



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 02:44 AM JST

PDB ID : 6KMW / pdb_00006kmw
EMDB ID : EMD-0726
Title : Structure of PSI from *H. hongdechloris* grown under white light condition
Authors : Kato, K.; Nagao, R.; Shen, J.R.; Miyazaki, N.; Akita, F.
Deposited on : 2019-08-01
Resolution : 2.35 Å (reported)
Based on initial model : 1JB0

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

We welcome your comments at validation@mail.wwpdb.org

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:

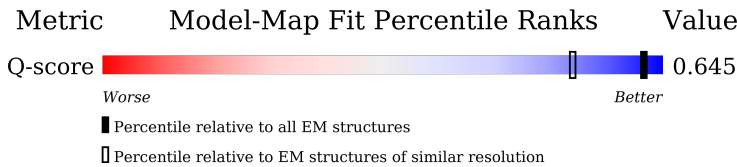
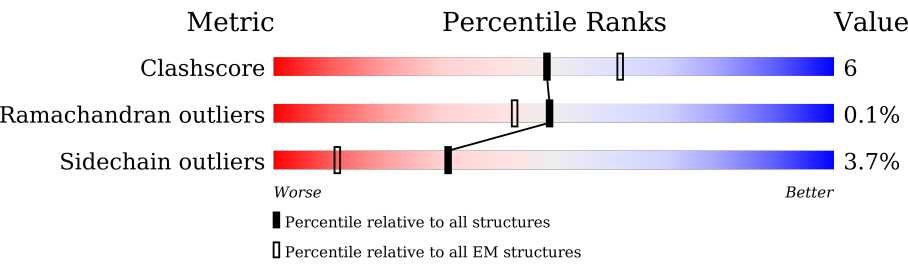
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4607 (1.85 - 2.85)

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

Mol	Chain	Length	Quality of chain
1	aA	764	13% 82%11%6%
1	bA	764	13% 83%11%6%
1	cA	764	13% 82%11%6%
2	aB	742	11% 86%13%

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Mol	Chain	Length	Quality of chain
2	bB	742	
2	cB	742	
3	aC	81	
3	bC	81	
3	cC	81	
4	aD	142	
4	bD	142	
4	cD	142	
5	aE	68	
5	bE	68	
5	cE	68	
6	aI	38	
6	bI	38	
6	cI	38	
7	aL	159	
7	bL	159	
7	cL	159	
8	aM	31	
8	bM	31	
8	cM	31	

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 64083 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	721	Total	C	N	O	S	0	0
			5629	3692	953	958	26		
1	bA	721	Total	C	N	O	S	0	0
			5629	3692	953	958	26		
1	cA	721	Total	C	N	O	S	0	0
			5629	3692	953	958	26		

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aI	38	Total	C	N	O	S	0	0
			305	210	41	51	3		
6	bI	38	Total	C	N	O	S	0	0
			305	210	41	51	3		
6	cI	38	Total	C	N	O	S	0	0
			305	210	41	51	3		

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

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

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

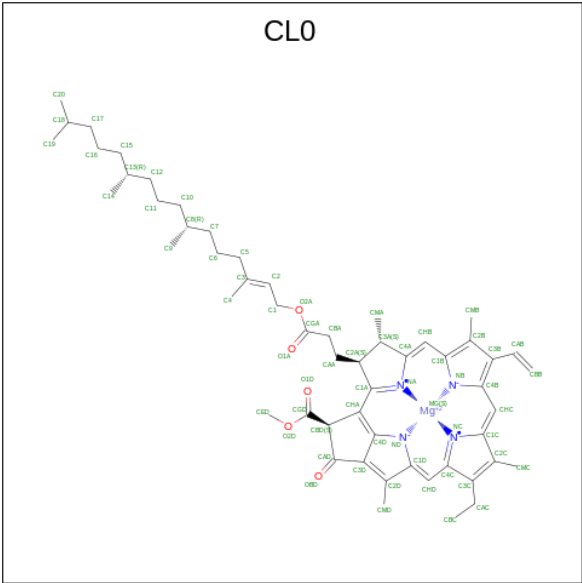
Mol	Chain	Residues	Atoms					AltConf	Trace
8	aM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		
8	bM	31	Total	C	N	O	S	0	0
			241	162	36	42	1		

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

- Molecule 9 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 10 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					AltConf
10	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aA	1	Total 50	C 40	Mg 1	N 4	O 5	0
10	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aA	1	Total 51	C 41	Mg 1	N 4	O 5	0
10	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aA	1	Total 41	C 33	Mg 1	N 4	O 3	0
10	aA	1	Total 52	C 42	Mg 1	N 4	O 5	0
10	aA	1	Total 49	C 39	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 57	C 47	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 54	C 44	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
10	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 56	C 46	Mg 1	N 4	O 5	0
10	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	aB	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	aB	1	Total 59	C 49	Mg 1	N 4	O 5	0
10	aB	1	Total 60	C 50	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 47	C 37	Mg 1	N 4	O 5	0
10	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	aB	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	aB	1	Total 54	C 44	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
10	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	aB	1	Total 60	C 50	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 47	C 37	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aL	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
10	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
10	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0
10	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
10	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bA	1	Total 50	C 40	Mg 1	N 4	O 5	0
10	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
10	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bA	1	Total 41	C 33	Mg 1	N 4	O 3	0
10	bA	1	Total 52	C 42	Mg 1	N 4	O 5	0
10	bA	1	Total 49	C 39	Mg 1	N 4	O 5	0
10	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bB	1	Total 57	C 47	Mg 1	N 4	O 5	0
10	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bB	1	Total 54	C 44	Mg 1	N 4	O 5	0
10	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
10	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bB	1	Total 58	C 48	Mg 1	N 4	O 5	0
10	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	bB	1	Total 60	C 50	Mg 1	N 4	O 5	0
10	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bB	1	Total 47	C 37	Mg 1	N 4	O 5	0
10	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bL	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 50	C 40	Mg 1	N 4	O 5	0
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 50	C 40	Mg 1	N 4	O 5	0
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cA	1	Total 41	C 33	Mg 1	N 4	O 3	0
10	cA	1	Total 52	C 42	Mg 1	N 4	O 5	0
10	cA	1	Total 49	C 39	Mg 1	N 4	O 5	0
10	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
10	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	cB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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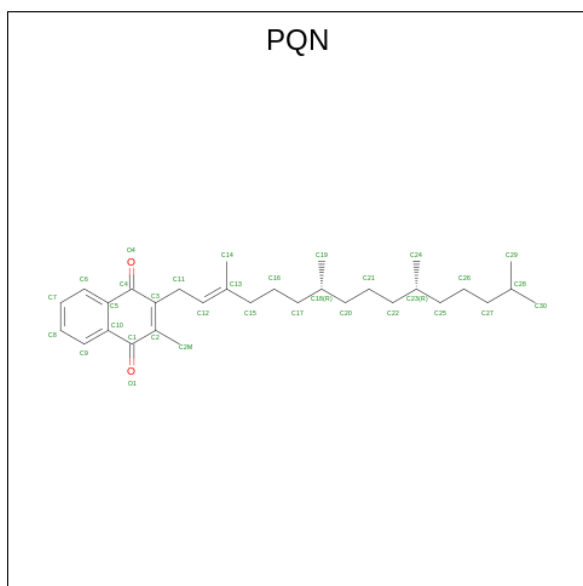
Mol	Chain	Residues	Atoms					AltConf
10	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	cB	1	Total 54	C 44	Mg 1	N 4	O 5	0
10	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cB	1	Total 58	C 48	Mg 1	N 4	O 5	0
10	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	cB	1	Total 60	C 50	Mg 1	N 4	O 5	0
10	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cB	1	Total 47	C 37	Mg 1	N 4	O 5	0
10	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cL	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	cL	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	cL	1	Total 65	C 55	Mg 1	N 4	O 5	0

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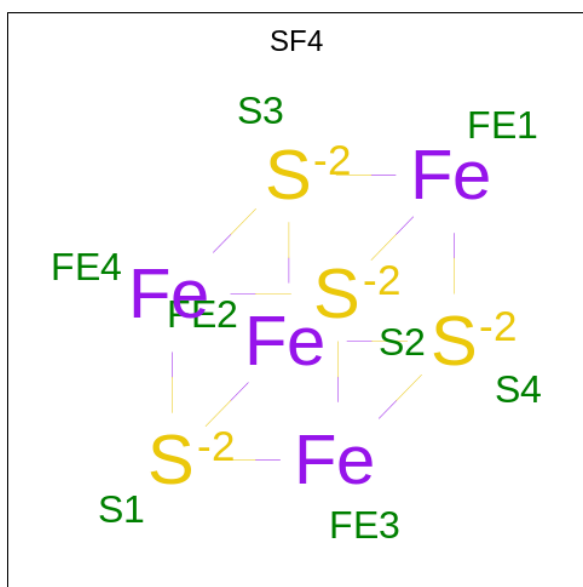
Mol	Chain	Residues	Atoms					AltConf
10	cL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 11 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



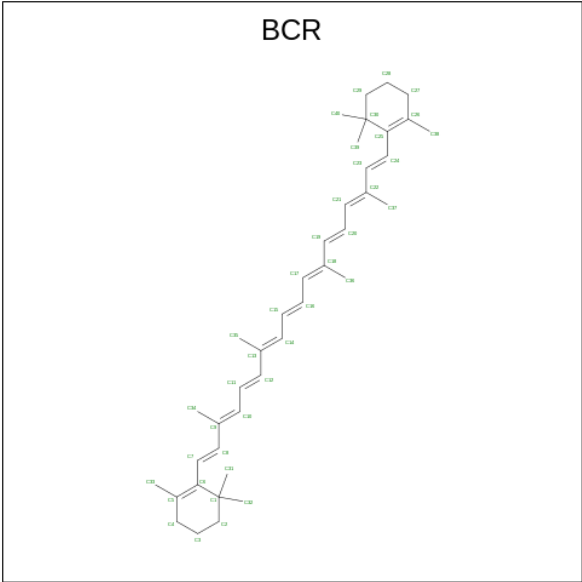
Mol	Chain	Residues	Atoms			AltConf
11	aA	1	Total	C	O	0
			33	31	2	
11	aB	1	Total	C	O	0
			33	31	2	
11	bA	1	Total	C	O	0
			33	31	2	
11	bB	1	Total	C	O	0
			33	31	2	
11	cA	1	Total	C	O	0
			33	31	2	
11	cB	1	Total	C	O	0
			33	31	2	

- Molecule 12 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 13 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms	AltConf
13	aA	1	Total C 40 40	0
13	aA	1	Total C 40 40	0
13	aA	1	Total C 40 40	0
13	aA	1	Total C 40 40	0
13	aA	1	Total C 40 40	0
13	aA	1	Total C 40 40	0
13	aB	1	Total C 40 40	0
13	aB	1	Total C 40 40	0
13	aB	1	Total C 40 40	0
13	aB	1	Total C 40 40	0
13	aB	1	Total C 40 40	0
13	aB	1	Total C 40 40	0
13	aB	1	Total C 40 40	0
13	aI	1	Total C 40 40	0
13	aI	1	Total C 40 40	0

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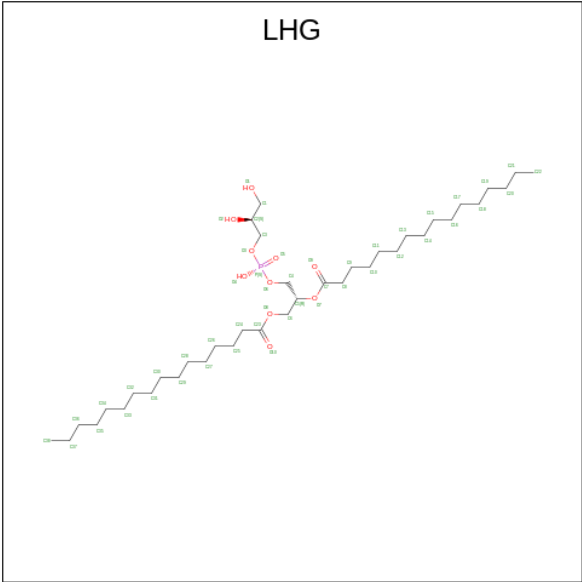
Mol	Chain	Residues	Atoms	AltConf
13	aL	1	Total C 40 40	0
13	aL	1	Total C 40 40	0
13	aM	1	Total C 40 40	0
13	bA	1	Total C 40 40	0
13	bA	1	Total C 40 40	0
13	bA	1	Total C 40 40	0
13	bA	1	Total C 40 40	0
13	bA	1	Total C 40 40	0
13	bA	1	Total C 40 40	0
13	bA	1	Total C 40 40	0
13	bB	1	Total C 40 40	0
13	bB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

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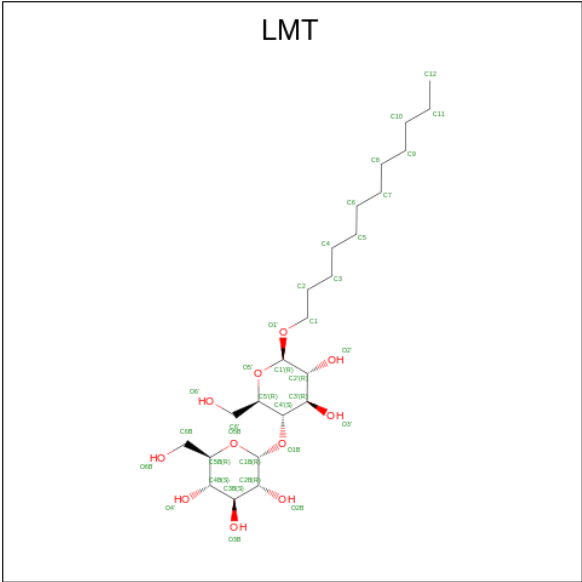
Mol	Chain	Residues	Atoms	AltConf
13	cA	1	Total C 40 40	0
13	cA	1	Total C 40 40	0
13	cA	1	Total C 40 40	0
13	cA	1	Total C 40 40	0
13	cA	1	Total C 40 40	0
13	cB	1	Total C 40 40	0
13	cB	1	Total C 40 40	0
13	cB	1	Total C 40 40	0
13	cB	1	Total C 40 40	0
13	cB	1	Total C 40 40	0
13	cB	1	Total C 40 40	0
13	cB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

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



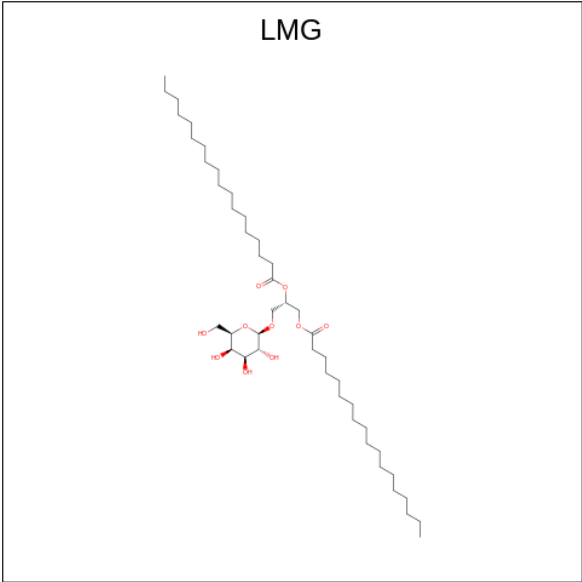
Mol	Chain	Residues	Atoms				AltConf
14	aA	1	Total	C	O	P	0
			49	38	10	1	
14	aA	1	Total	C	O	P	0
			27	16	10	1	
14	bA	1	Total	C	O	P	0
			49	38	10	1	
14	bA	1	Total	C	O	P	0
			27	16	10	1	
14	cA	1	Total	C	O	P	0
			49	38	10	1	
14	cA	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 15 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



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

- Molecule 17 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

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

- Molecule 18 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 19 is water.

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

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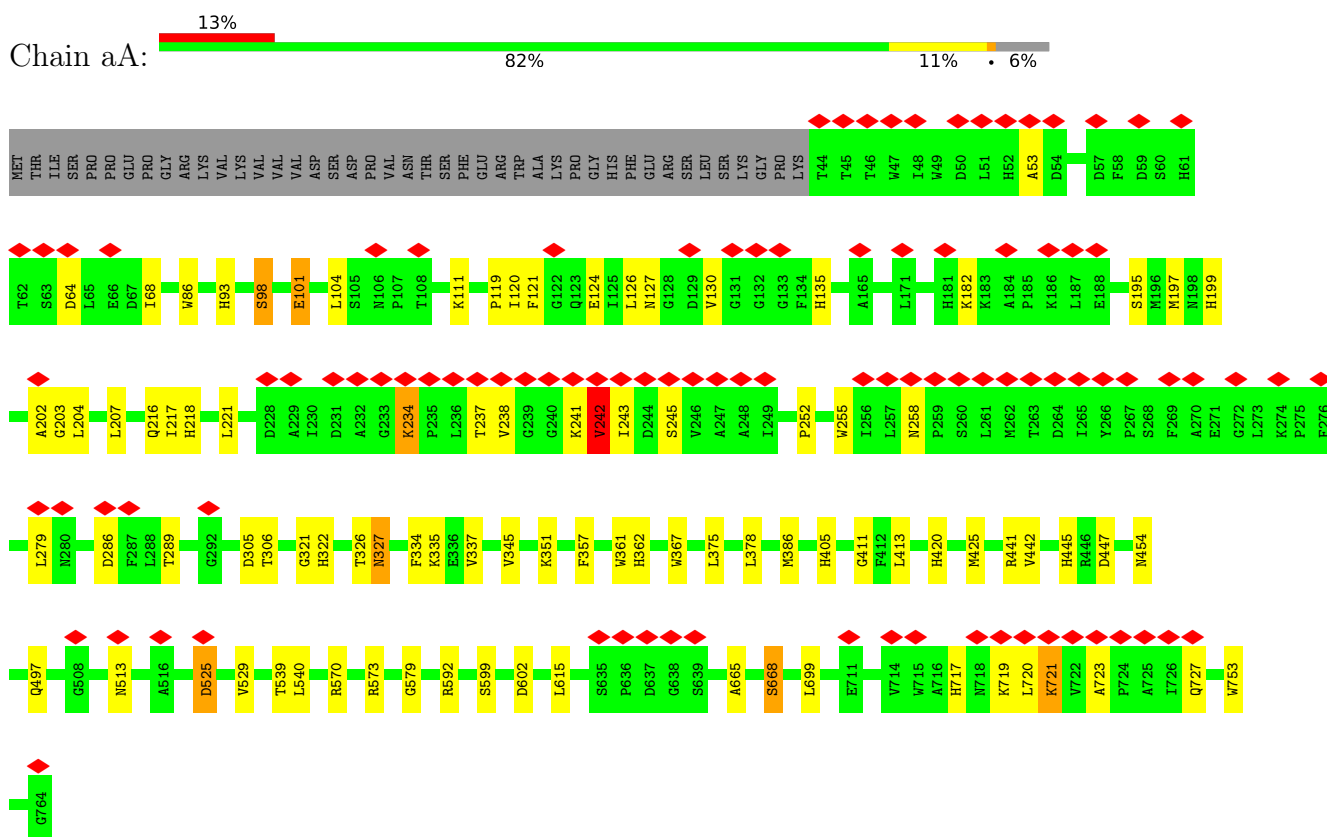
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Mol	Chain	Residues	Atoms		AltConf
19	aD	12	Total 12	O 12	0
19	aI	1	Total 1	O 1	0
19	aL	30	Total 30	O 30	0
19	aM	1	Total 1	O 1	0
19	bA	63	Total 63	O 63	0
19	bB	85	Total 85	O 85	0
19	bC	17	Total 17	O 17	0
19	bD	12	Total 12	O 12	0
19	bI	1	Total 1	O 1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

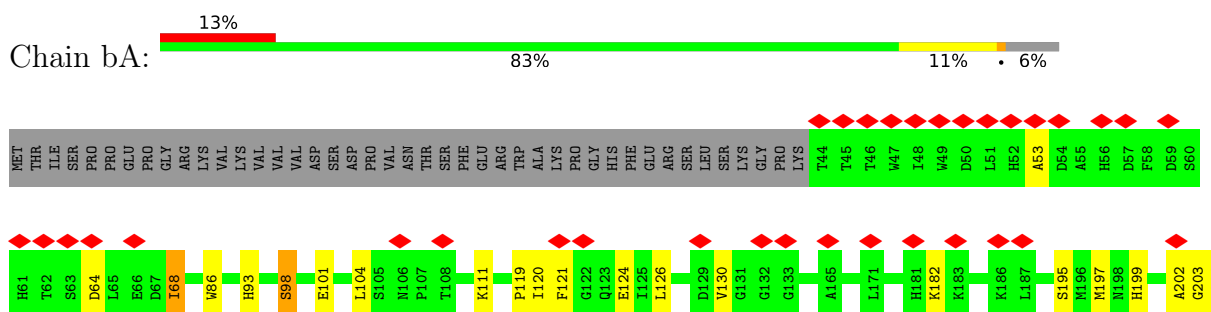
3 Residue-property plots

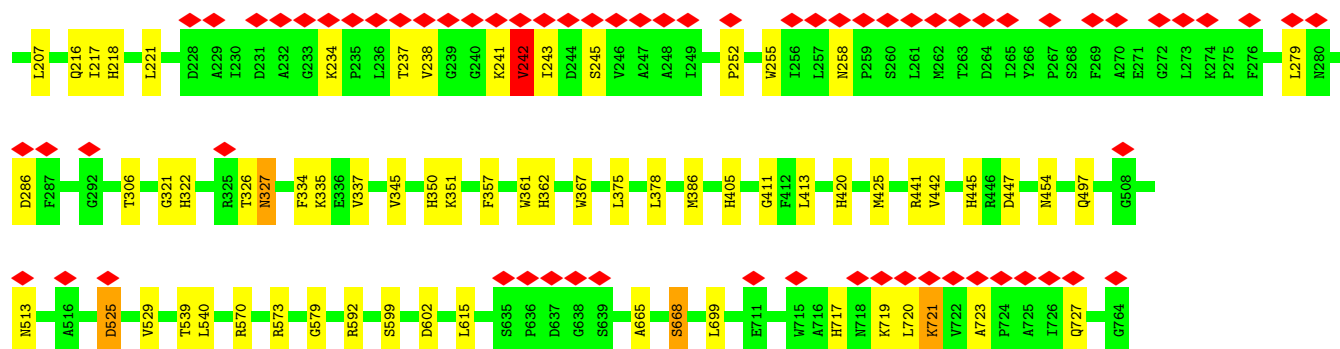
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

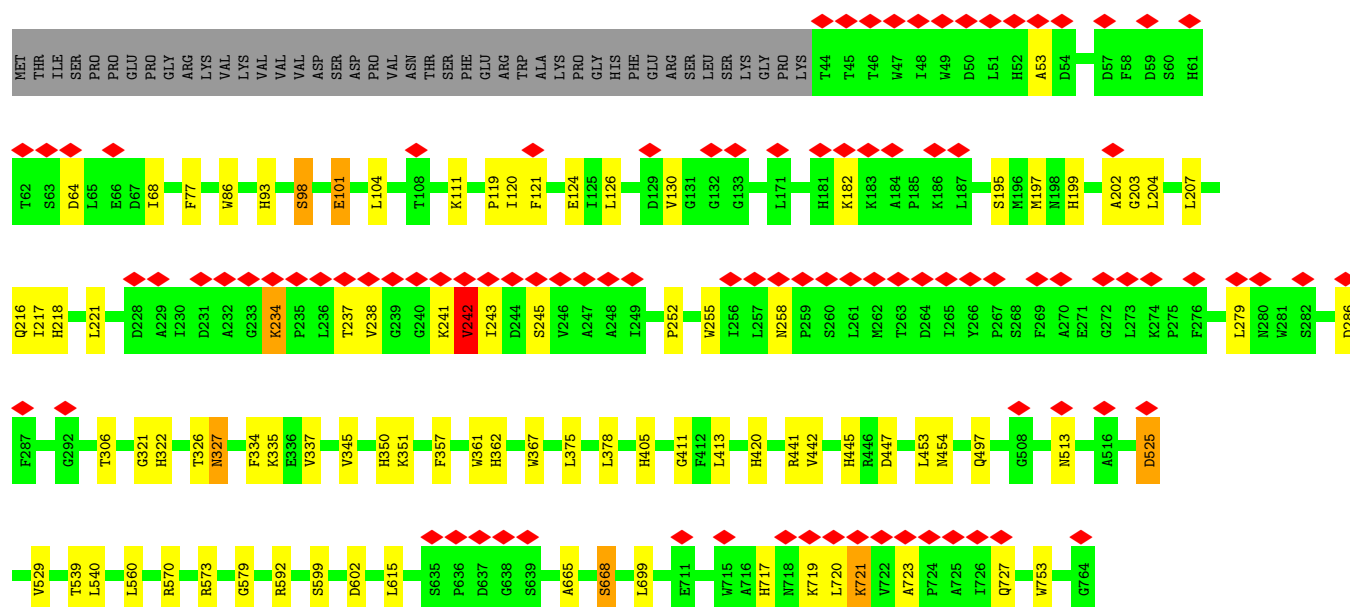
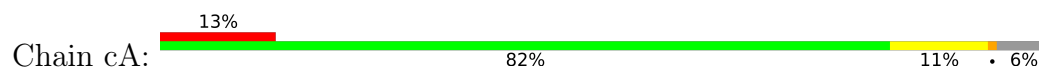


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

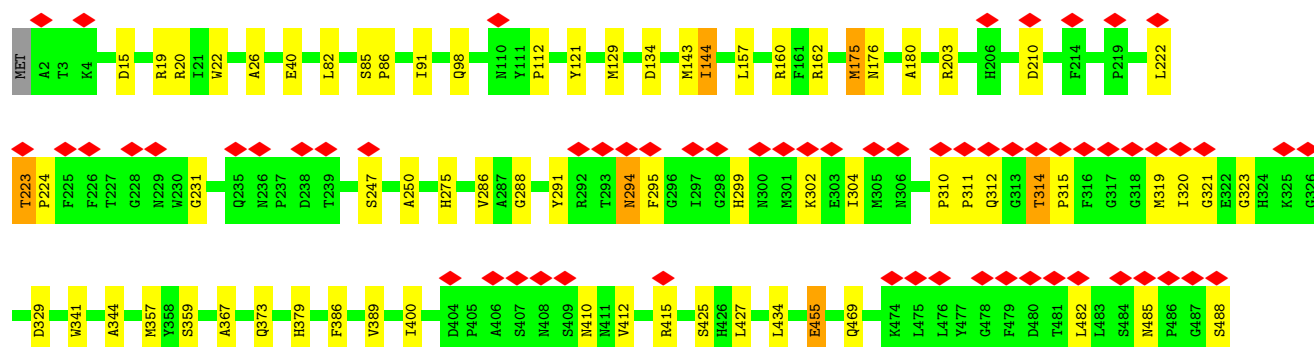
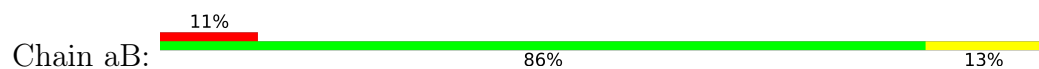


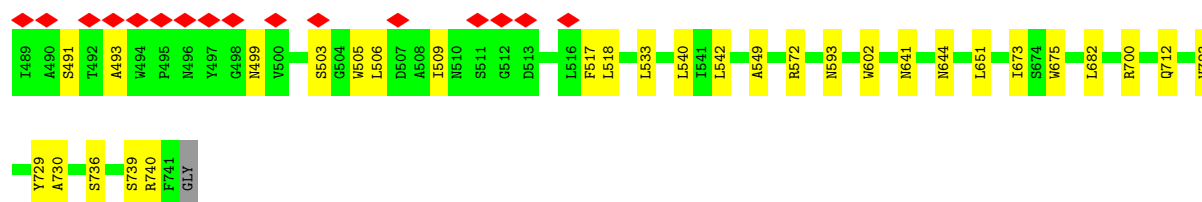


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

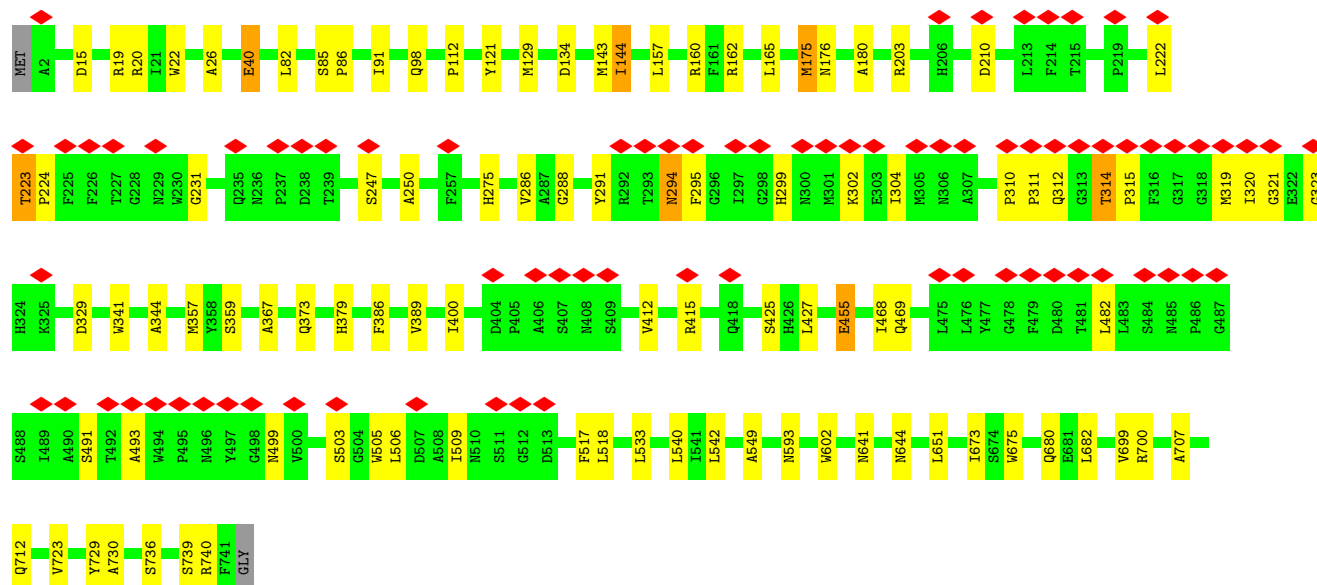
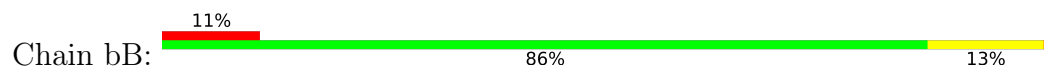


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

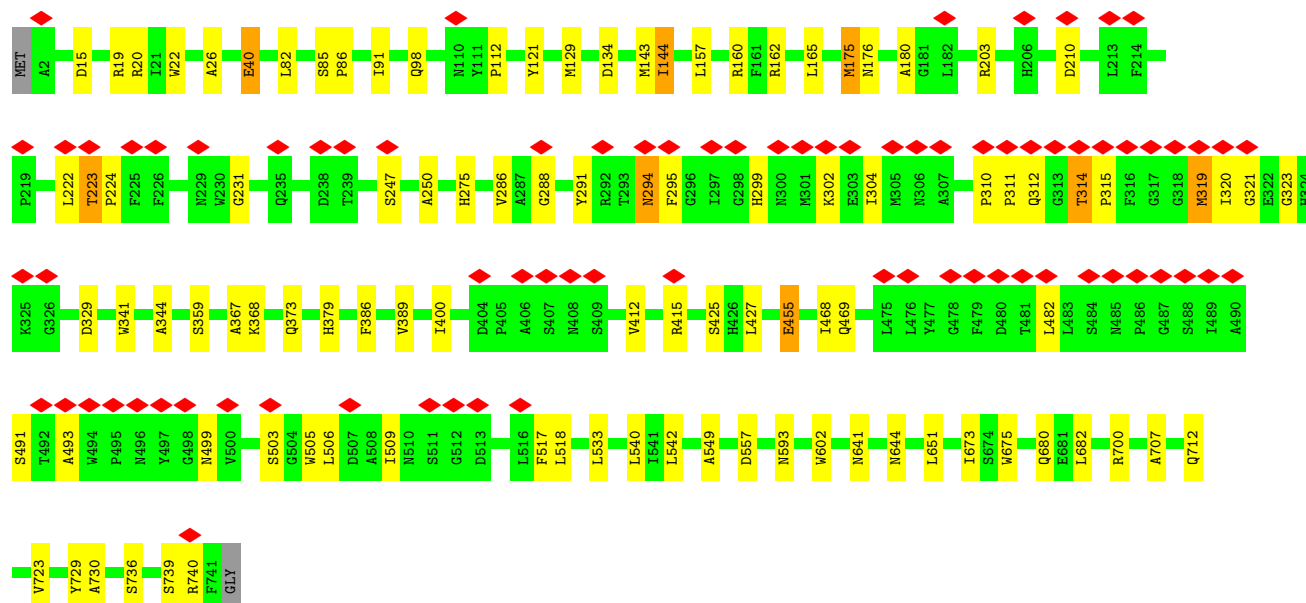
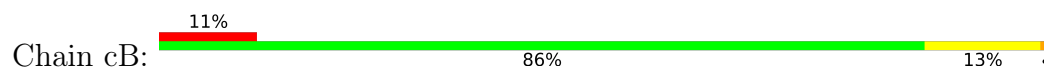




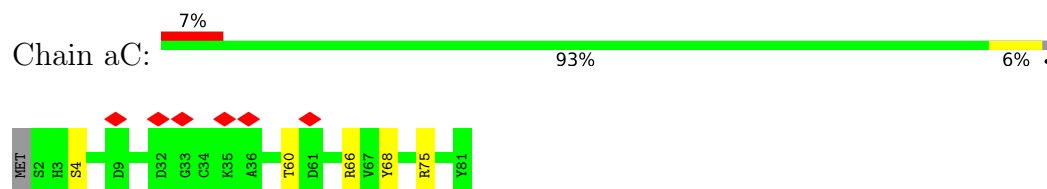
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



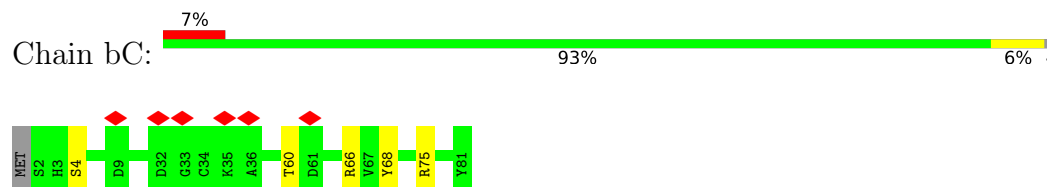
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



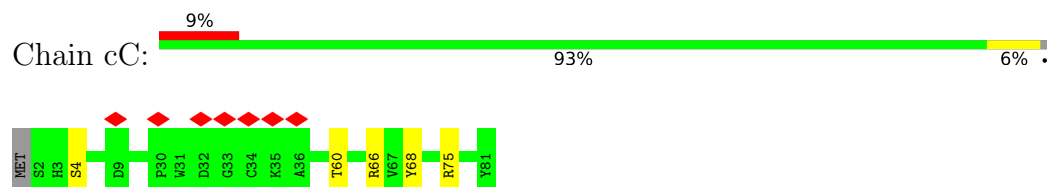
- Molecule 3: Photosystem I iron-sulfur center



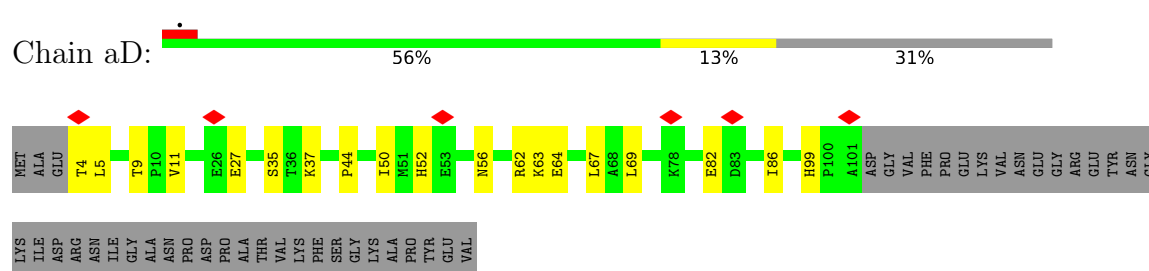
- Molecule 3: Photosystem I iron-sulfur center



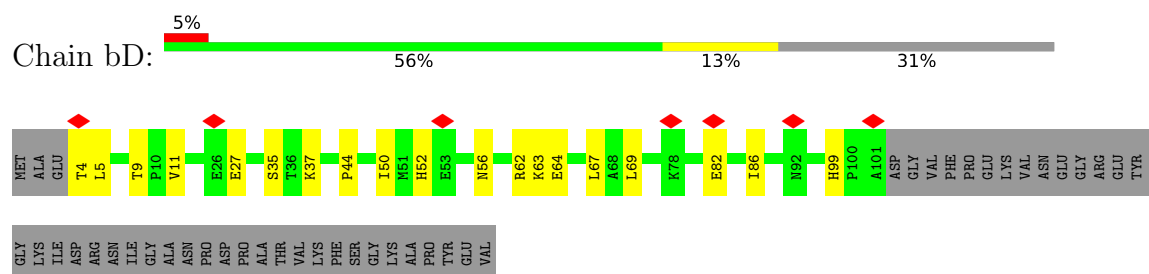
- Molecule 3: Photosystem I iron-sulfur center



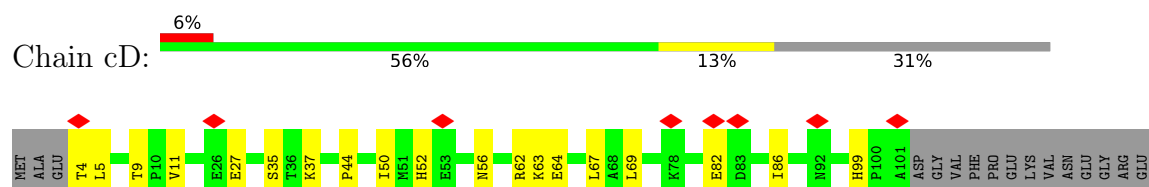
- Molecule 4: Photosystem I reaction center subunit II



- Molecule 4: Photosystem I reaction center subunit II



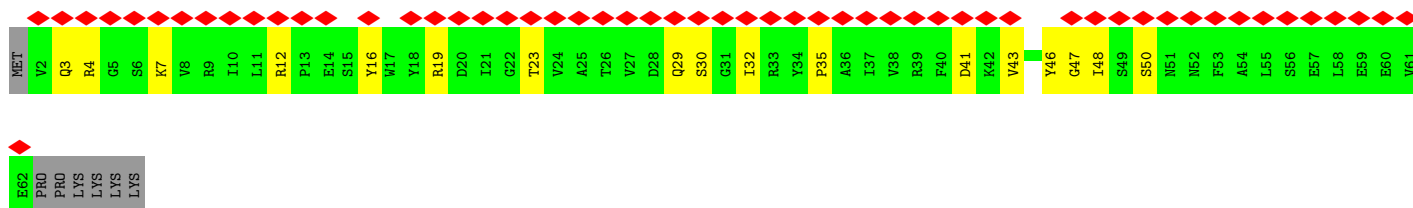
- Molecule 4: Photosystem I reaction center subunit II



ASN GLY LYS ILE ASP ARG ASN ILE GLY ALA ASN PRO ASP PRO THR VAL LYS PHE SER GLY LYS ALA PRO TYR GLU VAL

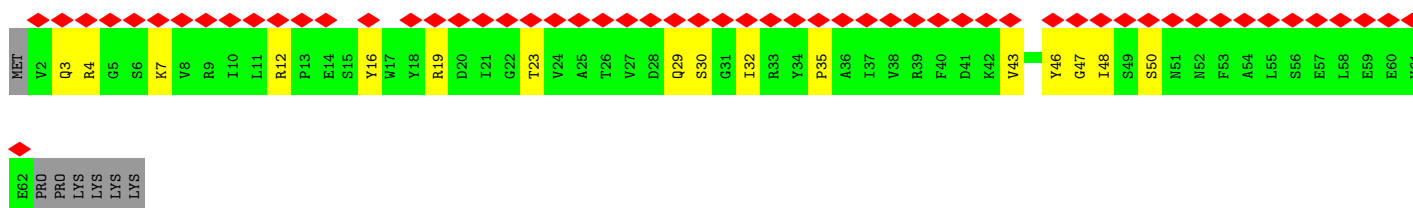
- Molecule 5: Photosystem I reaction center subunit IV

Chain aE: 



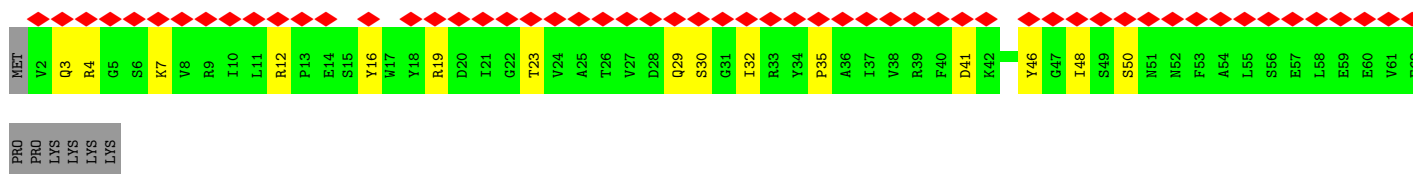
- Molecule 5: Photosystem I reaction center subunit IV

Chain bE: 



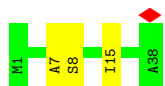
- Molecule 5: Photosystem I reaction center subunit IV

Chain cE: 



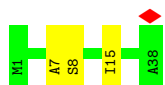
- Molecule 6: Photosystem I reaction center subunit VIII

Chain aI: 



- Molecule 6: Photosystem I reaction center subunit VIII

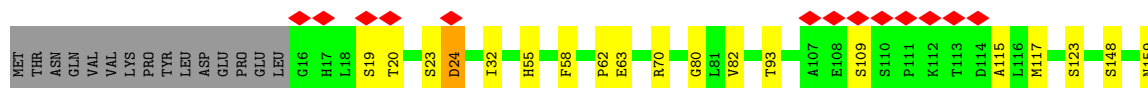
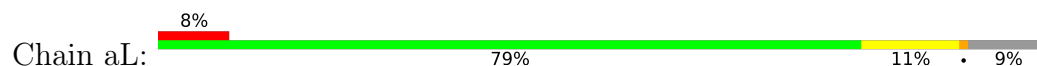
Chain bI: 



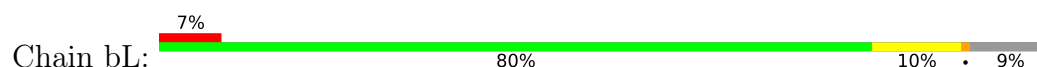
- Molecule 6: Photosystem I reaction center subunit VIII



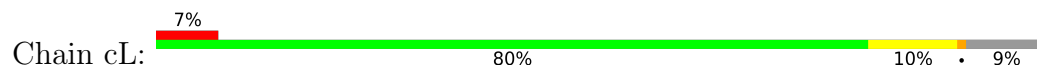
- Molecule 7: Photosystem I reaction center subunit XI



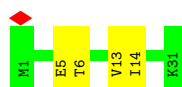
- Molecule 7: Photosystem I reaction center subunit XI



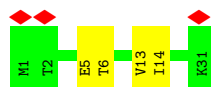
- Molecule 7: Photosystem I reaction center subunit XI



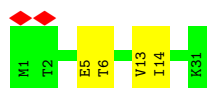
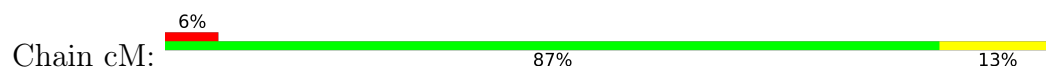
- Molecule 8: Photosystem I reaction center subunit XII



- Molecule 8: Photosystem I reaction center subunit XII



- Molecule 8: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	546366	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.453	Depositor
Minimum map value	-0.267	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	313.2, 313.2, 313.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.27	0/5825	0.52	2/7944 (0.0%)
1	bA	0.27	0/5825	0.52	2/7944 (0.0%)
1	cA	0.27	0/5825	0.52	2/7944 (0.0%)
2	aB	0.28	0/6105	0.54	8/8343 (0.1%)
2	bB	0.28	0/6105	0.54	8/8343 (0.1%)
2	cB	0.28	0/6105	0.54	8/8343 (0.1%)
3	aC	0.27	0/606	0.59	0/820
3	bC	0.27	0/606	0.59	0/820
3	cC	0.27	0/606	0.59	0/820
4	aD	0.22	0/785	0.44	0/1061
4	bD	0.22	0/785	0.44	0/1061
4	cD	0.22	0/785	0.44	0/1061
5	aE	0.25	0/509	0.61	1/689 (0.1%)
5	bE	0.24	0/509	0.61	1/689 (0.1%)
5	cE	0.24	0/509	0.61	1/689 (0.1%)
6	aI	0.32	0/317	0.56	0/436
6	bI	0.32	0/317	0.56	0/436
6	cI	0.32	0/317	0.57	0/436
7	aL	0.29	0/1093	0.52	0/1481
7	bL	0.29	0/1093	0.52	0/1481
7	cL	0.29	0/1093	0.53	0/1481
8	aM	0.25	0/244	0.56	0/332
8	bM	0.24	0/244	0.56	0/332
8	cM	0.25	0/244	0.56	0/332
All	All	0.27	0/46452	0.53	33/63318 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	aA	0	4
1	bA	0	4
1	cA	0	4
2	aB	0	3
2	bB	0	3
2	cB	0	3
All	All	0	21

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	bA	721	LYS	CA-C-N	6.92	134.43	121.97
1	bA	721	LYS	C-N-CA	6.92	134.43	121.97
1	cA	721	LYS	CA-C-N	6.91	134.41	121.97
1	cA	721	LYS	C-N-CA	6.91	134.41	121.97
1	aA	721	LYS	CA-C-N	6.90	134.40	121.97

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5629	0	5454	56	0
1	bA	5629	0	5454	52	0
1	cA	5629	0	5454	55	0
2	aB	5884	0	5623	60	0
2	bB	5884	0	5623	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	cB	5884	0	5623	62	0
3	aC	596	0	576	4	0
3	bC	596	0	576	4	0
3	cC	596	0	576	4	0
4	aD	768	0	774	9	0
4	bD	768	0	774	9	0
4	cD	768	0	774	9	0
5	aE	499	0	488	9	0
5	bE	499	0	488	7	0
5	cE	499	0	488	7	0
6	aI	305	0	304	1	0
6	bI	305	0	304	1	0
6	cI	305	0	304	1	0
7	aL	1065	0	1064	10	0
7	bL	1065	0	1064	8	0
7	cL	1065	0	1064	8	0
8	aM	241	0	266	3	0
8	bM	241	0	266	3	0
8	cM	241	0	266	3	0
9	aA	65	0	72	1	0
9	bA	65	0	72	1	0
9	cA	65	0	72	1	0
10	aA	2491	0	2400	62	0
10	aB	2357	0	2305	60	0
10	aL	250	0	265	6	0
10	bA	2491	0	2400	64	0
10	bB	2357	0	2305	62	0
10	bL	250	0	265	3	0
10	cA	2491	0	2400	59	0
10	cB	2357	0	2305	61	0
10	cL	250	0	265	6	0
11	aA	33	0	46	2	0
11	aB	33	0	46	1	0
11	bA	33	0	46	2	0
11	bB	33	0	46	0	0
11	cA	33	0	46	2	0
11	cB	33	0	46	0	0
12	aA	8	0	0	0	0
12	aC	16	0	0	0	0
12	bA	8	0	0	0	0
12	bC	16	0	0	0	0
12	cA	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	cC	16	0	0	0	0
13	aA	240	0	336	12	0
13	aB	240	0	333	17	0
13	aI	80	0	112	3	0
13	aL	80	0	112	2	0
13	aM	40	0	56	2	0
13	bA	240	0	336	11	0
13	bB	240	0	333	17	0
13	bI	80	0	112	4	0
13	bL	80	0	112	4	0
13	bM	40	0	56	2	0
13	cA	240	0	336	12	0
13	cB	240	0	333	16	0
13	cI	80	0	112	5	0
13	cL	80	0	112	3	0
13	cM	40	0	56	2	0
14	aA	76	0	98	2	0
14	bA	76	0	98	2	0
14	cA	76	0	98	2	0
15	aA	35	0	46	1	0
15	bA	35	0	46	1	0
15	cA	35	0	46	1	0
16	aB	55	0	84	1	0
16	bB	55	0	84	1	0
16	cB	55	0	84	1	0
17	aI	9	0	0	0	0
17	aL	56	0	0	0	0
17	bI	9	0	0	0	0
17	bL	56	0	0	0	0
17	cI	9	0	0	0	0
17	cL	56	0	0	0	0
18	aL	1	0	0	0	0
18	bL	1	0	0	0	0
18	cL	1	0	0	0	0
19	aA	64	0	0	1	0
19	aB	85	0	0	1	0
19	aC	16	0	0	0	0
19	aD	12	0	0	0	0
19	aI	1	0	0	0	0
19	aL	30	0	0	1	0
19	aM	1	0	0	0	0
19	bA	63	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	bB	85	0	0	1	0
19	bC	17	0	0	0	0
19	bD	12	0	0	0	0
19	bI	1	0	0	0	0
19	bL	30	0	0	0	0
19	bM	1	0	0	0	0
19	cA	63	0	0	1	0
19	cB	86	0	0	1	0
19	cC	15	0	0	0	0
19	cD	13	0	0	0	0
19	cI	1	0	0	0	0
19	cL	30	0	0	0	0
19	cM	1	0	0	0	0
All	All	64083	0	62580	728	0

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

The worst 5 of 728 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:aD:52:HIS:H	4:aD:56:ASN:HD21	1.34	0.76
4:bD:52:HIS:H	4:bD:56:ASN:HD21	1.34	0.75
4:cD:52:HIS:H	4:cD:56:ASN:HD21	1.34	0.75
10:bB:821:CLA:HBB1	13:bB:843:BCR:H14C	1.74	0.68
10:aB:821:CLA:HBB1	13:aB:843:BCR:H14C	1.74	0.68

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	48	59
1	bA	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	48	59
1	cA	719/764 (94%)	691 (96%)	27 (4%)	1 (0%)	48	59
2	aB	738/742 (100%)	705 (96%)	33 (4%)	0	100	100
2	bB	738/742 (100%)	705 (96%)	33 (4%)	0	100	100
2	cB	738/742 (100%)	705 (96%)	33 (4%)	0	100	100
3	aC	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
3	bC	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
3	cC	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	aD	96/142 (68%)	93 (97%)	3 (3%)	0	100	100
4	bD	96/142 (68%)	93 (97%)	3 (3%)	0	100	100
4	cD	96/142 (68%)	93 (97%)	3 (3%)	0	100	100
5	aE	59/68 (87%)	51 (86%)	8 (14%)	0	100	100
5	bE	59/68 (87%)	51 (86%)	8 (14%)	0	100	100
5	cE	59/68 (87%)	51 (86%)	8 (14%)	0	100	100
6	aI	36/38 (95%)	36 (100%)	0	0	100	100
6	bI	36/38 (95%)	36 (100%)	0	0	100	100
6	cI	36/38 (95%)	36 (100%)	0	0	100	100
7	aL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	18	20
7	bL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	18	20
7	cL	142/159 (89%)	138 (97%)	3 (2%)	1 (1%)	18	20
8	aM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
8	bM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
8	cM	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
All	All	5691/6075 (94%)	5442 (96%)	243 (4%)	6 (0%)	49	59

5 of 6 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	574/614 (94%)	551 (96%)	23 (4%)	28	37
1	bA	574/614 (94%)	551 (96%)	23 (4%)	28	37
1	cA	574/614 (94%)	551 (96%)	23 (4%)	28	37
2	aB	597/598 (100%)	579 (97%)	18 (3%)	36	48
2	bB	597/598 (100%)	579 (97%)	18 (3%)	36	48
2	cB	597/598 (100%)	579 (97%)	18 (3%)	36	48
3	aC	68/69 (99%)	68 (100%)	0	100	100
3	bC	68/69 (99%)	68 (100%)	0	100	100
3	cC	68/69 (99%)	68 (100%)	0	100	100
4	aD	80/115 (70%)	77 (96%)	3 (4%)	29	39
4	bD	80/115 (70%)	77 (96%)	3 (4%)	29	39
4	cD	80/115 (70%)	77 (96%)	3 (4%)	29	39
5	aE	54/61 (88%)	51 (94%)	3 (6%)	19	23
5	bE	54/61 (88%)	51 (94%)	3 (6%)	19	23
5	cE	54/61 (88%)	51 (94%)	3 (6%)	19	23
6	aI	32/32 (100%)	30 (94%)	2 (6%)	16	19
6	bI	32/32 (100%)	30 (94%)	2 (6%)	16	19
6	cI	32/32 (100%)	30 (94%)	2 (6%)	16	19
7	aL	108/123 (88%)	101 (94%)	7 (6%)	15	18
7	bL	108/123 (88%)	101 (94%)	7 (6%)	15	18
7	cL	108/123 (88%)	101 (94%)	7 (6%)	15	18
8	aM	27/27 (100%)	26 (96%)	1 (4%)	30	40
8	bM	27/27 (100%)	26 (96%)	1 (4%)	30	40
8	cM	27/27 (100%)	26 (96%)	1 (4%)	30	40
All	All	4620/4917 (94%)	4449 (96%)	171 (4%)	31	40

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	cA	68	ILE
2	cB	175	MET
1	cA	182	LYS
1	cA	335	LYS
2	cB	359	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	cA	492	GLN
2	cB	641	ASN
1	cA	571	ASN
2	cB	333	ASN
7	cL	98	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](#)

Of 366 ligands modelled in this entry, 15 are unknown and 3 are monoatomic - leaving 348 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	aA	803	1	49,53,73	2.45	21 (42%)	59,89,113	3.31	27 (45%)
13	BCR	bB	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	6 (10%)
10	CLA	bA	824	19	69,73,73	1.97	19 (27%)	83,113,113	2.85	27 (32%)
14	LHG	cA	855	10	26,26,48	0.83	0	29,32,54	1.33	3 (10%)
10	CLA	aA	813	1	49,53,73	2.43	20 (40%)	59,89,113	3.20	26 (44%)
10	CLA	cB	803	2	69,73,73	1.95	19 (27%)	83,113,113	2.86	32 (38%)
10	CLA	bA	816	1	58,62,73	2.19	20 (34%)	69,99,113	3.13	30 (43%)
10	CLA	aA	812	1	69,73,73	2.04	20 (28%)	83,113,113	2.87	30 (36%)
10	CLA	cB	831	2	49,53,73	2.43	19 (38%)	59,89,113	3.22	29 (49%)
10	CLA	cA	839	1	69,73,73	2.04	21 (30%)	83,113,113	2.82	29 (34%)
10	CLA	cA	809	10,1	49,53,73	2.41	19 (38%)	59,89,113	3.30	26 (44%)
10	CLA	bA	811	10,1	58,62,73	2.21	20 (34%)	69,99,113	3.00	29 (42%)
10	CLA	aA	824	19	69,73,73	1.97	19 (27%)	83,113,113	2.84	27 (32%)
10	CLA	bA	814	1	49,53,73	2.42	20 (40%)	59,89,113	3.22	26 (44%)
9	CL0	cA	801	1	69,73,73	1.94	18 (26%)	83,113,113	2.76	33 (39%)
10	CLA	bB	811	2	69,73,73	1.94	18 (26%)	83,113,113	2.65	26 (31%)
10	CLA	bA	823	1	69,73,73	2.02	19 (27%)	83,113,113	2.74	29 (34%)
10	CLA	aB	808	2	69,73,73	1.98	21 (30%)	83,113,113	2.78	30 (36%)
10	CLA	aB	809	2	69,73,73	1.98	20 (28%)	83,113,113	2.84	29 (34%)
10	CLA	aA	837	1	69,73,73	1.96	19 (27%)	83,113,113	2.80	30 (36%)
16	LMG	cB	848	10	55,55,55	0.76	1 (1%)	63,63,63	1.36	9 (14%)
10	CLA	bA	813	1	49,53,73	2.42	20 (40%)	59,89,113	3.21	26 (44%)
10	CLA	cB	834	2	49,53,73	2.42	20 (40%)	59,89,113	3.29	30 (50%)
11	PQN	bB	842	-	34,34,34	1.51	2 (5%)	42,45,45	1.05	3 (7%)
10	CLA	bL	203	7	69,73,73	2.01	20 (28%)	83,113,113	2.78	29 (34%)
13	BCR	bA	848	-	41,41,41	1.03	2 (4%)	56,56,56	1.29	8 (14%)
10	CLA	bA	817	1	58,62,73	2.21	19 (32%)	69,99,113	3.04	30 (43%)
10	CLA	aA	854	14	56,60,73	2.25	19 (33%)	67,97,113	3.15	29 (43%)
10	CLA	cA	835	1	69,73,73	2.03	18 (26%)	83,113,113	2.70	30 (36%)
10	CLA	aA	841	1	69,73,73	2.02	20 (28%)	83,113,113	2.77	29 (34%)
10	CLA	bB	838	2	69,73,73	2.01	19 (27%)	83,113,113	2.84	31 (37%)
10	CLA	cB	839	2	51,55,73	2.31	21 (41%)	61,91,113	3.23	27 (44%)
10	CLA	bA	818	1	69,73,73	2.06	19 (27%)	83,113,113	3.02	33 (39%)
10	CLA	cA	843	-	46,49,73	2.38	18 (39%)	55,83,113	3.27	24 (43%)
10	CLA	bB	803	2	69,73,73	1.96	19 (27%)	83,113,113	2.87	32 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	aA	802	1	49,53,73	2.43	20 (40%)	59,89,113	3.25	27 (45%)
13	BCR	cA	849	-	41,41,41	1.11	3 (7%)	56,56,56	1.27	7 (12%)
10	CLA	bA	835	1	69,73,73	2.02	18 (26%)	83,113,113	2.69	30 (36%)
13	BCR	bL	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	3 (5%)
13	BCR	cA	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.18	5 (8%)
10	CLA	bB	839	2	51,55,73	2.31	20 (39%)	61,91,113	3.23	27 (44%)
10	CLA	bA	856	1,2	53,57,73	2.35	20 (37%)	62,93,113	3.10	26 (41%)
10	CLA	cB	826	19	69,73,73	2.07	21 (30%)	83,113,113	2.89	33 (39%)
10	CLA	cB	813	2	49,53,73	2.42	21 (42%)	59,89,113	3.14	24 (40%)
10	CLA	cB	824	2	49,53,73	2.44	20 (40%)	59,89,113	3.21	26 (44%)
10	CLA	aA	834	1	58,62,73	2.17	18 (31%)	69,99,113	2.92	32 (46%)
10	CLA	cB	801	19	69,73,73	1.96	20 (28%)	83,113,113	2.81	30 (36%)
10	CLA	bB	816	2	49,53,73	2.39	19 (38%)	59,89,113	3.27	27 (45%)
10	CLA	bA	836	1	55,59,73	2.19	20 (36%)	66,96,113	5.74	33 (50%)
10	CLA	cA	834	1	58,62,73	2.17	18 (31%)	69,99,113	2.92	32 (46%)
10	CLA	cB	815	2	60,64,73	2.15	20 (33%)	72,102,113	2.91	30 (41%)
10	CLA	cB	840	19	69,73,73	1.97	20 (28%)	83,113,113	2.72	29 (34%)
10	CLA	bA	833	1	69,73,73	1.99	19 (27%)	83,113,113	2.92	31 (37%)
10	CLA	cA	808	1	49,53,73	2.37	20 (40%)	59,89,113	3.15	25 (42%)
10	CLA	bA	854	14	56,60,73	2.25	18 (32%)	67,97,113	3.15	29 (43%)
11	PQN	aB	842	-	34,34,34	1.51	2 (5%)	42,45,45	1.05	3 (7%)
10	CLA	cB	832	2	69,73,73	2.03	22 (31%)	83,113,113	2.83	31 (37%)
10	CLA	aB	804	19	61,65,73	2.08	19 (31%)	73,103,113	3.15	31 (42%)
10	CLA	cB	820	-	69,73,73	2.06	19 (27%)	83,113,113	2.70	30 (36%)
12	SF4	aC	101	3	0,12,12	-	-	-	-	-
10	CLA	cA	823	1	69,73,73	2.02	19 (27%)	83,113,113	2.75	29 (34%)
10	CLA	cB	835	-	49,53,73	2.43	19 (38%)	59,89,113	3.14	27 (45%)
12	SF4	bC	101	3	0,12,12	-	-	-	-	-
15	LMT	cA	853	-	36,36,36	0.45	0	47,47,47	0.91	3 (6%)
10	CLA	aA	818	1	69,73,73	2.07	19 (27%)	83,113,113	3.02	33 (39%)
10	CLA	aB	839	2	51,55,73	2.31	20 (39%)	61,91,113	3.22	27 (44%)
10	CLA	bA	842	19	69,73,73	1.96	19 (27%)	83,113,113	2.69	32 (38%)
10	CLA	bA	826	1	69,73,73	2.01	18 (26%)	83,113,113	2.79	28 (33%)
10	CLA	aA	814	1	49,53,73	2.42	20 (40%)	59,89,113	3.22	26 (44%)
10	CLA	bA	828	1	69,73,73	1.98	19 (27%)	83,113,113	2.74	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCR	bA	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.23	7 (12%)
10	CLA	aB	833	2	62,66,73	2.14	20 (32%)	74,104,113	2.97	32 (43%)
10	CLA	bA	805	1	69,73,73	2.01	20 (28%)	83,113,113	2.88	32 (38%)
10	CLA	bB	813	2	49,53,73	2.42	20 (40%)	59,89,113	3.15	24 (40%)
10	CLA	aA	856	1,2	53,57,73	2.35	20 (37%)	62,93,113	3.10	26 (41%)
10	CLA	bA	827	1	69,73,73	2.02	21 (30%)	83,113,113	2.87	30 (36%)
10	CLA	aA	806	1	55,59,73	2.28	19 (34%)	66,96,113	3.18	32 (48%)
10	CLA	bB	805	-	69,73,73	1.93	21 (30%)	83,113,113	2.72	26 (31%)
10	CLA	cA	804	1	69,73,73	1.98	21 (30%)	83,113,113	2.88	28 (33%)
10	CLA	bL	202	2	59,63,73	2.12	20 (33%)	71,101,113	2.99	30 (42%)
12	SF4	aC	102	3	0,12,12	-	-	-	-	-
10	CLA	cB	833	2	62,66,73	2.15	20 (32%)	74,104,113	2.97	31 (41%)
10	CLA	cB	810	2	59,63,73	2.11	18 (30%)	71,101,113	2.95	33 (46%)
10	CLA	cB	828	2	69,73,73	1.93	21 (30%)	83,113,113	2.81	30 (36%)
13	BCR	bA	849	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	7 (12%)
10	CLA	bA	809	10,1	49,53,73	2.41	19 (38%)	59,89,113	3.28	26 (44%)
10	CLA	bA	806	1	55,59,73	2.29	20 (36%)	66,96,113	3.19	33 (50%)
10	CLA	aA	804	1	69,73,73	1.98	20 (28%)	83,113,113	2.87	28 (33%)
10	CLA	aA	826	1	69,73,73	2.01	18 (26%)	83,113,113	2.79	29 (34%)
10	CLA	aA	830	1	54,58,73	2.25	19 (35%)	65,95,113	3.06	29 (44%)
12	SF4	cC	101	3	0,12,12	-	-	-	-	-
10	CLA	bB	841	2	69,73,73	1.96	19 (27%)	83,113,113	2.76	31 (37%)
12	SF4	cA	845	1,2	0,12,12	-	-	-	-	-
10	CLA	aA	821	1	53,57,73	2.30	19 (35%)	62,93,113	3.22	28 (45%)
10	CLA	cA	829	1	69,73,73	1.99	19 (27%)	83,113,113	2.76	28 (33%)
13	BCR	aA	849	-	41,41,41	1.11	3 (7%)	56,56,56	1.26	7 (12%)
10	CLA	aA	805	1	69,73,73	2.01	20 (28%)	83,113,113	2.88	32 (38%)
10	CLA	aB	837	2	64,68,73	2.06	20 (31%)	77,107,113	2.91	30 (38%)
10	CLA	cA	821	1	53,57,73	2.30	19 (35%)	62,93,113	3.22	28 (45%)
10	CLA	aA	827	1	69,73,73	2.02	21 (30%)	83,113,113	2.88	30 (36%)
12	SF4	bC	102	3	0,12,12	-	-	-	-	-
10	CLA	bB	802	-	69,73,73	1.97	20 (28%)	83,113,113	2.74	30 (36%)
10	CLA	aB	834	2	49,53,73	2.42	20 (40%)	59,89,113	3.30	30 (50%)
10	CLA	bA	843	-	46,49,73	2.39	18 (39%)	55,83,113	3.28	24 (43%)
10	CLA	aB	821	2	51,55,73	2.35	20 (39%)	61,91,113	3.08	29 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	bB	828	2	69,73,73	1.94	21 (30%)	83,113,113	2.81	30 (36%)
13	BCR	bB	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	3 (5%)
10	CLA	cB	836	-	49,53,73	2.45	20 (40%)	59,89,113	3.21	28 (47%)
10	CLA	bB	829	2	69,73,73	1.99	20 (28%)	83,113,113	2.60	27 (32%)
10	CLA	cA	806	1	55,59,73	2.28	19 (34%)	66,96,113	3.20	32 (48%)
13	BCR	aL	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	3 (5%)
10	CLA	bA	815	19	53,57,73	2.33	20 (37%)	62,93,113	3.15	26 (41%)
10	CLA	cA	803	1	49,53,73	2.45	21 (42%)	59,89,113	3.31	28 (47%)
11	PQN	bA	844	-	34,34,34	1.53	2 (5%)	42,45,45	1.22	4 (9%)
10	CLA	aB	824	2	49,53,73	2.44	20 (40%)	59,89,113	3.22	26 (44%)
10	CLA	aB	801	19	69,73,73	1.96	20 (28%)	83,113,113	2.81	30 (36%)
13	BCR	bI	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	6 (10%)
10	CLA	aL	205	19	69,73,73	1.99	21 (30%)	83,113,113	2.80	28 (33%)
10	CLA	aA	808	1	49,53,73	2.36	20 (40%)	59,89,113	3.16	26 (44%)
10	CLA	cA	837	1	69,73,73	1.96	19 (27%)	83,113,113	2.80	30 (36%)
10	CLA	aA	809	10,1	49,53,73	2.41	18 (36%)	59,89,113	3.29	26 (44%)
10	CLA	aB	815	2	60,64,73	2.15	20 (33%)	72,102,113	2.91	30 (41%)
10	CLA	bA	820	19	69,73,73	2.03	19 (27%)	83,113,113	2.70	29 (34%)
10	CLA	bB	817	2	59,63,73	2.18	20 (33%)	71,101,113	3.00	30 (42%)
10	CLA	aL	204	7	69,73,73	1.94	18 (26%)	83,113,113	2.88	29 (34%)
10	CLA	cB	825	2	58,62,73	2.19	20 (34%)	69,99,113	3.03	31 (44%)
13	BCR	aB	847	-	41,41,41	1.09	3 (7%)	56,56,56	1.30	6 (10%)
10	CLA	aB	819	2	64,68,73	2.08	18 (28%)	77,107,113	2.93	32 (41%)
13	BCR	bA	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.18	5 (8%)
10	CLA	bB	827	2	69,73,73	1.99	20 (28%)	83,113,113	2.86	30 (36%)
10	CLA	bB	835	-	49,53,73	2.43	20 (40%)	59,89,113	3.14	27 (45%)
10	CLA	aA	819	1	65,69,73	2.10	20 (30%)	78,108,113	2.82	28 (35%)
13	BCR	aB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.31	5 (8%)
10	CLA	aB	816	2	49,53,73	2.39	19 (38%)	59,89,113	3.27	27 (45%)
10	CLA	cA	819	1	65,69,73	2.10	20 (30%)	78,108,113	2.81	28 (35%)
10	CLA	bB	826	19	69,73,73	2.07	21 (30%)	83,113,113	2.88	33 (39%)
13	BCR	bB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
10	CLA	cA	833	1	69,73,73	1.98	19 (27%)	83,113,113	2.90	30 (36%)
10	CLA	bB	814	13,2	69,73,73	2.02	21 (30%)	83,113,113	2.78	31 (37%)
13	BCR	aB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	bA	831	1	69,73,73	1.98	19 (27%)	83,113,113	2.77	27 (32%)
10	CLA	aB	822	10,2	49,53,73	2.41	20 (40%)	59,89,113	3.35	26 (44%)
10	CLA	aA	816	1	58,62,73	2.19	20 (34%)	69,99,113	3.14	30 (43%)
10	CLA	cA	841	1	69,73,73	2.03	21 (30%)	83,113,113	2.76	29 (34%)
13	BCR	cL	206	-	41,41,41	1.03	2 (4%)	56,56,56	1.29	6 (10%)
10	CLA	bB	836	-	49,53,73	2.45	20 (40%)	59,89,113	3.21	28 (47%)
10	CLA	cA	816	1	58,62,73	2.19	19 (32%)	69,99,113	3.14	30 (43%)
10	CLA	cA	830	1	54,58,73	2.25	18 (33%)	65,95,113	3.06	29 (44%)
10	CLA	bA	808	1	49,53,73	2.36	20 (40%)	59,89,113	3.16	26 (44%)
10	CLA	bA	807	1	49,53,73	2.38	21 (42%)	59,89,113	3.32	29 (49%)
10	CLA	aB	814	13,2	69,73,73	2.03	22 (31%)	83,113,113	2.79	31 (37%)
10	CLA	bL	204	7	69,73,73	1.94	18 (26%)	83,113,113	2.88	29 (34%)
10	CLA	aB	803	2	69,73,73	1.95	19 (27%)	83,113,113	2.86	32 (38%)
10	CLA	bB	818	2	63,67,73	2.16	20 (31%)	75,105,113	2.93	29 (38%)
10	CLA	bB	810	2	59,63,73	2.11	18 (30%)	71,101,113	2.95	33 (46%)
10	CLA	cA	825	19	59,63,73	2.14	21 (35%)	71,101,113	3.06	28 (39%)
10	CLA	cA	813	1	49,53,73	2.43	20 (40%)	59,89,113	3.21	27 (45%)
12	SF4	bA	845	1,2	0,12,12	-	-	-	-	-
13	BCR	cB	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	3 (5%)
10	CLA	cB	806	2	58,62,73	2.16	20 (34%)	69,99,113	3.13	34 (49%)
10	CLA	cB	830	16,2	69,73,73	2.01	18 (26%)	83,113,113	2.69	30 (36%)
13	BCR	aI	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	5 (8%)
10	CLA	cB	817	2	59,63,73	2.17	20 (33%)	71,101,113	3.00	30 (42%)
10	CLA	bA	821	1	53,57,73	2.30	19 (35%)	62,93,113	3.22	28 (45%)
14	LHG	aA	852	-	48,48,48	0.67	2 (4%)	51,54,54	1.23	7 (13%)
10	CLA	aA	831	1	69,73,73	1.98	19 (27%)	83,113,113	2.77	27 (32%)
10	CLA	aA	832	1	69,73,73	1.97	19 (27%)	83,113,113	2.85	33 (39%)
10	CLA	cA	842	19	69,73,73	1.96	19 (27%)	83,113,113	2.69	32 (38%)
13	BCR	cA	848	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	8 (14%)
10	CLA	bA	804	1	69,73,73	1.99	20 (28%)	83,113,113	2.87	28 (33%)
10	CLA	cA	831	1	69,73,73	1.98	19 (27%)	83,113,113	2.77	27 (32%)
10	CLA	cL	203	7	69,73,73	2.01	20 (28%)	83,113,113	2.77	29 (34%)
10	CLA	cA	814	1	49,53,73	2.42	20 (40%)	59,89,113	3.23	26 (44%)
10	CLA	aB	806	2	58,62,73	2.17	20 (34%)	69,99,113	3.14	34 (49%)
10	CLA	aA	811	10,1	58,62,73	2.21	20 (34%)	69,99,113	3.00	29 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CL0	bA	801	1	69,73,73	1.94	18 (26%)	83,113,113	2.76	33 (39%)
14	LHG	cA	852	-	48,48,48	0.67	1 (2%)	51,54,54	1.23	7 (13%)
10	CLA	aB	825	2	58,62,73	2.18	20 (34%)	69,99,113	3.04	31 (44%)
10	CLA	aA	829	1	69,73,73	1.99	19 (27%)	83,113,113	2.77	28 (33%)
10	CLA	bB	808	2	69,73,73	1.98	20 (28%)	83,113,113	2.79	29 (34%)
10	CLA	bB	809	2	69,73,73	1.99	20 (28%)	83,113,113	2.84	29 (34%)
10	CLA	cB	804	19	61,65,73	2.07	19 (31%)	73,103,113	3.15	31 (42%)
13	BCR	aA	848	-	41,41,41	1.03	2 (4%)	56,56,56	1.29	8 (14%)
10	CLA	bA	840	-	55,59,73	2.32	20 (36%)	66,96,113	3.11	31 (46%)
10	CLA	cA	822	1	55,59,73	2.27	19 (34%)	66,96,113	3.15	30 (45%)
10	CLA	cL	204	7	69,73,73	1.95	18 (26%)	83,113,113	2.88	28 (33%)
10	CLA	cB	816	2	49,53,73	2.39	19 (38%)	59,89,113	3.27	27 (45%)
10	CLA	bB	831	2	49,53,73	2.42	19 (38%)	59,89,113	3.22	28 (47%)
10	CLA	cA	818	1	69,73,73	2.07	20 (28%)	83,113,113	3.02	33 (39%)
10	CLA	cA	810	1	69,73,73	2.06	20 (28%)	83,113,113	2.87	30 (36%)
10	CLA	aA	823	1	69,73,73	2.02	20 (28%)	83,113,113	2.74	29 (34%)
13	BCR	cB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.32	5 (8%)
10	CLA	cA	856	1,2	53,57,73	2.35	19 (35%)	62,93,113	3.09	26 (41%)
14	LHG	bA	855	10	26,26,48	0.83	0	29,32,54	1.33	3 (10%)
9	CL0	aA	801	1	69,73,73	1.94	18 (26%)	83,113,113	2.76	34 (40%)
10	CLA	cA	802	1	49,53,73	2.42	20 (40%)	59,89,113	3.24	27 (45%)
13	BCR	cB	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.30	6 (10%)
13	BCR	bM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	10 (17%)
10	CLA	cB	819	2	64,68,73	2.07	18 (28%)	77,107,113	2.93	32 (41%)
13	BCR	aB	849	10	41,41,41	1.02	2 (4%)	56,56,56	1.16	4 (7%)
13	BCR	cM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	10 (17%)
10	CLA	bA	803	1	49,53,73	2.45	21 (42%)	59,89,113	3.31	27 (45%)
10	CLA	aB	805	-	69,73,73	1.94	22 (31%)	83,113,113	2.72	26 (31%)
10	CLA	bB	807	2	69,73,73	1.98	21 (30%)	83,113,113	2.87	31 (37%)
10	CLA	aA	815	19	53,57,73	2.33	20 (37%)	62,93,113	3.15	26 (41%)
13	BCR	aL	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	6 (10%)
10	CLA	aB	829	2	69,73,73	1.99	20 (28%)	83,113,113	2.60	27 (32%)
10	CLA	cA	812	1	69,73,73	2.04	20 (28%)	83,113,113	2.86	30 (36%)
10	CLA	aA	810	1	69,73,73	2.06	20 (28%)	83,113,113	2.86	30 (36%)
10	CLA	cA	840	-	55,59,73	2.32	20 (36%)	66,96,113	3.12	30 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	bB	823	10,2	59,63,73	2.25	20 (33%)	71,101,113	2.97	29 (40%)
10	CLA	bA	832	1	69,73,73	1.97	19 (27%)	83,113,113	2.85	33 (39%)
10	CLA	cB	814	13,2	69,73,73	2.03	22 (31%)	83,113,113	2.79	30 (36%)
10	CLA	aB	832	2	69,73,73	2.04	21 (30%)	83,113,113	2.83	31 (37%)
10	CLA	aA	843	-	46,49,73	2.38	18 (39%)	55,83,113	3.28	24 (43%)
10	CLA	cB	823	10,2	59,63,73	2.25	20 (33%)	71,101,113	2.97	29 (40%)
10	CLA	bA	837	1	69,73,73	1.96	18 (26%)	83,113,113	2.80	30 (36%)
10	CLA	bA	812	1	69,73,73	2.04	20 (28%)	83,113,113	2.86	30 (36%)
10	CLA	cA	826	1	69,73,73	2.01	18 (26%)	83,113,113	2.79	29 (34%)
10	CLA	cB	802	-	69,73,73	1.98	20 (28%)	83,113,113	2.74	30 (36%)
10	CLA	cB	808	2	69,73,73	1.98	20 (28%)	83,113,113	2.79	29 (34%)
13	BCR	aI	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.27	6 (10%)
10	CLA	aA	828	1	69,73,73	1.98	19 (27%)	83,113,113	2.74	30 (36%)
10	CLA	cL	205	19	69,73,73	1.99	20 (28%)	83,113,113	2.80	28 (33%)
10	CLA	aA	840	-	55,59,73	2.32	20 (36%)	66,96,113	3.11	30 (45%)
11	PQN	cA	844	-	34,34,34	1.53	2 (5%)	42,45,45	1.21	4 (9%)
10	CLA	bA	830	1	54,58,73	2.25	19 (35%)	65,95,113	3.06	29 (44%)
16	LMG	bB	848	10	55,55,55	0.77	1 (1%)	63,63,63	1.36	9 (14%)
10	CLA	bB	833	2	62,66,73	2.15	20 (32%)	74,104,113	2.97	31 (41%)
10	CLA	cA	805	1	69,73,73	2.01	20 (28%)	83,113,113	2.87	32 (38%)
10	CLA	cA	832	1	69,73,73	1.97	19 (27%)	83,113,113	2.84	33 (39%)
10	CLA	cA	827	1	69,73,73	2.02	21 (30%)	83,113,113	2.87	30 (36%)
10	CLA	cA	820	19	69,73,73	2.04	18 (26%)	83,113,113	2.71	29 (34%)
10	CLA	bA	838	1	54,58,73	2.24	19 (35%)	65,95,113	3.41	33 (50%)
13	BCR	cI	102	-	41,41,41	1.08	3 (7%)	56,56,56	1.27	6 (10%)
10	CLA	bA	825	19	59,63,73	2.14	20 (33%)	71,101,113	3.07	28 (39%)
14	LHG	aA	855	10	26,26,48	0.83	0	29,32,54	1.33	3 (10%)
12	SF4	cC	102	3	0,12,12	-	-	-	-	-
10	CLA	cB	841	2	69,73,73	1.96	19 (27%)	83,113,113	2.76	31 (37%)
10	CLA	cA	811	10,1	58,62,73	2.21	20 (34%)	69,99,113	2.99	29 (42%)
13	BCR	bL	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.29	7 (12%)
10	CLA	aB	836	-	49,53,73	2.45	20 (40%)	59,89,113	3.21	28 (47%)
10	CLA	cB	812	2	49,53,73	2.38	18 (36%)	59,89,113	3.20	27 (45%)
11	PQN	aA	844	-	34,34,34	1.53	2 (5%)	42,45,45	1.22	4 (9%)
10	CLA	aB	811	2	69,73,73	1.94	18 (26%)	83,113,113	2.65	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	aB	810	2	59,63,73	2.11	18 (30%)	71,101,113	2.95	33 (46%)
10	CLA	bB	840	19	69,73,73	1.98	20 (28%)	83,113,113	2.72	29 (34%)
16	LMG	aB	848	10	55,55,55	0.76	1 (1%)	63,63,63	1.36	9 (14%)
10	CLA	aB	838	2	69,73,73	2.01	19 (27%)	83,113,113	2.85	31 (37%)
10	CLA	bA	829	1	69,73,73	1.99	19 (27%)	83,113,113	2.76	28 (33%)
10	CLA	cA	815	19	53,57,73	2.33	19 (35%)	62,93,113	3.15	26 (41%)
10	CLA	aB	830	16,2	69,73,73	2.01	19 (27%)	83,113,113	2.69	30 (36%)
10	CLA	aB	813	2	49,53,73	2.42	20 (40%)	59,89,113	3.15	24 (40%)
13	BCR	aA	846	-	41,41,41	1.11	3 (7%)	56,56,56	1.23	6 (10%)
10	CLA	cL	202	2	59,63,73	2.12	20 (33%)	71,101,113	2.99	30 (42%)
13	BCR	bA	851	-	41,41,41	1.06	2 (4%)	56,56,56	1.20	3 (5%)
13	BCR	aM	101	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	10 (17%)
13	BCR	bB	849	10	41,41,41	1.02	2 (4%)	56,56,56	1.15	4 (7%)
10	CLA	aB	827	2	69,73,73	1.99	20 (28%)	83,113,113	2.86	29 (34%)
13	BCR	cL	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	3 (5%)
13	BCR	cB	849	10	41,41,41	1.02	2 (4%)	56,56,56	1.15	4 (7%)
10	CLA	bB	812	2	49,53,73	2.38	18 (36%)	59,89,113	3.20	27 (45%)
10	CLA	aA	838	1	54,58,73	2.25	21 (38%)	65,95,113	3.42	33 (50%)
10	CLA	cA	807	1	49,53,73	2.38	21 (42%)	59,89,113	3.31	29 (49%)
10	CLA	aA	825	19	59,63,73	2.14	19 (32%)	71,101,113	3.06	28 (39%)
10	CLA	bA	822	1	55,59,73	2.27	19 (34%)	66,96,113	3.15	30 (45%)
10	CLA	bB	801	19	69,73,73	1.96	20 (28%)	83,113,113	2.81	31 (37%)
10	CLA	bB	832	2	69,73,73	2.03	21 (30%)	83,113,113	2.82	31 (37%)
10	CLA	bB	820	-	69,73,73	2.06	19 (27%)	83,113,113	2.71	30 (36%)
13	BCR	bB	844	-	41,41,41	1.04	2 (4%)	56,56,56	1.32	5 (8%)
10	CLA	aB	807	2	69,73,73	1.98	21 (30%)	83,113,113	2.87	31 (37%)
10	CLA	bA	810	1	69,73,73	2.06	20 (28%)	83,113,113	2.86	30 (36%)
12	SF4	aA	845	1,2	0,12,12	-	-	-	-	-
10	CLA	cB	818	2	63,67,73	2.16	21 (33%)	75,105,113	2.94	30 (40%)
10	CLA	bB	819	2	64,68,73	2.07	18 (28%)	77,107,113	2.92	32 (41%)
13	BCR	cB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)
10	CLA	bA	802	1	49,53,73	2.42	20 (40%)	59,89,113	3.24	27 (45%)
10	CLA	bB	837	2	64,68,73	2.06	20 (31%)	77,107,113	2.91	30 (38%)
10	CLA	aB	823	10,2	59,63,73	2.25	20 (33%)	71,101,113	2.96	29 (40%)
10	CLA	cB	822	10,2	49,53,73	2.42	20 (40%)	59,89,113	3.35	26 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	aB	831	2	49,53,73	2.43	19 (38%)	59,89,113	3.23	28 (47%)
10	CLA	aB	802	-	69,73,73	1.97	20 (28%)	83,113,113	2.74	30 (36%)
10	CLA	cA	836	1	55,59,73	2.20	20 (36%)	66,96,113	5.74	33 (50%)
10	CLA	cB	829	2	69,73,73	1.99	21 (30%)	83,113,113	2.60	27 (32%)
13	BCR	cB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
10	CLA	bB	830	16,2	69,73,73	2.01	19 (27%)	83,113,113	2.69	30 (36%)
13	BCR	aA	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.18	5 (8%)
14	LHG	bA	852	-	48,48,48	0.66	2 (4%)	51,54,54	1.23	7 (13%)
10	CLA	aB	828	2	69,73,73	1.94	21 (30%)	83,113,113	2.81	30 (36%)
13	BCR	bA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.30	5 (8%)
10	CLA	bB	824	2	49,53,73	2.43	20 (40%)	59,89,113	3.21	26 (44%)
10	CLA	cA	838	1	54,58,73	2.24	21 (38%)	65,95,113	3.41	33 (50%)
10	CLA	cB	805	-	69,73,73	1.93	21 (30%)	83,113,113	2.73	26 (31%)
10	CLA	aA	822	1	55,59,73	2.27	19 (34%)	66,96,113	3.16	29 (43%)
10	CLA	bB	815	2	60,64,73	2.14	20 (33%)	72,102,113	2.90	30 (41%)
15	LMT	aA	853	-	36,36,36	0.45	0	47,47,47	0.91	3 (6%)
10	CLA	aA	842	19	69,73,73	1.96	19 (27%)	83,113,113	2.69	32 (38%)
13	BCR	bB	843	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	4 (7%)
10	CLA	cB	821	2	51,55,73	2.35	20 (39%)	61,91,113	3.08	29 (47%)
10	CLA	aB	817	2	59,63,73	2.18	20 (33%)	71,101,113	3.01	30 (42%)
10	CLA	aB	841	2	69,73,73	1.96	19 (27%)	83,113,113	2.76	31 (37%)
10	CLA	cB	837	2	64,68,73	2.07	20 (31%)	77,107,113	2.92	30 (38%)
10	CLA	aA	807	1	49,53,73	2.37	21 (42%)	59,89,113	3.31	29 (49%)
10	CLA	bA	839	1	69,73,73	2.04	21 (30%)	83,113,113	2.81	29 (34%)
13	BCR	cI	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	5 (8%)
10	CLA	aL	202	2	59,63,73	2.12	20 (33%)	71,101,113	3.00	30 (42%)
10	CLA	cA	828	1	69,73,73	1.98	19 (27%)	83,113,113	2.74	30 (36%)
10	CLA	cB	838	2	69,73,73	2.01	19 (27%)	83,113,113	2.84	31 (37%)
13	BCR	cA	847	-	41,41,41	1.03	2 (4%)	56,56,56	1.29	5 (8%)
10	CLA	bB	806	2	58,62,73	2.17	20 (34%)	69,99,113	3.14	34 (49%)
13	BCR	bI	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
10	CLA	aA	817	1	58,62,73	2.21	19 (32%)	69,99,113	3.04	31 (44%)
10	CLA	aA	839	1	69,73,73	2.04	21 (30%)	83,113,113	2.82	29 (34%)
10	CLA	cB	827	2	69,73,73	1.99	20 (28%)	83,113,113	2.86	30 (36%)
10	CLA	aB	826	19	69,73,73	2.07	20 (28%)	83,113,113	2.89	33 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	bA	834	1	58,62,73	2.17	18 (31%)	69,99,113	2.91	32 (46%)
10	CLA	aA	820	19	69,73,73	2.03	18 (26%)	83,113,113	2.70	29 (34%)
10	CLA	bB	822	10,2	49,53,73	2.40	20 (40%)	59,89,113	3.35	26 (44%)
13	BCR	aA	847	-	41,41,41	1.04	2 (4%)	56,56,56	1.29	5 (8%)
10	CLA	cB	811	2	69,73,73	1.94	18 (26%)	83,113,113	2.65	26 (31%)
10	CLA	aA	833	1	69,73,73	1.98	19 (27%)	83,113,113	2.91	30 (36%)
10	CLA	bB	821	2	51,55,73	2.35	20 (39%)	61,91,113	3.07	29 (47%)
10	CLA	aA	835	1	69,73,73	2.03	18 (26%)	83,113,113	2.70	31 (37%)
10	CLA	cA	824	19	69,73,73	1.98	19 (27%)	83,113,113	2.84	27 (32%)
10	CLA	aB	840	19	69,73,73	1.98	20 (28%)	83,113,113	2.71	29 (34%)
10	CLA	bB	804	19	61,65,73	2.07	19 (31%)	73,103,113	3.15	31 (42%)
11	PQN	cB	842	-	34,34,34	1.50	2 (5%)	42,45,45	1.05	3 (7%)
10	CLA	cB	809	2	69,73,73	1.98	20 (28%)	83,113,113	2.84	29 (34%)
10	CLA	bB	834	2	49,53,73	2.42	20 (40%)	59,89,113	3.29	30 (50%)
13	BCR	aA	851	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	3 (5%)
15	LMT	bA	853	-	36,36,36	0.45	0	47,47,47	0.91	3 (6%)
13	BCR	aB	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	3 (5%)
10	CLA	aB	818	2	63,67,73	2.16	21 (33%)	75,105,113	2.94	30 (40%)
10	CLA	aB	835	-	49,53,73	2.44	19 (38%)	59,89,113	3.15	27 (45%)
10	CLA	aB	820	-	69,73,73	2.06	19 (27%)	83,113,113	2.71	31 (37%)
10	CLA	aL	203	7	69,73,73	2.01	20 (28%)	83,113,113	2.77	29 (34%)
10	CLA	cA	854	14	56,60,73	2.25	19 (33%)	67,97,113	3.16	29 (43%)
10	CLA	bB	825	2	58,62,73	2.18	19 (32%)	69,99,113	3.04	31 (44%)
13	BCR	cA	851	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	3 (5%)
10	CLA	cB	807	2	69,73,73	1.98	21 (30%)	83,113,113	2.86	32 (38%)
10	CLA	cA	817	1	58,62,73	2.22	20 (34%)	69,99,113	3.05	31 (44%)
13	BCR	aB	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
10	CLA	aA	836	1	55,59,73	2.20	20 (36%)	66,96,113	5.74	33 (50%)
10	CLA	bA	841	1	69,73,73	2.03	20 (28%)	83,113,113	2.77	29 (34%)
10	CLA	bL	205	19	69,73,73	1.99	20 (28%)	83,113,113	2.80	28 (33%)
10	CLA	bA	819	1	65,69,73	2.10	20 (30%)	78,108,113	2.81	28 (35%)
10	CLA	aB	812	2	49,53,73	2.38	18 (36%)	59,89,113	3.20	26 (44%)
13	BCR	cA	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.23	7 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	aA	803	1	-	5/15/91/115	-
13	BCR	bB	847	-	-	10/29/63/63	0/2/2/2
10	CLA	bA	824	19	-	13/39/115/115	-
14	LHG	cA	855	10	-	15/31/31/53	-
10	CLA	aA	813	1	-	1/15/91/115	-
10	CLA	cB	803	2	-	6/39/115/115	-
10	CLA	bA	816	1	-	12/26/102/115	-
10	CLA	aA	812	1	-	17/39/115/115	-
10	CLA	cB	831	2	-	8/15/91/115	-
10	CLA	cA	839	1	-	6/39/115/115	-
10	CLA	cA	809	10,1	-	4/15/91/115	-
10	CLA	bA	811	10,1	-	10/26/102/115	-
10	CLA	aA	824	19	-	13/39/115/115	-
10	CLA	bA	814	1	-	3/15/91/115	-
9	CL0	cA	801	1	-	8/39/115/115	-
10	CLA	bB	811	2	-	19/39/115/115	-
10	CLA	bA	823	1	-	14/39/115/115	-
10	CLA	aB	808	2	-	14/39/115/115	-
10	CLA	aB	809	2	-	8/39/115/115	-
10	CLA	aA	837	1	-	9/39/115/115	-
16	LMG	cB	848	10	-	19/50/70/70	0/1/1/1
10	CLA	bA	813	1	-	1/15/91/115	-
10	CLA	cB	834	2	-	0/15/91/115	-
11	PQN	bB	842	-	-	2/23/43/43	0/2/2/2
10	CLA	bL	203	7	-	13/39/115/115	-
13	BCR	bA	848	-	-	16/29/63/63	0/2/2/2
10	CLA	bA	817	1	-	12/26/102/115	-
10	CLA	aA	854	14	-	8/24/100/115	-
10	CLA	cA	835	1	-	12/39/115/115	-
10	CLA	aA	841	1	-	13/39/115/115	-
10	CLA	bB	838	2	-	11/39/115/115	-
10	CLA	cB	839	2	-	7/18/94/115	-
10	CLA	bA	818	1	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cA	843	-	-	4/9/81/115	-
10	CLA	bB	803	2	-	6/39/115/115	-
10	CLA	aA	802	1	-	9/15/91/115	-
13	BCR	cA	849	-	-	13/29/63/63	0/2/2/2
10	CLA	bA	835	1	-	12/39/115/115	-
13	BCR	bL	207	-	-	7/29/63/63	0/2/2/2
13	BCR	cA	850	-	-	9/29/63/63	0/2/2/2
10	CLA	bB	839	2	-	7/18/94/115	-
10	CLA	bA	856	1,2	-	9/20/96/115	-
10	CLA	cB	826	19	-	12/39/115/115	-
10	CLA	cB	813	2	-	6/15/91/115	-
10	CLA	cB	824	2	-	7/15/91/115	-
10	CLA	aA	834	1	-	10/26/102/115	-
10	CLA	cB	801	19	-	7/39/115/115	-
10	CLA	bB	816	2	-	4/15/91/115	-
10	CLA	bA	836	1	-	7/23/99/115	-
10	CLA	cA	834	1	-	10/26/102/115	-
10	CLA	cB	815	2	-	7/29/105/115	-
10	CLA	cB	840	19	-	2/39/115/115	-
10	CLA	bA	833	1	-	12/39/115/115	-
10	CLA	cA	808	1	-	4/15/91/115	-
10	CLA	bA	854	14	-	8/24/100/115	-
11	PQN	aB	842	-	-	2/23/43/43	0/2/2/2
10	CLA	cB	832	2	-	14/39/115/115	-
10	CLA	aB	804	19	-	14/30/106/115	-
10	CLA	cB	820	-	-	13/39/115/115	-
12	SF4	aC	101	3	-	-	0/6/5/5
10	CLA	cA	823	1	-	14/39/115/115	-
10	CLA	cB	835	-	-	7/15/91/115	-
12	SF4	bC	101	3	-	-	0/6/5/5
15	LMT	cA	853	-	-	9/21/61/61	0/2/2/2
10	CLA	aA	818	1	-	13/39/115/115	-
10	CLA	aB	839	2	-	7/18/94/115	-
10	CLA	bA	842	19	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	bA	826	1	-	10/39/115/115	-
10	CLA	aA	814	1	-	3/15/91/115	-
10	CLA	bA	828	1	-	6/39/115/115	-
13	BCR	bA	846	-	-	14/29/63/63	0/2/2/2
10	CLA	aB	833	2	-	16/31/107/115	-
10	CLA	bA	805	1	-	10/39/115/115	-
10	CLA	bB	813	2	-	6/15/91/115	-
10	CLA	aA	856	1,2	-	9/20/96/115	-
10	CLA	bA	827	1	-	17/39/115/115	-
10	CLA	aA	806	1	-	5/23/99/115	-
10	CLA	bB	805	-	-	12/39/115/115	-
10	CLA	cA	804	1	-	12/39/115/115	-
10	CLA	bL	202	2	-	7/27/103/115	-
12	SF4	aC	102	3	-	-	0/6/5/5
10	CLA	cB	833	2	-	16/31/107/115	-
10	CLA	cB	810	2	-	11/27/103/115	-
10	CLA	cB	828	2	-	13/39/115/115	-
13	BCR	bA	849	-	-	13/29/63/63	0/2/2/2
10	CLA	bA	809	10,1	-	4/15/91/115	-
10	CLA	bA	806	1	-	5/23/99/115	-
10	CLA	aA	804	1	-	12/39/115/115	-
10	CLA	aA	826	1	-	10/39/115/115	-
10	CLA	aA	830	1	-	7/21/97/115	-
12	SF4	cC	101	3	-	-	0/6/5/5
10	CLA	bB	841	2	-	11/39/115/115	-
12	SF4	cA	845	1,2	-	-	0/6/5/5
10	CLA	aA	821	1	-	6/20/96/115	-
10	CLA	cA	829	1	-	12/39/115/115	-
13	BCR	aA	849	-	-	13/29/63/63	0/2/2/2
10	CLA	aA	805	1	-	10/39/115/115	-
10	CLA	aB	837	2	-	12/33/109/115	-
10	CLA	cA	821	1	-	6/20/96/115	-
10	CLA	aA	827	1	-	17/39/115/115	-
12	SF4	bC	102	3	-	-	0/6/5/5
10	CLA	bB	802	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	aB	834	2	-	0/15/91/115	-
10	CLA	bA	843	-	-	4/9/81/115	-
10	CLA	aB	821	2	-	6/18/94/115	-
10	CLA	bB	828	2	-	13/39/115/115	-
13	BCR	bB	846	-	-	8/29/63/63	0/2/2/2
10	CLA	cB	836	-	-	4/15/91/115	-
10	CLA	bB	829	2	-	12/39/115/115	-
10	CLA	cA	806	1	-	5/23/99/115	-
13	BCR	aL	207	-	-	7/29/63/63	0/2/2/2
10	CLA	bA	815	19	-	5/20/96/115	-
10	CLA	cA	803	1	-	5/15/91/115	-
11	PQN	bA	844	-	-	8/23/43/43	0/2/2/2
10	CLA	aB	824	2	-	7/15/91/115	-
10	CLA	aB	801	19	-	7/39/115/115	-
13	BCR	bI	102	-	-	8/29/63/63	0/2/2/2
10	CLA	aL	205	19	-	13/39/115/115	-
10	CLA	aA	808	1	-	4/15/91/115	-
10	CLA	cA	837	1	-	9/39/115/115	-
10	CLA	aA	809	10,1	-	4/15/91/115	-
10	CLA	aB	815	2	-	7/29/105/115	-
10	CLA	bA	820	19	-	15/39/115/115	-
10	CLA	bB	817	2	-	12/27/103/115	-
10	CLA	aL	204	7	-	10/39/115/115	-
10	CLA	cB	825	2	-	8/26/102/115	-
13	BCR	aB	847	-	-	10/29/63/63	0/2/2/2
10	CLA	aB	819	2	-	12/33/109/115	-
13	BCR	bA	850	-	-	9/29/63/63	0/2/2/2
10	CLA	bB	827	2	-	9/39/115/115	-
10	CLA	bB	835	-	-	7/15/91/115	-
10	CLA	aA	819	1	-	13/35/111/115	-
13	BCR	aB	844	-	-	10/29/63/63	0/2/2/2
10	CLA	aB	816	2	-	4/15/91/115	-
10	CLA	cA	819	1	-	13/35/111/115	-
10	CLA	bB	826	19	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCR	bB	845	-	-	12/29/63/63	0/2/2/2
10	CLA	cA	833	1	-	12/39/115/115	-
10	CLA	bB	814	13,2	-	16/39/115/115	-
13	BCR	aB	843	-	-	11/29/63/63	0/2/2/2
10	CLA	bA	831	1	-	13/39/115/115	-
10	CLA	aB	822	10,2	-	9/15/91/115	-
10	CLA	aA	816	1	-	12/26/102/115	-
10	CLA	cA	841	1	-	13/39/115/115	-
13	BCR	cL	206	-	-	8/29/63/63	0/2/2/2
10	CLA	bB	836	-	-	4/15/91/115	-
10	CLA	cA	816	1	-	12/26/102/115	-
10	CLA	cA	830	1	-	7/21/97/115	-
10	CLA	bA	808	1	-	4/15/91/115	-
10	CLA	bA	807	1	-	9/15/91/115	-
10	CLA	aB	814	13,2	-	16/39/115/115	-
10	CLA	bL	204	7	-	10/39/115/115	-
10	CLA	aB	803	2	-	6/39/115/115	-
10	CLA	bB	818	2	-	12/32/108/115	-
10	CLA	bB	810	2	-	11/27/103/115	-
10	CLA	cA	825	19	-	11/27/103/115	-
10	CLA	cA	813	1	-	1/15/91/115	-
12	SF4	bA	845	1,2	-	-	0/6/5/5
13	BCR	cB	846	-	-	8/29/63/63	0/2/2/2
10	CLA	cB	806	2	-	11/26/102/115	-
10	CLA	cB	830	16,2	-	9/39/115/115	-
13	BCR	aI	102	-	-	8/29/63/63	0/2/2/2
10	CLA	cB	817	2	-	12/27/103/115	-
10	CLA	bA	821	1	-	6/20/96/115	-
14	LHG	aA	852	-	-	31/53/53/53	-
10	CLA	aA	831	1	-	13/39/115/115	-
10	CLA	aA	832	1	-	8/39/115/115	-
10	CLA	cA	842	19	-	15/39/115/115	-
13	BCR	cA	848	-	-	16/29/63/63	0/2/2/2
10	CLA	bA	804	1	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cA	831	1	-	13/39/115/115	-
10	CLA	cL	203	7	-	13/39/115/115	-
10	CLA	cA	814	1	-	3/15/91/115	-
10	CLA	aB	806	2	-	11/26/102/115	-
10	CLA	aA	811	10,1	-	10/26/102/115	-
9	CL0	bA	801	1	-	8/39/115/115	-
14	LHG	cA	852	-	-	31/53/53/53	-
10	CLA	aB	825	2	-	8/26/102/115	-
10	CLA	aA	829	1	-	12/39/115/115	-
10	CLA	bB	808	2	-	14/39/115/115	-
10	CLA	bB	809	2	-	8/39/115/115	-
10	CLA	cB	804	19	-	14/30/106/115	-
13	BCR	aA	848	-	-	16/29/63/63	0/2/2/2
10	CLA	bA	840	-	-	6/23/99/115	-
10	CLA	cA	822	1	-	10/23/99/115	-
10	CLA	cL	204	7	-	10/39/115/115	-
10	CLA	cB	816	2	-	4/15/91/115	-
10	CLA	bB	831	2	-	8/15/91/115	-
10	CLA	cA	818	1	-	13/39/115/115	-
10	CLA	cA	810	1	-	12/39/115/115	-
10	CLA	aA	823	1	-	14/39/115/115	-
13	BCR	cB	844	-	-	10/29/63/63	0/2/2/2
10	CLA	cA	856	1,2	-	9/20/96/115	-
14	LHG	bA	855	10	-	15/31/31/53	-
9	CL0	aA	801	1	-	8/39/115/115	-
10	CLA	cA	802	1	-	9/15/91/115	-
13	BCR	cB	847	-	-	10/29/63/63	0/2/2/2
13	BCR	bM	101	-	-	13/29/63/63	0/2/2/2
10	CLA	cB	819	2	-	12/33/109/115	-
13	BCR	aB	849	10	-	18/29/63/63	0/2/2/2
13	BCR	cM	101	-	-	13/29/63/63	0/2/2/2
10	CLA	bA	803	1	-	5/15/91/115	-
10	CLA	aB	805	-	-	12/39/115/115	-
10	CLA	bB	807	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	aA	815	19	-	5/20/96/115	-
13	BCR	aL	206	-	-	8/29/63/63	0/2/2/2
10	CLA	aB	829	2	-	12/39/115/115	-
10	CLA	cA	812	1	-	17/39/115/115	-
10	CLA	aA	810	1	-	12/39/115/115	-
10	CLA	cA	840	-	-	6/23/99/115	-
10	CLA	bB	823	10,2	-	15/27/103/115	-
10	CLA	bA	832	1	-	8/39/115/115	-
10	CLA	cB	814	13,2	-	16/39/115/115	-
10	CLA	aB	832	2	-	14/39/115/115	-
10	CLA	aA	843	-	-	4/9/81/115	-
10	CLA	cB	823	10,2	-	15/27/103/115	-
10	CLA	bA	837	1	-	9/39/115/115	-
10	CLA	bA	812	1	-	17/39/115/115	-
10	CLA	cA	826	1	-	10/39/115/115	-
10	CLA	cB	802	-	-	13/39/115/115	-
10	CLA	cB	808	2	-	14/39/115/115	-
13	BCR	aI	101	-	-	8/29/63/63	0/2/2/2
10	CLA	aA	828	1	-	6/39/115/115	-
10	CLA	cL	205	19	-	13/39/115/115	-
10	CLA	aA	840	-	-	6/23/99/115	-
11	PQN	cA	844	-	-	8/23/43/43	0/2/2/2
10	CLA	bA	830	1	-	7/21/97/115	-
16	LMG	bB	848	10	-	19/50/70/70	0/1/1/1
10	CLA	bB	833	2	-	16/31/107/115	-
10	CLA	cA	805	1	-	10/39/115/115	-
10	CLA	cA	832	1	-	8/39/115/115	-
10	CLA	cA	827	1	-	17/39/115/115	-
10	CLA	cA	820	19	-	15/39/115/115	-
10	CLA	bA	838	1	-	9/21/97/115	-
13	BCR	cI	102	-	-	8/29/63/63	0/2/2/2
10	CLA	bA	825	19	-	11/27/103/115	-
14	LHG	aA	855	10	-	15/31/31/53	-
12	SF4	cC	102	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cB	841	2	-	11/39/115/115	-
10	CLA	cA	811	10,1	-	10/26/102/115	-
13	BCR	bL	206	-	-	8/29/63/63	0/2/2/2
10	CLA	aB	836	-	-	4/15/91/115	-
10	CLA	cB	812	2	-	3/15/91/115	-
11	PQN	aA	844	-	-	8/23/43/43	0/2/2/2
10	CLA	aB	811	2	-	19/39/115/115	-
10	CLA	aB	810	2	-	11/27/103/115	-
10	CLA	bB	840	19	-	2/39/115/115	-
16	LMG	aB	848	10	-	19/50/70/70	0/1/1/1
10	CLA	aB	838	2	-	11/39/115/115	-
10	CLA	bA	829	1	-	12/39/115/115	-
10	CLA	cA	815	19	-	5/20/96/115	-
10	CLA	aB	830	16,2	-	9/39/115/115	-
10	CLA	aB	813	2	-	6/15/91/115	-
13	BCR	aA	846	-	-	14/29/63/63	0/2/2/2
10	CLA	cL	202	2	-	7/27/103/115	-
13	BCR	bA	851	-	-	13/29/63/63	0/2/2/2
13	BCR	aM	101	-	-	13/29/63/63	0/2/2/2
13	BCR	bB	849	10	-	18/29/63/63	0/2/2/2
10	CLA	aB	827	2	-	9/39/115/115	-
13	BCR	cL	207	-	-	7/29/63/63	0/2/2/2
13	BCR	cB	849	10	-	18/29/63/63	0/2/2/2
10	CLA	bB	812	2	-	3/15/91/115	-
10	CLA	aA	838	1	-	9/21/97/115	-
10	CLA	cA	807	1	-	9/15/91/115	-
10	CLA	aA	825	19	-	11/27/103/115	-
10	CLA	bA	822	1	-	10/23/99/115	-
10	CLA	bB	801	19	-	7/39/115/115	-
10	CLA	bB	832	2	-	14/39/115/115	-
10	CLA	bB	820	-	-	13/39/115/115	-
13	BCR	bB	844	-	-	10/29/63/63	0/2/2/2
10	CLA	aB	807	2	-	14/39/115/115	-
10	CLA	bA	810	1	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	SF4	aA	845	1,2	-	-	0/6/5/5
10	CLA	cB	818	2	-	12/32/108/115	-
10	CLA	bB	819	2	-	12/33/109/115	-
13	BCR	cB	843	-	-	11/29/63/63	0/2/2/2
10	CLA	bA	802	1	-	9/15/91/115	-
10	CLA	bB	837	2	-	12/33/109/115	-
10	CLA	aB	823	10,2	-	15/27/103/115	-
10	CLA	cB	822	10,2	-	9/15/91/115	-
10	CLA	aB	831	2	-	8/15/91/115	-
10	CLA	aB	802	-	-	13/39/115/115	-
10	CLA	cA	836	1	-	7/23/99/115	-
10	CLA	cB	829	2	-	12/39/115/115	-
13	BCR	cB	845	-	-	12/29/63/63	0/2/2/2
10	CLA	bB	830	16,2	-	9/39/115/115	-
13	BCR	aA	850	-	-	9/29/63/63	0/2/2/2
14	LHG	bA	852	-	-	31/53/53/53	-
10	CLA	aB	828	2	-	13/39/115/115	-
13	BCR	bA	847	-	-	9/29/63/63	0/2/2/2
10	CLA	bB	824	2	-	7/15/91/115	-
10	CLA	cA	838	1	-	9/21/97/115	-
10	CLA	cB	805	-	-	12/39/115/115	-
10	CLA	aA	822	1	-	10/23/99/115	-
10	CLA	bB	815	2	-	7/29/105/115	-
15	LMT	aA	853	-	-	9/21/61/61	0/2/2/2
10	CLA	aA	842	19	-	15/39/115/115	-
13	BCR	bB	843	-	-	11/29/63/63	0/2/2/2
10	CLA	cB	821	2	-	6/18/94/115	-
10	CLA	aB	817	2	-	12/27/103/115	-
10	CLA	aB	841	2	-	11/39/115/115	-
10	CLA	cB	837	2	-	12/33/109/115	-
10	CLA	aA	807	1	-	9/15/91/115	-
10	CLA	bA	839	1	-	6/39/115/115	-
13	BCR	cI	103	-	-	8/29/63/63	0/2/2/2
10	CLA	aL	202	2	-	7/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cA	828	1	-	6/39/115/115	-
10	CLA	cB	838	2	-	11/39/115/115	-
13	BCR	cA	847	-	-	9/29/63/63	0/2/2/2
10	CLA	bB	806	2	-	12/26/102/115	-
13	BCR	bI	101	-	-	8/29/63/63	0/2/2/2
10	CLA	aA	817	1	-	12/26/102/115	-
10	CLA	aA	839	1	-	6/39/115/115	-
10	CLA	cB	827	2	-	9/39/115/115	-
10	CLA	aB	826	19	-	12/39/115/115	-
10	CLA	bA	834	1	-	10/26/102/115	-
10	CLA	aA	820	19	-	15/39/115/115	-
10	CLA	bB	822	10,2	-	9/15/91/115	-
13	BCR	aA	847	-	-	9/29/63/63	0/2/2/2
10	CLA	cB	811	2	-	19/39/115/115	-
10	CLA	aA	833	1	-	12/39/115/115	-
10	CLA	bB	821	2	-	6/18/94/115	-
10	CLA	aA	835	1	-	12/39/115/115	-
10	CLA	cA	824	19	-	13/39/115/115	-
10	CLA	aB	840	19	-	2/39/115/115	-
10	CLA	bB	804	19	-	14/30/106/115	-
11	PQN	cB	842	-	-	2/23/43/43	0/2/2/2
10	CLA	cB	809	2	-	8/39/115/115	-
10	CLA	bB	834	2	-	0/15/91/115	-
13	BCR	aA	851	-	-	13/29/63/63	0/2/2/2
15	LMT	bA	853	-	-	9/21/61/61	0/2/2/2
13	BCR	aB	846	-	-	8/29/63/63	0/2/2/2
10	CLA	aB	818	2	-	12/32/108/115	-
10	CLA	aB	835	-	-	7/15/91/115	-
10	CLA	aB	820	-	-	13/39/115/115	-
10	CLA	aL	203	7	-	13/39/115/115	-
10	CLA	cA	854	14	-	8/24/100/115	-
10	CLA	bB	825	2	-	8/26/102/115	-
13	BCR	cA	851	-	-	13/29/63/63	0/2/2/2
10	CLA	cB	807	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	cA	817	1	-	12/26/102/115	-
13	BCR	aB	845	-	-	12/29/63/63	0/2/2/2
10	CLA	aA	836	1	-	7/23/99/115	-
10	CLA	bA	841	1	-	13/39/115/115	-
10	CLA	bL	205	19	-	13/39/115/115	-
10	CLA	bA	819	1	-	13/35/111/115	-
10	CLA	aB	812	2	-	3/15/91/115	-
13	BCR	cA	846	-	-	14/29/63/63	0/2/2/2

The worst 5 of 5429 bond length outliers are listed below:

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

The worst 5 of 8279 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 3439 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	aA	805	CLA	C1A-C2A-CAA-CBA
10	aA	806	CLA	C2B-C3B-CAB-CBB
10	aA	806	CLA	C4B-C3B-CAB-CBB
10	aA	806	CLA	C2-C3-C5-C6
10	aA	806	CLA	C4-C3-C5-C6

There are no ring outliers.

