	1/1/11/20	6/13/91/115	-
14	CLA	cB	826	2	1/1/15/20	20/37/115/115	-
14	CLA	dA	803	1	1/1/11/20	6/13/91/115	-
14	CLA	bB	819	2	1/1/14/20	8/31/109/115	-
14	CLA	dB	818	2	1/1/13/20	9/30/108/115	-
14	CLA	dB	824	2	1/1/11/20	6/13/91/115	-
14	CLA	bL	206	-	1/1/15/20	20/37/115/115	-
17	BCR	cB	844	-	-	9/29/63/63	0/2/2/2
14	CLA	bK	103	-	1/1/11/20	3/13/91/115	-
14	CLA	bB	840	2	-	1/16/94/115	-
19	LMG	cB	849	-	-	23/50/70/70	0/1/1/1
14	CLA	cB	835	-	1/1/11/20	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	aB	803	-	1/1/15/20	18/37/115/115	-
14	CLA	bA	819	1	1/1/15/20	19/37/115/115	-
14	CLA	dA	839	1	1/1/15/20	10/37/115/115	-
14	CLA	cA	831	1	1/1/12/20	2/19/97/115	-
14	CLA	cA	809	1	1/1/11/20	5/13/91/115	-
14	CLA	aL	204	-	1/1/12/20	8/22/100/115	-
14	CLA	bA	821	14	1/1/15/20	14/37/115/115	-
14	CLA	aA	811	14,1	1/1/15/20	11/37/115/115	-
14	CLA	aB	833	2	1/1/13/20	11/29/107/115	-
17	BCR	dL	207	-	-	9/29/63/63	0/2/2/2
16	SF4	aC	102	3	-	-	0/6/5/5
14	CLA	cB	822	-	1/1/13/20	12/25/103/115	-
15	PQN	aA	844	-	-	8/23/43/43	0/2/2/2
14	CLA	aA	808	1	1/1/11/20	4/13/91/115	-
14	CLA	aB	830	2	1/1/11/20	6/13/91/115	-
17	BCR	dF	202	-	-	11/29/63/63	0/2/2/2
18	LHG	cB	850	-	-	11/26/26/53	-
14	CLA	cA	807	1	1/1/12/20	2/21/99/115	-
14	CLA	bB	826	-	1/1/11/20	6/15/93/115	-
14	CLA	aF	201	-	1/1/12/20	5/21/99/115	-
14	CLA	cA	805	1	1/1/11/20	5/13/91/115	-
17	BCR	aA	849	-	-	18/29/63/63	0/2/2/2
14	CLA	bA	820	1	1/1/14/20	11/33/111/115	-
14	CLA	bA	810	1	1/1/11/20	5/13/91/115	-
14	CLA	aB	806	2	1/1/15/20	15/37/115/115	-
14	CLA	cB	829	2	1/1/15/20	13/37/115/115	-
14	CLA	aB	807	2	1/1/15/20	20/37/115/115	-
14	CLA	cB	833	2	1/1/13/20	11/29/107/115	-
14	CLA	cB	825	-	1/1/11/20	6/15/93/115	-
17	BCR	aI	101	-	-	14/29/63/63	0/2/2/2
14	CLA	aB	805	2	1/1/12/20	7/24/102/115	-
14	CLA	dF	201	-	1/1/12/20	5/21/99/115	-
14	CLA	aB	840	-	1/1/15/20	2/37/115/115	-
14	CLA	bB	811	2	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	aB	850	-	-	11/26/26/53	-
14	CLA	dA	831	1	1/1/12/20	2/19/97/115	-
17	BCR	aL	206	-	-	11/29/63/63	0/2/2/2
17	BCR	cA	848	-	-	8/29/63/63	0/2/2/2
14	CLA	aA	807	1	1/1/12/20	2/21/99/115	-
17	BCR	aA	850	-	-	9/29/63/63	0/2/2/2
14	CLA	dA	820	1	1/1/14/20	11/33/111/115	-
17	BCR	bB	847	-	-	17/29/63/63	0/2/2/2
14	CLA	aJ	102	-	1/1/8/20	0/2/76/115	-
14	CLA	aB	831	2	1/1/11/20	11/18/96/115	-
14	CLA	cB	806	2	1/1/15/20	15/37/115/115	-
14	CLA	aB	814	2	1/1/13/20	2/27/105/115	-
14	CLA	dJ	102	-	1/1/8/20	0/2/76/115	-
14	CLA	aA	832	1	1/1/15/20	11/37/115/115	-
17	BCR	bA	846	-	-	8/29/63/63	0/2/2/2
14	CLA	aL	202	10	1/1/15/20	10/37/115/115	-
14	CLA	bB	830	2	1/1/15/20	13/37/115/115	-
16	SF4	dC	101	3	-	-	0/6/5/5
14	CLA	cB	808	2	1/1/15/20	8/37/115/115	-
14	CLA	dB	822	2	1/1/11/20	5/13/91/115	-
17	BCR	bA	849	-	-	20/29/63/63	0/2/2/2
14	CLA	cB	804	-	1/1/15/20	13/37/115/115	-
14	CLA	aA	834	1	1/1/15/20	9/37/115/115	-
14	CLA	dB	813	2	1/1/11/20	6/13/91/115	-
14	CLA	bA	807	1	1/1/12/20	2/21/99/115	-
14	CLA	aF	203	-	1/1/11/20	4/13/91/115	-
14	CLA	aA	837	1	1/1/12/20	7/21/99/115	-
14	CLA	dA	819	1	1/1/15/20	19/37/115/115	-
14	CLA	cA	825	-	1/1/15/20	13/37/115/115	-
14	CLA	dA	821	14	1/1/15/20	14/37/115/115	-
14	CLA	cK	102	-	1/1/11/20	3/13/91/115	-
14	CLA	cA	816	-	-	8/18/96/115	-
14	CLA	bA	835	1	1/1/12/20	5/24/102/115	-
14	CLA	dA	828	1	1/1/15/20	6/37/115/115	-
14	CLA	cB	836	-	-	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	bA	842	-	1/1/15/20	12/37/115/115	-
14	CLA	dF	203	-	1/1/11/20	3/13/91/115	-
14	CLA	cB	832	2	1/1/15/20	15/37/115/115	-

The worst 5 of 3502 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bB	808	CLA	C4B-NB	7.89	1.42	1.35
14	bB	833	CLA	C4B-NB	7.83	1.42	1.35
14	dB	833	CLA	C4B-NB	7.81	1.42	1.35
14	aB	832	CLA	C4B-NB	7.80	1.42	1.35
14	cB	832	CLA	C4B-NB	7.78	1.42	1.35

The worst 5 of 3665 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	aB	804	CLA	C4A-NA-C1A	9.40	110.93	106.71
14	dB	804	CLA	C4A-NA-C1A	9.36	110.91	106.71
14	bB	804	CLA	C4A-NA-C1A	9.30	110.89	106.71
14	cB	804	CLA	C4A-NA-C1A	9.28	110.88	106.71
13	aA	801	CL0	C1D-ND-C4D	-8.96	99.97	106.33

5 of 366 chirality outliers are listed below:

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

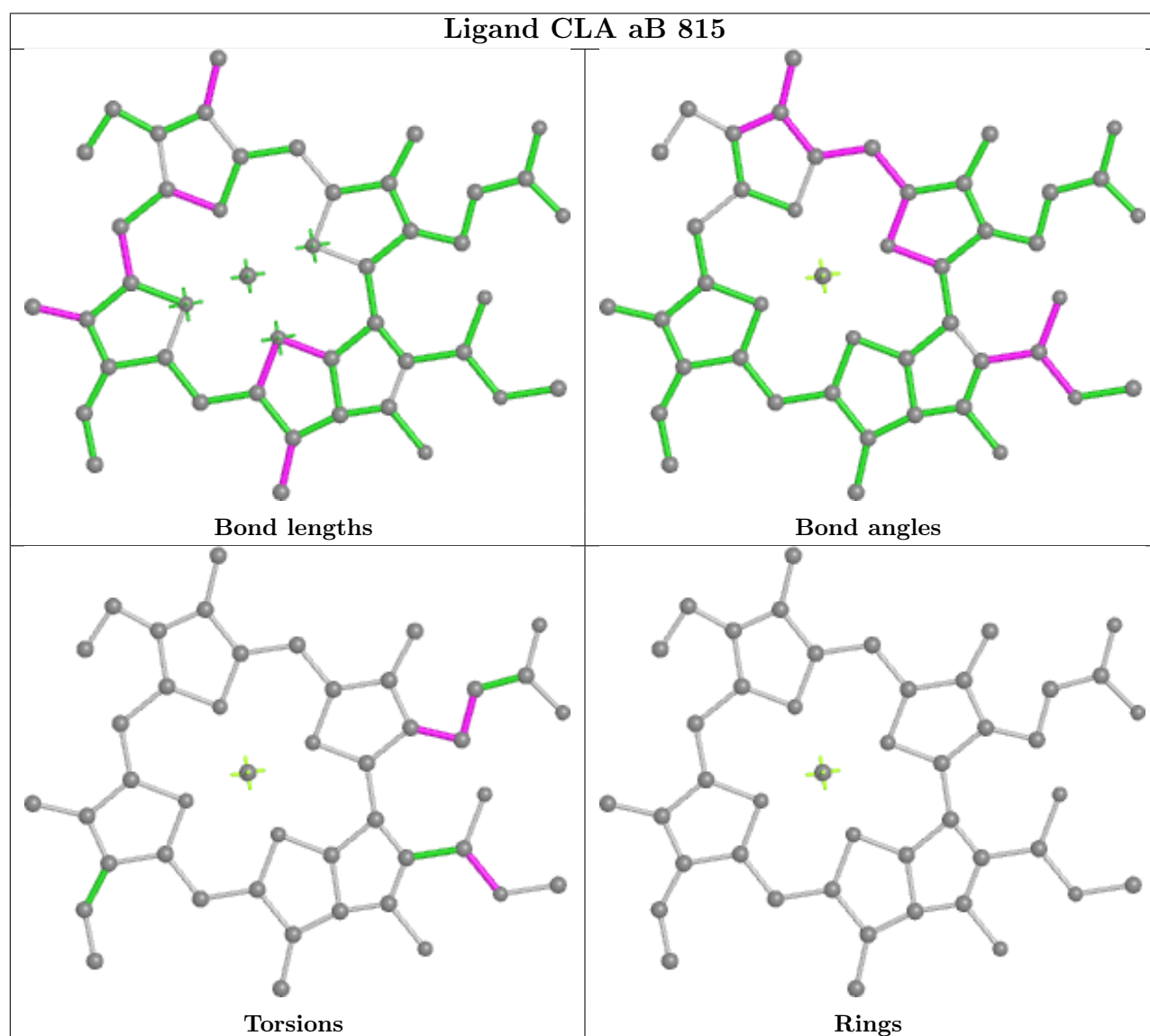
5 of 4615 torsion outliers are listed below:

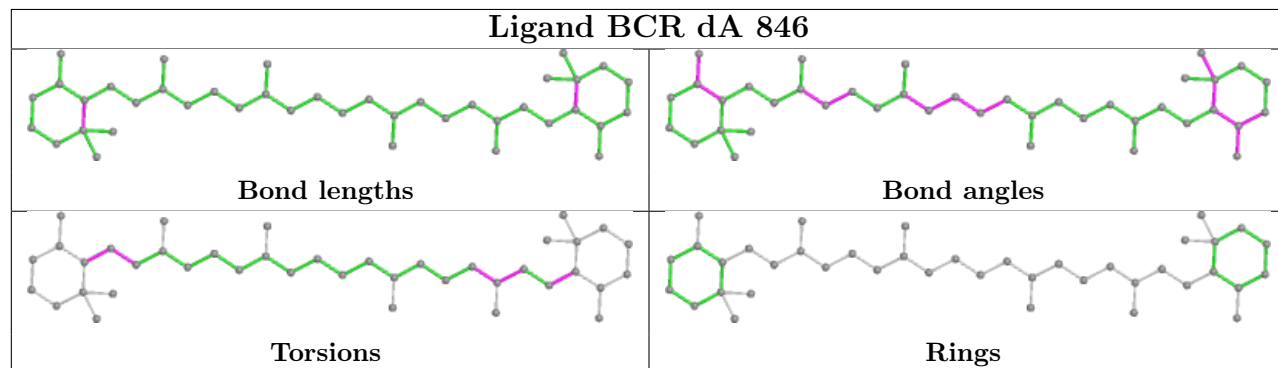
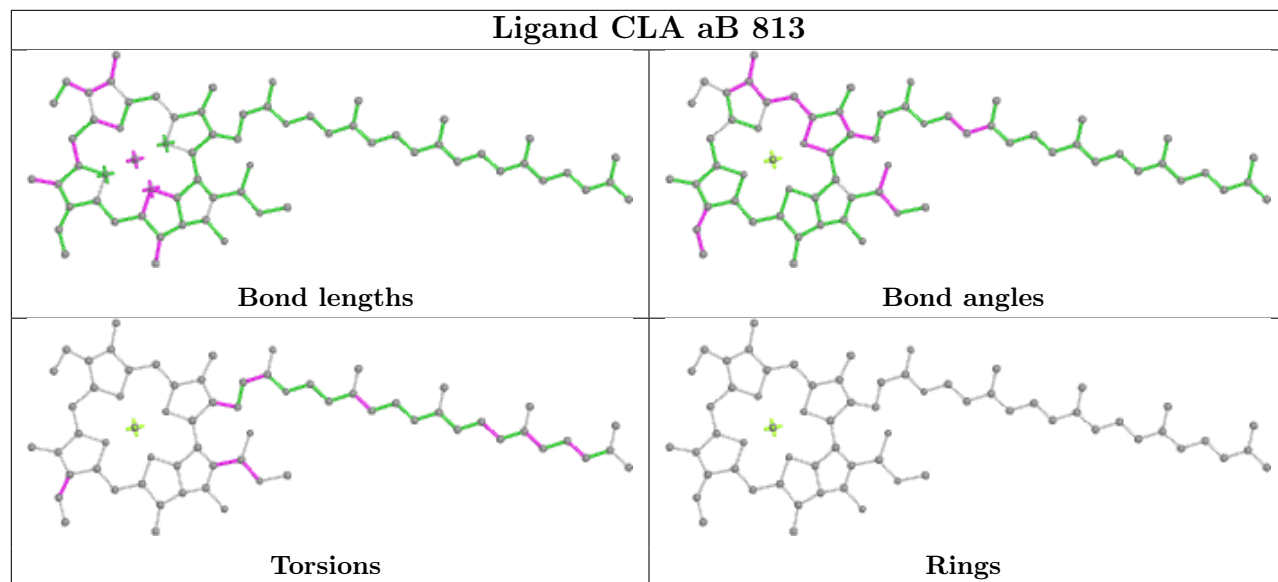
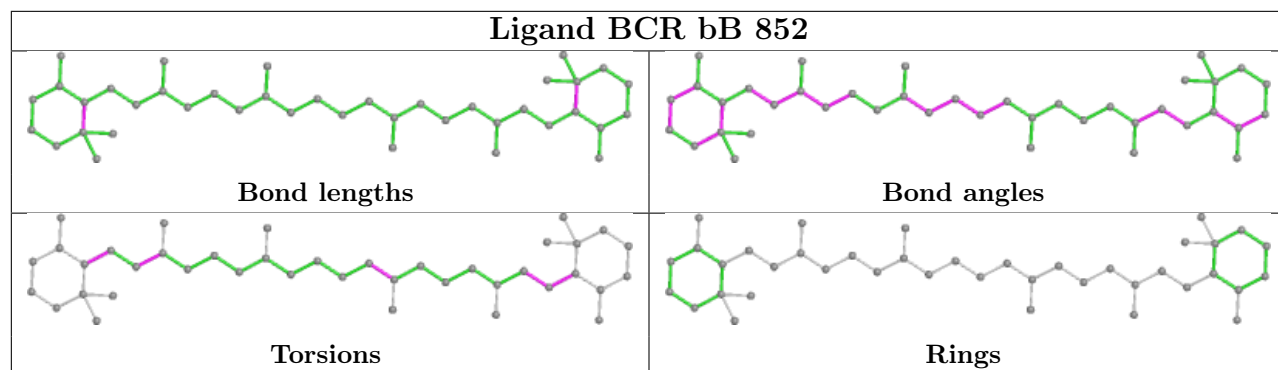
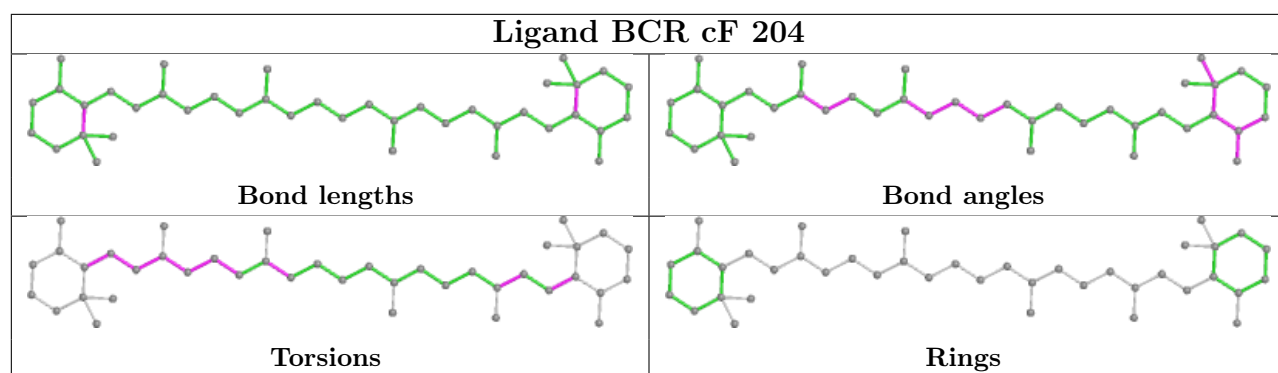
Mol	Chain	Res	Type	Atoms
14	aA	803	CLA	CHA-CBD-CGD-O1D
14	aA	803	CLA	CHA-CBD-CGD-O2D
14	aA	805	CLA	C1A-C2A-CAA-CBA
14	aA	805	CLA	C3A-C2A-CAA-CBA
14	aA	806	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

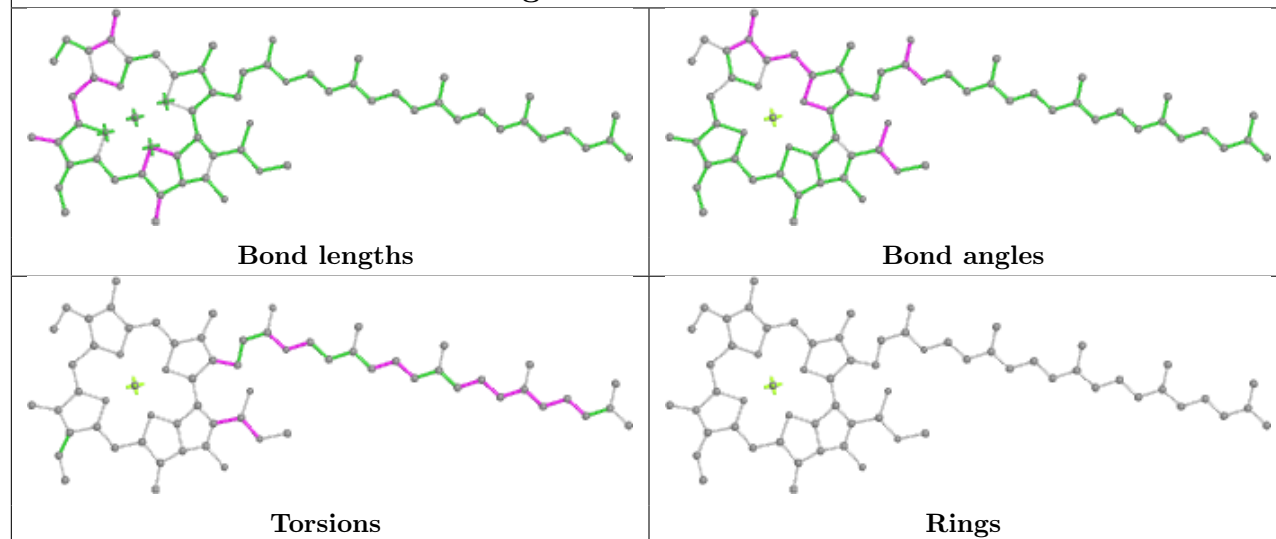
No monomer is involved in short contacts.

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.

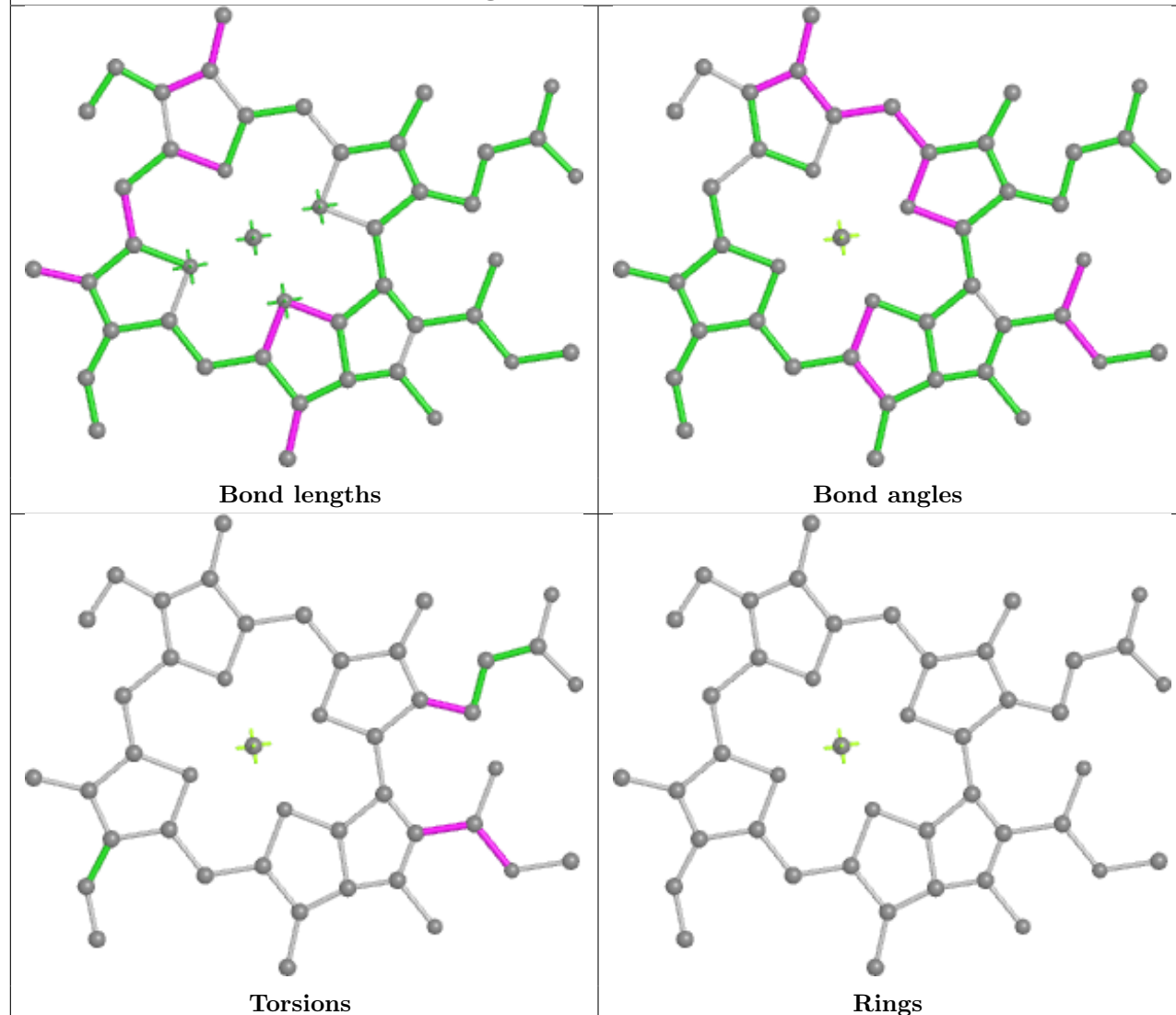




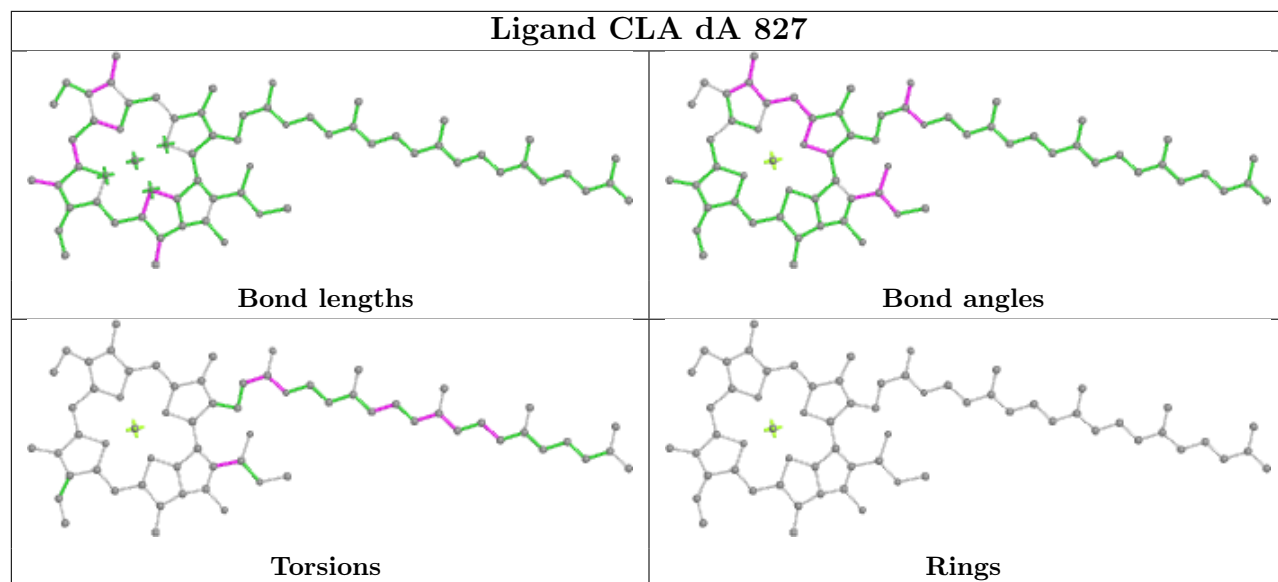
Ligand CLA dB 842



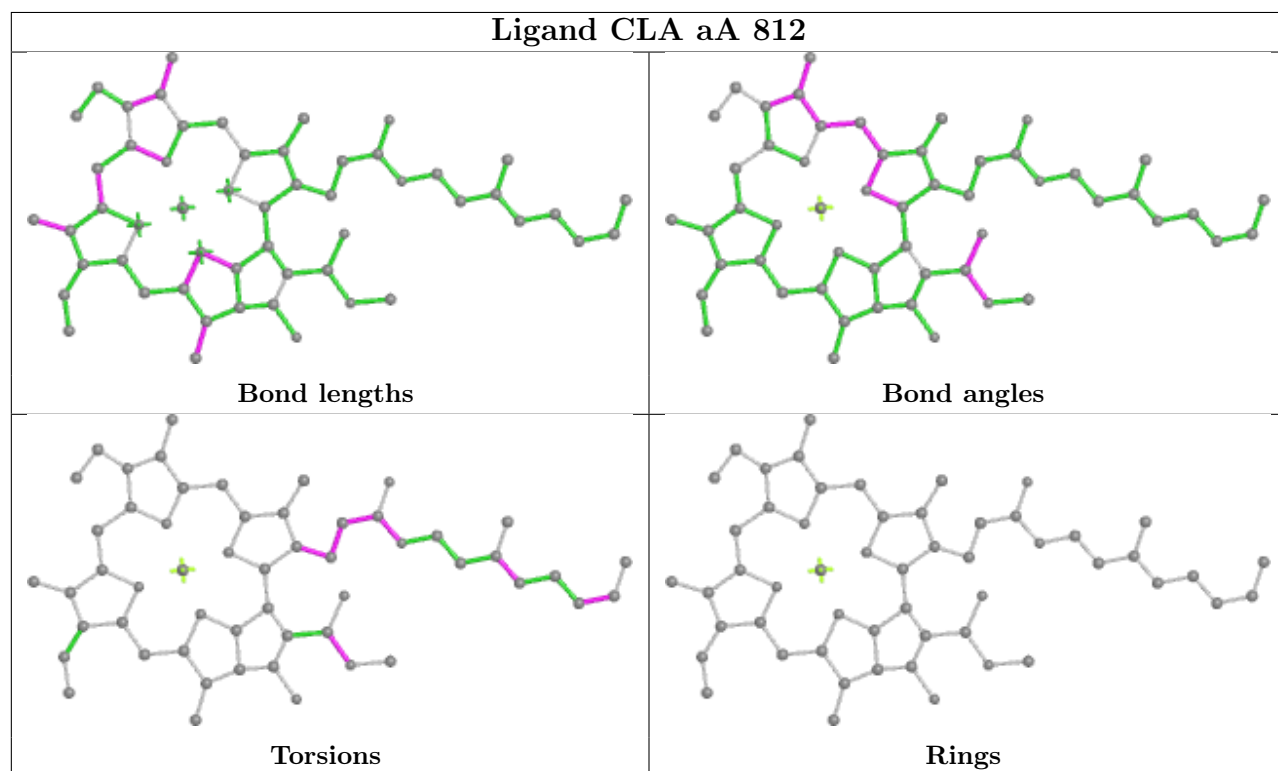
Ligand CLA aB 811



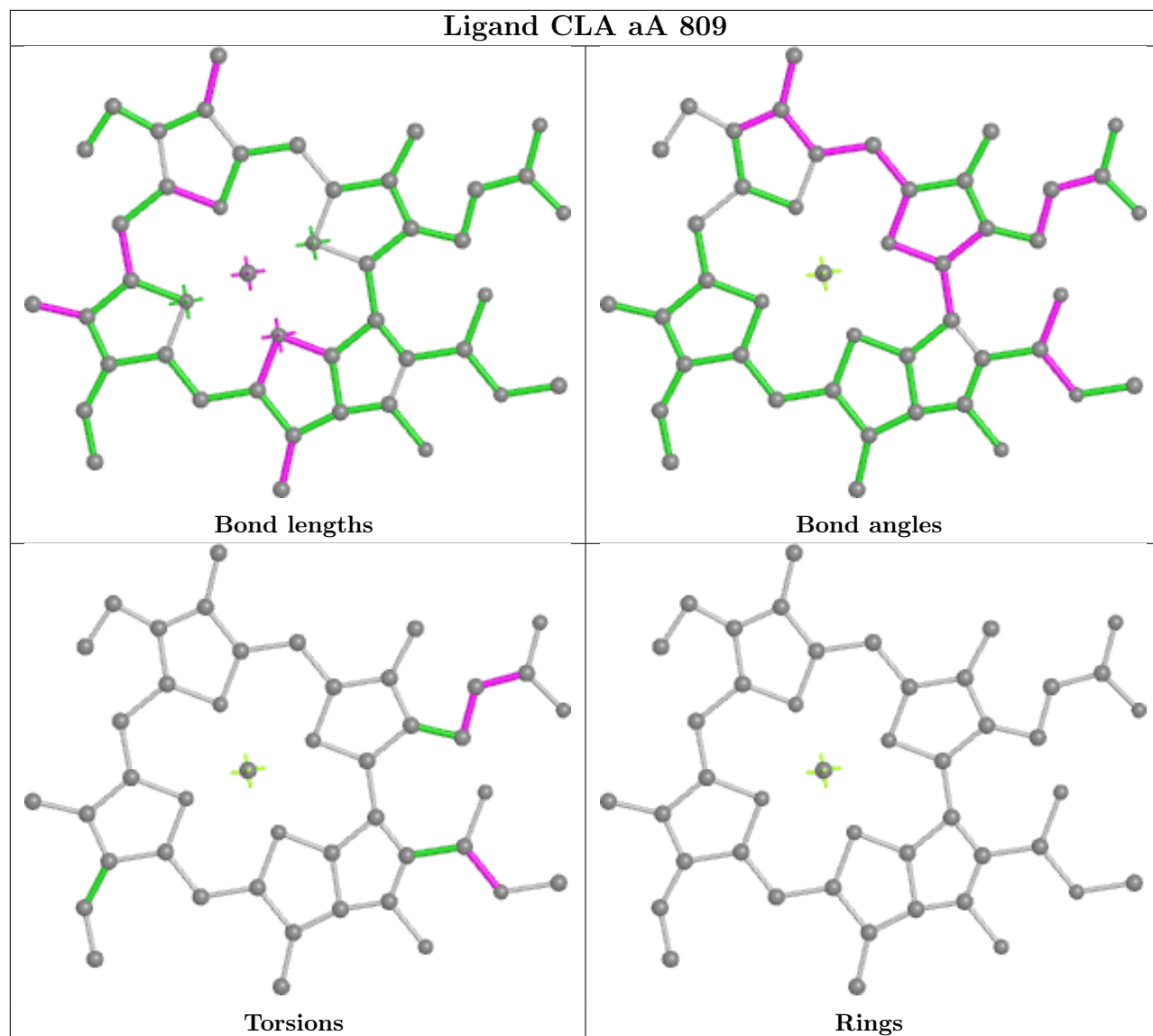
Ligand CLA dA 827

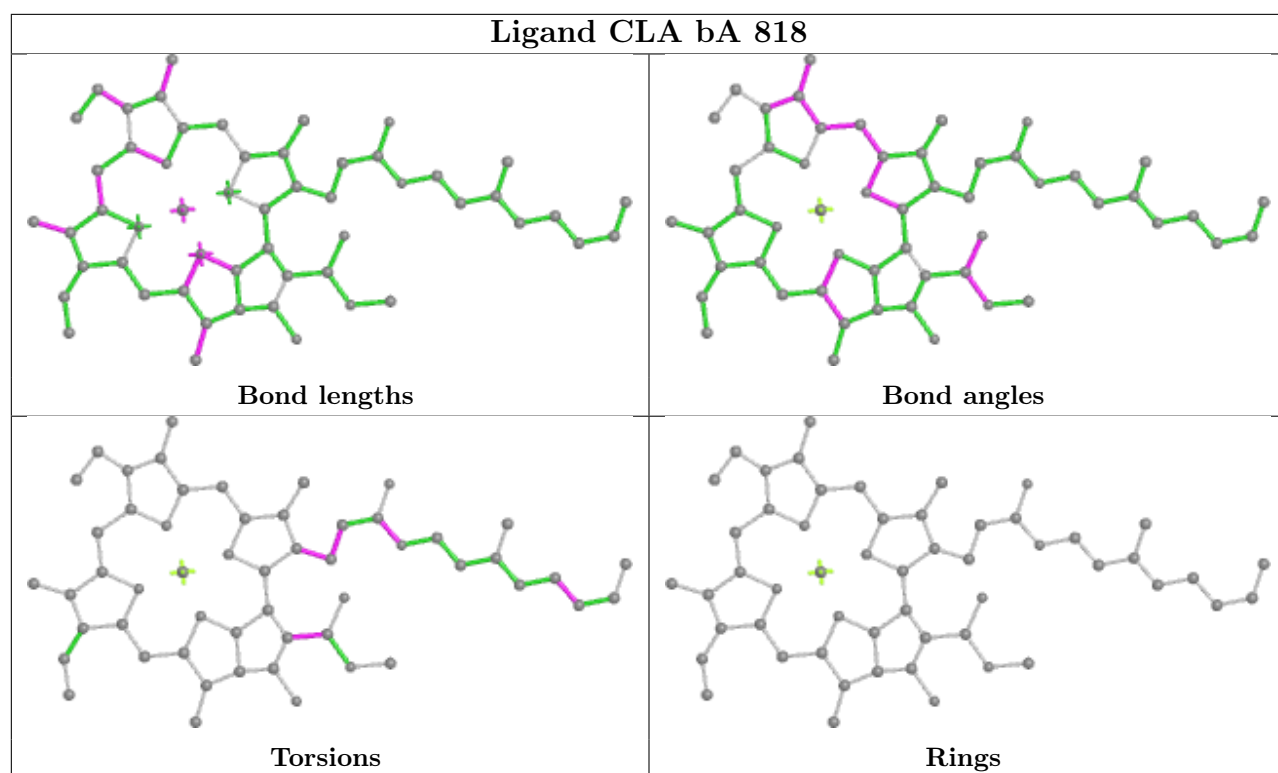


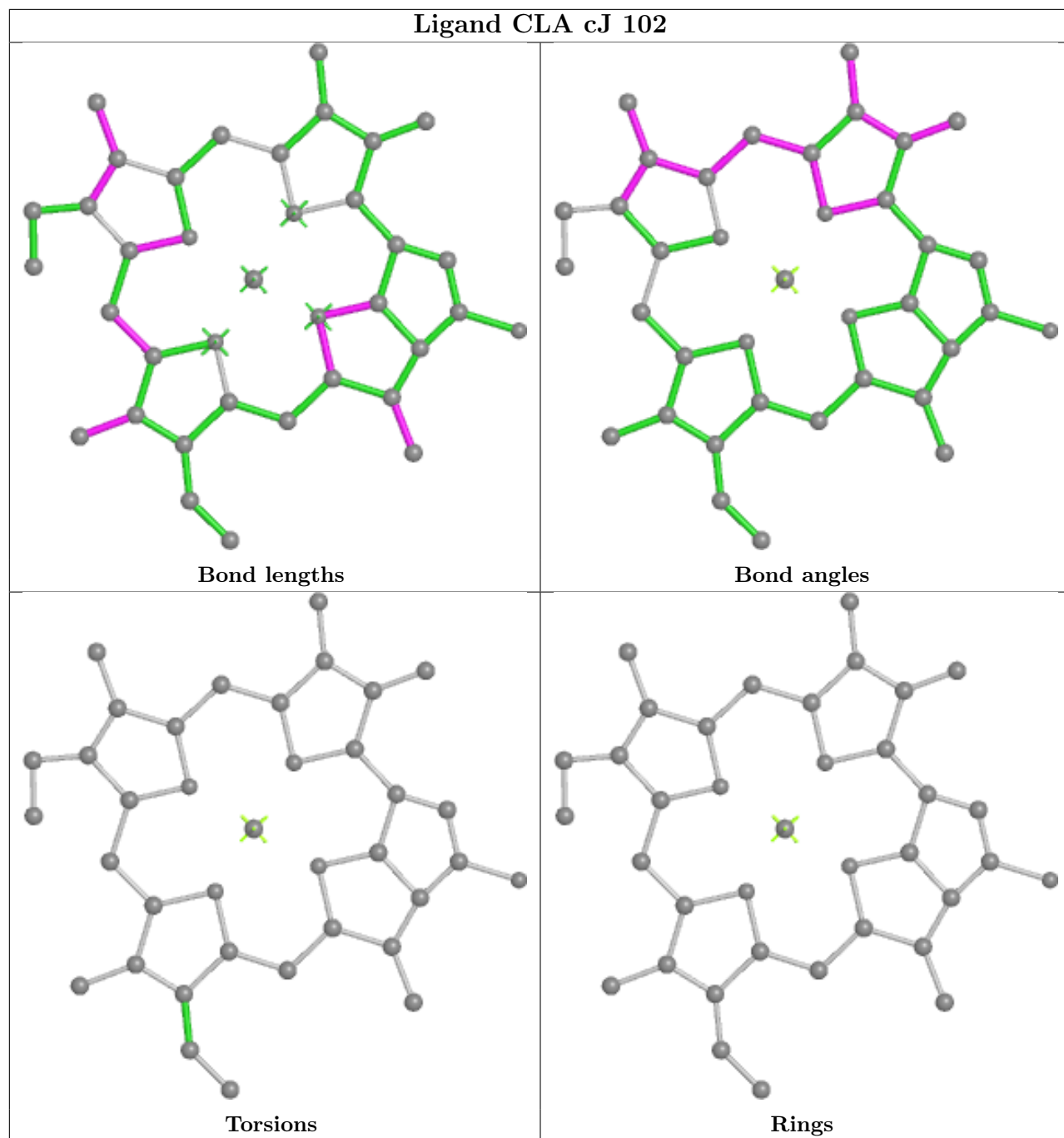
Ligand CLA aA 812



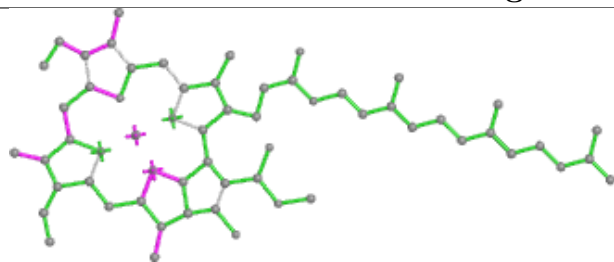
Ligand CLA aA 809



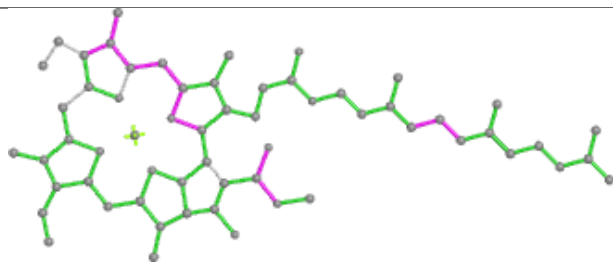




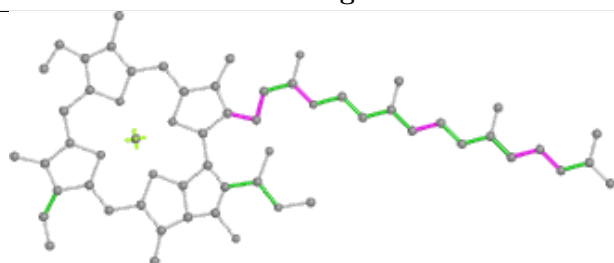
Ligand CLA aB 818



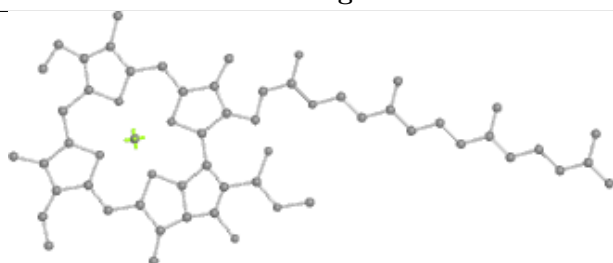
Bond lengths



Bond angles

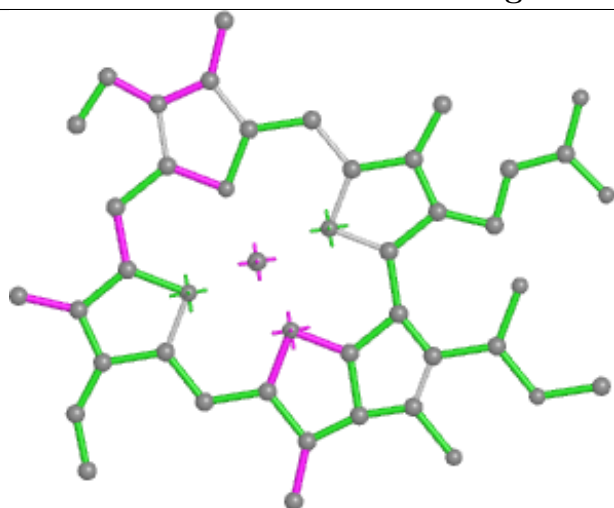


Torsions

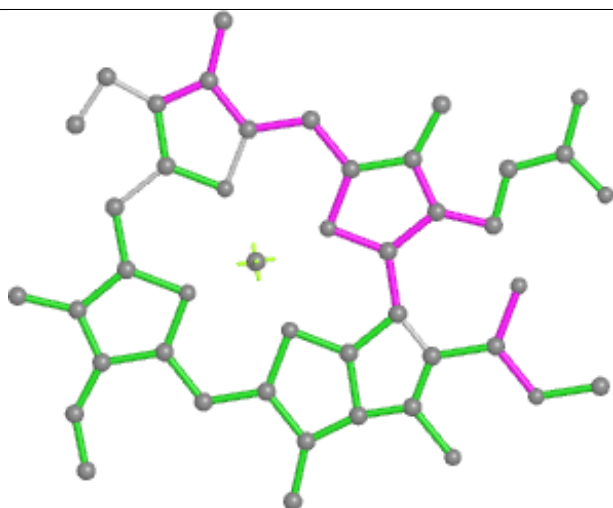


Rings

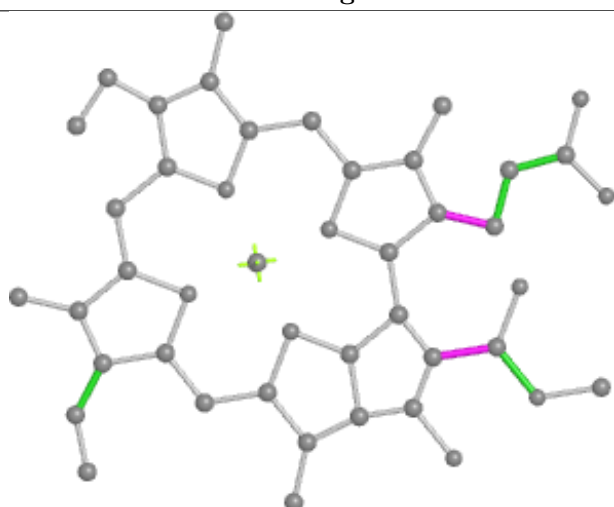
Ligand CLA aA 805



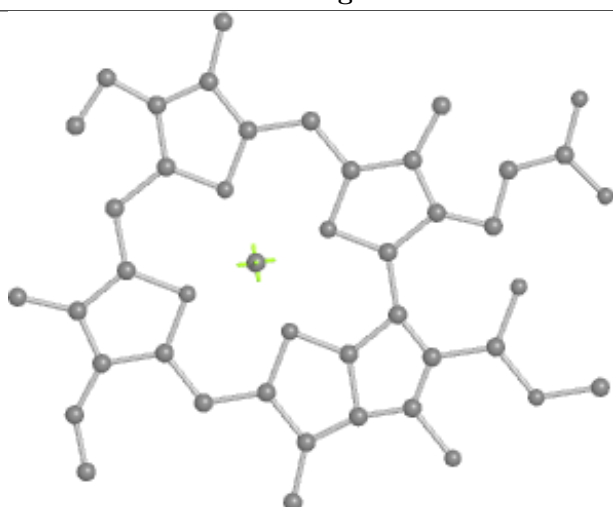
Bond lengths



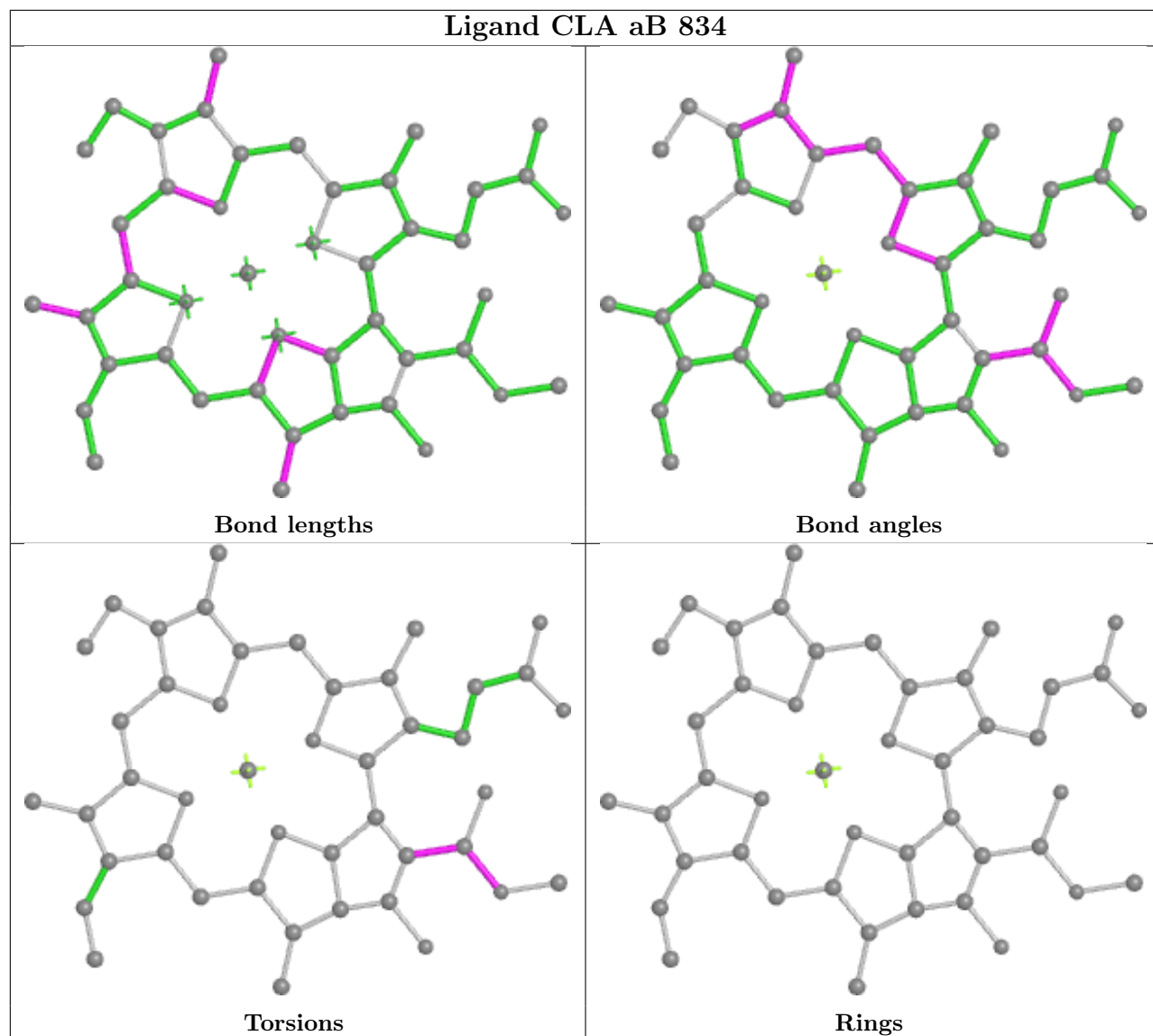
Bond angles



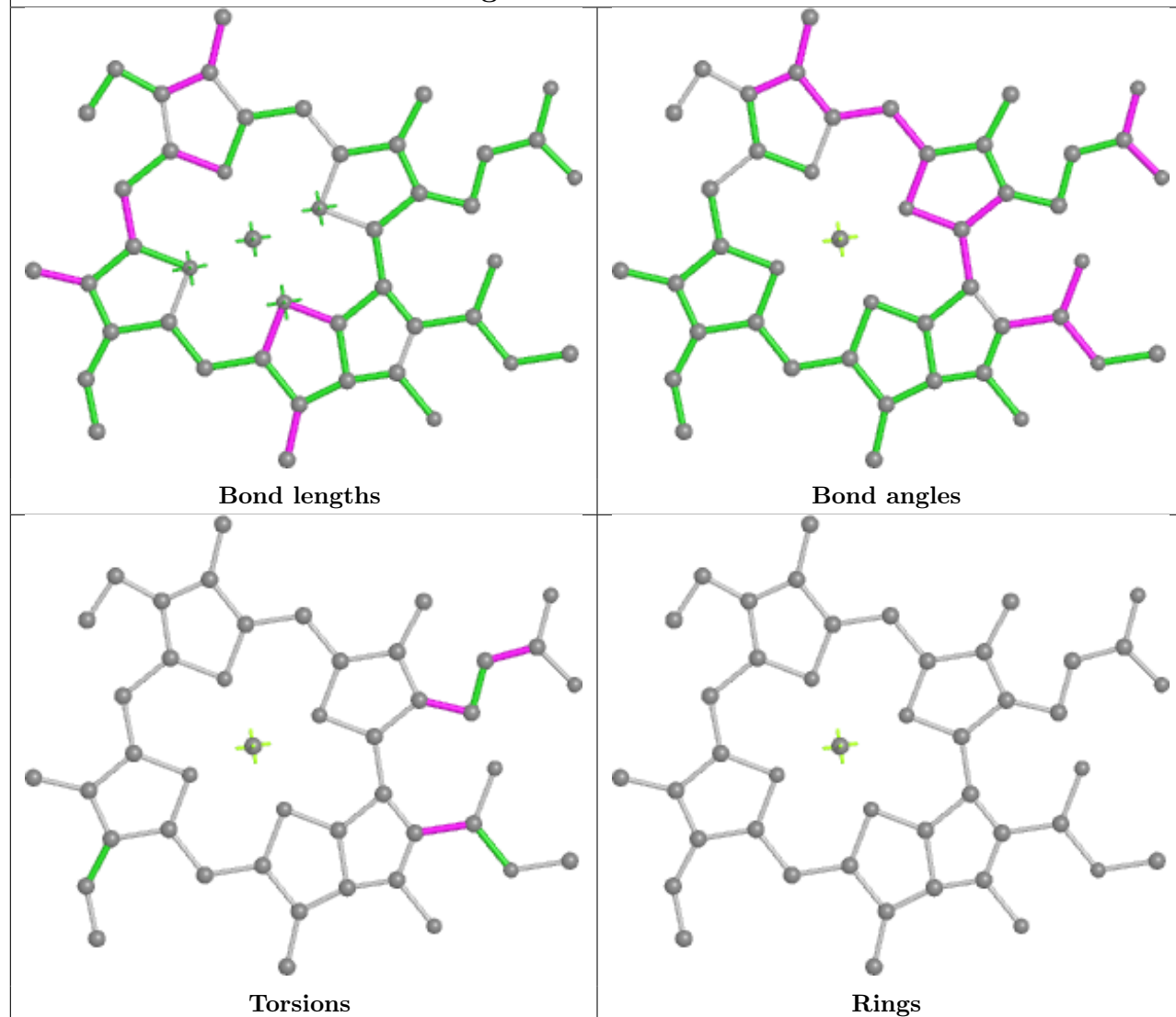
Torsions



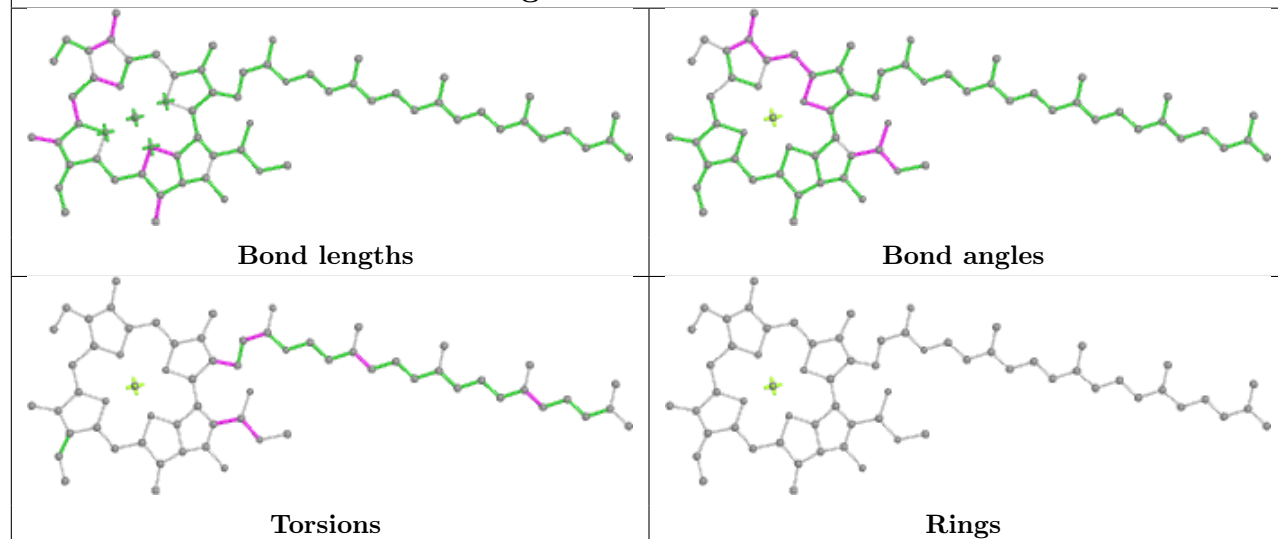
Rings

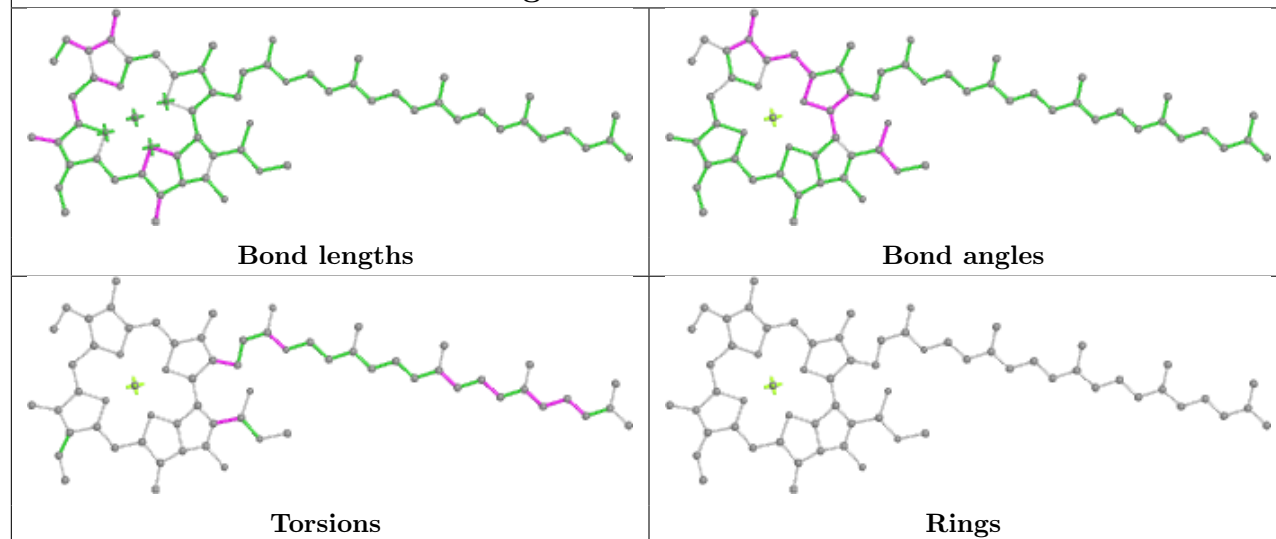
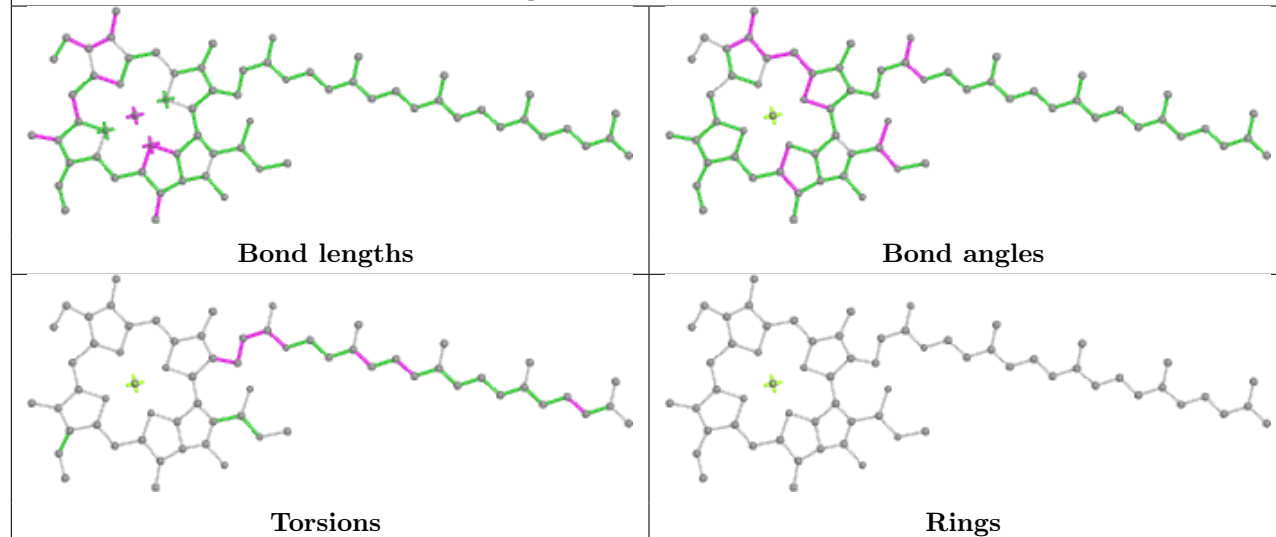


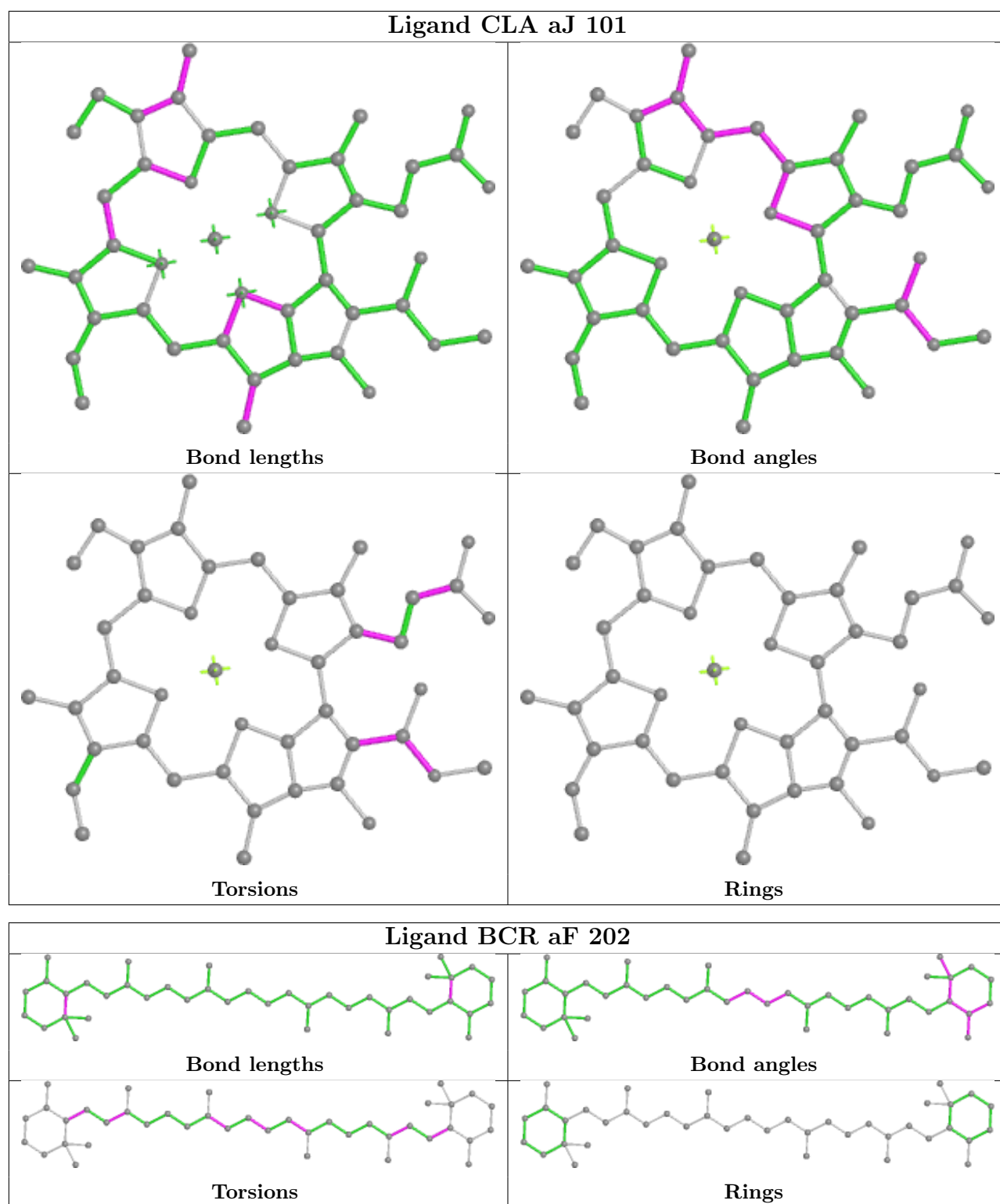
Ligand CLA aA 803

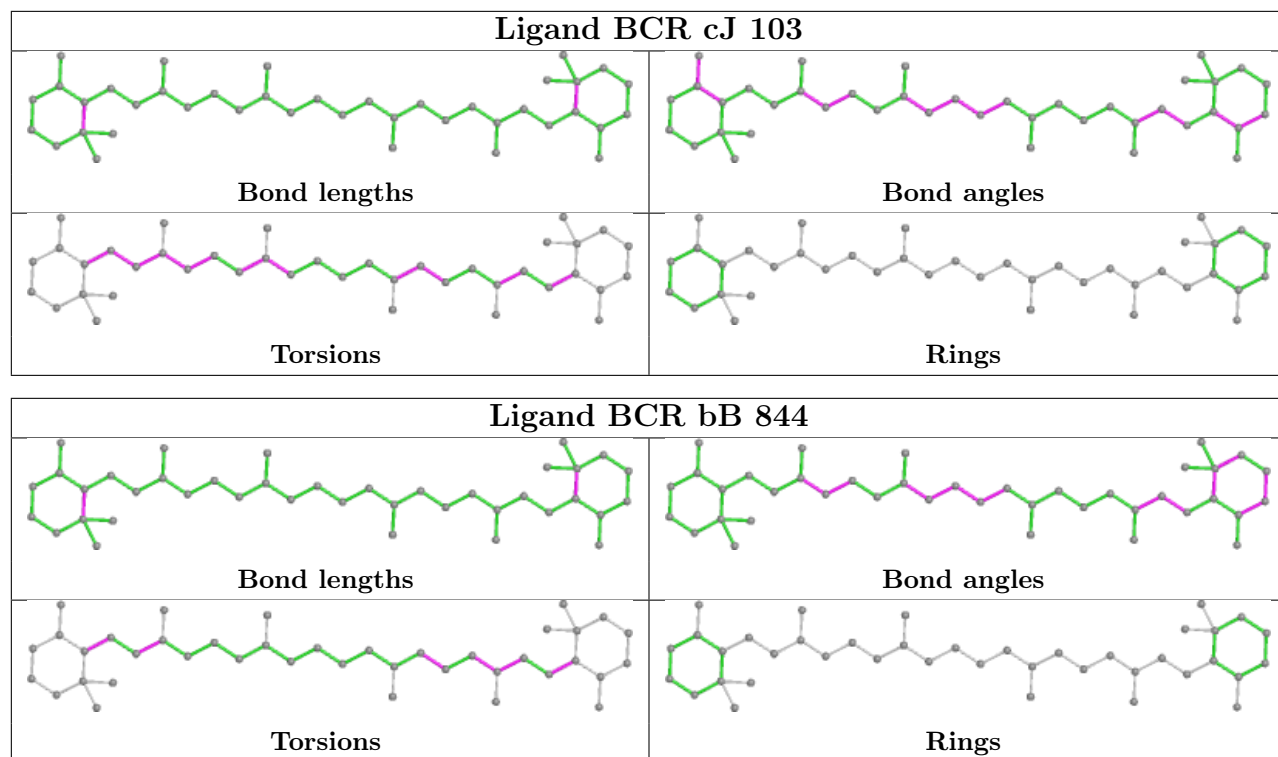


Ligand CLA bA 834

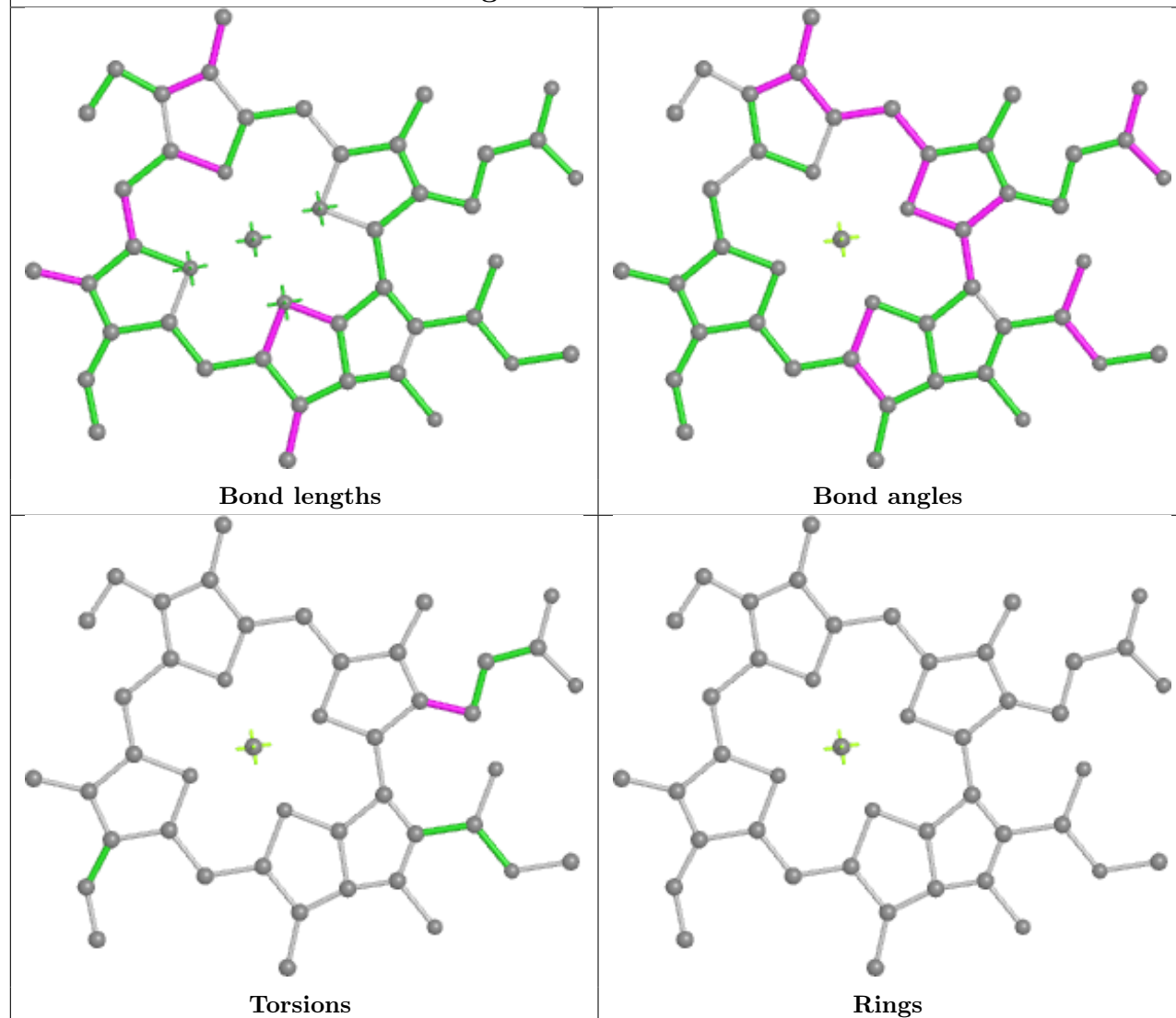


Ligand CLA aA 841**Ligand CLA dB 829**

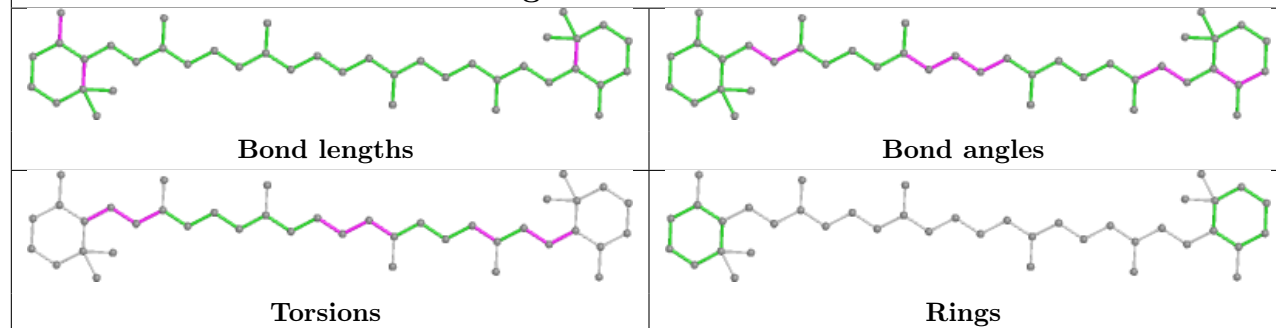


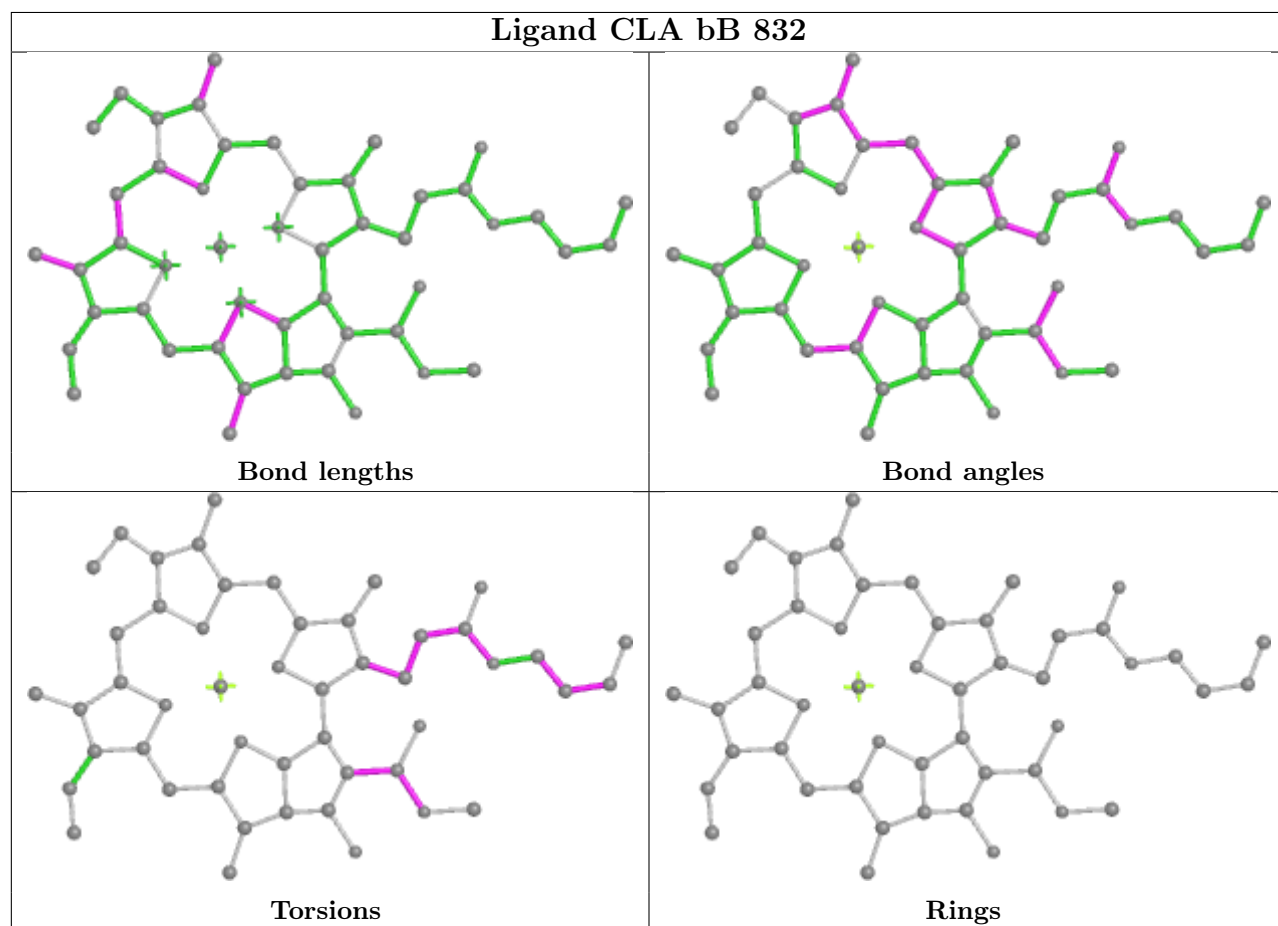
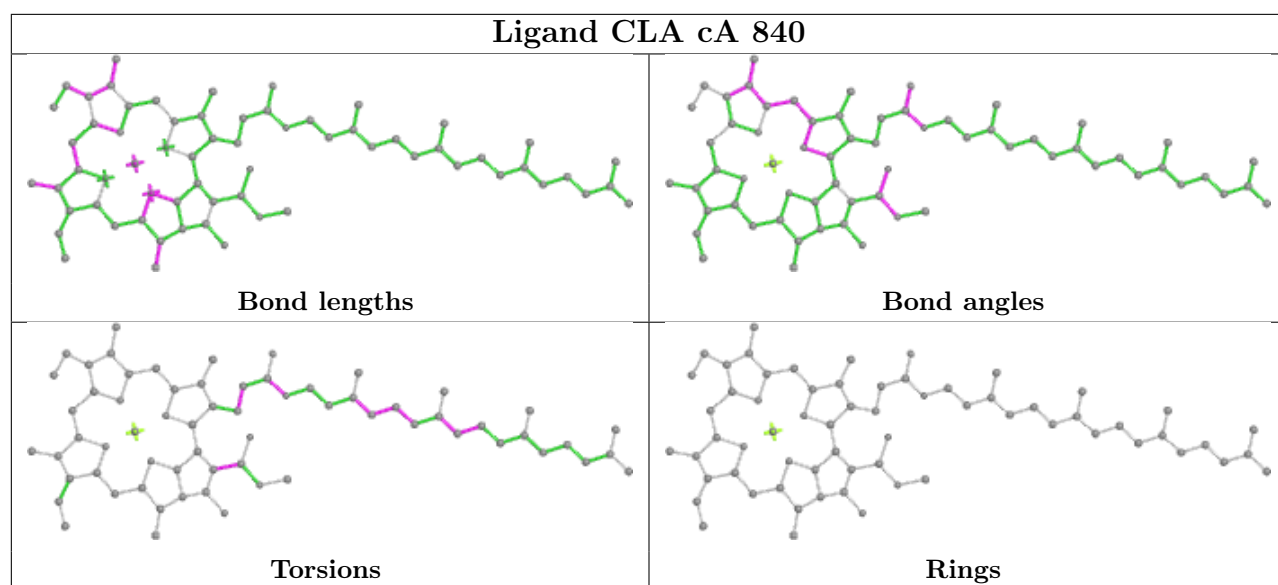


Ligand CLA bB 836

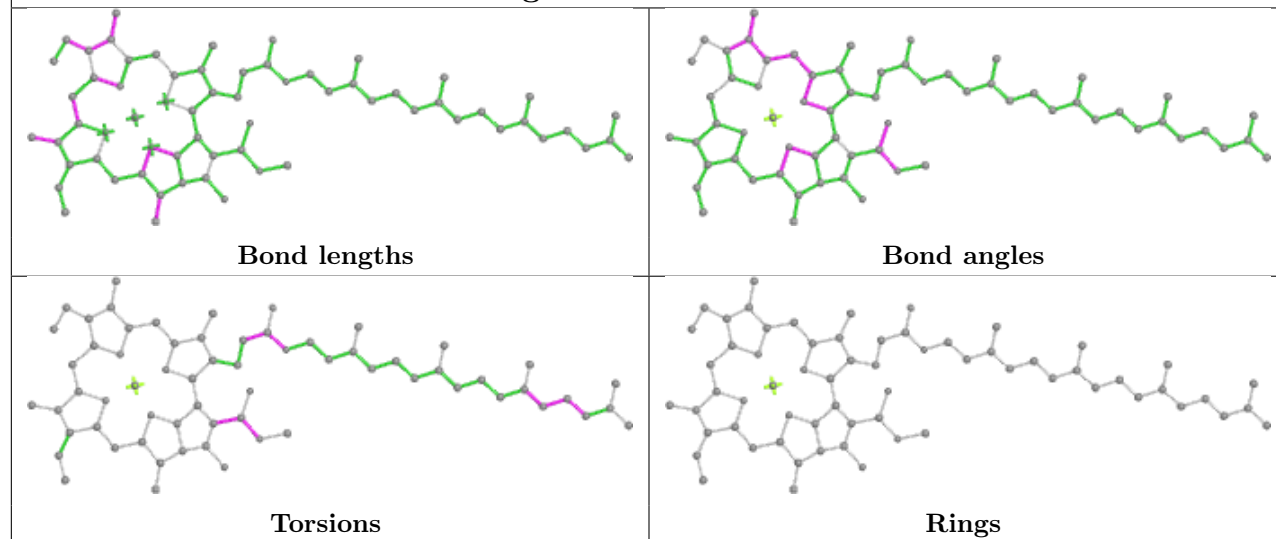


Ligand BCR dL 203

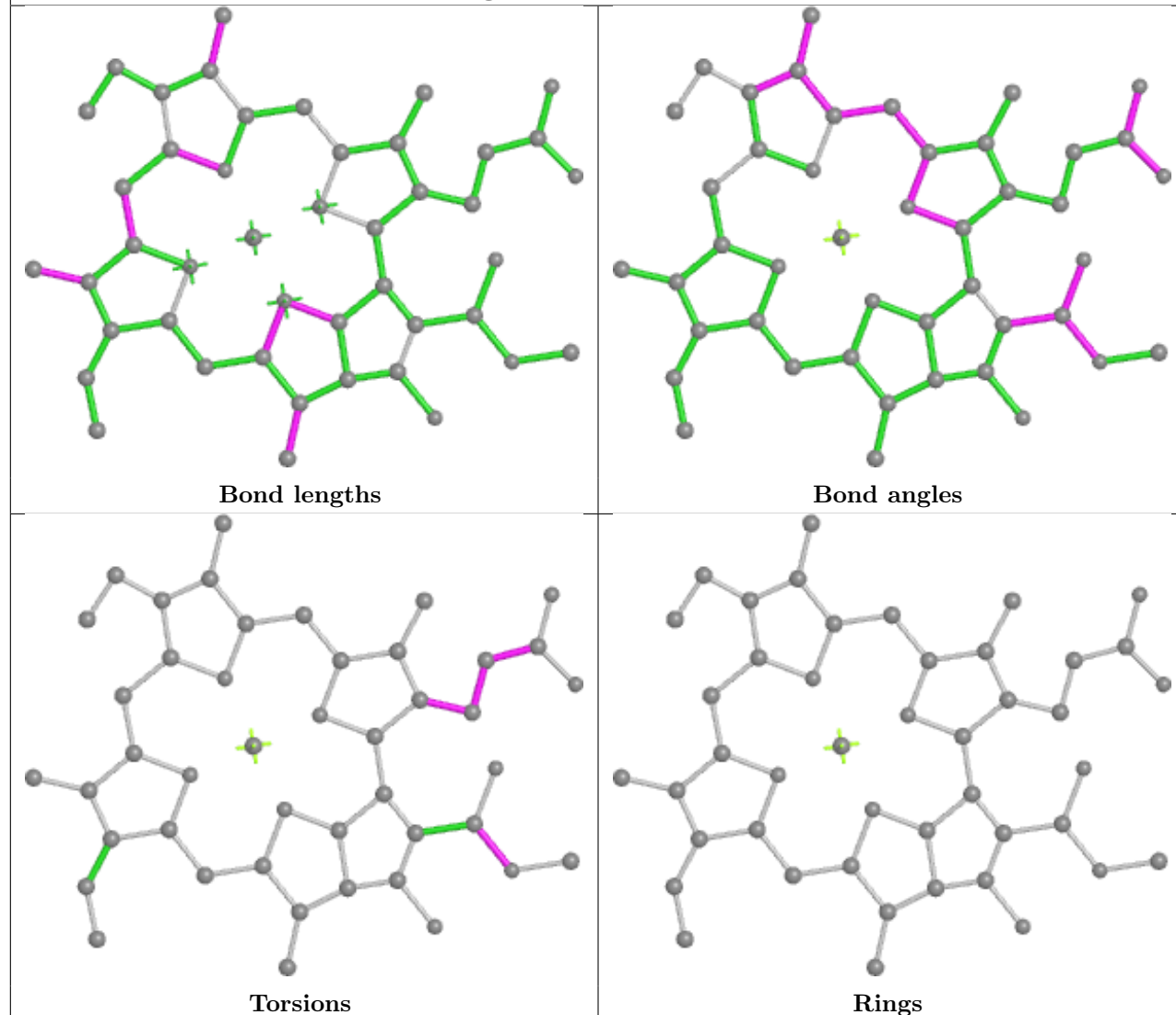


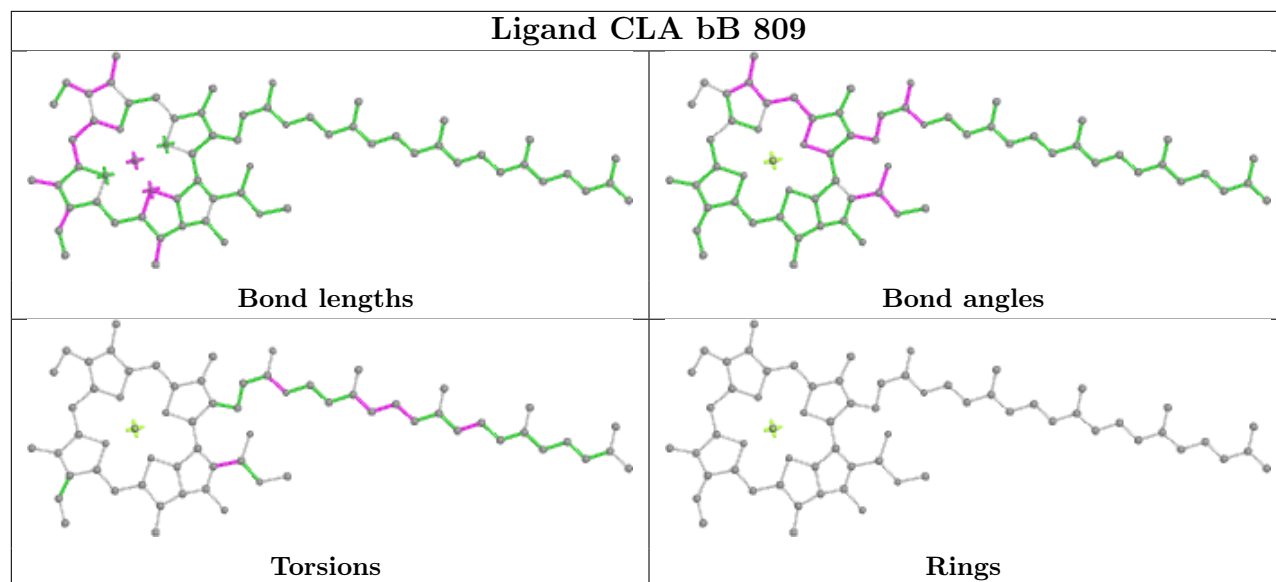
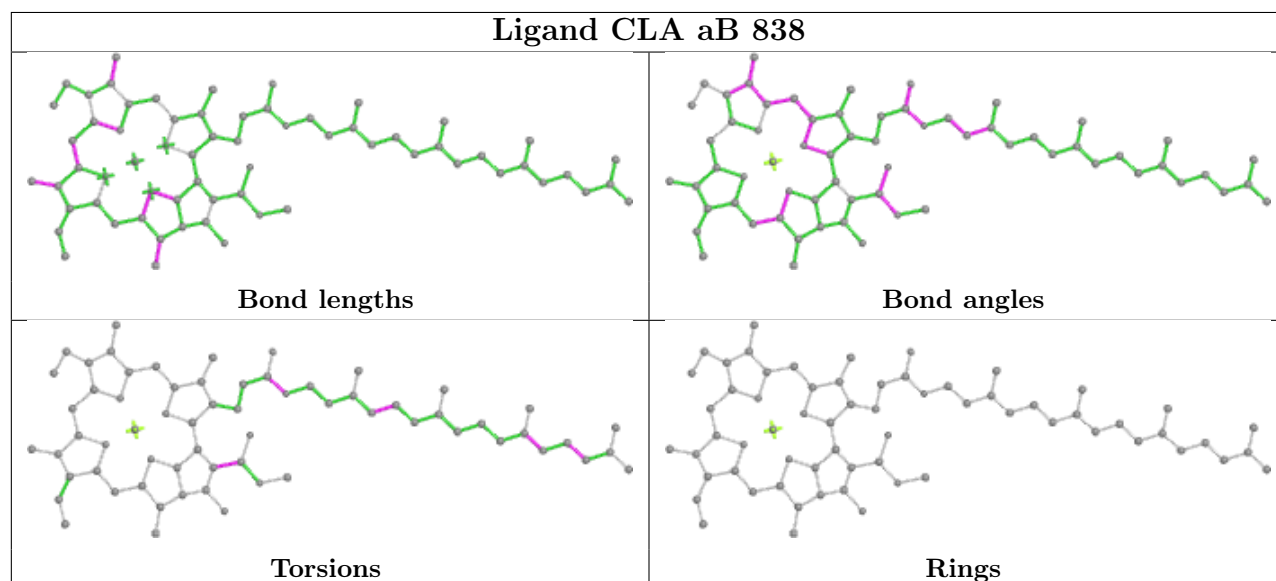


Ligand CLA dB 802

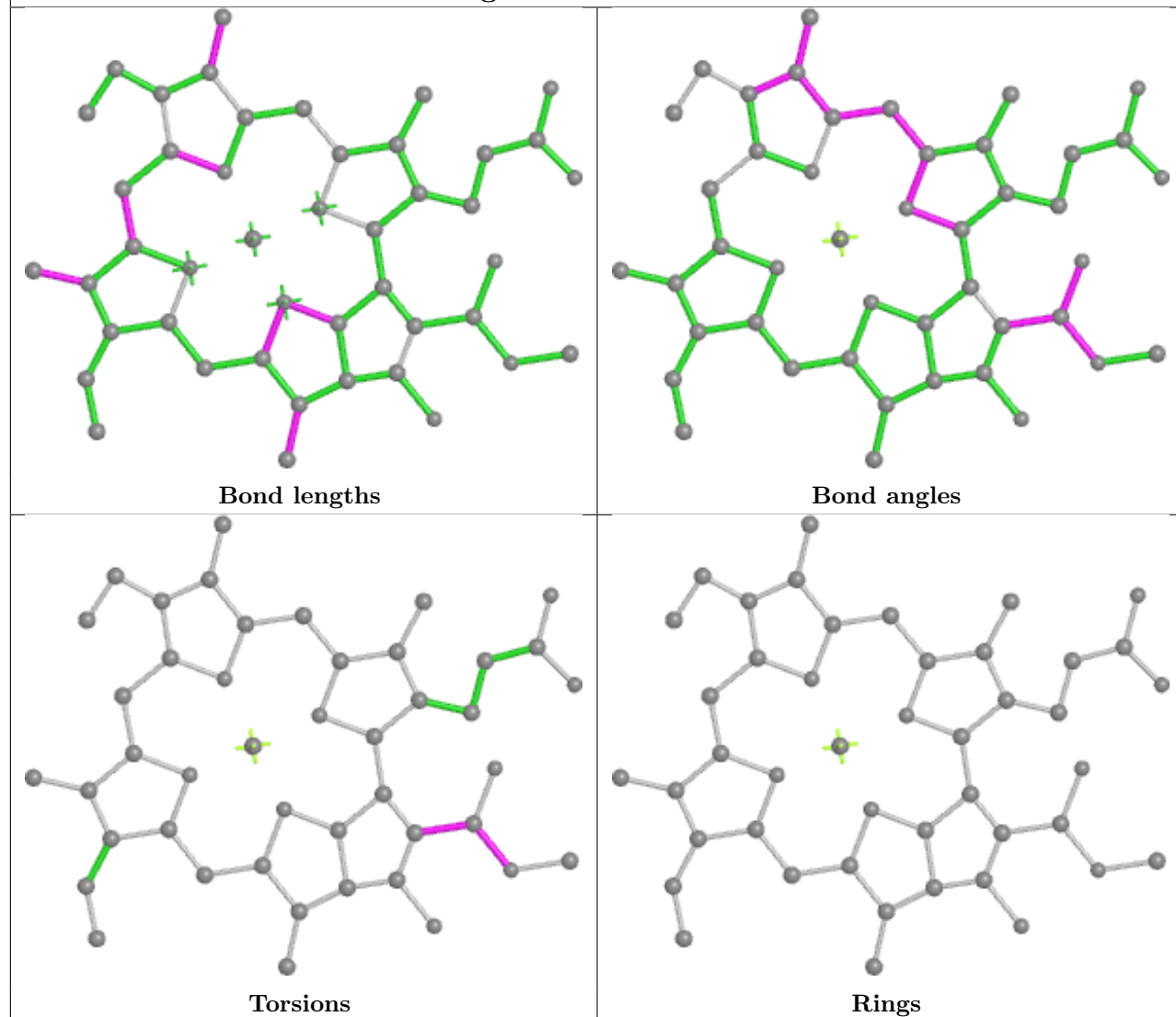


Ligand CLA bA 836

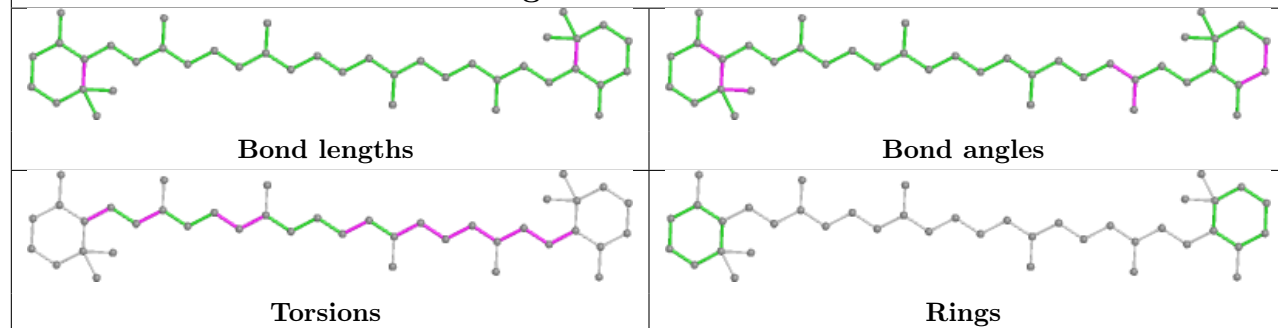


Ligand CLA bB 809**Ligand CLA aB 838**

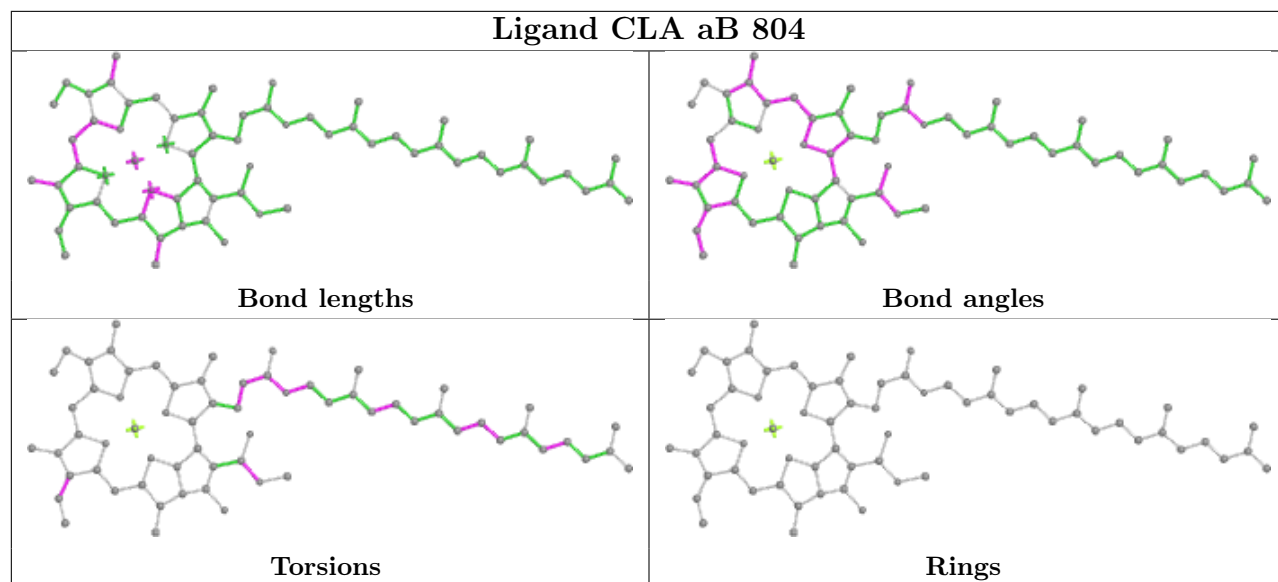
Ligand CLA dB 835



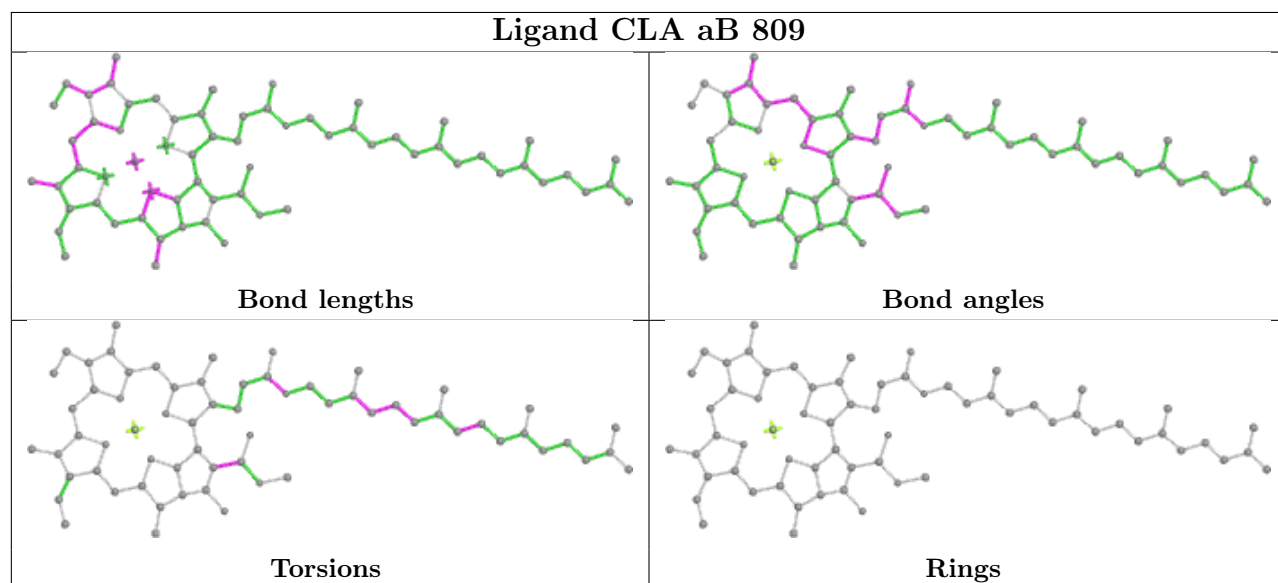
Ligand BCR cB 846



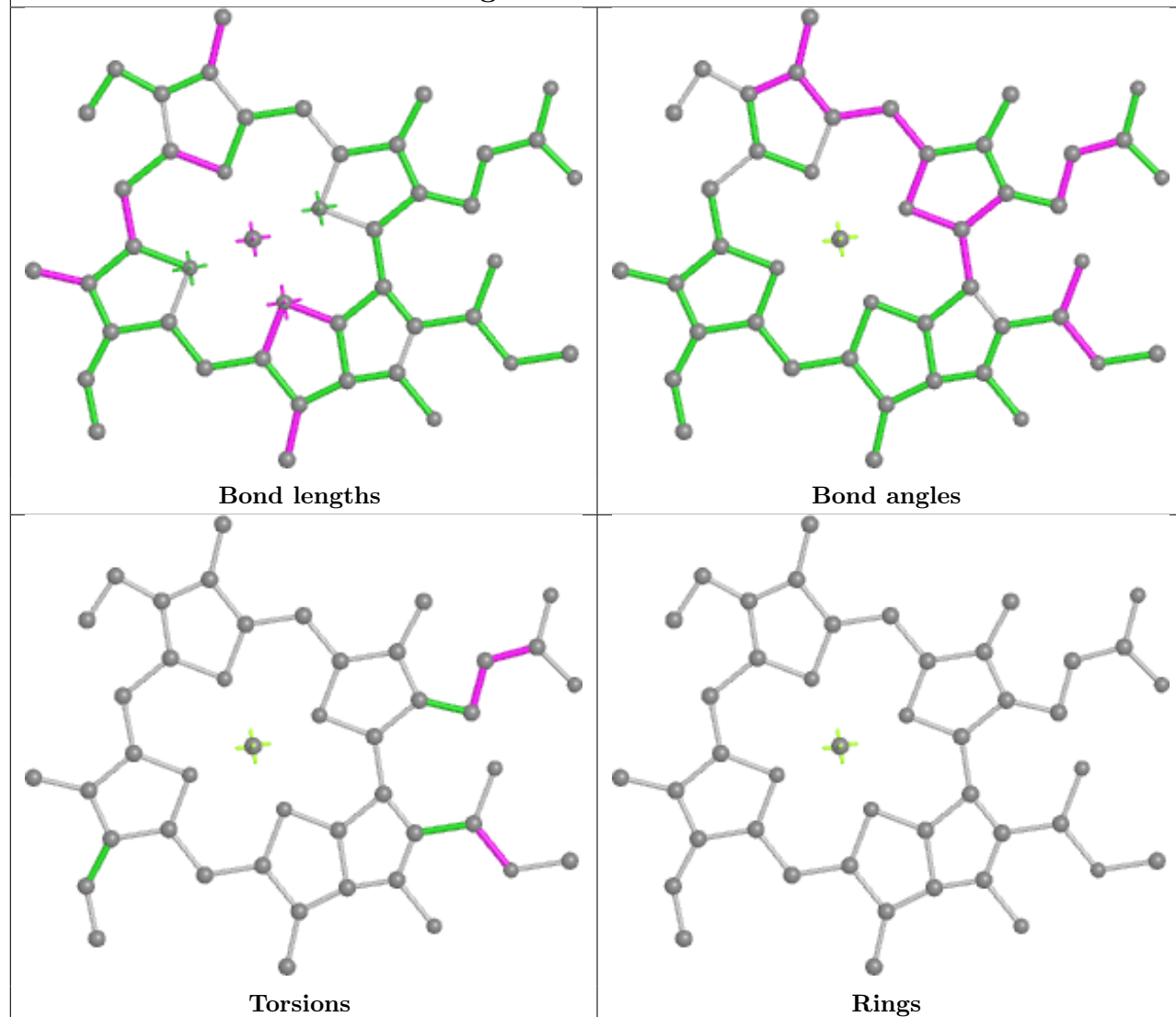
Ligand CLA aB 804



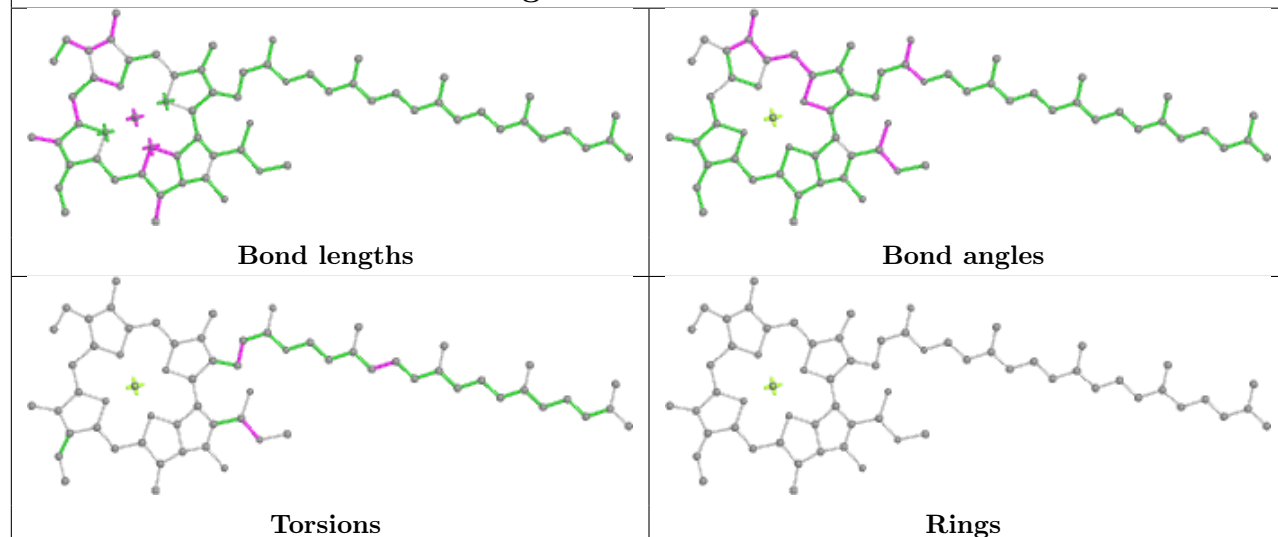
Ligand CLA aB 809

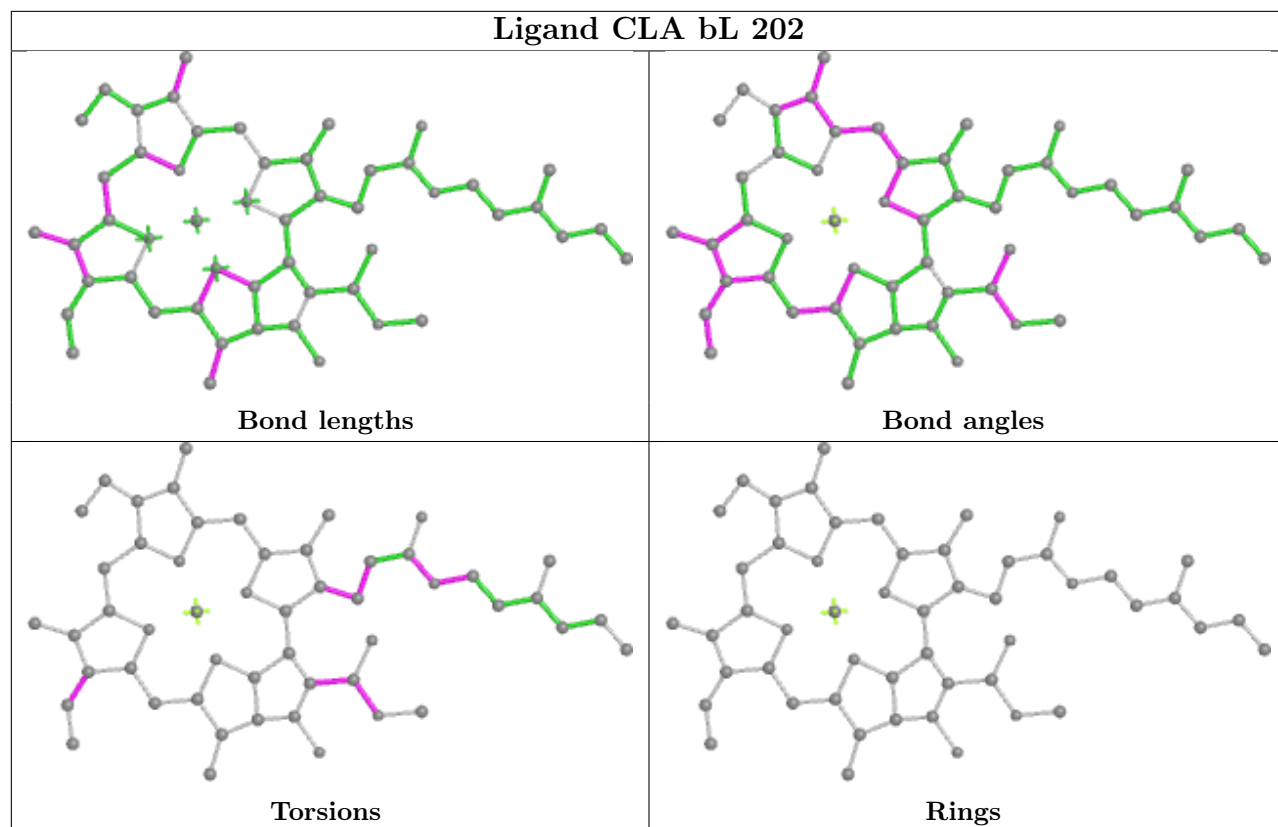


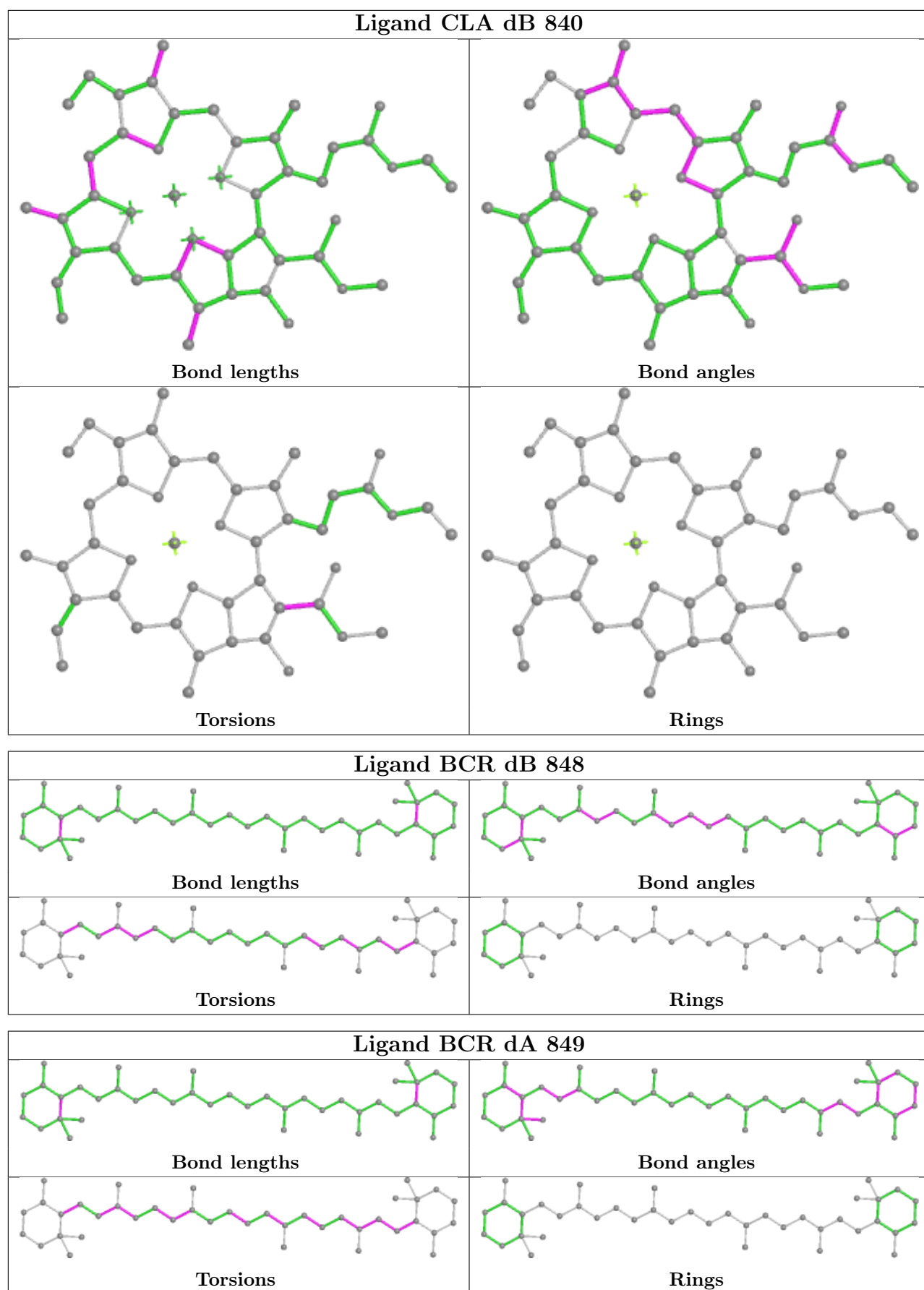
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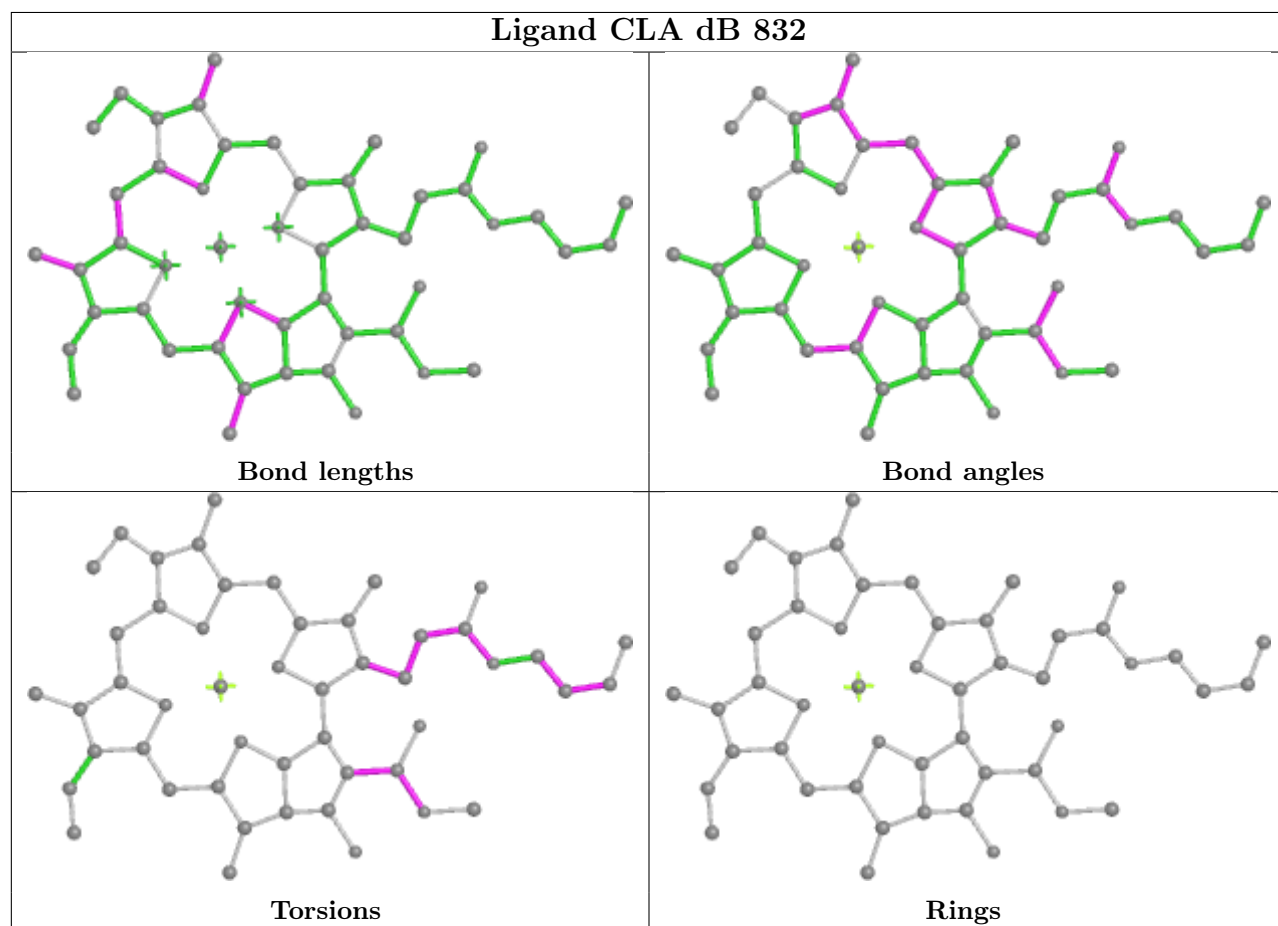
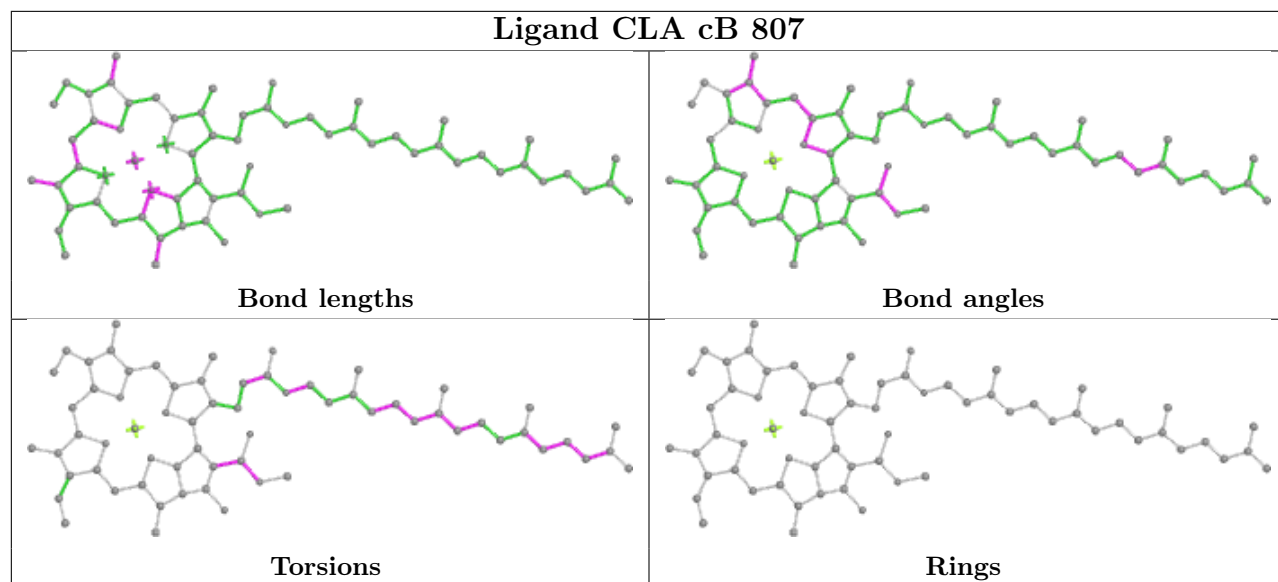


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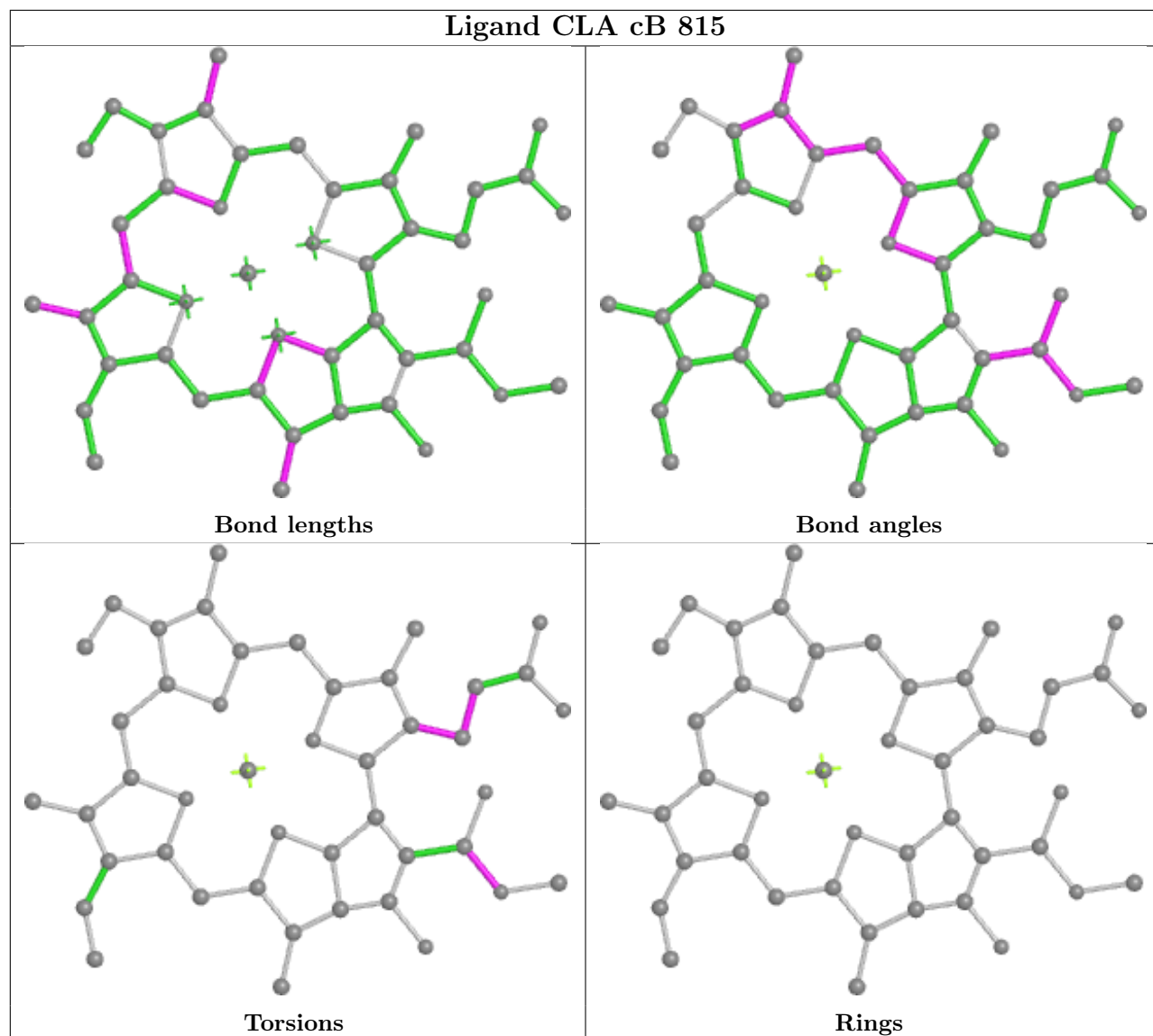


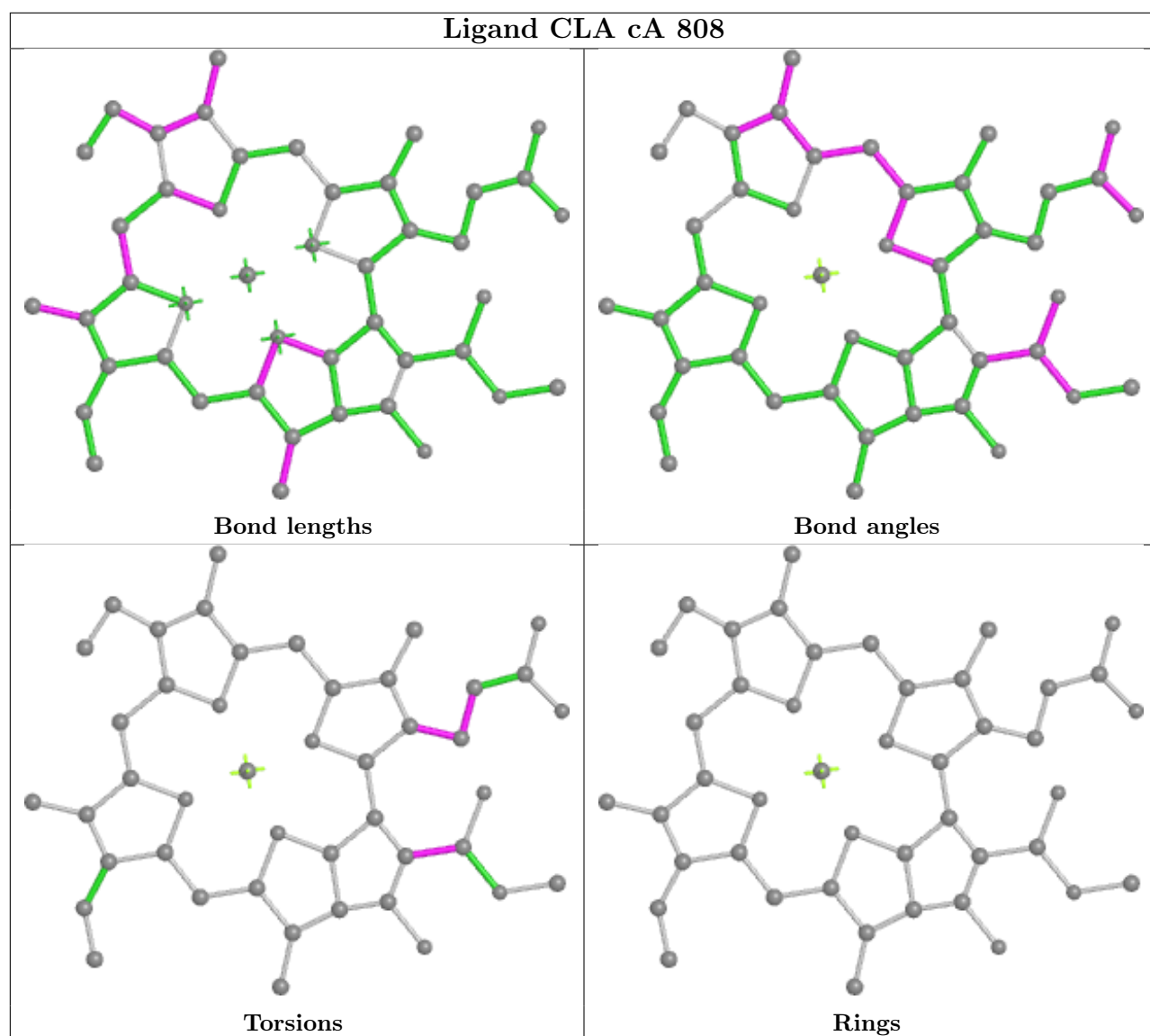


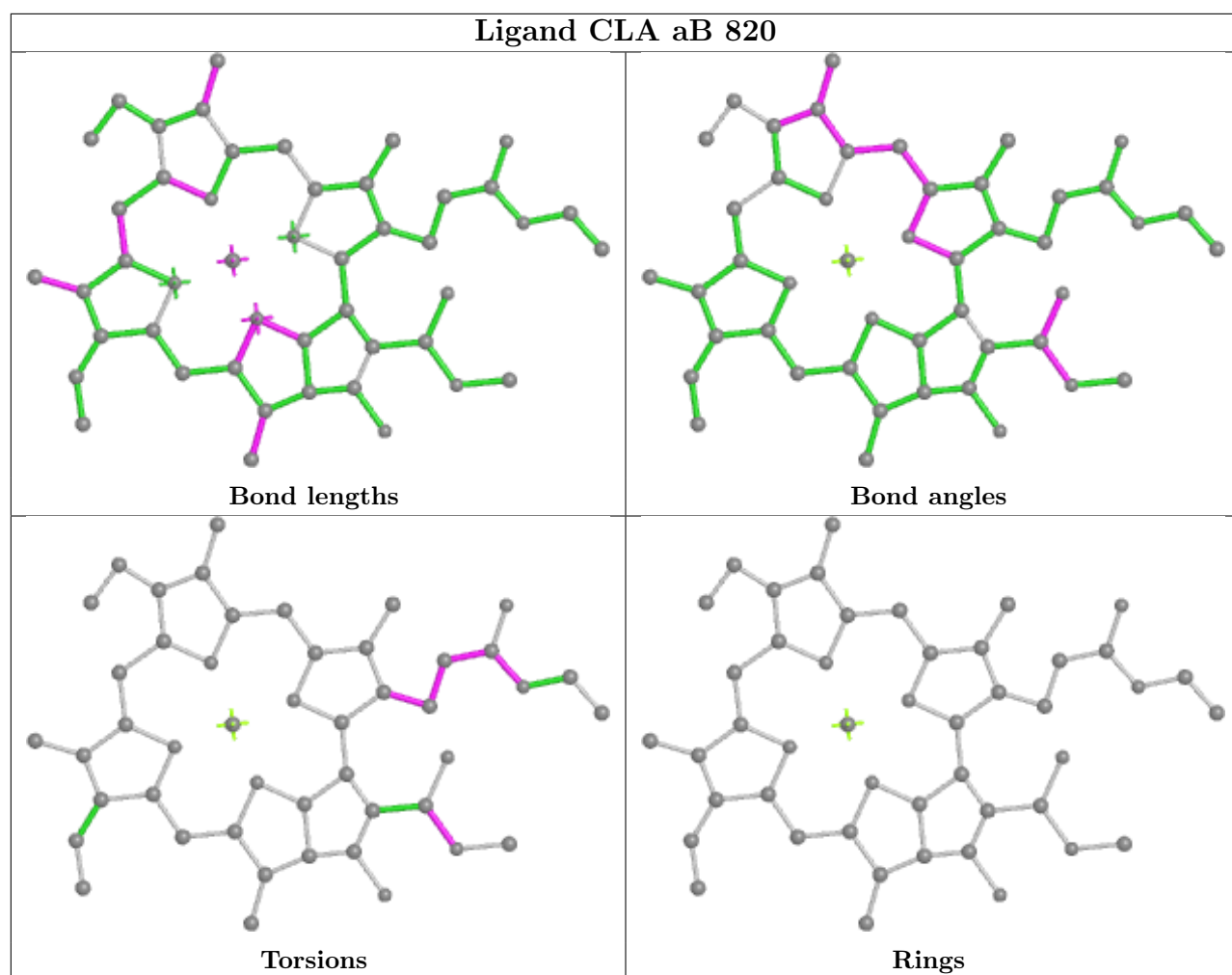


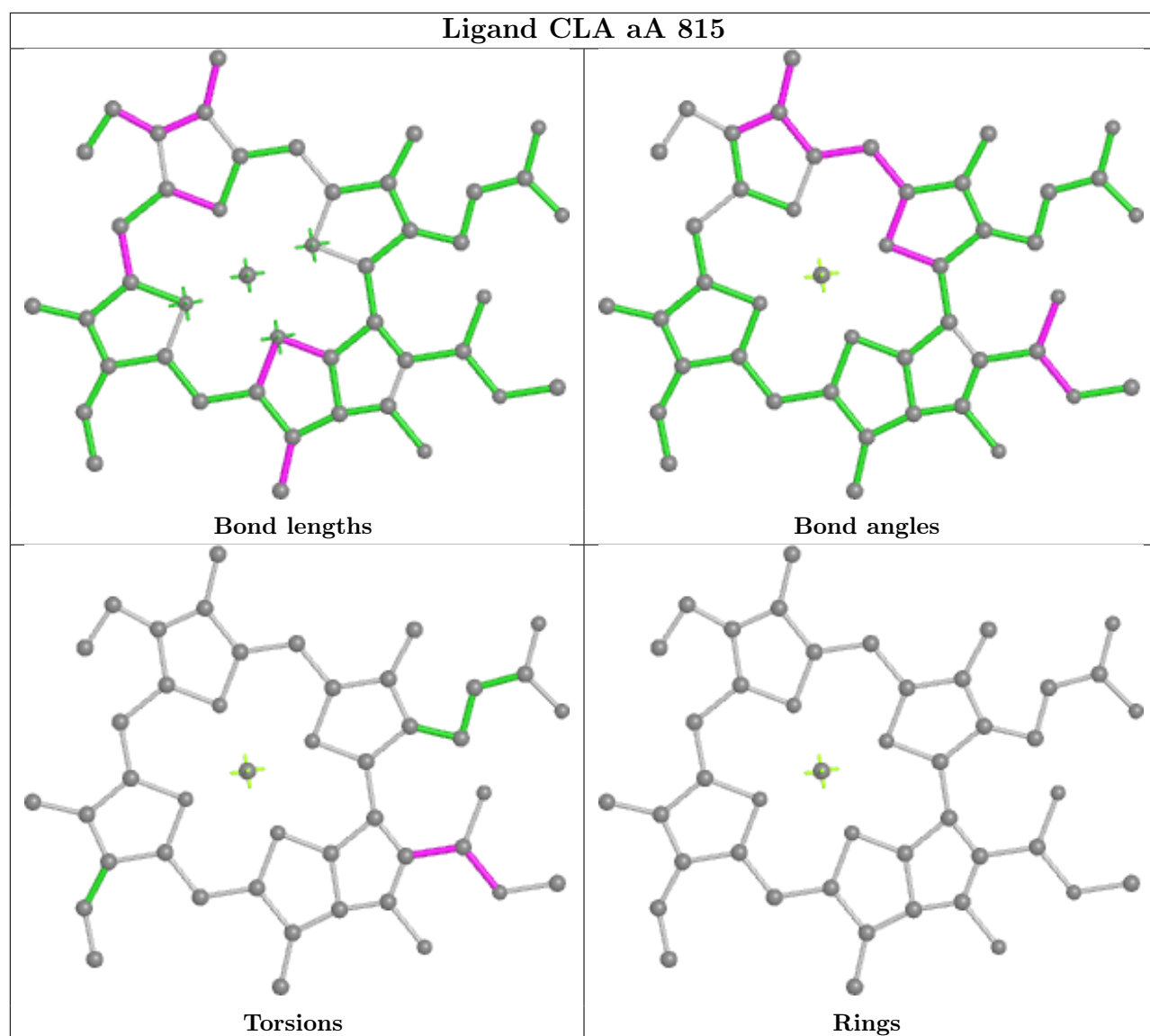


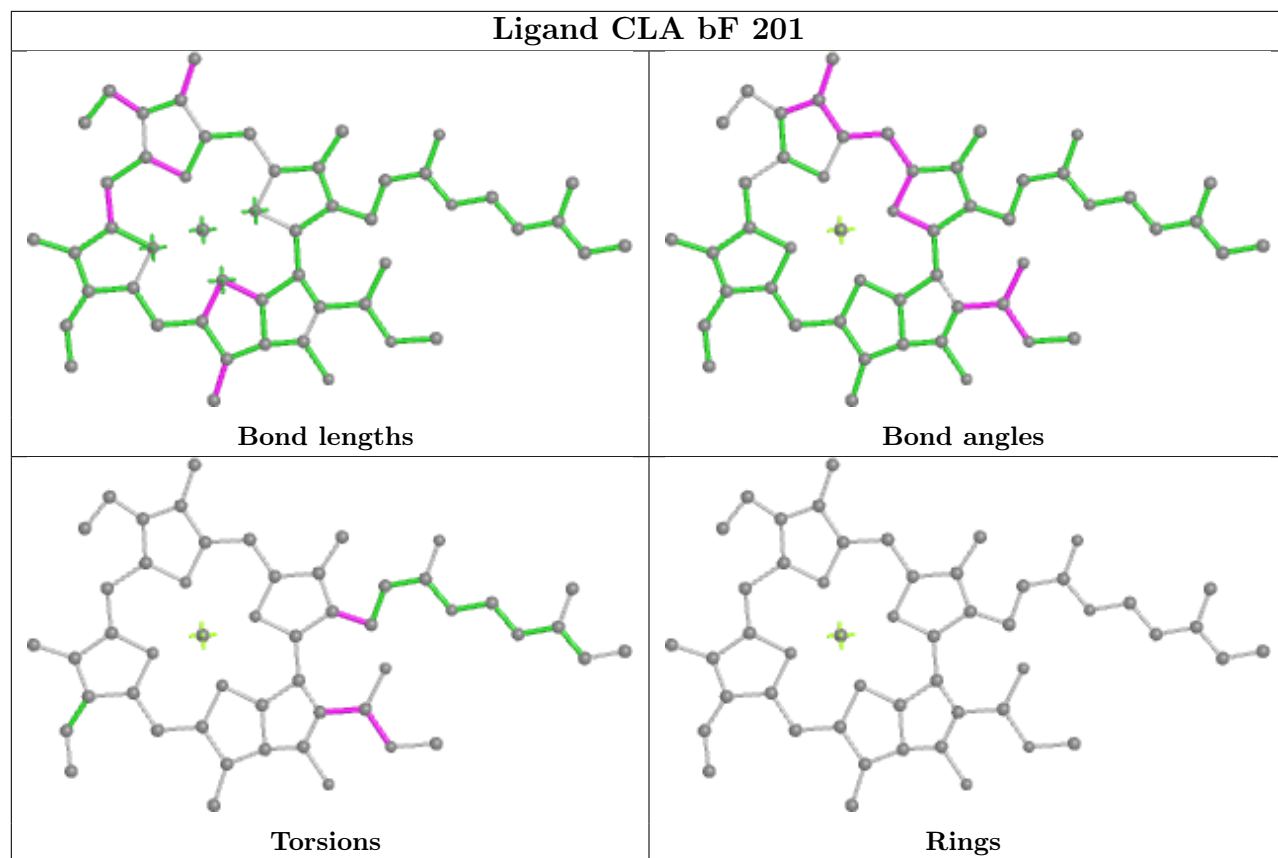
Ligand CLA cB 815



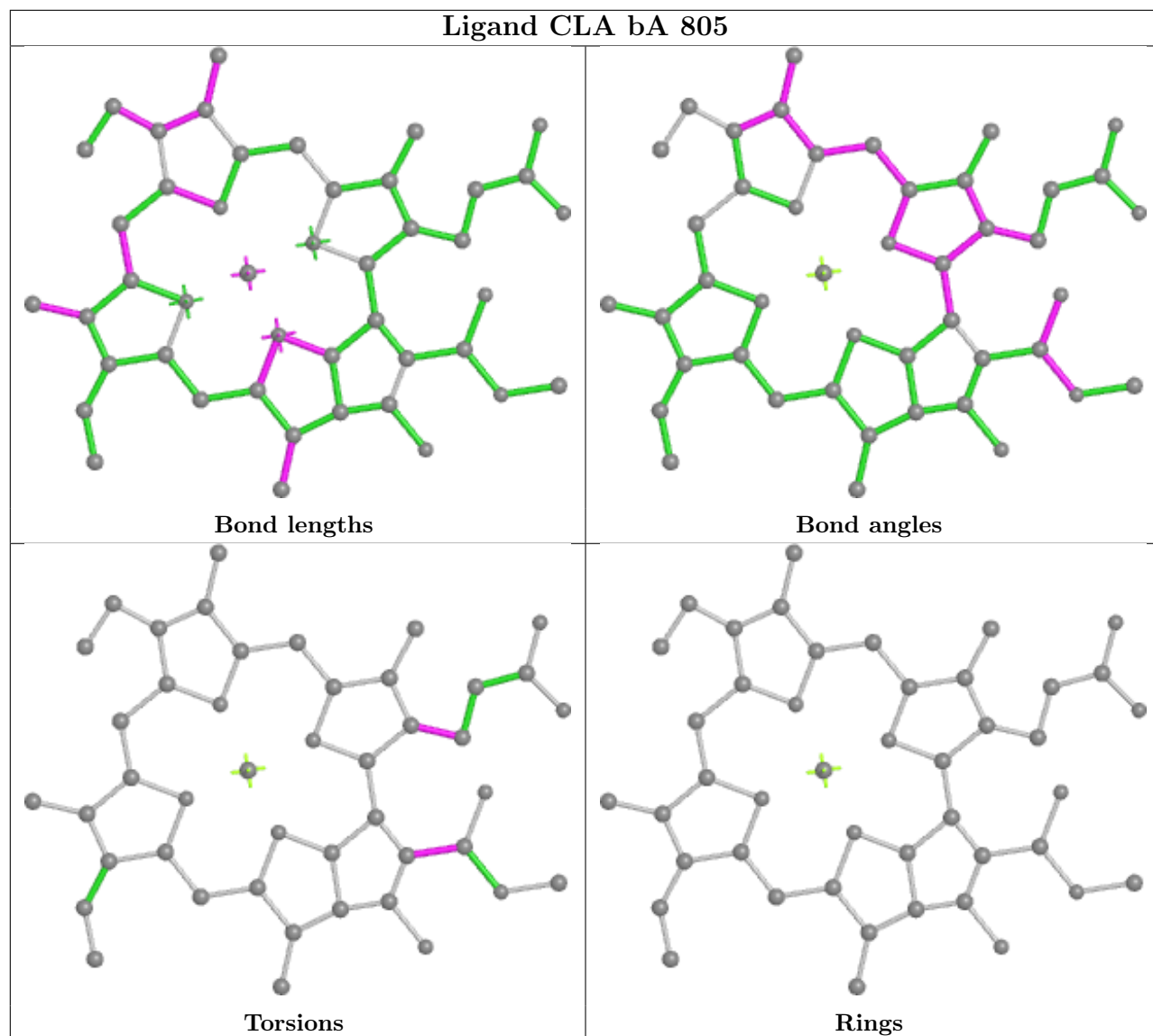


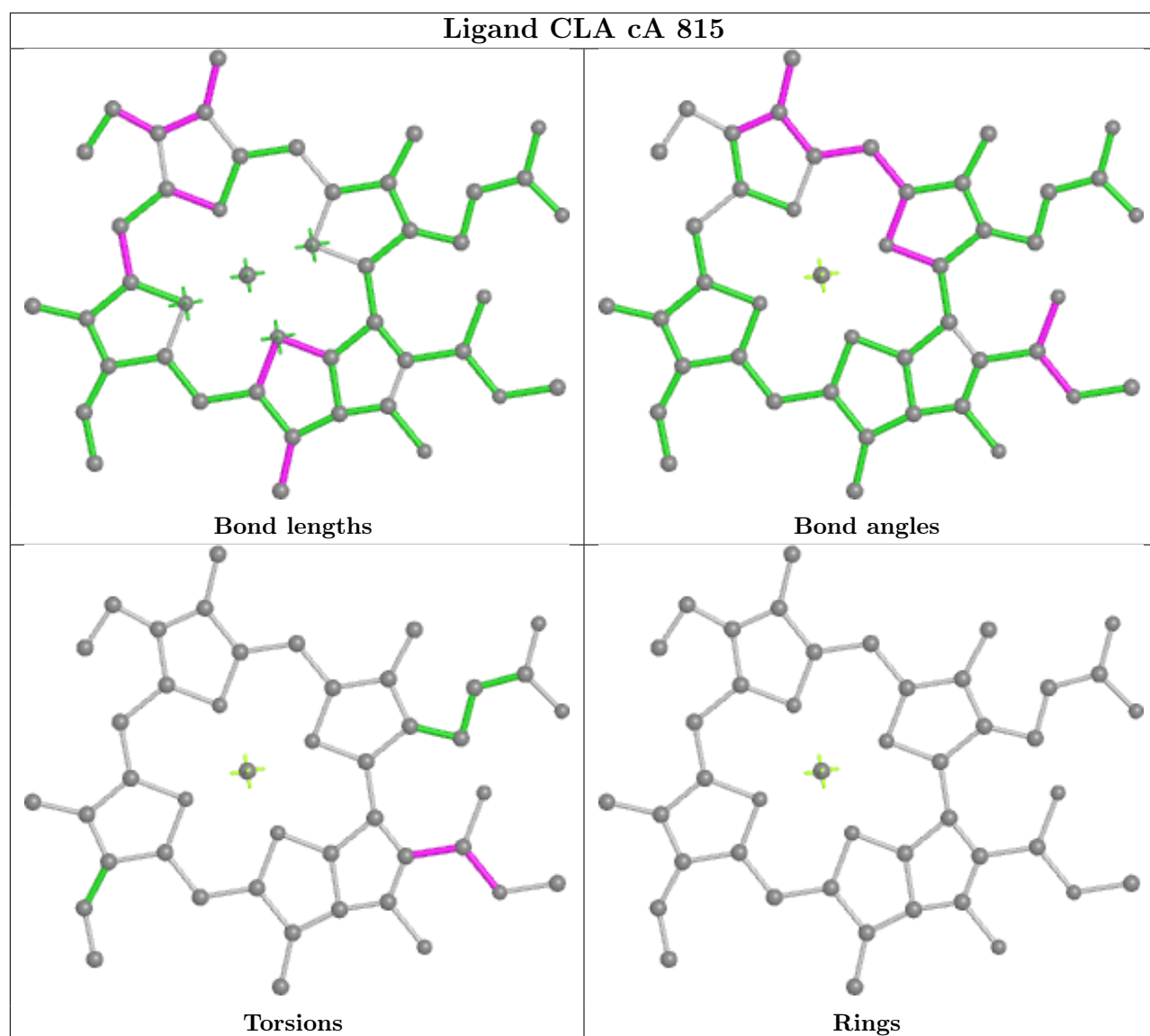




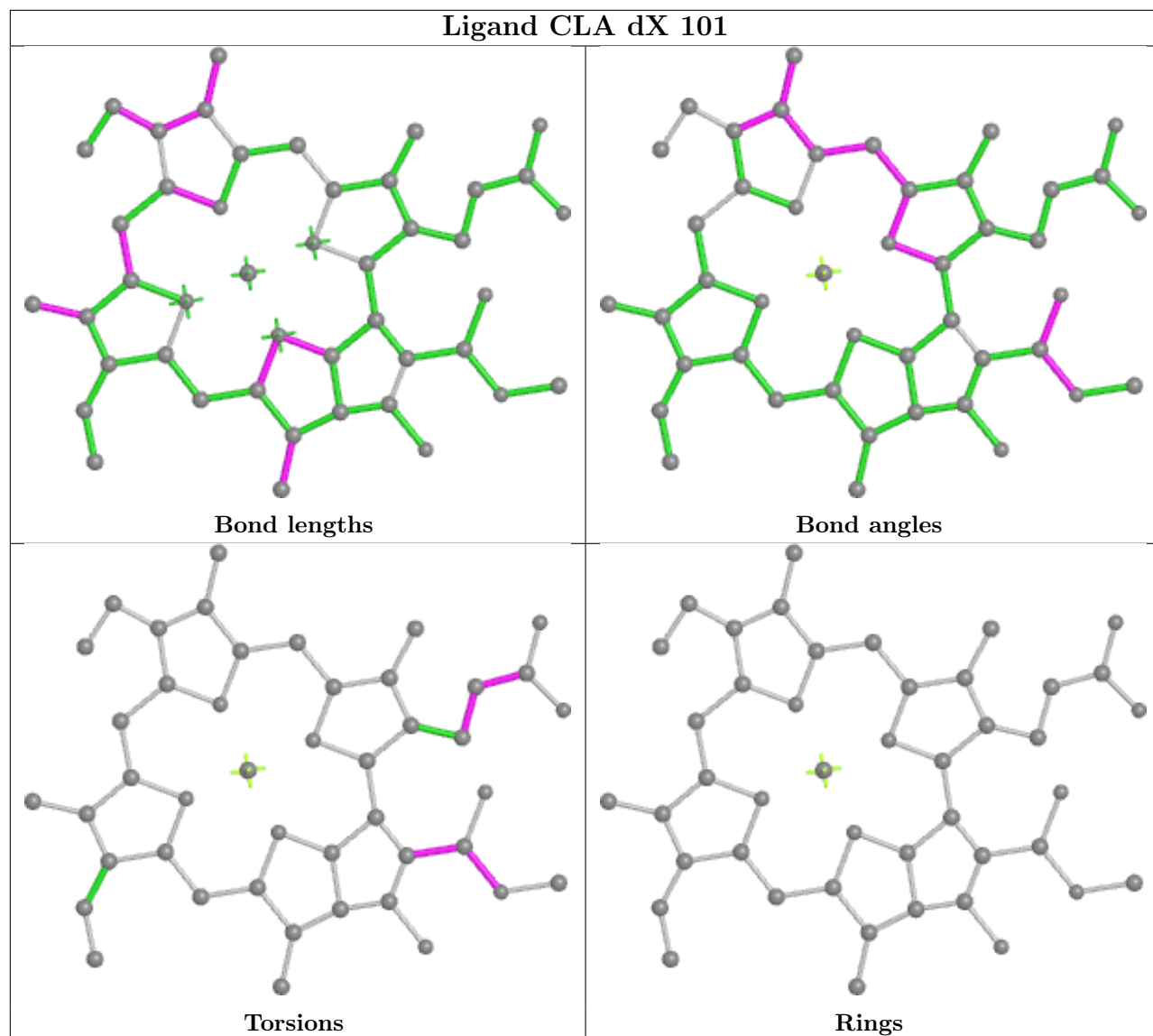


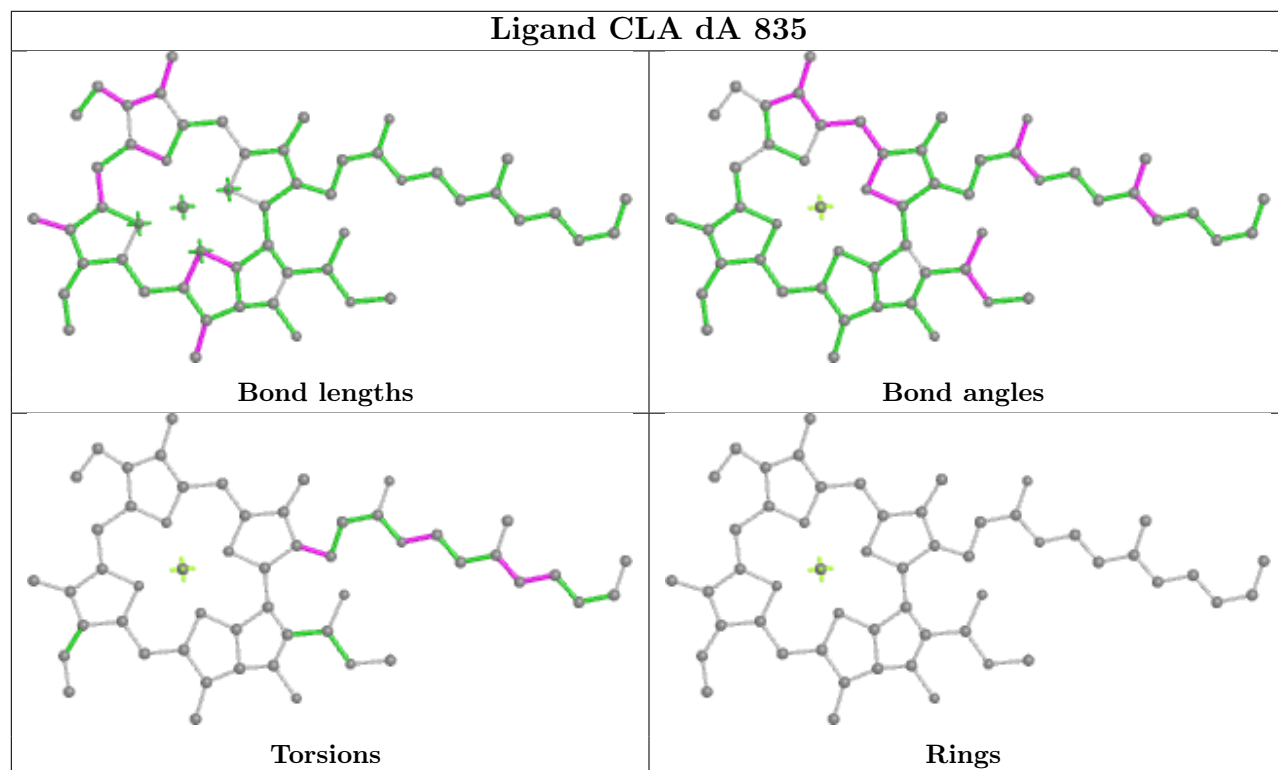
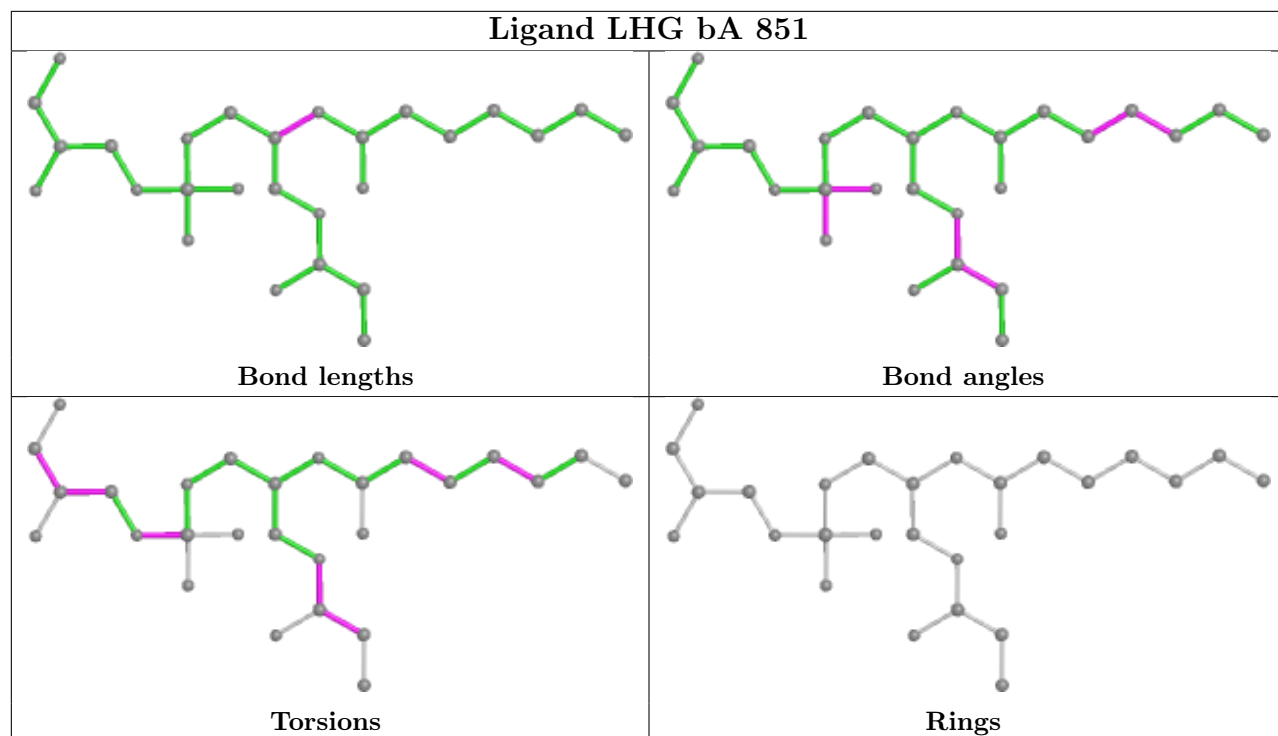
Ligand CLA bA 805