272 monomers are involved in 446 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	aA	803	CLA	1	0
13	bB	847	BCR	4	0
10	bA	824	CLA	3	0
14	cA	855	LHG	1	0
10	aA	813	CLA	1	0
10	cB	803	CLA	3	0
10	aA	812	CLA	4	0
10	cA	839	CLA	4	0
10	cA	809	CLA	1	0
10	aA	824	CLA	3	0
10	bA	814	CLA	1	0
9	cA	801	CL0	1	0
10	bB	811	CLA	2	0
10	bA	823	CLA	5	0
10	aB	808	CLA	3	0
10	aB	809	CLA	2	0
10	aA	837	CLA	3	0
16	cB	848	LMG	1	0
10	bA	813	CLA	1	0
10	cB	834	CLA	1	0
10	bL	203	CLA	1	0
13	bA	848	BCR	3	0
10	bA	817	CLA	1	0
10	cA	835	CLA	2	0
10	aA	841	CLA	2	0
10	bB	838	CLA	1	0
10	cB	839	CLA	1	0
10	bA	818	CLA	5	0
10	bB	803	CLA	3	0
10	aA	802	CLA	1	0
13	cA	849	BCR	2	0
10	bA	835	CLA	2	0
13	bL	207	BCR	2	0
13	cA	850	BCR	2	0
10	bB	839	CLA	2	0
10	cB	826	CLA	1	0
10	cB	813	CLA	3	0
10	cB	824	CLA	1	0
10	cB	801	CLA	1	0
10	bA	836	CLA	1	0
10	cB	815	CLA	1	0
10	cB	840	CLA	1	0
10	bA	833	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	cA	808	CLA	2	0
10	bA	854	CLA	1	0
11	aB	842	PQN	1	0
10	cB	832	CLA	2	0
10	aB	804	CLA	5	0
10	cB	820	CLA	2	0
10	cA	823	CLA	5	0
15	cA	853	LMT	1	0
10	aA	818	CLA	5	0
10	aB	839	CLA	2	0
10	bA	842	CLA	4	0
10	bA	826	CLA	1	0
10	aA	814	CLA	1	0
10	bA	828	CLA	2	0
10	bA	805	CLA	2	0
10	bB	813	CLA	3	0
10	bA	827	CLA	5	0
10	aA	806	CLA	1	0
10	bB	805	CLA	3	0
10	cA	804	CLA	4	0
10	bL	202	CLA	1	0
10	cB	810	CLA	3	0
10	cB	828	CLA	3	0
13	bA	849	BCR	1	0
10	bA	806	CLA	1	0
10	aA	804	CLA	4	0
10	aA	826	CLA	2	0
10	bB	841	CLA	1	0
10	aA	821	CLA	1	0
13	aA	849	BCR	1	0
10	aA	805	CLA	1	0
10	aB	837	CLA	2	0
10	aA	827	CLA	4	0
10	bB	802	CLA	2	0
10	aB	821	CLA	2	0
10	bB	828	CLA	1	0
13	bB	846	BCR	2	0
10	bB	829	CLA	4	0
10	cA	806	CLA	1	0
13	aL	207	BCR	1	0
11	bA	844	PQN	2	0
10	aB	824	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	aB	801	CLA	1	0
13	bI	102	BCR	2	0
10	aL	205	CLA	2	0
10	aA	808	CLA	2	0
10	cA	837	CLA	1	0
10	aB	815	CLA	2	0
10	bA	820	CLA	4	0
10	bB	817	CLA	2	0
10	aL	204	CLA	2	0
10	cB	825	CLA	4	0
13	aB	847	BCR	2	0
13	bA	850	BCR	3	0
10	bB	827	CLA	1	0
10	aA	819	CLA	2	0
13	aB	844	BCR	3	0
10	cA	819	CLA	2	0
10	bB	826	CLA	2	0
10	cA	833	CLA	1	0
10	bB	814	CLA	3	0
13	aB	843	BCR	7	0
10	bA	831	CLA	1	0
10	aB	822	CLA	1	0
10	cA	841	CLA	2	0
13	cL	206	BCR	3	0
10	bA	808	CLA	2	0
10	aB	814	CLA	3	0
10	bL	204	CLA	1	0
10	aB	803	CLA	4	0
10	bB	818	CLA	2	0
10	bB	810	CLA	3	0
10	cA	825	CLA	3	0
10	cA	813	CLA	1	0
13	cB	846	BCR	3	0
10	cB	830	CLA	2	0
13	aI	102	BCR	2	0
10	cB	817	CLA	3	0
14	aA	852	LHG	2	0
10	aA	831	CLA	2	0
10	cA	842	CLA	2	0
13	cA	848	BCR	2	0
10	bA	804	CLA	3	0
10	cA	831	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	cL	203	CLA	1	0
10	cA	814	CLA	1	0
9	bA	801	CL0	1	0
14	cA	852	LHG	1	0
10	aB	825	CLA	4	0
10	bB	808	CLA	3	0
10	bB	809	CLA	2	0
10	cB	804	CLA	5	0
13	aA	848	BCR	2	0
10	bA	840	CLA	2	0
10	cA	822	CLA	1	0
10	cL	204	CLA	2	0
10	bB	831	CLA	1	0
10	cA	818	CLA	4	0
10	cA	810	CLA	2	0
10	aA	823	CLA	3	0
13	cB	844	BCR	2	0
14	bA	855	LHG	1	0
9	aA	801	CL0	1	0
10	cA	802	CLA	1	0
13	cB	847	BCR	2	0
13	bM	101	BCR	2	0
10	cB	819	CLA	1	0
13	aB	849	BCR	3	0
13	cM	101	BCR	2	0
10	aB	805	CLA	4	0
10	bB	807	CLA	4	0
13	aL	206	BCR	1	0
10	aB	829	CLA	4	0
10	cA	812	CLA	4	0
10	aA	810	CLA	1	0
10	cA	840	CLA	2	0
10	bB	823	CLA	1	0
10	cB	814	CLA	4	0
10	aB	832	CLA	2	0
10	cB	823	CLA	1	0
10	bA	837	CLA	3	0
10	bA	812	CLA	4	0
10	cA	826	CLA	2	0
10	cB	802	CLA	1	0
10	cB	808	CLA	4	0
13	aI	101	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	aA	828	CLA	2	0
10	cL	205	CLA	2	0
10	aA	840	CLA	2	0
11	cA	844	PQN	2	0
16	bB	848	LMG	1	0
10	cA	805	CLA	2	0
10	cA	827	CLA	4	0
10	cA	820	CLA	4	0
10	bA	838	CLA	2	0
13	cI	102	BCR	3	0
10	bA	825	CLA	5	0
10	cB	841	CLA	2	0
13	bL	206	BCR	2	0
10	cB	812	CLA	2	0
11	aA	844	PQN	2	0
10	aB	810	CLA	3	0
10	bB	840	CLA	2	0
16	aB	848	LMG	1	0
10	aB	838	CLA	2	0
10	aB	830	CLA	2	0
10	aB	813	CLA	3	0
10	cL	202	CLA	1	0
13	bA	851	BCR	2	0
13	aM	101	BCR	2	0
13	bB	849	BCR	3	0
10	aB	827	CLA	1	0
13	cB	849	BCR	3	0
10	bB	812	CLA	2	0
10	aA	838	CLA	2	0
10	aA	825	CLA	5	0
10	bA	822	CLA	1	0
10	bB	801	CLA	1	0
10	bB	832	CLA	1	0
10	bB	820	CLA	4	0
13	bB	844	BCR	3	0
10	aB	807	CLA	3	0
10	bA	810	CLA	2	0
10	cB	818	CLA	2	0
10	bB	819	CLA	1	0
13	cB	843	BCR	6	0
10	bA	802	CLA	1	0
10	bB	837	CLA	1	0

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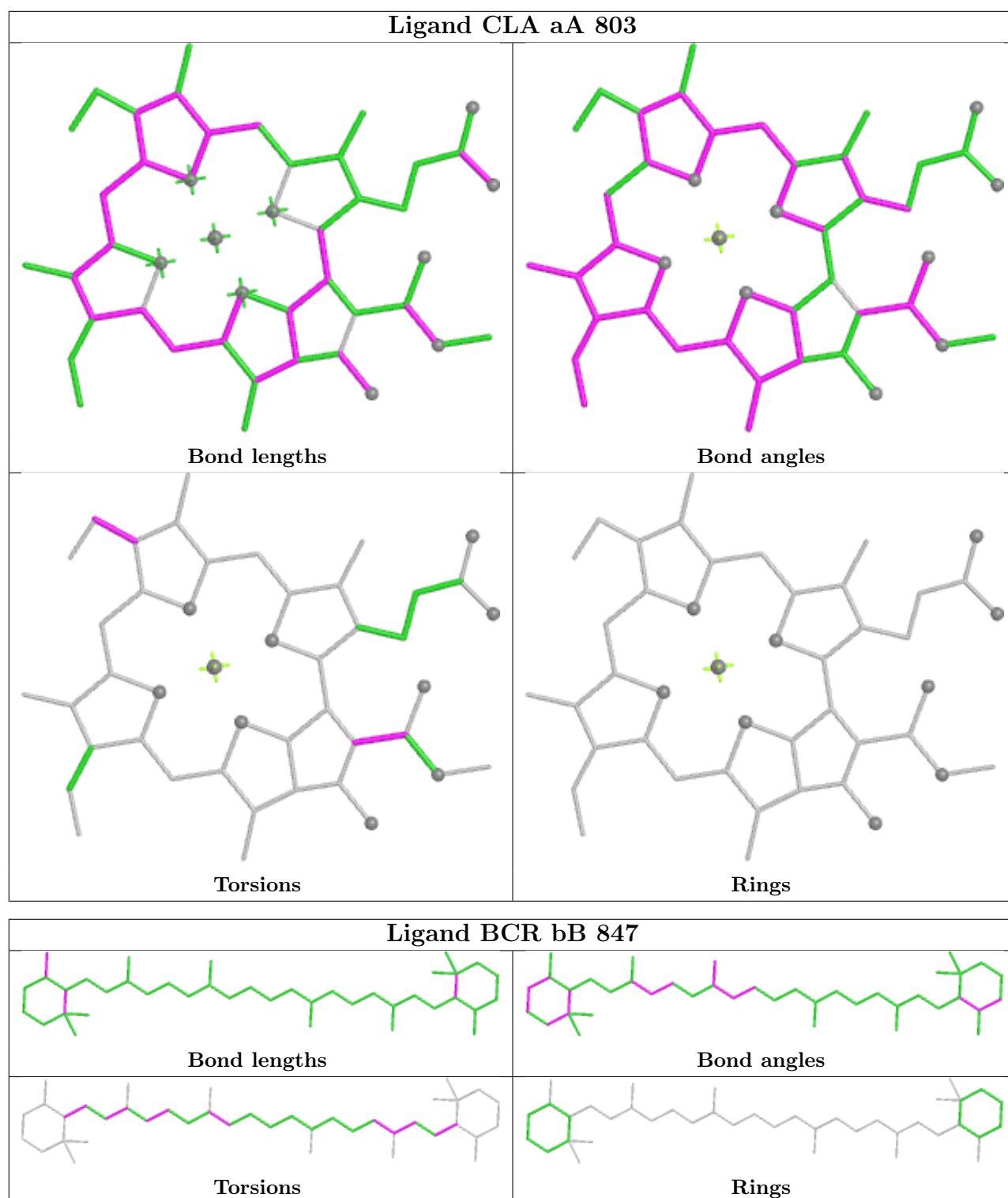
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	aB	823	CLA	1	0
10	cB	822	CLA	1	0
10	aB	802	CLA	1	0
10	cA	836	CLA	1	0
10	cB	829	CLA	4	0
13	cB	845	BCR	1	0
10	bB	830	CLA	2	0
13	aA	850	BCR	3	0
14	bA	852	LHG	1	0
10	aB	828	CLA	2	0
13	bA	847	BCR	2	0
10	bB	824	CLA	1	0
10	cA	838	CLA	2	0
10	cB	805	CLA	3	0
10	aA	822	CLA	1	0
10	bB	815	CLA	2	0
15	aA	853	LMT	1	0
10	aA	842	CLA	1	0
13	bB	843	BCR	6	0
10	cB	821	CLA	2	0
10	aB	817	CLA	3	0
10	aB	841	CLA	2	0
10	cB	837	CLA	2	0
10	aA	807	CLA	1	0
10	bA	839	CLA	4	0
13	cI	103	BCR	2	0
10	aL	202	CLA	1	0
10	cA	828	CLA	2	0
13	cA	847	BCR	2	0
13	bI	101	BCR	2	0
10	aA	817	CLA	1	0
10	aA	839	CLA	4	0
10	cB	827	CLA	1	0
10	aB	826	CLA	1	0
10	aA	820	CLA	4	0
10	bB	822	CLA	1	0
13	aA	847	BCR	3	0
10	aA	833	CLA	1	0
10	bB	821	CLA	2	0
10	aA	835	CLA	2	0
10	cA	824	CLA	3	0
10	aB	840	CLA	2	0

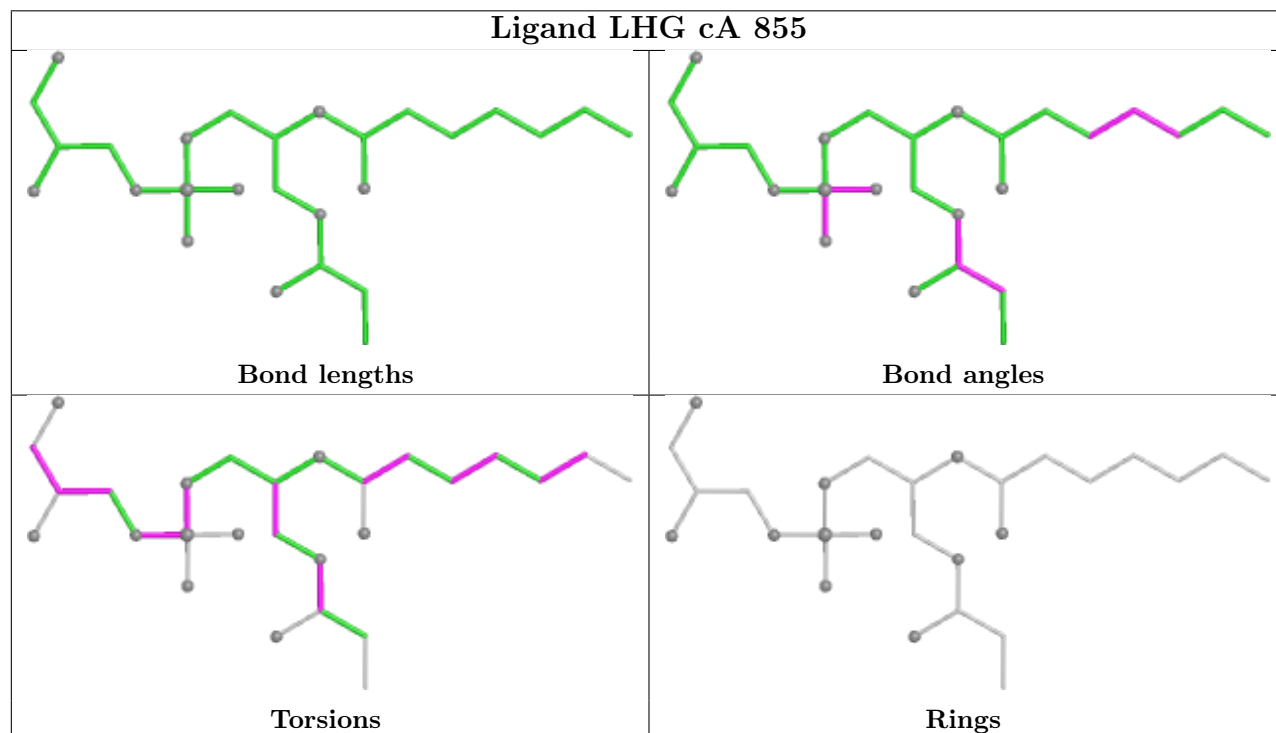
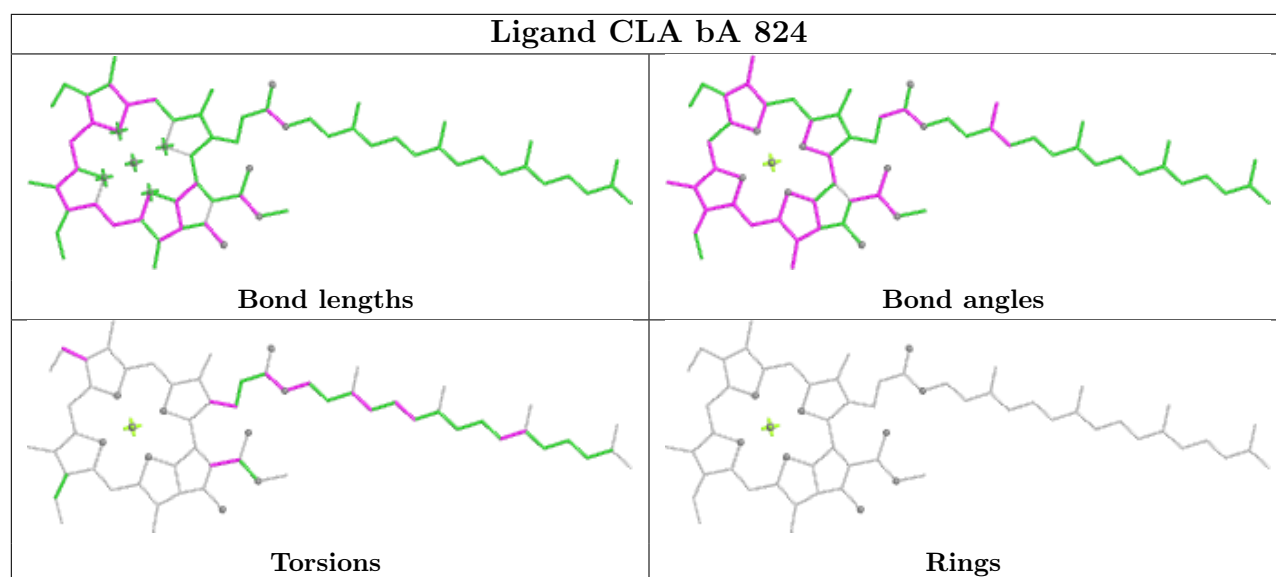
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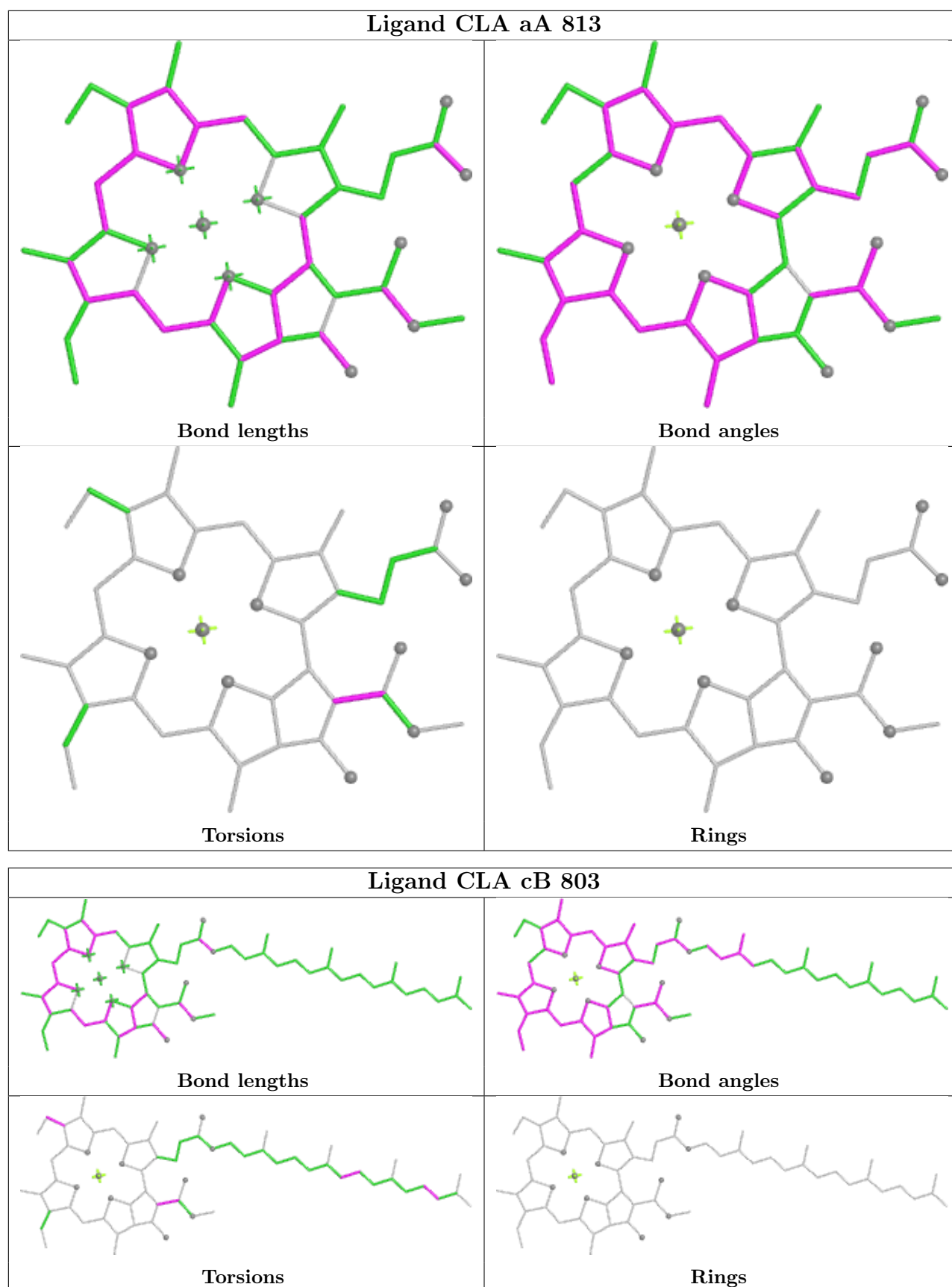
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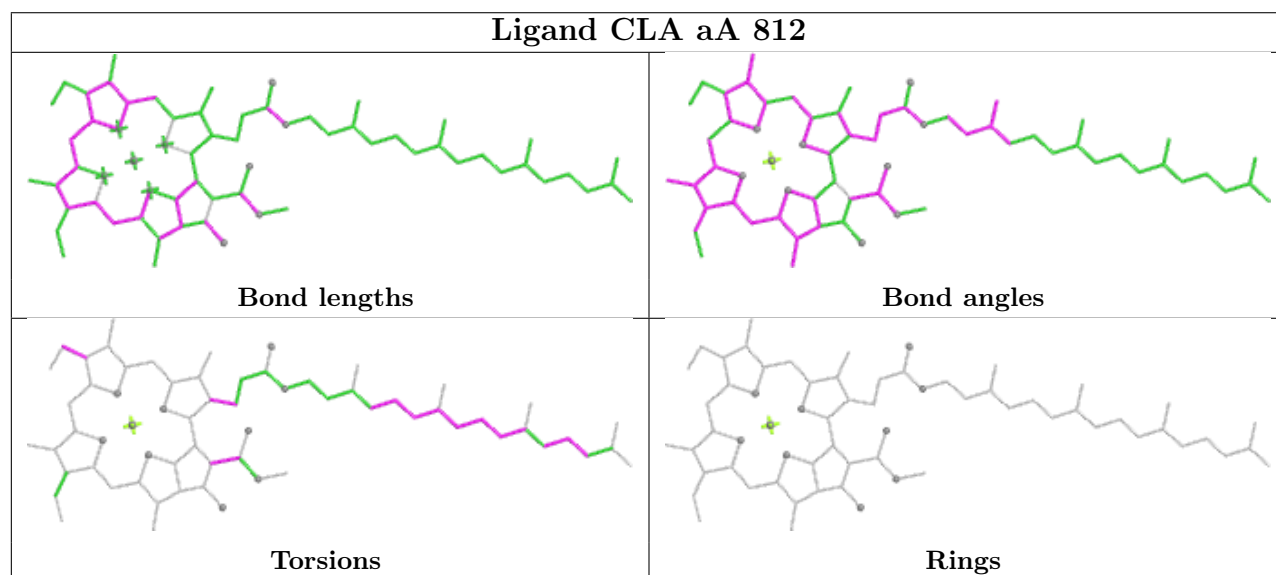
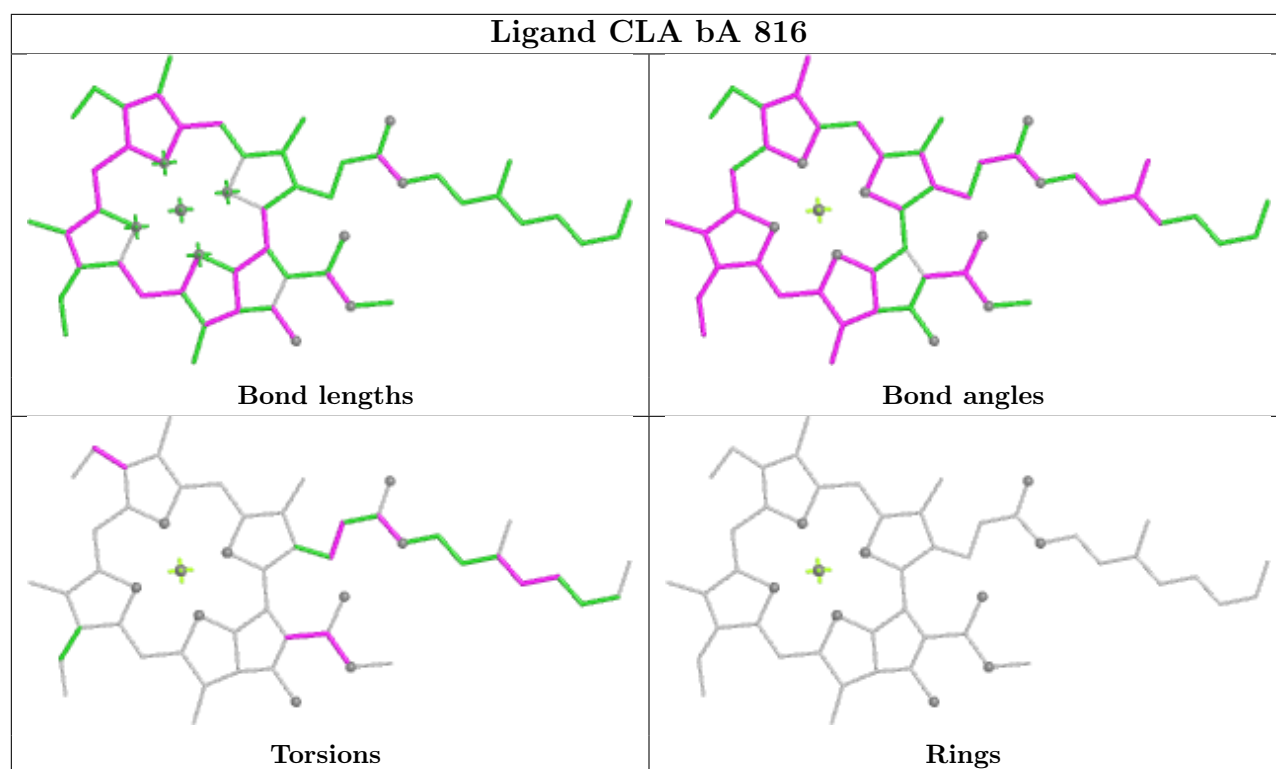
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	bB	804	CLA	4	0
10	cB	809	CLA	3	0
10	bB	834	CLA	1	0
13	aA	851	BCR	3	0
15	bA	853	LMT	1	0
13	aB	846	BCR	2	0
10	aB	818	CLA	1	0
10	aB	820	CLA	3	0
10	aL	203	CLA	1	0
10	bB	825	CLA	4	0
13	cA	851	BCR	3	0
10	cB	807	CLA	4	0
10	cA	817	CLA	1	0
13	aB	845	BCR	1	0
10	aA	836	CLA	1	0
10	bA	841	CLA	3	0
10	bA	819	CLA	1	0
10	aB	812	CLA	2	0
13	cA	846	BCR	1	0

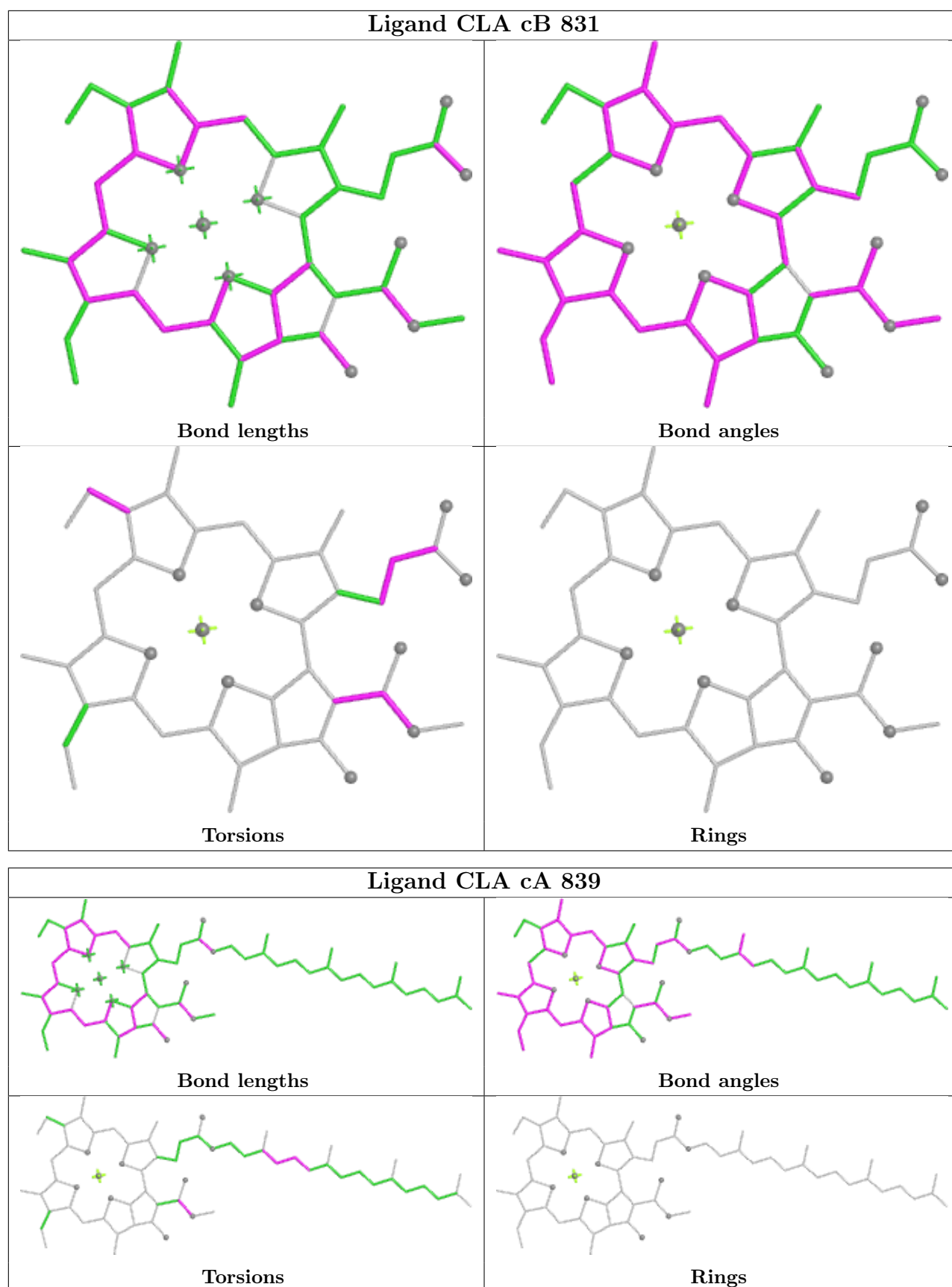
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

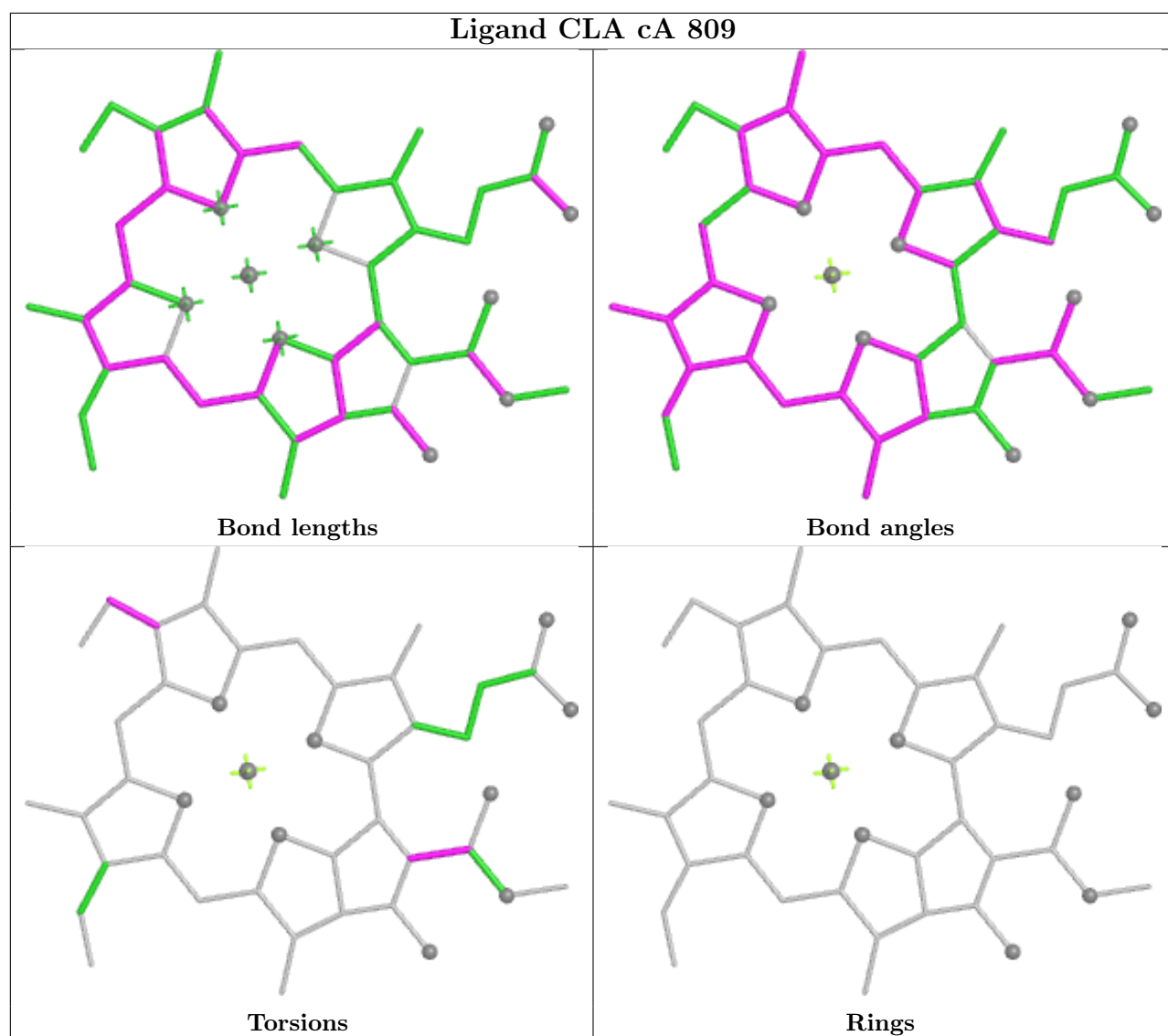


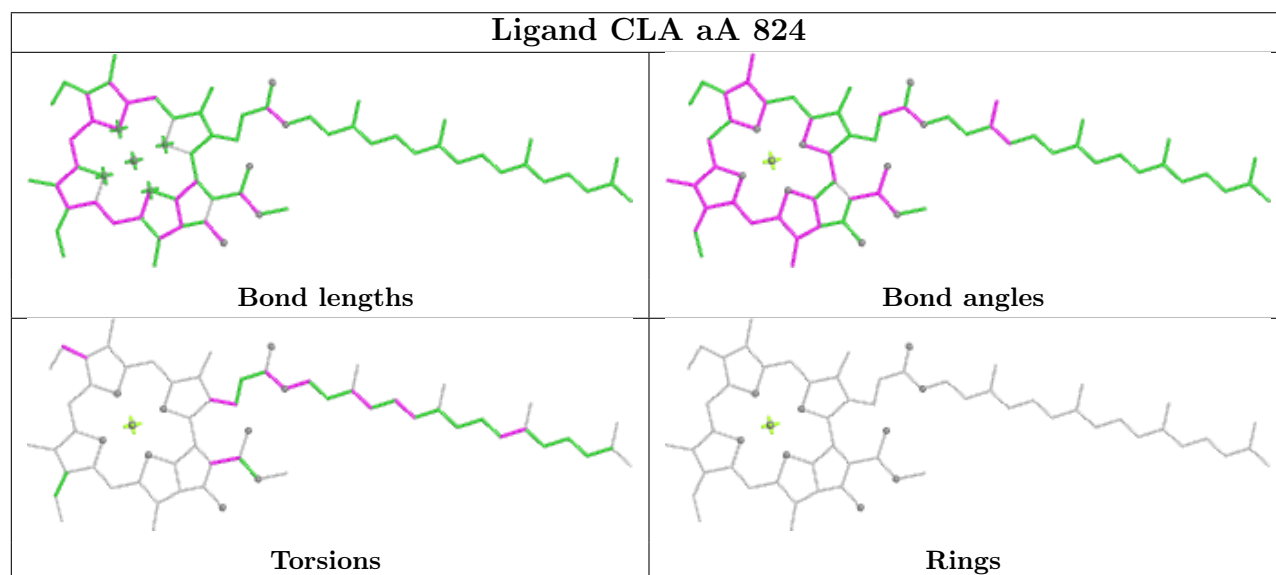
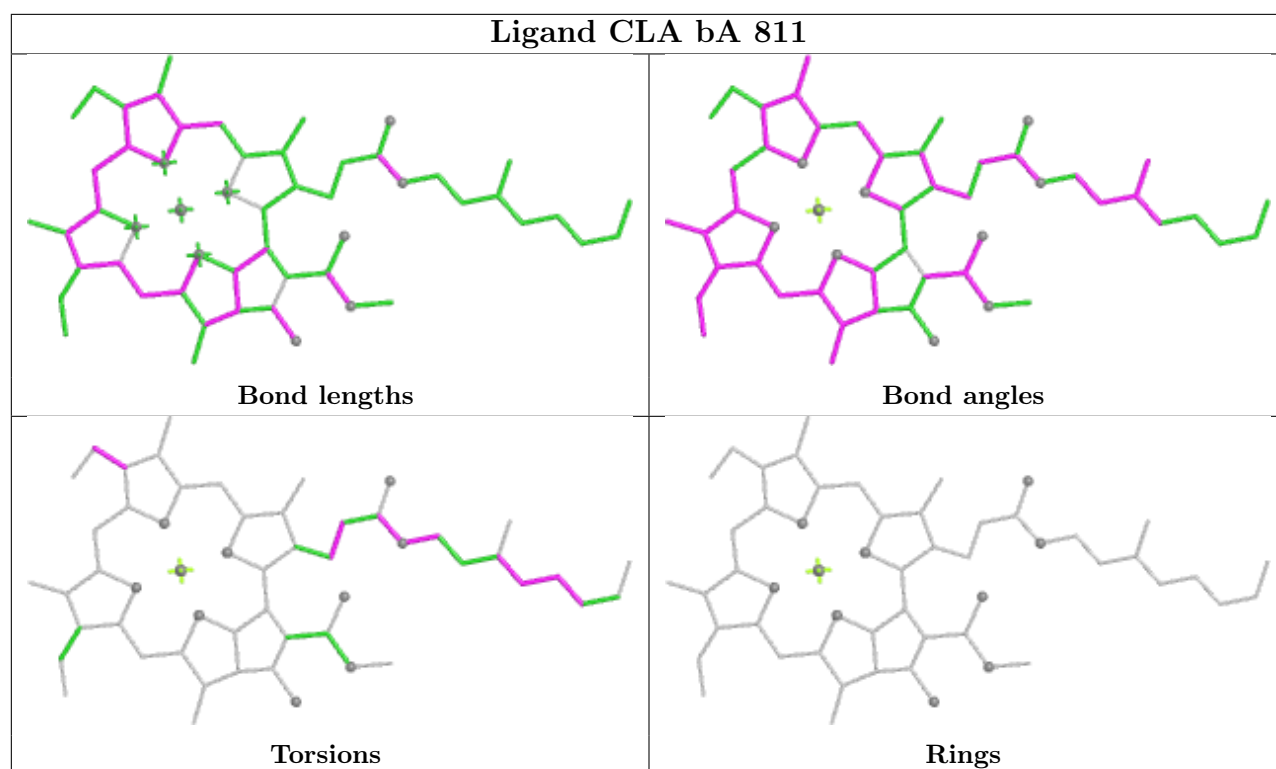




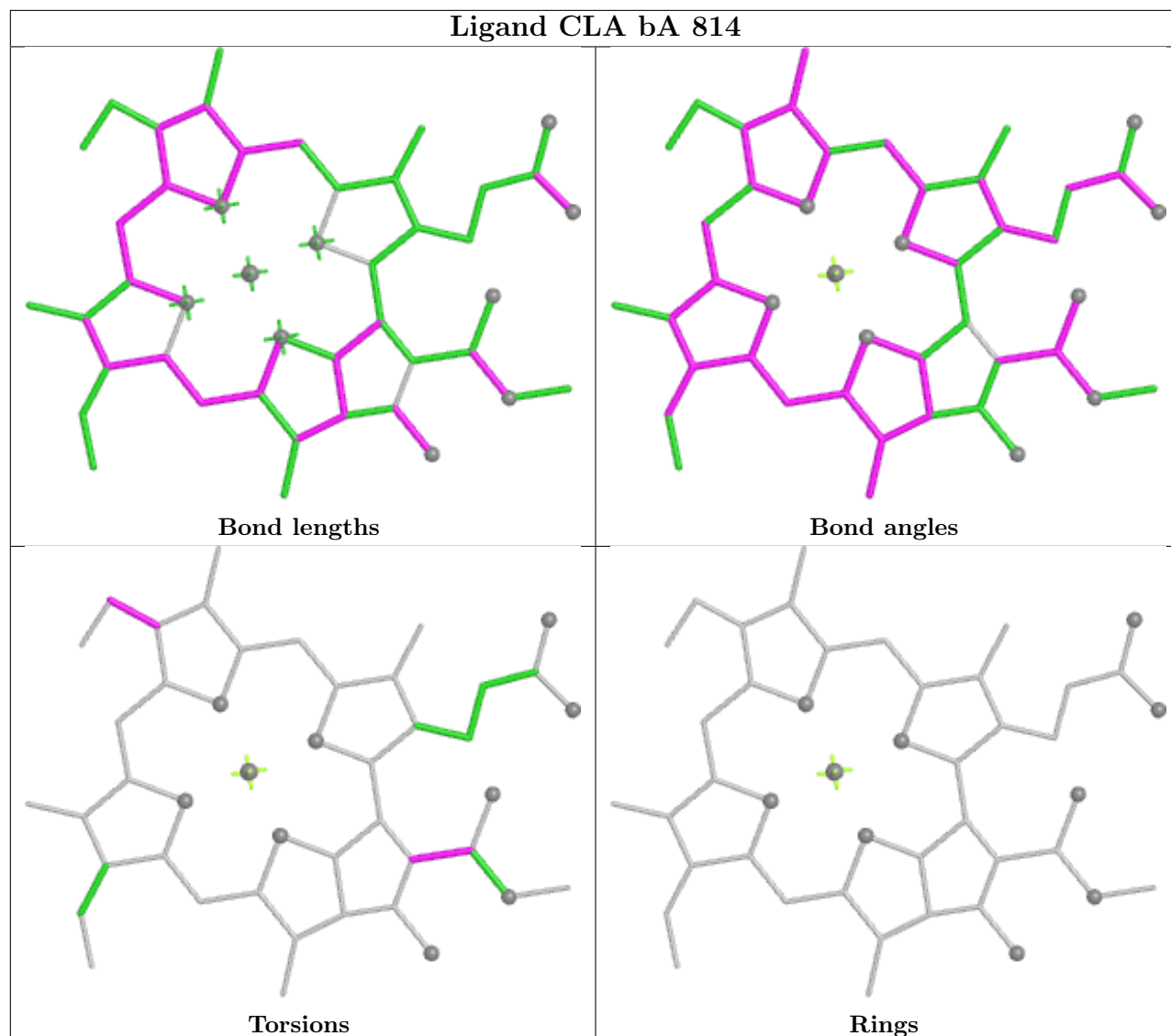




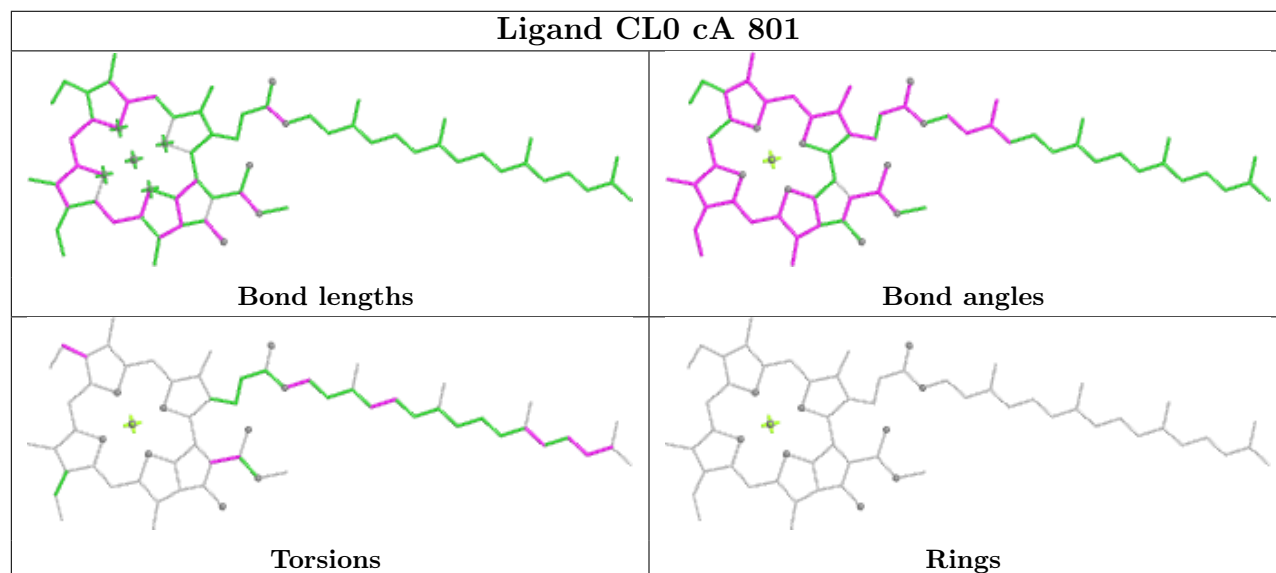


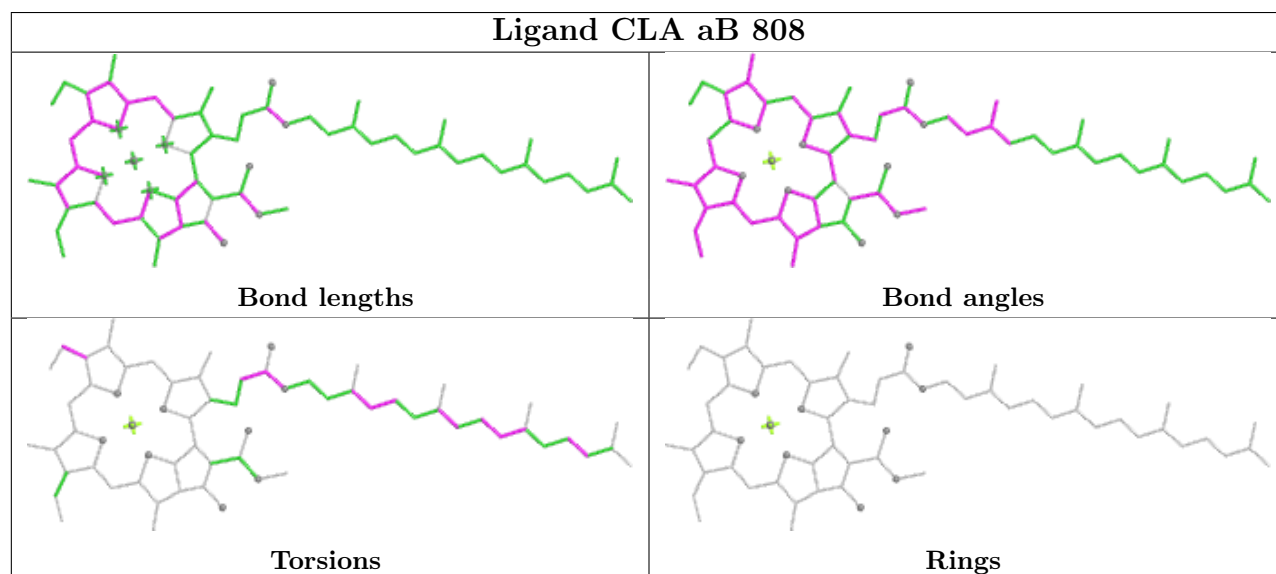
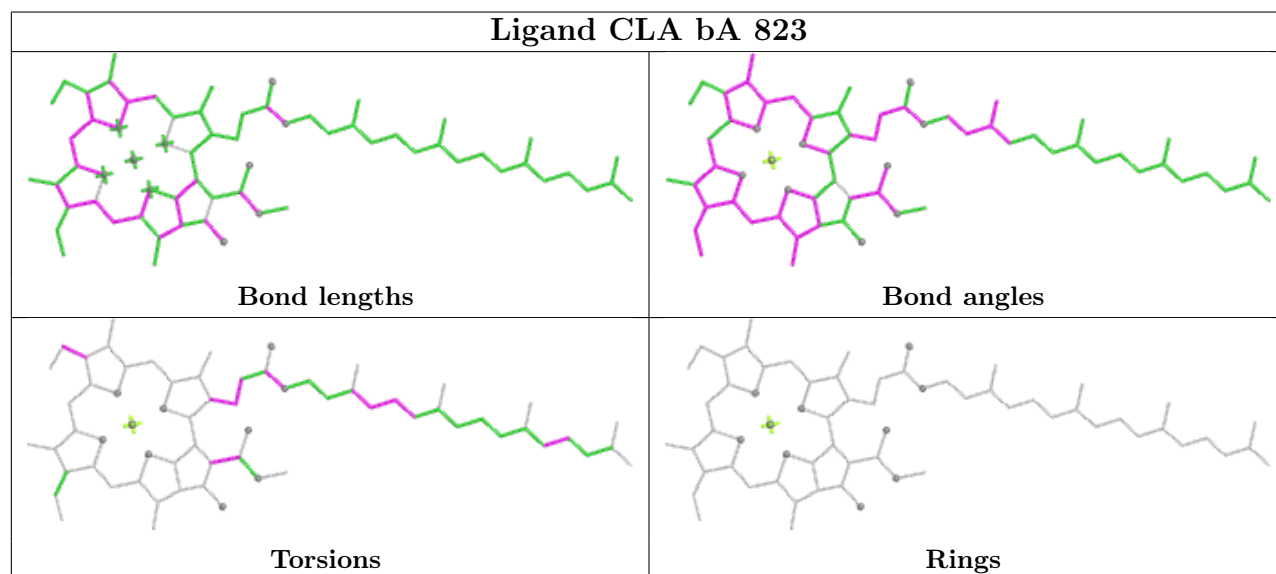
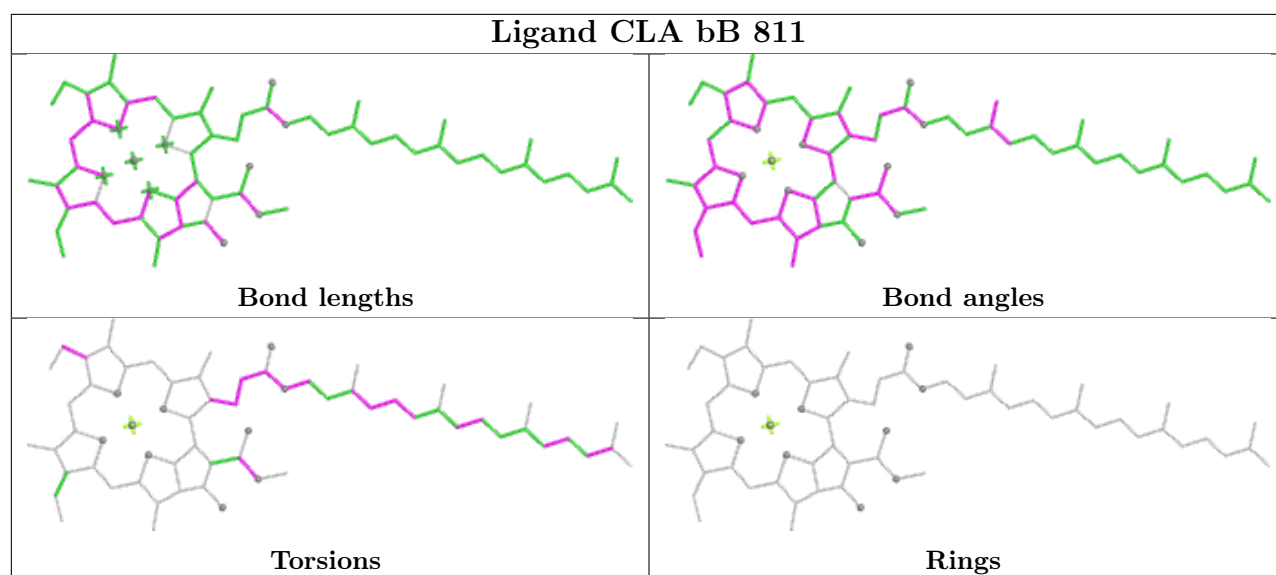


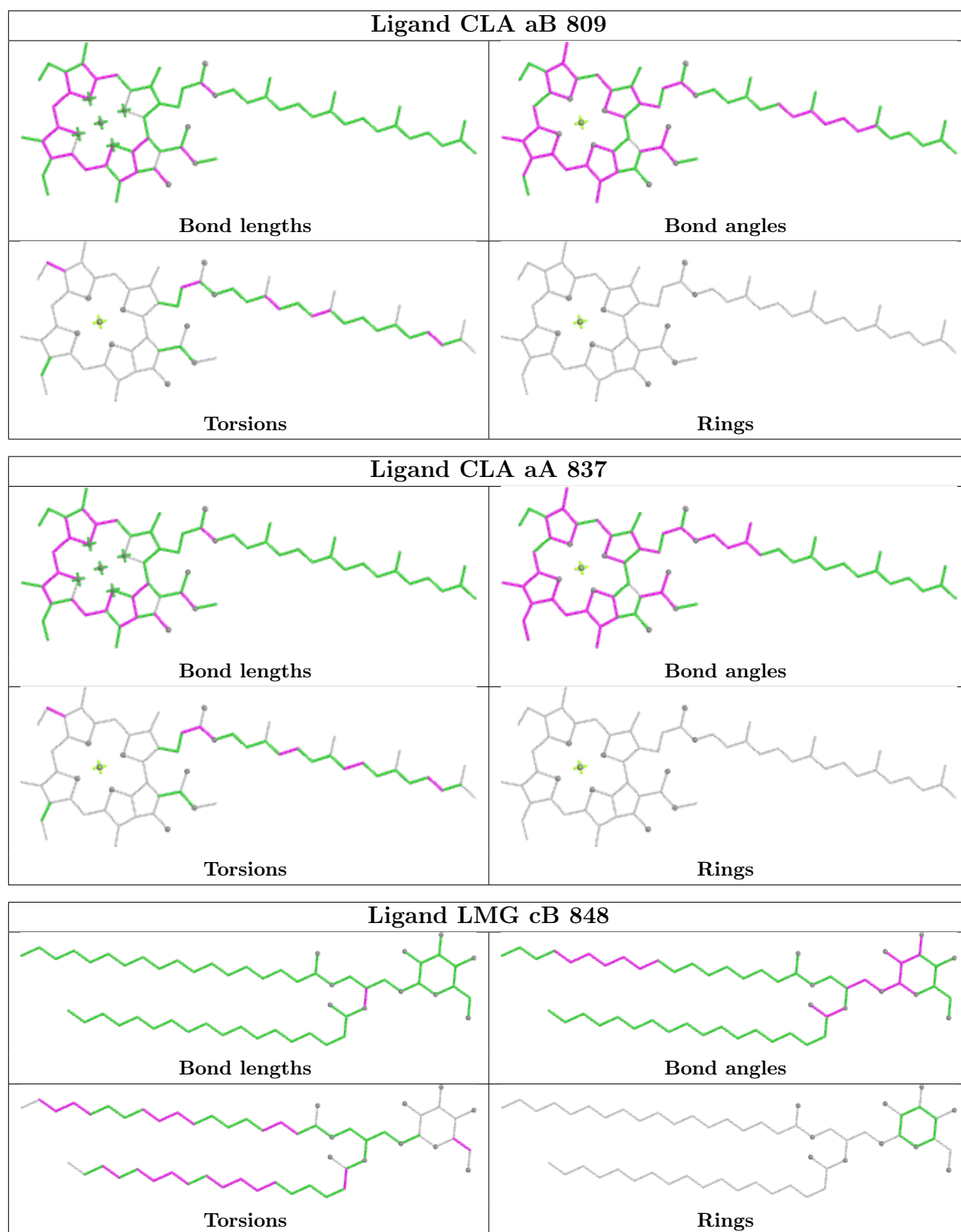
Ligand CLA bA 814

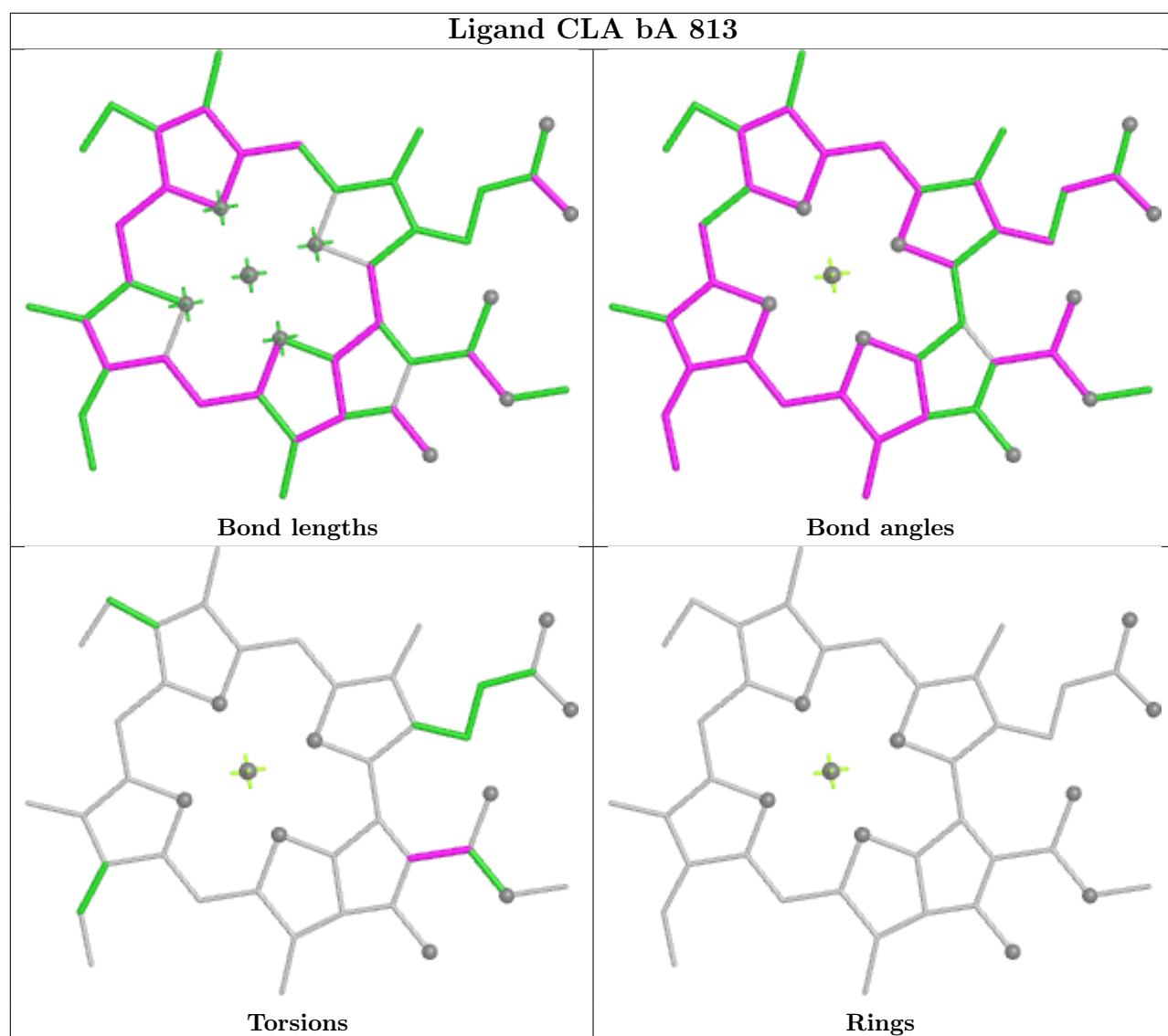


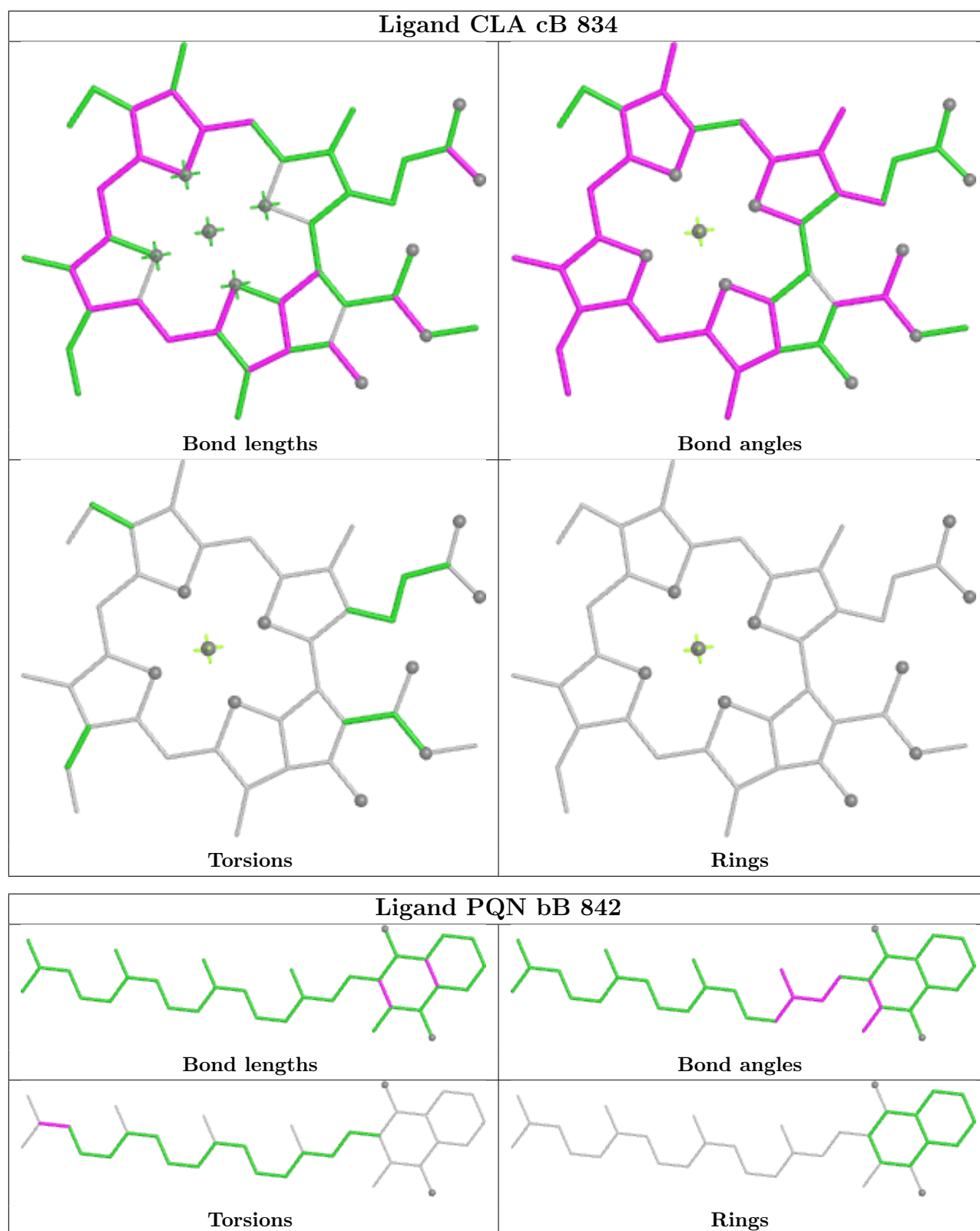
Ligand CL0 cA 801

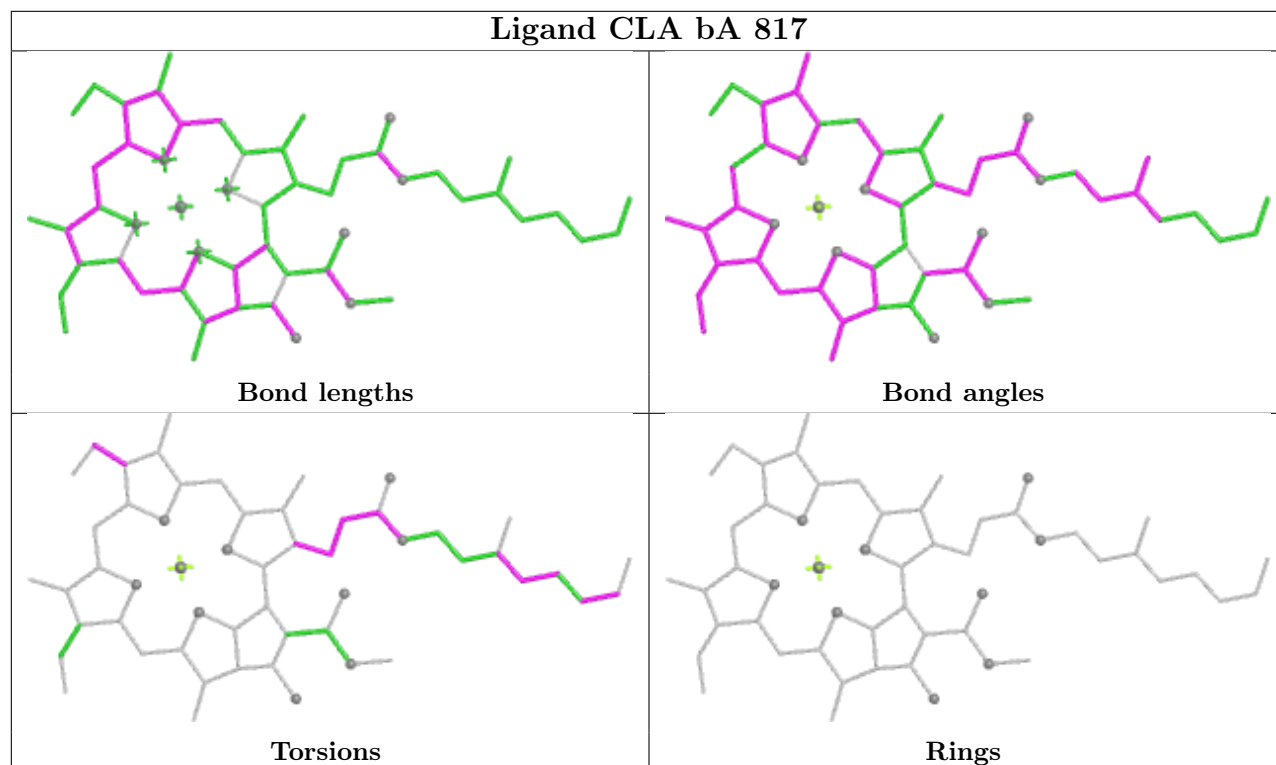
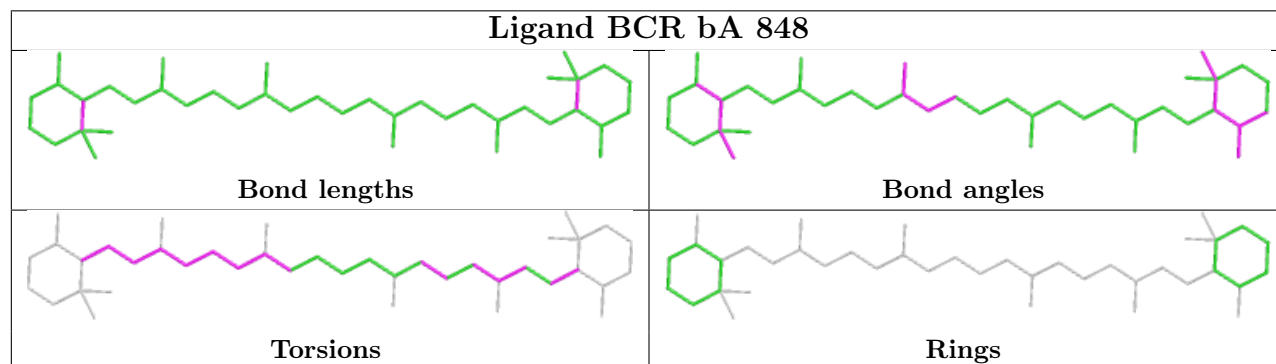
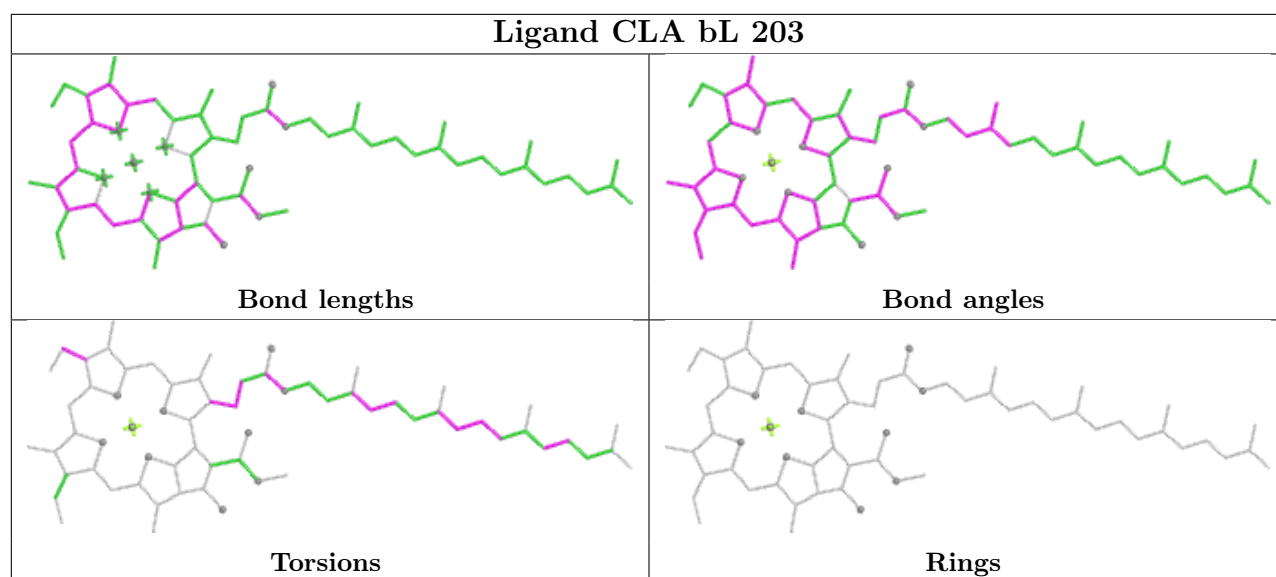


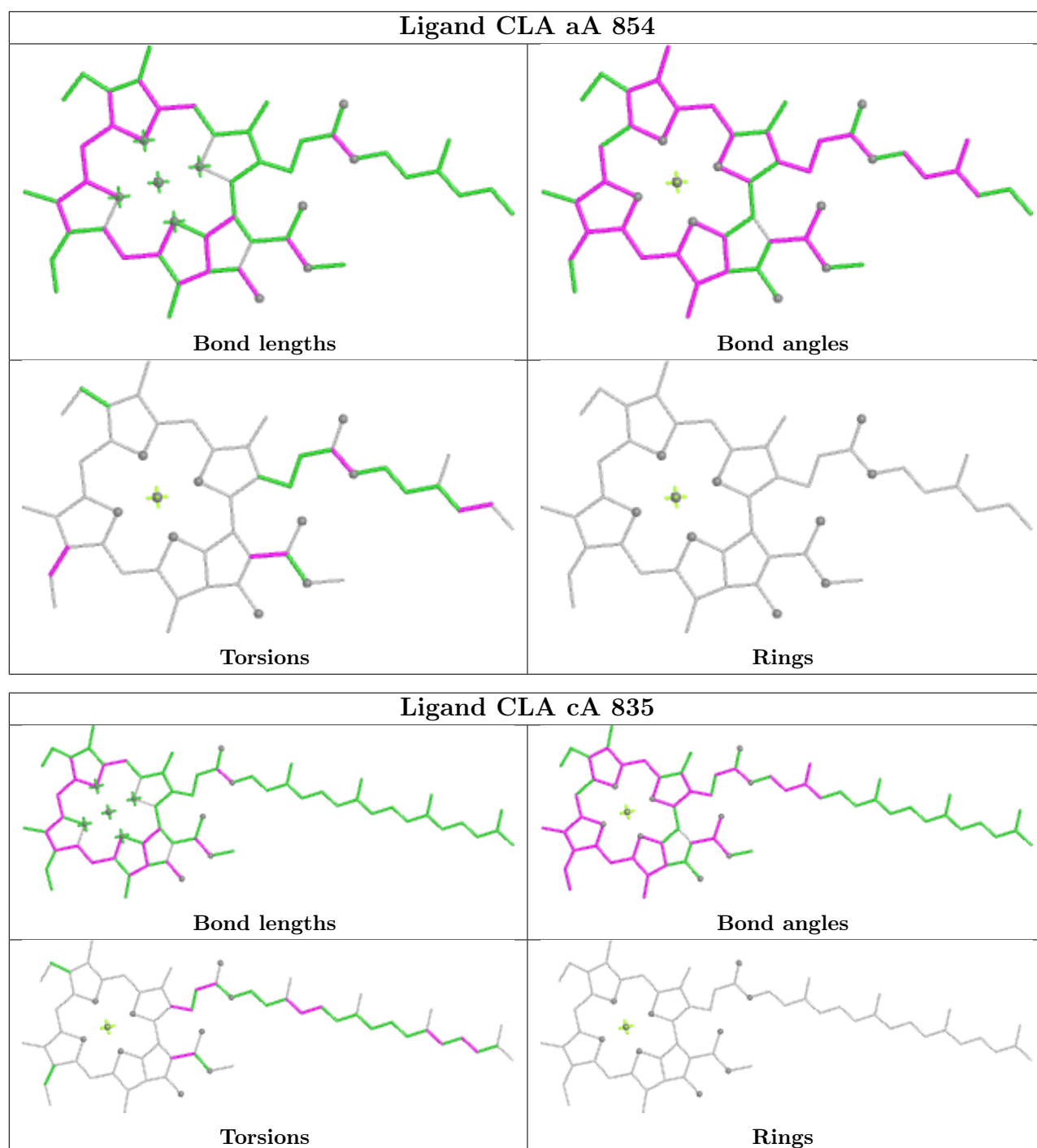


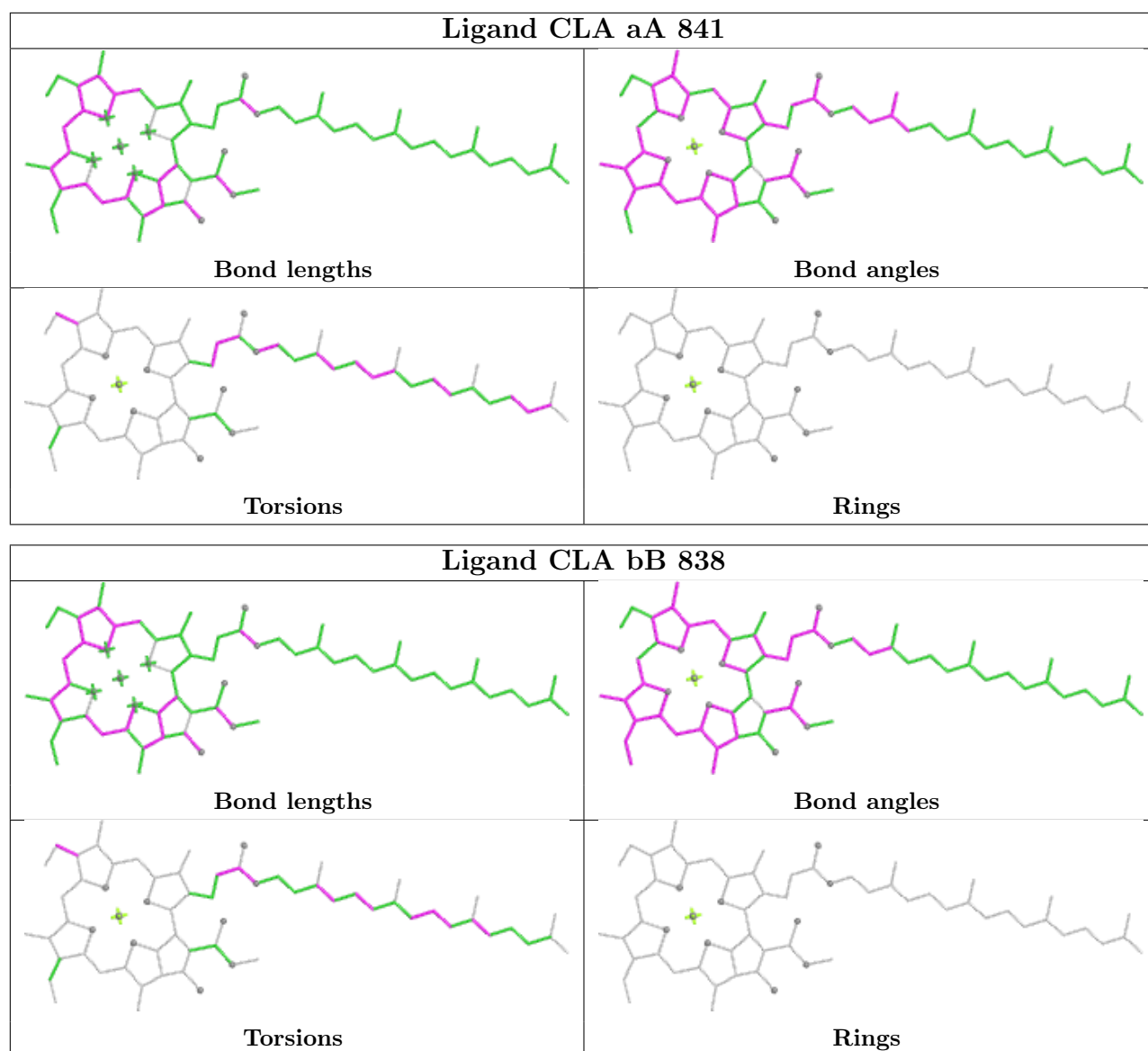




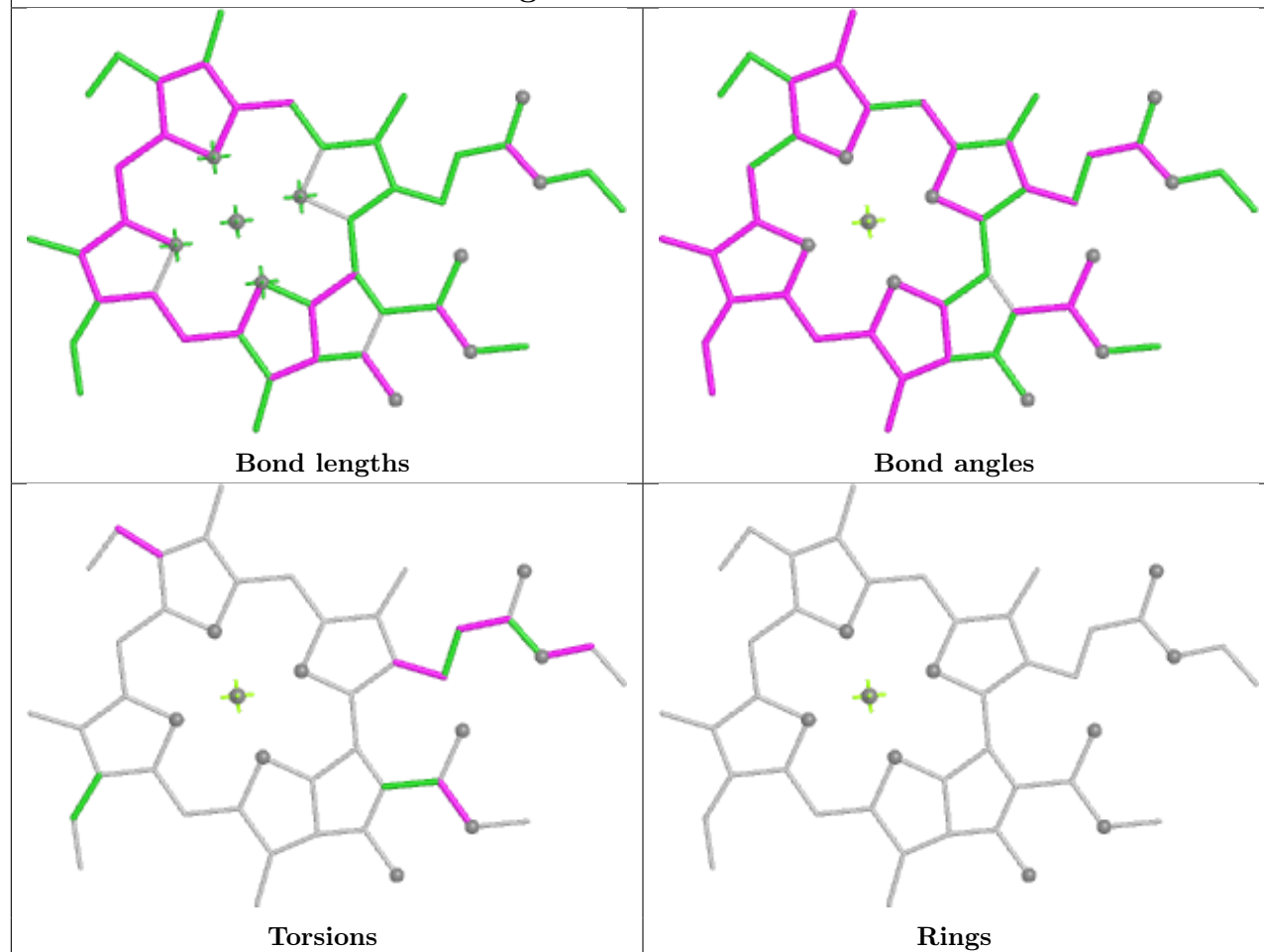




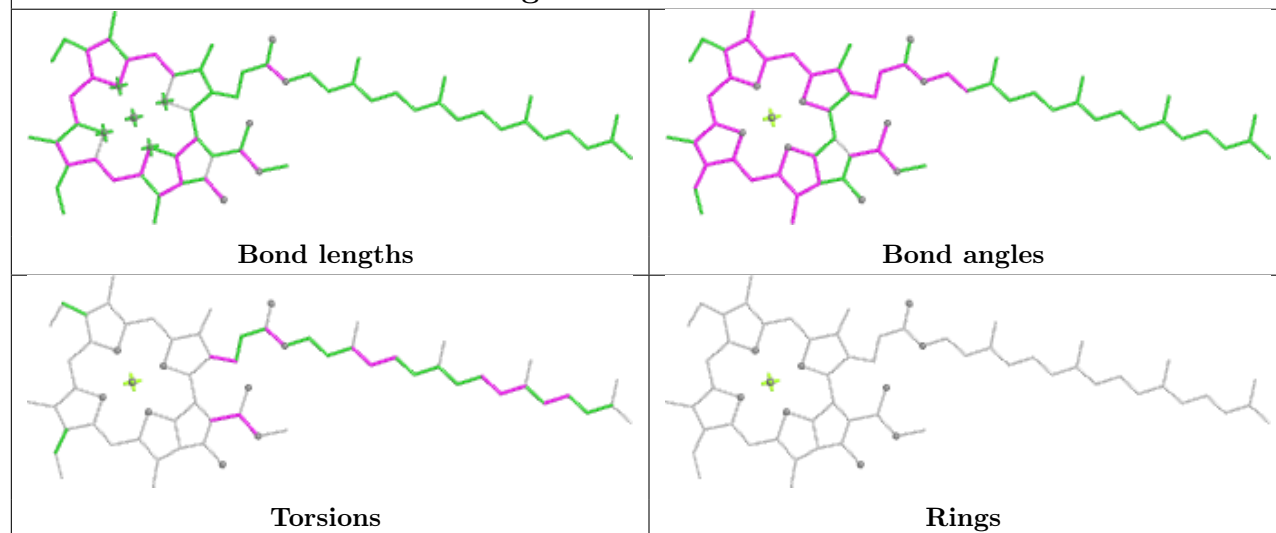


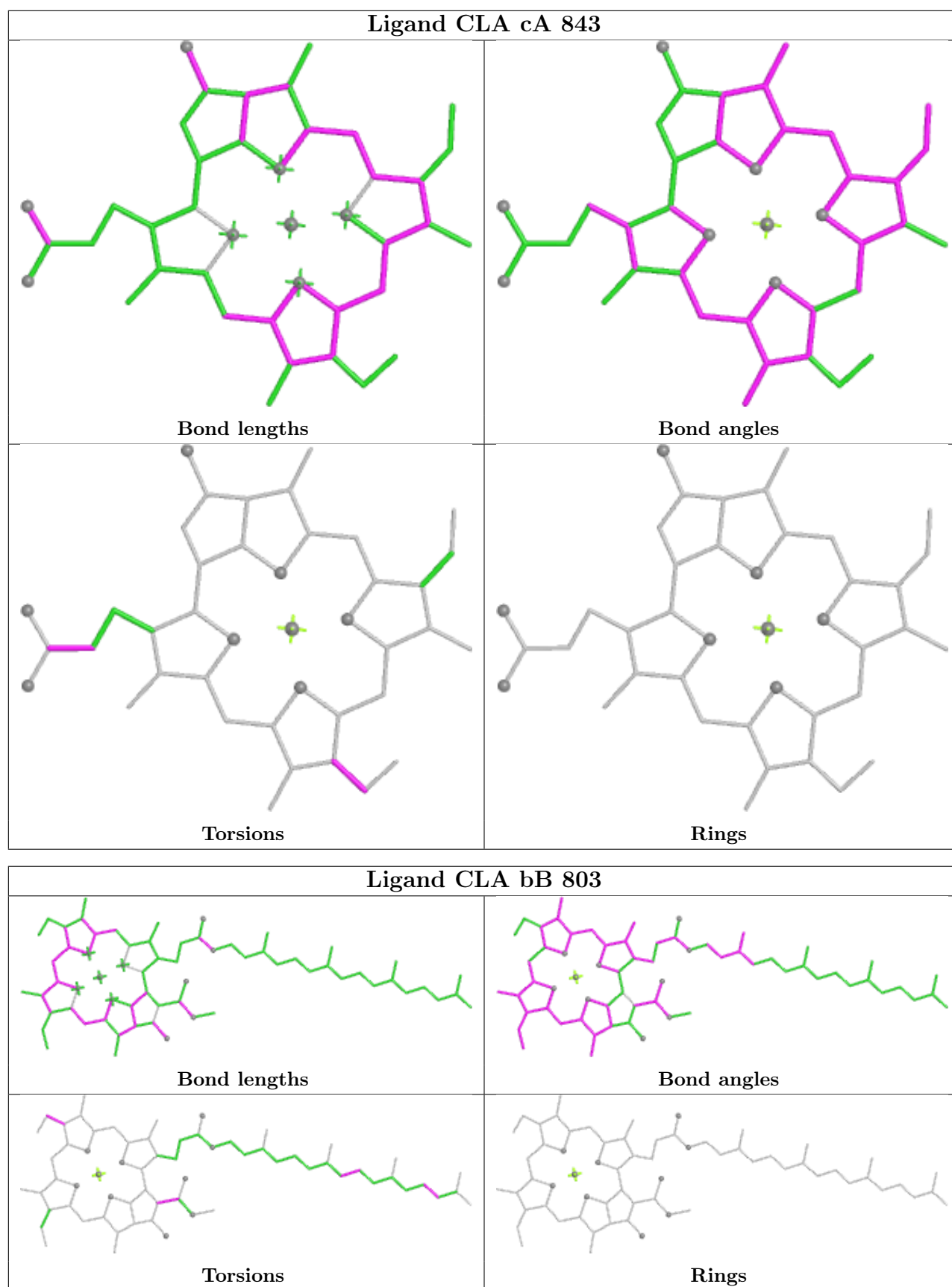


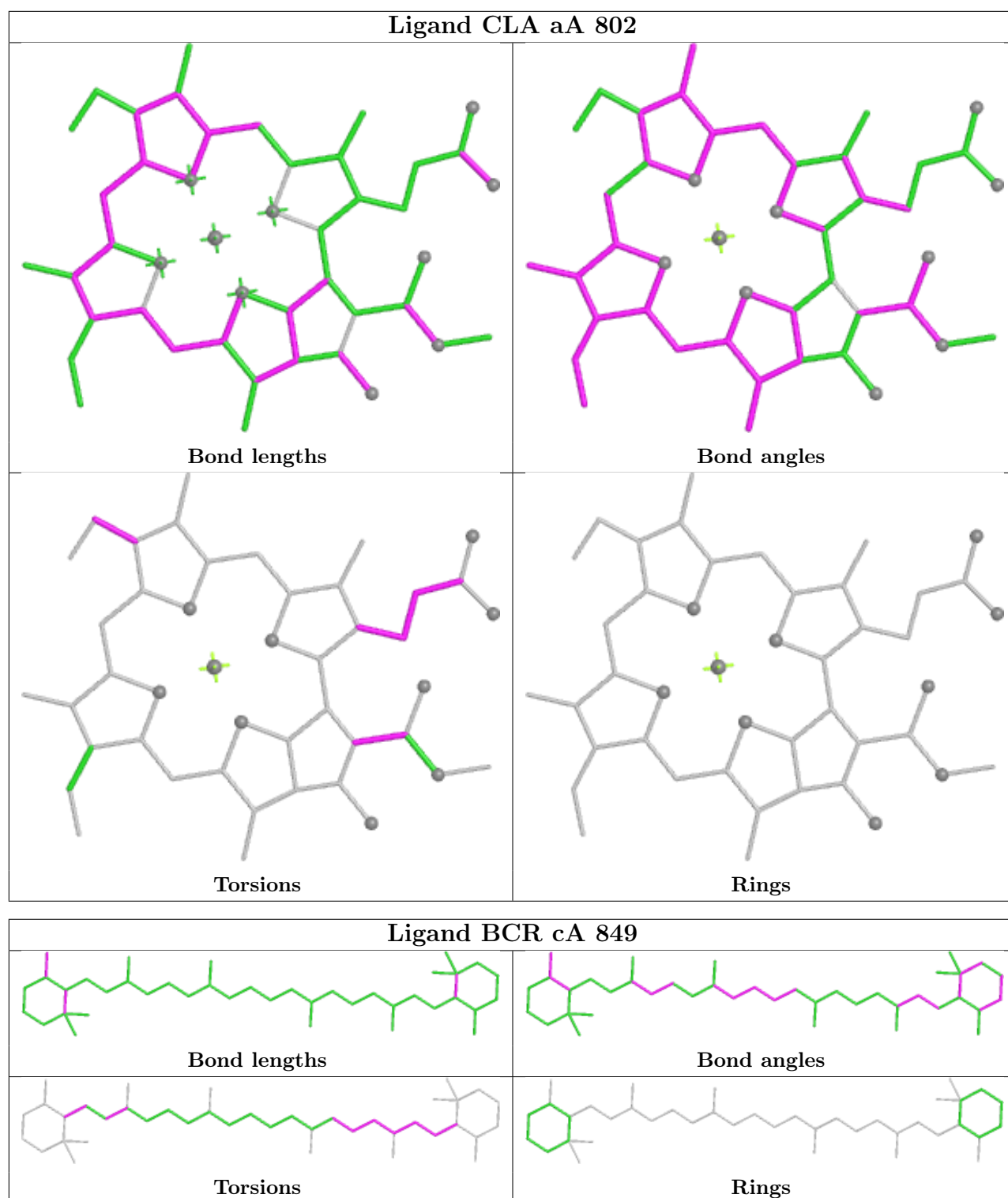
Ligand CLA cB 839

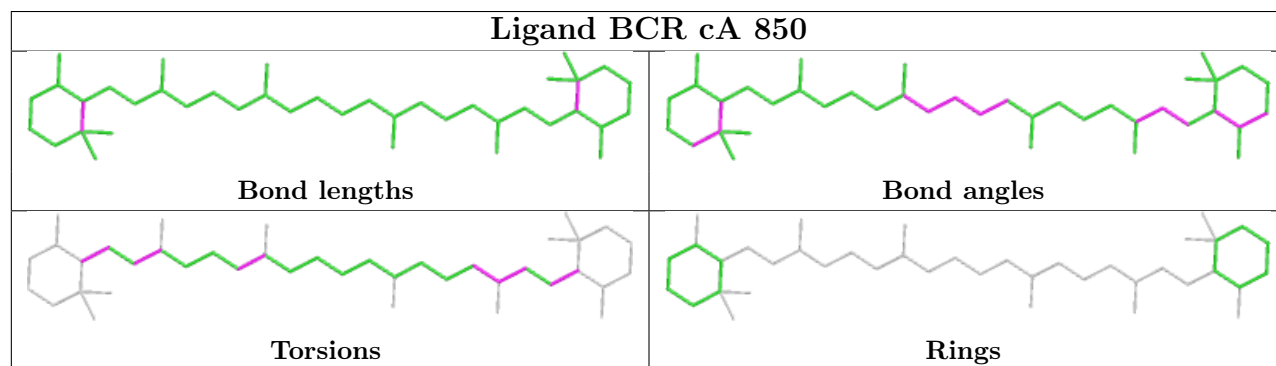
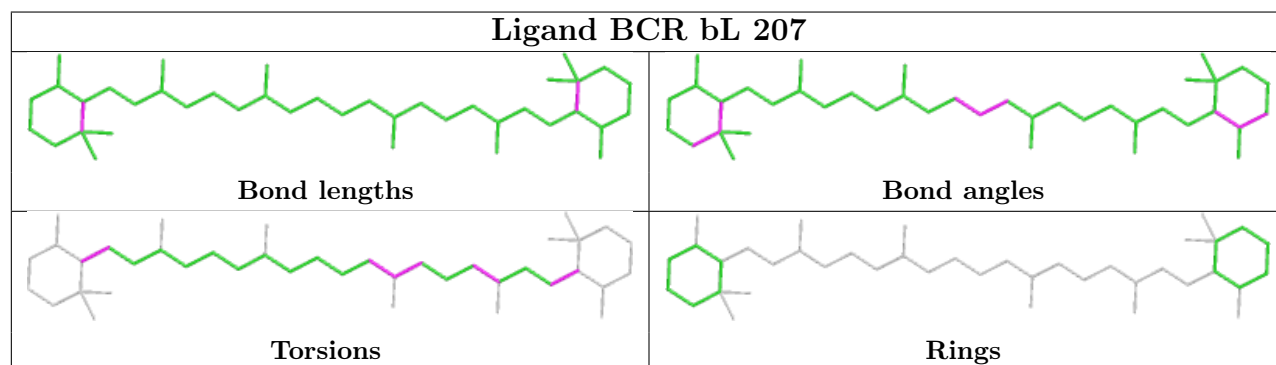
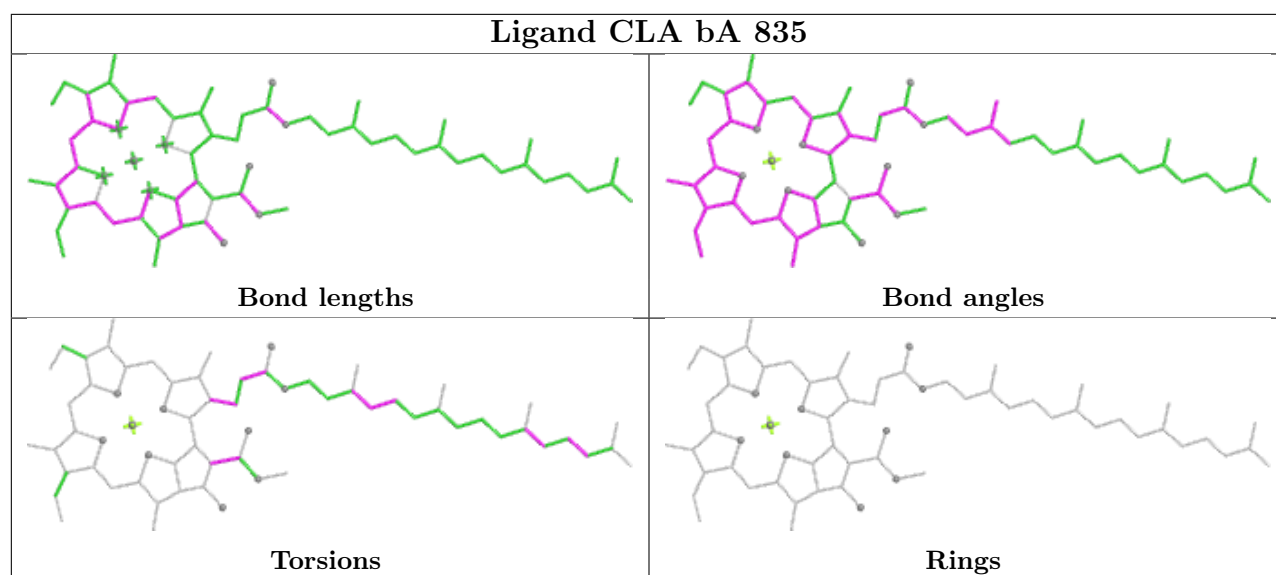


Ligand CLA bA 818

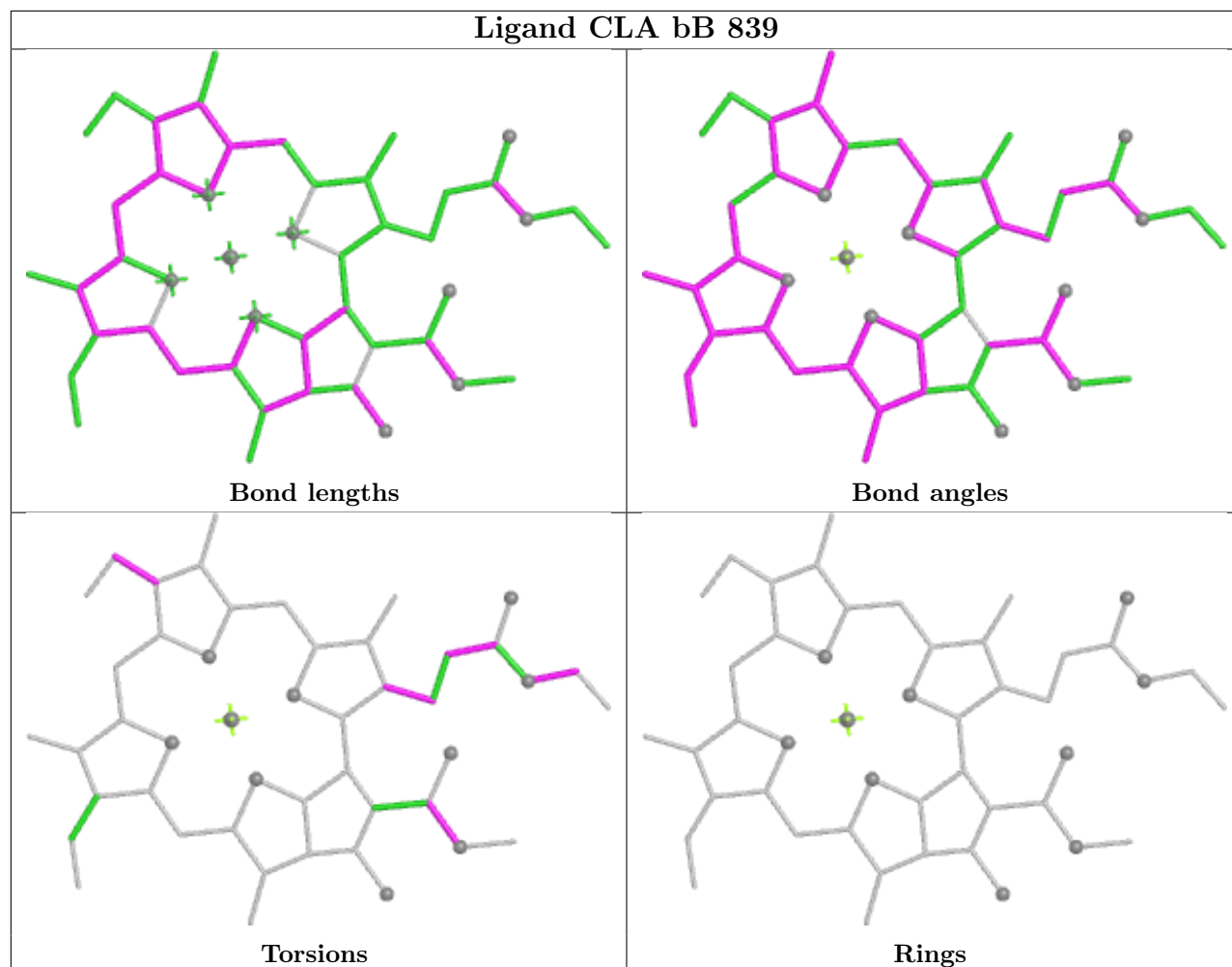




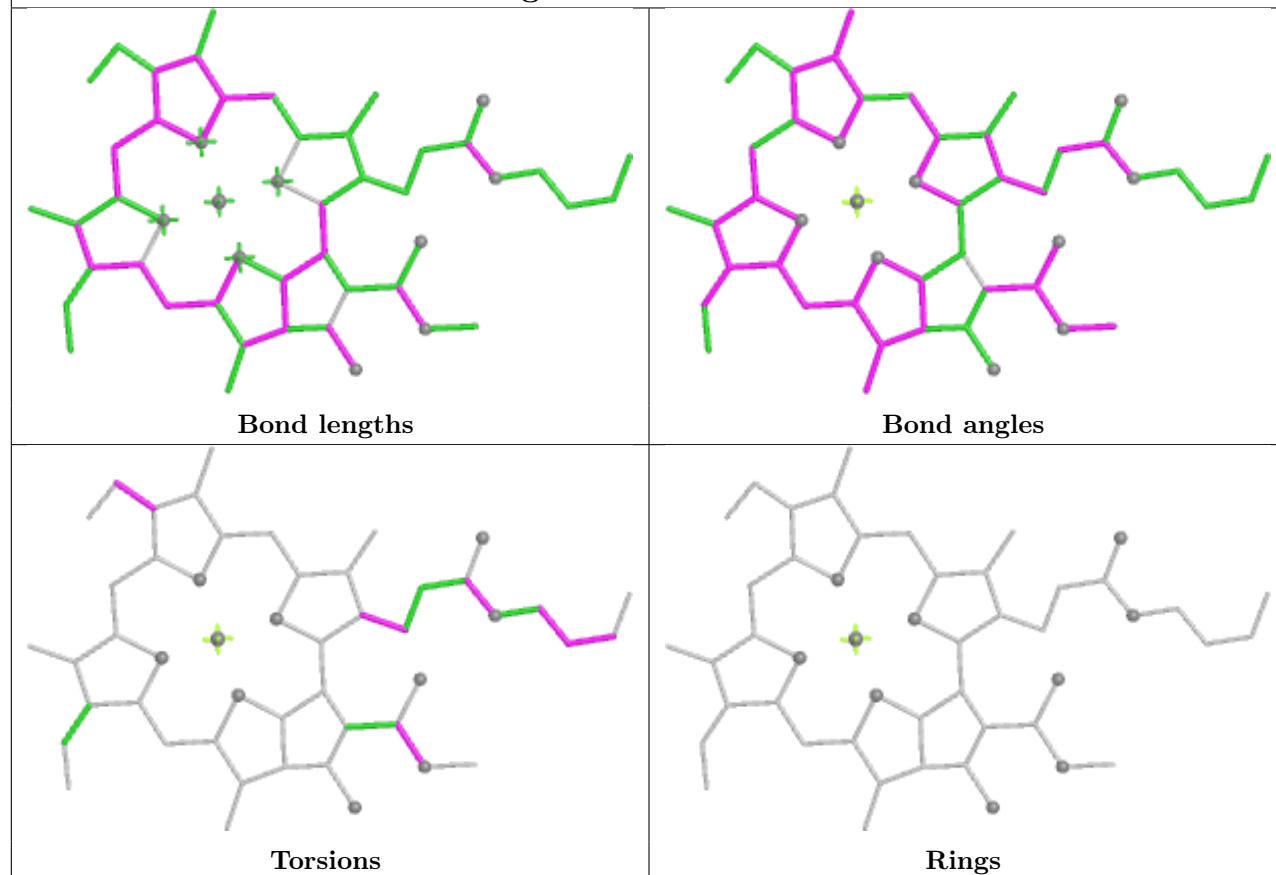




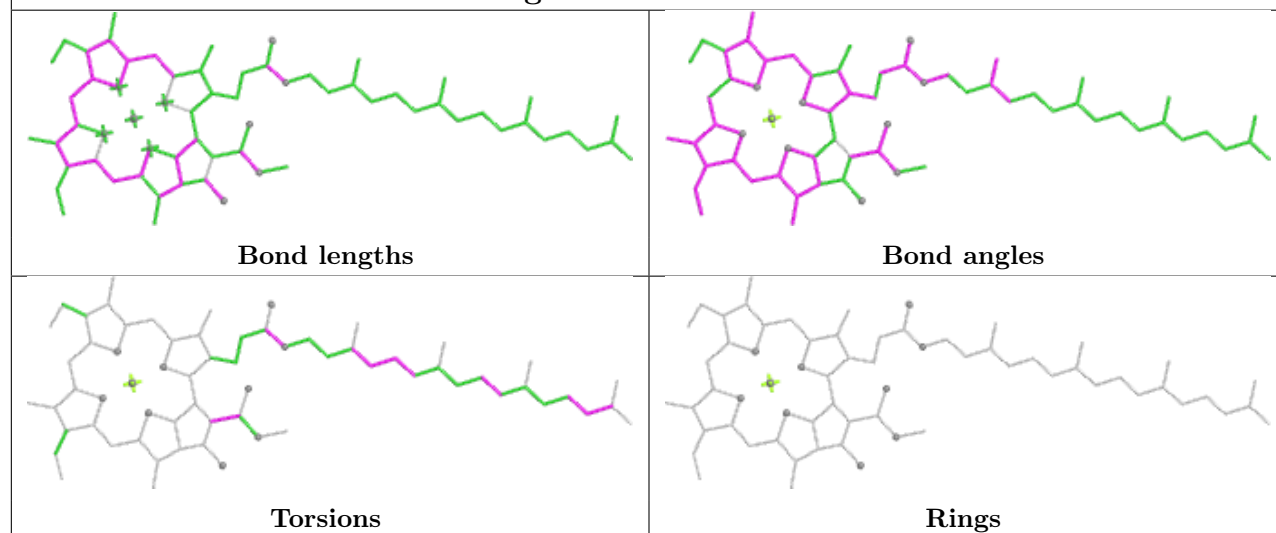
Ligand CLA bB 839

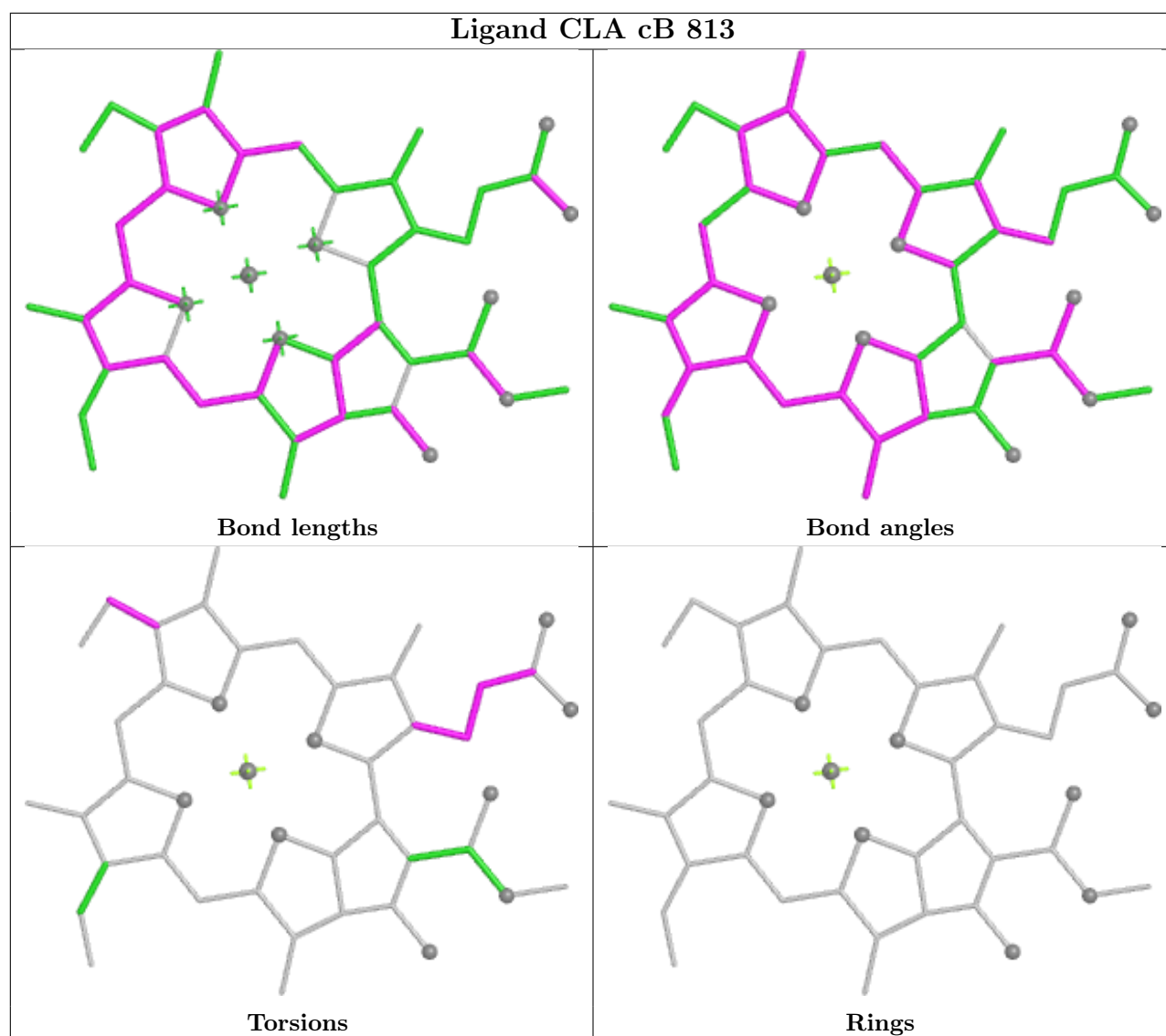


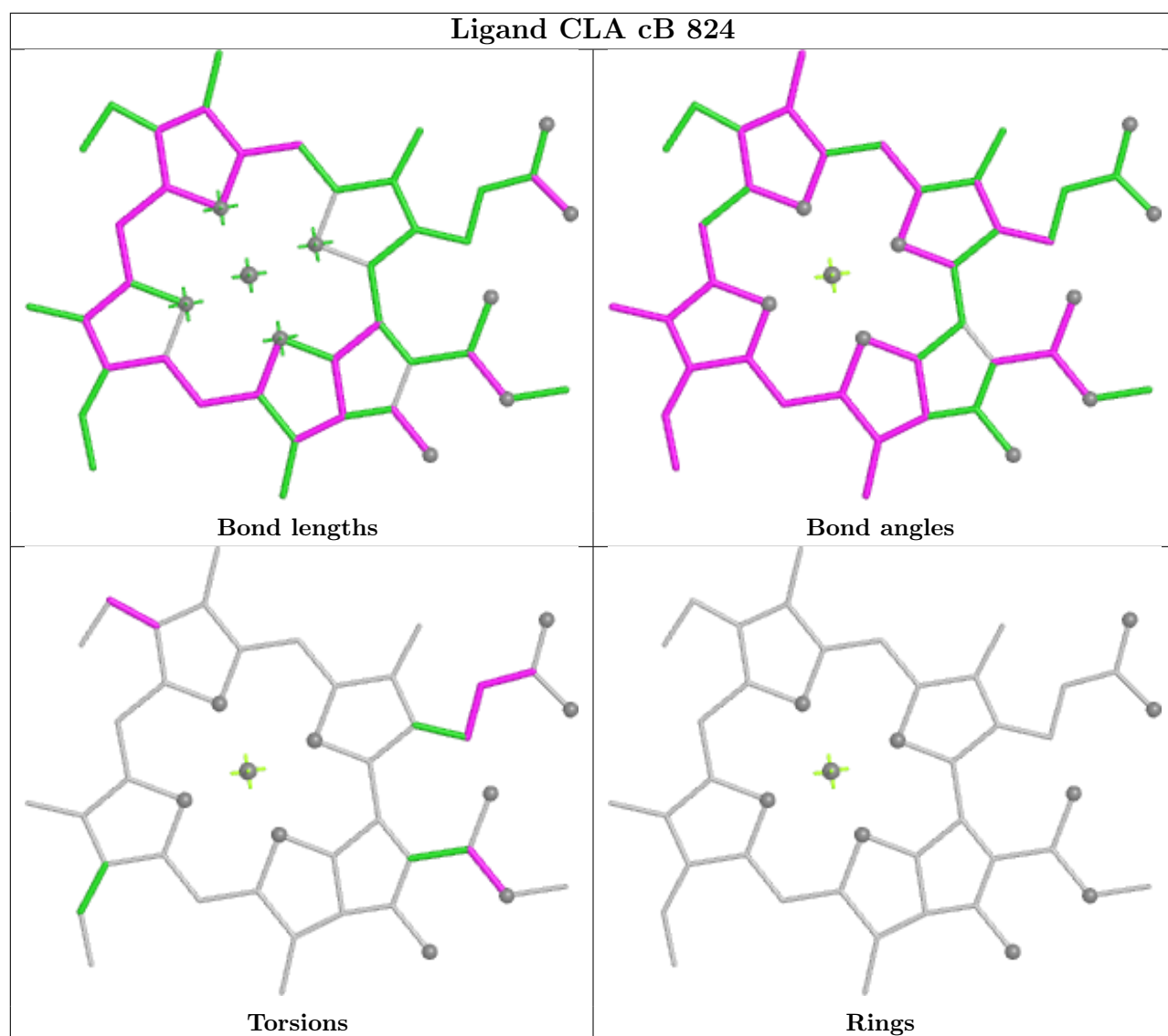
Ligand CLA bA 856

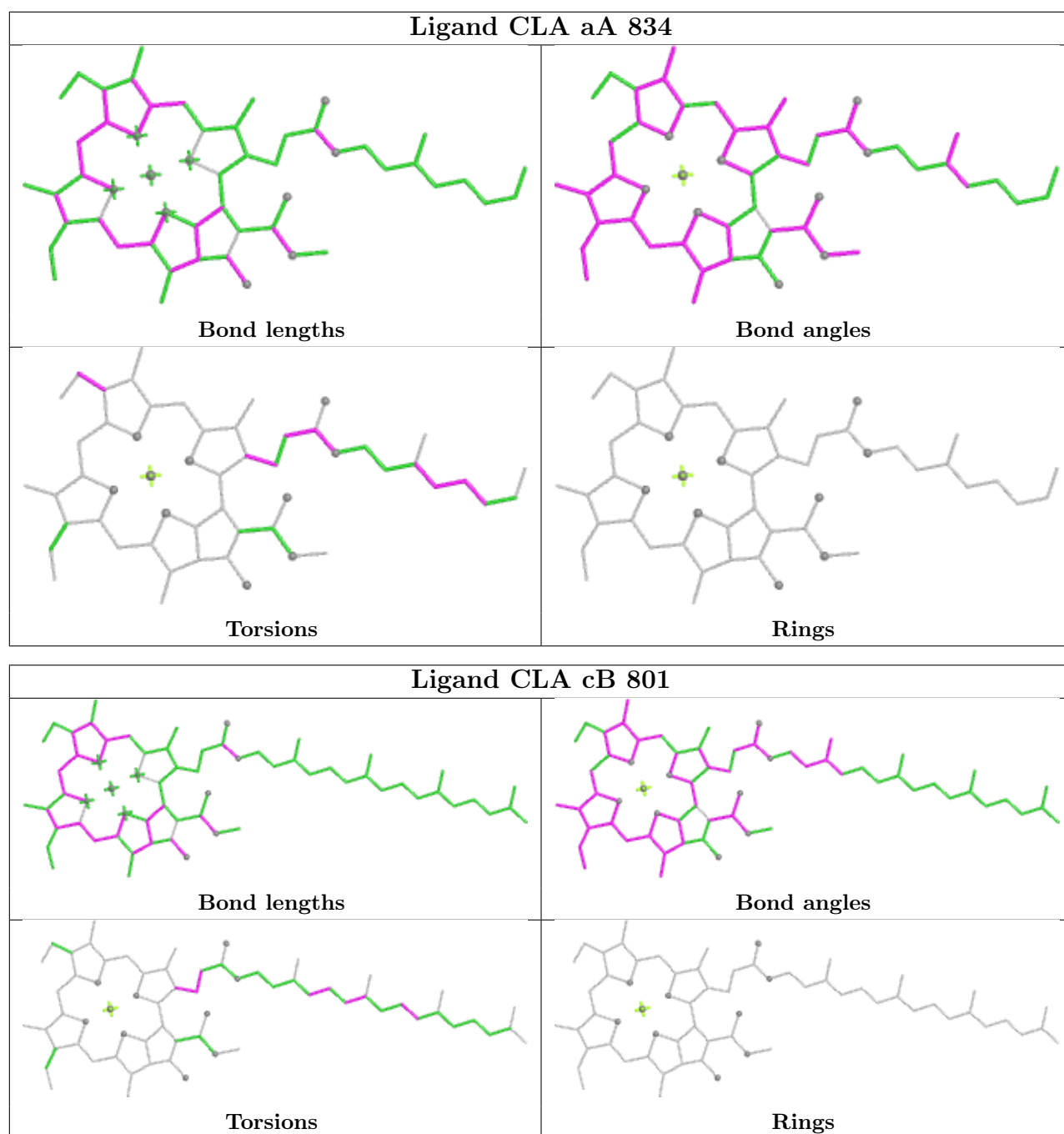


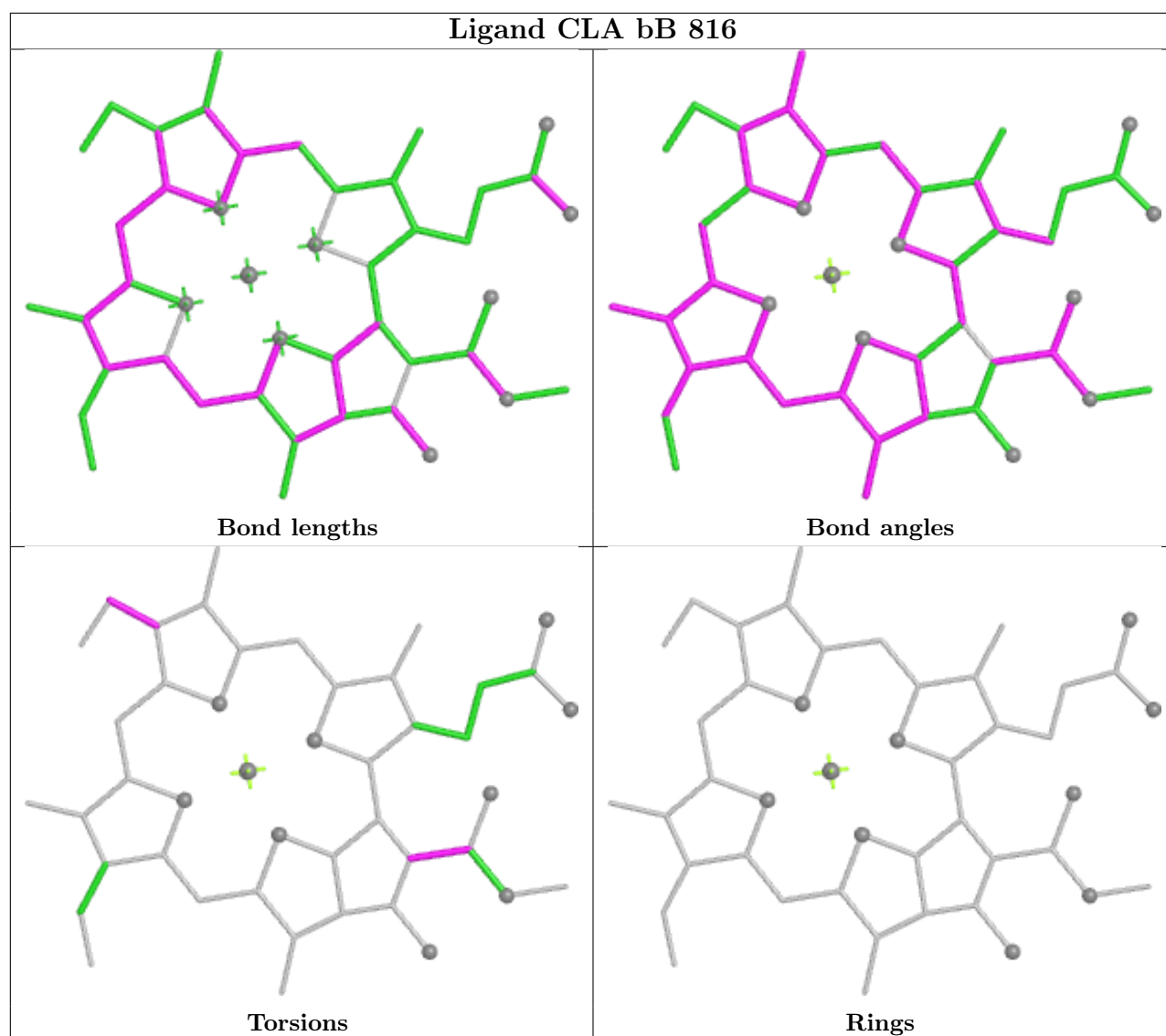
Ligand CLA cB 826

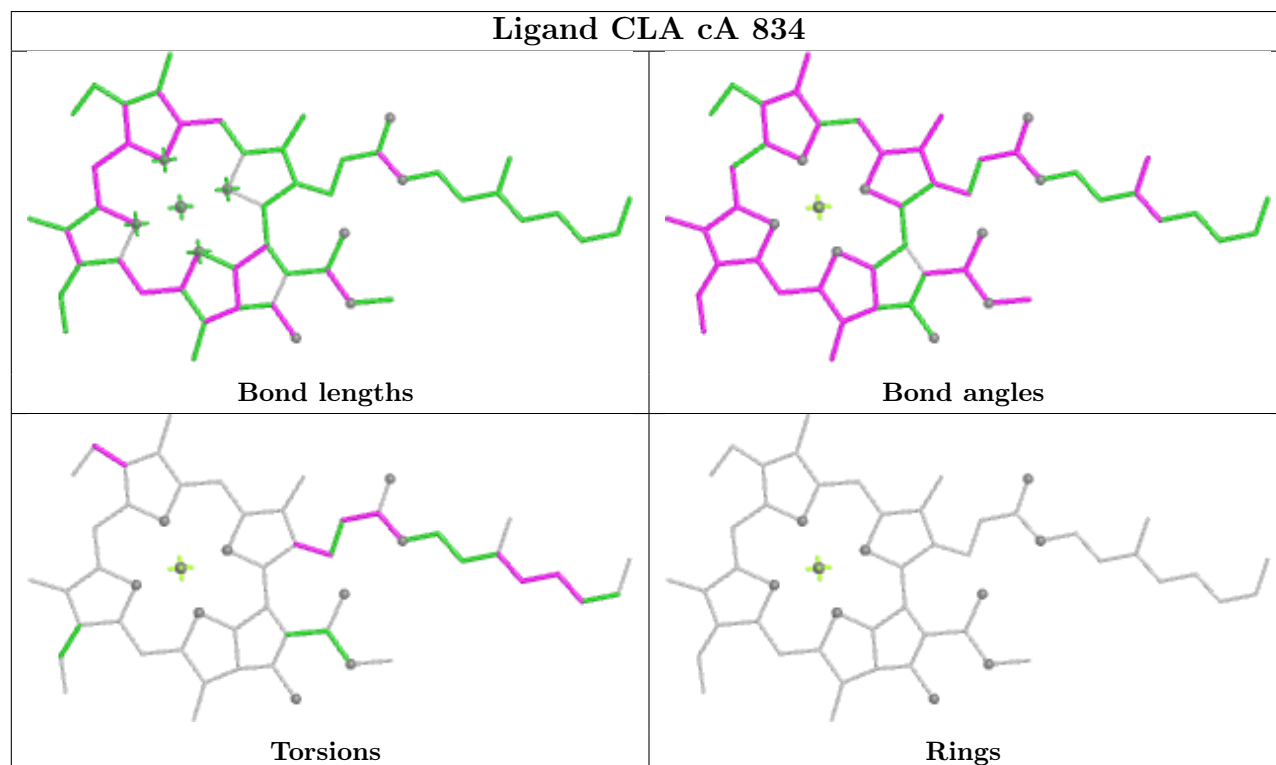
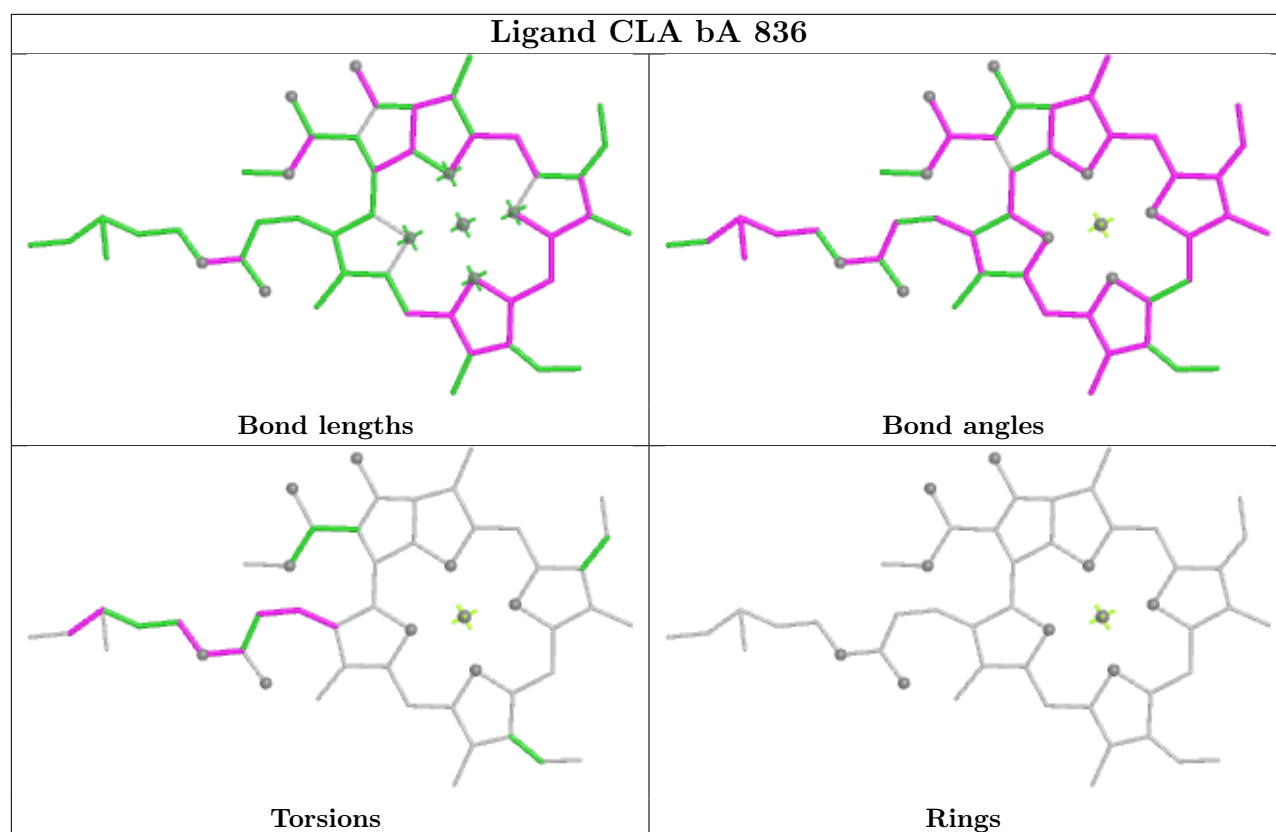


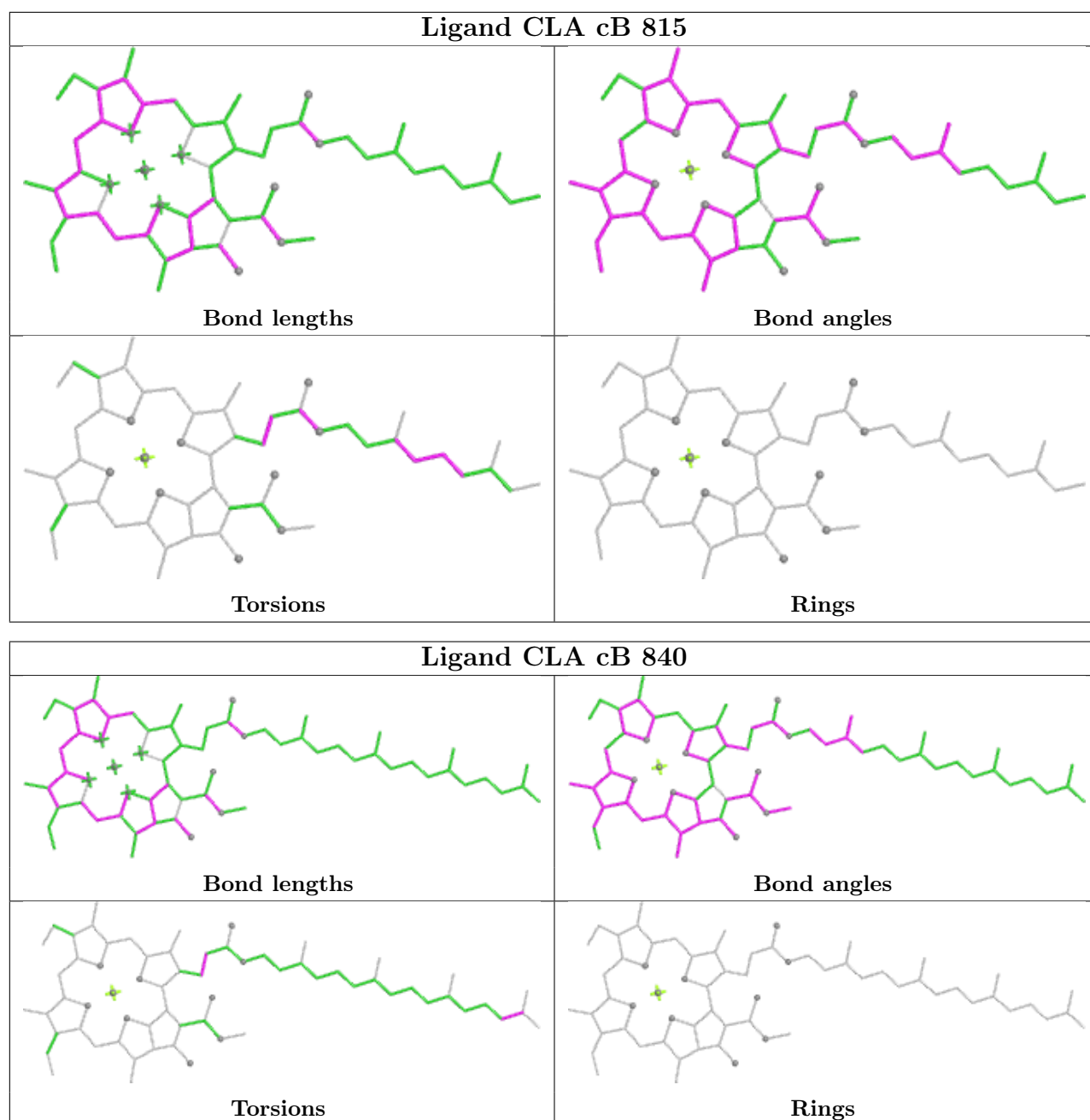


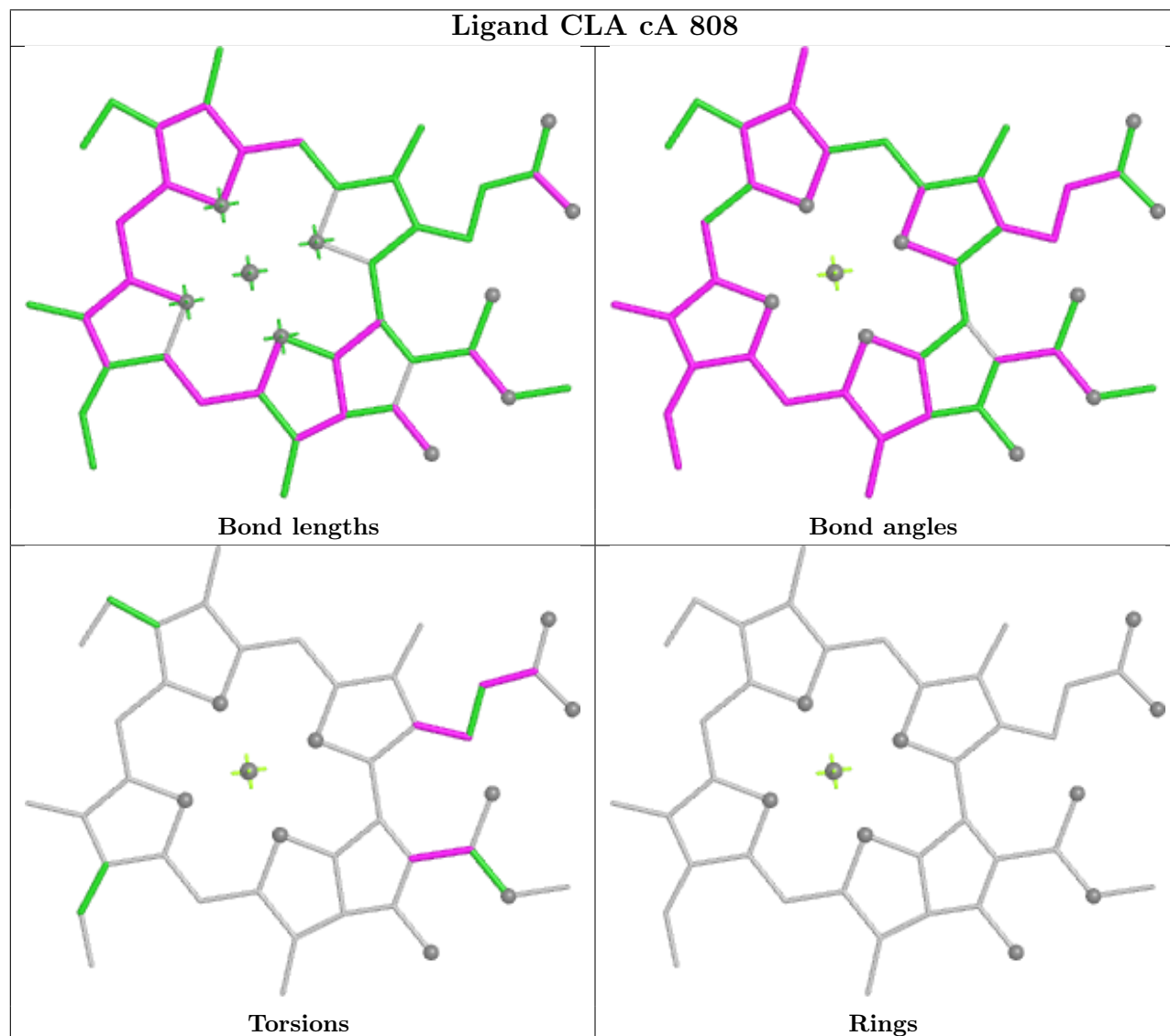
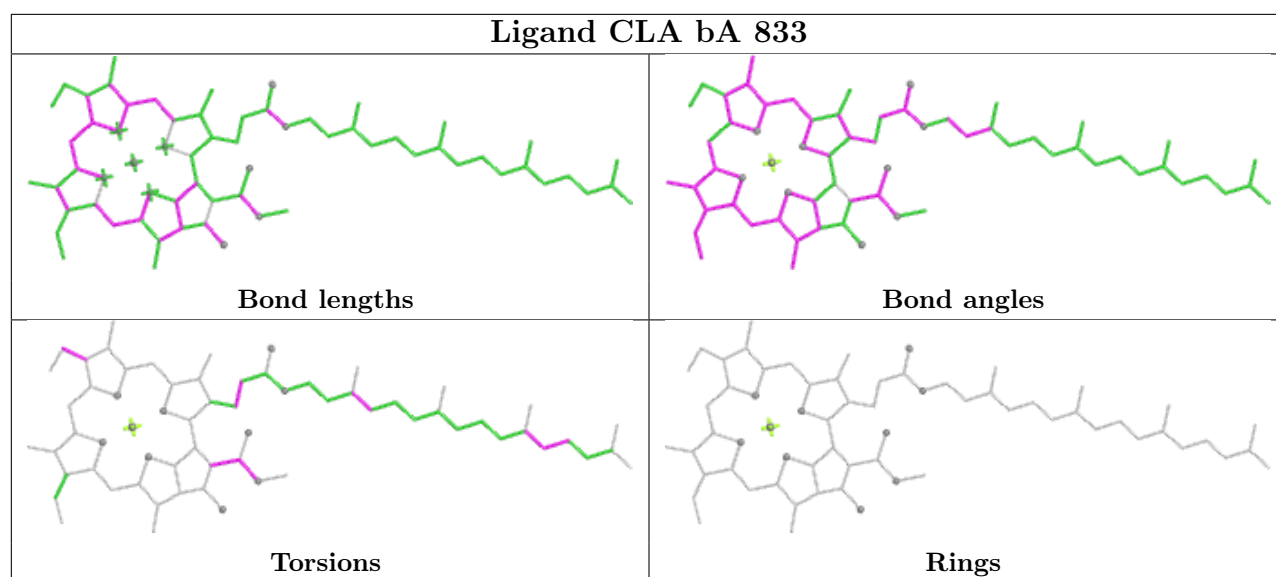


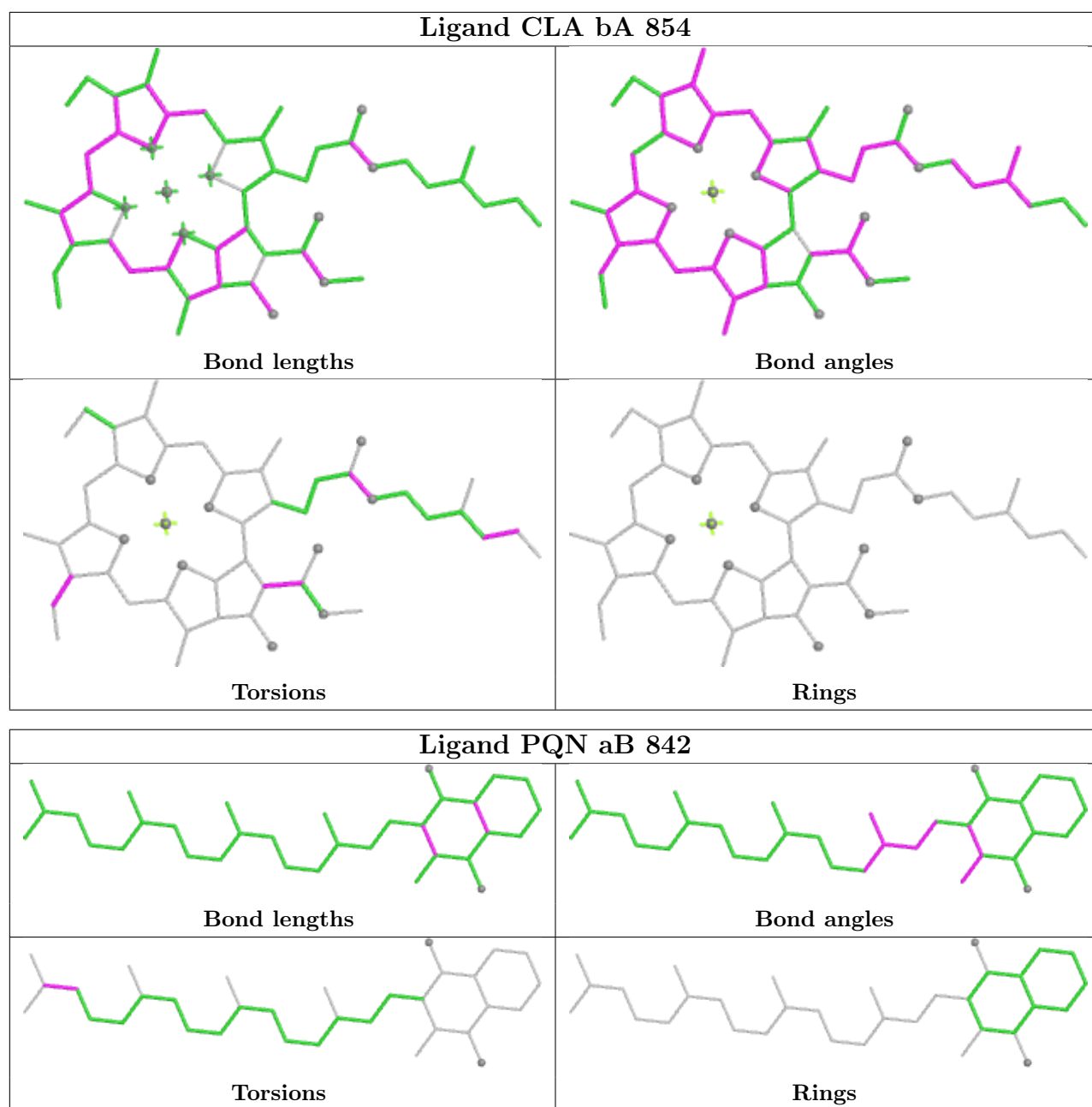


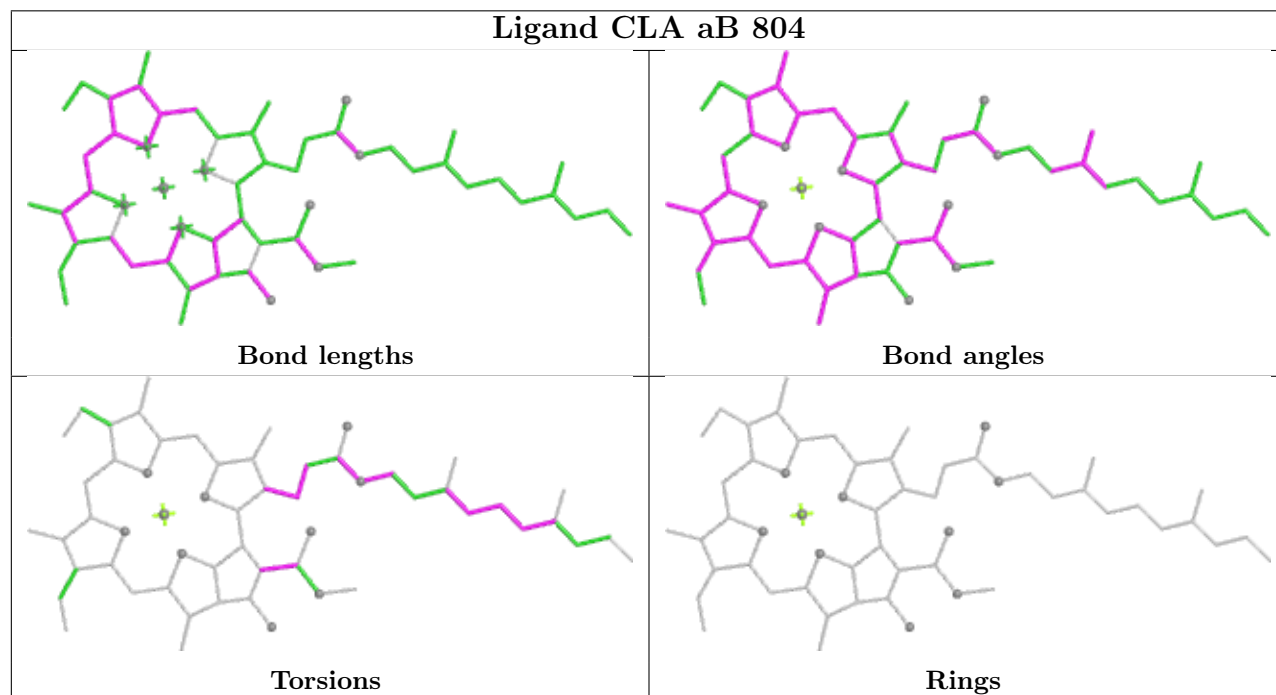
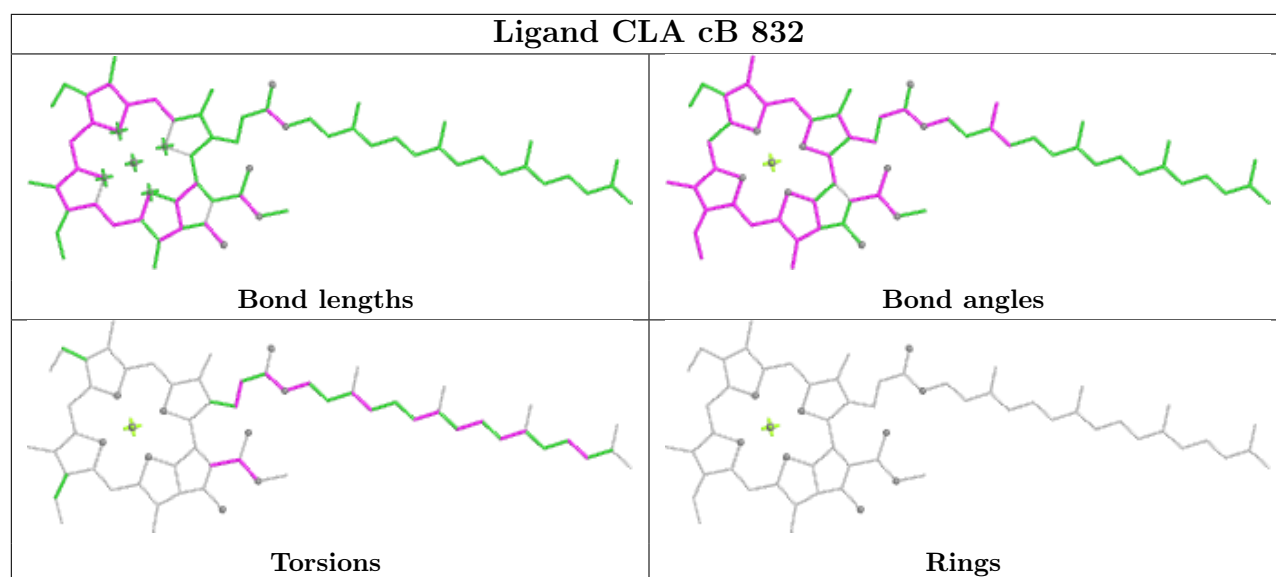


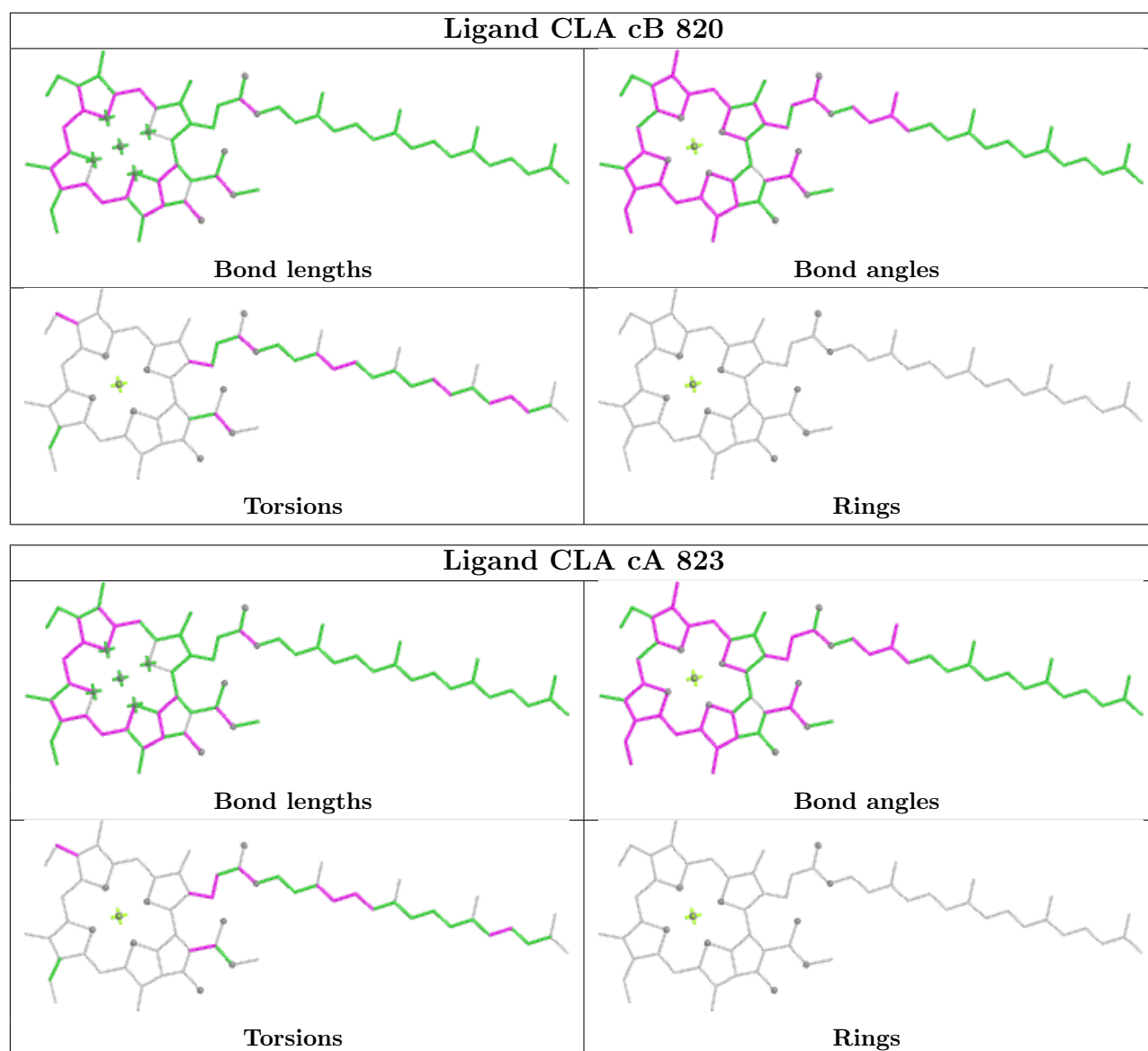


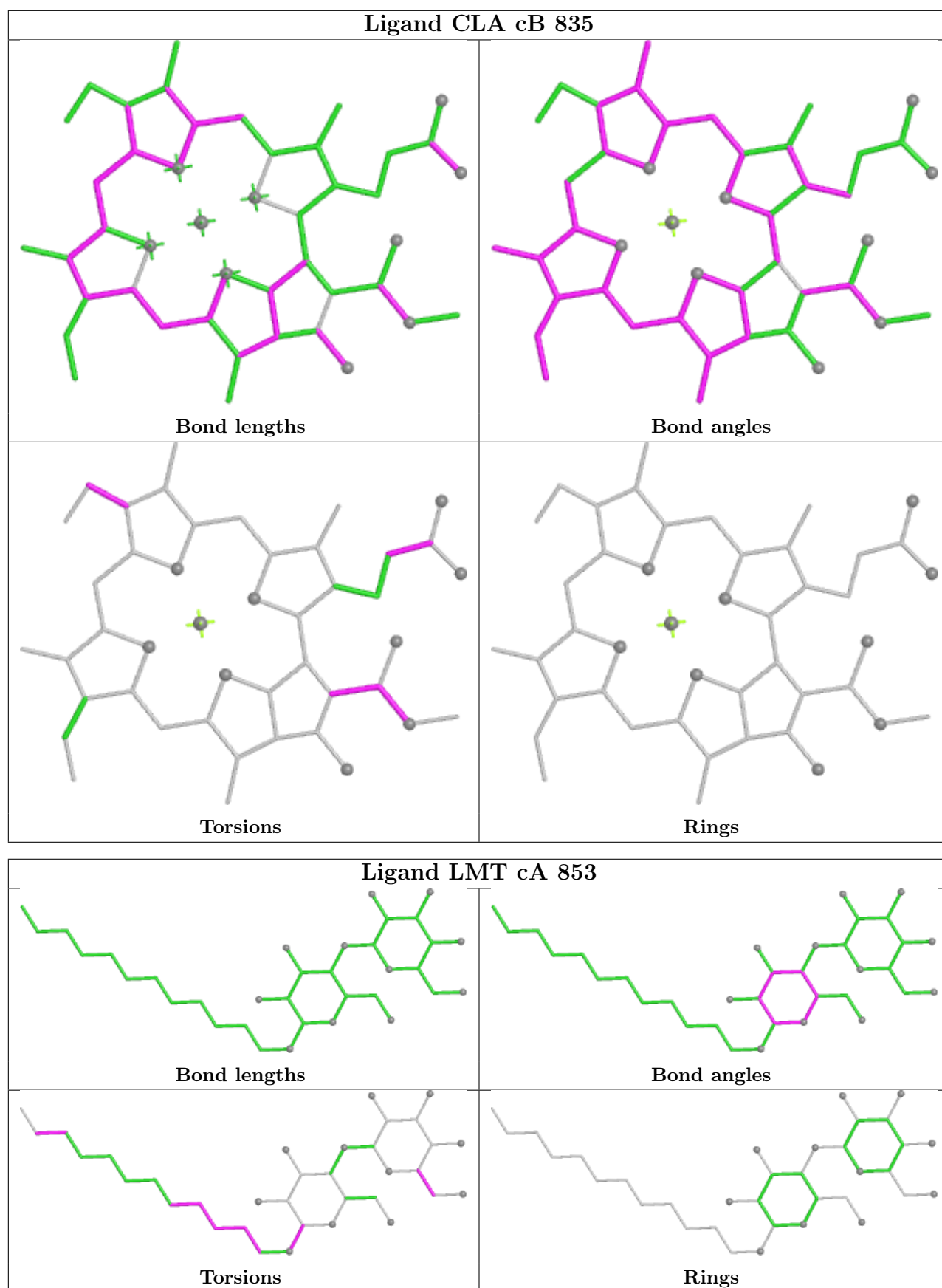


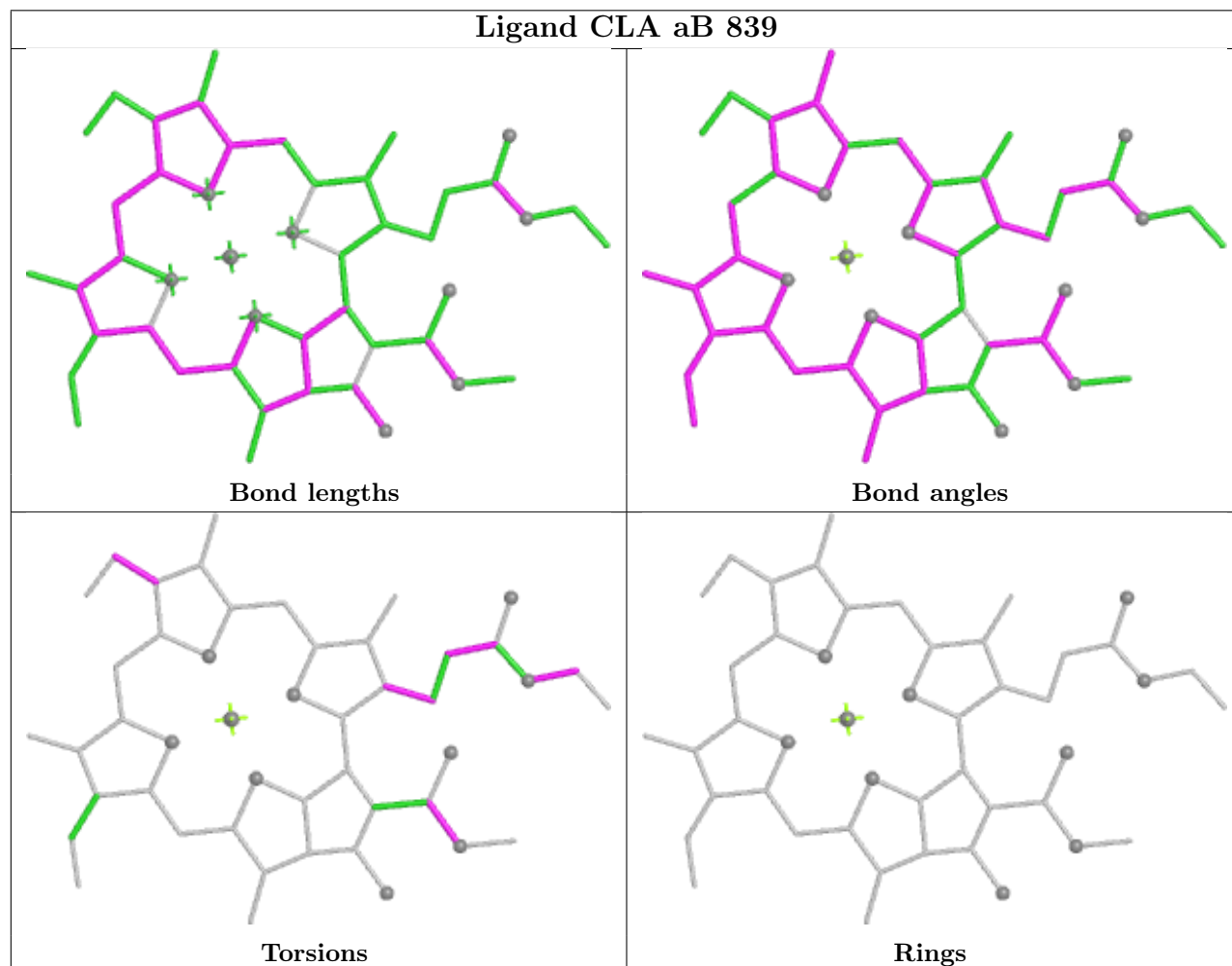
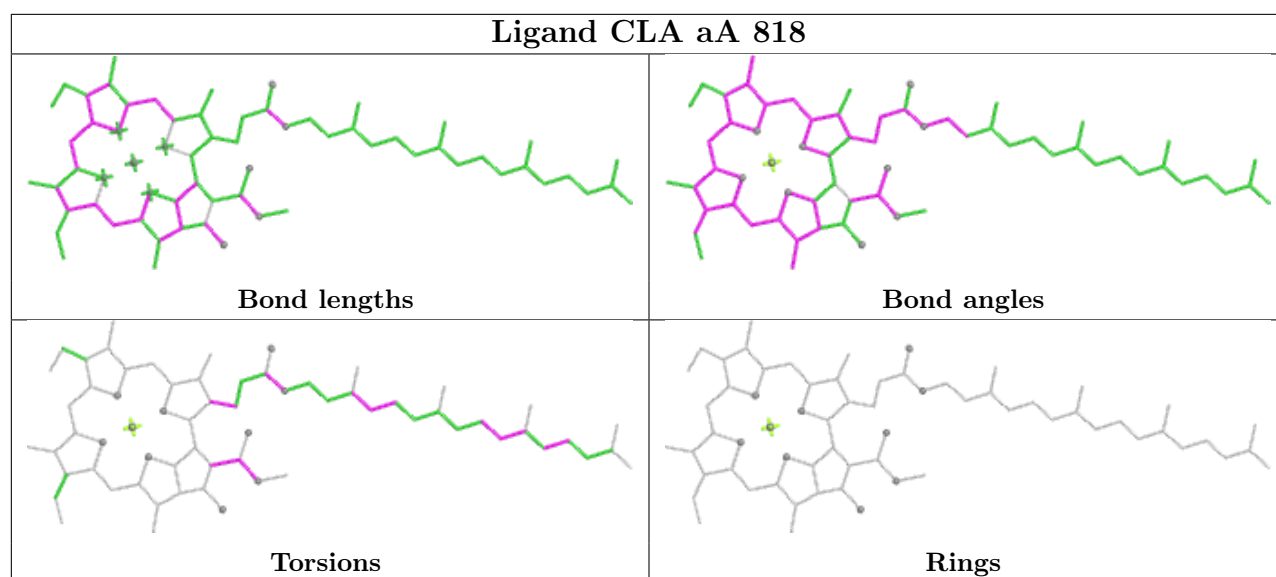


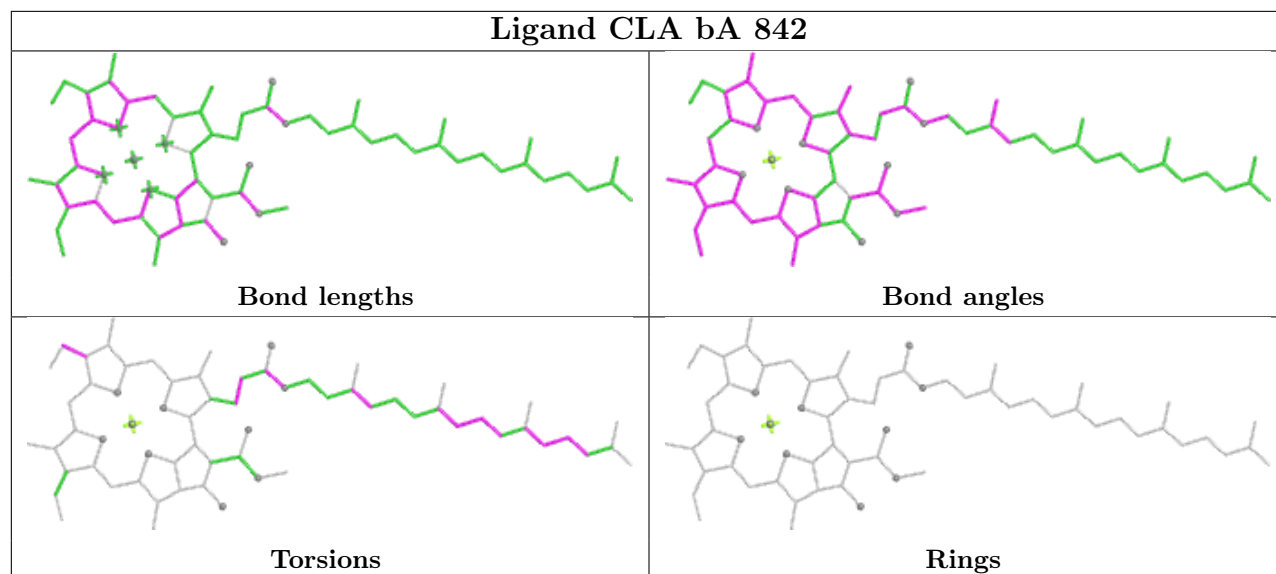
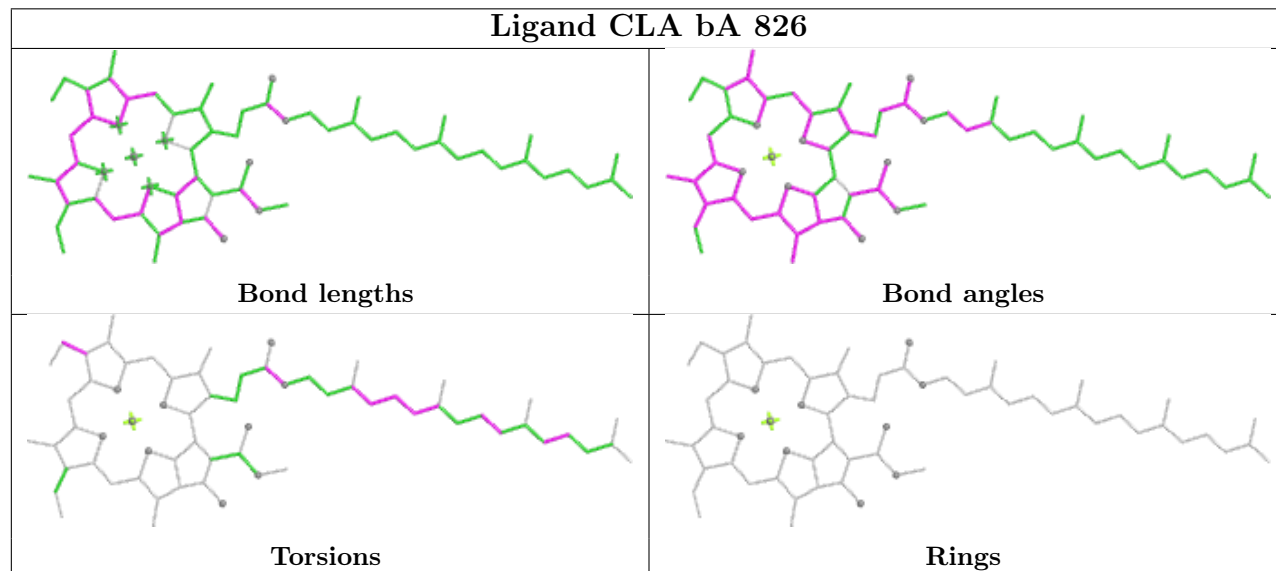




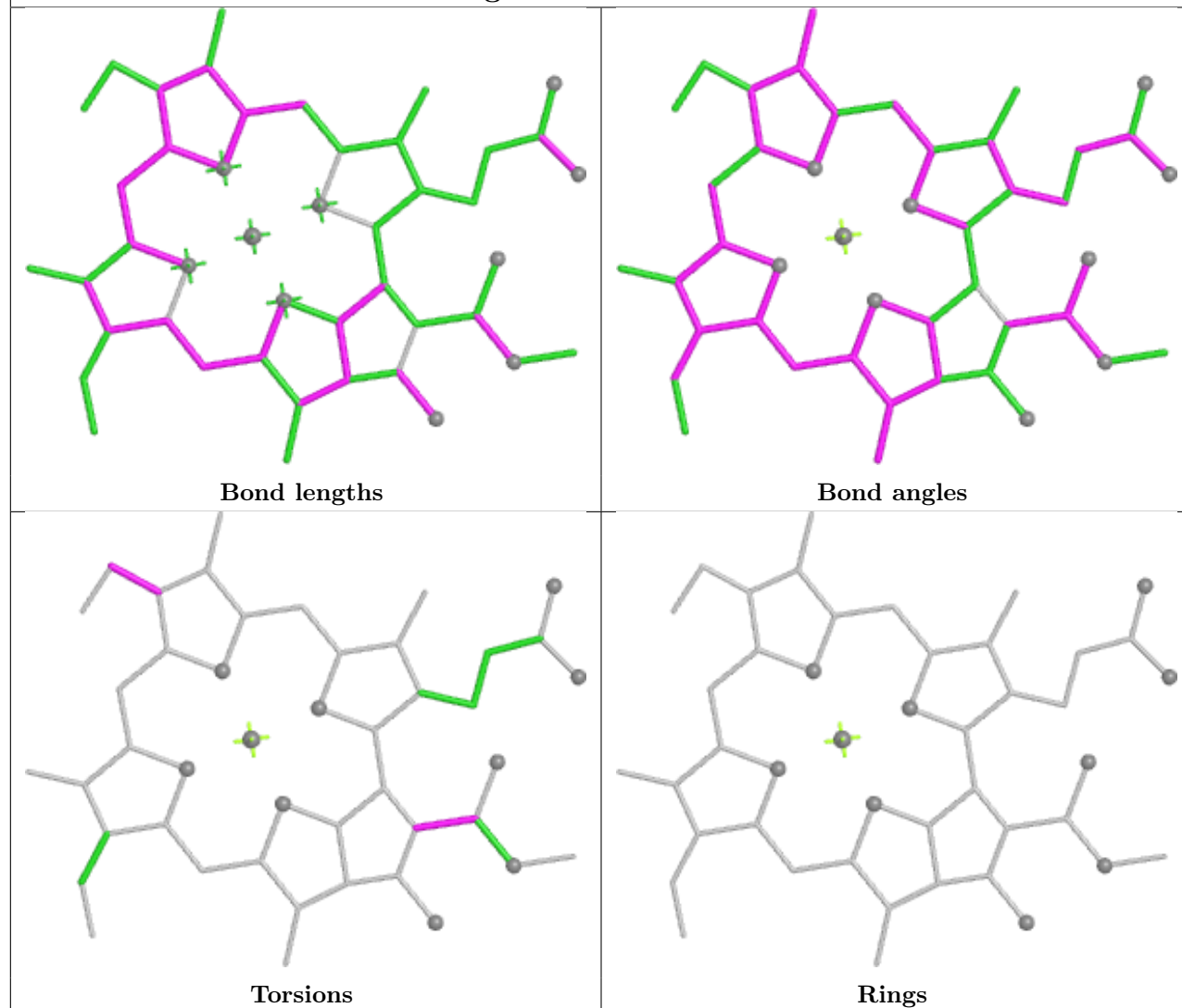




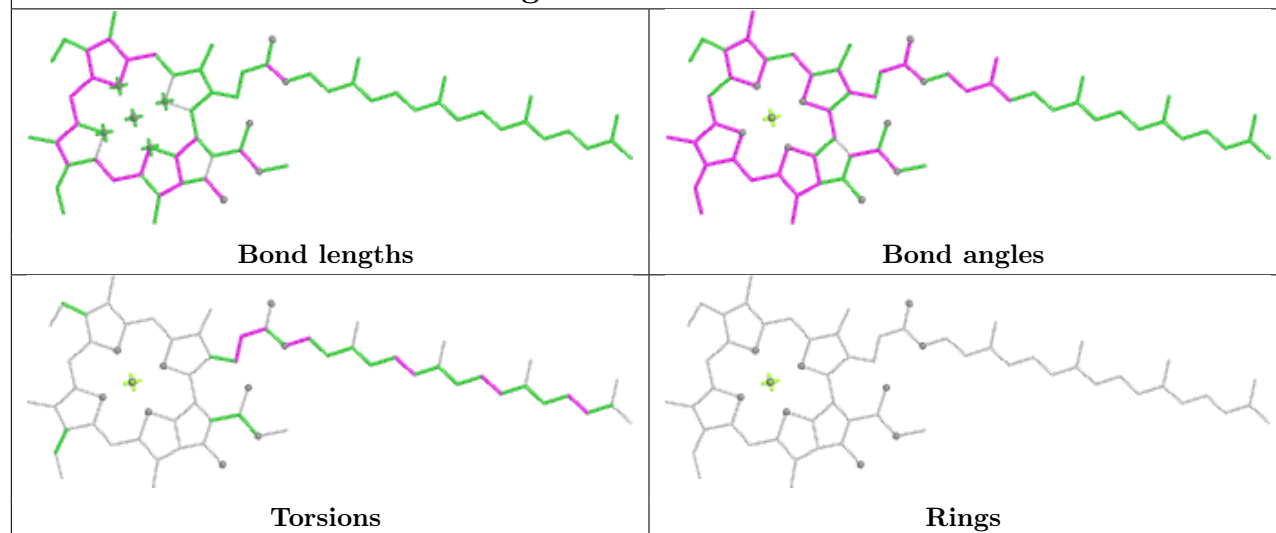


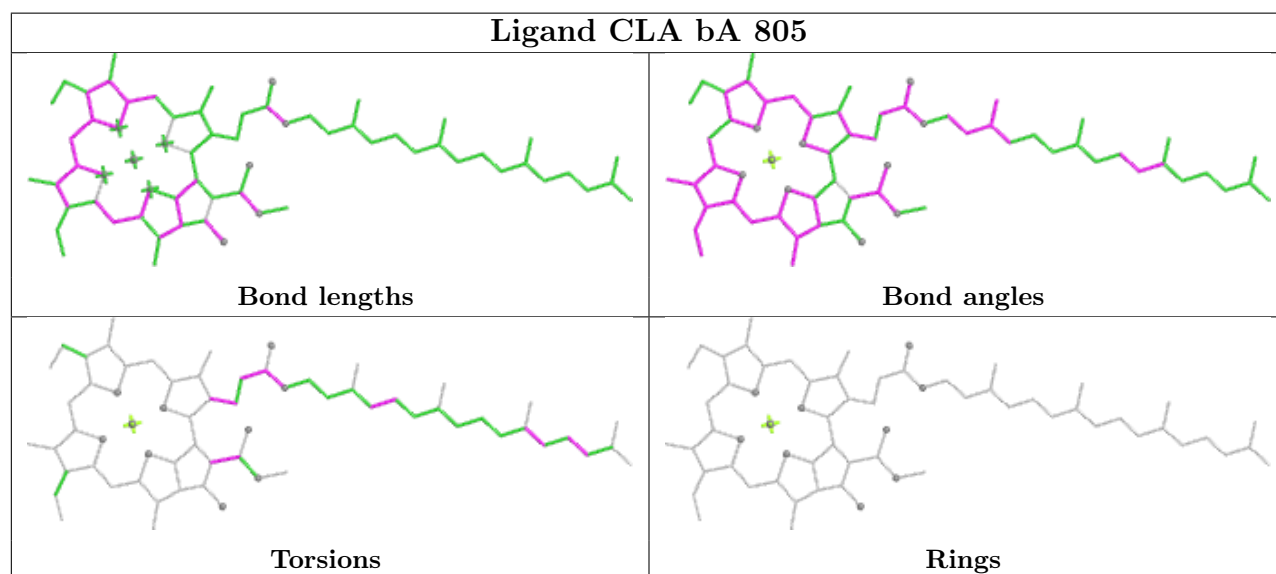
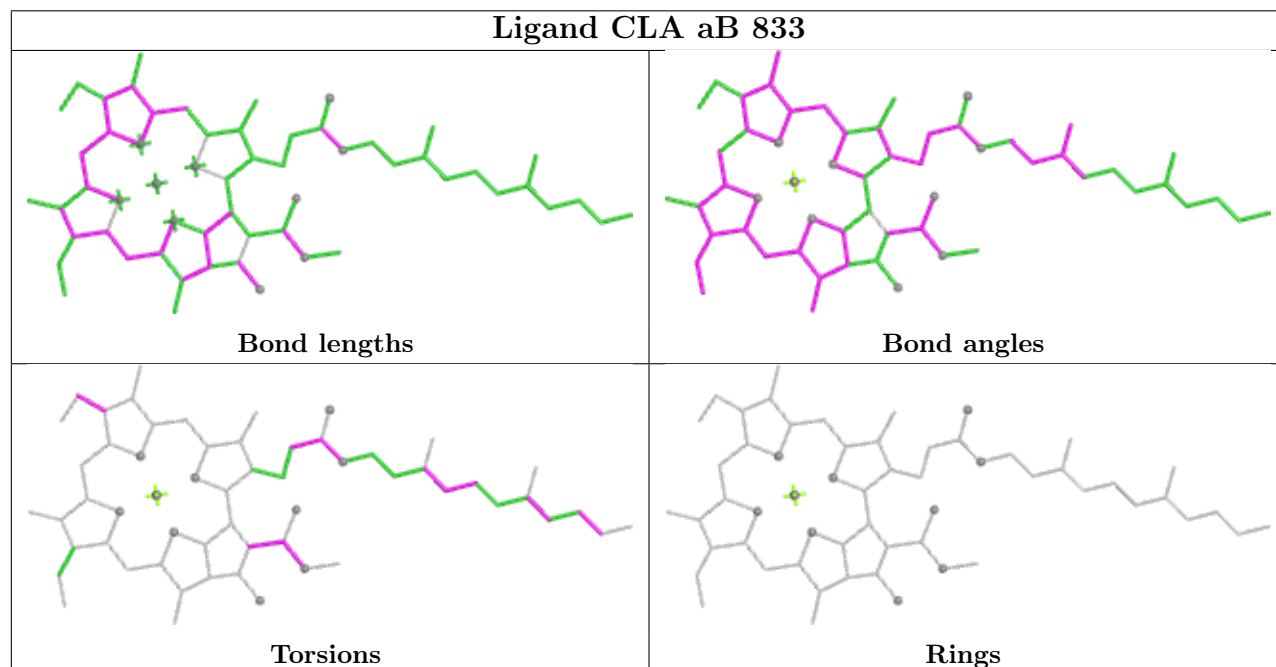
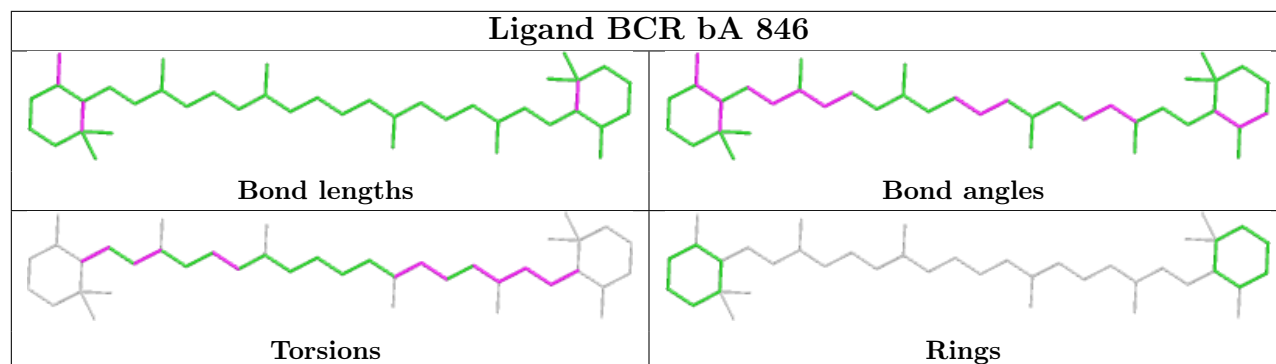
Ligand CLA bA 842**Ligand CLA bA 826**

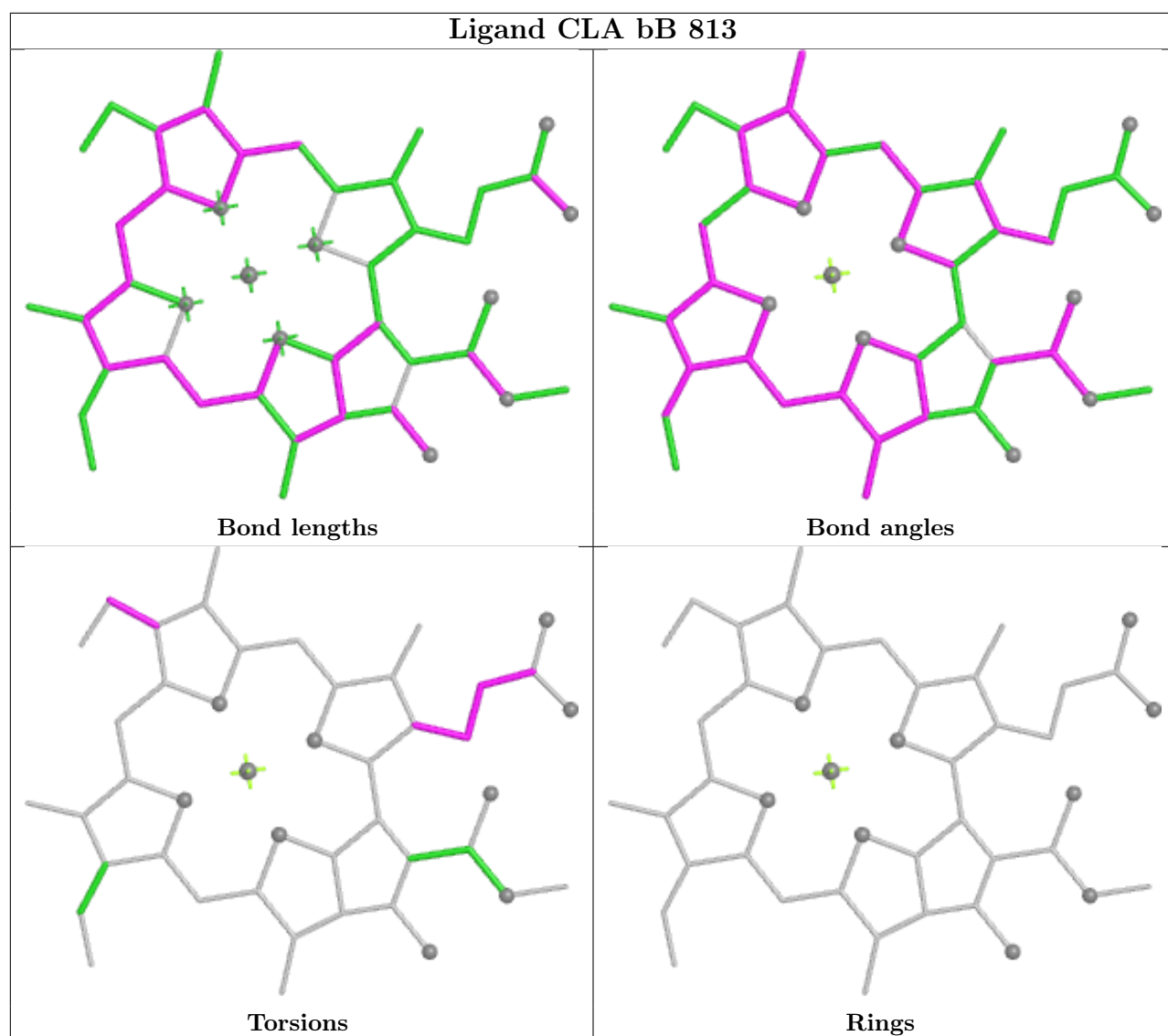
Ligand CLA aA 814



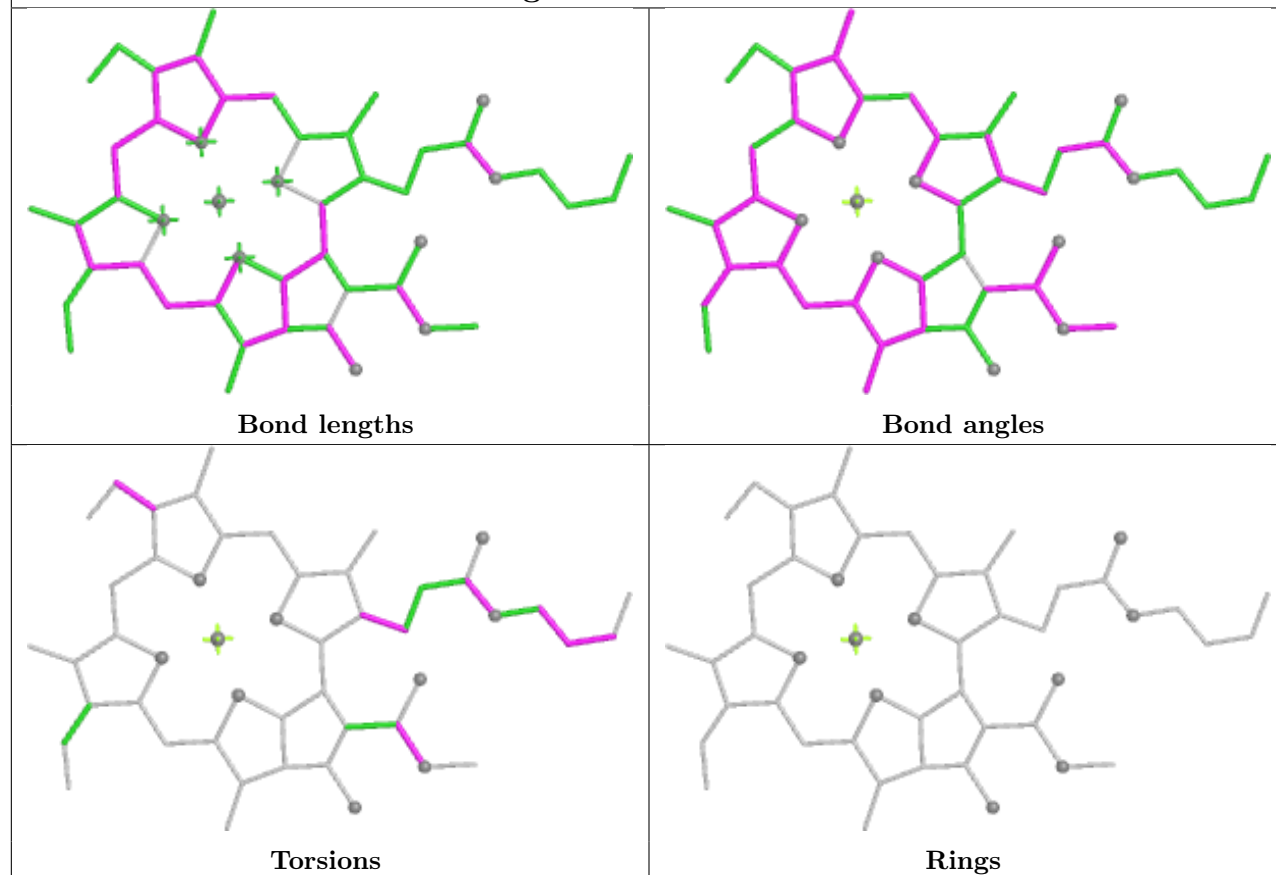
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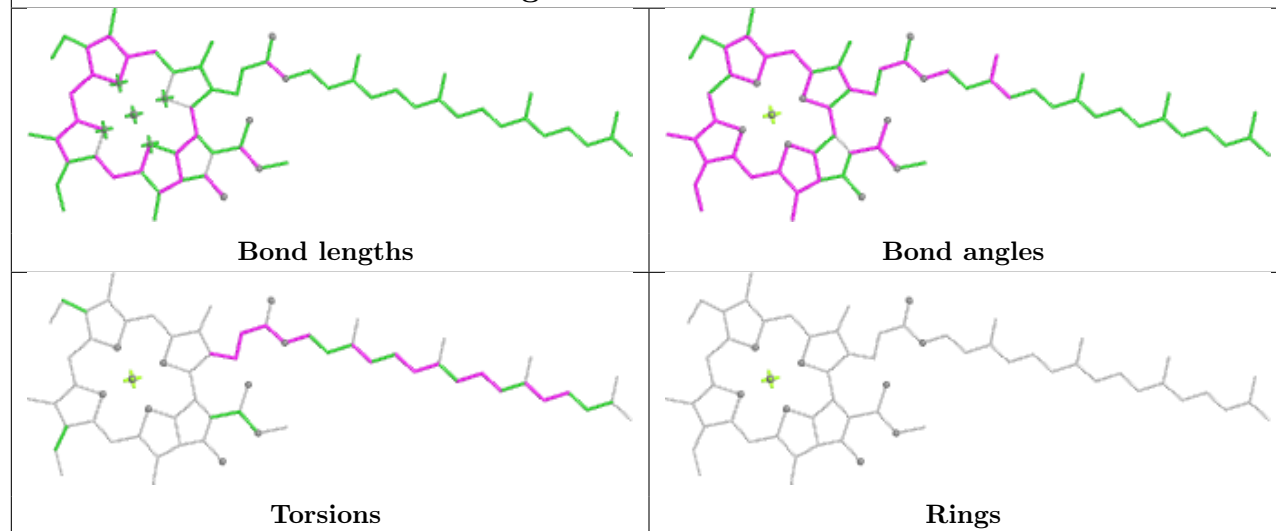


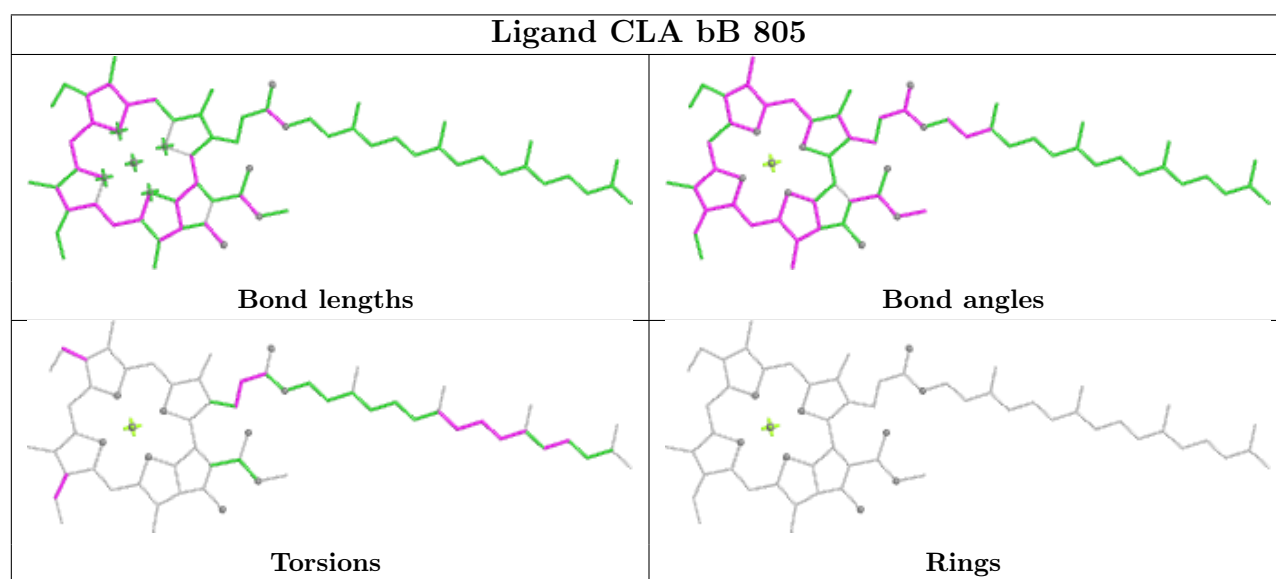
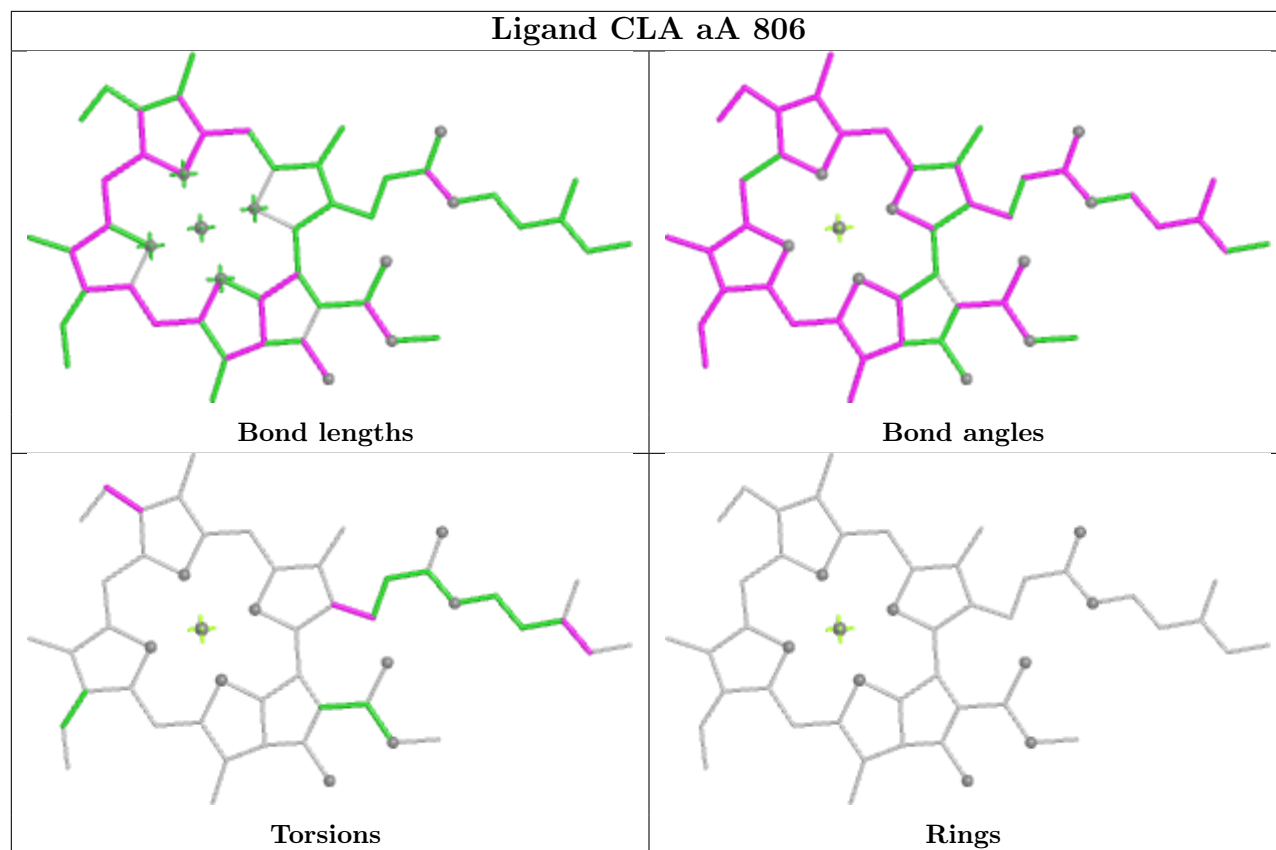


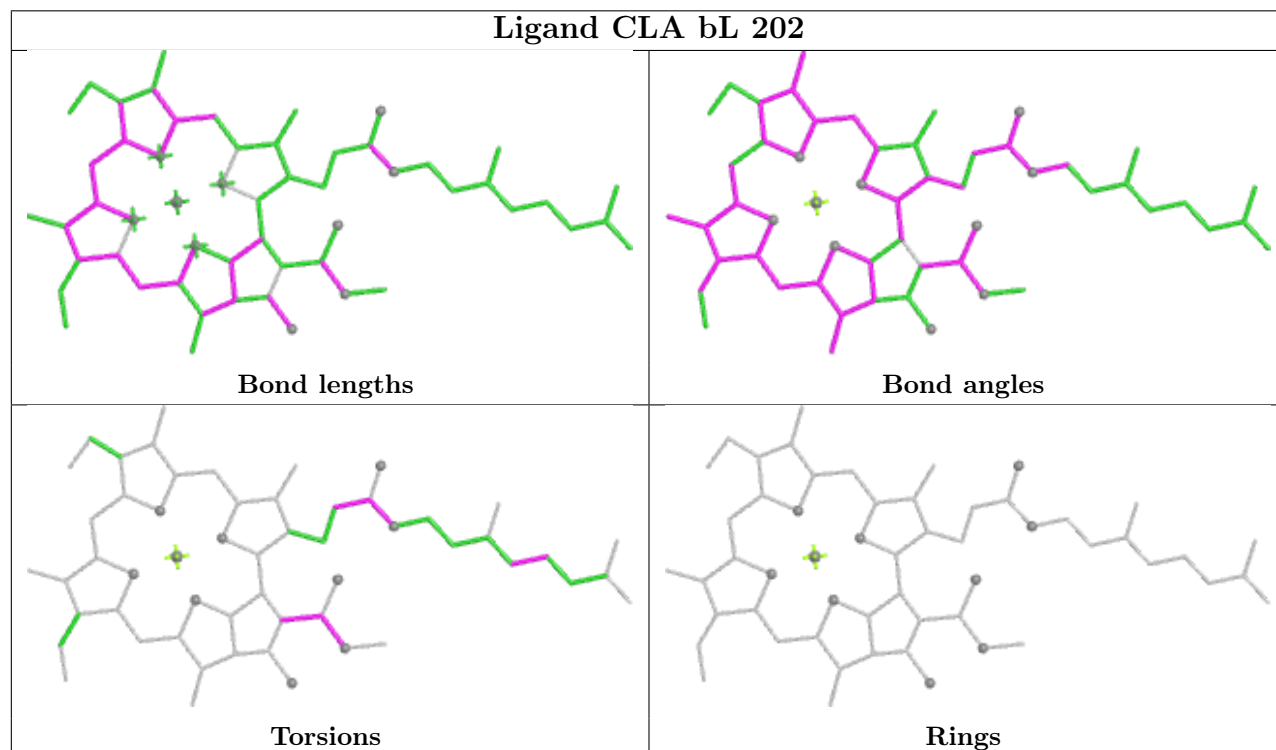
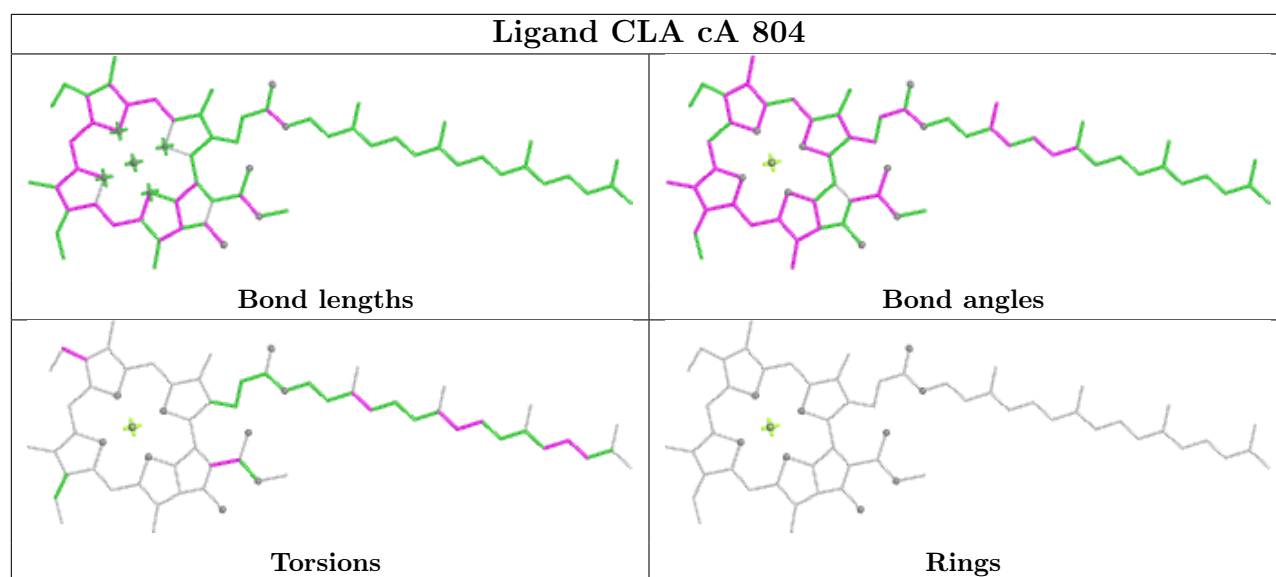
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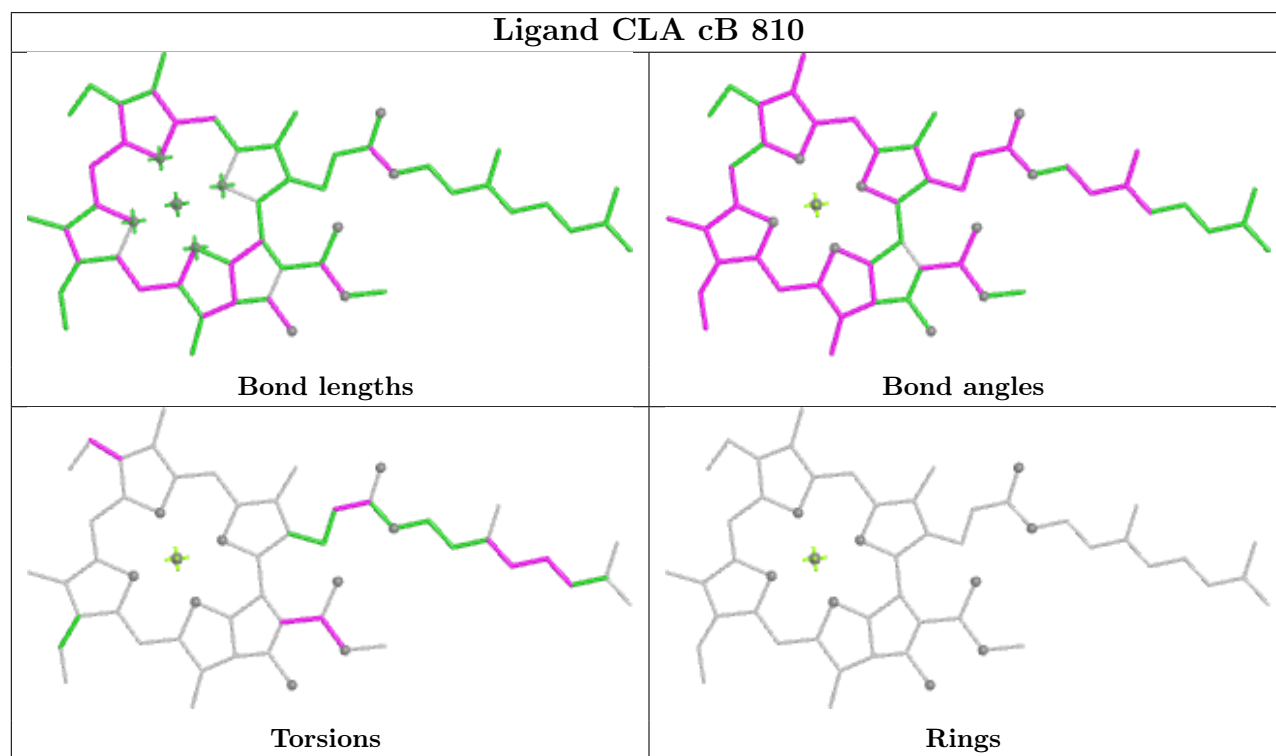
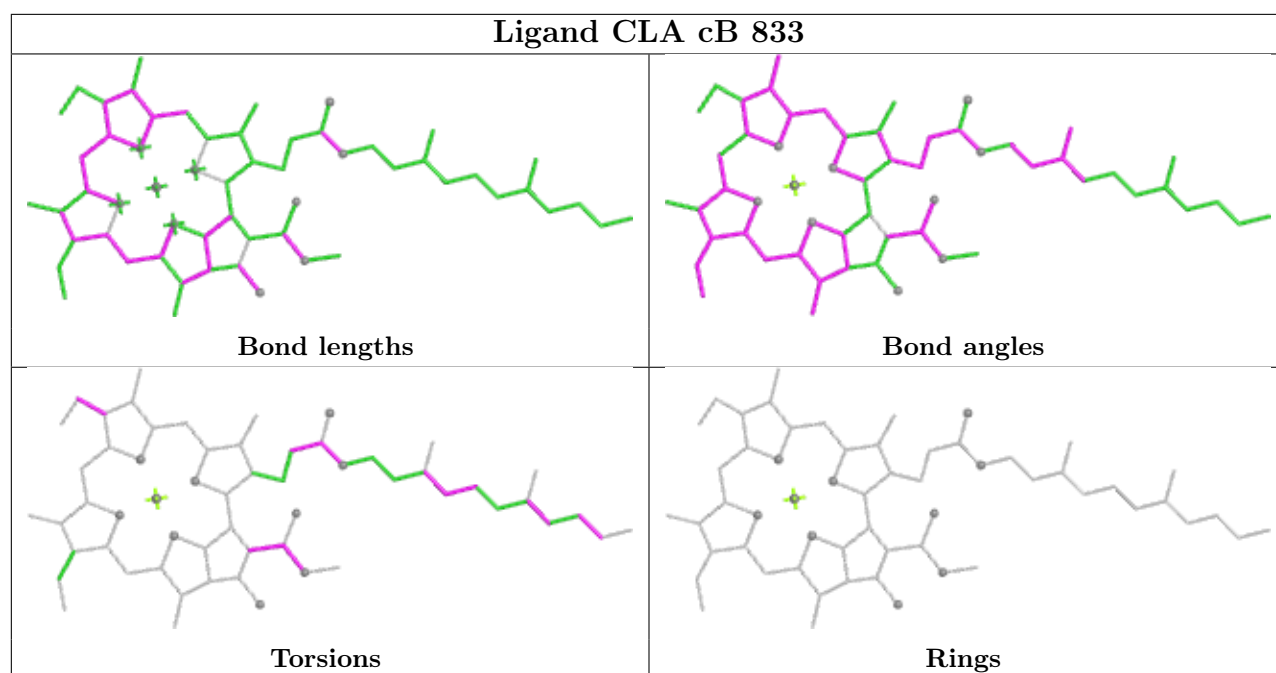


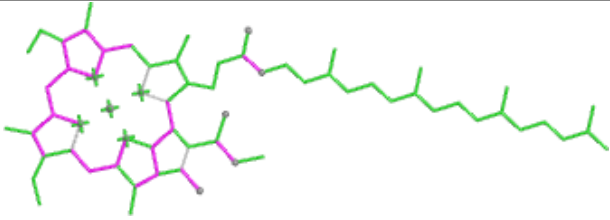
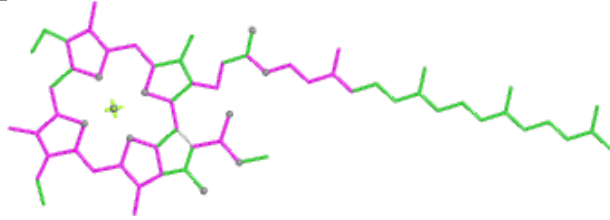
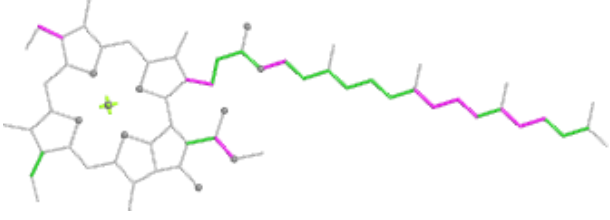
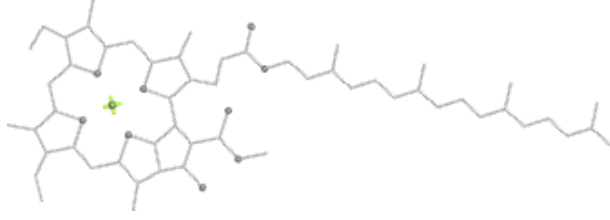
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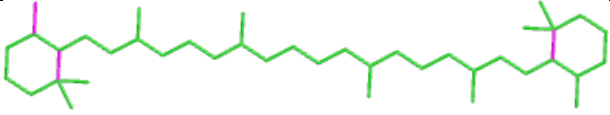
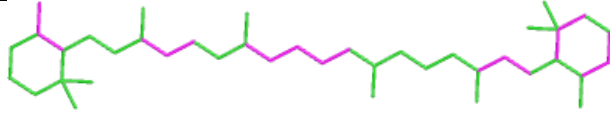
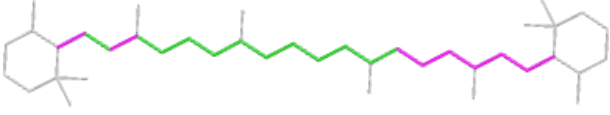
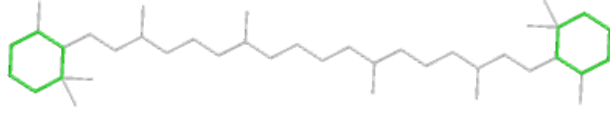


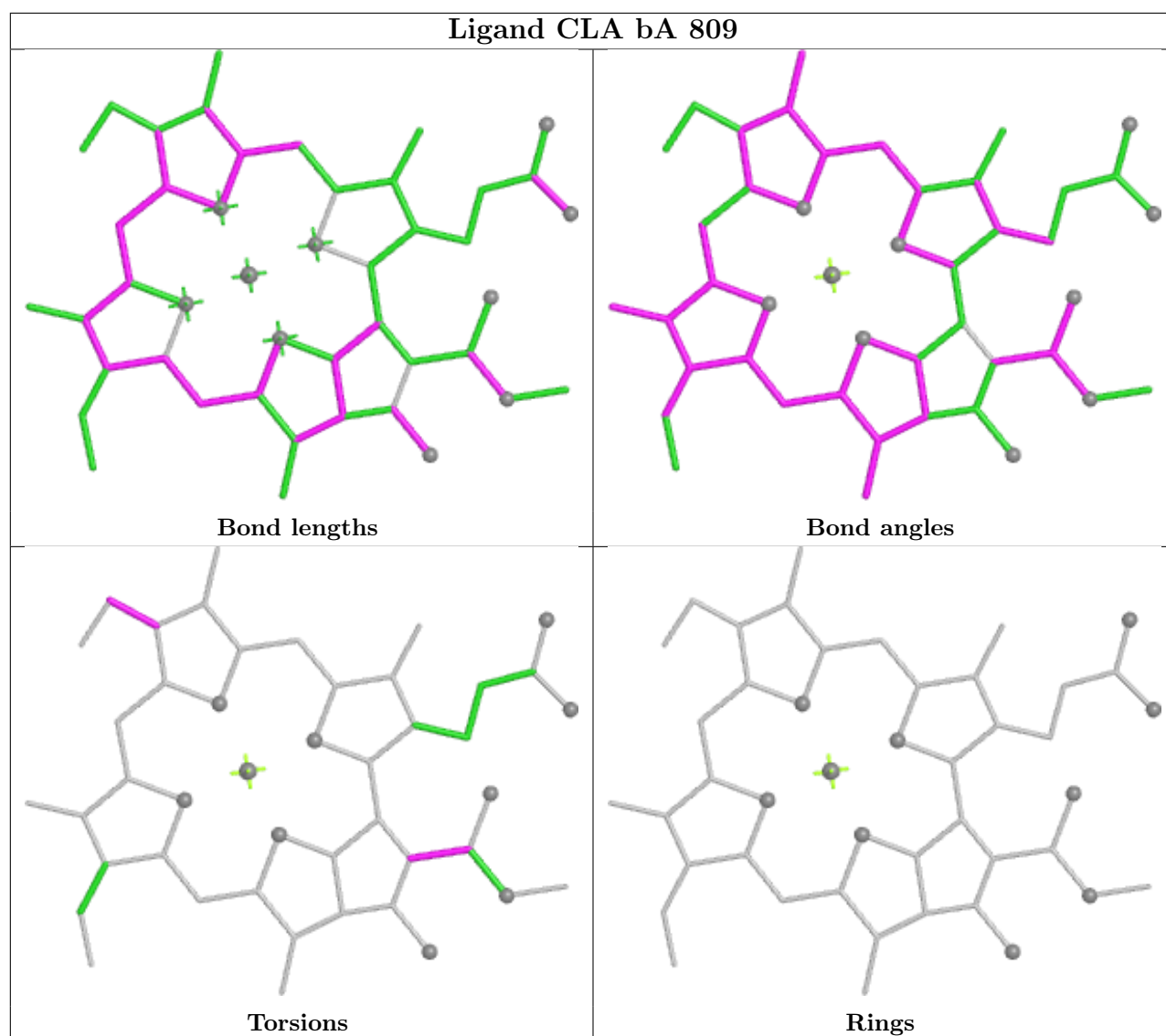


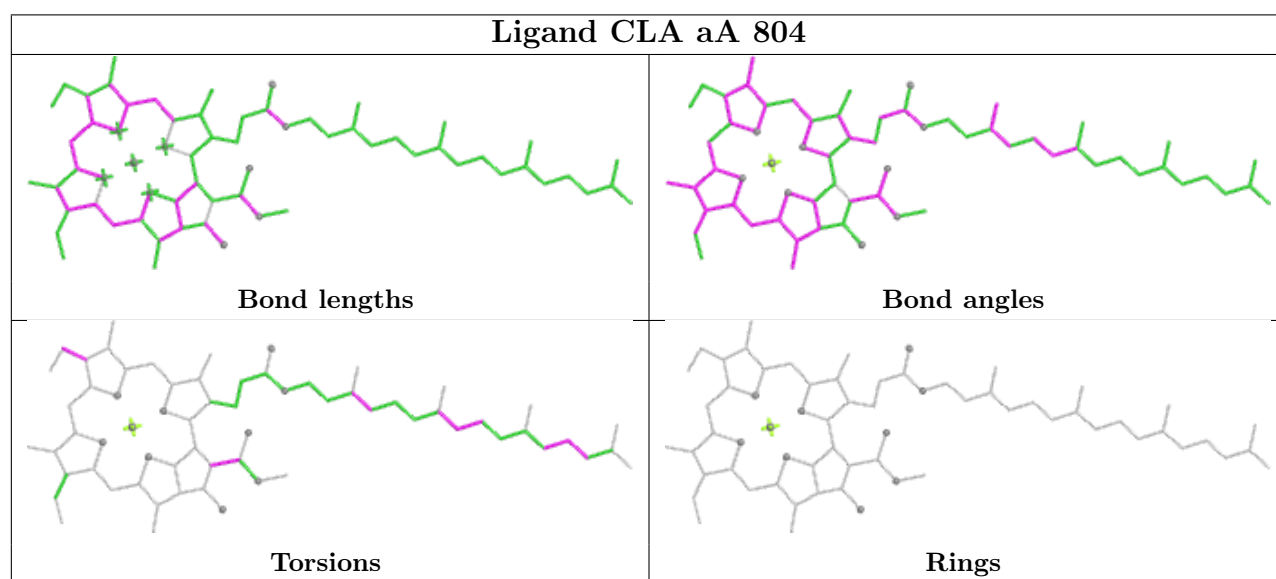
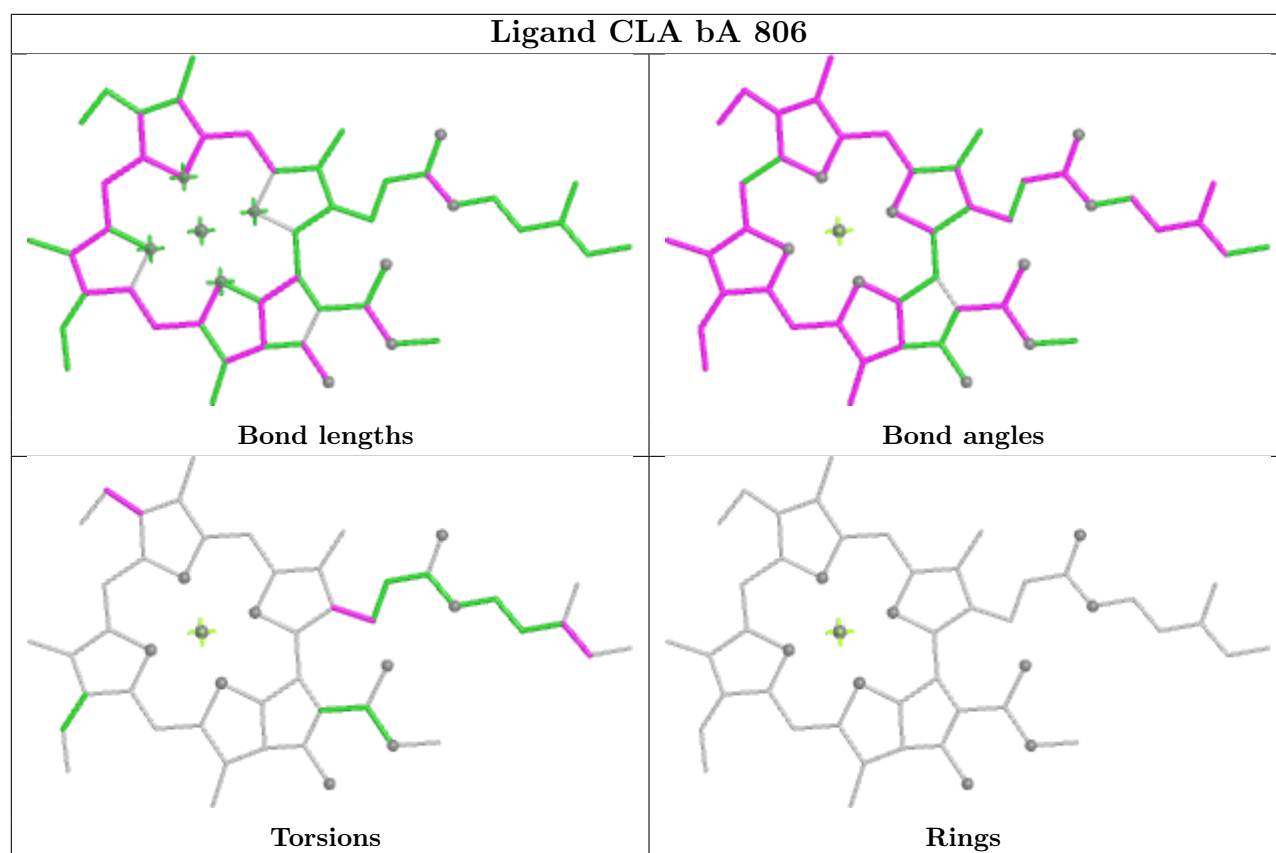




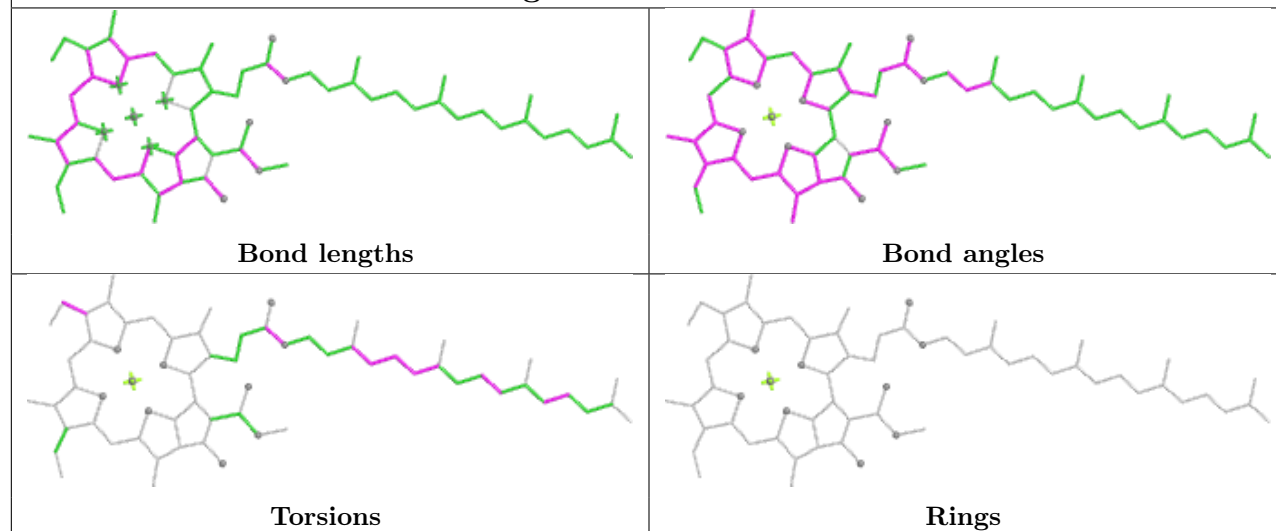
Ligand CLA cB 828			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand BCR bA 849			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

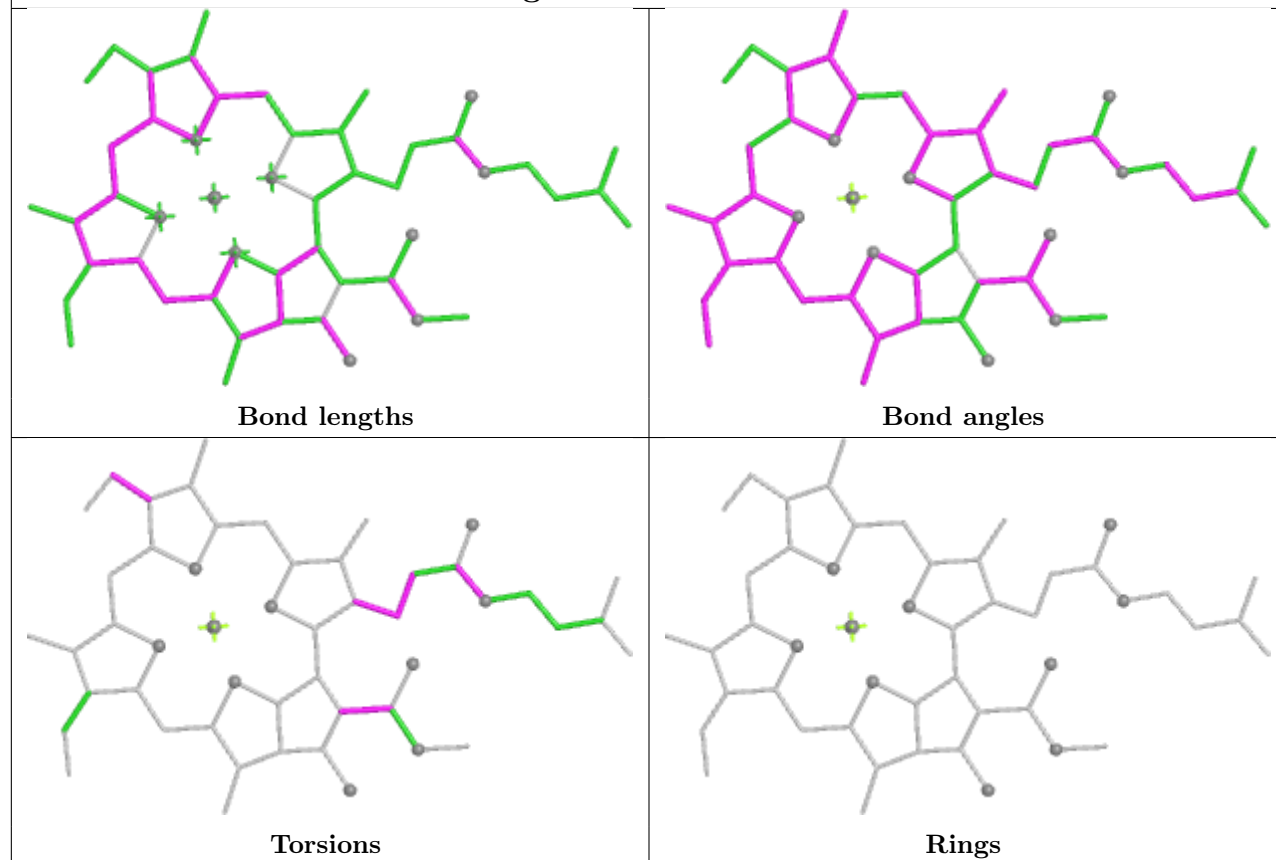




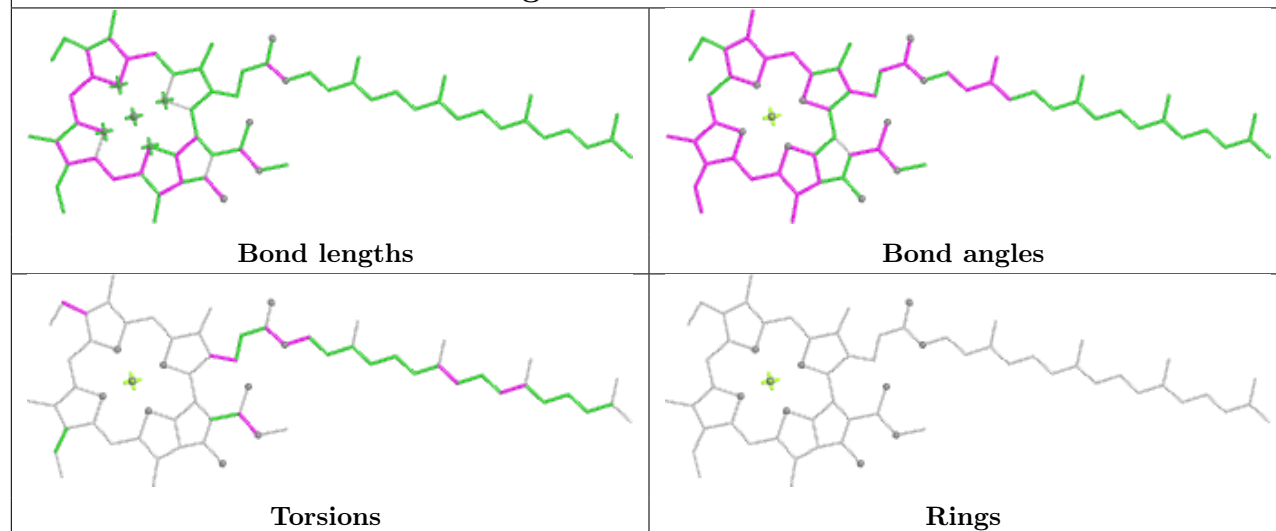
Ligand CLA aA 826



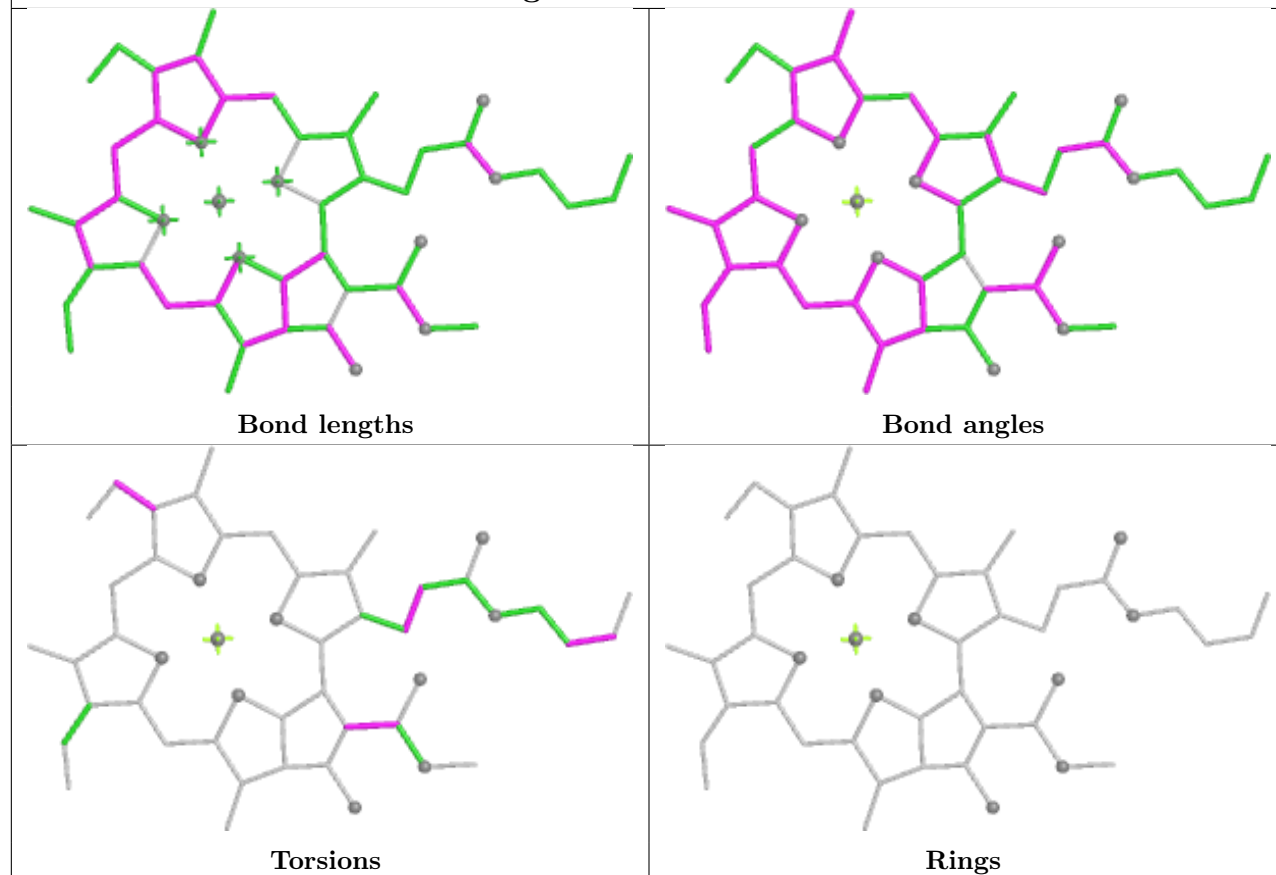
Ligand CLA aA 830

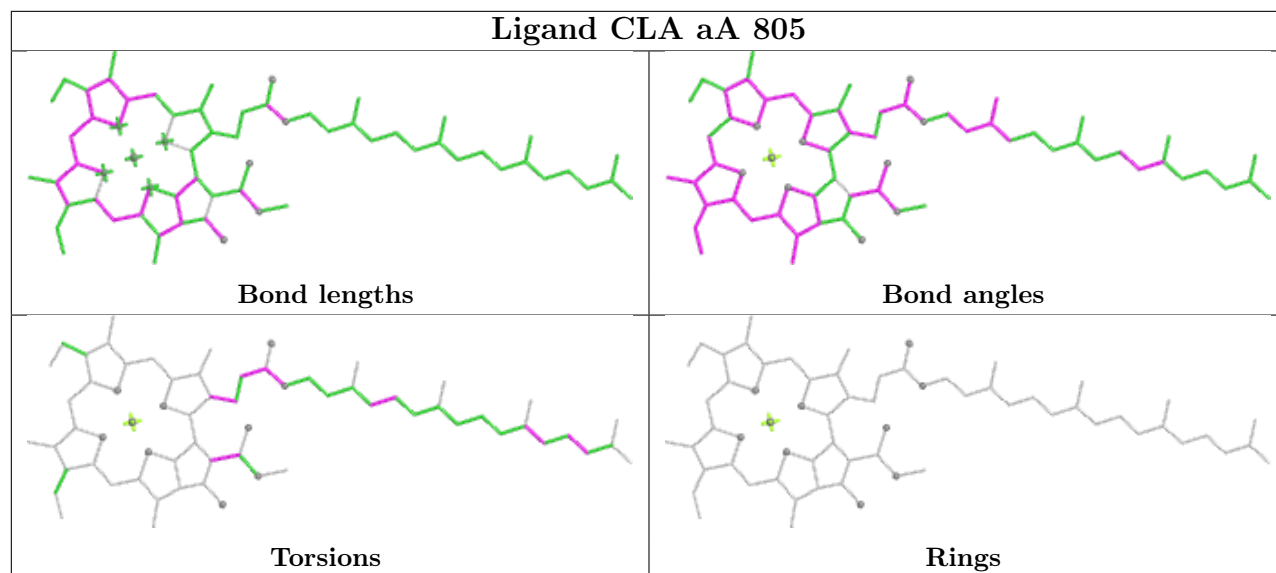
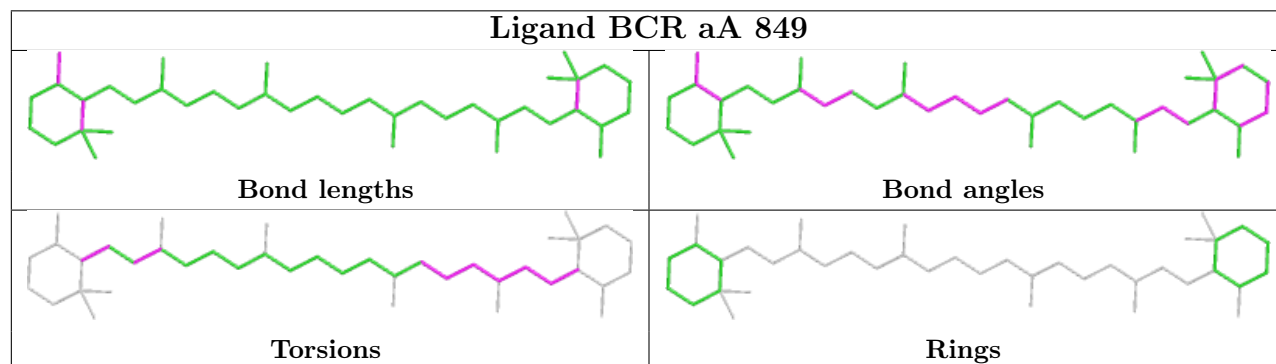
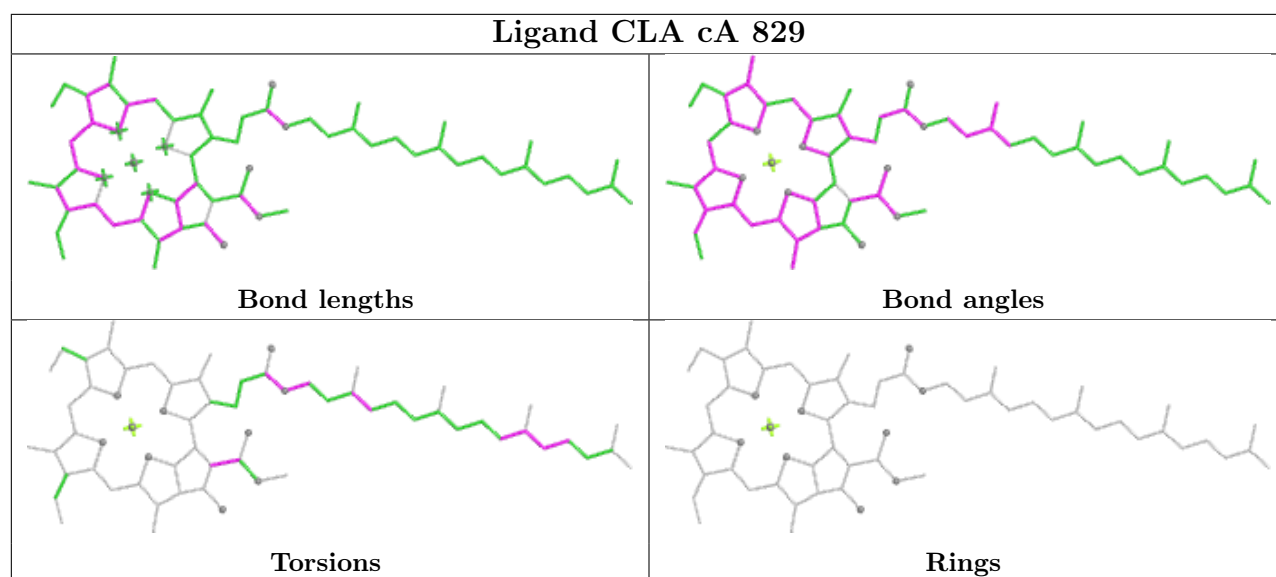


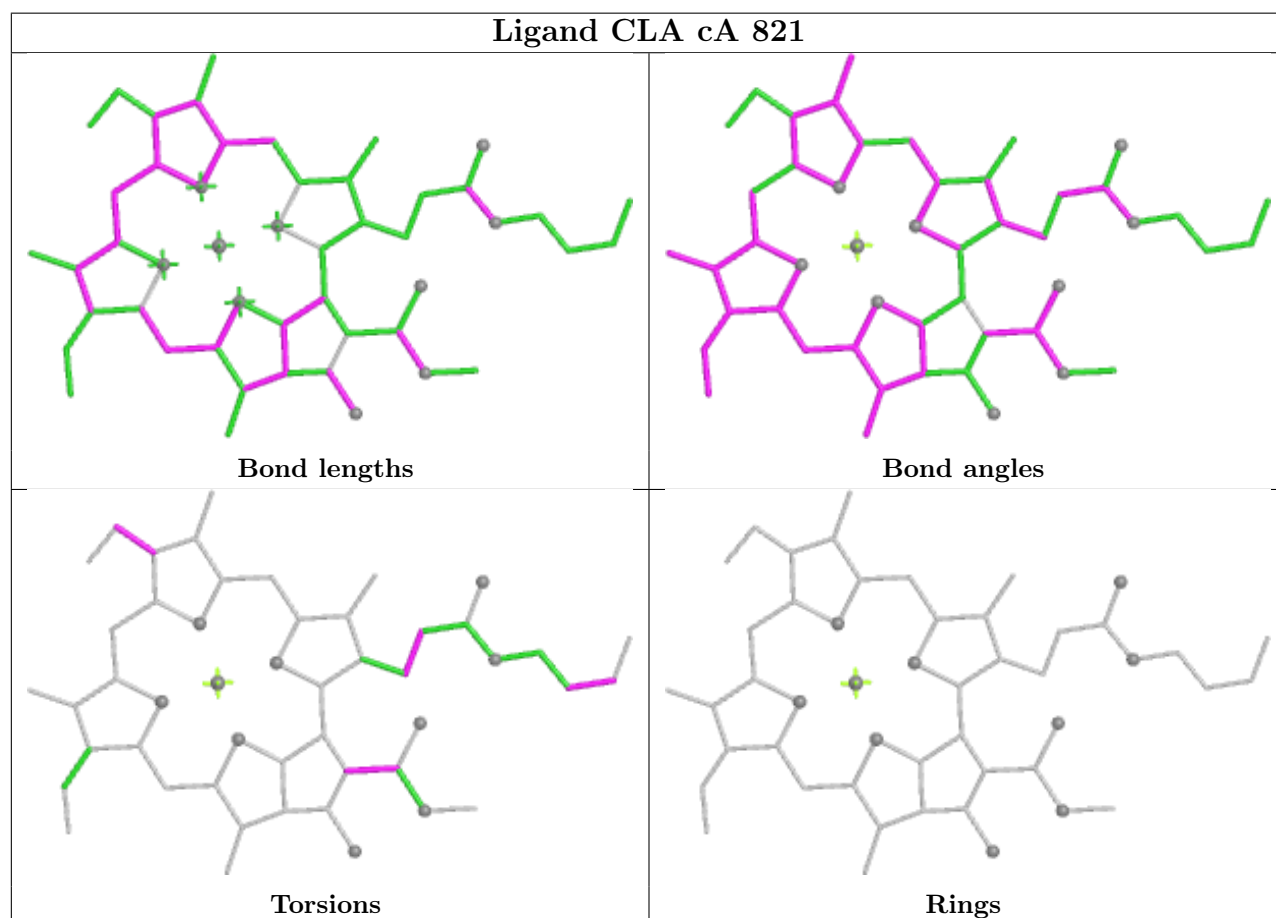
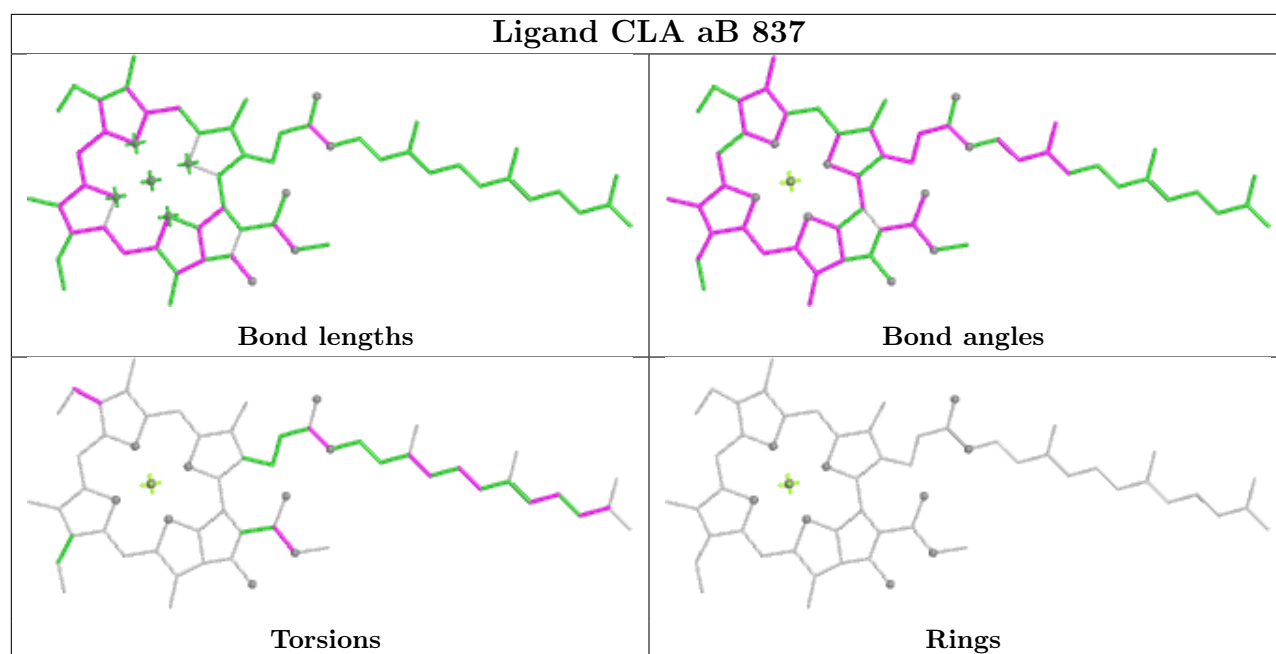
Ligand CLA bB 841

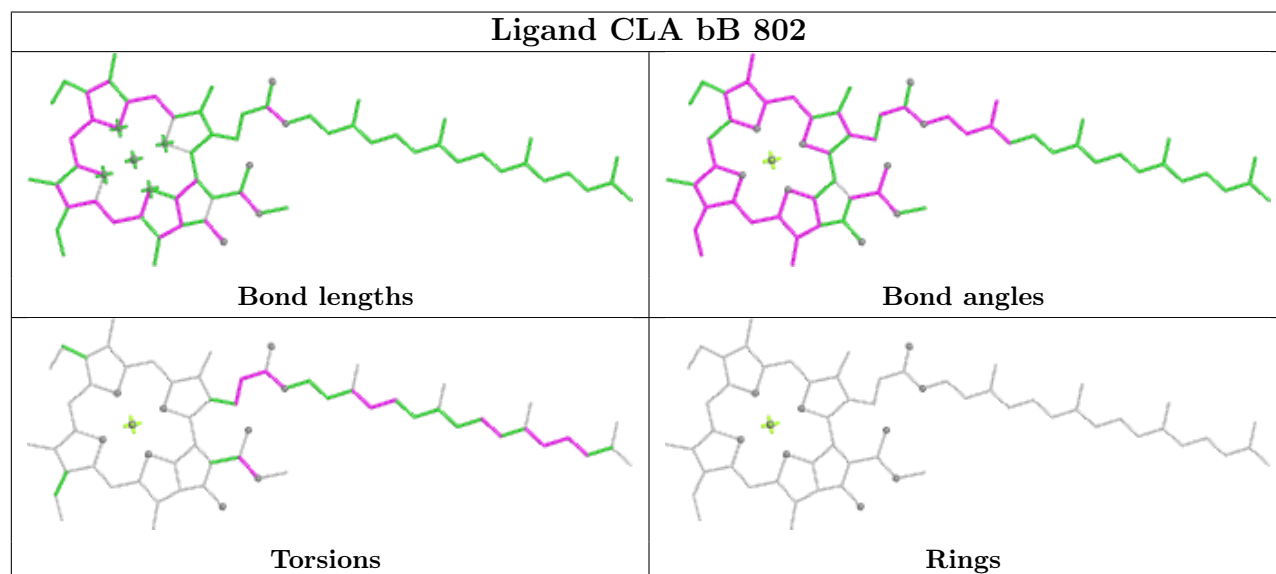
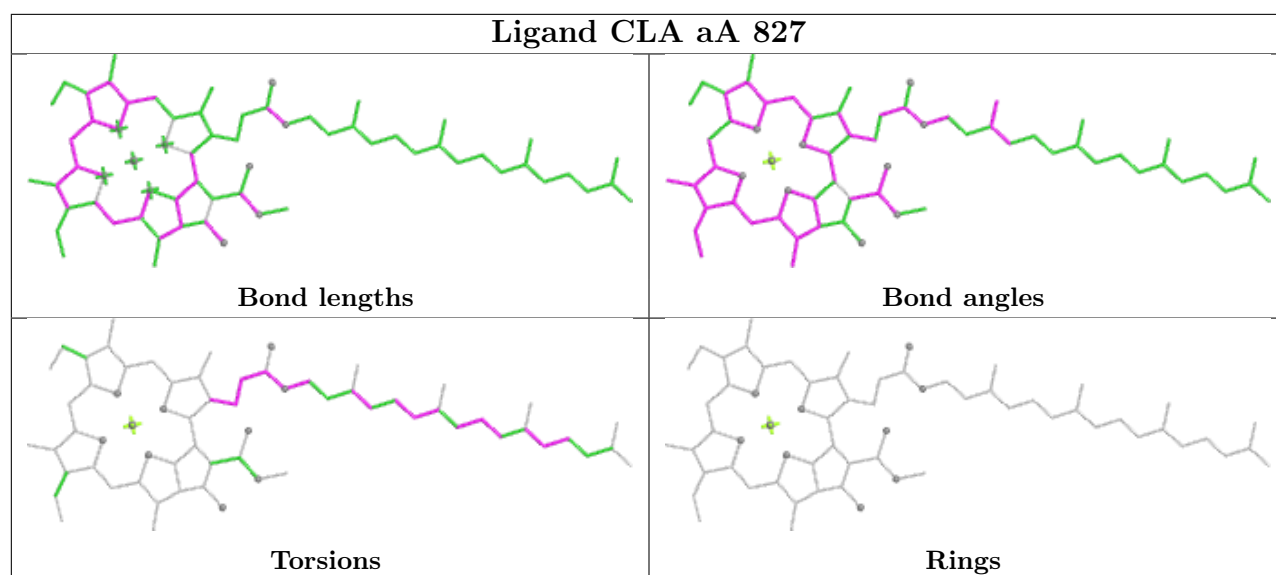