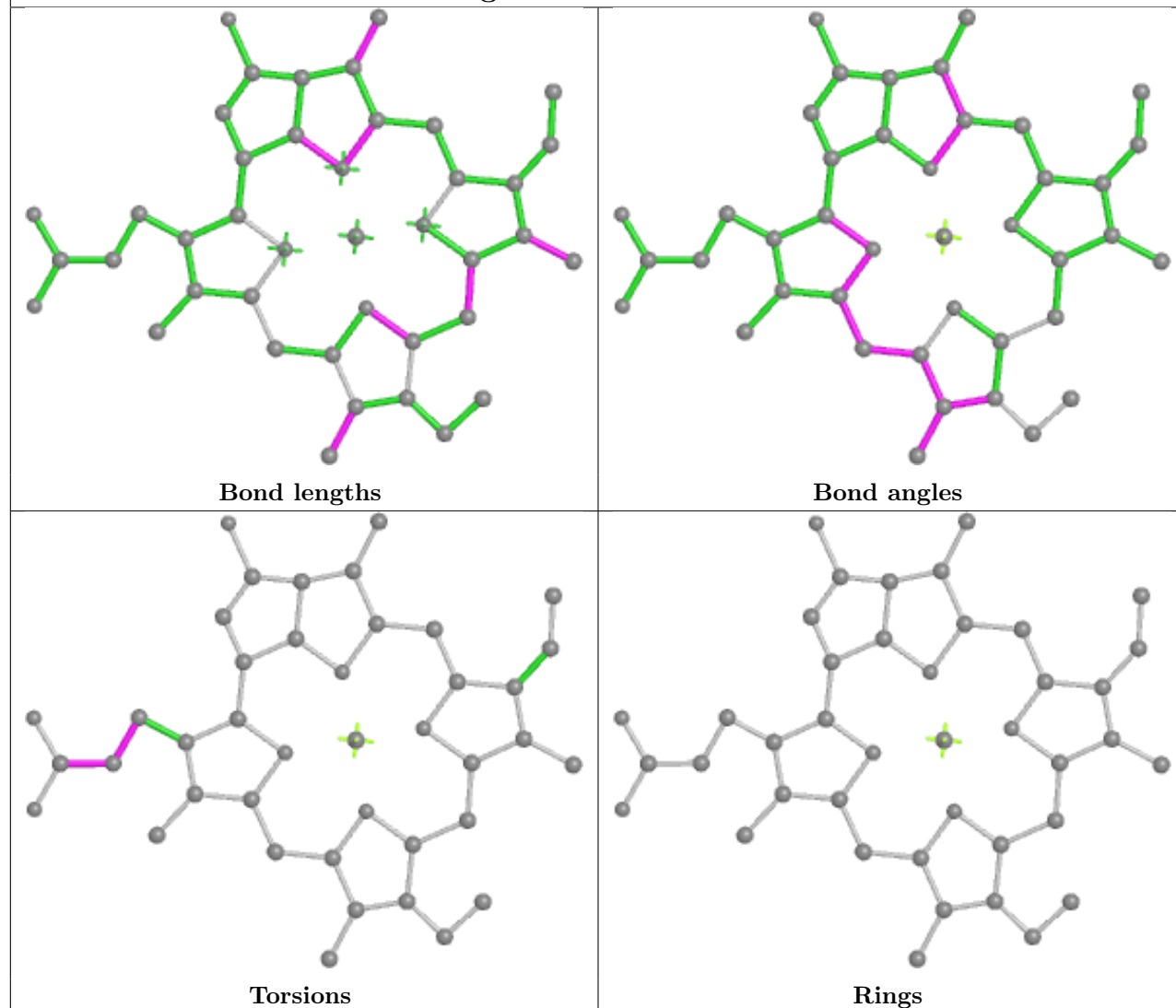


Ligand CLA dX 101

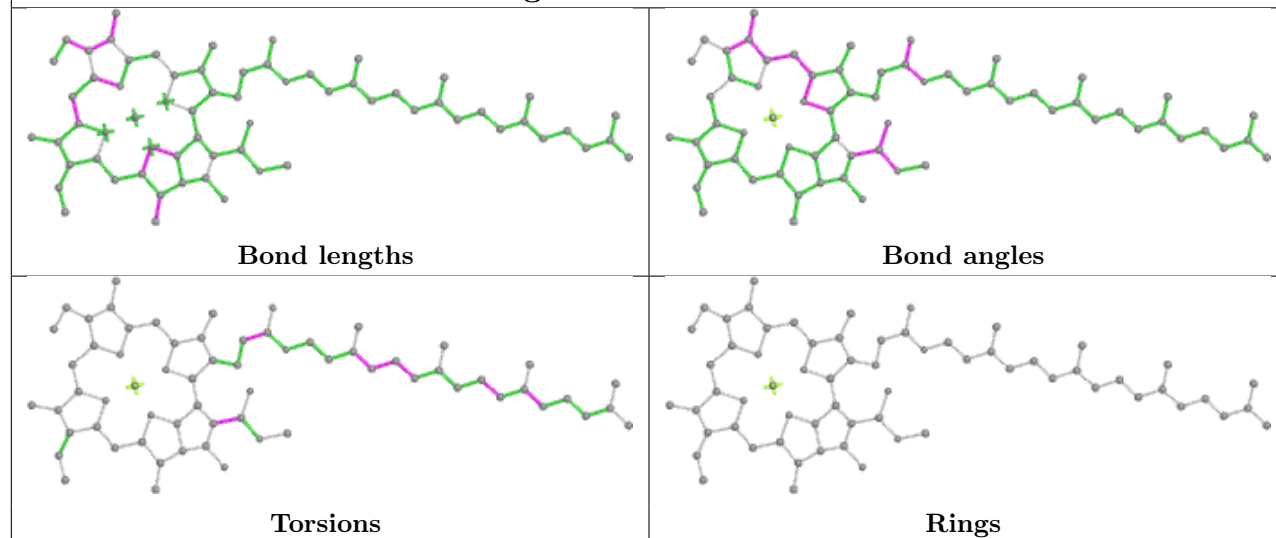


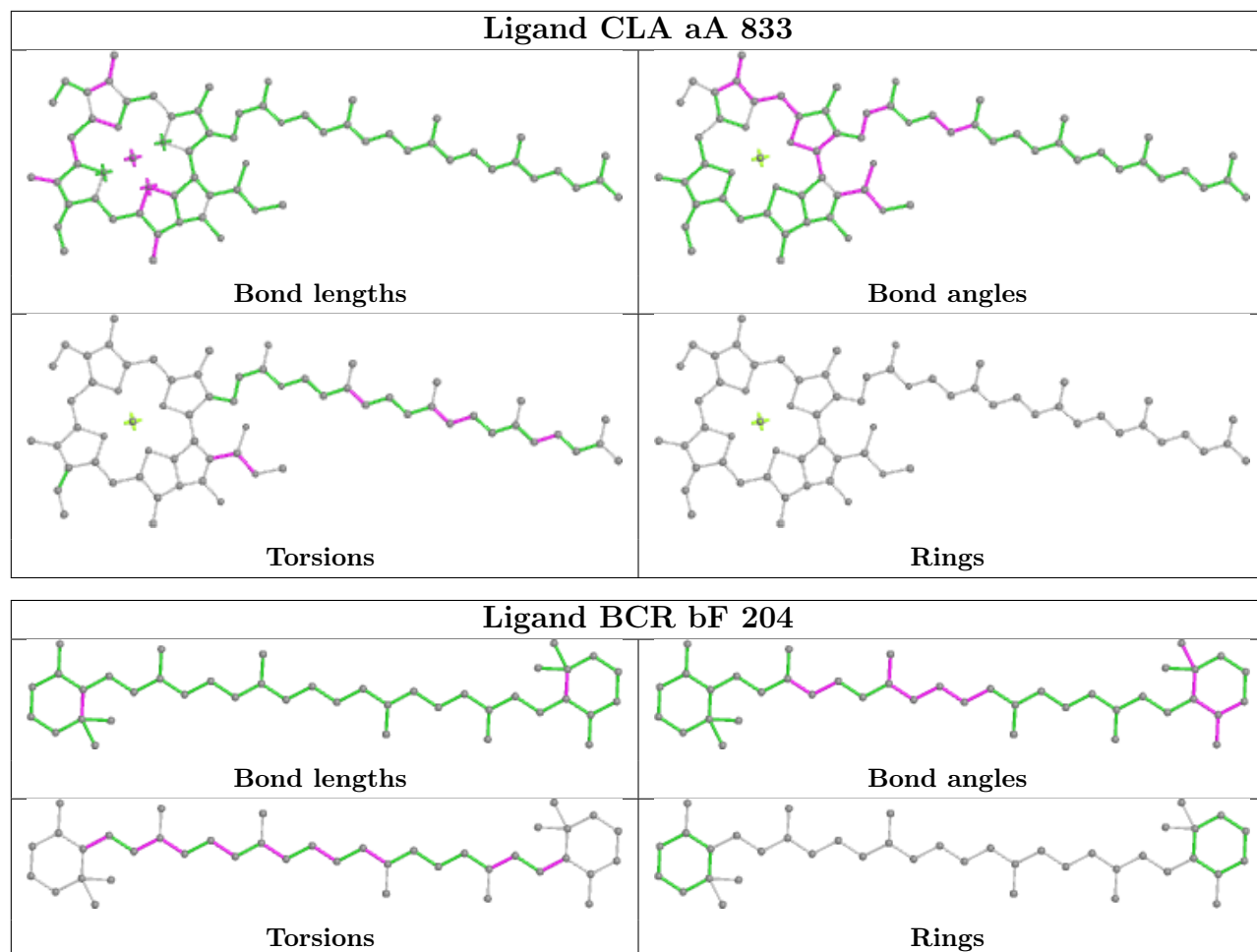


Ligand CLA bK 101

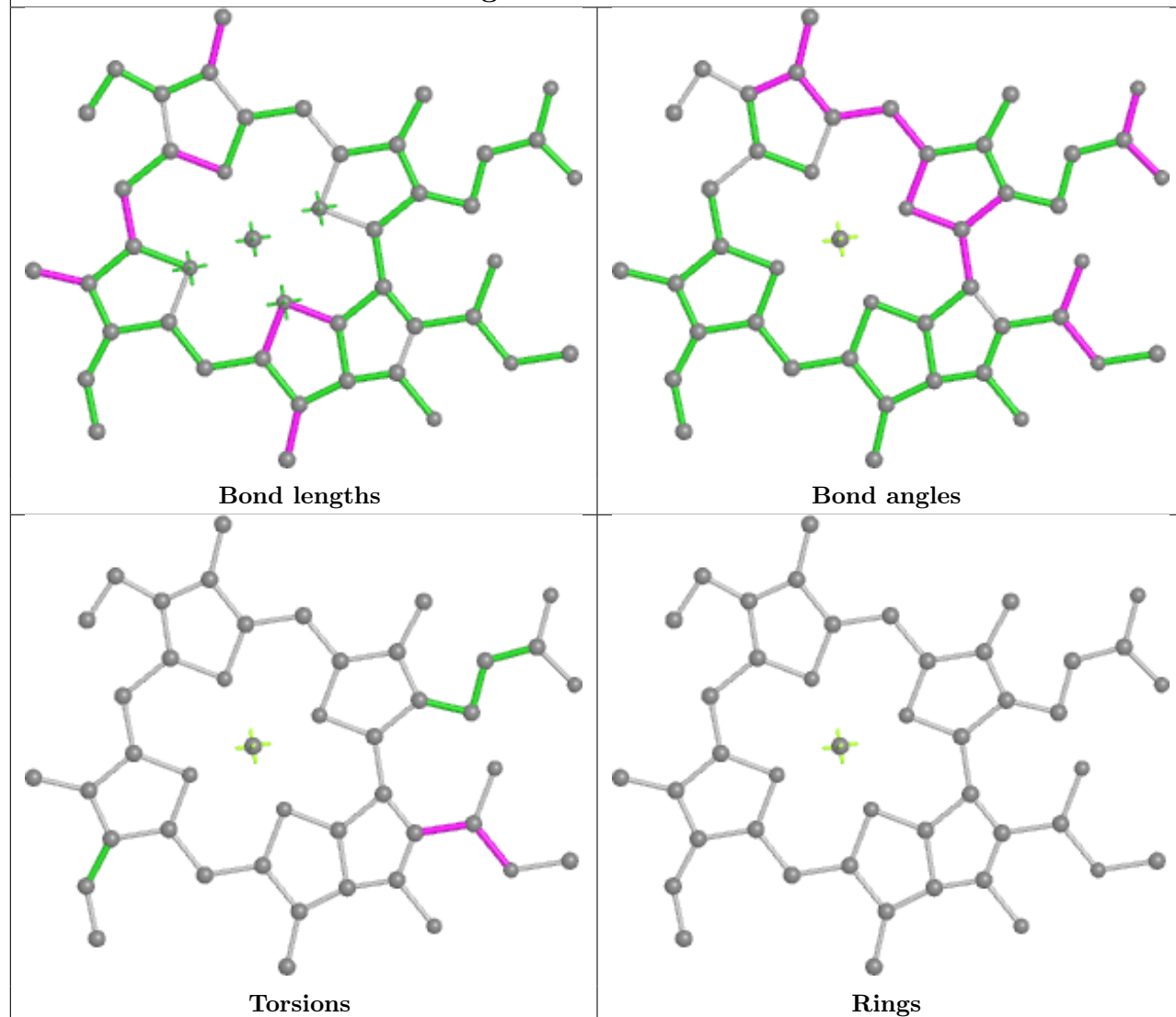


Ligand CLA cA 839

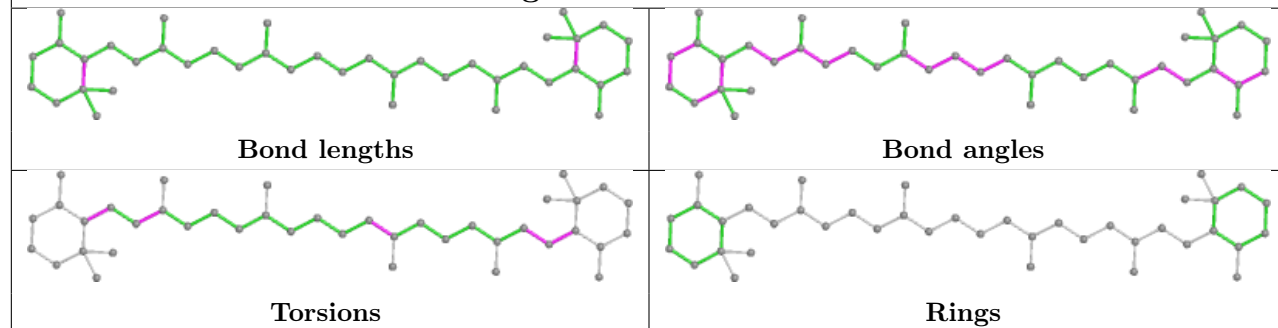




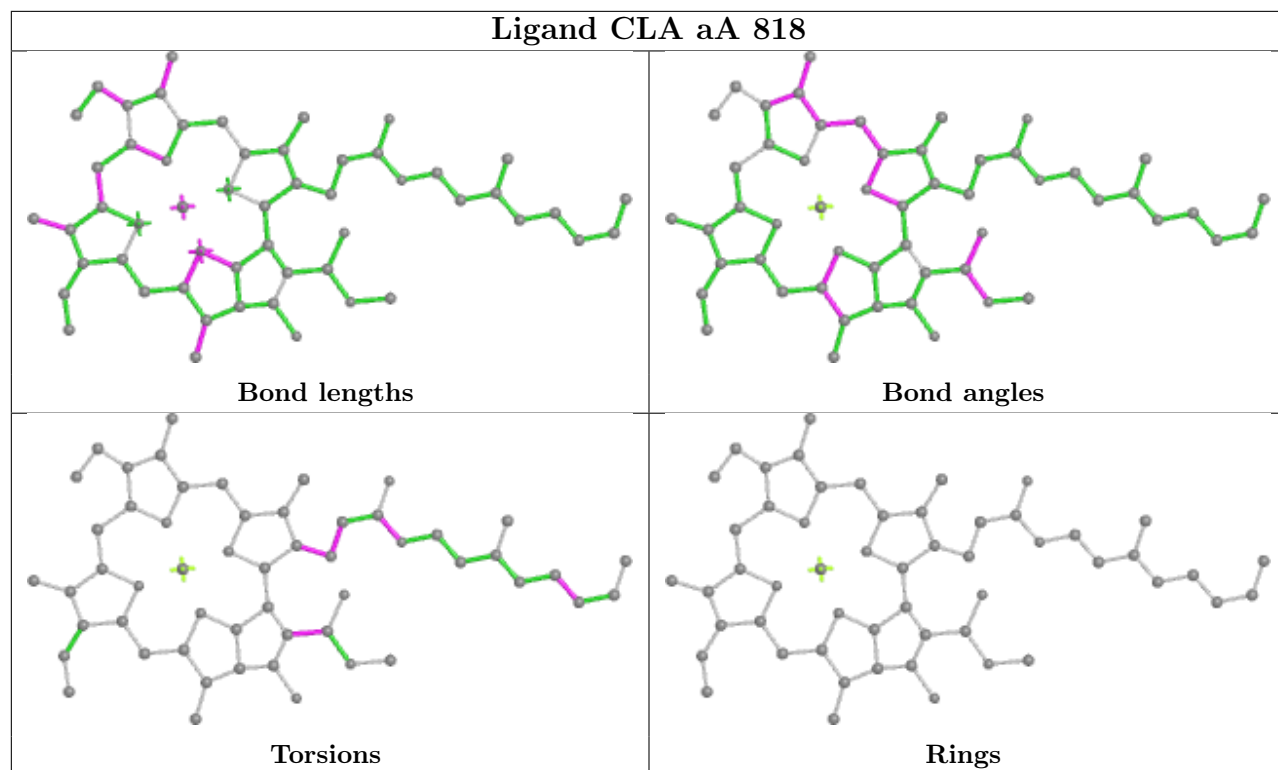
Ligand CLA aA 814



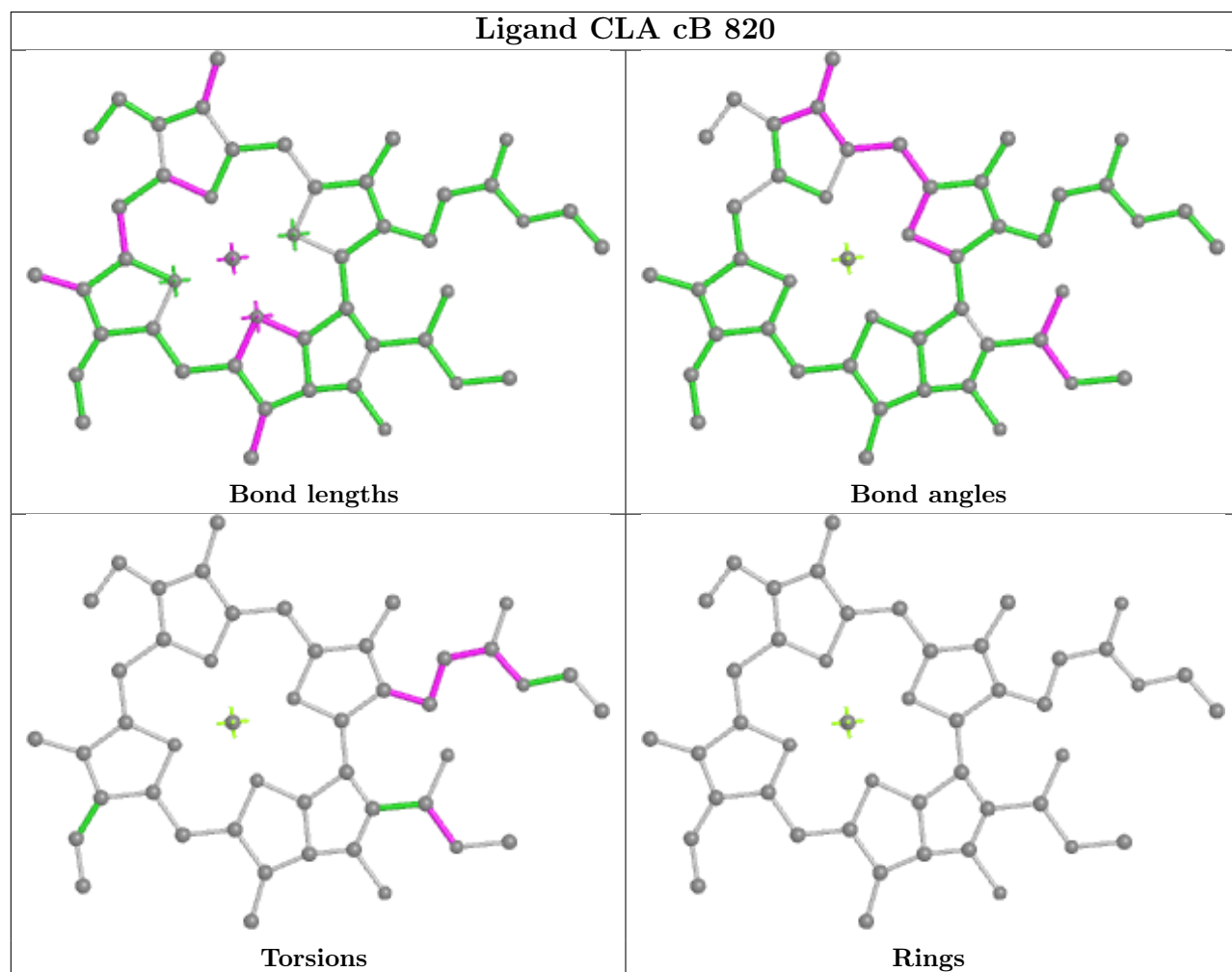
Ligand BCR aB 851



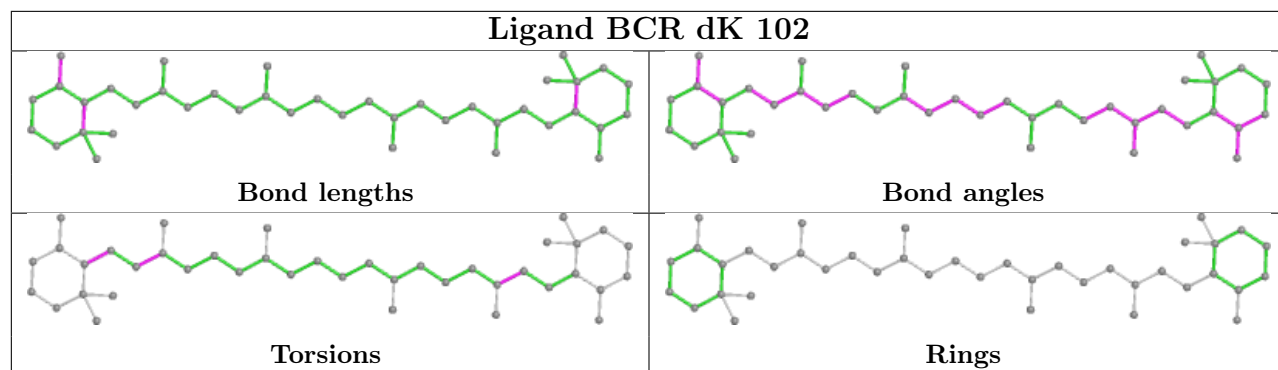
Ligand CLA aA 818



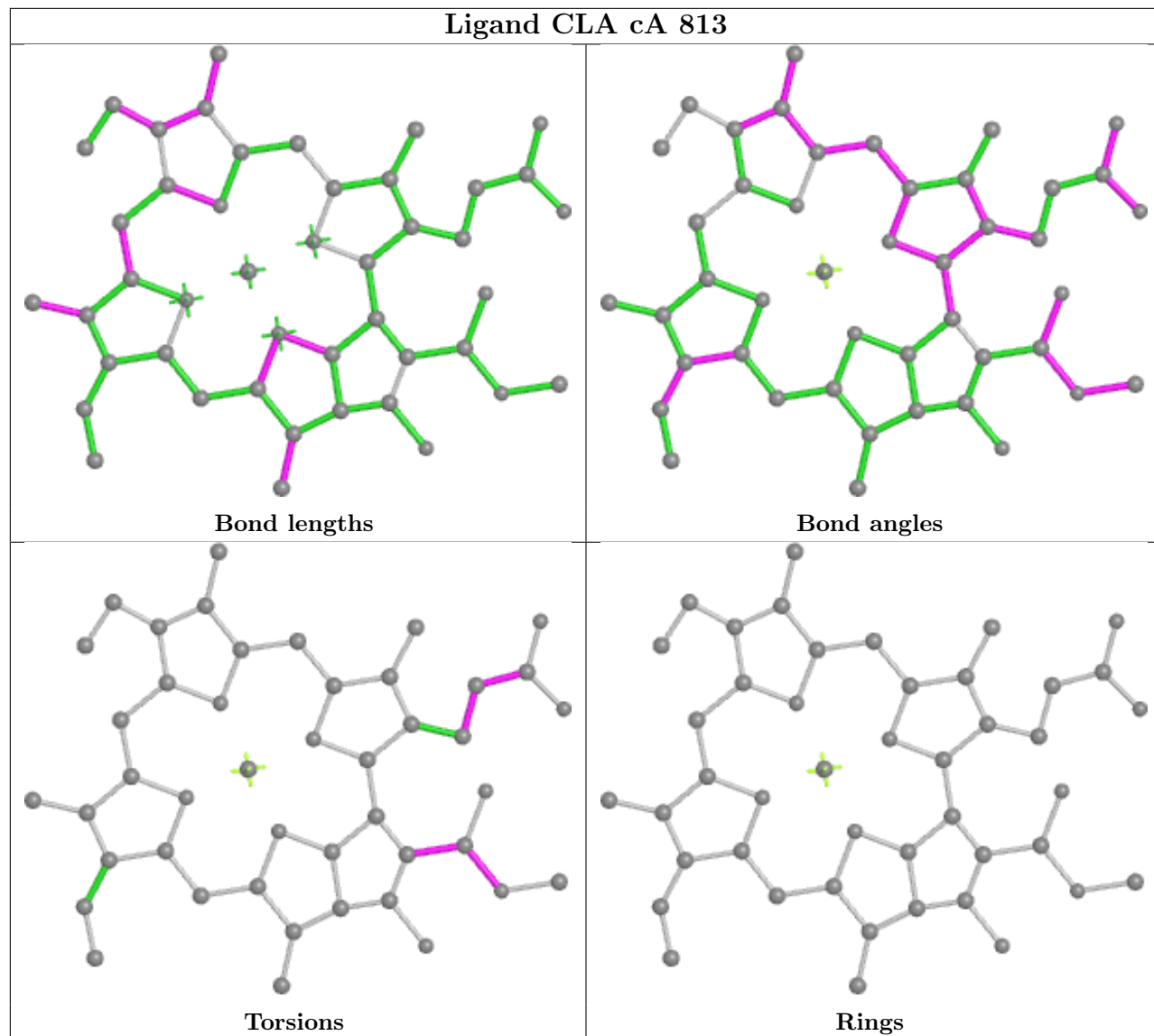
Ligand CLA cB 820

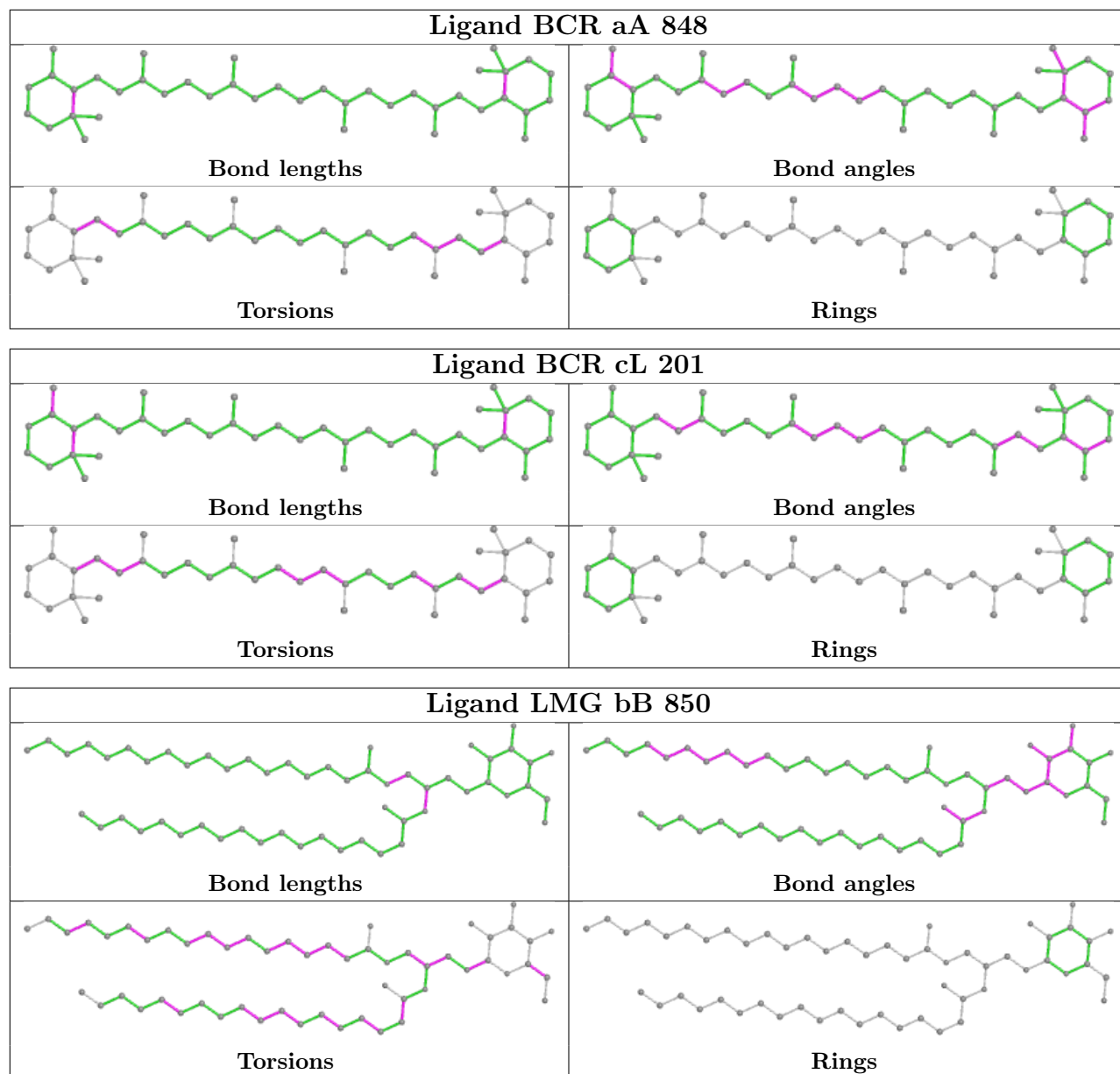


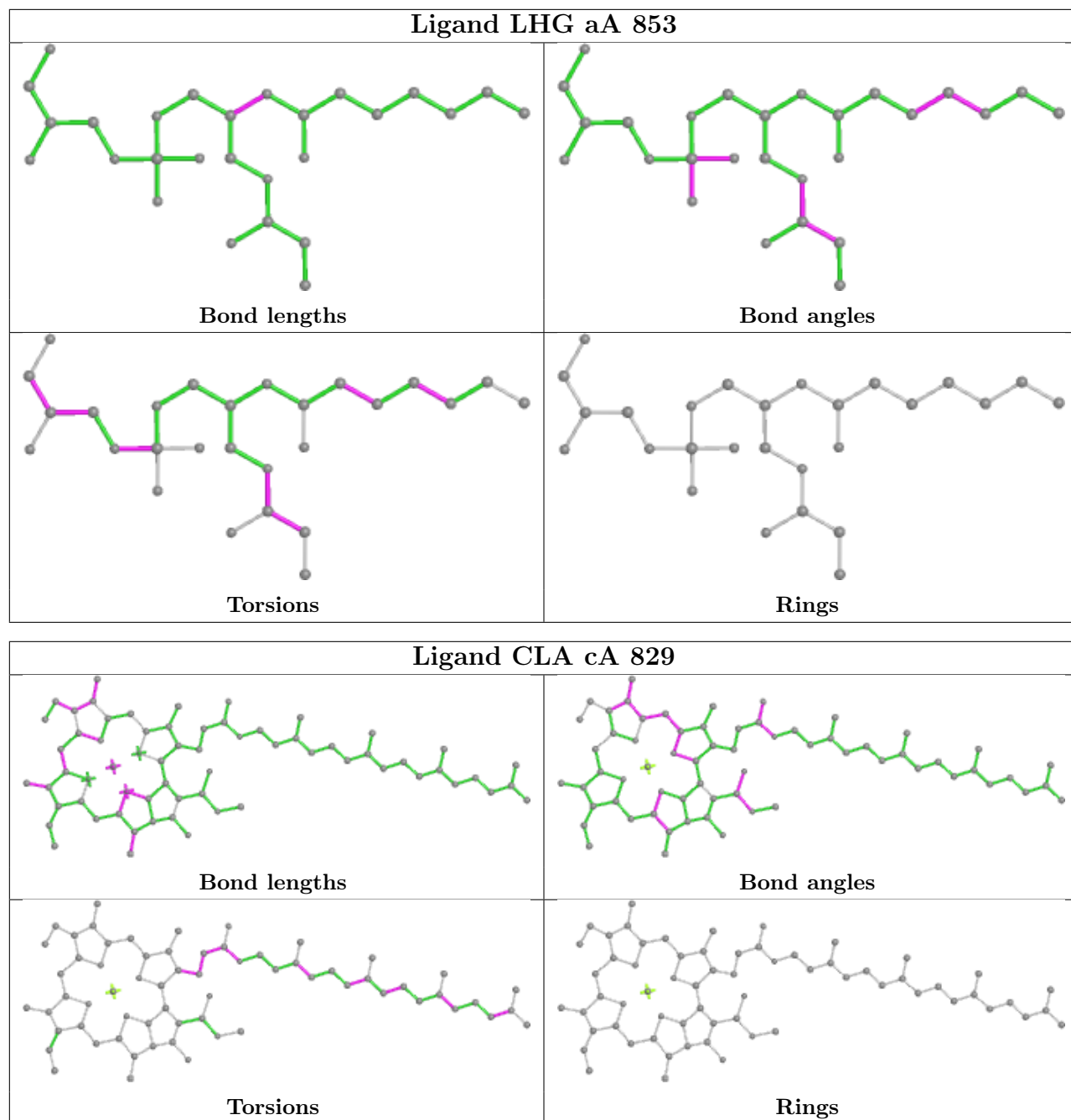
Ligand BCR dK 102



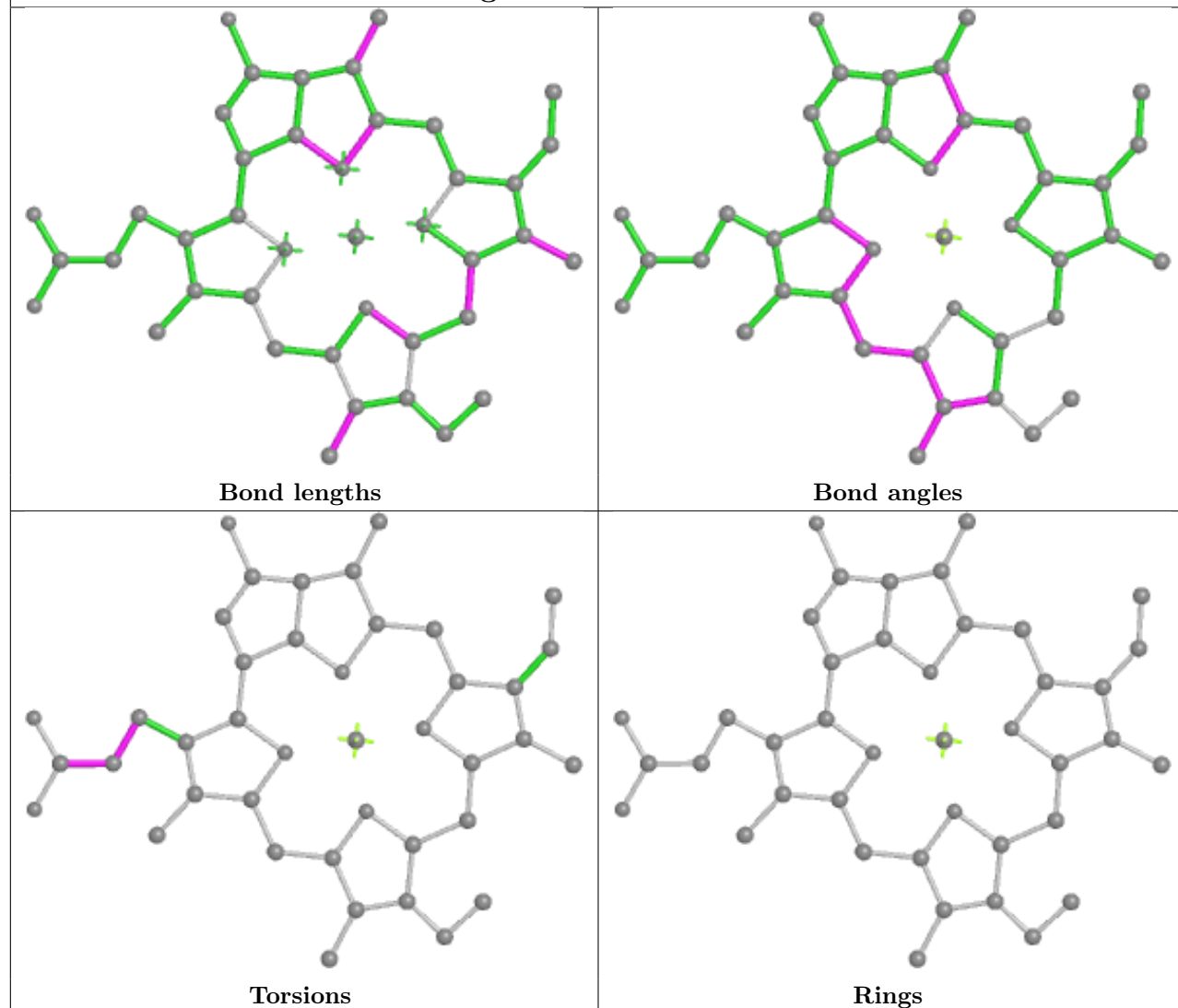
Ligand CLA cA 813



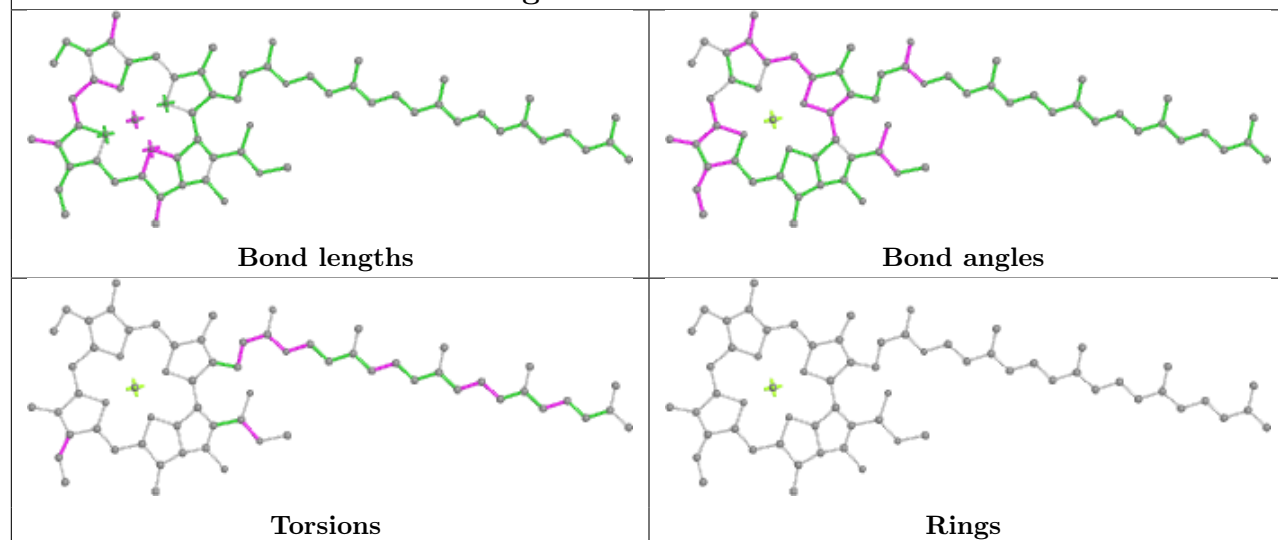


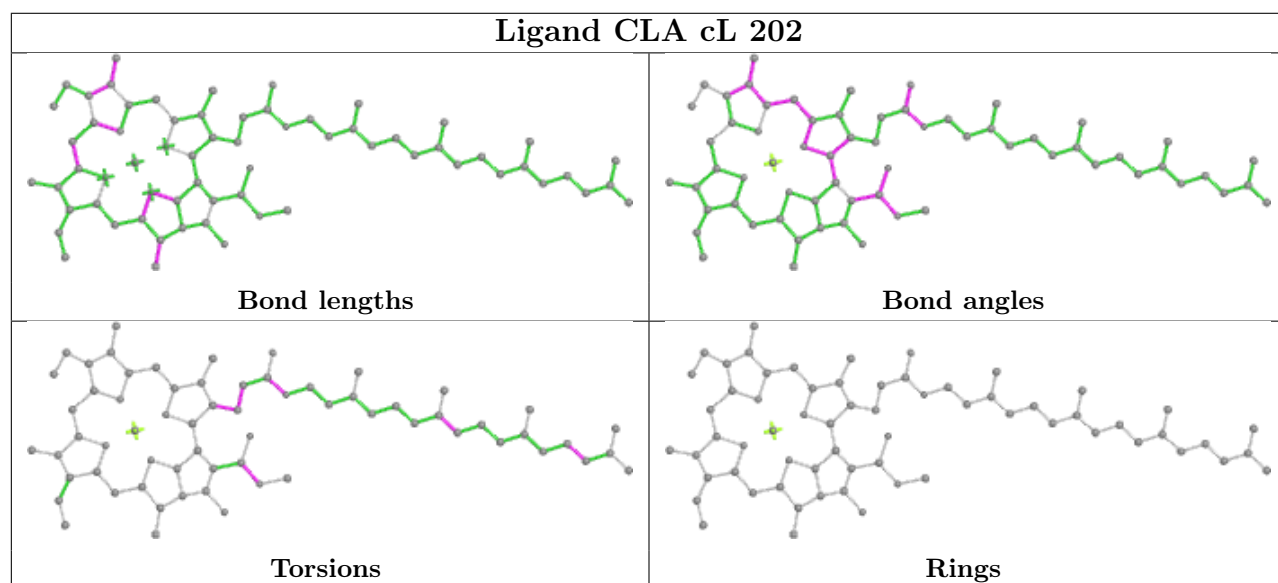
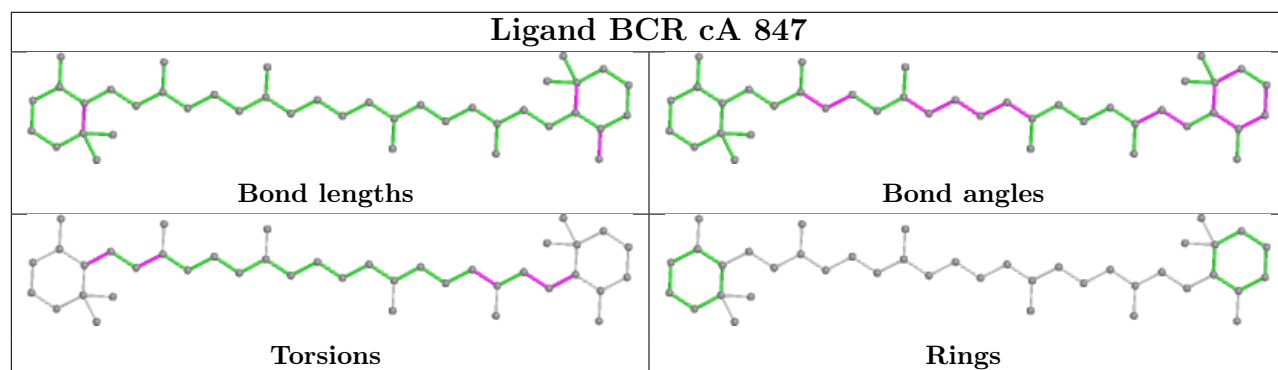
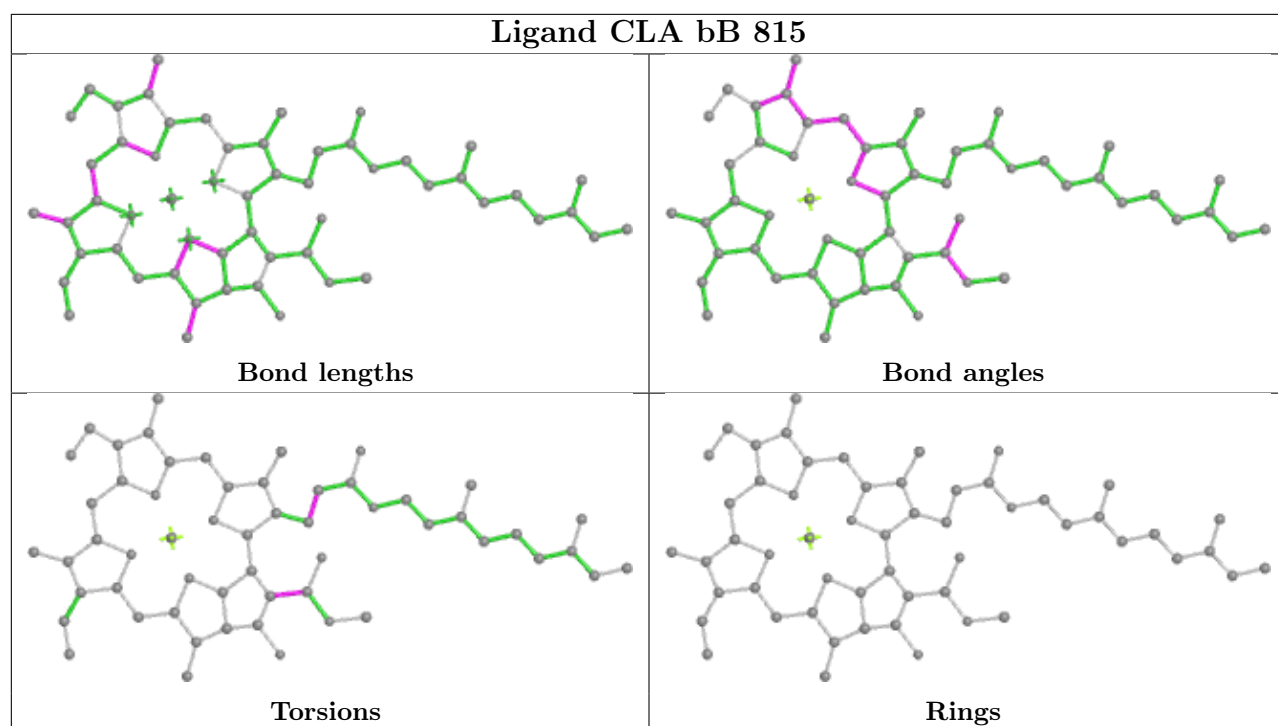


Ligand CLA dK 101

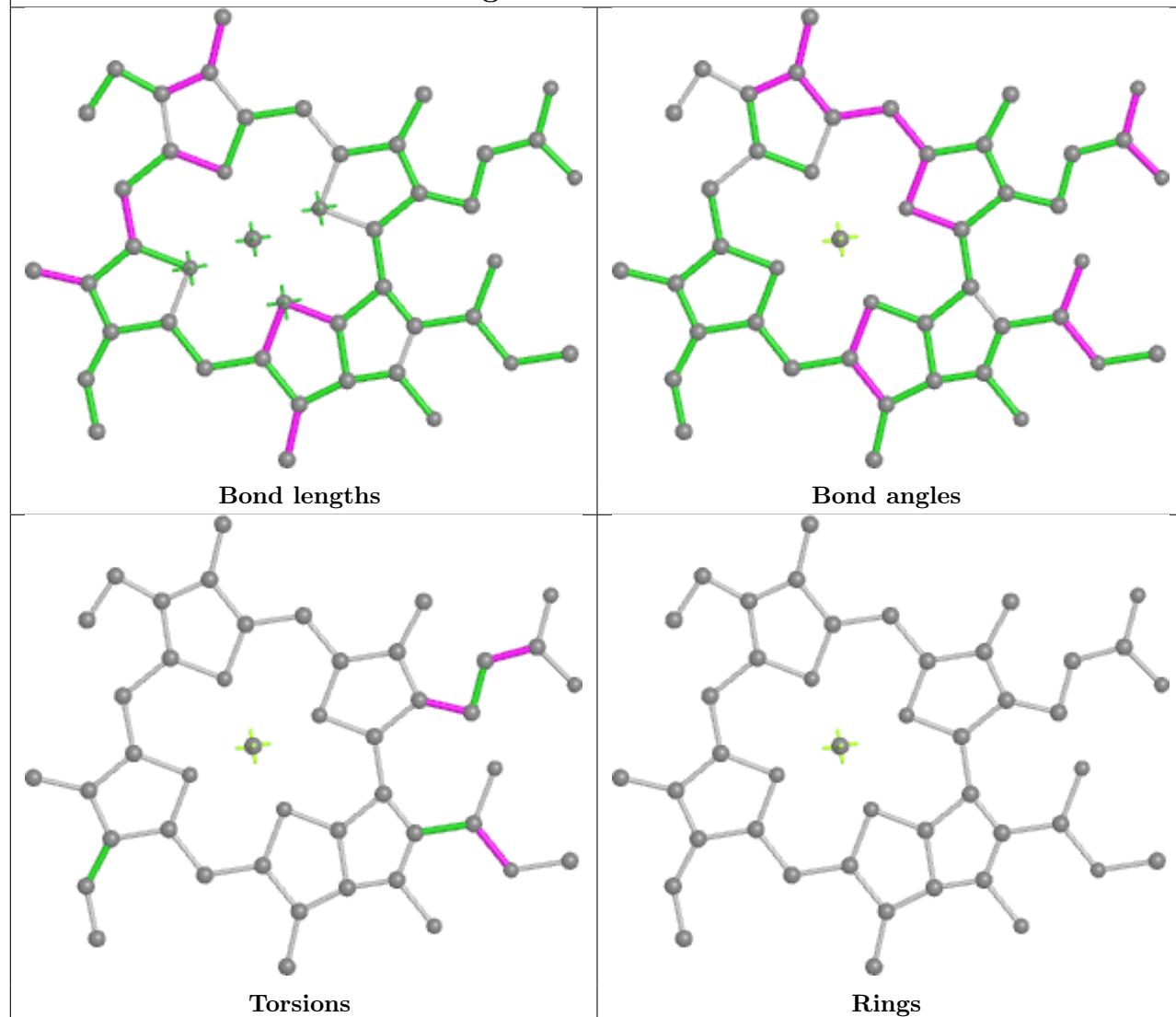


Ligand CLA bB 804

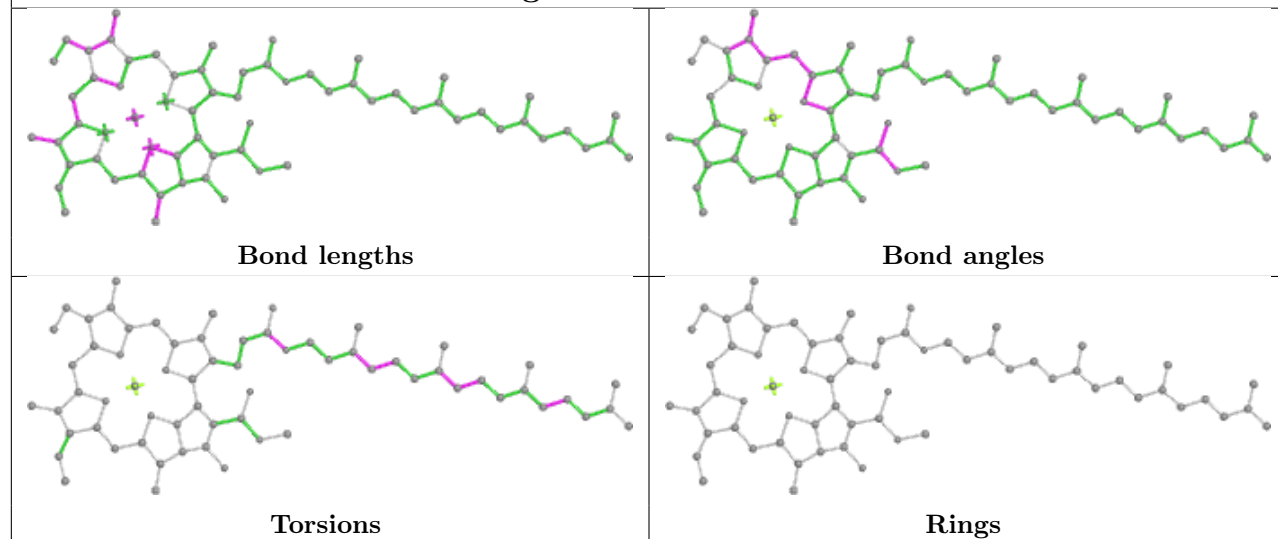




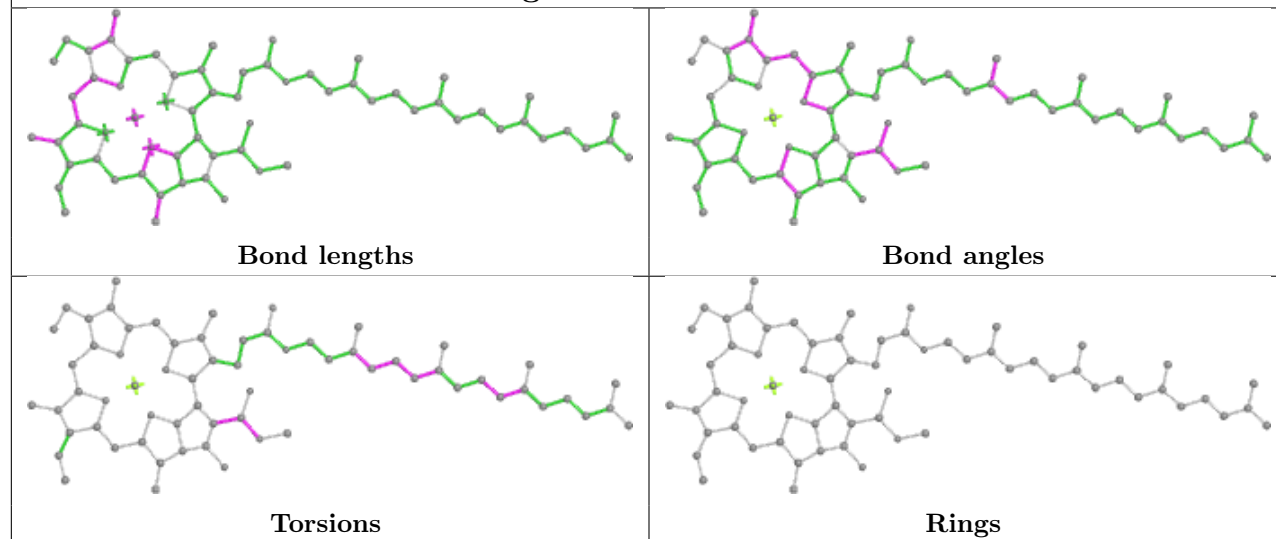
Ligand CLA cB 823



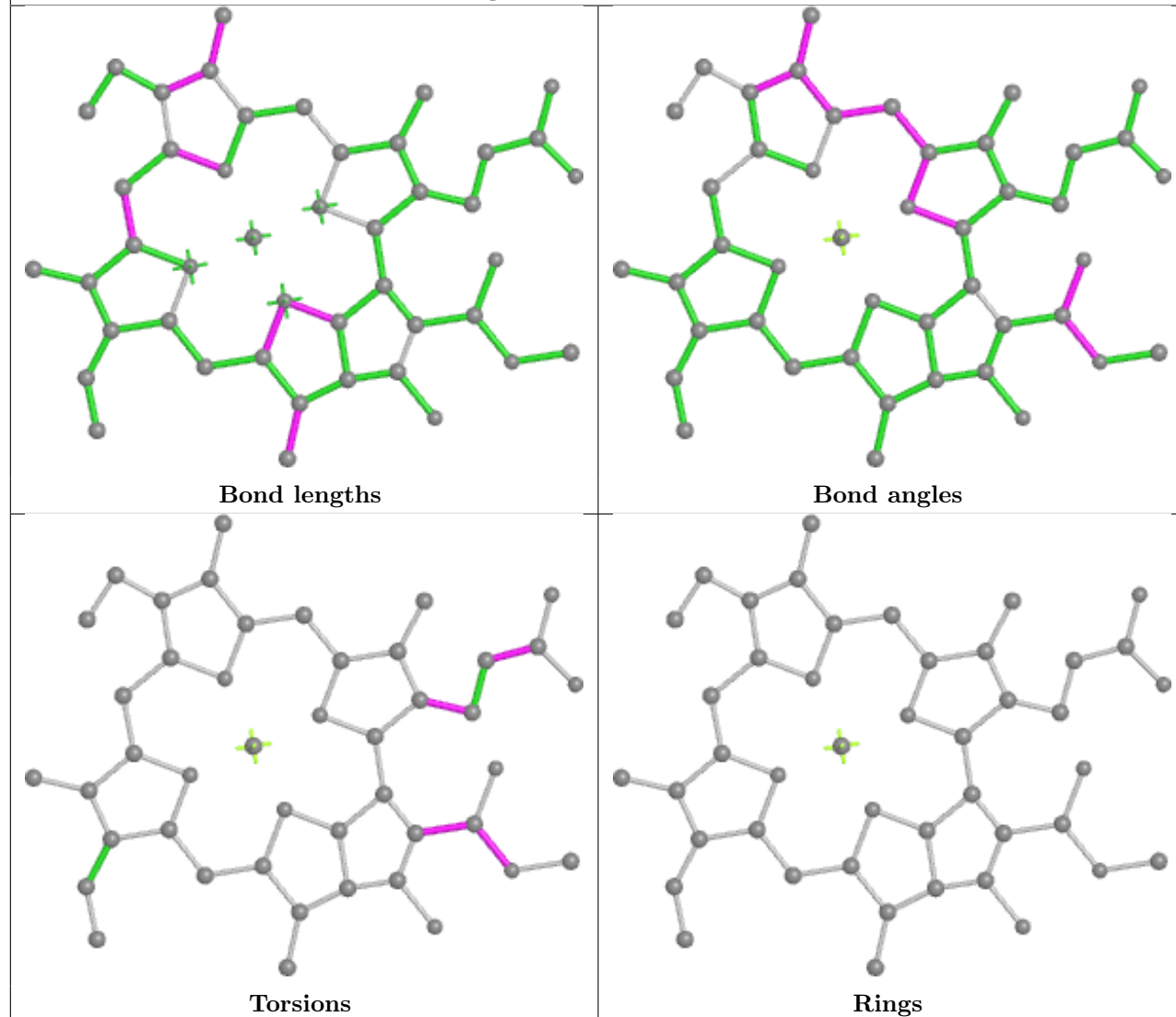
Ligand CLA dB 810

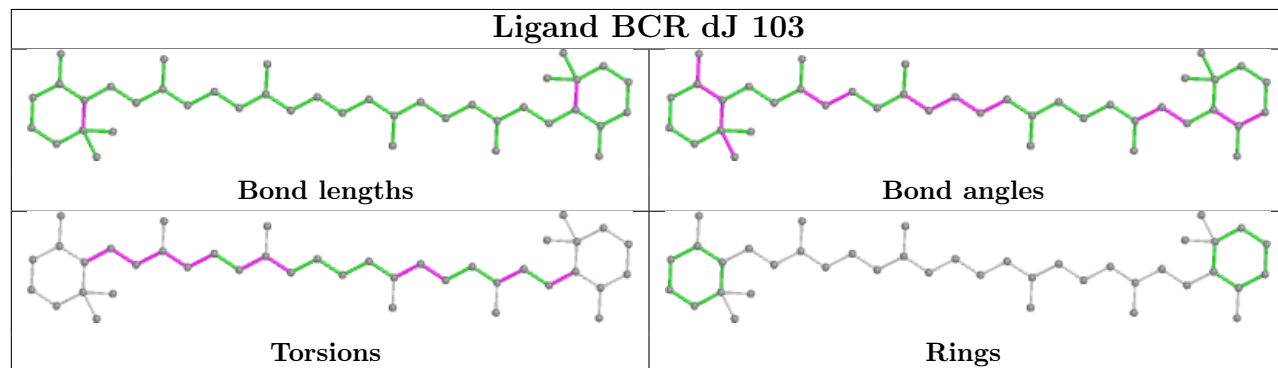
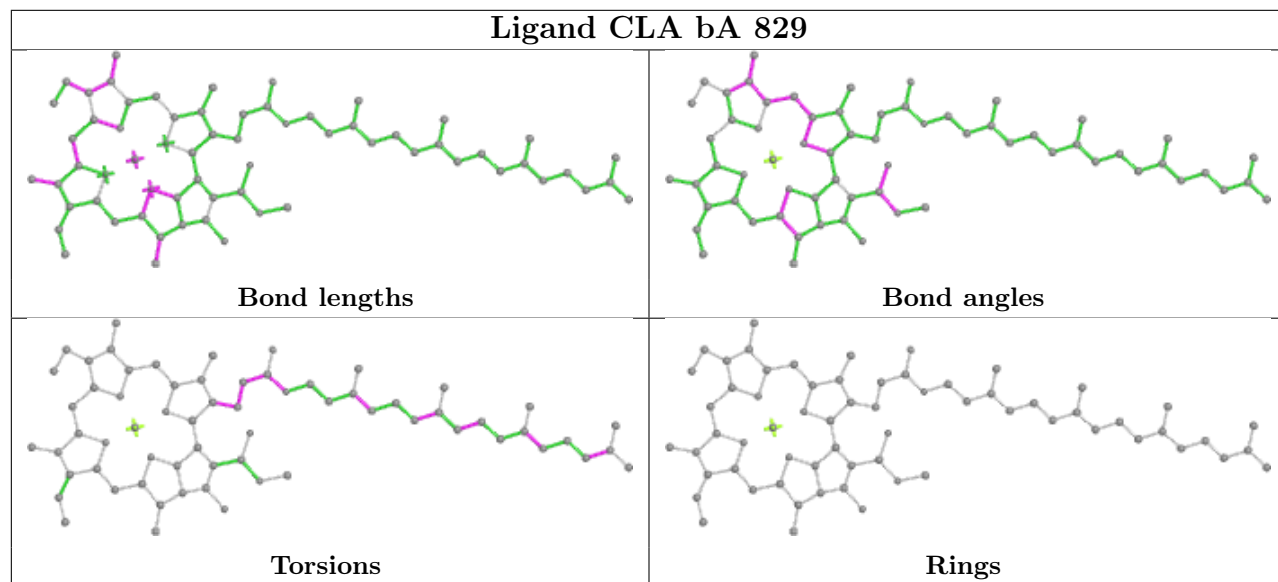
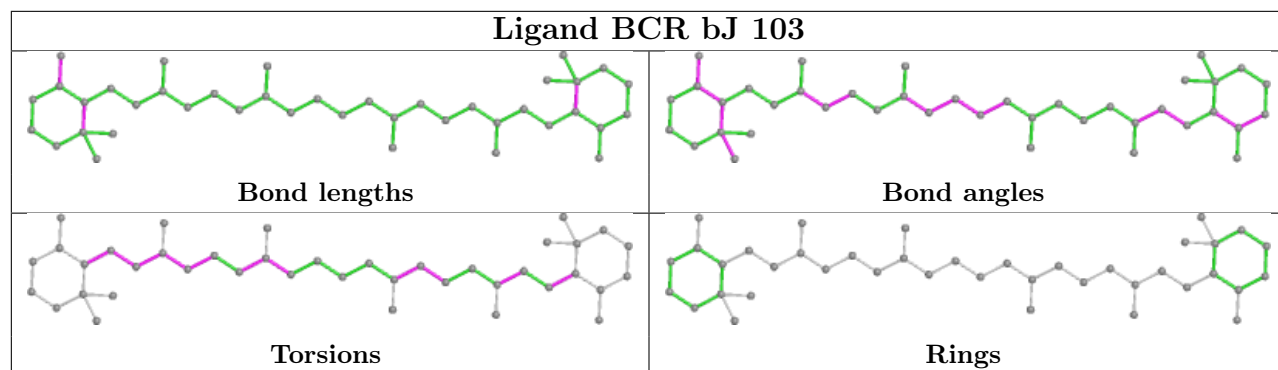
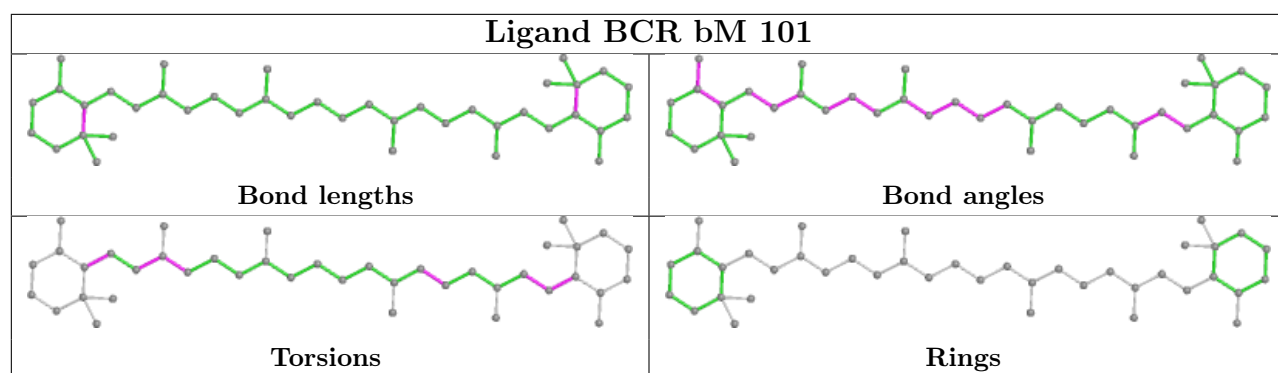


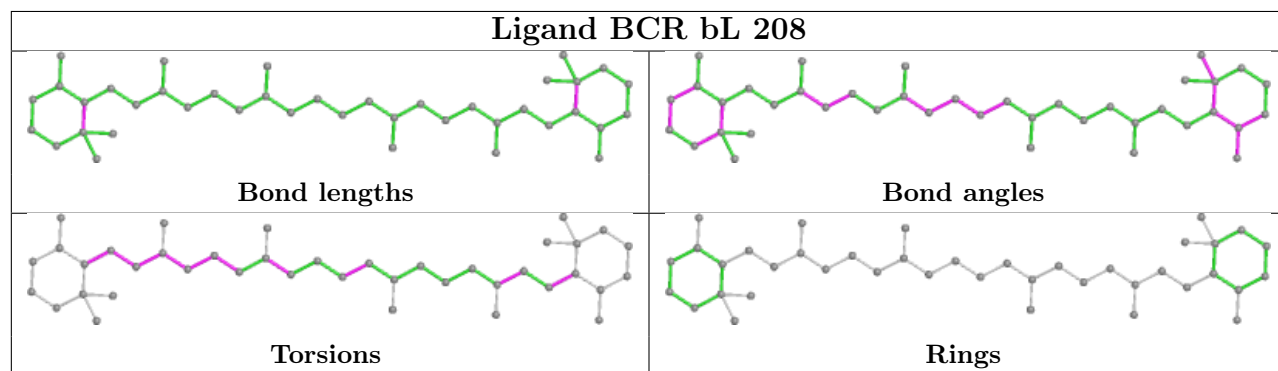
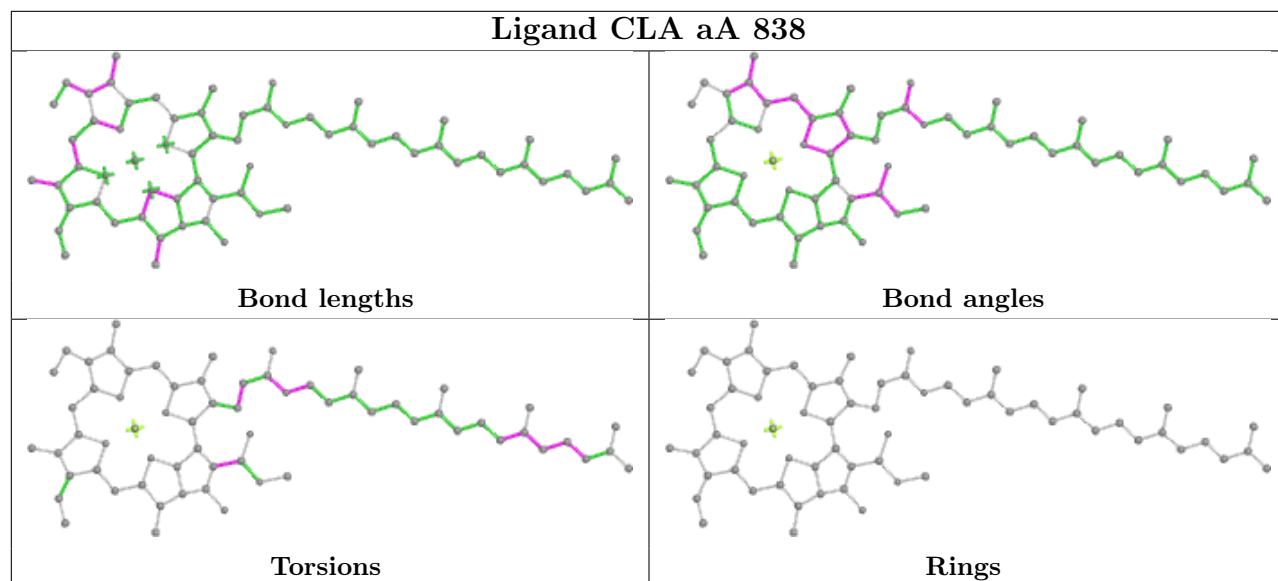
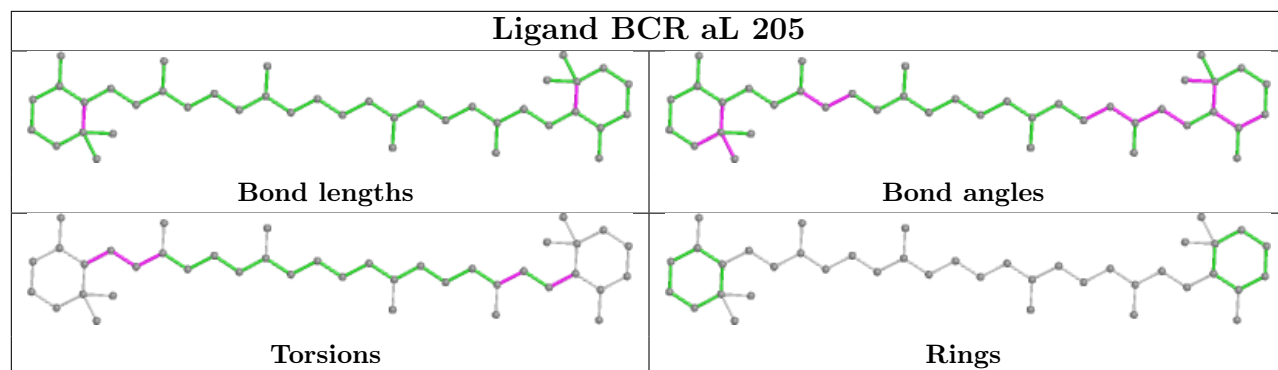
Ligand CLA dB 830



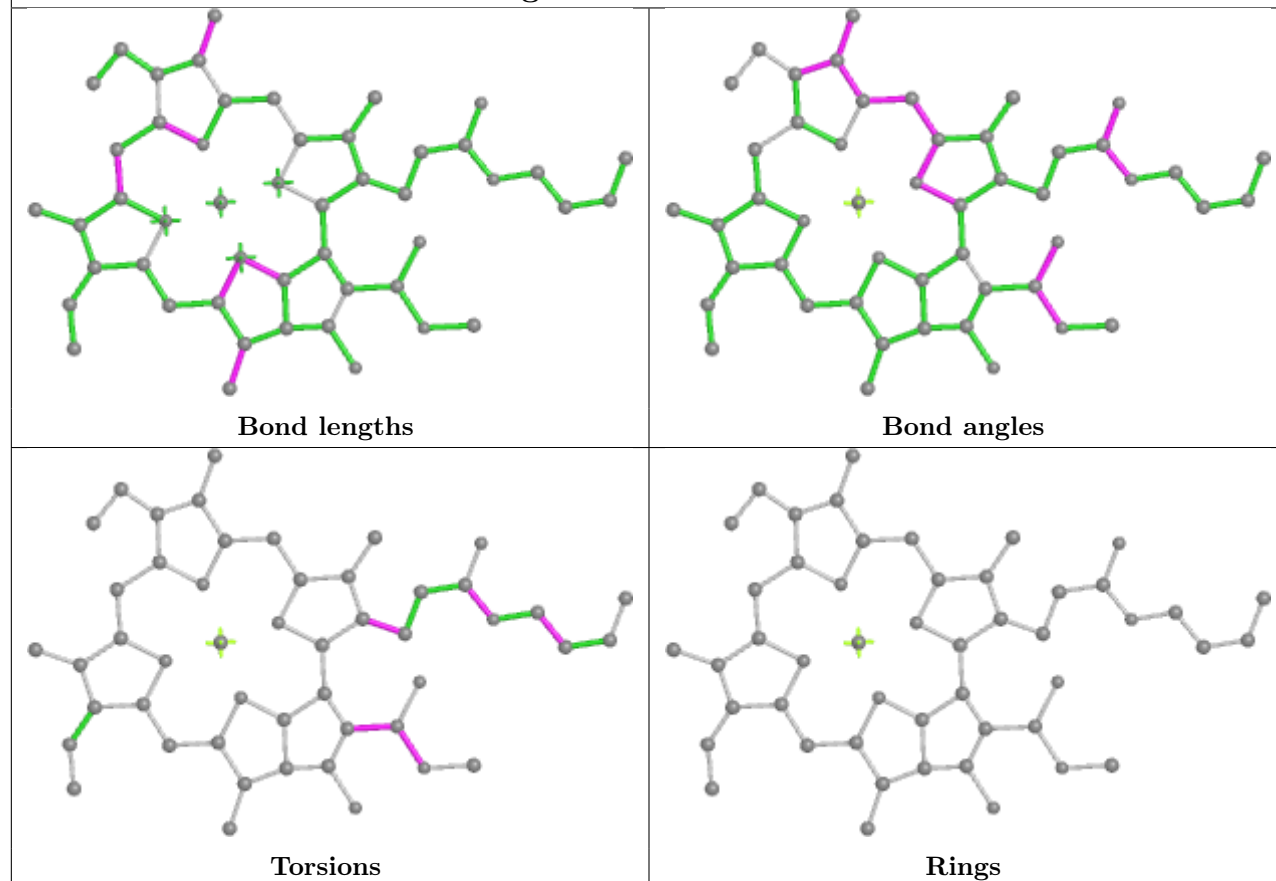
Ligand CLA dJ 101



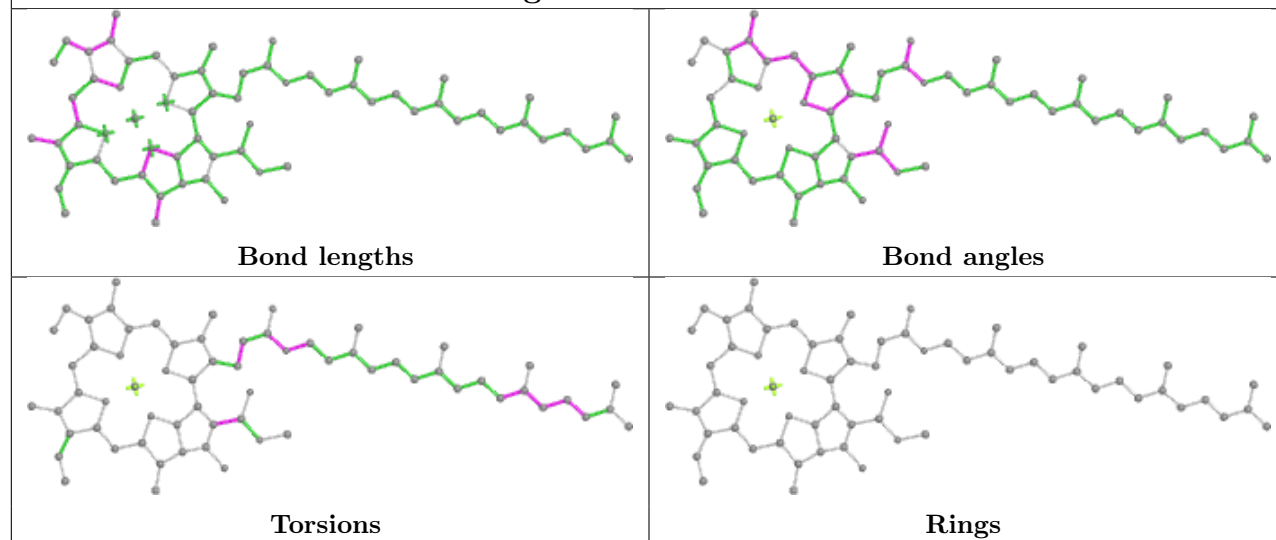




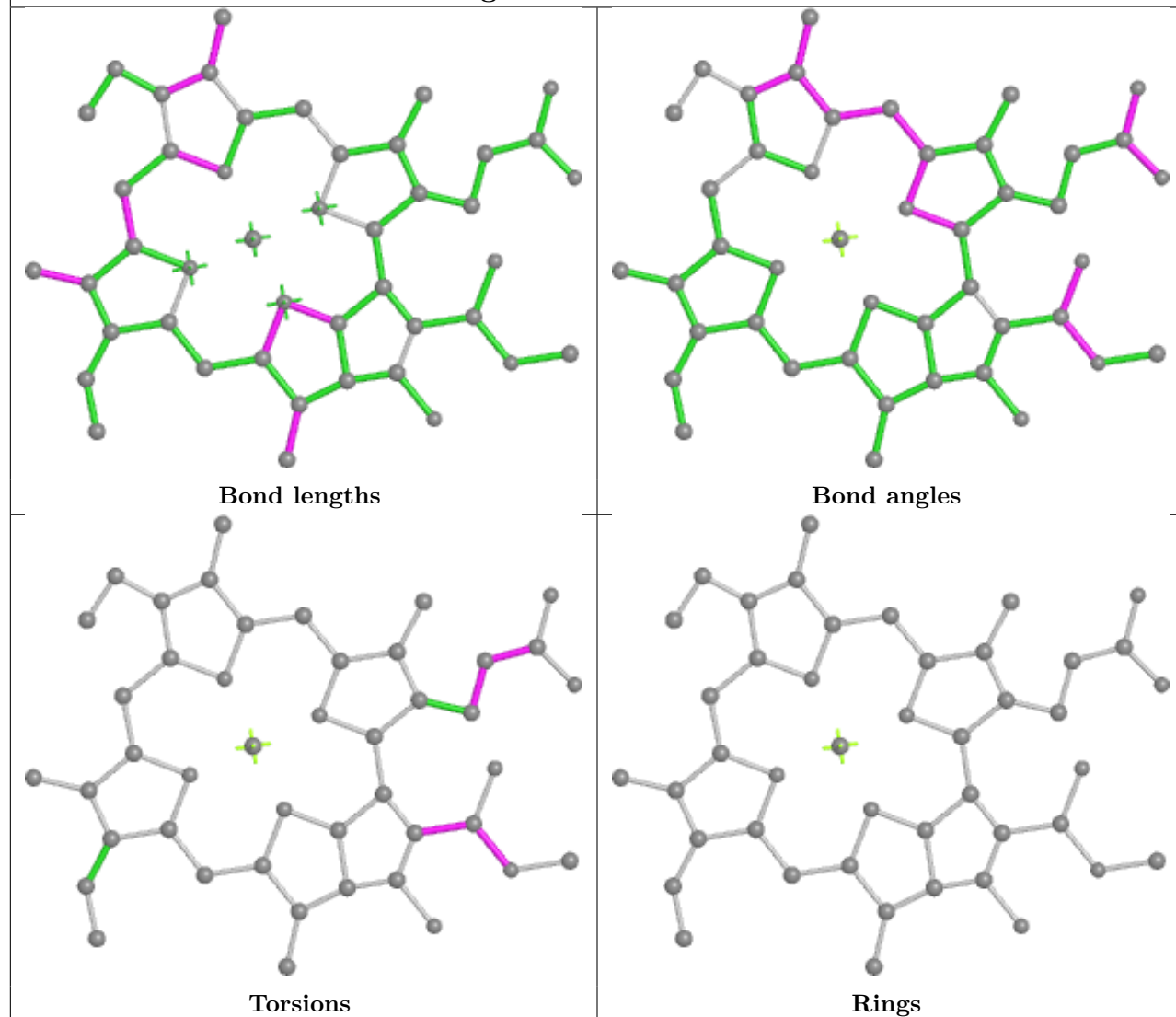
Ligand CLA bA 816



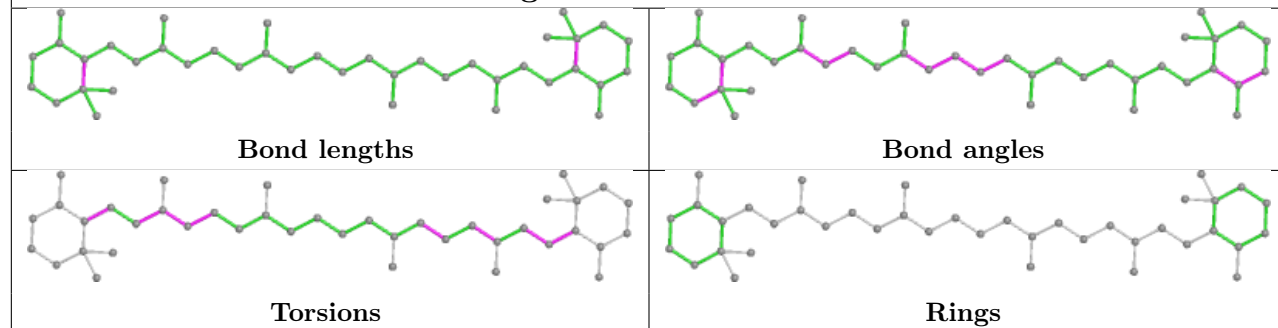
Ligand CLA cA 838

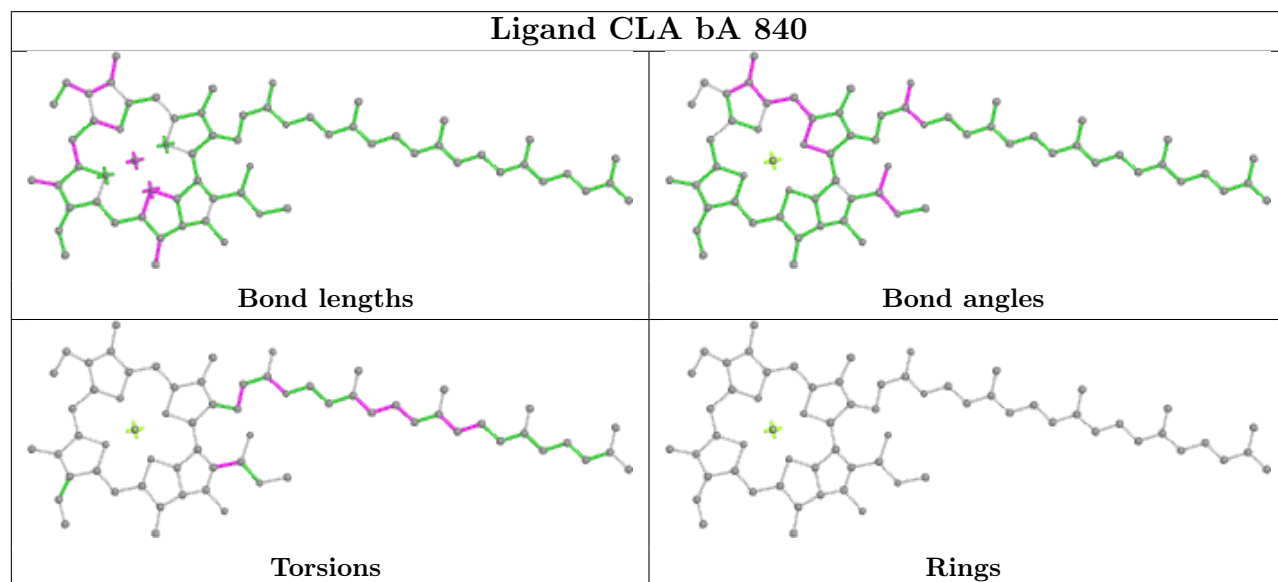
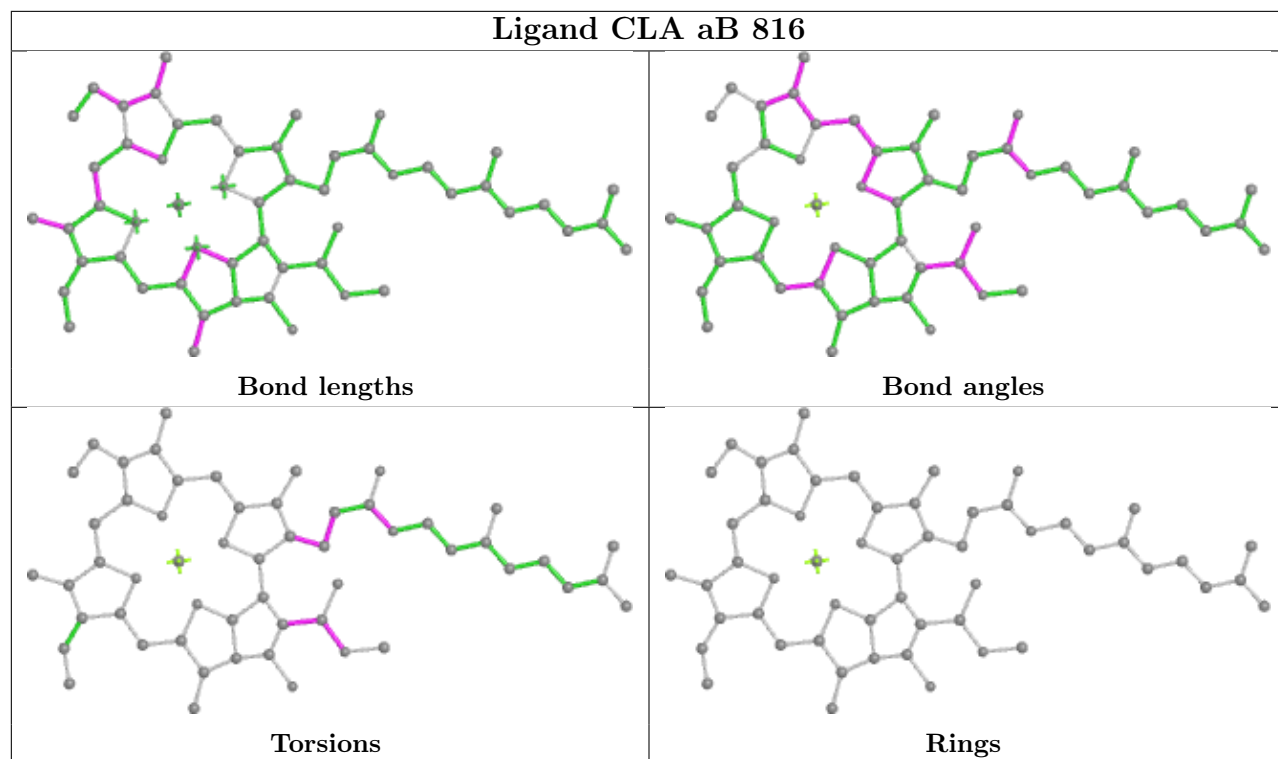


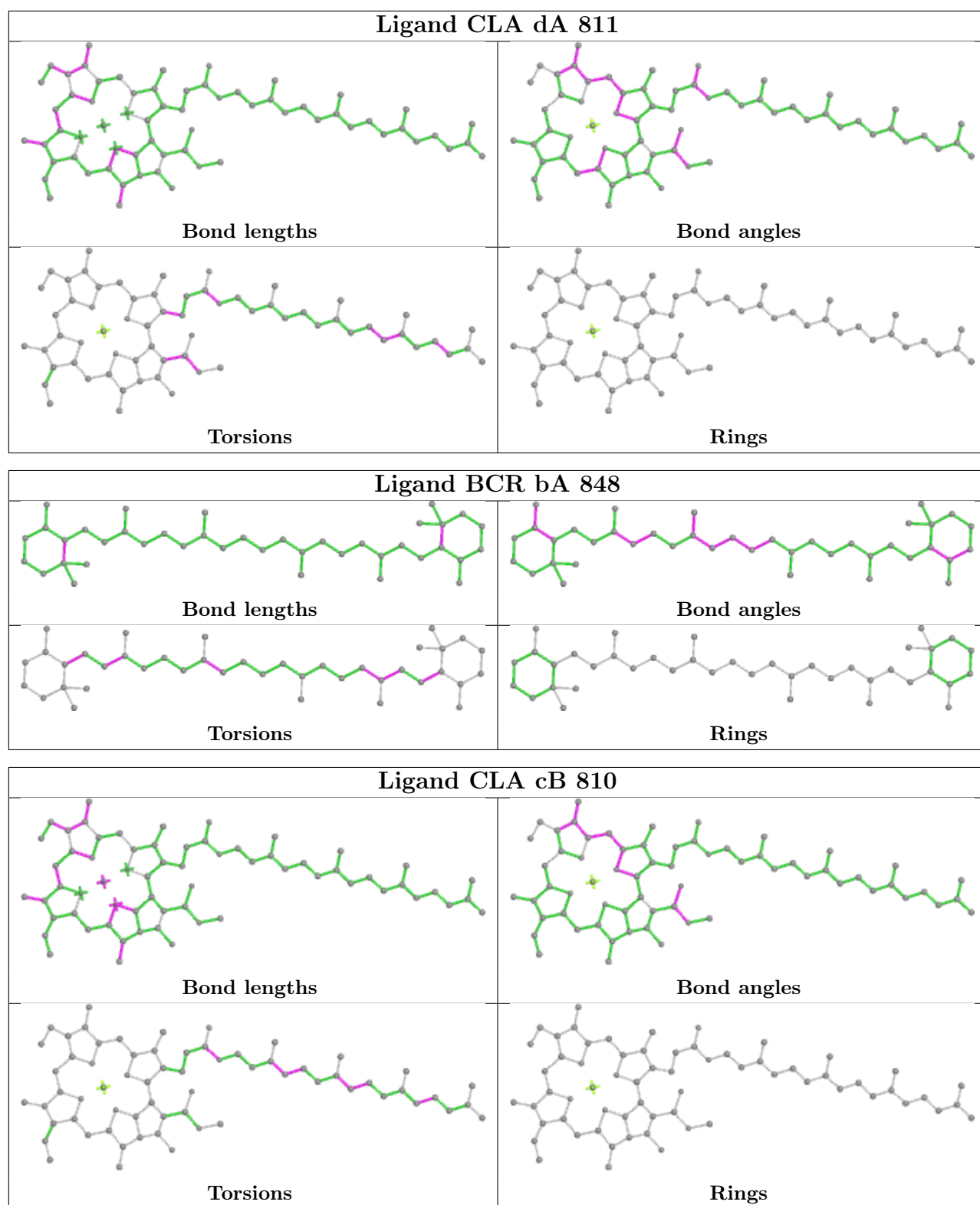
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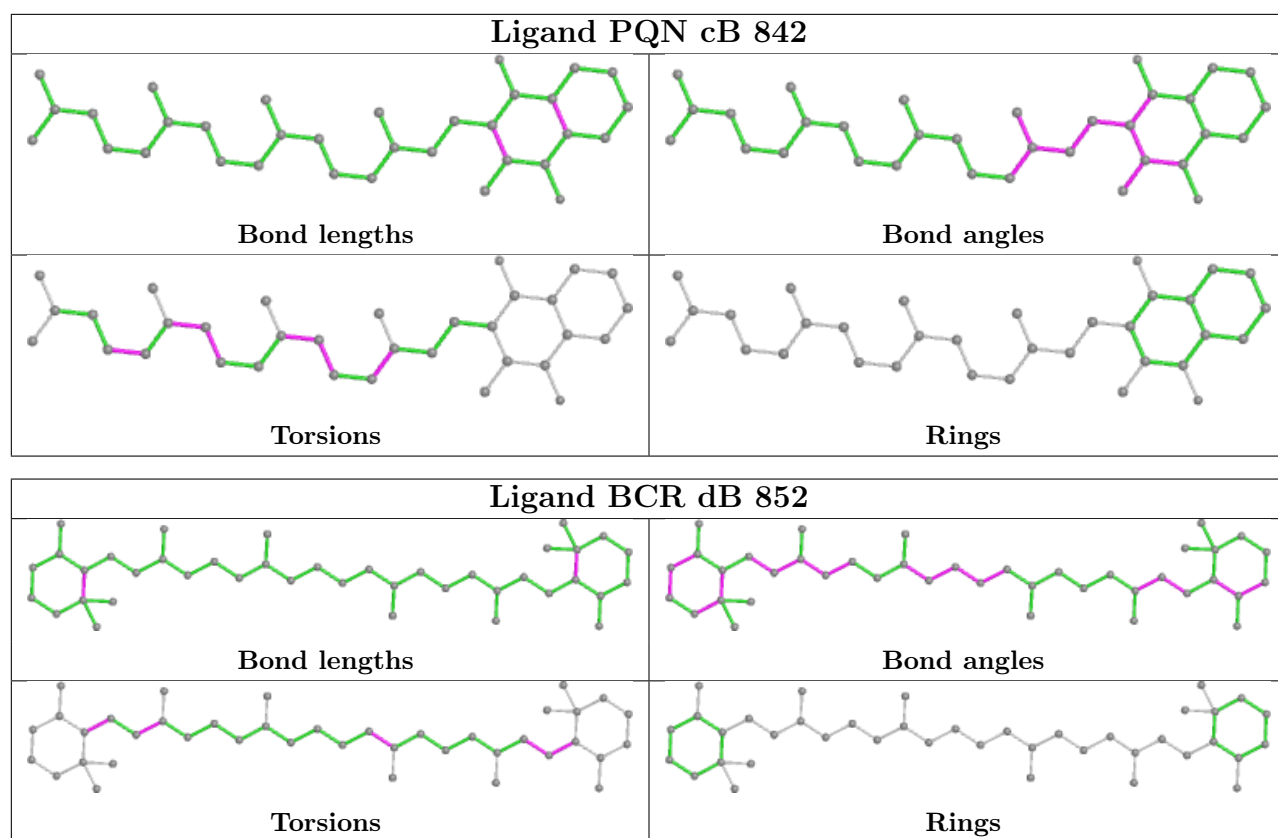


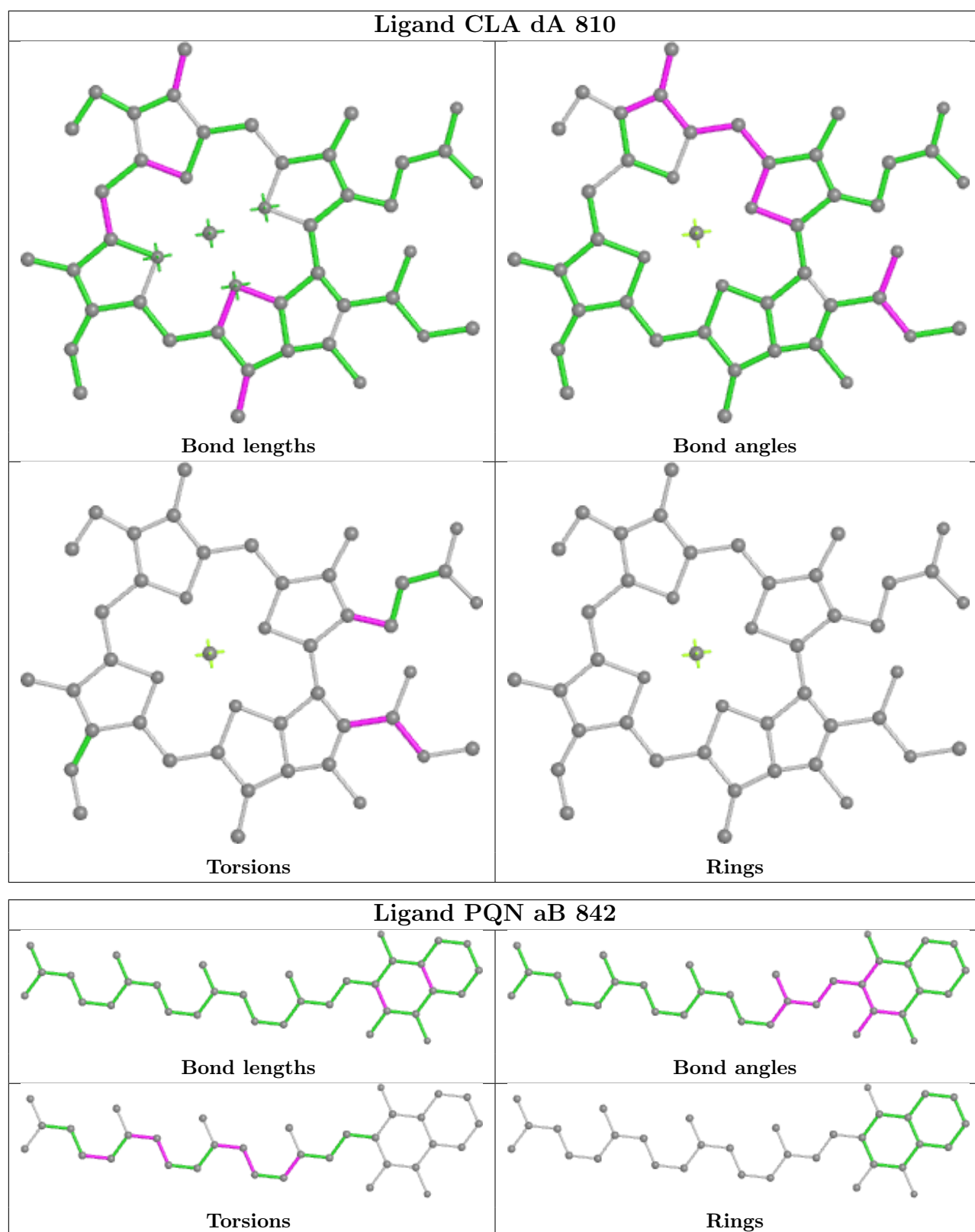
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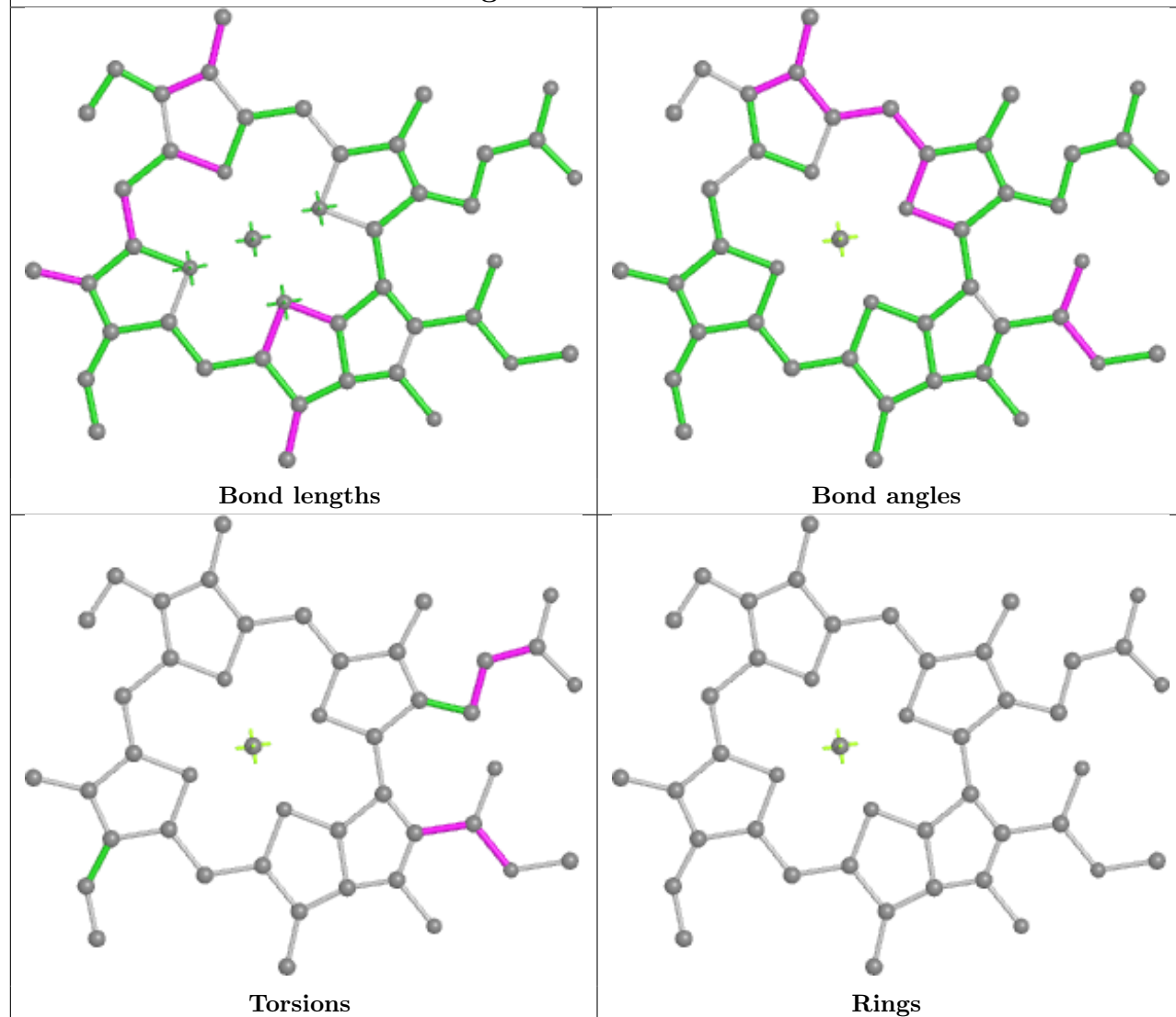




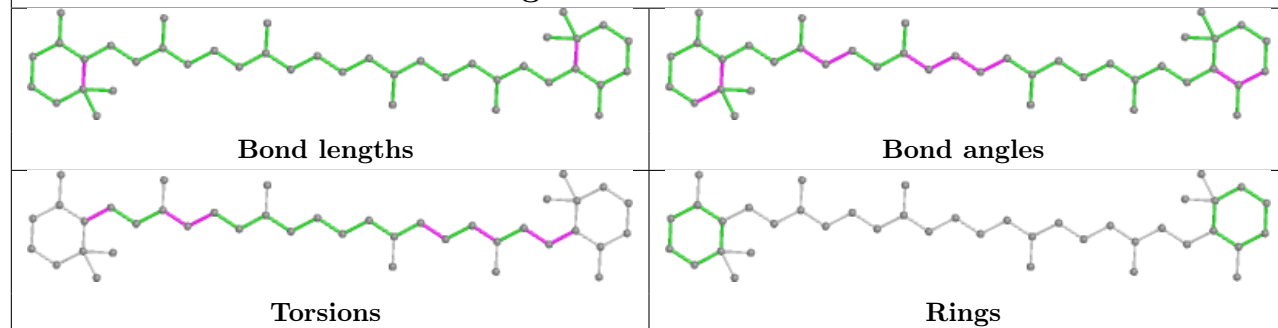


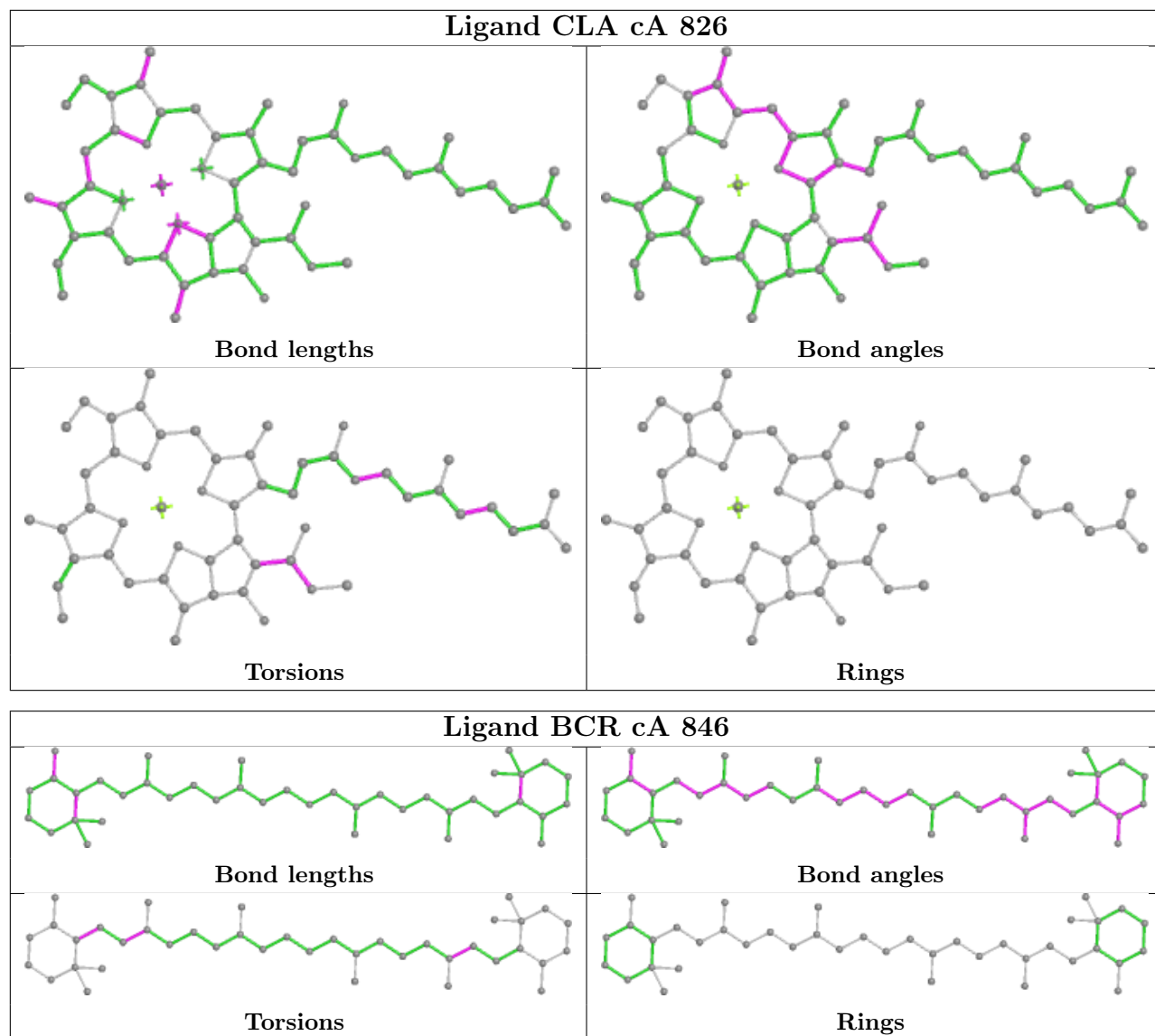


Ligand CLA aX 101

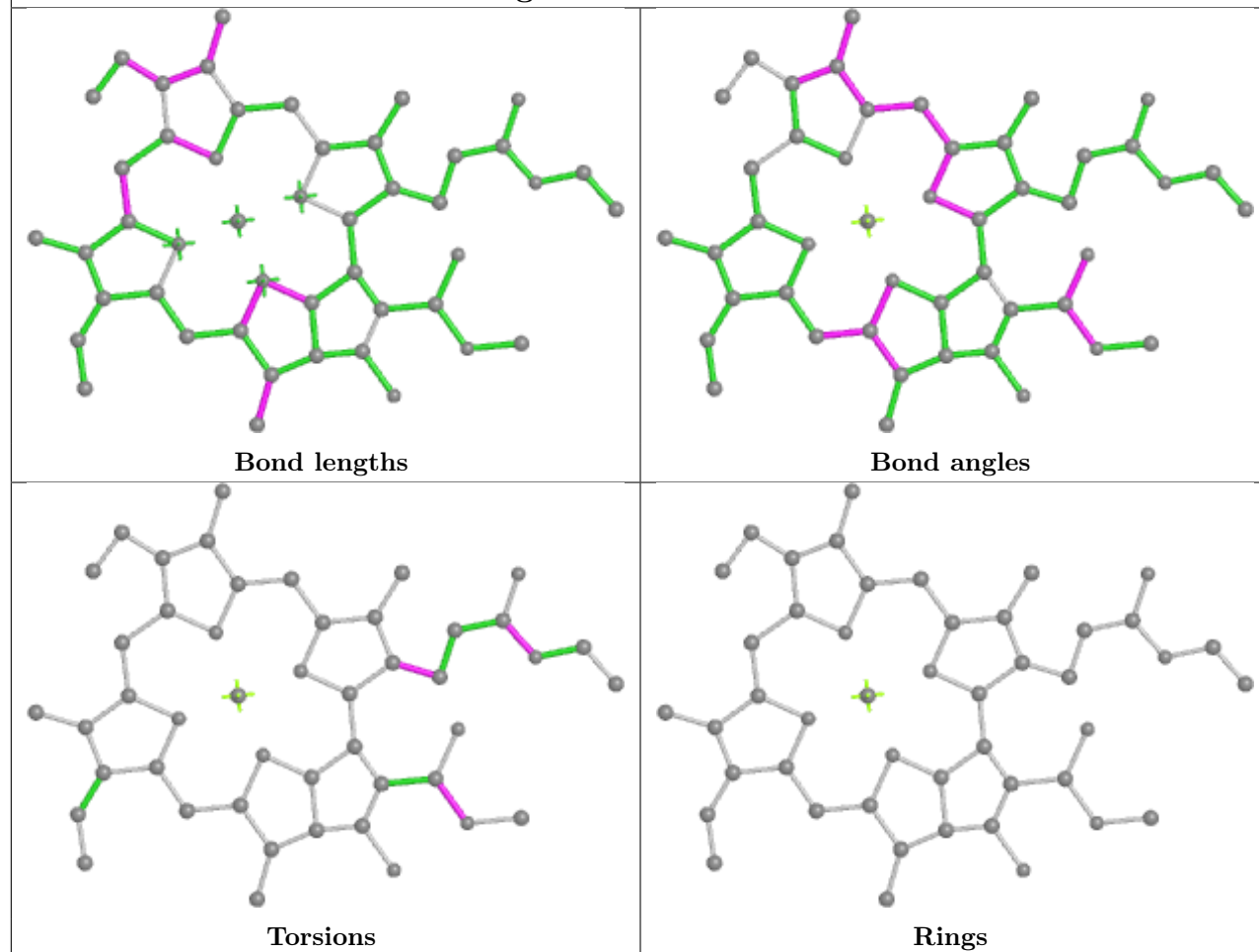


Ligand BCR aB 847

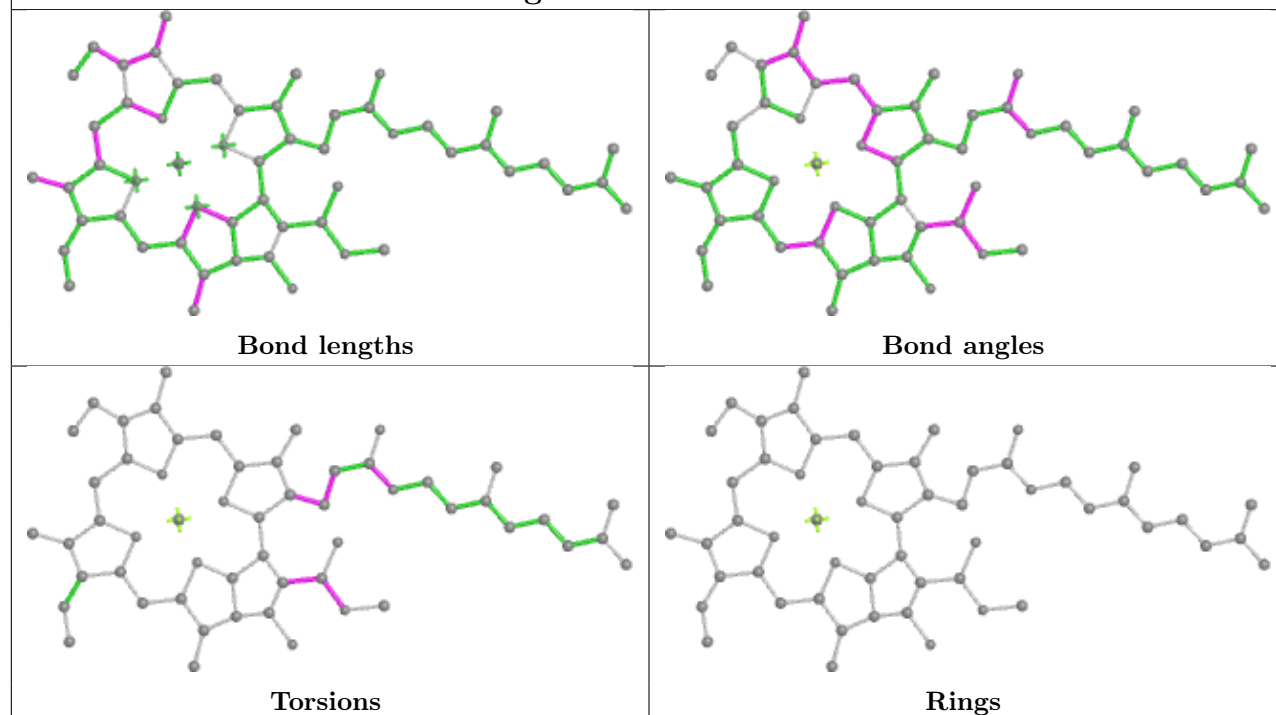


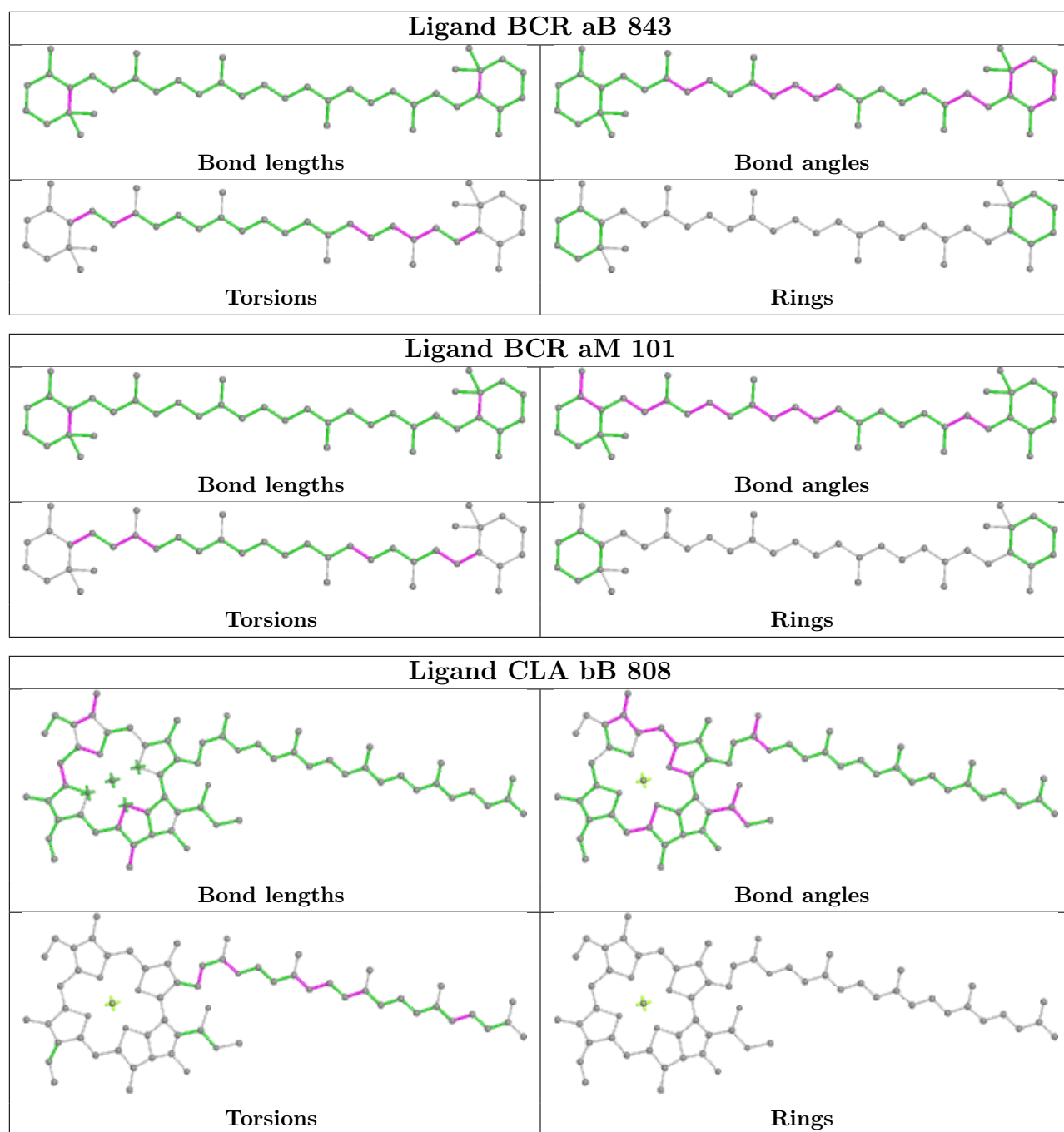


Ligand CLA aA 824

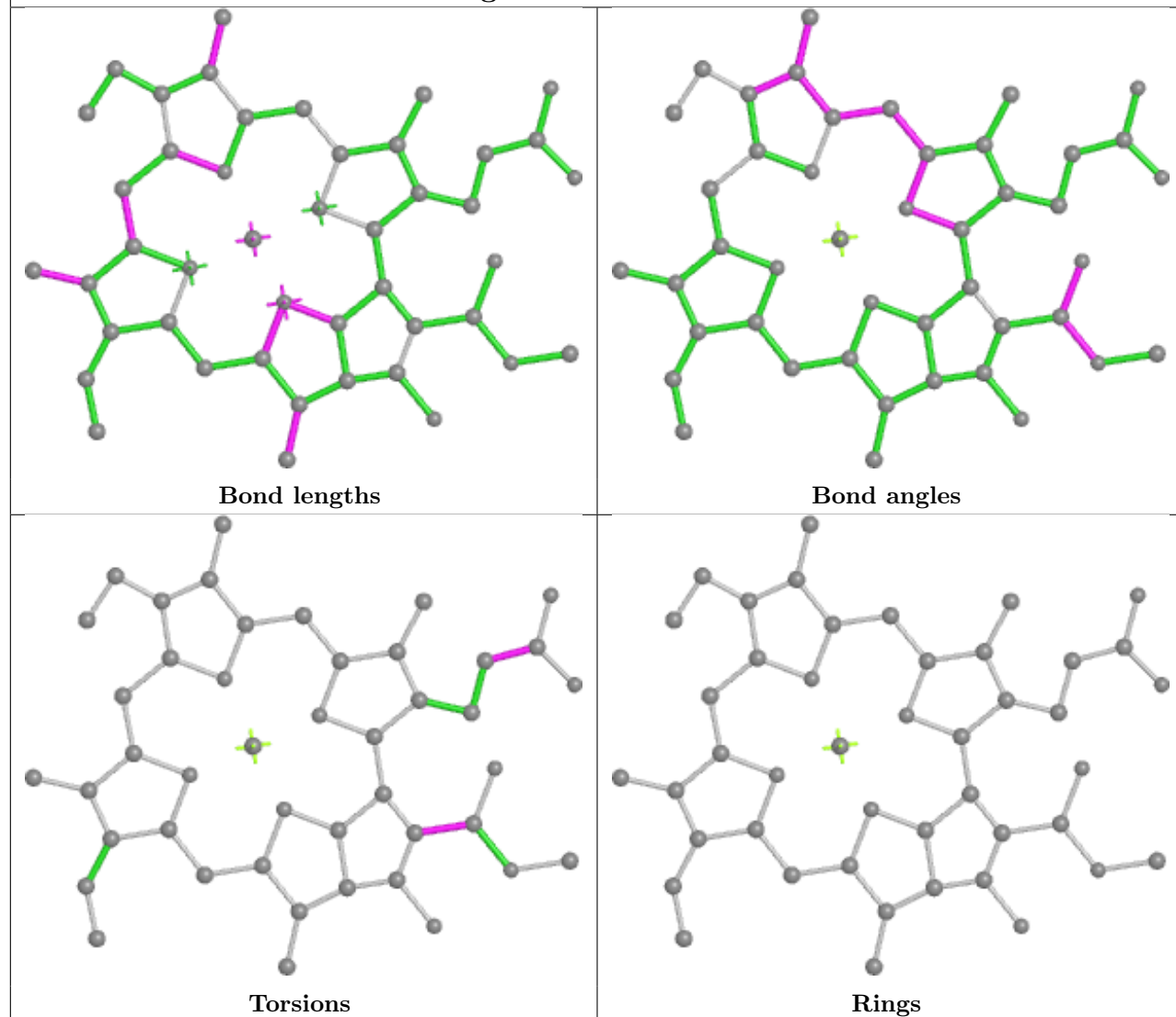


Ligand CLA cB 816

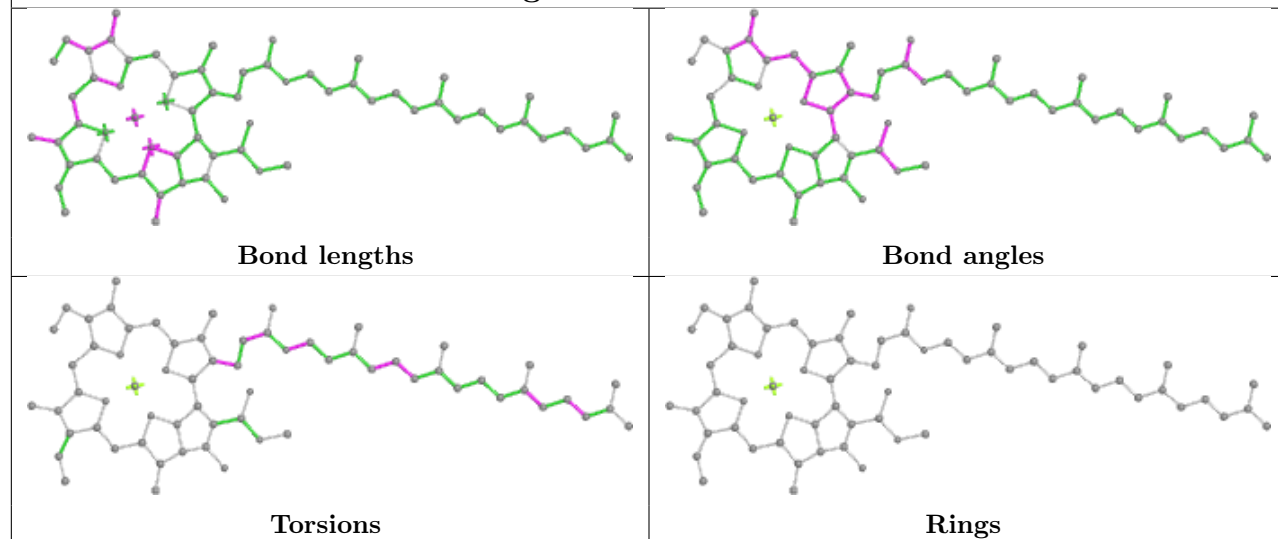




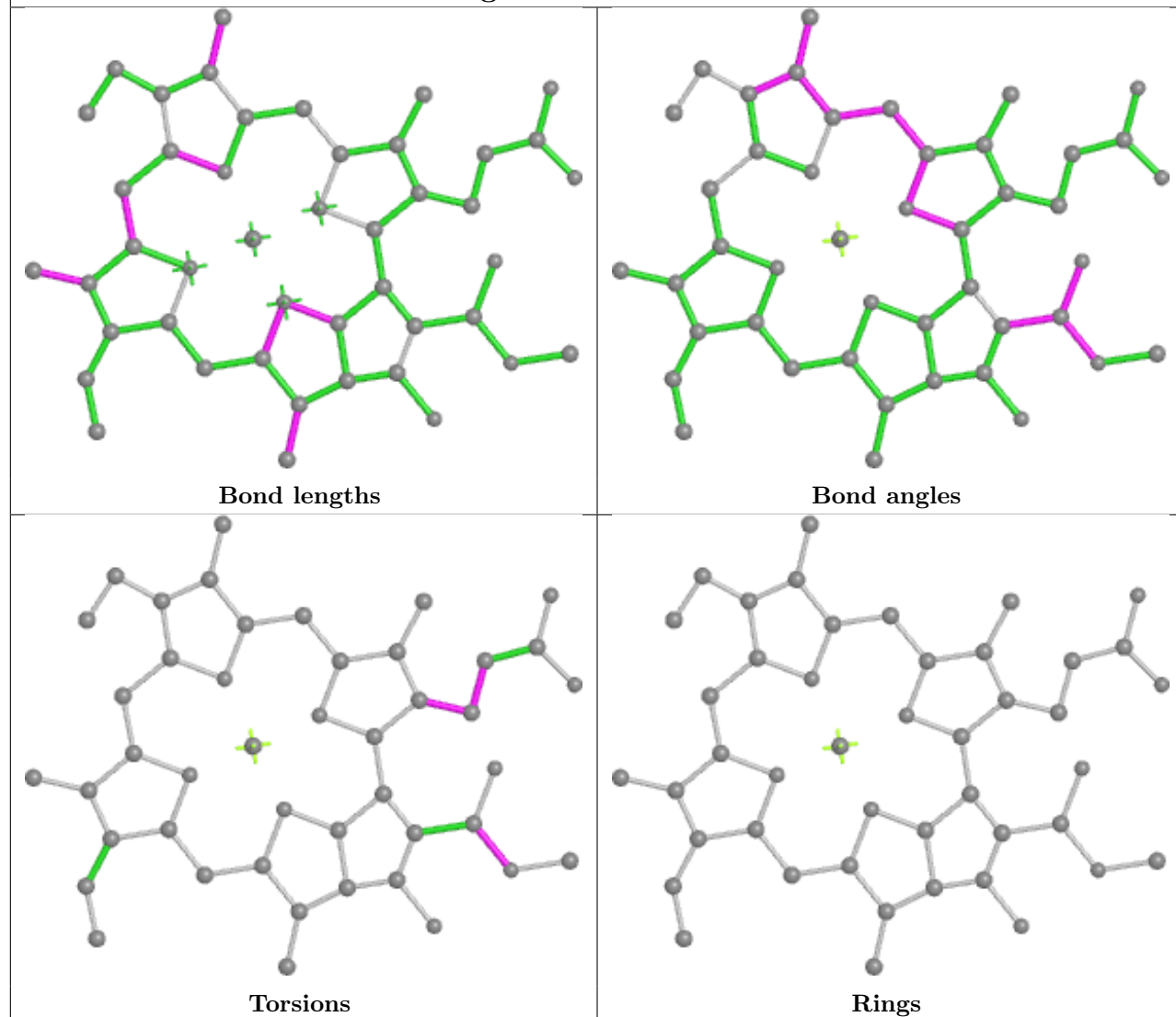
Ligand CLA aK 102



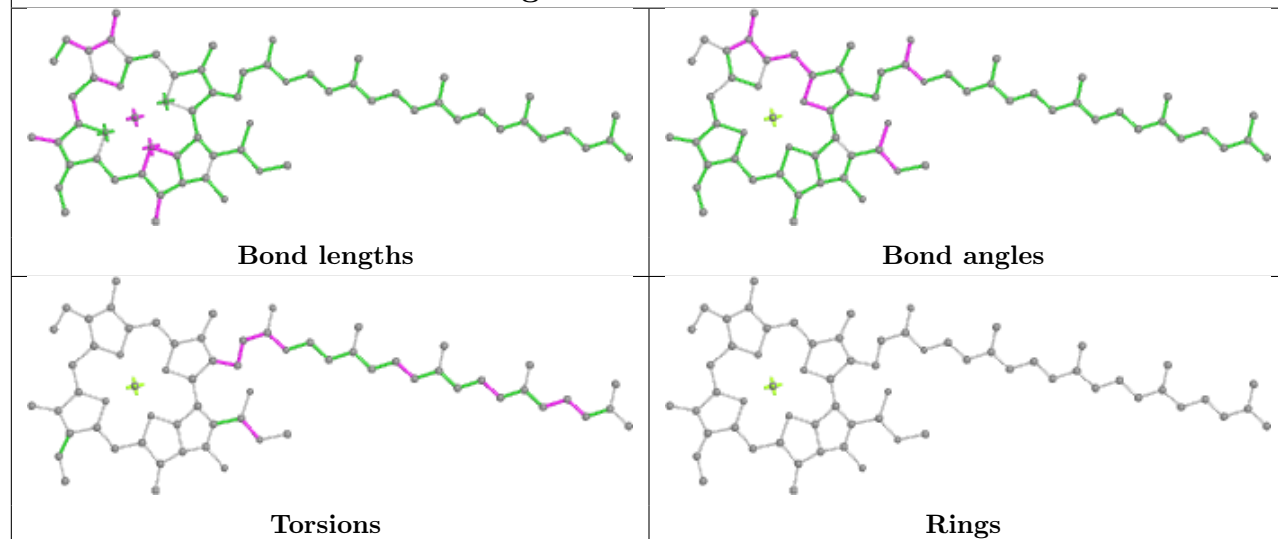
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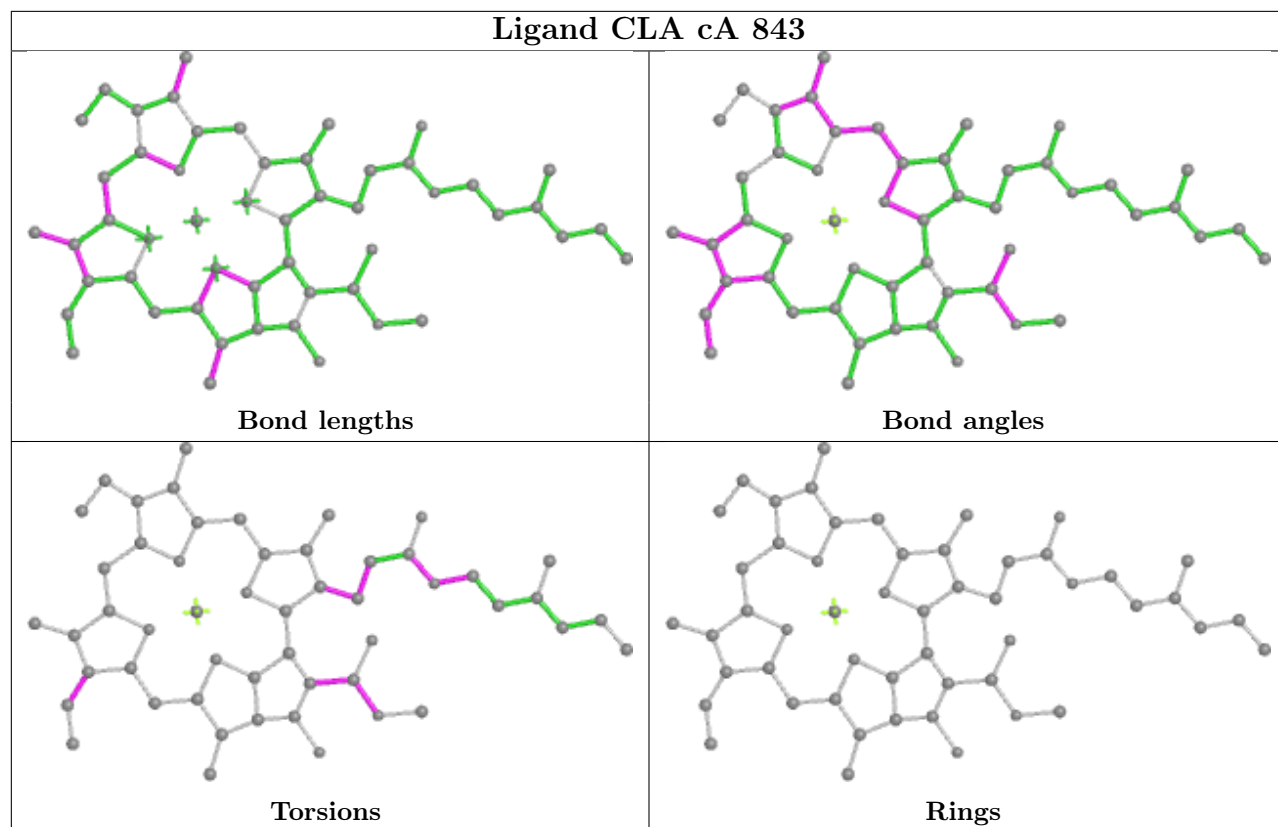


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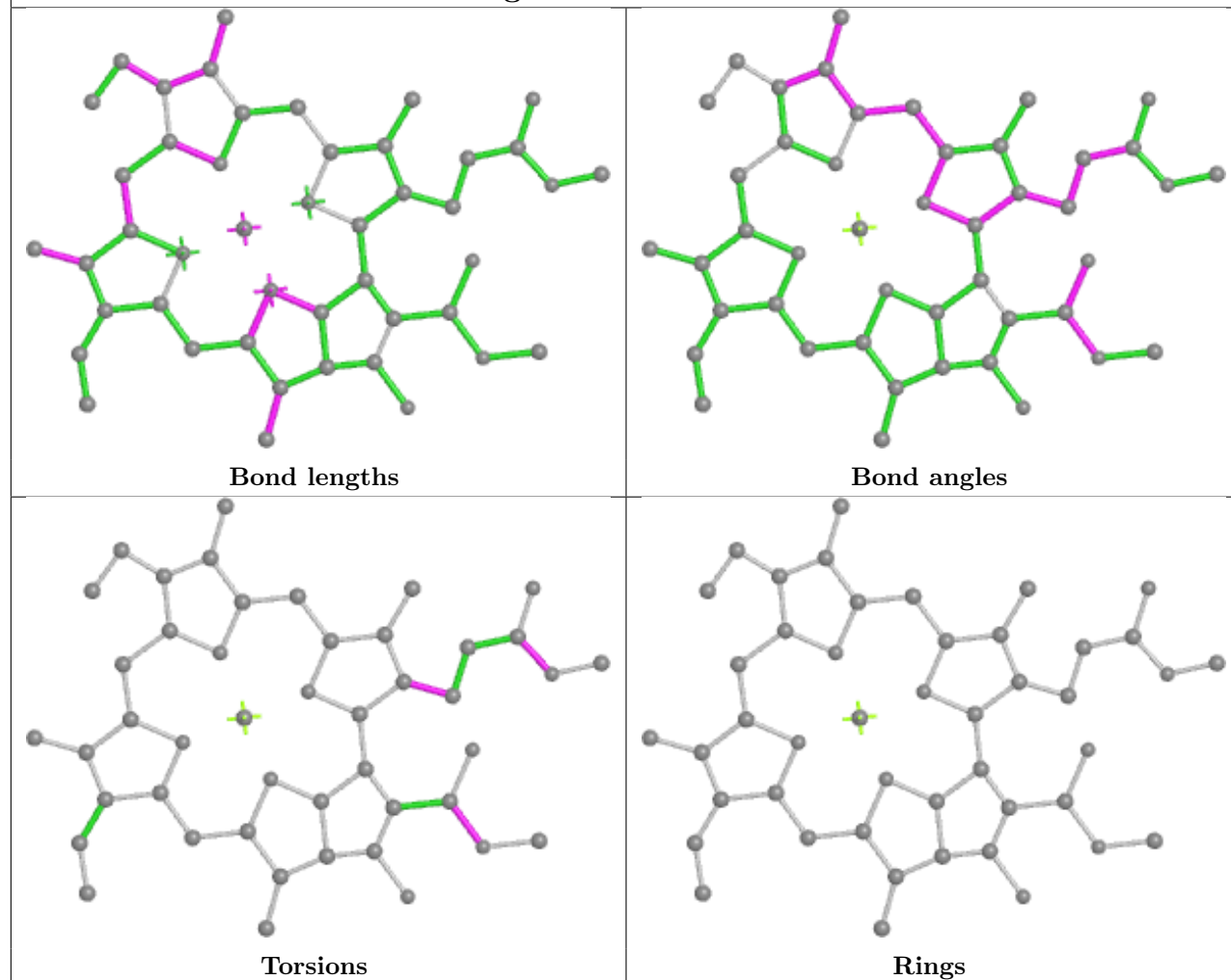


Ligand CLA dA 842

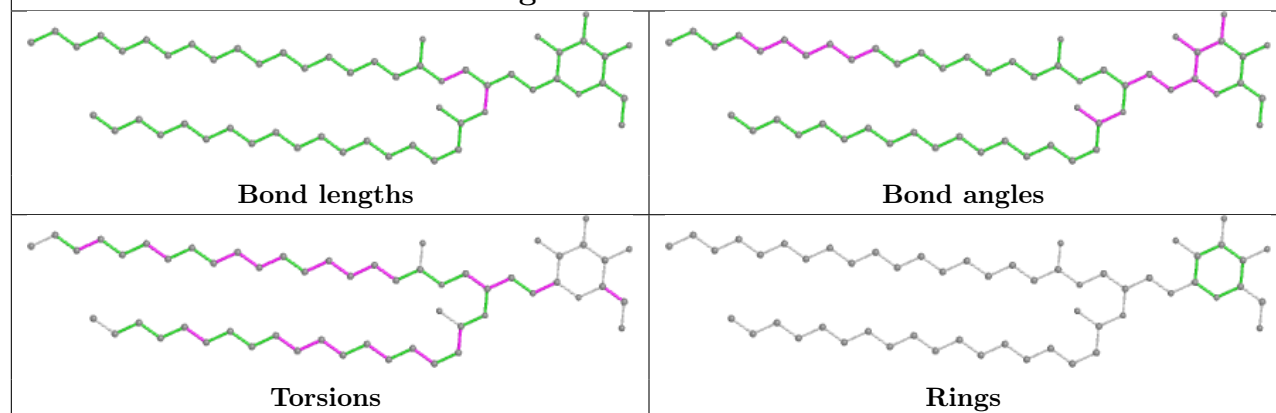


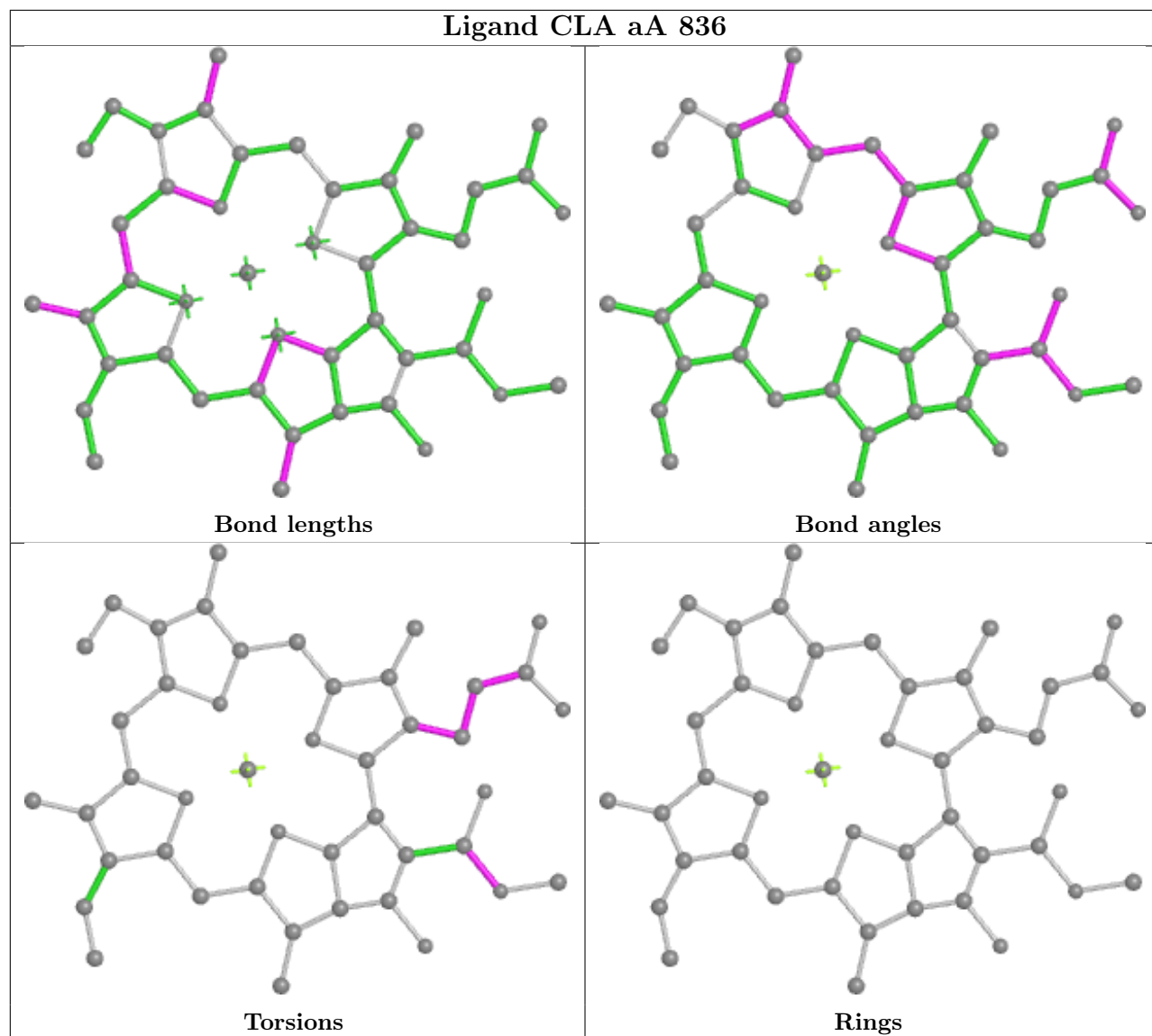
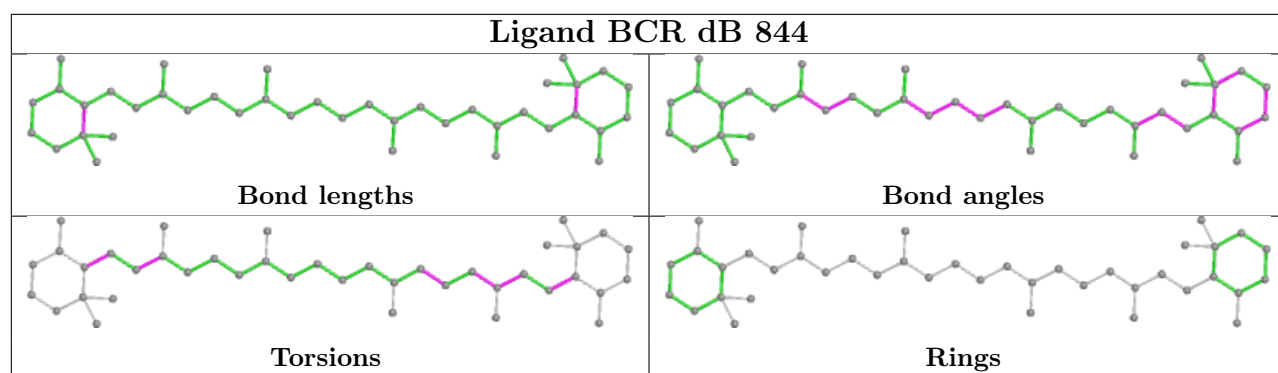


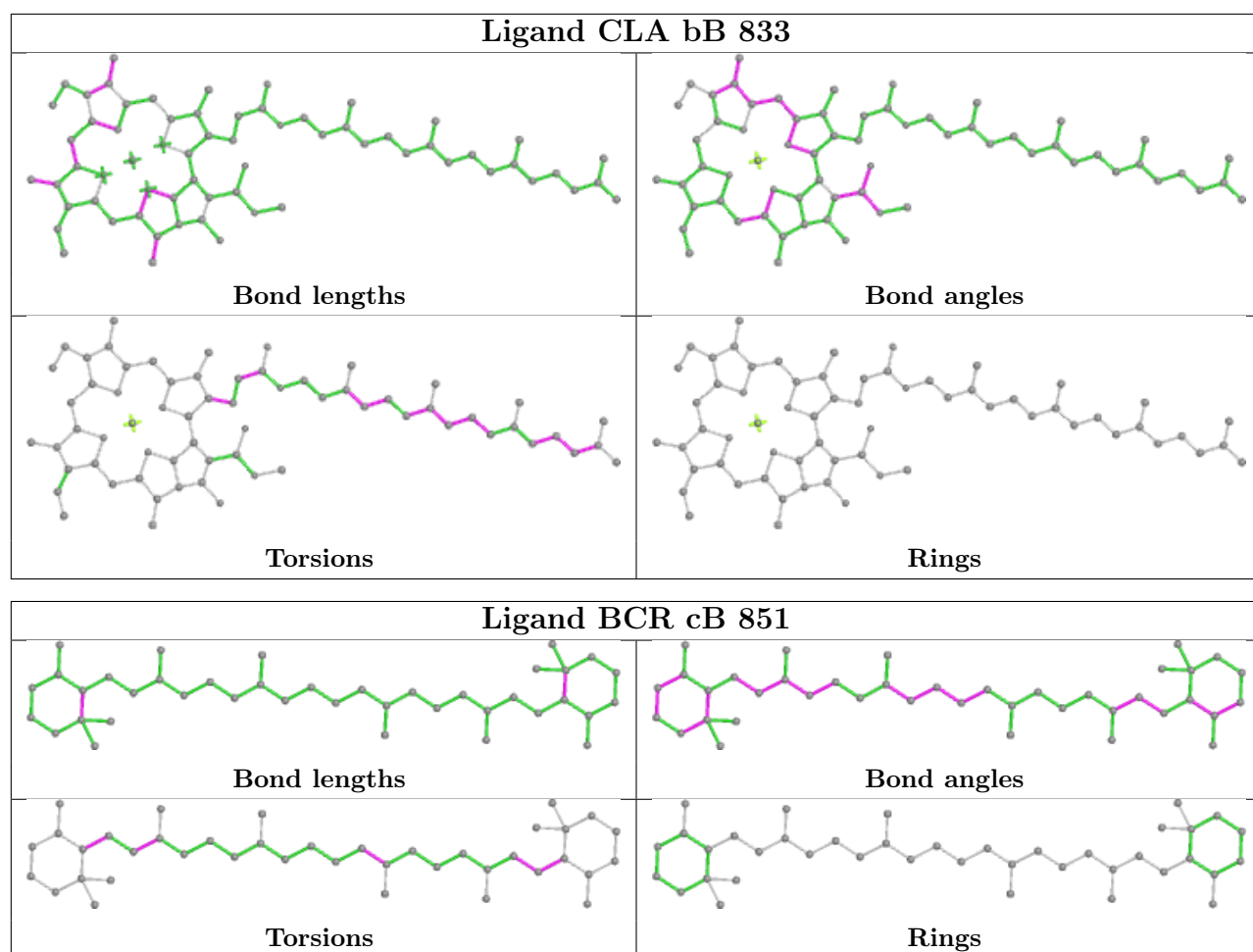
Ligand CLA dB 826

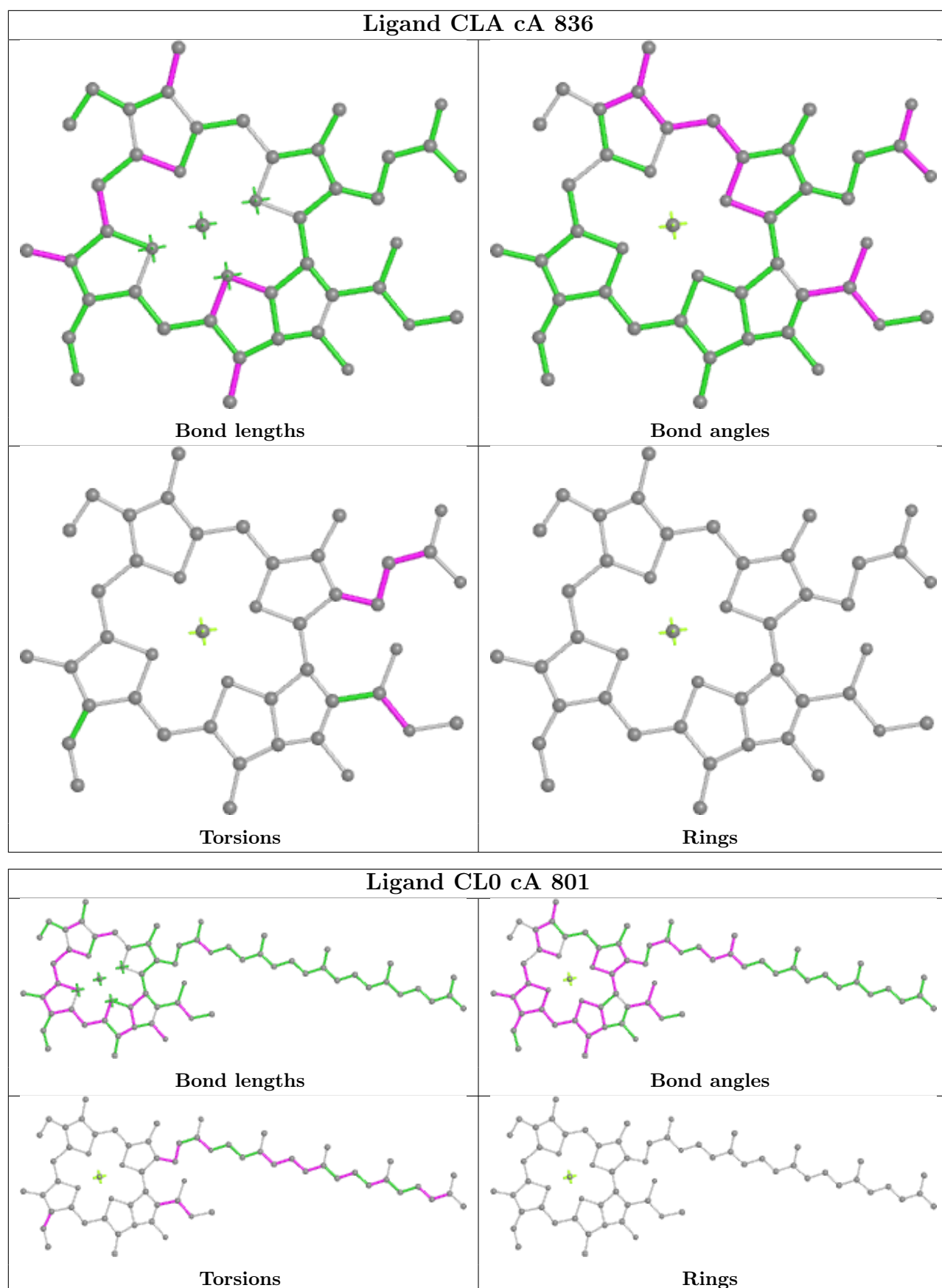


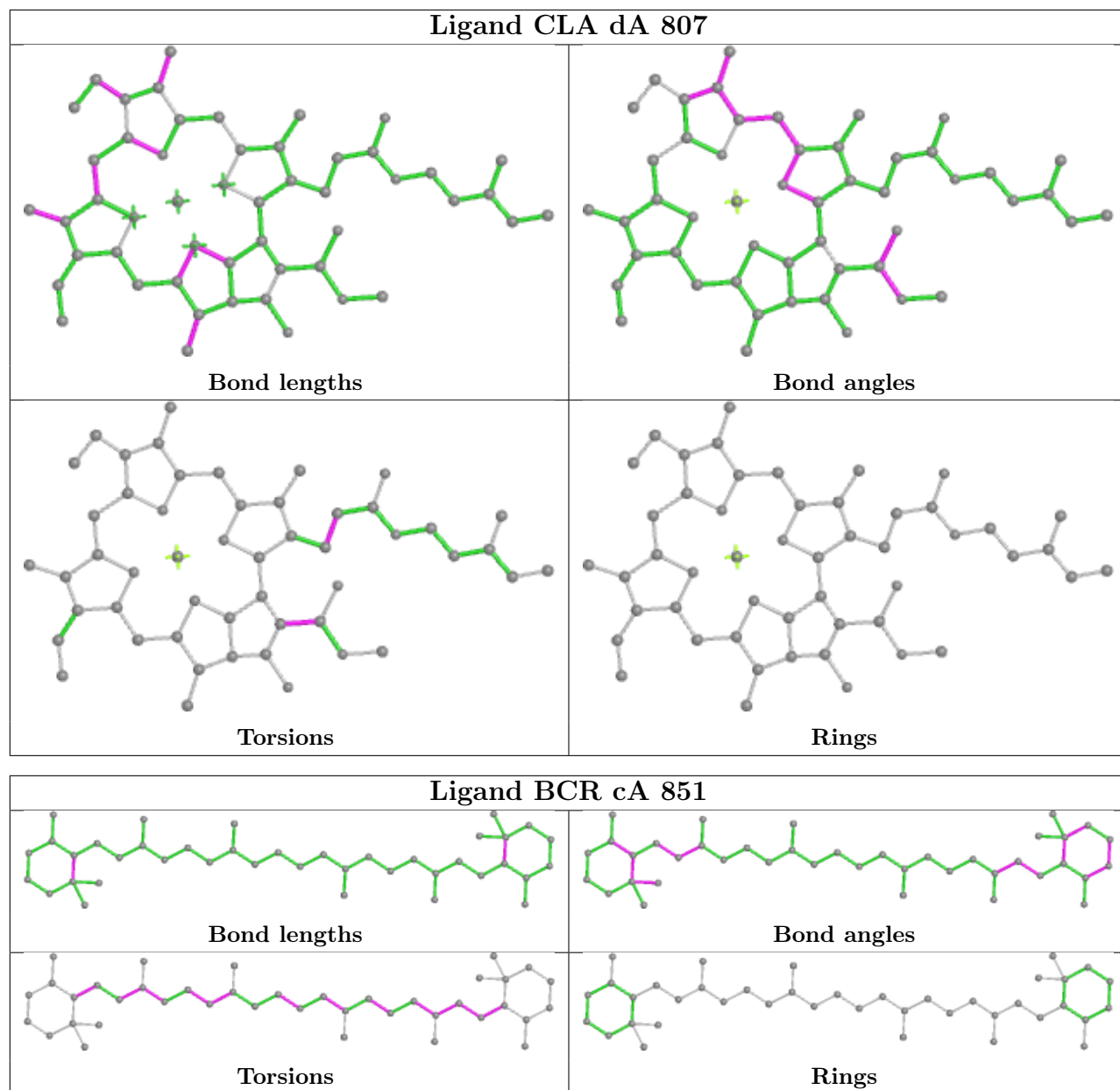
Ligand LMG aB 849



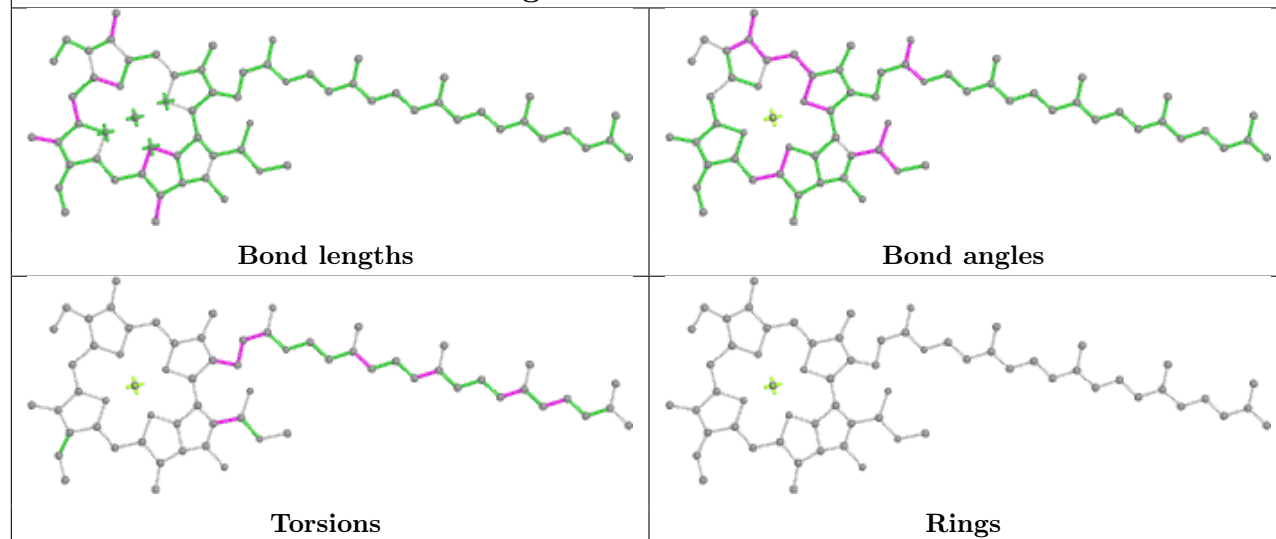




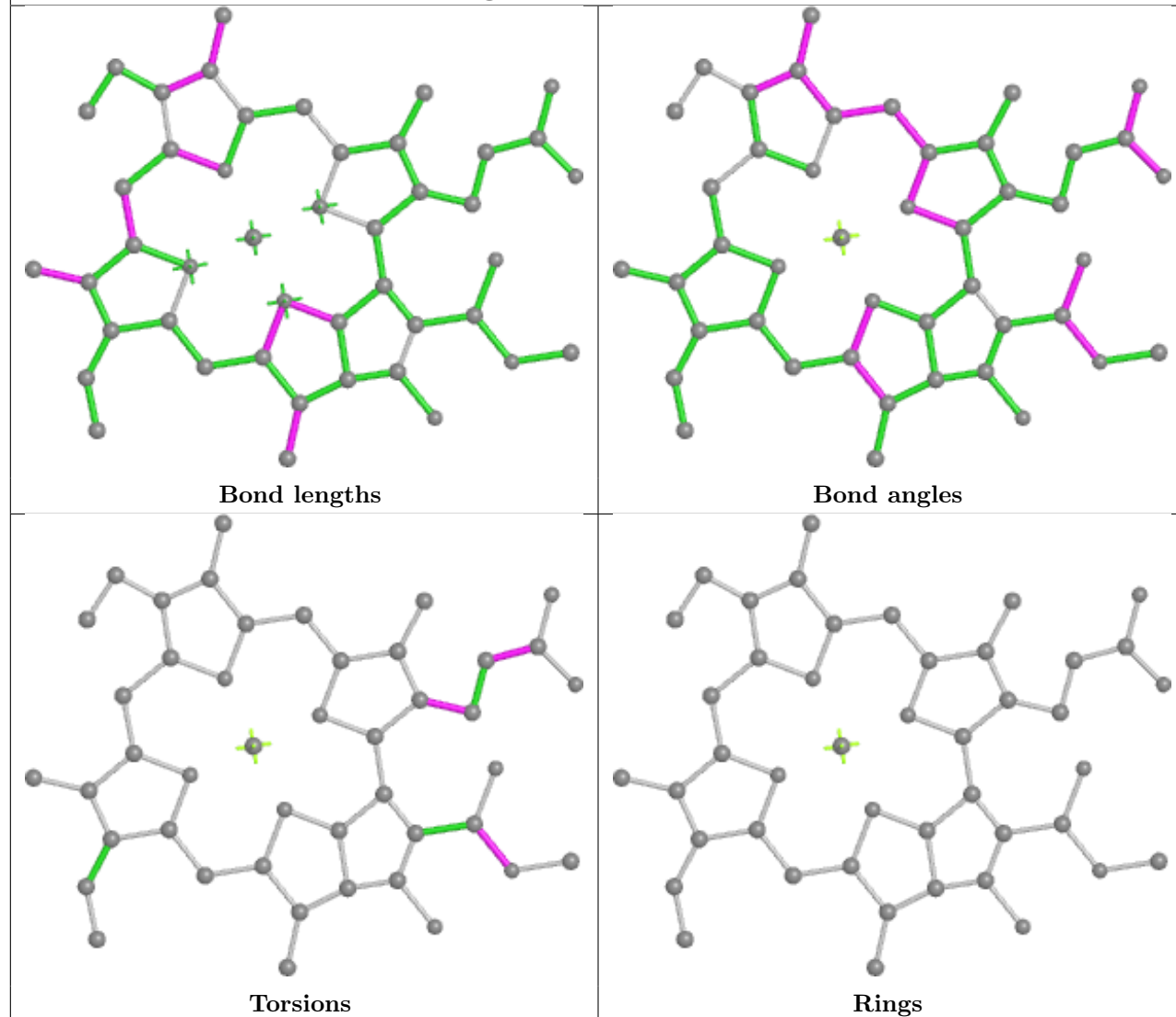


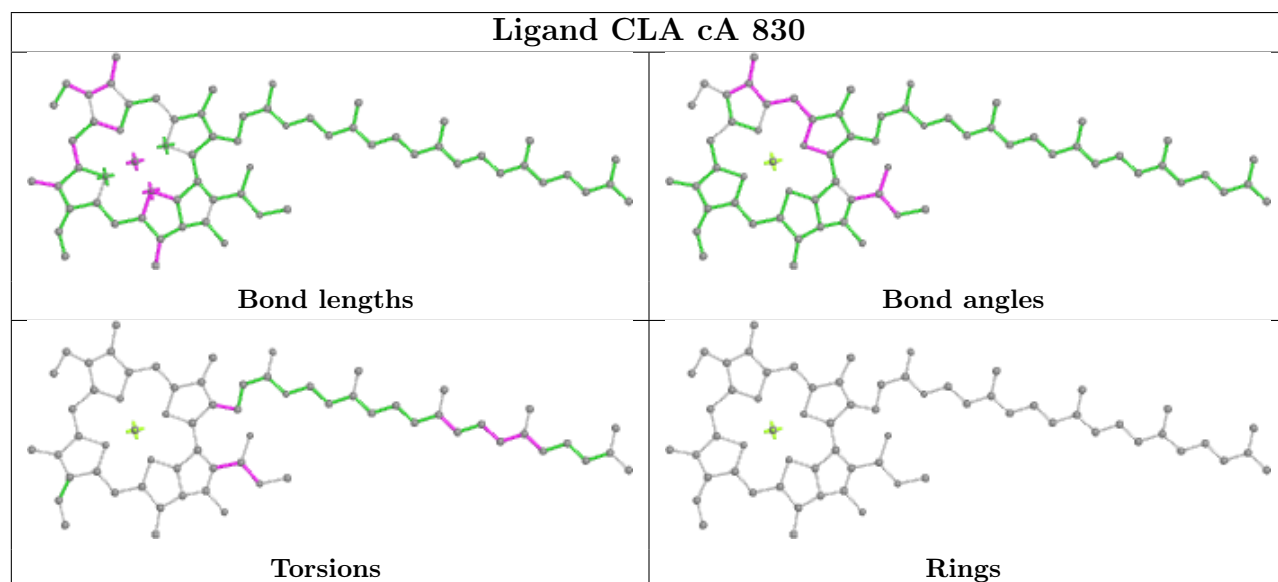
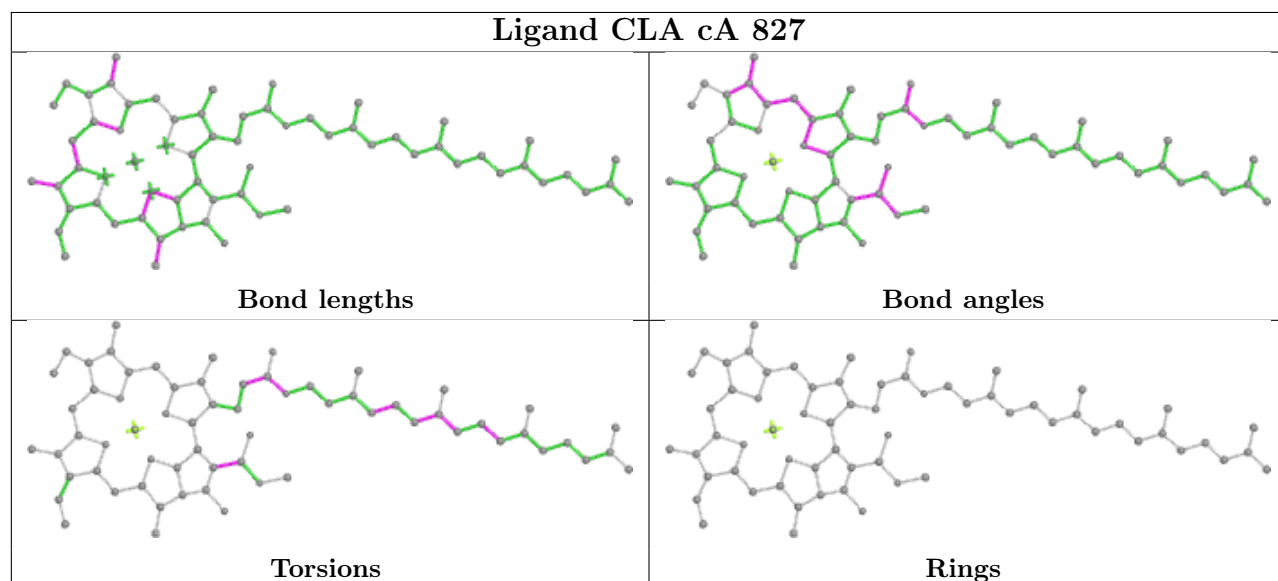
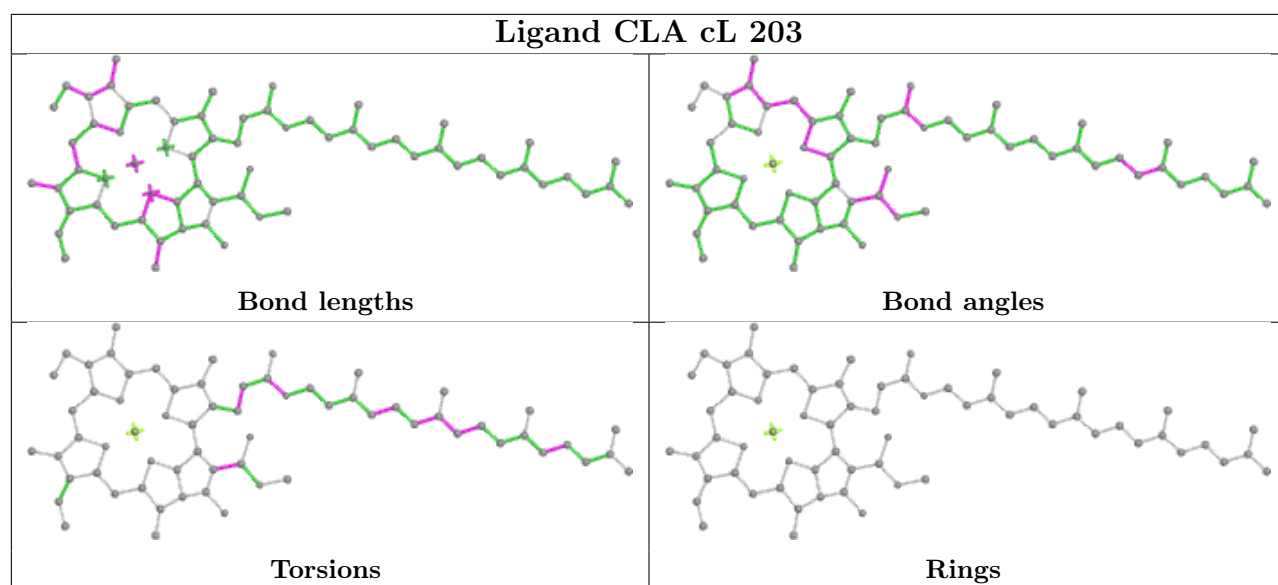