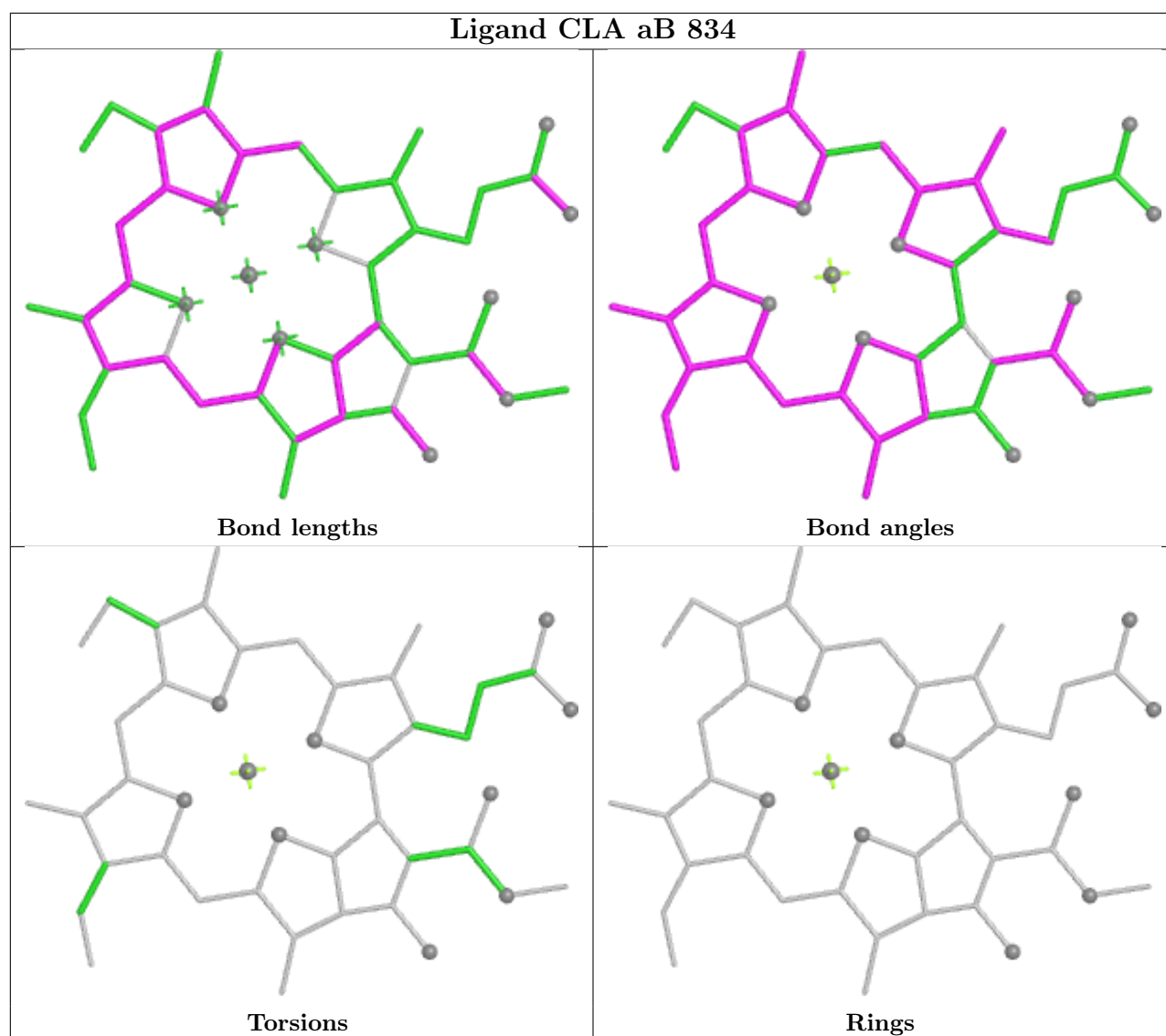
Ligand CLA aA 821

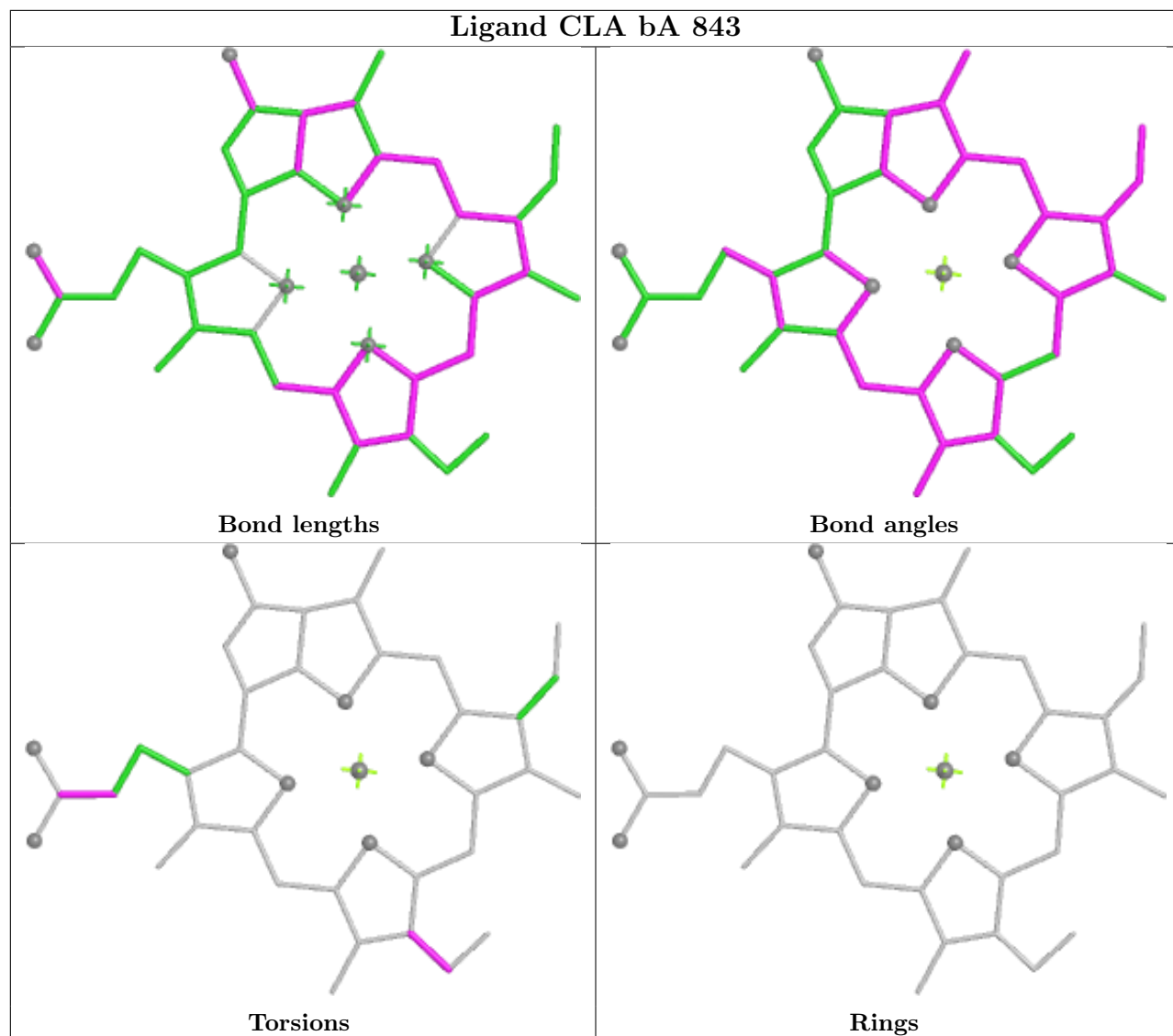




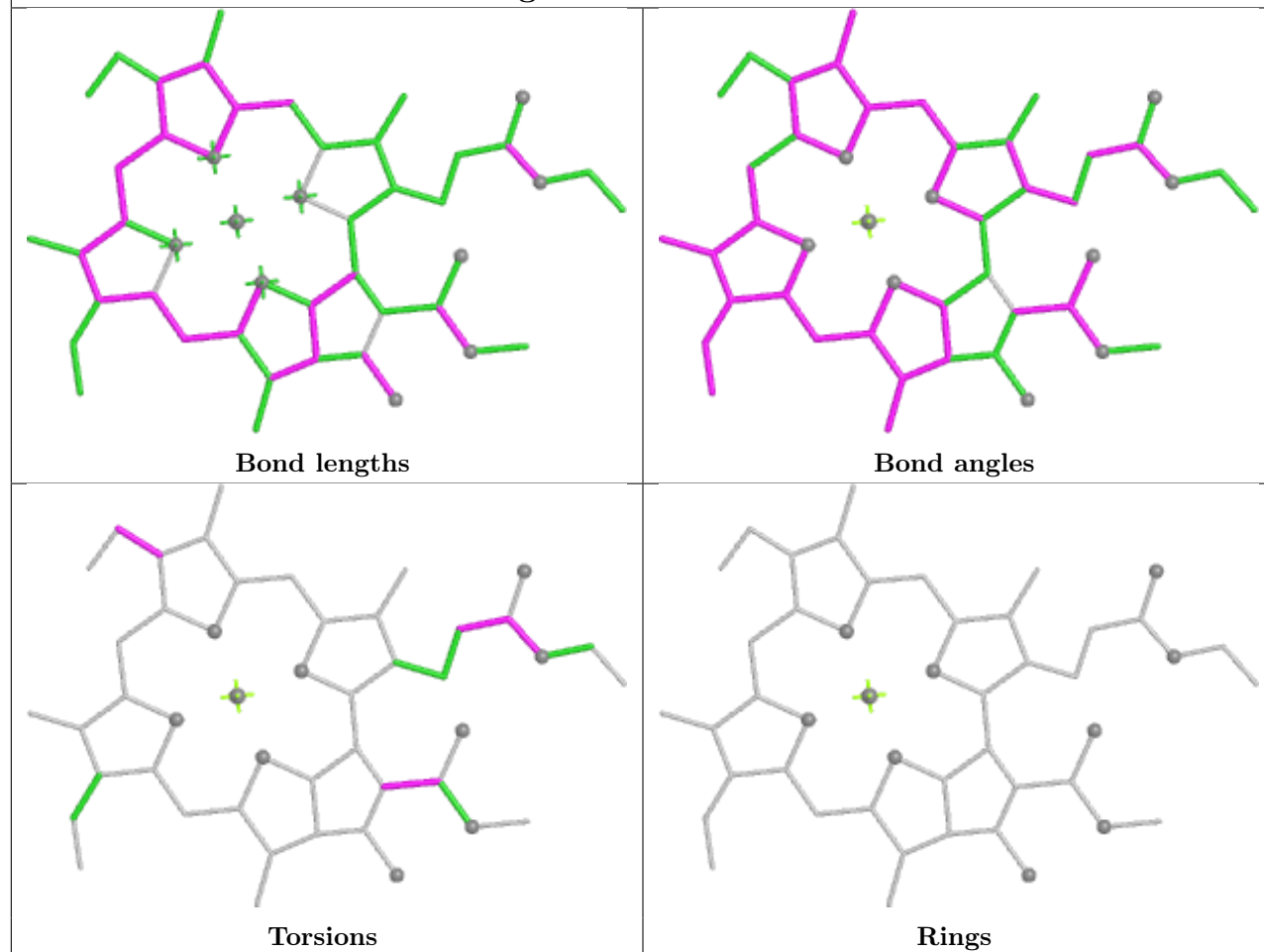




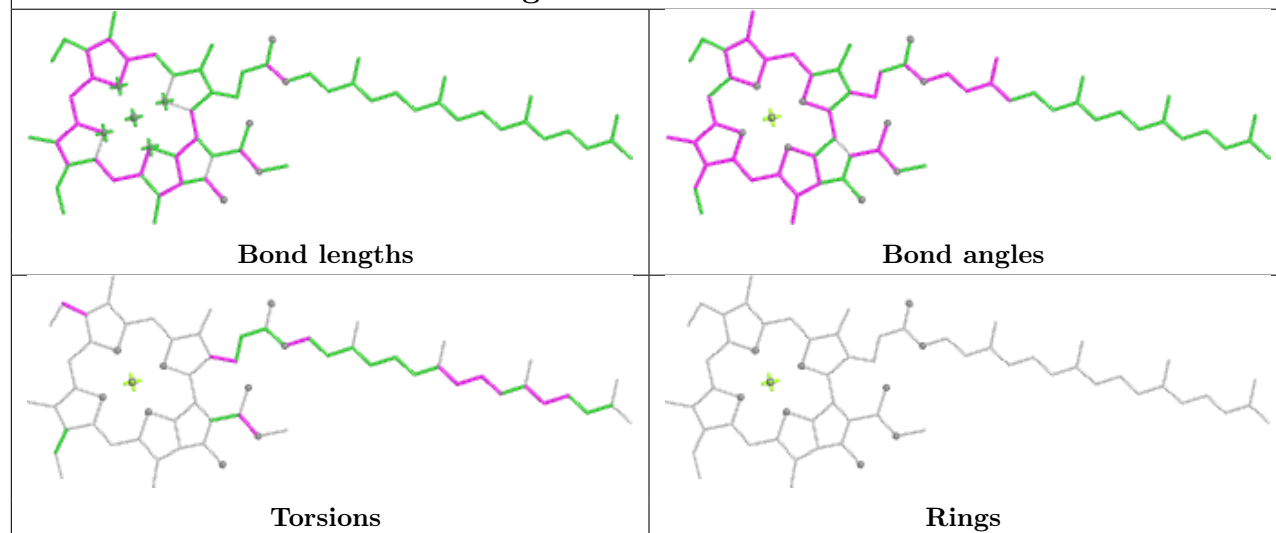


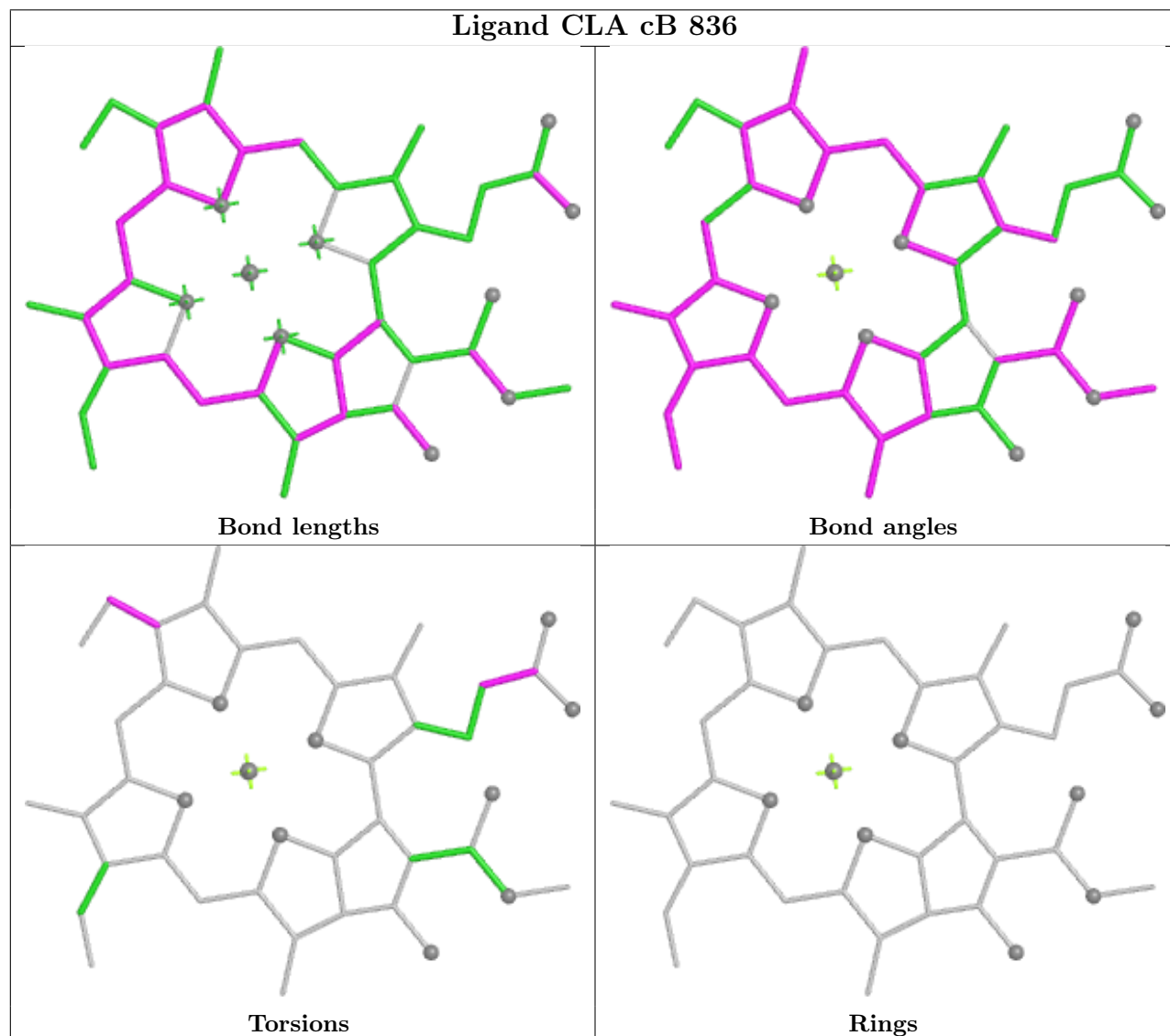
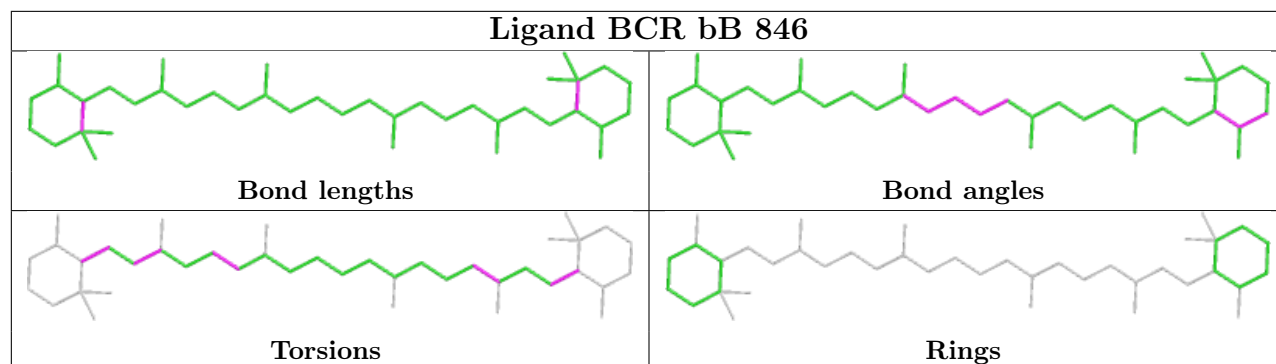


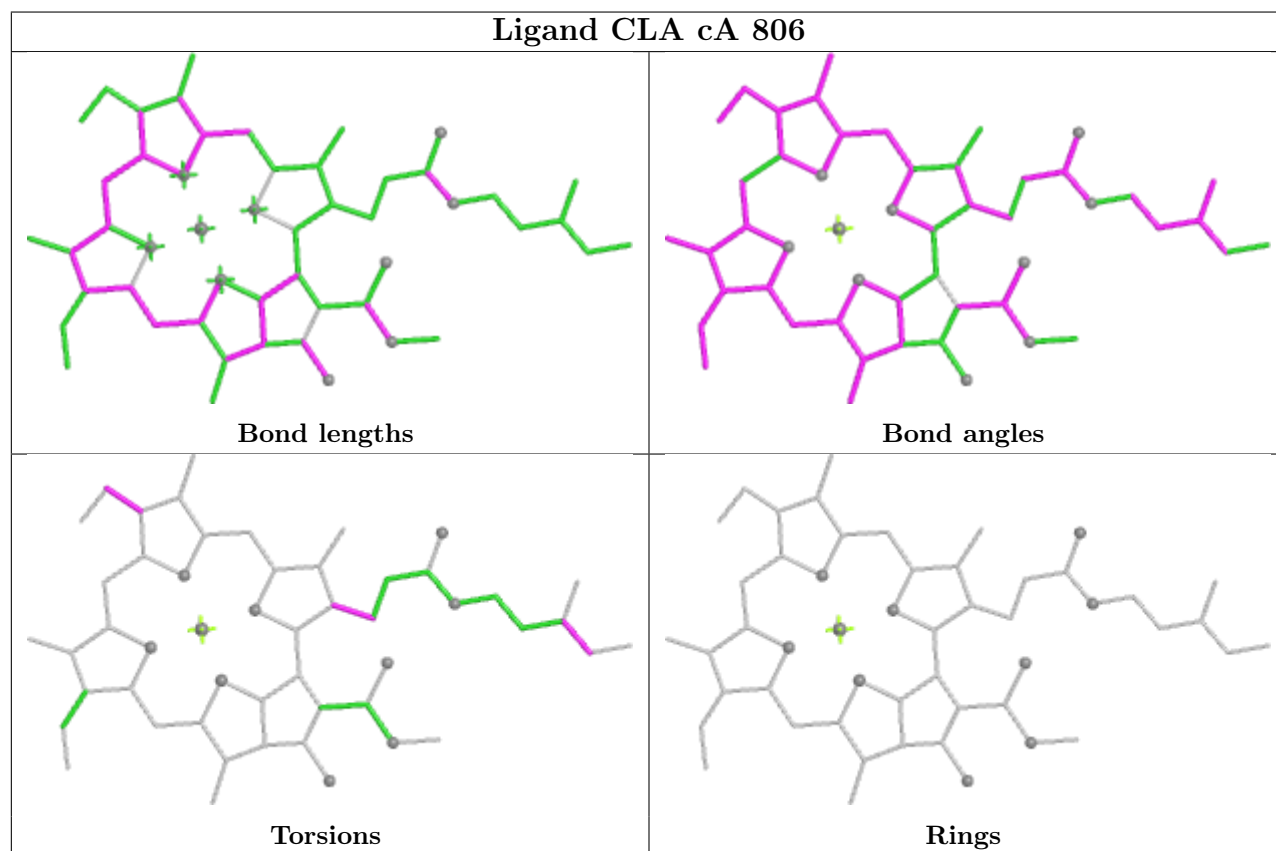
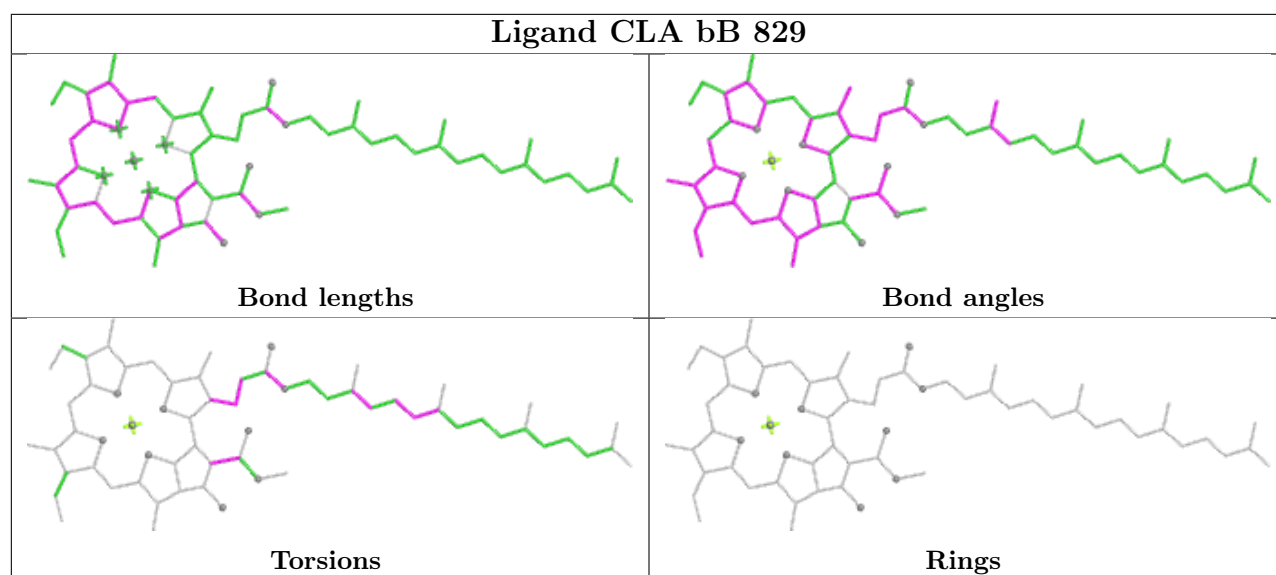
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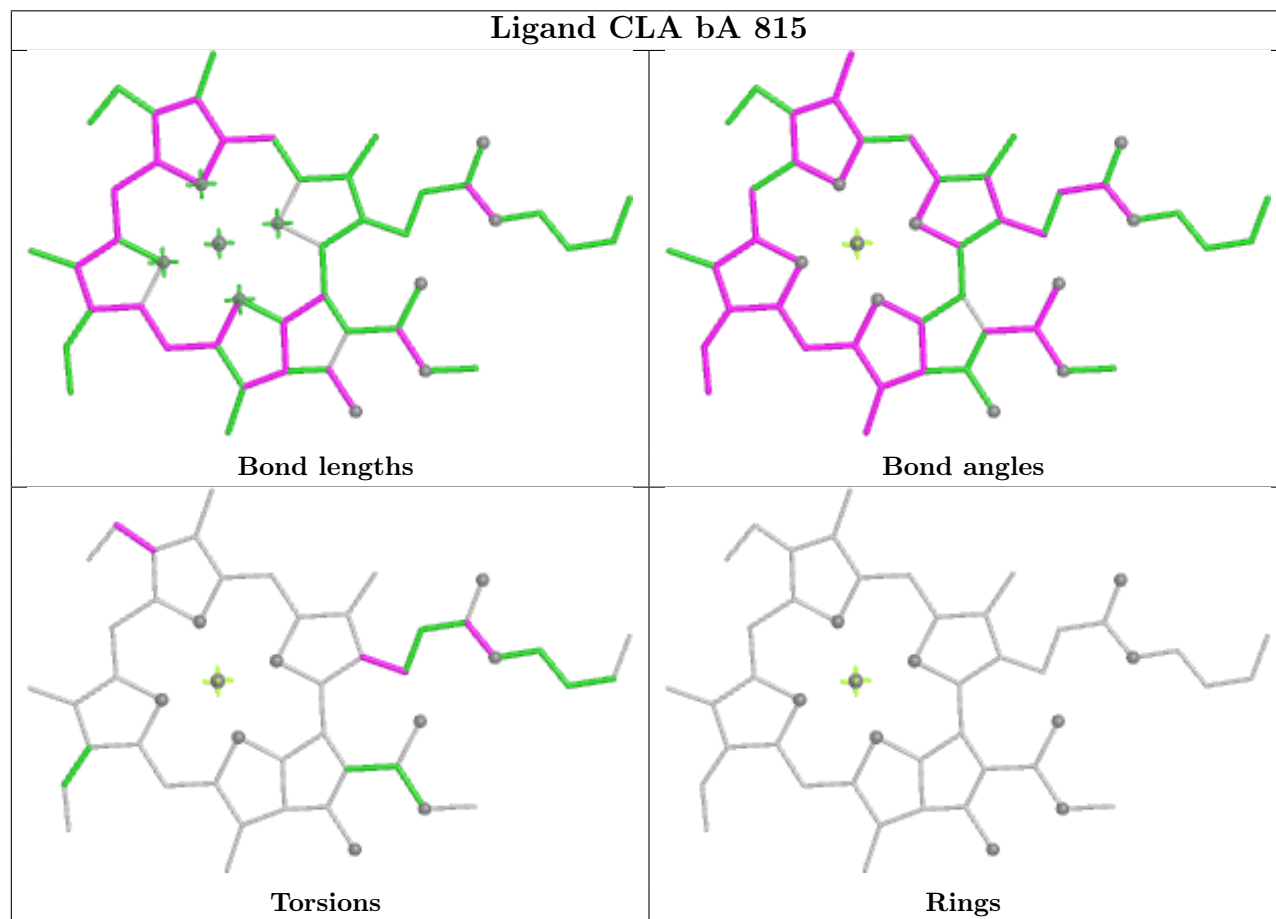
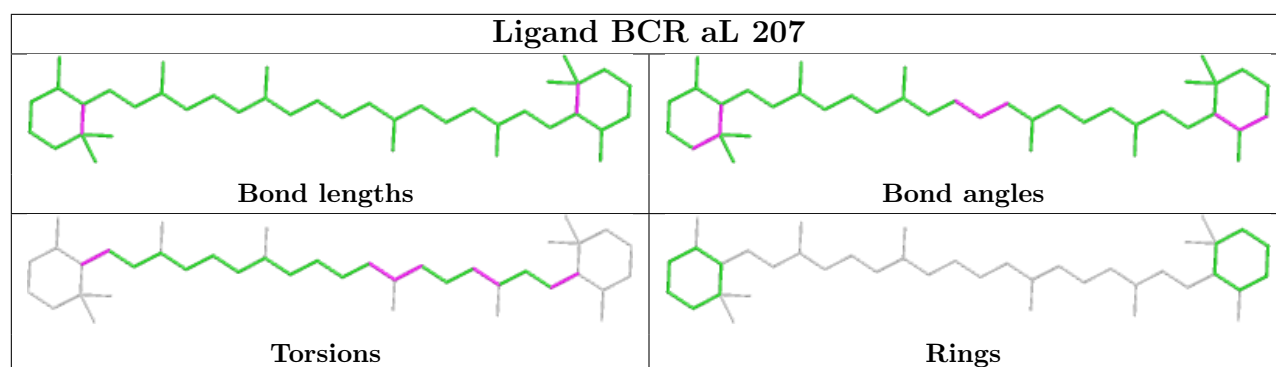


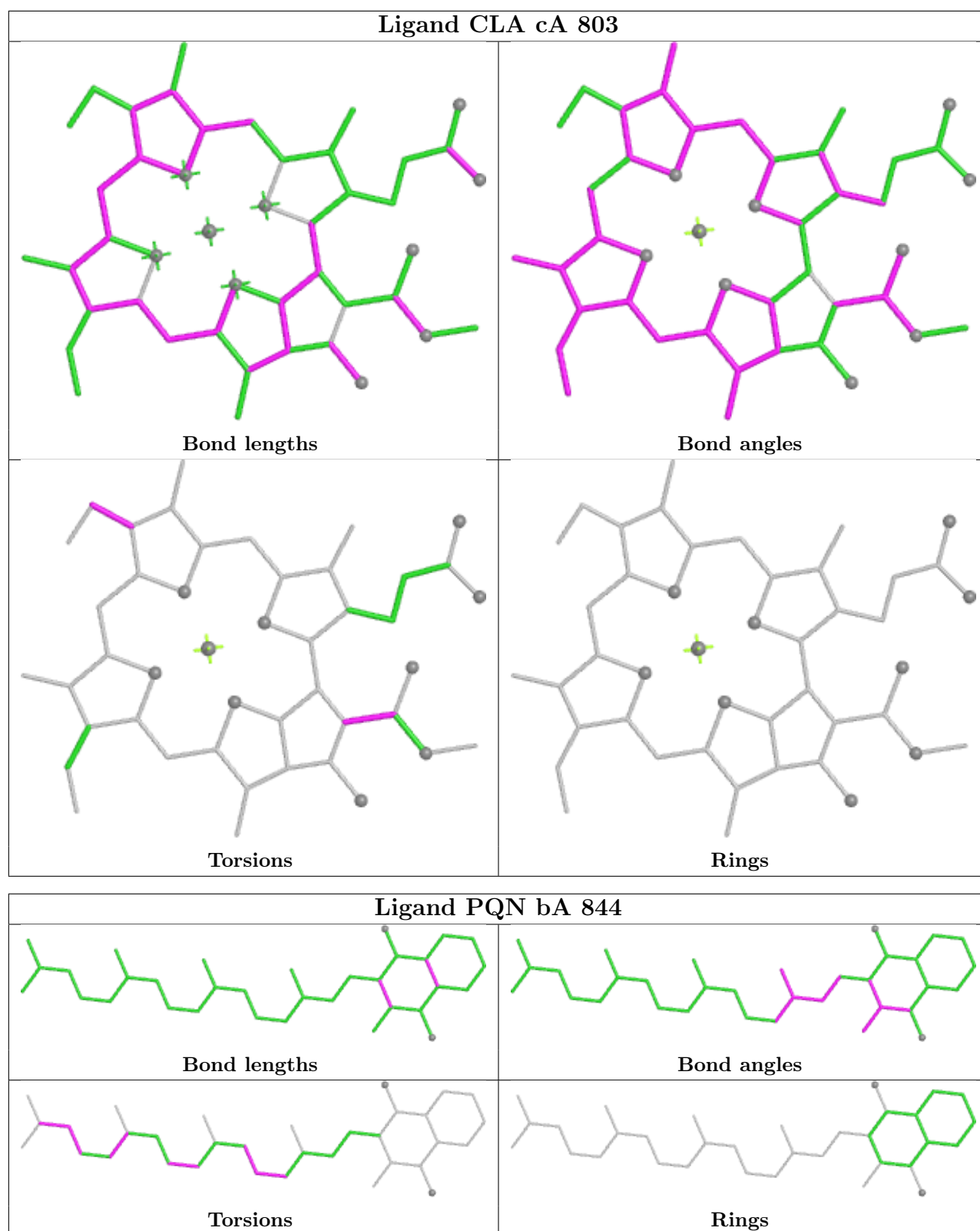
Ligand CLA bB 828

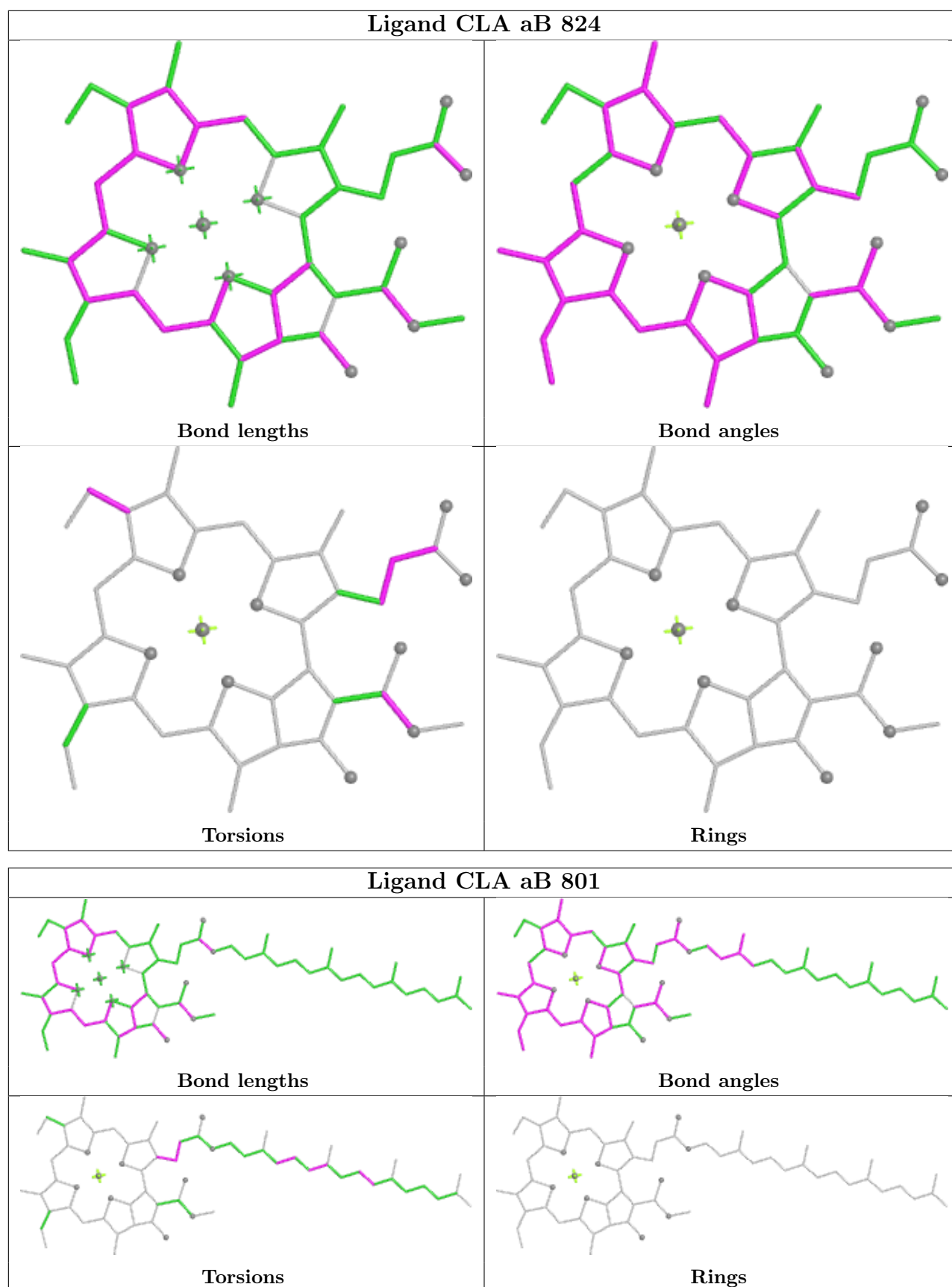


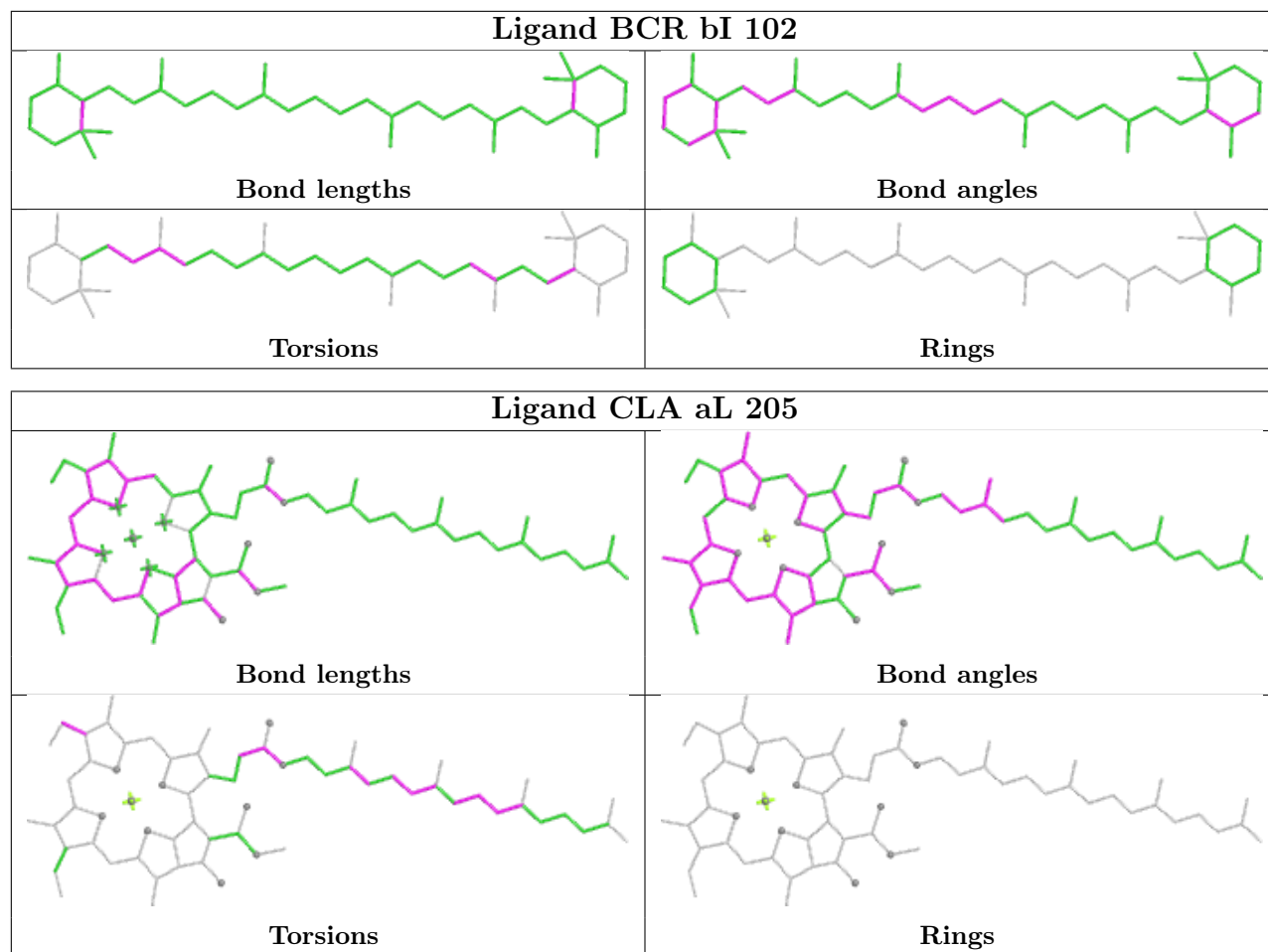




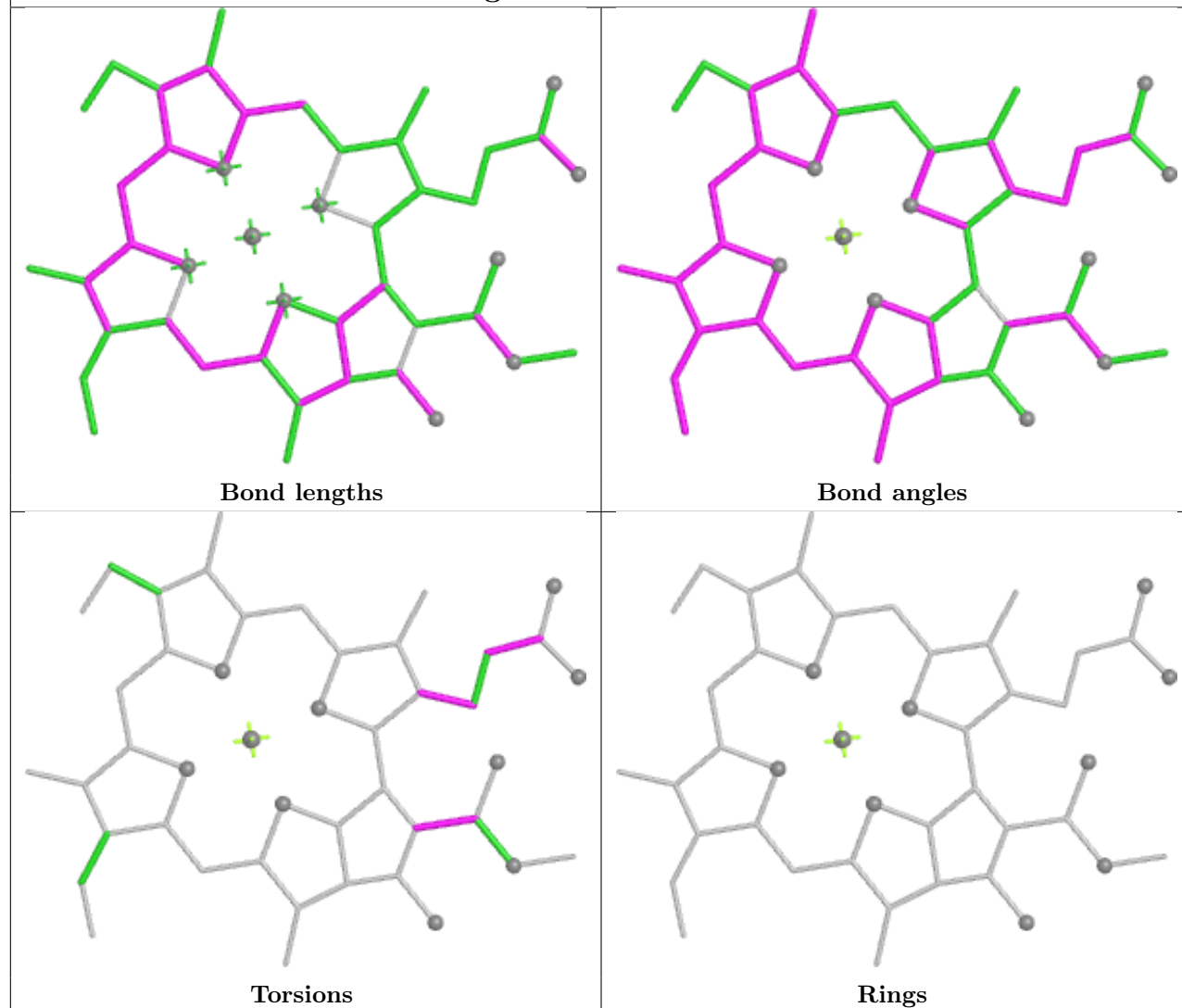




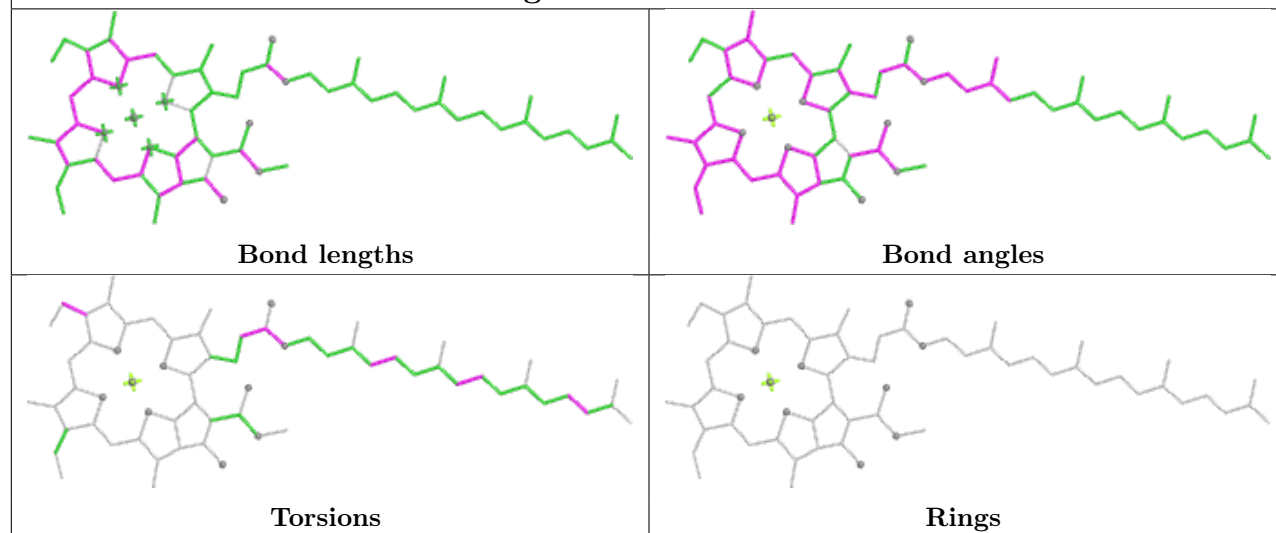




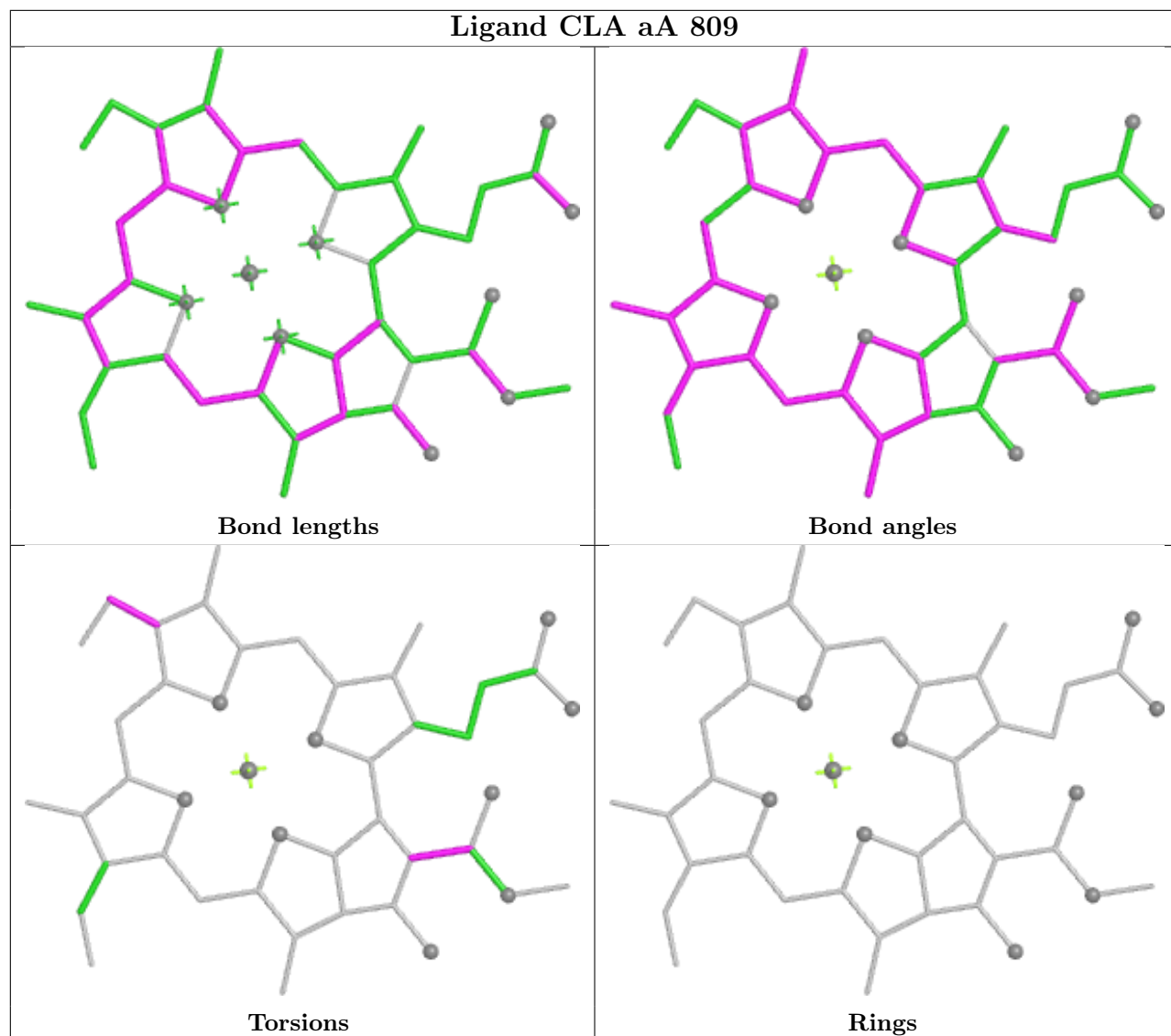
Ligand CLA aA 808

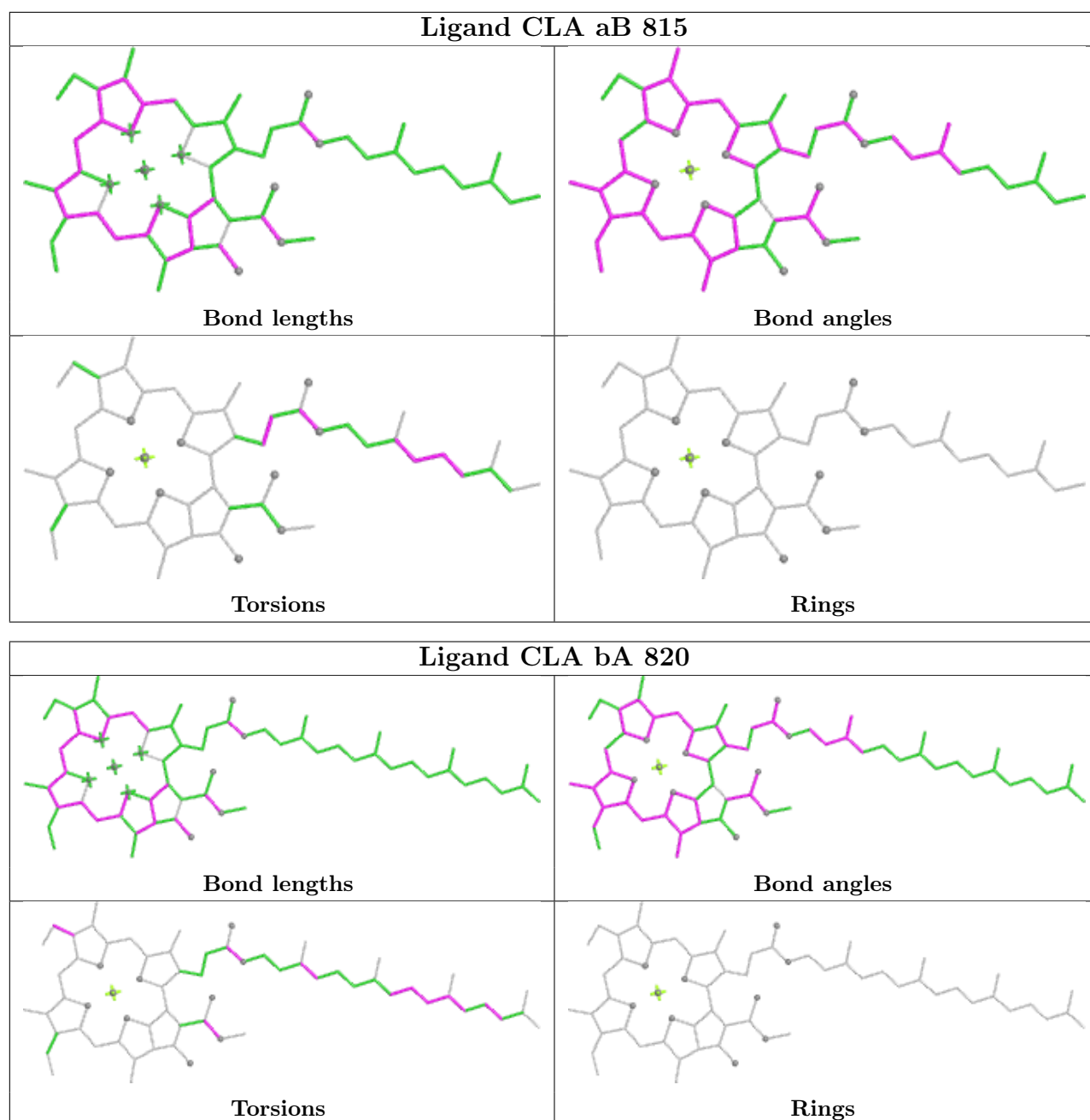


Ligand CLA cA 837

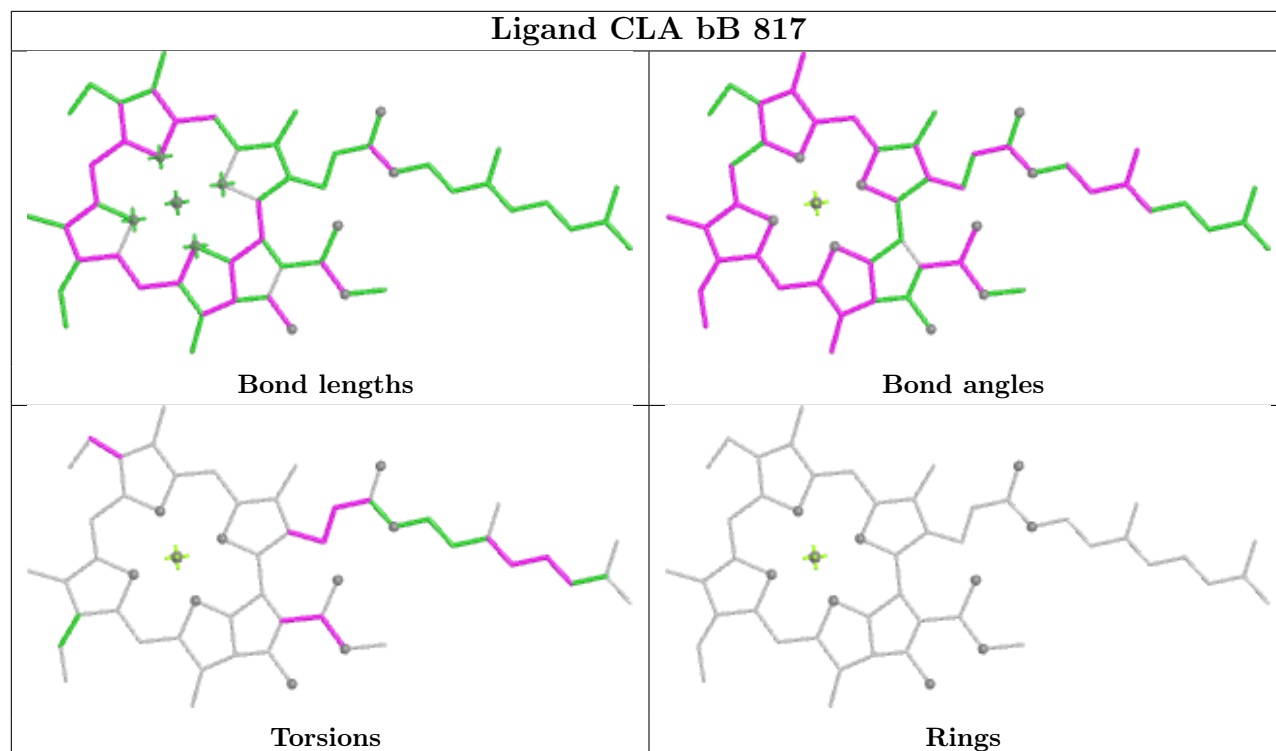


Ligand CLA aA 809

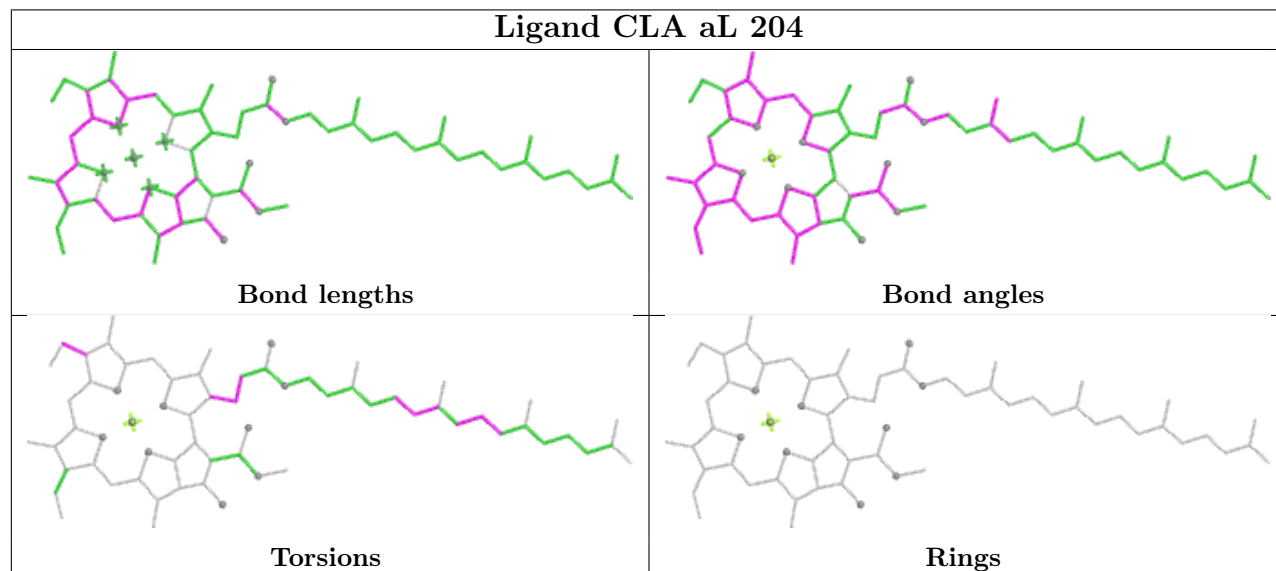


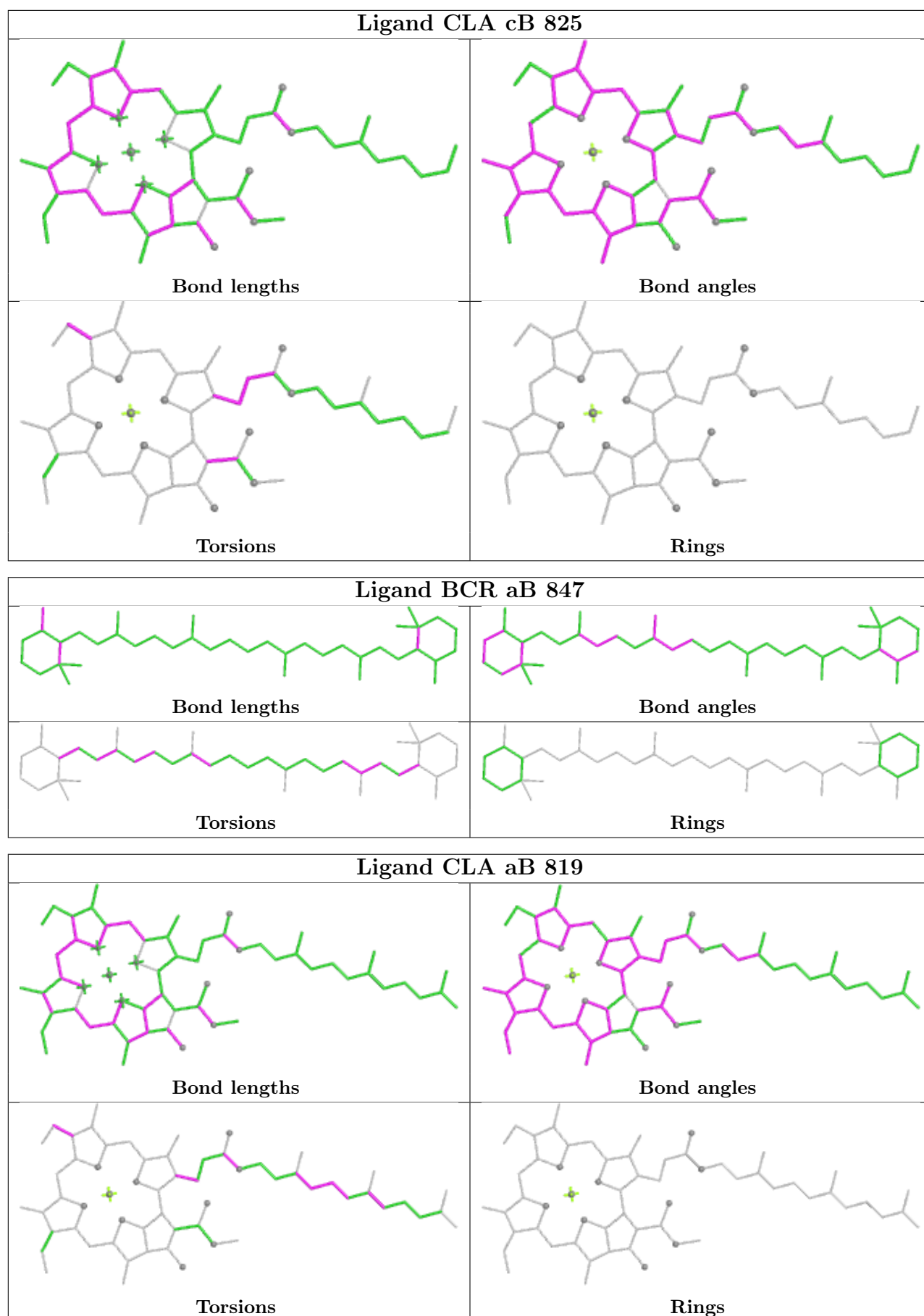


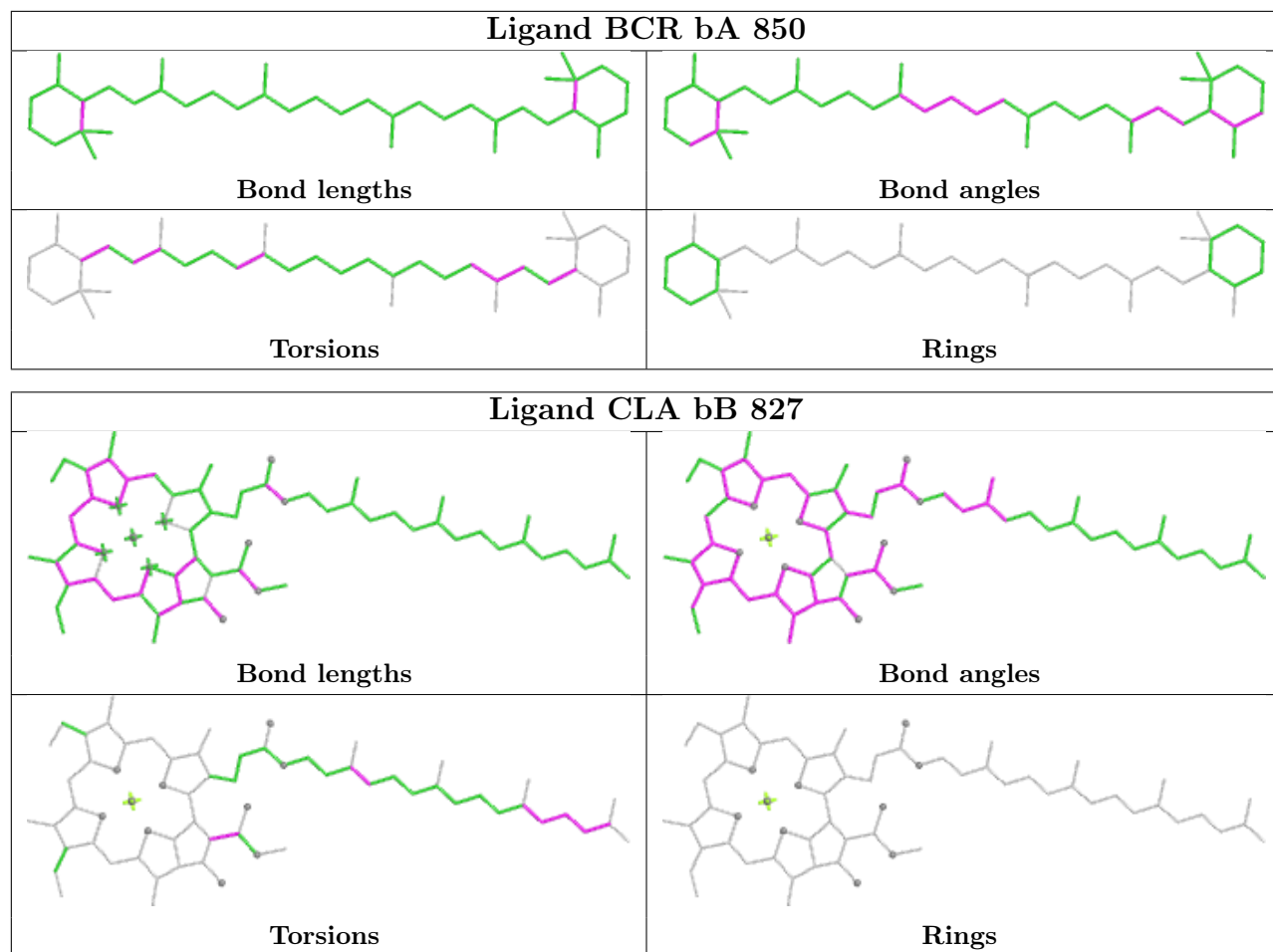
Ligand CLA bB 817



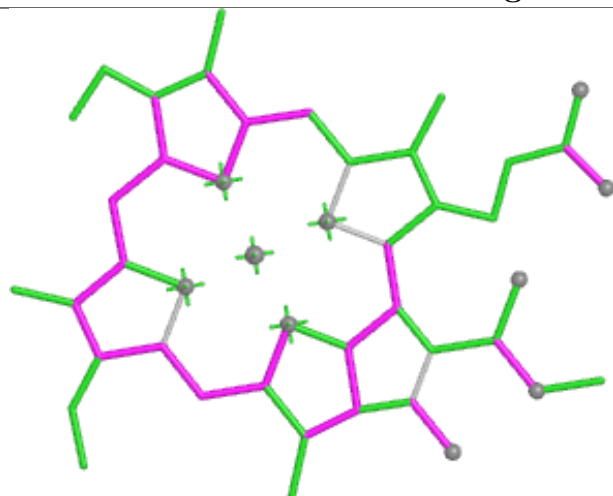
Ligand CLA aL 204



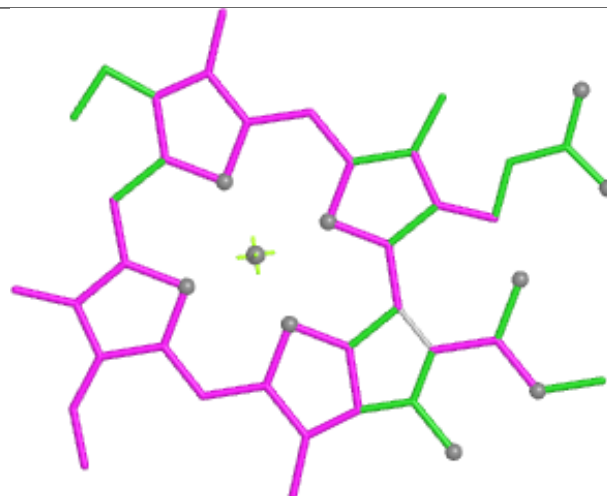




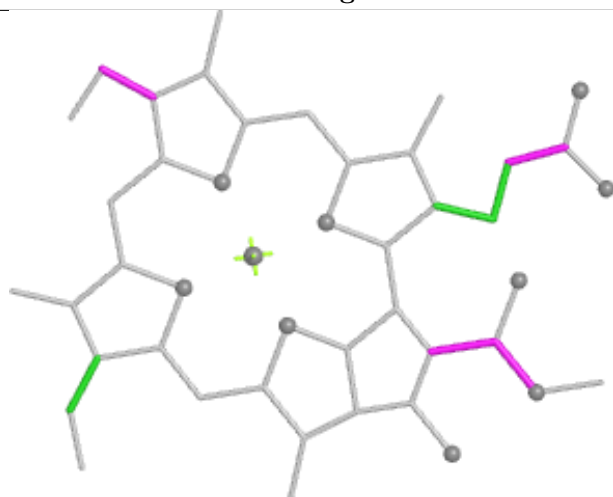
Ligand CLA bB 835



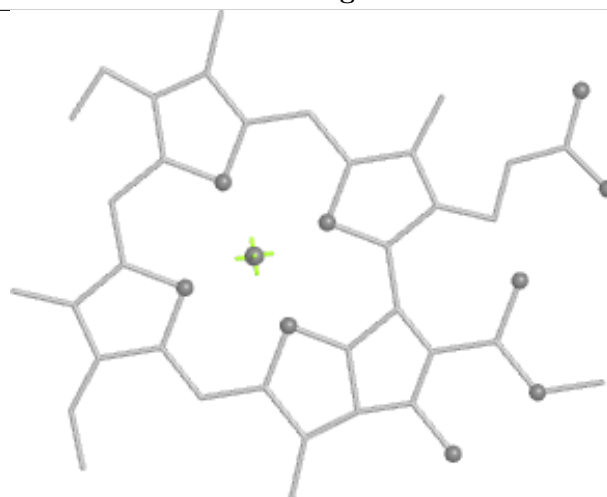
Bond lengths



Bond angles

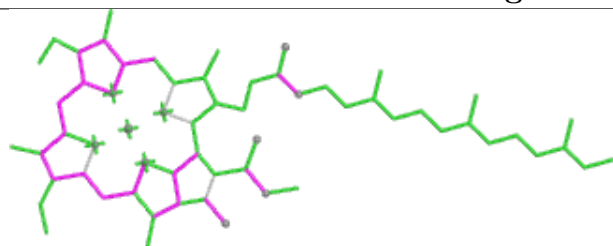


Torsions

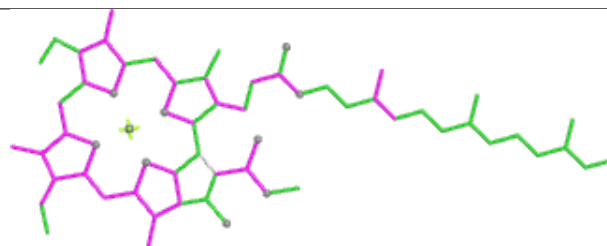


Rings

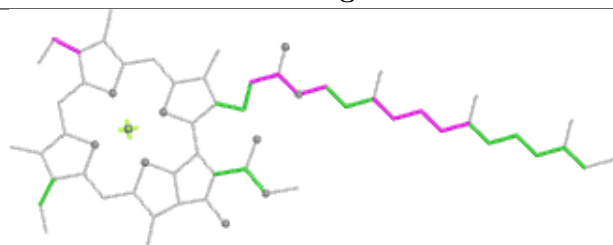
Ligand CLA aA 819



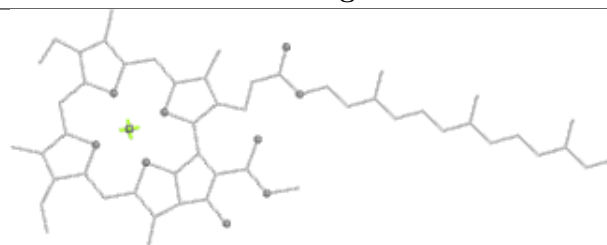
Bond lengths



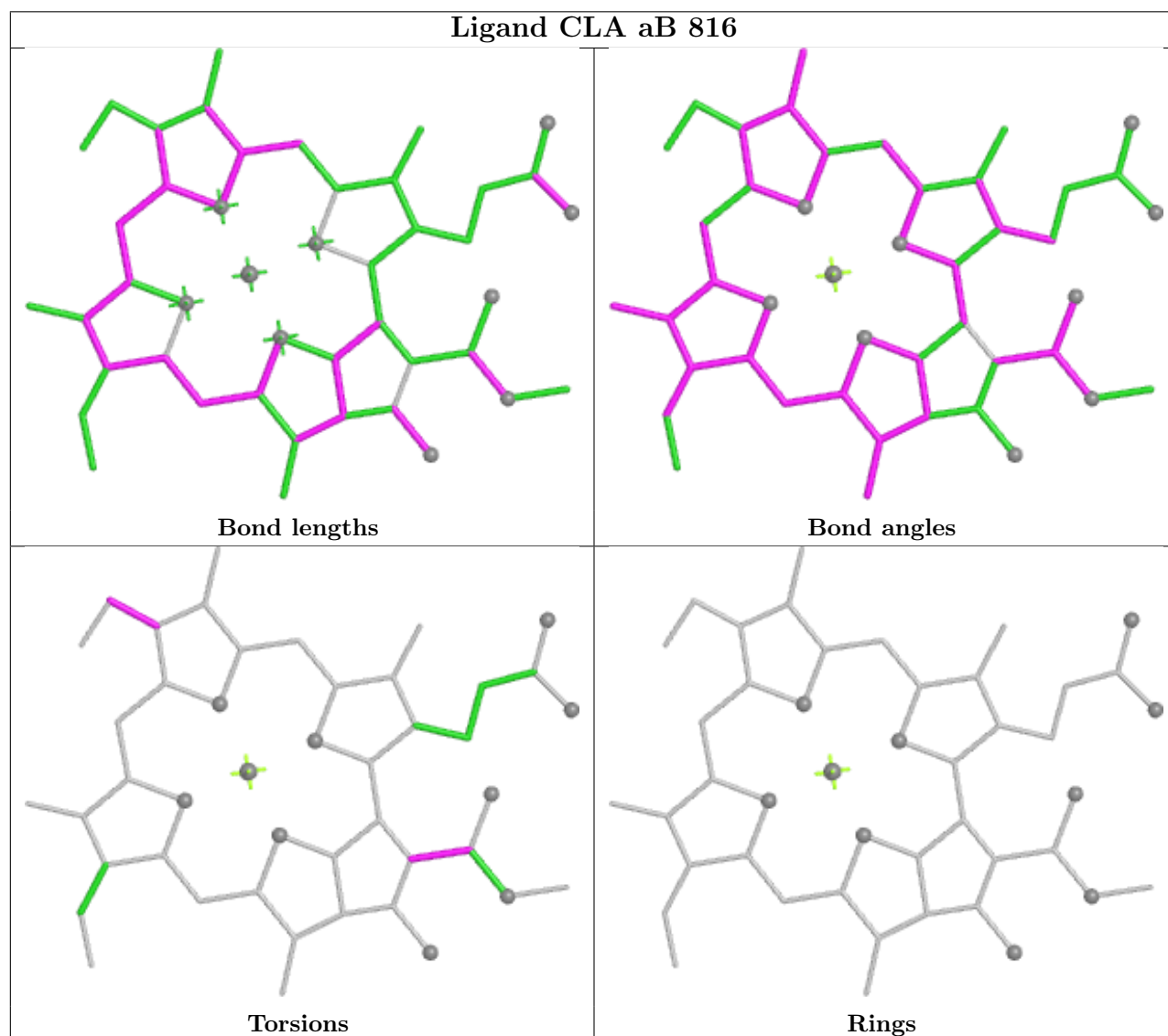
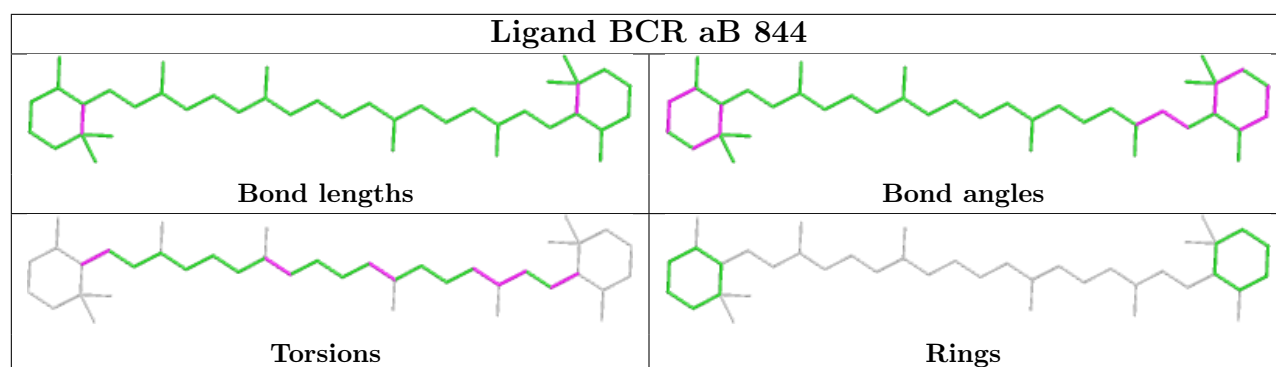
Bond angles

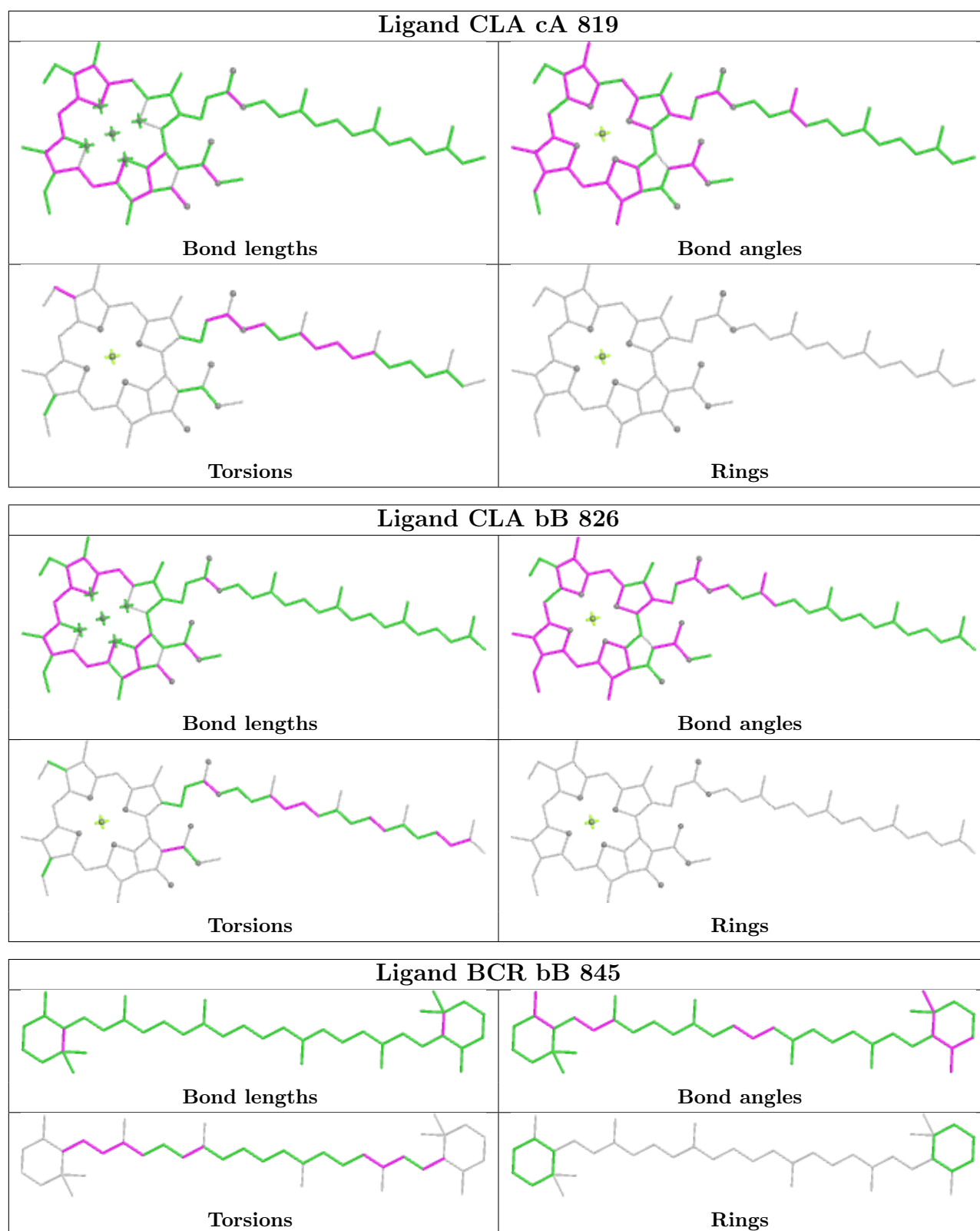


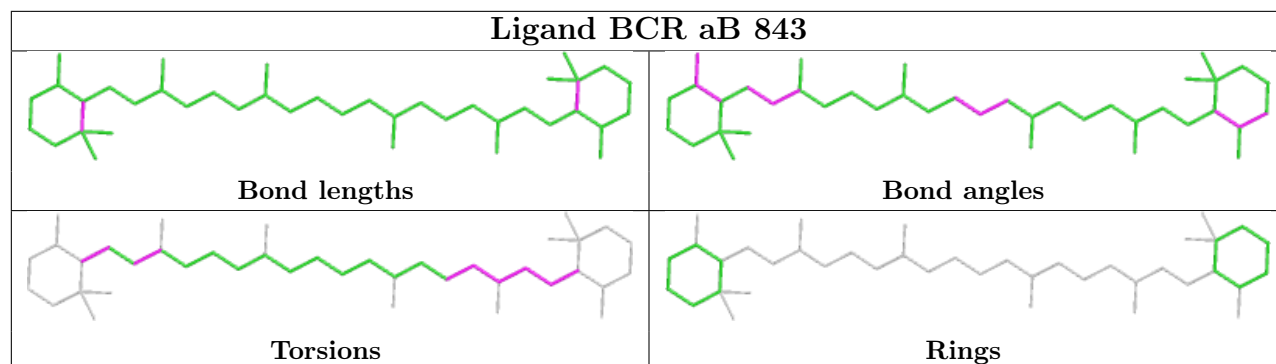
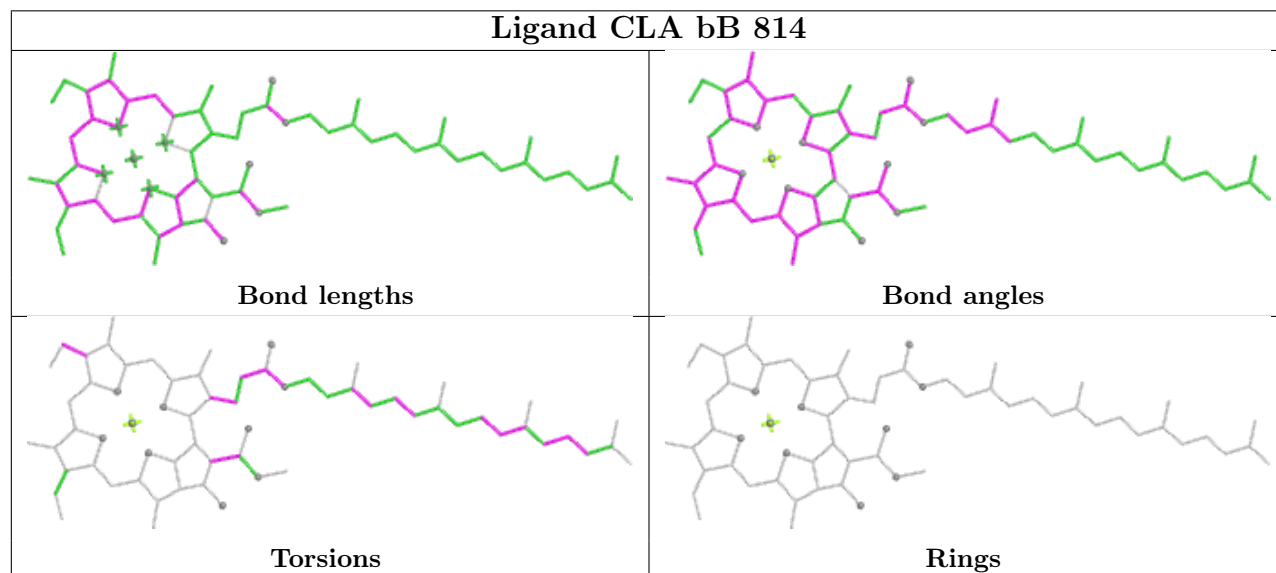
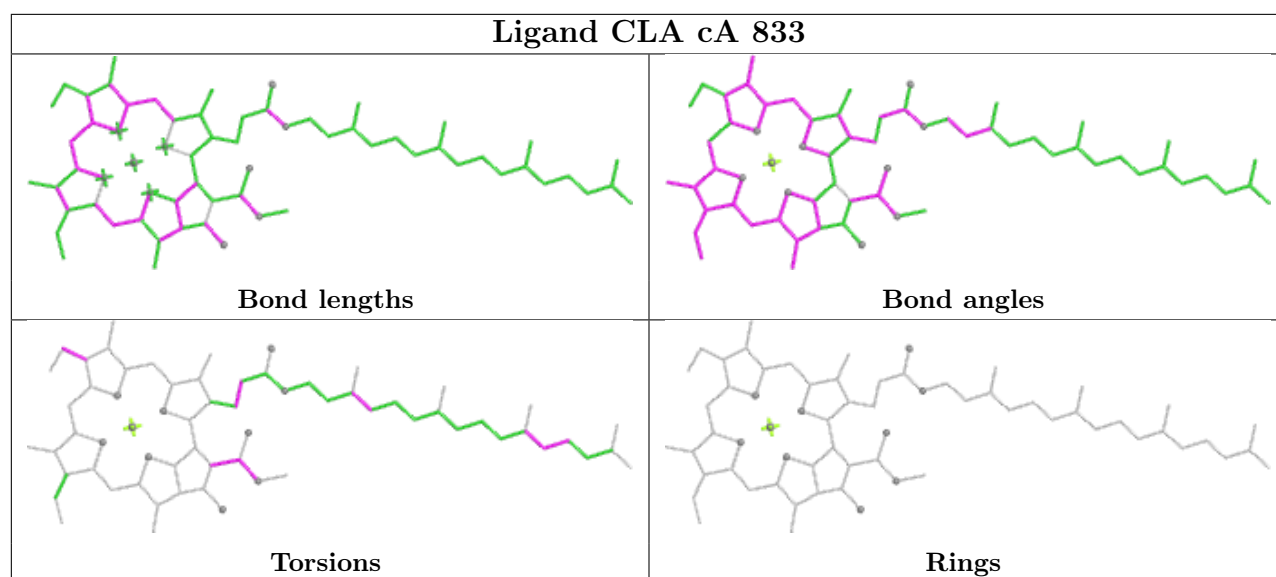
Torsions

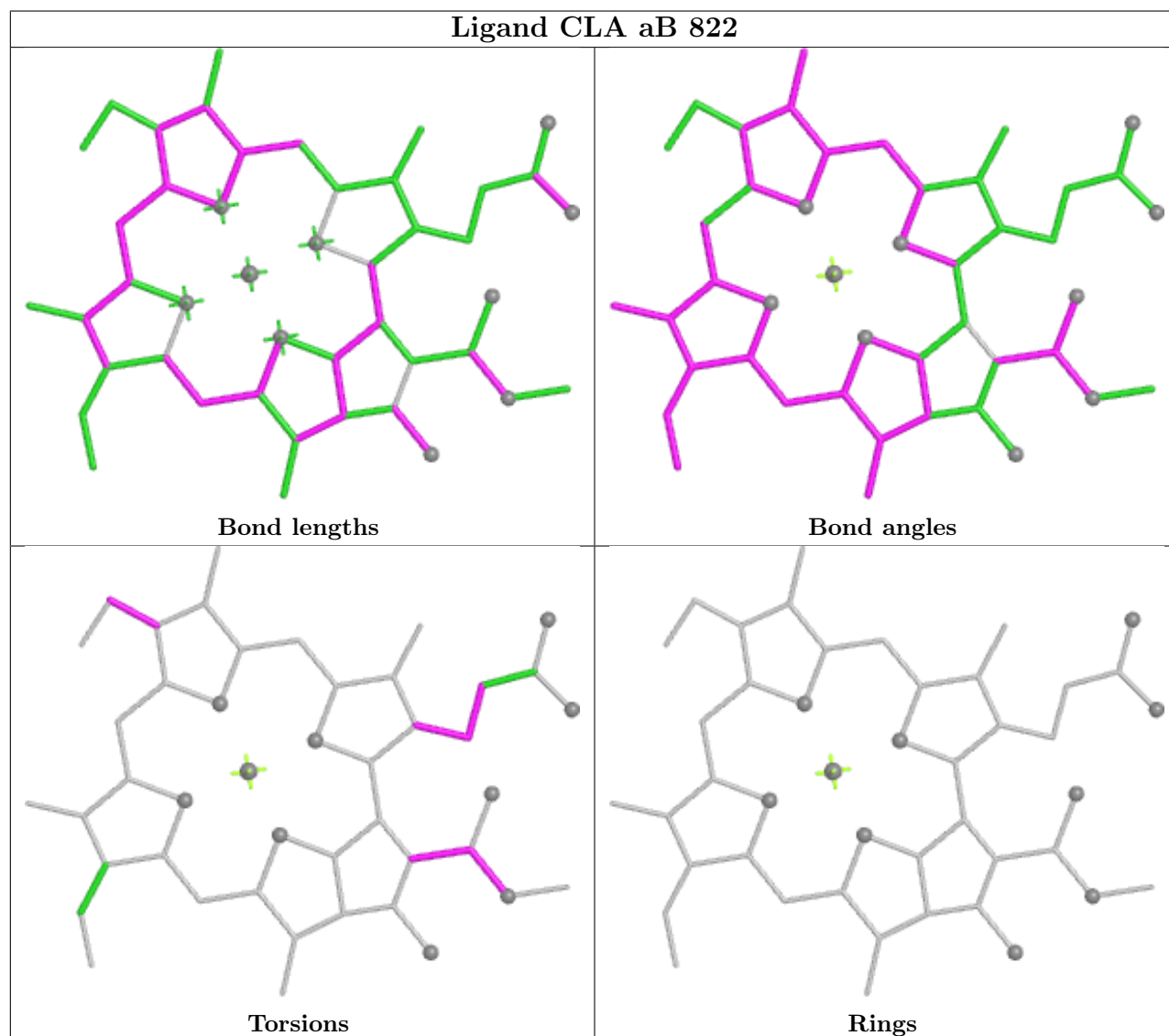
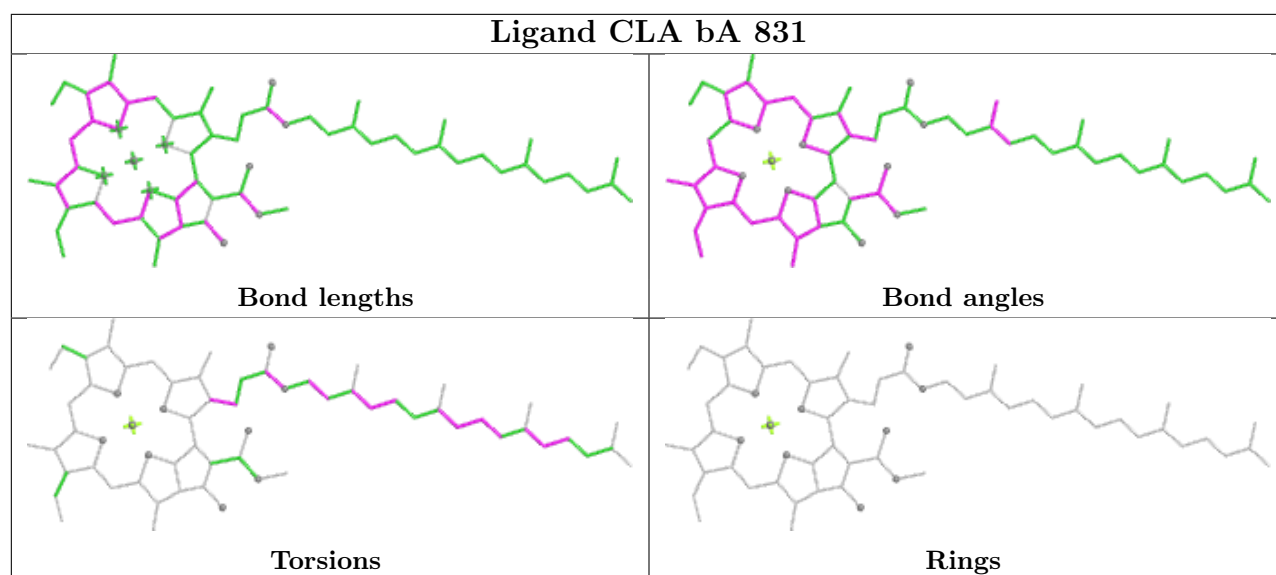


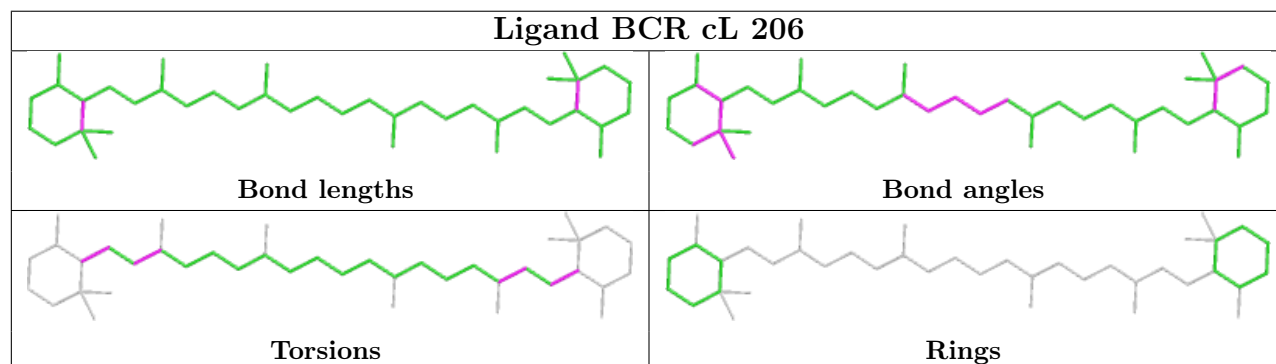
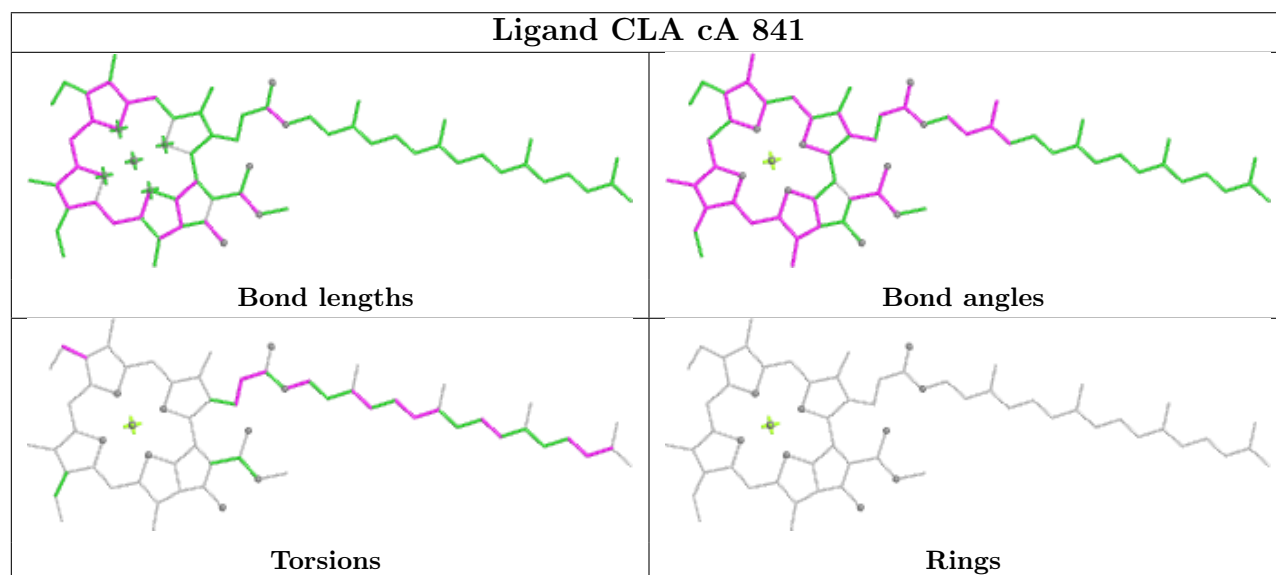
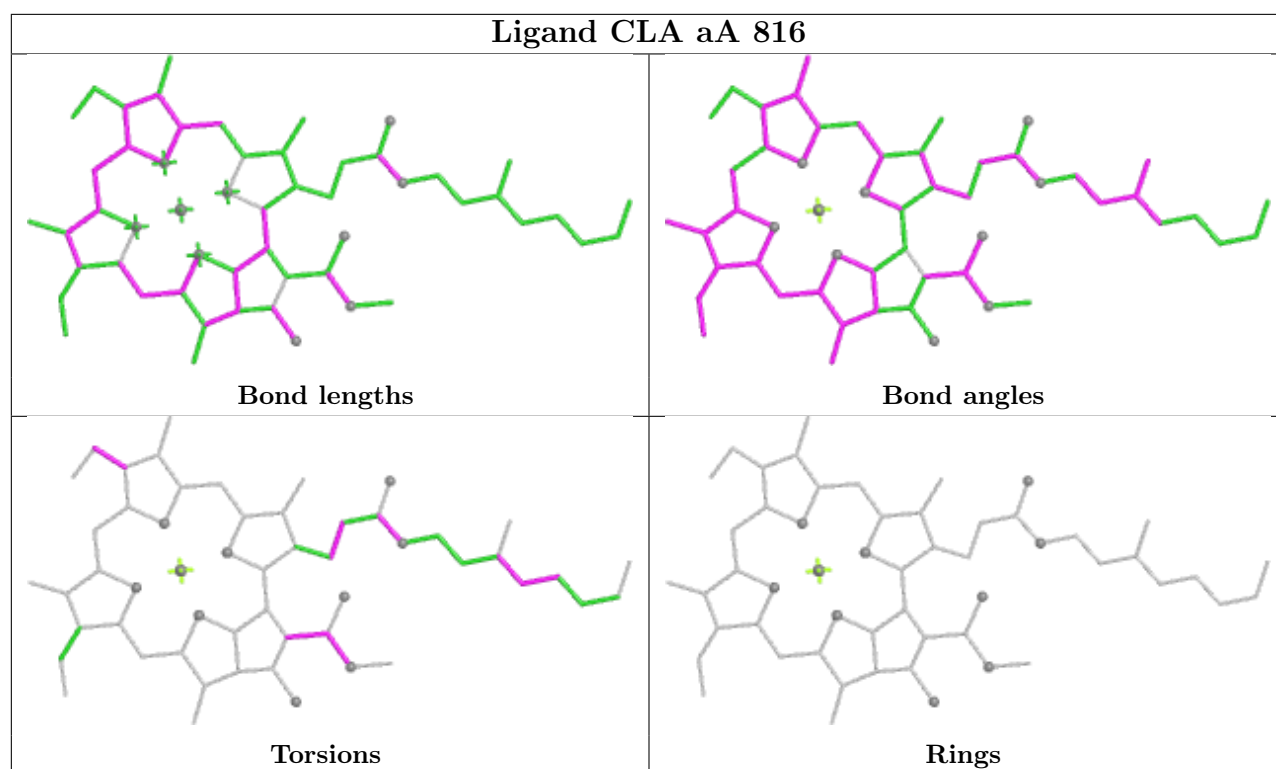
Rings



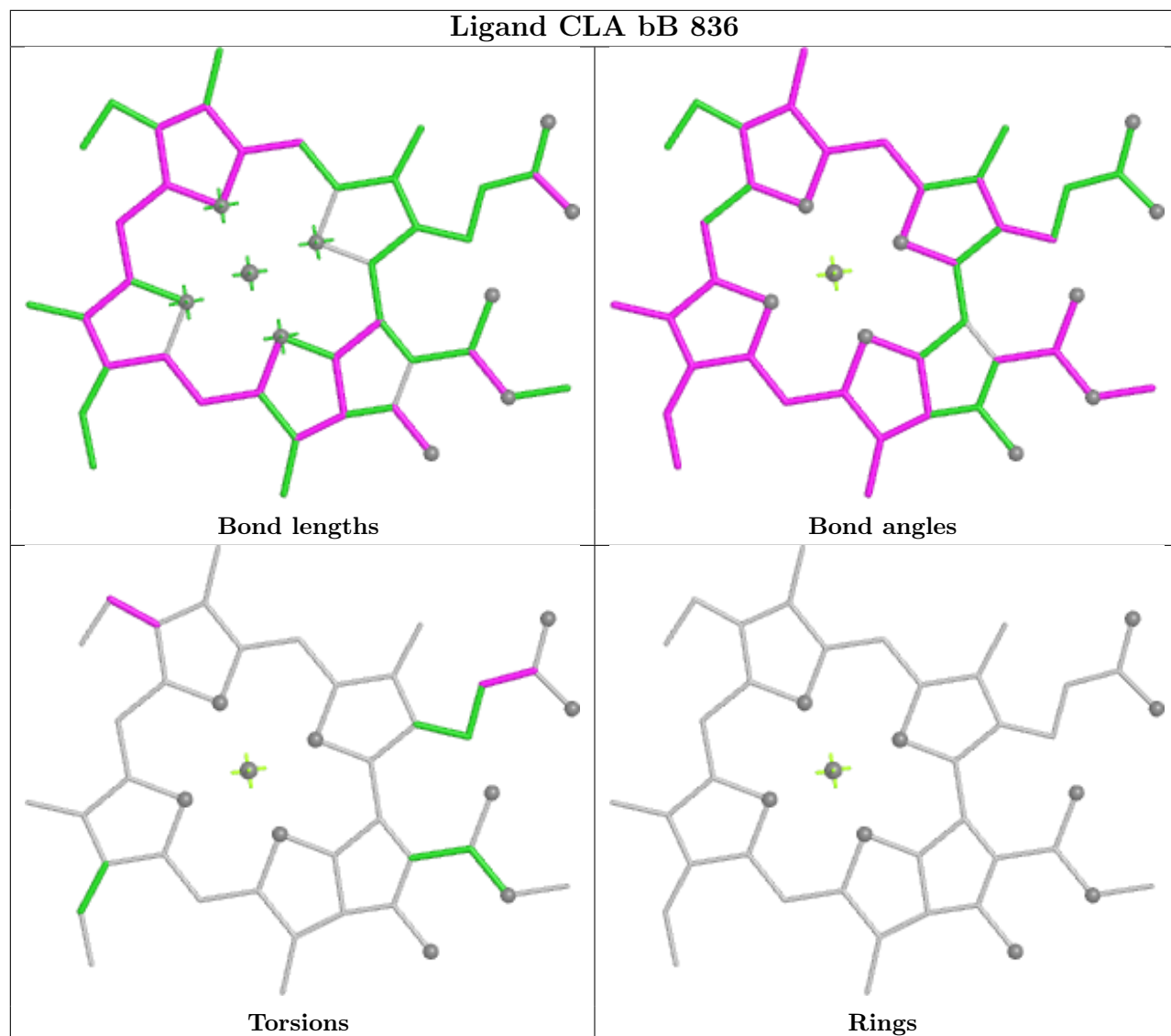


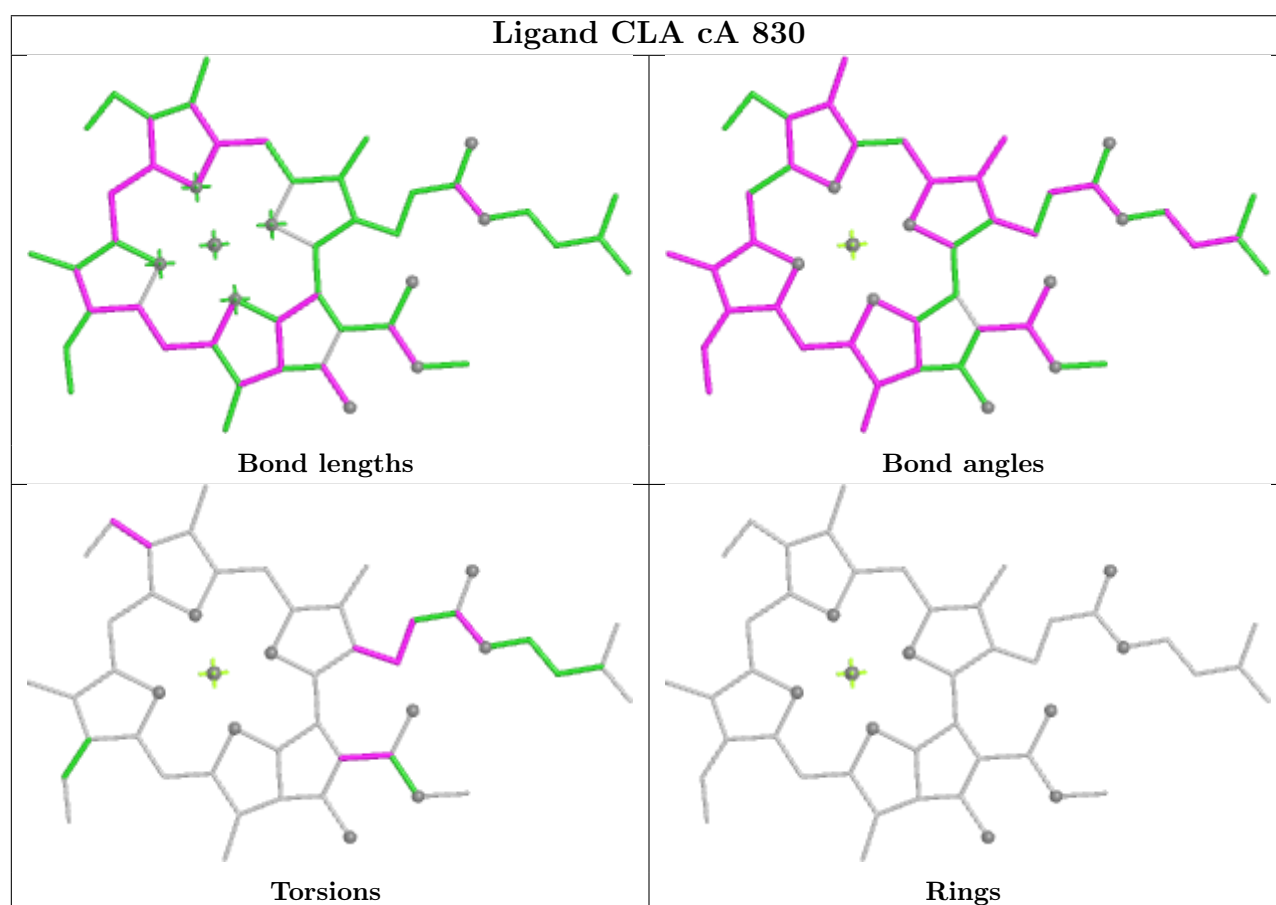
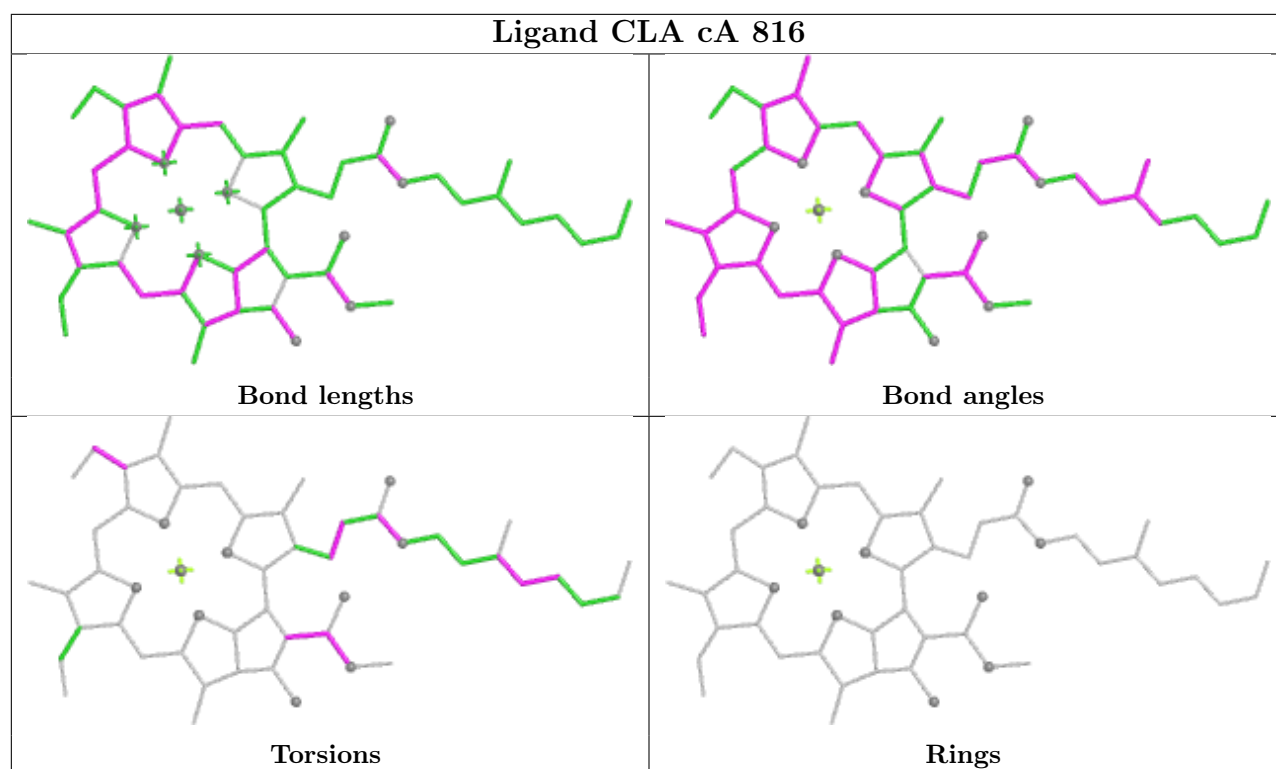


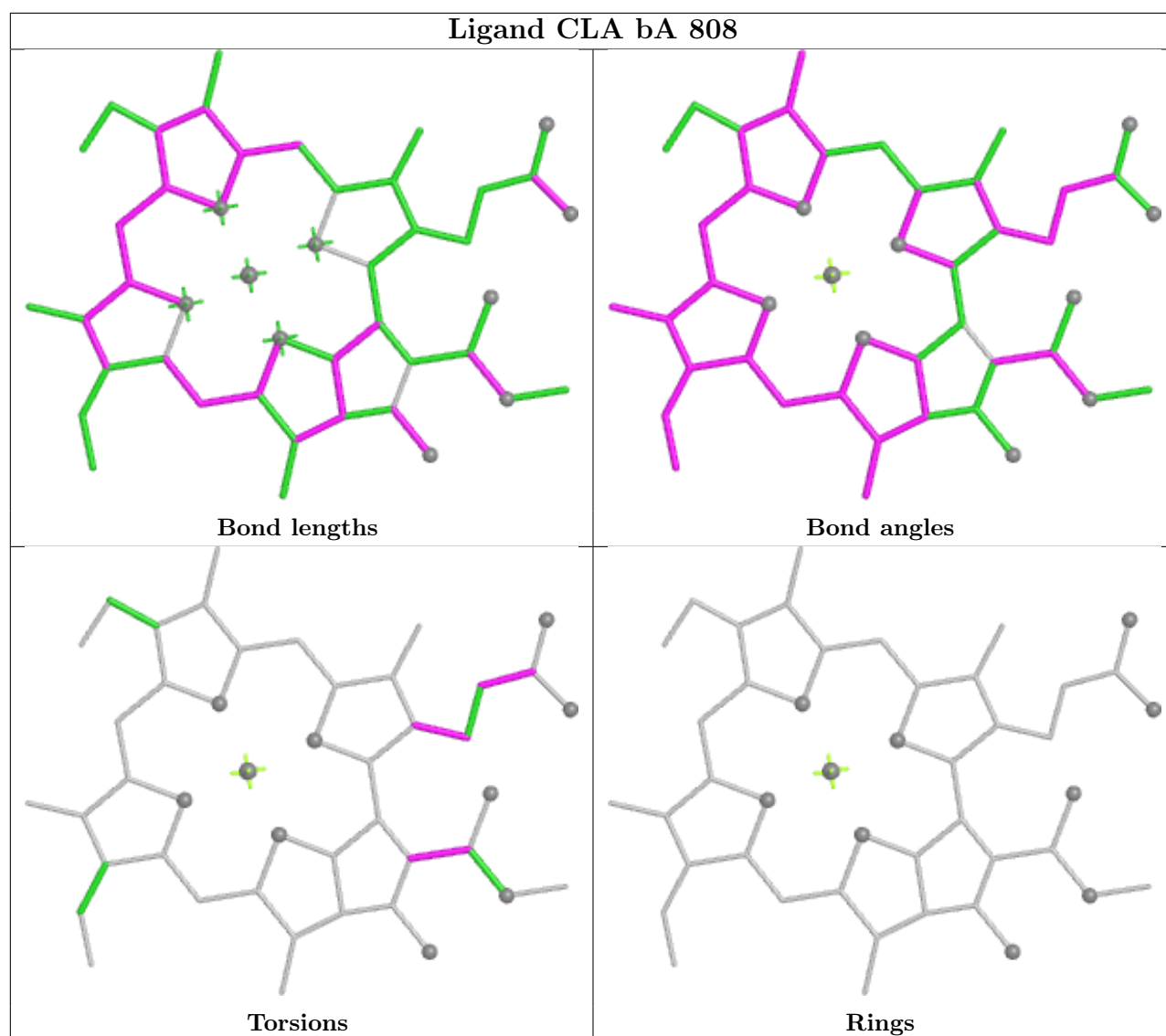




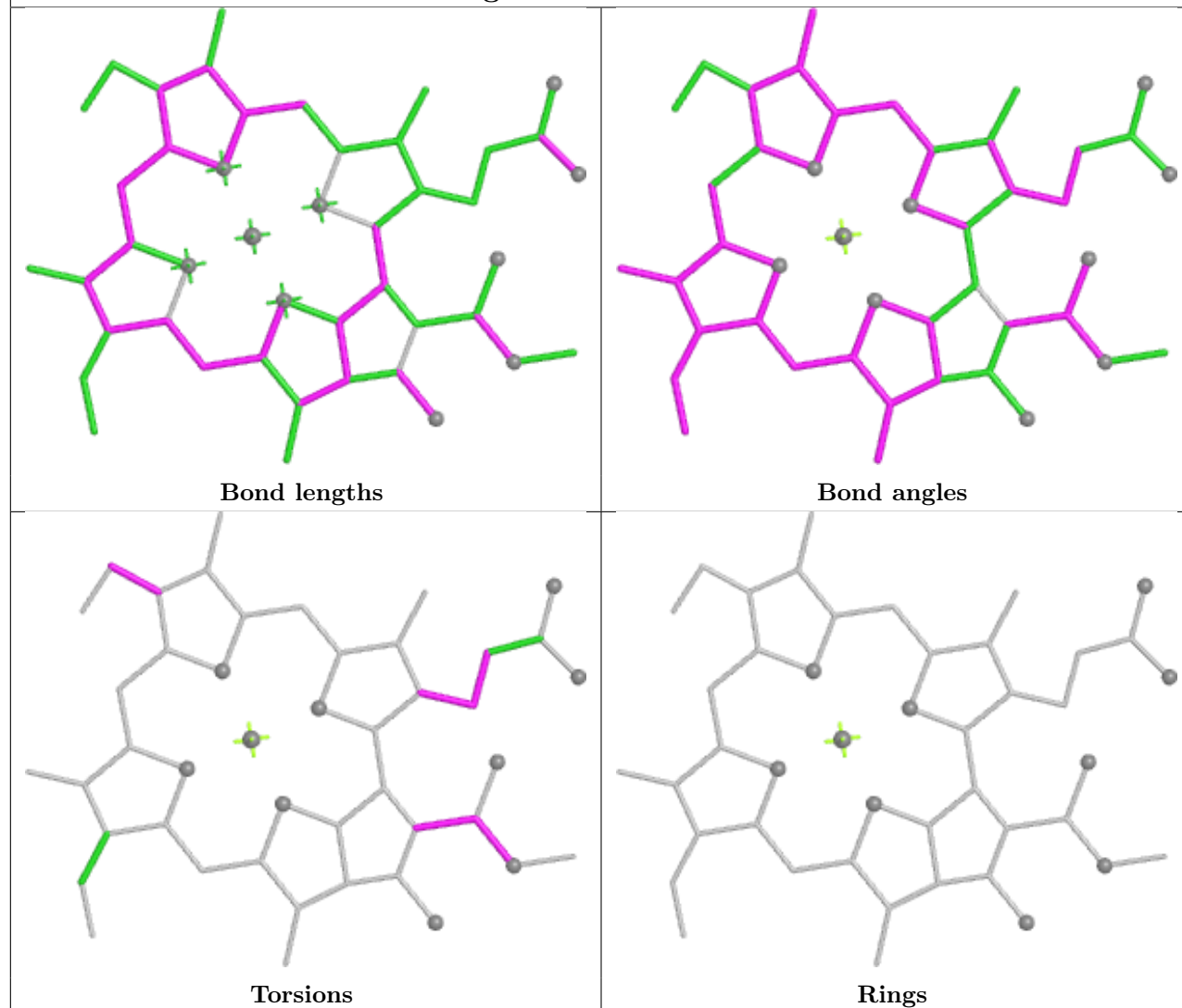
Ligand CLA bB 836



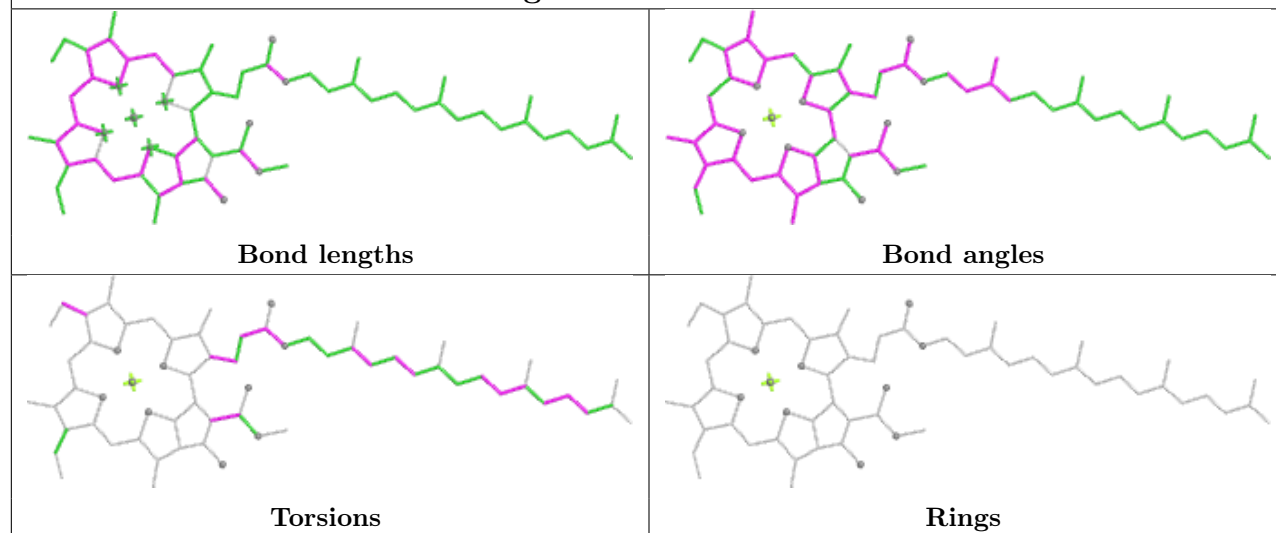


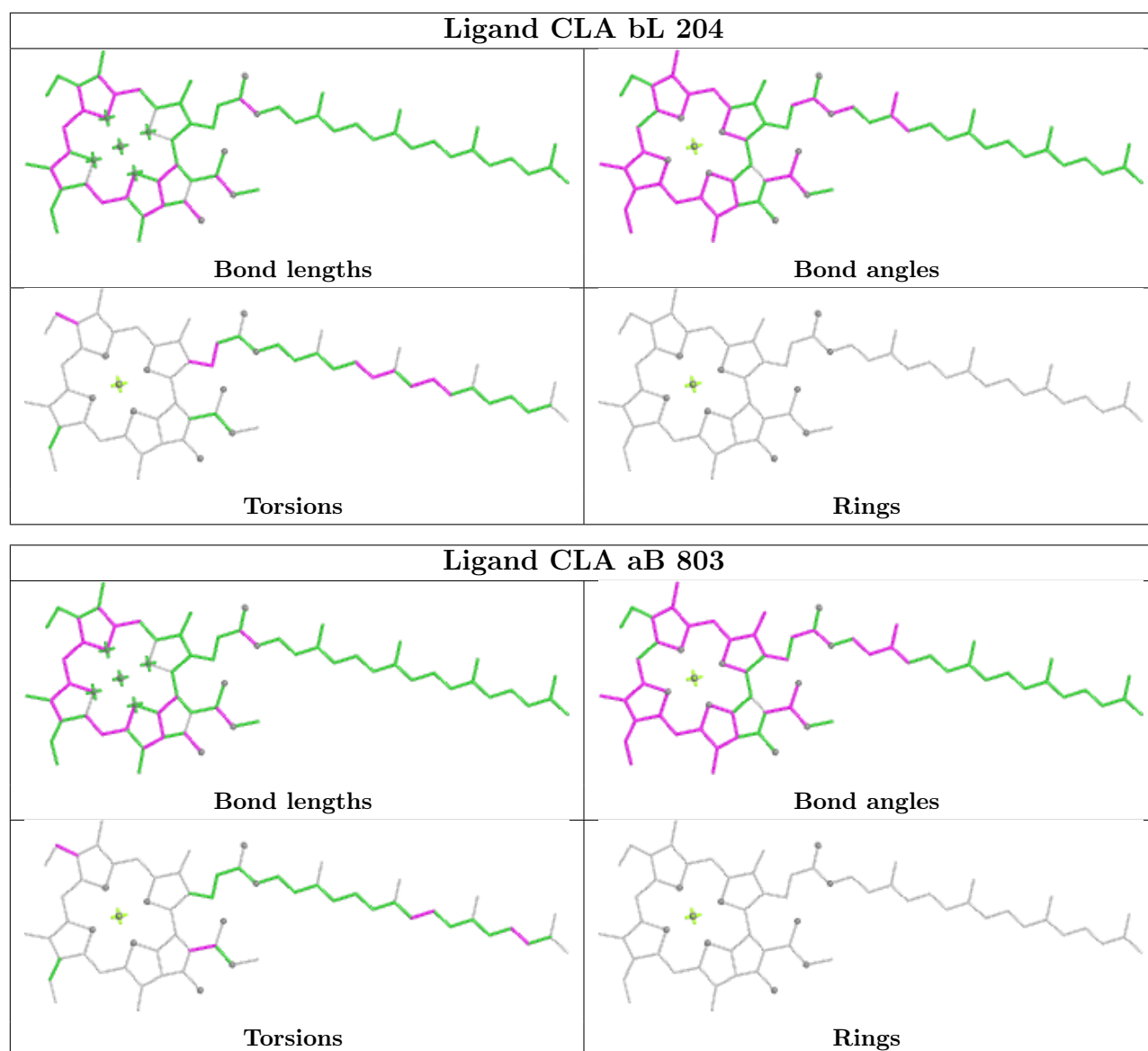


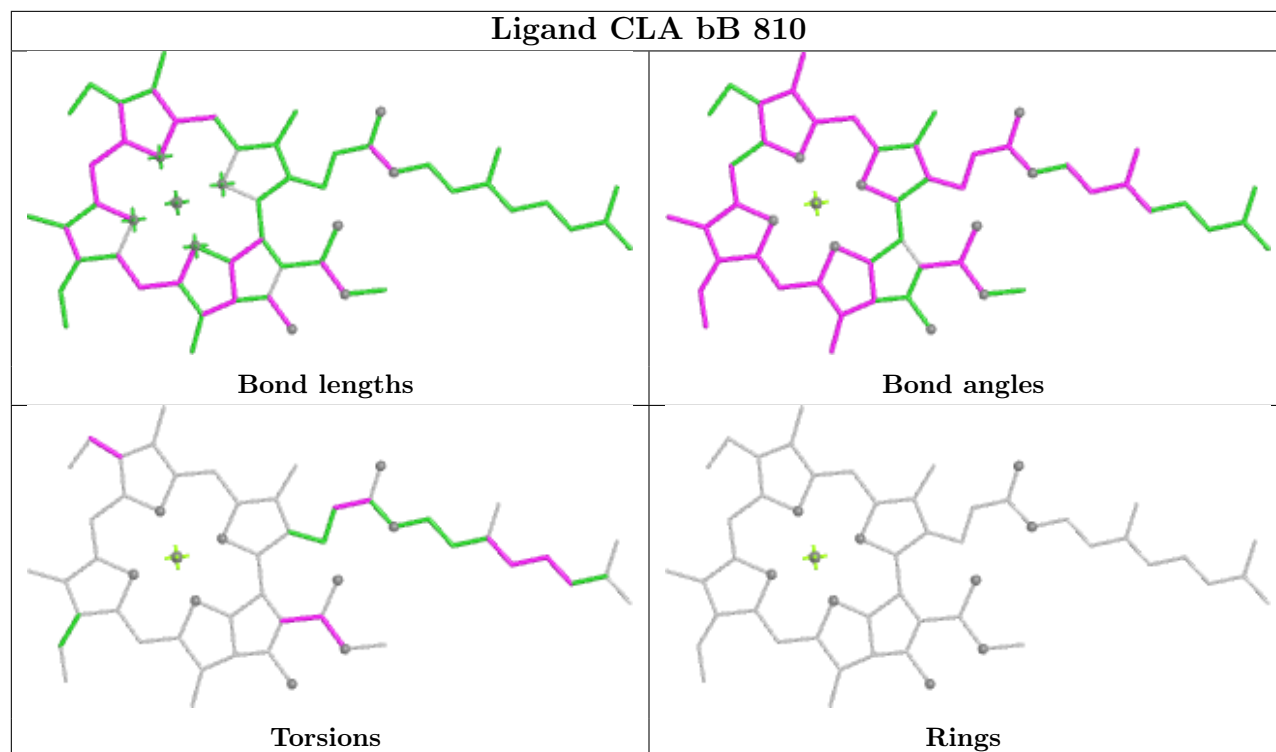
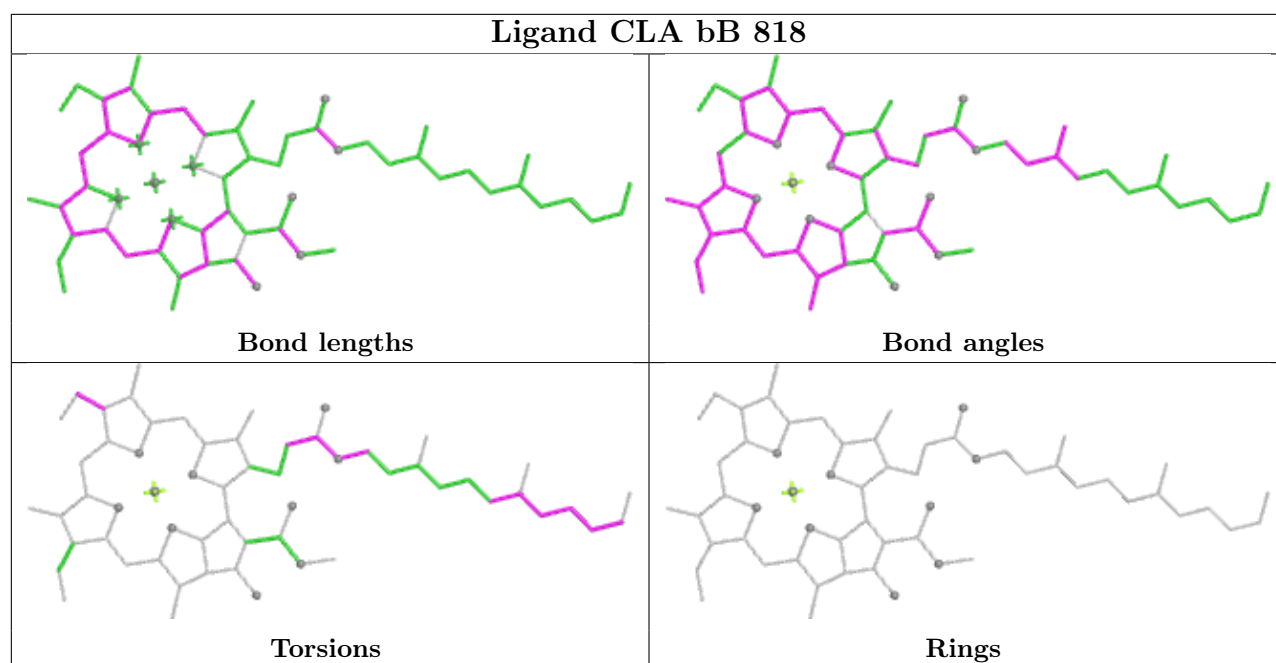
Ligand CLA bA 807

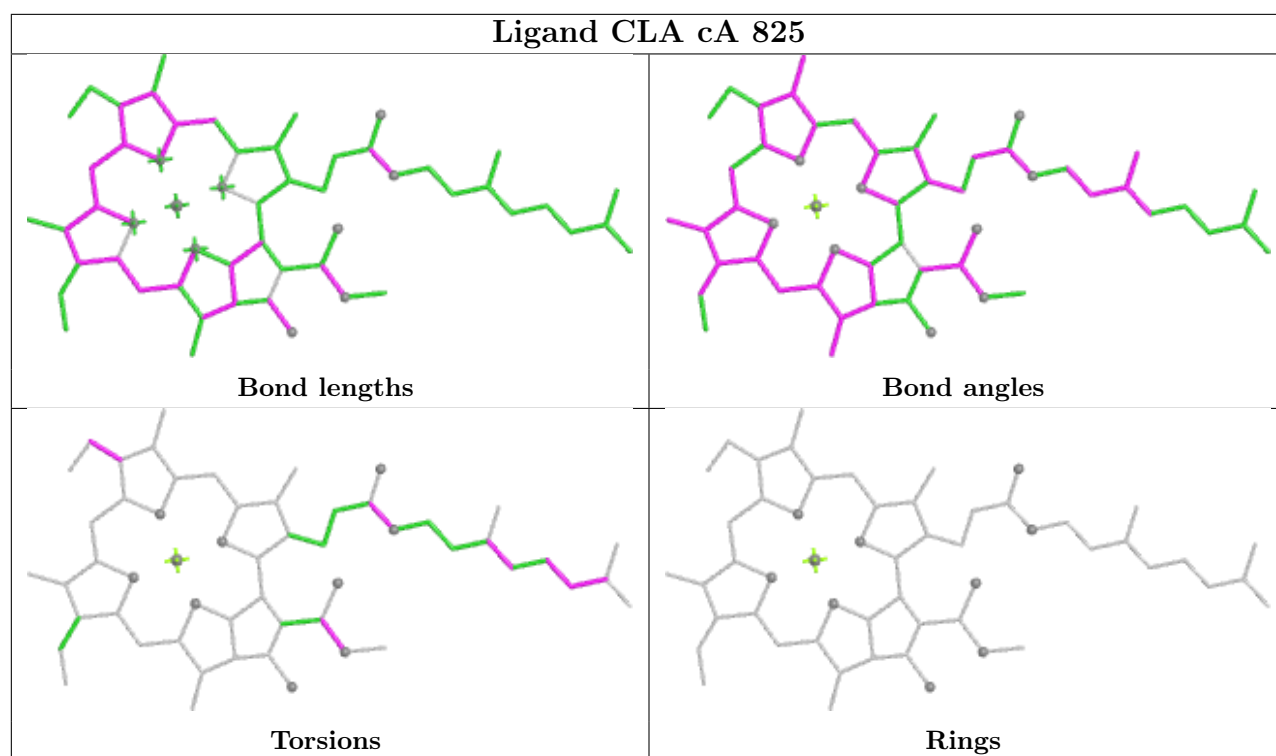


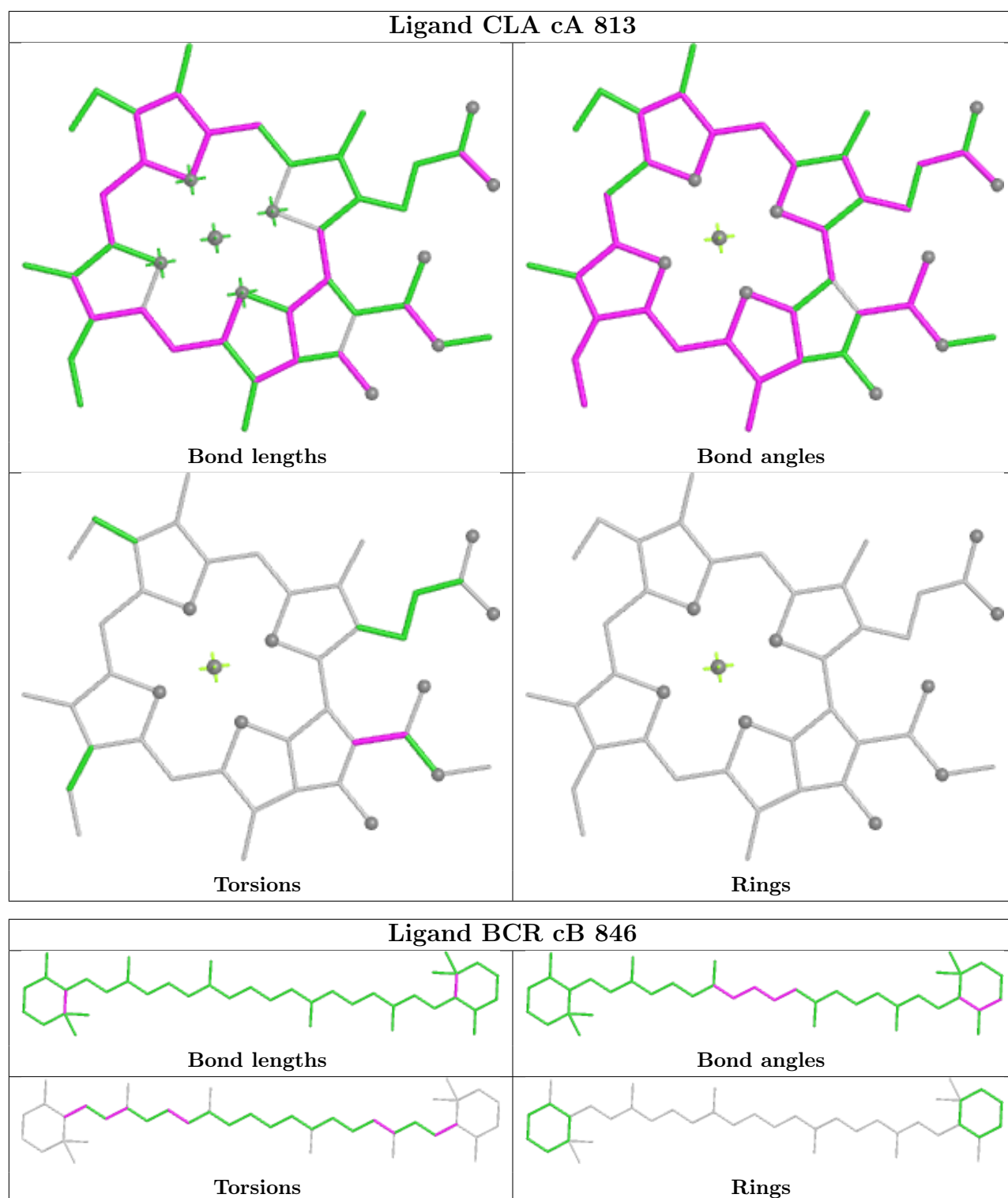
Ligand CLA aB 814

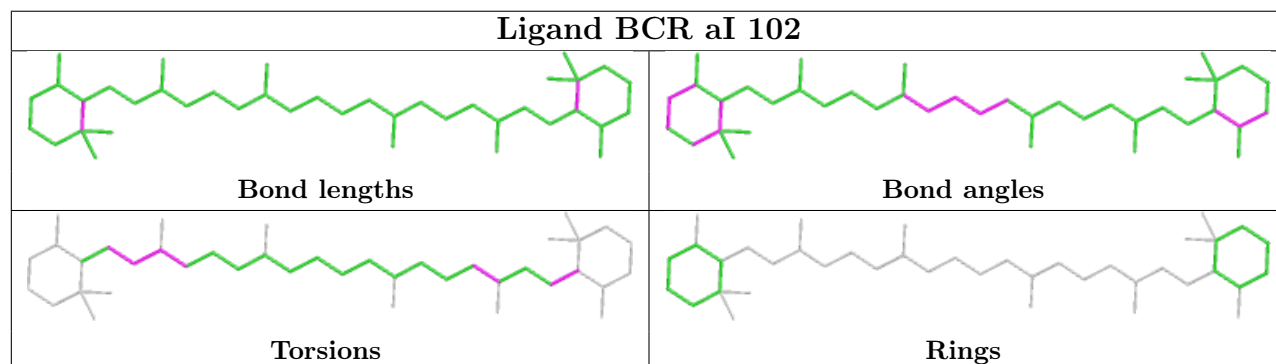
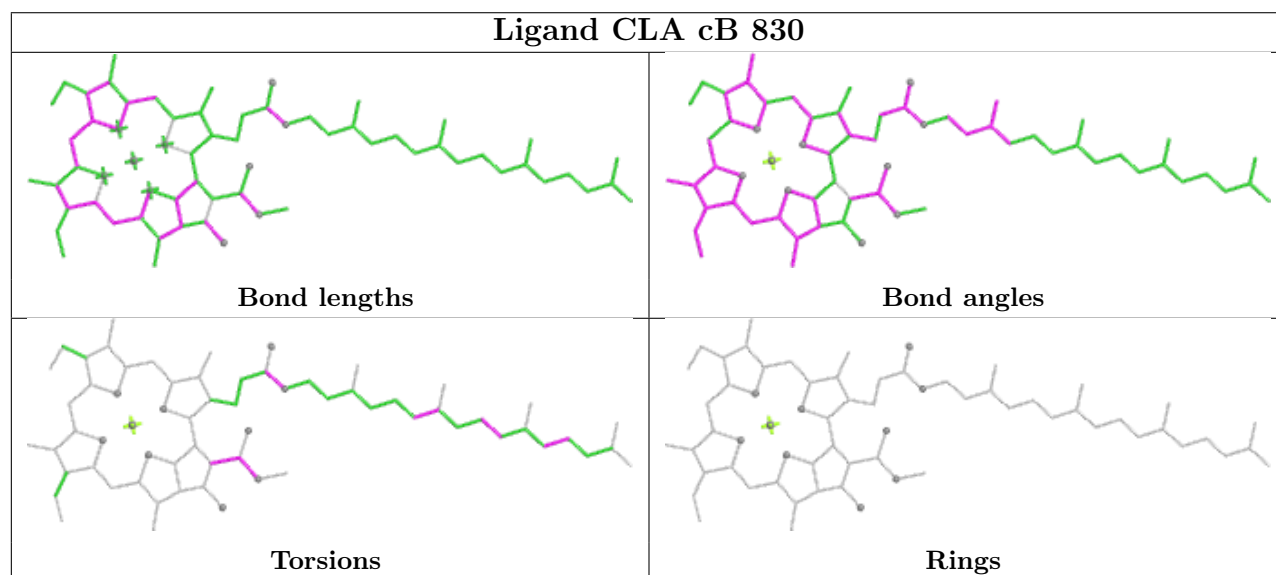
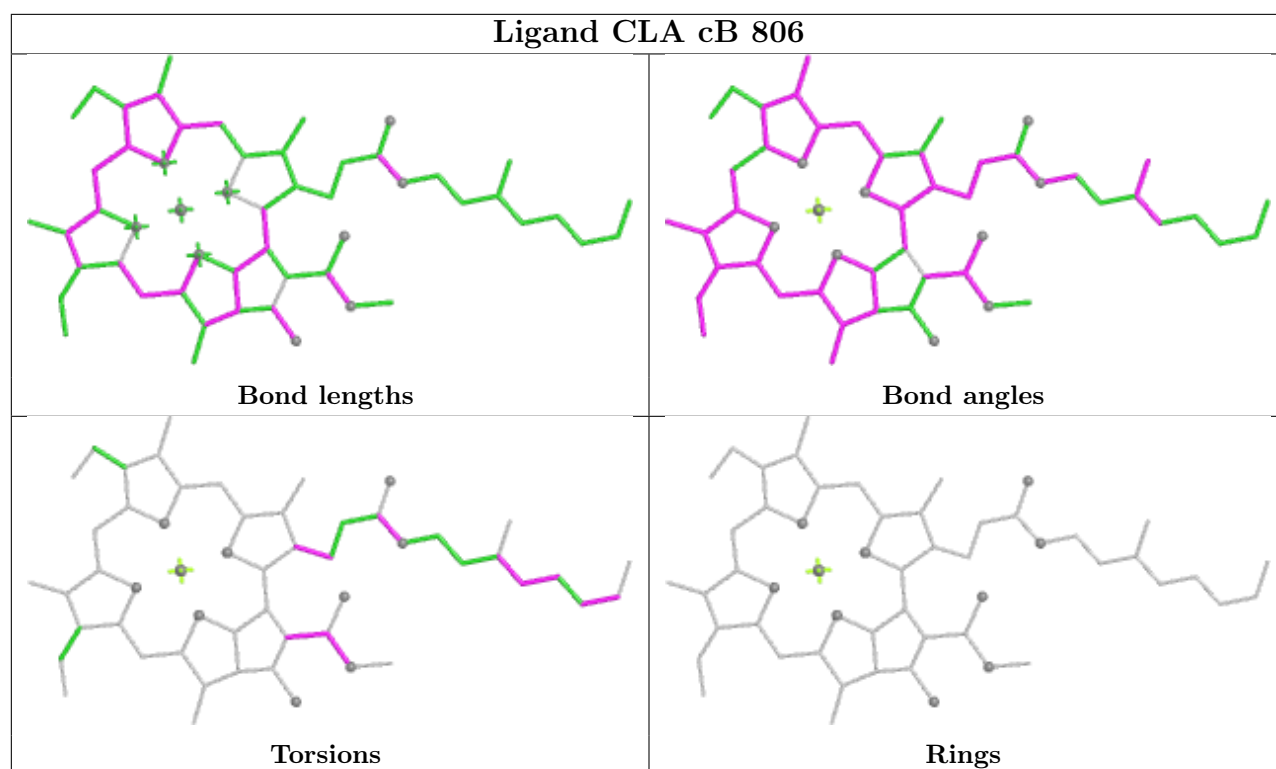




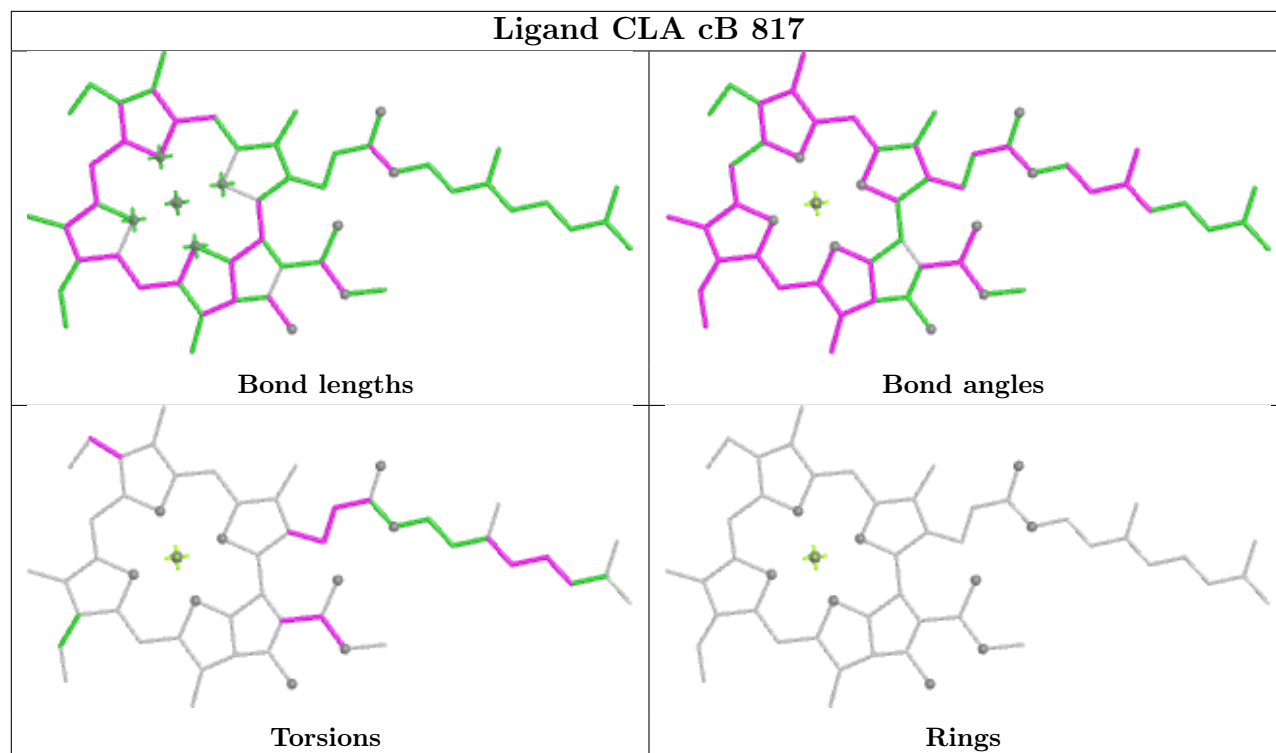




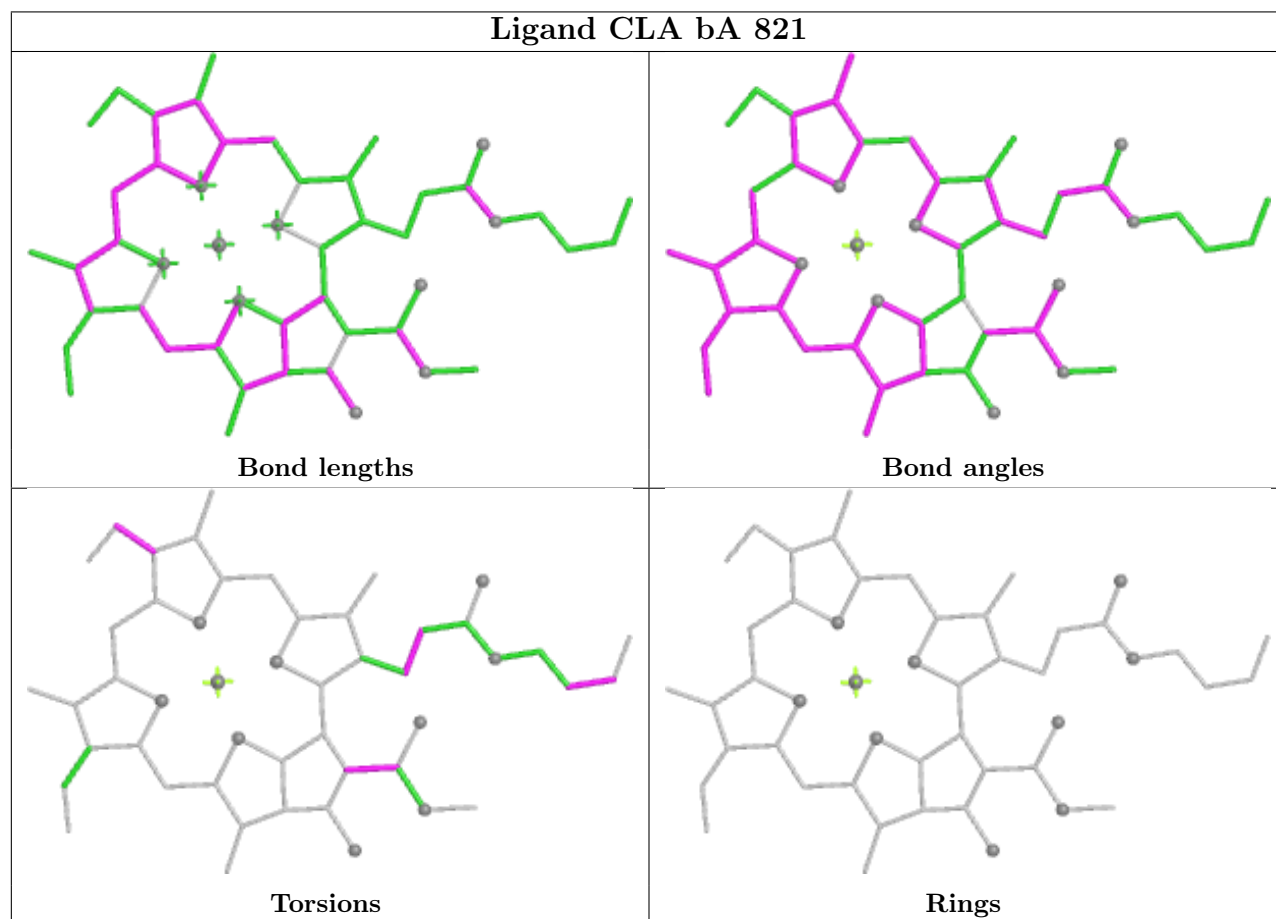


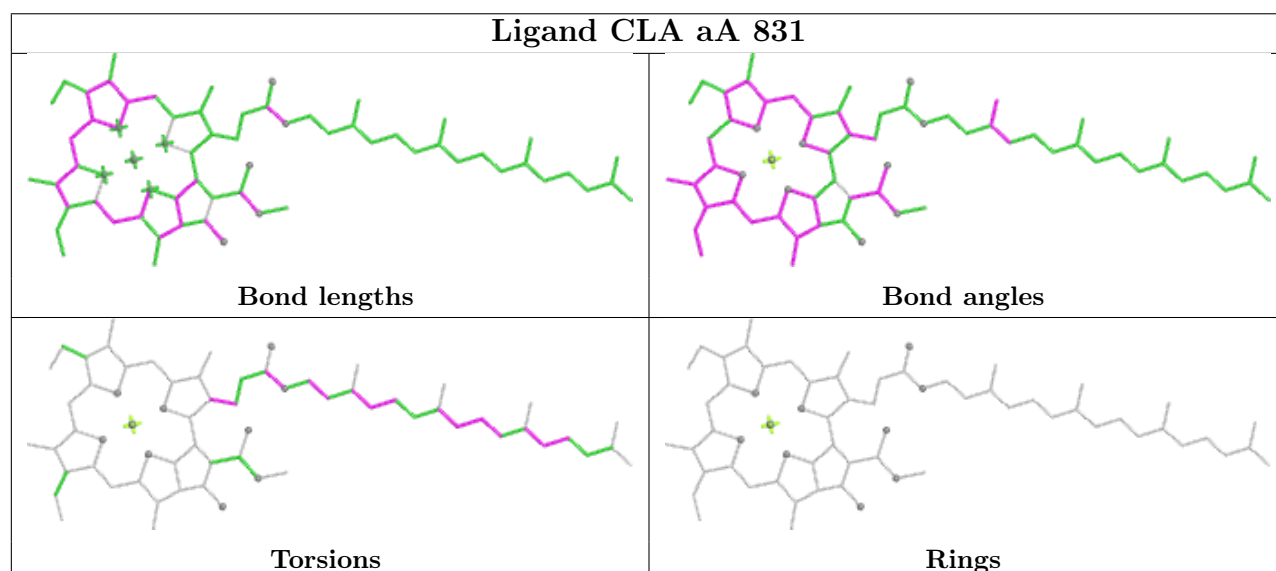
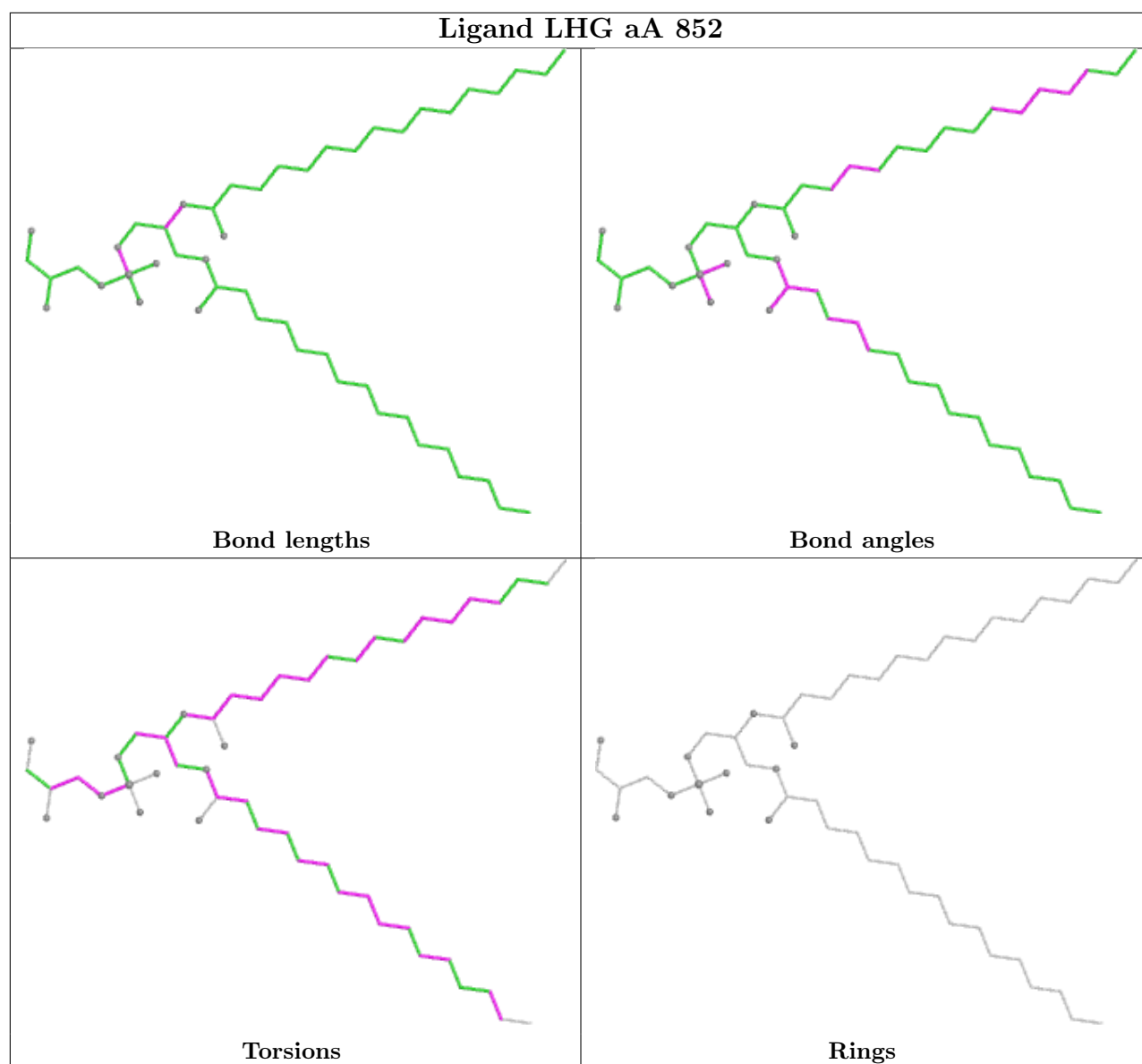


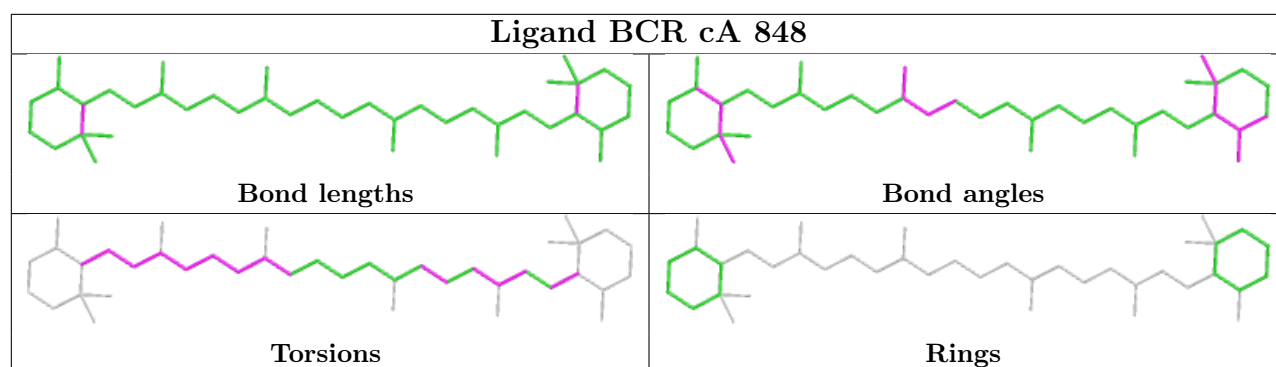
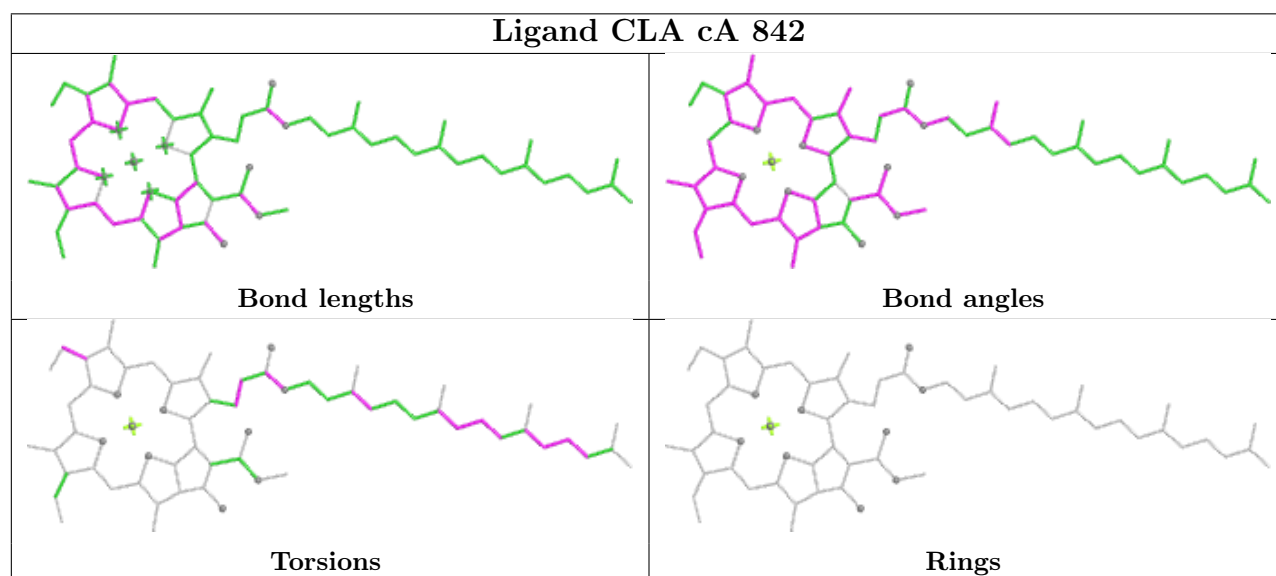
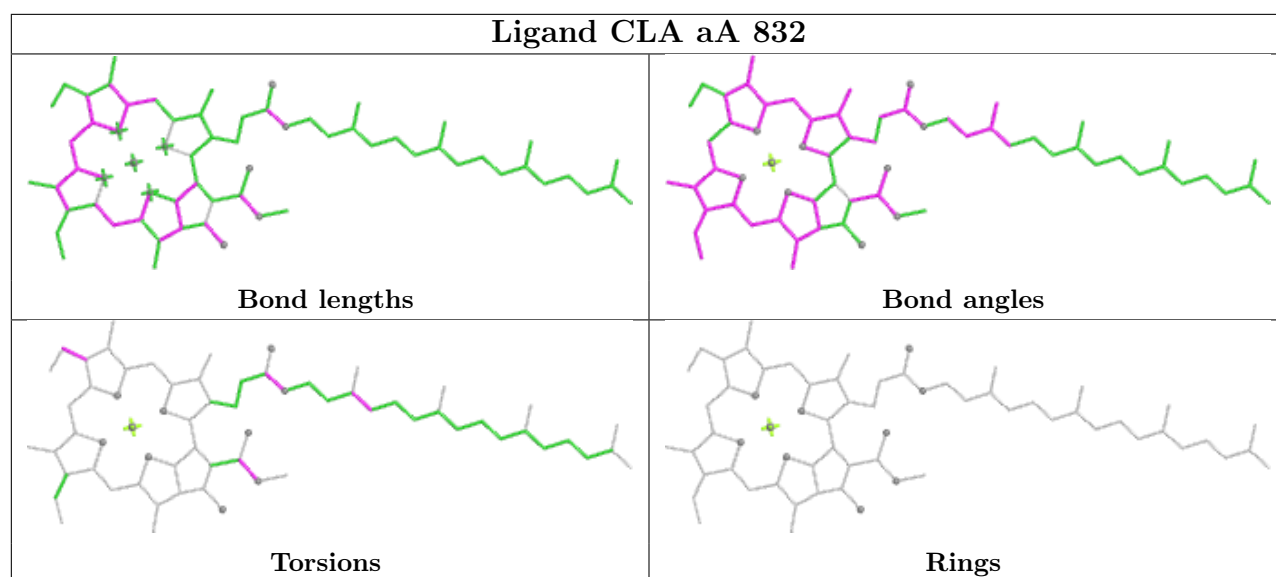
Ligand CLA cB 817

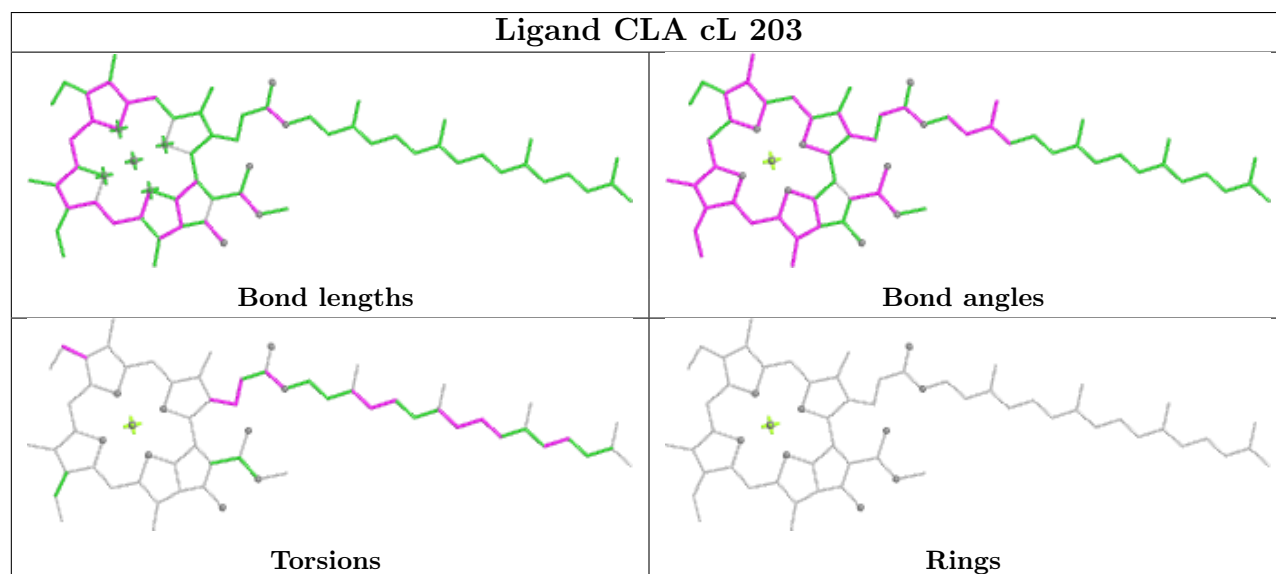
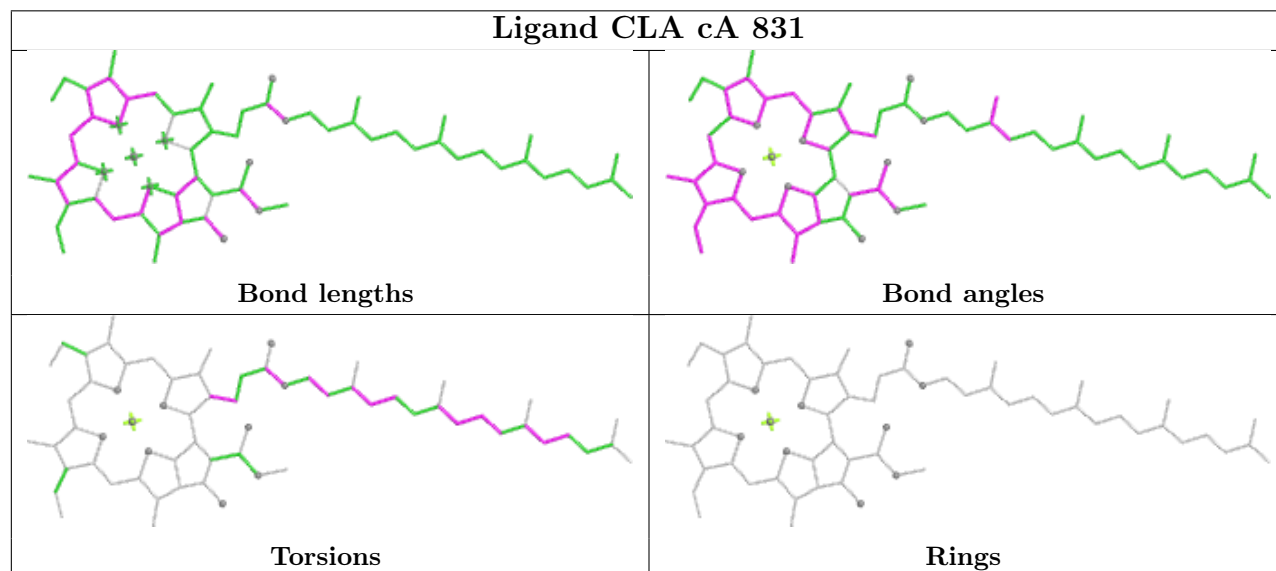
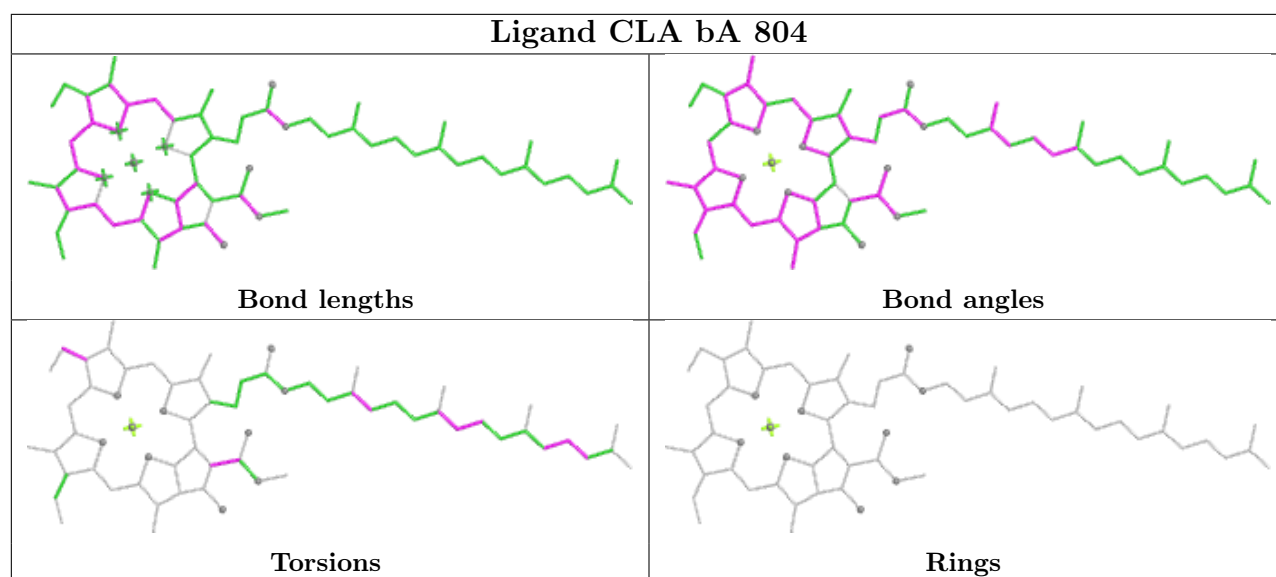


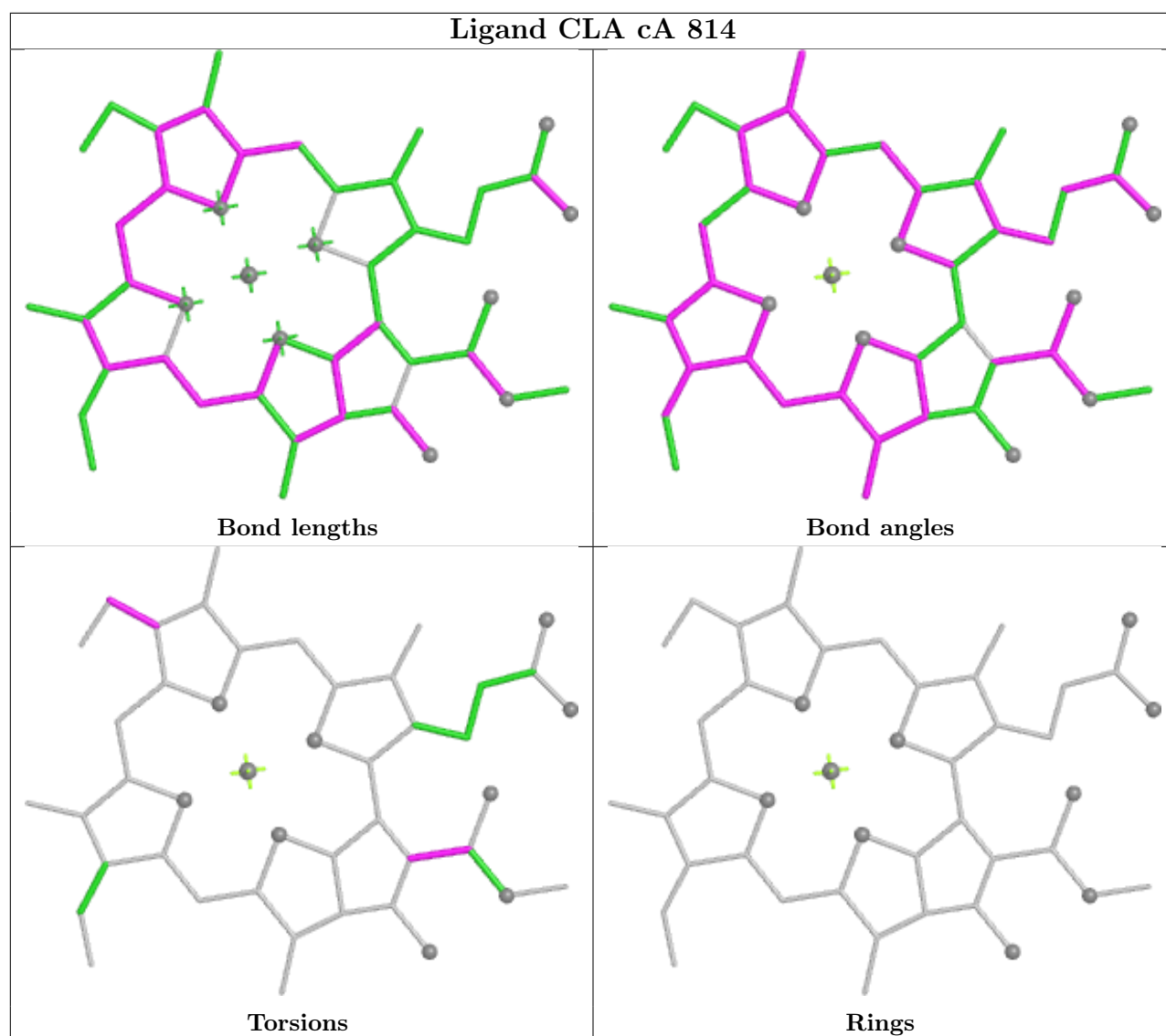
Ligand CLA bA 821

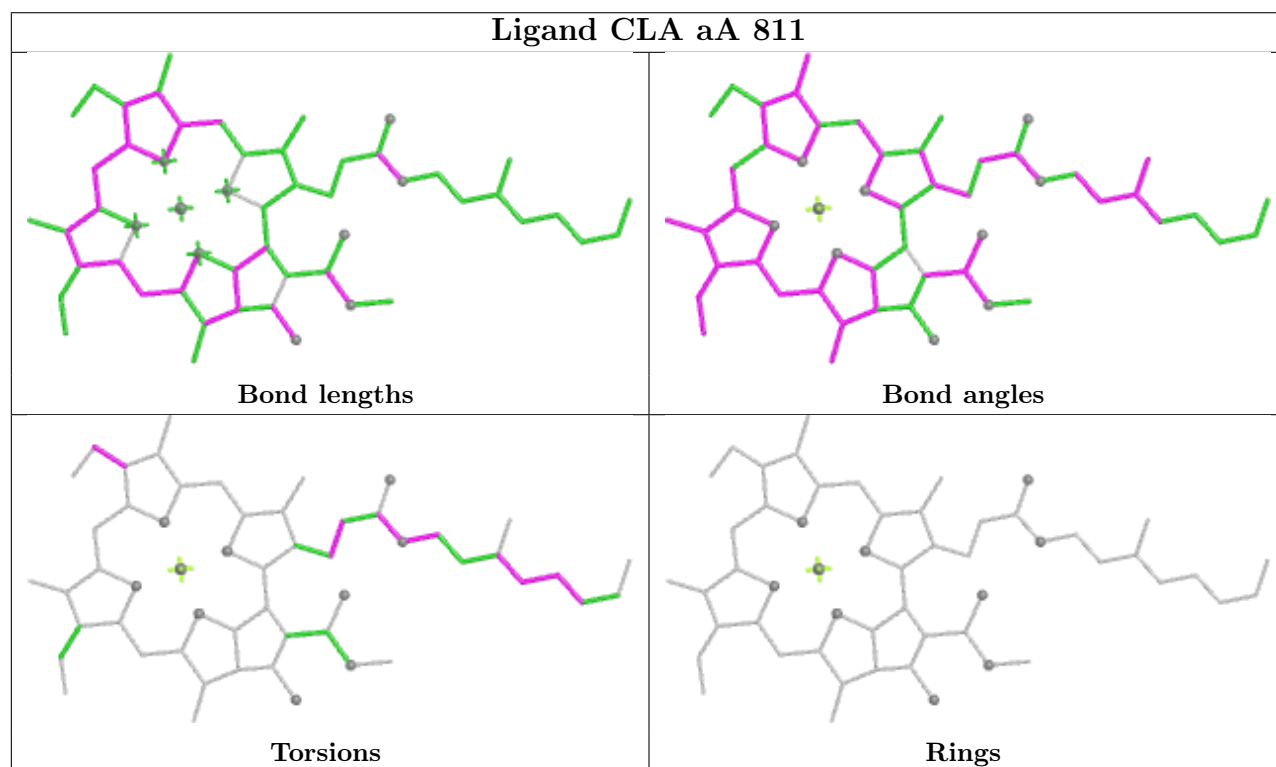
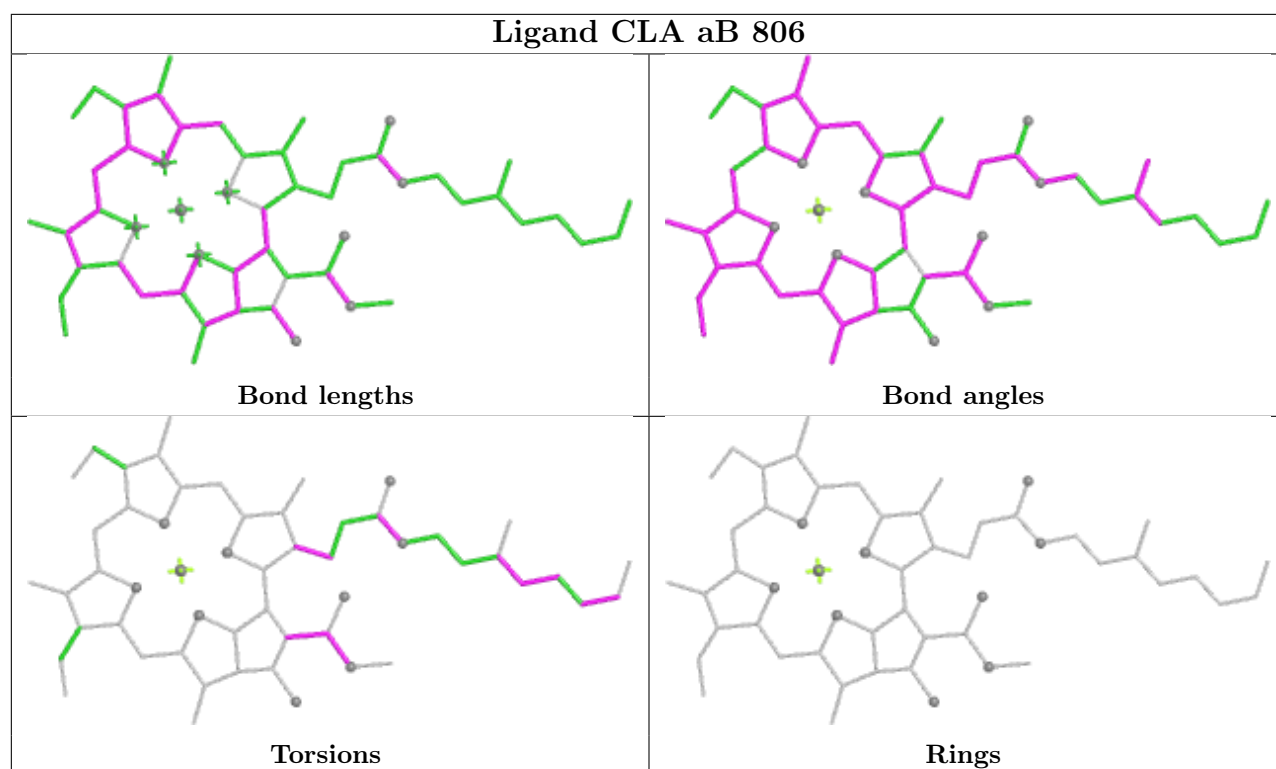


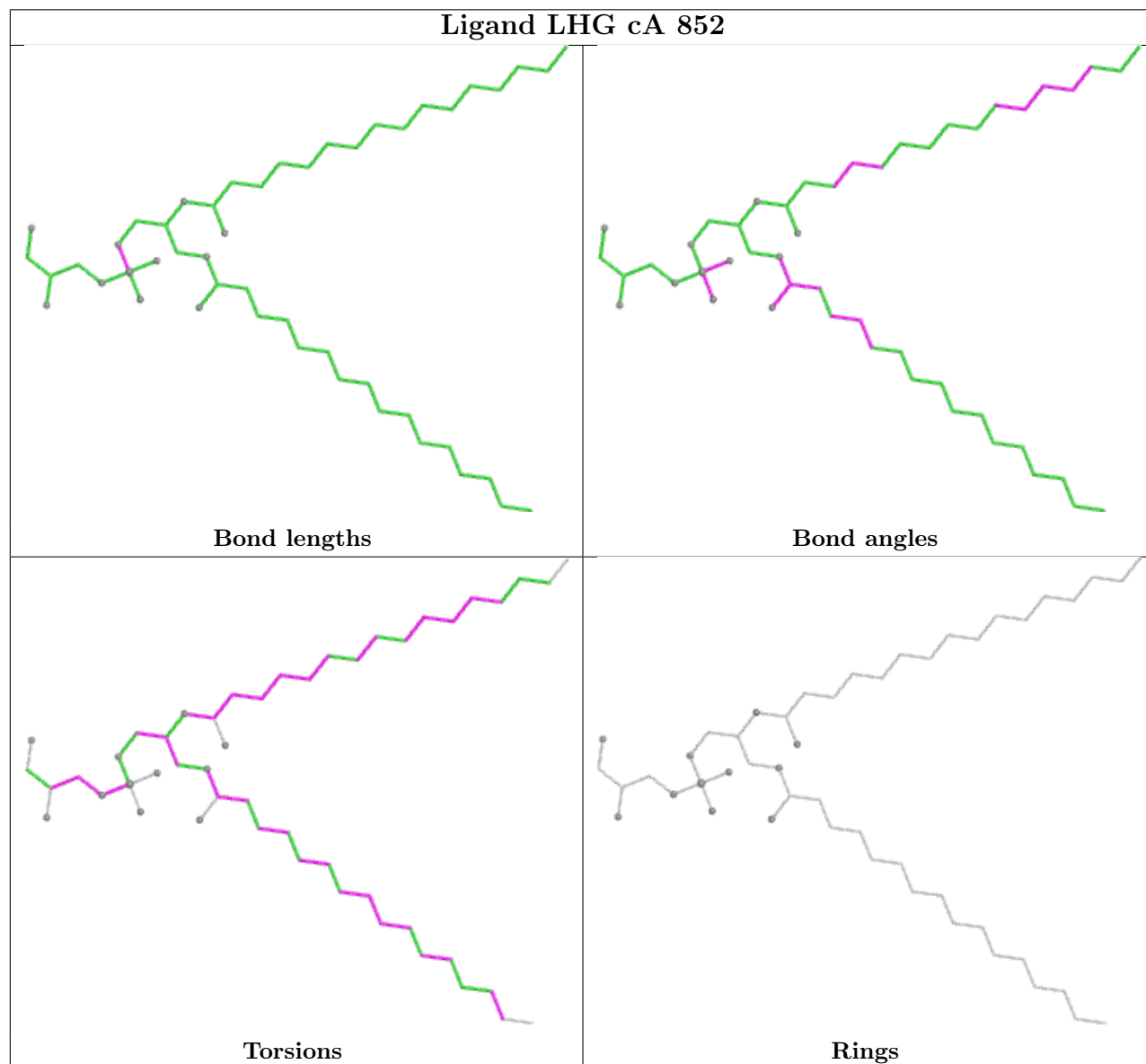
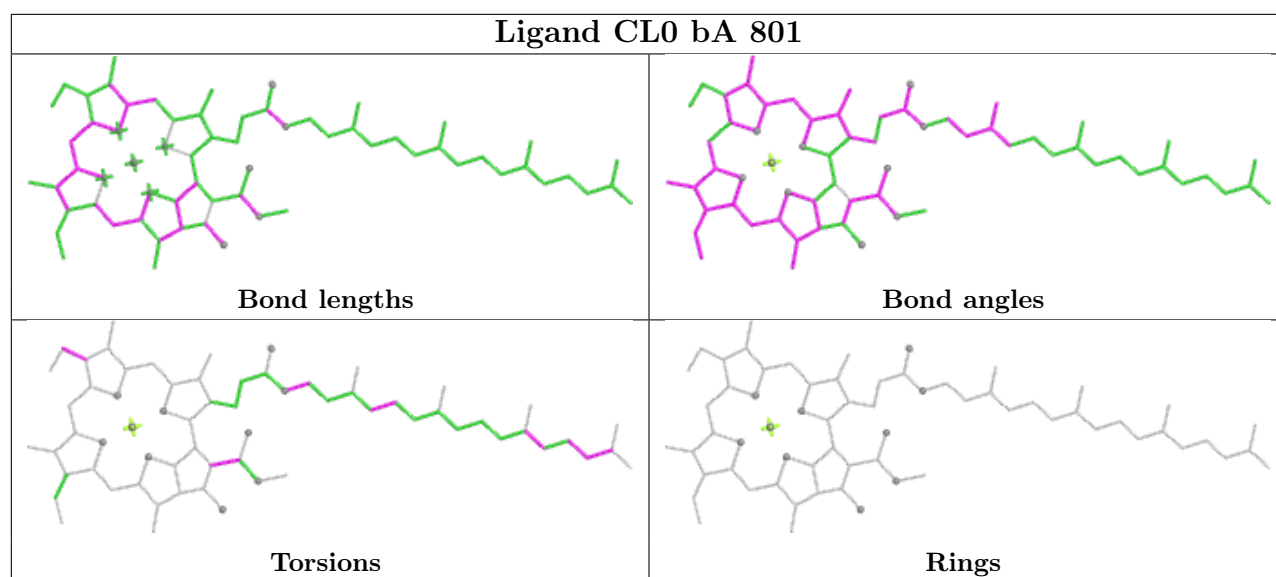


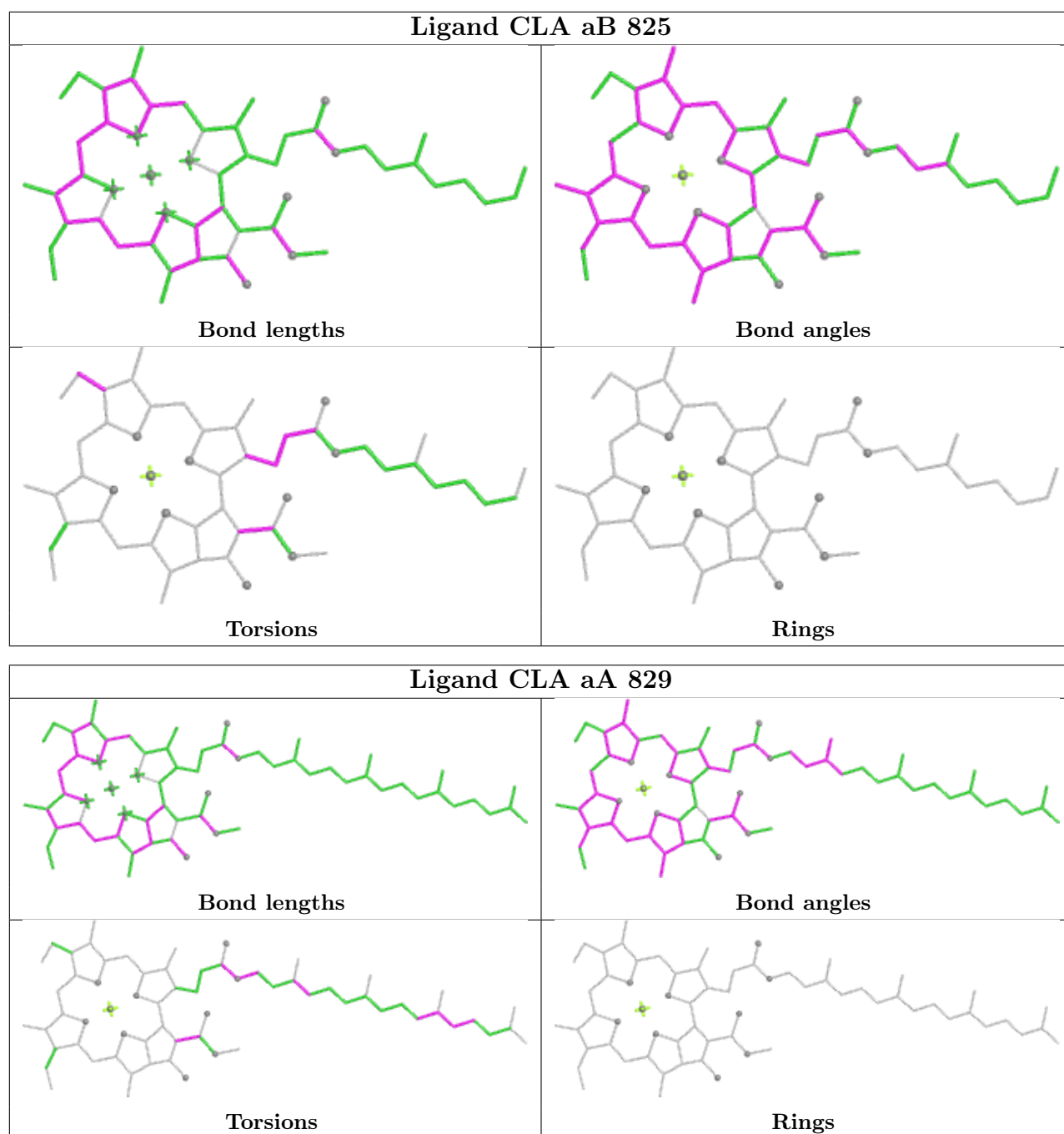


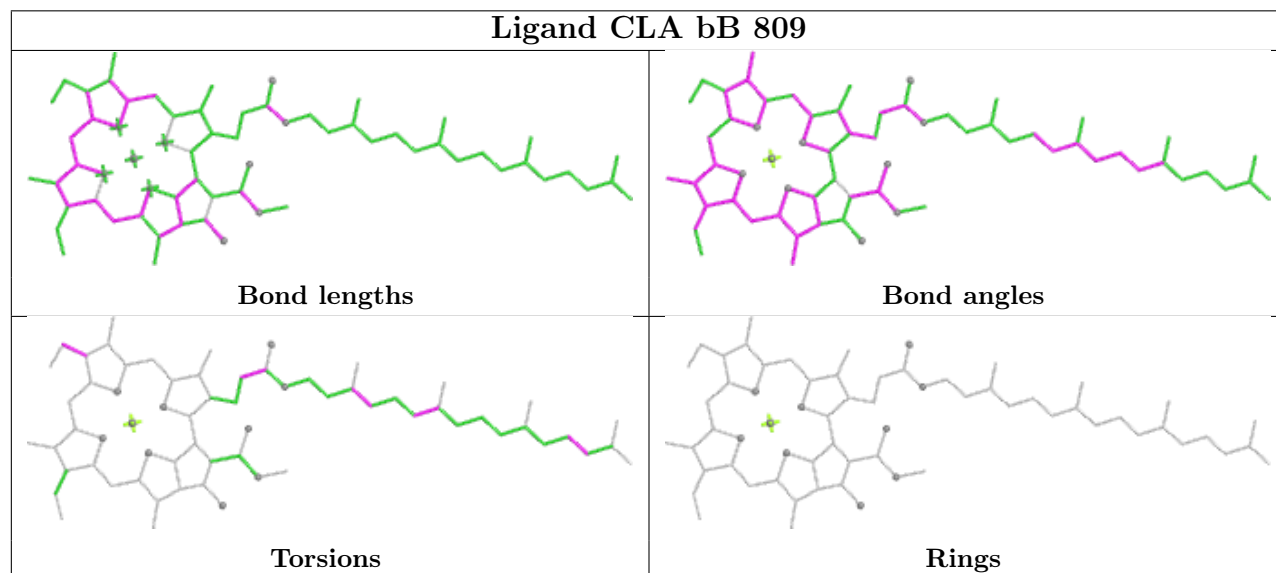
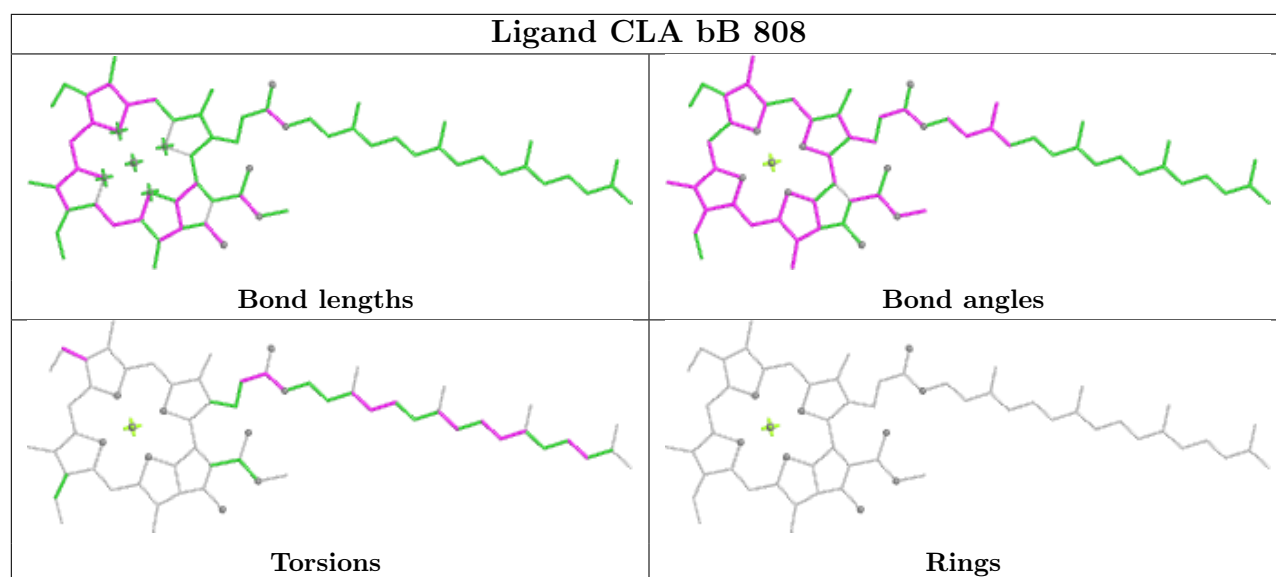


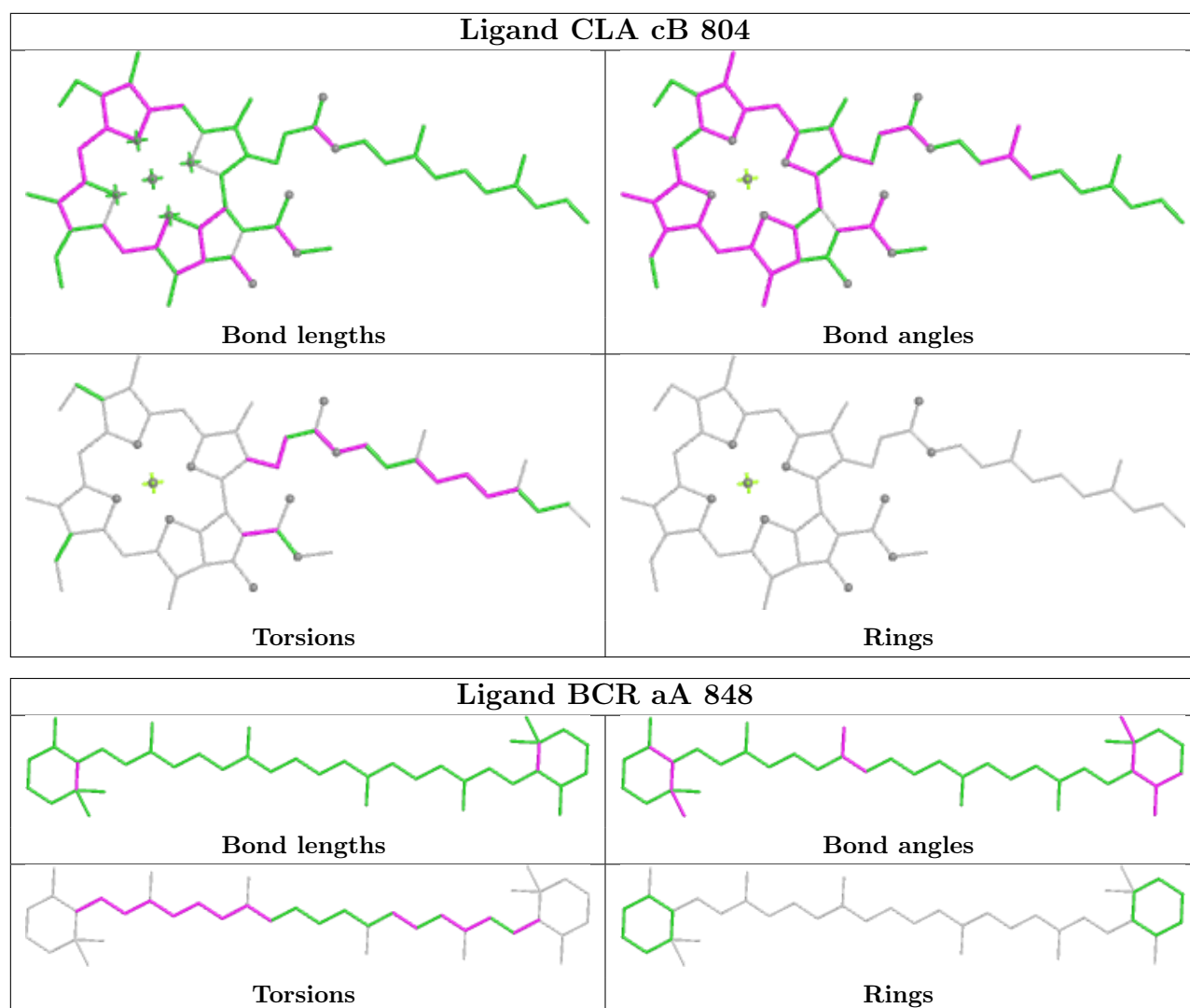




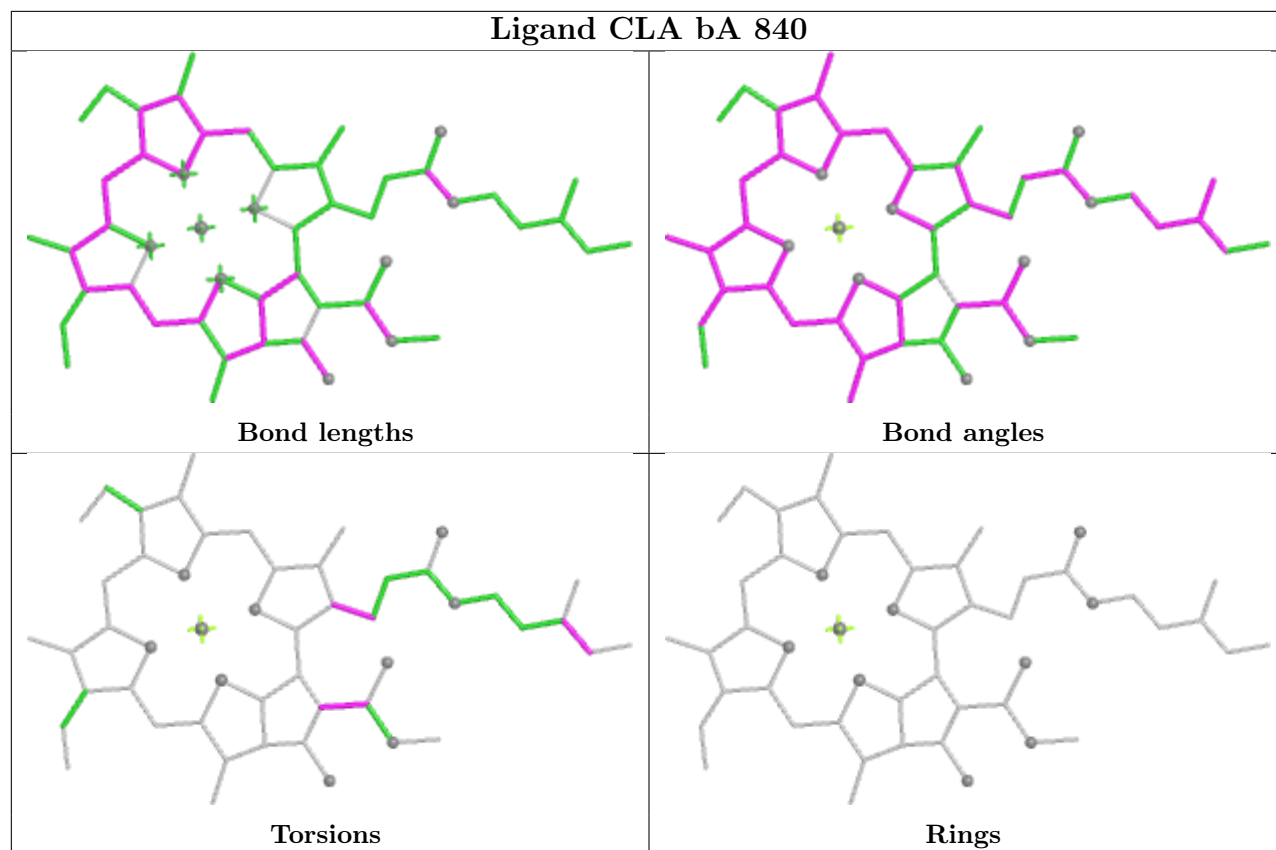




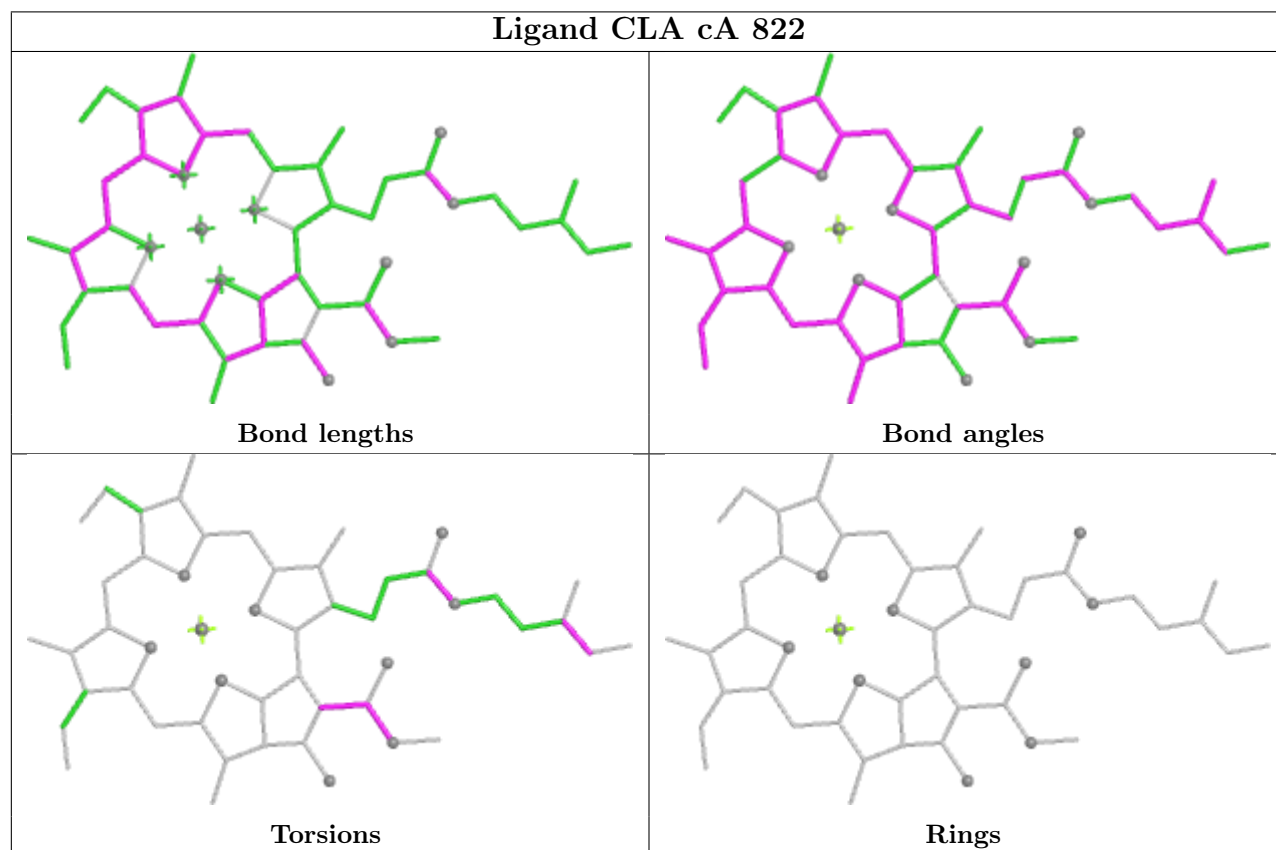


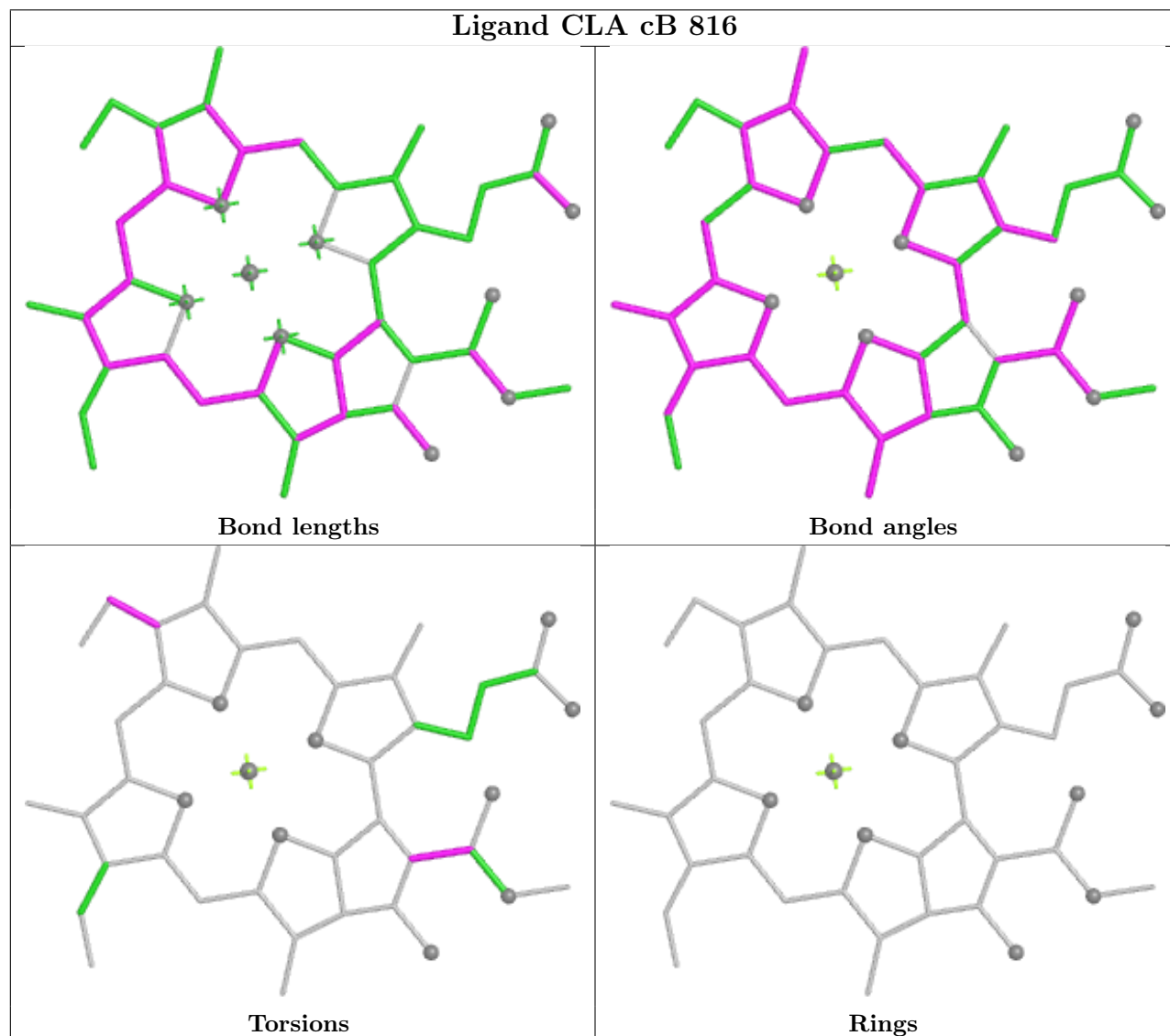
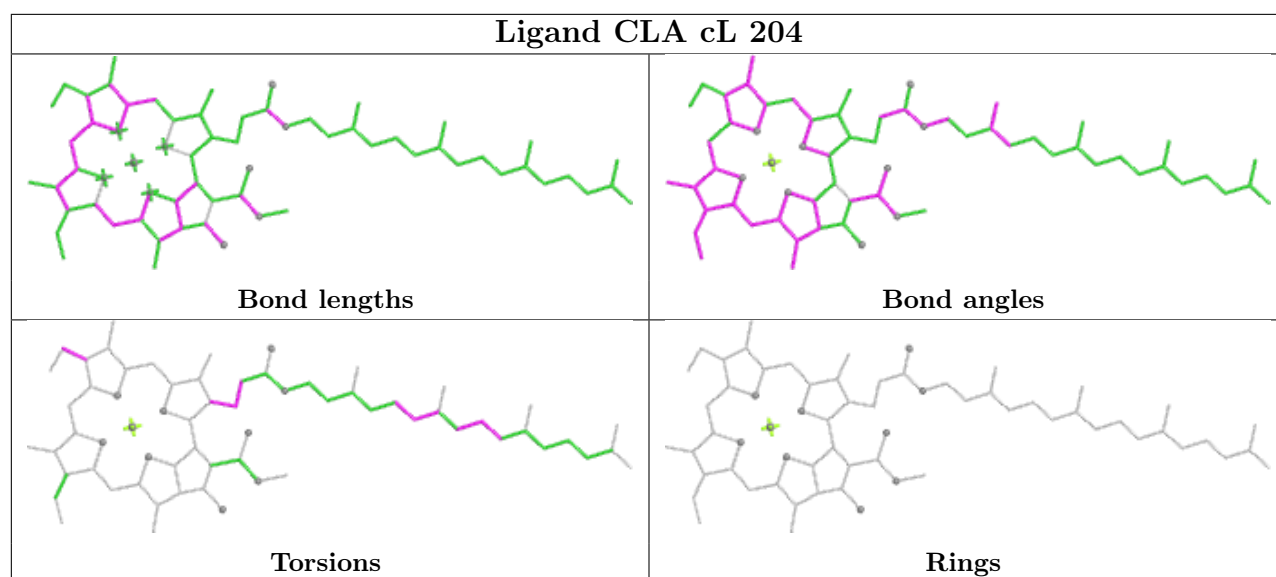


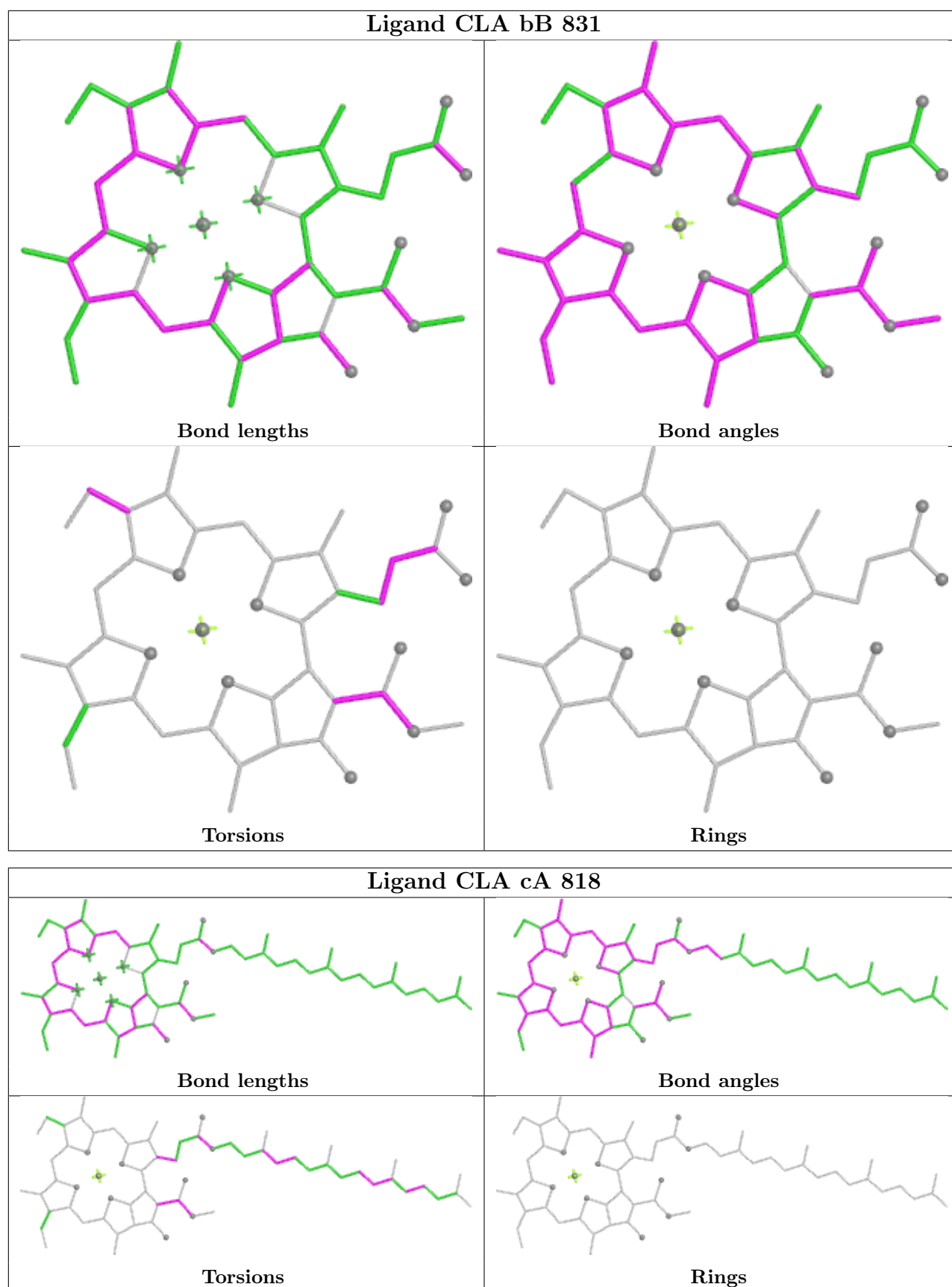
Ligand CLA bA 840

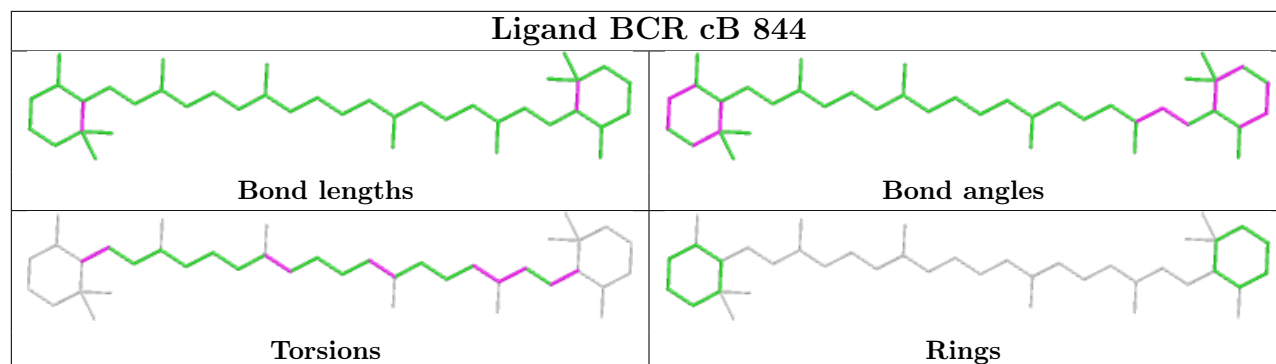
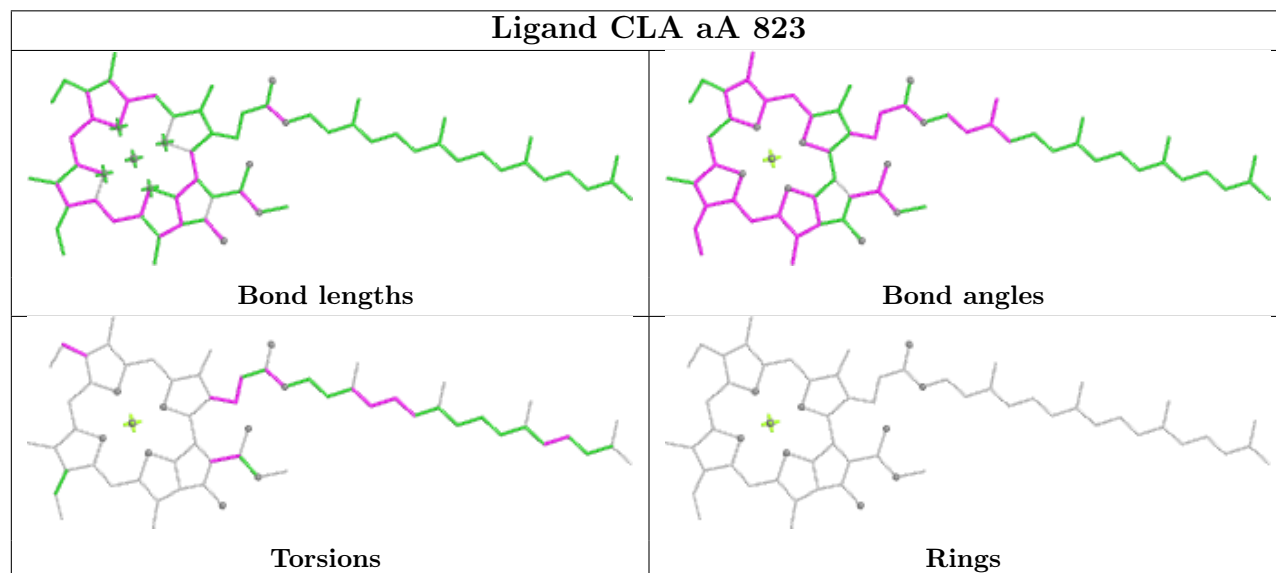
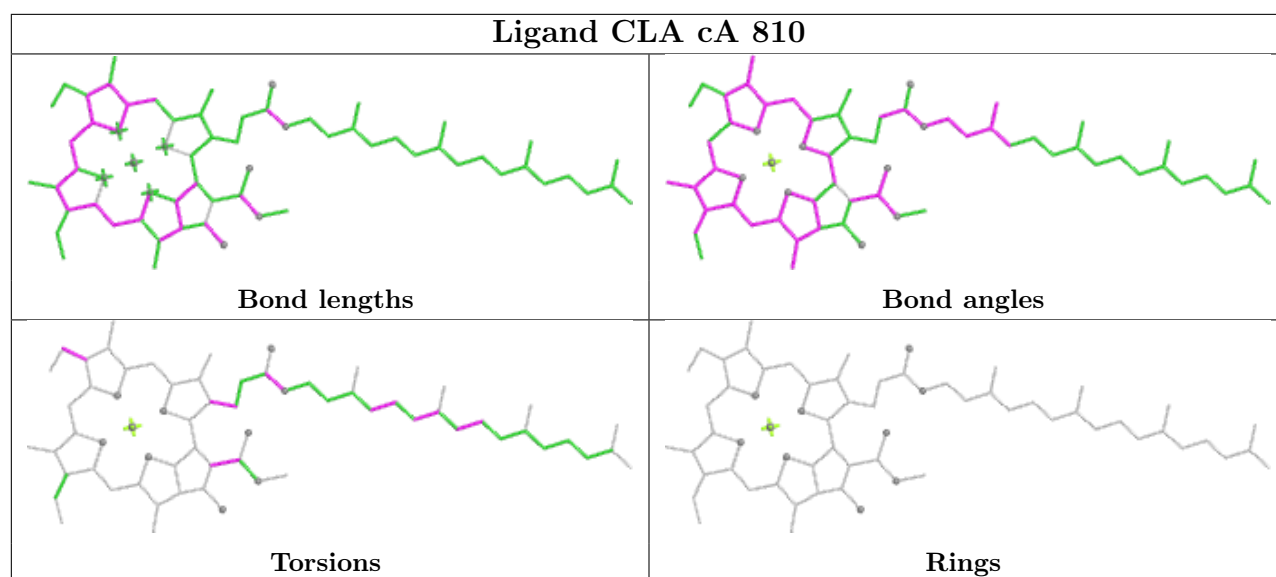


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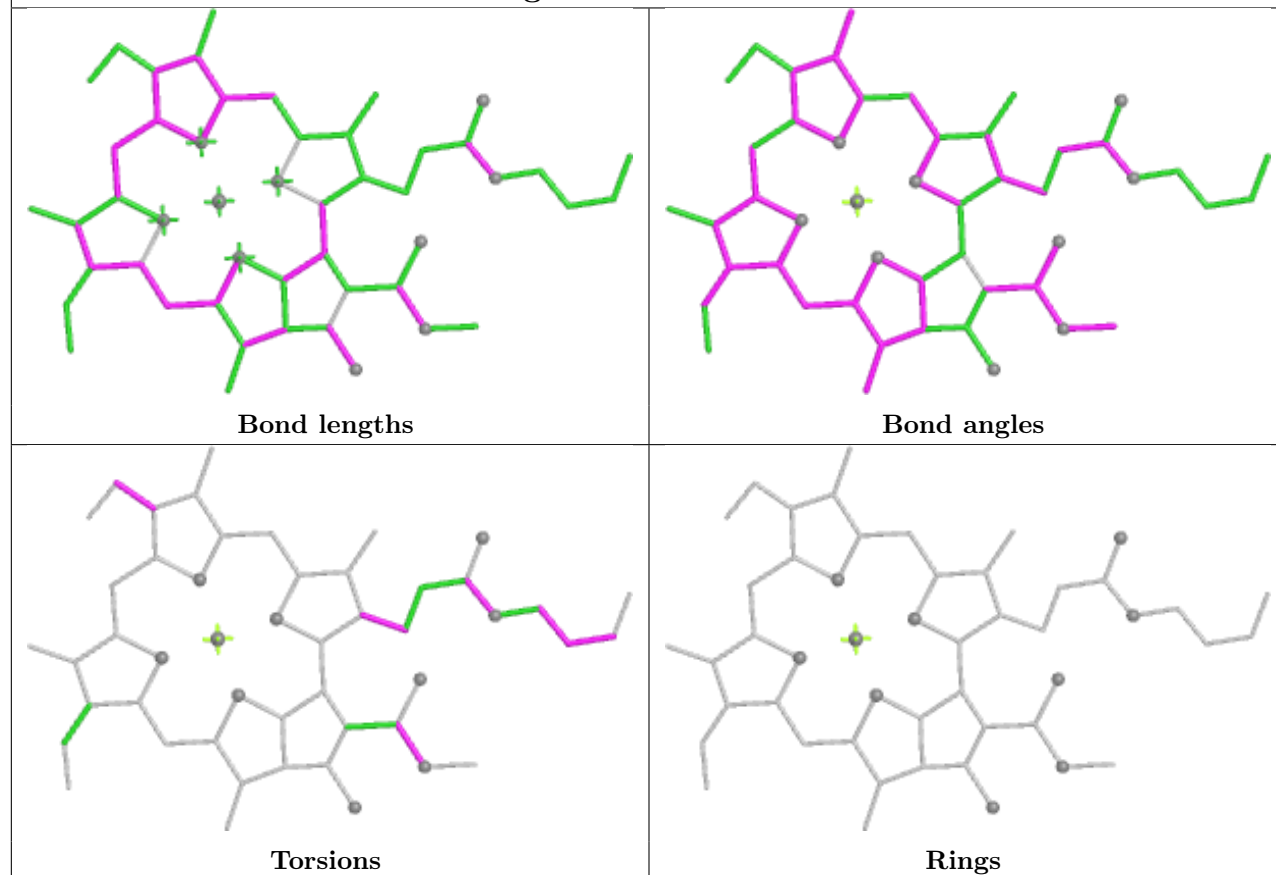




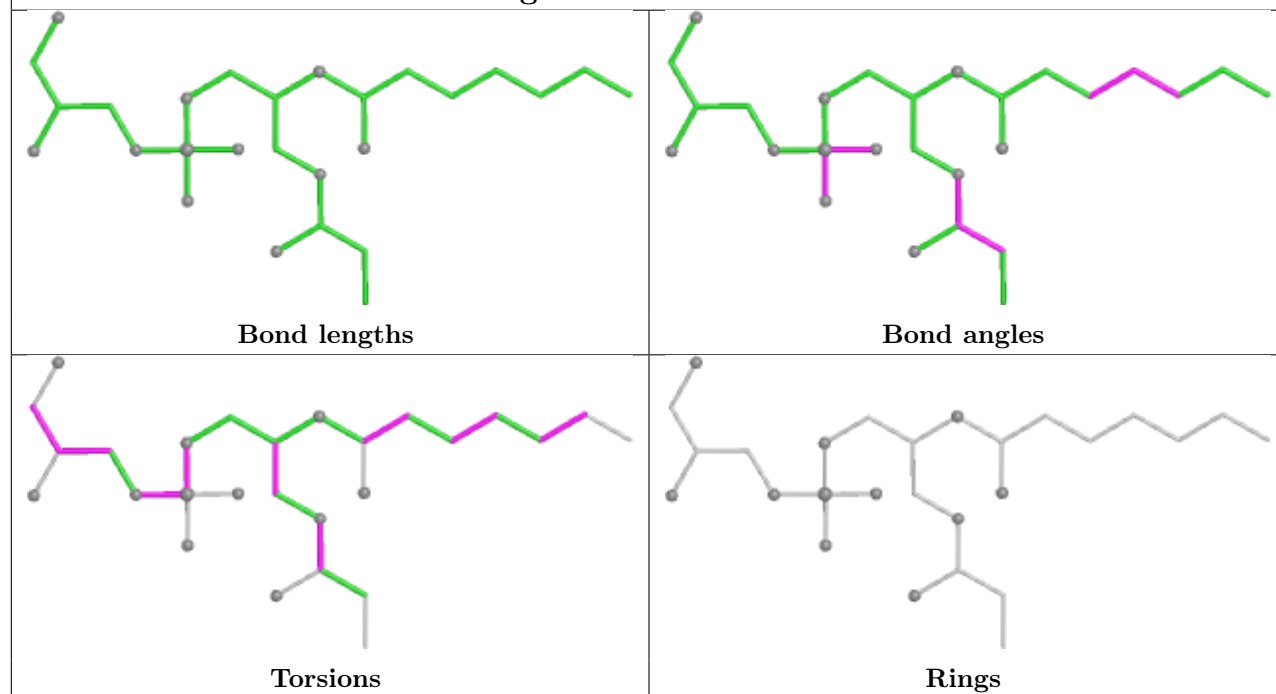


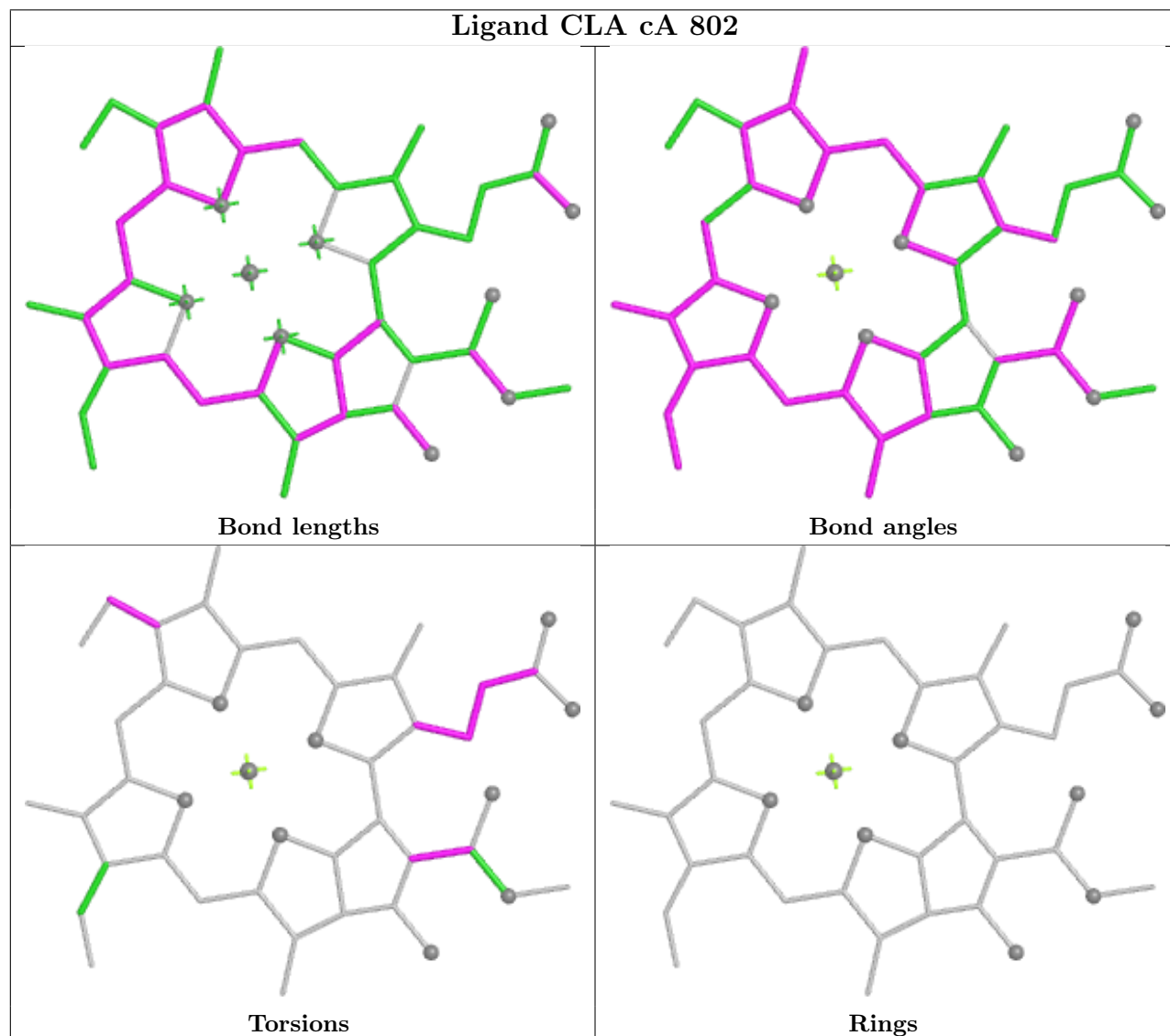
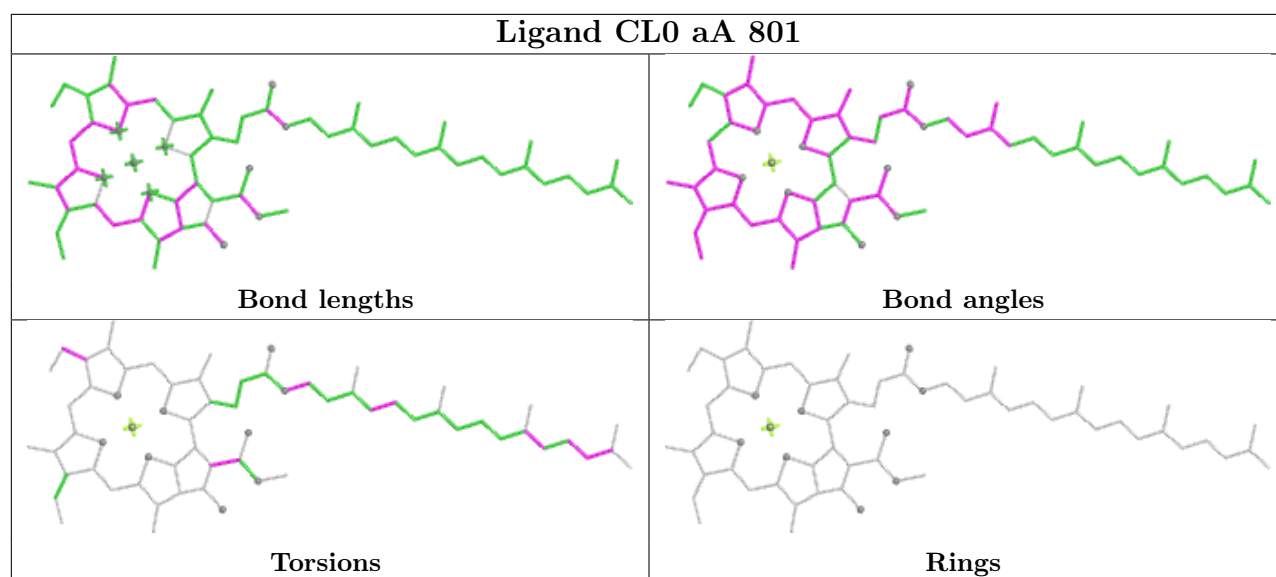


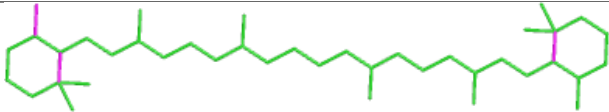
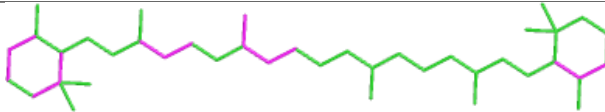
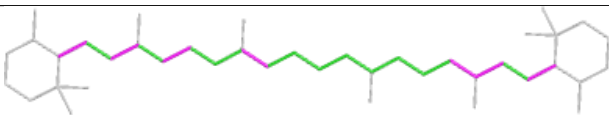
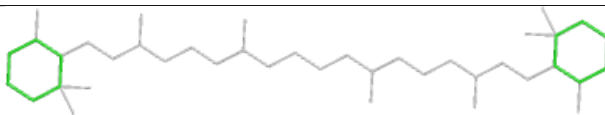
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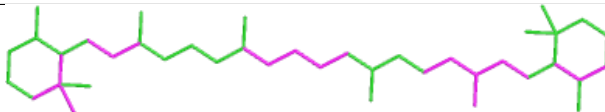
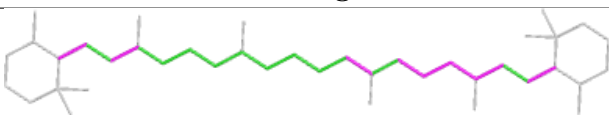
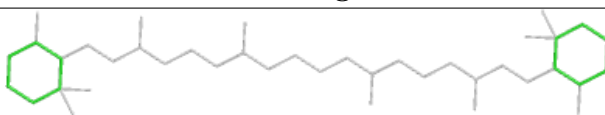


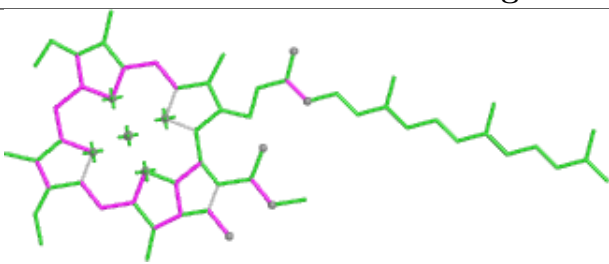
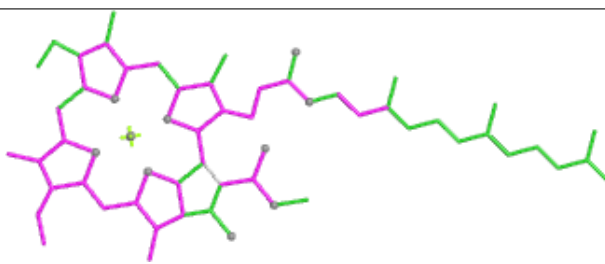
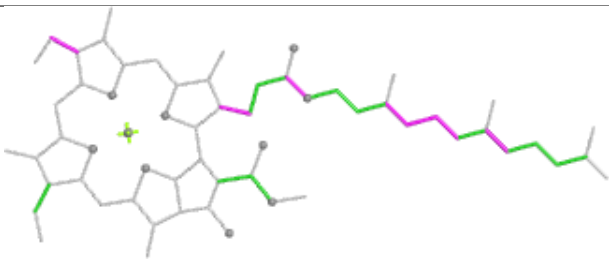
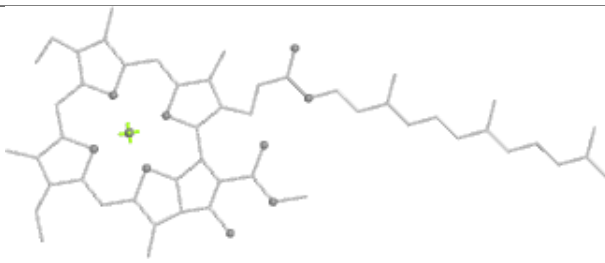
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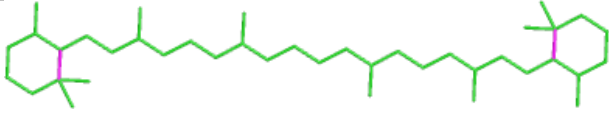
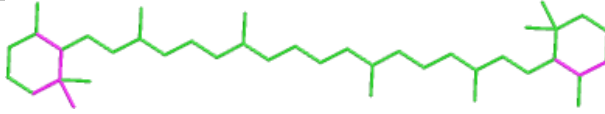
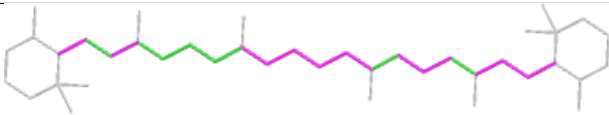
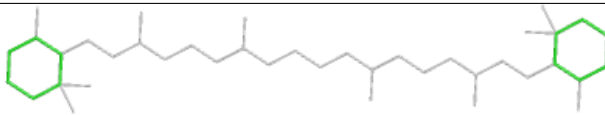


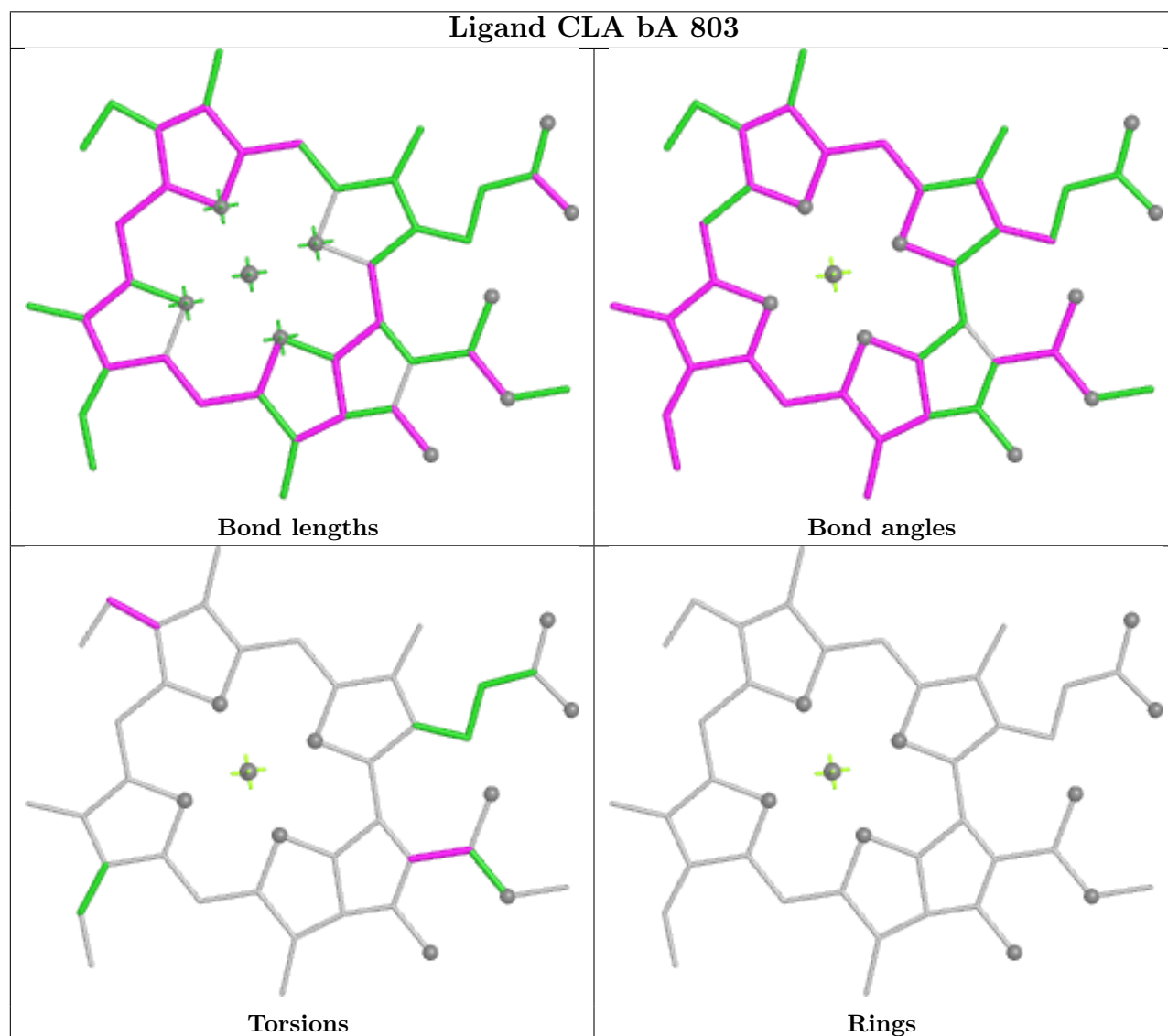
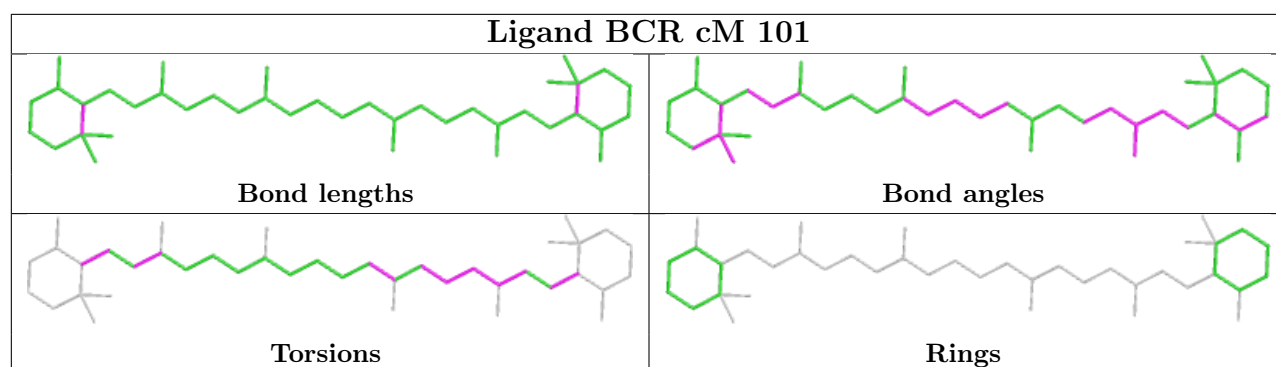


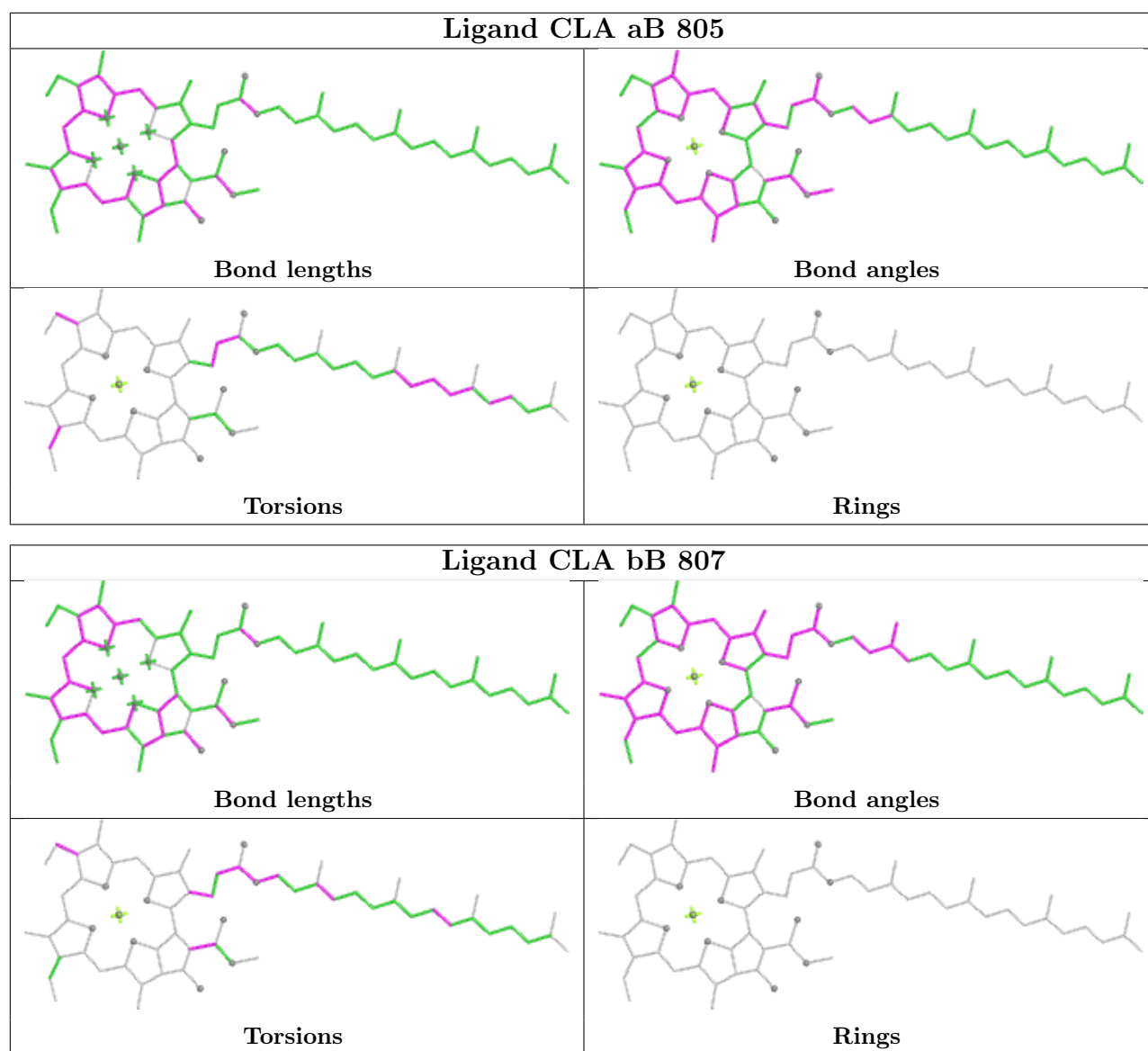
Ligand BCR cB 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