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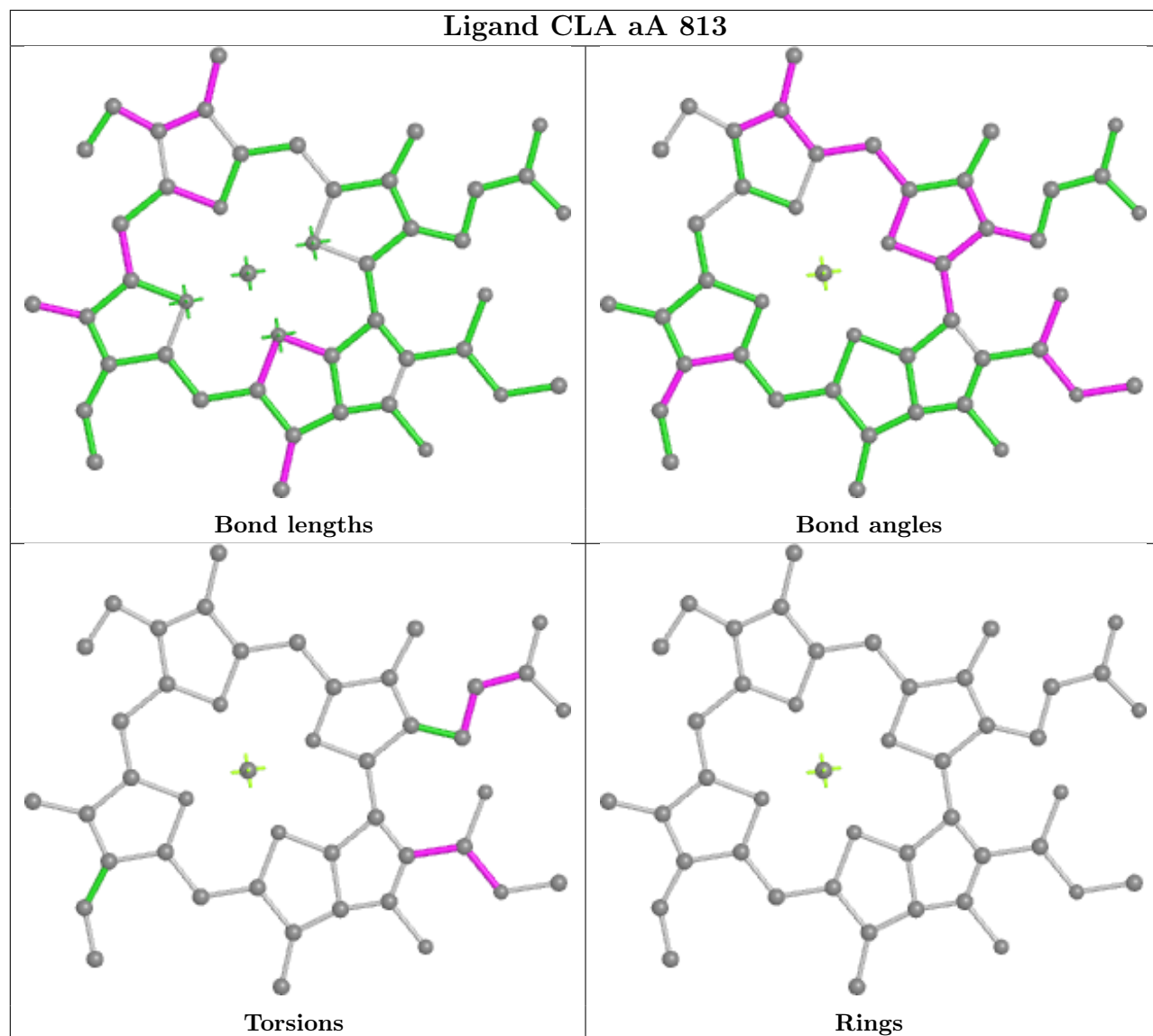


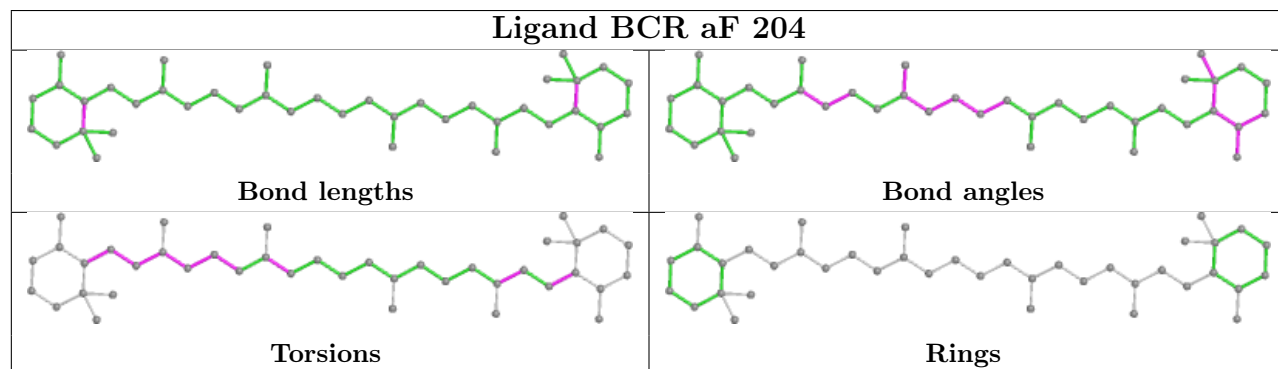
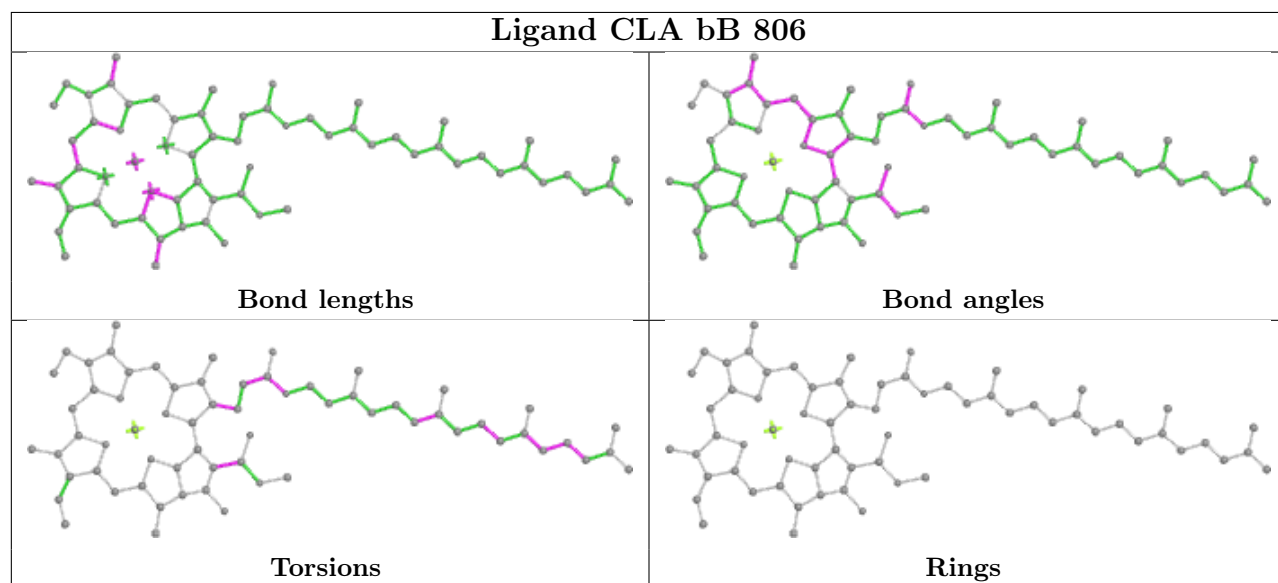
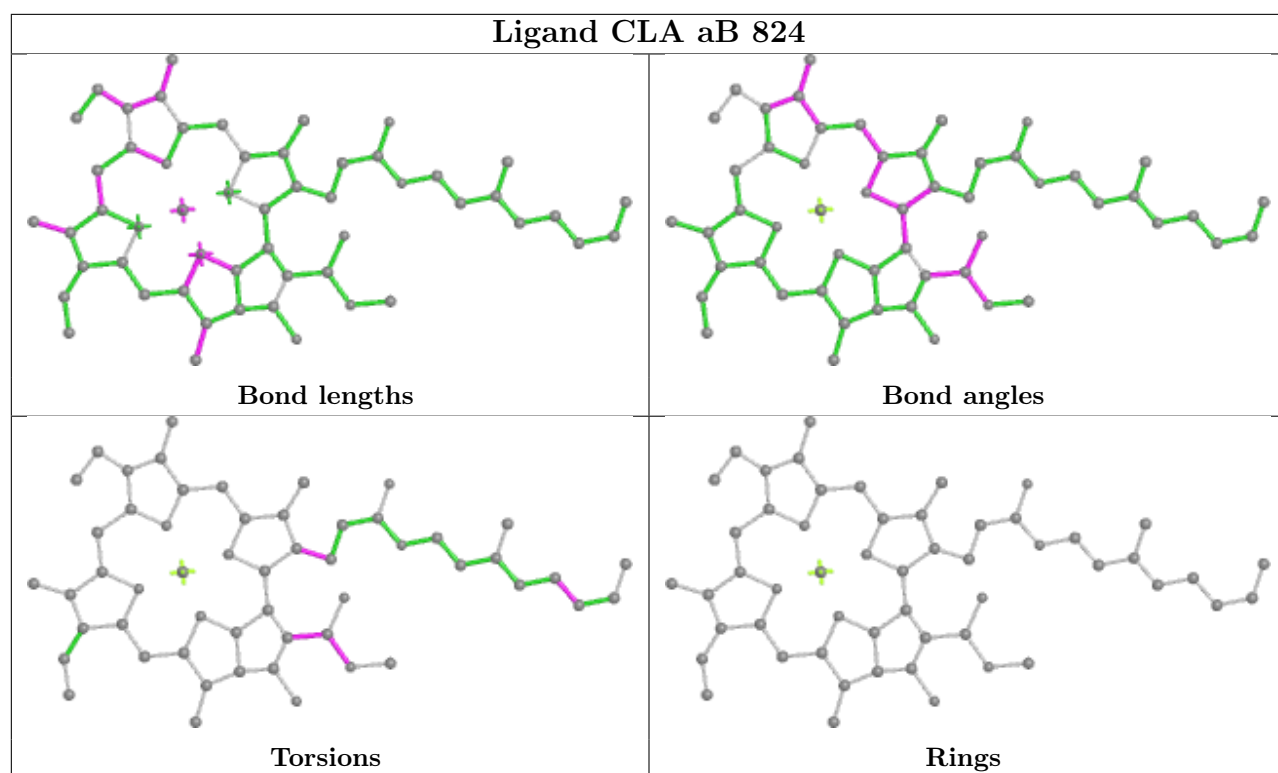
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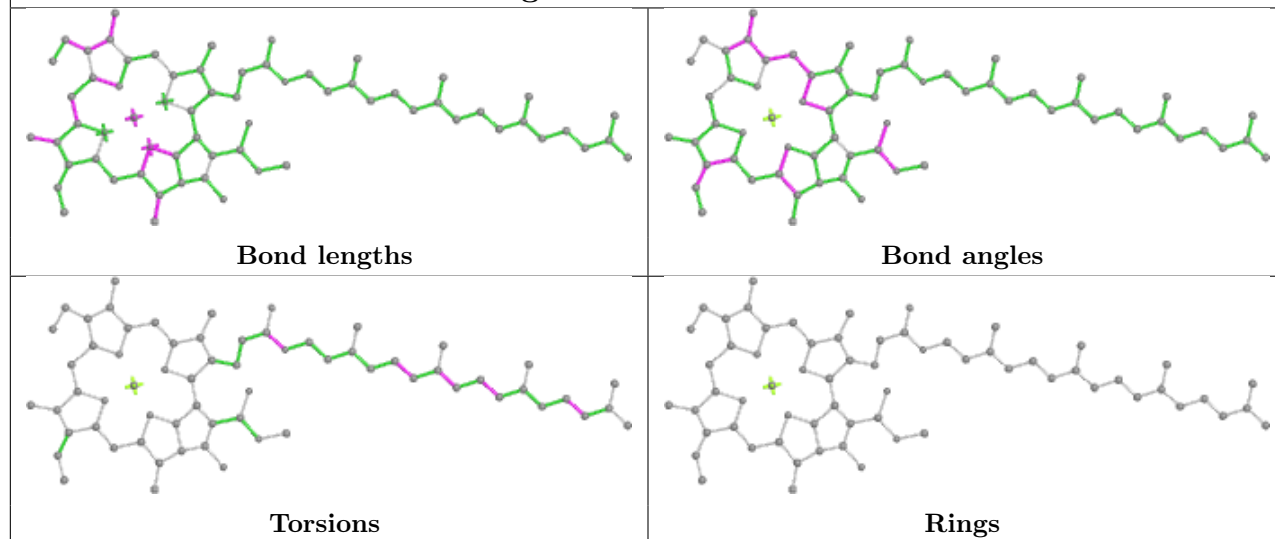
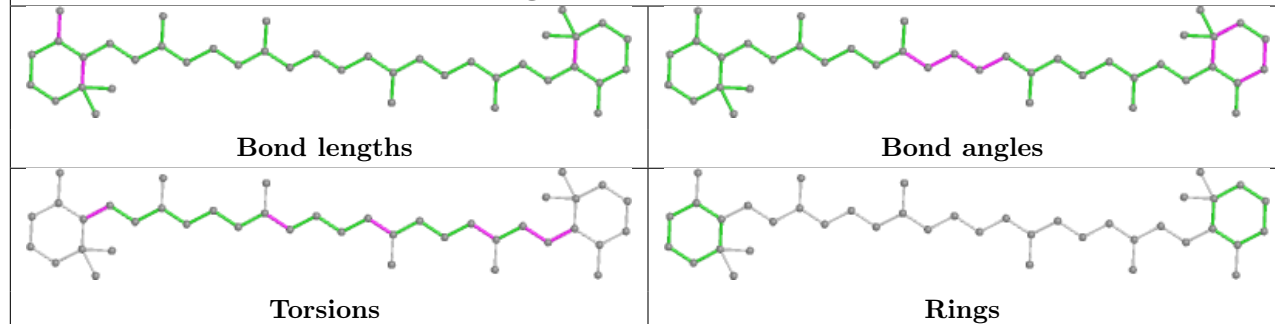
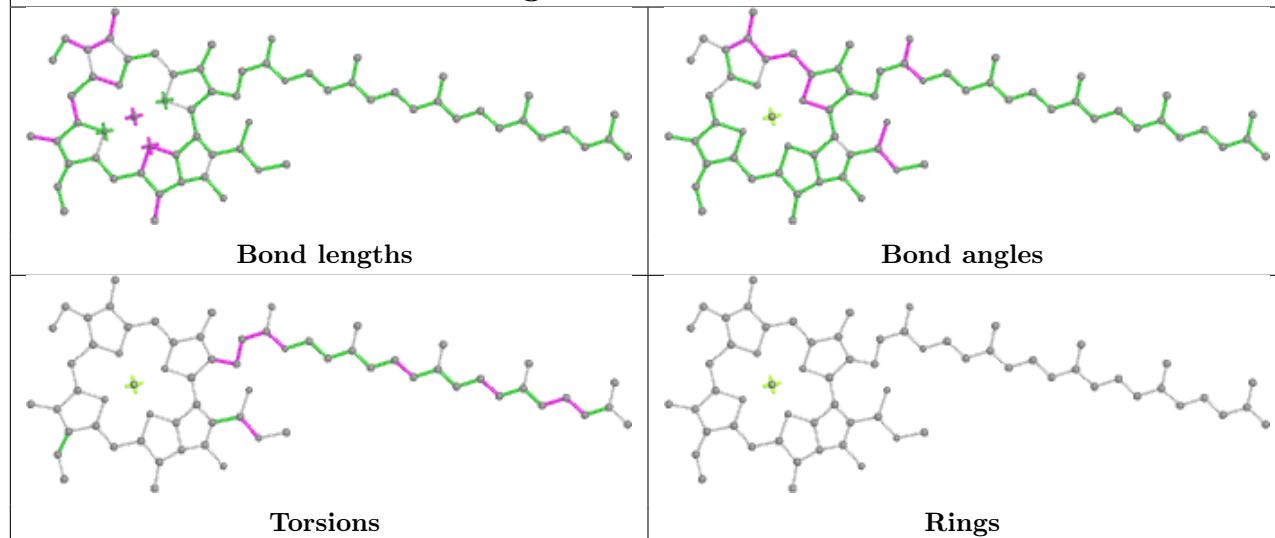


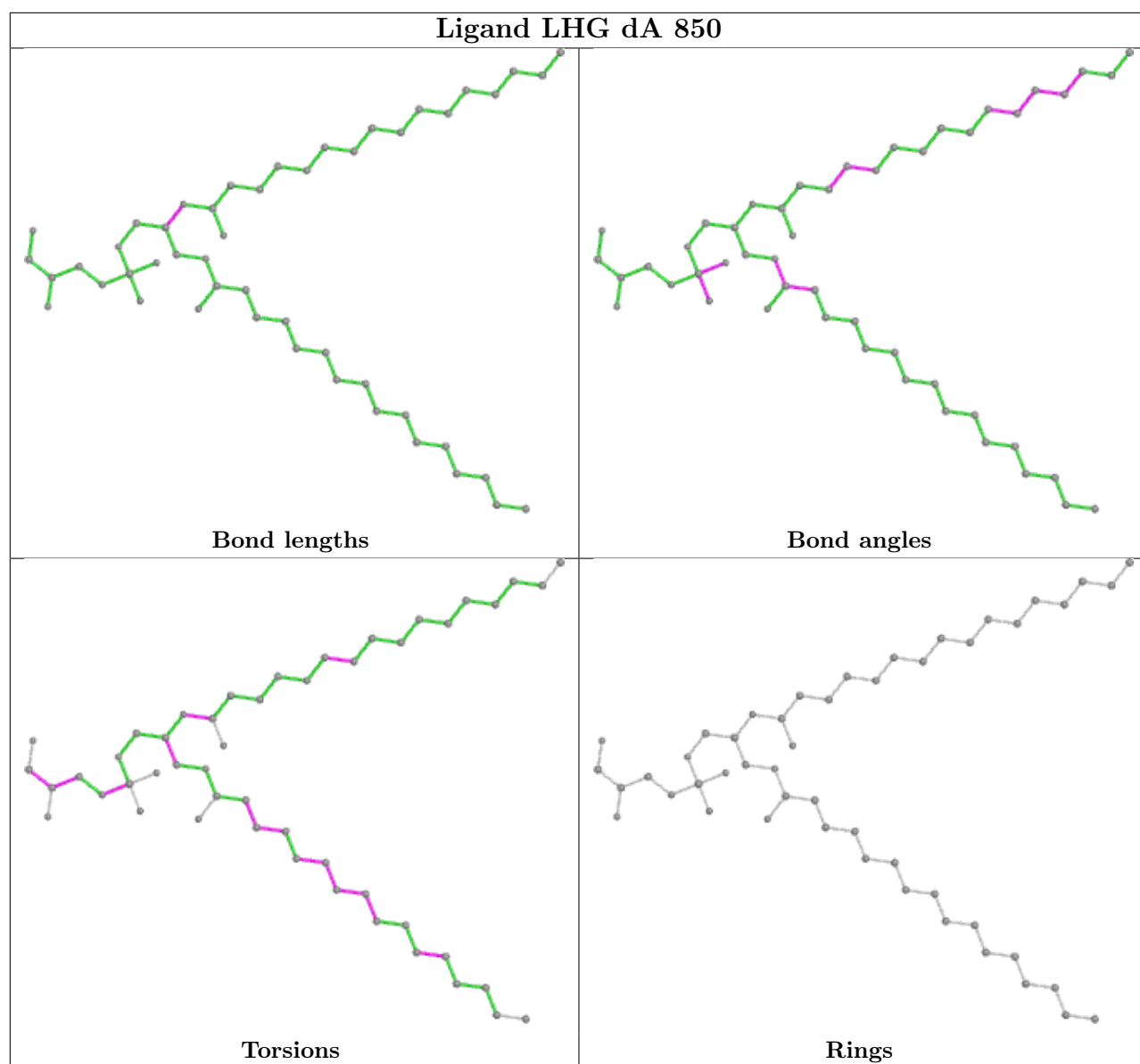


Ligand CLA aA 813

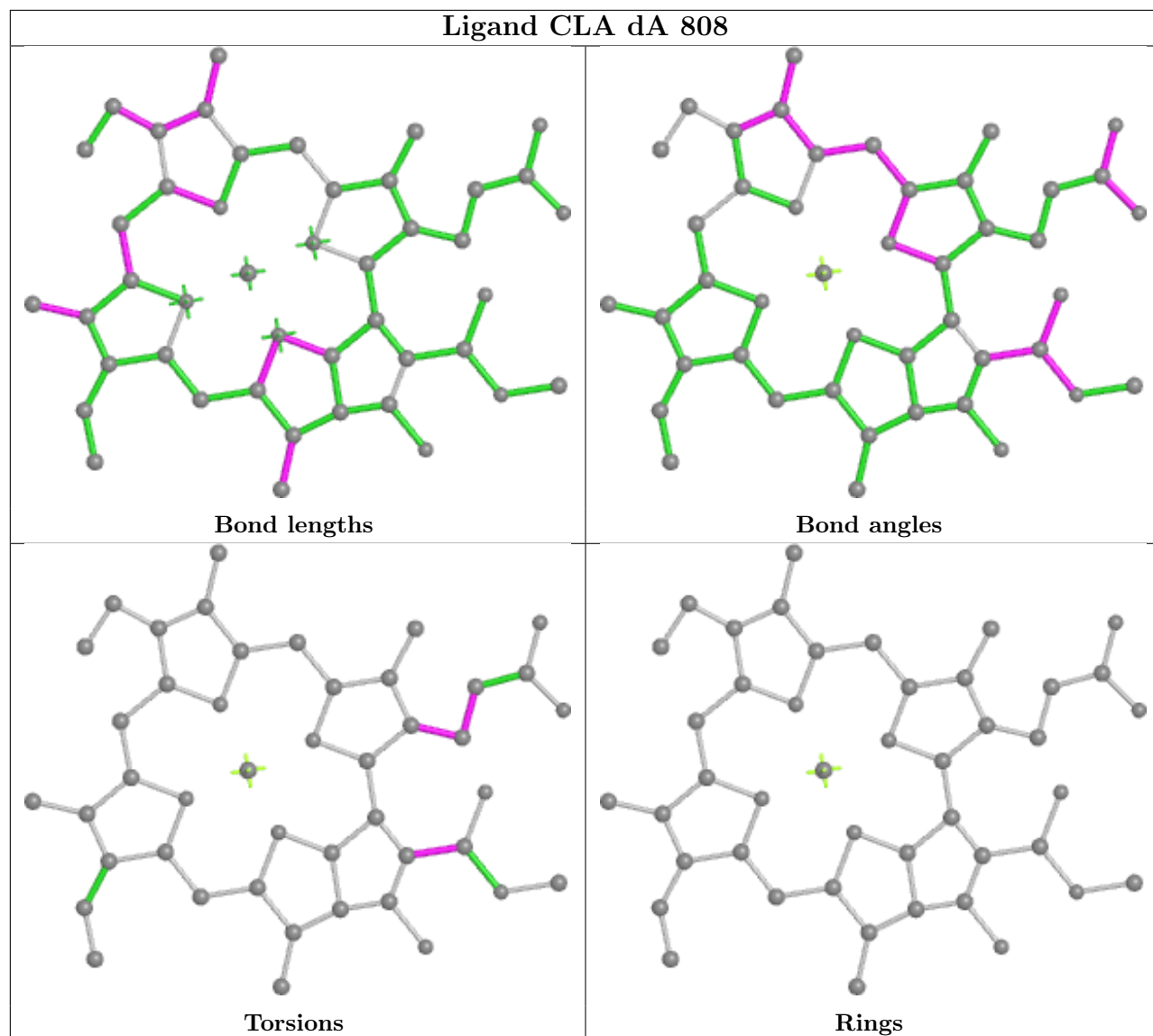


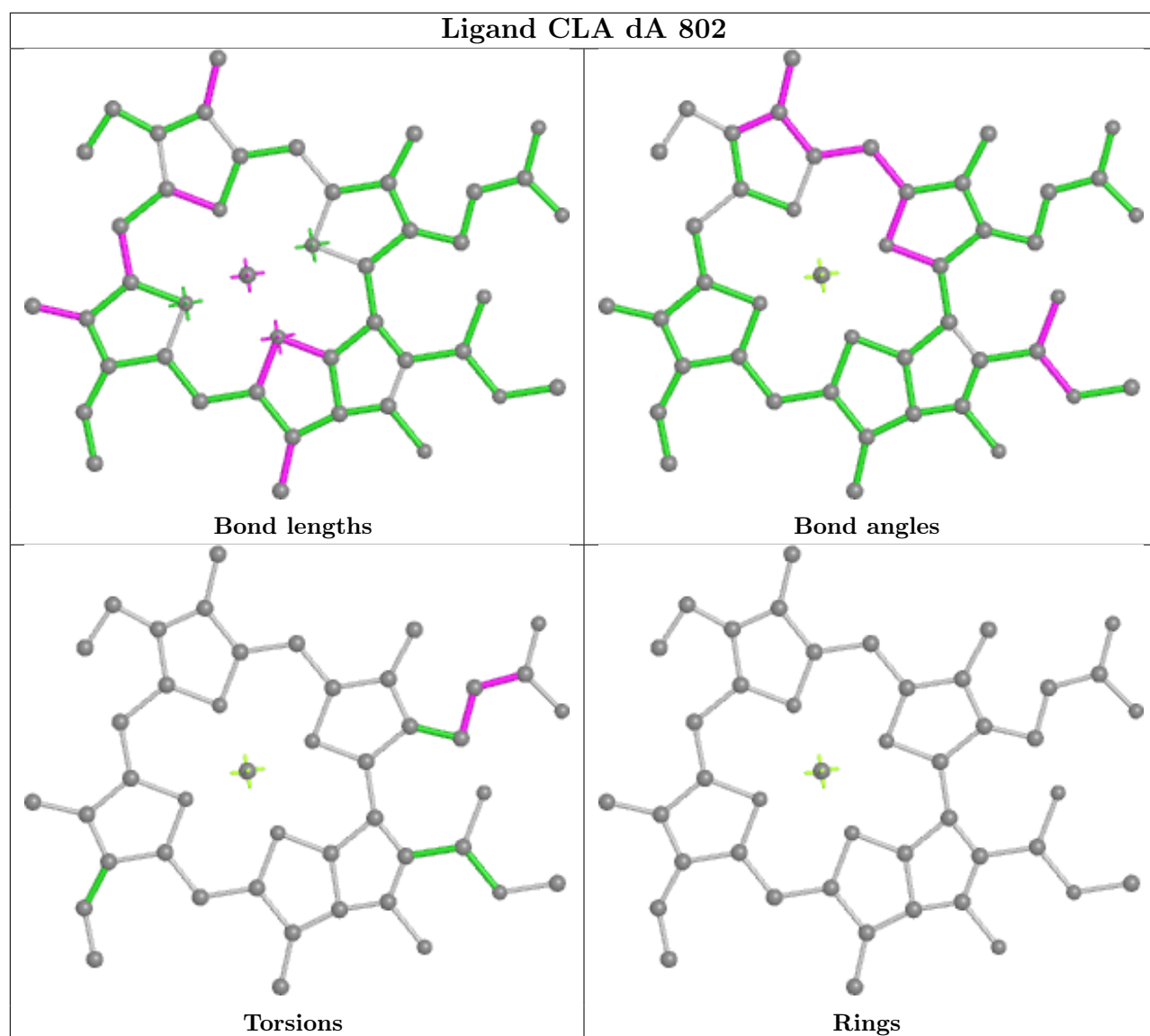


Ligand CLA dB 811**Ligand BCR dJ 104****Ligand CLA cA 842**

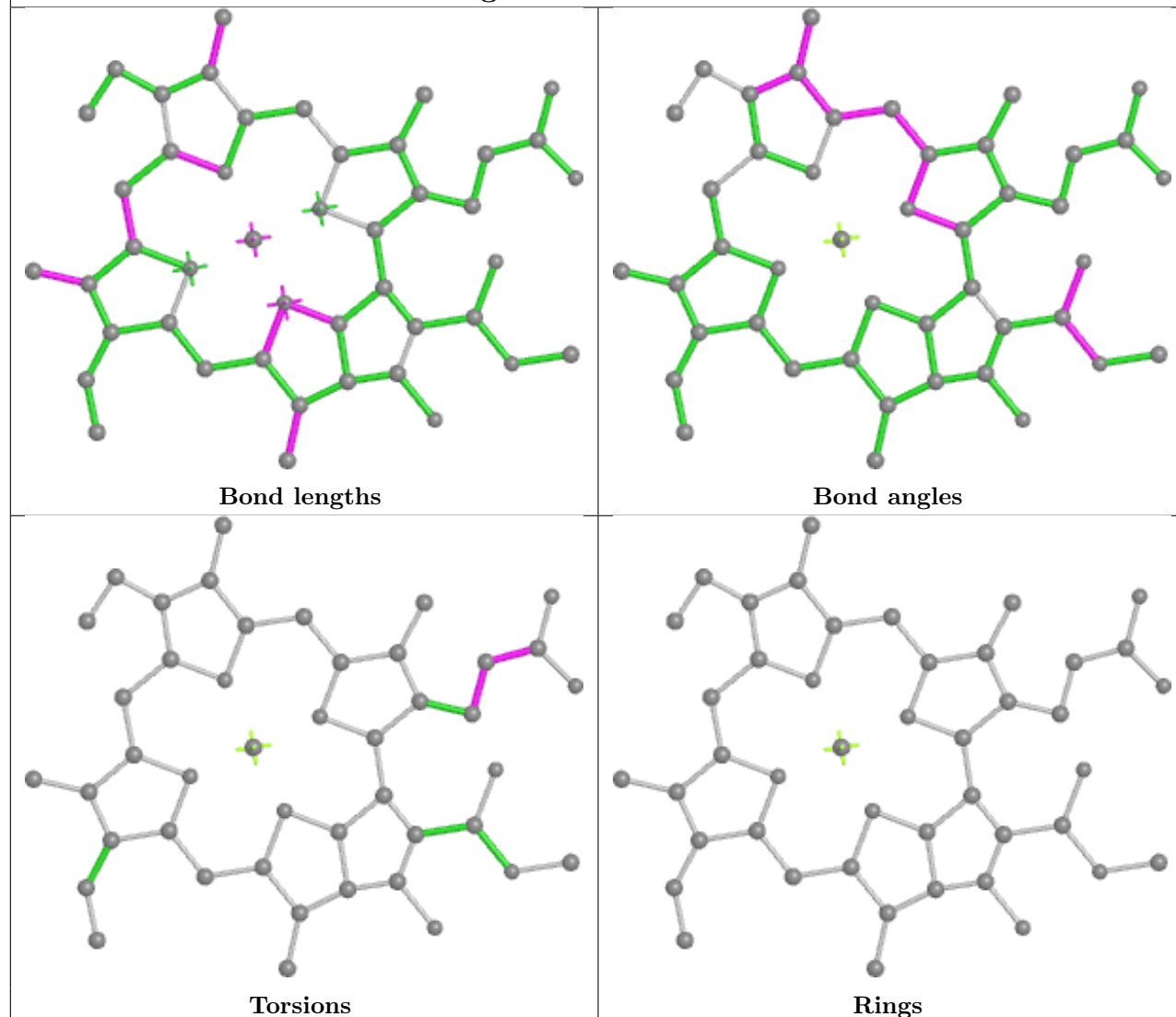


Ligand CLA dA 808

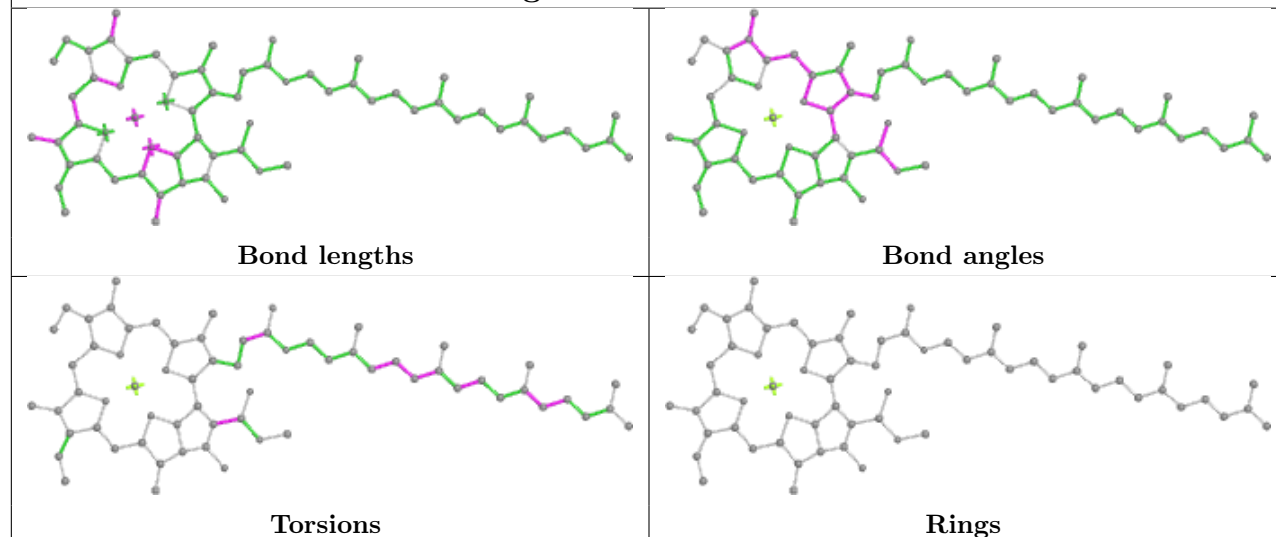


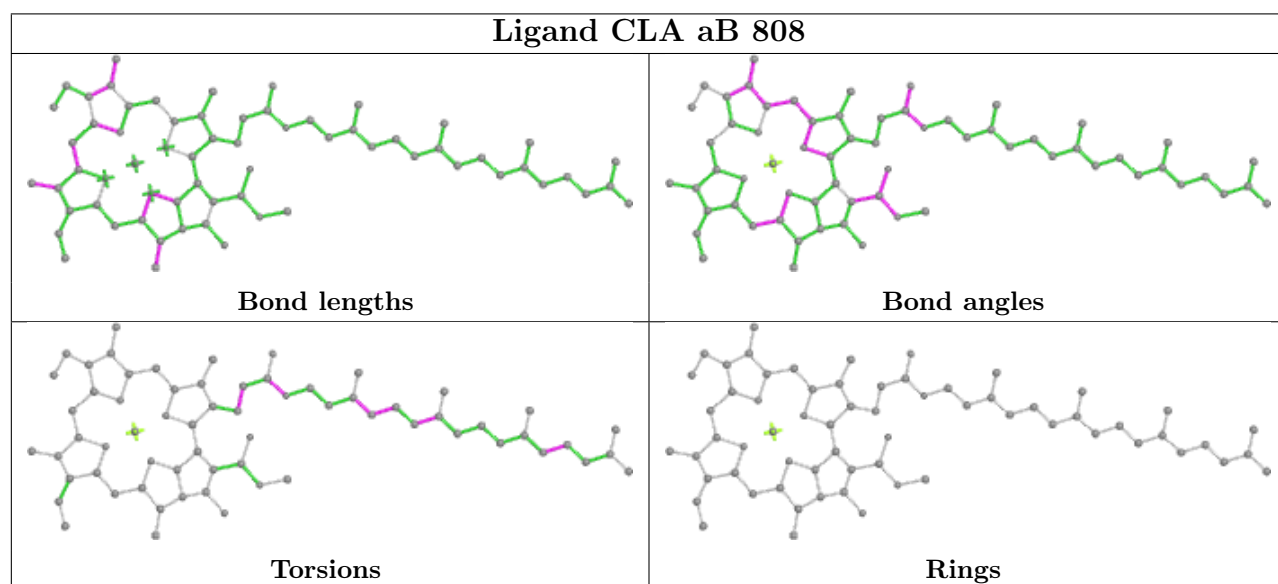
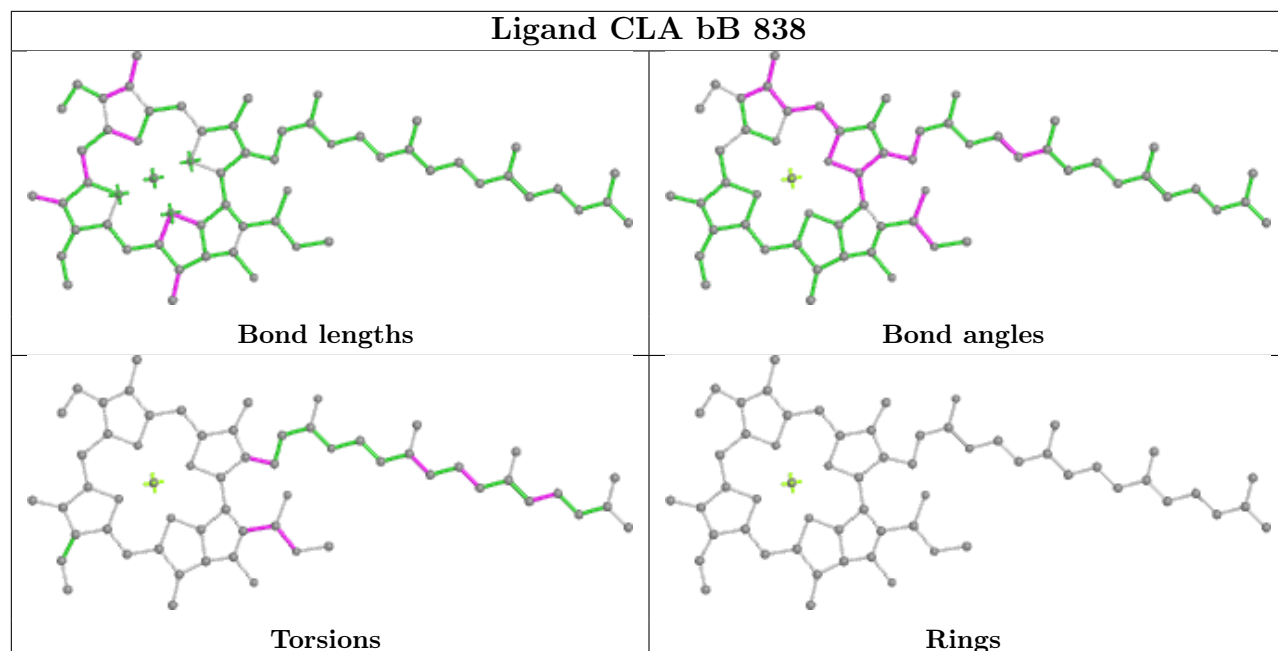
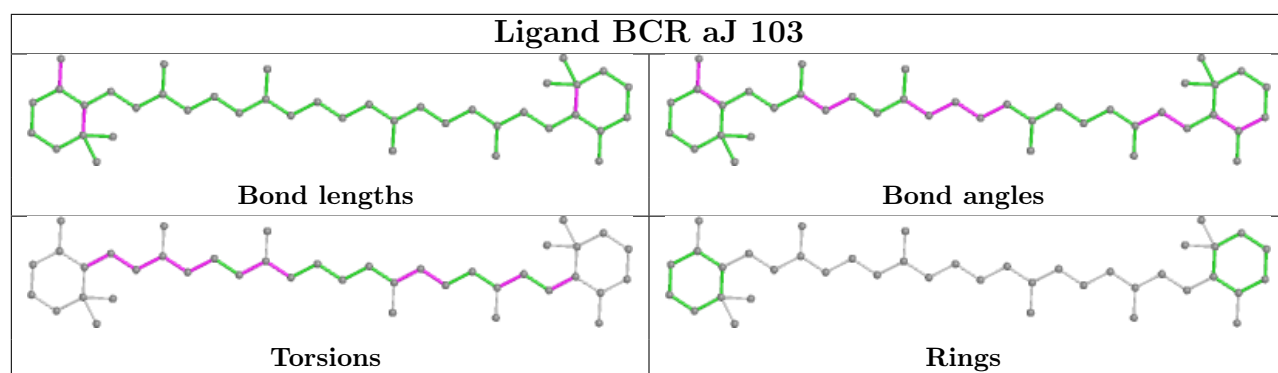


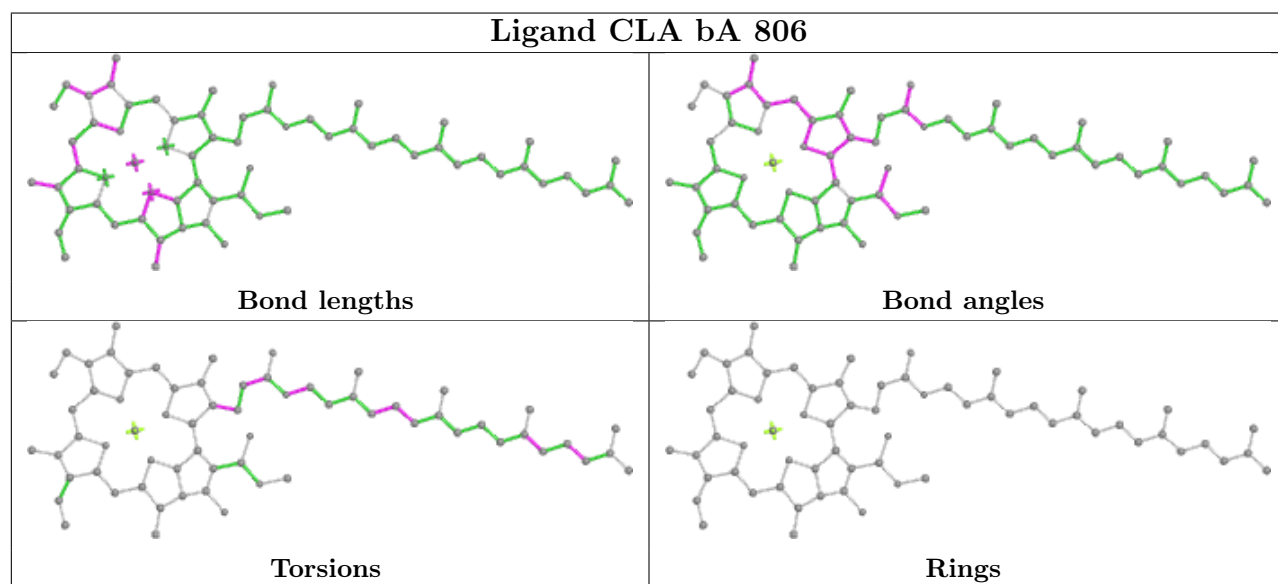
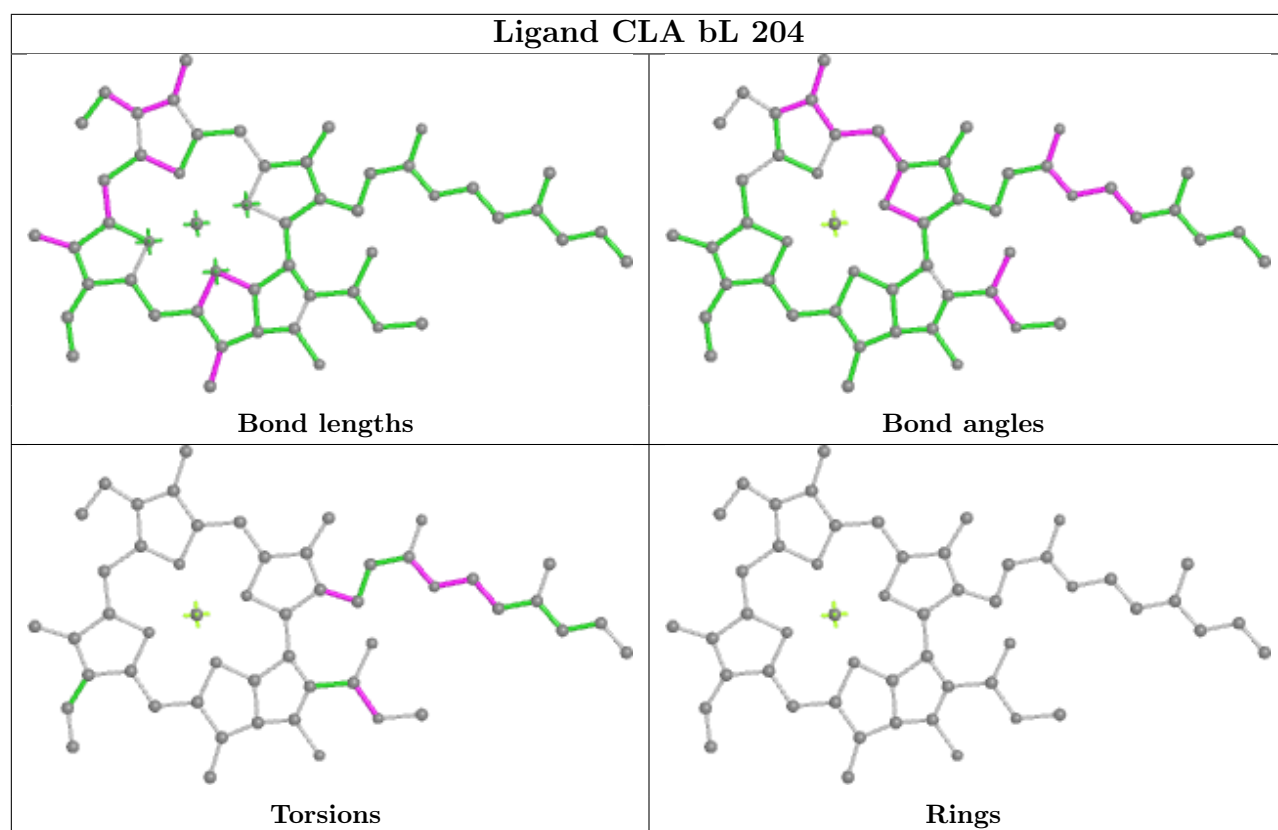
Ligand CLA bA 802

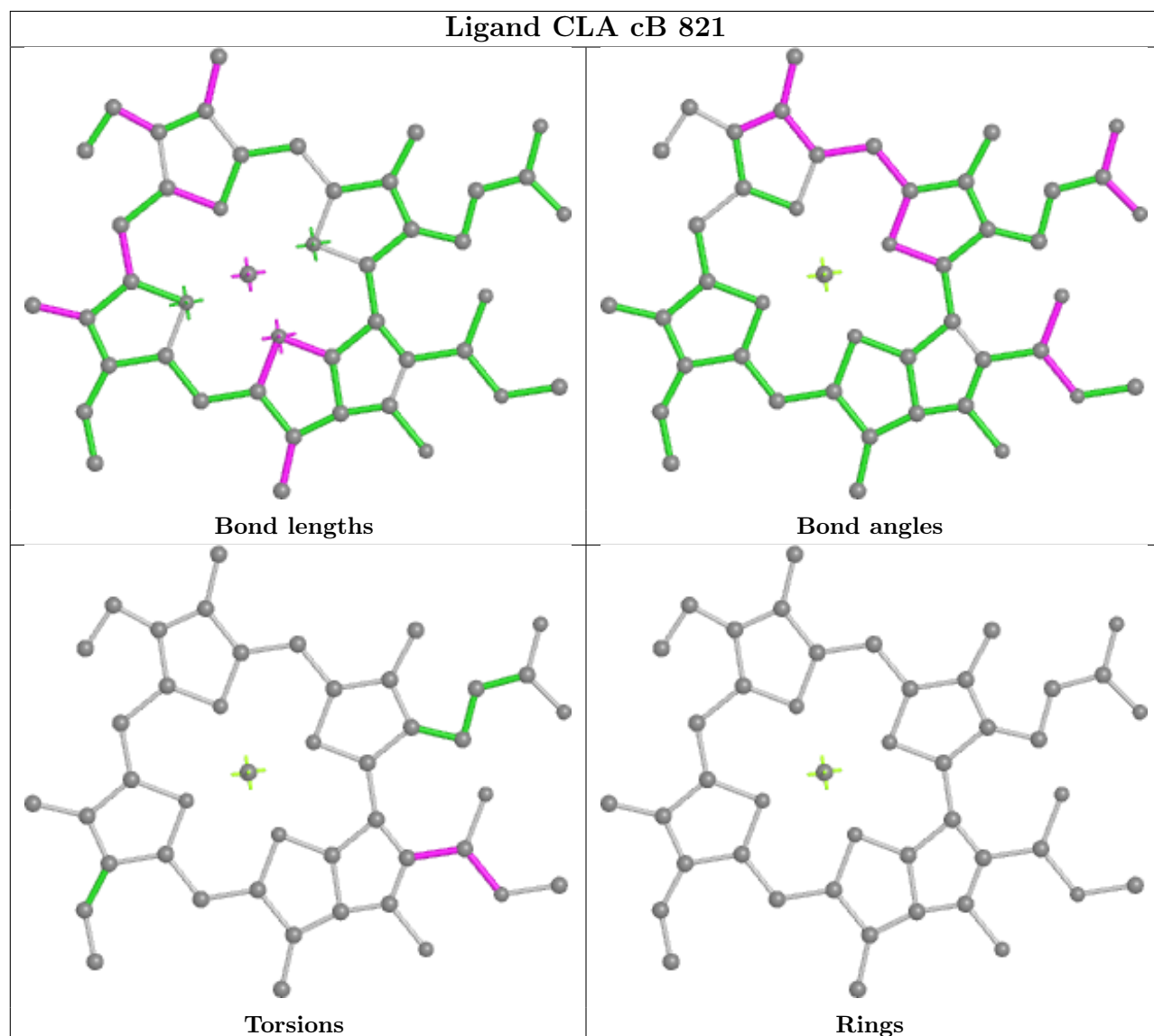
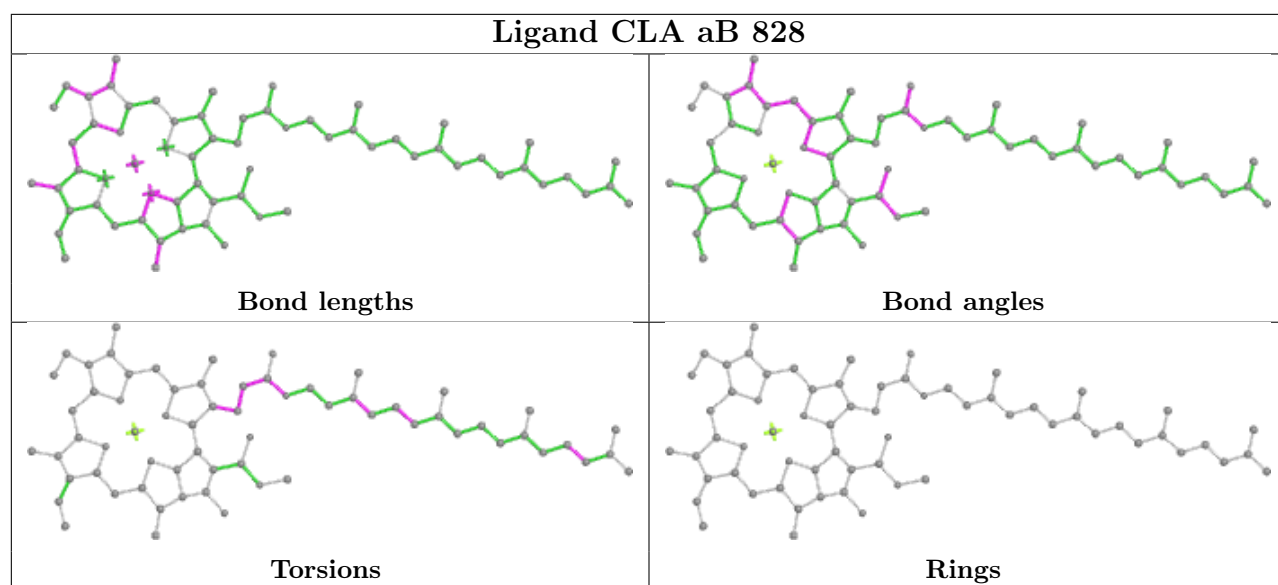


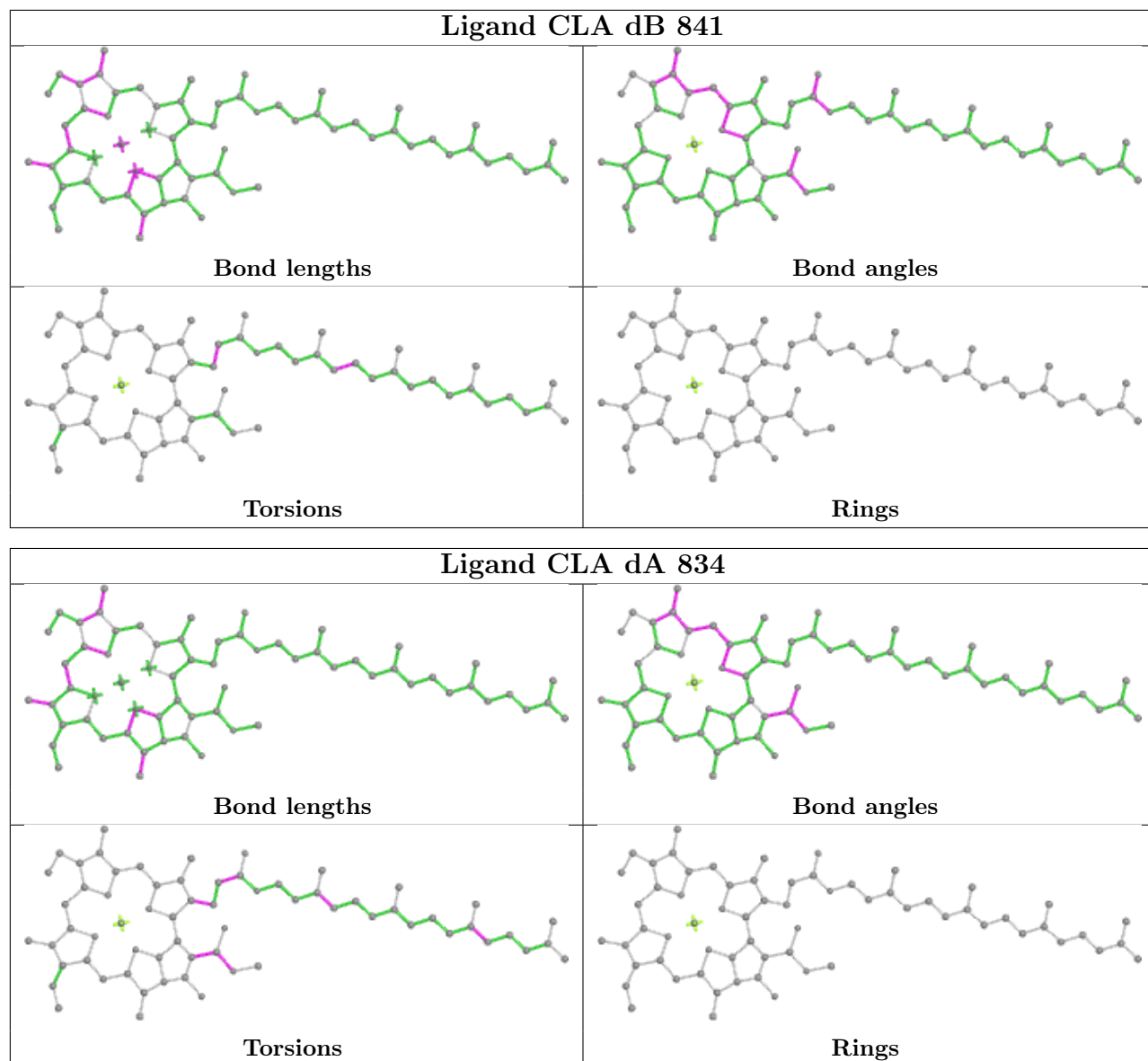
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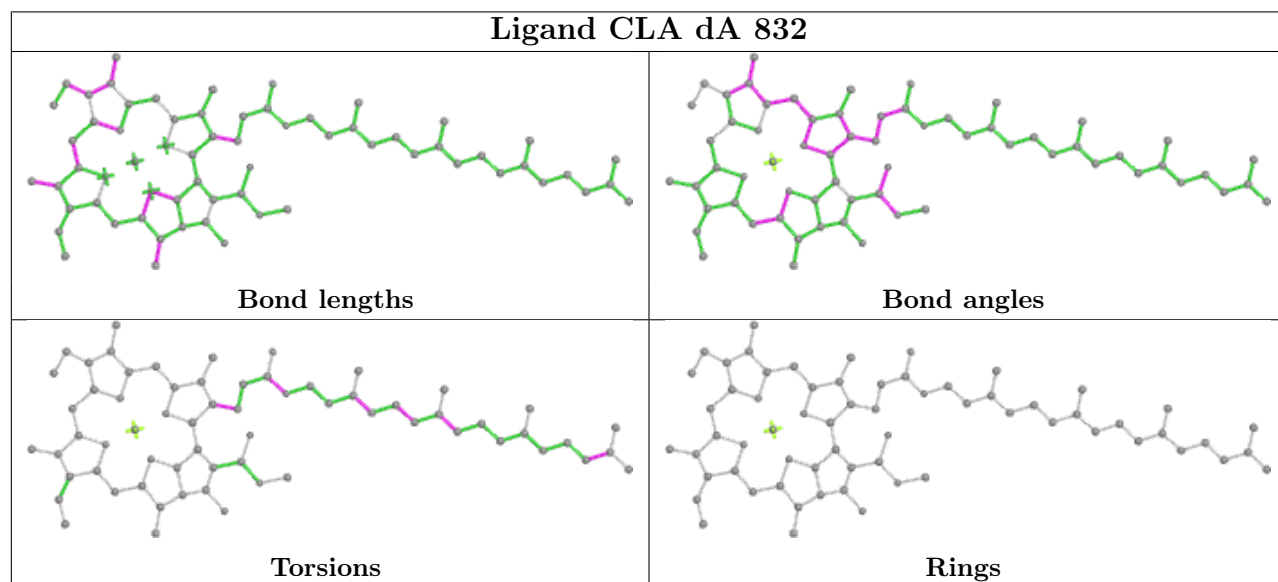
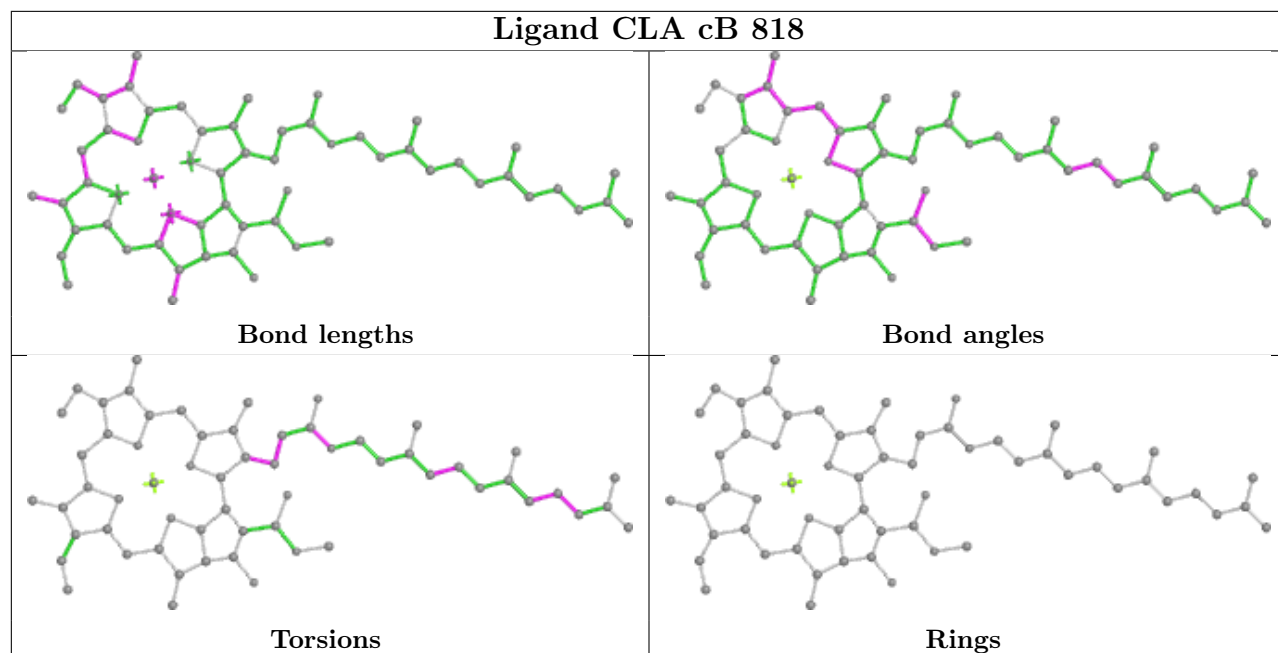




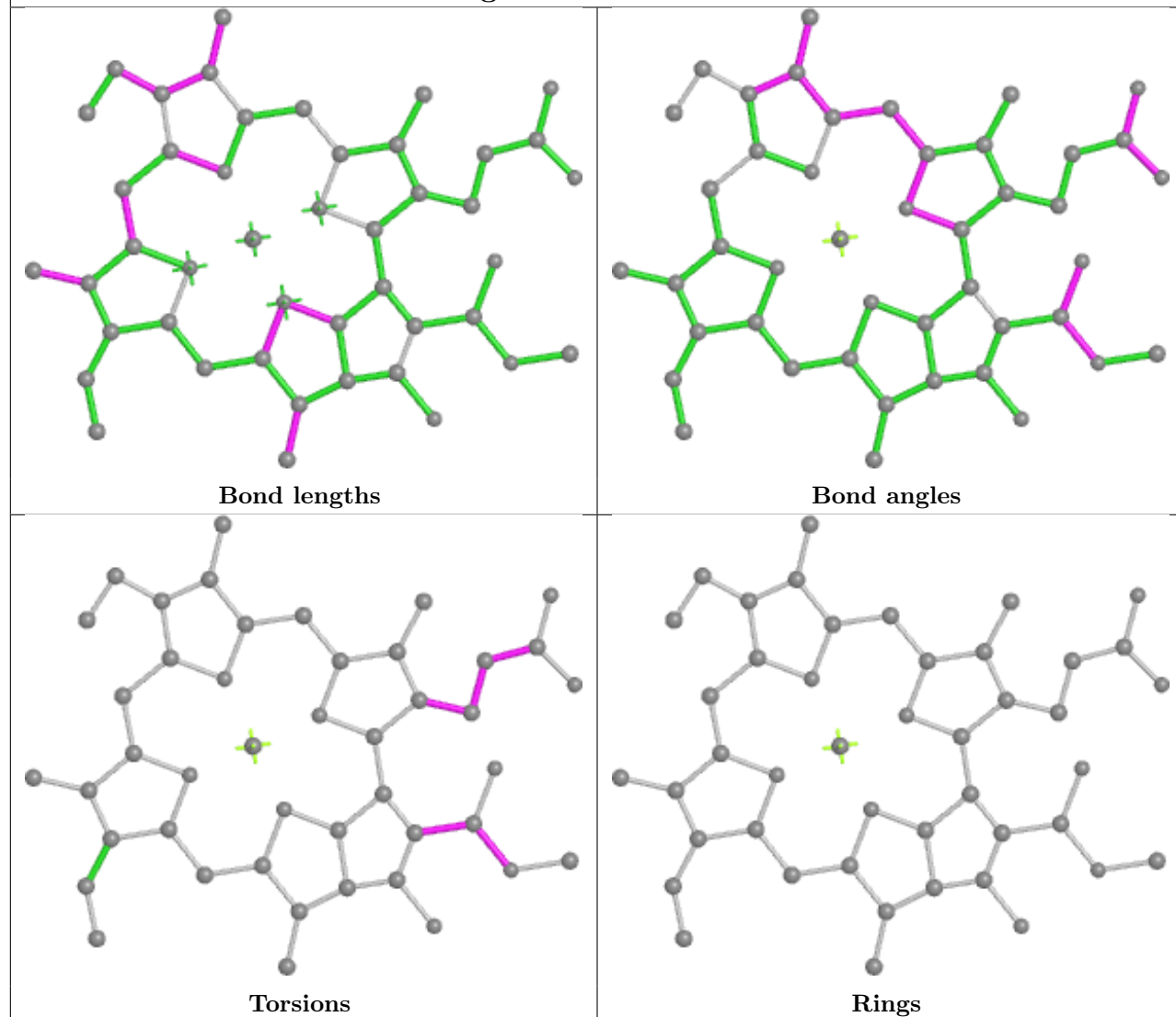




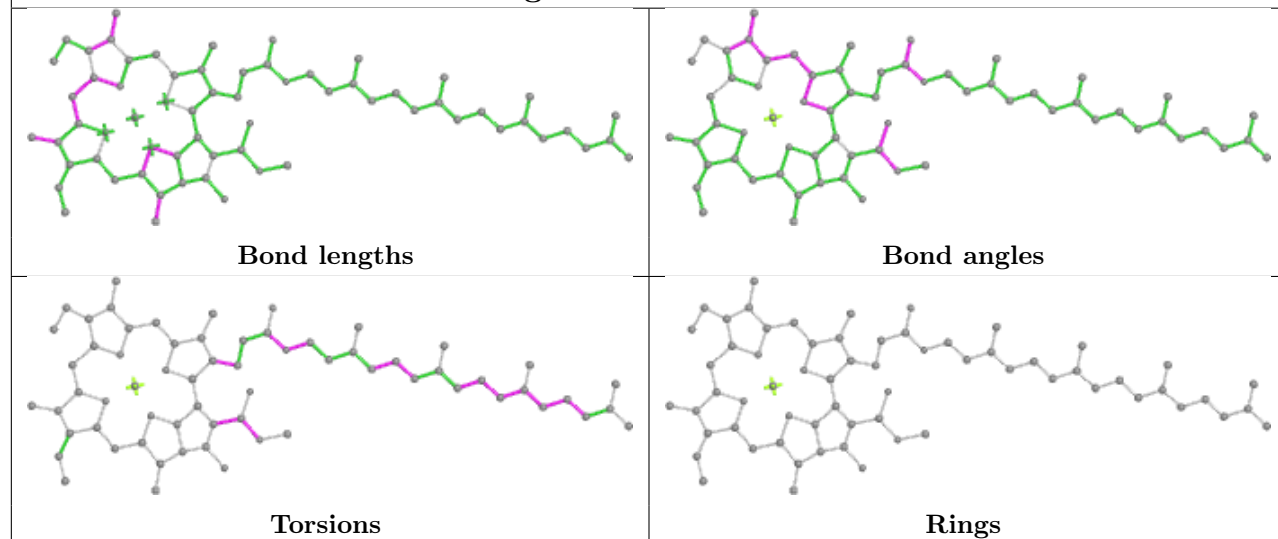


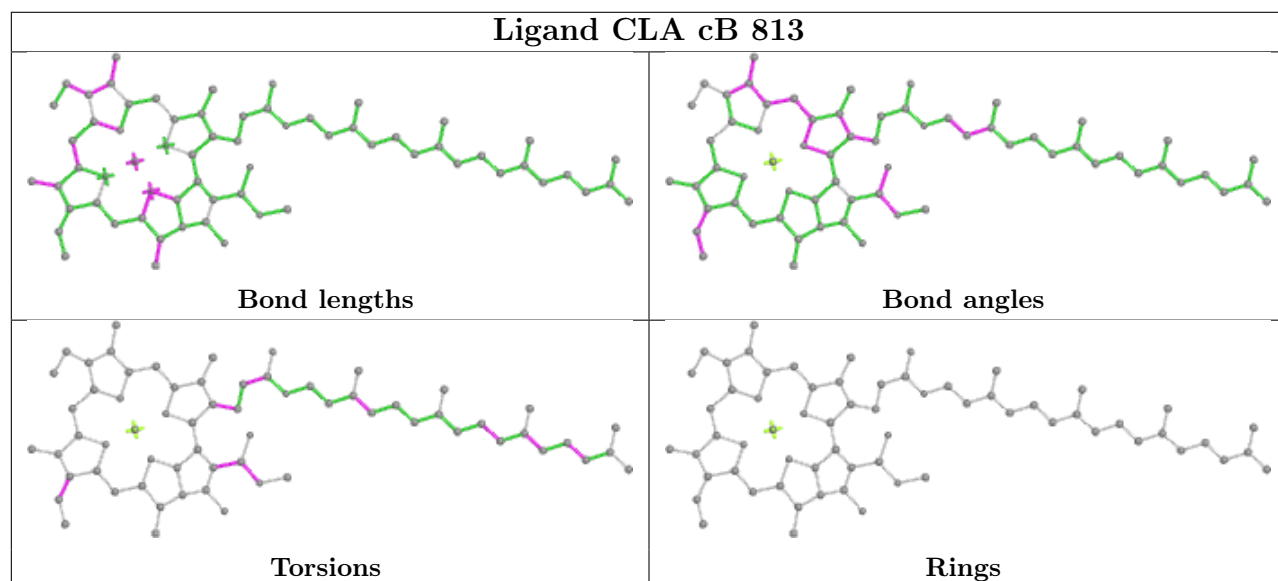
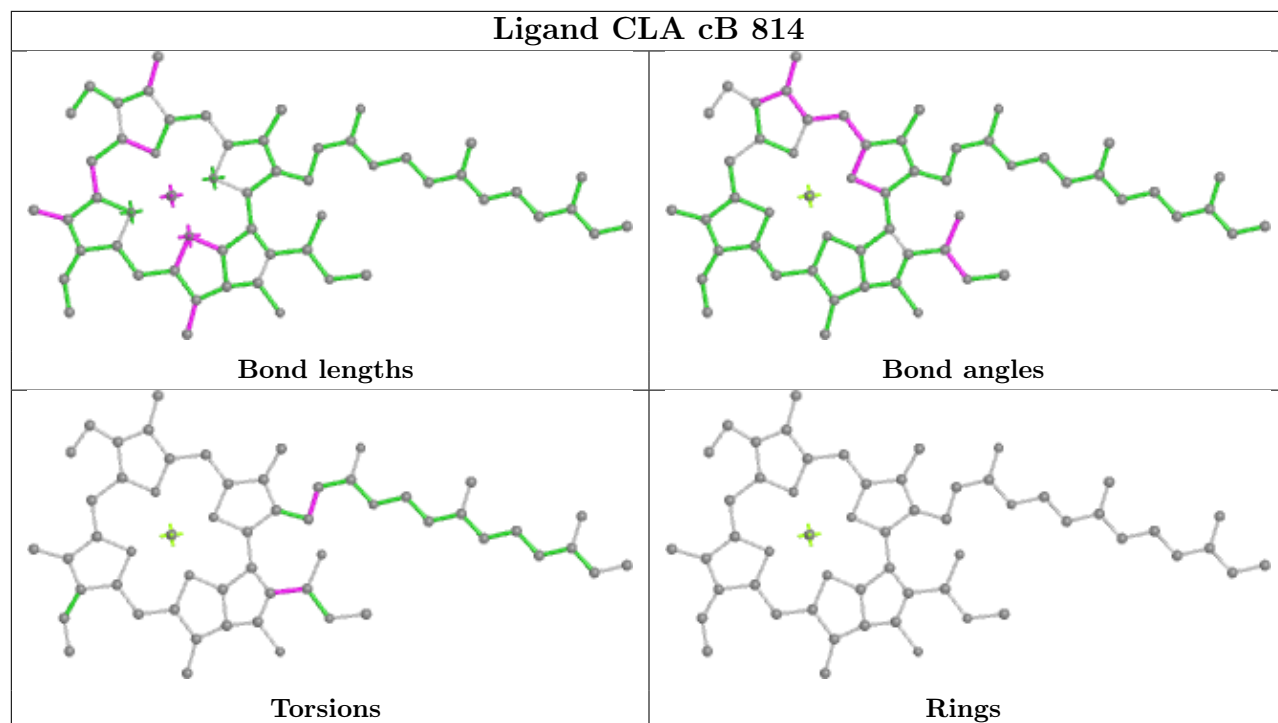


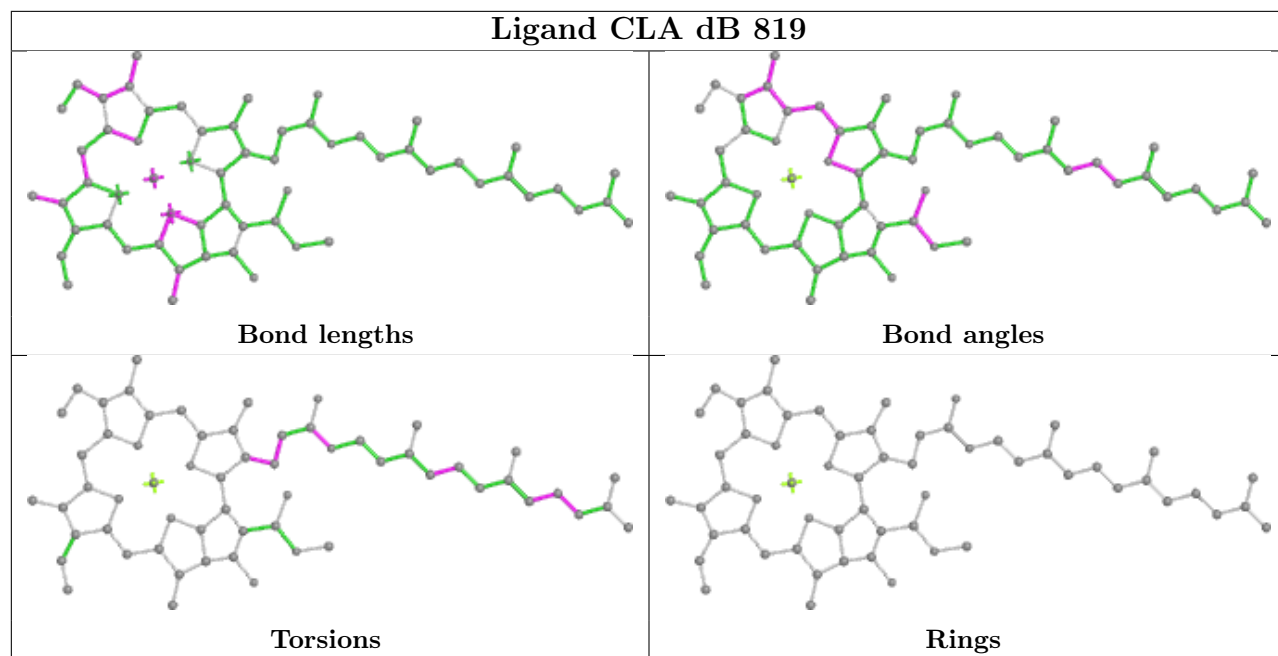
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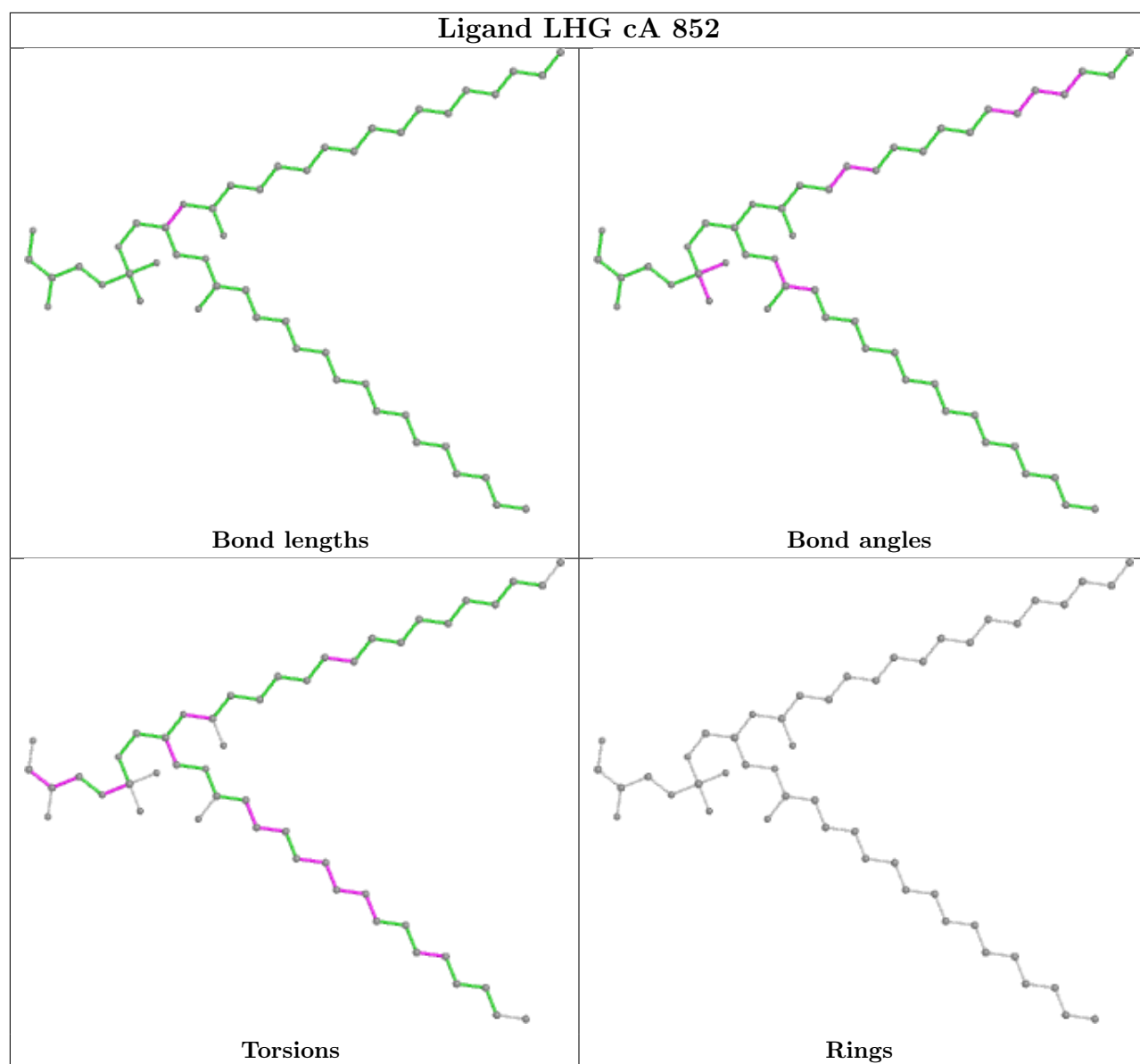


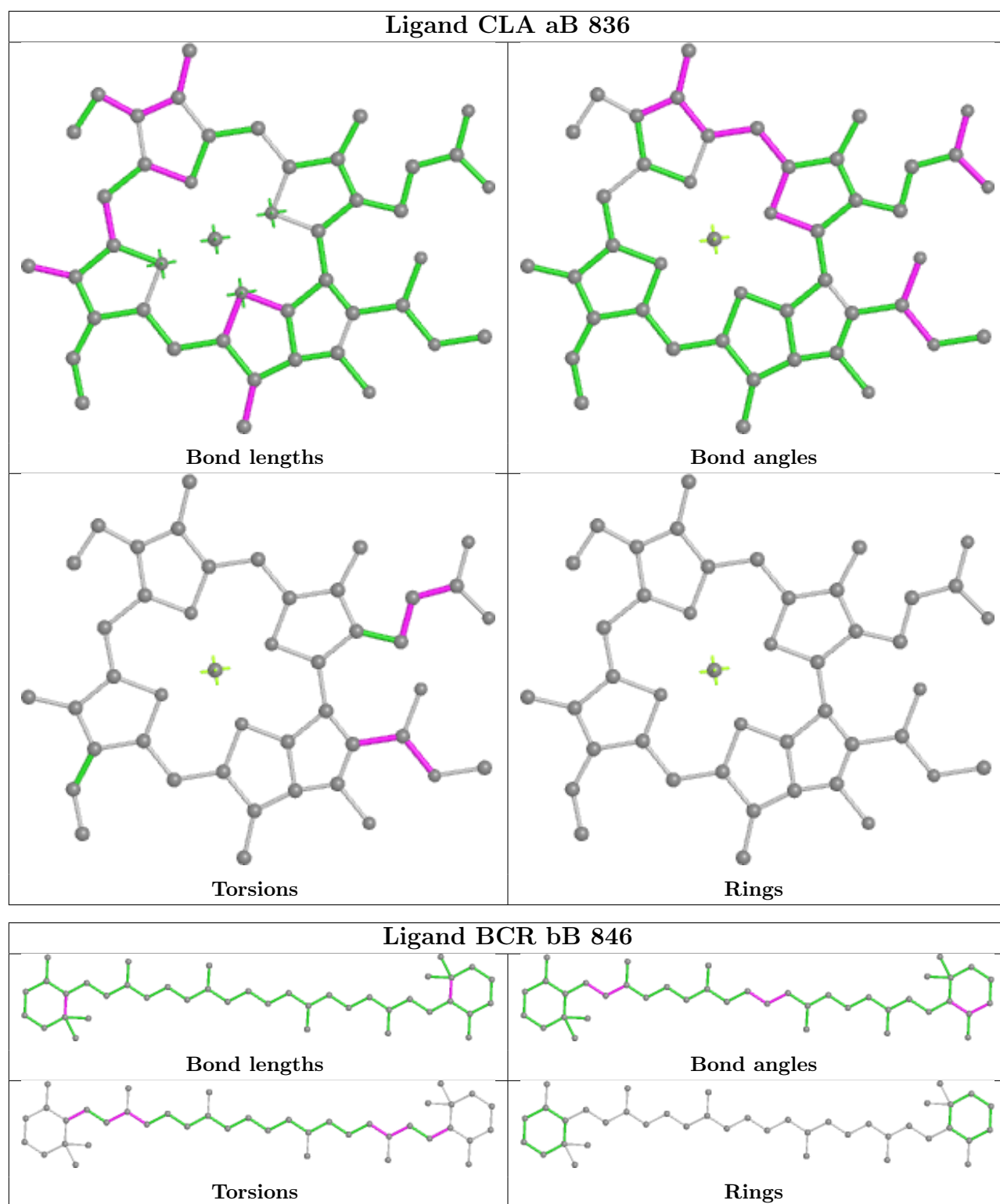
Ligand CLA cB 841



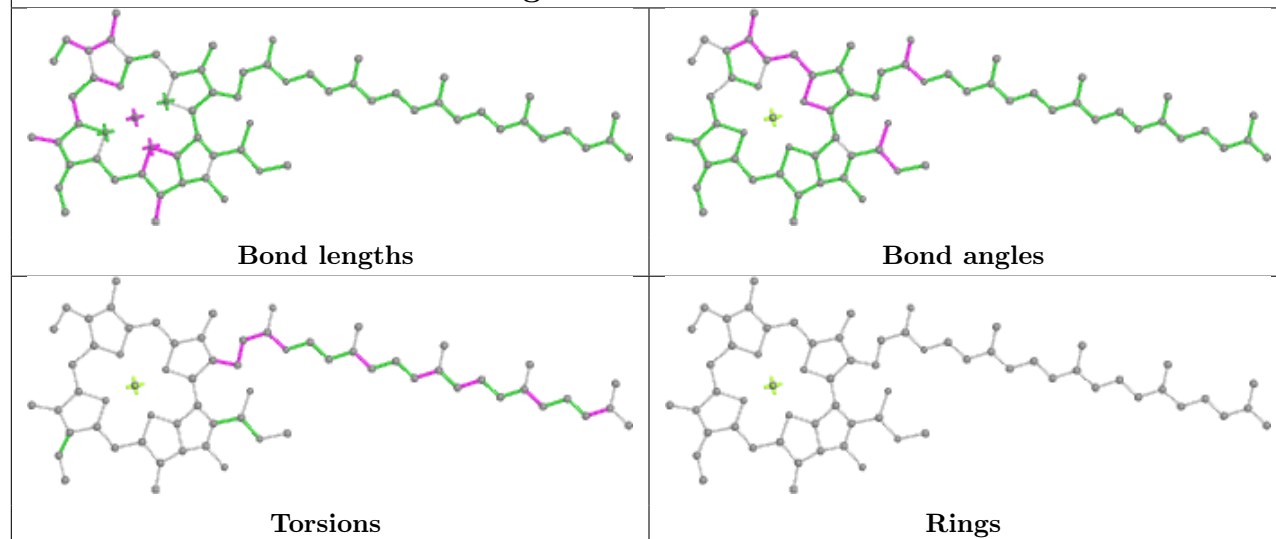




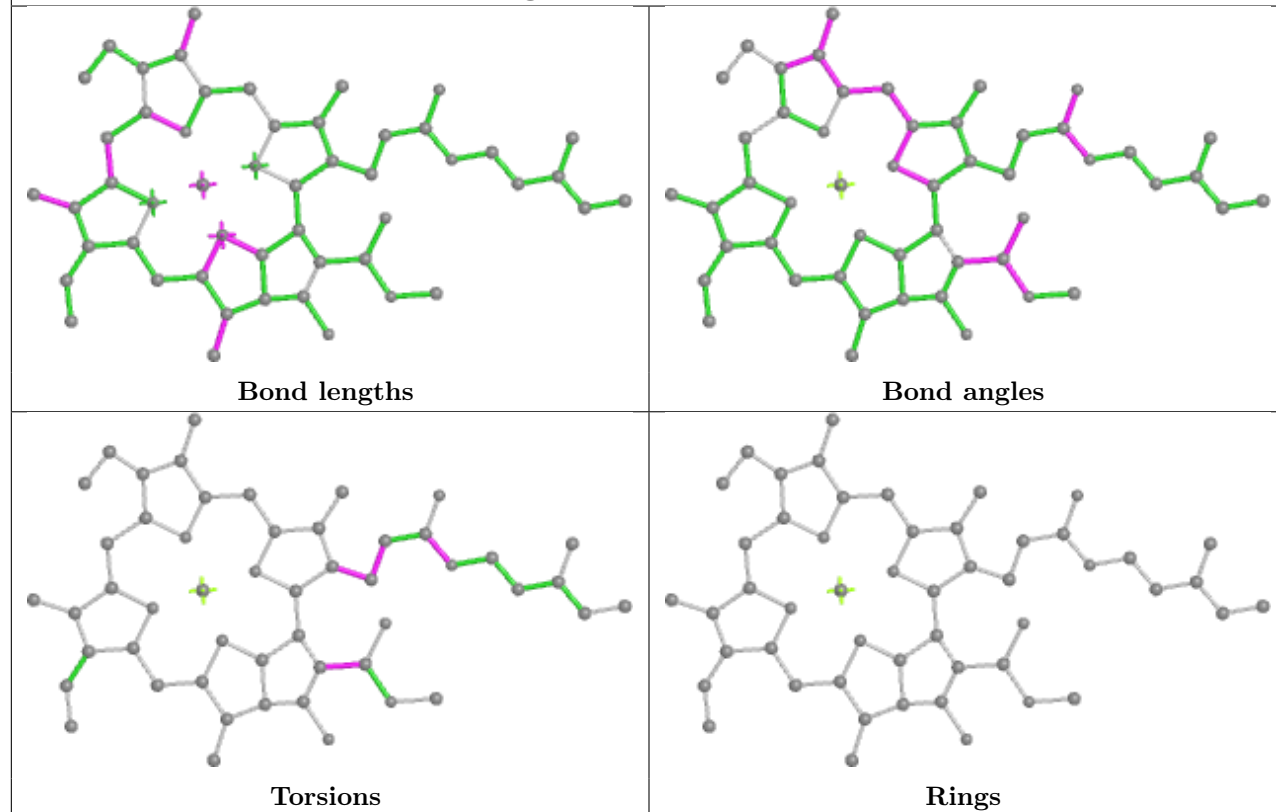


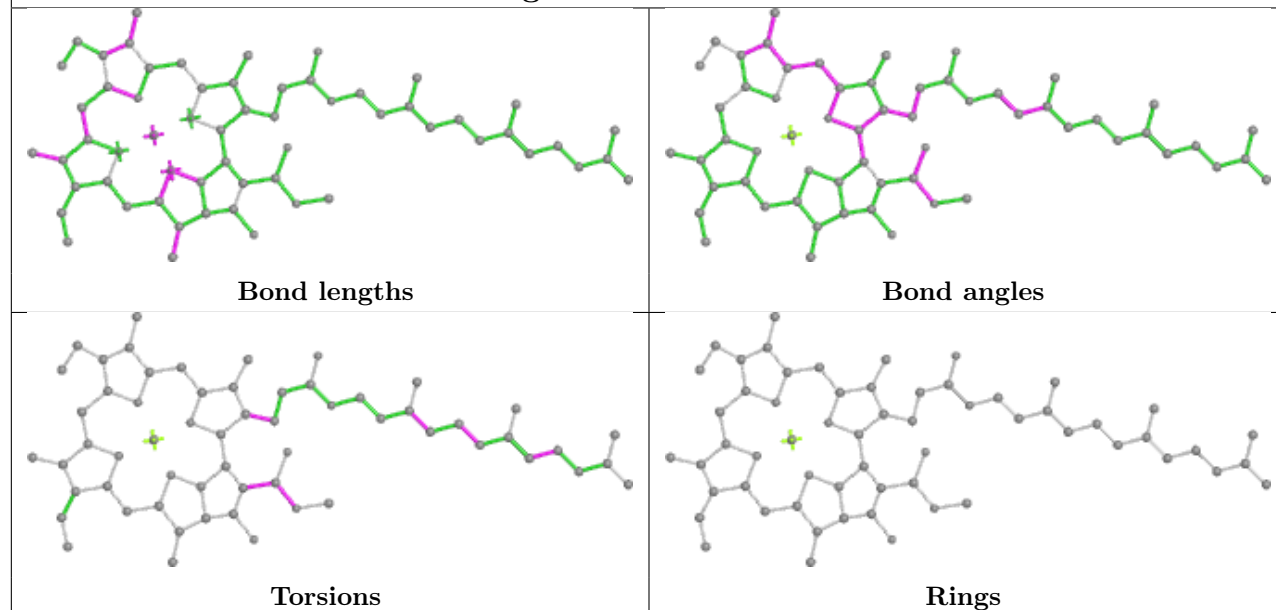
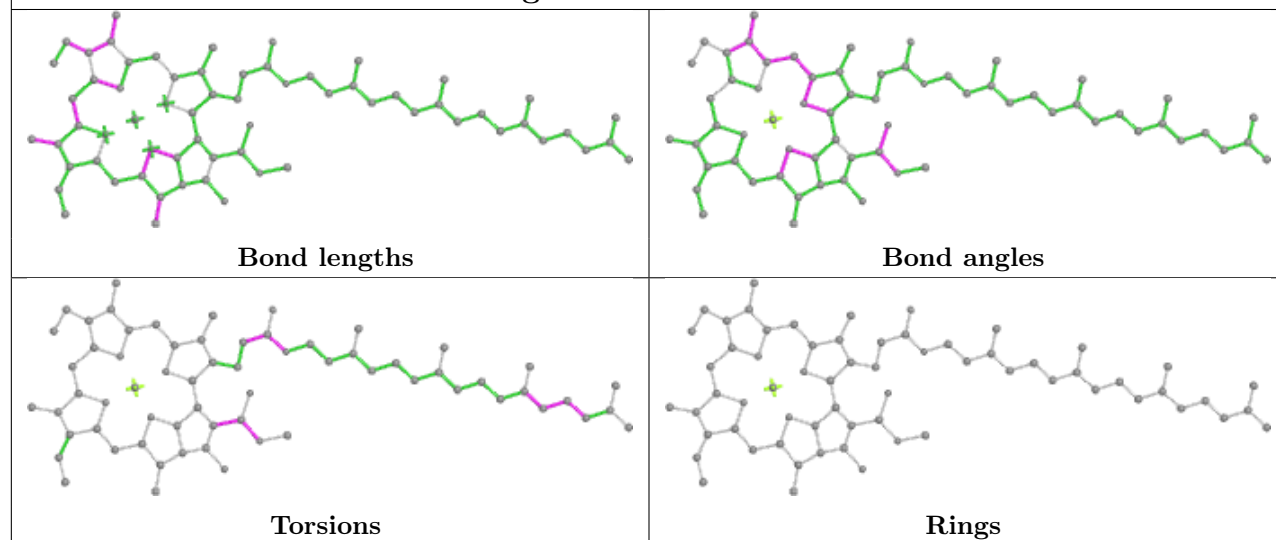


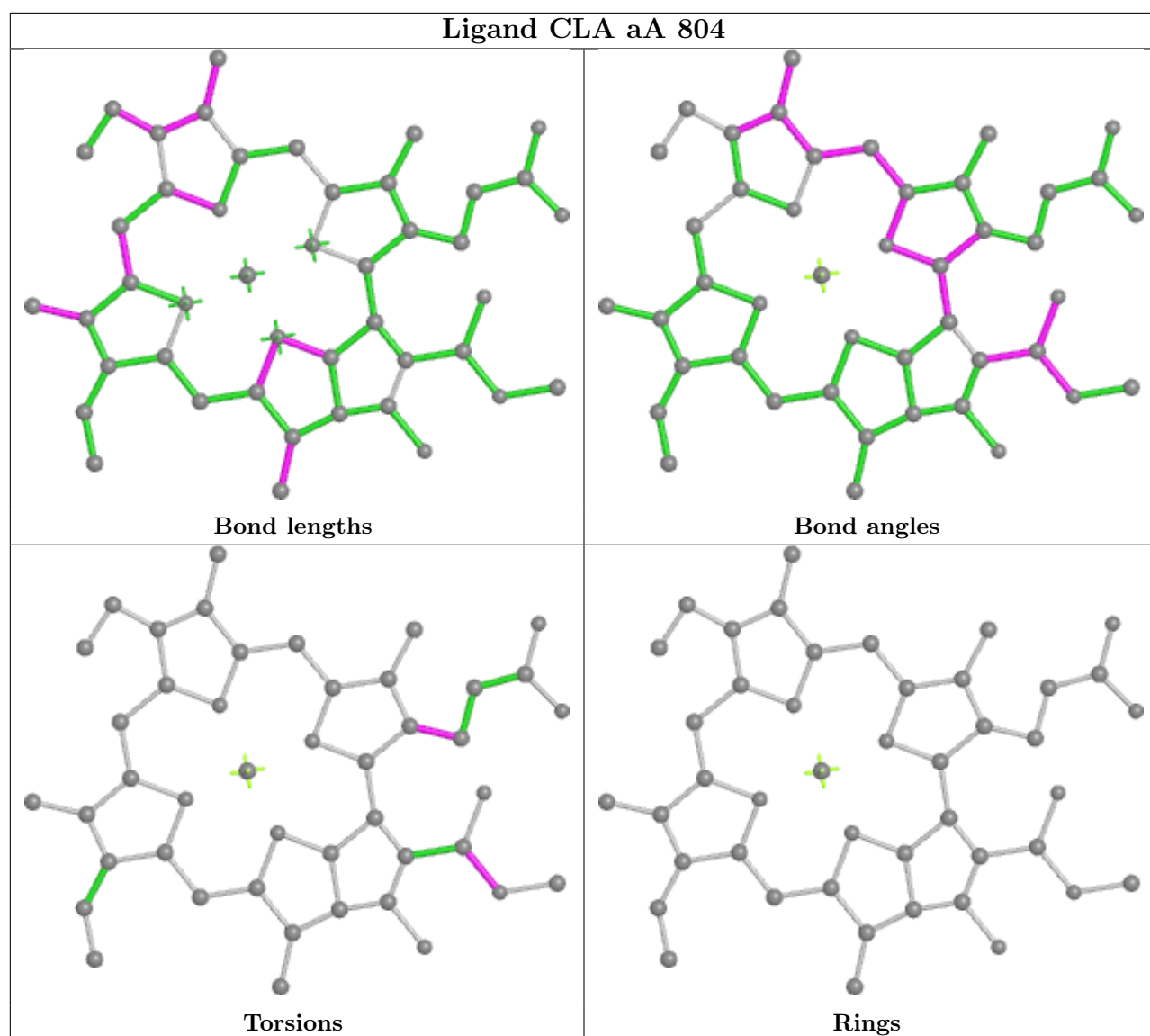
Ligand CLA aA 829



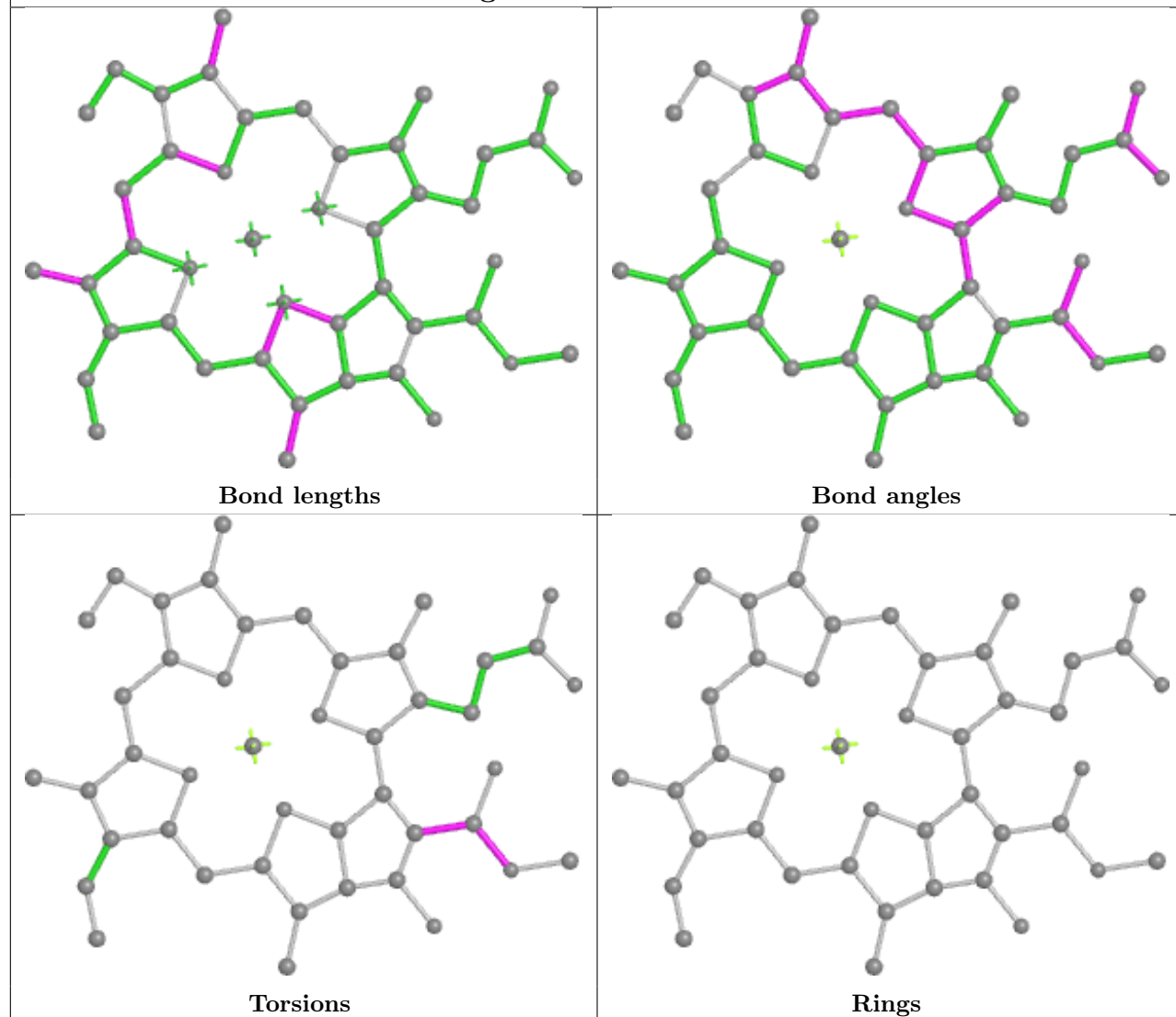
Ligand CLA dA 837



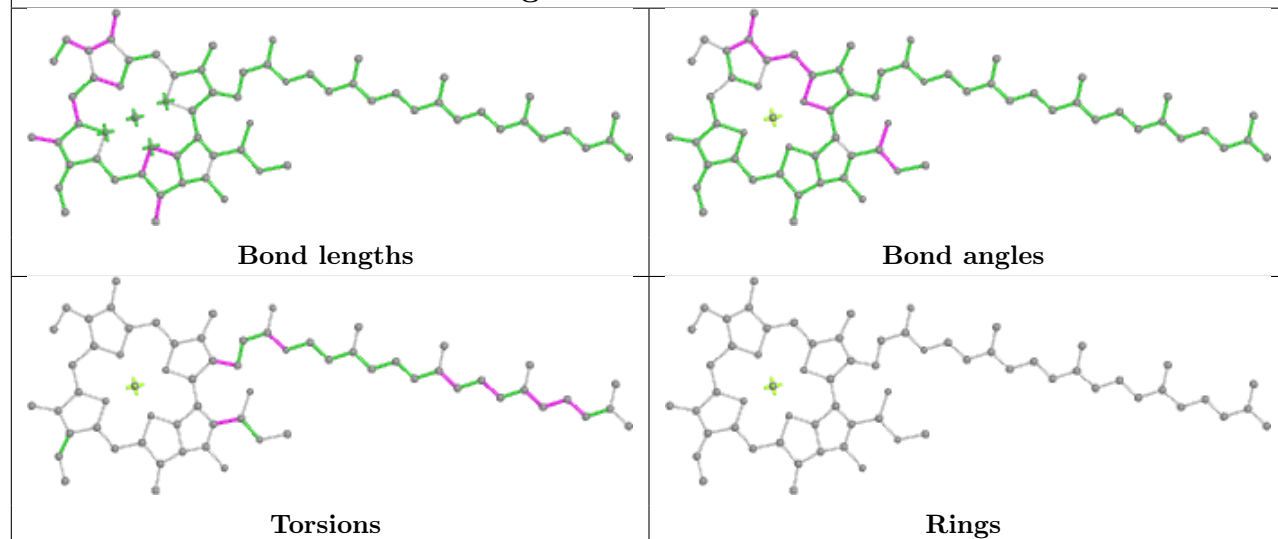
Ligand CLA dB 838**Ligand CLA bB 802**

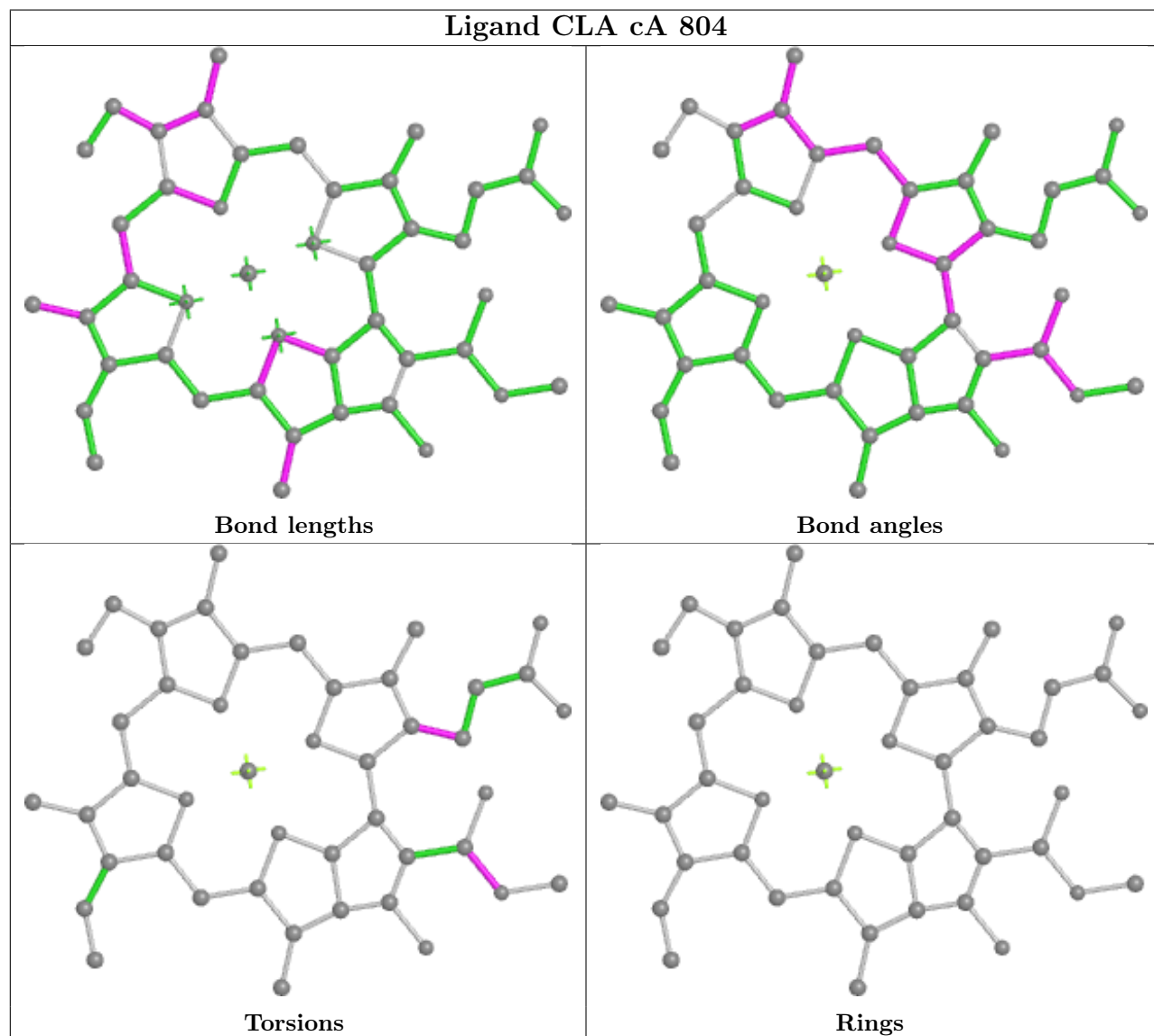
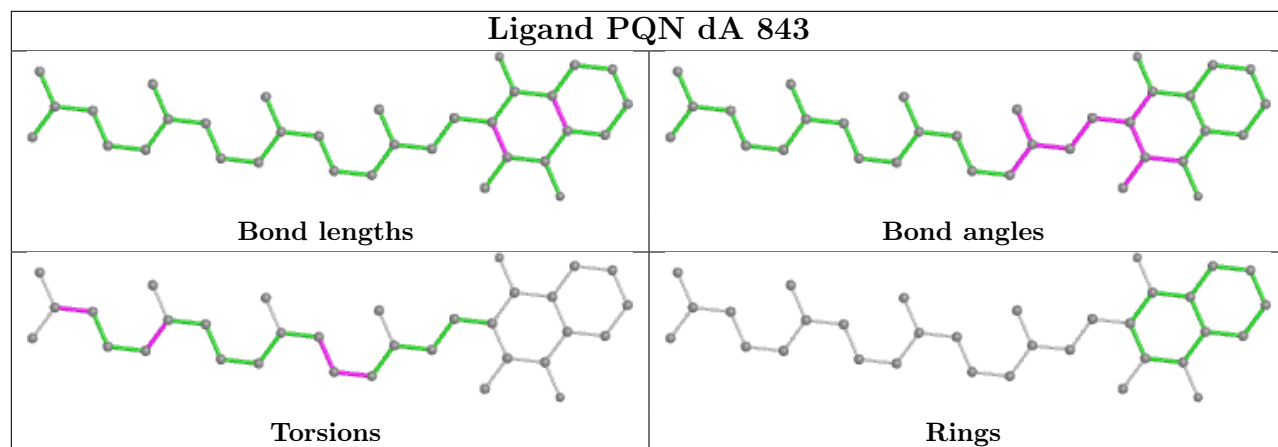


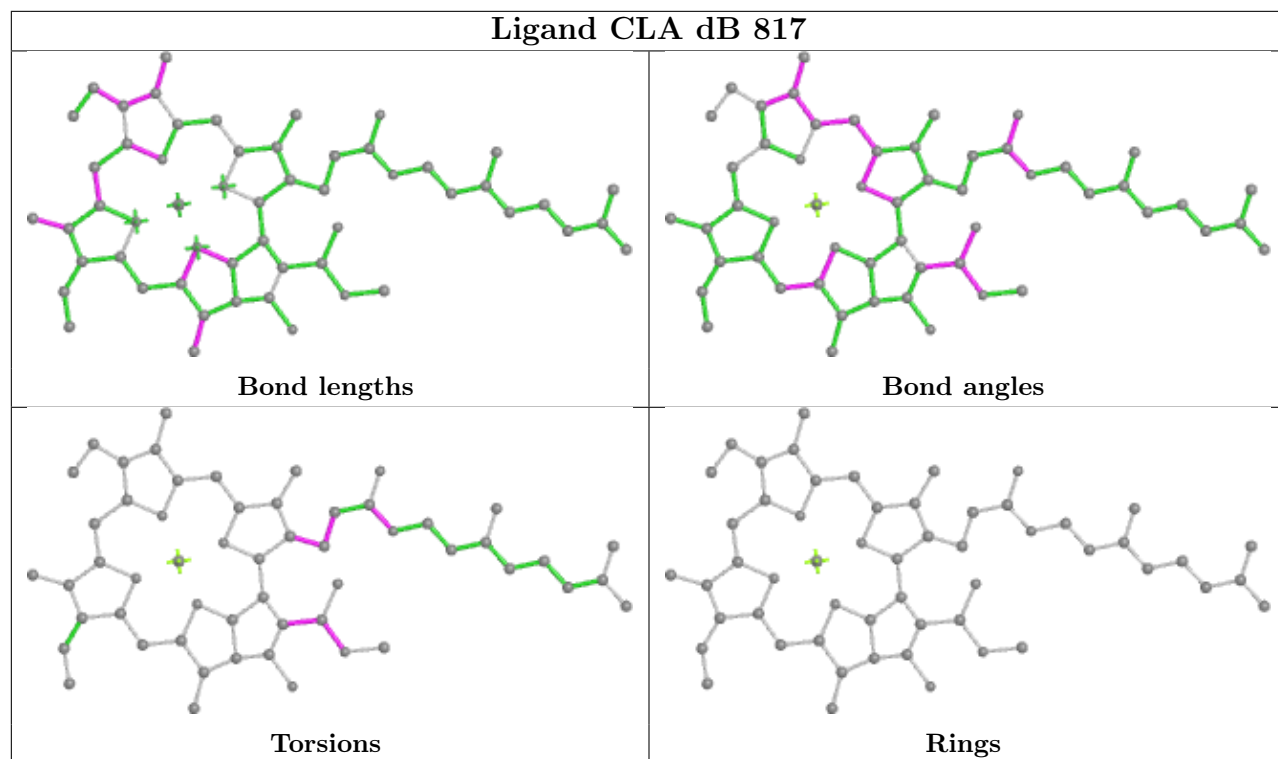
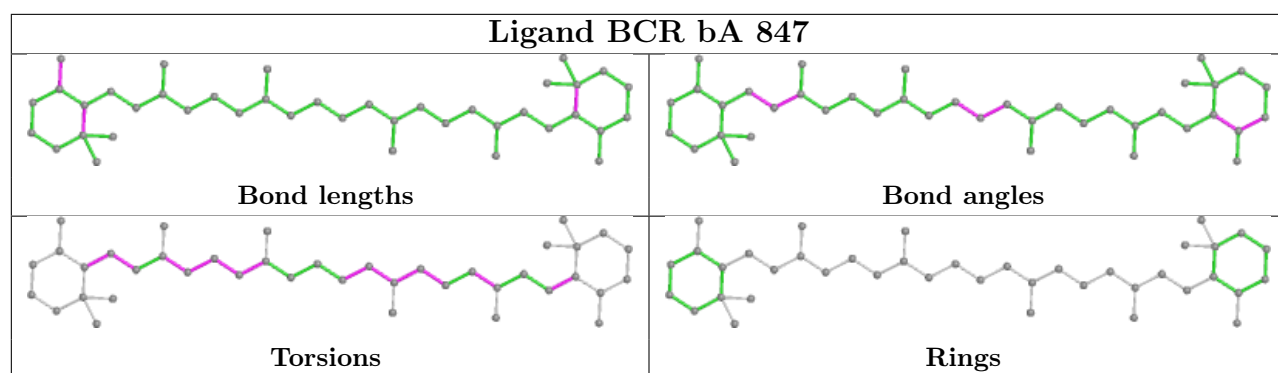
Ligand CLA bA 814



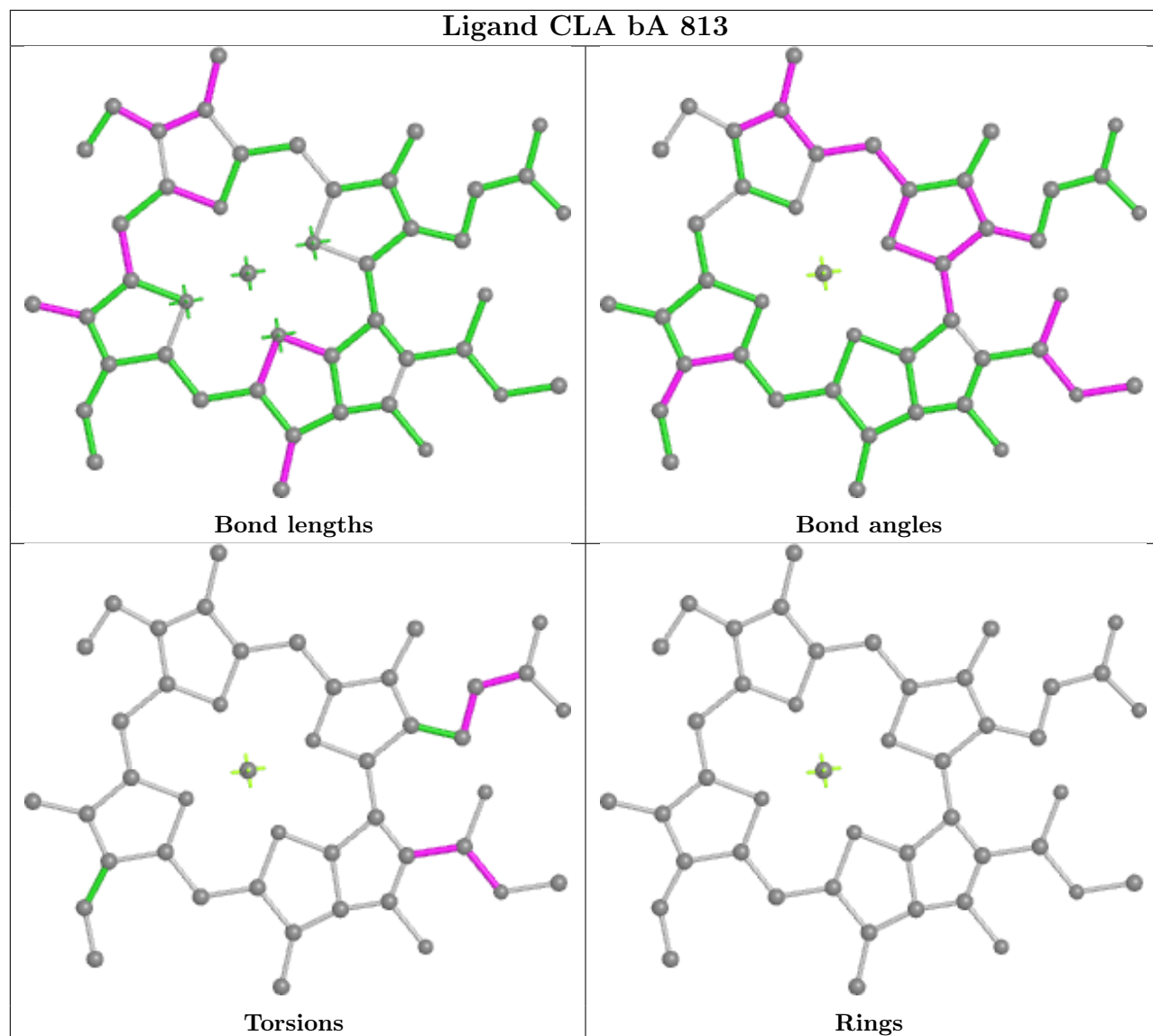
Ligand CLA dA 841

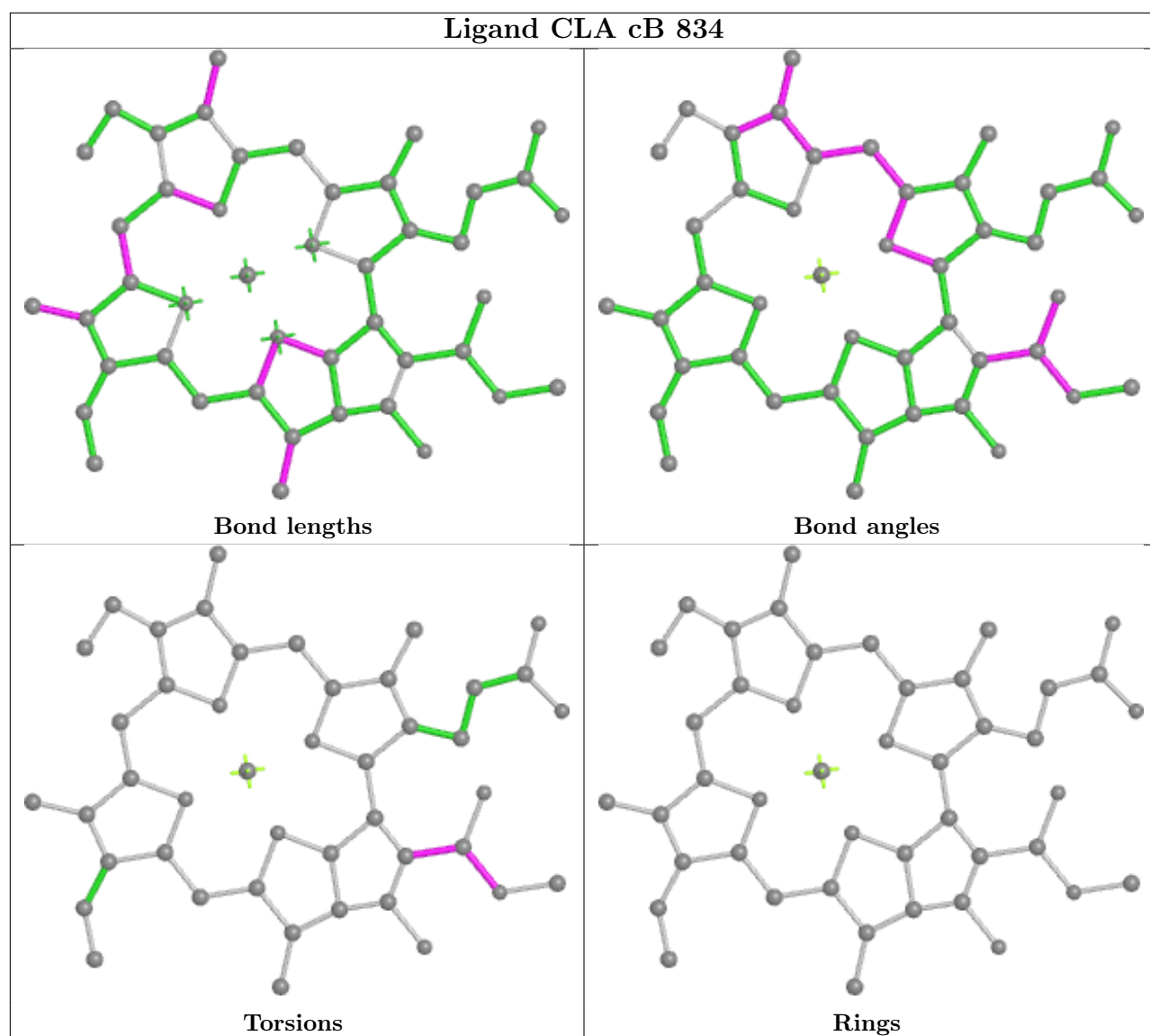




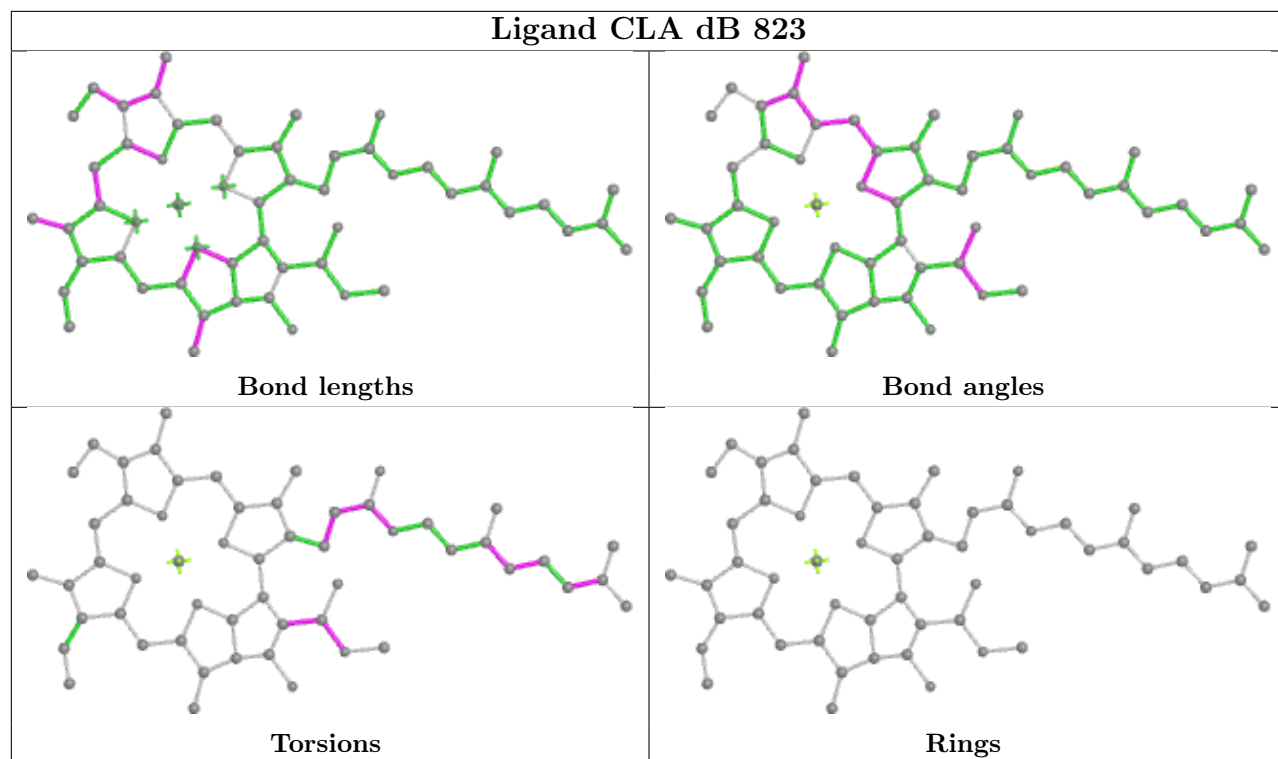


Ligand CLA bA 813

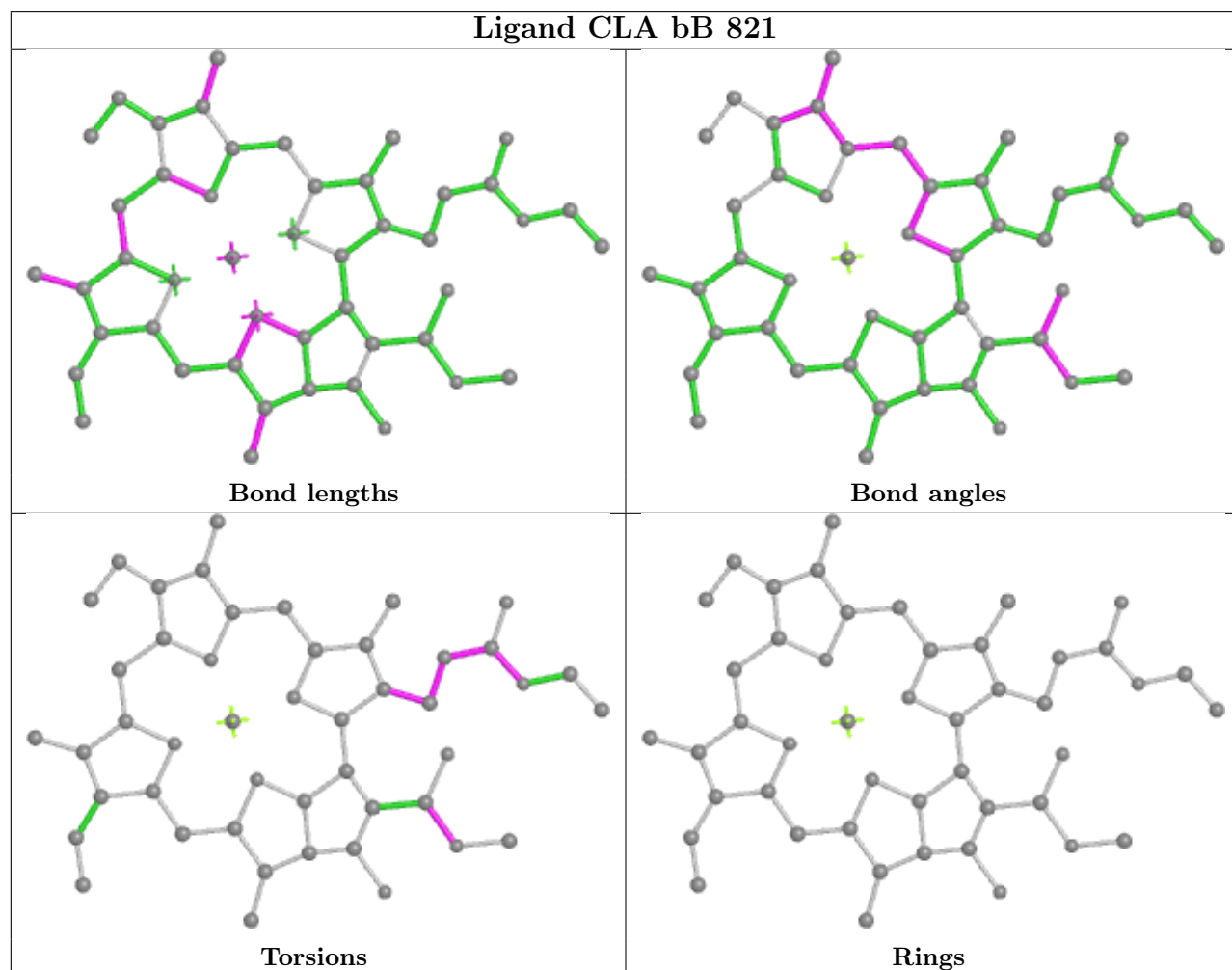


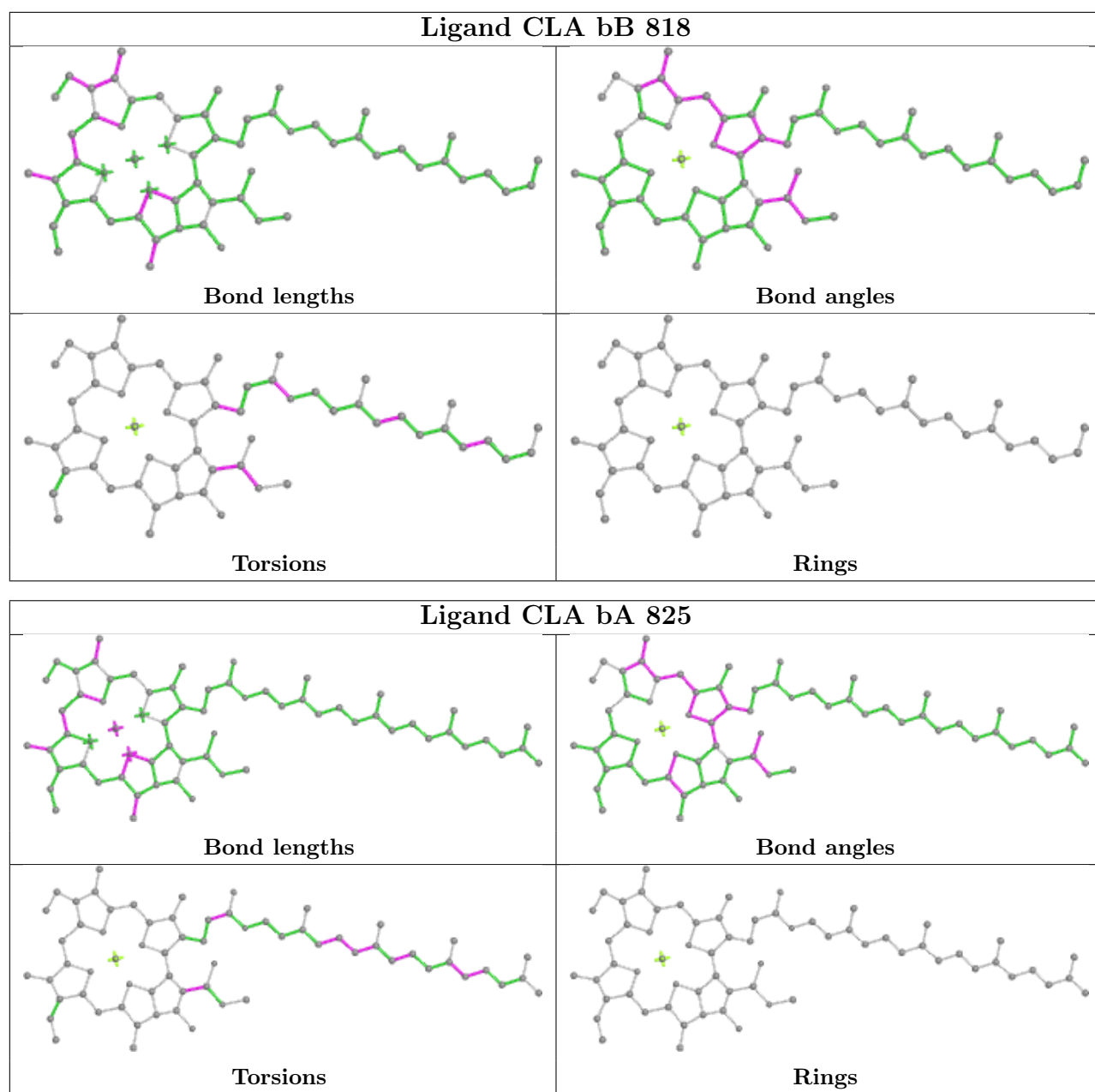


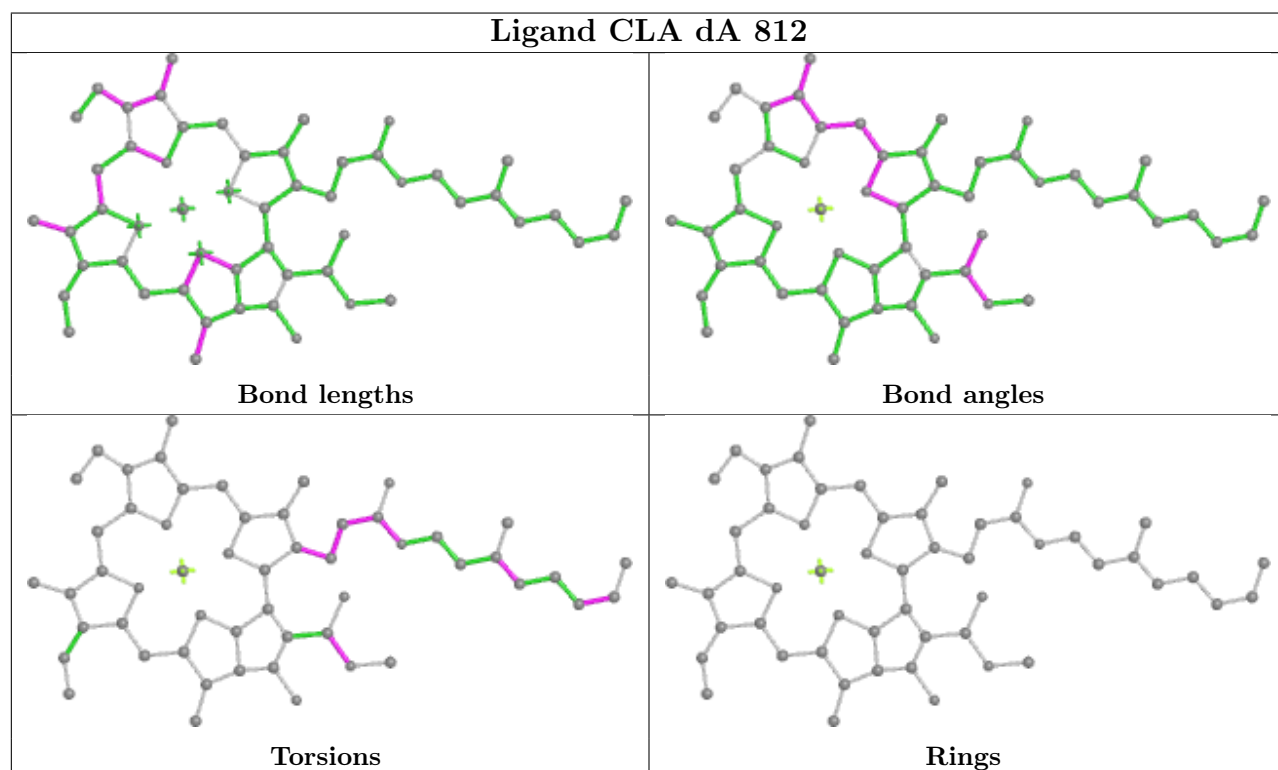
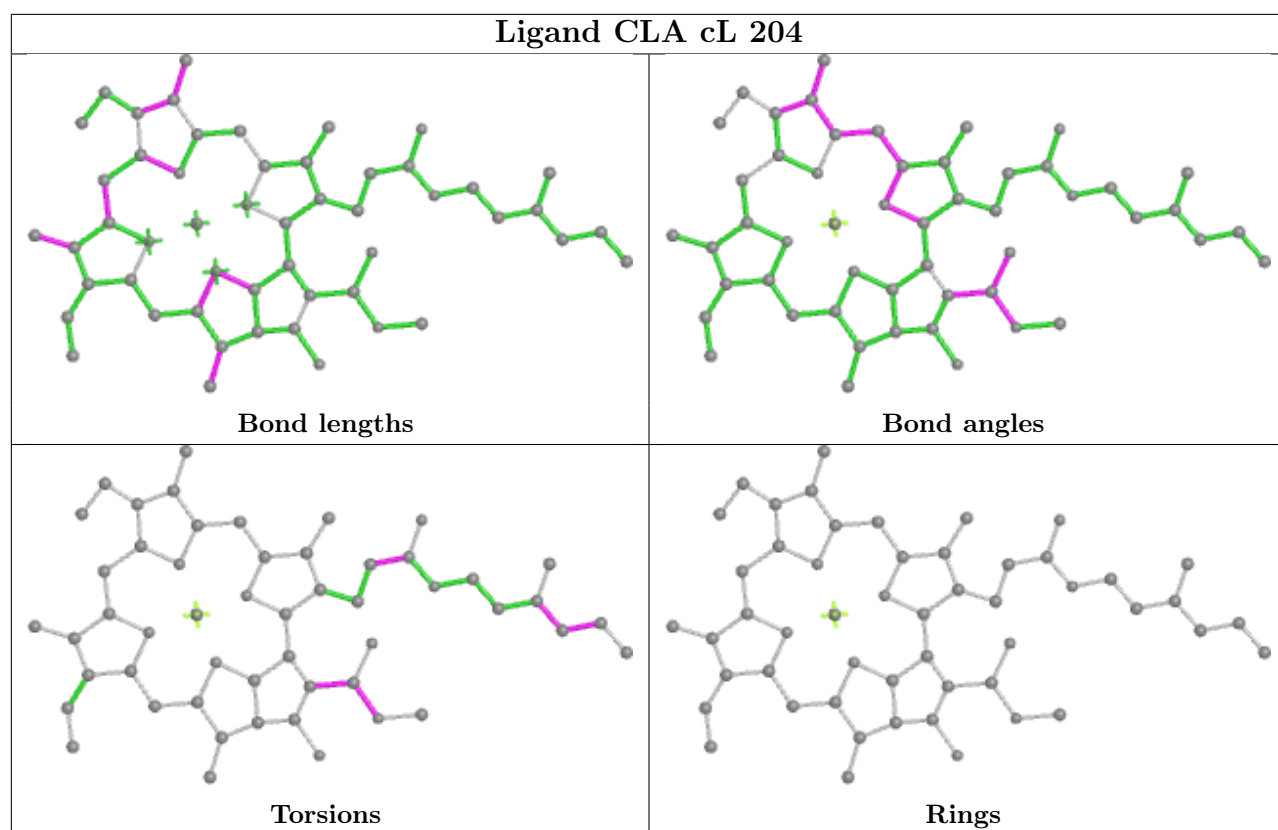
Ligand CLA dB 823

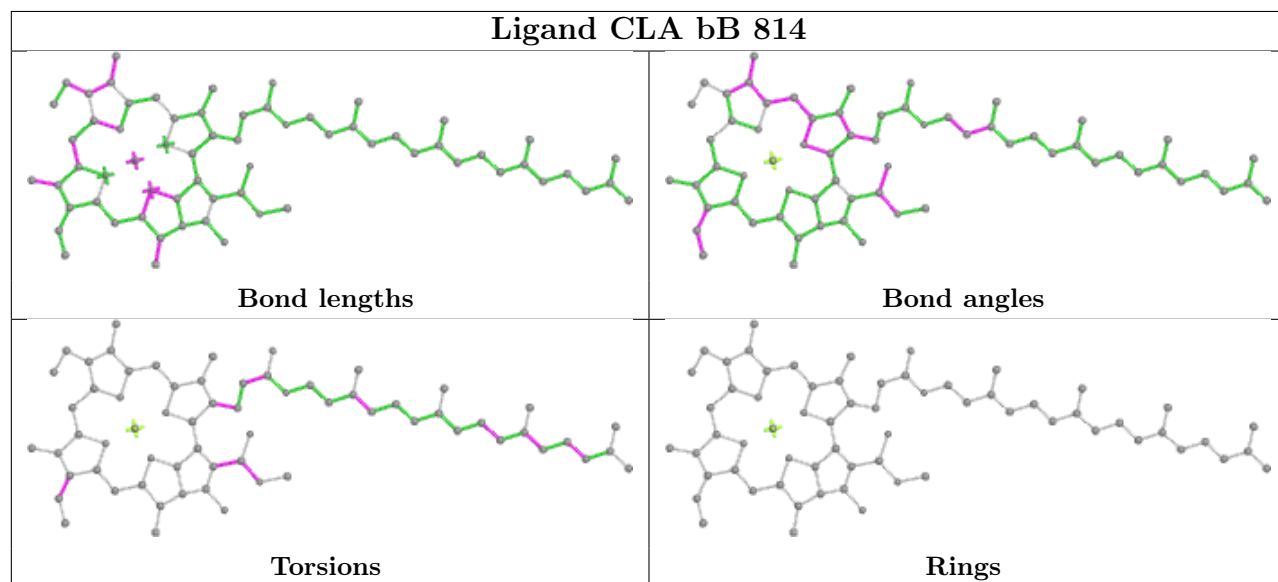
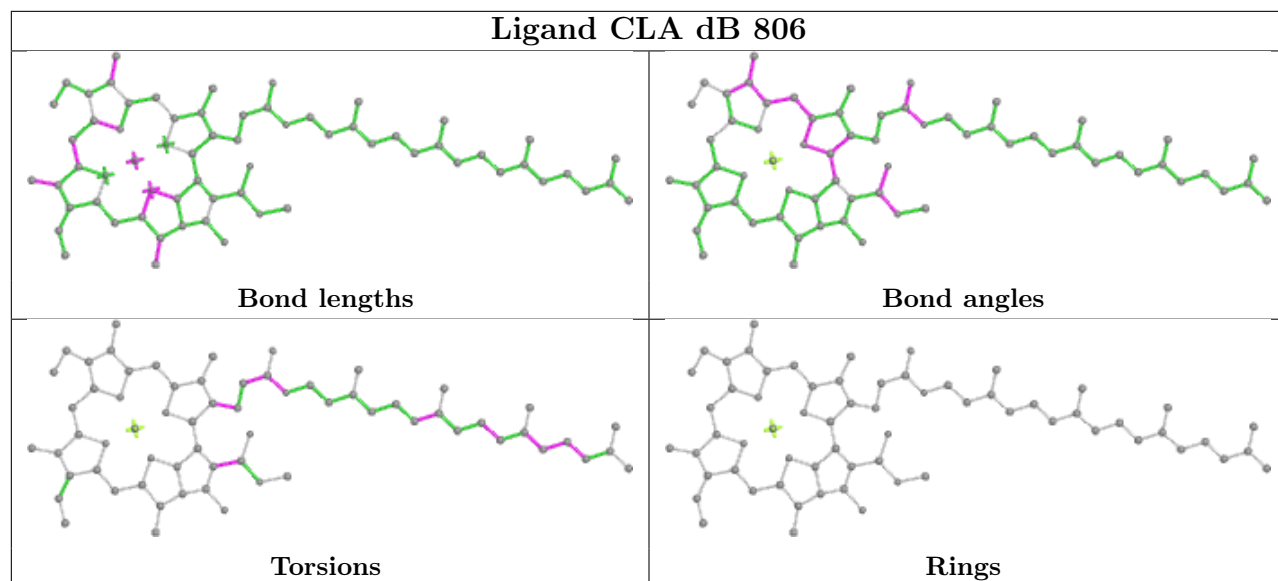
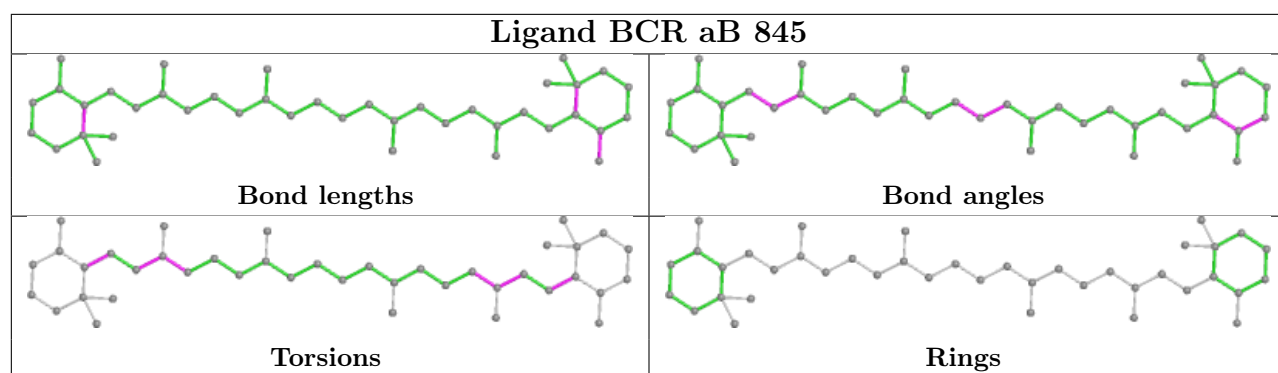


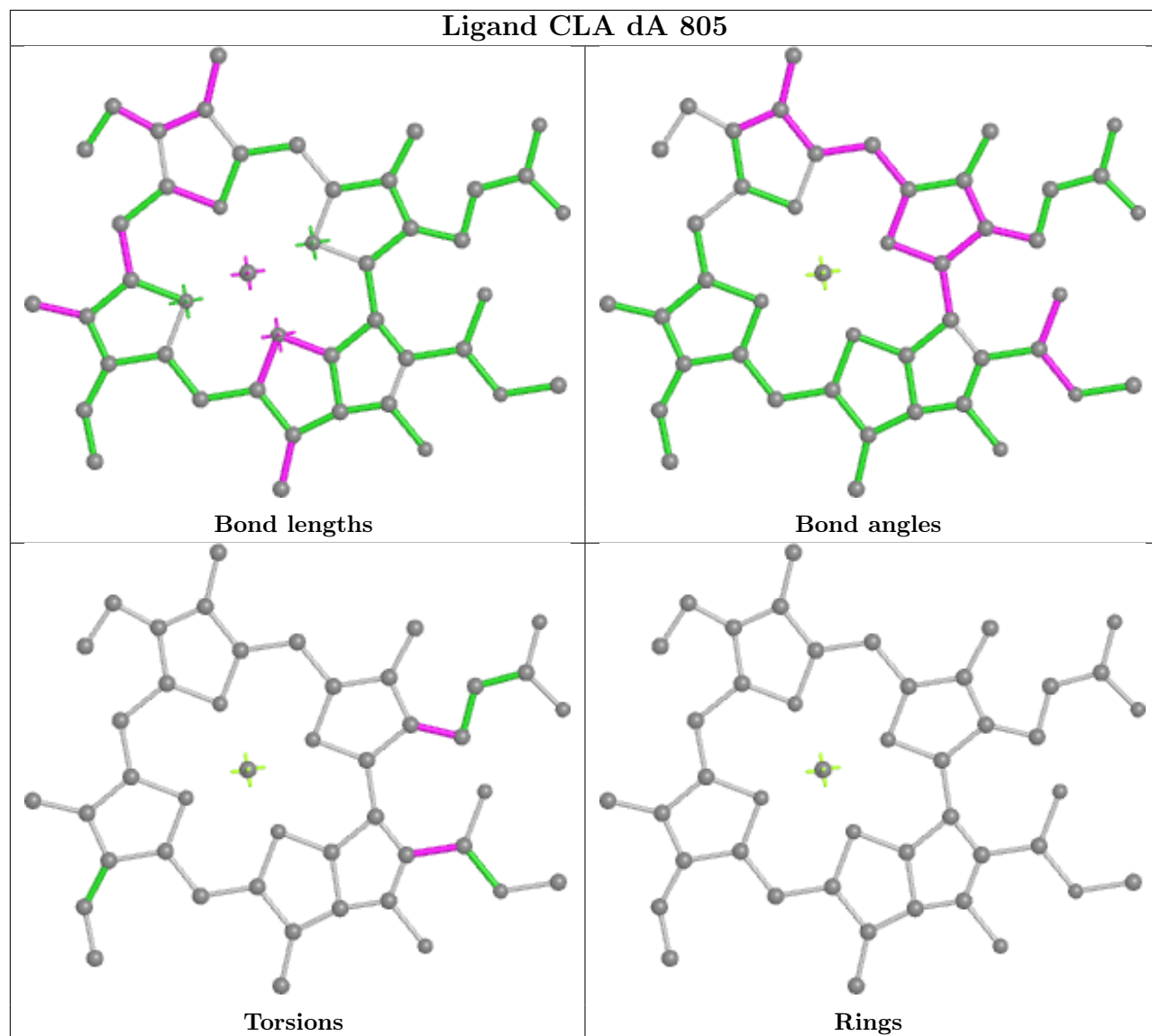
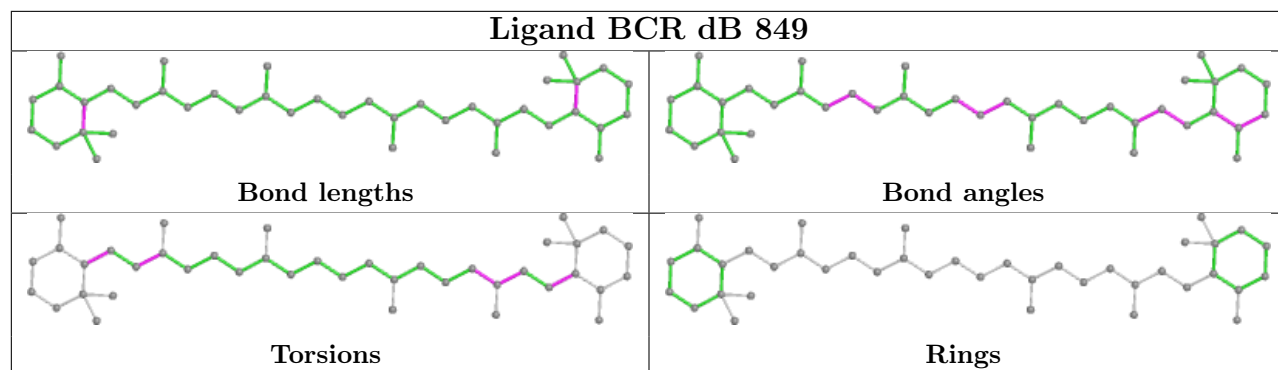
Ligand CLA bB 821