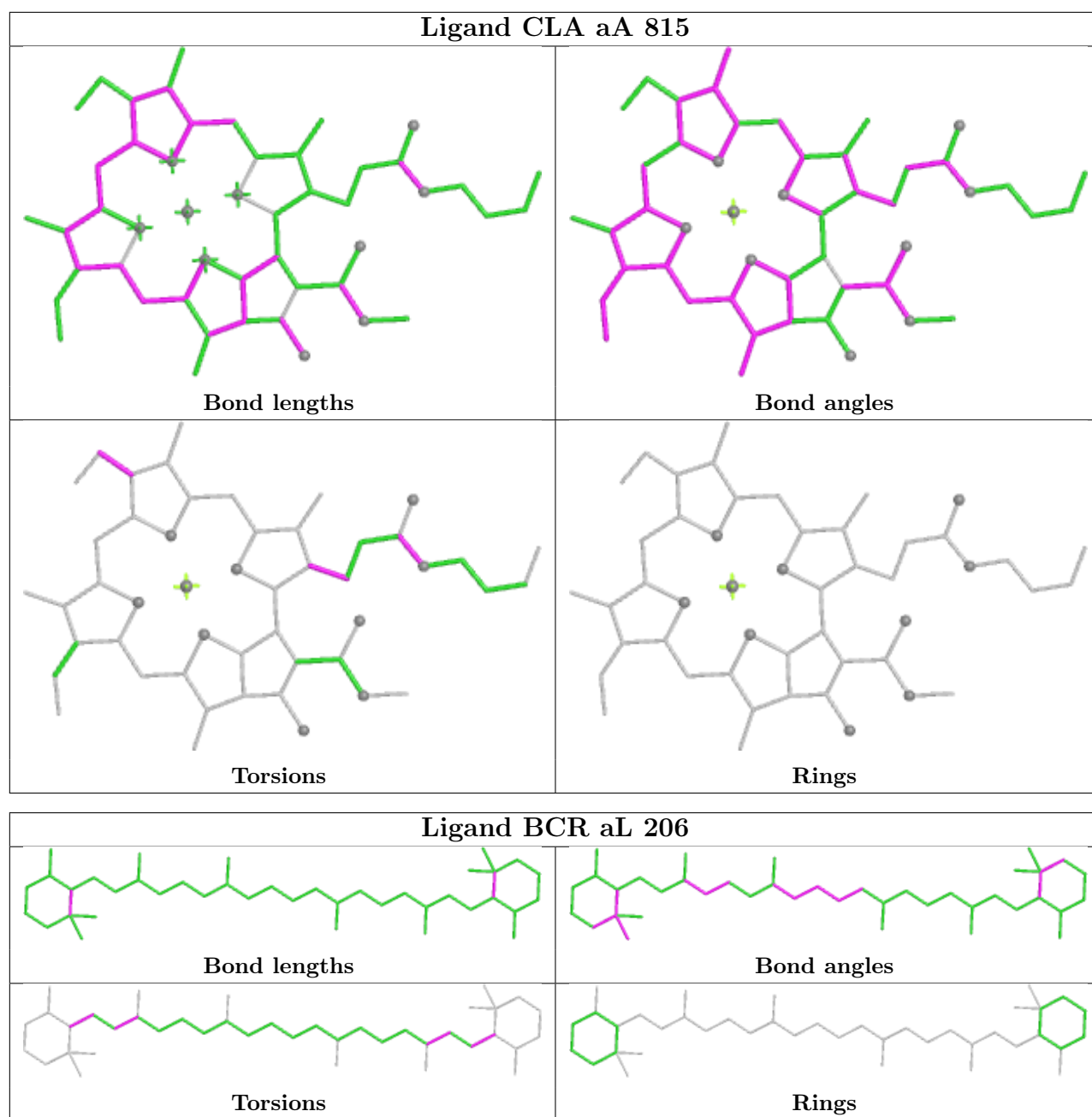
Ligand BCR bM 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

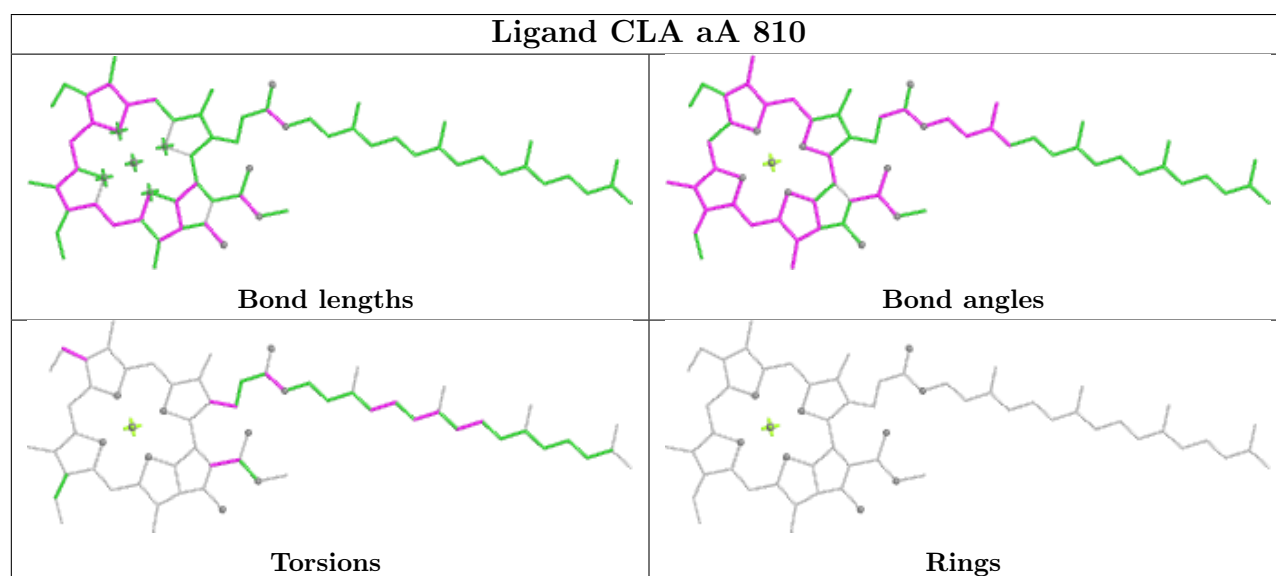
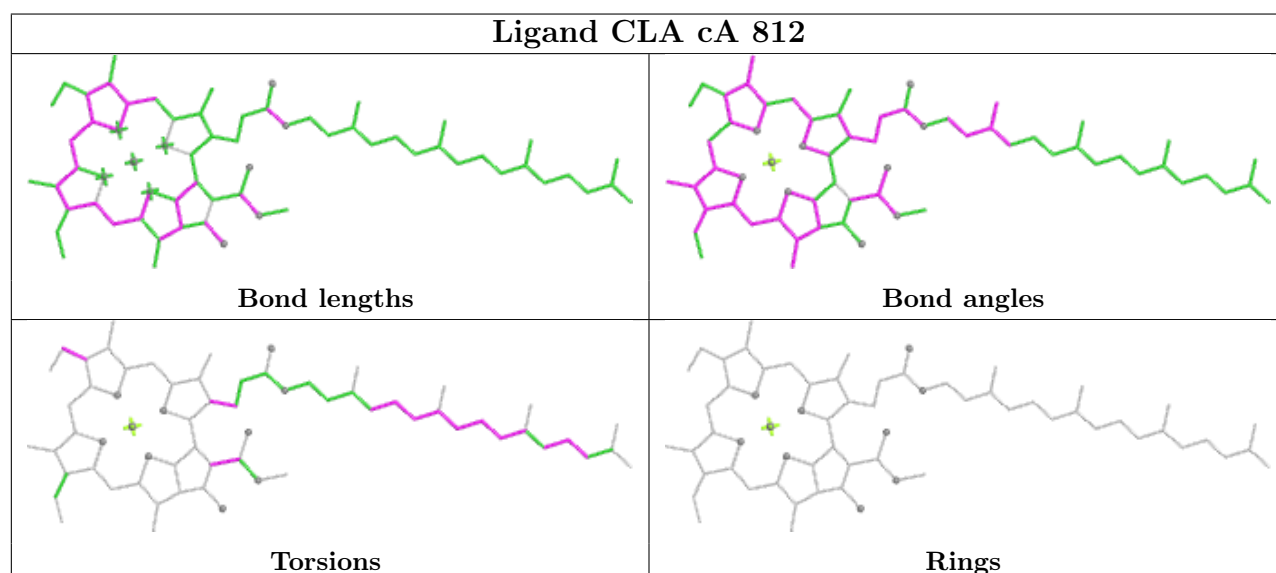
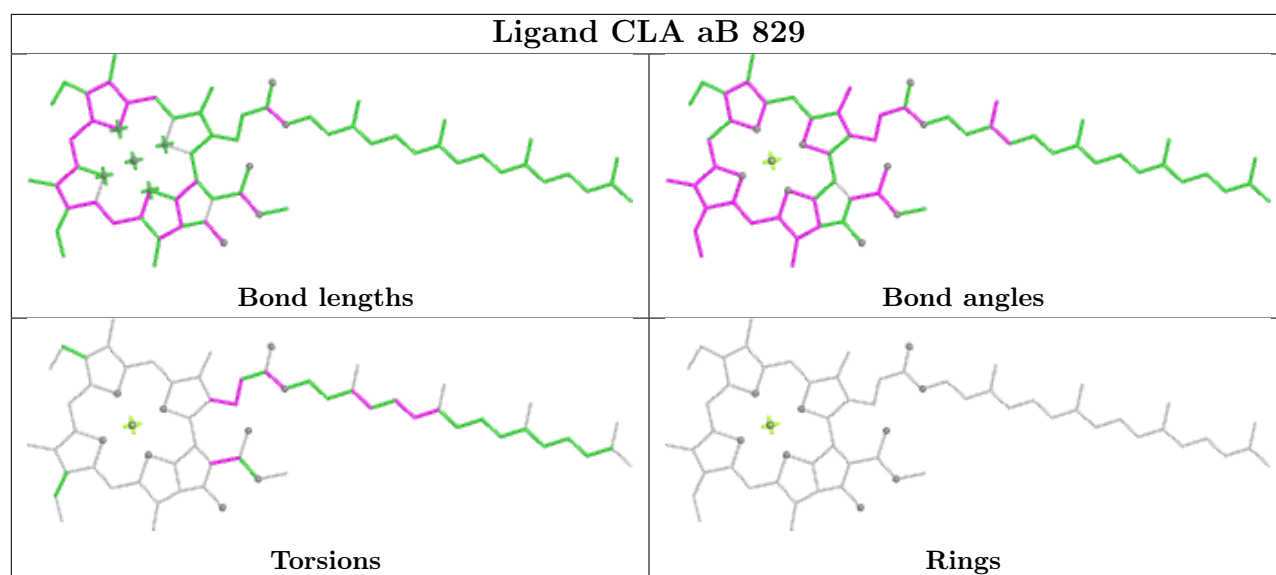
Ligand CLA cB 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR aB 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

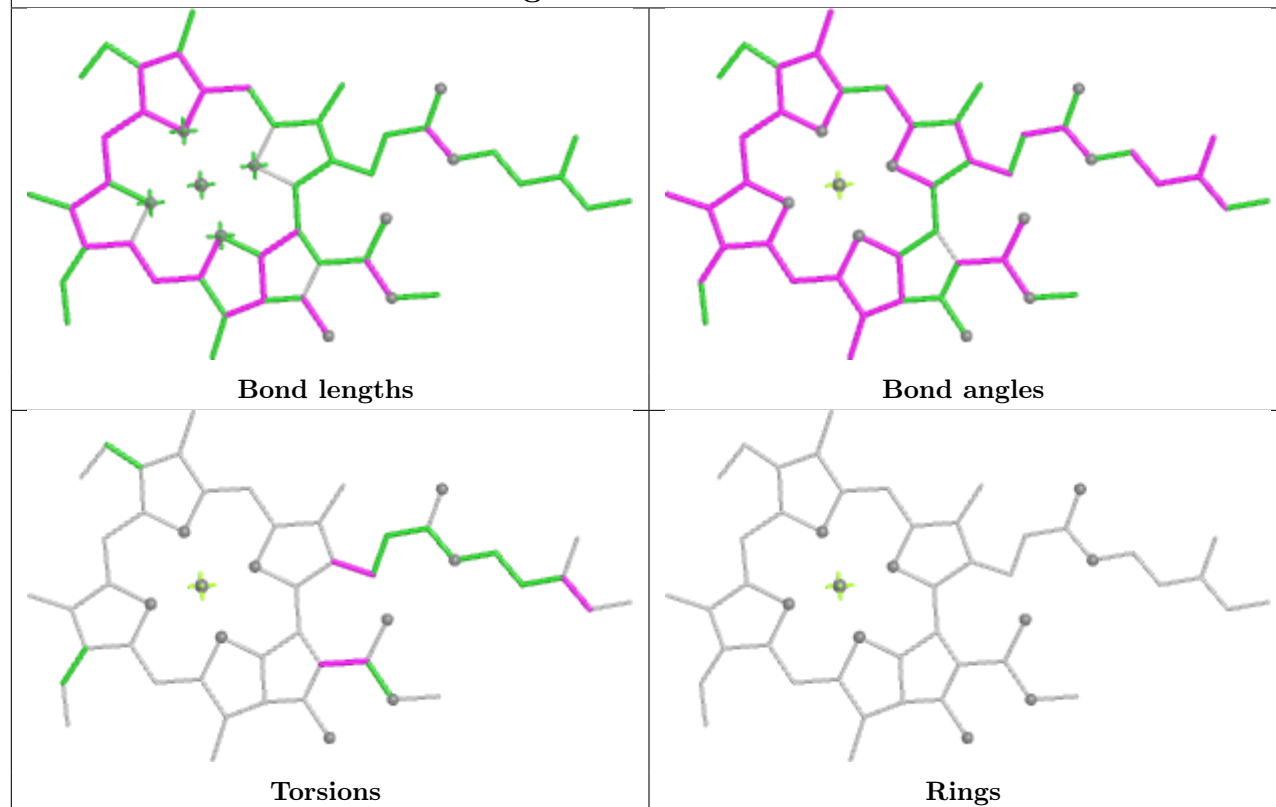




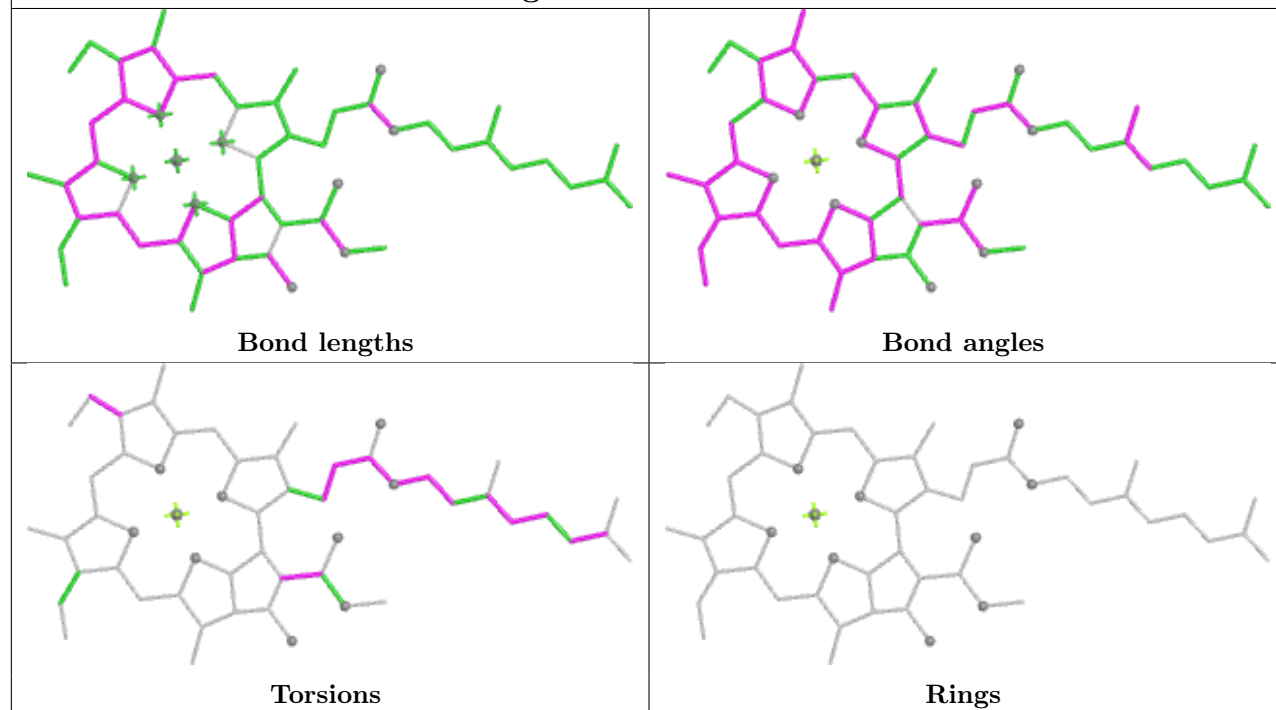


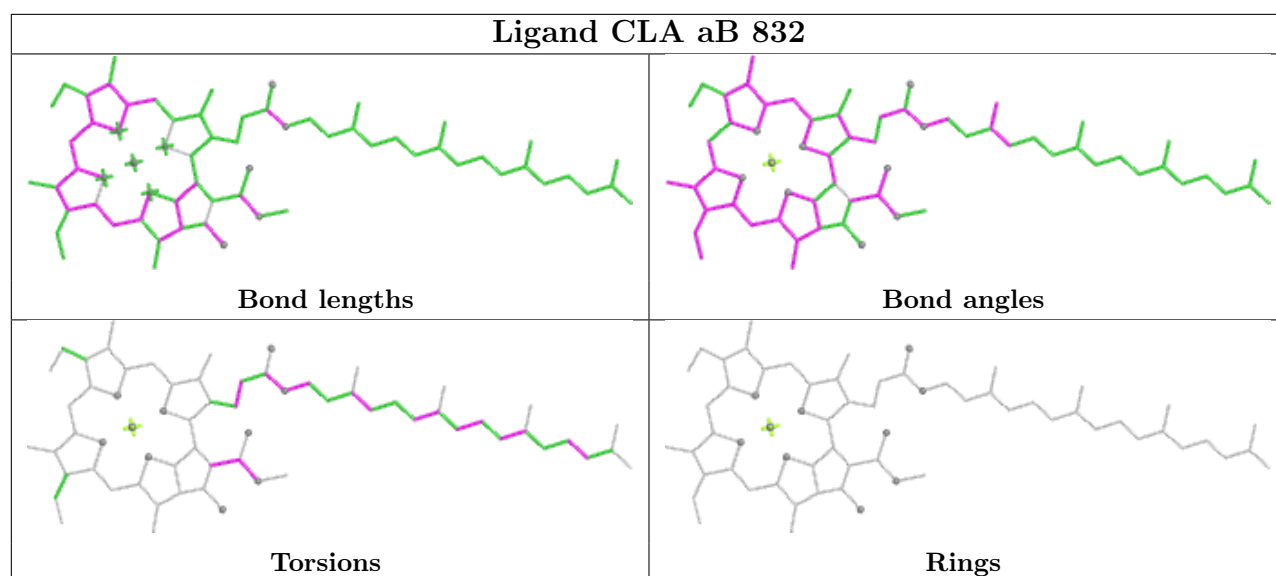
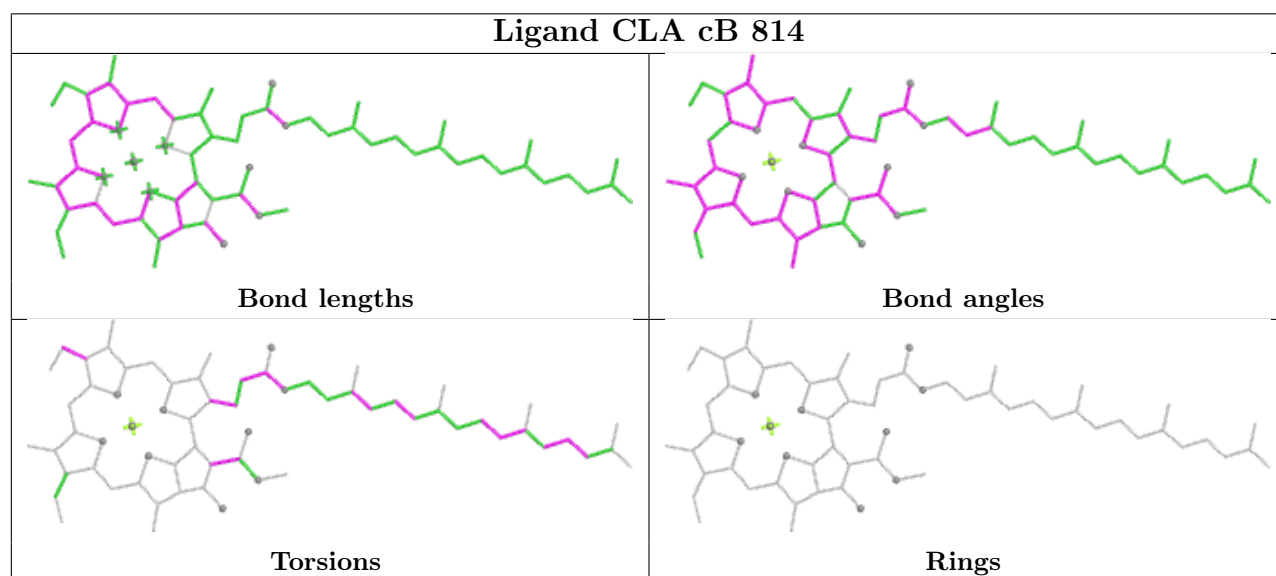
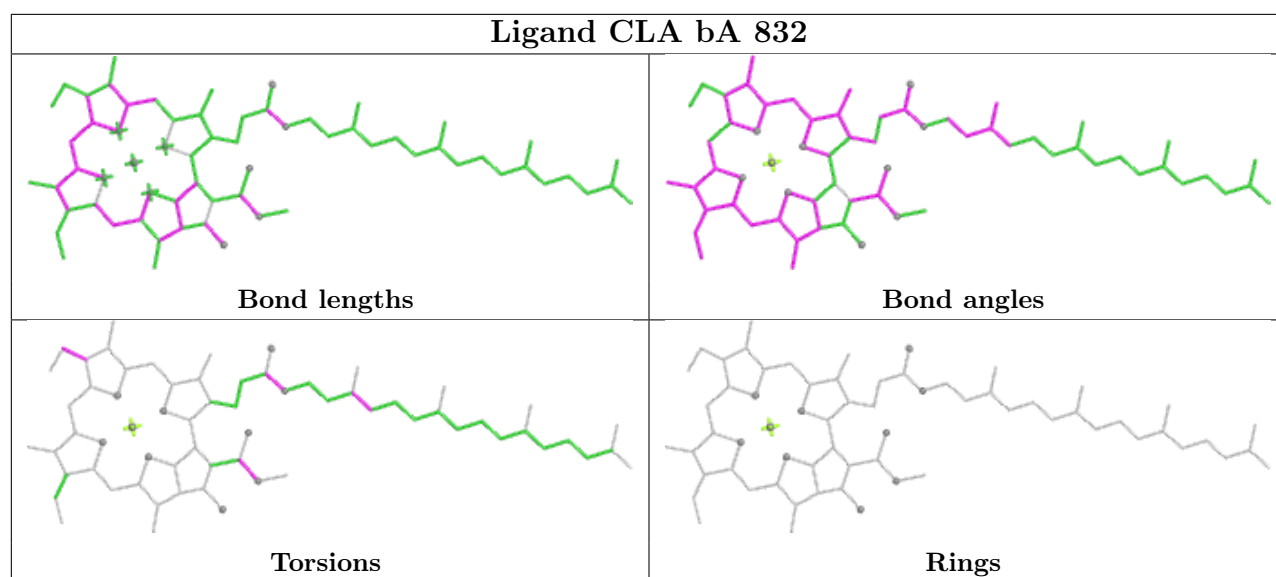


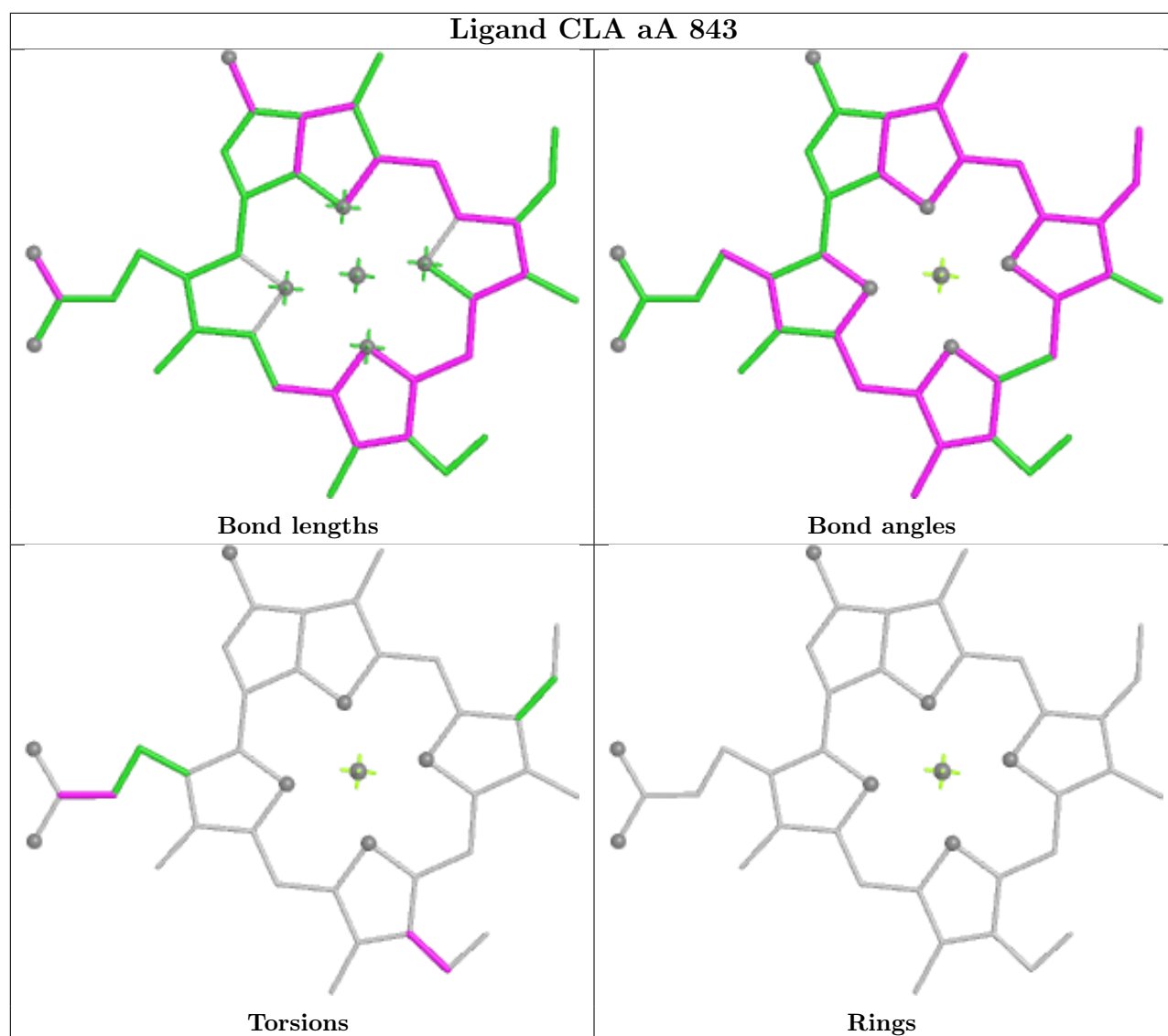
Ligand CLA cA 840

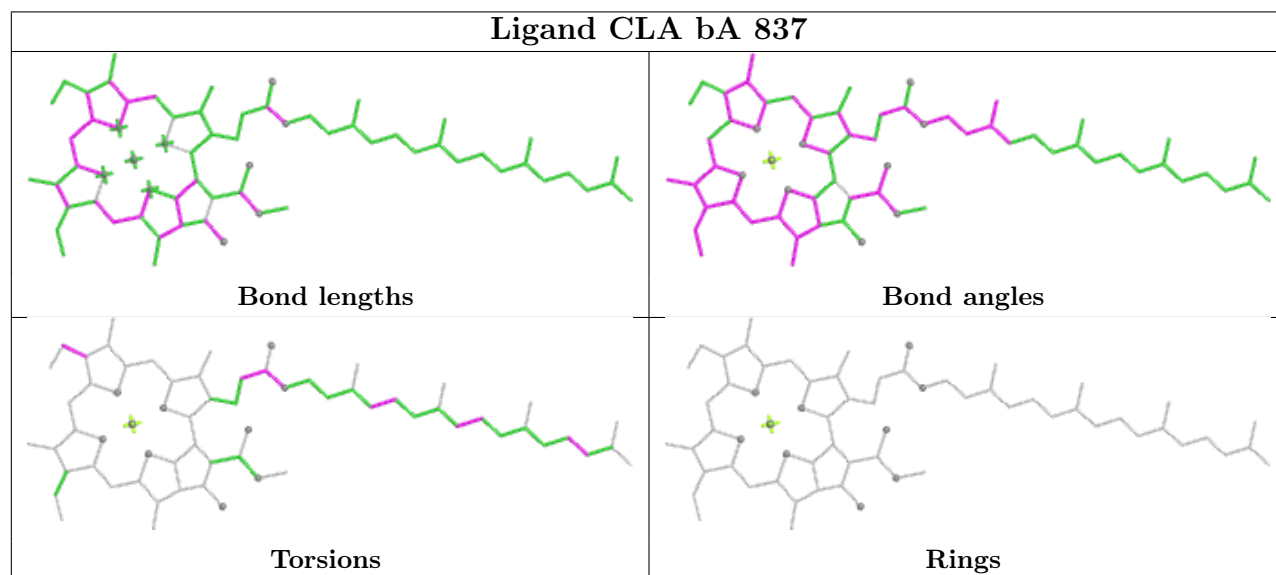
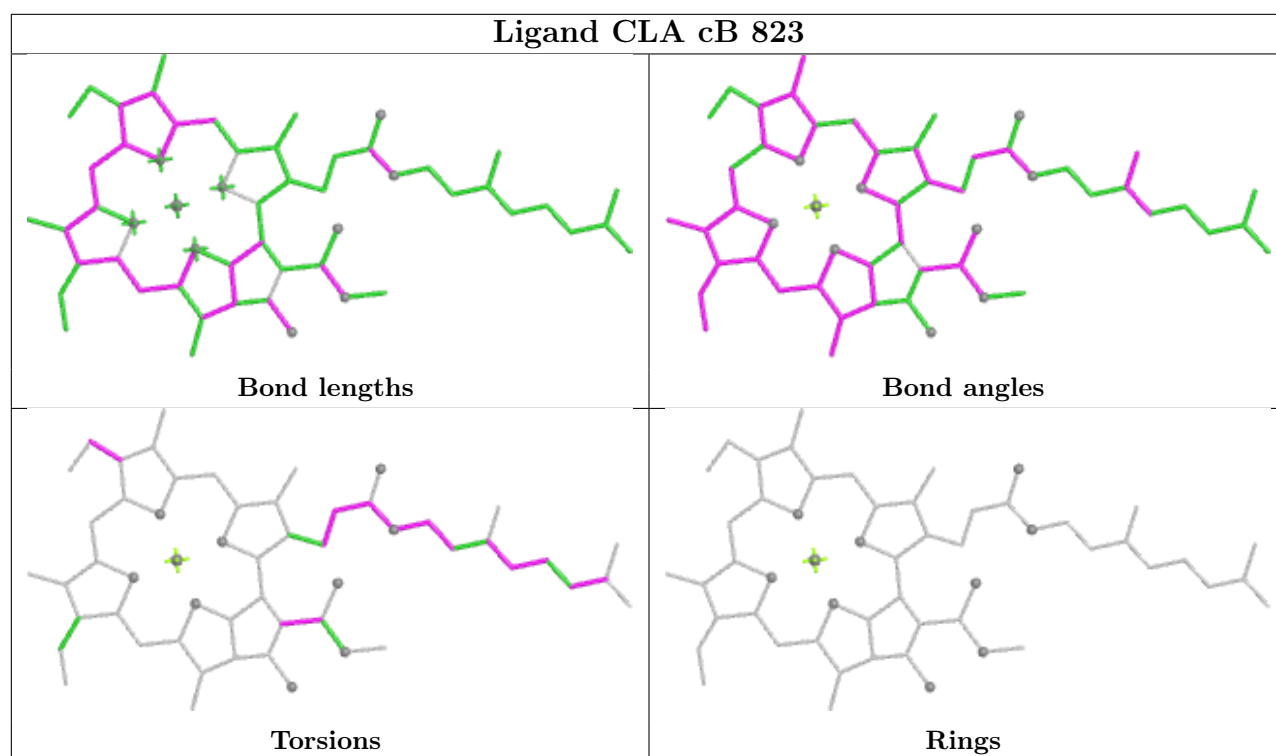


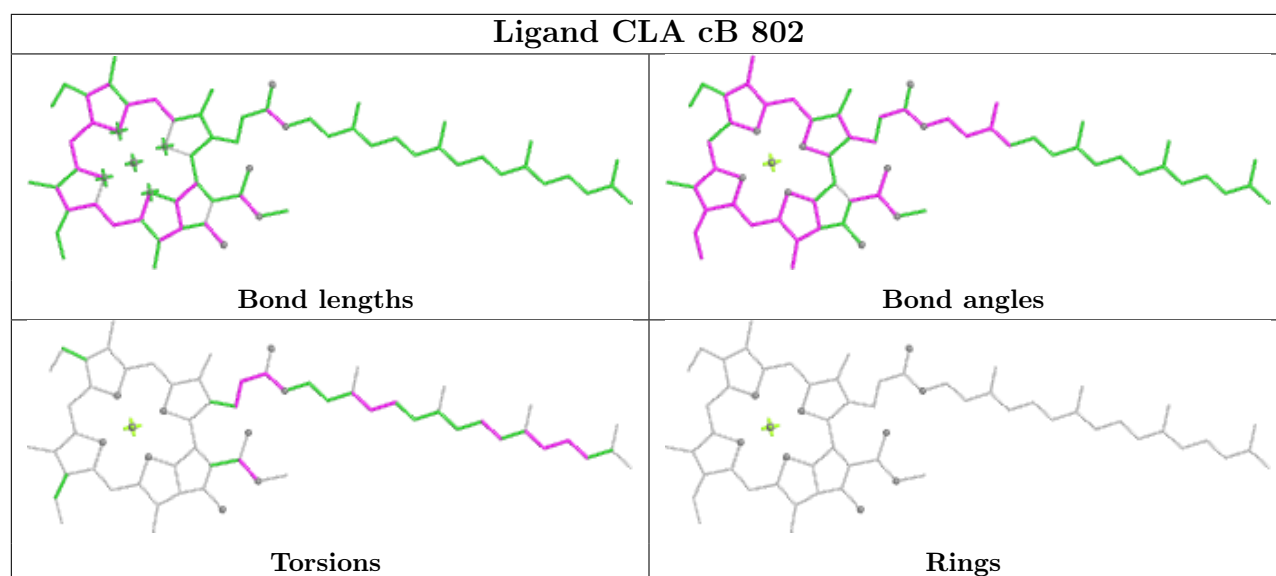
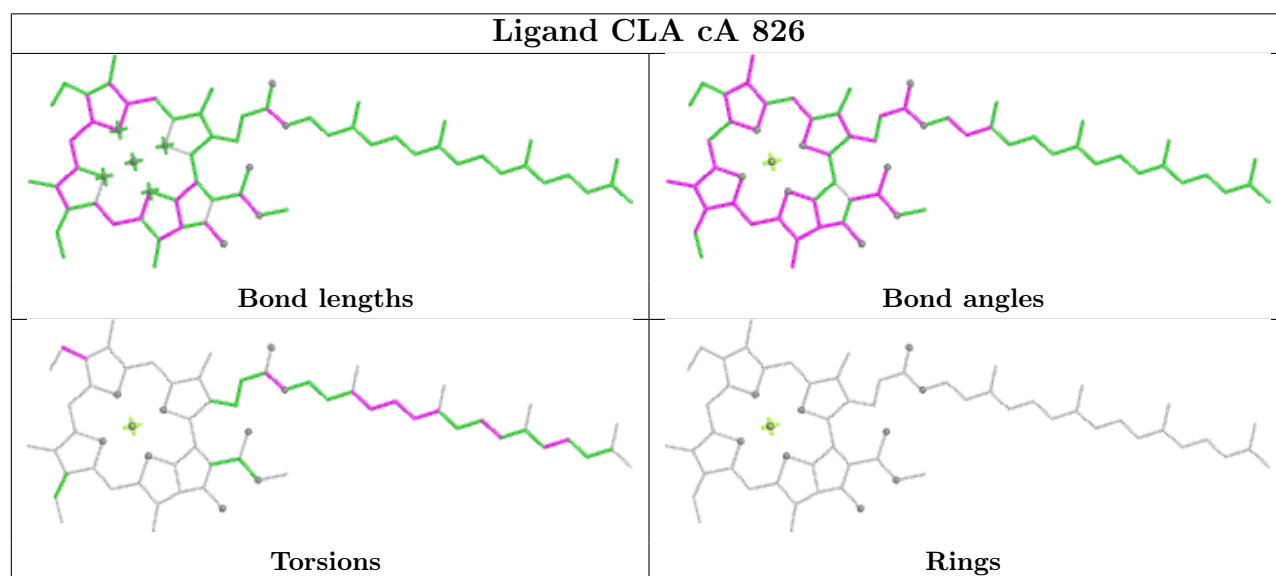
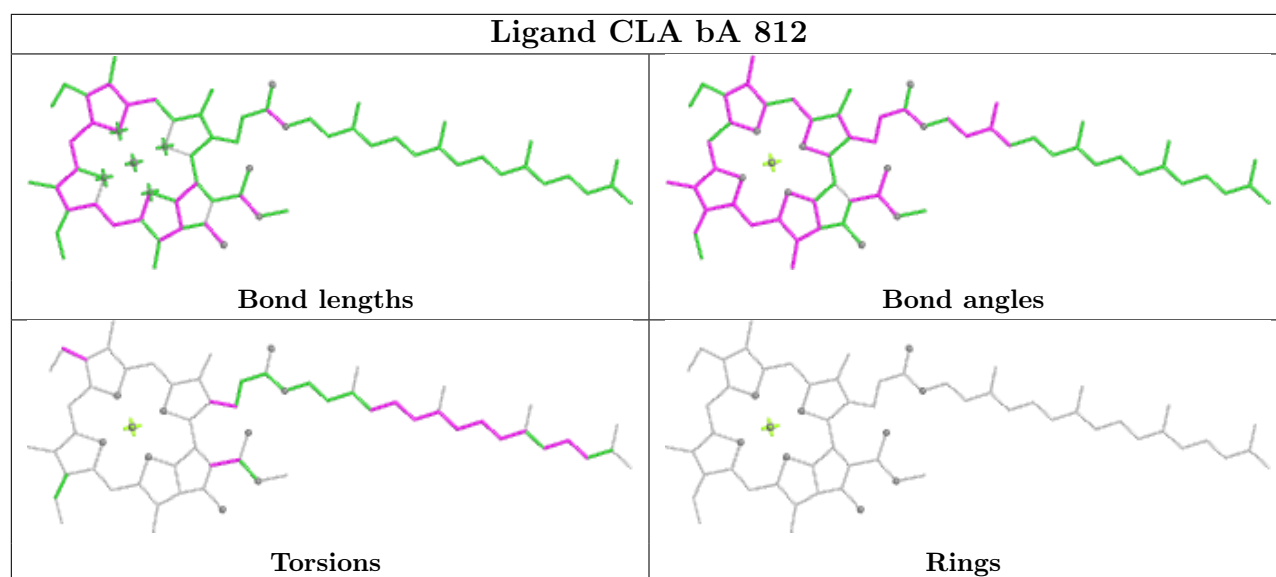
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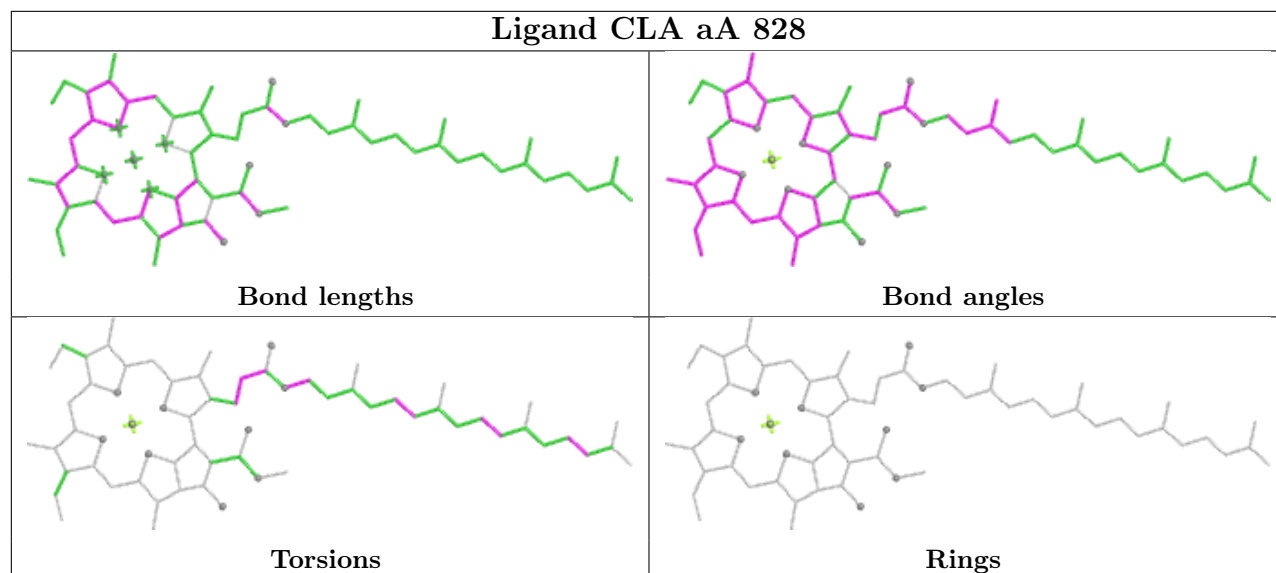
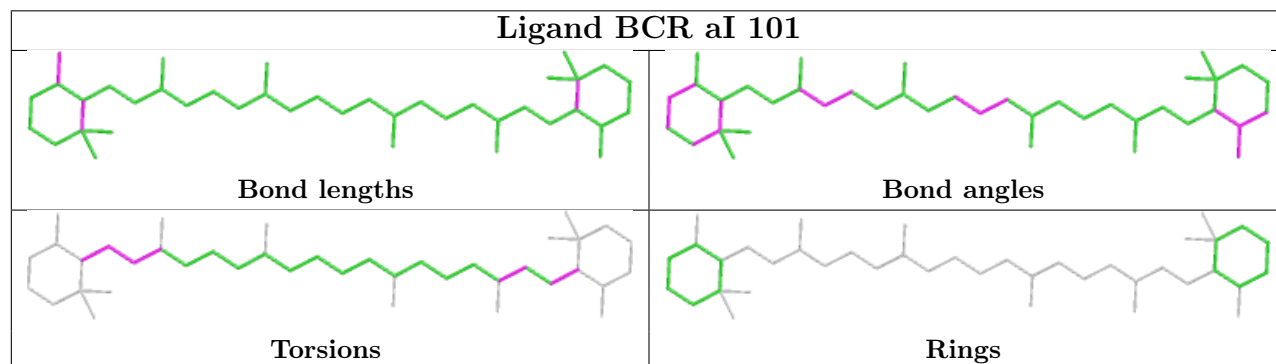
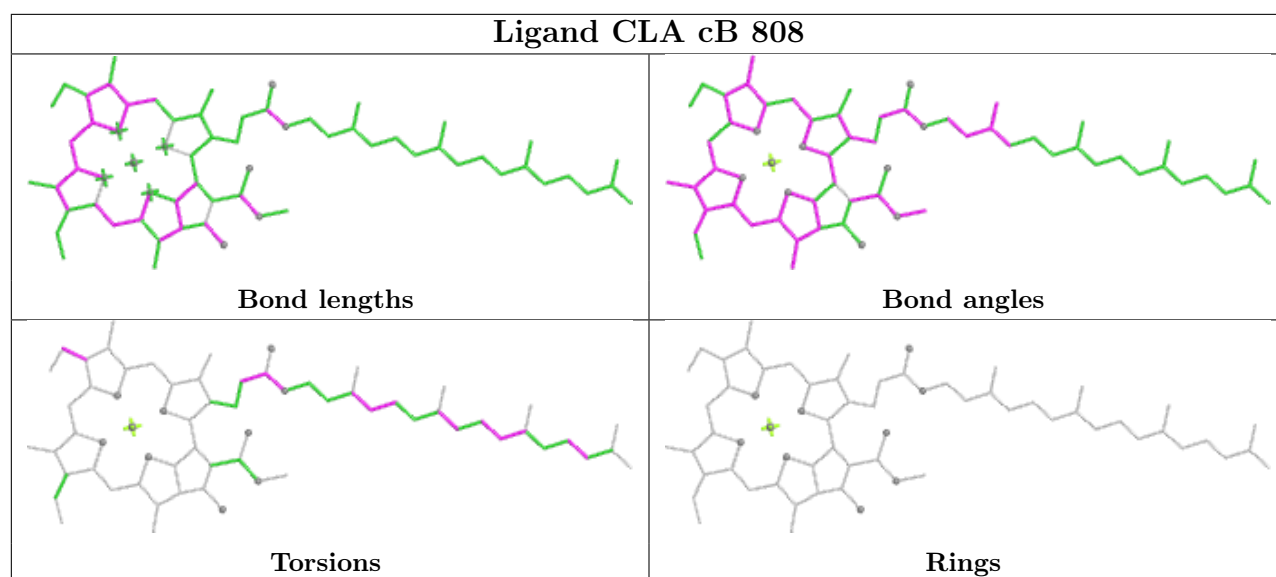


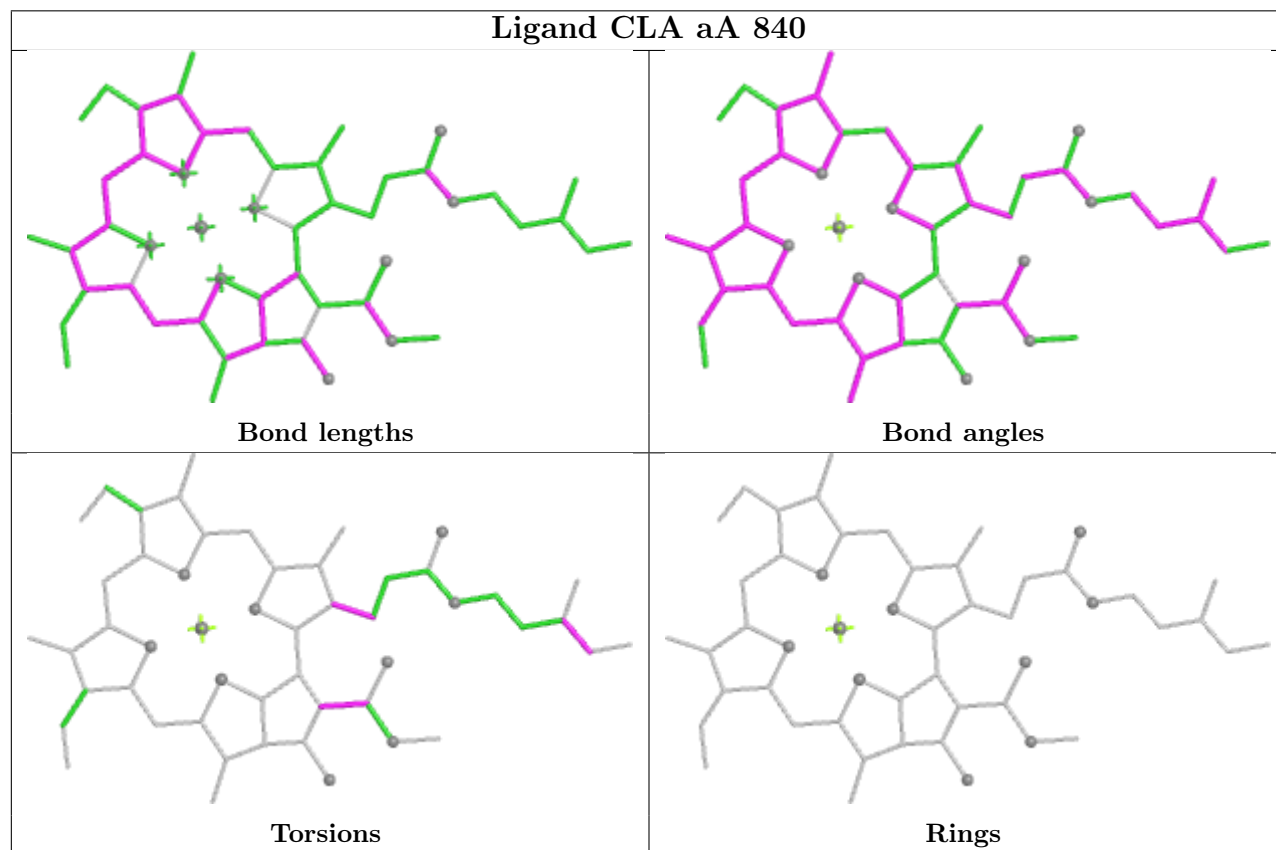
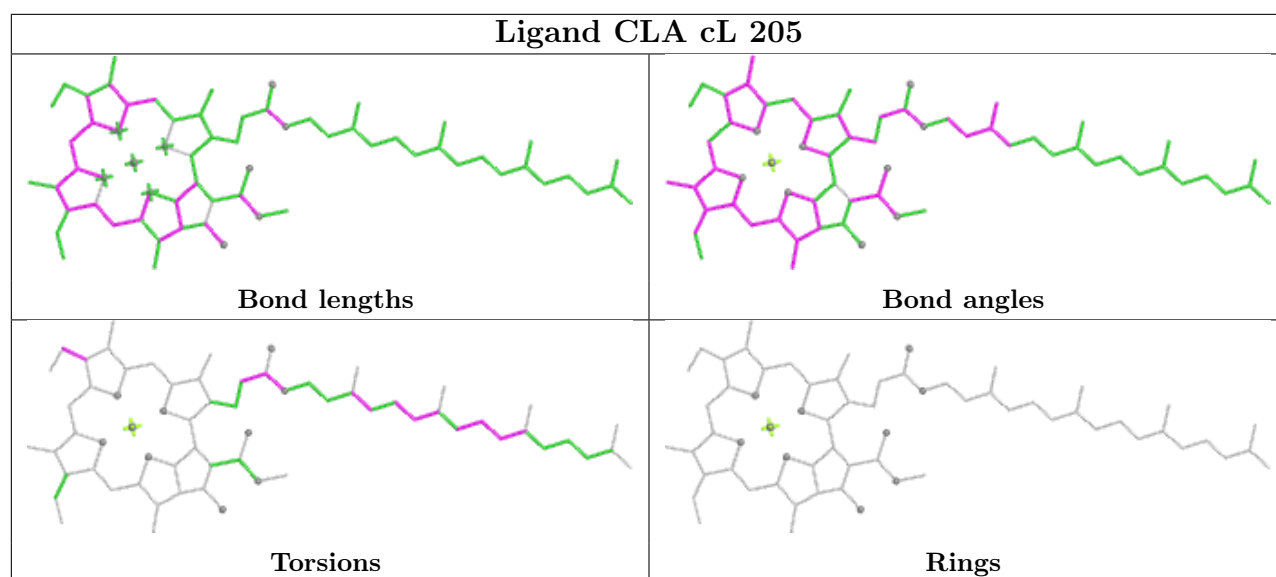


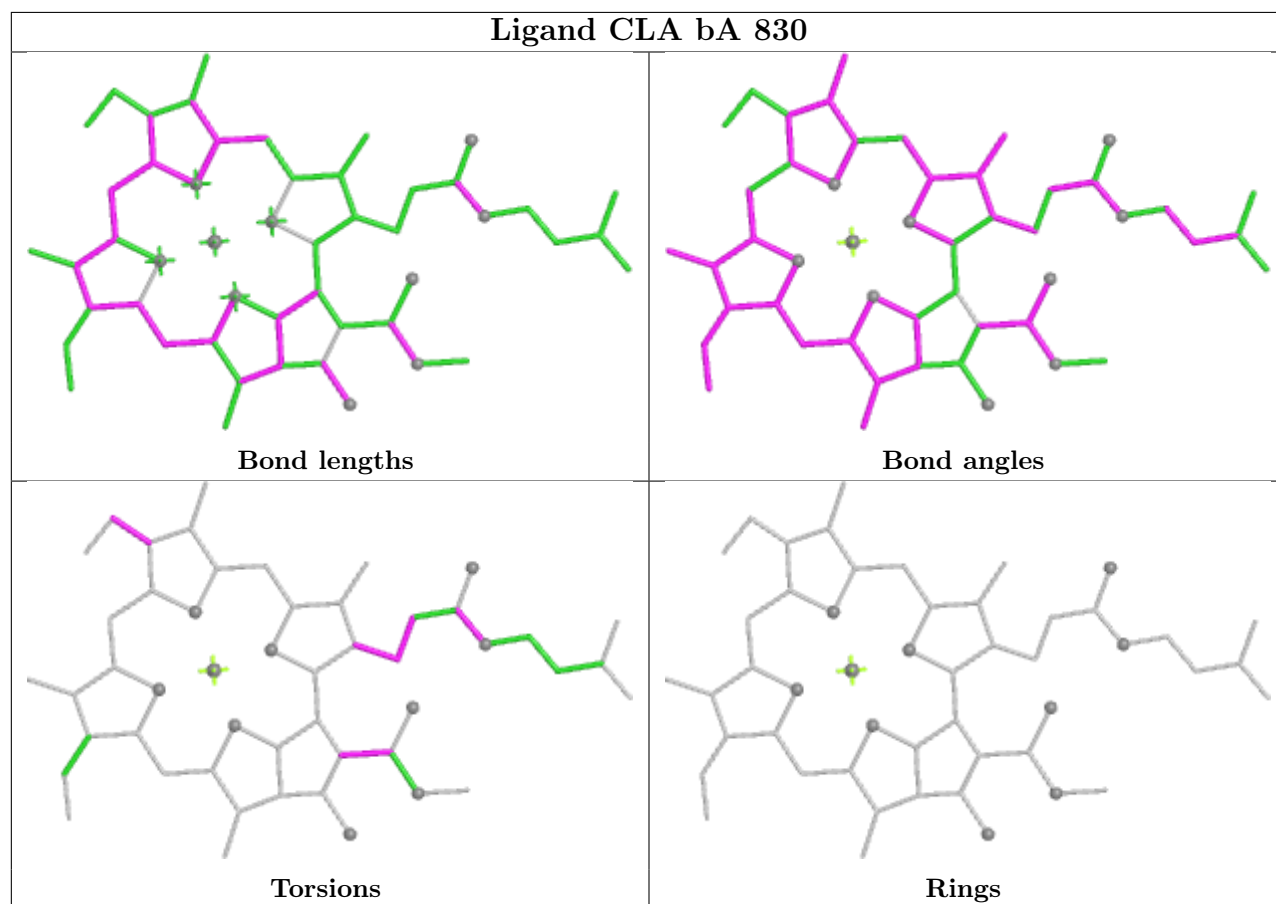
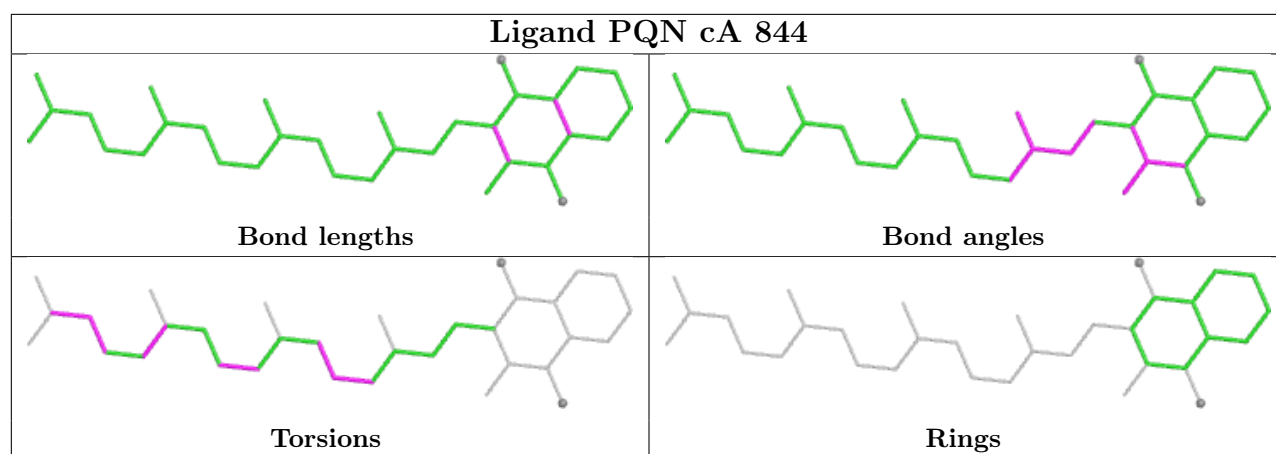


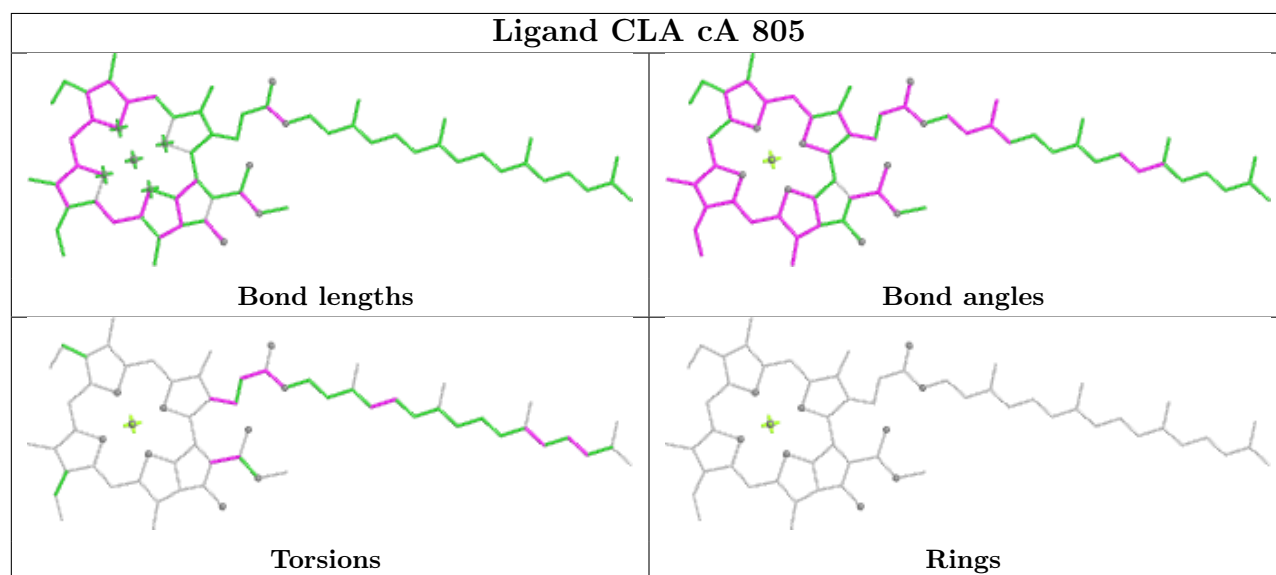
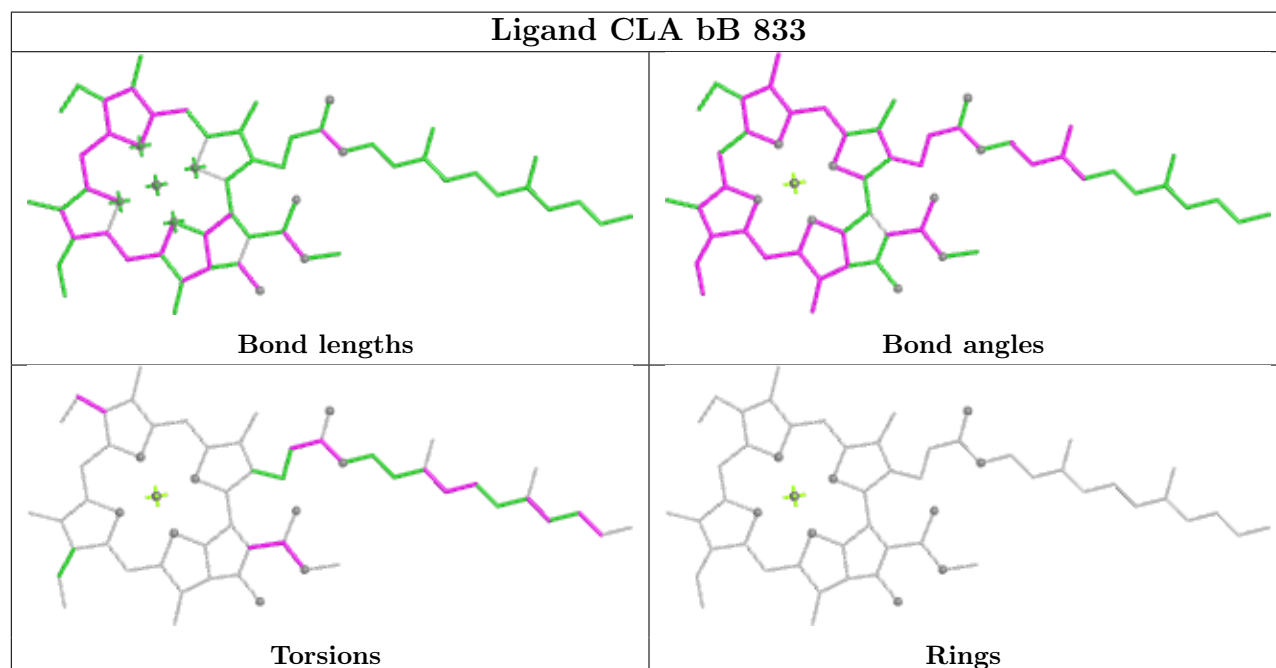
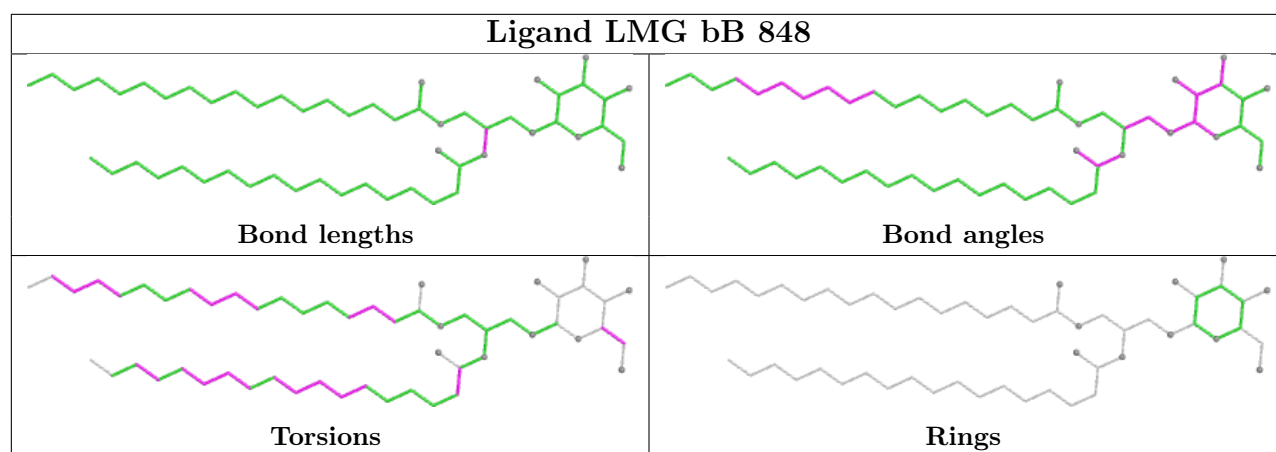


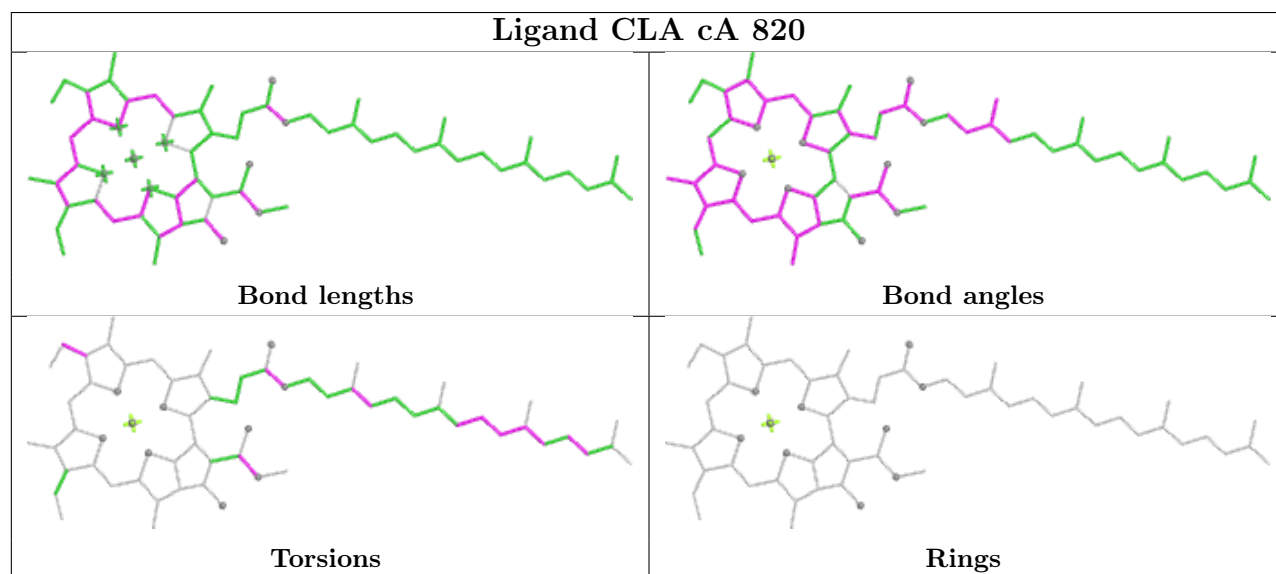
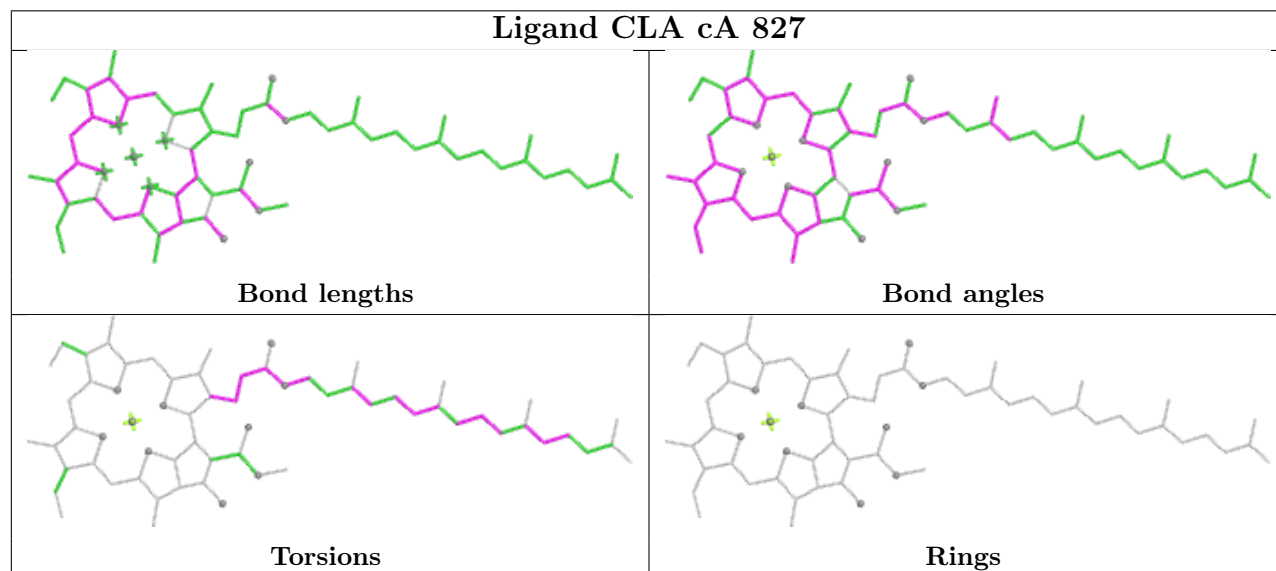
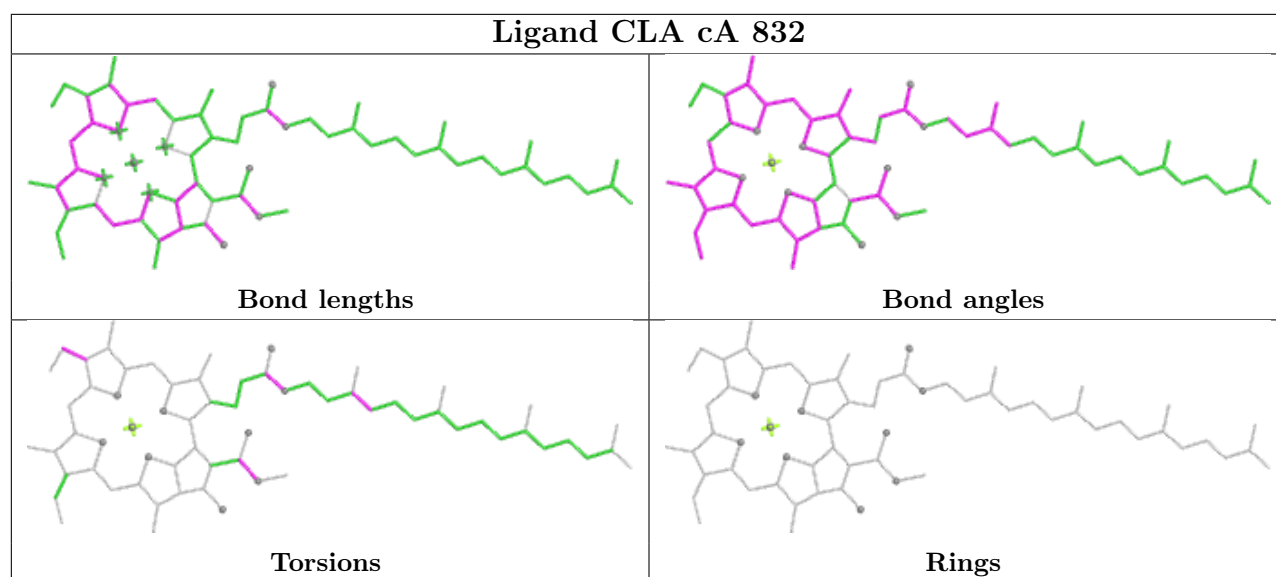


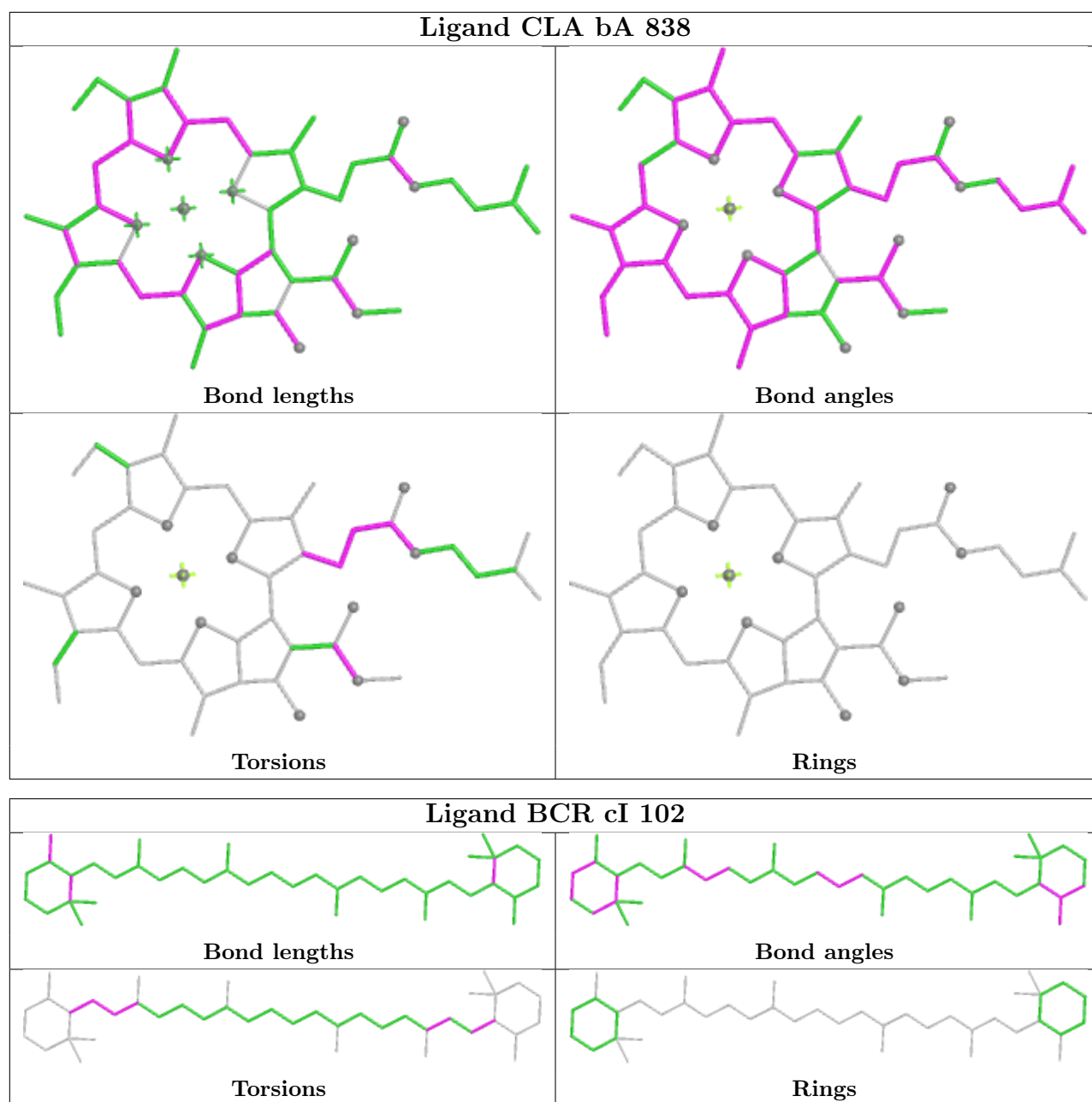


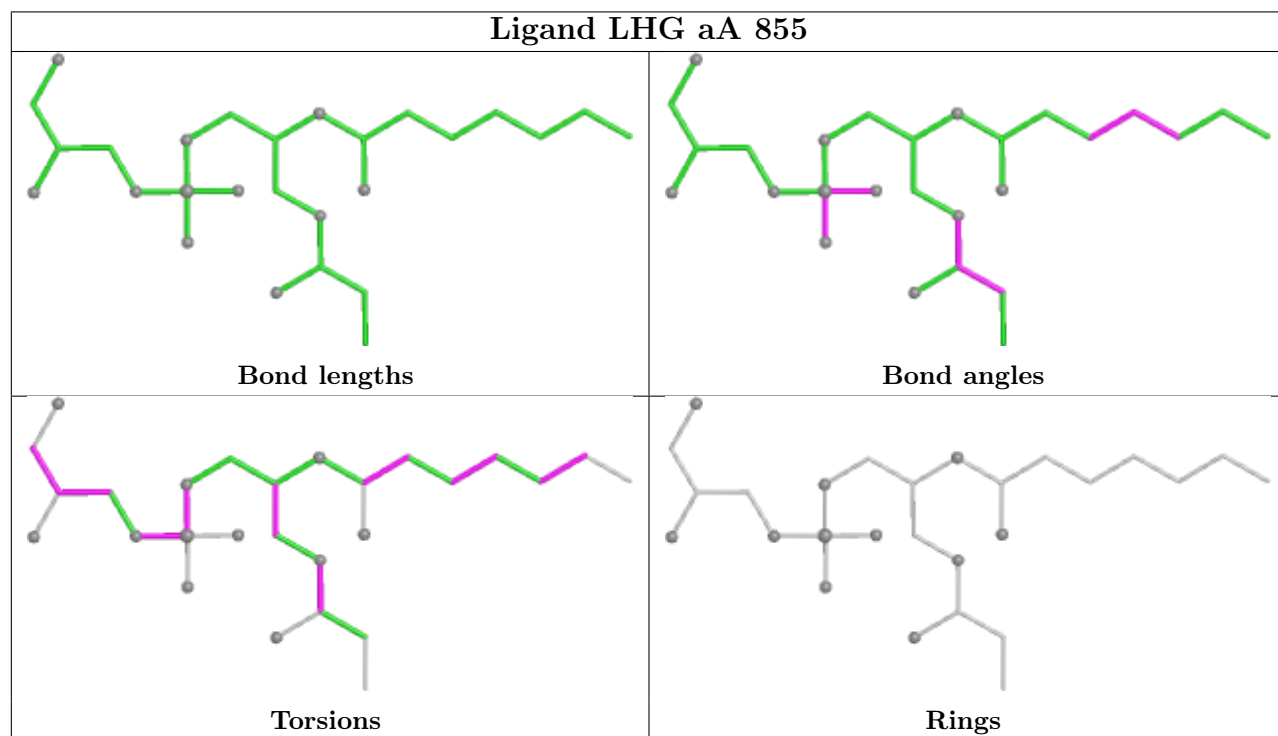
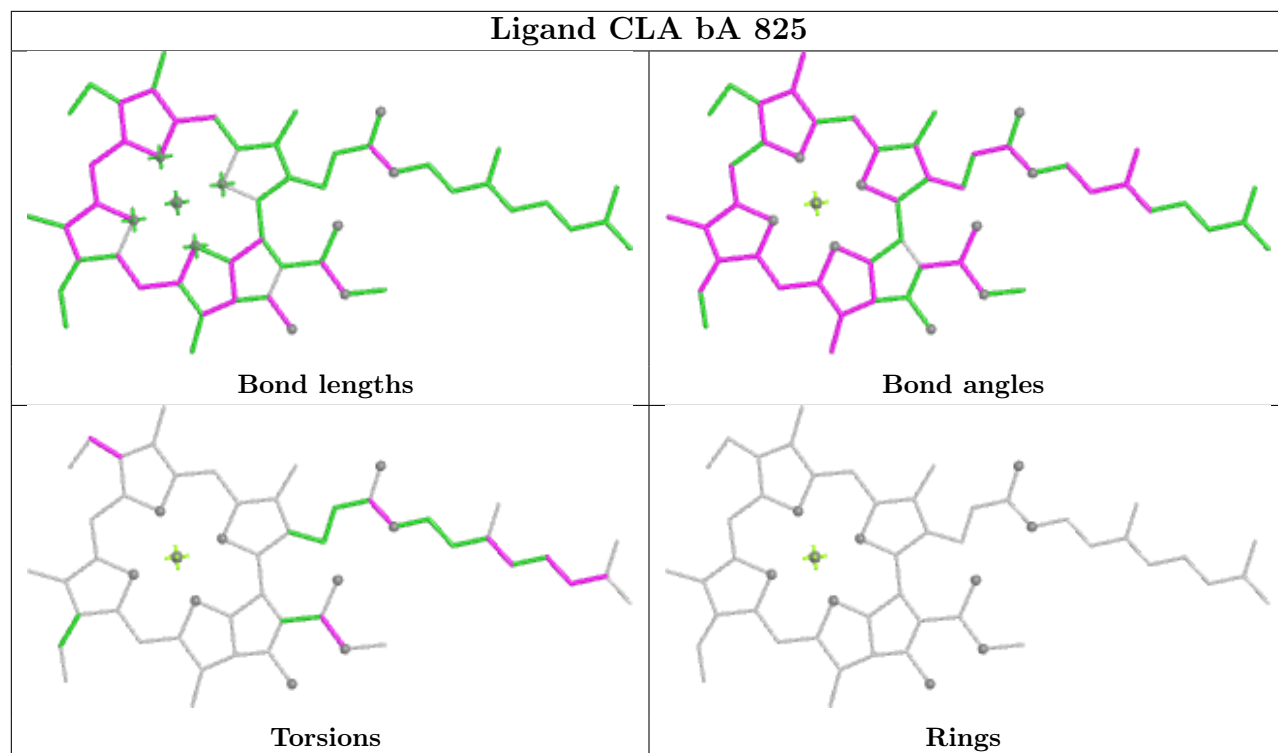


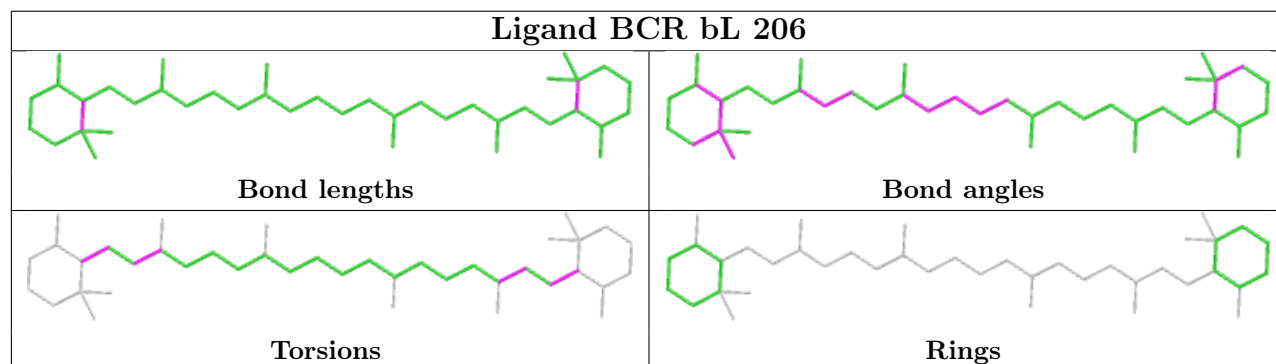
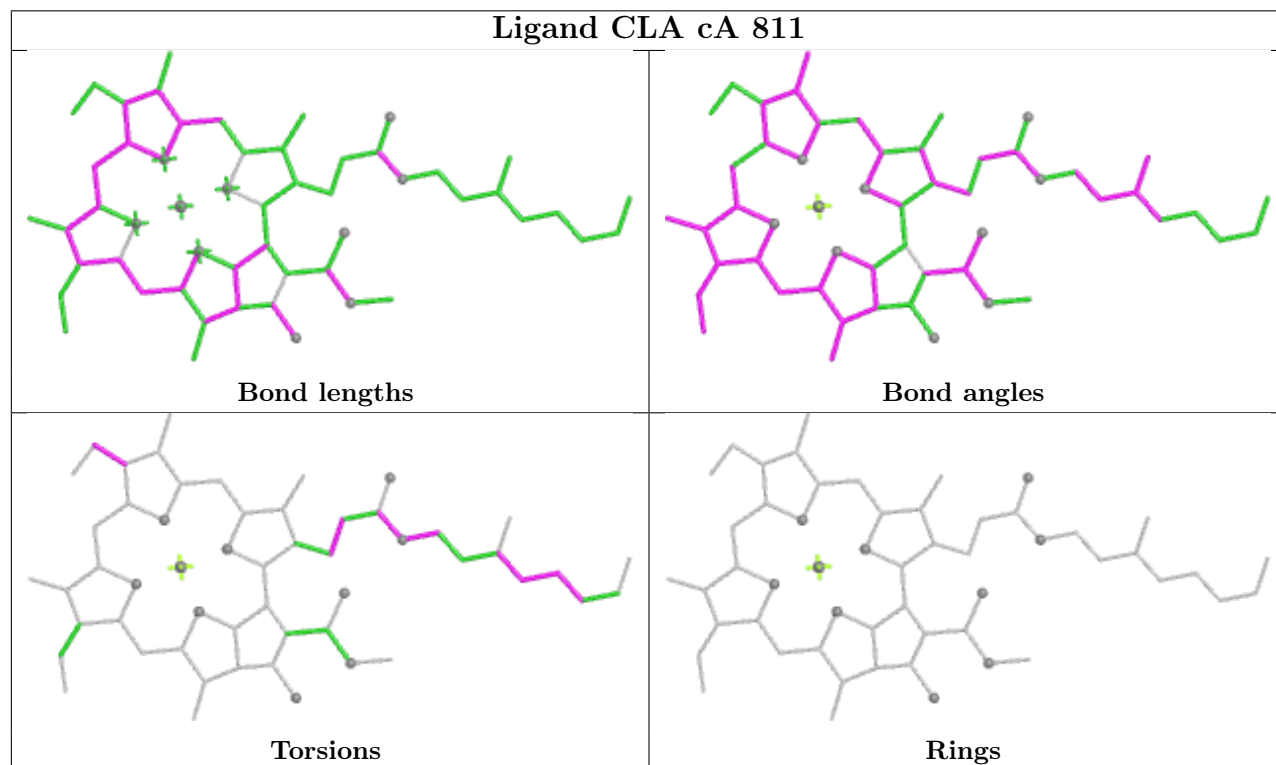
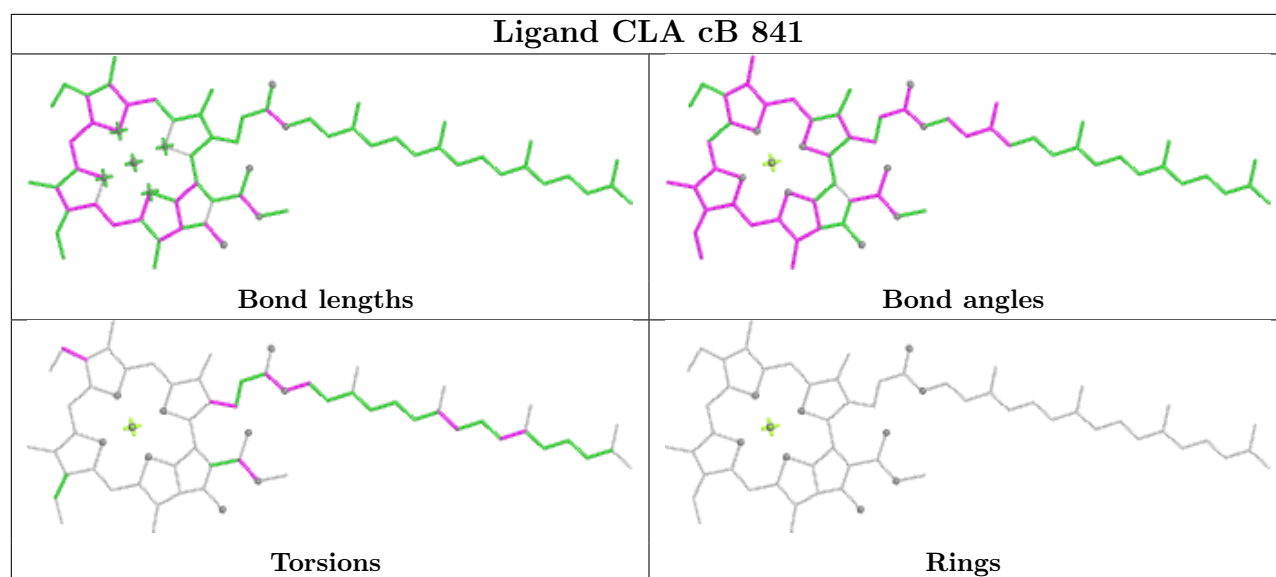


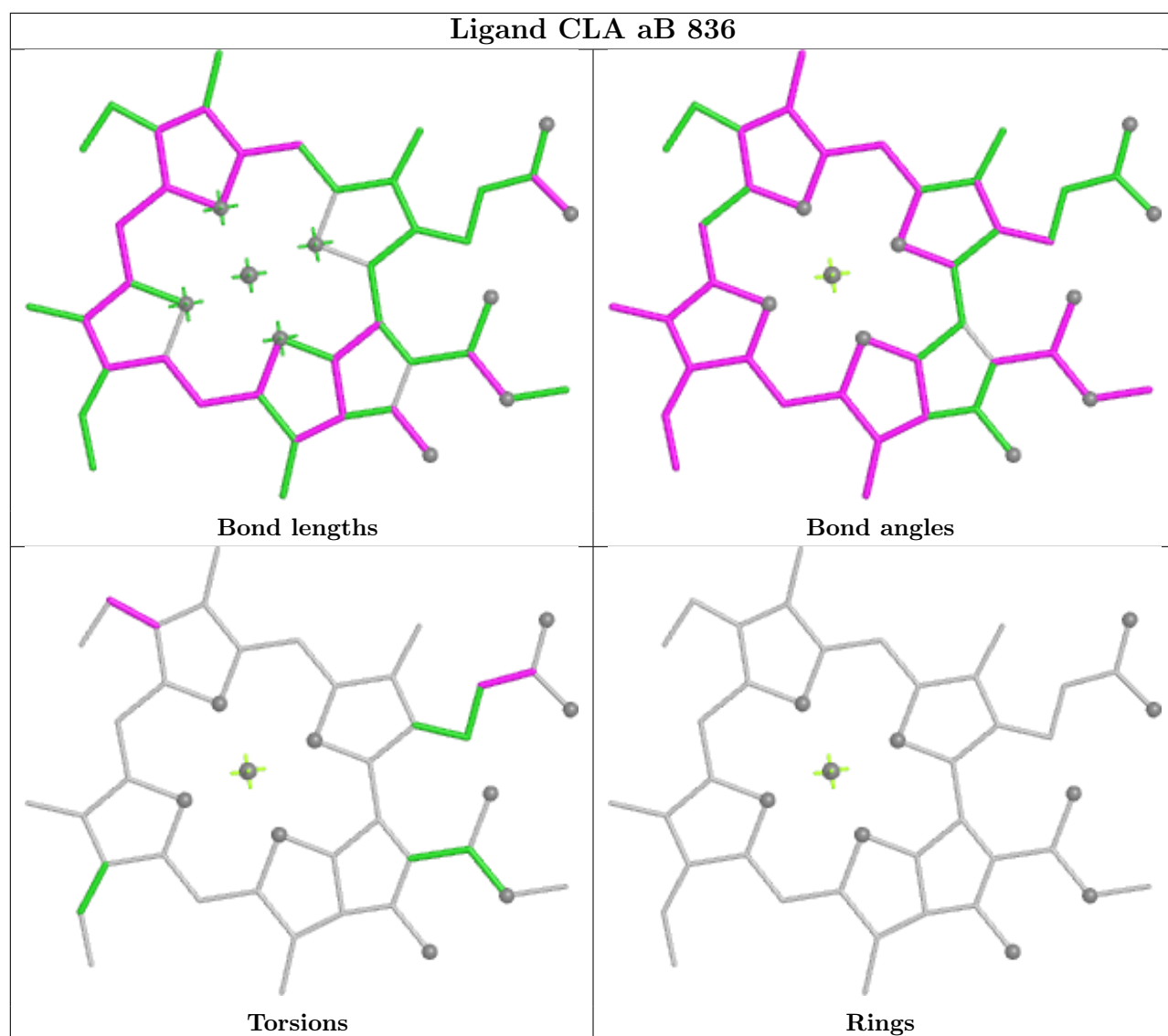


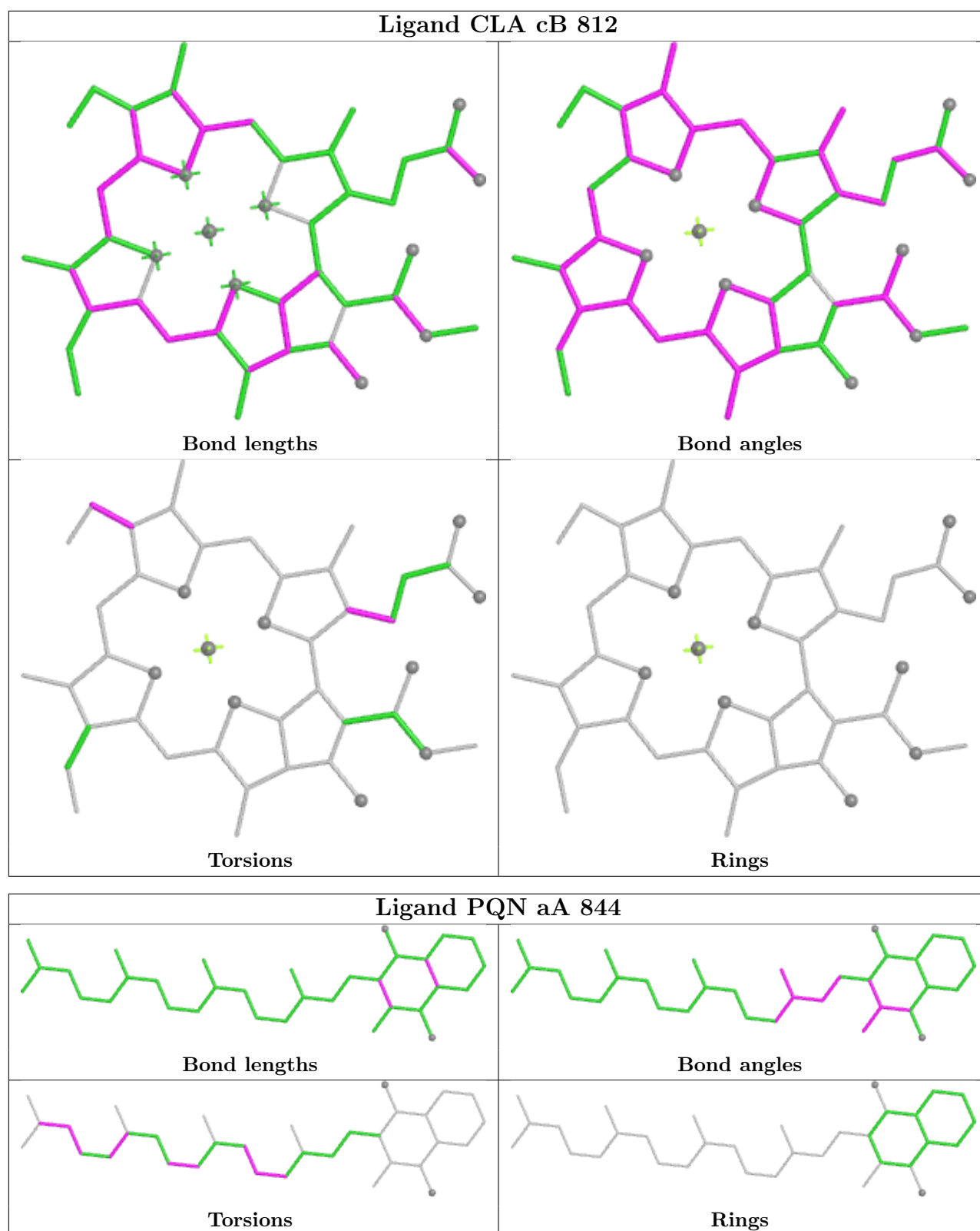


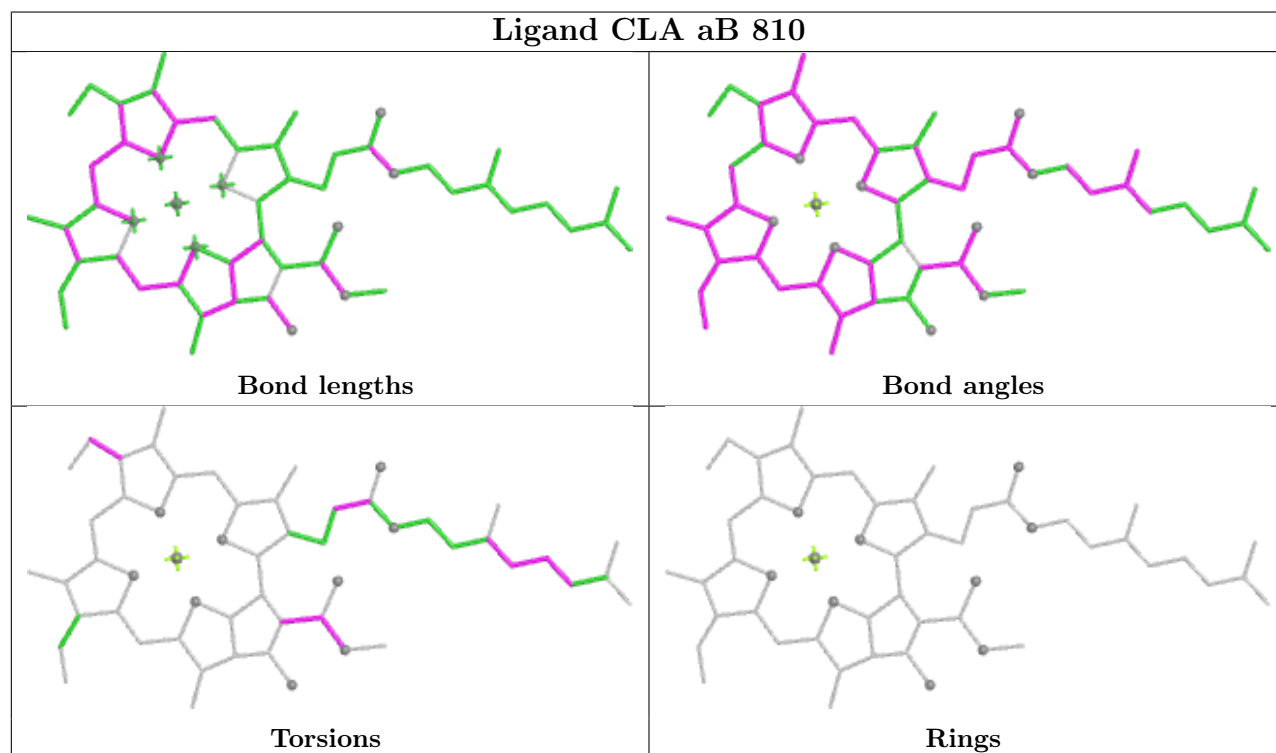
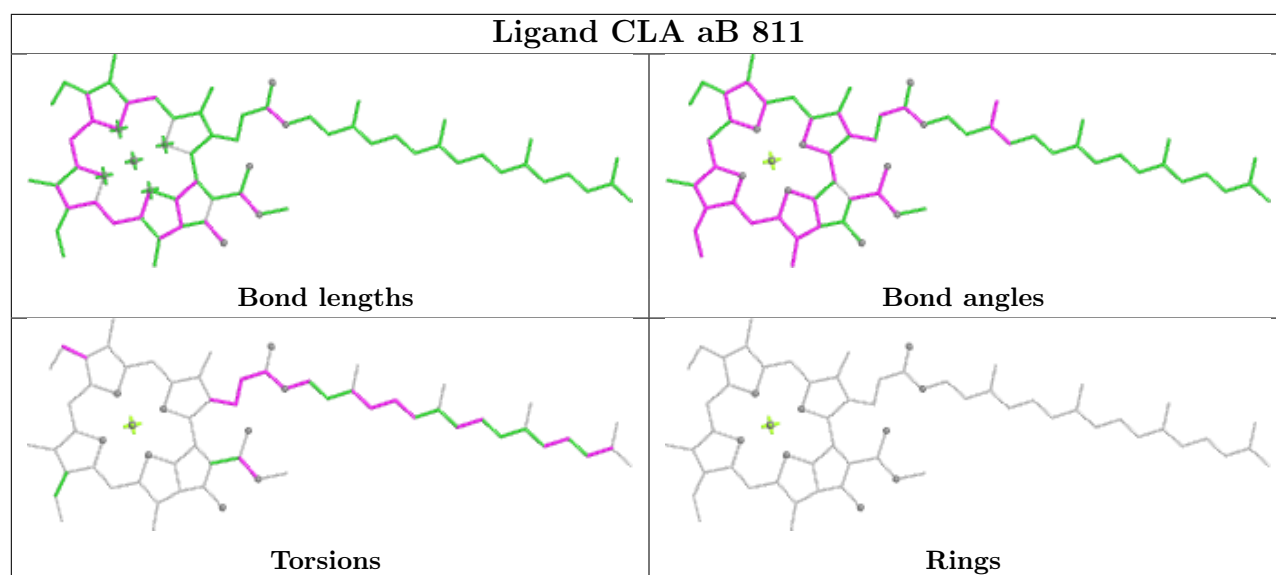


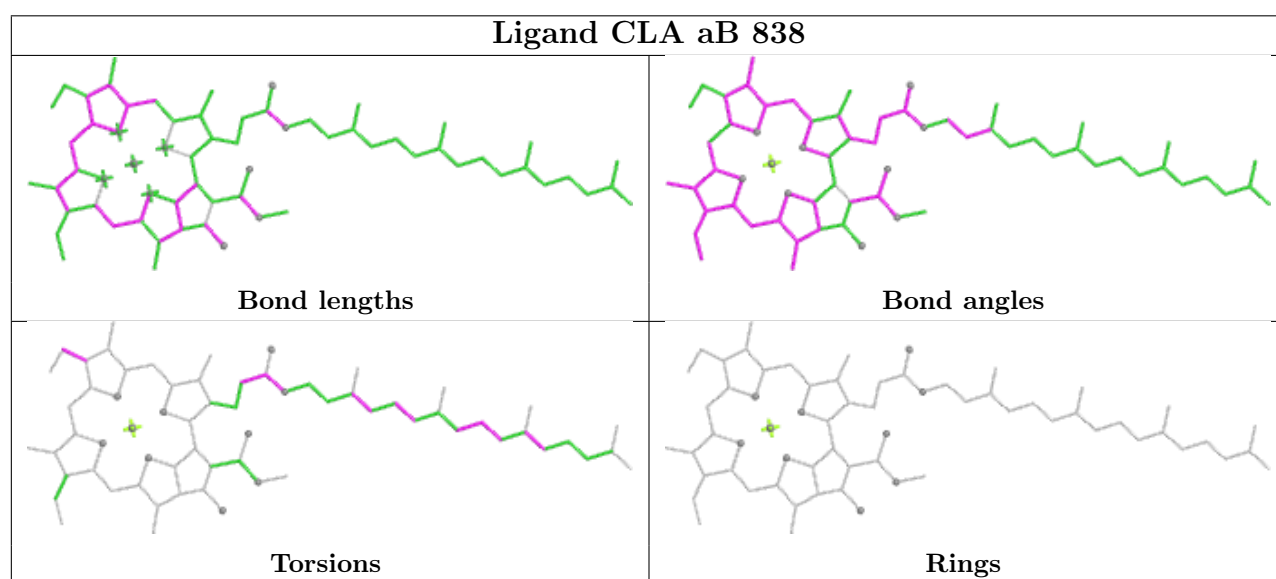
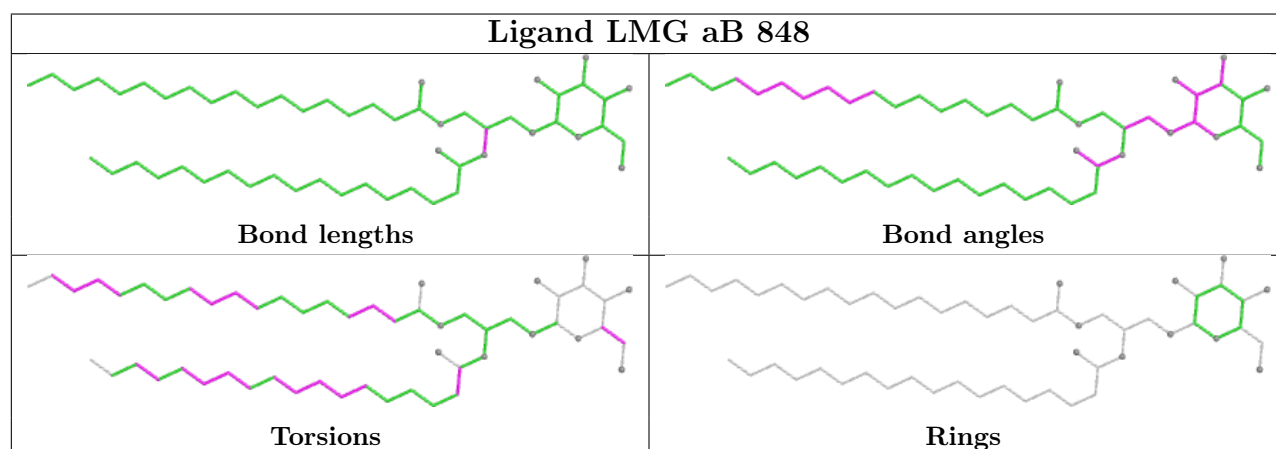
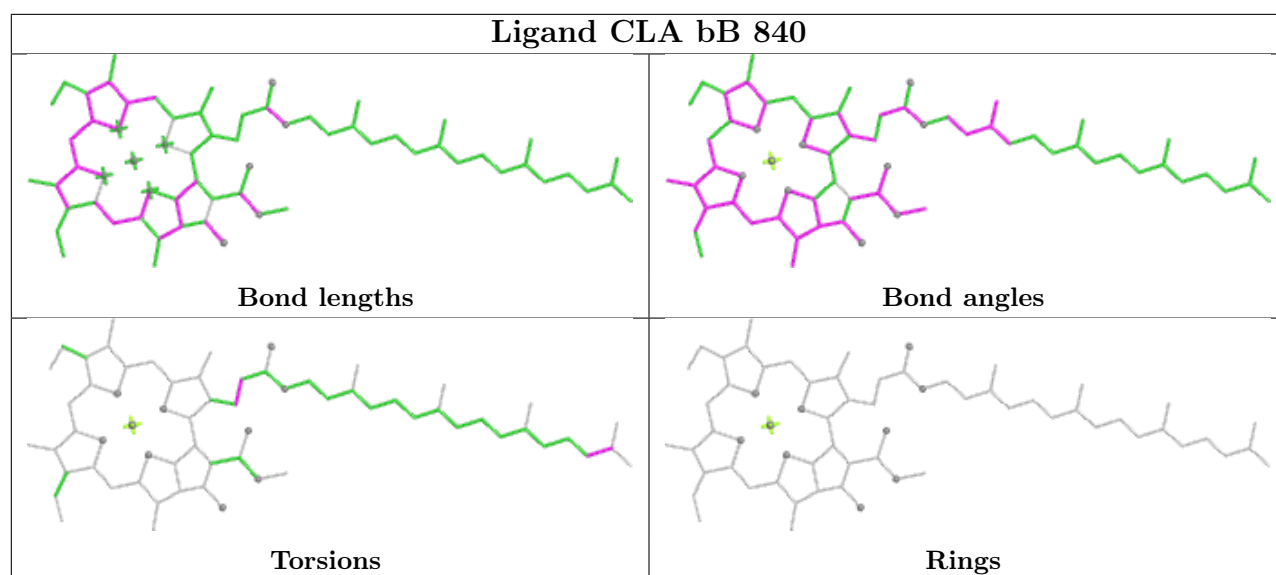




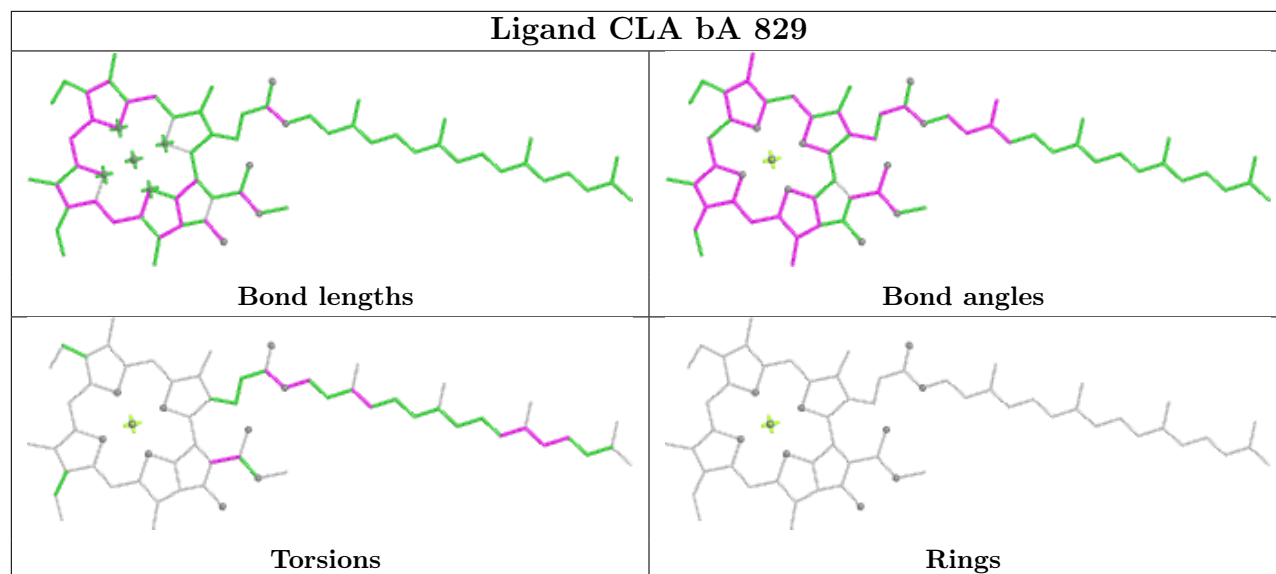




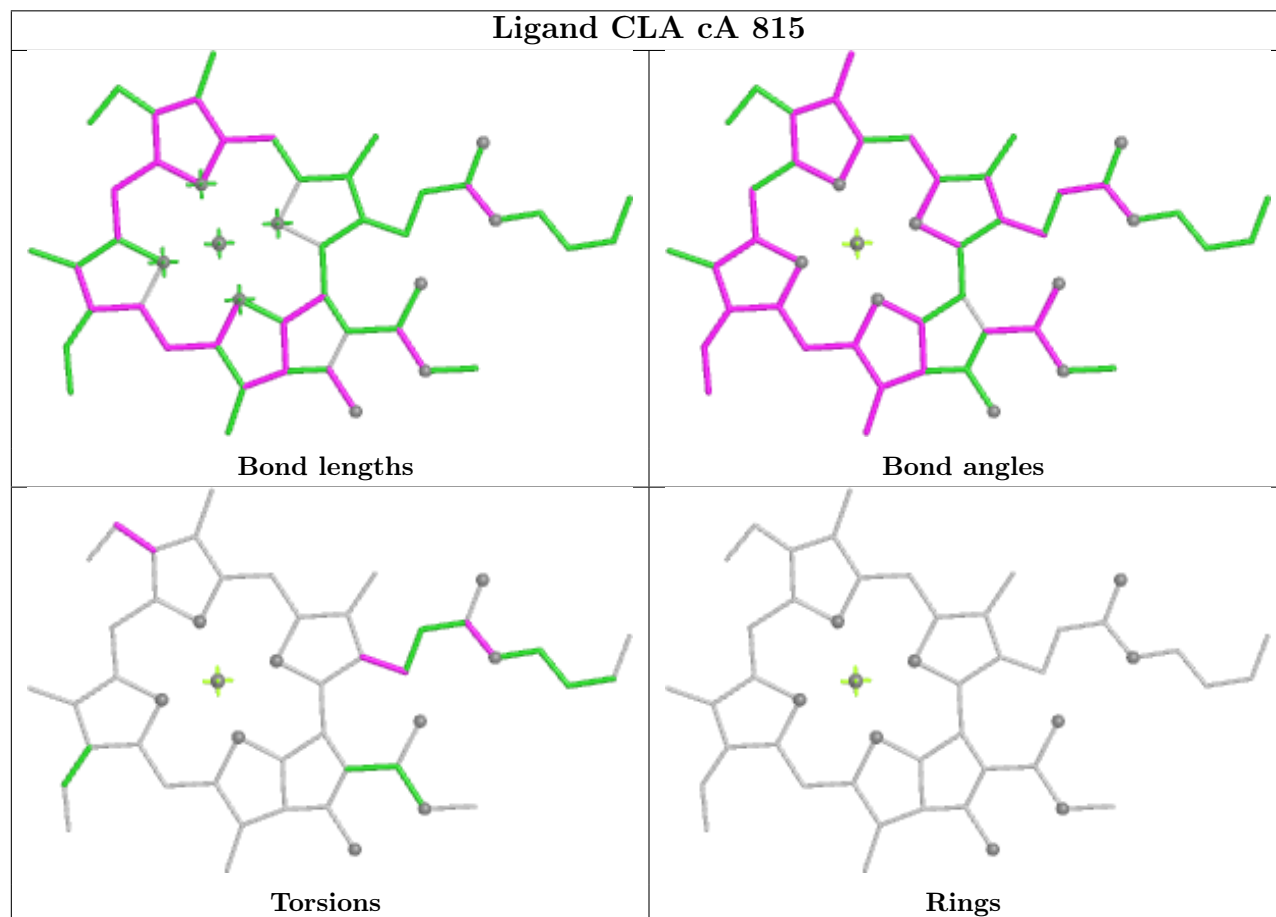


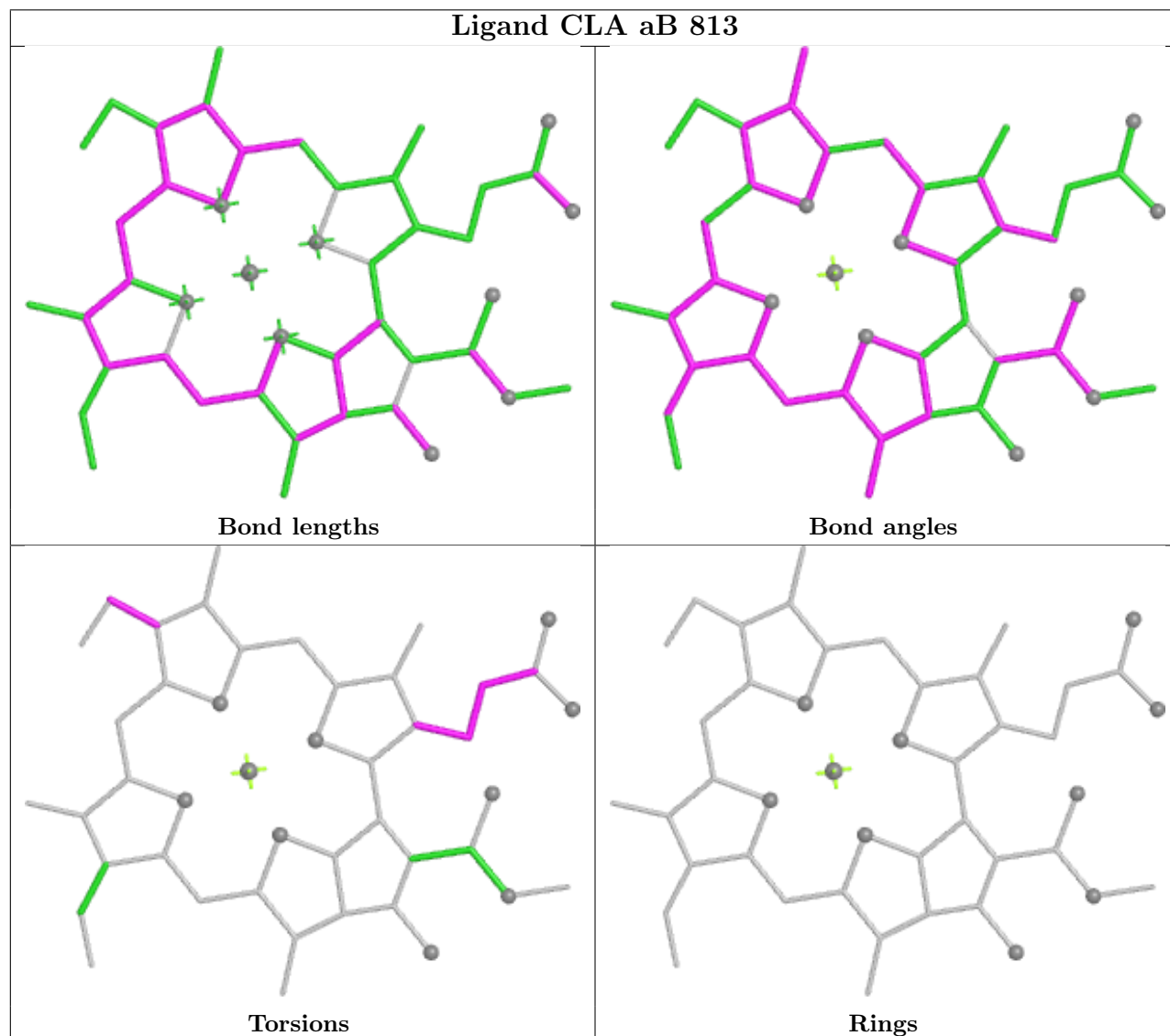
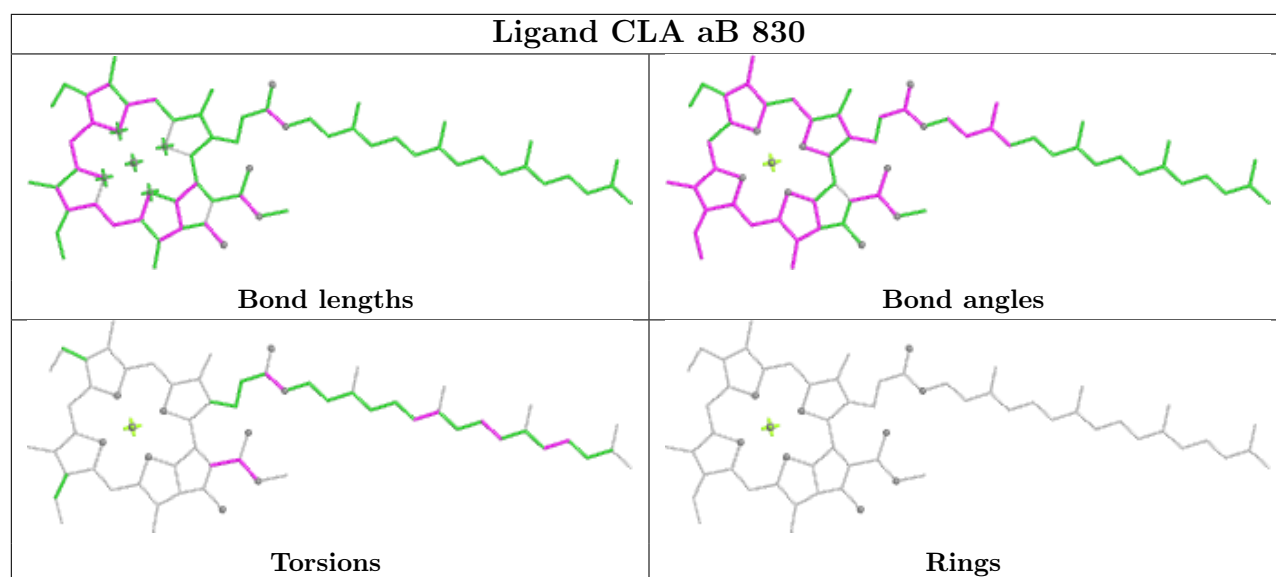