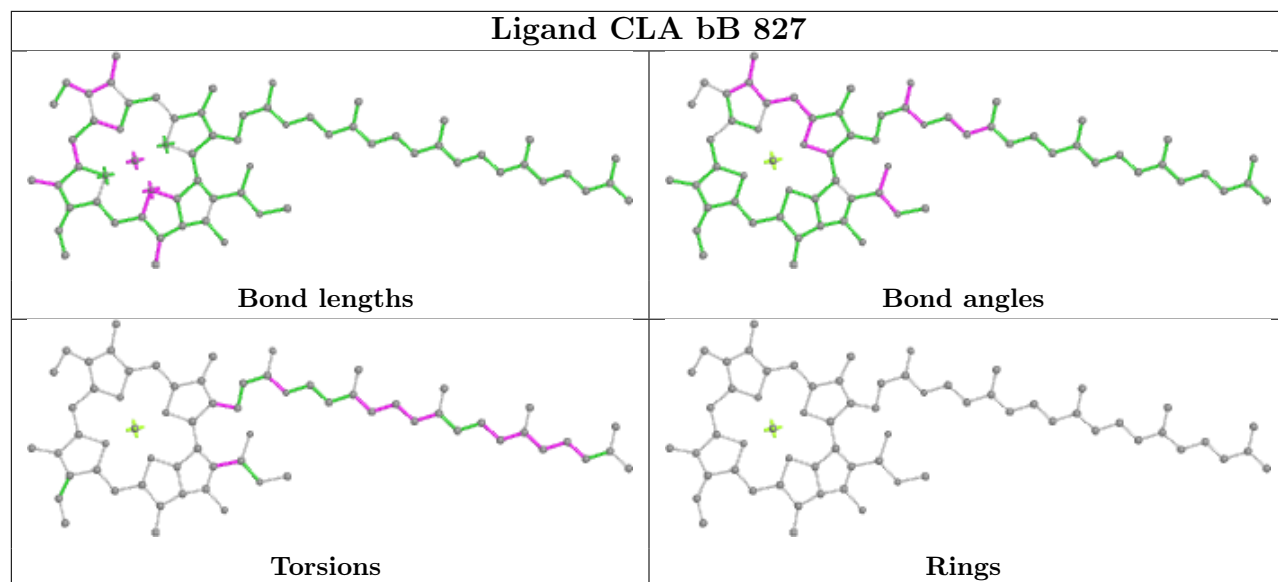


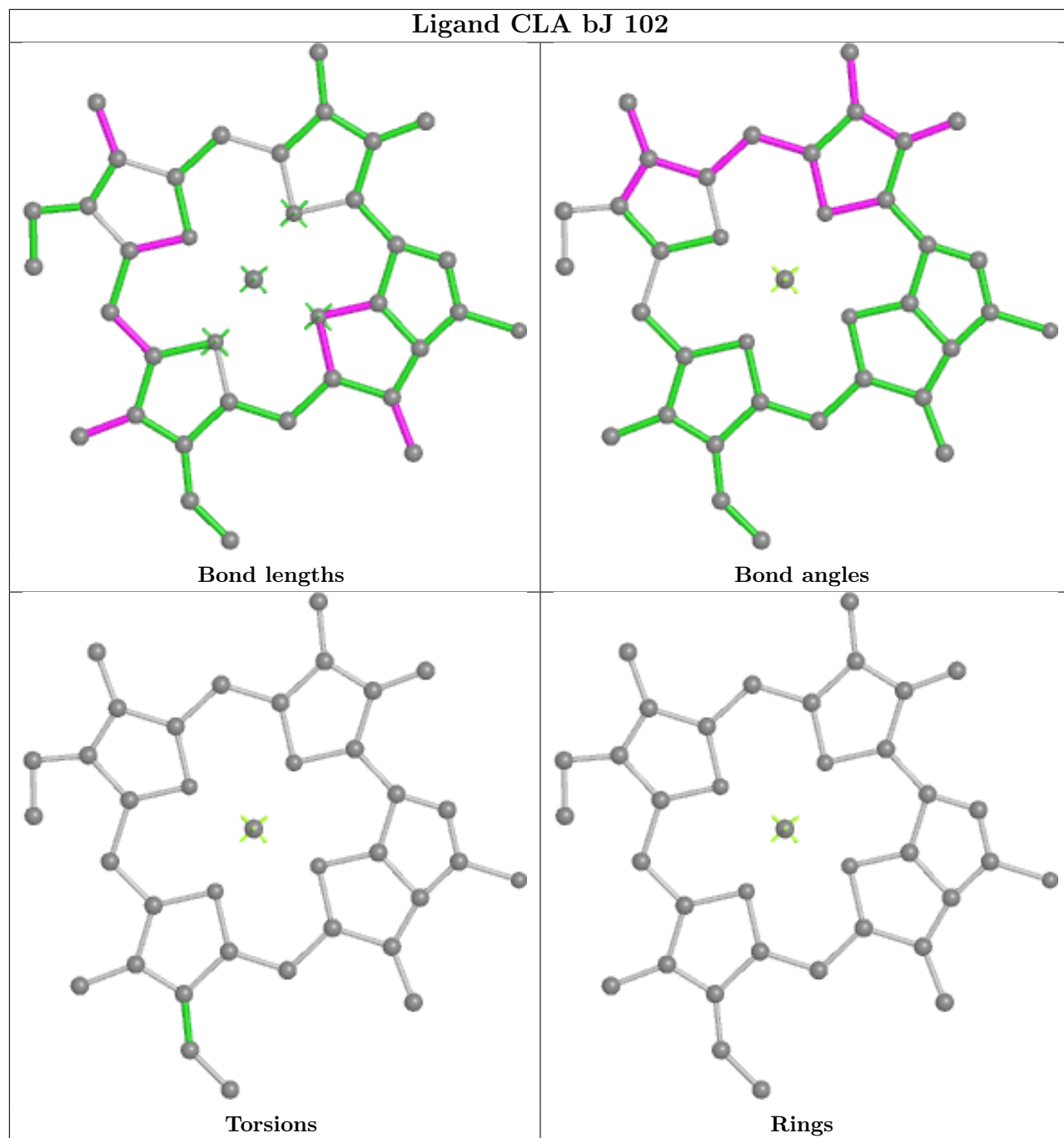


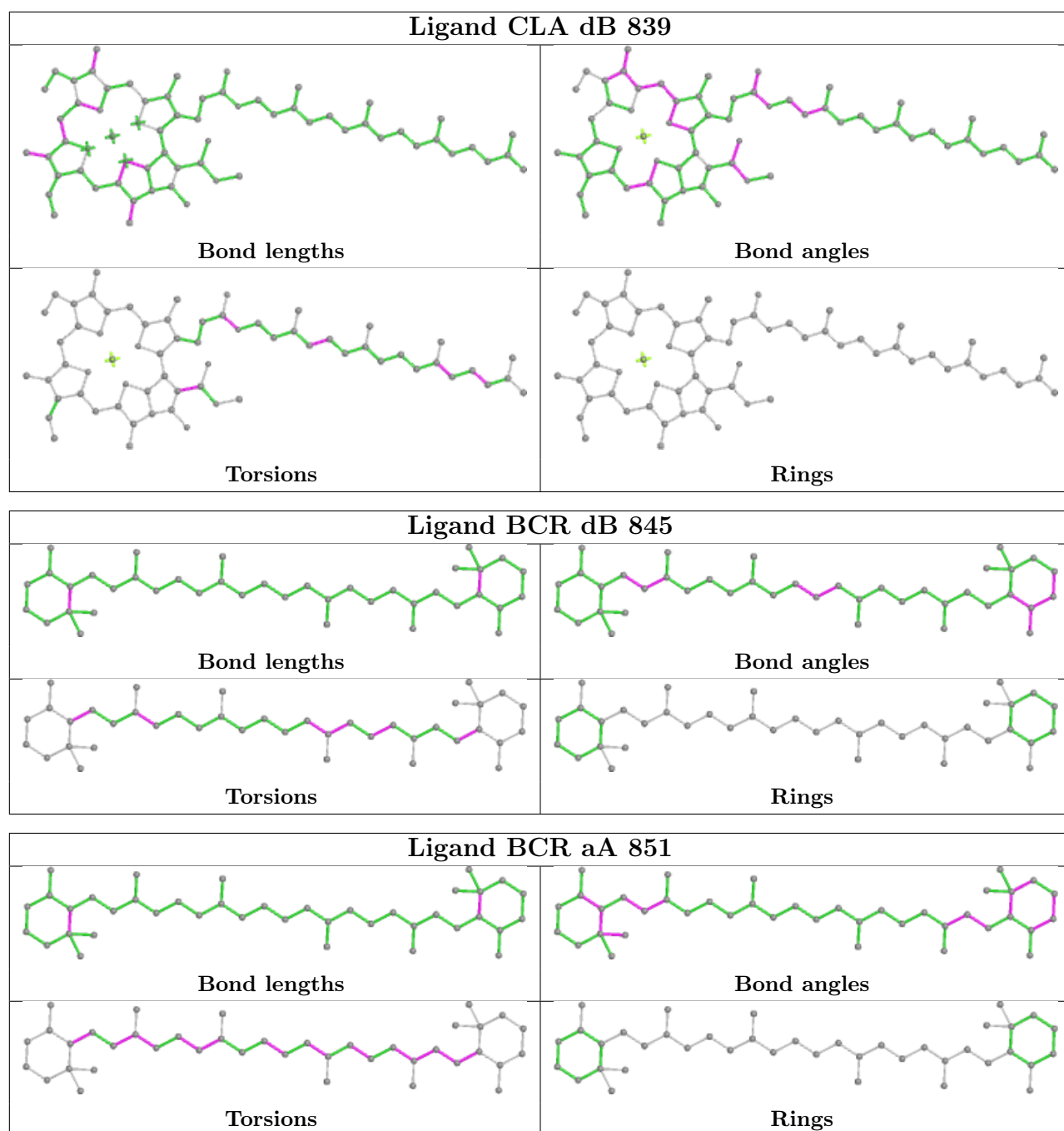




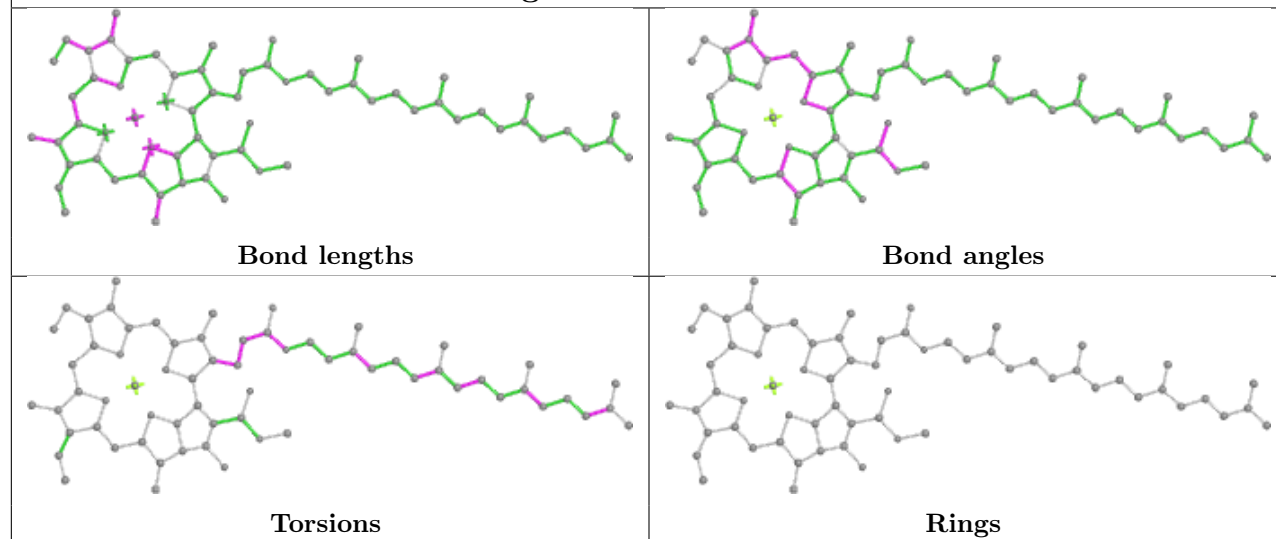




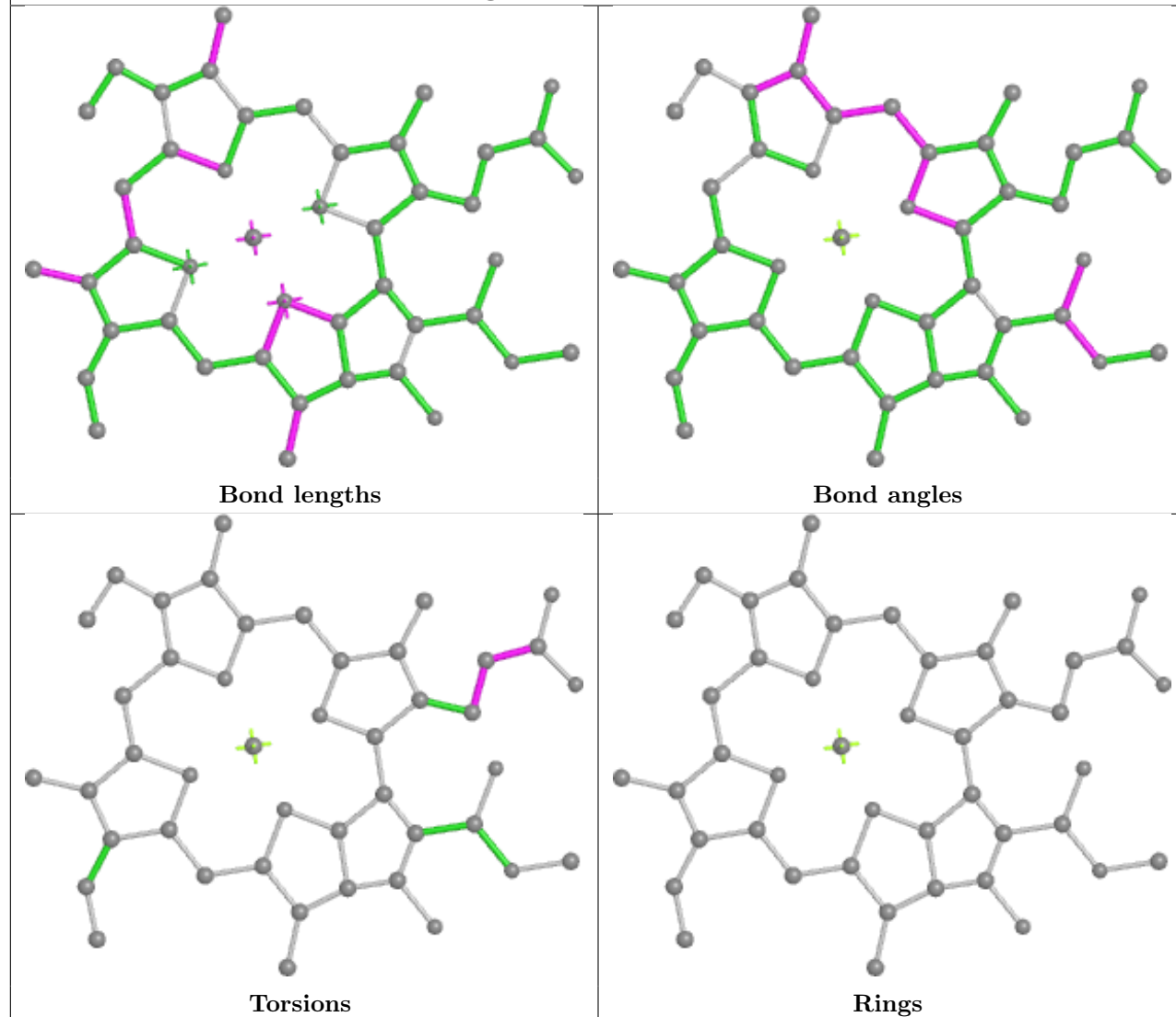


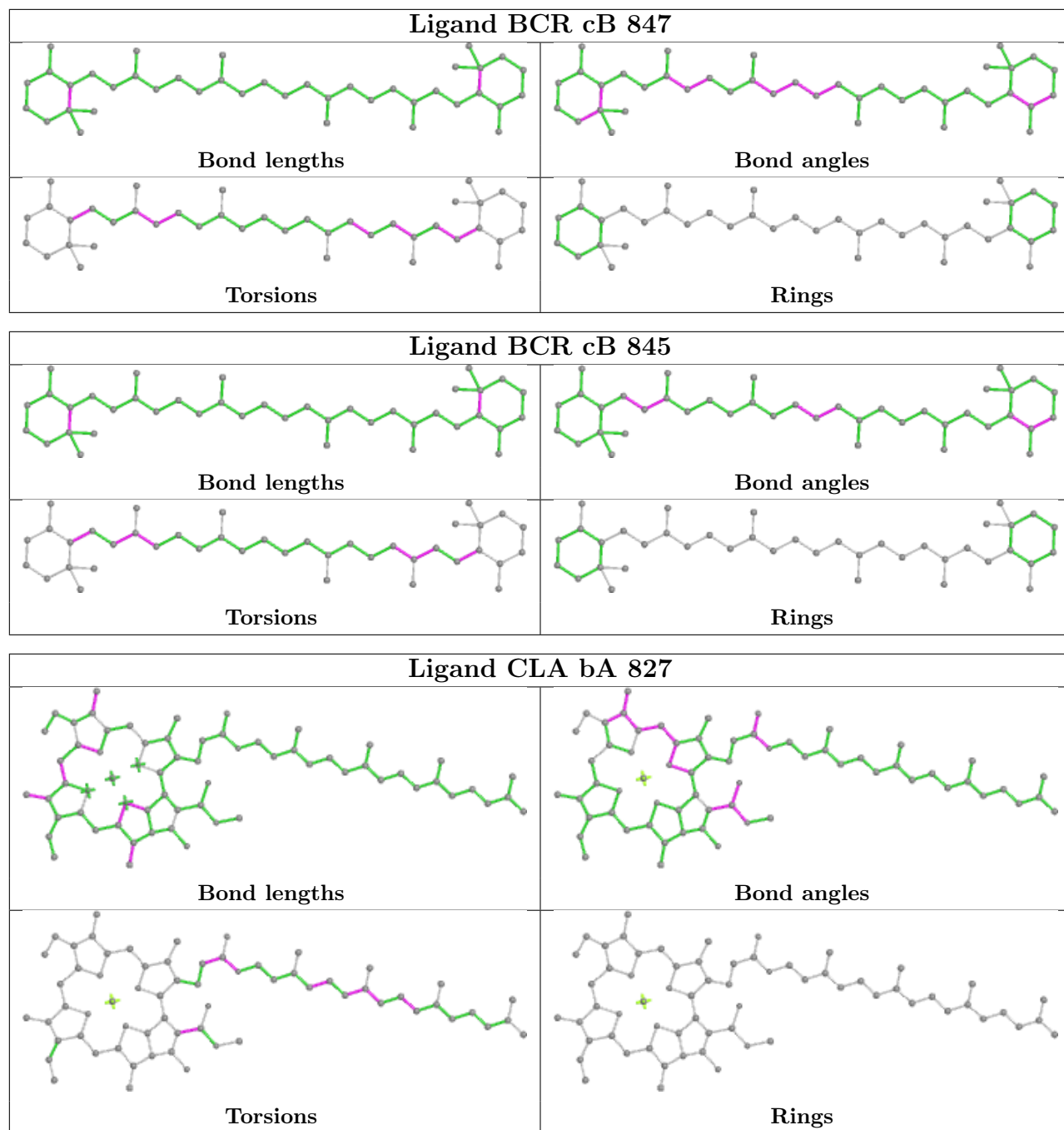


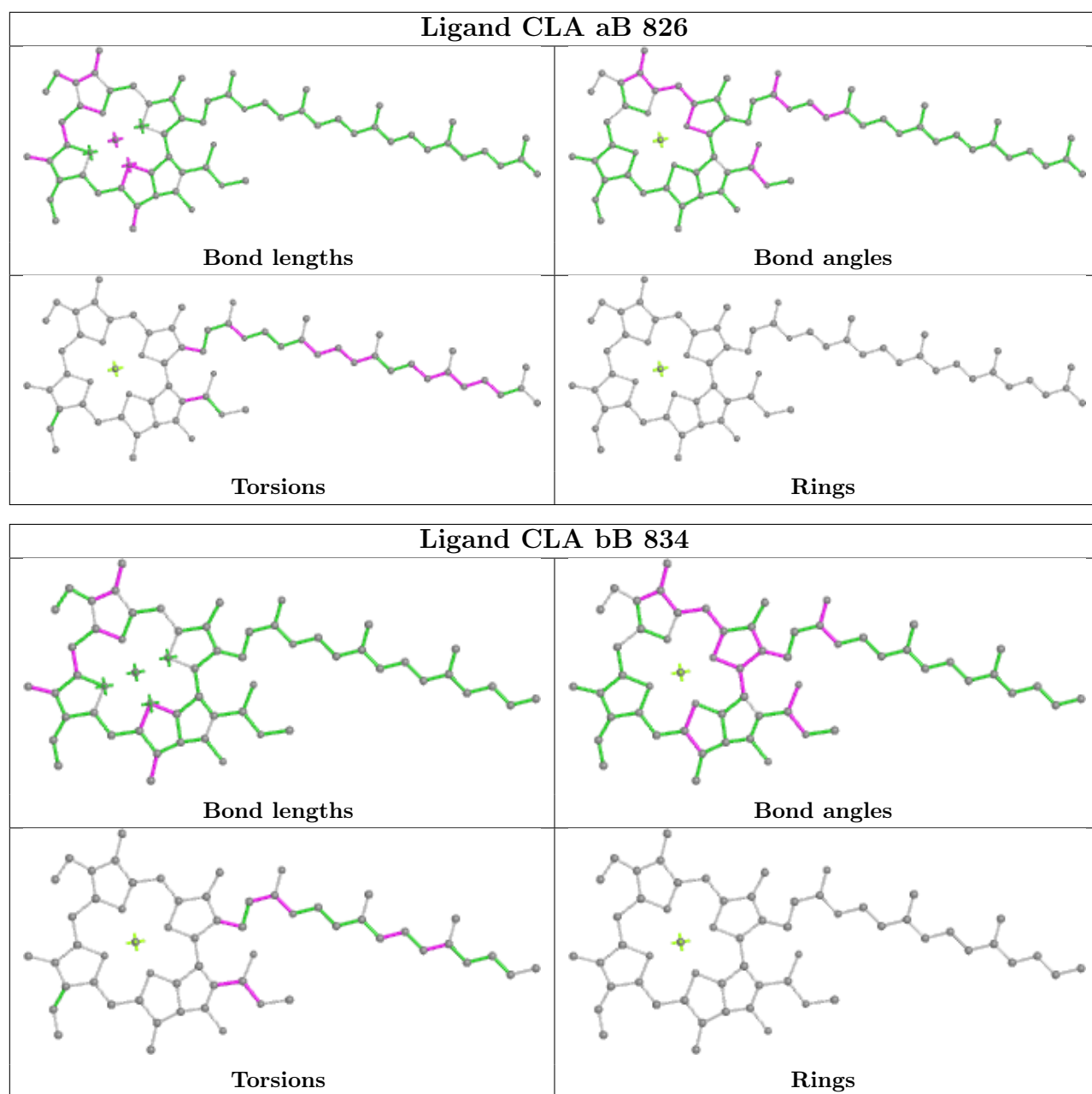
Ligand CLA dA 829

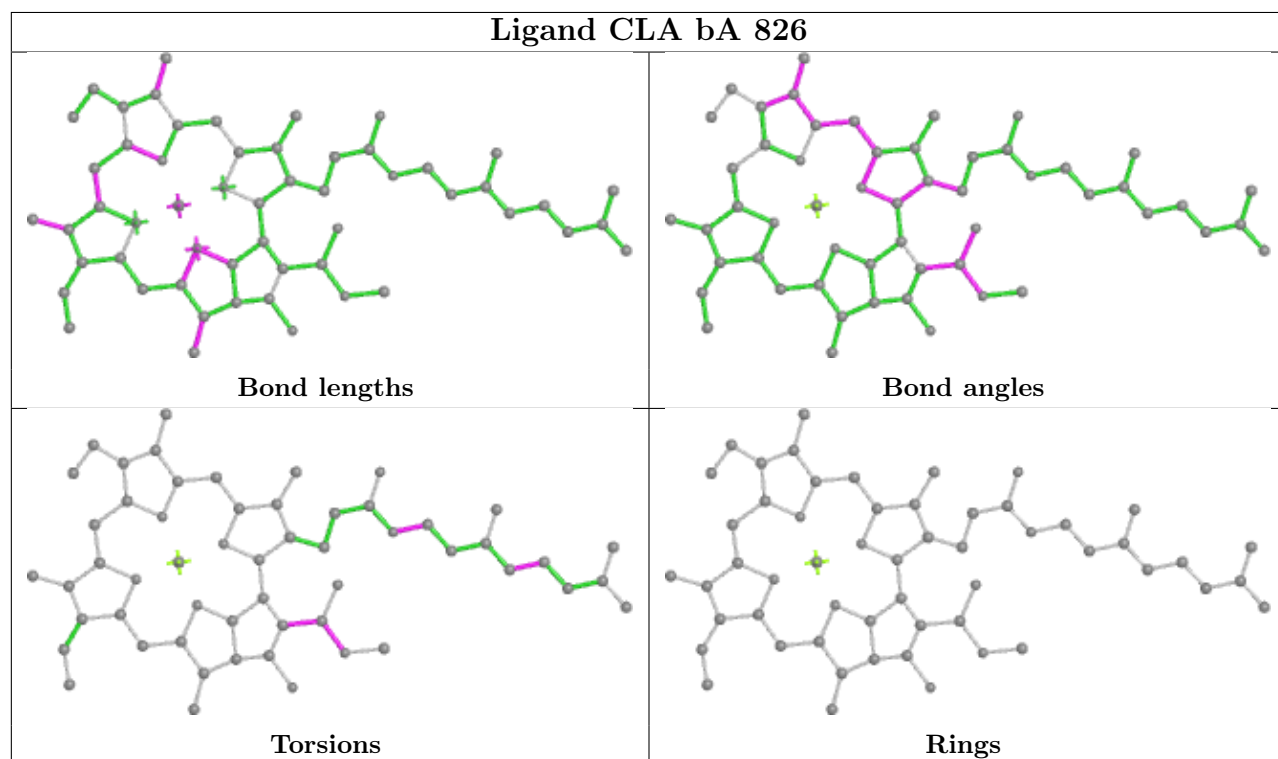
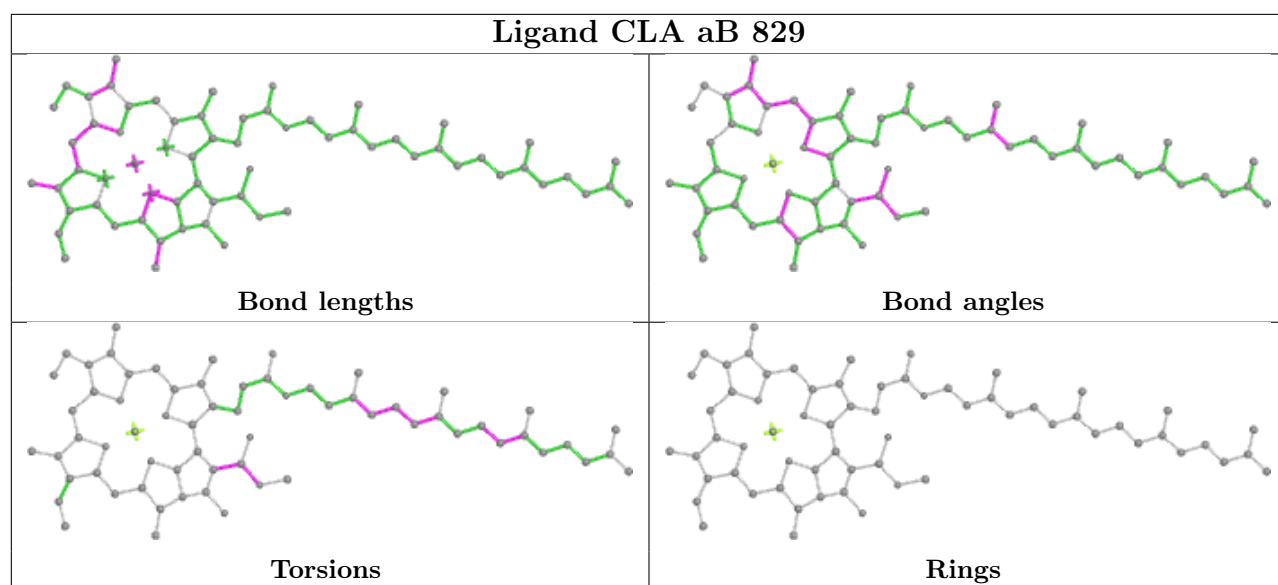


Ligand CLA cA 802

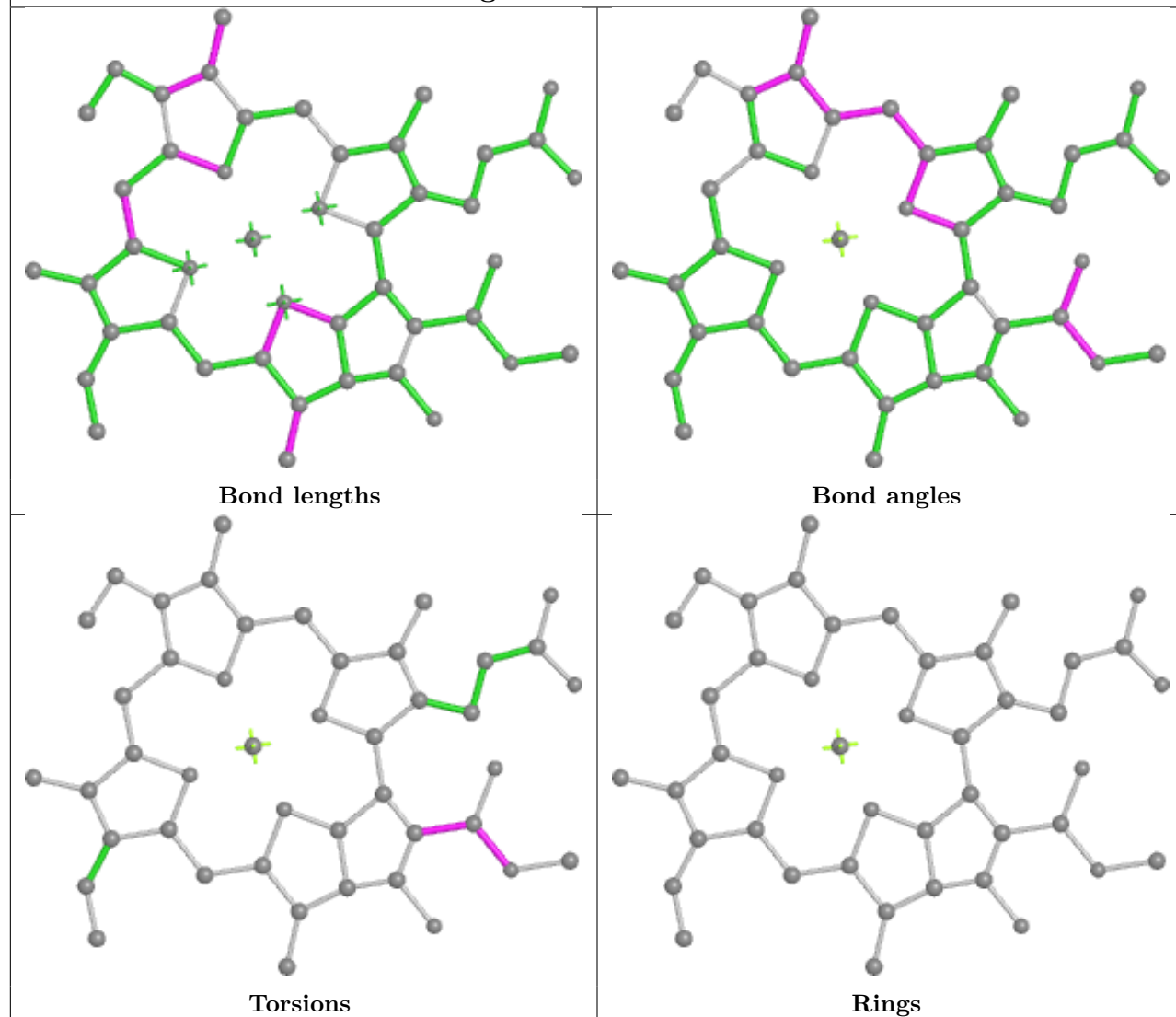




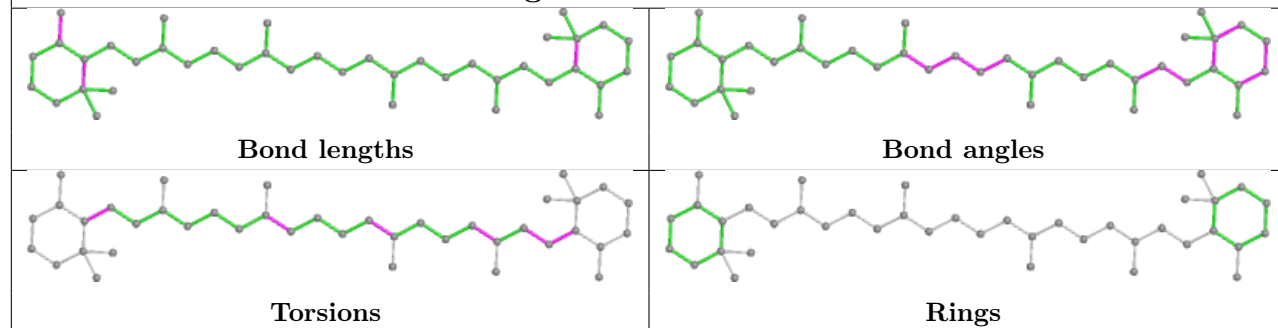




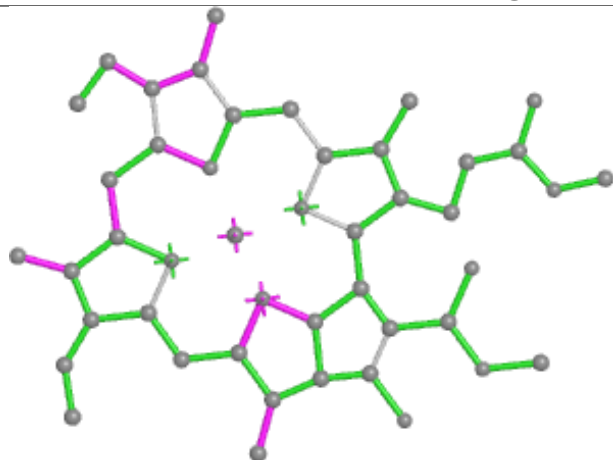
Ligand CLA dA 815



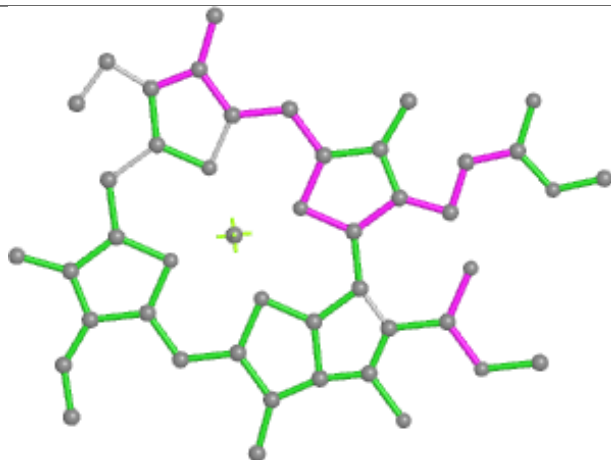
Ligand BCR bJ 104



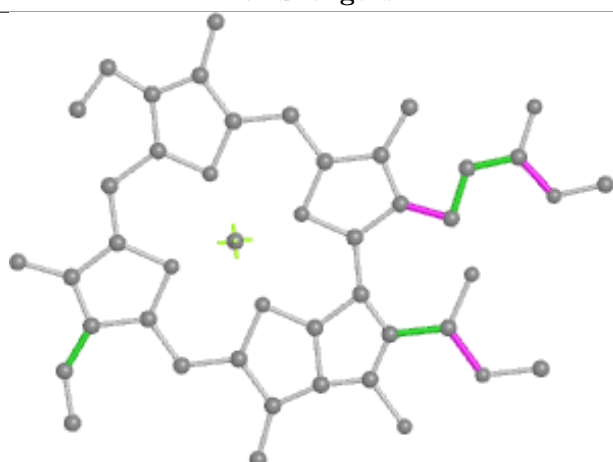
Ligand CLA aB 825



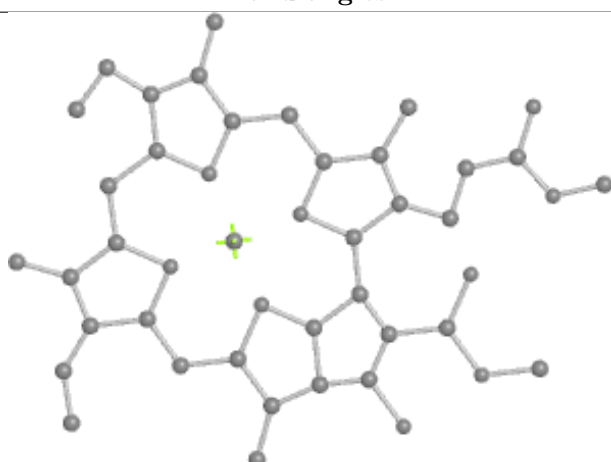
Bond lengths



Bond angles

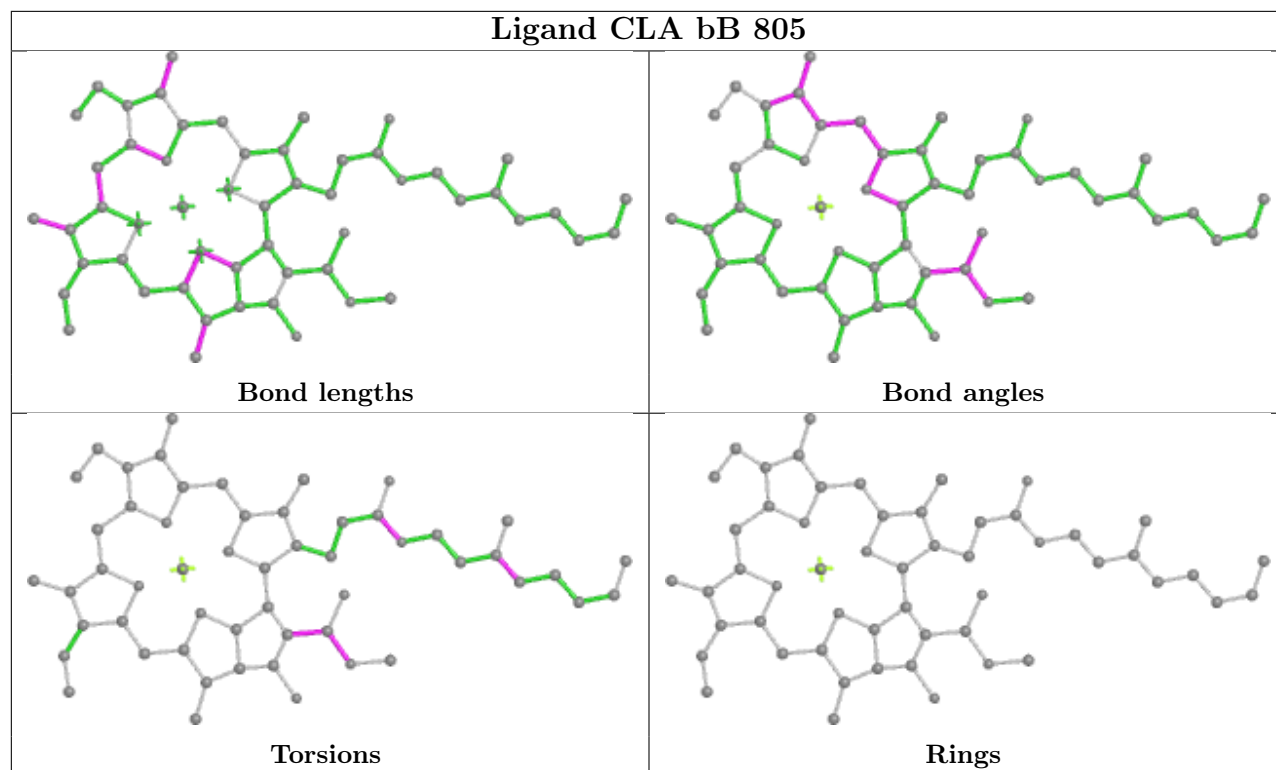


Torsions

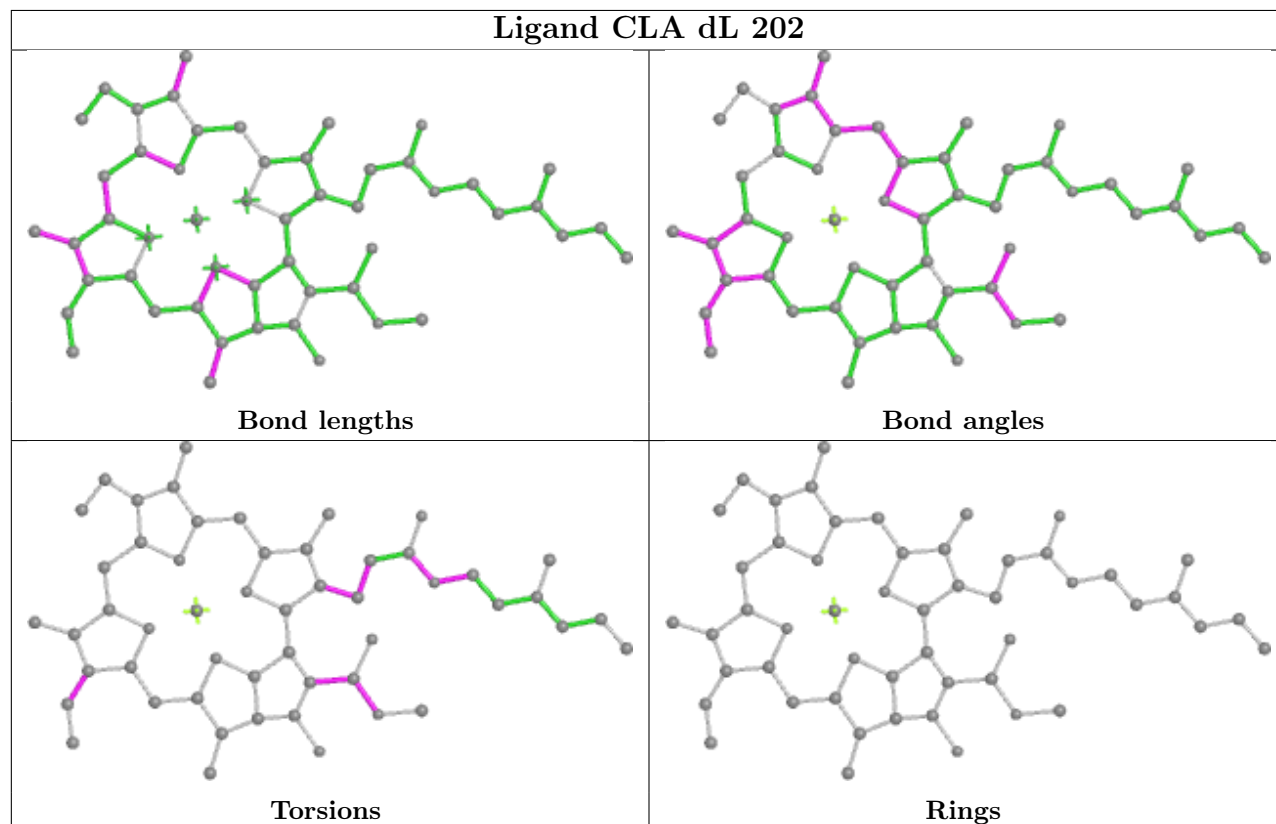


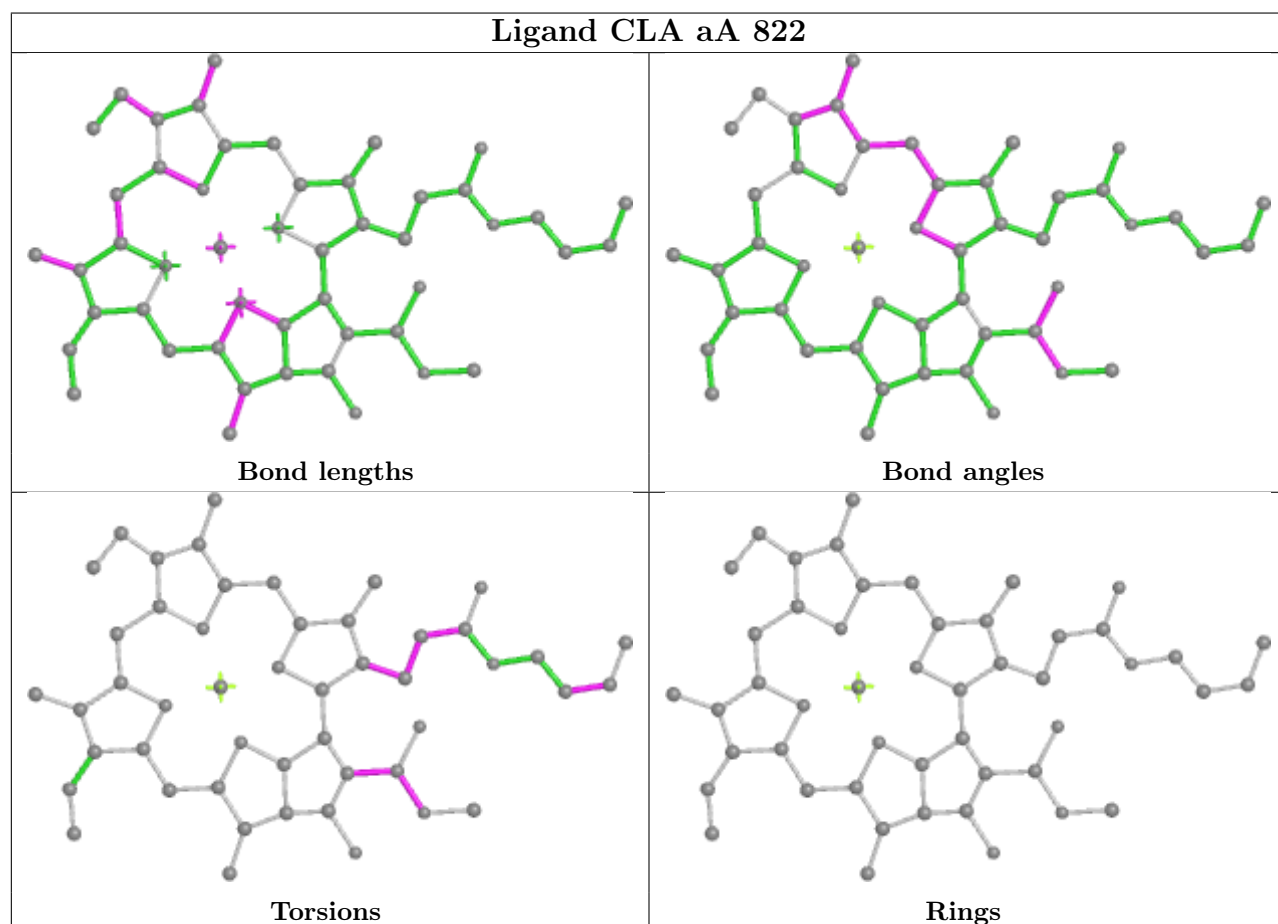
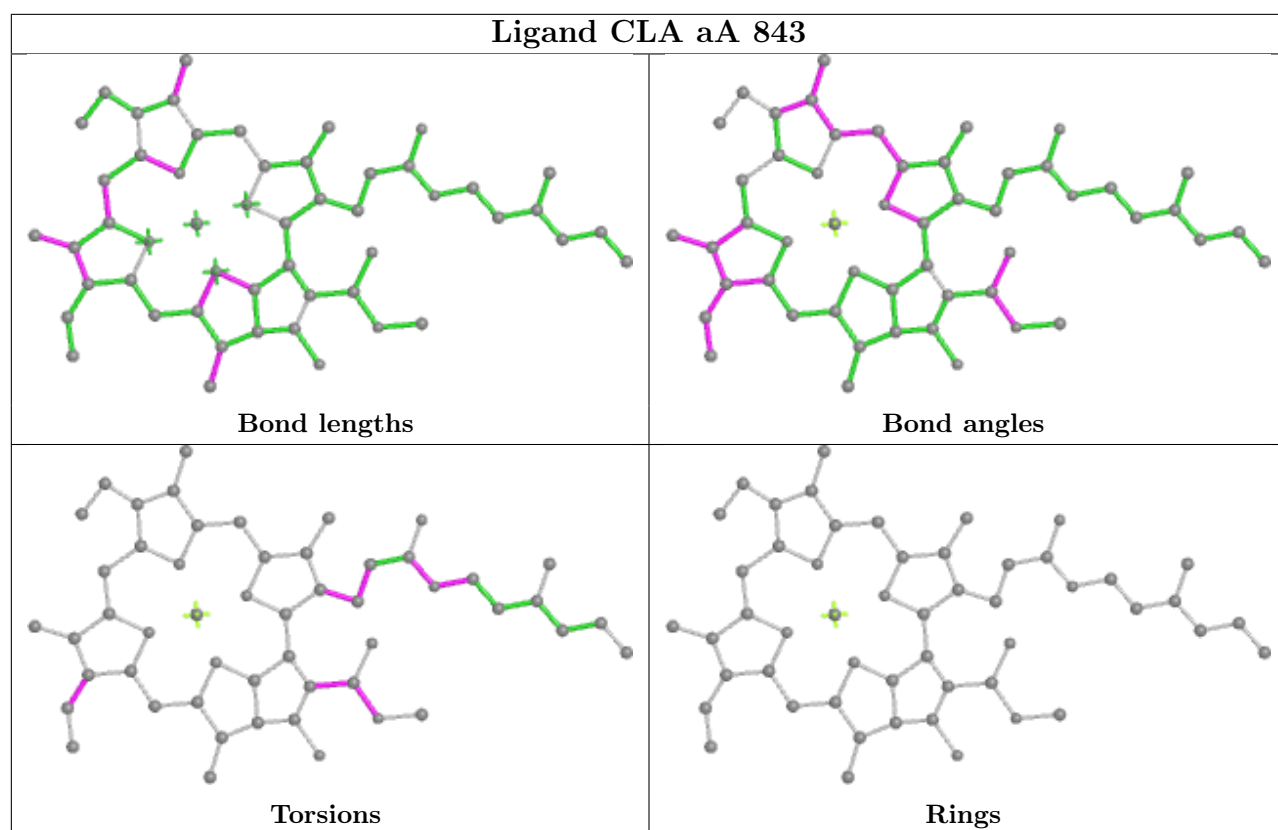
Rings

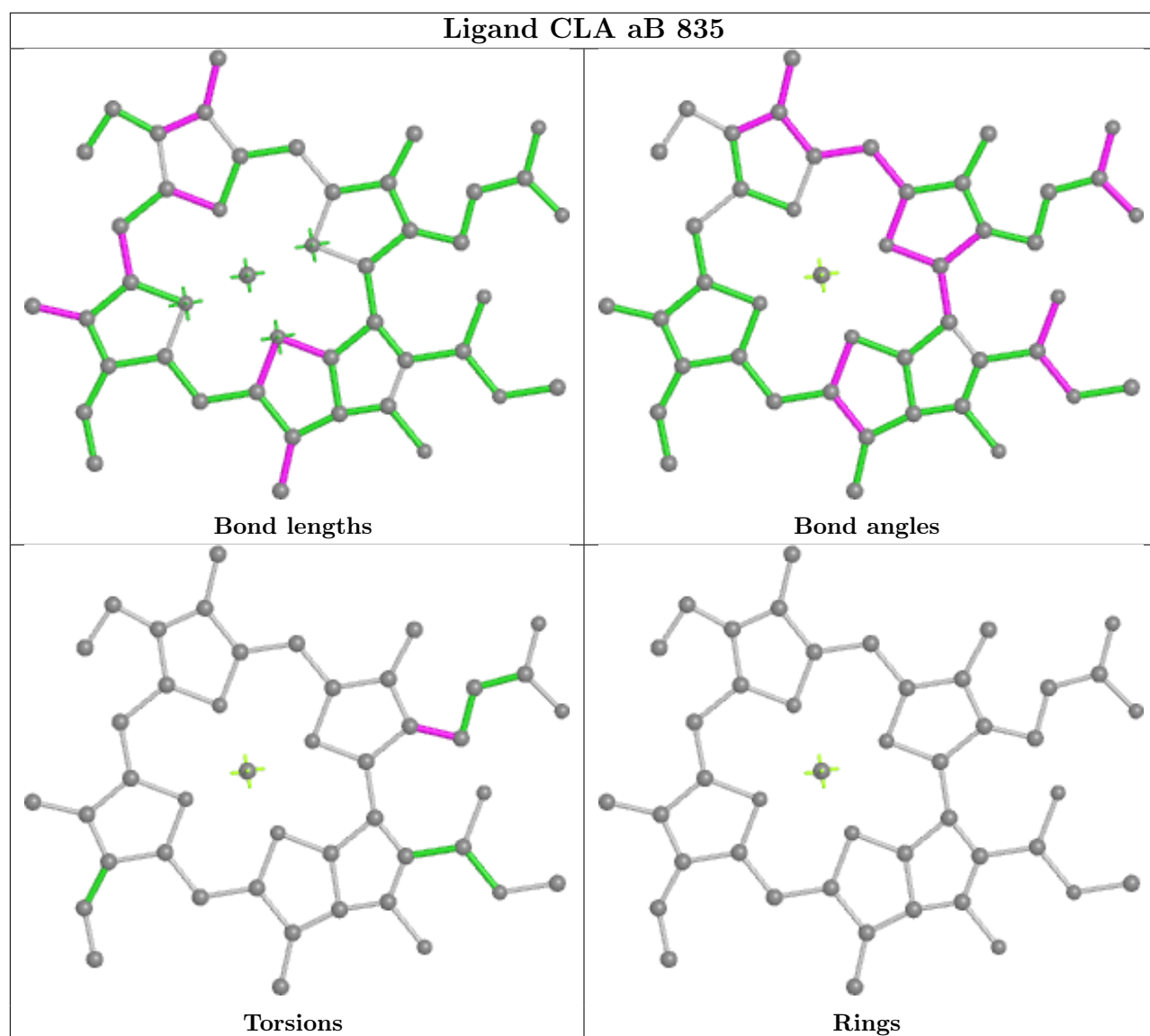
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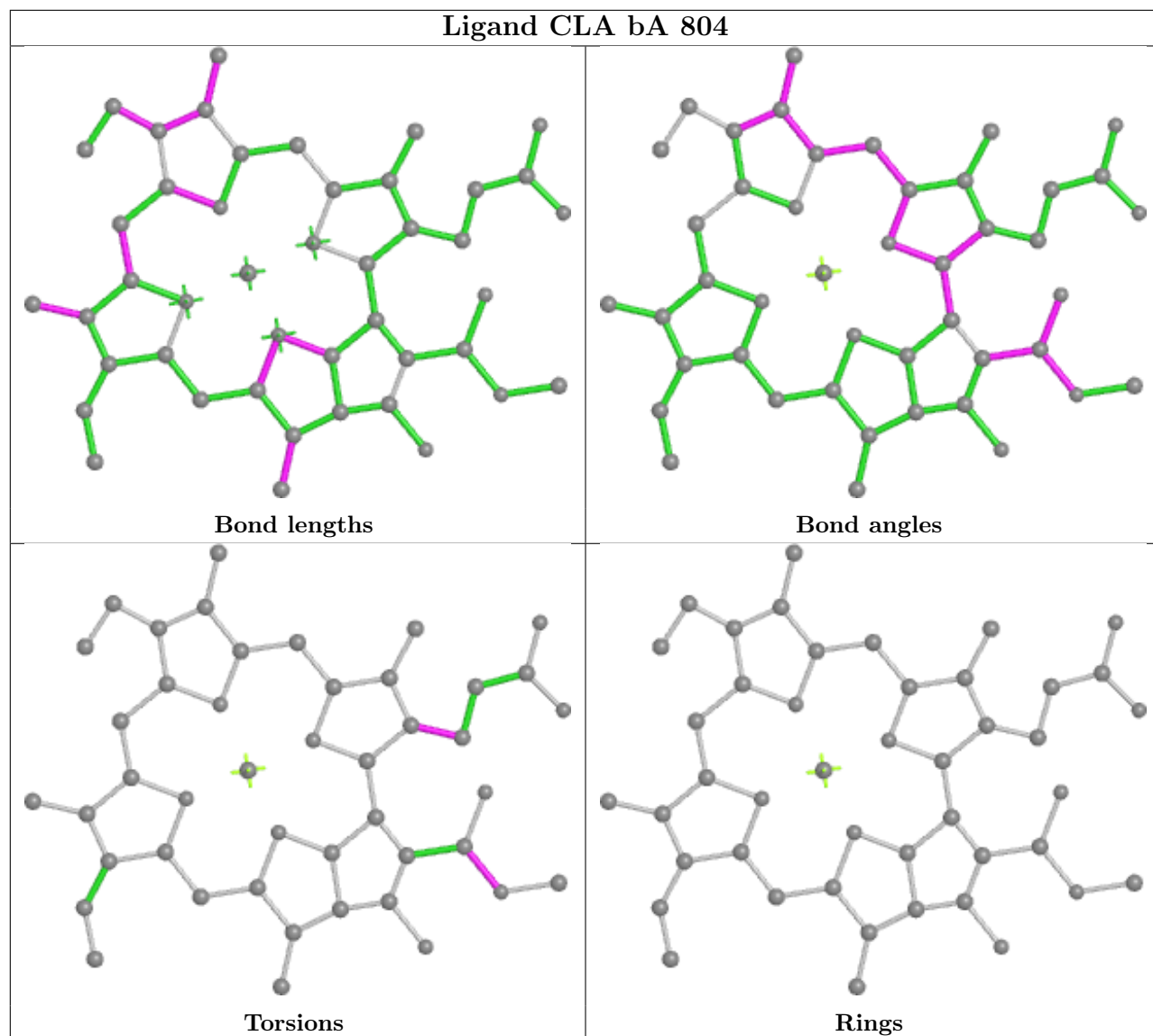
Ligand CLA dL 202

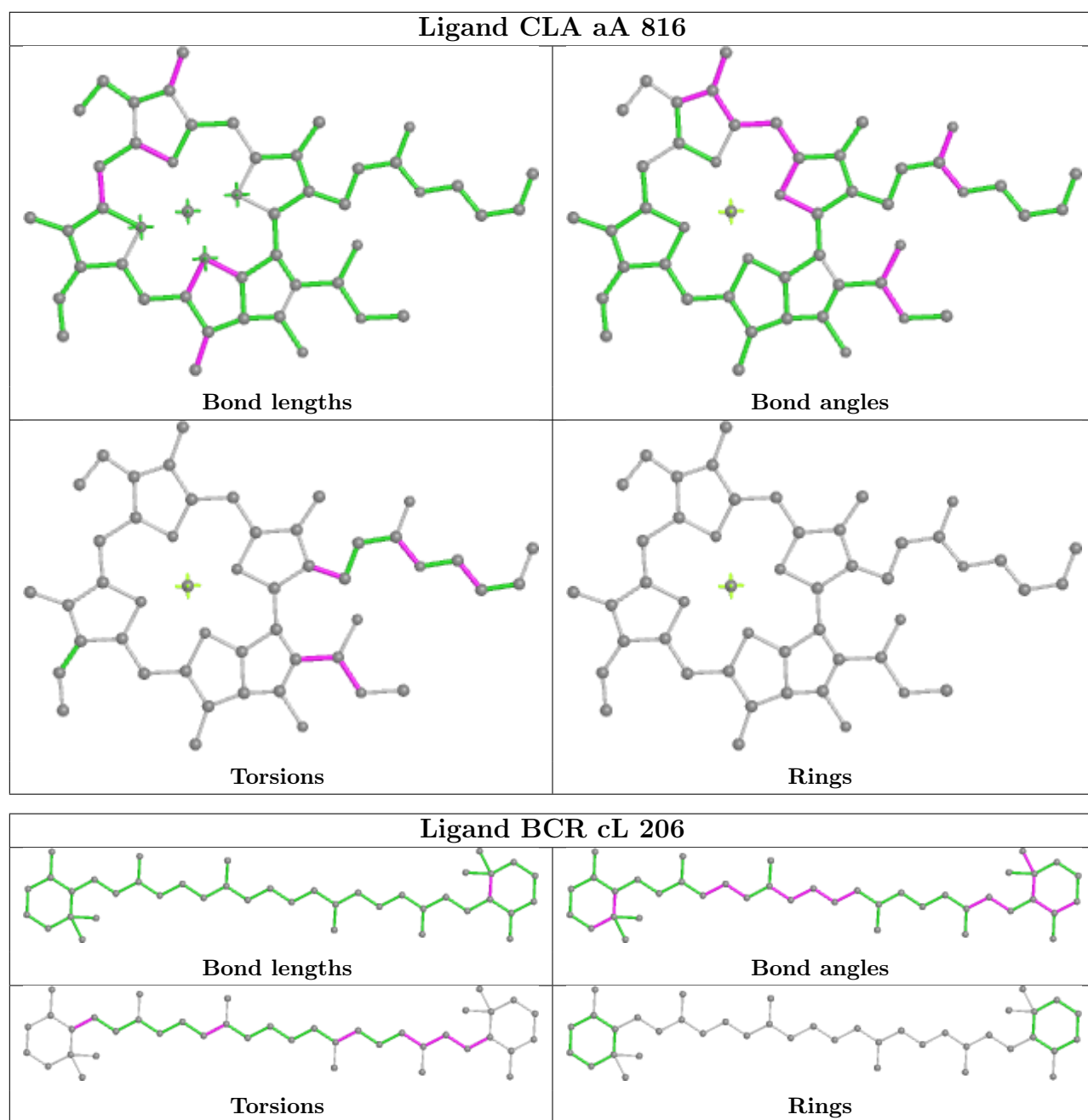


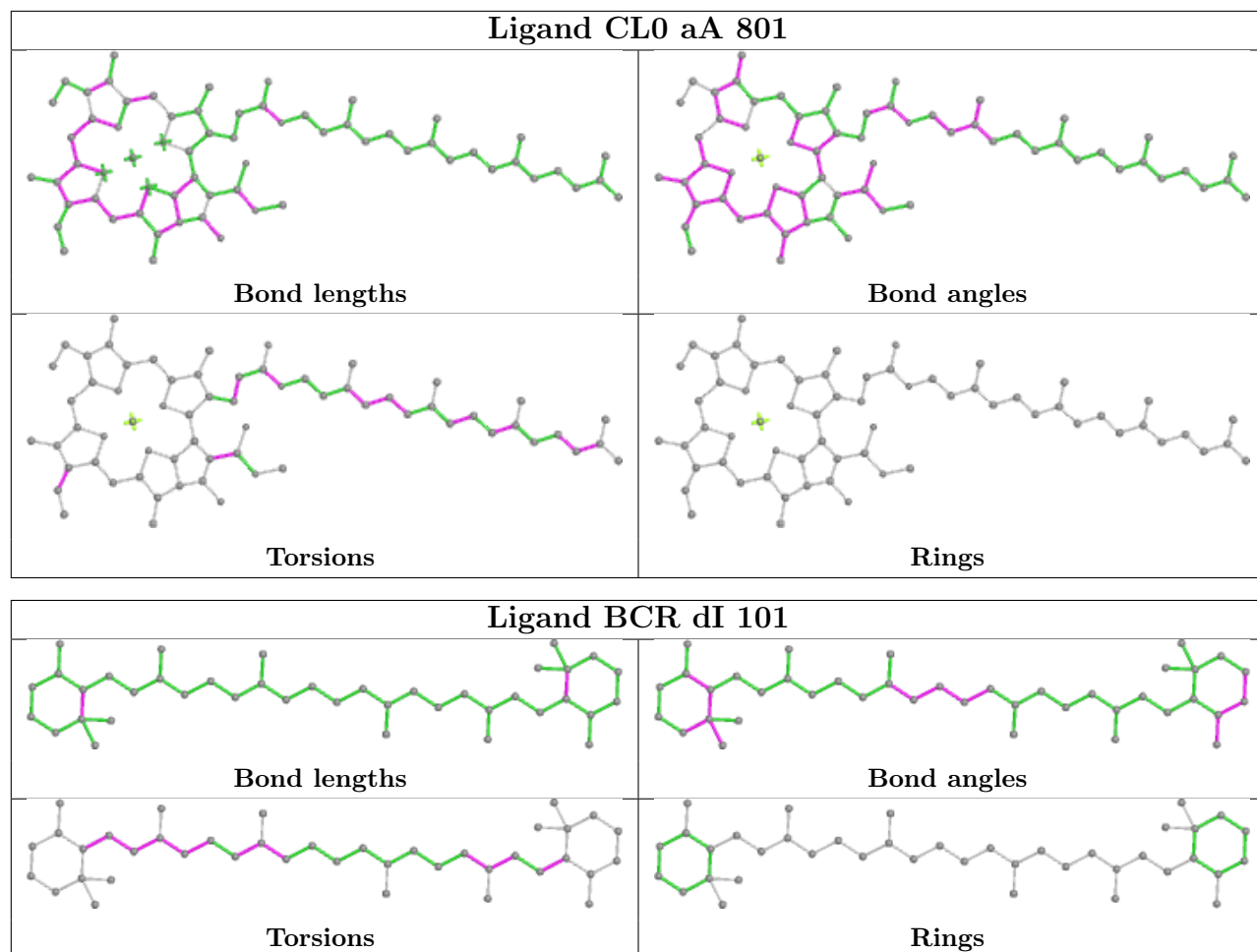




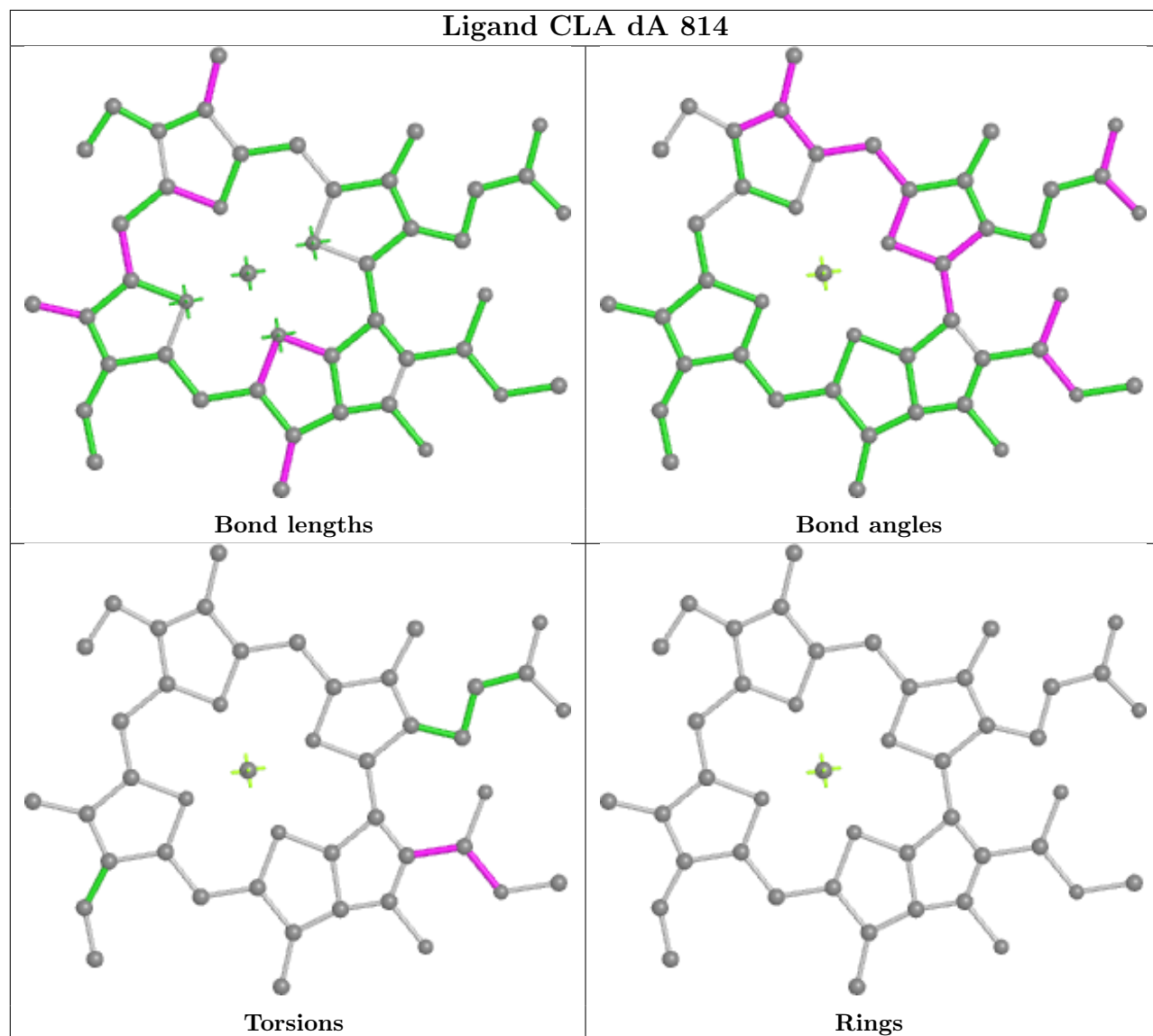
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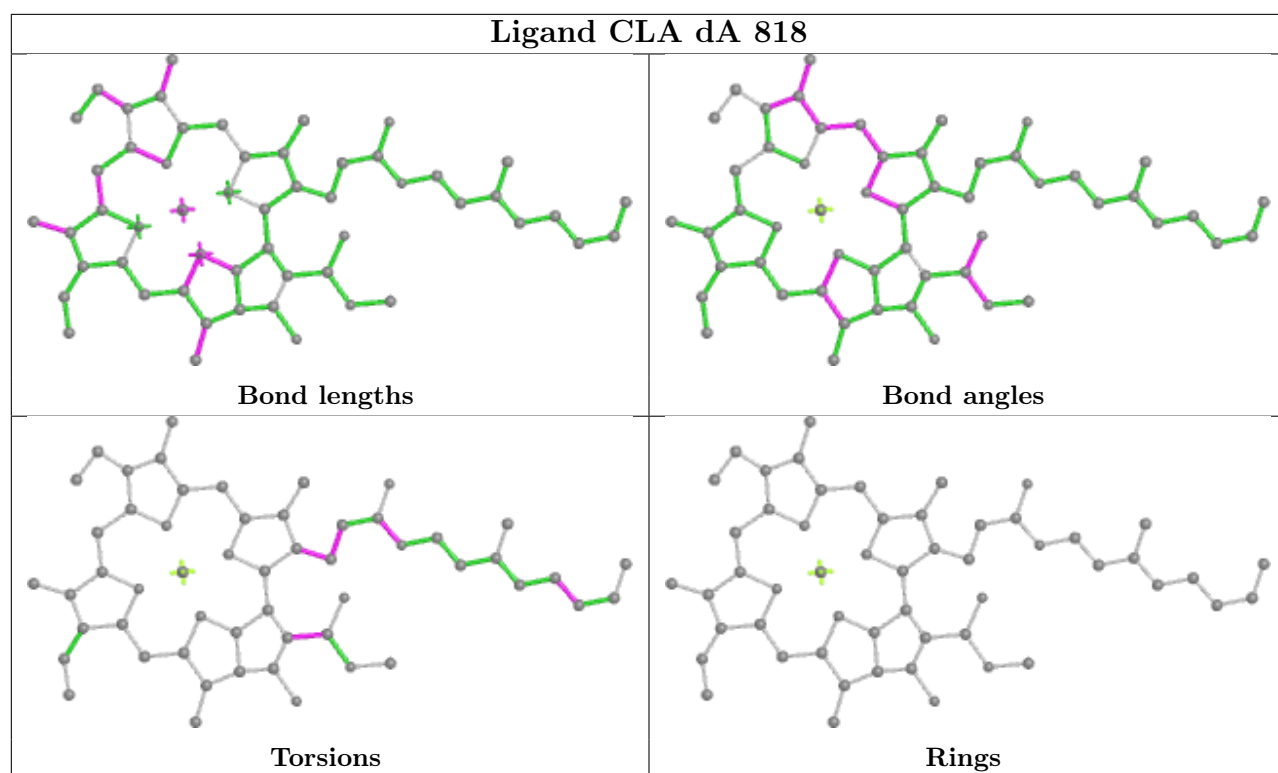




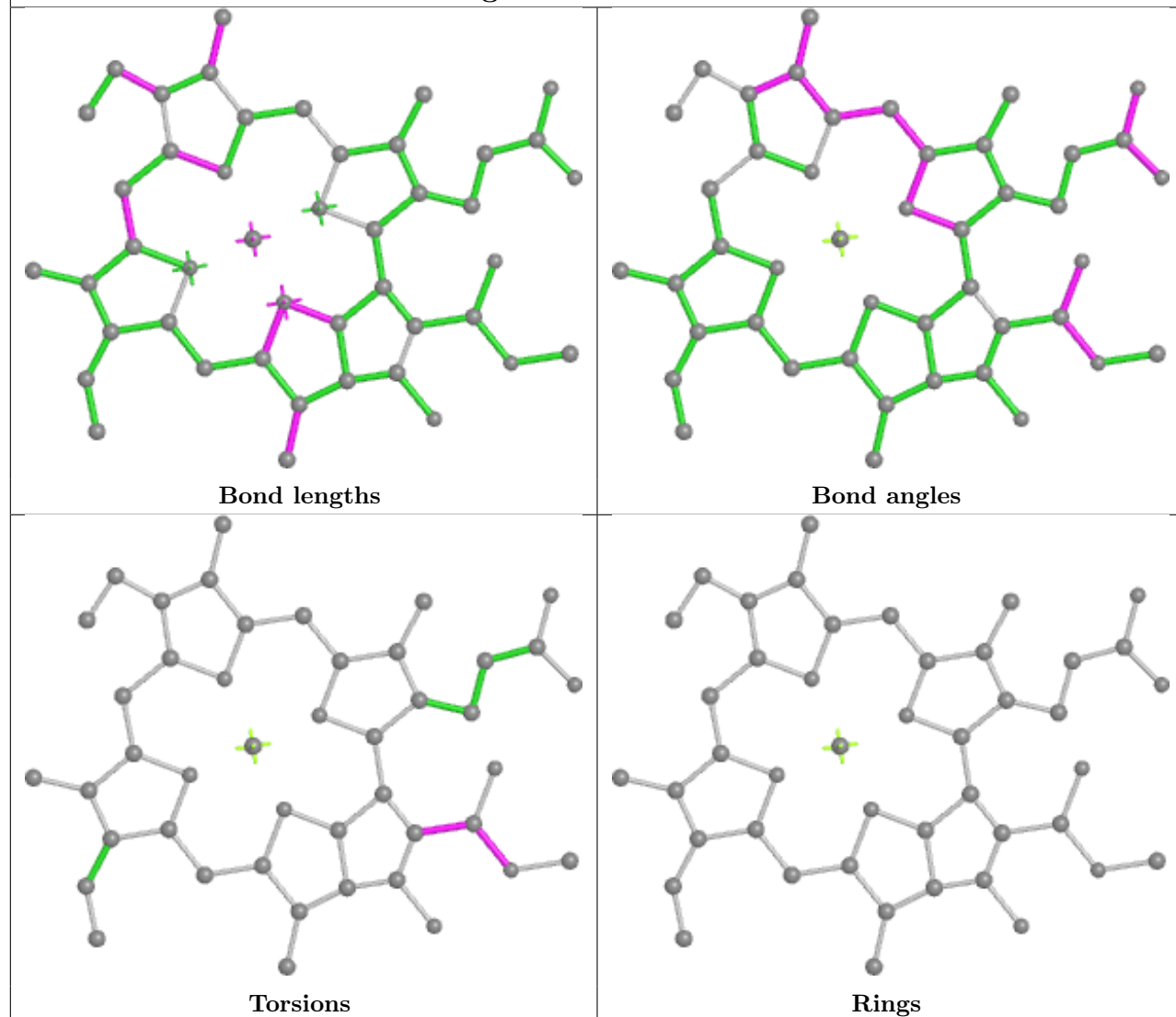


Ligand CLA dA 814

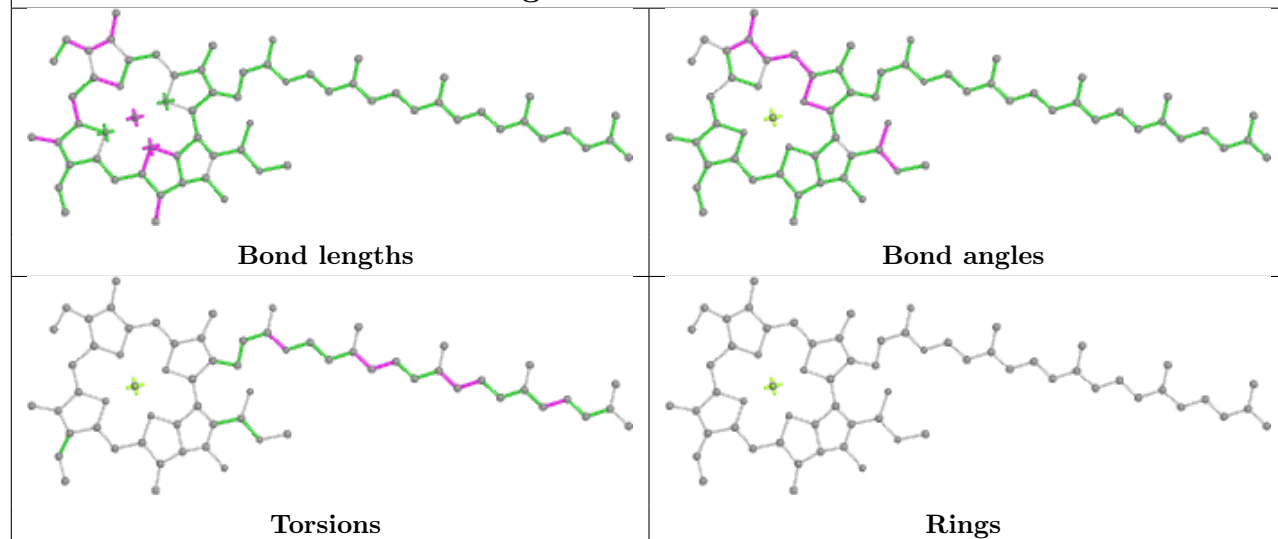


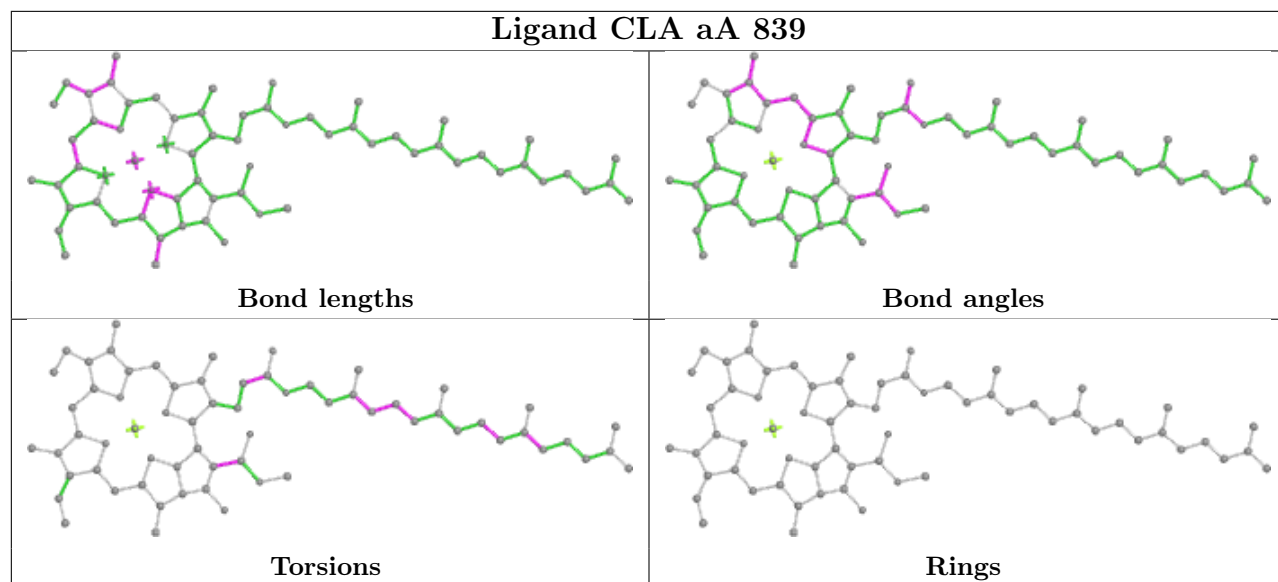
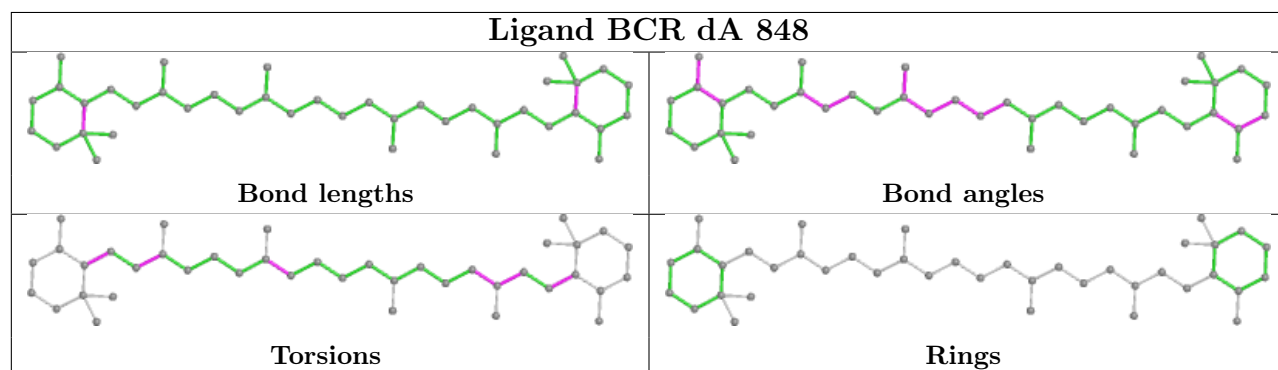
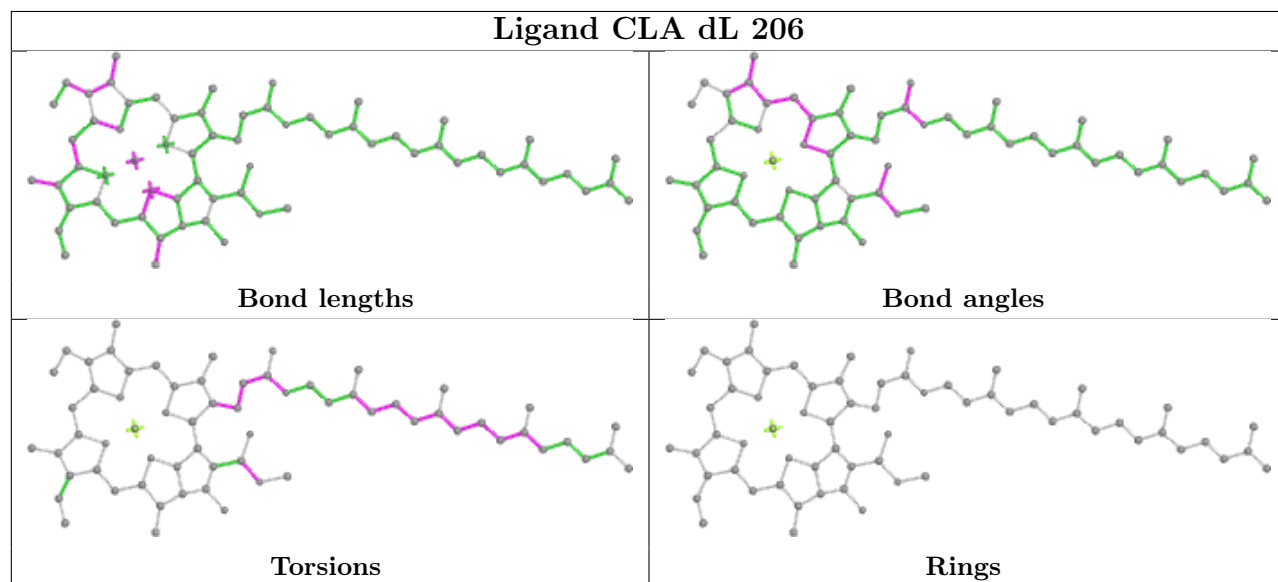


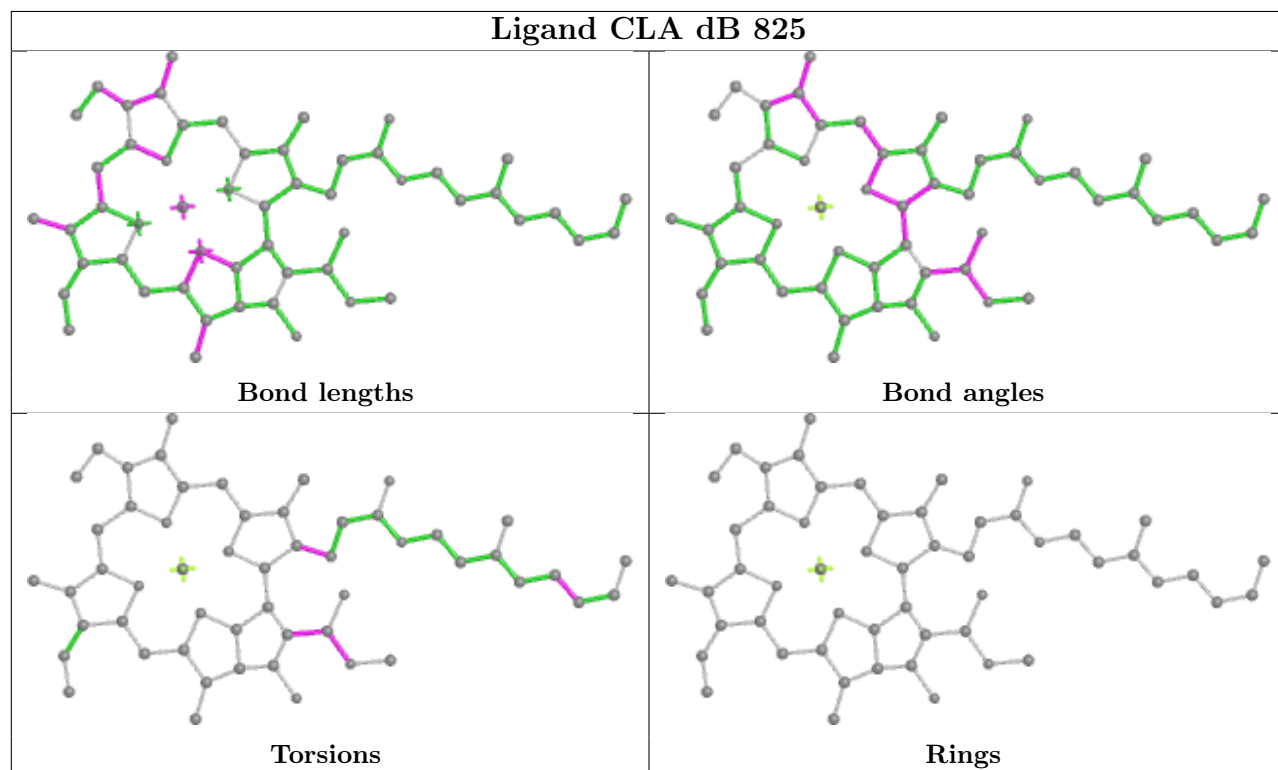
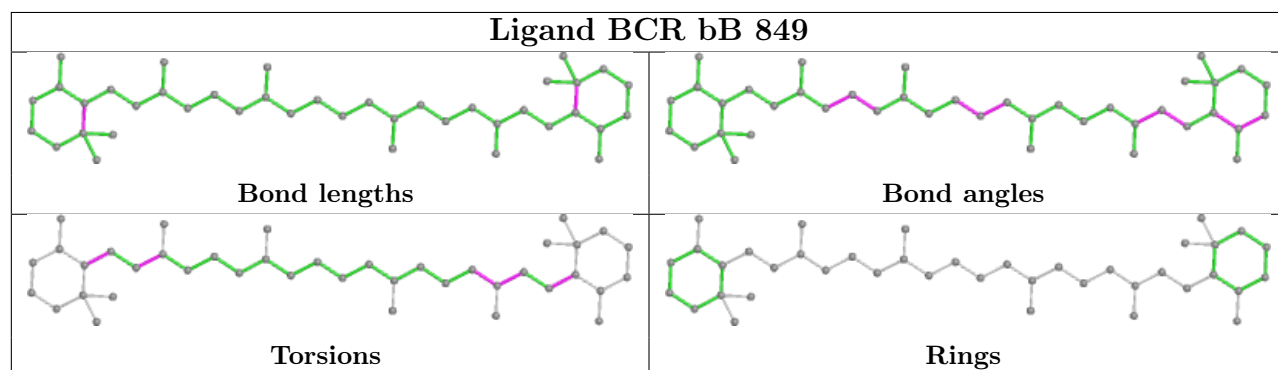
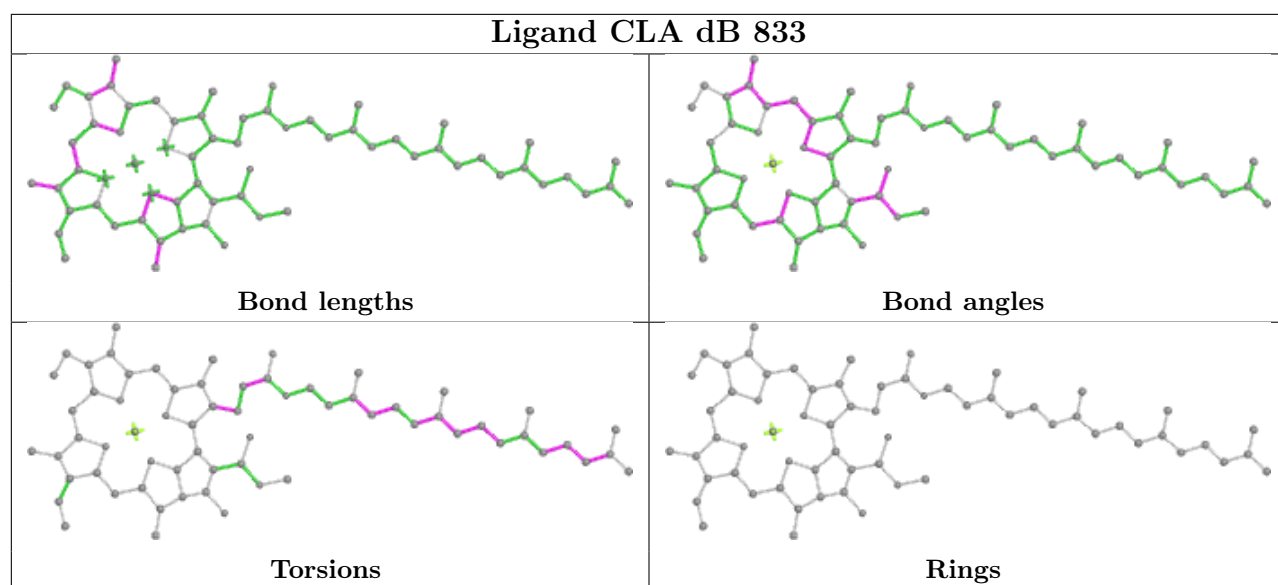
Ligand CLA aB 821

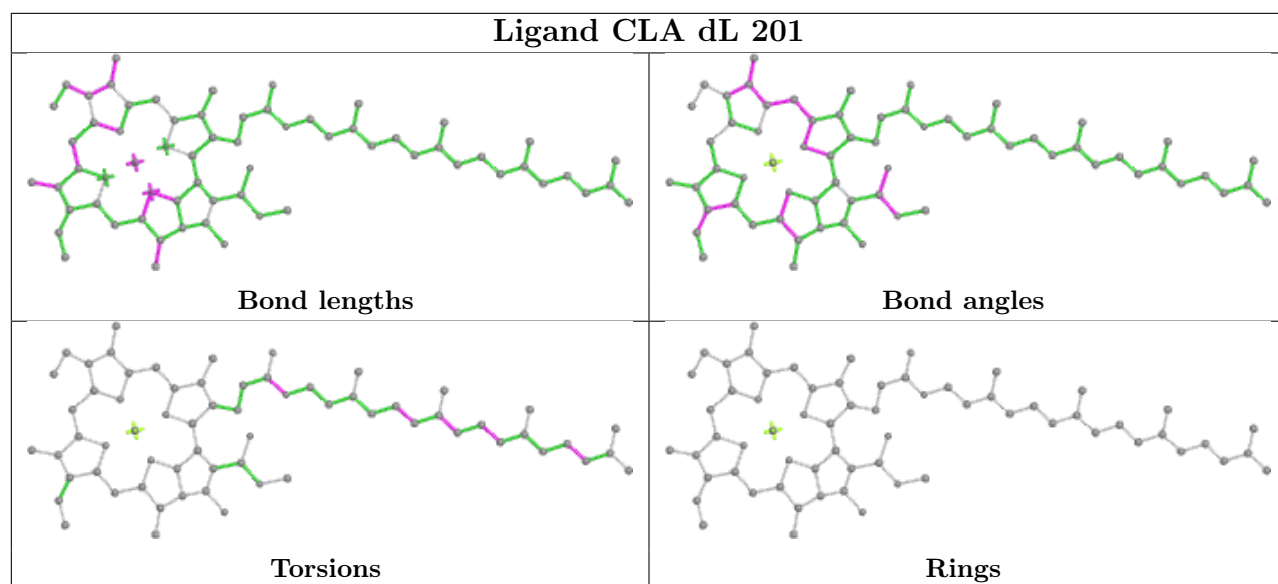
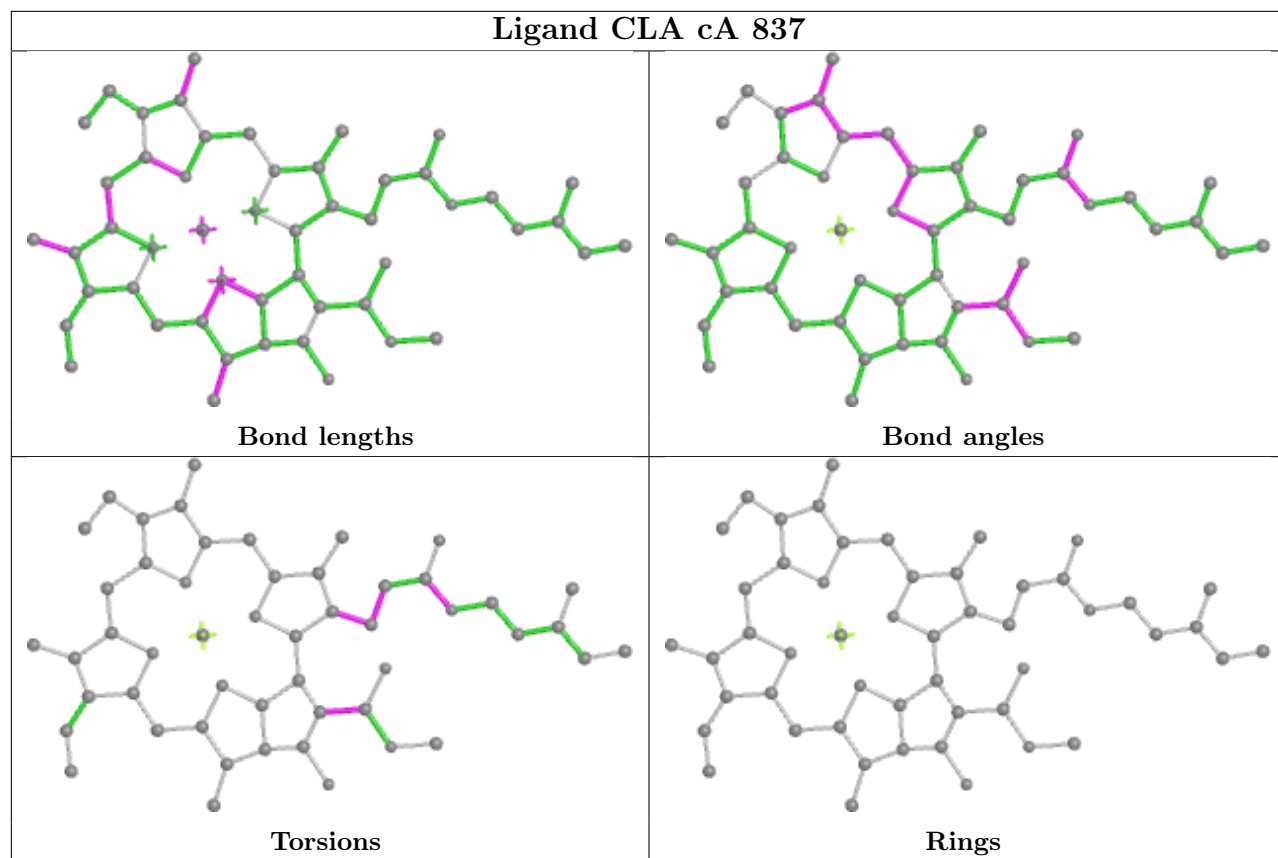


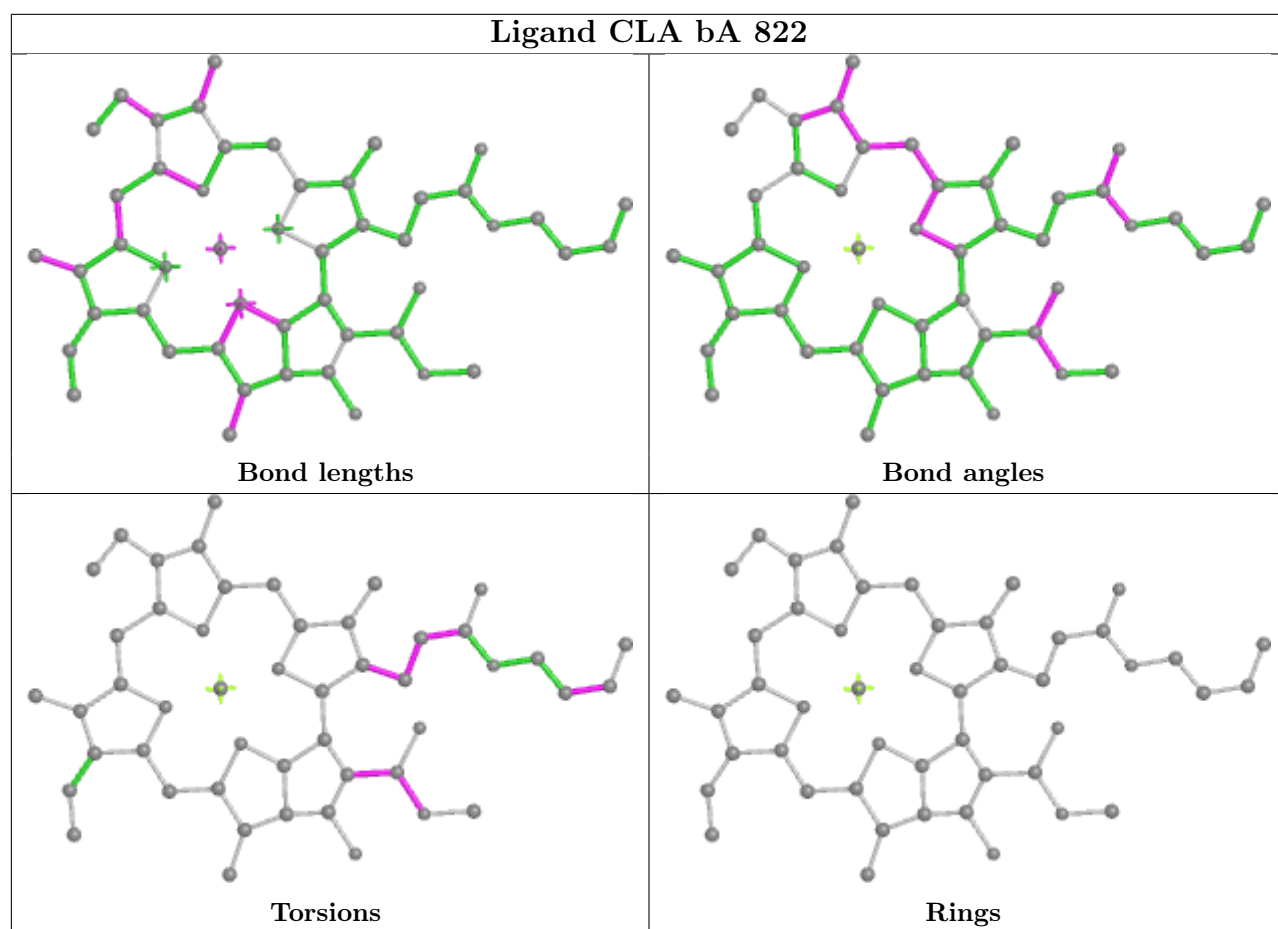
Ligand CLA bB 810



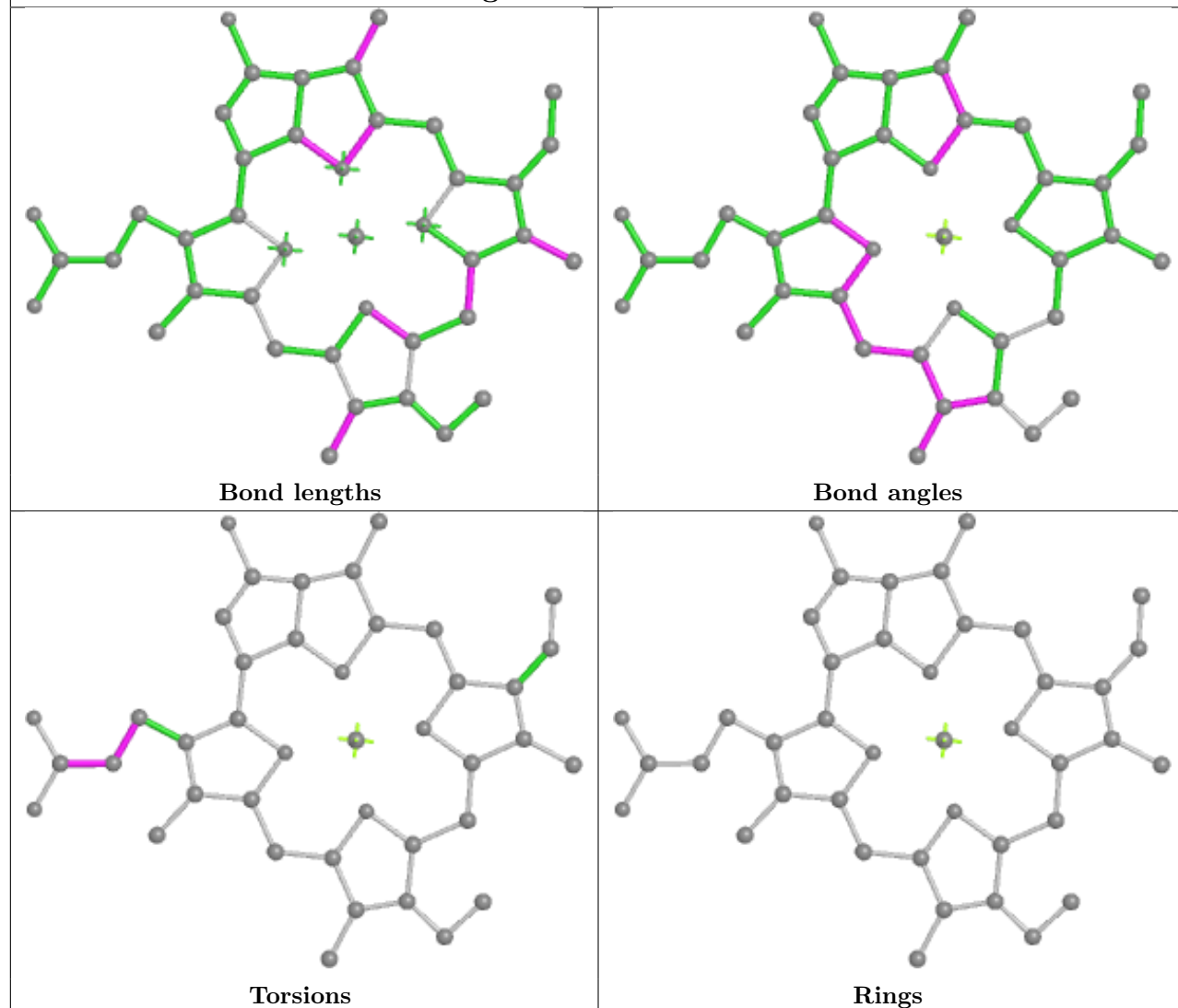
Ligand CLA aA 839**Ligand BCR dA 848****Ligand CLA dL 206**



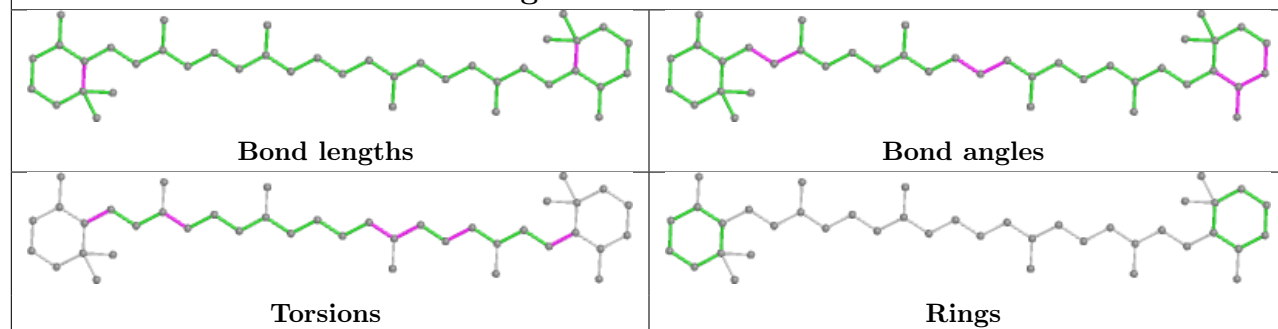


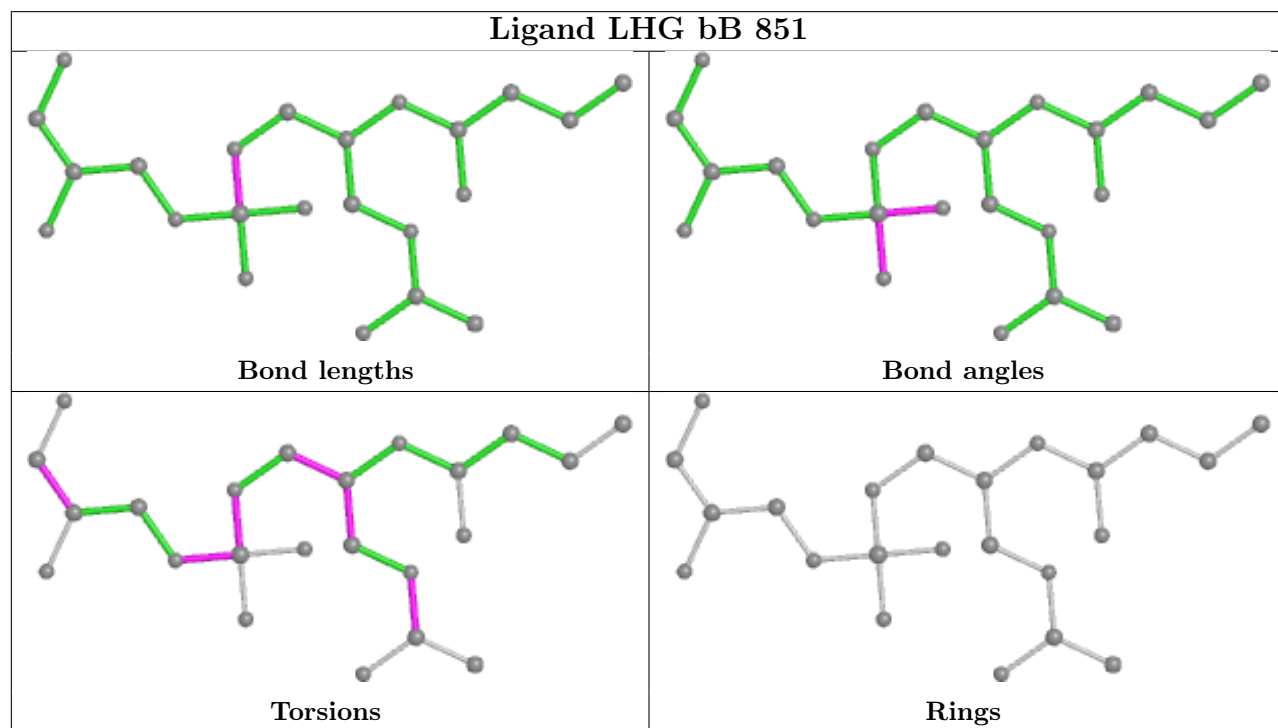
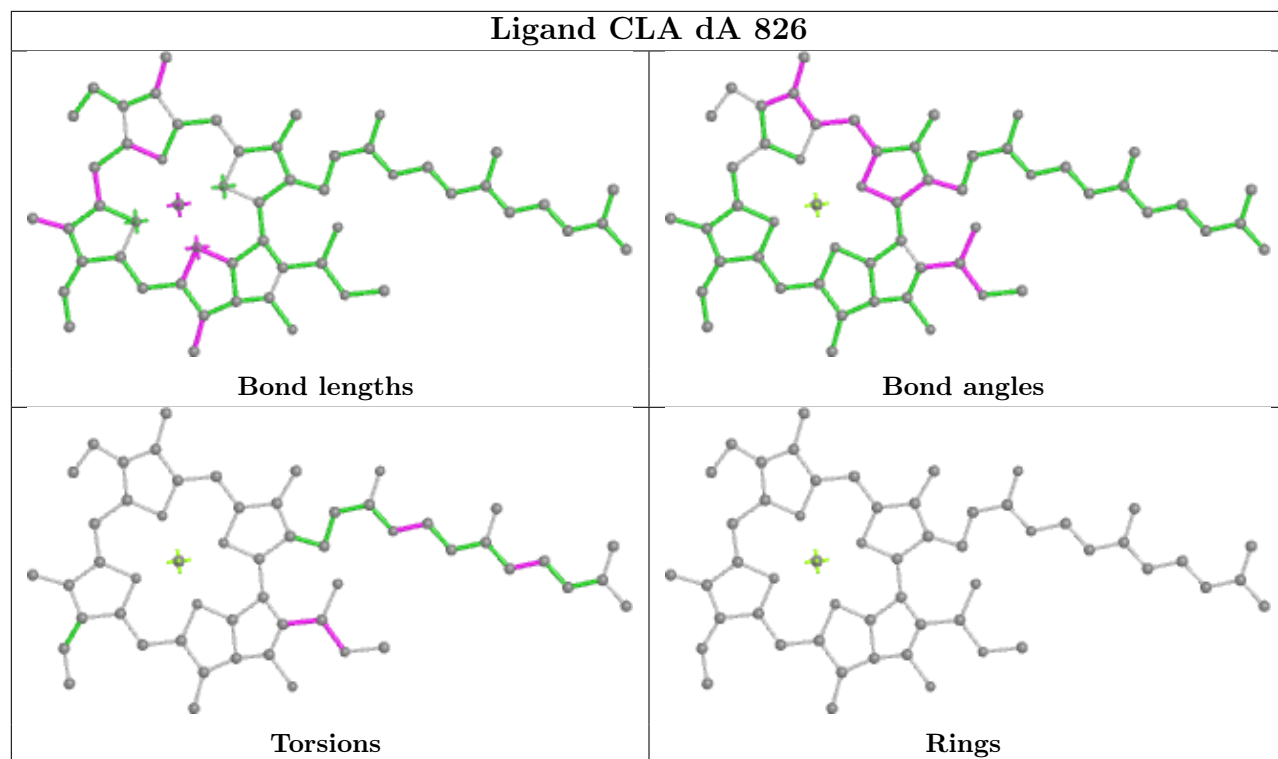


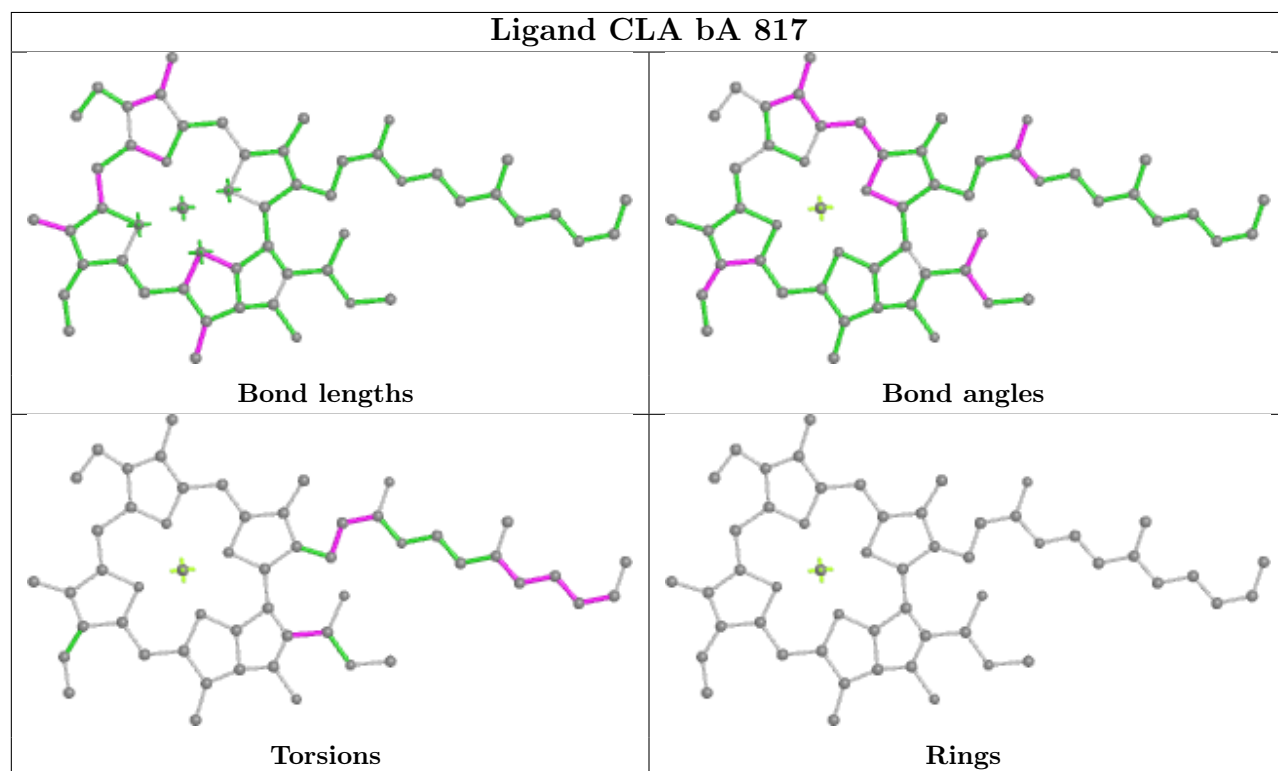
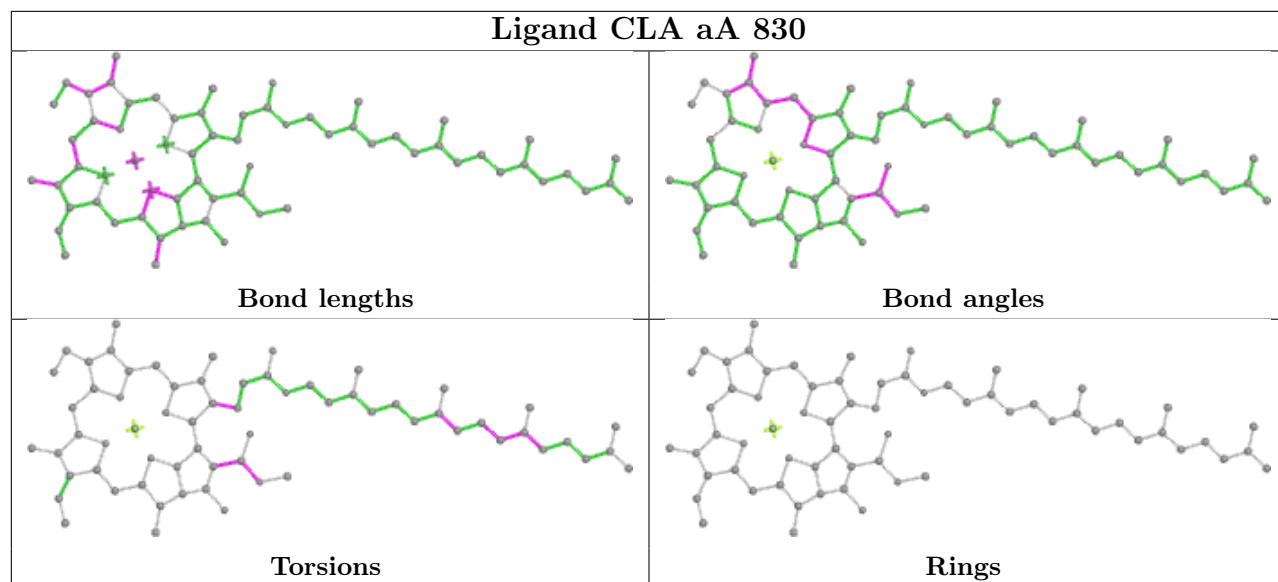
Ligand CLA cK 101

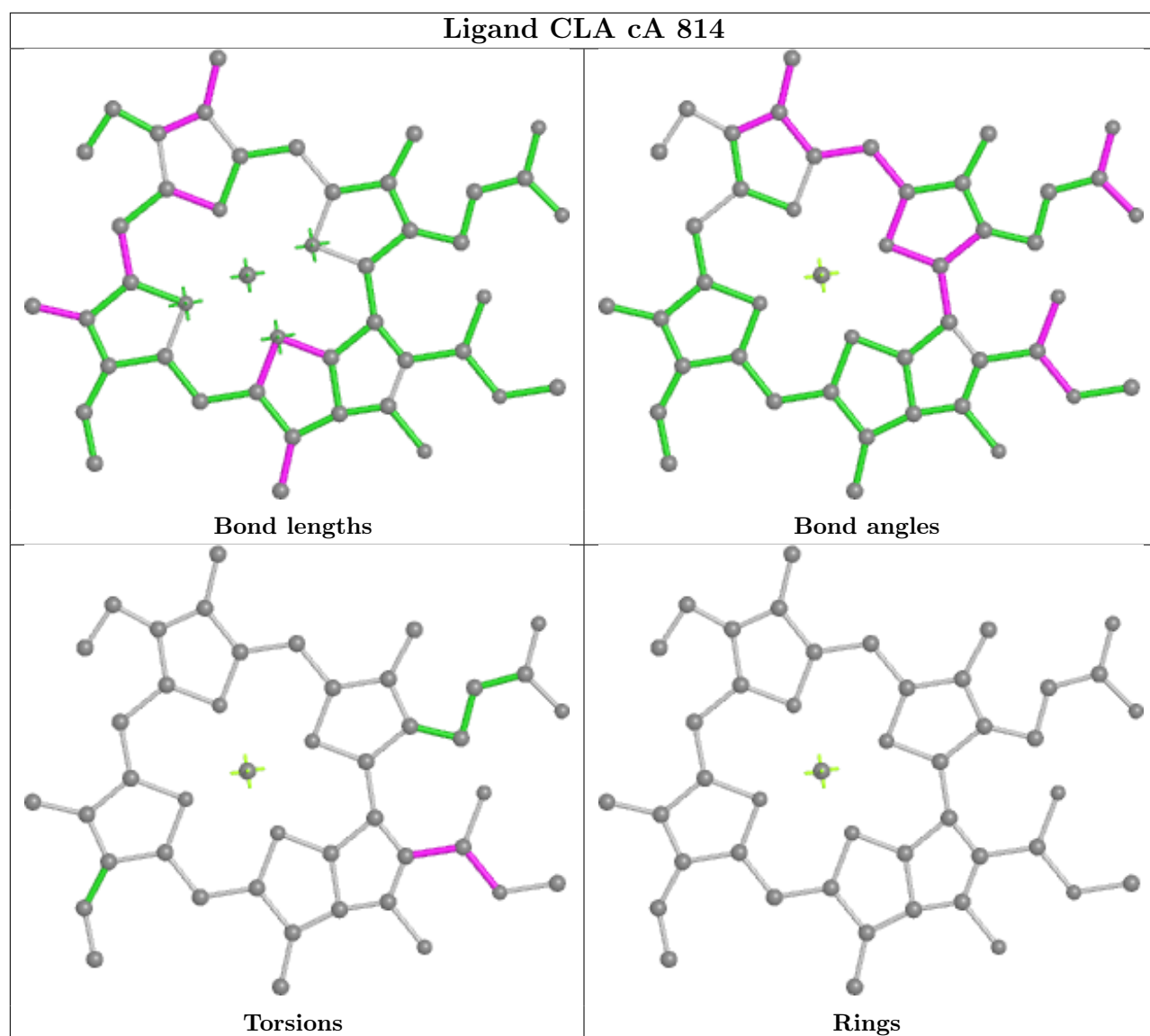


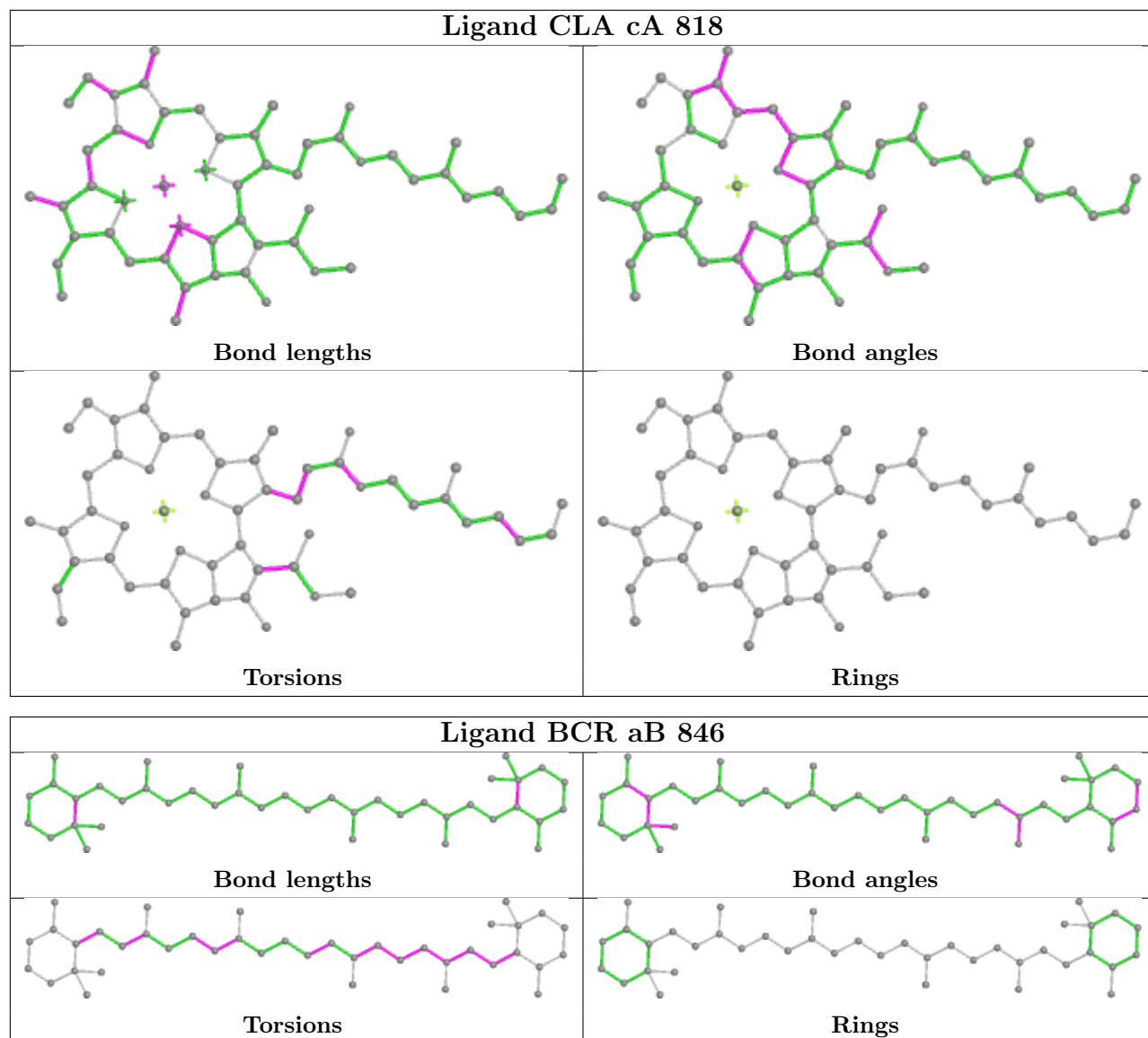
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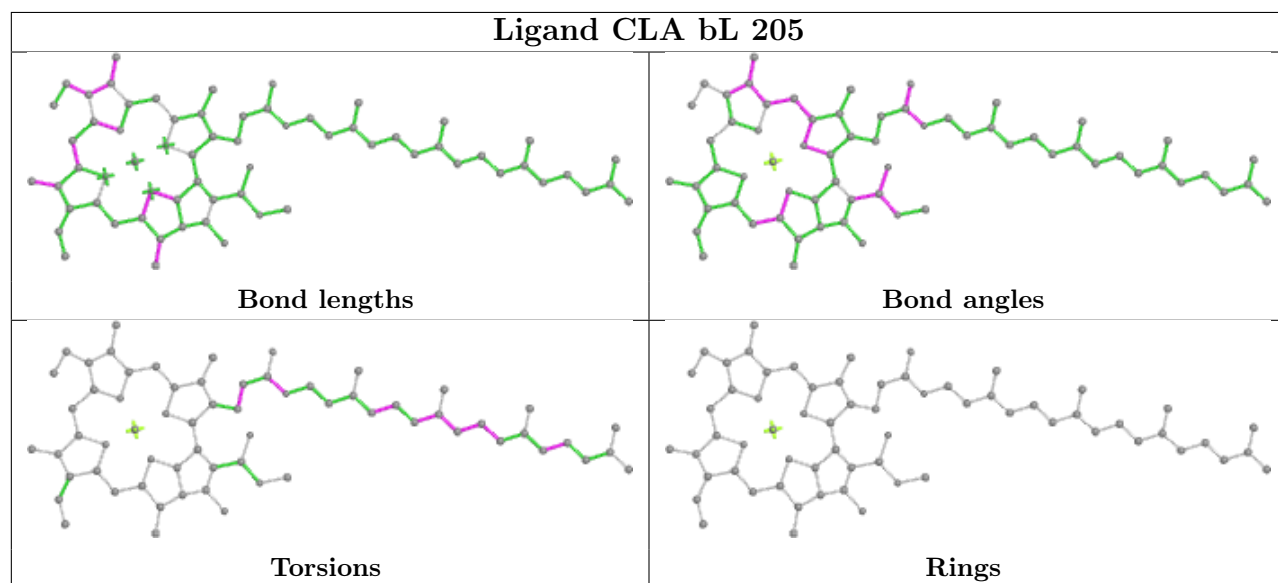
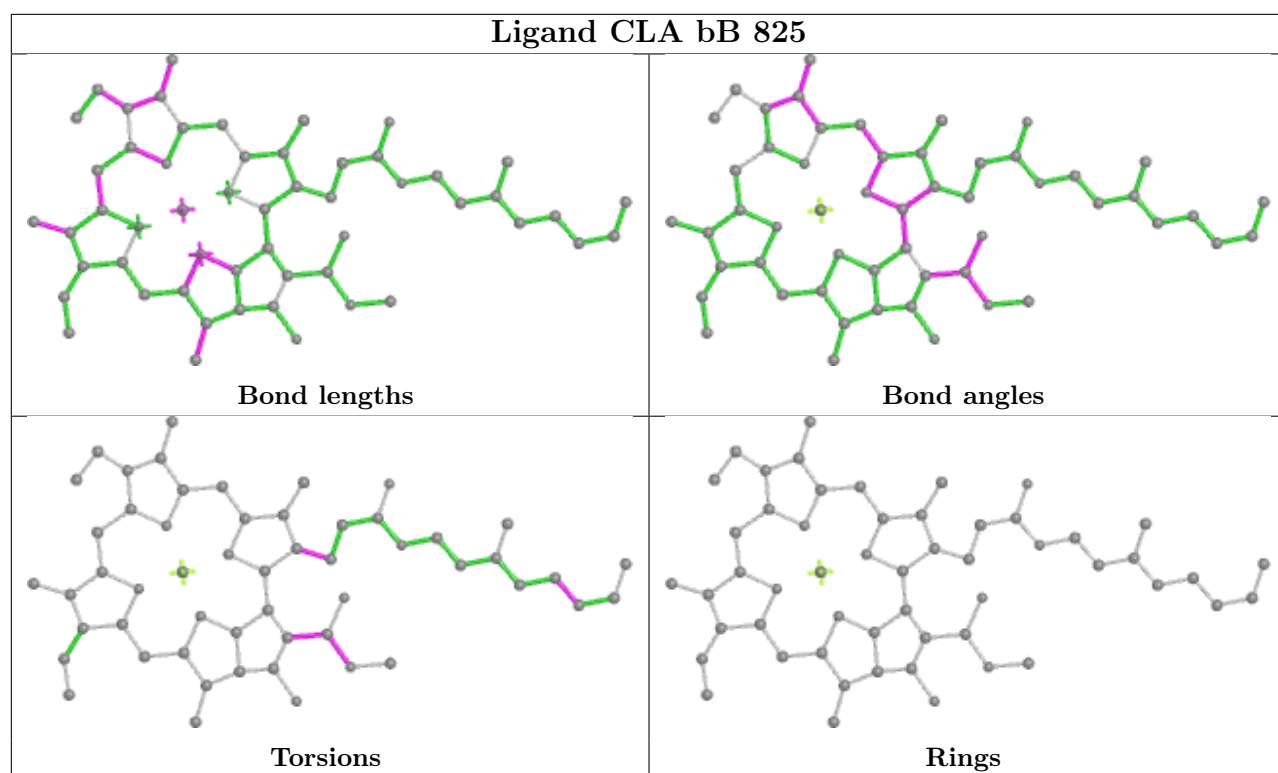




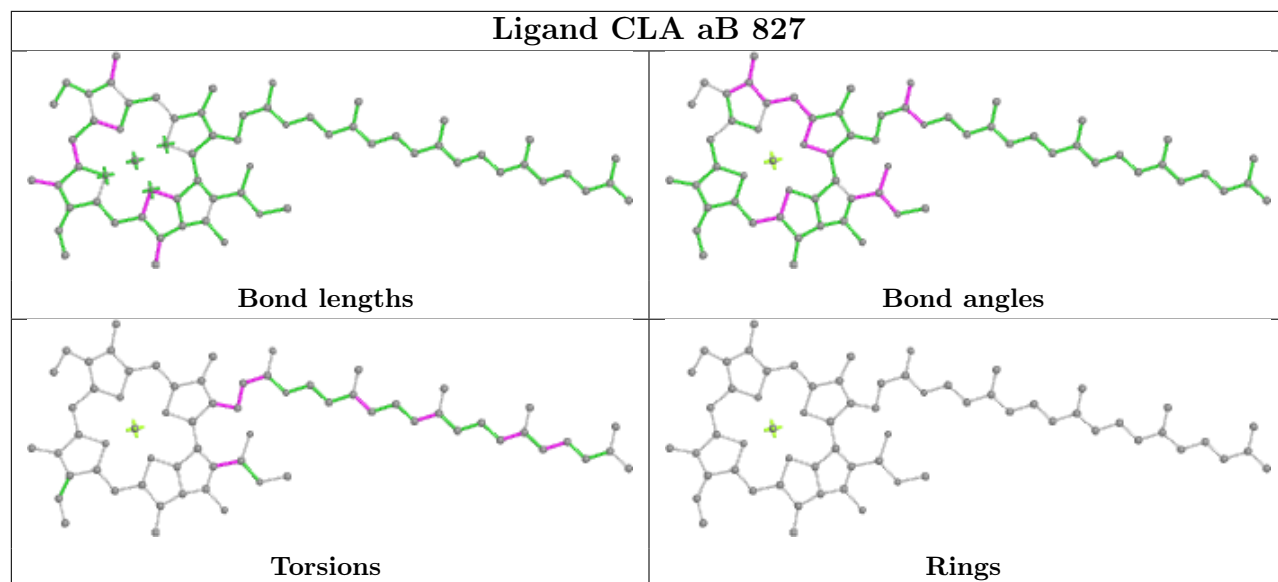




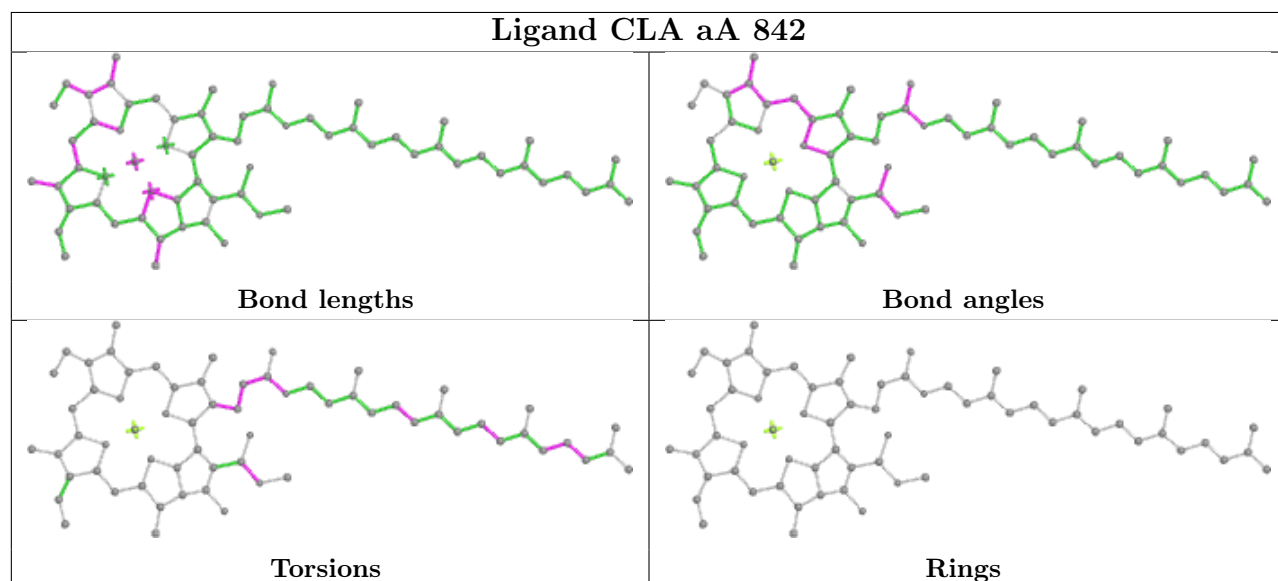




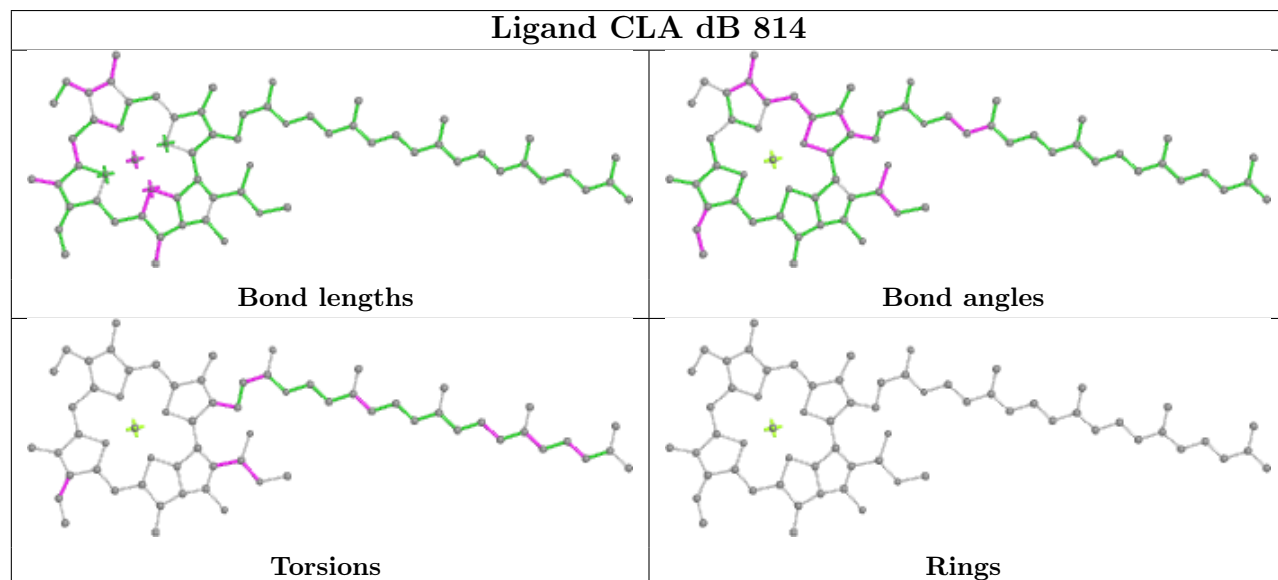
Ligand CLA aB 827

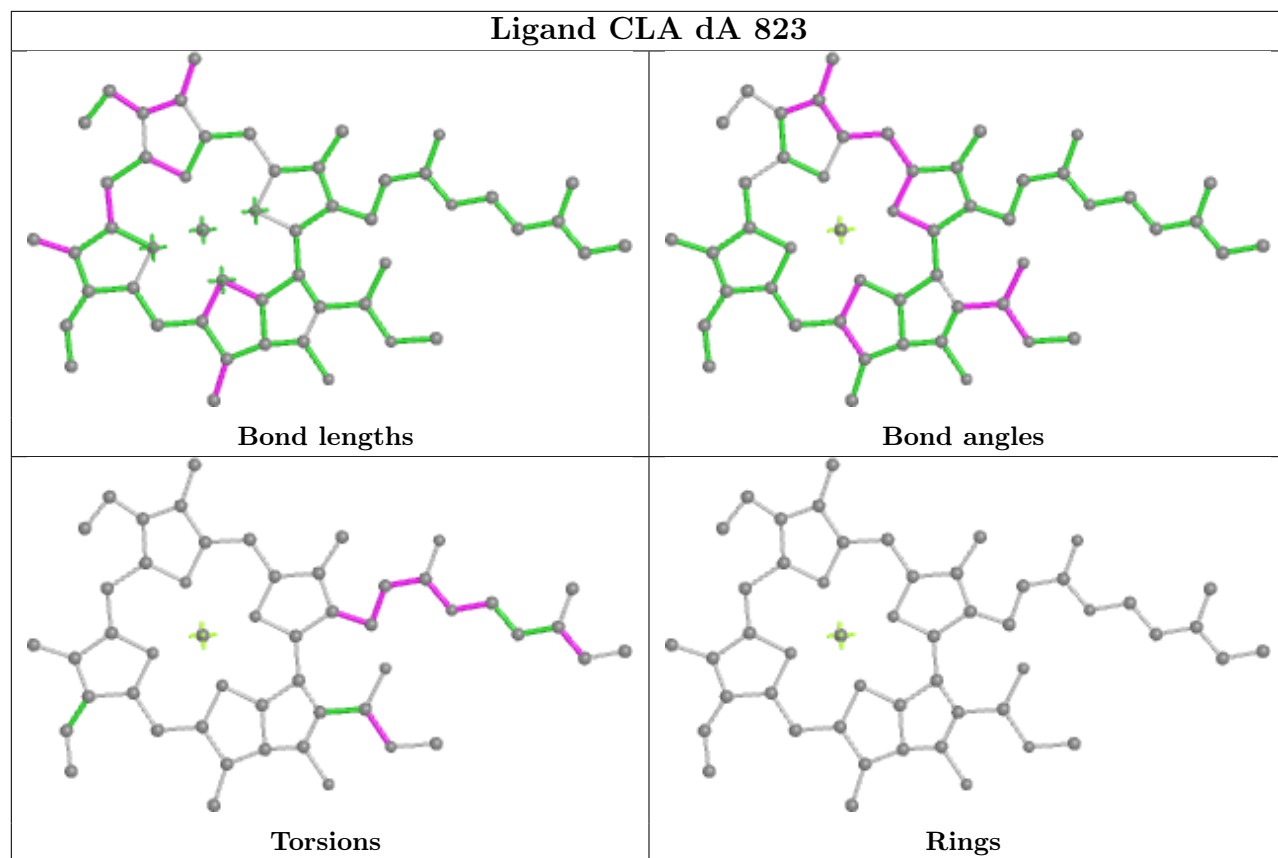


Ligand CLA aA 842

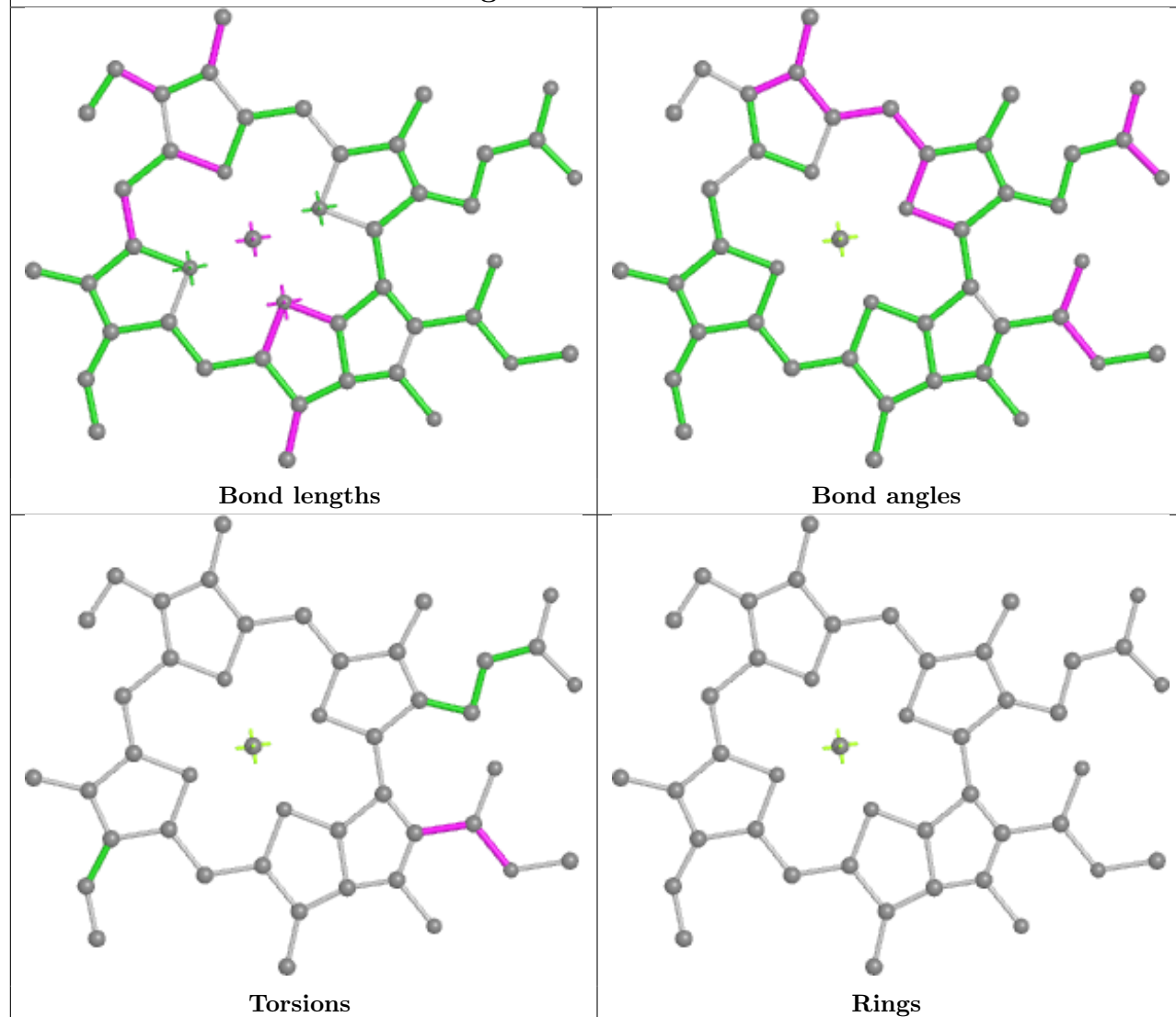


Ligand CLA dB 814

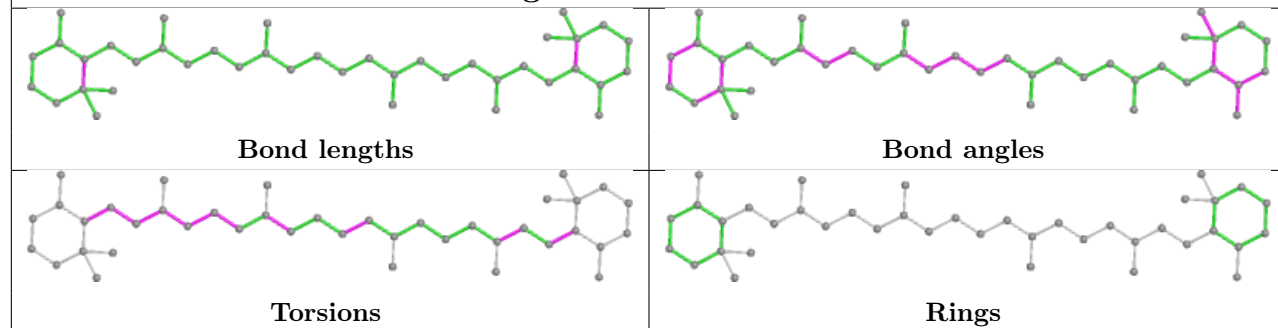


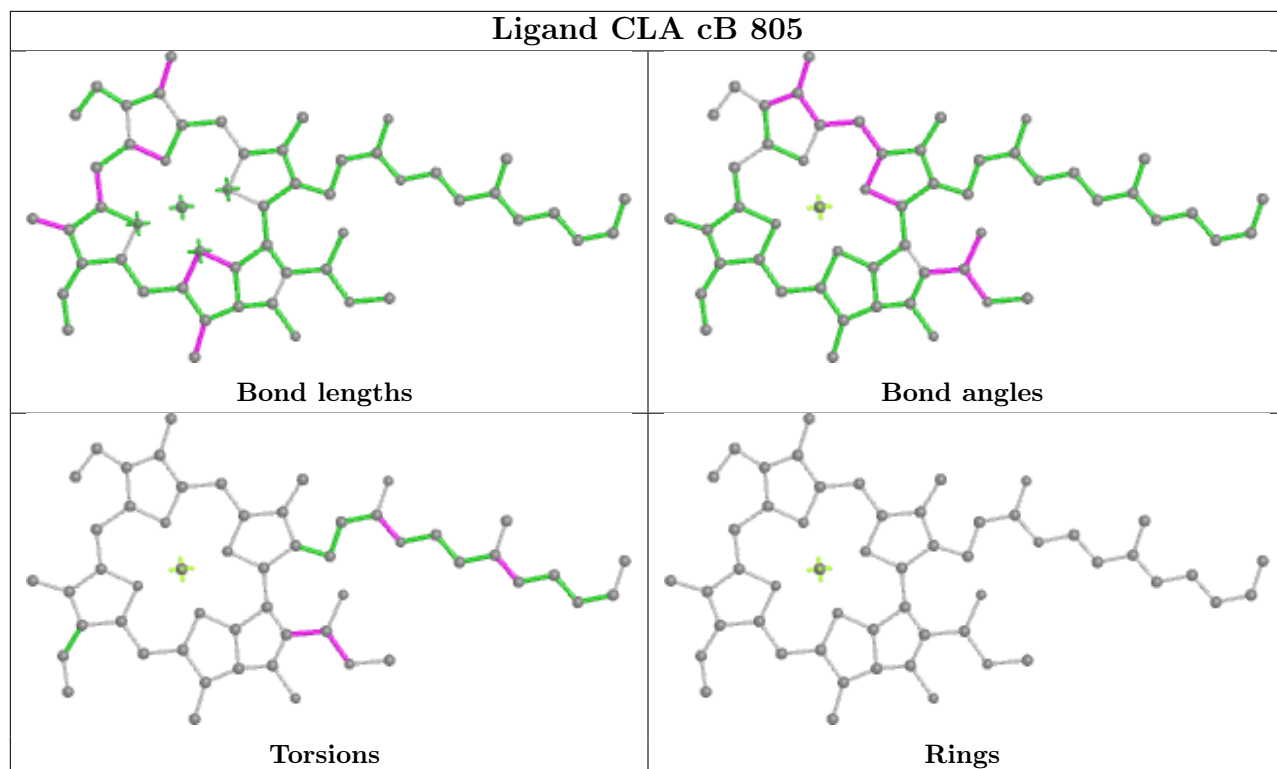
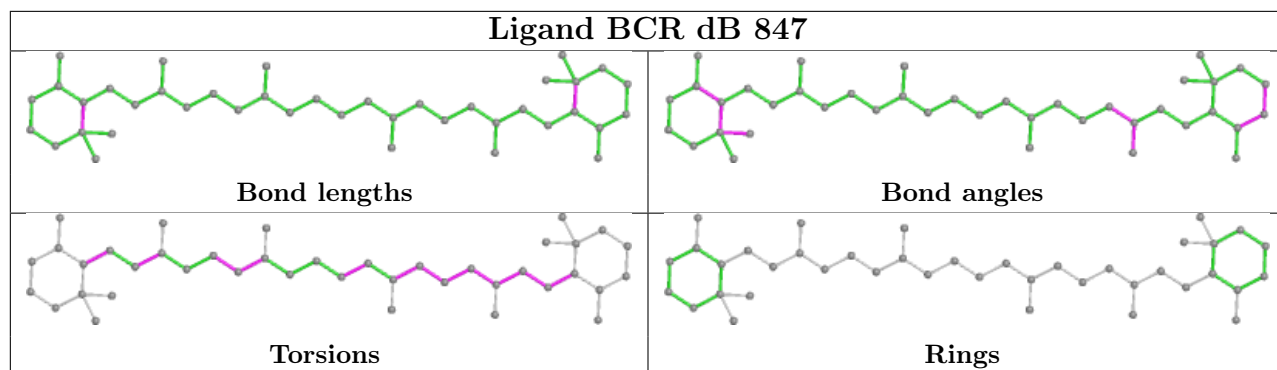


Ligand CLA bB 822

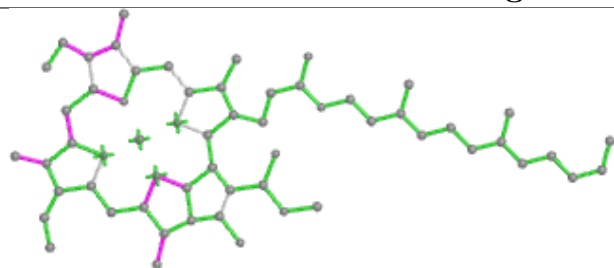


Ligand BCR dL 208

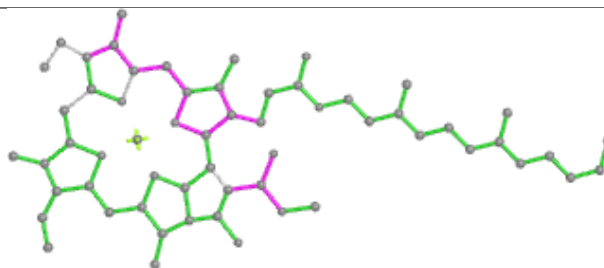




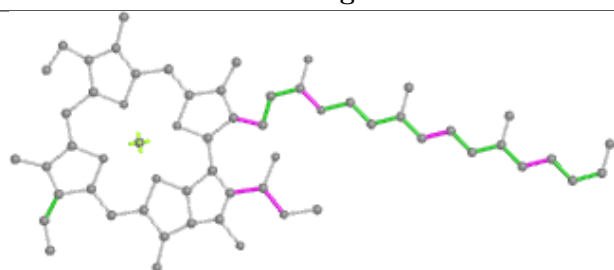
Ligand CLA aB 817



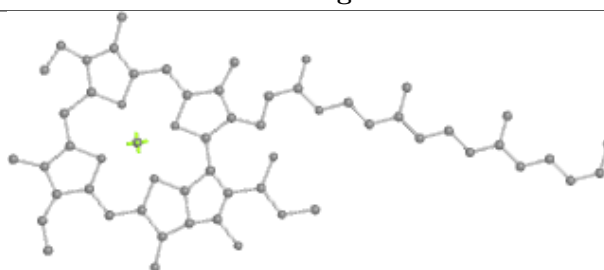
Bond lengths



Bond angles

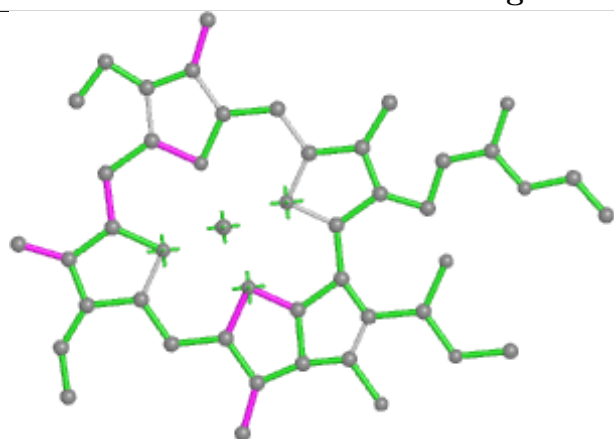


Torsions

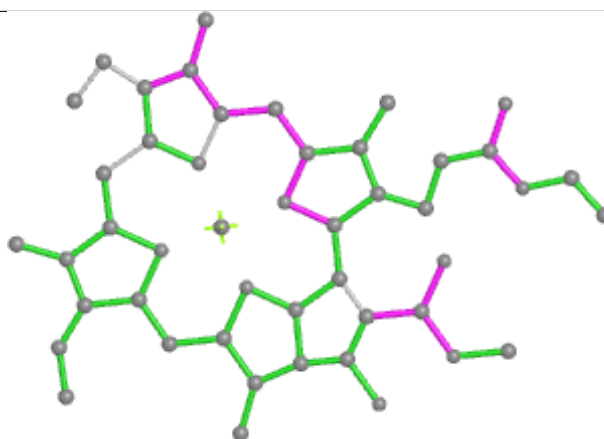


Rings

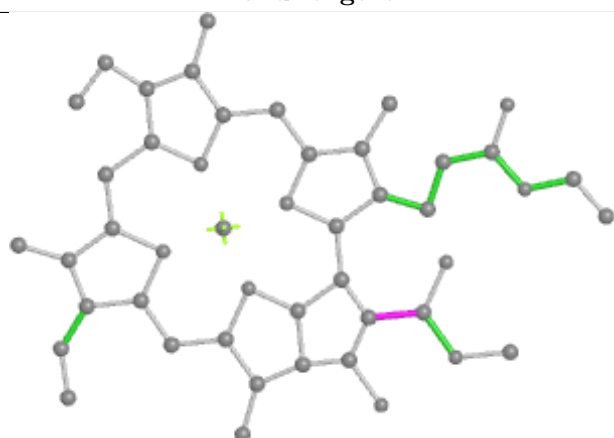
Ligand CLA cB 839



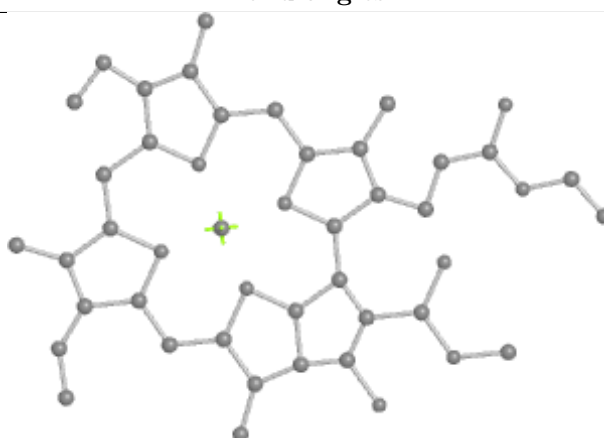
Bond lengths



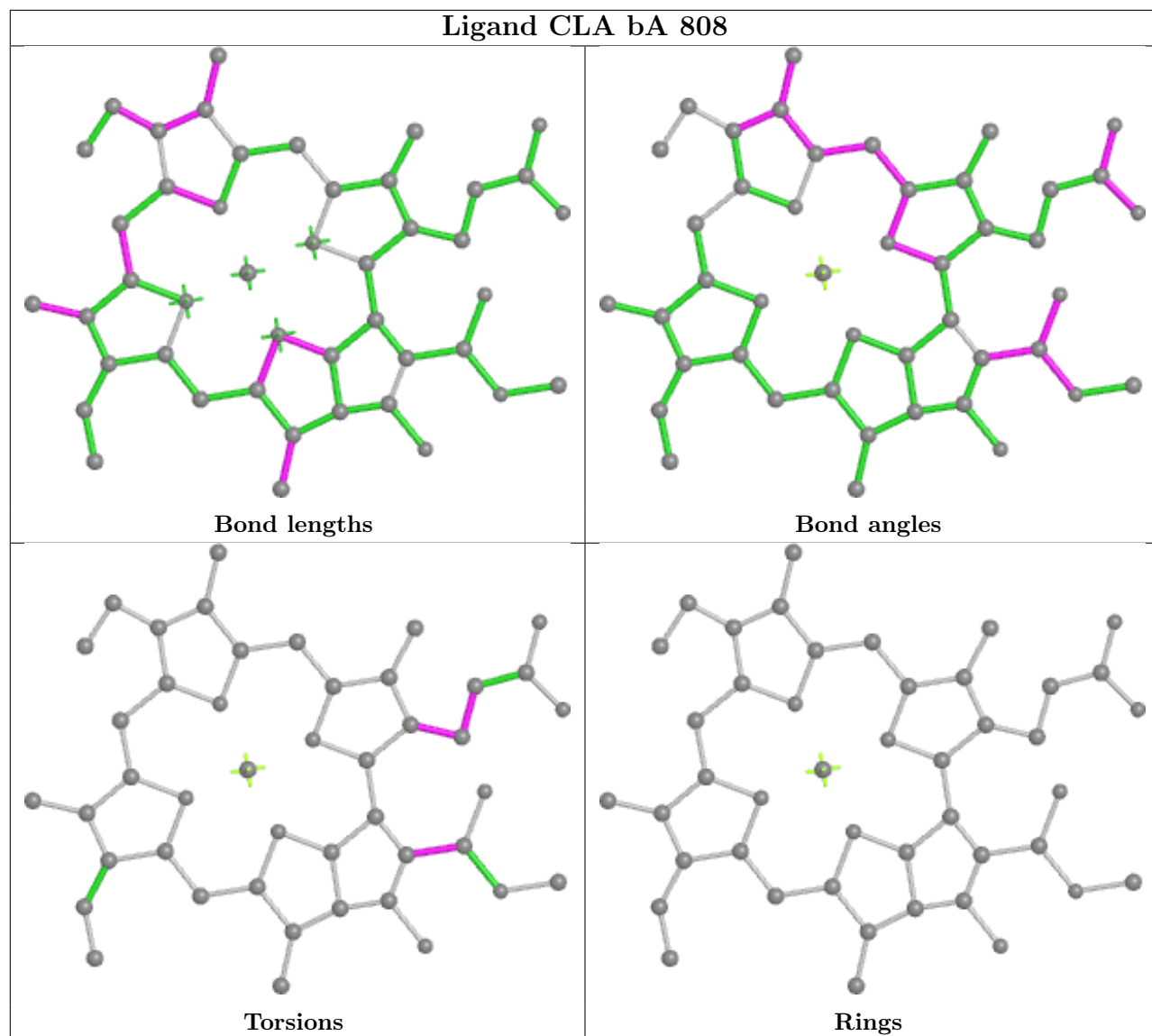
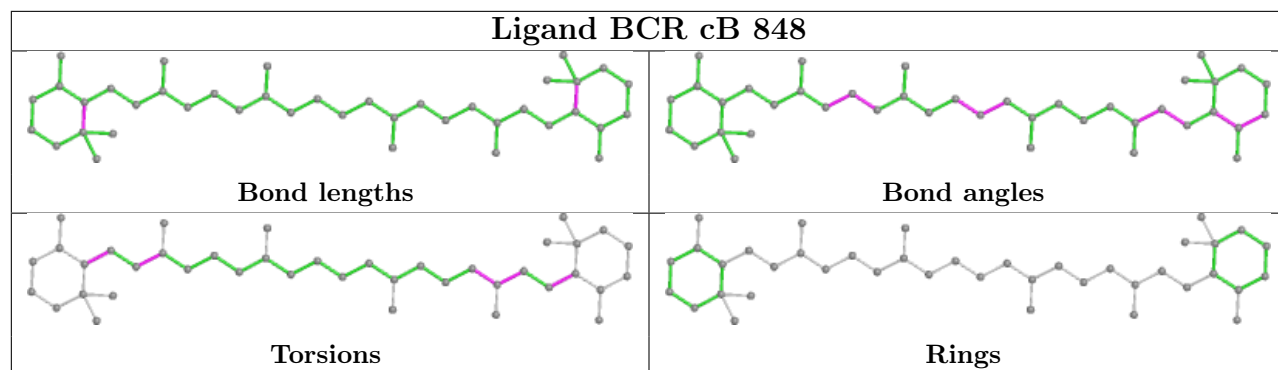
Bond angles



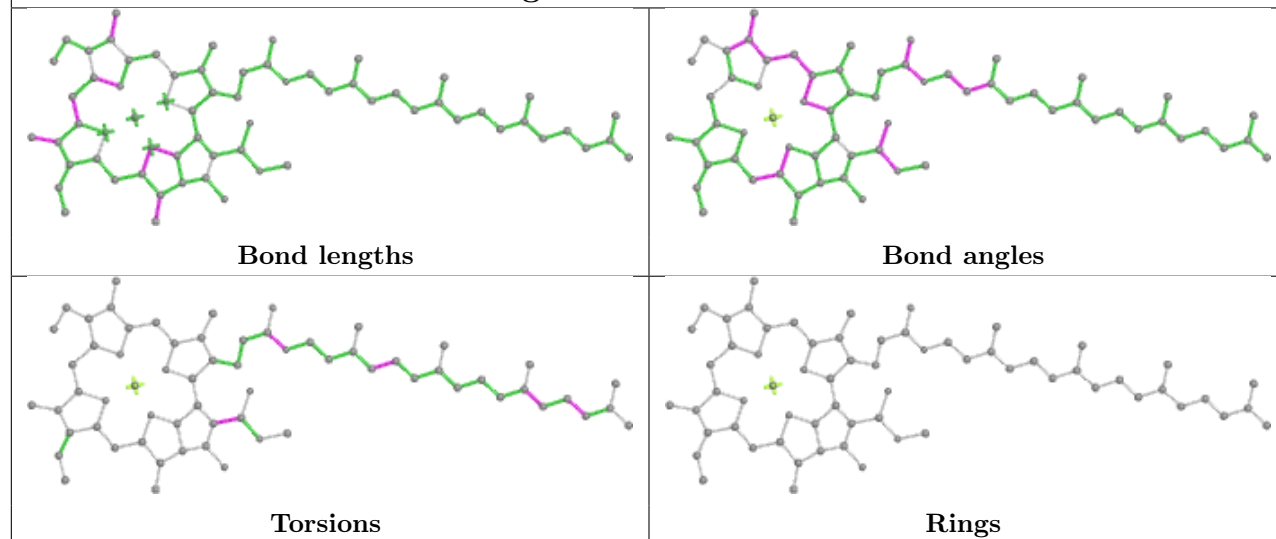
Torsions



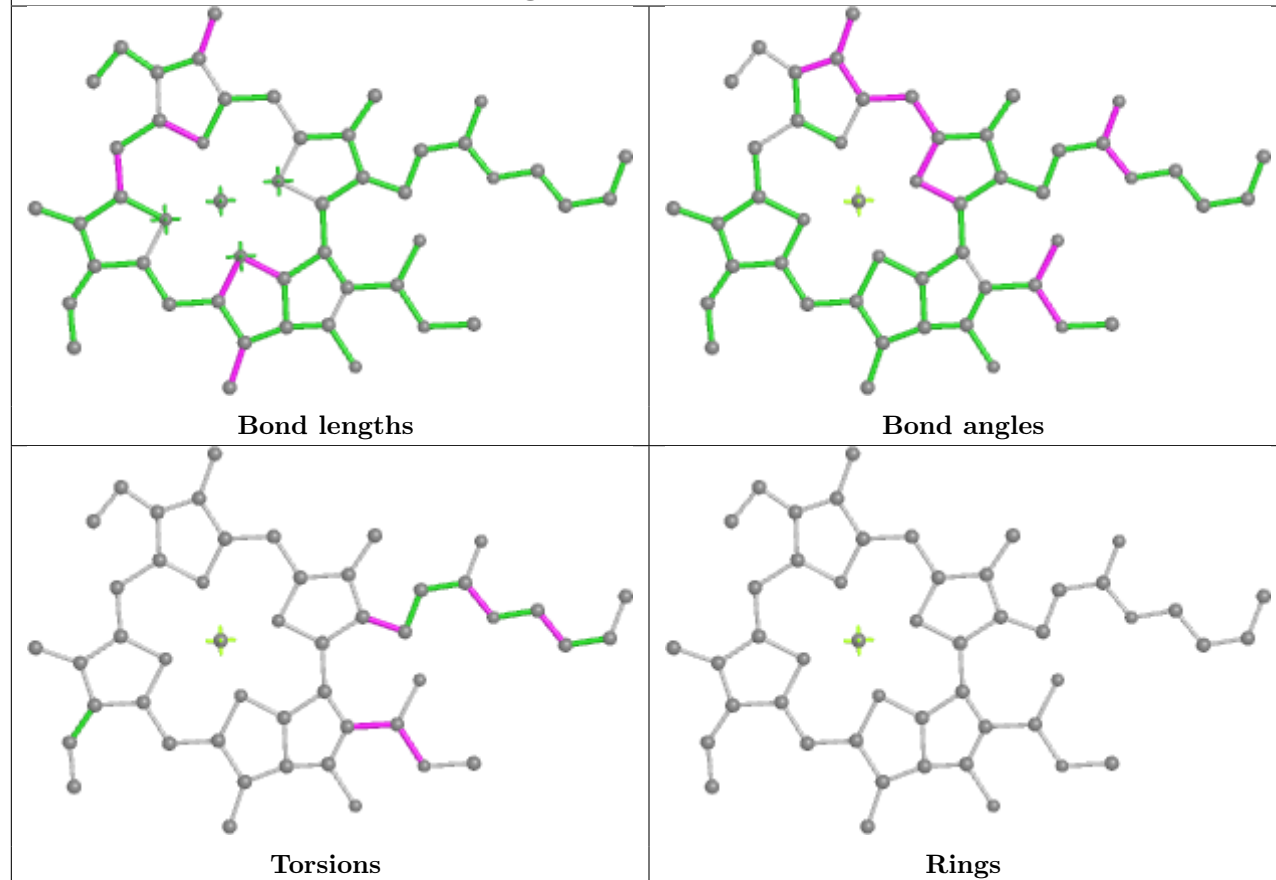
Rings



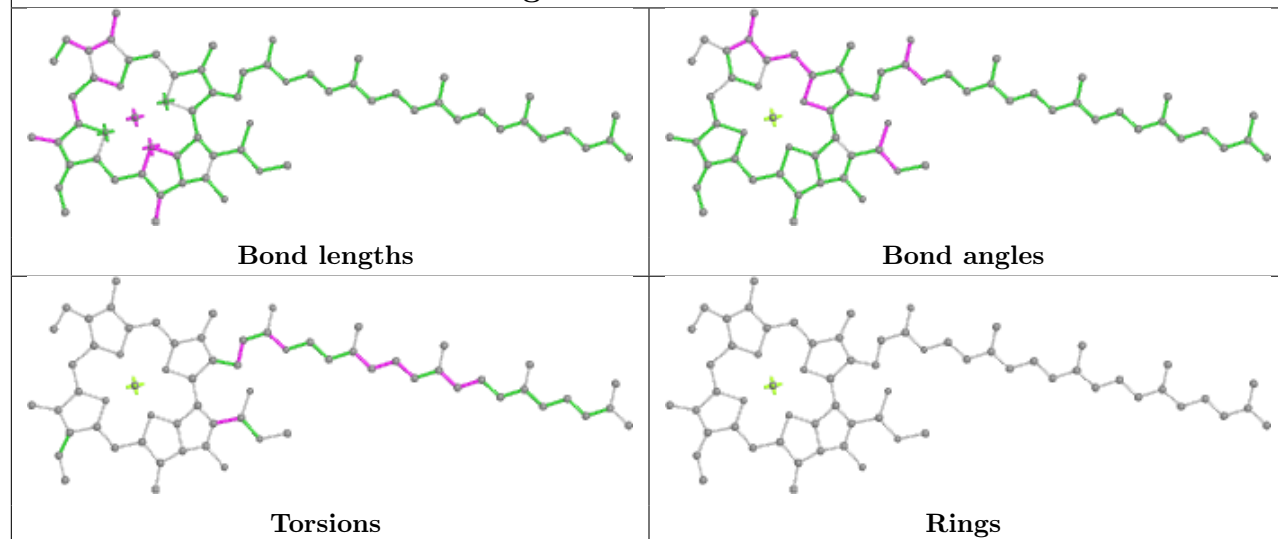
Ligand CLA bB 839



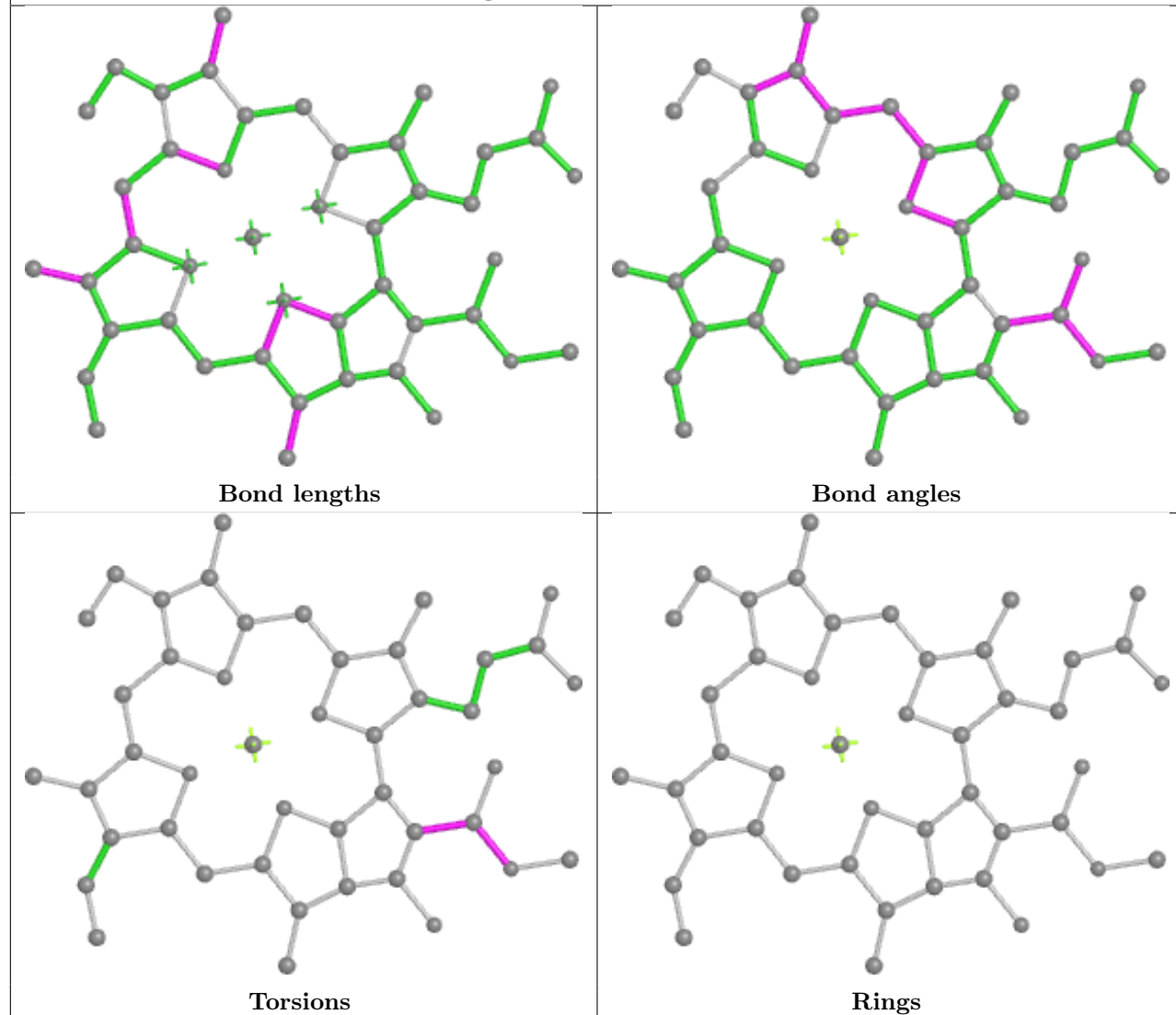
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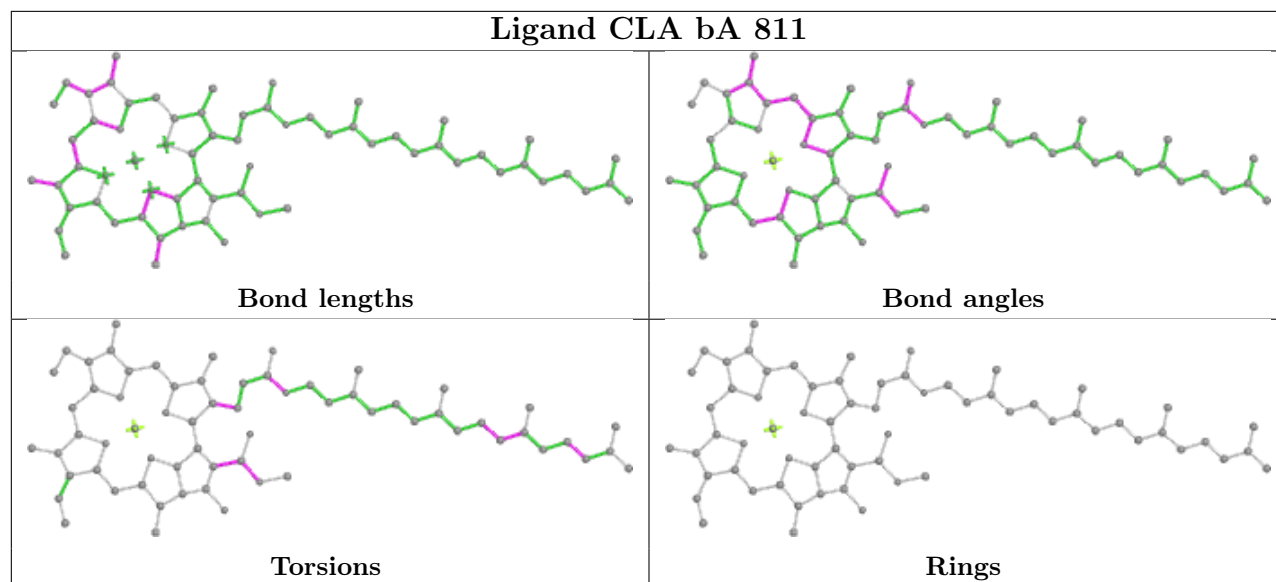
Ligand CLA aA 840



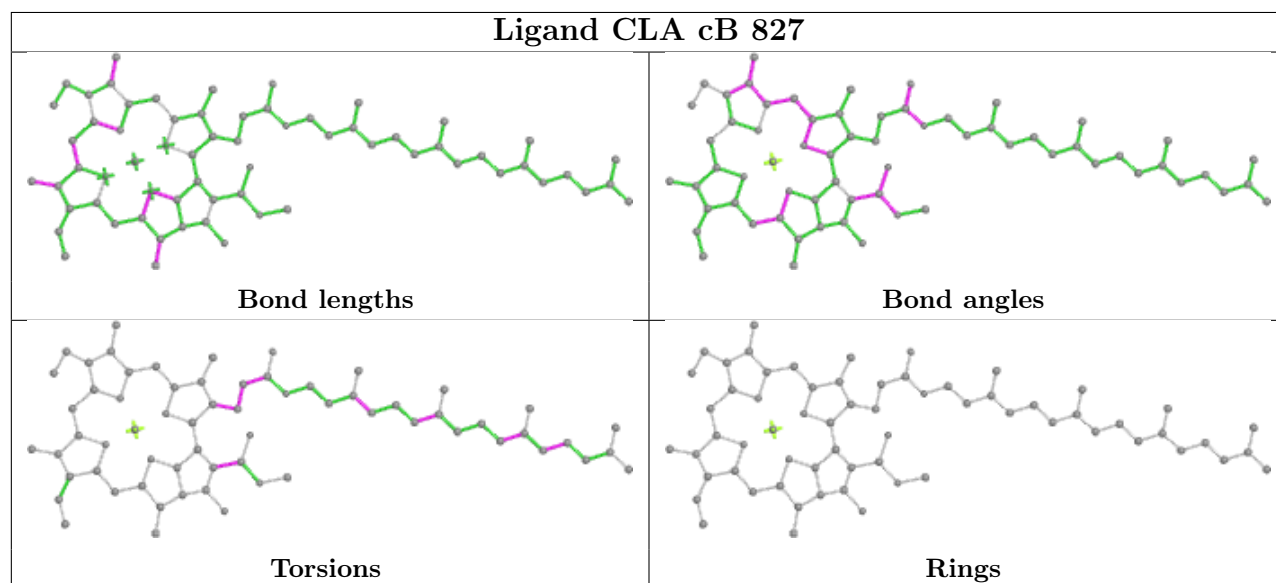
Ligand CLA bB 835

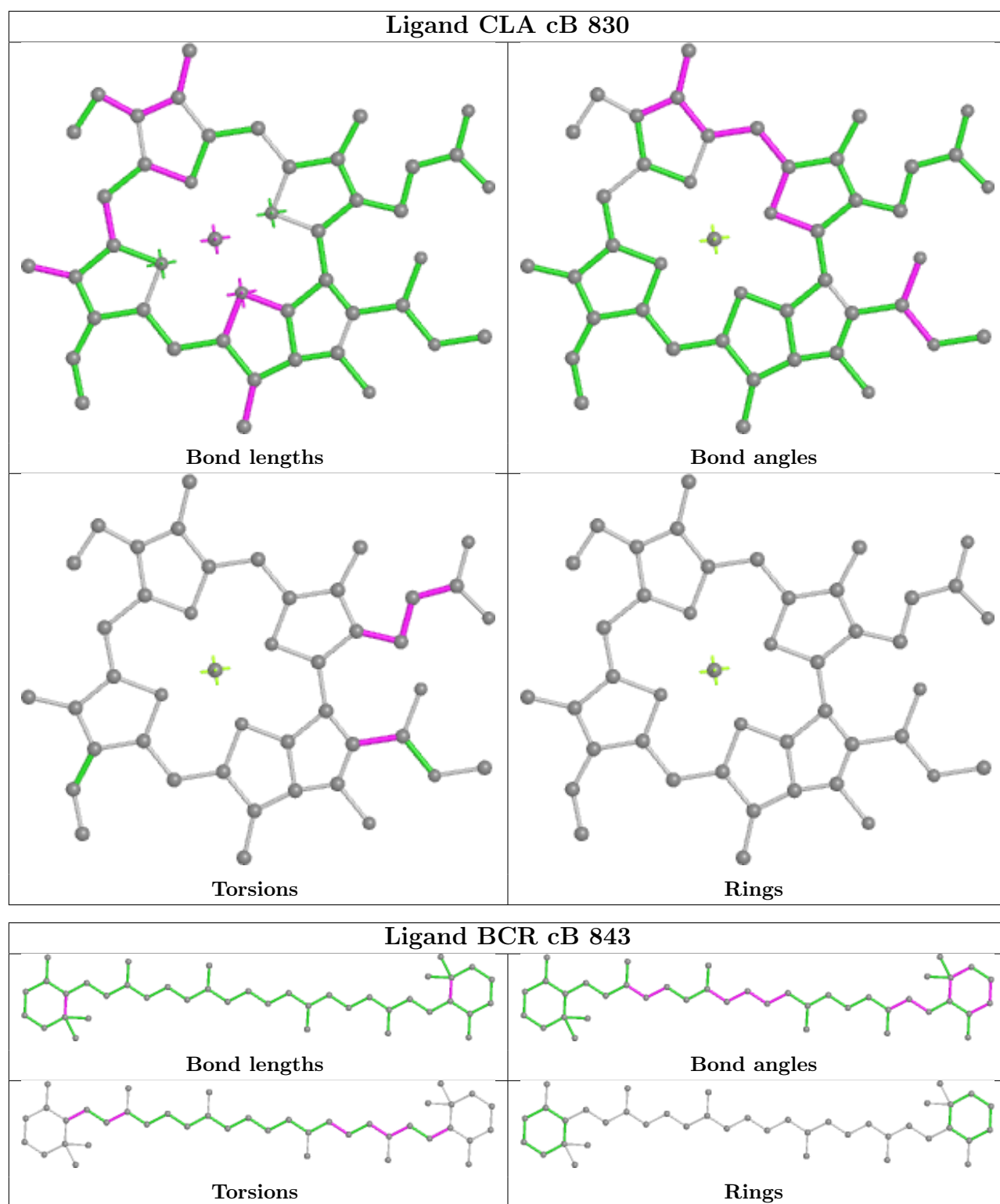


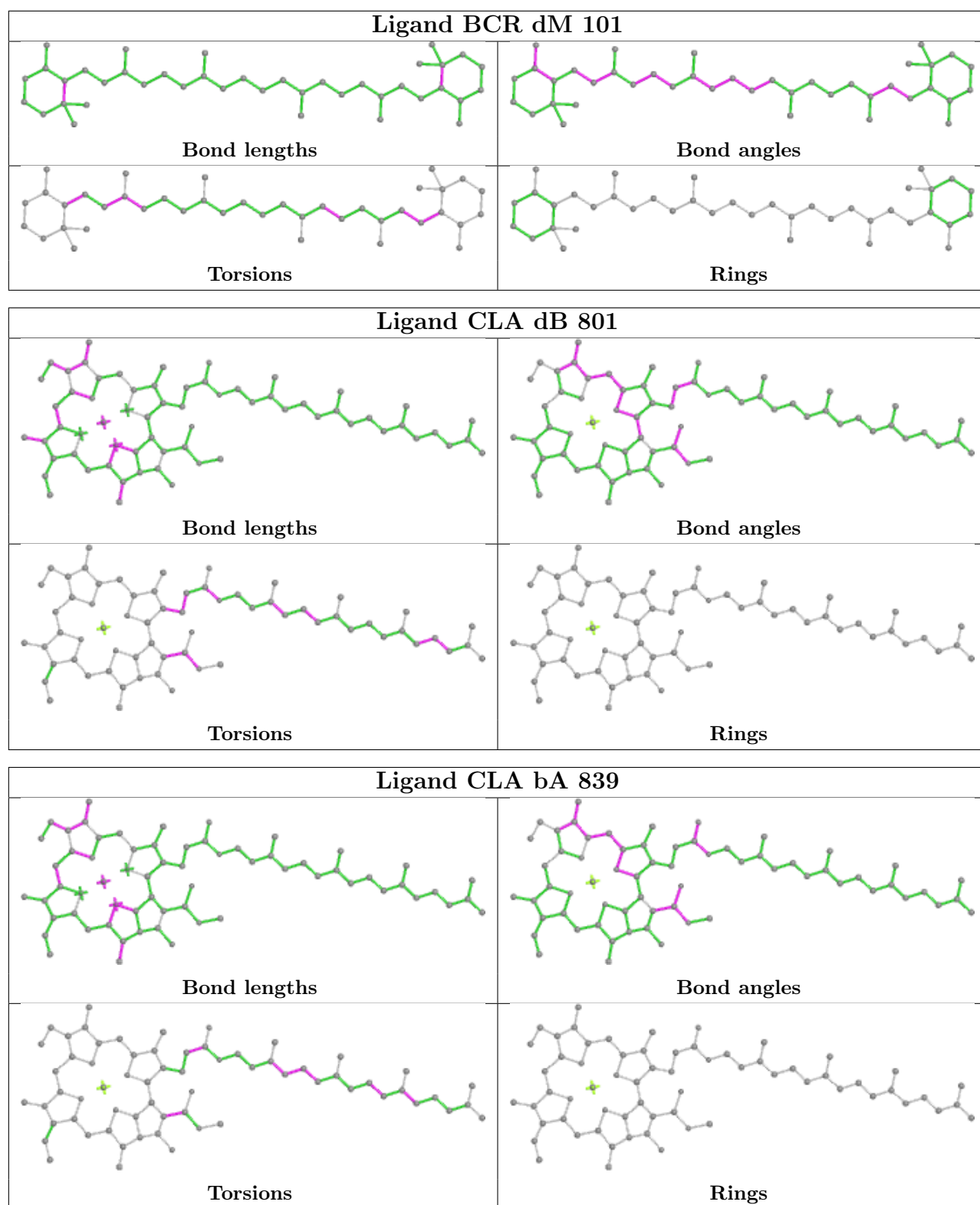
Ligand CLA bA 811

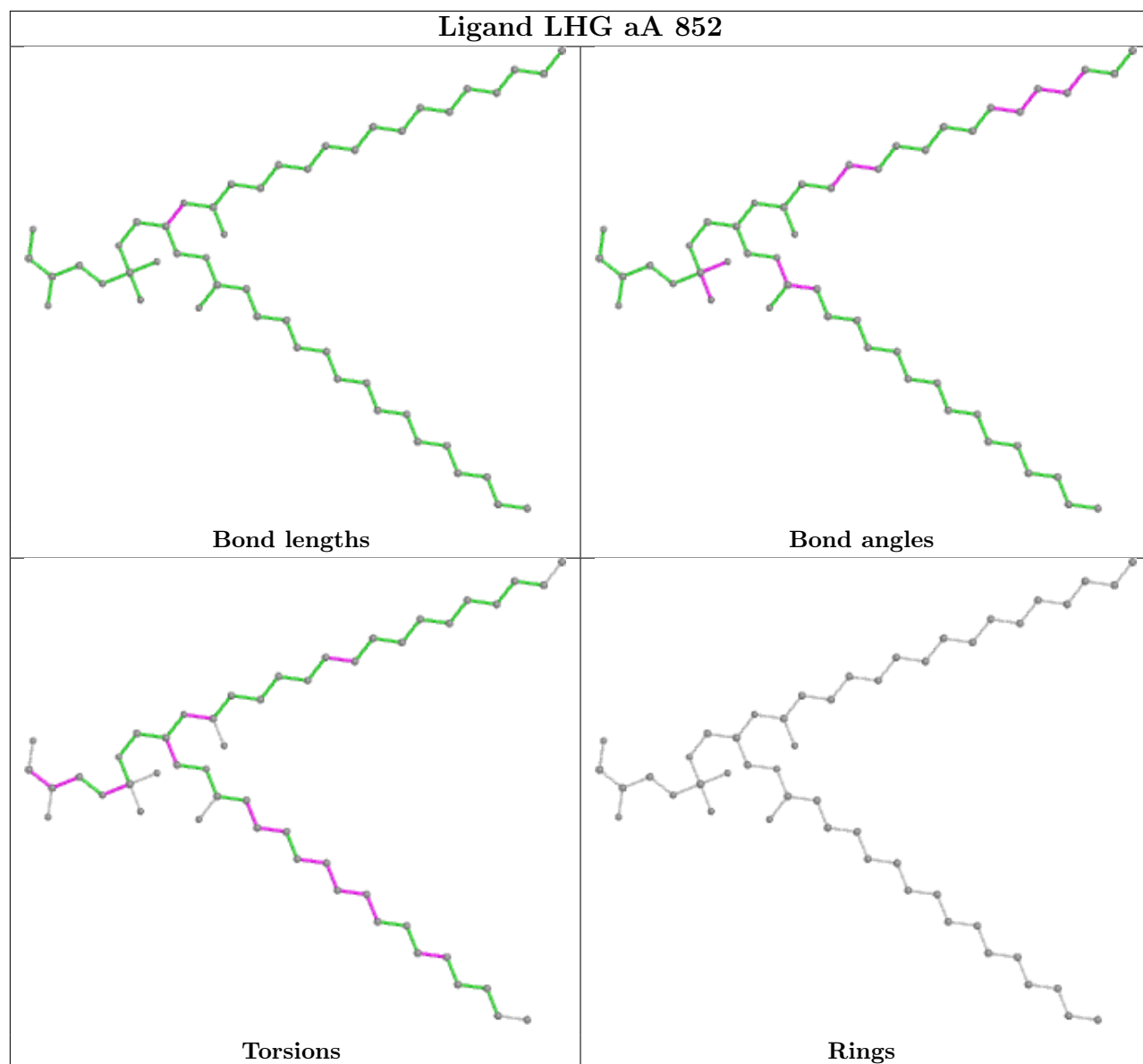
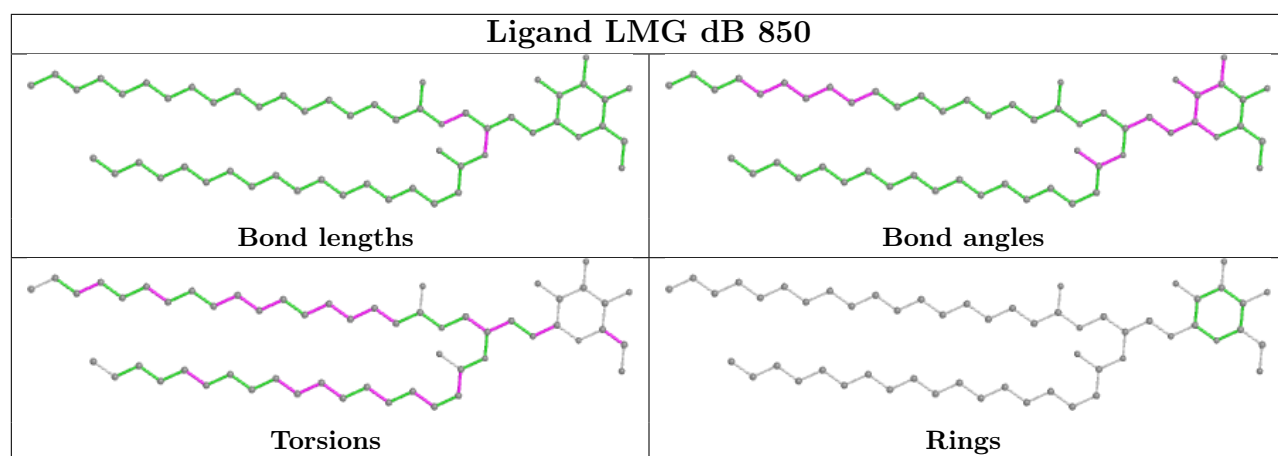


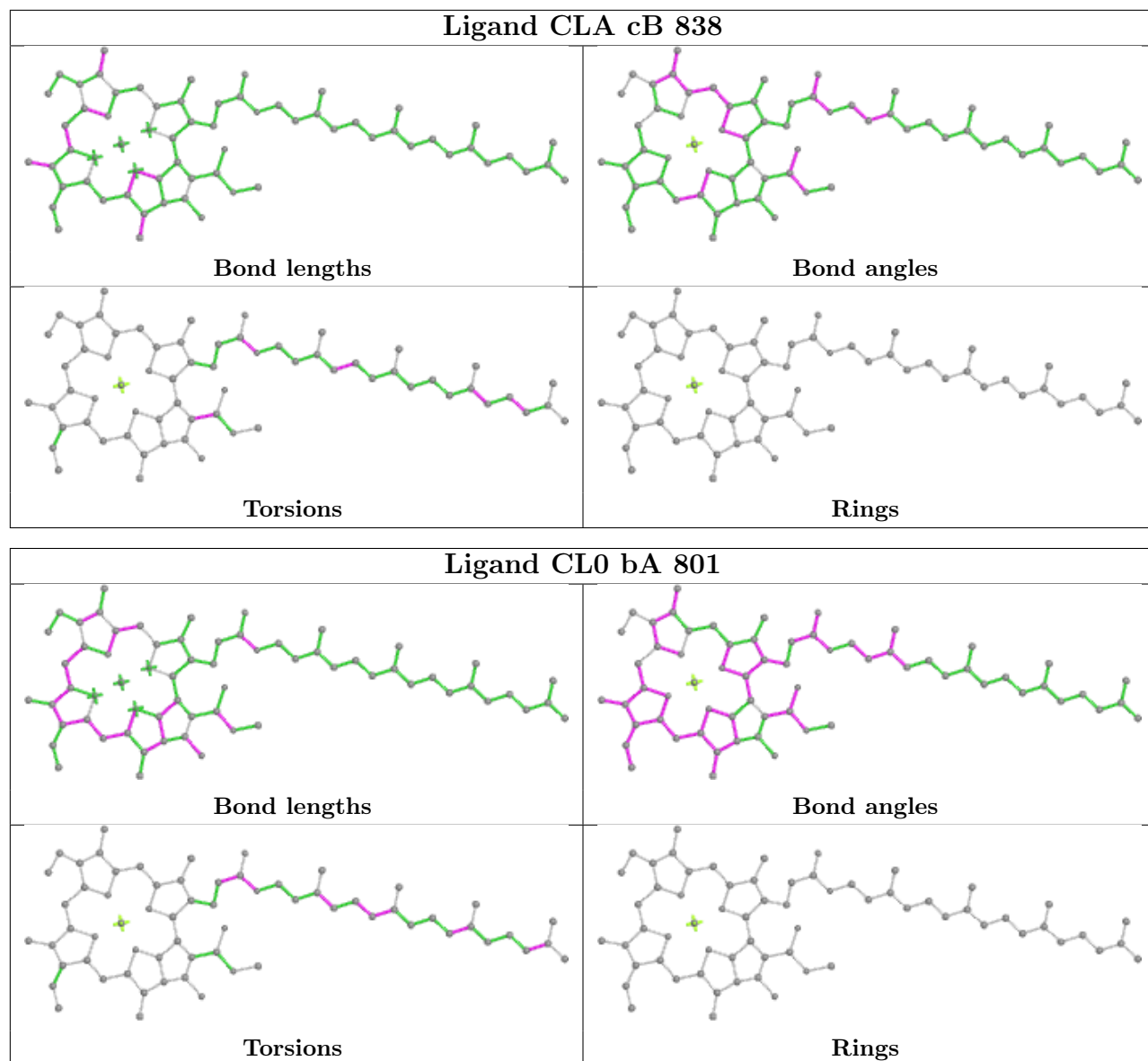
Ligand CLA cB 827

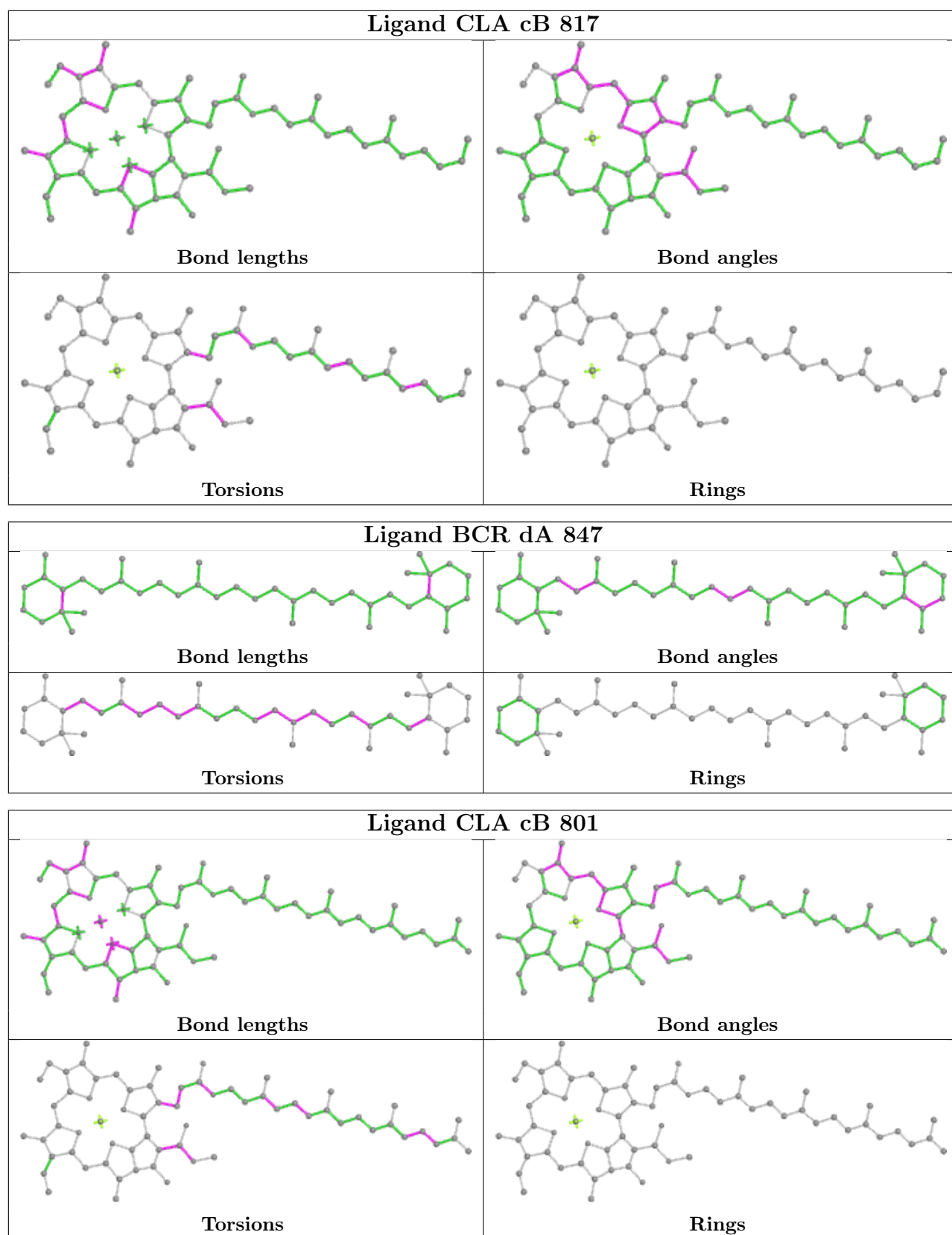


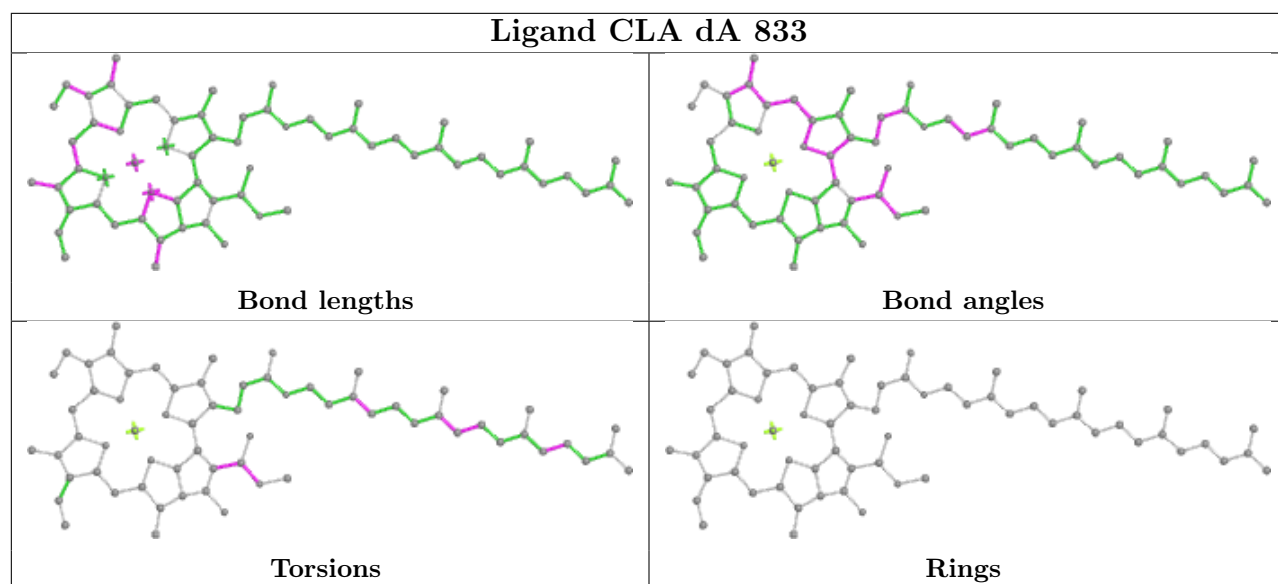
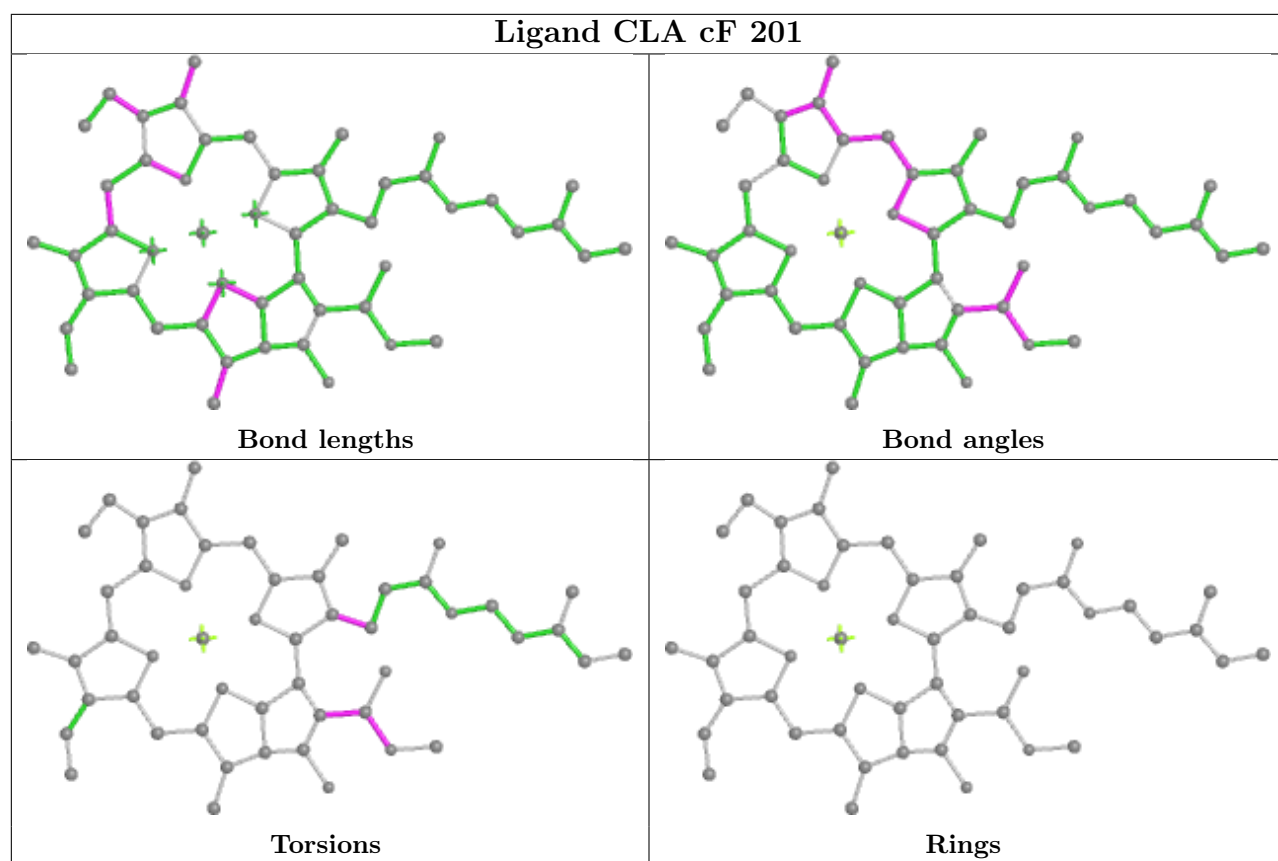


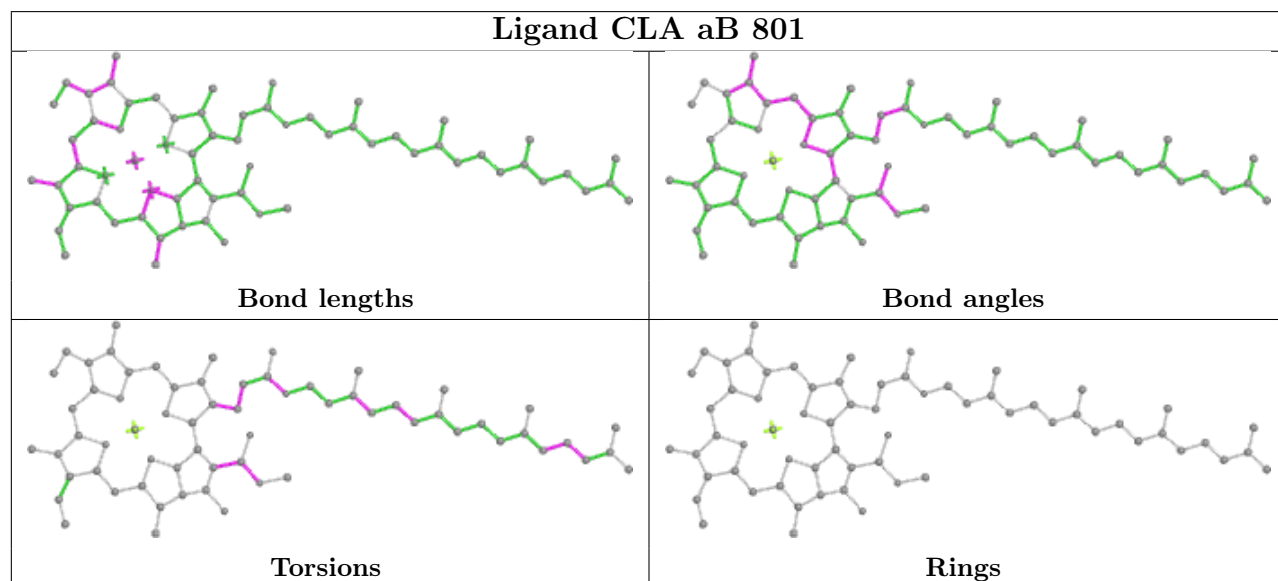
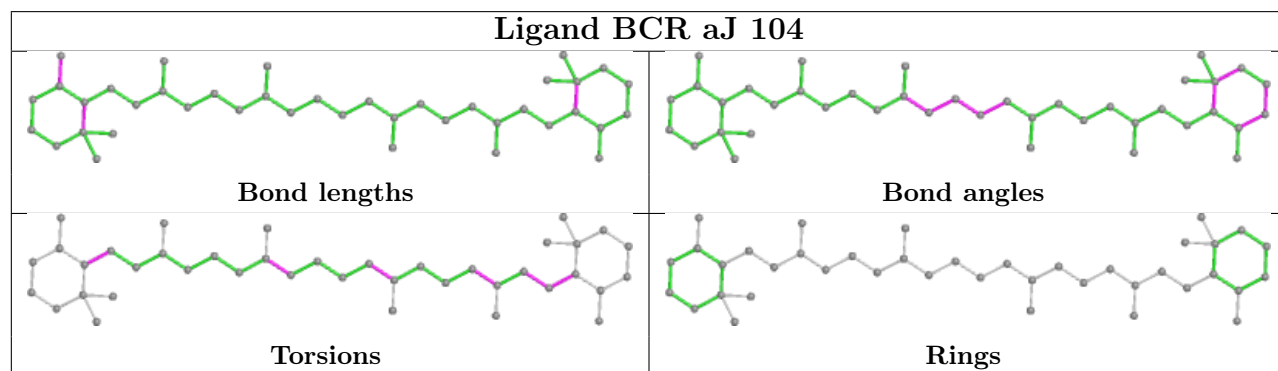
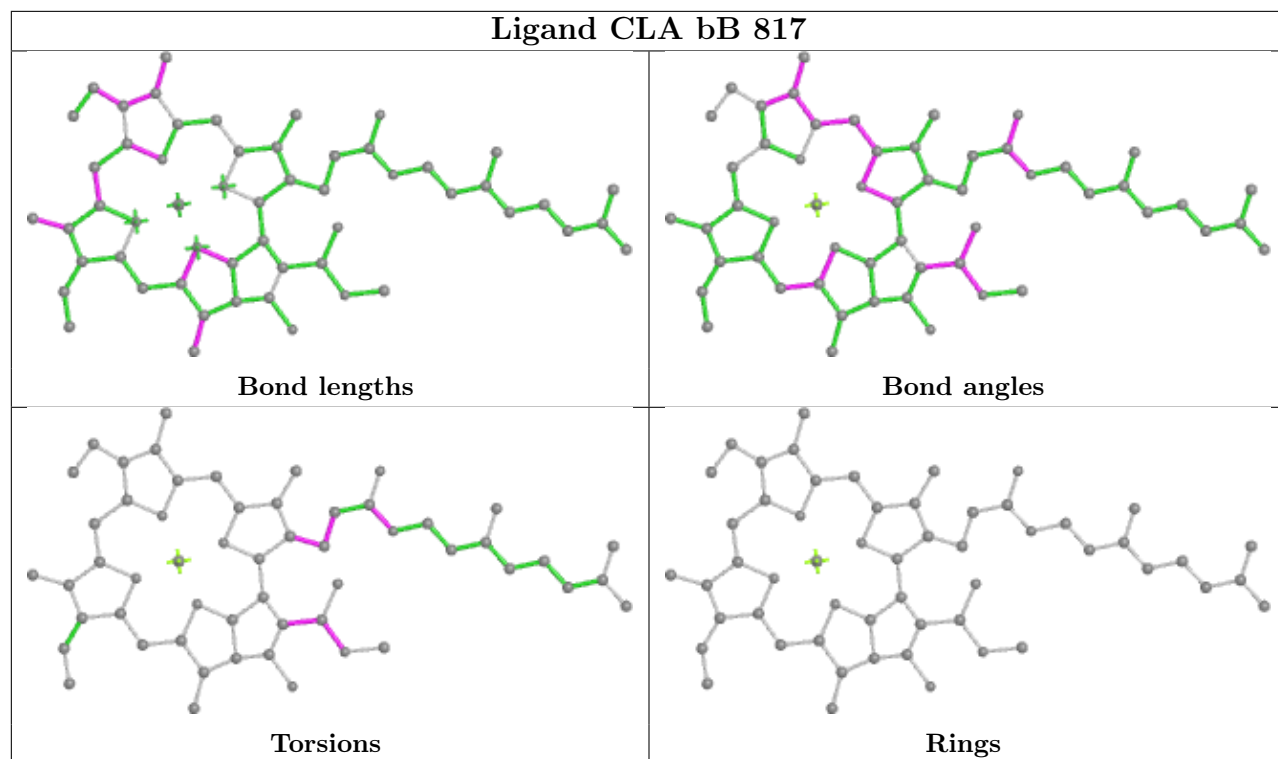




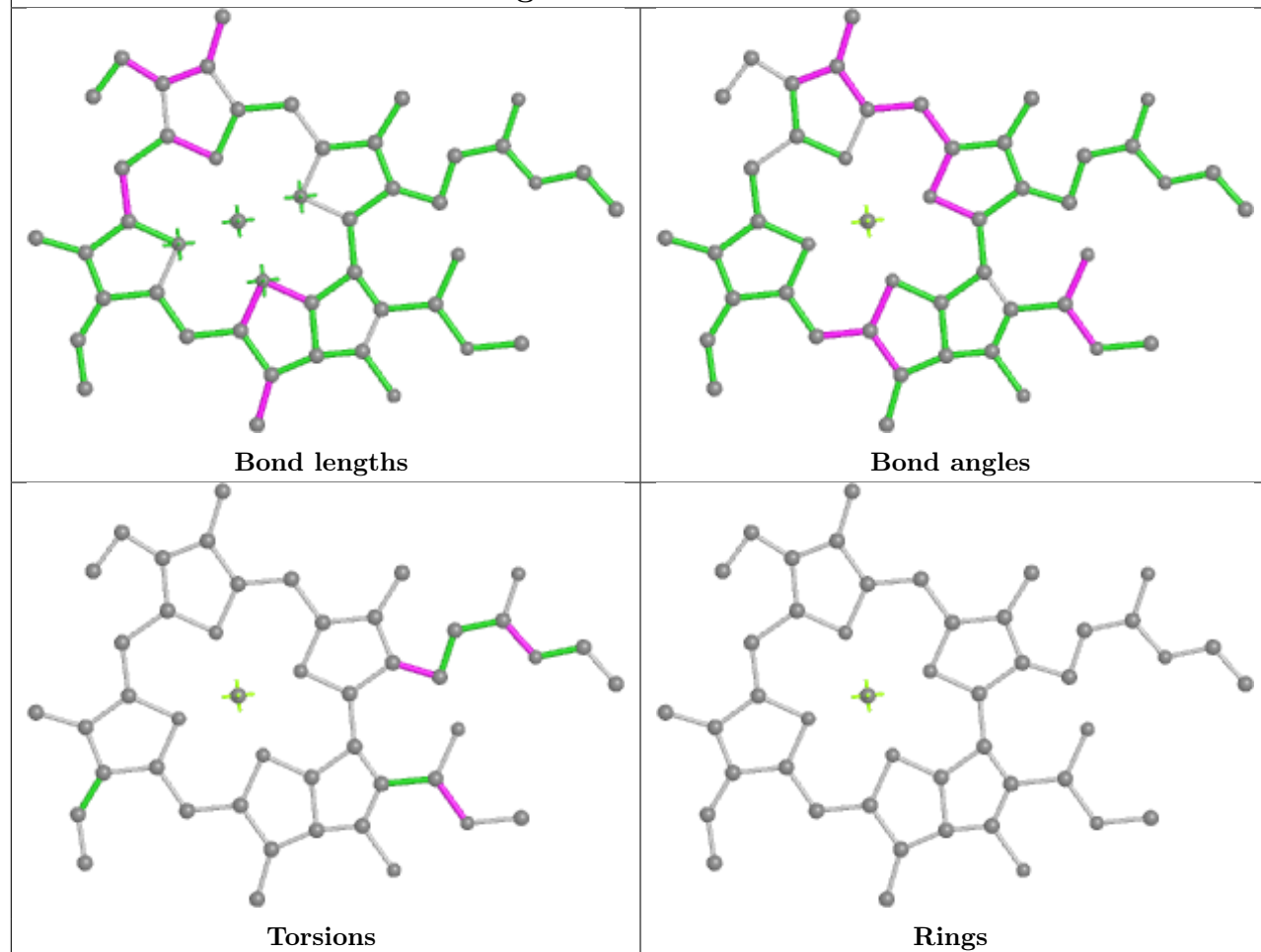




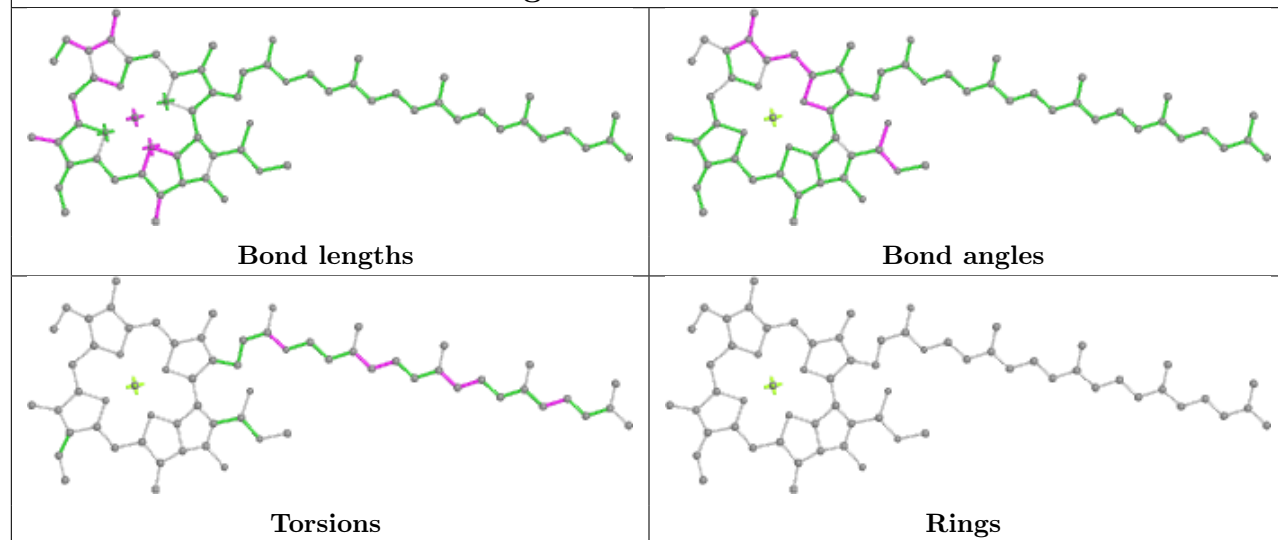


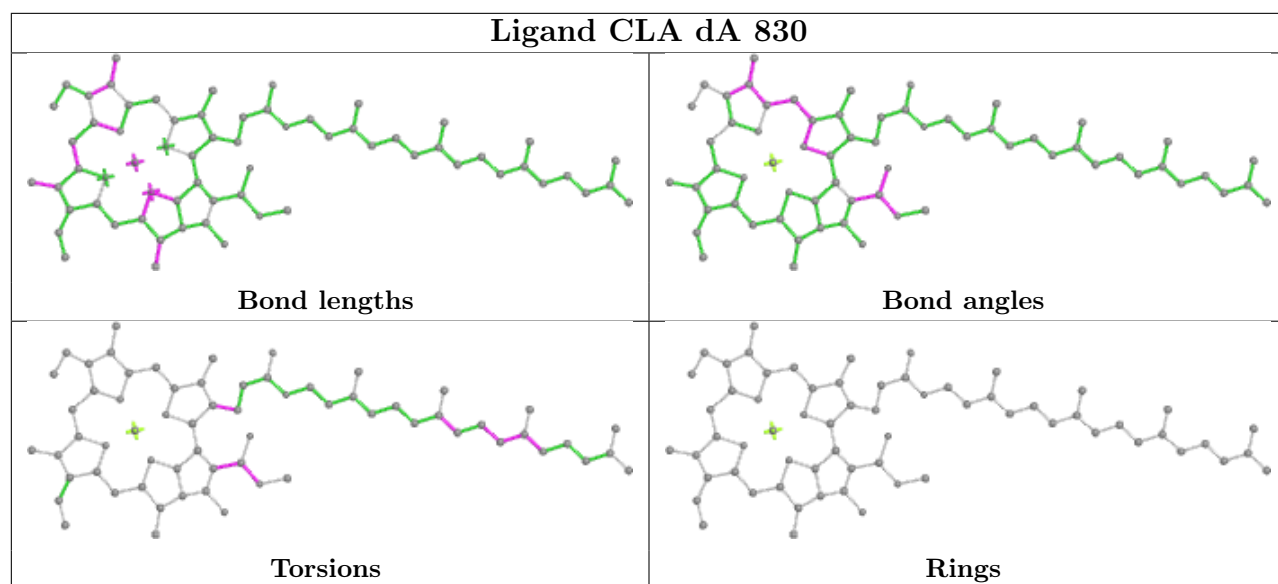
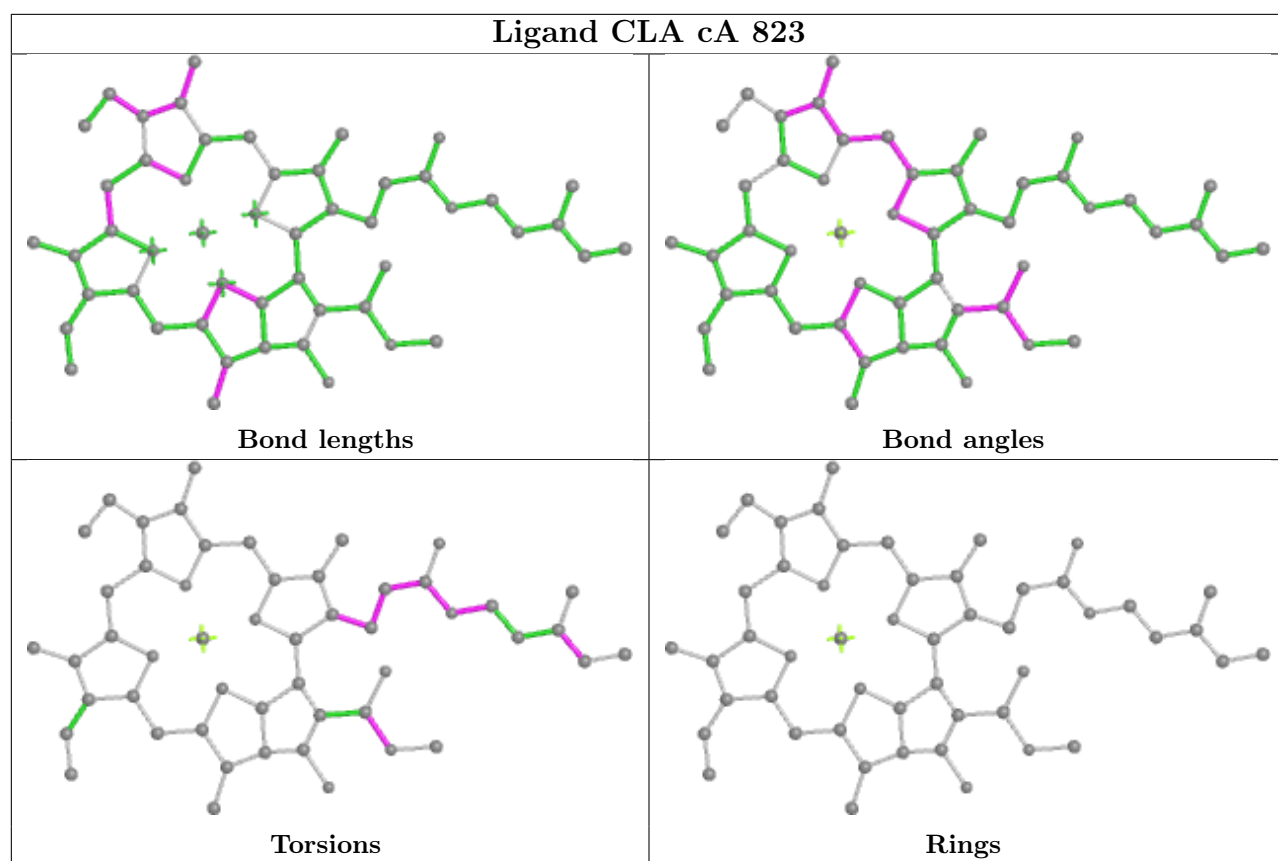


Ligand CLA cA 824

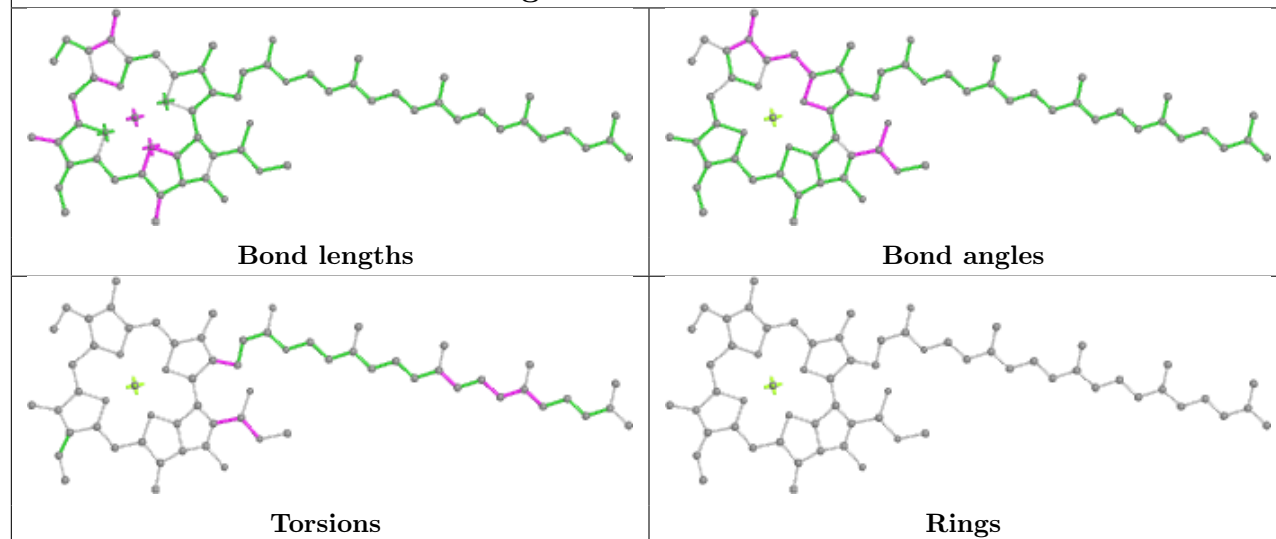


Ligand CLA aB 810

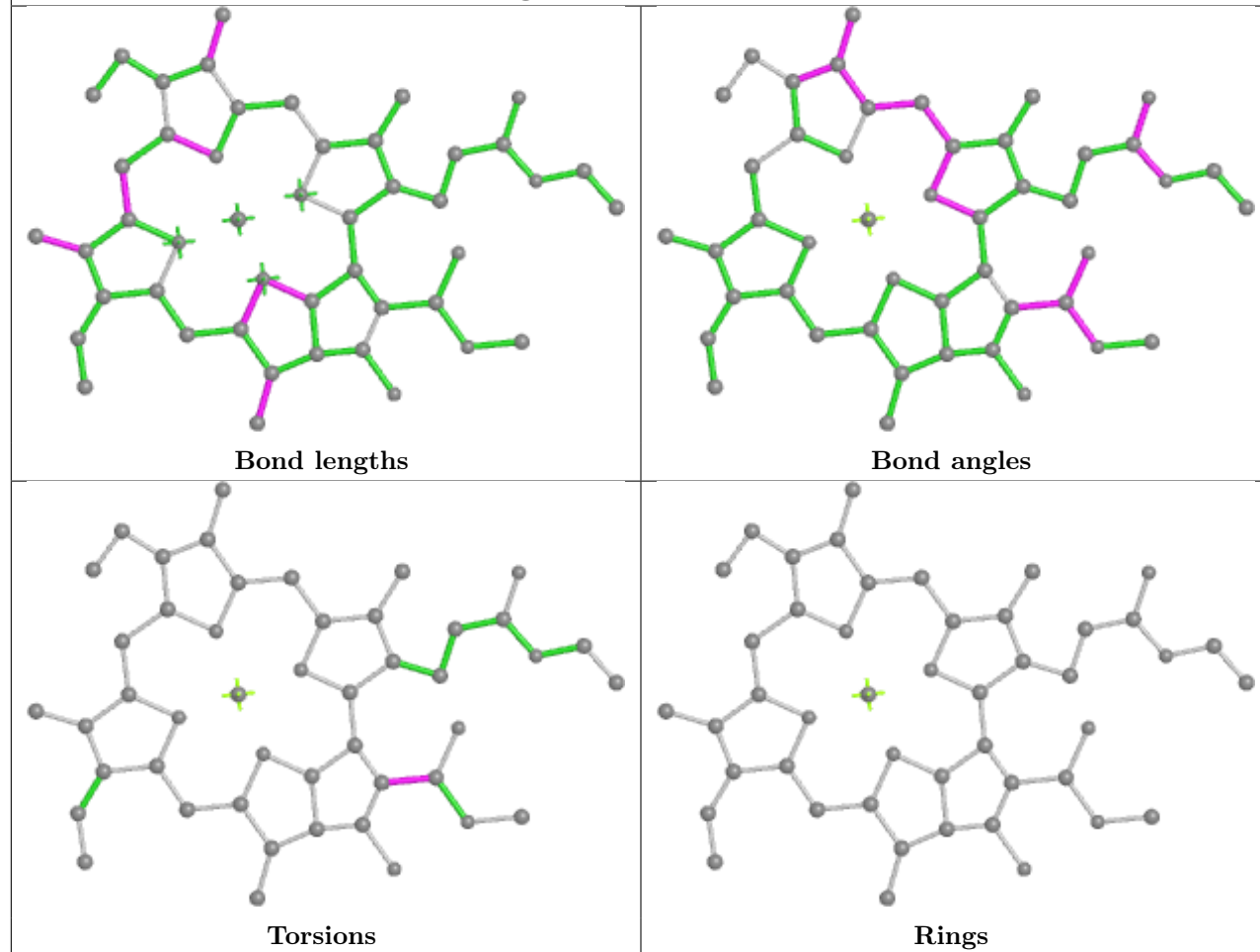




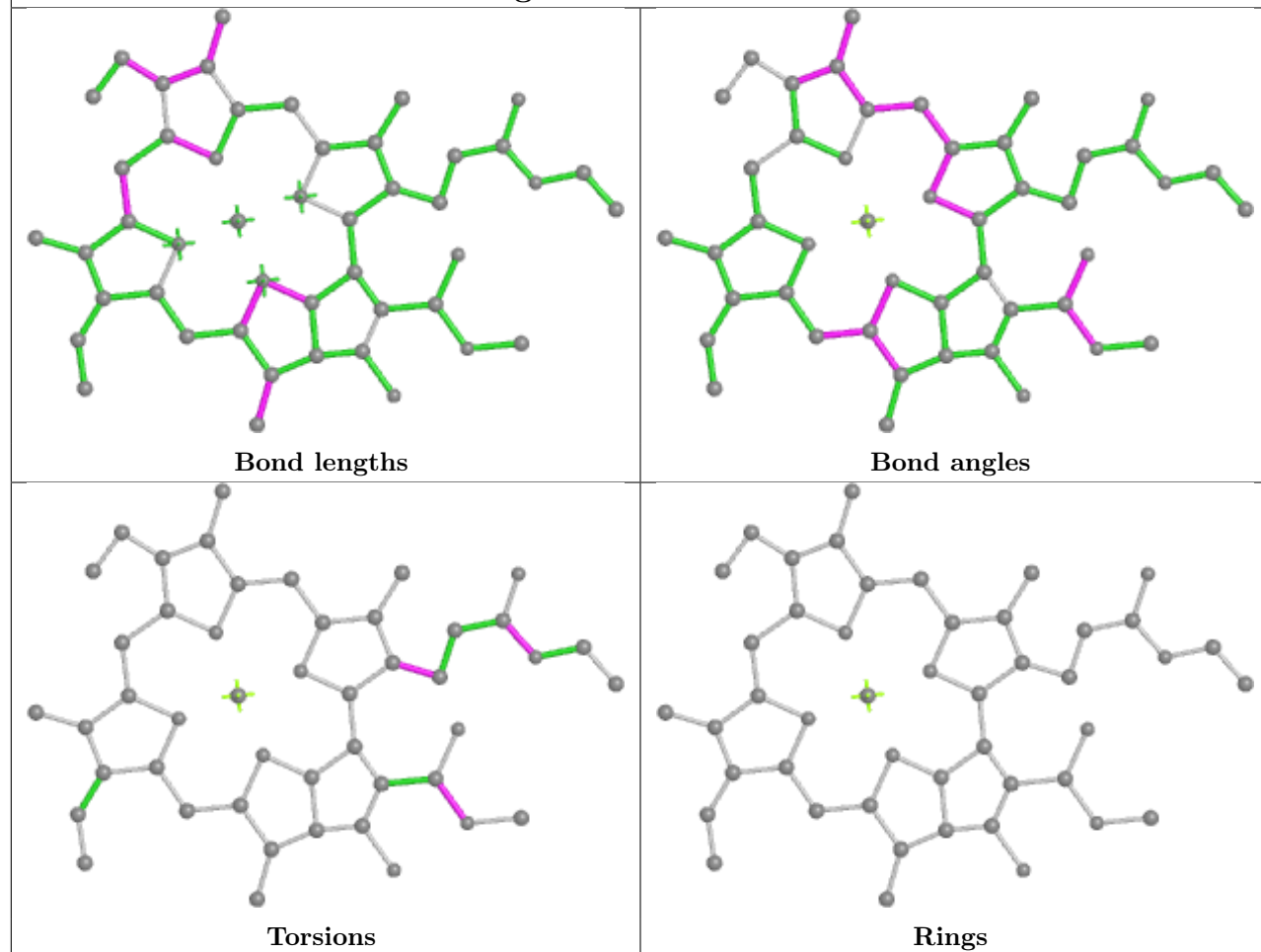
Ligand CLA bA 830



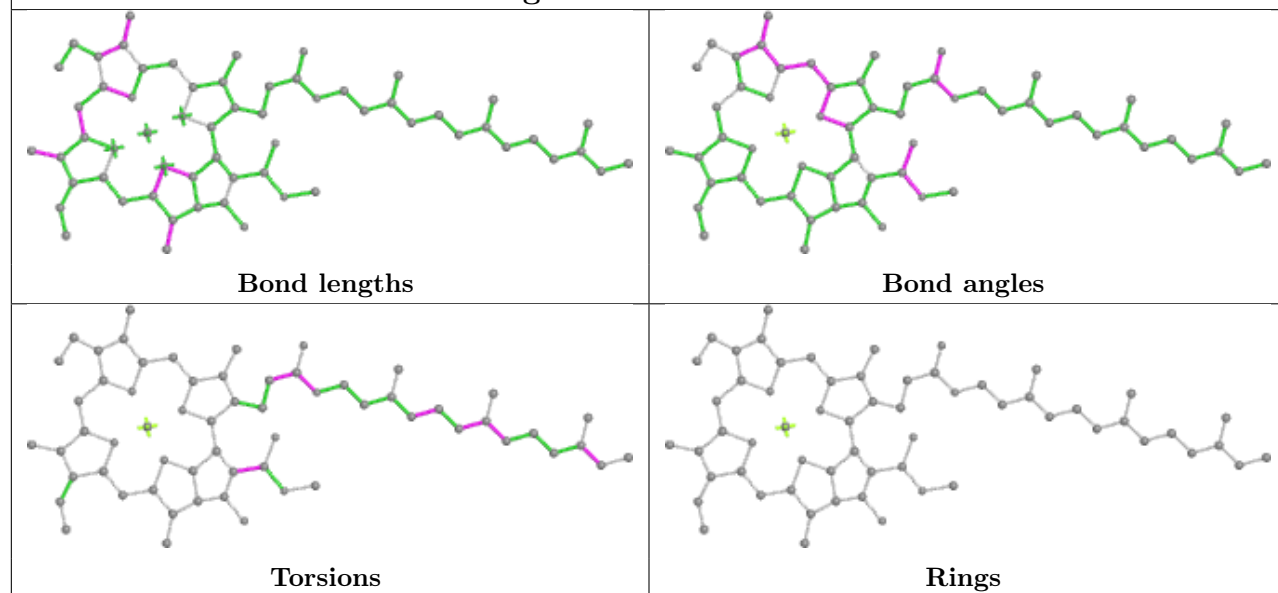
Ligand CLA aB 839

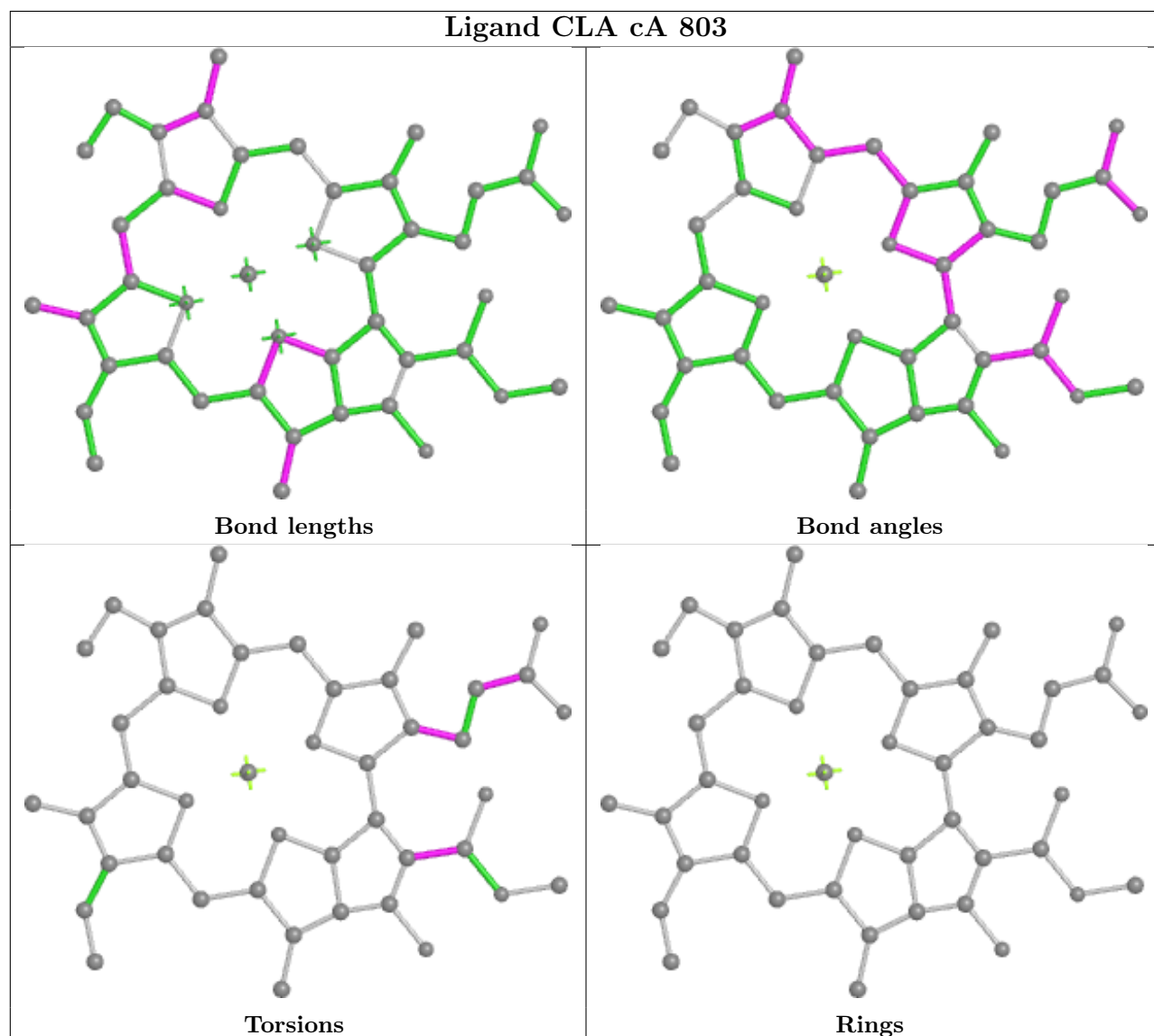
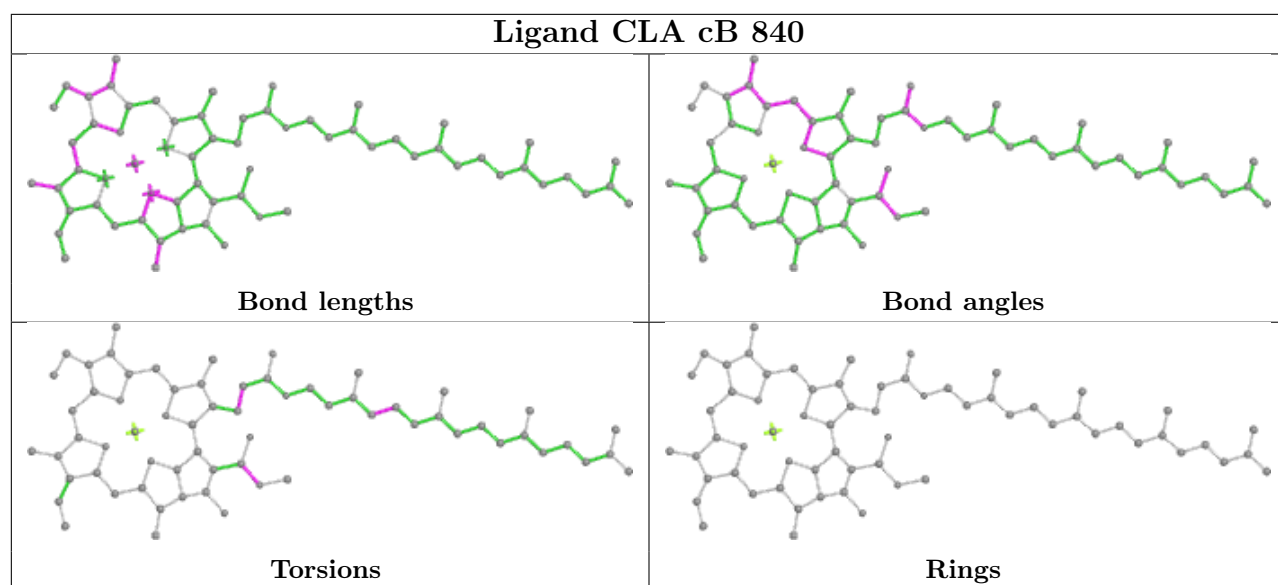


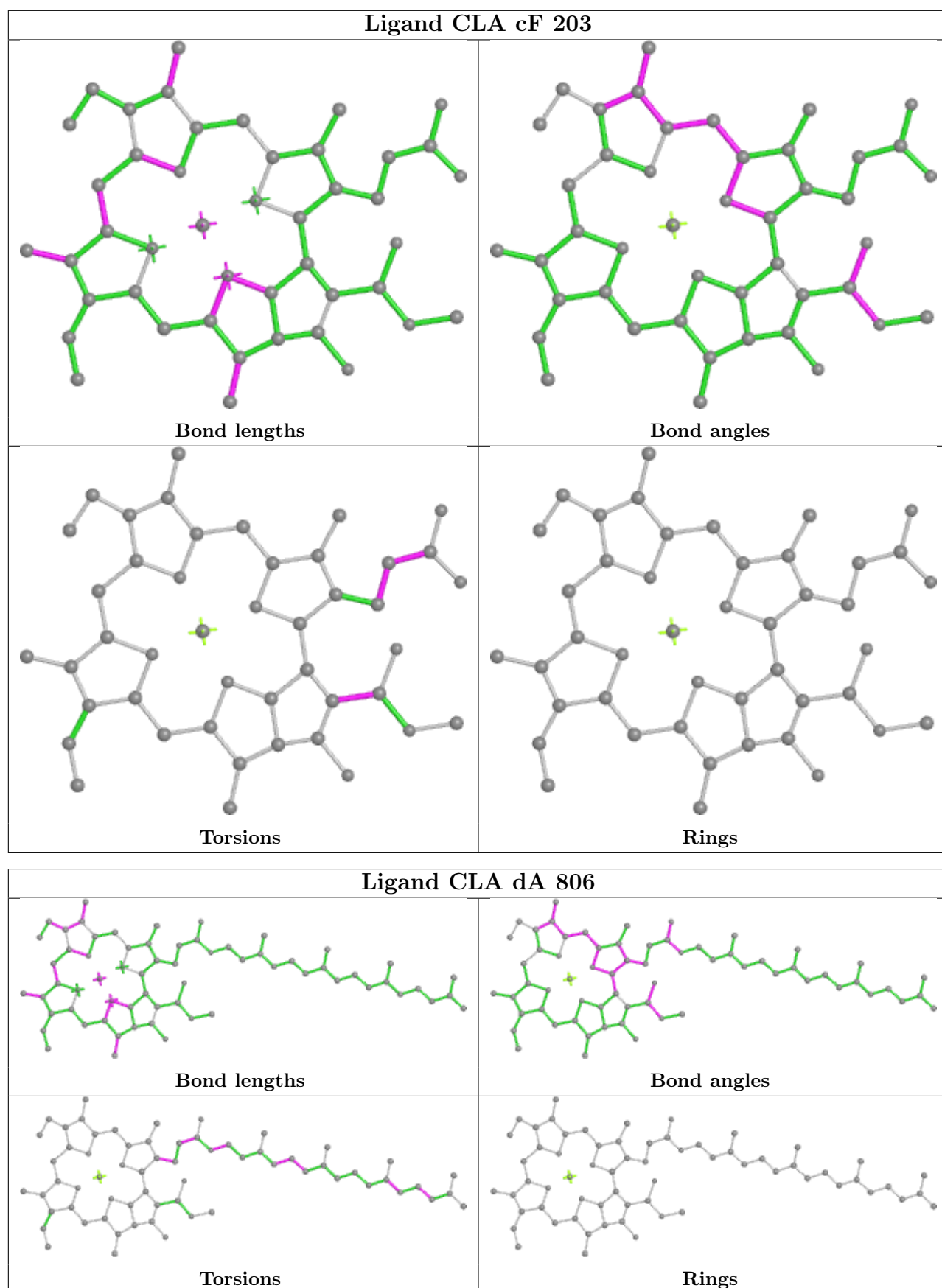
Ligand CLA dA 824

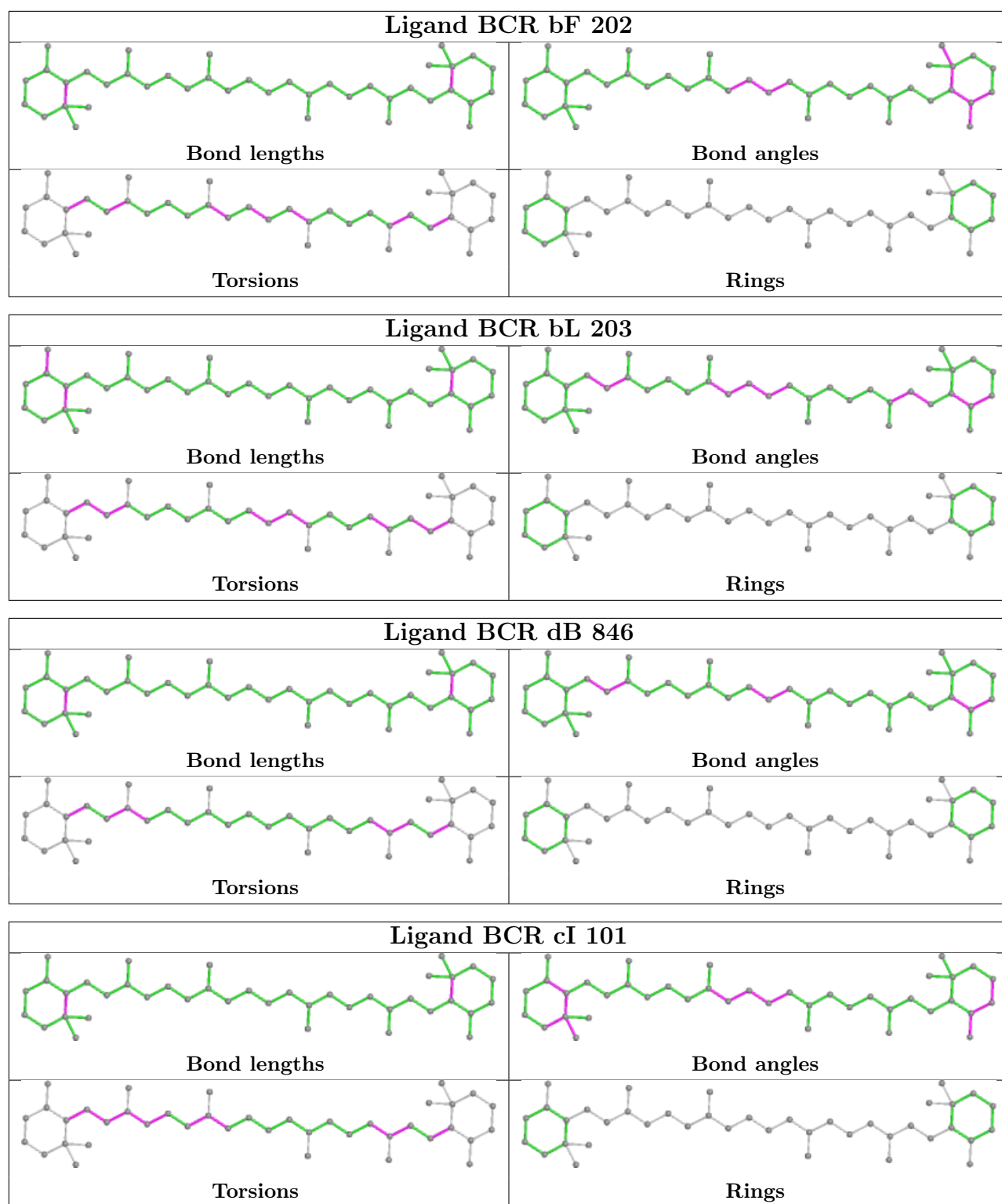


Ligand CLA aA 820

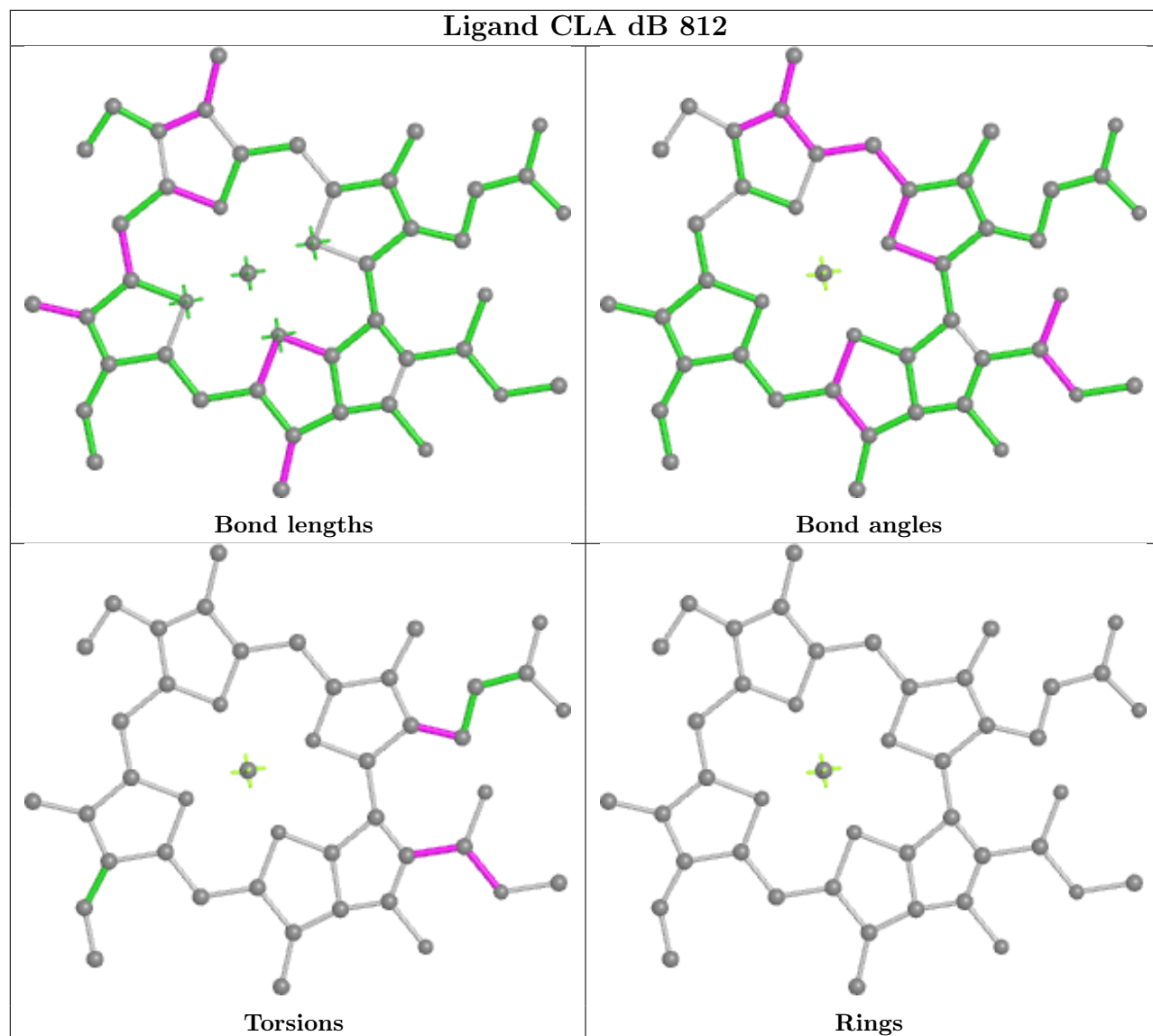


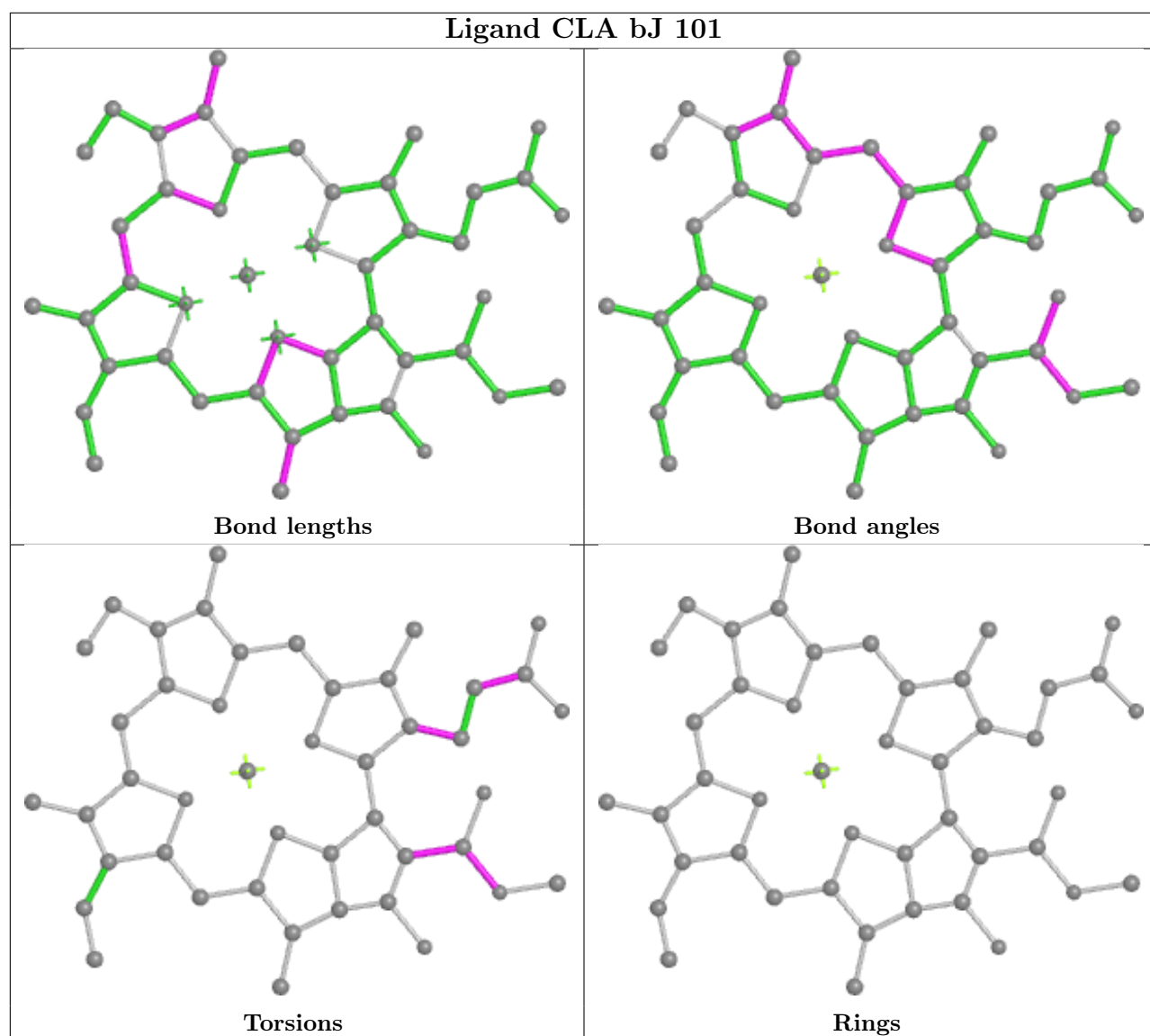




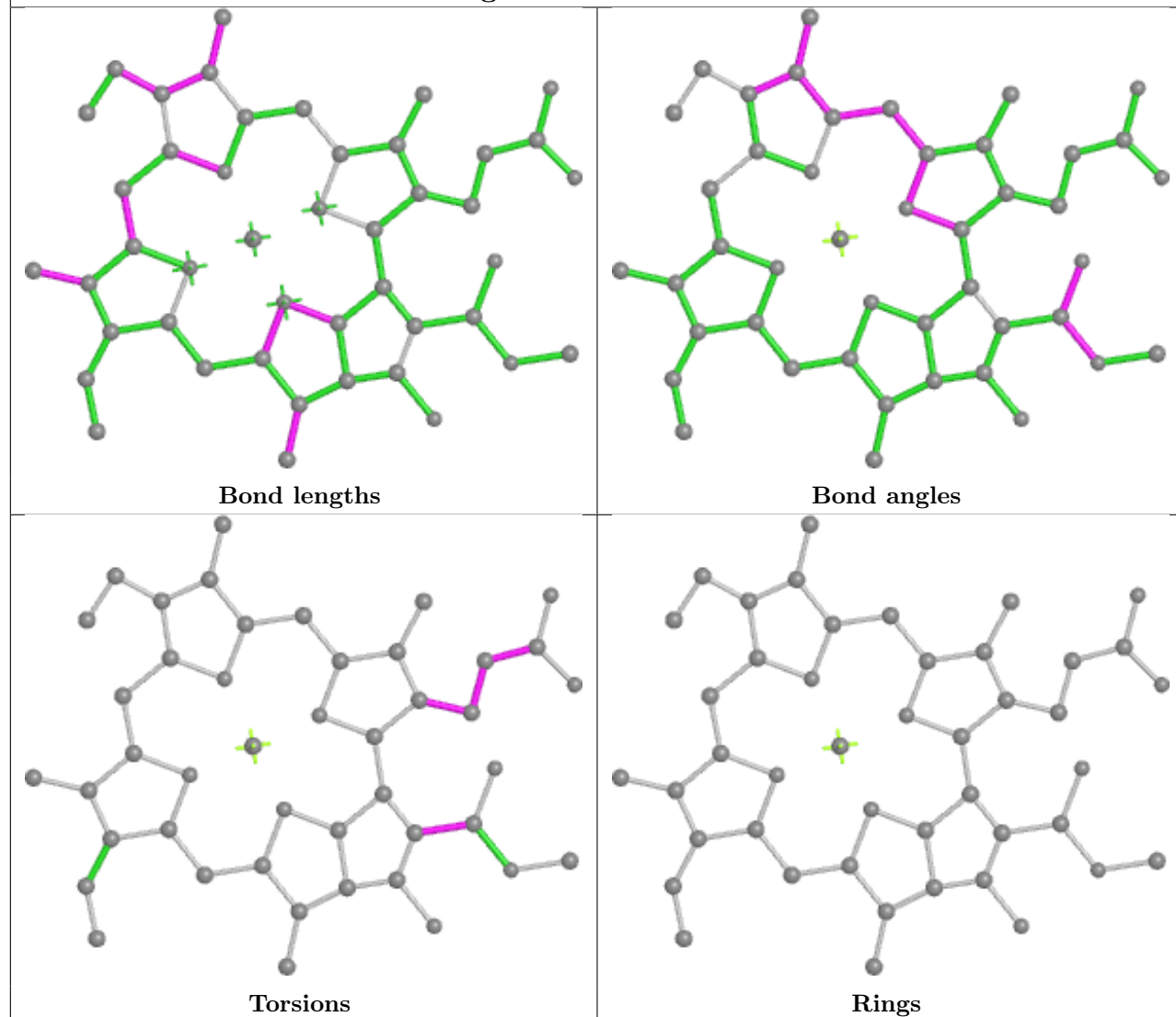


Ligand CLA dB 812

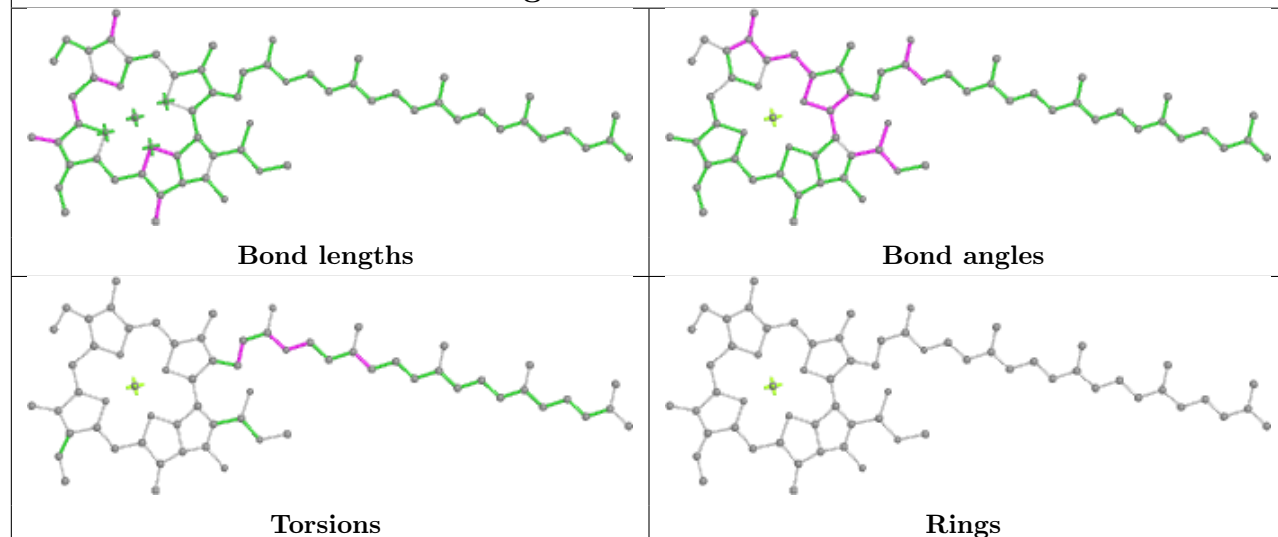




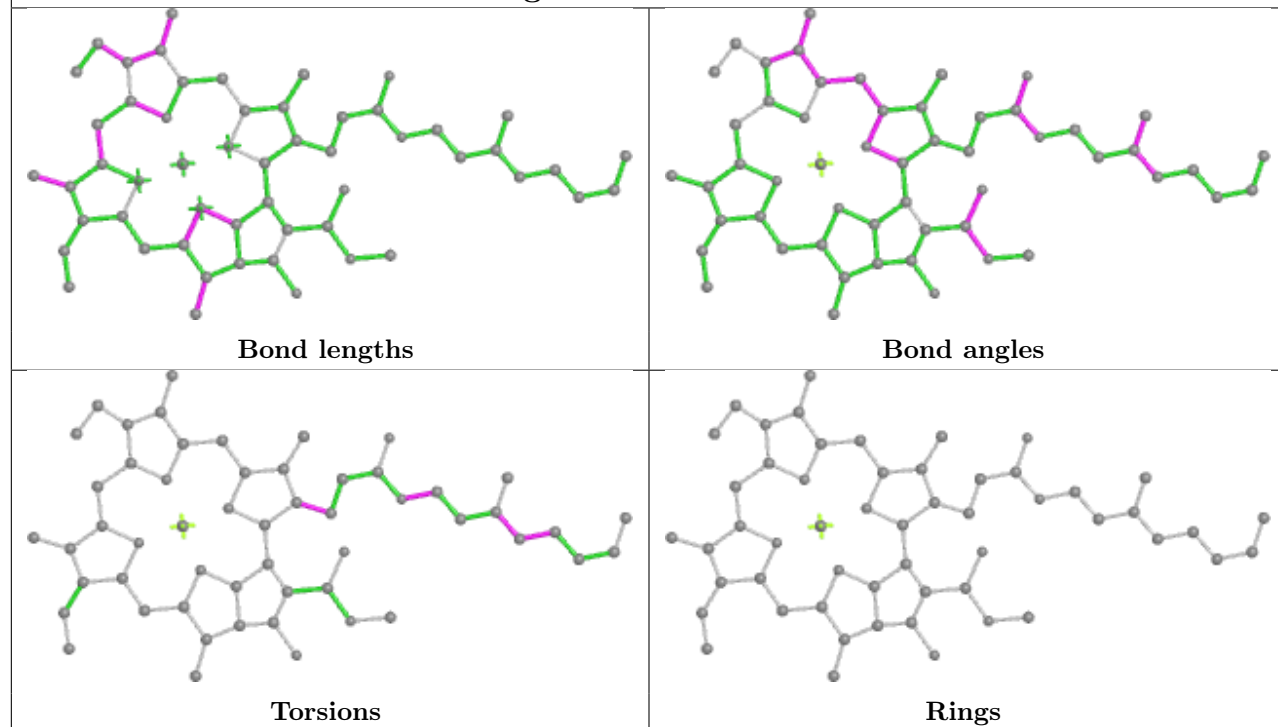
Ligand CLA dB 831



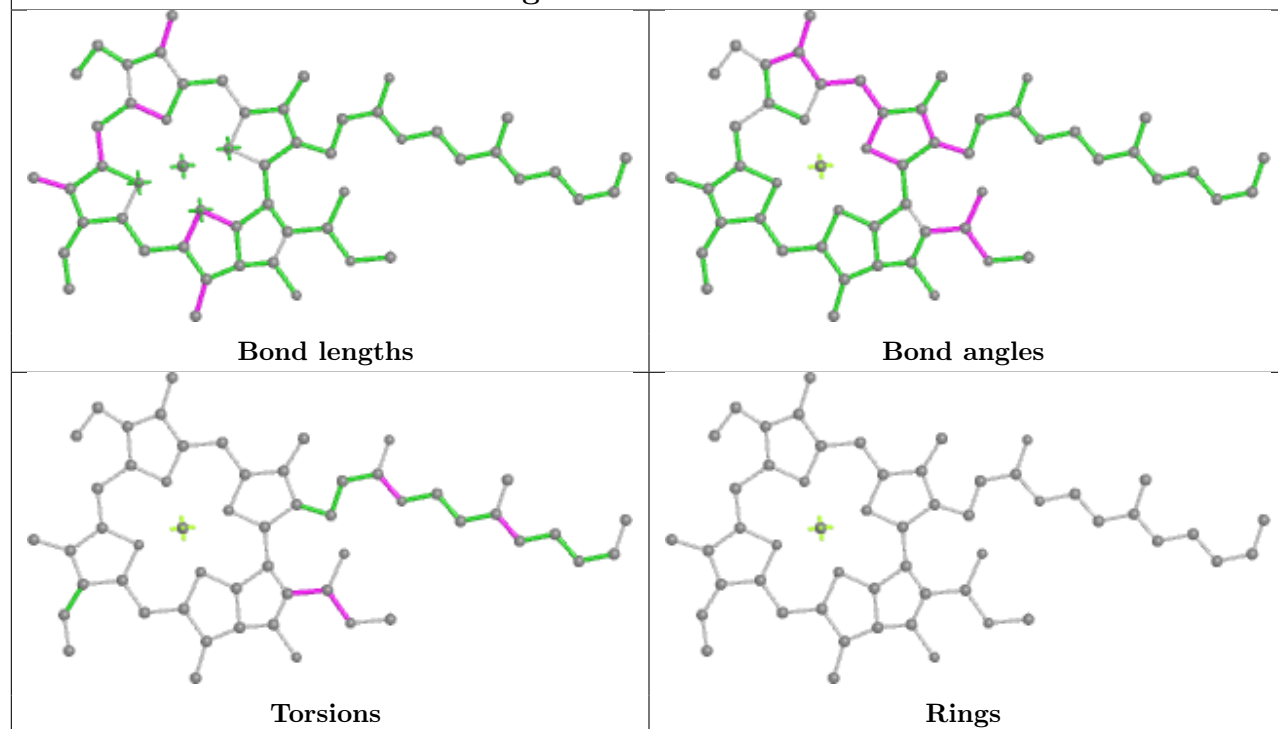
Ligand CLA cA 828

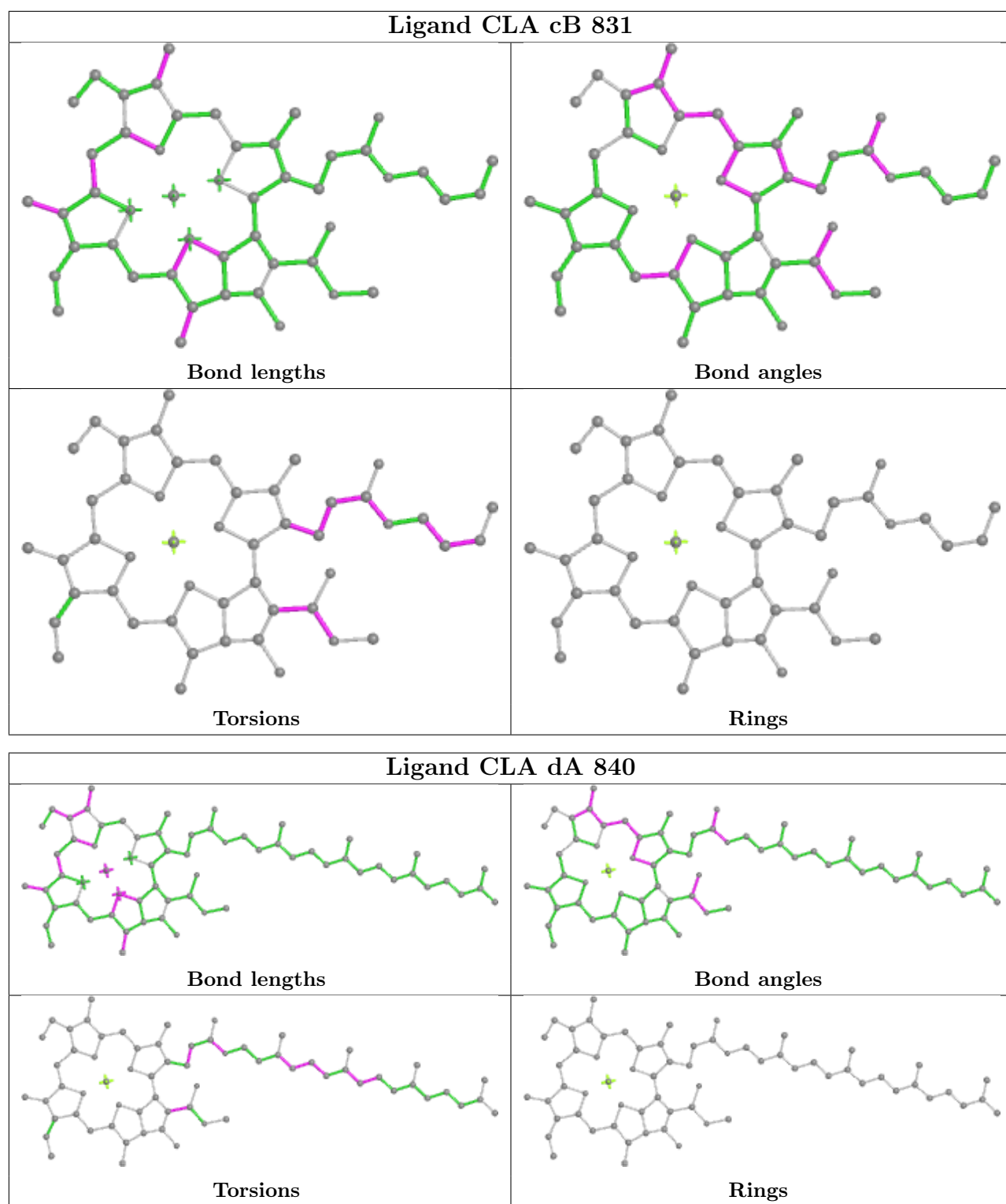


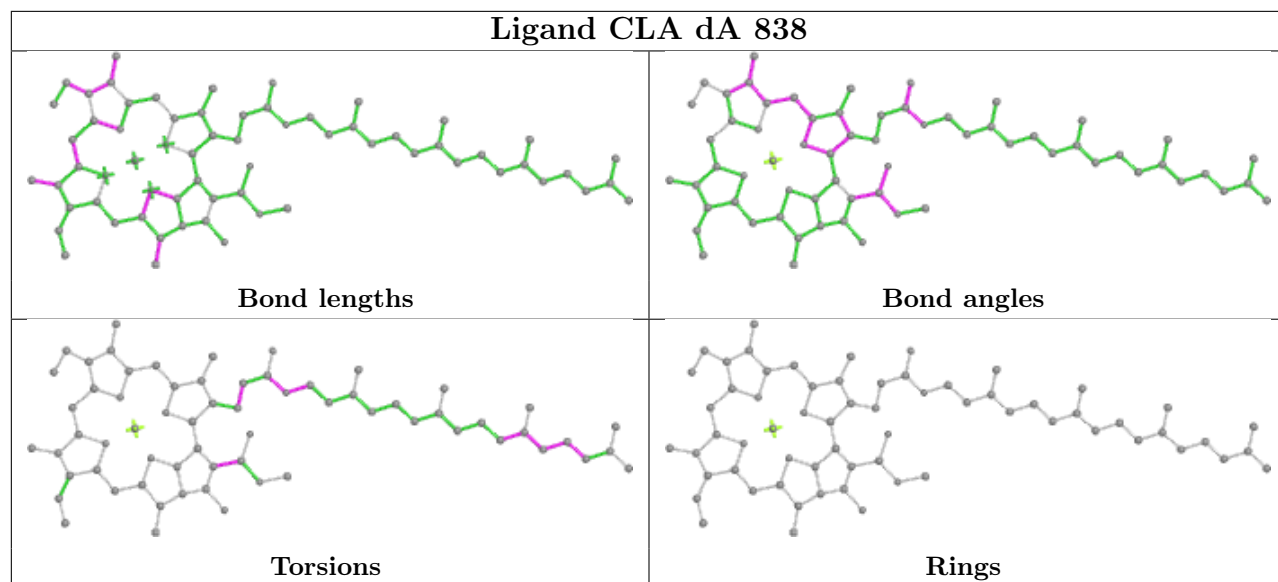
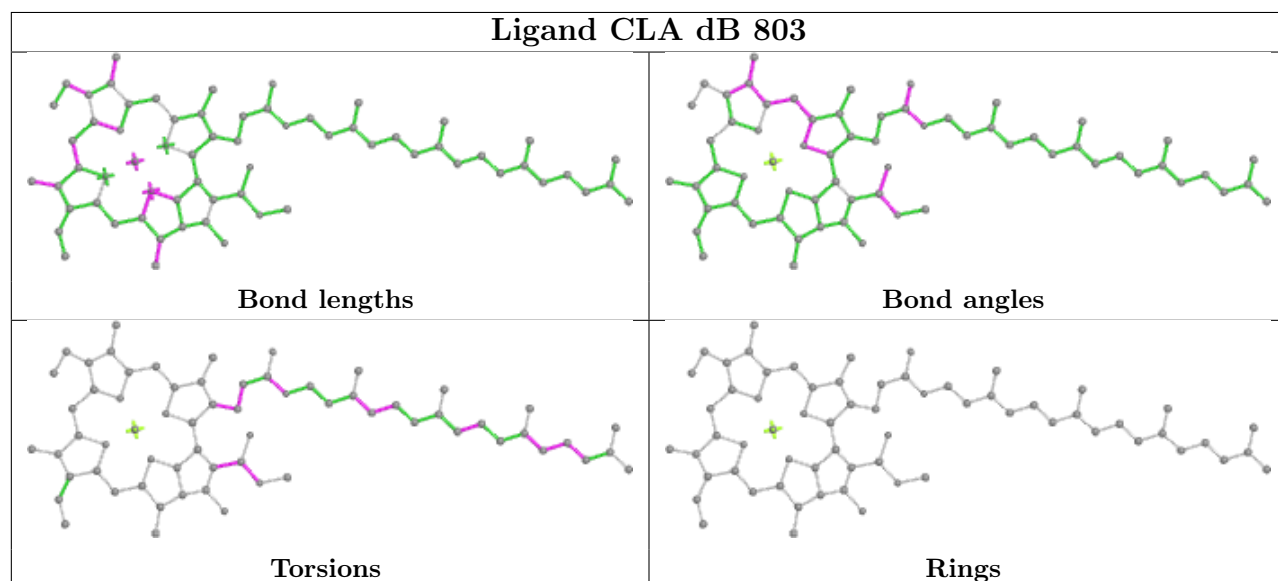
Ligand CLA cA 835

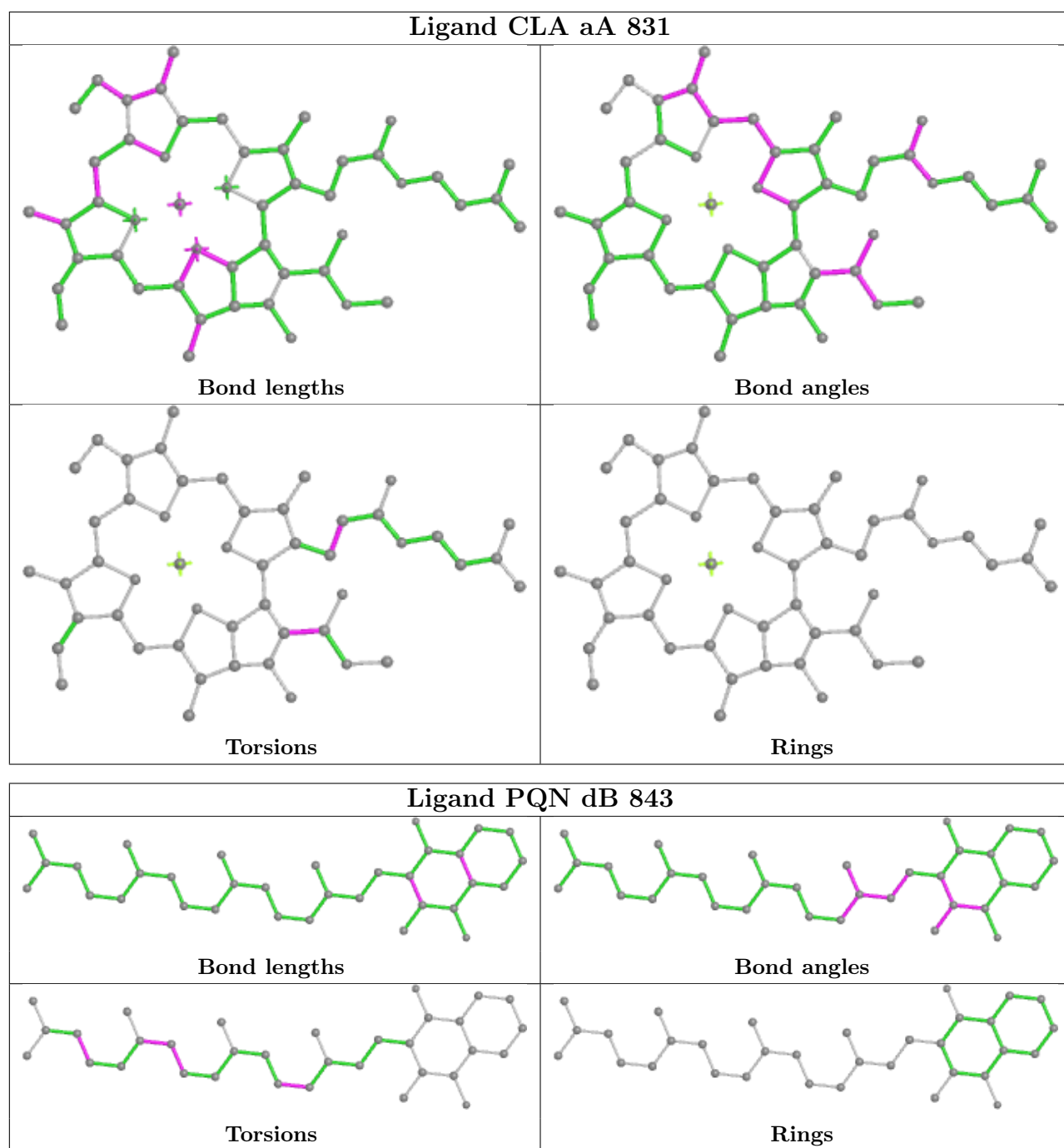


Ligand CLA dB 805

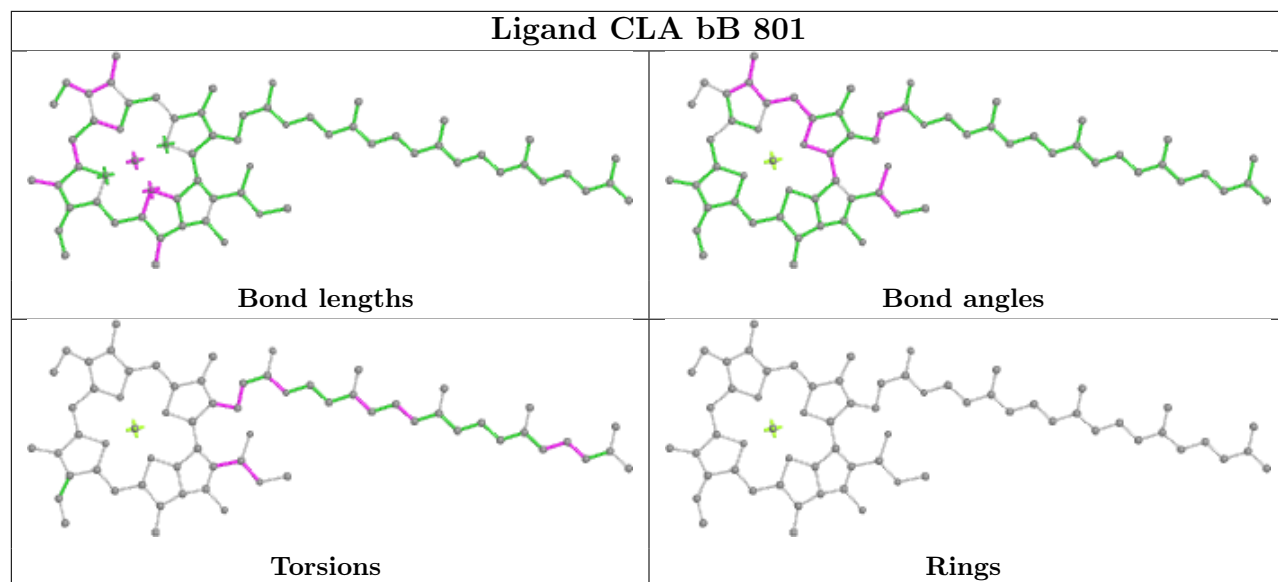




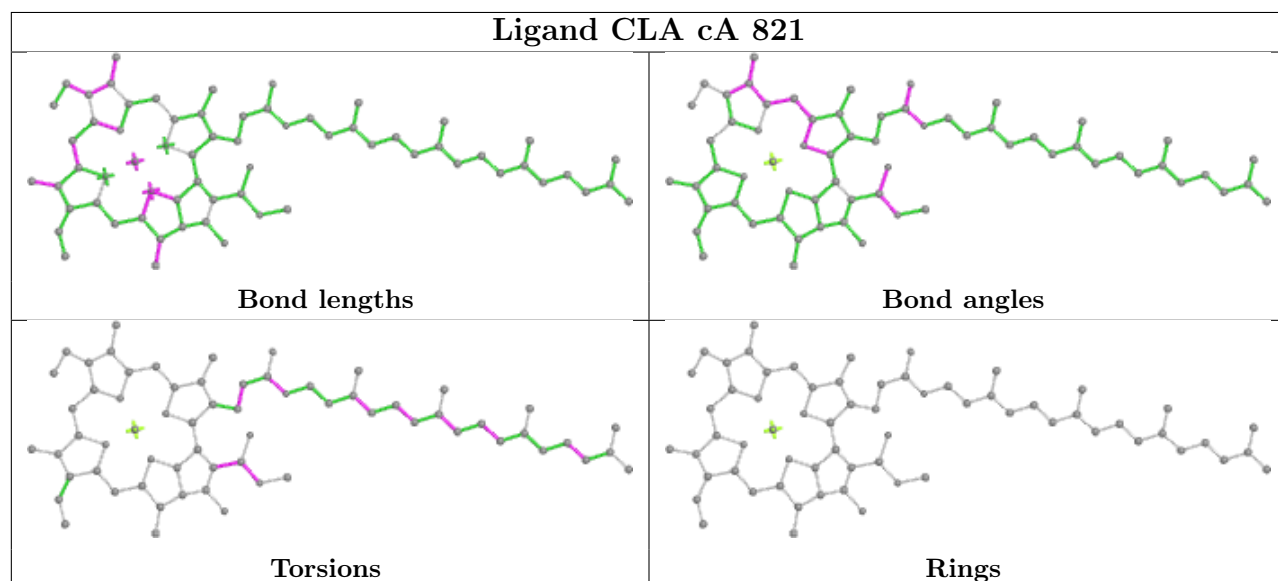
Ligand CLA dA 838**Ligand CLA dB 803**



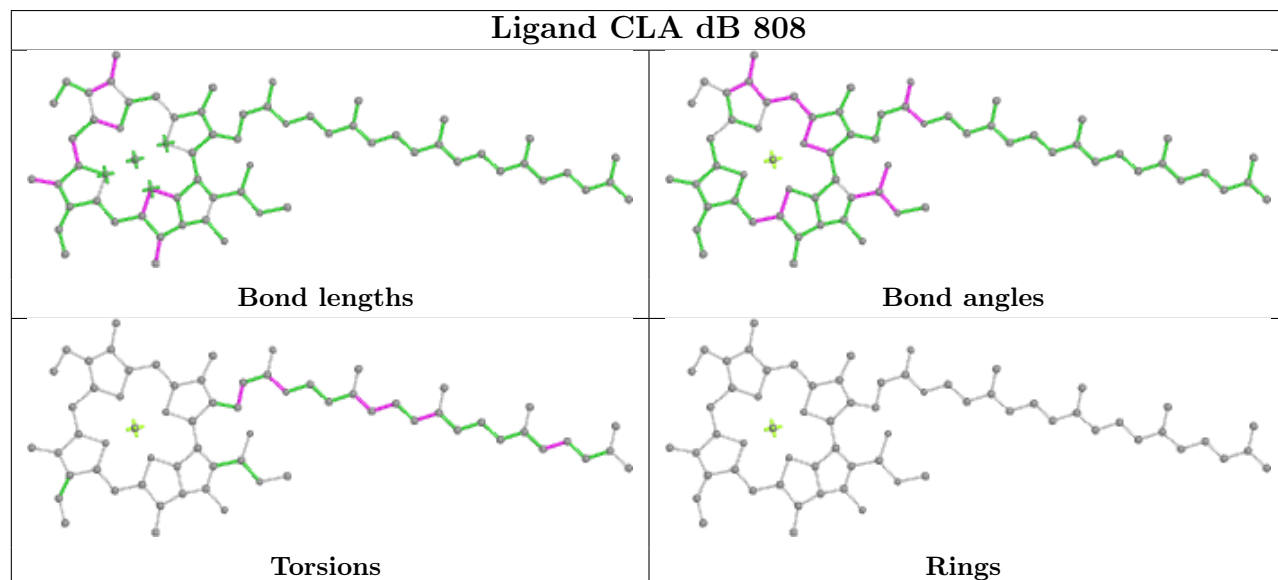
Ligand CLA bB 801

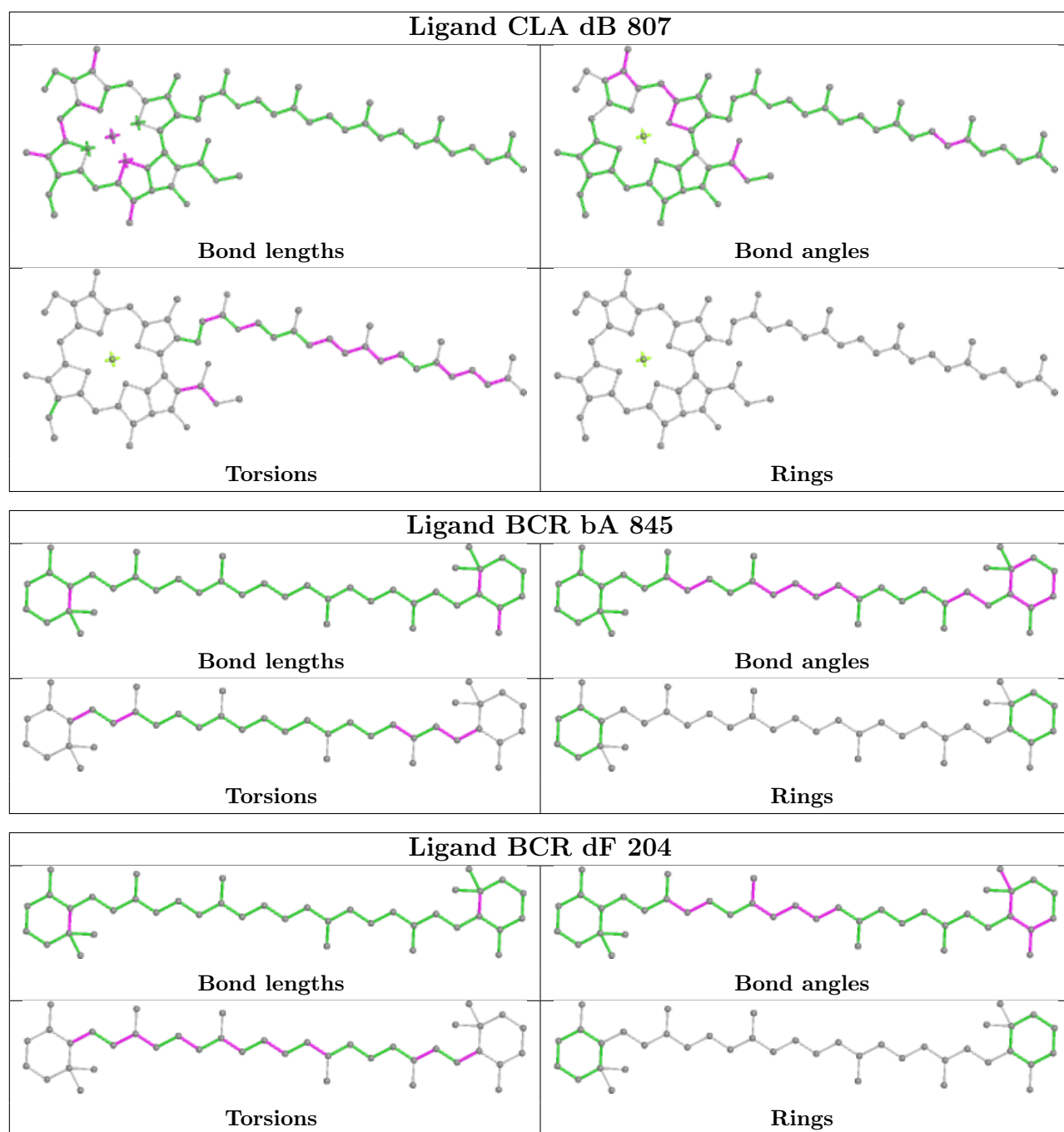


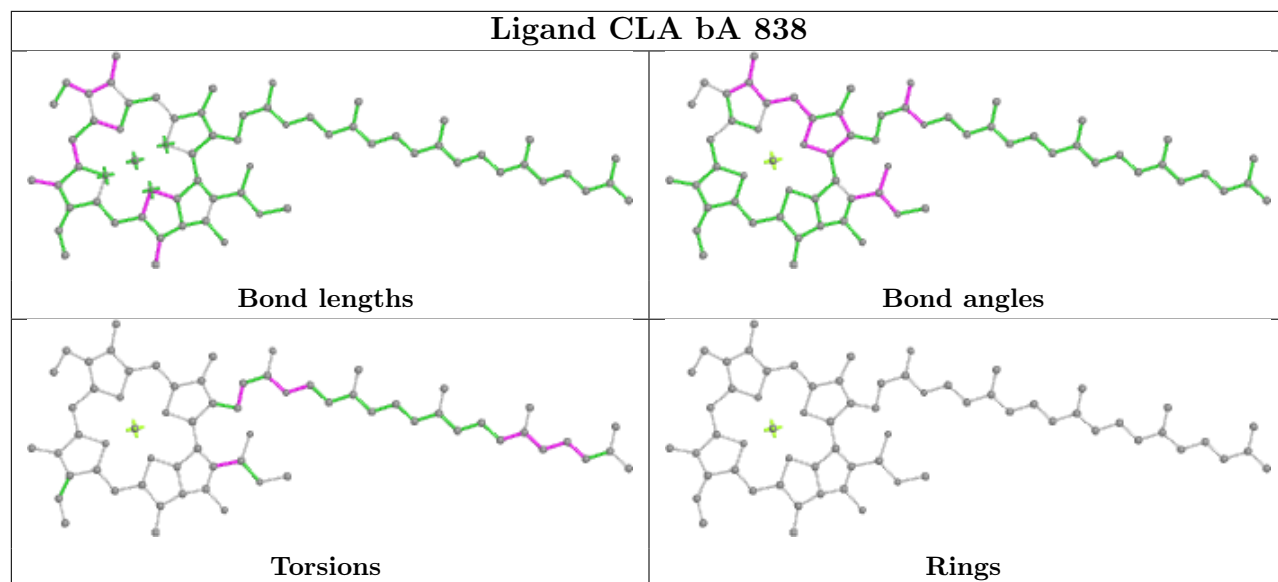
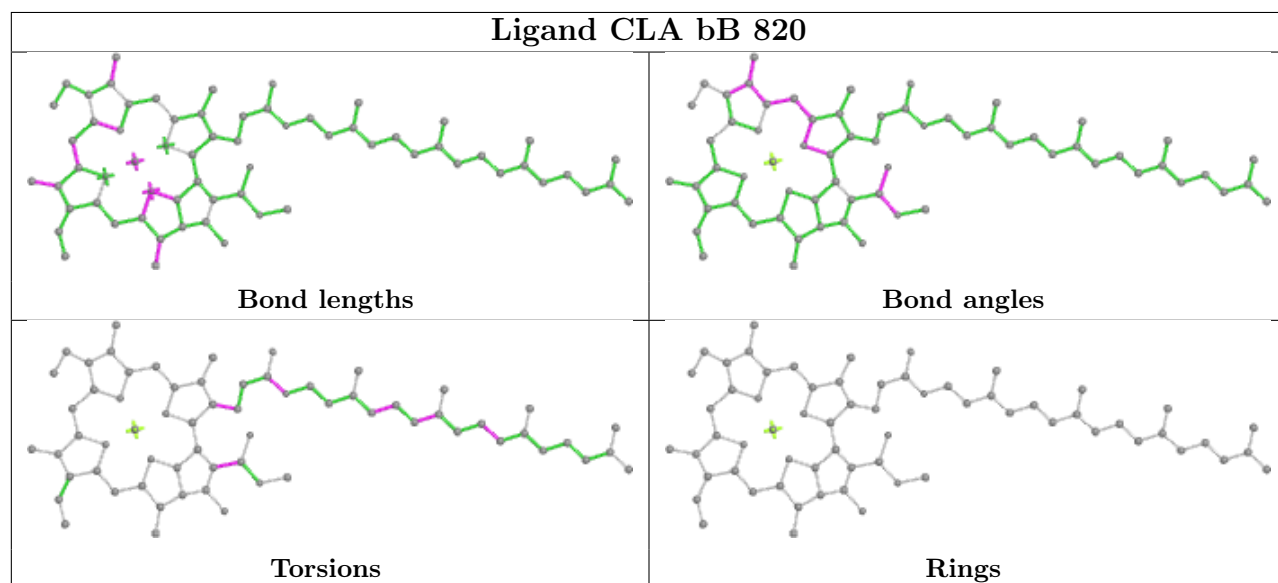
Ligand CLA cA 821