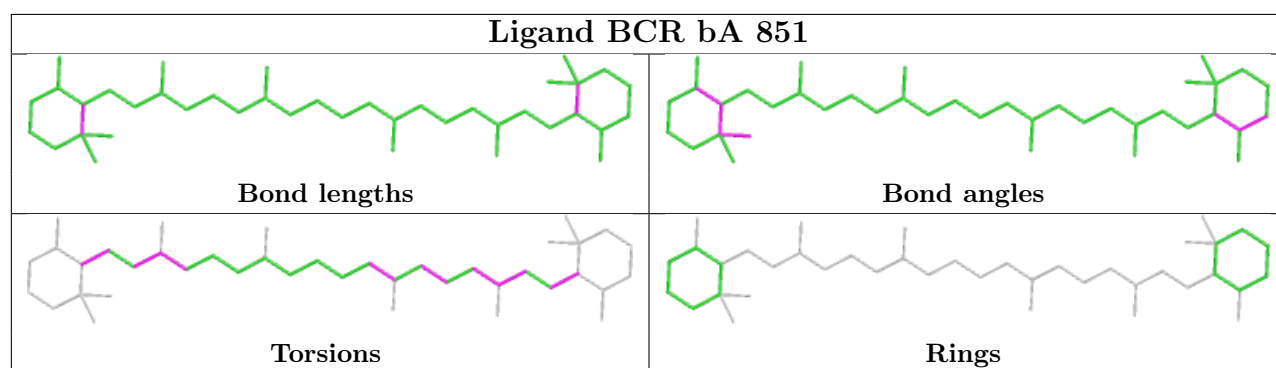
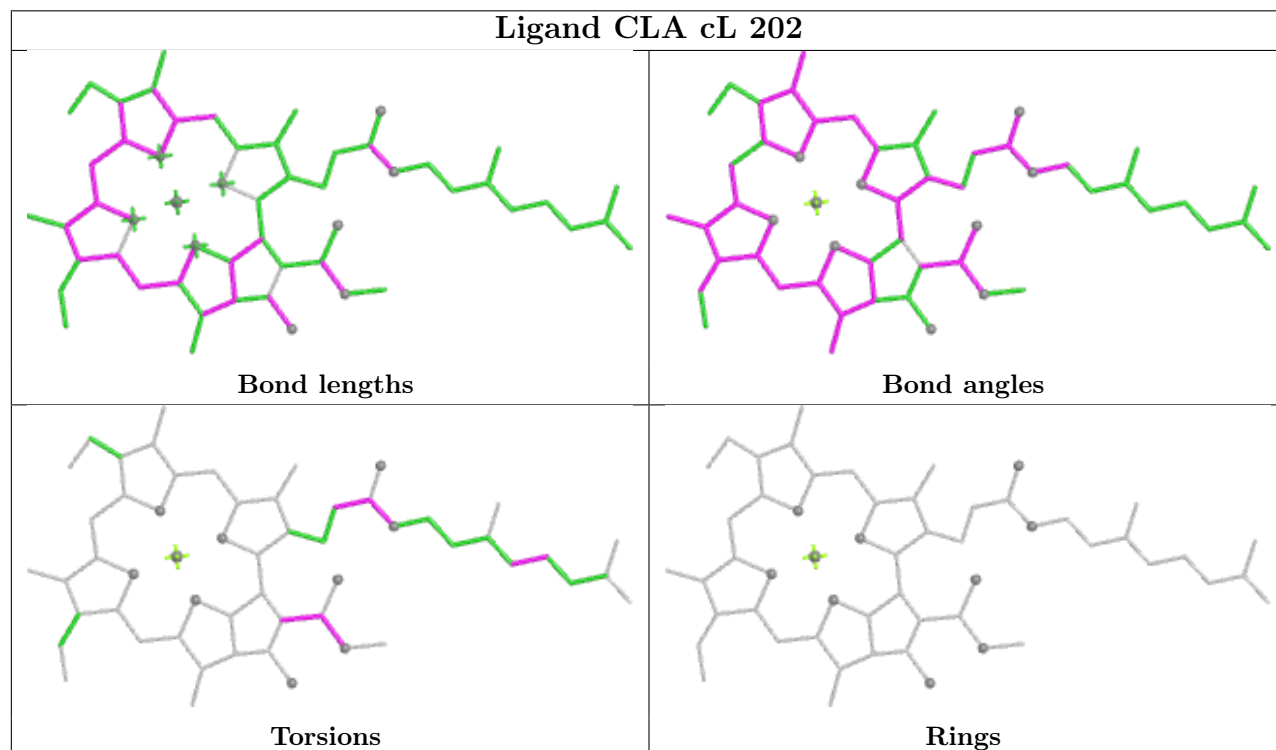
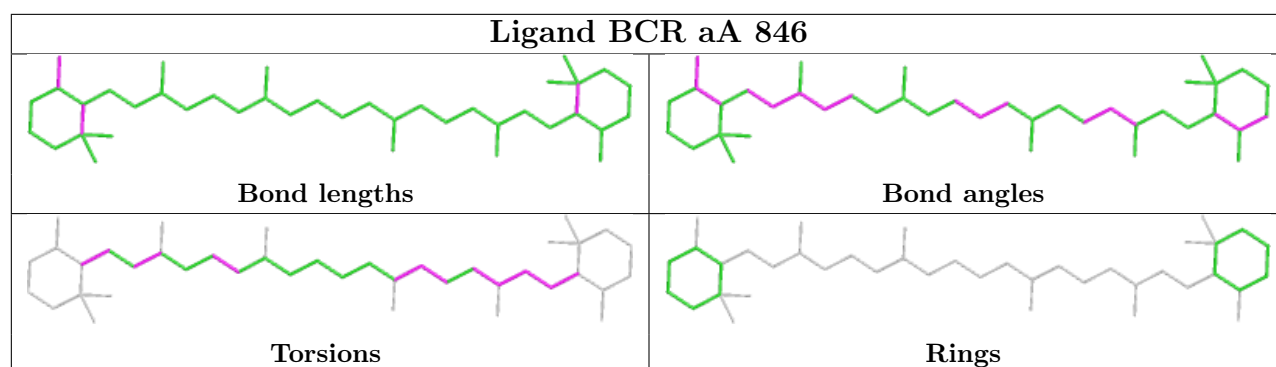
Ligand CLA bA 829

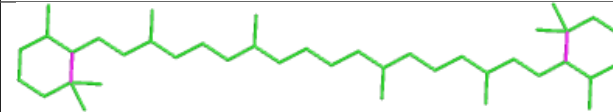
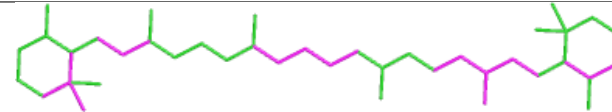
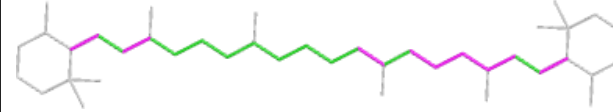
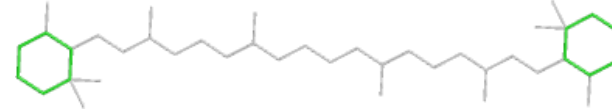


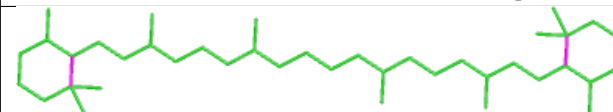
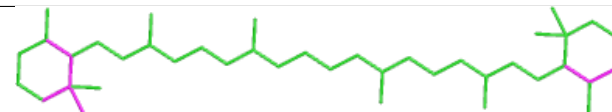
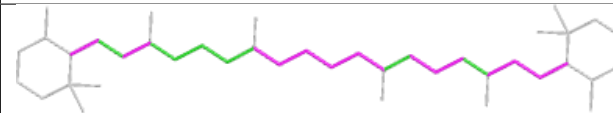
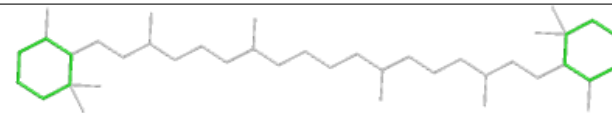
Ligand CLA cA 815

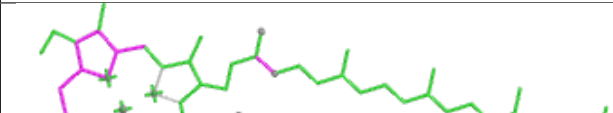
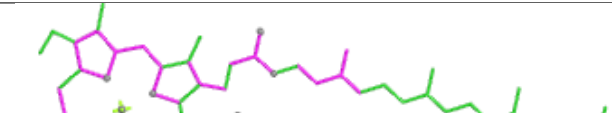
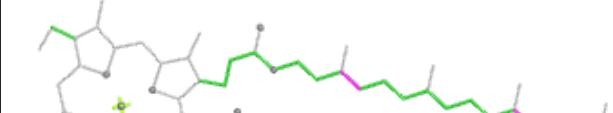
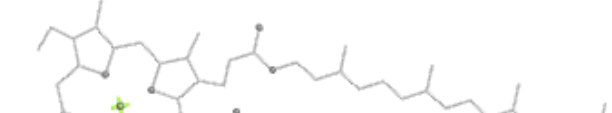


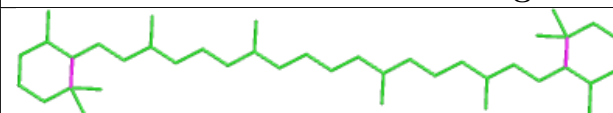
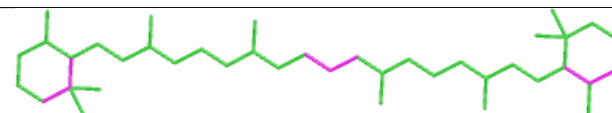
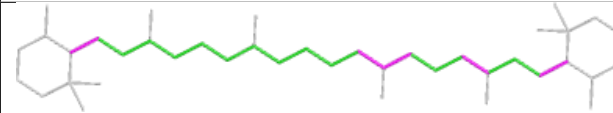
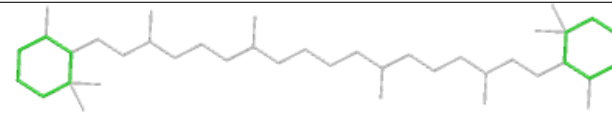


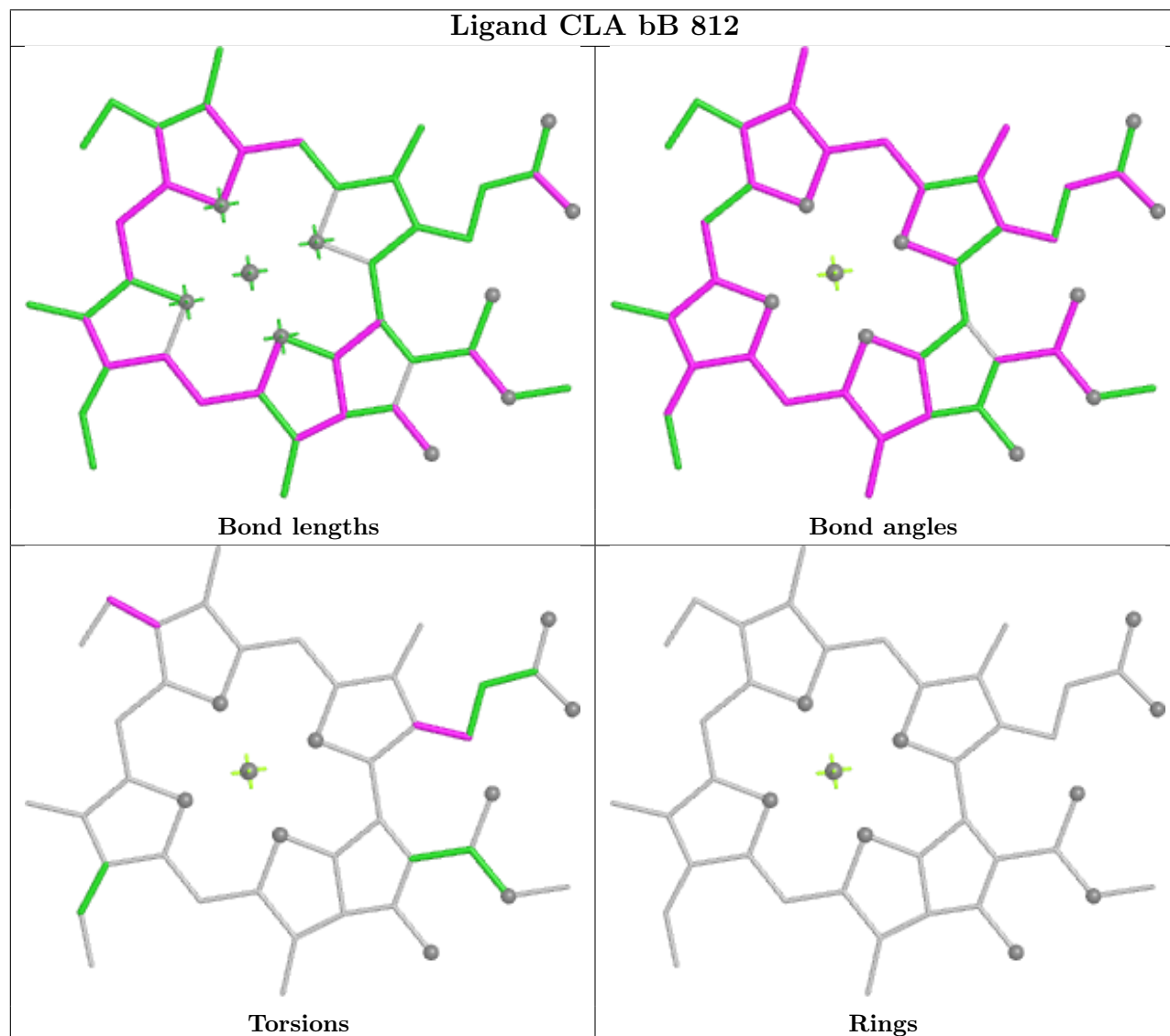
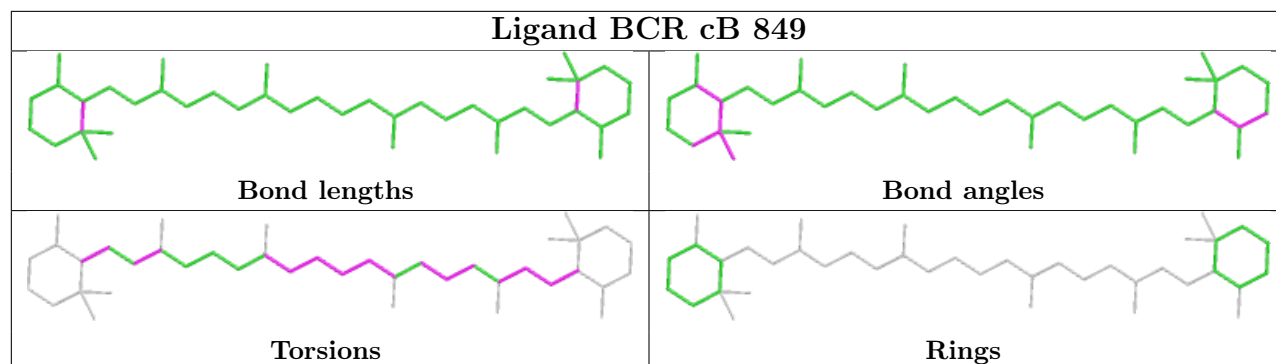


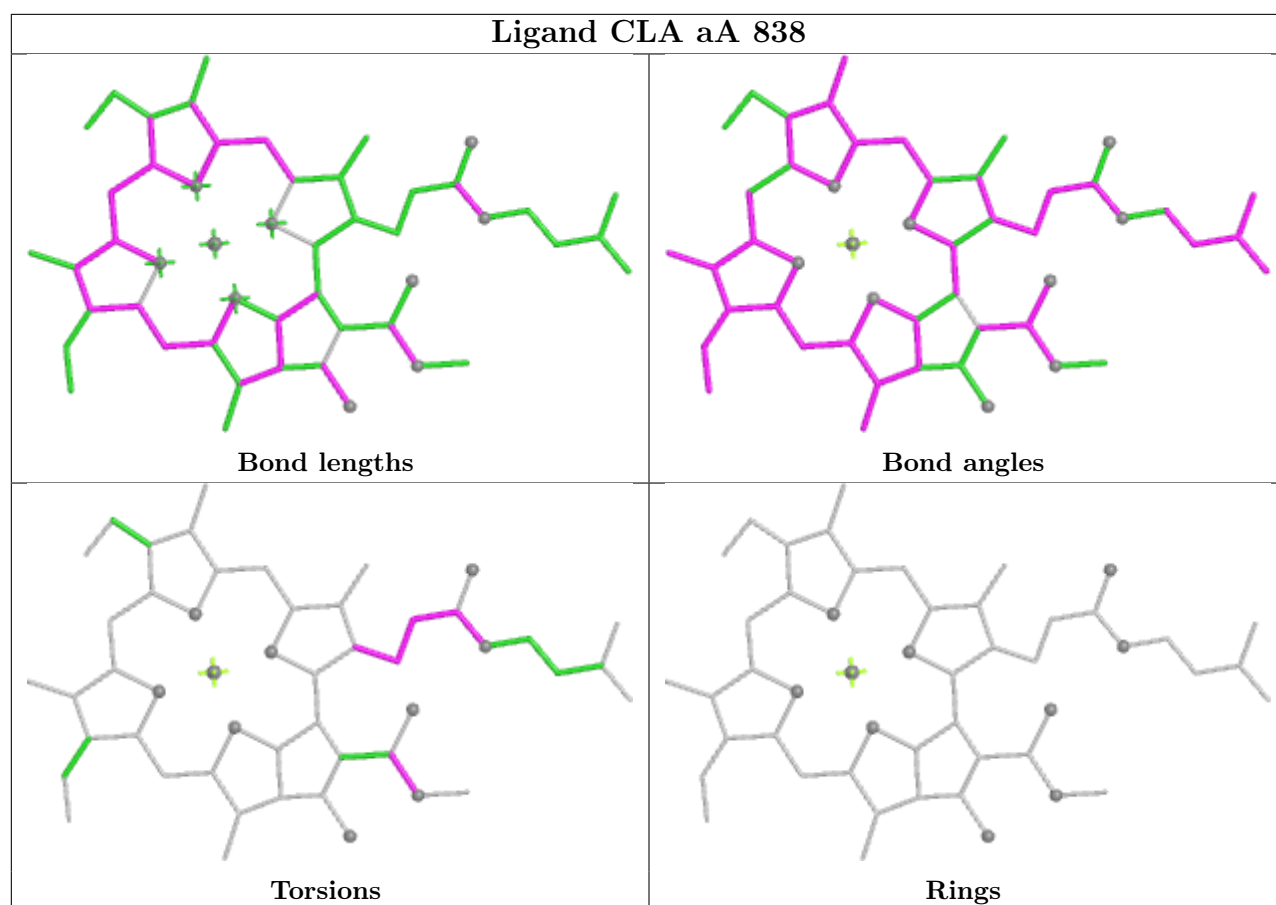
Ligand BCR aM 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

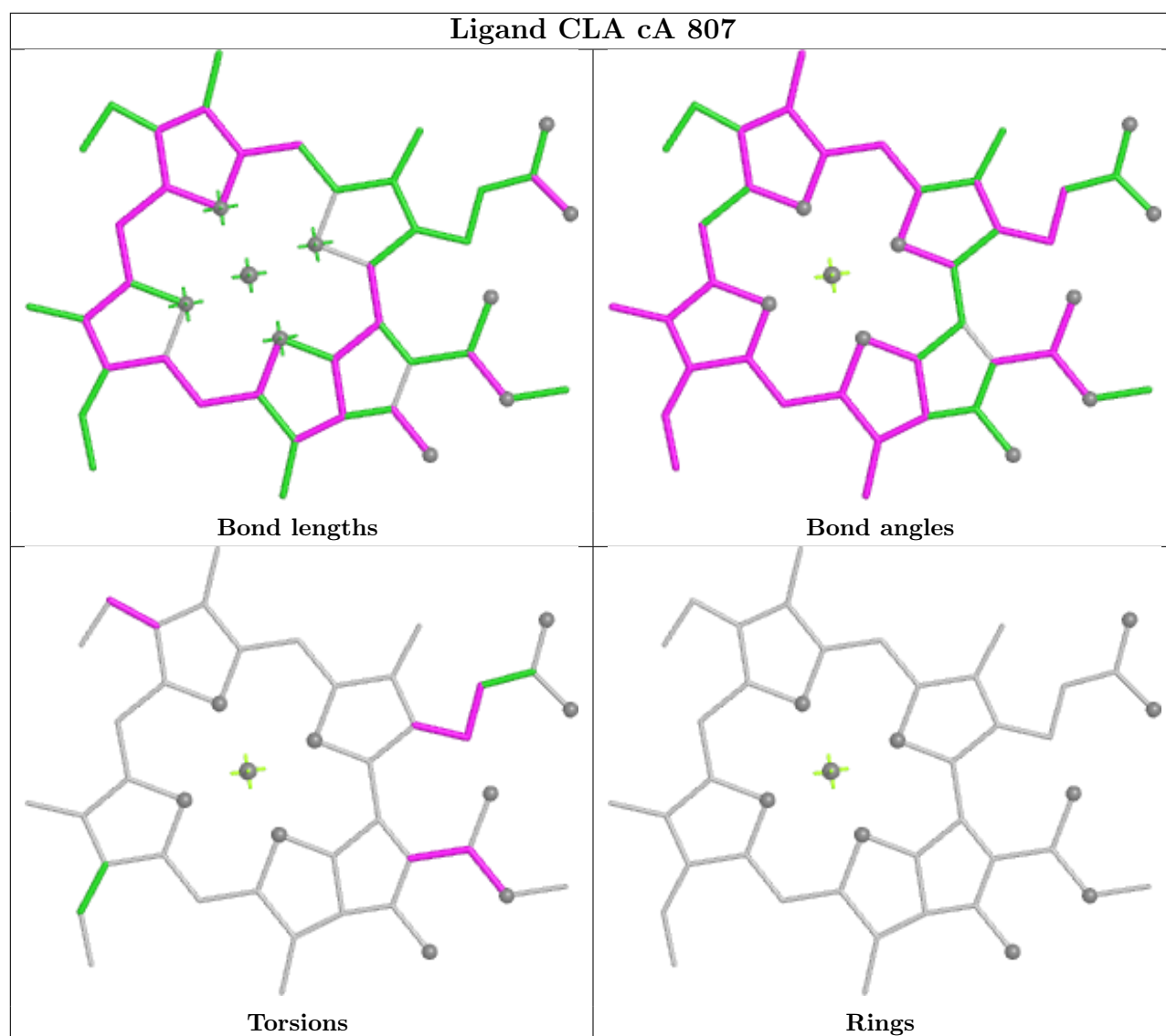
Ligand BCR bB 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA aB 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

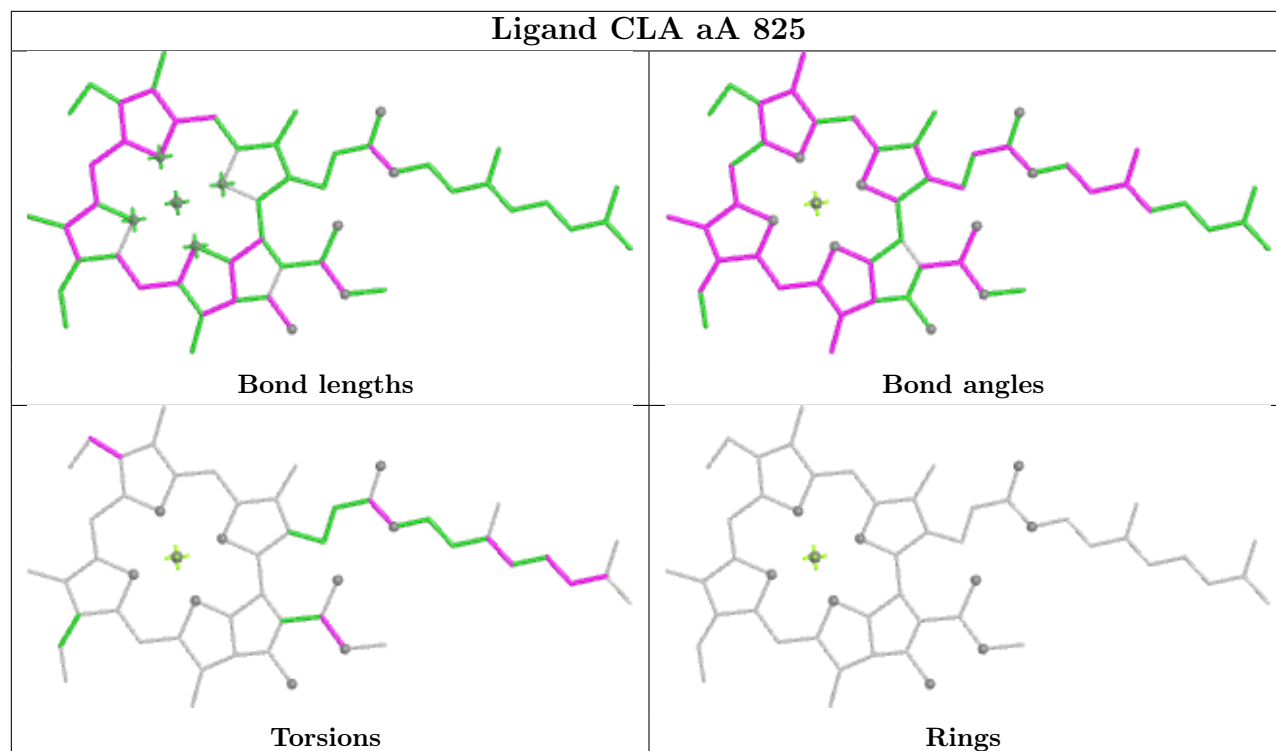
Ligand BCR cL 207	
	
Bond lengths	Bond angles
	
Torsions	Rings



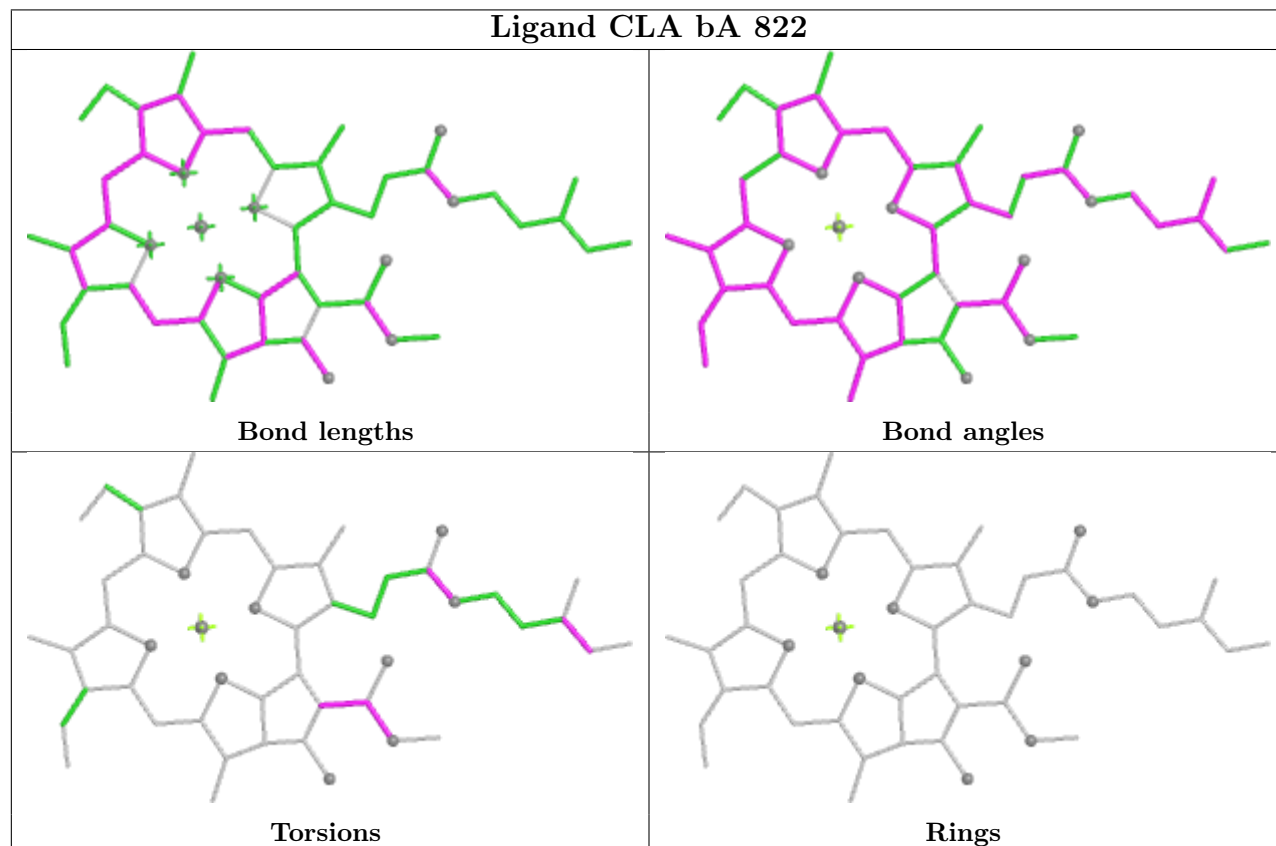


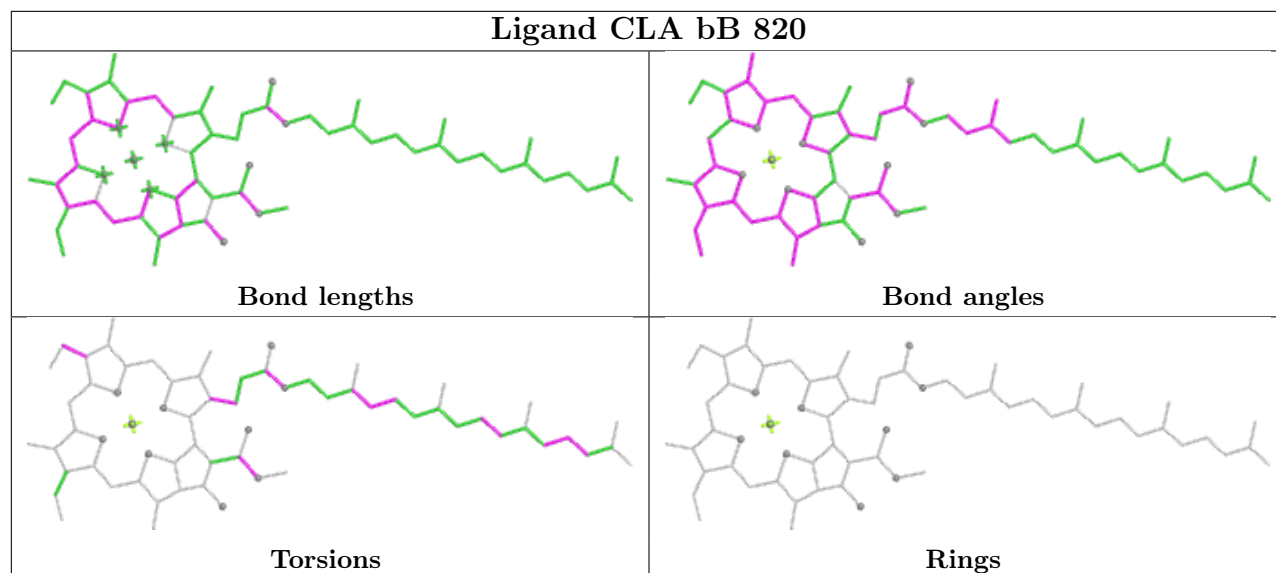
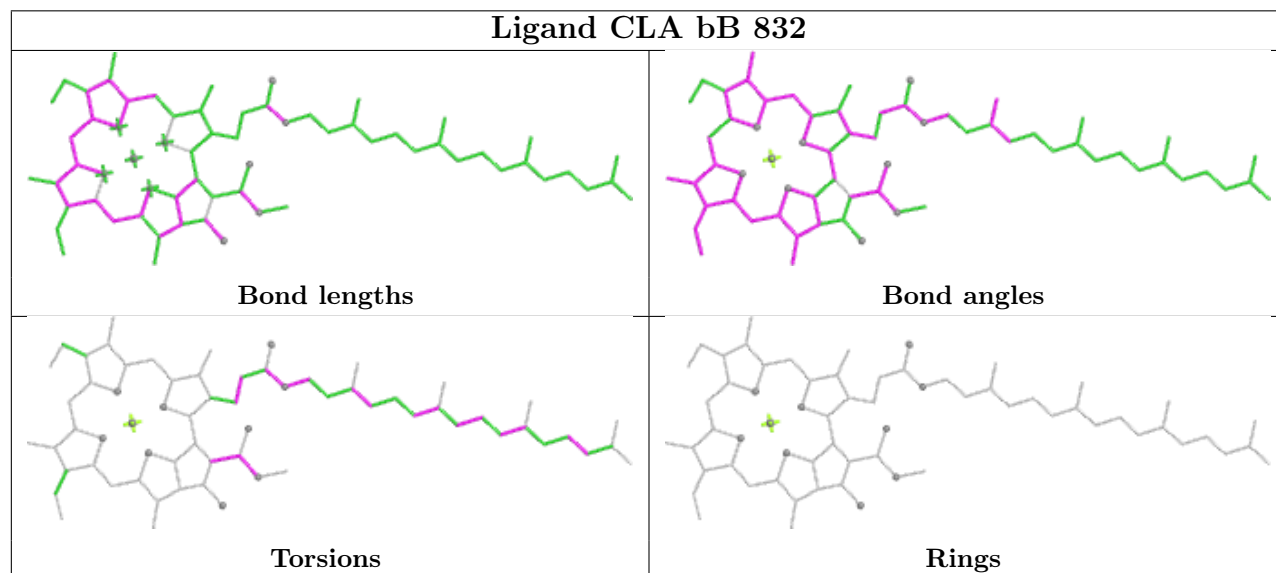
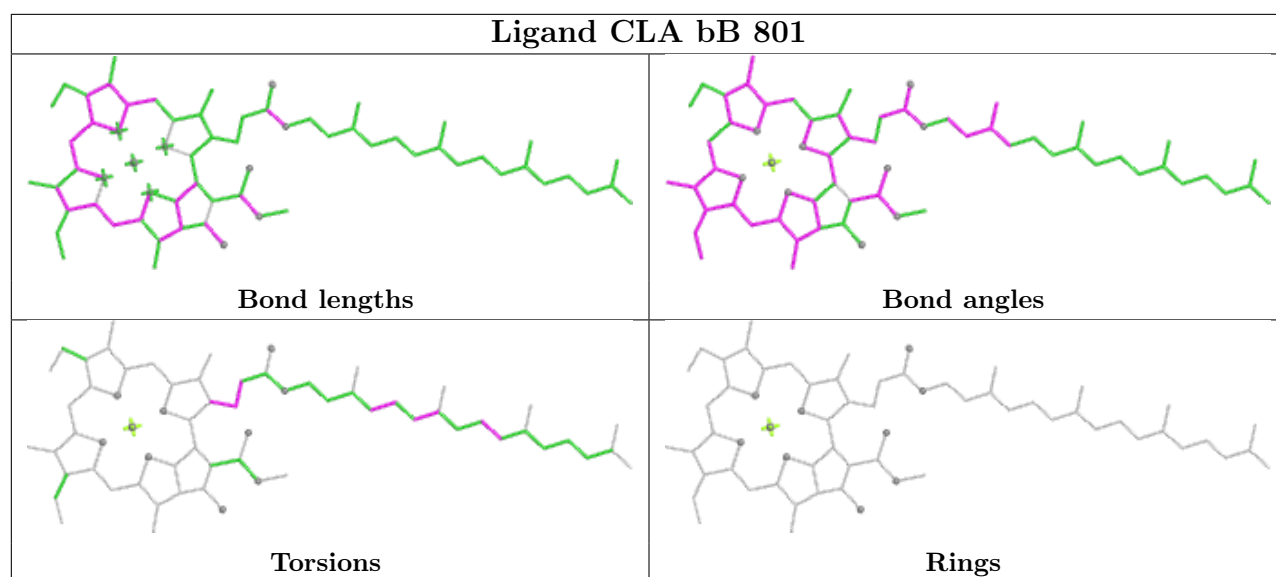


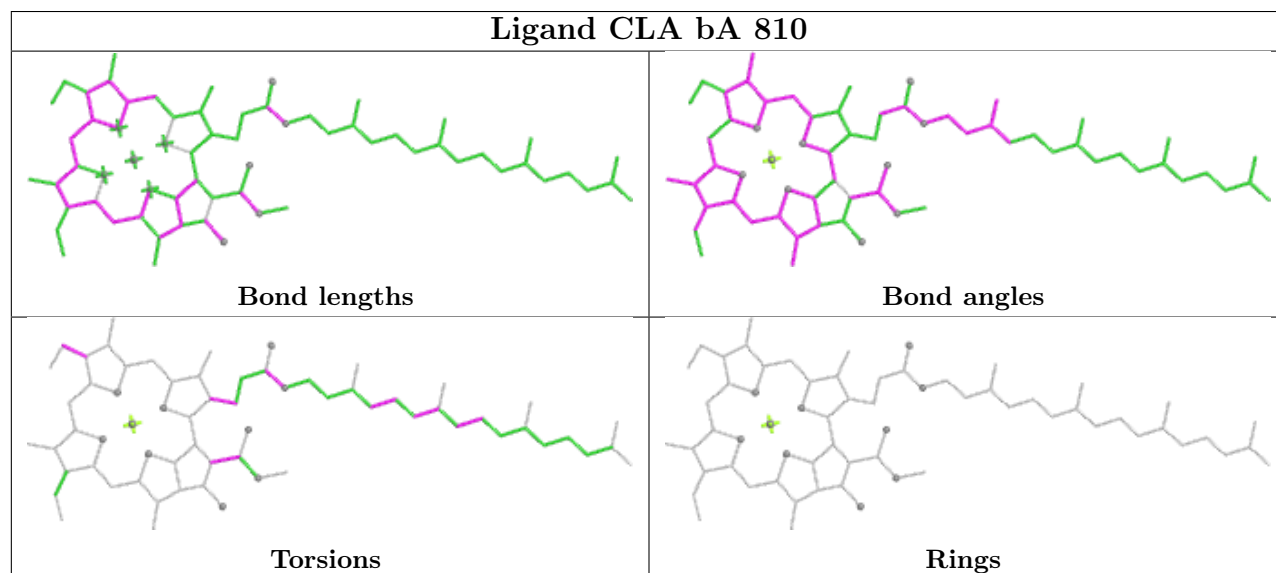
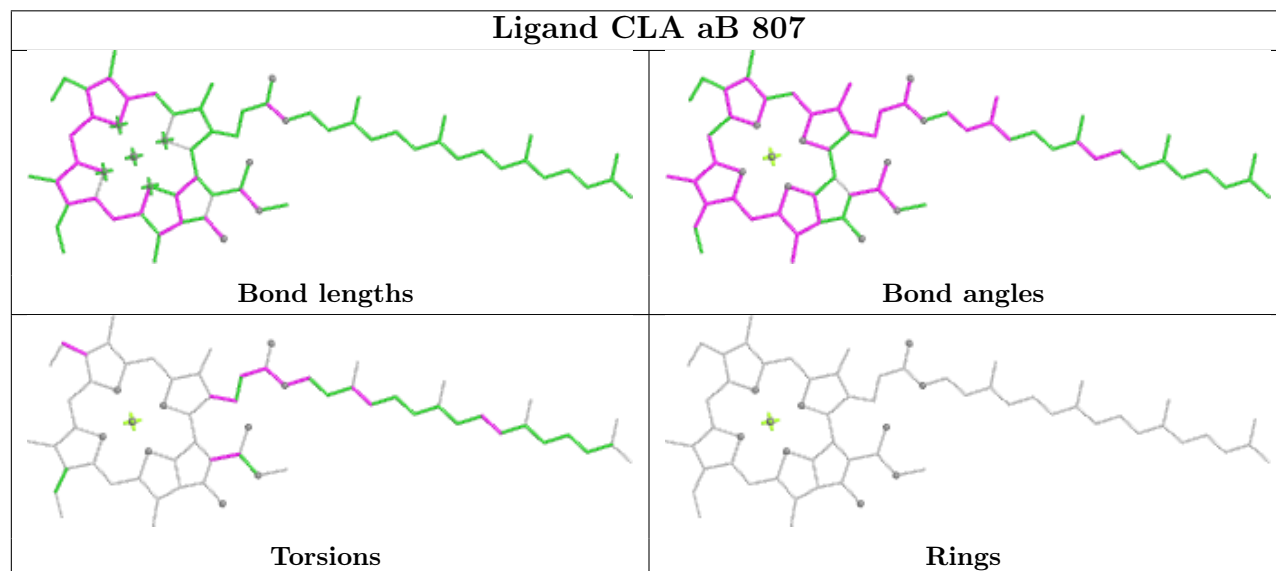
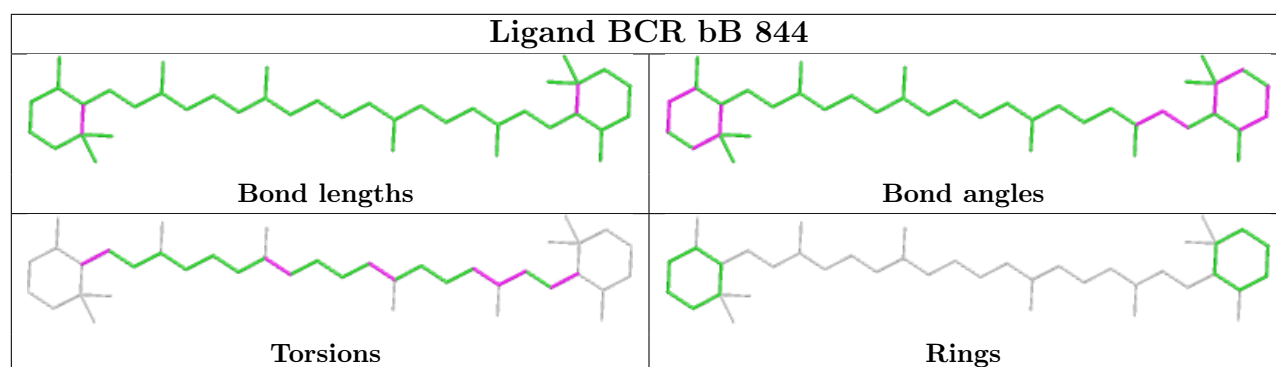
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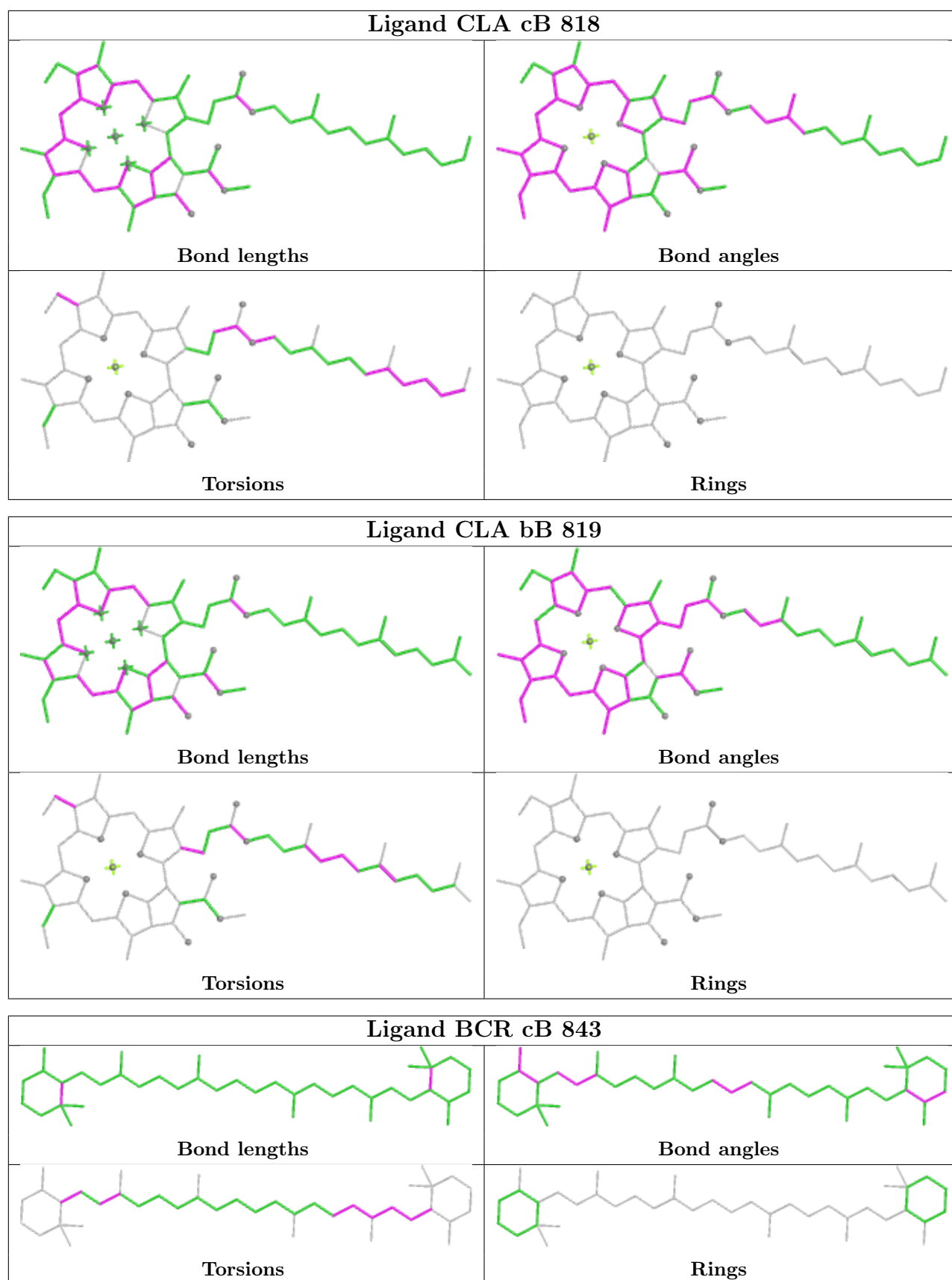


Ligand CLA bA 822

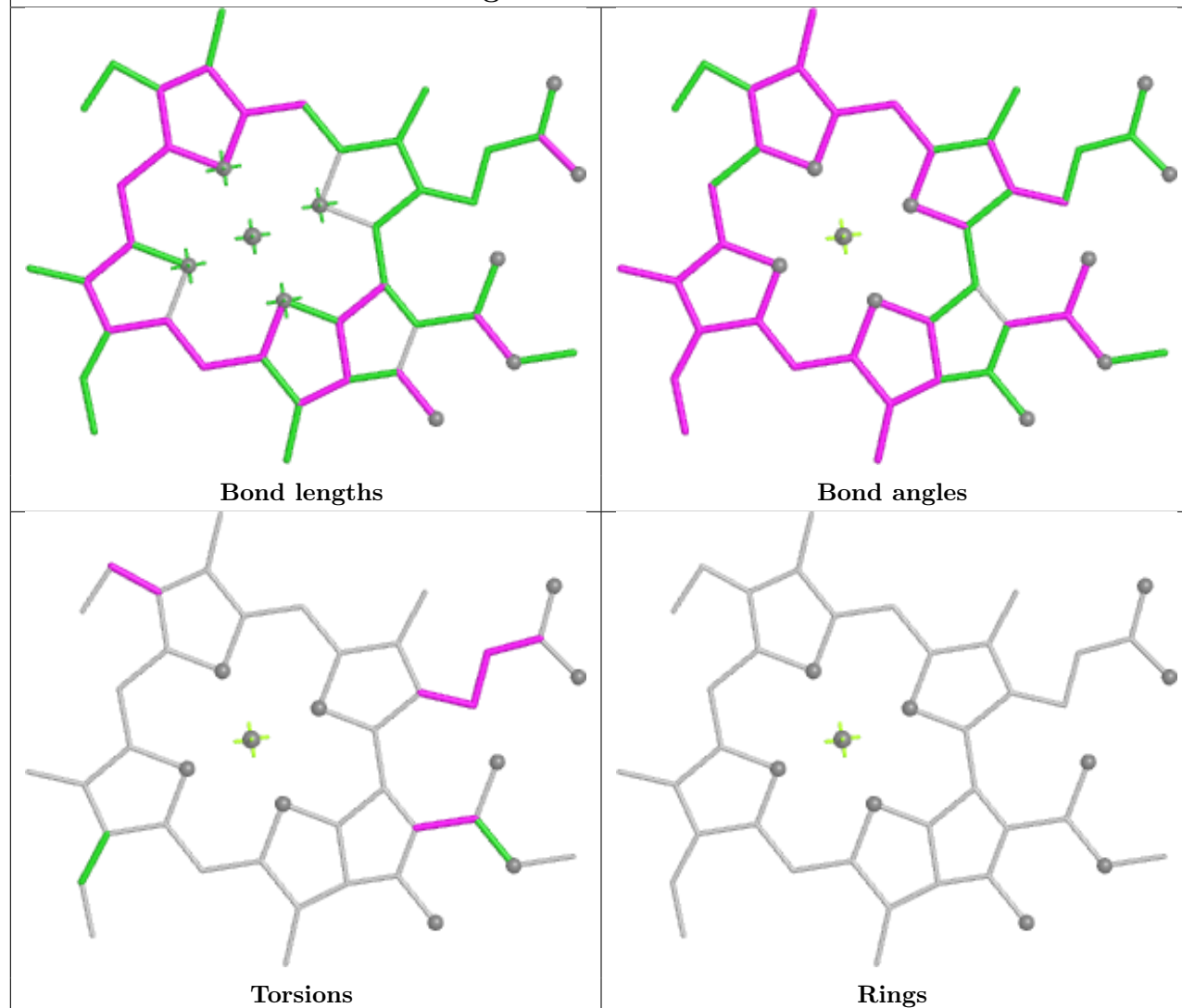




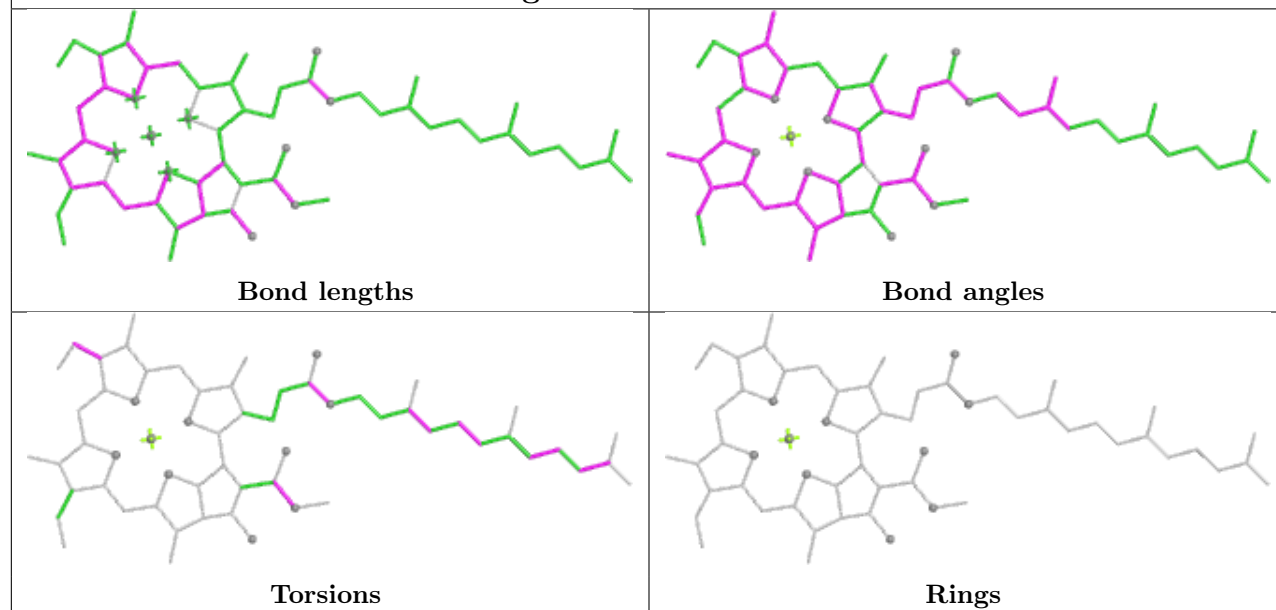


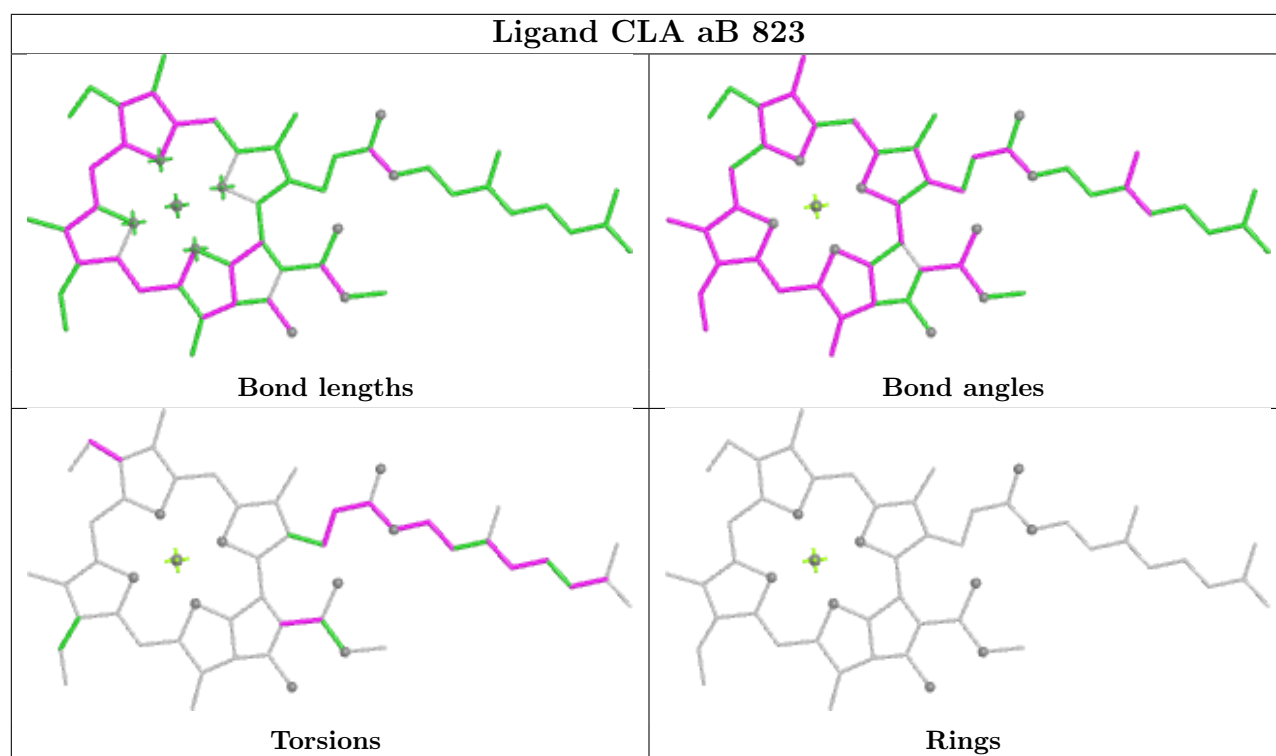


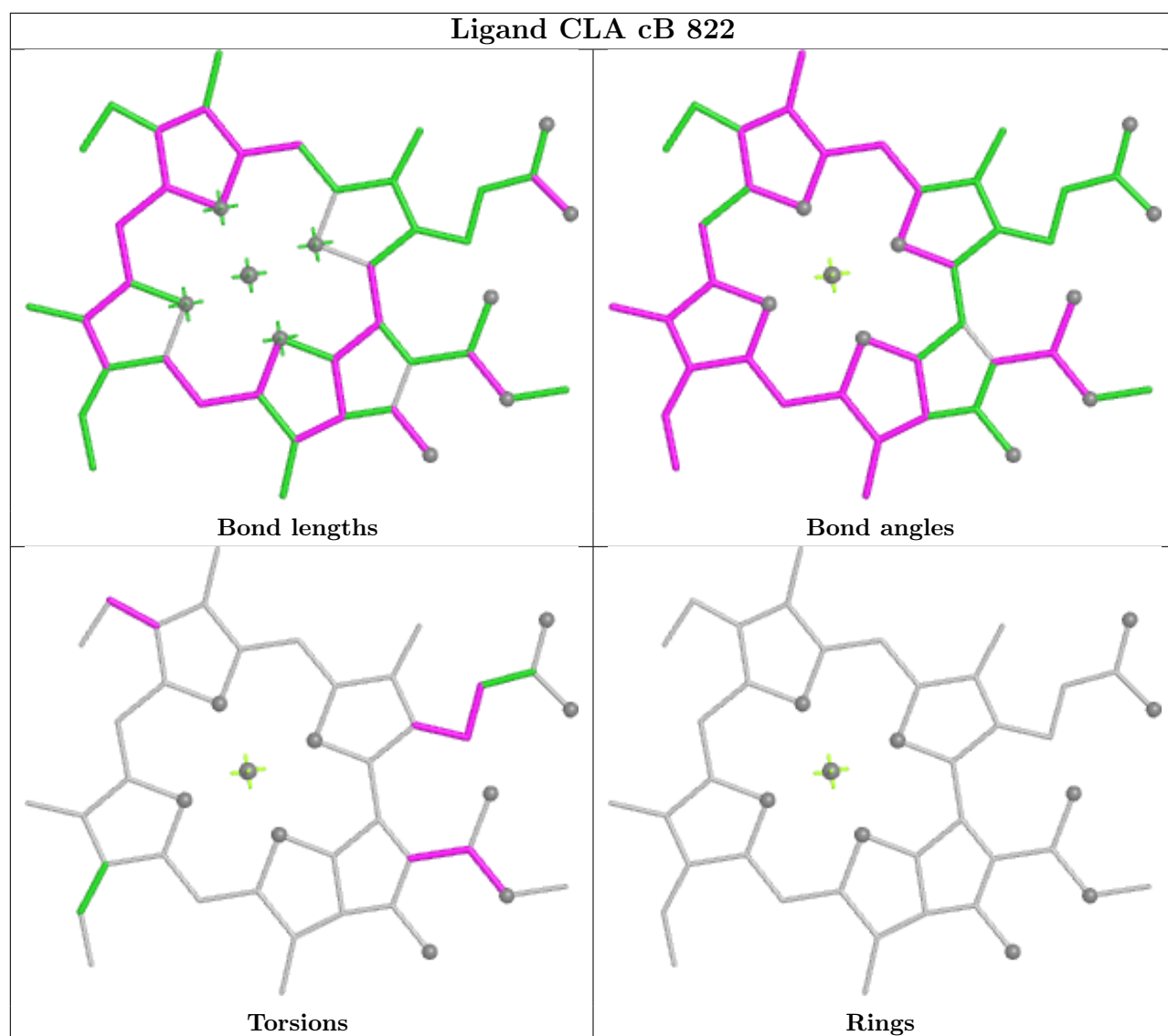
Ligand CLA bA 802

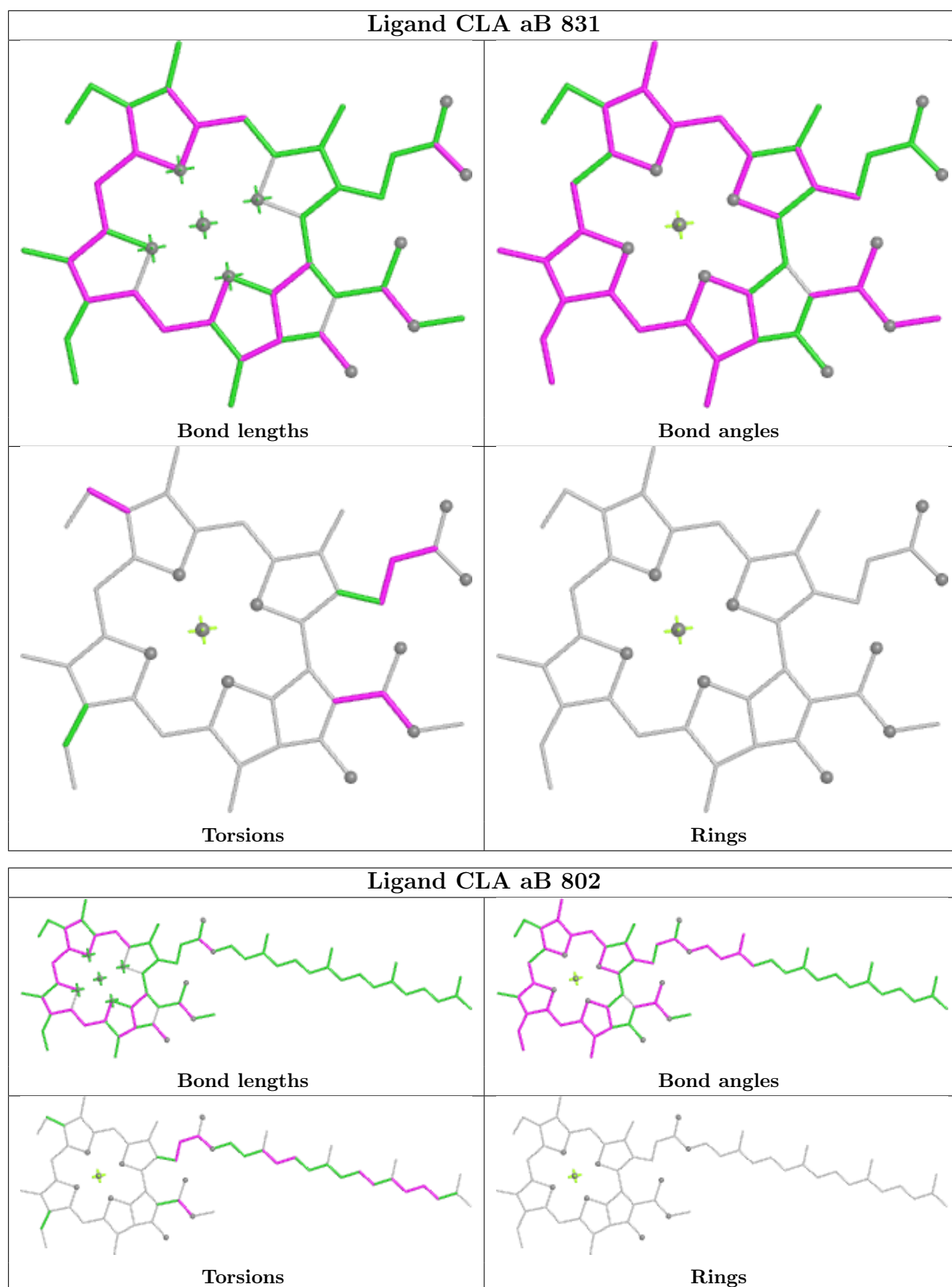


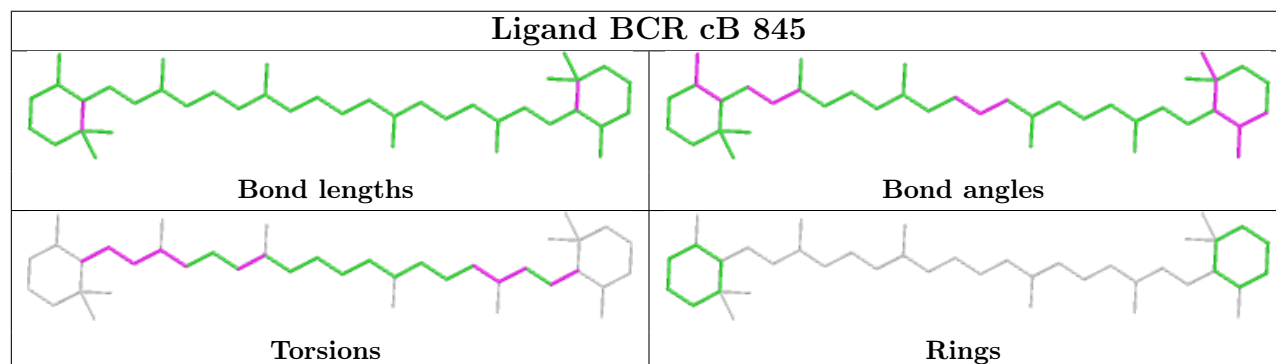
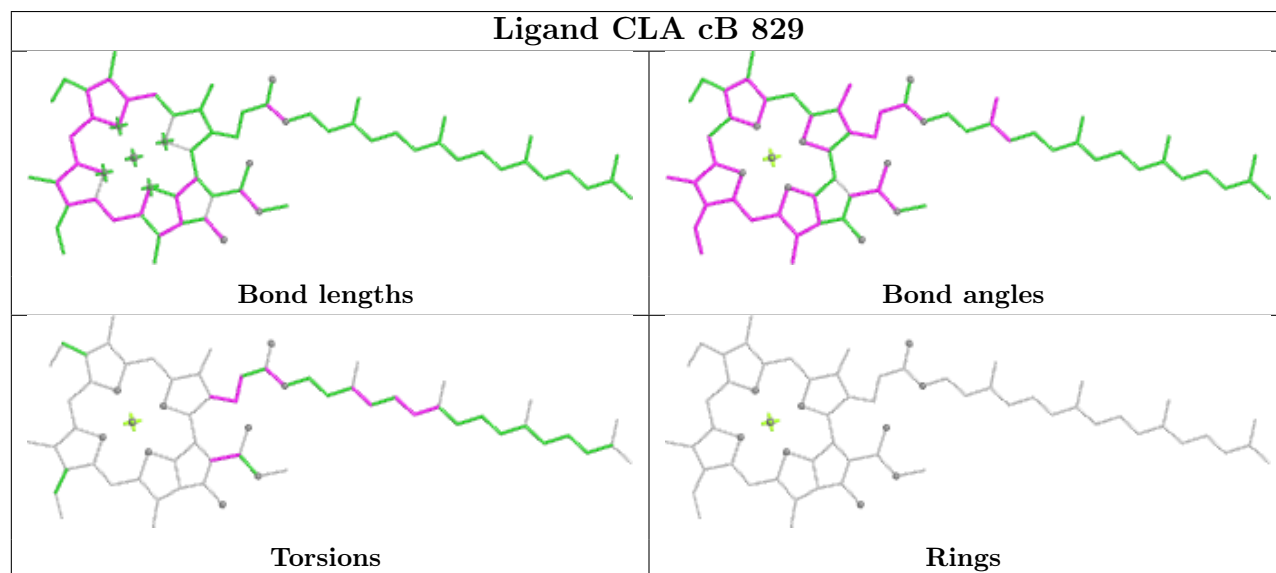
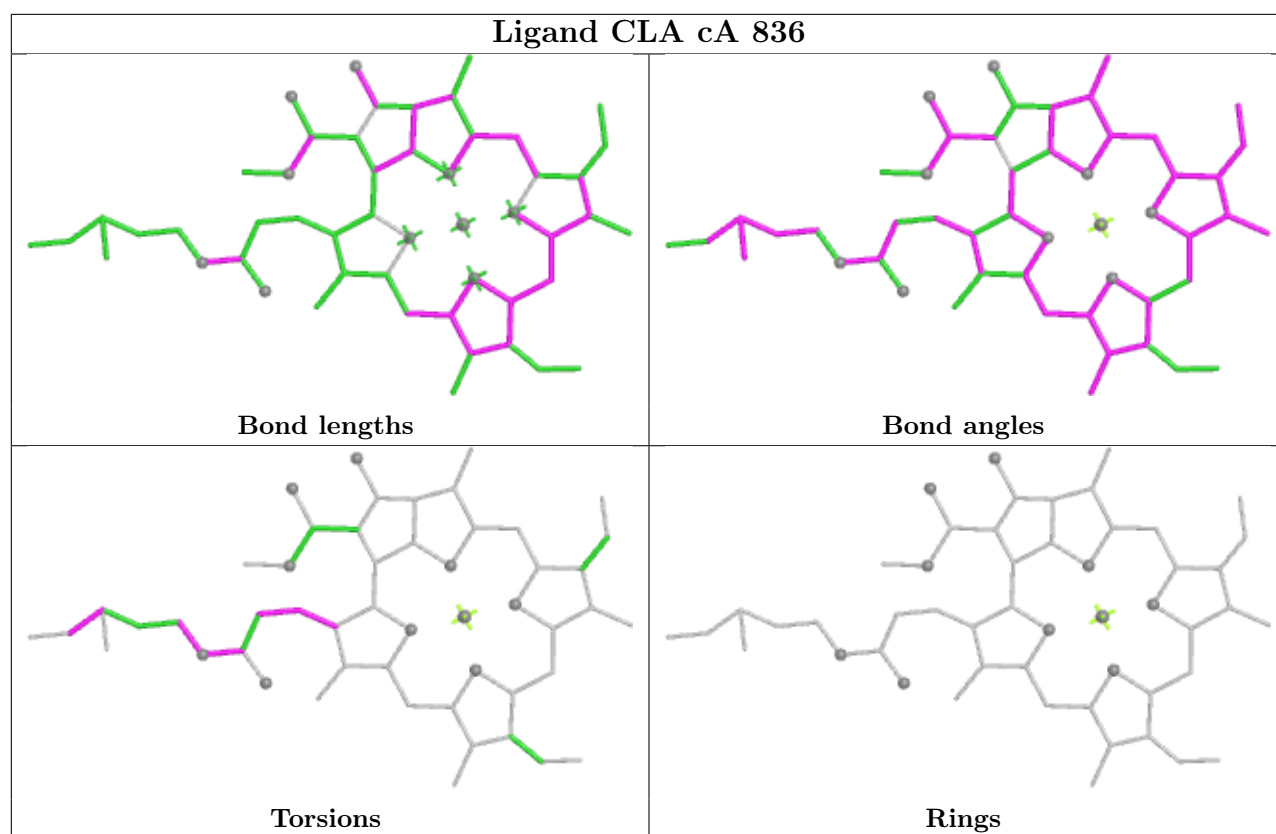
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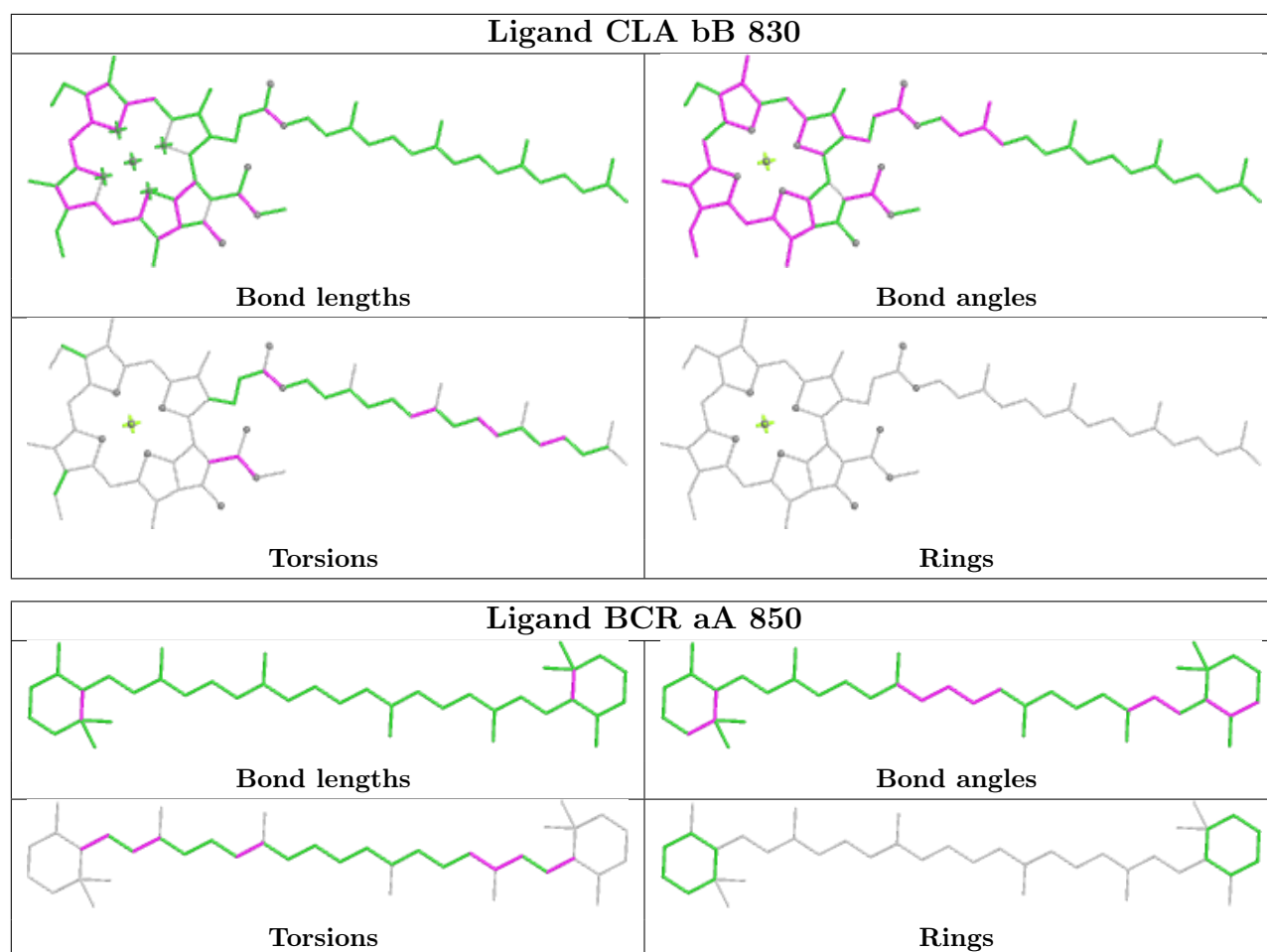


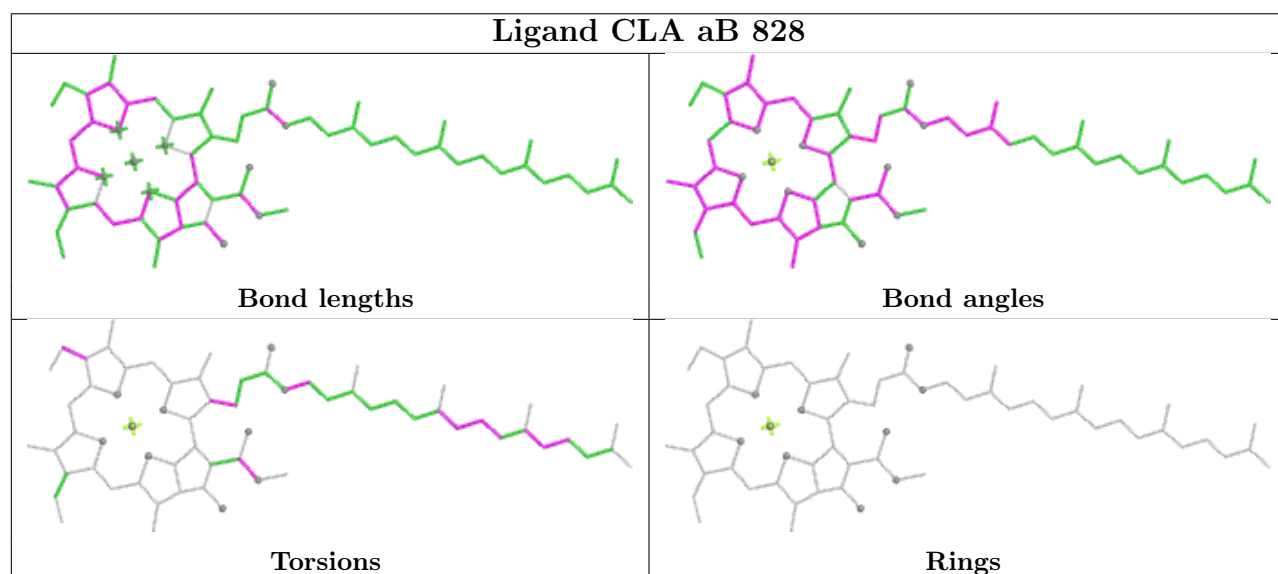
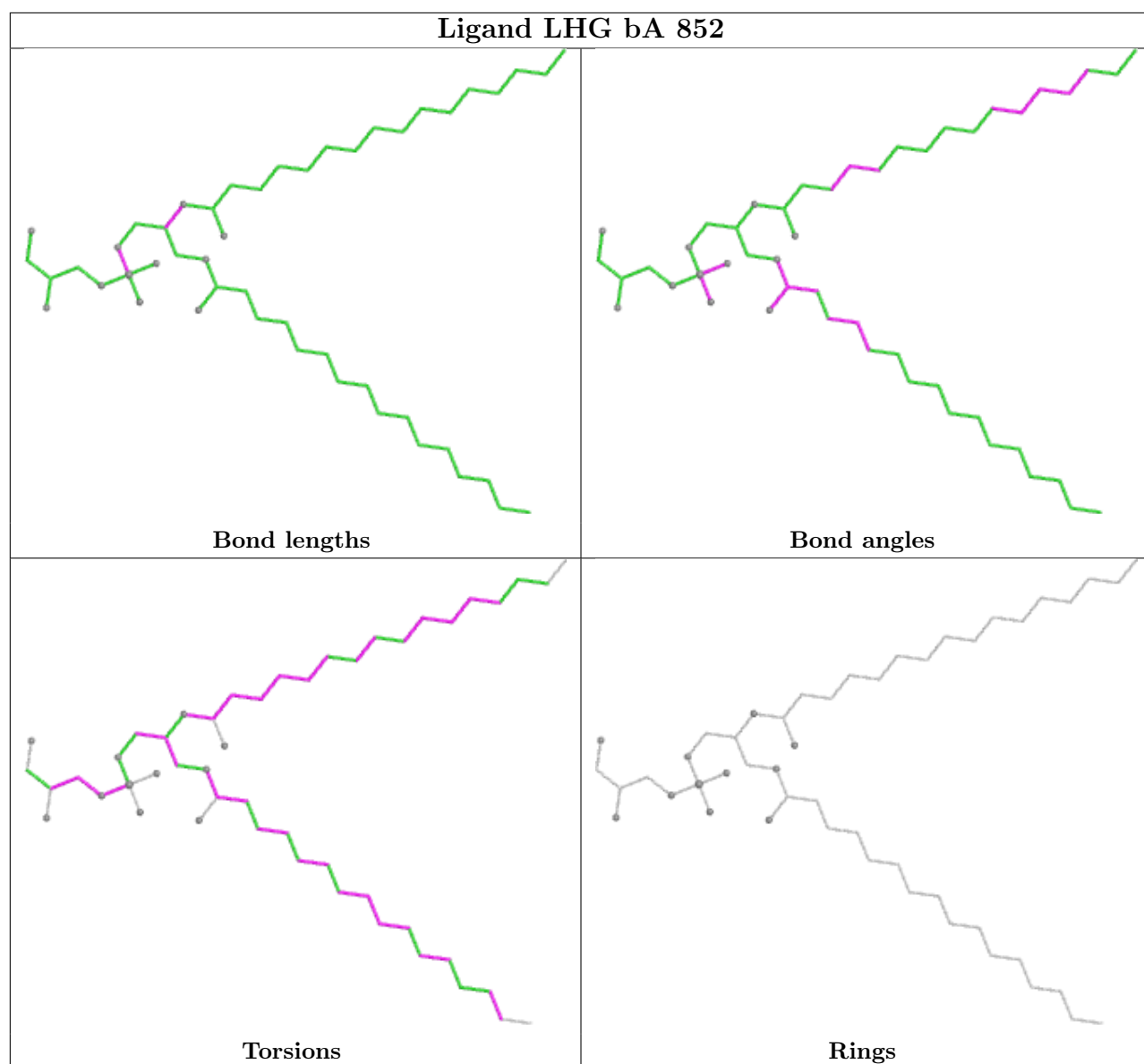


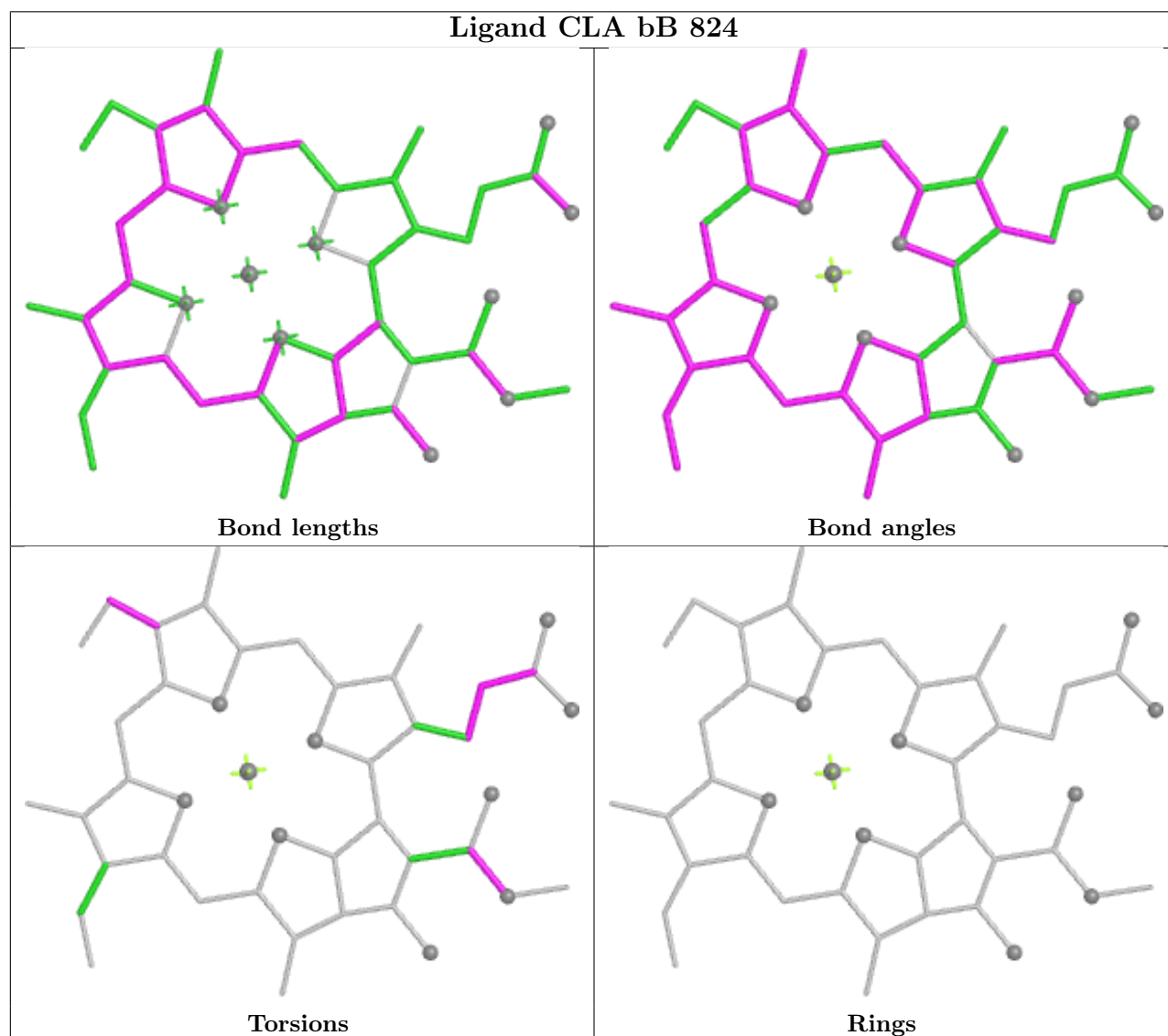
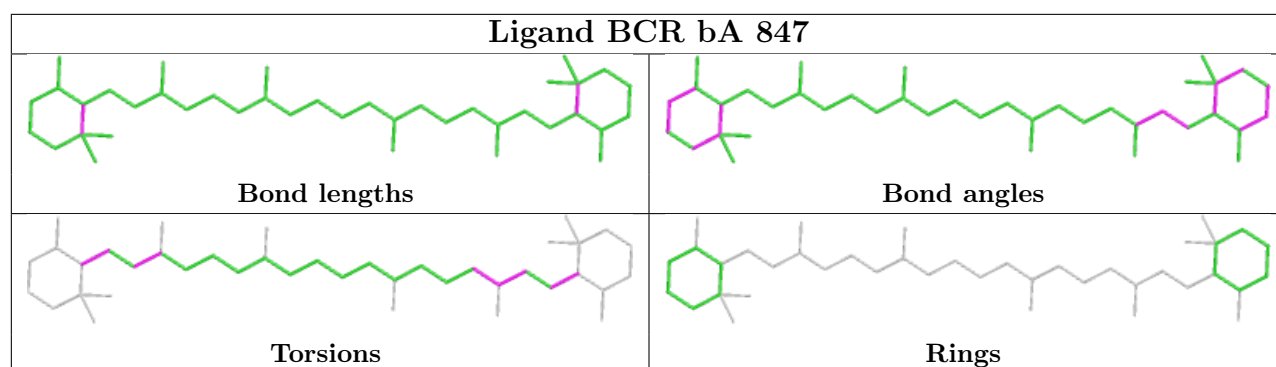




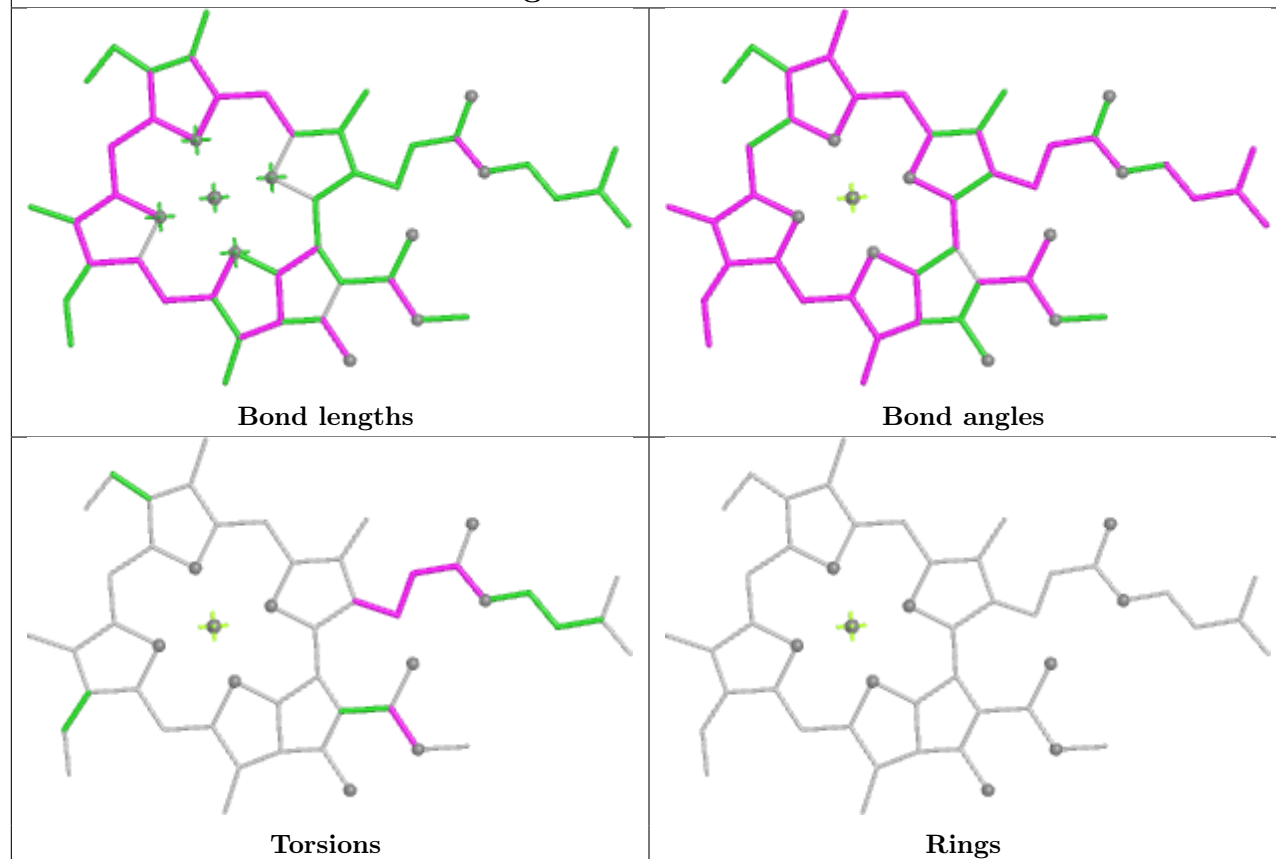




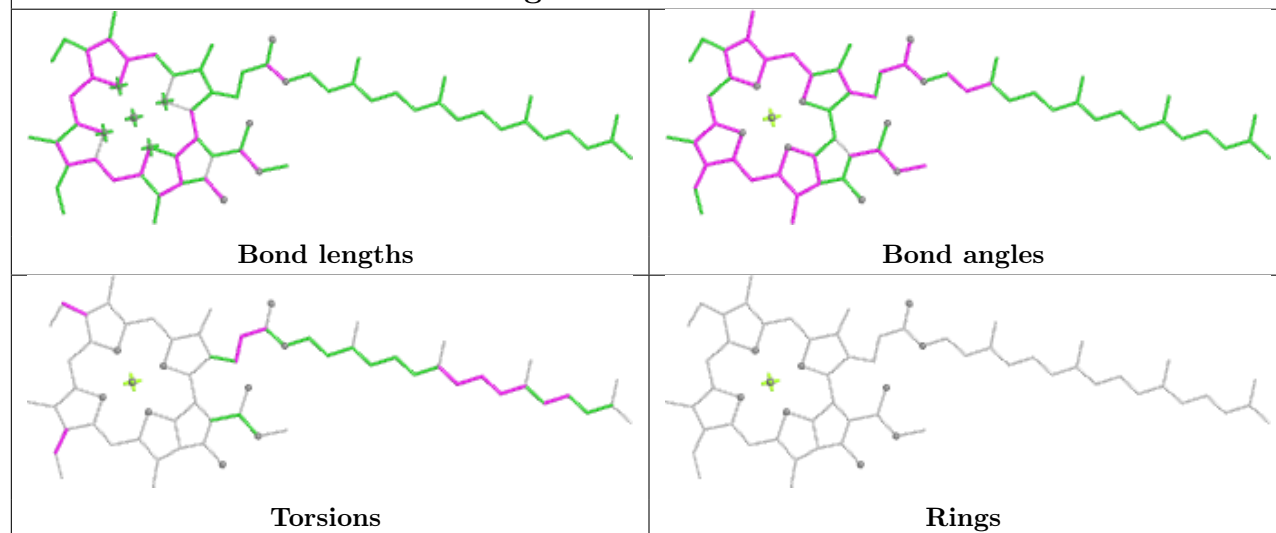




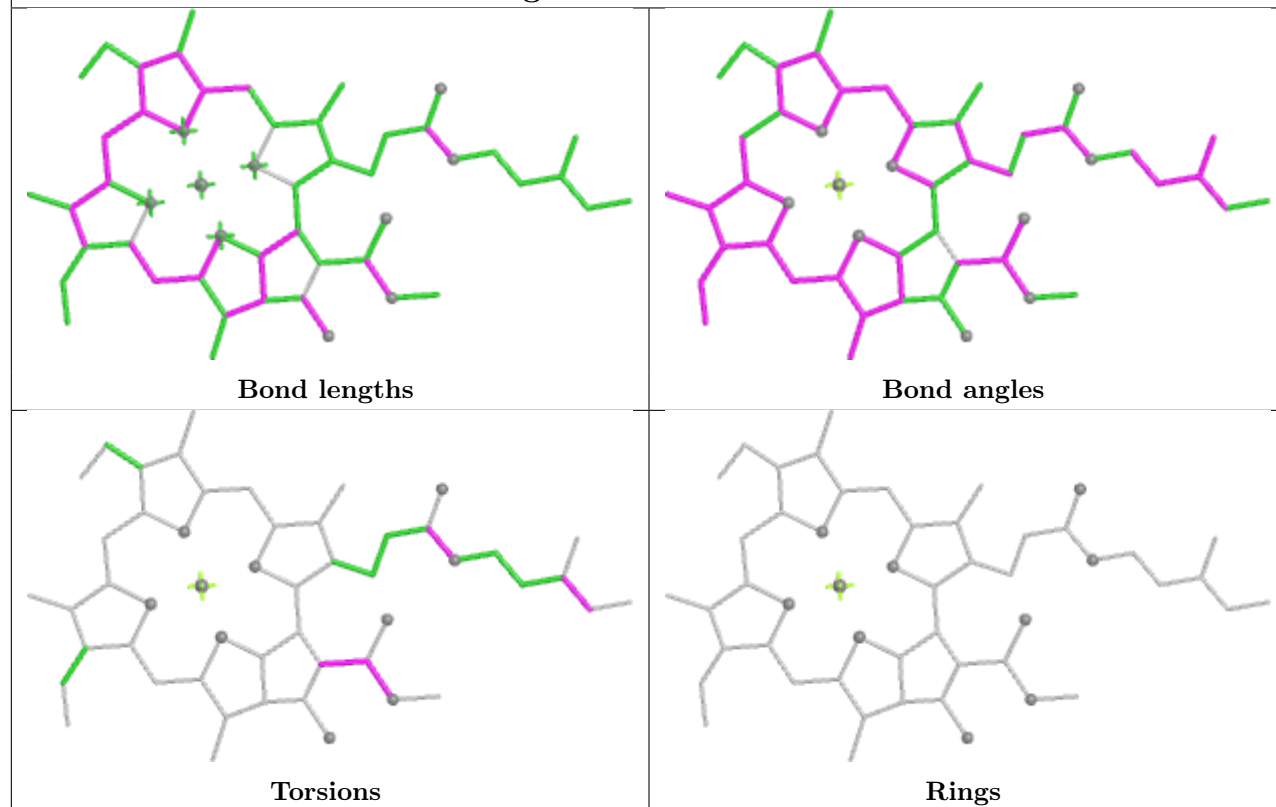
Ligand CLA cA 838



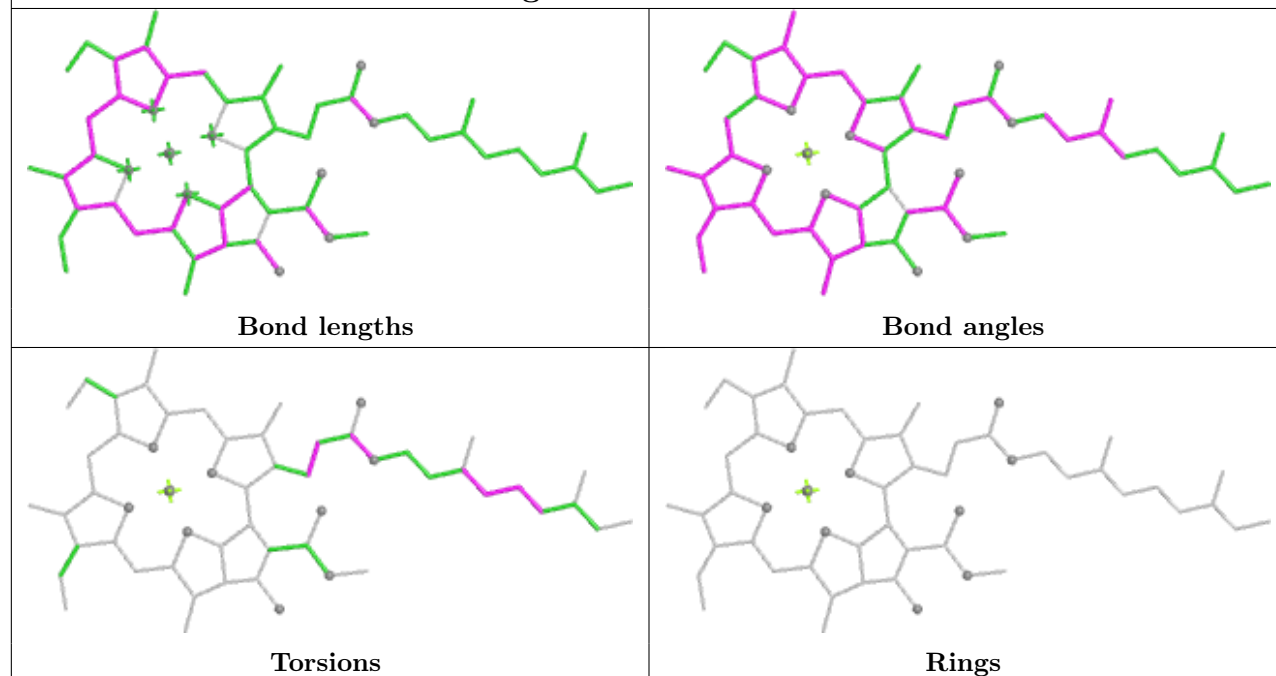
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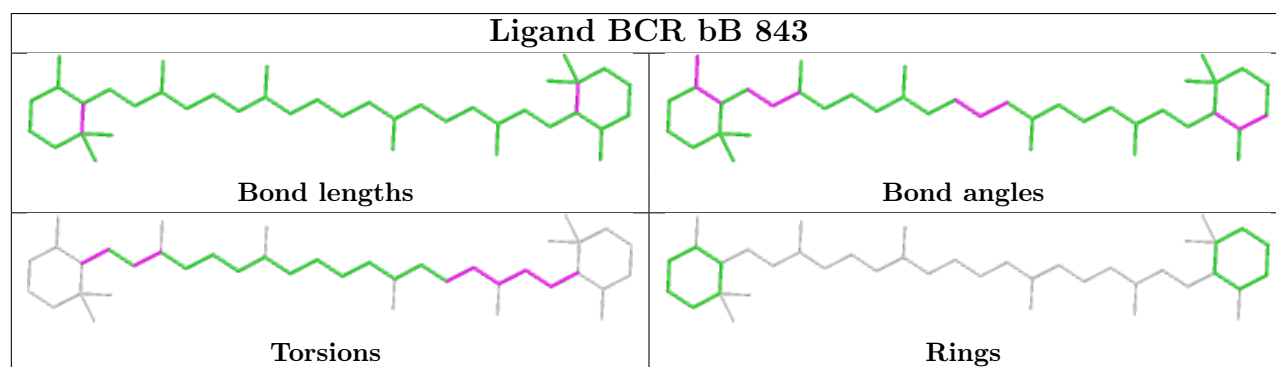
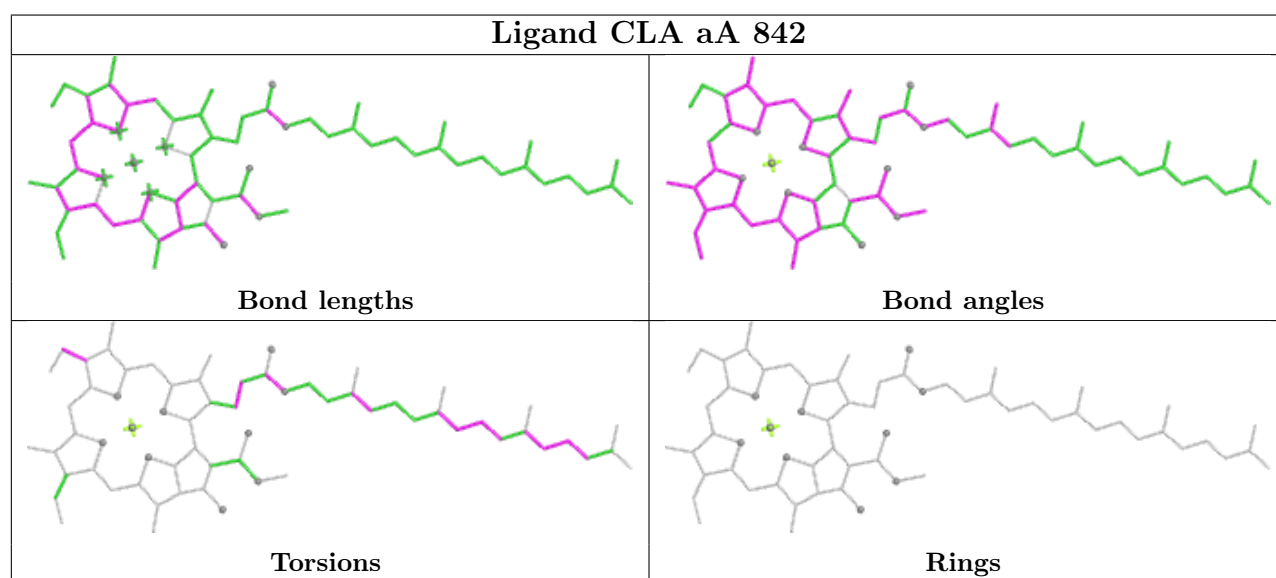
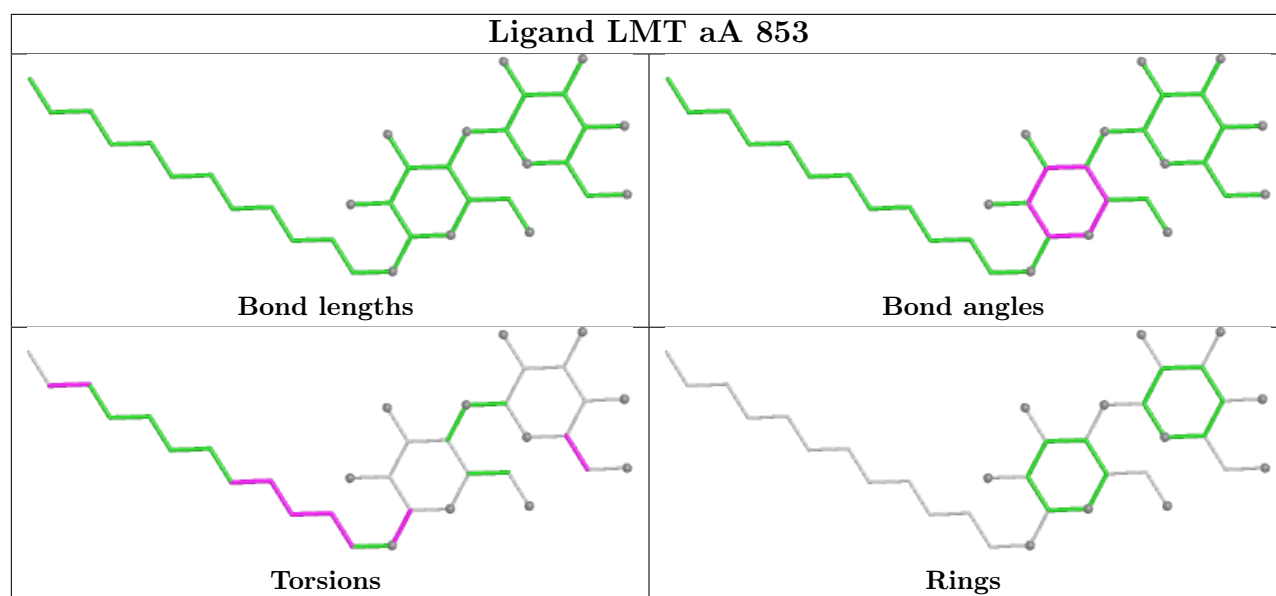


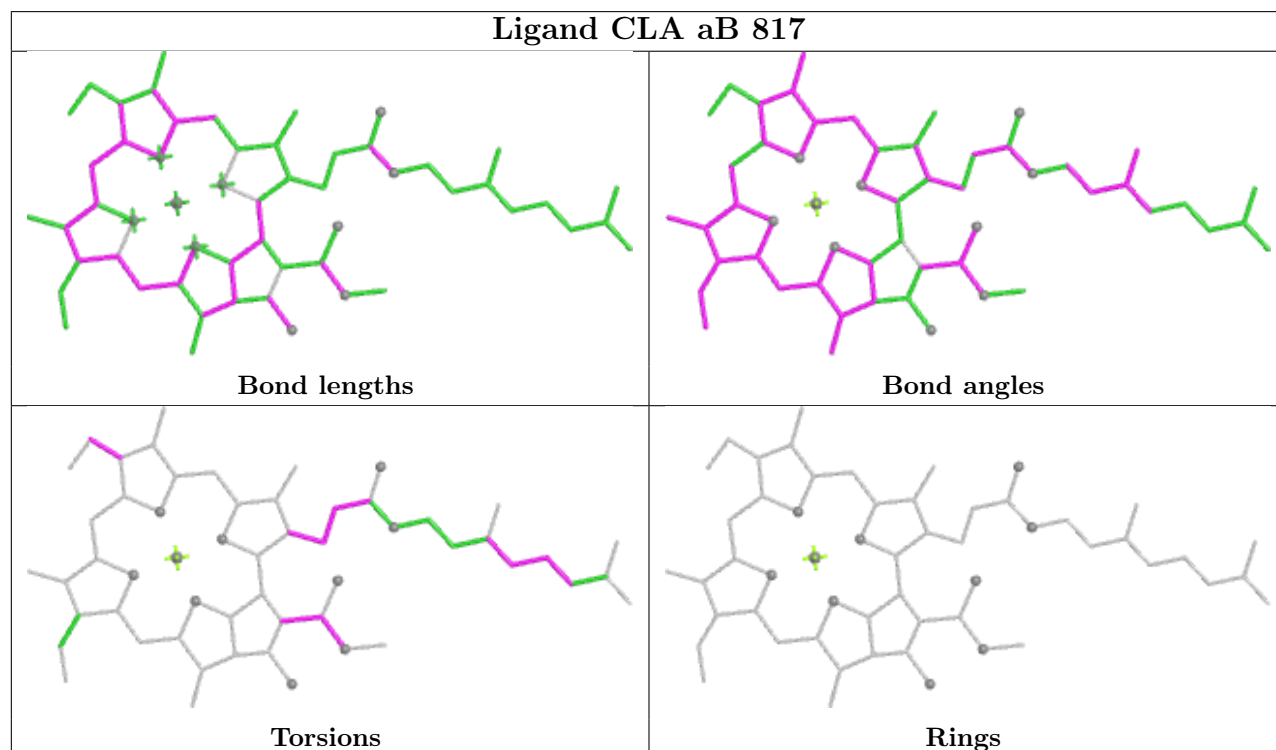
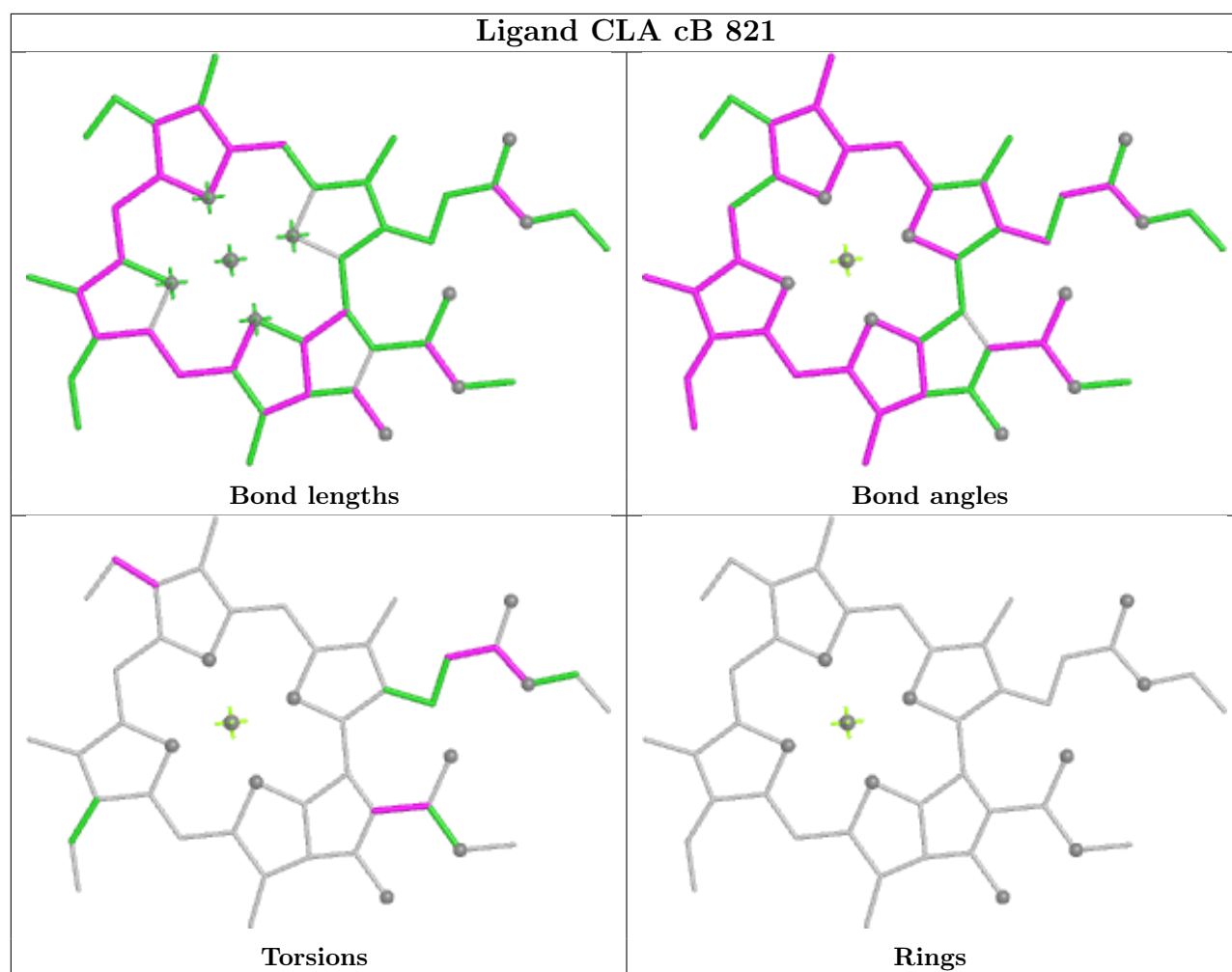
Ligand CLA aA 822

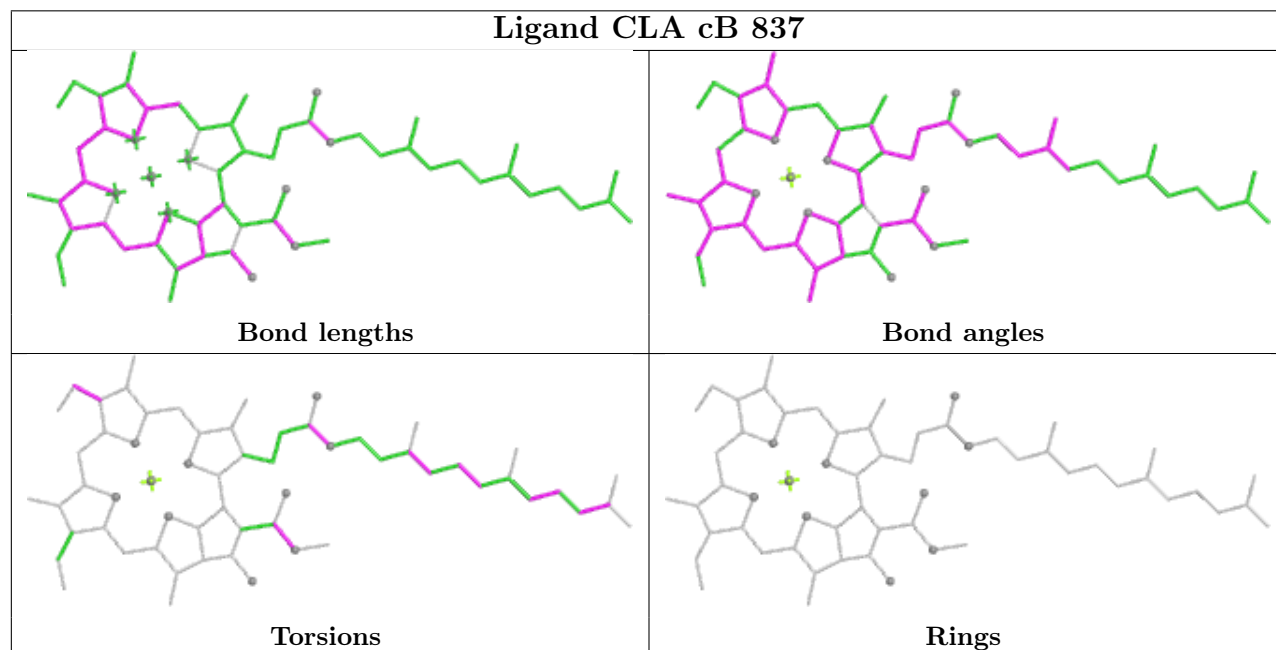
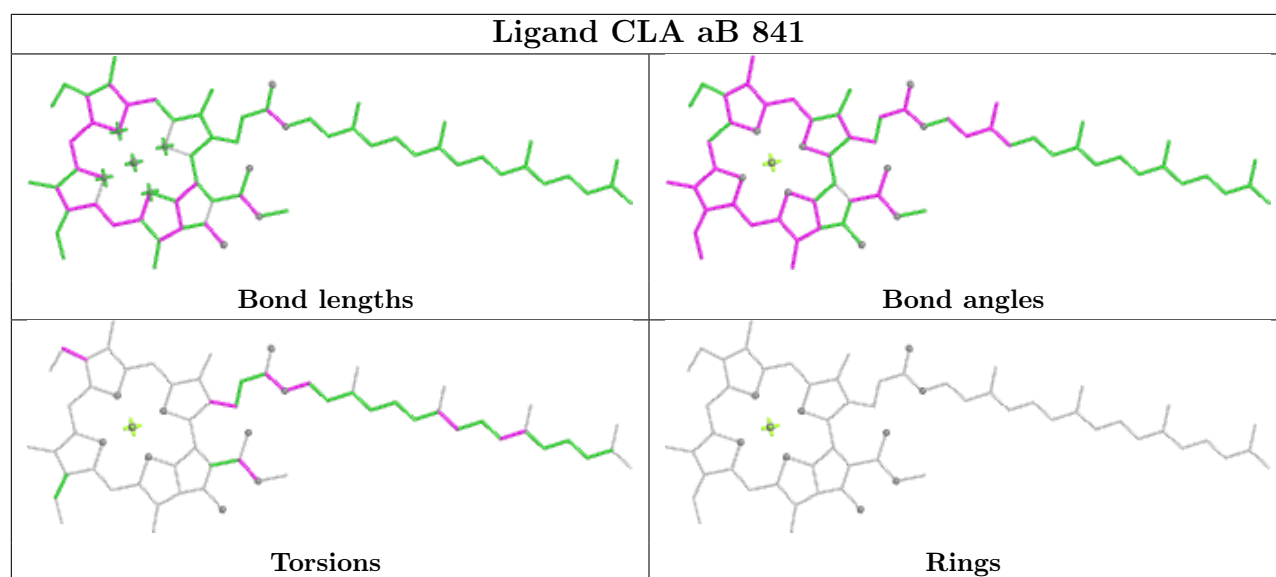


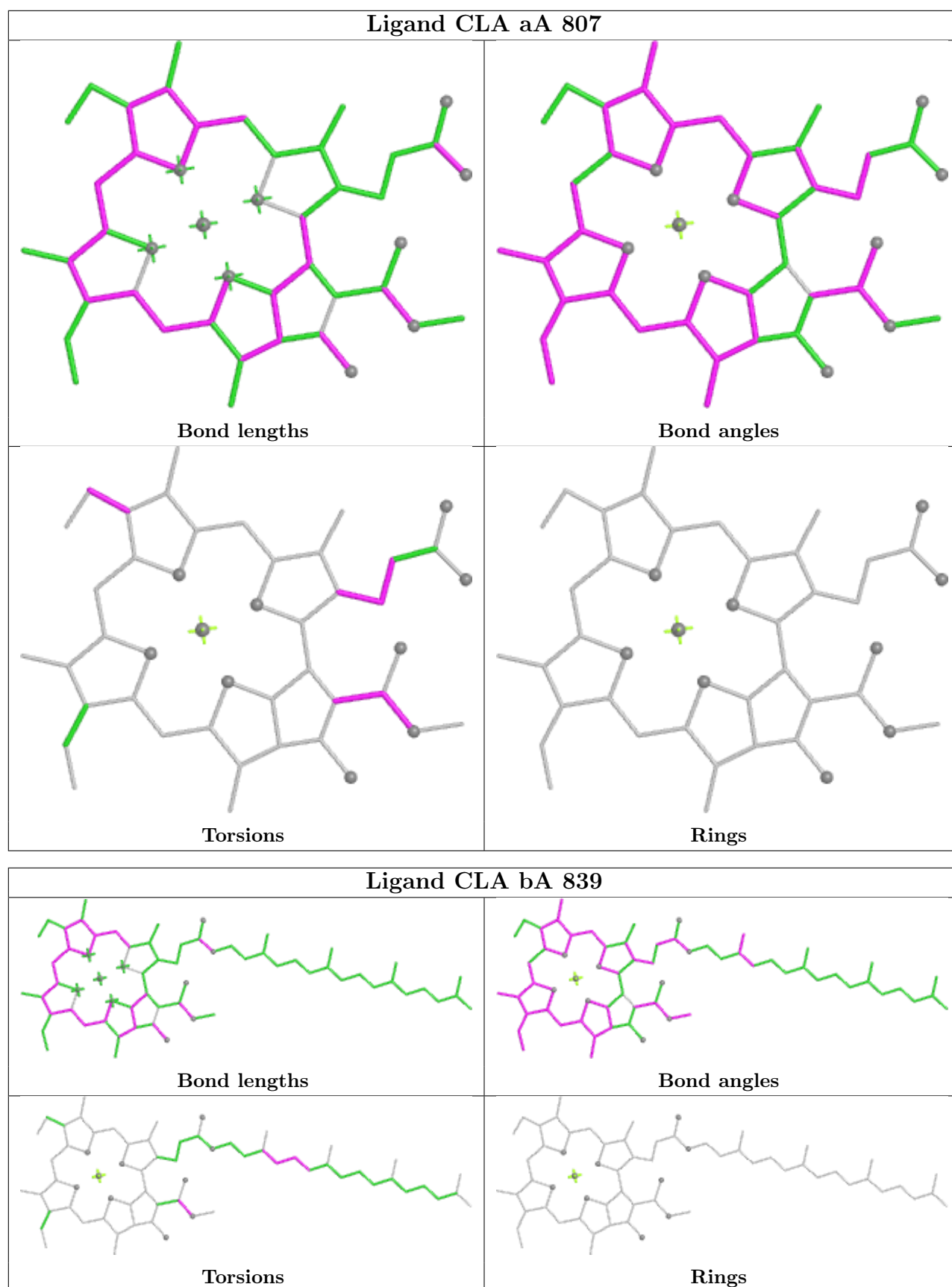
Ligand CLA bB 815

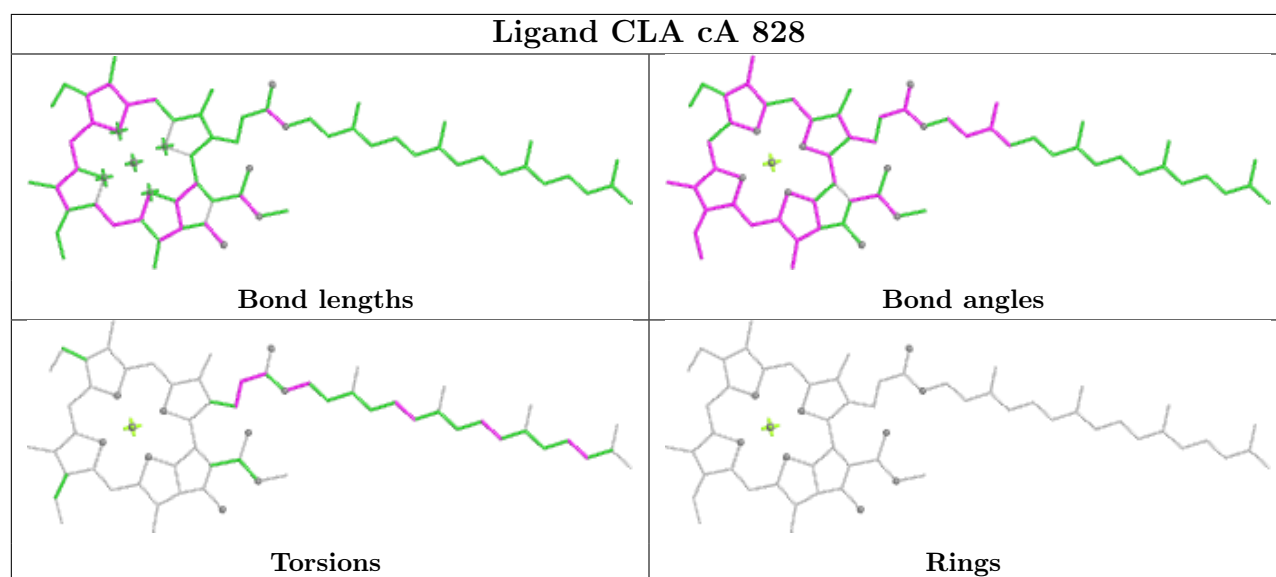
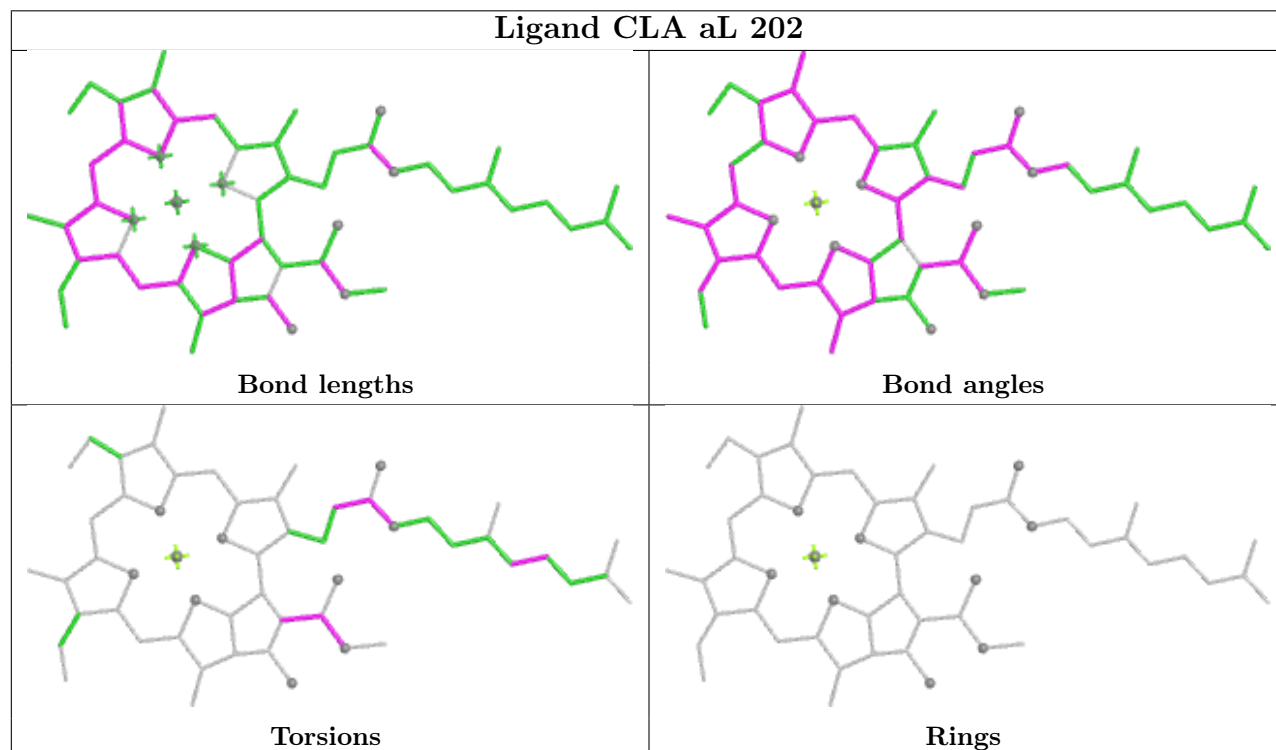
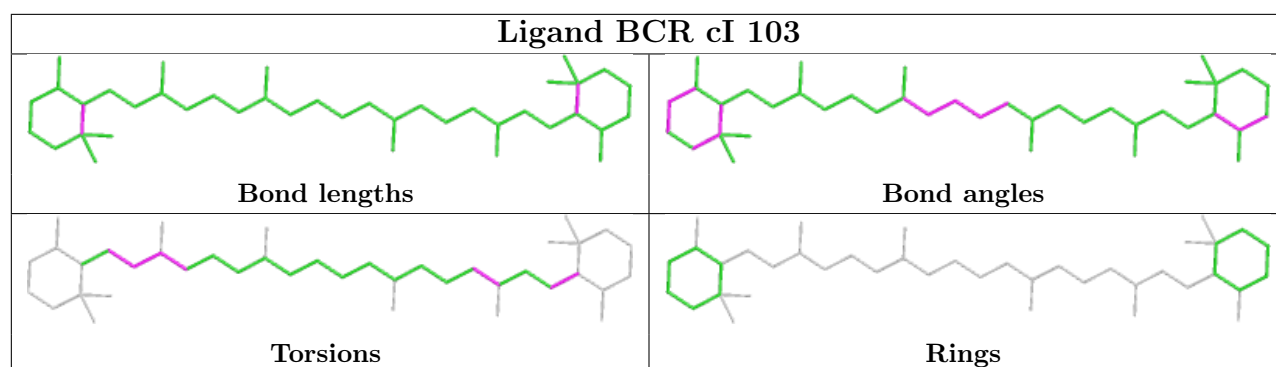