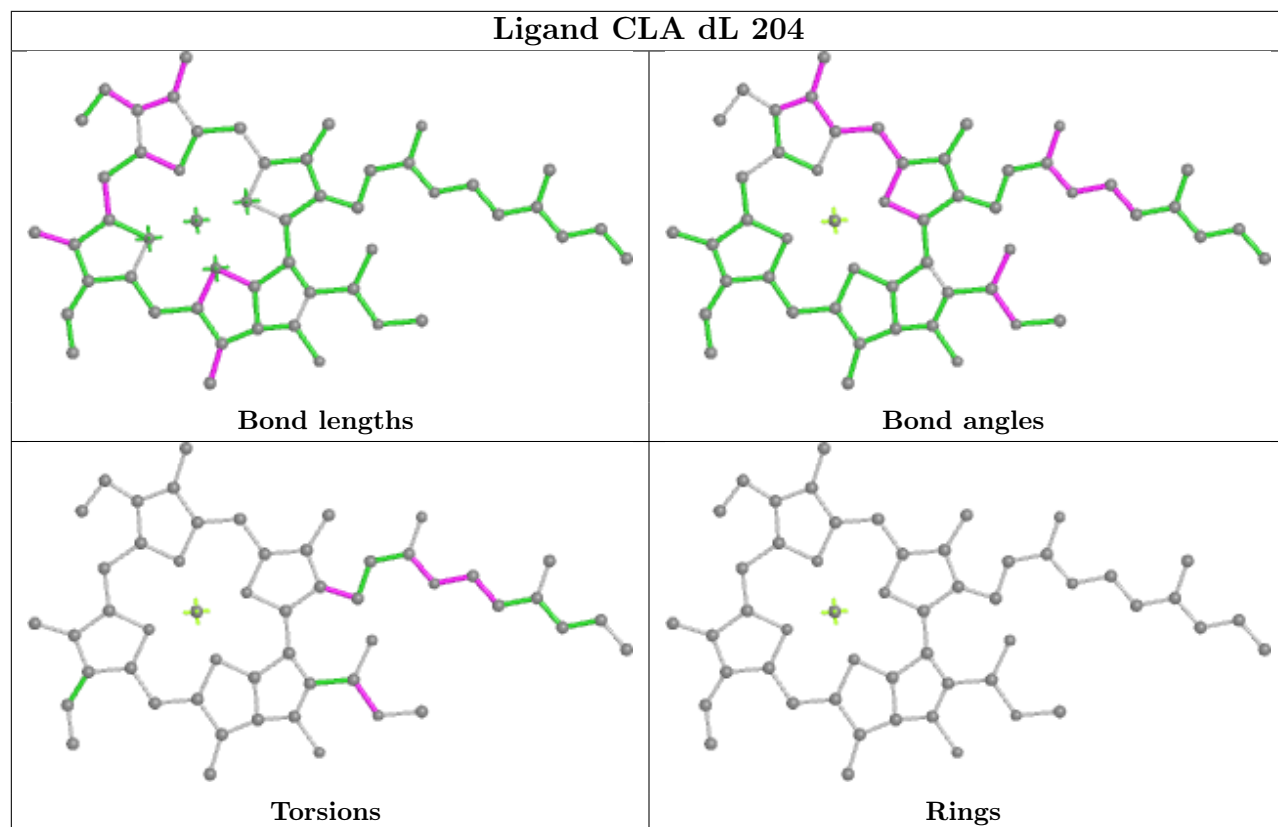


Ligand CLA dB 808

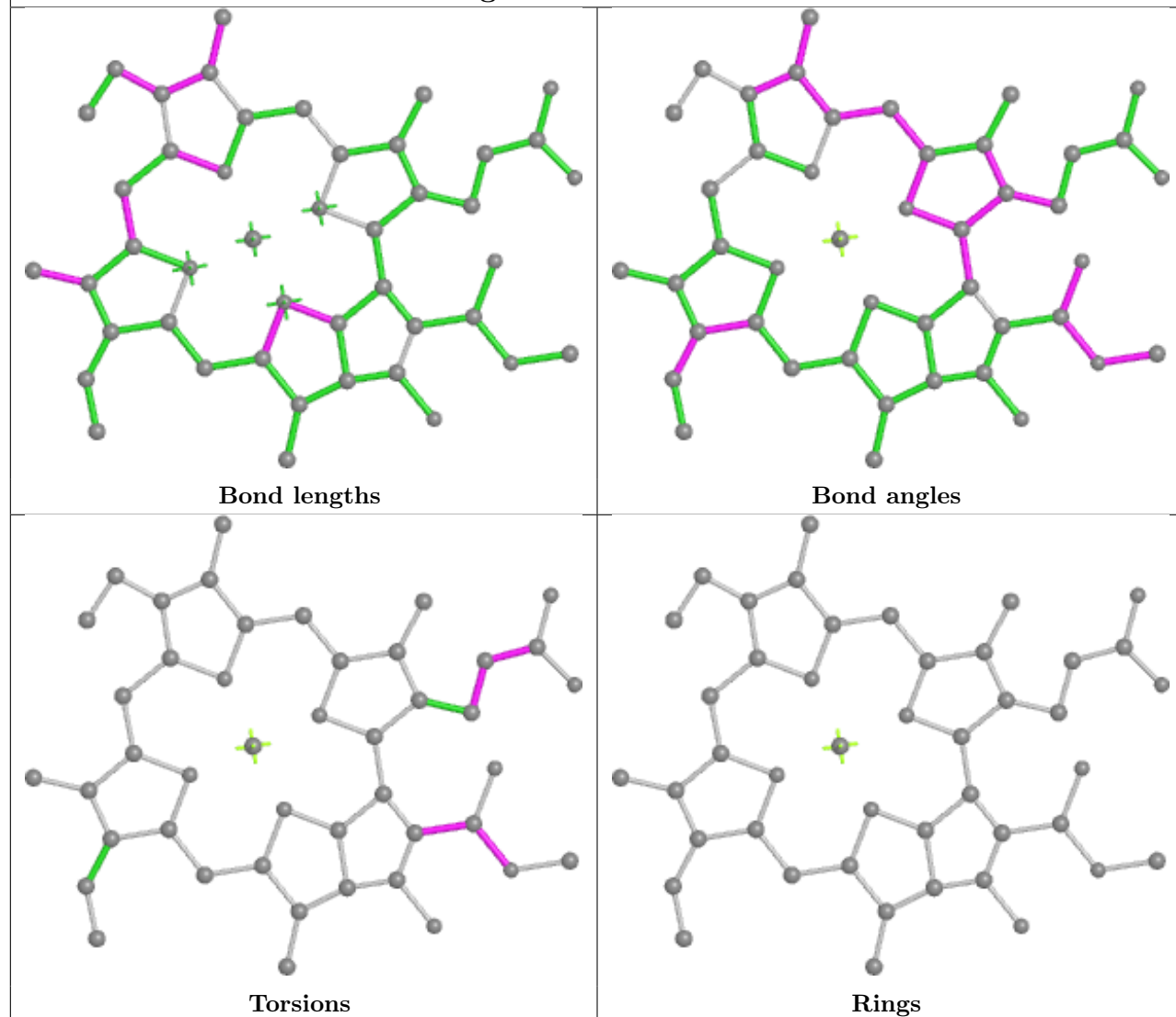




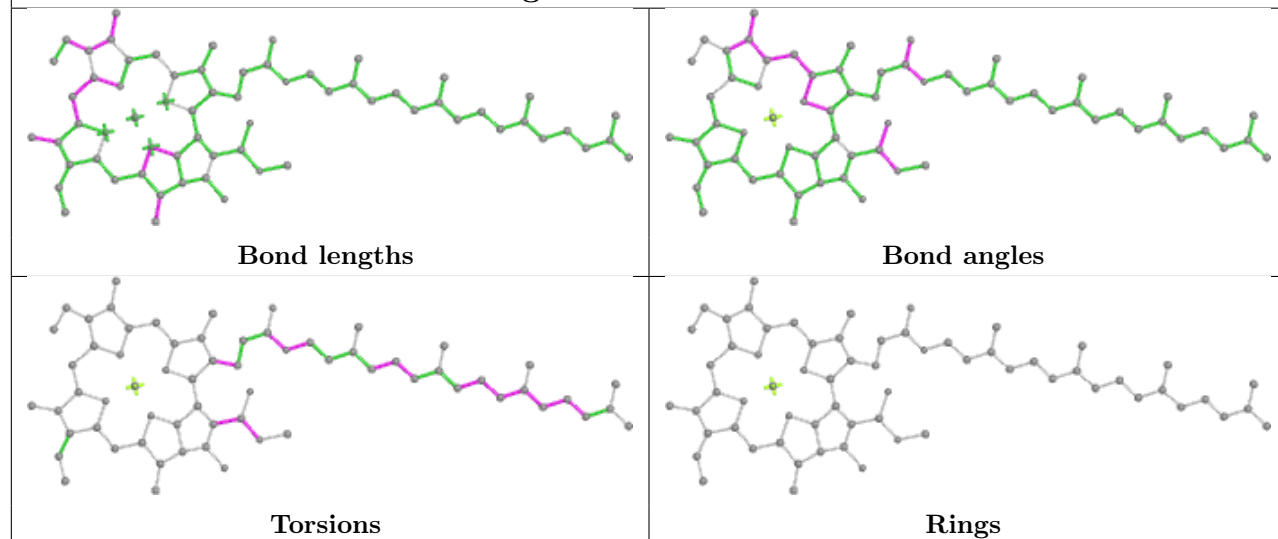
Ligand CLA bA 838**Ligand CLA bB 820**

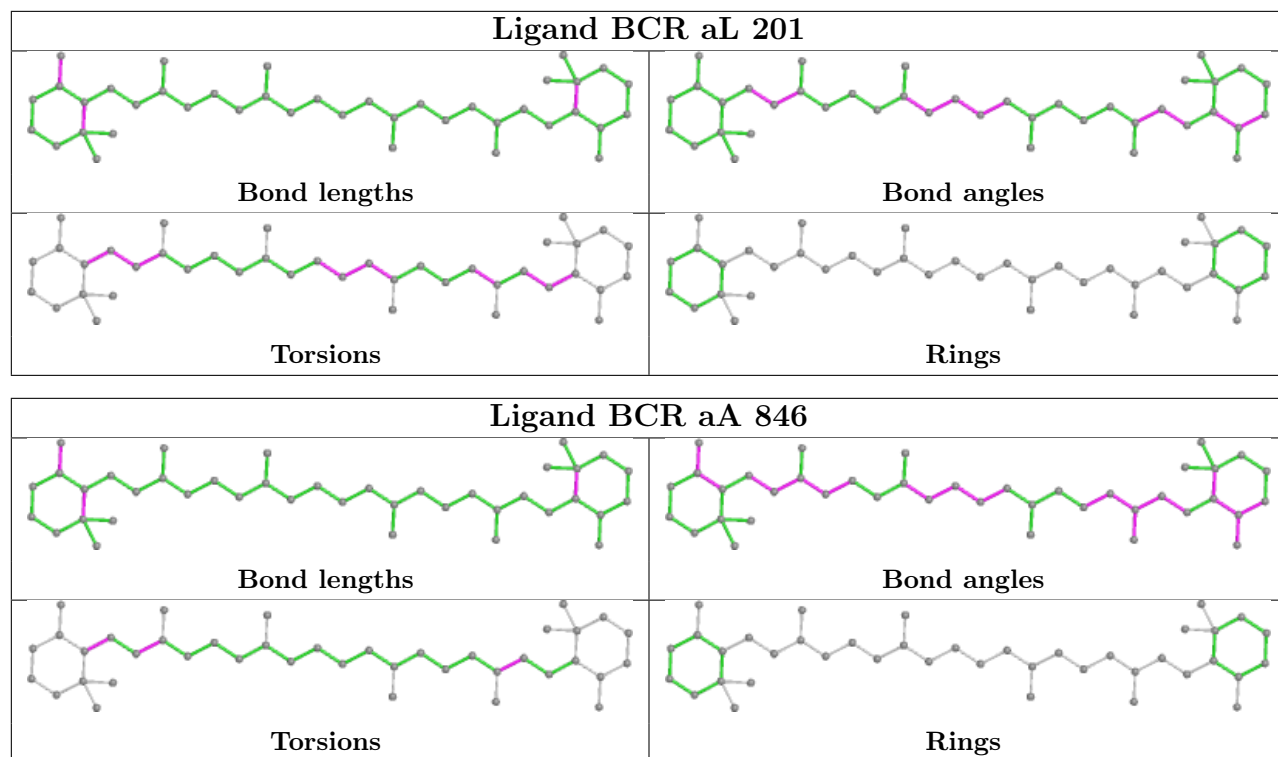


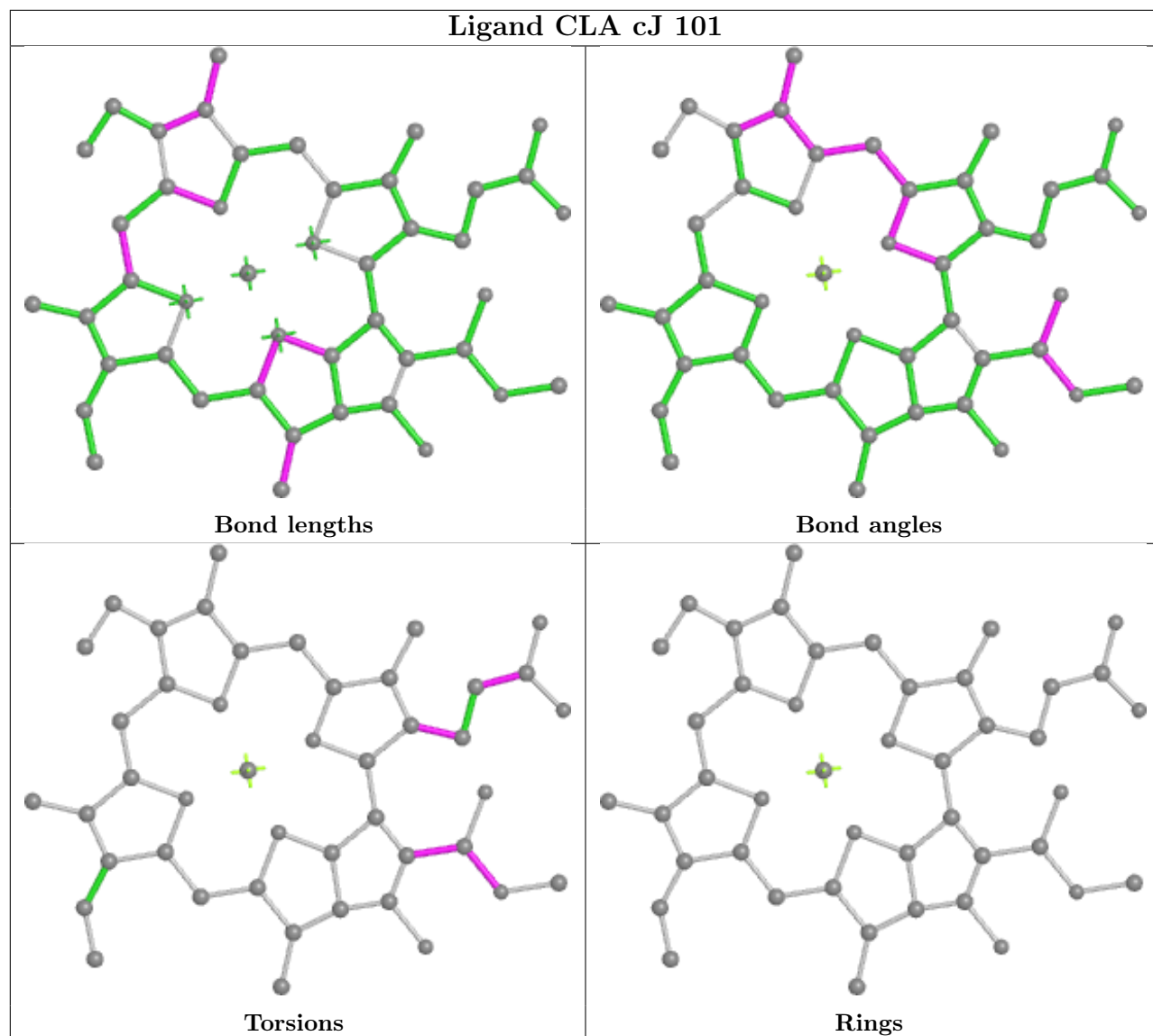
Ligand CLA dA 813



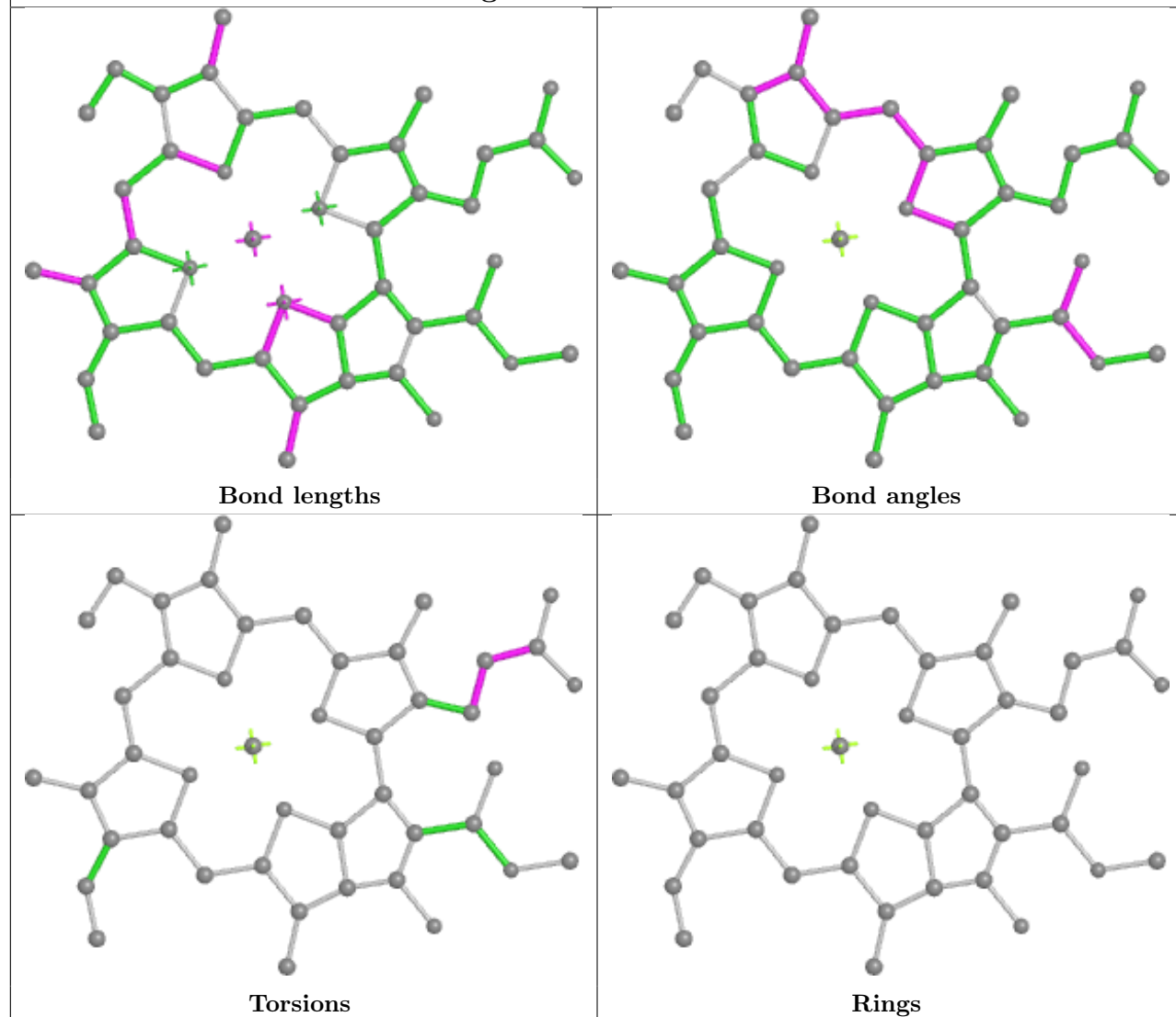
Ligand CLA bB 842



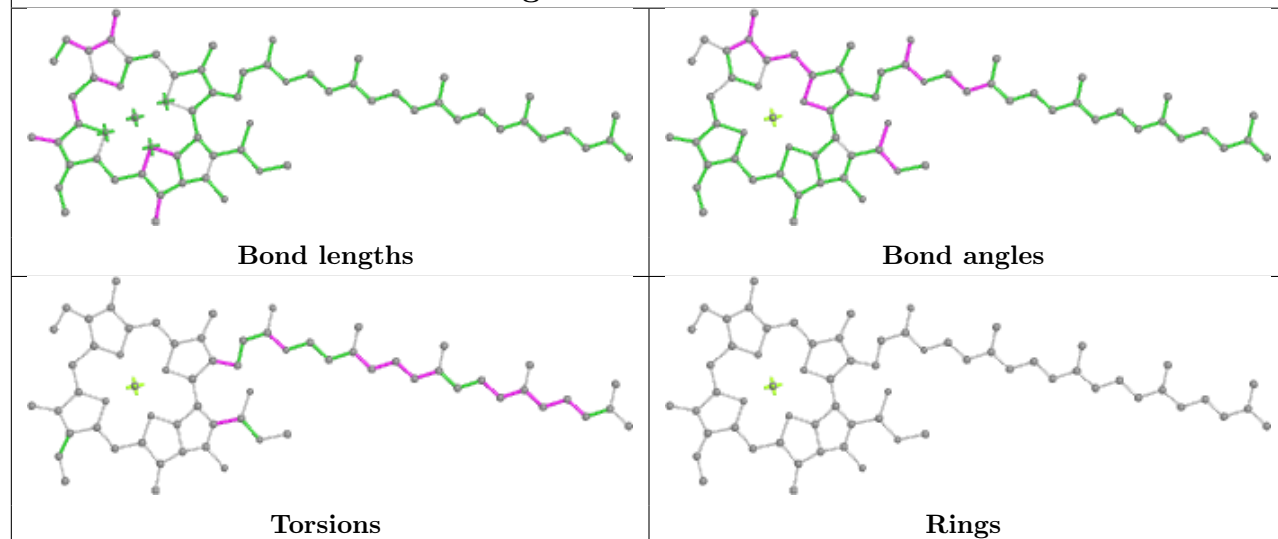




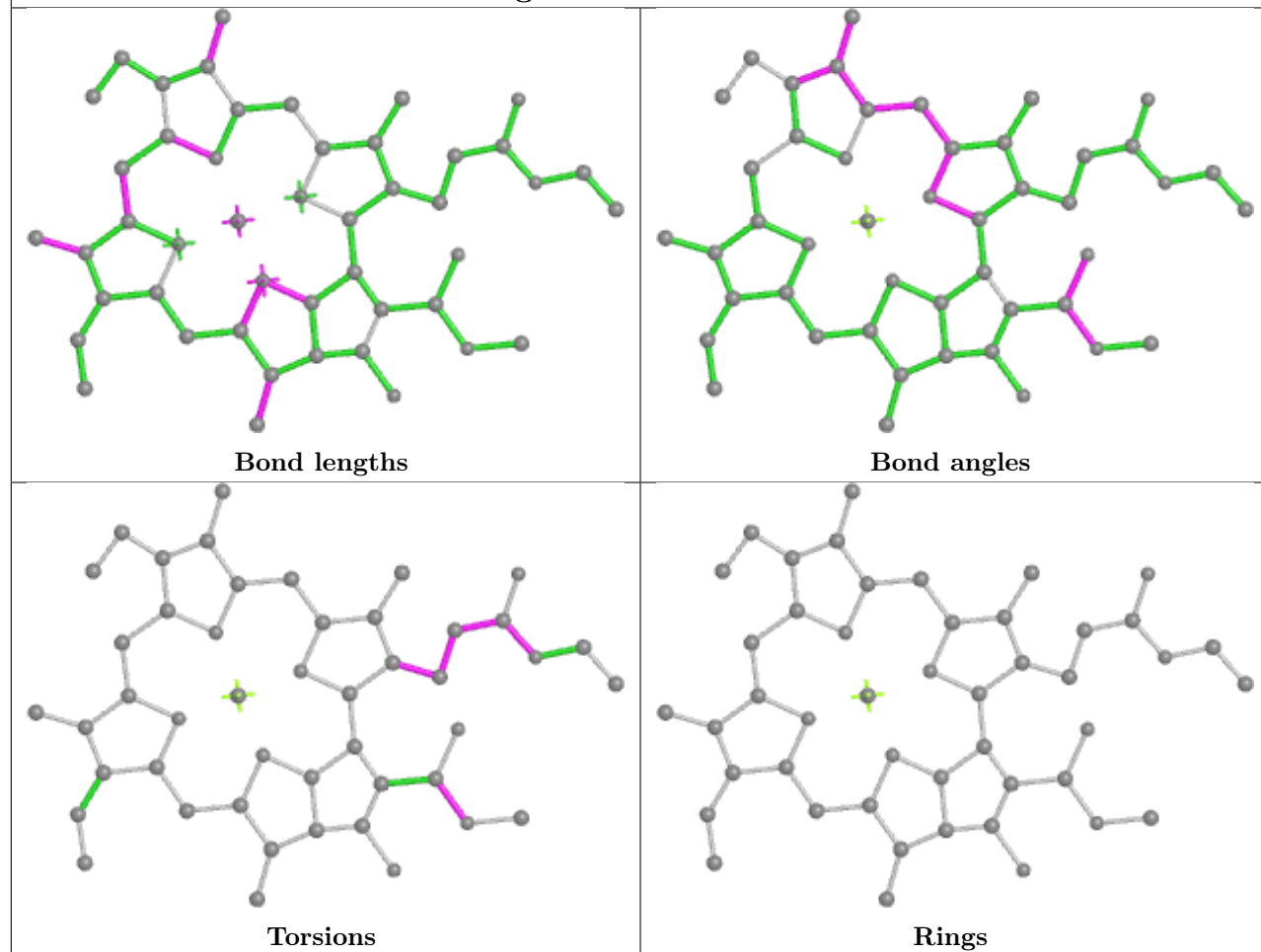
Ligand CLA aA 802



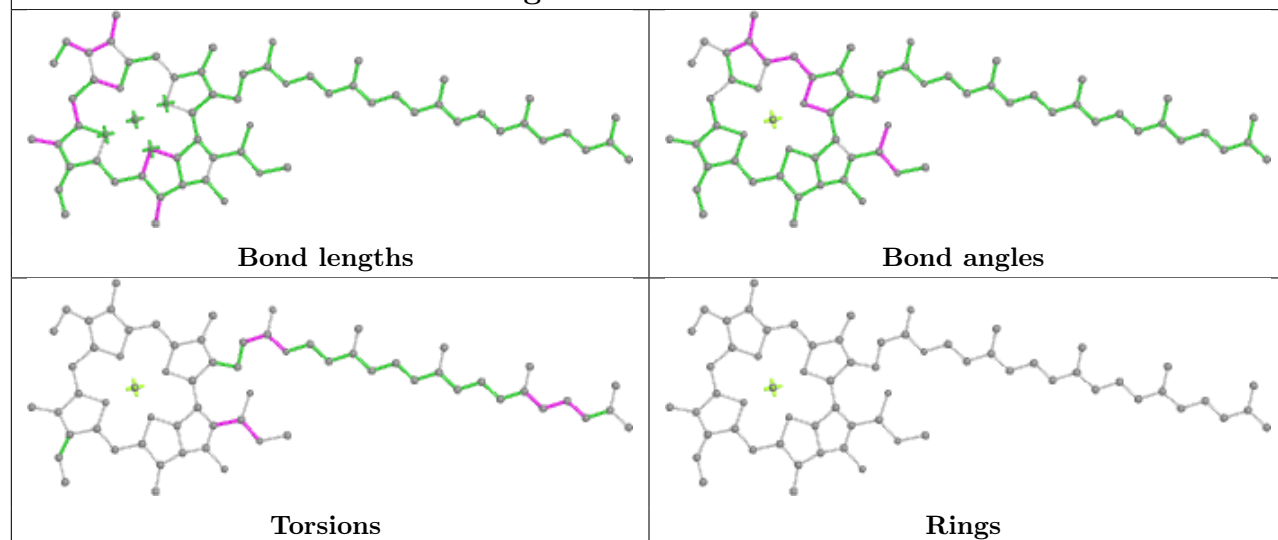
Ligand CLA dB 827



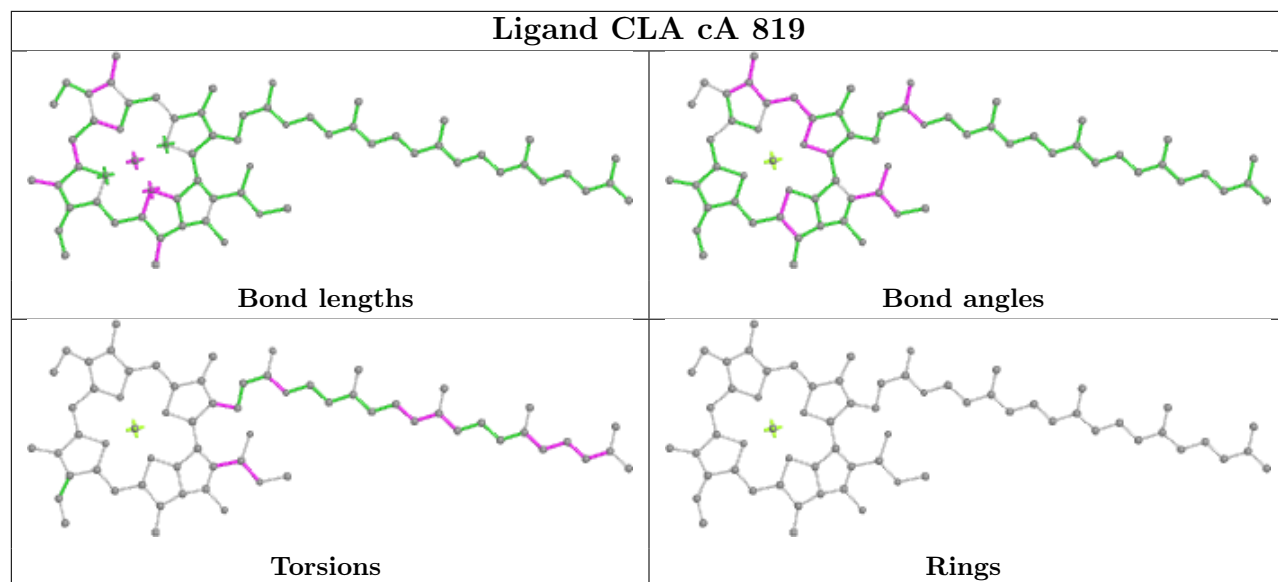
Ligand CLA dB 821



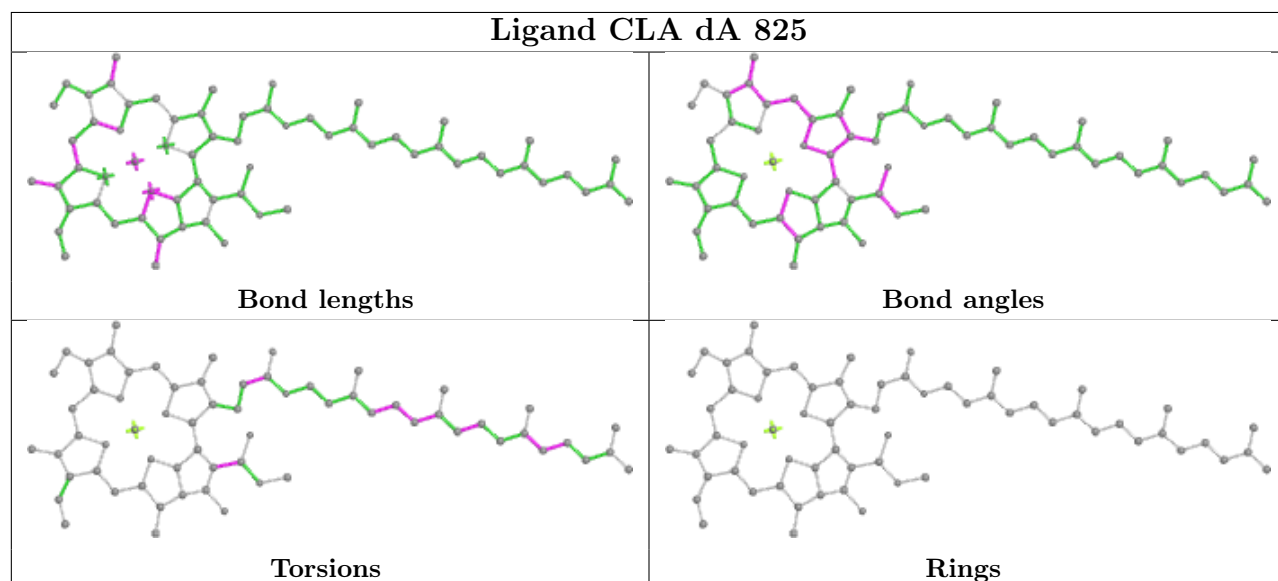
Ligand CLA aB 802



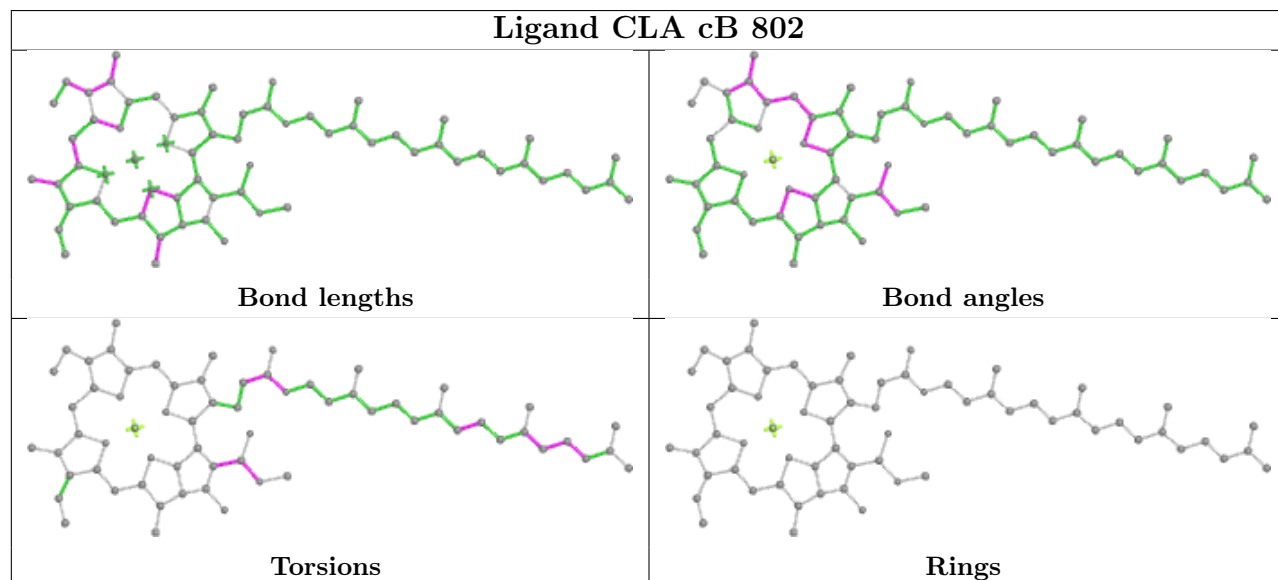
Ligand CLA cA 819



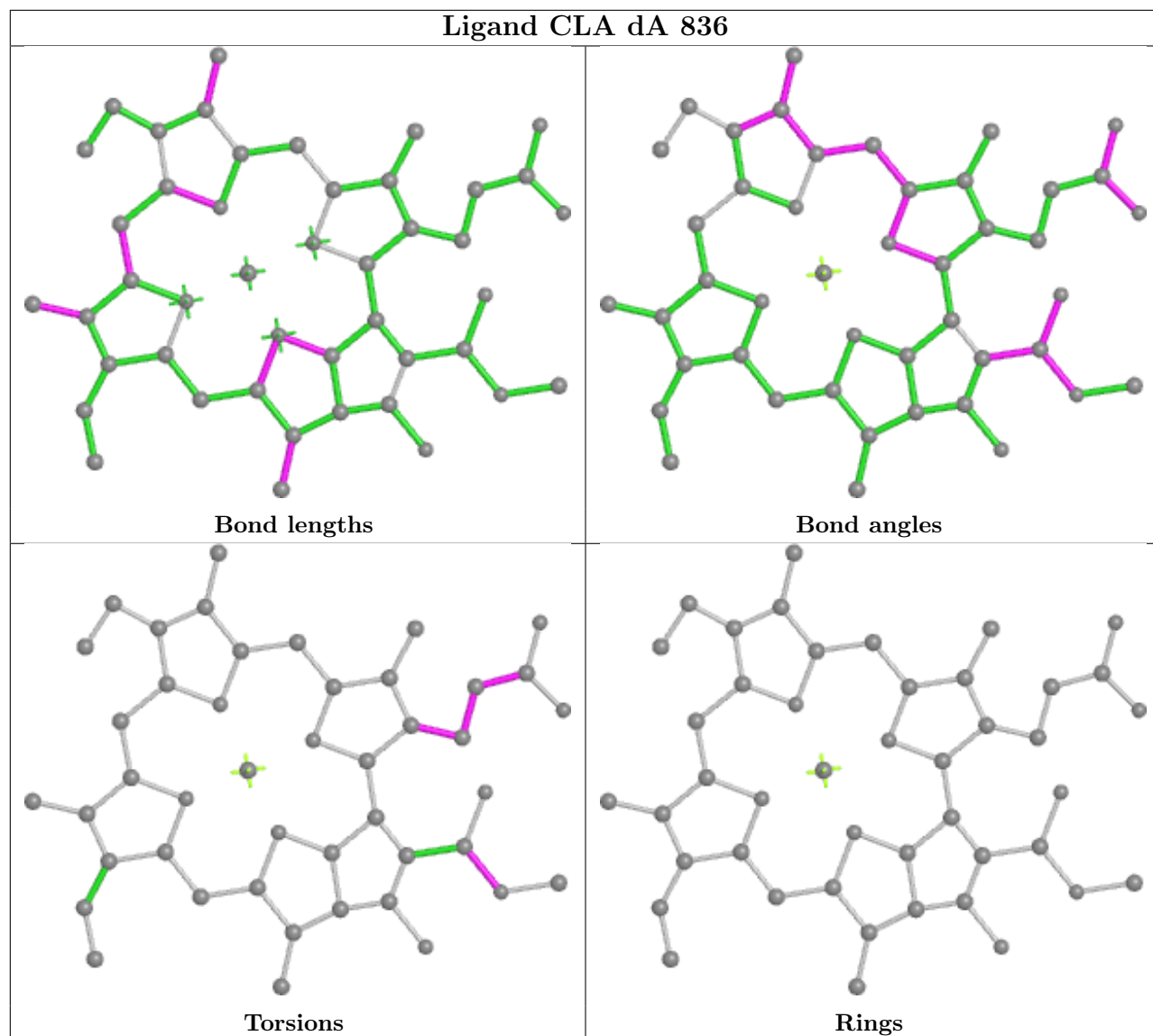
Ligand CLA dA 825



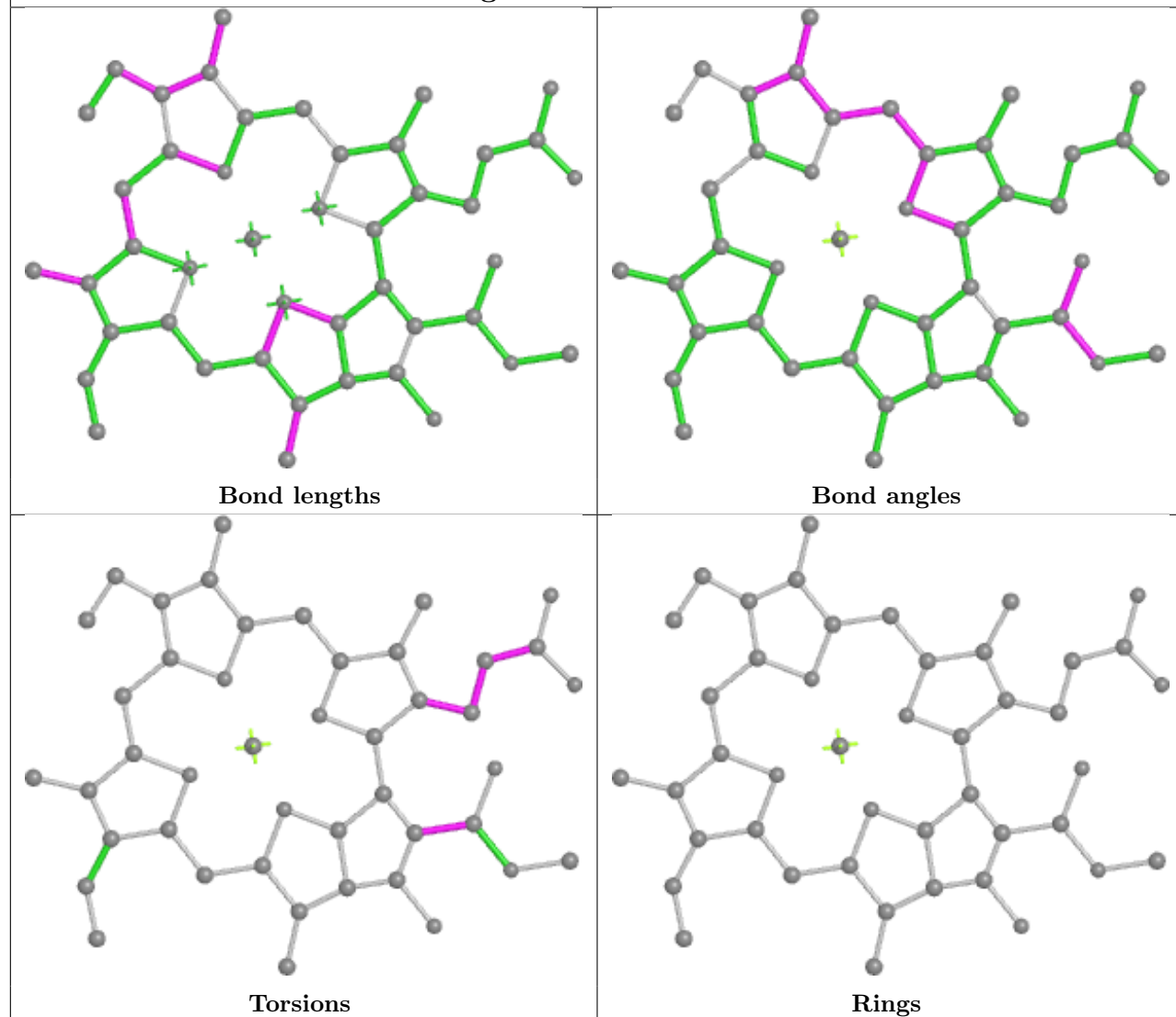
Ligand CLA cB 802



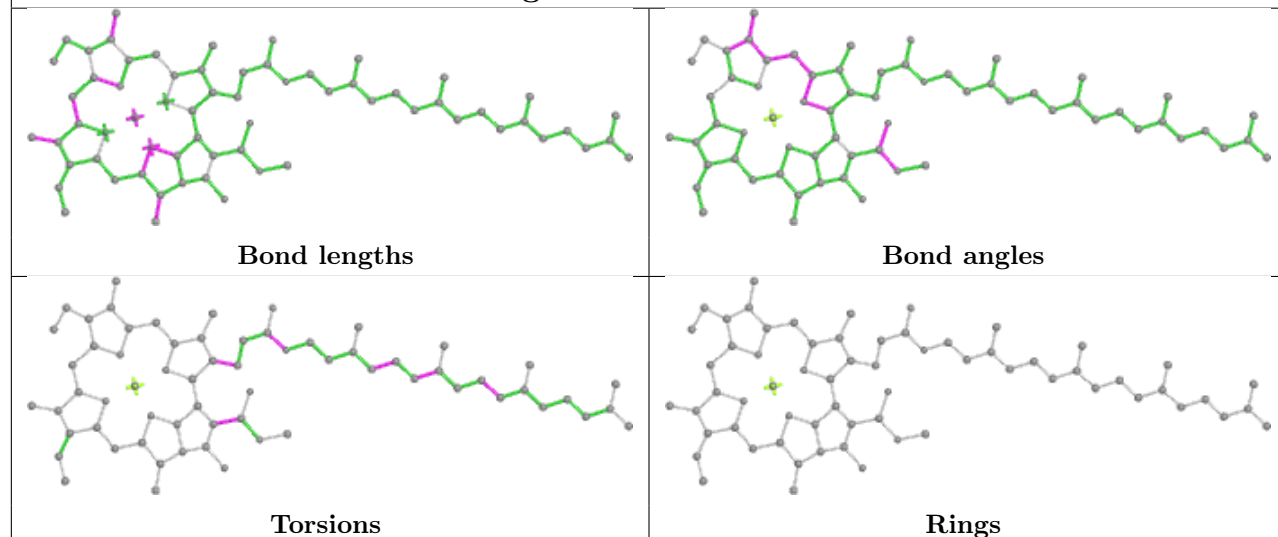
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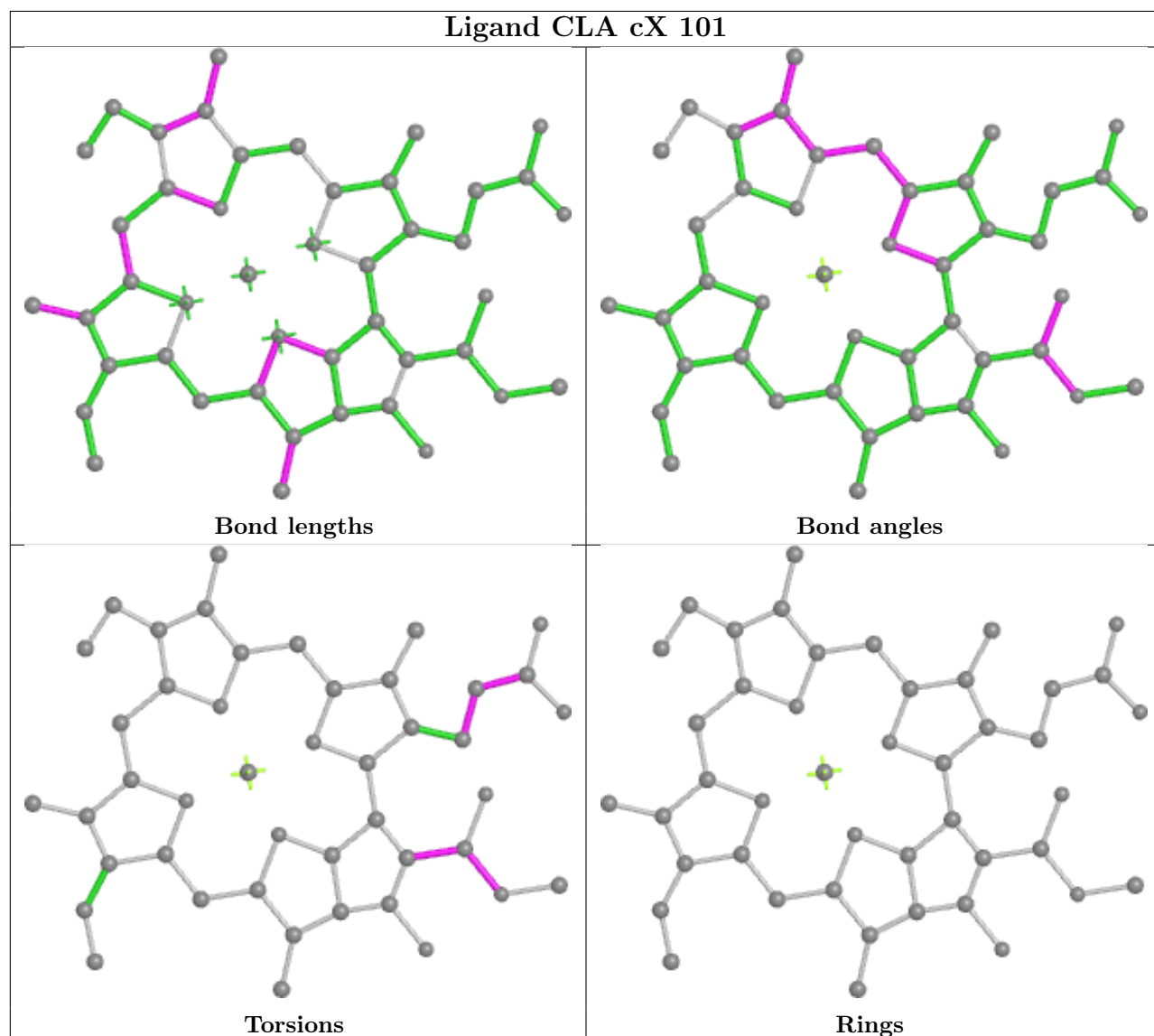
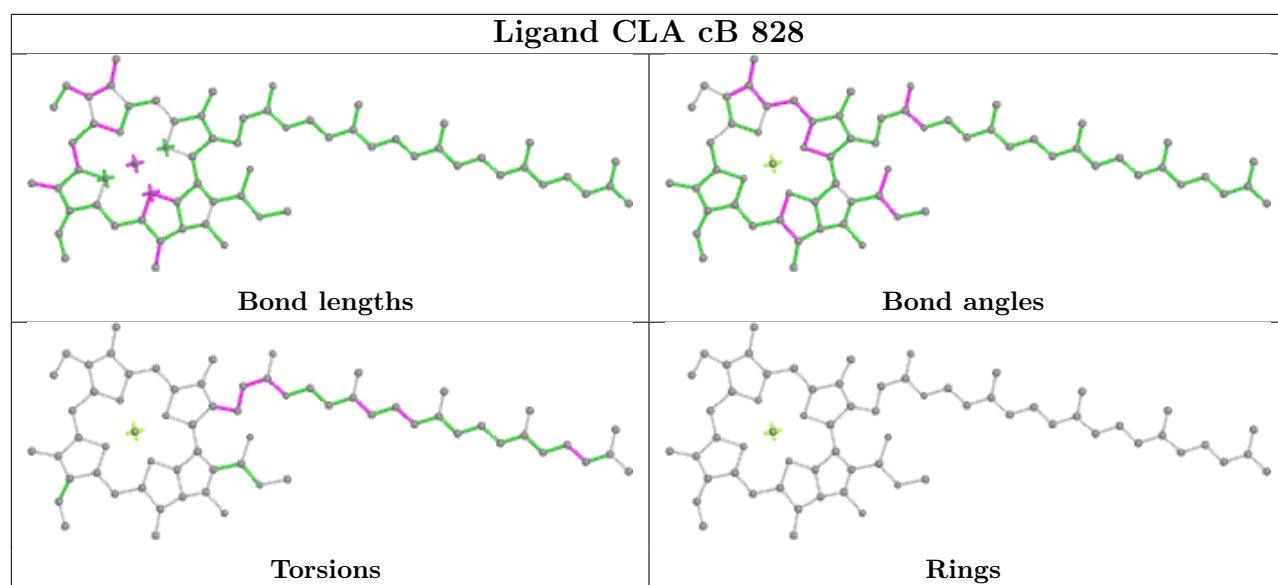


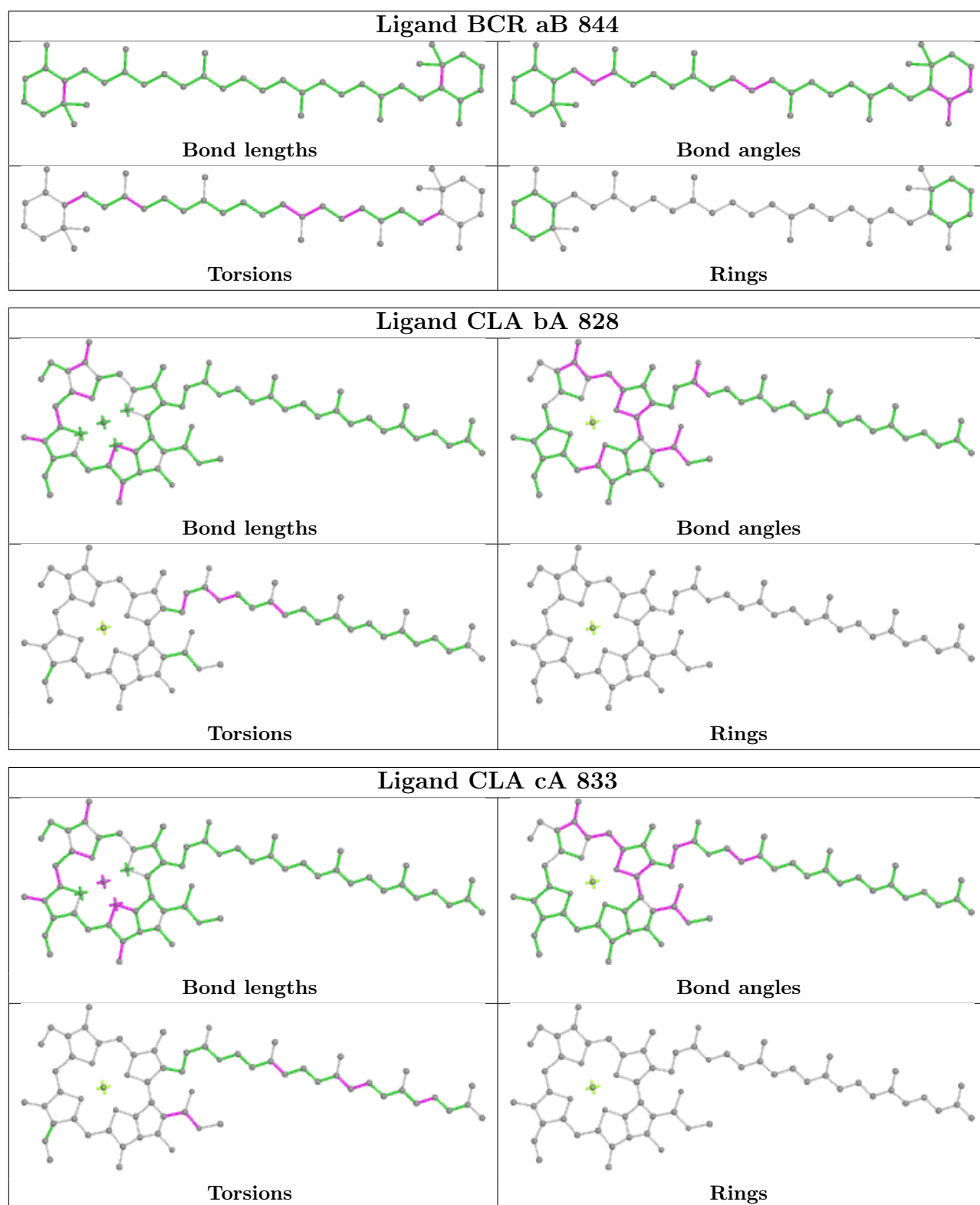
Ligand CLA bB 831



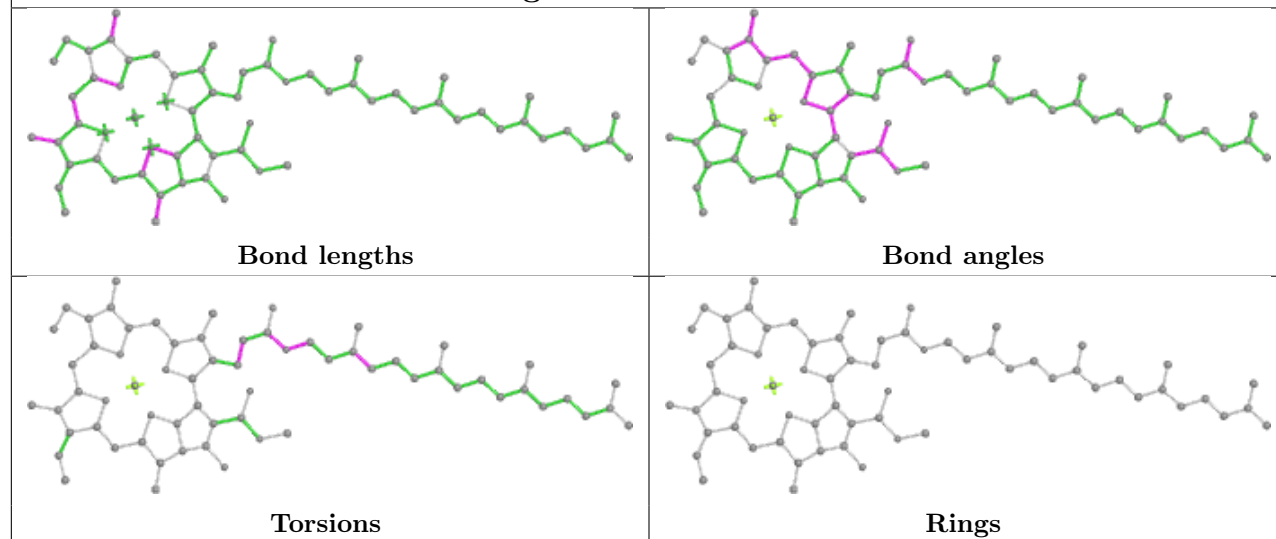
Ligand CLA dB 820



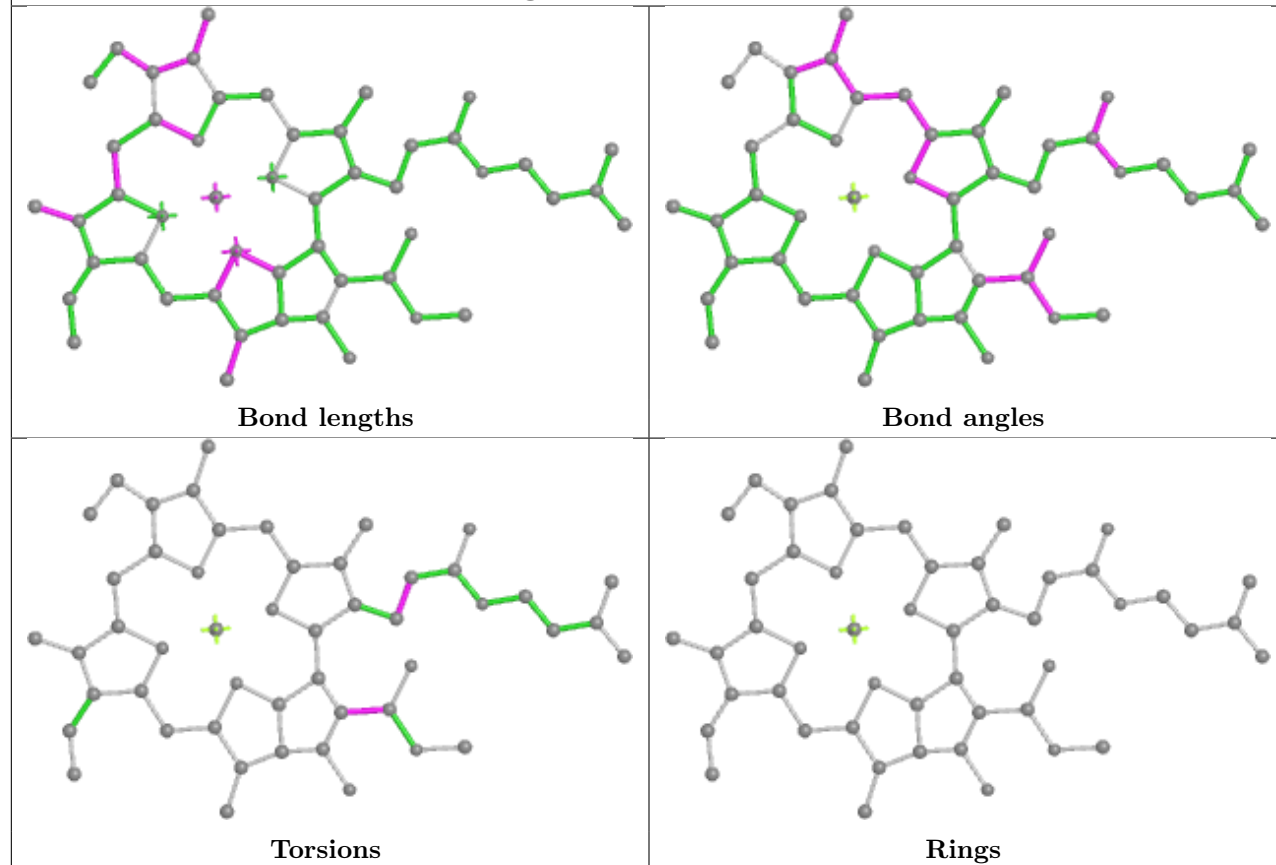


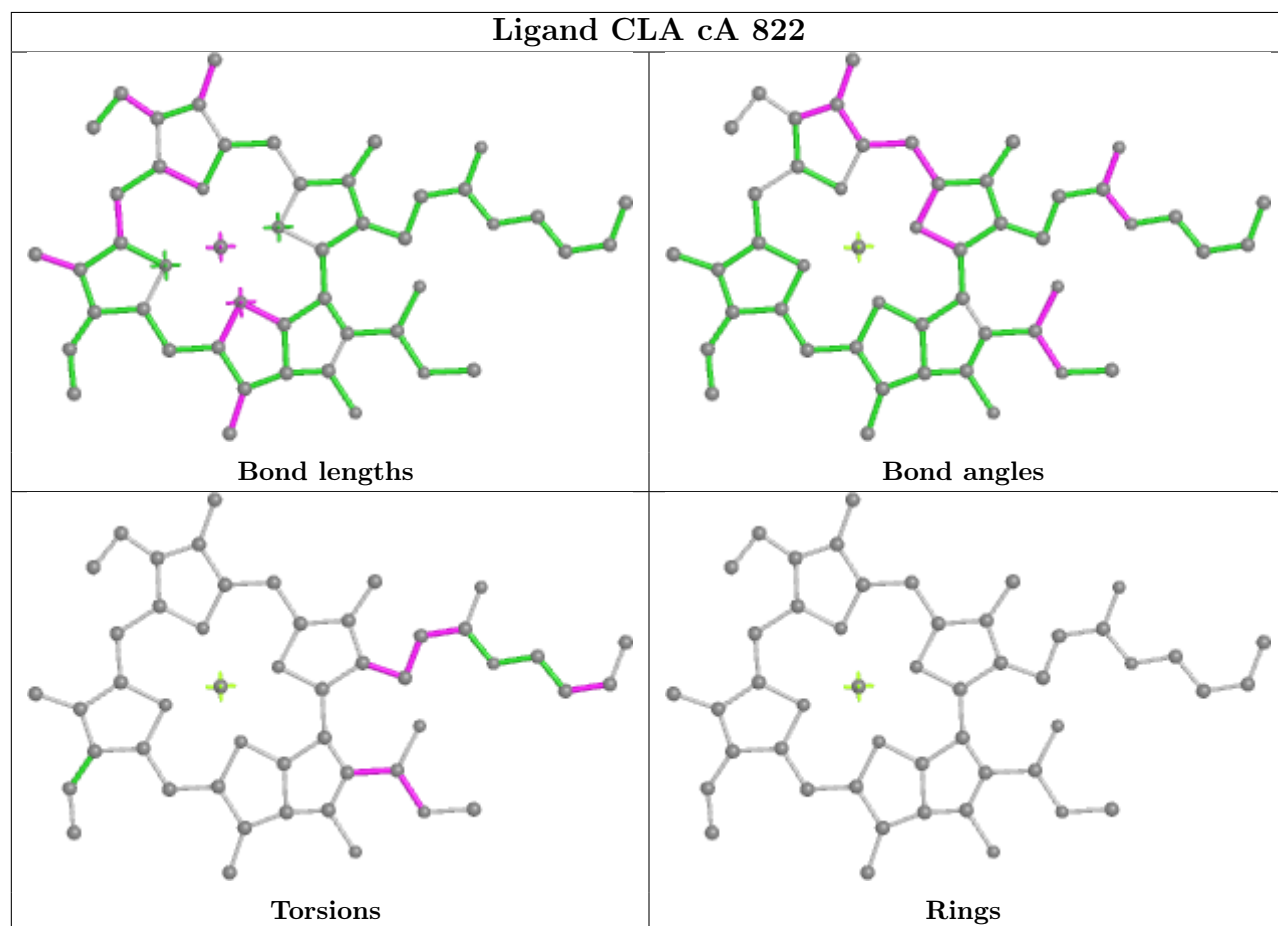
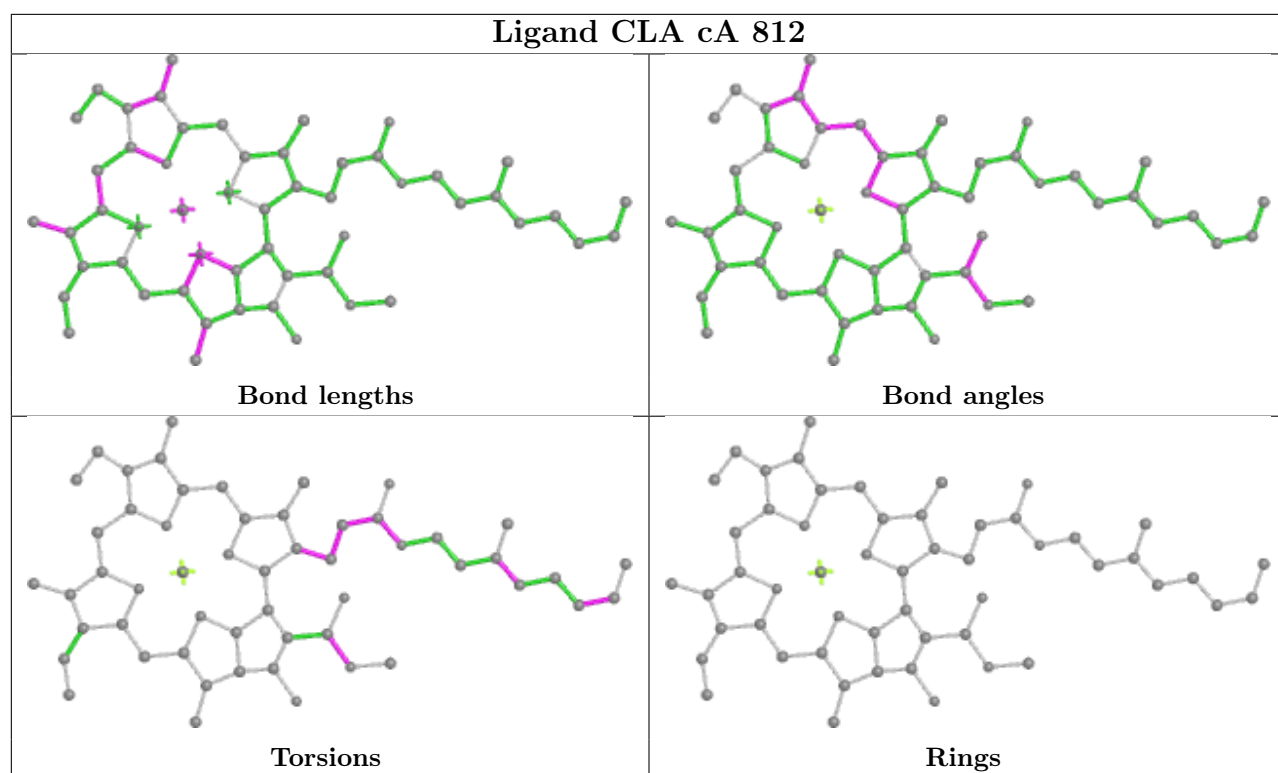


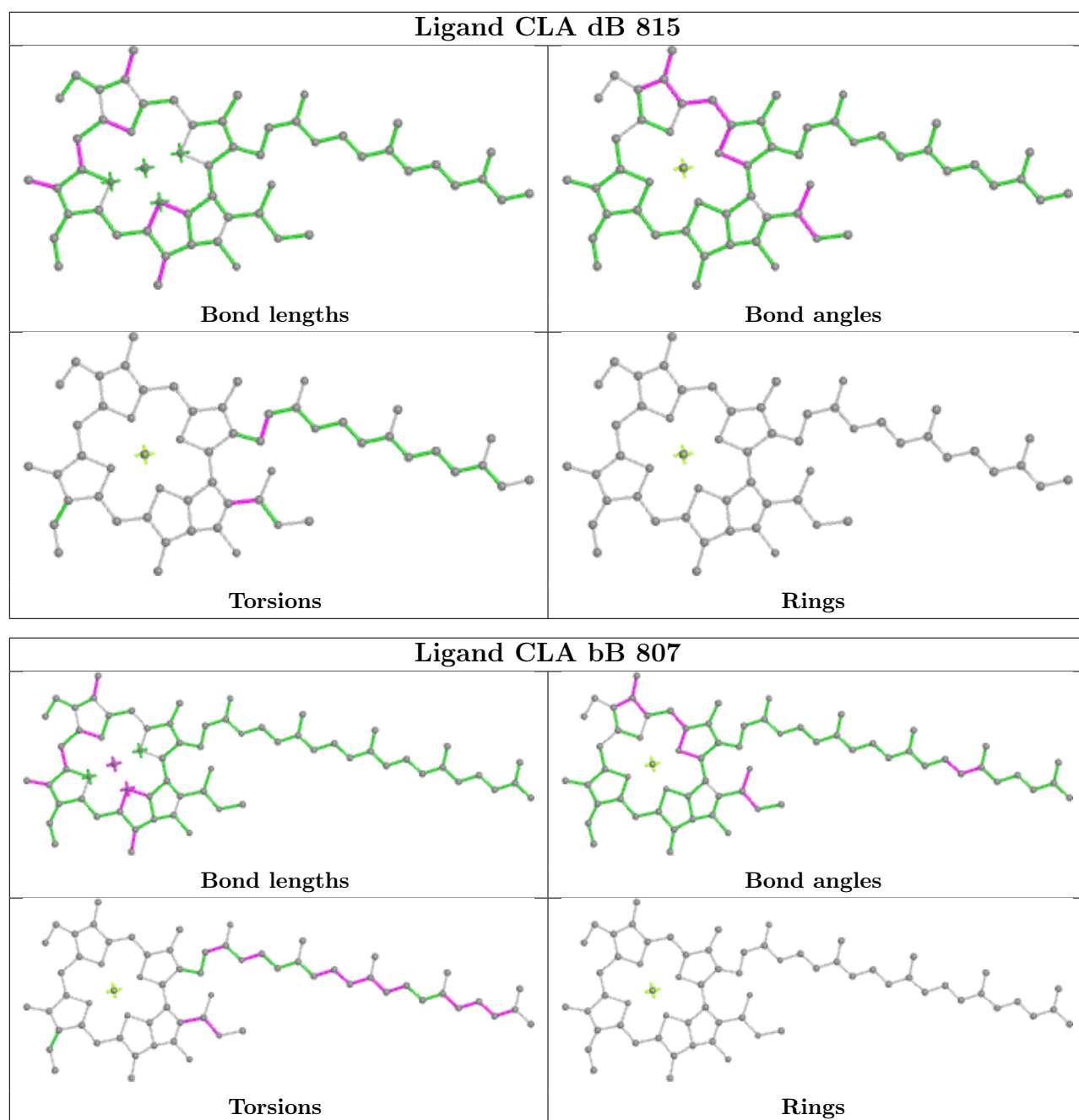
Ligand CLA aA 828



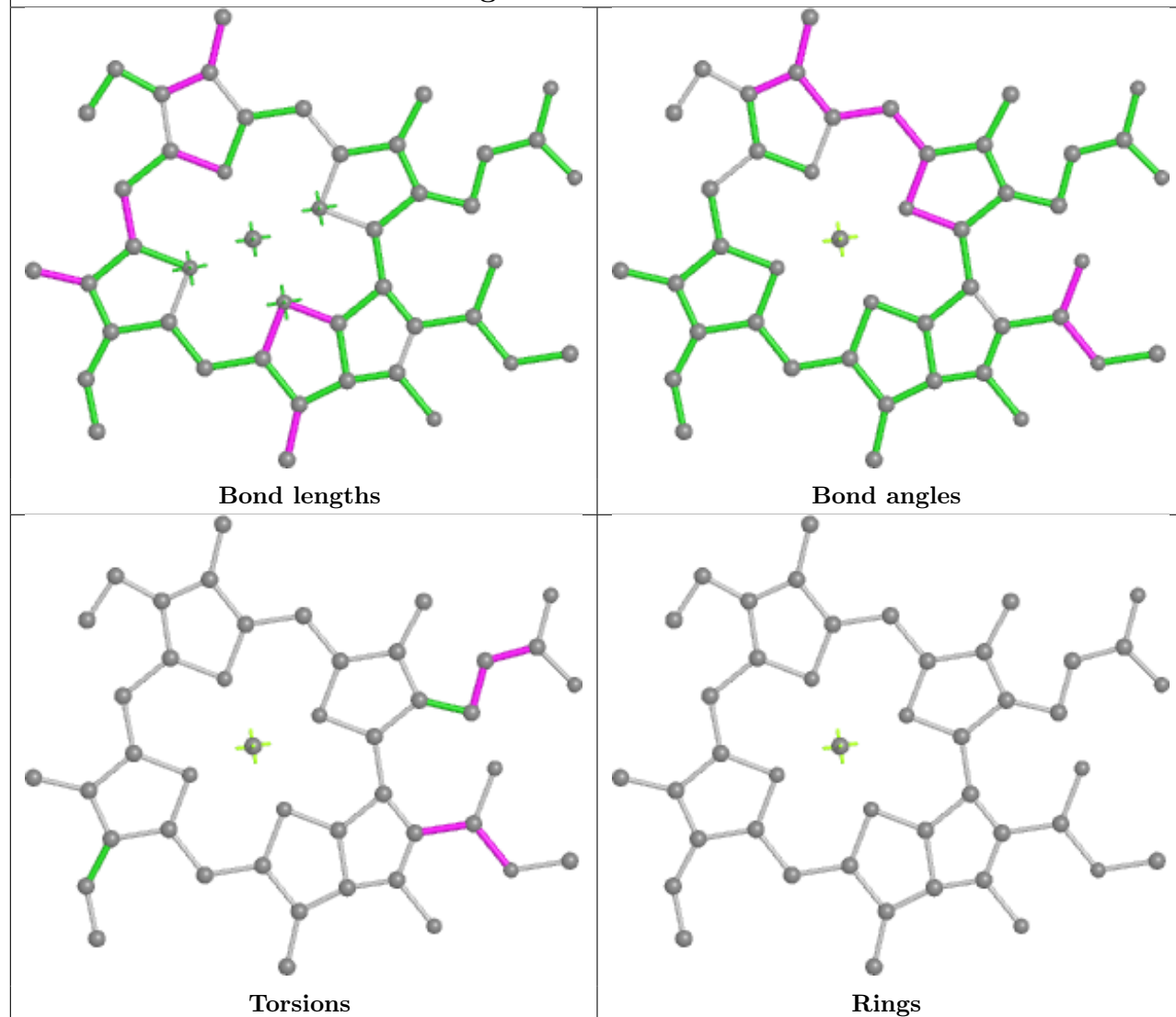
Ligand CLA bA 831



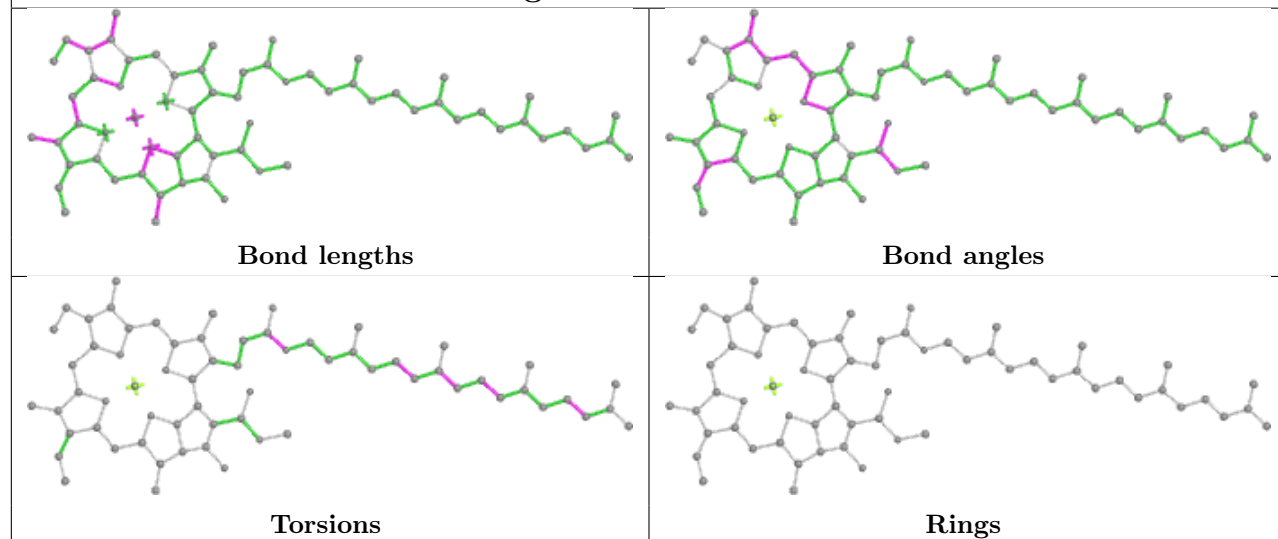


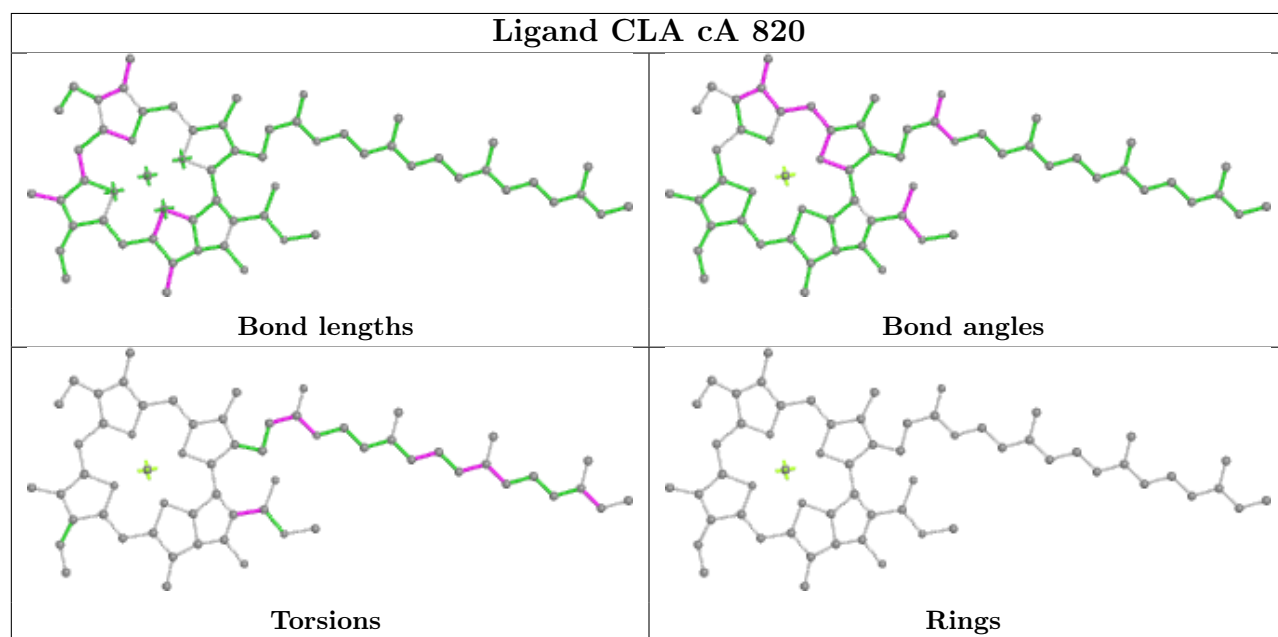
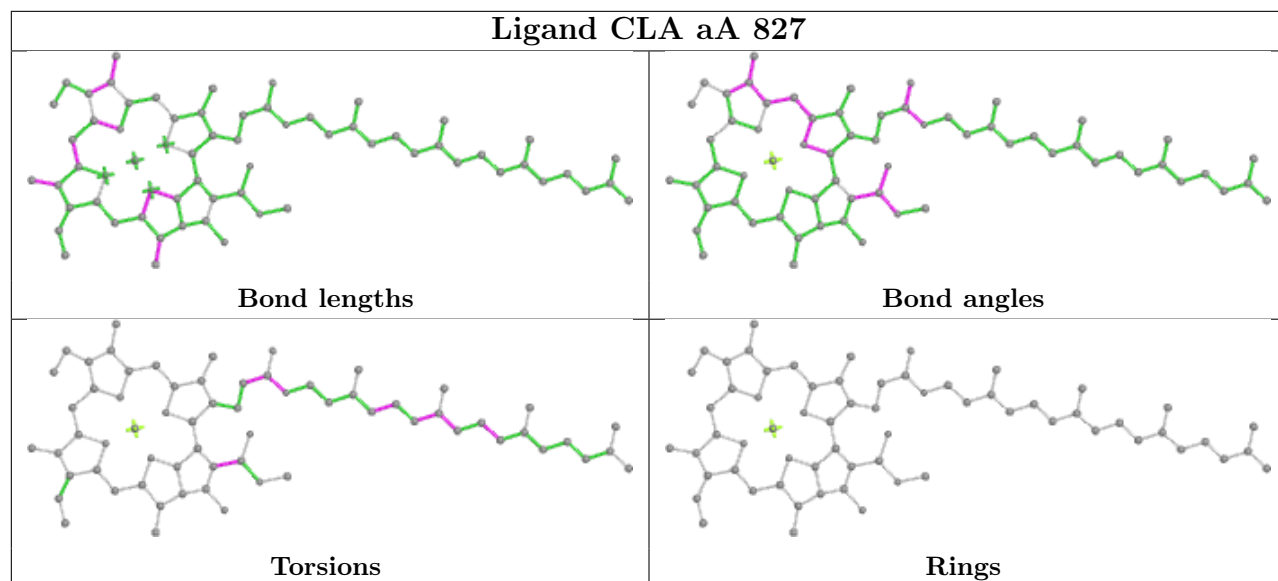
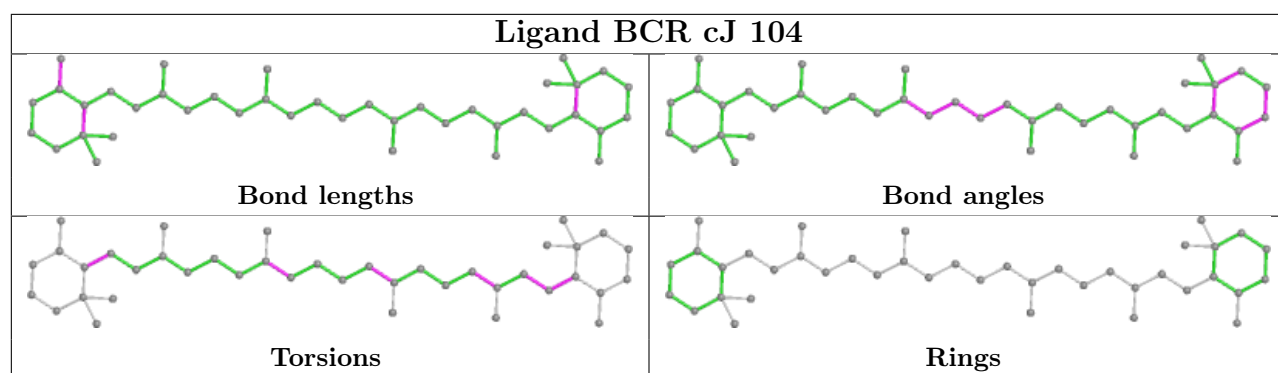


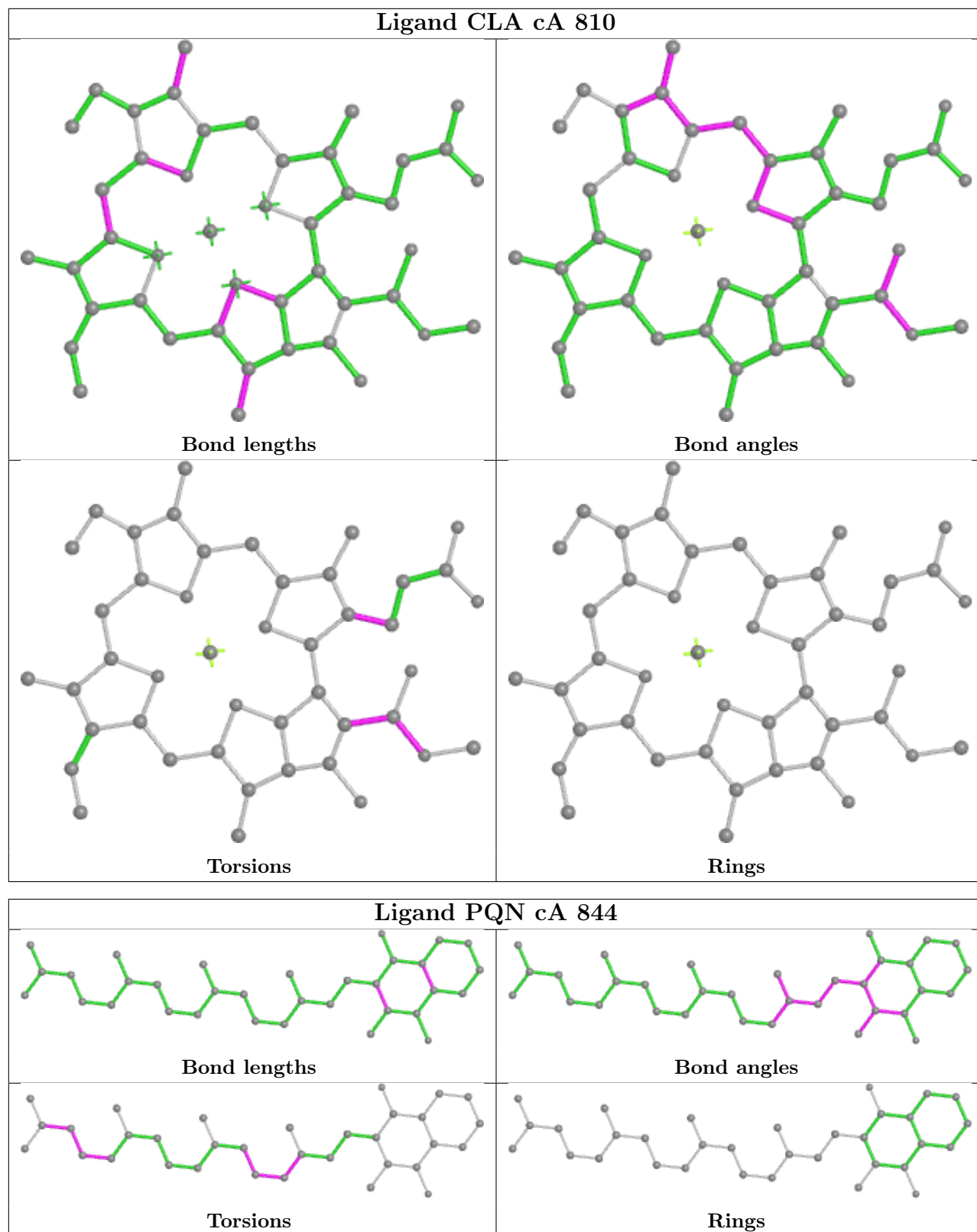
Ligand CLA bX 101

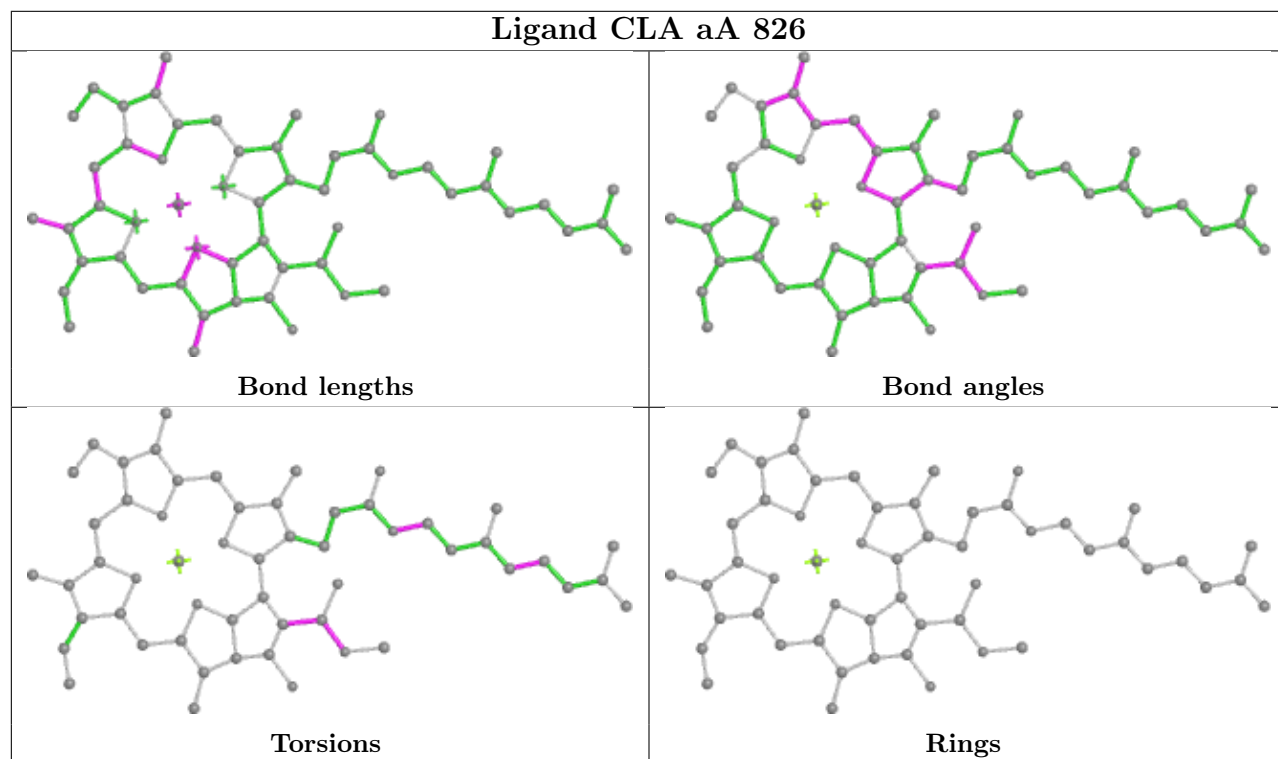
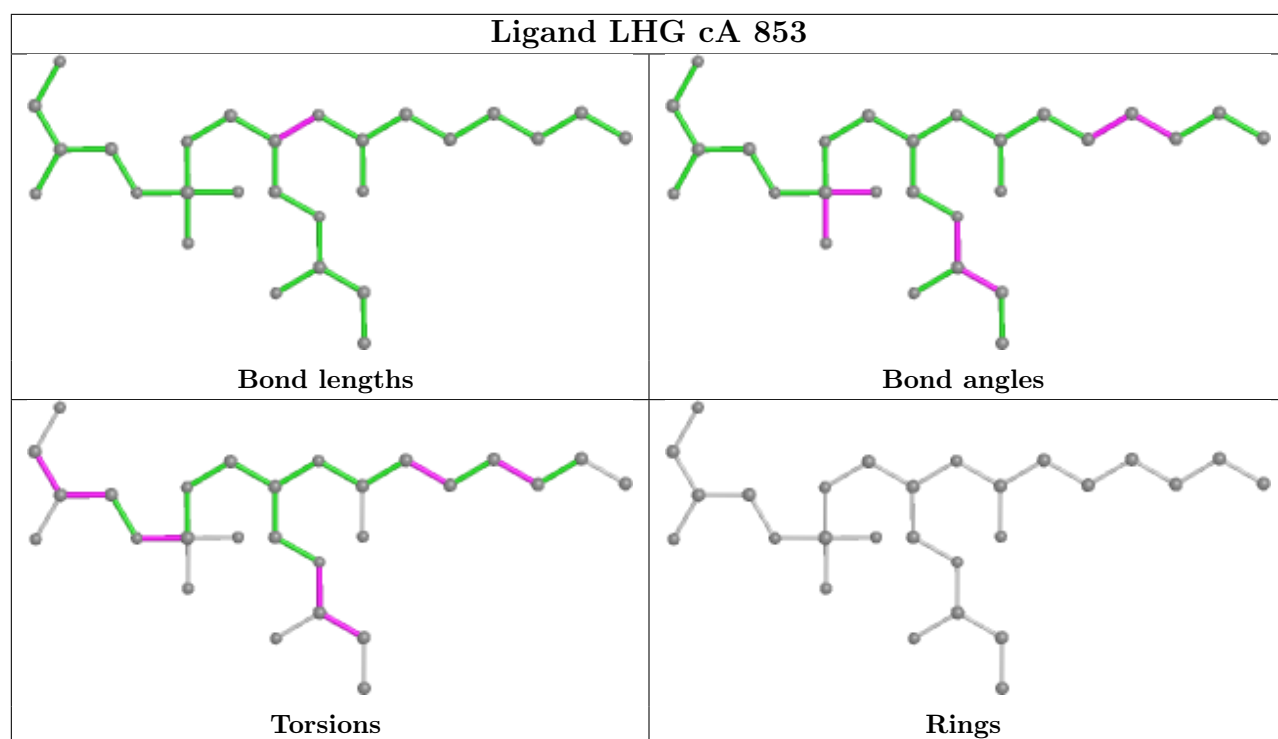


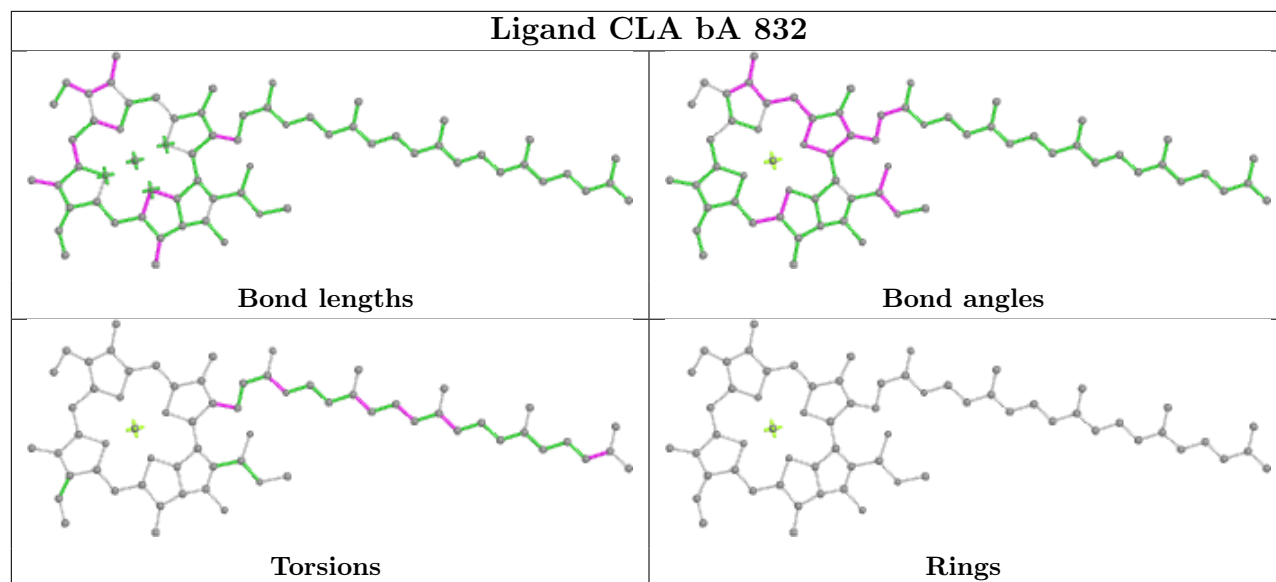
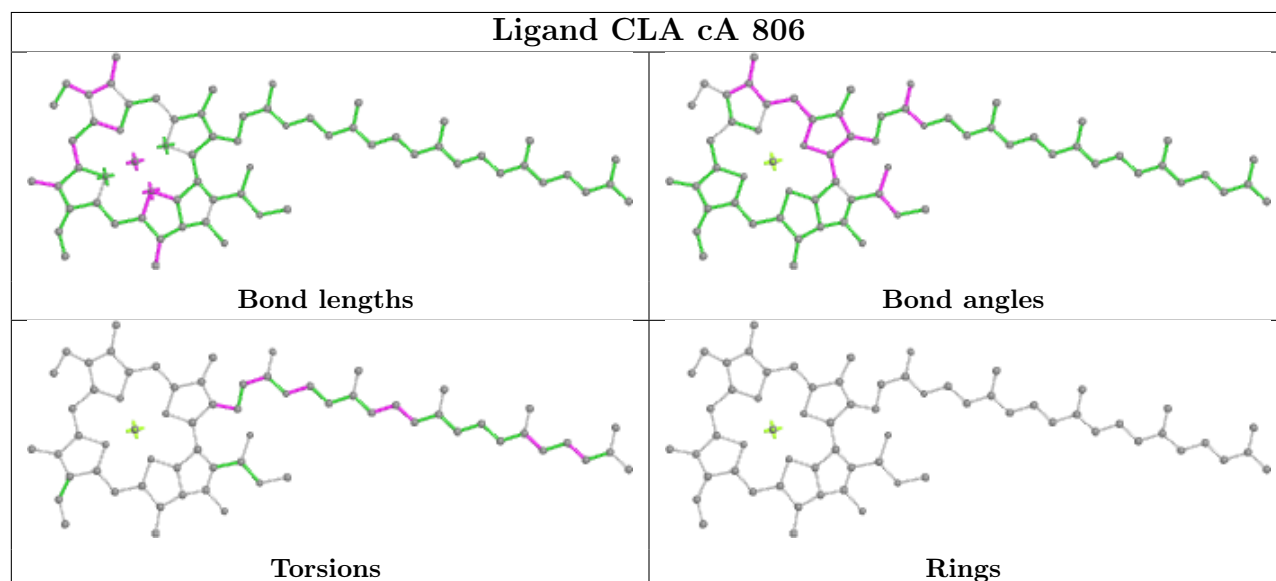
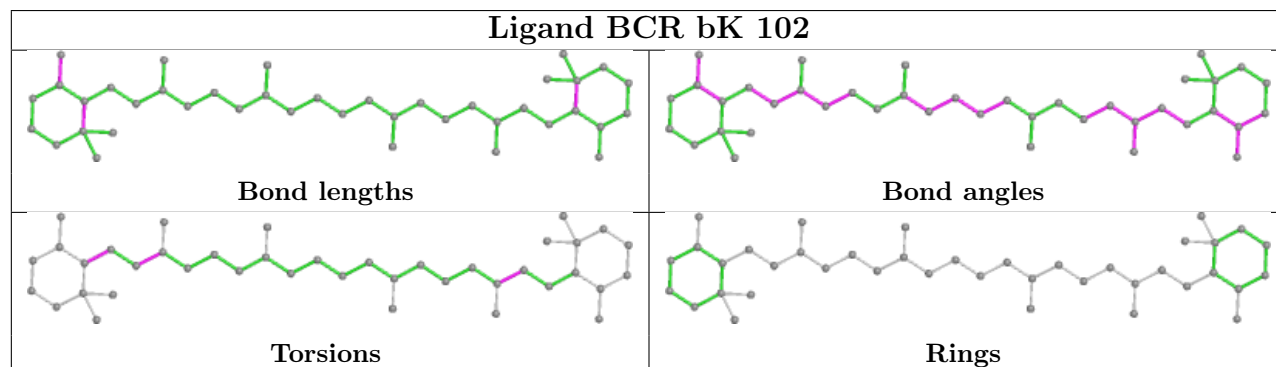
Ligand CLA bL 201

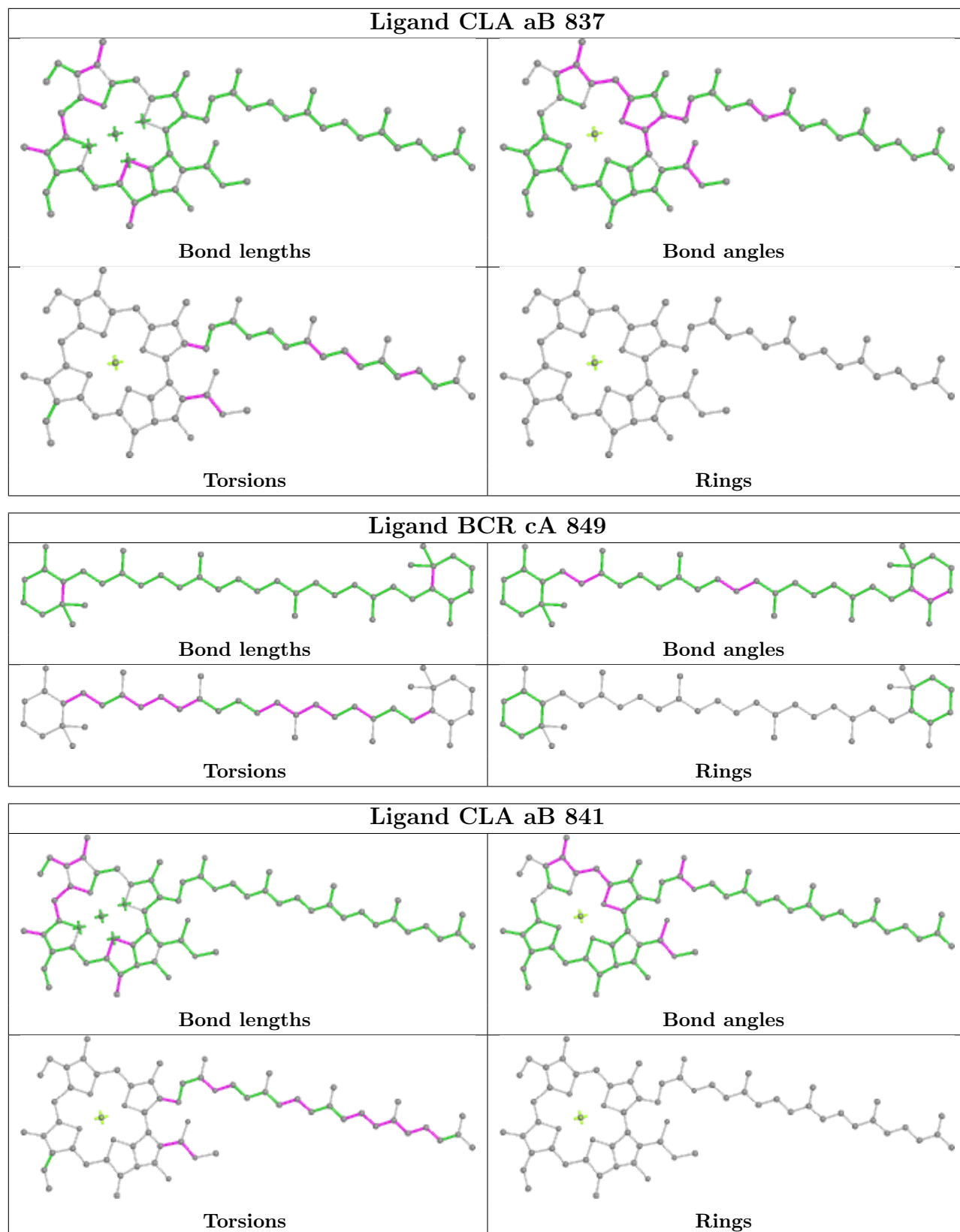




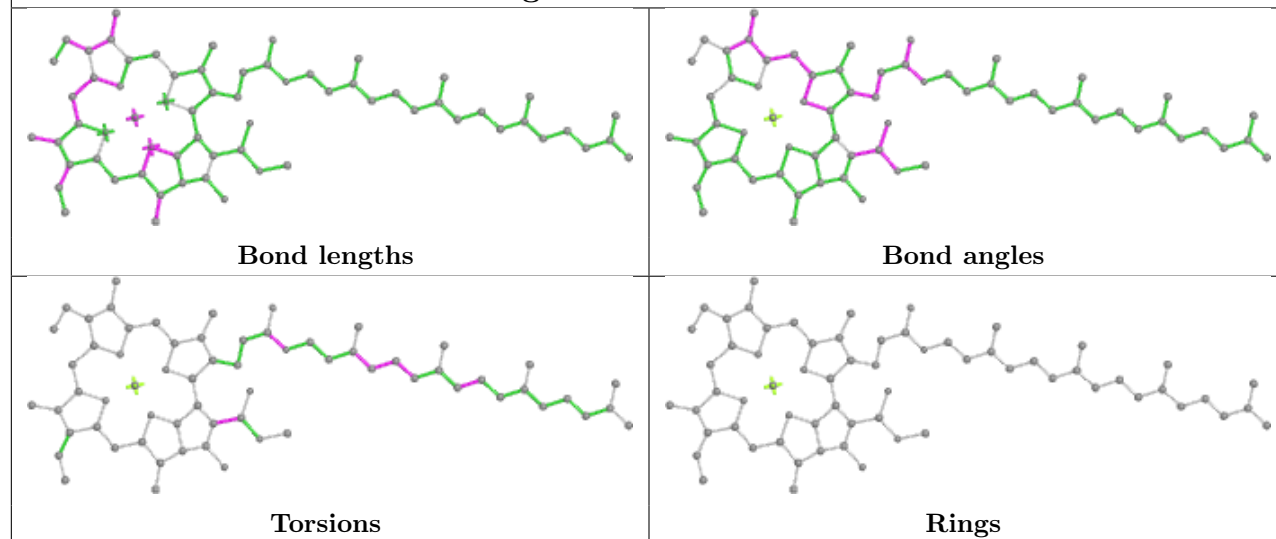




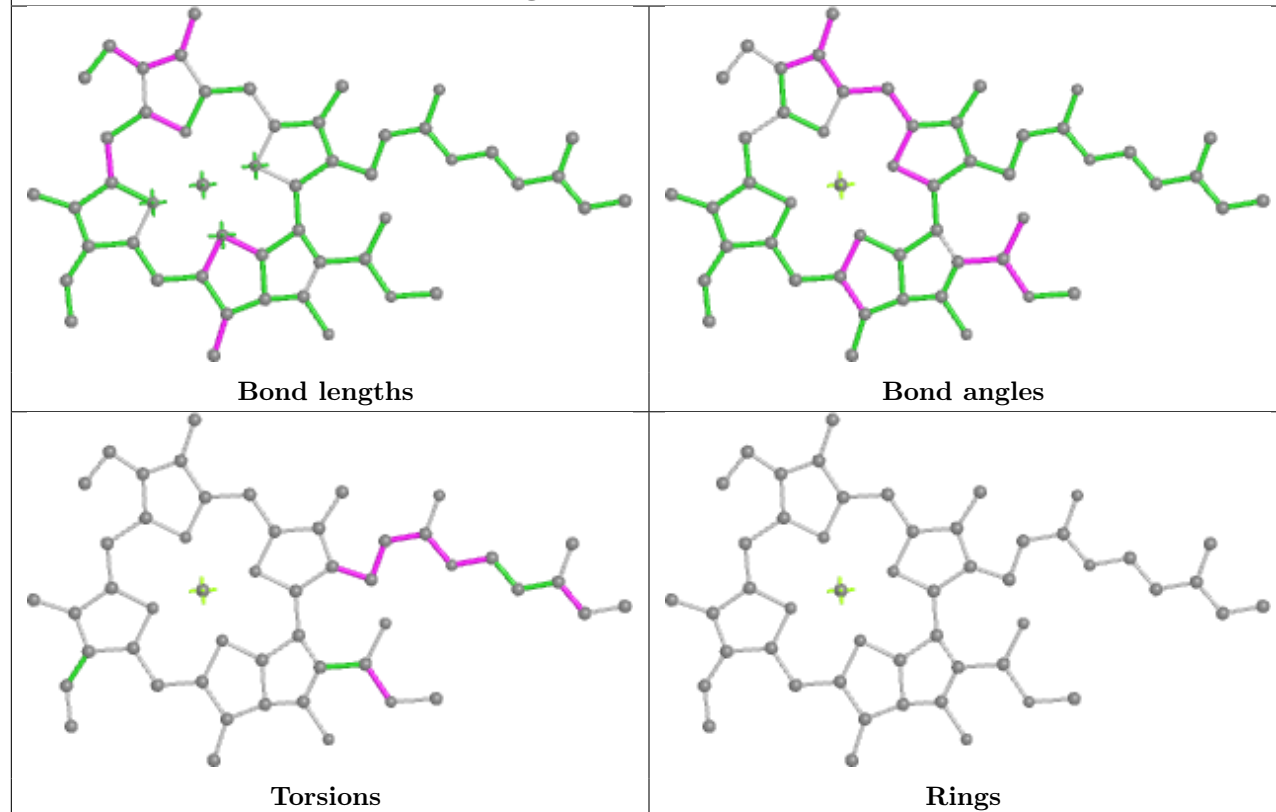
Ligand CLA bA 832**Ligand CLA cA 806****Ligand BCR bK 102**

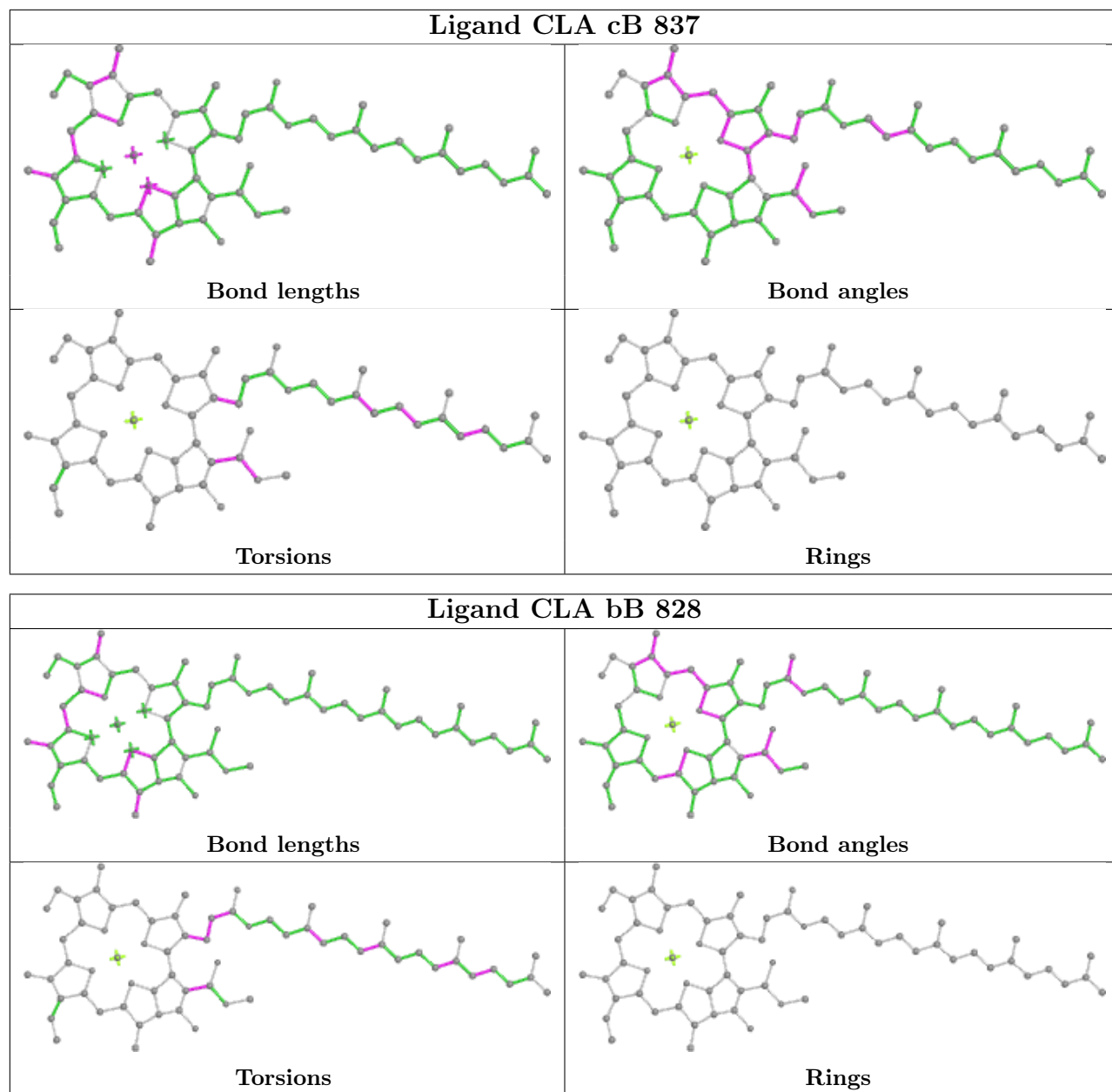


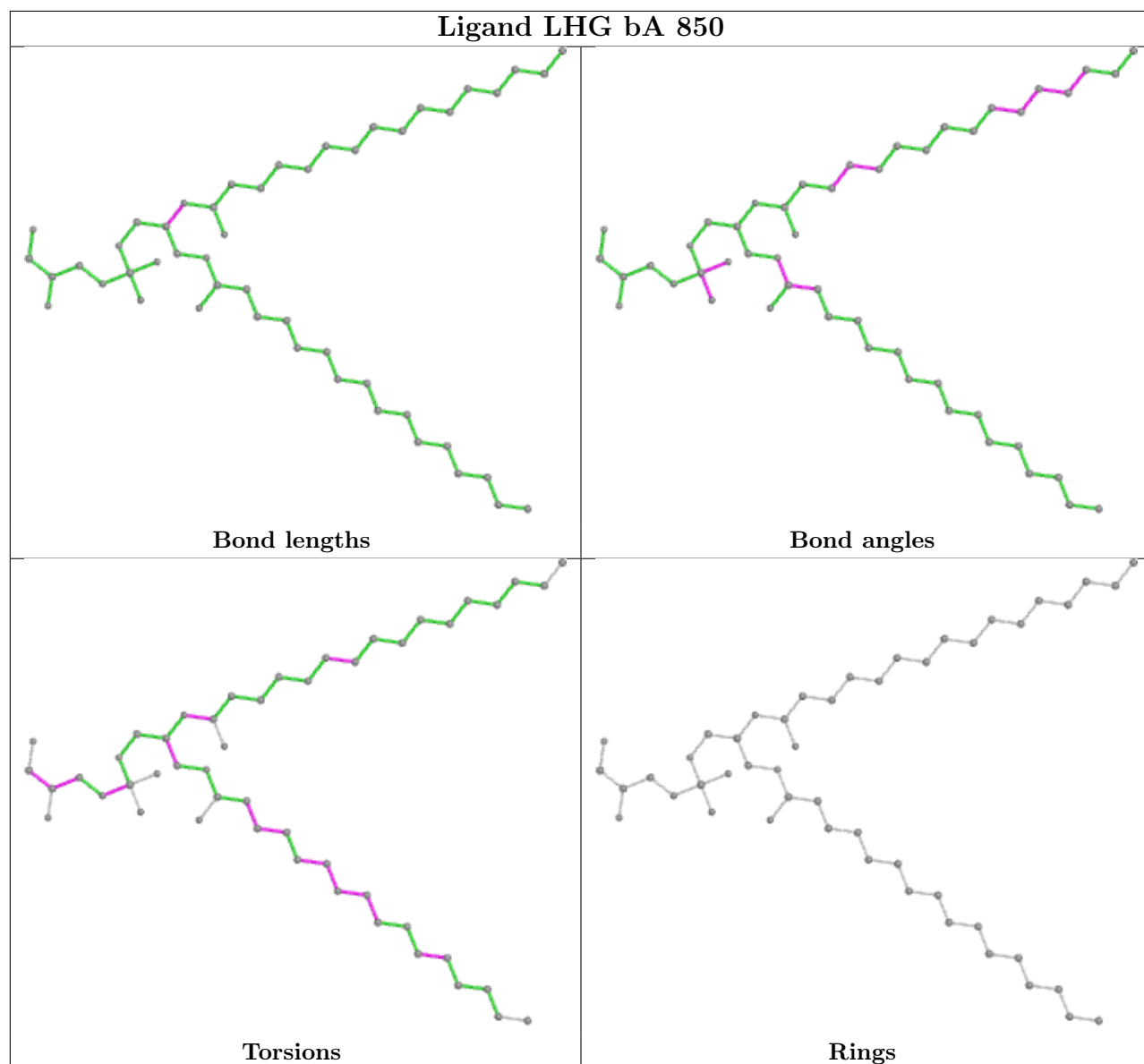
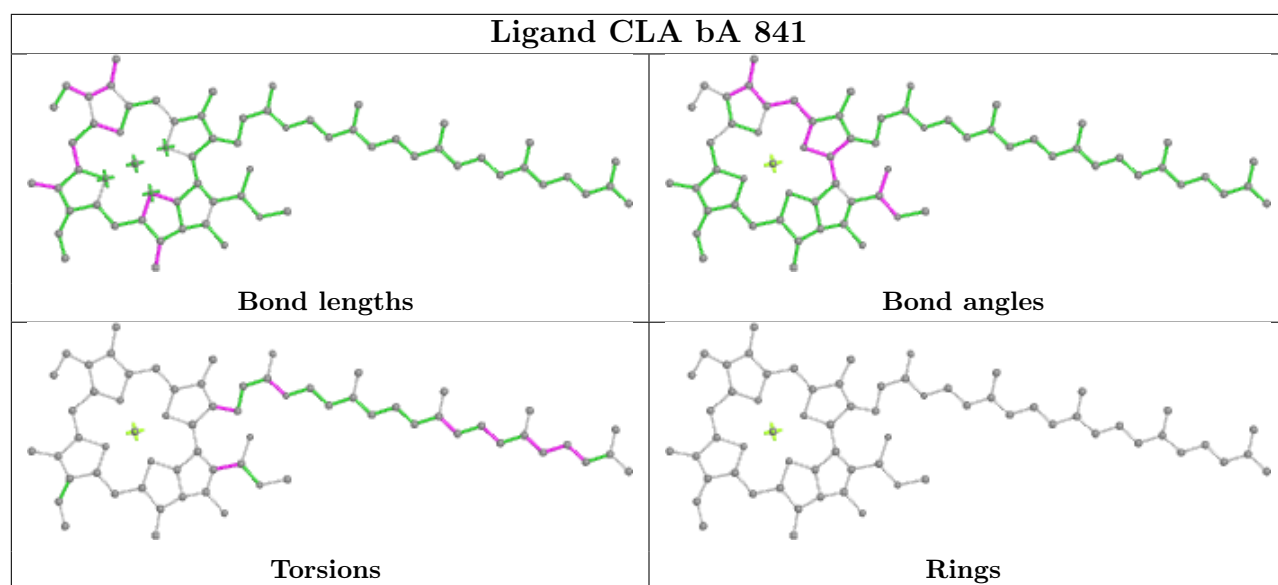
Ligand CLA dB 809



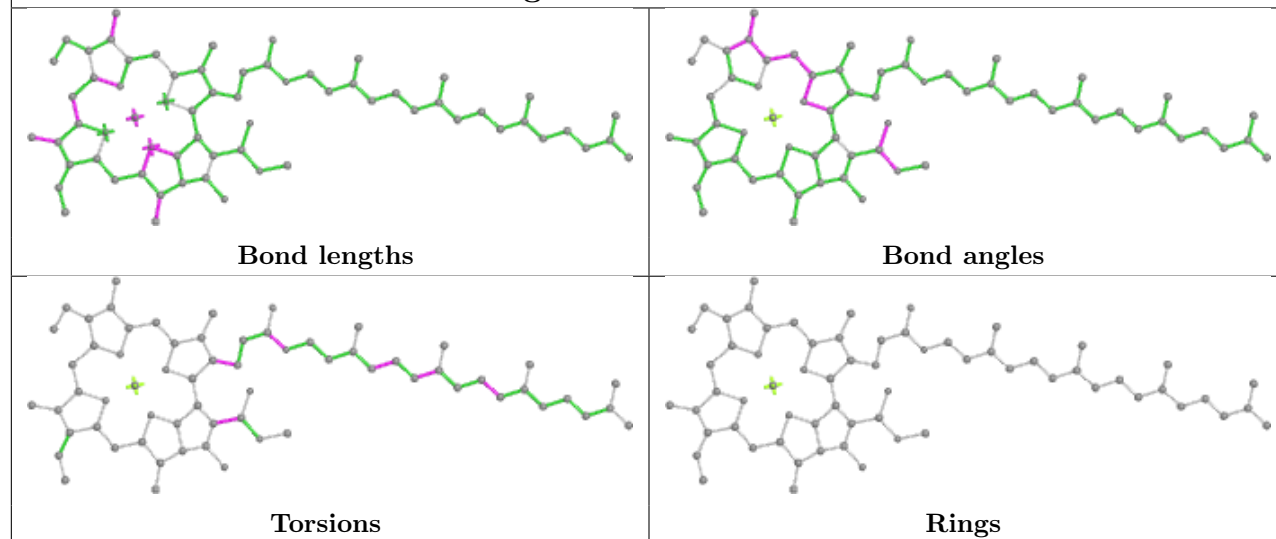
Ligand CLA aA 823



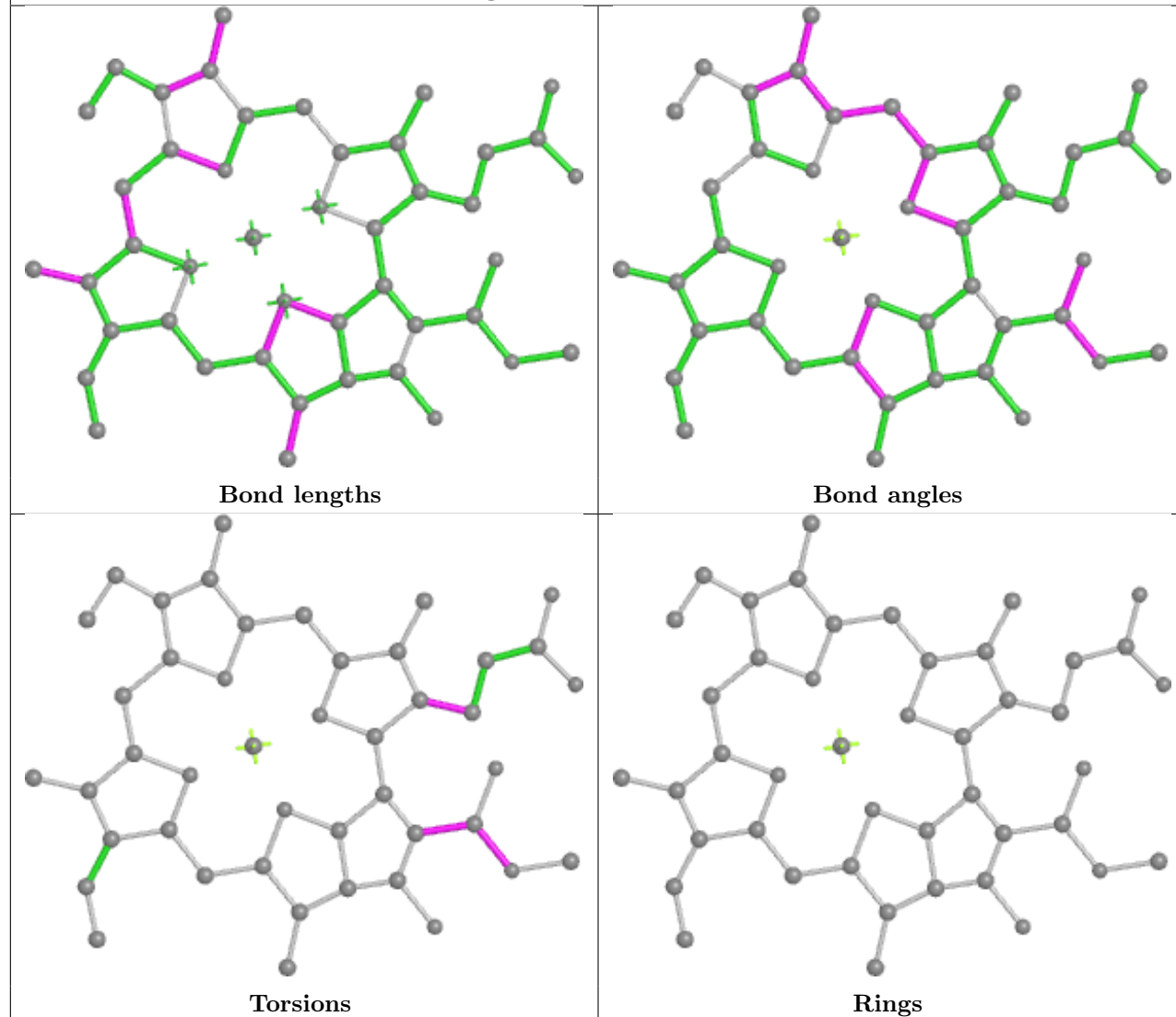




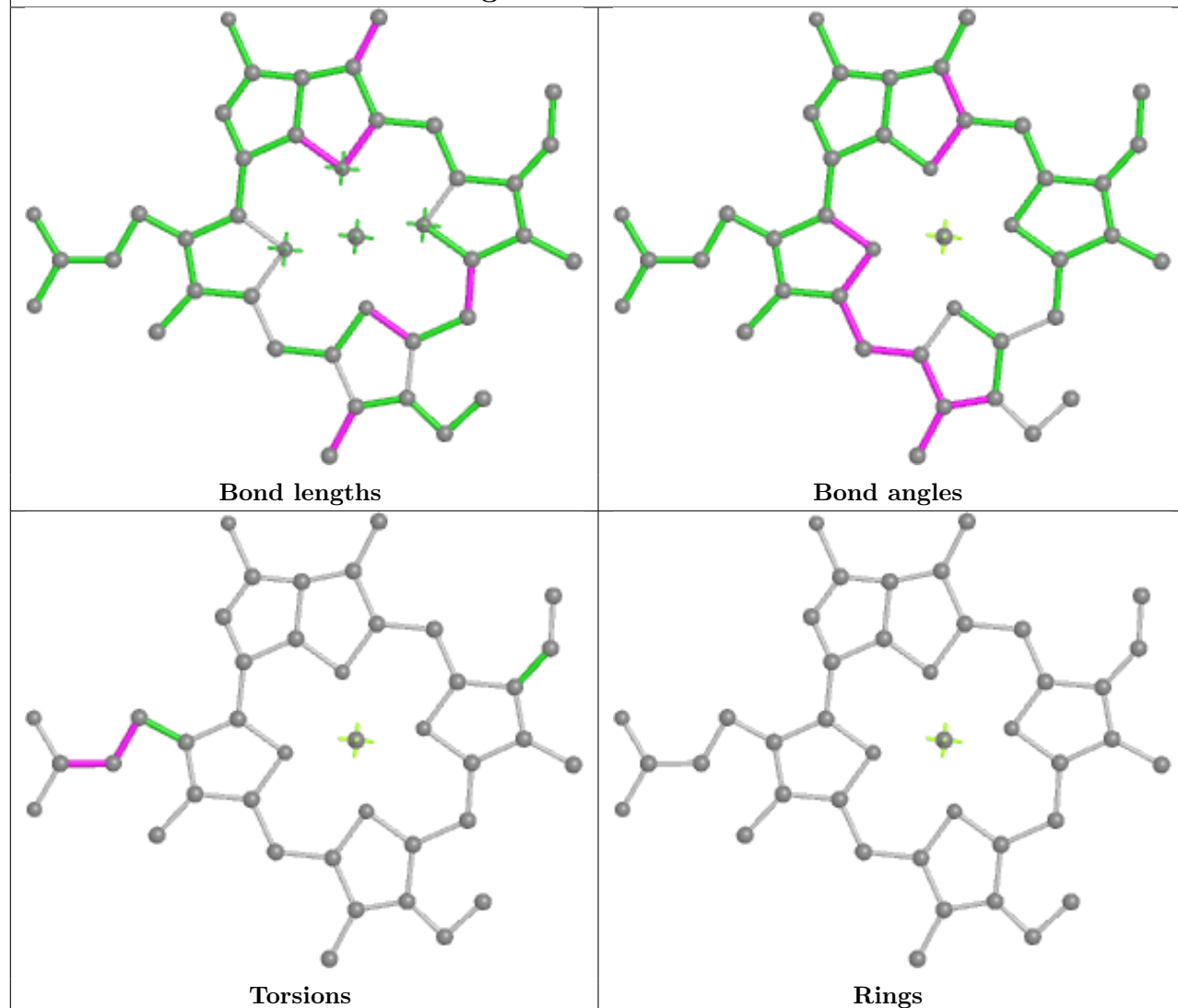
Ligand CLA aB 819



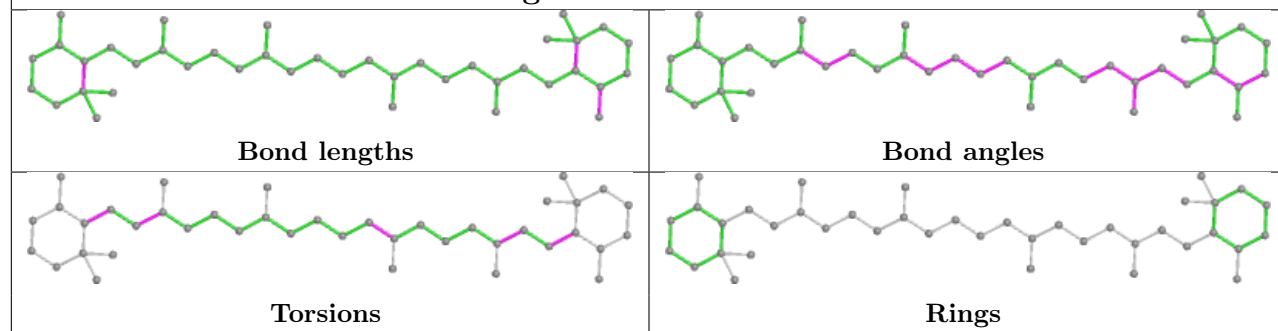
Ligand CLA cB 811

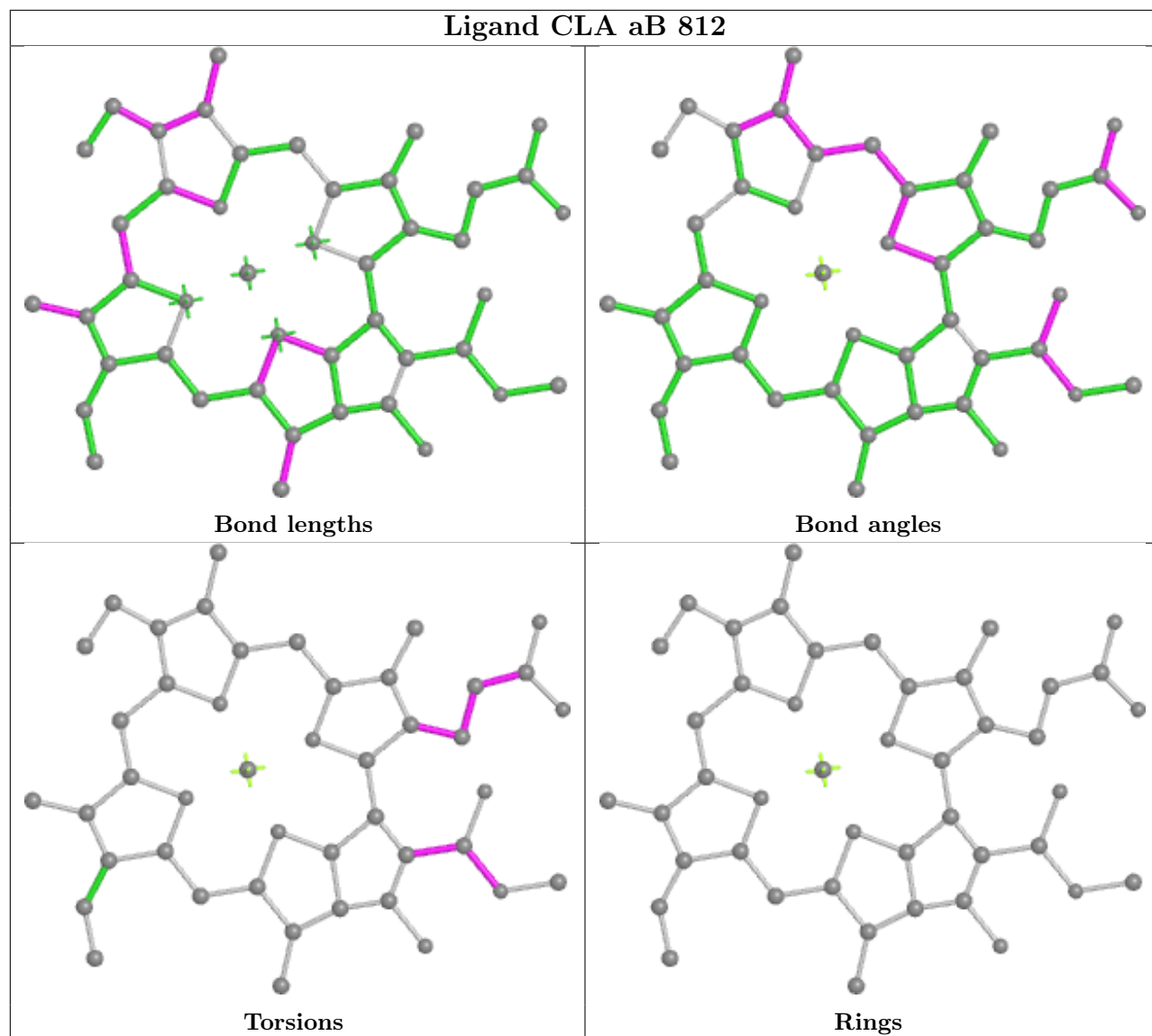
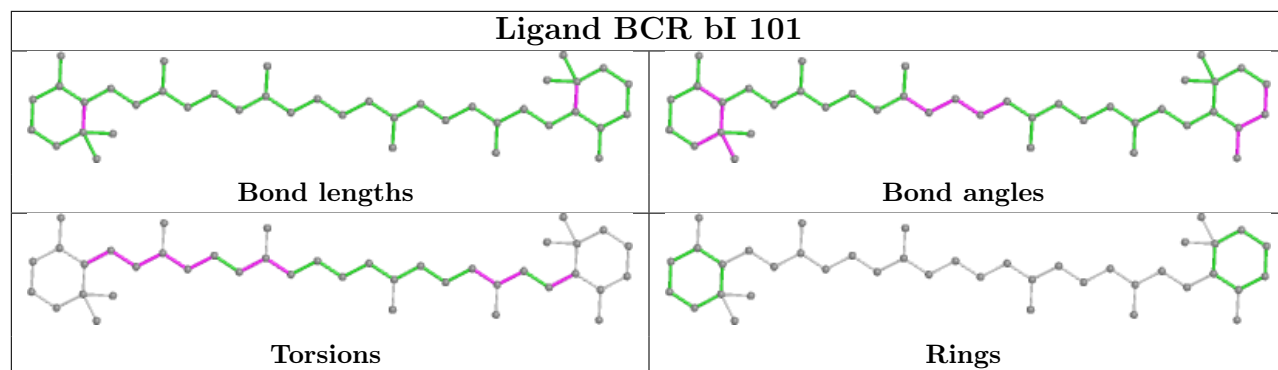


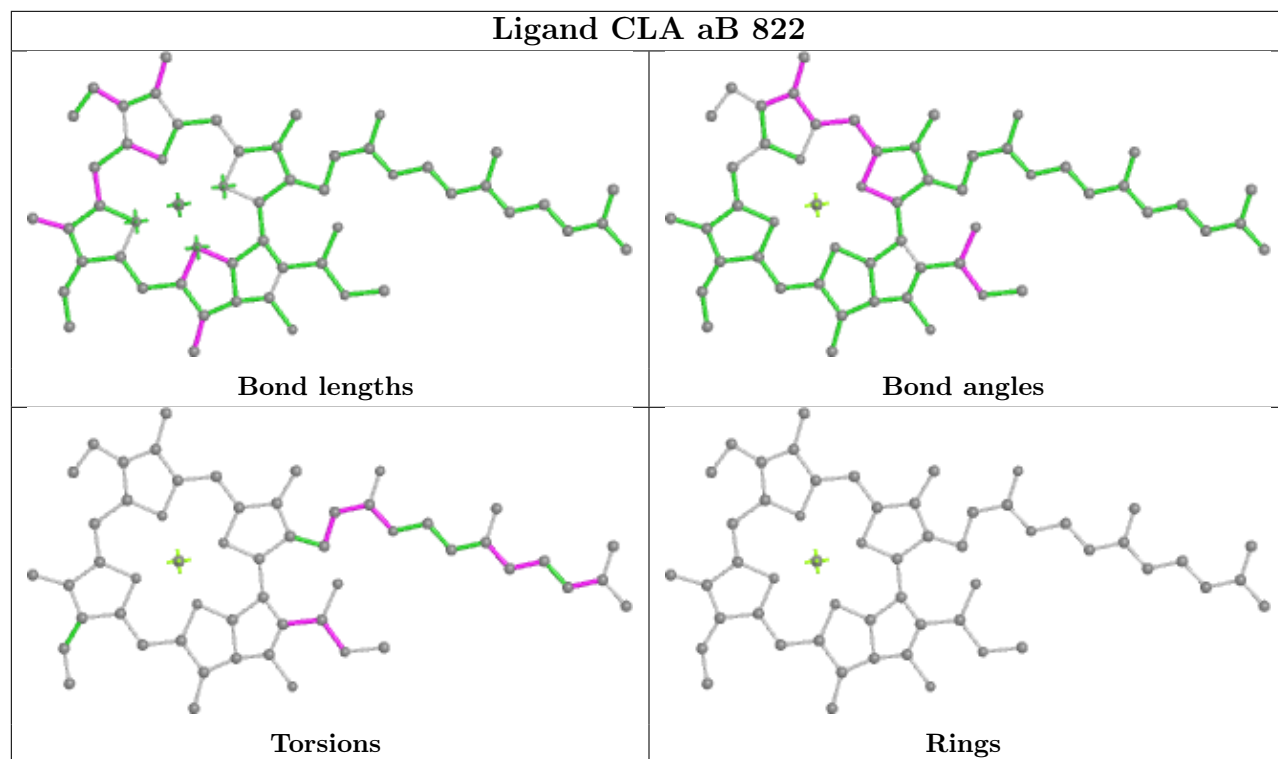
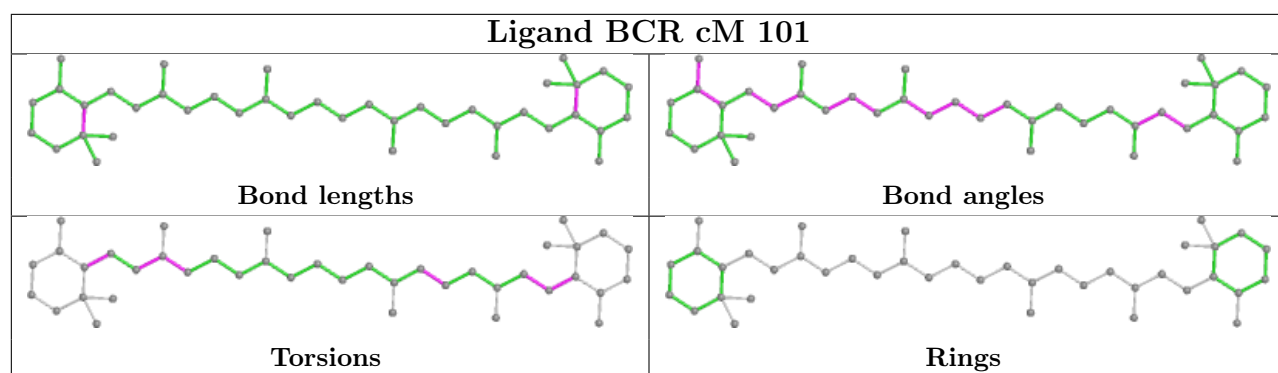
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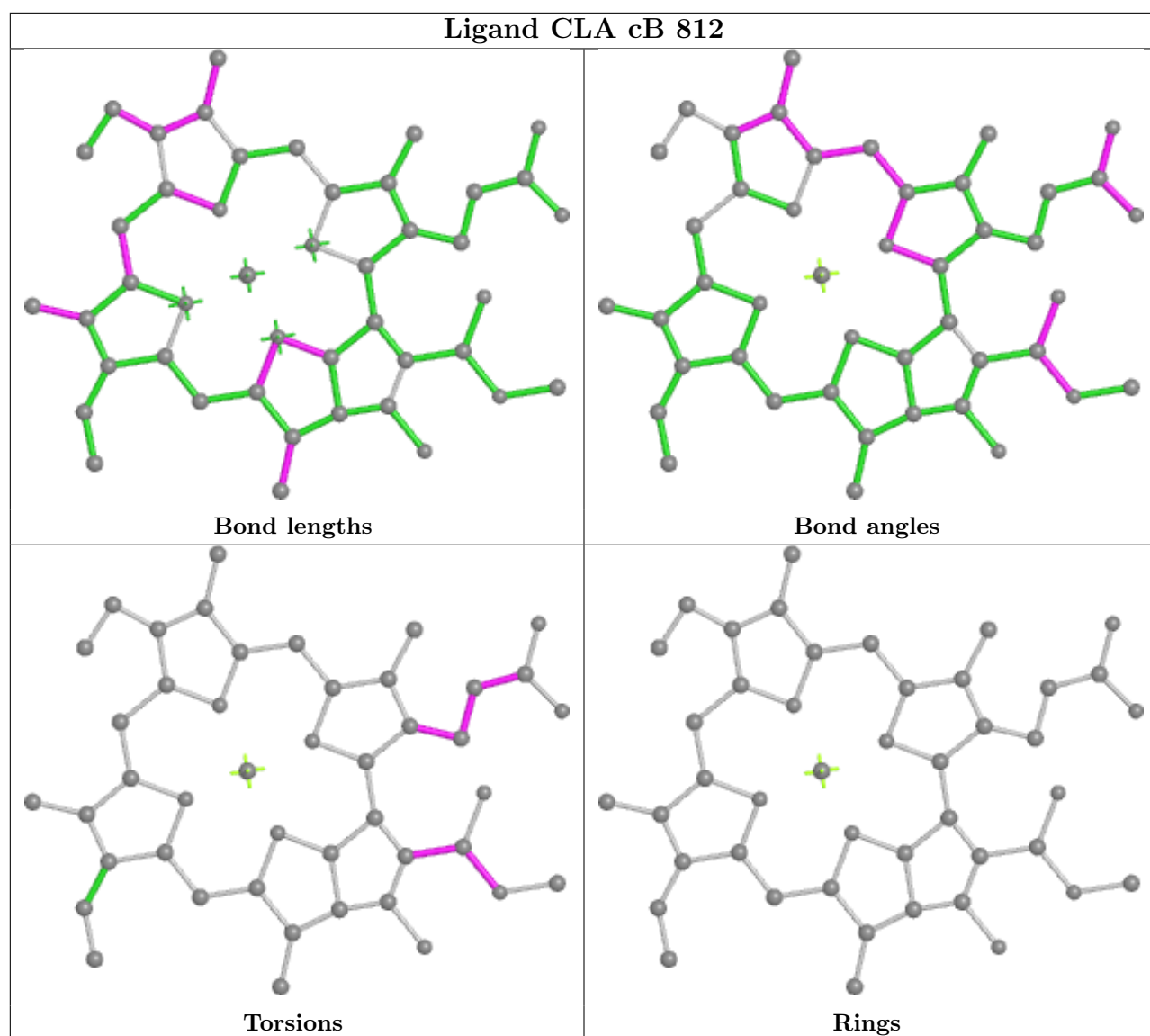


Ligand BCR bL 207

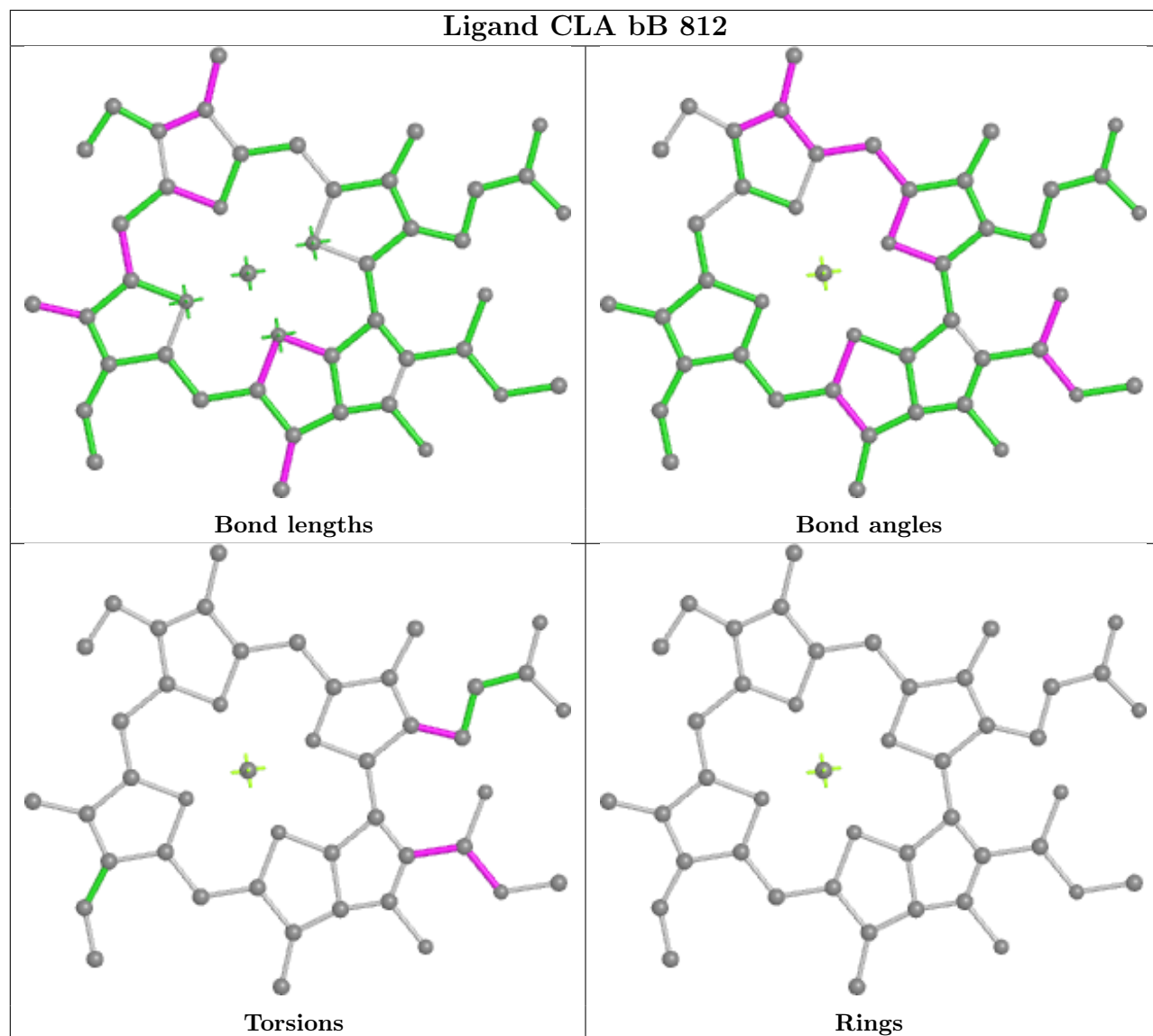


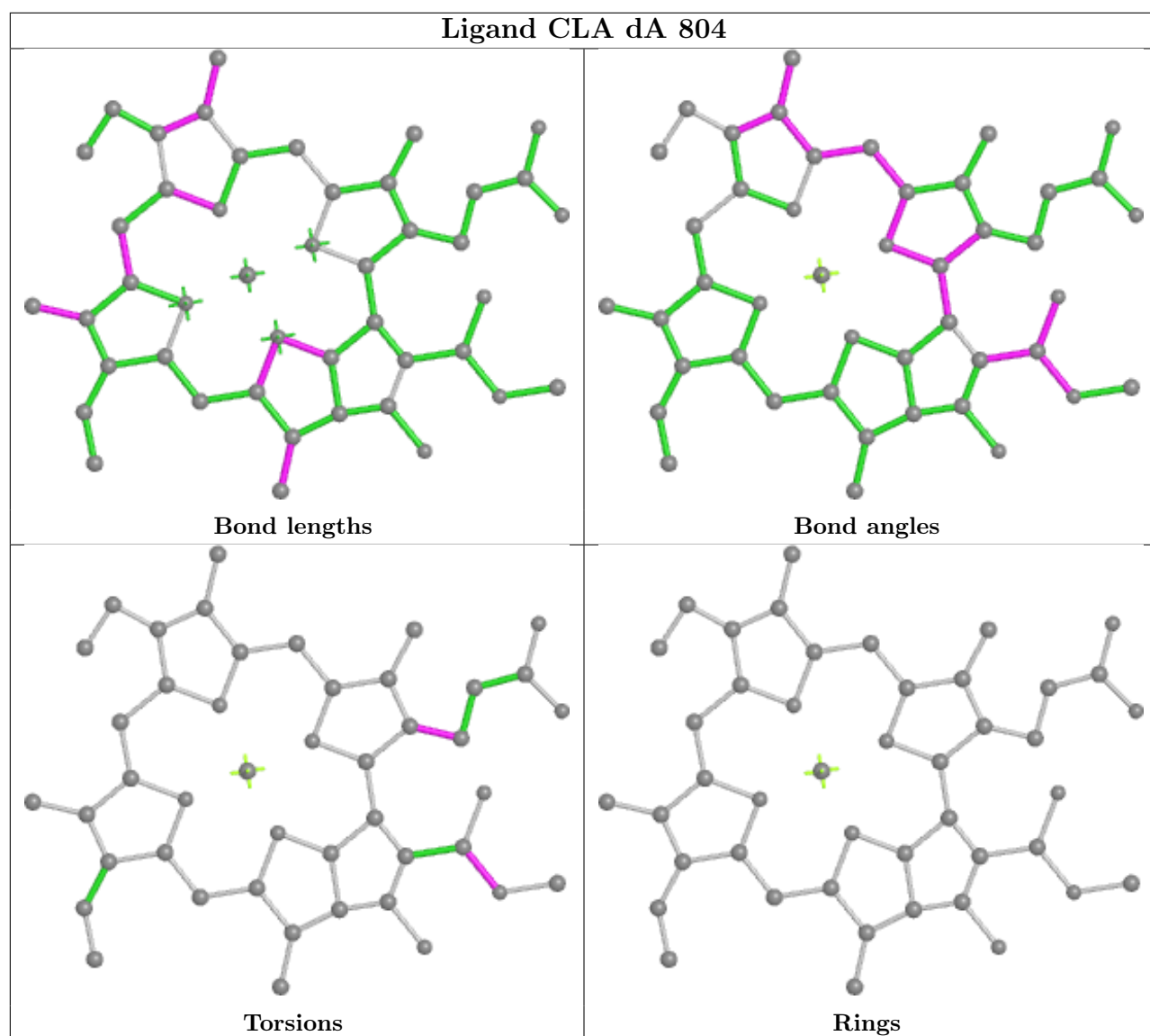




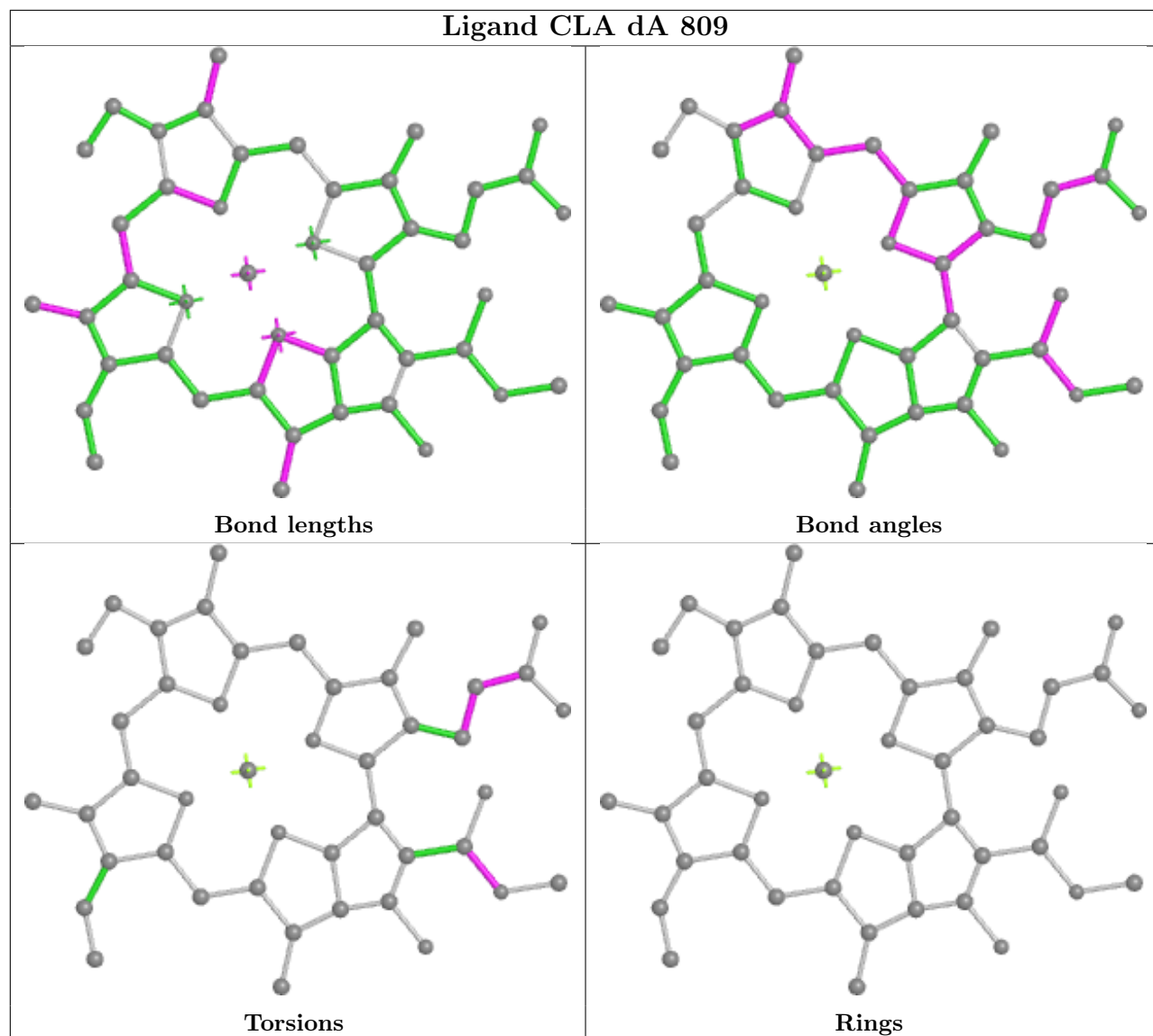


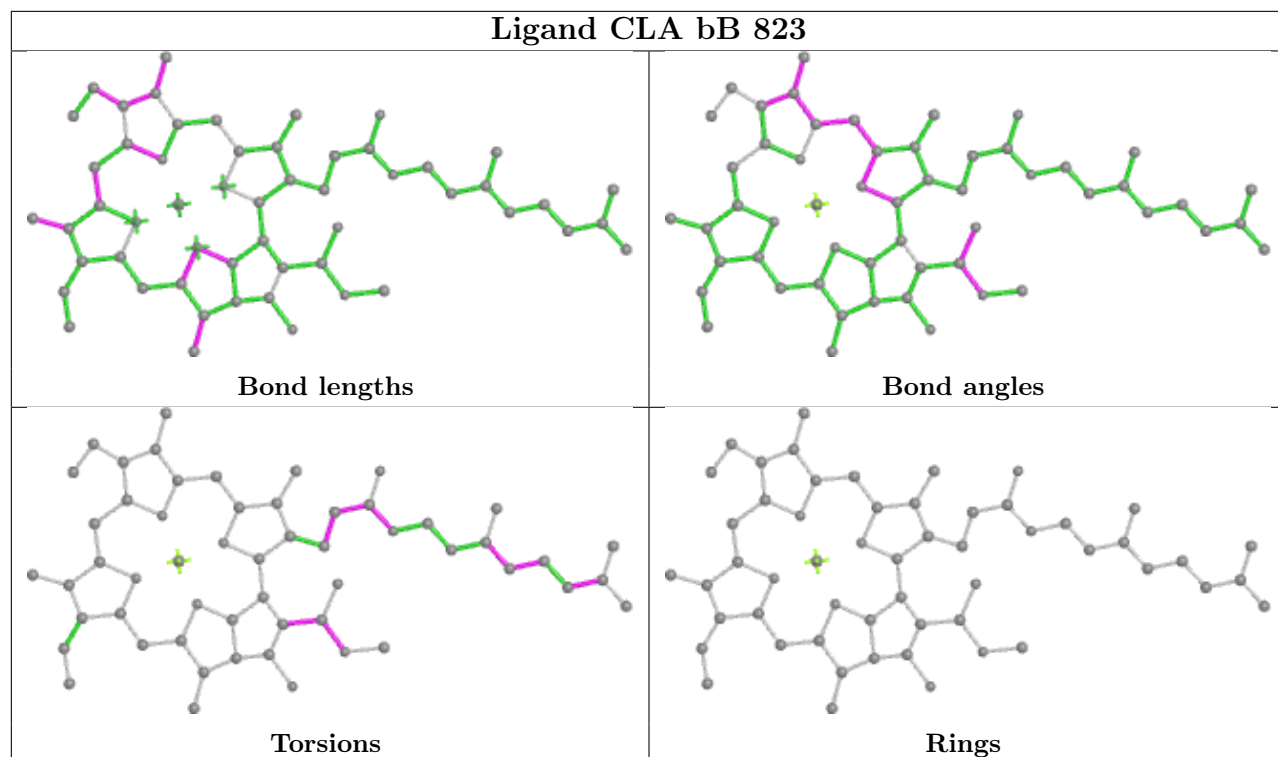
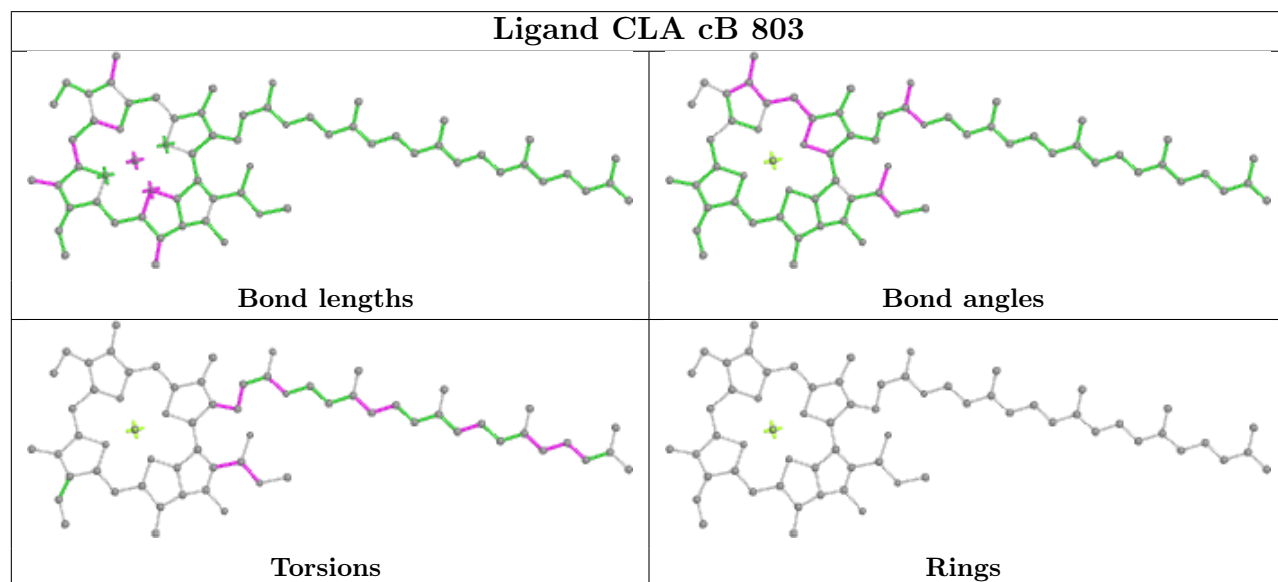
Ligand CLA bB 812

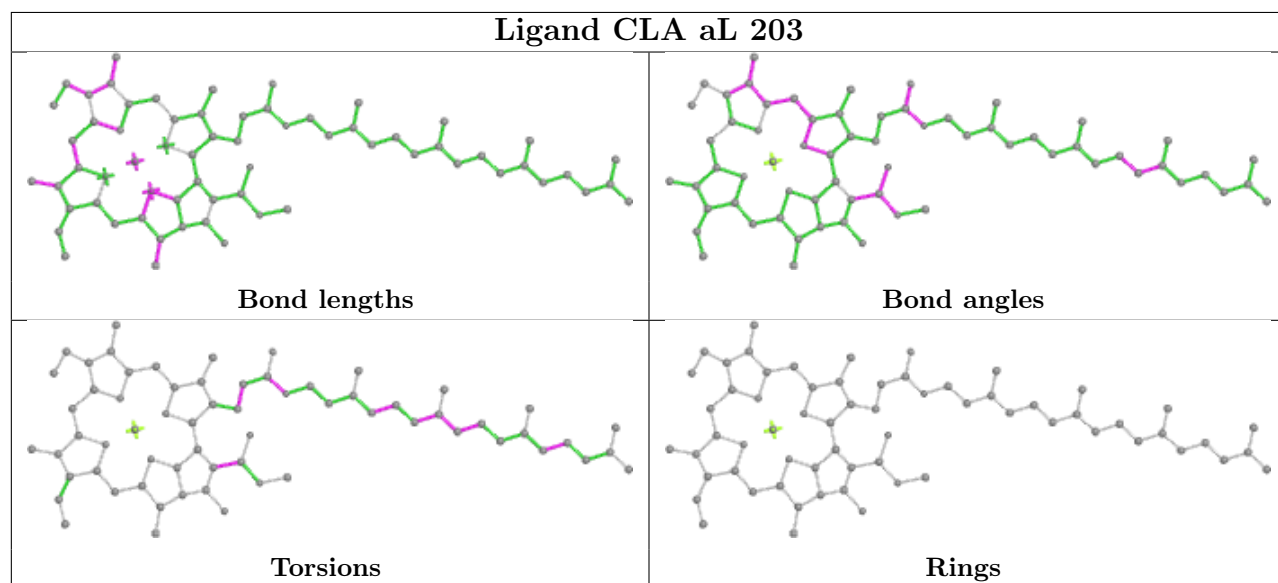
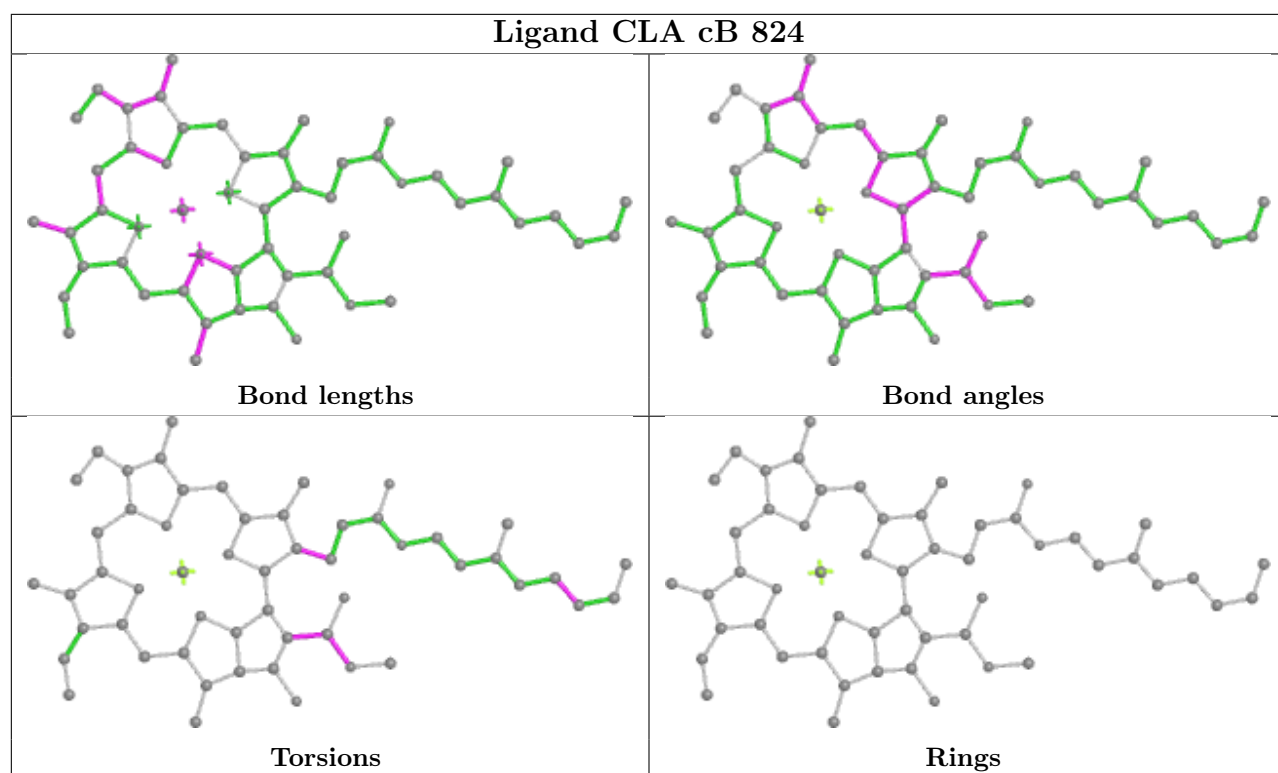


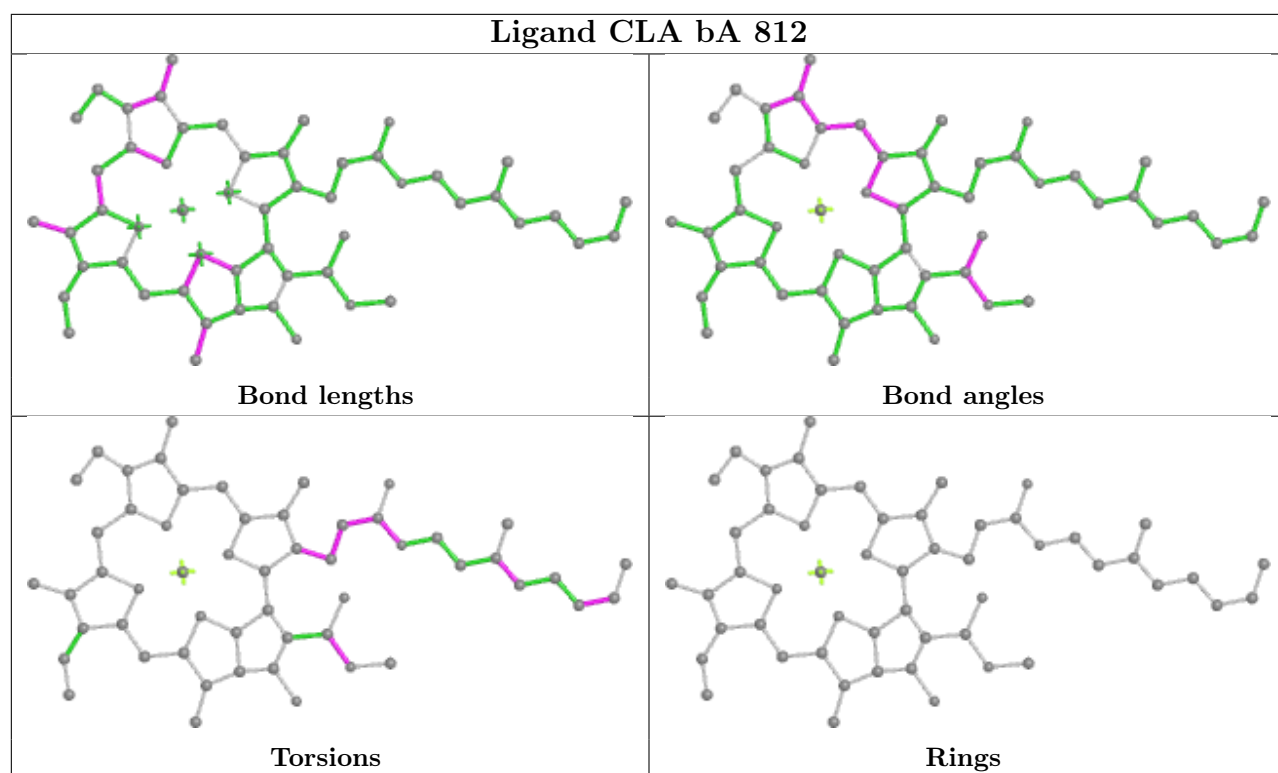


Ligand CLA dA 809

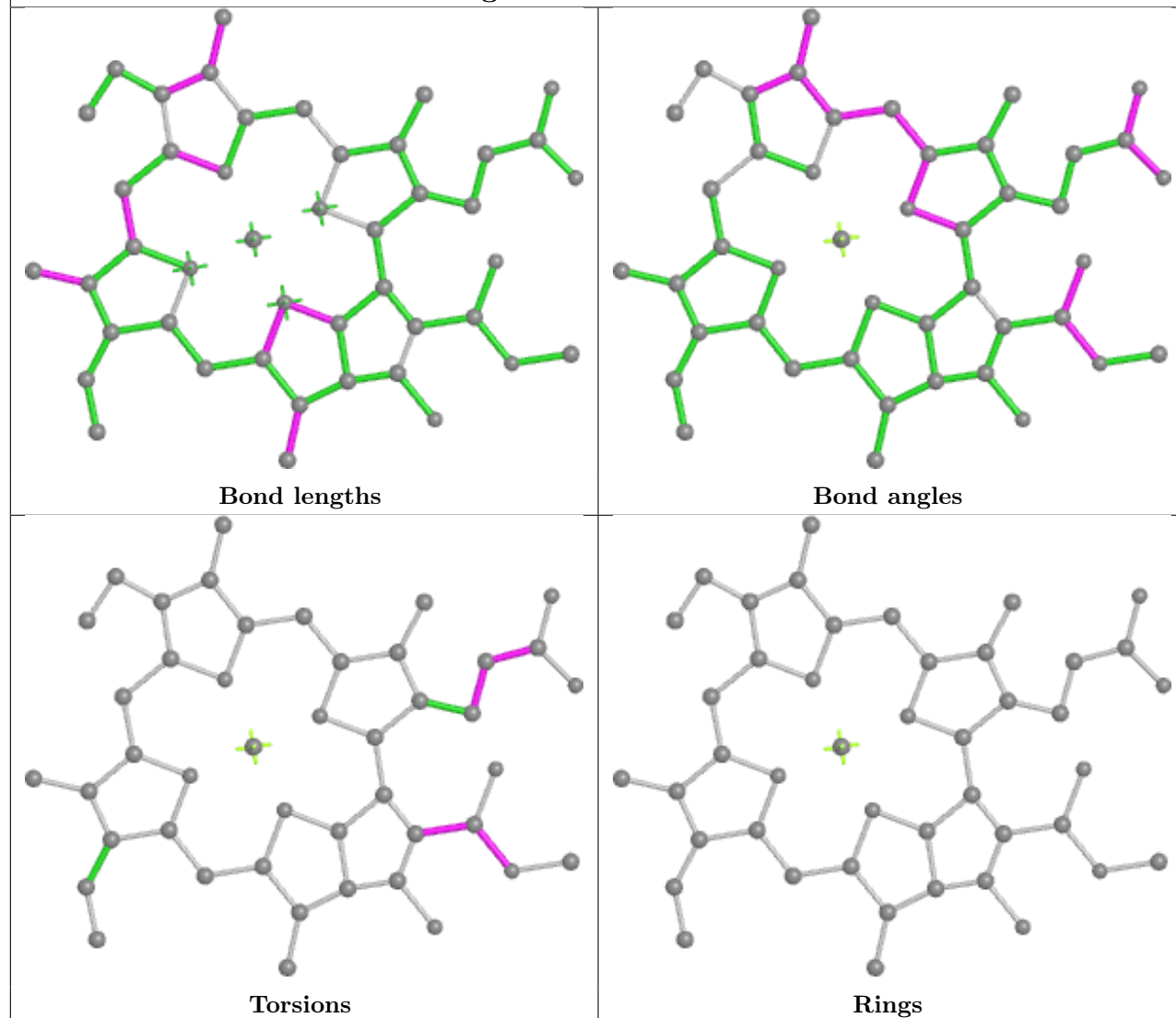


Ligand CLA bB 823**Ligand CLA cB 803**

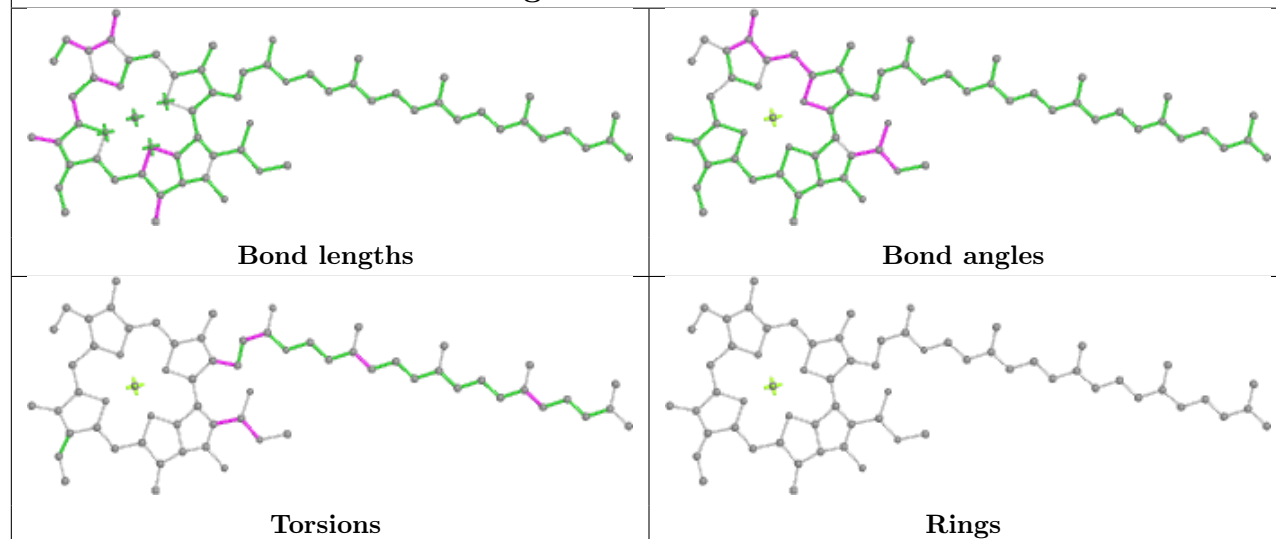


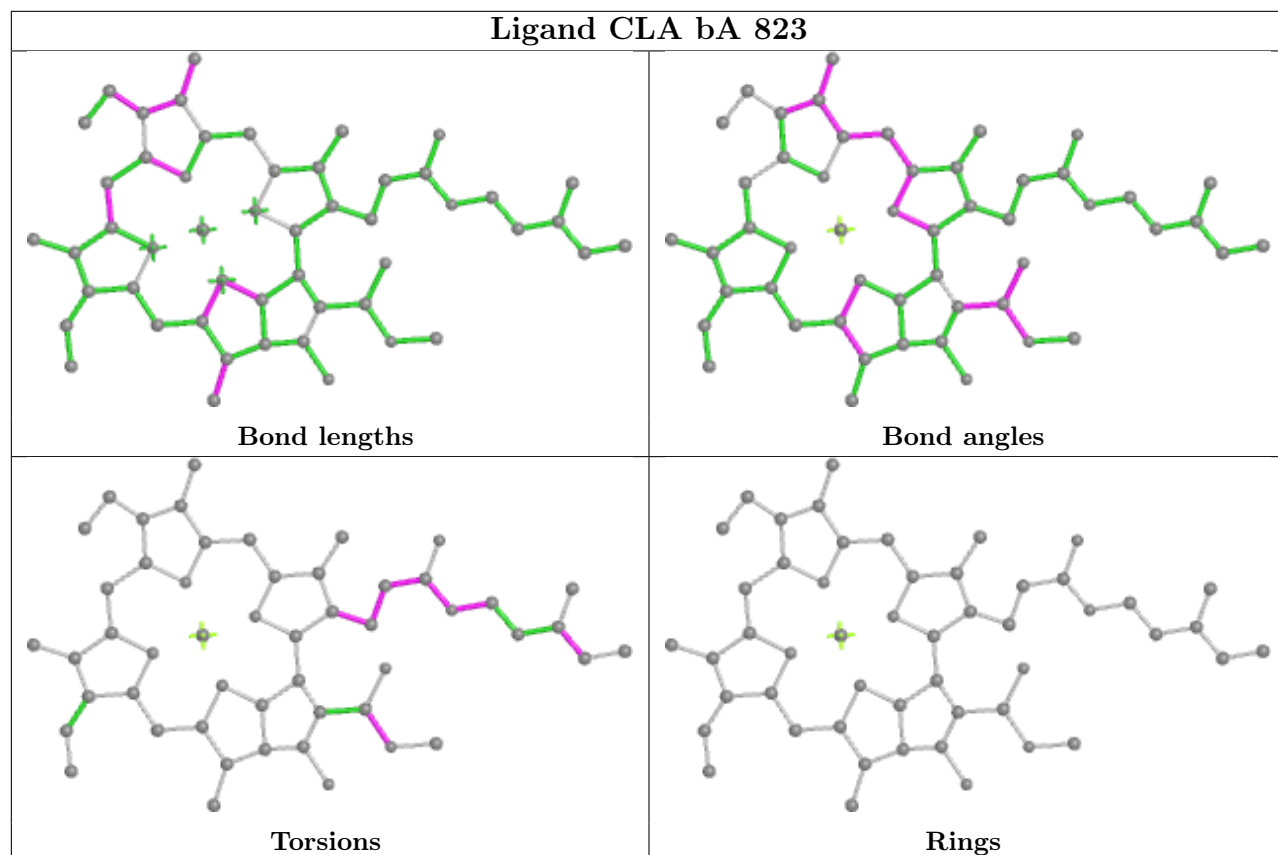
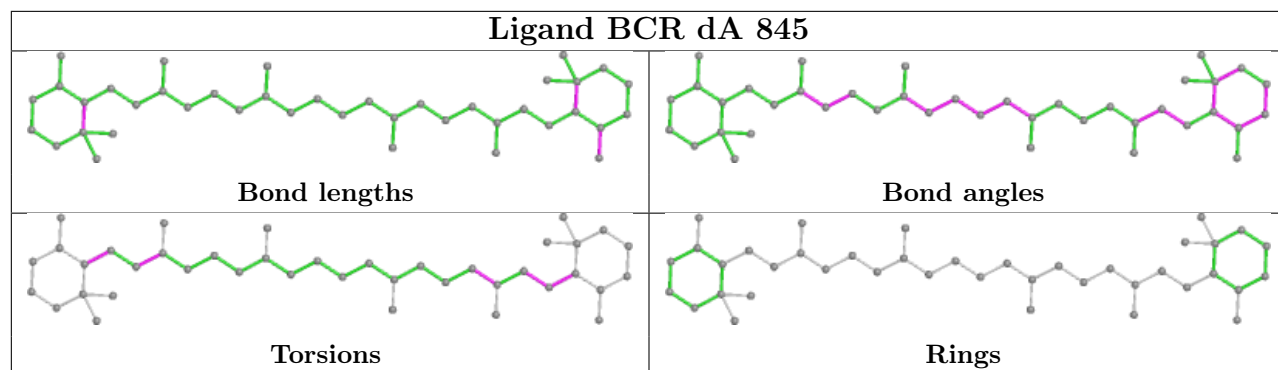


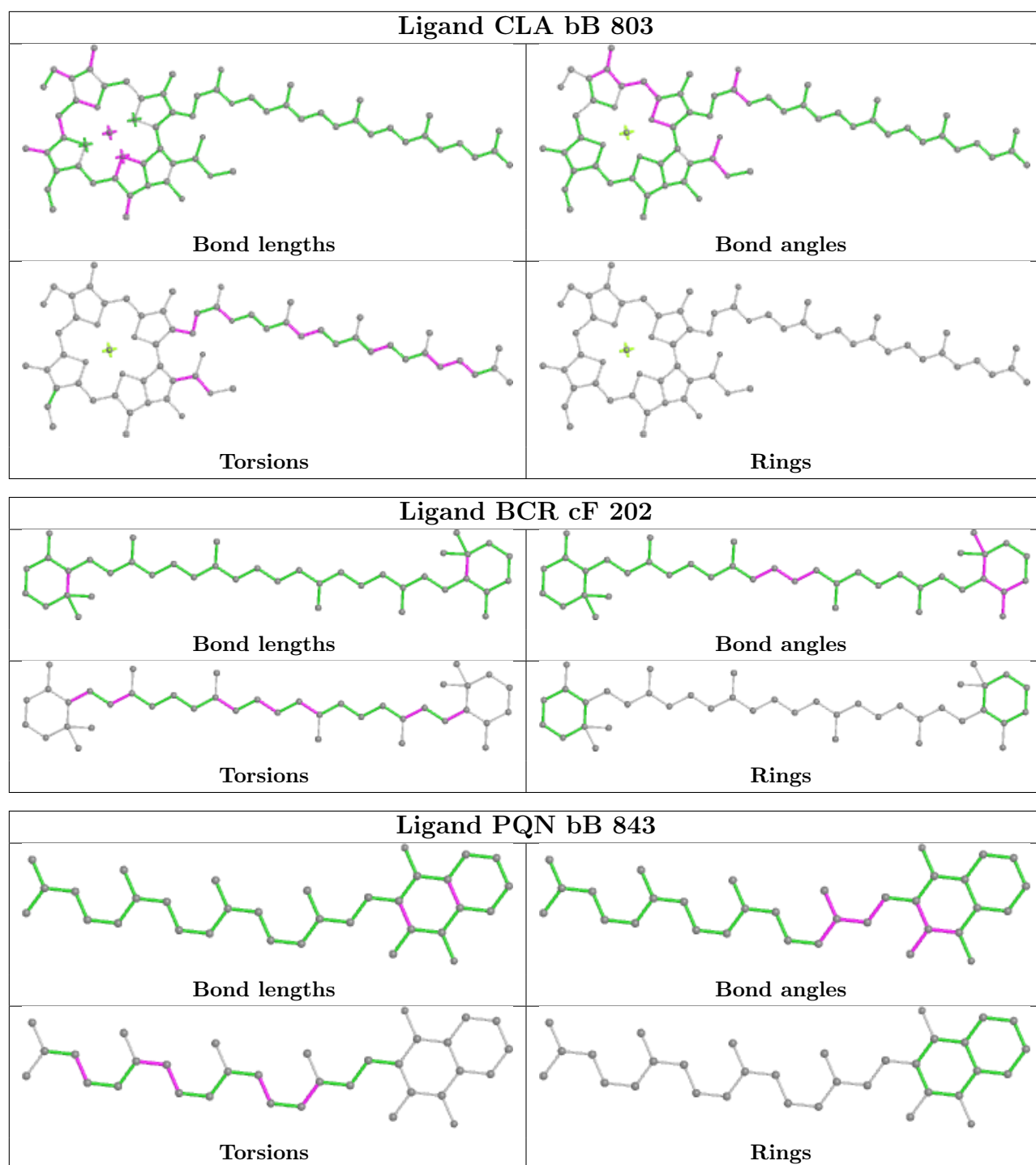
Ligand CLA bB 837

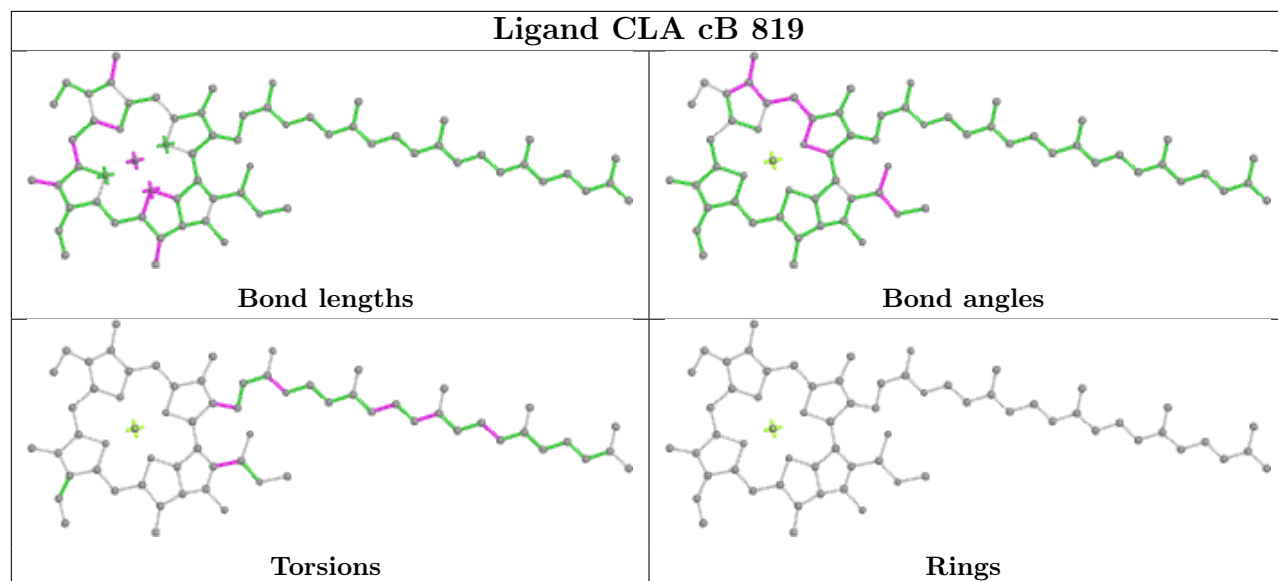
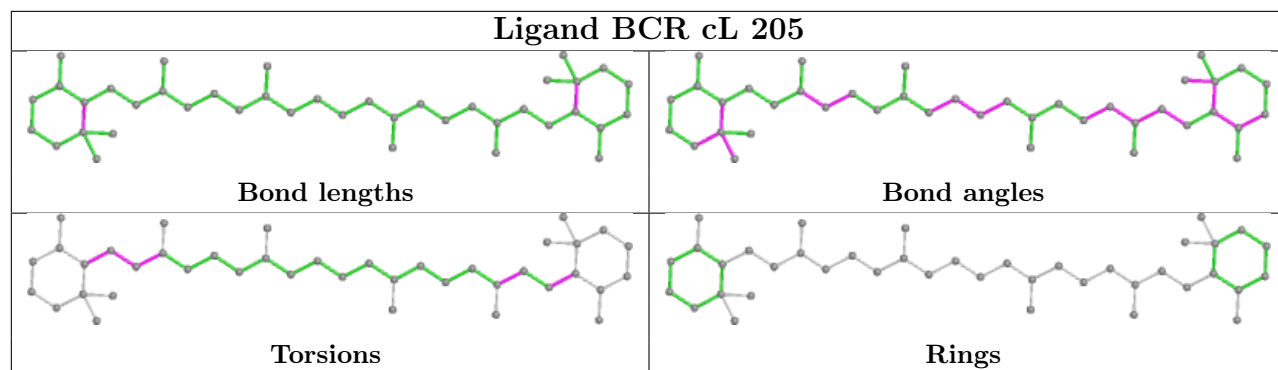


Ligand CLA cA 834

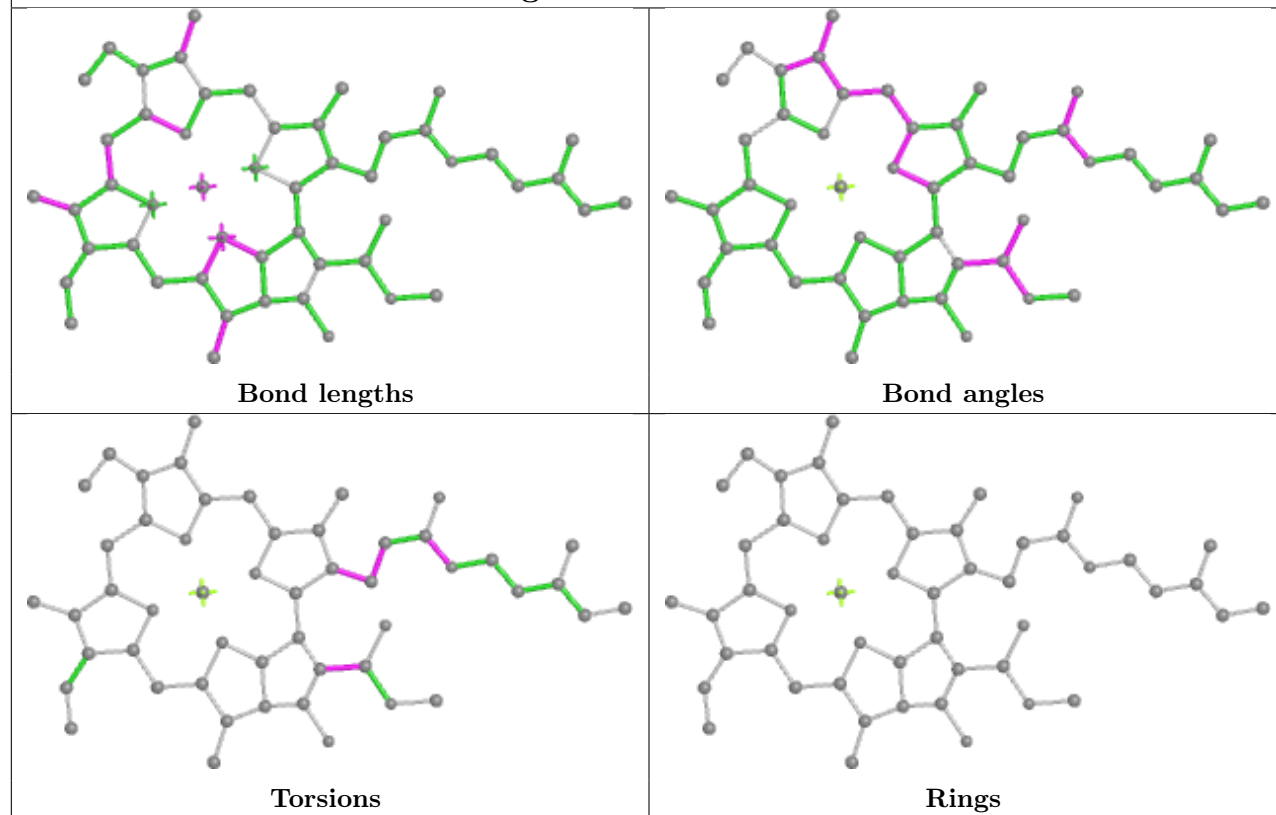




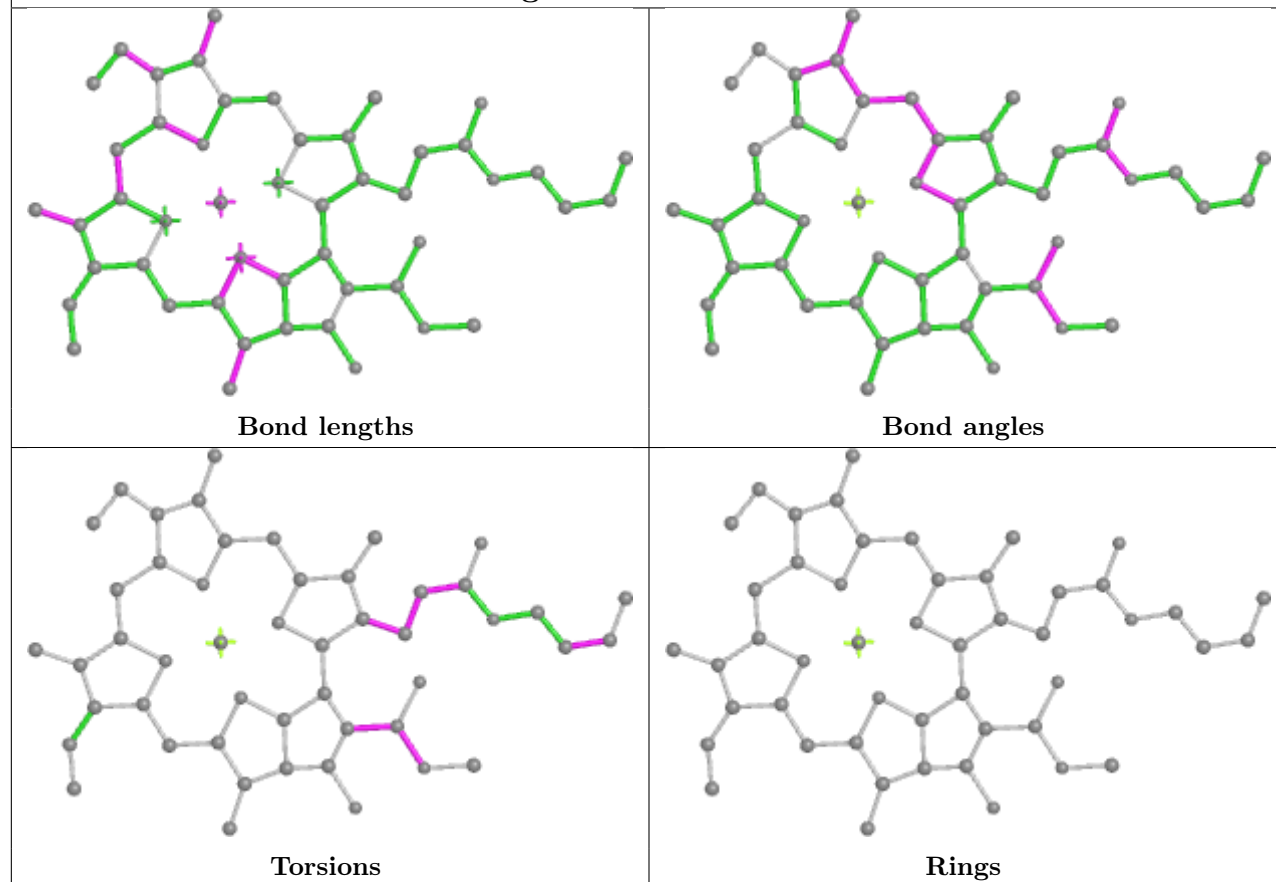




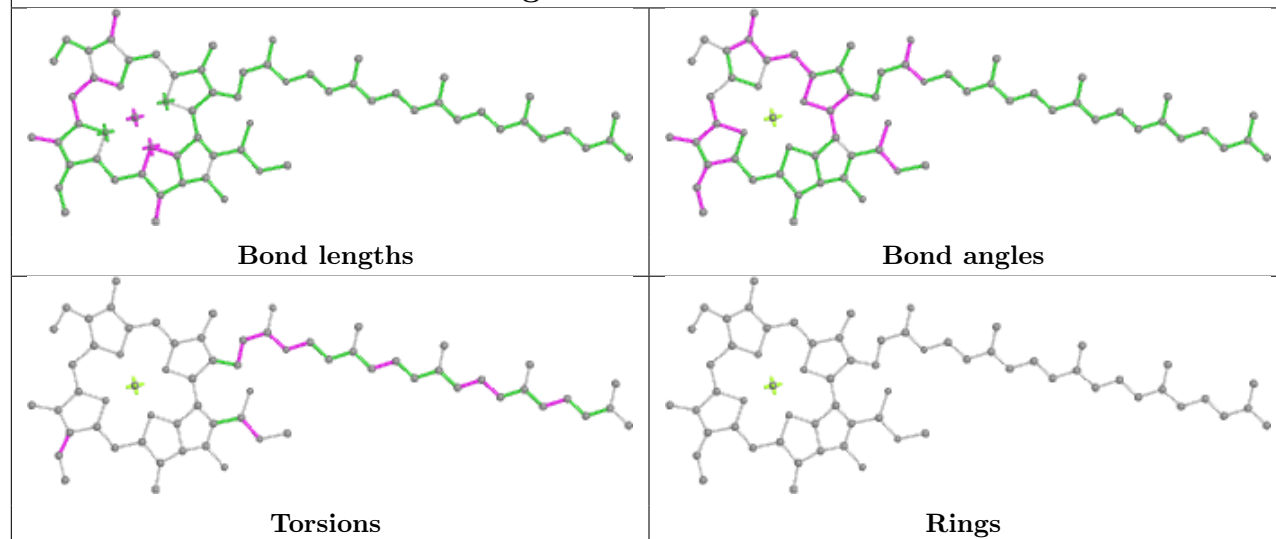
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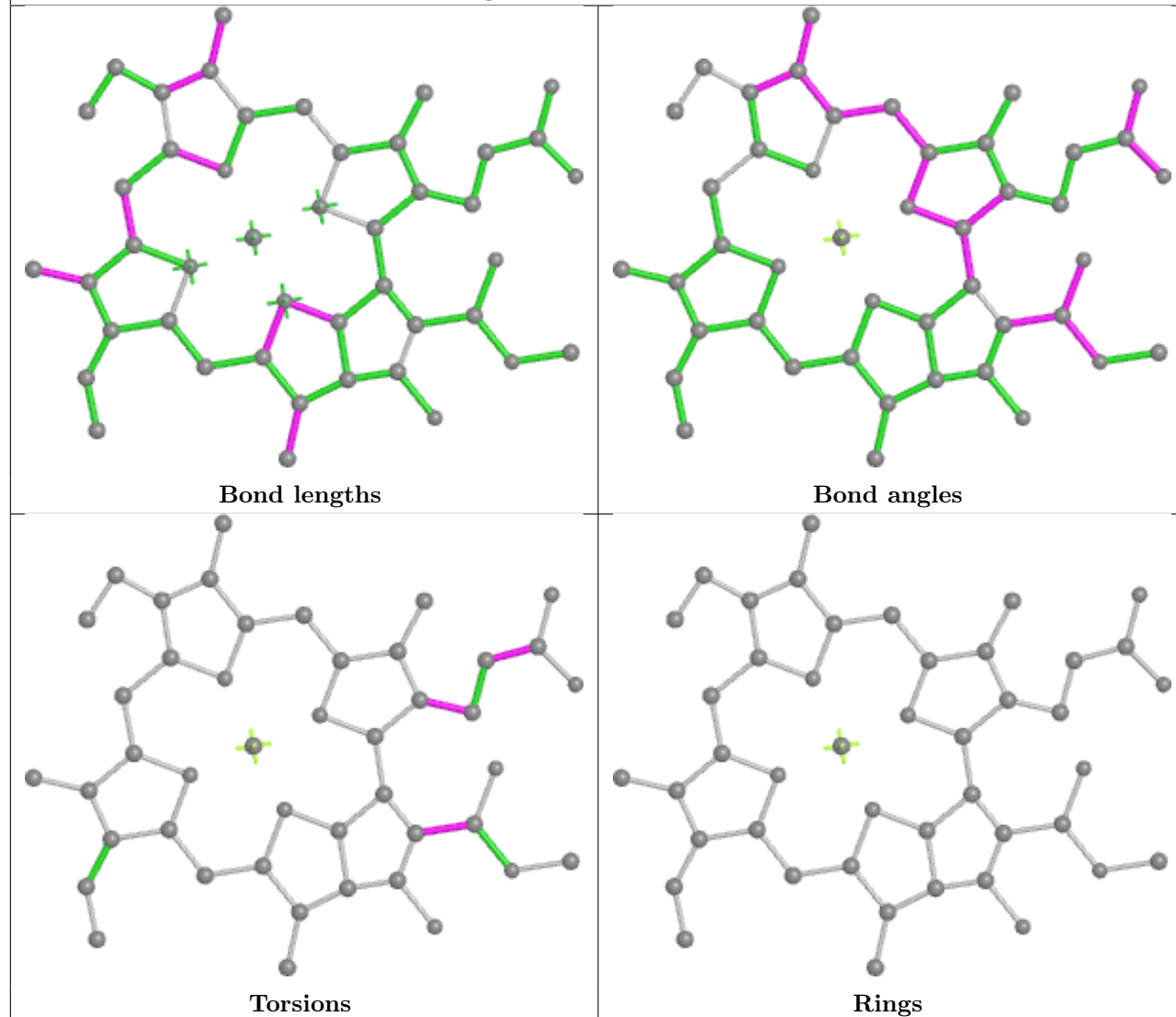
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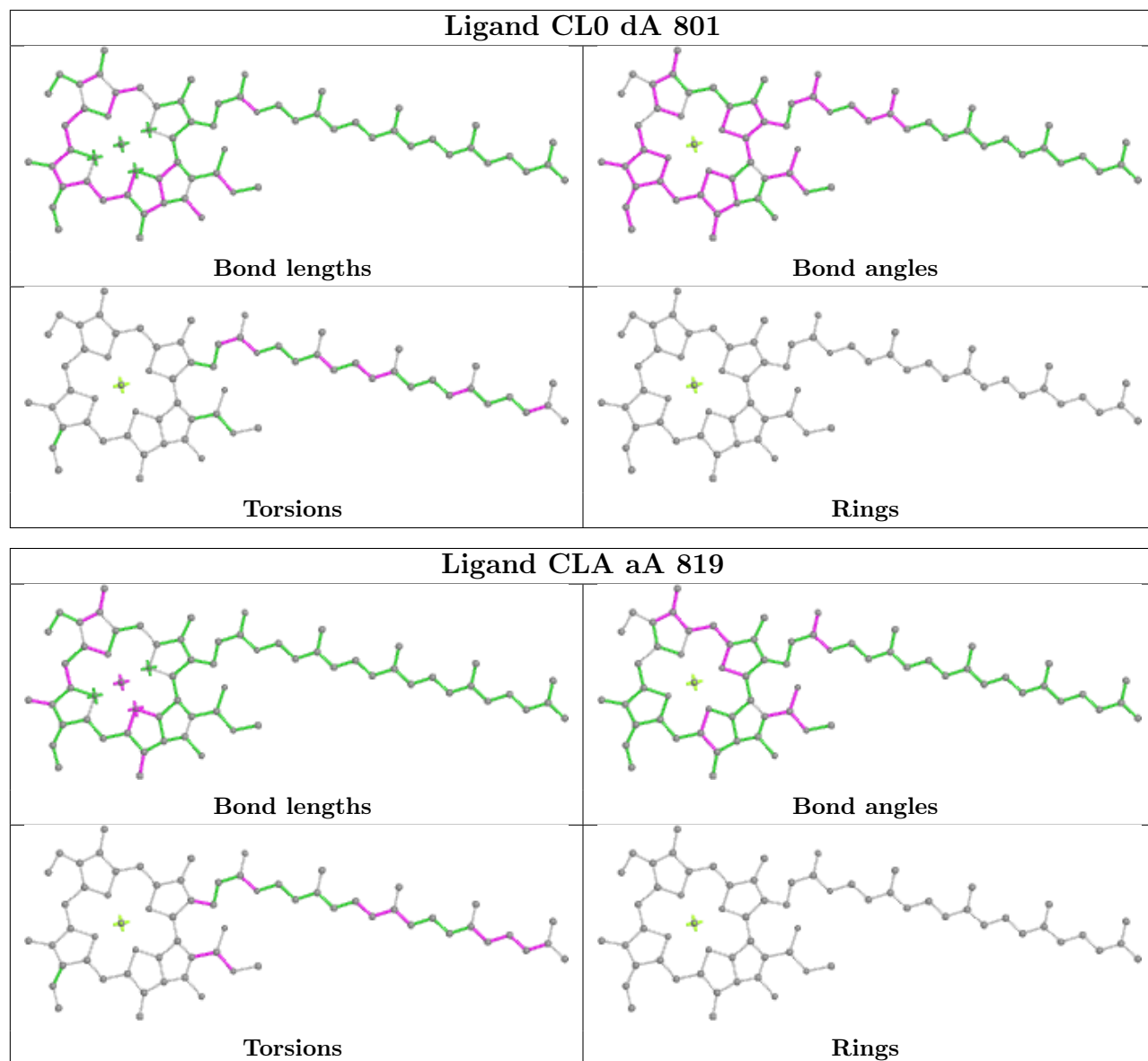


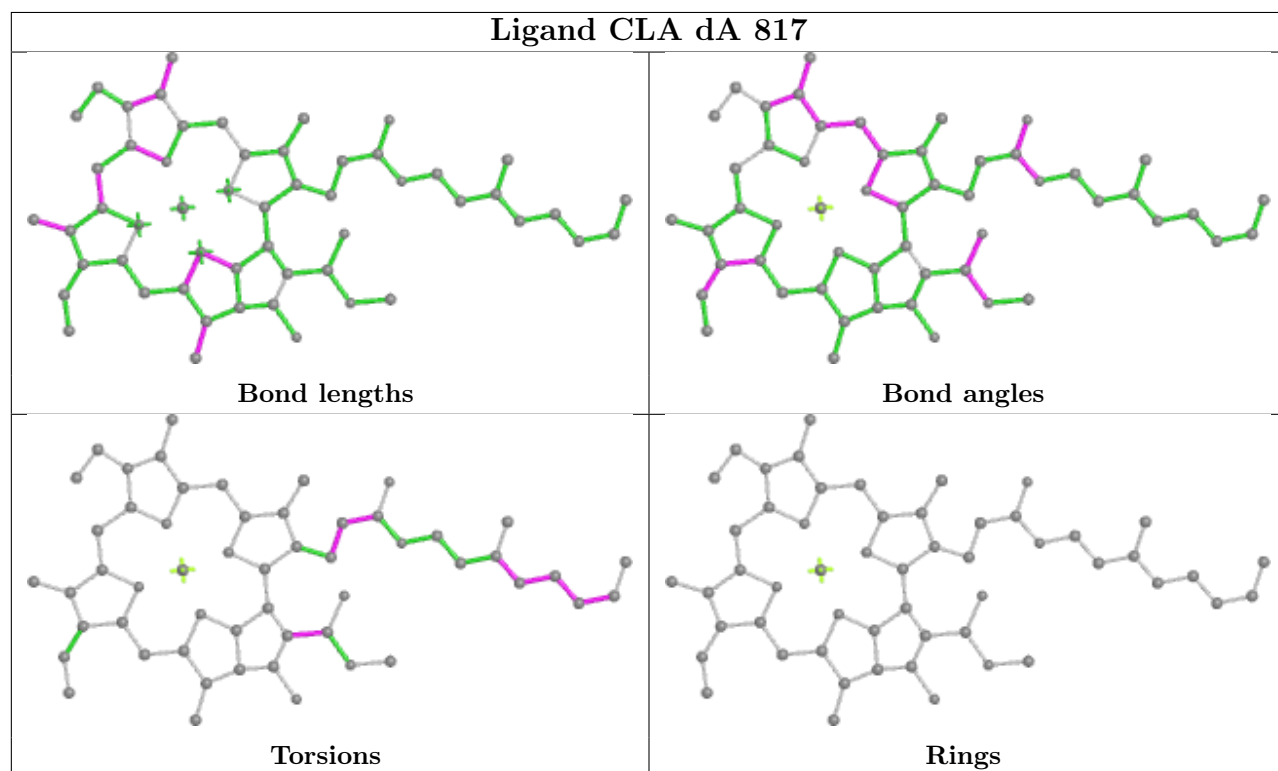
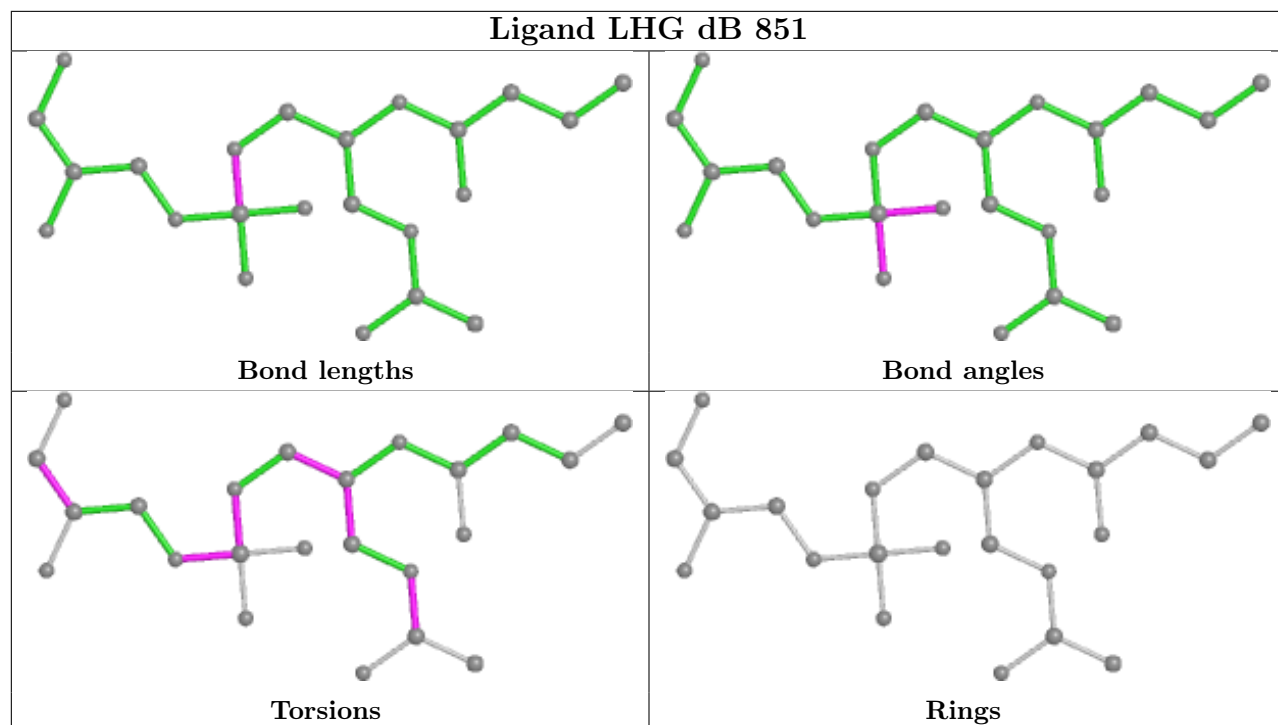
Ligand CLA dB 804

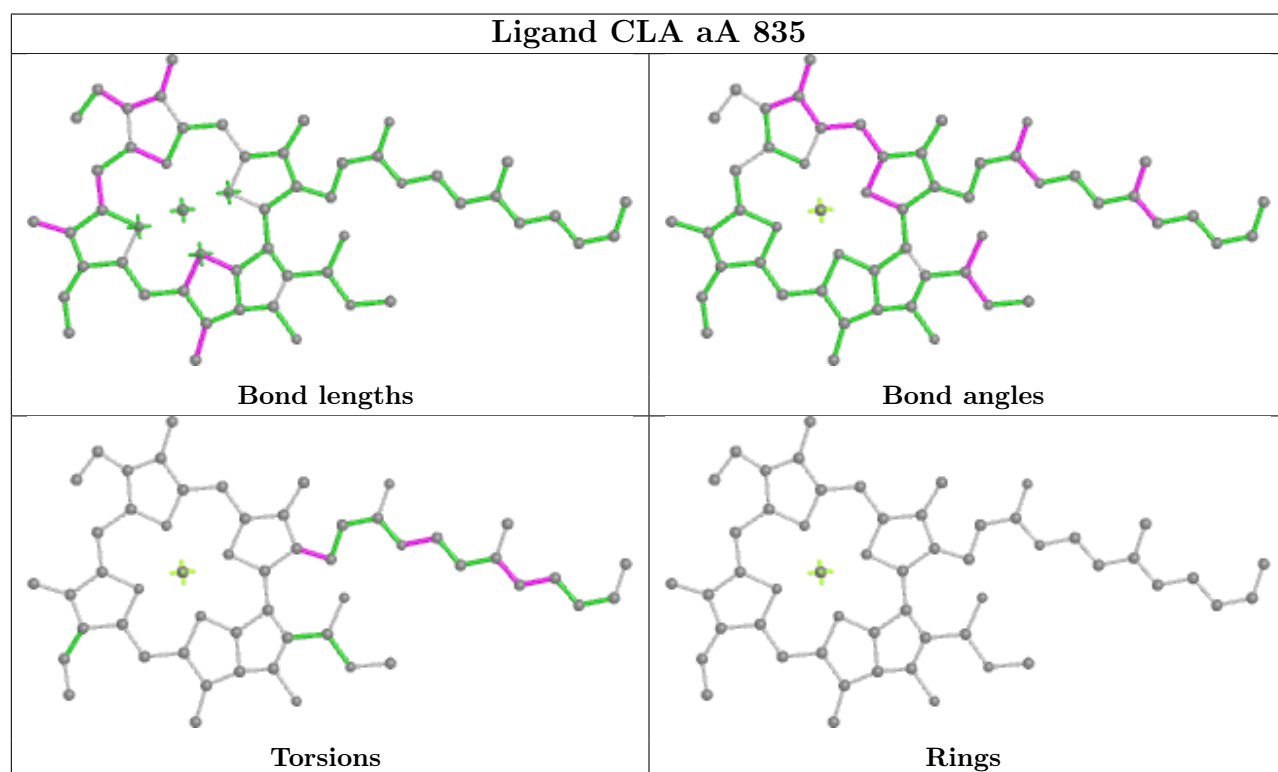
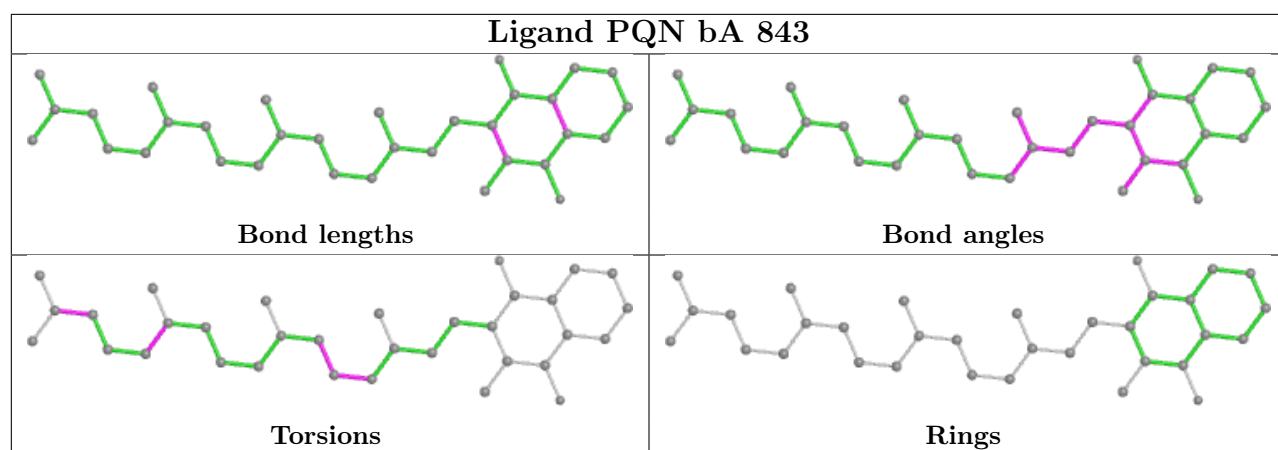


Ligand CLA bA 803

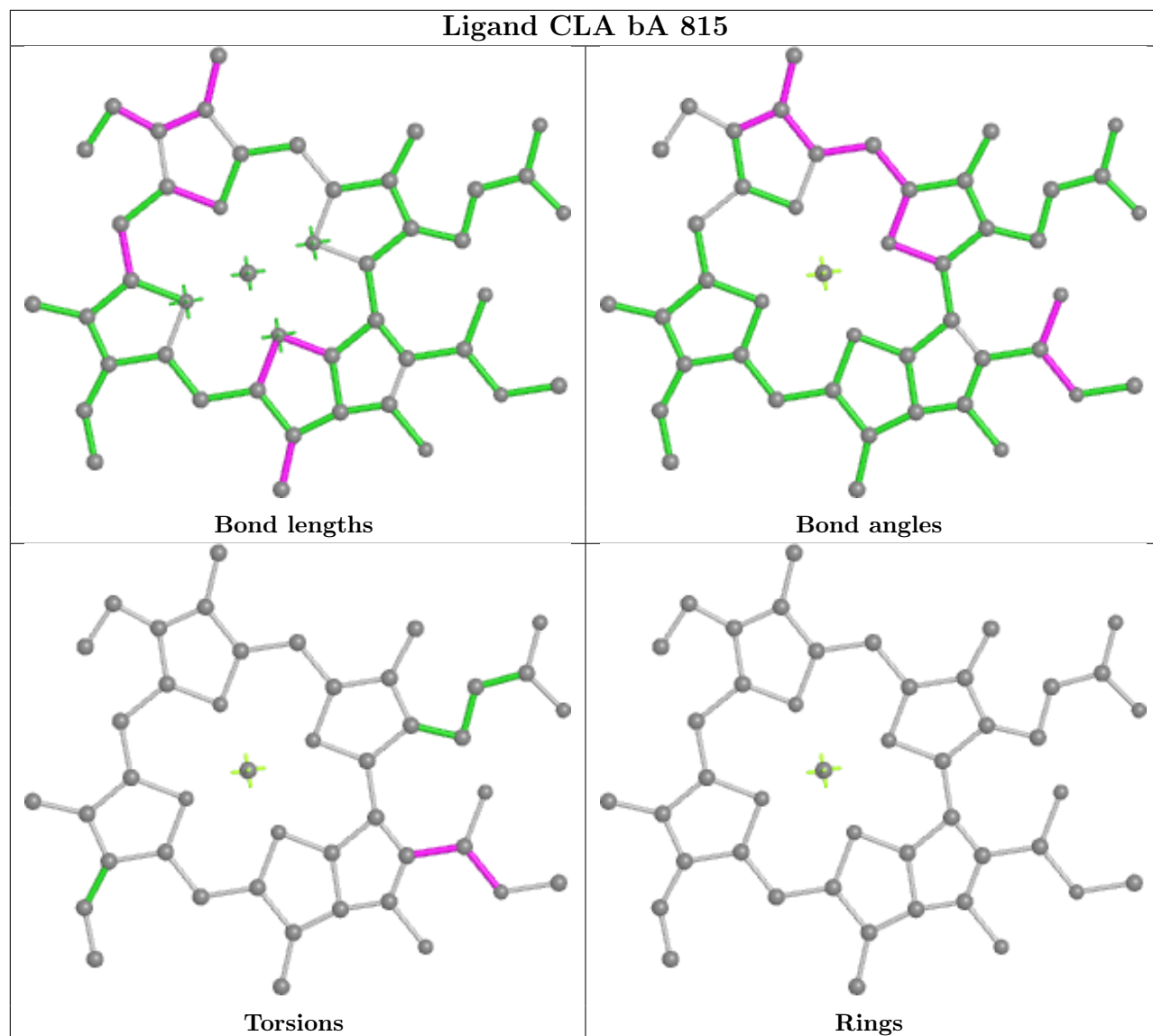


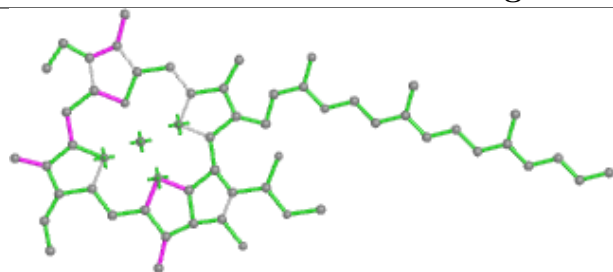
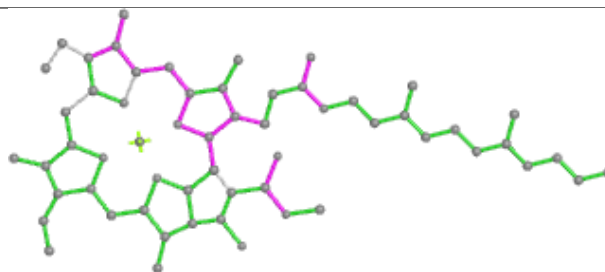
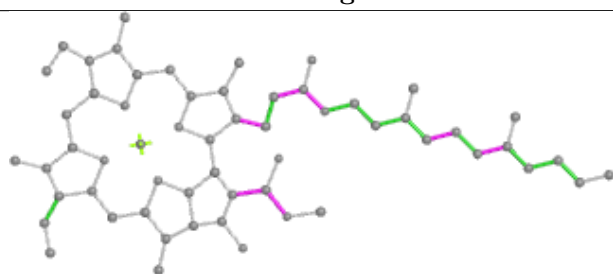
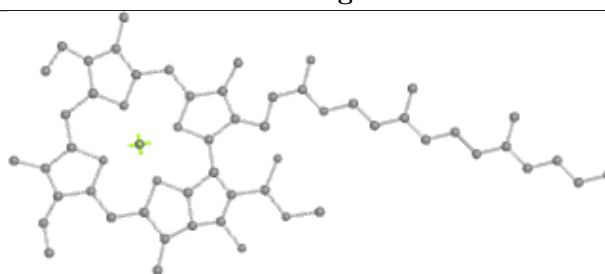
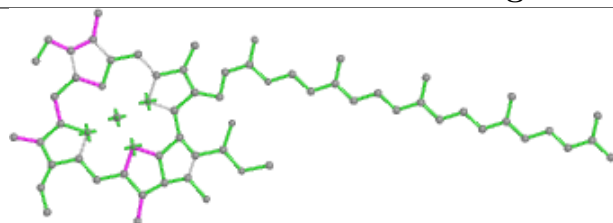
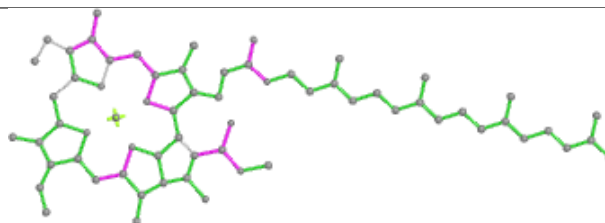
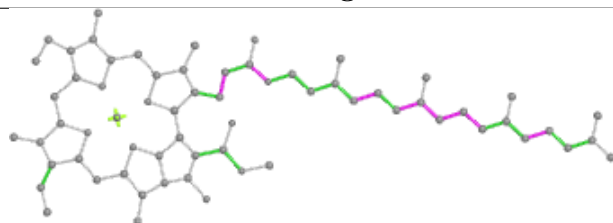
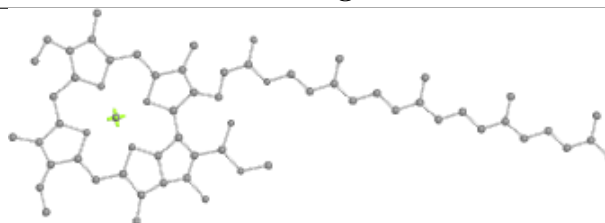


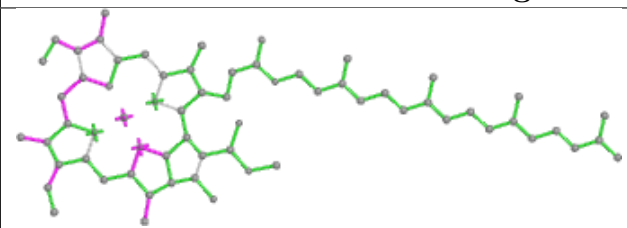
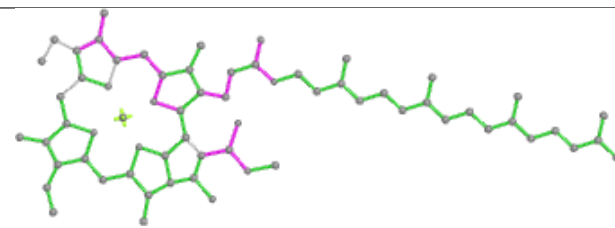
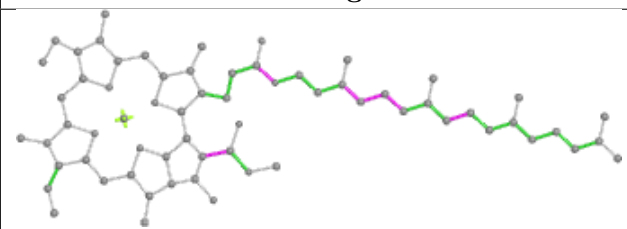
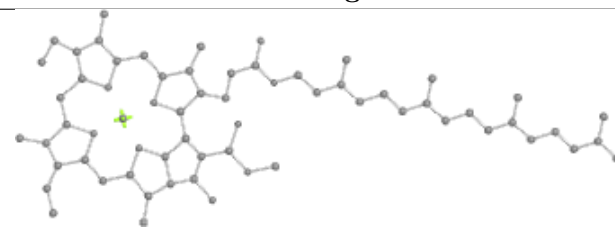


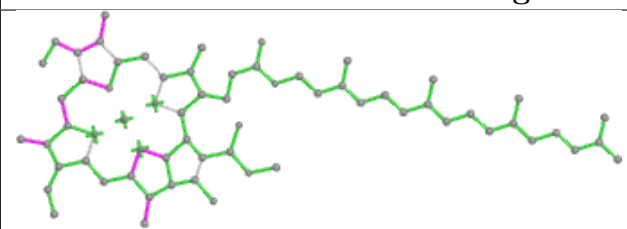
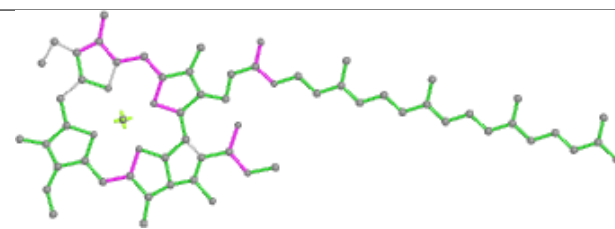
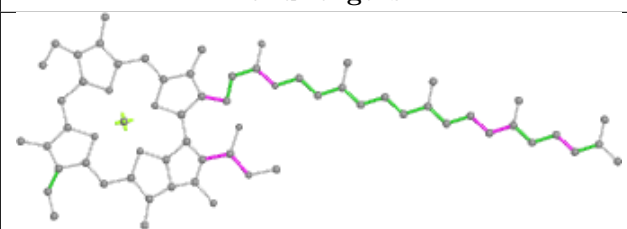
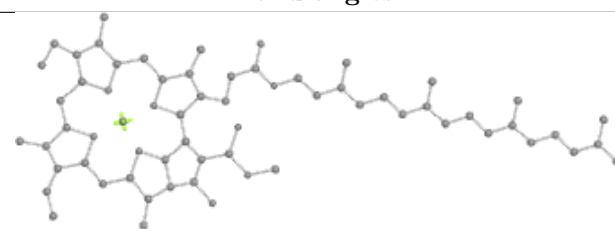


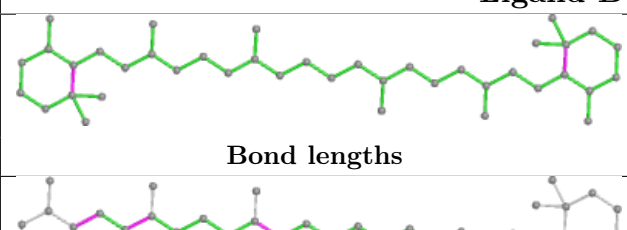
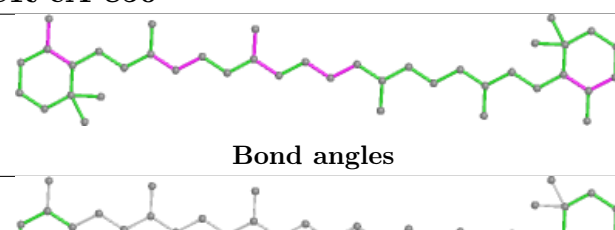
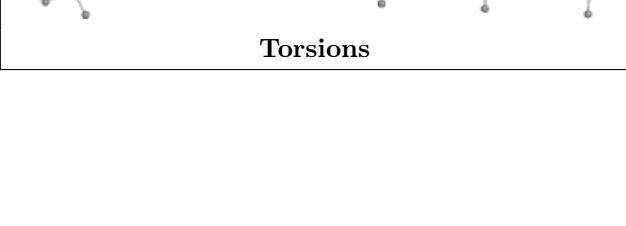
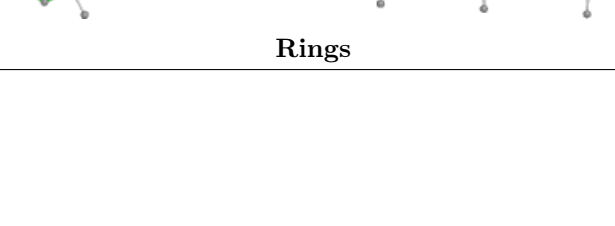
Ligand CLA bA 815



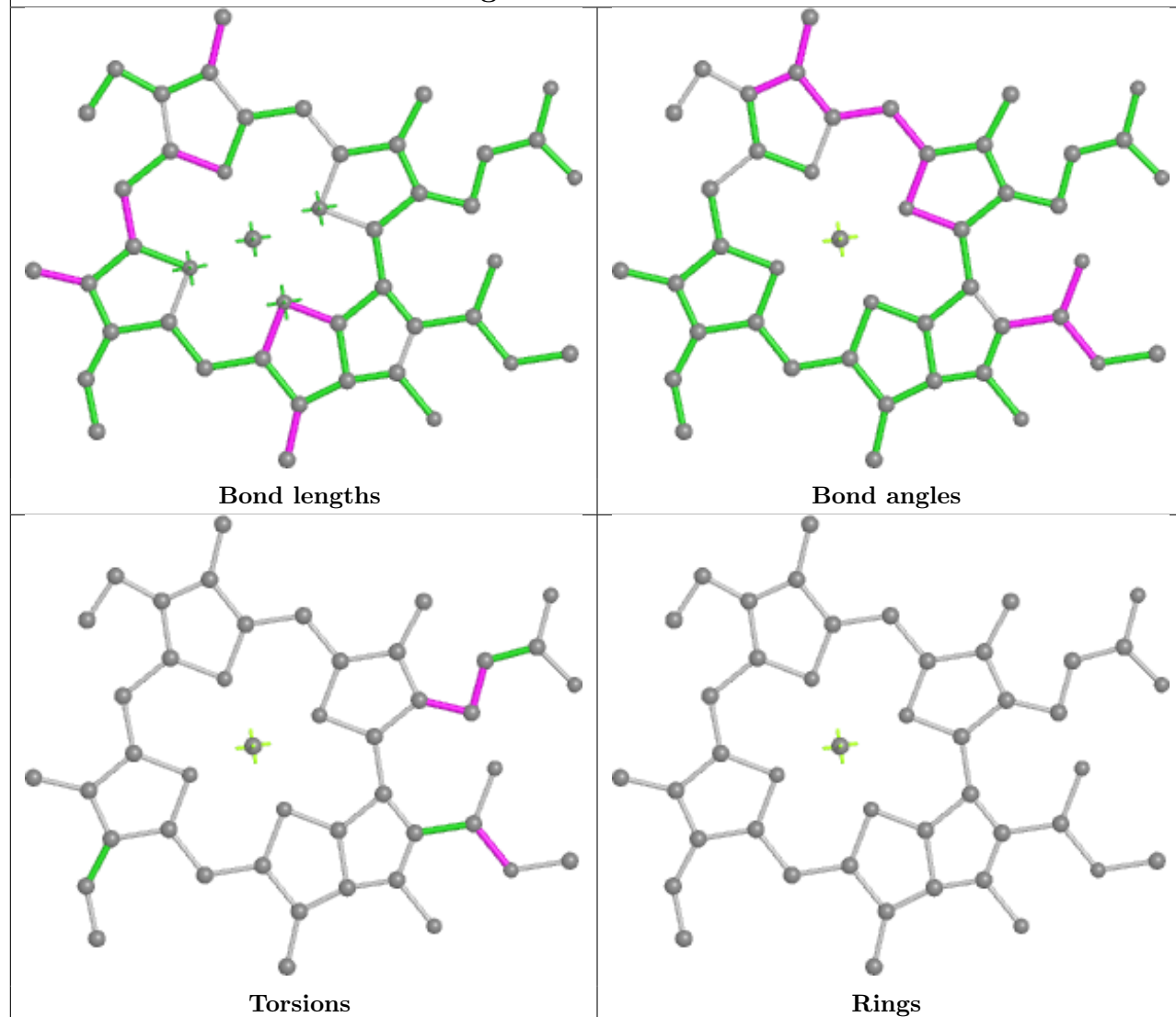
Ligand CLA dB 834**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA dL 205****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA cB 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

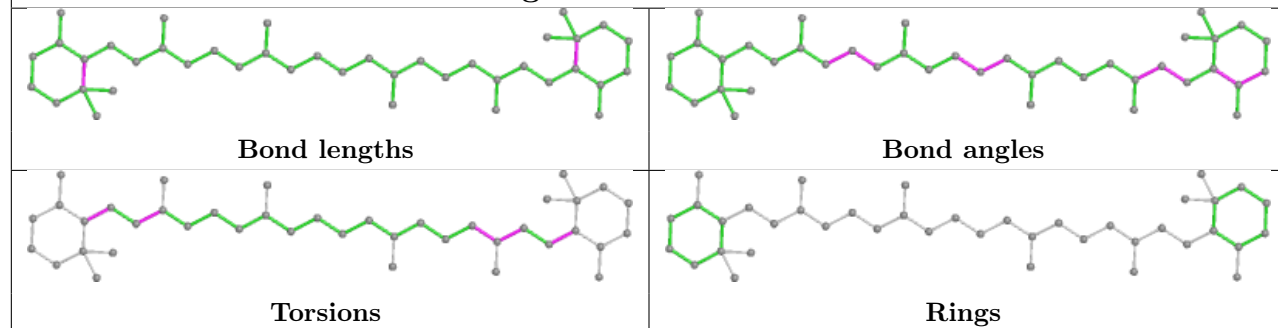
Ligand CLA cA 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

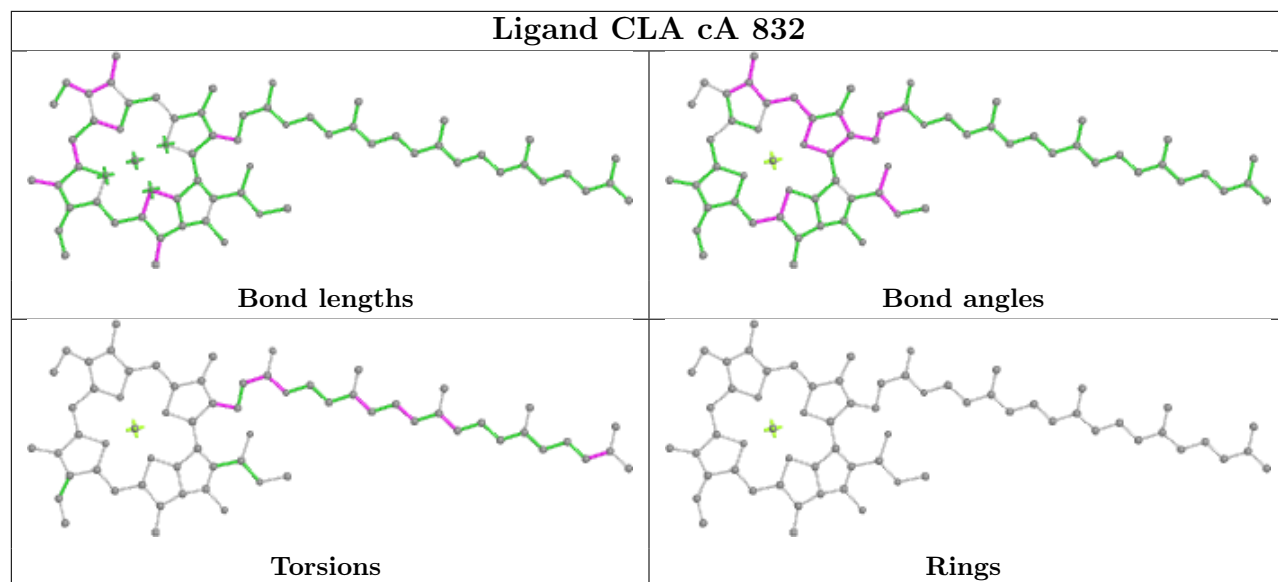
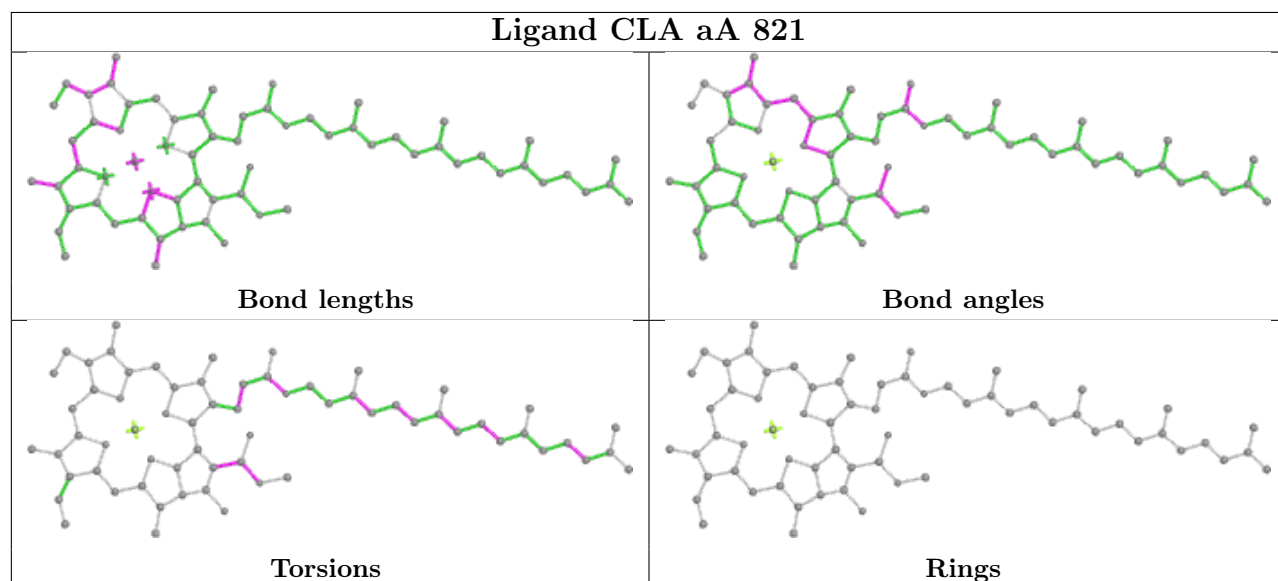
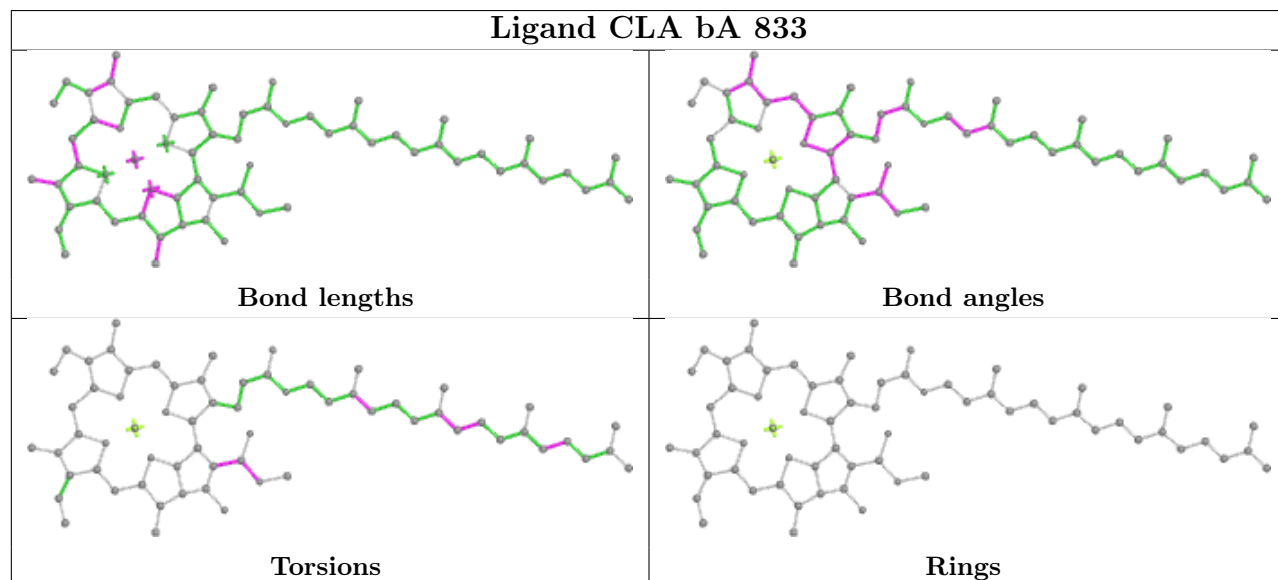
Ligand BCR cA 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA dB 816

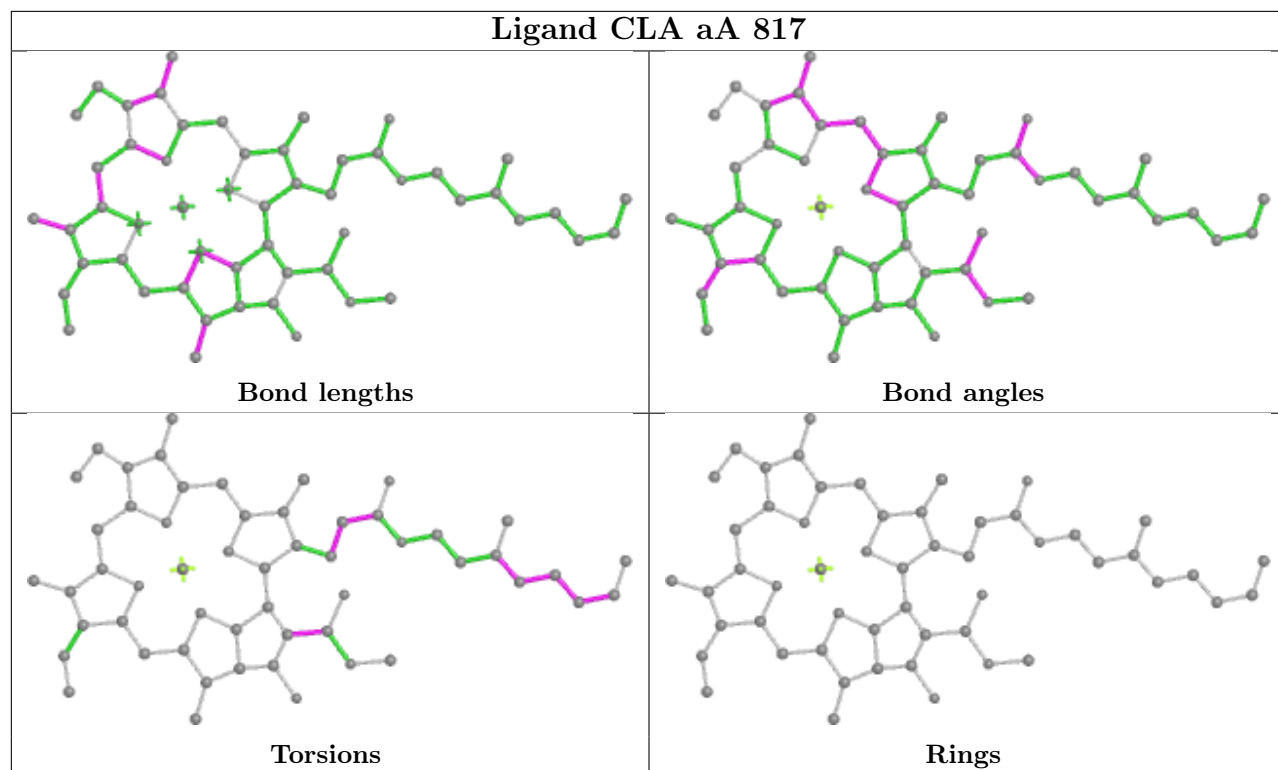


Ligand BCR aB 848

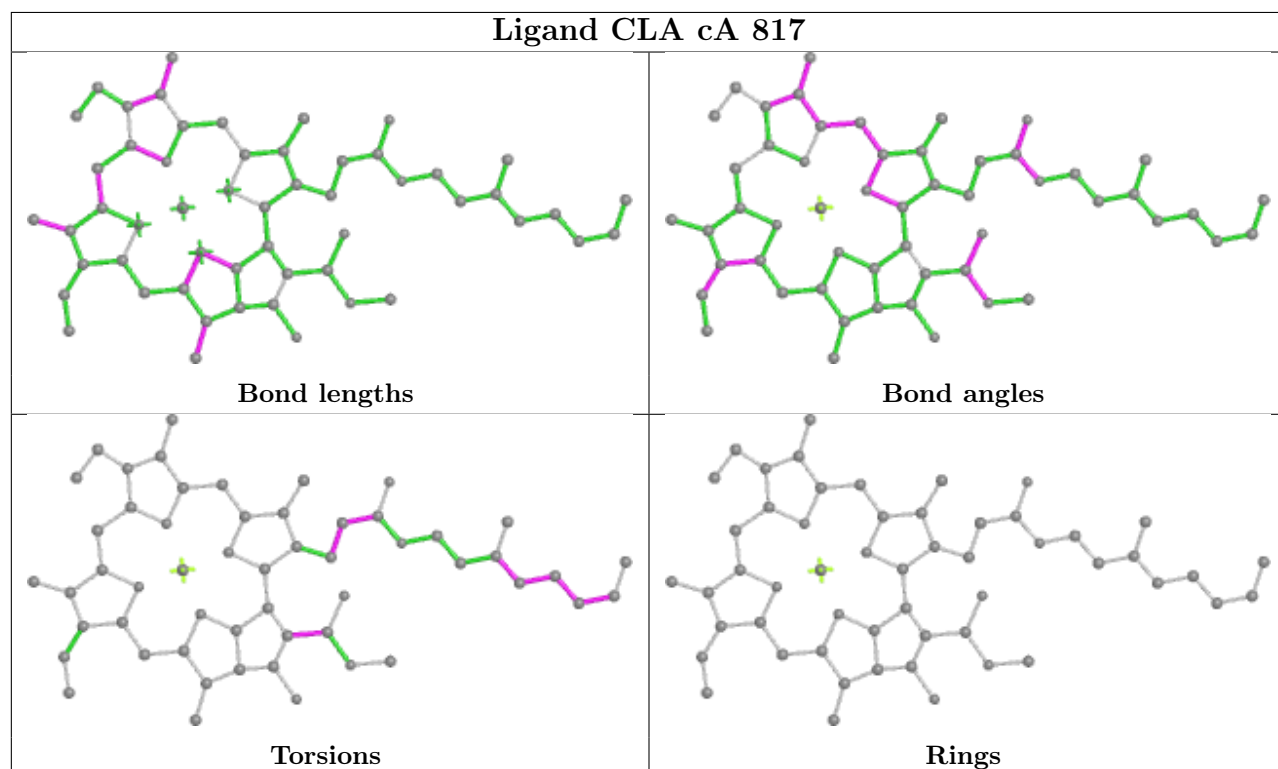


Ligand CLA cA 832**Ligand CLA aA 821****Ligand CLA bA 833**

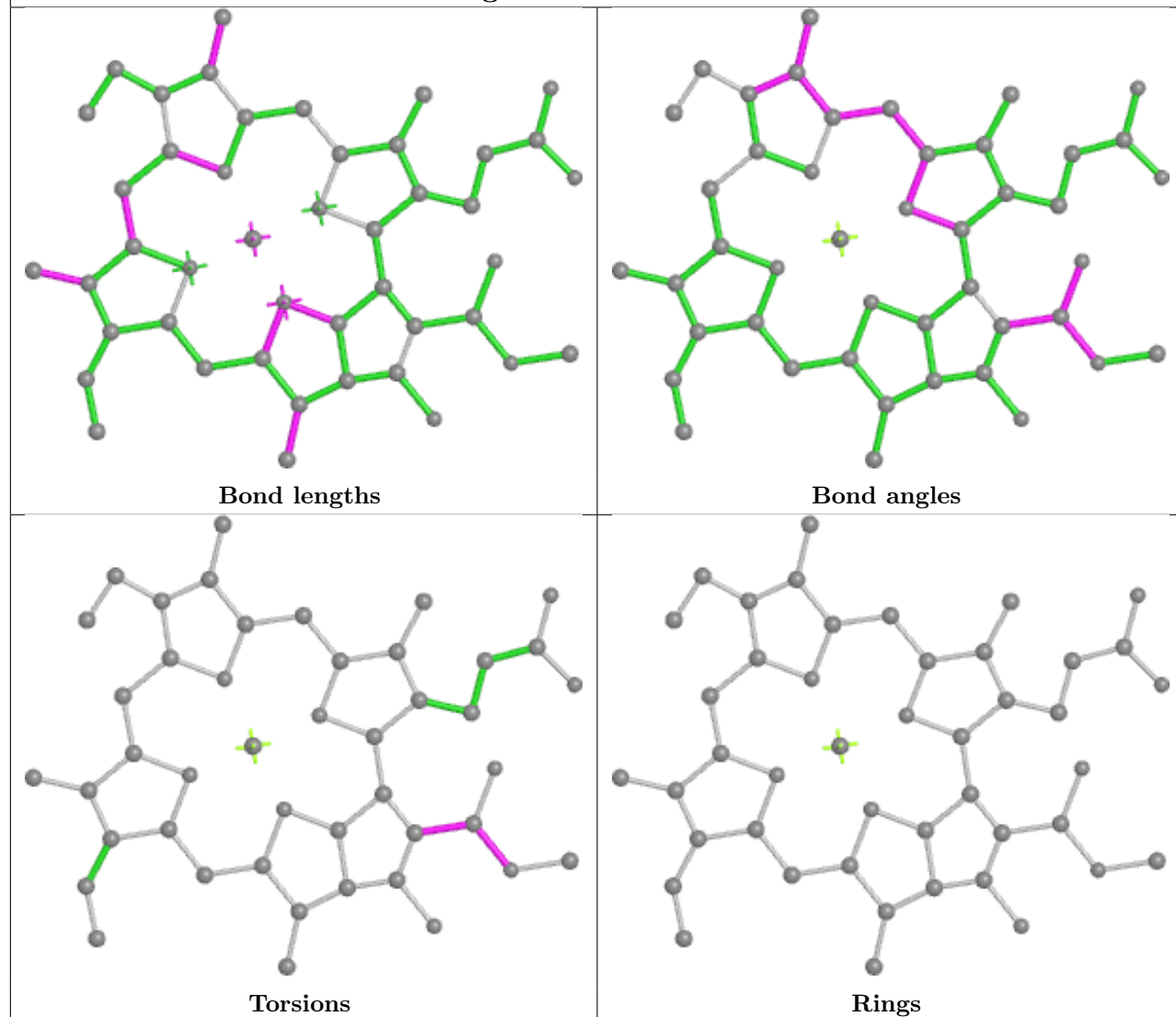
Ligand CLA aA 817



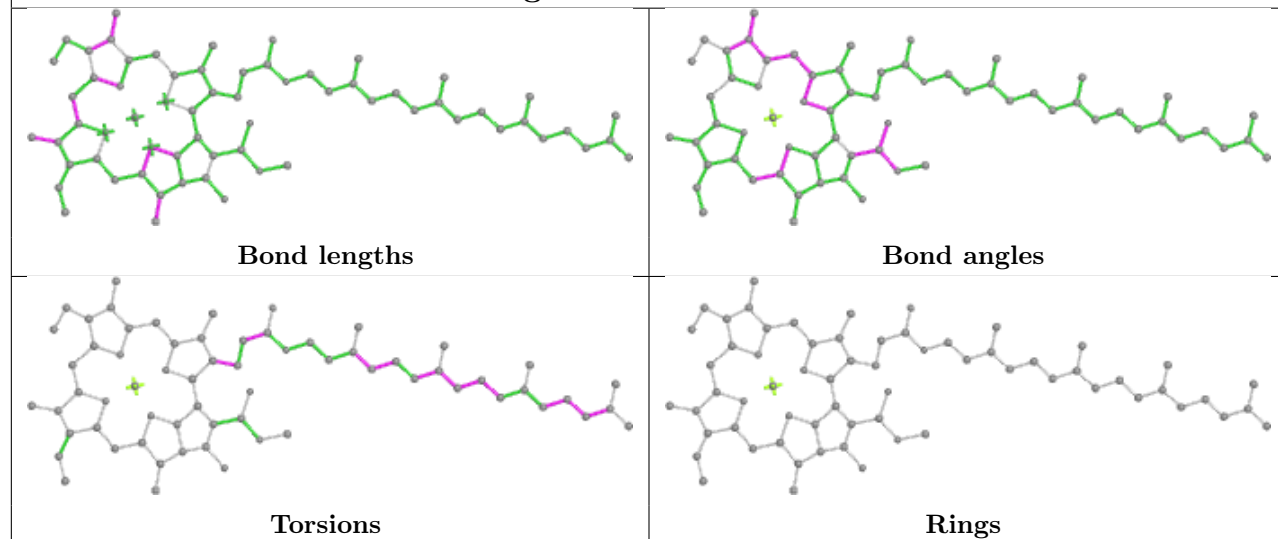
Ligand CLA cA 817



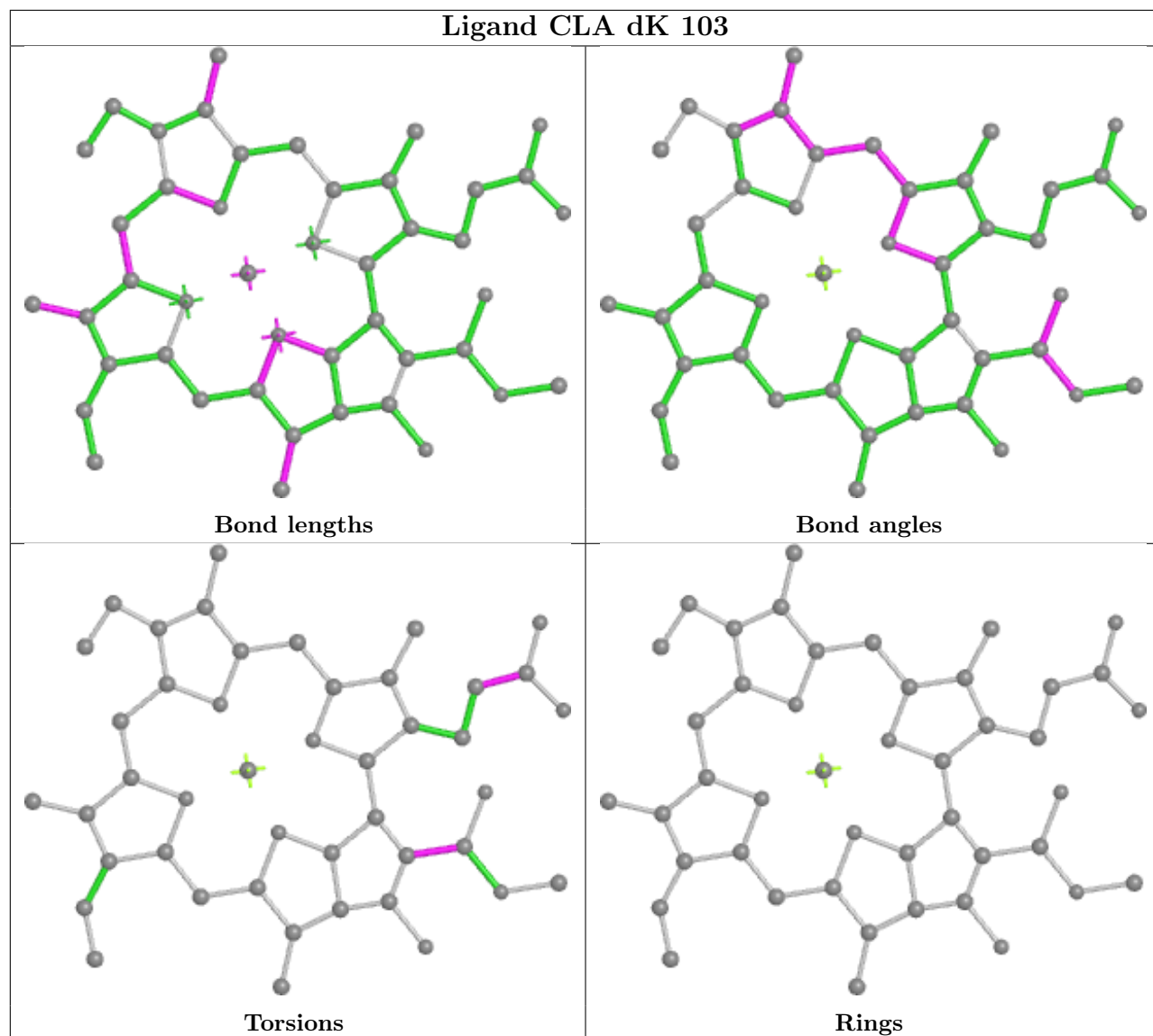
Ligand CLA bF 203

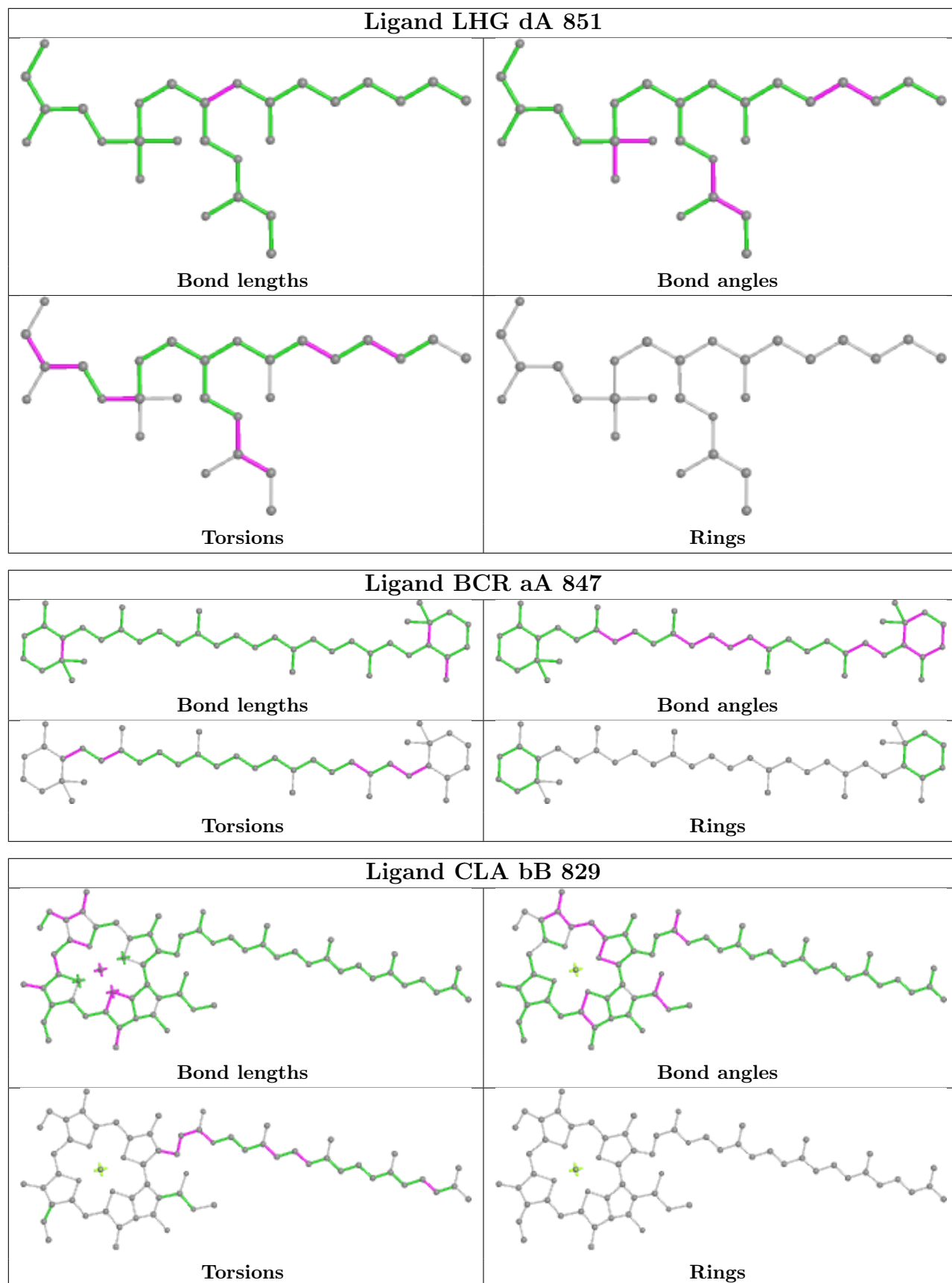


Ligand CLA aB 832

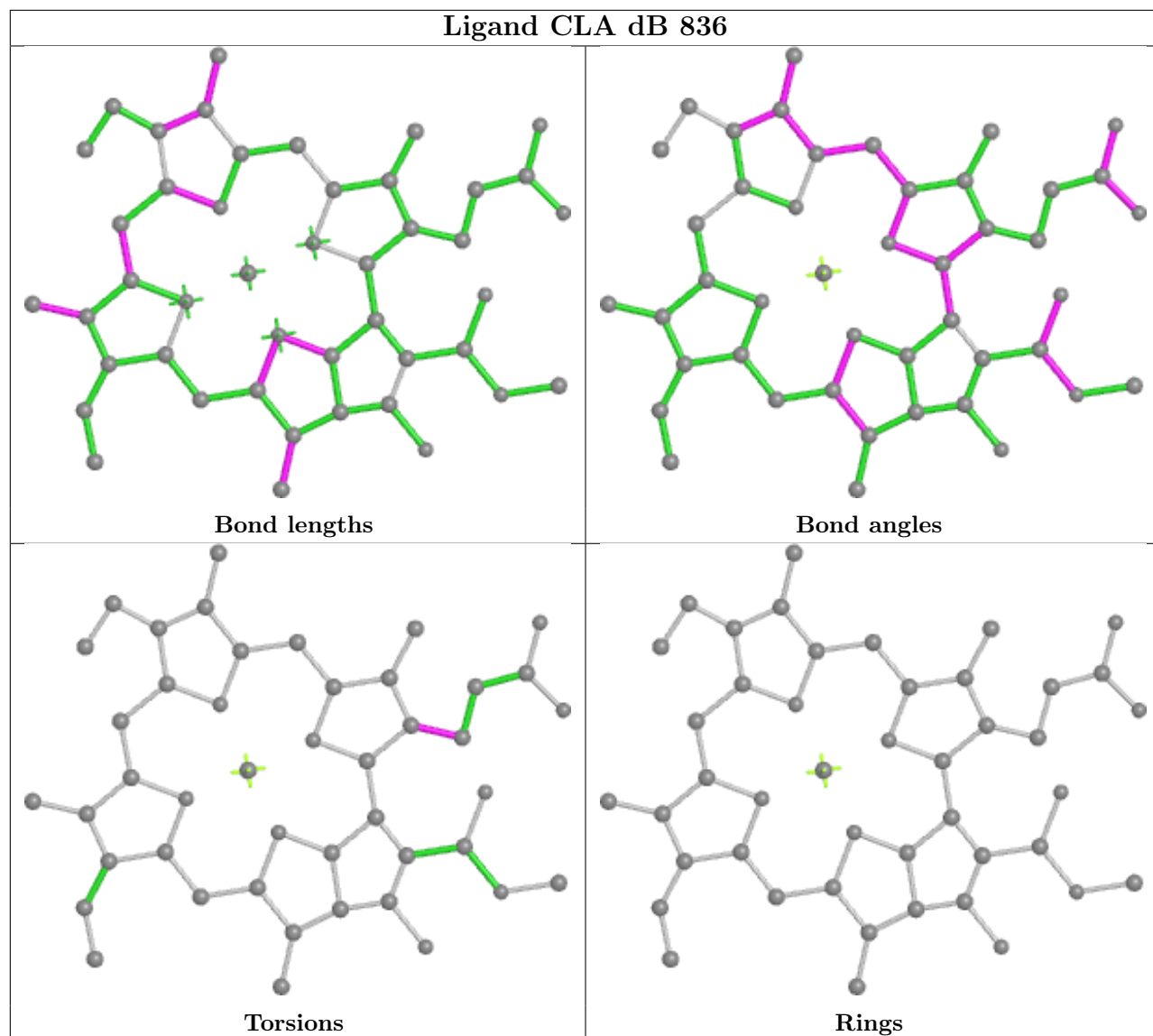


Ligand CLA dK 103

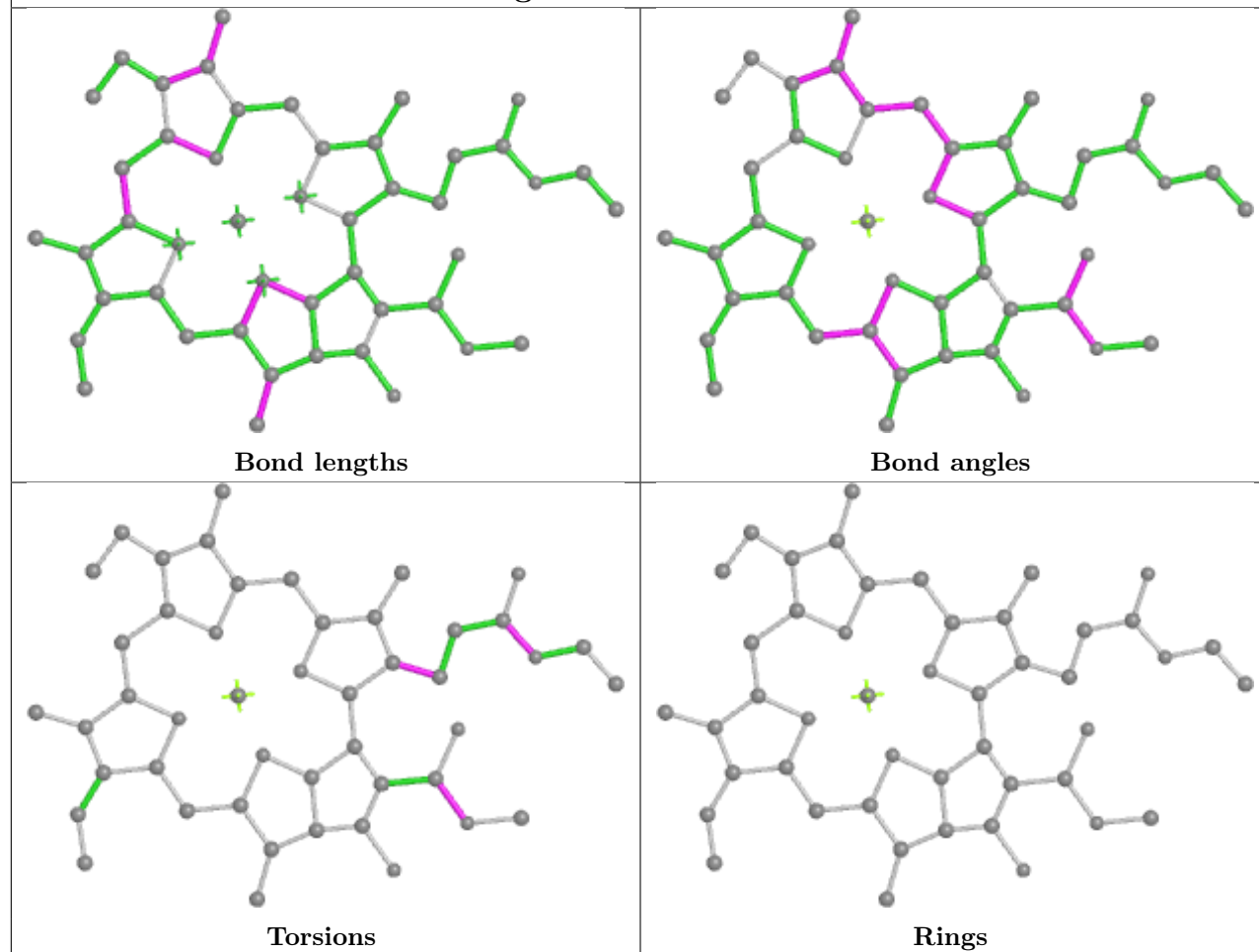




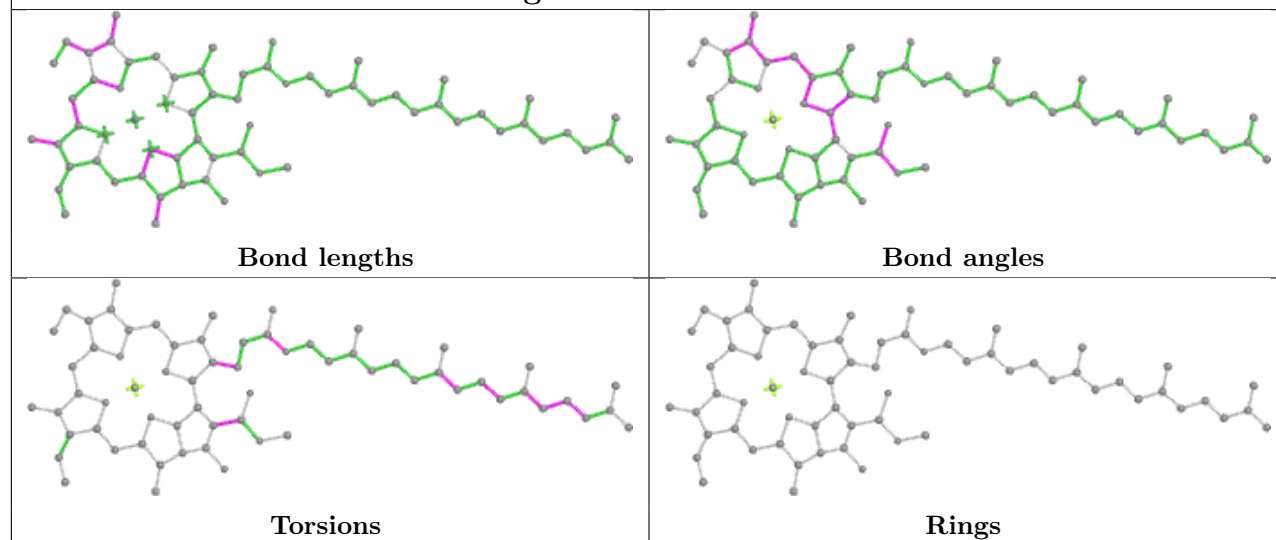
Ligand CLA dB 836



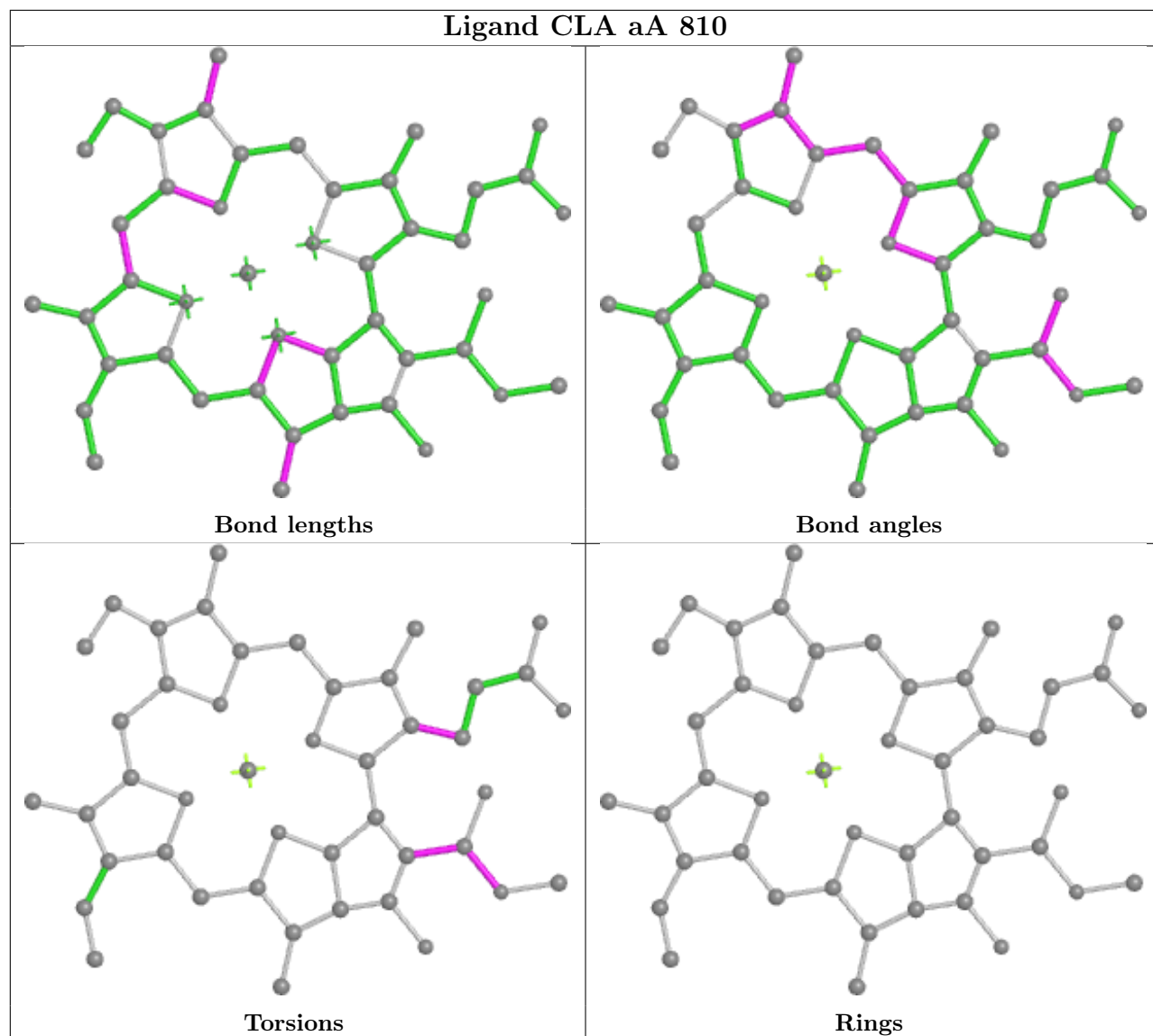
Ligand CLA bA 824



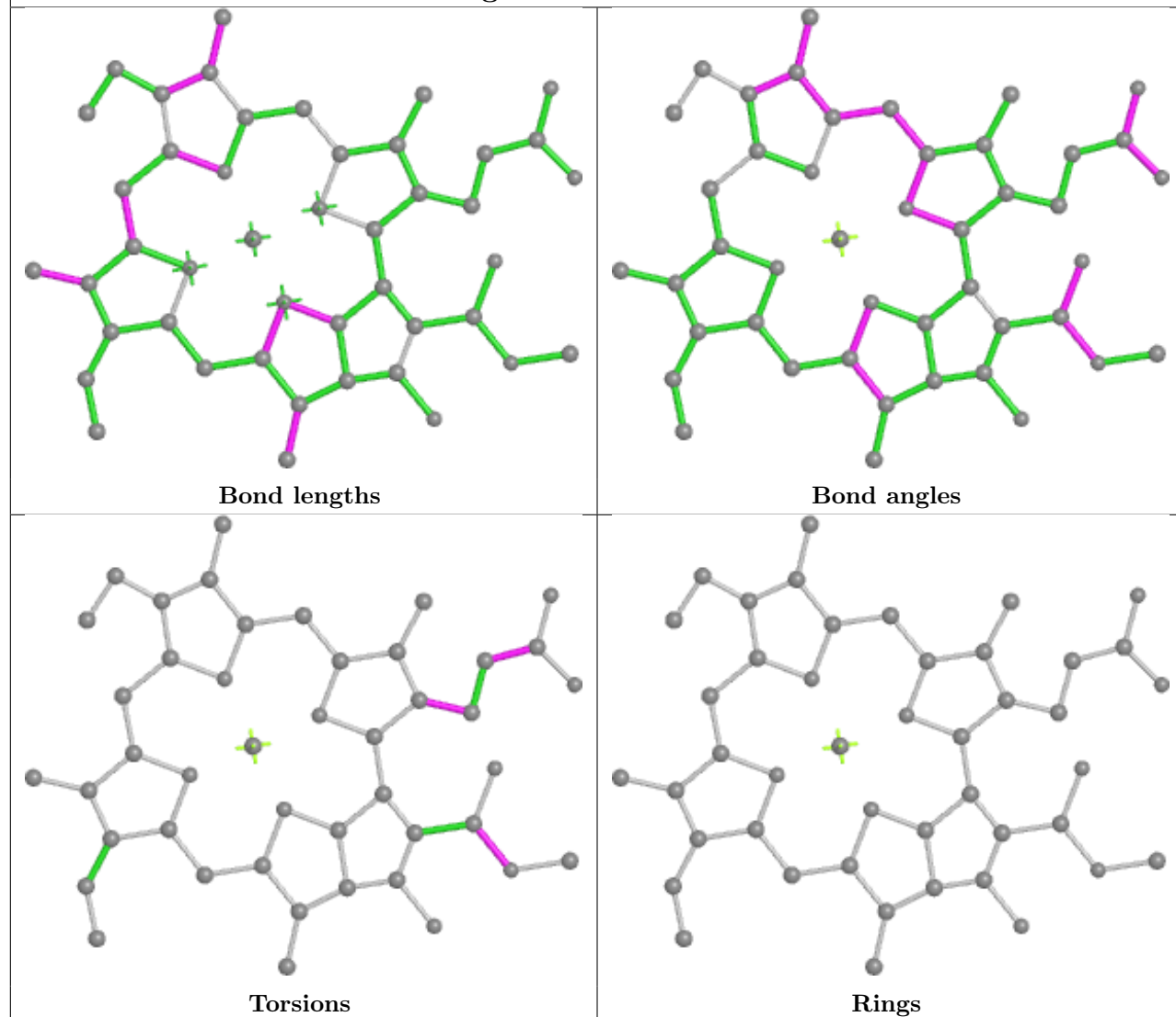
Ligand CLA cA 841



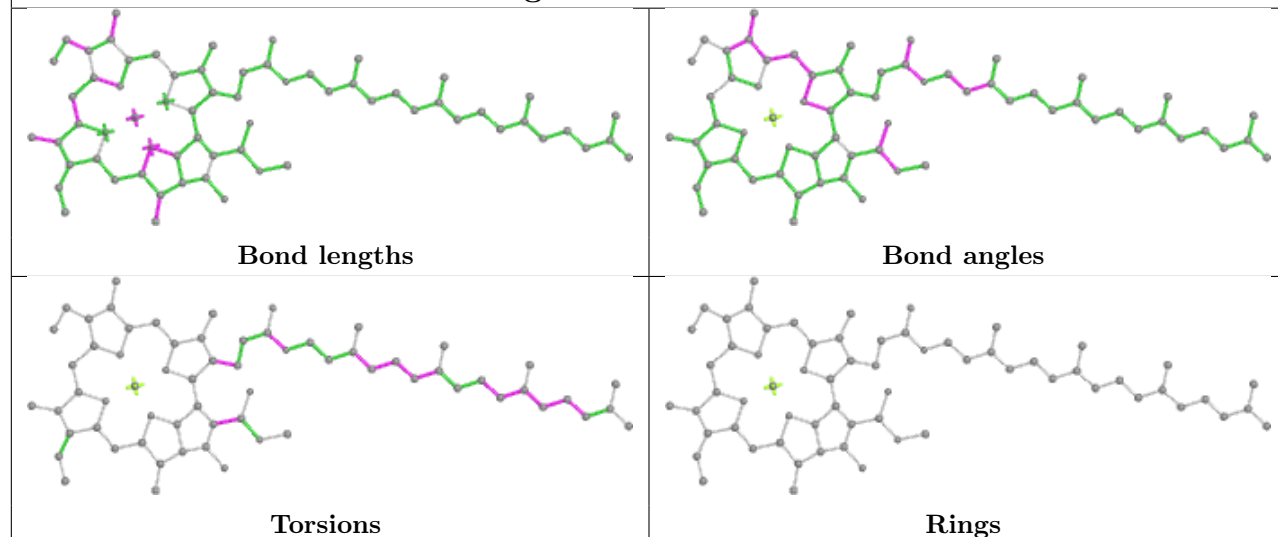
Ligand CLA aA 810



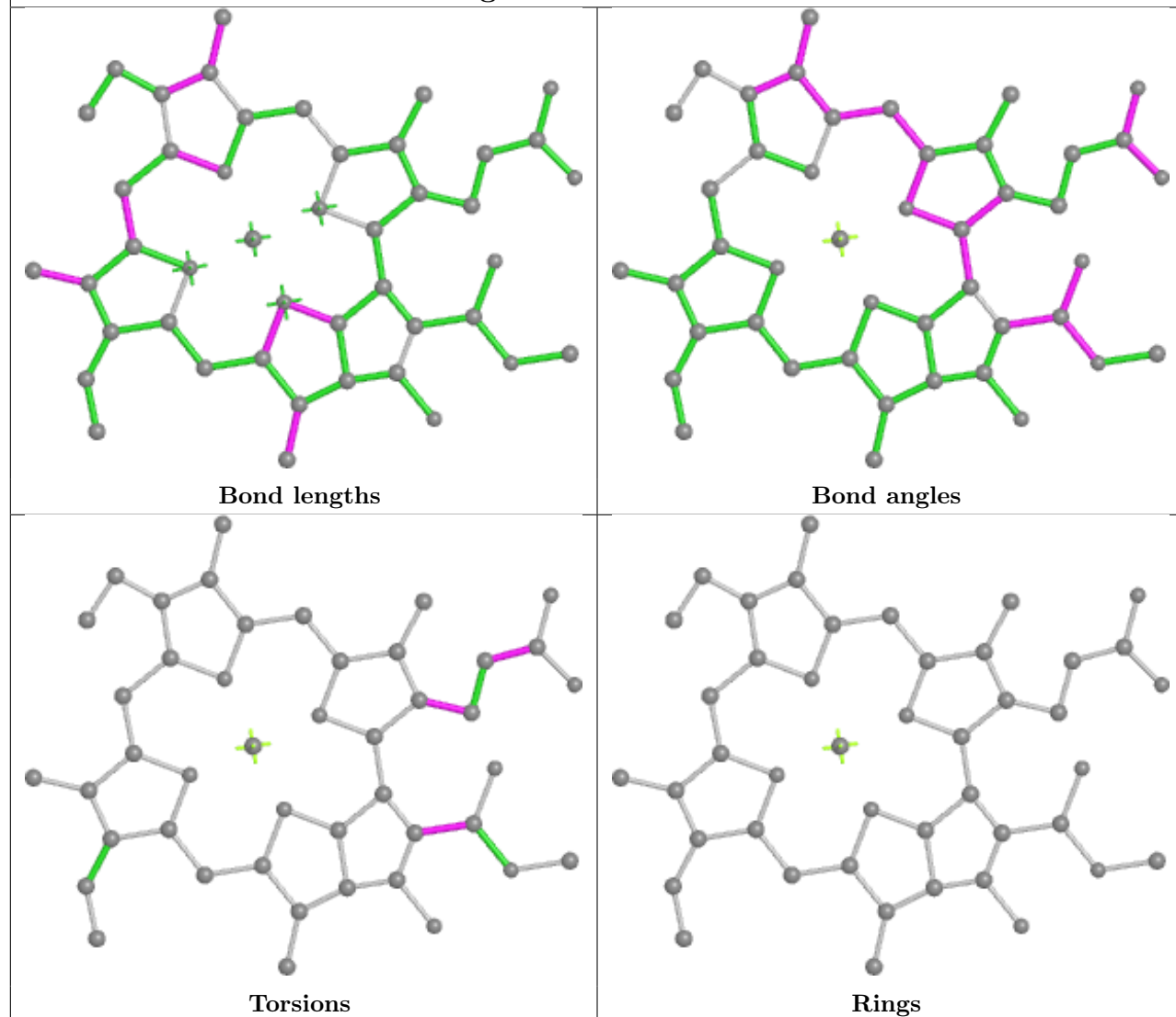
Ligand CLA aB 823



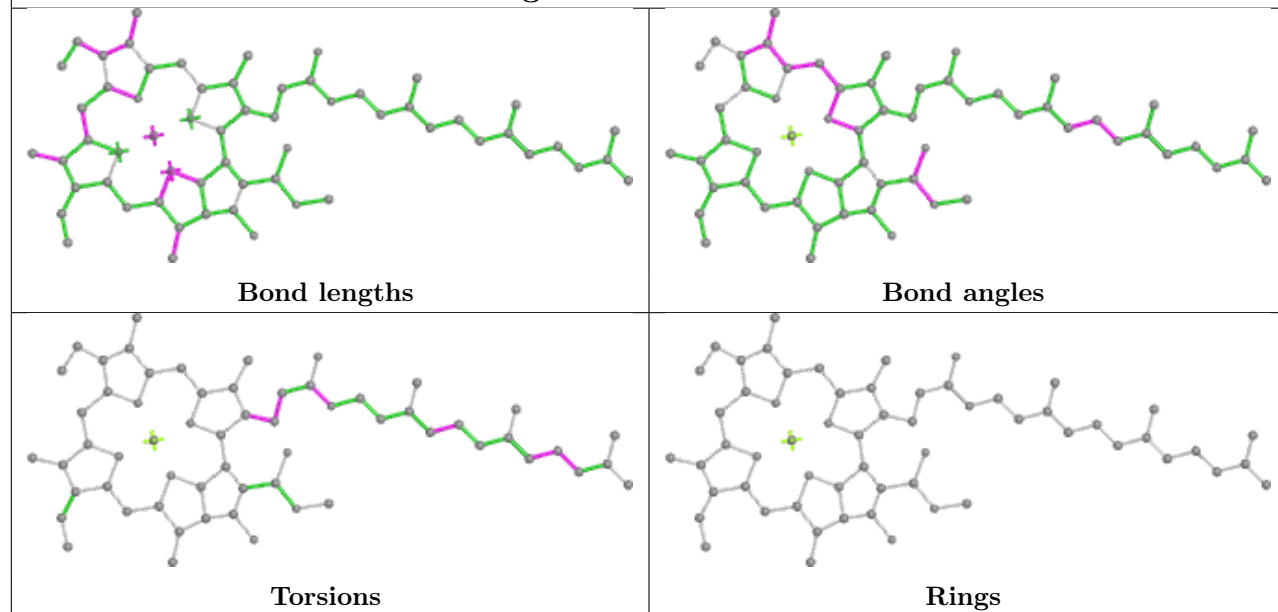
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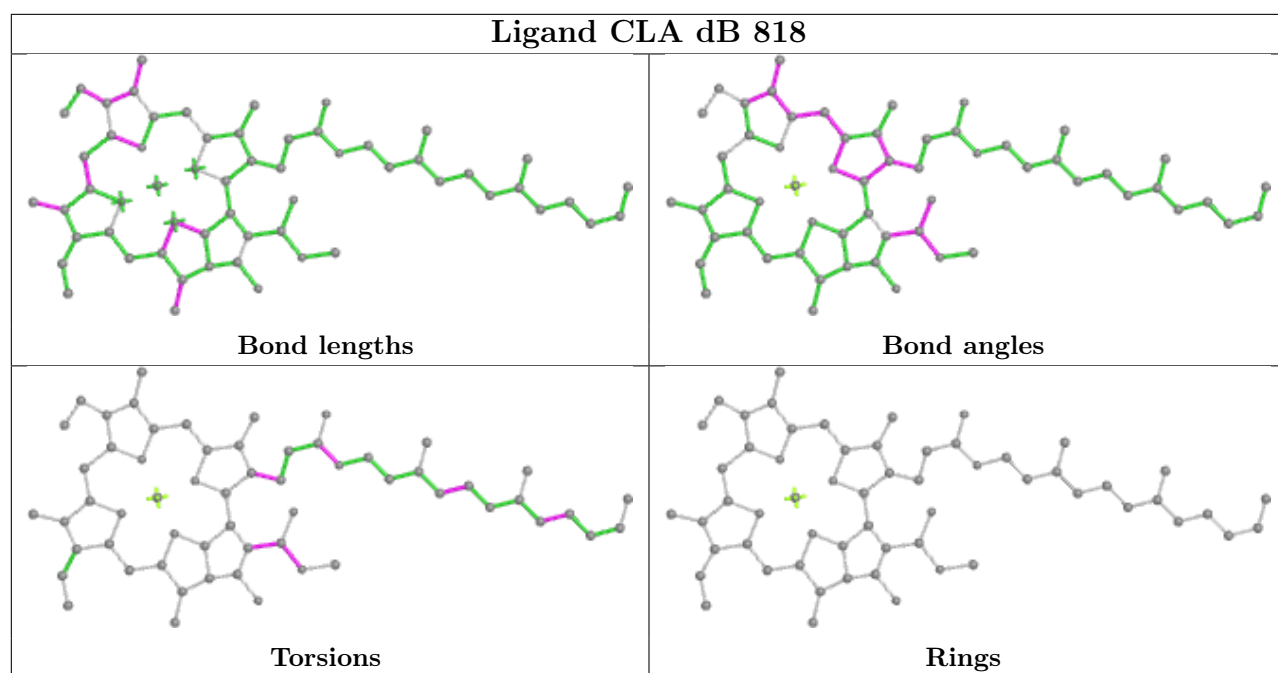


Ligand CLA dA 803

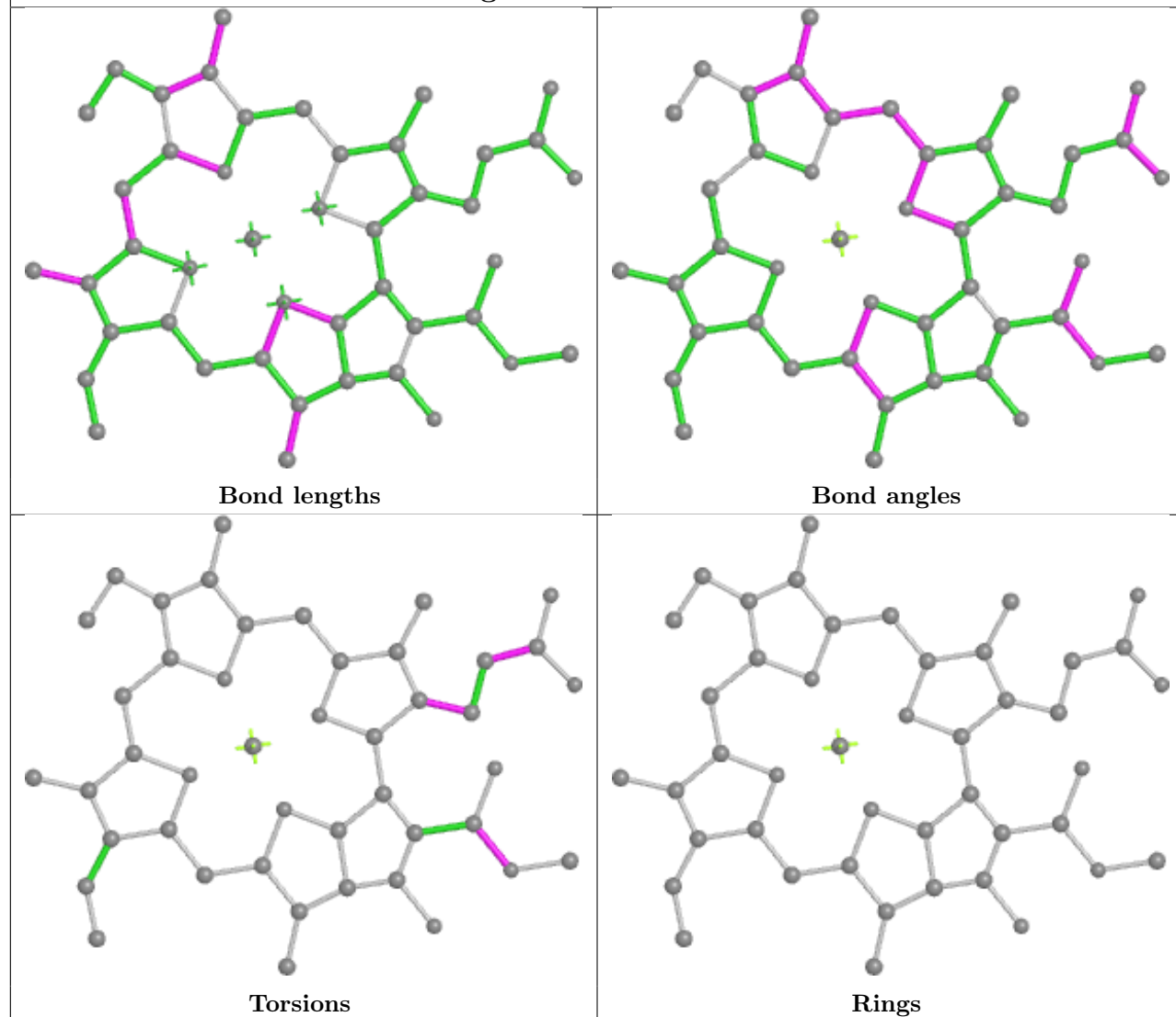


Ligand CLA bB 819

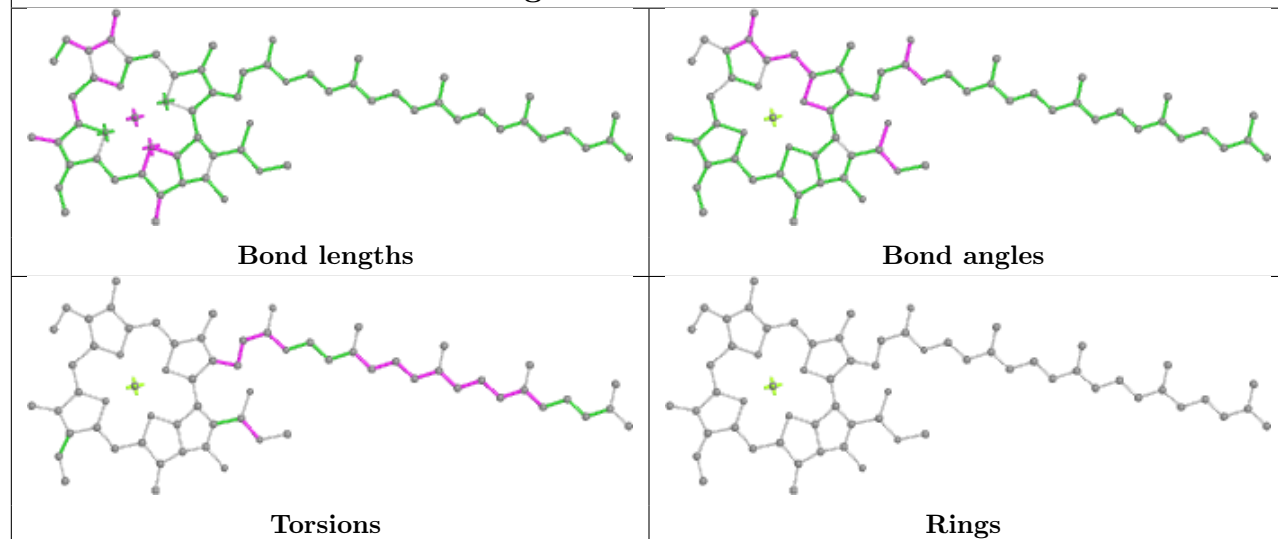


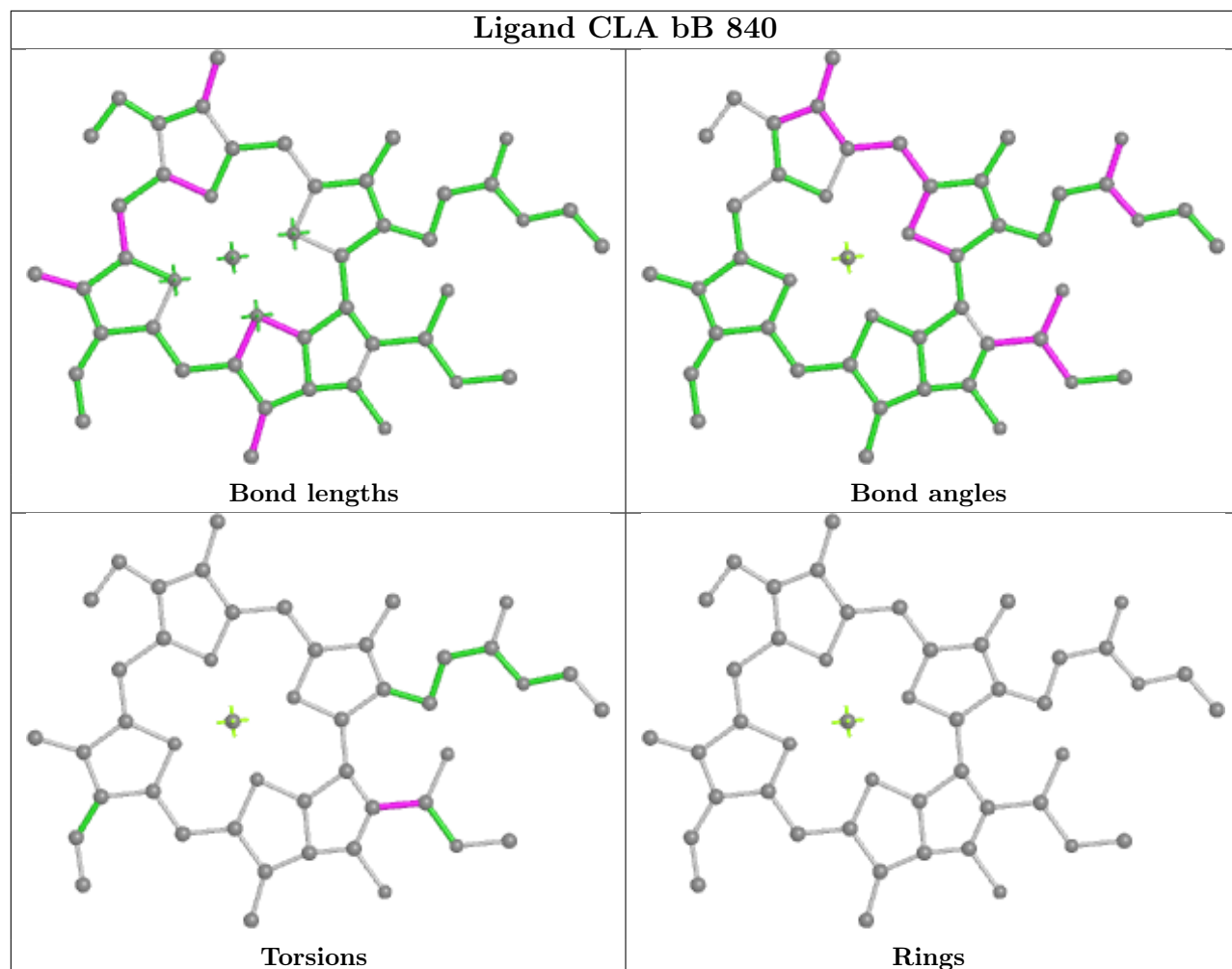
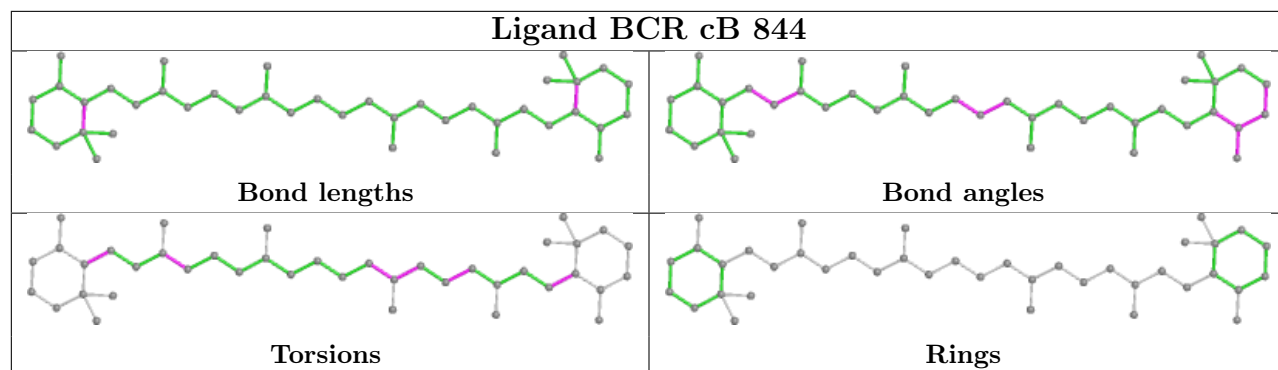


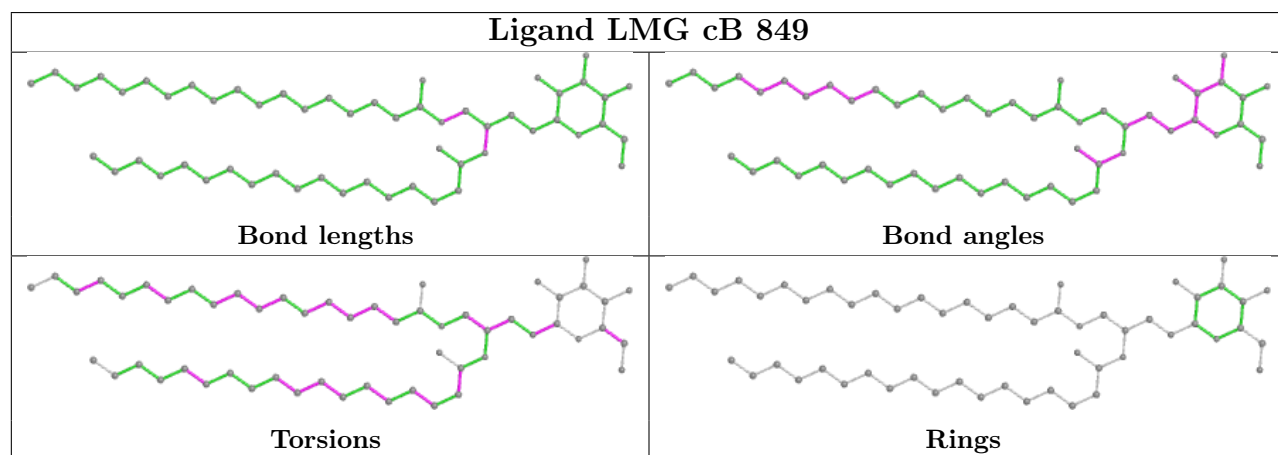
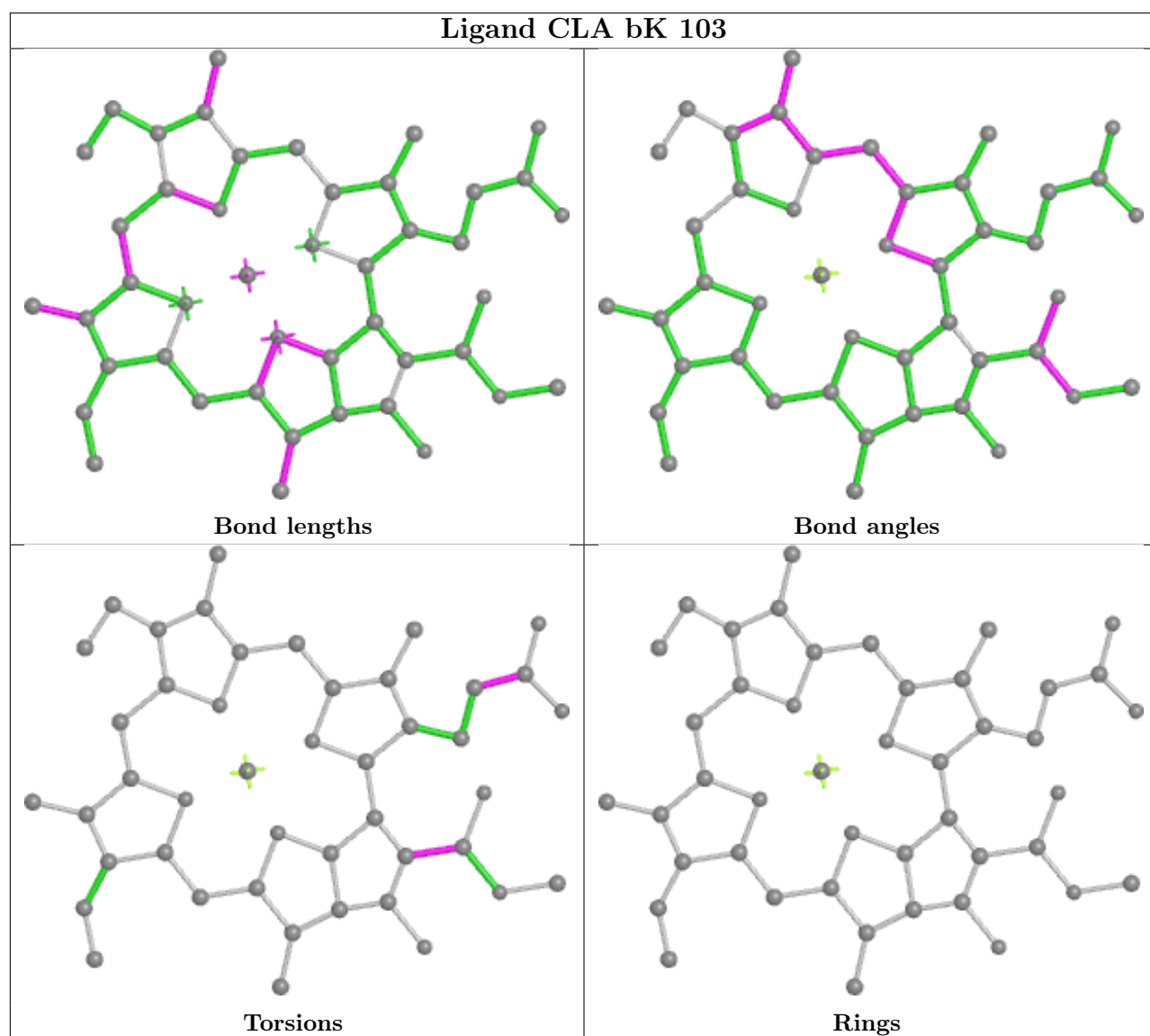
Ligand CLA dB 824



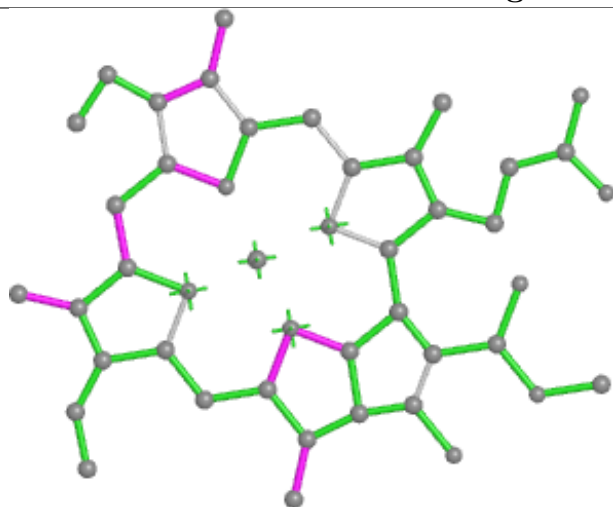
Ligand CLA bL 206



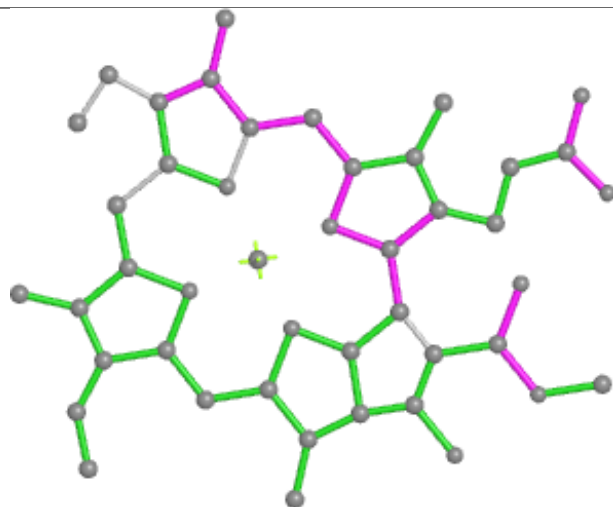




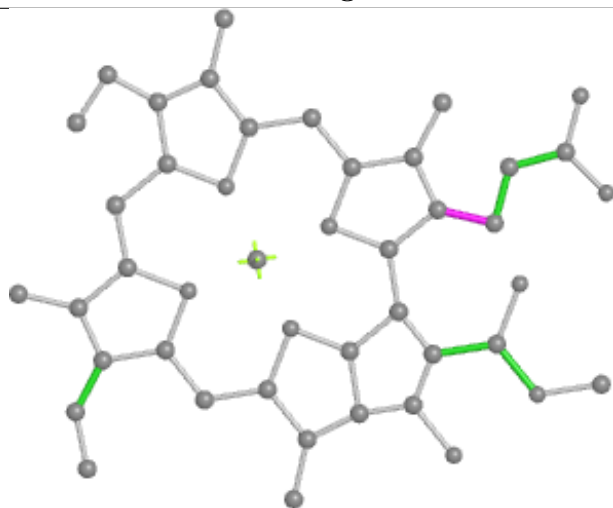
Ligand CLA cB 835



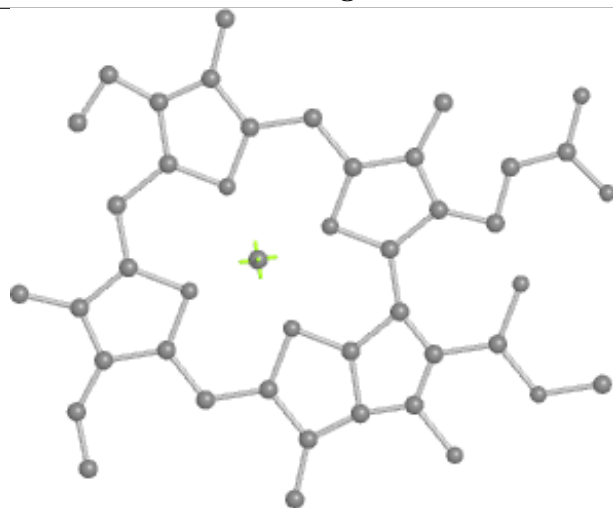
Bond lengths



Bond angles

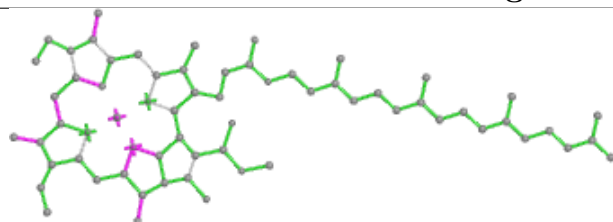


Torsions

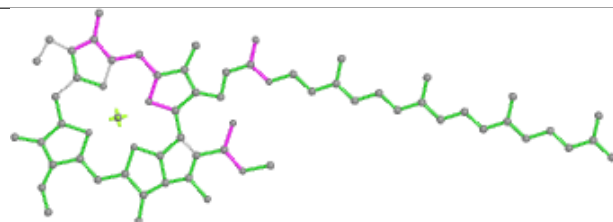


Rings

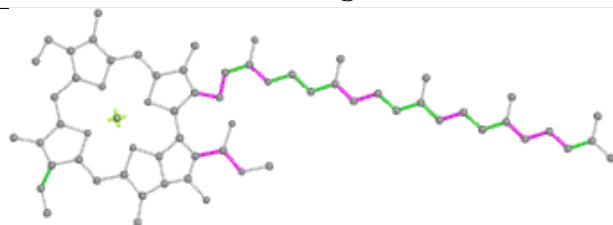
Ligand CLA aB 803



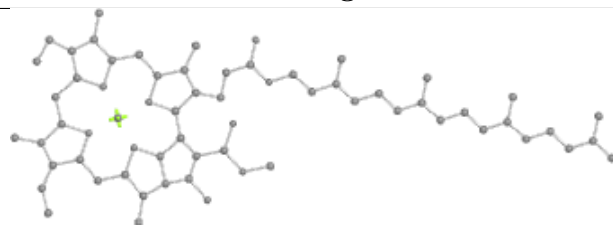
Bond lengths



Bond angles

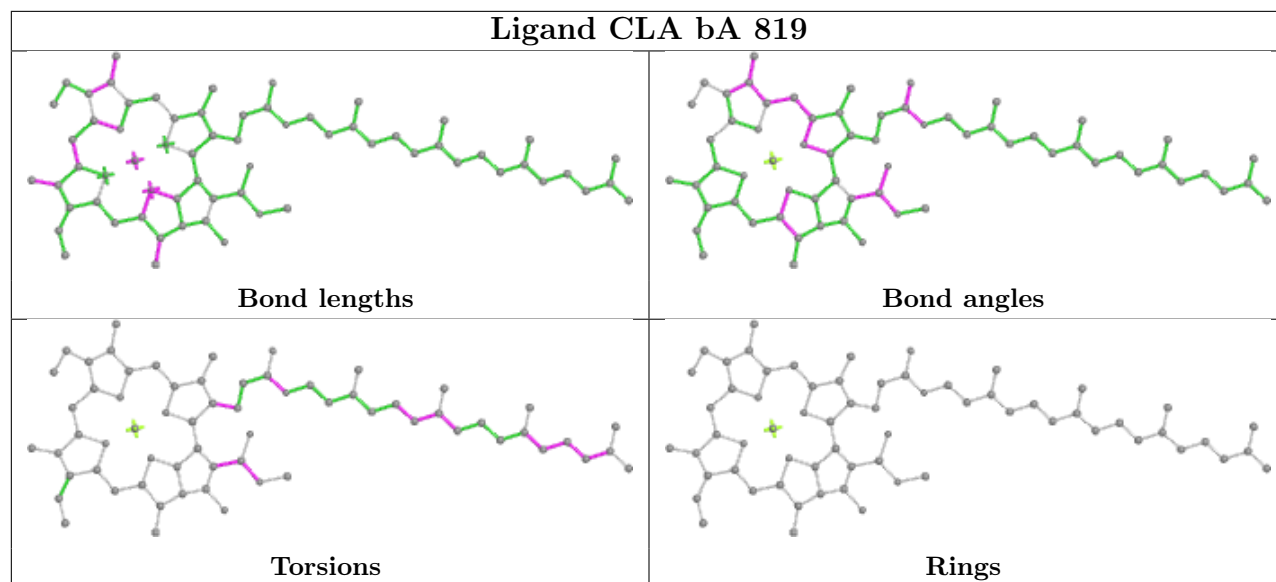


Torsions

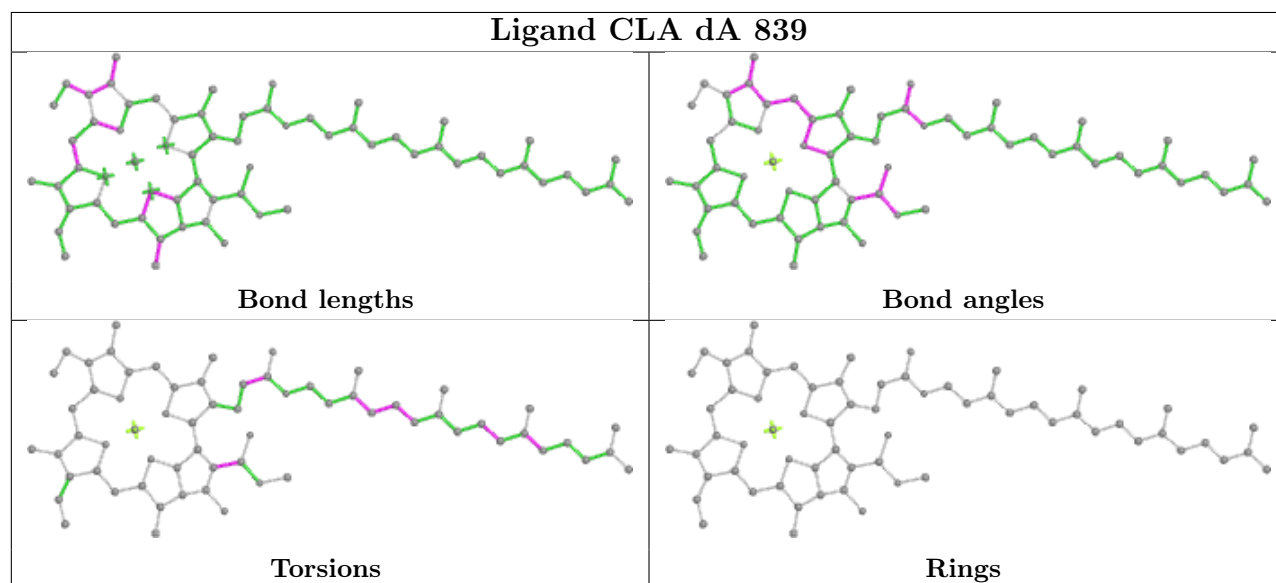


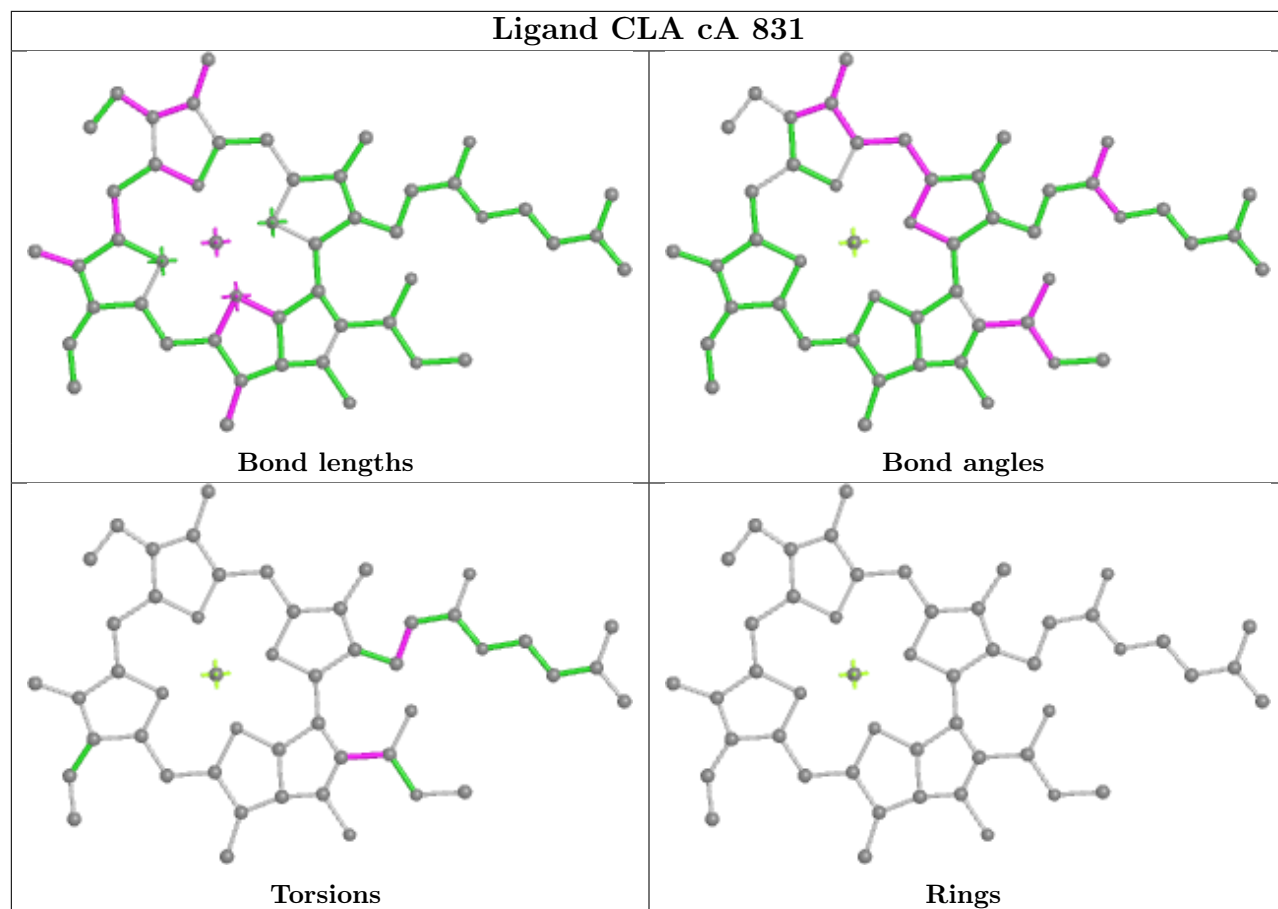
Rings

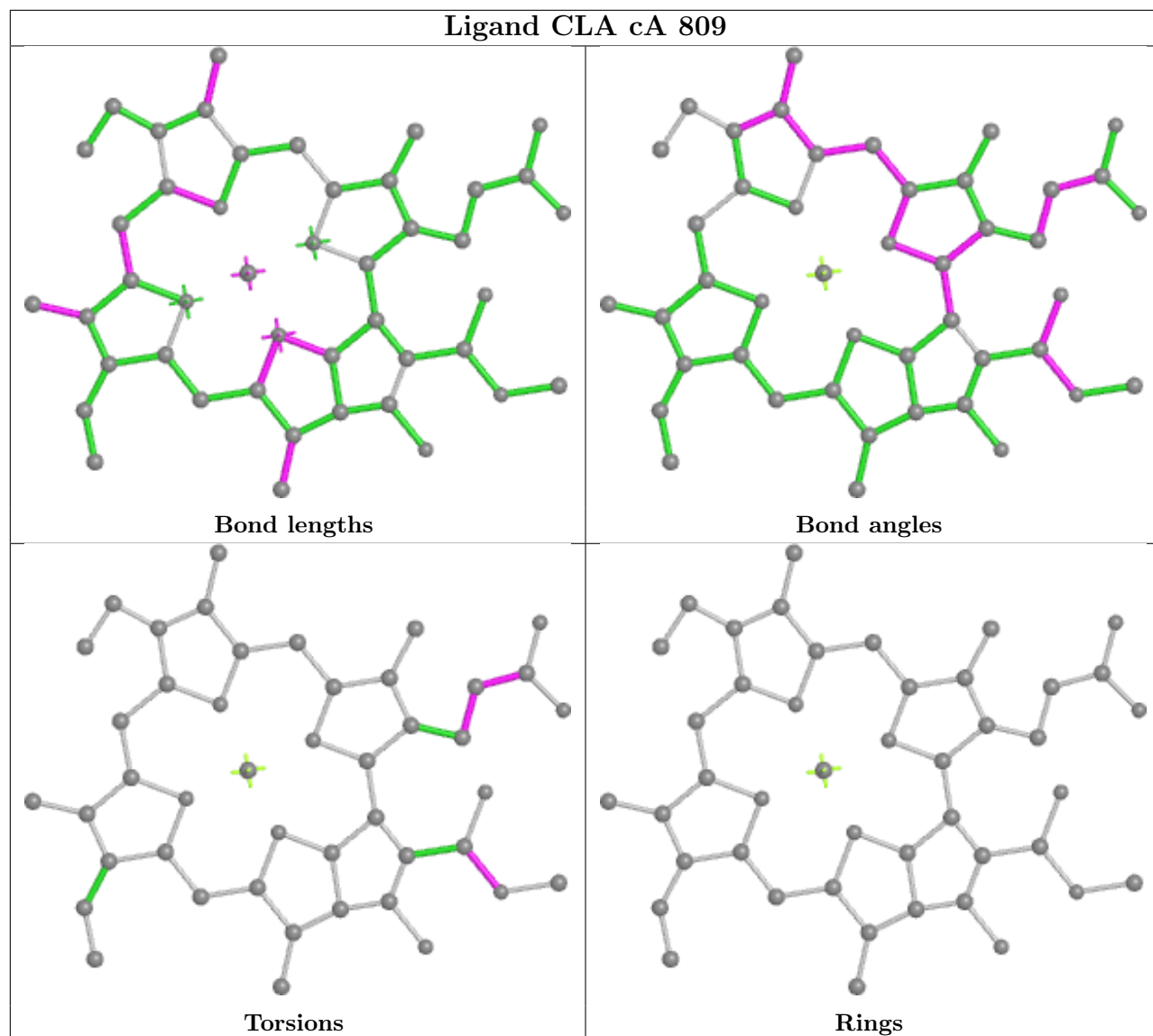
Ligand CLA bA 819

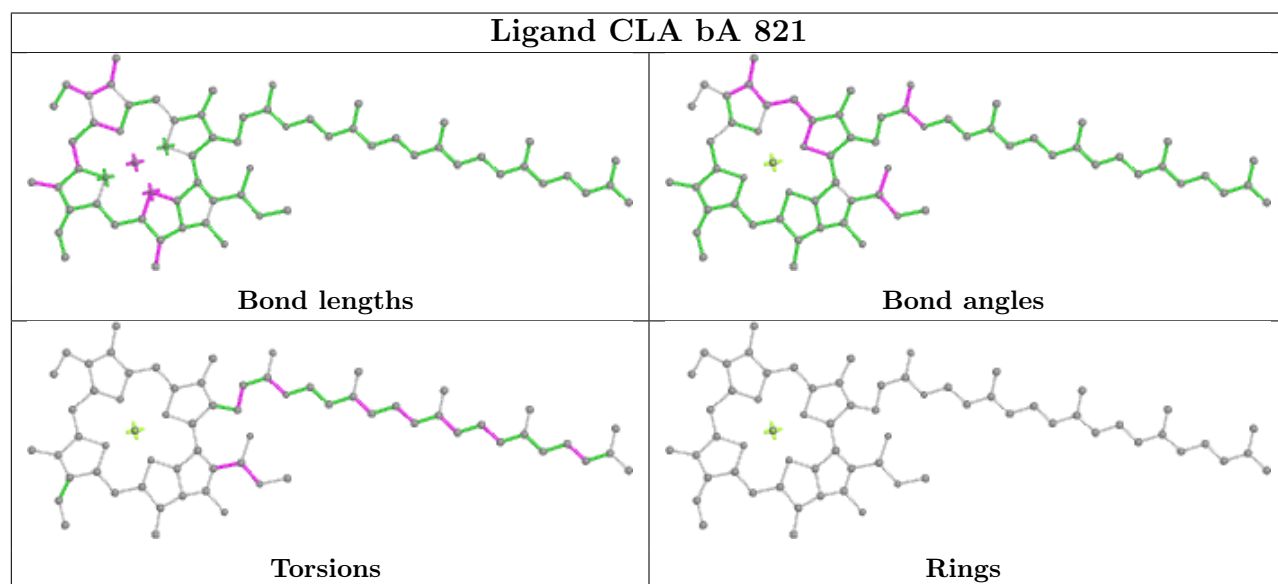
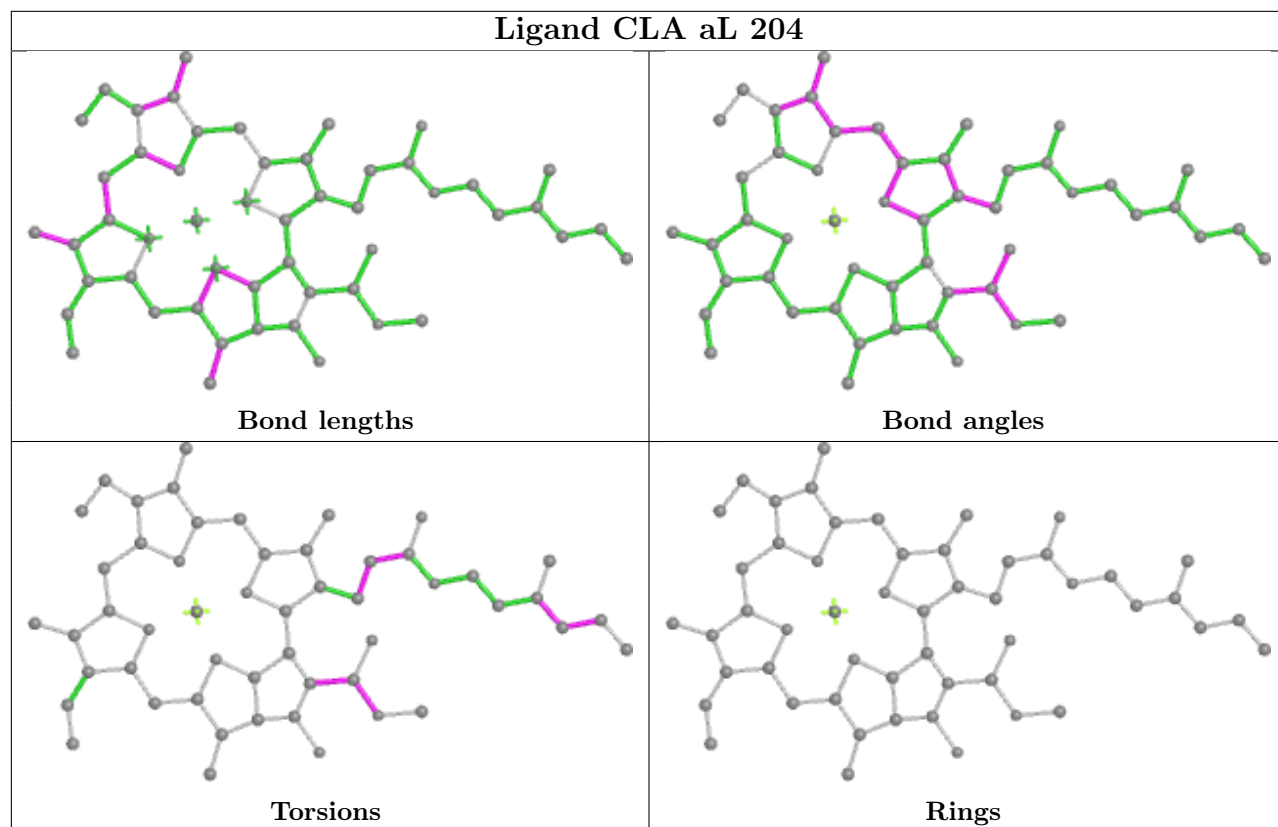