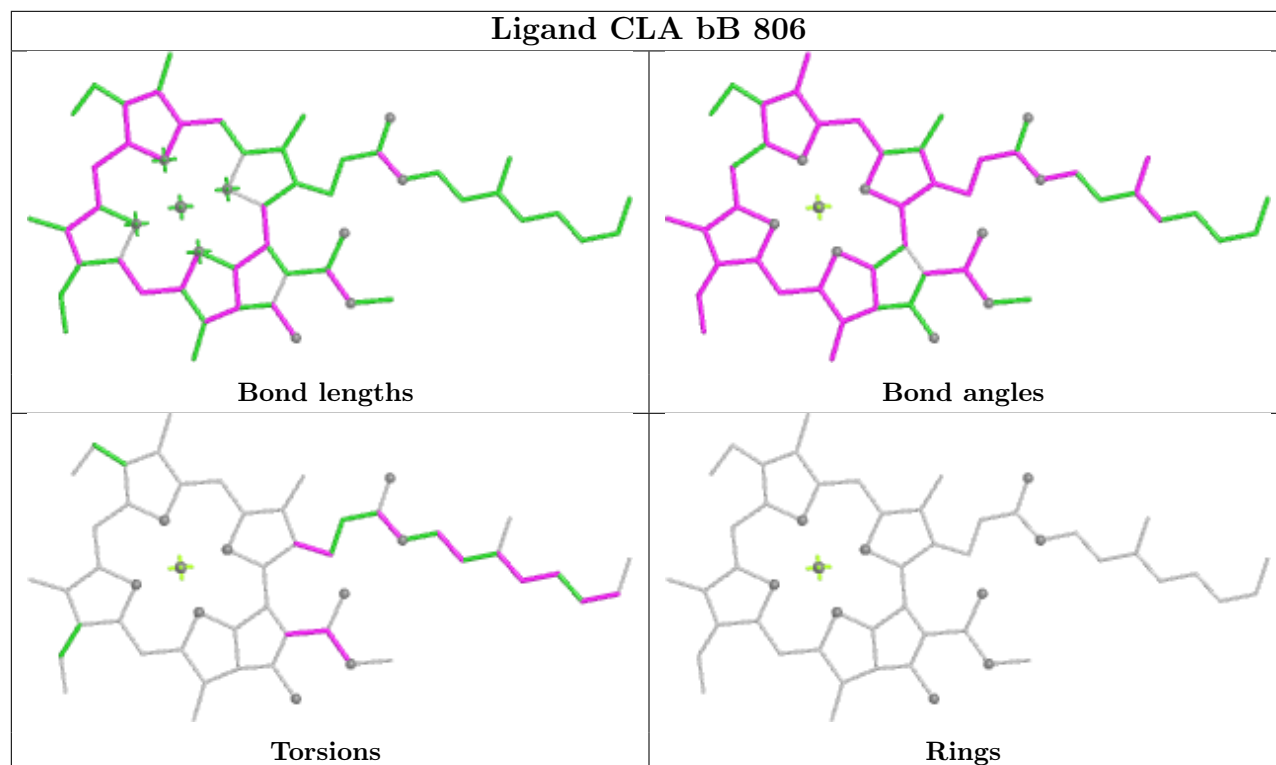
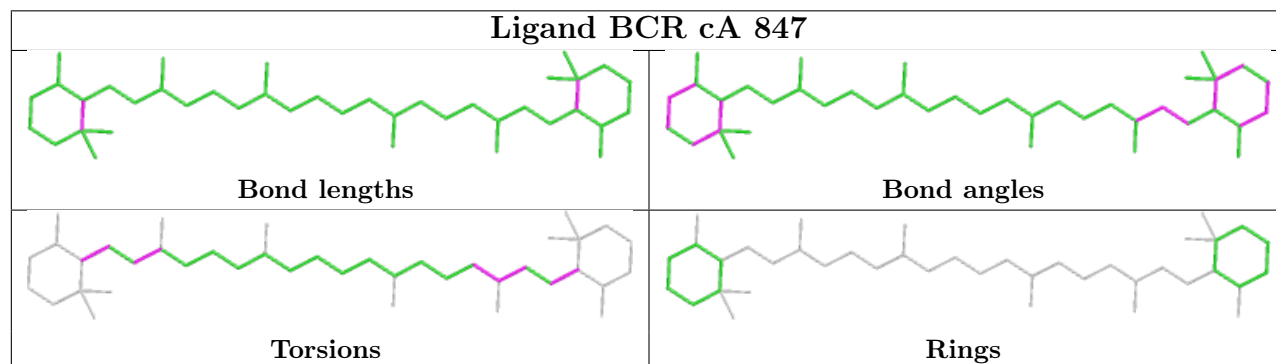
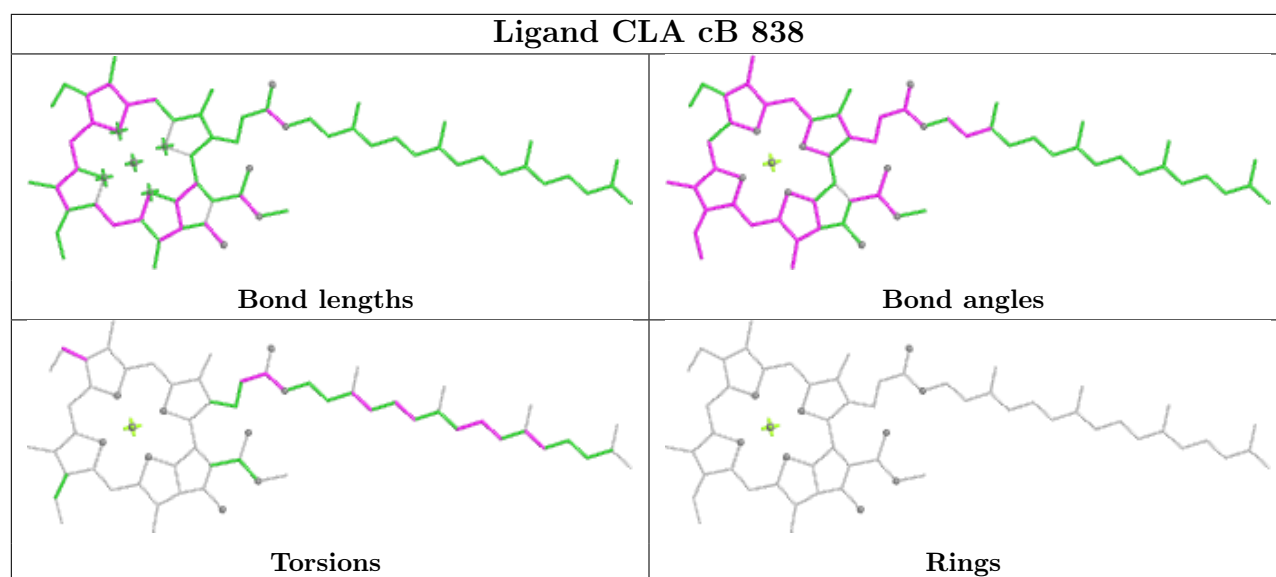


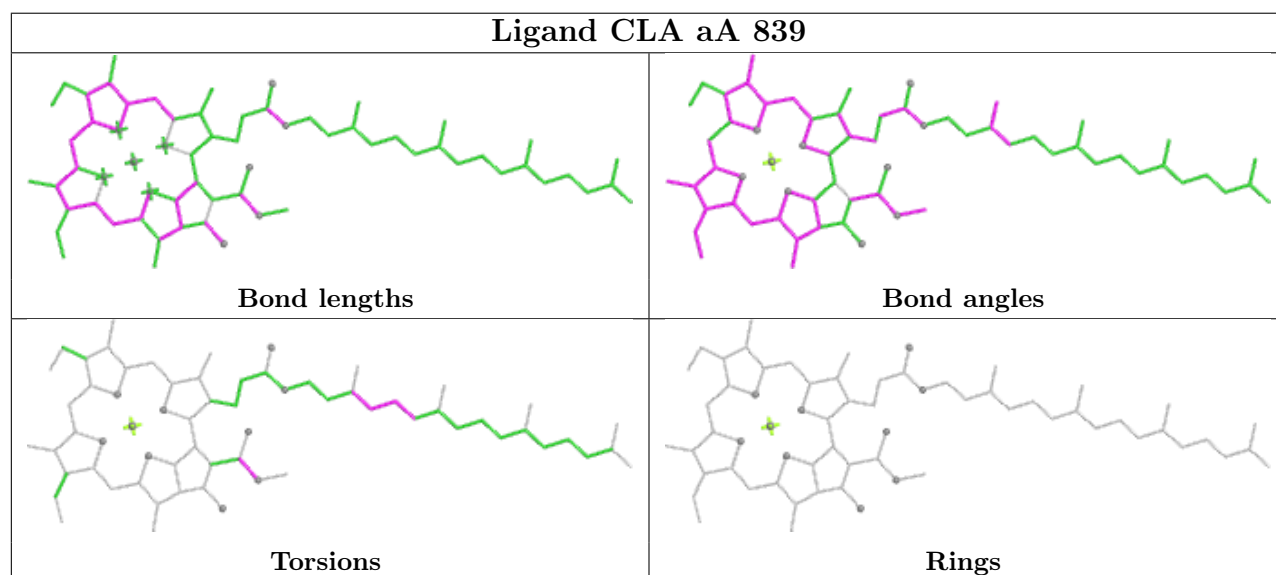
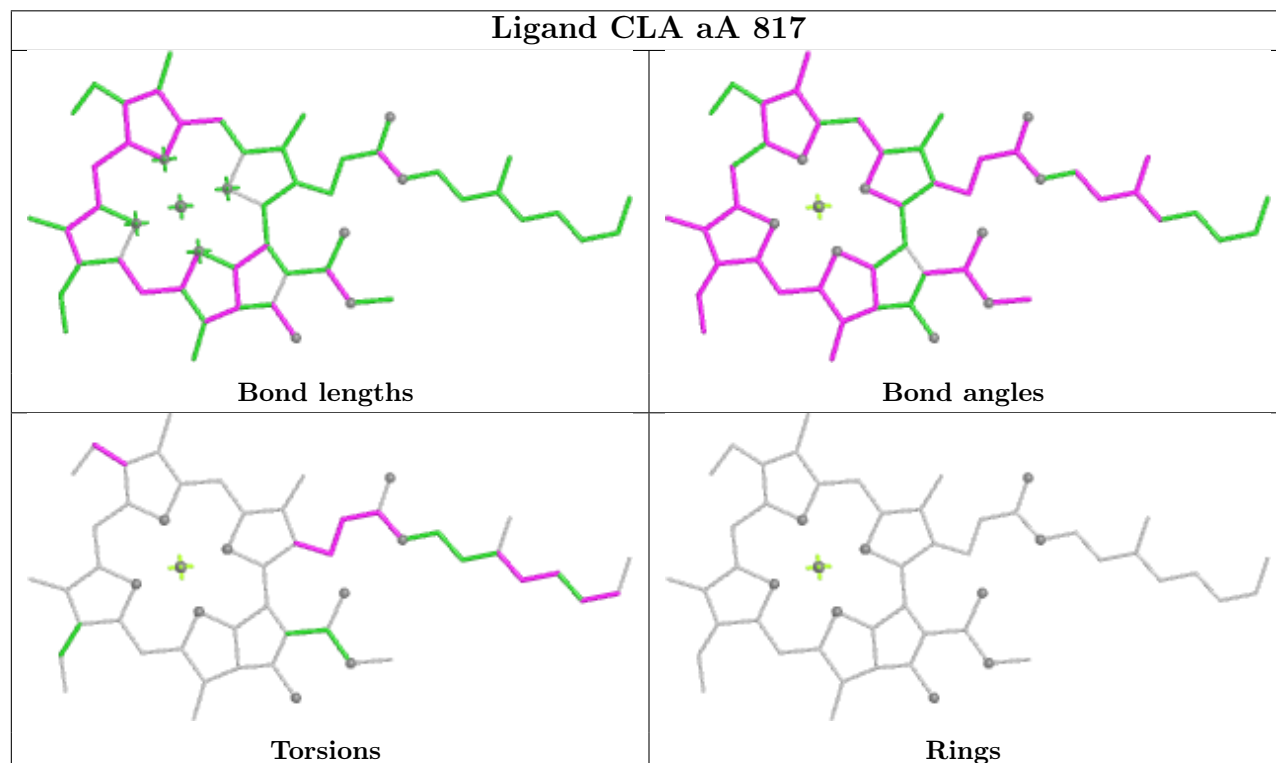
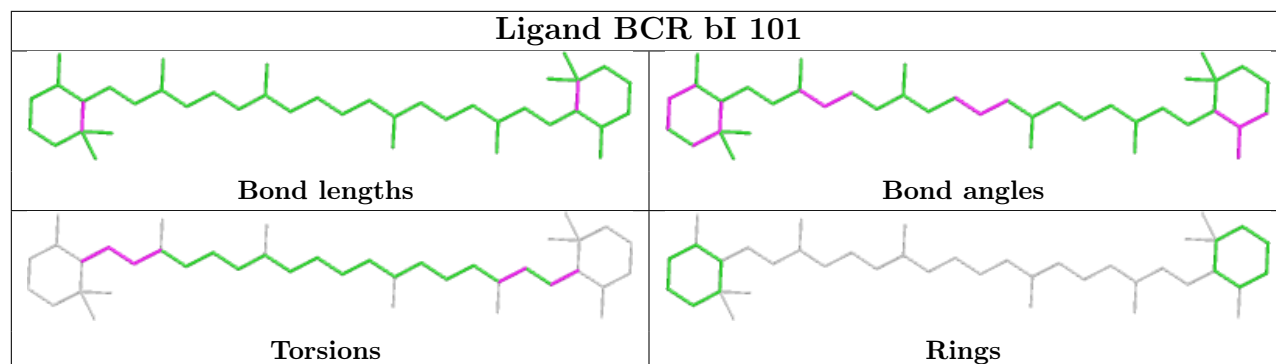


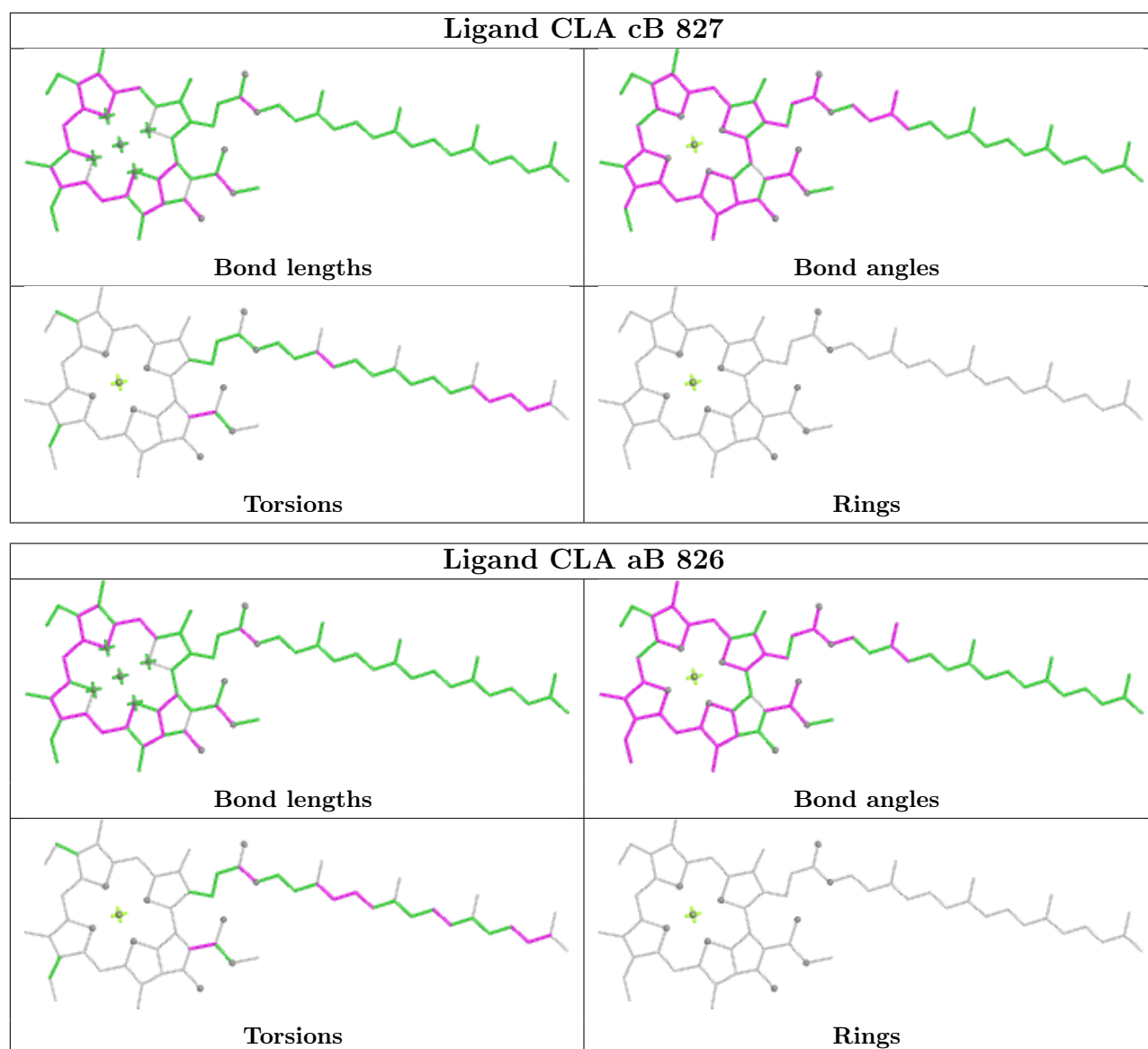


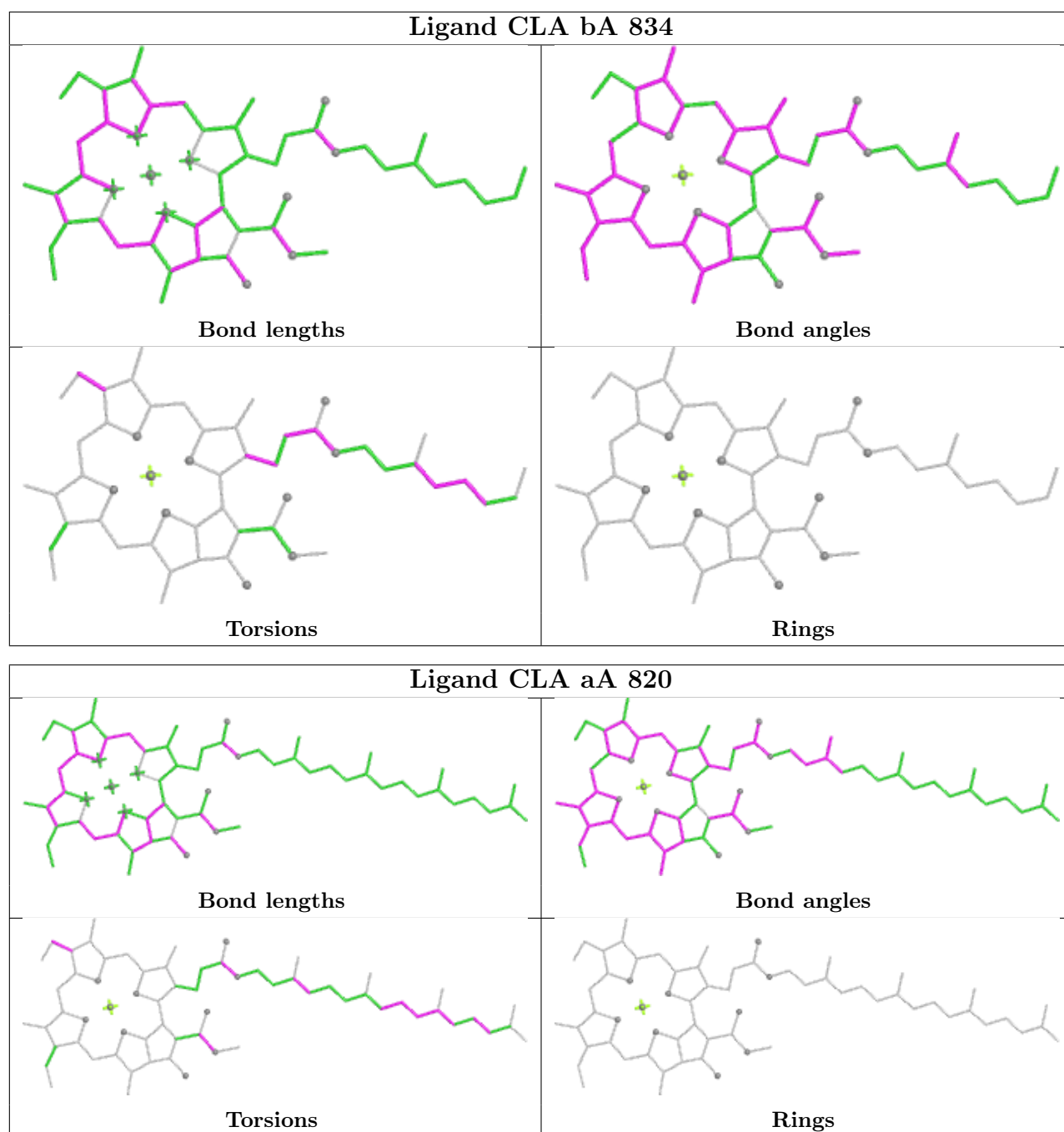


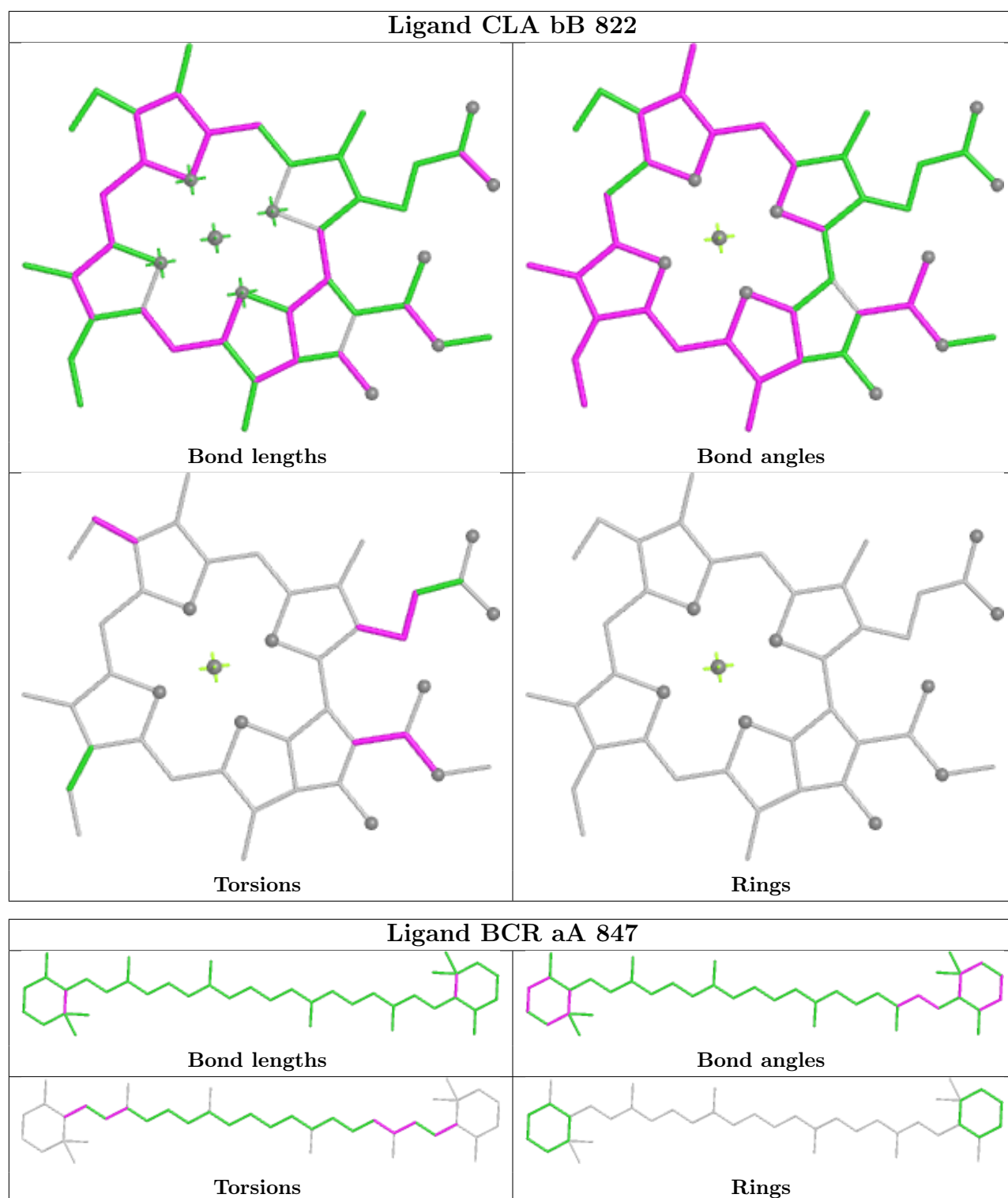


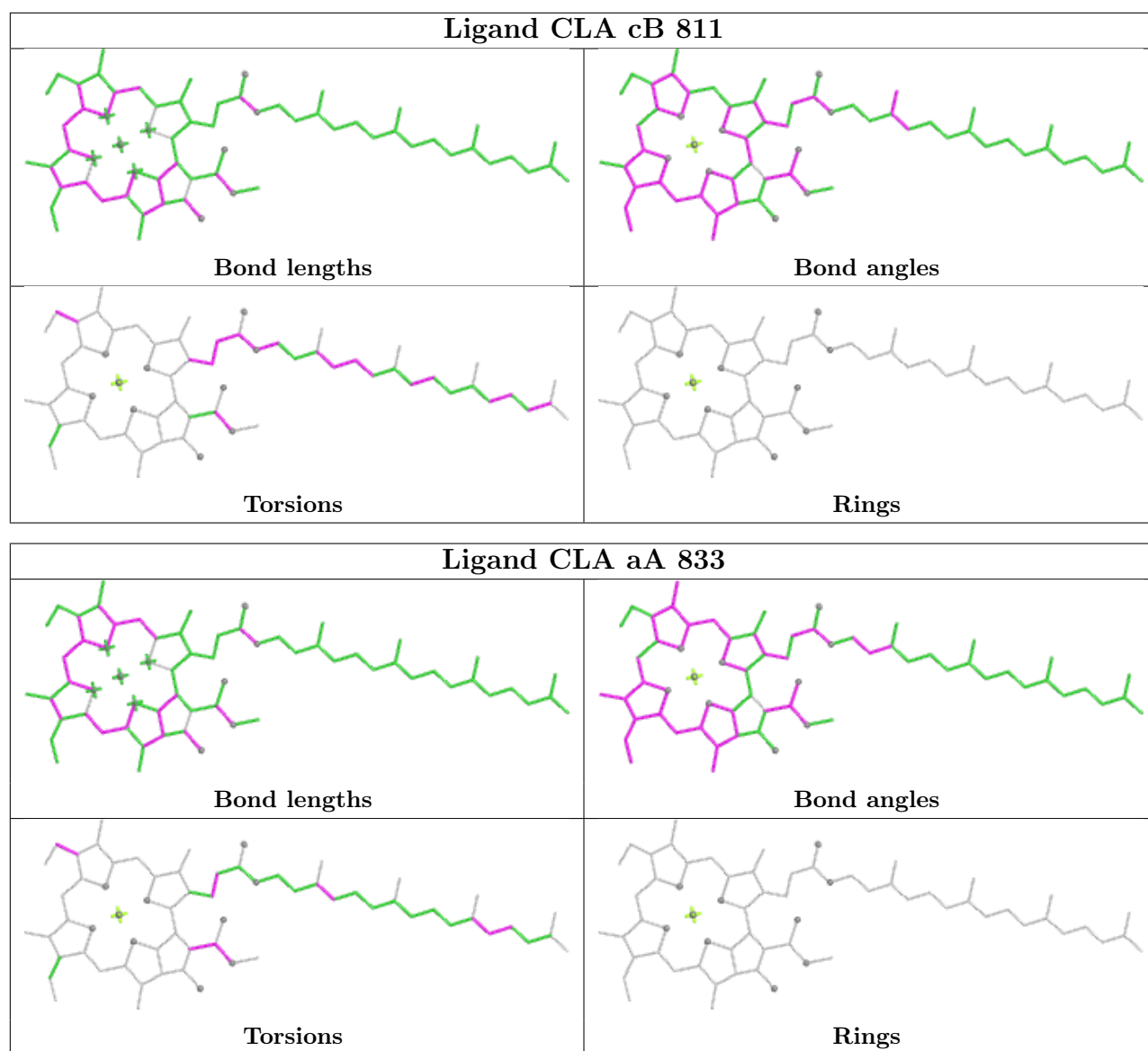




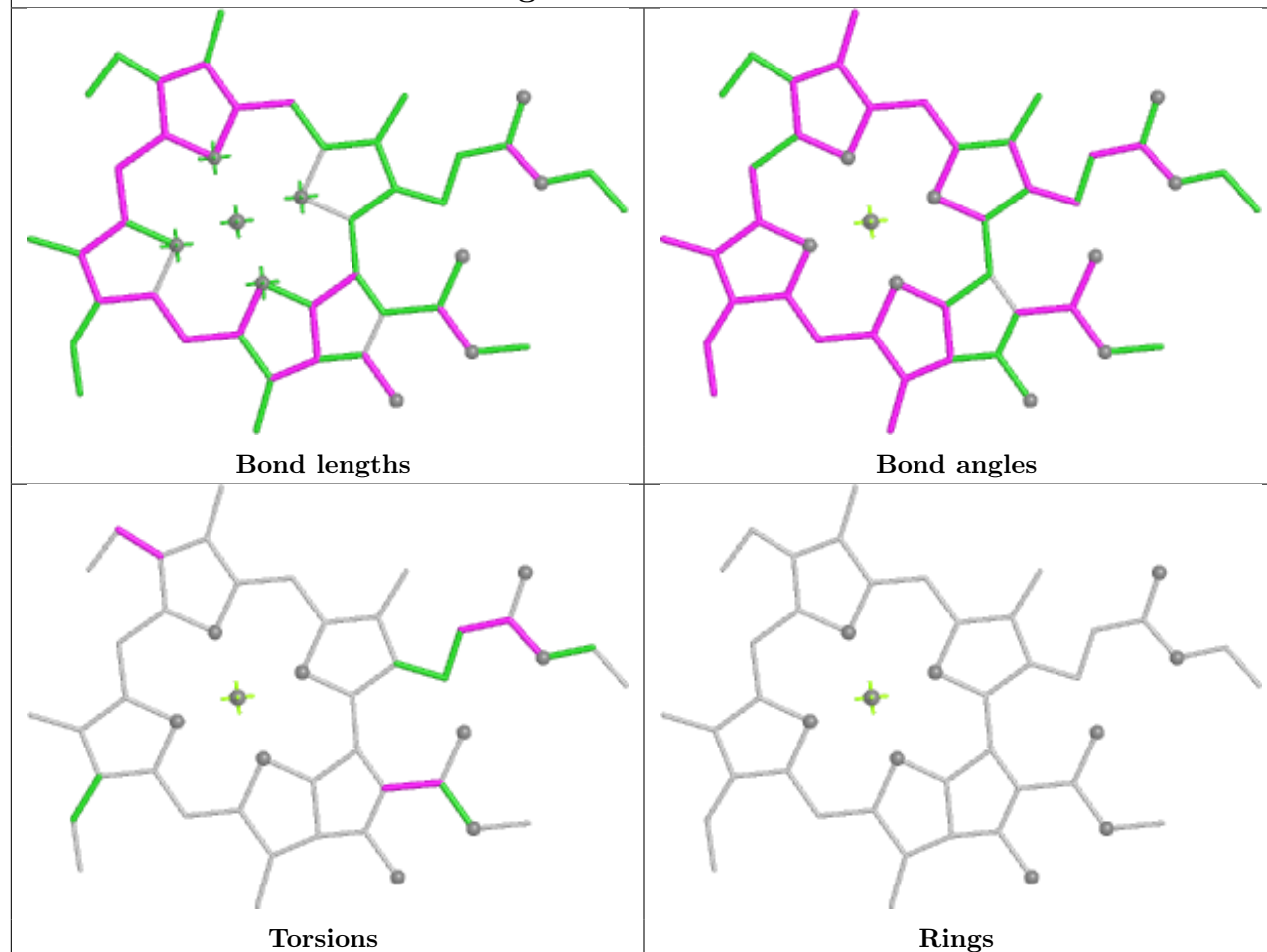




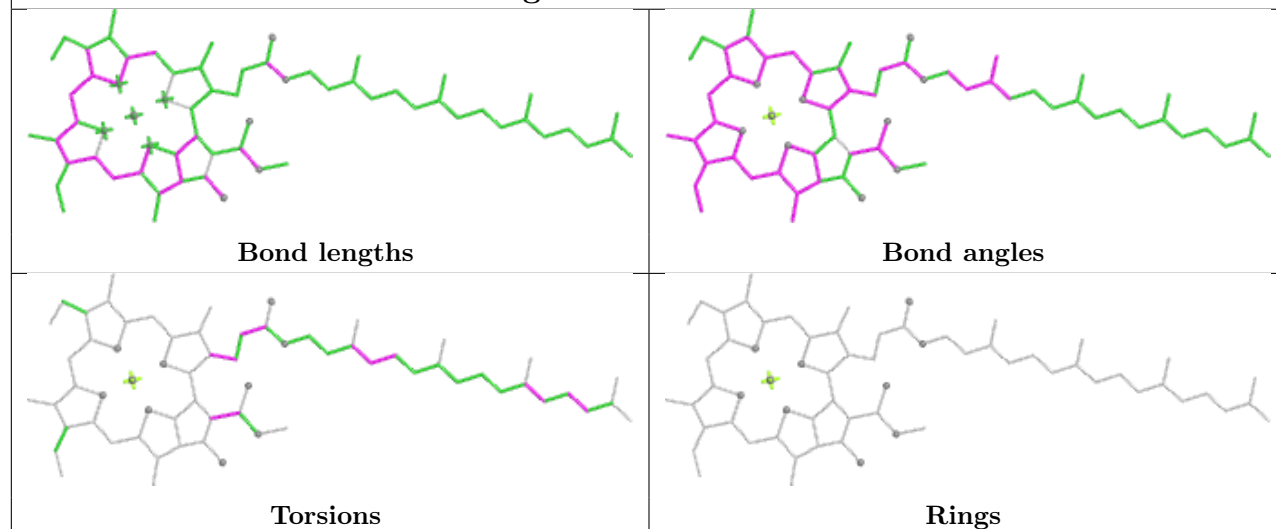


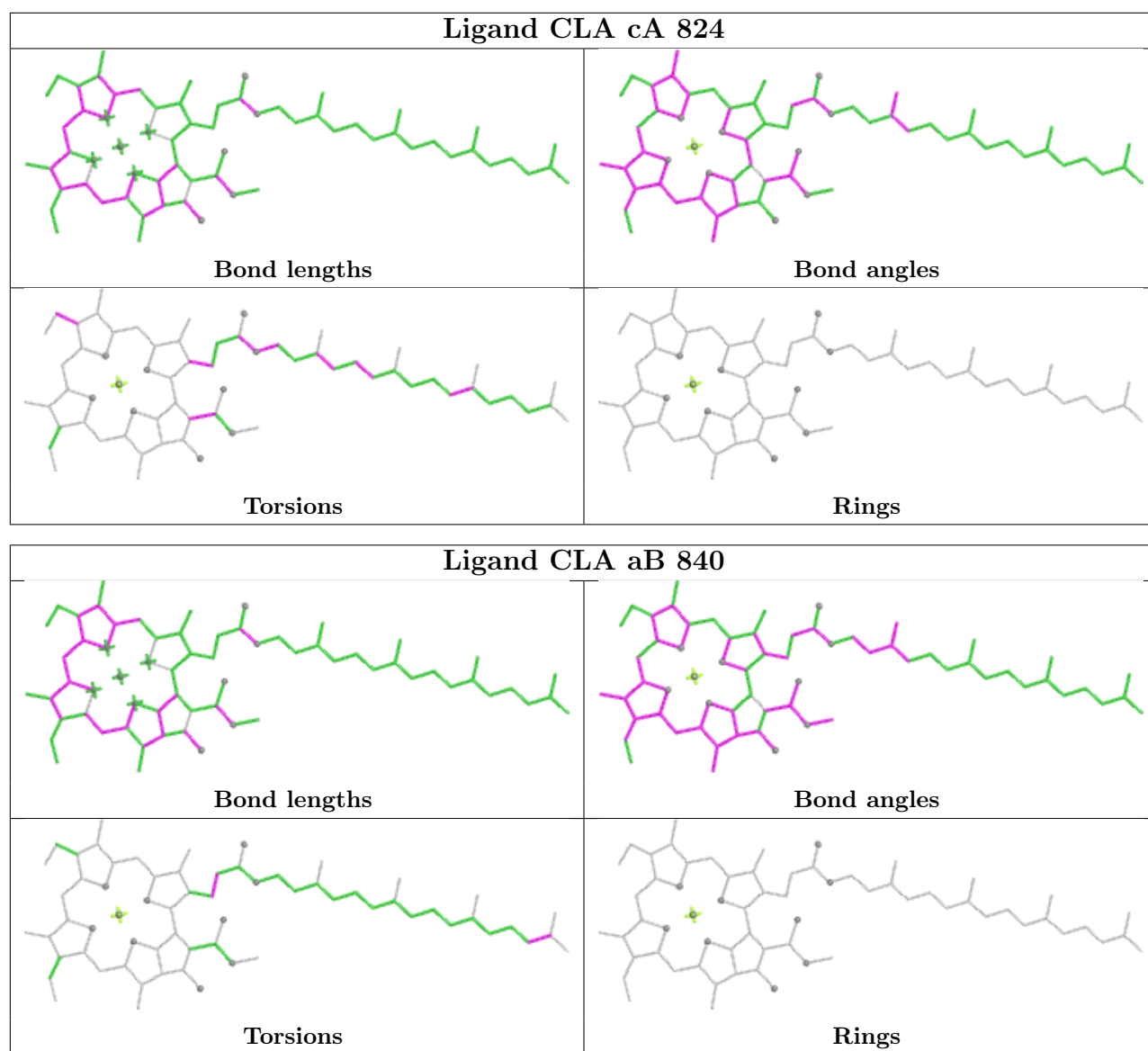


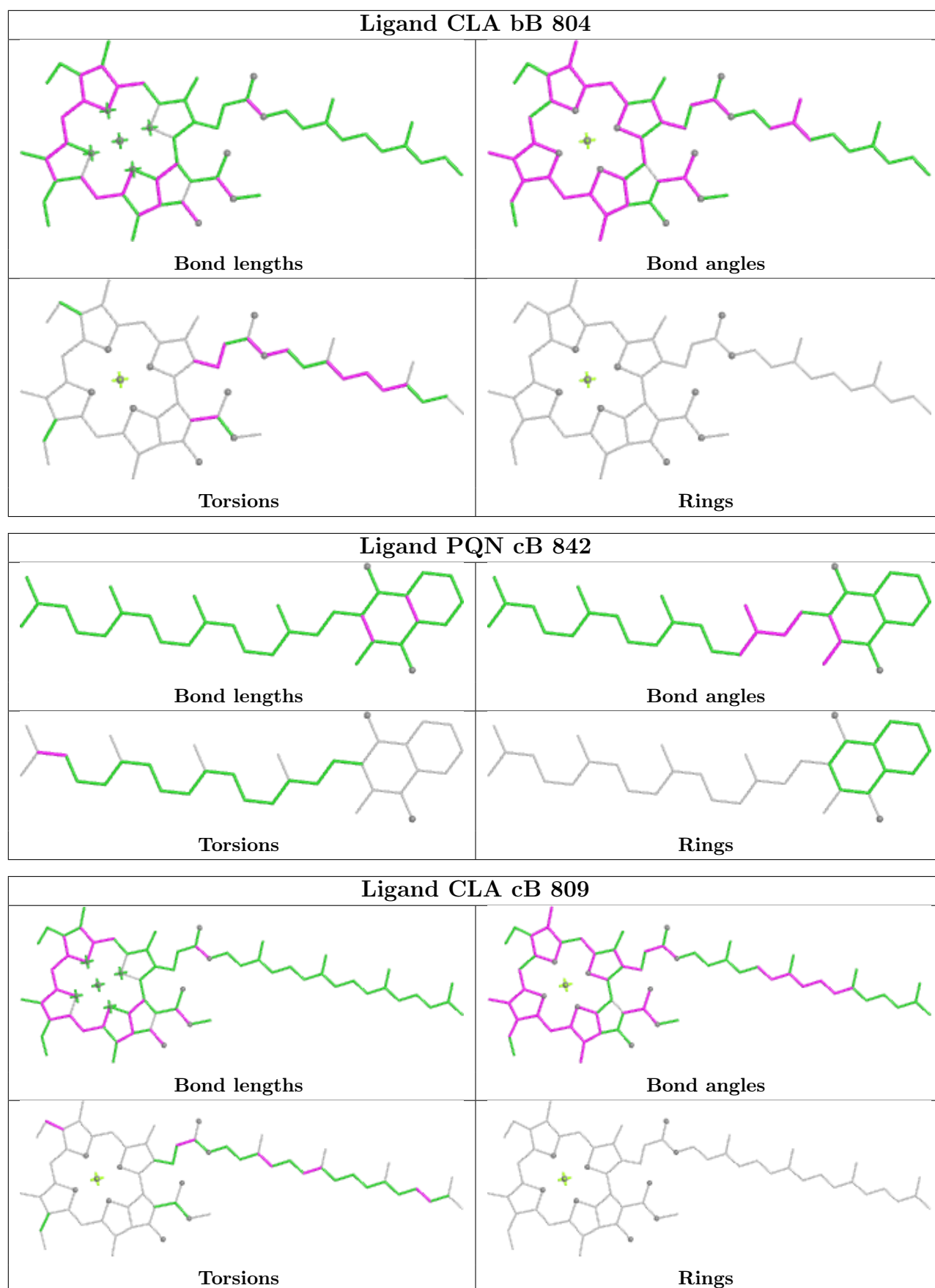
Ligand CLA bB 821

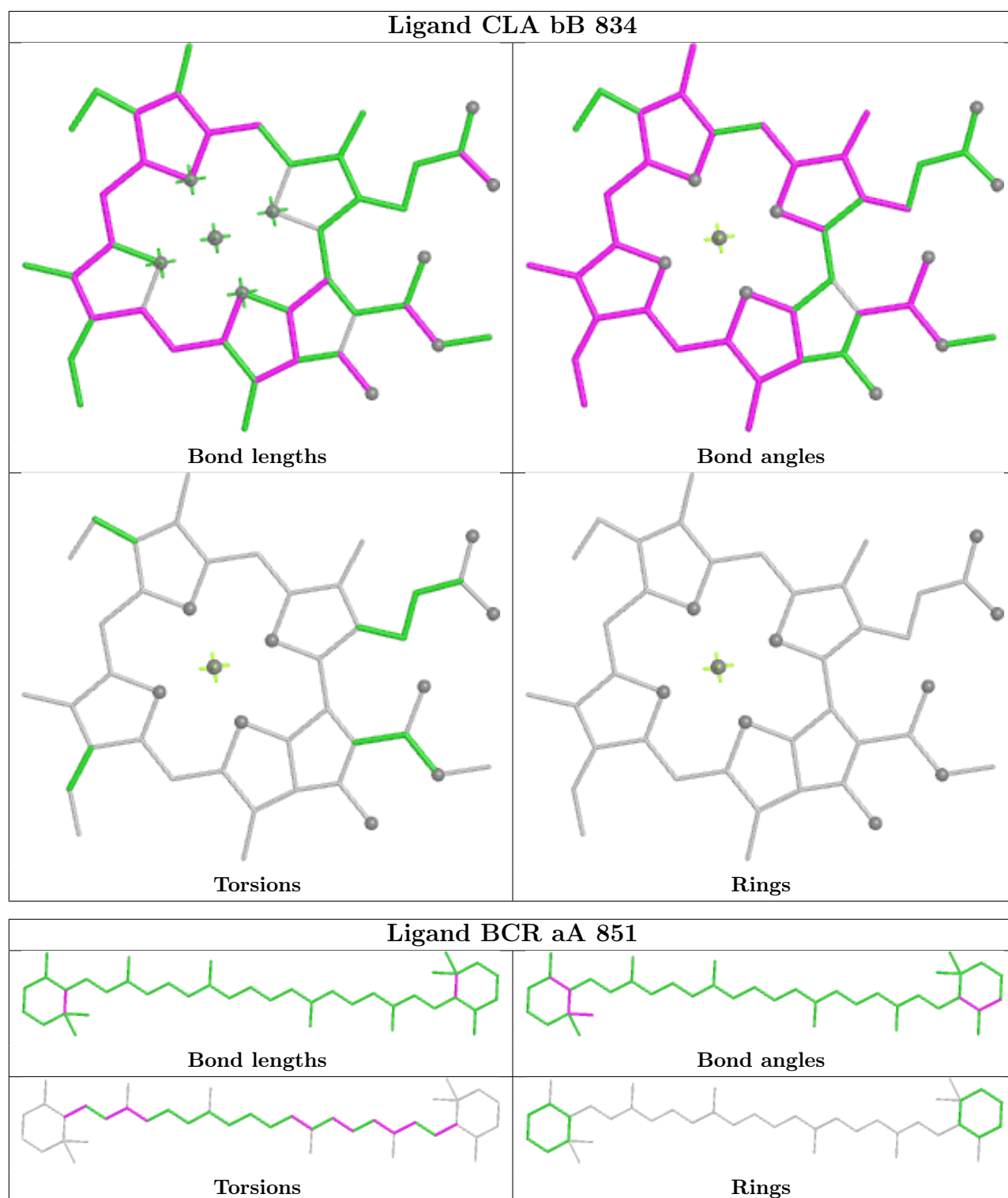


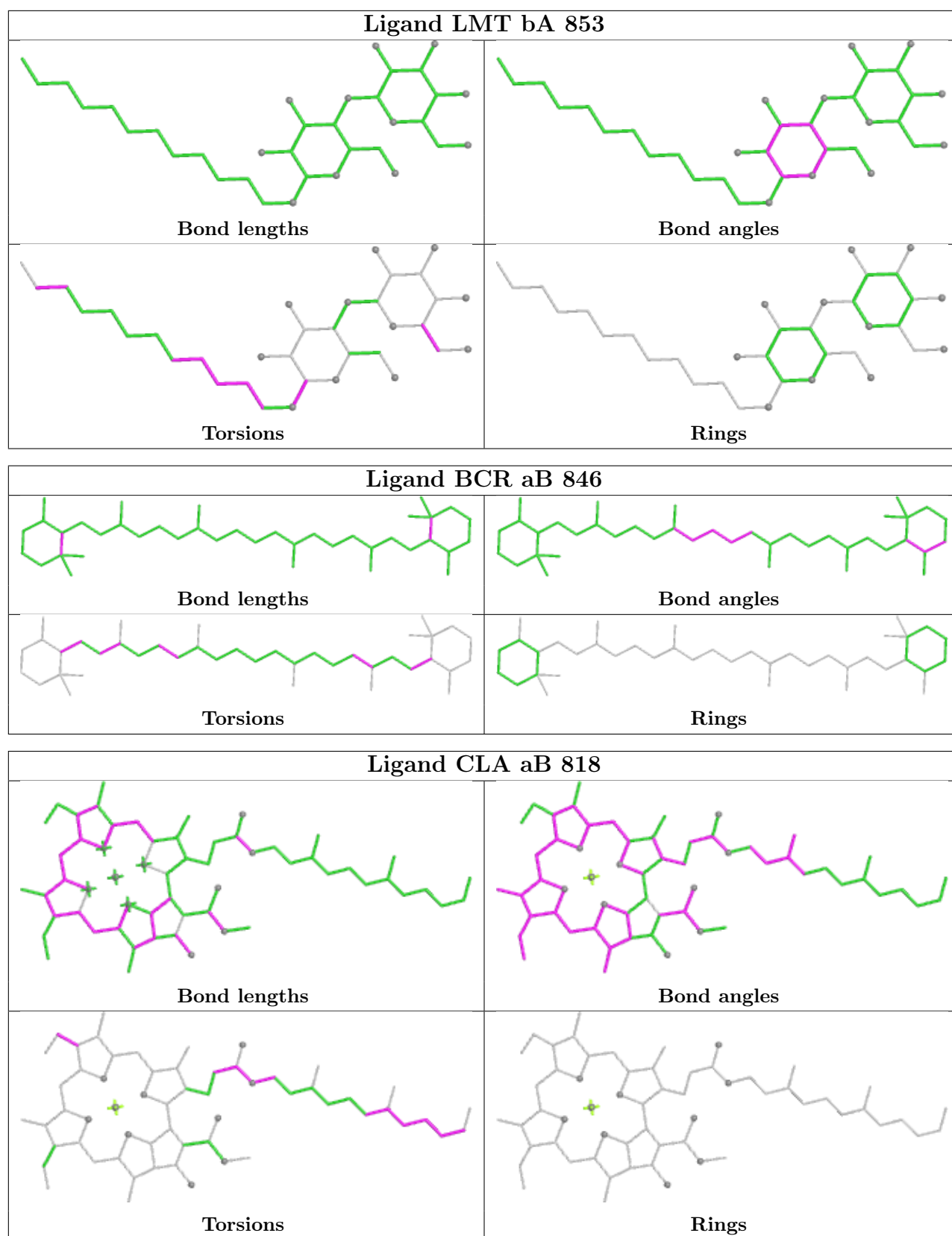
Ligand CLA aA 835

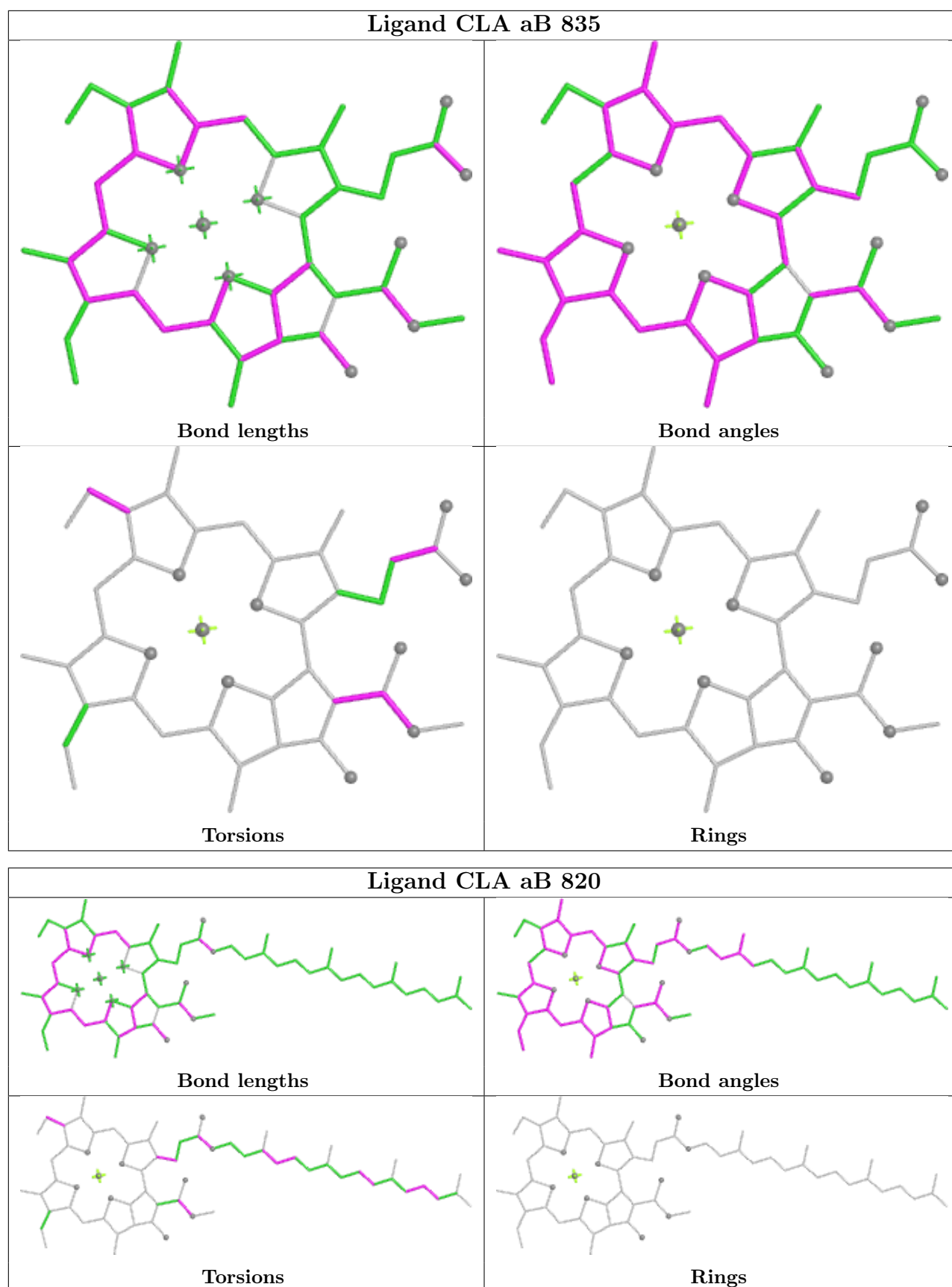


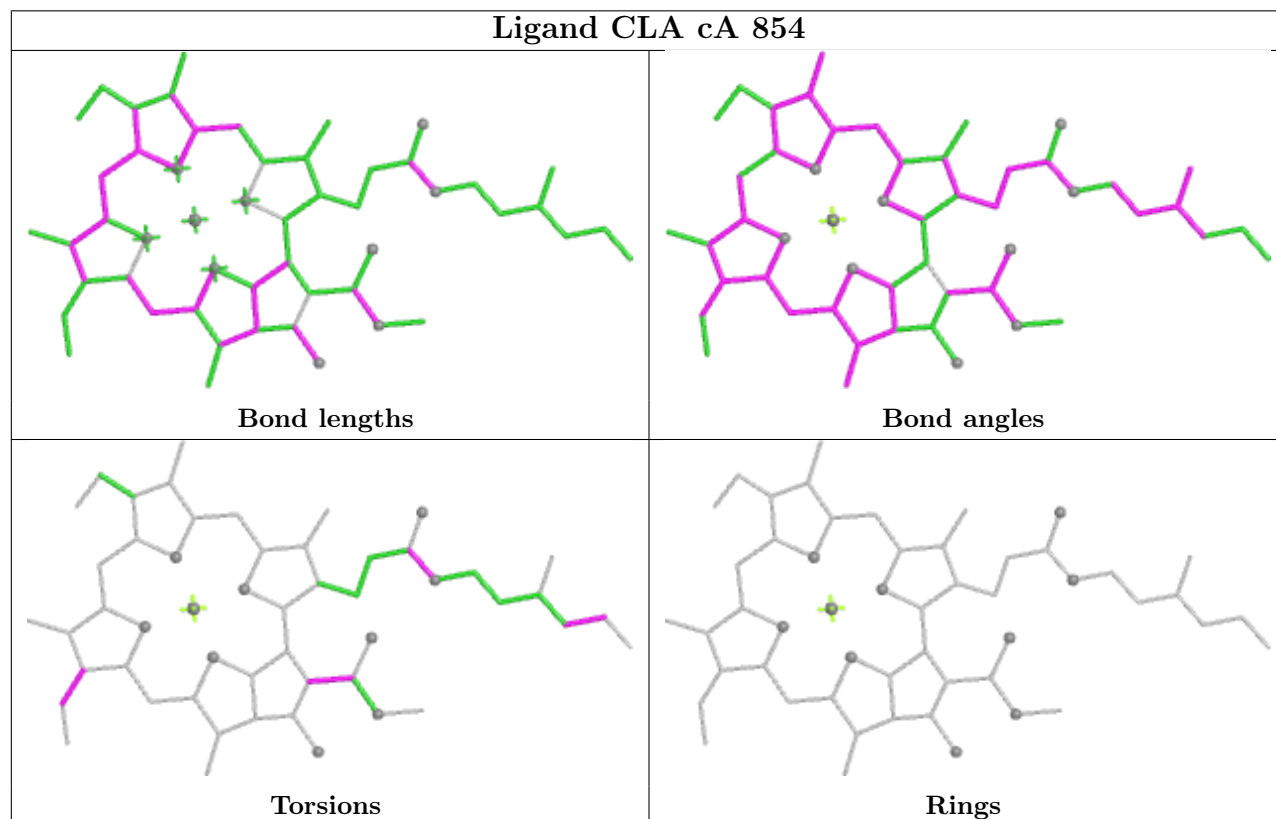
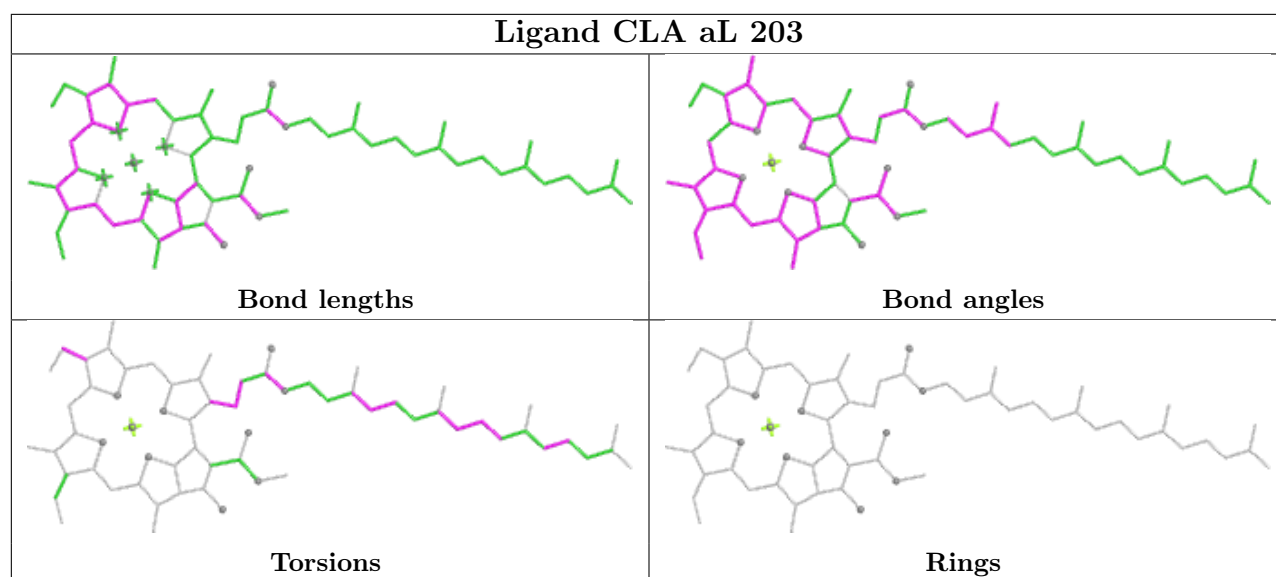


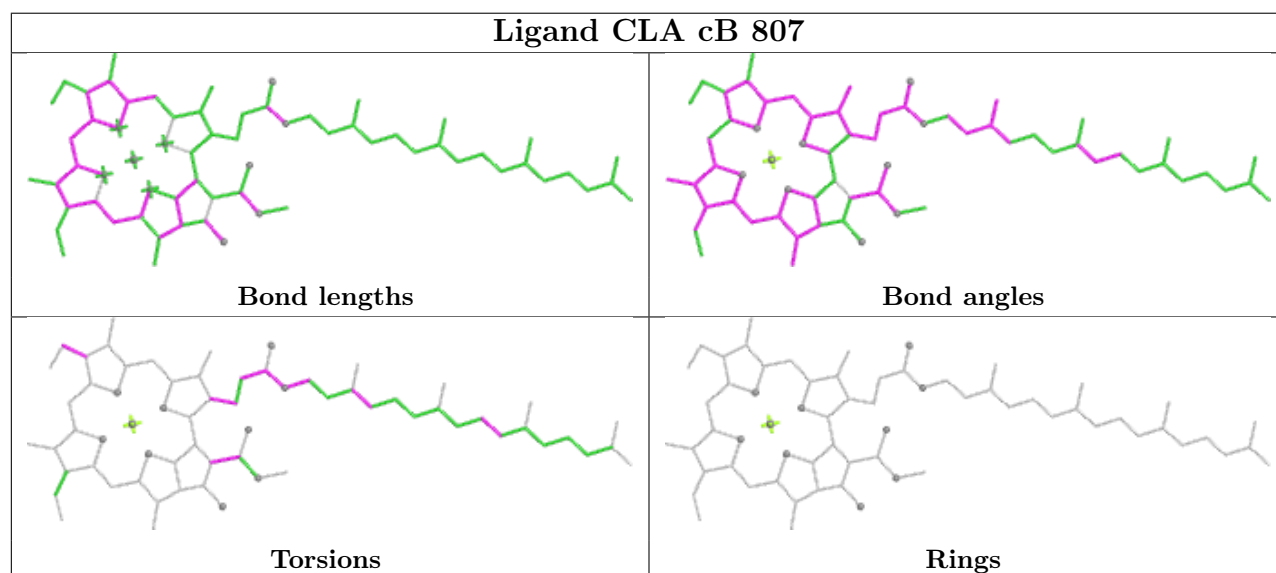
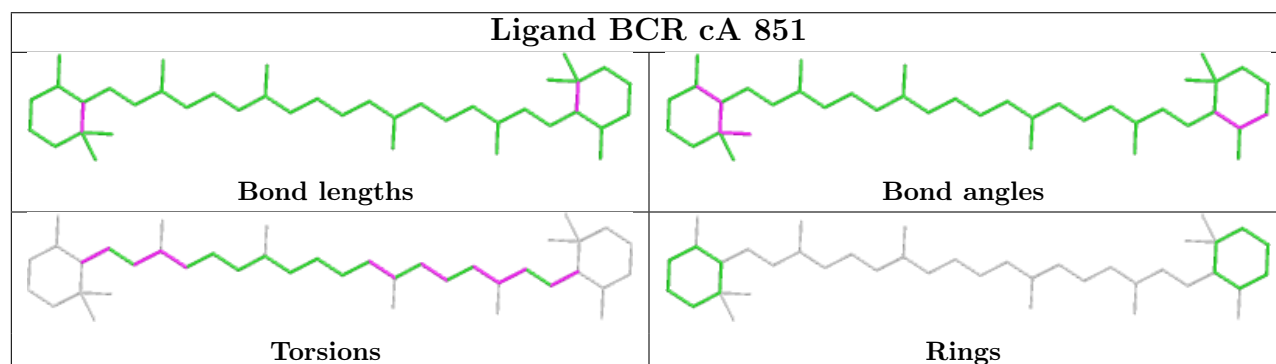
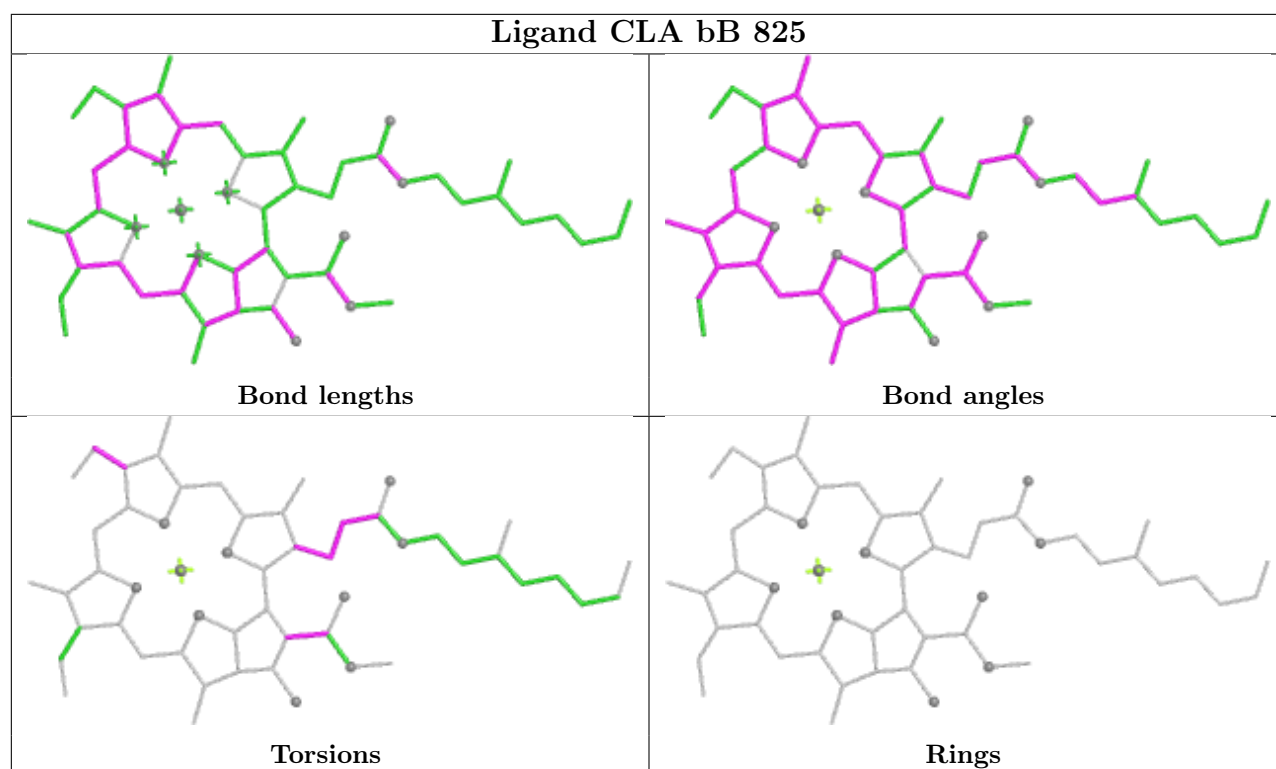


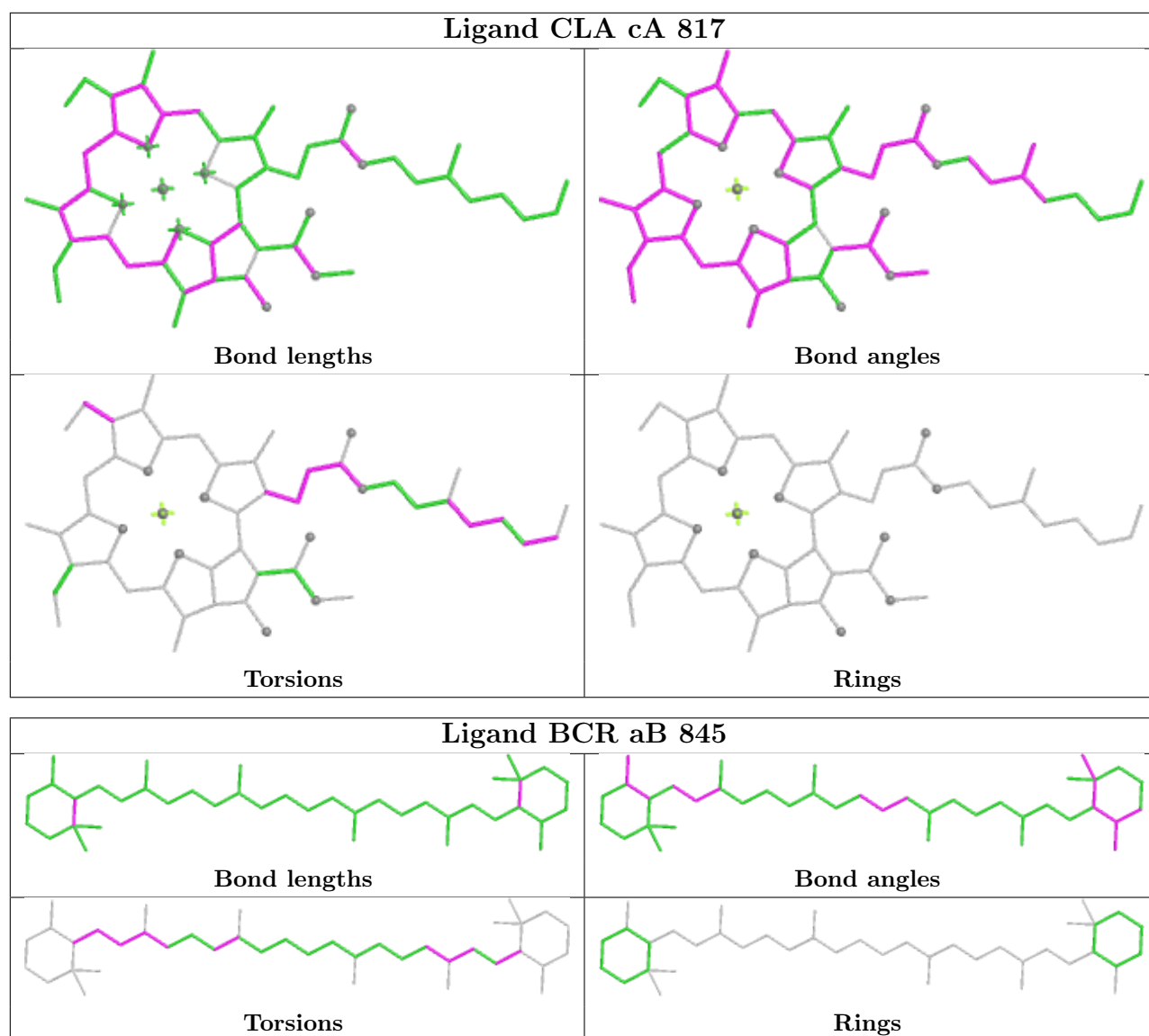


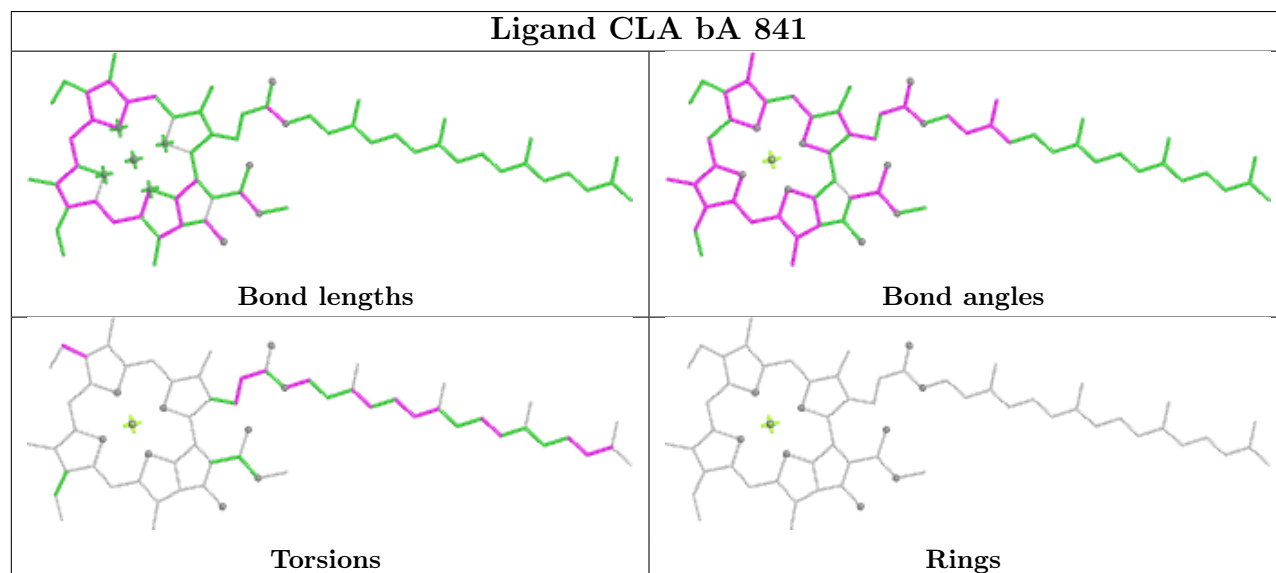
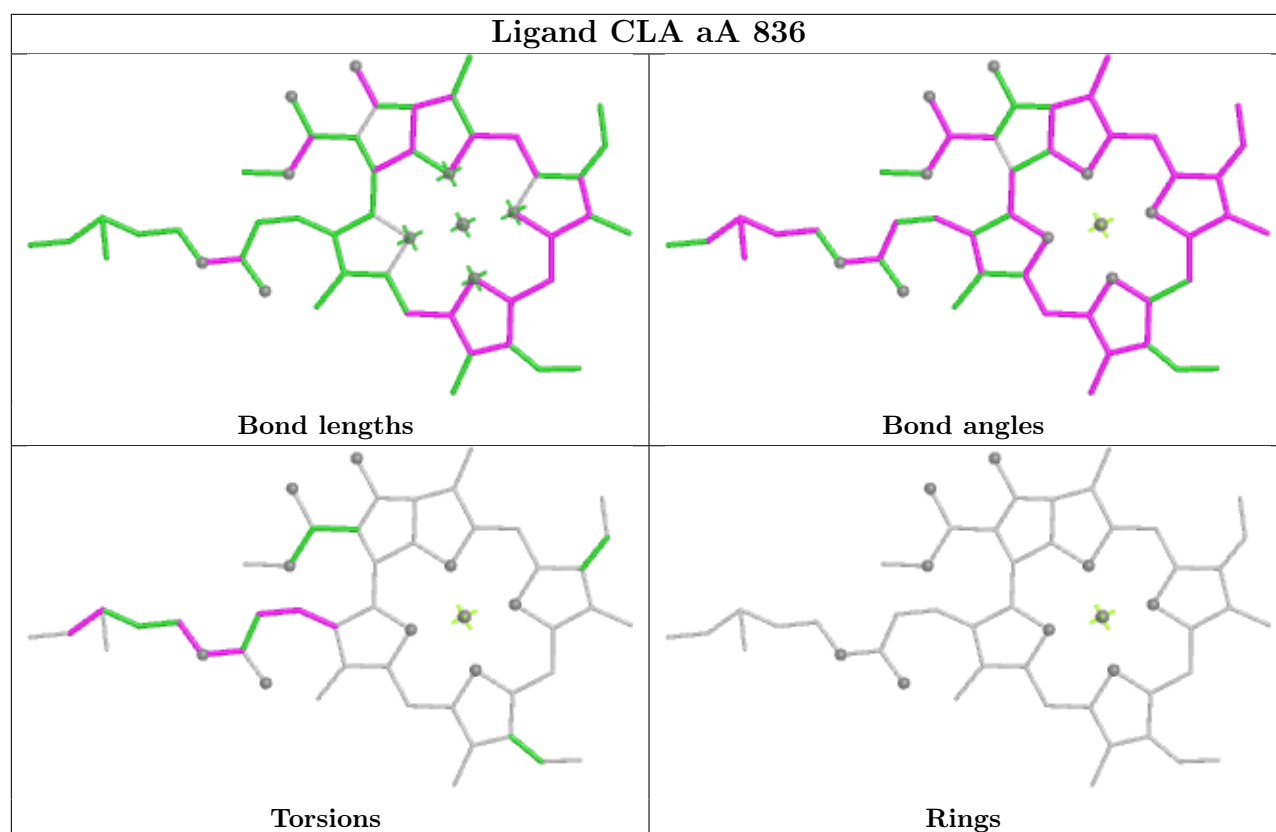


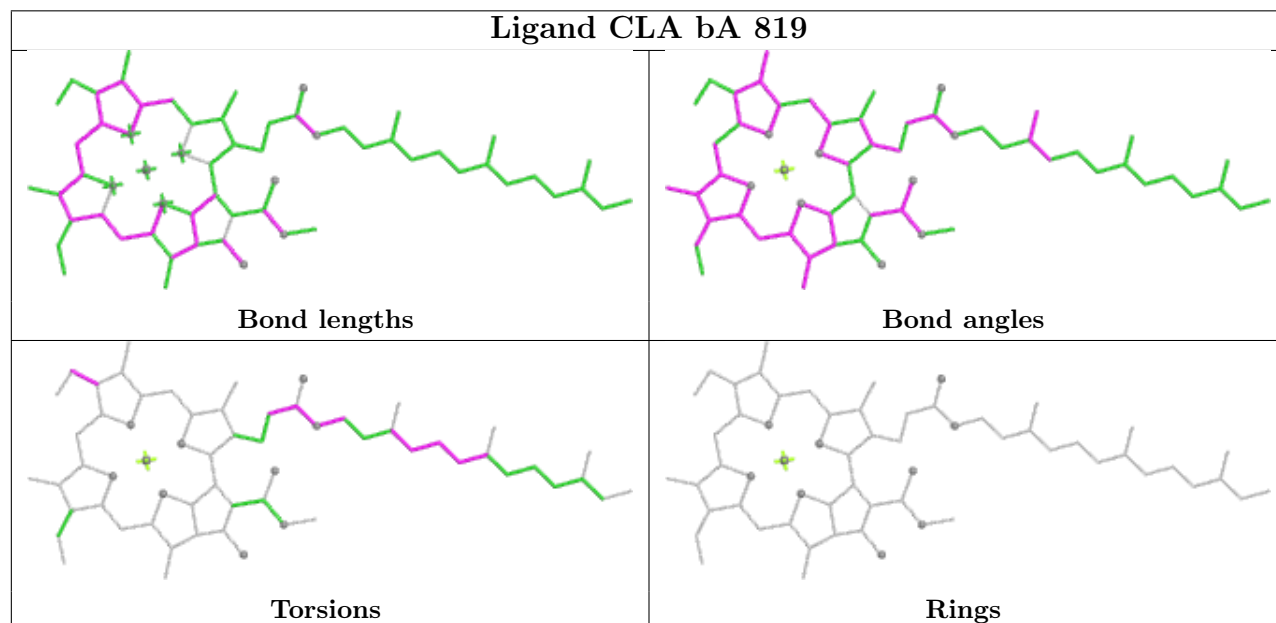
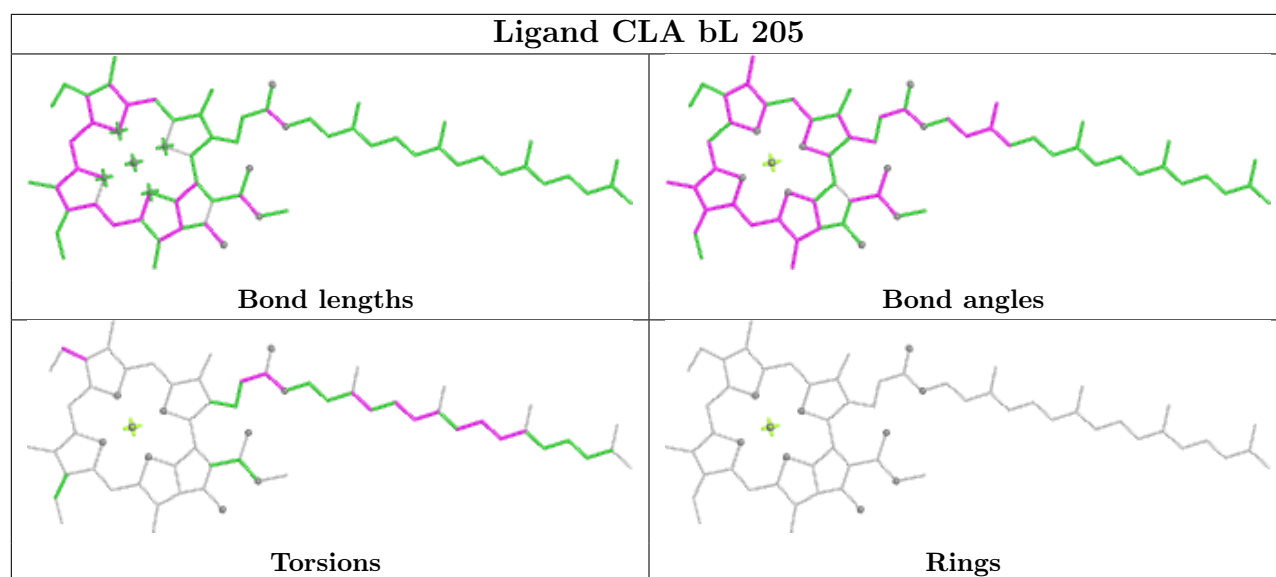


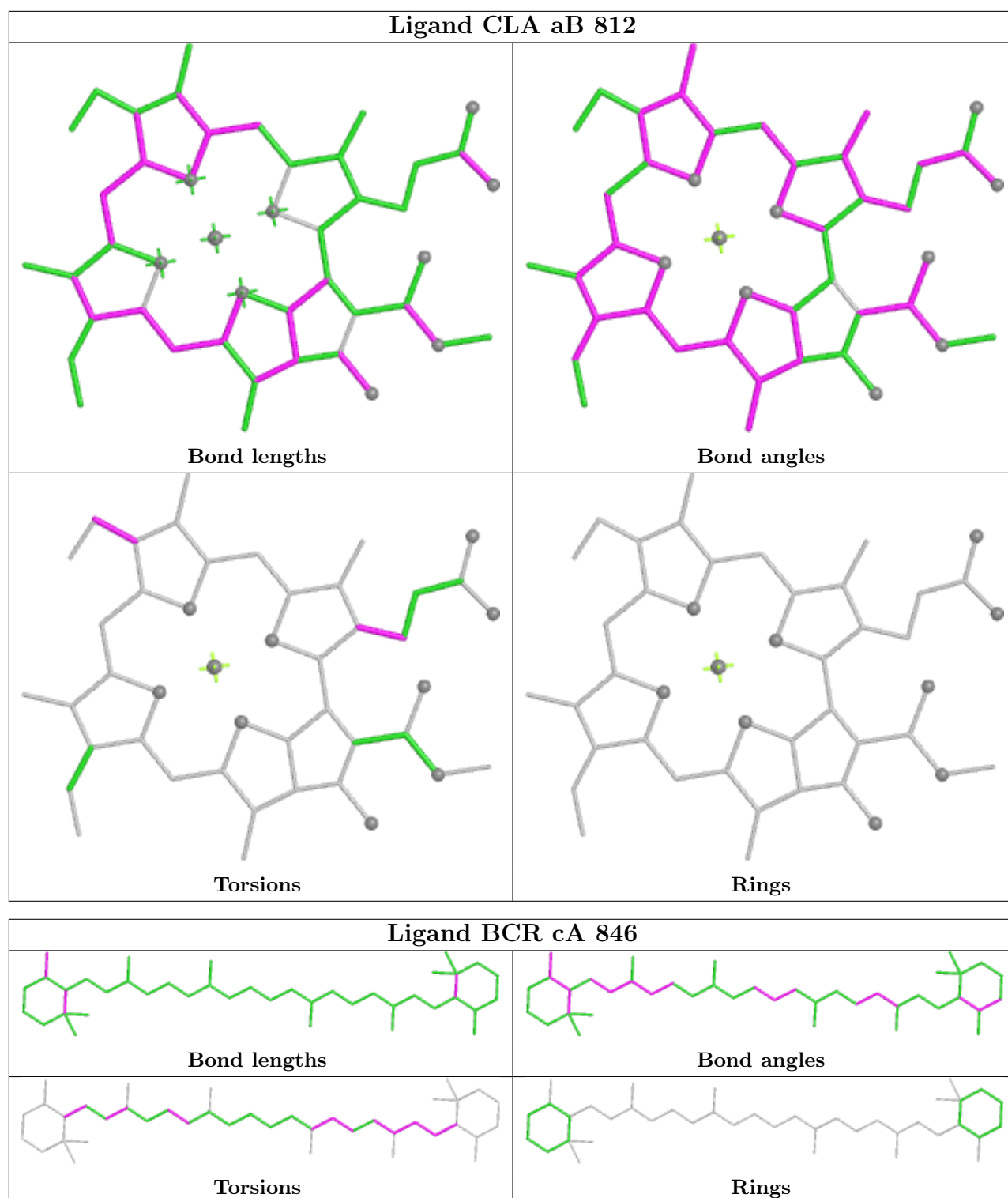












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

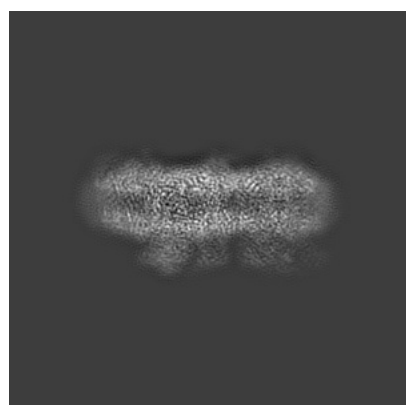
6 Map visualisation [i](#)

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

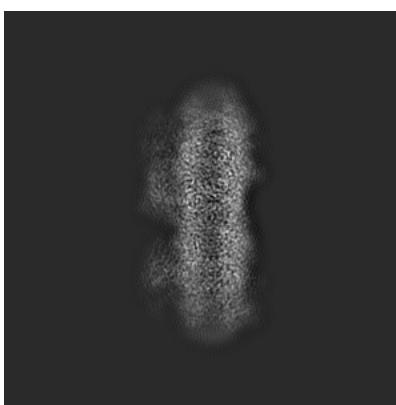
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

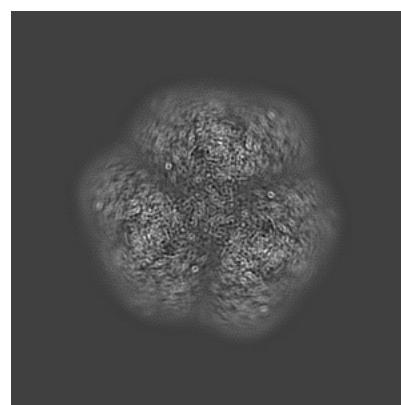
6.1.1 Primary map



X



Y

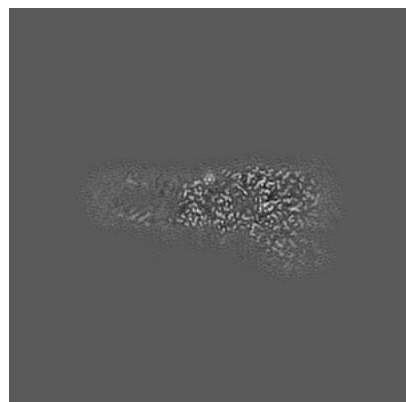


Z

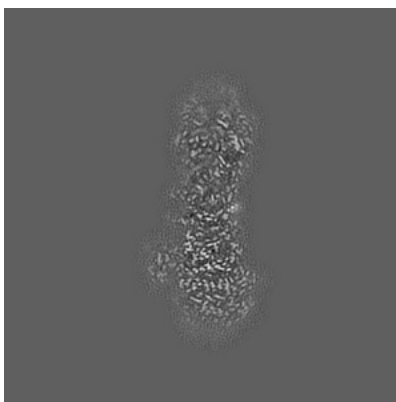
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

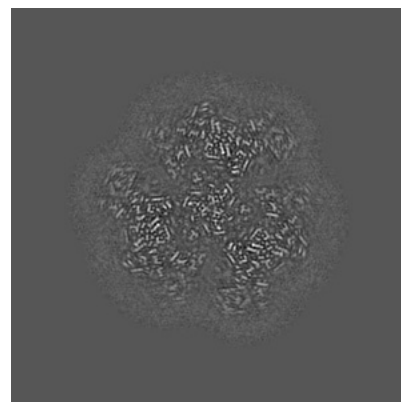
6.2.1 Primary map



X Index: 180



Y Index: 180

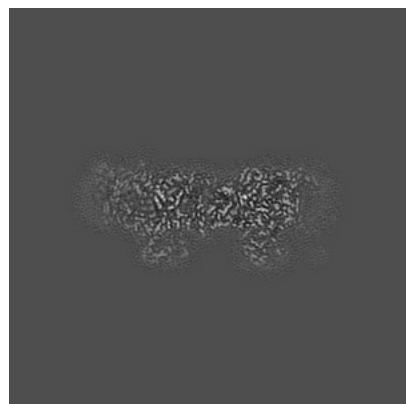


Z Index: 180

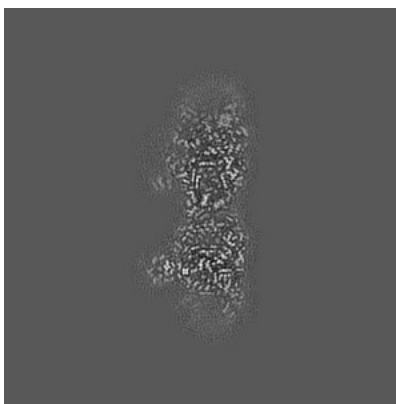
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

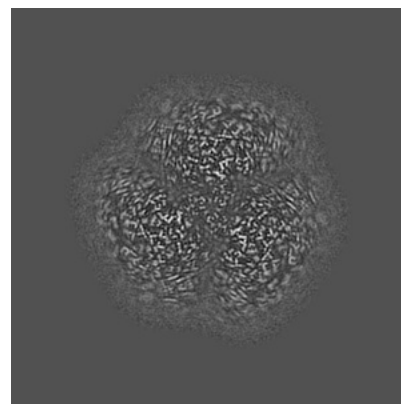
6.3.1 Primary map



X Index: 197



Y Index: 157

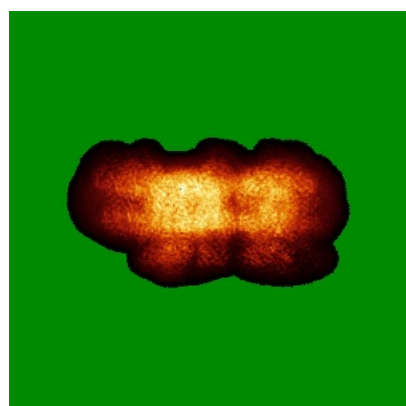


Z Index: 199

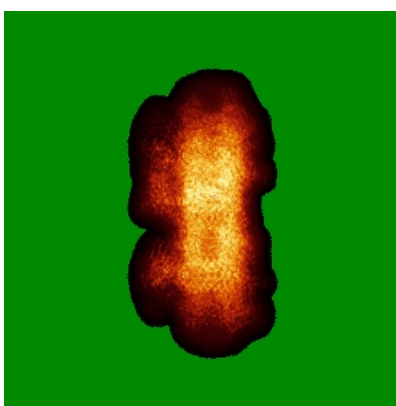
The images above show the largest variance slices of the map in three orthogonal directions.

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

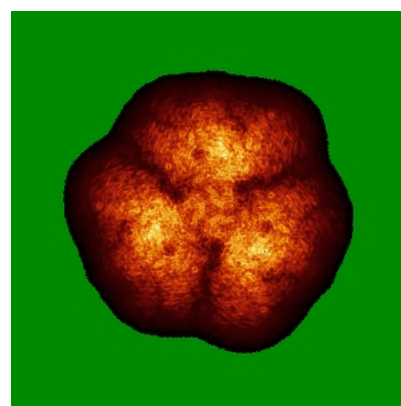
6.4.1 Primary map



X



Y

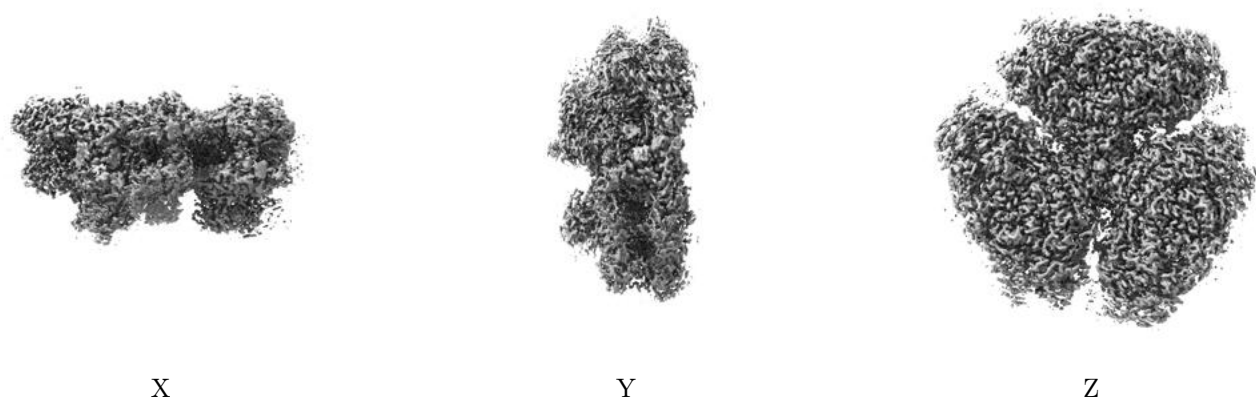


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

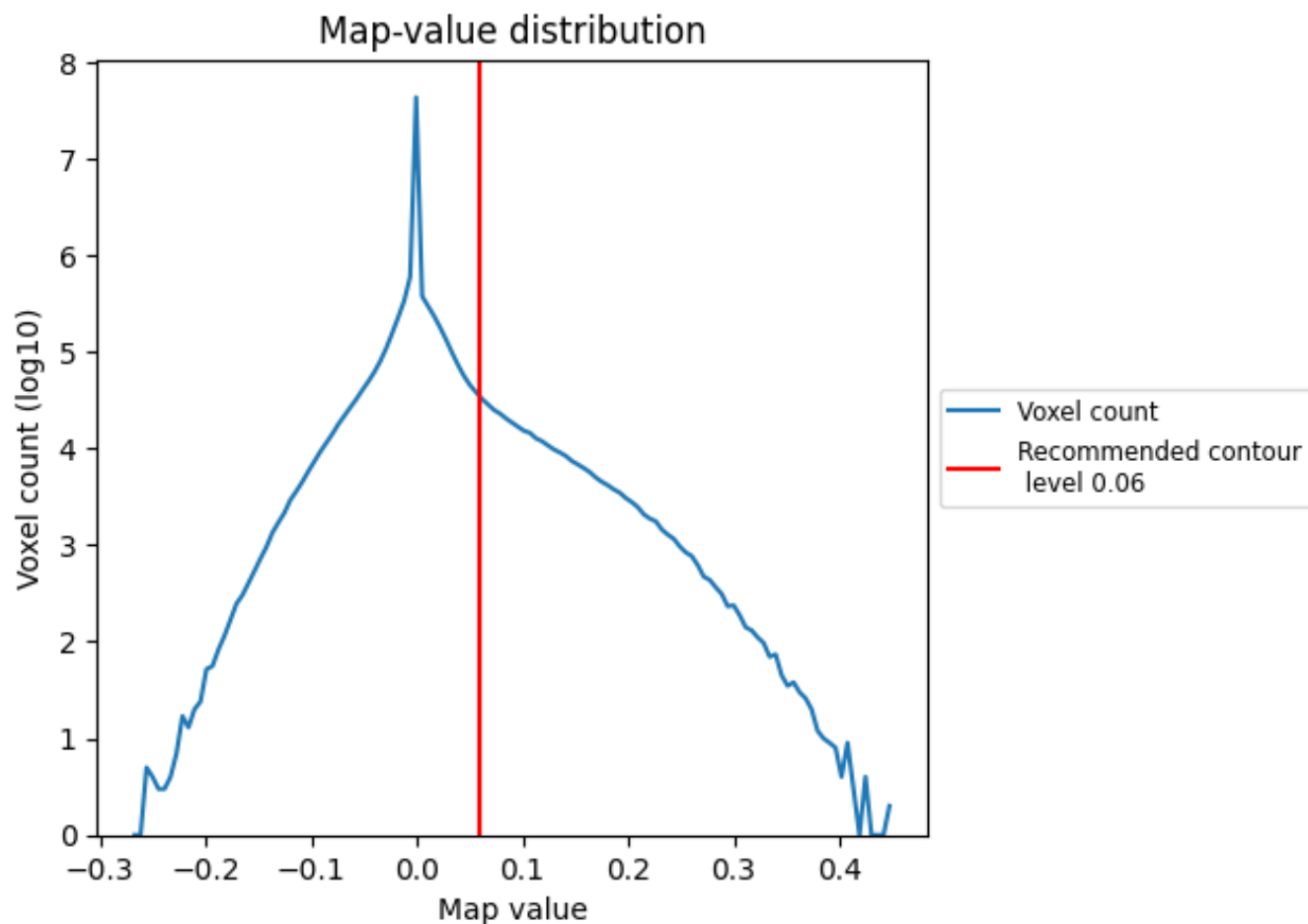
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

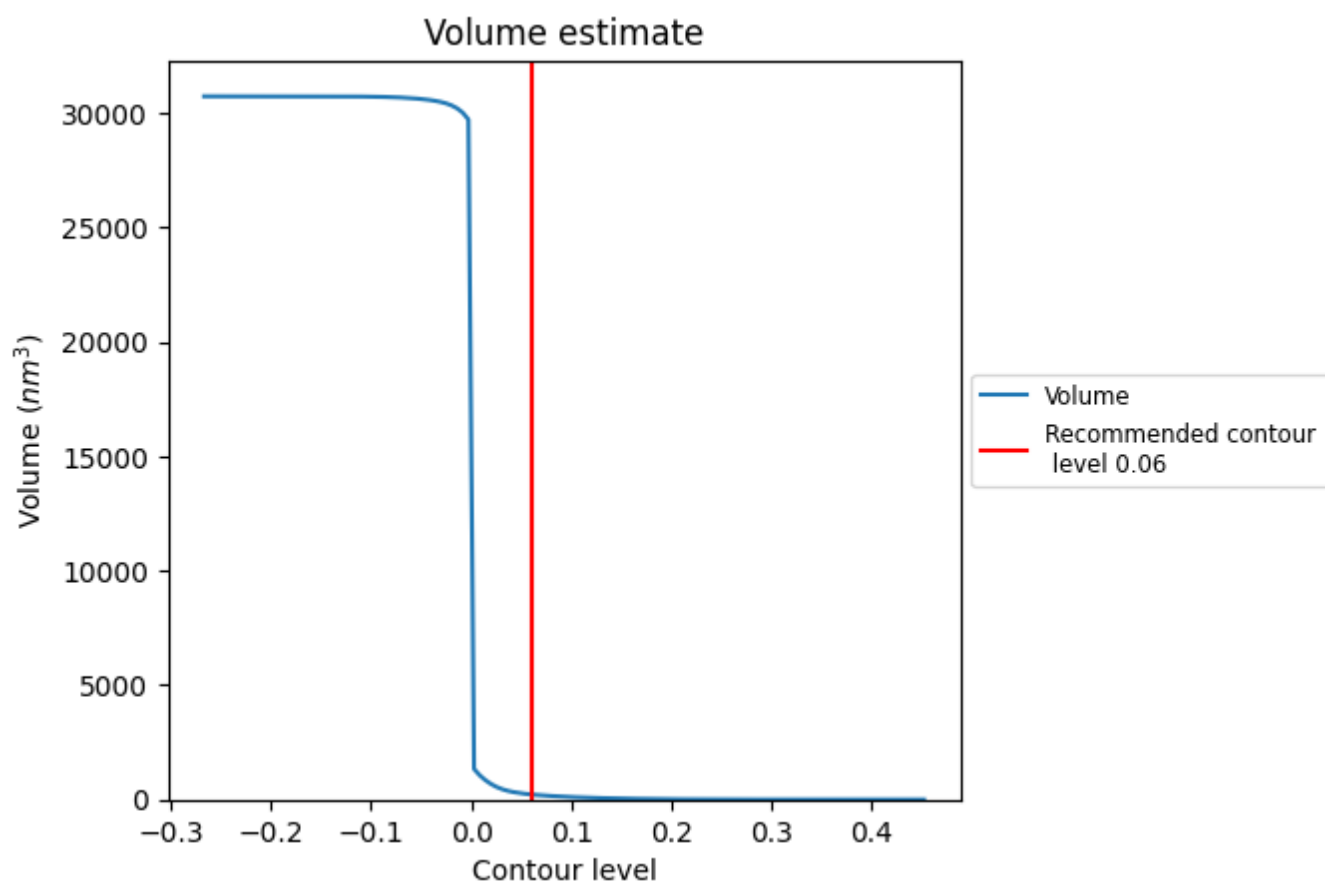
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

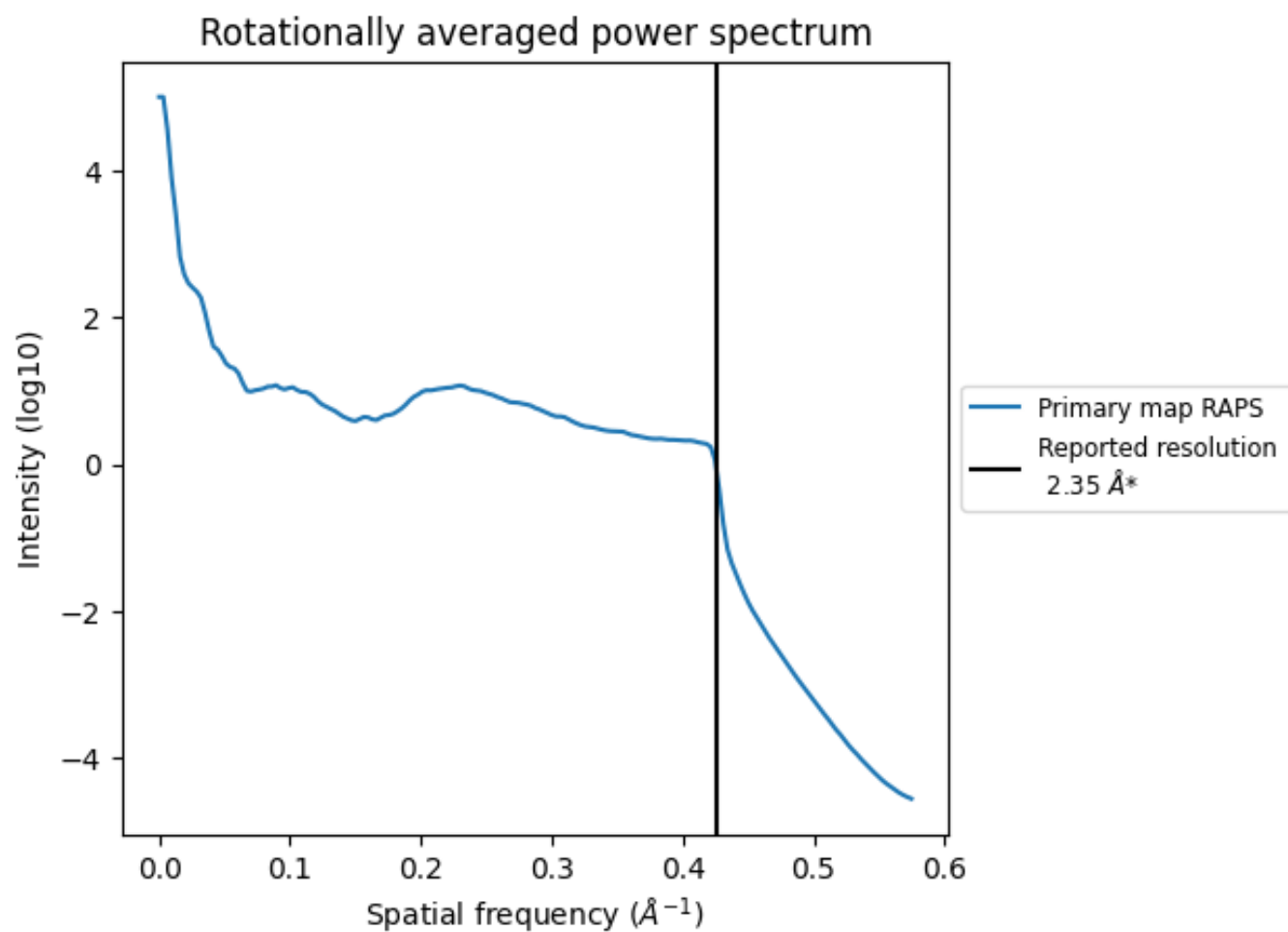
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

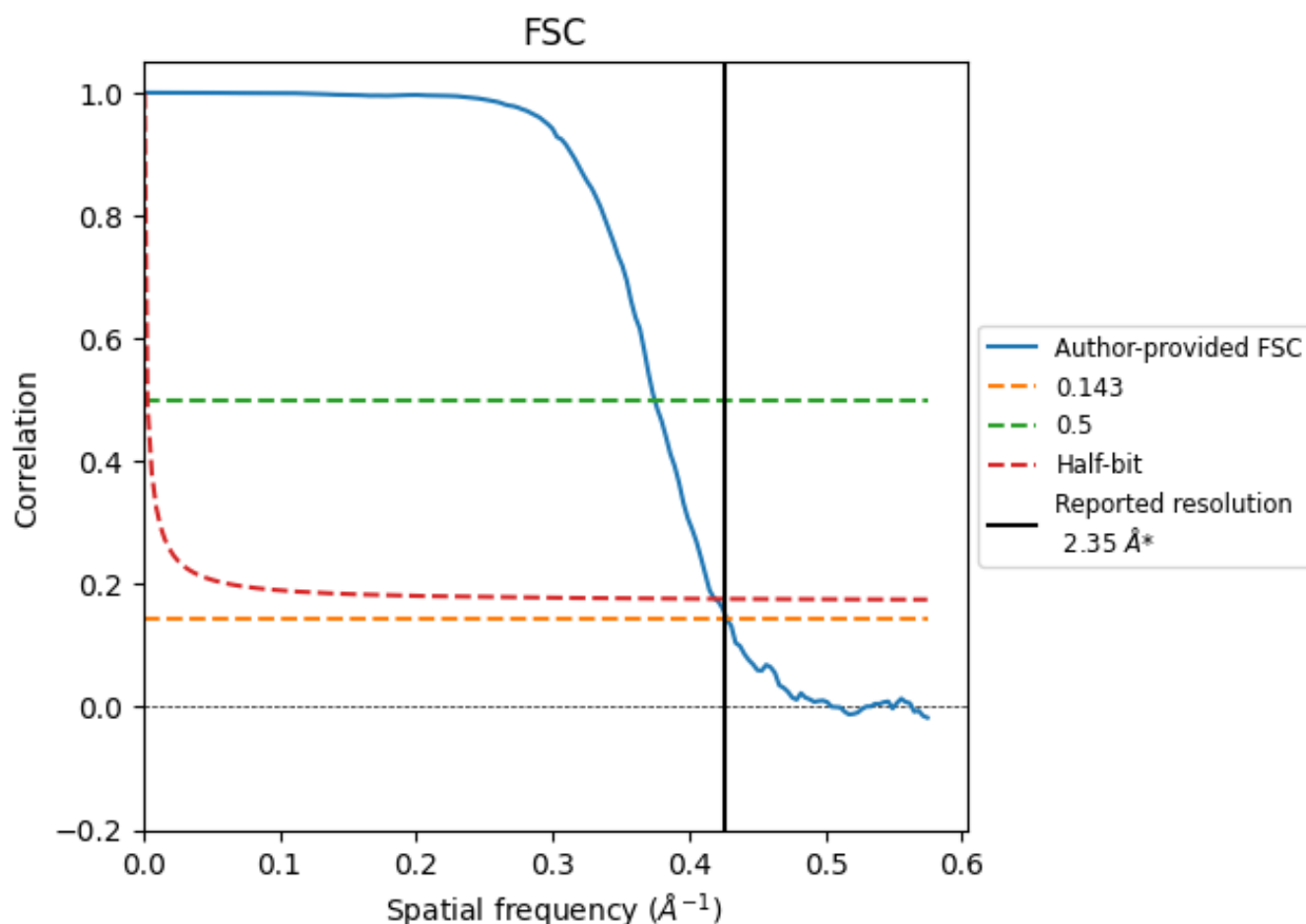


*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

8.2 Resolution estimates [i](#)

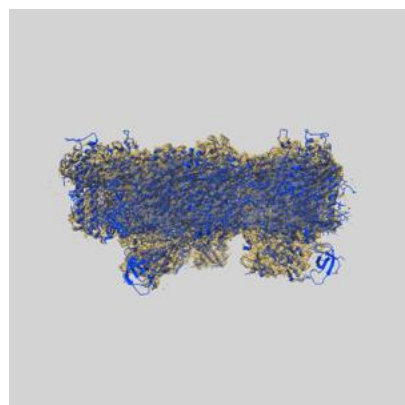
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.34	2.67	2.39
Unmasked-calculated*	-	-	-

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

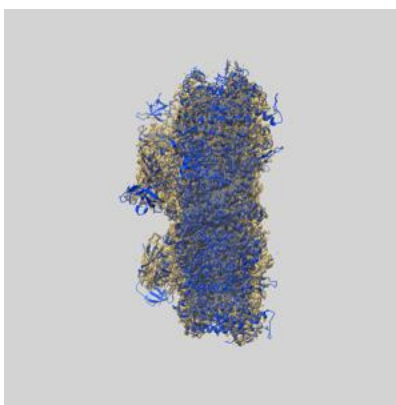
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0726 and PDB model 6KMW. Per-residue inclusion information can be found in section [3](#) on page [29](#).

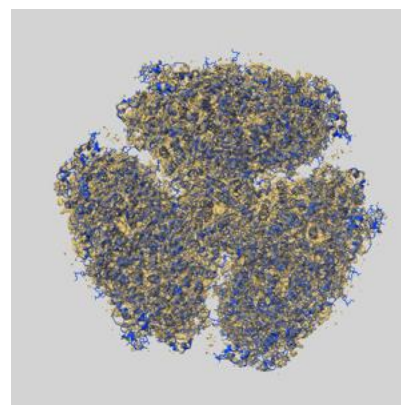
9.1 Map-model overlay [i](#)



X



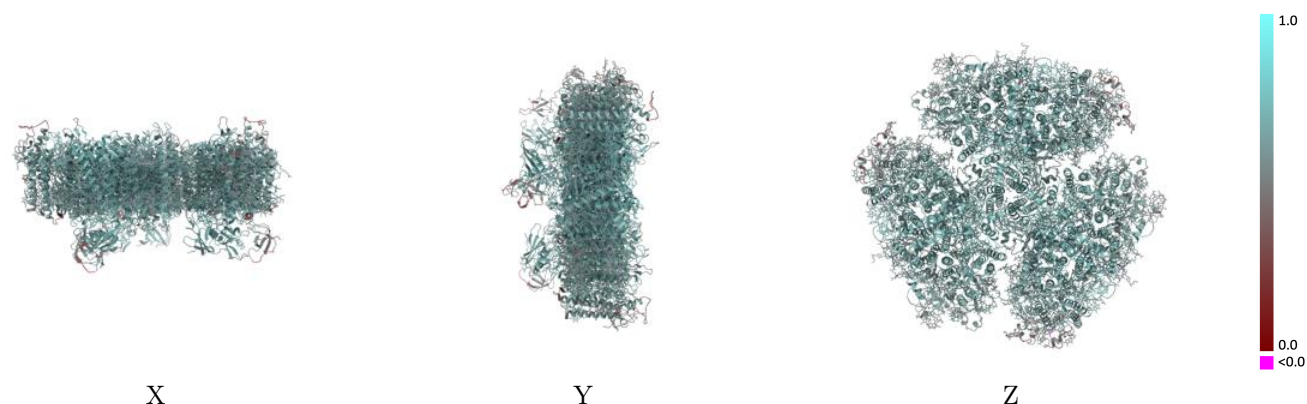
Y



Z

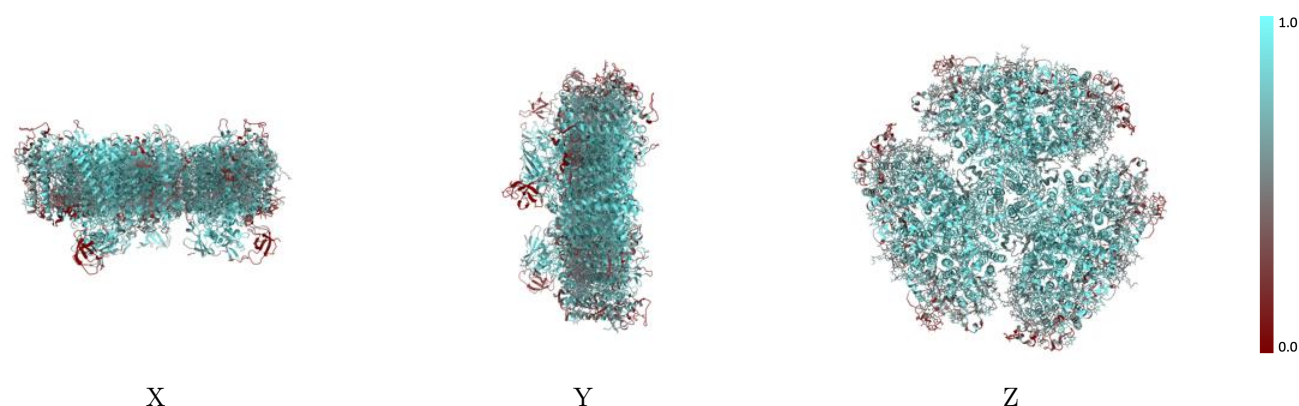
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



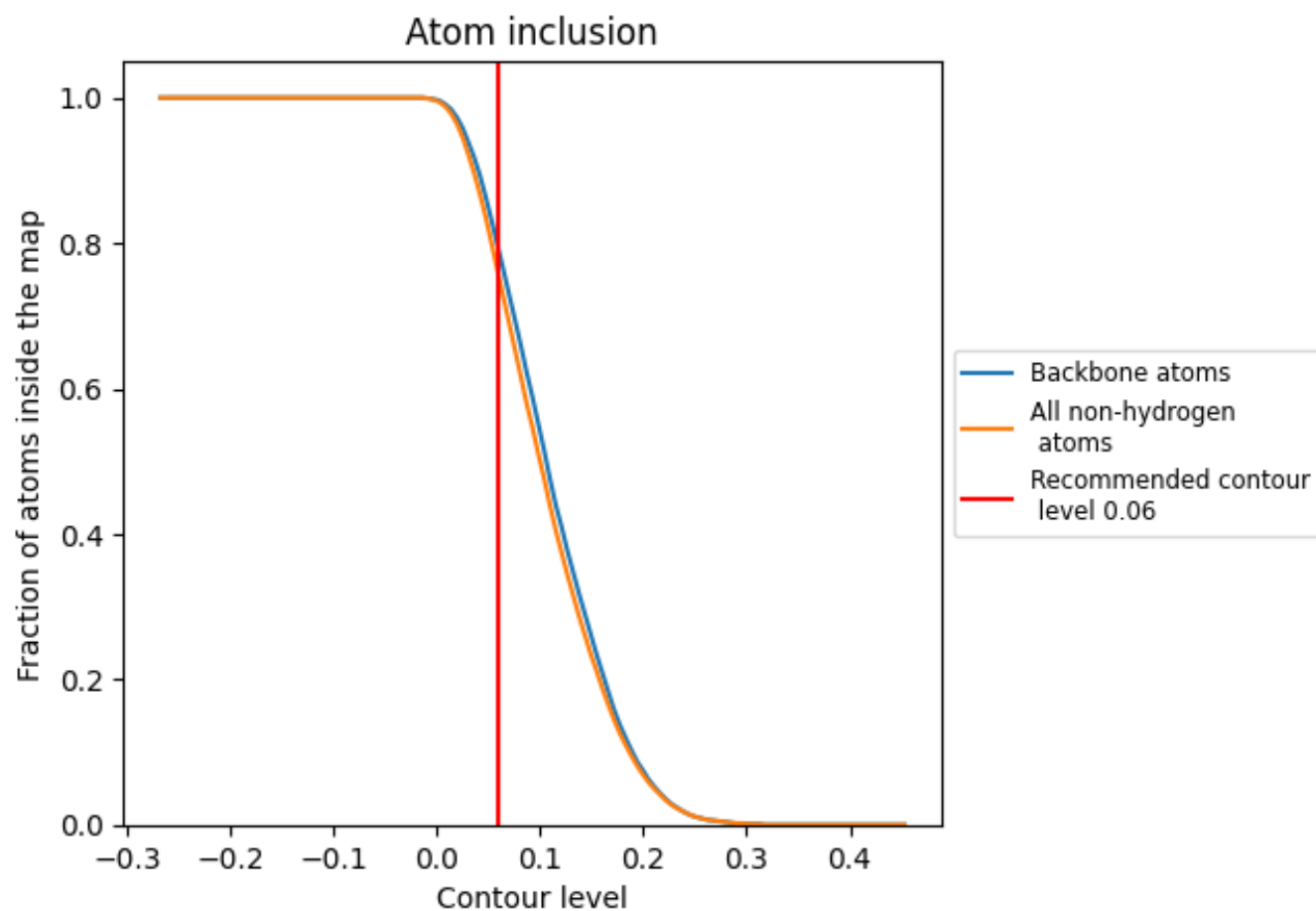
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

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

Chain	Atom inclusion	Q-score
All	 0.7580	 0.6450
aA	 0.7320	 0.6360
aB	 0.7850	 0.6540
aC	 0.8210	 0.6660
aD	 0.7860	 0.6530
aE	 0.1000	 0.4610
aI	 0.9150	 0.7050
aL	 0.8680	 0.6930
aM	 0.8020	 0.6590
bA	 0.7320	 0.6370
bB	 0.7850	 0.6520
bC	 0.8260	 0.6650
bD	 0.7820	 0.6530
bE	 0.1160	 0.4620
bI	 0.9230	 0.7070
bL	 0.8660	 0.6920
bM	 0.7990	 0.6590
cA	 0.7300	 0.6350
cB	 0.7840	 0.6520
cC	 0.8290	 0.6620
cD	 0.7780	 0.6510
cE	 0.1080	 0.4530
cI	 0.9230	 0.7060
cL	 0.8680	 0.6920
cM	 0.8130	 0.6580