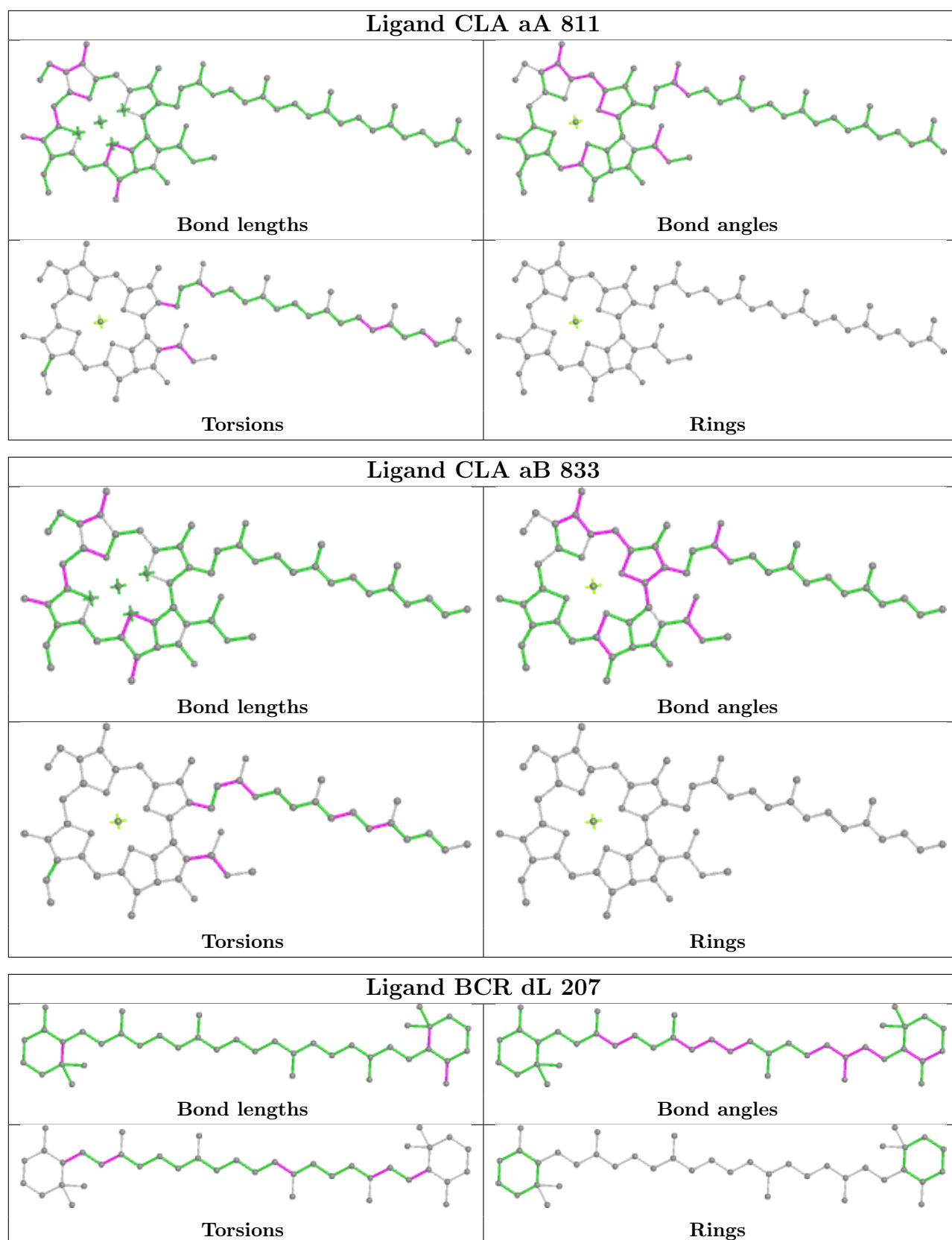
Ligand CLA dA 839

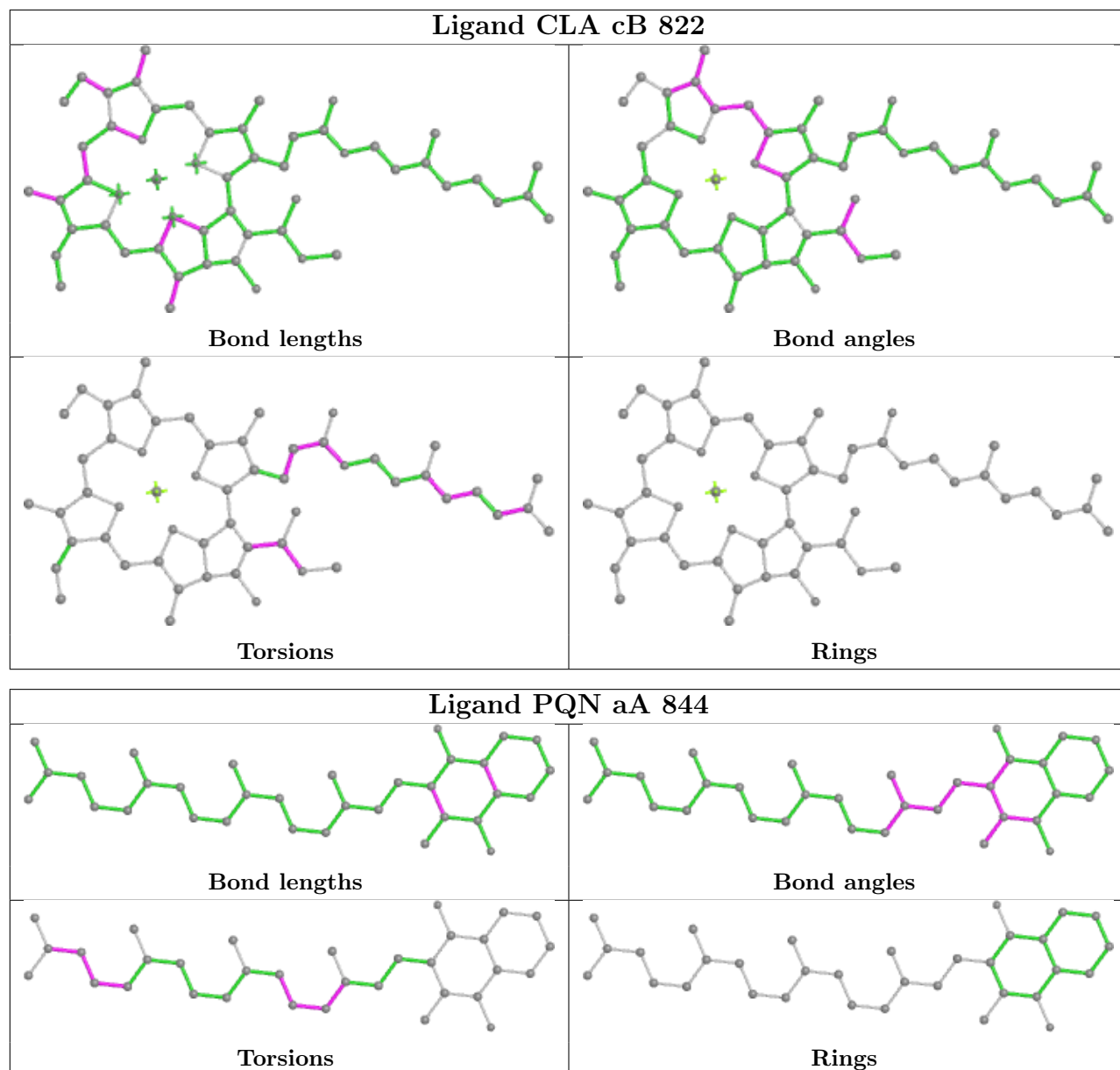




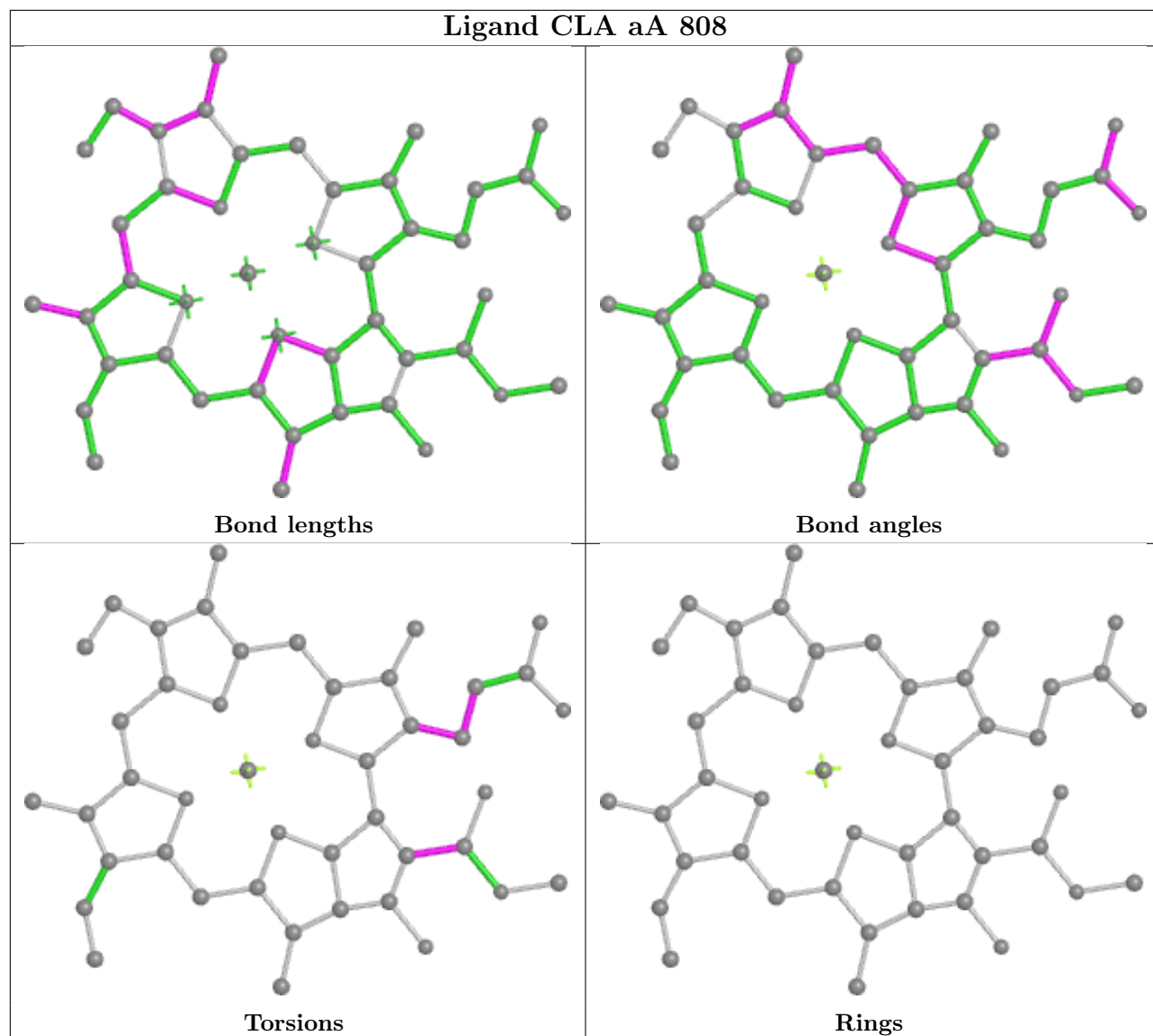




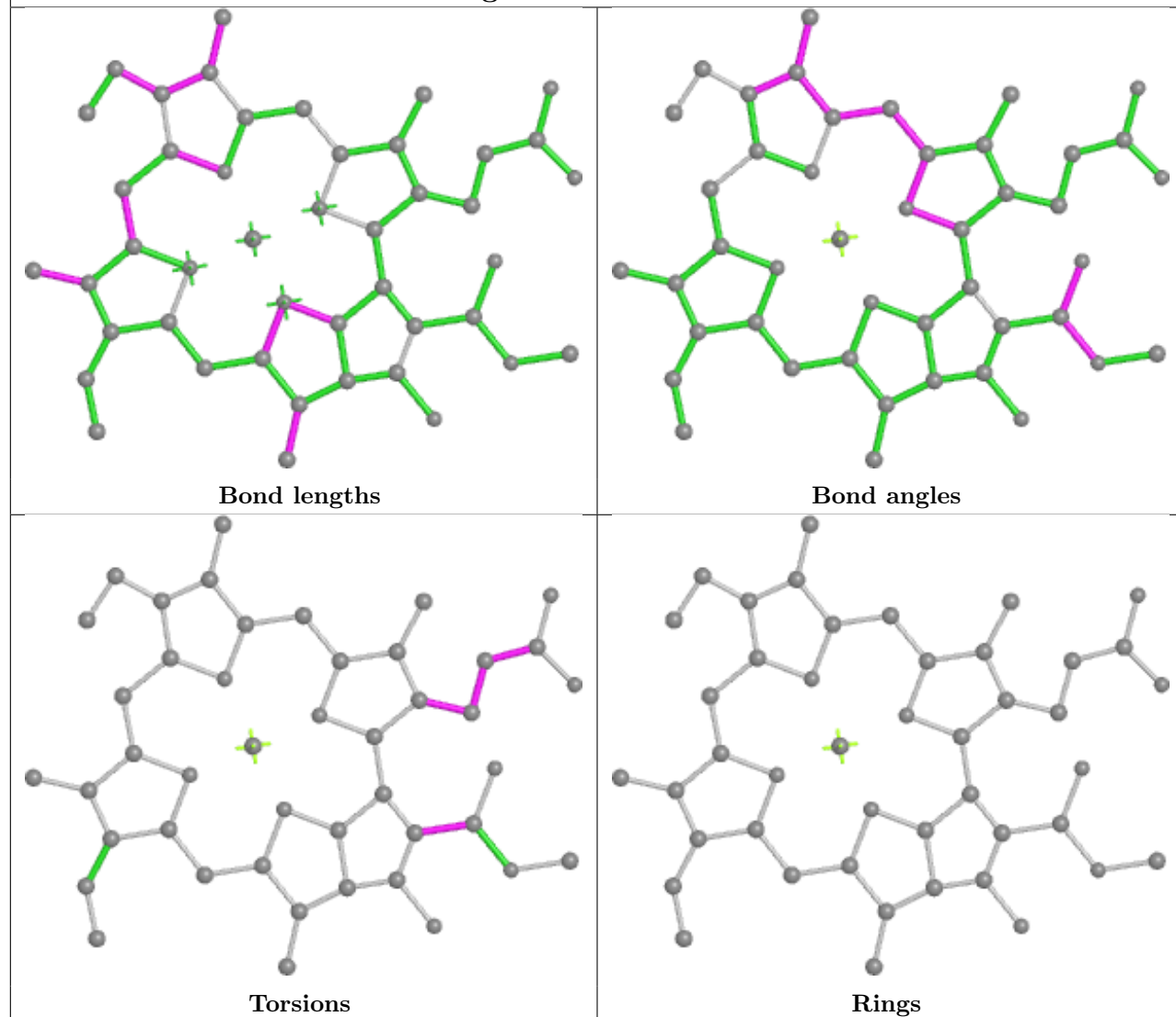




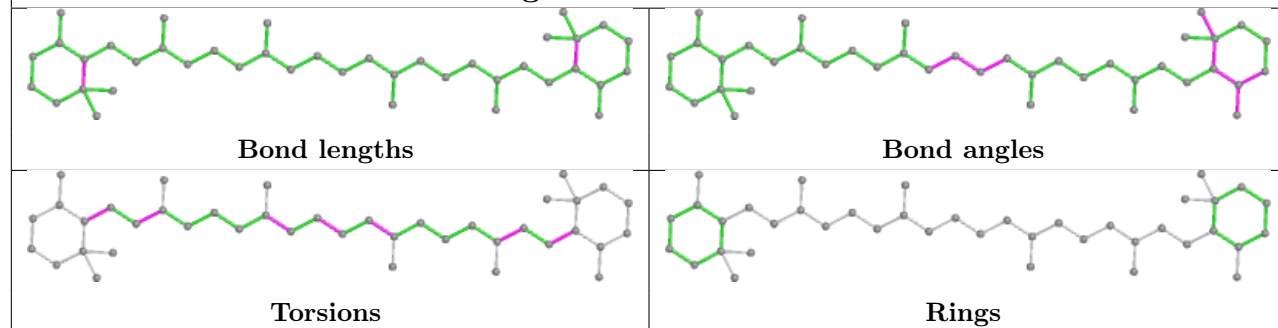
Ligand CLA aA 808

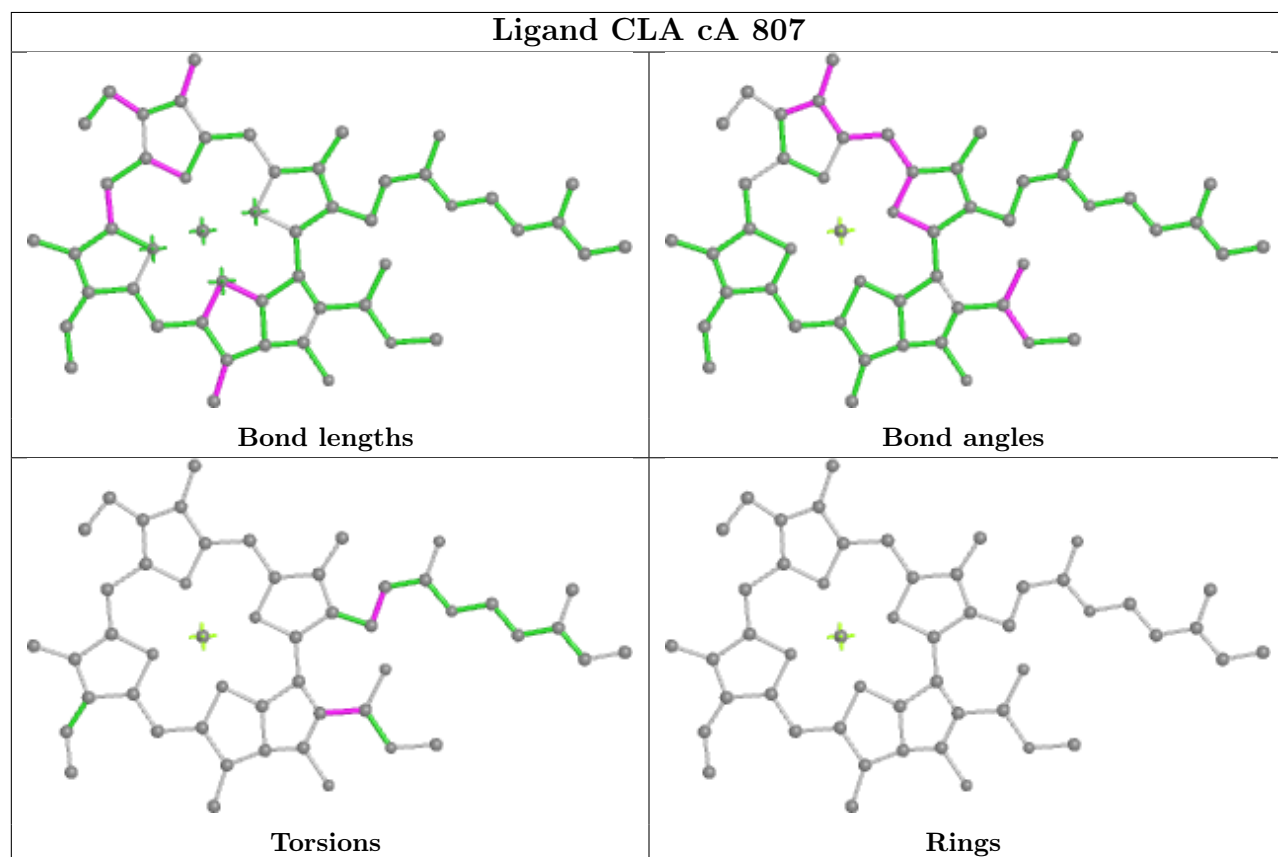
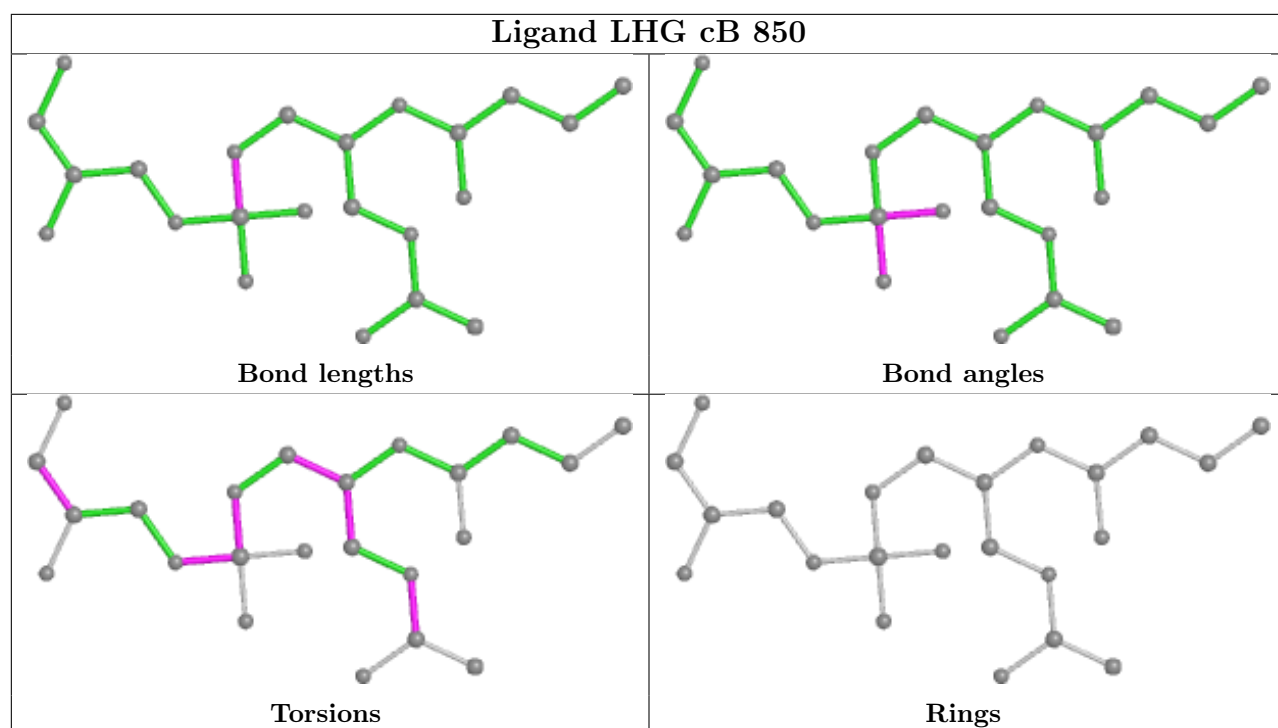


Ligand CLA aB 830

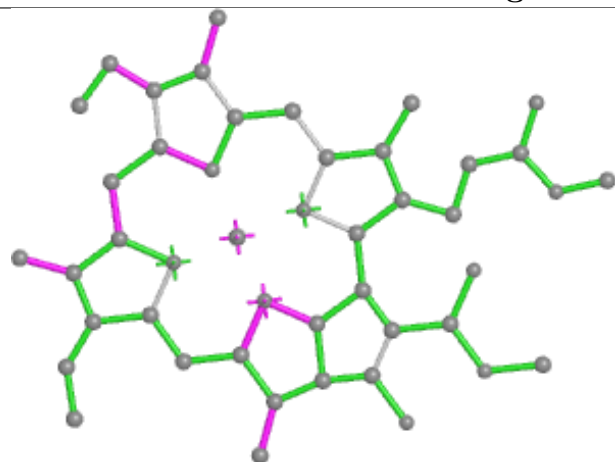


Ligand BCR dF 202

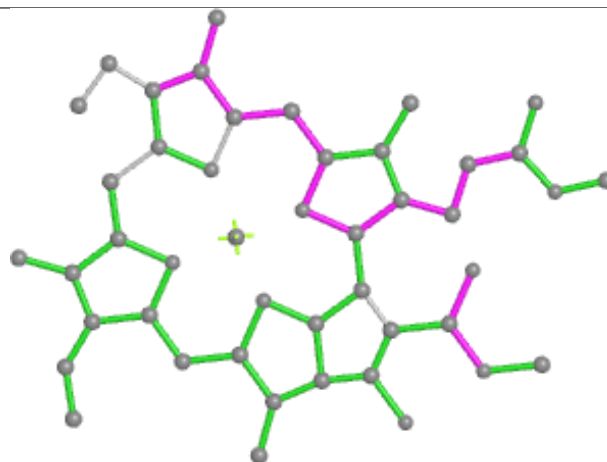




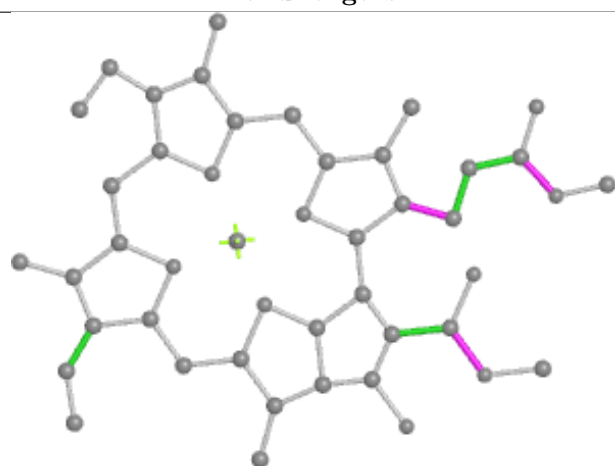
Ligand CLA bB 826



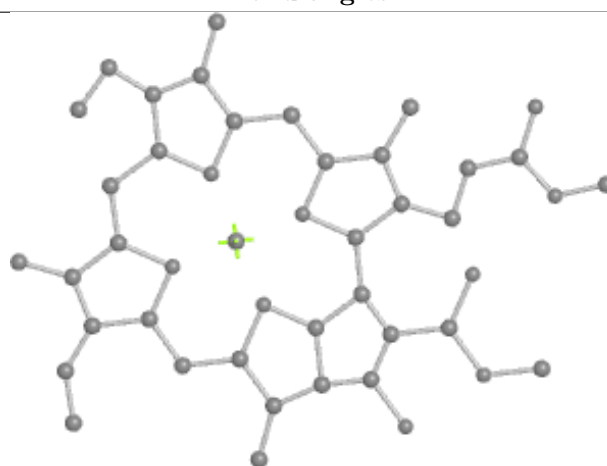
Bond lengths



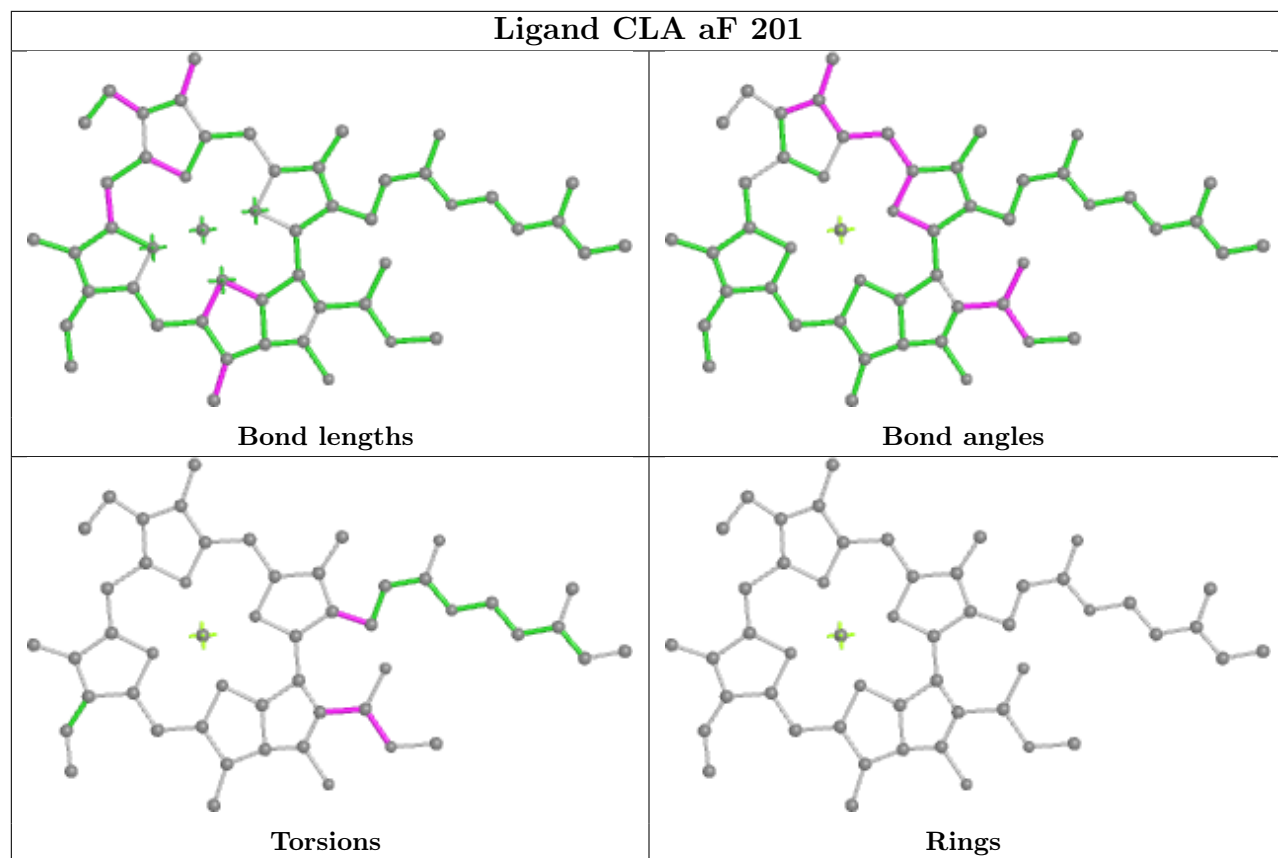
Bond angles



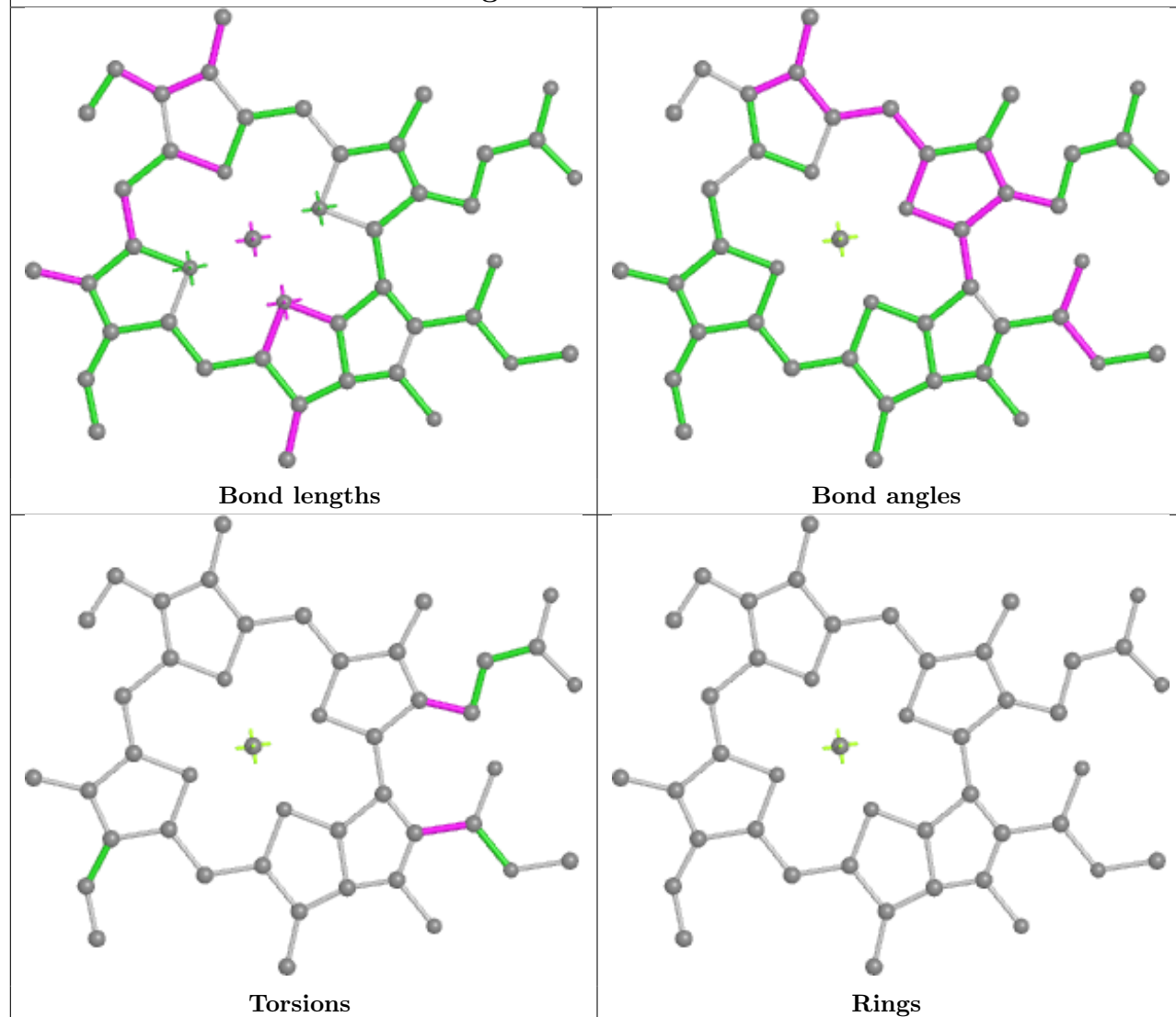
Torsions



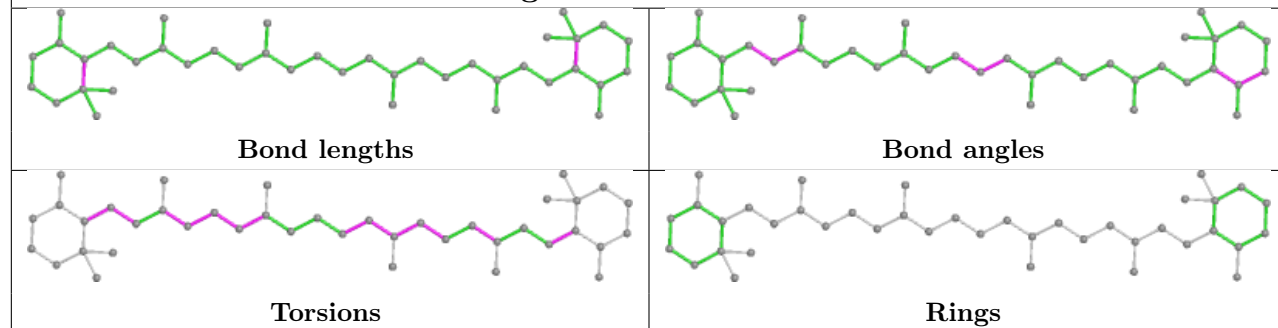
Rings



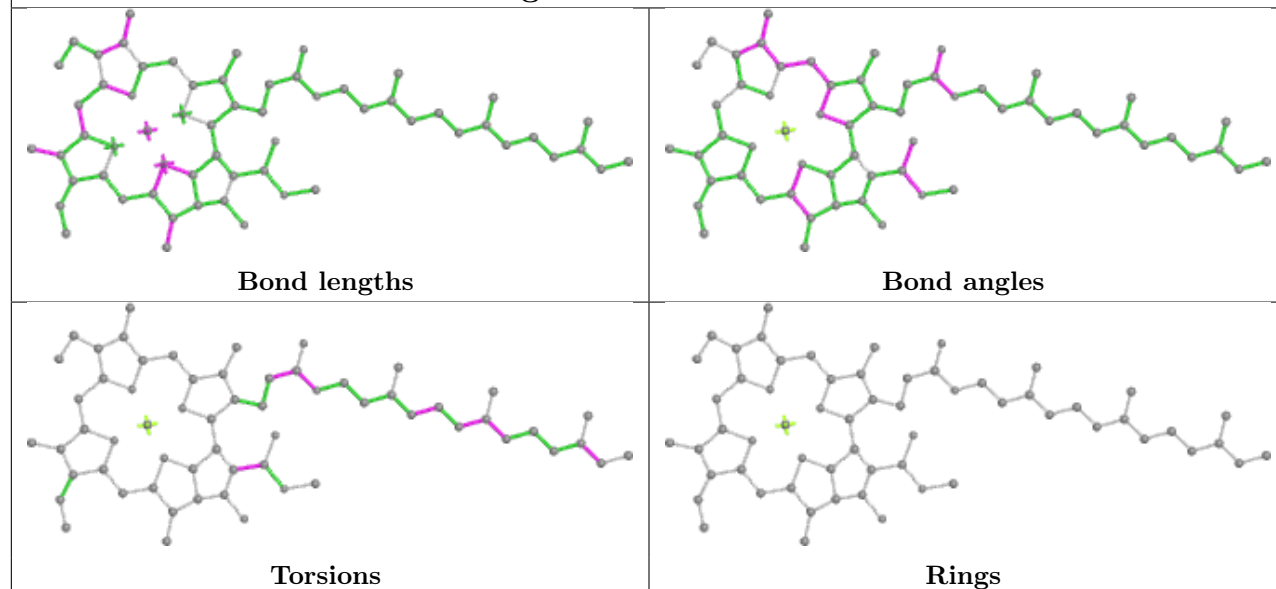
Ligand CLA cA 805



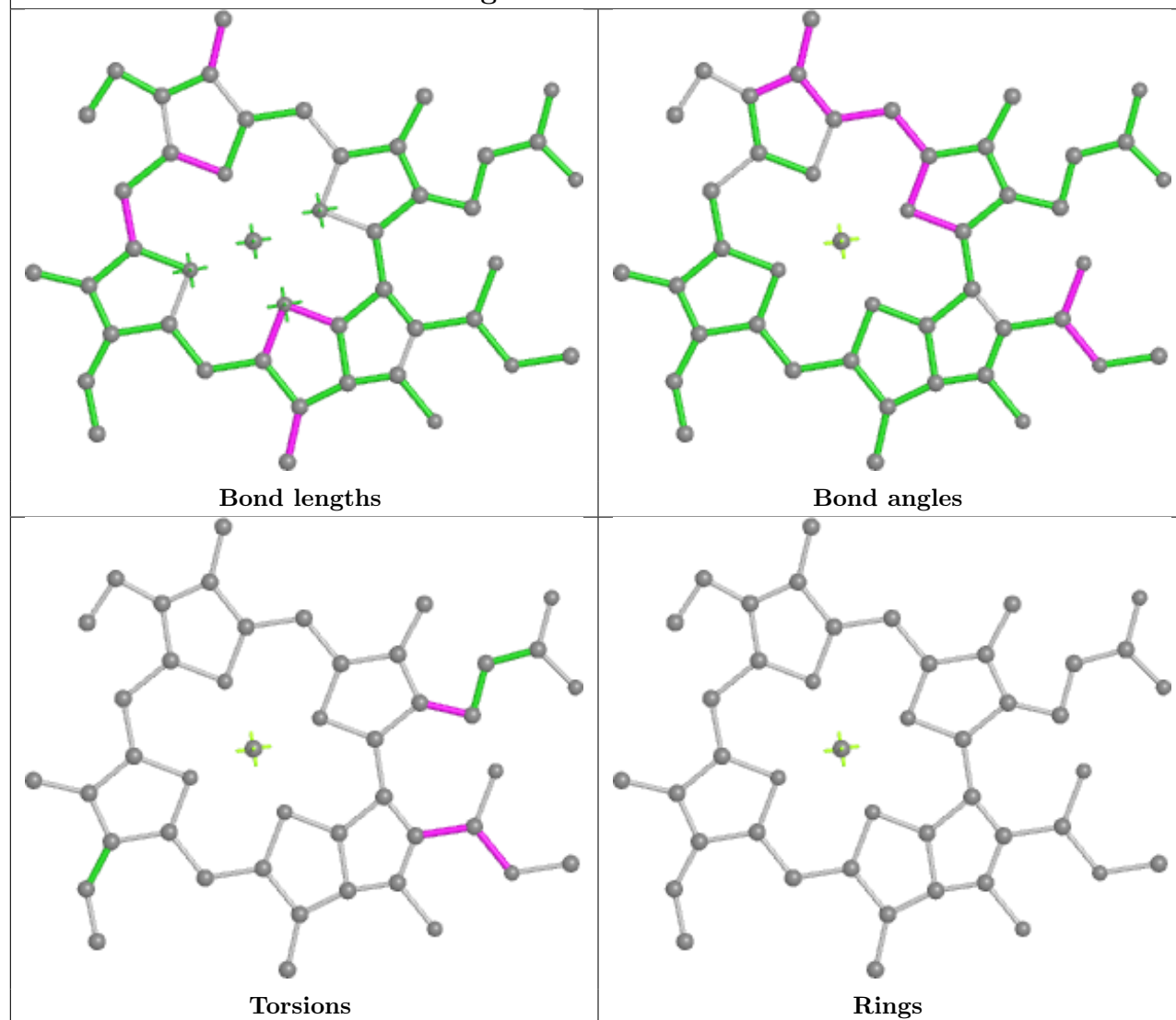
Ligand BCR aA 849

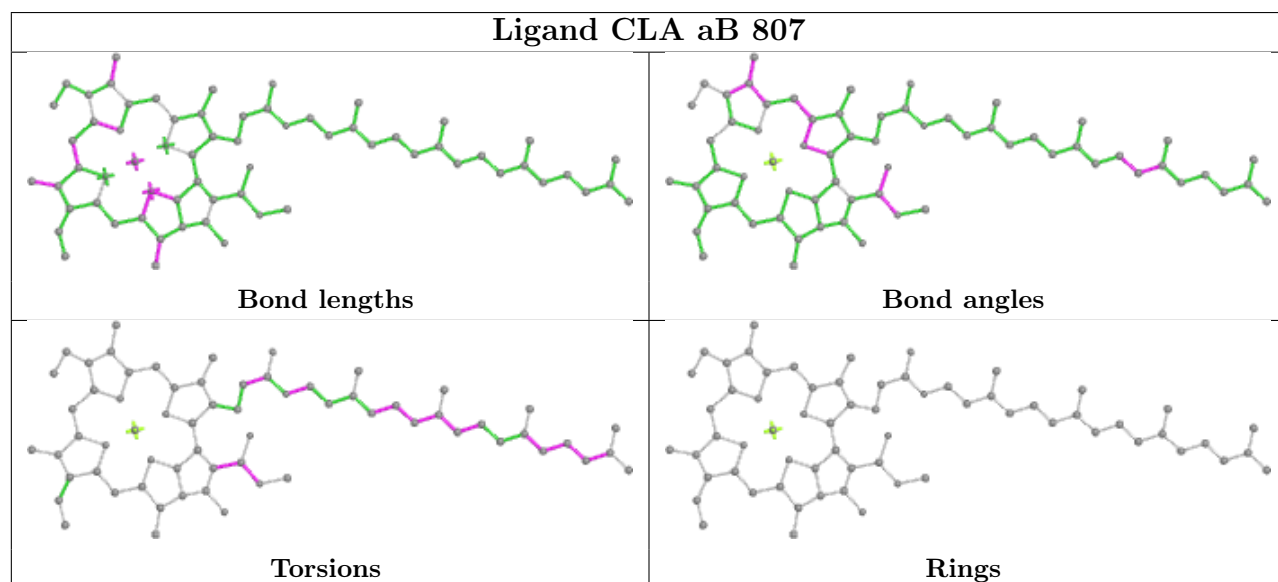
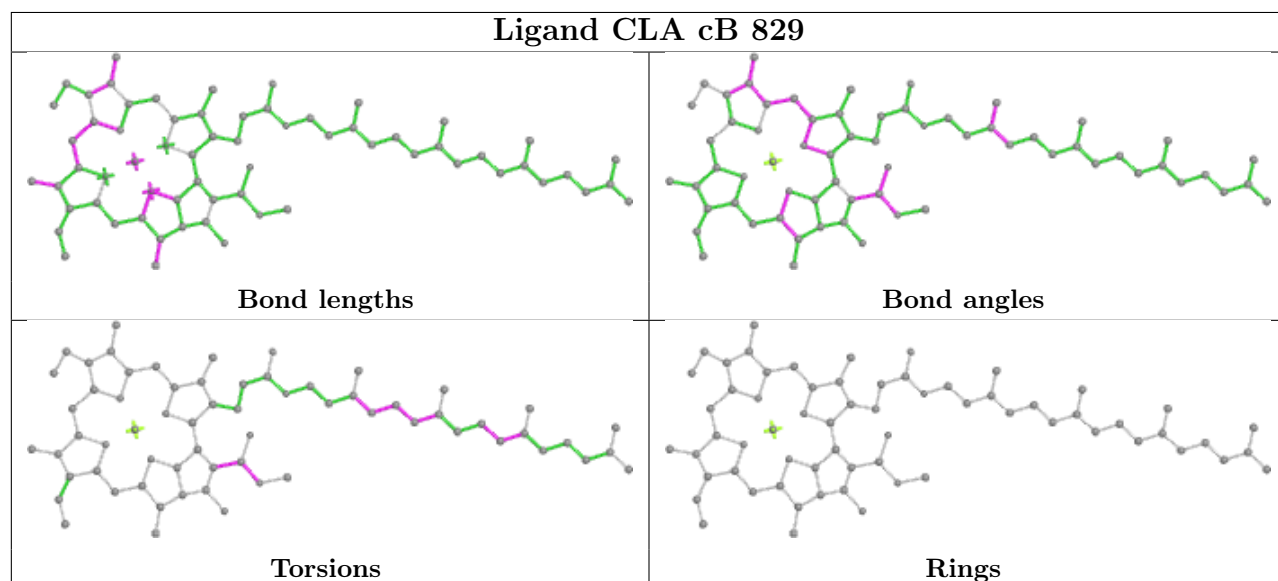
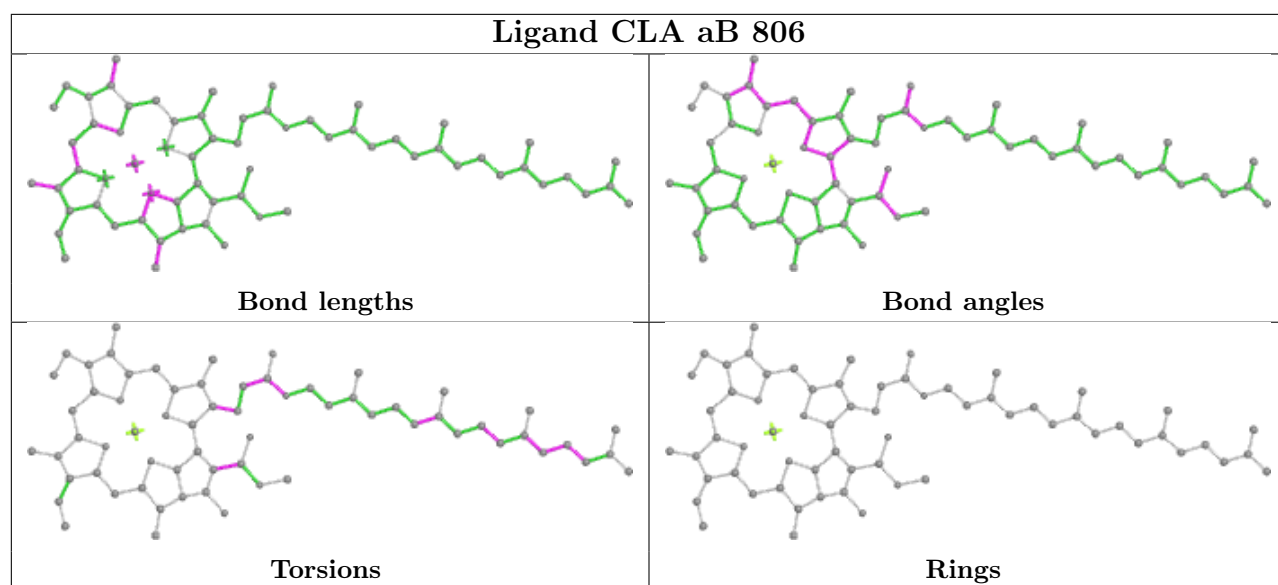


Ligand CLA bA 820

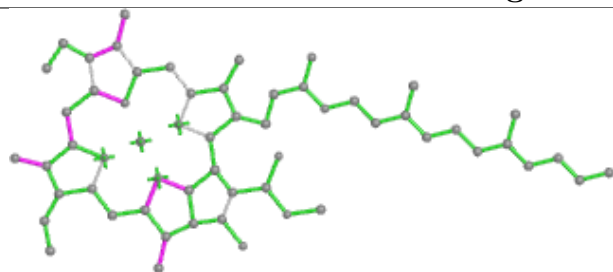


Ligand CLA bA 810

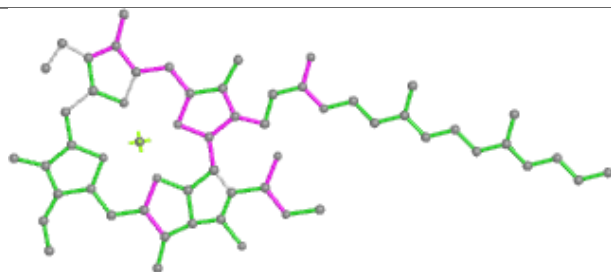




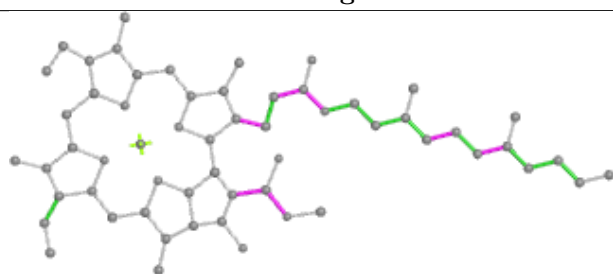
Ligand CLA cB 833



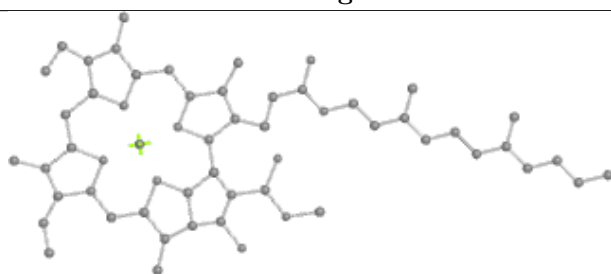
Bond lengths



Bond angles

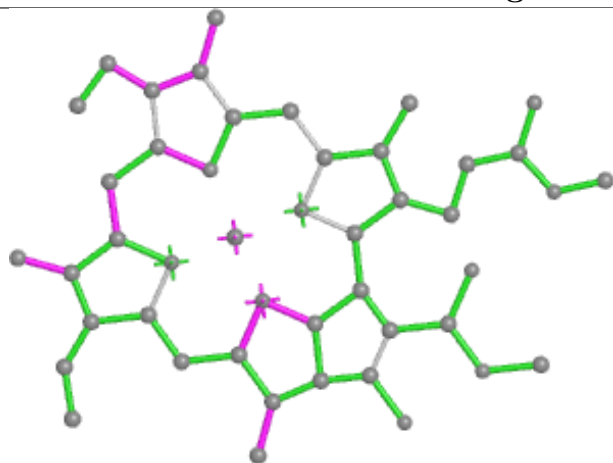


Torsions

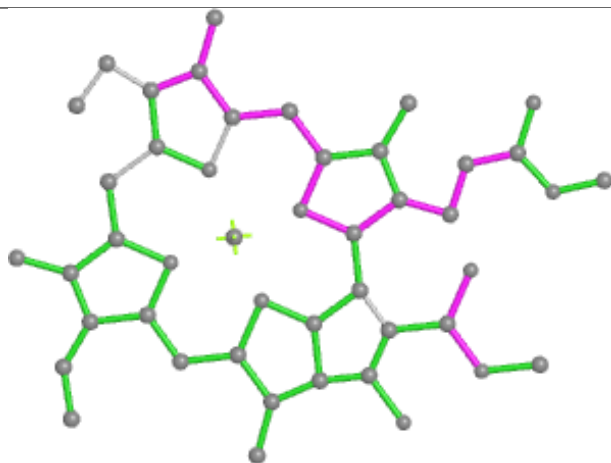


Rings

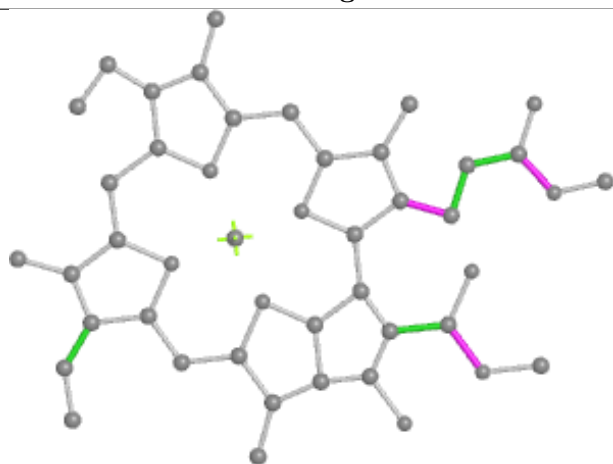
Ligand CLA cB 825



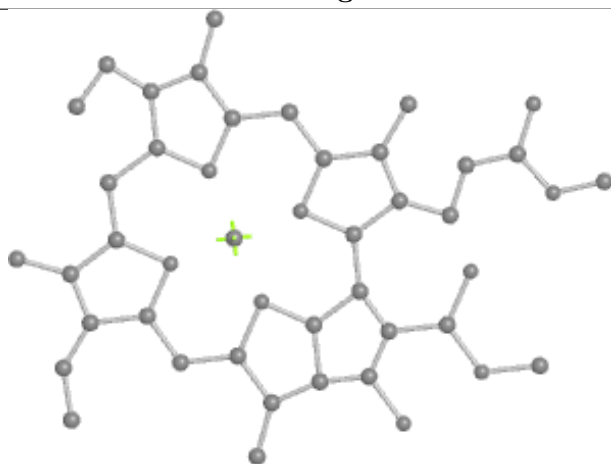
Bond lengths



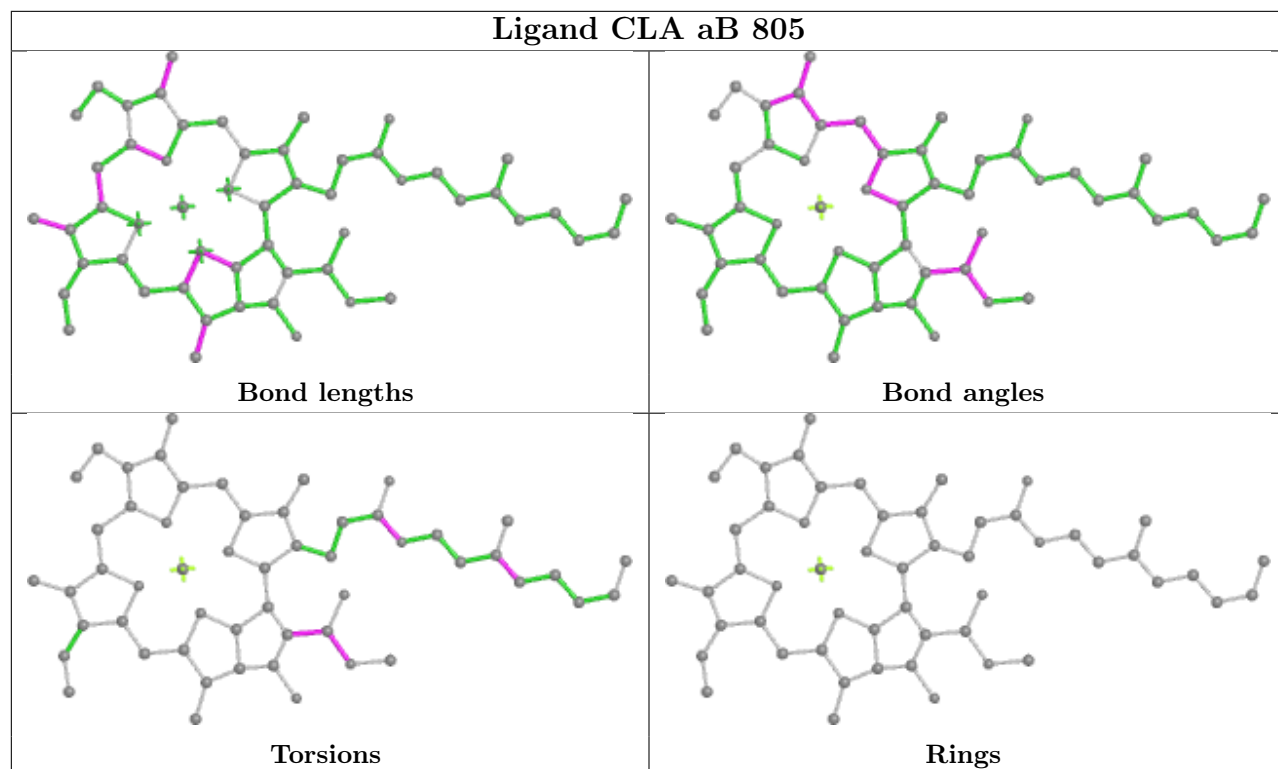
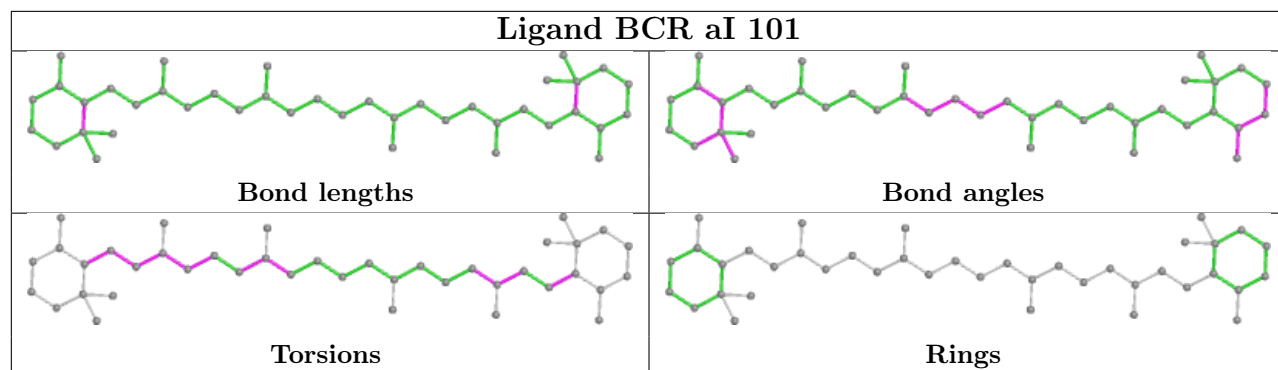
Bond angles

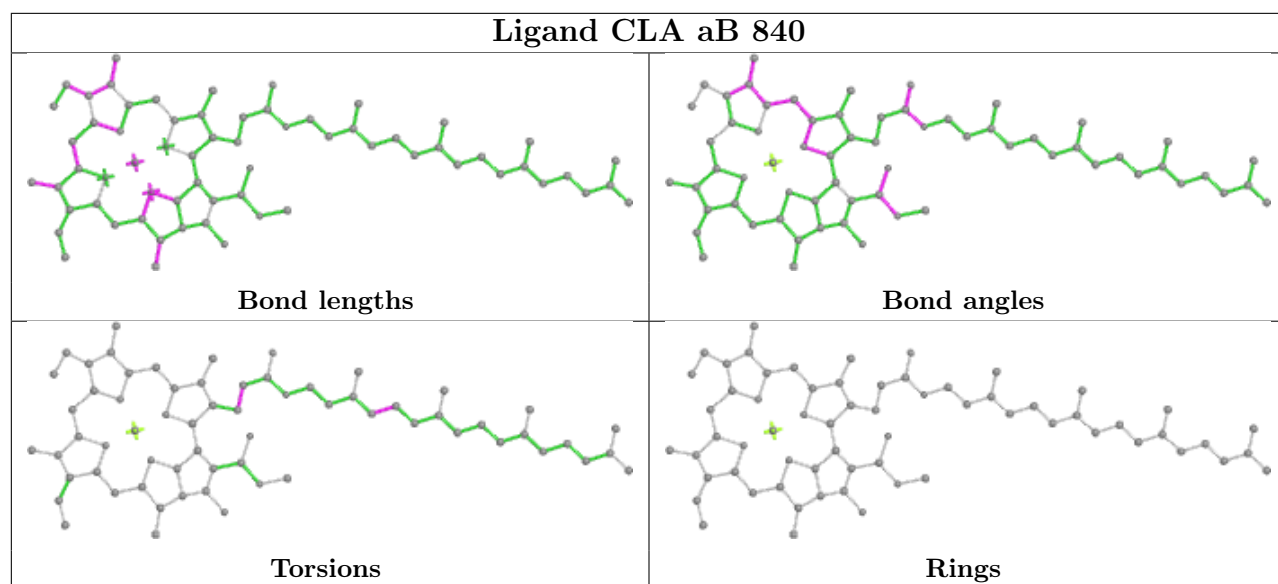
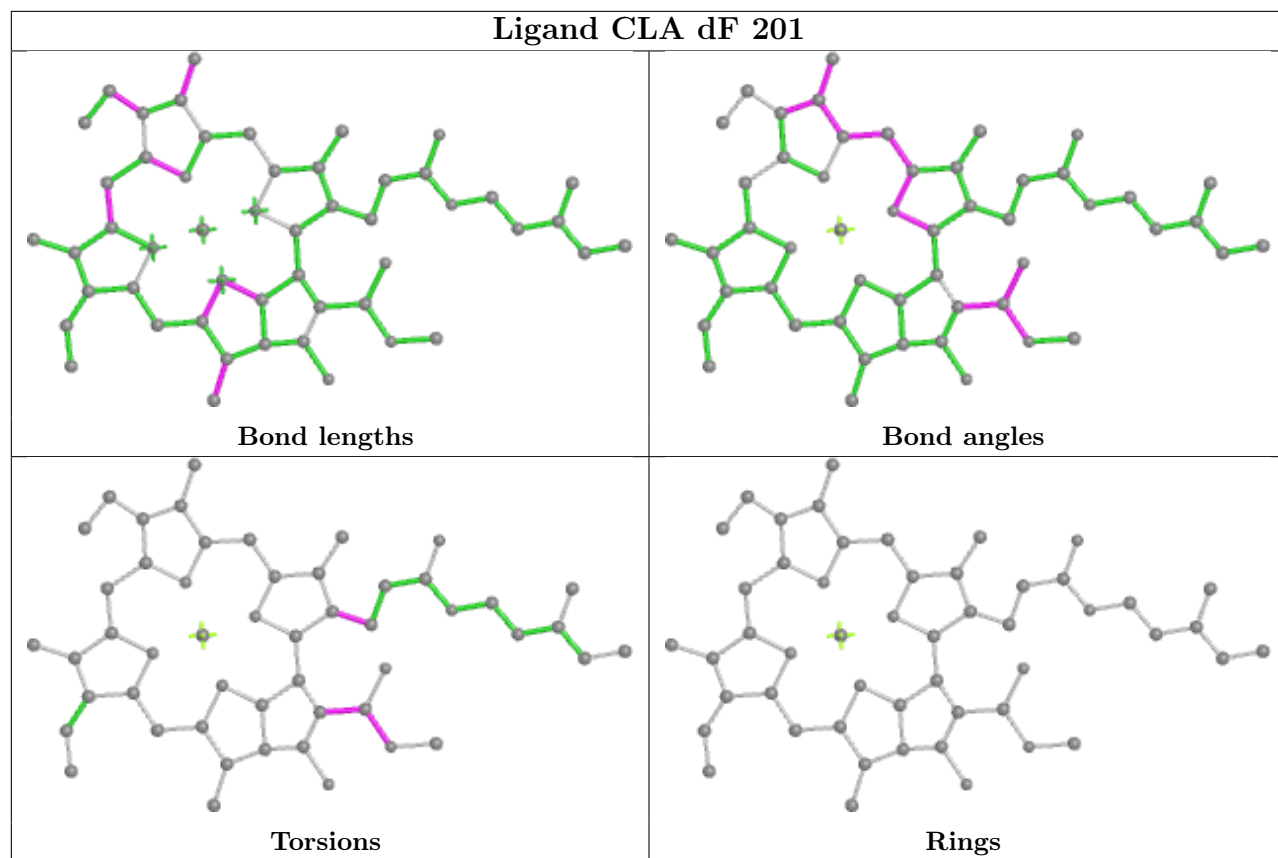


Torsions

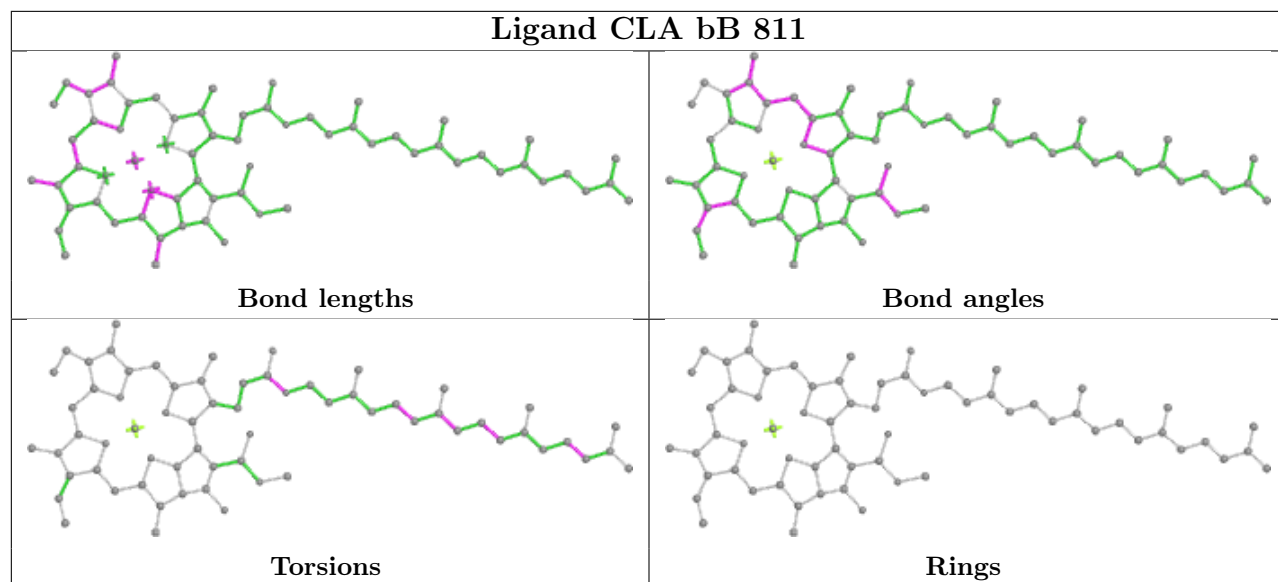


Rings

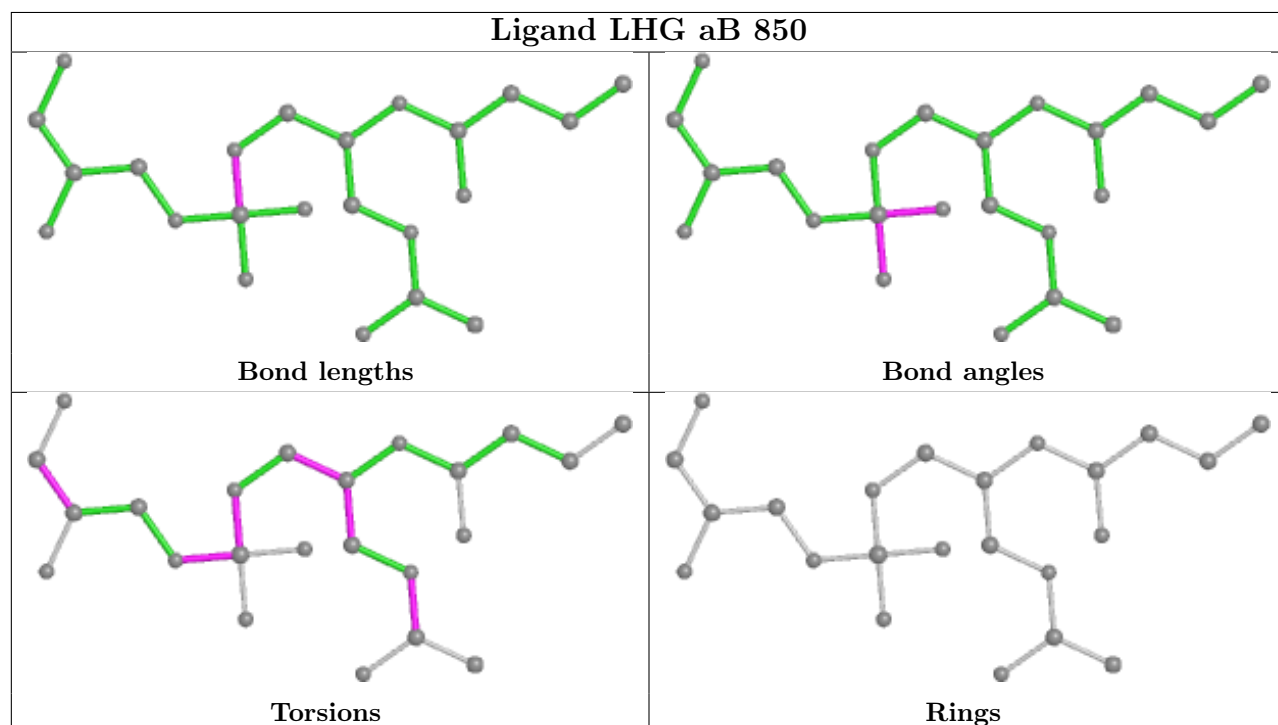


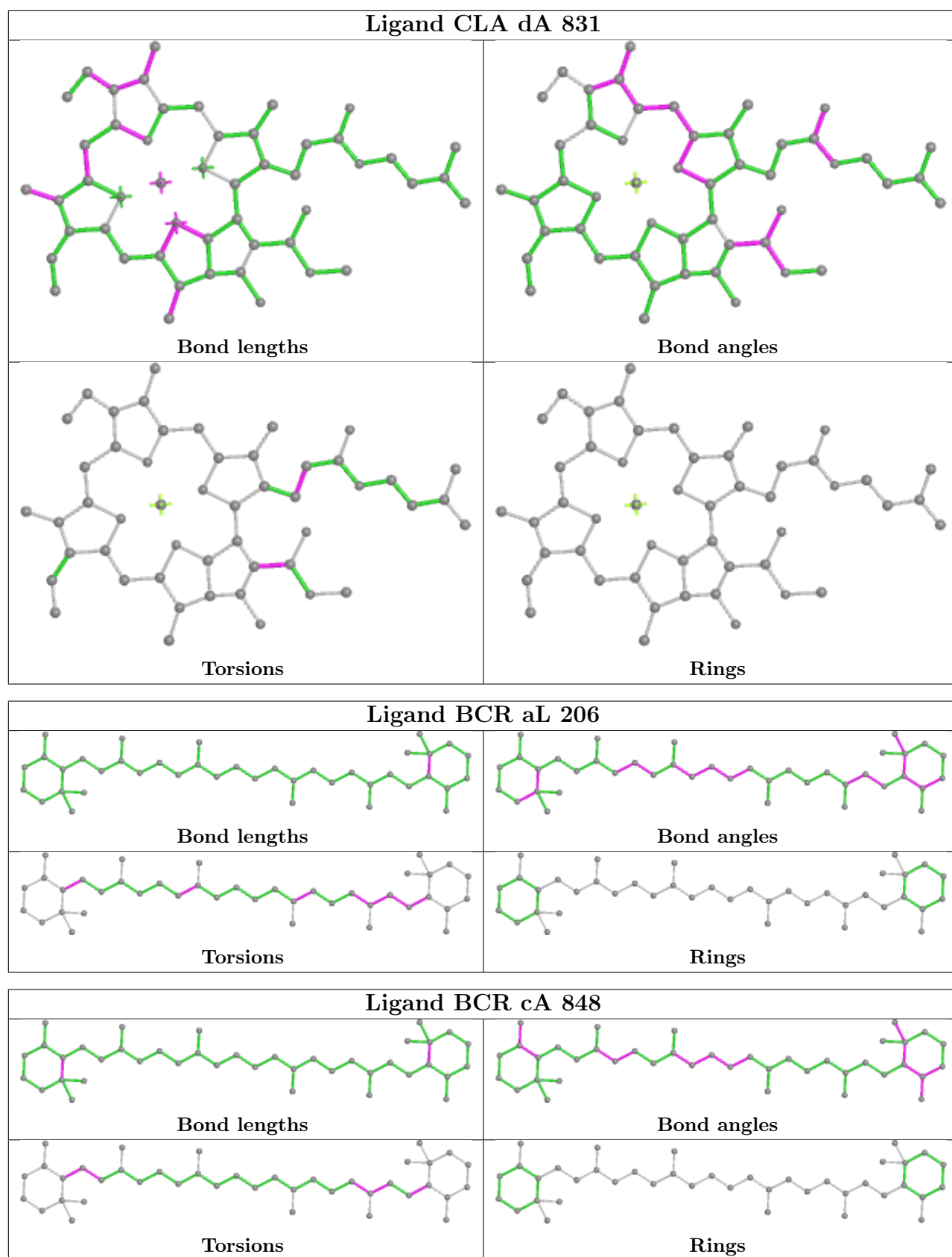


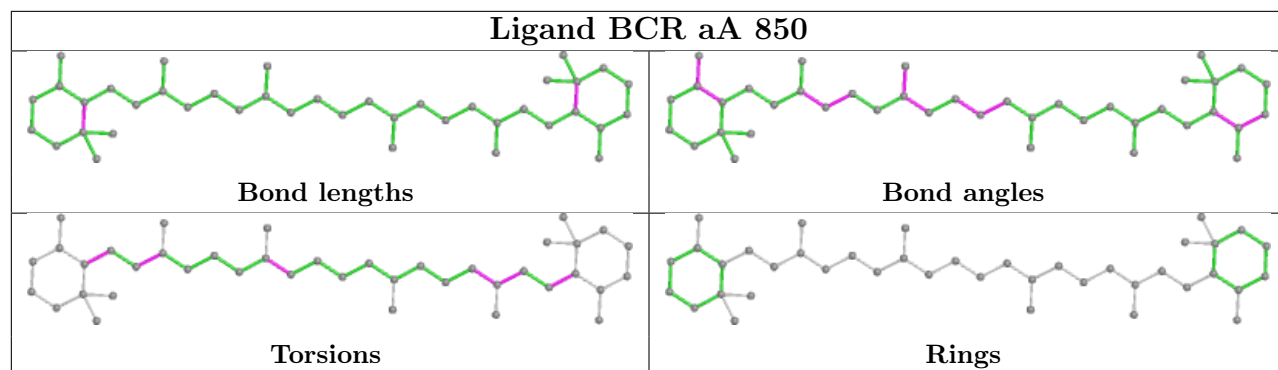
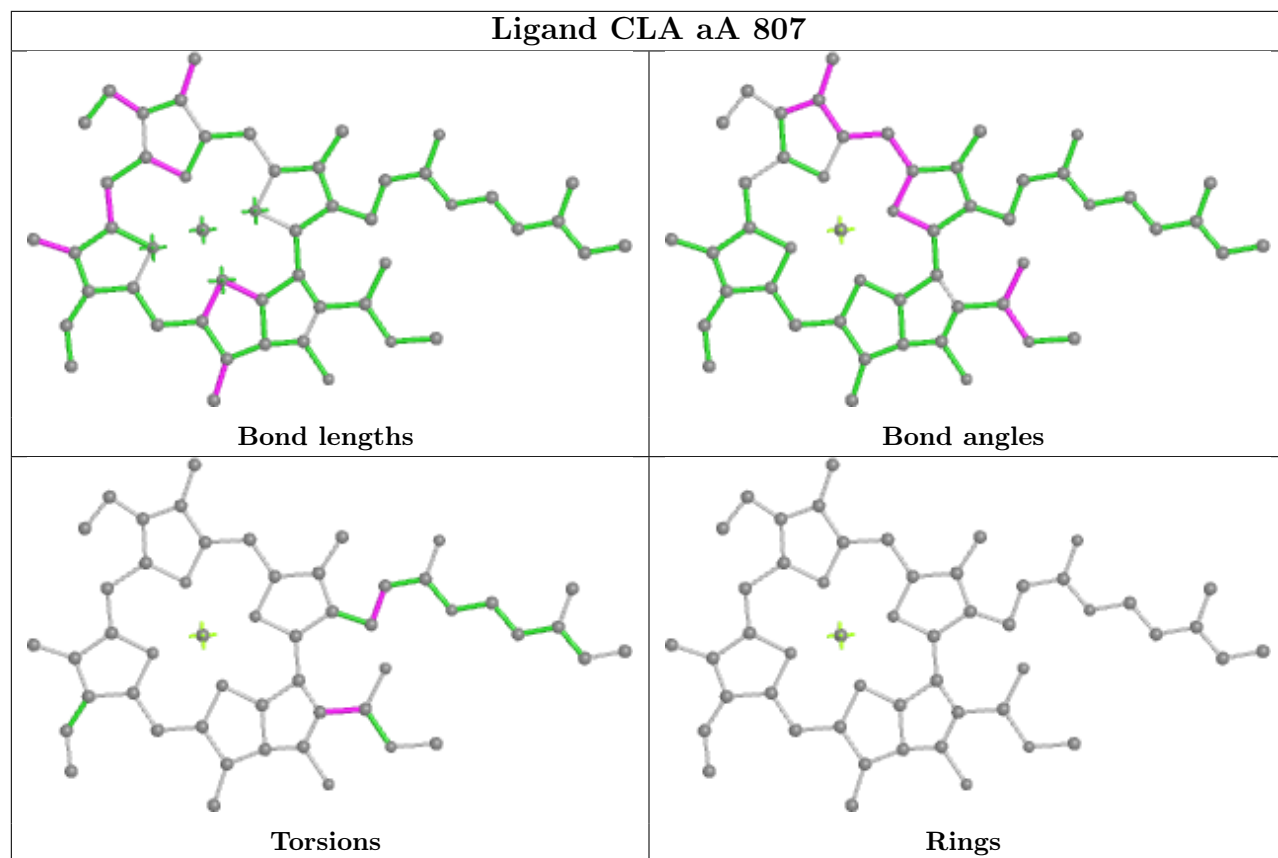
Ligand CLA bB 811

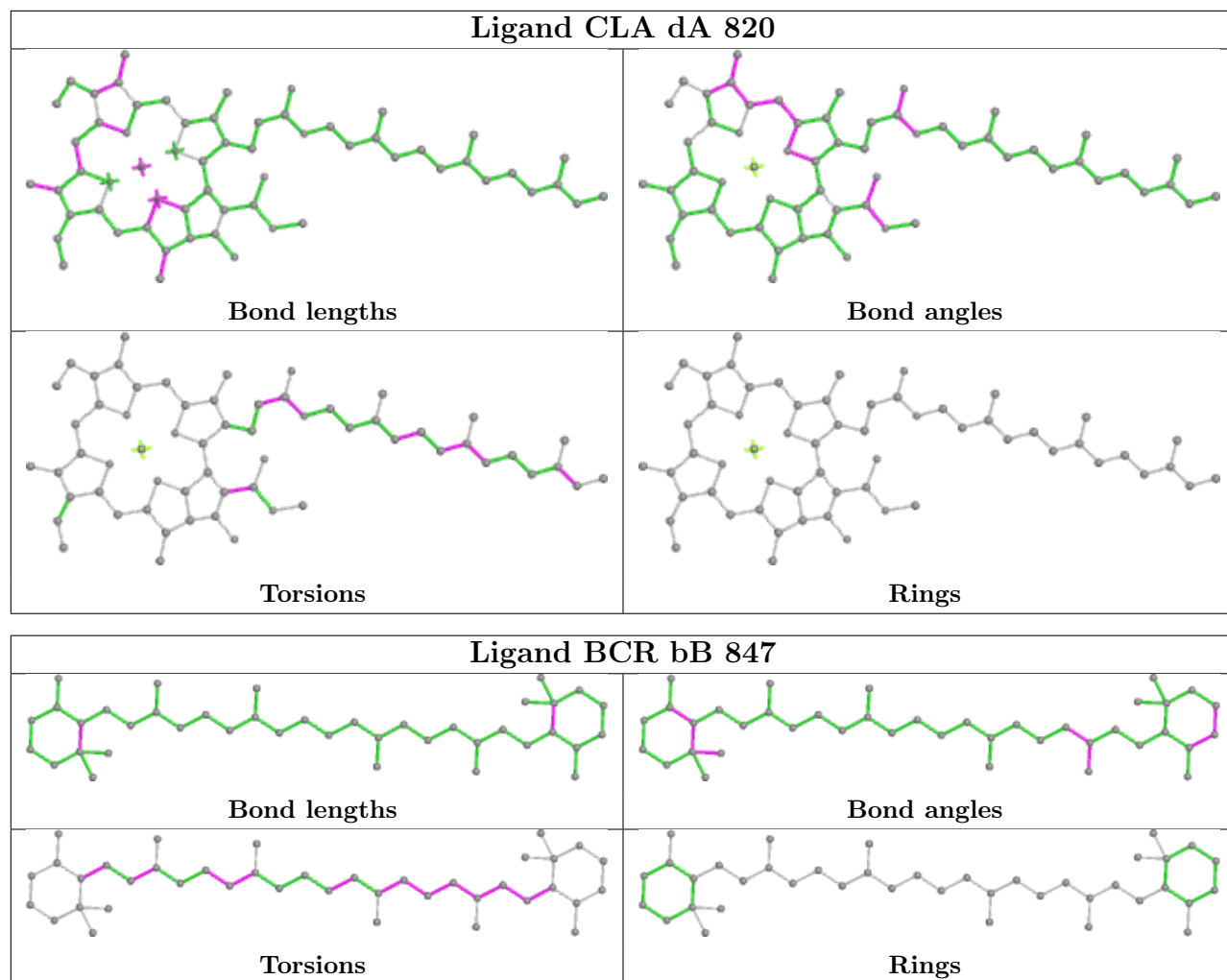


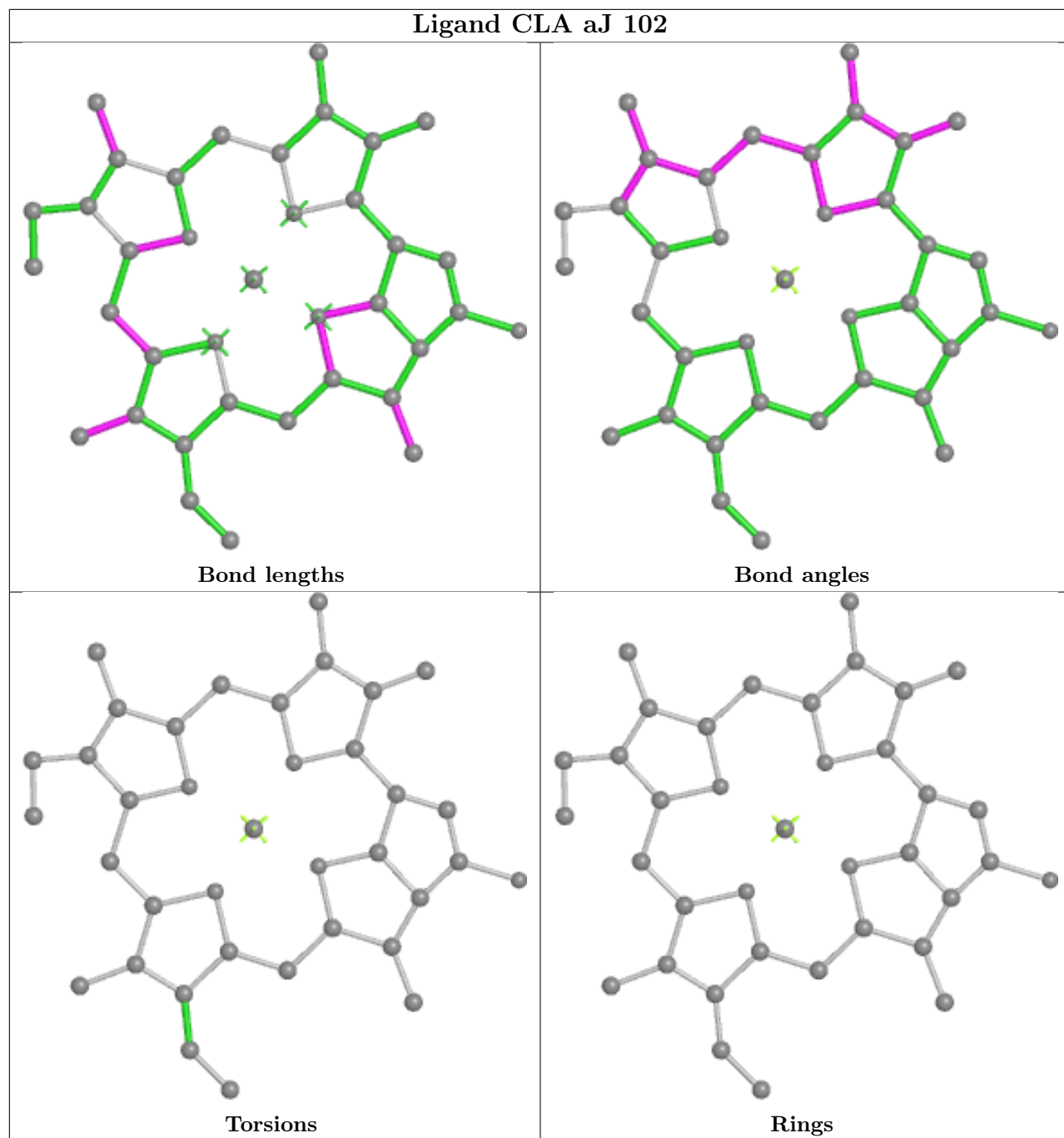
Ligand LHG aB 850

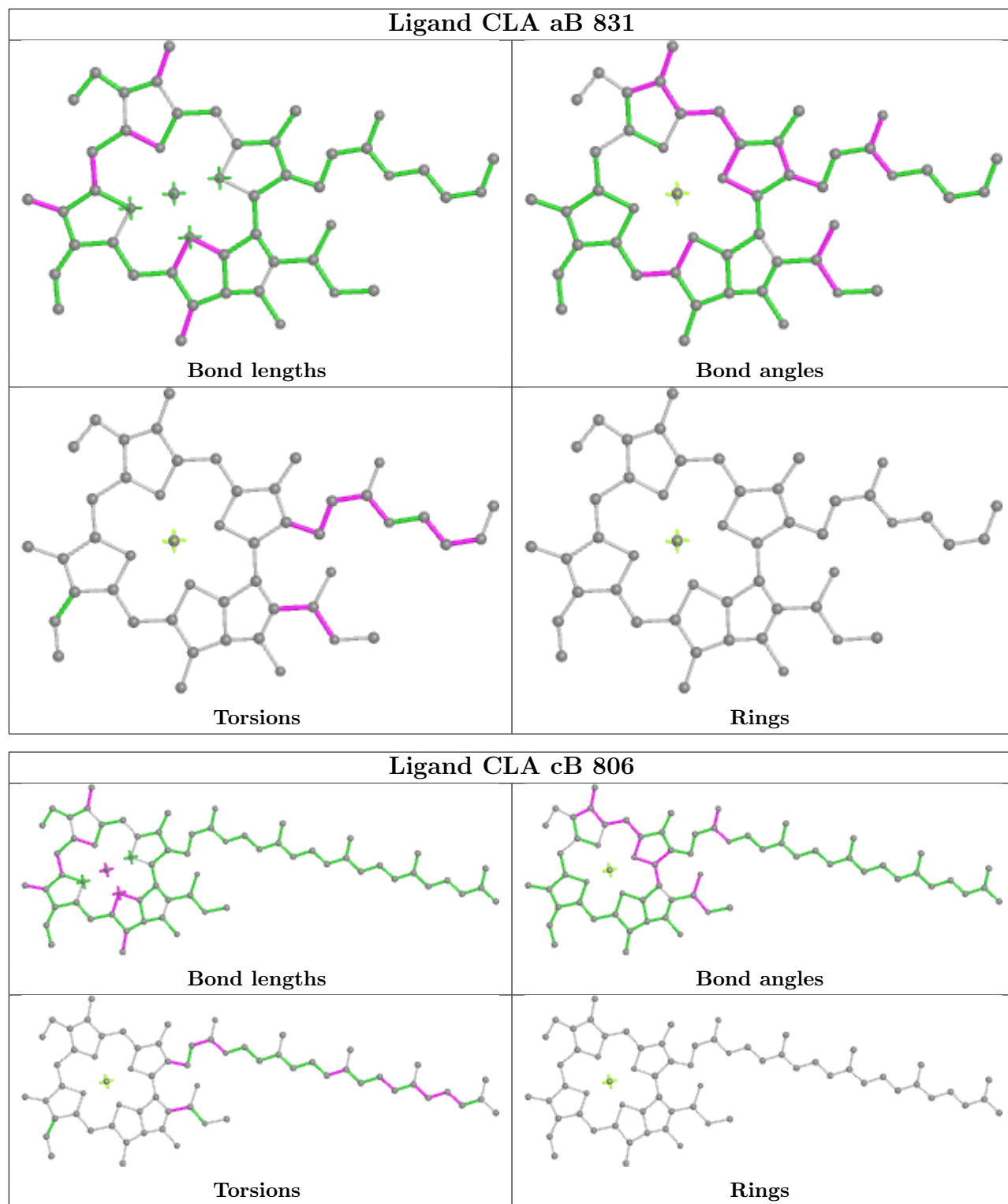


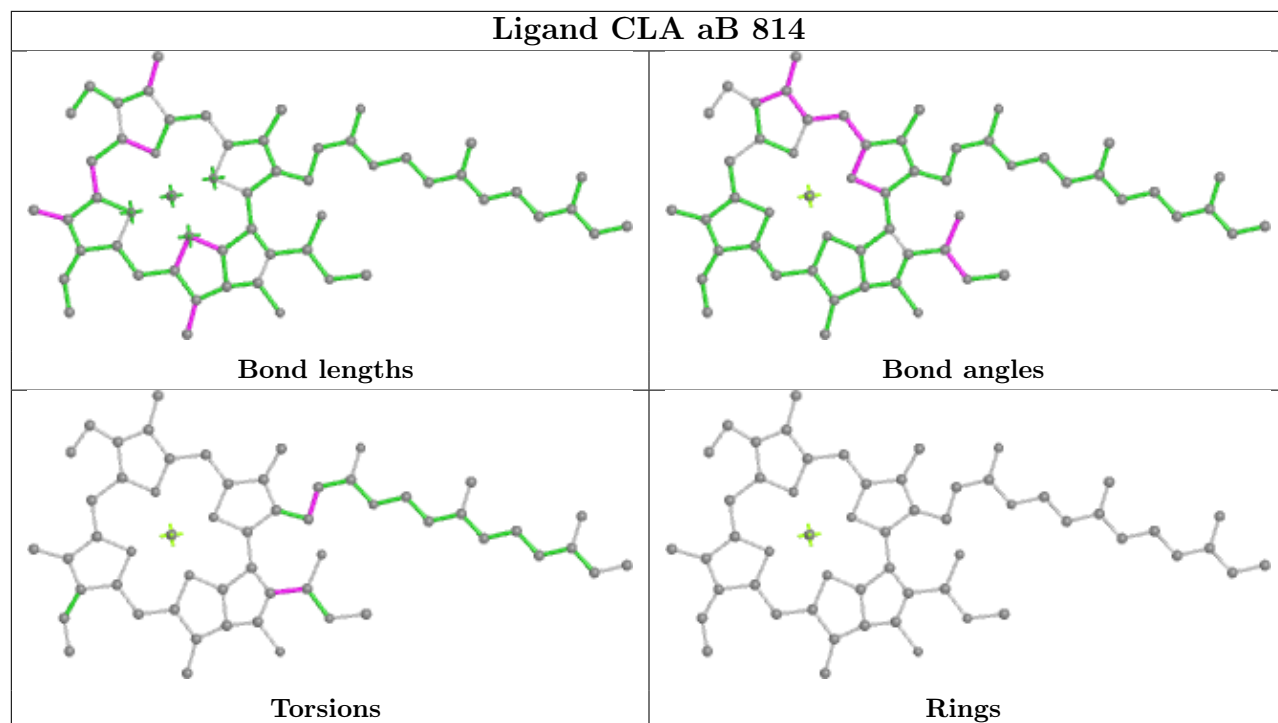


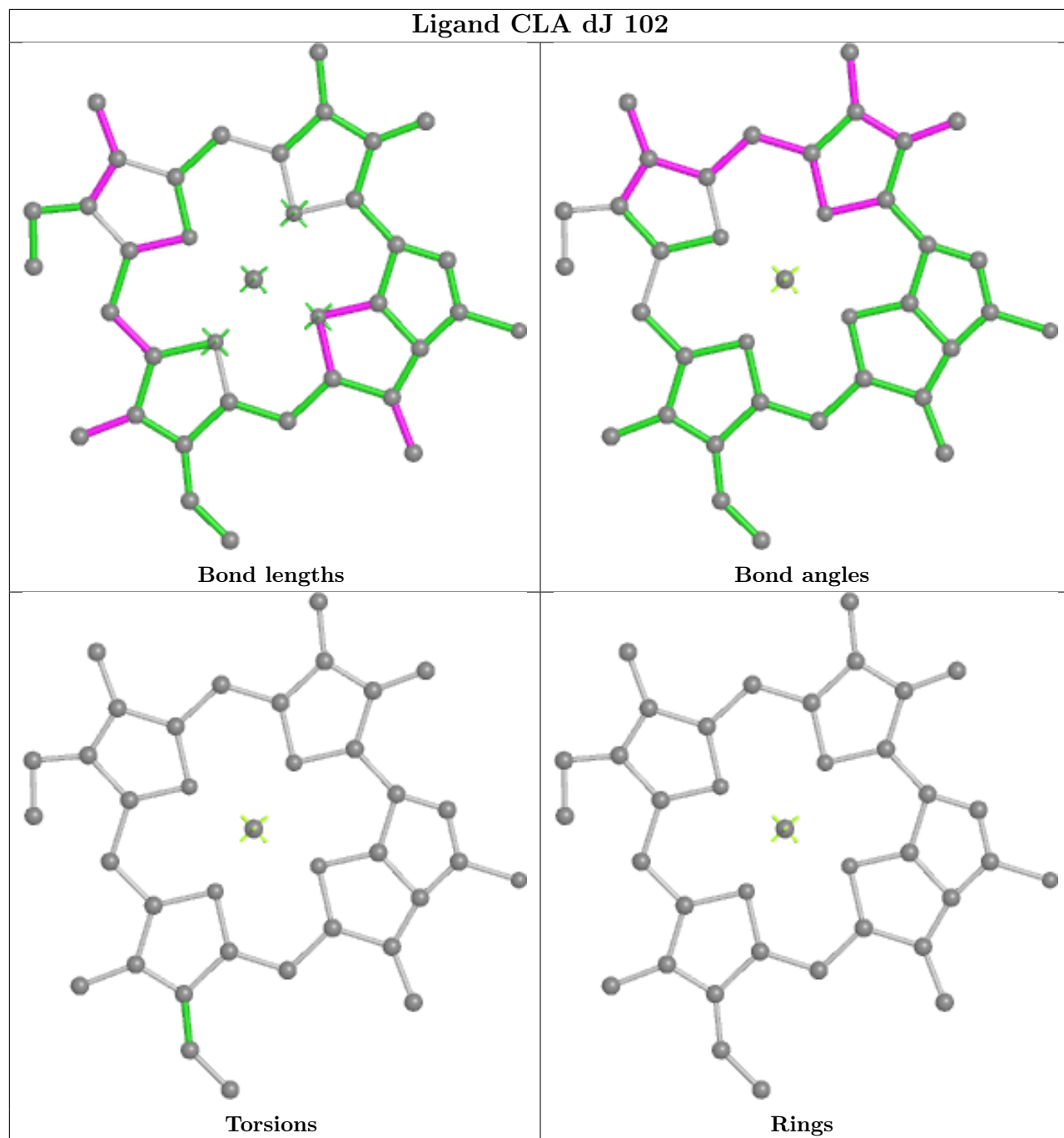


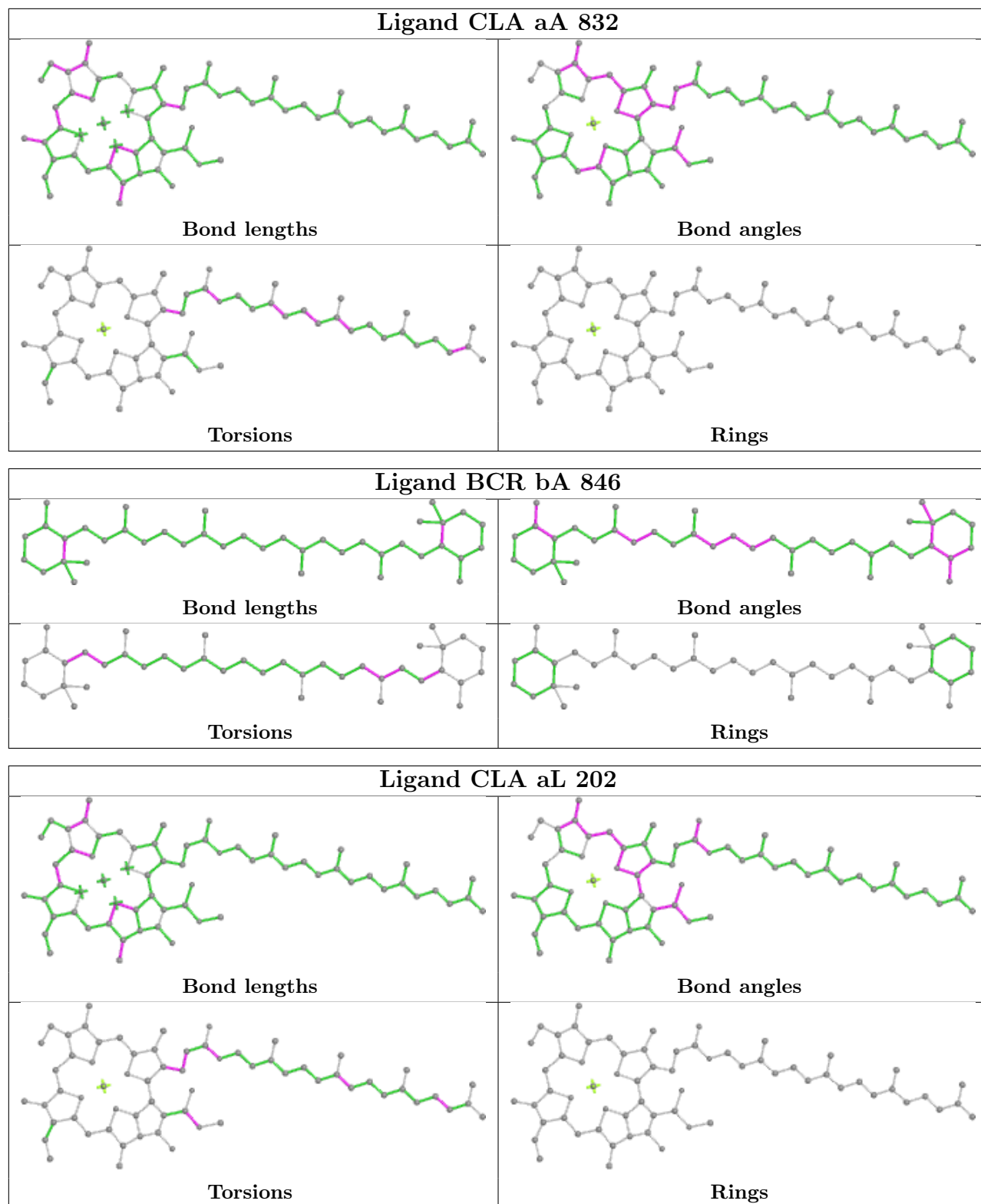


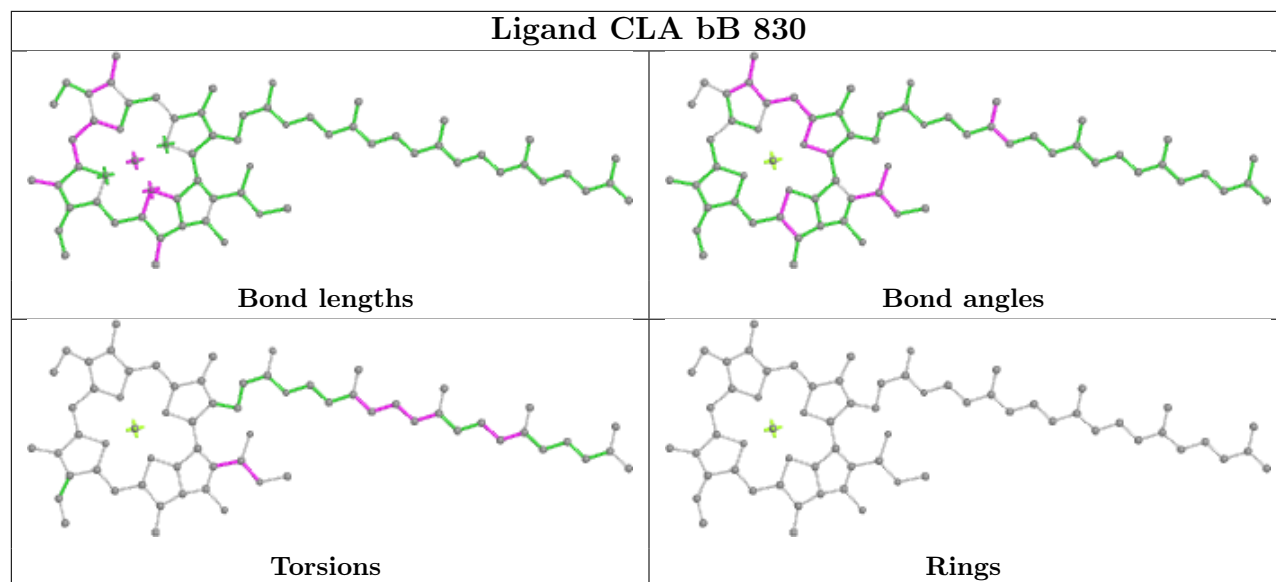
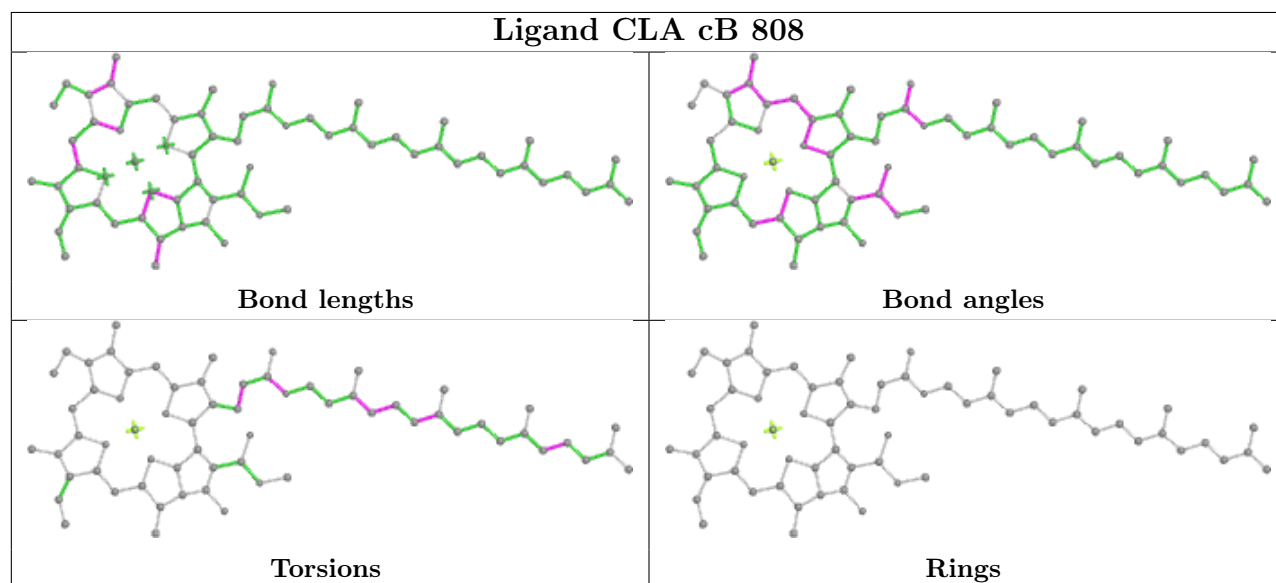




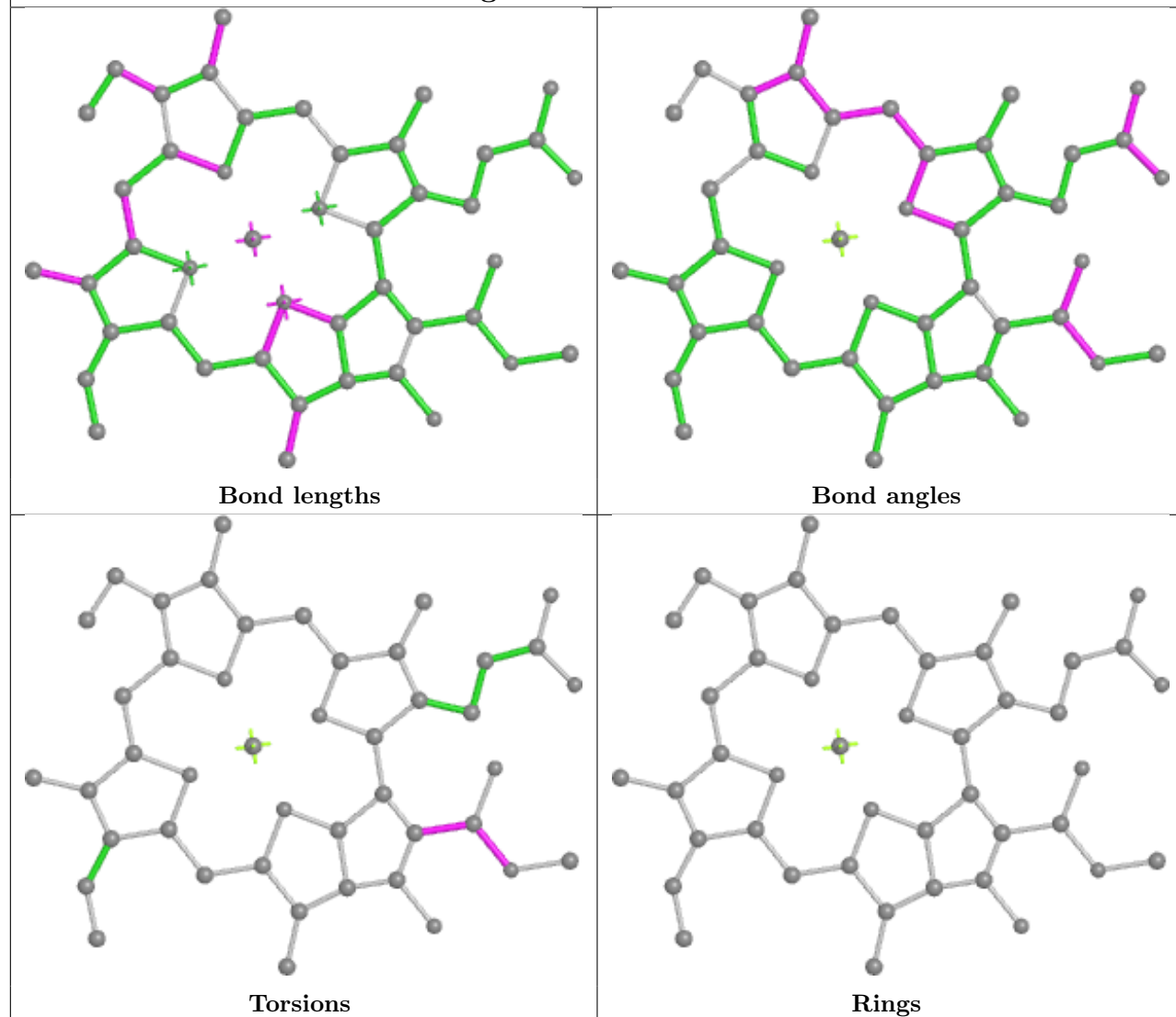




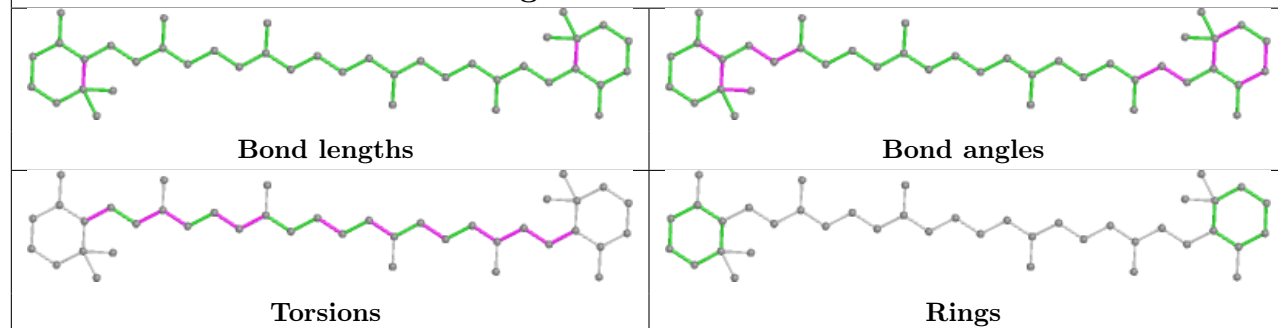


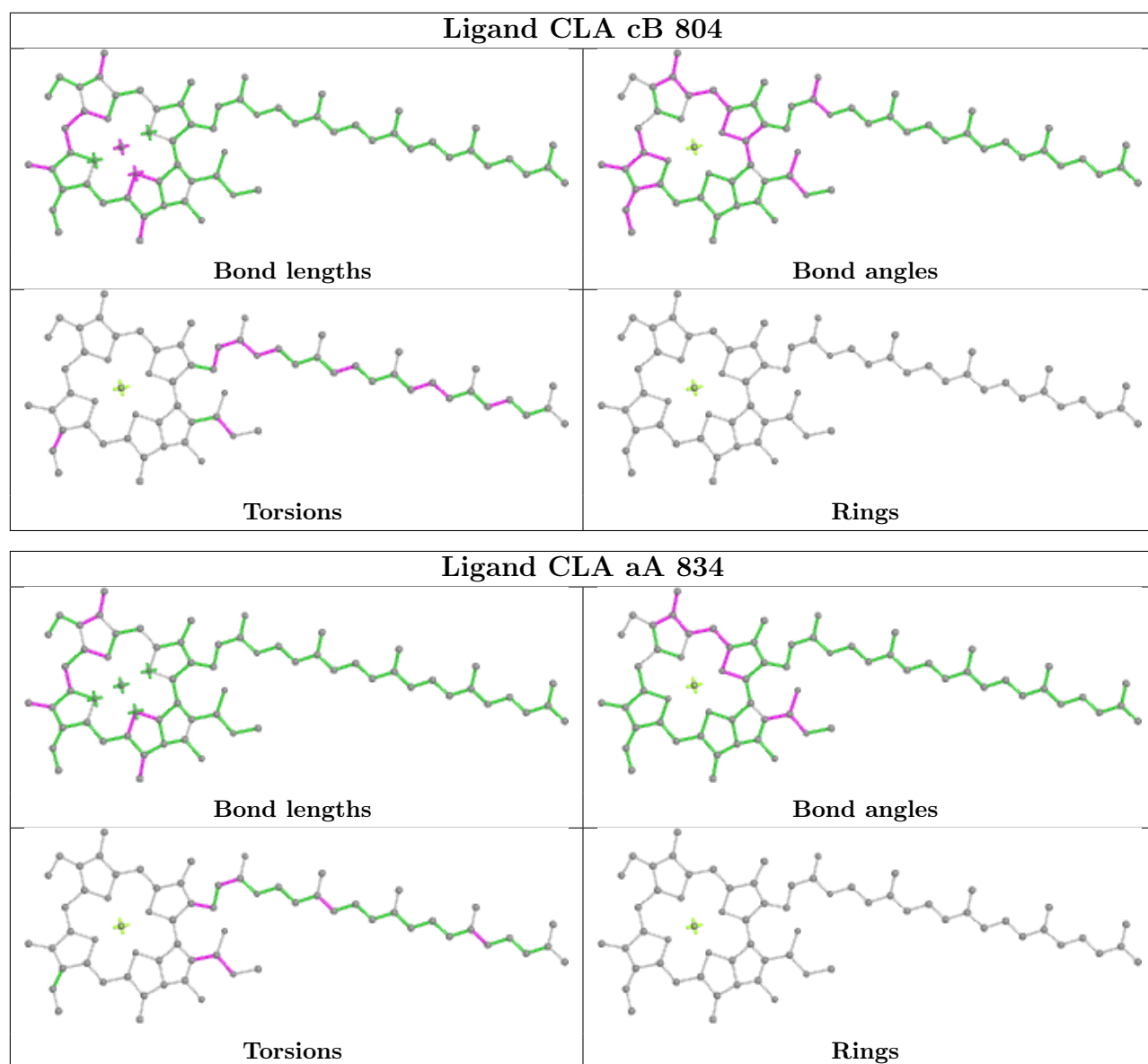
Ligand CLA bB 830**Ligand CLA cB 808**

Ligand CLA dB 822

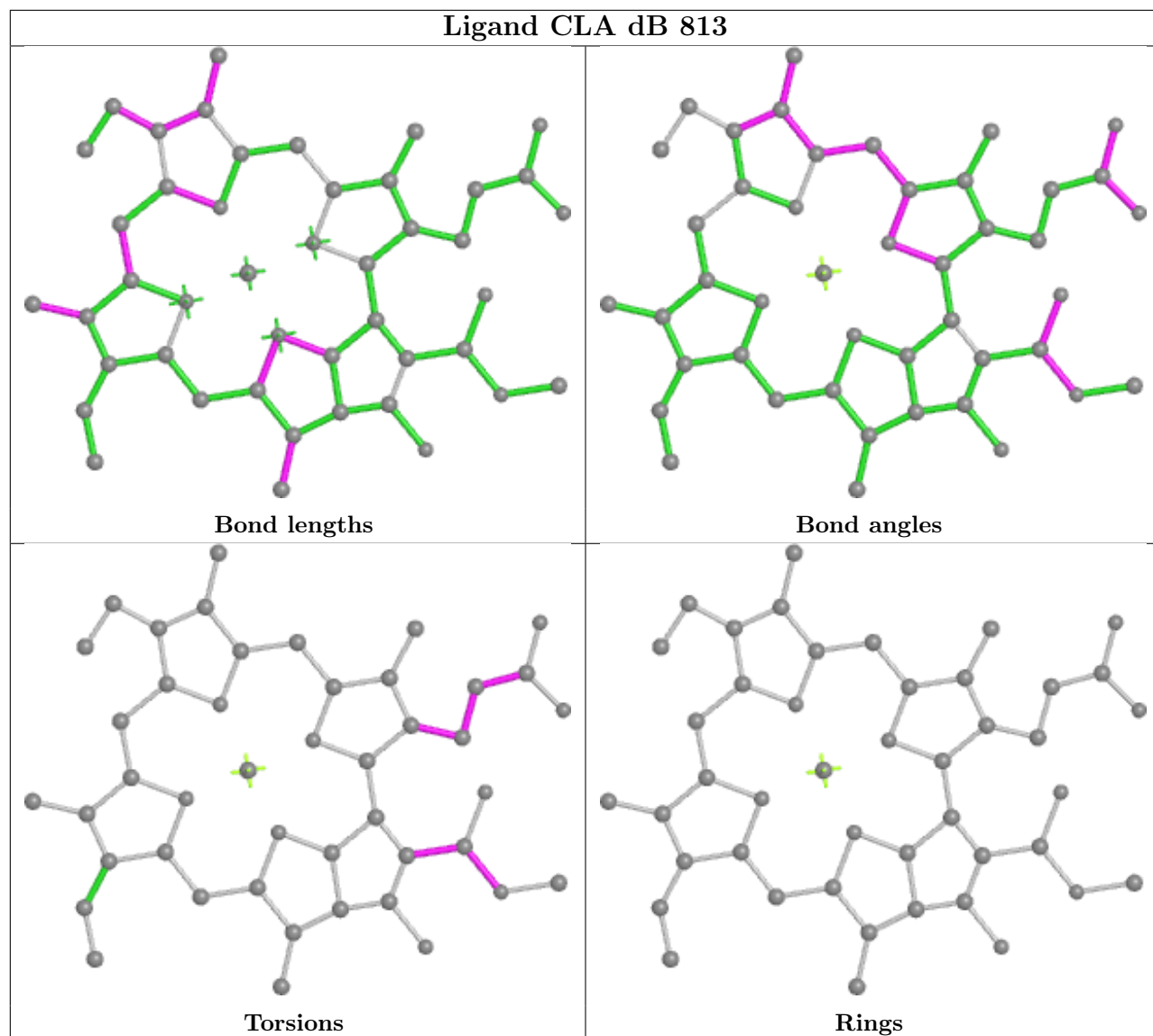


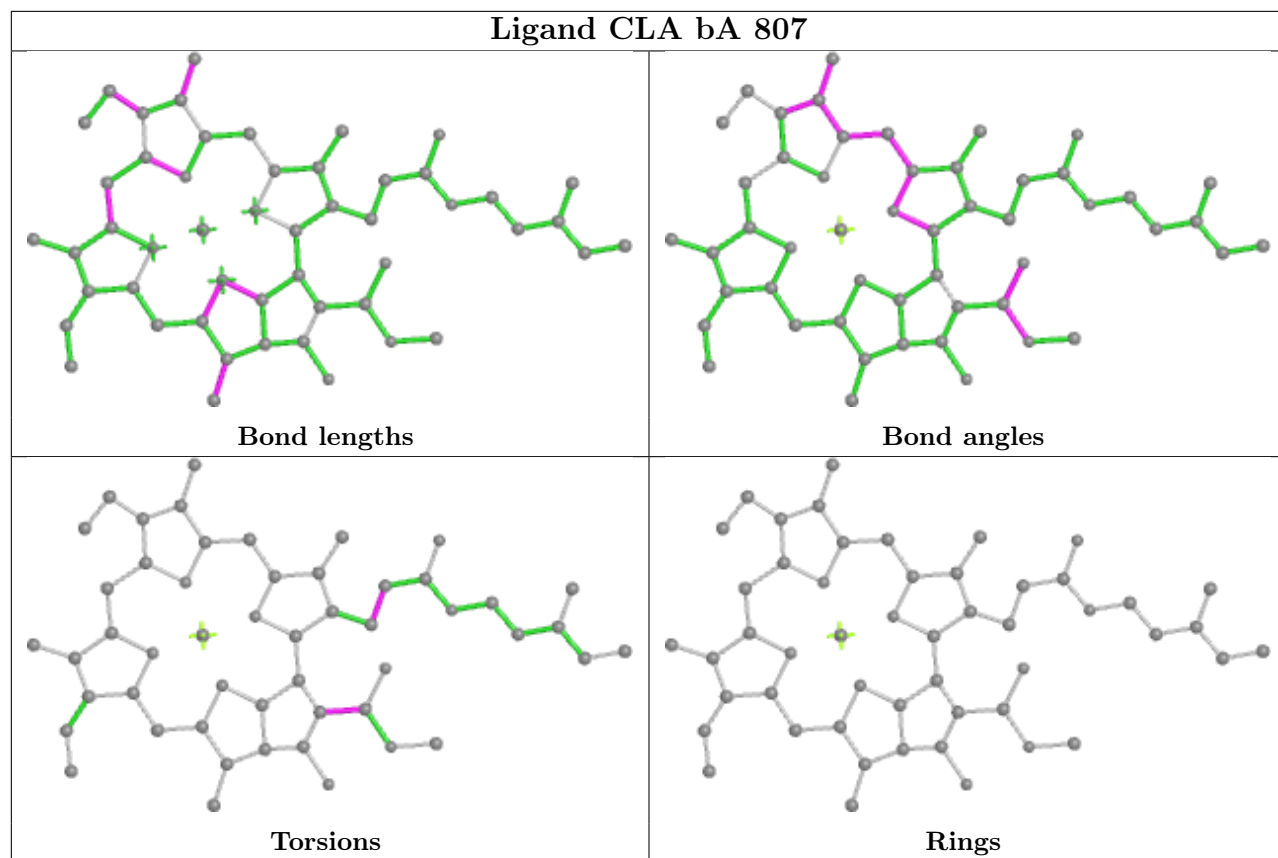
Ligand BCR bA 849

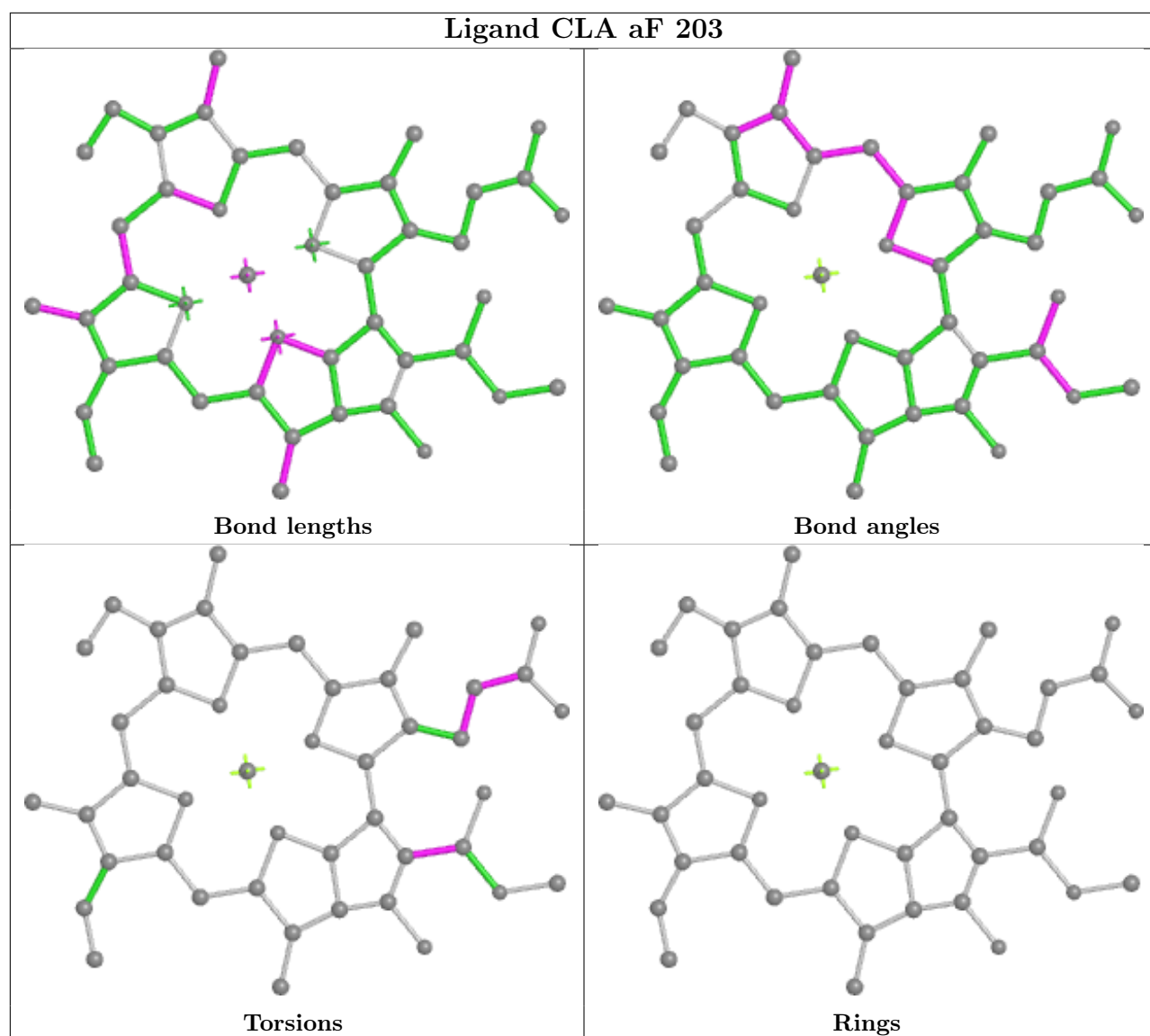


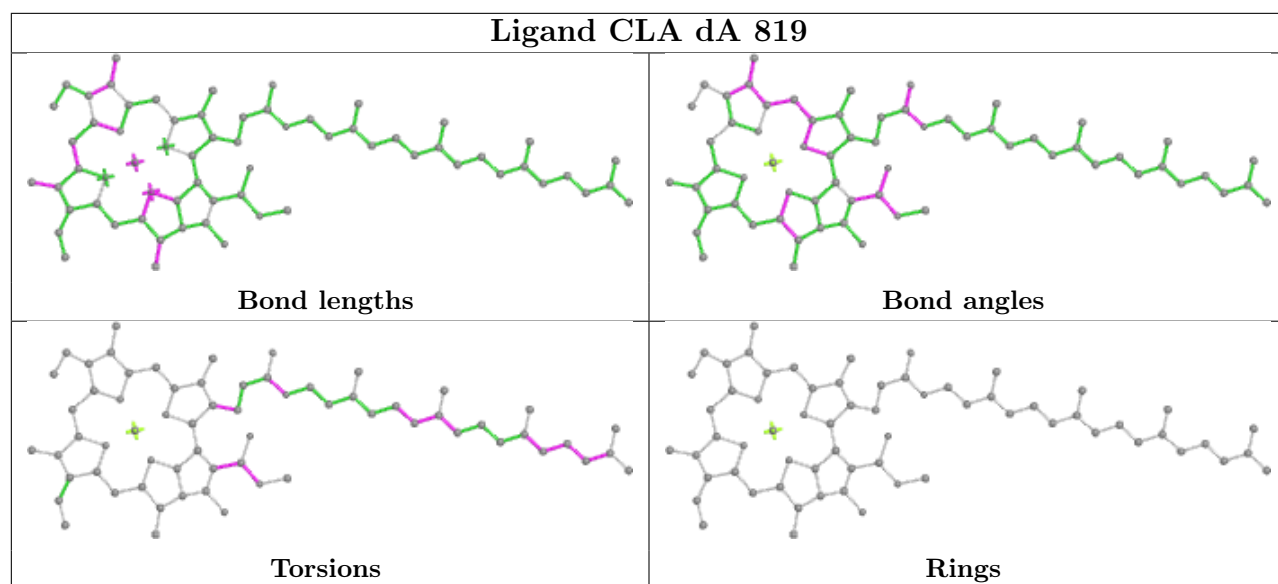
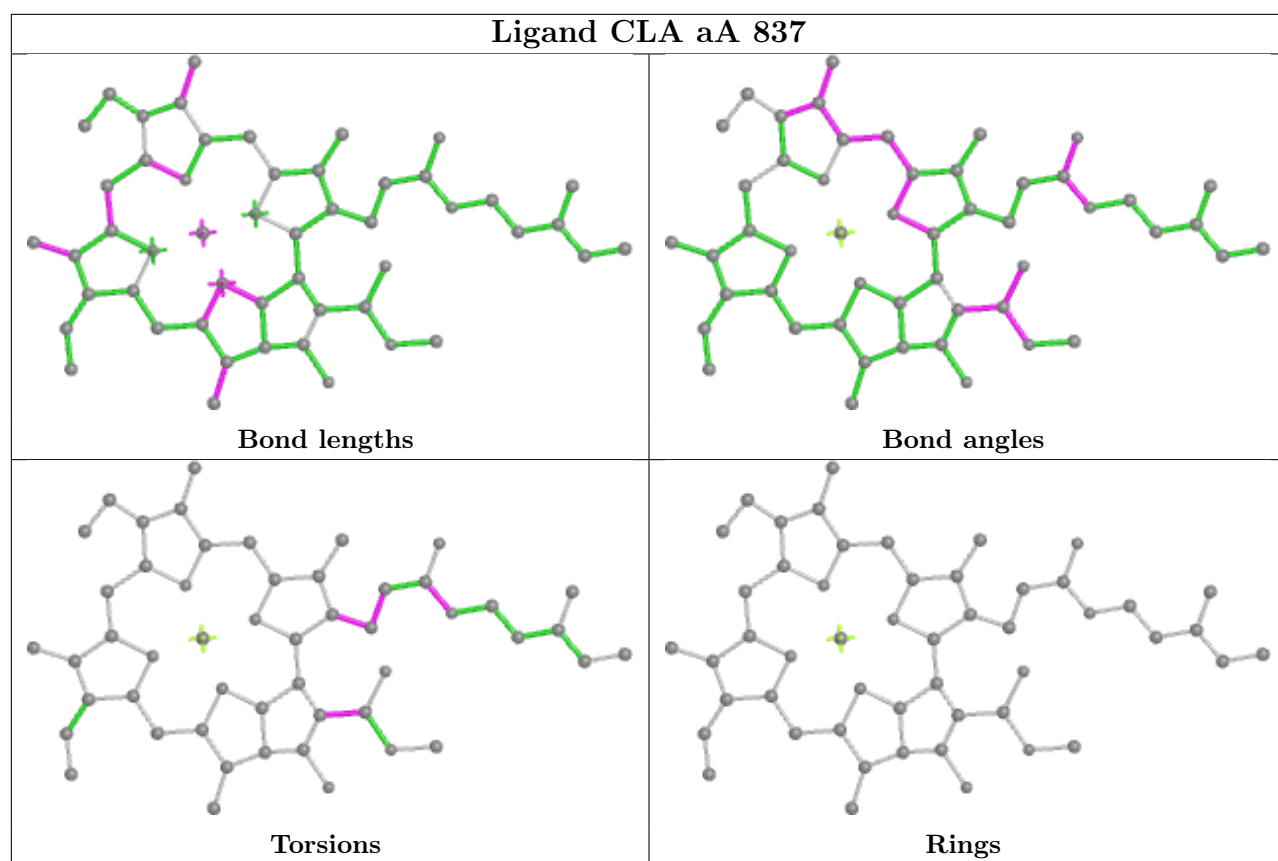


Ligand CLA dB 813

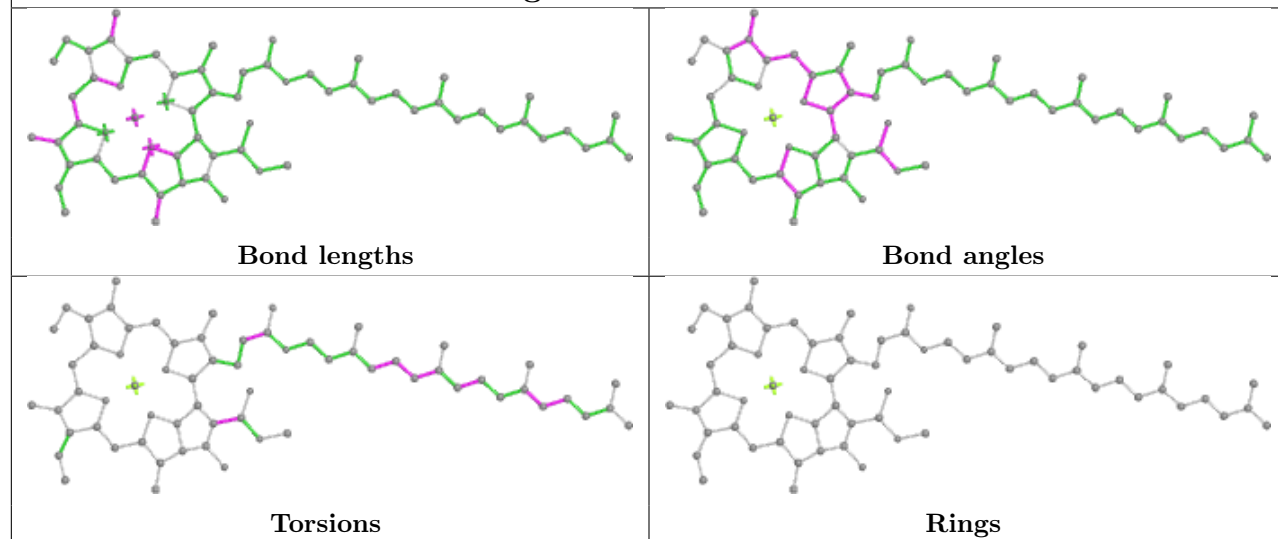




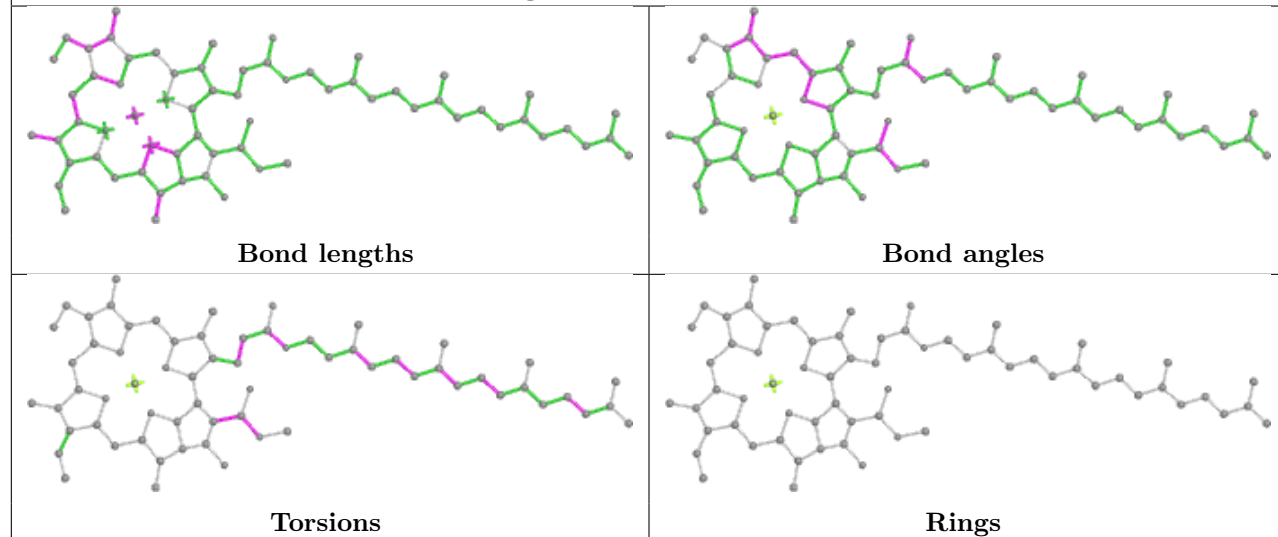




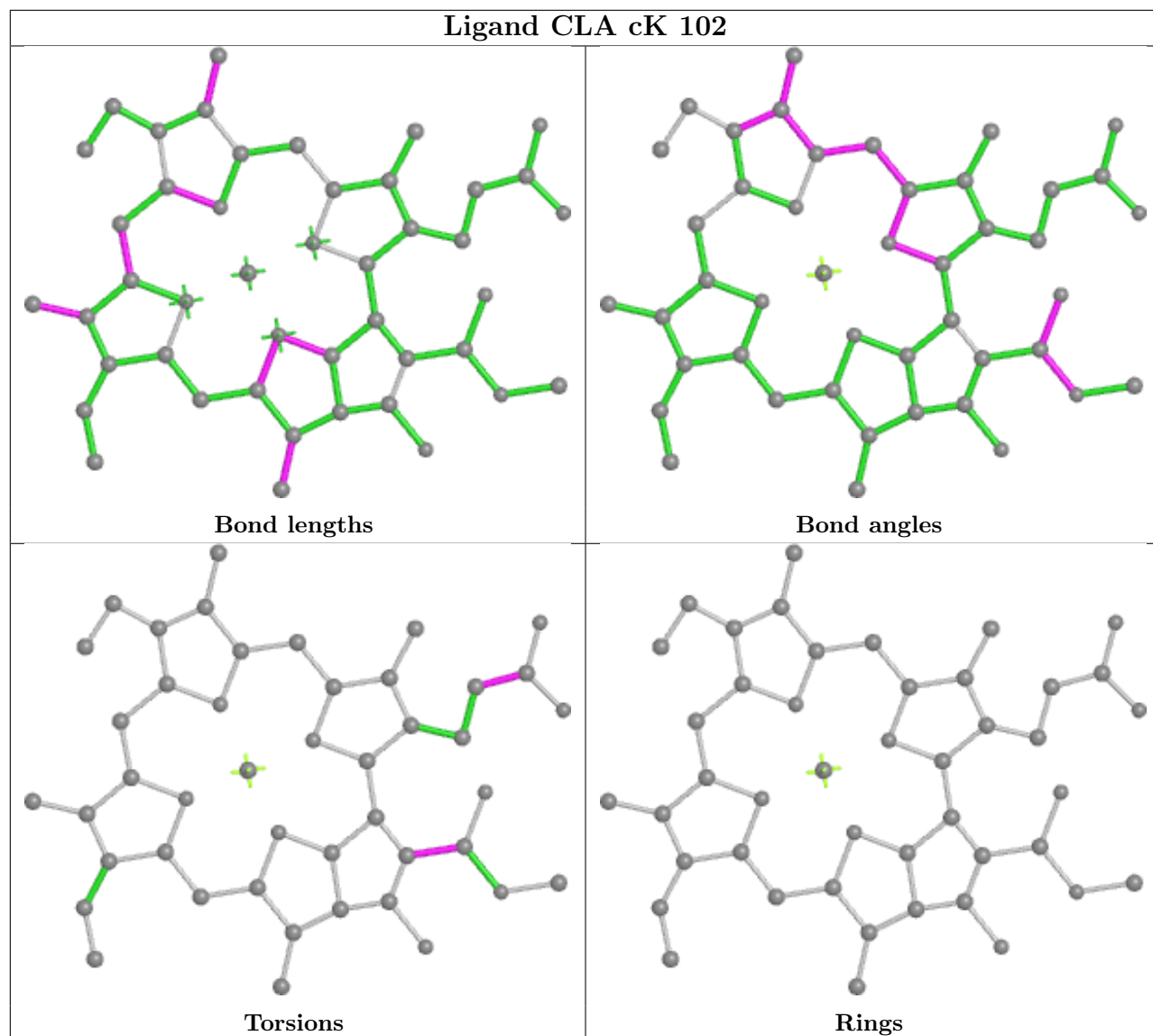
Ligand CLA cA 825



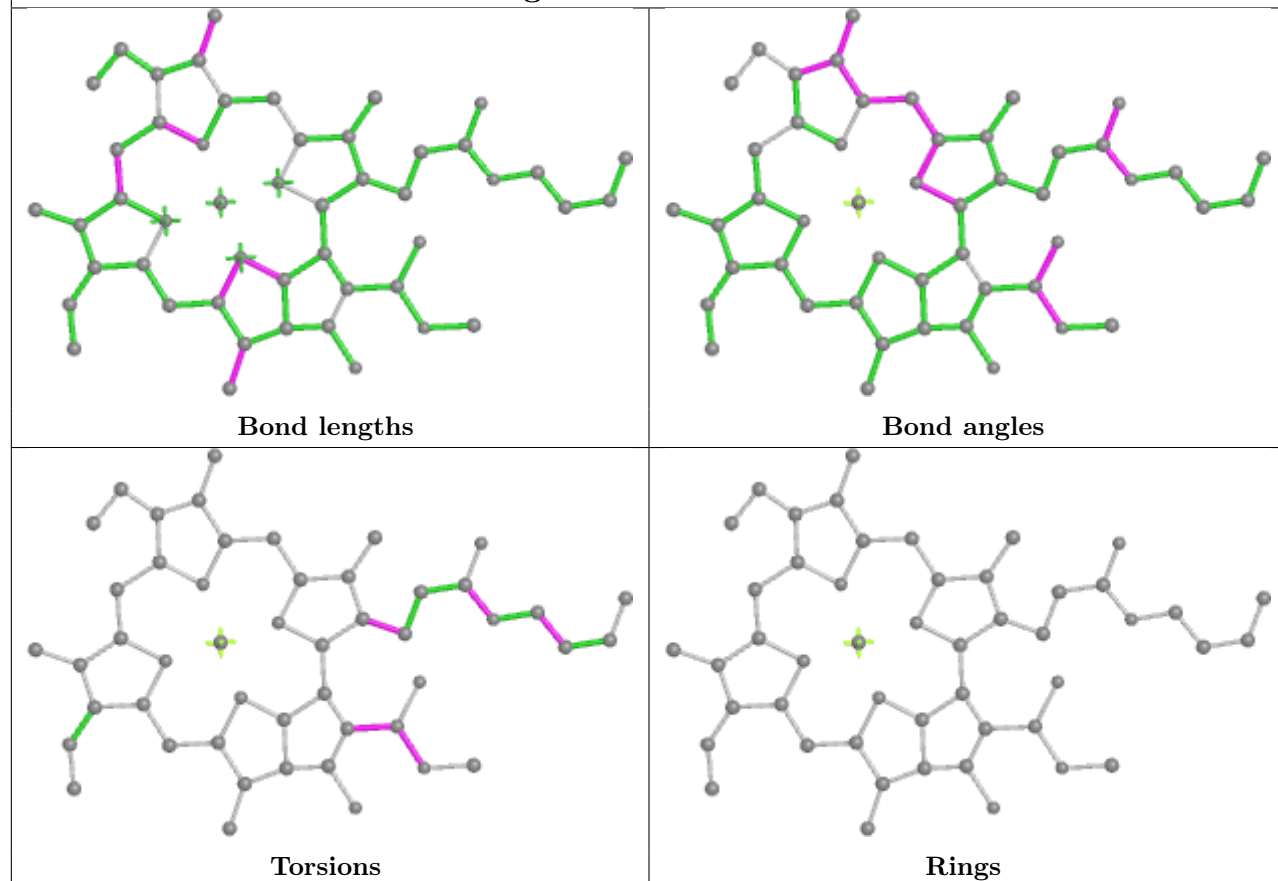
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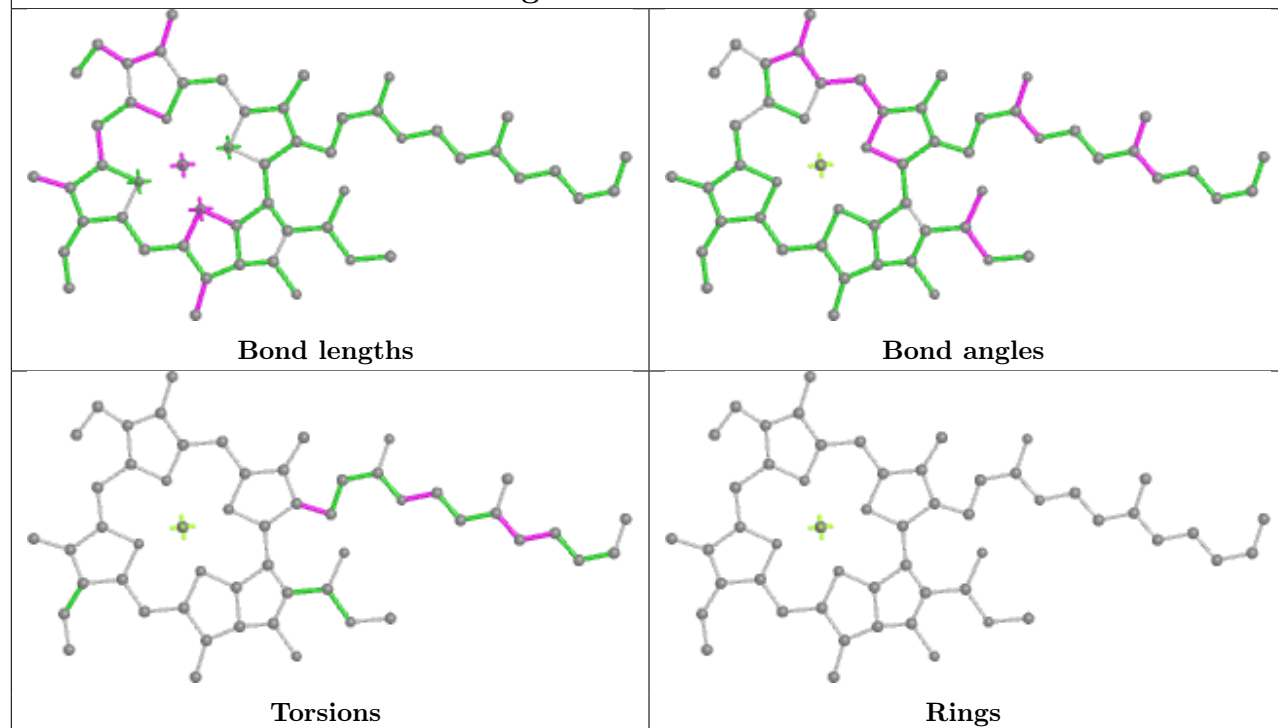
Ligand CLA cK 102



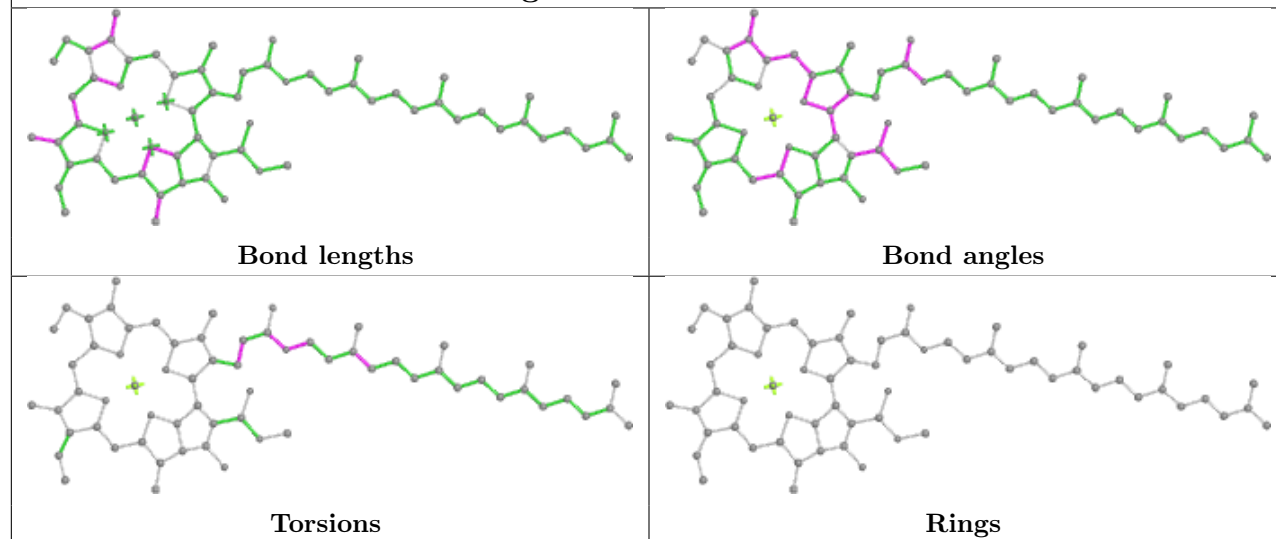
Ligand CLA cA 816



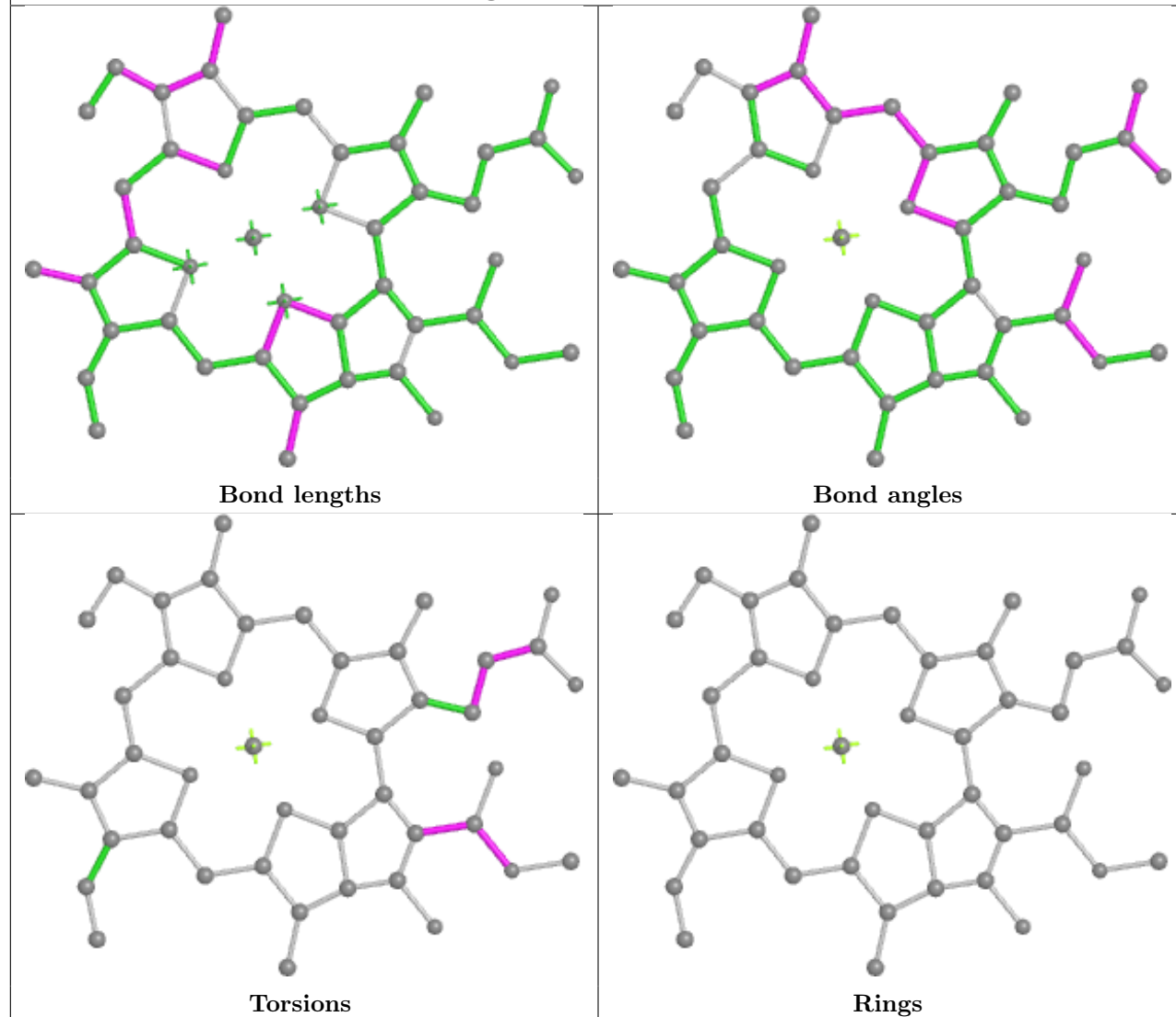
Ligand CLA bA 835



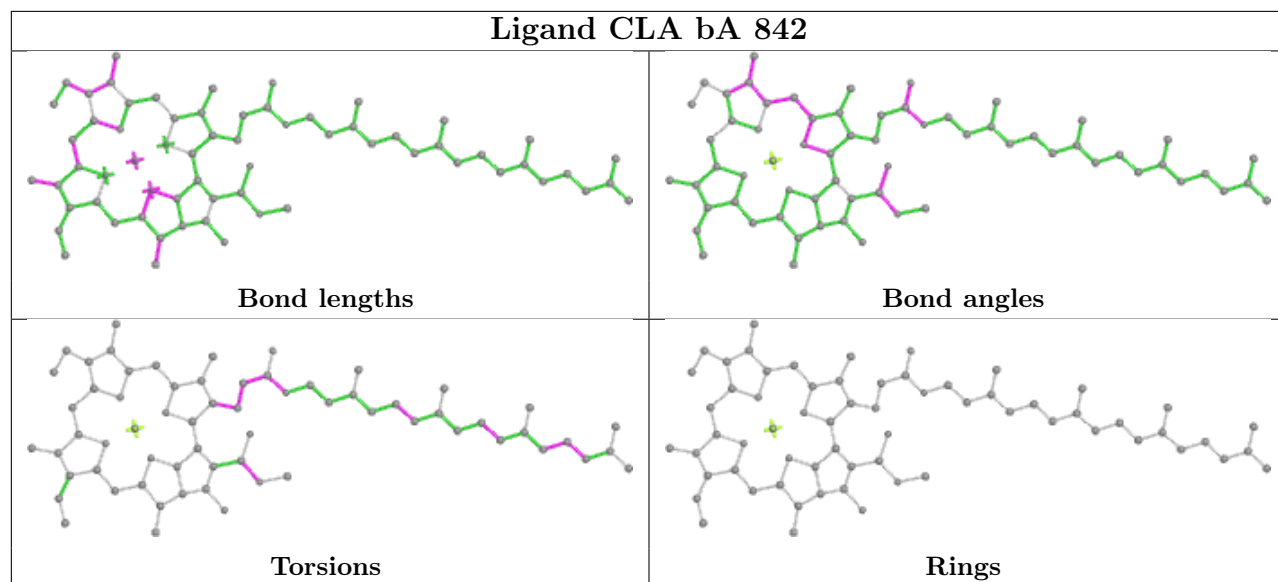
Ligand CLA dA 828



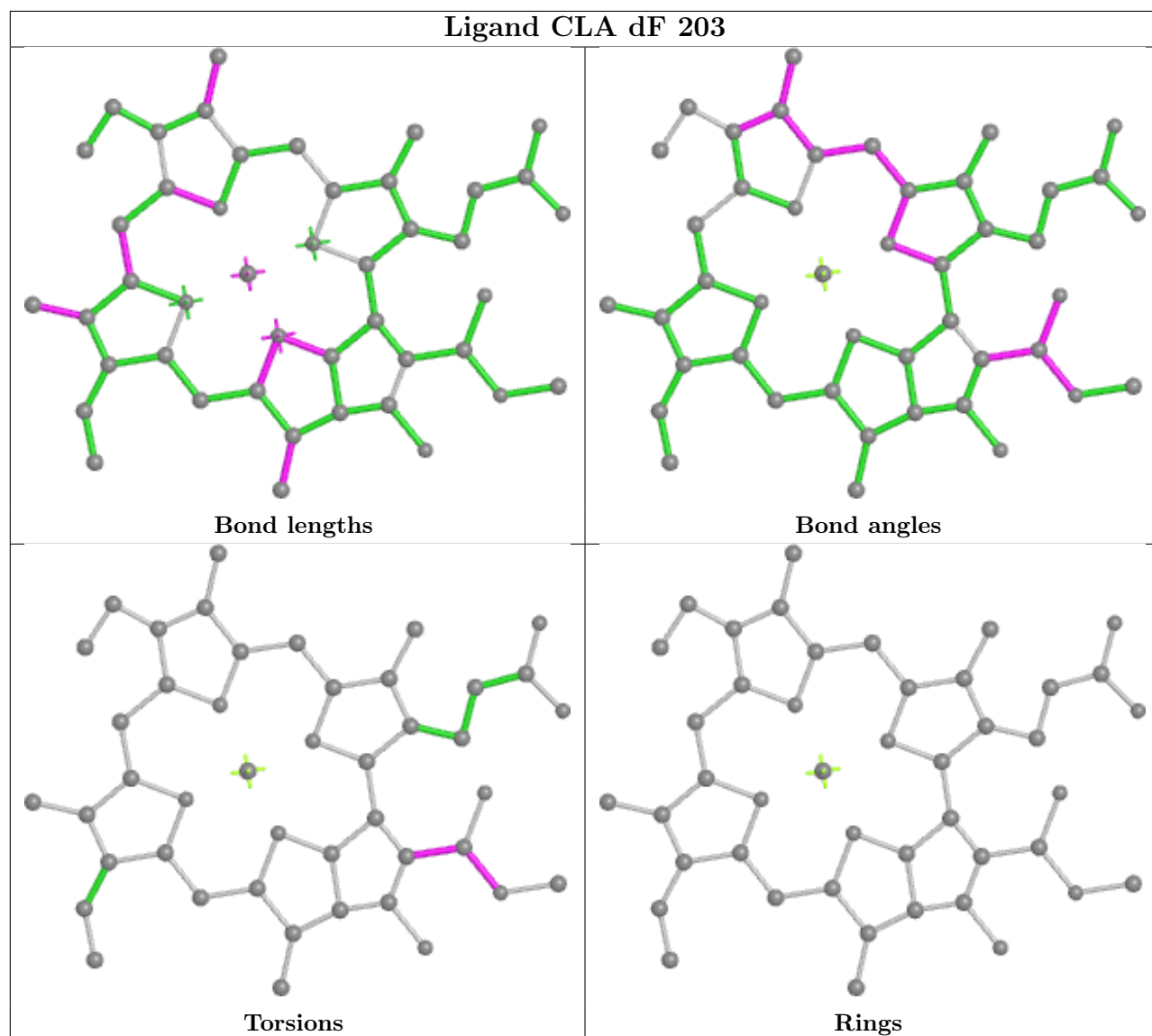
Ligand CLA cB 836

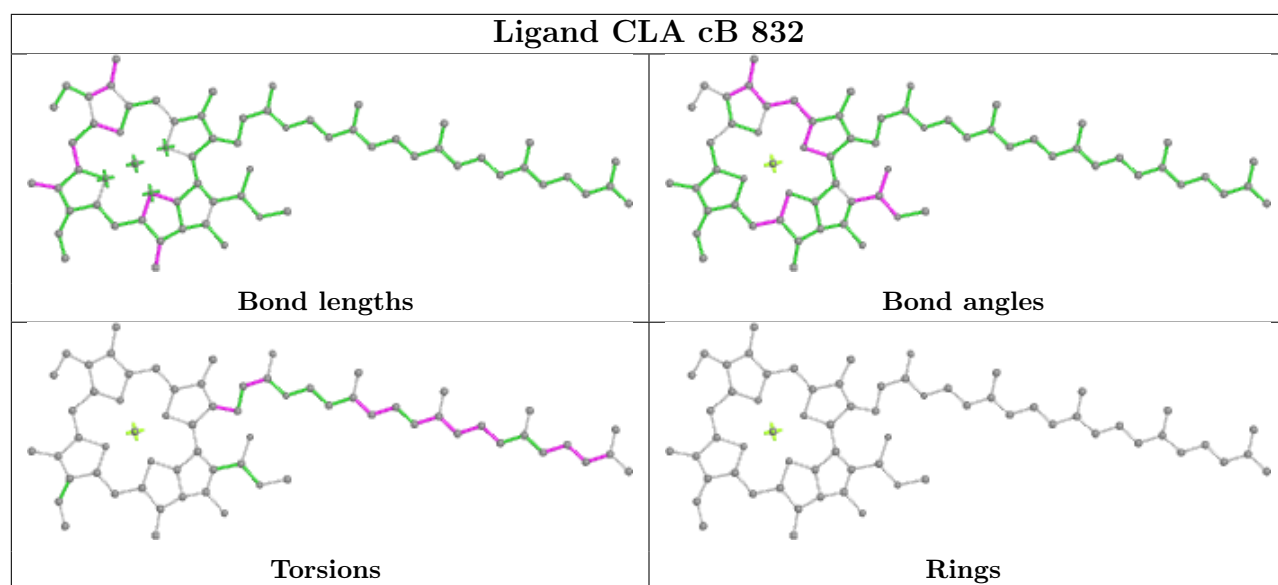


Ligand CLA bA 842



Ligand CLA dF 203





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

This section contains visualisations of the EMDB entry EMD-9807. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.